

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
# VectorValueType = 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 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
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 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
... ..
2 3 1 0 0 0 0
... ..
M END
> <CmpdID>
Test
```

\$\$\$


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

```
FingerprintsBitVector;ExtendedConnectivityBits;AtomicInvariantsAtomTypes;Radius2;1024;BinaryString;Ascending;00000000000000000000000000000000
```

```
FingerprintsVector;ExtendedConnectivity:FunctionalClassAtomTypes:Radiu
s2;57;AlphaNumericalValues;ValuesString;24769214 508787397 850393286 8
62102353 981185303 1231636850 1649386610 1941540674 263599683 32920567
1 571109041 639579325 683993318 723853089 810600886 885767127 90326012
7 958841485 981022393 1126908698 1152248391 1317567065 1421489994 1455
632544 1557272891 1826413669 1983319256 2015750777 2029559552 20404...
```

```
FingerprintsVector;ExtendedConnectivity:EStateAtomTypes:Radius2;62;Alp
haNumericalValues;ValuesString;25189973 528584866 662581668 671034184
926543080 1347067490 1738510057 1759600920 2034425745 2097234755 21450
44754 96779665 180364292 3471712110 345278822 386540408 387387308 50430
1706 617094135 771528807 957666640 997798220 1158349170 1291258082 134
1138533 1395329837 1420277211 1479584608 1486476397 1487556246 1566...
```

```
FingerprintsBitVector;MACCSKeyBits;166;BinaryString;Ascending;00000000
000000000000000000000000000000001001000010010000000010010000000011100
010010101011110001101100010011011000001101111010011011111111111011111
1111111111110111000
```

[illegible][illegible]

```
FingerprintsVector;MACCSKeyCount;322;OrderedNumericalValues;ValuesString;14 8 2 0 2 0 4 4 2 1 4 0 0 2 5 10 5 2 1 0 0 2 0 5 13 3 28 5 5 3 0 0  
0 4 2 1 1 0 1 1 0 0 2 1 0 0 0 0 0 0 0 0 0 0 0 0 0 22 5 3 0 0 0 1 0  
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0  
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11 0 2 0 0 0 0 0 0 0 0  
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 ...
```

```
FingerprintsBitVector;PathLengthBits:AtomicInvariantsAtomTypes:MinLeng  
thl:MaxLength8;1024;BinaryString;Ascending;001000010011010101011000110  
0100010101011000101001011100110001000010001001101000001001001001001000  
00101110100000111001001000001001010100100100000000011000000101001011100  
001000000010001010101000001001111001101101101100000001010111001101  
01011000110000000010001000001100001101100010000100001000000000...
```

```
FingerprintsVector;PathLengthCount:AtomicInvariantsAtomTypes:MinLength
1:MaxLength8;432;NumericalValues;IDsAndValuesPairsString;C.X1.BO1.H3 2
C.X2.BO2.H2 4 C.X2.BO3.H1 14 C.X3.BO3.H1 3 C.X3.BO4 10 F.X1.BO1 1 N.X
2.BO2.H1 1 N.X3.BO3 1 O.X1.BO1.H1 3 O.X1.BO2 2 C.X1.BO1.H3C.X3.BO3.H1
2 C.X2.BO2.H2C.X2.BO2.H2 1 C.X2.BO2.H2C.X3.BO3.H1 4 C.X2.BO2.H2C.X3.BO
4 1 C.X2.BO2.H2N.X3.BO3 1 C.X2.BO3.H1C.X2.BO3.H1 10 C.X2.BO3.H1C.X3.B...
```

```
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:MinDistance1: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 5 1 10 12 2 1 2 1 2 1 9 1 3 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:MinDistance1: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 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 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.B01.H3-C.X3.B03.H1-C.X3.B04-
C.X3.B04 C.X1.B01.H3-C.X3.B03.H1-C.X3.B04-N.X3.B03 C.X2.B02.H2-C.X2.B0
2.H2-C.X3.B03.H1-C.X2.B02.H2 C.X2.B02.H2-C.X2.B02.H2-C.X3.B03.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 2 1 1 2
```

```
FingerprintsVector;TopologicalAtomTriplets:AtomicInvariantsAtomTypes:M
inDistance1:MaxDistance10;3096;NumericalValues;IDsAndValuesString;C.X1
.B01.H3-D1-C.X1.B01.H3-D1-C.X3.B03.H1-D2 C.X1.B01.H3-D1-C.X2.B02.H2-D1
0-C.X3.B04-D9 C.X1.B01.H3-D1-C.X2.B02.H2-D3-N.X3.B03-D4 C.X1.B01.H3-D1
-C.X2.B02.H2-D4-C.X2.B02.H2-D5 C.X1.B01.H3-D1-C.X2.B02.H2-D6-C.X3...;
1 2 2 2 2 2 2 8 8 4 8 4 4 2 2 2 4 2 2 2 4 2 2 2 1 2 2 4 4 4 2 2
2 4 4 4 8 4 4 2 4 4 4 2 2 2 2 2 2 2 1 2 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 18 6 3 1 0 0 0 1
0 0 1 0 0 0 0 22 13 6 0 0 5 7 0 0 2 0 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 5 4 2 1 2 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 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

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SEE ALSO

FingerprintsFPFileIO.pm, FingerprintsSDFileIO.pm, FingerprintsTextFileIO.pm

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