

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 - H₂O, HCl, C₃H₇O₂N - other supported variations are: Ca₃(PO₄)₂, [PCl₄]⁺, [Fe(CN)₆]⁴⁻, C₃₇H₄₂N₂O₆+₂, Na₂CO₃.10H₂O, 8H₂S.46H₂O, 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: *H2O*. 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
```

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SEE ALSO

ElementalAnalysisSDFFiles.pl, ElementalAnalysisTextFiles.pl

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