NAME

SortSDFiles.pl - Sort SDFile(s) using values for a data field

SYNOPSIS

SortSDFiles.pl SDFile(s)...

SortSDFiles.pl [-d, --detail infolevel] [-h, --help] [-k, --key *SD data field name*] [--keydata numeric | alphanumeric] [-o, --overwrite] [-r, --root rootname] [-s, --sort ascending | descending] [-w, --workingdir dirname] SDFile(s)...

DESCRIPTION

Sort *SDFile(s)* using values for a specified data field name key. Only one SD data field name key can be specified for sorting. In an event of conflict during sorting process, two similar values for a SD data field name key are simply transferred to output files in order of their presence in input files. Additionally, compound records with no data field name, empty field values, or field values containing multiple lines are simply placed at the end. 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*.

-h, --help

Print this help message.

-k, --key *SD data field name*

SDFile(s) data field name used for sorting compound records. Default value: *first data field name*. Compound records with no *sdfieldname*, empty field values, field values containing multiple lines, or field values inappropriate for sorting are simply placed at the end.

--keydata *numeric* | *alphanumeric*

Data type for *sdfieldname* values. Possible values: *numeric or alphanumeric*. Default value: *numeric*. For *alphanumeric* data values, comparison is case insensitive.

-o, --overwrite

Overwrite existing files.

-r, --root *rootname*

New SD file name is generated using the root: <Root>.<Ext>. Default new file name: <InitialSDFileName>SortedByDataField.<Ext>. This option is ignored for multiple input files.

-s, --sort *ascending* | *descending*

Sorting order for SD data field values. Possible values: *ascending or descending*. Default value: *ascending*.

-w, --workingdir *dirname*

Location of working directory. Default: current directory.

EXAMPLES

To perform numerical sort in ascending order using first data field values and generate a new SD file NewSample1.sdf, type:

```
% SortSDFiles.pl -o -r NewSample1 Sample1.sdf
```

To perform numerical sort in descending order using MolWeight data field and generate a new SD text file NewSample1.sdf, type:

```
% SortSDFiles.pl -k MolWeight --keydata numeric -s descending
  -r NewSample1 -o Sample1.sdf
```

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SEE ALSO

JoinSDFiles.pl, MergeTextFilesWithSD.pl, SplitSDFiles.pl

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