# Adriana.CODE

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

**ADRIANA.Code** comprises a unique combination of methods for calculating molecular descriptors on a sound geometric and physicochemical basis. These descriptors can be used for a wide range of applications in all areas of chemistry, in particular in QSAR/QSPR.
**ADRIANA.Code** contains a series of methods for the generation of 3D structures and the calculation of physicochemical descriptors and molecular properties based on rapid empirical models. In addition, it contains a hierarchy of increasing levels of sophistication in representing chemical compounds from the constitution to the 3D structure of a molecule. At each level, a wide range of physicochemical effects are included in the molecular descriptors.

## Available descriptors

The following tables list the descriptors that are calculated by the OCHEM web service of **ADRIANA.Code**.
For further details about the descriptors availaible in **ADRIANA.Code**, their scientific and technical background and units, please refer to the ADRIANA.Code program manual.

### Global molecular descriptors

Global molecular descriptors represent a chemical structure by a structural, chemical or physicochemical feature or property of the molecule expressed by a single value.
The total number of global molecular descriptors is 19.

| **Descriptor** | **Short name in header line of *csv* descriptor file** | **Unit** | **References** |
|---|---|---|---|
| Molecular weight | Weight | [u], [Da] | [1] |
| Number of hydrogen bonding acceptors | HAcc | - | [2] |
| Number of oxygen atom-based hydrogen bonding acceptors | HAcc_O | - | [2] |
| Number of nitrogen atom-based hydrogen bonding acceptors | HAcc_N | - | [2] |
| Number of hydrogen bonding donors | HDon | - | [2] |
| Number of oxygen atom-based hydrogen bonding donors | HDon_O | - | [2] |
| Number of nitrogen atom-based hydrogen bonding donors | HDon_N | - | [2] |
| Octanol/water partition coefficient (logP) | XlogP | [log units] | [3] |
| Topological polar surface area | TPSA | [$Å^2$] | [4] |

| | | | |
|---|---|---|---|
| Mean molecular polarizability | Polariz | [Å$^3$] | [5-8] |
| Molecular dipole moment | Dipole | [Debey] | [9-15] |
| Aqueous solubility (logS) | LogS | [log units] | [16] |
| Number of rotatable bonds | NRotBond | - | [17] |
| Number of Ro5 violations | NViolationsRo5 | - | [2] |
| Number of extended Ro5 violations | NViolationsExtRo5 | - | [2] |
| Number of atoms | NAtoms | - | - |
| Number of tetrahedral stereocenters | NStereo | - | - |
| Molecular complexity | Complexity | - | [18] |
| Ring complexity | RComplexity | - | [19] |

## Shape and size descriptors

Shape and size descriptors characterize the size and the 3D shape of a molecule, *e.g.*, if a molecule has a more enlongated or a spherical shape. These descriptors represent a molecule by a single value.
The total number of shape- and size-related molecular descriptors is 8.

| **Descriptor** | **Short name in header line of *csv* descriptor file** | **Unit** | **References** |
|---|---|---|---|
| Molecular diameter | Diameter | [Å] | [20] |
| Principal moment of inertia of 1st principal axis | InertiaX | [Da·Å$^2$] | [21] |
| Principal moment of inertia of 2nd principal axis | InertiaX | [Da·Å$^2$] | [21] |
| Principal moment of inertia of 3rd principal axis | InertiaX | [Da·Å$^2$] | [21] |
| Molecular span | Span | [Å] | [22] |
| Molecular radius of gyration | Rgyr | [Å] | [22-23] |
| Molecular eccentricity | Eccentric | [Å] | [21] |
| Molecular asphericity | Aspheric | [Å] | [21] |

## Topological or 2D property-weighted autocorrelation descriptors

Topological or 2D property-weighted autocorrelation descriptors [24-25] are calculated from 0 - 10 topological distances (*i.e.*, the number of bonds on the shortest path between two atoms), and sampled for each topological

distance (11 distance bins). Thus, for each atom pair property a vector of 11 values (*n*) results.
The total number of 2D property-weighted autocorrelation descriptors is 88. The following table lists all 2D property-weighted autocorrelation descriptors.

| **Atom pair property** | **Short name in header line of *csv* descriptor file** | **References** |
|---|---|---|
| Identity, *i.e.*, "1" for an atom | 2DACorr_Ident_*n* | - |
| charge | 2DACorr_SigChg_*n* | [10-11] |
| charge | 2DACorr_PiChg_*n* | [12-14] |
| Total charge | 2DACorr_TotChg_*n* | [10-14] |
| electronegativity | 2DACorr_SigEN_*n* | [10-11] |
| electronegativity | 2DACorr_PiEN_*n* | [12-14] |
| Lone-pair electronegativity | 2DACorr_LpEN_*n* | [12-14] |
| Effective atom polarizability | 2DACorr_Polariz_*n* | [5-8] |

### Spatial or 3D property-weighted autocorrelation descriptors

Spatial or 3D property-weighted autocorrelation descriptors [26-27] are calculated from 1 - 13 Å and sampled in steps of 1 Å (12 distance bins). Thus, for each atom pair property a vector of 12 values (*n*) results.
The total number of 3D property-weighted autocorrelation descriptors is 96. The following table lists all 3D property-weighted autocorrelation descriptors.

| **Atom pair property** | **Short name in header line of *csv* descriptor file** | **References** |
|---|---|---|
| Identity, *i.e.*, "1" for an atom | 3DACorr_Ident_*n* | - |
| charge | 3DACorr_SigChg_*n* | [10-11] |
| charge | 3DACorr_PiChg_*n* | [12-14] |
| Total charge | 3DACorr_TotChg_*n* | [10-14] |
| electronegativity | 3DACorr_SigEN_*n* | [10-11] |
| electronegativity | 3DACorr_PiEN_*n* | [12-14] |
| Lone-pair electronegativity | 3DACorr_LpEN_*n* | [12-14] |
| Effective atom polarizability | 3DACorr_Polariz_*n* | [5-8] |

## References


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