NAME

AssignAtomTypes.pl - Assign atom types for SD files

SYNOPSIS

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

Multiple SDFile 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 ypes are assigned to all non-hydrogen atoms or all atoms in a molecule

OPTIONS

--AromaticityModel *MDLAromaticityModel* | *TriposAromaticityModel* | *MMFFAromaticityModel* | *ChemAxonBasicAromaticityModel* | *ChemAxonGeneralAromaticityModel* | *DaylightAromaticityModel* | *MayaChemToolsAromaticityModel*

Specify aromaticity model to use during detection of aromaticity. Possible values in the current release are: *MDLAromaticityModel, TriposAromaticityModel, 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 --CompoundIDMode specific and indicates how compound ID is generated.

For *DataField* value of --CompoundIDMode 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 --CompoundIDMode:

```
MolID
ExtReg
```

Examples for *LabelPrefix* or *MolNameOrLabelPrefix* value of --CompoundIDMode:

```
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 *SDFile(s)* datafield value; use molname line from *SDFile(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 --CompoundIDMode, molname line in *SDFile(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 *SDFiles(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 *SDFile(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 SDFile(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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