
NAME

InfoSDFFiles.pl - List information about SDFFile(s)

SYNOPSIS

InfoSDFFile.pl SDFFile(s)...

InfoSDFFile.pl [-a --all] [-c --count] [--chiral] [--datacheck] [-d --detail *infolevel*] [-e --empty] [-f, --fields] [-h, --help] [-i, --invalidatomnumbers] [-m, --mismatch] [-s, --salts] [-u, --unknownatoms] [-w, --workingdir *dirname*] SDFFile(s)...

DESCRIPTION

List information about *SDFFile(s)* contents: number of compounds, empty records and so on. Multiple SDFFile 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

-a, --all

List all the available information.

-c, --count

List number of compounds. This is default behavior.

--chiral

List number of empty atom/bond blocks for compounds with chiral flag set in count line.

-d, --detail *infolevel*

Level of information to print. Default: 1. Possible values: 1, 2, or 3.

--datacheck

List number of numerical and non-numerical values for each data field.

-e, --empty

List number of empty atom/bond blocks and data fields for compounds.

-f, --fields

List data field labels present for compounds.

-h, --help

Print this help message.

-i, --invalidatomnumbers

List number of bond blocks for compounds which contain invalid atom numbers.

-m, --mismatch

List number of atom/bond blocks for compounds which don't match with counts line information in header block.

-s, --salts

List number of atom blocks for compounds which contain salts identified as disconnected structural units.

-u, --unknownatoms

List number of atom blocks for compounds which contain special atom symbols such as L, O, *, ,LP, X, R#, or any other non periodic table symbols.

-w, --workingdir *dirname*

Location of working directory. Default: current directory.

EXAMPLES

To count compounds in SD file(s), type:

```
% InfoSDFfiles.pl Sample1.sdf
% InfoSDFfiles.pl Sample1.sdf Sample2.sdf
% InfoSDFfiles.pl *.sdf
```

To list all available information for SD file(s), type:

```
% InfoSDFfiles.pl -a *.sdf
```

To list all data fields present in sample.sdf, type:

```
% InfoSDFfiles.pl -f Sample.sdf
```

To count number of compounds which contain salts and list associated structural data, type:

```
% InfoSDFfiles.pl -s -d 3 Sample.sdf
```

AUTHOR

Manish Sud <msud@san.rr.com>

SEE ALSO

ExtractFromSDFfiles.pl, FilterSDFfiles.pl, MergeTextFilesWithSD.pl

COPYRIGHT

Copyright (C) 2022 Manish Sud. All rights reserved.

This file is part of MayaChemTools.

MayaChemTools is free software; you can redistribute it and/or modify it under the terms of the GNU Lesser General Public License as published by the Free Software Foundation; either version 3 of the License, or (at your option) any later version.