

NAME

AtomTypesFingerprints

SYNOPSIS

```
use AtomTypesFingerprints;

use AtomTypesFingerprints qw(:all);
```

DESCRIPTION

AtomTypesFingerprints class provides the following methods:

```
new, GenerateFingerprints, GetDescription, SetAtomIdentifierType, SetAtomTypesSetToUse,
SetAtomicInvariantsToUse, SetFunctionalClassesToUse, SetType, StringifyAtomTypesFingerprints
```

AtomTypesFingerprints is derived from Fingerprints class which in turn is derived from ObjectProperty base class that provides methods not explicitly defined in AtomNeighborhoodsFingerprints, Fingerprints or ObjectProperty classes using Perl's AUTOLOAD functionality. These methods are generated on-the-fly for a specified object property:

```
Set<PropertyName>(<PropertyValue>);
$PropertyValue = Get<PropertyName>();
Delete<PropertyName>();
```

The current release of MayaChemTools supports generation of AtomTypesFingerprints corresponding to following AtomIdentifierTypes:

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

Based on the values specified for AtomIdentifierType along with other specified parameters such as AtomicInvariantsToUse 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 Type, 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 is allowed:

```
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 *AtomIdentifierType*.

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 |

Combination of Type and AtomTypesSetToUse along with AtomIdentifierType allows generation of following different atom types fingerprints:

| Type | AtomIdentifierType | AtomTypesSetToUse |
|------|--------------------|-------------------|
|------|--------------------|-------------------|


```
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
```

```
FingerprintsVector;AtomTypesCount:UFFAtomTypes;124;OrderedNumerical
Values;IDsAndValuesString;He4+4 Li Be3+2 B_3 B_2 C_3 C_R C_2 C_1 N_3 N_
R N_2 N_1 O_3 O_3_z O_R O_2 O_1 F_ Ne4+4 Na Mg3+2 Al3 Si3 P_3+3 P_3+5 P
_3+q S_3+2 S_3+4 S_3+6 S_R S_2 Cl Ar4+4 K_ Ca6+2 Sc3+3 Ti3+4 Ti6+4 V_3+
;0 0 0 0 0 12 0 3 0 3 0 1 0 2 0 0 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ...
```

```
FingerprintsVector;AtomTypesCount:UFFAtomTypes:FixedSize;124;OrderedNu
mericalValues;IDsAndValuesString;He4+4 Li Be3+2 B_3 B_2 C_3 C_R C_2 C_
1 N_3 N_R N_2 N_1 O_3 O_3_z O_R O_2 O_1 F_ Ne4+4 Na Mg3+2 Al3 Si3 P_3+
3 P_3+5 P_3+q S_3+2 S_3+4 S_3+6 S_R S_2 Cl Ar4+4 K_ Ca6+2 Sc3+3 Ti...;
0 0 0 0 0 9 22 2 0 1 1 0 0 3 0 0 2 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0...
```

```
FingerprintsBitVector;AtomTypesBits:UFFAtomTypes:FixedSize;124;BinaryS
tring;Ascending;000001110110010010100000000000000000000000000000000
0000000000000000000000000000000000000000000000000000000000000000
```

METHODS

new

```
$NewAtomTypesFingerprints = new AtomTypesFingerprints(%NamesAndValues);
```

Using specified *AtomTypesFingerprints* property names and values hash, new method creates a new object and returns a reference to newly created PathLengthFingerprints object. By default, the following properties are initialized:

```
Molecule = '';
Type = ''
AtomIdentifierType = ''
AtomTypesSetToUse = ''
IgnoreHydrogens = 1
AtomicInvariantsToUse = ['AS', 'X', 'BO', 'H', 'FC', 'MN']
FunctionalClassesToUse = ['HBD', 'HBA', 'PI', 'NI', 'Ar', 'Hal']
```

Examples:

```
$AtomTypesFingerprints = new AtomTypesFingerprints(
    'Molecule' => $Molecule,
    'Type' => 'AtomTypesCount',
    'AtomIdentifierType' =>
        'AtomicInvariantsAtomTypes');

$AtomTypesFingerprints = new AtomTypesFingerprints(
    'Molecule' => $Molecule,
    'Type' => 'AtomTypesCount',
    'AtomIdentifierType' =>
        'AtomicInvariantsAtomTypes',
    'AtomicInvariantsToUse' =>
        ['AS', 'X', 'BO', 'H', 'FC'] );

$AtomTypesFingerprints = new AtomTypesFingerprints(
    'Molecule' => $Molecule,
    'Type' => 'AtomTypesCount',
    'AtomIdentifierType' =>
        'DREIDINGAtomTypes');

$AtomTypesFingerprints = new AtomTypesFingerprints(
    'Molecule' => $Molecule,
    'Type' => 'AtomTypesCount',
    'AtomIdentifierType' =>
        'EStateAtomTypes',
    'AtomTypesSetToUse' =>
```

```

        'ArbitrarySize');

$AtomTypesFingerprints = new AtomTypesFingerprints(
    'Molecule' => $Molecule,
    'Type' => 'AtomTypesCount',
    'AtomIdentifierType' =>
        'SLogPAtomTypes',
    'AtomTypesSetToUse' =>
        'FixedSize');

$AtomTypesFingerprints = new AtomTypesFingerprints(
    'Molecule' => $Molecule,
    'Type' => 'AtomTypesBits',
    'AtomIdentifierType' =>
        'MMFF94AtomTypes',
    'AtomTypesSetToUse' =>
        'FixedSize');

$AtomTypesFingerprints->GenerateFingerprints();
print "$AtomTypesFingerprints\n";

```

GenerateFingerprints

```
$AtomTypesFingerprints->GenerateFingerprints();
```

Generates atom types fingerprints and returns *AtomTypesFingerprints*.

GetDescription

```
$Description = $AtomTypesFingerprints->GetDescription();
```

Returns a string containing description of atom types fingerprints.

SetAtomIdentifierType

```
$AtomTypesFingerprints->SetAtomIdentifierType($IdentifierType);
```

Sets atom *IdentifierType* to use during atom types fingerprints generation and returns *AtomTypesFingerprints*.

Possible values: *AtomicInvariantsAtomTypes*, *DREIDINGAtomTypes*, *EStateAtomTypes*, *FunctionalClassAtomTypes*, *MMFF94AtomTypes*, *SLogPAtomTypes*, *SYBYLAtomTypes*, *TPSAAtomTypes*, *UFFAtomTypes*.

SetAtomTypesSetToUse

```
$AtomTypesFingerprints->SetAtomTypesSetToUse($Value);
```

Sets *Value* of *AtomTypesSetToUse* and returns *AtomTypesFingerprints*. Possible values: *ArbitrarySize* or *FixedSize*. Default for *AtomTypesCount* value of *AtomTypesSetToUse*: *ArbitrarySize*.

SetAtomicInvariantsToUse

```
$AtomTypesFingerprints->SetAtomicInvariantsToUse($ValuesRef);
$AtomTypesFingerprints->SetAtomicInvariantsToUse(@Values);
```

Sets atomic invariants to use during *AtomicInvariantsAtomTypes* value of *AtomIdentifierType* for atom neighborhood fingerprints generation and returns *AtomTypesFingerprints*.

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.

SetFunctionalClassesToUse

```
$AtomTypesFingerprints->SetFunctionalClassesToUse($ValuesRef);
$AtomTypesFingerprints->SetFunctionalClassesToUse(@Values);
```

Sets functional classes invariants to use during *FunctionalClassAtomTypes* value of *AtomIdentifierType* for atom types fingerprints generation and returns *AtomTypesFingerprints*.

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 or None

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

SetType

```
$AtomTypesFingerprints->SetType($Type);
```

Sets type of AtomTypes fingerprints and returns *AtomTypesFingerprints*. Possible values: *AtomTypesFingerprintsBits* or *AtomTypesFingerprintsCount*.

StringifyAtomTypesFingerprints

```
$String = $AtomTypesFingerprints->StringifyAtomTypesFingerprints();
```

Returns a string containing information about *AtomTypesFingerprints* object.

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SEE ALSO

Fingerprints.pm, FingerprintsStringUtil.pm, AtomNeighborhoodsFingerprints.pm, EStateIndicesFingerprints.pm, ExtendedConnectivityFingerprints.pm, MACCSKeys.pm, PathLengthFingerprints.pm, TopologicalAtomPairsFingerprints.pm, TopologicalAtomTripletsFingerprints.pm, TopologicalAtomTorsionsFingerprints.pm, TopologicalPharmacophoreAtomPairsFingerprints.pm, TopologicalPharmacophoreAtomTripletsFingerprints.pm

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