Supplementary Information for

Elucidation of inhibitor-binding pocket of D-amino acid oxidase using docking simulation and *N*-sulfanylethylanilide-based labeling technology

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kiyo.fukui@tokushima-u.ac.jp (K. Fukui)
aotaka@tokushima-u.ac.jp (A. Otaka)

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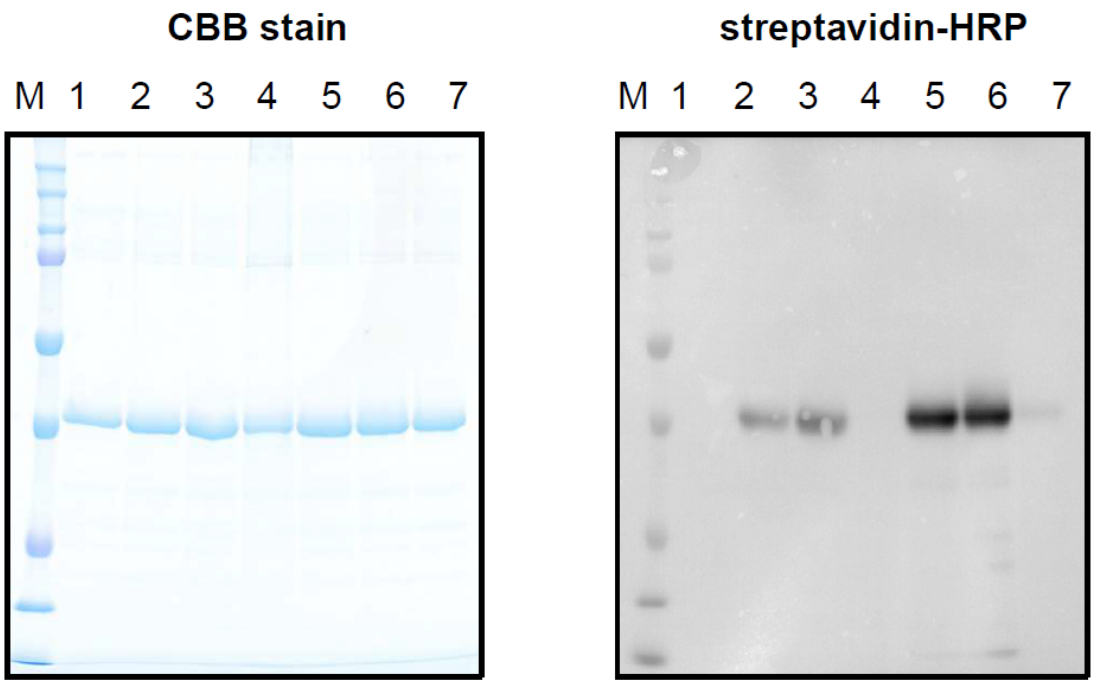
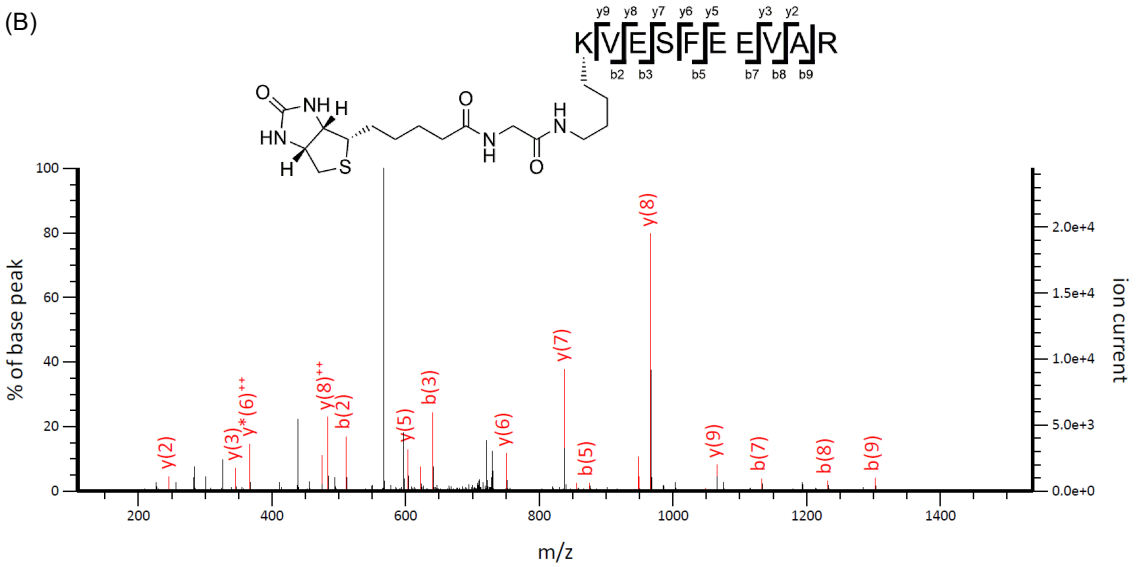


Fig. S1 An original picture of Fig. 4C. Lane 4 and 7 in Fig. S1 correspond to lane 1 and 2 in Fig. 4C, respectively.

(A)

[1]MRVVVIGAGV [11]IGLSTALCIH [21]ERYHSVLQPL [31]DIKVYADRFT
[41]PLTTTDVAAG [51]LWQPYLSDPN [61]NPQEADWSQQ [71]TFDYLLSHVH
[81]SPNAENLGLF [91]LISGYNLFHE [101]AIPDPSWKDT [111]VLGFRKLTPR
[121]ELDMFPDYGY [131]GWFHTSLILE [141]GKNYLQWLTE [151]RLTERGVKFF
[161]QRKVESFEEV [171]AREGADVIVN [181]CTGVWAGALQ [191]RDPLLQPGRG
[201]QIMKVDAPWM [211]KHFILTHDPE [221]RGIYNSPYII [231]PGTQTVTLGG
[241]IFQLGNWSEL [251]NNIQDHNTIW [261]EGCCRLEPTL [271]KNARIIGERT
[281]GFRPVRPQIR [291]LEREQLRTGP [301]SNTEVIHNYG [311]HGGYGLTIHW
[321]GCALEAAKLF [331]GRILEEKKLS [341]RMPPSHL

(B)



(C)

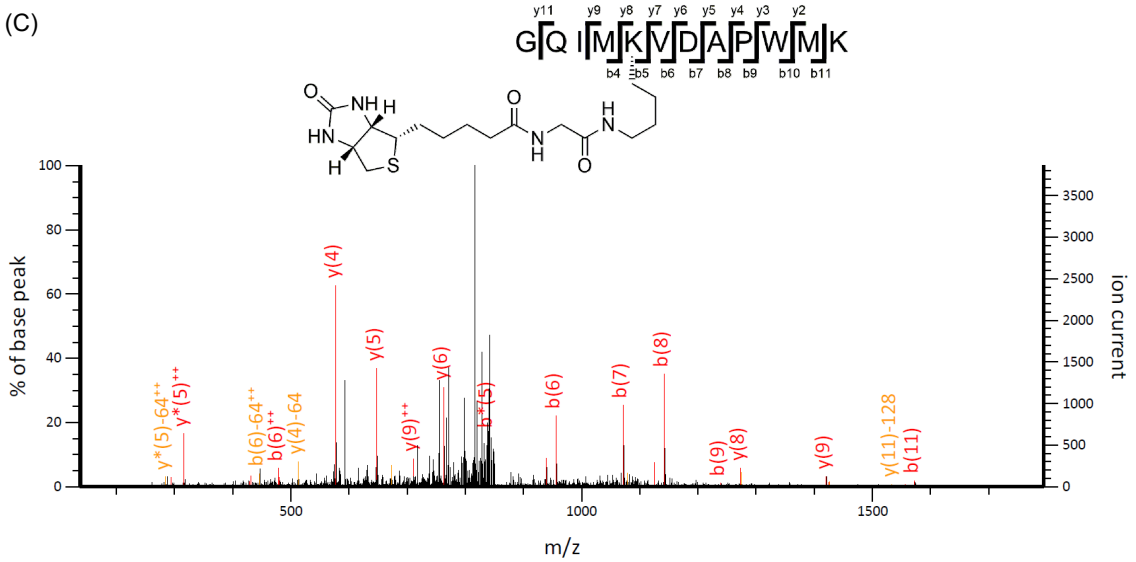
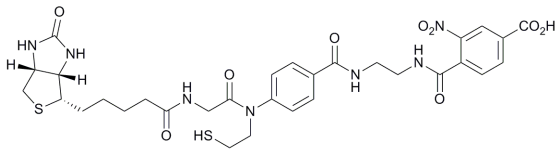


Fig. S2 Mass spectral analysis of the labeled residues of DAO using SEAL reagent **2**. (A) A primary sequence of DAO. (B and C) nanoLC-MS/MS analysis of the fragments labeled at Lys163 (B) and 204 (C).



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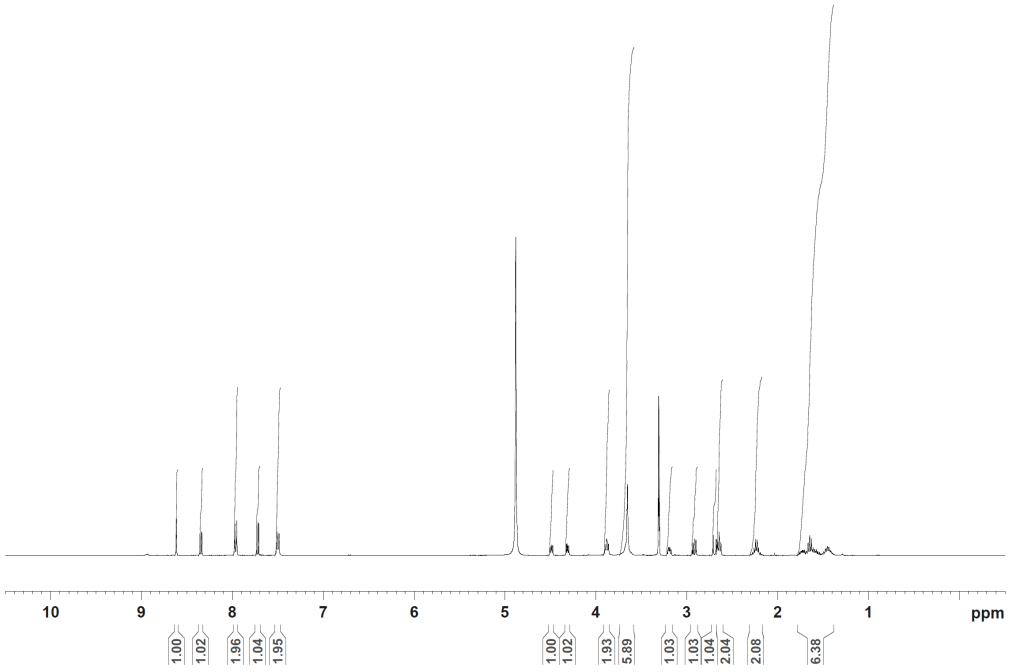
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8
7
6
5
4
3
2
1
ppm
1.00
1.02
1.96
1.04
1.95
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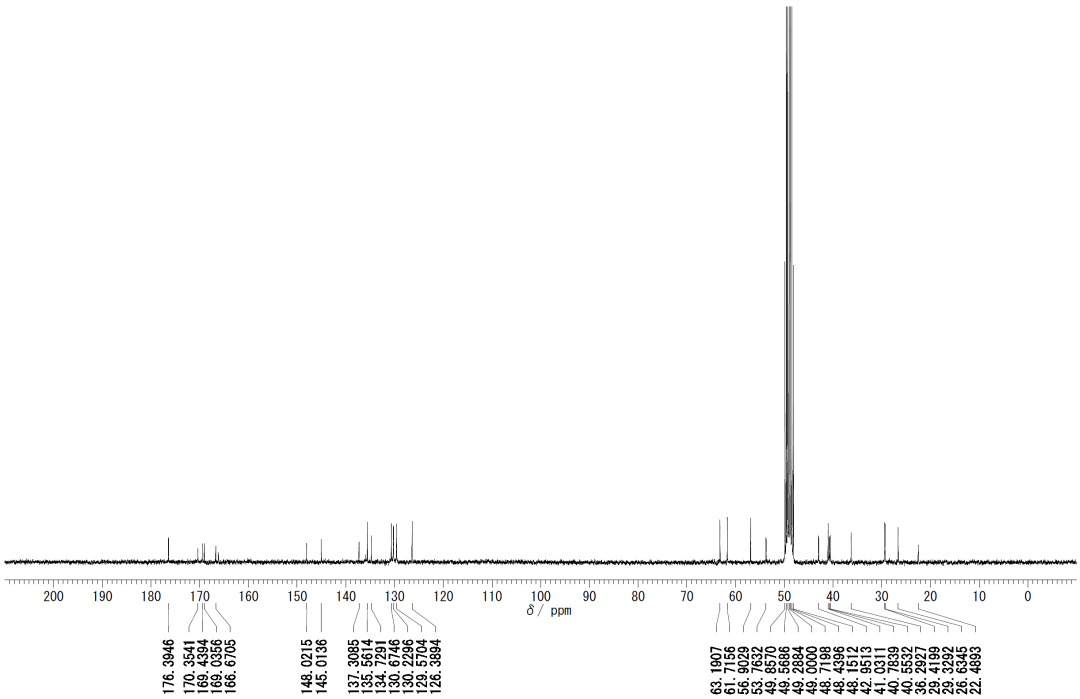
1.03
1.03
1.04
2.04
2.08
6.38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190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
δ / ppm
176.3946
170.3541
169.4394
169.0356
166.6705
148.0215
145.0136
137.3085
135.5614
134.7291
130.6746
130.2296
129.5704
126.3894
63.1907
61.7156
56.9029
53.7632
49.8570
49.5686
49.2884
49.0000
48.7198
48.4396
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29.4199
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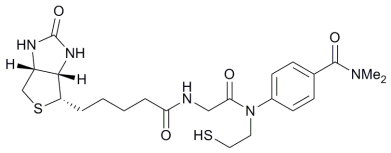
22.4693



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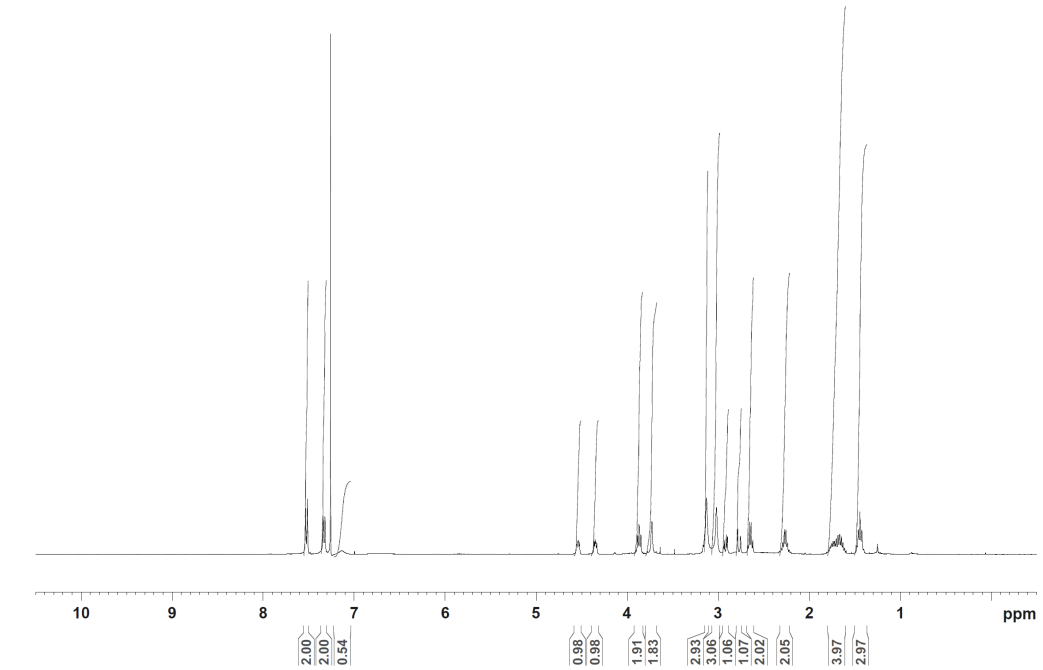
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8
7
6
5
4
3
2
1
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2.00
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0.98
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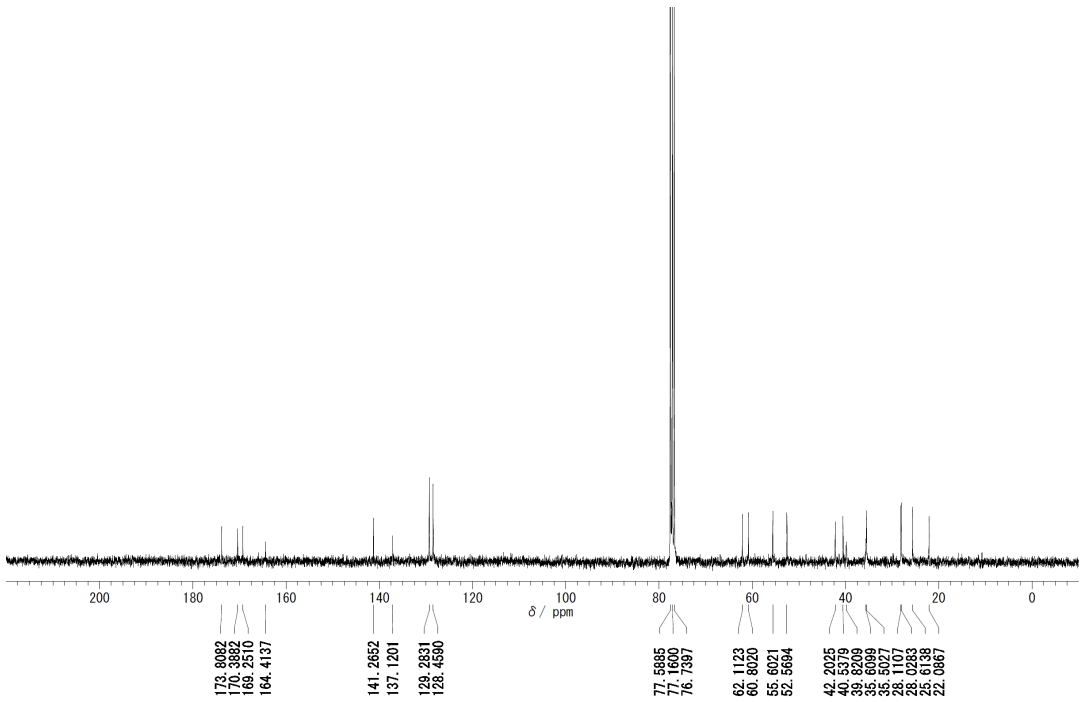
2.93
3.06
1.06
1.07
2.02
2.05
3.97
2.97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140
120
100
80
60
40
20
0
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141.2652
137.1201
129.2831
128.4590
77.5885
77.1600
76.7397
62.1123
60.8020
55.6021
52.5694
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40.5379
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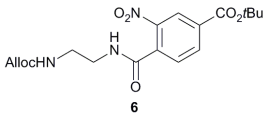
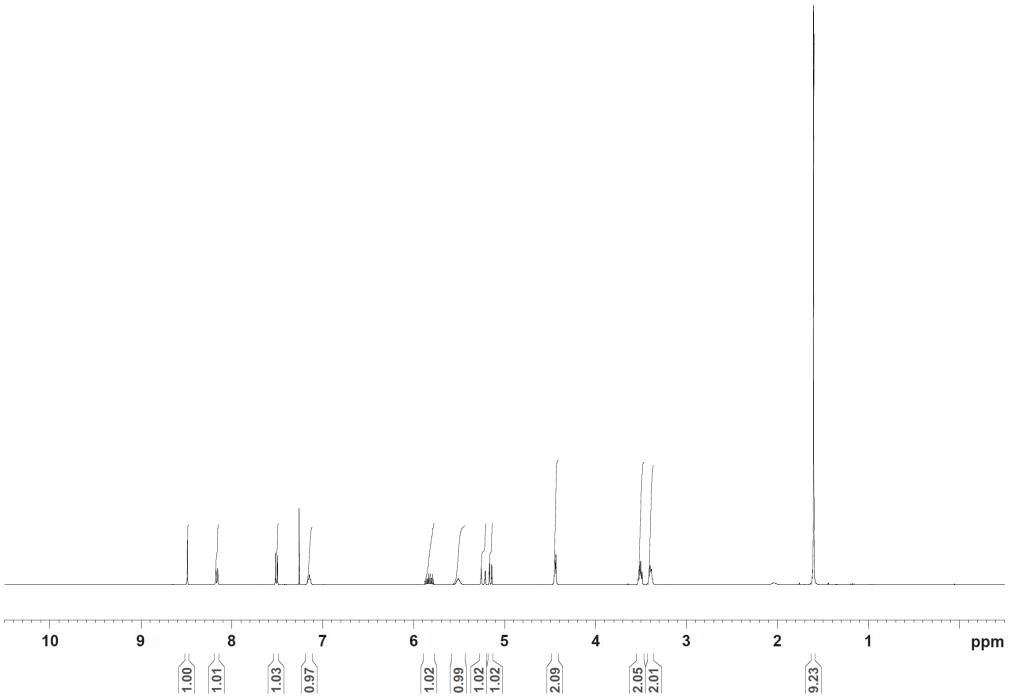
35.6099
35.5027
28.1107
28.0283
25.6138
22.0867


O2N
CO2tBu
H
N
AllocHN
O

6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1.02
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2.05
2.01
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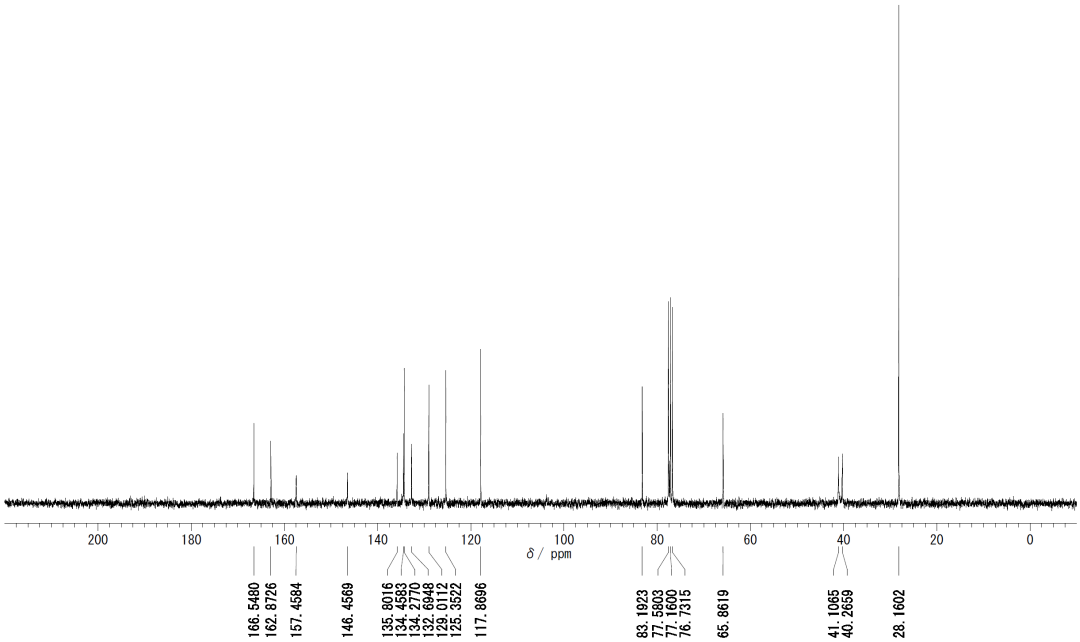
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80
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134.4583
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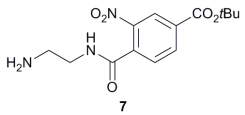
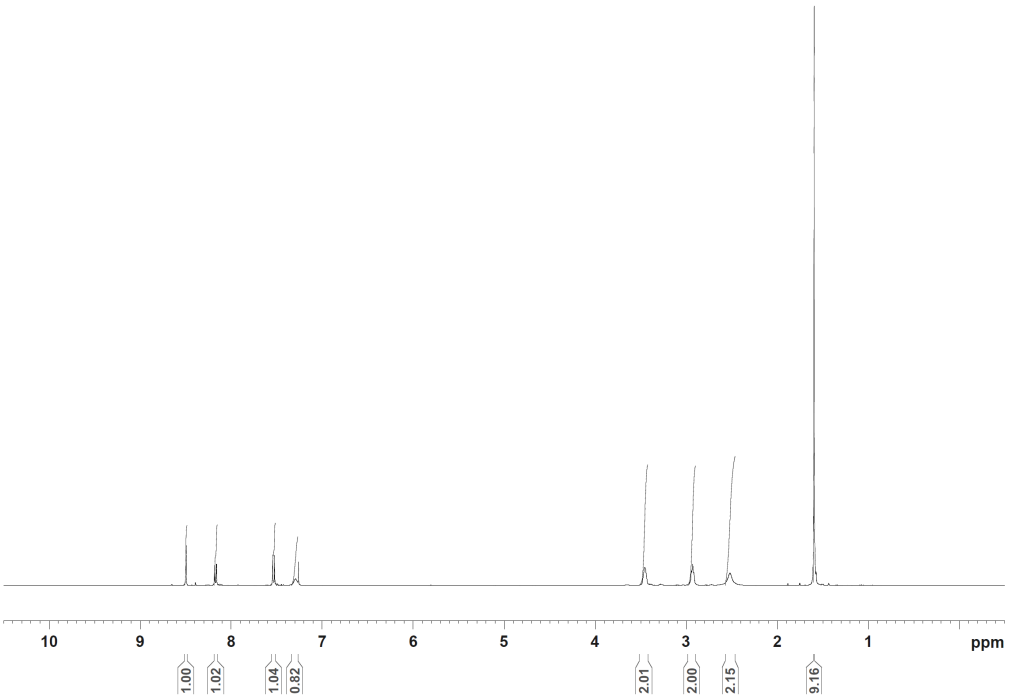
28.1602


O2N
CO2tBu
H
N
H2N
O

7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7
6
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4
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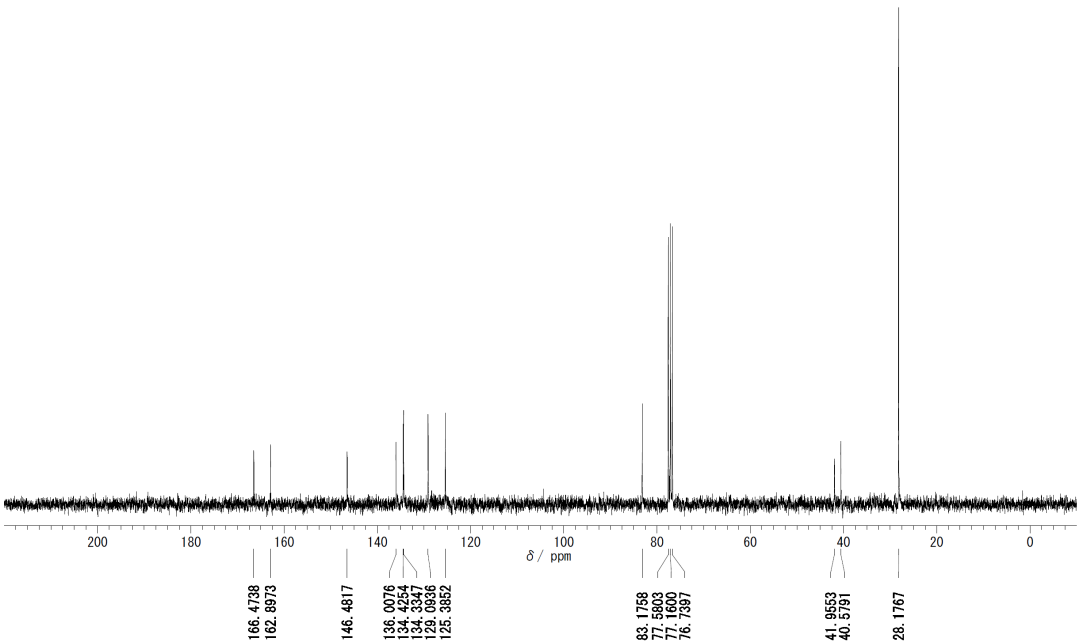
9.16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140
120
100
80
60
40
20
0
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134.4254
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129.0936
125.3852
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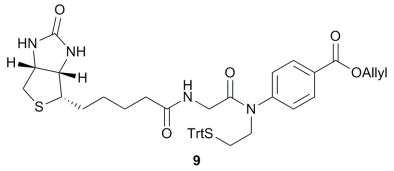
77.1600
76.7397
41.9553
40.5791
28.1767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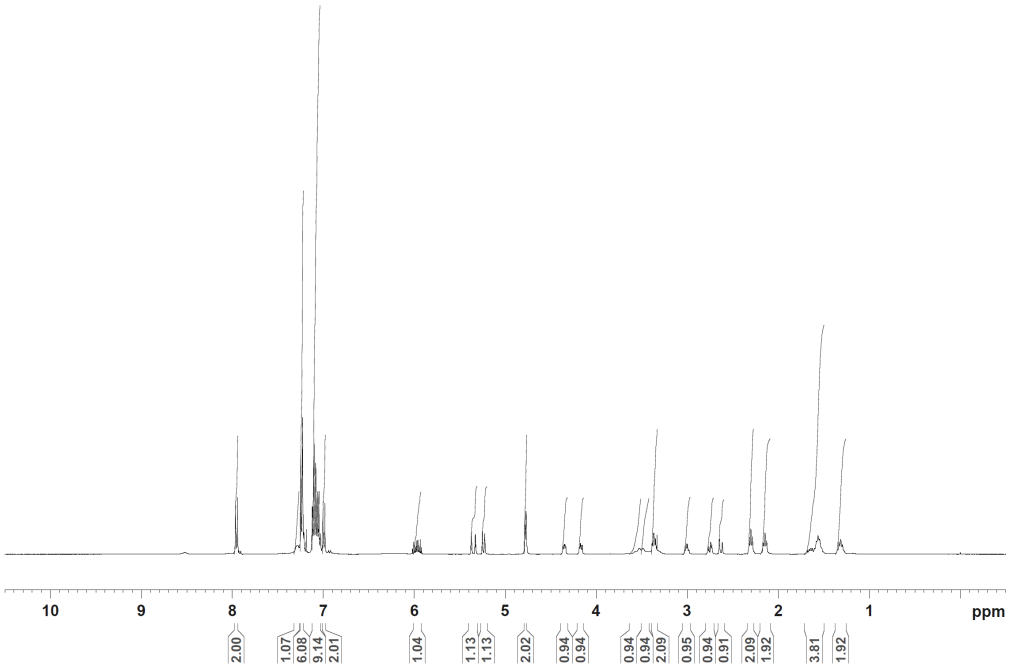
HN
NH
H
H
S
H
N
O
O
N
O
OAllyl
O
TrtS

9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8
7
6
5
4
3
2
1
ppm
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1.07
6.08
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2.01
1.04
1.13
1.13
2.02
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0.94
0.94
0.94
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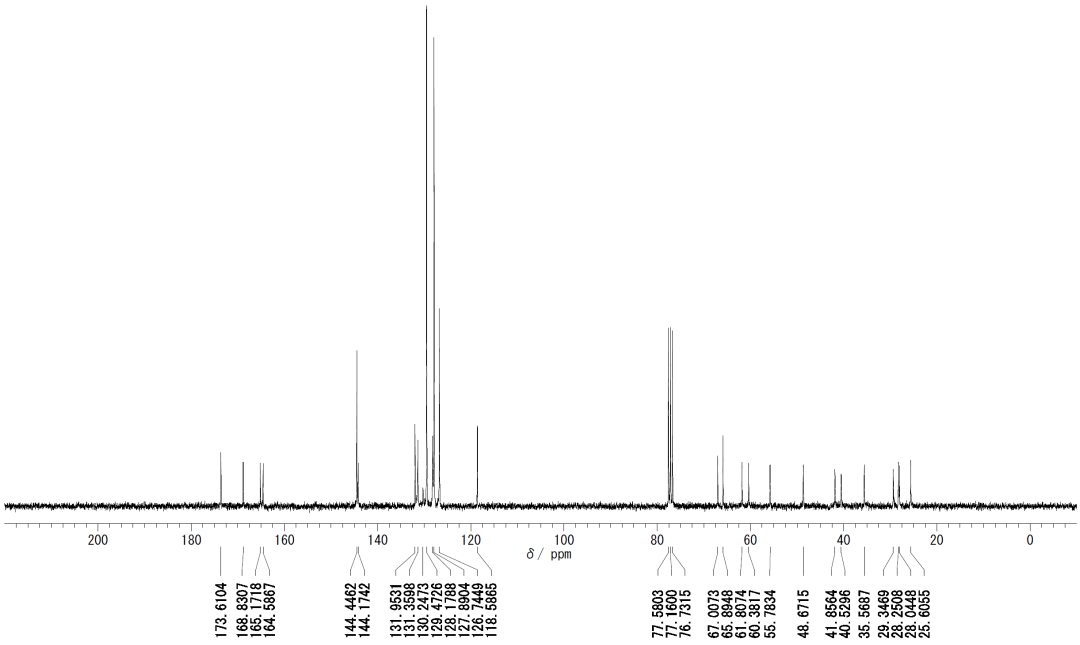
0.91
2.09
1.92
3.81
1.92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160
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120
100
80
60
40
20
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δ / ppm
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144.1742
131.9531
131.3598
130.2473
129.4726
128.1788
127.8904
126.7449
118.5865
77.5803
77.1600
76.7315
67.0073
65.8948
61.8074
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48.6715
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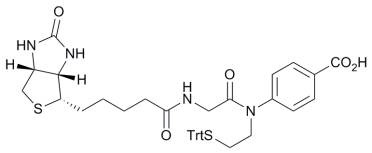
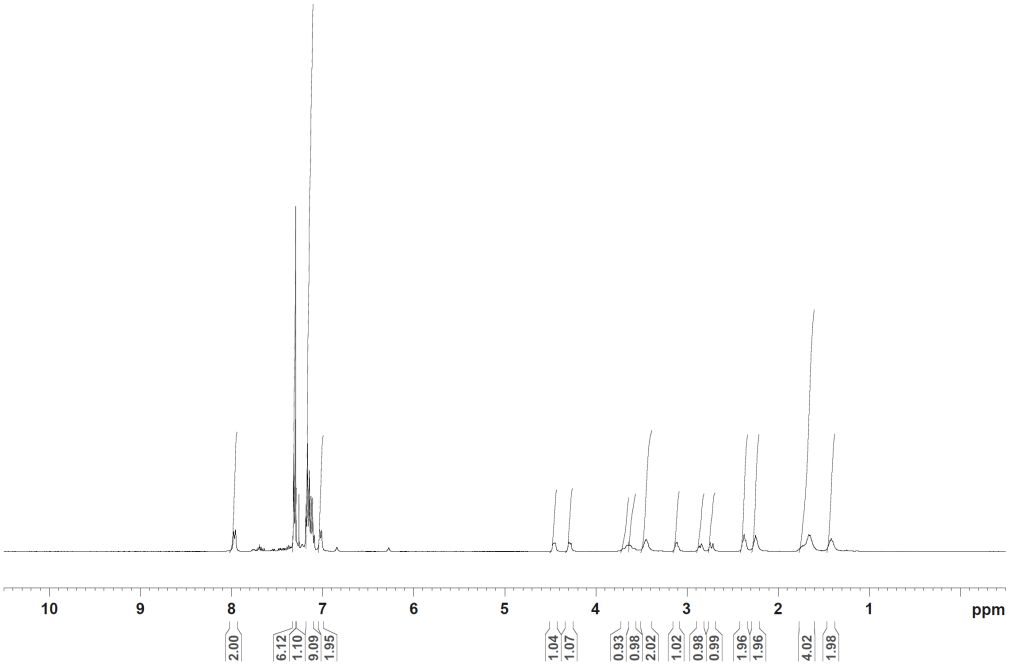
25.6055


O
HN
NH
H
H
S
H
N
O
O
N
CO2H
O
TrtS

10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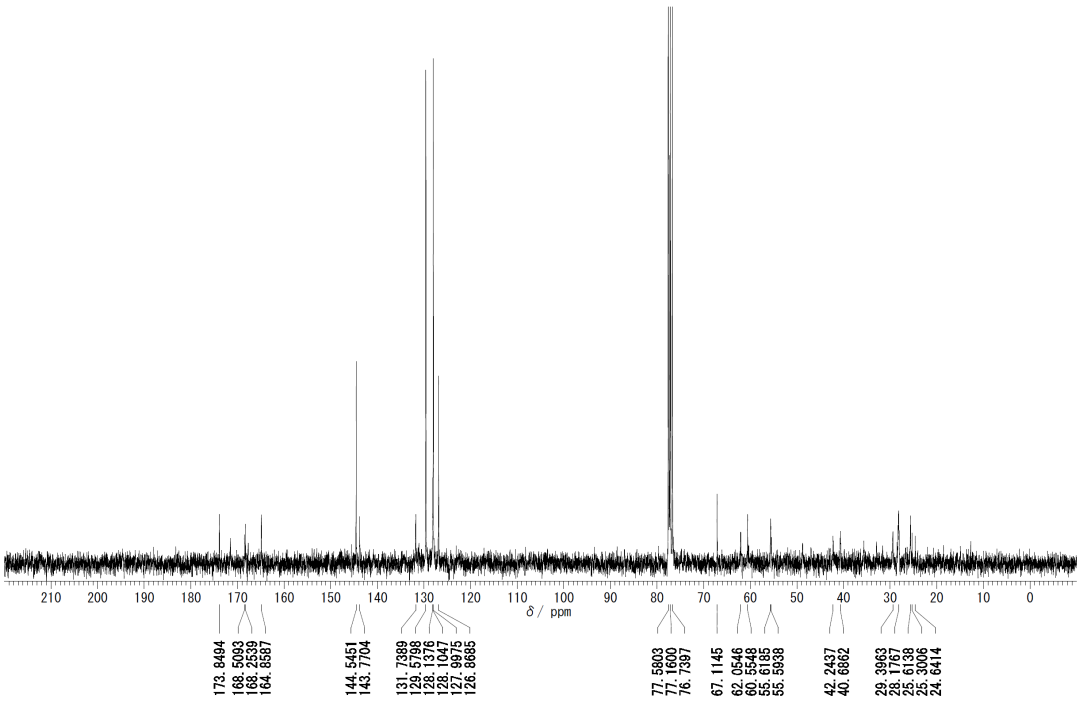
9
8
7
6
5
4
3
2
1
ppm
2.00
6.12
1.10
9.09
1.95
1.04
1.07
0.93
0.98
2.02
1.02
0.98
0.99
1.96
1.96
4.02
1.98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140
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120
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10
0
δ / ppm
173.8494
168.5093
168.2539
164.8587
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143.7704
131.7389
129.5798
128.1376
128.1047
127.9975
126.8885
77.5803
77.1600
76.7397
67.1145
62.0546
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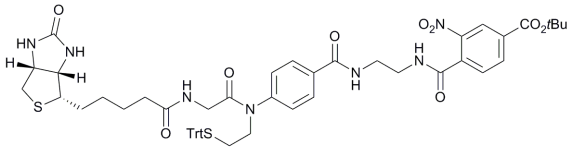

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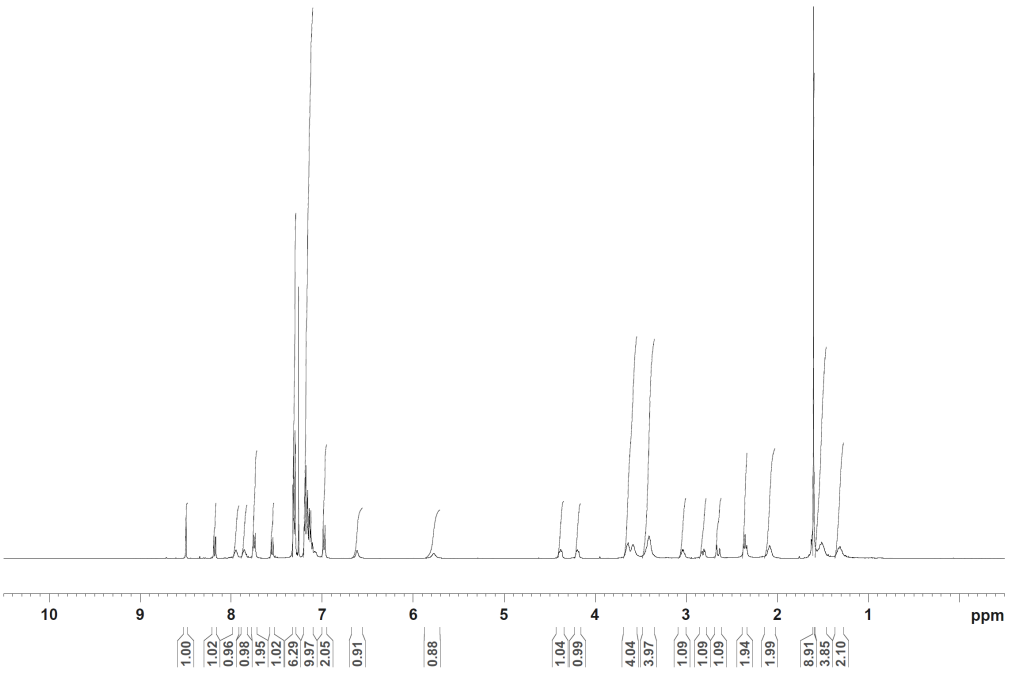
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7
6
5
4
3
2
1
ppm
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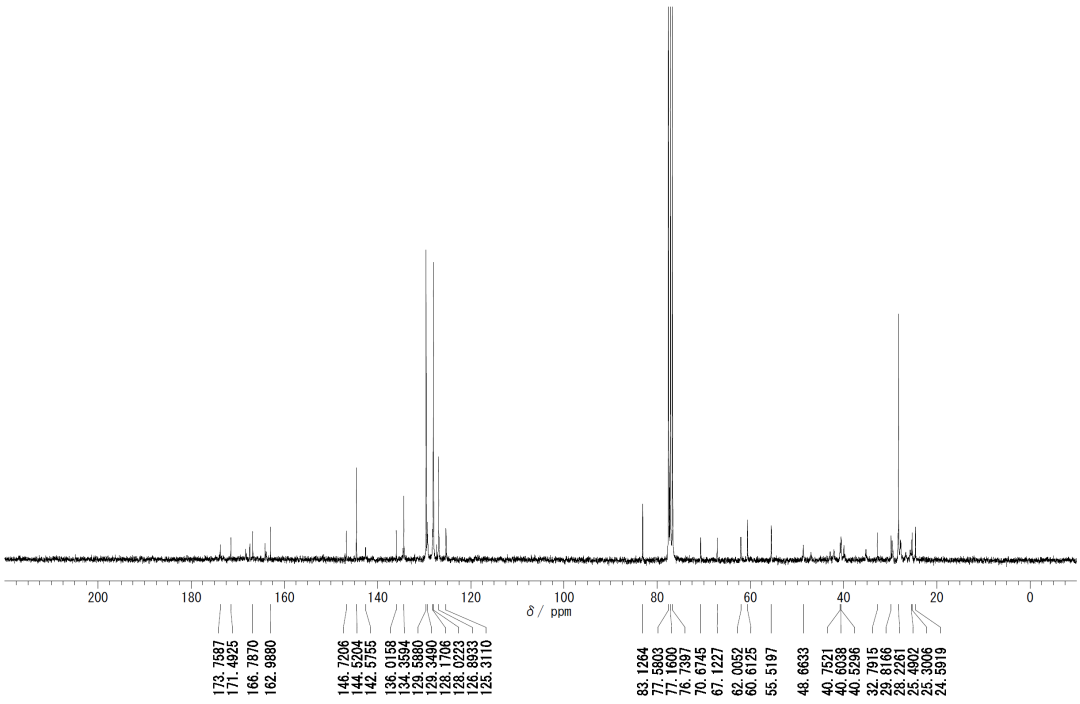
1.02
0.96
0.98
1.95
1.02
6.29
9.97
2.05
0.91
0.88
1.04
0.99
4.04
3.97
1.09
1.09
1.09
1.94
1.99
8.91
3.85
2.10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144.5204
142.5755
136.0158
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129.5880
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128.1706
128.0223
126.8933
125.3110
83.1284
77.5803
77.1600
76.7397
70.6745
67.1227
62.0052
60.6125
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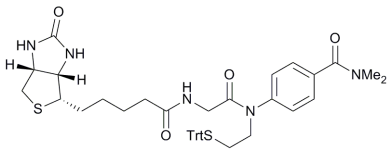
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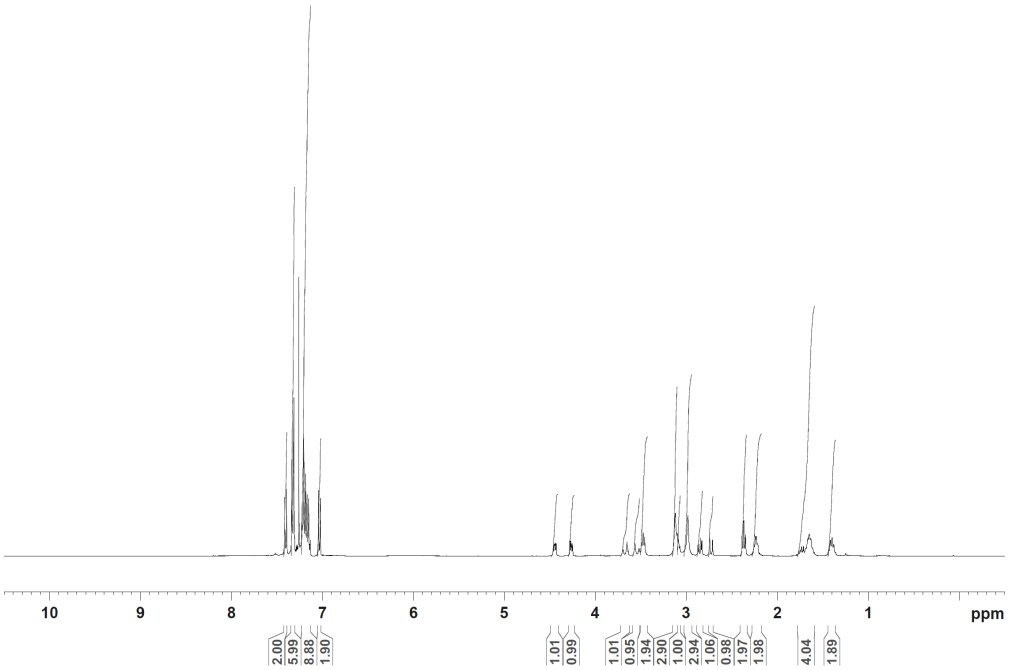
NH
H
H
S
H
N
O
N
O
NMe2
O
TrtS

12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8
7
6
5
4
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2
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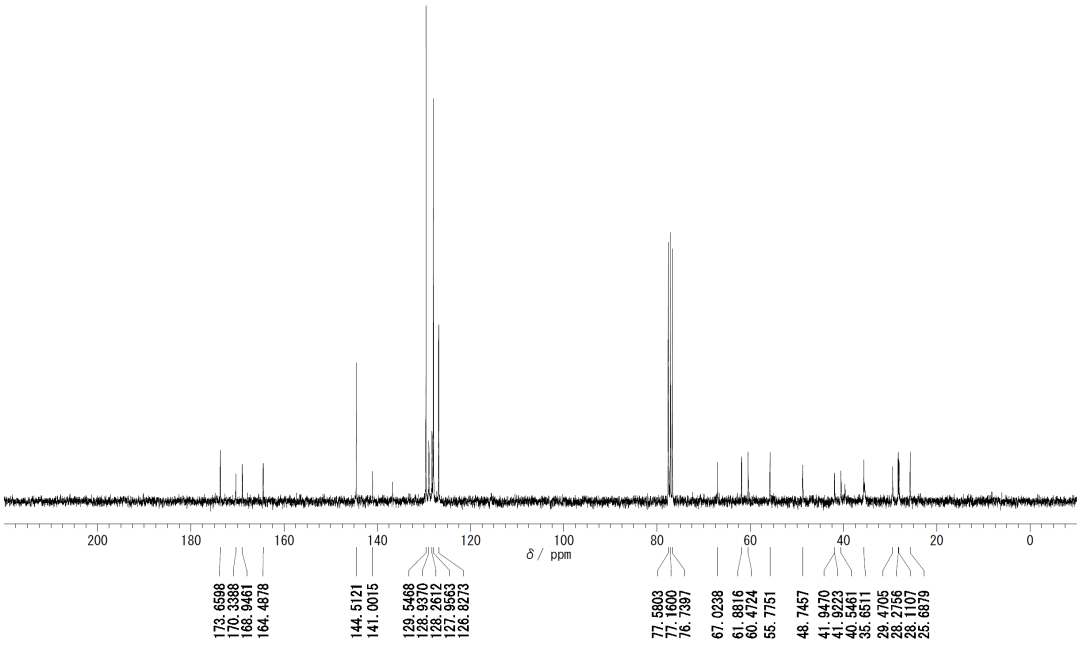
ppm
2.00
5.99
8.88
1.90
1.01
0.99
1.01
0.95
1.94
2.90
1.00
2.94
1.06
0.98
1.97
1.98
4.04
1.89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80
60
40
20
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δ / ppm
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141.0015
129.5468
128.9370
128.2612
127.9563
126.8273
77.5803
77.1600
76.7397
67.0238
61.8816
60.4724
55.7751
48.7457
41.9470
41.9223
40.5461
35.6511
29.4705
28.2756
28.1107
25.6879