LAMPIRAN

Lampiran. 1 Hasil *Docking*

1. Ligan NADPH

```
REMARK VINA RESULT:     -11.9      0.000      0.000
REMARK  16 active torsions:
REMARK  status: ('A' for Active; 'I' for Inactive)
REMARK    1  A    between atoms: PA_1919  and  O5B_1922
REMARK    2  A    between atoms: PA_1919  and  O3_1947
REMARK    3  A    between atoms: O5B_1922  and  C5B_1923
REMARK    4  A    between atoms: C5B_1923  and  C4B_1924
REMARK    5  A    between atoms: C3B_1926  and  O3B_1927
REMARK    6  A    between atoms: C2B_1929  and  O2B_1930
REMARK    7  A    between atoms: O2B_1930  and  P2B_1973
REMARK    8  A    between atoms: C1B_1931  and  N9A_1932
REMARK    9  A    between atoms: O3_1947  and  PN_1948
REMARK   10  A    between atoms: PN_1948  and  O5D_1951
REMARK   11  A    between atoms: O5D_1951  and  C5D_1952
REMARK   12  A    between atoms: C5D_1952  and  C4D_1953
REMARK   13  A    between atoms: C3D_1955  and  O3D_1956
REMARK   14  A    between atoms: C2D_1958  and  O2D_1959
REMARK   15  A    between atoms: C1D_1961  and  N1N_1962
REMARK   16  A    between atoms: C3N_1964  and  C7N_1965
REMARK       I    between atoms: C7N_1965  and  N7N_1967
ROOT
HETATM    1  PA  NDP A 201      11.485   7.855  28.694
1.00 12.85     0.418 P
HETATM    2  O1A NDP A 201      11.487   6.959  27.485
1.00 13.09    -0.624 OA
HETATM    3  O2A NDP A 201      10.408   7.707  29.732
1.00 12.69    -0.624 OA
ENDROOT
BRANCH   1   4
HETATM    4  O5B NDP A 201      12.893   7.782  29.470
1.00 13.35    -0.268 OA
BRANCH   4   5
HETATM    5  C5B NDP A 201      13.947   8.680  29.129
1.00 13.69     0.187 C
BRANCH   5   6
HETATM    6  C4B NDP A 201      15.043   8.342  30.116
1.00 13.97     0.177 C
HETATM    7  O4B NDP A 201      15.084   6.928  30.322
1.00 13.83    -0.331 OA
HETATM    8  C1B NDP A 201      16.440   6.510  30.518
1.00 14.26     0.238 C
HETATM    9  C2B NDP A 201      17.272   7.783  30.504
1.00 14.22     0.206 C
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HETATM   10  C3B NDP A 201      16.436   8.708  29.641
1.00 14.17     0.172 C
BRANCH   8  11
HETATM   11  N9A NDP A 201      16.868   5.602  29.414
1.00 14.52    -0.273 N
HETATM   12  C8A NDP A 201      16.547   5.706  28.111
1.00 14.86     0.158 A
HETATM   13  N7A NDP A 201      17.123   4.719  27.387
1.00 15.48    -0.333 N
HETATM   14  C5A NDP A 201      17.839   3.952  28.228
1.00 15.18     0.123 A
HETATM   15  H7A NDP A 201      17.030   4.580  26.380
1.00  0.00     0.168 HD
HETATM   16  C6A NDP A 201      18.690   2.739  28.122
1.00 15.29     0.131 A
HETATM   17  C4A NDP A 201      17.664   4.541  29.565
1.00 14.73     0.144 A
HETATM   18  N6A NDP A 201      18.915   2.113  26.936
1.00 15.76    -0.383 N
HETATM   19  N1A NDP A 201      19.249   2.281  29.262
1.00 14.97    -0.324 N
HETATM   20 2H6A NDP A 201      18.493   2.459  26.074
1.00  0.00     0.157 HD
HETATM   21 1H6A NDP A 201      19.499   1.281  26.863
1.00  0.00     0.157 HD
HETATM   22  C2A NDP A 201      19.052   2.875  30.459
1.00 15.02     0.153 A
HETATM   23  H1A NDP A 201      19.843   1.454  29.218
1.00  0.00     0.169 HD
HETATM   24  N3A NDP A 201      18.285   3.974  30.625
1.00 14.84    -0.323 N
HETATM   25  H3A NDP A 201      18.172   4.379  31.554
1.00  0.00     0.169 HD
ENDBRANCH   8  11
BRANCH   9  26
HETATM   26  O2B NDP A 201      17.379   8.265  31.843
1.00 14.39    -0.259 OA
BRANCH  26  27
HETATM   27  P2B NDP A 201      18.716   8.984  32.398
1.00 14.82     0.423 P
HETATM   28  O1X NDP A 201      19.843   8.070  31.971
1.00 15.20    -0.617 OA
HETATM   29  O2X NDP A 201      18.726  10.300  31.677
1.00 14.28    -0.617 OA
HETATM   30  O3X NDP A 201      18.487   9.076  33.885
1.00 15.33    -0.617 OA
ENDBRANCH  26  27
ENDBRANCH   9  26
BRANCH  10  31
HETATM   31  O3B NDP A 201      16.726  10.097  29.797
1.00 14.06    -0.380 OA
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HETATM   32  H3B NDP A 201      16.095  10.655  29.357
1.00  0.00      0.211 HD
ENDBRANCH  10  31
ENDBRANCH   5   6
ENDBRANCH   4   5
ENDBRANCH   1   4
BRANCH   1  33
HETATM   33  O3  NDP A 201      11.544   9.418  28.276
1.00 13.57    -0.180 OA
BRANCH  33  34
HETATM   34  PN  NDP A 201      10.814  10.227  27.100
1.00 14.04     0.418 P
HETATM   35  O1N NDP A 201      10.671  11.656  27.602
1.00 14.18    -0.624 OA
HETATM   36  O2N NDP A 201      11.506   9.977  25.784
1.00 14.31    -0.624 OA
BRANCH  34  37
HETATM   37  O5D NDP A 201       9.316   9.609  27.052
1.00 15.17    -0.268 OA
BRANCH  37  38
HETATM   38  C5D NDP A 201       8.242  10.334  27.651
1.00 18.01     0.187 C
BRANCH  38  39
HETATM   39  C4D NDP A 201       7.134  10.523  26.621
1.00 19.12     0.177 C
HETATM   40  O4D NDP A 201       6.534   9.249  26.358
1.00 20.16    -0.331 OA
HETATM   41  C1D NDP A 201       5.113   9.385  26.379
1.00 19.88     0.235 C
HETATM   42  C2D NDP A 201       4.825  10.544  27.324
1.00 20.78     0.190 C
HETATM   43  C3D NDP A 201       6.027  11.443  27.119
1.00 20.57     0.172 C
BRANCH  41  44
HETATM   44  N1N NDP A 201       4.433   8.151  26.784
1.00 19.09    -0.301 N
HETATM   45  C2N NDP A 201       3.270   7.895  26.171
1.00 18.47     0.083 A
HETATM   46  C3N NDP A 201       2.536   6.758  26.480
1.00 17.79     0.073 A
HETATM   47  C4N NDP A 201       3.025   5.865  27.441
1.00 17.96     0.008 A
HETATM   48  C5N NDP A 201       4.239   6.152  28.071
1.00 18.05     0.019 A
HETATM   49  C6N NDP A 201       4.933   7.313  27.719
1.00 18.76     0.078 A
BRANCH  46  50
HETATM   50  C7N NDP A 201       1.239   6.522  25.763
1.00 17.61     0.252 C
HETATM   51  O7N NDP A 201       0.750   5.408  25.803
1.00 17.08    -0.268 OA
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HETATM   52  N7N NDP A 201       0.655   7.536  25.108
1.00 17.22    -0.366 N
HETATM   53 2H7N NDP A 201       1.065   8.469  25.074
1.00  0.00     0.159 HD
HETATM   54 1H7N NDP A 201      -0.226   7.375  24.621
1.00  0.00     0.159 HD
ENDBRANCH  46  50
ENDBRANCH  41  44
BRANCH  42  55
HETATM   55  O2D NDP A 201       3.607  11.210  26.964
1.00 22.69    -0.378 OA
HETATM   56  H2D NDP A 201       2.852  10.652  27.108
1.00  0.00     0.211 HD
ENDBRANCH  42  55
BRANCH  43  57
HETATM   57  O3D NDP A 201       5.723  12.391  26.089
1.00 21.53    -0.380 OA
HETATM   58  H3D NDP A 201       5.079  13.005  26.422
1.00  0.00     0.211 HD
ENDBRANCH  43  57
ENDBRANCH  38  39
ENDBRANCH  37  38
ENDBRANCH  34  37
ENDBRANCH  33  34
ENDBRANCH   1  33
TORSDOF 16
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2. Obat pembanding *ketoconazole*

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MODEL 1
REMARK VINA RESULT:     -5.7      0.000      0.000
REMARK  7 active torsions:
REMARK  status: ('A' for Active; 'I' for Inactive)
REMARK    1  A    between atoms: O_5  and  C_16
REMARK    2  A    between atoms: O_5  and  C_24
REMARK    3  A    between atoms: N_7  and  C_21
REMARK       I    between atoms: N_8  and  C_25
REMARK    4  A    between atoms: N_9  and  C_14
REMARK    5  A    between atoms: C_11  and  C_14
REMARK    6  A    between atoms: C_11  and  C_15
REMARK    7  A    between atoms: C_12  and  C_16
ROOT
ATOM      1 CL   UNL d   1       7.852  10.722  29.950
0.00  0.00    -0.083 Cl
ATOM      2 CL   UNL d   1       8.968  13.581  31.556
0.00  0.00    -0.084 Cl
ATOM      3  C   UNL d   1       8.731  11.925  29.066
0.00  0.00     0.031 A
ATOM      4  C   UNL d   1       8.331  11.600  29.923
0.00  0.00     0.051 A
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ATOM      5  C   UNL d   1       9.210  12.802  29.039
0.00  0.00     0.012 A
ATOM      6  C   UNL d   1       8.410  12.152  30.753
0.00  0.00     0.040 A
ATOM      7  C   UNL d   1       9.289  13.354  29.869
0.00  0.00     0.020 A
ATOM      8  C   UNL d   1       8.889  13.029  30.726
0.00  0.00     0.042 A
ENDROOT
BRANCH   3   9
ATOM      9  C   UNL d   1       8.651  11.373  28.236
0.00  0.00     0.217 A
ATOM     10  O   UNL d   1       9.533  10.945  28.436
0.00  0.00    -0.334 OA
ATOM     11  C   UNL d   1       9.730  10.288  27.709
0.00  0.00     0.185 A
ATOM     12  C   UNL d   1       8.970  10.309  27.059
0.00  0.00     0.198 A
ATOM     13  O   UNL d   1       8.304  10.980  27.385
0.00  0.00    -0.341 OA
BRANCH  11  14
ATOM     14  C   UNL d   1      10.544   9.711  27.643
0.00  0.00     0.263 C
BRANCH  14  15
ATOM     15  O   UNL d   1      10.598   8.861  28.167
0.00  0.00    -0.489 OA
BRANCH  15  16
ATOM     16  C   UNL d   1      11.476   8.558  28.538
0.00  0.00     0.121 A
ATOM     17  C   UNL d   1      12.328   8.811  28.079
0.00  0.00     0.047 A
ATOM     18  C   UNL d   1      13.206   8.507  28.450
0.00  0.00     0.027 A
ATOM     19  C   UNL d   1      13.231   7.952  29.281
0.00  0.00     0.030 A
ATOM     20  C   UNL d   1      12.380   7.698  29.741
0.00  0.00     0.027 A
ATOM     21  C   UNL d   1      11.502   8.001  29.369
0.00  0.00     0.047 A
BRANCH  19  22
ATOM     22  N   UNL d   1      14.109   7.648  29.653
0.00  0.00    -0.327 N
ATOM     23  C   UNL d   1      14.497   8.105  30.454
0.00  0.00     0.124 A
ATOM     24  C   UNL d   1      15.374   7.802  30.826
0.00  0.00     0.126 A
ATOM     25  N   UNL d   1      15.864   7.042  30.398
0.00  0.00    -0.299 N
ATOM     26  C   UNL d   1      15.476   6.585  29.597
0.00  0.00     0.126 A
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ATOM      27  C   UNL d   1       16.741   6.739  30.770
0.00  0.00     0.213 C
ATOM      28  C   UNL d   1       14.599   6.888  29.225
0.00  0.00     0.124 A
ATOM      29  O   UNL d   1       17.129   7.196  31.570
0.00  0.00    -0.276 OA
ATOM      30  C   UNL d   1       17.230   5.979  30.342
0.00  0.00     0.109 C
ENDBRANCH  19  22
ENDBRANCH  15  16
ENDBRANCH  14  15
ENDBRANCH  11  14
BRANCH   9  31
ATOM      31  C   UNL d   1        7.838  11.950  28.302
0.00  0.00     0.193 C
BRANCH  31  32
ATOM      32  N   UNL d   1        7.367  12.247  27.471
0.00  0.00    -0.331 N
ATOM      33  C   UNL d   1        6.458  11.953  27.174
0.00  0.00     0.107 A
ATOM      34  C   UNL d   1        6.251  12.415  26.311
0.00  0.00     0.130 A
ATOM      35  N   UNL d   1        7.031  12.993  26.075
0.00  0.00    -0.244 NA
ATOM      36  C   UNL d   1        7.721  12.890  26.793
0.00  0.00     0.199 A
ENDBRANCH  31  32
ENDBRANCH   9  31
ENDBRANCH   3   9
TORSDOF 7
ENDMDL
```

3. Senyawa *Gallic acid*

```
MODEL 1
REMARK VINA RESULT:      -4.9      0.000      0.000
REMARK  6 active torsions:
REMARK  status: ('A' for Active; 'I' for Inactive)
REMARK    1  A    between atoms: O2_2  and  C1_7
REMARK    2  A    between atoms: O3_3  and  C2_8
REMARK    3  A    between atoms: O4_4  and  C4_10
REMARK    4  A    between atoms: O5_5  and  C5_11
REMARK    5  A    between atoms: O6_6  and  C6_12
REMARK    6  A    between atoms: C3_9  and  C6_12
ROOT
ATOM      1  O1  non d ame      15.118   7.048  28.879
0.00  0.00    -0.342 OA
ATOM      2  C1  non d ame      17.261   6.323  29.768
0.00  0.00     0.177 C
ATOM      3  C2  non d ame      17.318   7.557  30.697
0.00  0.00     0.179 C
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```
ATOM      4  C3  non d ame      16.431   6.590  28.507
0.00  0.00     0.178 C
ATOM      5  C4  non d ame      16.479   8.727  30.172
0.00  0.00     0.201 C
ATOM      6  C5  non d ame      15.092   8.186  29.744
0.00  0.00     0.279 C
ENDROOT
BRANCH   4   7
ATOM      7  C6  non d ame      16.244   5.329  27.655
0.00  0.00     0.190 C
BRANCH   7   8
ATOM      8  O6  non d ame      17.490   4.634  27.568
0.00  0.00    -0.393 OA
ATOM      9  H12 non d ame      18.125   5.180  28.071
0.00  0.00     0.210 HD
ENDBRANCH   7   8
ENDBRANCH   4   7
BRANCH   6  10
ATOM     10  O5  non d ame      14.315   7.836  30.885
0.00  0.00    -0.366 OA
ATOM     11  H11 non d ame      13.617   8.516  30.984
0.00  0.00     0.213 HD
ENDBRANCH   6  10
BRANCH   2  12
ATOM     12  O2  non d ame      16.695   5.225  30.514
0.00  0.00    -0.387 OA
ATOM     13  H8  non d ame      15.778   5.111  30.183
0.00  0.00     0.211 HD
ENDBRANCH   2  12
BRANCH   5  14
ATOM     14  O4  non d ame      17.163   9.370  29.094
0.00  0.00    -0.385 OA
ATOM     15  H10 non d ame      16.511   9.528  28.385
0.00  0.00     0.211 HD
ENDBRANCH   5  14
BRANCH   3  16
ATOM     16  O3  non d ame      16.833   7.203  32.007
0.00  0.00    -0.387 OA
ATOM     17  H9  non d ame      17.291   7.816  32.623
0.00  0.00     0.211 HD
ENDBRANCH   3  16
```

4. Senyawa *Clorogenic acid*

```
MODEL 1
REMARK VINA RESULT:      -8.5      0.000      0.000
REMARK  12 active torsions:
REMARK  status: ('A' for Active; 'I' for Inactive)
REMARK    1  A    between atoms: C_11  and  O_1
REMARK    2  A    between atoms: O_1  and  C_17
REMARK    3  A    between atoms: C_10  and  O_2
```

```
REMARK    4  A    between atoms: C_14  and  O_3
REMARK    5  A    between atoms: C_15  and  O_4
REMARK    6  A    between atoms: O_5  and  C_16
REMARK    7  A    between atoms: O_8  and  C_23
REMARK    8  A    between atoms: O_9  and  C_25
REMARK    9  A    between atoms: C_10  and  C_16
REMARK   10  A    between atoms: C_17  and  C_18
REMARK   11  A    between atoms: C_18  and  C_19
REMARK   12  A    between atoms: C_19  and  C_20
ROOT
ATOM      1  O   UNL d   1      11.667   8.995  27.637
0.00  0.00    -0.456 OA
ENDROOT
BRANCH   1   2
ATOM      2  C   UNL d   1      10.738   9.358  27.707
0.00  0.00     0.211 A
ATOM      3  C   UNL d   1      10.236   9.285  28.568
0.00  0.00     0.093 A
ATOM      4  C   UNL d   1       9.306   9.648  28.638
0.00  0.00     0.168 A
ATOM      5  C   UNL d   1       8.879  10.083  27.845
0.00  0.00     0.080 A
ATOM      6  C   UNL d   1       9.381  10.156  26.984
0.00  0.00     0.150 A
ATOM      7  C   UNL d   1      10.311   9.793  26.914
0.00  0.00     0.184 A
BRANCH   4   8
ATOM      8  O   UNL d   1       9.263   9.354  29.593
0.00  0.00    -0.377 OA
ATOM      9  H   UNL d   1       9.006   9.724  30.019
0.00  0.00     0.211 HD
ENDBRANCH   4   8
BRANCH   4  10
ATOM     10  C   UNL d   1       8.480   9.815  29.175
0.00  0.00     0.337 C
ATOM     11  O   UNL d   1       7.584   9.575  28.802
0.00  0.00    -0.248 OA
BRANCH  10  12
ATOM     12  O   UNL d   1       8.550  10.222  30.086
0.00  0.00    -0.479 OA
ATOM     13  H   UNL d   1       9.078  10.493  30.265
0.00  0.00     0.295 HD
ENDBRANCH  10  12
ENDBRANCH   4  10
BRANCH   6  14
ATOM     14  O   UNL d   1       8.954  10.591  26.191
0.00  0.00    -0.389 OA
ATOM     15  H   UNL d   1       8.948  10.300  25.644
0.00  0.00     0.210 HD
ENDBRANCH   6  14
BRANCH   7  16
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```
ATOM     16  O   UNL d   1      10.813   9.866  26.053
0.00  0.00    -0.386 OA
ATOM     17  H   UNL d   1      11.053   9.358  25.790
0.00  0.00     0.210 HD
ENDBRANCH   7  16
ENDBRANCH   1   2
BRANCH   1  18
ATOM     18  C   UNL d   1      11.850   8.040  27.870
0.00  0.00     0.332 C
ATOM     19  O   UNL d   1      11.401   7.307  27.360
0.00  0.00    -0.246 OA
BRANCH  18  20
ATOM     20  C   UNL d   1      12.481   7.819  28.614
0.00  0.00     0.092 C
BRANCH  20  21
ATOM     21  C   UNL d   1      13.429   7.575  28.408
0.00  0.00     0.015 C
BRANCH  21  22
ATOM     22  C   UNL d   1      14.067   7.376  29.153
0.00  0.00    -0.021 A
ATOM     23  C   UNL d   1      14.126   7.991  29.939
0.00  0.00     0.057 A
ATOM     24  C   UNL d   1      14.763   7.791  30.683
0.00  0.00     0.159 A
ATOM     25  C   UNL d   1      15.341   6.976  30.641
0.00  0.00     0.158 A
ATOM     26  C   UNL d   1      15.282   6.361  29.855
0.00  0.00     0.050 A
ATOM     27  C   UNL d   1      14.645   6.561  29.111
0.00  0.00     0.012 A
BRANCH  24  28
ATOM     28  O   UNL d   1      14.822   8.406  31.469
0.00  0.00    -0.503 OA
ATOM     29  H   UNL d   1      14.954   8.179  32.031
0.00  0.00     0.292 HD
ENDBRANCH  24  28
BRANCH  25  30
ATOM     30  O   UNL d   1      15.978   6.777  31.386
0.00  0.00    -0.503 OA
ATOM     31  H   UNL d   1      16.298   7.236  31.652
0.00  0.00     0.292 HD
ENDBRANCH  25  30
ENDBRANCH  21  22
ENDBRANCH  20  21
ENDBRANCH  18  20
ENDBRANCH   1  18
TORSDOF 12
ENDMDL
```

5. Senyawa *Myricetin*

```
MODEL 1
REMARK VINA RESULT:     -10.0      0.000      0.000
REMARK  7 active torsions:
REMARK  status: ('A' for Active; 'I' for Inactive)
REMARK    1  A    between atoms: O_2  and  C_13
REMARK    2  A    between atoms: O_3  and  C_15
REMARK    3  A    between atoms: O_5  and  C_19
REMARK    4  A    between atoms: O_6  and  C_21
REMARK    5  A    between atoms: O_7  and  C_22
REMARK    6  A    between atoms: O_8  and  C_23
REMARK    7  A    between atoms: C_10  and  C_12
ROOT
ATOM      1  O   UNL d   1      14.416   6.909  28.527
0.00  0.00    -0.451 OA
ATOM      2  O   UNL d   1      15.619   7.201  31.260
0.00  0.00    -0.283 OA
ATOM      3  C   UNL d   1      15.699   6.582  29.644
0.00  0.00     0.109 A
ATOM      4  C   UNL d   1      13.935   7.430  29.232
0.00  0.00     0.181 A
ATOM      5  C   UNL d   1      15.298   6.485  28.733
0.00  0.00     0.146 A
ATOM      6  C   UNL d   1      14.336   7.528  30.143
0.00  0.00     0.208 A
ATOM      7  C   UNL d   1      15.218   7.104  30.349
0.00  0.00     0.238 A
ATOM      8  C   UNL d   1      16.616   6.147  29.873
0.00  0.00     0.135 A
ATOM      9  C   UNL d   1      15.787   5.946  27.988
0.00  0.00     0.092 A
ATOM     10  C   UNL d   1      16.706   5.501  28.195
0.00  0.00     0.124 A
ATOM     11  C   UNL d   1      17.123   5.602  29.143
0.00  0.00     0.091 A
ENDROOT
BRANCH   4  12
ATOM     12  C   UNL d   1      13.053   7.854  29.026
0.00  0.00     0.028 A
ATOM     13  C   UNL d   1      13.001   8.607  28.369
0.00  0.00     0.061 A
ATOM     14  C   UNL d   1      12.119   9.031  28.163
0.00  0.00     0.163 A
ATOM     15  C   UNL d   1      11.289   8.702  28.614
0.00  0.00     0.201 A
ATOM     16  C   UNL d   1      11.341   7.950  29.271
0.00  0.00     0.163 A
ATOM     17  C   UNL d   1      12.223   7.526  29.477
0.00  0.00     0.061 A
BRANCH  14  18
ATOM     18  O   UNL d   1      12.067   9.783  27.506
0.00  0.00    -0.503 OA
```

```
ATOM      19  H   UNL d   1       12.563  10.142  27.406
0.00  0.00     0.292 HD
ENDBRANCH  14  18
BRANCH  15  20
ATOM      20  O   UNL d   1       10.407   9.126  28.408
0.00  0.00    -0.501 OA
ATOM      21  H   UNL d   1       10.378   9.607  28.018
0.00  0.00     0.292 HD
ENDBRANCH  15  20
BRANCH  16  22
ATOM      22  O   UNL d   1       10.511   7.622  29.722
0.00  0.00    -0.503 OA
ATOM      23  H   UNL d   1       10.530   7.111  30.072
0.00  0.00     0.292 HD
ENDBRANCH  16  22
ENDBRANCH   4  12
BRANCH   6  24
ATOM      24  O   UNL d   1       13.855   8.049  30.848
0.00  0.00    -0.501 OA
ATOM      25  H   UNL d   1       13.876   7.863  31.439
0.00  0.00     0.292 HD
ENDBRANCH   6  24
BRANCH   8  26
ATOM      26  O   UNL d   1       17.008   6.250  30.787
0.00  0.00    -0.506 OA
ATOM      27  H   UNL d   1       16.793   5.907  31.256
0.00  0.00     0.292 HD
ENDBRANCH   8  26
BRANCH  10  28
ATOM      28  O   UNL d   1       17.184   4.981  27.488
0.00  0.00    -0.506 OA
ATOM      29  H   UNL d   1       16.944   4.938  26.918
0.00  0.00     0.292 HD
ENDBRANCH  10  28
TORSDOF 7
ENDMDL
```

6. Senyawa *Kaemferol*

```
MODEL 1
REMARK VINA RESULT:      -9.5      0.000      0.000
REMARK  5 active torsions:
REMARK  status: ('A' for Active; 'I' for Inactive)
REMARK    1  A    between atoms: O_2  and  C_11
REMARK    2  A    between atoms: O_3  and  C_13
REMARK    3  A    between atoms: O_5  and  C_15
REMARK    4  A    between atoms: O_6  and  C_21
REMARK    5  A    between atoms: C_9  and  C_12
ROOT
ATOM      1  O   UNL d   1       14.562   6.852  28.284
0.00  0.00    -0.451 OA
```

```
ATOM      2  O   UNL d   1      15.339   7.049  31.175
0.00  0.00    -0.283 OA
ATOM      3  C   UNL d   1      15.649   6.463  29.575
0.00  0.00     0.109 A
ATOM      4  C   UNL d   1      15.390   6.397  28.611
0.00  0.00     0.146 A
ATOM      5  C   UNL d   1      13.993   7.373  28.920
0.00  0.00     0.181 A
ATOM      6  C   UNL d   1      15.080   6.983  30.211
0.00  0.00     0.238 A
ATOM      7  C   UNL d   1      14.252   7.438  29.884
0.00  0.00     0.208 A
ATOM      8  C   UNL d   1      16.509   5.994  29.930
0.00  0.00     0.135 A
ATOM      9  C   UNL d   1      15.973   5.859  27.936
0.00  0.00     0.092 A
ATOM     10  C   UNL d   1      16.837   5.382  28.269
0.00  0.00     0.124 A
ATOM     11  C   UNL d   1      17.107   5.450  29.272
0.00  0.00     0.091 A
ENDROOT
BRANCH   5  12
ATOM     12  C   UNL d   1      13.165   7.828  28.593
0.00  0.00     0.021 A
ATOM     13  C   UNL d   1      12.296   7.333  28.577
0.00  0.00     0.015 A
ATOM     14  C   UNL d   1      11.468   7.789  28.250
0.00  0.00     0.046 A
ATOM     15  C   UNL d   1      11.509   8.738  27.939
0.00  0.00     0.117 A
ATOM     16  C   UNL d   1      12.378   9.233  27.955
0.00  0.00     0.046 A
ATOM     17  C   UNL d   1      13.206   8.778  28.282
0.00  0.00     0.015 A
BRANCH  15  18
ATOM     18  O   UNL d   1      10.681   9.193  27.612
0.00  0.00    -0.507 OA
ATOM     19  H   UNL d   1      10.712   9.769  27.385
0.00  0.00     0.292 HD
ENDBRANCH  15  18
ENDBRANCH   5  12
BRANCH   7  20
ATOM     20  O   UNL d   1      13.683   7.959  30.520
0.00  0.00    -0.501 OA
ATOM     21  H   UNL d   1      13.389   7.668  30.982
0.00  0.00     0.292 HD
ENDBRANCH   7  20
BRANCH   8  22
ATOM     22  O   UNL d   1      16.758   6.066  30.895
0.00  0.00    -0.506 OA
```

```
ATOM     23  H   UNL d   1      16.431   5.760  31.323
0.00  0.00     0.292 HD
ENDBRANCH   8  22
BRANCH  10  24
ATOM     24  O   UNL d   1      17.404   4.862  27.630
0.00  0.00    -0.506 OA
ATOM     25  H   UNL d   1      17.820   5.154  27.277
0.00  0.00     0.292 HD
ENDBRANCH  10  24
TORSDOF 5
ENDMDL
```

7.Senyawa *Epichatecin*

```
MODEL 1
REMARK VINA RESULT:     -5.7      0.000      0.000
REMARK  6 active torsions:
REMARK  status: ('A' for Active; 'I' for Inactive)
REMARK    1  A    between atoms: C_7  and  O_2
REMARK    2  A    between atoms: O_3  and  C_13
REMARK    3  A    between atoms: O_4  and  C_18
REMARK    4  A    between atoms: O_5  and  C_19
REMARK    5  A    between atoms: O_6  and  C_21
REMARK    6  A    between atoms: C_8  and  C_12
ROOT
ATOM      1  O   UNL d   1      14.430   6.904  28.545
0.00  0.00    -0.481 OA
ATOM      2  C   UNL d   1      14.364   7.539  30.155
0.00  0.00     0.164 A
ATOM      3  C   UNL d   1      13.954   7.431  29.250
0.00  0.00     0.232 A
ATOM      4  C   UNL d   1      15.249   7.120  30.357
0.00  0.00     0.078 A
ATOM      5  C   UNL d   1      15.724   6.593  29.653
0.00  0.00     0.038 A
ATOM      6  C   UNL d   1      15.315   6.485  28.747
0.00  0.00     0.132 A
ATOM      7  C   UNL d   1      16.645   6.162  29.877
0.00  0.00     0.127 A
ATOM      8  C   UNL d   1      15.798   5.938  28.003
0.00  0.00     0.091 A
ATOM      9  C   UNL d   1      17.147   5.611  29.149
0.00  0.00     0.091 A
ATOM     10  C   UNL d   1      16.720   5.499  28.206
0.00  0.00     0.124 A
ENDROOT
BRANCH   3  11
ATOM     11  C   UNL d   1      13.069   7.851  29.048
0.00  0.00    -0.001 A
ATOM     12  C   UNL d   1      12.241   7.512  29.495
0.00  0.00     0.056 A
```

```
ATOM     13  C   UNL d   1      11.356   7.931  29.294
0.00  0.00     0.159 A
ATOM     14  C   UNL d   1      11.299   8.690  28.645
0.00  0.00     0.158 A
ATOM     15  C   UNL d   1      12.126   9.029  28.197
0.00  0.00     0.049 A
ATOM     16  C   UNL d   1      13.011   8.609  28.399
0.00  0.00     0.011 A
BRANCH  13  17
ATOM     17  O   UNL d   1      10.529   7.592  29.741
0.00  0.00    -0.503 OA
ATOM     18  H   UNL d   1      10.106   7.278  29.414
0.00  0.00     0.292 HD
ENDBRANCH  13  17
BRANCH  14  19
ATOM     19  O   UNL d   1      10.414   9.109  28.443
0.00  0.00    -0.503 OA
ATOM     20  H   UNL d   1      10.380   9.591  28.055
0.00  0.00     0.292 HD
ENDBRANCH  14  19
ENDBRANCH   3  11
BRANCH   2  21
ATOM     21  O   UNL d   1      13.888   8.066  30.860
0.00  0.00    -0.388 OA
ATOM     22  H   UNL d   1      14.074   8.642  30.994
0.00  0.00     0.210 HD
ENDBRANCH   2  21
BRANCH   7  23
ATOM     23  O   UNL d   1      17.045   6.276  30.787
0.00  0.00    -0.506 OA
ATOM     24  H   UNL d   1      17.386   5.821  31.034
0.00  0.00     0.292 HD
ENDBRANCH   7  23
BRANCH  10  25
ATOM     25  O   UNL d   1      17.193   4.972  27.499
0.00  0.00    -0.506 OA
ATOM     26  H   UNL d   1      17.587   5.254  27.113
0.00  0.00     0.292 HD
ENDBRANCH  10  25
TORSDOF 6
ENDMDL
```

8. Senyawa *Delpinidhin*

```
MODEL 1
REMARK VINA RESULT:     -10.0      0.000      0.000
REMARK  7 active torsions:
REMARK  status: ('A' for Active; 'I' for Inactive)
REMARK    1  A    between atoms: O_24  and  C_6
REMARK    2  A    between atoms: O_26  and  C_8
REMARK    3  A    between atoms: O_28  and  C_10
```

```
REMARK    4  A    between atoms: O_22  and  C_16
REMARK    5  A    between atoms: O_18  and  C_14
REMARK    6  A    between atoms: O_20  and  C_15
REMARK    7  A    between atoms: C_4  and  C_12
ROOT
ATOM      1  O   UNL d   1      14.416   6.909  28.527
0.00  0.00    -0.451 OA
ATOM      2  O   UNL d   1      15.619   7.201  31.260
0.00  0.00    -0.283 OA
ATOM      3  C   UNL d   1      15.699   6.582  29.644
0.00  0.00     0.109 A
ATOM      4  C   UNL d   1      13.935   7.430  29.232
0.00  0.00     0.181 A
ATOM      5  C   UNL d   1      15.298   6.485  28.733
0.00  0.00     0.146 A
ATOM      6  C   UNL d   1      14.336   7.528  30.143
0.00  0.00     0.208 A
ATOM      7  C   UNL d   1      15.218   7.104  30.349
0.00  0.00     0.238 A
ATOM      8  C   UNL d   1      16.616   6.147  29.873
0.00  0.00     0.135 A
ATOM      9  C   UNL d   1      15.787   5.946  27.988
0.00  0.00     0.092 A
ATOM     10  C   UNL d   1      16.706   5.501  28.195
0.00  0.00     0.124 A
ATOM     11  C   UNL d   1      17.123   5.602  29.143
0.00  0.00     0.091 A
ENDROOT
BRANCH   4  12
ATOM     12  C   UNL d   1      13.053   7.854  29.026
0.00  0.00     0.028 A
ATOM     13  C   UNL d   1      13.001   8.607  28.369
0.00  0.00     0.061 A
ATOM     14  C   UNL d   1      12.119   9.031  28.163
0.00  0.00     0.163 A
ATOM     15  C   UNL d   1      11.289   8.702  28.614
0.00  0.00     0.201 A
ATOM     16  C   UNL d   1      11.341   7.950  29.271
0.00  0.00     0.163 A
ATOM     17  C   UNL d   1      12.223   7.526  29.477
0.00  0.00     0.061 A
BRANCH  14  18
ATOM     18  O   UNL d   1      12.067   9.783  27.506
0.00  0.00    -0.503 OA
ATOM     19  H   UNL d   1      12.368  10.313  27.618
0.00  0.00     0.292 HD
ENDBRANCH  14  18
BRANCH  15  20
ATOM     20  O   UNL d   1      10.407   9.126  28.408
0.00  0.00    -0.501 OA
```

```
ATOM      21  H   UNL d   1       9.925   9.038  28.787
0.00  0.00     0.292 HD
ENDBRANCH  15  20
BRANCH  16  22
ATOM      22  O   UNL d   1      10.511   7.622  29.722
0.00  0.00    -0.503 OA
ATOM      23  H   UNL d   1      10.531   7.113  30.075
0.00  0.00     0.292 HD
ENDBRANCH  16  22
ENDBRANCH   4  12
BRANCH   6  24
ATOM      24  O   UNL d   1      13.855   8.049  30.848
0.00  0.00    -0.501 OA
ATOM      25  H   UNL d   1      14.175   8.330  31.298
0.00  0.00     0.292 HD
ENDBRANCH   6  24
BRANCH   8  26
ATOM      26  O   UNL d   1      17.008   6.250  30.787
0.00  0.00    -0.506 OA
ATOM      27  H   UNL d   1      16.820   5.881  31.248
0.00  0.00     0.292 HD
ENDBRANCH   8  26
BRANCH  10  28
ATOM      28  O   UNL d   1      17.184   4.981  27.488
0.00  0.00    -0.506 OA
ATOM      29  H   UNL d   1      17.675   5.226  27.201
0.00  0.00     0.292 HD
ENDBRANCH  10  28
TORSDOF 7
ENDMDL
```

9. Senyawa *procatecuice acid*

```
MODEL 1
REMARK VINA RESULT:      -5.7      0.000    ★ 0.000
REMARK  4 active torsions:
REMARK  status: ('A' for Active; 'I' for Inactive)
REMARK    1  A    between atoms: O_1  and  C_7
REMARK    2  A    between atoms: O_2  and  C_9
REMARK    3  A    between atoms: O_3  and  C_11
REMARK    4  A    between atoms: C_5  and  C_11
ROOT
ATOM      1  O   UNL d   1      10.420   7.756  29.713  0.00
0.00    -0.503 OA
ATOM      2  H   UNL d   1      10.382   7.518  30.285  0.00
0.00     0.292 HD
ENDROOT
BRANCH   1   3
ATOM      3  C   UNL d   1      11.309   8.014  29.337  0.00
0.00     0.159 A
```

```
ATOM      4  C   UNL d   1      12.150   7.721  29.793  0.00
0.00     0.064 A
ATOM      5  C   UNL d   1      13.039   7.980  29.416  0.00
0.00     0.063 A
ATOM      6  C   UNL d   1      13.088   8.532  28.584  0.00
0.00     0.019 A
ATOM      7  C   UNL d   1      12.248   8.825  28.128  0.00
0.00     0.050 A
ATOM      8  C   UNL d   1      11.359   8.567  28.505  0.00
0.00     0.158 A
BRANCH   5   9
ATOM      9  C   UNL d   1      13.879   7.686  29.872  0.00
0.00     0.337 C
ATOM     10  O   UNL d   1      14.097   8.026  30.787  0.00
0.00    -0.245 OA
BRANCH   9  11
ATOM     11  O   UNL d   1      14.502   7.053  29.413  0.00
0.00    -0.477 OA
ATOM     12  H   UNL d   1      14.347   6.456  29.350  0.00
0.00     0.295 HD
ENDBRANCH   9  11
ENDBRANCH   5   9
BRANCH   8  13
ATOM     13  O   UNL d   1      10.518   8.860  28.049  0.00
0.00    -0.503 OA
ATOM     14  H   UNL d   1      10.072   8.447  27.925  0.00
0.00     0.292 HD
ENDBRANCH   8  13
ENDBRANCH   1   3
TORSDOF 4
ENDMDL
```

10. Senyawa *Rutin*

```
MODEL 1
REMARK VINA RESULT:     -10.2      0.000      0.000
REMARK  16 active torsions:
REMARK  status: ('A' for Active; 'I' for Inactive)
REMARK    1  A    between atoms: C_22  and  O_2
REMARK    2  A    between atoms: O_2  and  C_26
REMARK    3  A    between atoms: C_18  and  O_4
REMARK    4  A    between atoms: C_19  and  O_5
REMARK    5  A    between atoms: C_25  and  O_6
REMARK    6  A    between atoms: O_6  and  C_29
REMARK    7  A    between atoms: C_20  and  O_7
REMARK    8  A    between atoms: C_21  and  O_8
REMARK    9  A    between atoms: C_23  and  O_9
REMARK   10  A    between atoms: C_24  and  O_10
REMARK   11  A    between atoms: O_13  and  C_35
REMARK   12  A    between atoms: O_14  and  C_40
REMARK   13  A    between atoms: O_15  and  C_41
```

```
REMARK   14  A    between atoms: O_16  and  C_43
REMARK   15  A    between atoms: C_17  and  C_26
REMARK   16  A    between atoms: C_30  and  C_33
ROOT
ATOM      1  O   UNL d   1       7.054  10.113  27.197  0.00
0.00    -0.331 OA
ATOM      2  C   UNL d   1       6.300   9.889  26.579  0.00
0.00     0.179 A
ATOM      3  C   UNL d   1       5.914  10.594  25.985  0.00
0.00     0.177 A
ATOM      4  C   UNL d   1       6.282  11.524  26.008  0.00
0.00     0.180 A
ATOM      5  C   UNL d   1       7.036  11.748  26.626  0.00
0.00     0.214 A
ATOM      6  C   UNL d   1       7.422  11.042  27.220  0.00
0.00     0.340 A
ENDROOT
BRANCH   2   7
ATOM      7  C   UNL d   1       5.932   8.959  26.556  0.00
0.00     0.197 C
BRANCH   7   8
ATOM      8  O   UNL d   1       5.587   8.537  27.395  0.00
0.00    -0.346 OA
BRANCH   8   9
ATOM      9  C   UNL d   1       4.935   7.780  27.342  0.00
0.00     0.282 A
ATOM     10  O   UNL d   1       4.400   7.639  26.509  0.00
0.00    -0.343 OA
ATOM     11  C   UNL d   1       3.748   6.882  26.456  0.00
0.00     0.149 A
ATOM     12  C   UNL d   1       3.633   6.266  27.236  0.00
0.00     0.174 A
ATOM     13  C   UNL d   1       3.213   6.740  25.624  0.00
0.00     0.040 C
ATOM     14  C   UNL d   1       4.168   6.408  28.069  0.00
0.00     0.179 A
ATOM     15  C   UNL d   1       4.820   7.165  28.121  0.00
0.00     0.201 A
BRANCH  12  16
ATOM     16  O   UNL d   1       2.981   5.509  27.183  0.00
0.00    -0.387 OA
ATOM     17  H   UNL d   1       2.624   5.442  26.681  0.00
0.00     0.210 HD
ENDBRANCH  12  16
BRANCH  14  18
ATOM     18  O   UNL d   1       4.053   5.792  28.848  0.00
0.00    -0.386 OA
ATOM     19  H   UNL d   1       4.202   5.193  28.795  0.00
0.00     0.210 HD
ENDBRANCH  14  18
BRANCH  15  20
```

```
ATOM     20  O   UNL d   1       5.355   7.306  28.954  0.00
0.00    -0.384 OA
ATOM     21  H   UNL d   1       5.926   7.547  28.918  0.00
0.00     0.210 HD
ENDBRANCH  15  20
ENDBRANCH   8   9
ENDBRANCH   7   8
ENDBRANCH   2   7
BRANCH   6  22
ATOM     22  O   UNL d   1       8.176  11.266  27.838  0.00
0.00    -0.453 OA
BRANCH  22  23
ATOM     23  C   UNL d   1       8.808  10.550  28.135  0.00
0.00     0.214 A
ATOM     24  C   UNL d   1       8.735  10.169  29.056  0.00
0.00     0.181 A
ATOM     25  O   UNL d   1       9.367   9.454  29.353  0.00
0.00    -0.451 OA
ATOM     26  C   UNL d   1      10.073   9.119  28.729  0.00
0.00     0.146 A
ATOM     27  C   UNL d   1      10.146   9.500  27.807  0.00
0.00     0.109 A
ATOM     28  C   UNL d   1      10.724   8.374  29.053  0.00
0.00     0.092 A
ATOM     29  C   UNL d   1       9.514  10.216  27.510  0.00
0.00     0.238 A
ATOM     30  C   UNL d   1      10.876   9.162  27.145  0.00
0.00     0.135 A
ATOM     31  O   UNL d   1       9.587  10.597  26.589  0.00
0.00    -0.283 OA
ATOM     32  C   UNL d   1      11.538   8.417  27.447  0.00
0.00     0.091 A
ATOM     33  C   UNL d   1      11.462   8.020  28.408  0.00
0.00     0.124 A
BRANCH  24  34
ATOM     34  C   UNL d   1       8.029  10.504  29.681  0.00
0.00     0.025 A
ATOM     35  C   UNL d   1       7.226   9.941  29.875  0.00
0.00     0.060 A
ATOM     36  C   UNL d   1       6.520  10.275  30.500  0.00
0.00     0.159 A
ATOM     37  C   UNL d   1       6.618  11.172  30.930  0.00
0.00     0.158 A
ATOM     38  C   UNL d   1       7.421  11.735  30.736  0.00
0.00     0.050 A
ATOM     39  C   UNL d   1       8.127  11.401  30.111  0.00
0.00     0.015 A
BRANCH  36  40
ATOM     40  O   UNL d   1       5.717   9.712  30.694  0.00
0.00    -0.503 OA
```

```
ATOM      41  H   UNL d   1       5.240   9.705  30.298  0.00
0.00     0.292 HD
ENDBRANCH  36  40
BRANCH  37  42
ATOM      42  O   UNL d   1       5.912  11.507  31.555  0.00
0.00    -0.503 OA
ATOM      43  H   UNL d   1       5.931  12.092  31.759  0.00
0.00     0.292 HD
ENDBRANCH  37  42
ENDBRANCH  24  34
BRANCH  30  44
ATOM      44  O   UNL d   1      10.940   9.551  26.226  0.00
0.00    -0.506 OA
ATOM      45  H   UNL d   1      11.456   9.845  26.049  0.00
0.00     0.292 HD
ENDBRANCH  30  44
BRANCH  33  46
ATOM      46  O   UNL d   1      12.092   7.305  28.708  0.00
0.00    -0.506 OA
ATOM      47  H   UNL d   1      12.633   7.458  28.969  0.00
0.00     0.292 HD
ENDBRANCH  33  46
ENDBRANCH  22  23
ENDBRANCH   6  22
BRANCH   3  48
ATOM      48  O   UNL d   1       5.160  10.370  25.368  0.00
0.00    -0.387 OA
ATOM      49  H   UNL d   1       5.022  10.749  24.896  0.00
0.00     0.210 HD
ENDBRANCH   3  48
BRANCH   5  50
ATOM      50  O   UNL d   1       7.404  12.677  26.649  0.00
0.00    -0.383 OA
ATOM      51  H   UNL d   1       7.796  12.844  27.100  0.00
0.00     0.210 HD
ENDBRANCH   5  50
BRANCH   4  52
ATOM      52  O   UNL d   1       5.896  12.229  25.414  0.00
0.00    -0.386 OA
ATOM      53  H   UNL d   1       6.107  12.297  24.835  0.00
0.00     0.210 HD
ENDBRANCH   4  52
TORSDOF 16
ENDMDL
```

11. Senyawa Quercetin

```
MODEL 1
REMARK VINA RESULT:      -8.5      0.000      0.000
REMARK  6 active torsions:
REMARK  status: ('A' for Active; 'I' for Inactive)
```

```
REMARK    1  A    between atoms: O1_2  and  C1_3
REMARK    2  A    between atoms: C3_5  and  O2_6
REMARK    3  A    between atoms: C6_11  and  O4_12
REMARK    4  A    between atoms: C7_14  and  C10_18
REMARK    5  A    between atoms: C12_20  and  O6_21
REMARK    6  A    between atoms: C13_23  and  O7_24
ROOT
ATOM      1  H1  non d ame      11.549  10.663  25.468  0.00
0.00     0.218 HD
ATOM      2  O1  non d ame      11.355  11.433  26.029  0.00
0.00    -0.280 OA
ENDROOT
BRANCH   2   3
ATOM      3  C1  non d ame      10.004  11.682  26.150  0.00
0.00     0.036 A
ATOM      4  C2  non d ame       9.504  12.934  26.089  0.00
0.00     0.068 A
ATOM      5  C3  non d ame       8.176  13.157  26.208  0.00
0.00     0.058 A
ATOM      6  C4  non d ame       7.343  12.103  26.390  0.00
0.00     0.029 A
ATOM      7  C5  non d ame       5.864  12.269  26.518  0.00
0.00     0.116 A
ATOM      8  C8  non d ame       7.837  10.842  26.462  0.00
0.00     0.061 A
ATOM      9  O3  non d ame       5.255  13.332  26.417  0.00
0.00    -0.277 OA
ATOM     10  C6  non d ame       5.064  11.045  26.786  0.00
0.00     0.069 A
ATOM     11  C7  non d ame       5.684   9.856  26.850  0.00
0.00     0.033 A
ATOM     12  O5  non d ame       7.047   9.718  26.664  0.00
0.00    -0.185 OA
ATOM     13  C9  non d ame       9.165  10.647  26.336  0.00
0.00     0.071 A
BRANCH   5  14
ATOM     14  O2  non d ame       7.700  14.454  26.148  0.00
0.00    -0.275 OA
ATOM     15  H3  non d ame       7.401  14.800  27.003  0.00
0.00     0.218 HD
ENDBRANCH   5  14
BRANCH  10  16
ATOM     16  O4  non d ame       3.697  11.204  26.926  0.00
0.00    -0.259 OA
ATOM     17  H4  non d ame       3.521  11.802  27.682  0.00
0.00     0.218 HD
ENDBRANCH  10  16
BRANCH  11  18
ATOM     18  C10 non d ame       5.003   8.584  27.072  0.00
0.00    -0.029 A
```

```
ATOM     19  C11 non d ame       5.101   7.923  28.252  0.00
0.00     0.074 A
ATOM     20  C12 non d ame       4.454   6.752  28.442  0.00
0.00     0.032 A
ATOM     21  C13 non d ame       3.698   6.234  27.449  0.00
0.00     0.034 A
ATOM     22  C14 non d ame       3.606   6.878  26.271  0.00
0.00     0.051 A
ATOM     23  C15 non d ame       4.257   8.042  26.080  0.00
0.00     0.032 A
BRANCH  20  24
ATOM     24  O6  non d ame       4.539   6.066  29.644  0.00
0.00    -0.275 OA
ATOM     25  H7  non d ame       4.425   5.109  29.519  0.00
0.00     0.218 HD
ENDBRANCH  20  24
BRANCH  21  26
ATOM     26  O7  non d ame       3.010   5.049  27.634  0.00
0.00    -0.275 OA
ATOM     27  H8  non d ame       3.374   4.583  28.410  0.00
0.00     0.218 HD
ENDBRANCH  21  26
ENDBRANCH  11  18
ENDBRANCH   2   3
TORSDOF 6
ENDMDL
```