

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, atom StereoParity 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

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