

NAME

GLStrGen.pl - Generate structures for Glycerolipids (GL)

SYNOPSIS

GLStrGen.pl GLAbbrev|GLAbbrevFileName ...

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

DESCRIPTION

Generate Glycerolipids (GL) 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 *-m*, *--mode* option to control the type of command line arguments.

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

SUPPORTED ABBREVIATIONS

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

o Monoradylglycerols

- . Monoacylglycerols
- . Monoalkylglycerols
- . Mono-(1Z-alkenyl)-glycerol

o Diradylglycerols

- . Diacylglycerols
- . Alkyl, acylglycerols
- . Dialkylglycerols
- . 1Z-alkenyl, acylglycerols

o Triradylglycerols

- . Triacylglycerols
- . Alkyl, diacylglycerols
- . Dialkyl, monoacylglycerols
- . 1Z-alkenyl, diacylglycerols

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: MG(16:0/0:0/0:0) DG(18:1(11E)/16:0/0:0)
 TG(16:0/16:0/18:1(9Z))
 Specific structures: MG(0-16:0/0:0/0:0) DG(0-16:1(1Z)/16:0/0:0)
 TG(0-20:0/16:0/18:1(9Z))
 Specific possibilities: DG(18:*/16:0/0:0) DG(18:1(*)/16:0/0:0)
 DG(*:*(9Z)/16:0/0:0)
 DG(*:*(9Z)/*:*(11E)/0:0)
 All TG possibilities: *(:*/*:*/*:*) or *(:*/*:*)
 All MG, DG and TG possibilities: "MG(*:*/0:0/0:0)"
 "DG(*:*/*:*/0:0)"
 "DG(*:*/0:0/*:*)"

Along 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: TG(*+*/*-:*/*:*)
 Odd and even number chains at sn1 and sn2 with length longer than 10 and 20: TG(*+>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:

MG(16:0/0:0/0:0)[rac] - racemic mixture
 DG(18:1(11E)/16:0/0:0)[S] - sn2 stereochemistry is S instead of default R
 TG(16:0/16:0/18:1(9Z))[U] - sn2 stereochemistry is unknown

To generate all isomers for specific chains in DG and TG, use of iso designation is also supported. Stereochemistry specification support is not available with isomeric structure generation. Examples:

DG(18:1(11E)/16:0/0:0)[iso2] - Two isomeric structures
 TG(16:0/16:0/18:1(9Z))[iso3] - Three isomeric structures
 TG(16:0/18:0/18:1(9Z))[iso6] - Six isomeric structures

Additionally, all isomeric structures can also be generated by explicit specification of chains at different positions:

DG(18:1(11E)/16:0/0:0) DG(16:0/18:1(11E)/0:0)
 TG(16:0/16:0/18:1(9Z)) TG(16:0/18:1(9Z)/16:0)
 TG(18:1(9Z)/16:0/16:0/)

Wild card chain abbreviations are supported with sn2 stereochemistry but not with isomer abbreviation.

-o, --overwrite

Overwrite existing files

-r, --root *rootname*

New file name is generated using the root: <Root>.sdf. Default for new file names: GLAbbrev.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 GLStructures.sdf file containing a structure specified by a command line GL abbreviation, type:

```
% GLStrGen.pl -r GLStructures -o "MG(16:0/0:0/0:0)"
```

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

```
% GLStrGen.pl -r GLStructures -o "MG(16:0/0:0/0:0)"
"DG(18:1(11E)/16:0/0:0)" "TG(16:0/16:0/18:1(9Z))"
```

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

```
% GLStrGen.pl -r GLStructures -o "MG(16:0/0:0/0:0)[rac]"
"DG(18:1(11E)/16:0/0:0)[S]" "TG(16:0/16:0/18:1(9Z))[U]"
```

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

```
% GLStrGen.pl -r GLStructures -o "DG(18:1(11E)/16:0/0:0)[iso2]"
"TG(16:0/16:0/18:1(9Z))[iso3]" "TG(16:0/16:0/18:1(9Z))[iso6]"
```

To enumerate all possible GL structures and generate a GLStructures.sdf file, type:

```
% GLStrGen.pl -r GLStructures -o "(*/*/*)"
```

or

```
% GLStrGen.pl -r GLStructures -o "(*:*/*:*/*:*)"
```

or

```
% GLStrGen.pl -r GLStructures -o "(*:*(*)/*:*(*)/*:*(*)")"
```

To enumerate all possible Monoradylglycerols structures and generate a MonoGLStructures.sdf file, type:

```
% GLStrGen.pl -r MonoGLStructures -o "MG(*/*:0/0:0)"
```

To enumerate all possible Diradylglycerols structures and generate a DiGLStructures.sdf file, type:

```
% GLStrGen.pl -r DiGLStructures -o "DG(*/*/*:0)"
```

To enumerate all possible Monoradylglycerols structures with one double bond on acyl chain and generate a GLStructures.sdf file, type:

```
% GLStrGen.pl -r MonoGLStructures -o "MG(*:1/0:0/0:0)"
```

To enumerate all possible Monoradylglycerols structures with even chain lengths and generate a GLStructures.sdf file, type:

```
% GLStrGen.pl -r MonoGLStructures -o "MG(*+/*:0/0:0)"
```

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

```
% GLStrGen.pl -r DiGLStructures -o "DG(*->10:*/*+>18:*/0:0)"
```

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SEE ALSO

GPStrGen.pl

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