NAME

AtomTypesFingerprints.pl - Generate atom types fingerprints for SD files

SYNOPSIS

AtomTypesFingerprints.pl SDFile(s)...

AtomTypesFingerprints.pl [--AromaticityModel AromaticityModelType] [-a, --AtomI dentifierType AtomicInvariantsAtomTypes | DREIDINGAtomTypes | EStateAtomTypes | MMFF94AtomTypes | SLogPAtomTypes | SYBYLAtomTypes | TPSAAtomTypes | UFFAtomTypes] [--AtomicInvariantsToUse "AtomicInvariant, AtomicInvariant..."] [--FunctionalClassesToUse "FunctionalClass1,FunctionalClass2..."] [--AtomTypesSetToUse ArbitrarySize | FixedSize] [--BitsOrder Ascending | Descending] [-b, --BitStringFormat BinaryString | HexadecimalString] [--CompoundI D DataFieldName or LabelPrefixString] [--CompoundI DLabel text] [--CompoundI DMode 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, --I gnoreHydrogens 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 fingerprints for *SDFile(s)* and create appropriate SD, FP or CSV/TSV text file(s) containing fingerprints bit-vector or vector strings corresponding to molecular fingerprints.

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 fingerpritns corresponding to following -a, --AtomI dentifierTypes:

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

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

Using the assigned atom types and specified -m, --Mode, one of the following types of fingerprints are generated:

```
AtomTypesCount - A vector containing count of atom types
AtomTypesBits - A bit vector indicating presence/absence of atom types
```

For *AtomTypesCount* fingerprints, two types of atom types set size are allowed as value of --AtomTypesSetToUse option:

```
ArbitrarySize - Corresponds to only atom types detected in molecule FixedSize - Corresponds to fixed number of atom types previously defined
```

For AtomTypesBits fingerprints, only FixedSize atom type set is allowed.

ArbitrarySize corresponds to atom types detected in a molecule where as FixedSize implies a fix number of all possible atom types previously defined for a specific -a, --AtomI dentifierType.

Fix number of all possible atom types for supported AtomIdentifierTypes in current release of MayaChemTools are:

AtomIdentifier	Total	TotalWithoutHydrogens
DREIDINGAtomTypes	37	34
EStateAtomTypes	109	87
MMFF94AtomTypes	212	171
SLogPAtomTypes	72	67
SYBYLAtomTypes	45	44

TPSAAtomTypes 47 47 UFFAtomTypes 126 124

The current release of MayaChemTools generates the following atom types fingerprints bit-vector and vector strings:

FingerprintsVector;AtomTypesCount:AtomicInvariantsAtomTypes:ArbitrarySize;10;NumericalValues;IDsAndValuesString;C.X1.B01.H3 C.X2.B02.H2 C.X2.B03.H1 C.X3.B03.H1 C.X3.B04 F.X1.B01 N.X2.B02.H1 N.X3.B03 O.X1.B01.H1 O.X1.B02;2 4 14 3 10 1 1 1 3 2

FingerprintsVector;AtomTypesCount:DREIDINGAtomTypes:ArbitrarySize;8;Nu
mericalValues;IDsAndValuesString;C_2 C_3 C_R F_ N_3 N_R O_2 O_3;2 9 22
1 1 1 2 3

FingerprintsVector;AtomTypesCount:EStateAtomTypes:ArbitrarySize;11;Num ericalValues;IDsAndValuesString;aaCH aasC aasN dO dssC sCH3 sF sOH ssC H2 ssNH sssCH;14 8 1 2 2 2 1 3 4 1 3

FingerprintsVector;AtomTypesCount:FunctionalClassAtomTypes:ArbitrarySize;8;NumericalValues;IDsAndValuesString;Ar Ar.HBA HBA HBA.HBD HBD Hal NI None;22 1 2 3 1 1 1 10

FingerprintsVector;AtomTypesCount:MMFF94AtomTypes:ArbitrarySize;13;Num ericalValues;IDsAndValuesString;C5A C5B C=ON CB COO CR F N5 NC=O O=CN O=CO OC=O OR;2 2 1 18 1 9 1 1 1 1 1 1 2

FingerprintsVector;AtomTypesCount:SLogPAtomTypes:ArbitrarySize;16;NumericalValues;IDsAndValuesString;C1 C10 C11 C14 C18 C20 C21 C22 C5 CS F N11 N4 O10 O2 O9;5 1 1 1 14 4 2 1 2 2 1 1 1 1 3 1

FingerprintsVector;AtomTypesCount:SYBYLAtomTypes:ArbitrarySize;9;Numer
icalValues;IDsAndValuesString;C.2 C.3 C.ar F N.am N.ar 0.2 0.3 0.co2;2
9 22 1 1 1 1 2 2

FingerprintsVector;AtomTypesCount:UFFAtomTypes:ArbitrarySize;8;Numeric
alValues;IDsAndValuesString;C_2 C_3 C_R F_ N_3 N_R O_2 O_3;2 9 22 1 1
1 2 3

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.

-a, --AtomI dentifierType AtomicInvariantsAtomTypes | DREIDINGAtomTypes | EStateAtomTypes | FunctionalClassAtomTypes | MMFF94AtomTypes | SLogPAtomTypes | SYBYLAtomTypes | TPSAAtomTypes | UFFAtomTypes

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. Default value: AtomicInvariantsAtomTypes.

-- Atomic Invariants To Use "Atomic Invariant, Atomic Invariant..."

This value is used during *AtomicInvariantsAtomTypes* value of a, --AtomI dentifierType 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
```

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

 ${\tt SB} \; : \; \; {\tt NumOfSingleBondsToNonHydrogenAtoms} \; \; {\tt or} \; \; {\tt NumOfSingleBondsToHeavyAtoms} \\$

 ${\tt DB} \; : \; {\tt NumOfDoubleBondsToNonHydrogenAtoms} \; \; {\tt or} \; \; {\tt NumOfDoubleBondsToHeavyAtoms}$

 ${\tt TB} \; : \; {\tt NumOfTripleBondsToNonHydrogenAtoms} \; \; {\tt or} \; \; {\tt NumOfTripleBondsToHeavyAtoms} \; \\$

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 a, --AtomI dentifierType 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(=0)OH, S(=0)OH, P(=0)OH
```

--AtomTypesSetToUse ArbitrarySize | FixedSize

Atom types set size to use during generation of atom types fingerprints.

Possible values for *AtomTypesCount* values of -m, --mode option: *ArbitrarySize | FixedSize*; Default value: *ArbitrarySize*.

Possible values for AtomTypesBits value of -m, --mode option: FixedSize; Default value: FixedSize.

FixedSize value is not supported for AtomicInvariantsAtomTypes value of -a, --AtomI dentifierType option.

 $\label{lem:arbitrarySize} \textit{ArbitrarySize} \ \textit{corresponds} \ \textit{to} \ \textit{only} \ \textit{atom} \ \textit{types} \ \textit{detected} \ \textit{in} \ \textit{molecule}; \ \textit{\textit{FixedSize}} \ \textit{corresponds} \ \textit{to} \ \textit{fixed} \ \textit{number} \ \textit{of} \ \textit{previously} \ \textit{defined} \ \textit{atom} \ \textit{types} \ \textit{for} \ \textit{specified} \ \textit{-a, --AtomI} \ \textit{dentifierType}.$

--BitsOrder Ascending | Descending

Bits order to use during generation of fingerprints bit-vector string for *AtomTypesBits* value of =item --BitsOrder *Ascending* | *Descending*

Bits order to use during generation of fingerprints bit-vector string for *AtomTypesBits* value of -m, --mode option. Possible values: *Ascending, Descending.* Default: *Ascending.*

Ascending bit order which corresponds to first bit in each byte as the lowest bit as opposed to the highest bit

Internally, bits are stored in *Ascending* order using Perl vec function. Regardless of machine order, big-endian or little-endian, vec function always considers first string byte as the lowest byte and first bit within each byte as the lowest bit.

-b, --BitStringFormat BinaryString | HexadecimalString

Format of fingerprints bit-vector string data in output SD, FP or CSV/TSV text file(s) specified by --output used during *AtomTypesBits* value of -m, --mode option. Possible values: *BinaryString, HexadecimalString*. Default value: *BinaryString*.

BinaryString corresponds to an ASCII string containing 1s and 0s. HexadecimalString contains bit values in ASCII hexadecimal format.

Examples:

-- Compound I D 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 --CompoundI DMode:

MolID ExtReg

Examples for LabelPrefix or MolNameOrLabelPrefix value of --CompoundI DMode:

Compound

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

--CompoundI DLabel text

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

--Compound I DMode 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 --CompoundI DMode, 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 fingerprints 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.

--FingerprintsLabelMode FingerprintsLabelOnly | FingerprintsLabelWithIDs

Specify how fingerprints label is generated in conjunction with --FingerprintsLabel option value: use fingerprints label generated only by --FingerprintsLabel option value or append atom type value IDs to --FingerprintsLabel option value.

Possible values: FingerprintsLabelOnly | FingerprintsLabelWithIDs. Default value: FingerprintsLabelOnly.

This option is only used for *FixedSize* value of -e, --AtomTypesSetToUse option during generation of *AtomTypesCount* fingerprints and ignored for *AtomTypesBits*.

Atom type IDs appended to --FingerprintsLabel value during *FingerprintsLabelWithIDs* values of --FingerprintsLabelMode correspond to fixed number of previously defined atom types.

--FingerprintsLabel text

SD data label or text file column label to use for fingerprints string in output SD or CSV/TSV text file(s) specified by --output. Default value: *AtomTypesFingerprints*.

-h, --help

Print this help message.

-i, --I gnoreHydrogens Yes | No

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

For yes value of -i, --I gnoreHydrogens, 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 AtomTypesCount | AtomTypesBits

Specify type of atom types fingerprints to generate for molecules in *SDFile(s)*. Possible values: *AtomTypesCount or AtomTypesBits*. Default value: *AtomTypesCount*.

For *AtomTypesCount* values of -m, --mode option, a fingerprint vector string is generated. The vector string corresponding to *AtomTypesCount* contains count of atom types.

For *AtomTypesBits* value of -m, --mode option, a fingerprint bit-vector string containing zeros and ones indicating presence or absence of atom types is generated.

For *AtomTypesCount* atom types fingerprints, two types of atom types set size can be specified using -a, --AtomTypesSetToUse option: *ArbitrarySize or FixedSize*. *ArbitrarySize* corrresponds to only atom types detected in molecule; *FixedSize* corresponds to fixed number of atom types previously defined.

For AtomTypesBits atom types fingeprints, only FixedSize is allowed.

Combination of -m, --Mode and --AtomTypesSetToUse along with -a, --AtomtomI dentifierType allows generation of following different atom types fingerprints:

Mode	AtomIdentifierType	AtomTypesSetToUse
AtomTypesCount	AtomicInvariantsAtomTypes	ArbitrarySize [Default]
AtomTypesCount AtomTypesCount AtomTypesBits	DREIDINGAtomTypes DREIDINGAtomTypes DREIDINGAtomTypes	ArbitrarySize FixedSize FixedSize
AtomTypesCount	EStateAtomTypes	ArbitrarySize

AtomTypesCount	EStateAtomTypes	FixedSize
AtomTypesBits	EStateAtomTypes	FixedSize
AtomTypesCount	FunctionalClassAtomTypes	ArbitrarySize
AtomTypesCount	MMFF94AtomTypes	ArbitrarySize
AtomTypesCount	MMFF94AtomTypes	FixedSize
AtomTypesBits	MMFF94AtomTypes	FixedSize
AtomTypesCount	SLogPAtomTypes	ArbitrarySize
AtomTypesCount	SLogPAtomTypes	FixedSize
AtomTypesBits	SLogPAtomTypes	FixedSize
AtomTypesCount	SYBYLAtomTypes	ArbitrarySize
AtomTypesCount	SYBYLAtomTypes	FixedSize
AtomTypesBits	SYBYLAtomTypes	FixedSize
AtomTypesCount AtomTypesBits	TPSAAtomTypes TPSAAtomTypes	FixedSize FixedSize
AtomTypesCount	UFFAtomTypes	ArbitrarySize
AtomTypesCount	UFFAtomTypes	FixedSize
AtomTypesBits	UFFAtomTypes	FixedSize

The default is to generate *AtomicInvariantAtomTypes* fingeprints corresponding to *ArbitrarySize* as value of --AtomTypesSetToUse option.

--OutDelim comma | tab | semicolon

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

--output SD | FP | text | all

Type of output files to generate. Possible values: SD, FP, 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><AtomTypesFP>.<Ext>. The file type determines <Ext> value. The sdf, fpf, csv, and tsv <Ext> values are used for SD, FP, comma/semicolon, and tab delimited text files, respectively. This option is ignored for multiple input files.

-v, --VectorStringFormat ValuesString | IDsAndValuesString | IDsAndValuesPairsString | ValuesAndIDsString | ValuesAndIDsPairsString

Format of fingerprints vector string data in output SD, FP or CSV/TSV text file(s) specified by --output used during <AtomTypesCount> value of -m, --mode option. Possible values: ValuesString, IDsAndValuesPairsString | ValuesAndIDsString | ValuesAndIDsPairsString.

Default value during *ArbitrarySize* value of -e, --AtomTypesSetToUse option: *IDsAndValuesString*. Default value during *FixedSize* value of -e, --AtomTypesSetToUse option: *ValuesString*.

Example of *SD* file containing atom types fingerprints string data:

```
1.4499
                      0.0000 C 0 0 0 0 0 0 0 0 0 0 0
 -3.3652
. . . . . .
2 3 1 0 0 0 0
. . . . . .
M END
> <CmpdID>
Cmpd1
> <AtomTypesFingerprints>
FingerprintsVector; AtomTypesCount: AtomicInvariantsAtomTypes: ArbitrarySi
ze;10;NumericalValues;IDsAndValuesString;C.X1.B01.H3 C.X2.B02.H2 C.X2.B
O3.H1 C.X3.BO3.H1 C.X3.BO4 F.X1.BO1 N.X2.BO2.H1 N.X3.BO3 O.X1.BO1.H1 O.
X1.B02;2 4 14 3 10 1 1 1 3 2
$$$$
. . . . . .
. . . . . .
```

Example of *FP* file containing atom types fingerprints string data:

```
# Package = MayaChemTools 7.4
# Release Date = Oct 21, 2010
# TimeStamp = Fri Mar 11 14:28:07 2011
# FingerprintsStringType = FingerprintsVector
# Description = AtomTypesCount:AtomicInvariantsAtomTypes:ArbitrarySize
# VectorStringFormat = IDsAndValuesString
# VectorValuesType = NumericalValues
Cmpd1 10;C.X1.B01.H3 C.X2.B02.H2 C.X2.B03.H1 C.X3.B03.H1 C.X3.B04 F...
Cmpd2 9; C.X1.B01.H3 C.X2.B02.H2 C.X3.B03.H1 C.X3.B04 N.X1.B01.H2 N....
. . . . . .
. . . . . .
```

Example of CSV Text file atom types containing fingerprints string data:

```
"CompoundID", "AtomTypesFingerprints"
"Cmpd1", "FingerprintsVector; AtomTypesCount: AtomicInvariantsAtomTypes: Ar
bitrarySize;10; NumericalValues; IDsAndValuesString; C.X1.BO1.H3 C.X2.BO2.
H2 C.X2.BO3.H1 C.X3.BO3.H1 C.X3.BO4 F.X1.BO1 N.X2.BO2.H1 N.X3.BO3 O.X1.
BO1.H1 O.X1.BO2;2 4 14 3 10 1 1 1 3 2"
O.X1.BO2;3 3 6 3 1 1 2 2 2"
. . . . . .
. . . . . .
```

Examples:

FingerprintsVector; AtomTypesCount: EStateAtomTypes: ArbitrarySize; 11; Num ericalValues;IDsAndValuesString;aaCH aasC aasN dO dssC sCH3 sF sOH ssC H2 ssNH sssCH;14 8 1 2 2 2 1 3 4 1 3

FingerprintsVector; AtomTypesCount: SYBYLAtomTypes: ArbitrarySize; 9; Numer icalValues; IDsAndValuesString; C.2 C.3 C.ar F N.am N.ar O.2 O.3 O.co2; 2 9 22 1 1 1 1 2 2

FingerprintsVector; AtomTypesCount: SYBYLAtomTypes: FixedSize; 44; OrderedN umericalValues; IDsAndValuesString; C.3 C.2 C.1 C.ar C.cat N.3 N.2 N.1 N .ar N.am N.pl3 N.4 O.3 O.2 O.co2 S.3 S.2 S.o S.o2 P.3 F Cl Br I ANY HA L HET Li Na Mg Al Si K Ca Cr.th Cr.oh Mn Fe Co.oh Cu Zn Se Mo Sn;9 2 0 0 0 0 0 0 0 0

-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
```

To generate functional class 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 -m AtomTypesCount -a FunctionalClassAtomTypes
-r SampleATFP -o Sample.sdf
```

To generate E-state 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 -m AtomTypesCount -a EStateAtomTypes
  --AtomTypesSetToUse ArbitrarySize -r SampleATFP -o Sample.sdf
```

To generate E-state atom types count fingerprints of fixed size in vector string with IDsAndValues format and create a SampleATFP.csv file containing sequential compound IDs along with fingerprints vector strings data, type:

```
% AtomTypesFingerprints.pl -m AtomTypesCount -a EStateAtomTypes
--AtomTypesSetToUse FixedSize -v IDsAndValuesString
-r SampleATFP -o Sample.sdf
```

To generate E-state atom types bits fingerprints of fixed size in bit-vector string format and create a SampleATFP.csv file containing sequential compound IDs along with fingerprints vector strings data, type:

```
% AtomTypesFingerprints.pl -m AtomTypesBits -a EStateAtomTypes
  --AtomTypesSetToUse FixedSize -r SampleATFP -o Sample.sdf
```

To generate MMFF94 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 -m AtomTypesCount -a MMFF94AtomTypes
  --AtomTypesSetToUse ArbitrarySize -r SampleATFP -o Sample.sdf
```

To generate MMFF94 atom types count fingerprints of fixed size in vector string format and create a SampleATFP.csv file containing sequential compound IDs along with fingerprints vector strings data, type:

```
% AtomTypesFingerprints.pl -m AtomTypesCount -a MMFF94AtomTypes
  --AtomTypesSetToUse FixedSize -r SampleATFP -o Sample.sdf
```

To generate MMFF94 atom types count fingerprints of fixed size in vector string with IDsAndValues format and create a SampleATFP.csv file containing sequential compound IDs along with fingerprints vector strings data, type:

```
% AtomTypesFingerprints.pl -m AtomTypesCount -a MMFF94AtomTypes
  --AtomTypesSetToUse FixedSize -v IDsAndValuesString
  -r SampleATFP -o Sample.sdf
```

To generate MMFF94 atom types bits fingerprints of fixed size in bit-vector string format and create a SampleATFP.csv file containing sequential compound IDs along with fingerprints vector strings data, type:

```
% AtomTypesFingerprints.pl -m AtomTypesBits -a MMFF94AtomTypes
  --AtomTypesSetToUse FixedSize -r SampleATFP -o Sample.sdf
```

To generate MMFF94 atom types count fingerprints of arbitrary size in vector string format and create a SampleATFP.csv file containing compound ID from molecule name line along with fingerprints vector strings data,

To generate MMFF94 atom types count fingerprints of arbitrary size in vector string format and create a SampleATFP.csv file containing compound IDs using specified data field along with fingerprints vector strings data, type:

```
% AtomTypesFingerprints.pl -m AtomTypesCount -a MMFF94AtomTypes
--DataFieldsMode CompoundID --CompoundIDMode DataField --CompoundID
Mol_ID -r SampleATFP -o Sample.sdf
```

To generate MMFF94 atom types count fingerprints of arbitrary size in vector string format and create a SampleATFP.csv file containing compound ID using combination of molecule name line and an explicit compound prefix along with fingerprints vector strings data, type:

```
% AtomTypesFingerprints.pl -m AtomTypesCount -a MMFF94AtomTypes
--DataFieldsMode CompoundID --CompoundIDMode MolnameOrLabelPrefix
--CompoundID Cmpd --CompoundIDLabel MolID -r SampleATFP -o Sample.sdf
```

To generate MMFF94 atom types count fingerprints of arbitrary size in vector string format and create a SampleATFP.csv file containing specific data fields columns along with fingerprints vector strings data, type:

```
% AtomTypesFingerprints.pl -m AtomTypesCount -a MMFF94AtomTypes
  --DataFieldsMode Specify --DataFields Mol_ID -r SampleATFP
  -o Sample.sdf
```

To generate MMFF94 atom types count fingerprints of arbitrary size in vector string format and create a SampleATFP.csv file containing common data fields columns along with fingerprints vector strings data, type:

```
% AtomTypesFingerprints.pl -m AtomTypesCount -a MMFF94AtomTypes
--DataFieldsMode Common -r SampleATFP -o Sample.sdf
```

To generate MMFF94 atom types count fingerprints of arbitrary size in vector string format and create SampleATFP.sdf, SampleATFP.fpf and SampleATFP.csv files containing all data fields columns in CSV file along with fingerprints vector strings data, type:

```
% AtomTypesFingerprints.pl -m AtomTypesCount -a MMFF94AtomTypes
  --DataFieldsMode All --output all -r SampleATFP -o Sample.sdf
```

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SEE ALSO

InfoFingerprintsFiles.pl, SimilarityMatricesFingerprints.pl, AtomNeighborhoodsFingerprints.pl, ExtendedConnectivityFingerprints.pl, MACCSKeysFingeprints.pl, PathLengthFingerprints.pl, TopologicalAtomPairsFingerprints.pl, TopologicalAtomTorsionsFingerprints.pl, TopologicalPharmacophoreAtomPairsFingerprints.pl, TopologicalPharmacophoreAtomPairsFingerprints.pl

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