

NAME

FingerprintsSDFFileIO

SYNOPSIS

```
use FileIO::FingerprintsSDFFileIO;

use FileIO::FingerprintsSDFFileIO qw(:all);
```

DESCRIPTION

FingerprintsSDFFileIO class provides the following methods:

new, GetCompoundString, GetFingerprints, GetFingerprintsString, IsFingerprintsDataValid, IsFingerprintsFileDataValid, IsFingerprintsSDFFile, Next, Read, SetBitStringFormat, SetBitsOrder, SetCompoundIDMode, SetCompoundString, SetDetailLevel, SetFingerprints, SetFingerprintsString, SetFingerprintsStringMode, SetVectorStringFormat, WriteFingerprints, WriteFingerprintsString

The following methods can also be used as functions:

IsFingerprintsSDFFile

FingerprintsSDFFileIO class is derived from *FileIO* class and uses its methods to support generic file related functionality.

The fingerprints SD file format with .sdf or .sd file extensions supports two types of fingerprints string data: fingerprints bit-vectors and fingerprints vector strings. The fingerprints string data is treated as value of a fingerprints data field label in a SD file.

Example of SD file format containing fingerprints 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
... ..
2 3 1 0 0 0 0
... ..
M END
> <CmpdID>
Test

> <PathLengthFingerprints>
FingerprintsBitVector;PathLengthBits:AtomicInvariantsAtomTypes:MinLength:MaxLength8;1024;HexadecimalString;Ascending;9c8460989ec8a49913991a6603130b0a19e8051c89184414953800cc2151082844a201042800130860308e8204d402800831048940e44281c00060449a5000ac80c894114e006321264401600846c05016446208190410805000304a10205b0100e04c0038ba0fad0209c0ca8b1200012268b61c0026a
aa0660a11014a011d46

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

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

```
FingerprintsVector;AtomNeighborhoods:AtomicInvariantsAtomTypes:MinRadius: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:NR1-C.X3.BO3.H1-ATC1:NR2-C.X1.BO1.H3-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.X2.BO2.H2-ATC1:NR2-N.X3.BO3-ATC1:NR2-O.X1.BO1.H1-ATC1 NR0-C.X2.B...
```

```
FingerprintsVector;AtomTypesCount:AtomicInvariantsAtomTypes:ArbitrarySize;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;NumericalValues;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 2 0 0 0 1 0 0 0 0 0 0 1 0 0 0 0...
```

```
FingerprintsVector;EStateIndicies:ArbitrarySize;11;NumericalValues;IDs
AndValuesString;SaasCH 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
```

```
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 2 1 1
```

```
FingerprintsBitVector;ExtendedConnectivityBits:AtomicInvariantsAtomTyp
es:Radius2;1024;BinaryString;Ascending;0000000000000000000000000000100
0000000001010000000011000000110000000000001000000000000000000000100001
1000000110000000000000000000000000000000000100110000000000000000000010000
0000000000000000000000000000000000000000000000000000000000000000000000
0000000000000000000000000000000000000000000000000000000000000000000000
00000000000100001000010000000000001010000000000000001000000000000000...
```

```
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
0000000000000000000000000000000000000000000000000000000000000000000000
01001010101111000110110001001101100000110111010011011111111111011111
1111111111110111000
```

```
FingerprintsBitVector;MACCSKeyBits;322;BinaryString;Ascending;11101011
1110011111100101111111000111011001100000000000000000000000000000000000
0000000000000000000000000000000000000000000000000000000000000000000000
0000000000000000000000000000000000000000000000000000000000000000000000
0000000000000000000000000000000000000000000000000000000000000000000000
0000000000000000000000000000000000000000000000000000000000000000000000
0000000000000000000000000000000000000000000000000000000000000000000000
```

```
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 00 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 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;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 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 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:MinLength1:MaxLength8;1024;BinaryString;Ascending;001000010011010101011000110
0100010101011000101001011100110001000010001001101000001001001001001000
001011010000011100100100000100101010010010000000011000000101001011100
0010000001000101010100000100111001101101101101100000010110111001101
01011000110000000100010000110000101000111011000010000100000000...

```

```

FingerprintsVector;PathLengthCount:AtomicInvariantsAtomTypes:MinLength1: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...

```

```

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=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.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 2 1 1 2 6 1 2 2 1 2 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:MinDistance1:MaxDistance10;144;NumericalValues;IDsAndValuesString;Ar-D1-Ar
Ar-D1-Ar.HBA Ar-D1-HBD Ar-D1-Ha1 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;Numerical
Values;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:MinDistance1: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
-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 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 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 0 100 101 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 ...
```

METHODS

new

```
$NewFingerprintsSDFFileIO = new FileIO::FingerprintsSDFFileIO(%IOParameters);
```

Using specified *IOParameters* names and values hash, new method creates a new object and returns a reference to a newly created FingerprintsSDFFileIO object. By default, the following properties are initialized during *Read* mode:

```
Name = '';
Mode = 'Read';
Status = 0;
FingerprintsStringMode = 'AutoDetect';
FingerprintsFieldLabel = 'AutoDetect';
CompoundIDMode = 'LabelPrefix';
CompoundIDFieldLabel = undef;
CompoundIDPrefix = 'Cmpd';
ValidateData = 1;
DetailLevel = 1;
```

During *Write* mode, the following properties get initialize by default:

```
FingerprintsStringMode = undef;

BitStringFormat = HexadecimalString;
BitsOrder = Ascending;

VectorStringFormat = NumericalValuesString or ValuesString;
```

Examples:

```
$NewFingerprintsSDFFileIO = new FileIO::FingerprintsSDFFileIO(
    'Name' => 'Sample.sdf',
    'Mode' => 'Read');

$NewFingerprintsSDFFileIO = new FileIO::FingerprintsSDFFileIO(
    'Name' => 'Sample.sdf',
    'Mode' => 'Read',;
    'FingerprintsStringMode' =>
        'AutoDetect',
```

```

'FingerprintsFieldLabel' =>
    'Fingerprints',
'CompoundIDMode' =>
    'DataField',
'CompoundIDFieldLabel' =>
    'CompoundID');

$NewFingerprintsSDFFileIO = new FileIO::FingerprintsSDFFileIO(
    'Name' => 'Sample.sdf',
    'Mode' => 'Write',
    'FingerprintsStringMode' =>
        'FingerprintsBitVectorString',
    'Overwrite' => 1,
    'BitStringFormat' => 'HexadecimalString',
    'BitsOrder' => 'Ascending');

$NewFingerprintsSDFFileIO = new FileIO::FingerprintsSDFFileIO(
    'Name' => 'Sample.sd',
    'Mode' => 'Write',
    'FingerprintsStringMode' =>
        'FingerprintsVectorString',
    'Overwrite' => 1,
    'VectorStringFormat' => 'IDsAndValuesString',
    'FingerprintsLabel' => 'Fingerprints');

```

GetCompoundString

```
$CompoundString = $FingerprintsSDFFileIO->GetCompoundString();
```

Returns CompoundString for current compound.

GetFingerprints

```
$FingerprintsObject = $FingerprintsSDFFileIO->GetFingerprints();
```

Returns FingerprintsObject generated for current compound using fingerprints bit-vector or vector string data. The fingerprints object corresponds to any of the supported fingerprints such as PathLengthFingerprints, ExtendedConnectivity, and so on.

GetFingerprintsString

```
$FingerprintsString = $FingerprintsSDFFileIO->GetFingerprintsString();
```

Returns FingerprintsString for current compound.

IsFingerprintsDataValid

```
$Status = $FingerprintsSDFFileIO->IsFingerprintsDataValid();
```

Returns 1 or 0 based on whether FingerprintsObject is valid.

IsFingerprintsFileDataValid

```
$Status = $FingerprintsSDFFileIO->IsFingerprintsFileDataValid();
```

Returns 1 or 0 based on whether fingerprints file contains valid fingerprints data.

IsFingerprintsSDFFile

```

$Status = $FingerprintsSDFFileIO->IsFingerprintsSDFFile($FileName);
$Status = FileIO::FingerprintsSDFFileIO::IsFingerprintsSDFFile($FileName);

```

Returns 1 or 0 based on whether *FileName* is a SD file.

Next or Read

```

$FingerprintsSDFFileIO = $FingerprintsSDFFileIO->Next();
$FingerprintsSDFFileIO = $FingerprintsSDFFileIO->Read();

```

Reads next available compound fingerprints in SD file, processes the data, generates appropriate fingerprints object, and returns FingerprintsSDFFileIO. The generated fingerprints object is available using method GetFingerprints.

SetBitStringFormat

```
$FingerprintsSDFFileIO->SetBitStringFormat($Format);
```

Sets bit string *Format* for fingerprints bit-vector string data in a SD file and returns FingerprintsSDFFileIO. Possible values for BitStringFormat: *BinaryString* or *HexadecimalString*.

SetBitsOrder

```
$FingerprintsSDFFileIO->SetBitsOrder($BitsOrder);
```

Sets *BitsOrder* for fingerprints bit-vector string data in SD file and returns FingerprintsSDFFileIO. Possible values for BitsOrder: *Ascending* or *Descending*.

SetCompoundIDMode

```
$FingerprintsSDFFileIO->SetCompoundIDMode($Mode);
```

Sets compound ID *Mode* for fingerprints bit-vector string data in a SD file and returns FingerprintsSDFFileIO. Possible values for CompoundIDMode: *DataField*, *MolName*, *LabelPrefix*, or *MolNameOrLabelPrefix*.

SetCompoundString

```
$FingerprintsSDFFileIO->SetCompoundString($CompoundString);
```

Sets *CompoundString* and returns FingerprintsSDFFileIO.

SetDetailLevel

```
$FingerprintsSDFFileIO->SetDetailLevel($Level);
```

Sets details *Level* for generating diagnostics messages during SD file processing and returns FingerprintsSDFFileIO. Possible values: *Positive integers*.

SetFingerprints

```
$FingerprintsSDFFileIO->SetFingerprints($FingerprintsObject);
```

Sets *FingerprintsObject* for current data line and returns FingerprintsSDFFileIO.

SetFingerprintsString

```
$FingerprintsSDFFileIO->SetFingerprintsString($FingerprintsString);
```

Sets *FingerprintsString* for current data line and returns FingerprintsSDFFileIO.

SetFingerprintsStringMode

```
$FingerprintsSDFFileIO->SetFingerprintsStringMode($Mode);
```

Sets *FingerprintsStringMode* for SD file and returns FingerprintsFPFileIO. Possible values: *AutoDetect*, *FingerprintsBitVectorString*, or *FingerprintsVectorString*

SetVectorStringFormat

```
$FingerprintsSDFFileIO->SetVectorStringFormat($Format);
```

Sets *VectorStringFormat* for SD file and returns FingerprintsFPFileIO. Possible values: *IDsAndValuesString*, *IDsAndValuesPairsString*, *ValuesAndIDsString*, *ValuesAndIDsPairsString*.

WriteFingerprints

```
$FingerprintsFPFileIO->WriteFingerprints($FingerprintsObject,  
                                         $CompoundID);
```

Writes fingerprints string generated from *FingerprintsObject* object and other data including *CompoundID* to SD file and returns FingerprintsSDFFileIO.

WriteFingerprintsString

```
$FingerprintsSDFFileIO->WriteFingerprints($FingerprintsString,  
                                         $CompoundID);
```

Writes *FingerprintsString* and other data including *CompoundID* to SD file and returns FingerprintsSDFFileIO.

Caveats:

- o FingerprintsStringMode, BitStringFormat, BitsOrder, VectorStringFormat values are ignored during writing of fingerprints and it's written to the file as it is.
- o CompoundString is not checked to remove any existing fingerprints data

AUTHOR

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SEE ALSO

FingerprintsTextFileIO.pm, FingerprintsFPFileIO.pm, SDFFileIO.pm

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