

NAME

SDFFileIO

SYNOPSIS

```
use FileIO::SDFFileIO;

use FileIO::SDFFileIO qw(:all);
```

DESCRIPTION

SDFFileIO class provides the following methods:

new, GenerateMoleculeString, IsSDFFile, ParseMoleculeString, ReadMolecule, ReadMoleculeString, WriteMolecule

The following methods can also be used as functions:

GenerateMoleculeString, IsSDFFile, ParseMoleculeString

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

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

SD data label and values are attached to Molecule object as a reference to a hash using SetDataFieldLabelAndValues and can be retrieved using GetDataFieldLabelAndValues method.

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

METHODS

new

```
$NewSDFFileIO = new FileIO::SDFFileIO(%NamesAndValues);
```

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

GenerateMoleculeString

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

Returns a MoleculeString in SD format corresponding to *Molecule*.

IsSDFFile

```
$Status = $SDFFileIO->IsSDFFile($FileName);
$Status = FileIO::SDFFileIO::IsSDFFile($FileName);
```

Returns 1 or 0 based on whether *FileName* is a SD file.

ParseMoleculeString

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

Parses *MoleculeString* and returns a Molecule object. SD data field label and value pairs are associated to Molecule object as a reference to a hash using:

```
$Molecule->SetDataFieldLabelAndValues(\%DataLabelsAndValues)
```

The reference to hash can be retrieved by:

```
$DataLabelsAndValues = $Molecule->GetDataFieldLabelAndValues();
for $DataLabel (sort keys %{ $DataLabelsAndValues }) {
    $DataValue = $DataLabelsAndValues->{ $DataLabel };
}
```

ReadMolecule

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

Reads data for the next compound in a file using already opened *FileHandle*, creates, and returns a

Molecule object.

ReadMoleculeString

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

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

WriteMolecule

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

Writes *Molecule* data to a file in MDLMol format and returns SDFFileIO.

AUTHOR

Manish Sud <msud@san.rr.com>

SEE ALSO

MoleculeFileIO.pm, MDLMolFileIO.pm

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