Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information for

$PhI(OAc)_2$-Mediated Trifluoromethylthiolation/Oxidative Cyclization of Ynamides

Shixuan Su,[a] Zhipeng Yan,[a] Xingyuan Ye,[a] Jingyang Wang[b], Yuan Li[a] and Guangke He*[,a]

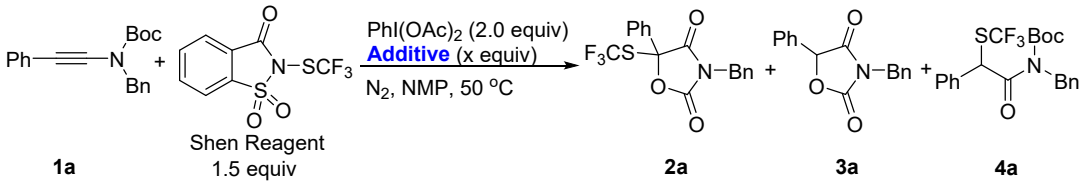
[a] *College of Chemistry and Molecular Engineering, Nanjing Tech University, Nanjing 211816, P. R. China.*

[b] *College of Energy Science and Engineering, Nanjing Tech University, Nanjing 211816, P. R. China.*

*E-mail: hegk@njtech.edu.cn

Contents

Table S1 The effect of additives on the trifluoromethylthiolation/oxidative cyclization of ynamides[a]



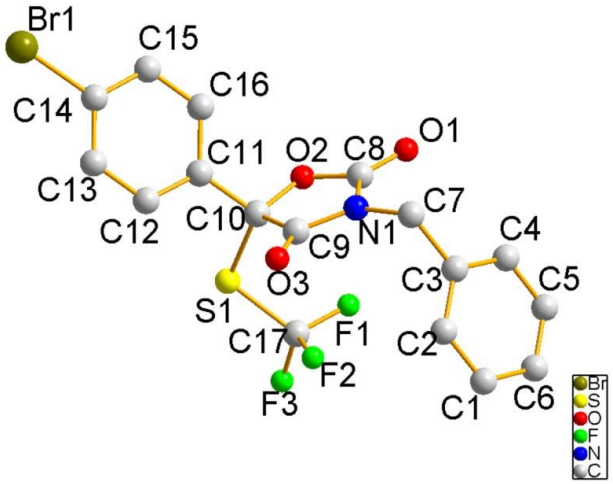
1a **2a** **3a** **4a**

Entry	**Additive** (x equiv.)	Time (h)	NMR yield of **2a**[b] (%)	Ratio of **2a**/**3a**/**4a**[b]
1[c]	–	24	61	75/25/0
2[d]	–	3	15	47/53/0
3[e]	–	3.5	0	0/99/0
4[f]	–	3.5	0	0/99/0
5[g]	–	11.5	0	0/100/0
6[h]	–	5	66	78/22/0
7[i]	–	4	78	82/18/0
8[j]	–	1.0	59	70/30/0
9[k]	–	1.0	67	80/20/0
10	Na_2CO_3 (0.2 equiv.)	13.5	50	86/7/7
11	K_2CO_3 (0.2 equiv.)	12	48	94/6/0
12	Cs_2CO_3 (0.2 equiv.)	11	46	84/7/9
13	Cs_2CO_3 (0.1 equiv.)	13.5	36	58/37/5
14	CH_3COOK (0.2 equiv)	6	62	74/23/3
15	K_3PO_4 (0.2 equiv.)	12	60	80/20/0
16	KPF_6 (0.2 equiv.)	6	64	76/22/2
17	NEt_3 (0.2 equiv)	6	46	74/10/16
18	PPh_3 (0.4 equiv)	6	55	65.5/27.5/7
19	PPh_3 (0.2 equiv)	6	62	71/23/6
20	PPh_3 (0.1 equiv)	6	62	73/23/4

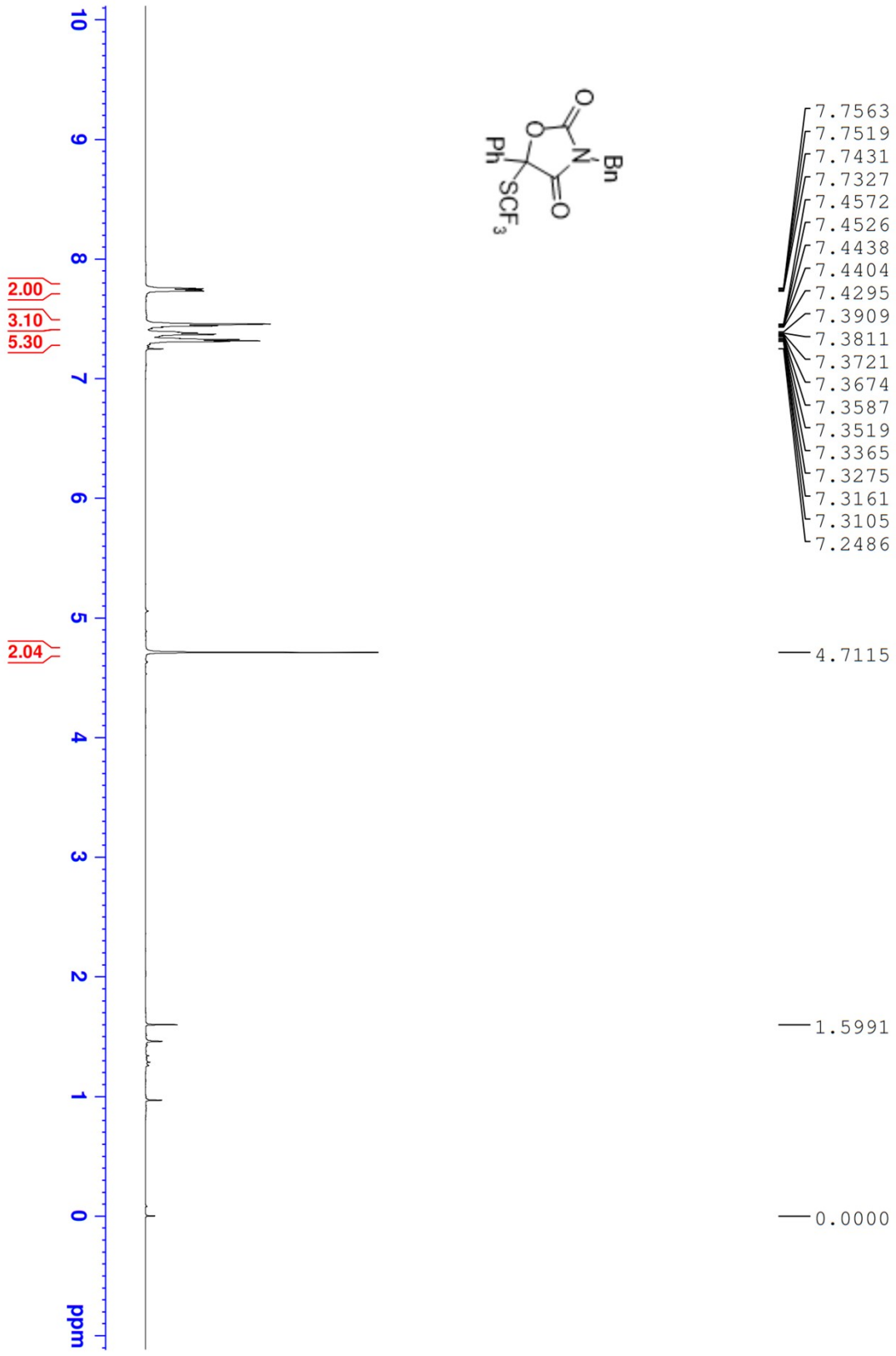
21	DBU (0.2 equiv.)	10	61	82/5/13
22	DIPEA (0.2 equiv)	11.5	39	72/15/13
23	2,6-Lutidine (0.2 equiv)	8	62	73/19/8
24	DMAP (0.2 equiv.)	6	52	56.5/14/29.5
25	TFIP (1.5 equiv)	3.5	49	91/0/9
26	TFIP (1.0 equiv)	5	60	90/0/10
27	TFIP (0.5 equiv)	3.5	60	92/0/8
28	TFIP (0.1 equiv)	3	60	90/0/10
29	H_2O (1.0 equiv)	6	48	69/31/0
30	H_2O (0.5 equiv)	3	63	76/24/0
31	H_2O (0.1 equiv)	3	65	77/23/0
32	$Pd(OAc)_2$ (0.5 mol%)	1	56	76/24/0
33	*m*-CPBA (1.0 equiv)	2.5	56	74/26/0
34	*t*-BuOH (1.0 equiv)	5	50	86/0/0

[a] Reaction conditions: **1a** (0.2 mmol), Shen Reagent (1.5 equiv.), and $PhI(OAc)_2$ (2.0 equiv.) in anhydrous NMP (2.0 mL) at 50 °C; [b] Determined by ^{19}F NMR and ^{1}H NMR analysis of the crude reaction mixture using benzotrifluoride and 1,3,5-trimethylbenzene as internal standards, respectively; [c] Temperature (r.t.); [d] Non-pretreated commercially available NMP; [e] Using MeOH instead of NMP; [f] Using benzyl alcohol instead of NMP; [g] Using HMPA instead of NMP;. [h] $PhI(OAc)_2$ (1.5 equiv.) was used; [i] $PhI(OAc)_2$ (3.0 equiv.) was used; [j] Shen Reagent (1.0 equiv.); [k] Shen Reagent (2.0 equiv.).

Fig. S1 X-ray structure of compound 2d



Crystal data for **2d**: $C_{17}H_{11}BrF_3NO_3S$, M = 446.24, monoclinic, space group $P2_1/c$, final R indices [I > 2σ(I)]: R_1 = 0.0668, wR_2 = 0.2057, R indices (all data): R_1 = 0.0885, wR_2 = 0.2603, a = 18.868(5), b = 12.831(4), c = 7.106(3) Å, β = 93.222(13) °, V = 1717.5(10) Å^3 , T = 296(2) K, Z = 4, reflections collected/unique: 9748/3813 (R_{int} = 0.0618), number of observations [I > 2σ(I)]: 3813, parameters: 235. **CCDC-2104187** contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_ request/cif.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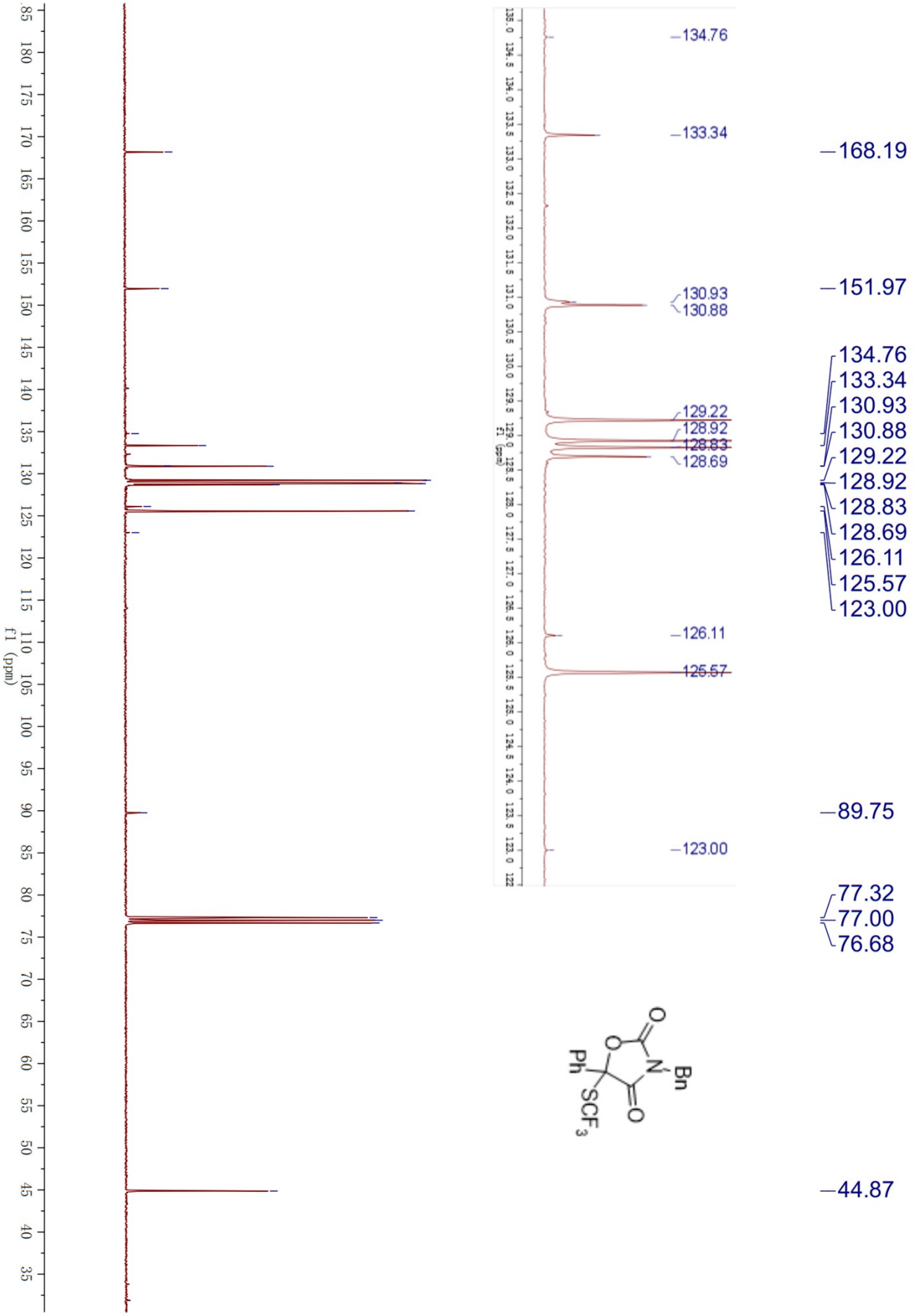
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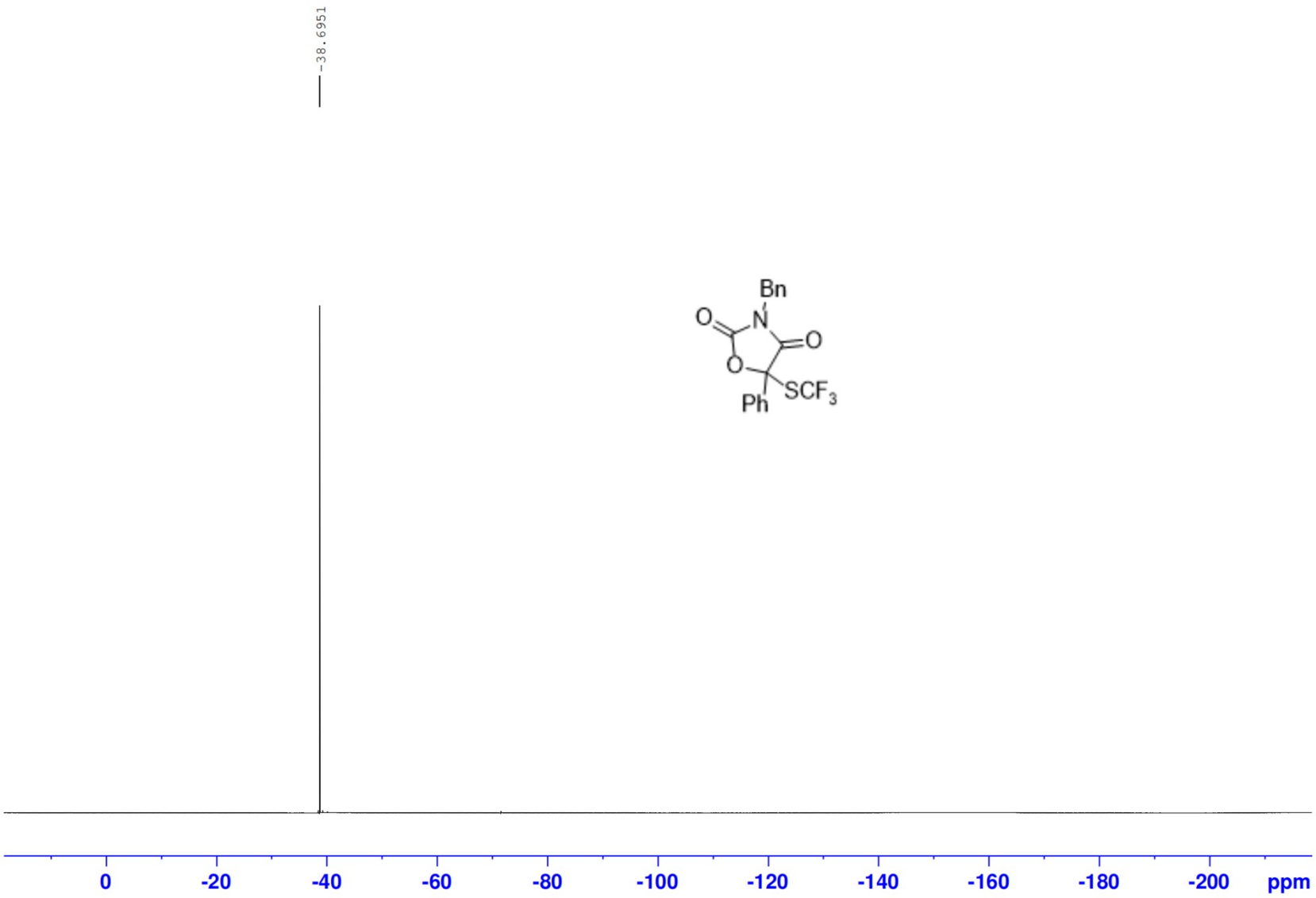
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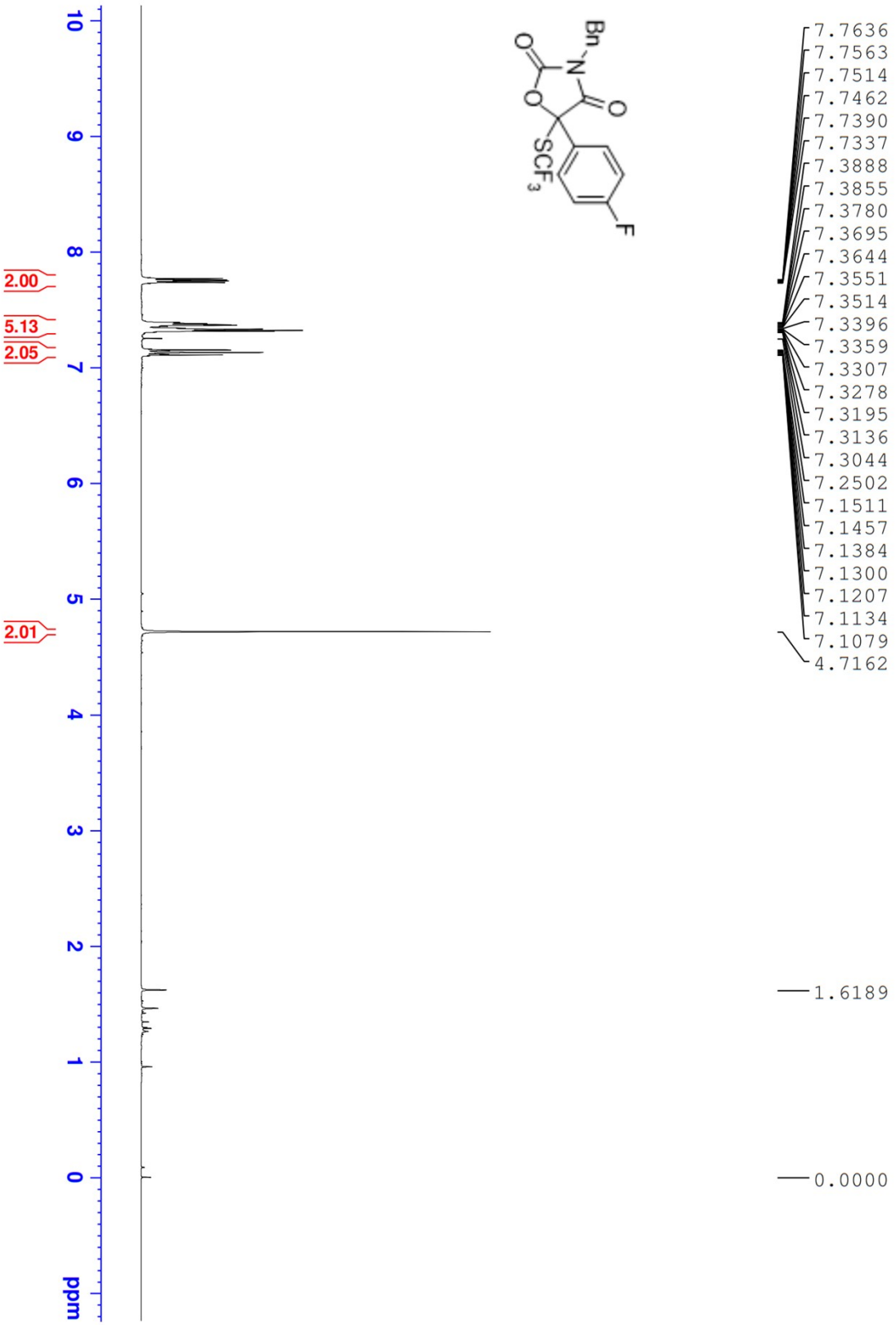
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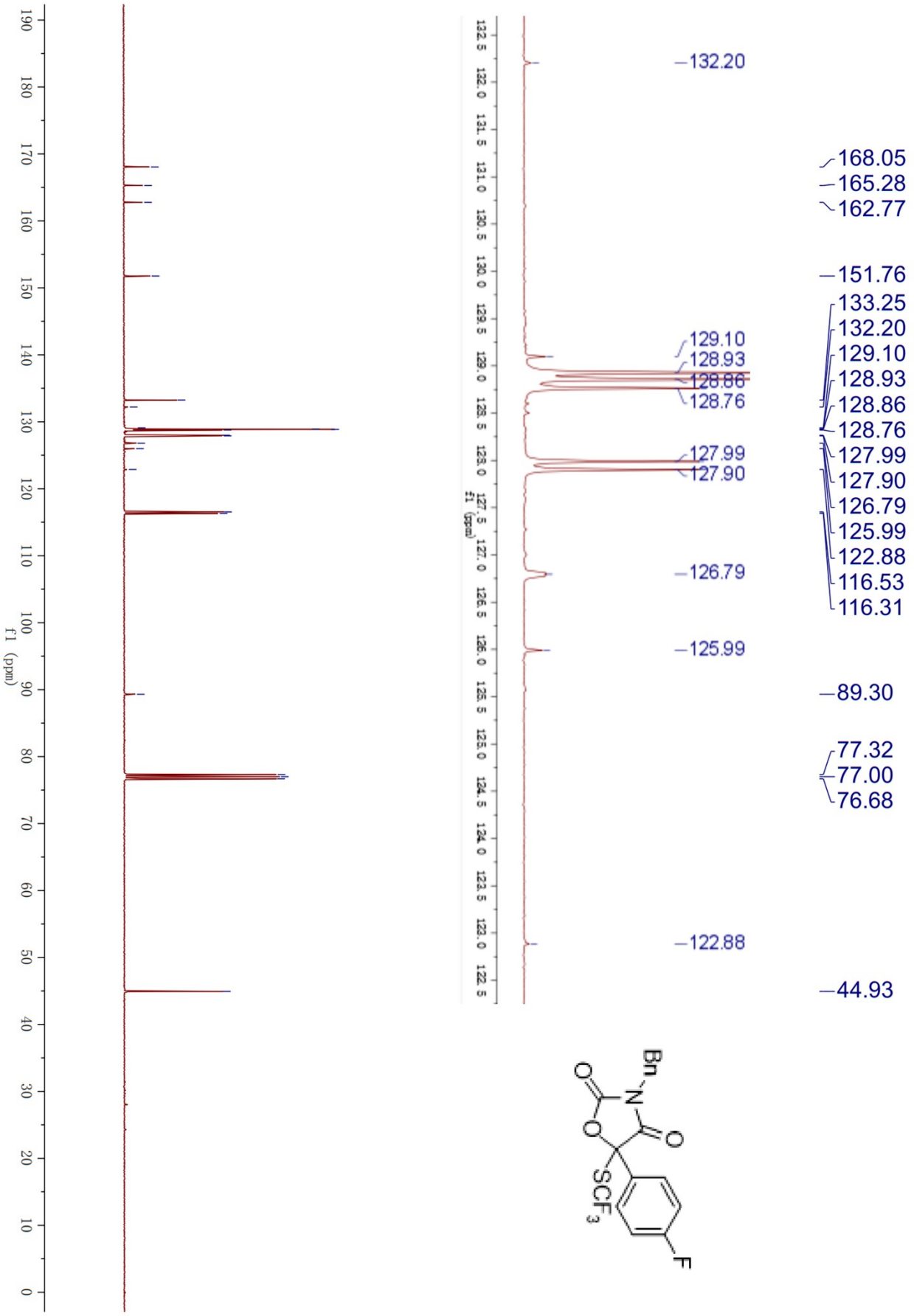
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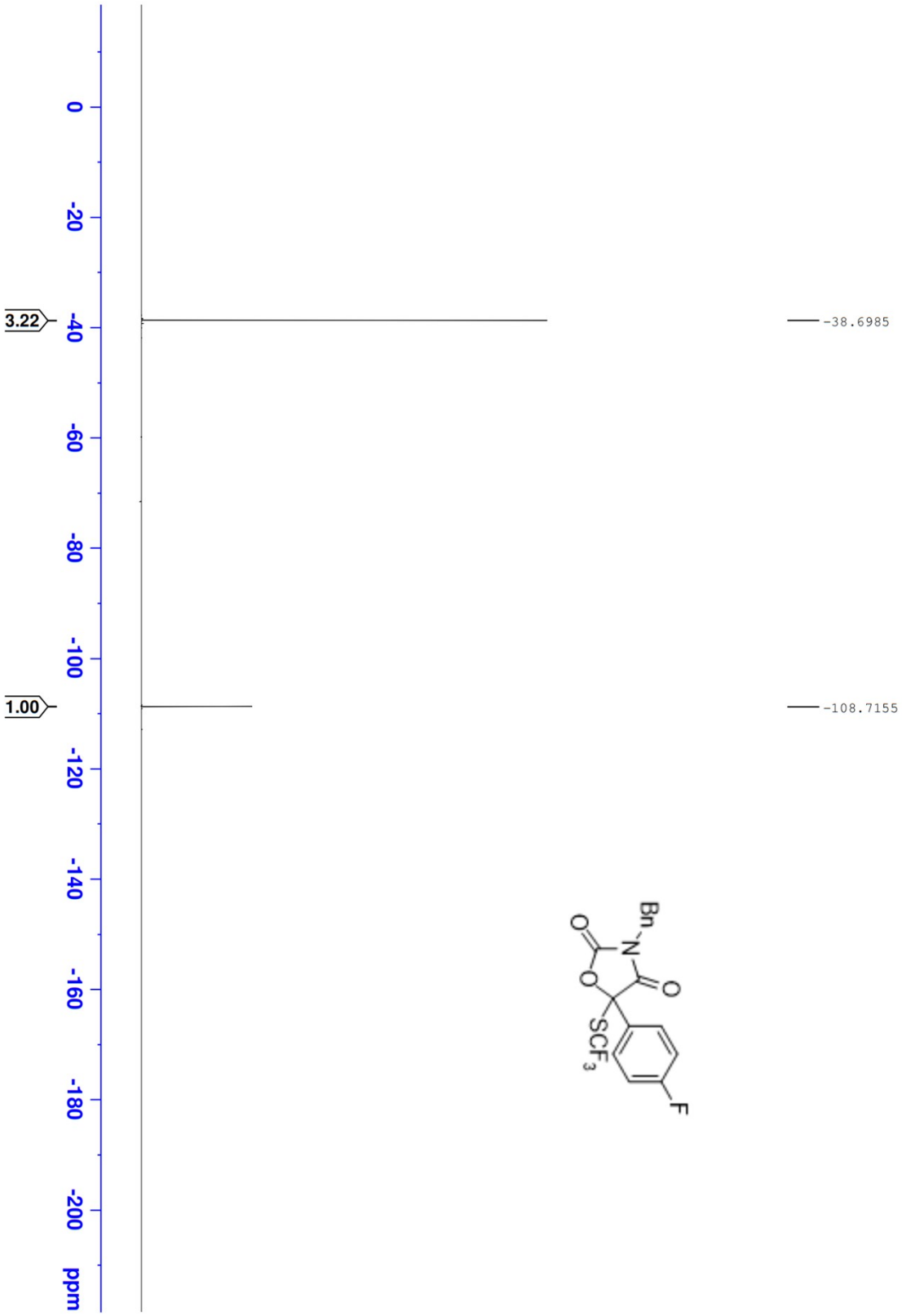
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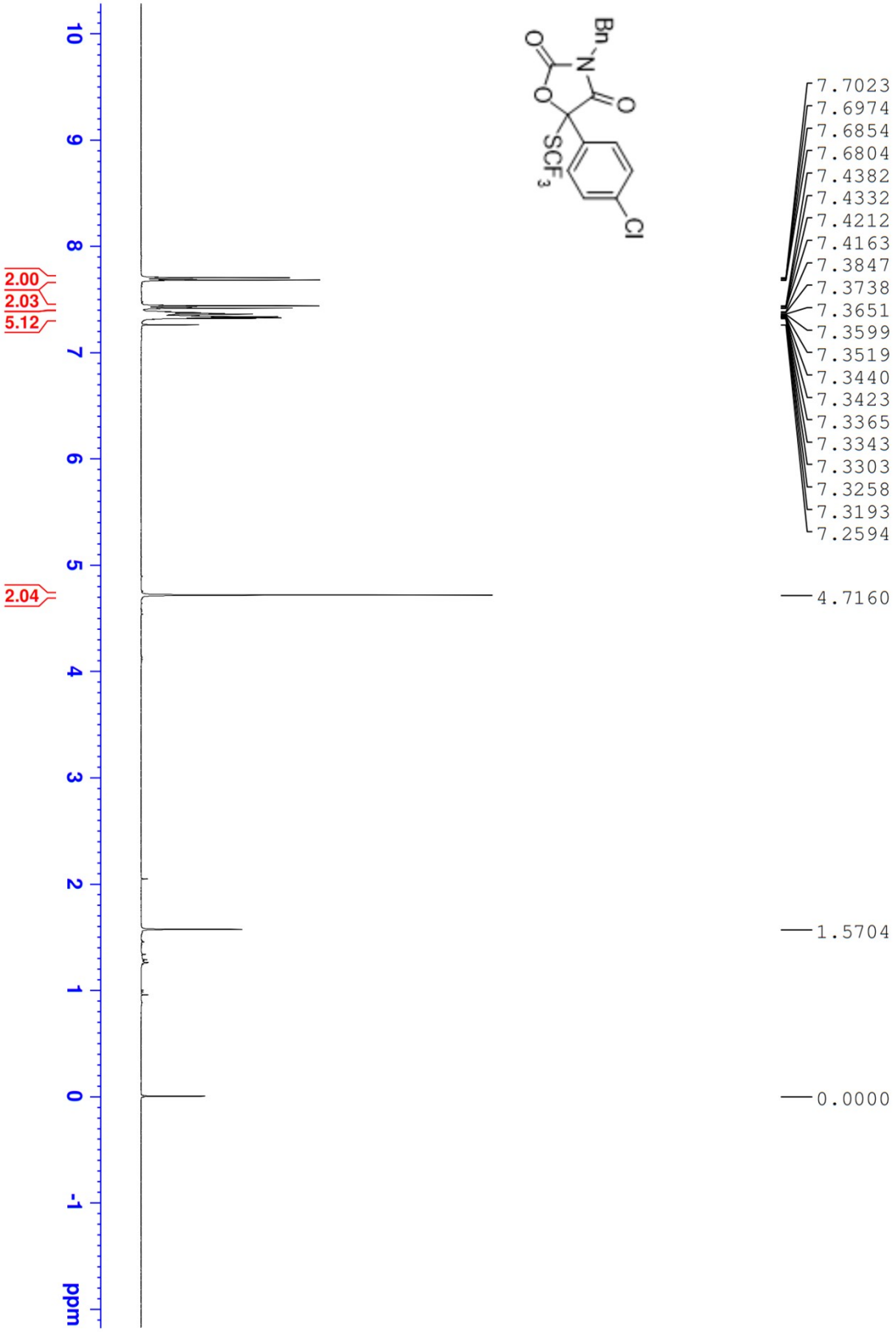
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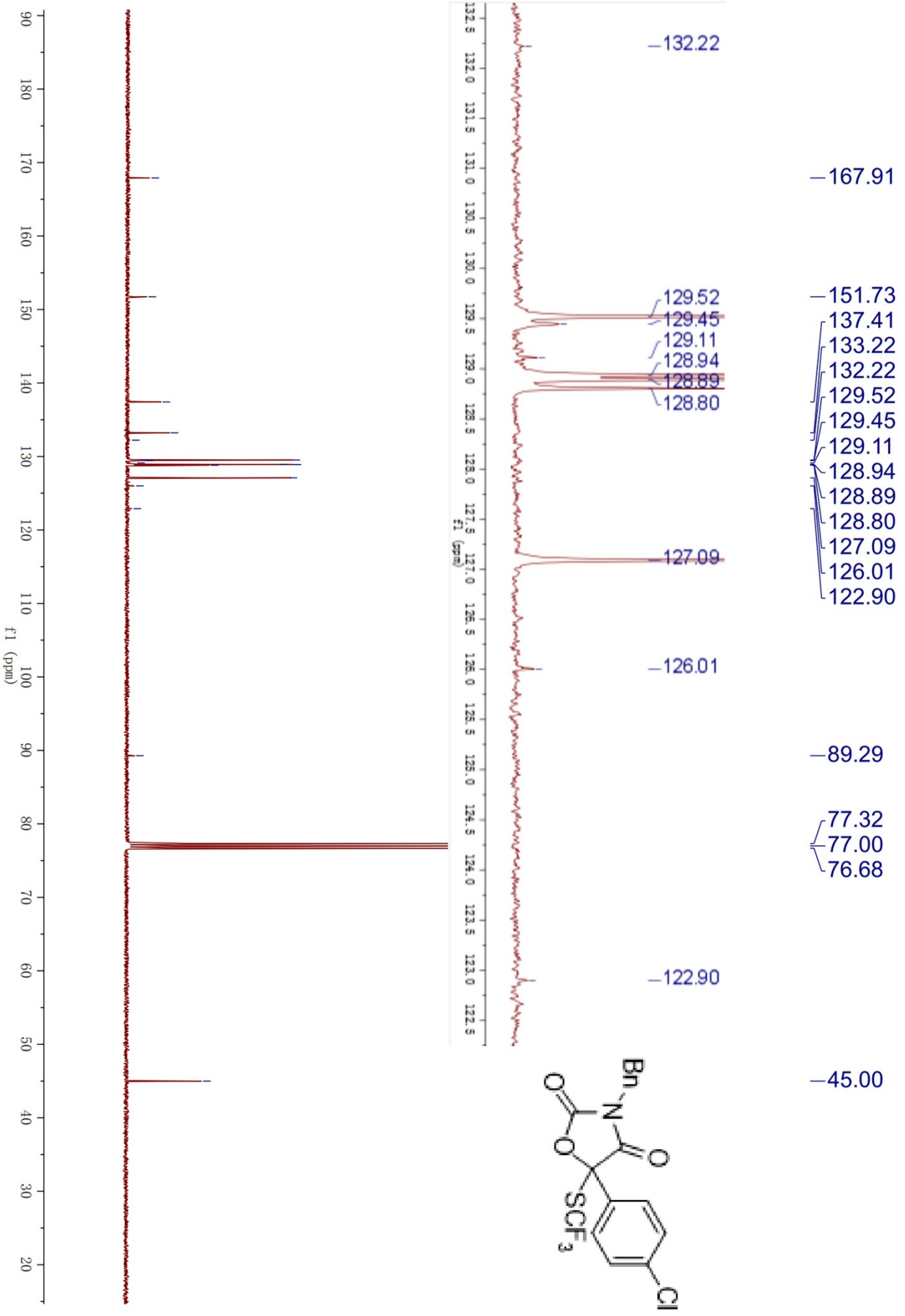
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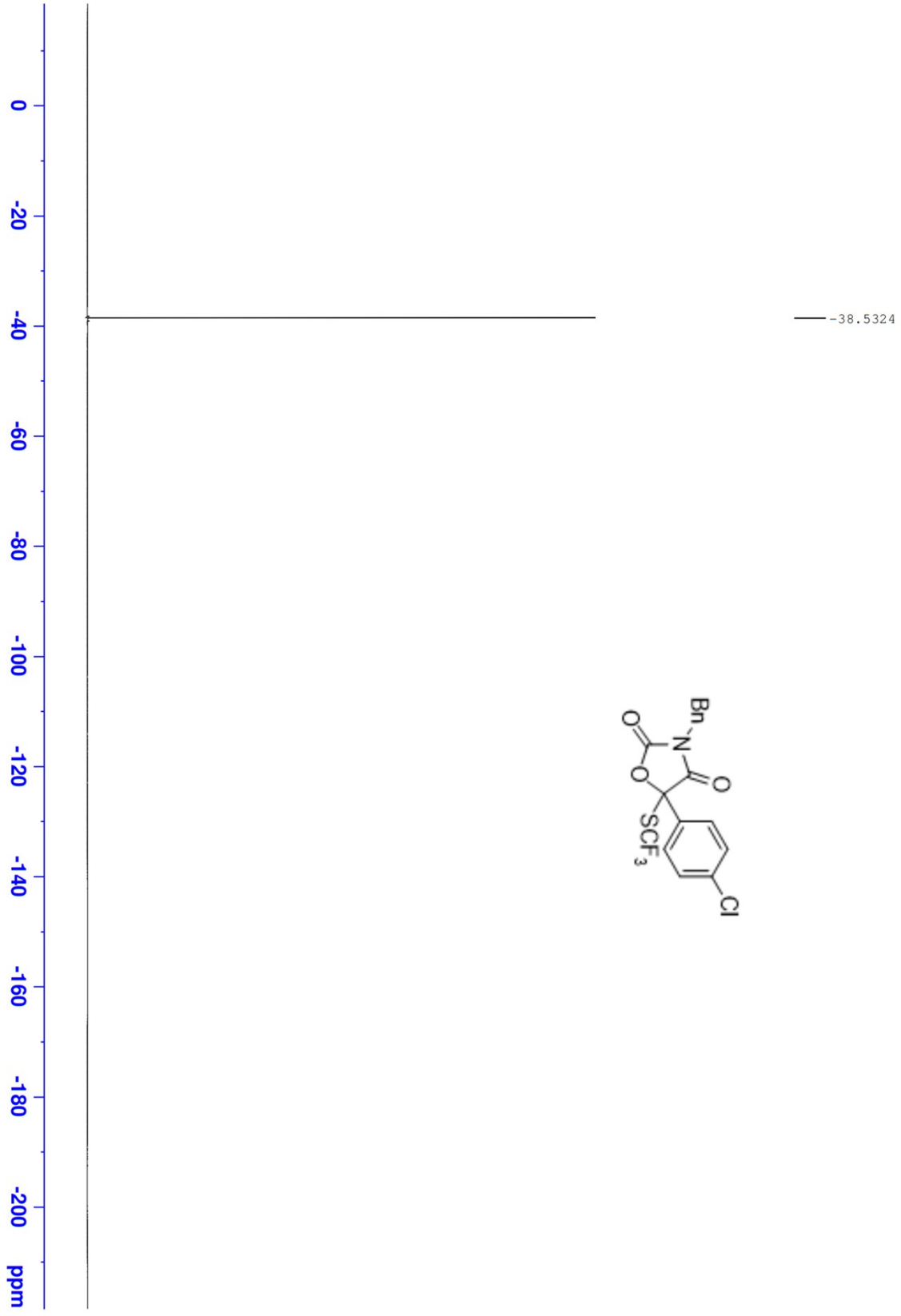
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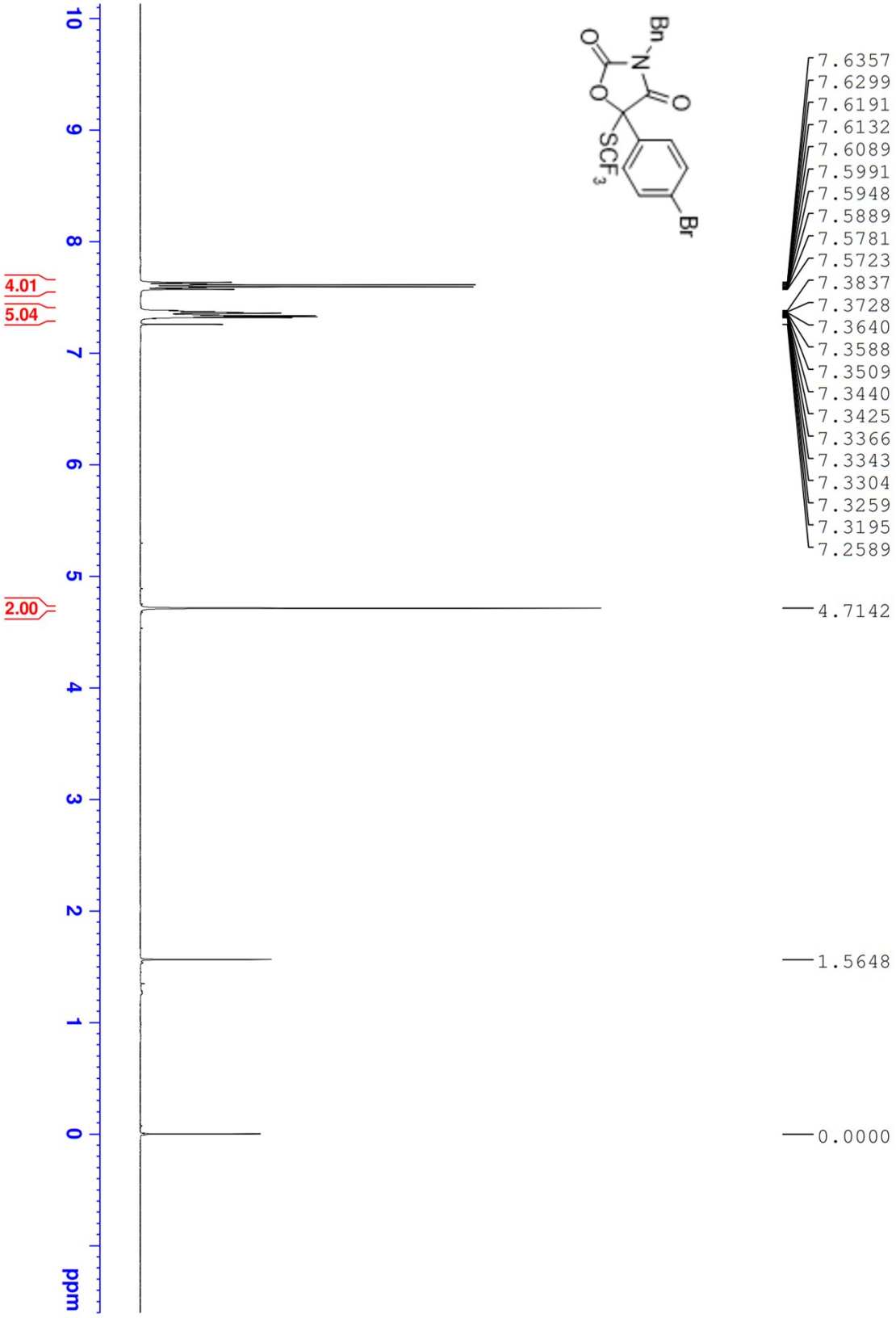
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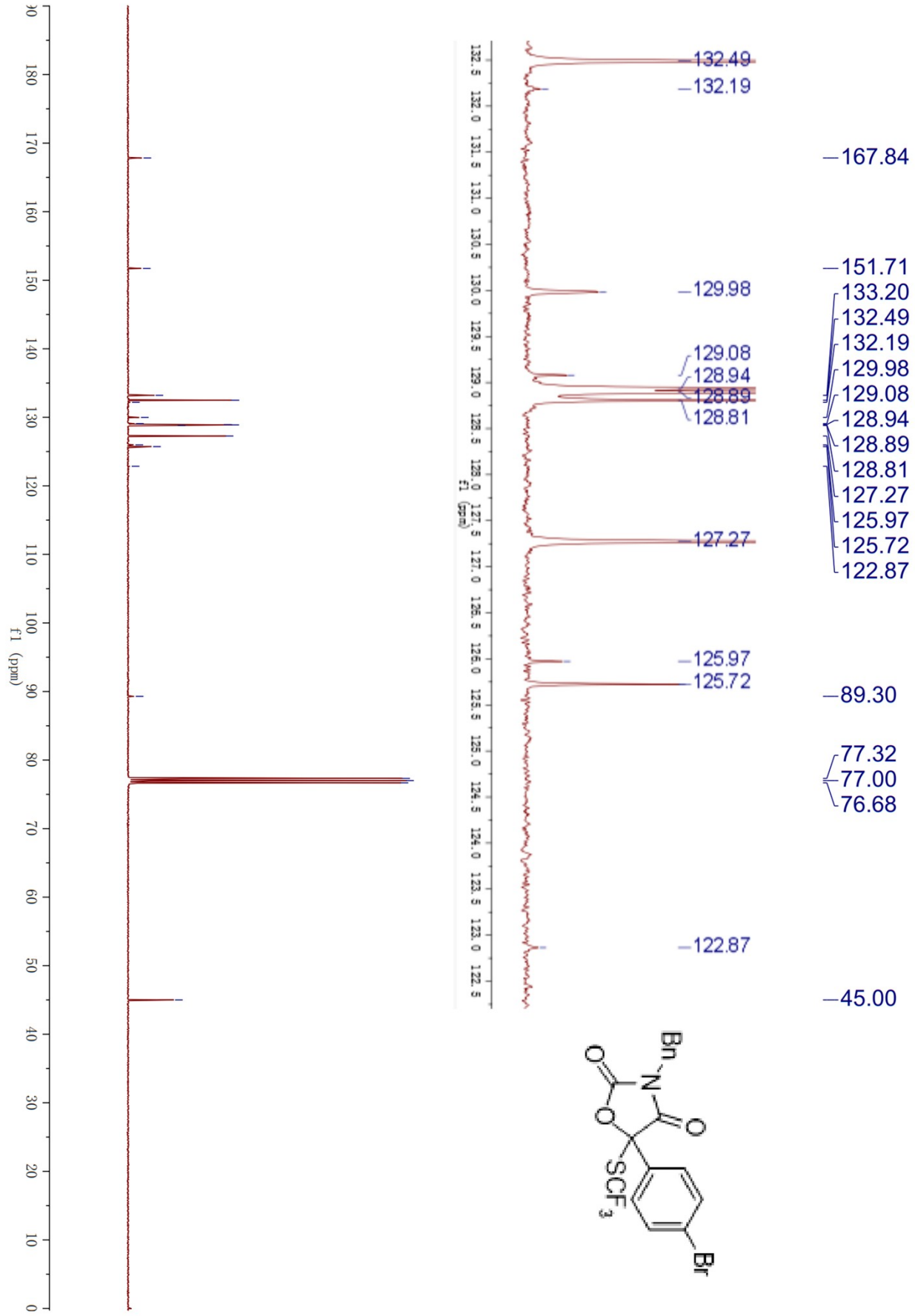
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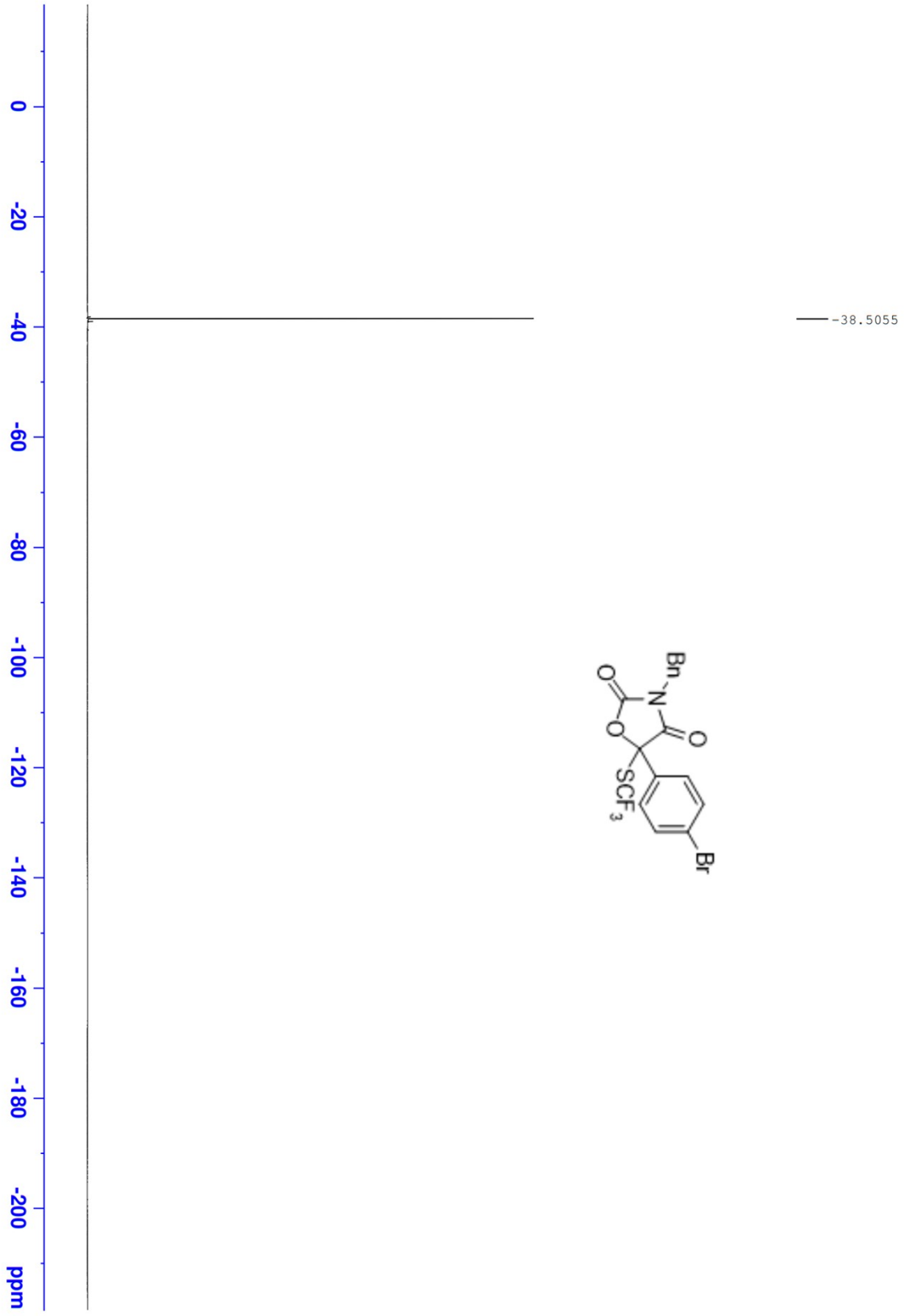
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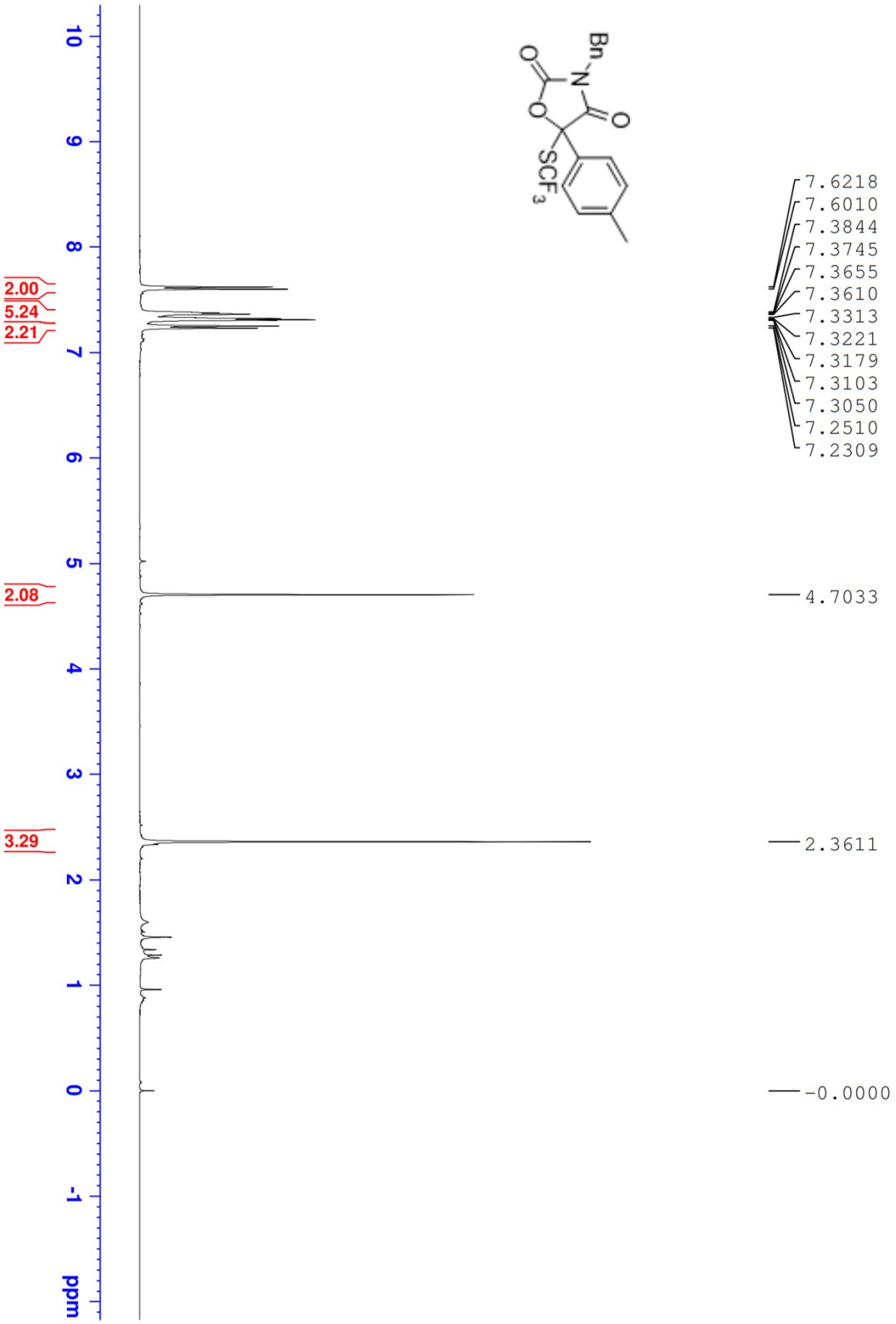
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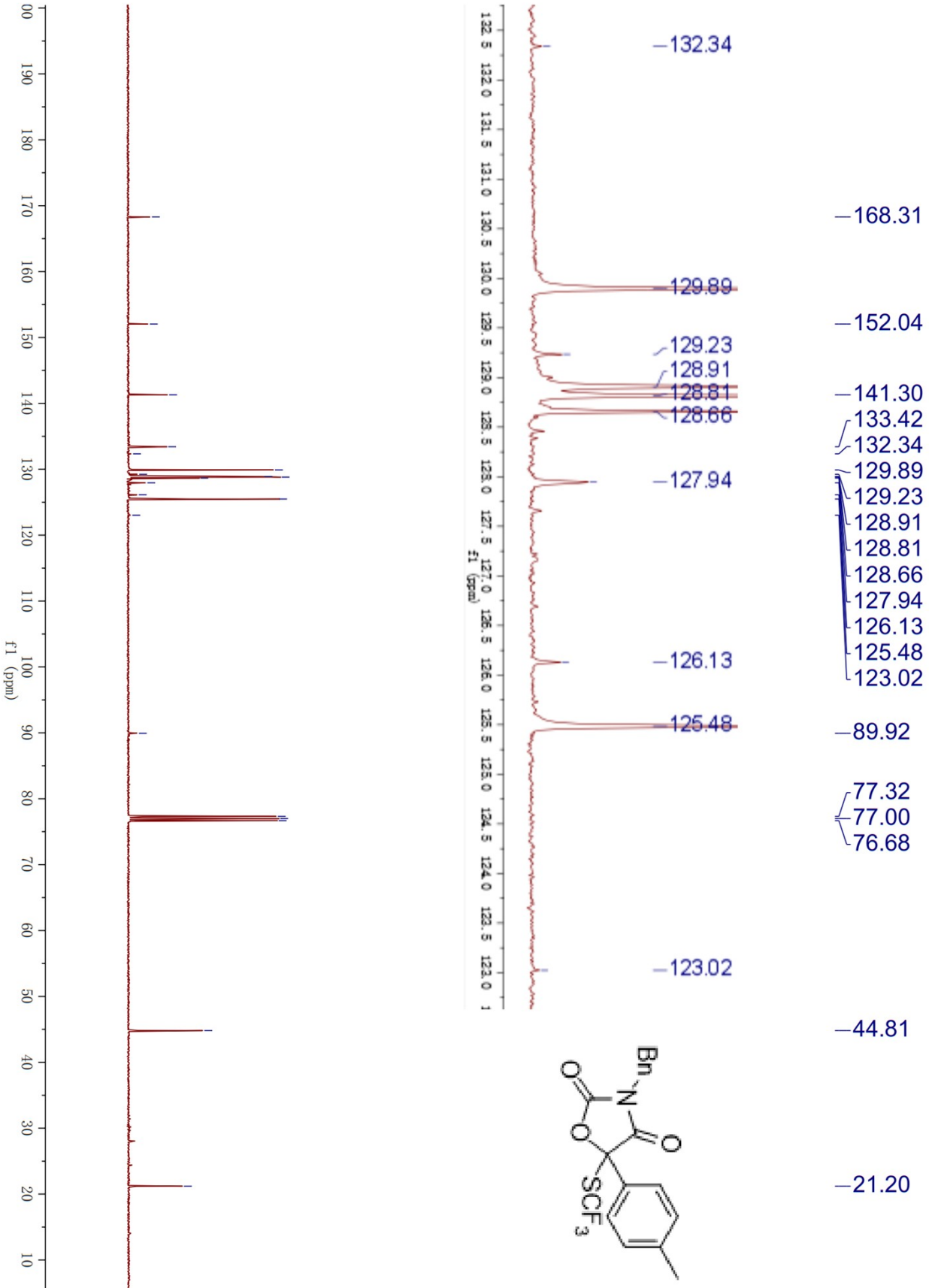
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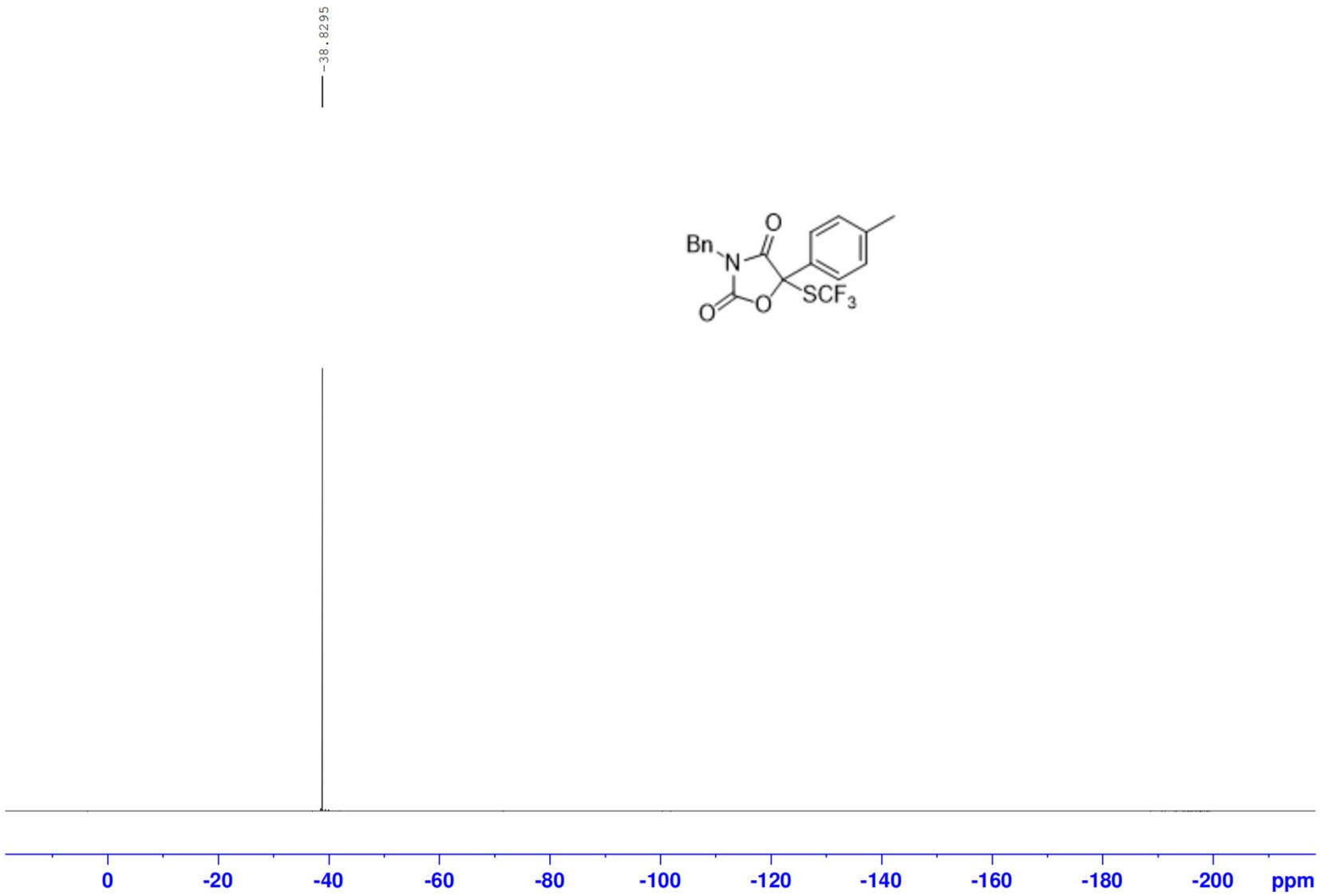
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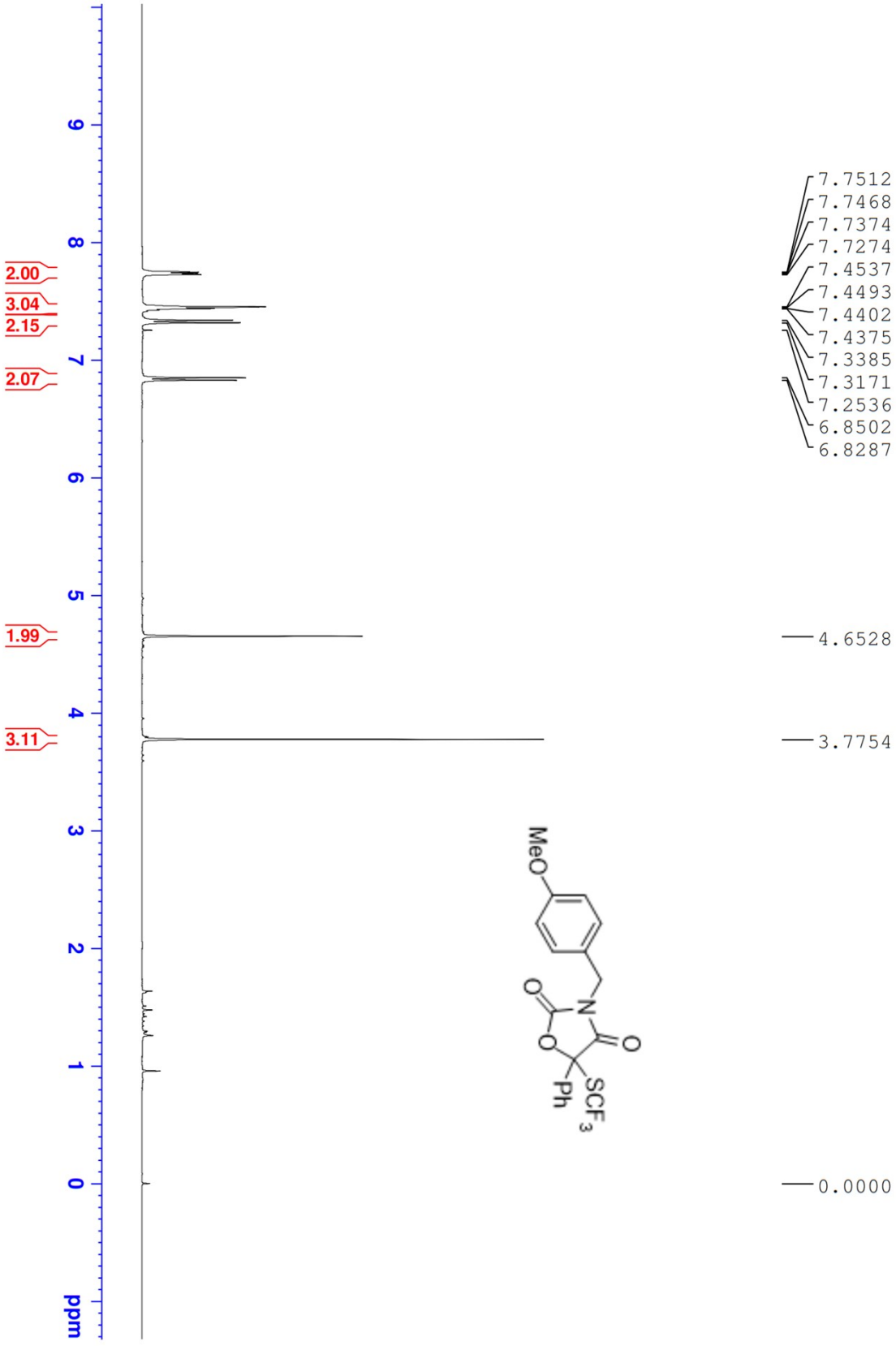
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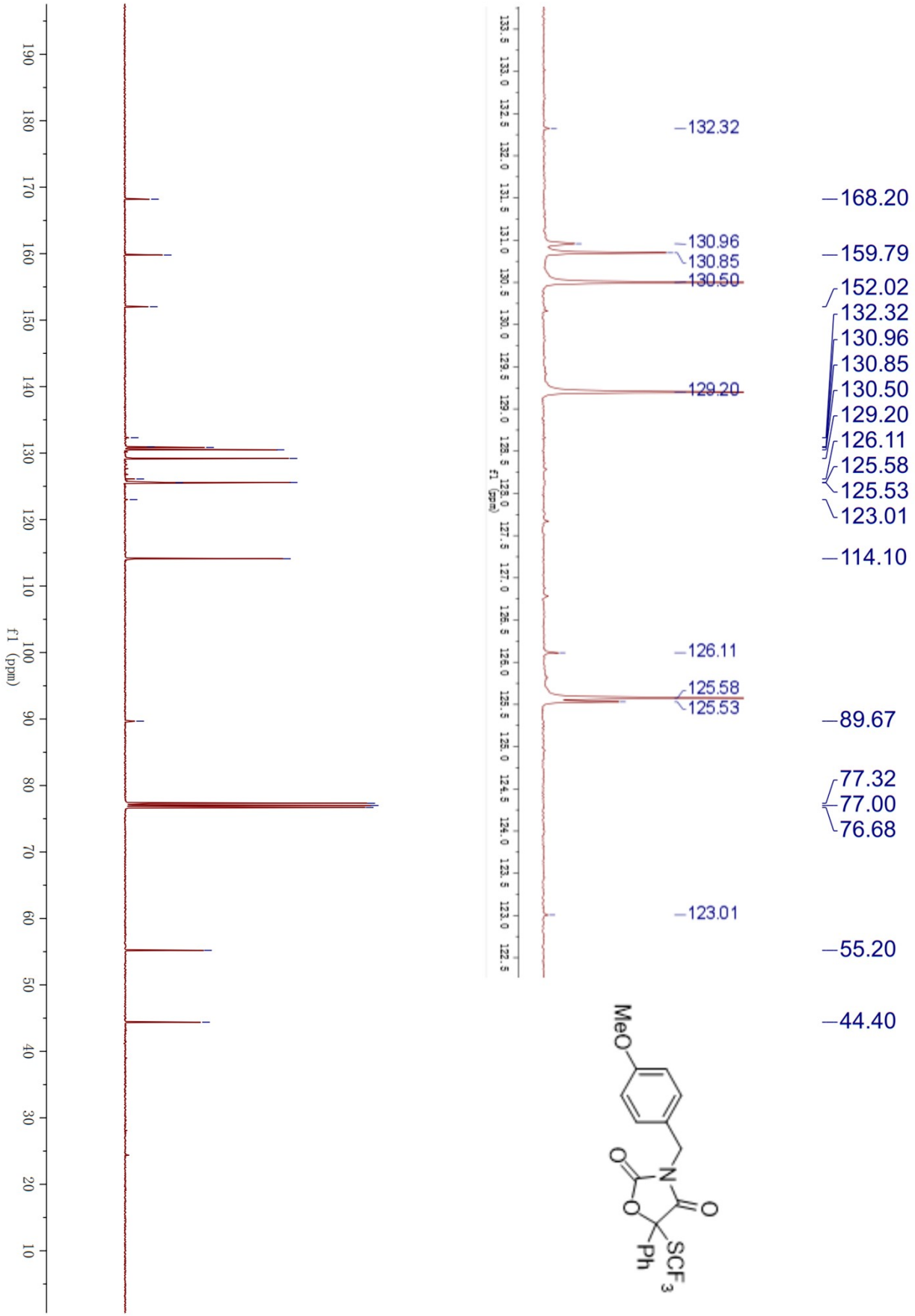
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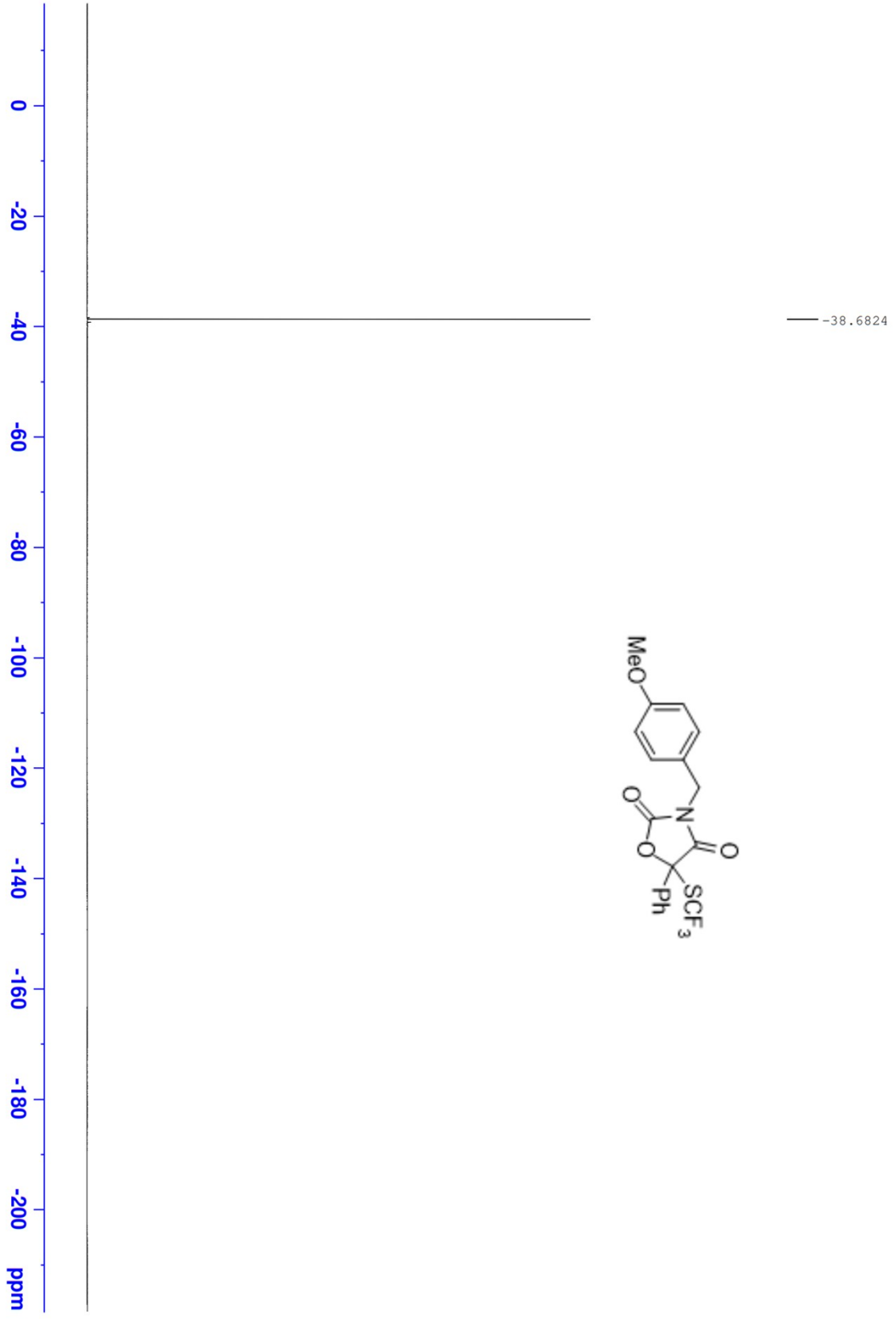
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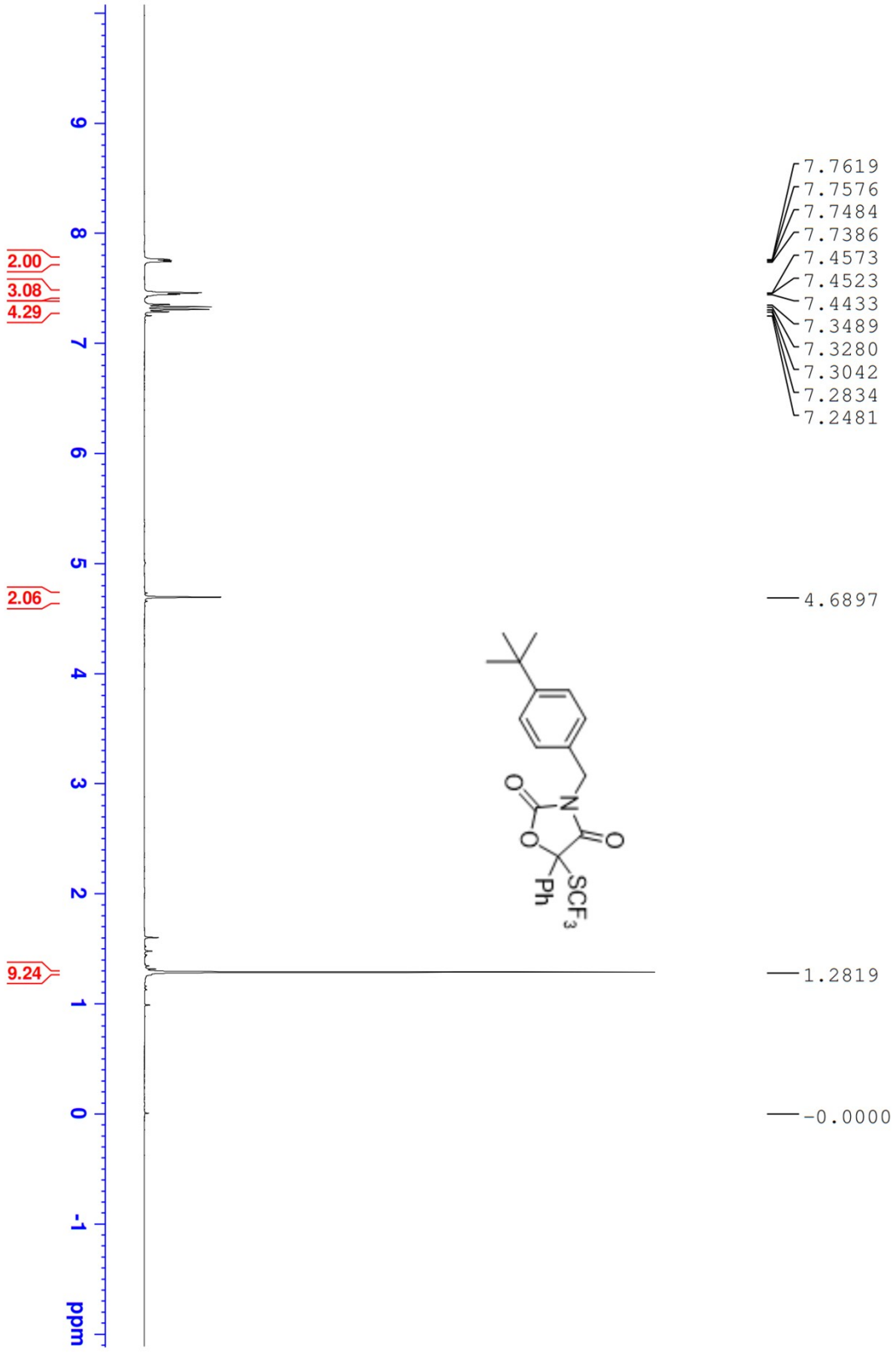
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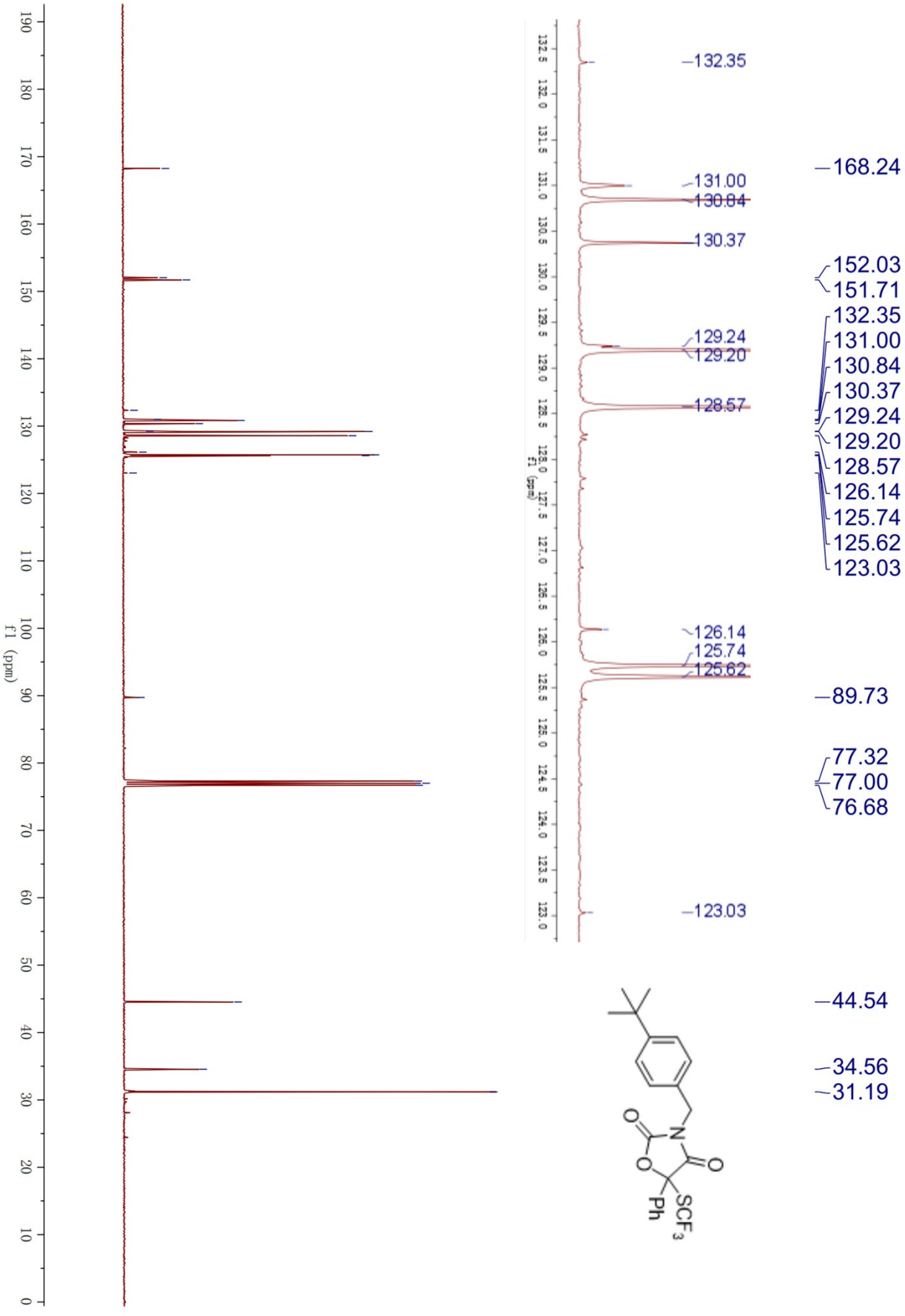
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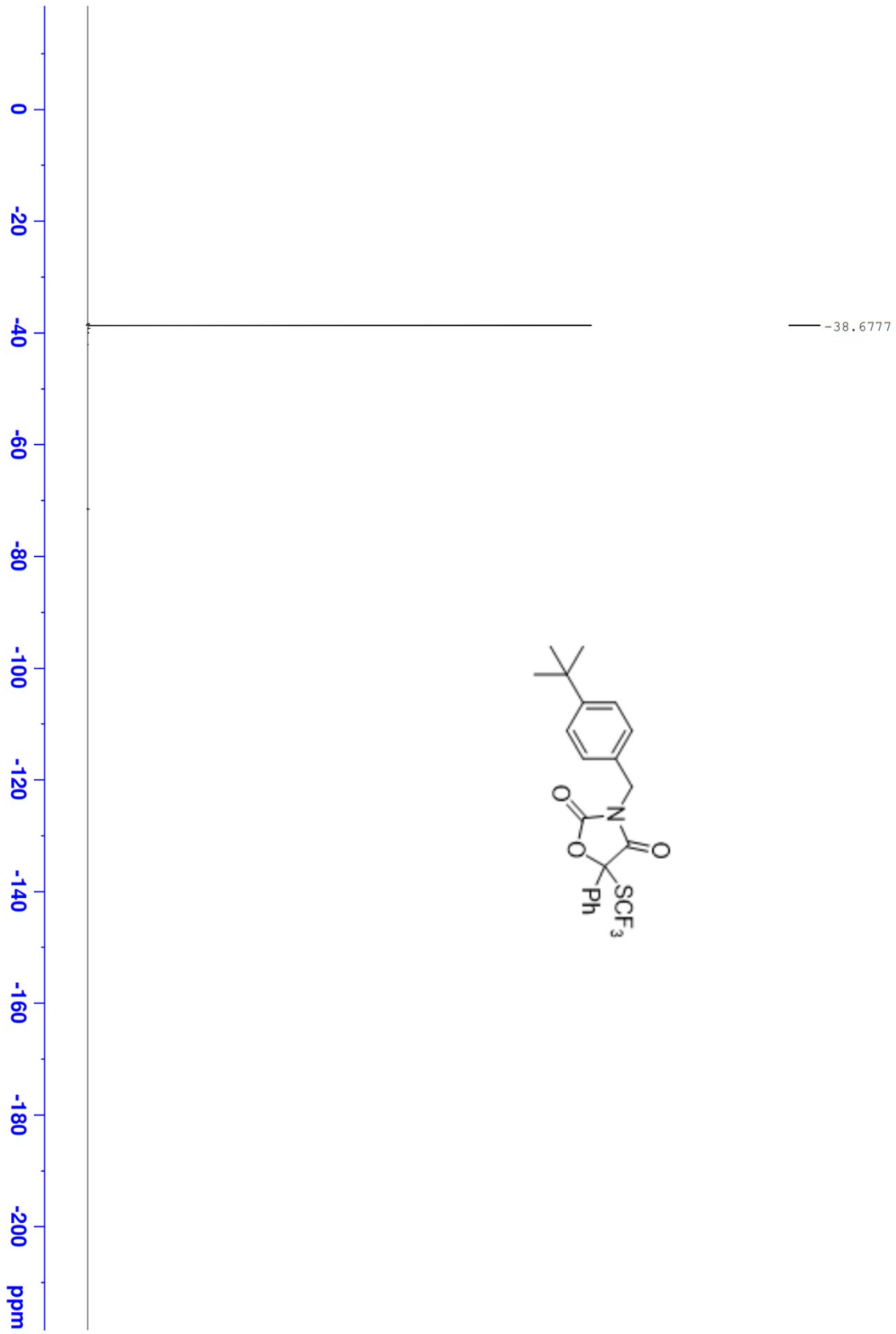
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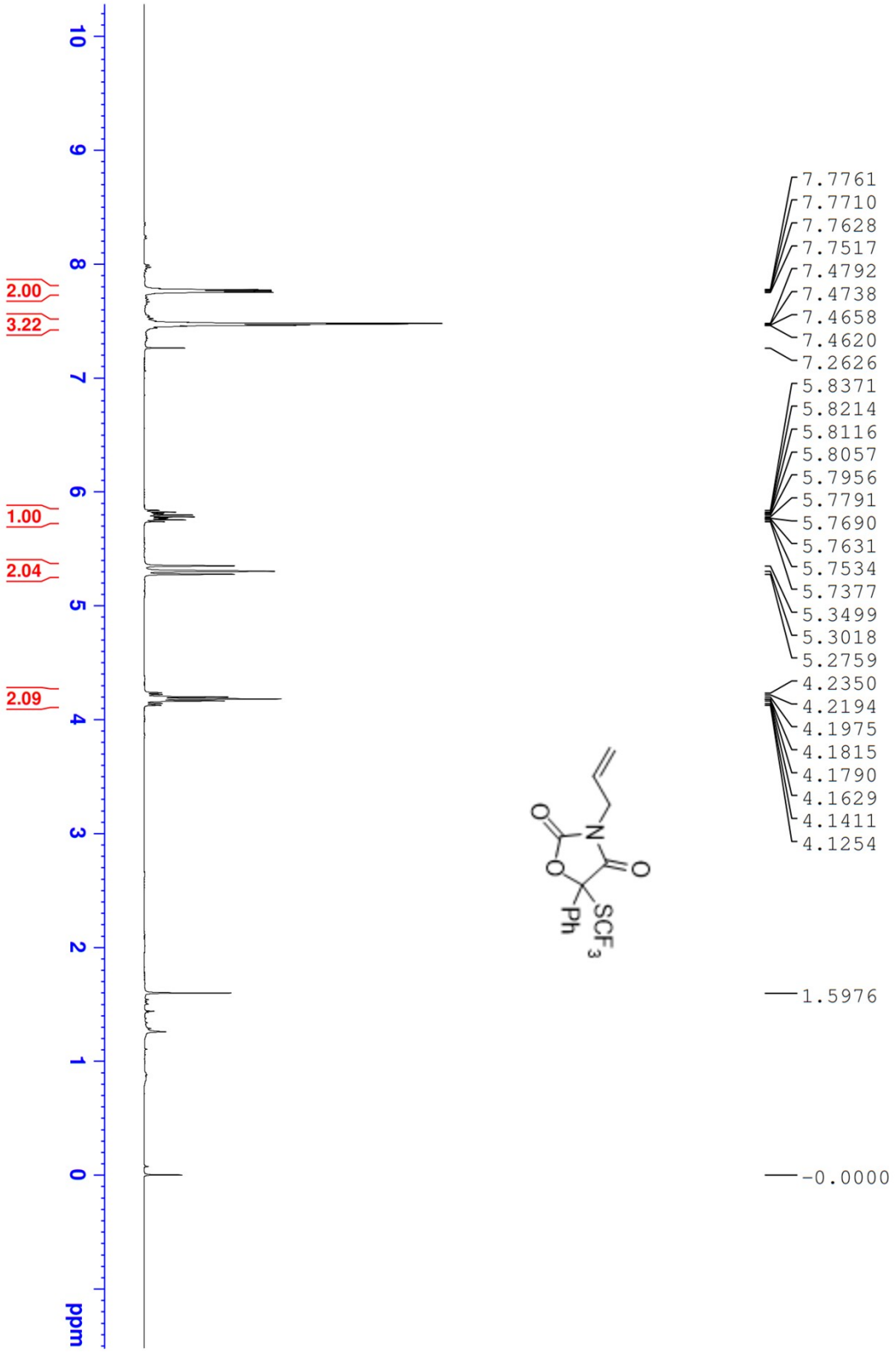
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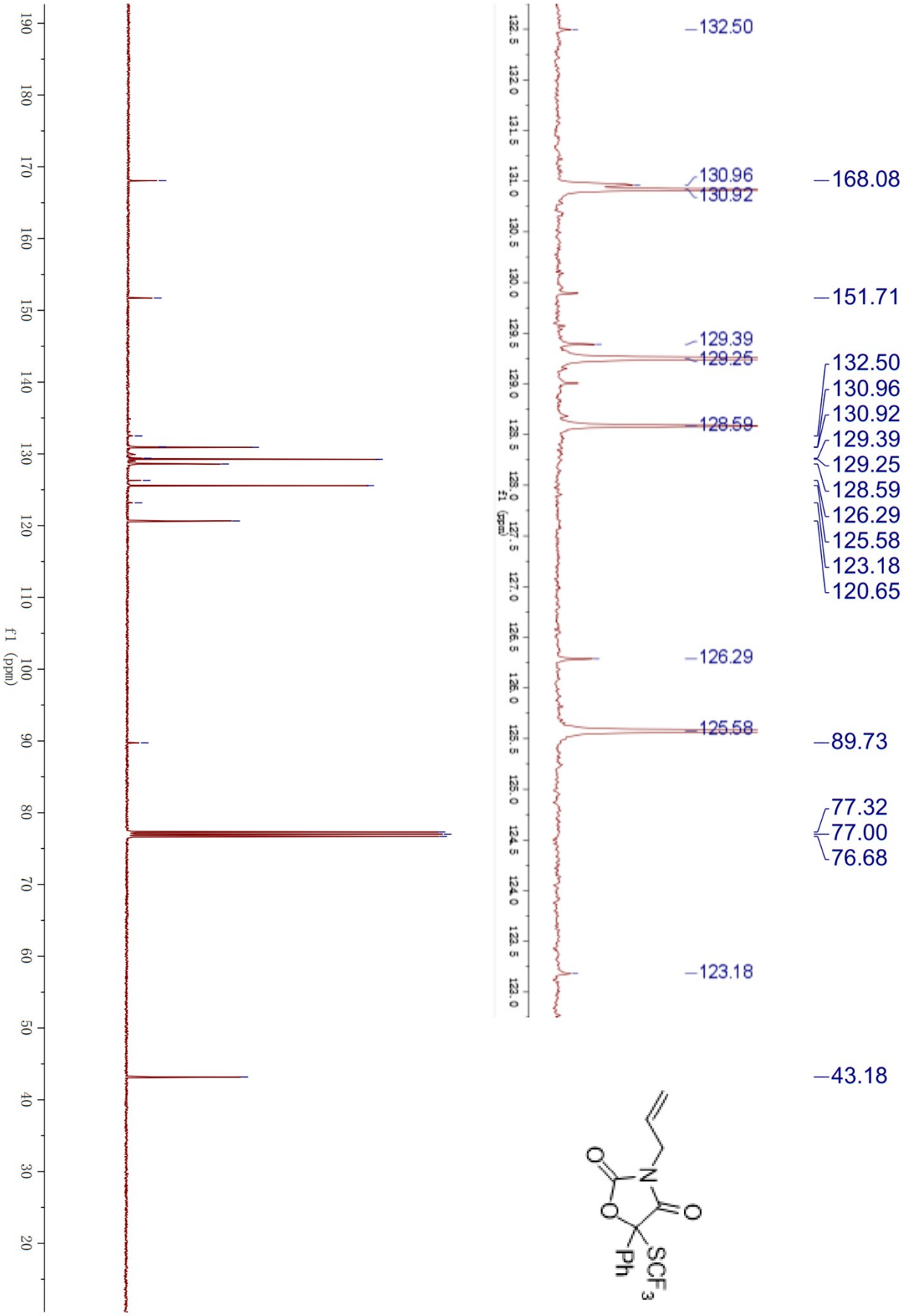
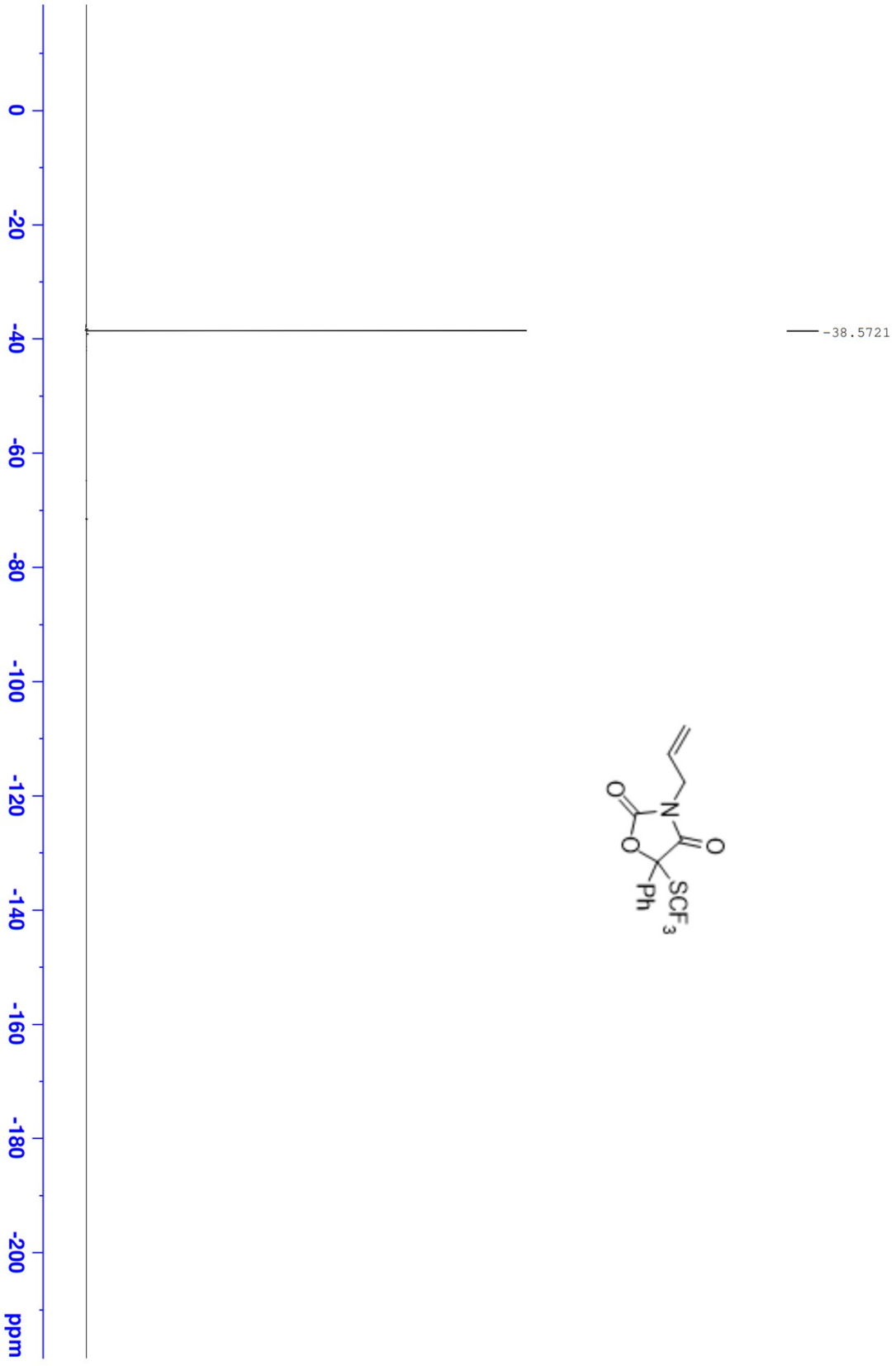
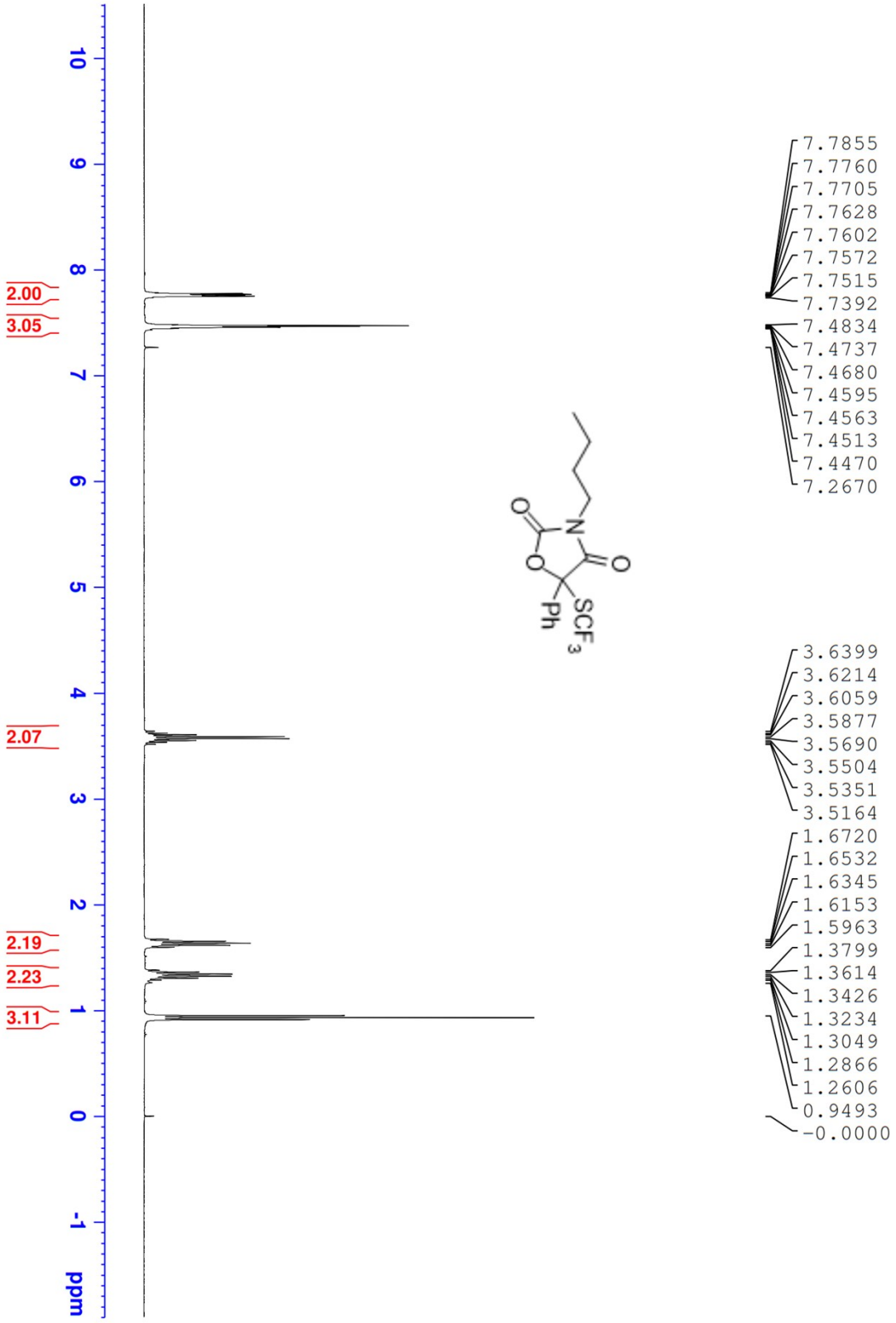
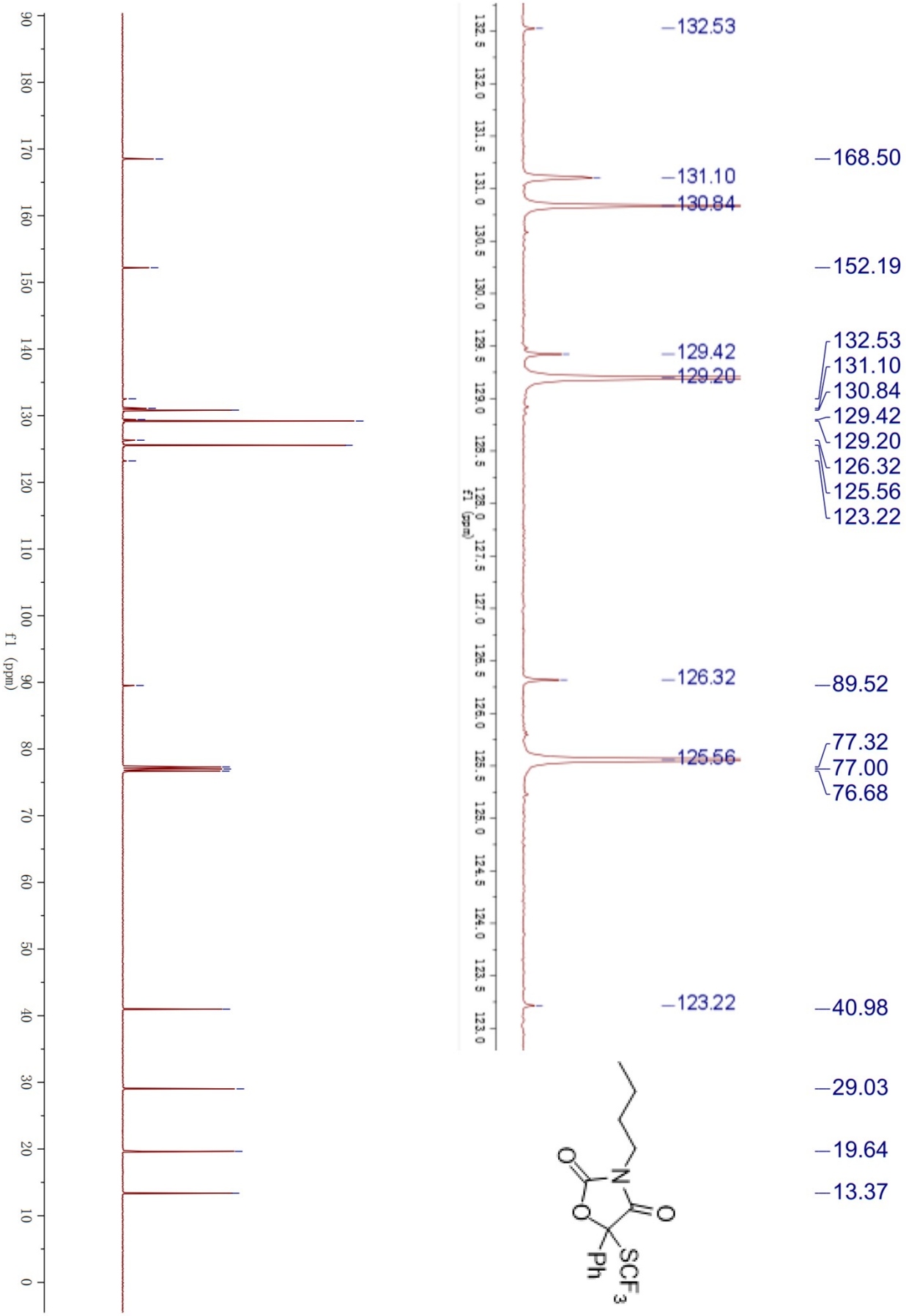
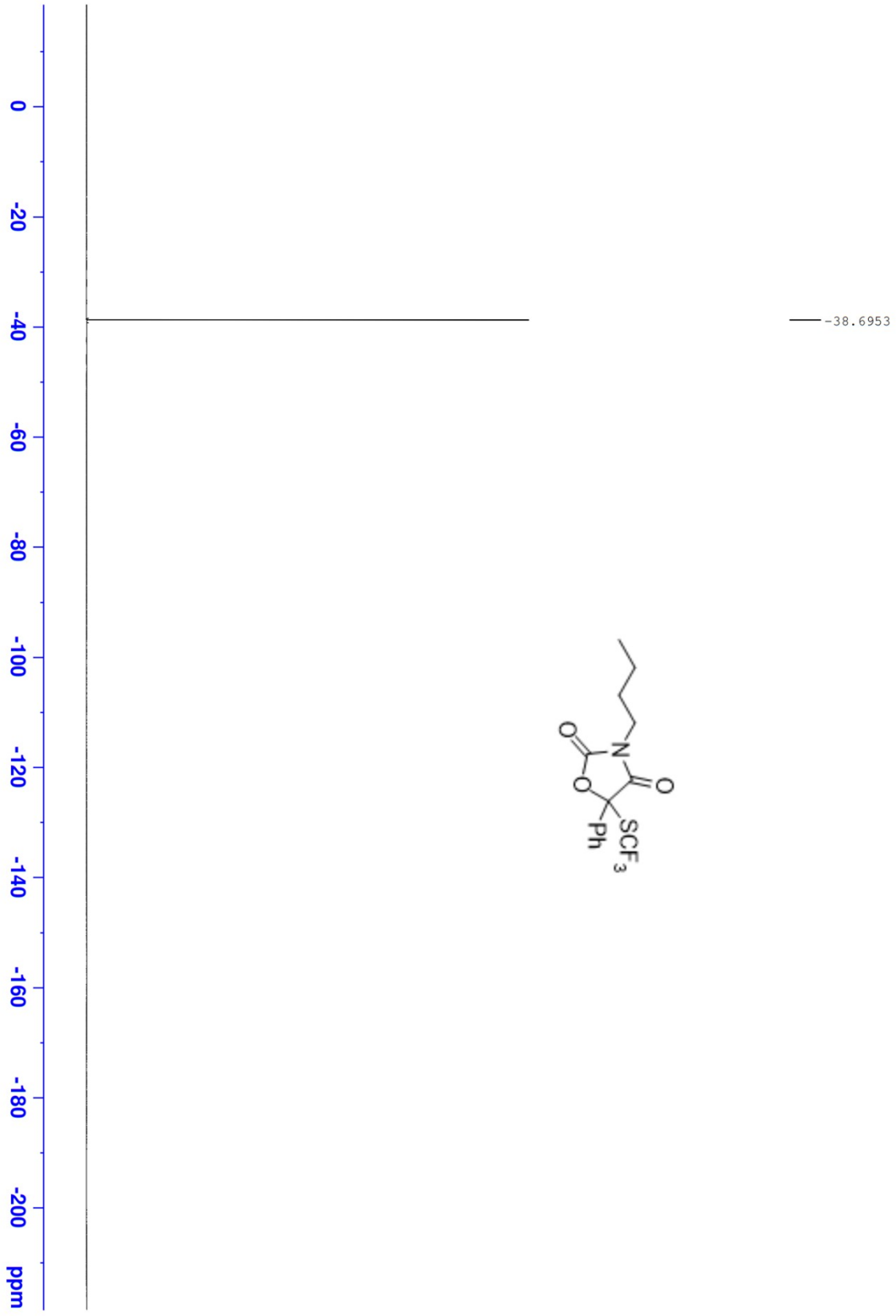
-0.0000
N
O
O
O
SCF3
Ph

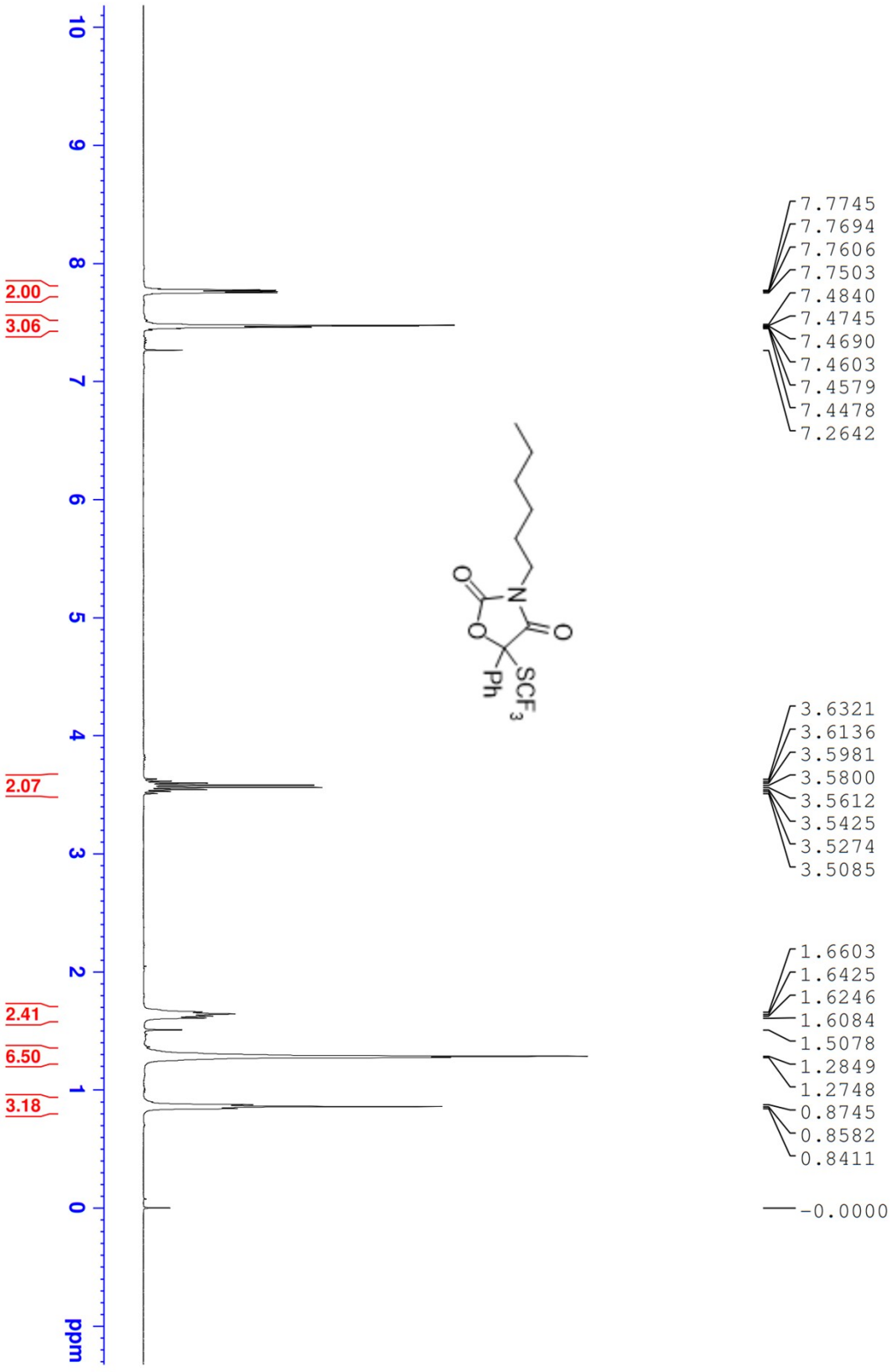

f1 (ppm)
132.50
130.96
130.92
168.08
151.71
129.39
129.25
132.50
130.96
130.92
129.39
129.25
128.59
128.59
126.29
125.58
123.18
120.65
126.29
125.58
89.73
77.32
77.00
76.68
123.18
43.18
O
N
O
O
SCF3
Ph

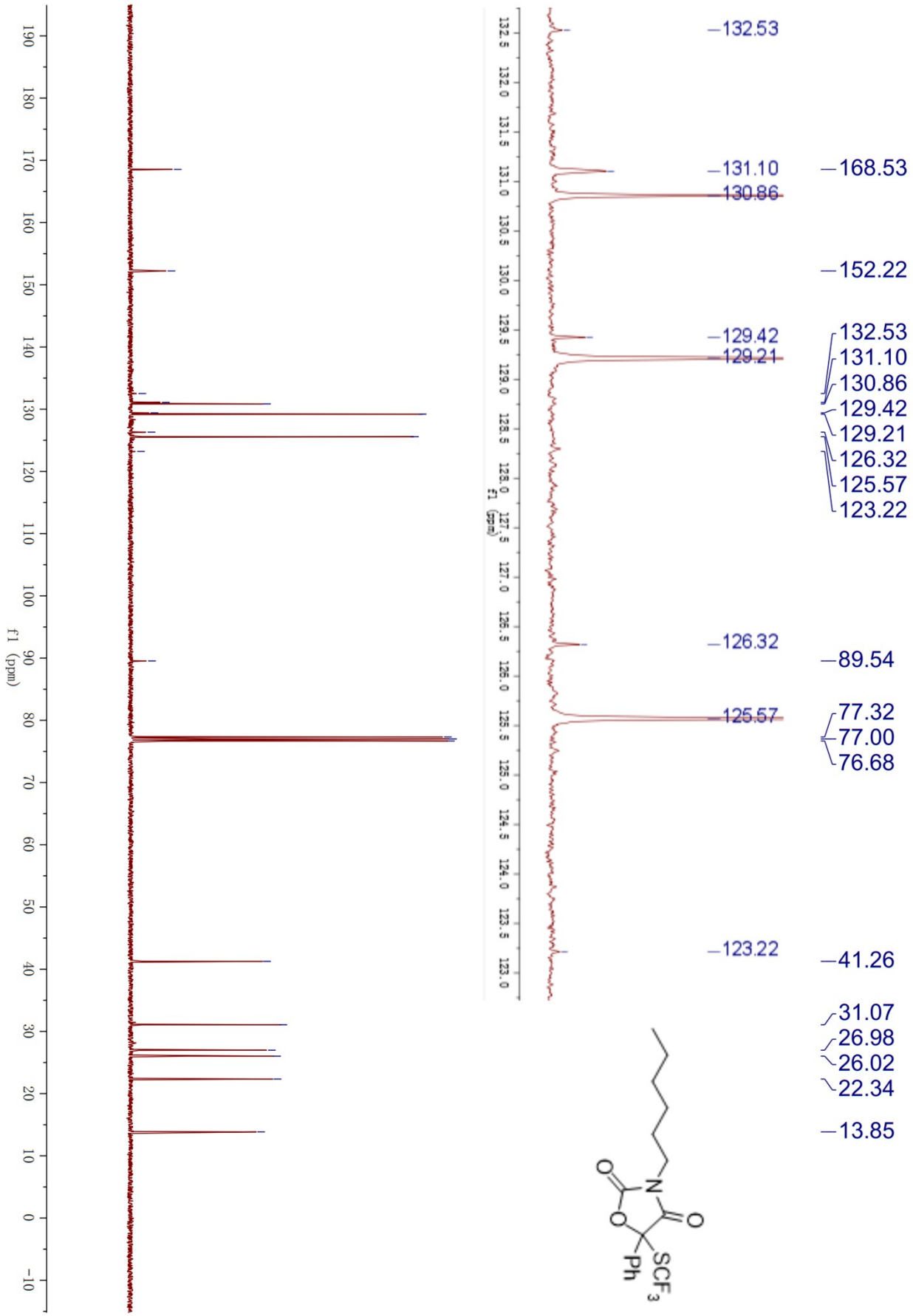

0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm
-38.5721
O
N
O
O
O
SCF3
Ph

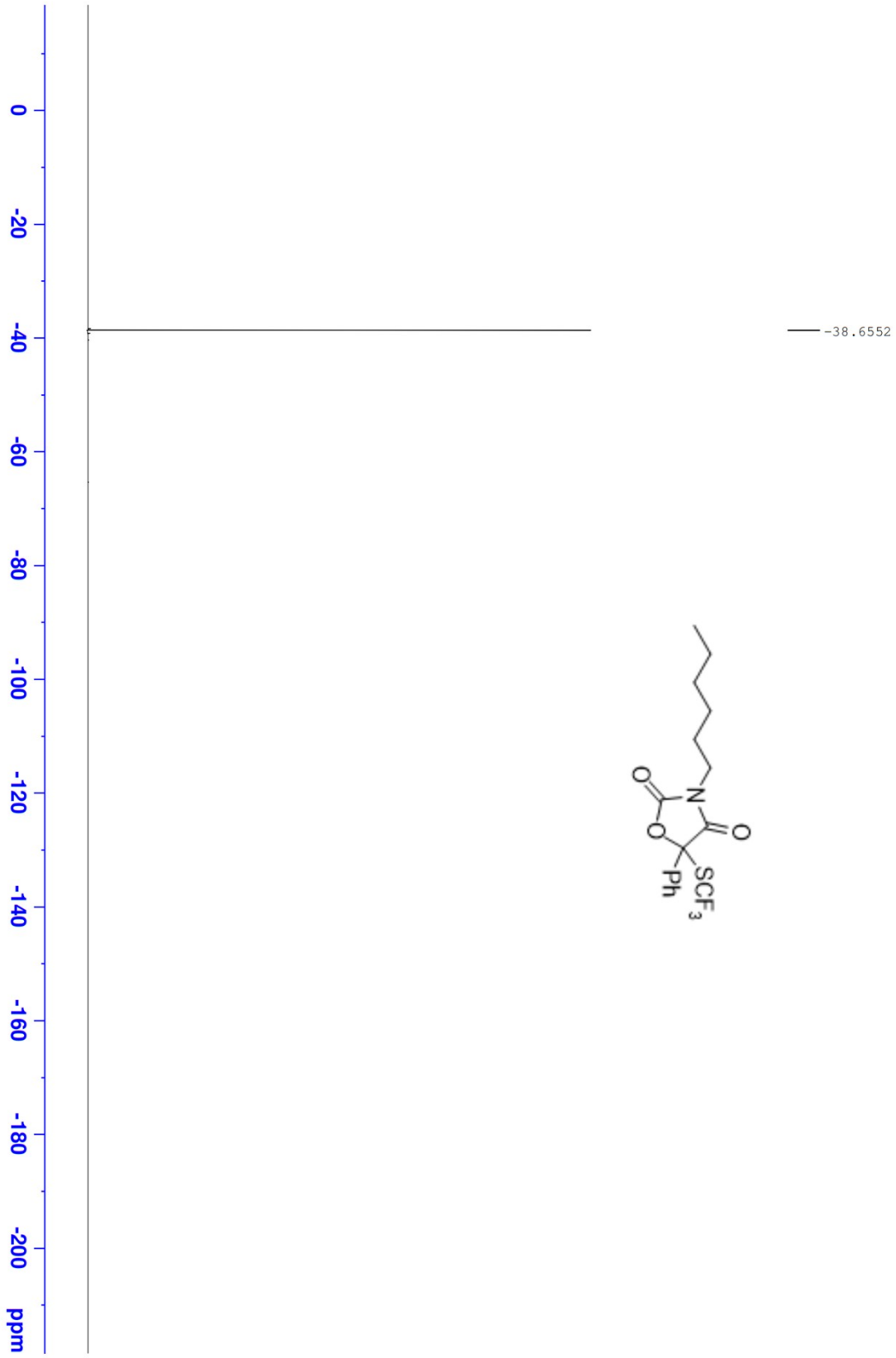

10
9
8
7
6
5
4
3
2
1
0
-1
ppm
2.00
3.05
2.07
2.19
2.23
3.11
7.7855
7.7760
7.7705
7.7628
7.7602
7.7572
7.7515
7.7392
7.4834
7.4737
7.4680
7.4595
7.4563
7.4513
7.4470
7.2670
3.6399
3.6214
3.6059
3.5877
3.5690
3.5504
3.5351
3.5164
1.6720
1.6532
1.6345
1.6153
1.5963
1.3799
1.3614
1.3426
1.3234
1.3049
1.2866
1.2606
0.9493
-0.0000
N
O
O
O
Ph
SCF3

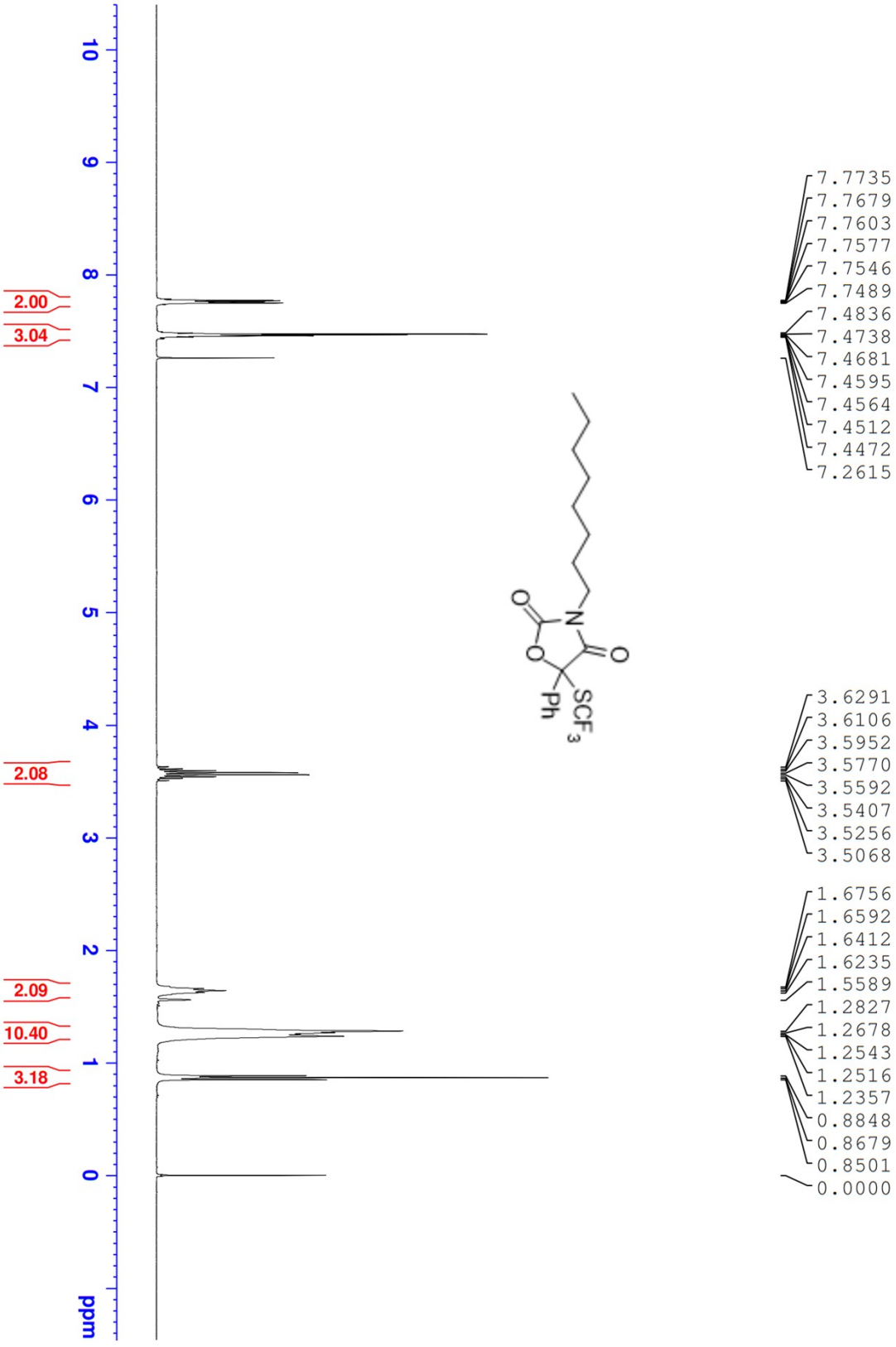

132.53
131.10
130.84
129.42
129.20
126.32
125.56
123.22
168.50
152.19
132.53
131.10
130.84
129.42
129.20
126.32
125.56
123.22
89.52
77.32
77.00
76.68
40.98
29.03
19.64
13.37
f1 (ppm)
O
N
O
O
SCF3
Ph

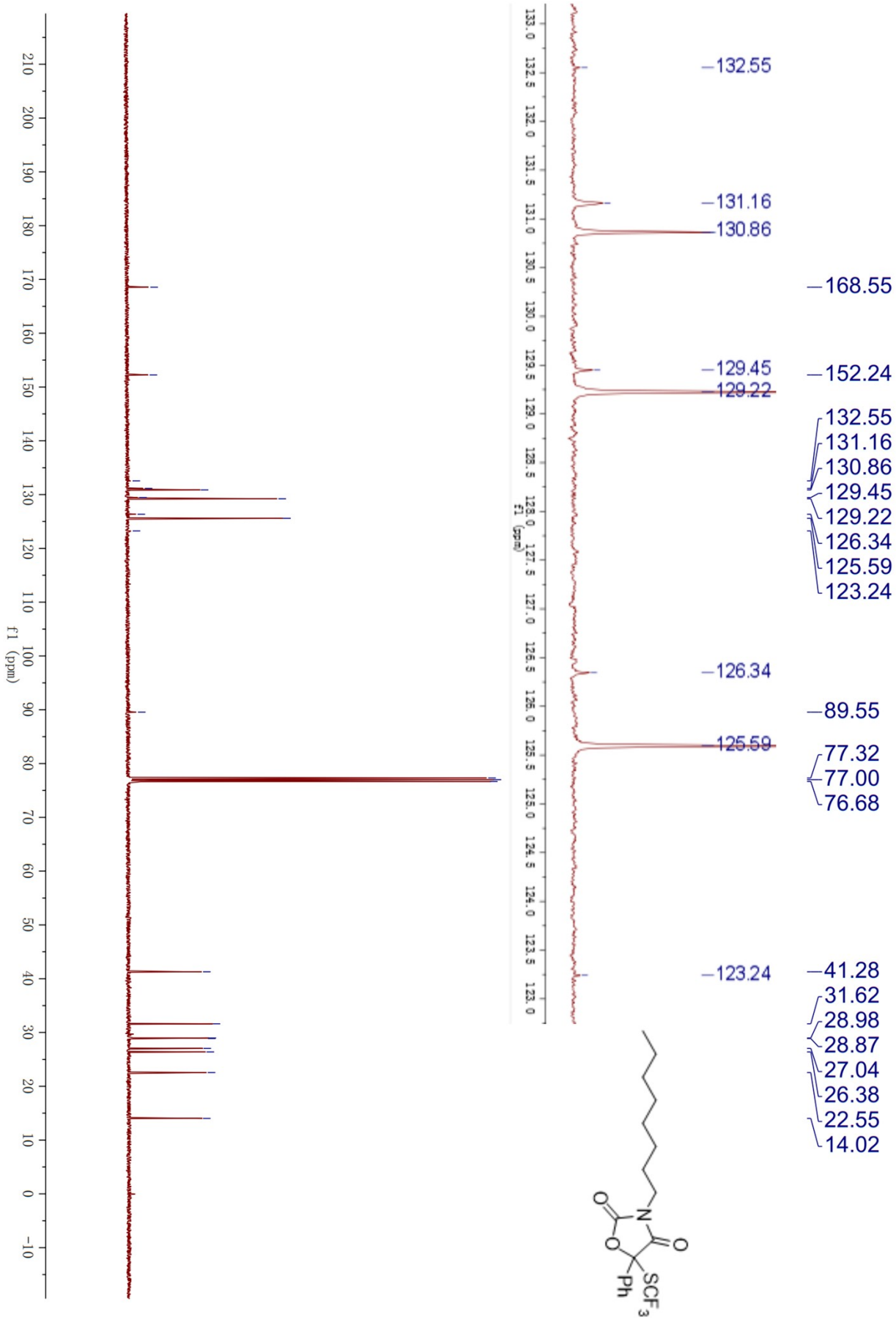

0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm
-38.6953
N
O
O
O
Ph
SCF3

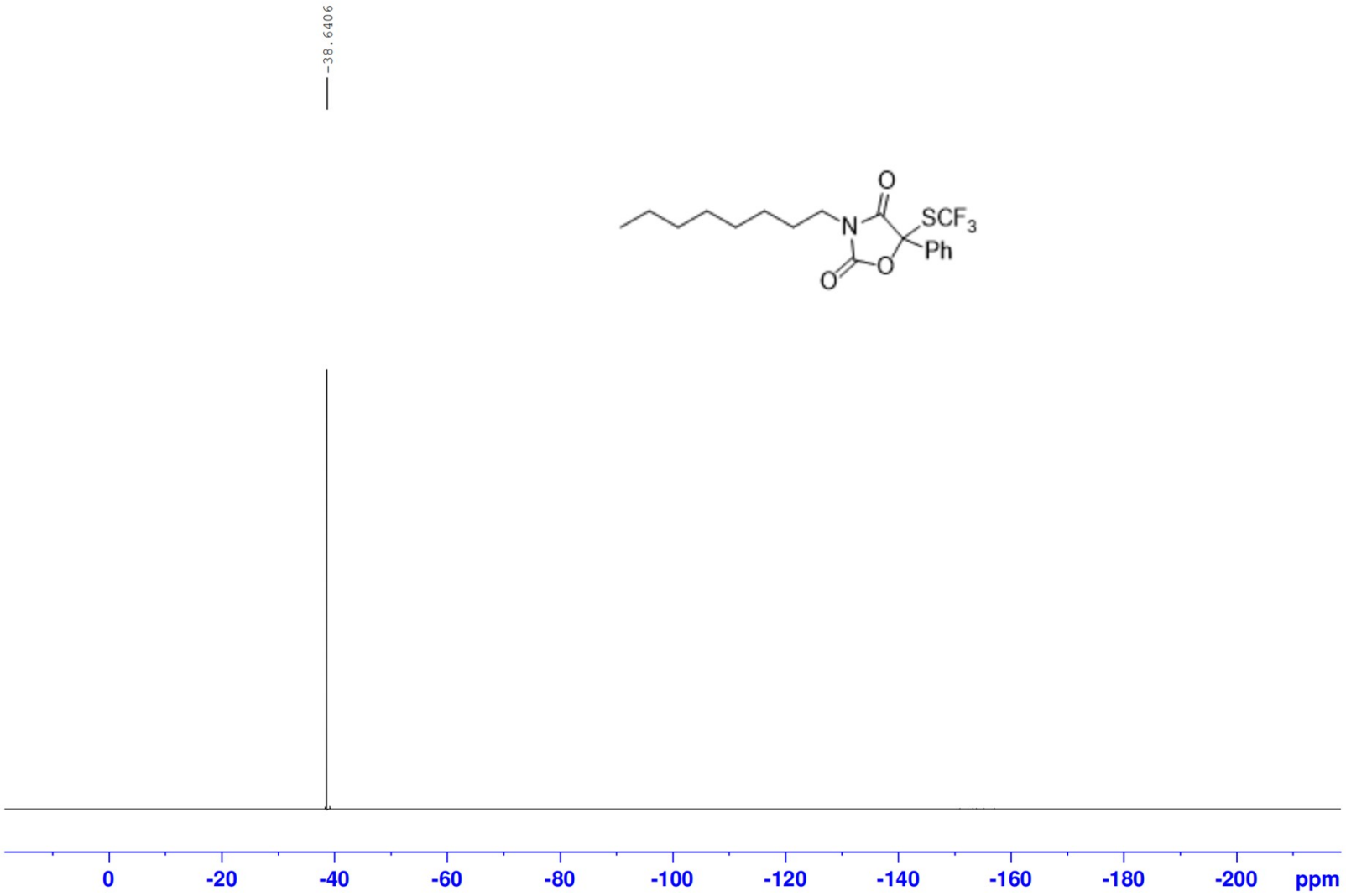

10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
3.06
2.07
2.41
6.50
3.18
7.7745
7.7694
7.7606
7.7503
7.4840
7.4745
7.4690
7.4603
7.4579
7.4478
7.2642
3.6321
3.6136
3.5981
3.5800
3.5612
3.5425
3.5274
3.5085
1.6603
1.6425
1.6246
1.6084
1.5078
1.2849
1.2748
0.8745
0.8582
0.8411
-0.0000
N
O
O
O
Ph
SCF3

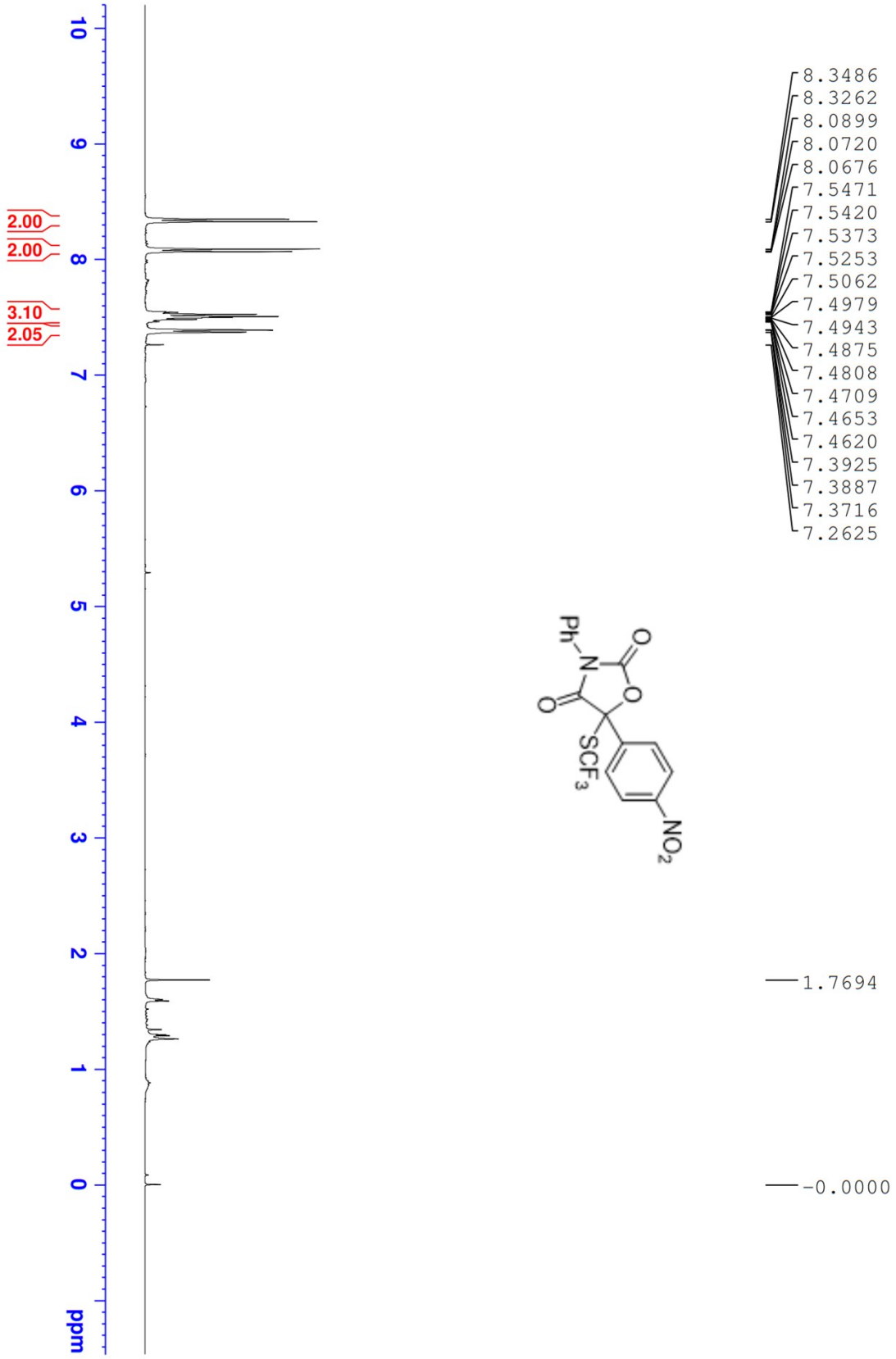

f1 (ppm)
132.53
131.10
130.86
129.42
129.21
126.32
125.57
123.22
168.53
152.22
132.53
131.10
130.86
129.42
129.21
126.32
125.57
123.22
89.54
77.32
77.00
76.68
41.26
31.07
26.98
26.02
22.34
13.85
O
N
O
O
O
Ph
SCF3

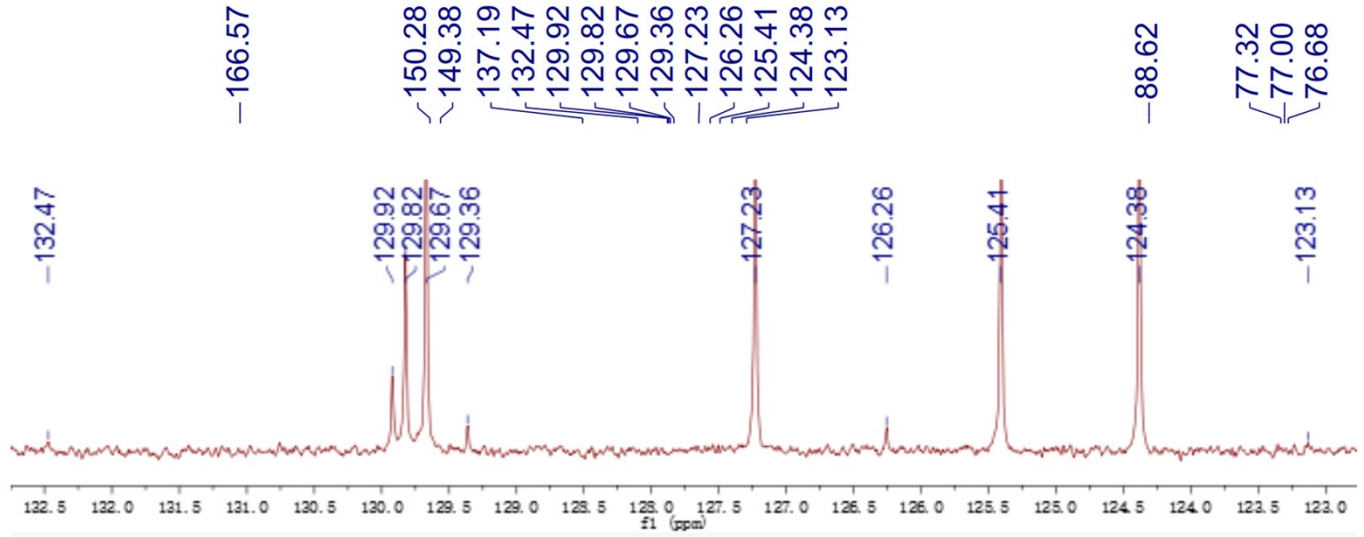

0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm
-38.6552
N
O
O
O
O
Ph
SCF3

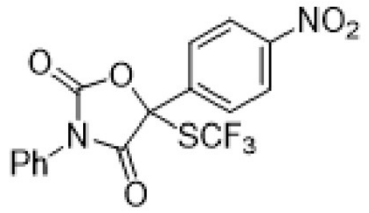

10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
3.04
2.08
2.09
10.40
3.18
O
N
O
O
O
Ph
SCF3
7.7735
7.7679
7.7603
7.7577
7.7546
7.7489
7.4836
7.4738
7.4681
7.4595
7.4564
7.4512
7.4472
7.2615
3.6291
3.6106
3.5952
3.5770
3.5592
3.5407
3.5256
3.5068
1.6756
1.6592
1.6412
1.6235
1.5589
1.2827
1.2678
1.2543
1.2516
1.2357
0.8848
0.8679
0.8501
0.0000

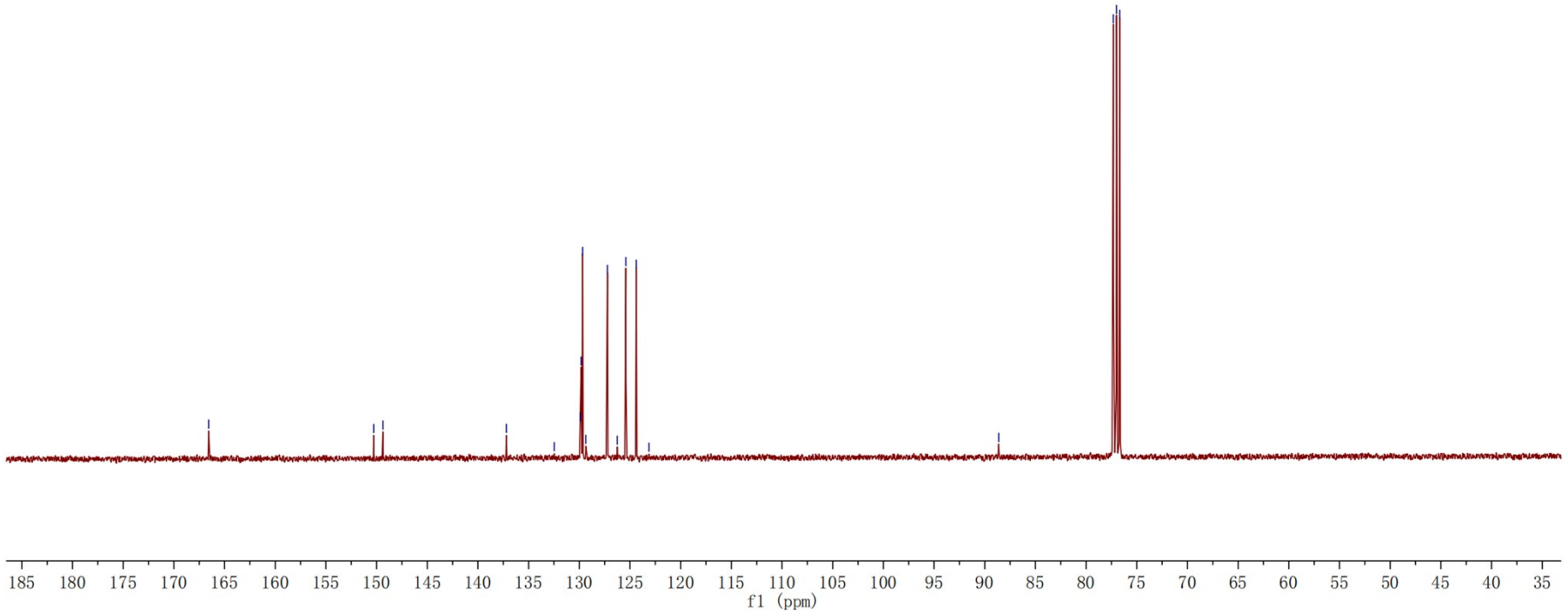

f1 (ppm)
132.55
131.16
130.86
129.45
129.22
126.34
125.59
123.24
168.55
152.24
89.55
77.32
77.00
76.68
41.28
31.62
28.98
28.87
27.04
26.38
22.55
14.02
O
N
O
O
Ph
SCF3

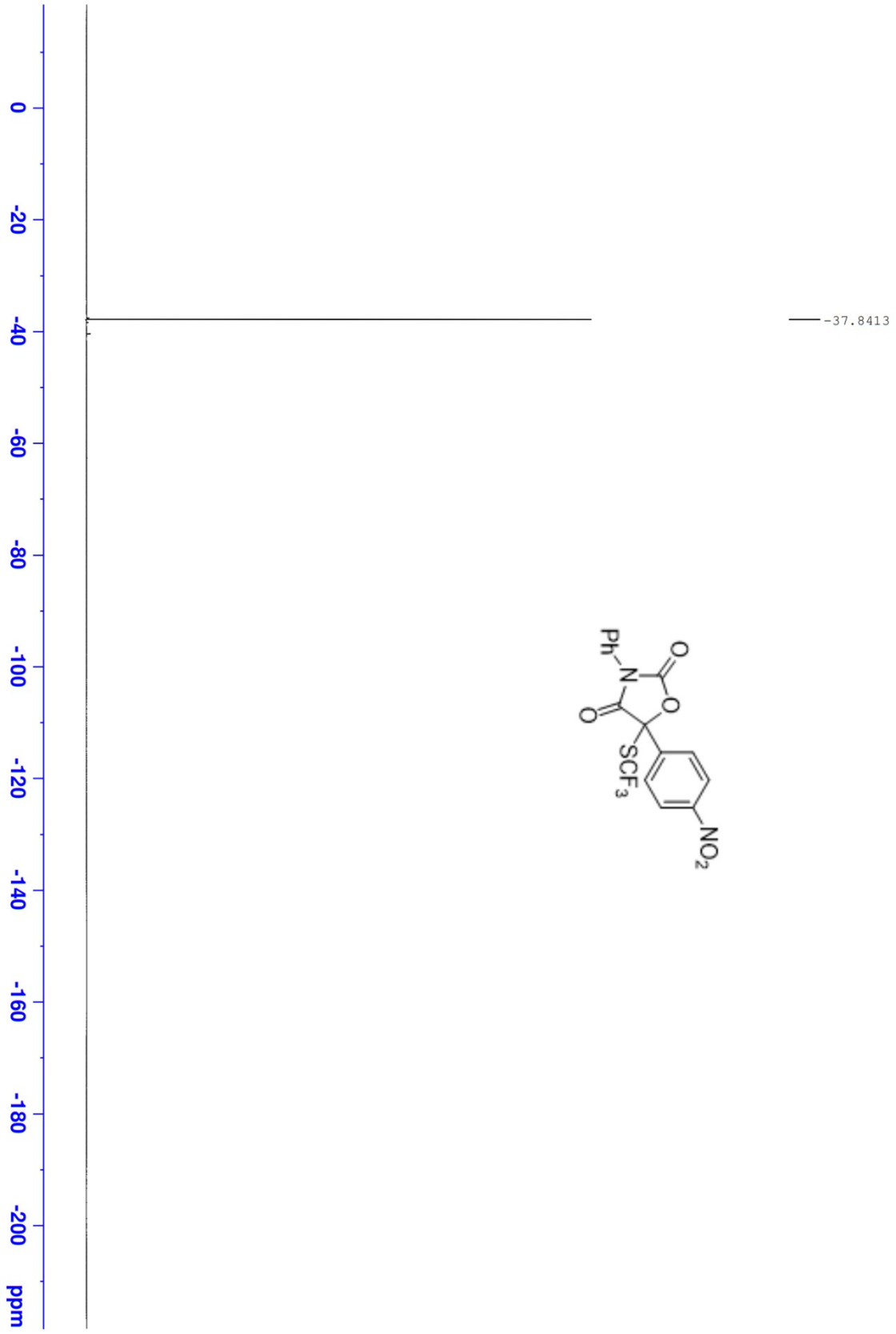

-38.6406
O
N
SCF3
Ph
O
O
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

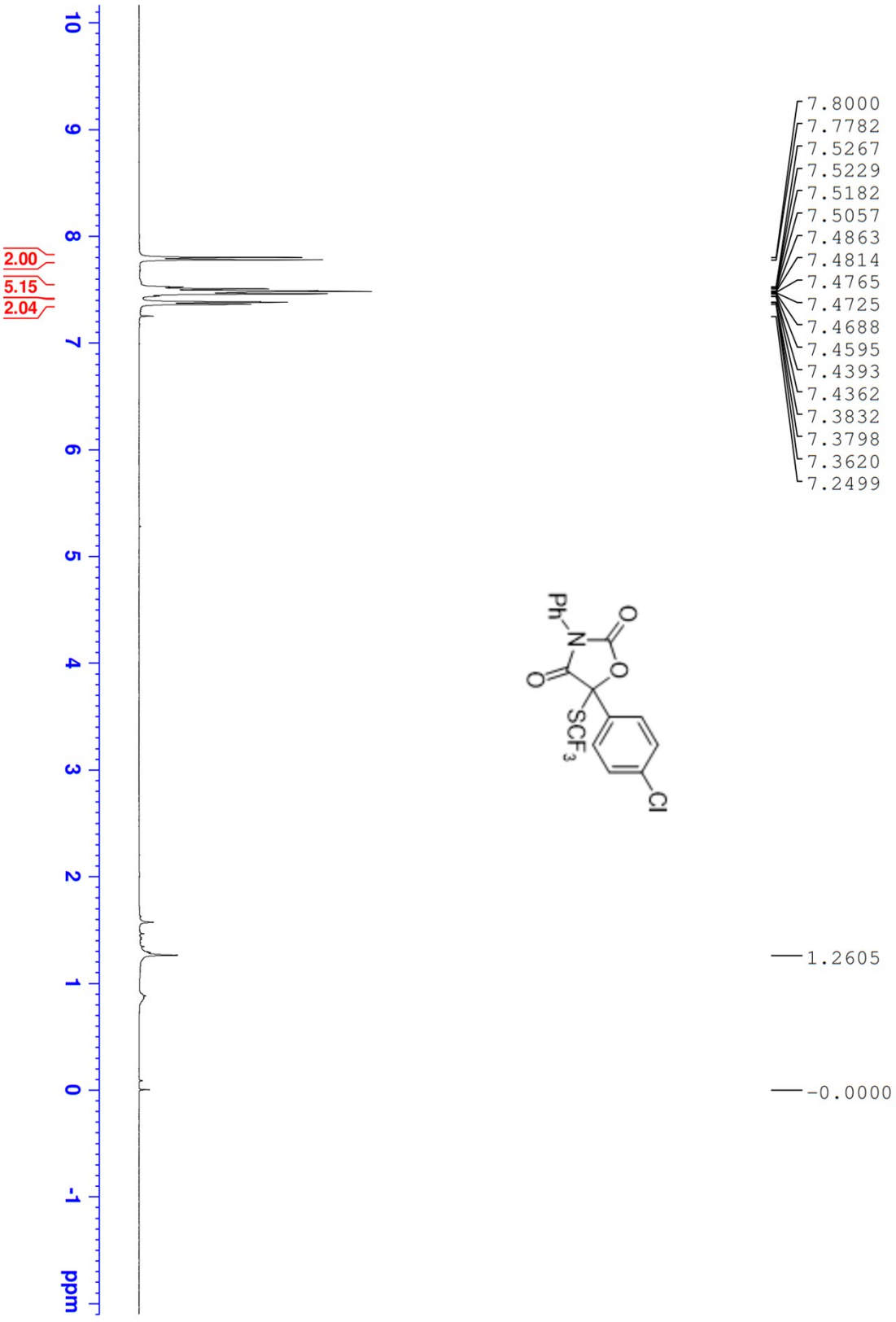

8.3486
8.3262
8.0899
8.0720
8.0676
7.5471
7.5420
7.5373
7.5253
7.5062
7.4979
7.4943
7.4875
7.4808
7.4709
7.4653
7.4620
7.3925
7.3887
7.3716
7.2625
2.00
2.00
3.10
2.05
Ph
N
O
O
O
O
SCF3
NO2
1.7694
-0.0000
10
9
8
7
6
5
4
3
2
1
0
ppm

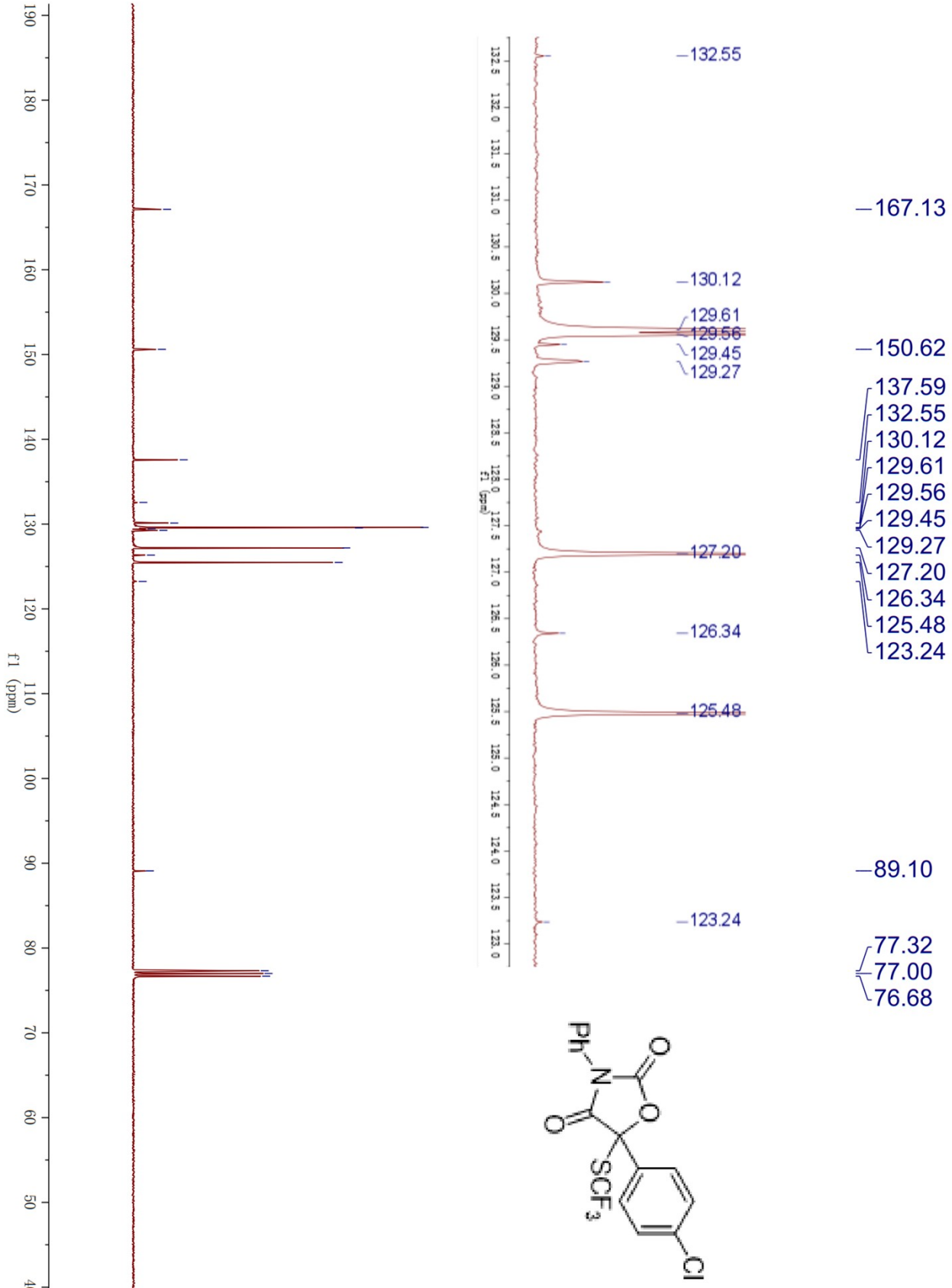

166.57
150.28
149.38
137.19
132.47
129.92
129.82
129.67
129.36
127.23
126.26
125.41
124.38
123.13
88.62
77.32
77.00
76.68
132.47
129.92
129.82
129.67
129.36
127.23
126.26
125.41
124.38
123.13
f1 (ppm)

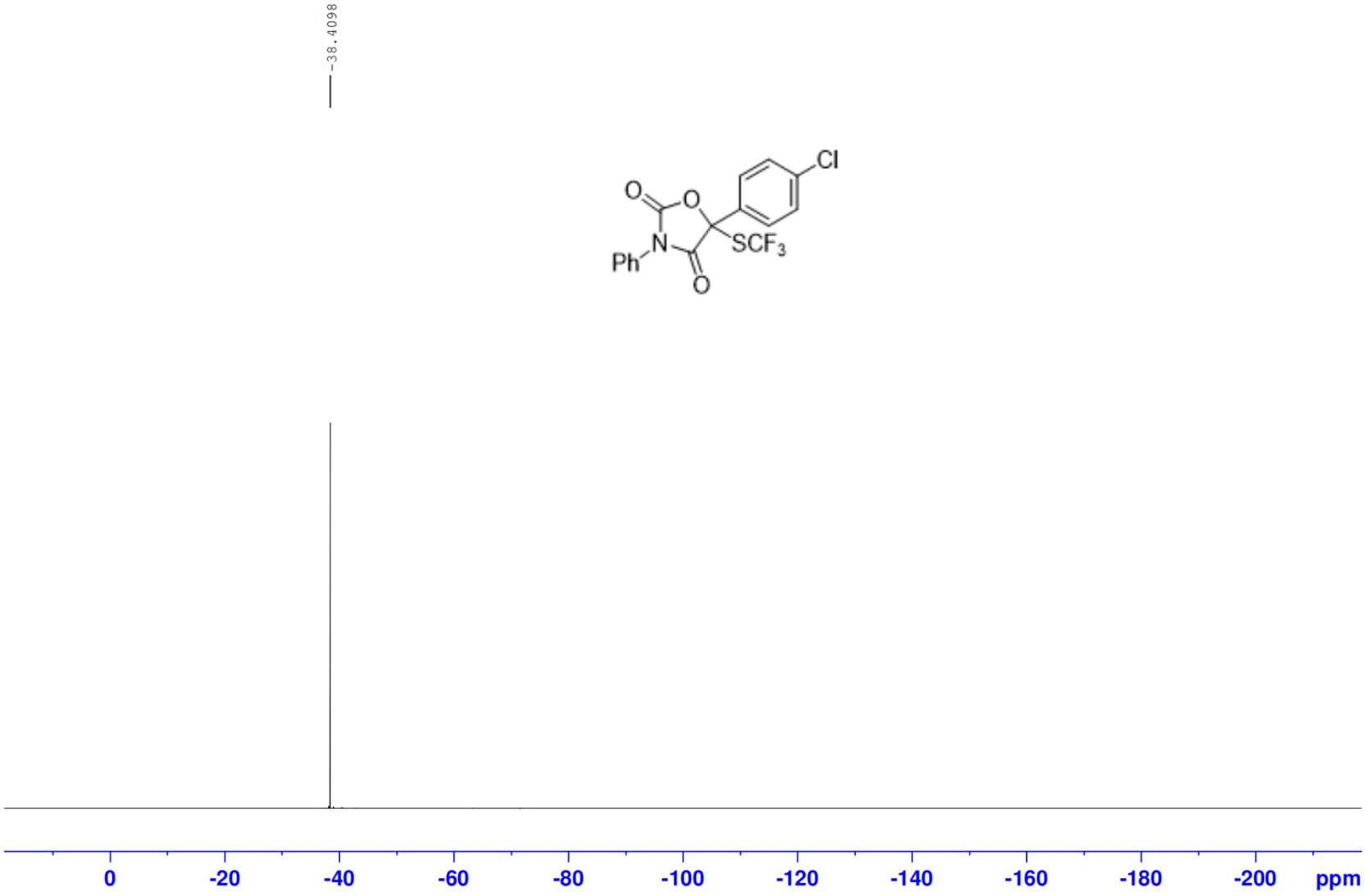

NO2
O
O
N
Ph
O
SCF3

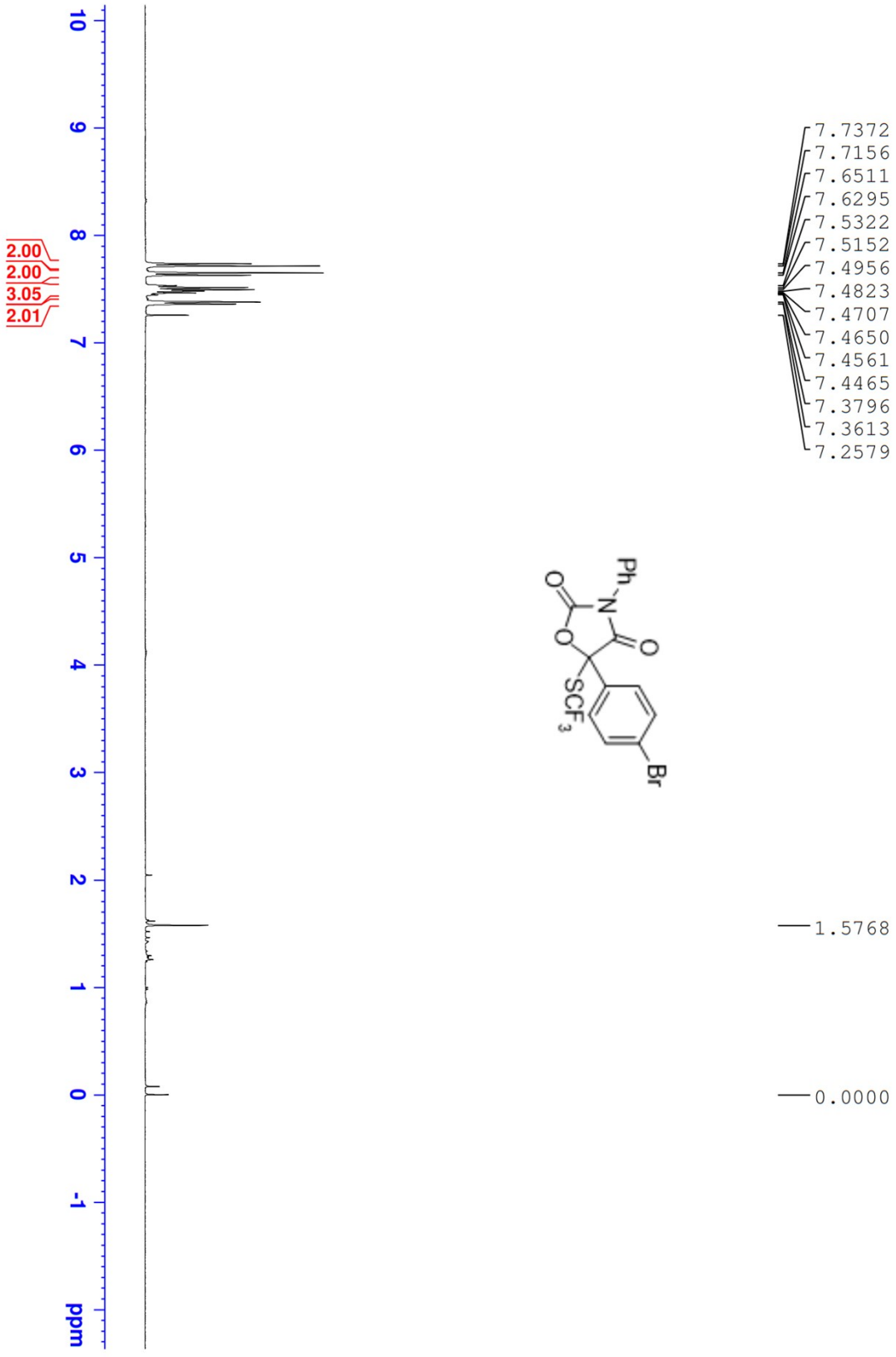

f1 (ppm)

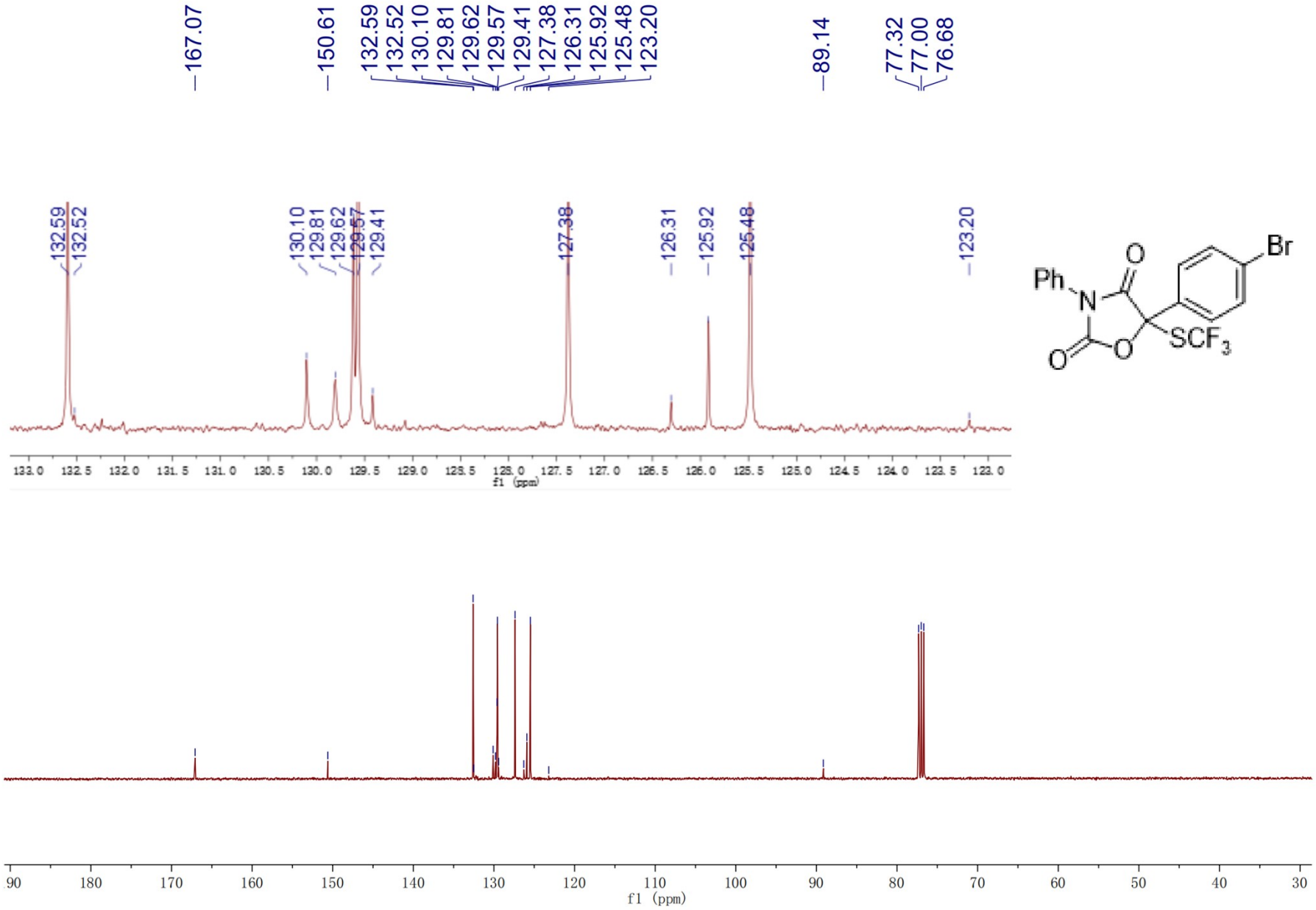

-37.8413
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm
Ph
N
O
O
O
O
SCF3
NO2

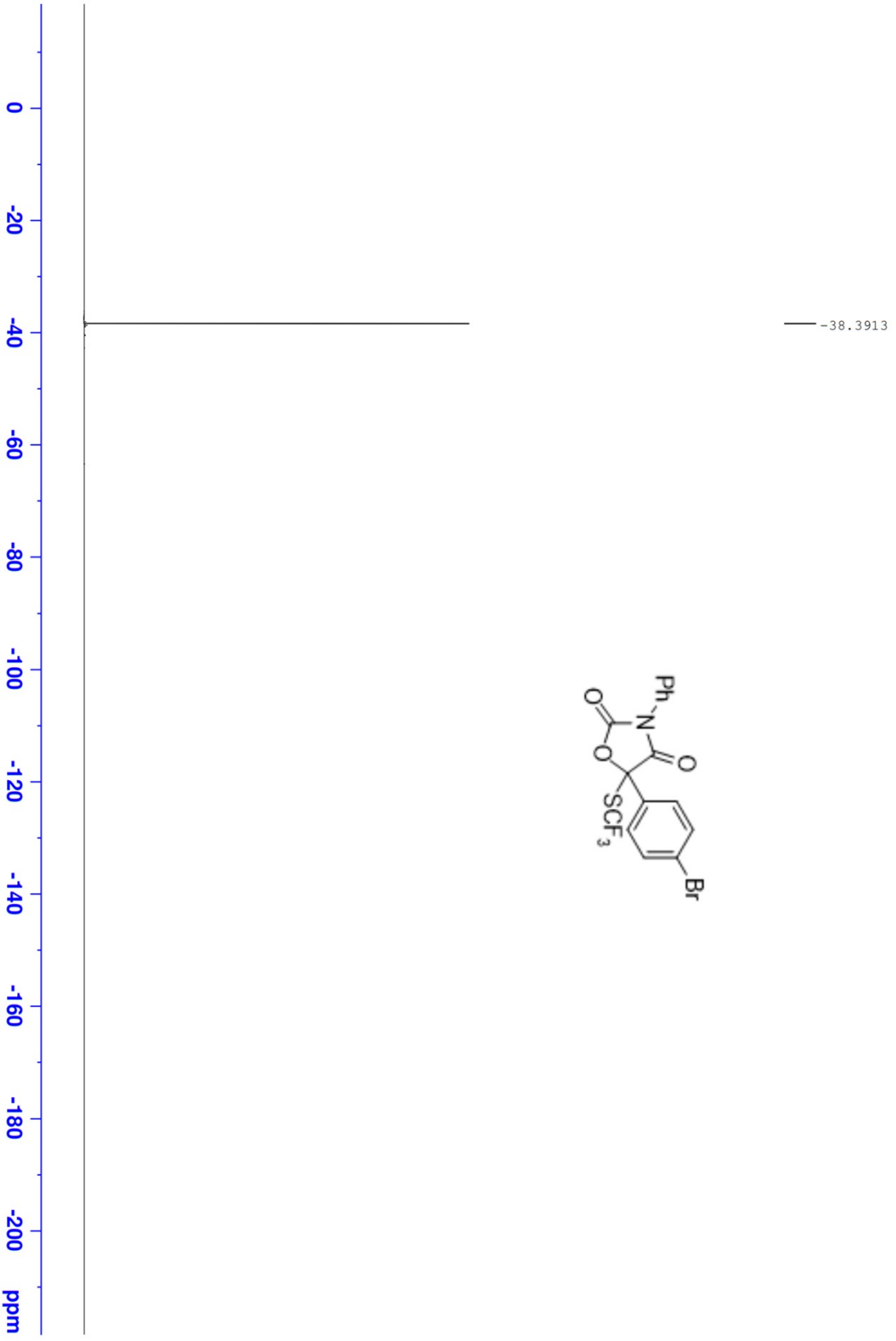

7.8000
7.7782
7.5267
7.5229
7.5182
7.5057
7.4863
7.4814
7.4765
7.4725
7.4688
7.4595
7.4393
7.4362
7.3832
7.3798
7.3620
7.2499
2.00
5.15
2.04
Ph
N
O
O
O
O
SCF3
Cl
1.2605
-0.0000
10
9
8
7
6
5
4
3
2
1
0
-1
ppm

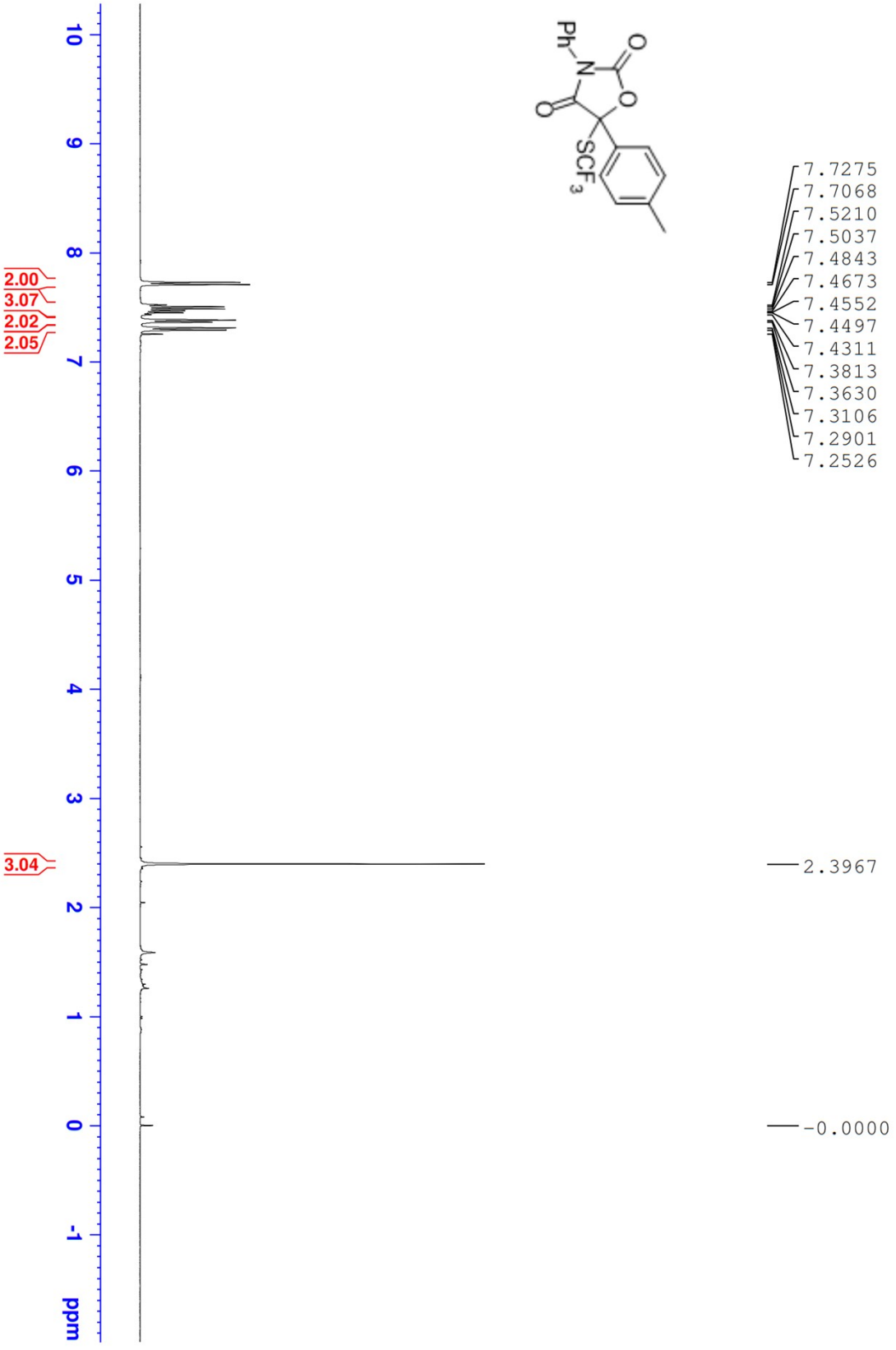

132.55
130.12
129.61
129.56
129.45
129.27
127.20
126.34
125.48
123.24
167.13
150.62
137.59
132.55
130.12
129.61
129.56
129.45
129.27
127.20
126.34
125.48
123.24
89.10
77.32
77.00
76.68
f1 (ppm)
Ph
N
O
O
O
SCF3
Cl

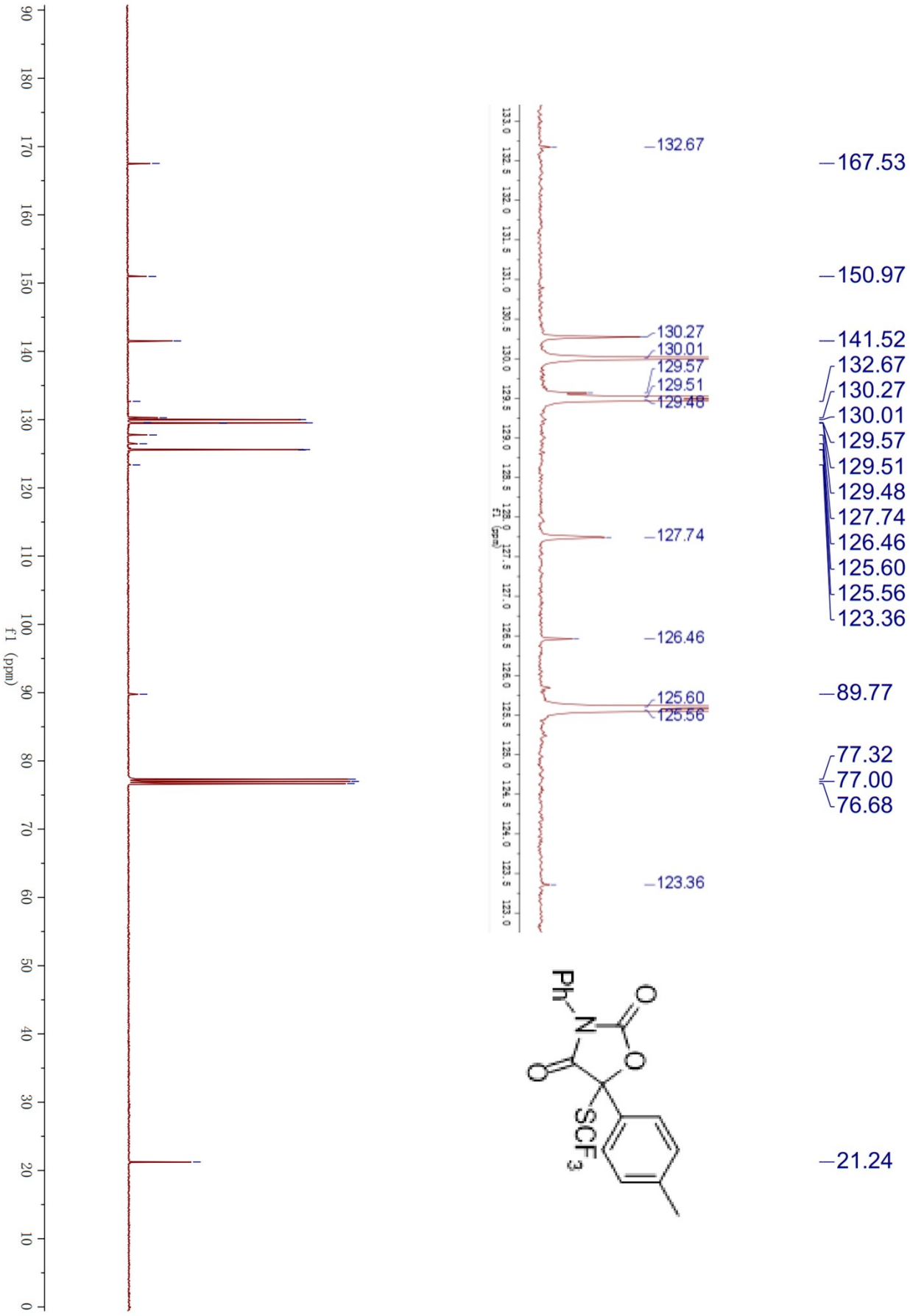

-38.4098
Cl
O
O
N
Ph
O
SCF3
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

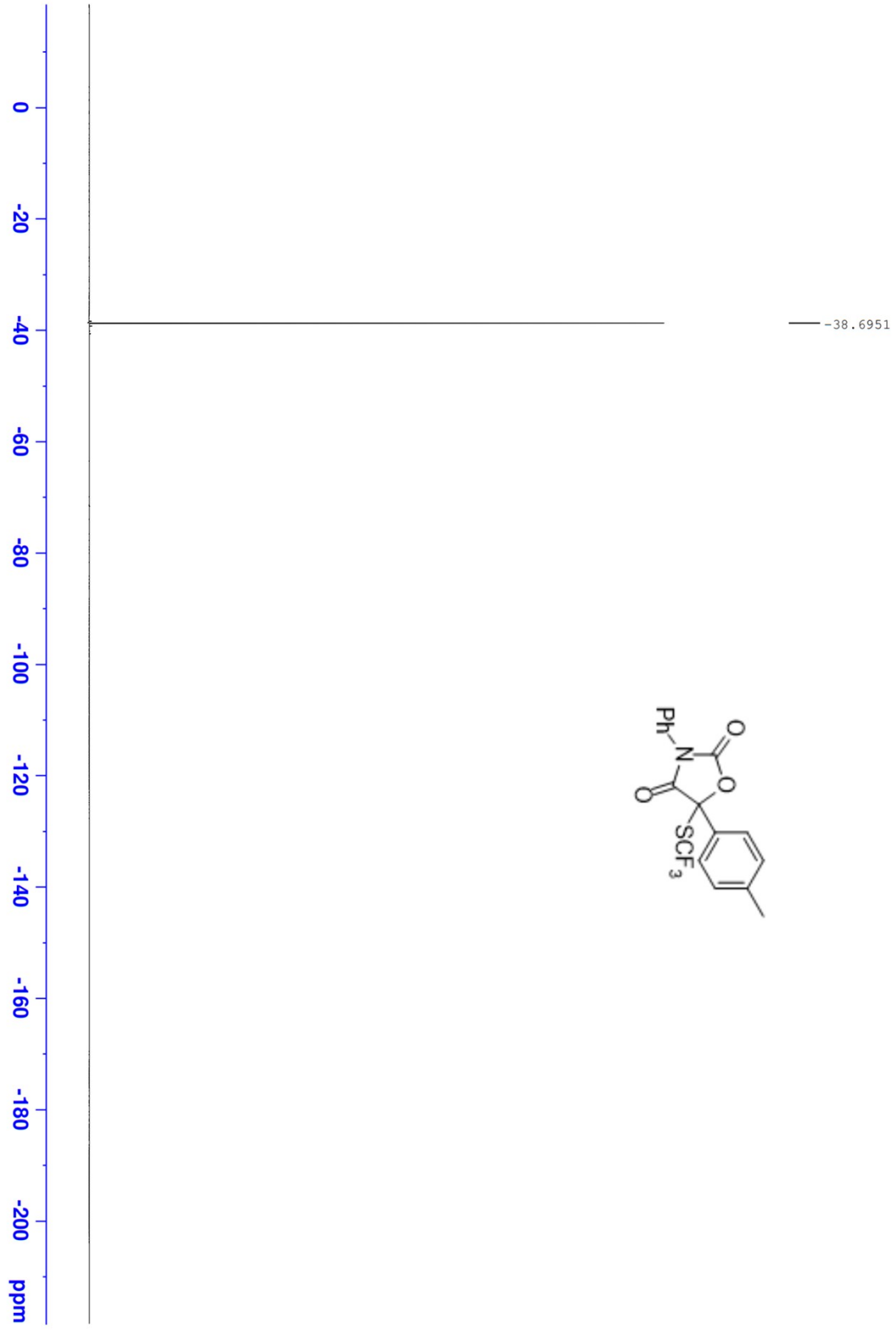

2.00
2.00
3.05
2.01
10
9
8
7
6
5
4
3
2
1
0
-1
ppm
7.7372
7.7156
7.6511
7.6295
7.5322
7.5152
7.4956
7.4823
7.4707
7.4650
7.4561
7.4465
7.3796
7.3613
7.2579
Ph
N
O
O
O
SCF3
Br
1.5768
0.0000

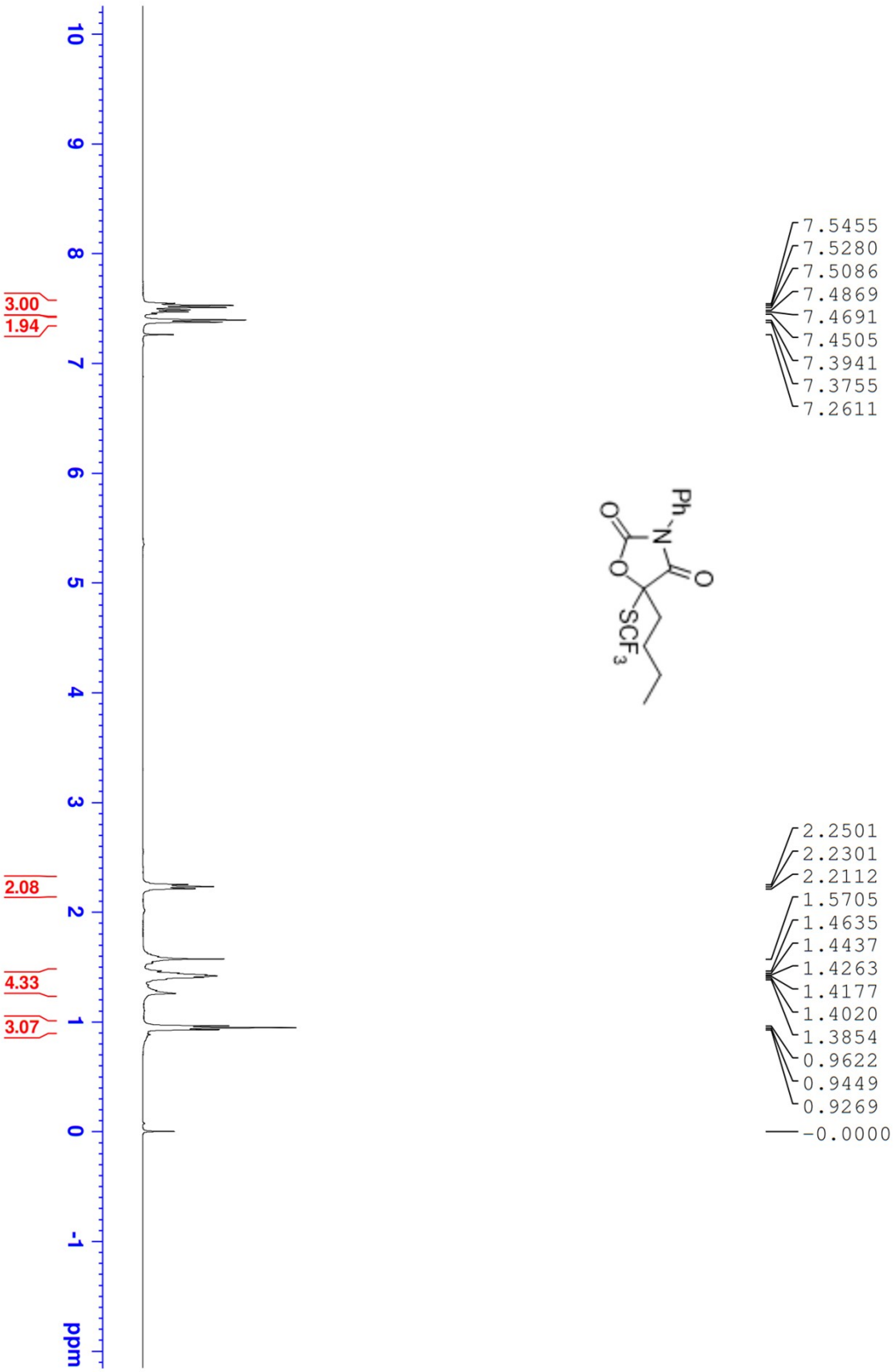

167.07
150.61
132.59
132.52
130.10
129.81
129.62
129.57
129.41
127.38
126.31
125.92
125.48
123.20
89.14
77.32
77.00
76.68
f1 (ppm)
Ph
N
O
O
O
O
SCF3
Br

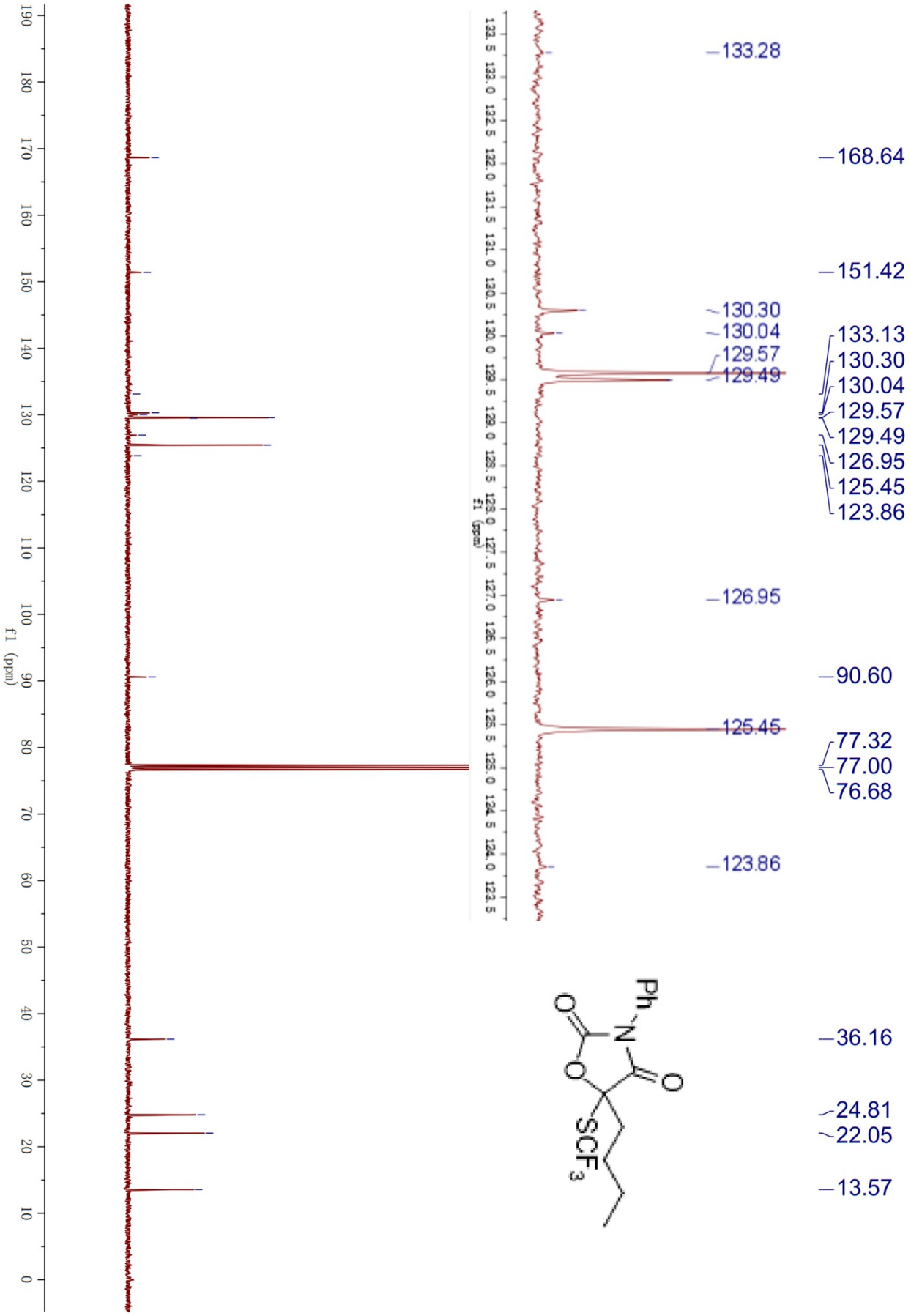

-38.3913
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm
Ph
N
O
O
O
O
SCF3
Br

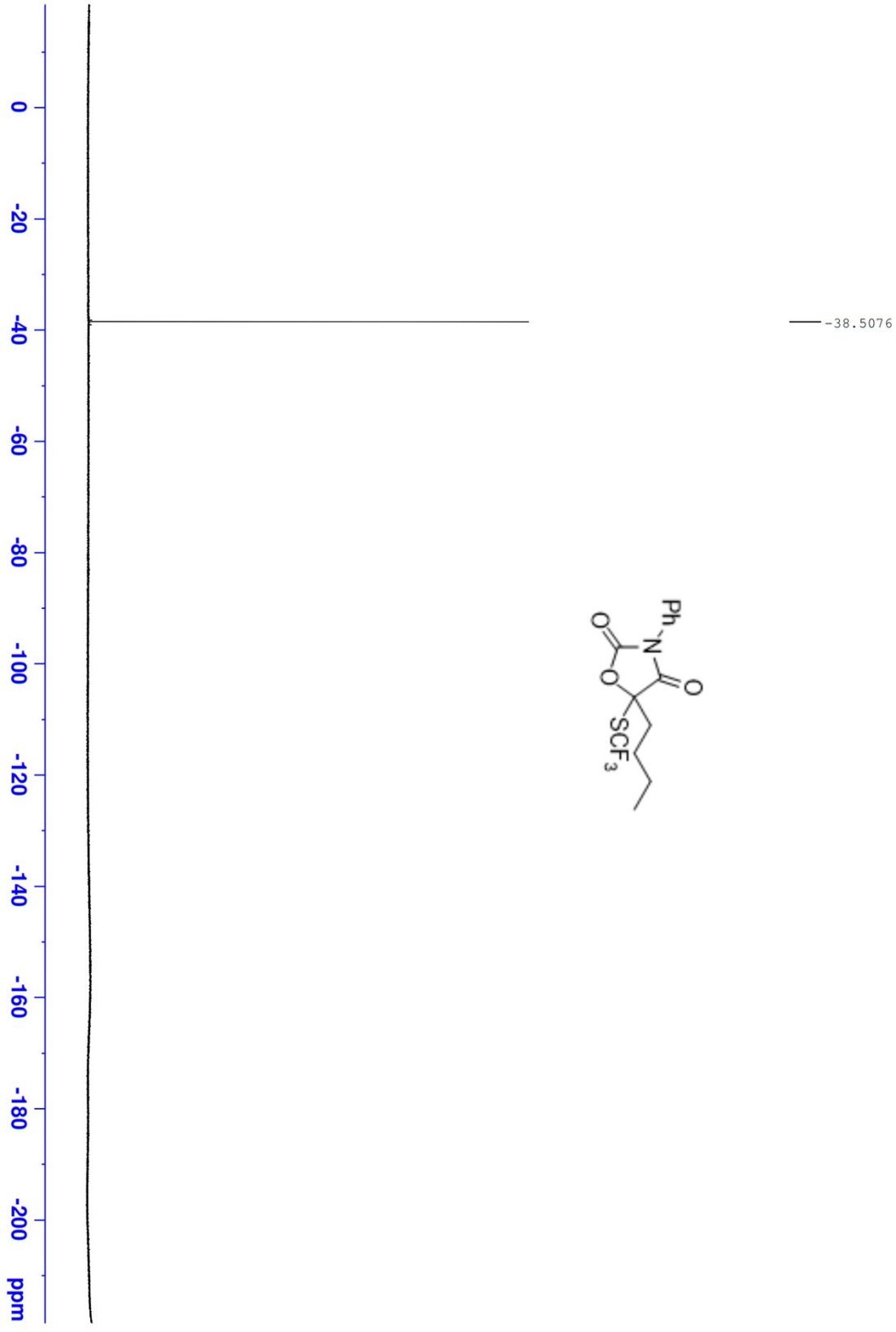

Ph
N
O
O
O
SCF3
7.7275
7.7068
7.5210
7.5037
7.4843
7.4673
7.4552
7.4497
7.4311
7.3813
7.3630
7.3106
7.2901
7.2526
2.00
3.07
2.02
2.05
3.04
2.3967
-0.0000
10
9
8
7
6
5
4
3
2
1
0
-1
ppm

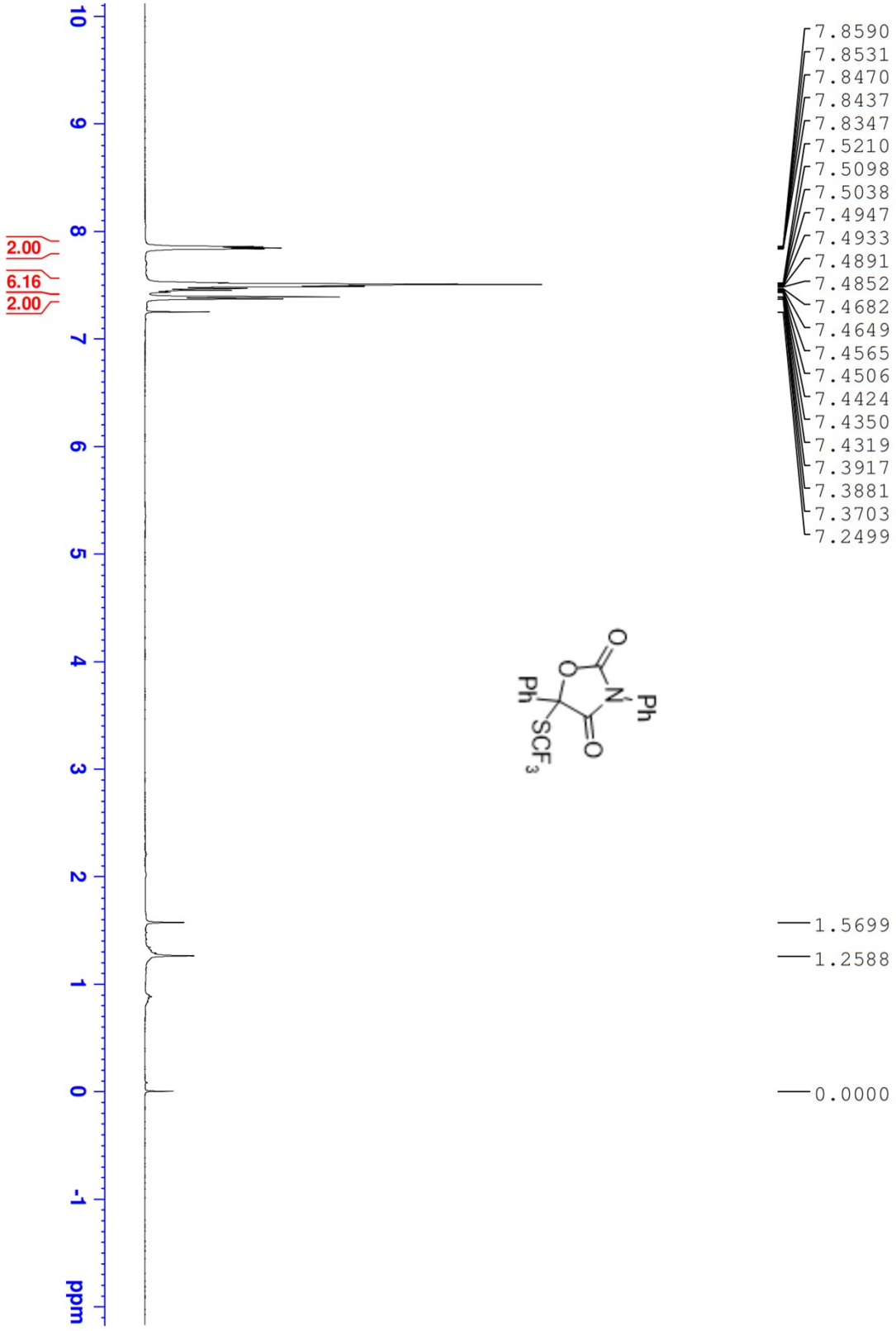

f1 (ppm)
132.67
130.27
130.01
129.57
129.51
129.48
127.74
126.46
125.60
125.56
123.36
167.53
150.97
141.52
132.67
130.27
130.01
129.57
129.51
129.48
127.74
126.46
125.60
125.56
123.36
89.77
77.32
77.00
76.68
21.24
Ph
N
O
O
O
SCF3

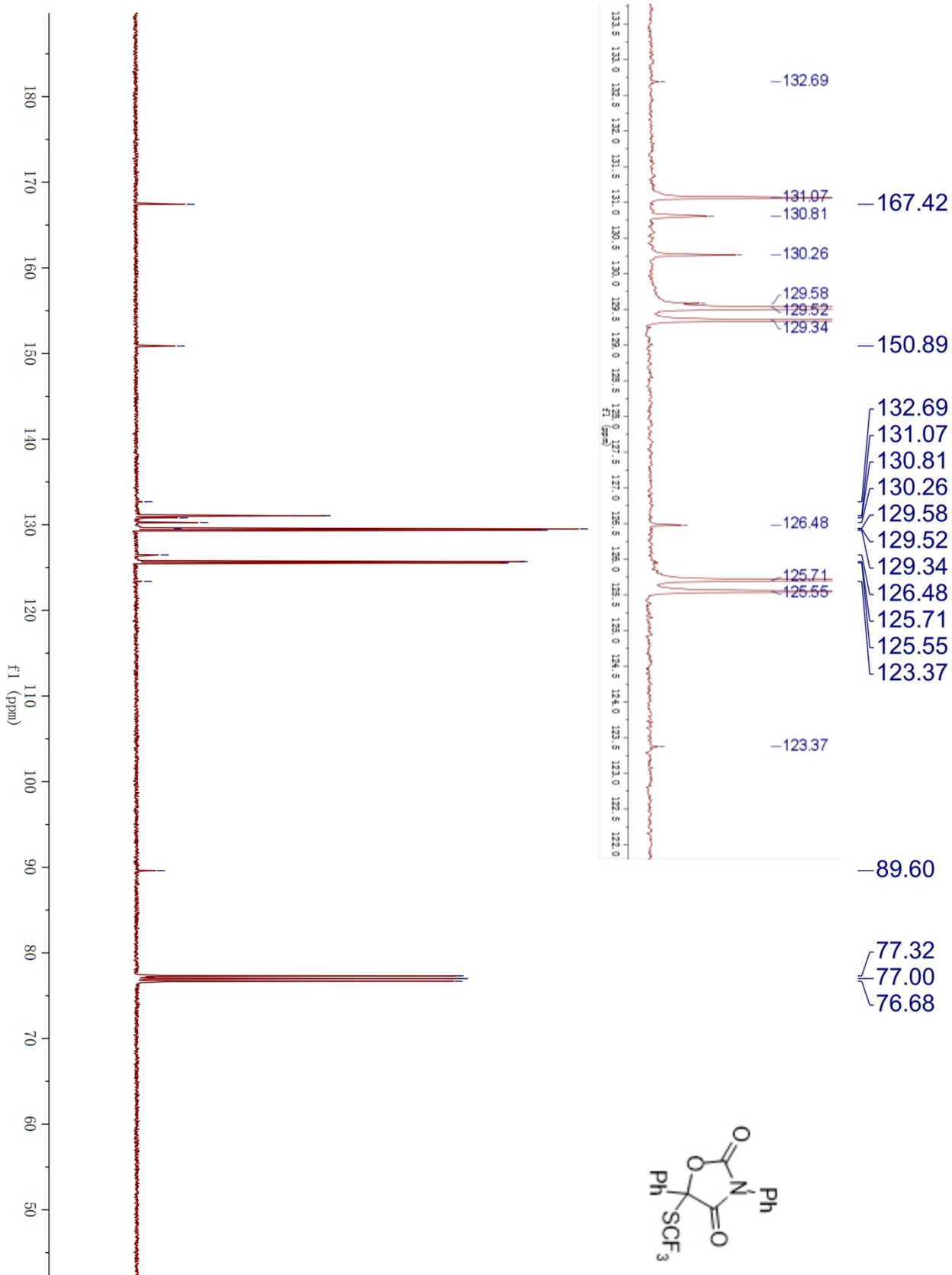

0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm
-38.6951
Ph
N
O
O
O
O
SCF3

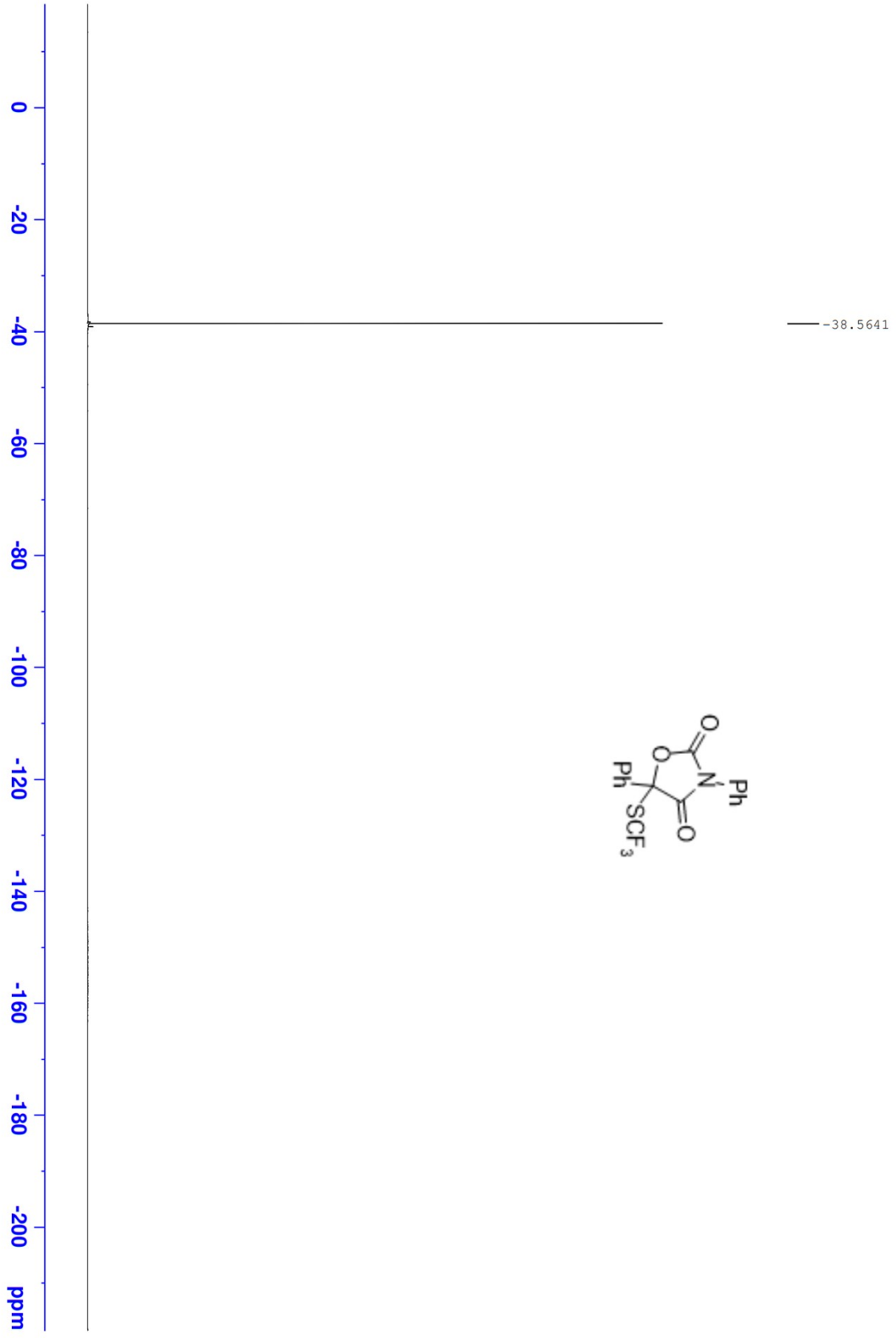

7.5455
7.5280
7.5086
7.4869
7.4691
7.4505
7.3941
7.3755
7.2611
Ph
N
O
O
O
SCF3
2.2501
2.2301
2.2112
1.5705
1.4635
1.4437
1.4263
1.4177
1.4020
1.3854
0.9622
0.9449
0.9269
-0.0000
3.00
1.94
2.08
4.33
3.07
10
9
8
7
6
5
4
3
2
1
0
-1
ppm

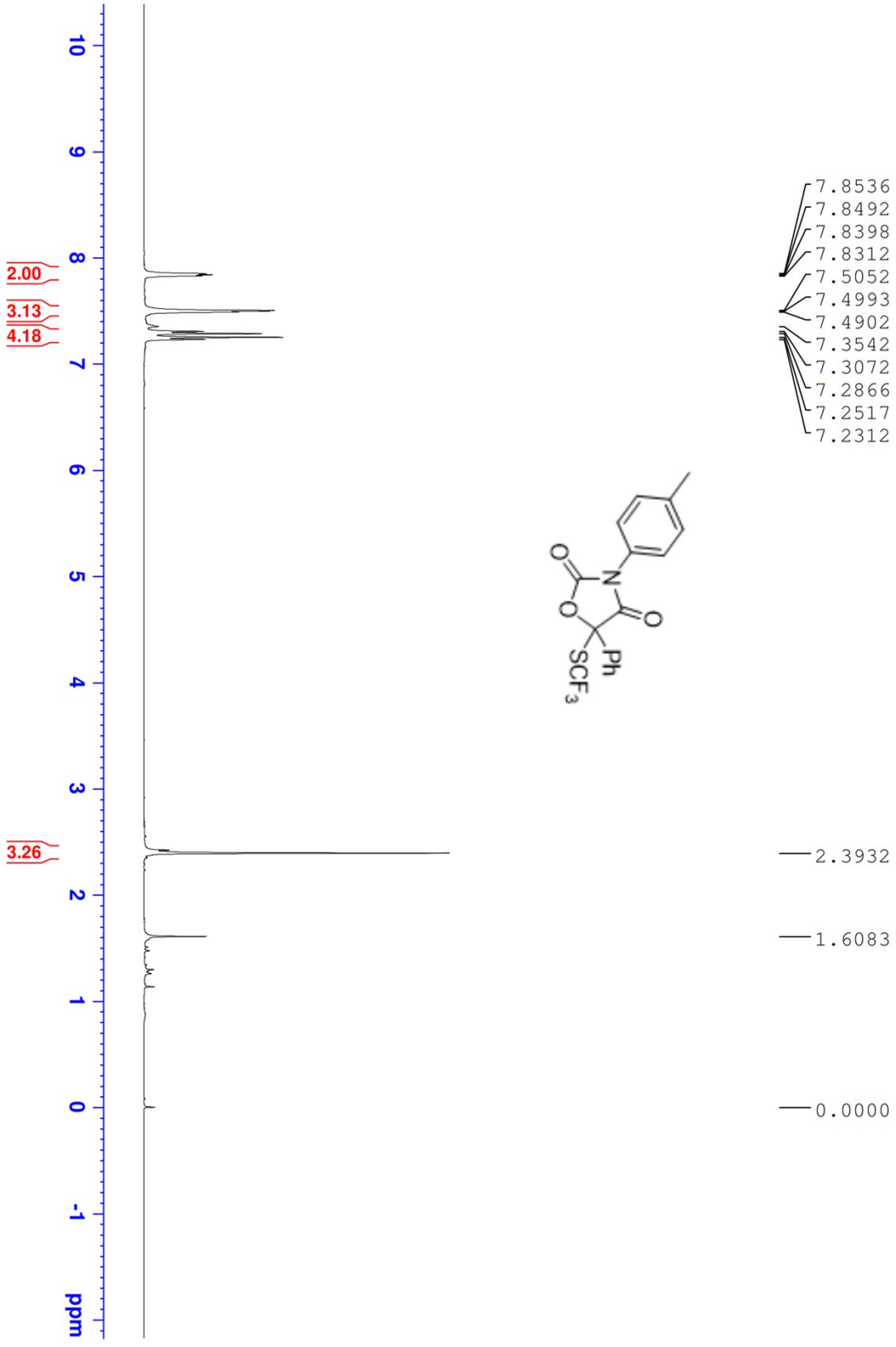

133.28
168.64
151.42
130.30
130.04
129.57
129.49
133.13
130.30
130.04
129.57
129.49
126.95
125.45
123.86
126.95
90.60
125.45
77.32
77.00
76.68
123.86
36.16
24.81
22.05
13.57
Ph
N
O
O
O
SCF3
f1 (ppm)

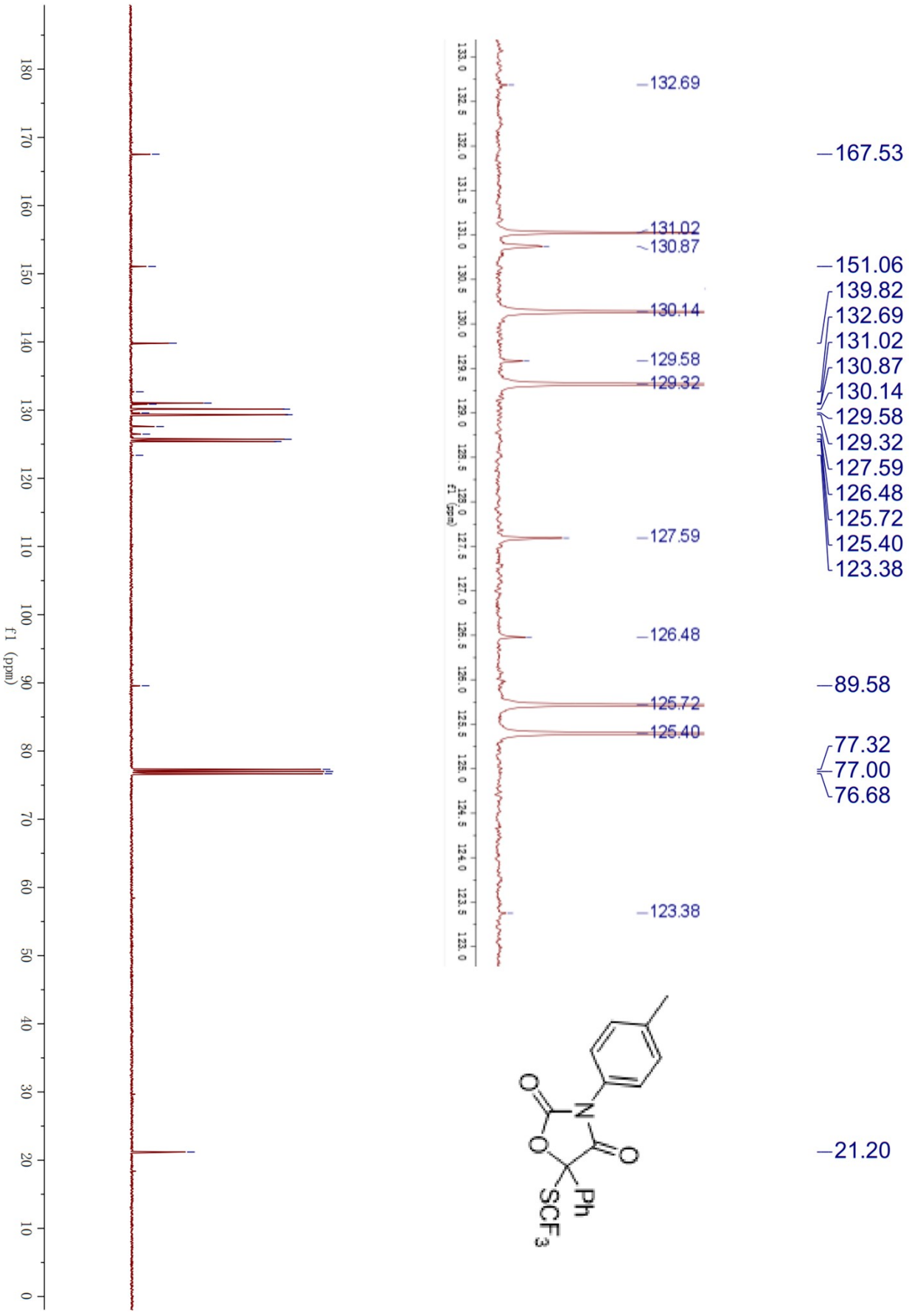

0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm
-38.5076
Ph
N
O
O
O
SCF3

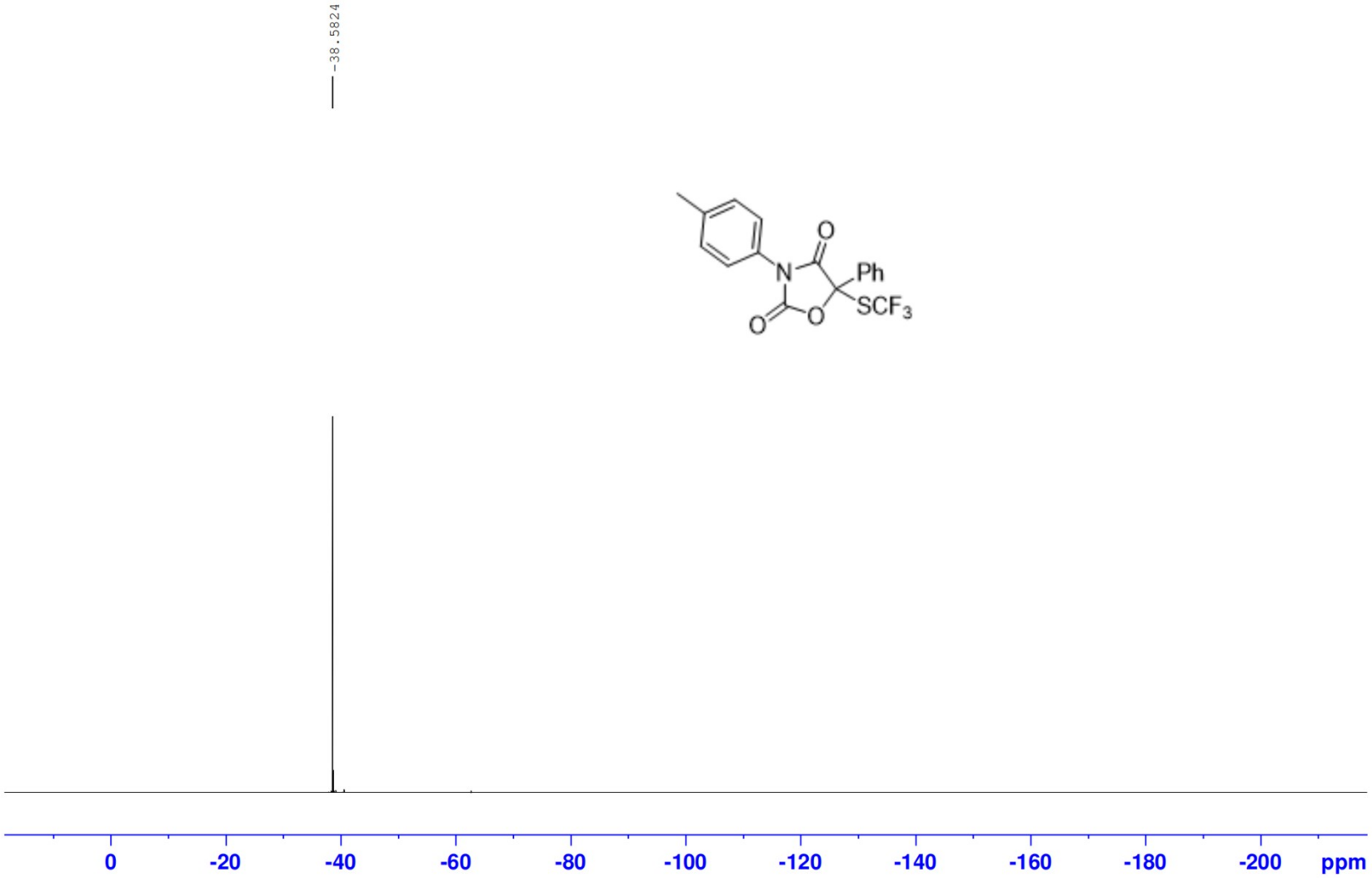

7.8590
7.8531
7.8470
7.8437
7.8347
7.5210
7.5098
7.5038
7.4947
7.4933
7.4891
7.4852
7.4682
7.4649
7.4565
7.4506
7.4424
7.4350
7.4319
7.3917
7.3881
7.3703
7.2499
2.00
6.16
2.00
1.5699
1.2588
0.0000
10
9
8
7
6
5
4
3
2
1
0
-1
ppm
O
O
N
Ph
O
Ph
SCF3

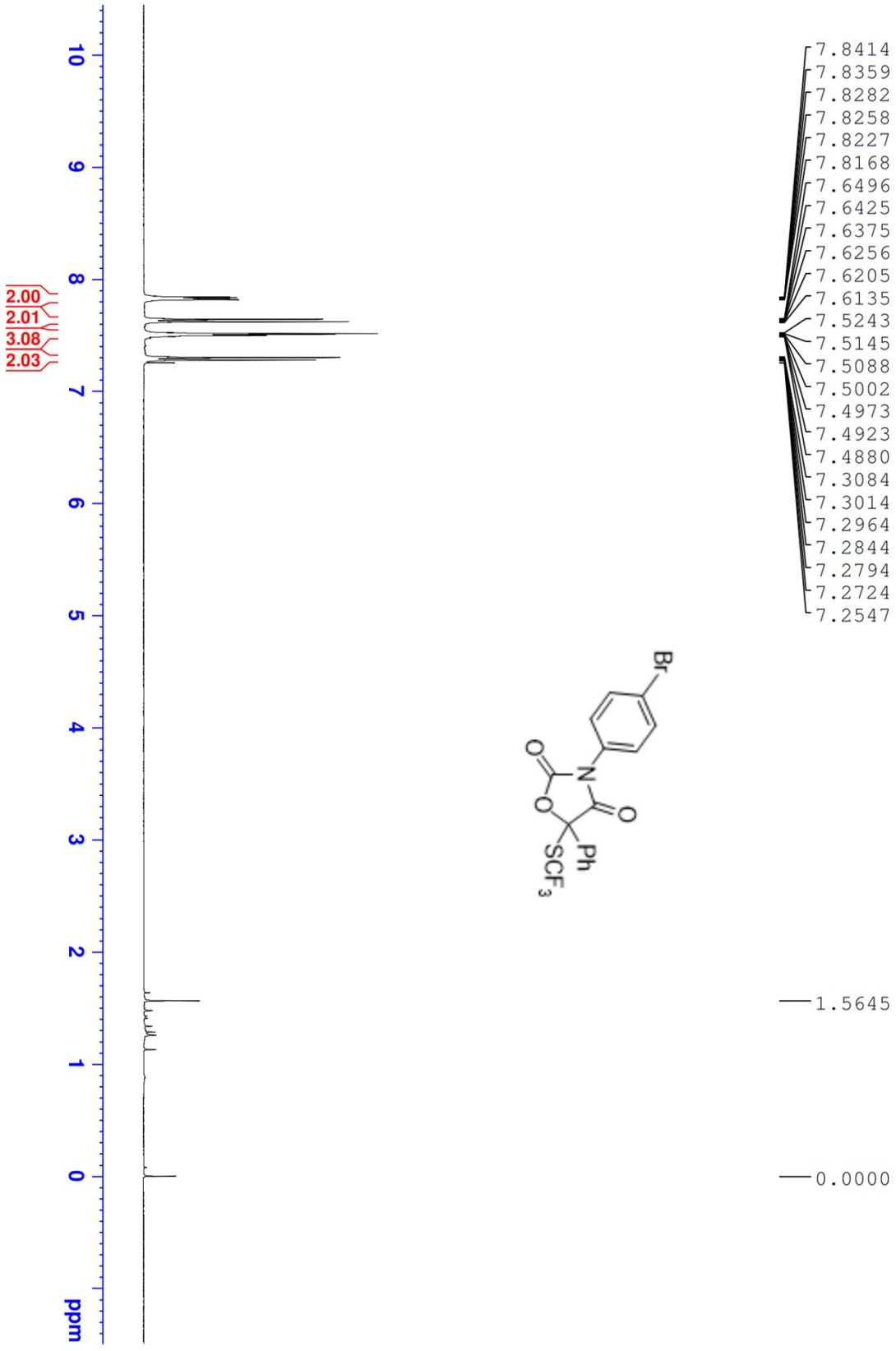

f1 (ppm)
132.69
131.07
130.81
130.26
129.58
129.52
129.34
126.48
125.71
125.55
123.37
167.42
150.89
89.60
77.32
77.00
76.68
Ph
Ph
SCF3
O
O
N
O
O

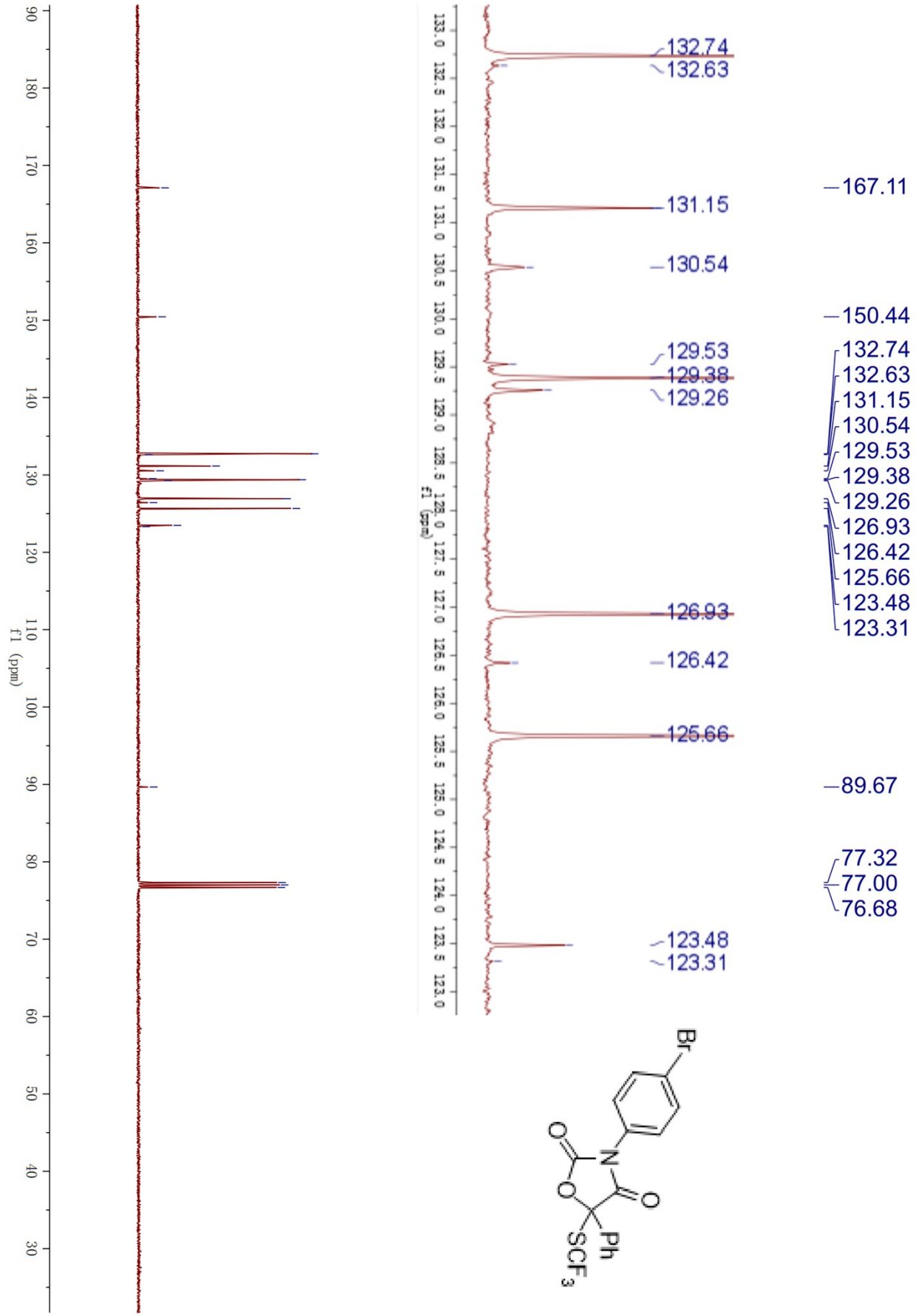

0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm
-38.5641
O
O
N
Ph
O
Ph
SCF3

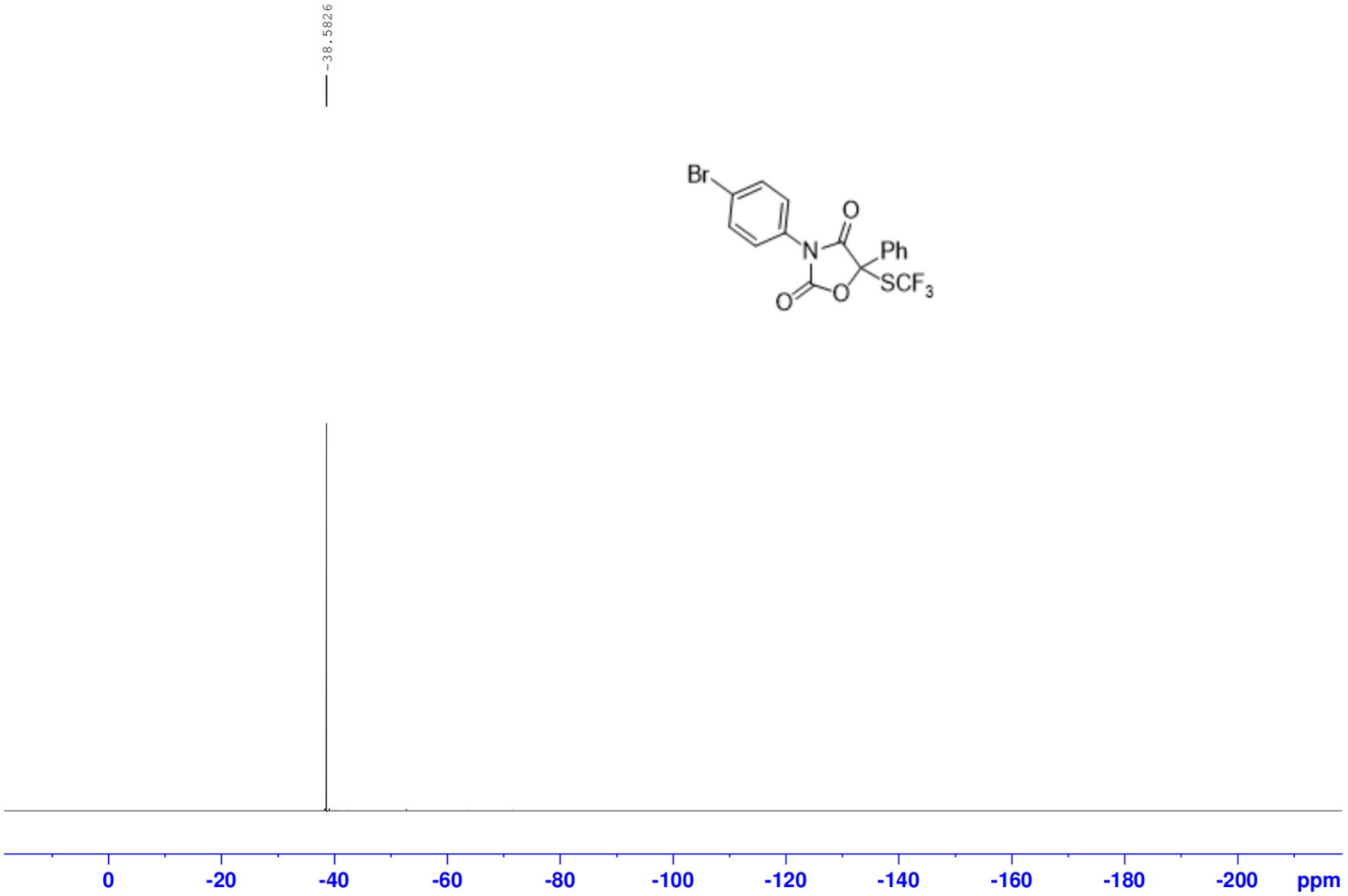

10
9
8
7
6
5
4
3
2
1
0
-1
ppm
2.00
3.13
4.18
3.26
7.8536
7.8492
7.8398
7.8312
7.5052
7.4993
7.4902
7.3542
7.3072
7.2866
7.2517
7.2312
2.3932
1.6083
0.0000
O
N
O
O
O
Ph
SCF3

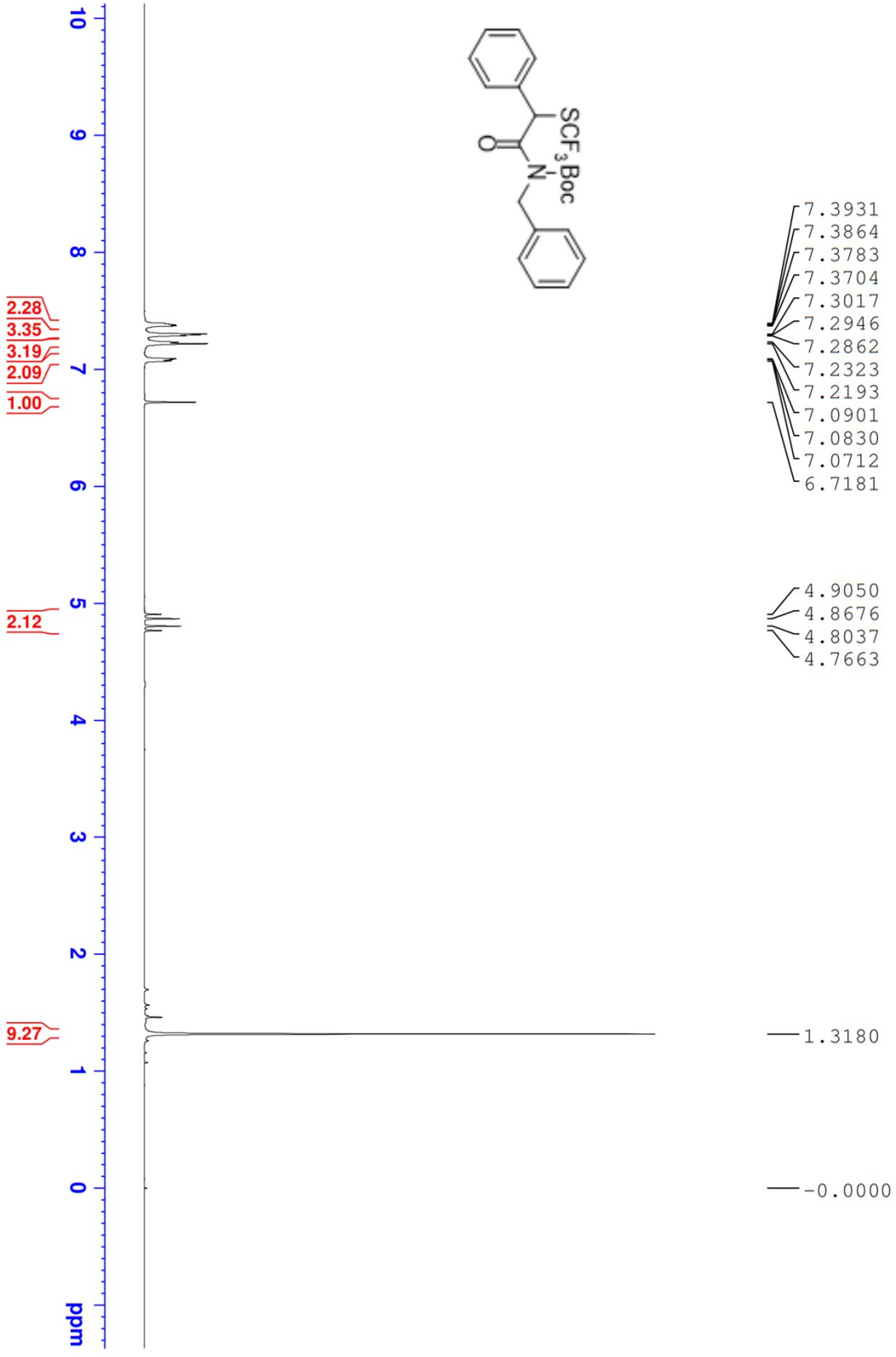

f1 (ppm)
132.69
131.02
130.87
130.14
129.58
129.32
127.59
126.48
125.72
125.40
123.38
167.53
151.06
139.82
132.69
131.02
130.87
130.14
129.58
129.32
127.59
126.48
125.72
125.40
123.38
89.58
77.32
77.00
76.68
21.20
O
N
O
O
Ph
SCF3

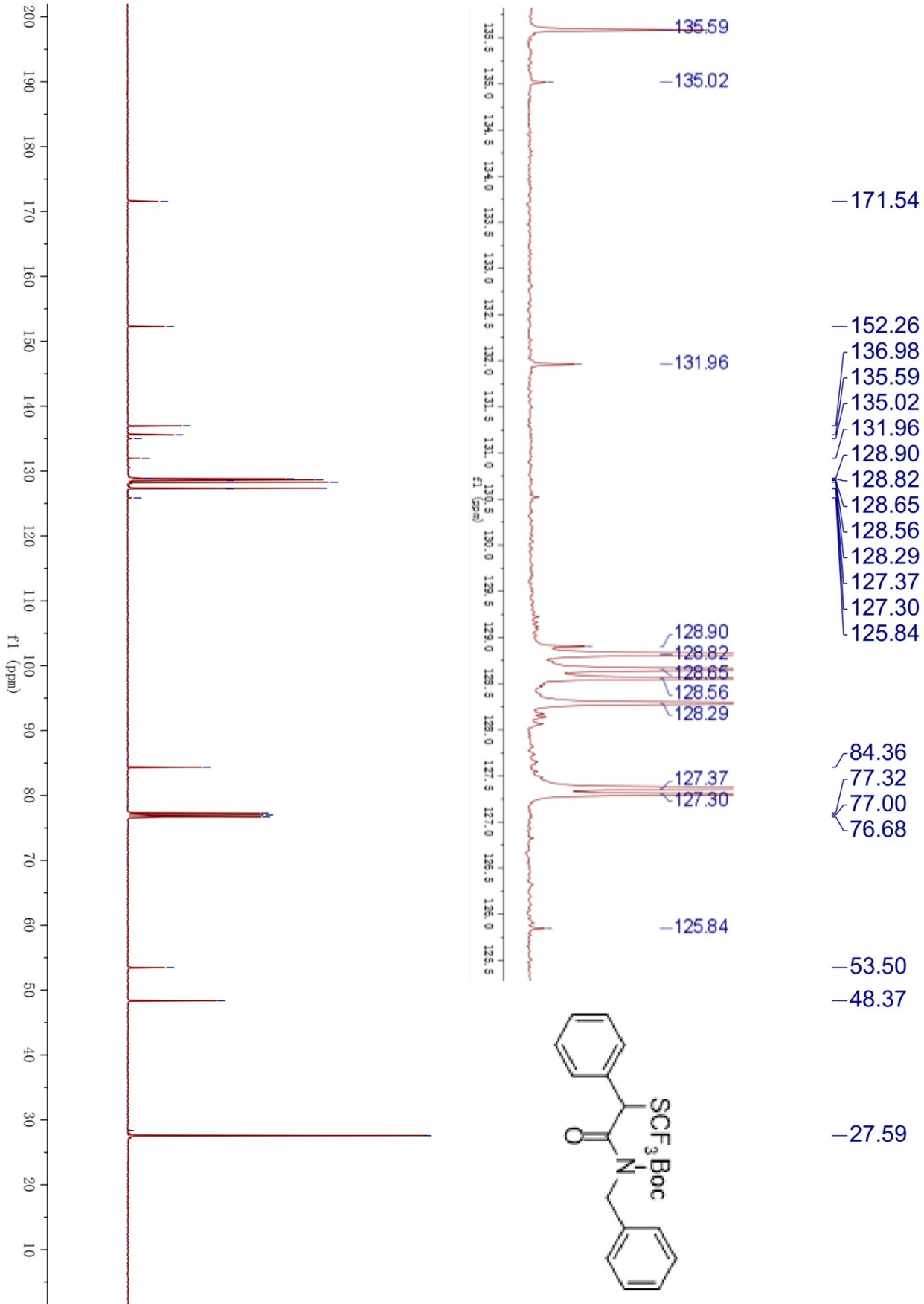

-38.5824
O
N
Ph
SCF3
O
O
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm


7.8414
7.8359
7.8282
7.8258
7.8227
7.8168
7.6496
7.6425
7.6375
7.6256
7.6205
7.6135
7.5243
7.5145
7.5088
7.5002
7.4973
7.4923
7.4880
7.3084
7.3014
7.2964
7.2844
7.2794
7.2724
7.2547
2.00
2.01
3.08
2.03
1.5645
0.0000
ppm
Br
N
O
O
O
Ph
SCF3

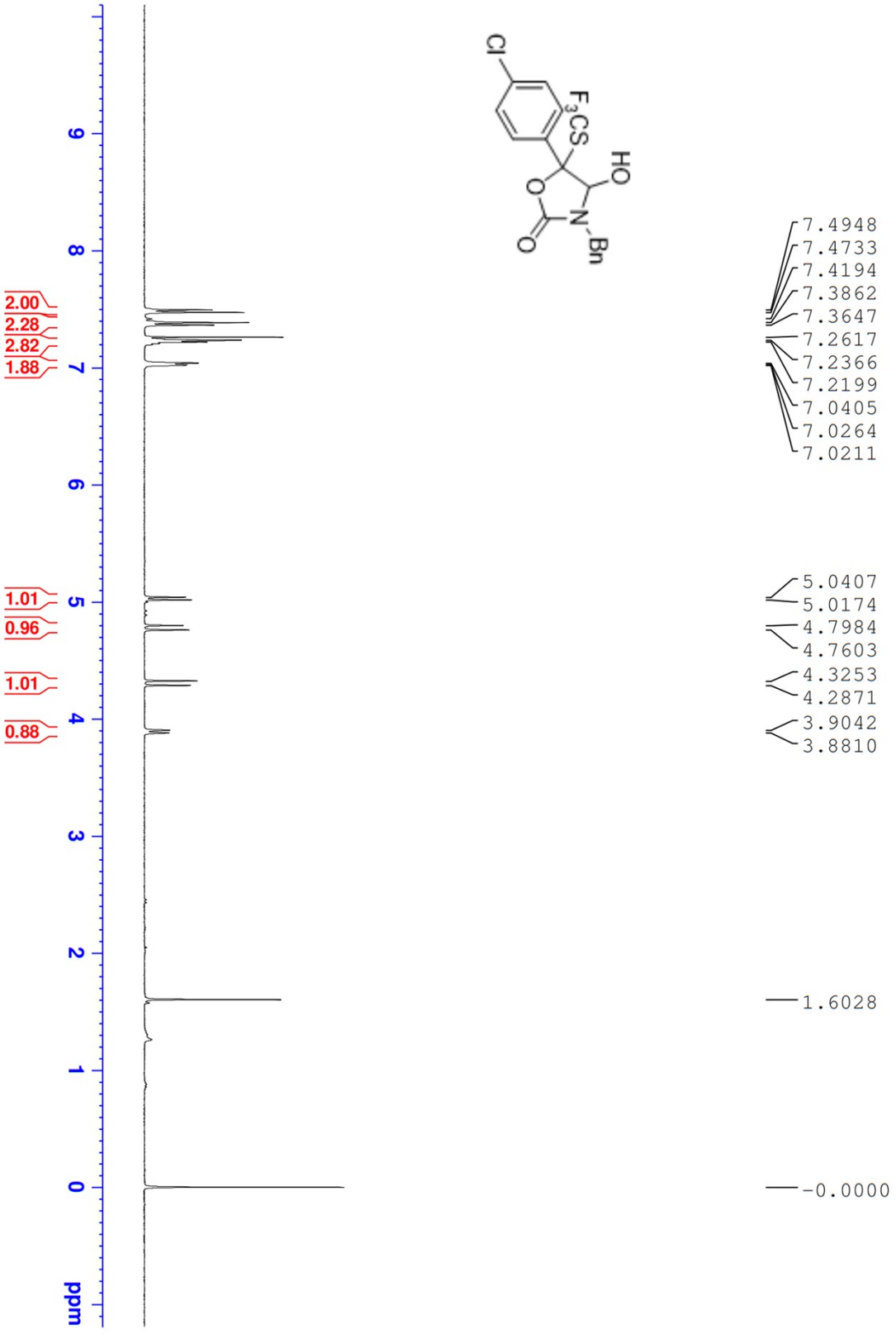

132.74
132.63
131.15
130.54
129.53
129.38
129.26
126.93
126.42
125.66
123.48
123.31
167.11
150.44
132.74
132.63
131.15
130.54
129.53
129.38
129.26
126.93
126.42
125.66
123.48
123.31
89.67
77.32
77.00
76.68
f1 (ppm)
Br
O
N
O
O
Ph
SCF3

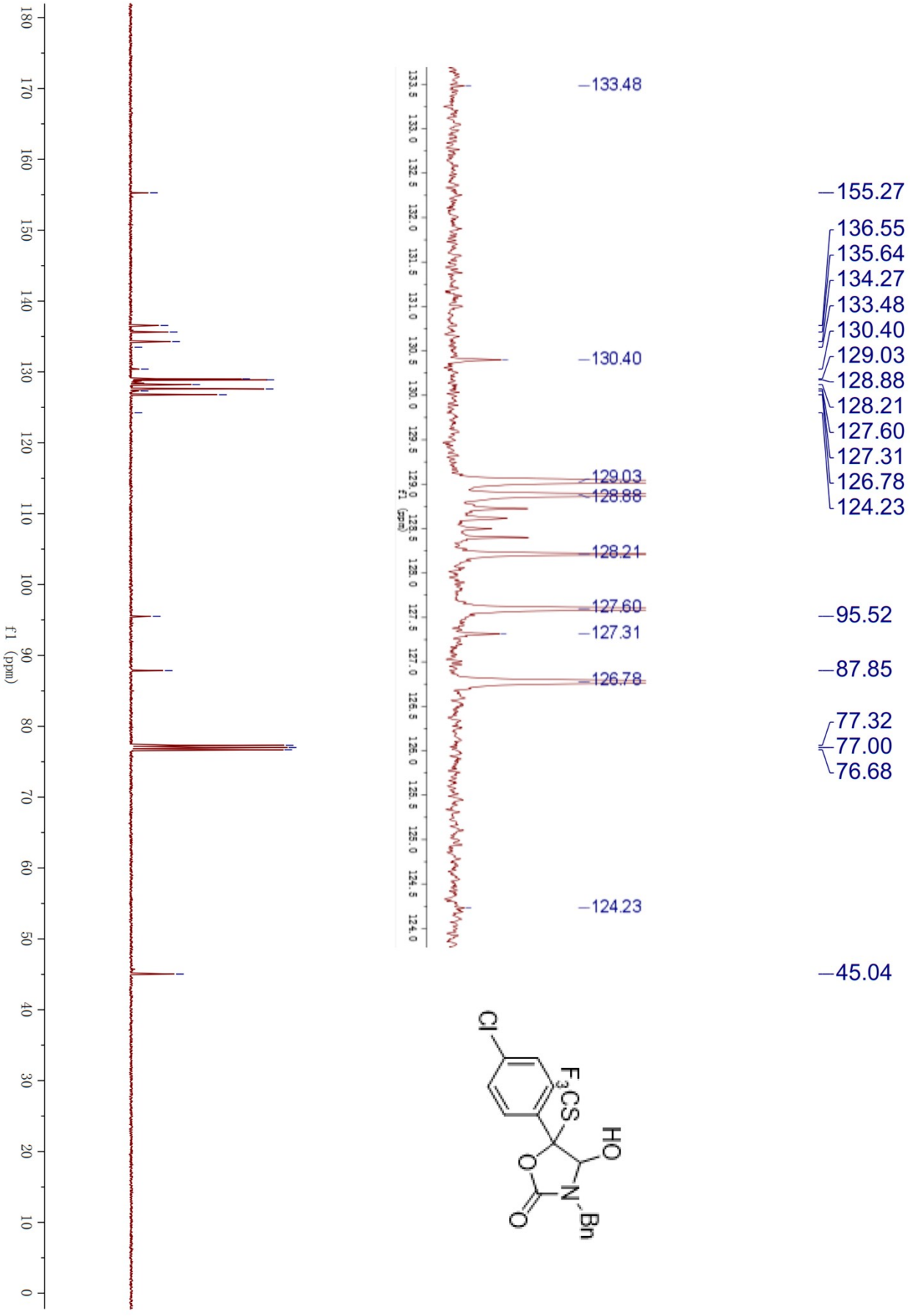

-38.5826
Br
O
N
Ph
SCF3
O
O
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

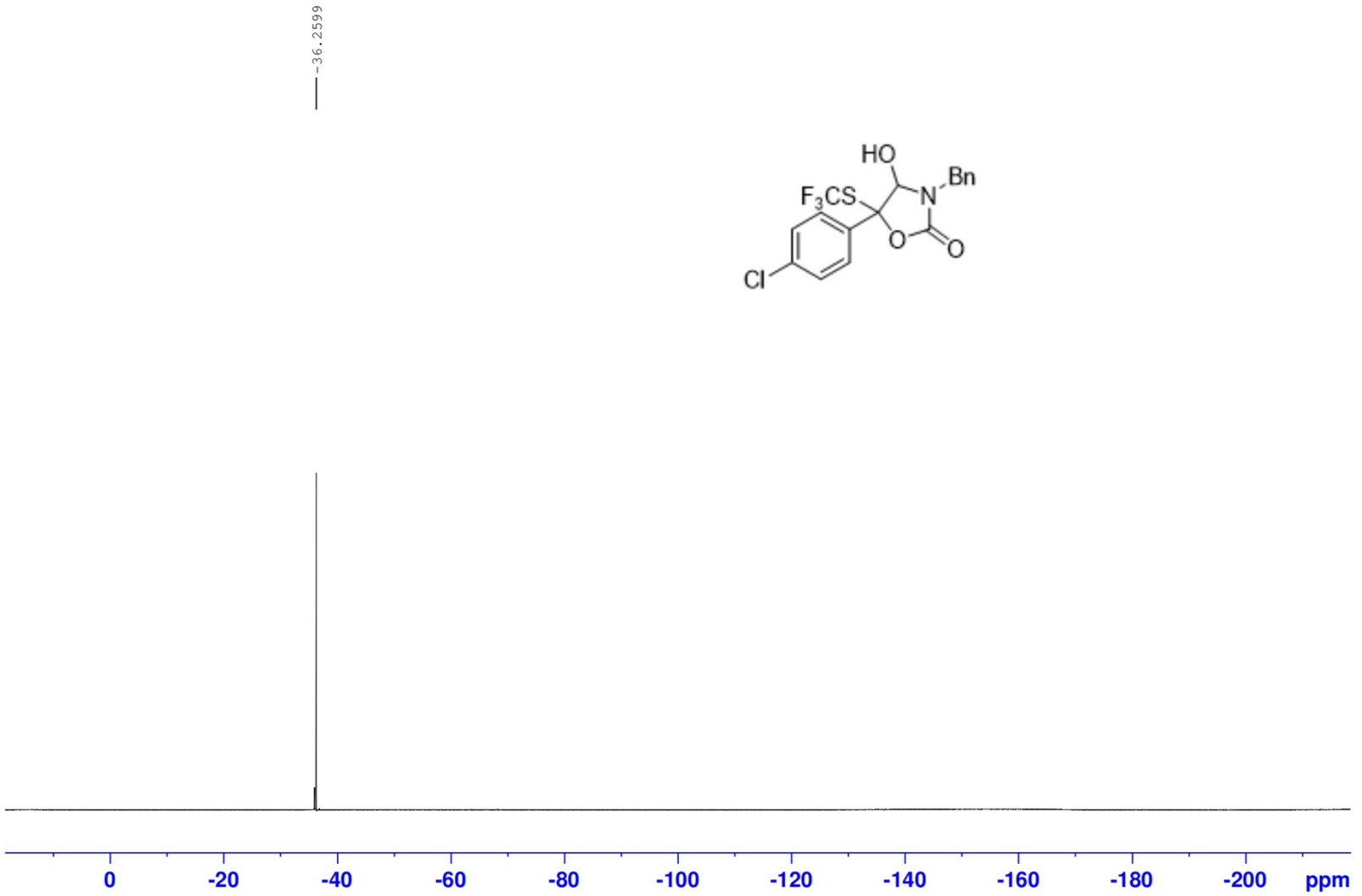

SCF3
Boc
N
7.3931
7.3864
7.3783
7.3704
7.3017
7.2946
7.2862
7.2323
7.2193
7.0901
7.0830
7.0712
6.7181
4.9050
4.8676
4.8037
4.7663
1.3180
-0.0000
2.28
3.35
3.19
2.09
1.00
2.12
9.27
10
9
8
7
6
5
4
3
2
1
0
ppm


135.59
135.02
131.96
128.90
128.82
128.65
128.56
128.29
127.37
127.30
125.84
171.54
152.26
136.98
135.59
135.02
131.96
128.90
128.82
128.65
128.56
128.29
127.37
127.30
125.84
84.36
77.32
77.00
76.68
53.50
48.37
27.59
f1 (ppm)
SCF3
Boc
N
O

-40.6330
SCF3
Boc
N
O
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm


Cl
F3CS
HO
O
N
Bn
O
2.00
2.28
2.82
1.88
1.01
0.96
1.01
0.88
9
8
7
6
5
4
3
2
1
0
ppm
7.4948
7.4733
7.4194
7.3862
7.3647
7.2617
7.2366
7.2199
7.0405
7.0264
7.0211
5.0407
5.0174
4.7984
4.7603
4.3253
4.2871
3.9042
3.8810
1.6028
-0.0000


f1 (ppm)
133.48
130.40
129.03
128.88
128.21
127.60
127.31
126.78
124.23
155.27
136.55
135.64
134.27
133.48
130.40
129.03
128.88
128.21
127.60
127.31
126.78
124.23
95.52
87.85
77.32
77.00
76.68
45.04
Cl
F3CS
HO
O
N
Bn
O


-36.2599
HO
Bn
F3CS
N
O
O
Cl
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm