


```
FingerprintsVector;ExtendedConnectivity:AtomicInvariantsAtomTypes;14;
AlphaNumericalValues;ValuesString;333564680 1142173602 14814699391
977749791 2006158649 291020918 443330853 692611812 816539344173
1657806 2039728782 931045615 1273931663 1317501190

FingerprintsVector;ExtendedConnectivity:FunctionalClassAtomTypes;11;
AlphaNumericalValues;ValuesString;862102353 981185303 12517955598
10600886 885767127 1452087973 1878436093 2029559552 1465773182
1530666307 2113761516

FingerprintsVector;TopologicalAtomPairs:AtomicInvariantsAtomTypes;23;
NumericalValues;IDsAndValuesString;C.X1.B01.H3-D1-C.X3.B04 C.X2.B03.H1-
D1-C.X2.B03.H1 C.X2.B03.H1-D1-C.X3.B04 C.X2.B03.H1-D1-N.X2.B02.H1
C.X3.B04-D1-C.X3.B04 C.X3.B04-D1-O.X1.B02 C.X1.B01.H3-D2-C.X2.B03.H1
C.X1.B01.H3-D2-C.X3.B04...; 1 1 2 2 1 1 1 1 3 1 1 1 1 1 1 1 2 1 1 1

FingerprintsVector;TopologicalAtomPairs:AtomicInvariantsAtomTypes;23;
NumericalValues;IDsAndValuesPairsString;C.X1.B01.H3-D1-C.X3.B04 1
C.X2.B03.H1-D1-C.X2.B03.H1 1 C.X2.B03.H1-D1-C.X3.B04 2 C.X2.B03.H1-
D1-N.X2.B02.H1 2 C.X3.B04-D1-C.X3.B04 1 C.X3.B04-D1-O.X1.B02 1
C.X1.B01.H3-D2-C.X2.B03.H1 1 C.X1.B01.H3-D2-C.X3.B04 1
C.X2.B03.H1-D2-C.X2.B03.H1 1 C.X2.B03.H1-D2-C.X3.B04 3...

FingerprintsVector;TopologicalAtomTorsions:AtomicInvariantsAtomTypes;11;
NumericalValues;IDsAndValuesString;C.X1.B01.H3-C.X3.B04-C.X2.B03.H1-
N.X2.B02.H1 C.X1.B01.H3-C.X3.B04-C.X2.B03.H1 C.X1.B01.H3-
C.X3.B04-C.X3.B04-O.X1.B02 C.X2.B03.H1-C.X2.B03.H1-C.X3.B04-C.X3.B04
C.X2.B03.H1-C.X2.B03.H1-C.X3.B04-O.X1.B02...;
1 1 1 1 1 1 1 1 1 1 1

FingerprintsVector;TopologicalAtomTorsions:AtomicInvariantsAtomTypes;11;
NumericalValues;IDsAndValuesPairsString;C.X1.B01.H3-C.X3.B04-C.X2.B03.H1-
N.X2.B02.H1 1 C.X1.B01.H3-C.X3.B04-C.X3.B04-C.X2.B03.H1 1 C.X1.B01.H3-
C.X3.B04-C.X3.B04-O.X1.B02 1 C.X2.B03.H1-C.X2.B03.H1-C.X3.B04-
C.X3.B04 1 C.X2.B03.H1-C.X2.B03.H1-C.X3.B04-O.X1.B02 1 C.X2.B03.H1-
C.X2.B03.H1-N.X2.B02.H1-C.X2.B03.H1 1 C.X2.B03.H1-C.X3.B04-C.X3.B04-
C.X2.B03.H1 1...

FingerprintsVector;TopologicalPharmacophoreAtomPairs;150;
OrderedNumericalValues;ValuesString;1 0 0 0 0 0 0 0 0 0 0 0 0 0 0
3 2 0 0 1 1 0 0 0 0 0 0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1 1 1 0 0
0 1 0 0 0 0 0 0 0 0 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0...

FingerprintsVector;TopologicalPharmacophoreAtomPairs;150;
OrderedNumericalValues;IDsAndValuesString;H-D1-H H-D1-HBA H-D1-HBD
H-D1-NI H-D1-PI HBA-D1-HBA HBA-D1-HBD HBA-D1-NI HBA-D1-PI HBD-D1-HBD
HBD-D1-NI HBD-D1-PI NI-D1-NI NI-D1-PI PI-D1-PI H-D2-H H-D2-HBA ...;
1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3 2 0 0 1 1 0 0 0 0 0 0 0 0 0 0 1 0
0 0 0 0 0 0 0 0 0 0 0 0 1 1 1 0 0 0 1 0 0 0 0 0 0 0 0 1 1 0 0 0 0 ...

FingerprintsVector;TopologicalPharmacophoreAtomTriplets;4960;
OrderedNumericalValues;ValuesString;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 1 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...

FingerprintsVector;TopologicalPharmacophoreAtomTriplets;4960;
OrderedNumericalValues;IDsAndValuesString;Ar1-Ar1-Ar1 Ar1-Ar1-H1
Ar1-Ar1-HBA1 Ar1-Ar1-HBD1 Ar1-Ar1-NI1 Ar1-Ar1-PI1 Ar1-H1-H1 ...;
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;AtomNeighborhoods;AtomicInvariantsAtomTypes;10;
AlphaNumericalValues;ValuesString;NR0-C.X2.BO3.H1-ATC1:NR1-C.X2.BO3.H1-
ATC1:NR1-C.X3.BO4-ATC1:NR2-C.X2.BO3.H1-ATC1:NR2-C.X3.BO4-ATC1:NR2-
N.X1.BO1.H2-ATC1 NR0-C.X2.BO3.H1-ATC1:NR1-C.X2.BO3.H1-ATC1:NR1-
C.X3.BO4-ATC1:NR2-C.X2.BO3.H1-ATC1:NR2-C.X3.BO4-ATC2 NR0-C.X2.BO3.H1-
ATC1:NR1-C.X2.BO3.H1-ATC2:NR2-C.X2.BO3.H1-ATC1:NR2-C.X3.BO4-ATC1...
```

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 rows containing fingerprints bit-vector or vector strings data. This is default behavior.
- c, --ColMode *ColNum* | *ColLabel*
Specify how columns are identified in *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 *TextFile(s)* containing fingerprints data. Possible values: *col number* or *col label*. Default value: *first column containing the word Fingerprints in its column 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.
- FingerprintsVectorValueType
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 a column name containing fingerprint substring, type:

```
% InfoFingerprintsTextFiles.pl SampleFPBin.csv
```

```
% InfoFingerprintsTextFiles.pl SampleFPHex.csv
```

```
% InfoFingerprintsTextFiles.pl SampleFPcount.csv
```

To list all available information about fingerprints bit-vector or vector strings data present in a column name containing fingerprint substring, type:

```
% InfoFingerprintsTextFiles.pl -a SampleFPHex.csv
```

```
% InfoFingerprintsTextFiles.pl -a SampleFPcount.csv
```

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

```
% InfoFingerprintsTextFiles.pl -a --ColMode ColLabel --FingerprintsCol  
Fingerprints SampleFPHex.csv
```

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

To list bit density, average bit density, and number of on bits for fingerprints bit-vector strings data present in a column named containing fingerprint substring, type:

```
% InfoFingerprintsTextFiles.pl --BitDensity --AverageBitDensity  
--NumOfOnBits SampleFPBin.csv
```

To list vector values type, format and number of non-zero values for fingerprints vector strings data present in a column named containing fingerprint substring along with fingerprints type and description, type:

```
% InfoFingerprintsTextFiles.pl --FingerprintsType --FingerprintsDescription  
--FingerprintsVectorValuesType --FingerprintsVectorValuesFormat  
--NumOfNonZeroValues SampleFPcount.csv
```

AUTHOR

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SEE ALSO

InfoFingerprintsSDFFiles.pl, SimilarityMatrixSDFFiles.pl, SimilarityMatrixTextFiles.pl,
AtomNeighborhoodsFingerprints.pl, ExtendedConnectivityFingerprints.pl, MACCSKeysFingerprints.pl,
PathLengthFingerprints.pl, TopologicalAtomPairsFingerprints.pl, TopologicalAtomTorsionsFingerprints.pl,
TopologicalPharmacophoreAtomPairsFingerprints.pl, TopologicalPharmacophoreAtomTripletsFingerprints.pl

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