NAME

EStateIndiciesFingerprints

SYNOPSIS

use Fingerprints::EStateIndiciesFingerprints;

use Fingerprints::EStateIndiciesFingerprints qw(:all);

DESCRIPTION

EStateIndiciesFingerprints [Ref 75-78] class provides the following methods:

new, GenerateFingerprints, GetDescription, SetEStateAtomTypesSetToUse, SetValuesPrecision, StringifyEStateIndiciesFingerprints

EStateIndiciesFingerprints 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>();
```

E-state atom types are assigned to all non-hydrogen atoms in a molecule using module AtomTypes::EStateAtomTypes.pm and E-state values are calculated using module AtomicDescriptors::EStateValues.pm. Using E-state atom types and E-state values, EStateIndiciesFingerprints constituting sum of E-state values for E-sate atom types are generated.

Two types of E-state atom types set size are allowed:

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

Module AtomTypes::EStateAtomTypes.pm, used to assign E-state atom types to non-hydrogen atoms in the molecule, is able to assign atom types to any valid atom group. However, for *FixedSize* value of EStateAtomTypesSetToUse, only a fixed set of E-state atom types corresponding to specific atom groups [Appendix III in Ref 77] are used for fingerprints.

The fixed size E-state atom type set size used during generation of fingerprints contains 87 E-state non-hydrogen atom types in EStateAtomTypes.csv data file distributed with MayaChemTools.

Combination of Type and EStateAtomTypesSetToUse allow generation of 2 different types of E-state indicies fingerprints:

```
Type                        EStateAtomTypesSetToUse

EStateIndicies              ArbitrarySize      [ default fingerprints ]
EStateIndicies              FixedSize
```

The current release of MayaChemTools generates the following types of E-state fingerprints vector strings:

```
FingerprintsVector;EStateIndicies:ArbitrarySize;11;NumericalValues;IDs
AndValuesString;SaaCH SaasC SaasN SdO SdssC SsCH3 SsF SsOH SssCH2 SssN
H SsssCH;24.778 4.387 1.993 25.023 -1.435 3.975 14.006 29.759 -0.073 3
.024 -2.270

FingerprintsVector;EStateIndicies:FixedSize;87;OrderedNumericalValues;
ValuesString;0 0 0 0 0 0 0 3.975 0 -0.073 0 0 24.778 -2.270 0 0 -1.435
4.387 0 0 0 0 0 0 3.024 0 0 0 0 0 0 0 1.993 0 29.759 25.023 0 0 0 0 1
4.006 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;EStateIndicies:FixedSize;87;OrderedNumericalValues;
IDsAndValuesString;SsLi SssBe SssssBem SsBH2 SssBH SssssB SssssBm SsCH3
SdCH2 SssCH2 StCH SdsCH SaaCH SssssCH SddC StsC SdssC SaasC SaaaC Sssss
C SsNH3p SsNH2 SssNH2p SdNH SssNH SaaNH StN SssssNHp SdsN SaaN SssssN Sd
0 0 0 0 0 0 0 3.975 0 -0.073 0 0 24.778 -2.270 0 0 -1.435 4.387 0 0 0
0 0 0 3.024 0 0 0 0 0 0 0 1.993 0 29.759 25.023 0 0 0 0 14.006 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...
```

METHODS

new

```
$EStateIndiciesFingerprints = new EStateIndiciesFingerprints(%NamesAndValues);
```

Using specified *EStateIndiciesFingerprints* 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 = 'EStateIndicies'
EStateAtomTypesSetToUse = 'ArbitrarySize'
ValuesPrecision = 3
```

Examples:

```
$EStateIndiciesFingerprints = new AtomTypesFingerprints(
                          'Molecule' => $Molecule,
                          'EStateAtomTypesSetToUse' =>
                                        'ArbitrarySize');

$EStateIndiciesFingerprints = new AtomTypesFingerprints(
                          'Molecule' => $Molecule,
                          'EStateAtomTypesSetToUse' =>
                                        'FixedSize');

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

GenerateFingerprints

```
$EStateIndiciesFingerprints = $EStateIndiciesFingerprints->
                              GenerateEStateIndiciesFingerprints();
```

Generates EState keys fingerprints and returns *EStateIndiciesFingerprints*.

GetDescription

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

Returns a string containing description of EState keys fingerprints.

SetEStateAtomTypesSetToUse

```
$EStateIndiciesFingerprints->SetEStateAtomTypesSetToUse($Value);
```

Sets *Value* of *EStateAtomTypesSetToUse* and returns *EStateIndiciesFingerprints*. Possible values: *ArbitrarySize or FixedSize*. Default value: *ArbitrarySize*.

SetValuesPrecision

```
$EStateIndiciesFingerprints->SetValuesPrecision($Precision);
```

Sets precesion of E-state values to use during generation of E-state indices fingerprints and returns *EStateIndiciesFingerprints*. Possible values: *Positive integers*. Default value: *3*.

StringifyEStateIndiciesFingerprints

```
$String = $EStateIndiciesFingerprints->StringifyEStateIndiciesFingerprints();
```

Returns a string containing information about *EStateIndiciesFingerprints* object.

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SEE ALSO

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

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