NAME

FingerprintsFileUtil

SYNOPSIS

use Fingerprints::FingerprintsFileUtil;

use Fingerprints::FingerprintsFileUtil qw(:all);

DESCRIPTION

FingerprintsFileUtil module provides the following functions:

GetFingerprintsFileType, NewFingerprintsFileIO, ReadAndProcessFingerpritsData

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 0000002494008400401000420110010019804l0c00000000l010088001120...
... ...
... ..
```

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 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  0999 V2000
 -3.3652    1.4499    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
... ...
2  3  1  0  0  0  0
... ...
M  END
>  <CmpdID>
Test
```

```
>  <PathLengthFingerprints>
FingerprintsBitVector;PathLengthBits:AtomicInvariantsAtomTypes:MinLengt
h1:MaxLength8;1024;HexadecimalString;Ascending;9c8460989ec8a49913991a66
03130b0a19e8051c89184414953800cc2151082844a2010428001308603 08e8204d4028
00831048940e44281c00060449a5000ac80c894114e006321264401600846c050164462
08190410805000304a10205b0100e04c0038ba0fad0209c0ca8b1200012268b61c0026a
aa0660a11014a011d46


$$$$
... ...
... ...
```

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

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

The current release of MayaChemTools supports the following types of fingerprint bit-vector and vector strings:

```
FingerprintsVector;AtomNeighborhoods:AtomicInvariantsAtomTypes:MinRadi
us0:MaxRadius2;41;AlphaNumericalValues;ValuesString;NR0-C.X1.BO1.H3-AT
C1:NR1-C.X3.BO3.H1-ATC1:NR2-C.X1.BO1.H3-ATC1:NR2-C.X3.BO4-ATC1 NR0-C.X
1.BO1.H3-ATC1:NR1-C.X3.BO3.H1-ATC1:NR2-C.X1.BO1.H3-ATC1:NR2-C.X3.BO4-A
TC1 NR0-C.X2.BO2.H2-ATC1:NR1-C.X2.BO2.H2-ATC1:NR1-C.X3.BO3.H1-ATC1:NR2
-C.X2.BO2.H2-ATC1:NR2-N.X3.BO3-ATC1:NR2-O.X1.BO1.H1-ATC1 NR0-C.X2.B...

FingerprintsVector;AtomTypesCount:AtomicInvariantsAtomTypes:ArbitraryS
ize;10;NumericalValues;IDsAndValuesString;C.X1.BO1.H3 C.X2.BO2.H2 C.X2
.BO3.H1 C.X3.BO3.H1 C.X3.BO4 F.X1.BO1 N.X2.BO2.H1 N.X3.BO3 O.X1.BO1.H1
O.X1.BO2;2 4 14 3 10 1 1 1 3 2

FingerprintsVector;AtomTypesCount:SLogPAtomTypes:ArbitrarySize;16;Nume
ricalValues;IDsAndValuesString;C1 C10 C11 C14 C18 C20 C21 C22 C5 CS F
N11 N4 O10 O2 O9;5 1 1 1 14 4 2 1 2 2 1 1 1 1 3 1

FingerprintsVector;AtomTypesCount:SLogPAtomTypes:FixedSize;67;OrderedN
umericalValues;IDsAndValuesString;C1 C2 C3 C4 C5 C6 C7 C8 C9 C10 C11 C
12 C13 C14 C15 C16 C17 C18 C19 C20 C21 C22 C23 C24 C25 C26 C27 CS N1 N
2 N3 N4 N5 N6 N7 N8 N9 N10 N11 N12 N13 N14 NS O1 O2 O3 O4 O5 O6 O7 O8
O9 O10 O11 O12 OS F Cl Br I Hal P S1 S2 S3 Me1 Me2;5 0 0 0 2 0 0 0 0 1
1 0 0 1 0 0 0 14 0 4 2 1 0 0 0 0 0 2 0 0 0 1 0 0 0 0 0 0 1 0 0 0 0...

FingerprintsVector;EStateIndicies:ArbitrarySize;11;NumericalValues;IDs
AndValuesString;SaaCH SaasC SaasN SdO SdssC SsCH3 SsF SsOH SssCH2 SssN
H SsssCH;24.778 4.387 1.993 25.023 -1.435 3.975 14.006 29.759 -0.073 3
.024 -2.270

FingerprintsVector;EStateIndicies:FixedSize;87;OrderedNumericalValues;
ValuesString;0 0 0 0 0 0 0 3.975 0 -0.073 0 0 24.778 -2.270 0 0 -1.435
4.387 0 0 0 0 0 0 3.024 0 0 0 0 0 0 0 1.993 0 29.759 25.023 0 0 0 0 1
4.006 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

FingerprintsVector;ExtendedConnectivity:AtomicInvariantsAtomTypes:Radi
us2;60;AlphaNumericalValues;ValuesString;73555770 333564680 352413391
666191900 1001270906 1371674323 1481469939 1977749791 2006158649 21414
08799 49532520 64643108 79385615 96062769 273726379 564565671 85514103
5 906706094 988546669 1018231313 1032696425 1197507444 1331250018 1338
532734 1455473691 1607485225 1609687129 1631614296 1670251330 17303...

FingerprintsVector;ExtendedConnectivityCount:AtomicInvariantsAtomTypes
:Radius2;60;NumericalValues;IDsAndValuesString;73555770 333564680 3524
13391 666191900 1001270906 1371674323 1481469939 1977749791 2006158649
2141408799 49532520 64643108 79385615 96062769 273726379 564565671...;
3 2 1 1 14 1 2 10 4 3 1 1 1 1 2 1 2 1 1 1 2 3 1 1 2 1 3 3 8 2 2 2 6 2
1 2 1 1 2 1 1 1 2 1 1 2 1 2 1 1 1 1 1 1 1 1 1 2 1 1

FingerprintsBitVector;ExtendedConnectivityBits:AtomicInvariantsAtomTyp
es:Radius2;1024;BinaryString;Ascending;00000000000000000000000000000100
```

```
0000000001010000000110000011000000000000010000000000000000000000100001
1000000110000000000000000000000000100110000000000000000000000000010000
0000000000000000000000000100000000000000000010000000000000000000000000
0000000000010000100001000000000000101000000000000000100000000000000...

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 341712110 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
0000000000000000000000000000000000100100001001000000000100100000000011100
0100101010111100011011000100110110000011011110100110111111111111011111
1111111111110111000

FingerprintsBitVector;MACCSKeyBits;322;BinaryString;Ascending;11101011
1110011111100101111111000111101100110000000000000011100010000000000000
0000000000000000000000000000000000000000000000101000000000000000000000
0000000000000000000000000000000000000000000000000000000000000000000000
0000000000000000000000000000000000000110000000000000000000000000000000
0000000000000000000000000000000000000000

FingerprintsVector;MACCSKeyCount;166;OrderedNumericalValues;ValuesStri
ng;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 1 0 0 3 0 0 0 0 4 0 0 2 0 0 0 0 0 0 0 0 2 0 0 2 0 0 0 0
0 0 0 0 1 1 8 0 0 0 1 0 0 1 0 1 0 1 0 3 1 3 1 0 0 0 1 2 0 11 1 0 0 0
5 0 0 1 2 0 1 1 0 0 0 0 0 1 1 0 1 1 1 1 0 4 0 0 1 1 0 4 6 1 1 1 2 1 1
3 5 2 2 0 5 3 5 1 1 2 5 1 2 1 2 4 8 3 5 5 2 2 0 3 5 4 1

FingerprintsVector;MACCSKeyCount;322;OrderedNumericalValues;ValuesStri
ng;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 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 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 0 0 0 0 ...

FingerprintsBitVector;PathLengthBits:AtomicInvariantsAtomTypes:MinLeng
th1:MaxLength8;1024;BinaryString;Ascending;001000010011010101011000110
0100010101011000101001011100110001000010001001101000001001001001001000
0010110100000111001001000000100101010010010000000001100000010100101110 0
0010000000100010101010000001001111001101110110110110000000101101110011 01
0101100011000000010001000011000010100011101100001000000100010000 0000...

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.H1:C.X2.BO3.H1 10 C.X2.BO3.H1:C....

FingerprintsVector;PathLengthCount:MMFF94AtomTypes:MinLength1:MaxLengt
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 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.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 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 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 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 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 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 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 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.

ReadAndProcessFingerpritsData

```
($CompoundIDsRef, $FingerprintsObjectRef) =
                ReadAndProcessFingerpritsData($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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