

MACCSKeys

## SYNOPSIS

```
use Fingerprints::MACCSKeys;
```

```
use Fingerprints::MACCSKeys qw(:all);
```

## DESCRIPTION

MACCSKeys [ Ref 45-47 ] class provides the following methods:

new, GenerateFingerprints, GenerateMACCSKeys, GetDescription, SetSize, SetType, StringifyMACCSKeys

MACCSKeys is derived from Fingerprints class which in turn is derived from ObjectProperty base class that provides methods not explicitly defined in MACCSKeys, Fingerprints or ObjectProperty classes using Perl's AUTOLOAD functionality. These methods are generated on-the-fly for a specified object property:

```
Set<PropertyName>(<PropertyValue>);
$PropertyValue = Get<PropertyName>();
Delete<PropertyName>();
```

For each MACCS (Molecular ACCess System) 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 Type 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* or *MACCSKeyCount* values for Type along with two possible 166 / 322 values of Size supports generation of four different types of MACCS keys fingerprint: *MACCS166KeyBits*, *MACCS166KeyCount*, *MACCS322KeyBits*, *MACCS322KeyCount*.

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

```
FingerprintsBitVector;MACCSKeyBits;166;BinaryString;Ascending;00000000  
000000000000000000000000000000001001000010010000000010010000000011100  
01001010101111000110110001001101100000110111101001101111111111011111  
11111111111110111000
```

```
FingerprintsBitVector;MACCSKeyBits;166;HexadecimalString;Ascending;000
0000000021210210e845f8d8c60b79dffbfbbfffd1
```

[illegible][illegible]

```
FingerprintsVector;MACCSKeyCount;166;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 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 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 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 1 1 0 1 1 1 1 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;ValuesStr  
ing;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 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 11 0 2 0 0 0 0 0 0 0
```

new

```
$NewMACCSKeys = new MACCSKeys(%NamesAndValues);
```

```
Molecule = ''
Type = ''
Size = ''
```

Examples:

```
$MACCSKeys = new MACCSKeys('Molecule' => $Molecule,  
                             'Type' => 'MACCSKeyBits',  
                             'Size' => 166);  
  
$MACCSKeys = new MACCSKeys('Molecule' => $Molecule,  
                             'Type' => 'MACCSKeyCount',  
                             'Size' => 166);  
  
$MACCSKeys = new MACCSKeys('Molecule' => $Molecule,  
                             'Type' => 'MACCSKeyBit',  
                             'Size' => 322);  
  
$MACCSKeys = new MACCSKeys('Molecule' => $Molecule,  
                             'Type' => 'MACCSKeyCount',  
                             'Size' => 322);  
  
$MACCSKeys->GenerateMACCSKeys();  
print "$MACCSKeys\n";
```

## GetDescription

```
$Description = $MACCSKeys->GetDescription();
```

Returns a string containing description of MACCS keys fingerprints.

### GenerateMACCSKeys or GenerateFingerprints

```
$MACCSKeys = $MACCSKeys->GenerateMACCSKeys();
```

Generates MACCS keys fingerprints and returns *MACCSKeys*.

For *MACCSKeyBits* value of Type, 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* or *MACCSKeyCount* values for Type option along with two possible 166 | 322 values of 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 QHAAQH  
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 NAAAN  
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:

- o 26 atom properties of type P, as listed in Table 1
- o 32 one-atom environments, as listed in Table 3
- o 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%not%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

#### SetSize

```
$MACCSKeys->SetSize($Size);
```

Sets size of MACCS keys and returns *MACCSKeys*. Possible values: *166* or *322*.

#### SetType

```
$MACCSKeys->SetType($Type);
```

Sets type of MACCS keys and returns *MACCSKeys*. Possible values: *MACCSKeysBits* or *MACCSKeysCount*.

#### StringifyMACCSKeys

```
$String = $MACCSKeys->StringifyMACCSKeys();
```

Returns a string containing information about *MACCSKeys* object.

#### AUTHOR

Manish Sud <msud@san.rr.com>

#### SEE ALSO

Fingerprints.pm, FingerprintsStringUtil.pm, AtomNeighborhoodsFingerprints.pm, AtomTypesFingerprints.pm, EStateIndicesFingerprints.pm, ExtendedConnectivityFingerprints.pm, PathLengthFingerprints.pm, TopologicalAtomPairsFingerprints.pm, TopologicalAtomTripletsFingerprints.pm, TopologicalAtomTorsionsFingerprints.pm, TopologicalPharmacophoreAtomPairsFingerprints.pm, TopologicalPharmacophoreAtomTripletsFingerprints.pm

#### COPYRIGHT

Copyright (C) 2022 Manish Sud. All rights reserved.

This file is part of MayaChemTools.

MayaChemTools is free software; you can redistribute it and/or modify it under the terms of the GNU Lesser General Public License as published by the Free Software Foundation; either version 3 of the License, or (at your option) any later version.