NAME

HydrogenBondsDescriptors

SYNOPSIS

use MolecularDescriptors::HydrogenBondsDescriptors;

use MolecularDescriptors::HydrogenBondsDescriptors qw(:all);

DESCRIPTION

HydrogenBondsDescriptors class provides the following methods:

new, GenerateDescriptors, GetDescriptorNames, SetHydrogenBondsType, StringifyHydrogenBondsDescriptors

HydrogenBondsDescriptors is derived from MolecularDescriptors class which in turn is derived from ObjectProperty base class that provides methods not explicitly defined in HydrogenBondsDescriptors, MolecularDescriptors or ObjectProperty classes using Perl's AUTOLOAD functionality. These methods are generated on-the-fly for a specified object property:

```
Set<PropertyName>(<PropertyValue>);
$PropertyValue = Get<PropertyName>();
Delete<PropertyName>();
```

The current release of MayaChemTools supports identification of two types of hydrogen bond donor and acceptor atoms with these names:

```
HBondsType1 or HydrogenBondsType1
HBondsType2 or HydrogenBondsType2
```

The names of these hydrogen bond types are rather arbitrary. However, their definitions have specific meaning and are as follows:

```
HydrogenBondsType1 [ Ref 60-61, Ref 65-66 ]:

    Donor: NH, NH2, OH - Any N and O with available H
    Acceptor: N[!H], O - Any N without available H and any O


HydrogenBondsType2 [ Ref 91 ]:

    Donor: NH, NH2, OH - N and O with available H
    Acceptor: N, O - And N and O
```

By default, *HydrogenBondsType2* is used to calculate number hydrogen bond donor and acceptor atoms. This corresponds to RuleOf5 definition of hydrogen bond donors and acceptors.

METHODS

new

```
$HydrogenBondsDescriptors = new MolecularDescriptors::
                            HydrogenBondsDescriptors(%NamesAndValues);
```

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

```
Molecule = ''
Type = 'HydrogenBonds'
HydrogenBondsType = 'HBondsType2'
@DescriptorNames = ('HydrogenBondDonors', 'HydrogenBondAcceptors')
@DescriptorValues = ('None', 'None')
```

Examples:

```
$HydrogenBondsDescriptors = new MolecularDescriptors::
                            HydrogenBondsDescriptors();

$HydrogenBondsDescriptors = new MolecularDescriptors::
                            HydrogenBondsDescriptors(
                            'HydrogenBondsType' => 'HBondsType2');
```

```
$HydrogenBondsDescriptors->SetMolecule($Molecule);
$HydrogenBondsDescriptors->GenerateDescriptors();
print "HydrogenBondsDescriptors: $HydrogenBondsDescriptors\n";
```

GenerateDescriptors

```
$HydrogenBondsDescriptors->GenerateDescriptors();
```

Calculates number of hydrogen bond donors and acceptors a molecule and returns *HydrogenBondsDescriptors*.

GetDescriptorNames

```
@DescriptorNames = $HydrogenBondsDescriptors->GetDescriptorNames();
@DescriptorNames = MolecularDescriptors::HydrogenBondsDescriptors::
                      GetDescriptorNames();
```

Returns all available descriptor names as an array.

SetHydrogenBondsType

```
$HydrogenBondsDescriptors->SetHydrogenBondsType($HBondsType);
```

Sets value of hydrogen bonds type to use during calculation of descriptors and returns *HydrogenBondsDescriptors*. Possible values: *HBondsType1, HydrogenBondsType1, HBondsType2, HydrogenBondsType2*.

StringifyHydrogenBondsDescriptors

```
$String = $HydrogenBondsDescriptors->
                      StringifyHydrogenBondsDescriptors();
```

Returns a string containing information about *HydrogenBondsDescriptors* object.

AUTHOR

Manish Sud <msud@san.rr.com>

SEE ALSO

MolecularDescriptors.pm, MolecularDescriptorsGenerator.pm

COPYRIGHT