

NAME

AssignAtomTypes.pl - Assign atom types for SD files

SYNOPSIS

AssignAtomTypes.pl SDFfile(s)...

```
AtomTypesFingerprints.pl [--AromaticityModel AromaticityModelType] [-a, --AtomIdentifierType
AtomicInvariantsAtomTypes | DREIDINGAtomTypes | EStateAtomTypes | MMFF94AtomTypes | SLogPAtomTypes |
SYBYLAtomTypes | TPSAAtomTypes | UFFAtomTypes] [--AtomicInvariantsToUse "AtomicInvariant,AtomicInvariant..." ] [
--FunctionalClassesToUse "FunctionalClass1,FunctionalClass2..." ] [--AtomTypesSetToUse ArbitrarySize | FixedSize] [
--BitsOrder Ascending | Descending] [-b, --BitStringFormat BinaryString | HexadecimalString] [--CompoundID
DataFieldName or LabelPrefixString] [--CompoundIDLabel text] [--CompoundIDMode DataField | MolName |
LabelPrefix | MolNameOrLabelPrefix] [--DataFields "FieldLabel1,FieldLabel2..." ] [-d, --DataFieldsMode All | Common |
Specify | CompoundID] [-f, --Filter Yes | No] [--FingerprintsLabelMode FingerprintsLabelOnly | FingerprintsLabelWithIDs
] [--FingerprintsLabel text] [-h, --help] [-k, --KeepLargestComponent Yes | No] [-m, --mode AtomTypesCount |
AtomTypesBits] [-i, --IgnoreHydrogens Yes | No] [--OutDelim comma | tab | semicolon] [--output SD | FP | text | all] [
-o, --overwrite] [-q, --quote Yes | No] [-r, --root RootName] [-s, --size number] [--ValuesPrecision number] [
-v, --VectorStringFormat IDsAndValuesString | IDsAndValuesPairsString | ValuesAndIDsString | ValuesAndIDsPairsString] [
-w, --WorkingDir DirName]
```

DESCRIPTION

Generate atom types for *SDFfile(s)* and create appropriate SD, or CSV/TSV text file(s) containing atom types assigned to atoms in molecules.

Multiple SDF file names are separated by spaces. The valid file extensions are *.sdf* and *.sd*. All other file names are ignored. All the SD files in a current directory can be specified either by **.sdf* or the current directory name.

The current release of MayaChemTools supports generation of atom types corresponding to following -a, --AtomIdentifierTypes:

```
AtomicInvariantsAtomTypes, DREIDINGAtomTypes, EStateAtomTypes,
FunctionalClassAtomTypes, MMFF94AtomTypes, SLogPAtomTypes,
SYBYLAtomTypes, TPSAAtomTypes, UFFAtomTypes
```

Based on the values specified for -a, --AtomIdentifierType along with other specified parameters such as --AtomicInvariantsToUse and --FunctionalClassesToUse, atom types are assigned to all non-hydrogen atoms or all atoms in a molecule

OPTIONS

```
--AromaticityModel MDLAromaticityModel | TripasAromaticityModel | MMFFAromaticityModel |
ChemAxonBasicAromaticityModel | ChemAxonGeneralAromaticityModel | DaylightAromaticityModel |
MayaChemToolsAromaticityModel
```

Specify aromaticity model to use during detection of aromaticity. Possible values in the current release are: *MDLAromaticityModel*, *TripasAromaticityModel*, *MMFFAromaticityModel*, *ChemAxonBasicAromaticityModel*, *ChemAxonGeneralAromaticityModel*, *DaylightAromaticityModel* or *MayaChemToolsAromaticityModel*. Default value: *MayaChemToolsAromaticityModel*.

The supported aromaticity model names along with model specific control parameters are defined in *AromaticityModelsData.csv*, which is distributed with the current release and is available under *lib/data* directory. Molecule.pm module retrieves data from this file during class instantiation and makes it available to method *DetectAromaticity* for detecting aromaticity corresponding to a specific model.

```
--AtomicInvariantsToUse "AtomicInvariant,AtomicInvariant..."
```

This value is used during *AtomicInvariantsAtomTypes* value of m, --mode option. It's a list of comma separated valid atomic invariant atom types.

Possible values for atomic invariants are: *AS, X, BO, LBO, SB, DB, TB, H, Ar, RA, FC, MN, SM*. Default value: *AS,X,BO,H,FC*.

The atomic invariants abbreviations correspond to:

```
AS = Atom symbol corresponding to element symbol
```

```
X<n> = Number of non-hydrogen atom neighbors or heavy atoms
```

BO<n> = Sum of bond orders to non-hydrogen atom neighbors or heavy atoms
 LBO<n> = Largest bond order of non-hydrogen atom neighbors or heavy atoms
 SB<n> = Number of single bonds to non-hydrogen atom neighbors or heavy atoms
 DB<n> = Number of double bonds to non-hydrogen atom neighbors or heavy atoms
 TB<n> = Number of triple bonds to non-hydrogen atom neighbors or heavy atoms
 H<n> = Number of implicit and explicit hydrogens for atom
 Ar = Aromatic annotation indicating whether atom is aromatic
 RA = Ring atom annotation indicating whether atom is a ring
 FC<+n/-n> = Formal charge assigned to atom
 MN<n> = Mass number indicating isotope other than most abundant isotope
 SM<n> = Spin multiplicity of atom. Possible values: 1 (singlet), 2 (doublet) or 3 (triplet)

Atom type generated by AtomTypes::AtomicInvariantsAtomTypes class corresponds to:

AS.X<n>.BO<n>.LBO<n>.<SB><n>.<DB><n>.<TB><n>.H<n>.Ar.RA.FC<+n/-n>.MN<n>.SM<n>

Except for AS which is a required atomic invariant in atom types, all other atomic invariants are optional. Atom type specification doesn't include atomic invariants with zero or undefined values.

In addition to usage of abbreviations for specifying atomic invariants, the following descriptive words are also allowed:

X : NumOfNonHydrogenAtomNeighbors or NumOfHeavyAtomNeighbors
 BO : SumOfBondOrdersToNonHydrogenAtoms or SumOfBondOrdersToHeavyAtoms
 LBO : LargestBondOrderToNonHydrogenAtoms or LargestBondOrderToHeavyAtoms
 SB : NumOfSingleBondsToNonHydrogenAtoms or NumOfSingleBondsToHeavyAtoms
 DB : NumOfDoubleBondsToNonHydrogenAtoms or NumOfDoubleBondsToHeavyAtoms
 TB : NumOfTripleBondsToNonHydrogenAtoms or NumOfTripleBondsToHeavyAtoms
 H : NumOfImplicitAndExplicitHydrogens
 Ar : Aromatic
 RA : RingAtom
 FC : FormalCharge
 MN : MassNumber
 SM : SpinMultiplicity

AtomTypes::AtomicInvariantsAtomTypes module is used to assign atomic invariant atom types.

--FunctionalClassesToUse "*FunctionalClass1,FunctionalClass2...*"

This value is used during *FunctionalClassAtomTypes* value of m, --mode option. It's a list of comma separated valid functional classes.

Possible values for atom functional classes are: *Ar, CA, H, HBA, HBD, Hal, NI, PI, RA*. Default value [Ref 24]: *HBD,HBA,PI,NI,Ar,Hal*.

The functional class abbreviations correspond to:

HBD: HydrogenBondDonor
 HBA: HydrogenBondAcceptor
 PI : PositivelyIonizable
 NI : NegativelyIonizable
 Ar : Aromatic
 Hal : Halogen
 H : Hydrophobic
 RA : RingAtom
 CA : ChainAtom

Functional class atom type specification for an atom corresponds to:

Ar.CA.H.HBA.HBD.Hal.NI.PI.RA

AtomTypes::FunctionalClassAtomTypes module is used to assign functional class atom types. It uses following definitions [Ref 60-61, Ref 65-66]:

HydrogenBondDonor: NH, NH2, OH
 HydrogenBondAcceptor: N[!H], O
 PositivelyIonizable: +, NH2
 NegativelyIonizable: -, C(=O)OH, S(=O)OH, P(=O)OH

--CompoundID *DataFieldName* or *LabelPrefixString*

This value is --CompoundID Mode specific and indicates how compound ID is generated.

For *DataField* value of --CompoundID Mode option, it corresponds to datafield label name whose value is used as compound ID; otherwise, it's a prefix string used for generating compound IDs like *LabelPrefixString*<Number>. Default value, *Cmpd*, generates compound IDs which look like *Cmpd*<Number>.

Examples for *DataField* value of --CompoundID Mode:

```
MolID
ExtReg
```

Examples for *LabelPrefix* or *MolNameOrLabelPrefix* value of --CompoundID Mode:

```
Compound
```

The value specified above generates compound IDs which correspond to *Compound*<Number> instead of default value of *Cmpd*<Number>.

--CompoundIDLabel *text*

Specify compound ID column label for FP or CSV/TSV text file(s) used during *CompoundID* value of --DataFieldsMode option. Default: *CompoundID*.

--CompoundIDMode *DataField* | *MolName* | *LabelPrefix* | *MolNameOrLabelPrefix*

Specify how to generate compound IDs and write to FP or CSV/TSV text file(s) along with generated fingerprints for *FP* | *text* | *all* values of --output option: use a *SDF* file(s) datafield value; use molname line from *SDF* file(s); generate a sequential ID with specific prefix; use combination of both *MolName* and *LabelPrefix* with usage of *LabelPrefix* values for empty molname lines.

Possible values: *DataField* | *MolName* | *LabelPrefix* | *MolNameOrLabelPrefix*. Default: *LabelPrefix*.

For *MolNameAndLabelPrefix* value of --CompoundID Mode, molname line in *SDF* file(s) takes precedence over sequential compound IDs generated using *LabelPrefix* and only empty molname values are replaced with sequential compound IDs.

This is only used for *CompoundID* value of --DataFieldsMode option.

--DataFields "*FieldLabel1,FieldLabel2,...*"

Comma delimited list of *SDF* file(s) data fields to extract and write to CSV/TSV text file(s) along with generated atom types for *text* | *all* values of --output option.

This is only used for *Specify* value of --DataFieldsMode option.

Examples:

```
Extreg
MolID,CompoundName
```

-d, --DataFieldsMode *All* | *Common* | *Specify* | *CompoundID*

Specify how data fields in *SDF* file(s) are transferred to output CSV/TSV text file(s) along with generated fingerprints for *text* | *all* values of --output option: transfer all SD data field; transfer SD data files common to all compounds; extract specified data fields; generate a compound ID using molname line, a compound prefix, or a combination of both. Possible values: *All* | *Common* | *specify* | *CompoundID*. Default value: *CompoundID*.

-f, --Filter *Yes* | *No*

Specify whether to check and filter compound data in *SDF* file(s). Possible values: *Yes* or *No*. Default value: *Yes*.

By default, compound data is checked before calculating fingerprints and compounds containing atom data corresponding to non-element symbols or no atom data are ignored.

-h, --help

Print this help message.

-i, --IgnoreHydrogens *Yes* | *No*

Ignore hydrogens during fingerprints generation. Possible values: *Yes* or *No*. Default value: *Yes*.

For **yes** value of **-i**, **--IgnoreHydrogens**, any explicit hydrogens are also used for generation of atom type fingerprints; implicit hydrogens are still ignored.

-k, --KeepLargestComponent *Yes / No*

Generate fingerprints for only the largest component in molecule. Possible values: **Yes** or **No**. Default value: **Yes**.

For molecules containing multiple connected components, fingerprints can be generated in two different ways: use all connected components or just the largest connected component. By default, all atoms except for the largest connected component are deleted before generation of fingerprints.

-m, --mode *AtomicInvariantsAtomTypes | DREIDINGAtomTypes | EStateAtomTypes | FunctionalClassAtomTypes | MMFF94AtomTypes | SLogPAtomTypes | SYBYLAtomTypes | TPSAAtomTypes | UFFAtomTypes | All*

Specify atom identifier type to use for assignment of atom types to hydrogen and/or non-hydrogen atoms during calculation of atom types fingerprints. Possible values in the current release are: *AtomicInvariantsAtomTypes*, *DREIDINGAtomTypes*, *EStateAtomTypes*, *FunctionalClassAtomTypes*, *MMFF94AtomTypes*, *SLogPAtomTypes*, *SYBYLAtomTypes*, *TPSAAtomTypes*, *UFFAtomTypes* or *All*. Default value: *AtomicInvariantsAtomTypes*.

--OutDelim *comma | tab | semicolon*

Delimiter for output CSV/TSV text file(s). Possible values: *comma*, *tab*, or *semicolon*. Default value: *comma*.

--output *SD | text | all*

Type of output files to generate. Possible values: *SD*, *text*, or *all*. Default value: *text*.

-o, --overwrite

Overwrite existing files.

-q, --quote *Yes / No*

Put quote around column values in output CSV/TSV text file(s). Possible values: **Yes** or **No**. Default value: **Yes**.

-r, --root *RootName*

New file name is generated using the root: *<Root>.<Ext>*. Default for new file names: *<SDFileName><AtomTypes>.<Ext>*. The file type determines *<Ext>* value. The *sdf*, *csv*, and *tsv* *<Ext>* values are used for *SD*, *comma/semicolon*, and *tab* delimited text files, respectively. This option is ignored for multiple input files.

-w, --WorkingDir *DirName*

Location of working directory. Default: current directory.

EXAMPLES

To generate atomic invariants atom types count fingerprints of arbitrary size in vector string format and create a *SampleATFP.csv* file containing sequential compound IDs along with fingerprints vector strings data, type:

```
% AtomTypesFingerprints.pl -r SampleATFP -o Sample.sdf
```

demo:

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SEE ALSO

AtomTypesFingerprints.pl

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