

## NAME

LMAPSStr - Glycerolipids (GL) structure generation methods

## SYNOPSIS

```
use LMAPSStr;
```

```
use LMAPSStr qw(:all);
```

## DESCRIPTION

LMAPSStr module provides these methods:

```
GenerateCmpdAtomLine - Generate SD file atom data line
GenerateCmpdBondLine - Generate SD file bond data line
GenerateCmpdCountsLine - Generate SD file count data line
GenerateCmpdMiscInfoLine - Generate SD file misc data line
ParseCmpdAtomLine - Parse SD file atom data line
ParseCmpdBondLine - Parse SD file bond data line
ParseCmpdCountsLine - Parse SD file count data line
RoundToNextInteger - Round up to next integer
SetupCmpdAbbrevs - Setup lipid abbreviations
SetupSDFileName - Setup SD file name
StandardizeStereochemistrySpec - Standardize stereochemistry
StandardizeStereochemistrySpec - Standardize ring stereochemistry
```

## METHODS

### GenerateCmpdAtomLine

```
$Line = GenerateCmpdAtomLine($AtomX, $AtomY, $AtomZ,
                              $AtomSymbol);
```

Return a formatted atom data line for SD file.

### GenerateCmpdBondLine

```
$Line = GenerateCmpdBondLine($FirstAtomNum, $SecondAtomNum,
                              $BondType, [$BondStereo]);
```

Return a formatted bond data line for SD file.

### GenerateCmpdCountsLine

```
$Line = GenerateCmpdCountsLine($AtomCount, $BondCount,
                                [$ChiralFlag, $PropertyCount, $Version]);
```

Return a formatted count data line for SD file.

### GenerateCmpdMiscInfoLine

```
$Line = GenerateCmpdMiscInfoLine();
```

Return a formatted miscellaneous data line for SD file. In addition to a time stamp, LipdMAPS name is used as the program name.

### ParseCmpdAtomLine

```
($AtomX, $AtomY, $AtomZ, $AtomSymbol) = ParseCmpdAtomLine($Line);
```

Parse SD file atom data line and return a list with these values: atom coordinates and element symbol.

### ParseCmpdBondLine

```
( $FirstAtomNum, $SecondAtomNum, $BondType, $BondStereo ) =  
  ParseCmpdBondLine( $Line );
```

Parse SD file atom bond data line and return a list containing these values: bond atom numbers and bond type.

### ParseCmpdCountsLine

```
( $AtomCount, $BondCount, $ChiralFlag, $PropertyCount, $Version ) =  
  ParseCmpdCountsLine( $Line );
```

Parse SD file count data line and return a list containing these values: atom/bond count and other miscellaneous count information.

### RoundToNextInteger

```
$IntegerValue = RoundToNextInteger( $Number );
```

Return an integer by rounding the number off to next integer.

### SetupCmpdAbbrevs

```
$AbbrevArrayRef = SetupCmpdAbbrevs( $CmdLineOptionsRef );
```

Return a reference to an array containing specified compound abbreviations by parsing command line arguments or processing files containing specified abbreviations.

### SetupSDFileName

```
$SDFilename = SetupSDFileName( $LipidCategory,  
  $CmdLineOptionsRef );
```

Return a SD file name by processing a specified *-r*, *--root* option or using default values.

### StandardizeStereochemistrySpec

```
$StandardizeSpec =  
  StandardizeStereochemistrySpec( $StereochemistrySpec );
```

Return a standardize stereochemistry specification containing R/S instead of a/b or alpha/beta.

### StandardizeRingStereochemistrySpec

```
$StandardizeSpec =  
  StandardizeRingStereochemistrySpec( $StereochemistrySpec );
```

Return a standardize stereochemistry specification containing alpha/beta instead of a/b or alpha/beta.

## AUTHOR

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## CONTRIBUTOR

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## SEE ALSO

ChainAbbrev.pm, ChainStr.pm

## COPYRIGHT

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