

NAME

FingerprintsFileUtil

SYNOPSIS

```
use Fingerprints::FingerprintsFileUtil;

use Fingerprints::FingerprintsFileUtil qw(:all);
```

DESCRIPTION

FingerprintsFileUtil module provides the following functions:

GetFingerprintsFileType, NewFingerprintsFileIO, ReadAndProcessFingerprintsData

FingerprintsFileUtil module provides function to handle fingerprints data strings in FP, SD and CSV/TSV text files present in one of the following two types: fingerprints bit-vectors and fingerprints vector strings

Example of FP file format containing fingerprints bit-vector string data:

```
#
# Package = MayaChemTools 7.4
# ReleaseDate = Oct 21, 2010
#
# TimeStamp = Mon Mar 7 15:14:01 2011
#
# FingerprintsStringType = FingerprintsBitVector
#
# Description = PathLengthBits:AtomicInvariantsAtomTypes:MinLength1:...
# Size = 1024
# BitStringFormat = HexadecimalString
# BitsOrder = Ascending
#
Cmpd1 9c8460989ec8a49913991a6603130b0a19e8051c89184414953800cc21510...
Cmpd2 000000249400840040100042011001001980410c000000001010088001120...
... ..
... ..
```

Example of FP file format containing fingerprints vector string data:

```
#
# Package = MayaChemTools 7.4
# ReleaseDate = Oct 21, 2010
#
# TimeStamp = Mon Mar 7 15:14:01 2011
#
# FingerprintsStringType = FingerprintsVector
#
# Description = PathLengthBits:AtomicInvariantsAtomTypes:MinLength1:...
# VectorStringFormat = IDsAndValuesString
# VectorValuesType = NumericalValues
#
Cmpd1 338;C F N O C:C C:N C=O CC CF CN CO C:C:C C:C:N C:CC C:CF C:CN C:
N:C C:NC CC:N CC=O CCC CCN CCO CNC NC=O O=CO C:C:C:C C:C:C:N C:C:CC...;
33 1 2 5 21 2 2 12 1 3 3 20 2 10 2 2 1 2 2 2 8 2 5 1 1 1 19 2 8 2 2 2 2
6 2 2 2 2 2 2 2 3 2 2 1 4 1 5 1 1 18 6 2 2 1 2 10 2 1 2 1 2 2 2 2 ...
Cmpd2 103;C N O C=N C=O CC CN CO CC=O CCC CCN CCO CNC N=CN NC=O NCN O=C
O C CC=O CCCC CCCN CCCO CCNC CNC=N CNC=O CNCN CCCC=O CCCCC CCCCN CC...;
15 4 4 1 2 13 5 2 2 15 5 3 2 2 1 1 1 2 17 7 6 5 1 1 1 2 15 8 5 7 2 2 2 2
1 2 1 1 3 15 7 6 8 3 4 4 3 2 2 1 2 3 14 2 4 7 4 4 4 4 1 1 1 2 1 1 1 ...
... ..
... ..
```

Example of SD file format containing fingerprints vector string data:

```
... ..
... ..
$$$$
... ..
... ..
... ..
41 44 0 0 0 0 0 0 0 0 0999 V2000
-3.3652 1.4499 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
... ..
```

```
"CompoundID", "PathLengthFingerprints"
"Cmpd1", "FingerprintsBitVector;PathLengthBits;AtomicInvariantsAtomTypes
:MinLength1:MaxLength8;1024;HexadecimalString;Ascending;9c8460989ec8a4
9913991a6603130b0a19e8051c89184414953800cc2151082844a20104280013086030
8e8204d402800831048940e44281c00060449a5000ac80c894114e006321264401..."
... ..
```

[illegible]

```
FingerprintsVector;PathLengthCount;AtomicInvariantsAtomTypes;MinLength
1:MaxLength8;432;NumericalValues;IDsAndValuesPairsString;C.X1.B01.H3 2
C.X2.B02.H2 4 C.X2.B03.H1 14 C.X3.B03.H1 3 C.X3.B04 10 F.X1.B01 1 N.X
2.B02.H1 1 N.X3.B03 1 O.X1.B01.H1 3 O.X1.B02 2 C.X1.B01.H3C.X3.B03.H1
2.C.X2.B02.H2C.X3.B02.H2 1 C.X2.B02.H2C.X3.B03.H1 4 C.X2.B02.H2C.X3.B0
4 1 C.X2.B02.H2N.X3.B03 1 C.X2.B03.H1C.X2.B03.H1 10 C.X2.B03.H1C.X
```

```
FingerprintsVector;PathLengthCount:MMFF94AtomTypes:MinLength1:MaxLength
h8;463;NumericalValues;IDsAndValuesPairsString;C5A 2 C5B 2 C=ON 1 CB 1
8 COO 1 CR 9 F 1 N5 1 NC=O 1 O=CN 1 O=CO 1 OC=O 1 OR 2 C5A:C5B 2 C5A:N
5 2 C5ACB 1 C5ACR 1 C5B:C5B 1 C5BC=ON 1 C5BCB 1 C=ON=O=CN 1 C=ONNC=O 1
CB:CB 18 CBF 1 CBNC=O 1 COO=O=CO 1 COOCR 1 COOOC=O 1 CRCR 7 CRN5 1 CR
OR 2 C5A:C5B:C5B 2 C5A:C5BC=ON 1 C5A:C5BCB 1 C5A:N5:C5A 1 C5A:N5CR ...
```

```
FingerprintsVector;TopologicalAtomPairs:AtomicInvariantsAtomTypes:MinD
istance1:MaxDistance10;223;NumericalValues;IDsAndValuesString;C.X1.BO1
.H3-D1-C.X3.BO3.H1 C.X2.BO2.H2-D1-C.X2.BO2.H2 C.X2.BO2.H2-D1-C.X3.BO3.
H1 C.X2.BO2.H2-D1-C.X3.BO4 C.X2.BO2.H2-D1-N.X3.BO3 C.X2.BO3.H1-D1-...;
2 1 4 1 1 10 8 1 2 6 1 2 2 1 2 1 2 1 2 1 5 1 10 12 2 2 1 2 1 9 1 3 1
1 1 2 2 1 3 6 1 6 14 2 2 2 3 1 3 1 8 2 2 1 3 2 6 1 2 2 5 1 3 1 23 1...
```

```
FingerprintsVector;TopologicalAtomPairs:FunctionalClassAtomTypes:MinDi
stance1:MaxDistance10;144;NumericalValues;IDsAndValuesString;Ar-D1-Ar
Ar-D1-Ar.HBA Ar-D1-HBD Ar-D1-Hal Ar-D1-None Ar.HBA-D1-None HBA-D1-NI H
BA-D1-None HBA.HBD-D1-NI HBA.HBD-D1-None HBD-D1-None NI-D1-None No...;
23 2 1 1 2 1 1 1 1 2 1 1 7 28 3 1 3 2 8 2 1 1 1 5 1 5 24 3 3 4 2 13 4
1 1 4 1 5 22 4 4 3 1 19 1 1 1 1 1 2 2 3 1 1 8 25 4 5 2 3 1 26 1 4 1 ...
```

```
FingerprintsVector;TopologicalAtomTorsions:AtomicInvariantsAtomTypes;3
3;NumericalValues;IDsAndValuesString;C.X1.BO1.H3-C.X3.BO3.H1-C.X3.BO4-
C.X3.BO4 C.X1.BO1.H3-C.X3.BO3.H1-C.X3.BO4-N.X3.BO3 C.X2.BO2.H2-C.X2.BO
2.H2-C.X3.BO3.H1-C.X2.BO2.H2 C.X2.BO2.H2-C.X2.BO2.H2-C.X3.BO3.H1-O...;
2 2 1 1 2 2 1 1 3 4 4 8 4 2 2 6 2 2 1 2 1 1 2 1 1 2 6 2 4 2 1 3 1
```

```
FingerprintsVector;TopologicalAtomTorsions:EStateAtomTypes;36;Numerica
lValues;IDsAndValuesString;aaCH-aaCH-aaCH-aaCH aaCH-aaCH-aaCH-aasC aaC
H-aaCH-aasC-aaCH aaCH-aaCH-aasC-aasC aaCH-aaCH-aasC-sF aaCH-aaCH-aasC-
ssNH aaCH-aasC-aasC-aasC aaCH-aasC-aasC-aasN aaCH-aasC-ssNH-dssC a...;
4 4 8 4 2 2 6 2 2 2 4 3 2 1 3 3 2 2 2 1 2 1 1 1 2 1 1 1 1 1 1 1 2 1 1 2
```

```
FingerprintsVector;TopologicalAtomTriplets:AtomicInvariantsAtomTypes:M
inDistance1:MaxDistance10;3096;NumericalValues;IDsAndValuesString;C.X1
.BO1.H3-D1-C.X1.BO1.H3-D1-C.X3.BO3.H1-D2 C.X1.BO1.H3-D1-C.X2.BO2.H2-D1
0-C.X3.BO4-D9 C.X1.BO1.H3-D1-C.X2.BO2.H2-D3-N.X3.BO3-D4 C.X1.BO1.H3-D1
-C.X2.BO2.H2-D4-C.X2.BO2.H2-D5 C.X1.BO1.H3-D1-C.X2.BO2.H2-D6-C.X3....;
1 2 2 2 2 2 2 8 8 4 8 4 4 2 2 2 2 4 2 2 2 4 2 2 2 2 1 2 2 4 4 4 2 2
2 4 4 4 8 4 4 2 4 4 4 2 4 4 2 2 2 2 2 2 2 1 2 2 2 2 2 2 2 2 2 8...
```

```
FingerprintsVector;TopologicalAtomTriplets:SYBYLAtomTypes:MinDistance1
:MaxDistance10;2332;NumericalValues;IDsAndValuesString;C.2-D1-C.2-D9-C
.3-D10 C.2-D1-C.2-D9-C.ar-D10 C.2-D1-C.3-D1-C.3-D2 C.2-D1-C.3-D10-C.3-
D9 C.2-D1-C.3-D2-C.3-D3 C.2-D1-C.3-D2-C.ar-D3 C.2-D1-C.3-D3-C.3-D4 C.2
-D1-C.3-D3-N.ar-D4 C.2-D1-C.3-D3-O.3-D2 C.2-D1-C.3-D4-C.3-D5 C.2-D1-C.
3-D5-C.3-D6 C.2-D1-C.3-D5-O.3-D4 C.2-D1-C.3-D6-C.3-D7 C.2-D1-C.3-D7...
```

```
FingerprintsVector;TopologicalPharmacophoreAtomPairs:ArbitrarySize:Min
Distance1:MaxDistance10;54;NumericalValues;IDsAndValuesString;H-D1-H H
-D1-NI HBA-D1-NI HBD-D1-NI H-D2-H H-D2-HBA H-D2-HBD HBA-D2-HBA HBA-D2-
HBD H-D3-H H-D3-HBA H-D3-HBD H-D3-NI HBA-D3-NI HBD-D3-NI H-D4-H H-D4-H
BA H-D4-HBD HBA-D4-HBA HBA-D4-HBD HBD-D4-HBD H-D5-H H-D5-HBA H-D5-...;
18 1 2 1 22 12 8 1 2 18 6 3 1 1 1 22 13 6 5 7 2 28 9 5 1 1 1 36 16 10
3 4 1 37 10 8 1 35 10 9 3 3 1 28 7 7 4 18 16 12 5 1 2 1
```

```
FingerprintsVector;TopologicalPharmacophoreAtomPairs:FixedSize:MinDist
ance1:MaxDistance10;150;OrderedNumericalValues;ValuesString;18 0 0 1 0
0 0 2 0 0 1 0 0 0 0 22 12 8 0 0 1 2 0 0 0 0 0 0 0 0 0 18 6 3 1 0 0 0 1
0 0 1 0 0 0 0 22 13 6 0 0 5 7 0 0 0 2 0 0 0 0 0 28 9 5 1 0 0 0 1 0 0 1 0
0 0 0 36 16 10 0 0 3 4 0 0 1 0 0 0 0 0 37 10 8 0 0 0 0 1 0 0 0 0 0 0
0 35 10 9 0 0 3 3 0 0 1 0 0 0 0 0 28 7 7 4 0 0 0 0 0 0 0 0 0 0 0 18...
```

```
FingerprintsVector;TopologicalPharmacophoreAtomTriplets:ArbitrarySize:
MinDistance1:MaxDistance10;696;NumericalValues;IDsAndValuesString;Ar1-
Ar1-Ar1 Ar1-Ar1-H1 Ar1-Ar1-HBA1 Ar1-Ar1-HBD1 Ar1-H1-H1 Ar1-H1-HBA1 Ar1
-H1-HBD1 Ar1-HBA1-HBD1 H1-H1-H1 H1-H1-HBA1 H1-H1-HBD1 H1-HBA1-HBA1 H1-
HBA1-HBD1 H1-HBA1-NI1 H1-HBD1-NI1 HBA1-HBA1-NI1 HBA1-HBD1-NI1 Ar1-...;
46 106 8 3 83 11 4 1 21 5 3 1 2 2 1 1 1 100 101 18 11 145 132 26 14 23
```

```
28 3 3 5 4 61 45 10 4 16 20 7 5 1 3 4 5 3 1 1 1 1 5 4 2 1 2 2 1 1 1
119 123 24 15 185 202 41 25 22 17 3 5 85 95 18 11 23 17 3 1 1 6 4 ...
```

```
FingerprintsVector;TopologicalPharmacophoreAtomTriplets:FixedSize:MinD
istance1:MaxDistance10;2692;OrderedNumericalValues;ValuesString;46 106
8 3 0 0 83 11 4 0 0 0 1 0 0 0 0 0 0 0 0 21 5 3 0 0 1 2 2 0 0 1 0 0 0
0 0 0 1 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 100 101 18 11 0 0 145 132 26
14 0 0 23 28 3 3 0 0 5 4 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 61 45 10 4 0
0 16 20 7 5 1 0 3 4 5 3 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 1 0 0 5 ...
```

FUNCTIONS

GetFingerprintsFileType

```
$FileType = GetFingerprintsFileType($FileName);
```

Returns fingerprints FileType of *FileName* determined using extension of file name. Possible FileType values: *FP*, *SD*, *Text*. Supported file name extensions for various file types are: FP - *fpf*, *fp*; SD - *sdf*, *sd*; Text - *csv*, *tsv*.

NewFingerprintsFileIO

```
$FingerprintsFileIO = NewFingerprintsFileIO(%IOParameters);
```

Using specified *IOParameters* property names and values hash, NewFingerprintsFileIO method creates a new object using appropriate fingerprints file IO class - FingerprintsFPFileIO, FingerprintsSDFileIO, or FingerprintsTextFileIO - and returns a reference to a newly created FingerprintsFileIO object.

The *IOParameters* hash must contain *Name* and *Mode* as key/value pairs to create a new FingerprintsFileIO object.

Based on type of file - FP, SD or Text - NewFingerprintsFileIO use new method from appropriate class - FingerprintsFPFileIO - along with *IOParameters* to create FingerprintsFileIO object.

ReadAndProcessFingerprintsData

```
($CompoundIDsRef, $FingerprintsObjectRef) =
    ReadAndProcessFingerprintsData($FingerprintsFileIO);
```

Processes fingerprints bit-vector and vector string data in a file using *FingerprintsFileIO* object and returns a references to arrays of CompoundIDs and *FingerprintsObjects*.

The file open and close is automatically performed during processing.

AUTHOR

Manish Sud <msud@san.rr.com>

SEE ALSO

FingerprintsFPFileIO.pm, FingerprintsSDFileIO.pm, FingerprintsTextFileIO.pm

COPYRIGHT

Copyright (C) 2018 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.