NAME

> InfoSDFiles.pl - List information about SDFile(s)

SYNOPSIS

> InfoSDFile.pl SDFile(s)...

> InfoSDFile.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] SDFile(s)...

DESCRIPTION

> List information about *SDFile(s)* contents: number of compounds, empty records and so on. Multiple SDFile 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, Q, * ,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:
>
> ```
> % InfoSDFiles.pl Sample1.sdf
> % InfoSDFiles.pl Sample1.sdf Sample2.sdf
> % InfoSDFiles.pl *.sdf
> ```

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

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

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

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

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

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

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SEE ALSO

ExtractFromSDFiles.pl, FilterSDFiles.pl, MergeTextFilesWithSD.pl

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