

## NAME

SPStrGen.pl - Generate structures for Sphingophospholipids (SP)

## SYNOPSIS

SPStrGen.pl SPAbbrev|SPAbbrevFileName ...

SPStrGen.pl [-c, --ChainAbbrevMode *MostLikely | Arbitrary*] [-h, --help] [-m, --mode *Abbrev | AbbrevFileName*] [-p, --ProcessMode *WriteSDFile | CountOnly*] [-o, --overwrite] [-r, --root rootname] [-w, --workingdir dirname] <arguments>...

## DESCRIPTION

Generate Sphingophospholipids (SP) structures using compound abbreviations specified on a command line or in a CSV/TSV Text file. All the command line arguments represent either compound abbreviations or file name containing abbreviations. Use mode option to control the type of command line arguments.

A SD file, containing structures for all SP abbreviations along with ontological information, is generated as an output.

## SUPPORTED ABBREVIATIONS

Current support for SP structure generation include these main classes and sub classes:

### o Sphingoid bases

- . Sphing-4-enines (Sphingosines)
- . Sphinganines
- . 4-Hydroxysphinganines (Phytosphingosines)
- . Sphingoid base homologs and variants
- . Sphingoid base 1-phosphates
- . Lysosphingomyelins and lysoglycosphingolipids

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- . Sphingoid base 1-phosphates
- . Lysosphingomyelins and lysoglycosphingolipids
- . Sphingoid base analogs

### o Ceramides

- . N-acylsphingosines (ceramides)
- . N-acylsphinganines (dihydroceramides)
- . N-acyl-4-hydroxysphinganines (phytoceramides)
- . Ceramide 1-phosphates

### o Phosphosphingolipids

- . Ceramide phosphocholines (sphingomyelins)
- . Ceramide phosphoethanolamines
- . Ceramide phosphoinositols

### o Neutral glycosphingolipids

- . Simple Glc series (GlcCer, LacCer, etc)

- . GalNAcb1-3GalA1-4Galb1-4Glc- (Globo series)
- . GalNAcb1-4Galb1-4Glc- (Ganglio series)
- . Galb1-3GlcNAcb1-3Galb1-4Glc- (Lacto series)
- . Galb1-4GlcNAcb1-3Galb1-4Glc- (Neolacto series)
- . GalNAcb1-3GalA1-3Galb1-4Glc- (Isoglobo series)
- . GlcNAcb1-2ManA1-3Manb1-4Glc- (Mollu series)
- . GalNAcb1-4GlcNAcb1-3Manb1-4Glc- (Arthro series)
- . Gal- (Gala series)

#### o Acidic glycosphingolipids

- . Gangliosides

## OPTIONS

### **-c, --ChainAbbrevMode** *MostLikely|Arbitrary*

Specify what types of acyl chain abbreviations are allowed during processing of complete abbreviations: allow most likely chain abbreviations containing specific double bond geometry specifications; allow any acyl chain abbreviation with valid chain length and double bond geometry specifications. Possible values: *MostLikely* or *Arbitrary*. Default value: *MostLikely*.

*Arbitrary* value of **-c, --ChainAbbrevMode** option is not allowed during processing of abbreviations containing wild cards.

During *MostLikely* value of **-c, --ChainAbbrevMode** option, only the most likely acyl chain abbreviations specified in ChainAbbrev.pm module are allowed. However, during *Arbitrary* value of **-c, --ChainAbbrevMode** option, any acyl chain abbreviations with valid chain length and double bond geometry can be specified. The current release of lipidmapstools support chain lengths from 2 to 50 as specified in ChainAbbrev.pm module.

In addition to double bond geometry specifications, valid substituents can be specified for in the acyl chain abbreviations.

### **-h, --help**

Print this help message

### **-m, --mode** *Abbrev|AbbrevFileName*

Controls interpretation of command line arguments. Two different methods are provided: specify compound abbreviations or a file name containing compound abbreviations. Possible values: *Abbrev* or *AbbrevFileName*. Default: *Abbrev*

In *AbbrevFileName* mode, a single line in CSV/TSV files can contain multiple compound abbreviations. The file extension determines delimiter used to process data lines: comma for CSV and tab for TSV. For files with TXT extension, only one compound abbreviation per line is allowed.

Wild card character, \*, is also supported in compound abbreviations.

Examples:

```
Specific structures: Cer(d18:0/0:0) Cer(d18:1(4E)/0:0)
                   Cer(d19:1(4E)/24:4(5Z,8Z,11Z,14Z))
Specific structures: SM(d18:0/16:0) SM(d19:0/24:1(15Z))
Specific possibilities: Cer(*0:0) Cer(d18:1(4E)/*)
All possibilities: *((*//*) or *((*//*)
```

With wild card character, +/- can also be used for chain lengths to indicate even and odd lengths at sn1/sn2/sn3 positions; additionally > and < qualifiers are also allowed to specify length requirements. Examples:

```
Odd and even number chains at sn1 and sn2: *((-:*/+*:*)
Odd and even number chains at sn1 and sn2 with length longer than
```

18

```
and 22: *( *->18:*/*+>22:*)
```

**-p, --ProcessMode** *WriteSDFfile|CountOnly*

Specify how abbreviations are processed: generate structures for specified abbreviations along with generating a SD file or just count the number of structures corresponding to specified abbreviations without generating any SD file. Possible values: *WriteSDFfile* or *CountOnly*. Default: *WriteSDFfile*.

It can take substantial amount of time for generating all the structures and writing out a SD file for abbreviations containing wild cards. *CountOnly* value of **--ProcessMode** option can be used to get a quick count of number of structures to be generated without writing out any SD file.

**-o, --overwrite**

Overwrite existing files

**-r, --root** *rootname*

New file name is generated using the root: <Root>.sdf. Default for new file names: SPAbbrev.sdf, <AbbrevFileName>.sdf, or <FirstAbbrevFileName>1To<Count>.sdf.

**-w, --workingdir** *dirname*

Location of working directory. Default: current directory

**EXAMPLES**

On some systems, command line scripts may need to be invoked using *perl -s SPStrGen.pl*; however, all the examples assume direct invocation of command line script works.

To generate a SPStructures.sdf file containing a structure specified by a command line SP abbreviation, type:

```
% SPStrGen.pl -r SPStructures -o "Cer(d18:0/0:0)"
```

To generate a SPStructures.sdf file containing structures specified by a command line SP abbreviations, type:

```
% SPStrGen.pl -r SPStructures -o "SM(d18:0/16:0)" "SM(d19:0/24:1(15Z))"
```

To enumerate all possible SP structures and generate a SPStructures.sdf file, type:

```
% SPStrGen.pl -r SPStructures -o "**(*/*)"
```

or

```
% SPStrGen.pl -r SPStructures -o "**(*:*/*:*)"
```

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**SEE ALSO**

CLStrGen.pl, FAStrGen.pl, GLStrGen.pl, GPStrGen.pl, STStrGen.pl

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