

NAME

AtomNeighborhoodsFingerprints

SYNOPSIS

```
use Fingerprints::AtomNeighborhoodsFingerprints;

use Fingerprints::AtomNeighborhoodsFingerprints qw(:all);
```

DESCRIPTION

AtomNeighborhoodsFingerprints [Ref 53-56, Ref 73] class provides the following methods:

new, GenerateFingerprints, GetDescription, SetAtomIdentifierType, SetAtomicInvariantsToUse, SetFunctionalClassesToUse, SetMaxNeighborhoodRadius, SetMinNeighborhoodRadius, StringifyAtomNeighborhoodsFingerprints

AtomNeighborhoodsFingerprints 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 AtomNeighborhoodsFingerprints corresponding to following AtomIdentifierTypes:

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

Based on the values specified for AtomIdentifierType along with other specified such as AtomicInvariantsToUse and FunctionalClassesToUse, initial atom types are assigned to all non-hydrogen atoms in a molecule. Using atom neighborhoods around each non-hydrogen central atom corresponding to radii between specified values MinNeighborhoodRadius and MaxNeighborhoodRadius, unique atom types at each radii level are counted and an atom neighborhood identifier is generated.

The format of an atom neighborhood identifier around a central non-hydrogen atom at a specific radius is:

```
NR<n>-<AtomType>-ATC<n>

NR: Neighborhood radius
AtomType: Assigned atom type
ATC: Atom type count
```

The atom neighborhood identifier for non-hydrogen central atom corresponding to all specified radii is generated by concatenating neighborhood identifiers at each radii by colon as a delimiter:

```
NR<n>-<AtomType>-ATC<n>:NR<n>-<AtomType>-ATC<n>:...
```

The atom neighborhood identifiers for all non-hydrogen central atoms at all specified radii are concatenated using space as a delimiter and constitute atom neighborhood fingerprint of the molecule.

The current release of MayaChemTools generates the following types of atom neighborhoods fingerprints vector strings:

```
FingerprintsVector;AtomNeighborhoods:AtomicInvariantsAtomTypes:MinRadius0:MaxRadius2;41;AlphaNumericalValues;ValuesString;NR0-C.X1.BO1.H3-ATC1:NR1-C.X3.BO3.H1-ATC1:NR2-C.X1.BO1.H3-ATC1:NR2-C.X3.BO4-ATC1 NR0-C.X1.BO1.H3-ATC1:NR1-C.X3.BO3.H1-ATC1:NR2-C.X1.BO1.H3-ATC1:NR2-C.X3.BO4-ATC1 NR0-C.X2.BO2.H2-ATC1:NR1-C.X2.BO2.H2-ATC1:NR1-C.X3.BO3.H1-ATC1:NR2-C.X2.BO2.H2-ATC1:NR2-N.X3.BO3-ATC1:NR2-O.X1.BO1.H1-ATC1 NR0-C.X2.B...
```

```
FingerprintsVector;AtomNeighborhoods:DREIDINGAtomTypes:MinRadius0:MaxRadius2;41;AlphaNumericalValues;ValuesString;NR0-C_2-ATC1:NR1-C_3-ATC1:NR1-O_2-ATC1:NR1-O_3-ATC1:NR2-C_3-ATC1 NR0-C_2-ATC1:NR1-C_R-ATC1:NR1-N_3-ATC1:NR1-O_2-ATC1:NR2-C_R-ATC3 NR0-C_3-ATC1:NR1-C_2-ATC1:NR1-C_3-AT
```

```
C1:NR2-C_3-ATC1:NR2-O_2-ATC1:NR2-O_3-ATC2 NR0-C_3-ATC1:NR1-C_3-ATC1:NR1-N_R-ATC1:NR2-C_3-ATC1:NR2-C_R-ATC2 NR0-C_3-ATC1:NR1-C_3-ATC1:NR2-...
```

```
FingerprintsVector;AtomNeighborhoods:EStateAtomTypes:MinRadius0:MaxRadius2;41;AlphaNumericalValues;ValuesString;NR0-aaCH-ATC1:NR1-aaCH-ATC1:NR1-aasC-ATC1:NR2-aaCH-ATC1:NR2-aasC-ATC1:NR2-sF-ATC1 NR0-aaCH-ATC1:NR1-aaCH-ATC1:NR1-aasC-ATC1:NR2-aaCH-ATC1:NR2-aasC-ATC1:NR2-sF-ATC1 NR0-aaCH-ATC1:NR1-aaCH-ATC1:NR1-aasC-ATC1:NR2-aaCH-ATC1:NR2-aasC-ATC2 NR0-aaCH-ATC1:NR1-aaCH-ATC1:NR1-aasC-ATC1:NR2-aaCH-ATC1:NR2-aasC-ATC2 N...
```

```
FingerprintsVector;AtomNeighborhoods:FunctionalClassAtomTypes:MinRadius0:MaxRadius2;41;AlphaNumericalValues;ValuesString;NR0-Ar-ATC1:NR1-Ar-ATC1:NR1-Ar.HBA-ATC1:NR1-None-ATC1:NR2-Ar-ATC2:NR2-None-ATC4 NR0-Ar-ATC1:NR1-Ar-ATC2:NR1-Ar.HBA-ATC1:NR2-Ar-ATC5:NR2-None-ATC1 NR0-Ar-ATC1:NR1-Ar-ATC2:NR1-HBD-ATC1:NR2-Ar-ATC2:NR2-None-ATC1 NR0-Ar-ATC1:NR1-Ar-ATC2:NR1-Hal-ATC1:NR2-Ar-ATC2 NR0-Ar-ATC1:NR1-Ar-ATC2:NR1-None-ATC1:...
```

```
FingerprintsVector;AtomNeighborhoods:MMFF94AtomTypes:MinRadius0:MaxRadius2;41;AlphaNumericalValues;ValuesString;NR0-C5A-ATC1:NR1-C5B-ATC1:NR1-CB-ATC1:NR1-N5-ATC1:NR2-C5A-ATC1:NR2-C5B-ATC1:NR2-CB-ATC3:NR2-CR-ATC1 NR0-C5A-ATC1:NR1-C5B-ATC1:NR1-CR-ATC1:NR1-N5-ATC1:NR2-C5A-ATC1:NR2-C5B-ATC1:NR2-C=ON-ATC1:NR2-CR-ATC3 NR0-C5B-ATC1:NR1-C5A-ATC1:NR1-C5B-ATC1:NR1-C=ON-ATC1:NR2-C5A-ATC1:NR2-CB-ATC1:NR2-CR-ATC1:NR2-N5-ATC1:N...
```

```
FingerprintsVector;AtomNeighborhoods:SLogPAtomTypes:MinRadius0:MaxRadius2;41;AlphaNumericalValues;ValuesString;NR0-C1-ATC1:NR1-C10-ATC1:NR1-CS-ATC1:NR2-C1-ATC1:NR2-N11-ATC1:NR2-O2-ATC1 NR0-C1-ATC1:NR1-C11-ATC1:NR2-C1-ATC1:NR2-C21-ATC1 NR0-C1-ATC1:NR1-C11-ATC1:NR2-C1-ATC1:NR2-C21-ATC1 NR0-C1-ATC1:NR1-C5-ATC1:NR1-CS-ATC1:NR2-C1-ATC1:NR2-O2-ATC2:NR2-O9-ATC1 NR0-C1-ATC1:NR1-CS-ATC2:NR2-C1-ATC2:NR2-O2-ATC2 NR0-C10-ATC1:...
```

```
FingerprintsVector;AtomNeighborhoods:SYBYLAtomTypes:MinRadius0:MaxRadius2;41;AlphaNumericalValues;ValuesString;NR0-C.2-ATC1:NR1-C.3-ATC1:NR1-O.co2-ATC2:NR2-C.3-ATC1 NR0-C.2-ATC1:NR1-C.ar-ATC1:NR1-N.am-ATC1:NR1-O.2-ATC1:NR2-C.ar-ATC3 NR0-C.3-ATC1:NR1-C.2-ATC1:NR1-C.3-ATC1:NR2-C.3-ATC1:NR2-O.3-ATC1:NR2-O.co2-ATC2 NR0-C.3-ATC1:NR1-C.3-ATC1:NR1-N.ar-ATC1:NR2-C.3-ATC1:NR2-C.ar-ATC2 NR0-C.3-ATC1:NR1-C.3-ATC1:NR2-C.3-ATC1:...
```

```
FingerprintsVector;AtomNeighborhoods:TPSAAtomTypes:MinRadius0:MaxRadius2;41;AlphaNumericalValues;ValuesString;NR0-N21-ATC1:NR1-None-ATC3:NR2-None-ATC5 NR0-N7-ATC1:NR1-None-ATC2:NR2-None-ATC3:NR2-O3-ATC1 NR0-None-ATC1:NR1-N21-ATC1:NR1-None-ATC1:NR2-None-ATC3 NR0-None-ATC1:NR1-N21-ATC1:NR1-None-ATC2:NR2-None-ATC6 NR0-None-ATC1:NR1-N21-ATC1:NR1-None-ATC2:NR2-None-ATC6 NR0-None-ATC1:NR1-N7-ATC1:NR1-None-ATC1:NR1-O3-ATC1:...
```

```
FingerprintsVector;AtomNeighborhoods:UFFAAtomTypes:MinRadius0:MaxRadius2;41;AlphaNumericalValues;ValuesString;NR0-C_2-ATC1:NR1-C_3-ATC1:NR1-O_2-ATC1:NR1-O_3-ATC1:NR2-C_3-ATC1 NR0-C_2-ATC1:NR1-C_R-ATC1:NR1-N_3-ATC1:NR1-O_2-ATC1:NR2-C_R-ATC3 NR0-C_3-ATC1:NR1-C_2-ATC1:NR1-C_3-ATC1:NR2-C_3-ATC1:NR2-O_2-ATC1:NR2-O_3-ATC2 NR0-C_3-ATC1:NR1-C_3-ATC1:NR1-N_R-ATC1:NR2-C_3-ATC1:NR2-C_R-ATC2 NR0-C_3-ATC1:NR1-C_3-ATC1:NR2-C_3-A...
```

METHODS

new

```
$NewAtomNeighborhoodsFingerprints = new AtomNeighborhoodsFingerprints(
    %NamesAndValues);
```

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

```
Molecule = ''
Type = 'AtomNeighborhoods'
MinNeighborhoodRadius = 0
MaxNeighborhoodRadius = 2
```

```

AtomIdentifierType = ''
AtomicInvariantsToUse = ['AS', 'X', 'BO', 'H', 'FC', 'MN']
FunctionalClassesToUse = ['HBD', 'HBA', 'PI', 'NI', 'Ar', 'Hal']

```

Examples:

```

$AtomNeighborhoodsFingerprints = new AtomNeighborhoodsFingerprints(
    'Molecule' => $Molecule,
    'AtomIdentifierType' =>
        "AtomicInvariantsAtomTypes");

$AtomNeighborhoodsFingerprints = new AtomNeighborhoodsFingerprints(
    'Molecule' => $Molecule,
    'MinNeighborhoodRadius' => 0,
    'MaxNeighborhoodRadius' => 2,
    'AtomIdentifierType' =>
        'AtomicInvariantsAtomTypes',
    'AtomicInvariantsToUse' =>
        ['AS', 'X', 'BO', 'H', 'FC'] );

$AtomNeighborhoodsFingerprints = new AtomNeighborhoodsFingerprints(
    'Molecule' => $Molecule,
    'AtomIdentifierType' =>
        'SYBYLAtomTypes');

$AtomNeighborhoodsFingerprints = new AtomNeighborhoodsFingerprints(
    'Molecule' => $Molecule,
    'AtomIdentifierType' =>
        'MMFF94AtomTypes');

$AtomNeighborhoodsFingerprints = new AtomNeighborhoodsFingerprints(
    'Molecule' => $Molecule,
    'AtomIdentifierType' =>
        'AtomicInvariantsAtomTypes');

$AtomNeighborhoodsFingerprints = new AtomNeighborhoodsFingerprints(
    'Molecule' => $Molecule,
    'MinNeighborhoodRadius' => 0,
    'MaxNeighborhoodRadius' => 2,
    'AtomIdentifierType' =>
        'FunctionalClassAtomTypes',
    'FunctionalClassesToUse' =>
        ['HBD', 'HBA', 'PI', 'NI', 'Ar', 'Hal'] );

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

```

GenerateFingerprints

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

Generates atom neighborhood fingerprints and returns *AtomNeighborhoodsFingerprints*.

GetDescription

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

Returns a string containing description of atom neighborhood fingerprints.

SetAtomIdentifierType

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

Sets atom *IdentifierType* to use during atom neighborhood fingerprints generation and returns *AtomNeighborhoodsFingerprints*.

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

SetAtomicInvariantsToUse

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

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

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

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

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

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

SetMaxNeighborhoodRadius

```
$AtomNeighborhoodsFingerprints->SetMaxNeighborhoodRadius($Radius);
```

Sets maximum neighborhood radius to use during atom neighborhood fingerprints generation and returns *AtomNeighborhoodsFingerprints*.

SetMinNeighborhoodRadius

```
$AtomNeighborhoodsFingerprints->SetMinNeighborhoodRadius($Radius);
```

Sets minimum neighborhood radius to use during atom neighborhood fingerprints generation and returns *AtomNeighborhoodsFingerprints*.

StringifyAtomNeighborhoodsFingerprints

```
$String = $Fingerprints->StringifyAtomNeighborhoodsFingerprints();
```

Returns a string containing information about *AtomNeighborhoodsFingerprints* object.

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SEE ALSO

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

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