
NAME

ElementalAnalysisSDFiles.pl - Perform elemental analysis using formula data field in SDFFile(s)

SYNOPSIS

ElementalAnalysisSDFiles.pl SDFFile(s)...

ElementalAnalysisSDFiles.pl [-d, --detail infolevel] [--fast] [-f, --formulafield SD data field name] [-m, --mode All | "ElementalAnalysis, [MolecularWeight, ExactMass]"] [-h, --help] [-o, --overwrite] [-r, --root rootname] [-v --valuefieldnames Name, Label, [Name, Label,...]] [-w, --workingdir dirname] SDFFile(s)...

DESCRIPTION

Perform elemental analysis using molecular formula specified by a data field name in *SDFFile(s)*.

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.

The file names are separated by space. The valid file extensions are *.sdf* and *.sd*. All other file names are ignored. All the SD files in a current directory can be specified either by **.sdf* or the current directory name.

OPTIONS

-d, --detail *infolevel*

Level of information to print about compound records being ignored. Default: 1. Possible values: 1, 2 or 3

--fast

In this mode, the formula data field specified using -f, --formulafield option is assumed to contain valid molecular formula data and initial formula validation check is skipped.

-f, --formulafield *SD data field name*

SDFFile(s) data field name containing molecular formulas used for performing elemental analysis. Default value: *SD data field containing the word formula in its name*.

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

Specify what values to calculate using molecular formula data field in *TextFile(s)*: calculate all supported values or specify a comma delimited list of values. Possible values: *All | "ElementalAnalysis, [MolecularWeight, ExactMass]"*. Default: *All*

-h, --help

Print this help message

-o, --overwrite

Overwrite existing files

-p, --precision *number*

Precision of calculated values in the output file. Default: up to 2 decimal places. Valid values: positive integers.

-r, --root *rootname*

New SD file name is generated using the root: <Root>.<Ext>. Default new file name: <InitialSDFFileName>ElementalAnalysis.<Ext>. This option is ignored for multiple input files.

-v --valuefieldnames *Name,Label,[Name,Label,...]*

Specify SD data field names to use for calculated values. In general, it's a comma delimited list of value name and SD field name 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 using SD field name value with the word Formula in its name and generate a new SD file NewSample1.sdf, type:

```
% ElementalAnalysisSDFiles.pl -o -r NewSample1 Sample1.sdf
```

To perform elemental analysis using formulas in SD field name Formula, use field name Analysis for calculated data, and generate a new SD file NewSample1.sdf, type:

```
% ElementalAnalysisSDFFiles.pl --m ElementalAnalysis --formulafield  
Formula --valuefieldnames "ElementalAnalysis,Analysis" -o  
-r NewSample1 Sample1.sdf
```

To calculate molecular weight, using formulas in SD field name Formula, with four decimal precision and generate a new SD file NewSample1.sdf, type

```
% ElementalAnalysisSDFFiles.pl --m MolecularWeight --formulafield  
Formula --precision 4 -o -r NewSample1 Sample1.sdf
```

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SEE ALSO

AnalyzeSDFFilesData.pl, InfoSDFFiles.pl, ExtractFromSDFFiles.pl

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