

NAME

MoleculeFileIO

SYNOPSIS

```
use MoleculeFileIO;

use MoleculeFileIO qw(:all);
```

DESCRIPTION

MoleculeFileIO class provides the following methods:

new, Close, IsSupportedMoleculeFileFormat, Open, ReadMolecule, ReadMoleculeString, WriteMolecule

The following methods can also be used as functions:

IsSupportedMoleculeFileFormat

METHODS

new

```
$NewMoleculeFileIO = new MoleculeFileIO([%PropertyNameAndValues]);
```

Using specified *MoleculeFileIO* property names and values hash, new method creates a new object and returns a reference to newly created MoleculeFileIO object. By default, following properties are initialized:

```
Name = ""
Mode = ""
FileIORef = ""
```

Based on extension of specified file *Name*, an input class is automatically associated to provide molecule read and write methods.

Examples:

```
$Name = "Water.mol";
$Mode = "Read";
$MoleculeFileIO = new MoleculeFileIO('Name' => $Name,
                                         'Mode' => $Mode);

$MoleculeFileIO->Open();
$Molecule = $MoleculeFileIO->ReadMolecule();
$Molecule->DetectRings();
print "$Molecule\n";
$MoleculeFileIO->Close();

$MoleculeFileIO = new MoleculeFileIO('Name' => 'Sample1.sdf',
                                         'Mode' => 'Read');

$MoleculeFileIO->Open();
while ($Molecule = $MoleculeFileIO->ReadMolecule()) {
    $Molecule->DetectRings();
    print "$Molecule\n";

    $DataLabelsAndValuesRef =
        $Molecule->GetDataFieldLabelAndValues();
    for $DataLabel (sort keys %{ $DataLabelsAndValuesRef } ) {
        $DataValue = $DataLabelsAndValuesRef->{ $DataLabel };
        print "<DataLabel: $DataLabel; DataValue: $DataValue>; ";
    }
    print "\n";
}
$MoleculeFileIO->Close();
```

Close

```
$MoleculeFileIO->Close();
```

Closes an open file

IsSupportedMoleculeFileFormat

```
$Status = $MoleculeFileIO->IsSupportedMoleculeFileFormat($Name);
$Status = MoleculeFileIO::IsSupportedMoleculeFileFormat($Name);
($Status, $FormatType, $IOClassName) =
    MoleculeFileIO::IsSupportedMoleculeFileFormat($Name);
```

Returns 1 or 0 based on whether input file *Name* format is supported. In list context, value of supported format type and

name of associated IO class is also returned.

File extension is used to determine file format. Currently, following file extensions are supported:

FileExts - FormatType - AssociatedIOClassName

.mol - MDLMOL - MDLMolFileIO

.sdf, .sd - SDF - SDFFileIO

Open

```
$MoleculeFileIO->Open([$Mode]);
```

Opens a file in a specified *Mode*. Default mode value: *Read*. Supported mode values:

Read, Write, Append, <, >, >>, r, w, or a

ReadMolecule

```
$Molecule = $MoleculeFileIO->ReadMolecule();
```

Reads molecule data from the file and returns a *Molecule* object.

ReadMoleculeString

```
$MoleculeString = $MoleculeFileIO->ReadMoleculeString();
```

Reads molecule data from a file and returns a *Molecule* string.

WriteMolecule

```
$MoleculeFileIO->WriteMolecule();
```

Write molecule data to a file for a *Molecule*.

AUTHOR

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SEE ALSO

FileIO.pm, MDLMolFileIO.pm, SDFFileIO.pm

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