


```

FingerprintsVector;TopologicalAtomPairs:AtomicInvariantsAtomTypes;23;
NumericalValues;IDsAndValuesPairsString;C.X1.BO1.H3-D1-C.X3.BO4 1
C.X2.BO3.H1-D1-C.X2.BO3.H1 1 C.X2.BO3.H1-D1-C.X3.BO4 2 C.X2.BO3.H1-
D1-N.X2.BO2.H1 2 C.X3.BO4-D1-C.X3.BO4 1 C.X3.BO4-D1-O.X1.BO2 1
C.X1.BO1.H3-D2-C.X2.BO3.H1 1 C.X1.BO1.H3-D2-C.X3.BO4 1
C.X2.BO3.H1-D2-C.X2.BO3.H1 1 C.X2.BO3.H1-D2-C.X3.BO4 3...

FingerprintsVector;TopologicalAtomTorsions:AtomicInvariantsAtomTypes;11;
NumericalValues;IDsAndValuesString;C.X1.BO1.H3-C.X3.BO4-C.X2.BO3.H1-
N.X2.BO2.H1 C.X1.BO1.H3-C.X3.BO4-C.X3.BO4-C.X2.BO3.H1 C.X1.BO1.H3-
C.X3.BO4-C.X3.BO4-O.X1.BO2 C.X2.BO3.H1-C.X2.BO3.H1-C.X3.BO4-C.X3.BO4
C.X2.BO3.H1-C.X2.BO3.H1-C.X3.BO4-O.X1.BO2...;
1 1 1 1 1 1 1 1 1 1 1

FingerprintsVector;TopologicalAtomTorsions:AtomicInvariantsAtomTypes;11;
NumericalValues;IDsAndValuesPairsString;C.X1.BO1.H3-C.X3.BO4-C.X2.BO3.H1-
N.X2.BO2.H1 1 C.X1.BO1.H3-C.X3.BO4-C.X3.BO4-C.X2.BO3.H1 1 C.X1.BO1.H3-
C.X3.BO4-C.X3.BO4-O.X1.BO2 1 C.X2.BO3.H1-C.X2.BO3.H1-C.X3.BO4-
C.X3.BO4 1 C.X2.BO3.H1-C.X2.BO3.H1-C.X3.BO4-O.X1.BO2 1 C.X2.BO3.H1-
C.X2.BO3.H1-N.X2.BO2.H1-C.X2.BO3.H1 1 C.X2.BO3.H1-C.X3.BO4-C.X3.BO4-
C.X2.BO3.H1 1...

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

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 1 0 0 1 1 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.
- 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.

- 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.
- 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 data field with Fingerprint substring in its label, type:

```
% InfoFingerprintsSDFFiles.pl SampleFPBin.sdf
% InfoFingerprintsSDFFiles.pl SampleFPHex.sdf
% InfoFingerprintsSDFFiles.pl SampleFPcount.sdf
```

To list all available information about fingerprints bit-vector or vector strings data present in a data field with Fingerprint substring in its label, type:

```
% InfoFingerprintsSDFFiles.pl -a SampleFPHex.sdf
% InfoFingerprintsSDFFiles.pl -a SampleFPcount.sdf
```

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

```
% InfoFingerprintsSDFFiles.pl -a --FingerprintsField Fingerprints
SampleFPHex.sdf
% InfoFingerprintsSDFFiles.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 a data field with Fingerprint substring in its label, type:

```
% InfoFingerprintsSDFFiles.pl --BitDensity --AverageBitDensity
--NumOfOnBits SampleFPBin.sdf
```

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

```
% InfoFingerprintsSDFiles.pl --FingerprintsType --FingerprintsDescription  
--FingerprintsVectorValuesType --FingerprintsVectorValuesFormat  
--NumOfNonZeroValues SampleFPcount.sdf
```

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SEE ALSO

InfoFingerprintsTextFiles.pl, SimilarityMatrixSDFiles.pl, SimilarityMatrixTextFiles.pl, AtomNeighborhoodsFingerprints.pl, ExtendedConnectivityFingerprints.pl, MACCSKeysFingerprints.pl, PathLengthFingerprints.pl, TopologicalAtomPairsFingerprints.pl, TopologicalAtomTorsionsFingerprints.pl, TopologicalPharmacophoreAtomPairsFingerprints.pl, TopologicalPharmacophoreAtomTripletsFingerprints.pl

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