NAME

GLStr - Glycerolipids (GL) structure generation methods

SYNOPSIS

use GLStr;

use GLStr qw(:all);

DESCRIPTION

GLStr module provides these methods:

```
GenerateCmpdOntologyData - Generate ontology data
GenerateCmpdOntologySDDataLines - Generate ontology data lines for SD
file
GenerateGLChainStrData - Generate chain structure data
GenerateSDFile - Generate SD file
IsGLAbbrevSupported - Is it a supported GL abbreviation
ParseGLAbrev - Parse GL abbreviation
ProcessGLCmpdAbbrevs - Process GL abbreviation
SetupGLCmpdAbbrevTemplateDataMap - Setup template structure data map
ValidateGLAbbrev - Validate GL abbreviation
```

METHODS

ExpandGLCmpdAbbrevs

```
$ExpandedAbbrevArrayRef = ExpandGLCmpdAbbrevs($CmpdAbbrev);
```

Return a reference to an array containing complete GL abbreviations. Wild card characters in GL abbreviation name are expanded to generate fully qualified GL abbreviations.

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

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

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

GenerateGLChainStrData

```
($AtomLinesArrayRef, $BondLinesArrayRef) =
    GenerateGLChainStrData($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.

IsGLAbbrevSupported

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

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

ParseGLAbrev

```
($GLType, $ChainsAbbrev, $AbbrevModifier) =
ParseGLAbrev($Abbrev);
```

Parse GL abbreviation and return these values: GLType, ChainsAbbrev, AbbrevModifier.

ProcessGLCmpdAbbrevs

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

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

SetupGLCmpdAbbrevTemplateDataMap

```
$AbbrevTemplateDataMapRef =
    SetupGLCmpdAbbrevTemplateDataMap($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.

ValidateGLAbbrev

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

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

AUTHOR

Manish Sud

CONTRIBUTOR

Eoin Fahy

SEE ALSO

ChainAbbrev.pm, ChainStr.pm, LMAPSStr.pm

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