

NAME

ChainAbbrev - Methods for processing chain abbreviations

SYNOPSIS

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

DESCRIPTION

ChainAbbrev module provides these methods:

```
ChainAbbrevNameExists - Is it a supported chain abbreviation  
ExpandChainAbbrev - Expand wild cards in chain abbreviation  
GetChainAbbrevToNameMap - Get chain name  
GetChainLenAbbrevSupportedMap - Get reference to supported chain  
                                abbreviations data  
GetChainLenAbbrevDbleBondGeometyDataMap - Get reference to supported  
chain                                double bond geometry data  
GetSubstituentsAbbrevToNameMap - Get substituents name  
GetSupportedChainLenList - Get supported chain lengths  
IsAlkylChainAbbrev - Is it a alkyl chain abbreviation  
IsAlkenylChainAbbrev - Is it a alkenyl chain abbreviation  
IsChainAbbrevOkay - Is it a valid chain abbreviation  
IsWildCardInChainAbbrev - Does chain abbreviation contains a wild card  
ParseChainAbbrev - Parse chain abbreviation  
ParseSubstituentAbbrev - Parse substituent abbreviation
```

METHODS

ChainAbbrevNameExists

```
$Status = ChainAbbrevNameExists($ChainAbbrev);
```

Return 1 or 0 based on whether it's a supported chain name.

ExpandChainAbbrev

```
$AbbrevArrayRef = ExpandChainAbbrev($Abbrev);
```

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

GetChainAbbrevToNameMap

```
$AbbrevNameHashRef = GetChainAbbrevToNameMap();
```

Return a reference to hash with chain abbreviation/name as key/value pair.

GetChainLenAbbrevSupportedMap

```
$ChainLenHashRef = GetChainLenAbbrevSupportedMap();
```

Return a reference to hash with supported chain length as hash key.

GetChainLenAbbrevDbleBondGeometyDataMap

```
$ChainLenDblBondHashRef =  
GetChainLenAbbrevDbleBondGeometyDataMap();
```

Return a reference to hash containing information about chain length, number of double bonds and geometry of double bonds.

GetSubstituentsAbbrevToNameMap

```
$AbbrevNameHashRef = GetSubstituentsAbbrevToNameMap();
```

Return a reference to hash with substituents abbreviation/name as key/value pair.

GetSupportedChainLenList

```
$ChainLengthListRef = GetSupportedChainLenList();
```

Return a reference to a sorted list containing supported chain lengths.

IsAlkylChainAbbrev

```
$Status = IsAlkylChainAbbrev($ChainAbbrev);
```

Return 1 or 0 based on whether it's a alkyl chain abbreviation.

IsAlkenylChainAbbrev

```
$Status = IsAlkenylChainAbbrev($ChainAbbrev);
```

Return 1 or 0 based on whether it's a alkenyl chain abbreviation.

IsChainAbbrevOkay

```
$Status = IsChainAbbrevOkay($ChainAbbrev);
```

Return 1 or 0 based on whether chain abbreviation is valid.

IsWildCardInChainAbbrev

```
$Status = IsWildCardInChainAbbrev($ChainAbbrev);
```

Return 1 or 0 based on whether chain abbreviation contains any wild card character.

ParseChainAbbrev

```
($ChainLength, $DoubleBondCount, $DoubleBondGeometry) =  
    ParseChainAbbrev($ChainAbbrev);
```

Parse chain abbreviation and return these values: chain length, number of double bonds, and geometry of double bonds.

ParseSubstituentAbbrev

```
($Pos, $Name, $StereoChemistry) =  
    ParseSubstituentAbbrev($SubstituentAbbrev);
```

Parse substituent abbreviation and return these values: position of the substituent on the chain, name, and stereochemistry of the substituent.

AUTHOR

Manish Sud

CONTRIBUTOR

Eoin Fahy

SEE ALSO

LMAPSStr.pm, ChainStr.pm

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