

NAME

InfoFingerprintsFiles.pl - List information about fingerprints data in SD, FP and CSV/TSV text file(s)

SYNOPSIS

InfoFingerprintsFiles.pl SDFFile(s) FPFile(s) TextFile(s)...

```
InfoFingerprintsFiles.pl [-a, --all] [--AverageBitDensity] [--BitDensity] [-c, --count] [-c, --ColMode ColNum /
ColLabel] [--DataCheck] [-d, --detail InfoLevel] [-e, --empty] [--FingerprintsCol col number | col name] [
--FingerprintsField FieldLabel] [--FingerprintsType] [--FingerprintsDescription] [--FingerprintsSize] [
--FingerprintsBitStringFormat] [--FingerprintsBitOrder] [--FingerprintsVectorValuesType] [
--FingerprintsVectorValuesFormat] [-h, --help] [--InDelim comma | semicolon] [--NumOfOnBits] [
--NumOfNonZeroValues] [-w, --WorkingDir dirname] SDFFile(s) FPFile(s) TextFile(s)...
```

DESCRIPTION

List information about fingerprints data in *SD*, *FP* and *CSV/TSV* text file(s): number of rows containing fingerprints data, type of fingerprints vector, description and size of fingerprints, bit density and average bit density for bit-vector fingerprints strings, and so on.

The scripts *InfoFingerprintsSDFiles.pl* and *InfoFingerprintsTextFiles.pl* have been removed from the current release of *MayaChemTools* and their functionality merged with this script.

The valid *SDFFile* extensions are *.sdf* and *.sd*. All SD files in a current directory can be specified either by **.sdf* or the current directory name.

The valid *FPFile* extensions are *.fpf* and *.fp*. All FP files in a current directory can be specified either by **.fpf* or the current directory name.

The valid *TextFile* extensions are *.csv* and *.tsv* for comma/semicolon and tab delimited text files respectively. All other file names are ignored. All text files in a current directory can be specified by **.csv*, **.tsv*, or the current directory name. The *--indelim* option determines the format of *TextFile(s)*. Any file which doesn't correspond to the format indicated by *--indelim* option is ignored.

Format of fingerprint strings data in *SDFFile(s)*, *FPFile(s)* and *TextFile(s)* is automatically detected.

Example of *FP* file 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 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
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 ...
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 4 1 1 1 2 1 1 1 ...
... ..
... ..
```

Example of *SD* file containing fingerprints bit-vector string data:

```
... ..
... ..
$$$$
... ..
... ..
... ..
41 44 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
-3.3652 1.4499 0.0000 C 0 0 0 0 0 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>
Cmpd1

> <PathLengthFingerprints>
FingerprintsBitVector;PathLengthBits:AtomicInvariantsAtomTypes:MinLengt
h1:MaxLength8;1024;HexadecimalString;Ascending;9c8460989ec8a49913991a66
03130b0a19e8051c89184414953800cc2151082844a201042800130860308e8204d4028
00831048940e44281c00060449a5000ac80c894114e006321264401600846c050164462
08190410805000304a10205b0100e04c0038ba0fad0209c0ca8b1200012268b61c0026a
aa0660a11014a011d46

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

Example of CSV *Text* file 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...
```



```
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.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 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-D4-
HBD H-D3-H H-D3-HBA H-D3-HBD H-D3-NI HBA-D3-NI HBA-D3-NI H-D4-H H-D4-
HBA 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 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 0 100 101 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 0 0 1 1 1 0 0 5 ...
```

OPTIONS

- a, --all**
List all the available information.
- AverageBitDensity**
List average bit density of fingerprint bit-vector strings.
- BitDensity**
List bit density of fingerprints bit-vector strings data in each row.
- count**
List number of data entries containing fingerprints bit-vector or vector strings data. This is default behavior.
- c, --ColMode *ColNum | ColLabel***
Specify how columns are identified in CSV/TSV *TextFile(s)*: using column number or column label. Possible values: *ColNum* or *ColLabel*. Default value: *ColNum*
- d, --detail *InfoLevel***
Level of information to print about lines being ignored. Default: *1*. Possible values: *1, 2 or 3*.
- DataCheck**
Validate fingerprints data specified using **--FingerprintsCol** and list information about missing and invalid data.
- e, --empty**
List number of rows containing no fingerprints data.
- FingerprintsCol *col number | col name***
This value is **-c, --colmode** specific. It corresponds to column in CSV/TSV *TextFile(s)* containing fingerprints data. Possible values: *col number* or *col label*. Default value: *first column containing the word Fingerprints in its column label*.
- FingerprintsField *FieldLabel***
Fingerprints field label to use during listing of fingerprints information for *SDFFile(s)*. Default value: *first data field label containing the word Fingerprints in its label*.
- FingerprintsType**
List types of fingerprint strings: FingerprintsBitVector or FingerprintsVector.
- FingerprintsDescription**
List types of fingerprints: PathLengthBits, PathLengthCount, MACCSKeyCount, ExtendedConnectivity and so on.
- FingerprintsSize**
List size of fingerprints.
- FingerprintsBitStringFormat**
List format of fingerprint bit-vector strings: BinaryString or HexadecimalString.
- FingerprintsBitOrder**
List order of bits data in fingerprint bit-vector bit strings: Ascending or Descending.
- FingerprintsVectorValuesType**
List type of values in fingerprint vector strings: OrderedNumericalValues, NumericalValues or AlphaNumericalValues.
- FingerprintsVectorValuesFormat**
List format of values in fingerprint vector strings: ValuesString, IDsAndValuesString, IDsAndValuesPairsString, ValuesAndIDsString or ValuesAndIDsPairsString.

-
- h, --help
Print this help message.
- InDelim *comma | semicolon*
Input delimiter for CSV *TextFile(s)*. Possible values: *comma or semicolon*. Default value: *comma*. For TSV files, this option is ignored and *tab* is used as a delimiter.
- NumOfOnBits
List number of on bits in fingerprints bit-vector strings data in each row.
- NumOfNonZeroValues
List number of non-zero values in fingerprints vector strings data in each row.
- w, --WorkingDir *DirName*
Location of working directory. Default: current directory.

EXAMPLES

To count number of lines containing fingerprints bit-vector or vector strings data present in FP file, in a column name containing Fingerprint substring in text file, and in a data field with Fingerprint substring in its label, type:

```
% InfoFingerprintsFiles.pl SampleFPBin.csv

% InfoFingerprintsFiles.pl SampleFPBin.sdf SampleFPBin.fpf
SampleFPBin.csv

% InfoFingerprintsFiles.pl SampleFPHex.sdf SampleFPHex.fpf
SampleFPHex.csv

% InfoFingerprintsFiles.pl SampleFPcount.sdf SampleFPcount.fpf
SampleFPcount.csv
```

To list all available information about fingerprints bit-vector or vector strings data present in FP file, in a column name containing Fingerprint substring in text file, and in a data field with Fingerprint substring in its label, type:

```
% InfoFingerprintsFiles.pl -a SampleFPHex.sdf SampleFPHex.fpf
SampleFPHex.csv

% InfoFingerprintsFiles.pl -a SampleFPcount.sdf SampleFPcount.fpf
SampleFPcount.csv
```

To list all available information about fingerprints bit-vector or vector strings data present in a column named Fingerprints in text file, type:

```
% InfoFingerprintsFiles.pl -a --ColMode ColLabel --FingerprintsCol
Fingerprints SampleFPHex.sdf

% InfoFingerprintsFiles.pl -a --ColMode ColLabel --FingerprintsCol
Fingerprints SampleFPcount.csv
```

To list all available information about fingerprints bit-vector or vector strings data present in a data field names Fingerprints in SD file, type:

```
% InfoFingerprintsFiles.pl -a --FingerprintsField Fingerprints
SampleFPHex.sdf

% InfoFingerprintsFiles.pl -a --FingerprintsField Fingerprints
SampleFPcount.sdf
```

To list bit density, average bit density, and number of on bits for fingerprints bit-vector strings data present in FP

file, in a column name containing Fingerprint substring in text file, and in a data field with Fingerprint substring in its label, type:

```
% InfoFingerprintsFiles.pl --BitDensity --AverageBitDensity
--NumOfOnBits SampleFPBin.csv SampleFPBin.sdf SampleFPBin.fpf
```

To list vector values type, format and number of non-zero values for fingerprints vector strings data present in FP file, in a column name containing Fingerprint substring in text file, and in a data field with Fingerprint substring in its label along with fingerprints type and description, type:

```
% InfoFingerprintsFiles.pl --FingerprintsType --FingerprintsDescription
--FingerprintsVectorValuesType --FingerprintsVectorValuesFormat
--NumOfNonZeroValues SampleFPcount.csv SampleFPcount.sdf
SampleFPcount.fpf
```

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SEE ALSO

SimilarityMatricesFingerprints.pl, SimilaritySearchingFingerprints.pl, AtomNeighborhoodsFingerprints.pl, AtomNeighborhoodsFingerprints.pl, ExtendedConnectivityFingerprints.pl, MACCSKeysFingerprints.pl, PathLengthFingerprints.pl, TopologicalAtomPairsFingerprints.pl, TopologicalAtomTorsionsFingerprints.pl, TopologicalPharmacophoreAtomPairsFingerprints.pl, TopologicalPharmacophoreAtomTripletsFingerprints.pl

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