

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:

```
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  
SetupTemplateDataMap - Set up template data for a compound abbreviation
```

METHODS

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.

SetupTemplateDataMap

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

Setup compound abbreviation template data using a supported template.

AUTHOR

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CONTRIBUTOR

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SEE ALSO

GLStr.pm, GPStr.pm

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