NAME

ExtendedConnectivityFingerprints

SYNOPSIS

use Fingerprints::ExtendedConnectivityFingerprints;

use Fingerprints::ExtendedConnectivityFingerprints qw(:all);

DESCRIPTION

ExtendedConnectivityFingerprints [Ref 48, Ref 52] class provides the following methods:

new, GenerateFingerprints, GetDescription, SetAtomIdentifierType, SetAtomicInvariantsToUse, SetFunctionalClassesToUse, SetNeighborhoodRadius, StringifyExtendedConnectivityFingerprints

ExtendedConnectivityFingerprints is derived from Fingerprints class which in turn is derived from ObjectProperty base class that provides methods not explicitly defined in ExtendedConnectivityFingerprints, 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 ExtendedConnectivityFingerprints corresponding to following AtomtomIdentifierTypes:

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

Based on the values specified for AtomIdentifierType, AtomicInvariantsToUse and FunctionalClassesToUse, initial atom types are assigned to all non-hydrogen atoms in a molecule and these atom types strings are converted into initial atom identifier integers using TextUtil::HashCode function. The duplicate atom identifiers are removed.

For NeighborhoodRadius value of *0*, the initial set of unique atom identifiers comprises the molecule fingerprints. Otherwise, atom neighborhoods are generated for each non-hydrogen atom up-to specified NeighborhoodRadius value. For each non-hydrogen central atom at a specific radius, its neighbors at next radius level along with their bond orders and previously calculated atom identifiers are collected which in turn are used to generate a new integer atom identifier; the bond orders and atom identifier pairs list is first sorted by bond order followed by atom identifiers to make these values graph invariant.

After integer atom identifiers have been generated for all non-hydrogen atoms at all specified neighborhood radii, the duplicate integer atom identifiers corresponding to same hash code value generated using TextUtil::HashCode are tracked by keeping the atom identifiers at lower radius. Additionally, all structurally duplicate integer atom identifiers at each specified radius are also tracked by identifying equivalent atom and bonds corresponding to substructures used for generating atom identifier and keeping integer atom identifier with lowest value.

For *ExtendedConnnectivity* value of fingerprints Type, the duplicate identifiers are removed from the list and the unique atom identifiers constitute the extended connectivity fingerprints of a molecule.

For *ExtendedConnnectivityCount* value of fingerprints Type, the occurrence of each unique atom identifiers appears is counted and the unique atom identifiers along with their count constitute the extended connectivity fingerprints of a molecule.

For *ExtendedConnectivityBits* value of fingerprints -m, --mode, the unique atom identifiers are used as a random number seed to generate a random integer value between 0 and --Size which in turn is used to set corresponding bits in the fingerprint bit-vector string.

The current release of MayaChemTools generates the following types of extended connectivity fingerprints vector strings:

```
FingerprintsVector;ExtendedConnectivity:AtomicInvariantsAtomTypes:Radi
us2;60;AlphaNumericalValues;ValuesString;73555770 333564680 352413391
666191900 1001270906 1371674323 1481469939 1977749791 2006158649 21414
08799 49532520 64643108 79385615 96062769 273726379 564565671 85514103
5 906706094 988546669 1018231313 1032696425 1197507444 1331250018 1338
532734 1455473691 1607485225 1609687129 1631614296 1670251330 17303...
```

FingerprintsVector;ExtendedConnectivityCount:AtomicInvariantsAtomTypes
:Radius2;60;NumericalValues;IDsAndValuesString;73555770 333564680 3524
13391 666191900 1001270906 1371674323 1481469939 1977749791 2006158649
2141408799 49532520 64643108 79385615 96062769 273726379 564565671...;
3 2 1 1 14 1 2 10 4 3 1 1 1 1 2 1 2 1 1 1 2 3 1 1 2 1 3 3 8 2 2 2 6 2
1 2 1 1 2 1 1 1 2 1 1 2 1 2 1 1 1 1 1 1 1 1 1 2 1 1

FingerprintsBitVector;ExtendedConnectivityBits:AtomicInvariantsAtomTyp
es:Radius2;1024;BinaryString;Ascending;0000000000000000000000000000100
0000000001010000000110000011000000000000100000000000000000000000100001
1000000110000000000000000000000000001001100000000000000000000000010000
0000000000000000000000000010000000000000000001000000000000000000000000
0000000000010000100001000000000000101000000000000000100000000000000...

FingerprintsBitVector;ExtendedConnectivityBits:AtomicInvariantsAtomTyp
es:Radius2;1024;HexadecimalString;Ascending;000000010050c0600800000803
0300000091000004000000020000100000000124008200020000000040020000000000
2080000000820040010020000000008040000000000080001000000000400000000000
4040000090000061010000000800200000000000014000000000200800000000000020
00008020200000408000

FingerprintsVector;ExtendedConnectivity:FunctionalClassAtomTypes:Radiu
s2;57;AlphaNumericalValues;ValuesString;24769214 508787397 850393286 8
62102353 981185303 1231636850 1649386610 1941540674 263599683 32920567
1 571109041 639579325 683993318 723853089 810600886 885767127 90326012
7 958841485 981022393 1126908698 1152248391 1317567065 1421489994 1455
632544 1557272891 1826413669 1983319256 2015750777 2029559552 20404...

FingerprintsVector;ExtendedConnectivityCount:FunctionalClassAtomTypes:
Radius2;57;NumericalValues;IDsAndValuesString;24769214 508787397 85039
3286 862102353 981185303 1231636850 1649386610 1941540674 263599683 32
9205671 571109041 639579325 683993318 723853089 810600886 885767127...;
1 1 1 10 2 22 3 1 3 3 1 1 1 3 2 2 1 2 2 2 3 1 1 1 1 1 14 1 1 1 1 1 1 2
1 2 1 1 2 2 1 1 2 1 1 1 2 1 1 2 1 1 1 1 1 1 1

FingerprintsBitVector;ExtendedConnectivityBits:FunctionalClassAtomType
s:Radius2;1024;BinaryString;Ascending;0000000000000000000100000000000
0000000001000100000000001000000000000000000000000000000000101000000010
0000001000000000001000000000000000000000000000000000000000000000000100
0000000000001000000000000001000000000001001000000000000000000000000000
0000000000000000100000000000001000000000000000000000000000000000000...

FingerprintsVector;ExtendedConnectivity:DREIDINGAtomTypes:Radius2;56;A
lphaNumericalValues;ValuesString;280305427 357928343 721790579 1151822
898 1207111054 1380963747 1568213839 1603445250 4559268 55012922 18094
0813 335715751 534801009 684609658 829361048 972945982 999881534 10076
55741 1213692591 1222032501 1224517934 1235687794 1244268533 152812070
0 1629595024 1856308891 1978806036 2001865095 2096549435 172675415 ...

FingerprintsVector;ExtendedConnectivity:EStateAtomTypes:Radius2;62;Alp
haNumericalValues;ValuesString;25189973 528584866 662581668 671034184
926543080 1347067490 1738510057 1759600920 2034425745 2097234755 21450
44754 96779665 180364292 341712110 345278822 386540408 387387308 50430
1706 617094135 771528807 957666640 997798220 1158349170 1291258082 134
1138533 1395329837 1420277211 1479584608 1486476397 1487556246 1566...

FingerprintsVector;ExtendedConnectivity:MMFF94AtomTypes:Radius2;64;Alp
haNumericalValues;ValuesString;224051550 746527773 998750766 103704190
2 1239701709 1248384926 1259447756 1521678386 1631549126 1909437580 20
37095052 2104274756 2117729376 8770364 31445800 81450228 314289324 344
041929 581773587 638555787 692022098 811840536 929651561 936421792 988
636432 1048624296 1054288509 1369487579 1454058929 1519352190 17271...

FingerprintsVector;ExtendedConnectivity:SLogPAtomTypes:Radius2;71;Alph
aNumericalValues;ValuesString;78989290 116507218 489454042 888737940 1

```
162561799 1241797255 1251494264 1263717127 1471206899 1538061784 17654
07295 1795036542 1809833874 2020454493 2055310842 2117729376 11868981
56731842 149505242 184525155 196984339 288181334 481409282 556716568 6
41915747 679881756 721736571 794256218 908276640 992898760 10987549...

FingerprintsVector;ExtendedConnectivity:SYBYLAtomTypes:Radius2;58;Alph
aNumericalValues;ValuesString;199957044 313356892 455463968 465982819
1225318176 1678585943 1883366064 1963811677 2117729376 113784599 19153
8837 196629033 263865277 416380653 477036669 681527491 730724924 90906
5537 1021959189 1133014972 1174311016 1359441203 1573452838 1661585138
1668649038 1684198062 1812312554 1859266290 1891651106 2072549404 ...

FingerprintsVector;ExtendedConnectivity:TPSAAtomTypes:Radius2;47;Alpha
NumericalValues;ValuesString;20818206 259344053 862102353 1331904542 1
700688206 265614156 363161397 681332588 810600886 885767127 950172500
951454814 1059668746 1247054493 1382302230 1399502637 1805025917 19189
39561 2114677228 2126402271 8130483 17645742 32278373 149975755 160327
654 256360355 279492740 291251259 317592700 333763396 972105960 101...

FingerprintsVector;ExtendedConnectivity:UFFAtomTypes:Radius2;56;AlphaN
umericalValues;ValuesString;280305427 357928343 721790579 1151822898 1
207111054 1380963747 1568213839 1603445250 4559268 55012922 180940813
335715751 534801009 684609658 829361048 972945982 999881534 1007655741
1213692591 1222032501 1224517934 1235687794 1244268533 1528120700 162
9595024 1856308891 1978806036 2001865095 2096549435 172675415 18344...
```

METHODS

new

```
$NewExtendedConnectivityFingerprints = new ExtendedConnectivityFingerprints(
                                                    %NamesAndValues);
```

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

```
Molecule = ''
Type = 'ExtendedConnectivity'
NeighborhoodRadius = 2
AtomIdentifierType = ''
AtomicInvariantsToUse = ['AS', 'X', 'BO', 'H', 'FC', 'MN']
FunctionalClassesToUse = ['HBD', 'HBA', 'PI', 'NI', 'Ar', 'Hal']
```

Examples:

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

$ExtendedConnectivityFingerprints = new ExtendedConnectivityFingerprints(
                            'Type' => 'ExtendedConnectivityCount',
                            'Molecule' => $Molecule,
                            'AtomIdentifierType' =>
                                        'AtomicInvariantsAtomTypes');

$ExtendedConnectivityFingerprints = new ExtendedConnectivityFingerprints(
                            'Type' => 'ExtendedConnectivityBits',
                            'Molecule' => $Molecule,
                            'Size' => 1024,
                            'AtomIdentifierType' =>
                                        'AtomicInvariantsAtomTypes');

$ExtendedConnectivityFingerprints = new ExtendedConnectivityFingerprints(
                            'Type' => 'ExtendedConnectivity',
                            'Molecule' => $Molecule,
                            'NeighborhoodRadius' => 2,
                            'AtomIdentifierType' =>
```

```
                                        'AtomicInvariantsAtomTypes',
                                'AtomicInvariantsToUse' =>
                                        ['AS', 'X', 'BO', 'H', 'FC', 'MN'] );

        $ExtendedConnectivityFingerprints = new ExtendedConnectivityFingerprints(
                                'Type' => 'ExtendedConnectivity',
                                'Molecule' => $Molecule,
                                'NeighborhoodRadius' => 2,
                                'AtomIdentifierType' =>
                                        'FunctionalClassAtomTypes',
                                'FunctionalClassesToUse' =>
                                        ['HBD', 'HBA', 'PI', 'NI', 'Ar', 'Hal'] );

        $ExtendedConnectivityFingerprints = new ExtendedConnectivityFingerprints(
                                'Type' => 'ExtendedConnectivity',
                                'Molecule' => $Molecule,;
                                'AtomIdentifierType' =>
                                        'MMFF94AtomTypes');

        $ExtendedConnectivityFingerprints = new ExtendedConnectivityFingerprints(
                                'Type' => 'ExtendedConnectivityCount',
                                'Molecule' => $Molecule,;
                                'AtomIdentifierType' =>
                                        'MMFF94AtomTypes');

        $ExtendedConnectivityFingerprints = new ExtendedConnectivityFingerprints(
                                'Type' => 'ExtendedConnectivityCount',
                                'Molecule' => $Molecule,;
                                'AtomIdentifierType' =>
                                        'SLogPAtomTypes');

        $ExtendedConnectivityFingerprints = new ExtendedConnectivityFingerprints(
                                'Type' => 'ExtendedConnectivity',
                                'Molecule' => $Molecule,;
                                'AtomIdentifierType' =>
                                        'SLogPAtomTypes');

        $ExtendedConnectivityFingerprints = new ExtendedConnectivityFingerprints(
                                'Type' => 'ExtendedConnectivity',
                                'Molecule' => $Molecule,;
                                'AtomIdentifierType' =>
                                        'SYBYLAtomTypes');

        $ExtendedConnectivityFingerprints->GenerateFingerprints();
        print "$ExtendedConnectivityFingerprints\n";
```

GenerateFingerprints

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

Generates extended connectivity fingerprints and returns *ExtendedConnectivityFingerprints*.

GetDescription

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

Returns a string containing description of extended connectivity fingerprints fingerprints.

SetAtomIdentifierType

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

Sets atom *IdentifierType* to use during extended connectivity fingerprints generation and returns *ExtendedConnectivityFingerprints*.

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

SetAtomicInvariantsToUse

```
        $ExtendedConnectivityFingerprints->SetAtomicInvariantsToUse($ValuesRef);
```

```
$ExtendedConnectivityFingerprints->SetAtomicInvariantsToUse(@Values);
```

Sets atomic invariants to use during *AtomicInvariantsAtomTypes* value of *AtomIdentifierType* for extended connectivity fingerprints generation and returns *ExtendedConnectivityFingerprints*.

Possible values for atomic invariants are: *AS, X, BO, LBO, SB, DB, TB, H, Ar, RA, FC, MN, SM*. Default value [Ref 24]: *AS,X,BO,H,FC,MN*.

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

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

Sets functional classes invariants to use during *FunctionalClassAtomTypes* value of *AtomIdentifierType* for extended connectivity fingerprints generation and returns *ExtendedConnectivityFingerprints*.

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
```

SetNeighborhoodRadius

```
$ExtendedConnectivityFingerprints->SetNeighborhoodRadius($Radius);
```

Sets neighborhood radius to use during extended connectivity fingerprints generation and returns *ExtendedConnectivityFingerprints*.

StringifyExtendedConnectivityFingerprints

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

Returns a string containing information about *ExtendedConnectivityFingerprints* object.

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SEE ALSO

Fingerprints.pm, FingerprintsStringUtil.pm, AtomNeighborhoodsFingerprints.pm, AtomTypesFingerprints.pm, EStateIndiciesFingerprints.pm, MACCSKeys.pm, PathLengthFingerprints.pm, TopologicalAtomPairsFingerprints.pm, TopologicalAtomTripletsFingerprints.pm, TopologicalAtomTorsionsFingerprints.pm, TopologicalPharmacophoreAtomPairsFingerprints.pm, TopologicalPharmacophoreAtomTripletsFingerprints.pm

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