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

ElementalAnalysisSDFiles.pl, ElementalAnalysisTextFiles.pl

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