Molecular descriptors

Molecular descriptors are numerical features of chemical compounds.

OCHEM supports the calculation of many different descriptor packages:

- Adriana.CODE
- alvaDesc
- ALogPS
- CDK
- Chemaxon descriptors
- Chemaxon scaffolds
- Custom descriptors from a file
- Dragon
- ECFP fingerprints
- ESTATE
- Experimental values of other properties
- Functional groups
- GSFrag
- Inductive Descriptors
- ISIDA Fragments
- MERA descriptors
- MERSY descriptors
- MolPrint
- MOPAC-derived descriptors
- OEState
- QNPR
- Silicos-It scaffolds
- Spectrophores
- ToxAlerts
- MAP4
- JPLOGP
- RDKit descriptors
- MOE
- CDDD
- PyDescriptor
- CDK22
- SIRMS
- CDK2
- RDKit additional descriptors
- MORDRED
- MOPAC2016-derived descriptors

You can select one or more descriptor packages to calculate for the same dataset. The calculation time for descriptors depends on many factors including the size of the dataset, the package selected, and the availability of computational resources.

Model editor
Select model template and training set

Select the molecular descriptors:

Suggested descriptors:

- [x] E-state

E-State types:
- [x] Atom indices
- [x] Bonds indices
- [ ] Atom counts
- [ ] Bonds counts

Aromatize structures: Chemaxon Basic

- [x] ALogPS (2)
- [ ] GSFragment (1138)
- [ ] Dragon v. 6.0 (4885/3D)
- [ ] ISIDA fragments
- [ ] ADRIANA.Code *(211/3D)*
- [ ] CDK descriptors (246/3D)
- [ ] 'Inductive' descriptors *(54/3D)*
- [ ] MERA descriptors *(529/3D)*
- [ ] MERSY descriptors *(42/3D)*
- [ ] Chemaxon descriptors (499/3D)
- [ ] QNPR
- [ ] Spectrophores (144/3D)

Additional or obsolete descriptors:

- [ ] OEState
- [ ] MolPrint
- [ ] Dragon v. 5.4 (1630/3D)
- [ ] Dragon v. 5.5 (3190/3D)
- [ ] Structural alerts (ToxAlerts)
- [ ] MOPAC descriptors *(21/3D)*
- [ ] ShapeSignatures *(3D)*

Experimental descriptors (use only if you know how to use them):

- [ ] Custom descriptors from a file
- [ ] AMBIT Descriptors
- [ ] ISIDA fragments (2011)
- [ ] Chiral Descriptors (/3D)
- [ ] Scaffold Hunter Descriptors
- [ ] ECFP Fingerprints
- [ ] Chemaxon Scaffolds
- [ ] Silicos-It Scaffolds *Not supported by your installation*
- [ ] Functional Groups
- [ ] ETM descriptors *Not supported by your installation*
- [ ] DockingDescriptors (pre-pre-alfa) *Not supported by your installation*
- [ ] Experimental values of other properties *Not supported by your installation*