Cl
2 CN
*
4 OH
(±)-5 diastereomer = 65:35
abundance
4.20
1.29
0.34
0.42
0.37
0.98
0.61
0.24
1.94
1.06
7.377
7.371
7.367
7.355
7.349
7.322
7.316
7.309
7.305
7.300
7.289
7.260
4.175
4.164
4.152
4.147
4.135
4.060
4.046
4.036
4.022
3.640
3.632
3.625
3.616
3.608
3.601
3.592
1.978
1.971
1.950
1.943
1.922
1.860
1.849
1.834
1.824
1.519
1.503
1.297
1.282
1.237
1.221
-0.000
X : parts per Million : 1H

Cl
2
CN
*
4
OH
(±)-5 diastereomer = 65:35
abundance
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
134.459
134.058
133.858
133.696
129.203
129.184
129.032
128.440
121.124
120.352
77.258
77.000
76.742
65.726
64.972
63.875
44.703
43.845
33.677
32.723
23.843
23.585
15.115
X : parts per Million : Carbon13

Cl
4 CN
*
2 OTs
(±)-3 diastereomer = 65:35
abundance
1.00
0.51
3.32
1.10
0.28
0.55
0.28
0.27
0.50
2.27
1.84
1.60
1.40
7.868
7.848
7.793
7.772
7.396
7.375
7.354
7.333
7.267
7.260
7.246
7.223
7.203
4.835
4.826
4.819
4.813
4.804
4.797
4.788
4.552
4.549
4.543
3.913
3.899
3.891
3.877
3.833
3.819
3.808
3.794
2.467
2.071
2.058
2.044
2.036
1.542
1.330
1.314
1.276
1.260
-0.000
X : parts per Million : 1H

Cl
4
CN
*
2
OTs
(±)-3 diastereomer = 65:35
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
144.951
144.827
129.804
129.680
129.070
129.032
128.822
128.249
127.486
127.334
119.818
119.083
77.258
77.200
77.000
76.742
76.590
75.741
73.509
42.929
42.347
41.393
33.000
31.884
21.621
21.296
20.648
20.285
X : parts per Million : Carbon13

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
X : parts per Million : 1H
7.322
7.317
7.306
7.300
7.261
7.209
7.204
7.193
7.187
2.00
2.08
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
1.601
1.589
1.580
1.567
1.554
1.543
1.534
1.487
1.472
1.443
1.418
1.414
1.388
2.01
3.11
1.03
-0.000
Cl
1
CN
2
(1R*, 2S*)-4

Cl
1
CN
2
(1R*, 2S*)-4
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
1.5
1.6
1.7
1.8
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
135.203
133.123
128.850
126.761
120.361
77.258
77.210
77.000
76.752
25.340
25.274
19.999
15.878
X : parts per Million : Carbon13

Cl
CN
1
2
(1R*, 2R*)-4
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
2.93
1.69
0.95
0.98
1.05
3.00
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.363
7.357
7.346
7.341
7.336
7.283
7.278
7.261
1.893
1.888
1.877
1.872
1.855
1.757
1.743
1.734
1.721
1.541
1.277
1.262
1.245
0.842
0.826
-0.000
X : parts per Million : 1H

Cl
1
CN
2
(1R*, 2R*)-4
abundance
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
134.125
131.006
130.748
128.927
123.223
77.248
77.000
76.742
23.204
19.875
17.452
13.608
X : parts per Million : Carbon13

Cl
1
CO2H
2
(1R*,2S*)-6
5.49
4.00
2.05
abundance
3.0
2.0
1.0
0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.270
7.260
1.662
1.641
1.633
1.613
1.577
1.576
1.562
1.552
1.537
1.377
1.356
1.341
1.327
1.312
-0.000
X : parts per Million : 1H

Cl
1
CO2H
2
(1R*,2S*)-6
abundance
0.3
0.2
0.1
0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
178.650
139.018
133.057
131.607
128.335
77.258
77.000
76.752
33.706
25.302
22.565
12.712
X : parts per Million : Carbon13

Cl
CO2H
(1R*, 2R*)-6
abundance
1.89
1.98
0.91
1.09
0.99
3.00
7.313
7.292
7.260
7.209
7.188
1.947
1.926
1.908
1.820
1.809
1.797
1.787
1.108
1.096
1.091
1.079
0.837
0.821
-0.000
X : parts per Million : 1H

Cl
CO2H
(1R*, 2R*)-6
abundance
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
181.092
133.858
133.219
132.742
128.268
77.258
77.000
76.752
32.857
24.072
23.347
15.335
X : parts per Million : Carbon13

Cl
O
CN
O
O
(1R*,2S*)-8
17.66
1.00
2.20
2.77
1.60
abundance
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.385
7.378
7.362
7.260
7.233
7.217
7.206
7.021
7.001
6.981
6.339
6.314
2.046
1.617
1.606
1.536
1.348
1.324
1.314
1.308
1.268
1.253
-0.000
X : parts per Million : 1H

Cl
O
CN
O
O
(1R*,2S*)-8
abundance
0.4
0.3
0.2
0.1
0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
170.209
170.161
158.162
157.990
156.321
156.206
137.969
131.445
129.957
128.450
124.100
123.957
121.554
121.439
120.151
120.056
119.388
119.188
116.956
116.937
77.248
77.000
76.742
62.664
62.559
33.896
33.763
25.159
25.035
22.679
22.479
12.855
12.807
X : parts per Million : Carbon13

Cl
O
CN
O
O
(1R*,2R*)-8
abundance
3.0
2.0
1.0
0
8.85
3.99
0.94
0.98
0.99
0.90
3.00
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.388
7.364
7.268
7.260
7.249
7.174
7.142
7.030
7.026
6.319
6.294
1.951
1.930
1.909
1.860
1.846
1.829
1.815
1.814
1.783
1.546
1.157
1.155
1.132
0.853
0.836
0.816
-0.000
X : parts per Million : 1H

Cl
O
CN
O
O
(1R*,2R*)-8
abundance
0.4
0.3
0.2
0.1
0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
172.202
172.183
171.096
158.104
156.225
156.159
133.457
133.114
132.656
130.548
129.947
128.412
124.033
121.525
121.410
120.066
119.989
119.341
119.302
116.918
116.803
115.840
77.258
77.000
76.742
62.626
60.346
32.742
24.329
24.148
23.576
15.249
15.192
14.162
X : parts per Million : Carbon13

abundance
X : parts per Million : 1H
7.288
7.273
7.260
7.250
3.919
3.892
3.754
3.726
1.548
1.317
1.302
1.270
1.258
1.243
1.236
1.221
1.031
1.018
1.010
0.998
0.577
0.565
0.551
-0.000
3.49
1.00
1.00
4.94
0.90
0.99
Cl
OH
(1R*,2S*)-7

Cl
OH
(1R*,2S*)-7
abundance
0
0.1
0.2
0.3
0.4
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
143.082
132.093
130.281
128.898
128.440
77.258
77.000
76.742
66.899
66.718
31.245
19.226
19.026
18.864
13.904
X : parts per Million : Carbon13

Cl
OH
(1R*,2R*)-7
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.73
0.74
1.00
1.04
0.94
0.92
0.98
2.97
0.95
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.317
7.296
7.260
7.241
3.793
3.779
3.766
3.751
3.406
3.390
3.377
3.361
1.537
1.321
1.306
1.290
1.089
0.984
0.971
0.962
0.951
0.804
0.788
0.624
0.613
-0.000
X : parts per Million : 1H

Cl
OH
(1R*,2R*)-7
abundance
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9 2.0
140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0
138.322
138.074
132.322
132.179
131.969
131.750
130.644
130.214
128.497
128.307
128.183
126.542
77.258
77.000
76.742
71.954
71.668
66.441
33.448
32.847
30.777
29.604
19.121
18.959
16.708
16.126
15.373
13.790
X : parts per Million : Carbon13

Cl
O
O
(1R*,2S*)-9
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
5.08
4.55
2.67
1.04
2.28
1.00
0.99
4.22
0.92
1.01
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.359
7.340
7.319
7.259
7.228
7.206
7.189
7.167
7.115
7.006
6.986
6.895
4.425
4.402
3.745
3.719
3.528
3.502
1.533
1.229
1.217
1.030
1.017
0.544
0.530
0.519
0.000
X : parts per Million : 1H

Cl
O
O
(1R*,2S*)-9
abundance
0.4
0.3
0.2
0.1
0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
157.370
157.093
143.949
140.573
131.540
129.823
129.728
129.537
128.068
123.289
122.097
118.988
117.824
117.614
77.248
77.000
76.742
73.871
72.412
28.841
19.732
19.541
14.133
X : parts per Million : Carbon13

Cl
O
O
(1R*,2R*)-9
abundance
4.34
1.71
0.93
1.91
2.79
2.07
1.01
0.99
1.535
0.97
1.02
3.00
0.99
7.363
7.343
7.323
7.259
7.240
7.226
7.117
7.005
6.985
6.914
6.897
6.878
6.855
4.418
4.387
4.382
4.349
3.544
3.520
3.344
3.320
0.954
0.943
0.934
0.921
0.767
0.753
0.631
0.619
0.000
X : parts per Million : 1H

Cl
O
O
(1R*,2R*)-9
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
157.294
157.046
140.592
138.856
132.036
131.912
129.652
129.489
128.049
123.194
121.859
118.892
117.700
117.385
79.013
78.879
77.258
77.000
76.742
72.097
30.472
17.033
16.851
16.317
16.136
15.373
15.239
15.154
X : parts per Million : Carbon13

EtO
O
O
(1R,2R)-10
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
3.20
1.93
1.93
1.98
1.99
0.97
0.90
2.05
2.00
1.00
1.00
3.02
3.00
1.00
1.00
1.00
1.00
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.353
7.335
7.313
7.258
7.233
7.213
7.191
7.101
7.001
6.982
6.935
6.883
6.811
6.789
4.388
4.005
3.987
3.970
3.552
3.528
3.353
3.329
1.533
1.415
1.397
1.380
1.254
0.916
0.905
0.884
0.778
0.763
0.594
-0.000
X : parts per Million : 1H

EtO
O
O
(1R,2R)-10
abundance
0.4
0.3
0.2
0.1
0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
157.437
157.236
157.170
140.897
132.246
131.531
129.671
129.489
123.156
122.002
118.883
117.662
117.595
113.885
79.270
77.258
77.000
76.742
72.126
63.236
30.234
16.956
16.203
15.440
14.906
X : parts per Million : Carbon13