

NAME

ChainStr - Fatty Acyls (FA), Glycerolipids (GL) and Glycerophospholipids (GP) structure data generation methods

SYNOPSIS

```
use ChainStr;
```

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

DESCRIPTION

ChainStr module provides these methods:

```
AssignSubstituentStereoChemistry - Assign stereochemistry to
substituents
GenerateAtomBlockLines - Generate SD file atom data lines
GenerateBondBlockLines - Generate SD file bond data lines
GenerateChainStrData - Generate structure data for chains
GenerateCmpdCountsLine - Generate SD file count data line
IsAnySubstituentSpecifiedWithStereoChemistry - Check stereochemistry of
substituents
SetupTemplateDataMap - Set up template data for a compound abbreviation
```

METHODS

AssignSubstituentStereoChemistry

```
AssignSubstituentStereoChemistry($CmpdAbbrevTemplateDataMapRef,
    $CmdDataLinesRef);
```

Assign stereochemistry to substituents using structure and stereochemistry data available via \$CmpdAbbrevTemplateDataMapRef and \$CmdDataLinesRef. And add new lines to existing structure data using \$CmdDataLinesRef.

GenerateAtomBlockLines

```
$AtomDataLines =
GenerateAtomBlockLines($CmpdAbbrevTemplateDataMapRef,
    $Sn1AtomLinesRef, $Sn2AtomLinesRef, $Sn3AtomLinesRef);
```

Return atom data lines suitable for writing to SD file. Atom data for all appropriate chains is merged into a single string using new line character as delimiter.

GenerateBondBlockLines

```
$BondDataLines =
GenerateBondBlockLines($CmpdAbbrevTemplateDataMapRef,
    $Sn1BondLinesRef, $Sn2AtomLinesRef, $Sn3AtomLinesRef);
```

Return bond data lines suitable for writing to SD file. Bond data for all appropriate chains is merged into a single string using new line character as delimiter.

GenerateChainStrData

```
($AtomLinesArrayRef, $BondLinesArrayRef) =
GenerateChainStrData($ChainType,
    $CmpdAbbrevTemplateDataMapRef);
```

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.

GenerateCmpdCountsLine

```
$RetVal =  
GenerateCmpdCountsLine($CmpdAbbrevTemplateDataMapRef);
```

Return a formatted count data line for SD file.

IsAnySubstituentSpecifiedWithStereoChemistry

```
$Status = IsAnySubstituentSpecifiedWithStereoChemistry(  
$CmpdAbbrevTemplateDataMapRef);
```

Return 1 or 0 based on whether stereochemistry is specified for any substituent.

SetupTemplateDataMap

```
SetupTemplateDataMap($TemplateType, $AbbrevTemplateDataMapRef,  
$TemplateData);
```

Setup compound abbreviation template data using a supported template.

AUTHOR

Manish Sud

CONTRIBUTOR

Eoin Fahy

SEE ALSO

FAStr.pm, GLStr.pm, GPStr.pm, LMAPSStr.pm, SPStr.pm

COPYRIGHT

Copyright (C) 2006-2017. The Regents of the University of California. All Rights Reserved.

LICENSE

Modified BSD License