

NAME

SPStr - Spingolipids (SP) structure generation methods

SYNOPSIS

```
use SPStr;
```

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

DESCRIPTION

SPStr module provides these methods:

```
GenerateCmpdOntologyData - Generate ontology data
GenerateCmpdOntologySDDataLines - Generate ontology data lines for SD
file
GenerateSPChainStrData - Generate chain structure data
GenerateSDFile - Generate SD file
GetSPTemplatesData - Get templates data
GetSPSupportedHeadGroupMap - Get supported headgroups data
GetSPTemplateID - Get templates ID
IsSPChainsAbbrevSupported - Is it a supported SP abbreviation
ParseSPAbbrev - Parse SP abbreviation
ProcessSPCmpdAbbrevs - Process SP abbreviation
SetupSPCmpdAbbrevTemplateDataMap - Setup template structure data map
ValidateSPAbbrev - Validate SP 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.

GenerateSPChainStrData

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

GetSPTemplatesData

```
$TemplatesDataRef = GetSPTemplatesData();
```

Return a reference to a hash containing SP templates data

GetSPSupportedHeadGroupMap

```
$SupportedHeadGroupDataRef = GetSPSupportedHeadGroupMap();
```

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

GetSPTemplateID

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

Return a supported template ID for compound abbreviation.

IsSPChainsAbbrevSupported

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

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

ParseSPAbbrev

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

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

ProcessSPCmpdAbbrevs

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

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

SetupSPCmpdAbbrevTemplateDataMap

```
$AbbrevTemplateDataMapRef =  
SetupSPCmpdAbbrevTemplateDataMap($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.

ValidateSPAbbrev

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

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

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SEE ALSO

ChainStr.pm

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