

## 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

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## SEE ALSO

Molecule.pm

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