

NAME

EStateIndicesFingerprints

SYNOPSIS

```
use Fingerprints::EStateIndicesFingerprints;

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

DESCRIPTION

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

new, GenerateFingerprints, GetDescription, SetEStateAtomTypesSetToUse, SetValuesPrecision, StringifyEStateIndicesFingerprints

EStateIndicesFingerprints 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, EStateIndicesFingerprints constituting sum of E-state values for E-state 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 indices fingerprints:

Type	EStateAtomTypesSetToUse
EStateIndices	ArbitrarySize [default fingerprints]
EStateIndices	FixedSize

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

```
FingerprintsVector;EStateIndices: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;EStateIndices: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 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
```

```
FingerprintsVector;EStateIndicies:FixedSize;87;OrderedNumericalValues;  
IDsAndValuesString;SsLi SssBe SssssBem SsBH2 SssBH SsssB SssssBm ScCH3  
SdCH2 SsssCH2 StCH SdsCH SaaCH SssssCH SddC StcC Sdssc SaasC SaaaC Sssss  
C SsnNH3p SsnH2 SssNH2p SdNH SssNH SaaNH StN SssssNHp SdsN SaaN SssssN Sd  
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 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 ...
```

METHODS

new

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

Using specified *EStateIndicesFingerprints* 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";
```

Generate Fingerprints

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

Generates EState keys fingerprints and returns *EStateIndicesFingerprints*.

GetDescription

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

Returns a string containing description of EState keys fingerprints.

SetEStateAtomTypesSetToUse

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

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

SetValuesPrecision

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

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

StringifyEStateIndicesFingerprints

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

Returns a string containing information about *EStateIndicesFingerprints* object.

AUTHOR

Manish Sud <msud@san.rr.com>

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

COPYRIGHT

Copyright (C) 2024 Manish Sud. All rights reserved.

This file is part of MayaChemTools.

MayaChemTools is free software; you can redistribute it and/or modify it under the terms of the GNU Lesser General Public License as published by the Free Software Foundation; either version 3 of the License, or (at your option) any later version.