NAME

MACCSKeysFingerprints.pl - Generate MACCS key fingerprints for SD files

SYNOPSIS

MACCSKeysFingerprints.pl SDFile(s)...

MACCSKeysFingerprints.pl [--AromaticityModel *AromaticityModelType*] [--BitsOrder *Ascending* | *Descending*] [-b, --BitStringFormat *BinaryString* | *HexadecimalString*] [--CompoundID *DataFieldName or LabelPrefixString*] [--CompoundIDLabel *text*] [--CompoundIDMode *DataField* | *MolName* | *LabelPrefix* | *MolNameOrLabelPrefix*] [--DataFields *"FieldLabel1,FieldLabel2,..."*] [-d, --DataFieldsMode *All* | *Common* | *Specify* | *CompoundID*] [-f, --Filter *Yes* | *No*] [--FingerprintsLabel *text*] [-h, --help] [-k, --KeepLargestComponent *Yes* | *No*] [-m, --mode *MACCSKeyBits* | *MACCSKeyCount*] [--OutDelim *comma* | *tab* | *semicolon*] [--output *SD* | *FP* | *text* | *all*] [-o, --overwrite] [-q, --quote *Yes* | *No*] [-r, --root *RootName*] [-s, --size *number*] [-v, --VectorStringFormat *IDsAndValuesString* | *IDsAndValuesPairsString* | *ValuesAndIDsString* | *ValuesAndIDsPairsString*] [-w, --WorkingDir *DirName*]

DESCRIPTION

Generate MACCS (Molecular ACCess System) keys fingerprints [Ref 45-47] for *SDFile(s)* and create appropriate SD, FP or CSV/TSV text file(s) containing fingerprints bit-vector or vector strings corresponding to molecular fingerprints.

Multiple SDFile names are separated by spaces. The valid file extensions are *.sdf* and *.sd*. All other file names are ignored. All the SD files in a current directory can be specified either by **.sdf* or the current directory name.

For each MACCS keys definition, atoms are processed to determine their membership to the key and the appropriate molecular fingerprints strings are generated. An atom can belong to multiple MACCS keys.

For *MACCSKeyBits* value of -m, --mode option, a fingerprint bit-vector string containing zeros and ones is generated and for *MACCSKeyCount* value, a fingerprint vector string corresponding to number of MACCS keys [Ref 45-47] is generated.

MACCSKeyBits | *MACCSKeyCount* values for -m, --mode option along with two possible *166* | *322* values of -s, --size supports generation of four different types of MACCS keys fingerprint: *MACCS166KeyBits, MACCS166KeyCount, MACCS322KeyBits, MACCS322KeyCount*.

Example of *SD* file containing MAACS keys fingerprints string data:

```
... ...
... ...
$$$$
... ...
... ...
... ...
41 44  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>
Cmpd1

>  <MACCSKeysFingerprints>
FingerprintsBitVector;MACCSKeyBits;166;BinaryString;Ascending;000000000
000000000000000000000000000000010010000100100000000100100000000001110001
001010101111000110110001001101100000110111101001101111111111111011111111
11111111110111000

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

Example of *FP* file containing MAACS keys fingerprints string data:

```
#
# Package = MayaChemTools 7.4
# Release Date = Oct 21, 2010
#
# TimeStamp = Fri Mar 11 14:57:24 2011
#
# FingerprintsStringType = FingerprintsBitVector
#
# Description = MACCSKeyBits
# Size = 166
# BitStringFormat = BinaryString
# BitsOrder = Ascending
#
Cmpd1 00000000000000000000000000000000000000000001001000010010000000001...
Cmpd2 00000000000000000000000010000000010000000100000000010000000000...
... ...
... ..
```

Example of CSV *Text* file containing MAACS keys fingerprints string data:

```
"CompoundID","MACCSKeysFingerprints"
"Cmpd1","FingerprintsBitVector;MACCSKeyBits;166;BinaryString;Ascending;
00000000000000000000000000000000000000000001001000010010000000001001000000
00111000100101010111100011011000100110110000011011110100110111111111111111
01111111111111111110111000"
... ...
... ...
```

The current release of MayaChemTools generates the following types of MACCS keys fingerprints bit-vector and vector strings:

```
FingerprintsBitVector;MACCSKeyBits;166;BinaryString;Ascending;00000000
00000000000000000000000000000000001001000010010000000010010000000011100
01001010101111000110110001001101100000110111101001101111111111111011111
11111111111110111000


FingerprintsBitVector;MACCSKeyBits;166;HexadecimalString;Ascending;000
000000021210210e845f8d8c60b79dffbffffd1


FingerprintsBitVector;MACCSKeyBits;322;BinaryString;Ascending;11101011
11100111111001011111110001111011001100000000000000011100010000000000000
00000000000000000000000000000000000000000000000010100000000000000000000
00000000000000000000000000000000000000000000000000000000000000000000000
00000000000000000000000000000000000000011000000000000000000000000000000
00000000000000000000000000000000000000


FingerprintsBitVector;MACCSKeyBits;322;HexadecimalString;Ascending;7d7
e7af3edc000c11000000000000005000000000000000000000000000000003000000000
000000000


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 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 0 1 1 8 0 0 0 1 0 0 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 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;ValuesStri
ng;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 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 0 0 0 0 0 0 ...
```

OPTIONS

--AromaticityModel *MDLAromaticityModel* | *TriposAromaticityModel* | *MMFFAromaticityModel* | *ChemAxonBasicAromaticityModel* | *ChemAxonGeneralAromaticityModel* | *DaylightAromaticityModel* | *MayaChemToolsAromaticityModel*

Specify aromaticity model to use during detection of aromaticity. Possible values in the current release are: *MDLAromaticityModel, TriposAromaticityModel, MMFFAromaticityModel, ChemAxonBasicAromaticityModel, ChemAxonGeneralAromaticityModel, DaylightAromaticityModel or MayaChemToolsAromaticityModel*. Default value: *MayaChemToolsAromaticityModel*.

The supported aromaticity model names along with model specific control parameters are defined in AromaticityModelsData.csv, which is distributed with the current release and is available under lib/data directory. Molecule.pm module retrieves data from this file during class instantiation and makes it available to method DetectAromaticity for detecting aromaticity corresponding to a specific model.

--BitsOrder *Ascending* | *Descending*

Bits order to use during generation of fingerprints bit-vector string for *MACCSKeyBits* value of -m, --mode option. Possible values: *Ascending, Descending*. Default: *Ascending*.

Ascending bit order which corresponds to first bit in each byte as the lowest bit as opposed to the highest bit.

Internally, bits are stored in *Ascending* order using Perl vec function. Regardless of machine order, big-endian or little-endian, vec function always considers first string byte as the lowest byte and first bit within each byte as the lowest bit.

-b, --BitStringFormat *BinaryString* | *HexadecimalString*

Format of fingerprints bit-vector string data in output SD, FP or CSV/TSV text file(s) specified by --output used during *MACCSKeyBits* value of -m, --mode option. Possible values: *BinaryString, HexadecimalString*. Default value: *BinaryString*.

BinaryString corresponds to an ASCII string containing 1s and 0s. *HexadecimalString* contains bit values in ASCII hexadecimal format.

Examples:

```
FingerprintsBitVector;MACCSKeyBits;166;BinaryString;Ascending;00000000
000000000000000000000000000000000100100001001000000001001000000000011100
010010101011110001101100010011011000001101111010011011111111111111011111
11111111111110111000

FingerprintsBitVector;MACCSKeyBits;166;HexadecimalString;Ascending;000
000000021210210e845f8d8c60b79dffbffffd1

FingerprintsBitVector;MACCSKeyBits;322;BinaryString;Ascending;11101011
111001111110010111111100011110110011000000000000001110001000000000000000
000000000000000000000000000000000000000000000001010000000000000000000000
000000000000000000000000000000000000000000000000000000000000000000000000
000000000000000000000000000000000000011000000000000000000000000000000000
00000000000000000000000000000000000000

FingerprintsBitVector;MACCSKeyBits;322;HexadecimalString;Ascending;7d7
e7af3edc000c11000000000000005000000000000000000000000000000000300000000
000000000
```

--CompoundID *DataFieldName or LabelPrefixString*

This value is --CompoundIDMode specific and indicates how compound ID is generated.

For *DataField* value of --CompoundIDMode option, it corresponds to datafield label name whose value is used as compound ID; otherwise, it's a prefix string used for generating compound IDs like LabelPrefixString<Number>. Default value, *Cmpd*, generates compound IDs which look like Cmpd<Number>.

Examples for *DataField* value of --CompoundIDMode:

```
MolID
ExtReg
```

Examples for *LabelPrefix* or *MolNameOrLabelPrefix* value of --CompoundIDMode:

```
Compound
```

The value specified above generates compound IDs which correspond to Compound<Number> instead of default value of Cmpd<Number>.

--CompoundIDLabel *text*

Specify compound ID column label for FP or CSV/TSV text file(s) used during *CompoundID* value of --DataFieldsMode option. Default: *CompoundID*.

--CompoundIDMode *DataField* | *MolName* | *LabelPrefix* | *MolNameOrLabelPrefix*

Specify how to generate compound IDs and write to FP or CSV/TSV text file(s) along with generated fingerprints for *FP* | *text* | *all* values of --output option: use a *SDFile(s)* datafield value; use molname line from *SDFile(s)*; generate a sequential ID with specific prefix; use combination of both MolName and LabelPrefix with usage of LabelPrefix values for empty molname lines.

Possible values: *DataField* | *MolName* | *LabelPrefix* | *MolNameOrLabelPrefix*. Default: *LabelPrefix*.

For *MolNameAndLabelPrefix* value of --CompoundIDMode, molname line in *SDFile(s)* takes precedence over sequential compound IDs generated using *LabelPrefix* and only empty molname values are replaced with sequential compound IDs.

This is only used for *CompoundID* value of --DataFieldsMode option.

--DataFields *"FieldLabel1,FieldLabel2,..."*

Comma delimited list of *SDFiles(s)* data fields to extract and write to CSV/TSV text file(s) along with generated fingerprints for *text* | *all* values of --output option.

This is only used for *Specify* value of --DataFieldsMode option.

Examples:

```
Extreg
MolID,CompoundName
```

-d, --DataFieldsMode *All* | *Common* | *Specify* | *CompoundID*

Specify how data fields in *SDFile(s)* are transferred to output CSV/TSV text file(s) along with generated fingerprints for *text* | *all* values of --output option: transfer all SD data field; transfer SD data files common to all compounds; extract specified data fields; generate a compound ID using molname line, a compound prefix, or a combination of both. Possible values: *All* | *Common* | *specify* | *CompoundID*. Default value: *CompoundID*.

-f, --Filter *Yes* | *No*

Specify whether to check and filter compound data in SDFile(s). Possible values: *Yes or No*. Default value: *Yes*.

By default, compound data is checked before calculating fingerprints and compounds containing atom data corresponding to non-element symbols or no atom data are ignored.

--FingerprintsLabel *text*

SD data label or text file column label to use for fingerprints string in output SD or CSV/TSV text file(s) specified by --output. Default value: *MACCSKeyFingerprints*.

-h, --help

Print this help message.

-k, --KeepLargestComponent *Yes* | *No*

Generate fingerprints for only the largest component in molecule. Possible values: *Yes or No*. Default value: *Yes*.

For molecules containing multiple connected components, fingerprints can be generated in two different ways: use all connected components or just the largest connected component. By default, all atoms except for the largest connected component are deleted before generation of fingerprints.

-m, --mode *MACCSKeyBits* | *MACCSKeyCount*

Specify type of MACCS keys [Ref 45-47] fingerprints to generate for molecules in *SDFile(s)*. Possible values: *MACCSKeyBits, MACCSKeyCount*. Default value: *MACCSKeyBits*.

For *MACCSKeyBits* value of -m, --mode option, a fingerprint bit-vector string containing zeros and ones is generated and for *MACCSKeyCount* value, a fingerprint vector string corresponding to number of MACCS keys is generated.

MACCSKeyBits | *MACCSKeyCount* values for -m, --mode option along with two possible *166* | *322* values of -s, --size supports generation of four different types of MACCS keys fingerprint: *MACCS166KeyBits, MACCS166KeyCount, MACCS322KeyBits, MACCS322KeyCount*.

Definition of MACCS keys uses the following atom and bond symbols to define atom and bond environments:

```
Atom symbols for 166 keys [ Ref 47 ]:

A : Any valid periodic table element symbol
Q  : Hetro atoms; any non-C or non-H atom
X  : Halogens; F, Cl, Br, I
Z  : Others; other than H, C, N, O, Si, P, S, F, Cl, Br, I

Atom symbols for 322 keys [ Ref 46 ]:

A : Any valid periodic table element symbol
Q  : Hetro atoms; any non-C or non-H atom
X  : Others; other than H, C, N, O, Si, P, S, F, Cl, Br, I
Z is neither defined nor used

Bond types:

-  : Single
=  : Double
T  : Triple
#  : Triple
~  : Single or double query bond
%  : An aromatic query bond

None : Any bond type; no explicit bond specified

$  : Ring bond; $ before a bond type specifies ring bond
!  : Chain or non-ring bond; ! before a bond type specifies chain bond

@  : A ring linkage and the number following it specifies the
     atoms position in the line, thus @1 means linked back to the first
     atom in the list.

Aromatic: Kekule or Arom5

Kekule: Bonds in 6-membered rings with alternate single/double bonds
        or perimeter bonds
Arom5:  Bonds in 5-membered rings with two double bonds and a hetro
        atom at the apex of the ring.
```

MACCS 166 keys [Ref 45-47] are defined as follows:

```
Key Description

1 ISOTOPE
2 103 < ATOMIC NO. < 256
3 GROUP IVA,VA,VIA PERIODS 4-6 (Ge...)
4 ACTINIDE
5 GROUP IIIB,IVB (Sc...)
6 LANTHANIDE
7 GROUP VB,VIB,VIIB (V...)
8 QAAA@1
```

```
9 GROUP VIII (Fe...)
10 GROUP IIA (ALKALINE EARTH)
11 4M RING
12 GROUP IB,IIB (Cu...)
13 ON(C)C
14 S-S
15 OC(O)O
16 QAA@1
17 CTC
18 GROUP IIIA (B...)
19 7M RING
20 SI
21 C=C(Q)Q
22 3M RING
23 NC(O)O
24 N-O
25 NC(N)N
26 C$=C($A)$A
27 I
28 QCH2Q
29 P
30 CQ(C)(C)A
31 QX
32 CSN
33 NS
34 CH2=A
35 GROUP IA (ALKALI METAL)
36 S HETEROCYCLE
37 NC(O)N
38 NC(C)N
39 OS(O)O
40 S-O
41 CTN
42 F
43 QHAQH
44 OTHER
45 C=CN
46 BR
47 SAN
48 OQ(O)O
49 CHARGE
50 C=C(C)C
51 CSO
52 NN
53 QHAAAQH
54 QHAAQH
55 OSO
56 ON(O)C
57 O HETEROCYCLE
58 QSQ
59 Snot%A%A
60 S=O
61 AS(A)A
62 A$A!A$A
63 N=O
64 A$A!S
65 C%N
66 CC(C)(C)A
67 QS
68 QHQH (&...)
69 QQH
70 QNQ
71 NO
72 OAAO
```

```
 73 S=A
 74 CH3ACH3
 75 A!N$A
 76 C=C(A)A
 77 NAN
 78 C=N
 79 NAAN
 80 NAAAN
 81 SA(A)A
 82 ACH2QH
 83  QAAAA@1
 84 NH2
 85 CN(C)C
 86 CH2QCH2
 87 X!A$A
 88 S
 89 OAAAO
 90 QHAACH2A
 91 QHAAACH2A
 92 OC(N)C
 93 QCH3
 94 QN
 95 NAAO
 96 5M RING
 97 NAAAO
 98 QAAAAA@1
 99 C=C
100 ACH2N
101 8M RING
102 QO
103 CL
104 QHACH2A
105 A$A($A)$A
106 QA(Q)Q
107 XA(A)A
108 CH3AAACH2A
109 ACH2O
110 NCO
111 NACH2A
112 AA(A)(A)A
113 Onot%A%A
114 CH3CH2A
115 CH3ACH2A
116 CH3AACH2A
117 NAO
118 ACH2CH2A > 1
119 N=A
120 HETEROCYCLIC ATOM > 1 (&...)
121 N HETEROCYCLE
122 AN(A)A
123 OCO
124 QQ
125 AROMATIC RING > 1
126 A!O!A
127 A$A!O > 1 (&...)
128 ACH2AAACH2A
129 ACH2AACH2A
130 QQ > 1 (&...)
131 QH > 1
132 OACH2A
133 A$A!N
134 X (HALOGEN)
135 Nnot%A%A
136 O=A > 1
```

```
137 HETEROCYCLE
138 QCH2A > 1 (&...)
139 OH
140 O > 3 (&...)
141 CH3 > 2 (&...)
142 N > 1
143 A$A!O
144 Anot%A%Anot%A
145 6M RING > 1
146 O > 2
147 ACH2CH2A
148 AQ(A)A
149 CH3 > 1
150 A!A$A!A
151 NH
152 OC(C)C
153 QCH2A
154 C=O
155 A!CH2!A
156 NA(A)A
157 C-O
158 C-N
159 O > 1
160 CH3
161 N
162 AROMATIC
163 6M RING
164 O
165 RING
166  FRAGMENTS
```

MACCS 322 keys set as defined in tables 1, 2 and 3 [Ref 46] include:

```
. 26 atom properties of type P, as listed in Table 1
. 32 one-atom environments, as listed in Table 3
. 264 atom-bond-atom combinations listed in Table 4
```

Total number of keys in three tables is : 322

Atom symbol, X, used for 322 keys [Ref 46] doesn't refer to Halogens as it does for 166 keys. In order to keep the definition of 322 keys consistent with the published definitions, the symbol X is used to imply "others" atoms, but it's internally mapped to symbol X as defined for 166 keys during the generation of key values.

Atom properties-based keys (26):

```
Key   Description
1     A(AAA) or AA(A)A - atom with at least three neighbors
2     Q - heteroatom
3     Anot%not-A - atom involved in one or more multiple bonds, not aromatic
4     A(AAAA) or AA(A)(A)A - atom with at least four neighbors
5     A(QQ) or QA(Q) - atom with at least two heteroatom neighbors
6     A(QQQ) or QA(Q)Q - atom with at least three heteroatom neighbors
7     QH - heteroatom with at least one hydrogen attached
8     CH2(AA) or ACH2A - carbon with at least two single bonds and at least
      two hydrogens attached
9     CH3(A) or ACH3 - carbon with at least one single bond and at least three
      hydrogens attached
10    Halogen
11    A(-A-A-A) or A-A(-A)-A - atom has at least three single bonds
12    AAAAAA@1 > 2 - atom is in at least two different six-membered rings
13    A($A$A$A) or A$A($A)$A - atom has more than two ring bonds
14    A$A!A$A - atom is at a ring/chain boundary. When a comparison is done
      with another atom the path passes through the chain bond.
15    Anot%A%Anot%A - atom is at an aromatic/nonaromatic boundary. When a
      comparison is done with another atom the path
```

```
      passes through the aromatic bond.
16    A!A!A  - atom with more than one chain bond
17    A!A$A!A - atom is at a ring/chain boundary. When a comparison is done
      with another atom the path passes through the ring bond.
18    A%Anot%A%A - atom is at an aromatic/nonaromatic boundary. When a
      comparison is done with another atom the
      path passes through the nonaromatic bond.
19    HETEROCYCLE - atom is a heteroatom in a ring.
20    rare properties: atom with five or more neighbors, atom in
      four or more rings, or atom types other than
      H, C, N, O, S, F, Cl, Br, or I
21    rare properties: atom has a charge, is an isotope, has two or
      more multiple bonds, or has a triple bond.
22    N - nitrogen
23    S - sulfur
24    O - oxygen
25    A(AA)A(A)A(AA) - atom has two neighbors, each with three or
      more neighbors (including the central atom).
26    CHACH2 - atom has two hydrocarbon (CH2) neighbors
```

Atomic environments properties-based keys (32):

```
Key   Description
27    C(CC)
28    C(CCC)
29    C(CN)
30    C(CCN)
31    C(NN)
32    C(NNC)
33    C(NNN)
34    C(CO)
35    C(CCO)
36    C(NO)
37    C(NCO)
38    C(NNO)
39    C(OO)
40    C(COO)
41    C(NOO)
42    C(OOO)
43    Q(CC)
44    Q(CCC)
45    Q(CN)
46    Q(CCN)
47    Q(NN)
48    Q(CNN)
49    Q(NNN)
50    Q(CO)
51    Q(CCO)
52    Q(NO)
53    Q(CNO)
54    Q(NNO)
55    Q(OO)
56    Q(COO)
57    Q(NOO)
58    Q(OOO)
```

Note: The first symbol is the central atom, with atoms bonded to the central atom listed in parentheses. Q is any non-C, non-H atom. If only two atoms are in parentheses, there is no implication concerning the other atoms bonded to the central atom.

Atom-Bond-Atom properties-based keys: (264)

```
Key   Description
59    C-C
60    C-N
```

```
61    C-O
62    C-S
63    C-Cl
64    C-P
65    C-F
66    C-Br
67    C-Si
68    C-I
69    C-X
70    N-N
71    N-O
72    N-S
73    N-Cl
74    N-P
75    N-F
76    N-Br
77    N-Si
78    N-I
79    N-X
80    O-O
81    O-S
82    O-Cl
83    O-P
84    O-F
85    O-Br
86    O-Si
87    O-I
88    O-X
89    S-S
90    S-Cl
91    S-P
92    S-F
93    S-Br
94    S-Si
95    S-I
96    S-X
97    Cl-Cl
98    Cl-P
99    Cl-F
100   Cl-Br
101   Cl-Si
102   Cl-I
103   Cl-X
104   P-P
105   P-F
106   P-Br
107   P-Si
108   P-I
109   P-X
110   F-F
111   F-Br
112   F-Si
113   F-I
114   F-X
115   Br-Br
116   Br-Si
117   Br-I
118   Br-X
119   Si-Si
120   Si-I
121   Si-X
122   I-I
123   I-X
124   X-X
```

```
125   C=C
126   C=N
127   C=O
128   C=S
129   C=Cl
130   C=P
131   C=F
132   C=Br
133   C=Si
134   C=I
135   C=X
136   N=N
137   N=O
138   N=S
139   N=Cl
140   N=P
141   N=F
142   N=Br
143   N=Si
144   N=I
145   N=X
146   O=O
147   O=S
148   O=Cl
149   O=P
150   O=F
151   O=Br
152   O=Si
153   O=I
154   O=X
155   S=S
156   S=Cl
157   S=P
158   S=F
159   S=Br
160   S=Si
161   S=I
162   S=X
163   Cl=Cl
164   Cl=P
165   Cl=F
166   Cl=Br
167   Cl=Si
168   Cl=I
169   Cl=X
170   P=P
171   P=F
172   P=Br
173   P=Si
174   P=I
175   P=X
176   F=F
177   F=Br
178   F=Si
179   F=I
180   F=X
181   Br=Br
182   Br=Si
183   Br=I
184   Br=X
185   Si=Si
186   Si=I
187   Si=X
188   I=I
```

```
189   I=X
190   X=X
191   C#C
192   C#N
193   C#O
194   C#S
195   C#Cl
196   C#P
197   C#F
198   C#Br
199   C#Si
200   C#I
201   C#X
202   N#N
203   N#O
204   N#S
205   N#Cl
206   N#P
207   N#F
208   N#Br
209   N#Si
210   N#I
211   N#X
212   O#O
213   O#S
214   O#Cl
215   O#P
216   O#F
217   O#Br
218   O#Si
219   O#I
220   O#X
221   S#S
222   S#Cl
223   S#P
224   S#F
225   S#Br
226   S#Si
227   S#I
228   S#X
229   Cl#Cl
230   Cl#P
231   Cl#F
232   Cl#Br
233   Cl#Si
234   Cl#I
235   Cl#X
236   P#P
237   P#F
238   P#Br
239   P#Si
240   P#I
241   P#X
242   F#F
243   F#Br
244   F#Si
245   F#I
246   F#X
247   Br#Br
248   Br#Si
249   Br#I
250   Br#X
251   Si#Si
252   Si#I
```

```
253   Si#X
254   I#I
255   I#X
256   X#X
257   C$C
258   C$N
259   C$O
260   C$S
261   C$Cl
262   C$P
263   C$F
264   C$Br
265   C$Si
266   C$I
267   C$X
268   N$N
269   N$O
270   N$S
271   N$Cl
272   N$P
273   N$F
274   N$Br
275   N$Si
276   N$I
277   N$X
278   O$O
279   O$S
280   O$Cl
281   O$P
282   O$F
283   O$Br
284   O$Si
285   O$I
286   O$X
287   S$S
288   S$Cl
289   S$P
290   S$F
291   S$Br
292   S$Si
293   S$I
294   S$X
295   Cl$Cl
296   Cl$P
297   Cl$F
298   Cl$Br
299   Cl$Si
300   Cl$I
301   Cl$X
302   P$P
303   P$F
304   P$Br
305   P$Si
306   P$I
307   P$X
308   F$F
309   F$Br
310   F$Si
311   F$I
312   F$X
313   Br$Br
314   Br$Si
315   Br$I
316   Br$X
```

```
317   Si$Si
318   Si$I
319   Si$X
320   I$I
321   I$X
322   X$X
```

--OutDelim *comma | tab | semicolon*

Delimiter for output CSV/TSV text file(s). Possible values: *comma, tab, or semicolon* Default value: *comma*.

--output *SD | FP | text | all*

Type of output files to generate. Possible values: *SD, FP, text, or all*. Default value: *text*.

-o, --overwrite

Overwrite existing files.

-q, --quote *Yes | No*

Put quote around column values in output CSV/TSV text file(s). Possible values: *Yes or No*. Default value: *Yes*.

-r, --root *RootName*

New file name is generated using the root: <Root>.<Ext>. Default for new file names: <SDFileName><MACCSKeysFP>.<Ext>. The file type determines <Ext> value. The sdf, fpf, csv, and tsv <Ext> values are used for SD, FP, comma/semicolon, and tab delimited text files, respectively.This option is ignored for multiple input files.

-s, --size *number*

Size of MACCS keys [Ref 45-47] set to use during fingerprints generation. Possible values: *166 or 322*. Default value: *166*.

-v, --VectorStringFormat *ValuesString | IDsAndValuesString | IDsAndValuesPairsString | ValuesAndIDsString | ValuesAndIDsPairsString*

Format of fingerprints vector string data in output SD, FP or CSV/TSV text file(s) specified by --output used during *MACCSKeyCount* value of -m, --mode option. Possible values: *ValuesString, IDsAndValuesString | IDsAndValuesPairsString | ValuesAndIDsString | ValuesAndIDsPairsString*. Defaultvalue: *ValuesString*.

Examples:

```
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 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 0 0 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 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;ValuesStri
ng;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 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 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 0 0 0 ...
```

-w, --WorkingDir *DirName*

Location of working directory. Default: current directory.

EXAMPLES

To generate MACCS keys fingerprints of size 166 in binary bit-vector string format and create a SampleMACCS166FPBin.csv file containing sequential compound IDs along with fingerprints bit-vector strings data, type:

```
% MACCSKeysFingerprints.pl -r SampleMACCS166FPBin -o Sample.sdf
```

To generate MACCS keys fingerprints of size 166 in binary bit-vector string format and create SampleMACCS166FPBin.sdf, SampleMACCS166FPBin.csv and SampleMACCS166FPBin.csv files containing sequential compound IDs in CSV file along with fingerprints bit-vector strings data, type:

```
% MACCSKeysFingerprints.pl --output all -r SampleMACCS166FPBin
  -o Sample.sdf
```

To generate MACCS keys fingerprints of size 322 in binary bit-vector string format and create a SampleMACCS322FPBin.csv file containing sequential compound IDs along with fingerprints bit-vector strings data, type:

```
% MACCSKeysFingerprints.pl -size 322 -r SampleMACCS322FPBin -o Sample.sdf
```

To generate MACCS keys fingerprints of size 166 corresponding to count of keys in ValuesString format and create a SampleMACCS166FPCount.csv file containing sequential compound IDs along with fingerprints vector strings data, type:

```
% MACCSKeysFingerprints.pl -m MACCSKeyCount -r SampleMACCS166FPCount
  -o Sample.sdf
```

To generate MACCS keys fingerprints of size 322 corresponding to count of keys in ValuesString format and create a SampleMACCS322FPCount.csv file containing sequential compound IDs along with fingerprints vector strings data, type:

```
% MACCSKeysFingerprints.pl -m MACCSKeyCount -size 322
  -r SampleMACCS322FPCount -o Sample.sdf
```

To generate MACCS keys fingerprints of size 166 in hexadecimal bit-vector string format with ascending bits order and create a SampleMACCS166FPHex.csv file containing compound IDs from MolName along with fingerprints bit-vector strings data, type:

```
% MACCSKeysFingerprints.pl -m MACCSKeyBits --size 166 --BitStringFormat
  HexadecimalString --BitsOrder Ascending --DataFieldsMode CompoundID
  --CompoundIDMode MolName -r SampleMACCS166FPBin -o Sample.sdf
```

To generate MACCS keys fingerprints of size 166 corresponding to count of keys in IDsAndValuesString format and create a SampleMACCS166FPCount.csv file containing compound IDs from MolName line along with fingerprints vector strings data, type:

```
% MACCSKeysFingerprints.pl -m MACCSKeyCount --size 166
  --VectorStringFormat IDsAndValuesString  --DataFieldsMode CompoundID
  --CompoundIDMode MolName -r SampleMACCS166FPCount -o Sample.sdf
```

To generate MACCS keys fingerprints of size 166 corresponding to count of keys in IDsAndValuesString format and create a SampleMACCS166FPCount.csv file containing compound IDs using specified data field along with fingerprints vector strings data, type:

```
% MACCSKeysFingerprints.pl -m MACCSKeyCount --size 166
  --VectorStringFormat IDsAndValuesString  --DataFieldsMode CompoundID
  --CompoundIDMode DataField --CompoundID Mol_ID -r
  SampleMACCS166FPCount -o Sample.sdf
```

To generate MACCS keys fingerprints of size 322 corresponding to count of keys in ValuesString format and create a SampleMACCS322FPCount.tsv file containing compound IDs derived from combination of molecule name line and an explicit compound prefix along with fingerprints vector strings data in a column labels MACCSKeyCountFP, type:

```
% MACCSKeysFingerprints.pl -m MACCSKeyCount -size 322 --DataFieldsMode
  CompoundID --CompoundIDMode MolnameOrLabelPrefix --CompoundID Cmpd
  --CompoundIDLabel MolID --FingerprintsLabel MACCSKeyCountFP --OutDelim
  Tab -r SampleMACCS322FPCount -o Sample.sdf
```

To generate MACCS keys fingerprints of size 166 corresponding to count of keys in ValuesString format and create

a SampleMACCS166FPCount.csv file containing specific data fields columns along with fingerprints vector strings data, type:

```
% MACCSKeysFingerprints.pl -m MACCSKeyCount --size 166
  --VectorStringFormat ValuesString --DataFieldsMode Specify --DataFields
  Mol_ID  -r SampleMACCS166FPCount -o Sample.sdf
```

To generate MACCS keys fingerprints of size 322 corresponding to count of keys in ValuesString format and create a SampleMACCS322FPCount.csv file containing common data fields columns along with fingerprints vector strings data, type:

```
% MACCSKeysFingerprints.pl -m MACCSKeyCount --size 322
  --VectorStringFormat ValuesString --DataFieldsMode Common -r
  SampleMACCS322FPCount -o Sample.sdf
```

To generate MACCS keys fingerprints of size 166 corresponding to count of keys in ValuesString format and create SampleMACCS166FPCount.sdf, SampleMACCS166FPCount.fpf and SampleMACCS166FPCount.csv files containing all data fields columns in CSV file along with fingerprints vector strings data, type:

```
% MACCSKeysFingerprints.pl -m MACCSKeyCount --size 166 --output all
  --VectorStringFormat ValuesString --DataFieldsMode All -r
  SampleMACCS166FPCount -o Sample.sdf
```

AUTHOR

Manish Sud <msud@san.rr.com>

SEE ALSO

InfoFingerprintsFiles.pl, SimilarityMatricesFingerprints.pl, AtomNeighborhoodsFingerprints.pl, ExtendedConnectivityFingerprints.pl, PathLengthFingerprints.pl, TopologicalAtomPairsFingerprints.pl, TopologicalAtomTorsionsFingerprints.pl, TopologicalPharmacophoreAtomPairsFingerprints.pl, TopologicalPharmacophoreAtomTripletsFingerprints.pl

COPYRIGHT