

NAME

MDLMolFileIO

SYNOPSIS

```
use MDLMolFileIO;

use MDLMolFileIO qw(:all);
```

DESCRIPTION

MDLMolFileIO class provides the following methods:

`new`, `GenerateMoleculeString`, `IsMDLMolFile`, `ParseMoleculeString`, `ReadMolecule`, `ReadMoleculeString`, `WriteMolecule`

The following methods can also be used as functions:

`GenerateMoleculeString`, `IsMDLMolFile`, `ParseMoleculeString`

Data specific to MDLMolFileIO class not directly used by `Molecule`, `Atom` and `Bond` objects - data label/value pairs, `atomSteroParity` and so on - is associated to and retrieved from appropriate objects using following methods:

```
SetMDL<PropertyName>
GetMDL<PropertyName>.
```

MDLMolFileIO class is derived from `FileIO` class and uses its methods to support generic file related functionality.

METHODS

`new`

```
$NewMDLMolFileIO = new MDLMolFileIO(%NamesAndValues);
```

Using specified `MDLMolFileIO` property names and values hash, `new` method creates a new object and returns a reference to newly created MDLMolFileIO object.

`GenerateMoleculeString`

```
$MoleculeString = $MDLMolFileIO->GenerateMoleculeString($Molecule);
MoleculeString = MDLMolFileIO::GenerateMoleculeString($Molecule);
```

Returns a `MoleculeString` in MDLMol format corresponding to `Molecule`.

`IsMDLMolFile`

```
$Status = $MDLMolFileIO->IsMDLMolFile($FileName);
Status = MDLMolFileIO::IsMDLMolFile($FileName);
```

Returns 1 or 0 based on whether `FileName` is a MDLMol file.

`ParseMoleculeString`

```
$Molecule = $MDLMolFileIO->ParseMoleculeString($MoleculeString);
Molecule = MDLMolFileIO::ParseMoleculeString($MoleculeString);
```

Parses `MoleculeString` and returns a `Molecule` object.

`ReadMolecule`

```
$Molecule = $MDLMolFileIO->ReadMolecule($FileHandle);
```

Reads data for the compound in a file using already opened `FileHandle`, creates, and returns a `Molecule` object.

`ReadMoleculeString`

```
$MoleculeString = $MDLMolFileIO->ReadMoleculeString($FileHandle);
```

Reads data for the compound in a file using already opened `FileHandle` and returns a `MoleculeString` corresponding to compound structure and other associated data.

`WriteMolecule`

```
$MDLMolFileIO->WriteMolecule($Molecule);
```

Writes `Molecule` data to a file in MDLMol format and returns MDLMolFileIO.

AUTHOR

Manish Sud <msud@san.rr.com>

SEE ALSO

`MoleculeFileIO.pm`, `SDFFileIO.pm`

COPYRIGHT

Copyright (C) 2004-2012 Manish Sud. All rights reserved.

This file is part of MayaChemTools.

MayaChemTools is free software; you can redistribute it and/or modify it under the terms of the GNU Lesser General Public License as published by the Free Software Foundation; either version 3 of the License, or (at your option) any later version.