

## NAME

ElementalAnalysis.pl - Perform elemental analysis using specified formulas

## SYNOPSIS

ElementalAnalysis.pl Formula(s)...

```
ElementalAnalysis.pl [-h, --help] [-m, --mode All | "ElementalAnalysis, [MolecularWeight, ExactMass]"] [--outdelim comma | tab
| semicolon] [--output STDOUT | File] [--outputstyle FormulaBlock | FormulaRows] [-o, --overwrite] [--precision number] [-q,
--quote yes | no] [-r, --root rootname] [-v --valueLabels [Name, Label, [Name, Label,...]]] [-w, --workingdir dirname]
Formula(s)...
```

## DESCRIPTION

Perform elemental analysis using molecular formula(s) specified on the command line.

In addition to straightforward molecular formulas - H<sub>2</sub>O, HCl, C<sub>3</sub>H<sub>7</sub>O<sub>2</sub>N - other supported variations are: Ca<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub>, [PCl<sub>4</sub>]<sup>+</sup>, [Fe(CN)<sub>6</sub>]<sup>4-</sup>, C<sub>37</sub>H<sub>42</sub>N<sub>2</sub>O<sub>6</sub>+<sub>2</sub>, Na<sub>2</sub>CO<sub>3</sub>·10H<sub>2</sub>O, 8H<sub>2</sub>S·46H<sub>2</sub>O, and so on. Charges are simply ignored. Isotope symbols in formulas specification, including D and T, are not supported.

## PARAMETERS

Formulas *Formula1 [Formula2...]*

*Formulas* is a space delimited list of molecular formulas to use for elemental analysis.

Input value format is: *Formula1 [Formula2 Formula3...]*. Default: *H<sub>2</sub>O*. Examples:

```
HCl
HCl, C3H7O2N
H2O2 Ca3(PO4)2 [PCl4]+
```

## OPTIONS

-h, --help

Print this help message.

--fast

In this mode, the specified formulas are considered valid and initial formula validation check is skipped.

-m, --mode *All | "ElementalAnalysis,[MolecularWeight,ExactMass]"*

Specify what values to calculate using molecular formulas specified on command line: calculate all supported values or specify a comma delimited list of values. Possible values: *All | "ElementalAnalysis, [MolecularWeight, ExactMass]"*. Default: *All*.

--outdelim *comma | tab | semicolon*

Output text file delimiter. Possible values: *comma, tab, or semicolon* Default value: *comma*.

--output *STDOUT | File*

List information at STDOUT or write it to a file. Possible values: *STDOUT or File*. Default: *STDOUT*. -r, --root option is used to generate output file name.

--outputstyle *FormulaBlock | FormulaRows*

Specify how to list calculated values: add a new line for each property and present it as a block for each formula; or include all properties in one line and show it as a single line.

Possible values: *FormulaBlock | FormulaRows*. Default: *FormulaBlock*

An example for *FormulaBlock* output style:

```
Formula: H2O
ElementalAnalysis: H: H: 11.1898%; O: 88.8102%
MolecularWeight: 18.0153
ExactMass: 18.0106
... ..
... ..
... ..

Formula: H2O2
ElementalAnalysis: H: 5.9265%; O: 94.0735%
MolecularWeight: 34.0147
ExactMass: 34.0055
... ..
... ..
... ..
```

An example for *FormulaRows* output style:

```
Formula,ElementalAnalysis,MolecularWeight,ExactMass
```

```
H2O,H: 11.1898%; O: 88.8102%,18.0153,18.0106
H2O2,H: 5.9265%; O: 94.0735%,34.0147,34.0055
```

`-o, --overwrite`

Overwrite existing files.

`--precision number`

Precision for listing numerical values. Default: up to 4 decimal places. Valid values: positive integers.

`-r, --root rootname`

New text file name is generated using the root: `<Root>.<Ext>`. File name is only used during *File* value of `-o, --output` option.

Default file name: `FormulsElementalAnalysis.<Ext>`. The `csv`, and `tsv` `<Ext>` values are used for comma/semicolon, and tab delimited text files respectively.

`-v --valuelabels Name,Label,[Name,Label,...]`

Specify labels to use for calculated values. In general, it's a comma delimited list of value name and column label pairs.

Supported value names: *ElementalAnalysis*, *MolecularWeight*, and *ExactMass*. Default labels: *ElementalAnalysis*, *MolecularWeight*, and *ExactMass*.

`-w, --workingdir dirname`

Location of working directory. Default: current directory.

## EXAMPLES

To perform elemental analysis, calculate molecular weight and exact mass for H2O, type:

```
% ElementalAnalysis.pl
```

To perform elemental analysis, calculate molecular weight and exact mass for Ca3(PO4)2 and [PCl4]+, type:

```
% ElementalAnalysis.pl "Ca3(PO4)2" "[PCl4]+"
```

To perform elemental analysis, use label analysis for calculated data, and generate a new CSV file ElementalAnalysis.csv for H2O and H2O2, type:

```
% ElementalAnalysis.pl --m ElementalAnalysis --output File
--valuelabels "ElementalAnalysis,Analysis" -o -r ElementalAnalysis.csv
H2O H2O2
```

To calculate molecular weight and exact mass with four decimal precision and generate a new CSV file WeightAndMass.csv with data rows for H2O and H2O2, type:

```
% ElementalAnalysis.pl --m "MolecularWeight,ExactMass" --output File
--outputstyle FormulaRows -o -r WeightAndMass.csv
H2O H2O2
```

## AUTHOR

Manish Sud <msud@san.rr.com>

## SEE ALSO

ElementalAnalysisSDFFiles.pl, ElementalAnalysisTextFiles.pl

## 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.