

NAME

GPStr - Glycerolipids (GP) structure generation methods

SYNOPSIS

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

DESCRIPTION

GPStr module provides these methods:

```
GenerateCmpdOntologyData - Generate ontology data  
GenerateCmpdOntologySDDataLines - Generate ontology data lines for SD file  
GenerateGPChainStrData - Generate chain structure data  
GenerateSDFile - Generate SD file  
GetGPTemplatesData - Get templates data  
GetGPSupportedHeadGroupMap - Get supported headgroups data  
GetGPTemplateID - Get templates ID  
IsGPChainsAbbrevSupported - Is it a supported GP abbreviation  
ParseGPAbbrev - Parse GP abbreviation  
ProcessGPCmpdAbbrevs - Process GP abbreviation  
SetupGPCmpdAbbrevTemplateDataMap - Setup template structure data map  
ValidateGPAbbrev - Validate GP abbreviation
```

METHODS

GenerateCmpdOntologyData

```
$DataHashRef = GenerateCmpdOntologyData($CmpdDataRef);
```

Return a reference to a hash containing ontology data with hash keys and values corresponding to property names and values.

GenerateCmpdOntologySDDataLines

```
$DataLinesArrayRef = GenerateCmpdOntologySDDataLines($CmpdDataRef);
```

Return a reference to an array containing ontology data lines suitable for generate SD file data block.

GenerateGPChainStrData

```
($AtomLinesArrayRef, $BondLinesArrayRef) =  
    GenerateGPChainStrData($ChainType, $CmpdDataRef);
```

Return array references containing atom and bond data lines for SD file. Appropriate atom and bond data lines are generated using chain type and abbreviation template data.

GenerateSDFile

```
GenerateSDFile($SDFileName, $CmdAbbrevsRef);
```

Generate a SD file for compound abbreviations. Structure data for specified abbreviation is generated sequentially and written to SD file.

GetGPTemplatesData

```
$TemplatesDataRef = GetGPTemplatesData();
```

Return a reference to a hash containing GP templates data

GetGPSupportedHeadGroupMap

```
$SupportedHeadGroupDataRef = GetGPSupportedHeadGroupMap();
```

Return a reference to a hash containing supported head groups data.

GetGPTemplateID

```
$HeadGroupID = GetGPTemplateID($HeadGroupAbbrev, $ChainsAbbrev);
```

Return a supported template ID for compound abbreviation.

IsGPChainsAbbrevSupported

```
$Status = IsGPChainsAbbrevSupported($Abbrev, $PrintWarning);
```

Return 1 or 0 based on whether GP abbreviated is supported. For unsupported GP abbreviations, a warning is printed unless PrintWarning flag is set.

ParseGPAbbrev

```
($HeadGroup, $ChainsAbbrev, $AbbrevModifier) =  
ParseGPAbbrev($Abbrev);
```

Parse GP abbreviation and return these values: HeadGroup, ChainsAbbrev, AbbrevModifier.

ProcessGPCmpdAbbrevs

```
ProcessGPCmpdAbbrevs($CmpdAbbrevsRef, $AllowArbitraryChainAbbrev,  
$WriteSDFile, $SDFileName);
```

Process specified GP abbreviations to generate structures and write them out either a SD file or simply report number of valid abbreviations.

SetupGPCmpdAbbrevTemplateDataMap

```
$AbbrevTemplateDataMapRef =  
SetupGPCmpdAbbrevTemplateDataMap($Abbrev);
```

Return a reference to a hash containing template data for compound abbreviation. The template data is used to generate SD file for compound abbreviation.

ValidateGPAbbrev

```
$Status = ValidateGPAbbrev($Abbrev);
```

Return 1 or 0 based on whether a GP abbreviation is valid.

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CONTRIBUTOR

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SEE ALSO

ChainAbbrev.pm, ChainStr.pm, LMAPSStr.pm

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