
NAME

TorsionAlertsUtil

SYNOPSIS

import TorsionAlertsUtil

DESCRIPTION

TorsionAlertsUtil module provides the following functions:

CalculateTorsionAngleDifference, DoesSMARTSContainValidSubClassMappedAtoms, DoesSMARTSContainValidTorsionRuleMappedAtoms, DoesSMARTSContainsMappedAtoms, FilterSubstructureMatchesByAtomMapNumbers, GetAtomPositions, GetGenericHierarchyClassElementNode, GetHeavyAtomNeighbors, IdentifyRotatableBondsForTorsionLibraryMatch, IsSpecificHierarchyClass, ListTorsionLibraryInfo, RemoveLastHierarchyClassElementNodeFromTracking, RemoveLastHierarchySubClassElementNodeFromTracking, RetrieveTorsionLibraryInfo, SetupHierarchyClassAndSubClassNamesForRotatableBond, SetupHierarchySubClassElementPatternMol, SetupTorsionLibraryInfoForMatchingRotatableBonds, SetupTorsionRuleAnglesInfo, SetupTorsionRuleElementPatternMol, TrackHierarchyClassElementNode, TrackHierarchySubClassElementNode

FUNCTIONS**CalculateTorsionAngleDifference**

```
CalculateTorsionAngleDifference(TorsionAngle1, TorsionAngle2)
```

Calculate torsion angle difference in the range from 0 to 180.

Arguments:

```
TorsionAngle1 (float): First torsion angle.  
TorsionAngle2 (float): Second torsion angle.
```

Returns:

```
float: Difference between first and second torsion angle.
```

DoesSMARTSContainValidSubClassMappedAtoms

```
DoesSMARTSContainValidSubClassMappedAtoms(SMARTS)
```

Check for the presence of two central mapped atoms in SMARTS pattern. A valid SMARTS pattern must contain only two mapped atoms corresponding to map atom numbers ':2' and ':3'.

Arguments:

```
SMARTS (str): SMARTS pattern for sub class in torsion library XML tree.
```

Returns:

```
bool: True - A valid pattern; Otherwise, false.
```

DoesSMARTSContainValidTorsionRuleMappedAtoms

```
DoesSMARTSContainValidTorsionRuleMappedAtoms(SMARTS)
```

Check for the presence of four mapped atoms in a SMARTS pattern. A valid SMARTS pattern must contain only four mapped atoms corresponding to map atom numbers ':1', ':2', ':3' and ':4'.

Arguments:

```
SMARTS (str): SMARTS pattern for torsion rule in torsion library XML  
tree.
```

Returns:

```
bool: True - A valid pattern; Otherwise, false.
```

DoesSMARTSContainsMappedAtoms

```
DoesSMARTSContainsMappedAtoms(SMARTS, MappedAtomNumsList)
```

Check for the presence of specified mapped atoms in SMARTS pattern. The mapped atom numbers in the list are specified as ':1', ':2', ':3' etc.

Arguments:

SMARTS (str): SMARTS pattern in torsion library XML tree.
MappedAtoms (list): Mapped atom numbers as ":1", ":2" etc.

Returns:

bool: True - All mapped atoms present in pattern; Otherwise, false.

FilterSubstructureMatchesByAtomMapNumbers

FilterSubstructureMatchesByAtomMapNumbers(Mol, PatternMol, AtomIndicesList)

Filter a list of lists containing matched atom indices by map atom numbers present in a pattern molecule. The list of atom indices correspond to a list retrieved by RDKit function GetSubstructureMatches using SMILES/SMARTS pattern. The atom map numbers are mapped to appropriate atom indices during the generation of molecules. For example:
[O:1]=[S:2](=[O])[C:3][C:4].

Arguments:

Mol (object): RDKit molecule object.
PatternMol (object): RDKit molecule object for a SMILES/SMARTS pattern.
AtomIndicesList (list): A list of lists containing atom indices.

Returns:

list : A list of lists containing filtered atom indices.

GetAtomPositions

GetAtomPositions(Mol, ConfID = -1)

Retrieve a list of lists containing coordinates of all atoms in a molecule.

Arguments:

Mol (object): RDKit molecule object.
ConfID (int): Conformer number.

Returns:

list : List of lists containing atom positions.

Example(s):

```
for AtomPosition in TorsionAlertsUtil.GetAtomPositions(Mol):  
    print("X: %s; Y: %s; Z: %s" % (AtomPosition[0], AtomPosition[1],  
    AtomPosition[2]))
```

GetGenericHierarchyClassElementNode

GetGenericHierarchyClassElementNode(TorsionLibraryInfo)

Get generic hierarchy class element node.

Arguments:

TorsionLibraryInfo (dict): A dictionary containing information for matching rotatable bonds.

Returns:

object: Generic hierarchy class element node in torsion library XML tree.

GetHeavyAtomNeighbors

GetHeavyAtomNeighbors(Atom)

Get a list of heavy atom neighbors.

Arguments:

Atom (object): RDKit atom object.

Returns:

list : List of heavy atom neighbors.

IdentifyRotatableBondsForTorsionLibraryMatch

```
IdentifyRotatableBondsForTorsionLibraryMatch(TorsionLibraryInfo, Mol,
RotBondsPatternMol)
```

Identify rotatable bonds in a molecule for torsion library match.

Arguments:

TorsionLibraryInfo (dict): A dictionary containing information for matching rotatable bonds.
 Mol (object): RDKit molecule object.
 RotBondsPatternMol (object): RDKit molecule object for SMARTS pattern corresponding to rotatable bonds.

Returns:

bool: True - Rotatable bonds present in molecule; Otherwise, false.
 None or dict: None - For no rotatable bonds in molecule; otherwise, a dictionary containing the following informations for rotatable bonds matched to RotBondsPatternMol:

```
RotBondsInfo["IDs"] = []
RotBondsInfo["AtomIndices"] = {}
RotBondsInfo["HierarchyClass"] = {}
```

IsSpecificHierarchyClass

```
IsSpecificHierarchyClass(TorsionLibraryInfo, HierarchyClass)
```

Check whether it's a specific hierarchy class.

Arguments:

TorsionLibraryInfo (dict): A dictionary containing information for matching rotatable bonds.
 HierarchyClass (str): Hierarchy class name.

Returns:

bool: True - A valid hierarchy class name; Otherwise, false.

ListTorsionLibraryInfo

```
ListTorsionLibraryInfo(TorsionLibElementTree)
```

List torsion library information using XML tree object. The following information is listed:

Summary:

```
Total number of HierarchyClass nodes: <Number>
Total number of HierarchyClassSubClass nodes: <Number>
Total number of TorsionRule nodes: <Number>
```

Details:

```
HierarchyClass: <Name>; HierarchySubClass nodes: <Number>;
TorsionRule nodes: <SMARTS>
... ..
```

Arguments:

TorsionLibElementTree (object): XML tree object.

Returns:

Nothing.

RemoveLastHierarchyClassElementNodeFromTracking

```
RemoveLastHierarchyClassElementNodeFromTracking(TorsionLibraryInfo)
```

Remove last hierarchy class element node from tracking by removing it from a stack.

Arguments:

`TorsionLibraryInfo (dict)`: A dictionary containing information for matching rotatable bonds.

Returns:

Nothing. The torsion library info is updated.

RemoveLastHierarchySubClassElementNodeFromTracking

`RemoveLastHierarchySubClassElementNodeFromTracking(TorsionLibraryInfo)`

Remove last hierarchy sub class element node from tracking by removing it from a stack.

Arguments:

`TorsionLibraryInfo (dict)`: A dictionary containing information for matching rotatable bonds.

Returns:

Nothing. The torsion library info is updated.

RetrieveTorsionLibraryInfo

`RetrieveTorsionLibraryInfo(TorsionLibraryFilePath, Quiet = True)`

Retrieve torsion library information.

Arguments:

`TorsionLibraryFilePath (str)`: Torsion library XML file path.

Returns:

object: An object returned by `xml.etree.ElementTree.parse` function.

The XML file is parsed using `xml.etree.ElementTree.parse` function and object created by the parse function is simply returned.

SetupHierarchyClassAndSubClassNamesForRotatableBond

`SetupHierarchyClassAndSubClassNamesForRotatableBond(TorsionLibraryInfo)`

Setup hierarchy class and subclass names for a rotatable bond matched to a torsion rule element node.

Returns:

`TorsionLibraryInfo (dict)`: A dictionary containing information for matching rotatable bonds.

`str`: A back slash delimited string containing hierarchy class names at the level of torsion rule element node.

`str`: A back slash delimited string containing hierarchy sub class names at the level of torsion rule element node.

SetupHierarchySubClassElementPatternMol

`SetupHierarchySubClassElementPatternMol(TorsionLibraryInfo, ElementNode)`

Setup pattern molecule for SMARTS pattern in hierarchy subclass element.

Arguments:

`TorsionLibraryInfo (dict)`: A dictionary containing information for matching rotatable bonds.

`ElementNode (object)`: A hierarchy sub class element node being matched in torsion library XML tree.

Returns:

object: RDKit molecule object corresponding to SMARTS pattern for hierarchy sub class element node.

SetupTorsionLibraryInfoForMatchingRotatableBonds

`SetupTorsionLibraryInfoForMatchingRotatableBonds(TorsionLibraryInfo)`

Setup torsion library information for matching rotatable bonds. The following information is initialized and updated in torsion library dictionary for matching rotatable bonds:

```
TorsionLibraryInfo["GenericClass"] = None
TorsionLibraryInfo["GenericClassElementNode"] = None

TorsionLibraryInfo["SpecificClasses"] = {}
TorsionLibraryInfo["SpecificClasses"]["Names"] = []
TorsionLibraryInfo["SpecificClasses"]["ElementNode"] = {}

TorsionLibraryInfo["HierarchyClassNodes"] = []
TorsionLibraryInfo["HierarchySubClassNodes"] = []

TorsionLibraryInfo["DataCache"] = {}
TorsionLibraryInfo["DataCache"]["SubClassPatternMol"] = {}

TorsionLibraryInfo["DataCache"]["TorsionRulePatternMol"] = {}
TorsionLibraryInfo["DataCache"]["TorsionRuleAnglesInfo"] = {}
```

Arguments:

TorsionLibraryInfo (dict): A dictionary containing root node for torsion library element tree.

Returns:

Nothing. The torsion library information dictionary is updated.

SetupTorsionRuleAnglesInfo

```
SetupTorsionRuleAnglesInfo(TorsionLibraryInfo, TorsionRuleElementNode)
```

Setup torsion angles and energy info for matching a torsion rule.

Arguments:

TorsionLibraryInfo (dict): A dictionary containing information for matching rotatable bonds.

TorsionRuleElementNode (object): A torsion rule element node being matched in torsion library XML tree.

Returns:

dict: A dictionary containing the following information for torsion rule being matched to a rotatable bond:

```
RuleAnglesInfo = {}

RuleAnglesInfo["IDs"] = []
RuleAnglesInfo["Value"] = {}
RuleAnglesInfo["Score"] = {}
RuleAnglesInfo["Tolerance1"] = {}
RuleAnglesInfo["Tolerance2"] = {}

RuleAnglesInfo["ValuesList"] = []
RuleAnglesInfo["ValuesIn360RangeList"] = []
RuleAnglesInfo["Tolerances1List"] = []
RuleAnglesInfo["Tolerances2List"] = []

# Strain energy calculations...
RuleAnglesInfo["EnergyMethod"] = None
RuleAnglesInfo["EnergyMethodExact"] = None
RuleAnglesInfo["EnergyMethodApproximate"] = None

# For approximate strain energy calculation...
RuleAnglesInfo["Beta1"] = {}
RuleAnglesInfo["Beta2"] = {}
RuleAnglesInfo["Theta0"] = {}

# For exact strain energy calculation...
RuleAnglesInfo["HistogramEnergy"] = []
RuleAnglesInfo["HistogramEnergyLowerBound"] = []
```

```
RuleAnglesInfo["HistogramEnergyUpperBound"] = []
```

SetupTorsionRuleElementPatternMol

```
SetupTorsionRuleElementPatternMol(TorsionLibraryInfo, ElementNode,  
TorsionRuleNodeID, TorsionSMARTSPattern)
```

Setup pattern molecule for SMARTS pattern in torsion rule element.

Arguments:

TorsionLibraryInfo (dict): A dictionary containing information for matching rotatable bonds.
ElementNode (object): A torsion rule element node being matched in torsion library XML tree.
TorsionRuleNodeID (int): Torsion rule element node ID.
TorsionSMARTSPattern (str): SMARTS pattern for torsion rule element node.

Returns:

object: RDKit molecule object corresponding to SMARTS pattern for torsion rule element node.

TrackHierarchyClassElementNode

```
TrackHierarchyClassElementNode(TorsionLibraryInfo, ElementNode)
```

Track hierarchy class element node using a stack.

Arguments:

TorsionLibraryInfo (dict): A dictionary containing information for matching rotatable bonds.
ElementNode (object): Hierarchy class element node in torsion library XML tree.

Returns:

Nothing. The torsion library info is updated.

TrackHierarchySubClassElementNode

```
TrackHierarchySubClassElementNode(TorsionLibraryInfo, ElementNode)
```

Track hierarchy sub class element node using a stack.

Arguments:

TorsionLibraryInfo (dict): A dictionary containing information for matching rotatable bonds.
ElementNode (object): Hierarchy sub class element node in torsion library XML tree.

Returns:

Nothing. The torsion library info is updated.

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