NAME

SDToMolFiles.pl - Generate MDLMOL file(s) from SD file(s)

SYNOPSIS

SDToMolFiles.pl SDFile(s)...

SDToMolFiles.pl [-d, --DataField DataFieldName] [-m, --mode DataField | MolName | RootPrefix] [-h, --help] [-o, --overwrite] [-r, --root rootname] [-w, --workingdir dirname] SDFile(s)...

DESCRIPTION

Generate MDLMOL file(s) from *SDFile(s)*. All header data labels and values in SDFile(s) are simply ignored; other appopriate data from SDFile(s) is transferred to MDLMOL files. Multiple *SDFile(s)* names are separated by spaces. 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, --DataField *DataFieldName*

Specify *SDFile(s)* datafield label name whose value is used for generation of MDLMOL file names. Default value: *None*.

-h, --help

Print this help message.

-m, --mode *DataField | MolName | RootPrefix*

Specify how to generate MDLMOL file names: use a *SDFile(s)* datafield value; use molname line from *SDFile(s)*; generate a sequential ID using root prefix specified by -r, --root option.

Possible values: *DataField | MolName | RootPrefix | RootPrefix*. Default: *RootPrefix*.

For empty *MolName* and *DataField* values during these specified modes, file name is automatically generated using *RootPrefix*.

For *RootPrefix* value of -m, --mode option, MDLMOL file names are generated using by appending compound record number to value of -r, --root option. For example: *RootName*Cmd<RecordNumber>.mol.

Allowed characters in file names are: a-zA-Z0-9_. All other characters in datafield values, molname line, and root prefix are ignore during generation of file names.

-o, --overwrite

Overwrite existing files.

-r, --root *rootname*

Specify root name to used during *RootPrefix* -m, --mode option value. New MDLMOL file names are generated using the root: <Root>Cmpd<RecordNumber>.mol Default for new file names: <InitialSDFileName>Cmpd<RecordNumber>.mol. This option is ignored for multiple input files.

-w, --workingdir *dirname*

Location of working directory. Default: current directory.

EXAMPLES

To generate MDLMOL files from Sample1*.sdf and Sample2*.sd files, type:

```
% SDToMolFiles.pl -o Sample1*.sdf Sample2*.sd
```

To generate Sample*.mol files from Sample1.sdf, type:

```
% SDToMolFiles.pl -r Sample -o Sample1.sdf
```

To generate MOL files from Sample1.sdf using molname line data for generating MOL file names, type:

```
% SDToMolFiles.pl -m MolName -r Sample -o Sample1.sdf
```

To generate MOL files from Sample1.sdf using a specific data field values for generating MOL file names, type:

```
% SDToMolFiles.pl -m DataField --DataField MolID -r Sample
  -o Sample1.sdf
```

AUTHOR

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SEE ALSO

InfoSDFiles.pl, MolFilesToSD.pl

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