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:

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 1 19 2 8 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:

> <PathLengthFingerprints>

FingerprintsBitVector; PathLengthBits: AtomicInvariantsAtomTypes: MinLength1: MaxLength8; 1024; HexadecimalString; Ascending; 9c8460989ec8a49913991a6603130b0a19e8051c89184414953800cc2151082844a201042800130860308e8204d402800831048940e44281c00060449a5000ac80c894114e006321264401600846c05016446208190410805000304a10205b0100e04c0038ba0fad0209c0ca8b1200012268b61c0026aaa0660a11014a011d46

\$\$\$\$

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:MinRadius0:MaxRadius2;41;AlphaNumericalValues;ValuesString;NR0-C.X1.BO1.H3-ATC1:NR1-C.X3.BO3.H1-ATC1:NR2-C.X1.BO1.H3-ATC1:NR2-C.X3.BO4-ATC1 NR0-C.X1.BO1.H3-ATC1:NR2-C.X3.BO3.H1-ATC1:NR2-C.X3.BO4-ATC1 NR0-C.X3.BO3.H1-ATC1:NR2-C.X3.BO4-ATC1 NR0-C.X2.BO2.H2-ATC1:NR1-C.X2.BO2.H2-ATC1:NR1-C.X3.BO3.H1-ATC1:NR2-C.X3.BO3.H1-ATC1:N

FingerprintsVector;AtomTypesCount:AtomicInvariantsAtomTypes:ArbitrarySize;10;NumericalValues;IDsAndValuesString;C.X1.B01.H3 C.X2.B02.H2 C.X2.B03.H1 C.X3.B03.H1 C.X3.B04 F.X1.B01 N.X2.B02.H1 N.X3.B03 O.X1.B01.H1 O.X1.B02;2 4 14 3 10 1 1 1 3 2

FingerprintsVector;AtomTypesCount:SLogPAtomTypes:ArbitrarySize;16;NumericalValues;IDsAndValuesString;Cl Cl0 Cl1 Cl4 Cl8 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; 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; ExtendedConnectivity: AtomicInvariantsAtomTypes: Radius2;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; 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...

 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.X2.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.H1:C.X2.B03.H1 10 C.X2.B03.H1:C.X2.B03.H1

FingerprintsVector; PathLengthCount: MMFF94AtomTypes: MinLength1: MaxLength8; 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=CO 1 COOCR 1 COOCC=O 1 CRCR 7 CRN5 1 CR OR 2 C5A: C5B: C5B 2 C5A: C5BC=ON 1 C5A: N5: C5A 1 C5A: N5: C5A 1 C5A: N5: C5A 1 C5A: N5: C5A 1 C5A: N5: C5A

FingerprintsVector; TopologicalAtomPairs: AtomicInvariantsAtomTypes: MinD istance1: MaxDistance10; 223; NumericalValues; IDsAndValuesString; C.X1.B01.H3-D1-C.X3.B03.H1 C.X2.B02.H2-D1-C.X2.B02.H2 C.X2.B02.H2-D1-C.X3.B03.H1 C.X2.B02.H2-D1-C.X3.B04 C.X2.B02.H2-D1-N.X3.B03 C.X2.B03.H1-D1-...; 2 1 4 1 1 10 8 1 2 6 1 2 2 1 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:MinDistancel:MaxDistancel0;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 HBA-D1-None HBA-D1-None HBA-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.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.B02.H2-C.X2.B02.H2-C.X3.B03.H1-C.X2.B02.H2-C.X3.B03.H1-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

 ${\tt FingerprintsVector; Topological AtomTriplets: AtomicInvariants AtomTypes: Matter and the property of the$

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 HBD-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; 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-HBA1-HBD1 H1-HBA1-HBA1 H1-HBA1-HBD1 H1-HBA1-NI1 H1-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 ...

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

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