NAME

MolFilesToSD.pl - Generate a SD file from MDLMOL File(s)

SYNOPSIS

MolFilesToSD.pl MDLMOLFile(s)…

MolFilesToSD.pl [-c, --compoundid usefileprefix | idlabel] [-d, --datafieldlabel fieldlabel] [-h, --help] [-m, --mode molnameline | datafield | both | none] [-o, --overwrite] [-r, --root rootname] [-w, --workingdir dirname] MDLMOLFile(s)…

DESCRIPTION

Generate a SD file from *MDLMOL File(s)*. Multiple file names are separated by spaces. The valid file extension is *.mol*. All other file names are ignored. All the files in a current directory can be specified by **.mol*, or the current directory name.

OPTIONS

-c, --compoundid *usefileprefix | idlabel*

Specify how to generate compound IDs: use MOL filename prefix or generate a new compound ID by combining *idlabel* with compound number. Possible values: *usefileprefix | idlabel*. By default, *Cmd* is used as a *idlabel* to generate these types of compound IDs: Cmpd1, Cmpd2 and so on.

Example: To generate compound IDs like Mol_ID1, Mol_ID2 and so on, specify "MolID" value for this option.

-d, --datafieldlabel *fieldlabel*

Specify data field label for adding compound ID field into SD file during *datafield | both* values of -m, --mode option. Default: <Cmpd_ID>.

-h, --help

Print this help message.

-m, --mode *molnameline | datafield | both | none*

Specify how to add compopund ID into SD file: relplace the molname line, add a new data field, replace the molname line and add data field, or do nothing. Possible values: *molnameline | datafield | both | none*. Default: *nothing*.

Use -c, --compoundid to specify compound ID generation process.

-o, --overwrite

Overwrite existing files.

-r, --root *rootname*

New SD file name is generated using the root: <Root>.sdf. Default new file name: <InitialMOLFileName>1To<Count>.sdf.

-w, --workingdir *dirname*

Location of working directory. Default: current directory.

EXAMPLES

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

```
% MolFilesToSD.pl  -r NewSample -o Sample*.mol
```

To generate NewSample.sdf with Cmpd1, Cmpd2 and so on as compound ID in MolName line and Cmpd_ID datafield from Sample*.mol files, type:

```
% MolFilesToSD.pl  -r NewSample -m both -o Sample*.mol
```

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SEE ALSO

InfoSDFiles.pl, SDToMolFiles.pl

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