

NAME

CLStr - Cardiolipins (CL) structure generation methods

SYNOPSIS

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

DESCRIPTION

CLStr module provides these methods:

```
GenerateCmpdOntologyData - Generate ontology data  
GenerateCmpdOntologySDDataLines - Generate ontology data lines for  
                                SD file  
GenerateCLChainStrData - Generate chain structure data  
GenerateSDFile - Generate SD file  
GetCLTemplatesData - Get templates data  
GetCLSupportedHeadGroupMap - Get supported headgroups data  
GetCLTemplateID - Get templates ID  
IsCLChainsAbbrevSupported - Is it a supported CL abbreviation  
ParseCLAbbrev - Parse CL abbreviation  
ProcessCLCmpdAbbrevs - Process CL abbreviation  
SetupCLCmpdAbbrevTemplateDataMap - Setup template structure data map  
ValidateCLAbbrev - Validate CL 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.

GenerateCLChainStrData

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

GetCLTemplatesData

```
$TemplatesDataRef = GetCLTemplatesData();
```

Return a reference to a hash containing CL templates data

GetCLSupportedHeadGroupMap

```
$SupportedHeadGroupDataRef = GetCLSupportedHeadGroupMap();
```

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

GetCLTemplateID

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

Return a supported template ID for compound abbreviation.

IsCLChainsAbbrevSupported

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

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

ParseCLAbbrev

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

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

ProcessCLCmpdAbbrevs

```
ProcessCLCmpdAbbrevs($CmpdAbbrevsRef, $AllowArbitraryChainAbbrev,  
$WriteSDFFile, $SDFFileName);
```

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

SetupCLCmpdAbbrevTemplateDataMap

```
$AbbrevTemplateDataMapRef =  
SetupCLCmpdAbbrevTemplateDataMap($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.

ValidateCLAbbrev

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

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

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CONTRIBUTOR

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SEE ALSO

ChainAbbrev.pm, ChainStr.pm, LMAPSStr.pm

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