alvaDesc

alvaDesc calculates almost 4000 descriptors independent of 3-dimensional information such as constitutional, topological, pharmacophore. It includes ETA and Atom-type E-state indices together with atom pairs, functional groups and fragment counts. Furthermore, alvaDesc implements almost 1500 3-dimensional descriptors such as 3D-autocorrelation, Weighted Holistic Invariant Molecular descriptors (WHIM), GETAWAY and CATS3D descriptors.

alvaDesc provides the calculation of several model-based physicochemical properties such as molar refractivity, topological polar surface area (TPSA), molecular volume estimations, two LogP models (Moriguchi and Ghose-Chippen octanol-water partition coefficient) and provides also a significant list of drug-like and lead-like alerts including the well-known Lipinski alert index. **alvaDesc** calculates molecular descriptors both on full-connected and non-full-connected molecular structures, such as salts, mixtures, ionic liquids and metal complexes.

Molecular descriptors are divided into 30 logical blocks.

Block name (# of descriptors)

- Constitutional indices (48)
- Ring descriptors (32)
- Topological indices (79)
- Walk and path counts (46)
- Connectivity indices (37)
- Information indices (50)
- 2D matrix-based descriptors (607)
- 2D autocorrelations (213)
- Burden eigenvalues (96)
- P_VSA-like descriptors (55)
- ETA indices (38)
- Edge adjacency indices (324)
- Geometrical descriptors (38)
- 3D matrix-based descriptors (99)
- 3D autocorrelations (80)
- RDF descriptors (210)
- 3D-MoRSE descriptors (224)
- WHIM descriptors (114)
- GETAWAY descriptors (273)
- Randic molecular profiles (41)
- Functional group counts (154)
- Atom-centred fragments (115)
- Atom-type E-state indices (172)
- Pharmacophore descriptors (165)
- 2D Atom Pairs (1596)
- 3D Atom Pairs (36)
- Charge descriptors (15)
- Molecular properties (20)
- Drug-like indices (28)
- CATS 3D descriptors (300)

See the full list of descriptors here

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