NAME

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

SYNOPSIS

ElementalAnalysisSDFiles.pl SDFile(s)...

ElementalAnalysisSDFiles.pl [-d, --detail infolevel] [--fast] [--formulafield SD data field name] [-f, --formulamode *DataField* | *StructureData*] [--formulaout yes or no] [-m, --mode All | "ElementalAnalysis, [MolecularWeight, ExactMass]"] [-h, --help] [-o, --overwrite] [-r, --root rootname] [-v --valuefieldnames Name, Label, [Name, Label,...]] [-w, --workingdir dirname] SDFile(s)...

DESCRIPTION

Perform elemental analysis using molecular formula specified by a data field name or generated from structure data in *SDFile(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.

--formulafield *SD data field name*

SDFile(s) data field name containing molecular formulas used for performing elemental analysis during *DataField* value of -f, --formulamode option. Default value: *SD data field containing the word formula in its name*.

This option is ignore during *StructureData* value of -f, --formulamode option.

-f, --formulamode *DataField* | *StructureData*

Specify source of molecular formula used for performing elemental analysis: retrieve formula using *SDFile(s)* data field name or generate formula from structure. Possible values: *DataField or StructureData*. Default value: *DataField*.

--formulaout *yes or no*

Specify whether to write out formula to SD file during *StructureData* value of -f, --formulamode option. Possible values: *Yes or No*. Default: *No*.

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

Specify what values to calculate using molecular formula data field or structure data from *SDFile(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: <InitialSDFileName>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, ExactMass, and MolecularFormula*. Default labels: *ElementalAnalysis, MolecularWeight, ExactMass, and MolecularFormula*.

MolecularFormula label is only used during *StructureData* value of -f, --formulamode option.

-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, calculate molecular weight and exact mass using structure data in SD file and generate a new SD file NewSample1.sdf, type:

```
% ElementalAnalysisSDFiles.pl --formulamode StructureData -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:

```
% ElementalAnalysisSDFiles.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

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

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SEE ALSO

AnalyzeSDFilesData.pl, InfoSDFiles.pl, ExtractFromSDFiles.pl

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