LAMPIRAN

Lampiran 1. Hasil *Docking*

1. Obat pembanding ketoconazole

```
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
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
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
```

2. 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
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
```

3. 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
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
```

4. 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
```

5. 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
```

6. 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
```

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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
```

7. 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
```