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**NAME**

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

**SYNOPSIS**

ElementalAnalysisSDFFiles.pl SDFFile(s)...

ElementalAnalysisSDFFiles.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 - 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>3</sub>H<sub>4</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.

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

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## 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:

```
% ElementalAnalysisSDFfiles.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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