
NAME

GPStrGen.pl - Generate structures for Glycerophospholipids (GP)

SYNOPSIS

GPStrGen.pl GPAbbrev|GPAbbrevFileName ...

GPStrGen.pl [-h, --help] [-o, --overwrite] [-r, --root rootname] [-w, --workingdir dirname] <arguments>...

DESCRIPTION

Generate Glycerophospholipids (GP) 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 GP abbreviations along with ontological information, is generated as an output.

SUPPORTED ABBREVIATIONS

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

o Glycerophosphocholines (GPCho)

- . Diacylglycerophosphocholines
- . 1-alkyl, 2-acylglycerophosphocholines
- . 1Z-alkenyl, 2-acylglycerophosphocholines
- . Dialkylglycerophosphocholines
- . Monoacylglycerophosphocholines
- . 1-alkyl glycerophosphocholines
- . 1Z-alkenylglycerophosphocholines

o Glycerophosphoethanolamines (GPEtn)

- . Diacylglycerophosphoethanolamines
- . 1-alkyl, 2-acylglycerophosphoethanolamines
- . 1Z-alkenyl, 2-acylglycerophosphoethanolamines
- . Dialkylglycerophosphoethanolamines
- . Monoacylglycerophosphoethanolamines
- . 1-alkyl glycerophosphoethanolamines
- . 1Z-alkenylglycerophosphoethanolamines

o Glycerophosphoserines (GPSer)

- . Diacylglycerophosphoserines
- . 1-alkyl, 2-acylglycerophosphoserines
- . 1Z-alkenyl, 2-acylglycerophosphoserines
- . Dialkylglycerophosphoserines
- . Monoacylglycerophosphoserines
- . 1-alkyl glycerophosphoserines
- . 1Z-alkenylglycerophosphoserines

o Glycerophosphoglycerols (GPGro)

- . Diacylglycerophosphoglycerols
- . 1-alkyl, 2-acylglycerophosphoglycerols
- . 1Z-alkenyl, 2-acylglycerophosphoglycerols
- . Dialkylglycerophosphoglycerols

- . Monoacylglycerophosphoglycerols
- . 1-alkyl glycerophosphoglycerols
- . 1Z-alkenylglycerophosphoglycerols

o Glycerophosphoglycerophosphates (GPGroP)

- . Diacylglycerophosphoglycerophosphates
- . 1-alkyl, 2-acylglycerophosphoglycerophosphates
- . 1Z-alkenyl, 2-acylglycerophosphoglycerophosphates
- . Dialkylglycerophosphoglycerophosphates
- . Monoacylglycerophosphoglycerophosphates
- . 1-alkyl glycerophosphoglycerophosphates
- . 1Z-alkenylglycerophosphoglycerophosphates

o Glycerophosphoinositols (GPIIns)

- . Diacylglycerophosphoinositols
- . 1-alkyl, 2-acylglycerophosphoinositols
- . 1Z-alkenyl, 2-acylglycerophosphoinositols
- . Dialkylglycerophosphoinositols
- . Monoacylglycerophosphoinositols
- . 1-alkyl glycerophosphoinositols
- . 1Z-alkenylglycerophosphoinositols

o Glycerophosphoinositol monophosphates (GPIInsP)

- . Diacylglycerophosphoinositol monophosphates
- . 1-alkyl, 2-acylglycerophosphoinositol monophosphates
- . 1Z-alkenyl, 2-acylglycerophosphoinositol monophosphates
- . Dialkylglycerophosphoinositol monophosphates
- . Monoacylglycerophosphoinositol monophosphates
- . 1-alkyl glycerophosphoinositol monophosphates
- . 1Z-alkenylglycerophosphoinositol monophosphates

o Glycerophosphates (GPA)

- . Diacylglycerophosphates
- . 1-alkyl, 2-acylglycerophosphates
- . 1Z-alkenyl, 2-acylglycerophosphates
- . Dialkylglycerophosphates
- . Monoacylglycerophosphates
- . 1-alkyl glycerophosphates
- . 1Z-alkenylglycerophosphates

o Glyceropyrophosphates (GPP)

- . Diacylglyceropyrophosphates
- . Monoacylglyceropyrophosphates

o Glycerophosphonocholines (GPnCho)

- . Diacylglycerophosphonocholines
- . 1-alkyl, 2-acylglycerophosphonocholines
- . 1Z-alkenyl, 2-acylglycerophosphonocholines
- . Dialkylglycerophosphonocholines
- . Monoacylglycerophosphonocholines
- . 1-alkyl glycerophosphonocholines

- . 1Z-alkenylglycerophosphonocholines
- o Glycerophosphonoethanolamines (GPnEtn)
 - . Diacylglycerophosphonoethanolamines
 - . 1-alkyl, 2-acylglycerophosphonoethanolamines
 - . 1Z-alkenyl, 2-acylglycerophosphonoethanolamines
 - . Dialkylglycerophosphonoethanolamines
 - . Monoacylglycerophosphonoethanolamines
 - . 1-alkyl glycerophosphonoethanolamines
 - . 1Z-alkenylglycerophosphonoethanolamines

OPTIONS

-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: GPCho(12:0/13:0) GPCho(17:1(9Z)/0:0)
                    GPA(13:0/0:0)
Specific structures: GPCho(0-16:0/13:0) GPCho(0-16:1(1Z)/0:0)
Specific possibilities: GPCho(21:0/22:*) GPA(17:*/0:0)
                      GPEtn(0-18:0/*:*)
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
10
and 20: *(+>10:*/->20:*)
```

Default sn2 stereochemistry is R. However, abbreviation format also supports these additional stereochemistry specifications for sn2 position: S; U - unknown; rac - racemic mixture.

Examples:

```
GPCho(12:0/13:0)[rac]
GPCho(17:1(9Z)/14:0)[S]
GPA(13:0/12:0)[U]
```

-o, --overwrite

Overwrite existing files

-r, --root *rootname*

New file name is generated using the root: <Root>.sdf. Default for new file names:

GPAbbrev.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 GPStructures.sdf file containing a structure specified by a command line GP abbreviation, type:

```
% GPStrGen.pl -r GPStructures -o "GPCho(16:0/0:0)"
```

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

```
% GPStrGen.pl -r GPStructures -o "GPCho(16:0/0:0)"
"GPEtn(18:1(11E)/16:0)"
```

To generate a GPStructures.sdf file containing structures specified by a command line GP abbreviations with specific stereochemistry, type:

```
% GPStrGen.pl -r GPStructures -o "GPCho(16:0/0:0)[U]"
"GPEtn(18:1(11E)/16:0)[S]"
```

To enumerate all possible GP structures and generate a GPStructures.sdf file, type:

```
% GPStrGen.pl -r GPStructures -o "**(*/*)"
```

or

```
% GPStrGen.pl -r GPStructures -o "**(*:*/*:*)"
```

or

```
% GPStrGen.pl -r GPStructures -o "**(*:*(*)/*:*(*))"
```

To enumerate all possible GP structures with a sn1 chain, and generate a GPStructures.sdf file, type:

```
% GPStrGen.pl -r GPStructures -o "**(*/*:0)"
```

To enumerate all possible GP structures with a sn1 chain containing one double bond, and generate a GPStructures.sdf file, type:

```
% GPStrGen.pl -r GPStructures -o "**(*:1/0:0)"
```

To enumerate all possible GP structures with even chain length larger than 10 at sn1 position, and generate and generate a GPStructures.sdf file, type:

```
% GPStrGen.pl -r GPStructures -o "**(*+:*/0:0/0:0)"
```

To enumerate all possible GP structures with odd chains longer than 10 at sn1 and even chains longer than 18 at sn2, and generate a GPStructures.sdf file, type:

```
% GPStrGen.pl -r GPStructures -o "**(*->10:*/*+>18:*)"
```

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SEE ALSO

GLStrGen.pl

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