

NAME

MolecularFormula

SYNOPSIS

```
use MolecularFormula;

use MolecularFormula qw(:all);
```

DESCRIPTION

MolecularFormula module provides the following functions:

CalculateElementalComposition, CalculateExactMass, CalculateMolecularWeight, FormatCompositionInformation, 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*.

FormatCompositionInformation

```
$FormattedString = FormatCompositionInformation($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 based on whether it's a valid *MolecularFormula*.

AUTHOR

Manish Sud <msud@san.rr.com>

SEE ALSO

Molecule.pm

COPYRIGHT

Copyright (C) 2004-2012 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.