List of descriptors

Full list of alvaDesc descriptors

No.	Name	Description	Block	Sub-Block
1	MW	molecular weight	Constitutional indices	Basic descriptors
2	AMW	average molecular weight	Constitutional indices	Basic descriptors
3	Sv	sum of atomic van der Waals volumes (scaled on Carbon atom)	Constitutional indices	Basic descriptors
4	Se	sum of atomic Sanderson electronegativities (scaled on Carbon atom)	Constitutional indices	Basic descriptors
5	Sp	sum of atomic polarizabilities (scaled on Carbon atom)	Constitutional indices	Basic descriptors
6	Si	sum of first ionization potentials (scaled on Carbon atom)	Constitutional indices	Basic descriptors
7	Mv	mean atomic van der Waals volume (scaled on Carbon atom)	Constitutional indices	Basic descriptors
8	Me	mean atomic Sanderson electronegativity (scaled on Carbon atom)	Constitutional indices	Basic descriptors
9	Mp	mean atomic polarizability (scaled on Carbon atom)	Constitutional indices	Basic descriptors
10	Mi	mean first ionization potential (scaled on Carbon atom)	Constitutional indices	Basic descriptors
11	GD	graph density	Constitutional indices	Basic descriptors
12	nAT	number of atoms	Constitutional indices	Basic descriptors
13	nSK	number of non-H atoms	Constitutional indices	Basic descriptors
14	nTA	number of terminal atoms	Constitutional indices	Basic descriptors
15	nBT	number of bonds	Constitutional indices	Basic descriptors
16	nBO	number of non-H bonds	Constitutional indices	Basic descriptors
17	nBM	number of multiple bonds	Constitutional indices	Basic descriptors

18	SCBO	sum of conventional bond orders (H-depleted)	Constitutional indices	Basic descriptors
19	RBN	number of rotatable bonds	Constitutional indices	Basic descriptors
20	RBF	rotatable bond fraction	Constitutional indices	Basic descriptors
21	nDB	number of double bonds	Constitutional indices	Basic descriptors
22	nTB	number of triple bonds	Constitutional indices	Basic descriptors
23	nAB	number of aromatic bonds	Constitutional indices	Basic descriptors
24	nH	number of Hydrogen atoms	Constitutional indices	Basic descriptors
25	nC	number of Carbon atoms	Constitutional indices	Basic descriptors
26	nN	number of Nitrogen atoms	Constitutional indices	Basic descriptors
27	nO	number of Oxygen atoms	Constitutional indices	Basic descriptors
28	nP	number of Phosphorous atoms	Constitutional indices	Basic descriptors
29	nS	number of Sulfur atoms	Constitutional indices	Basic descriptors
30	nF	number of Fluorine atoms	Constitutional indices	Basic descriptors
31	nCL	number of Chlorine atoms	Constitutional indices	Basic descriptors
32	nBR	number of Bromine atoms	Constitutional indices	Basic descriptors
33	nI	number of Iodine atoms	Constitutional indices	Basic descriptors
34	nB	number of Boron atoms	Constitutional indices	Basic descriptors
35	nHM	number of heavy atoms	Constitutional indices	Basic descriptors
36	nHet	number of heteroatoms	Constitutional indices	Basic descriptors
37	nX	number of halogen atoms	Constitutional indices	Basic descriptors

38	H%	percentage of H atoms	Constitutional indices	Basic descriptors
39	C%	percentage of C atoms	Constitutional indices	Basic descriptors
40	N%	percentage of N atoms	Constitutional indices	Basic descriptors
41	O%	percentage of O atoms	Constitutional indices	Basic descriptors
42	X%	percentage of halogen atoms	Constitutional indices	Basic descriptors
43	nCsp3	number of sp3 hybridized Carbon atoms	Constitutional indices	Basic descriptors
44	nCsp2	number of sp2 hybridized Carbon atoms	Constitutional indices	Basic descriptors
45	nCsp	number of sp hybridized Carbon atoms	Constitutional indices	Basic descriptors
46	max_conj_path	maximum number of atoms that can be in conjugation with each other	Constitutional indices	Basic descriptors
47	nStructures	number of disconnected structures	Constitutional indices	Basic descriptors
48	totalcharge	total charge	Constitutional indices	Basic descriptors
49	nCIC	number of rings (cyclomatic number)	Ring descriptors	Basic descriptors
50	nCIR	number of circuits	Ring descriptors	Basic descriptors
51	TRS	total ring size	Ring descriptors	Basic descriptors
52	Rperim	ring perimeter	Ring descriptors	Basic descriptors
53	Rbrid	ring bridge count	Ring descriptors	Basic descriptors
54	MCD	molecular cyclized degree	Ring descriptors	Basic descriptors
55	RFD	ring fusion density	Ring descriptors	Basic descriptors
56	RCI	ring complexity index	Ring descriptors	Basic descriptors
57	NRS	number of ring systems	Ring descriptors	Basic descriptors

58	NNRS	normalized number of ring systems	Ring descriptors	Basic descriptors
59	nR03	number of 3-membered rings	Ring descriptors	Basic descriptors
60	nR04	number of 4-membered rings	Ring descriptors	Basic descriptors
61	nR05	number of 5-membered rings	Ring descriptors	Basic descriptors
62	nR06	number of 6-membered rings	Ring descriptors	Basic descriptors
63	nR07	number of 7-membered rings	Ring descriptors	Basic descriptors
64	nR08	number of 8-membered rings	Ring descriptors	Basic descriptors
65	nR09	number of 9-membered rings	Ring descriptors	Basic descriptors
66	nR10	number of 10-membered rings	Ring descriptors	Basic descriptors
67	nR11	number of 11-membered rings	Ring descriptors	Basic descriptors
68	nR12	number of 12-membered rings	Ring descriptors	Basic descriptors
69	nBnz	number of benzene-like rings	Ring descriptors	Basic descriptors
70	ARR	aromatic ratio	Ring descriptors	Basic descriptors
71	D/Dtr03	distance/detour ring index of order 3	Ring descriptors	Basic descriptors
72	D/Dtr04	distance/detour ring index of order 4	Ring descriptors	Basic descriptors
73	D/Dtr05	distance/detour ring index of order 5	Ring descriptors	Basic descriptors
74	D/Dtr06	distance/detour ring index of order 6	Ring descriptors	Basic descriptors
75	D/Dtr07	distance/detour ring index of order 7	Ring descriptors	Basic descriptors
76	D/Dtr08	distance/detour ring index of order 8	Ring descriptors	Basic descriptors
77	D/Dtr09	distance/detour ring index of order 9	Ring descriptors	Basic descriptors

78	D/Dtr10	distance/detour ring index of order 10	Ring descriptors	Basic descriptors
79	D/Dtr11	distance/detour ring index of order 11	Ring descriptors	Basic descriptors
80	D/Dtr12	distance/detour ring index of order 12	Ring descriptors	Basic descriptors
81	ZM1	first Zagreb index	Topological indices	Vertex degree-based indices
82	ZM1V	first Zagreb index by valence vertex degrees	Topological indices	Vertex degree-based indices
83	ZM1Kup	first Zagreb index by Kupchik vertex degrees	Topological indices	Vertex degree-based indices
84	ZM1Mad	first Zagreb index by Madan vertex degrees	Topological indices	Vertex degree-based indices
85	ZM1Per	first Zagreb index by perturbation vertex degrees	Topological indices	Vertex degree-based indices
86	ZM1MulPer	first Zagreb index by multiplicative perturbation vertex degrees	Topological indices	Vertex degree-based indices
87	ZM2	second Zagreb index	Topological indices	Vertex degree-based indices
88	ZM2V	second Zagreb index by valence vertex degrees	Topological indices	Vertex degree-based indices
89	ZM2Kup	second Zagreb index by Kupchik vertex degrees	Topological indices	Vertex degree-based indices
90	ZM2Mad	second Zagreb index by Madan vertex degrees	Topological indices	Vertex degree-based indices
91	ZM2Per	second Zagreb index by perturbation vertex degrees	Topological indices	Vertex degree-based indices
92	ZM2MulPer	second Zagreb index by multiplicative perturbation vertex degrees	Topological indices	Vertex degree-based indices
93	ON0	overall modified Zagreb index of order 0	Topological indices	Vertex degree-based indices
94	ON0V	overall modified Zagreb index of order 0 by valence vertex degrees	Topological indices	Vertex degree-based indices
95	ON1	overall modified Zagreb index of order 1	Topological indices	Vertex degree-based indices
96	ON1V	overall modified Zagreb index of order 1 by valence vertex degrees	Topological indices	Vertex degree-based indices
97	Qindex	quadratic index	Topological indices	Vertex degree-based indices

98	BBI	Bertz branching index	Topological indices	Vertex degree-based indices
99	DBI	Dragon branching index	Topological indices	Vertex degree-based indices
100	SNar	Narumi simple topological index (log function)	Topological indices	Vertex degree-based indices
101	HNar	Narumi harmonic topological index	Topological indices	Vertex degree-based indices
102	GNar	Narumi geometric topological index	Topological indices	Vertex degree-based indices
103	Xt	total structure connectivity index	Topological indices	Vertex degree-based indices
104	Dz	Pogliani index	Topological indices	Vertex degree-based indices
105	Ram	ramification index	Topological indices	Vertex degree-based indices
106	BLI	Kier benzene-likeliness index	Topological indices	Vertex degree-based indices
107	Pol	polarity number	Topological indices	Distance-based indices
108	LPRS	log of product of row sums (PRS)	Topological indices	Distance-based indices
109	MSD	mean square distance index (Balaban)	Topological indices	Distance-based indices
110	SPI	superpendentic index	Topological indices	Distance-based indices
111	PJI2	2D Petitjean shape index	Topological indices	Distance-based indices
112	ECC	eccentricity	Topological indices	Distance-based indices
113	AECC	average eccentricity	Topological indices	Distance-based indices
114	DECC	eccentric	Topological indices	Distance-based indices
115	MDDD	mean distance degree deviation	Topological indices	Distance-based indices
116	UNIP	unipolarity	Topological indices	Distance-based indices
117	CENT	centralization	Topological indices	Distance-based indices

118	VAR	variation	Topological indices	Distance-based indices
119	ICR	radial centric information index	Topological indices	Distance-based indices
120	MaxTD	max topological distance	Topological indices	Distance-based indices
121	MeanTD	mean pairwise topological distance	Topological indices	Distance-based indices
122	MaxDD	max detour distance	Topological indices	Distance-based indices
123	MeanDD	mean pairwise detour distance	Topological indices	Distance-based indices
124	SMTI	Schultz Molecular Topological Index (MTI)	Topological indices	MTI indices
125	SMTIV	Schultz Molecular Topological Index by valence vertex degrees	Topological indices	MTI indices
126	GMTI	Gutman Molecular Topological Index	Topological indices	MTI indices
127	GMTIV	Gutman Molecular Topological Index by valence vertex degrees	Topological indices	MTI indices
128	Xu	Xu index	Topological indices	MTI indices
129	CSI	eccentric connectivity index	Topological indices	MTI indices
130	Wap	all-path Wiener index	Topological indices	Path/walk indices
131	S1K	1-path Kier alpha-modified shape index	Topological indices	Path/walk indices
132	S2K	2-path Kier alpha-modified shape index	Topological indices	Path/walk indices
133	S3K	3-path Kier alpha-modified shape index	Topological indices	Path/walk indices
134	PHI	Kier flexibility index	Topological indices	Path/walk indices
135	PW2	path/walk 2 - Randic shape index	Topological indices	Path/walk indices
136	PW3	path/walk 3 - Randic shape index	Topological indices	Path/walk indices
137	PW4	path/walk 4 - Randic shape index	Topological indices	Path/walk indices

138	PW5	path/walk 5 - Randic shape index	Topological indices	Path/walk indices
139	MAXDN	maximal electrotopological negative variation	Topological indices	E-state indices
140	MAXDP	maximal electrotopological positive variation	Topological indices	E-state indices
141	DELS	molecular electrotopological variation	Topological indices	E-state indices
142	TIE	E-state topological parameter	Topological indices	E-state indices
143	Psi_i_s	intrinsic state pseudoconnectivity index - type S	Topological indices	E-state indices
144	Psi_i_A	intrinsic state pseudoconnectivity index - type S average	Topological indices	E-state indices
145	Psi_i_0	intrinsic state pseudoconnectivity index - type 0	Topological indices	E-state indices
146	Psi_i_1	intrinsic state pseudoconnectivity index - type 1	Topological indices	E-state indices
147	Psi_i_t	intrinsic state pseudoconnectivity index - type T	Topological indices	E-state indices
148	Psi_i_0d	intrinsic state pseudoconnectivity index - type 0d	Topological indices	E-state indices
149	Psi_i_1d	intrinsic state pseudoconnectivity index - type 1d	Topological indices	E-state indices
150	Psi_i_1s	intrinsic state pseudoconnectivity index - type 1s	Topological indices	E-state indices
151	Psi_e_A	electrotopological state pseudoconnectivity index - type S average	Topological indices	E-state indices
152	Psi_e_0	electrotopological state pseudoconnectivity index - type 0	Topological indices	E-state indices
153	Psi_e_1	electrotopological state pseudoconnectivity index - type 1	Topological indices	E-state indices
154	Psi_e_t	electrotopological state pseudoconnectivity index - type T	Topological indices	E-state indices
155	Psi_e_0d	electrotopological state pseudoconnectivity index - type 0d	Topological indices	E-state indices
156	Psi_e_1d	electrotopological state pseudoconnectivity index - type 1d	Topological indices	E-state indices
157	Psi_e_1s	electrotopological state pseudoconnectivity index - type 1s	Topological indices	E-state indices

158	BAC	Balaban centric index	Topological indices	Centric indices
159	LOC	lopping centric index	Topological indices	Centric indices
160	MWC01	molecular walk count of order 1	Walk and path counts	Walk counts
161	MWC02	molecular walk count of order 2	Walk and path counts	Walk counts
162	MWC03	molecular walk count of order 3	Walk and path counts	Walk counts
163	MWC04	molecular walk count of order 4	Walk and path counts	Walk counts
164	MWC05	molecular walk count of order 5	Walk and path counts	Walk counts
165	MWC06	molecular walk count of order 6	Walk and path counts	Walk counts
166	MWC07	molecular walk count of order 7	Walk and path counts	Walk counts
167	MWC08	molecular walk count of order 8	Walk and path counts	Walk counts
168	MWC09	molecular walk count of order 9	Walk and path counts	Walk counts
169	MWC10	molecular walk count of order 10	Walk and path counts	Walk counts
170	SRW02	self-returning walk count of order 2	Walk and path counts	Self-returning walk counts
171	SRW03	self-returning walk count of order 3	Walk and path counts	Self-returning walk counts
172	SRW04	self-returning walk count of order 4	Walk and path counts	Self-returning walk counts
173	SRW05	self-returning walk count of order 5	Walk and path counts	Self-returning walk counts
174	SRW06	self-returning walk count of order 6	Walk and path counts	Self-returning walk counts
175	SRW07	self-returning walk count of order 7	Walk and path counts	Self-returning walk counts
176	SRW08	self-returning walk count of order 8	Walk and path counts	Self-returning walk counts
177	SRW09	self-returning walk count of order 9	Walk and path counts	Self-returning walk counts

178	SRW10	self-returning walk count of order 10	Walk and path counts	Self-returning walk counts
179	MPC01	molecular path count of order 1 (no. of non-H bonds)	Walk and path counts	Path counts
180	MPC02	molecular path count of order 2 (Gordon-Scantlebury index)	Walk and path counts	Path counts
181	MPC03	molecular path count of order 3	Walk and path counts	Path counts
182	MPC04	molecular path count of order 4	Walk and path counts	Path counts
183	MPC05	molecular path count of order 5	Walk and path counts	Path counts
184	MPC06	molecular path count of order 6	Walk and path counts	Path counts
185	MPC07	molecular path count of order 7	Walk and path counts	Path counts
186	MPC08	molecular path count of order 8	Walk and path counts	Path counts
187	MPC09	molecular path count of order 9	Walk and path counts	Path counts
188	MPC10	molecular path count of order 10	Walk and path counts	Path counts
189	piPC01	molecular multiple path count of order 1	Walk and path counts	Multiple path counts
190	piPC02	molecular multiple path count of order 2	Walk and path counts	Multiple path counts
191	piPC03	molecular multiple path count of order 3	Walk and path counts	Multiple path counts
192	piPC04	molecular multiple path count of order 4	Walk and path counts	Multiple path counts
193	piPC05	molecular multiple path count of order 5	Walk and path counts	Multiple path counts
194	piPC06	molecular multiple path count of order 6	Walk and path counts	Multiple path counts
195	piPC07	molecular multiple path count of order 7	Walk and path counts	Multiple path counts
196	piPC08	molecular multiple path count of order 8	Walk and path counts	Multiple path counts
197	piPC09	molecular multiple path count of order 9	Walk and path counts	Multiple path counts

198	piPC10	molecular multiple path count of order 10	Walk and path counts	Multiple path counts
199	TWC	total walk count	Walk and path counts	ID numbers
200	TPC	total path count	Walk and path counts	ID numbers
201	piID	conventional bond order ID number	Walk and path counts	ID numbers
202	PCR	ratio of multiple path count over path count	Walk and path counts	ID numbers
203	PCD	difference between multiple path count and path count	Walk and path counts	ID numbers
204	CID	Randic ID number	Walk and path counts	ID numbers
205	BID	Balaban ID number	Walk and path counts	ID numbers
206	X0	connectivity index of order 0	Connectivity indices	Kier-Hall molecular connectivity indices
207	X1	connectivity index of order 1 (Randic connectivity index)	Connectivity indices	Kier-Hall molecular connectivity indices
208	X2	connectivity index of order 2	Connectivity indices	Kier-Hall molecular connectivity indices
209	X3	connectivity index of order 3	Connectivity indices	Kier-Hall molecular connectivity indices
210	X4	connectivity index of order 4	Connectivity indices	Kier-Hall molecular connectivity indices
211	X5	connectivity index of order 5	Connectivity indices	Kier-Hall molecular connectivity indices
212	X0A	average connectivity index of order 0	Connectivity indices	Kier-Hall molecular connectivity indices
213	X1A	average connectivity index of order 1	Connectivity indices	Kier-Hall molecular connectivity indices
214	X2A	average connectivity index of order 2	Connectivity indices	Kier-Hall molecular connectivity indices
215	X3A	average connectivity index of order 3	Connectivity indices	Kier-Hall molecular connectivity indices
216	X4A	average connectivity index of order 4	Connectivity indices	Kier-Hall molecular connectivity indices
217	X5A	average connectivity index of order 5	Connectivity indices	Kier-Hall molecular connectivity indices

218	X0v	valence connectivity index of order 0	Connectivity indices	Kier-Hall molecular connectivity indices
219	X1v	valence connectivity index of order 1	Connectivity indices	Kier-Hall molecular connectivity indices
220	X2v	valence connectivity index of order 2	Connectivity indices	Kier-Hall molecular connectivity indices
221	X3v	valence connectivity index of order 3	Connectivity indices	Kier-Hall molecular connectivity indices
222	X4v	valence connectivity index of order 4	Connectivity indices	Kier-Hall molecular connectivity indices
223	X5v	valence connectivity index of order 5	Connectivity indices	Kier-Hall molecular connectivity indices
224	X0Av	average valence connectivity index of order 0	Connectivity indices	Kier-Hall molecular connectivity indices
225	X1Av	average valence connectivity index of order 1	Connectivity indices	Kier-Hall molecular connectivity indices
226	X2Av	average valence connectivity index of order 2	Connectivity indices	Kier-Hall molecular connectivity indices
227	X3Av	average valence connectivity index of order 3	Connectivity indices	Kier-Hall molecular connectivity indices
228	X4Av	average valence connectivity index of order 4	Connectivity indices	Kier-Hall molecular connectivity indices
229	X5Av	average valence connectivity index of order 5	Connectivity indices	Kier-Hall molecular connectivity indices
230	X0sol	solvation connectivity index of order 0	Connectivity indices	Solvation connectivity indices
231	X1sol	solvation connectivity index of order 1	Connectivity indices	Solvation connectivity indices
232	X2sol	solvation connectivity index of order 2	Connectivity indices	Solvation connectivity indices
233	X3sol	solvation connectivity index of order 3	Connectivity indices	Solvation connectivity indices
234	X4sol	solvation connectivity index of order 4	Connectivity indices	Solvation connectivity indices
235	X5sol	solvation connectivity index of order 5	Connectivity indices	Solvation connectivity indices
236	XMOD	modified Randic index	Connectivity indices	Randic-like connectivity indices
237	RDCHI	reciprocal distance sum Randic-like index	Connectivity indices	Randic-like connectivity indices

238	RDSQ	reciprocal distance sum inverse Randic-like index	Connectivity indices	Randic-like connectivity indices
239	X1Kup	Kupchik connectivity index	Connectivity indices	Randic-like connectivity indices
240	X1Mad	connectivity topochemical index	Connectivity indices	Randic-like connectivity indices
241	X1Per	perturbation connectivity index	Connectivity indices	Randic-like connectivity indices
242	X1MulPer	multiplicative perturbation connectivity index	Connectivity indices	Randic-like connectivity indices
243	ISIZ	information index on molecular size	Information indices	Basic descriptors
244	IAC	total information index on atomic composition	Information indices	Basic descriptors
245	AAC	mean information index on atomic composition	Information indices	Basic descriptors
246	IDE	mean information content on the distance equality	Information indices	Basic descriptors
247	IDM	mean information content on the distance magnitude	Information indices	Basic descriptors
248	IDDE	mean information content on the distance degree equality	Information indices	Basic descriptors
249	IDDM	mean information content on the distance degree magnitude	Information indices	Basic descriptors
250	IDET	total information content on the distance equality	Information indices	Basic descriptors
251	IDMT	total information content on the distance magnitude	Information indices	Basic descriptors
252	IVDE	mean information content on the vertex degree equality	Information indices	Basic descriptors
253	IVDM	mean information content on the vertex degree magnitude	Information indices	Basic descriptors
254	Ges	Number of symmetry classes (based on electrotopological state)	Information indices	Basic descriptors
255	rGes	Relative number of symmetry classes (based on electrotopological state)	Information indices	Basic descriptors
256	S0K	Kier symmetry index	Information indices	Basic descriptors
257	HVcpx	graph vertex complexity index	Information indices	Basic descriptors

258	HDcpx	graph distance complexity index (log function)	Information indices	Basic descriptors
259	Uindex	Balaban U index	Information indices	Basic descriptors
260	Vindex	Balaban V index	Information indices	Basic descriptors
261	Xindex	Balaban X index	Information indices	Basic descriptors
262	Yindex	Balaban Y index	Information indices	Basic descriptors
263	IC0	Information Content index (neighborhood symmetry of 0-order)	Information indices	Indices of neighborhood symmetry
264	IC1	Information Content index (neighborhood symmetry of 1-order)	Information indices	Indices of neighborhood symmetry
265	IC2	Information Content index (neighborhood symmetry of 2-order)	Information indices	Indices of neighborhood symmetry
266	IC3	Information Content index (neighborhood symmetry of 3-order)	Information indices	Indices of neighborhood symmetry
267	IC4	Information Content index (neighborhood symmetry of 4-order)	Information indices	Indices of neighborhood symmetry
268	IC5	Information Content index (neighborhood symmetry of 5-order)	Information indices	Indices of neighborhood symmetry
269	TIC0	Total Information Content index (neighborhood symmetry of 0-order)	Information indices	Indices of neighborhood symmetry
270	TIC1	Total Information Content index (neighborhood symmetry of 1-order)	Information indices	Indices of neighborhood symmetry
271	TIC2	Total Information Content index (neighborhood symmetry of 2-order)	Information indices	Indices of neighborhood symmetry
272	TIC3	Total Information Content index (neighborhood symmetry of 3-order)	Information indices	Indices of neighborhood symmetry
273	TIC4	Total Information Content index (neighborhood symmetry of 4-order)	Information indices	Indices of neighborhood symmetry

274	TIC5	Total Information Content index (neighborhood symmetry of 5-order)	Information indices	Indices of neighborhood symmetry
275	SIC0	Structural Information Content index (neighborhood symmetry of 0-order)	Information indices	Indices of neighborhood symmetry
276	SIC1	Structural Information Content index (neighborhood symmetry of 1-order)	Information indices	Indices of neighborhood symmetry
277	SIC2	Structural Information Content index (neighborhood symmetry of 2-order)	Information indices	Indices of neighborhood symmetry
278	SIC3	Structural Information Content index (neighborhood symmetry of 3-order)	Information indices	Indices of neighborhood symmetry
279	SIC4	Structural Information Content index (neighborhood symmetry of 4-order)	Information indices	Indices of neighborhood symmetry
280	SIC5	Structural Information Content index (neighborhood symmetry of 5-order)	Information indices	Indices of neighborhood symmetry
281	CIC0	Complementary Information Content index (neighborhood symmetry of 0-order)	Information indices	Indices of neighborhood symmetry
282	CIC1	Complementary Information Content index (neighborhood symmetry of 1-order)	Information indices	Indices of neighborhood symmetry
283	CIC2	Complementary Information Content index (neighborhood symmetry of 2-order)	Information indices	Indices of neighborhood symmetry
284	CIC3	Complementary Information Content index (neighborhood symmetry of 3-order)	Information indices	Indices of neighborhood symmetry
285	CIC4	Complementary Information Content index (neighborhood symmetry of 4-order)	Information indices	Indices of neighborhood symmetry
286	CIC5	Complementary Information Content index (neighborhood symmetry of 5-order)	Information indices	Indices of neighborhood symmetry
287	BIC0	Bond Information Content index (neighborhood symmetry of 0-order)	Information indices	Indices of neighborhood symmetry
288	BIC1	Bond Information Content index (neighborhood symmetry of 1-order)	Information indices	Indices of neighborhood symmetry

289	BIC2	Bond Information Content index (neighborhood symmetry of 2-order)	Information indices	Indices of neighborhood symmetry
290	BIC3	Bond Information Content index (neighborhood symmetry of 3-order)	Information indices	Indices of neighborhood symmetry
291	BIC4	Bond Information Content index (neighborhood symmetry of 4-order)	Information indices	Indices of neighborhood symmetry
292	BIC5	Bond Information Content index (neighborhood symmetry of 5-order)	Information indices	Indices of neighborhood symmetry
293	J_A	Balaban-like index from adjacency matrix	2D matrix-based descriptors	Adjacency matrix (A)
294	SpPos_A	spectral positive sum from adjacency matrix	2D matrix-based descriptors	Adjacency matrix (A)
295	SpPosA_A	normalized spectral positive sum from adjacency matrix	2D matrix-based descriptors	Adjacency matrix (A)
296	SpPosLog_A	logarithmic spectral positive sum from adjacency matrix	2D matrix-based descriptors	Adjacency matrix (A)
297	SpMax_A	leading eigenvalue from adjacency matrix (Lovasz-Pelikan index)	2D matrix-based descriptors	Adjacency matrix (A)
298	SpMaxA_A	normalized leading eigenvalue from adjacency matrix	2D matrix-based descriptors	Adjacency matrix (A)
299	SpDiam_A	spectral diameter from adjacency matrix	2D matrix-based descriptors	Adjacency matrix (A)
300	SpAD_A	spectral absolute deviation from adjacency matrix	2D matrix-based descriptors	Adjacency matrix (A)
301	SpMAD_A	spectral mean absolute deviation from adjacency matrix	2D matrix-based descriptors	Adjacency matrix (A)
302	Ho_A	Hosoya-like index (log function) from adjacency matrix	2D matrix-based descriptors	Adjacency matrix (A)
303	EE_A	Estrada-like index (log function) from adjacency matrix	2D matrix-based descriptors	Adjacency matrix (A)

304	VE1_A	coefficient sum of the last eigenvector (absolute values) from adjacency matrix	2D matrix-based descriptors	Adjacency matrix (A)
305	VE2_A	average coefficient of the last eigenvector (absolute values) from adjacency matrix	2D matrix-based descriptors	Adjacency matrix (A)
306	VE3_A	logarithmic coefficient sum of the last eigenvector (absolute values) from adjacency matrix	2D matrix-based descriptors	Adjacency matrix (A)
307	VE1sign_A	coefficient sum of the last eigenvector from adjacency matrix	2D matrix-based descriptors	Adjacency matrix (A)
308	VE2sign_A	average coefficient of the last eigenvector from adjacency matrix	2D matrix-based descriptors	Adjacency matrix (A)
309	VE3sign_A	logarithmic coefficient sum of the last eigenvector from adjacency matrix	2D matrix-based descriptors	Adjacency matrix (A)
310	VR1_A	Randic-like eigenvector-based index from adjacency matrix	2D matrix-based descriptors	Adjacency matrix (A)
311	VR2_A	normalized Randic-like eigenvector-based index from adjacency matrix	2D matrix-based descriptors	Adjacency matrix (A)
312	VR3_A	logarithmic Randic-like eigenvector-based index from adjacency matrix	2D matrix-based descriptors	Adjacency matrix (A)
313	Wi_D	Wiener-like index from topological distance matrix (Wiener index)	2D matrix-based descriptors	Topological distance matrix (D)
314	WiA_D	average Wiener-like index from topological distance matrix	2D matrix-based descriptors	Topological distance matrix (D)
315	AVS_D	average vertex sum from topological distance matrix	2D matrix-based descriptors	Topological distance matrix (D)
316	H_D	Harary-like index from topological distance matrix (Harary index)	2D matrix-based descriptors	Topological distance matrix (D)
317	Chi_D	Randic-like index from topological distance matrix	2D matrix-based descriptors	Topological distance matrix (D)
318	ChiA_D	average Randic-like index from topological distance matrix	2D matrix-based descriptors	Topological distance matrix (D)

319	J_D	Balaban-like index from topological distance matrix (Balaban distance connectivity index)	2D matrix-based descriptors	Topological distance matrix (D)
320	HyWi_D	hyper-Wiener-like index (log function) from topological distance matrix	2D matrix-based descriptors	Topological distance matrix (D)
321	SpPos_D	spectral positive sum from topological distance matrix	2D matrix-based descriptors	Topological distance matrix (D)
322	SpPosA_D	normalized spectral positive sum from topological distance matrix	2D matrix-based descriptors	Topological distance matrix (D)
323	SpPosLog_D	logarithmic spectral positive sum from topological distance matrix	2D matrix-based descriptors	Topological distance matrix (D)
324	SpMax_D	leading eigenvalue from topological distance matrix	2D matrix-based descriptors	Topological distance matrix (D)
325	SpMaxA_D	normalized leading eigenvalue from topological distance matrix	2D matrix-based descriptors	Topological distance matrix (D)
326	SpDiam_D	spectral diameter from topological distance matrix	2D matrix-based descriptors	Topological distance matrix (D)
327	SpAD_D	spectral absolute deviation from topological distance matrix	2D matrix-based descriptors	Topological distance matrix (D)
328	SpMAD_D	spectral mean absolute deviation from topological distance matrix	2D matrix-based descriptors	Topological distance matrix (D)
329	Ho_D	Hosoya-like index (log function) from topological distance matrix	2D matrix-based descriptors	Topological distance matrix (D)
330	EE_D	Estrada-like index (log function) from topological distance matrix	2D matrix-based descriptors	Topological distance matrix (D)
331	SM2_D	spectral moment of order 2 from topological distance matrix	2D matrix-based descriptors	Topological distance matrix (D)
332	SM3_D	spectral moment of order 3 from topological distance matrix	2D matrix-based descriptors	Topological distance matrix (D)
333	SM4_D	spectral moment of order 4 from topological distance matrix	2D matrix-based descriptors	Topological distance matrix (D)

334	SM5_D	spectral moment of order 5 from topological distance matrix	2D matrix-based descriptors	Topological distance matrix (D)
335	SM6_D	spectral moment of order 6 from topological distance matrix	2D matrix-based descriptors	Topological distance matrix (D)
336	VE1_D	coefficient sum of the last eigenvector (absolute values) from topological distance matrix	2D matrix-based descriptors	Topological distance matrix (D)
337	VE2_D	average coefficient of the last eigenvector (absolute values) from topological distance matrix	2D matrix-based descriptors	Topological distance matrix (D)
338	VE3_D	logarithmic coefficient sum of the last eigenvector (absolute values) from topological distance matrix	2D matrix-based descriptors	Topological distance matrix (D)
339	VE1sign_D	coefficient sum of the last eigenvector from topological distance matrix	2D matrix-based descriptors	Topological distance matrix (D)
340	VE2sign_D	average coefficient of the last eigenvector from topological distance matrix	2D matrix-based descriptors	Topological distance matrix (D)
341	VE3sign_D	logarithmic coefficient sum of the last eigenvector from topological distance matrix	2D matrix-based descriptors	Topological distance matrix (D)
342	VR1_D	Randic-like eigenvector-based index from topological distance matrix	2D matrix-based descriptors	Topological distance matrix (D)
343	VR2_D	normalized Randic-like eigenvector-based index from topological distance matrix	2D matrix-based descriptors	Topological distance matrix (D)
344	VR3_D	logarithmic Randic-like eigenvector-based index from topological distance matrix	2D matrix-based descriptors	Topological distance matrix (D)
345	QW_L	quasi-Wiener index (Kirchhoff number) from Laplace matrix	2D matrix-based descriptors	Laplace matrix (L)
346	TI1_L	first Mohar index from Laplace matrix	2D matrix-based descriptors	Laplace matrix (L)
347	TI2_L	second Mohar index from Laplace matrix	2D matrix-based descriptors	Laplace matrix (L)
348	STN_L	spanning tree number (log function) from Laplace matrix	2D matrix-based descriptors	Laplace matrix (L)

349	SpPos_L	spectral positive sum from Laplace matrix	2D matrix-based descriptors	Laplace matrix (L)
350	SpPosA_L	normalized spectral positive sum from Laplace matrix	2D matrix-based descriptors	Laplace matrix (L)
351	SpPosLog_L	logarithmic spectral positive sum from Laplace matrix	2D matrix-based descriptors	Laplace matrix (L)
352	SpMax_L	leading eigenvalue from Laplace matrix	2D matrix-based descriptors	Laplace matrix (L)
353	SpMaxA_L	normalized leading eigenvalue from Laplace matrix	2D matrix-based descriptors	Laplace matrix (L)
354	SpDiam_L	spectral diameter from Laplace matrix	2D matrix-based descriptors	Laplace matrix (L)
355	SpAD_L	spectral absolute deviation from Laplace matrix	2D matrix-based descriptors	Laplace matrix (L)
356	SpMAD_L	spectral mean absolute deviation from Laplace matrix	2D matrix-based descriptors	Laplace matrix (L)
357	Ho_L	Hosoya-like index (log function) from Laplace matrix	2D matrix-based descriptors	Laplace matrix (L)
358	EE_L	Estrada-like index (log function) from Laplace matrix	2D matrix-based descriptors	Laplace matrix (L)
359	SM2_L	spectral moment of order 2 from Laplace matrix	2D matrix-based descriptors	Laplace matrix (L)
360	SM3_L	spectral moment of order 3 from Laplace matrix	2D matrix-based descriptors	Laplace matrix (L)
361	SM4_L	spectral moment of order 4 from Laplace matrix	2D matrix-based descriptors	Laplace matrix (L)
362	SM5_L	spectral moment of order 5 from Laplace matrix	2D matrix-based descriptors	Laplace matrix (L)
363	SM6_L	spectral moment of order 6 from Laplace matrix	2D matrix-based descriptors	Laplace matrix (L)

364	VE1_L	coefficient sum of the last eigenvector (absolute values) from Laplace matrix	2D matrix-based descriptors	Laplace matrix (L)
365	VE2_L	average coefficient of the last eigenvector (absolute values) from Laplace matrix	2D matrix-based descriptors	Laplace matrix (L)
366	VE3_L	logarithmic coefficient sum of the last eigenvector (absolute values) from Laplace matrix	2D matrix-based descriptors	Laplace matrix (L)
367	VE1sign_L	coefficient sum of the last eigenvector from Laplace matrix	2D matrix-based descriptors	Laplace matrix (L)
368	VE2sign_L	average coefficient of the last eigenvector from Laplace matrix	2D matrix-based descriptors	Laplace matrix (L)
369	VE3sign_L	logarithmic coefficient sum of the last eigenvector from Laplace matrix	2D matrix-based descriptors	Laplace matrix (L)
370	VR1_L	Randic-like eigenvector-based index from Laplace matrix	2D matrix-based descriptors	Laplace matrix (L)
371	VR2_L	normalized Randic-like eigenvector-based index from Laplace matrix	2D matrix-based descriptors	Laplace matrix (L)
372	VR3_L	logarithmic Randic-like eigenvector-based index from Laplace matrix	2D matrix-based descriptors	Laplace matrix (L)
373	AVS_X	average vertex sum from chi matrix	2D matrix-based descriptors	Chi matrix (X)
374	H_X	Harary-like index from chi matrix	2D matrix-based descriptors	Chi matrix (X)
375	Chi_X	Randic-like index from chi matrix	2D matrix-based descriptors	Chi matrix (X)
376	ChiA_X	average Randic-like index from chi matrix	2D matrix-based descriptors	Chi matrix (X)
377	J_X	Balaban-like index from chi matrix	2D matrix-based descriptors	Chi matrix (X)
378	HyWi_X	hyper-Wiener-like index (log function) from chi matrix	2D matrix-based descriptors	Chi matrix (X)

379	SpPos_X	spectral positive sum from chi matrix	2D matrix-based descriptors	Chi matrix (X)
380	SpPosA_X	normalized spectral positive sum from chi matrix	2D matrix-based descriptors	Chi matrix (X)
381	SpPosLog_X	logarithmic spectral positive sum from chi matrix	2D matrix-based descriptors	Chi matrix (X)
382	SpMax_X	leading eigenvalue from chi matrix	2D matrix-based descriptors	Chi matrix (X)
383	SpMaxA_X	normalized leading eigenvalue from chi matrix	2D matrix-based descriptors	Chi matrix (X)
384	SpDiam_X	spectral diameter from chi matrix	2D matrix-based descriptors	Chi matrix (X)
385	SpAD_X	spectral absolute deviation from chi matrix	2D matrix-based descriptors	Chi matrix (X)
386	SpMAD_X	spectral mean absolute deviation from chi matrix	2D matrix-based descriptors	Chi matrix (X)
387	Ho_X	Hosoya-like index (log function) from chi matrix	2D matrix-based descriptors	Chi matrix (X)
388	EE_X	Estrada-like index (log function) from chi matrix	2D matrix-based descriptors	Chi matrix (X)
389	SM2_X	spectral moment of order 2 from chi matrix	2D matrix-based descriptors	Chi matrix (X)
390	SM3_X	spectral moment of order 3 from chi matrix	2D matrix-based descriptors	Chi matrix (X)
391	SM4_X	spectral moment of order 4 from chi matrix	2D matrix-based descriptors	Chi matrix (X)
392	SM5_X	spectral moment of order 5 from chi matrix	2D matrix-based descriptors	Chi matrix (X)
393	SM6_X	spectral moment of order 6 from chi matrix	2D matrix-based descriptors	Chi matrix (X)

394	VE1_X	coefficient sum of the last eigenvector (absolute values) from chi matrix	2D matrix-based descriptors	Chi matrix (X)
395	VE2_X	average coefficient of the last eigenvector (absolute values) from chi matrix	2D matrix-based descriptors	Chi matrix (X)
396	VE3_X	logarithmic coefficient sum of the last eigenvector (absolute values) from chi matrix	2D matrix-based descriptors	Chi matrix (X)
397	VE1sign_X	coefficient sum of the last eigenvector from chi matrix	2D matrix-based descriptors	Chi matrix (X)
398	VE2sign_X	average coefficient of the last eigenvector from chi matrix	2D matrix-based descriptors	Chi matrix (X)
399	VE3sign_X	logarithmic coefficient sum of the last eigenvector from chi matrix	2D matrix-based descriptors	Chi matrix (X)
400	VR1_X	Randic-like eigenvector-based index from chi matrix	2D matrix-based descriptors	Chi matrix (X)
401	VR2_X	normalized Randic-like eigenvector-based index from chi matrix	2D matrix-based descriptors	Chi matrix (X)
402	VR3_X	logarithmic Randic-like eigenvector-based index from chi matrix	2D matrix-based descriptors	Chi matrix (X)
403	Wi_H2	Wiener-like index from reciprocal squared distance matrix	2D matrix-based descriptors	Reciprocal squared distance matrix (H2)
404	WiA_H2	average Wiener-like index from reciprocal squared distance matrix	2D matrix-based descriptors	Reciprocal squared distance matrix (H2)
405	AVS_H2	average vertex sum from reciprocal squared distance matrix	2D matrix-based descriptors	Reciprocal squared distance matrix (H2)
406	Chi_H2	Randic-like index from reciprocal squared distance matrix	2D matrix-based descriptors	Reciprocal squared distance matrix (H2)
407	ChiA_H2	average Randic-like index from reciprocal squared distance matrix	2D matrix-based descriptors	Reciprocal squared distance matrix (H2)
408	J_H2	Balaban-like index from reciprocal squared distance matrix	2D matrix-based descriptors	Reciprocal squared distance matrix (H2)

409	HyWi_H2	hyper-Wiener-like index (log function) from reciprocal squared distance matrix	2D matrix-based descriptors	Reciprocal squared distance matrix (H2)
410	SpPos_H2	spectral positive sum from reciprocal squared distance matrix	2D matrix-based descriptors	Reciprocal squared distance matrix (H2)
411	SpPosA_H2	normalized spectral positive sum from reciprocal squared distance matrix	2D matrix-based descriptors	Reciprocal squared distance matrix (H2)
412	SpPosLog_H2	logarithmic spectral positive sum from reciprocal squared distance matrix	2D matrix-based descriptors	Reciprocal squared distance matrix (H2)
413	SpMax_H2	leading eigenvalue from reciprocal squared distance matrix	2D matrix-based descriptors	Reciprocal squared distance matrix (H2)
414	SpMaxA_H2	normalized leading eigenvalue from reciprocal squared distance matrix	2D matrix-based descriptors	Reciprocal squared distance matrix (H2)
415	SpDiam_H2	spectral diameter from reciprocal squared distance matrix	2D matrix-based descriptors	Reciprocal squared distance matrix (H2)
416	SpAD_H2	spectral absolute deviation from reciprocal squared distance matrix	2D matrix-based descriptors	Reciprocal squared distance matrix (H2)
417	SpMAD_H2	spectral mean absolute deviation from reciprocal squared distance matrix	2D matrix-based descriptors	Reciprocal squared distance matrix (H2)
418	Ho_H2	Hosoya-like index (log function) from reciprocal squared distance matrix	2D matrix-based descriptors	Reciprocal squared distance matrix (H2)
419	EE_H2	Estrada-like index (log function) from reciprocal squared distance matrix	2D matrix-based descriptors	Reciprocal squared distance matrix (H2)
420	SM2_H2	spectral moment of order 2 from reciprocal squared distance matrix	2D matrix-based descriptors	Reciprocal squared distance matrix (H2)
421	SM3_H2	spectral moment of order 3 from reciprocal squared distance matrix	2D matrix-based descriptors	Reciprocal squared distance matrix (H2)
422	SM4_H2	spectral moment of order 4 from reciprocal squared distance matrix	2D matrix-based descriptors	Reciprocal squared distance matrix (H2)
423	SM5_H2	spectral moment of order 5 from reciprocal squared distance matrix	2D matrix-based descriptors	Reciprocal squared distance matrix (H2)

424	SM6_H2	spectral moment of order 6 from reciprocal squared distance matrix	2D matrix-based descriptors	Reciprocal squared distance matrix (H2)
425	VE1_H2	coefficient sum of the last eigenvector (absolute values) from reciprocal squared distance matrix	2D matrix-based descriptors	Reciprocal squared distance matrix (H2)
426	VE2_H2	average coefficient of the last eigenvector (absolute values) from reciprocal squared distance matrix	2D matrix-based descriptors	Reciprocal squared distance matrix (H2)
427	VE3_H2	logarithmic coefficient sum of the last eigenvector (absolute values) from reciprocal squared distance matrix	2D matrix-based descriptors	Reciprocal squared distance matrix (H2)
428	VE1sign_H2	coefficient sum of the last eigenvector from reciprocal squared distance matrix	2D matrix-based descriptors	Reciprocal squared distance matrix (H2)
429	VE2sign_H2	average coefficient of the last eigenvector from reciprocal squared distance matrix	2D matrix-based descriptors	Reciprocal squared distance matrix (H2)
430	VE3sign_H2	logarithmic coefficient sum of the last eigenvector from reciprocal squared distance matrix	2D matrix-based descriptors	Reciprocal squared distance matrix (H2)
431	VR1_H2	Randic-like eigenvector-based index from reciprocal squared distance matrix	2D matrix-based descriptors	Reciprocal squared distance matrix (H2)
432	VR2_H2	normalized Randic-like eigenvector-based index from reciprocal squared distance matrix	2D matrix-based descriptors	Reciprocal squared distance matrix (H2)
433	VR3_H2	logarithmic Randic-like eigenvector-based index from reciprocal squared distance matrix	2D matrix-based descriptors	Reciprocal squared distance matrix (H2)
434	Wi_Dt	Wiener-like index from detour matrix (detour index)	2D matrix-based descriptors	Detour matrix (Dt)
435	WiA_Dt	average Wiener-like index from detour matrix	2D matrix-based descriptors	Detour matrix (Dt)
436	AVS_Dt	average vertex sum from detour matrix	2D matrix-based descriptors	Detour matrix (Dt)
437	H_Dt	Harary-like index from detour matrix	2D matrix-based descriptors	Detour matrix (Dt)
438	Chi_Dt	Randic-like index from detour matrix	2D matrix-based descriptors	Detour matrix (Dt)

439	ChiA_Dt	average Randic-like index from detour matrix	2D matrix-based descriptors	Detour matrix (Dt)
440	J_Dt	Balaban-like index from detour matrix	2D matrix-based descriptors	Detour matrix (Dt)
441	HyWi_Dt	hyper-Wiener-like index (log function) from detour matrix	2D matrix-based descriptors	Detour matrix (Dt)
442	SpPos_Dt	spectral positive sum from detour matrix	2D matrix-based descriptors	Detour matrix (Dt)
443	SpPosA_Dt	normalized spectral positive sum from detour matrix	2D matrix-based descriptors	Detour matrix (Dt)
444	SpPosLog_Dt	logarithmic spectral positive sum from detour matrix	2D matrix-based descriptors	Detour matrix (Dt)
445	SpMax_Dt	leading eigenvalue from detour matrix	2D matrix-based descriptors	Detour matrix (Dt)
446	SpMaxA_Dt	normalized leading eigenvalue from detour matrix	2D matrix-based descriptors	Detour matrix (Dt)
447	SpDiam_Dt	spectral diameter from detour matrix	2D matrix-based descriptors	Detour matrix (Dt)
448	SpAD_Dt	spectral absolute deviation from detour matrix	2D matrix-based descriptors	Detour matrix (Dt)
449	SpMAD_Dt	spectral mean absolute deviation from detour matrix	2D matrix-based descriptors	Detour matrix (Dt)
450	Ho_Dt	Hosoya-like index (log function) from detour matrix	2D matrix-based descriptors	Detour matrix (Dt)
451	EE_Dt	Estrada-like index (log function) from detour matrix	2D matrix-based descriptors	Detour matrix (Dt)
452	SM2_Dt	spectral moment of order 2 from detour matrix	2D matrix-based descriptors	Detour matrix (Dt)
453	SM3_Dt	spectral moment of order 3 from detour matrix	2D matrix-based descriptors	Detour matrix (Dt)

454	SM4_Dt	spectral moment of order 4 from detour matrix	2D matrix-based descriptors	Detour matrix (Dt)
455	SM5_Dt	spectral moment of order 5 from detour matrix	2D matrix-based descriptors	Detour matrix (Dt)
456	SM6_Dt	spectral moment of order 6 from detour matrix	2D matrix-based descriptors	Detour matrix (Dt)
457	VE1_Dt	coefficient sum of the last eigenvector (absolute values) from detour matrix	2D matrix-based descriptors	Detour matrix (Dt)
458	VE2_Dt	average coefficient of the last eigenvector (absolute values) from detour matrix	2D matrix-based descriptors	Detour matrix (Dt)
459	VE3_Dt	logarithmic coefficient sum of the last eigenvector (absolute values) from detour matrix	2D matrix-based descriptors	Detour matrix (Dt)
460	VE1sign_Dt	coefficient sum of the last eigenvector from detour matrix	2D matrix-based descriptors	Detour matrix (Dt)
461	VE2sign_Dt	average coefficient of the last eigenvector from detour matrix	2D matrix-based descriptors	Detour matrix (Dt)
462	VE3sign_Dt	logarithmic coefficient sum of the last eigenvector from detour matrix	2D matrix-based descriptors	Detour matrix (Dt)
463	VR1_Dt	Randic-like eigenvector-based index from detour matrix	2D matrix-based descriptors	Detour matrix (Dt)
464	VR2_Dt	normalized Randic-like eigenvector-based index from detour matrix	2D matrix-based descriptors	Detour matrix (Dt)
465	VR3_Dt	logarithmic Randic-like eigenvector-based index from detour matrix	2D matrix-based descriptors	Detour matrix (Dt)
466	Wi_D/Dt	Wiener-like index from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)
467	WiA_D/Dt	average Wiener-like index from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)
468	AVS_D/Dt	average vertex sum from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)

469	H_D/Dt	Harary-like index from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)
470	Chi_D/Dt	Randic-like index from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)
471	ChiA_D/Dt	average Randic-like index from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)
472	J_D/Dt	Balaban-like index from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)
473	HyWi_D/Dt	hyper-Wiener-like index (log function) from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)
474	SpPos_D/Dt	spectral positive sum from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)
475	SpPosA_D/Dt	normalized spectral positive sum from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)
476	SpPosLog_D/Dt	logarithmic spectral positive sum from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)
477	SpMax_D/Dt	leading eigenvalue from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)
478	SpMaxA_D/Dt	normalized leading eigenvalue from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)
479	SpDiam_D/Dt	spectral diameter from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)
480	SpAD_D/Dt	spectral absolute deviation from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)
481	SpMAD_D/Dt	spectral mean absolute deviation from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)
482	Ho_D/Dt	Hosoya-like index (log function) from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)
483	EE_D/Dt	Estrada-like index (log function) from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)

484	SM2_D/Dt	spectral moment of order 2 from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)
485	SM3_D/Dt	spectral moment of order 3 from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)
486	SM4_D/Dt	spectral moment of order 4 from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)
487	SM5_D/Dt	spectral moment of order 5 from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)
488	SM6_D/Dt	spectral moment of order 6 from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)
489	VE1_D/Dt	coefficient sum of the last eigenvector (absolute values) from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)
490	VE2_D/Dt	average coefficient of the last eigenvector (absolute values) from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)
491	VE3_D/Dt	logarithmic coefficient sum of the last eigenvector (absolute values) from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)
492	VE1sign_D/Dt	coefficient sum of the last eigenvector from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)
493	VE2sign_D/Dt	average coefficient of the last eigenvector from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)
494	VE3sign_D/Dt	logarithmic coefficient sum of the last eigenvector from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)
495	VR1_D/Dt	Randic-like eigenvector-based index from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)
496	VR2_D/Dt	normalized Randic-like eigenvector-based index from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)
497	VR3_D/Dt	logarithmic Randic-like eigenvector-based index from distance/detour matrix	2D matrix-based descriptors	Distance / detour matrix (D/Dt)
498	Wi_Dz(Z)	Wiener-like index from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))

499	WiA_Dz(Z)	average Wiener-like index from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))
500	AVS_Dz(Z)	average vertex sum from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))
501	H_Dz(Z)	Harary-like index from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))
502	Chi_Dz(Z)	Randic-like index from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))
503	ChiA_Dz(Z)	average Randic-like index from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))
504	J_Dz(Z)	Balaban-like index from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))
505	HyWi_Dz(Z)	hyper-Wiener-like index (log function) from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))
506	SpAbs_Dz(Z)	graph energy from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))
507	SpPos_Dz(Z)	spectral positive sum from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))
508	SpPosA_Dz(Z)	normalized spectral positive sum from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))
509	SpPosLog_Dz(Z)	logarithmic spectral positive sum from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))
510	SpMax_Dz(Z)	leading eigenvalue from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))
511	SpMaxA_Dz(Z)	normalized leading eigenvalue from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))
512	SpDiam_Dz(Z)	spectral diameter from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))
513	SpAD_Dz(Z)	spectral absolute deviation from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))

514	SpMAD_Dz(Z)	spectral mean absolute deviation from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))
515	Ho_Dz(Z)	Hosoya-like index (log function) from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))
516	EE_Dz(Z)	Estrada-like index (log function) from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))
517	SM1_Dz(Z)	spectral moment of order 1 from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))
518	SM2_Dz(Z)	spectral moment of order 2 from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))
519	SM3_Dz(Z)	spectral moment of order 3 from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))
520	SM4_Dz(Z)	spectral moment of order 4 from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))
521	SM5_Dz(Z)	spectral moment of order 5 from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))
522	SM6_Dz(Z)	spectral moment of order 6 from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))
523	VE1_Dz(Z)	coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))
524	VE2_Dz(Z)	average coefficient of the last eigenvector (absolute values) from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))
525	VE3_Dz(Z)	logarithmic coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))
526	VE1sign_Dz(Z)	coefficient sum of the last eigenvector from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))
527	VE2sign_Dz(Z)	average coefficient of the last eigenvector from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))
528	VE3sign_Dz(Z)	logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))

529	VR1_Dz(Z)	Randic-like eigenvector-based index from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))
530	VR2_Dz(Z)	normalized Randic-like eigenvector-based index from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))
531	VR3_Dz(Z)	logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by atomic number	2D matrix-based descriptors	Barysz matrix weighted by atomic number (Dz(Z))
532	Wi_Dz(m)	Wiener-like index from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
533	WiA_Dz(m)	average Wiener-like index from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
534	AVS_Dz(m)	average vertex sum from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
535	H_Dz(m)	Harary-like index from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
536	Chi_Dz(m)	Randic-like index from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
537	ChiA_Dz(m)	average Randic-like index from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
538	J_Dz(m)	Balaban-like index from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
539	HyWi_Dz(m)	hyper-Wiener-like index (log function) from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
540	SpAbs_Dz(m)	graph energy from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
541	SpPos_Dz(m)	spectral positive sum from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
542	SpPosA_Dz(m)	normalized spectral positive sum from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
543	SpPosLog_Dz(m)	logarithmic spectral positive sum from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))

544	SpMax_Dz(m)	leading eigenvalue from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
545	SpMaxA_Dz(m)	normalized leading eigenvalue from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
546	SpDiam_Dz(m)	spectral diameter from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
547	SpAD_Dz(m)	spectral absolute deviation from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
548	SpMAD_Dz(m)	spectral mean absolute deviation from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
549	Ho_Dz(m)	Hosoya-like index (log function) from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
550	EE_Dz(m)	Estrada-like index (log function) from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
551	SM1_Dz(m)	spectral moment of order 1 from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
552	SM2_Dz(m)	spectral moment of order 2 from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
553	SM3_Dz(m)	spectral moment of order 3 from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
554	SM4_Dz(m)	spectral moment of order 4 from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
555	SM5_Dz(m)	spectral moment of order 5 from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
556	SM6_Dz(m)	spectral moment of order 6 from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
557	VE1_Dz(m)	coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
558	VE2_Dz(m)	average coefficient of the last eigenvector (absolute values) from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))

559	VE3_Dz(m)	logarithmic coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
560	VE1sign_Dz(m)	coefficient sum of the last eigenvector from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
561	VE2sign_Dz(m)	average coefficient of the last eigenvector from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
562	VE3sign_Dz(m)	logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
563	VR1_Dz(m)	Randic-like eigenvector-based index from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
564	VR2_Dz(m)	normalized Randic-like eigenvector-based index from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
565	VR3_Dz(m)	logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by mass	2D matrix-based descriptors	Barysz matrix weighted by mass (Dz(m))
566	Wi_Dz(v)	Wiener-like index from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
567	WiA_Dz(v)	average Wiener-like index from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
568	AVS_Dz(v)	average vertex sum from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
569	H_Dz(v)	Harary-like index from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
570	Chi_Dz(v)	Randic-like index from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
571	ChiA_Dz(v)	average Randic-like index from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
572	J_Dz(v)	Balaban-like index from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
573	HyWi_Dz(v)	hyper-Wiener-like index (log function) from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))

574	SpAbs_Dz(v)	graph energy from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
575	SpPos_Dz(v)	spectral positive sum from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
576	SpPosA_Dz(v)	normalized spectral positive sum from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
577	SpPosLog_Dz(v)	logarithmic spectral positive sum from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
578	SpMax_Dz(v)	leading eigenvalue from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
579	SpMaxA_Dz(v)	normalized leading eigenvalue from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
580	SpDiam_Dz(v)	spectral diameter from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
581	SpAD_Dz(v)	spectral absolute deviation from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
582	SpMAD_Dz(v)	spectral mean absolute deviation from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
583	Ho_Dz(v)	Hosoya-like index (log function) from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
584	EE_Dz(v)	Estrada-like index (log function) from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
585	SM1_Dz(v)	spectral moment of order 1 from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
586	SM2_Dz(v)	spectral moment of order 2 from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
587	SM3_Dz(v)	spectral moment of order 3 from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
588	SM4_Dz(v)	spectral moment of order 4 from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))

589	SM5_Dz(v)	spectral moment of order 5 from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
590	SM6_Dz(v)	spectral moment of order 6 from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
591	VE1_Dz(v)	coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
592	VE2_Dz(v)	average coefficient of the last eigenvector (absolute values) from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
593	VE3_Dz(v)	logarithmic coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
594	VE1sign_Dz(v)	coefficient sum of the last eigenvector from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
595	VE2sign_Dz(v)	average coefficient of the last eigenvector from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
596	VE3sign_Dz(v)	logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
597	VR1_Dz(v)	Randic-like eigenvector-based index from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
598	VR2_Dz(v)	normalized Randic-like eigenvector-based index from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
599	VR3_Dz(v)	logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by van der Waals volume	2D matrix-based descriptors	Barysz matrix weighted by Van der Waals volume (Dz(v))
600	Wi_Dz(e)	Wiener-like index from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))
601	WiA_Dz(e)	average Wiener-like index from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))

602	AVS_Dz(e)	average vertex sum from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))
603	H_Dz(e)	Harary-like index from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))
604	Chi_Dz(e)	Randic-like index from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))
605	ChiA_Dz(e)	average Randic-like index from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))
606	J_Dz(e)	Balaban-like index from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))
607	HyWi_Dz(e)	hyper-Wiener-like index (log function) from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))
608	SpAbs_Dz(e)	graph energy from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))
609	SpPos_Dz(e)	spectral positive sum from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))
610	SpPosA_Dz(e)	normalized spectral positive sum from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))

611	SpPosLog_Dz(e)	logarithmic spectral positive sum from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))
612	SpMax_Dz(e)	leading eigenvalue from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))
613	SpMaxA_Dz(e)	normalized leading eigenvalue from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))
614	SpDiam_Dz(e)	spectral diameter from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))
615	SpAD_Dz(e)	spectral absolute deviation from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))
616	SpMAD_Dz(e)	spectral mean absolute deviation from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))
617	Ho_Dz(e)	Hosoya-like index (log function) from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))
618	EE_Dz(e)	Estrada-like index (log function) from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))
619	SM1_Dz(e)	spectral moment of order 1 from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))

620	SM2_Dz(e)	spectral moment of order 2 from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))
621	SM3_Dz(e)	spectral moment of order 3 from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))
622	SM4_Dz(e)	spectral moment of order 4 from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))
623	SM5_Dz(e)	spectral moment of order 5 from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))
624	SM6_Dz(e)	spectral moment of order 6 from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))
625	VE1_Dz(e)	coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))
626	VE2_Dz(e)	average coefficient of the last eigenvector (absolute values) from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))
627	VE3_Dz(e)	logarithmic coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))
628	VE1sign_Dz(e)	coefficient sum of the last eigenvector from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))

629	VE2sign_Dz(e)	average coefficient of the last eigenvector from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))
630	VE3sign_Dz(e)	logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))
631	VR1_Dz(e)	Randic-like eigenvector-based index from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))
632	VR2_Dz(e)	normalized Randic-like eigenvector-based index from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))
633	VR3_Dz(e)	logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Barysz matrix weighted by Sanderson electronegativity (Dz(e))
634	Wi_Dz(p)	Wiener-like index from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
635	WiA_Dz(p)	average Wiener-like index from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
636	AVS_Dz(p)	average vertex sum from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
637	H_Dz(p)	Harary-like index from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
638	Chi_Dz(p)	Randic-like index from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
639	ChiA_Dz(p)	average Randic-like index from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
640	J_Dz(p)	Balaban-like index from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))

641	HyWi_Dz(p)	hyper-Wiener-like index (log function) from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
642	SpAbs_Dz(p)	graph energy from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
643	SpPos_Dz(p)	spectral positive sum from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
644	SpPosA_Dz(p)	normalized spectral positive sum from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
645	SpPosLog_Dz(p)	logarithmic spectral positive sum from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
646	SpMax_Dz(p)	leading eigenvalue from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
647	SpMaxA_Dz(p)	normalized leading eigenvalue from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
648	SpDiam_Dz(p)	spectral diameter from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
649	SpAD_Dz(p)	spectral absolute deviation from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
650	SpMAD_Dz(p)	spectral mean absolute deviation from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
651	Ho_Dz(p)	Hosoya-like index (log function) from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
652	EE_Dz(p)	Estrada-like index (log function) from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
653	SM1_Dz(p)	spectral moment of order 1 from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
654	SM2_Dz(p)	spectral moment of order 2 from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
655	SM3_Dz(p)	spectral moment of order 3 from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))

656	SM4_Dz(p)	spectral moment of order 4 from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
657	SM5_Dz(p)	spectral moment of order 5 from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
658	SM6_Dz(p)	spectral moment of order 6 from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
659	VE1_Dz(p)	coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
660	VE2_Dz(p)	average coefficient of the last eigenvector (absolute values) from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
661	VE3_Dz(p)	logarithmic coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
662	VE1sign_Dz(p)	coefficient sum of the last eigenvector from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
663	VE2sign_Dz(p)	average coefficient of the last eigenvector from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
664	VE3sign_Dz(p)	logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
665	VR1_Dz(p)	Randic-like eigenvector-based index from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
666	VR2_Dz(p)	normalized Randic-like eigenvector-based index from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
667	VR3_Dz(p)	logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by polarizability	2D matrix-based descriptors	Barysz matrix weighted by polarizability (Dz(p))
668	Wi_Dz(i)	Wiener-like index from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))
669	WiA_Dz(i)	average Wiener-like index from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))

670	AVS_Dz(i)	average vertex sum from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))
671	H_Dz(i)	Harary-like index from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))
672	Chi_Dz(i)	Randic-like index from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))
673	ChiA_Dz(i)	average Randic-like index from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))
674	J_Dz(i)	Balaban-like index from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))
675	HyWi_Dz(i)	hyper-Wiener-like index (log function) from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))
676	SpAbs_Dz(i)	graph energy from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))
677	SpPos_Dz(i)	spectral positive sum from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))
678	SpPosA_Dz(i)	normalized spectral positive sum from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))
679	SpPosLog_Dz(i)	logarithmic spectral positive sum from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))
680	SpMax_Dz(i)	leading eigenvalue from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))
681	SpMaxA_Dz(i)	normalized leading eigenvalue from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))

682	SpDiam_Dz(i)	spectral diameter from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))
683	SpAD_Dz(i)	spectral absolute deviation from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))
684	SpMAD_Dz(i)	spectral mean absolute deviation from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))
685	Ho_Dz(i)	Hosoya-like index (log function) from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))
686	EE_Dz(i)	Estrada-like index (log function) from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))
687	SM1_Dz(i)	spectral moment of order 1 from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))
688	SM2_Dz(i)	spectral moment of order 2 from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))
689	SM3_Dz(i)	spectral moment of order 3 from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))
690	SM4_Dz(i)	spectral moment of order 4 from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))
691	SM5_Dz(i)	spectral moment of order 5 from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))
692	SM6_Dz(i)	spectral moment of order 6 from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))
693	VE1_Dz(i)	coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))

694	VE2_Dz(i)	average coefficient of the last eigenvector (absolute values) from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))
695	VE3_Dz(i)	logarithmic coefficient sum of the last eigenvector (absolute values) from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))
696	VE1sign_Dz(i)	coefficient sum of the last eigenvector from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))
697	VE2sign_Dz(i)	average coefficient of the last eigenvector from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))
698	VE3sign_Dz(i)	logarithmic coefficient sum of the last eigenvector from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))
699	VR1_Dz(i)	Randic-like eigenvector-based index from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))
700	VR2_Dz(i)	normalized Randic-like eigenvector-based index from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))
701	VR3_Dz(i)	logarithmic Randic-like eigenvector-based index from Barysz matrix weighted by ionization potential	2D matrix-based descriptors	Barysz matrix weighted by ionization potential (Dz(i))
702	Wi_B(m)	Wiener-like index from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))
703	WiA_B(m)	average Wiener-like index from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))
704	AVS_B(m)	average vertex sum from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))
705	Chi_B(m)	Randic-like index from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))
706	ChiA_B(m)	average Randic-like index from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))

707	J_B(m)	Balaban-like index from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))
708	HyWi_B(m)	hyper-Wiener-like index (log function) from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))
709	SpAbs_B(m)	graph energy from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))
710	SpPos_B(m)	spectral positive sum from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))
711	SpPosA_B(m)	normalized spectral positive sum from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))
712	SpPosLog_B(m)	logarithmic spectral positive sum from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))
713	SpMax_B(m)	leading eigenvalue from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))
714	SpMaxA_B(m)	normalized leading eigenvalue from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))
715	SpDiam_B(m)	spectral diameter from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))
716	SpAD_B(m)	spectral absolute deviation from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))
717	SpMAD_B(m)	spectral mean absolute deviation from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))
718	Ho_B(m)	Hosoya-like index (log function) from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))
719	EE_B(m)	Estrada-like index (log function) from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))
720	SM1_B(m)	spectral moment of order 1 from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))
721	SM2_B(m)	spectral moment of order 2 from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))

722	SM3_B(m)	spectral moment of order 3 from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))
723	SM4_B(m)	spectral moment of order 4 from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))
724	SM5_B(m)	spectral moment of order 5 from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))
725	SM6_B(m)	spectral moment of order 6 from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))
726	VE1_B(m)	coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))
727	VE2_B(m)	average coefficient of the last eigenvector (absolute values) from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))
728	VE3_B(m)	logarithmic coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))
729	VE1sign_B(m)	coefficient sum of the last eigenvector from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))
730	VE2sign_B(m)	average coefficient of the last eigenvector from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))
731	VE3sign_B(m)	logarithmic coefficient sum of the last eigenvector from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))
732	VR1_B(m)	Randic-like eigenvector-based index from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))
733	VR2_B(m)	normalized Randic-like eigenvector-based index from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))
734	VR3_B(m)	logarithmic Randic-like eigenvector-based index from Burden matrix weighted by mass	2D matrix-based descriptors	Burden matrix weighted by mass (B(m))
735	Wi_B(v)	Wiener-like index from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))
736	WiA_B(v)	average Wiener-like index from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))

737	AVS_B(v)	average vertex sum from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))
738	Chi_B(v)	Randic-like index from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))
739	ChiA_B(v)	average Randic-like index from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))
740	J_B(v)	Balaban-like index from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))
741	HyWi_B(v)	hyper-Wiener-like index (log function) from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))
742	SpAbs_B(v)	graph energy from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))
743	SpPos_B(v)	spectral positive sum from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))
744	SpPosA_B(v)	normalized spectral positive sum from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))
745	SpPosLog_B(v)	logarithmic spectral positive sum from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))
746	SpMax_B(v)	leading eigenvalue from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))
747	SpMaxA_B(v)	normalized leading eigenvalue from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))
748	SpDiam_B(v)	spectral diameter from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))
749	SpAD_B(v)	spectral absolute deviation from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))
750	SpMAD_B(v)	spectral mean absolute deviation from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))
751	Ho_B(v)	Hosoya-like index (log function) from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))

752	EE_B(v)	Estrada-like index (log function) from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))
753	SM1_B(v)	spectral moment of order 1 from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))
754	SM2_B(v)	spectral moment of order 2 from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))
755	SM3_B(v)	spectral moment of order 3 from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))
756	SM4_B(v)	spectral moment of order 4 from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))
757	SM5_B(v)	spectral moment of order 5 from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))
758	SM6_B(v)	spectral moment of order 6 from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))
759	VE1_B(v)	coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))
760	VE2_B(v)	average coefficient of the last eigenvector (absolute values) from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))
761	VE3_B(v)	logarithmic coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))
762	VE1sign_B(v)	coefficient sum of the last eigenvector from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))
763	VE2sign_B(v)	average coefficient of the last eigenvector from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))
764	VE3sign_B(v)	logarithmic coefficient sum of the last eigenvector from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))
765	VR1_B(v)	Randic-like eigenvector-based index from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))
766	VR2_B(v)	normalized Randic-like eigenvector-based index from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))

767	VR3_B(v)	logarithmic Randic-like eigenvector-based index from Burden matrix weighted by van der Waals volume	2D matrix-based descriptors	Burden matrix weighted by Van der Waals volume (B(v))
768	Wi_B(e)	Wiener-like index from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))
769	WiA_B(e)	average Wiener-like index from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))
770	AVS_B(e)	average vertex sum from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))
771	Chi_B(e)	Randic-like index from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))
772	ChiA_B(e)	average Randic-like index from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))
773	J_B(e)	Balaban-like index from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))
774	HyWi_B(e)	hyper-Wiener-like index (log function) from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))
775	SpAbs_B(e)	graph energy from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))
776	SpPos_B(e)	spectral positive sum from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))

777	SpPosA_B(e)	normalized spectral positive sum from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))
778	SpPosLog_B(e)	logarithmic spectral positive sum from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))
779	SpMax_B(e)	leading eigenvalue from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))
780	SpMaxA_B(e)	normalized leading eigenvalue from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))
781	SpDiam_B(e)	spectral diameter from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))
782	SpAD_B(e)	spectral absolute deviation from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))
783	SpMAD_B(e)	spectral mean absolute deviation from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))
784	Ho_B(e)	Hosoya-like index (log function) from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))
785	EE_B(e)	Estrada-like index (log function) from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))

786	SM1_B(e)	spectral moment of order 1 from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))
787	SM2_B(e)	spectral moment of order 2 from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))
788	SM3_B(e)	spectral moment of order 3 from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))
789	SM4_B(e)	spectral moment of order 4 from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))
790	SM5_B(e)	spectral moment of order 5 from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))
791	SM6_B(e)	spectral moment of order 6 from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))
792	VE1_B(e)	coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))
793	VE2_B(e)	average coefficient of the last eigenvector (absolute values) from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))
794	VE3_B(e)	logarithmic coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))

795	VE1sign_B(e)	coefficient sum of the last eigenvector from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))
796	VE2sign_B(e)	average coefficient of the last eigenvector from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))
797	VE3sign_B(e)	logarithmic coefficient sum of the last eigenvector from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))
798	VR1_B(e)	Randic-like eigenvector-based index from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))
799	VR2_B(e)	normalized Randic-like eigenvector-based index from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))
800	VR3_B(e)	logarithmic Randic-like eigenvector-based index from Burden matrix weighted by Sanderson electronegativity	2D matrix-based descriptors	Burden matrix weighted by Sanderson electronegativity (B(e))
801	Wi_B(p)	Wiener-like index from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))
802	WiA_B(p)	average Wiener-like index from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))
803	AVS_B(p)	average vertex sum from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))
804	Chi_B(p)	Randic-like index from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))
805	ChiA_B(p)	average Randic-like index from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))
806	J_B(p)	Balaban-like index from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))

807	HyWi_B(p)	hyper-Wiener-like index (log function) from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))
808	SpAbs_B(p)	graph energy from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))
809	SpPos_B(p)	spectral positive sum from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))
810	SpPosA_B(p)	normalized spectral positive sum from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))
811	SpPosLog_B(p)	logarithmic spectral positive sum from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))
812	SpMax_B(p)	leading eigenvalue from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))
813	SpMaxA_B(p)	normalized leading eigenvalue from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))
814	SpDiam_B(p)	spectral diameter from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))
815	SpAD_B(p)	spectral absolute deviation from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))
816	SpMAD_B(p)	spectral mean absolute deviation from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))
817	Ho_B(p)	Hosoya-like index (log function) from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))
818	EE_B(p)	Estrada-like index (log function) from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))
819	SM1_B(p)	spectral moment of order 1 from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))
820	SM2_B(p)	spectral moment of order 2 from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))
821	SM3_B(p)	spectral moment of order 3 from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))

822	SM4_B(p)	spectral moment of order 4 from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))
823	SM5_B(p)	spectral moment of order 5 from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))
824	SM6_B(p)	spectral moment of order 6 from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))
825	VE1_B(p)	coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))
826	VE2_B(p)	average coefficient of the last eigenvector (absolute values) from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))
827	VE3_B(p)	logarithmic coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))
828	VE1sign_B(p)	coefficient sum of the last eigenvector from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))
829	VE2sign_B(p)	average coefficient of the last eigenvector from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))
830	VE3sign_B(p)	logarithmic coefficient sum of the last eigenvector from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))
831	VR1_B(p)	Randic-like eigenvector-based index from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))
832	VR2_B(p)	normalized Randic-like eigenvector-based index from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))
833	VR3_B(p)	logarithmic Randic-like eigenvector-based index from Burden matrix weighted by polarizability	2D matrix-based descriptors	Burden matrix weighted by polarizability (B(p))
834	Wi_B(i)	Wiener-like index from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))
835	WiA_B(i)	average Wiener-like index from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))

836	AVS_B(i)	average vertex sum from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))
837	Chi_B(i)	Randic-like index from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))
838	ChiA_B(i)	average Randic-like index from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))
839	J_B(i)	Balaban-like index from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))
840	HyWi_B(i)	hyper-Wiener-like index (log function) from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))
841	SpAbs_B(i)	graph energy from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))
842	SpPos_B(i)	spectral positive sum from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))
843	SpPosA_B(i)	normalized spectral positive sum from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))
844	SpPosLog_B(i)	logarithmic spectral positive sum from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))
845	SpMax_B(i)	leading eigenvalue from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))
846	SpMaxA_B(i)	normalized leading eigenvalue from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))
847	SpDiam_B(i)	spectral diameter from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))

848	SpAD_B(i)	spectral absolute deviation from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))
849	SpMAD_B(i)	spectral mean absolute deviation from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))
850	Ho_B(i)	Hosoya-like index (log function) from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))
851	EE_B(i)	Estrada-like index (log function) from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))
852	SM1_B(i)	spectral moment of order 1 from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))
853	SM2_B(i)	spectral moment of order 2 from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))
854	SM3_B(i)	spectral moment of order 3 from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))
855	SM4_B(i)	spectral moment of order 4 from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))
856	SM5_B(i)	spectral moment of order 5 from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))
857	SM6_B(i)	spectral moment of order 6 from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))
858	VE1_B(i)	coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))
859	VE2_B(i)	average coefficient of the last eigenvector (absolute values) from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))

860	VE3_B(i)	logarithmic coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))
861	VE1sign_B(i)	coefficient sum of the last eigenvector from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))
862	VE2sign_B(i)	average coefficient of the last eigenvector from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))
863	VE3sign_B(i)	logarithmic coefficient sum of the last eigenvector from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))
864	VR1_B(i)	Randic-like eigenvector-based index from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))
865	VR2_B(i)	normalized Randic-like eigenvector-based index from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))
866	VR3_B(i)	logarithmic Randic-like eigenvector-based index from Burden matrix weighted by ionization potential	2D matrix-based descriptors	Burden matrix weighted by ionization potential (B(i))
867	Wi_B(s)	Wiener-like index from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))
868	WiA_B(s)	average Wiener-like index from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))
869	AVS_B(s)	average vertex sum from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))
870	Chi_B(s)	Randic-like index from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))
871	ChiA_B(s)	average Randic-like index from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))
872	J_B(s)	Balaban-like index from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))

873	HyWi_B(s)	hyper-Wiener-like index (log function) from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))
874	SpAbs_B(s)	graph energy from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))
875	SpPos_B(s)	spectral positive sum from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))
876	SpPosA_B(s)	normalized spectral positive sum from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))
877	SpPosLog_B(s)	logarithmic spectral positive sum from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))
878	SpMax_B(s)	leading eigenvalue from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))
879	SpMaxA_B(s)	normalized leading eigenvalue from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))
880	SpDiam_B(s)	spectral diameter from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))
881	SpAD_B(s)	spectral absolute deviation from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))
882	SpMAD_B(s)	spectral mean absolute deviation from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))
883	Ho_B(s)	Hosoya-like index (log function) from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))
884	EE_B(s)	Estrada-like index (log function) from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))
885	SM1_B(s)	spectral moment of order 1 from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))
886	SM2_B(s)	spectral moment of order 2 from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))
887	SM3_B(s)	spectral moment of order 3 from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))

888	SM4_B(s)	spectral moment of order 4 from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))
889	SM5_B(s)	spectral moment of order 5 from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))
890	SM6_B(s)	spectral moment of order 6 from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))
891	VE1_B(s)	coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))
892	VE2_B(s)	average coefficient of the last eigenvector (absolute values) from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))
893	VE3_B(s)	logarithmic coefficient sum of the last eigenvector (absolute values) from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))
894	VE1sign_B(s)	coefficient sum of the last eigenvector from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))
895	VE2sign_B(s)	average coefficient of the last eigenvector from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))
896	VE3sign_B(s)	logarithmic coefficient sum of the last eigenvector from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))
897	VR1_B(s)	Randic-like eigenvector-based index from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))
898	VR2_B(s)	normalized Randic-like eigenvector-based index from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))
899	VR3_B(s)	logarithmic Randic-like eigenvector-based index from Burden matrix weighted by I-State	2D matrix-based descriptors	Burden matrix weighted by I-state (B(s))
900	ATS1m	Broto-Moreau autocorrelation of lag 1 (log function) weighted by mass	2D autocorrelations	Broto-Moreau autocorrelations
901	ATS2m	Broto-Moreau autocorrelation of lag 2 (log function) weighted by mass	2D autocorrelations	Broto-Moreau autocorrelations
902	ATS3m	Broto-Moreau autocorrelation of lag 3 (log function) weighted by mass	2D autocorrelations	Broto-Moreau autocorrelations
903	ATS4m	Broto-Moreau autocorrelation of lag 4 (log function) weighted by mass	2D autocorrelations	Broto-Moreau autocorrelations

904	ATS5m	Broto-Moreau autocorrelation of lag 5 (log function) weighted by mass	2D autocorrelations	Broto-Moreau autocorrelations
905	ATS6m	Broto-Moreau autocorrelation of lag 6 (log function) weighted by mass	2D autocorrelations	Broto-Moreau autocorrelations
906	ATS7m	Broto-Moreau autocorrelation of lag 7 (log function) weighted by mass	2D autocorrelations	Broto-Moreau autocorrelations
907	ATS8m	Broto-Moreau autocorrelation of lag 8 (log function) weighted by mass	2D autocorrelations	Broto-Moreau autocorrelations
908	ATS1v	Broto-Moreau autocorrelation of lag 1 (log function) weighted by van der Waals volume	2D autocorrelations	Broto-Moreau autocorrelations
909	ATS2v	Broto-Moreau autocorrelation of lag 2 (log function) weighted by van der Waals volume	2D autocorrelations	Broto-Moreau autocorrelations
910	ATS3v	Broto-Moreau autocorrelation of lag 3 (log function) weighted by van der Waals volume	2D autocorrelations	Broto-Moreau autocorrelations
911	ATS4v	Broto-Moreau autocorrelation of lag 4 (log function) weighted by van der Waals volume	2D autocorrelations	Broto-Moreau autocorrelations
912	ATS5v	Broto-Moreau autocorrelation of lag 5 (log function) weighted by van der Waals volume	2D autocorrelations	Broto-Moreau autocorrelations
913	ATS6v	Broto-Moreau autocorrelation of lag 6 (log function) weighted by van der Waals volume	2D autocorrelations	Broto-Moreau autocorrelations
914	ATS7v	Broto-Moreau autocorrelation of lag 7 (log function) weighted by van der Waals volume	2D autocorrelations	Broto-Moreau autocorrelations
915	ATS8v	Broto-Moreau autocorrelation of lag 8 (log function) weighted by van der Waals volume	2D autocorrelations	Broto-Moreau autocorrelations
916	ATS1e	Broto-Moreau autocorrelation of lag 1 (log function) weighted by Sanderson electronegativity	2D autocorrelations	Broto-Moreau autocorrelations
917	ATS2e	Broto-Moreau autocorrelation of lag 2 (log function) weighted by Sanderson electronegativity	2D autocorrelations	Broto-Moreau autocorrelations
918	ATS3e	Broto-Moreau autocorrelation of lag 3 (log function) weighted by Sanderson electronegativity	2D autocorrelations	Broto-Moreau autocorrelations
919	ATS4e	Broto-Moreau autocorrelation of lag 4 (log function) weighted by Sanderson electronegativity	2D autocorrelations	Broto-Moreau autocorrelations

920	ATS5e	Broto-Moreau autocorrelation of lag 5 (log function) weighted by Sanderson electronegativity	2D autocorrelations	Broto-Moreau autocorrelations
921	ATS6e	Broto-Moreau autocorrelation of lag 6 (log function) weighted by Sanderson electronegativity	2D autocorrelations	Broto-Moreau autocorrelations
922	ATS7e	Broto-Moreau autocorrelation of lag 7 (log function) weighted by Sanderson electronegativity	2D autocorrelations	Broto-Moreau autocorrelations
923	ATS8e	Broto-Moreau autocorrelation of lag 8 (log function) weighted by Sanderson electronegativity	2D autocorrelations	Broto-Moreau autocorrelations
924	ATS1p	Broto-Moreau autocorrelation of lag 1 (log function) weighted by polarizability	2D autocorrelations	Broto-Moreau autocorrelations
925	ATS2p	Broto-Moreau autocorrelation of lag 2 (log function) weighted by polarizability	2D autocorrelations	Broto-Moreau autocorrelations
926	ATS3p	Broto-Moreau autocorrelation of lag 3 (log function) weighted by polarizability	2D autocorrelations	Broto-Moreau autocorrelations
927	ATS4p	Broto-Moreau autocorrelation of lag 4 (log function) weighted by polarizability	2D autocorrelations	Broto-Moreau autocorrelations
928	ATS5p	Broto-Moreau autocorrelation of lag 5 (log function) weighted by polarizability	2D autocorrelations	Broto-Moreau autocorrelations
929	ATS6p	Broto-Moreau autocorrelation of lag 6 (log function) weighted by polarizability	2D autocorrelations	Broto-Moreau autocorrelations
930	ATS7p	Broto-Moreau autocorrelation of lag 7 (log function) weighted by polarizability	2D autocorrelations	Broto-Moreau autocorrelations
931	ATS8p	Broto-Moreau autocorrelation of lag 8 (log function) weighted by polarizability	2D autocorrelations	Broto-Moreau autocorrelations
932	ATS1i	Broto-Moreau autocorrelation of lag 1 (log function) weighted by ionization potential	2D autocorrelations	Broto-Moreau autocorrelations
933	ATS2i	Broto-Moreau autocorrelation of lag 2 (log function) weighted by ionization potential	2D autocorrelations	Broto-Moreau autocorrelations
934	ATS3i	Broto-Moreau autocorrelation of lag 3 (log function) weighted by ionization potential	2D autocorrelations	Broto-Moreau autocorrelations
935	ATS4i	Broto-Moreau autocorrelation of lag 4 (log function) weighted by ionization potential	2D autocorrelations	Broto-Moreau autocorrelations
936	ATS5i	Broto-Moreau autocorrelation of lag 5 (log function) weighted by ionization potential	2D autocorrelations	Broto-Moreau autocorrelations
937	ATS6i	Broto-Moreau autocorrelation of lag 6 (log function) weighted by ionization potential	2D autocorrelations	Broto-Moreau autocorrelations
938	ATS7i	Broto-Moreau autocorrelation of lag 7 (log function) weighted by ionization potential	2D autocorrelations	Broto-Moreau autocorrelations

939	ATS8i	Broto-Moreau autocorrelation of lag 8 (log function) weighted by ionization potential	2D autocorrelations	Broto-Moreau autocorrelations
940	ATS1s	Broto-Moreau autocorrelation of lag 1 (log function) weighted by I-state	2D autocorrelations	Broto-Moreau autocorrelations
941	ATS2s	Broto-Moreau autocorrelation of lag 2 (log function) weighted by I-state	2D autocorrelations	Broto-Moreau autocorrelations
942	ATS3s	Broto-Moreau autocorrelation of lag 3 (log function) weighted by I-state	2D autocorrelations	Broto-Moreau autocorrelations
943	ATS4s	Broto-Moreau autocorrelation of lag 4 (log function) weighted by I-state	2D autocorrelations	Broto-Moreau autocorrelations
944	ATS5s	Broto-Moreau autocorrelation of lag 5 (log function) weighted by I-state	2D autocorrelations	Broto-Moreau autocorrelations
945	ATS6s	Broto-Moreau autocorrelation of lag 6 (log function) weighted by I-state	2D autocorrelations	Broto-Moreau autocorrelations
946	ATS7s	Broto-Moreau autocorrelation of lag 7 (log function) weighted by I-state	2D autocorrelations	Broto-Moreau autocorrelations
947	ATS8s	Broto-Moreau autocorrelation of lag 8 (log function) weighted by I-state	2D autocorrelations	Broto-Moreau autocorrelations
948	ATSC1m	Centred Broto-Moreau autocorrelation of lag 1 weighted by mass	2D autocorrelations	Centred Broto-Moreau autocorrelations
949	ATSC2m	Centred Broto-Moreau autocorrelation of lag 2 weighted by mass	2D autocorrelations	Centred Broto-Moreau autocorrelations
950	ATSC3m	Centred Broto-Moreau autocorrelation of lag 3 weighted by mass	2D autocorrelations	Centred Broto-Moreau autocorrelations
951	ATSC4m	Centred Broto-Moreau autocorrelation of lag 4 weighted by mass	2D autocorrelations	Centred Broto-Moreau autocorrelations
952	ATSC5m	Centred Broto-Moreau autocorrelation of lag 5 weighted by mass	2D autocorrelations	Centred Broto-Moreau autocorrelations
953	ATSC6m	Centred Broto-Moreau autocorrelation of lag 6 weighted by mass	2D autocorrelations	Centred Broto-Moreau autocorrelations
954	ATSC7m	Centred Broto-Moreau autocorrelation of lag 7 weighted by mass	2D autocorrelations	Centred Broto-Moreau autocorrelations
955	ATSC8m	Centred Broto-Moreau autocorrelation of lag 8 weighted by mass	2D autocorrelations	Centred Broto-Moreau autocorrelations

956	ATSC1v	Centred Broto-Moreau autocorrelation of lag 1 weighted by van der Waals volume	2D autocorrelations	Centred Broto-Moreau autocorrelations
957	ATSC2v	Centred Broto-Moreau autocorrelation of lag 2 weighted by van der Waals volume	2D autocorrelations	Centred Broto-Moreau autocorrelations
958	ATSC3v	Centred Broto-Moreau autocorrelation of lag 3 weighted by van der Waals volume	2D autocorrelations	Centred Broto-Moreau autocorrelations
959	ATSC4v	Centred Broto-Moreau autocorrelation of lag 4 weighted by van der Waals volume	2D autocorrelations	Centred Broto-Moreau autocorrelations
960	ATSC5v	Centred Broto-Moreau autocorrelation of lag 5 weighted by van der Waals volume	2D autocorrelations	Centred Broto-Moreau autocorrelations
961	ATSC6v	Centred Broto-Moreau autocorrelation of lag 6 weighted by van der Waals volume	2D autocorrelations	Centred Broto-Moreau autocorrelations
962	ATSC7v	Centred Broto-Moreau autocorrelation of lag 7 weighted by van der Waals volume	2D autocorrelations	Centred Broto-Moreau autocorrelations
963	ATSC8v	Centred Broto-Moreau autocorrelation of lag 8 weighted by van der Waals volume	2D autocorrelations	Centred Broto-Moreau autocorrelations
964	ATSC1e	Centred Broto-Moreau autocorrelation of lag 1 weighted by Sanderson electronegativity	2D autocorrelations	Centred Broto-Moreau autocorrelations
965	ATSC2e	Centred Broto-Moreau autocorrelation of lag 2 weighted by Sanderson electronegativity	2D autocorrelations	Centred Broto-Moreau autocorrelations
966	ATSC3e	Centred Broto-Moreau autocorrelation of lag 3 weighted by Sanderson electronegativity	2D autocorrelations	Centred Broto-Moreau autocorrelations
967	ATSC4e	Centred Broto-Moreau autocorrelation of lag 4 weighted by Sanderson electronegativity	2D autocorrelations	Centred Broto-Moreau autocorrelations
968	ATSC5e	Centred Broto-Moreau autocorrelation of lag 5 weighted by Sanderson electronegativity	2D autocorrelations	Centred Broto-Moreau autocorrelations
969	ATSC6e	Centred Broto-Moreau autocorrelation of lag 6 weighted by Sanderson electronegativity	2D autocorrelations	Centred Broto-Moreau autocorrelations
970	ATSC7e	Centred Broto-Moreau autocorrelation of lag 7 weighted by Sanderson electronegativity	2D autocorrelations	Centred Broto-Moreau autocorrelations

971	ATSC8e	Centred Broto-Moreau autocorrelation of lag 8 weighted by Sanderson electronegativity	2D autocorrelations	Centred Broto-Moreau autocorrelations
972	ATSC1p	Centred Broto-Moreau autocorrelation of lag 1 weighted by polarizability	2D autocorrelations	Centred Broto-Moreau autocorrelations
973	ATSC2p	Centred Broto-Moreau autocorrelation of lag 2 weighted by polarizability	2D autocorrelations	Centred Broto-Moreau autocorrelations
974	ATSC3p	Centred Broto-Moreau autocorrelation of lag 3 weighted by polarizability	2D autocorrelations	Centred Broto-Moreau autocorrelations
975	ATSC4p	Centred Broto-Moreau autocorrelation of lag 4 weighted by polarizability	2D autocorrelations	Centred Broto-Moreau autocorrelations
976	ATSC5p	Centred Broto-Moreau autocorrelation of lag 5 weighted by polarizability	2D autocorrelations	Centred Broto-Moreau autocorrelations
977	ATSC6p	Centred Broto-Moreau autocorrelation of lag 6 weighted by polarizability	2D autocorrelations	Centred Broto-Moreau autocorrelations
978	ATSC7p	Centred Broto-Moreau autocorrelation of lag 7 weighted by polarizability	2D autocorrelations	Centred Broto-Moreau autocorrelations
979	ATSC8p	Centred Broto-Moreau autocorrelation of lag 8 weighted by polarizability	2D autocorrelations	Centred Broto-Moreau autocorrelations
980	ATSC1i	Centred Broto-Moreau autocorrelation of lag 1 weighted by ionization potential	2D autocorrelations	Centred Broto-Moreau autocorrelations
981	ATSC2i	Centred Broto-Moreau autocorrelation of lag 2 weighted by ionization potential	2D autocorrelations	Centred Broto-Moreau autocorrelations
982	ATSC3i	Centred Broto-Moreau autocorrelation of lag 3 weighted by ionization potential	2D autocorrelations	Centred Broto-Moreau autocorrelations
983	ATSC4i	Centred Broto-Moreau autocorrelation of lag 4 weighted by ionization potential	2D autocorrelations	Centred Broto-Moreau autocorrelations
984	ATSC5i	Centred Broto-Moreau autocorrelation of lag 5 weighted by ionization potential	2D autocorrelations	Centred Broto-Moreau autocorrelations
985	ATSC6i	Centred Broto-Moreau autocorrelation of lag 6 weighted by ionization potential	2D autocorrelations	Centred Broto-Moreau autocorrelations

986	ATSC7i	Centred Broto-Moreau autocorrelation of lag 7 weighted by ionization potential	2D autocorrelations	Centred Broto-Moreau autocorrelations
987	ATSC8i	Centred Broto-Moreau autocorrelation of lag 8 weighted by ionization potential	2D autocorrelations	Centred Broto-Moreau autocorrelations
988	ATSC1s	Centred Broto-Moreau autocorrelation of lag 1 weighted by I-state	2D autocorrelations	Centred Broto-Moreau autocorrelations
989	ATSC2s	Centred Broto-Moreau autocorrelation of lag 2 weighted by I-state	2D autocorrelations	Centred Broto-Moreau autocorrelations
990	ATSC3s	Centred Broto-Moreau autocorrelation of lag 3 weighted by I-state	2D autocorrelations	Centred Broto-Moreau autocorrelations
991	ATSC4s	Centred Broto-Moreau autocorrelation of lag 4 weighted by I-state	2D autocorrelations	Centred Broto-Moreau autocorrelations
992	ATSC5s	Centred Broto-Moreau autocorrelation of lag 5 weighted by I-state	2D autocorrelations	Centred Broto-Moreau autocorrelations
993	ATSC6s	Centred Broto-Moreau autocorrelation of lag 6 weighted by I-state	2D autocorrelations	Centred Broto-Moreau autocorrelations
994	ATSC7s	Centred Broto-Moreau autocorrelation of lag 7 weighted by I-state	2D autocorrelations	Centred Broto-Moreau autocorrelations
995	ATSC8s	Centred Broto-Moreau autocorrelation of lag 8 weighted by I-state	2D autocorrelations	Centred Broto-Moreau autocorrelations
996	MATS1m	Moran autocorrelation of lag 1 weighted by mass	2D autocorrelations	Moran autocorrelations
997	MATS2m	Moran autocorrelation of lag 2 weighted by mass	2D autocorrelations	Moran autocorrelations
998	MATS3m	Moran autocorrelation of lag 3 weighted by mass	2D autocorrelations	Moran autocorrelations
999	MATS4m	Moran autocorrelation of lag 4 weighted by mass	2D autocorrelations	Moran autocorrelations
1000	MATS5m	Moran autocorrelation of lag 5 weighted by mass	2D autocorrelations	Moran autocorrelations
1001	MATS6m	Moran autocorrelation of lag 6 weighted by mass	2D autocorrelations	Moran autocorrelations
1002	MATS7m	Moran autocorrelation of lag 7 weighted by mass	2D autocorrelations	Moran autocorrelations

1003	MATS8m	Moran autocorrelation of lag 8 weighted by mass	2D autocorrelations	Moran autocorrelations
1004	MATS1v	Moran autocorrelation of lag 1 weighted by van der Waals volume	2D autocorrelations	Moran autocorrelations
1005	MATS2v	Moran autocorrelation of lag 2 weighted by van der Waals volume	2D autocorrelations	Moran autocorrelations
1006	MATS3v	Moran autocorrelation of lag 3 weighted by van der Waals volume	2D autocorrelations	Moran autocorrelations
1007	MATS4v	Moran autocorrelation of lag 4 weighted by van der Waals volume	2D autocorrelations	Moran autocorrelations
1008	MATS5v	Moran autocorrelation of lag 5 weighted by van der Waals volume	2D autocorrelations	Moran autocorrelations
1009	MATS6v	Moran autocorrelation of lag 6 weighted by van der Waals volume	2D autocorrelations	Moran autocorrelations
1010	MATS7v	Moran autocorrelation of lag 7 weighted by van der Waals volume	2D autocorrelations	Moran autocorrelations
1011	MATS8v	Moran autocorrelation of lag 8 weighted by van der Waals volume	2D autocorrelations	Moran autocorrelations
1012	MATS1e	Moran autocorrelation of lag 1 weighted by Sanderson electronegativity	2D autocorrelations	Moran autocorrelations
1013	MATS2e	Moran autocorrelation of lag 2 weighted by Sanderson electronegativity	2D autocorrelations	Moran autocorrelations
1014	MATS3e	Moran autocorrelation of lag 3 weighted by Sanderson electronegativity	2D autocorrelations	Moran autocorrelations
1015	MATS4e	Moran autocorrelation of lag 4 weighted by Sanderson electronegativity	2D autocorrelations	Moran autocorrelations
1016	MATS5e	Moran autocorrelation of lag 5 weighted by Sanderson electronegativity	2D autocorrelations	Moran autocorrelations
1017	MATS6e	Moran autocorrelation of lag 6 weighted by Sanderson electronegativity	2D autocorrelations	Moran autocorrelations
1018	MATS7e	Moran autocorrelation of lag 7 weighted by Sanderson electronegativity	2D autocorrelations	Moran autocorrelations
1019	MATS8e	Moran autocorrelation of lag 8 weighted by Sanderson electronegativity	2D autocorrelations	Moran autocorrelations
1020	MATS1p	Moran autocorrelation of lag 1 weighted by polarizability	2D autocorrelations	Moran autocorrelations
1021	MATS2p	Moran autocorrelation of lag 2 weighted by polarizability	2D autocorrelations	Moran autocorrelations
1022	MATS3p	Moran autocorrelation of lag 3 weighted by polarizability	2D autocorrelations	Moran autocorrelations

1023	MATS4p	Moran autocorrelation of lag 4 weighted by polarizability	2D autocorrelations	Moran autocorrelations
1024	MATS5p	Moran autocorrelation of lag 5 weighted by polarizability	2D autocorrelations	Moran autocorrelations
1025	MATS6p	Moran autocorrelation of lag 6 weighted by polarizability	2D autocorrelations	Moran autocorrelations
1026	MATS7p	Moran autocorrelation of lag 7 weighted by polarizability	2D autocorrelations	Moran autocorrelations
1027	MATS8p	Moran autocorrelation of lag 8 weighted by polarizability	2D autocorrelations	Moran autocorrelations
1028	MATS1i	Moran autocorrelation of lag 1 weighted by ionization potential	2D autocorrelations	Moran autocorrelations
1029	MATS2i	Moran autocorrelation of lag 2 weighted by ionization potential	2D autocorrelations	Moran autocorrelations
1030	MATS3i	Moran autocorrelation of lag 3 weighted by ionization potential	2D autocorrelations	Moran autocorrelations
1031	MATS4i	Moran autocorrelation of lag 4 weighted by ionization potential	2D autocorrelations	Moran autocorrelations
1032	MATS5i	Moran autocorrelation of lag 5 weighted by ionization potential	2D autocorrelations	Moran autocorrelations
1033	MATS6i	Moran autocorrelation of lag 6 weighted by ionization potential	2D autocorrelations	Moran autocorrelations
1034	MATS7i	Moran autocorrelation of lag 7 weighted by ionization potential	2D autocorrelations	Moran autocorrelations
1035	MATS8i	Moran autocorrelation of lag 8 weighted by ionization potential	2D autocorrelations	Moran autocorrelations
1036	MATS1s	Moran autocorrelation of lag 1 weighted by I-state	2D autocorrelations	Moran autocorrelations
1037	MATS2s	Moran autocorrelation of lag 2 weighted by I-state	2D autocorrelations	Moran autocorrelations
1038	MATS3s	Moran autocorrelation of lag 3 weighted by I-state	2D autocorrelations	Moran autocorrelations
1039	MATS4s	Moran autocorrelation of lag 4 weighted by I-state	2D autocorrelations	Moran autocorrelations
1040	MATS5s	Moran autocorrelation of lag 5 weighted by I-state	2D autocorrelations	Moran autocorrelations
1041	MATS6s	Moran autocorrelation of lag 6 weighted by I-state	2D autocorrelations	Moran autocorrelations
1042	MATS7s	Moran autocorrelation of lag 7 weighted by I-state	2D autocorrelations	Moran autocorrelations

1043	MATS8s	Moran autocorrelation of lag 8 weighted by I-state	2D autocorrelations	Moran autocorrelations
1044	GATS1m	Geary autocorrelation of lag 1 weighted by mass	2D autocorrelations	Geary autocorrelations
1045	GATS2m	Geary autocorrelation of lag 2 weighted by mass	2D autocorrelations	Geary autocorrelations
1046	GATS3m	Geary autocorrelation of lag 3 weighted by mass	2D autocorrelations	Geary autocorrelations
1047	GATS4m	Geary autocorrelation of lag 4 weighted by mass	2D autocorrelations	Geary autocorrelations
1048	GATS5m	Geary autocorrelation of lag 5 weighted by mass	2D autocorrelations	Geary autocorrelations
1049	GATS6m	Geary autocorrelation of lag 6 weighted by mass	2D autocorrelations	Geary autocorrelations
1050	GATS7m	Geary autocorrelation of lag 7 weighted by mass	2D autocorrelations	Geary autocorrelations
1051	GATS8m	Geary autocorrelation of lag 8 weighted by mass	2D autocorrelations	Geary autocorrelations
1052	GATS1v	Geary autocorrelation of lag 1 weighted by van der Waals volume	2D autocorrelations	Geary autocorrelations
1053	GATS2v	Geary autocorrelation of lag 2 weighted by van der Waals volume	2D autocorrelations	Geary autocorrelations
1054	GATS3v	Geary autocorrelation of lag 3 weighted by van der Waals volume	2D autocorrelations	Geary autocorrelations
1055	GATS4v	Geary autocorrelation of lag 4 weighted by van der Waals volume	2D autocorrelations	Geary autocorrelations
1056	GATS5v	Geary autocorrelation of lag 5 weighted by van der Waals volume	2D autocorrelations	Geary autocorrelations
1057	GATS6v	Geary autocorrelation of lag 6 weighted by van der Waals volume	2D autocorrelations	Geary autocorrelations
1058	GATS7v	Geary autocorrelation of lag 7 weighted by van der Waals volume	2D autocorrelations	Geary autocorrelations
1059	GATS8v	Geary autocorrelation of lag 8 weighted by van der Waals volume	2D autocorrelations	Geary autocorrelations
1060	GATS1e	Geary autocorrelation of lag 1 weighted by Sanderson electronegativity	2D autocorrelations	Geary autocorrelations
1061	GATS2e	Geary autocorrelation of lag 2 weighted by Sanderson electronegativity	2D autocorrelations	Geary autocorrelations
1062	GATS3e	Geary autocorrelation of lag 3 weighted by Sanderson electronegativity	2D autocorrelations	Geary autocorrelations

1063	GATS4e	Geary autocorrelation of lag 4 weighted by Sanderson electronegativity	2D autocorrelations	Geary autocorrelations
1064	GATS5e	Geary autocorrelation of lag 5 weighted by Sanderson electronegativity	2D autocorrelations	Geary autocorrelations
1065	GATS6e	Geary autocorrelation of lag 6 weighted by Sanderson electronegativity	2D autocorrelations	Geary autocorrelations
1066	GATS7e	Geary autocorrelation of lag 7 weighted by Sanderson electronegativity	2D autocorrelations	Geary autocorrelations
1067	GATS8e	Geary autocorrelation of lag 8 weighted by Sanderson electronegativity	2D autocorrelations	Geary autocorrelations
1068	GATS1p	Geary autocorrelation of lag 1 weighted by polarizability	2D autocorrelations	Geary autocorrelations
1069	GATS2p	Geary autocorrelation of lag 2 weighted by polarizability	2D autocorrelations	Geary autocorrelations
1070	GATS3p	Geary autocorrelation of lag 3 weighted by polarizability	2D autocorrelations	Geary autocorrelations
1071	GATS4p	Geary autocorrelation of lag 4 weighted by polarizability	2D autocorrelations	Geary autocorrelations
1072	GATS5p	Geary autocorrelation of lag 5 weighted by polarizability	2D autocorrelations	Geary autocorrelations
1073	GATS6p	Geary autocorrelation of lag 6 weighted by polarizability	2D autocorrelations	Geary autocorrelations
1074	GATS7p	Geary autocorrelation of lag 7 weighted by polarizability	2D autocorrelations	Geary autocorrelations
1075	GATS8p	Geary autocorrelation of lag 8 weighted by polarizability	2D autocorrelations	Geary autocorrelations
1076	GATS1i	Geary autocorrelation of lag 1 weighted by ionization potential	2D autocorrelations	Geary autocorrelations
1077	GATS2i	Geary autocorrelation of lag 2 weighted by ionization potential	2D autocorrelations	Geary autocorrelations
1078	GATS3i	Geary autocorrelation of lag 3 weighted by ionization potential	2D autocorrelations	Geary autocorrelations
1079	GATS4i	Geary autocorrelation of lag 4 weighted by ionization potential	2D autocorrelations	Geary autocorrelations
1080	GATS5i	Geary autocorrelation of lag 5 weighted by ionization potential	2D autocorrelations	Geary autocorrelations
1081	GATS6i	Geary autocorrelation of lag 6 weighted by ionization potential	2D autocorrelations	Geary autocorrelations
1082	GATS7i	Geary autocorrelation of lag 7 weighted by ionization potential	2D autocorrelations	Geary autocorrelations

1083	GATS8i	Geary autocorrelation of lag 8 weighted by ionization potential	2D autocorrelations	Geary autocorrelations
1084	GATS1s	Geary autocorrelation of lag 1 weighted by I-state	2D autocorrelations	Geary autocorrelations
1085	GATS2s	Geary autocorrelation of lag 2 weighted by I-state	2D autocorrelations	Geary autocorrelations
1086	GATS3s	Geary autocorrelation of lag 3 weighted by I-state	2D autocorrelations	Geary autocorrelations
1087	GATS4s	Geary autocorrelation of lag 4 weighted by I-state	2D autocorrelations	Geary autocorrelations
1088	GATS5s	Geary autocorrelation of lag 5 weighted by I-state	2D autocorrelations	Geary autocorrelations
1089	GATS6s	Geary autocorrelation of lag 6 weighted by I-state	2D autocorrelations	Geary autocorrelations
1090	GATS7s	Geary autocorrelation of lag 7 weighted by I-state	2D autocorrelations	Geary autocorrelations
1091	GATS8s	Geary autocorrelation of lag 8 weighted by I-state	2D autocorrelations	Geary autocorrelations
1092	GGI1	topological charge index of order 1	2D autocorrelations	Topological charge autocorrelations
1093	GGI2	topological charge index of order 2	2D autocorrelations	Topological charge autocorrelations
1094	GGI3	topological charge index of order 3	2D autocorrelations	Topological charge autocorrelations
1095	GGI4	topological charge index of order 4	2D autocorrelations	Topological charge autocorrelations
1096	GGI5	topological charge index of order 5	2D autocorrelations	Topological charge autocorrelations
1097	GGI6	topological charge index of order 6	2D autocorrelations	Topological charge autocorrelations
1098	GGI7	topological charge index of order 7	2D autocorrelations	Topological charge autocorrelations
1099	GGI8	topological charge index of order 8	2D autocorrelations	Topological charge autocorrelations
1100	GGI9	topological charge index of order 9	2D autocorrelations	Topological charge autocorrelations
1101	GGI10	topological charge index of order 10	2D autocorrelations	Topological charge autocorrelations
1102	JGI1	mean topological charge index of order 1	2D autocorrelations	Topological charge autocorrelations

1103	JGI2	mean topological charge index of order 2	2D autocorrelations	Topological charge autocorrelations
1104	JGI3	mean topological charge index of order 3	2D autocorrelations	Topological charge autocorrelations
1105	JGI4	mean topological charge index of order 4	2D autocorrelations	Topological charge autocorrelations
1106	JGI5	mean topological charge index of order 5	2D autocorrelations	Topological charge autocorrelations
1107	JGI6	mean topological charge index of order 6	2D autocorrelations	Topological charge autocorrelations
1108	JGI7	mean topological charge index of order 7	2D autocorrelations	Topological charge autocorrelations
1109	JGI8	mean topological charge index of order 8	2D autocorrelations	Topological charge autocorrelations
1110	JGI9	mean topological charge index of order 9	2D autocorrelations	Topological charge autocorrelations
1111	JGI10	mean topological charge index of order 10	2D autocorrelations	Topological charge autocorrelations
1112	JGT	global topological charge index	2D autocorrelations	Topological charge autocorrelations
1113	SpMax1_Bh(m)	largest eigenvalue n. 1 of Burden matrix weighted by mass	Burden eigenvalues	Largest eigenvalues
1114	SpMax2_Bh(m)	largest eigenvalue n. 2 of Burden matrix weighted by mass	Burden eigenvalues	Largest eigenvalues
1115	SpMax3_Bh(m)	largest eigenvalue n. 3 of Burden matrix weighted by mass	Burden eigenvalues	Largest eigenvalues
1116	SpMax4_Bh(m)	largest eigenvalue n. 4 of Burden matrix weighted by mass	Burden eigenvalues	Largest eigenvalues
1117	SpMax5_Bh(m)	largest eigenvalue n. 5 of Burden matrix weighted by mass	Burden eigenvalues	Largest eigenvalues
1118	SpMax6_Bh(m)	largest eigenvalue n. 6 of Burden matrix weighted by mass	Burden eigenvalues	Largest eigenvalues
1119	SpMax7_Bh(m)	largest eigenvalue n. 7 of Burden matrix weighted by mass	Burden eigenvalues	Largest eigenvalues
1120	SpMax8_Bh(m)	largest eigenvalue n. 8 of Burden matrix weighted by mass	Burden eigenvalues	Largest eigenvalues
1121	SpMax1_Bh(v)	largest eigenvalue n. 1 of Burden matrix weighted by van der Waals volume	Burden eigenvalues	Largest eigenvalues
1122	SpMax2_Bh(v)	largest eigenvalue n. 2 of Burden matrix weighted by van der Waals volume	Burden eigenvalues	Largest eigenvalues

1123	SpMax3_Bh(v)	largest eigenvalue n. 3 of Burden matrix weighted by van der Waals volume	Burden eigenvalues	Largest eigenvalues
1124	SpMax4_Bh(v)	largest eigenvalue n. 4 of Burden matrix weighted by van der Waals volume	Burden eigenvalues	Largest eigenvalues
1125	SpMax5_Bh(v)	largest eigenvalue n. 5 of Burden matrix weighted by van der Waals volume	Burden eigenvalues	Largest eigenvalues
1126	SpMax6_Bh(v)	largest eigenvalue n. 6 of Burden matrix weighted by van der Waals volume	Burden eigenvalues	Largest eigenvalues
1127	SpMax7_Bh(v)	largest eigenvalue n. 7 of Burden matrix weighted by van der Waals volume	Burden eigenvalues	Largest eigenvalues
1128	SpMax8_Bh(v)	largest eigenvalue n. 8 of Burden matrix weighted by van der Waals volume	Burden eigenvalues	Largest eigenvalues
1129	SpMax1_Bh(e)	largest eigenvalue n. 1 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues	Largest eigenvalues
1130	SpMax2_Bh(e)	largest eigenvalue n. 2 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues	Largest eigenvalues
1131	SpMax3_Bh(e)	largest eigenvalue n. 3 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues	Largest eigenvalues
1132	SpMax4_Bh(e)	largest eigenvalue n. 4 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues	Largest eigenvalues
1133	SpMax5_Bh(e)	largest eigenvalue n. 5 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues	Largest eigenvalues
1134	SpMax6_Bh(e)	largest eigenvalue n. 6 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues	Largest eigenvalues
1135	SpMax7_Bh(e)	largest eigenvalue n. 7 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues	Largest eigenvalues
1136	SpMax8_Bh(e)	largest eigenvalue n. 8 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues	Largest eigenvalues
1137	SpMax1_Bh(p)	largest eigenvalue n. 1 of Burden matrix weighted by polarizability	Burden eigenvalues	Largest eigenvalues
1138	SpMax2_Bh(p)	largest eigenvalue n. 2 of Burden matrix weighted by polarizability	Burden eigenvalues	Largest eigenvalues
1139	SpMax3_Bh(p)	largest eigenvalue n. 3 of Burden matrix weighted by polarizability	Burden eigenvalues	Largest eigenvalues
1140	SpMax4_Bh(p)	largest eigenvalue n. 4 of Burden matrix weighted by polarizability	Burden eigenvalues	Largest eigenvalues
1141	SpMax5_Bh(p)	largest eigenvalue n. 5 of Burden matrix weighted by polarizability	Burden eigenvalues	Largest eigenvalues
1142	SpMax6_Bh(p)	largest eigenvalue n. 6 of Burden matrix weighted by polarizability	Burden eigenvalues	Largest eigenvalues

1143	SpMax7_Bh(p)	largest eigenvalue n. 7 of Burden matrix weighted by polarizability	Burden eigenvalues	Largest eigenvalues
1144	SpMax8_Bh(p)	largest eigenvalue n. 8 of Burden matrix weighted by polarizability	Burden eigenvalues	Largest eigenvalues
1145	SpMax1_Bh(i)	largest eigenvalue n. 1 of Burden matrix weighted by ionization potential	Burden eigenvalues	Largest eigenvalues
1146	SpMax2_Bh(i)	largest eigenvalue n. 2 of Burden matrix weighted by ionization potential	Burden eigenvalues	Largest eigenvalues
1147	SpMax3_Bh(i)	largest eigenvalue n. 3 of Burden matrix weighted by ionization potential	Burden eigenvalues	Largest eigenvalues
1148	SpMax4_Bh(i)	largest eigenvalue n. 4 of Burden matrix weighted by ionization potential	Burden eigenvalues	Largest eigenvalues
1149	SpMax5_Bh(i)	largest eigenvalue n. 5 of Burden matrix weighted by ionization potential	Burden eigenvalues	Largest eigenvalues
1150	SpMax6_Bh(i)	largest eigenvalue n. 6 of Burden matrix weighted by ionization potential	Burden eigenvalues	Largest eigenvalues
1151	SpMax7_Bh(i)	largest eigenvalue n. 7 of Burden matrix weighted by ionization potential	Burden eigenvalues	Largest eigenvalues
1152	SpMax8_Bh(i)	largest eigenvalue n. 8 of Burden matrix weighted by ionization potential	Burden eigenvalues	Largest eigenvalues
1153	SpMax1_Bh(s)	largest eigenvalue n. 1 of Burden matrix weighted by I-state	Burden eigenvalues	Largest eigenvalues
1154	SpMax2_Bh(s)	largest eigenvalue n. 2 of Burden matrix weighted by I-state	Burden eigenvalues	Largest eigenvalues
1155	SpMax3_Bh(s)	largest eigenvalue n. 3 of Burden matrix weighted by I-state	Burden eigenvalues	Largest eigenvalues
1156	SpMax4_Bh(s)	largest eigenvalue n. 4 of Burden matrix weighted by I-state	Burden eigenvalues	Largest eigenvalues
1157	SpMax5_Bh(s)	largest eigenvalue n. 5 of Burden matrix weighted by I-state	Burden eigenvalues	Largest eigenvalues
1158	SpMax6_Bh(s)	largest eigenvalue n. 6 of Burden matrix weighted by I-state	Burden eigenvalues	Largest eigenvalues
1159	SpMax7_Bh(s)	largest eigenvalue n. 7 of Burden matrix weighted by I-state	Burden eigenvalues	Largest eigenvalues
1160	SpMax8_Bh(s)	largest eigenvalue n. 8 of Burden matrix weighted by I-state	Burden eigenvalues	Largest eigenvalues
1161	SpMin1_Bh(m)	smallest eigenvalue n. 1 of Burden matrix weighted by mass	Burden eigenvalues	Smallest eigenvalues
1162	SpMin2_Bh(m)	smallest eigenvalue n. 2 of Burden matrix weighted by mass	Burden eigenvalues	Smallest eigenvalues

1163	SpMin3_Bh(m)	smallest eigenvalue n. 3 of Burden matrix weighted by mass	Burden eigenvalues	Smallest eigenvalues
1164	SpMin4_Bh(m)	smallest eigenvalue n. 4 of Burden matrix weighted by mass	Burden eigenvalues	Smallest eigenvalues
1165	SpMin5_Bh(m)	smallest eigenvalue n. 5 of Burden matrix weighted by mass	Burden eigenvalues	Smallest eigenvalues
1166	SpMin6_Bh(m)	smallest eigenvalue n. 6 of Burden matrix weighted by mass	Burden eigenvalues	Smallest eigenvalues
1167	SpMin7_Bh(m)	smallest eigenvalue n. 7 of Burden matrix weighted by mass	Burden eigenvalues	Smallest eigenvalues
1168	SpMin8_Bh(m)	smallest eigenvalue n. 8 of Burden matrix weighted by mass	Burden eigenvalues	Smallest eigenvalues
1169	SpMin1_Bh(v)	smallest eigenvalue n. 1 of Burden matrix weighted by van der Waals volume	Burden eigenvalues	Smallest eigenvalues
1170	SpMin2_Bh(v)	smallest eigenvalue n. 2 of Burden matrix weighted by van der Waals volume	Burden eigenvalues	Smallest eigenvalues
1171	SpMin3_Bh(v)	smallest eigenvalue n. 3 of Burden matrix weighted by van der Waals volume	Burden eigenvalues	Smallest eigenvalues
1172	SpMin4_Bh(v)	smallest eigenvalue n. 4 of Burden matrix weighted by van der Waals volume	Burden eigenvalues	Smallest eigenvalues
1173	SpMin5_Bh(v)	smallest eigenvalue n. 5 of Burden matrix weighted by van der Waals volume	Burden eigenvalues	Smallest eigenvalues
1174	SpMin6_Bh(v)	smallest eigenvalue n. 6 of Burden matrix weighted by van der Waals volume	Burden eigenvalues	Smallest eigenvalues
1175	SpMin7_Bh(v)	smallest eigenvalue n. 7 of Burden matrix weighted by van der Waals volume	Burden eigenvalues	Smallest eigenvalues
1176	SpMin8_Bh(v)	smallest eigenvalue n. 8 of Burden matrix weighted by van der Waals volume	Burden eigenvalues	Smallest eigenvalues
1177	SpMin1_Bh(e)	smallest eigenvalue n. 1 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues	Smallest eigenvalues
1178	SpMin2_Bh(e)	smallest eigenvalue n. 2 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues	Smallest eigenvalues
1179	SpMin3_Bh(e)	smallest eigenvalue n. 3 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues	Smallest eigenvalues
1180	SpMin4_Bh(e)	smallest eigenvalue n. 4 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues	Smallest eigenvalues
1181	SpMin5_Bh(e)	smallest eigenvalue n. 5 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues	Smallest eigenvalues
1182	SpMin6_Bh(e)	smallest eigenvalue n. 6 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues	Smallest eigenvalues

1183	SpMin7_Bh(e)	smallest eigenvalue n. 7 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues	Smallest eigenvalues
1184	SpMin8_Bh(e)	smallest eigenvalue n. 8 of Burden matrix weighted by Sanderson electronegativity	Burden eigenvalues	Smallest eigenvalues
1185	SpMin1_Bh(p)	smallest eigenvalue n. 1 of Burden matrix weighted by polarizability	Burden eigenvalues	Smallest eigenvalues
1186	SpMin2_Bh(p)	smallest eigenvalue n. 2 of Burden matrix weighted by polarizability	Burden eigenvalues	Smallest eigenvalues
1187	SpMin3_Bh(p)	smallest eigenvalue n. 3 of Burden matrix weighted by polarizability	Burden eigenvalues	Smallest eigenvalues
1188	SpMin4_Bh(p)	smallest eigenvalue n. 4 of Burden matrix weighted by polarizability	Burden eigenvalues	Smallest eigenvalues
1189	SpMin5_Bh(p)	smallest eigenvalue n. 5 of Burden matrix weighted by polarizability	Burden eigenvalues	Smallest eigenvalues
1190	SpMin6_Bh(p)	smallest eigenvalue n. 6 of Burden matrix weighted by polarizability	Burden eigenvalues	Smallest eigenvalues
1191	SpMin7_Bh(p)	smallest eigenvalue n. 7 of Burden matrix weighted by polarizability	Burden eigenvalues	Smallest eigenvalues
1192	SpMin8_Bh(p)	smallest eigenvalue n. 8 of Burden matrix weighted by polarizability	Burden eigenvalues	Smallest eigenvalues
1193	SpMin1_Bh(i)	smallest eigenvalue n. 1 of Burden matrix weighted by ionization potential	Burden eigenvalues	Smallest eigenvalues
1194	SpMin2_Bh(i)	smallest eigenvalue n. 2 of Burden matrix weighted by ionization potential	Burden eigenvalues	Smallest eigenvalues
1195	SpMin3_Bh(i)	smallest eigenvalue n. 3 of Burden matrix weighted by ionization potential	Burden eigenvalues	Smallest eigenvalues
1196	SpMin4_Bh(i)	smallest eigenvalue n. 4 of Burden matrix weighted by ionization potential	Burden eigenvalues	Smallest eigenvalues
1197	SpMin5_Bh(i)	smallest eigenvalue n. 5 of Burden matrix weighted by ionization potential	Burden eigenvalues	Smallest eigenvalues
1198	SpMin6_Bh(i)	smallest eigenvalue n. 6 of Burden matrix weighted by ionization potential	Burden eigenvalues	Smallest eigenvalues
1199	SpMin7_Bh(i)	smallest eigenvalue n. 7 of Burden matrix weighted by ionization potential	Burden eigenvalues	Smallest eigenvalues
1200	SpMin8_Bh(i)	smallest eigenvalue n. 8 of Burden matrix weighted by ionization potential	Burden eigenvalues	Smallest eigenvalues
1201	SpMin1_Bh(s)	smallest eigenvalue n. 1 of Burden matrix weighted by I-state	Burden eigenvalues	Smallest eigenvalues
1202	SpMin2_Bh(s)	smallest eigenvalue n. 2 of Burden matrix weighted by I-state	Burden eigenvalues	Smallest eigenvalues

1203	SpMin3_Bh(s)	smallest eigenvalue n. 3 of Burden matrix weighted by I-state	Burden eigenvalues	Smallest eigenvalues
1204	SpMin4_Bh(s)	smallest eigenvalue n. 4 of Burden matrix weighted by I-state	Burden eigenvalues	Smallest eigenvalues
1205	SpMin5_Bh(s)	smallest eigenvalue n. 5 of Burden matrix weighted by I-state	Burden eigenvalues	Smallest eigenvalues
1206	SpMin6_Bh(s)	smallest eigenvalue n. 6 of Burden matrix weighted by I-state	Burden eigenvalues	Smallest eigenvalues
1207	SpMin7_Bh(s)	smallest eigenvalue n. 7 of Burden matrix weighted by I-state	Burden eigenvalues	Smallest eigenvalues
1208	SpMin8_Bh(s)	smallest eigenvalue n. 8 of Burden matrix weighted by I-state	Burden eigenvalues	Smallest eigenvalues
1209	P_VSA_LogP_1	P_VSA-like on LogP, bin 1	P_VSA-like descriptors	LogP
1210	P_VSA_LogP_2	P_VSA-like on LogP, bin 2	P_VSA-like descriptors	LogP
1211	P_VSA_LogP_3	P_VSA-like on LogP, bin 3	P_VSA-like descriptors	LogP
1212	P_VSA_LogP_4	P_VSA-like on LogP, bin 4	P_VSA-like descriptors	LogP
1213	P_VSA_LogP_5	P_VSA-like on LogP, bin 5	P_VSA-like descriptors	LogP
1214	P_VSA_LogP_6	P_VSA-like on LogP, bin 6	P_VSA-like descriptors	LogP
1215	P_VSA_LogP_7	P_VSA-like on LogP, bin 7	P_VSA-like descriptors	LogP
1216	P_VSA_LogP_8	P_VSA-like on LogP, bin 8	P_VSA-like descriptors	LogP
1217	P_VSA_MR_1	P_VSA-like on Molar Refractivity, bin 1	P_VSA-like descriptors	Molar Refractivity
1218	P_VSA_MR_2	P_VSA-like on Molar Refractivity, bin 2	P_VSA-like descriptors	Molar Refractivity
1219	P_VSA_MR_3	P_VSA-like on Molar Refractivity, bin 3	P_VSA-like descriptors	Molar Refractivity
1220	P_VSA_MR_4	P_VSA-like on Molar Refractivity, bin 4	P_VSA-like descriptors	Molar Refractivity
1221	P_VSA_MR_5	P_VSA-like on Molar Refractivity, bin 5	P_VSA-like descriptors	Molar Refractivity
1222	P_VSA_MR_6	P_VSA-like on Molar Refractivity, bin 6	P_VSA-like descriptors	Molar Refractivity

1223	P_VSA_MR_7	P_VSA-like on Molar Refractivity, bin 7	P_VSA-like descriptors	Molar Refractivity
1224	P_VSA_MR_8	P_VSA-like on Molar Refractivity, bin 8	P_VSA-like descriptors	Molar Refractivity
1225	P_VSA_m_1	P_VSA-like on mass, bin 1	P_VSA-like descriptors	Mass
1226	P_VSA_m_2	P_VSA-like on mass, bin 2	P_VSA-like descriptors	Mass
1227	P_VSA_m_3	P_VSA-like on mass, bin 3	P_VSA-like descriptors	Mass
1228	P_VSA_m_4	P_VSA-like on mass, bin 4	P_VSA-like descriptors	Mass
1229	P_VSA_m_5	P_VSA-like on mass, bin 5	P_VSA-like descriptors	Mass
1230	P_VSA_v_1	P_VSA-like on van der Waals volume, bin 1	P_VSA-like descriptors	Van der Waals volume
1231	P_VSA_v_2	P_VSA-like on van der Waals volume, bin 2	P_VSA-like descriptors	Van der Waals volume
1232	P_VSA_v_3	P_VSA-like on van der Waals volume, bin 3	P_VSA-like descriptors	Van der Waals volume
1233	P_VSA_v_4	P_VSA-like on van der Waals volume, bin 4	P_VSA-like descriptors	Van der Waals volume
1234	P_VSA_e_1	P_VSA-like on Sanderson electronegativity, bin 1	P_VSA-like descriptors	Sanderson electronegativity
1235	P_VSA_e_2	P_VSA-like on Sanderson electronegativity, bin 2	P_VSA-like descriptors	Sanderson electronegativity
1236	P_VSA_e_3	P_VSA-like on Sanderson electronegativity, bin 3	P_VSA-like descriptors	Sanderson electronegativity
1237	P_VSA_e_4	P_VSA-like on Sanderson electronegativity, bin 4	P_VSA-like descriptors	Sanderson electronegativity
1238	P_VSA_e_5	P_VSA-like on Sanderson electronegativity, bin 5	P_VSA-like descriptors	Sanderson electronegativity
1239	P_VSA_e_6	P_VSA-like on Sanderson electronegativity, bin 6	P_VSA-like descriptors	Sanderson electronegativity
1240	P_VSA_p_1	P_VSA-like on polarizability, bin 1	P_VSA-like descriptors	Polarizability
1241	P_VSA_p_2	P_VSA-like on polarizability, bin 2	P_VSA-like descriptors	Polarizability
1242	P_VSA_p_3	P_VSA-like on polarizability, bin 3	P_VSA-like descriptors	Polarizability

1243	P_VSA_p_4	P_VSA-like on polarizability, bin 4	P_VSA-like descriptors	Polarizability
1244	P_VSA_i_1	P_VSA-like on ionization potential, bin 1	P_VSA-like descriptors	Ionization Potential
1245	P_VSA_i_2	P_VSA-like on ionization potential, bin 2	P_VSA-like descriptors	Ionization Potential
1246	P_VSA_i_3	P_VSA-like on ionization potential, bin 3	P_VSA-like descriptors	Ionization Potential
1247	P_VSA_i_4	P_VSA-like on ionization potential, bin 4	P_VSA-like descriptors	Ionization Potential
1248	P_VSA_s_1	P_VSA-like on I-state, bin 1	P_VSA-like descriptors	Intrinsic State
1249	P_VSA_s_2	P_VSA-like on I-state, bin 2	P_VSA-like descriptors	Intrinsic State
1250	P_VSA_s_3	P_VSA-like on I-state, bin 3	P_VSA-like descriptors	Intrinsic State
1251	P_VSA_s_4	P_VSA-like on I-state, bin 4	P_VSA-like descriptors	Intrinsic State
1252	P_VSA_s_5	P_VSA-like on I-state, bin 5	P_VSA-like descriptors	Intrinsic State
1253	P_VSA_s_6	P_VSA-like on I-state, bin 6	P_VSA-like descriptors	Intrinsic State
1254	P_VSA_ppp_L	P_VSA-like on potential pharmacophore points, L - lipophilic	P_VSA-like descriptors	Potential Pharmacophore Points
1255	P_VSA_ppp_P	P_VSA-like on potential pharmacophore points, P - positive	P_VSA-like descriptors	Potential Pharmacophore Points
1256	P_VSA_ppp_N	P_VSA-like on potential pharmacophore points, N - negative	P_VSA-like descriptors	Potential Pharmacophore Points
1257	P_VSA_ppp_D	P_VSA-like on potential pharmacophore points, D - hydrogen-bond donor	P_VSA-like descriptors	Potential Pharmacophore Points
1258	P_VSA_ppp_A	P_VSA-like on potential pharmacophore points, A - hydrogen-bond acceptor	P_VSA-like descriptors	Potential Pharmacophore Points
1259	P_VSA_ppp_ar	P_VSA-like on potential pharmacophore points, ar - aromatic atoms	P_VSA-like descriptors	Potential Pharmacophore Points
1260	P_VSA_ppp_con	P_VSA-like on potential pharmacophore points, con - conjugated atoms	P_VSA-like descriptors	Potential Pharmacophore Points

1261	P_VSA_ppp_hal	P_VSA-like on potential pharmacophore points, hal - halogen atoms	P_VSA-like descriptors	Potential Pharmacophore Points
1262	P_VSA_ppp_cyc	P_VSA-like on potential pharmacophore points, cyc - atoms belonging to cycles	P_VSA-like descriptors	Potential Pharmacophore Points
1263	P_VSA_ppp_ter	P_VSA-like on potential pharmacophore points, ter - terminal atoms	P_VSA-like descriptors	Potential Pharmacophore Points
1264	Eta_alpha	eta core count	ETA indices	Basic descriptors
1265	Eta_alpha_A	eta average core count	ETA indices	Basic descriptors
1266	Eta_epsi	eta electronegativity measure	ETA indices	Basic descriptors
1267	Eta_epsi_A	eta average electronegativity measure	ETA indices	Basic descriptors
1268	Eta_betaS	eta sigma VEM count	ETA indices	Basic descriptors
1269	Eta_betaS_A	eta sigma average VEM coun	ETA indices	Basic descriptors
1270	Eta_betaP	eta pi and lone pair VEM count	ETA indices	Basic descriptors
1271	Eta_betaP_A	eta pi and lone pair average VEM count	ETA indices	Basic descriptors
1272	Eta_beta	eta VEM count	ETA indices	Basic descriptors
1273	Eta_beta_A	eta average VEM count	ETA indices	Basic descriptors
1274	Eta_C	eta composite index	ETA indices	Basic descriptors
1275	Eta_C_A	eta average composite index	ETA indices	Basic descriptors
1276	Eta_L	eta local composite index	ETA indices	Basic descriptors
1277	Eta_L_A	eta average local composite index	ETA indices	Basic descriptors
1278	Eta_F	eta functionality index	ETA indices	Basic descriptors
1279	Eta_F_A	eta average functionality index	ETA indices	Basic descriptors
1280	Eta_FL	eta local functionality index	ETA indices	Basic descriptors
1281	Eta_FL_A	eta average local functionality index	ETA indices	Basic descriptors
1282	Eta_B	eta branching index	ETA indices	Basic descriptors
1283	Eta_B_A	eta average branching index	ETA indices	Basic descriptors
1284	Eta_sh_p	eta p shape index	ETA indices	Basic descriptors
1285	Eta_sh_y	eta y shape index	ETA indices	Basic descriptors
1286	Eta_sh_x	eta x shape index	ETA indices	Basic descriptors
1287	Eta_D_AlphaA	eta delta alpha a index	ETA indices	Basic descriptors
1288	Eta_D_AlphaB	eta delta alpha b index	ETA indices	Basic descriptors

1289	Eta_epsi_2	eta electronegativity measure 2	ETA indices	Basic descriptors
1290	Eta_epsi_3	eta electronegativity measure 3	ETA indices	Basic descriptors
1291	Eta_epsi_4	eta electronegativity measure 4	ETA indices	Basic descriptors
1292	Eta_epsi_5	eta electronegativity measure 5	ETA indices	Basic descriptors
1293	Eta_D_epsiA	eta measure of unsaturation and electronegative atom count	ETA indices	Basic descriptors
1294	Eta_D_epsiB	eta measure of unsaturation	ETA indices	Basic descriptors
1295	Eta_D_epsiC	eta measure of electronegativity	ETA indices	Basic descriptors
1296	Eta_D_epsiD	eta measure of hydrogen bond donor atoms	ETA indices	Basic descriptors
1297	Eta_psi1	eta measure of hydrogen bonding propensity and/or polar surface area	ETA indices	Basic descriptors
1298	Eta_D_psiA	eta measure of hydrogen bonding propensity	ETA indices	Basic descriptors
1299	Eta_D_psiB	eta measure of hydrogen bonding propensity	ETA indices	Basic descriptors
1300	Eta_D_beta	eta measure of electronic features	ETA indices	Basic descriptors
1301	Eta_D_beta_A	eta average measure of electronic features	ETA indices	Basic descriptors
1302	SpMax_EA	leading eigenvalue from edge adjacency mat.	Edge adjacency indices	Spectral indices
1303	SpMaxA_EA	normalized leading eigenvalue from edge adjacency mat.	Edge adjacency indices	Spectral indices
1304	SpDiam_EA	spectral diameter from edge adjacency mat.	Edge adjacency indices	Spectral indices
1305	SpAD_EA	spectral absolute deviation from edge adjacency mat.	Edge adjacency indices	Spectral indices
1306	SpMAD_EA	spectral mean absolute deviation from edge adjacency mat.	Edge adjacency indices	Spectral indices
1307	SpMax_EA(ed)	leading eigenvalue from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral indices
1308	SpMaxA_EA(ed)	normalized leading eigenvalue from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral indices

1309	SpDiam_EA(ed)	spectral diameter from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral indices
1310	SpAD_EA(ed)	spectral absolute deviation from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral indices
1311	SpMAD_EA(ed)	spectral mean absolute deviation from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral indices
1312	SpMax_EA(bo)	leading eigenvalue from edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral indices
1313	SpMaxA_EA(bo)	normalized leading eigenvalue from edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral indices
1314	SpDiam_EA(bo)	spectral diameter from edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral indices
1315	SpAD_EA(bo)	spectral absolute deviation from edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral indices
1316	SpMAD_EA(bo)	spectral mean absolute deviation from edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral indices
1317	SpMax_EA(dm)	leading eigenvalue from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral indices
1318	SpMaxA_EA(dm)	normalized leading eigenvalue from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral indices
1319	SpDiam_EA(dm)	spectral diameter from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral indices
1320	SpAD_EA(dm)	spectral absolute deviation from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral indices
1321	SpMAD_EA(dm)	spectral mean absolute deviation from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral indices
1322	SpMax_EA(ri)	leading eigenvalue from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral indices
1323	SpMaxA_EA(ri)	normalized leading eigenvalue from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral indices

1324	SpDiam_EA(ri)	spectral diameter from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral indices
1325	SpAD_EA(ri)	spectral absolute deviation from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral indices
1326	SpMAD_EA(ri)	spectral mean absolute deviation from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral indices
1327	SpMax_AEA(ed)	leading eigenvalue from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral indices
1328	SpMaxA_AEA(ed)	normalized leading eigenvalue from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral indices
1329	SpDiam_AEA(ed)	spectral diameter from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral indices
1330	SpAD_AEA(ed)	spectral absolute deviation from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral indices
1331	SpMAD_AEA(ed)	spectral mean absolute deviation from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral indices
1332	SpMax_AEA(bo)	leading eigenvalue from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral indices
1333	SpMaxA_AEA(bo)	normalized leading eigenvalue from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral indices
1334	SpDiam_AEA(bo)	spectral diameter from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral indices
1335	SpAD_AEA(bo)	spectral absolute deviation from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral indices
1336	SpMAD_AEA(bo)	spectral mean absolute deviation from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral indices
1337	SpMax_AEA(dm)	leading eigenvalue from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral indices
1338	SpMaxA_AEA(dm)	normalized leading eigenvalue from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral indices

1339	SpDiam_AEA(dm)	spectral diameter from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral indices
1340	SpAD_AEA(dm)	spectral absolute deviation from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral indices
1341	SpMAD_AEA(dm)	spectral mean absolute deviation from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral indices
1342	SpMax_AEA(ri)	leading eigenvalue from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral indices
1343	SpMaxA_AEA(ri)	normalized leading eigenvalue from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral indices
1344	SpDiam_AEA(ri)	spectral diameter from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral indices
1345	SpAD_AEA(ri)	spectral absolute deviation from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral indices
1346	SpMAD_AEA(ri)	spectral mean absolute deviation from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral indices
1347	Chi0_EA	connectivity-like index of order 0 from edge adjacency mat.	Edge adjacency indices	Connectivity-like indices
1348	Chi1_EA	connectivity-like index of order 1 from edge adjacency mat.	Edge adjacency indices	Connectivity-like indices
1349	Chi0_EA(ed)	connectivity-like index of order 0 from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Connectivity-like indices
1350	Chi1_EA(ed)	connectivity-like index of order 1 from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Connectivity-like indices
1351	Chi0_EA(bo)	connectivity-like index of order 0 from edge adjacency mat. weighted by bond order	Edge adjacency indices	Connectivity-like indices
1352	Chi1_EA(bo)	connectivity-like index of order 1 from edge adjacency mat. weighted by bond order	Edge adjacency indices	Connectivity-like indices
1353	Chi0_EA(dm)	connectivity-like index of order 0 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Connectivity-like indices

1354	Chi1_EA(dm)	connectivity-like index of order 1 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Connectivity-like indices
1355	Chi0_EA(ri)	connectivity-like index of order 0 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Connectivity-like indices
1356	Chi1_EA(ri)	connectivity-like index of order 1 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Connectivity-like indices
1357	Chi0_AEA(ed)	connectivity-like index of order 0 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Connectivity-like indices
1358	Chi1_AEA(ed)	connectivity-like index of order 1 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Connectivity-like indices
1359	Chi0_AEA(bo)	connectivity-like index of order 0 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Connectivity-like indices
1360	Chi1_AEA(bo)	connectivity-like index of order 1 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Connectivity-like indices
1361	Chi0_AEA(dm)	connectivity-like index of order 0 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Connectivity-like indices
1362	Chi1_AEA(dm)	connectivity-like index of order 1 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Connectivity-like indices
1363	Chi0_AEA(ri)	connectivity-like index of order 0 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Connectivity-like indices
1364	Chi1_AEA(ri)	connectivity-like index of order 1 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Connectivity-like indices
1365	SM02_EA	spectral moment of order 2 from edge adjacency mat.	Edge adjacency indices	Spectral moments
1366	SM03_EA	spectral moment of order 3 from edge adjacency mat.	Edge adjacency indices	Spectral moments
1367	SM04_EA	spectral moment of order 4 from edge adjacency mat.	Edge adjacency indices	Spectral moments
1368	SM05_EA	spectral moment of order 5 from edge adjacency mat.	Edge adjacency indices	Spectral moments

1369	SM06_EA	spectral moment of order 6 from edge adjacency mat.	Edge adjacency indices	Spectral moments
1370	SM07_EA	spectral moment of order 7 from edge adjacency mat.	Edge adjacency indices	Spectral moments
1371	SM08_EA	spectral moment of order 8 from edge adjacency mat.	Edge adjacency indices	Spectral moments
1372	SM09_EA	spectral moment of order 9 from edge adjacency mat.	Edge adjacency indices	Spectral moments
1373	SM10_EA	spectral moment of order 10 from edge adjacency mat.	Edge adjacency indices	Spectral moments
1374	SM11_EA	spectral moment of order 11 from edge adjacency mat.	Edge adjacency indices	Spectral moments
1375	SM12_EA	spectral moment of order 12 from edge adjacency mat.	Edge adjacency indices	Spectral moments
1376	SM13_EA	spectral moment of order 13 from edge adjacency mat.	Edge adjacency indices	Spectral moments
1377	SM14_EA	spectral moment of order 14 from edge adjacency mat.	Edge adjacency indices	Spectral moments
1378	SM15_EA	spectral moment of order 15 from edge adjacency mat.	Edge adjacency indices	Spectral moments
1379	SM02_EA(ed)	spectral moment of order 2 from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral moments
1380	SM03_EA(ed)	spectral moment of order 3 from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral moments
1381	SM04_EA(ed)	spectral moment of order 4 from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral moments
1382	SM05_EA(ed)	spectral moment of order 5 from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral moments
1383	SM06_EA(ed)	spectral moment of order 6 from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral moments

1384	SM07_EA(ed)	spectral moment of order 7 from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral moments
1385	SM08_EA(ed)	spectral moment of order 8 from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral moments
1386	SM09_EA(ed)	spectral moment of order 9 from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral moments
1387	SM10_EA(ed)	spectral moment of order 10 from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral moments
1388	SM11_EA(ed)	spectral moment of order 11 from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral moments
1389	SM12_EA(ed)	spectral moment of order 12 from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral moments
1390	SM13_EA(ed)	spectral moment of order 13 from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral moments
1391	SM14_EA(ed)	spectral moment of order 14 from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral moments
1392	SM15_EA(ed)	spectral moment of order 15 from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral moments
1393	SM02_EA(bo)	spectral moment of order 2 from edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral moments
1394	SM03_EA(bo)	spectral moment of order 3 from edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral moments
1395	SM04_EA(bo)	spectral moment of order 4 from edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral moments
1396	SM05_EA(bo)	spectral moment of order 5 from edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral moments
1397	SM06_EA(bo)	spectral moment of order 6 from edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral moments
1398	SM07_EA(bo)	spectral moment of order 7 from edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral moments

1399	SM08_EA(bo)	spectral moment of order 8 from edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral moments
1400	SM09_EA(bo)	spectral moment of order 9 from edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral moments
1401	SM10_EA(bo)	spectral moment of order 10 from edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral moments
1402	SM11_EA(bo)	spectral moment of order 11 from edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral moments
1403	SM12_EA(bo)	spectral moment of order 12 from edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral moments
1404	SM13_EA(bo)	spectral moment of order 13 from edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral moments
1405	SM14_EA(bo)	spectral moment of order 14 from edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral moments
1406	SM15_EA(bo)	spectral moment of order 15 from edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral moments
1407	SM02_EA(dm)	spectral moment of order 2 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral moments
1408	SM03_EA(dm)	spectral moment of order 3 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral moments
1409	SM04_EA(dm)	spectral moment of order 4 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral moments
1410	SM05_EA(dm)	spectral moment of order 5 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral moments
1411	SM06_EA(dm)	spectral moment of order 6 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral moments
1412	SM07_EA(dm)	spectral moment of order 7 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral moments
1413	SM08_EA(dm)	spectral moment of order 8 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral moments

1414	SM09_EA(dm)	spectral moment of order 9 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral moments
1415	SM10_EA(dm)	spectral moment of order 10 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral moments
1416	SM11_EA(dm)	spectral moment of order 11 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral moments
1417	SM12_EA(dm)	spectral moment of order 12 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral moments
1418	SM13_EA(dm)	spectral moment of order 13 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral moments
1419	SM14_EA(dm)	spectral moment of order 14 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral moments
1420	SM15_EA(dm)	spectral moment of order 15 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral moments
1421	SM02_EA(ri)	spectral moment of order 2 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral moments
1422	SM03_EA(ri)	spectral moment of order 3 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral moments
1423	SM04_EA(ri)	spectral moment of order 4 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral moments
1424	SM05_EA(ri)	spectral moment of order 5 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral moments
1425	SM06_EA(ri)	spectral moment of order 6 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral moments
1426	SM07_EA(ri)	spectral moment of order 7 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral moments
1427	SM08_EA(ri)	spectral moment of order 8 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral moments
1428	SM09_EA(ri)	spectral moment of order 9 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral moments

1429	SM10_EA(ri)	spectral moment of order 10 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral moments
1430	SM11_EA(ri)	spectral moment of order 11 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral moments
1431	SM12_EA(ri)	spectral moment of order 12 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral moments
1432	SM13_EA(ri)	spectral moment of order 13 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral moments
1433	SM14_EA(ri)	spectral moment of order 14 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral moments
1434	SM15_EA(ri)	spectral moment of order 15 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral moments
1435	SM02_AEA(ed)	spectral moment of order 2 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral moments
1436	SM03_AEA(ed)	spectral moment of order 3 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral moments
1437	SM04_AEA(ed)	spectral moment of order 4 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral moments
1438	SM05_AEA(ed)	spectral moment of order 5 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral moments
1439	SM06_AEA(ed)	spectral moment of order 6 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral moments
1440	SM07_AEA(ed)	spectral moment of order 7 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral moments
1441	SM08_AEA(ed)	spectral moment of order 8 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral moments
1442	SM09_AEA(ed)	spectral moment of order 9 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral moments
1443	SM10_AEA(ed)	spectral moment of order 10 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral moments

1444	SM11_AEA(ed)	spectral moment of order 11 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral moments
1445	SM12_AEA(ed)	spectral moment of order 12 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral moments
1446	SM13_AEA(ed)	spectral moment of order 13 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral moments
1447	SM14_AEA(ed)	spectral moment of order 14 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral moments
1448	SM15_AEA(ed)	spectral moment of order 15 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Spectral moments
1449	SM02_AEA(bo)	spectral moment of order 2 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral moments
1450	SM03_AEA(bo)	spectral moment of order 3 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral moments
1451	SM04_AEA(bo)	spectral moment of order 4 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral moments
1452	SM05_AEA(bo)	spectral moment of order 5 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral moments
1453	SM06_AEA(bo)	spectral moment of order 6 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral moments
1454	SM07_AEA(bo)	spectral moment of order 7 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral moments
1455	SM08_AEA(bo)	spectral moment of order 8 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral moments
1456	SM09_AEA(bo)	spectral moment of order 9 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral moments
1457	SM10_AEA(bo)	spectral moment of order 10 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral moments
1458	SM11_AEA(bo)	spectral moment of order 11 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral moments

1459	SM12_AEA(bo)	spectral moment of order 12 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral moments
1460	SM13_AEA(bo)	spectral moment of order 13 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral moments
1461	SM14_AEA(bo)	spectral moment of order 14 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral moments
1462	SM15_AEA(bo)	spectral moment of order 15 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Spectral moments
1463	SM02_AEA(dm)	spectral moment of order 2 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral moments
1464	SM03_AEA(dm)	spectral moment of order 3 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral moments
1465	SM04_AEA(dm)	spectral moment of order 4 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral moments
1466	SM05_AEA(dm)	spectral moment of order 5 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral moments
1467	SM06_AEA(dm)	spectral moment of order 6 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral moments
1468	SM07_AEA(dm)	spectral moment of order 7 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral moments
1469	SM08_AEA(dm)	spectral moment of order 8 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral moments
1470	SM09_AEA(dm)	spectral moment of order 9 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral moments
1471	SM10_AEA(dm)	spectral moment of order 10 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral moments
1472	SM11_AEA(dm)	spectral moment of order 11 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral moments
1473	SM12_AEA(dm)	spectral moment of order 12 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral moments

1474	SM13_AEA(dm)	spectral moment of order 13 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral moments
1475	SM14_AEA(dm)	spectral moment of order 14 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral moments
1476	SM15_AEA(dm)	spectral moment of order 15 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Spectral moments
1477	SM02_AEA(ri)	spectral moment of order 2 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral moments
1478	SM03_AEA(ri)	spectral moment of order 3 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral moments
1479	SM04_AEA(ri)	spectral moment of order 4 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral moments
1480	SM05_AEA(ri)	spectral moment of order 5 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral moments
1481	SM06_AEA(ri)	spectral moment of order 6 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral moments
1482	SM07_AEA(ri)	spectral moment of order 7 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral moments
1483	SM08_AEA(ri)	spectral moment of order 8 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral moments
1484	SM09_AEA(ri)	spectral moment of order 9 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral moments
1485	SM10_AEA(ri)	spectral moment of order 10 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral moments
1486	SM11_AEA(ri)	spectral moment of order 11 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral moments
1487	SM12_AEA(ri)	spectral moment of order 12 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral moments
1488	SM13_AEA(ri)	spectral moment of order 13 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral moments

1489	SM14_AEA(ri)	spectral moment of order 14 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral moments
1490	SM15_AEA(ri)	spectral moment of order 15 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Spectral moments
1491	Eig01_EA	eigenvalue n. 1 from edge adjacency mat.	Edge adjacency indices	Eigenvalues
1492	Eig02_EA	eigenvalue n. 2 from edge adjacency mat.	Edge adjacency indices	Eigenvalues
1493	Eig03_EA	eigenvalue n. 3 from edge adjacency mat.	Edge adjacency indices	Eigenvalues
1494	Eig04_EA	eigenvalue n. 4 from edge adjacency mat.	Edge adjacency indices	Eigenvalues
1495	Eig05_EA	eigenvalue n. 5 from edge adjacency mat.	Edge adjacency indices	Eigenvalues
1496	Eig06_EA	eigenvalue n. 6 from edge adjacency mat.	Edge adjacency indices	Eigenvalues
1497	Eig07_EA	eigenvalue n. 7 from edge adjacency mat.	Edge adjacency indices	Eigenvalues
1498	Eig08_EA	eigenvalue n. 8 from edge adjacency mat.	Edge adjacency indices	Eigenvalues
1499	Eig09_EA	eigenvalue n. 9 from edge adjacency mat.	Edge adjacency indices	Eigenvalues
1500	Eig10_EA	eigenvalue n. 10 from edge adjacency mat.	Edge adjacency indices	Eigenvalues
1501	Eig11_EA	eigenvalue n. 11 from edge adjacency mat.	Edge adjacency indices	Eigenvalues
1502	Eig12_EA	eigenvalue n. 12 from edge adjacency mat.	Edge adjacency indices	Eigenvalues
1503	Eig13_EA	eigenvalue n. 13 from edge adjacency mat.	Edge adjacency indices	Eigenvalues

1504	Eig14_EA	eigenvalue n. 14 from edge adjacency mat.	Edge adjacency indices	Eigenvalues
1505	Eig15_EA	eigenvalue n. 15 from edge adjacency mat.	Edge adjacency indices	Eigenvalues
1506	Eig01_EA(ed)	eigenvalue n. 1 from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Eigenvalues
1507	Eig02_EA(ed)	eigenvalue n. 2 from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Eigenvalues
1508	Eig03_EA(ed)	eigenvalue n. 3 from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Eigenvalues
1509	Eig04_EA(ed)	eigenvalue n. 4 from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Eigenvalues
1510	Eig05_EA(ed)	eigenvalue n. 5 from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Eigenvalues
1511	Eig06_EA(ed)	eigenvalue n. 6 from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Eigenvalues
1512	Eig07_EA(ed)	eigenvalue n. 7 from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Eigenvalues
1513	Eig08_EA(ed)	eigenvalue n. 8 from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Eigenvalues
1514	Eig09_EA(ed)	eigenvalue n. 9 from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Eigenvalues
1515	Eig10_EA(ed)	eigenvalue n. 10 from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Eigenvalues
1516	Eig11_EA(ed)	eigenvalue n. 11 from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Eigenvalues
1517	Eig12_EA(ed)	eigenvalue n. 12 from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Eigenvalues
1518	Eig13_EA(ed)	eigenvalue n. 13 from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Eigenvalues

1519	Eig14_EA(ed)	eigenvalue n. 14 from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Eigenvalues
1520	Eig15_EA(ed)	eigenvalue n. 15 from edge adjacency mat. weighted by edge degree	Edge adjacency indices	Eigenvalues
1521	Eig01_EA(bo)	eigenvalue n. 1 from edge adjacency mat. weighted by bond order	Edge adjacency indices	Eigenvalues
1522	Eig02_EA(bo)	eigenvalue n. 2 from edge adjacency mat. weighted by bond order	Edge adjacency indices	Eigenvalues
1523	Eig03_EA(bo)	eigenvalue n. 3 from edge adjacency mat. weighted by bond order	Edge adjacency indices	Eigenvalues
1524	Eig04_EA(bo)	eigenvalue n. 4 from edge adjacency mat. weighted by bond order	Edge adjacency indices	Eigenvalues
1525	Eig05_EA(bo)	eigenvalue n. 5 from edge adjacency mat. weighted by bond order	Edge adjacency indices	Eigenvalues
1526	Eig06_EA(bo)	eigenvalue n. 6 from edge adjacency mat. weighted by bond order	Edge adjacency indices	Eigenvalues
1527	Eig07_EA(bo)	eigenvalue n. 7 from edge adjacency mat. weighted by bond order	Edge adjacency indices	Eigenvalues
1528	Eig08_EA(bo)	eigenvalue n. 8 from edge adjacency mat. weighted by bond order	Edge adjacency indices	Eigenvalues
1529	Eig09_EA(bo)	eigenvalue n. 9 from edge adjacency mat. weighted by bond order	Edge adjacency indices	Eigenvalues
1530	Eig10_EA(bo)	eigenvalue n. 10 from edge adjacency mat. weighted by bond order	Edge adjacency indices	Eigenvalues
1531	Eig11_EA(bo)	eigenvalue n. 11 from edge adjacency mat. weighted by bond order	Edge adjacency indices	Eigenvalues
1532	Eig12_EA(bo)	eigenvalue n. 12 from edge adjacency mat. weighted by bond order	Edge adjacency indices	Eigenvalues
1533	Eig13_EA(bo)	eigenvalue n. 13 from edge adjacency mat. weighted by bond order	Edge adjacency indices	Eigenvalues

1534	Eig14_EA(bo)	eigenvalue n. 14 from edge adjacency mat. weighted by bond order	Edge adjacency indices	Eigenvalues
1535	Eig15_EA(bo)	eigenvalue n. 15 from edge adjacency mat. weighted by bond order	Edge adjacency indices	Eigenvalues
1536	Eig01_EA(dm)	eigenvalue n. 1 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Eigenvalues
1537	Eig02_EA(dm)	eigenvalue n. 2 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Eigenvalues
1538	Eig03_EA(dm)	eigenvalue n. 3 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Eigenvalues
1539	Eig04_EA(dm)	eigenvalue n. 4 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Eigenvalues
1540	Eig05_EA(dm)	eigenvalue n. 5 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Eigenvalues
1541	Eig06_EA(dm)	eigenvalue n. 6 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Eigenvalues
1542	Eig07_EA(dm)	eigenvalue n. 7 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Eigenvalues
1543	Eig08_EA(dm)	eigenvalue n. 8 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Eigenvalues
1544	Eig09_EA(dm)	eigenvalue n. 9 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Eigenvalues
1545	Eig10_EA(dm)	eigenvalue n. 10 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Eigenvalues
1546	Eig11_EA(dm)	eigenvalue n. 11 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Eigenvalues
1547	Eig12_EA(dm)	eigenvalue n. 12 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Eigenvalues
1548	Eig13_EA(dm)	eigenvalue n. 13 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Eigenvalues

1549	Eig14_EA(dm)	eigenvalue n. 14 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Eigenvalues
1550	Eig15_EA(dm)	eigenvalue n. 15 from edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Eigenvalues
1551	Eig01_EA(ri)	eigenvalue n. 1 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Eigenvalues
1552	Eig02_EA(ri)	eigenvalue n. 2 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Eigenvalues
1553	Eig03_EA(ri)	eigenvalue n. 3 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Eigenvalues
1554	Eig04_EA(ri)	eigenvalue n. 4 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Eigenvalues
1555	Eig05_EA(ri)	eigenvalue n. 5 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Eigenvalues
1556	Eig06_EA(ri)	eigenvalue n. 6 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Eigenvalues
1557	Eig07_EA(ri)	eigenvalue n. 7 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Eigenvalues
1558	Eig08_EA(ri)	eigenvalue n. 8 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Eigenvalues
1559	Eig09_EA(ri)	eigenvalue n. 9 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Eigenvalues
1560	Eig10_EA(ri)	eigenvalue n. 10 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Eigenvalues
1561	Eig11_EA(ri)	eigenvalue n. 11 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Eigenvalues
1562	Eig12_EA(ri)	eigenvalue n. 12 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Eigenvalues
1563	Eig13_EA(ri)	eigenvalue n. 13 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Eigenvalues

1564	Eig14_EA(ri)	eigenvalue n. 14 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Eigenvalues
1565	Eig15_EA(ri)	eigenvalue n. 15 from edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Eigenvalues
1566	Eig01_AEA(ed)	eigenvalue n. 1 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Eigenvalues
1567	Eig02_AEA(ed)	eigenvalue n. 2 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Eigenvalues
1568	Eig03_AEA(ed)	eigenvalue n. 3 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Eigenvalues
1569	Eig04_AEA(ed)	eigenvalue n. 4 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Eigenvalues
1570	Eig05_AEA(ed)	eigenvalue n. 5 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Eigenvalues
1571	Eig06_AEA(ed)	eigenvalue n. 6 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Eigenvalues
1572	Eig07_AEA(ed)	eigenvalue n. 7 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Eigenvalues
1573	Eig08_AEA(ed)	eigenvalue n. 8 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Eigenvalues
1574	Eig09_AEA(ed)	eigenvalue n. 9 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Eigenvalues
1575	Eig10_AEA(ed)	eigenvalue n. 10 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Eigenvalues
1576	Eig11_AEA(ed)	eigenvalue n. 11 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Eigenvalues
1577	Eig12_AEA(ed)	eigenvalue n. 12 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Eigenvalues
1578	Eig13_AEA(ed)	eigenvalue n. 13 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Eigenvalues

1579	Eig14_AEA(ed)	eigenvalue n. 14 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Eigenvalues
1580	Eig15_AEA(ed)	eigenvalue n. 15 from augmented edge adjacency mat. weighted by edge degree	Edge adjacency indices	Eigenvalues
1581	Eig01_AEA(bo)	eigenvalue n. 1 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Eigenvalues
1582	Eig02_AEA(bo)	eigenvalue n. 2 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Eigenvalues
1583	Eig03_AEA(bo)	eigenvalue n. 3 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Eigenvalues
1584	Eig04_AEA(bo)	eigenvalue n. 4 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Eigenvalues
1585	Eig05_AEA(bo)	eigenvalue n. 5 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Eigenvalues
1586	Eig06_AEA(bo)	eigenvalue n. 6 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Eigenvalues
1587	Eig07_AEA(bo)	eigenvalue n. 7 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Eigenvalues
1588	Eig08_AEA(bo)	eigenvalue n. 8 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Eigenvalues
1589	Eig09_AEA(bo)	eigenvalue n. 9 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Eigenvalues
1590	Eig10_AEA(bo)	eigenvalue n. 10 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Eigenvalues
1591	Eig11_AEA(bo)	eigenvalue n. 11 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Eigenvalues
1592	Eig12_AEA(bo)	eigenvalue n. 12 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Eigenvalues
1593	Eig13_AEA(bo)	eigenvalue n. 13 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Eigenvalues

1594	Eig14_AEA(bo)	eigenvalue n. 14 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Eigenvalues
1595	Eig15_AEA(bo)	eigenvalue n. 15 from augmented edge adjacency mat. weighted by bond order	Edge adjacency indices	Eigenvalues
1596	Eig01_AEA(dm)	eigenvalue n. 1 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Eigenvalues
1597	Eig02_AEA(dm)	eigenvalue n. 2 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Eigenvalues
1598	Eig03_AEA(dm)	eigenvalue n. 3 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Eigenvalues
1599	Eig04_AEA(dm)	eigenvalue n. 4 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Eigenvalues
1600	Eig05_AEA(dm)	eigenvalue n. 5 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Eigenvalues
1601	Eig06_AEA(dm)	eigenvalue n. 6 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Eigenvalues
1602	Eig07_AEA(dm)	eigenvalue n. 7 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Eigenvalues
1603	Eig08_AEA(dm)	eigenvalue n. 8 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Eigenvalues
1604	Eig09_AEA(dm)	eigenvalue n. 9 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Eigenvalues
1605	Eig10_AEA(dm)	eigenvalue n. 10 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Eigenvalues
1606	Eig11_AEA(dm)	eigenvalue n. 11 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Eigenvalues
1607	Eig12_AEA(dm)	eigenvalue n. 12 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Eigenvalues
1608	Eig13_AEA(dm)	eigenvalue n. 13 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Eigenvalues

1609	Eig14_AEA(dm)	eigenvalue n. 14 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Eigenvalues
1610	Eig15_AEA(dm)	eigenvalue n. 15 from augmented edge adjacency mat. weighted by dipole moment	Edge adjacency indices	Eigenvalues
1611	Eig01_AEA(ri)	eigenvalue n. 1 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Eigenvalues
1612	Eig02_AEA(ri)	eigenvalue n. 2 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Eigenvalues
1613	Eig03_AEA(ri)	eigenvalue n. 3 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Eigenvalues
1614	Eig04_AEA(ri)	eigenvalue n. 4 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Eigenvalues
1615	Eig05_AEA(ri)	eigenvalue n. 5 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Eigenvalues
1616	Eig06_AEA(ri)	eigenvalue n. 6 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Eigenvalues
1617	Eig07_AEA(ri)	eigenvalue n. 7 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Eigenvalues
1618	Eig08_AEA(ri)	eigenvalue n. 8 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Eigenvalues
1619	Eig09_AEA(ri)	eigenvalue n. 9 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Eigenvalues
1620	Eig10_AEA(ri)	eigenvalue n. 10 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Eigenvalues
1621	Eig11_AEA(ri)	eigenvalue n. 11 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Eigenvalues
1622	Eig12_AEA(ri)	eigenvalue n. 12 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Eigenvalues
1623	Eig13_AEA(ri)	eigenvalue n. 13 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Eigenvalues

1624	Eig14_AEA(ri)	eigenvalue n. 14 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Eigenvalues
1625	Eig15_AEA(ri)	eigenvalue n. 15 from augmented edge adjacency mat. weighted by resonance integral	Edge adjacency indices	Eigenvalues
1626	G1	gravitational index G1	Geometrical descriptors	Size indices
1627	G2	gravitational index G2 (bond-restricted)	Geometrical descriptors	Size indices
1628	RGyr	radius of gyration (mass weighted)	Geometrical descriptors	Size indices
1629	SPAN	span R	Geometrical descriptors	Size indices
1630	SPAM	average span R	Geometrical descriptors	Shape indices
1631	MEcc	molecular eccentricity	Geometrical descriptors	Shape indices
1632	SPH	spherosity	Geometrical descriptors	Shape indices
1633	ASP	asphericity	Geometrical descriptors	Shape indices
1634	PJI3	3D Petitjean shape index	Geometrical descriptors	Shape indices
1635	L/Bw	length-to-breadth ratio by WHIM	Geometrical descriptors	Shape indices
1636	HOMA	Harmonic Oscillator Model of Aromaticity index	Geometrical descriptors	Delocalization-degree indices
1637	CMBL	conjugated maximum bond length	Geometrical descriptors	Delocalization-degree indices
1638	AROM	aromaticity index	Geometrical descriptors	Delocalization-degree indices
1639	HOMT	HOMA total	Geometrical descriptors	Delocalization-degree indices
1640	DISPm	displacement value / weighted by mass	Geometrical descriptors	COMMA descriptors
1641	QXXm	quadrupole x-component value / weighted by mass	Geometrical descriptors	COMMA descriptors
1642	QYYm	quadrupole y-component value / weighted by mass	Geometrical descriptors	COMMA descriptors

1643	QZZm	quadrupole z-component value / weighted by mass	Geometrical descriptors	COMMA descriptors
1644	DISPv	displacement value / weighted by van der Waals volume	Geometrical descriptors	COMMA descriptors
1645	QXXv	quadrupole x-component value / weighted by van der Waals volume	Geometrical descriptors	COMMA descriptors
1646	QYYv	quadrupole y-component value / weighted by van der Waals volume	Geometrical descriptors	COMMA descriptors
1647	QZZv	quadrupole z-component value / weighted by van der Waals volume	Geometrical descriptors	COMMA descriptors
1648	DISPe	displacement value / weighted by Sanderson electronegativity	Geometrical descriptors	COMMA descriptors
1649	QXXe	quadrupole x-component value / weighted by Sanderson electronegativity	Geometrical descriptors	COMMA descriptors
1650	QYYe	quadrupole y-component value / weighted by Sanderson electronegativity	Geometrical descriptors	COMMA descriptors
1651	QZZe	quadrupole z-component value / weighted by Sanderson electronegativity	Geometrical descriptors	COMMA descriptors
1652	DISPp	displacement value / weighted by polarizability	Geometrical descriptors	COMMA descriptors
1653	QXXp	quadrupole x-component value / weighted by polarizability	Geometrical descriptors	COMMA descriptors
1654	QYYp	quadrupole y-component value / weighted by polarizability	Geometrical descriptors	COMMA descriptors
1655	QZZp	quadrupole z-component value / weighted by polarizability	Geometrical descriptors	COMMA descriptors
1656	DISPi	displacement value / weighted by ionization potential	Geometrical descriptors	COMMA descriptors
1657	QXXi	quadrupole x-component value / weighted by ionization potential	Geometrical descriptors	COMMA descriptors
1658	QYYi	quadrupole y-component value / weighted by ionization potential	Geometrical descriptors	COMMA descriptors
1659	QZZi	quadrupole z-component value / weighted by ionization potential	Geometrical descriptors	COMMA descriptors
1660	DISPs	displacement value / weighted by I-state	Geometrical descriptors	COMMA descriptors
1661	QXXs	quadrupole x-component value / weighted by I-state	Geometrical descriptors	COMMA descriptors
1662	QYYs	quadrupole y-component value / weighted by I-state	Geometrical descriptors	COMMA descriptors

1663	QZZs	quadrupole z-component value / weighted by I-state	Geometrical descriptors	COMMA descriptors
1664	Wi_G	Wiener-like index from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)
1665	WiA_G	average Wiener-like index from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)
1666	AVS_G	average vertex sum from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)
1667	H_G	Harary-like index from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)
1668	Chi_G	Randic-like index from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)
1669	ChiA_G	average Randic-like index from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)
1670	J_G	Balaban-like index from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)
1671	HyWi_G	hyper-Wiener-like index from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)
1672	SpAbs_G	graph energy from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)
1673	SpPos_G	spectral positive sum from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)
1674	SpPosA_G	normalized spectral positive sum from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)
1675	SpPosLog_G	logarithmic spectral positive sum from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)
1676	SpMax_G	leading eigenvalue from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)
1677	SpMaxA_G	normalized leading eigenvalue from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)

1678	SpDiam_G	spectral diameter from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)
1679	SpAD_G	spectral absolute deviation from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)
1680	SpMAD_G	spectral mean absolute deviation from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)
1681	Ho_G	Hosoya-like index (log function) from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)
1682	EE_G	Estrada-like index (log function) from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)
1683	SM2_G	spectral moment of order 2 from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)
1684	SM3_G	spectral moment of order 3 from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)
1685	SM4_G	spectral moment of order 4 from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)
1686	SM5_G	spectral moment of order 5 from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)
1687	SM6_G	spectral moment of order 6 from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)
1688	VE1_G	coefficient sum of the last eigenvector (absolute values) from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)
1689	VE2_G	average coefficient of the last eigenvector (absolute values) from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)
1690	VE3_G	logarithmic coefficient sum of the last eigenvector (absolute values) from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)
1691	VE1sign_G	coefficient sum of the last eigenvector from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)
1692	VE2sign_G	average coefficient of the last eigenvector from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)

1693	VE3sign_G	logarithmic coefficient sum of the last eigenvector from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)
1694	VR1_G	Randic-like eigenvector-based index from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)
1695	VR2_G	normalized Randic-like eigenvector-based index from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)
1696	VR3_G	logarithmic Randic-like eigenvector-based index from geometrical matrix	3D matrix-based descriptors	Geometrical distance matrix (G)
1697	Wi_RG	Wiener-like index from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)
1698	WiA_RG	average Wiener-like index from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)
1699	AVS_RG	average vertex sum from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)
1700	H_RG	Harary-like index from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)
1701	Chi_RG	Randic-like index from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)
1702	ChiA_RG	average Randic-like index from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)
1703	J_RG	Balaban-like index from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)
1704	HyWi_RG	hyper-Wiener-like index from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)
1705	SpAbs_RG	graph energy from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)
1706	SpPos_RG	spectral positive sum from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)
1707	SpPosA_RG	normalized spectral positive sum from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)

1708	SpPosLog_RG	logarithmic spectral positive sum from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)
1709	SpMax_RG	leading eigenvalue from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)
1710	SpMaxA_RG	normalized leading eigenvalue from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)
1711	SpDiam_RG	spectral diameter from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)
1712	SpAD_RG	spectral absolute deviation from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)
1713	SpMAD_RG	spectral mean absolute deviation from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)
1714	Ho_RG	Hosoya-like index (log function) from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)
1715	EE_RG	Estrada-like index (log function) from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)
1716	SM2_RG	spectral moment of order 2 from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)
1717	SM3_RG	spectral moment of order 3 from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)
1718	SM4_RG	spectral moment of order 4 from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)
1719	SM5_RG	spectral moment of order 5 from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)
1720	SM6_RG	spectral moment of order 6 from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)
1721	VE1_RG	coefficient sum of the last eigenvector (absolute values) from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)
1722	VE2_RG	average coefficient of the last eigenvector (absolute values) from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)

1723	VE3_RG	logarithmic coefficient sum of the last eigenvector (absolute values) from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)
1724	VE1sign_RG	coefficient sum of the last eigenvector from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)
1725	VE2sign_RG	average coefficient of the last eigenvector from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)
1726	VE3sign_RG	logarithmic coefficient sum of the last eigenvector from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)
1727	VR1_RG	Randic-like eigenvector-based index from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)
1728	VR2_RG	normalized Randic-like eigenvector-based index from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)
1729	VR3_RG	logarithmic Randic-like eigenvector-based index from reciprocal squared geometrical matrix	3D matrix-based descriptors	Reciprocal squared geometrical distance matrix (RG)
1730	Wi_G/D	Wiener-like index from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)
1731	WiA_G/D	average Wiener-like index from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)
1732	AVS_G/D	average vertex sum from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)
1733	H_G/D	Harary-like index from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)
1734	Chi_G/D	Randic-like index from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)
1735	ChiA_G/D	average Randic-like index from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)
1736	J_G/D	Balaban-like index from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)
1737	HyWi_G/D	hyper-Wiener-like index from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)

1738	SpAbs_G/D	graph energy from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)
1739	SpPos_G/D	spectral positive sum from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)
1740	SpPosA_G/D	normalized spectral positive sum from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)
1741	SpPosLog_G/D	logarithmic spectral positive sum from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)
1742	SpMax_G/D	leading eigenvalue from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)
1743	SpMaxA_G/D	normalized leading eigenvalue from distance/distance matrix (folding degree index)	3D matrix-based descriptors	Distance/distance matrix (G/D)
1744	SpDiam_G/D	spectral diameter from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)
1745	SpAD_G/D	spectral absolute deviation from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)
1746	SpMAD_G/D	spectral mean absolute deviation from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)
1747	Ho_G/D	Hosoya-like index (log function) from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)
1748	EE_G/D	Estrada-like index (log function) from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)
1749	SM2_G/D	spectral moment of order 2 from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)
1750	SM3_G/D	spectral moment of order 3 from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)
1751	SM4_G/D	spectral moment of order 4 from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)
1752	SM5_G/D	spectral moment of order 5 from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)

1753	SM6_G/D	spectral moment of order 6 from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)
1754	VE1_G/D	coefficient sum of the last eigenvector (absolute values) from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)
1755	VE2_G/D	average coefficient of the last eigenvector (absolute values) from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)
1756	VE3_G/D	logarithmic coefficient sum of the last eigenvector (absolute values) from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)
1757	VE1sign_G/D	coefficient sum of the last eigenvector from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)
1758	VE2sign_G/D	average coefficient of the last eigenvector from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)
1759	VE3sign_G/D	logarithmic coefficient sum of the last eigenvector from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)
1760	VR1_G/D	Randic-like eigenvector-based index from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)
1761	VR2_G/D	normalized Randic-like eigenvector-based index from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)
1762	VR3_G/D	logarithmic Randic-like eigenvector-based index from distance/distance matrix	3D matrix-based descriptors	Distance/distance matrix (G/D)
1763	TDB01u	3D Topological distance based descriptors - lag 1 unweighted	3D autocorrelations	TDB autocorrelations
1764	TDB02u	3D Topological distance based descriptors - lag 2 unweighted	3D autocorrelations	TDB autocorrelations
1765	TDB03u	3D Topological distance based descriptors - lag 3 unweighted	3D autocorrelations	TDB autocorrelations
1766	TDB04u	3D Topological distance based descriptors - lag 4 unweighted	3D autocorrelations	TDB autocorrelations
1767	TDB05u	3D Topological distance based descriptors - lag 5 unweighted	3D autocorrelations	TDB autocorrelations
1768	TDB06u	3D Topological distance based descriptors - lag 6 unweighted	3D autocorrelations	TDB autocorrelations
1769	TDB07u	3D Topological distance based descriptors - lag 7 unweighted	3D autocorrelations	TDB autocorrelations

1770	TDB08u	3D Topological distance based descriptors - lag 8 unweighted	3D autocorrelations	TDB autocorrelations
1771	TDB09u	3D Topological distance based descriptors - lag 9 unweighted	3D autocorrelations	TDB autocorrelations
1772	TDB10u	3D Topological distance based descriptors - lag 10 unweighted	3D autocorrelations	TDB autocorrelations
1773	TDB01m	3D Topological distance based descriptors - lag 1 weighted by mass	3D autocorrelations	TDB autocorrelations
1774	TDB02m	3D Topological distance based descriptors - lag 2 weighted by mass	3D autocorrelations	TDB autocorrelations
1775	TDB03m	3D Topological distance based descriptors - lag 3 weighted by mass	3D autocorrelations	TDB autocorrelations
1776	TDB04m	3D Topological distance based descriptors - lag 4 weighted by mass	3D autocorrelations	TDB autocorrelations
1777	TDB05m	3D Topological distance based descriptors - lag 5 weighted by mass	3D autocorrelations	TDB autocorrelations
1778	TDB06m	3D Topological distance based descriptors - lag 6 weighted by mass	3D autocorrelations	TDB autocorrelations
1779	TDB07m	3D Topological distance based descriptors - lag 7 weighted by mass	3D autocorrelations	TDB autocorrelations
1780	TDB08m	3D Topological distance based descriptors - lag 8 weighted by mass	3D autocorrelations	TDB autocorrelations
1781	TDB09m	3D Topological distance based descriptors - lag 9 weighted by mass	3D autocorrelations	TDB autocorrelations
1782	TDB10m	3D Topological distance based descriptors - lag 10 weighted by mass	3D autocorrelations	TDB autocorrelations
1783	TDB01v	3D Topological distance based descriptors - lag 1 weighted by van der Waals volume	3D autocorrelations	TDB autocorrelations
1784	TDB02v	3D Topological distance based descriptors - lag 2 weighted by van der Waals volume	3D autocorrelations	TDB autocorrelations
1785	TDB03v	3D Topological distance based descriptors - lag 3 weighted by van der Waals volume	3D autocorrelations	TDB autocorrelations
1786	TDB04v	3D Topological distance based descriptors - lag 4 weighted by van der Waals volume	3D autocorrelations	TDB autocorrelations
1787	TDB05v	3D Topological distance based descriptors - lag 5 weighted by van der Waals volume	3D autocorrelations	TDB autocorrelations
1788	TDB06v	3D Topological distance based descriptors - lag 6 weighted by van der Waals volume	3D autocorrelations	TDB autocorrelations
1789	TDB07v	3D Topological distance based descriptors - lag 7 weighted by van der Waals volume	3D autocorrelations	TDB autocorrelations

1790	TDB08v	3D Topological distance based descriptors - lag 8 weighted by van der Waals volume	3D autocorrelations	TDB autocorrelations
1791	TDB09v	3D Topological distance based descriptors - lag 9 weighted by van der Waals volume	3D autocorrelations	TDB autocorrelations
1792	TDB10v	3D Topological distance based descriptors - lag 10 weighted by van der Waals volume	3D autocorrelations	TDB autocorrelations
1793	TDB01e	3D Topological distance based descriptors - lag 1 weighted by Sanderson electronegativity	3D autocorrelations	TDB autocorrelations
1794	TDB02e	3D Topological distance based descriptors - lag 2 weighted by Sanderson electronegativity	3D autocorrelations	TDB autocorrelations
1795	TDB03e	3D Topological distance based descriptors - lag 3 weighted by Sanderson electronegativity	3D autocorrelations	TDB autocorrelations
1796	TDB04e	3D Topological distance based descriptors - lag 4 weighted by Sanderson electronegativity	3D autocorrelations	TDB autocorrelations
1797	TDB05e	3D Topological distance based descriptors - lag 5 weighted by Sanderson electronegativity	3D autocorrelations	TDB autocorrelations
1798	TDB06e	3D Topological distance based descriptors - lag 6 weighted by Sanderson electronegativity	3D autocorrelations	TDB autocorrelations
1799	TDB07e	3D Topological distance based descriptors - lag 7 weighted by Sanderson electronegativity	3D autocorrelations	TDB autocorrelations
1800	TDB08e	3D Topological distance based descriptors - lag 8 weighted by Sanderson electronegativity	3D autocorrelations	TDB autocorrelations
1801	TDB09e	3D Topological distance based descriptors - lag 9 weighted by Sanderson electronegativity	3D autocorrelations	TDB autocorrelations
1802	TDB10e	3D Topological distance based descriptors - lag 10 weighted by Sanderson electronegativity	3D autocorrelations	TDB autocorrelations
1803	TDB01p	3D Topological distance based descriptors - lag 1 weighted by polarizability	3D autocorrelations	TDB autocorrelations
1804	TDB02p	3D Topological distance based descriptors - lag 2 weighted by polarizability	3D autocorrelations	TDB autocorrelations
1805	TDB03p	3D Topological distance based descriptors - lag 3 weighted by polarizability	3D autocorrelations	TDB autocorrelations
1806	TDB04p	3D Topological distance based descriptors - lag 4 weighted by polarizability	3D autocorrelations	TDB autocorrelations

1807	TDB05p	3D Topological distance based descriptors - lag 5 weighted by polarizability	3D autocorrelations	TDB autocorrelations
1808	TDB06p	3D Topological distance based descriptors - lag 6 weighted by polarizability	3D autocorrelations	TDB autocorrelations
1809	TDB07p	3D Topological distance based descriptors - lag 7 weighted by polarizability	3D autocorrelations	TDB autocorrelations
1810	TDB08p	3D Topological distance based descriptors - lag 8 weighted by polarizability	3D autocorrelations	TDB autocorrelations
1811	TDB09p	3D Topological distance based descriptors - lag 9 weighted by polarizability	3D autocorrelations	TDB autocorrelations
1812	TDB10p	3D Topological distance based descriptors - lag 10 weighted by polarizability	3D autocorrelations	TDB autocorrelations
1813	TDB01i	3D Topological distance based descriptors - lag 1 weighted by ionization potential	3D autocorrelations	TDB autocorrelations
1814	TDB02i	3D Topological distance based descriptors - lag 2 weighted by ionization potential	3D autocorrelations	TDB autocorrelations
1815	TDB03i	3D Topological distance based descriptors - lag 3 weighted by ionization potential	3D autocorrelations	TDB autocorrelations
1816	TDB04i	3D Topological distance based descriptors - lag 4 weighted by ionization potential	3D autocorrelations	TDB autocorrelations
1817	TDB05i	3D Topological distance based descriptors - lag 5 weighted by ionization potential	3D autocorrelations	TDB autocorrelations
1818	TDB06i	3D Topological distance based descriptors - lag 6 weighted by ionization potential	3D autocorrelations	TDB autocorrelations
1819	TDB07i	3D Topological distance based descriptors - lag 7 weighted by ionization potential	3D autocorrelations	TDB autocorrelations
1820	TDB08i	3D Topological distance based descriptors - lag 8 weighted by ionization potential	3D autocorrelations	TDB autocorrelations
1821	TDB09i	3D Topological distance based descriptors - lag 9 weighted by ionization potential	3D autocorrelations	TDB autocorrelations
1822	TDB10i	3D Topological distance based descriptors - lag 10 weighted by ionization potential	3D autocorrelations	TDB autocorrelations
1823	TDB01s	3D Topological distance based descriptors - lag 1 weighted by I-state	3D autocorrelations	TDB autocorrelations
1824	TDB02s	3D Topological distance based descriptors - lag 2 weighted by I-state	3D autocorrelations	TDB autocorrelations
1825	TDB03s	3D Topological distance based descriptors - lag 3 weighted by I-state	3D autocorrelations	TDB autocorrelations
1826	TDB04s	3D Topological distance based descriptors - lag 4 weighted by I-state	3D autocorrelations	TDB autocorrelations

1827	TDB05s	3D Topological distance based descriptors - lag 5 weighted by I-state	3D autocorrelations	TDB autocorrelations
1828	TDB06s	3D Topological distance based descriptors - lag 6 weighted by I-state	3D autocorrelations	TDB autocorrelations
1829	TDB07s	3D Topological distance based descriptors - lag 7 weighted by I-state	3D autocorrelations	TDB autocorrelations
1830	TDB08s	3D Topological distance based descriptors - lag 8 weighted by I-state	3D autocorrelations	TDB autocorrelations
1831	TDB09s	3D Topological distance based descriptors - lag 9 weighted by I-state	3D autocorrelations	TDB autocorrelations
1832	TDB10s	3D Topological distance based descriptors - lag 10 weighted by I-state	3D autocorrelations	TDB autocorrelations
1833	TDB01r	3D Topological distance based descriptors - lag 1 weighted by covalent radius	3D autocorrelations	TDB autocorrelations
1834	TDB02r	3D Topological distance based descriptors - lag 2 weighted by covalent radius	3D autocorrelations	TDB autocorrelations
1835	TDB03r	3D Topological distance based descriptors - lag 3 weighted by covalent radius	3D autocorrelations	TDB autocorrelations
1836	TDB04r	3D Topological distance based descriptors - lag 4 weighted by covalent radius	3D autocorrelations	TDB autocorrelations
1837	TDB05r	3D Topological distance based descriptors - lag 5 weighted by covalent radius	3D autocorrelations	TDB autocorrelations
1838	TDB06r	3D Topological distance based descriptors - lag 6 weighted by covalent radius	3D autocorrelations	TDB autocorrelations
1839	TDB07r	3D Topological distance based descriptors - lag 7 weighted by covalent radius	3D autocorrelations	TDB autocorrelations
1840	TDB08r	3D Topological distance based descriptors - lag 8 weighted by covalent radius	3D autocorrelations	TDB autocorrelations
1841	TDB09r	3D Topological distance based descriptors - lag 9 weighted by covalent radius	3D autocorrelations	TDB autocorrelations
1842	TDB10r	3D Topological distance based descriptors - lag 10 weighted by covalent radius	3D autocorrelations	TDB autocorrelations
1843	RDF010u	Radial Distribution Function - 010 / unweighted	RDF descriptors	Unweighted
1844	RDF015u	Radial Distribution Function - 015 / unweighted	RDF descriptors	Unweighted
1845	RDF020u	Radial Distribution Function - 020 / unweighted	RDF descriptors	Unweighted
1846	RDF025u	Radial Distribution Function - 025 / unweighted	RDF descriptors	Unweighted

1847	RDF030u	Radial Distribution Function - 030 / unweighted	RDF descriptors	Unweighted
1848	RDF035u	Radial Distribution Function - 035 / unweighted	RDF descriptors	Unweighted
1849	RDF040u	Radial Distribution Function - 040 / unweighted	RDF descriptors	Unweighted
1850	RDF045u	Radial Distribution Function - 045 / unweighted	RDF descriptors	Unweighted
1851	RDF050u	Radial Distribution Function - 050 / unweighted	RDF descriptors	Unweighted
1852	RDF055u	Radial Distribution Function - 055 / unweighted	RDF descriptors	Unweighted
1853	RDF060u	Radial Distribution Function - 060 / unweighted	RDF descriptors	Unweighted
1854	RDF065u	Radial Distribution Function - 065 / unweighted	RDF descriptors	Unweighted
1855	RDF070u	Radial Distribution Function - 070 / unweighted	RDF descriptors	Unweighted
1856	RDF075u	Radial Distribution Function - 075 / unweighted	RDF descriptors	Unweighted
1857	RDF080u	Radial Distribution Function - 080 / unweighted	RDF descriptors	Unweighted
1858	RDF085u	Radial Distribution Function - 085 / unweighted	RDF descriptors	Unweighted
1859	RDF090u	Radial Distribution Function - 090 / unweighted	RDF descriptors	Unweighted
1860	RDF095u	Radial Distribution Function - 095 / unweighted	RDF descriptors	Unweighted
1861	RDF100u	Radial Distribution Function - 100 / unweighted	RDF descriptors	Unweighted
1862	RDF105u	Radial Distribution Function - 105 / unweighted	RDF descriptors	Unweighted
1863	RDF110u	Radial Distribution Function - 110 / unweighted	RDF descriptors	Unweighted
1864	RDF115u	Radial Distribution Function - 115 / unweighted	RDF descriptors	Unweighted
1865	RDF120u	Radial Distribution Function - 120 / unweighted	RDF descriptors	Unweighted
1866	RDF125u	Radial Distribution Function - 125 / unweighted	RDF descriptors	Unweighted

1867	RDF130u	Radial Distribution Function - 130 / unweighted	RDF descriptors	Unweighted
1868	RDF135u	Radial Distribution Function - 135 / unweighted	RDF descriptors	Unweighted
1869	RDF140u	Radial Distribution Function - 140 / unweighted	RDF descriptors	Unweighted
1870	RDF145u	Radial Distribution Function - 145 / unweighted	RDF descriptors	Unweighted
1871	RDF150u	Radial Distribution Function - 150 / unweighted	RDF descriptors	Unweighted
1872	RDF155u	Radial Distribution Function - 155 / unweighted	RDF descriptors	Unweighted
1873	RDF010m	Radial Distribution Function - 010 / weighted by mass	RDF descriptors	Weighted by mass
1874	RDF015m	Radial Distribution Function - 015 / weighted by mass	RDF descriptors	Weighted by mass
1875	RDF020m	Radial Distribution Function - 020 / weighted by mass	RDF descriptors	Weighted by mass
1876	RDF025m	Radial Distribution Function - 025 / weighted by mass	RDF descriptors	Weighted by mass
1877	RDF030m	Radial Distribution Function - 030 / weighted by mass	RDF descriptors	Weighted by mass
1878	RDF035m	Radial Distribution Function - 035 / weighted by mass	RDF descriptors	Weighted by mass
1879	RDF040m	Radial Distribution Function - 040 / weighted by mass	RDF descriptors	Weighted by mass
1880	RDF045m	Radial Distribution Function - 045 / weighted by mass	RDF descriptors	Weighted by mass
1881	RDF050m	Radial Distribution Function - 050 / weighted by mass	RDF descriptors	Weighted by mass
1882	RDF055m	Radial Distribution Function - 055 / weighted by mass	RDF descriptors	Weighted by mass
1883	RDF060m	Radial Distribution Function - 060 / weighted by mass	RDF descriptors	Weighted by mass
1884	RDF065m	Radial Distribution Function - 065 / weighted by mass	RDF descriptors	Weighted by mass
1885	RDF070m	Radial Distribution Function - 070 / weighted by mass	RDF descriptors	Weighted by mass
1886	RDF075m	Radial Distribution Function - 075 / weighted by mass	RDF descriptors	Weighted by mass

1887	RDF080m	Radial Distribution Function - 080 / weighted by mass	RDF descriptors	Weighted by mass
1888	RDF085m	Radial Distribution Function - 085 / weighted by mass	RDF descriptors	Weighted by mass
1889	RDF090m	Radial Distribution Function - 090 / weighted by mass	RDF descriptors	Weighted by mass
1890	RDF095m	Radial Distribution Function - 095 / weighted by mass	RDF descriptors	Weighted by mass
1891	RDF100m	Radial Distribution Function - 100 / weighted by mass	RDF descriptors	Weighted by mass
1892	RDF105m	Radial Distribution Function - 105 / weighted by mass	RDF descriptors	Weighted by mass
1893	RDF110m	Radial Distribution Function - 110 / weighted by mass	RDF descriptors	Weighted by mass
1894	RDF115m	Radial Distribution Function - 115 / weighted by mass	RDF descriptors	Weighted by mass
1895	RDF120m	Radial Distribution Function - 120 / weighted by mass	RDF descriptors	Weighted by mass
1896	RDF125m	Radial Distribution Function - 125 / weighted by mass	RDF descriptors	Weighted by mass
1897	RDF130m	Radial Distribution Function - 130 / weighted by mass	RDF descriptors	Weighted by mass
1898	RDF135m	Radial Distribution Function - 135 / weighted by mass	RDF descriptors	Weighted by mass
1899	RDF140m	Radial Distribution Function - 140 / weighted by mass	RDF descriptors	Weighted by mass
1900	RDF145m	Radial Distribution Function - 145 / weighted by mass	RDF descriptors	Weighted by mass
1901	RDF150m	Radial Distribution Function - 150 / weighted by mass	RDF descriptors	Weighted by mass
1902	RDF155m	Radial Distribution Function - 155 / weighted by mass	RDF descriptors	Weighted by mass
1903	RDF010v	Radial Distribution Function - 010 / weighted by van der Waals volume	RDF descriptors	Weighted by van der Waals volume
1904	RDF015v	Radial Distribution Function - 015 / weighted by van der Waals volume	RDF descriptors	Weighted by van der Waals volume
1905	RDF020v	Radial Distribution Function - 020 / weighted by van der Waals volume	RDF descriptors	Weighted by van der Waals volume
1906	RDF025v	Radial Distribution Function - 025 / weighted by van der Waals volume	RDF descriptors	Weighted by van der Waals volume

1907	RDF030v	Radial Distribution Function - 030 / weighted by van der Waals volume	RDF descriptors	Weighted by van der Waals volume
1908	RDF035v	Radial Distribution Function - 035 / weighted by van der Waals volume	RDF descriptors	Weighted by van der Waals volume
1909	RDF040v	Radial Distribution Function - 040 / weighted by van der Waals volume	RDF descriptors	Weighted by van der Waals volume
1910	RDF045v	Radial Distribution Function - 045 / weighted by van der Waals volume	RDF descriptors	Weighted by van der Waals volume
1911	RDF050v	Radial Distribution Function - 050 / weighted by van der Waals volume	RDF descriptors	Weighted by van der Waals volume
1912	RDF055v	Radial Distribution Function - 055 / weighted by van der Waals volume	RDF descriptors	Weighted by van der Waals volume
1913	RDF060v	Radial Distribution Function - 060 / weighted by van der Waals volume	RDF descriptors	Weighted by van der Waals volume
1914	RDF065v	Radial Distribution Function - 065 / weighted by van der Waals volume	RDF descriptors	Weighted by van der Waals volume
1915	RDF070v	Radial Distribution Function - 070 / weighted by van der Waals volume	RDF descriptors	Weighted by van der Waals volume
1916	RDF075v	Radial Distribution Function - 075 / weighted by van der Waals volume	RDF descriptors	Weighted by van der Waals volume
1917	RDF080v	Radial Distribution Function - 080 / weighted by van der Waals volume	RDF descriptors	Weighted by van der Waals volume
1918	RDF085v	Radial Distribution Function - 085 / weighted by van der Waals volume	RDF descriptors	Weighted by van der Waals volume
1919	RDF090v	Radial Distribution Function - 090 / weighted by van der Waals volume	RDF descriptors	Weighted by van der Waals volume
1920	RDF095v	Radial Distribution Function - 095 / weighted by van der Waals volume	RDF descriptors	Weighted by van der Waals volume
1921	RDF100v	Radial Distribution Function - 100 / weighted by van der Waals volume	RDF descriptors	Weighted by van der Waals volume
1922	RDF105v	Radial Distribution Function - 105 / weighted by van der Waals volume	RDF descriptors	Weighted by van der Waals volume
1923	RDF110v	Radial Distribution Function - 110 / weighted by van der Waals volume	RDF descriptors	Weighted by van der Waals volume
1924	RDF115v	Radial Distribution Function - 115 / weighted by van der Waals volume	RDF descriptors	Weighted by van der Waals volume
1925	RDF120v	Radial Distribution Function - 120 / weighted by van der Waals volume	RDF descriptors	Weighted by van der Waals volume
1926	RDF125v	Radial Distribution Function - 125 / weighted by van der Waals volume	RDF descriptors	Weighted by van der Waals volume

1927	RDF130v	Radial Distribution Function - 130 / weighted by van der Waals volume	RDF descriptors	Weighted by van der Waals volume
1928	RDF135v	Radial Distribution Function - 135 / weighted by van der Waals volume	RDF descriptors	Weighted by van der Waals volume
1929	RDF140v	Radial Distribution Function - 140 / weighted by van der Waals volume	RDF descriptors	Weighted by van der Waals volume
1930	RDF145v	Radial Distribution Function - 145 / weighted by van der Waals volume	RDF descriptors	Weighted by van der Waals volume
1931	RDF150v	Radial Distribution Function - 150 / weighted by van der Waals volume	RDF descriptors	Weighted by van der Waals volume
1932	RDF155v	Radial Distribution Function - 155 / weighted by van der Waals volume	RDF descriptors	Weighted by van der Waals volume
1933	RDF010e	Radial Distribution Function - 010 / weighted by Sanderson electronegativity	RDF descriptors	Weighted by Sanderson electronegativity
1934	RDF015e	Radial Distribution Function - 015 / weighted by Sanderson electronegativity	RDF descriptors	Weighted by Sanderson electronegativity
1935	RDF020e	Radial Distribution Function - 020 / weighted by Sanderson electronegativity	RDF descriptors	Weighted by Sanderson electronegativity
1936	RDF025e	Radial Distribution Function - 025 / weighted by Sanderson electronegativity	RDF descriptors	Weighted by Sanderson electronegativity
1937	RDF030e	Radial Distribution Function - 030 / weighted by Sanderson electronegativity	RDF descriptors	Weighted by Sanderson electronegativity
1938	RDF035e	Radial Distribution Function - 035 / weighted by Sanderson electronegativity	RDF descriptors	Weighted by Sanderson electronegativity
1939	RDF040e	Radial Distribution Function - 040 / weighted by Sanderson electronegativity	RDF descriptors	Weighted by Sanderson electronegativity
1940	RDF045e	Radial Distribution Function - 045 / weighted by Sanderson electronegativity	RDF descriptors	Weighted by Sanderson electronegativity
1941	RDF050e	Radial Distribution Function - 050 / weighted by Sanderson electronegativity	RDF descriptors	Weighted by Sanderson electronegativity
1942	RDF055e	Radial Distribution Function - 055 / weighted by Sanderson electronegativity	RDF descriptors	Weighted by Sanderson electronegativity

1943	RDF060e	Radial Distribution Function - 060 / weighted by Sanderson electronegativity	RDF descriptors	Weighted by Sanderson electronegativity
1944	RDF065e	Radial Distribution Function - 065 / weighted by Sanderson electronegativity	RDF descriptors	Weighted by Sanderson electronegativity
1945	RDF070e	Radial Distribution Function - 070 / weighted by Sanderson electronegativity	RDF descriptors	Weighted by Sanderson electronegativity
1946	RDF075e	Radial Distribution Function - 075 / weighted by Sanderson electronegativity	RDF descriptors	Weighted by Sanderson electronegativity
1947	RDF080e	Radial Distribution Function - 080 / weighted by Sanderson electronegativity	RDF descriptors	Weighted by Sanderson electronegativity
1948	RDF085e	Radial Distribution Function - 085 / weighted by Sanderson electronegativity	RDF descriptors	Weighted by Sanderson electronegativity
1949	RDF090e	Radial Distribution Function - 090 / weighted by Sanderson electronegativity	RDF descriptors	Weighted by Sanderson electronegativity
1950	RDF095e	Radial Distribution Function - 095 / weighted by Sanderson electronegativity	RDF descriptors	Weighted by Sanderson electronegativity
1951	RDF100e	Radial Distribution Function - 100 / weighted by Sanderson electronegativity	RDF descriptors	Weighted by Sanderson electronegativity
1952	RDF105e	Radial Distribution Function - 105 / weighted by Sanderson electronegativity	RDF descriptors	Weighted by Sanderson electronegativity
1953	RDF110e	Radial Distribution Function - 110 / weighted by Sanderson electronegativity	RDF descriptors	Weighted by Sanderson electronegativity
1954	RDF115e	Radial Distribution Function - 115 / weighted by Sanderson electronegativity	RDF descriptors	Weighted by Sanderson electronegativity
1955	RDF120e	Radial Distribution Function - 120 / weighted by Sanderson electronegativity	RDF descriptors	Weighted by Sanderson electronegativity
1956	RDF125e	Radial Distribution Function - 125 / weighted by Sanderson electronegativity	RDF descriptors	Weighted by Sanderson electronegativity
1957	RDF130e	Radial Distribution Function - 130 / weighted by Sanderson electronegativity	RDF descriptors	Weighted by Sanderson electronegativity

1958	RDF135e	Radial Distribution Function - 135 / weighted by Sanderson electronegativity	RDF descriptors	Weighted by Sanderson electronegativity
1959	RDF140e	Radial Distribution Function - 140 / weighted by Sanderson electronegativity	RDF descriptors	Weighted by Sanderson electronegativity
1960	RDF145e	Radial Distribution Function - 145 / weighted by Sanderson electronegativity	RDF descriptors	Weighted by Sanderson electronegativity
1961	RDF150e	Radial Distribution Function - 150 / weighted by Sanderson electronegativity	RDF descriptors	Weighted by Sanderson electronegativity
1962	RDF155e	Radial Distribution Function - 155 / weighted by Sanderson electronegativity	RDF descriptors	Weighted by Sanderson electronegativity
1963	RDF010p	Radial Distribution Function - 010 / weighted by polarizability	RDF descriptors	Weighted by polarizability
1964	RDF015p	Radial Distribution Function - 015 / weighted by polarizability	RDF descriptors	Weighted by polarizability
1965	RDF020p	Radial Distribution Function - 020 / weighted by polarizability	RDF descriptors	Weighted by polarizability
1966	RDF025p	Radial Distribution Function - 025 / weighted by polarizability	RDF descriptors	Weighted by polarizability
1967	RDF030p	Radial Distribution Function - 030 / weighted by polarizability	RDF descriptors	Weighted by polarizability
1968	RDF035p	Radial Distribution Function - 035 / weighted by polarizability	RDF descriptors	Weighted by polarizability
1969	RDF040p	Radial Distribution Function - 040 / weighted by polarizability	RDF descriptors	Weighted by polarizability
1970	RDF045p	Radial Distribution Function - 045 / weighted by polarizability	RDF descriptors	Weighted by polarizability
1971	RDF050p	Radial Distribution Function - 050 / weighted by polarizability	RDF descriptors	Weighted by polarizability
1972	RDF055p	Radial Distribution Function - 055 / weighted by polarizability	RDF descriptors	Weighted by polarizability
1973	RDF060p	Radial Distribution Function - 060 / weighted by polarizability	RDF descriptors	Weighted by polarizability
1974	RDF065p	Radial Distribution Function - 065 / weighted by polarizability	RDF descriptors	Weighted by polarizability
1975	RDF070p	Radial Distribution Function - 070 / weighted by polarizability	RDF descriptors	Weighted by polarizability

1976	RDF075p	Radial Distribution Function - 075 / weighted by polarizability	RDF descriptors	Weighted by polarizability
1977	RDF080p	Radial Distribution Function - 080 / weighted by polarizability	RDF descriptors	Weighted by polarizability
1978	RDF085p	Radial Distribution Function - 085 / weighted by polarizability	RDF descriptors	Weighted by polarizability
1979	RDF090p	Radial Distribution Function - 090 / weighted by polarizability	RDF descriptors	Weighted by polarizability
1980	RDF095p	Radial Distribution Function - 095 / weighted by polarizability	RDF descriptors	Weighted by polarizability
1981	RDF100p	Radial Distribution Function - 100 / weighted by polarizability	RDF descriptors	Weighted by polarizability
1982	RDF105p	Radial Distribution Function - 105 / weighted by polarizability	RDF descriptors	Weighted by polarizability
1983	RDF110p	Radial Distribution Function - 110 / weighted by polarizability	RDF descriptors	Weighted by polarizability
1984	RDF115p	Radial Distribution Function - 115 / weighted by polarizability	RDF descriptors	Weighted by polarizability
1985	RDF120p	Radial Distribution Function - 120 / weighted by polarizability	RDF descriptors	Weighted by polarizability
1986	RDF125p	Radial Distribution Function - 125 / weighted by polarizability	RDF descriptors	Weighted by polarizability
1987	RDF130p	Radial Distribution Function - 130 / weighted by polarizability	RDF descriptors	Weighted by polarizability
1988	RDF135p	Radial Distribution Function - 135 / weighted by polarizability	RDF descriptors	Weighted by polarizability
1989	RDF140p	Radial Distribution Function - 140 / weighted by polarizability	RDF descriptors	Weighted by polarizability
1990	RDF145p	Radial Distribution Function - 145 / weighted by polarizability	RDF descriptors	Weighted by polarizability
1991	RDF150p	Radial Distribution Function - 150 / weighted by polarizability	RDF descriptors	Weighted by polarizability
1992	RDF155p	Radial Distribution Function - 155 / weighted by polarizability	RDF descriptors	Weighted by polarizability
1993	RDF010i	Radial Distribution Function - 010 / weighted by ionization potential	RDF descriptors	Weighted by ionization potential
1994	RDF015i	Radial Distribution Function - 015 / weighted by ionization potential	RDF descriptors	Weighted by ionization potential
1995	RDF020i	Radial Distribution Function - 020 / weighted by ionization potential	RDF descriptors	Weighted by ionization potential

1996	RDF025i	Radial Distribution Function - 025 / weighted by ionization potential	RDF descriptors	Weighted by ionization potential
1997	RDF030i	Radial Distribution Function - 030 / weighted by ionization potential	RDF descriptors	Weighted by ionization potential
1998	RDF035i	Radial Distribution Function - 035 / weighted by ionization potential	RDF descriptors	Weighted by ionization potential
1999	RDF040i	Radial Distribution Function - 040 / weighted by ionization potential	RDF descriptors	Weighted by ionization potential
2000	RDF045i	Radial Distribution Function - 045 / weighted by ionization potential	RDF descriptors	Weighted by ionization potential
2001	RDF050i	Radial Distribution Function - 050 / weighted by ionization potential	RDF descriptors	Weighted by ionization potential
2002	RDF055i	Radial Distribution Function - 055 / weighted by ionization potential	RDF descriptors	Weighted by ionization potential
2003	RDF060i	Radial Distribution Function - 060 / weighted by ionization potential	RDF descriptors	Weighted by ionization potential
2004	RDF065i	Radial Distribution Function - 065 / weighted by ionization potential	RDF descriptors	Weighted by ionization potential
2005	RDF070i	Radial Distribution Function - 070 / weighted by ionization potential	RDF descriptors	Weighted by ionization potential
2006	RDF075i	Radial Distribution Function - 075 / weighted by ionization potential	RDF descriptors	Weighted by ionization potential
2007	RDF080i	Radial Distribution Function - 080 / weighted by ionization potential	RDF descriptors	Weighted by ionization potential
2008	RDF085i	Radial Distribution Function - 085 / weighted by ionization potential	RDF descriptors	Weighted by ionization potential
2009	RDF090i	Radial Distribution Function - 090 / weighted by ionization potential	RDF descriptors	Weighted by ionization potential
2010	RDF095i	Radial Distribution Function - 095 / weighted by ionization potential	RDF descriptors	Weighted by ionization potential
2011	RDF100i	Radial Distribution Function - 100 / weighted by ionization potential	RDF descriptors	Weighted by ionization potential
2012	RDF105i	Radial Distribution Function - 105 / weighted by ionization potential	RDF descriptors	Weighted by ionization potential
2013	RDF110i	Radial Distribution Function - 110 / weighted by ionization potential	RDF descriptors	Weighted by ionization potential
2014	RDF115i	Radial Distribution Function - 115 / weighted by ionization potential	RDF descriptors	Weighted by ionization potential
2015	RDF120i	Radial Distribution Function - 120 / weighted by ionization potential	RDF descriptors	Weighted by ionization potential

2016	RDF125i	Radial Distribution Function - 125 / weighted by ionization potential	RDF descriptors	Weighted by ionization potential
2017	RDF130i	Radial Distribution Function - 130 / weighted by ionization potential	RDF descriptors	Weighted by ionization potential
2018	RDF135i	Radial Distribution Function - 135 / weighted by ionization potential	RDF descriptors	Weighted by ionization potential
2019	RDF140i	Radial Distribution Function - 140 / weighted by ionization potential	RDF descriptors	Weighted by ionization potential
2020	RDF145i	Radial Distribution Function - 145 / weighted by ionization potential	RDF descriptors	Weighted by ionization potential
2021	RDF150i	Radial Distribution Function - 150 / weighted by ionization potential	RDF descriptors	Weighted by ionization potential
2022	RDF155i	Radial Distribution Function - 155 / weighted by ionization potential	RDF descriptors	Weighted by ionization potential
2023	RDF010s	Radial Distribution Function - 010 / weighted by I-state	RDF descriptors	Weighted by I-state
2024	RDF015s	Radial Distribution Function - 015 / weighted by I-state	RDF descriptors	Weighted by I-state
2025	RDF020s	Radial Distribution Function - 020 / weighted by I-state	RDF descriptors	Weighted by I-state
2026	RDF025s	Radial Distribution Function - 025 / weighted by I-state	RDF descriptors	Weighted by I-state
2027	RDF030s	Radial Distribution Function - 030 / weighted by I-state	RDF descriptors	Weighted by I-state
2028	RDF035s	Radial Distribution Function - 035 / weighted by I-state	RDF descriptors	Weighted by I-state
2029	RDF040s	Radial Distribution Function - 040 / weighted by I-state	RDF descriptors	Weighted by I-state
2030	RDF045s	Radial Distribution Function - 045 / weighted by I-state	RDF descriptors	Weighted by I-state
2031	RDF050s	Radial Distribution Function - 050 / weighted by I-state	RDF descriptors	Weighted by I-state
2032	RDF055s	Radial Distribution Function - 055 / weighted by I-state	RDF descriptors	Weighted by I-state
2033	RDF060s	Radial Distribution Function - 060 / weighted by I-state	RDF descriptors	Weighted by I-state
2034	RDF065s	Radial Distribution Function - 065 / weighted by I-state	RDF descriptors	Weighted by I-state
2035	RDF070s	Radial Distribution Function - 070 / weighted by I-state	RDF descriptors	Weighted by I-state

2036	RDF075s	Radial Distribution Function - 075 / weighted by I-state	RDF descriptors	Weighted by I-state
2037	RDF080s	Radial Distribution Function - 080 / weighted by I-state	RDF descriptors	Weighted by I-state
2038	RDF085s	Radial Distribution Function - 085 / weighted by I-state	RDF descriptors	Weighted by I-state
2039	RDF090s	Radial Distribution Function - 090 / weighted by I-state	RDF descriptors	Weighted by I-state
2040	RDF095s	Radial Distribution Function - 095 / weighted by I-state	RDF descriptors	Weighted by I-state
2041	RDF100s	Radial Distribution Function - 100 / weighted by I-state	RDF descriptors	Weighted by I-state
2042	RDF105s	Radial Distribution Function - 105 / weighted by I-state	RDF descriptors	Weighted by I-state
2043	RDF110s	Radial Distribution Function - 110 / weighted by I-state	RDF descriptors	Weighted by I-state
2044	RDF115s	Radial Distribution Function - 115 / weighted by I-state	RDF descriptors	Weighted by I-state
2045	RDF120s	Radial Distribution Function - 120 / weighted by I-state	RDF descriptors	Weighted by I-state
2046	RDF125s	Radial Distribution Function - 125 / weighted by I-state	RDF descriptors	Weighted by I-state
2047	RDF130s	Radial Distribution Function - 130 / weighted by I-state	RDF descriptors	Weighted by I-state
2048	RDF135s	Radial Distribution Function - 135 / weighted by I-state	RDF descriptors	Weighted by I-state
2049	RDF140s	Radial Distribution Function - 140 / weighted by I-state	RDF descriptors	Weighted by I-state
2050	RDF145s	Radial Distribution Function - 145 / weighted by I-state	RDF descriptors	Weighted by I-state
2051	RDF150s	Radial Distribution Function - 150 / weighted by I-state	RDF descriptors	Weighted by I-state
2052	RDF155s	Radial Distribution Function - 155 / weighted by I-state	RDF descriptors	Weighted by I-state
2053	Mor01u	signal 01 / unweighted	3D-MoRSE descriptors	Unweighted
2054	Mor02u	signal 02 / unweighted	3D-MoRSE descriptors	Unweighted
2055	Mor03u	signal 03 / unweighted	3D-MoRSE descriptors	Unweighted

2056	Mor04u	signal 04 / unweighted	3D-MoRSE descriptors	Unweighted
2057	Mor05u	signal 05 / unweighted	3D-MoRSE descriptors	Unweighted
2058	Mor06u	signal 06 / unweighted	3D-MoRSE descriptors	Unweighted
2059	Mor07u	signal 07 / unweighted	3D-MoRSE descriptors	Unweighted
2060	Mor08u	signal 08 / unweighted	3D-MoRSE descriptors	Unweighted
2061	Mor09u	signal 09 / unweighted	3D-MoRSE descriptors	Unweighted
2062	Mor10u	signal 10 / unweighted	3D-MoRSE descriptors	Unweighted
2063	Mor11u	signal 11 / unweighted	3D-MoRSE descriptors	Unweighted
2064	Mor12u	signal 12 / unweighted	3D-MoRSE descriptors	Unweighted
2065	Mor13u	signal 13 / unweighted	3D-MoRSE descriptors	Unweighted
2066	Mor14u	signal 14 / unweighted	3D-MoRSE descriptors	Unweighted
2067	Mor15u	signal 15 / unweighted	3D-MoRSE descriptors	Unweighted
2068	Mor16u	signal 16 / unweighted	3D-MoRSE descriptors	Unweighted
2069	Mor17u	signal 17 / unweighted	3D-MoRSE descriptors	Unweighted
2070	Mor18u	signal 18 / unweighted	3D-MoRSE descriptors	Unweighted
2071	Mor19u	signal 19 / unweighted	3D-MoRSE descriptors	Unweighted
2072	Mor20u	signal 20 / unweighted	3D-MoRSE descriptors	Unweighted
2073	Mor21u	signal 21 / unweighted	3D-MoRSE descriptors	Unweighted
2074	Mor22u	signal 22 / unweighted	3D-MoRSE descriptors	Unweighted
2075	Mor23u	signal 23 / unweighted	3D-MoRSE descriptors	Unweighted

2076	Mor24u	signal 24 / unweighted	3D-MoRSE descriptors	Unweighted
2077	Mor25u	signal 25 / unweighted	3D-MoRSE descriptors	Unweighted
2078	Mor26u	signal 26 / unweighted	3D-MoRSE descriptors	Unweighted
2079	Mor27u	signal 27 / unweighted	3D-MoRSE descriptors	Unweighted
2080	Mor28u	signal 28 / unweighted	3D-MoRSE descriptors	Unweighted
2081	Mor29u	signal 29 / unweighted	3D-MoRSE descriptors	Unweighted
2082	Mor30u	signal 30 / unweighted	3D-MoRSE descriptors	Unweighted
2083	Mor31u	signal 31 / unweighted	3D-MoRSE descriptors	Unweighted
2084	Mor32u	signal 32 / unweighted	3D-MoRSE descriptors	Unweighted
2085	Mor01m	signal 01 / weighted by mass	3D-MoRSE descriptors	Weighted by mass
2086	Mor02m	signal 02 / weighted by mass	3D-MoRSE descriptors	Weighted by mass
2087	Mor03m	signal 03 / weighted by mass	3D-MoRSE descriptors	Weighted by mass
2088	Mor04m	signal 04 / weighted by mass	3D-MoRSE descriptors	Weighted by mass
2089	Mor05m	signal 05 / weighted by mass	3D-MoRSE descriptors	Weighted by mass
2090	Mor06m	signal 06 / weighted by mass	3D-MoRSE descriptors	Weighted by mass
2091	Mor07m	signal 07 / weighted by mass	3D-MoRSE descriptors	Weighted by mass
2092	Mor08m	signal 08 / weighted by mass	3D-MoRSE descriptors	Weighted by mass
2093	Mor09m	signal 09 / weighted by mass	3D-MoRSE descriptors	Weighted by mass
2094	Mor10m	signal 10 / weighted by mass	3D-MoRSE descriptors	Weighted by mass
2095	Mor11m	signal 11 / weighted by mass	3D-MoRSE descriptors	Weighted by mass

2096	Mor12m	signal 12 / weighted by mass	3D-MoRSE descriptors	Weighted by mass
2097	Mor13m	signal 13 / weighted by mass	3D-MoRSE descriptors	Weighted by mass
2098	Mor14m	signal 14 / weighted by mass	3D-MoRSE descriptors	Weighted by mass
2099	Mor15m	signal 15 / weighted by mass	3D-MoRSE descriptors	Weighted by mass
2100	Mor16m	signal 16 / weighted by mass	3D-MoRSE descriptors	Weighted by mass
2101	Mor17m	signal 17 / weighted by mass	3D-MoRSE descriptors	Weighted by mass
2102	Mor18m	signal 18 / weighted by mass	3D-MoRSE descriptors	Weighted by mass
2103	Mor19m	signal 19 / weighted by mass	3D-MoRSE descriptors	Weighted by mass
2104	Mor20m	signal 20 / weighted by mass	3D-MoRSE descriptors	Weighted by mass
2105	Mor21m	signal 21 / weighted by mass	3D-MoRSE descriptors	Weighted by mass
2106	Mor22m	signal 22 / weighted by mass	3D-MoRSE descriptors	Weighted by mass
2107	Mor23m	signal 23 / weighted by mass	3D-MoRSE descriptors	Weighted by mass
2108	Mor24m	signal 24 / weighted by mass	3D-MoRSE descriptors	Weighted by mass
2109	Mor25m	signal 25 / weighted by mass	3D-MoRSE descriptors	Weighted by mass
2110	Mor26m	signal 26 / weighted by mass	3D-MoRSE descriptors	Weighted by mass
2111	Mor27m	signal 27 / weighted by mass	3D-MoRSE descriptors	Weighted by mass
2112	Mor28m	signal 28 / weighted by mass	3D-MoRSE descriptors	Weighted by mass
2113	Mor29m	signal 29 / weighted by mass	3D-MoRSE descriptors	Weighted by mass
2114	Mor30m	signal 30 / weighted by mass	3D-MoRSE descriptors	Weighted by mass
2115	Mor31m	signal 31 / weighted by mass	3D-MoRSE descriptors	Weighted by mass

2116	Mor32m	signal 32 / weighted by mass	3D-MoRSE descriptors	Weighted by mass
2117	Mor01v	signal 01 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume
2118	Mor02v	signal 02 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume
2119	Mor03v	signal 03 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume
2120	Mor04v	signal 04 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume
2121	Mor05v	signal 05 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume
2122	Mor06v	signal 06 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume
2123	Mor07v	signal 07 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume
2124	Mor08v	signal 08 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume
2125	Mor09v	signal 09 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume
2126	Mor10v	signal 10 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume
2127	Mor11v	signal 11 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume
2128	Mor12v	signal 12 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume
2129	Mor13v	signal 13 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume
2130	Mor14v	signal 14 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume
2131	Mor15v	signal 15 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume
2132	Mor16v	signal 16 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume
2133	Mor17v	signal 17 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume
2134	Mor18v	signal 18 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume
2135	Mor19v	signal 19 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume

2136	Mor20v	signal 20 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume
2137	Mor21v	signal 21 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume
2138	Mor22v	signal 22 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume
2139	Mor23v	signal 23 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume
2140	Mor24v	signal 24 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume
2141	Mor25v	signal 25 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume
2142	Mor26v	signal 26 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume
2143	Mor27v	signal 27 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume
2144	Mor28v	signal 28 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume
2145	Mor29v	signal 29 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume
2146	Mor30v	signal 30 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume
2147	Mor31v	signal 31 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume
2148	Mor32v	signal 32 / weighted by van der Waals volume	3D-MoRSE descriptors	Weighted by van der Waals volume
2149	Mor01e	signal 01 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity
2150	Mor02e	signal 02 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity
2151	Mor03e	signal 03 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity
2152	Mor04e	signal 04 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity
2153	Mor05e	signal 05 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity

2154	Mor06e	signal 06 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity
2155	Mor07e	signal 07 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity
2156	Mor08e	signal 08 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity
2157	Mor09e	signal 09 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity
2158	Mor10e	signal 10 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity
2159	Mor11e	signal 11 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity
2160	Mor12e	signal 12 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity
2161	Mor13e	signal 13 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity
2162	Mor14e	signal 14 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity
2163	Mor15e	signal 15 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity
2164	Mor16e	signal 16 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity
2165	Mor17e	signal 17 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity
2166	Mor18e	signal 18 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity
2167	Mor19e	signal 19 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity
2168	Mor20e	signal 20 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity

2169	Mor21e	signal 21 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity
2170	Mor22e	signal 22 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity
2171	Mor23e	signal 23 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity
2172	Mor24e	signal 24 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity
2173	Mor25e	signal 25 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity
2174	Mor26e	signal 26 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity
2175	Mor27e	signal 27 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity
2176	Mor28e	signal 28 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity
2177	Mor29e	signal 29 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity
2178	Mor30e	signal 30 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity
2179	Mor31e	signal 31 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity
2180	Mor32e	signal 32 / weighted by Sanderson electronegativity	3D-MoRSE descriptors	Weighted by Sanderson electronegativity
2181	Mor01p	signal 01 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability
2182	Mor02p	signal 02 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability
2183	Mor03p	signal 03 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability
2184	Mor04p	signal 04 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability

2185	Mor05p	signal 05 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability
2186	Mor06p	signal 06 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability
2187	Mor07p	signal 07 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability
2188	Mor08p	signal 08 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability
2189	Mor09p	signal 09 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability
2190	Mor10p	signal 10 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability
2191	Mor11p	signal 11 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability
2192	Mor12p	signal 12 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability
2193	Mor13p	signal 13 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability
2194	Mor14p	signal 14 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability
2195	Mor15p	signal 15 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability
2196	Mor16p	signal 16 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability
2197	Mor17p	signal 17 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability
2198	Mor18p	signal 18 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability
2199	Mor19p	signal 19 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability
2200	Mor20p	signal 20 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability
2201	Mor21p	signal 21 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability
2202	Mor22p	signal 22 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability
2203	Mor23p	signal 23 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability
2204	Mor24p	signal 24 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability

2205	Mor25p	signal 25 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability
2206	Mor26p	signal 26 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability
2207	Mor27p	signal 27 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability
2208	Mor28p	signal 28 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability
2209	Mor29p	signal 29 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability
2210	Mor30p	signal 30 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability
2211	Mor31p	signal 31 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability
2212	Mor32p	signal 32 / weighted by polarizability	3D-MoRSE descriptors	Weighted by polarizability
2213	Mor01i	signal 01 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential
2214	Mor02i	signal 02 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential
2215	Mor03i	signal 03 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential
2216	Mor04i	signal 04 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential
2217	Mor05i	signal 05 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential
2218	Mor06i	signal 06 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential
2219	Mor07i	signal 07 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential
2220	Mor08i	signal 08 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential
2221	Mor09i	signal 09 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential
2222	Mor10i	signal 10 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential
2223	Mor11i	signal 11 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential
2224	Mor12i	signal 12 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential

2225	Mor13i	signal 13 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential
2226	Mor14i	signal 14 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential
2227	Mor15i	signal 15 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential
2228	Mor16i	signal 16 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential
2229	Mor17i	signal 17 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential
2230	Mor18i	signal 18 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential
2231	Mor19i	signal 19 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential
2232	Mor20i	signal 20 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential
2233	Mor21i	signal 21 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential
2234	Mor22i	signal 22 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential
2235	Mor23i	signal 23 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential
2236	Mor24i	signal 24 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential
2237	Mor25i	signal 25 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential
2238	Mor26i	signal 26 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential
2239	Mor27i	signal 27 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential
2240	Mor28i	signal 28 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential
2241	Mor29i	signal 29 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential
2242	Mor30i	signal 30 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential
2243	Mor31i	signal 31 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential
2244	Mor32i	signal 32 / weighted by ionization potential	3D-MoRSE descriptors	Weighted by ionization potential

2245	Mor01s	signal 01 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state
2246	Mor02s	signal 02 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state
2247	Mor03s	signal 03 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state
2248	Mor04s	signal 04 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state
2249	Mor05s	signal 05 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state
2250	Mor06s	signal 06 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state
2251	Mor07s	signal 07 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state
2252	Mor08s	signal 08 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state
2253	Mor09s	signal 09 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state
2254	Mor10s	signal 10 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state
2255	Mor11s	signal 11 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state
2256	Mor12s	signal 12 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state
2257	Mor13s	signal 13 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state
2258	Mor14s	signal 14 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state
2259	Mor15s	signal 15 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state
2260	Mor16s	signal 16 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state
2261	Mor17s	signal 17 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state
2262	Mor18s	signal 18 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state
2263	Mor19s	signal 19 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state
2264	Mor20s	signal 20 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state

2265	Mor21s	signal 21 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state
2266	Mor22s	signal 22 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state
2267	Mor23s	signal 23 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state
2268	Mor24s	signal 24 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state
2269	Mor25s	signal 25 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state
2270	Mor26s	signal 26 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state
2271	Mor27s	signal 27 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state
2272	Mor28s	signal 28 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state
2273	Mor29s	signal 29 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state
2274	Mor30s	signal 30 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state
2275	Mor31s	signal 31 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state
2276	Mor32s	signal 32 / weighted by I-state	3D-MoRSE descriptors	Weighted by I-state
2277	L1u	1st component size directional WHIM index / unweighted	WHIM descriptors	Directional descriptors
2278	L2u	2nd component size directional WHIM index / unweighted	WHIM descriptors	Directional descriptors
2279	L3u	3rd component size directional WHIM index / unweighted	WHIM descriptors	Directional descriptors
2280	P1u	1st component shape directional WHIM index / unweighted	WHIM descriptors	Directional descriptors
2281	P2u	2nd component shape directional WHIM index / unweighted	WHIM descriptors	Directional descriptors
2282	G1u	1st component symmetry directional WHIM index / unweighted	WHIM descriptors	Directional descriptors
2283	G2u	2nd component symmetry directional WHIM index / unweighted	WHIM descriptors	Directional descriptors
2284	G3u	3rd component symmetry directional WHIM index / unweighted	WHIM descriptors	Directional descriptors

2285	E1u	1st component accessibility directional WHIM index / unweighted	WHIM descriptors	Directional descriptors
2286	E2u	2nd component accessibility directional WHIM index / unweighted	WHIM descriptors	Directional descriptors
2287	E3u	3rd component accessibility directional WHIM index / unweighted	WHIM descriptors	Directional descriptors
2288	L1m	1st component size directional WHIM index / weighted by mass	WHIM descriptors	Directional descriptors
2289	L2m	2nd component size directional WHIM index / weighted by mass	WHIM descriptors	Directional descriptors
2290	L3m	3rd component size directional WHIM index / weighted by mass	WHIM descriptors	Directional descriptors
2291	P1m	1st component shape directional WHIM index / weighted by mass	WHIM descriptors	Directional descriptors
2292	P2m	2nd component shape directional WHIM index / weighted by mass	WHIM descriptors	Directional descriptors
2293	G1m	1st component symmetry directional WHIM index / weighted by mass	WHIM descriptors	Directional descriptors
2294	G2m	2nd component symmetry directional WHIM index / weighted by mass	WHIM descriptors	Directional descriptors
2295	G3m	3rd component symmetry directional WHIM index / weighted by mass	WHIM descriptors	Directional descriptors
2296	E1m	1st component accessibility directional WHIM index / weighted by mass	WHIM descriptors	Directional descriptors
2297	E2m	2nd component accessibility directional WHIM index / weighted by mass	WHIM descriptors	Directional descriptors
2298	E3m	3rd component accessibility directional WHIM index / weighted by mass	WHIM descriptors	Directional descriptors
2299	L1v	1st component size directional WHIM index / weighted by van der Waals volume	WHIM descriptors	Directional descriptors
2300	L2v	2nd component size directional WHIM index / weighted by van der Waals volume	WHIM descriptors	Directional descriptors
2301	L3v	3rd component size directional WHIM index / weighted by van der Waals volume	WHIM descriptors	Directional descriptors
2302	P1v	1st component shape directional WHIM index / weighted by van der Waals volume	WHIM descriptors	Directional descriptors
2303	P2v	2nd component shape directional WHIM index / weighted by van der Waals volume	WHIM descriptors	Directional descriptors
2304	G1v	1st component symmetry directional WHIM index / weighted by van der Waals volume	WHIM descriptors	Directional descriptors

2305	G2v	2nd component symmetry directional WHIM index / weighted by van der Waals volume	WHIM descriptors	Directional descriptors
2306	G3v	3rd component symmetry directional WHIM index / weighted by van der Waals volume	WHIM descriptors	Directional descriptors
2307	E1v	1st component accessibility directional WHIM index / weighted by van der Waals volume	WHIM descriptors	Directional descriptors
2308	E2v	2nd component accessibility directional WHIM index / weighted by van der Waals volume	WHIM descriptors	Directional descriptors
2309	E3v	3rd component accessibility directional WHIM index / weighted by van der Waals volume	WHIM descriptors	Directional descriptors
2310	L1e	1st component size directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors	Directional descriptors
2311	L2e	2nd component size directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors	Directional descriptors
2312	L3e	3rd component size directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors	Directional descriptors
2313	P1e	1st component shape directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors	Directional descriptors
2314	P2e	2nd component shape directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors	Directional descriptors
2315	G1e	1st component symmetry directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors	Directional descriptors
2316	G2e	2nd component symmetry directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors	Directional descriptors
2317	G3e	3rd component symmetry directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors	Directional descriptors
2318	E1e	1st component accessibility directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors	Directional descriptors
2319	E2e	2nd component accessibility directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors	Directional descriptors

2320	E3e	3rd component accessibility directional WHIM index / weighted by Sanderson electronegativity	WHIM descriptors	Directional descriptors
2321	L1p	1st component size directional WHIM index / weighted by polarizability	WHIM descriptors	Directional descriptors
2322	L2p	2nd component size directional WHIM index / weighted by polarizability	WHIM descriptors	Directional descriptors
2323	L3p	3rd component size directional WHIM index / weighted by polarizability	WHIM descriptors	Directional descriptors
2324	P1p	1st component shape directional WHIM index / weighted by polarizability	WHIM descriptors	Directional descriptors
2325	P2p	2nd component shape directional WHIM index / weighted by polarizability	WHIM descriptors	Directional descriptors
2326	G1p	1st component symmetry directional WHIM index / weighted by polarizability	WHIM descriptors	Directional descriptors
2327	G2p	2nd component symmetry directional WHIM index / weighted by polarizability	WHIM descriptors	Directional descriptors
2328	G3p	3rd component symmetry directional WHIM index / weighted by polarizability	WHIM descriptors	Directional descriptors
2329	E1p	1st component accessibility directional WHIM index / weighted by polarizability	WHIM descriptors	Directional descriptors
2330	E2p	2nd component accessibility directional WHIM index / weighted by polarizability	WHIM descriptors	Directional descriptors
2331	E3p	3rd component accessibility directional WHIM index / weighted by polarizability	WHIM descriptors	Directional descriptors
2332	L1i	1st component size directional WHIM index / weighted by ionization potential	WHIM descriptors	Directional descriptors
2333	L2i	2nd component size directional WHIM index / weighted by ionization potential	WHIM descriptors	Directional descriptors
2334	L3i	3rd component size directional WHIM index / weighted by ionization potential	WHIM descriptors	Directional descriptors
2335	P1i	1st component shape directional WHIM index / weighted by ionization potential	WHIM descriptors	Directional descriptors
2336	P2i	2nd component shape directional WHIM index / weighted by ionization potential	WHIM descriptors	Directional descriptors
2337	G1i	1st component symmetry directional WHIM index / weighted by ionization potential	WHIM descriptors	Directional descriptors
2338	G2i	2nd component symmetry directional WHIM index / weighted by ionization potential	WHIM descriptors	Directional descriptors

2339	G3i	3rd component symmetry directional WHIM index / weighted by ionization potential	WHIM descriptors	Directional descriptors
2340	E1i	1st component accessibility directional WHIM index / weighted by ionization potential	WHIM descriptors	Directional descriptors
2341	E2i	2nd component accessibility directional WHIM index / weighted by ionization potential	WHIM descriptors	Directional descriptors
2342	E3i	3rd component accessibility directional WHIM index / weighted by ionization potential	WHIM descriptors	Directional descriptors
2343	L1s	1st component size directional WHIM index / weighted by I-state	WHIM descriptors	Directional descriptors
2344	L2s	2nd component size directional WHIM index / weighted by I-state	WHIM descriptors	Directional descriptors
2345	L3s	3rd component size directional WHIM index / weighted by I-state	WHIM descriptors	Directional descriptors
2346	P1s	1st component shape directional WHIM index / weighted by I-state	WHIM descriptors	Directional descriptors
2347	P2s	2nd component shape directional WHIM index / weighted by I-state	WHIM descriptors	Directional descriptors
2348	G1s	1st component symmetry directional WHIM index / weighted by I-state	WHIM descriptors	Directional descriptors
2349	G2s	2nd component symmetry directional WHIM index / weighted by I-state	WHIM descriptors	Directional descriptors
2350	G3s	3rd component symmetry directional WHIM index / weighted by I-state	WHIM descriptors	Directional descriptors
2351	E1s	1st component accessibility directional WHIM index / weighted by I-state	WHIM descriptors	Directional descriptors
2352	E2s	2nd component accessibility directional WHIM index / weighted by I-state	WHIM descriptors	Directional descriptors
2353	E3s	3rd component accessibility directional WHIM index / weighted by I-state	WHIM descriptors	Directional descriptors
2354	Tu	T total size index / unweighted	WHIM descriptors	Global descriptors
2355	Tm	T total size index / weighted by mass	WHIM descriptors	Global descriptors
2356	Tv	T total size index / weighted by van der Waals volume	WHIM descriptors	Global descriptors
2357	Te	T total size index / weighted by Sanderson electronegativity	WHIM descriptors	Global descriptors

2358	Tp	T total size index / weighted by polarizability	WHIM descriptors	Global descriptors
2359	Ti	T total size index / weighted by ionization potential	WHIM descriptors	Global descriptors
2360	Ts	T total size index / weighted by I-state	WHIM descriptors	Global descriptors
2361	Au	A total size index / unweighted	WHIM descriptors	Global descriptors
2362	Am	A total size index / weighted by mass	WHIM descriptors	Global descriptors
2363	Av	A total size index / weighted by van der Waals volume	WHIM descriptors	Global descriptors
2364	Ae	A total size index / weighted by Sanderson electronegativity	WHIM descriptors	Global descriptors
2365	Ap	A total size index / weighted by polarizability	WHIM descriptors	Global descriptors
2366	Ai	A total size index / weighted by ionization potential	WHIM descriptors	Global descriptors
2367	As	A total size index / weighted by I-state	WHIM descriptors	Global descriptors
2368	Gu	total symmetry index / unweighted	WHIM descriptors	Global descriptors
2369	Gm	total symmetry index / weighted by mass	WHIM descriptors	Global descriptors
2370	Ku	K global shape index / unweighted	WHIM descriptors	Global descriptors
2371	Km	K global shape index / weighted by mass	WHIM descriptors	Global descriptors
2372	Kv	K global shape index / weighted by van der Waals volume	WHIM descriptors	Global descriptors
2373	Ke	K global shape index / weighted by Sanderson electronegativity	WHIM descriptors	Global descriptors
2374	Kp	K global shape index / weighted by polarizability	WHIM descriptors	Global descriptors
2375	Ki	K global shape index / weighted by ionization potential	WHIM descriptors	Global descriptors
2376	Ks	K global shape index / weighted by I-state	WHIM descriptors	Global descriptors
2377	Du	D total accessibility index / unweighted	WHIM descriptors	Global descriptors

2378	Dm	D total accessibility index / weighted by mass	WHIM descriptors	Global descriptors
2379	Dv	D total accessibility index / weighted by van der Waals volume	WHIM descriptors	Global descriptors
2380	De	D total accessibility index / weighted by Sanderson electronegativity	WHIM descriptors	Global descriptors
2381	Dp	D total accessibility index / weighted by polarizability	WHIM descriptors	Global descriptors
2382	Di	D total accessibility index / weighted by ionization potential	WHIM descriptors	Global descriptors
2383	Ds	D total accessibility index / weighted by I-state	WHIM descriptors	Global descriptors
2384	Vu	V total size index / unweighted	WHIM descriptors	Global descriptors
2385	Vm	V total size index / weighted by mass	WHIM descriptors	Global descriptors
2386	Vv	V total size index / weighted by van der Waals volume	WHIM descriptors	Global descriptors
2387	Ve	V total size index / weighted by Sanderson electronegativity	WHIM descriptors	Global descriptors
2388	Vp	V total size index / weighted by polarizability	WHIM descriptors	Global descriptors
2389	Vi	V total size index / weighted by ionization potential	WHIM descriptors	Global descriptors
2390	Vs	V total size index / weighted by I-state	WHIM descriptors	Global descriptors
2391	ITH	total information content on the leverage equality	GETAWAY descriptors	Basic descriptors
2392	ISH	standardized information content on the leverage equality	GETAWAY descriptors	Basic descriptors
2393	HIC	mean information content on the leverage magnitude	GETAWAY descriptors	Basic descriptors
2394	HGM	geometric mean on the leverage magnitude	GETAWAY descriptors	Basic descriptors
2395	H0u	H autocorrelation of lag 0 / unweighted	GETAWAY descriptors	H-indices
2396	H1u	H autocorrelation of lag 1 / unweighted	GETAWAY descriptors	H-indices
2397	H2u	H autocorrelation of lag 2 / unweighted	GETAWAY descriptors	H-indices

2398	H3u	H autocorrelation of lag 3 / unweighted	GETAWAY descriptors	H-indices
2399	H4u	H autocorrelation of lag 4 / unweighted	GETAWAY descriptors	H-indices
2400	H5u	H autocorrelation of lag 5 / unweighted	GETAWAY descriptors	H-indices
2401	H6u	H autocorrelation of lag 6 / unweighted	GETAWAY descriptors	H-indices
2402	H7u	H autocorrelation of lag 7 / unweighted	GETAWAY descriptors	H-indices
2403	H8u	H autocorrelation of lag 8 / unweighted	GETAWAY descriptors	H-indices
2404	HTu	H total index / unweighted	GETAWAY descriptors	H-indices
2405	HATS0u	leverage-weighted autocorrelation of lag 0 / unweighted	GETAWAY descriptors	H-indices
2406	HATS1u	leverage-weighted autocorrelation of lag 1 / unweighted	GETAWAY descriptors	H-indices
2407	HATS2u	leverage-weighted autocorrelation of lag 2 / unweighted	GETAWAY descriptors	H-indices
2408	HATS3u	leverage-weighted autocorrelation of lag 3 / unweighted	GETAWAY descriptors	H-indices
2409	HATS4u	leverage-weighted autocorrelation of lag 4 / unweighted	GETAWAY descriptors	H-indices
2410	HATS5u	leverage-weighted autocorrelation of lag 5 / unweighted	GETAWAY descriptors	H-indices
2411	HATS6u	leverage-weighted autocorrelation of lag 6 / unweighted	GETAWAY descriptors	H-indices
2412	HATS7u	leverage-weighted autocorrelation of lag 7 / unweighted	GETAWAY descriptors	H-indices
2413	HATS8u	leverage-weighted autocorrelation of lag 8 / unweighted	GETAWAY descriptors	H-indices
2414	HATSu	leverage-weighted total index / unweighted	GETAWAY descriptors	H-indices
2415	H0m	H autocorrelation of lag 0 / weighted by mass	GETAWAY descriptors	H-indices
2416	H1m	H autocorrelation of lag 1 / weighted by mass	GETAWAY descriptors	H-indices
2417	H2m	H autocorrelation of lag 2 / weighted by mass	GETAWAY descriptors	H-indices

2418	H3m	H autocorrelation of lag 3 / weighted by mass	GETAWAY descriptors	H-indices
2419	H4m	H autocorrelation of lag 4 / weighted by mass	GETAWAY descriptors	H-indices
2420	H5m	H autocorrelation of lag 5 / weighted by mass	GETAWAY descriptors	H-indices
2421	H6m	H autocorrelation of lag 6 / weighted by mass	GETAWAY descriptors	H-indices
2422	H7m	H autocorrelation of lag 7 / weighted by mass	GETAWAY descriptors	H-indices
2423	H8m	H autocorrelation of lag 8 / weighted by mass	GETAWAY descriptors	H-indices
2424	HTm	H total index / weighted by mass	GETAWAY descriptors	H-indices
2425	HATS0m	leverage-weighted autocorrelation of lag 0 / weighted by mass	GETAWAY descriptors	H-indices
2426	HATS1m	leverage-weighted autocorrelation of lag 1 / weighted by mass	GETAWAY descriptors	H-indices
2427	HATS2m	leverage-weighted autocorrelation of lag 2 / weighted by mass	GETAWAY descriptors	H-indices
2428	HATS3m	leverage-weighted autocorrelation of lag 3 / weighted by mass	GETAWAY descriptors	H-indices
2429	HATS4m	leverage-weighted autocorrelation of lag 4 / weighted by mass	GETAWAY descriptors	H-indices
2430	HATS5m	leverage-weighted autocorrelation of lag 5 / weighted by mass	GETAWAY descriptors	H-indices
2431	HATS6m	leverage-weighted autocorrelation of lag 6 / weighted by mass	GETAWAY descriptors	H-indices
2432	HATS7m	leverage-weighted autocorrelation of lag 7 / weighted by mass	GETAWAY descriptors	H-indices
2433	HATS8m	leverage-weighted autocorrelation of lag 8 / weighted by mass	GETAWAY descriptors	H-indices
2434	HATSm	leverage-weighted total index / weighted by mass	GETAWAY descriptors	H-indices
2435	H0v	H autocorrelation of lag 0 / weighted by van der Waals volume	GETAWAY descriptors	H-indices
2436	H1v	H autocorrelation of lag 1 / weighted by van der Waals volume	GETAWAY descriptors	H-indices
2437	H2v	H autocorrelation of lag 2 / weighted by van der Waals volume	GETAWAY descriptors	H-indices

2438	H3v	H autocorrelation of lag 3 / weighted by van der Waals volume	GETAWAY descriptors	H-indices
2439	H4v	H autocorrelation of lag 4 / weighted by van der Waals volume	GETAWAY descriptors	H-indices
2440	H5v	H autocorrelation of lag 5 / weighted by van der Waals volume	GETAWAY descriptors	H-indices
2441	H6v	H autocorrelation of lag 6 / weighted by van der Waals volume	GETAWAY descriptors	H-indices
2442	H7v	H autocorrelation of lag 7 / weighted by van der Waals volume	GETAWAY descriptors	H-indices
2443	H8v	H autocorrelation of lag 8 / weighted by van der Waals volume	GETAWAY descriptors	H-indices
2444	HTv	H total index / weighted by van der Waals volume	GETAWAY descriptors	H-indices
2445	HATS0v	leverage-weighted autocorrelation of lag 0 / weighted by van der Waals volume	GETAWAY descriptors	H-indices
2446	HATS1v	leverage-weighted autocorrelation of lag 1 / weighted by van der Waals volume	GETAWAY descriptors	H-indices
2447	HATS2v	leverage-weighted autocorrelation of lag 2 / weighted by van der Waals volume	GETAWAY descriptors	H-indices
2448	HATS3v	leverage-weighted autocorrelation of lag 3 / weighted by van der Waals volume	GETAWAY descriptors	H-indices
2449	HATS4v	leverage-weighted autocorrelation of lag 4 / weighted by van der Waals volume	GETAWAY descriptors	H-indices
2450	HATS5v	leverage-weighted autocorrelation of lag 5 / weighted by van der Waals volume	GETAWAY descriptors	H-indices
2451	HATS6v	leverage-weighted autocorrelation of lag 6 / weighted by van der Waals volume	GETAWAY descriptors	H-indices
2452	HATS7v	leverage-weighted autocorrelation of lag 7 / weighted by van der Waals volume	GETAWAY descriptors	H-indices
2453	HATS8v	leverage-weighted autocorrelation of lag 8 / weighted by van der Waals volume	GETAWAY descriptors	H-indices
2454	HATSv	leverage-weighted total index / weighted by van der Waals volume	GETAWAY descriptors	H-indices
2455	H0e	H autocorrelation of lag 0 / weighted by Sanderson electronegativity	GETAWAY descriptors	H-indices
2456	H1e	H autocorrelation of lag 1 / weighted by Sanderson electronegativity	GETAWAY descriptors	H-indices
2457	H2e	H autocorrelation of lag 2 / weighted by Sanderson electronegativity	GETAWAY descriptors	H-indices

2458	H3e	H autocorrelation of lag 3 / weighted by Sanderson electronegativity	GETAWAY descriptors	H-indices
2459	H4e	H autocorrelation of lag 4 / weighted by Sanderson electronegativity	GETAWAY descriptors	H-indices
2460	H5e	H autocorrelation of lag 5 / weighted by Sanderson electronegativity	GETAWAY descriptors	H-indices
2461	H6e	H autocorrelation of lag 6 / weighted by Sanderson electronegativity	GETAWAY descriptors	H-indices
2462	H7e	H autocorrelation of lag 7 / weighted by Sanderson electronegativity	GETAWAY descriptors	H-indices
2463	H8e	H autocorrelation of lag 8 / weighted by Sanderson electronegativity	GETAWAY descriptors	H-indices
2464	HTe	H total index / weighted by Sanderson electronegativity	GETAWAY descriptors	H-indices
2465	HATS0e	leverage-weighted autocorrelation of lag 0 / weighted by Sanderson electronegativity	GETAWAY descriptors	H-indices
2466	HATS1e	leverage-weighted autocorrelation of lag 1 / weighted by Sanderson electronegativity	GETAWAY descriptors	H-indices
2467	HATS2e	leverage-weighted autocorrelation of lag 2 / weighted by Sanderson electronegativity	GETAWAY descriptors	H-indices
2468	HATS3e	leverage-weighted autocorrelation of lag 3 / weighted by Sanderson electronegativity	GETAWAY descriptors	H-indices
2469	HATS4e	leverage-weighted autocorrelation of lag 4 / weighted by Sanderson electronegativity	GETAWAY descriptors	H-indices
2470	HATS5e	leverage-weighted autocorrelation of lag 5 / weighted by Sanderson electronegativity	GETAWAY descriptors	H-indices
2471	HATS6e	leverage-weighted autocorrelation of lag 6 / weighted by Sanderson electronegativity	GETAWAY descriptors	H-indices
2472	HATS7e	leverage-weighted autocorrelation of lag 7 / weighted by Sanderson electronegativity	GETAWAY descriptors	H-indices
2473	HATS8e	leverage-weighted autocorrelation of lag 8 / weighted by Sanderson electronegativity	GETAWAY descriptors	H-indices
2474	HATSe	leverage-weighted total index / weighted by Sanderson electronegativity	GETAWAY descriptors	H-indices
2475	H0p	H autocorrelation of lag 0 / weighted by polarizability	GETAWAY descriptors	H-indices
2476	H1p	H autocorrelation of lag 1 / weighted by polarizability	GETAWAY descriptors	H-indices
2477	H2p	H autocorrelation of lag 2 / weighted by polarizability	GETAWAY descriptors	H-indices

2478	H3p	H autocorrelation of lag 3 / weighted by polarizability	GETAWAY descriptors	H-indices
2479	H4p	H autocorrelation of lag 4 / weighted by polarizability	GETAWAY descriptors	H-indices
2480	H5p	H autocorrelation of lag 5 / weighted by polarizability	GETAWAY descriptors	H-indices
2481	H6p	H autocorrelation of lag 6 / weighted by polarizability	GETAWAY descriptors	H-indices
2482	H7p	H autocorrelation of lag 7 / weighted by polarizability	GETAWAY descriptors	H-indices
2483	H8p	H autocorrelation of lag 8 / weighted by polarizability	GETAWAY descriptors	H-indices
2484	HTp	H total index / weighted by polarizability	GETAWAY descriptors	H-indices
2485	HATS0p	leverage-weighted autocorrelation of lag 0 / weighted by polarizability	GETAWAY descriptors	H-indices
2486	HATS1p	leverage-weighted autocorrelation of lag 1 / weighted by polarizability	GETAWAY descriptors	H-indices
2487	HATS2p	leverage-weighted autocorrelation of lag 2 / weighted by polarizability	GETAWAY descriptors	H-indices
2488	HATS3p	leverage-weighted autocorrelation of lag 3 / weighted by polarizability	GETAWAY descriptors	H-indices
2489	HATS4p	leverage-weighted autocorrelation of lag 4 / weighted by polarizability	GETAWAY descriptors	H-indices
2490	HATS5p	leverage-weighted autocorrelation of lag 5 / weighted by polarizability	GETAWAY descriptors	H-indices
2491	HATS6p	leverage-weighted autocorrelation of lag 6 / weighted by polarizability	GETAWAY descriptors	H-indices
2492	HATS7p	leverage-weighted autocorrelation of lag 7 / weighted by polarizability	GETAWAY descriptors	H-indices
2493	HATS8p	leverage-weighted autocorrelation of lag 8 / weighted by polarizability	GETAWAY descriptors	H-indices
2494	HATSp	leverage-weighted total index / weighted by polarizability	GETAWAY descriptors	H-indices
2495	H0i	H autocorrelation of lag 0 / weighted by ionization potential	GETAWAY descriptors	H-indices
2496	H1i	H autocorrelation of lag 1 / weighted by ionization potential	GETAWAY descriptors	H-indices
2497	H2i	H autocorrelation of lag 2 / weighted by ionization potential	GETAWAY descriptors	H-indices

2498	H3i	H autocorrelation of lag 3 / weighted by ionization potential	GETAWAY descriptors	H-indices
2499	H4i	H autocorrelation of lag 4 / weighted by ionization potential	GETAWAY descriptors	H-indices
2500	H5i	H autocorrelation of lag 5 / weighted by ionization potential	GETAWAY descriptors	H-indices
2501	H6i	H autocorrelation of lag 6 / weighted by ionization potential	GETAWAY descriptors	H-indices
2502	H7i	H autocorrelation of lag 7 / weighted by ionization potential	GETAWAY descriptors	H-indices
2503	H8i	H autocorrelation of lag 8 / weighted by ionization potential	GETAWAY descriptors	H-indices
2504	HTi	H total index / weighted by ionization potential	GETAWAY descriptors	H-indices
2505	HATS0i	leverage-weighted autocorrelation of lag 0 / weighted by ionization potential	GETAWAY descriptors	H-indices
2506	HATS1i	leverage-weighted autocorrelation of lag 1 / weighted by ionization potential	GETAWAY descriptors	H-indices
2507	HATS2i	leverage-weighted autocorrelation of lag 2 / weighted by ionization potential	GETAWAY descriptors	H-indices
2508	HATS3i	leverage-weighted autocorrelation of lag 3 / weighted by ionization potential	GETAWAY descriptors	H-indices
2509	HATS4i	leverage-weighted autocorrelation of lag 4 / weighted by ionization potential	GETAWAY descriptors	H-indices
2510	HATS5i	leverage-weighted autocorrelation of lag 5 / weighted by ionization potential	GETAWAY descriptors	H-indices
2511	HATS6i	leverage-weighted autocorrelation of lag 6 / weighted by ionization potential	GETAWAY descriptors	H-indices
2512	HATS7i	leverage-weighted autocorrelation of lag 7 / weighted by ionization potential	GETAWAY descriptors	H-indices
2513	HATS8i	leverage-weighted autocorrelation of lag 8 / weighted by ionization potential	GETAWAY descriptors	H-indices
2514	HATSi	leverage-weighted total index / weighted by ionization potential	GETAWAY descriptors	H-indices
2515	H0s	H autocorrelation of lag 0 / weighted by I-state	GETAWAY descriptors	H-indices
2516	H1s	H autocorrelation of lag 1 / weighted by I-state	GETAWAY descriptors	H-indices
2517	H2s	H autocorrelation of lag 2 / weighted by I-state	GETAWAY descriptors	H-indices

2518	H3s	H autocorrelation of lag 3 / weighted by I-state	GETAWAY descriptors	H-indices
2519	H4s	H autocorrelation of lag 4 / weighted by I-state	GETAWAY descriptors	H-indices
2520	H5s	H autocorrelation of lag 5 / weighted by I-state	GETAWAY descriptors	H-indices
2521	H6s	H autocorrelation of lag 6 / weighted by I-state	GETAWAY descriptors	H-indices
2522	H7s	H autocorrelation of lag 7 / weighted by I-state	GETAWAY descriptors	H-indices
2523	H8s	H autocorrelation of lag 8 / weighted by I-state	GETAWAY descriptors	H-indices
2524	HTs	H total index / weighted by I-state	GETAWAY descriptors	H-indices
2525	HATS0s	leverage-weighted autocorrelation of lag 0 / weighted by I-state	GETAWAY descriptors	H-indices
2526	HATS1s	leverage-weighted autocorrelation of lag 1 / weighted by I-state	GETAWAY descriptors	H-indices
2527	HATS2s	leverage-weighted autocorrelation of lag 2 / weighted by I-state	GETAWAY descriptors	H-indices
2528	HATS3s	leverage-weighted autocorrelation of lag 3 / weighted by I-state	GETAWAY descriptors	H-indices
2529	HATS4s	leverage-weighted autocorrelation of lag 4 / weighted by I-state	GETAWAY descriptors	H-indices
2530	HATS5s	leverage-weighted autocorrelation of lag 5 / weighted by I-state	GETAWAY descriptors	H-indices
2531	HATS6s	leverage-weighted autocorrelation of lag 6 / weighted by I-state	GETAWAY descriptors	H-indices
2532	HATS7s	leverage-weighted autocorrelation of lag 7 / weighted by I-state	GETAWAY descriptors	H-indices
2533	HATS8s	leverage-weighted autocorrelation of lag 8 / weighted by I-state	GETAWAY descriptors	H-indices
2534	HATSs	leverage-weighted total index / weighted by I-state	GETAWAY descriptors	H-indices
2535	RCON	Randic-type R matrix connectivity	GETAWAY descriptors	R-indices
2536	RARS	R matrix average row sum	GETAWAY descriptors	R-indices
2537	REIG	first eigenvalue of the R matrix	GETAWAY descriptors	R-indices

2538	R1u	R autocorrelation of lag 1 / unweighted	GETAWAY descriptors	R-indices
2539	R2u	R autocorrelation of lag 2 / unweighted	GETAWAY descriptors	R-indices
2540	R3u	R autocorrelation of lag 3 / unweighted	GETAWAY descriptors	R-indices
2541	R4u	R autocorrelation of lag 4 / unweighted	GETAWAY descriptors	R-indices
2542	R5u	R autocorrelation of lag 5 / unweighted	GETAWAY descriptors	R-indices
2543	R6u	R autocorrelation of lag 6 / unweighted	GETAWAY descriptors	R-indices
2544	R7u	R autocorrelation of lag 7 / unweighted	GETAWAY descriptors	R-indices
2545	R8u	R autocorrelation of lag 8 / unweighted	GETAWAY descriptors	R-indices
2546	RTu	R total index / unweighted	GETAWAY descriptors	R-indices
2547	R1u+	R maximal autocorrelation of lag 1 / unweighted	GETAWAY descriptors	R-indices
2548	R2u+	R maximal autocorrelation of lag 2 / unweighted	GETAWAY descriptors	R-indices
2549	R3u+	R maximal autocorrelation of lag 3 / unweighted	GETAWAY descriptors	R-indices
2550	R4u+	R maximal autocorrelation of lag 4 / unweighted	GETAWAY descriptors	R-indices
2551	R5u+	R maximal autocorrelation of lag 5 / unweighted	GETAWAY descriptors	R-indices
2552	R6u+	R maximal autocorrelation of lag 6 / unweighted	GETAWAY descriptors	R-indices
2553	R7u+	R maximal autocorrelation of lag 7 / unweighted	GETAWAY descriptors	R-indices
2554	R8u+	R maximal autocorrelation of lag 8 / unweighted	GETAWAY descriptors	R-indices
2555	RTu+	R maximal index / unweighted	GETAWAY descriptors	R-indices
2556	R1m	R autocorrelation of lag 1 / weighted by mass	GETAWAY descriptors	R-indices
2557	R2m	R autocorrelation of lag 2 / weighted by mass	GETAWAY descriptors	R-indices

2558	R3m	R autocorrelation of lag 3 / weighted by mass	GETAWAY descriptors	R-indices
2559	R4m	R autocorrelation of lag 4 / weighted by mass	GETAWAY descriptors	R-indices
2560	R5m	R autocorrelation of lag 5 / weighted by mass	GETAWAY descriptors	R-indices
2561	R6m	R autocorrelation of lag 6 / weighted by mass	GETAWAY descriptors	R-indices
2562	R7m	R autocorrelation of lag 7 / weighted by mass	GETAWAY descriptors	R-indices
2563	R8m	R autocorrelation of lag 8 / weighted by mass	GETAWAY descriptors	R-indices
2564	RTm	R total index / weighted by mass	GETAWAY descriptors	R-indices
2565	R1m+	R maximal autocorrelation of lag 1 / weighted by mass	GETAWAY descriptors	R-indices
2566	R2m+	R maximal autocorrelation of lag 2 / weighted by mass	GETAWAY descriptors	R-indices
2567	R3m+	R maximal autocorrelation of lag 3 / weighted by mass	GETAWAY descriptors	R-indices
2568	R4m+	R maximal autocorrelation of lag 4 / weighted by mass	GETAWAY descriptors	R-indices
2569	R5m+	R maximal autocorrelation of lag 5 / weighted by mass	GETAWAY descriptors	R-indices
2570	R6m+	R maximal autocorrelation of lag 6 / weighted by mass	GETAWAY descriptors	R-indices
2571	R7m+	R maximal autocorrelation of lag 7 / weighted by mass	GETAWAY descriptors	R-indices
2572	R8m+	R maximal autocorrelation of lag 8 / weighted by mass	GETAWAY descriptors	R-indices
2573	RTm+	R maximal index / weighted by mass	GETAWAY descriptors	R-indices
2574	R1v	R autocorrelation of lag 1 / weighted by van der Waals volume	GETAWAY descriptors	R-indices
2575	R2v	R autocorrelation of lag 2 / weighted by van der Waals volume	GETAWAY descriptors	R-indices
2576	R3v	R autocorrelation of lag 3 / weighted by van der Waals volume	GETAWAY descriptors	R-indices
2577	R4v	R autocorrelation of lag 4 / weighted by van der Waals volume	GETAWAY descriptors	R-indices

2578	R5v	R autocorrelation of lag 5 / weighted by van der Waals volume	GETAWAY descriptors	R-indices
2579	R6v	R autocorrelation of lag 6 / weighted by van der Waals volume	GETAWAY descriptors	R-indices
2580	R7v	R autocorrelation of lag 7 / weighted by van der Waals volume	GETAWAY descriptors	R-indices
2581	R8v	R autocorrelation of lag 8 / weighted by van der Waals volume	GETAWAY descriptors	R-indices
2582	RTv	R total index / weighted by van der Waals volume	GETAWAY descriptors	R-indices
2583	R1v+	R maximal autocorrelation of lag 1 / weighted by van der Waals volume	GETAWAY descriptors	R-indices
2584	R2v+	R maximal autocorrelation of lag 2 / weighted by van der Waals volume	GETAWAY descriptors	R-indices
2585	R3v+	R maximal autocorrelation of lag 3 / weighted by van der Waals volume	GETAWAY descriptors	R-indices
2586	R4v+	R maximal autocorrelation of lag 4 / weighted by van der Waals volume	GETAWAY descriptors	R-indices
2587	R5v+	R maximal autocorrelation of lag 5 / weighted by van der Waals volume	GETAWAY descriptors	R-indices
2588	R6v+	R maximal autocorrelation of lag 6 / weighted by van der Waals volume	GETAWAY descriptors	R-indices
2589	R7v+	R maximal autocorrelation of lag 7 / weighted by van der Waals volume	GETAWAY descriptors	R-indices
2590	R8v+	R maximal autocorrelation of lag 8 / weighted by van der Waals volume	GETAWAY descriptors	R-indices
2591	RTv+	R maximal index / weighted by van der Waals volume	GETAWAY descriptors	R-indices
2592	R1e	R autocorrelation of lag 1 / weighted by Sanderson electronegativity	GETAWAY descriptors	R-indices
2593	R2e	R autocorrelation of lag 2 / weighted by Sanderson electronegativity	GETAWAY descriptors	R-indices
2594	R3e	R autocorrelation of lag 3 / weighted by Sanderson electronegativity	GETAWAY descriptors	R-indices
2595	R4e	R autocorrelation of lag 4 / weighted by Sanderson electronegativity	GETAWAY descriptors	R-indices
2596	R5e	R autocorrelation of lag 5 / weighted by Sanderson electronegativity	GETAWAY descriptors	R-indices
2597	R6e	R autocorrelation of lag 6 / weighted by Sanderson electronegativity	GETAWAY descriptors	R-indices

2598	R7e	R autocorrelation of lag 7 / weighted by Sanderson electronegativity	GETAWAY descriptors	R-indices
2599	R8e	R autocorrelation of lag 8 / weighted by Sanderson electronegativity	GETAWAY descriptors	R-indices
2600	RTe	R total index / weighted by Sanderson electronegativity	GETAWAY descriptors	R-indices
2601	R1e+	R maximal autocorrelation of lag 1 / weighted by Sanderson electronegativity	GETAWAY descriptors	R-indices
2602	R2e+	R maximal autocorrelation of lag 2 / weighted by Sanderson electronegativity	GETAWAY descriptors	R-indices
2603	R3e+	R maximal autocorrelation of lag 3 / weighted by Sanderson electronegativity	GETAWAY descriptors	R-indices
2604	R4e+	R maximal autocorrelation of lag 4 / weighted by Sanderson electronegativity	GETAWAY descriptors	R-indices
2605	R5e+	R maximal autocorrelation of lag 5 / weighted by Sanderson electronegativity	GETAWAY descriptors	R-indices
2606	R6e+	R maximal autocorrelation of lag 6 / weighted by Sanderson electronegativity	GETAWAY descriptors	R-indices
2607	R7e+	R maximal autocorrelation of lag 7 / weighted by Sanderson electronegativity	GETAWAY descriptors	R-indices
2608	R8e+	R maximal autocorrelation of lag 8 / weighted by Sanderson electronegativity	GETAWAY descriptors	R-indices
2609	RTe+	R maximal index / weighted by Sanderson electronegativity	GETAWAY descriptors	R-indices
2610	R1p	R autocorrelation of lag 1 / weighted by polarizability	GETAWAY descriptors	R-indices
2611	R2p	R autocorrelation of lag 2 / weighted by polarizability	GETAWAY descriptors	R-indices
2612	R3p	R autocorrelation of lag 3 / weighted by polarizability	GETAWAY descriptors	R-indices
2613	R4p	R autocorrelation of lag 4 / weighted by polarizability	GETAWAY descriptors	R-indices
2614	R5p	R autocorrelation of lag 5 / weighted by polarizability	GETAWAY descriptors	R-indices
2615	R6p	R autocorrelation of lag 6 / weighted by polarizability	GETAWAY descriptors	R-indices
2616	R7p	R autocorrelation of lag 7 / weighted by polarizability	GETAWAY descriptors	R-indices
2617	R8p	R autocorrelation of lag 8 / weighted by polarizability	GETAWAY descriptors	R-indices

2618	RTp	R total index / weighted by polarizability	GETAWAY descriptors	R-indices
2619	R1p+	R maximal autocorrelation of lag 1 / weighted by polarizability	GETAWAY descriptors	R-indices
2620	R2p+	R maximal autocorrelation of lag 2 / weighted by polarizability	GETAWAY descriptors	R-indices
2621	R3p+	R maximal autocorrelation of lag 3 / weighted by polarizability	GETAWAY descriptors	R-indices
2622	R4p+	R maximal autocorrelation of lag 4 / weighted by polarizability	GETAWAY descriptors	R-indices
2623	R5p+	R maximal autocorrelation of lag 5 / weighted by polarizability	GETAWAY descriptors	R-indices
2624	R6p+	R maximal autocorrelation of lag 6 / weighted by polarizability	GETAWAY descriptors	R-indices
2625	R7p+	R maximal autocorrelation of lag 7 / weighted by polarizability	GETAWAY descriptors	R-indices
2626	R8p+	R maximal autocorrelation of lag 8 / weighted by polarizability	GETAWAY descriptors	R-indices
2627	RTp+	R maximal index / weighted by polarizability	GETAWAY descriptors	R-indices
2628	R1i	R autocorrelation of lag 1 / weighted by ionization potential	GETAWAY descriptors	R-indices
2629	R2i	R autocorrelation of lag 2 / weighted by ionization potential	GETAWAY descriptors	R-indices
2630	R3i	R autocorrelation of lag 3 / weighted by ionization potential	GETAWAY descriptors	R-indices
2631	R4i	R autocorrelation of lag 4 / weighted by ionization potential	GETAWAY descriptors	R-indices
2632	R5i	R autocorrelation of lag 5 / weighted by ionization potential	GETAWAY descriptors	R-indices
2633	R6i	R autocorrelation of lag 6 / weighted by ionization potential	GETAWAY descriptors	R-indices
2634	R7i	R autocorrelation of lag 7 / weighted by ionization potential	GETAWAY descriptors	R-indices
2635	R8i	R autocorrelation of lag 8 / weighted by ionization potential	GETAWAY descriptors	R-indices
2636	RTi	R total index / weighted by ionization potential	GETAWAY descriptors	R-indices
2637	R1i+	R maximal autocorrelation of lag 1 / weighted by ionization potential	GETAWAY descriptors	R-indices

2638	R2i+	R maximal autocorrelation of lag 2 / weighted by ionization potential	GETAWAY descriptors	R-indices
2639	R3i+	R maximal autocorrelation of lag 3 / weighted by ionization potential	GETAWAY descriptors	R-indices
2640	R4i+	R maximal autocorrelation of lag 4 / weighted by ionization potential	GETAWAY descriptors	R-indices
2641	R5i+	R maximal autocorrelation of lag 5 / weighted by ionization potential	GETAWAY descriptors	R-indices
2642	R6i+	R maximal autocorrelation of lag 6 / weighted by ionization potential	GETAWAY descriptors	R-indices
2643	R7i+	R maximal autocorrelation of lag 7 / weighted by ionization potential	GETAWAY descriptors	R-indices
2644	R8i+	R maximal autocorrelation of lag 8 / weighted by ionization potential	GETAWAY descriptors	R-indices
2645	RTi+	R maximal index / weighted by ionization potential	GETAWAY descriptors	R-indices
2646	R1s	R autocorrelation of lag 1 / weighted by I-state	GETAWAY descriptors	R-indices
2647	R2s	R autocorrelation of lag 2 / weighted by I-state	GETAWAY descriptors	R-indices
2648	R3s	R autocorrelation of lag 3 / weighted by I-state	GETAWAY descriptors	R-indices
2649	R4s	R autocorrelation of lag 4 / weighted by I-state	GETAWAY descriptors	R-indices
2650	R5s	R autocorrelation of lag 5 / weighted by I-state	GETAWAY descriptors	R-indices
2651	R6s	R autocorrelation of lag 6 / weighted by I-state	GETAWAY descriptors	R-indices
2652	R7s	R autocorrelation of lag 7 / weighted by I-state	GETAWAY descriptors	R-indices
2653	R8s	R autocorrelation of lag 8 / weighted by I-state	GETAWAY descriptors	R-indices
2654	RTs	R total index / weighted by I-state	GETAWAY descriptors	R-indices
2655	R1s+	R maximal autocorrelation of lag 1 / weighted by I-state	GETAWAY descriptors	R-indices
2656	R2s+	R maximal autocorrelation of lag 2 / weighted by I-state	GETAWAY descriptors	R-indices
2657	R3s+	R maximal autocorrelation of lag 3 / weighted by I-state	GETAWAY descriptors	R-indices

2658	R4s+	R maximal autocorrelation of lag 4 / weighted by I-state	GETAWAY descriptors	R-indices
2659	R5s+	R maximal autocorrelation of lag 5 / weighted by I-state	GETAWAY descriptors	R-indices
2660	R6s+	R maximal autocorrelation of lag 6 / weighted by I-state	GETAWAY descriptors	R-indices
2661	R7s+	R maximal autocorrelation of lag 7 / weighted by I-state	GETAWAY descriptors	R-indices
2662	R8s+	R maximal autocorrelation of lag 8 / weighted by I-state	GETAWAY descriptors	R-indices
2663	RTs+	R maximal index / weighted by I-state	GETAWAY descriptors	R-indices
2664	DP01	molecular profile no. 1	Randic molecular profiles	Molecular profiles
2665	DP02	molecular profile no. 2	Randic molecular profiles	Molecular profiles
2666	DP03	molecular profile no. 3	Randic molecular profiles	Molecular profiles
2667	DP04	molecular profile no. 4	Randic molecular profiles	Molecular profiles
2668	DP05	molecular profile no. 5	Randic molecular profiles	Molecular profiles
2669	DP06	molecular profile no. 6	Randic molecular profiles	Molecular profiles
2670	DP07	molecular profile no. 7	Randic molecular profiles	Molecular profiles
2671	DP08	molecular profile no. 8	Randic molecular profiles	Molecular profiles
2672	DP09	molecular profile no. 9	Randic molecular profiles	Molecular profiles
2673	DP10	molecular profile no. 10	Randic molecular profiles	Molecular profiles

2674	DP11	molecular profile no. 11	Randic molecular profiles	Molecular profiles
2675	DP12	molecular profile no. 12	Randic molecular profiles	Molecular profiles
2676	DP13	molecular profile no. 13	Randic molecular profiles	Molecular profiles
2677	DP14	molecular profile no. 14	Randic molecular profiles	Molecular profiles
2678	DP15	molecular profile no. 15	Randic molecular profiles	Molecular profiles
2679	DP16	molecular profile no. 16	Randic molecular profiles	Molecular profiles
2680	DP17	molecular profile no. 17	Randic molecular profiles	Molecular profiles
2681	DP18	molecular profile no. 18	Randic molecular profiles	Molecular profiles
2682	DP19	molecular profile no. 19	Randic molecular profiles	Molecular profiles
2683	DP20	molecular profile no. 20	Randic molecular profiles	Molecular profiles
2684	SP01	shape profile no. 1	Randic molecular profiles	Shape profiles
2685	SP02	shape profile no. 2	Randic molecular profiles	Shape profiles
2686	SP03	shape profile no. 3	Randic molecular profiles	Shape profiles
2687	SP04	shape profile no. 4	Randic molecular profiles	Shape profiles
2688	SP05	shape profile no. 5	Randic molecular profiles	Shape profiles

2689	SP06	shape profile no. 6	Randic molecular profiles	Shape profiles
2690	SP07	shape profile no. 7	Randic molecular profiles	Shape profiles
2691	SP08	shape profile no. 8	Randic molecular profiles	Shape profiles
2692	SP09	shape profile no. 9	Randic molecular profiles	Shape profiles
2693	SP10	shape profile no. 10	Randic molecular profiles	Shape profiles
2694	SP11	shape profile no. 11	Randic molecular profiles	Shape profiles
2695	SP12	shape profile no. 12	Randic molecular profiles	Shape profiles
2696	SP13	shape profile no. 13	Randic molecular profiles	Shape profiles
2697	SP14	shape profile no. 14	Randic molecular profiles	Shape profiles
2698	SP15	shape profile no. 15	Randic molecular profiles	Shape profiles
2699	SP16	shape profile no. 16	Randic molecular profiles	Shape profiles
2700	SP17	shape profile no. 17	Randic molecular profiles	Shape profiles
2701	SP18	shape profile no. 18	Randic molecular profiles	Shape profiles
2702	SP19	shape profile no. 19	Randic molecular profiles	Shape profiles
2703	SP20	shape profile no. 20	Randic molecular profiles	Shape profiles

2704	SHP2	average shape profile index of order 2	Randic molecular profiles	Shape profiles
2705	nCp	number of terminal primary C(sp3)	Functional group counts	Basic descriptors
2706	nCs	number of total secondary C(sp3)	Functional group counts	Basic descriptors
2707	nCt	number of total tertiary C(sp3)	Functional group counts	Basic descriptors
2708	nCq	number of total quaternary C(sp3)	Functional group counts	Basic descriptors
2709	nCrs	number of ring secondary C(sp3)	Functional group counts	Basic descriptors
2710	nCrt	number of ring tertiary C(sp3)	Functional group counts	Basic descriptors
2711	nCrq	number of ring quaternary C(sp3)	Functional group counts	Basic descriptors
2712	nCar	number of aromatic C(sp2)	Functional group counts	Basic descriptors
2713	nCbH	number of unsubstituted benzene C(sp2)	Functional group counts	Basic descriptors
2714	nCb-	number of substituted benzene C(sp2)	Functional group counts	Basic descriptors
2715	nCconj	number of non-aromatic conjugated C(sp2)	Functional group counts	Basic descriptors
2716	nR=Cp	number of terminal primary C(sp2)	Functional group counts	Basic descriptors
2717	nR=Cs	number of aliphatic secondary C(sp2)	Functional group counts	Basic descriptors
2718	nR=Ct	number of aliphatic tertiary C(sp2)	Functional group counts	Basic descriptors
2719	n=C=	number of allenes groups	Functional group counts	Basic descriptors
2720	nR#CH/X	number of terminal C(sp)	Functional group counts	Basic descriptors
2721	nR#C-	number of non-terminal C(sp)	Functional group counts	Basic descriptors
2722	nROCN	number of cyanates (aliphatic)	Functional group counts	Basic descriptors
2723	nArOCN	number of cyanates (aromatic)	Functional group counts	Basic descriptors

2724	nRNCO	number of isocyanates (aliphatic)	Functional group counts	Basic descriptors
2725	nArNCO	number of isocyanates (aromatic)	Functional group counts	Basic descriptors
2726	nRSCN	number of thiocyanates (aliphatic)	Functional group counts	Basic descriptors
2727	nArSCN	number of thiocyanates (aromatic)	Functional group counts	Basic descriptors
2728	nRNCS	number of isothiocyanates (aliphatic)	Functional group counts	Basic descriptors
2729	nArNCS	number of isothiocyanates (aromatic)	Functional group counts	Basic descriptors
2730	nRCOOH	number of carboxylic acids (aliphatic)	Functional group counts	Basic descriptors
2731	nArCOOH	number of carboxylic acids (aromatic)	Functional group counts	Basic descriptors
2732	nRCOOR	number of esters (aliphatic)	Functional group counts	Basic descriptors
2733	nArCOOR	number of esters (aromatic)	Functional group counts	Basic descriptors
2734	nRCONH2	number of primary amides (aliphatic)	Functional group counts	Basic descriptors
2735	nArCONH2	number of primary amides (aromatic)	Functional group counts	Basic descriptors
2736	nRCONHR	number of secondary amides (aliphatic)	Functional group counts	Basic descriptors
2737	nArCONHR	number of secondary amides (aromatic)	Functional group counts	Basic descriptors
2738	nRCONR2	number of tertiary amides (aliphatic)	Functional group counts	Basic descriptors
2739	nArCONR2	number of tertiary amides (aromatic)	Functional group counts	Basic descriptors
2740	nROCON	number of (thio-) carbamates (aliphatic)	Functional group counts	Basic descriptors
2741	nArOCON	number of (thio-) carbamates (aromatic)	Functional group counts	Basic descriptors
2742	nRCOX	number of acyl halogenides (aliphatic)	Functional group counts	Basic descriptors
2743	nArCOX	number of acyl halogenides (aromatic)	Functional group counts	Basic descriptors

2744	nRCSOH	number of thioacids (aliphatic)	Functional group counts	Basic descriptors
2745	nArCSOH	number of thioacids (aromatic)	Functional group counts	Basic descriptors
2746	nRCSSH	number of dithioacids (aliphatic)	Functional group counts	Basic descriptors
2747	nArCSSH	number of dithioacids (aromatic)	Functional group counts	Basic descriptors
2748	nRCOSR	number of thioesters (aliphatic)	Functional group counts	Basic descriptors
2749	nArCOSR	number of thioesters (aromatic)	Functional group counts	Basic descriptors
2750	nRCSSR	number of dithioesters (aliphatic)	Functional group counts	Basic descriptors
2751	nArCSSR	number of dithioesters (aromatic)	Functional group counts	Basic descriptors
2752	nRCHO	number of aldehydes (aliphatic)	Functional group counts	Basic descriptors
2753	nArCHO	number of aldehydes (aromatic)	Functional group counts	Basic descriptors
2754	nRCO	number of ketones (aliphatic)	Functional group counts	Basic descriptors
2755	nArCO	number of ketones (aromatic)	Functional group counts	Basic descriptors
2756	nCONN	number of urea (-thio) derivatives	Functional group counts	Basic descriptors
2757	nC=O(O)2	number of carbonate (-thio) derivatives	Functional group counts	Basic descriptors
2758	nN=C-N<	number of amidine derivatives	Functional group counts	Basic descriptors
2759	nC(=N)N2	number of guanidine derivatives	Functional group counts	Basic descriptors
2760	nRC=N	number of imines (aliphatic)	Functional group counts	Basic descriptors
2761	nArC=N	number of imines (aromatic)	Functional group counts	Basic descriptors
2762	nRCNO	number of oximes (aliphatic)	Functional group counts	Basic descriptors
2763	nArCNO	number of oximes (aromatic)	Functional group counts	Basic descriptors

2764	nRNH2	number of primary amines (aliphatic)	Functional group counts	Basic descriptors
2765	nArNH2	number of primary amines (aromatic)	Functional group counts	Basic descriptors
2766	nRNHR	number of secondary amines (aliphatic)	Functional group counts	Basic descriptors
2767	nArNHR	number of secondary amines (aromatic)	Functional group counts	Basic descriptors
2768	nRNR2	number of tertiary amines (aliphatic)	Functional group counts	Basic descriptors
2769	nArNR2	number of tertiary amines (aromatic)	Functional group counts	Basic descriptors
2770	nN-N	number of N hydrazines	Functional group counts	Basic descriptors
2771	nN=N	number of N azo-derivatives	Functional group counts	Basic descriptors
2772	nRCN	number of nitriles (aliphatic)	Functional group counts	Basic descriptors
2773	nArCN	number of nitriles (aromatic)	Functional group counts	Basic descriptors
2774	nN+	number of positively charged N	Functional group counts	Basic descriptors
2775	nNq	number of quaternary N	Functional group counts	Basic descriptors
2776	nRNHO	number of hydroxylamines (aliphatic)	Functional group counts	Basic descriptors
2777	nArNHO	number of hydroxylamines (aromatic)	Functional group counts	Basic descriptors
2778	nRNNOx	number of N-nitroso groups (aliphatic)	Functional group counts	Basic descriptors
2779	nArNNOx	number of N-nitroso groups (aromatic)	Functional group counts	Basic descriptors
2780	nRNO	number of nitroso groups (aliphatic)	Functional group counts	Basic descriptors
2781	nArNO	number of nitroso groups (aromatic)	Functional group counts	Basic descriptors
2782	nRNO2	number of nitro groups (aliphatic)	Functional group counts	Basic descriptors
2783	nArNO2	number of nitro groups (aromatic)	Functional group counts	Basic descriptors

2784	nN(CO)2	number of imides (-thio)	Functional group counts	Basic descriptors
2785	nC=N-N<	number of hydrazones	Functional group counts	Basic descriptors
2786	nROH	number of hydroxyl groups	Functional group counts	Basic descriptors
2787	nArOH	number of aromatic hydroxyls	Functional group counts	Basic descriptors
2788	nOHp	number of primary alcohols	Functional group counts	Basic descriptors
2789	nOHs	number of secondary alcohols	Functional group counts	Basic descriptors
2790	nOHt	number of tertiary alcohols	Functional group counts	Basic descriptors
2791	nROR	number of ethers (aliphatic)	Functional group counts	Basic descriptors
2792	nArOR	number of ethers (aromatic)	Functional group counts	Basic descriptors
2793	nROX	number of hypohalogenides (aliphatic)	Functional group counts	Basic descriptors
2794	nArOX	number of hypohalogenides (aromatic)	Functional group counts	Basic descriptors
2795	nO(C=O)2	number of anhydrides (-thio)	Functional group counts	Basic descriptors
2796	nH2O	number of water molecules	Functional group counts	Basic descriptors
2797	nSH	number of thiols	Functional group counts	Basic descriptors
2798	nC=S	number of thioketones	Functional group counts	Basic descriptors
2799	nRSR	number of sulfides	Functional group counts	Basic descriptors
2800	nRSSR	number of disulfides	Functional group counts	Basic descriptors
2801	nSO	number of sulfoxides	Functional group counts	Basic descriptors
2802	nS(=O)2	number of sulfones	Functional group counts	Basic descriptors
2803	nSOH	number of sulfenic (thio-) acids	Functional group counts	Basic descriptors

2804	nSOOH	number of sulfinic (thio-/dithio-) acids	Functional group counts	Basic descriptors
2805	nSO2OH	number of sulfonic (thio-/dithio-) acids	Functional group counts	Basic descriptors
2806	nSO3OH	number of sulfuric (thio-/dithio-) acids	Functional group counts	Basic descriptors
2807	nSO2	number of sulfites (thio-/dithio-)	Functional group counts	Basic descriptors
2808	nSO3	number of sulfonates (thio-/dithio-)	Functional group counts	Basic descriptors
2809	nSO4	number of sulfates (thio-/dithio-)	Functional group counts	Basic descriptors
2810	nSO2N	number of sulfonamides (thio-/dithio-)	Functional group counts	Basic descriptors
2811	nPO3	number of phosphites/thiophosphites	Functional group counts	Basic descriptors
2812	nPO4	number of phosphates/thiophosphates	Functional group counts	Basic descriptors
2813	nPR3	number of phosphanes	Functional group counts	Basic descriptors
2814	nP(=O)O2R	number of phosphonates (thio-)	Functional group counts	Basic descriptors
2815	nP(=O)R3/nPR5	number of phosphoranes (thio-)	Functional group counts	Basic descriptors
2816	nCH2RX	number of CH2RX	Functional group counts	Basic descriptors
2817	nCHR2X	number of CHR2X	Functional group counts	Basic descriptors
2818	nCR3X	number of CR3X	Functional group counts	Basic descriptors
2819	nR=CHX	number of R=CHX	Functional group counts	Basic descriptors
2820	nR=CRX	number of R=CRX	Functional group counts	Basic descriptors
2821	nR#CX	number of R#CX	Functional group counts	Basic descriptors
2822	nCHRX2	number of CHRX2	Functional group counts	Basic descriptors
2823	nCR2X2	number of CR2X2	Functional group counts	Basic descriptors

2824	nR=CX2	number of R=CX2	Functional group counts	Basic descriptors
2825	nCRX3	number of CRX3	Functional group counts	Basic descriptors
2826	nArX	number of X on aromatic ring	Functional group counts	Basic descriptors
2827	nCXr	number of X on ring C(sp3)	Functional group counts	Basic descriptors
2828	nCXr=	number of X on ring C(sp2)	Functional group counts	Basic descriptors
2829	nCconjX	number of X on exo-conjugated C	Functional group counts	Basic descriptors
2830	nAziridines	number of Aziridines	Functional group counts	Basic descriptors
2831	nOxiranes	number of Oxiranes	Functional group counts	Basic descriptors
2832	nThiranes	number of Thiranes	Functional group counts	Basic descriptors
2833	nAzetidines	number of Azetidines	Functional group counts	Basic descriptors
2834	nOxetanes	number of Oxetanes	Functional group counts	Basic descriptors
2835	nThioethanes	number of Thioethanes	Functional group counts	Basic descriptors
2836	nBeta-Lactams	number of Beta-Lactams	Functional group counts	Basic descriptors
2837	nPyrrolidines	number of Pyrrolidines	Functional group counts	Basic descriptors
2838	nOxolanes	number of Oxolanes	Functional group counts	Basic descriptors
2839	ntH-Thiophenes	number of tetrahydro-thiophenes	Functional group counts	Basic descriptors
2840	nPyrroles	number of Pyrroles	Functional group counts	Basic descriptors
2841	nPyrazoles	number of Pyrazoles	Functional group counts	Basic descriptors
2842	nImidazoles	number of Imidazoles	Functional group counts	Basic descriptors
2843	nFuranes	number of Furanes	Functional group counts	Basic descriptors

2844	nThiophenes	number of Thiophenes	Functional group counts	Basic descriptors
2845	nOxazoles	number of Oxazoles	Functional group counts	Basic descriptors
2846	nIsoxazoles	number of Isoxazoles	Functional group counts	Basic descriptors
2847	nThiazoles	number of Thiazoles	Functional group counts	Basic descriptors
2848	nIsothiazoles	number of Isothiazoles	Functional group counts	Basic descriptors
2849	nTriazoles	number of Triazoles	Functional group counts	Basic descriptors
2850	nPyridines	number of Pyridines	Functional group counts	Basic descriptors
2851	nPyridazines	number of Pyridazines	Functional group counts	Basic descriptors
2852	nPyrimidines	number of Pyrimidines	Functional group counts	Basic descriptors
2853	nPyrazines	number of Pyrazines	Functional group counts	Basic descriptors
2854	n135-Triazines	number of 1-3-5-Triazines	Functional group counts	Basic descriptors
2855	n124-Triazines	number of 1-2-4-Triazines	Functional group counts	Basic descriptors
2856	nHDon	number of donor atoms for H-bonds (N and O)	Functional group counts	Basic descriptors
2857	nHAcc	number of acceptor atoms for H-bonds (N,O,F)	Functional group counts	Basic descriptors
2858	nHBonds	number of intramolecular H-bonds (with N,O,F)	Functional group counts	Basic descriptors
2859	C-001	CH3R / CH4	Atom-centred fragments	Basic descriptors
2860	C-002	CH2R2	Atom-centred fragments	Basic descriptors
2861	C-003	CHR3	Atom-centred fragments	Basic descriptors
2862	C-004	CR4	Atom-centred fragments	Basic descriptors
2863	C-005	CH3X	Atom-centred fragments	Basic descriptors

2864	C-006	CH2RX	Atom-centred fragments	Basic descriptors
2865	C-007	CH2X2	Atom-centred fragments	Basic descriptors
2866	C-008	CHR2X	Atom-centred fragments	Basic descriptors
2867	C-009	CHRX2	Atom-centred fragments	Basic descriptors
2868	C-010	CHX3	Atom-centred fragments	Basic descriptors
2869	C-011	CR3X	Atom-centred fragments	Basic descriptors
2870	C-012	CR2X2	Atom-centred fragments	Basic descriptors
2871	C-013	CRX3	Atom-centred fragments	Basic descriptors
2872	C-014	CX4	Atom-centred fragments	Basic descriptors
2873	C-015	=CH2	Atom-centred fragments	Basic descriptors
2874	C-016	=CHR	Atom-centred fragments	Basic descriptors
2875	C-017	=CR2	Atom-centred fragments	Basic descriptors
2876	C-018	=CHX	Atom-centred fragments	Basic descriptors
2877	C-019	=CRX	Atom-centred fragments	Basic descriptors
2878	C-020	=CX2	Atom-centred fragments	Basic descriptors
2879	C-021	#CH	Atom-centred fragments	Basic descriptors
2880	C-022	#CR / R=C=R	Atom-centred fragments	Basic descriptors
2881	C-023	#CX	Atom-centred fragments	Basic descriptors
2882	C-024	R--CH--R	Atom-centred fragments	Basic descriptors
2883	C-025	R--CR--R	Atom-centred fragments	Basic descriptors

2884	C-026	R--CX--R	Atom-centred fragments	Basic descriptors
2885	C-027	R--CH--X	Atom-centred fragments	Basic descriptors
2886	C-028	R--CR--X	Atom-centred fragments	Basic descriptors
2887	C-029	R--CX--X	Atom-centred fragments	Basic descriptors
2888	C-030	X--CH--X	Atom-centred fragments	Basic descriptors
2889	C-031	X--CR--X	Atom-centred fragments	Basic descriptors
2890	C-032	X--CX--X	Atom-centred fragments	Basic descriptors
2891	C-033	R--CH..X	Atom-centred fragments	Basic descriptors
2892	C-034	R--CR..X	Atom-centred fragments	Basic descriptors
2893	C-035	R--CX..X	Atom-centred fragments	Basic descriptors
2894	C-036	Al-CH=X	Atom-centred fragments	Basic descriptors
2895	C-037	Ar-CH=X	Atom-centred fragments	Basic descriptors
2896	C-038	Al-C(=X)-Al	Atom-centred fragments	Basic descriptors
2897	C-039	Ar-C(=X)-R	Atom-centred fragments	Basic descriptors
2898	C-040	R-C(=X)-X / R-C#X / X=C=X	Atom-centred fragments	Basic descriptors
2899	C-041	X-C(=X)-X	Atom-centred fragments	Basic descriptors
2900	C-042	X--CH..X	Atom-centred fragments	Basic descriptors
2901	C-043	X--CR..X	Atom-centred fragments	Basic descriptors
2902	C-044	X--CX..X	Atom-centred fragments	Basic descriptors
2903	H-046	H attached to C0(sp3) no X attached to next C	Atom-centred fragments	Basic descriptors

2904	H-047	H attached to C1(sp3)/C0(sp2)	Atom-centred fragments	Basic descriptors
2905	H-048	H attached to C2(sp3)/C1(sp2)/C0(sp)	Atom-centred fragments	Basic descriptors
2906	H-049	H attached to C3(sp3)/C2(sp2)/C3(sp2)/C3(sp)	Atom-centred fragments	Basic descriptors
2907	H-050	H attached to heteroatom	Atom-centred fragments	Basic descriptors
2908	H-051	H attached to alpha-C	Atom-centred fragments	Basic descriptors
2909	H-052	H attached to C0(sp3) with 1X attached to next C	Atom-centred fragments	Basic descriptors
2910	H-053	H attached to C0(sp3) with 2X attached to next C	Atom-centred fragments	Basic descriptors
2911	H-054	H attached to C0(sp3) with 3X attached to next C	Atom-centred fragments	Basic descriptors
2912	H-055	H attached to C0(sp3) with 4X attached to next C	Atom-centred fragments	Basic descriptors
2913	O-056	alcohol	Atom-centred fragments	Basic descriptors
2914	O-057	phenol / enol / carboxyl OH	Atom-centred fragments	Basic descriptors
2915	O-058	#NAME?	Atom-centred fragments	Basic descriptors
2916	O-059	Al-O-Al	Atom-centred fragments	Basic descriptors
2917	O-060	Al-O-Ar / Ar-O-Ar / R..O..R / R-O-C=X	Atom-centred fragments	Basic descriptors
2918	O-061	O--	Atom-centred fragments	Basic descriptors
2919	O-062	O- (negatively charged)	Atom-centred fragments	Basic descriptors
2920	O-063	R-O-O-R	Atom-centred fragments	Basic descriptors
2921	Se-064	Any-Se-Any	Atom-centred fragments	Basic descriptors
2922	Se-065	#NAME?	Atom-centred fragments	Basic descriptors
2923	N-066	Al-NH2	Atom-centred fragments	Basic descriptors

2924	N-067	Al2-NH	Atom-centred fragments	Basic descriptors
2925	N-068	Al3-N	Atom-centred fragments	Basic descriptors
2926	N-069	Ar-NH2 / X-NH2	Atom-centred fragments	Basic descriptors
2927	N-070	Ar-NH-Al	Atom-centred fragments	Basic descriptors
2928	N-071	Ar-NAl2	Atom-centred fragments	Basic descriptors
2929	N-072	RCO-N< / >N-X=X	Atom-centred fragments	Basic descriptors
2930	N-073	Ar2NH / Ar3N / Ar2N-Al / R..N..R	Atom-centred fragments	Basic descriptors
2931	N-074	R#N / R=N-	Atom-centred fragments	Basic descriptors
2932	N-075	R--N--R / R--N--X	Atom-centred fragments	Basic descriptors
2933	N-076	Ar-NO2 / R--N(--R)--O / RO-NO	Atom-centred fragments	Basic descriptors
2934	N-077	Al-NO2	Atom-centred fragments	Basic descriptors
2935	N-078	Ar-N=X / X-N=X	Atom-centred fragments	Basic descriptors
2936	N-079	N+ (positively charged)	Atom-centred fragments	Basic descriptors
2937	F-081	F attached to C1(sp3)	Atom-centred fragments	Basic descriptors
2938	F-082	F attached to C2(sp3)	Atom-centred fragments	Basic descriptors
2939	F-083	F attached to C3(sp3)	Atom-centred fragments	Basic descriptors
2940	F-084	F attached to C1(sp2)	Atom-centred fragments	Basic descriptors
2941	F-085	F attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X	Atom-centred fragments	Basic descriptors
2942	Cl-086	Cl attached to C1(sp3)	Atom-centred fragments	Basic descriptors
2943	Cl-087	Cl attached to C2(sp3)	Atom-centred fragments	Basic descriptors

2944	Cl-088	Cl attached to C3(sp3)	Atom-centred fragments	Basic descriptors
2945	Cl-089	Cl attached to C1(sp2)	Atom-centred fragments	Basic descriptors
2946	Cl-090	Cl attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X	Atom-centred fragments	Basic descriptors
2947	Br-091	Br attached to C1(sp3)	Atom-centred fragments	Basic descriptors
2948	Br-092	Br attached to C2(sp3)	Atom-centred fragments	Basic descriptors
2949	Br-093	Br attached to C3(sp3)	Atom-centred fragments	Basic descriptors
2950	Br-094	Br attached to C1(sp2)	Atom-centred fragments	Basic descriptors
2951	Br-095	Br attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X	Atom-centred fragments	Basic descriptors
2952	I-096	I attached to C1(sp3)	Atom-centred fragments	Basic descriptors
2953	I-097	I attached to C2(sp3)	Atom-centred fragments	Basic descriptors
2954	I-098	I attached to C3(sp3)	Atom-centred fragments	Basic descriptors
2955	I-099	I attached to C1(sp2)	Atom-centred fragments	Basic descriptors
2956	I-100	I attached to C2(sp2)-C4(sp2)/C1(sp)/C4(sp3)/X	Atom-centred fragments	Basic descriptors
2957	F-101	fluoride ion	Atom-centred fragments	Basic descriptors
2958	Cl-102	chloride ion	Atom-centred fragments	Basic descriptors
2959	Br-103	bromide ion	Atom-centred fragments	Basic descriptors
2960	I-104	iodide ion	Atom-centred fragments	Basic descriptors
2961	S-106	R-SH	Atom-centred fragments	Basic descriptors
2962	S-107	R2S / RS-SR	Atom-centred fragments	Basic descriptors
2963	S-108	R=S	Atom-centred fragments	Basic descriptors

2964	S-109	R-SO-R	Atom-centred fragments	Basic descriptors
2965	S-110	R-SO2-R	Atom-centred fragments	Basic descriptors
2966	Si-111	>Si<	Atom-centred fragments	Basic descriptors
2967	B-112	>B- as in boranes	Atom-centred fragments	Basic descriptors
2968	P-115	P ylids	Atom-centred fragments	Basic descriptors
2969	P-116	R3-P=X	Atom-centred fragments	Basic descriptors
2970	P-117	X3-P=X (phosphate)	Atom-centred fragments	Basic descriptors
2971	P-118	PX3 (phosphite)	Atom-centred fragments	Basic descriptors
2972	P-119	PR3 (phosphine)	Atom-centred fragments	Basic descriptors
2973	P-120	C-P(X)2=X (phosphonate)	Atom-centred fragments	Basic descriptors
2974	SsCH3	Sum of sCH3 E-states	Atom-type E-state indices	E-State sums
2975	SdCH2	Sum of dCH2 E-states	Atom-type E-state indices	E-State sums
2976	SssCH2	Sum of ssCH2 E-states	Atom-type E-state indices	E-State sums
2977	StCH	Sum of tCH E-states	Atom-type E-state indices	E-State sums
2978	SdsCH	Sum of dsCH E-states	Atom-type E-state indices	E-State sums
2979	SaaCH	Sum of aaCH E-states	Atom-type E-state indices	E-State sums
2980	SsssCH	Sum of sssCH E-states	Atom-type E-state indices	E-State sums
2981	SddC	Sum of ddC E-states	Atom-type E-state indices	E-State sums
2982	StsC	Sum of tsC E-states	Atom-type E-state indices	E-State sums
2983	SdssC	Sum of dssC E-states	Atom-type E-state indices	E-State sums

2984	SaasC	Sum of aasC E-states	Atom-type E-state indices	E-State sums
2985	SaaaC	Sum of aaaC E-states	Atom-type E-state indices	E-State sums
2986	SssssC	Sum of ssssC E-states	Atom-type E-state indices	E-State sums
2987	SsNH2	Sum of sNH2 E-states	Atom-type E-state indices	E-State sums
2988	SssNH	Sum of ssNH E-states	Atom-type E-state indices	E-State sums
2989	SdNH	Sum of dNH E-states	Atom-type E-state indices	E-State sums
2990	SsssN	Sum of sssN E-states	Atom-type E-state indices	E-State sums
2991	SdsN	Sum of dsN E-states	Atom-type E-state indices	E-State sums
2992	SaaN	Sum of aaN E-states	Atom-type E-state indices	E-State sums
2993	StN	Sum of tN E-states	Atom-type E-state indices	E-State sums
2994	SsNH3+	Sum of sNH3+ E-states	Atom-type E-state indices	E-State sums
2995	SssNH2+	Sum of ssNH2+ E-states	Atom-type E-state indices	E-State sums
2996	SdNH2+	Sum of dNH2+ E-states	Atom-type E-state indices	E-State sums
2997	SsssNH+	Sum of sssNH+ E-states	Atom-type E-state indices	E-State sums
2998	SssssN+	Sum of ssssN+ E-states	Atom-type E-state indices	E-State sums
2999	SddsN	Sum of ddsN E-states	Atom-type E-state indices	E-State sums
3000	SaadN	Sum of aadN E-states	Atom-type E-state indices	E-State sums
3001	SaasN	Sum of aasN E-states	Atom-type E-state indices	E-State sums
3002	SaaNH	Sum of aaNH E-states	Atom-type E-state indices	E-State sums
3003	SsOH	Sum of sOH E-states	Atom-type E-state indices	E-State sums

3004	SdO	Sum of dO E-states	Atom-type E-state indices	E-State sums
3005	SssO	Sum of ssO E-states	Atom-type E-state indices	E-State sums
3006	SaaO	Sum of aaO E-states	Atom-type E-state indices	E-State sums
3007	SsPH2	Sum of sPH2 E-states	Atom-type E-state indices	E-State sums
3008	SssPH	Sum of ssPH E-states	Atom-type E-state indices	E-State sums
3009	SsssP	Sum of sssP E-states	Atom-type E-state indices	E-State sums
3010	SdsssP	Sum of dsssP E-states	Atom-type E-state indices	E-State sums
3011	SddsP	Sum of ddsP E-states	Atom-type E-state indices	E-State sums
3012	SsssssP	Sum of sssssP E-states	Atom-type E-state indices	E-State sums
3013	SsSH	Sum of sSH E-states	Atom-type E-state indices	E-State sums
3014	SdS	Sum of dS E-states	Atom-type E-state indices	E-State sums
3015	SssS	Sum of ssS E-states	Atom-type E-state indices	E-State sums
3016	SaaS	Sum of aaS E-states	Atom-type E-state indices	E-State sums
3017	SdssS	Sum of dssS E-states	Atom-type E-state indices	E-State sums
3018	SddssS	Sum of ddssS E-states	Atom-type E-state indices	E-State sums
3019	SsssssS	Sum of ssssssS E-states	Atom-type E-state indices	E-State sums
3020	SsF	Sum of sF E-states	Atom-type E-state indices	E-State sums
3021	SsCl	Sum of sCl E-states	Atom-type E-state indices	E-State sums
3022	SsBr	Sum of sBr E-states	Atom-type E-state indices	E-State sums
3023	SsI	Sum of sI E-states	Atom-type E-state indices	E-State sums

3024	SsLi	Sum of sLi E-states	Atom-type E-state indices	E-State sums
3025	SssBe	Sum of ssBe E-states	Atom-type E-state indices	E-State sums
3026	SssssBe-	Sum of ssssBe- E-states	Atom-type E-state indices	E-State sums
3027	SsBH2	Sum of sBH2 E-states	Atom-type E-state indices	E-State sums
3028	SssBH	Sum of ssBH E-states	Atom-type E-state indices	E-State sums
3029	SsssB	Sum of sssB E-states	Atom-type E-state indices	E-State sums
3030	SssssB-	Sum of ssssB- E-states	Atom-type E-state indices	E-State sums
3031	SsGeH3	Sum of sGeH3 E-states	Atom-type E-state indices	E-State sums
3032	SssGeH2	Sum of ssGeH2 E-states	Atom-type E-state indices	E-State sums
3033	SsssGeH	Sum of sssGeH E-states	Atom-type E-state indices	E-State sums
3034	SssssGe	Sum of ssssGe E-states	Atom-type E-state indices	E-State sums
3035	SsAsH2	Sum of sAsH2 E-states	Atom-type E-state indices	E-State sums
3036	SssAsH	Sum of ssAsH E-states	Atom-type E-state indices	E-State sums
3037	SsssAs	Sum of sssAs E-states	Atom-type E-state indices	E-State sums
3038	SsssssAs	Sum of sssssAs E-states	Atom-type E-state indices	E-State sums
3039	SdsssAs	Sum of dsssAs E-states	Atom-type E-state indices	E-State sums
3040	SddsAs	Sum of ddsAs E-states	Atom-type E-state indices	E-State sums
3041	SsSeH	Sum of sSeH E-states	Atom-type E-state indices	E-State sums
3042	SdSe	Sum of dSe E-states	Atom-type E-state indices	E-State sums
3043	SssSe	Sum of ssSe E-states	Atom-type E-state indices	E-State sums

3044	SaaSe	Sum of aaSe E-states	Atom-type E-state indices	E-State sums
3045	SdssSe	Sum of dssSe E-states	Atom-type E-state indices	E-State sums
3046	SsssssSe	Sum of ssssssSe E-states	Atom-type E-state indices	E-State sums
3047	SddssSe	Sum of ddssSe E-states	Atom-type E-state indices	E-State sums
3048	SsSnH3	Sum of sSnH3 E-states	Atom-type E-state indices	E-State sums
3049	SssSnH2	Sum of ssSnH2 E-states	Atom-type E-state indices	E-State sums
3050	SsssSnH	Sum of sssSnH E-states	Atom-type E-state indices	E-State sums
3051	SssssSn	Sum of ssssSn E-states	Atom-type E-state indices	E-State sums
3052	SsPbH3	Sum of sPbH3 E-states	Atom-type E-state indices	E-State sums
3053	SssPbH2	Sum of ssPbH2 E-states	Atom-type E-state indices	E-State sums
3054	SsssPbH	Sum of sssPbH E-states	Atom-type E-state indices	E-State sums
3055	SssssPb	Sum of ssssPb E-states	Atom-type E-state indices	E-State sums
3056	SsSiH3	Sum of sSiH3 E-states	Atom-type E-state indices	E-State sums
3057	SssSiH2	Sum of ssSiH2 E-states	Atom-type E-state indices	E-State sums
3058	SsssSiH	Sum of sssSiH E-states	Atom-type E-state indices	E-State sums
3059	SssssSi	Sum of ssssSi E-states	Atom-type E-state indices	E-State sums
3060	NsCH3	Number of atoms of type sCH3	Atom-type E-state indices	Atom-type counts
3061	NdCH2	Number of atoms of type dCH2	Atom-type E-state indices	Atom-type counts
3062	NssCH2	Number of atoms of type ssCH2	Atom-type E-state indices	Atom-type counts
3063	NtCH	Number of atoms of type tCH	Atom-type E-state indices	Atom-type counts

3064	NdsCH	Number of atoms of type dsCH	Atom-type E-state indices	Atom-type counts
3065	NaaCH	Number of atoms of type aaCH	Atom-type E-state indices	Atom-type counts
3066	NsssCH	Number of atoms of type sssCH	Atom-type E-state indices	Atom-type counts
3067	NddC	Number of atoms of type ddC	Atom-type E-state indices	Atom-type counts
3068	NtsC	Number of atoms of type tsC	Atom-type E-state indices	Atom-type counts
3069	NdssC	Number of atoms of type dssC	Atom-type E-state indices	Atom-type counts
3070	NaasC	Number of atoms of type aasC	Atom-type E-state indices	Atom-type counts
3071	NaaaC	Number of atoms of type aaaC	Atom-type E-state indices	Atom-type counts
3072	NssssC	Number of atoms of type ssssC	Atom-type E-state indices	Atom-type counts
3073	NsNH2	Number of atoms of type sNH2	Atom-type E-state indices	Atom-type counts
3074	NssNH	Number of atoms of type ssNH	Atom-type E-state indices	Atom-type counts
3075	NdNH	Number of atoms of type dNH	Atom-type E-state indices	Atom-type counts
3076	NsssN	Number of atoms of type sssN	Atom-type E-state indices	Atom-type counts
3077	NdsN	Number of atoms of type dsN	Atom-type E-state indices	Atom-type counts
3078	NaaN	Number of atoms of type aaN	Atom-type E-state indices	Atom-type counts
3079	NtN	Number of atoms of type tN	Atom-type E-state indices	Atom-type counts
3080	NsNH3+	Number of atoms of type sNH3+	Atom-type E-state indices	Atom-type counts
3081	NssNH2+	Number of atoms of type ssNH2+	Atom-type E-state indices	Atom-type counts
3082	NdNH2+	Number of atoms of type dNH2+	Atom-type E-state indices	Atom-type counts
3083	NsssNH+	Number of atoms of type sssNH+	Atom-type E-state indices	Atom-type counts

3084	NssssN+	Number of atoms of type ssssN+	Atom-type E-state indices	Atom-type counts
3085	NddsN	Number of atoms of type ddsN	Atom-type E-state indices	Atom-type counts
3086	NaadN	Number of atoms of type aadN	Atom-type E-state indices	Atom-type counts
3087	NaasN	Number of atoms of type aasN	Atom-type E-state indices	Atom-type counts
3088	NaaNH	Number of atoms of type aaNH	Atom-type E-state indices	Atom-type counts
3089	NsOH	Number of atoms of type sOH	Atom-type E-state indices	Atom-type counts
3090	NdO	Number of atoms of type dO	Atom-type E-state indices	Atom-type counts
3091	NssO	Number of atoms of type ssO	Atom-type E-state indices	Atom-type counts
3092	NaaO	Number of atoms of type aaO	Atom-type E-state indices	Atom-type counts
3093	NsPH2	Number of atoms of type sPH2	Atom-type E-state indices	Atom-type counts
3094	NssPH	Number of atoms of type ssPH	Atom-type E-state indices	Atom-type counts
3095	NsssP	Number of atoms of type sssP	Atom-type E-state indices	Atom-type counts
3096	NdsssP	Number of atoms of type dsssP	Atom-type E-state indices	Atom-type counts
3097	NddsP	Number of atoms of type ddsP	Atom-type E-state indices	Atom-type counts
3098	NsssssP	Number of atoms of type sssssP	Atom-type E-state indices	Atom-type counts
3099	NsSH	Number of atoms of type sSH	Atom-type E-state indices	Atom-type counts
3100	NdS	Number of atoms of type dS	Atom-type E-state indices	Atom-type counts
3101	NssS	Number of atoms of type ssS	Atom-type E-state indices	Atom-type counts
3102	NaaS	Number of atoms of type aaS	Atom-type E-state indices	Atom-type counts
3103	NdssS	Number of atoms of type dssS	Atom-type E-state indices	Atom-type counts

3104	NddssS	Number of atoms of type ddssS	Atom-type E-state indices	Atom-type counts
3105	NsssssssS	Number of atoms of type sssssssS	Atom-type E-state indices	Atom-type counts
3106	NsF	Number of atoms of type sF	Atom-type E-state indices	Atom-type counts
3107	NsCl	Number of atoms of type sCl	Atom-type E-state indices	Atom-type counts
3108	NsBr	Number of atoms of type sBr	Atom-type E-state indices	Atom-type counts
3109	NsI	Number of atoms of type sI	Atom-type E-state indices	Atom-type counts
3110	NsLi	Number of atoms of type sLi	Atom-type E-state indices	Atom-type counts
3111	NssBe	Number of atoms of type ssBe	Atom-type E-state indices	Atom-type counts
3112	NssssBe-	Number of atoms of type ssssBe-	Atom-type E-state indices	Atom-type counts
3113	NsBH2	Number of atoms of type sBH2	Atom-type E-state indices	Atom-type counts
3114	NssBH	Number of atoms of type ssBH	Atom-type E-state indices	Atom-type counts
3115	NsssB	Number of atoms of type sssB	Atom-type E-state indices	Atom-type counts
3116	NssssB-	Number of atoms of type ssssB-	Atom-type E-state indices	Atom-type counts
3117	NsGeH3	Number of atoms of type sGeH3	Atom-type E-state indices	Atom-type counts
3118	NssGeH2	Number of atoms of type ssGeH2	Atom-type E-state indices	Atom-type counts
3119	NsssGeH	Number of atoms of type sssGeH	Atom-type E-state indices	Atom-type counts
3120	NssssGe	Number of atoms of type ssssGe	Atom-type E-state indices	Atom-type counts
3121	NsAsH2	Number of atoms of type sAsH2	Atom-type E-state indices	Atom-type counts
3122	NssAsH	Number of atoms of type ssAsH	Atom-type E-state indices	Atom-type counts
3123	NsssAs	Number of atoms of type sssAs	Atom-type E-state indices	Atom-type counts

3124	NsssssAs	Number of atoms of type sssssAs	Atom-type E-state indices	Atom-type counts
3125	NdsssAs	Number of atoms of type dsssAs	Atom-type E-state indices	Atom-type counts
3126	NddsAs	Number of atoms of type ddsAs	Atom-type E-state indices	Atom-type counts
3127	NsSeH	Number of atoms of type sSeH	Atom-type E-state indices	Atom-type counts
3128	NdSe	Number of atoms of type dSe	Atom-type E-state indices	Atom-type counts
3129	NssSe	Number of atoms of type ssSe	Atom-type E-state indices	Atom-type counts
3130	NaaSe	Number of atoms of type aaSe	Atom-type E-state indices	Atom-type counts
3131	NdssSe	Number of atoms of type dssSe	Atom-type E-state indices	Atom-type counts
3132	NssssssSe	Number of atoms of type ssssssSe	Atom-type E-state indices	Atom-type counts
3133	NddssSe	Number of atoms of type ddssSe	Atom-type E-state indices	Atom-type counts
3134	NsSnH3	Number of atoms of type sSnH3	Atom-type E-state indices	Atom-type counts
3135	NssSnH2	Number of atoms of type ssSnH2	Atom-type E-state indices	Atom-type counts
3136	NsssSnH	Number of atoms of type sssSnH	Atom-type E-state indices	Atom-type counts
3137	NssssSn	Number of atoms of type ssssSn	Atom-type E-state indices	Atom-type counts
3138	NsPbH3	Number of atoms of type sPbH3	Atom-type E-state indices	Atom-type counts
3139	NssPbH2	Number of atoms of type ssPbH2	Atom-type E-state indices	Atom-type counts
3140	NsssPbH	Number of atoms of type sssPbH	Atom-type E-state indices	Atom-type counts
3141	NssssPb	Number of atoms of type ssssPb	Atom-type E-state indices	Atom-type counts
3142	NsSiH3	Number of atoms of type sSiH3	Atom-type E-state indices	Atom-type counts
3143	NssSiH2	Number of atoms of type ssSiH2	Atom-type E-state indices	Atom-type counts

3144	NsssSiH	Number of atoms of type sssSiH	Atom-type E-state indices	Atom-type counts
3145	NssssSi	Number of atoms of type ssssSi	Atom-type E-state indices	Atom-type counts
3146	CATS2D_00_DD	CATS2D Donor-Donor at lag 00	Pharmacophore descriptors	CATS 2D descriptors
3147	CATS2D_01_DD	CATS2D Donor-Donor at lag 01	Pharmacophore descriptors	CATS 2D descriptors
3148	CATS2D_02_DD	CATS2D Donor-Donor at lag 02	Pharmacophore descriptors	CATS 2D descriptors
3149	CATS2D_03_DD	CATS2D Donor-Donor at lag 03	Pharmacophore descriptors	CATS 2D descriptors
3150	CATS2D_04_DD	CATS2D Donor-Donor at lag 04	Pharmacophore descriptors	CATS 2D descriptors
3151	CATS2D_05_DD	CATS2D Donor-Donor at lag 05	Pharmacophore descriptors	CATS 2D descriptors
3152	CATS2D_06_DD	CATS2D Donor-Donor at lag 06	Pharmacophore descriptors	CATS 2D descriptors
3153	CATS2D_07_DD	CATS2D Donor-Donor at lag 07	Pharmacophore descriptors	CATS 2D descriptors
3154	CATS2D_08_DD	CATS2D Donor-Donor at lag 08	Pharmacophore descriptors	CATS 2D descriptors
3155	CATS2D_09_DD	CATS2D Donor-Donor at lag 09	Pharmacophore descriptors	CATS 2D descriptors
3156	CATS2D_00_DA	CATS2D Donor-Acceptor at lag 00	Pharmacophore descriptors	CATS 2D descriptors
3157	CATS2D_01_DA	CATS2D Donor-Acceptor at lag 01	Pharmacophore descriptors	CATS 2D descriptors
3158	CATS2D_02_DA	CATS2D Donor-Acceptor at lag 02	Pharmacophore descriptors	CATS 2D descriptors
3159	CATS2D_03_DA	CATS2D Donor-Acceptor at lag 03	Pharmacophore descriptors	CATS 2D descriptors
3160	CATS2D_04_DA	CATS2D Donor-Acceptor at lag 04	Pharmacophore descriptors	CATS 2D descriptors
3161	CATS2D_05_DA	CATS2D Donor-Acceptor at lag 05	Pharmacophore descriptors	CATS 2D descriptors
3162	CATS2D_06_DA	CATS2D Donor-Acceptor at lag 06	Pharmacophore descriptors	CATS 2D descriptors
3163	CATS2D_07_DA	CATS2D Donor-Acceptor at lag 07	Pharmacophore descriptors	CATS 2D descriptors

3164	CATS2D_08_DA	CATS2D Donor-Acceptor at lag 08	Pharmacophore descriptors	CATS 2D descriptors
3165	CATS2D_09_DA	CATS2D Donor-Acceptor at lag 09	Pharmacophore descriptors	CATS 2D descriptors
3166	CATS2D_00_DP	CATS2D Donor-Positive at lag 00	Pharmacophore descriptors	CATS 2D descriptors
3167	CATS2D_01_DP	CATS2D Donor-Positive at lag 01	Pharmacophore descriptors	CATS 2D descriptors
3168	CATS2D_02_DP	CATS2D Donor-Positive at lag 02	Pharmacophore descriptors	CATS 2D descriptors
3169	CATS2D_03_DP	CATS2D Donor-Positive at lag 03	Pharmacophore descriptors	CATS 2D descriptors
3170	CATS2D_04_DP	CATS2D Donor-Positive at lag 04	Pharmacophore descriptors	CATS 2D descriptors
3171	CATS2D_05_DP	CATS2D Donor-Positive at lag 05	Pharmacophore descriptors	CATS 2D descriptors
3172	CATS2D_06_DP	CATS2D Donor-Positive at lag 06	Pharmacophore descriptors	CATS 2D descriptors
3173	CATS2D_07_DP	CATS2D Donor-Positive at lag 07	Pharmacophore descriptors	CATS 2D descriptors
3174	CATS2D_08_DP	CATS2D Donor-Positive at lag 08	Pharmacophore descriptors	CATS 2D descriptors
3175	CATS2D_09_DP	CATS2D Donor-Positive at lag 09	Pharmacophore descriptors	CATS 2D descriptors
3176	CATS2D_00_DN	CATS2D Donor-Negative at lag 00	Pharmacophore descriptors	CATS 2D descriptors
3177	CATS2D_01_DN	CATS2D Donor-Negative at lag 01	Pharmacophore descriptors	CATS 2D descriptors
3178	CATS2D_02_DN	CATS2D Donor-Negative at lag 02	Pharmacophore descriptors	CATS 2D descriptors
3179	CATS2D_03_DN	CATS2D Donor-Negative at lag 03	Pharmacophore descriptors	CATS 2D descriptors
3180	CATS2D_04_DN	CATS2D Donor-Negative at lag 04	Pharmacophore descriptors	CATS 2D descriptors
3181	CATS2D_05_DN	CATS2D Donor-Negative at lag 05	Pharmacophore descriptors	CATS 2D descriptors
3182	CATS2D_06_DN	CATS2D Donor-Negative at lag 06	Pharmacophore descriptors	CATS 2D descriptors
3183	CATS2D_07_DN	CATS2D Donor-Negative at lag 07	Pharmacophore descriptors	CATS 2D descriptors

3184	CATS2D_08_DN	CATS2D Donor-Negative at lag 08	Pharmacophore descriptors	CATS 2D descriptors
3185	CATS2D_09_DN	CATS2D Donor-Negative at lag 09	Pharmacophore descriptors	CATS 2D descriptors
3186	CATS2D_00_DL	CATS2D Donor-Lipophilic at lag 00	Pharmacophore descriptors	CATS 2D descriptors
3187	CATS2D_01_DL	CATS2D Donor-Lipophilic at lag 01	Pharmacophore descriptors	CATS 2D descriptors
3188	CATS2D_02_DL	CATS2D Donor-Lipophilic at lag 02	Pharmacophore descriptors	CATS 2D descriptors
3189	CATS2D_03_DL	CATS2D Donor-Lipophilic at lag 03	Pharmacophore descriptors	CATS 2D descriptors
3190	CATS2D_04_DL	CATS2D Donor-Lipophilic at lag 04	Pharmacophore descriptors	CATS 2D descriptors
3191	CATS2D_05_DL	CATS2D Donor-Lipophilic at lag 05	Pharmacophore descriptors	CATS 2D descriptors
3192	CATS2D_06_DL	CATS2D Donor-Lipophilic at lag 06	Pharmacophore descriptors	CATS 2D descriptors
3193	CATS2D_07_DL	CATS2D Donor-Lipophilic at lag 07	Pharmacophore descriptors	CATS 2D descriptors
3194	CATS2D_08_DL	CATS2D Donor-Lipophilic at lag 08	Pharmacophore descriptors	CATS 2D descriptors
3195	CATS2D_09_DL	CATS2D Donor-Lipophilic at lag 09	Pharmacophore descriptors	CATS 2D descriptors
3196	CATS2D_00_AA	CATS2D Acceptor-Acceptor at lag 00	Pharmacophore descriptors	CATS 2D descriptors
3197	CATS2D_01_AA	CATS2D Acceptor-Acceptor at lag 01	Pharmacophore descriptors	CATS 2D descriptors
3198	CATS2D_02_AA	CATS2D Acceptor-Acceptor at lag 02	Pharmacophore descriptors	CATS 2D descriptors
3199	CATS2D_03_AA	CATS2D Acceptor-Acceptor at lag 03	Pharmacophore descriptors	CATS 2D descriptors
3200	CATS2D_04_AA	CATS2D Acceptor-Acceptor at lag 04	Pharmacophore descriptors	CATS 2D descriptors
3201	CATS2D_05_AA	CATS2D Acceptor-Acceptor at lag 05	Pharmacophore descriptors	CATS 2D descriptors
3202	CATS2D_06_AA	CATS2D Acceptor-Acceptor at lag 06	Pharmacophore descriptors	CATS 2D descriptors
3203	CATS2D_07_AA	CATS2D Acceptor-Acceptor at lag 07	Pharmacophore descriptors	CATS 2D descriptors

3204	CATS2D_08_AA	CATS2D Acceptor-Acceptor at lag 08	Pharmacophore descriptors	CATS 2D descriptors
3205	CATS2D_09_AA	CATS2D Acceptor-Acceptor at lag 09	Pharmacophore descriptors	CATS 2D descriptors
3206	CATS2D_00_AP	CATS2D Acceptor-Positive at lag 00	Pharmacophore descriptors	CATS 2D descriptors
3207	CATS2D_01_AP	CATS2D Acceptor-Positive at lag 01	Pharmacophore descriptors	CATS 2D descriptors
3208	CATS2D_02_AP	CATS2D Acceptor-Positive at lag 02	Pharmacophore descriptors	CATS 2D descriptors
3209	CATS2D_03_AP	CATS2D Acceptor-Positive at lag 03	Pharmacophore descriptors	CATS 2D descriptors
3210	CATS2D_04_AP	CATS2D Acceptor-Positive at lag 04	Pharmacophore descriptors	CATS 2D descriptors
3211	CATS2D_05_AP	CATS2D Acceptor-Positive at lag 05	Pharmacophore descriptors	CATS 2D descriptors
3212	CATS2D_06_AP	CATS2D Acceptor-Positive at lag 06	Pharmacophore descriptors	CATS 2D descriptors
3213	CATS2D_07_AP	CATS2D Acceptor-Positive at lag 07	Pharmacophore descriptors	CATS 2D descriptors
3214	CATS2D_08_AP	CATS2D Acceptor-Positive at lag 08	Pharmacophore descriptors	CATS 2D descriptors
3215	CATS2D_09_AP	CATS2D Acceptor-Positive at lag 09	Pharmacophore descriptors	CATS 2D descriptors
3216	CATS2D_00_AN	CATS2D Acceptor-Negative at lag 00	Pharmacophore descriptors	CATS 2D descriptors
3217	CATS2D_01_AN	CATS2D Acceptor-Negative at lag 01	Pharmacophore descriptors	CATS 2D descriptors
3218	CATS2D_02_AN	CATS2D Acceptor-Negative at lag 02	Pharmacophore descriptors	CATS 2D descriptors
3219	CATS2D_03_AN	CATS2D Acceptor-Negative at lag 03	Pharmacophore descriptors	CATS 2D descriptors
3220	CATS2D_04_AN	CATS2D Acceptor-Negative at lag 04	Pharmacophore descriptors	CATS 2D descriptors
3221	CATS2D_05_AN	CATS2D Acceptor-Negative at lag 05	Pharmacophore descriptors	CATS 2D descriptors
3222	CATS2D_06_AN	CATS2D Acceptor-Negative at lag 06	Pharmacophore descriptors	CATS 2D descriptors
3223	CATS2D_07_AN	CATS2D Acceptor-Negative at lag 07	Pharmacophore descriptors	CATS 2D descriptors

3224	CATS2D_08_AN	CATS2D Acceptor-Negative at lag 08	Pharmacophore descriptors	CATS 2D descriptors
3225	CATS2D_09_AN	CATS2D Acceptor-Negative at lag 09	Pharmacophore descriptors	CATS 2D descriptors
3226	CATS2D_00_AL	CATS2D Acceptor-Lipophilic at lag 00	Pharmacophore descriptors	CATS 2D descriptors
3227	CATS2D_01_AL	CATS2D Acceptor-Lipophilic at lag 01	Pharmacophore descriptors	CATS 2D descriptors
3228	CATS2D_02_AL	CATS2D Acceptor-Lipophilic at lag 02	Pharmacophore descriptors	CATS 2D descriptors
3229	CATS2D_03_AL	CATS2D Acceptor-Lipophilic at lag 03	Pharmacophore descriptors	CATS 2D descriptors
3230	CATS2D_04_AL	CATS2D Acceptor-Lipophilic at lag 04	Pharmacophore descriptors	CATS 2D descriptors
3231	CATS2D_05_AL	CATS2D Acceptor-Lipophilic at lag 05	Pharmacophore descriptors	CATS 2D descriptors
3232	CATS2D_06_AL	CATS2D Acceptor-Lipophilic at lag 06	Pharmacophore descriptors	CATS 2D descriptors
3233	CATS2D_07_AL	CATS2D Acceptor-Lipophilic at lag 07	Pharmacophore descriptors	CATS 2D descriptors
3234	CATS2D_08_AL	CATS2D Acceptor-Lipophilic at lag 08	Pharmacophore descriptors	CATS 2D descriptors
3235	CATS2D_09_AL	CATS2D Acceptor-Lipophilic at lag 09	Pharmacophore descriptors	CATS 2D descriptors
3236	CATS2D_00_PP	CATS2D Positive-Positive at lag 00	Pharmacophore descriptors	CATS 2D descriptors
3237	CATS2D_01_PP	CATS2D Positive-Positive at lag 01	Pharmacophore descriptors	CATS 2D descriptors
3238	CATS2D_02_PP	CATS2D Positive-Positive at lag 02	Pharmacophore descriptors	CATS 2D descriptors
3239	CATS2D_03_PP	CATS2D Positive-Positive at lag 03	Pharmacophore descriptors	CATS 2D descriptors
3240	CATS2D_04_PP	CATS2D Positive-Positive at lag 04	Pharmacophore descriptors	CATS 2D descriptors
3241	CATS2D_05_PP	CATS2D Positive-Positive at lag 05	Pharmacophore descriptors	CATS 2D descriptors
3242	CATS2D_06_PP	CATS2D Positive-Positive at lag 06	Pharmacophore descriptors	CATS 2D descriptors
3243	CATS2D_07_PP	CATS2D Positive-Positive at lag 07	Pharmacophore descriptors	CATS 2D descriptors

3244	CATS2D_08_PP	CATS2D Positive-Positive at lag 08	Pharmacophore descriptors	CATS 2D descriptors
3245	CATS2D_09_PP	CATS2D Positive-Positive at lag 09	Pharmacophore descriptors	CATS 2D descriptors
3246	CATS2D_00_PN	CATS2D Positive-Negative at lag 00	Pharmacophore descriptors	CATS 2D descriptors
3247	CATS2D_01_PN	CATS2D Positive-Negative at lag 01	Pharmacophore descriptors	CATS 2D descriptors
3248	CATS2D_02_PN	CATS2D Positive-Negative at lag 02	Pharmacophore descriptors	CATS 2D descriptors
3249	CATS2D_03_PN	CATS2D Positive-Negative at lag 03	Pharmacophore descriptors	CATS 2D descriptors
3250	CATS2D_04_PN	CATS2D Positive-Negative at lag 04	Pharmacophore descriptors	CATS 2D descriptors
3251	CATS2D_05_PN	CATS2D Positive-Negative at lag 05	Pharmacophore descriptors	CATS 2D descriptors
3252	CATS2D_06_PN	CATS2D Positive-Negative at lag 06	Pharmacophore descriptors	CATS 2D descriptors
3253	CATS2D_07_PN	CATS2D Positive-Negative at lag 07	Pharmacophore descriptors	CATS 2D descriptors
3254	CATS2D_08_PN	CATS2D Positive-Negative at lag 08	Pharmacophore descriptors	CATS 2D descriptors
3255	CATS2D_09_PN	CATS2D Positive-Negative at lag 09	Pharmacophore descriptors	CATS 2D descriptors
3256	CATS2D_00_PL	CATS2D Positive-Lipophilic at lag 00	Pharmacophore descriptors	CATS 2D descriptors
3257	CATS2D_01_PL	CATS2D Positive-Lipophilic at lag 01	Pharmacophore descriptors	CATS 2D descriptors
3258	CATS2D_02_PL	CATS2D Positive-Lipophilic at lag 02	Pharmacophore descriptors	CATS 2D descriptors
3259	CATS2D_03_PL	CATS2D Positive-Lipophilic at lag 03	Pharmacophore descriptors	CATS 2D descriptors
3260	CATS2D_04_PL	CATS2D Positive-Lipophilic at lag 04	Pharmacophore descriptors	CATS 2D descriptors
3261	CATS2D_05_PL	CATS2D Positive-Lipophilic at lag 05	Pharmacophore descriptors	CATS 2D descriptors
3262	CATS2D_06_PL	CATS2D Positive-Lipophilic at lag 06	Pharmacophore descriptors	CATS 2D descriptors
3263	CATS2D_07_PL	CATS2D Positive-Lipophilic at lag 07	Pharmacophore descriptors	CATS 2D descriptors

3264	CATS2D_08_PL	CATS2D Positive-Lipophilic at lag 08	Pharmacophore descriptors	CATS 2D descriptors
3265	CATS2D_09_PL	CATS2D Positive-Lipophilic at lag 09	Pharmacophore descriptors	CATS 2D descriptors
3266	CATS2D_00_NN	CATS2D Negative-Negative at lag 00	Pharmacophore descriptors	CATS 2D descriptors
3267	CATS2D_01_NN	CATS2D Negative-Negative at lag 01	Pharmacophore descriptors	CATS 2D descriptors
3268	CATS2D_02_NN	CATS2D Negative-Negative at lag 02	Pharmacophore descriptors	CATS 2D descriptors
3269	CATS2D_03_NN	CATS2D Negative-Negative at lag 03	Pharmacophore descriptors	CATS 2D descriptors
3270	CATS2D_04_NN	CATS2D Negative-Negative at lag 04	Pharmacophore descriptors	CATS 2D descriptors
3271	CATS2D_05_NN	CATS2D Negative-Negative at lag 05	Pharmacophore descriptors	CATS 2D descriptors
3272	CATS2D_06_NN	CATS2D Negative-Negative at lag 06	Pharmacophore descriptors	CATS 2D descriptors
3273	CATS2D_07_NN	CATS2D Negative-Negative at lag 07	Pharmacophore descriptors	CATS 2D descriptors
3274	CATS2D_08_NN	CATS2D Negative-Negative at lag 08	Pharmacophore descriptors	CATS 2D descriptors
3275	CATS2D_09_NN	CATS2D Negative-Negative at lag 09	Pharmacophore descriptors	CATS 2D descriptors
3276	CATS2D_00_NL	CATS2D Negative-Lipophilic at lag 00	Pharmacophore descriptors	CATS 2D descriptors
3277	CATS2D_01_NL	CATS2D Negative-Lipophilic at lag 01	Pharmacophore descriptors	CATS 2D descriptors
3278	CATS2D_02_NL	CATS2D Negative-Lipophilic at lag 02	Pharmacophore descriptors	CATS 2D descriptors
3279	CATS2D_03_NL	CATS2D Negative-Lipophilic at lag 03	Pharmacophore descriptors	CATS 2D descriptors
3280	CATS2D_04_NL	CATS2D Negative-Lipophilic at lag 04	Pharmacophore descriptors	CATS 2D descriptors
3281	CATS2D_05_NL	CATS2D Negative-Lipophilic at lag 05	Pharmacophore descriptors	CATS 2D descriptors
3282	CATS2D_06_NL	CATS2D Negative-Lipophilic at lag 06	Pharmacophore descriptors	CATS 2D descriptors
3283	CATS2D_07_NL	CATS2D Negative-Lipophilic at lag 07	Pharmacophore descriptors	CATS 2D descriptors

3284	CATS2D_08_NL	CATS2D Negative-Lipophilic at lag 08	Pharmacophore descriptors	CATS 2D descriptors
3285	CATS2D_09_NL	CATS2D Negative-Lipophilic at lag 09	Pharmacophore descriptors	CATS 2D descriptors
3286	CATS2D_00_LL	CATS2D Lipophilic-Lipophilic at lag 00	Pharmacophore descriptors	CATS 2D descriptors
3287	CATS2D_01_LL	CATS2D Lipophilic-Lipophilic at lag 01	Pharmacophore descriptors	CATS 2D descriptors
3288	CATS2D_02_LL	CATS2D Lipophilic-Lipophilic at lag 02	Pharmacophore descriptors	CATS 2D descriptors
3289	CATS2D_03_LL	CATS2D Lipophilic-Lipophilic at lag 03	Pharmacophore descriptors	CATS 2D descriptors
3290	CATS2D_04_LL	CATS2D Lipophilic-Lipophilic at lag 04	Pharmacophore descriptors	CATS 2D descriptors
3291	CATS2D_05_LL	CATS2D Lipophilic-Lipophilic at lag 05	Pharmacophore descriptors	CATS 2D descriptors
3292	CATS2D_06_LL	CATS2D Lipophilic-Lipophilic at lag 06	Pharmacophore descriptors	CATS 2D descriptors
3293	CATS2D_07_LL	CATS2D Lipophilic-Lipophilic at lag 07	Pharmacophore descriptors	CATS 2D descriptors
3294	CATS2D_08_LL	CATS2D Lipophilic-Lipophilic at lag 08	Pharmacophore descriptors	CATS 2D descriptors
3295	CATS2D_09_LL	CATS2D Lipophilic-Lipophilic at lag 09	Pharmacophore descriptors	CATS 2D descriptors
3296	SHED_DD	SHED Donor-Donor	Pharmacophore descriptors	SHED descriptors
3297	SHED_DA	SHED Donor-Acceptor	Pharmacophore descriptors	SHED descriptors
3298	SHED_DP	SHED Donor-Positive	Pharmacophore descriptors	SHED descriptors
3299	SHED_DN	SHED Donor-Negative	Pharmacophore descriptors	SHED descriptors
3300	SHED_DL	SHED Donor-Lipophilic	Pharmacophore descriptors	SHED descriptors
3301	SHED_AA	SHED Acceptor-Acceptor	Pharmacophore descriptors	SHED descriptors
3302	SHED_AP	SHED Acceptor-Positive	Pharmacophore descriptors	SHED descriptors
3303	SHED_AN	SHED Acceptor-Negative	Pharmacophore descriptors	SHED descriptors

3304	SHED_AL	SHED Acceptor-Lipophilic	Pharmacophore descriptors	SHED descriptors
3305	SHED_PP	SHED Positive-Positive	Pharmacophore descriptors	SHED descriptors
3306	SHED_PN	SHED Positive-Negative	Pharmacophore descriptors	SHED descriptors
3307	SHED_PL	SHED Positive-Lipophilic	Pharmacophore descriptors	SHED descriptors
3308	SHED_NN	SHED Negative-Negative	Pharmacophore descriptors	SHED descriptors
3309	SHED_NL	SHED Negative-Lipophilic	Pharmacophore descriptors	SHED descriptors
3310	SHED_LL	SHED Lipophilic-Lipophilic	Pharmacophore descriptors	SHED descriptors
3311	T(N..N)	sum of topological distances between N..N	2D Atom Pairs	Weighted topological atom pairs
3312	T(N..O)	sum of topological distances between N..O	2D Atom Pairs	Weighted topological atom pairs
3313	T(N..S)	sum of topological distances between N..S	2D Atom Pairs	Weighted topological atom pairs
3314	T(N..P)	sum of topological distances between N..P	2D Atom Pairs	Weighted topological atom pairs
3315	T(N..F)	sum of topological distances between N..F	2D Atom Pairs	Weighted topological atom pairs
3316	T(N..Cl)	sum of topological distances between N..Cl	2D Atom Pairs	Weighted topological atom pairs
3317	T(N..Br)	sum of topological distances between N..Br	2D Atom Pairs	Weighted topological atom pairs
3318	T(N..I)	sum of topological distances between N..I	2D Atom Pairs	Weighted topological atom pairs
3319	T(O..O)	sum of topological distances between O..O	2D Atom Pairs	Weighted topological atom pairs
3320	T(O..S)	sum of topological distances between O..S	2D Atom Pairs	Weighted topological atom pairs
3321	T(O..P)	sum of topological distances between O..P	2D Atom Pairs	Weighted topological atom pairs
3322	T(O..F)	sum of topological distances between O..F	2D Atom Pairs	Weighted topological atom pairs
3323	T(O..Cl)	sum of topological distances between O..Cl	2D Atom Pairs	Weighted topological atom pairs

3324	T(O..Br)	sum of topological distances between O..Br	2D Atom Pairs	Weighted topological atom pairs
3325	T(O..I)	sum of topological distances between O..I	2D Atom Pairs	Weighted topological atom pairs
3326	T(S..S)	sum of topological distances between S..S	2D Atom Pairs	Weighted topological atom pairs
3327	T(S..P)	sum of topological distances between S..P	2D Atom Pairs	Weighted topological atom pairs
3328	T(S..F)	sum of topological distances between S..F	2D Atom Pairs	Weighted topological atom pairs
3329	T(S..Cl)	sum of topological distances between S..Cl	2D Atom Pairs	Weighted topological atom pairs
3330	T(S..Br)	sum of topological distances between S..Br	2D Atom Pairs	Weighted topological atom pairs
3331	T(S..I)	sum of topological distances between S..I	2D Atom Pairs	Weighted topological atom pairs
3332	T(P..P)	sum of topological distances between P..P	2D Atom Pairs	Weighted topological atom pairs
3333	T(P..F)	sum of topological distances between P..F	2D Atom Pairs	Weighted topological atom pairs
3334	T(P..Cl)	sum of topological distances between P..Cl	2D Atom Pairs	Weighted topological atom pairs
3335	T(P..Br)	sum of topological distances between P..Br	2D Atom Pairs	Weighted topological atom pairs
3336	T(P..I)	sum of topological distances between P..I	2D Atom Pairs	Weighted topological atom pairs
3337	T(F..F)	sum of topological distances between F..F	2D Atom Pairs	Weighted topological atom pairs
3338	T(F..Cl)	sum of topological distances between F..Cl	2D Atom Pairs	Weighted topological atom pairs
3339	T(F..Br)	sum of topological distances between F..Br	2D Atom Pairs	Weighted topological atom pairs
3340	T(F..I)	sum of topological distances between F..I	2D Atom Pairs	Weighted topological atom pairs
3341	T(Cl..Cl)	sum of topological distances between Cl..Cl	2D Atom Pairs	Weighted topological atom pairs
3342	T(Cl..Br)	sum of topological distances between Cl..Br	2D Atom Pairs	Weighted topological atom pairs
3343	T(Cl..I)	sum of topological distances between Cl..I	2D Atom Pairs	Weighted topological atom pairs

3344	T(Br..Br)	sum of topological distances between Br..Br	2D Atom Pairs	Weighted topological atom pairs
3345	T(Br..I)	sum of topological distances between Br..I	2D Atom Pairs	Weighted topological atom pairs
3346	T(I..I)	sum of topological distances between I..I	2D Atom Pairs	Weighted topological atom pairs
3347	B01[C-C]	Presence/absence of C - C at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3348	B01[C-N]	Presence/absence of C - N at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3349	B01[C-O]	Presence/absence of C - O at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3350	B01[C-S]	Presence/absence of C - S at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3351	B01[C-P]	Presence/absence of C - P at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3352	B01[C-F]	Presence/absence of C - F at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3353	B01[C-Cl]	Presence/absence of C - Cl at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3354	B01[C-Br]	Presence/absence of C - Br at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3355	B01[C-I]	Presence/absence of C - I at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3356	B01[C-B]	Presence/absence of C - B at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3357	B01[C-Si]	Presence/absence of C - Si at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3358	B01[C-X]	Presence/absence of C - X at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3359	B01[N-N]	Presence/absence of N - N at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3360	B01[N-O]	Presence/absence of N - O at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3361	B01[N-S]	Presence/absence of N - S at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3362	B01[N-P]	Presence/absence of N - P at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3363	B01[N-F]	Presence/absence of N - F at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1

3364	B01[N-Cl]	Presence/absence of N - Cl at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3365	B01[N-Br]	Presence/absence of N - Br at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3366	B01[N-I]	Presence/absence of N - I at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3367	B01[N-B]	Presence/absence of N - B at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3368	B01[N-Si]	Presence/absence of N - Si at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3369	B01[N-X]	Presence/absence of N - X at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3370	B01[O-O]	Presence/absence of O - O at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3371	B01[O-S]	Presence/absence of O - S at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3372	B01[O-P]	Presence/absence of O - P at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3373	B01[O-F]	Presence/absence of O - F at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3374	B01[O-Cl]	Presence/absence of O - Cl at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3375	B01[O-Br]	Presence/absence of O - Br at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3376	B01[O-I]	Presence/absence of O - I at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3377	B01[O-B]	Presence/absence of O - B at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3378	B01[O-Si]	Presence/absence of O - Si at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3379	B01[O-X]	Presence/absence of O - X at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3380	B01[S-S]	Presence/absence of S - S at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3381	B01[S-P]	Presence/absence of S - P at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3382	B01[S-F]	Presence/absence of S - F at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3383	B01[S-Cl]	Presence/absence of S - Cl at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1

3384	B01[S-Br]	Presence/absence of S - Br at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3385	B01[S-I]	Presence/absence of S - I at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3386	B01[S-B]	Presence/absence of S - B at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3387	B01[S-Si]	Presence/absence of S - Si at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3388	B01[S-X]	Presence/absence of S - X at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3389	B01[P-P]	Presence/absence of P - P at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3390	B01[P-F]	Presence/absence of P - F at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3391	B01[P-Cl]	Presence/absence of P - Cl at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3392	B01[P-Br]	Presence/absence of P - Br at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3393	B01[P-I]	Presence/absence of P - I at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3394	B01[P-B]	Presence/absence of P - B at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3395	B01[P-Si]	Presence/absence of P - Si at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3396	B01[P-X]	Presence/absence of P - X at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3397	B01[F-F]	Presence/absence of F - F at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3398	B01[F-Cl]	Presence/absence of F - Cl at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3399	B01[F-Br]	Presence/absence of F - Br at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3400	B01[F-I]	Presence/absence of F - I at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3401	B01[F-B]	Presence/absence of F - B at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3402	B01[F-Si]	Presence/absence of F - Si at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3403	B01[F-X]	Presence/absence of F - X at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1

3404	B01[Cl-Cl]	Presence/absence of Cl - Cl at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3405	B01[Cl-Br]	Presence/absence of Cl - Br at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3406	B01[Cl-I]	Presence/absence of Cl - I at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3407	B01[Cl-B]	Presence/absence of Cl - B at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3408	B01[Cl-Si]	Presence/absence of Cl - Si at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3409	B01[Cl-X]	Presence/absence of Cl - X at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3410	B01[Br-Br]	Presence/absence of Br - Br at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3411	B01[Br-I]	Presence/absence of Br - I at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3412	B01[Br-B]	Presence/absence of Br - B at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3413	B01[Br-Si]	Presence/absence of Br - Si at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3414	B01[Br-X]	Presence/absence of Br - X at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3415	B01[I-I]	Presence/absence of I - I at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3416	B01[I-B]	Presence/absence of I - B at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3417	B01[I-Si]	Presence/absence of I - Si at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3418	B01[I-X]	Presence/absence of I - X at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3419	B01[B-B]	Presence/absence of B - B at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3420	B01[B-Si]	Presence/absence of B - Si at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3421	B01[B-X]	Presence/absence of B - X at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3422	B01[Si-Si]	Presence/absence of Si - Si at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3423	B01[Si-X]	Presence/absence of Si - X at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1

3424	B01[X-X]	Presence/absence of X - X at topological distance 1	2D Atom Pairs	Binary Atom Pairs of order 1
3425	B02[C-C]	Presence/absence of C - C at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3426	B02[C-N]	Presence/absence of C - N at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3427	B02[C-O]	Presence/absence of C - O at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3428	B02[C-S]	Presence/absence of C - S at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3429	B02[C-P]	Presence/absence of C - P at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3430	B02[C-F]	Presence/absence of C - F at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3431	B02[C-Cl]	Presence/absence of C - Cl at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3432	B02[C-Br]	Presence/absence of C - Br at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3433	B02[C-I]	Presence/absence of C - I at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3434	B02[C-B]	Presence/absence of C - B at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3435	B02[C-Si]	Presence/absence of C - Si at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3436	B02[C-X]	Presence/absence of C - X at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3437	B02[N-N]	Presence/absence of N - N at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3438	B02[N-O]	Presence/absence of N - O at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3439	B02[N-S]	Presence/absence of N - S at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3440	B02[N-P]	Presence/absence of N - P at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3441	B02[N-F]	Presence/absence of N - F at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3442	B02[N-Cl]	Presence/absence of N - Cl at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3443	B02[N-Br]	Presence/absence of N - Br at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2

3444	B02[N-I]	Presence/absence of N - I at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3445	B02[N-B]	Presence/absence of N - B at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3446	B02[N-Si]	Presence/absence of N - Si at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3447	B02[N-X]	Presence/absence of N - X at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3448	B02[O-O]	Presence/absence of O - O at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3449	B02[O-S]	Presence/absence of O - S at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3450	B02[O-P]	Presence/absence of O - P at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3451	B02[O-F]	Presence/absence of O - F at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3452	B02[O-Cl]	Presence/absence of O - Cl at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3453	B02[O-Br]	Presence/absence of O - Br at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3454	B02[O-I]	Presence/absence of O - I at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3455	B02[O-B]	Presence/absence of O - B at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3456	B02[O-Si]	Presence/absence of O - Si at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3457	B02[O-X]	Presence/absence of O - X at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3458	B02[S-S]	Presence/absence of S - S at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3459	B02[S-P]	Presence/absence of S - P at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3460	B02[S-F]	Presence/absence of S - F at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3461	B02[S-Cl]	Presence/absence of S - Cl at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3462	B02[S-Br]	Presence/absence of S - Br at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3463	B02[S-I]	Presence/absence of S - I at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2

3464	B02[S-B]	Presence/absence of S - B at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3465	B02[S-Si]	Presence/absence of S - Si at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3466	B02[S-X]	Presence/absence of S - X at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3467	B02[P-P]	Presence/absence of P - P at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3468	B02[P-F]	Presence/absence of P - F at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3469	B02[P-Cl]	Presence/absence of P - Cl at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3470	B02[P-Br]	Presence/absence of P - Br at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3471	B02[P-I]	Presence/absence of P - I at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3472	B02[P-B]	Presence/absence of P - B at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3473	B02[P-Si]	Presence/absence of P - Si at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3474	B02[P-X]	Presence/absence of P - X at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3475	B02[F-F]	Presence/absence of F - F at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3476	B02[F-Cl]	Presence/absence of F - Cl at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3477	B02[F-Br]	Presence/absence of F - Br at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3478	B02[F-I]	Presence/absence of F - I at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3479	B02[F-B]	Presence/absence of F - B at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3480	B02[F-Si]	Presence/absence of F - Si at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3481	B02[F-X]	Presence/absence of F - X at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3482	B02[Cl-Cl]	Presence/absence of Cl - Cl at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3483	B02[Cl-Br]	Presence/absence of Cl - Br at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2

3484	B02[Cl-I]	Presence/absence of Cl - I at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3485	B02[Cl-B]	Presence/absence of Cl - B at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3486	B02[Cl-Si]	Presence/absence of Cl - Si at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3487	B02[Cl-X]	Presence/absence of Cl - X at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3488	B02[Br-Br]	Presence/absence of Br - Br at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3489	B02[Br-I]	Presence/absence of Br - I at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3490	B02[Br-B]	Presence/absence of Br - B at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3491	B02[Br-Si]	Presence/absence of Br - Si at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3492	B02[Br-X]	Presence/absence of Br - X at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3493	B02[I-I]	Presence/absence of I - I at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3494	B02[I-B]	Presence/absence of I - B at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3495	B02[I-Si]	Presence/absence of I - Si at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3496	B02[I-X]	Presence/absence of I - X at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3497	B02[B-B]	Presence/absence of B - B at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3498	B02[B-Si]	Presence/absence of B - Si at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3499	B02[B-X]	Presence/absence of B - X at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3500	B02[Si-Si]	Presence/absence of Si - Si at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3501	B02[Si-X]	Presence/absence of Si - X at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3502	B02[X-X]	Presence/absence of X - X at topological distance 2	2D Atom Pairs	Binary Atom Pairs of order 2
3503	B03[C-C]	Presence/absence of C - C at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3

3504	B03[C-N]	Presence/absence of C - N at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3505	B03[C-O]	Presence/absence of C - O at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3506	B03[C-S]	Presence/absence of C - S at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3507	B03[C-P]	Presence/absence of C - P at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3508	B03[C-F]	Presence/absence of C - F at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3509	B03[C-Cl]	Presence/absence of C - Cl at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3510	B03[C-Br]	Presence/absence of C - Br at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3511	B03[C-I]	Presence/absence of C - I at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3512	B03[C-B]	Presence/absence of C - B at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3513	B03[C-Si]	Presence/absence of C - Si at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3514	B03[C-X]	Presence/absence of C - X at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3515	B03[N-N]	Presence/absence of N - N at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3516	B03[N-O]	Presence/absence of N - O at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3517	B03[N-S]	Presence/absence of N - S at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3518	B03[N-P]	Presence/absence of N - P at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3519	B03[N-F]	Presence/absence of N - F at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3520	B03[N-Cl]	Presence/absence of N - Cl at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3521	B03[N-Br]	Presence/absence of N - Br at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3522	B03[N-I]	Presence/absence of N - I at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3523	B03[N-B]	Presence/absence of N - B at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3

3524	B03[N-Si]	Presence/absence of N - Si at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3525	B03[N-X]	Presence/absence of N - X at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3526	B03[O-O]	Presence/absence of O - O at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3527	B03[O-S]	Presence/absence of O - S at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3528	B03[O-P]	Presence/absence of O - P at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3529	B03[O-F]	Presence/absence of O - F at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3530	B03[O-Cl]	Presence/absence of O - Cl at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3531	B03[O-Br]	Presence/absence of O - Br at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3532	B03[O-I]	Presence/absence of O - I at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3533	B03[O-B]	Presence/absence of O - B at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3534	B03[O-Si]	Presence/absence of O - Si at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3535	B03[O-X]	Presence/absence of O - X at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3536	B03[S-S]	Presence/absence of S - S at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3537	B03[S-P]	Presence/absence of S - P at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3538	B03[S-F]	Presence/absence of S - F at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3539	B03[S-Cl]	Presence/absence of S - Cl at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3540	B03[S-Br]	Presence/absence of S - Br at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3541	B03[S-I]	Presence/absence of S - I at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3542	B03[S-B]	Presence/absence of S - B at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3543	B03[S-Si]	Presence/absence of S - Si at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3

3544	B03[S-X]	Presence/absence of S - X at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3545	B03[P-P]	Presence/absence of P - P at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3546	B03[P-F]	Presence/absence of P - F at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3547	B03[P-Cl]	Presence/absence of P - Cl at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3548	B03[P-Br]	Presence/absence of P - Br at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3549	B03[P-I]	Presence/absence of P - I at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3550	B03[P-B]	Presence/absence of P - B at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3551	B03[P-Si]	Presence/absence of P - Si at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3552	B03[P-X]	Presence/absence of P - X at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3553	B03[F-F]	Presence/absence of F - F at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3554	B03[F-Cl]	Presence/absence of F - Cl at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3555	B03[F-Br]	Presence/absence of F - Br at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3556	B03[F-I]	Presence/absence of F - I at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3557	B03[F-B]	Presence/absence of F - B at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3558	B03[F-Si]	Presence/absence of F - Si at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3559	B03[F-X]	Presence/absence of F - X at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3560	B03[Cl-Cl]	Presence/absence of Cl - Cl at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3561	B03[Cl-Br]	Presence/absence of Cl - Br at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3562	B03[Cl-I]	Presence/absence of Cl - I at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3563	B03[Cl-B]	Presence/absence of Cl - B at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3

3564	B03[Cl-Si]	Presence/absence of Cl - Si at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3565	B03[Cl-X]	Presence/absence of Cl - X at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3566	B03[Br-Br]	Presence/absence of Br - Br at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3567	B03[Br-I]	Presence/absence of Br - I at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3568	B03[Br-B]	Presence/absence of Br - B at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3569	B03[Br-Si]	Presence/absence of Br - Si at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3570	B03[Br-X]	Presence/absence of Br - X at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3571	B03[I-I]	Presence/absence of I - I at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3572	B03[I-B]	Presence/absence of I - B at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3573	B03[I-Si]	Presence/absence of I - Si at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3574	B03[I-X]	Presence/absence of I - X at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3575	B03[B-B]	Presence/absence of B - B at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3576	B03[B-Si]	Presence/absence of B - Si at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3577	B03[B-X]	Presence/absence of B - X at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3578	B03[Si-Si]	Presence/absence of Si - Si at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3579	B03[Si-X]	Presence/absence of Si - X at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3580	B03[X-X]	Presence/absence of X - X at topological distance 3	2D Atom Pairs	Binary Atom Pairs of order 3
3581	B04[C-C]	Presence/absence of C - C at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3582	B04[C-N]	Presence/absence of C - N at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3583	B04[C-O]	Presence/absence of C - O at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4

3584	B04[C-S]	Presence/absence of C - S at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3585	B04[C-P]	Presence/absence of C - P at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3586	B04[C-F]	Presence/absence of C - F at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3587	B04[C-Cl]	Presence/absence of C - Cl at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3588	B04[C-Br]	Presence/absence of C - Br at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3589	B04[C-I]	Presence/absence of C - I at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3590	B04[C-B]	Presence/absence of C - B at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3591	B04[C-Si]	Presence/absence of C - Si at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3592	B04[C-X]	Presence/absence of C - X at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3593	B04[N-N]	Presence/absence of N - N at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3594	B04[N-O]	Presence/absence of N - O at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3595	B04[N-S]	Presence/absence of N - S at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3596	B04[N-P]	Presence/absence of N - P at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3597	B04[N-F]	Presence/absence of N - F at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3598	B04[N-Cl]	Presence/absence of N - Cl at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3599	B04[N-Br]	Presence/absence of N - Br at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3600	B04[N-I]	Presence/absence of N - I at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3601	B04[N-B]	Presence/absence of N - B at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3602	B04[N-Si]	Presence/absence of N - Si at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3603	B04[N-X]	Presence/absence of N - X at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4

3604	B04[O-O]	Presence/absence of O - O at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3605	B04[O-S]	Presence/absence of O - S at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3606	B04[O-P]	Presence/absence of O - P at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3607	B04[O-F]	Presence/absence of O - F at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3608	B04[O-Cl]	Presence/absence of O - Cl at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3609	B04[O-Br]	Presence/absence of O - Br at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3610	B04[O-I]	Presence/absence of O - I at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3611	B04[O-B]	Presence/absence of O - B at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3612	B04[O-Si]	Presence/absence of O - Si at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3613	B04[O-X]	Presence/absence of O - X at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3614	B04[S-S]	Presence/absence of S - S at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3615	B04[S-P]	Presence/absence of S - P at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3616	B04[S-F]	Presence/absence of S - F at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3617	B04[S-Cl]	Presence/absence of S - Cl at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3618	B04[S-Br]	Presence/absence of S - Br at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3619	B04[S-I]	Presence/absence of S - I at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3620	B04[S-B]	Presence/absence of S - B at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3621	B04[S-Si]	Presence/absence of S - Si at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3622	B04[S-X]	Presence/absence of S - X at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3623	B04[P-P]	Presence/absence of P - P at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4

3624	B04[P-F]	Presence/absence of P - F at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3625	B04[P-Cl]	Presence/absence of P - Cl at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3626	B04[P-Br]	Presence/absence of P - Br at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3627	B04[P-I]	Presence/absence of P - I at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3628	B04[P-B]	Presence/absence of P - B at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3629	B04[P-Si]	Presence/absence of P - Si at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3630	B04[P-X]	Presence/absence of P - X at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3631	B04[F-F]	Presence/absence of F - F at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3632	B04[F-Cl]	Presence/absence of F - Cl at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3633	B04[F-Br]	Presence/absence of F - Br at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3634	B04[F-I]	Presence/absence of F - I at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3635	B04[F-B]	Presence/absence of F - B at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3636	B04[F-Si]	Presence/absence of F - Si at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3637	B04[F-X]	Presence/absence of F - X at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3638	B04[Cl-Cl]	Presence/absence of Cl - Cl at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3639	B04[Cl-Br]	Presence/absence of Cl - Br at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3640	B04[Cl-I]	Presence/absence of Cl - I at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3641	B04[Cl-B]	Presence/absence of Cl - B at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3642	B04[Cl-Si]	Presence/absence of Cl - Si at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3643	B04[Cl-X]	Presence/absence of Cl - X at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4

3644	B04[Br-Br]	Presence/absence of Br - Br at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3645	B04[Br-I]	Presence/absence of Br - I at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3646	B04[Br-B]	Presence/absence of Br - B at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3647	B04[Br-Si]	Presence/absence of Br - Si at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3648	B04[Br-X]	Presence/absence of Br - X at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3649	B04[I-I]	Presence/absence of I - I at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3650	B04[I-B]	Presence/absence of I - B at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3651	B04[I-Si]	Presence/absence of I - Si at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3652	B04[I-X]	Presence/absence of I - X at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3653	B04[B-B]	Presence/absence of B - B at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3654	B04[B-Si]	Presence/absence of B - Si at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3655	B04[B-X]	Presence/absence of B - X at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3656	B04[Si-Si]	Presence/absence of Si - Si at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3657	B04[Si-X]	Presence/absence of Si - X at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3658	B04[X-X]	Presence/absence of X - X at topological distance 4	2D Atom Pairs	Binary Atom Pairs of order 4
3659	B05[C-C]	Presence/absence of C - C at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3660	B05[C-N]	Presence/absence of C - N at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3661	B05[C-O]	Presence/absence of C - O at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3662	B05[C-S]	Presence/absence of C - S at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3663	B05[C-P]	Presence/absence of C - P at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5

3664	B05[C-F]	Presence/absence of C - F at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3665	B05[C-Cl]	Presence/absence of C - Cl at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3666	B05[C-Br]	Presence/absence of C - Br at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3667	B05[C-I]	Presence/absence of C - I at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3668	B05[C-B]	Presence/absence of C - B at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3669	B05[C-Si]	Presence/absence of C - Si at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3670	B05[C-X]	Presence/absence of C - X at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3671	B05[N-N]	Presence/absence of N - N at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3672	B05[N-O]	Presence/absence of N - O at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3673	B05[N-S]	Presence/absence of N - S at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3674	B05[N-P]	Presence/absence of N - P at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3675	B05[N-F]	Presence/absence of N - F at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3676	B05[N-Cl]	Presence/absence of N - Cl at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3677	B05[N-Br]	Presence/absence of N - Br at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3678	B05[N-I]	Presence/absence of N - I at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3679	B05[N-B]	Presence/absence of N - B at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3680	B05[N-Si]	Presence/absence of N - Si at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3681	B05[N-X]	Presence/absence of N - X at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3682	B05[O-O]	Presence/absence of O - O at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3683	B05[O-S]	Presence/absence of O - S at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5

3684	B05[O-P]	Presence/absence of O - P at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3685	B05[O-F]	Presence/absence of O - F at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3686	B05[O-Cl]	Presence/absence of O - Cl at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3687	B05[O-Br]	Presence/absence of O - Br at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3688	B05[O-I]	Presence/absence of O - I at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3689	B05[O-B]	Presence/absence of O - B at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3690	B05[O-Si]	Presence/absence of O - Si at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3691	B05[O-X]	Presence/absence of O - X at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3692	B05[S-S]	Presence/absence of S - S at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3693	B05[S-P]	Presence/absence of S - P at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3694	B05[S-F]	Presence/absence of S - F at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3695	B05[S-Cl]	Presence/absence of S - Cl at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3696	B05[S-Br]	Presence/absence of S - Br at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3697	B05[S-I]	Presence/absence of S - I at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3698	B05[S-B]	Presence/absence of S - B at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3699	B05[S-Si]	Presence/absence of S - Si at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3700	B05[S-X]	Presence/absence of S - X at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3701	B05[P-P]	Presence/absence of P - P at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3702	B05[P-F]	Presence/absence of P - F at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3703	B05[P-Cl]	Presence/absence of P - Cl at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5

3704	B05[P-Br]	Presence/absence of P - Br at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3705	B05[P-I]	Presence/absence of P - I at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3706	B05[P-B]	Presence/absence of P - B at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3707	B05[P-Si]	Presence/absence of P - Si at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3708	B05[P-X]	Presence/absence of P - X at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3709	B05[F-F]	Presence/absence of F - F at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3710	B05[F-Cl]	Presence/absence of F - Cl at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3711	B05[F-Br]	Presence/absence of F - Br at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3712	B05[F-I]	Presence/absence of F - I at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3713	B05[F-B]	Presence/absence of F - B at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3714	B05[F-Si]	Presence/absence of F - Si at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3715	B05[F-X]	Presence/absence of F - X at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3716	B05[Cl-Cl]	Presence/absence of Cl - Cl at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3717	B05[Cl-Br]	Presence/absence of Cl - Br at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3718	B05[Cl-I]	Presence/absence of Cl - I at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3719	B05[Cl-B]	Presence/absence of Cl - B at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3720	B05[Cl-Si]	Presence/absence of Cl - Si at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3721	B05[Cl-X]	Presence/absence of Cl - X at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3722	B05[Br-Br]	Presence/absence of Br - Br at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3723	B05[Br-I]	Presence/absence of Br - I at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5

3724	B05[Br-B]	Presence/absence of Br - B at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3725	B05[Br-Si]	Presence/absence of Br - Si at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3726	B05[Br-X]	Presence/absence of Br - X at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3727	B05[I-I]	Presence/absence of I - I at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3728	B05[I-B]	Presence/absence of I - B at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3729	B05[I-Si]	Presence/absence of I - Si at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3730	B05[I-X]	Presence/absence of I - X at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3731	B05[B-B]	Presence/absence of B - B at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3732	B05[B-Si]	Presence/absence of B - Si at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3733	B05[B-X]	Presence/absence of B - X at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3734	B05[Si-Si]	Presence/absence of Si - Si at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3735	B05[Si-X]	Presence/absence of Si - X at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3736	B05[X-X]	Presence/absence of X - X at topological distance 5	2D Atom Pairs	Binary Atom Pairs of order 5
3737	B06[C-C]	Presence/absence of C - C at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3738	B06[C-N]	Presence/absence of C - N at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3739	B06[C-O]	Presence/absence of C - O at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3740	B06[C-S]	Presence/absence of C - S at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3741	B06[C-P]	Presence/absence of C - P at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3742	B06[C-F]	Presence/absence of C - F at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3743	B06[C-Cl]	Presence/absence of C - Cl at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6

3744	B06[C-Br]	Presence/absence of C - Br at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3745	B06[C-I]	Presence/absence of C - I at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3746	B06[C-B]	Presence/absence of C - B at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3747	B06[C-Si]	Presence/absence of C - Si at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3748	B06[C-X]	Presence/absence of C - X at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3749	B06[N-N]	Presence/absence of N - N at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3750	B06[N-O]	Presence/absence of N - O at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3751	B06[N-S]	Presence/absence of N - S at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3752	B06[N-P]	Presence/absence of N - P at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3753	B06[N-F]	Presence/absence of N - F at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3754	B06[N-Cl]	Presence/absence of N - Cl at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3755	B06[N-Br]	Presence/absence of N - Br at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3756	B06[N-I]	Presence/absence of N - I at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3757	B06[N-B]	Presence/absence of N - B at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3758	B06[N-Si]	Presence/absence of N - Si at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3759	B06[N-X]	Presence/absence of N - X at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3760	B06[O-O]	Presence/absence of O - O at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3761	B06[O-S]	Presence/absence of O - S at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3762	B06[O-P]	Presence/absence of O - P at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3763	B06[O-F]	Presence/absence of O - F at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6

3764	B06[O-Cl]	Presence/absence of O - Cl at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3765	B06[O-Br]	Presence/absence of O - Br at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3766	B06[O-I]	Presence/absence of O - I at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3767	B06[O-B]	Presence/absence of O - B at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3768	B06[O-Si]	Presence/absence of O - Si at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3769	B06[O-X]	Presence/absence of O - X at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3770	B06[S-S]	Presence/absence of S - S at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3771	B06[S-P]	Presence/absence of S - P at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3772	B06[S-F]	Presence/absence of S - F at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3773	B06[S-Cl]	Presence/absence of S - Cl at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3774	B06[S-Br]	Presence/absence of S - Br at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3775	B06[S-I]	Presence/absence of S - I at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3776	B06[S-B]	Presence/absence of S - B at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3777	B06[S-Si]	Presence/absence of S - Si at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3778	B06[S-X]	Presence/absence of S - X at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3779	B06[P-P]	Presence/absence of P - P at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3780	B06[P-F]	Presence/absence of P - F at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3781	B06[P-Cl]	Presence/absence of P - Cl at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3782	B06[P-Br]	Presence/absence of P - Br at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3783	B06[P-I]	Presence/absence of P - I at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6

3784	B06[P-B]	Presence/absence of P - B at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3785	B06[P-Si]	Presence/absence of P - Si at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3786	B06[P-X]	Presence/absence of P - X at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3787	B06[F-F]	Presence/absence of F - F at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3788	B06[F-Cl]	Presence/absence of F - Cl at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3789	B06[F-Br]	Presence/absence of F - Br at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3790	B06[F-I]	Presence/absence of F - I at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3791	B06[F-B]	Presence/absence of F - B at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3792	B06[F-Si]	Presence/absence of F - Si at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3793	B06[F-X]	Presence/absence of F - X at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3794	B06[Cl-Cl]	Presence/absence of Cl - Cl at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3795	B06[Cl-Br]	Presence/absence of Cl - Br at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3796	B06[Cl-I]	Presence/absence of Cl - I at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3797	B06[Cl-B]	Presence/absence of Cl - B at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3798	B06[Cl-Si]	Presence/absence of Cl - Si at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3799	B06[Cl-X]	Presence/absence of Cl - X at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3800	B06[Br-Br]	Presence/absence of Br - Br at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3801	B06[Br-I]	Presence/absence of Br - I at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3802	B06[Br-B]	Presence/absence of Br - B at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3803	B06[Br-Si]	Presence/absence of Br - Si at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6

3804	B06[Br-X]	Presence/absence of Br - X at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3805	B06[I-I]	Presence/absence of I - I at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3806	B06[I-B]	Presence/absence of I - B at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3807	B06[I-Si]	Presence/absence of I - Si at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3808	B06[I-X]	Presence/absence of I - X at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3809	B06[B-B]	Presence/absence of B - B at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3810	B06[B-Si]	Presence/absence of B - Si at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3811	B06[B-X]	Presence/absence of B - X at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3812	B06[Si-Si]	Presence/absence of Si - Si at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3813	B06[Si-X]	Presence/absence of Si - X at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3814	B06[X-X]	Presence/absence of X - X at topological distance 6	2D Atom Pairs	Binary Atom Pairs of order 6
3815	B07[C-C]	Presence/absence of C - C at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3816	B07[C-N]	Presence/absence of C - N at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3817	B07[C-O]	Presence/absence of C - O at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3818	B07[C-S]	Presence/absence of C - S at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3819	B07[C-P]	Presence/absence of C - P at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3820	B07[C-F]	Presence/absence of C - F at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3821	B07[C-Cl]	Presence/absence of C - Cl at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3822	B07[C-Br]	Presence/absence of C - Br at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3823	B07[C-I]	Presence/absence of C - I at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7

3824	B07[C-B]	Presence/absence of C - B at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3825	B07[C-Si]	Presence/absence of C - Si at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3826	B07[C-X]	Presence/absence of C - X at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3827	B07[N-N]	Presence/absence of N - N at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3828	B07[N-O]	Presence/absence of N - O at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3829	B07[N-S]	Presence/absence of N - S at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3830	B07[N-P]	Presence/absence of N - P at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3831	B07[N-F]	Presence/absence of N - F at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3832	B07[N-Cl]	Presence/absence of N - Cl at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3833	B07[N-Br]	Presence/absence of N - Br at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3834	B07[N-I]	Presence/absence of N - I at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3835	B07[N-B]	Presence/absence of N - B at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3836	B07[N-Si]	Presence/absence of N - Si at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3837	B07[N-X]	Presence/absence of N - X at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3838	B07[O-O]	Presence/absence of O - O at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3839	B07[O-S]	Presence/absence of O - S at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3840	B07[O-P]	Presence/absence of O - P at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3841	B07[O-F]	Presence/absence of O - F at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3842	B07[O-Cl]	Presence/absence of O - Cl at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3843	B07[O-Br]	Presence/absence of O - Br at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7

3844	B07[O-I]	Presence/absence of O - I at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3845	B07[O-B]	Presence/absence of O - B at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3846	B07[O-Si]	Presence/absence of O - Si at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3847	B07[O-X]	Presence/absence of O - X at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3848	B07[S-S]	Presence/absence of S - S at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3849	B07[S-P]	Presence/absence of S - P at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3850	B07[S-F]	Presence/absence of S - F at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3851	B07[S-Cl]	Presence/absence of S - Cl at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3852	B07[S-Br]	Presence/absence of S - Br at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3853	B07[S-I]	Presence/absence of S - I at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3854	B07[S-B]	Presence/absence of S - B at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3855	B07[S-Si]	Presence/absence of S - Si at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3856	B07[S-X]	Presence/absence of S - X at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3857	B07[P-P]	Presence/absence of P - P at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3858	B07[P-F]	Presence/absence of P - F at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3859	B07[P-Cl]	Presence/absence of P - Cl at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3860	B07[P-Br]	Presence/absence of P - Br at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3861	B07[P-I]	Presence/absence of P - I at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3862	B07[P-B]	Presence/absence of P - B at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3863	B07[P-Si]	Presence/absence of P - Si at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7

3864	B07[P-X]	Presence/absence of P - X at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3865	B07[F-F]	Presence/absence of F - F at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3866	B07[F-Cl]	Presence/absence of F - Cl at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3867	B07[F-Br]	Presence/absence of F - Br at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3868	B07[F-I]	Presence/absence of F - I at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3869	B07[F-B]	Presence/absence of F - B at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3870	B07[F-Si]	Presence/absence of F - Si at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3871	B07[F-X]	Presence/absence of F - X at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3872	B07[Cl-Cl]	Presence/absence of Cl - Cl at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3873	B07[Cl-Br]	Presence/absence of Cl - Br at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3874	B07[Cl-I]	Presence/absence of Cl - I at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3875	B07[Cl-B]	Presence/absence of Cl - B at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3876	B07[Cl-Si]	Presence/absence of Cl - Si at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3877	B07[Cl-X]	Presence/absence of Cl - X at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3878	B07[Br-Br]	Presence/absence of Br - Br at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3879	B07[Br-I]	Presence/absence of Br - I at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3880	B07[Br-B]	Presence/absence of Br - B at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3881	B07[Br-Si]	Presence/absence of Br - Si at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3882	B07[Br-X]	Presence/absence of Br - X at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3883	B07[I-I]	Presence/absence of I - I at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7

3884	B07[I-B]	Presence/absence of I - B at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3885	B07[I-Si]	Presence/absence of I - Si at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3886	B07[I-X]	Presence/absence of I - X at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3887	B07[B-B]	Presence/absence of B - B at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3888	B07[B-Si]	Presence/absence of B - Si at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3889	B07[B-X]	Presence/absence of B - X at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3890	B07[Si-Si]	Presence/absence of Si - Si at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3891	B07[Si-X]	Presence/absence of Si - X at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3892	B07[X-X]	Presence/absence of X - X at topological distance 7	2D Atom Pairs	Binary Atom Pairs of order 7
3893	B08[C-C]	Presence/absence of C - C at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3894	B08[C-N]	Presence/absence of C - N at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3895	B08[C-O]	Presence/absence of C - O at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3896	B08[C-S]	Presence/absence of C - S at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3897	B08[C-P]	Presence/absence of C - P at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3898	B08[C-F]	Presence/absence of C - F at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3899	B08[C-Cl]	Presence/absence of C - Cl at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3900	B08[C-Br]	Presence/absence of C - Br at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3901	B08[C-I]	Presence/absence of C - I at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3902	B08[C-B]	Presence/absence of C - B at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3903	B08[C-Si]	Presence/absence of C - Si at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8

3904	B08[C-X]	Presence/absence of C - X at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3905	B08[N-N]	Presence/absence of N - N at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3906	B08[N-O]	Presence/absence of N - O at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3907	B08[N-S]	Presence/absence of N - S at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3908	B08[N-P]	Presence/absence of N - P at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3909	B08[N-F]	Presence/absence of N - F at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3910	B08[N-Cl]	Presence/absence of N - Cl at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3911	B08[N-Br]	Presence/absence of N - Br at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3912	B08[N-I]	Presence/absence of N - I at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3913	B08[N-B]	Presence/absence of N - B at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3914	B08[N-Si]	Presence/absence of N - Si at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3915	B08[N-X]	Presence/absence of N - X at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3916	B08[O-O]	Presence/absence of O - O at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3917	B08[O-S]	Presence/absence of O - S at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3918	B08[O-P]	Presence/absence of O - P at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3919	B08[O-F]	Presence/absence of O - F at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3920	B08[O-Cl]	Presence/absence of O - Cl at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3921	B08[O-Br]	Presence/absence of O - Br at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3922	B08[O-I]	Presence/absence of O - I at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3923	B08[O-B]	Presence/absence of O - B at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8

3924	B08[O-Si]	Presence/absence of O - Si at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3925	B08[O-X]	Presence/absence of O - X at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3926	B08[S-S]	Presence/absence of S - S at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3927	B08[S-P]	Presence/absence of S - P at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3928	B08[S-F]	Presence/absence of S - F at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3929	B08[S-Cl]	Presence/absence of S - Cl at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3930	B08[S-Br]	Presence/absence of S - Br at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3931	B08[S-I]	Presence/absence of S - I at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3932	B08[S-B]	Presence/absence of S - B at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3933	B08[S-Si]	Presence/absence of S - Si at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3934	B08[S-X]	Presence/absence of S - X at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3935	B08[P-P]	Presence/absence of P - P at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3936	B08[P-F]	Presence/absence of P - F at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3937	B08[P-Cl]	Presence/absence of P - Cl at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3938	B08[P-Br]	Presence/absence of P - Br at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3939	B08[P-I]	Presence/absence of P - I at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3940	B08[P-B]	Presence/absence of P - B at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3941	B08[P-Si]	Presence/absence of P - Si at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3942	B08[P-X]	Presence/absence of P - X at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3943	B08[F-F]	Presence/absence of F - F at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8

3944	B08[F-Cl]	Presence/absence of F - Cl at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3945	B08[F-Br]	Presence/absence of F - Br at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3946	B08[F-I]	Presence/absence of F - I at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3947	B08[F-B]	Presence/absence of F - B at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3948	B08[F-Si]	Presence/absence of F - Si at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3949	B08[F-X]	Presence/absence of F - X at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3950	B08[Cl-Cl]	Presence/absence of Cl - Cl at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3951	B08[Cl-Br]	Presence/absence of Cl - Br at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3952	B08[Cl-I]	Presence/absence of Cl - I at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3953	B08[Cl-B]	Presence/absence of Cl - B at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3954	B08[Cl-Si]	Presence/absence of Cl - Si at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3955	B08[Cl-X]	Presence/absence of Cl - X at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3956	B08[Br-Br]	Presence/absence of Br - Br at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3957	B08[Br-I]	Presence/absence of Br - I at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3958	B08[Br-B]	Presence/absence of Br - B at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3959	B08[Br-Si]	Presence/absence of Br - Si at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3960	B08[Br-X]	Presence/absence of Br - X at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3961	B08[I-I]	Presence/absence of I - I at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3962	B08[I-B]	Presence/absence of I - B at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3963	B08[I-Si]	Presence/absence of I - Si at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8

3964	B08[I-X]	Presence/absence of I - X at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3965	B08[B-B]	Presence/absence of B - B at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3966	B08[B-Si]	Presence/absence of B - Si at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3967	B08[B-X]	Presence/absence of B - X at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3968	B08[Si-Si]	Presence/absence of Si - Si at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3969	B08[Si-X]	Presence/absence of Si - X at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3970	B08[X-X]	Presence/absence of X - X at topological distance 8	2D Atom Pairs	Binary Atom Pairs of order 8
3971	B09[C-C]	Presence/absence of C - C at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
3972	B09[C-N]	Presence/absence of C - N at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
3973	B09[C-O]	Presence/absence of C - O at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
3974	B09[C-S]	Presence/absence of C - S at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
3975	B09[C-P]	Presence/absence of C - P at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
3976	B09[C-F]	Presence/absence of C - F at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
3977	B09[C-Cl]	Presence/absence of C - Cl at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
3978	B09[C-Br]	Presence/absence of C - Br at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
3979	B09[C-I]	Presence/absence of C - I at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
3980	B09[C-B]	Presence/absence of C - B at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
3981	B09[C-Si]	Presence/absence of C - Si at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
3982	B09[C-X]	Presence/absence of C - X at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
3983	B09[N-N]	Presence/absence of N - N at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9

3984	B09[N-O]	Presence/absence of N - O at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
3985	B09[N-S]	Presence/absence of N - S at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
3986	B09[N-P]	Presence/absence of N - P at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
3987	B09[N-F]	Presence/absence of N - F at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
3988	B09[N-Cl]	Presence/absence of N - Cl at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
3989	B09[N-Br]	Presence/absence of N - Br at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
3990	B09[N-I]	Presence/absence of N - I at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
3991	B09[N-B]	Presence/absence of N - B at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
3992	B09[N-Si]	Presence/absence of N - Si at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
3993	B09[N-X]	Presence/absence of N - X at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
3994	B09[O-O]	Presence/absence of O - O at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
3995	B09[O-S]	Presence/absence of O - S at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
3996	B09[O-P]	Presence/absence of O - P at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
3997	B09[O-F]	Presence/absence of O - F at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
3998	B09[O-Cl]	Presence/absence of O - Cl at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
3999	B09[O-Br]	Presence/absence of O - Br at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4000	B09[O-I]	Presence/absence of O - I at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4001	B09[O-B]	Presence/absence of O - B at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4002	B09[O-Si]	Presence/absence of O - Si at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4003	B09[O-X]	Presence/absence of O - X at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9

4004	B09[S-S]	Presence/absence of S - S at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4005	B09[S-P]	Presence/absence of S - P at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4006	B09[S-F]	Presence/absence of S - F at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4007	B09[S-Cl]	Presence/absence of S - Cl at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4008	B09[S-Br]	Presence/absence of S - Br at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4009	B09[S-I]	Presence/absence of S - I at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4010	B09[S-B]	Presence/absence of S - B at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4011	B09[S-Si]	Presence/absence of S - Si at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4012	B09[S-X]	Presence/absence of S - X at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4013	B09[P-P]	Presence/absence of P - P at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4014	B09[P-F]	Presence/absence of P - F at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4015	B09[P-Cl]	Presence/absence of P - Cl at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4016	B09[P-Br]	Presence/absence of P - Br at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4017	B09[P-I]	Presence/absence of P - I at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4018	B09[P-B]	Presence/absence of P - B at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4019	B09[P-Si]	Presence/absence of P - Si at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4020	B09[P-X]	Presence/absence of P - X at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4021	B09[F-F]	Presence/absence of F - F at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4022	B09[F-Cl]	Presence/absence of F - Cl at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4023	B09[F-Br]	Presence/absence of F - Br at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9

4024	B09[F-I]	Presence/absence of F - I at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4025	B09[F-B]	Presence/absence of F - B at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4026	B09[F-Si]	Presence/absence of F - Si at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4027	B09[F-X]	Presence/absence of F - X at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4028	B09[Cl-Cl]	Presence/absence of Cl - Cl at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4029	B09[Cl-Br]	Presence/absence of Cl - Br at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4030	B09[Cl-I]	Presence/absence of Cl - I at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4031	B09[Cl-B]	Presence/absence of Cl - B at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4032	B09[Cl-Si]	Presence/absence of Cl - Si at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4033	B09[Cl-X]	Presence/absence of Cl - X at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4034	B09[Br-Br]	Presence/absence of Br - Br at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4035	B09[Br-I]	Presence/absence of Br - I at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4036	B09[Br-B]	Presence/absence of Br - B at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4037	B09[Br-Si]	Presence/absence of Br - Si at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4038	B09[Br-X]	Presence/absence of Br - X at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4039	B09[I-I]	Presence/absence of I - I at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4040	B09[I-B]	Presence/absence of I - B at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4041	B09[I-Si]	Presence/absence of I - Si at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4042	B09[I-X]	Presence/absence of I - X at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4043	B09[B-B]	Presence/absence of B - B at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9

4044	B09[B-Si]	Presence/absence of B - Si at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4045	B09[B-X]	Presence/absence of B - X at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4046	B09[Si-Si]	Presence/absence of Si - Si at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4047	B09[Si-X]	Presence/absence of Si - X at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4048	B09[X-X]	Presence/absence of X - X at topological distance 9	2D Atom Pairs	Binary Atom Pairs of order 9
4049	B10[C-C]	Presence/absence of C - C at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4050	B10[C-N]	Presence/absence of C - N at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4051	B10[C-O]	Presence/absence of C - O at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4052	B10[C-S]	Presence/absence of C - S at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4053	B10[C-P]	Presence/absence of C - P at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4054	B10[C-F]	Presence/absence of C - F at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4055	B10[C-Cl]	Presence/absence of C - Cl at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4056	B10[C-Br]	Presence/absence of C - Br at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4057	B10[C-I]	Presence/absence of C - I at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4058	B10[C-B]	Presence/absence of C - B at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4059	B10[C-Si]	Presence/absence of C - Si at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4060	B10[C-X]	Presence/absence of C - X at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4061	B10[N-N]	Presence/absence of N - N at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4062	B10[N-O]	Presence/absence of N - O at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4063	B10[N-S]	Presence/absence of N - S at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10

4064	B10[N-P]	Presence/absence of N - P at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4065	B10[N-F]	Presence/absence of N - F at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4066	B10[N-Cl]	Presence/absence of N - Cl at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4067	B10[N-Br]	Presence/absence of N - Br at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4068	B10[N-I]	Presence/absence of N - I at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4069	B10[N-B]	Presence/absence of N - B at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4070	B10[N-Si]	Presence/absence of N - Si at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4071	B10[N-X]	Presence/absence of N - X at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4072	B10[O-O]	Presence/absence of O - O at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4073	B10[O-S]	Presence/absence of O - S at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4074	B10[O-P]	Presence/absence of O - P at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4075	B10[O-F]	Presence/absence of O - F at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4076	B10[O-Cl]	Presence/absence of O - Cl at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4077	B10[O-Br]	Presence/absence of O - Br at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4078	B10[O-I]	Presence/absence of O - I at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4079	B10[O-B]	Presence/absence of O - B at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4080	B10[O-Si]	Presence/absence of O - Si at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4081	B10[O-X]	Presence/absence of O - X at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4082	B10[S-S]	Presence/absence of S - S at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4083	B10[S-P]	Presence/absence of S - P at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10

4084	B10[S-F]	Presence/absence of S - F at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4085	B10[S-Cl]	Presence/absence of S - Cl at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4086	B10[S-Br]	Presence/absence of S - Br at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4087	B10[S-I]	Presence/absence of S - I at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4088	B10[S-B]	Presence/absence of S - B at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4089	B10[S-Si]	Presence/absence of S - Si at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4090	B10[S-X]	Presence/absence of S - X at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4091	B10[P-P]	Presence/absence of P - P at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4092	B10[P-F]	Presence/absence of P - F at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4093	B10[P-Cl]	Presence/absence of P - Cl at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4094	B10[P-Br]	Presence/absence of P - Br at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4095	B10[P-I]	Presence/absence of P - I at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4096	B10[P-B]	Presence/absence of P - B at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4097	B10[P-Si]	Presence/absence of P - Si at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4098	B10[P-X]	Presence/absence of P - X at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4099	B10[F-F]	Presence/absence of F - F at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4100	B10[F-Cl]	Presence/absence of F - Cl at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4101	B10[F-Br]	Presence/absence of F - Br at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4102	B10[F-I]	Presence/absence of F - I at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4103	B10[F-B]	Presence/absence of F - B at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10

4104	B10[F-Si]	Presence/absence of F - Si at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4105	B10[F-X]	Presence/absence of F - X at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4106	B10[Cl-Cl]	Presence/absence of Cl - Cl at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4107	B10[Cl-Br]	Presence/absence of Cl - Br at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4108	B10[Cl-I]	Presence/absence of Cl - I at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4109	B10[Cl-B]	Presence/absence of Cl - B at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4110	B10[Cl-Si]	Presence/absence of Cl - Si at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4111	B10[Cl-X]	Presence/absence of Cl - X at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4112	B10[Br-Br]	Presence/absence of Br - Br at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4113	B10[Br-I]	Presence/absence of Br - I at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4114	B10[Br-B]	Presence/absence of Br - B at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4115	B10[Br-Si]	Presence/absence of Br - Si at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4116	B10[Br-X]	Presence/absence of Br - X at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4117	B10[I-I]	Presence/absence of I - I at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4118	B10[I-B]	Presence/absence of I - B at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4119	B10[I-Si]	Presence/absence of I - Si at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4120	B10[I-X]	Presence/absence of I - X at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4121	B10[B-B]	Presence/absence of B - B at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4122	B10[B-Si]	Presence/absence of B - Si at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4123	B10[B-X]	Presence/absence of B - X at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10

4124	B10[Si-Si]	Presence/absence of Si - Si at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4125	B10[Si-X]	Presence/absence of Si - X at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4126	B10[X-X]	Presence/absence of X - X at topological distance 10	2D Atom Pairs	Binary Atom Pairs of order 10
4127	F01[C-C]	Frequency of C - C at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4128	F01[C-N]	Frequency of C - N at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4129	F01[C-O]	Frequency of C - O at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4130	F01[C-S]	Frequency of C - S at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4131	F01[C-P]	Frequency of C - P at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4132	F01[C-F]	Frequency of C - F at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4133	F01[C-Cl]	Frequency of C - Cl at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4134	F01[C-Br]	Frequency of C - Br at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4135	F01[C-I]	Frequency of C - I at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4136	F01[C-B]	Frequency of C - B at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4137	F01[C-Si]	Frequency of C - Si at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4138	F01[C-X]	Frequency of C - X at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4139	F01[N-N]	Frequency of N - N at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4140	F01[N-O]	Frequency of N - O at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4141	F01[N-S]	Frequency of N - S at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4142	F01[N-P]	Frequency of N - P at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4143	F01[N-F]	Frequency of N - F at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1

4144	F01[N-Cl]	Frequency of N - Cl at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4145	F01[N-Br]	Frequency of N - Br at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4146	F01[N-I]	Frequency of N - I at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4147	F01[N-B]	Frequency of N - B at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4148	F01[N-Si]	Frequency of N - Si at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4149	F01[N-X]	Frequency of N - X at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4150	F01[O-O]	Frequency of O - O at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4151	F01[O-S]	Frequency of O - S at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4152	F01[O-P]	Frequency of O - P at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4153	F01[O-F]	Frequency of O - F at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4154	F01[O-Cl]	Frequency of O - Cl at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4155	F01[O-Br]	Frequency of O - Br at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4156	F01[O-I]	Frequency of O - I at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4157	F01[O-B]	Frequency of O - B at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4158	F01[O-Si]	Frequency of O - Si at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4159	F01[O-X]	Frequency of O - X at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4160	F01[S-S]	Frequency of S - S at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4161	F01[S-P]	Frequency of S - P at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4162	F01[S-F]	Frequency of S - F at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4163	F01[S-Cl]	Frequency of S - Cl at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1

4164	F01[S-Br]	Frequency of S - Br at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4165	F01[S-I]	Frequency of S - I at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4166	F01[S-B]	Frequency of S - B at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4167	F01[S-Si]	Frequency of S - Si at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4168	F01[S-X]	Frequency of S - X at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4169	F01[P-P]	Frequency of P - P at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4170	F01[P-F]	Frequency of P - F at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4171	F01[P-Cl]	Frequency of P - Cl at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4172	F01[P-Br]	Frequency of P - Br at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4173	F01[P-I]	Frequency of P - I at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4174	F01[P-B]	Frequency of P - B at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4175	F01[P-Si]	Frequency of P - Si at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4176	F01[P-X]	Frequency of P - X at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4177	F01[F-F]	Frequency of F - F at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4178	F01[F-Cl]	Frequency of F - Cl at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4179	F01[F-Br]	Frequency of F - Br at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4180	F01[F-I]	Frequency of F - I at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4181	F01[F-B]	Frequency of F - B at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4182	F01[F-Si]	Frequency of F - Si at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4183	F01[F-X]	Frequency of F - X at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1

4184	F01[Cl-Cl]	Frequency of Cl - Cl at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4185	F01[Cl-Br]	Frequency of Cl - Br at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4186	F01[Cl-I]	Frequency of Cl - I at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4187	F01[Cl-B]	Frequency of Cl - B at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4188	F01[Cl-Si]	Frequency of Cl - Si at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4189	F01[Cl-X]	Frequency of Cl - X at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4190	F01[Br-Br]	Frequency of Br - Br at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4191	F01[Br-I]	Frequency of Br - I at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4192	F01[Br-B]	Frequency of Br - B at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4193	F01[Br-Si]	Frequency of Br - Si at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4194	F01[Br-X]	Frequency of Br - X at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4195	F01[I-I]	Frequency of I - I at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4196	F01[I-B]	Frequency of I - B at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4197	F01[I-Si]	Frequency of I - Si at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4198	F01[I-X]	Frequency of I - X at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4199	F01[B-B]	Frequency of B - B at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4200	F01[B-Si]	Frequency of B - Si at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4201	F01[B-X]	Frequency of B - X at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4202	F01[Si-Si]	Frequency of Si - Si at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4203	F01[Si-X]	Frequency of Si - X at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1

4204	F01[X-X]	Frequency of X - X at topological distance 1	2D Atom Pairs	Frequency Atom Pairs of order 1
4205	F02[C-C]	Frequency of C - C at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4206	F02[C-N]	Frequency of C - N at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4207	F02[C-O]	Frequency of C - O at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4208	F02[C-S]	Frequency of C - S at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4209	F02[C-P]	Frequency of C - P at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4210	F02[C-F]	Frequency of C - F at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4211	F02[C-Cl]	Frequency of C - Cl at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4212	F02[C-Br]	Frequency of C - Br at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4213	F02[C-I]	Frequency of C - I at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4214	F02[C-B]	Frequency of C - B at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4215	F02[C-Si]	Frequency of C - Si at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4216	F02[C-X]	Frequency of C - X at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4217	F02[N-N]	Frequency of N - N at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4218	F02[N-O]	Frequency of N - O at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4219	F02[N-S]	Frequency of N - S at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4220	F02[N-P]	Frequency of N - P at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4221	F02[N-F]	Frequency of N - F at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4222	F02[N-Cl]	Frequency of N - Cl at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4223	F02[N-Br]	Frequency of N - Br at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2

4224	F02[N-I]	Frequency of N - I at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4225	F02[N-B]	Frequency of N - B at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4226	F02[N-Si]	Frequency of N - Si at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4227	F02[N-X]	Frequency of N - X at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4228	F02[O-O]	Frequency of O - O at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4229	F02[O-S]	Frequency of O - S at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4230	F02[O-P]	Frequency of O - P at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4231	F02[O-F]	Frequency of O - F at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4232	F02[O-Cl]	Frequency of O - Cl at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4233	F02[O-Br]	Frequency of O - Br at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4234	F02[O-I]	Frequency of O - I at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4235	F02[O-B]	Frequency of O - B at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4236	F02[O-Si]	Frequency of O - Si at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4237	F02[O-X]	Frequency of O - X at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4238	F02[S-S]	Frequency of S - S at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4239	F02[S-P]	Frequency of S - P at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4240	F02[S-F]	Frequency of S - F at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4241	F02[S-Cl]	Frequency of S - Cl at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4242	F02[S-Br]	Frequency of S - Br at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4243	F02[S-I]	Frequency of S - I at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2

4244	F02[S-B]	Frequency of S - B at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4245	F02[S-Si]	Frequency of S - Si at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4246	F02[S-X]	Frequency of S - X at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4247	F02[P-P]	Frequency of P - P at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4248	F02[P-F]	Frequency of P - F at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4249	F02[P-Cl]	Frequency of P - Cl at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4250	F02[P-Br]	Frequency of P - Br at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4251	F02[P-I]	Frequency of P - I at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4252	F02[P-B]	Frequency of P - B at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4253	F02[P-Si]	Frequency of P - Si at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4254	F02[P-X]	Frequency of P - X at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4255	F02[F-F]	Frequency of F - F at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4256	F02[F-Cl]	Frequency of F - Cl at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4257	F02[F-Br]	Frequency of F - Br at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4258	F02[F-I]	Frequency of F - I at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4259	F02[F-B]	Frequency of F - B at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4260	F02[F-Si]	Frequency of F - Si at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4261	F02[F-X]	Frequency of F - X at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4262	F02[Cl-Cl]	Frequency of Cl - Cl at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4263	F02[Cl-Br]	Frequency of Cl - Br at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2

4264	F02[Cl-I]	Frequency of Cl - I at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4265	F02[Cl-B]	Frequency of Cl - B at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4266	F02[Cl-Si]	Frequency of Cl - Si at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4267	F02[Cl-X]	Frequency of Cl - X at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4268	F02[Br-Br]	Frequency of Br - Br at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4269	F02[Br-I]	Frequency of Br - I at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4270	F02[Br-B]	Frequency of Br - B at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4271	F02[Br-Si]	Frequency of Br - Si at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4272	F02[Br-X]	Frequency of Br - X at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4273	F02[I-I]	Frequency of I - I at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4274	F02[I-B]	Frequency of I - B at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4275	F02[I-Si]	Frequency of I - Si at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4276	F02[I-X]	Frequency of I - X at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4277	F02[B-B]	Frequency of B - B at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4278	F02[B-Si]	Frequency of B - Si at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4279	F02[B-X]	Frequency of B - X at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4280	F02[Si-Si]	Frequency of Si - Si at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4281	F02[Si-X]	Frequency of Si - X at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4282	F02[X-X]	Frequency of X - X at topological distance 2	2D Atom Pairs	Frequency Atom Pairs of order 2
4283	F03[C-C]	Frequency of C - C at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3

4284	F03[C-N]	Frequency of C - N at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4285	F03[C-O]	Frequency of C - O at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4286	F03[C-S]	Frequency of C - S at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4287	F03[C-P]	Frequency of C - P at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4288	F03[C-F]	Frequency of C - F at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4289	F03[C-Cl]	Frequency of C - Cl at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4290	F03[C-Br]	Frequency of C - Br at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4291	F03[C-I]	Frequency of C - I at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4292	F03[C-B]	Frequency of C - B at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4293	F03[C-Si]	Frequency of C - Si at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4294	F03[C-X]	Frequency of C - X at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4295	F03[N-N]	Frequency of N - N at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4296	F03[N-O]	Frequency of N - O at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4297	F03[N-S]	Frequency of N - S at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4298	F03[N-P]	Frequency of N - P at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4299	F03[N-F]	Frequency of N - F at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4300	F03[N-Cl]	Frequency of N - Cl at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4301	F03[N-Br]	Frequency of N - Br at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4302	F03[N-I]	Frequency of N - I at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4303	F03[N-B]	Frequency of N - B at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3

4304	F03[N-Si]	Frequency of N - Si at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4305	F03[N-X]	Frequency of N - X at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4306	F03[O-O]	Frequency of O - O at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4307	F03[O-S]	Frequency of O - S at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4308	F03[O-P]	Frequency of O - P at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4309	F03[O-F]	Frequency of O - F at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4310	F03[O-Cl]	Frequency of O - Cl at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4311	F03[O-Br]	Frequency of O - Br at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4312	F03[O-I]	Frequency of O - I at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4313	F03[O-B]	Frequency of O - B at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4314	F03[O-Si]	Frequency of O - Si at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4315	F03[O-X]	Frequency of O - X at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4316	F03[S-S]	Frequency of S - S at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4317	F03[S-P]	Frequency of S - P at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4318	F03[S-F]	Frequency of S - F at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4319	F03[S-Cl]	Frequency of S - Cl at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4320	F03[S-Br]	Frequency of S - Br at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4321	F03[S-I]	Frequency of S - I at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4322	F03[S-B]	Frequency of S - B at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4323	F03[S-Si]	Frequency of S - Si at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3

4324	F03[S-X]	Frequency of S - X at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4325	F03[P-P]	Frequency of P - P at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4326	F03[P-F]	Frequency of P - F at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4327	F03[P-Cl]	Frequency of P - Cl at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4328	F03[P-Br]	Frequency of P - Br at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4329	F03[P-I]	Frequency of P - I at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4330	F03[P-B]	Frequency of P - B at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4331	F03[P-Si]	Frequency of P - Si at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4332	F03[P-X]	Frequency of P - X at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4333	F03[F-F]	Frequency of F - F at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4334	F03[F-Cl]	Frequency of F - Cl at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4335	F03[F-Br]	Frequency of F - Br at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4336	F03[F-I]	Frequency of F - I at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4337	F03[F-B]	Frequency of F - B at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4338	F03[F-Si]	Frequency of F - Si at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4339	F03[F-X]	Frequency of F - X at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4340	F03[Cl-Cl]	Frequency of Cl - Cl at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4341	F03[Cl-Br]	Frequency of Cl - Br at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4342	F03[Cl-I]	Frequency of Cl - I at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4343	F03[Cl-B]	Frequency of Cl - B at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3

4344	F03[Cl-Si]	Frequency of Cl - Si at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4345	F03[Cl-X]	Frequency of Cl - X at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4346	F03[Br-Br]	Frequency of Br - Br at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4347	F03[Br-I]	Frequency of Br - I at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4348	F03[Br-B]	Frequency of Br - B at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4349	F03[Br-Si]	Frequency of Br - Si at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4350	F03[Br-X]	Frequency of Br - X at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4351	F03[I-I]	Frequency of I - I at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4352	F03[I-B]	Frequency of I - B at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4353	F03[I-Si]	Frequency of I - Si at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4354	F03[I-X]	Frequency of I - X at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4355	F03[B-B]	Frequency of B - B at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4356	F03[B-Si]	Frequency of B - Si at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4357	F03[B-X]	Frequency of B - X at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4358	F03[Si-Si]	Frequency of Si - Si at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4359	F03[Si-X]	Frequency of Si - X at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4360	F03[X-X]	Frequency of X - X at topological distance 3	2D Atom Pairs	Frequency Atom Pairs of order 3
4361	F04[C-C]	Frequency of C - C at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4362	F04[C-N]	Frequency of C - N at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4363	F04[C-O]	Frequency of C - O at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4

4364	F04[C-S]	Frequency of C - S at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4365	F04[C-P]	Frequency of C - P at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4366	F04[C-F]	Frequency of C - F at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4367	F04[C-Cl]	Frequency of C - Cl at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4368	F04[C-Br]	Frequency of C - Br at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4369	F04[C-I]	Frequency of C - I at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4370	F04[C-B]	Frequency of C - B at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4371	F04[C-Si]	Frequency of C - Si at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4372	F04[C-X]	Frequency of C - X at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4373	F04[N-N]	Frequency of N - N at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4374	F04[N-O]	Frequency of N - O at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4375	F04[N-S]	Frequency of N - S at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4376	F04[N-P]	Frequency of N - P at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4377	F04[N-F]	Frequency of N - F at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4378	F04[N-Cl]	Frequency of N - Cl at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4379	F04[N-Br]	Frequency of N - Br at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4380	F04[N-I]	Frequency of N - I at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4381	F04[N-B]	Frequency of N - B at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4382	F04[N-Si]	Frequency of N - Si at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4383	F04[N-X]	Frequency of N - X at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4

4384	F04[O-O]	Frequency of O - O at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4385	F04[O-S]	Frequency of O - S at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4386	F04[O-P]	Frequency of O - P at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4387	F04[O-F]	Frequency of O - F at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4388	F04[O-Cl]	Frequency of O - Cl at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4389	F04[O-Br]	Frequency of O - Br at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4390	F04[O-I]	Frequency of O - I at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4391	F04[O-B]	Frequency of O - B at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4392	F04[O-Si]	Frequency of O - Si at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4393	F04[O-X]	Frequency of O - X at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4394	F04[S-S]	Frequency of S - S at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4395	F04[S-P]	Frequency of S - P at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4396	F04[S-F]	Frequency of S - F at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4397	F04[S-Cl]	Frequency of S - Cl at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4398	F04[S-Br]	Frequency of S - Br at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4399	F04[S-I]	Frequency of S - I at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4400	F04[S-B]	Frequency of S - B at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4401	F04[S-Si]	Frequency of S - Si at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4402	F04[S-X]	Frequency of S - X at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4403	F04[P-P]	Frequency of P - P at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4

4404	F04[P-F]	Frequency of P - F at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4405	F04[P-Cl]	Frequency of P - Cl at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4406	F04[P-Br]	Frequency of P - Br at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4407	F04[P-I]	Frequency of P - I at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4408	F04[P-B]	Frequency of P - B at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4409	F04[P-Si]	Frequency of P - Si at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4410	F04[P-X]	Frequency of P - X at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4411	F04[F-F]	Frequency of F - F at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4412	F04[F-Cl]	Frequency of F - Cl at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4413	F04[F-Br]	Frequency of F - Br at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4414	F04[F-I]	Frequency of F - I at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4415	F04[F-B]	Frequency of F - B at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4416	F04[F-Si]	Frequency of F - Si at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4417	F04[F-X]	Frequency of F - X at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4418	F04[Cl-Cl]	Frequency of Cl - Cl at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4419	F04[Cl-Br]	Frequency of Cl - Br at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4420	F04[Cl-I]	Frequency of Cl - I at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4421	F04[Cl-B]	Frequency of Cl - B at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4422	F04[Cl-Si]	Frequency of Cl - Si at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4423	F04[Cl-X]	Frequency of Cl - X at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4

4424	F04[Br-Br]	Frequency of Br - Br at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4425	F04[Br-I]	Frequency of Br - I at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4426	F04[Br-B]	Frequency of Br - B at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4427	F04[Br-Si]	Frequency of Br - Si at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4428	F04[Br-X]	Frequency of Br - X at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4429	F04[I-I]	Frequency of I - I at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4430	F04[I-B]	Frequency of I - B at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4431	F04[I-Si]	Frequency of I - Si at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4432	F04[I-X]	Frequency of I - X at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4433	F04[B-B]	Frequency of B - B at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4434	F04[B-Si]	Frequency of B - Si at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4435	F04[B-X]	Frequency of B - X at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4436	F04[Si-Si]	Frequency of Si - Si at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4437	F04[Si-X]	Frequency of Si - X at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4438	F04[X-X]	Frequency of X - X at topological distance 4	2D Atom Pairs	Frequency Atom Pairs of order 4
4439	F05[C-C]	Frequency of C - C at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4440	F05[C-N]	Frequency of C - N at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4441	F05[C-O]	Frequency of C - O at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4442	F05[C-S]	Frequency of C - S at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4443	F05[C-P]	Frequency of C - P at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5

4444	F05[C-F]	Frequency of C - F at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4445	F05[C-Cl]	Frequency of C - Cl at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4446	F05[C-Br]	Frequency of C - Br at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4447	F05[C-I]	Frequency of C - I at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4448	F05[C-B]	Frequency of C - B at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4449	F05[C-Si]	Frequency of C - Si at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4450	F05[C-X]	Frequency of C - X at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4451	F05[N-N]	Frequency of N - N at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4452	F05[N-O]	Frequency of N - O at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4453	F05[N-S]	Frequency of N - S at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4454	F05[N-P]	Frequency of N - P at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4455	F05[N-F]	Frequency of N - F at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4456	F05[N-Cl]	Frequency of N - Cl at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4457	F05[N-Br]	Frequency of N - Br at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4458	F05[N-I]	Frequency of N - I at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4459	F05[N-B]	Frequency of N - B at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4460	F05[N-Si]	Frequency of N - Si at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4461	F05[N-X]	Frequency of N - X at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4462	F05[O-O]	Frequency of O - O at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4463	F05[O-S]	Frequency of O - S at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5

4464	F05[O-P]	Frequency of O - P at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4465	F05[O-F]	Frequency of O - F at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4466	F05[O-Cl]	Frequency of O - Cl at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4467	F05[O-Br]	Frequency of O - Br at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4468	F05[O-I]	Frequency of O - I at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4469	F05[O-B]	Frequency of O - B at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4470	F05[O-Si]	Frequency of O - Si at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4471	F05[O-X]	Frequency of O - X at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4472	F05[S-S]	Frequency of S - S at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4473	F05[S-P]	Frequency of S - P at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4474	F05[S-F]	Frequency of S - F at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4475	F05[S-Cl]	Frequency of S - Cl at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4476	F05[S-Br]	Frequency of S - Br at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4477	F05[S-I]	Frequency of S - I at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4478	F05[S-B]	Frequency of S - B at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4479	F05[S-Si]	Frequency of S - Si at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4480	F05[S-X]	Frequency of S - X at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4481	F05[P-P]	Frequency of P - P at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4482	F05[P-F]	Frequency of P - F at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4483	F05[P-Cl]	Frequency of P - Cl at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5

4484	F05[P-Br]	Frequency of P - Br at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4485	F05[P-I]	Frequency of P - I at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4486	F05[P-B]	Frequency of P - B at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4487	F05[P-Si]	Frequency of P - Si at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4488	F05[P-X]	Frequency of P - X at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4489	F05[F-F]	Frequency of F - F at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4490	F05[F-Cl]	Frequency of F - Cl at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4491	F05[F-Br]	Frequency of F - Br at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4492	F05[F-I]	Frequency of F - I at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4493	F05[F-B]	Frequency of F - B at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4494	F05[F-Si]	Frequency of F - Si at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4495	F05[F-X]	Frequency of F - X at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4496	F05[Cl-Cl]	Frequency of Cl - Cl at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4497	F05[Cl-Br]	Frequency of Cl - Br at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4498	F05[Cl-I]	Frequency of Cl - I at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4499	F05[Cl-B]	Frequency of Cl - B at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4500	F05[Cl-Si]	Frequency of Cl - Si at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4501	F05[Cl-X]	Frequency of Cl - X at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4502	F05[Br-Br]	Frequency of Br - Br at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4503	F05[Br-I]	Frequency of Br - I at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5

4504	F05[Br-B]	Frequency of Br - B at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4505	F05[Br-Si]	Frequency of Br - Si at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4506	F05[Br-X]	Frequency of Br - X at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4507	F05[I-I]	Frequency of I - I at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4508	F05[I-B]	Frequency of I - B at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4509	F05[I-Si]	Frequency of I - Si at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4510	F05[I-X]	Frequency of I - X at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4511	F05[B-B]	Frequency of B - B at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4512	F05[B-Si]	Frequency of B - Si at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4513	F05[B-X]	Frequency of B - X at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4514	F05[Si-Si]	Frequency of Si - Si at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4515	F05[Si-X]	Frequency of Si - X at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4516	F05[X-X]	Frequency of X - X at topological distance 5	2D Atom Pairs	Frequency Atom Pairs of order 5
4517	F06[C-C]	Frequency of C - C at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4518	F06[C-N]	Frequency of C - N at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4519	F06[C-O]	Frequency of C - O at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4520	F06[C-S]	Frequency of C - S at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4521	F06[C-P]	Frequency of C - P at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4522	F06[C-F]	Frequency of C - F at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4523	F06[C-Cl]	Frequency of C - Cl at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6

4524	F06[C-Br]	Frequency of C - Br at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4525	F06[C-I]	Frequency of C - I at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4526	F06[C-B]	Frequency of C - B at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4527	F06[C-Si]	Frequency of C - Si at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4528	F06[C-X]	Frequency of C - X at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4529	F06[N-N]	Frequency of N - N at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4530	F06[N-O]	Frequency of N - O at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4531	F06[N-S]	Frequency of N - S at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4532	F06[N-P]	Frequency of N - P at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4533	F06[N-F]	Frequency of N - F at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4534	F06[N-Cl]	Frequency of N - Cl at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4535	F06[N-Br]	Frequency of N - Br at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4536	F06[N-I]	Frequency of N - I at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4537	F06[N-B]	Frequency of N - B at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4538	F06[N-Si]	Frequency of N - Si at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4539	F06[N-X]	Frequency of N - X at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4540	F06[O-O]	Frequency of O - O at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4541	F06[O-S]	Frequency of O - S at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4542	F06[O-P]	Frequency of O - P at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4543	F06[O-F]	Frequency of O - F at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6

4544	F06[O-Cl]	Frequency of O - Cl at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4545	F06[O-Br]	Frequency of O - Br at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4546	F06[O-I]	Frequency of O - I at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4547	F06[O-B]	Frequency of O - B at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4548	F06[O-Si]	Frequency of O - Si at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4549	F06[O-X]	Frequency of O - X at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4550	F06[S-S]	Frequency of S - S at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4551	F06[S-P]	Frequency of S - P at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4552	F06[S-F]	Frequency of S - F at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4553	F06[S-Cl]	Frequency of S - Cl at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4554	F06[S-Br]	Frequency of S - Br at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4555	F06[S-I]	Frequency of S - I at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4556	F06[S-B]	Frequency of S - B at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4557	F06[S-Si]	Frequency of S - Si at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4558	F06[S-X]	Frequency of S - X at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4559	F06[P-P]	Frequency of P - P at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4560	F06[P-F]	Frequency of P - F at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4561	F06[P-Cl]	Frequency of P - Cl at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4562	F06[P-Br]	Frequency of P - Br at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4563	F06[P-I]	Frequency of P - I at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6

4564	F06[P-B]	Frequency of P - B at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4565	F06[P-Si]	Frequency of P - Si at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4566	F06[P-X]	Frequency of P - X at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4567	F06[F-F]	Frequency of F - F at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4568	F06[F-Cl]	Frequency of F - Cl at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4569	F06[F-Br]	Frequency of F - Br at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4570	F06[F-I]	Frequency of F - I at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4571	F06[F-B]	Frequency of F - B at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4572	F06[F-Si]	Frequency of F - Si at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4573	F06[F-X]	Frequency of F - X at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4574	F06[Cl-Cl]	Frequency of Cl - Cl at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4575	F06[Cl-Br]	Frequency of Cl - Br at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4576	F06[Cl-I]	Frequency of Cl - I at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4577	F06[Cl-B]	Frequency of Cl - B at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4578	F06[Cl-Si]	Frequency of Cl - Si at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4579	F06[Cl-X]	Frequency of Cl - X at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4580	F06[Br-Br]	Frequency of Br - Br at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4581	F06[Br-I]	Frequency of Br - I at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4582	F06[Br-B]	Frequency of Br - B at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4583	F06[Br-Si]	Frequency of Br - Si at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6

4584	F06[Br-X]	Frequency of Br - X at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4585	F06[I-I]	Frequency of I - I at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4586	F06[I-B]	Frequency of I - B at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4587	F06[I-Si]	Frequency of I - Si at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4588	F06[I-X]	Frequency of I - X at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4589	F06[B-B]	Frequency of B - B at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4590	F06[B-Si]	Frequency of B - Si at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4591	F06[B-X]	Frequency of B - X at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4592	F06[Si-Si]	Frequency of Si - Si at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4593	F06[Si-X]	Frequency of Si - X at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4594	F06[X-X]	Frequency of X - X at topological distance 6	2D Atom Pairs	Frequency Atom Pairs of order 6
4595	F07[C-C]	Frequency of C - C at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4596	F07[C-N]	Frequency of C - N at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4597	F07[C-O]	Frequency of C - O at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4598	F07[C-S]	Frequency of C - S at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4599	F07[C-P]	Frequency of C - P at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4600	F07[C-F]	Frequency of C - F at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4601	F07[C-Cl]	Frequency of C - Cl at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4602	F07[C-Br]	Frequency of C - Br at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4603	F07[C-I]	Frequency of C - I at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7

4604	F07[C-B]	Frequency of C - B at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4605	F07[C-Si]	Frequency of C - Si at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4606	F07[C-X]	Frequency of C - X at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4607	F07[N-N]	Frequency of N - N at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4608	F07[N-O]	Frequency of N - O at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4609	F07[N-S]	Frequency of N - S at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4610	F07[N-P]	Frequency of N - P at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4611	F07[N-F]	Frequency of N - F at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4612	F07[N-Cl]	Frequency of N - Cl at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4613	F07[N-Br]	Frequency of N - Br at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4614	F07[N-I]	Frequency of N - I at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4615	F07[N-B]	Frequency of N - B at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4616	F07[N-Si]	Frequency of N - Si at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4617	F07[N-X]	Frequency of N - X at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4618	F07[O-O]	Frequency of O - O at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4619	F07[O-S]	Frequency of O - S at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4620	F07[O-P]	Frequency of O - P at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4621	F07[O-F]	Frequency of O - F at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4622	F07[O-Cl]	Frequency of O - Cl at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4623	F07[O-Br]	Frequency of O - Br at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7

4624	F07[O-I]	Frequency of O - I at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4625	F07[O-B]	Frequency of O - B at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4626	F07[O-Si]	Frequency of O - Si at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4627	F07[O-X]	Frequency of O - X at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4628	F07[S-S]	Frequency of S - S at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4629	F07[S-P]	Frequency of S - P at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4630	F07[S-F]	Frequency of S - F at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4631	F07[S-Cl]	Frequency of S - Cl at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4632	F07[S-Br]	Frequency of S - Br at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4633	F07[S-I]	Frequency of S - I at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4634	F07[S-B]	Frequency of S - B at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4635	F07[S-Si]	Frequency of S - Si at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4636	F07[S-X]	Frequency of S - X at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4637	F07[P-P]	Frequency of P - P at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4638	F07[P-F]	Frequency of P - F at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4639	F07[P-Cl]	Frequency of P - Cl at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4640	F07[P-Br]	Frequency of P - Br at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4641	F07[P-I]	Frequency of P - I at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4642	F07[P-B]	Frequency of P - B at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4643	F07[P-Si]	Frequency of P - Si at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7

4644	F07[P-X]	Frequency of P - X at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4645	F07[F-F]	Frequency of F - F at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4646	F07[F-Cl]	Frequency of F - Cl at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4647	F07[F-Br]	Frequency of F - Br at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4648	F07[F-I]	Frequency of F - I at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4649	F07[F-B]	Frequency of F - B at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4650	F07[F-Si]	Frequency of F - Si at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4651	F07[F-X]	Frequency of F - X at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4652	F07[Cl-Cl]	Frequency of Cl - Cl at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4653	F07[Cl-Br]	Frequency of Cl - Br at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4654	F07[Cl-I]	Frequency of Cl - I at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4655	F07[Cl-B]	Frequency of Cl - B at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4656	F07[Cl-Si]	Frequency of Cl - Si at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4657	F07[Cl-X]	Frequency of Cl - X at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4658	F07[Br-Br]	Frequency of Br - Br at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4659	F07[Br-I]	Frequency of Br - I at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4660	F07[Br-B]	Frequency of Br - B at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4661	F07[Br-Si]	Frequency of Br - Si at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4662	F07[Br-X]	Frequency of Br - X at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4663	F07[I-I]	Frequency of I - I at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7

4664	F07[I-B]	Frequency of I - B at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4665	F07[I-Si]	Frequency of I - Si at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4666	F07[I-X]	Frequency of I - X at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4667	F07[B-B]	Frequency of B - B at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4668	F07[B-Si]	Frequency of B - Si at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4669	F07[B-X]	Frequency of B - X at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4670	F07[Si-Si]	Frequency of Si - Si at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4671	F07[Si-X]	Frequency of Si - X at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4672	F07[X-X]	Frequency of X - X at topological distance 7	2D Atom Pairs	Frequency Atom Pairs of order 7
4673	F08[C-C]	Frequency of C - C at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4674	F08[C-N]	Frequency of C - N at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4675	F08[C-O]	Frequency of C - O at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4676	F08[C-S]	Frequency of C - S at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4677	F08[C-P]	Frequency of C - P at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4678	F08[C-F]	Frequency of C - F at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4679	F08[C-Cl]	Frequency of C - Cl at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4680	F08[C-Br]	Frequency of C - Br at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4681	F08[C-I]	Frequency of C - I at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4682	F08[C-B]	Frequency of C - B at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4683	F08[C-Si]	Frequency of C - Si at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8

4684	F08[C-X]	Frequency of C - X at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4685	F08[N-N]	Frequency of N - N at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4686	F08[N-O]	Frequency of N - O at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4687	F08[N-S]	Frequency of N - S at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4688	F08[N-P]	Frequency of N - P at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4689	F08[N-F]	Frequency of N - F at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4690	F08[N-Cl]	Frequency of N - Cl at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4691	F08[N-Br]	Frequency of N - Br at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4692	F08[N-I]	Frequency of N - I at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4693	F08[N-B]	Frequency of N - B at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4694	F08[N-Si]	Frequency of N - Si at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4695	F08[N-X]	Frequency of N - X at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4696	F08[O-O]	Frequency of O - O at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4697	F08[O-S]	Frequency of O - S at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4698	F08[O-P]	Frequency of O - P at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4699	F08[O-F]	Frequency of O - F at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4700	F08[O-Cl]	Frequency of O - Cl at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4701	F08[O-Br]	Frequency of O - Br at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4702	F08[O-I]	Frequency of O - I at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4703	F08[O-B]	Frequency of O - B at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8

4704	F08[O-Si]	Frequency of O - Si at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4705	F08[O-X]	Frequency of O - X at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4706	F08[S-S]	Frequency of S - S at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4707	F08[S-P]	Frequency of S - P at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4708	F08[S-F]	Frequency of S - F at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4709	F08[S-Cl]	Frequency of S - Cl at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4710	F08[S-Br]	Frequency of S - Br at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4711	F08[S-I]	Frequency of S - I at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4712	F08[S-B]	Frequency of S - B at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4713	F08[S-Si]	Frequency of S - Si at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4714	F08[S-X]	Frequency of S - X at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4715	F08[P-P]	Frequency of P - P at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4716	F08[P-F]	Frequency of P - F at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4717	F08[P-Cl]	Frequency of P - Cl at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4718	F08[P-Br]	Frequency of P - Br at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4719	F08[P-I]	Frequency of P - I at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4720	F08[P-B]	Frequency of P - B at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4721	F08[P-Si]	Frequency of P - Si at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4722	F08[P-X]	Frequency of P - X at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4723	F08[F-F]	Frequency of F - F at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8

4724	F08[F-Cl]	Frequency of F - Cl at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4725	F08[F-Br]	Frequency of F - Br at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4726	F08[F-I]	Frequency of F - I at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4727	F08[F-B]	Frequency of F - B at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4728	F08[F-Si]	Frequency of F - Si at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4729	F08[F-X]	Frequency of F - X at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4730	F08[Cl-Cl]	Frequency of Cl - Cl at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4731	F08[Cl-Br]	Frequency of Cl - Br at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4732	F08[Cl-I]	Frequency of Cl - I at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4733	F08[Cl-B]	Frequency of Cl - B at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4734	F08[Cl-Si]	Frequency of Cl - Si at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4735	F08[Cl-X]	Frequency of Cl - X at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4736	F08[Br-Br]	Frequency of Br - Br at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4737	F08[Br-I]	Frequency of Br - I at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4738	F08[Br-B]	Frequency of Br - B at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4739	F08[Br-Si]	Frequency of Br - Si at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4740	F08[Br-X]	Frequency of Br - X at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4741	F08[I-I]	Frequency of I - I at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4742	F08[I-B]	Frequency of I - B at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4743	F08[I-Si]	Frequency of I - Si at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8

4744	F08[I-X]	Frequency of I - X at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4745	F08[B-B]	Frequency of B - B at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4746	F08[B-Si]	Frequency of B - Si at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4747	F08[B-X]	Frequency of B - X at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4748	F08[Si-Si]	Frequency of Si - Si at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4749	F08[Si-X]	Frequency of Si - X at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4750	F08[X-X]	Frequency of X - X at topological distance 8	2D Atom Pairs	Frequency Atom Pairs of order 8
4751	F09[C-C]	Frequency of C - C at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4752	F09[C-N]	Frequency of C - N at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4753	F09[C-O]	Frequency of C - O at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4754	F09[C-S]	Frequency of C - S at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4755	F09[C-P]	Frequency of C - P at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4756	F09[C-F]	Frequency of C - F at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4757	F09[C-Cl]	Frequency of C - Cl at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4758	F09[C-Br]	Frequency of C - Br at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4759	F09[C-I]	Frequency of C - I at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4760	F09[C-B]	Frequency of C - B at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4761	F09[C-Si]	Frequency of C - Si at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4762	F09[C-X]	Frequency of C - X at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4763	F09[N-N]	Frequency of N - N at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9

4764	F09[N-O]	Frequency of N - O at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4765	F09[N-S]	Frequency of N - S at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4766	F09[N-P]	Frequency of N - P at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4767	F09[N-F]	Frequency of N - F at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4768	F09[N-Cl]	Frequency of N - Cl at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4769	F09[N-Br]	Frequency of N - Br at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4770	F09[N-I]	Frequency of N - I at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4771	F09[N-B]	Frequency of N - B at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4772	F09[N-Si]	Frequency of N - Si at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4773	F09[N-X]	Frequency of N - X at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4774	F09[O-O]	Frequency of O - O at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4775	F09[O-S]	Frequency of O - S at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4776	F09[O-P]	Frequency of O - P at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4777	F09[O-F]	Frequency of O - F at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4778	F09[O-Cl]	Frequency of O - Cl at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4779	F09[O-Br]	Frequency of O - Br at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4780	F09[O-I]	Frequency of O - I at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4781	F09[O-B]	Frequency of O - B at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4782	F09[O-Si]	Frequency of O - Si at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4783	F09[O-X]	Frequency of O - X at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9

4784	F09[S-S]	Frequency of S - S at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4785	F09[S-P]	Frequency of S - P at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4786	F09[S-F]	Frequency of S - F at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4787	F09[S-Cl]	Frequency of S - Cl at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4788	F09[S-Br]	Frequency of S - Br at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4789	F09[S-I]	Frequency of S - I at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4790	F09[S-B]	Frequency of S - B at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4791	F09[S-Si]	Frequency of S - Si at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4792	F09[S-X]	Frequency of S - X at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4793	F09[P-P]	Frequency of P - P at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4794	F09[P-F]	Frequency of P - F at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4795	F09[P-Cl]	Frequency of P - Cl at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4796	F09[P-Br]	Frequency of P - Br at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4797	F09[P-I]	Frequency of P - I at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4798	F09[P-B]	Frequency of P - B at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4799	F09[P-Si]	Frequency of P - Si at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4800	F09[P-X]	Frequency of P - X at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4801	F09[F-F]	Frequency of F - F at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4802	F09[F-Cl]	Frequency of F - Cl at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4803	F09[F-Br]	Frequency of F - Br at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9

4804	F09[F-I]	Frequency of F - I at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4805	F09[F-B]	Frequency of F - B at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4806	F09[F-Si]	Frequency of F - Si at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4807	F09[F-X]	Frequency of F - X at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4808	F09[Cl-Cl]	Frequency of Cl - Cl at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4809	F09[Cl-Br]	Frequency of Cl - Br at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4810	F09[Cl-I]	Frequency of Cl - I at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4811	F09[Cl-B]	Frequency of Cl - B at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4812	F09[Cl-Si]	Frequency of Cl - Si at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4813	F09[Cl-X]	Frequency of Cl - X at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4814	F09[Br-Br]	Frequency of Br - Br at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4815	F09[Br-I]	Frequency of Br - I at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4816	F09[Br-B]	Frequency of Br - B at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4817	F09[Br-Si]	Frequency of Br - Si at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4818	F09[Br-X]	Frequency of Br - X at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4819	F09[I-I]	Frequency of I - I at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4820	F09[I-B]	Frequency of I - B at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4821	F09[I-Si]	Frequency of I - Si at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4822	F09[I-X]	Frequency of I - X at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4823	F09[B-B]	Frequency of B - B at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9

4824	F09[B-Si]	Frequency of B - Si at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4825	F09[B-X]	Frequency of B - X at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4826	F09[Si-Si]	Frequency of Si - Si at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4827	F09[Si-X]	Frequency of Si - X at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4828	F09[X-X]	Frequency of X - X at topological distance 9	2D Atom Pairs	Frequency Atom Pairs of order 9
4829	F10[C-C]	Frequency of C - C at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4830	F10[C-N]	Frequency of C - N at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4831	F10[C-O]	Frequency of C - O at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4832	F10[C-S]	Frequency of C - S at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4833	F10[C-P]	Frequency of C - P at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4834	F10[C-F]	Frequency of C - F at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4835	F10[C-Cl]	Frequency of C - Cl at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4836	F10[C-Br]	Frequency of C - Br at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4837	F10[C-I]	Frequency of C - I at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4838	F10[C-B]	Frequency of C - B at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4839	F10[C-Si]	Frequency of C - Si at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4840	F10[C-X]	Frequency of C - X at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4841	F10[N-N]	Frequency of N - N at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4842	F10[N-O]	Frequency of N - O at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4843	F10[N-S]	Frequency of N - S at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10

4844	F10[N-P]	Frequency of N - P at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4845	F10[N-F]	Frequency of N - F at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4846	F10[N-Cl]	Frequency of N - Cl at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4847	F10[N-Br]	Frequency of N - Br at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4848	F10[N-I]	Frequency of N - I at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4849	F10[N-B]	Frequency of N - B at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4850	F10[N-Si]	Frequency of N - Si at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4851	F10[N-X]	Frequency of N - X at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4852	F10[O-O]	Frequency of O - O at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4853	F10[O-S]	Frequency of O - S at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4854	F10[O-P]	Frequency of O - P at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4855	F10[O-F]	Frequency of O - F at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4856	F10[O-Cl]	Frequency of O - Cl at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4857	F10[O-Br]	Frequency of O - Br at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4858	F10[O-I]	Frequency of O - I at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4859	F10[O-B]	Frequency of O - B at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4860	F10[O-Si]	Frequency of O - Si at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4861	F10[O-X]	Frequency of O - X at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4862	F10[S-S]	Frequency of S - S at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4863	F10[S-P]	Frequency of S - P at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10

4864	F10[S-F]	Frequency of S - F at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4865	F10[S-Cl]	Frequency of S - Cl at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4866	F10[S-Br]	Frequency of S - Br at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4867	F10[S-I]	Frequency of S - I at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4868	F10[S-B]	Frequency of S - B at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4869	F10[S-Si]	Frequency of S - Si at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4870	F10[S-X]	Frequency of S - X at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4871	F10[P-P]	Frequency of P - P at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4872	F10[P-F]	Frequency of P - F at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4873	F10[P-Cl]	Frequency of P - Cl at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4874	F10[P-Br]	Frequency of P - Br at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4875	F10[P-I]	Frequency of P - I at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4876	F10[P-B]	Frequency of P - B at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4877	F10[P-Si]	Frequency of P - Si at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4878	F10[P-X]	Frequency of P - X at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4879	F10[F-F]	Frequency of F - F at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4880	F10[F-Cl]	Frequency of F - Cl at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4881	F10[F-Br]	Frequency of F - Br at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4882	F10[F-I]	Frequency of F - I at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4883	F10[F-B]	Frequency of F - B at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10

4884	F10[F-Si]	Frequency of F - Si at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4885	F10[F-X]	Frequency of F - X at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4886	F10[Cl-Cl]	Frequency of Cl - Cl at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4887	F10[Cl-Br]	Frequency of Cl - Br at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4888	F10[Cl-I]	Frequency of Cl - I at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4889	F10[Cl-B]	Frequency of Cl - B at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4890	F10[Cl-Si]	Frequency of Cl - Si at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4891	F10[Cl-X]	Frequency of Cl - X at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4892	F10[Br-Br]	Frequency of Br - Br at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4893	F10[Br-I]	Frequency of Br - I at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4894	F10[Br-B]	Frequency of Br - B at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4895	F10[Br-Si]	Frequency of Br - Si at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4896	F10[Br-X]	Frequency of Br - X at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4897	F10[I-I]	Frequency of I - I at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4898	F10[I-B]	Frequency of I - B at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4899	F10[I-Si]	Frequency of I - Si at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4900	F10[I-X]	Frequency of I - X at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4901	F10[B-B]	Frequency of B - B at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4902	F10[B-Si]	Frequency of B - Si at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4903	F10[B-X]	Frequency of B - X at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10

4904	F10[Si-Si]	Frequency of Si - Si at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4905	F10[Si-X]	Frequency of Si - X at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4906	F10[X-X]	Frequency of X - X at topological distance 10	2D Atom Pairs	Frequency Atom Pairs of order 10
4907	G(N..N)	sum of geometrical distances between N..N	3D Atom Pairs	Weighted geometrical atom pairs
4908	G(N..O)	sum of geometrical distances between N..O	3D Atom Pairs	Weighted geometrical atom pairs
4909	G(N..S)	sum of geometrical distances between N..S	3D Atom Pairs	Weighted geometrical atom pairs
4910	G(N..P)	sum of geometrical distances between N..P	3D Atom Pairs	Weighted geometrical atom pairs
4911	G(N..F)	sum of geometrical distances between N..F	3D Atom Pairs	Weighted geometrical atom pairs
4912	G(N..Cl)	sum of geometrical distances between N..Cl	3D Atom Pairs	Weighted geometrical atom pairs
4913	G(N..Br)	sum of geometrical distances between N..Br	3D Atom Pairs	Weighted geometrical atom pairs
4914	G(N..I)	sum of geometrical distances between N..I	3D Atom Pairs	Weighted geometrical atom pairs
4915	G(O..O)	sum of geometrical distances between O..O	3D Atom Pairs	Weighted geometrical atom pairs
4916	G(O..S)	sum of geometrical distances between O..S	3D Atom Pairs	Weighted geometrical atom pairs
4917	G(O..P)	sum of geometrical distances between O..P	3D Atom Pairs	Weighted geometrical atom pairs
4918	G(O..F)	sum of geometrical distances between O..F	3D Atom Pairs	Weighted geometrical atom pairs

4919	G(O..Cl)	sum of geometrical distances between O..Cl	3D Atom Pairs	Weighted geometrical atom pairs
4920	G(O..Br)	sum of geometrical distances between O..Br	3D Atom Pairs	Weighted geometrical atom pairs
4921	G(O..I)	sum of geometrical distances between O..I	3D Atom Pairs	Weighted geometrical atom pairs
4922	G(S..S)	sum of geometrical distances between S..S	3D Atom Pairs	Weighted geometrical atom pairs
4923	G(S..P)	sum of geometrical distances between S..P	3D Atom Pairs	Weighted geometrical atom pairs
4924	G(S..F)	sum of geometrical distances between S..F	3D Atom Pairs	Weighted geometrical atom pairs
4925	G(S..Cl)	sum of geometrical distances between S..Cl	3D Atom Pairs	Weighted geometrical atom pairs
4926	G(S..Br)	sum of geometrical distances between S..Br	3D Atom Pairs	Weighted geometrical atom pairs
4927	G(S..I)	sum of geometrical distances between S..I	3D Atom Pairs	Weighted geometrical atom pairs
4928	G(P..P)	sum of geometrical distances between P..P	3D Atom Pairs	Weighted geometrical atom pairs
4929	G(P..F)	sum of geometrical distances between P..F	3D Atom Pairs	Weighted geometrical atom pairs
4930	G(P..Cl)	sum of geometrical distances between P..Cl	3D Atom Pairs	Weighted geometrical atom pairs
4931	G(P..Br)	sum of geometrical distances between P..Br	3D Atom Pairs	Weighted geometrical atom pairs
4932	G(P..I)	sum of geometrical distances between P..I	3D Atom Pairs	Weighted geometrical atom pairs
4933	G(F..F)	sum of geometrical distances between F..F	3D Atom Pairs	Weighted geometrical atom pairs

4934	G(F..Cl)	sum of geometrical distances between F..Cl	3D Atom Pairs	Weighted geometrical atom pairs
4935	G(F..Br)	sum of geometrical distances between F..Br	3D Atom Pairs	Weighted geometrical atom pairs
4936	G(F..I)	sum of geometrical distances between F..I	3D Atom Pairs	Weighted geometrical atom pairs
4937	G(Cl..Cl)	sum of geometrical distances between Cl..Cl	3D Atom Pairs	Weighted geometrical atom pairs
4938	G(Cl..Br)	sum of geometrical distances between Cl..Br	3D Atom Pairs	Weighted geometrical atom pairs
4939	G(Cl..I)	sum of geometrical distances between Cl..I	3D Atom Pairs	Weighted geometrical atom pairs
4940	G(Br..Br)	sum of geometrical distances between Br..Br	3D Atom Pairs	Weighted geometrical atom pairs
4941	G(Br..I)	sum of geometrical distances between Br..I	3D Atom Pairs	Weighted geometrical atom pairs
4942	G(I..I)	sum of geometrical distances between I..I	3D Atom Pairs	Weighted geometrical atom pairs
4943	qpmax	maximum positive charge	Charge descriptors	Basic descriptors
4944	qnmax	maximum negative charge	Charge descriptors	Basic descriptors
4945	Qpos	total positive charge	Charge descriptors	Basic descriptors
4946	Qneg	total negative charge	Charge descriptors	Basic descriptors
4947	Qtot	total absolute charge (electronic charge index - ECI)	Charge descriptors	Basic descriptors
4948	Qmean	mean absolute charge (charge polarization)	Charge descriptors	Basic descriptors
4949	Q2	total squared charge	Charge descriptors	Basic descriptors
4950	RPCG	relative positive charge	Charge descriptors	Basic descriptors

4951	RNCG	relative negative charge	Charge descriptors	Basic descriptors
4952	SPP	submolecular polarity parameter	Charge descriptors	Basic descriptors
4953	TE1	topographic electronic descriptor	Charge descriptors	Basic descriptors
4954	TE2	topographic electronic descriptor (bond resctricted)	Charge descriptors	Basic descriptors
4955	PCWTE1	partial charge weighted topological electronic index	Charge descriptors	Basic descriptors
4956	PCWTE2	partial charge weighted topological electronic index (bond resctricted)	Charge descriptors	Basic descriptors
4957	LDI	local dipole index	Charge descriptors	Basic descriptors
4958	Uc	unsaturation count	Molecular properties	Basic descriptors
4959	Ui	unsaturation index	Molecular properties	Basic descriptors
4960	Hy	hydrophilic factor	Molecular properties	Basic descriptors
4961	AMR	Ghose-Crippen molar refractivity	Molecular properties	Basic descriptors
4962	TPSA(NO)	topological polar surface area using N,O polar contributions	Molecular properties	Basic descriptors
4963	TPSA(Tot)	topological polar surface area using N,O,S,P polar contributions	Molecular properties	Basic descriptors
4964	MLOGP	Moriguchi octanol-water partition coeff. (logP)	Molecular properties	Basic descriptors
4965	MLOGP2	squared Moriguchi octanol-water partition coeff. (logP^2)	Molecular properties	Basic descriptors
4966	ALOGP	Ghose-Crippen octanol-water partition coeff. (logP)	Molecular properties	Basic descriptors
4967	ALOGP2	squared Ghose-Crippen octanol-water partition coeff. (logP^2)	Molecular properties	Basic descriptors
4968	SAtot	total surface area from P_VSA-like descriptors	Molecular properties	Basic descriptors
4969	SAacc	surface area of acceptor atoms from P_VSA-like descriptors	Molecular properties	Basic descriptors
4970	SAdon	surface area of donor atoms from P_VSA-like descriptors	Molecular properties	Basic descriptors

4971	Vx	McGowan volume	Molecular properties	Basic descriptors
4972	VvdwMG	van der Waals volume from McGowan volume	Molecular properties	Basic descriptors
4973	VvdwZAZ	van der Waals volume from Zhao-Abraham-Zissimos equation	Molecular properties	Basic descriptors
4974	PDI	packing density index	Molecular properties	Basic descriptors
4975	BLTF96	Verhaar Fish base-line toxicity from MLOGP (mmol/l)	Molecular properties	Basic descriptors
4976	BLTD48	Verhaar Daphnia base-line toxicity from MLOGP (mmol/l)	Molecular properties	Basic descriptors
4977	BLTA96	Verhaar Algae base-line toxicity from MLOGP (mmol/l)	Molecular properties	Basic descriptors
4978	Ro5	Lipinski Rule of 5	Drug-like indices	Basic indices
4979	cRo5	Complementary Lipinski Alert index	Drug-like indices	Basic indices
4980	DLS_01	modified drug-like score from Lipinski (4 rules)	Drug-like indices	Basic indices
4981	DLS_02	modified drug-like score from Oprea et al. (6 rules)	Drug-like indices	Basic indices
4982	DLS_03	modified drug-like score from Walters et al. (6 rules)	Drug-like indices	Basic indices
4983	DLS_04	modified drug-like score from Chen et al. (7 rules)	Drug-like indices	Basic indices
4984	DLS_05	modified drug-like score from Zheng et al. (2 rules)	Drug-like indices	Basic indices
4985	DLS_06	modified drug-like score from Rishton (6 rules)	Drug-like indices	Basic indices
4986	DLS_07	modified drug-like score from Veber et al. (2 rules)	Drug-like indices	Basic indices
4987	DLS_cons	DRAGON consensus drug-like score	Drug-like indices	Basic indices
4988	LLS_01	modified lead-like score from Congreve et al. (6 rules)	Drug-like indices	Basic indices
4989	LLS_02	modified lead-like score from Monge et al. (8 rules)	Drug-like indices	Basic indices
4990	CMC-80	Ghose-Viswanadhan-Wendoloski CMC drug-like index at 80%	Drug-like indices	Basic indices

4991	CMC-50	Ghose-Viswanadhan-Wendoloski CMC drug-like index at 50%	Drug-like indices	Basic indices
4992	Inflammat-80	Ghose-Viswanadhan-Wendoloski antiinflammatory-like index at 80%	Drug-like indices	Basic indices
4993	Inflammat-50	Ghose-Viswanadhan-Wendoloski antiinflammatory-like index at 50%	Drug-like indices	Basic indices
4994	Depressant-80	Ghose-Viswanadhan-Wendoloski antidepressant-like index at 80%	Drug-like indices	Basic indices
4995	Depressant-50	Ghose-Viswanadhan-Wendoloski antidepressant-like index at 50%	Drug-like indices	Basic indices
4996	Psychotic-80	Ghose-Viswanadhan-Wendoloski antipsychotic-like index at 80%	Drug-like indices	Basic indices
4997	Psychotic-50	Ghose-Viswanadhan-Wendoloski antipsychotic-like index at 50%	Drug-like indices	Basic indices
4998	Hypertens-80	Ghose-Viswanadhan-Wendoloski antihypertensive-like index at 80%	Drug-like indices	Basic indices
4999	Hypertens-50	Ghose-Viswanadhan-Wendoloski antihypertensive-like index at 50%	Drug-like indices	Basic indices
5000	Hypnotic-80	Ghose-Viswanadhan-Wendoloski hypnotic-like index at 80%	Drug-like indices	Basic indices
5001	Hypnotic-50	Ghose-Viswanadhan-Wendoloski hypnotic-like index at 50%	Drug-like indices	Basic indices
5002	Neoplastic-80	Ghose-Viswanadhan-Wendoloski antineoplastic-like index at 80%	Drug-like indices	Basic indices
5003	Neoplastic-50	Ghose-Viswanadhan-Wendoloski antineoplastic-like index at 50%	Drug-like indices	Basic indices
5004	Infective-80	Ghose-Viswanadhan-Wendoloski antiinfective-like index at 80%	Drug-like indices	Basic indices
5005	Infective-50	Ghose-Viswanadhan-Wendoloski antiinfective-like index at 50%	Drug-like indices	Basic indices
5006	CATS3D_00_DD	CATS3D Donor-Donor BIN 00 (0.000 - 1.000 Ã…)	CATS 3D descriptors	Basic descriptors
5007	CATS3D_01_DD	CATS3D Donor-Donor BIN 01 (1.000 - 2.000 Ã…)	CATS 3D descriptors	Basic descriptors
5008	CATS3D_02_DD	CATS3D Donor-Donor BIN 02 (2.000 - 3.000 Ã…)	CATS 3D descriptors	Basic descriptors
5009	CATS3D_03_DD	CATS3D Donor-Donor BIN 03 (3.000 - 4.000 Ã…)	CATS 3D descriptors	Basic descriptors
5010	CATS3D_04_DD	CATS3D Donor-Donor BIN 04 (4.000 - 5.000 Ã…)	CATS 3D descriptors	Basic descriptors

5011	CATS3D_05_DD	CATS3D Donor-Donor BIN 05 (5.000 - 6.000 Ã…)	CATS 3D descriptors	Basic descriptors
5012	CATS3D_06_DD	CATS3D Donor-Donor BIN 06 (6.000 - 7.000 Ã…)	CATS 3D descriptors	Basic descriptors
5013	CATS3D_07_DD	CATS3D Donor-Donor BIN 07 (7.000 - 8.000 Ã…)	CATS 3D descriptors	Basic descriptors
5014	CATS3D_08_DD	CATS3D Donor-Donor BIN 08 (8.000 - 9.000 Ã…)	CATS 3D descriptors	Basic descriptors
5015	CATS3D_09_DD	CATS3D Donor-Donor BIN 09 (9.000 - 10.000 Ã…)	CATS 3D descriptors	Basic descriptors
5016	CATS3D_10_DD	CATS3D Donor-Donor BIN 10 (10.000 - 11.000 Ã…)	CATS 3D descriptors	Basic descriptors
5017	CATS3D_11_DD	CATS3D Donor-Donor BIN 11 (11.000 - 12.000 Ã…)	CATS 3D descriptors	Basic descriptors
5018	CATS3D_12_DD	CATS3D Donor-Donor BIN 12 (12.000 - 13.000 Ã…)	CATS 3D descriptors	Basic descriptors
5019	CATS3D_13_DD	CATS3D Donor-Donor BIN 13 (13.000 - 14.000 Ã…)	CATS 3D descriptors	Basic descriptors
5020	CATS3D_14_DD	CATS3D Donor-Donor BIN 14 (14.000 - 15.000 Ã…)	CATS 3D descriptors	Basic descriptors
5021	CATS3D_15_DD	CATS3D Donor-Donor BIN 15 (15.000 - 16.000 Ã…)	CATS 3D descriptors	Basic descriptors
5022	CATS3D_16_DD	CATS3D Donor-Donor BIN 16 (16.000 - 17.000 Ã…)	CATS 3D descriptors	Basic descriptors
5023	CATS3D_17_DD	CATS3D Donor-Donor BIN 17 (17.000 - 18.000 Ã…)	CATS 3D descriptors	Basic descriptors
5024	CATS3D_18_DD	CATS3D Donor-Donor BIN 18 (18.000 - 19.000 Ã…)	CATS 3D descriptors	Basic descriptors
5025	CATS3D_19_DD	CATS3D Donor-Donor BIN 19 (19.000 - 20.000 Ã…)	CATS 3D descriptors	Basic descriptors
5026	CATS3D_00_DA	CATS3D Donor-Acceptor BIN 00 (0.000 - 1.000 Ã…)	CATS 3D descriptors	Basic descriptors
5027	CATS3D_01_DA	CATS3D Donor-Acceptor BIN 01 (1.000 - 2.000 Ã…)	CATS 3D descriptors	Basic descriptors
5028	CATS3D_02_DA	CATS3D Donor-Acceptor BIN 02 (2.000 - 3.000 Ã…)	CATS 3D descriptors	Basic descriptors
5029	CATS3D_03_DA	CATS3D Donor-Acceptor BIN 03 (3.000 - 4.000 Ã…)	CATS 3D descriptors	Basic descriptors
5030	CATS3D_04_DA	CATS3D Donor-Acceptor BIN 04 (4.000 - 5.000 Ã…)	CATS 3D descriptors	Basic descriptors

5031	CATS3D_05_DA	CATS3D Donor-Acceptor BIN 05 (5.000 - 6.000 Ã…)	CATS 3D descriptors	Basic descriptors
5032	CATS3D_06_DA	CATS3D Donor-Acceptor BIN 06 (6.000 - 7.000 Ã…)	CATS 3D descriptors	Basic descriptors
5033	CATS3D_07_DA	CATS3D Donor-Acceptor BIN 07 (7.000 - 8.000 Ã…)	CATS 3D descriptors	Basic descriptors
5034	CATS3D_08_DA	CATS3D Donor-Acceptor BIN 08 (8.000 - 9.000 Ã…)	CATS 3D descriptors	Basic descriptors
5035	CATS3D_09_DA	CATS3D Donor-Acceptor BIN 09 (9.000 - 10.000 Ã…)	CATS 3D descriptors	Basic descriptors
5036	CATS3D_10_DA	CATS3D Donor-Acceptor BIN 10 (10.000 - 11.000 Ã…)	CATS 3D descriptors	Basic descriptors
5037	CATS3D_11_DA	CATS3D Donor-Acceptor BIN 11 (11.000 - 12.000 Ã…)	CATS 3D descriptors	Basic descriptors
5038	CATS3D_12_DA	CATS3D Donor-Acceptor BIN 12 (12.000 - 13.000 Ã…)	CATS 3D descriptors	Basic descriptors
5039	CATS3D_13_DA	CATS3D Donor-Acceptor BIN 13 (13.000 - 14.000 Ã…)	CATS 3D descriptors	Basic descriptors
5040	CATS3D_14_DA	CATS3D Donor-Acceptor BIN 14 (14.000 - 15.000 Ã…)	CATS 3D descriptors	Basic descriptors
5041	CATS3D_15_DA	CATS3D Donor-Acceptor BIN 15 (15.000 - 16.000 Ã…)	CATS 3D descriptors	Basic descriptors
5042	CATS3D_16_DA	CATS3D Donor-Acceptor BIN 16 (16.000 - 17.000 Ã…)	CATS 3D descriptors	Basic descriptors
5043	CATS3D_17_DA	CATS3D Donor-Acceptor BIN 17 (17.000 - 18.000 Ã…)	CATS 3D descriptors	Basic descriptors
5044	CATS3D_18_DA	CATS3D Donor-Acceptor BIN 18 (18.000 - 19.000 Ã…)	CATS 3D descriptors	Basic descriptors
5045	CATS3D_19_DA	CATS3D Donor-Acceptor BIN 19 (19.000 - 20.000 Ã…)	CATS 3D descriptors	Basic descriptors
5046	CATS3D_00_DP	CATS3D Donor-Positive BIN 00 (0.000 - 1.000 Ã…)	CATS 3D descriptors	Basic descriptors
5047	CATS3D_01_DP	CATS3D Donor-Positive BIN 01 (1.000 - 2.000 Ã…)	CATS 3D descriptors	Basic descriptors
5048	CATS3D_02_DP	CATS3D Donor-Positive BIN 02 (2.000 - 3.000 Ã…)	CATS 3D descriptors	Basic descriptors
5049	CATS3D_03_DP	CATS3D Donor-Positive BIN 03 (3.000 - 4.000 Ã…)	CATS 3D descriptors	Basic descriptors
5050	CATS3D_04_DP	CATS3D Donor-Positive BIN 04 (4.000 - 5.000 Ã…)	CATS 3D descriptors	Basic descriptors

5051	CATS3D_05_DP	CATS3D Donor-Positive BIN 05 (5.000 - 6.000 Ã…)	CATS 3D descriptors	Basic descriptors
5052	CATS3D_06_DP	CATS3D Donor-Positive BIN 06 (6.000 - 7.000 Ã…)	CATS 3D descriptors	Basic descriptors
5053	CATS3D_07_DP	CATS3D Donor-Positive BIN 07 (7.000 - 8.000 Ã…)	CATS 3D descriptors	Basic descriptors
5054	CATS3D_08_DP	CATS3D Donor-Positive BIN 08 (8.000 - 9.000 Ã…)	CATS 3D descriptors	Basic descriptors
5055	CATS3D_09_DP	CATS3D Donor-Positive BIN 09 (9.000 - 10.000 Ã…)	CATS 3D descriptors	Basic descriptors
5056	CATS3D_10_DP	CATS3D Donor-Positive BIN 10 (10.000 - 11.000 Ã…)	CATS 3D descriptors	Basic descriptors
5057	CATS3D_11_DP	CATS3D Donor-Positive BIN 11 (11.000 - 12.000 Ã…)	CATS 3D descriptors	Basic descriptors
5058	CATS3D_12_DP	CATS3D Donor-Positive BIN 12 (12.000 - 13.000 Ã…)	CATS 3D descriptors	Basic descriptors
5059	CATS3D_13_DP	CATS3D Donor-Positive BIN 13 (13.000 - 14.000 Ã…)	CATS 3D descriptors	Basic descriptors
5060	CATS3D_14_DP	CATS3D Donor-Positive BIN 14 (14.000 - 15.000 Ã…)	CATS 3D descriptors	Basic descriptors
5061	CATS3D_15_DP	CATS3D Donor-Positive BIN 15 (15.000 - 16.000 Ã…)	CATS 3D descriptors	Basic descriptors
5062	CATS3D_16_DP	CATS3D Donor-Positive BIN 16 (16.000 - 17.000 Ã…)	CATS 3D descriptors	Basic descriptors
5063	CATS3D_17_DP	CATS3D Donor-Positive BIN 17 (17.000 - 18.000 Ã…)	CATS 3D descriptors	Basic descriptors
5064	CATS3D_18_DP	CATS3D Donor-Positive BIN 18 (18.000 - 19.000 Ã…)	CATS 3D descriptors	Basic descriptors
5065	CATS3D_19_DP	CATS3D Donor-Positive BIN 19 (19.000 - 20.000 Ã…)	CATS 3D descriptors	Basic descriptors
5066	CATS3D_00_DN	CATS3D Donor-Negative BIN 00 (0.000 - 1.000 Ã…)	CATS 3D descriptors	Basic descriptors
5067	CATS3D_01_DN	CATS3D Donor-Negative BIN 01 (1.000 - 2.000 Ã…)	CATS 3D descriptors	Basic descriptors
5068	CATS3D_02_DN	CATS3D Donor-Negative BIN 02 (2.000 - 3.000 Ã…)	CATS 3D descriptors	Basic descriptors
5069	CATS3D_03_DN	CATS3D Donor-Negative BIN 03 (3.000 - 4.000 Ã…)	CATS 3D descriptors	Basic descriptors
5070	CATS3D_04_DN	CATS3D Donor-Negative BIN 04 (4.000 - 5.000 Ã…)	CATS 3D descriptors	Basic descriptors

5071	CATS3D_05_DN	CATS3D Donor-Negative BIN 05 (5.000 - 6.000 Ã…)	CATS 3D descriptors	Basic descriptors
5072	CATS3D_06_DN	CATS3D Donor-Negative BIN 06 (6.000 - 7.000 Ã…)	CATS 3D descriptors	Basic descriptors
5073	CATS3D_07_DN	CATS3D Donor-Negative BIN 07 (7.000 - 8.000 Ã…)	CATS 3D descriptors	Basic descriptors
5074	CATS3D_08_DN	CATS3D Donor-Negative BIN 08 (8.000 - 9.000 Ã…)	CATS 3D descriptors	Basic descriptors
5075	CATS3D_09_DN	CATS3D Donor-Negative BIN 09 (9.000 - 10.000 Ã…)	CATS 3D descriptors	Basic descriptors
5076	CATS3D_10_DN	CATS3D Donor-Negative BIN 10 (10.000 - 11.000 Ã…)	CATS 3D descriptors	Basic descriptors
5077	CATS3D_11_DN	CATS3D Donor-Negative BIN 11 (11.000 - 12.000 Ã…)	CATS 3D descriptors	Basic descriptors
5078	CATS3D_12_DN	CATS3D Donor-Negative BIN 12 (12.000 - 13.000 Ã…)	CATS 3D descriptors	Basic descriptors
5079	CATS3D_13_DN	CATS3D Donor-Negative BIN 13 (13.000 - 14.000 Ã…)	CATS 3D descriptors	Basic descriptors
5080	CATS3D_14_DN	CATS3D Donor-Negative BIN 14 (14.000 - 15.000 Ã…)	CATS 3D descriptors	Basic descriptors
5081	CATS3D_15_DN	CATS3D Donor-Negative BIN 15 (15.000 - 16.000 Ã…)	CATS 3D descriptors	Basic descriptors
5082	CATS3D_16_DN	CATS3D Donor-Negative BIN 16 (16.000 - 17.000 Ã…)	CATS 3D descriptors	Basic descriptors
5083	CATS3D_17_DN	CATS3D Donor-Negative BIN 17 (17.000 - 18.000 Ã…)	CATS 3D descriptors	Basic descriptors
5084	CATS3D_18_DN	CATS3D Donor-Negative BIN 18 (18.000 - 19.000 Ã…)	CATS 3D descriptors	Basic descriptors
5085	CATS3D_19_DN	CATS3D Donor-Negative BIN 19 (19.000 - 20.000 Ã…)	CATS 3D descriptors	Basic descriptors
5086	CATS3D_00_DL	CATS3D Donor-Lipophilic BIN 00 (0.000 - 1.000 Ã…)	CATS 3D descriptors	Basic descriptors
5087	CATS3D_01_DL	CATS3D Donor-Lipophilic BIN 01 (1.000 - 2.000 Ã…)	CATS 3D descriptors	Basic descriptors
5088	CATS3D_02_DL	CATS3D Donor-Lipophilic BIN 02 (2.000 - 3.000 Ã…)	CATS 3D descriptors	Basic descriptors
5089	CATS3D_03_DL	CATS3D Donor-Lipophilic BIN 03 (3.000 - 4.000 Ã…)	CATS 3D descriptors	Basic descriptors
5090	CATS3D_04_DL	CATS3D Donor-Lipophilic BIN 04 (4.000 - 5.000 Ã…)	CATS 3D descriptors	Basic descriptors

5091	CATS3D_05_DL	CATS3D Donor-Lipophilic BIN 05 (5.000 - 6.000 Ã…)	CATS 3D descriptors	Basic descriptors
5092	CATS3D_06_DL	CATS3D Donor-Lipophilic BIN 06 (6.000 - 7.000 Ã…)	CATS 3D descriptors	Basic descriptors
5093	CATS3D_07_DL	CATS3D Donor-Lipophilic BIN 07 (7.000 - 8.000 Ã…)	CATS 3D descriptors	Basic descriptors
5094	CATS3D_08_DL	CATS3D Donor-Lipophilic BIN 08 (8.000 - 9.000 Ã…)	CATS 3D descriptors	Basic descriptors
5095	CATS3D_09_DL	CATS3D Donor-Lipophilic BIN 09 (9.000 - 10.000 Ã…)	CATS 3D descriptors	Basic descriptors
5096	CATS3D_10_DL	CATS3D Donor-Lipophilic BIN 10 (10.000 - 11.000 Ã…)	CATS 3D descriptors	Basic descriptors
5097	CATS3D_11_DL	CATS3D Donor-Lipophilic BIN 11 (11.000 - 12.000 Ã…)	CATS 3D descriptors	Basic descriptors
5098	CATS3D_12_DL	CATS3D Donor-Lipophilic BIN 12 (12.000 - 13.000 Ã…)	CATS 3D descriptors	Basic descriptors
5099	CATS3D_13_DL	CATS3D Donor-Lipophilic BIN 13 (13.000 - 14.000 Ã…)	CATS 3D descriptors	Basic descriptors
5100	CATS3D_14_DL	CATS3D Donor-Lipophilic BIN 14 (14.000 - 15.000 Ã…)	CATS 3D descriptors	Basic descriptors
5101	CATS3D_15_DL	CATS3D Donor-Lipophilic BIN 15 (15.000 - 16.000 Ã…)	CATS 3D descriptors	Basic descriptors
5102	CATS3D_16_DL	CATS3D Donor-Lipophilic BIN 16 (16.000 - 17.000 Ã…)	CATS 3D descriptors	Basic descriptors
5103	CATS3D_17_DL	CATS3D Donor-Lipophilic BIN 17 (17.000 - 18.000 Ã…)	CATS 3D descriptors	Basic descriptors
5104	CATS3D_18_DL	CATS3D Donor-Lipophilic BIN 18 (18.000 - 19.000 Ã…)	CATS 3D descriptors	Basic descriptors
5105	CATS3D_19_DL	CATS3D Donor-Lipophilic BIN 19 (19.000 - 20.000 Ã…)	CATS 3D descriptors	Basic descriptors
5106	CATS3D_00_AA	CATS3D Acceptor-Acceptor BIN 00 (0.000 - 1.000 Ã…)	CATS 3D descriptors	Basic descriptors
5107	CATS3D_01_AA	CATS3D Acceptor-Acceptor BIN 01 (1.000 - 2.000 Ã…)	CATS 3D descriptors	Basic descriptors
5108	CATS3D_02_AA	CATS3D Acceptor-Acceptor BIN 02 (2.000 - 3.000 Ã…)	CATS 3D descriptors	Basic descriptors
5109	CATS3D_03_AA	CATS3D Acceptor-Acceptor BIN 03 (3.000 - 4.000 Ã…)	CATS 3D descriptors	Basic descriptors
5110	CATS3D_04_AA	CATS3D Acceptor-Acceptor BIN 04 (4.000 - 5.000 Ã…)	CATS 3D descriptors	Basic descriptors

5111	CATS3D_05_AA	CATS3D Acceptor-Acceptor BIN 05 (5.000 - 6.000 Ã…)	CATS 3D descriptors	Basic descriptors
5112	CATS3D_06_AA	CATS3D Acceptor-Acceptor BIN 06 (6.000 - 7.000 Ã…)	CATS 3D descriptors	Basic descriptors
5113	CATS3D_07_AA	CATS3D Acceptor-Acceptor BIN 07 (7.000 - 8.000 Ã…)	CATS 3D descriptors	Basic descriptors
5114	CATS3D_08_AA	CATS3D Acceptor-Acceptor BIN 08 (8.000 - 9.000 Ã…)	CATS 3D descriptors	Basic descriptors
5115	CATS3D_09_AA	CATS3D Acceptor-Acceptor BIN 09 (9.000 - 10.000 Ã…)	CATS 3D descriptors	Basic descriptors
5116	CATS3D_10_AA	CATS3D Acceptor-Acceptor BIN 10 (10.000 - 11.000 Ã…)	CATS 3D descriptors	Basic descriptors
5117	CATS3D_11_AA	CATS3D Acceptor-Acceptor BIN 11 (11.000 - 12.000 Ã…)	CATS 3D descriptors	Basic descriptors
5118	CATS3D_12_AA	CATS3D Acceptor-Acceptor BIN 12 (12.000 - 13.000 Ã…)	CATS 3D descriptors	Basic descriptors
5119	CATS3D_13_AA	CATS3D Acceptor-Acceptor BIN 13 (13.000 - 14.000 Ã…)	CATS 3D descriptors	Basic descriptors
5120	CATS3D_14_AA	CATS3D Acceptor-Acceptor BIN 14 (14.000 - 15.000 Ã…)	CATS 3D descriptors	Basic descriptors
5121	CATS3D_15_AA	CATS3D Acceptor-Acceptor BIN 15 (15.000 - 16.000 Ã…)	CATS 3D descriptors	Basic descriptors
5122	CATS3D_16_AA	CATS3D Acceptor-Acceptor BIN 16 (16.000 - 17.000 Ã…)	CATS 3D descriptors	Basic descriptors
5123	CATS3D_17_AA	CATS3D Acceptor-Acceptor BIN 17 (17.000 - 18.000 Ã…)	CATS 3D descriptors	Basic descriptors
5124	CATS3D_18_AA	CATS3D Acceptor-Acceptor BIN 18 (18.000 - 19.000 Ã…)	CATS 3D descriptors	Basic descriptors
5125	CATS3D_19_AA	CATS3D Acceptor-Acceptor BIN 19 (19.000 - 20.000 Ã…)	CATS 3D descriptors	Basic descriptors
5126	CATS3D_00_AP	CATS3D Acceptor-Positive BIN 00 (0.000 - 1.000 Ã…)	CATS 3D descriptors	Basic descriptors
5127	CATS3D_01_AP	CATS3D Acceptor-Positive BIN 01 (1.000 - 2.000 Ã…)	CATS 3D descriptors	Basic descriptors
5128	CATS3D_02_AP	CATS3D Acceptor-Positive BIN 02 (2.000 - 3.000 Ã…)	CATS 3D descriptors	Basic descriptors
5129	CATS3D_03_AP	CATS3D Acceptor-Positive BIN 03 (3.000 - 4.000 Ã…)	CATS 3D descriptors	Basic descriptors
5130	CATS3D_04_AP	CATS3D Acceptor-Positive BIN 04 (4.000 - 5.000 Ã…)	CATS 3D descriptors	Basic descriptors

5131	CATS3D_05_AP	CATS3D Acceptor-Positive BIN 05 (5.000 - 6.000 Ã…)	CATS 3D descriptors	Basic descriptors
5132	CATS3D_06_AP	CATS3D Acceptor-Positive BIN 06 (6.000 - 7.000 Ã…)	CATS 3D descriptors	Basic descriptors
5133	CATS3D_07_AP	CATS3D Acceptor-Positive BIN 07 (7.000 - 8.000 Ã…)	CATS 3D descriptors	Basic descriptors
5134	CATS3D_08_AP	CATS3D Acceptor-Positive BIN 08 (8.000 - 9.000 Ã…)	CATS 3D descriptors	Basic descriptors
5135	CATS3D_09_AP	CATS3D Acceptor-Positive BIN 09 (9.000 - 10.000 Ã…)	CATS 3D descriptors	Basic descriptors
5136	CATS3D_10_AP	CATS3D Acceptor-Positive BIN 10 (10.000 - 11.000 Ã…)	CATS 3D descriptors	Basic descriptors
5137	CATS3D_11_AP	CATS3D Acceptor-Positive BIN 11 (11.000 - 12.000 Ã…)	CATS 3D descriptors	Basic descriptors
5138	CATS3D_12_AP	CATS3D Acceptor-Positive BIN 12 (12.000 - 13.000 Ã…)	CATS 3D descriptors	Basic descriptors
5139	CATS3D_13_AP	CATS3D Acceptor-Positive BIN 13 (13.000 - 14.000 Ã…)	CATS 3D descriptors	Basic descriptors
5140	CATS3D_14_AP	CATS3D Acceptor-Positive BIN 14 (14.000 - 15.000 Ã…)	CATS 3D descriptors	Basic descriptors
5141	CATS3D_15_AP	CATS3D Acceptor-Positive BIN 15 (15.000 - 16.000 Ã…)	CATS 3D descriptors	Basic descriptors
5142	CATS3D_16_AP	CATS3D Acceptor-Positive BIN 16 (16.000 - 17.000 Ã…)	CATS 3D descriptors	Basic descriptors
5143	CATS3D_17_AP	CATS3D Acceptor-Positive BIN 17 (17.000 - 18.000 Ã…)	CATS 3D descriptors	Basic descriptors
5144	CATS3D_18_AP	CATS3D Acceptor-Positive BIN 18 (18.000 - 19.000 Ã…)	CATS 3D descriptors	Basic descriptors
5145	CATS3D_19_AP	CATS3D Acceptor-Positive BIN 19 (19.000 - 20.000 Ã…)	CATS 3D descriptors	Basic descriptors
5146	CATS3D_00_AN	CATS3D Acceptor-Negative BIN 00 (0.000 - 1.000 Ã…)	CATS 3D descriptors	Basic descriptors
5147	CATS3D_01_AN	CATS3D Acceptor-Negative BIN 01 (1.000 - 2.000 Ã…)	CATS 3D descriptors	Basic descriptors
5148	CATS3D_02_AN	CATS3D Acceptor-Negative BIN 02 (2.000 - 3.000 Ã…)	CATS 3D descriptors	Basic descriptors
5149	CATS3D_03_AN	CATS3D Acceptor-Negative BIN 03 (3.000 - 4.000 Ã…)	CATS 3D descriptors	Basic descriptors
5150	CATS3D_04_AN	CATS3D Acceptor-Negative BIN 04 (4.000 - 5.000 Ã…)	CATS 3D descriptors	Basic descriptors

5151	CATS3D_05_AN	CATS3D Acceptor-Negative BIN 05 (5.000 - 6.000 Ã…)	CATS 3D descriptors	Basic descriptors
5152	CATS3D_06_AN	CATS3D Acceptor-Negative BIN 06 (6.000 - 7.000 Ã…)	CATS 3D descriptors	Basic descriptors
5153	CATS3D_07_AN	CATS3D Acceptor-Negative BIN 07 (7.000 - 8.000 Ã…)	CATS 3D descriptors	Basic descriptors
5154	CATS3D_08_AN	CATS3D Acceptor-Negative BIN 08 (8.000 - 9.000 Ã…)	CATS 3D descriptors	Basic descriptors
5155	CATS3D_09_AN	CATS3D Acceptor-Negative BIN 09 (9.000 - 10.000 Ã…)	CATS 3D descriptors	Basic descriptors
5156	CATS3D_10_AN	CATS3D Acceptor-Negative BIN 10 (10.000 - 11.000 Ã…)	CATS 3D descriptors	Basic descriptors
5157	CATS3D_11_AN	CATS3D Acceptor-Negative BIN 11 (11.000 - 12.000 Ã…)	CATS 3D descriptors	Basic descriptors
5158	CATS3D_12_AN	CATS3D Acceptor-Negative BIN 12 (12.000 - 13.000 Ã…)	CATS 3D descriptors	Basic descriptors
5159	CATS3D_13_AN	CATS3D Acceptor-Negative BIN 13 (13.000 - 14.000 Ã…)	CATS 3D descriptors	Basic descriptors
5160	CATS3D_14_AN	CATS3D Acceptor-Negative BIN 14 (14.000 - 15.000 Ã…)	CATS 3D descriptors	Basic descriptors
5161	CATS3D_15_AN	CATS3D Acceptor-Negative BIN 15 (15.000 - 16.000 Ã…)	CATS 3D descriptors	Basic descriptors
5162	CATS3D_16_AN	CATS3D Acceptor-Negative BIN 16 (16.000 - 17.000 Ã…)	CATS 3D descriptors	Basic descriptors
5163	CATS3D_17_AN	CATS3D Acceptor-Negative BIN 17 (17.000 - 18.000 Ã…)	CATS 3D descriptors	Basic descriptors
5164	CATS3D_18_AN	CATS3D Acceptor-Negative BIN 18 (18.000 - 19.000 Ã…)	CATS 3D descriptors	Basic descriptors
5165	CATS3D_19_AN	CATS3D Acceptor-Negative BIN 19 (19.000 - 20.000 Ã…)	CATS 3D descriptors	Basic descriptors
5166	CATS3D_00_AL	CATS3D Acceptor-Lipophilic BIN 00 (0.000 - 1.000 Ã…)	CATS 3D descriptors	Basic descriptors
5167	CATS3D_01_AL	CATS3D Acceptor-Lipophilic BIN 01 (1.000 - 2.000 Ã…)	CATS 3D descriptors	Basic descriptors
5168	CATS3D_02_AL	CATS3D Acceptor-Lipophilic BIN 02 (2.000 - 3.000 Ã…)	CATS 3D descriptors	Basic descriptors
5169	CATS3D_03_AL	CATS3D Acceptor-Lipophilic BIN 03 (3.000 - 4.000 Ã…)	CATS 3D descriptors	Basic descriptors
5170	CATS3D_04_AL	CATS3D Acceptor-Lipophilic BIN 04 (4.000 - 5.000 Ã…)	CATS 3D descriptors	Basic descriptors

5171	CATS3D_05_AL	CATS3D Acceptor-Lipophilic BIN 05 (5.000 - 6.000 Ã…)	CATS 3D descriptors	Basic descriptors
5172	CATS3D_06_AL	CATS3D Acceptor-Lipophilic BIN 06 (6.000 - 7.000 Ã…)	CATS 3D descriptors	Basic descriptors
5173	CATS3D_07_AL	CATS3D Acceptor-Lipophilic BIN 07 (7.000 - 8.000 Ã…)	CATS 3D descriptors	Basic descriptors
5174	CATS3D_08_AL	CATS3D Acceptor-Lipophilic BIN 08 (8.000 - 9.000 Ã…)	CATS 3D descriptors	Basic descriptors
5175	CATS3D_09_AL	CATS3D Acceptor-Lipophilic BIN 09 (9.000 - 10.000 Ã…)	CATS 3D descriptors	Basic descriptors
5176	CATS3D_10_AL	CATS3D Acceptor-Lipophilic BIN 10 (10.000 - 11.000 Ã…)	CATS 3D descriptors	Basic descriptors
5177	CATS3D_11_AL	CATS3D Acceptor-Lipophilic BIN 11 (11.000 - 12.000 Ã…)	CATS 3D descriptors	Basic descriptors
5178	CATS3D_12_AL	CATS3D Acceptor-Lipophilic BIN 12 (12.000 - 13.000 Ã…)	CATS 3D descriptors	Basic descriptors
5179	CATS3D_13_AL	CATS3D Acceptor-Lipophilic BIN 13 (13.000 - 14.000 Ã…)	CATS 3D descriptors	Basic descriptors
5180	CATS3D_14_AL	CATS3D Acceptor-Lipophilic BIN 14 (14.000 - 15.000 Ã…)	CATS 3D descriptors	Basic descriptors
5181	CATS3D_15_AL	CATS3D Acceptor-Lipophilic BIN 15 (15.000 - 16.000 Ã…)	CATS 3D descriptors	Basic descriptors
5182	CATS3D_16_AL	CATS3D Acceptor-Lipophilic BIN 16 (16.000 - 17.000 Ã…)	CATS 3D descriptors	Basic descriptors
5183	CATS3D_17_AL	CATS3D Acceptor-Lipophilic BIN 17 (17.000 - 18.000 Ã…)	CATS 3D descriptors	Basic descriptors
5184	CATS3D_18_AL	CATS3D Acceptor-Lipophilic BIN 18 (18.000 - 19.000 Ã…)	CATS 3D descriptors	Basic descriptors
5185	CATS3D_19_AL	CATS3D Acceptor-Lipophilic BIN 19 (19.000 - 20.000 Ã…)	CATS 3D descriptors	Basic descriptors
5186	CATS3D_00_PP	CATS3D Positive-Positive BIN 00 (0.000 - 1.000 Ã…)	CATS 3D descriptors	Basic descriptors
5187	CATS3D_01_PP	CATS3D Positive-Positive BIN 01 (1.000 - 2.000 Ã…)	CATS 3D descriptors	Basic descriptors
5188	CATS3D_02_PP	CATS3D Positive-Positive BIN 02 (2.000 - 3.000 Ã…)	CATS 3D descriptors	Basic descriptors
5189	CATS3D_03_PP	CATS3D Positive-Positive BIN 03 (3.000 - 4.000 Ã…)	CATS 3D descriptors	Basic descriptors
5190	CATS3D_04_PP	CATS3D Positive-Positive BIN 04 (4.000 - 5.000 Ã…)	CATS 3D descriptors	Basic descriptors

5191	CATS3D_05_PP	CATS3D Positive-Positive BIN 05 (5.000 - 6.000 Ã…)	CATS 3D descriptors	Basic descriptors
5192	CATS3D_06_PP	CATS3D Positive-Positive BIN 06 (6.000 - 7.000 Ã…)	CATS 3D descriptors	Basic descriptors
5193	CATS3D_07_PP	CATS3D Positive-Positive BIN 07 (7.000 - 8.000 Ã…)	CATS 3D descriptors	Basic descriptors
5194	CATS3D_08_PP	CATS3D Positive-Positive BIN 08 (8.000 - 9.000 Ã…)	CATS 3D descriptors	Basic descriptors
5195	CATS3D_09_PP	CATS3D Positive-Positive BIN 09 (9.000 - 10.000 Ã…)	CATS 3D descriptors	Basic descriptors
5196	CATS3D_10_PP	CATS3D Positive-Positive BIN 10 (10.000 - 11.000 Ã…)	CATS 3D descriptors	Basic descriptors
5197	CATS3D_11_PP	CATS3D Positive-Positive BIN 11 (11.000 - 12.000 Ã…)	CATS 3D descriptors	Basic descriptors
5198	CATS3D_12_PP	CATS3D Positive-Positive BIN 12 (12.000 - 13.000 Ã…)	CATS 3D descriptors	Basic descriptors
5199	CATS3D_13_PP	CATS3D Positive-Positive BIN 13 (13.000 - 14.000 Ã…)	CATS 3D descriptors	Basic descriptors
5200	CATS3D_14_PP	CATS3D Positive-Positive BIN 14 (14.000 - 15.000 Ã…)	CATS 3D descriptors	Basic descriptors
5201	CATS3D_15_PP	CATS3D Positive-Positive BIN 15 (15.000 - 16.000 Ã…)	CATS 3D descriptors	Basic descriptors
5202	CATS3D_16_PP	CATS3D Positive-Positive BIN 16 (16.000 - 17.000 Ã…)	CATS 3D descriptors	Basic descriptors
5203	CATS3D_17_PP	CATS3D Positive-Positive BIN 17 (17.000 - 18.000 Ã…)	CATS 3D descriptors	Basic descriptors
5204	CATS3D_18_PP	CATS3D Positive-Positive BIN 18 (18.000 - 19.000 Ã…)	CATS 3D descriptors	Basic descriptors
5205	CATS3D_19_PP	CATS3D Positive-Positive BIN 19 (19.000 - 20.000 Ã…)	CATS 3D descriptors	Basic descriptors
5206	CATS3D_00_PN	CATS3D Positive-Negative BIN 00 (0.000 - 1.000 Ã…)	CATS 3D descriptors	Basic descriptors
5207	CATS3D_01_PN	CATS3D Positive-Negative BIN 01 (1.000 - 2.000 Ã…)	CATS 3D descriptors	Basic descriptors
5208	CATS3D_02_PN	CATS3D Positive-Negative BIN 02 (2.000 - 3.000 Ã…)	CATS 3D descriptors	Basic descriptors
5209	CATS3D_03_PN	CATS3D Positive-Negative BIN 03 (3.000 - 4.000 Ã…)	CATS 3D descriptors	Basic descriptors
5210	CATS3D_04_PN	CATS3D Positive-Negative BIN 04 (4.000 - 5.000 Ã…)	CATS 3D descriptors	Basic descriptors

5211	CATS3D_05_PN	CATS3D Positive-Negative BIN 05 (5.000 - 6.000 Ã…)	CATS 3D descriptors	Basic descriptors
5212	CATS3D_06_PN	CATS3D Positive-Negative BIN 06 (6.000 - 7.000 Ã…)	CATS 3D descriptors	Basic descriptors
5213	CATS3D_07_PN	CATS3D Positive-Negative BIN 07 (7.000 - 8.000 Ã…)	CATS 3D descriptors	Basic descriptors
5214	CATS3D_08_PN	CATS3D Positive-Negative BIN 08 (8.000 - 9.000 Ã…)	CATS 3D descriptors	Basic descriptors
5215	CATS3D_09_PN	CATS3D Positive-Negative BIN 09 (9.000 - 10.000 Ã…)	CATS 3D descriptors	Basic descriptors
5216	CATS3D_10_PN	CATS3D Positive-Negative BIN 10 (10.000 - 11.000 Ã…)	CATS 3D descriptors	Basic descriptors
5217	CATS3D_11_PN	CATS3D Positive-Negative BIN 11 (11.000 - 12.000 Ã…)	CATS 3D descriptors	Basic descriptors
5218	CATS3D_12_PN	CATS3D Positive-Negative BIN 12 (12.000 - 13.000 Ã…)	CATS 3D descriptors	Basic descriptors
5219	CATS3D_13_PN	CATS3D Positive-Negative BIN 13 (13.000 - 14.000 Ã…)	CATS 3D descriptors	Basic descriptors
5220	CATS3D_14_PN	CATS3D Positive-Negative BIN 14 (14.000 - 15.000 Ã…)	CATS 3D descriptors	Basic descriptors
5221	CATS3D_15_PN	CATS3D Positive-Negative BIN 15 (15.000 - 16.000 Ã…)	CATS 3D descriptors	Basic descriptors
5222	CATS3D_16_PN	CATS3D Positive-Negative BIN 16 (16.000 - 17.000 Ã…)	CATS 3D descriptors	Basic descriptors
5223	CATS3D_17_PN	CATS3D Positive-Negative BIN 17 (17.000 - 18.000 Ã…)	CATS 3D descriptors	Basic descriptors
5224	CATS3D_18_PN	CATS3D Positive-Negative BIN 18 (18.000 - 19.000 Ã…)	CATS 3D descriptors	Basic descriptors
5225	CATS3D_19_PN	CATS3D Positive-Negative BIN 19 (19.000 - 20.000 Ã…)	CATS 3D descriptors	Basic descriptors
5226	CATS3D_00_PL	CATS3D Positive-Lipophilic BIN 00 (0.000 - 1.000 Ã…)	CATS 3D descriptors	Basic descriptors
5227	CATS3D_01_PL	CATS3D Positive-Lipophilic BIN 01 (1.000 - 2.000 Ã…)	CATS 3D descriptors	Basic descriptors
5228	CATS3D_02_PL	CATS3D Positive-Lipophilic BIN 02 (2.000 - 3.000 Ã…)	CATS 3D descriptors	Basic descriptors
5229	CATS3D_03_PL	CATS3D Positive-Lipophilic BIN 03 (3.000 - 4.000 Ã…)	CATS 3D descriptors	Basic descriptors
5230	CATS3D_04_PL	CATS3D Positive-Lipophilic BIN 04 (4.000 - 5.000 Ã…)	CATS 3D descriptors	Basic descriptors

5231	CATS3D_05_PL	CATS3D Positive-Lipophilic BIN 05 (5.000 - 6.000 Ã…)	CATS 3D descriptors	Basic descriptors
5232	CATS3D_06_PL	CATS3D Positive-Lipophilic BIN 06 (6.000 - 7.000 Ã…)	CATS 3D descriptors	Basic descriptors
5233	CATS3D_07_PL	CATS3D Positive-Lipophilic BIN 07 (7.000 - 8.000 Ã…)	CATS 3D descriptors	Basic descriptors
5234	CATS3D_08_PL	CATS3D Positive-Lipophilic BIN 08 (8.000 - 9.000 Ã…)	CATS 3D descriptors	Basic descriptors
5235	CATS3D_09_PL	CATS3D Positive-Lipophilic BIN 09 (9.000 - 10.000 Ã…)	CATS 3D descriptors	Basic descriptors
5236	CATS3D_10_PL	CATS3D Positive-Lipophilic BIN 10 (10.000 - 11.000 Ã…)	CATS 3D descriptors	Basic descriptors
5237	CATS3D_11_PL	CATS3D Positive-Lipophilic BIN 11 (11.000 - 12.000 Ã…)	CATS 3D descriptors	Basic descriptors
5238	CATS3D_12_PL	CATS3D Positive-Lipophilic BIN 12 (12.000 - 13.000 Ã…)	CATS 3D descriptors	Basic descriptors
5239	CATS3D_13_PL	CATS3D Positive-Lipophilic BIN 13 (13.000 - 14.000 Ã…)	CATS 3D descriptors	Basic descriptors
5240	CATS3D_14_PL	CATS3D Positive-Lipophilic BIN 14 (14.000 - 15.000 Ã…)	CATS 3D descriptors	Basic descriptors
5241	CATS3D_15_PL	CATS3D Positive-Lipophilic BIN 15 (15.000 - 16.000 Ã…)	CATS 3D descriptors	Basic descriptors
5242	CATS3D_16_PL	CATS3D Positive-Lipophilic BIN 16 (16.000 - 17.000 Ã…)	CATS 3D descriptors	Basic descriptors
5243	CATS3D_17_PL	CATS3D Positive-Lipophilic BIN 17 (17.000 - 18.000 Ã…)	CATS 3D descriptors	Basic descriptors
5244	CATS3D_18_PL	CATS3D Positive-Lipophilic BIN 18 (18.000 - 19.000 Ã…)	CATS 3D descriptors	Basic descriptors
5245	CATS3D_19_PL	CATS3D Positive-Lipophilic BIN 19 (19.000 - 20.000 Ã…)	CATS 3D descriptors	Basic descriptors
5246	CATS3D_00_NN	CATS3D Negative-Negative BIN 00 (0.000 - 1.000 Ã…)	CATS 3D descriptors	Basic descriptors
5247	CATS3D_01_NN	CATS3D Negative-Negative BIN 01 (1.000 - 2.000 Ã…)	CATS 3D descriptors	Basic descriptors
5248	CATS3D_02_NN	CATS3D Negative-Negative BIN 02 (2.000 - 3.000 Ã…)	CATS 3D descriptors	Basic descriptors
5249	CATS3D_03_NN	CATS3D Negative-Negative BIN 03 (3.000 - 4.000 Ã…)	CATS 3D descriptors	Basic descriptors
5250	CATS3D_04_NN	CATS3D Negative-Negative BIN 04 (4.000 - 5.000 Ã…)	CATS 3D descriptors	Basic descriptors

5251	CATS3D_05_NN	CATS3D Negative-Negative BIN 05 (5.000 - 6.000 Ã…)	CATS 3D descriptors	Basic descriptors
5252	CATS3D_06_NN	CATS3D Negative-Negative BIN 06 (6.000 - 7.000 Ã…)	CATS 3D descriptors	Basic descriptors
5253	CATS3D_07_NN	CATS3D Negative-Negative BIN 07 (7.000 - 8.000 Ã…)	CATS 3D descriptors	Basic descriptors
5254	CATS3D_08_NN	CATS3D Negative-Negative BIN 08 (8.000 - 9.000 Ã…)	CATS 3D descriptors	Basic descriptors
5255	CATS3D_09_NN	CATS3D Negative-Negative BIN 09 (9.000 - 10.000 Ã…)	CATS 3D descriptors	Basic descriptors
5256	CATS3D_10_NN	CATS3D Negative-Negative BIN 10 (10.000 - 11.000 Ã…)	CATS 3D descriptors	Basic descriptors
5257	CATS3D_11_NN	CATS3D Negative-Negative BIN 11 (11.000 - 12.000 Ã…)	CATS 3D descriptors	Basic descriptors
5258	CATS3D_12_NN	CATS3D Negative-Negative BIN 12 (12.000 - 13.000 Ã…)	CATS 3D descriptors	Basic descriptors
5259	CATS3D_13_NN	CATS3D Negative-Negative BIN 13 (13.000 - 14.000 Ã…)	CATS 3D descriptors	Basic descriptors
5260	CATS3D_14_NN	CATS3D Negative-Negative BIN 14 (14.000 - 15.000 Ã…)	CATS 3D descriptors	Basic descriptors
5261	CATS3D_15_NN	CATS3D Negative-Negative BIN 15 (15.000 - 16.000 Ã…)	CATS 3D descriptors	Basic descriptors
5262	CATS3D_16_NN	CATS3D Negative-Negative BIN 16 (16.000 - 17.000 Ã…)	CATS 3D descriptors	Basic descriptors
5263	CATS3D_17_NN	CATS3D Negative-Negative BIN 17 (17.000 - 18.000 Ã…)	CATS 3D descriptors	Basic descriptors
5264	CATS3D_18_NN	CATS3D Negative-Negative BIN 18 (18.000 - 19.000 Ã…)	CATS 3D descriptors	Basic descriptors
5265	CATS3D_19_NN	CATS3D Negative-Negative BIN 19 (19.000 - 20.000 Ã…)	CATS 3D descriptors	Basic descriptors
5266	CATS3D_00_NL	CATS3D Negative-Lipophilic BIN 00 (0.000 - 1.000 Ã…)	CATS 3D descriptors	Basic descriptors
5267	CATS3D_01_NL	CATS3D Negative-Lipophilic BIN 01 (1.000 - 2.000 Ã…)	CATS 3D descriptors	Basic descriptors
5268	CATS3D_02_NL	CATS3D Negative-Lipophilic BIN 02 (2.000 - 3.000 Ã…)	CATS 3D descriptors	Basic descriptors
5269	CATS3D_03_NL	CATS3D Negative-Lipophilic BIN 03 (3.000 - 4.000 Ã…)	CATS 3D descriptors	Basic descriptors
5270	CATS3D_04_NL	CATS3D Negative-Lipophilic BIN 04 (4.000 - 5.000 Ã…)	CATS 3D descriptors	Basic descriptors

5271	CATS3D_05_NL	CATS3D Negative-Lipophilic BIN 05 (5.000 - 6.000 Ã…)	CATS 3D descriptors	Basic descriptors
5272	CATS3D_06_NL	CATS3D Negative-Lipophilic BIN 06 (6.000 - 7.000 Ã…)	CATS 3D descriptors	Basic descriptors
5273	CATS3D_07_NL	CATS3D Negative-Lipophilic BIN 07 (7.000 - 8.000 Ã…)	CATS 3D descriptors	Basic descriptors
5274	CATS3D_08_NL	CATS3D Negative-Lipophilic BIN 08 (8.000 - 9.000 Ã…)	CATS 3D descriptors	Basic descriptors
5275	CATS3D_09_NL	CATS3D Negative-Lipophilic BIN 09 (9.000 - 10.000 Ã…)	CATS 3D descriptors	Basic descriptors
5276	CATS3D_10_NL	CATS3D Negative-Lipophilic BIN 10 (10.000 - 11.000 Ã…)	CATS 3D descriptors	Basic descriptors
5277	CATS3D_11_NL	CATS3D Negative-Lipophilic BIN 11 (11.000 - 12.000 Ã…)	CATS 3D descriptors	Basic descriptors
5278	CATS3D_12_NL	CATS3D Negative-Lipophilic BIN 12 (12.000 - 13.000 Ã…)	CATS 3D descriptors	Basic descriptors
5279	CATS3D_13_NL	CATS3D Negative-Lipophilic BIN 13 (13.000 - 14.000 Ã…)	CATS 3D descriptors	Basic descriptors
5280	CATS3D_14_NL	CATS3D Negative-Lipophilic BIN 14 (14.000 - 15.000 Ã…)	CATS 3D descriptors	Basic descriptors
5281	CATS3D_15_NL	CATS3D Negative-Lipophilic BIN 15 (15.000 - 16.000 Ã…)	CATS 3D descriptors	Basic descriptors
5282	CATS3D_16_NL	CATS3D Negative-Lipophilic BIN 16 (16.000 - 17.000 Ã…)	CATS 3D descriptors	Basic descriptors
5283	CATS3D_17_NL	CATS3D Negative-Lipophilic BIN 17 (17.000 - 18.000 Ã…)	CATS 3D descriptors	Basic descriptors
5284	CATS3D_18_NL	CATS3D Negative-Lipophilic BIN 18 (18.000 - 19.000 Ã…)	CATS 3D descriptors	Basic descriptors
5285	CATS3D_19_NL	CATS3D Negative-Lipophilic BIN 19 (19.000 - 20.000 Ã…)	CATS 3D descriptors	Basic descriptors
5286	CATS3D_00_LL	CATS3D Lipophilic-Lipophilic BIN 00 (0.000 - 1.000 Ã…)	CATS 3D descriptors	Basic descriptors
5287	CATS3D_01_LL	CATS3D Lipophilic-Lipophilic BIN 01 (1.000 - 2.000 Ã…)	CATS 3D descriptors	Basic descriptors
5288	CATS3D_02_LL	CATS3D Lipophilic-Lipophilic BIN 02 (2.000 - 3.000 Ã…)	CATS 3D descriptors	Basic descriptors
5289	CATS3D_03_LL	CATS3D Lipophilic-Lipophilic BIN 03 (3.000 - 4.000 Ã…)	CATS 3D descriptors	Basic descriptors
5290	CATS3D_04_LL	CATS3D Lipophilic-Lipophilic BIN 04 (4.000 - 5.000 Ã…)	CATS 3D descriptors	Basic descriptors

5291	CATS3D_05_LL	CATS3D Lipophilic-Lipophilic BIN 05 (5.000 - 6.000 Ã…)	CATS 3D descriptors	Basic descriptors
5292	CATS3D_06_LL	CATS3D Lipophilic-Lipophilic BIN 06 (6.000 - 7.000 Ã…)	CATS 3D descriptors	Basic descriptors
5293	CATS3D_07_LL	CATS3D Lipophilic-Lipophilic BIN 07 (7.000 - 8.000 Ã…)	CATS 3D descriptors	Basic descriptors
5294	CATS3D_08_LL	CATS3D Lipophilic-Lipophilic BIN 08 (8.000 - 9.000 Ã…)	CATS 3D descriptors	Basic descriptors
5295	CATS3D_09_LL	CATS3D Lipophilic-Lipophilic BIN 09 (9.000 - 10.000 Ã…)	CATS 3D descriptors	Basic descriptors
5296	CATS3D_10_LL	CATS3D Lipophilic-Lipophilic BIN 10 (10.000 - 11.000 Ã…)	CATS 3D descriptors	Basic descriptors
5297	CATS3D_11_LL	CATS3D Lipophilic-Lipophilic BIN 11 (11.000 - 12.000 Ã…)	CATS 3D descriptors	Basic descriptors
5298	CATS3D_12_LL	CATS3D Lipophilic-Lipophilic BIN 12 (12.000 - 13.000 Ã…)	CATS 3D descriptors	Basic descriptors
5299	CATS3D_13_LL	CATS3D Lipophilic-Lipophilic BIN 13 (13.000 - 14.000 Ã…)	CATS 3D descriptors	Basic descriptors
5300	CATS3D_14_LL	CATS3D Lipophilic-Lipophilic BIN 14 (14.000 - 15.000 Ã…)	CATS 3D descriptors	Basic descriptors
5301	CATS3D_15_LL	CATS3D Lipophilic-Lipophilic BIN 15 (15.000 - 16.000 Ã…)	CATS 3D descriptors	Basic descriptors
5302	CATS3D_16_LL	CATS3D Lipophilic-Lipophilic BIN 16 (16.000 - 17.000 Ã…)	CATS 3D descriptors	Basic descriptors
5303	CATS3D_17_LL	CATS3D Lipophilic-Lipophilic BIN 17 (17.000 - 18.000 Ã…)	CATS 3D descriptors	Basic descriptors
5304	CATS3D_18_LL	CATS3D Lipophilic-Lipophilic BIN 18 (18.000 - 19.000 Ã…)	CATS 3D descriptors	Basic descriptors
5305	CATS3D_19_LL	CATS3D Lipophilic-Lipophilic BIN 19 (19.000 - 20.000 Ã…)	CATS 3D descriptors	Basic descriptors

table { }td { padding-top: 1px; padding-right: 1px; padding-left: 1px; color: black; font-size: 12pt; font-weight: 400; font-style: normal; text-decoration: none; font-family: Calibri, sans-serif; vertical-align: bottom; border: medium none; white-space: nowrap; }