Chemaxon descriptors

N.B.! These descriptors can be only used for model development on OCHEM web site and cannot be exported.

Most of Chemaxon descriptors (also known as: Chemaxon calculators) are implemented in OCHEM platform and can be calculated for any set of molecules. Desscriptors implemented are those which return munerical or boolean results. Unimplemented descriptors are those which return results not suitable for modeling purposes such as molecules, formula, or fingerprints. Also calculators that require specific input parameters are not implemented. Example of these calculators are those that check whether certain atom is assymetric, whether 2 atoms are connected, or calculate the angle between 3 specified atoms.

The implemented descriptors are divided into 7 groups: Elemental Analysis, Charge, Geometry, Partitioning, Protonation, Isomers, and Others

Descriptor Name	Descriptor class	Definition	Considers pH during calculation
atomcount	Elemental Analysis	Number of atoms in the molecule	no
exactmass	Elemental Analysis	Exact molecule mass calculation based on the most frequent natural isotopes of the elements	no
mass	Elemental Analysis	Molecule mass calculation	no
			no
averagemolecularpolarizability	Charge	Average molecular polarizability calculation	yes
formalcharge	Charge	Formal charge calculation	yes
molecularpolarizability	Charge	Molecular polarizability calculation	yes
			no
aliphaticatomcount	Geometry	Aliphatic atom count	no
aliphaticbondcount	Geometry	Aliphatic bond count	no
aliphaticringcount	Geometry	Aliphatic ring count	no
aliphaticringcountofsize	Geometry	Aliphatic ring count of size	no
aromaticatomcount	Geometry	Aromatic atom count	no
aromaticbondcount	Geometry	Aromatic bond count	no
aromaticringcount	Geometry	Aromatic ring count	no
aromaticringcountofsize	Geometry	Aromatic ring count of size	no
asymmetricatomcount	Geometry	The number of asymmetric atoms	no
balabanindex	Geometry	The Balaban index	no

bondcount	Geometry	Bond count	no
carboaliphaticringcount	Geometry	Carboaliphatic ring count	no
carboaromaticringcount	Geometry	Carboaromatic ring count	no
carboringcount	Geometry	Carbo ring count	no
chainatomcount	Geometry	Chain atom count	no
chainbondcount	Geometry	Chain bond count	no
chiralcentercount	Geometry	The number of tetrahedral stereogenic center atoms	no
dreidingenergy	Geometry	Calculates the dreiding energy of a conformer of the molecule in kcal/mol	no
fragmentcount	Geometry	Fragment count	no
fusedaliphaticringcount	Geometry	The number of fused aliphatic rings (SSSR smallest set of smallest aliphatic rings)	no
fusedaromaticringcount	Geometry	The number of fused aromatic rings (SSSR smallest set of smallest aromatic rings)	no
fusedringcount	Geometry	The number of fused rings (SSSR smallest set of smallest rings)	no
hararyindex	Geometry	Harary index	no
heteroaliphaticringcount	Geometry	Heteroaliphatic ring count	no
heteroaromaticringcount	Geometry	Heteroaromatic ring count	no
heteroringcount	Geometry	Hetero ring count	no
hyperwienerindex	Geometry	Hyper Wiener index	no
largestringsize	Geometry	Largest ring size	no
largestringsystemsize	Geometry	Largest ring system size	no
maximalprojectionarea	Geometry	Calculates the maximal projection area	no
maximalprojectionradius	Geometry	Calculates the maximal projection radius	no
maximalprojectionsize	Geometry		no
minimalprojectionarea	Geometry	Calculates the minimal projection area	no
minimalprojectionradius	Geometry	Calculates the minimal projection radius	no
minimalprojectionsize	Geometry		no
molecularsurfacearea	Geometry	Molecular Surface Area calculation (3D)	yes
plattindex	Geometry	The Platt index	no

randicindex	Geometry	The Randic index	no
polarsurfacearea	Geometry	Topological Polar Surface Area calculation (2D)	yes
ringatomcount	Geometry	Ring atom count	no
ringbondcount	Geometry	Ring bond count	no
ringcount	Geometry	Ring count	no
ringcountofsize	Geometry	Ring count of size	no
ringsystemcount	Geometry	The number of ring systems	no
ringsystemcountofsize	Geometry	Ring system count of size	no
rotatablebondcount	Geometry	Rotatable bond count	no
smallestringsize	Geometry	Size of smallest ring	no
smallestringsystemsize	Geometry	Smallest ring system size	no
stereodoublebondcount	Geometry	The number of stereo double bonds	no
szegedindex	Geometry	Szeged index	no
volume	Geometry	Calculate the van der Waals volume of the molecule	no
wienerindex	Geometry	Wiener index	no
wienerpolarity	Geometry	Wiener polarity	no
vdwsa	Geometry	Van der Waals Surface Area calculation	yes
			no
logp	Partitioning	logP calculation: logP of uncharged species, or, in the case of zwitterions, logD at pI	no
logd	Partitioning	logD calculation	yes
			no
isoelectricpoint	protonationDescriptors	Isoelectric point calculation	no
			no
doublebondstereoisomercount	Isomers	The number of double-bond stereoisomers of the molecule	no
stereoisomercount	Isomers	The number of stereoisomers of the molecule	no
tautomercount	Isomers	The number of tautomers	no
tetrahedralstereoisomercount	Isomers	The number of tetrahedral stereoisomers of the molecule	no
			no

acceptorcount	Others	Hydrogen bond acceptor atom count in molecule	yes
acceptorsitecount	Others	Hydrogen bond acceptor multiplicity in molecule	no
donorcount	Others	Hydrogen bond donor atom count in molecule	yes
donorsitecount	Others	Hydrogen bond donor multiplicity in molecule	yes
hmopienergy	Others	HMO Pi energy	yes
pienergy *	Others	Pi energy	yes
msacc	Others	Hydrogen bond acceptor average multiplicity over microspecies by pH	no
msdon	Others	Hydrogen bond donor average multiplicity over microspecies by pH	no
resonantcount	Others	The number of resonant structures	no

- - Descriptors that will not be supported in in future versions.

pH descriptors

Calculation of some descriptors require consideration of pH value. User is allowed 3 options for pH:

- All: This calculates the value of the descriptor over the pH range from 0 to 14 taking 1 pH unit increments at a time. Additionally, the descriptor value at pH 7.4 is calculated.
- Specific value: calculates the value of the descriptor at the speicifed pH.
- Specific range: calculates the value of the descriptor over the pH range specified between "from" until "to" taking pH unit increments equal to the value specifid in "step". Additionally, the descriptor value at pH 7.4 is calculated.

Descriptors which consider pH value during their calculation are: veragemolecularpolarizability, formalcharge, molecularpolarizability, molecularsurfacearea, polarsurfacearea, vdwsa, logd, acceptorcount, acceptorsitecount, donorcount, donorsitecount, hmopienergy, pienergy

Ring size

The following descriptors measure the ring size: aliphaticringcountofsize, aromaticringcountofsize, ringcountofsize, ringsystemcountofsize They are calculated for 3-, 4-, 5-, 6-, 7-, and 8-membered rings.

The following calculators are unable to handle molecules with multiple fragments, instead OCHEM platform replaces it with a "missing descriptor value". Currently this value is set to 0. We plan to allow the user to specify such value in the future or even skip the whole molecule altogether from the dataset.