NAME

MolecularFormula

SYNOPSIS

use MolecularFormula;

use MolecularFormula qw(:all);

DESCRIPTION

MolecularFormula module provides the following functions:

CalculateElementalComposition, CalculateExactMass, CalculateMolecularWeight, FormatCompositionInfomation, GetElementsAndCount, IsMolecularFormula

FUNCTIONS

CalculateMolecularWeight

```
$MolecularWeight = CalculateMolecularWeight($MolecularFormula);
```

Calculates and returns the molecular weight for a specified *MolecularFormula*.

CalculateElementalComposition

```
($ElementsRef, $ElementCompositionRef) =
   CalculateElementalComposition($MolecularFormula);
```

Calculates the percent composition in a specified *MolecularFormula* and returns references to arrays containing elements and their percent composition.

CalculateExactMass

```
$ExactMass = CalculateMolecularWeight($MolecularFormula);
```

Calculates and returns the exact mass for a specified *MolecularFormula*.

FormatCompositionInfomation

```
$FormattedString = FormatCompositionInfomation($ElementsRef,
                   $ElementCompositionRef, [$Precision]);
```

Returns a formatted elemental composition string using references to elements and elemental composition arrays. Precision is an optional parameter; its default value is *2*.

GetElementsAndCount

```
($ElementsRef, $ElementCountRef) = GetElementsAndCount(
                                   $MolecularFormula);
```

Retrieves elements and their count composition in a specified *MolecularFormula* and returns references to arrays containing elements and their count.

IsMolecularFormula

```
$Status = IsMolecularFormula($MolecularFormula);
($Status, $ErrorMsg) = IsMolecularFormula($MolecularFormula);
```

Returns 1 or 0 a based on whether it's a valid *MolecularFormula*.

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SEE ALSO

Molecule.pm

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