

NAME

PathLengthFingerprints

SYNOPSIS

```
use Fingerprints::PathLengthFingerprints;

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

DESCRIPTION

PathLengthFingerprints class provides the following methods:

new, GenerateFingerprints, , GetDescription, SetAtomIdentifierType, SetAtomicInvariantsToUse, SetFunctionalClassesToUse, SetMaxLength, SetMinLength, SetNumOfBitsToSetPerPath, SetType, StringifyPathLengthFingerprints

PathLengthFingerprints is derived from Fingerprints class which in turn is derived from ObjectProperty base class that provides methods not explicitly defined in PathLengthFingerprints, 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 Type, AtomIdentifierTypes, MinPathLength and MaxPathLength, all appropriate atom paths are generated for each atom in the molecule and collected in a list and the list is filtered to remove any structurally duplicate paths as indicated by the value of UseUniquePaths.

For molecules containing rings, atom paths starting from each atom can be traversed in four different ways:

- o Atom paths without any rings and sharing of bonds in traversed paths.
- o Atom paths containing rings and without any sharing of bonds in traversed paths
- o All possible atom paths without any rings and sharing of bonds in traversed paths
- o All possible atom paths containing rings and with sharing of bonds in traversed paths.

Atom path traversal is terminated at the last ring atom. For molecules containing no rings, first two and last two types described above are equivalent.

AllowSharedBonds and AllowRings allow generation of different types of paths to be used for fingerprints generation.

The combination of AllowSharedBonds, AllowRings, and UseBondSymbols allows generation of 8 different types of path length fingerprints:

AllowSharedBonds	AllowRings	UseBondSymbols	
0	0	1	- AtomPathsNoCyclesWithBondSymbols
0	1	1	- AtomPathsWithCyclesWithBondSymbols
1	0	1	- AllAtomPathsNoCyclesWithBondSymbols
1	1	1	- AllAtomPathsWithCyclesWithBondSymbols [DEFAULT]
0	0	0	- AtomPathsNoCyclesNoBondSymbols
0	1	0	- AtomPathsWithCyclesNoBondSymbols
1	0	0	- AllAtomPathsNoCyclesNoBondSymbols

For each atom path in the filtered atom paths list, an atom path string is created using value of AtomIdentifierType and specified values to use for a particular atom identifier type. Value of UseBondSymbols controls whether bond order symbols are used during generation of atom path string. Atom symbol corresponds to element symbol and characters used to represent bond order are: 1 - *None*; 2 - '='; 3 - '#'; 1.5 or aromatic - ':'; *others: bond order value*. By default, bond symbols are included in atom path strings. Exclusion of bond symbols in atom path strings results in fingerprints which correspond purely to atom paths without considering bonds.

For *PathLengthBits* value of *Type*, each atom path is hashed to a 32 bit unsigned integer key using `TextUtil::HashCode` function. Using the hash key as a seed for a random number generator, a random integer value between 0 and *Size* is used to set corresponding bits in the fingerprint bit-vector string. Value of *NumOfBitsToSetPerPaths* option controls the number of time a random number is generated to set corresponding bits.

The current release of MayaChemTools generates the following types of path length fingerprints bit-vector and vector strings:

```
FingerprintsBitVector;PathLengthBits:AtomicInvariantsAtomTypes:MinLength1:MaxLength8;1024;HexadecimalString;Ascending;48caa1315d82d91122b02942861c9409a4208182d12015509767bd0867653604481a8b12880000560905836030789ccdaae54e26596889ab121309800900490515224208421502120a0dd9200509723ae8900024181b86c0122821d4e4880c38620dab280824b455404009f082003d52c212b4e6d6ea05280140069c780290c43
```

```
FingerprintsVector;PathLengthCount:AtomicInvariantsAtomTypes:MinLength
1:MaxLength8;432:NumericalValues;IDsAndValuesPairsString;C.X1.B01.H3 2
C.X2.B02.H2 4 C.X2.B03.H1 14 C.X3.B03.H1 3 C.X3.B04 10 F.X1.B01 1 N.X
2.B02.H1 1 N.X3.B03 1 O.X1.B01.H1 3 O.X1.B02 2 C.X1.B01.H3C.X3.B03.H1
2 C.X2.B02.H2C.X2.B02.H2 1 C.X2.B02.H2C.X3.H1 4 C.X2.B02.H2C.X3.B0
4 1 C.X2.B02.H2N.X3.B03 1 C.X2.B03.H1C.X2.B03.H1 10 C.X2.B03.H1C.X...
```

```
FingerprintsVector;PathLengthCount:DREIDINGAtomTypes:MinLength1:MaxLen
gth8;410;NumericalValues;IDsAndValuesPairsString;C_2 2 C_3 9 C_R 22 F_
1 N_3 1 N_R 1 O_2 2 O_3 3 C_2=O_2 2 C_2C_3 1 C_2C_R 1 C_2N_3 1 C_2O_3
1 C_3C_3 7 C_3C_R 1 C_3N_R 1 C_3O_3 2 C_R:C_R 21 C_R:N_R 2 C_RC_R 2 C
_RF_ 1 C_RN_3 1 C_2C_3C_3 1 C_2C_R:C_R 2 C_2N_3C_R 1 C_3C_2=O_2 1 C_3C
_2O_3 1 C_3C_3C_3 5 C_3C_3C_R 2 C_3C_3N_R 1 C_3C_3O_3 4 C_3C_R:C_R .
```

```
FingerprintsVector;PathLengthCount:EStateAtomTypes:MinLength1:MaxLength
h8;454;NumericalValues;IDsAndValuesPairsString;aaCH 14 aasC 8 aasN 1 d
O 2 dssC 2 sCH3 2 sF 1 sOH 3 ssCH2 4 ssNH 1 sssCH 3 aaCH:aACH 10 aACH:
aasC 8 aasC:aasC 3 aasC:aasN 2 aasCaasC 2 aasCdssC 1 aasCsF 1 aasCssh
1 aasCsshCH 1 aasNsshCH2 1 dO=dssC 2 dssCsOH 1 dssCsshCH2 1 dssCsshNH
1 sCH3ssssCH 2 sOHssssCH 2 ssCH2ssCH2 1 ssCH2ssssCH 4 aaCH:aACH:aACH 6 a...
```

```
FingerprintsVector;PathLengthCount;FunctionalClassAtomTypes;MinLength1
:MaxLength8;404;NumericalValues;IDsAndValuesPairsString;Ar 22 Ar.HBA 1
HBA 2 HBA.HBD 3 HBD 1 Hal 1 NI 1 None 10 Ar.HBA:Ar 2 Ar.HBANone 1 Ar:
Ar 21 ArAr 2 ArHBD 1 ArHal 1 ArNone 2 HBA.HBDNI 1 HBA.HBDNone 2 HBA=NI
```

```
1 HBA=None 1 HBDNone 1 NINone 1 NoneNone 7 Ar.HBA:Ar:Ar 2 Ar.HBA:ArAr
1 Ar.HBA:ArNone 1 Ar.HBANoneNone 1 Ar:Ar.HBA:Ar 1 Ar:Ar.HBANone 2 ...
```

```
FingerprintsVector;PathLengthCount:MMFF94AtomTypes:MinLength1:MaxLength
8;463;NumericalValues;IDsAndValuesPairsString;C5A 2 C5B 2 C=ON 1 CB 1
8 COO 1 CR 9 F 1 N5 1 NC=O 1 O=CN 1 O=CO 1 OC=O 1 OR 2 C5A:C5B 2 C5A:N
5 2 C5ACB 1 C5ACR 1 C5B:C5B 1 C5BC=ON 1 C5BCB 1 C=ON=O=CN 1 C=ONNC=O 1
CB:CB 18 CBF 1 CBNC=O 1 COO=O=CO 1 COOCR 1 COOOC=O 1 CRCR 7 CRN5 1 CR
OR 2 C5A:C5B:C5B 2 C5A:C5BC=ON 1 C5A:C5BCB 1 C5A:N5:C5A 1 C5A:N5CR ...
```

```
FingerprintsVector;PathLengthCount:SLogPAtomTypes:MinLength1:MaxLength
8;518;NumericalValues;IDsAndValuesPairsString;C1 5 C10 1 C11 1 C14 1 C
18 14 C20 4 C21 2 C22 1 C5 2 CS 2 F 1 N11 1 N4 1 O10 1 O2 3 O9 1 C10C1
1 C10N11 1 C11C1 2 C11C21 1 C14:C18 2 C14F 1 C18:C18 10 C18:C20 4 C18
:C22 2 C1C5 1 C1CS 4 C20:C20 1 C20:C21 1 C20:N11 1 C20C20 2 C21:C21 1
C21:N11 1 C21C5 1 C22N4 1 C5=O10 1 C5=O9 1 C5N4 1 C5O2 1 CSO2 2 C10...
```

```
FingerprintsVector;PathLengthCount:SYBYLAtomTypes:MinLength1:MaxLength
8;412;NumericalValues;IDsAndValuesPairsString;C.2 2 C.3 9 C.ar 22 F 1
N.am 1 N.ar 1 O.2 1 O.3 2 O.co2 2 C.2=O.2 1 C.2=O.co2 1 C.2C.3 1 C.2C.
ar 1 C.2N.am 1 C.2O.co2 1 C.3C.3 7 C.3C.ar 1 C.3N.ar 1 C.3O.3 2 C.ar:C
.ar 21 C.ar:N.ar 2 C.arC.ar 2 C.arF 1 C.arN.am 1 C.2C.3C.3 1 C.2C.ar:C
.ar 2 C.2N.amC.ar 1 C.3C.2=O.co2 1 C.3C.2O.co2 1 C.3C.3C.3 5 C.3C.3...
```

```
FingerprintsVector;PathLengthCount:TPSAAAtomTypes:MinLength1:MaxLength8
;331;NumericalValues;IDsAndValuesPairsString;N21 1 N7 1 None 34 O3 2 O
4 3 N21:None 2 N21None 1 N7None 2 None:None 21 None=O3 2 NoneNone 13 N
oneO4 3 N21:None:None 2 N21:NoneNone 2 N21NoneNone 1 N7None:None 2 N7N
one=O3 1 N7NoneNone 1 None:N21:None 1 None:N21None 2 None:None:None 20
None:NoneNone 12 NoneN7None 1 NoneNone=O3 2 NoneNoneNone 8 NoneNon...
```

```
FingerprintsVector;PathLengthCount:UFFAtomTypes:MinLength1:MaxLength8;
410;NumericalValues;IDsAndValuesPairsString;C_2 2 C_3 9 C_R 22 F_ 1 N_
3 1 N_R 1 O_2 2 O_3 3 C_2=O_2 2 C_2C_3 1 C_2C_R 1 C_2N_3 1 C_2O_3 1 C_
3C_3 7 C_3C_R 1 C_3N_R 1 C_3O_3 2 C_R:C_R 21 C_R:N_R 2 C_RC_R 2 C_RF_
1 C_RN_3 1 C_2C_3C_3 1 C_2C_R:C_R 2 C_2N_3C_R 1 C_3C_2=O_2 1 C_3C_2O_3
1 C_3C_3C_3 5 C_3C_3C_R 2 C_3C_3N_R 1 C_3C_3O_3 4 C_3C_R:C_R 1 C_3...
```

METHODS

new

```
$NewPathLengthFingerprints = new PathLengthFingerprints(
                                %NamesAndValues);
```

Using specified *PathLengthFingerprints* 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 = ''
Size = 1024
MinSize = 32
MaxSize = 2**32
NumOfBitsToSetPerPath = 1
MinLength = 1
MaxLength = 8
AllowSharedBonds = 1
AllowRings = 1
UseBondSymbols = 1
UseUniquePaths = ''
AtomIdentifierType = ''
SetAtomicInvariantsToUse = ['AS']
FunctionalClassesToUse = ['HBD', 'HBA', 'PI', 'NI', 'Ar', 'Hal']
```

Examples:

```
$PathLengthFingerprints = new PathLengthFingerprints(
                                'Molecule' => $Molecule,
```

```
'Type' => 'PathLengthBits',
'AtomIdentifierType' =
    'AtomicInvariantsAtomTypes');

$PathLengthFingerprints = new PathLengthFingerprints(
    'Molecule' => $Molecule,
    'Type' => 'PathLengthBits',
    'Size' => 1024,
    'MinLength' => 1,
    'MaxLength' => 8,
    'AllowRings' => 1,
    'AllowSharedBonds' => 1,
    'UseBondSymbols' => 1,
    'UseUniquePaths' => 1,
    'AtomIdentifierType' =
        'AtomicInvariantsAtomTypes',
    'AtomicInvariantsToUse' => ['AS']);

$PathLengthFingerprints = new PathLengthFingerprints(
    'Molecule' => $Molecule,
    'Type' => 'PathLengthCount',
    'MinLength' => 1,
    'MaxLength' => 8,
    'AllowRings' => 1,
    'AllowSharedBonds' => 1,
    'UseBondSymbols' => 1,
    'UseUniquePaths' => 1,
    'AtomIdentifierType' =>
        'AtomicInvariantsAtomTypes',
    'AtomicInvariantsToUse' => ['AS']);

$PathLengthFingerprints = new PathLengthFingerprints(
    'Molecule' => $Molecule,
    'Type' => 'PathLengthBits',
    'AtomIdentifierType' =
        'SLogPAtomTypes');

$PathLengthFingerprints = new PathLengthFingerprints(
    'Molecule' => $Molecule,
    'Type' => 'PathLengthCount',
    'AtomIdentifierType' =
        'SYBYLAtomTypes');

$PathLengthFingerprints = new PathLengthFingerprints(
    'Molecule' => $Molecule,
    'Type' => 'PathLengthBits',
    'AtomIdentifierType' =
        'FunctionalClassAtomTypes',
    'FunctionalClassesToUse' => ['HBD', 'HBA', 'Ar']);

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

GetDescription

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

Returns a string containing description of path length fingerprints.

GenerateFingerprints

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

Generates path length fingerprints and returns *PathLengthFingerprints*.

SetMaxLength

```
$PathLengthFingerprints->SetMaxLength($Length);
```

Sets maximum value of atom path length to be used during atom path length fingerprints generation

and returns *PathLengthFingerprints*

SetAtomIdentifierType

```
$PathLengthFingerprints->SetAtomIdentifierType();
```

Sets atom *IdentifierType* to use during path length fingerprints generation and returns *PathLengthFingerprints*.

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

SetAtomicInvariantsToUse

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

Sets atomic invariants to use during *AtomicInvariantsAtomTypes* value of *AtomIdentifierType* for path length fingerprints generation and returns *PathLengthFingerprints*.

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

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

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

Sets functional classes invariants to use during *FunctionalClassAtomTypes* value of *AtomIdentifierType* for path length fingerprints generation and returns *PathLengthFingerprints*.

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
```

SetMinLength

```
$PathLengthFingerprints->SetMinLength($Length);
```

Sets minimum value of atom path length to be used during atom path length fingerprints generation and returns *PathLengthFingerprints*.

SetMaxLength

```
$PathLengthFingerprints->SetMaxLength($Length);
```

Sets maximum value of atom path length to be used during atom path length fingerprints generation and returns *PathLengthFingerprints*.

SetNumOfBitsToSetPerPath

```
$PathLengthFingerprints->SetNumOfBitsToSetPerPath($NumOfBits);
```

Sets number of bits to set for each path during *PathLengthBits* Type during path length fingerprints generation and returns *PathLengthFingerprints*.

SetType

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

Sets type of path length fingerprints and returns *PathLengthFingerprints*. Possible values: *PathLengthBits* or *PathLengthCount*.

StringifyPathLengthFingerprints

```
$String = $PathLengthFingerprints->StringifyPathLengthFingerprints();
```

Returns a string containing information about *PathLengthFingerprints* object.

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SEE ALSO

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

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