NAME

> WeightAndMassDescriptors

SYNOPSIS

> use MolecularDescriptors::WeightAndMassDescriptors;
>
> use MolecularDescriptors::WeightAndMassDescriptors qw(:all);

DESCRIPTION

> WeightAndMassDescriptors class provides the following methods:
>
> new, GenerateDescriptors, GetDescriptorNames, StringifyWeightAndMassDescriptors
>
> WeightAndMassDescriptors is derived from MolecularDescriptors class which in turn is derived from ObjectProperty base class that provides methods not explicitly defined in WeightAndMassDescriptors, MolecularDescriptors 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>();
```

> WeightAndMassDescriptors calculates molecular weight and exact mass descriptors using methods available in Molecule class.

METHODS

> new

```
$NewWeightAndMassDescriptors = new MolecularDescriptors::
                               WeightAndMassDescriptors(
                               %NamesAndValues);
```

> > Using specified *WeightAndMassDescriptors* property names and values hash, new method creates a new object and returns a reference to newly created WeightAndMassDescriptors object. By default, the following properties are initialized:

```
Molecule = ''
Type = 'WeightAndMass'
WeightPrecision = 2;
MassPrecision = 4;

@DescriptorNames = ('MolecularWeight', 'ExactMass')
@DescriptorValues = ('None', 'None')
```

> > Examples:

```
$WeightAndMassDescriptors = new MolecularDescriptors::
                               WeightAndMassDescriptors(
                               'Molecule' => $Molecule);

$WeightAndMassDescriptors = new MolecularDescriptors::
                               WeightAndMassDescriptors();

$WeightAndMassDescriptors->SetMolecule($Molecule);
$WeightAndMassDescriptors->GenerateDescriptors();
print "WeightAndMassDescriptors: $WeightAndMassDescriptors\n";
```

> GenerateDescriptors

```
$WeightAndMassDescriptors->GenerateDescriptors();
```

> > Calculates molecular weight and exact mass of a molecule and returns *WeightAndMassDescriptors*.

> GetDescriptorNames

```
@DescriptorNames = $WeightAndMassDescriptors->GetDescriptorNames();
@DescriptorNames = MolecularDescriptors::WeightAndMassDescriptors::
                   GetDescriptorNames();
```

> > Returns all available descriptor names as an array.

> SetMassPrecision

```
$WeightAndMassDescriptors->SetMassPrecision($Precision);
```

> > Sets precision for calculated exact mass value and returns *WeightAndMassDescriptors*.

> SetWeightPrecision

```
$WeightAndMassDescriptors->SetWeightPrecision($Precision);
```

Sets precision for calculated molecular weight value and returns *WeightAndMassDescriptors*.

StringifyWeightAndMassDescriptors

```
$String = $WeightAndMassDescriptors->StringifyWeightAndMassDescriptors();
```

Returns a string containing information about *WeightAndMassDescriptors* object.

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SEE ALSO

MolecularDescriptors.pm, MolecularDescriptorsGenerator.pm

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