

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 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 CCCC CCNC CNC=N CNC=O CNCN CCCC=O CCCCC CCCC CN 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 CSV *Text* file containing fingerprints bit-vector string data:

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

```
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 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

```
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.X...
```

```
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: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.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
O-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 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 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 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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