

NAME

CLStrGen.pl - Generate structures for Glycerophosphoglycerophosphoglycerols (Cardiolipins)

SYNOPSIS

CLStrGen.pl CLAbbrev|CLAbbrevFileName ...

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

DESCRIPTION

Generate Cardiolipins (CL) 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 CL abbreviations along with ontological information, is generated as an output.

SUPPORTED ABBREVIATIONS

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

o Glycerophosphoglycerophosphoglycerols (Cardiolipins)

- . Diacylglycerophosphoglycerophosphodiradylglycerols
- . Diacylglycerophosphoglycerophosphomonoradylglycerols
- . 1-alkyl,2-acylglycerophosphoglycerophosphodiradylglycerols
- . 1-alkyl,2-acylglycerophosphoglycerophosphomonoradylglycerols
- . 1Z-alkenyl,2-acylglycerophosphoglycerophosphodiradylglycerols
- . 1Z-alkenyl,2-acylglycerophosphoglycerophosphomonoradylglycerols
- . Monoacylglycerophosphoglycerophosphomonoradylglycerols
- . 1-alkyl glycerophosphoglycerophosphodiradylglycerols
- . 1-alkyl glycerophosphoglycerophosphomonoradylglycerols
- . 1Z-alkenylglycerophosphoglycerophosphodiradylglycerols
- . 1Z-alkenylglycerophosphoglycerophosphomonoradylglycerols

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: CL(1'-[18:2(9Z,12Z)/18:2(9Z,12Z)],
                    3'-[18:2(9Z,12Z)/18:2(9Z,12Z)])
All possibilities: *(1'-[**/**],3'-[**/**]) or
                  *(1'-[*/],3'-[*/])
```

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/even number chains at sn1/sn3 and sn2/sn4: *(1'-[+*/*/*-*],
                                                3'-[+*/*/*-*])
Odd/even number chains at sn1/sn3 and sn2/sn4 with length longer
than 20 and 22: *(1'-[+*>20/*/*->22:*],3'-[+*>20/*/*->22:*])
```

-p, --ProcessMode *WriteSDFile|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: *WriteSDFile* or *CountOnly*. Default: *WriteSDFile*.

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: CLAbbrev.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 GLStrGen.pl*; however, all the examples assume direct invocation of command line script works.

To generate a CLStructures.sdf file containing a structure specified by a command line CL abbreviation for Diacylglycerophosphoglycerophosphodiradylglycerols, type:

```
% CLStrGen.pl -r CLStructures -o "CL(1'-[18:2(9Z,12Z)/18:2(9Z,12Z)],
  3'-[18:2(9Z,12Z)/18:2(9Z,12Z)])"
```

To generate a CLStructures.sdf file containing a structure specified by a command line CL abbreviation for Diacylglycerophosphoglycerophosphomonoradylglycerols, type:

```
% CLStrGen.pl -r CLStructures -o "CL(1'-[18:2(9Z,12Z)/18:2(9Z,12Z)],  
3'-[18:2(9Z,12Z)/0:0])"
```

To generate a CLStructures.sdf file containing a structure specified by a command line CL abbreviation for 1-alkyl,2-acylglycerophosphoglycerophosphodiradylglycerols, type:

```
% CLStrGen.pl -r CLStructures -o "CL(1'-[O-16:0/18:2(9Z,12Z)],  
3'-[18:2(9Z,12Z)/18:2(9Z,12Z)])"
```

To generate a CLStructures.sdf file containing a structure specified by a command line CL abbreviation for 1-alkyl,2-acylglycerophosphoglycerophosphomonoradylglycerols, type:

```
% CLStrGen.pl -r CLStructures -o "CL(1'-[O-16:0/18:2(9Z,12Z)],  
3'-[18:2(9Z,12Z)/0:0])"
```

To generate a CLStructures.sdf file containing a structure specified by a command line CL abbreviation for 1Z-alkenyl,2-acylglycerophosphoglycerophosphodiradylglycerols, type:

```
% CLStrGen.pl -r CLStructures -o "CL(1'-[P-16:0/18:2(9Z,12Z)],  
3'-[18:2(9Z,12Z)/18:2(9Z,12Z)])"
```

To generate a CLStructures.sdf file containing a structure specified by a command line CL abbreviation for 1Z-alkenyl,2-acylglycerophosphoglycerophosphomonoradylglycerols, type:

```
% CLStrGen.pl -r CLStructures -o "CL(1'-[P-16:0/18:2(9Z,12Z)],  
3'-[18:2(9Z,12Z)/0:0])"
```

To generate a CLStructures.sdf file containing a structure specified by a command line CL abbreviation for Monoacylglycerophosphoglycerophosphomonoradylglycerols, type:

```
% CLStrGen.pl -r CLStructures -o "CL(1'-[18:2(9Z,12Z)/0:0],  
3'-[18:2(9Z,12Z)/0:0])"
```

To generate a CLStructures.sdf file containing a structure specified by a command line CL abbreviation for 1-alkyl glycerophosphoglycerophosphodiradylglycerols, type:

```
% CLStrGen.pl -r CLStructures -o "CL(1'-[O-16:0/0:0],  
3'-[18:2(9Z,12Z)/18:2(9Z,12Z)])"
```

To generate a CLStructures.sdf file containing a structure specified by a command line CL abbreviation for 1-alkyl glycerophosphoglycerophosphomonoradylglycerols, type:

```
% CLStrGen.pl -r CLStructures -o "CL(1'-[O-16:0/0:0],  
3'-[18:2(9Z,12Z)/0:0])"
```

To generate a CLStructures.sdf file containing a structure specified by a command line CL abbreviation for 1Z-alkenylglycerophosphoglycerophosphodiradylglycerols, type:

```
% CLStrGen.pl -r CLStructures -o "CL(1'-[P-16:0/0:0],  
3'-[18:2(9Z,12Z)/18:2(9Z,12Z)])"
```

To generate a CLStructures.sdf file containing a structure specified by a command line CL abbreviation for 1Z-alkenylglycerophosphoglycerophosphomonoradylglycerols, type:

```
% CLStrGen.pl -r CLStructures -o "CL(1'-[P-16:0/0:0],  
3'-[18:2(9Z,12Z)/0:0])"
```

To enumerate all possible CL structures and generate a CLStructures.sdf file, type:

```
% CLStrGen.pl -r CLStructures -o "(1'-[*/*],3'-[*/*])"
```

or

```
% CLStrGen.pl -r CLStructures -o "(1'-[**/*:*],3'-[**/*:*])"
```

or

```
% CLStrGen.pl -r CLStructures -o "(1'-[**(*)/*:(*)],  
3'-[**(*)/*:(*)])"
```

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SEE ALSO

FAStrGen.pl, GLStrGen.pl, GPStrGen.pl, SPStrGen.pl, STStrGen.pl

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