Electronic Supplementary Material (ESI) for ChemComm.

An unexpected reaction of 2-alkynylaryldiazonium tetrafluoroborate with sulfur dioxide

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Supporting Information

General experimental methods:

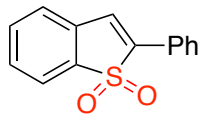
Unless otherwise stated, all commercial reagents were used as received. All solvents were dried and distilled according to standard procedures. Flash column chromatography was performed using silica gel (60-Å pore size, 32–63μm, standard grade). Analytical thin–layer chromatography was performed using glass plates pre-coated with 0.25 mm 230–400 mesh silica gel impregnated with a fluorescent indicator (254 nm). Thin layer chromatography plates were visualized by exposure to ultraviolet light. Organic solutions were concentrated on rotary evaporators at ~20 Torr at 25–35°C. Nuclear magnetic resonance (NMR) spectra are recorded in parts per million from internal tetramethylsilane on the δ scale. ^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ on a Bruker DRX-400 spectrometer operating at 400 MHz and 100 MHz, respectively. All chemical shift values are quoted in ppm and coupling constants quoted in Hz. High resolution mass spectrometry (HRMS) spectra were obtained on a micrOTOF II Instrument.

*General experimental procedure for the copper(I)-catalyzed reaction of 2-alkynylphenyldiazonium tetrafluoroborate **1** with DABCO-bis(sulfur dioxide) **2***

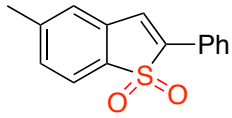
1 **2** **3**

2-Alkynylphenyldiazonium **1** (0.48 mmol) in CH_3CN (2.0 mL) was added dropwisely to a solution of DABCO-bis(sulfur dioxide) **2** (0.24 mmol) and morpholin-4-amine **2** (0.40 mmol) in CH_3CN (5.0 mL) in 10 minutes. After the mixture was stirred at room temperature for another 15 minutes, NaOAc (1.20 mmol) and CuBr (0.04 mmol) were added to the suspension. The mixture was allowed to stir under reflux overnight. After completion of the reaction as indicated by TLC, the solvent was evaporated and the residue was purified directly by flash column chromatograph (*n*-hexane/ethyl acetate = 6:1) to give

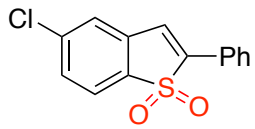
the desired product **3**.



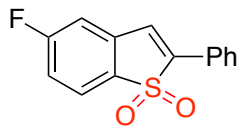
2-Phenylbenzo[*b*]thiophene 1,1-dioxide (**3a**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, J = 5.6 Hz, 2H), 7.75 (d, J = 7.2 Hz, 1H), 7.54 (d, J = 7.2 Hz, 1H), 7.50-7.45 (m, 4H), 7.39 (d, J = 7.2 Hz, 1H), 7.28 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.5, 137.0, 133.7, 131.1, 130.3, 129.9, 129.2, 127.1, 126.5, 125.0, 123.7, 121.4. HRMS (ESI) calcd for $C_{14}H_{11}O_2S^+$: 243.0474 ($M + H^+$), found: 243.0478.



5-Methyl-2-phenylbenzo[*b*]thiophene 1,1-dioxide (**3b**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81-7.79 (m, 2H), 7.61 (d, J = 7.6 Hz, 1H), 7.44-7.42 (m, 3H), 7.25-7.23 (m, 1H), 7.21-7.20 (m, 1H), 7.15 (s, 1H), 2.39 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.7, 142.7, 134.3, 131.3, 130.3, 130.1, 129.1, 127.2, 126.4, 125.7, 123.7, 121.2, 21.6. HRMS (ESI) calcd for $C_{15}H_{13}O_2S^+$: 257.0631 ($M + H^+$), found: 257.0635.

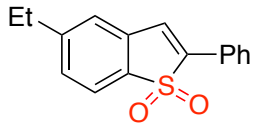


5-Chloro-2-phenylbenzo[*b*]thiophene 1,1-dioxide (**3c**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83-7.81 (m, 2H), 7.69 (d, J = 8.0 Hz, 1H), 7.48-7.47 (m, 4H), 7.39-7.38 (m, 1H), 7.23 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.0, 135.1, 133.0, 130.7, 129.6, 129.3, 128.7, 128.5, 126.6, 125.2, 122.5, 122.2. HRMS (ESI) calcd for $C_{14}H_9ClNaO_2S^+$: 298.9904 ($M + Na^+$), found: 298.9900.

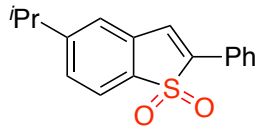


5-Fluoro-2-phenylbenzo[*b*]thiophene 1,1-dioxide (**3d**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83-7.81 (m, 2H), 7.76-7.73 (m, 1H), 7.48-7.46 (m, 3H), 7.26 (s, 1H), 7.18-7.13 (m, 1H), 7.10-7.08 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.9 (d, J_{CF} = 253.7 Hz),

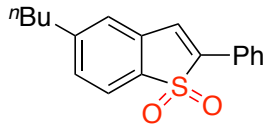
144.6, 134.2, 132.7, 130.7, 129.3, 126.1, 123.6 (d, J_{CF} = 9.8 Hz), 122.2, 116.5 (d, J_{CF} = 23.7 Hz), 112.6 (d, J_{CF} = 24.6 Hz). HRMS (ESI) calcd for $C_{14}H_9FNaO_2S^+$: 283.0199 (M + Na^+), found: 283.0201.



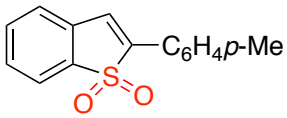
5-Ethyl-2-phenylbenzo[*b*]thiophene 1,1-dioxide (**3e**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83-7.81 (m, 2H), 7.65 (d, J = 8.0 Hz, 1H), 7.46-7.44 (m, 3H), 7.29 (d, J = 8.0 Hz, 1H), 7.24 (s, 1H), 7.21(s, 1H), 2.71 (q, J = 7.6 Hz, 2H), 1.26 (t, J = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.9, 132.4, 131.4, 130.2, 130.2, 129.3, 129.1, 128.2, 126.5, 124.6, 123.8, 121.4, 29.0, 15.2.



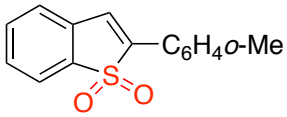
5-Isopropyl-2-phenylbenzo[*b*]thiophene 1,1-dioxide (**3f**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (dd, J = 8.4 Hz, 1.8 Hz, 2H), 7.66 (d, J = 7.6 Hz, 1H), 7.46-7.43 (m, 3H), 7.34-7.31 (m, 1H), 7.26-7.25 (m, 2H), 2.99-2.95 (m, 1H), 1.27 (d, J = 7.2 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.3, 142.4, 134.3, 131.1, 129.8, 128.8, 127.7, 127.0, 126.2, 123.6, 123.0, 121.1, 34.0, 23.3. HRMS (ESI) calcd for $C_{17}H_{17}O_2S^+$: 285.0944 (M + H^+), found: 285.0965.



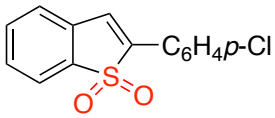
5-Butyl-2-phenylbenzo[*b*]thiophene 1,1-dioxide (**3g**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83-7.80 (m, 2H), 7.64 (d, J = 7.6 Hz, 1H), 7.47-7.42 (m, 3H), 7.26 (d, J = 8.0 Hz, 1H), 7.23(s, 1H), 7.19 (s, 1H), 2.66 (t, J = 7.6 Hz, 2H), 1.62-1.57 (m, 2H), 1.38-1.32 (m, 2H), 0.93 (t, J = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.7, 142.7, 134.4, 131.3, 130.1, 129.8, 129.1, 127.3, 126.4, 125.1, 123.8, 121.3, 35.6, 33.1, 22.1, 13.8.



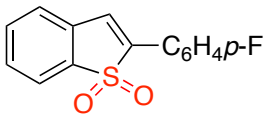
2-(*p*-Tolyl)benzo[*b*]thiophene 1,1-dioxide (**3h**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73-7.69 (m, 3H), 7.53-7.49 (m, 1H), 7.44 (t, J = 7.6 Hz, 1H), 7.34 (d, J = 7.6 Hz, 1H), 7.25 (d, J = 8.0 Hz, 2H), 7.20 (s, 1H), 2.38 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.7, 133.6, 131.3, 129.9, 129.6, 129.0, 128.5, 126.3, 124.8, 124.2, 122.6, 121.3, 21.4. HRMS (ESI) calcd for $C_{15}H_{12}NaO_2S^+$: 279.0450 (M + Na^+), found: 279.0449.



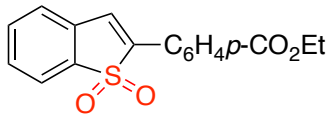
2-(*o*-Tolyl)benzo[*b*]thiophene 1,1-dioxide (**3i**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, J = 7.6 Hz, 1H), 7.69 (t, J = 7.6 Hz, 1H), 7.59-7.55 (m, 1H), 7.52-7.48 (m, 1H), 7.40-7.27 (m, 4H), 7.03 (s, 1H), 2.45 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.6, 138.0, 136.3, 133.6, 131.0, 130.0, 129.4, 128.2, 126.4, 126.1, 125.0, 121.6, 20.6. HRMS (ESI) calcd for $C_{15}H_{13}O_2S^+$: 257.0631 (M + H^+), found: 257.0625.



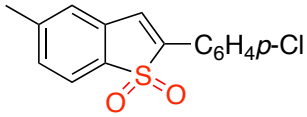
2-(4-Chlorophenyl)benzo[*b*]thiophene 1,1-dioxide (**3j**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, J = 8.8 Hz, 3H), 7.56-7.47 (m, 2H), 7.41 (d, J = 8.8 Hz, 2H), 7.36 (d, J = 7.2 Hz, 1H), 7.26 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.4, 136.4, 133.8, 130.8, 130.1, 129.5, 128.6, 127.8, 125.5, 125.2, 124.1, 121.4, 20.6. HRMS (ESI) calcd for $C_{14}H_9ClNaO_2S^+$: 298.9904 (M + Na^+), found: 298.9905.



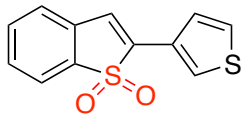
2-(4-Fluorophenyl)benzo[*b*]thiophene 1,1-dioxide (**3k**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81-7.78 (m, 2H), 7.73 (d, J = 7.2 Hz, 1H), 7.55-7.45 (m, 2H), 7.35 (d, J = 7.2 Hz, 1H), 7.20 (s, 1H), 7.13 (t, J = 8.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.7 (d, J_{CF} = 250.9 Hz), 141.4, 136.7, 133.8, 130.9, 129.9, 128.6 (d, J_{CF} = 8.4 Hz), 125.0, 123.5, 123.3, 121.4, 116.4 (d, J_{CF} = 22.0 Hz). HRMS (ESI) calcd for $C_{14}H_9FNaO_2S^+$: 283.0199 (M + Na^+), found: 283.0202.



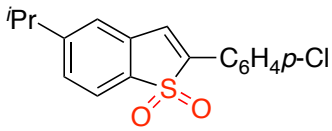
Ethyl 4-(1,1-dioxidobenzo[*b*]thiophen-2-yl)benzoate (**3l**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, J = 8.4 Hz, 2H), 7.90 (d, J = 8.4 Hz, 2H), 7.78 (d, J = 7.2 Hz, 1H), 7.61-7.52 (m, 2H), 7.45-7.41 (m, 2H), 4.41 (q, J = 7.2 Hz, 2H), 1.42 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.7, 141.6, 137.1, 133.9, 131.7, 131.2, 130.4, 130.3, 127.9, 126.3, 125.6, 125.4, 121.5, 61.3, 14.3. HRMS (ESI) calcd for $C_{17}H_{15}O_4S^+$: 315.0686 ($M + H^+$), found: 315.0691.



2-(4-Chlorophenyl)-5-methylbenzo[*b*]thiophene 1,1-dioxide (**3m**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75-7.73 (m, 2H), 7.63 (d, J = 7.6 Hz, 1H), 7.43-7.40 (m, 2H), 7.30-7.28 (m, 1H), 7.21 (s, 1H), 7.17 (s, 1H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.9, 141.7, 136.3, 134.2, 131.2, 130.5, 129.5, 127.7, 125.9, 125.7, 124.2, 121.4, 21.7. HRMS (ESI) calcd for $C_{15}H_{11}ClNaO_2S^+$: 313.0060 ($M + Na^+$), found: 313.0044.

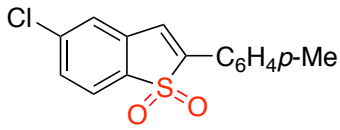


2-(Thiophen-3-yl)benzo[*b*]thiophene 1,1-dioxide (**3n**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95-7.94 (m, 1H), 7.75 (d, J = 7.6 Hz, 1H), 7.57-7.52 (m, 1H), 7.49-7.43 (m, 2H), 7.40-7.36 (m, 2H), 7.12 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.4, 133.8, 131.6, 129.6, 128.7, 127.2, 125.4, 125.2, 125.0, 122.0, 121.5. HRMS (ESI) calcd for $C_{12}H_8NaO_2S_2^+$: 270.9858 ($M + Na^+$), found: 270.9863.

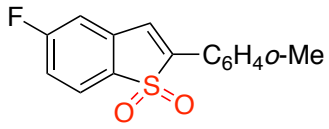


2-(4-Chlorophenyl)-5-isopropylbenzo[*b*]thiophene 1,1-dioxide (**3o**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, J = 8.8 Hz, 2H), 7.67 (d, J = 7.6 Hz, 1H), 7.44 (d, J = 8.8 Hz, 2H), 7.36-7.34 (m, 1H), 7.26-7.25 (m, 2H), 3.00-2.97 (m, 1H), 1.28 (d, J = 7.2 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.8, 136.3, 131.6, 131.2, 129.5, 128.6,

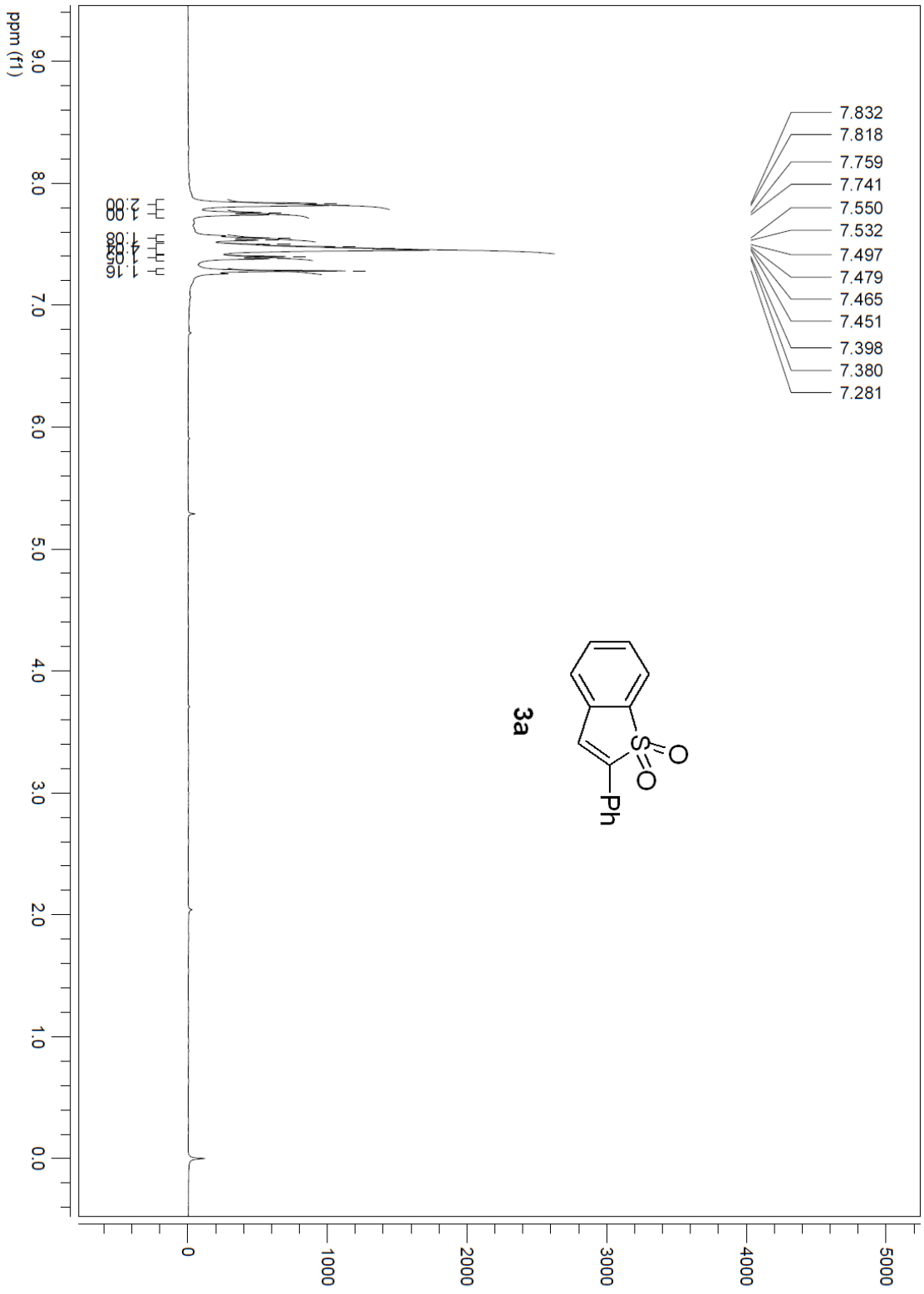
128.5, 128.3, 127.7, 124.4, 123.4, 121.5, 34.4, 23.6.



5-Chloro-2-(*p*-tolyl)benzo[*b*]thiophene 1,1-dioxide (**3p**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71-7.66 (m, 3H), 7.44-7.42 (m, 1H), 7.34-7.33 (m, 1H), 7.28-7.20 (m, 2H), 7.16 (s, 1H), 2.40 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.3, 139.9, 133.3, 130.0, 129.4, 129.2, 128.3, 126.5, 125.0, 123.9, 122.5, 121.1, 21.5. HRMS (ESI) calcd for $C_{15}H_{11}ClNaO_2S^+$: 313.0060 ($M + Na^+$), found: 313.0050.



5-Fluoro-2-(*o*-tolyl)benzo[*b*]thiophene 1,1-dioxide (**3q**). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75-7.72 (m, 1H), 7.69-7.67 (m, 1H), 7.36-7.29 (m, 3H), 7.11-7.08 (m, 1H), 7.11-7.08 (m, 1H), 6.99 (s, 1H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.7 (d, J_{CF} = 253.4 Hz), 144.5, 138.0, 134.0 (d, J_{CF} = 9.9 Hz), 131.1, 130.3, 129.3, 126.8, 126.2, 126.0, 123.7 (d, J_{CF} = 9.7 Hz), 116.6 (d, J_{CF} = 23.6 Hz), 112.7 (d, J_{CF} = 24.6 Hz), 20.6. HRMS (ESI) calcd for $C_{15}H_{11}FNaO_2S^+$: 297.0356 ($M + Na^+$), found: 297.0350.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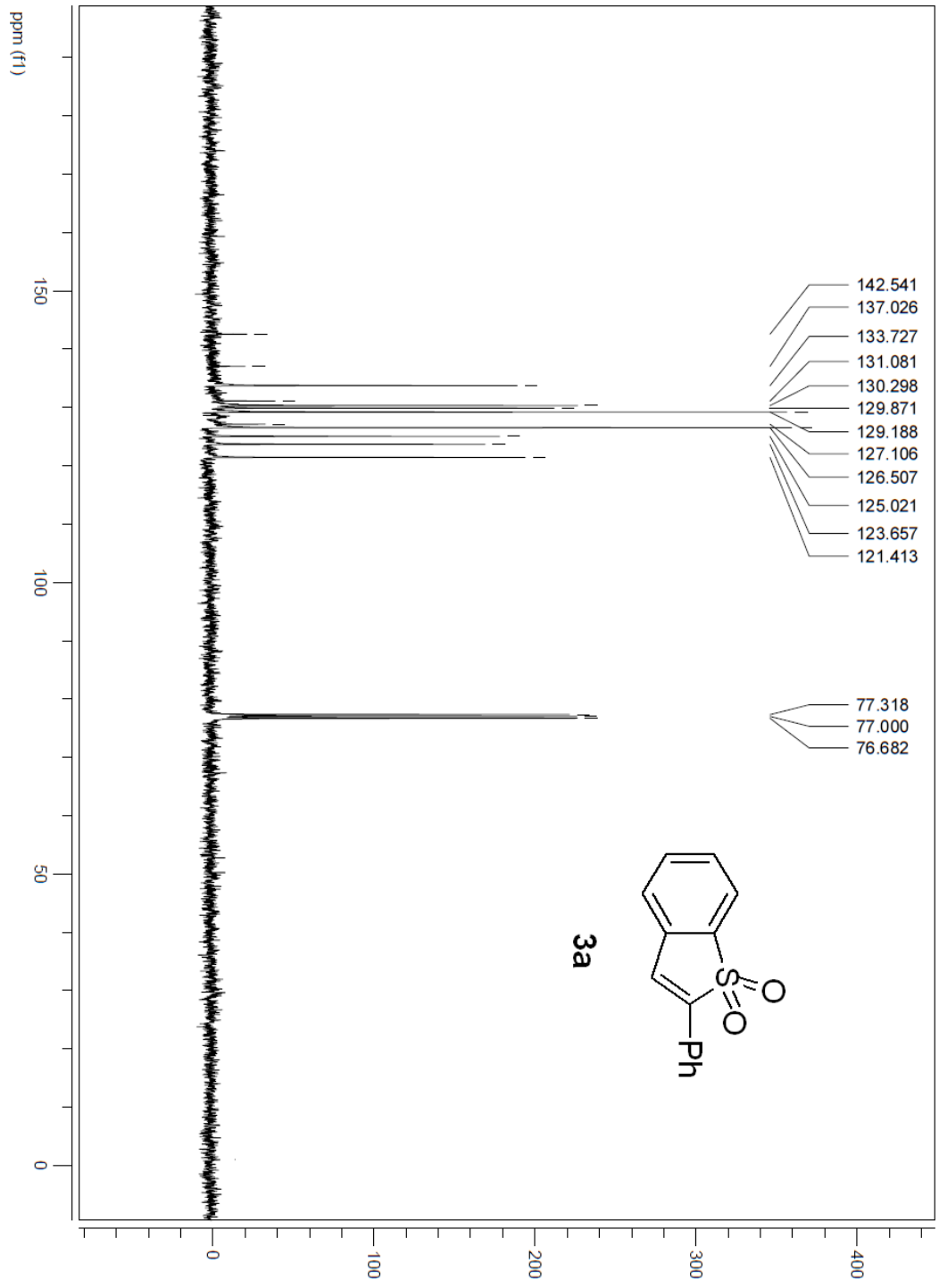
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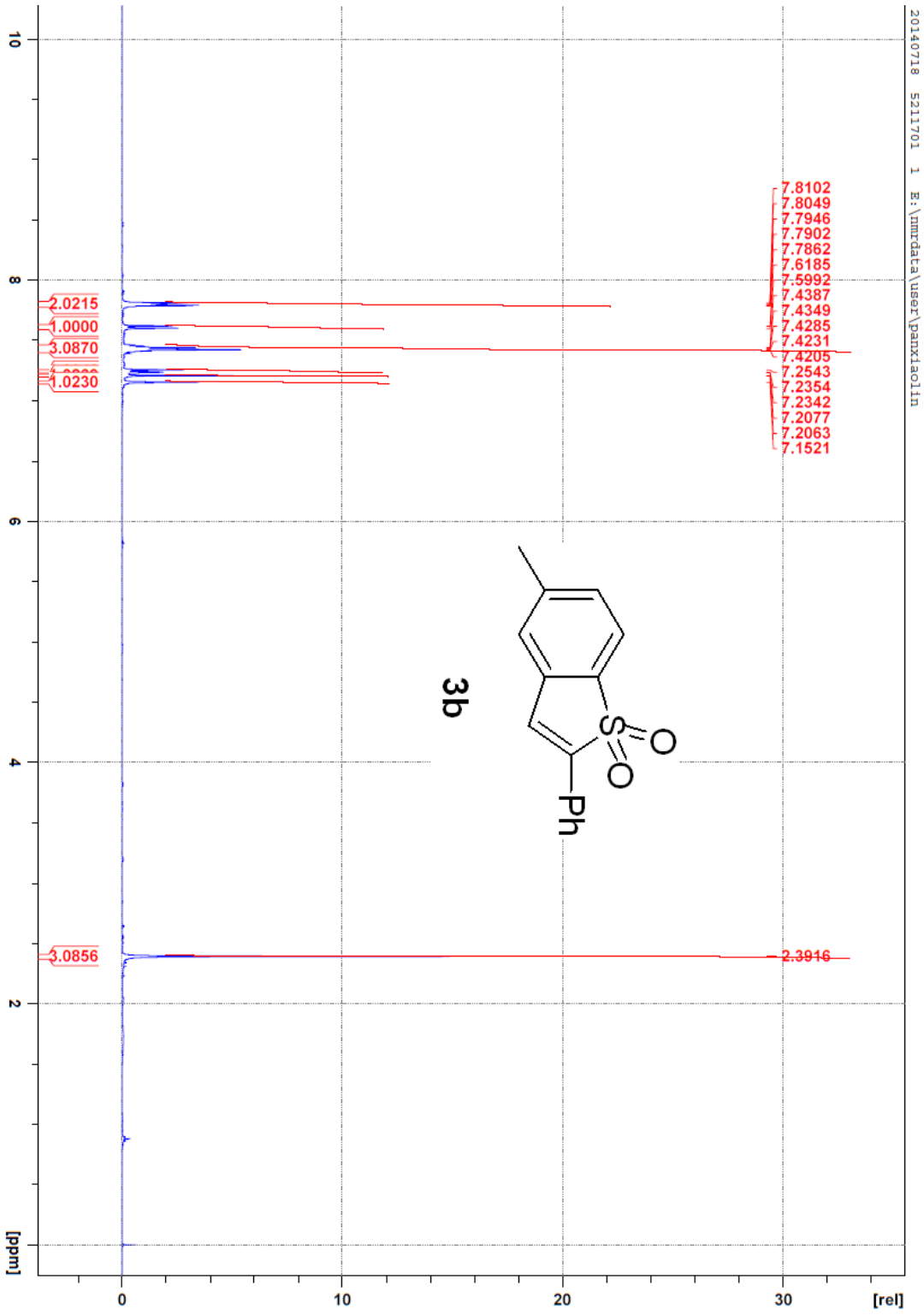
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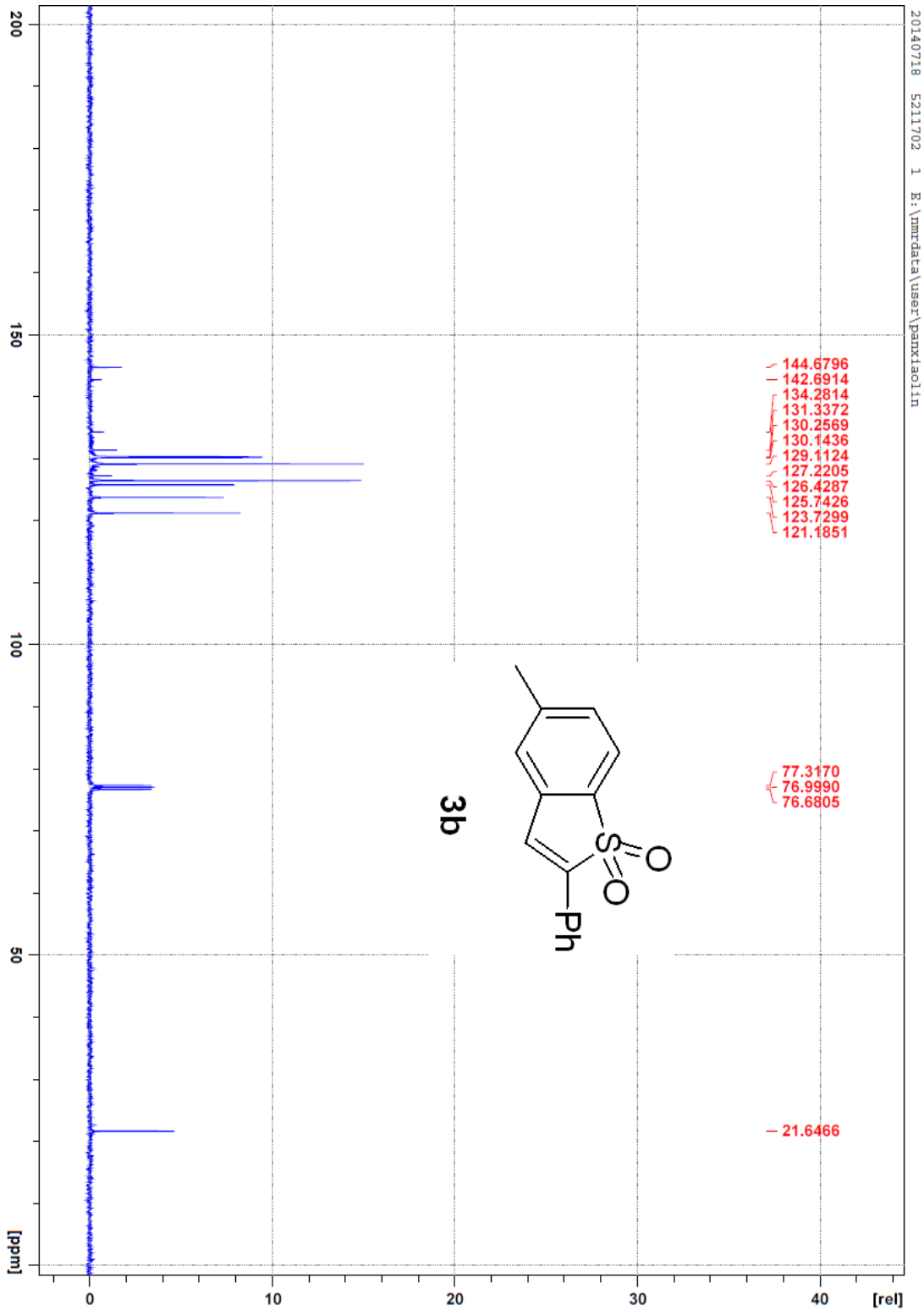
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134.2814
131.3372
130.2569
130.1436
129.1124
127.2205
126.4287
125.7426
123.7299
121.1851
77.3170
76.9990
76.6805
21.6466
3b
S
O
O
Ph
200
150
100
50
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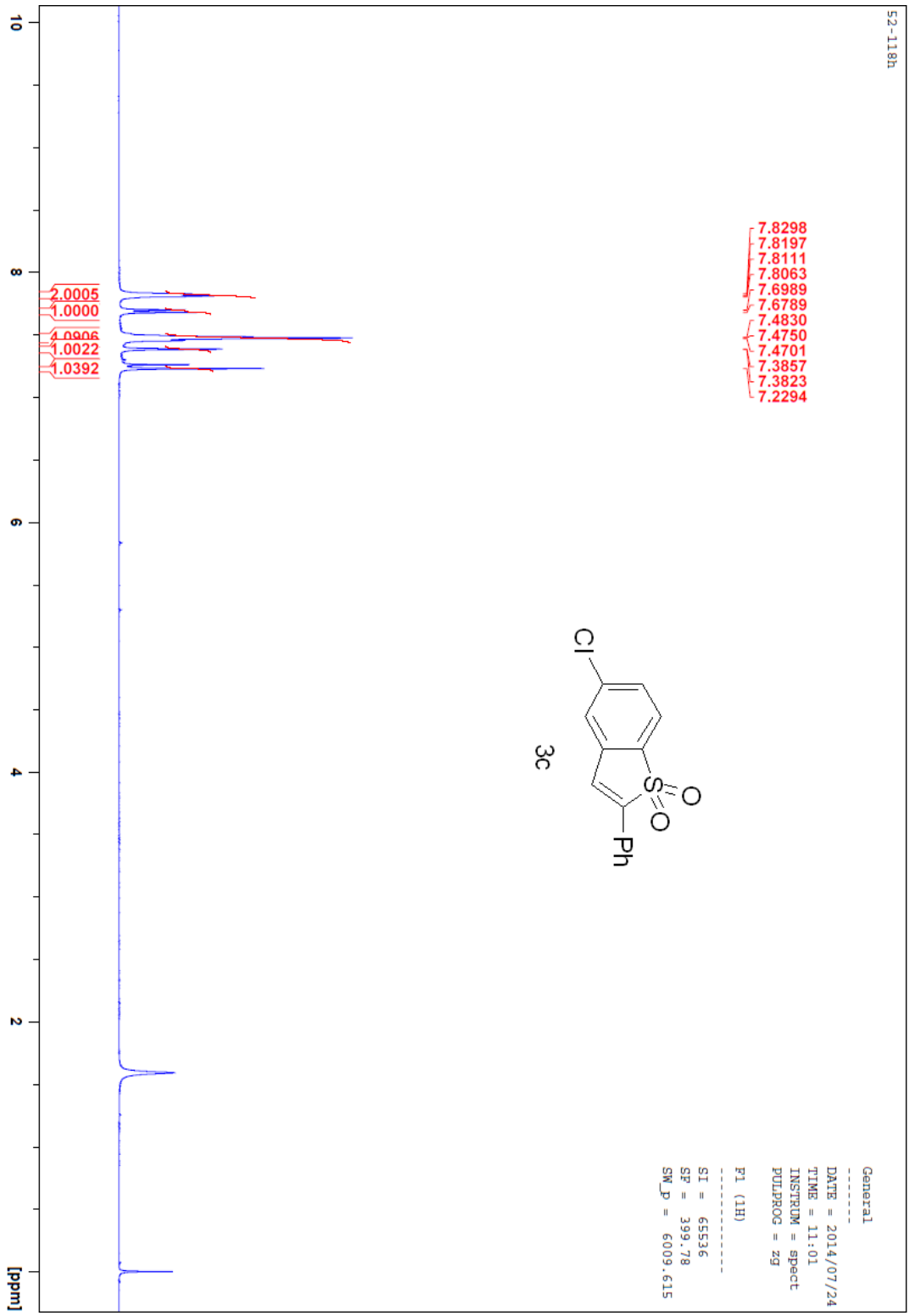
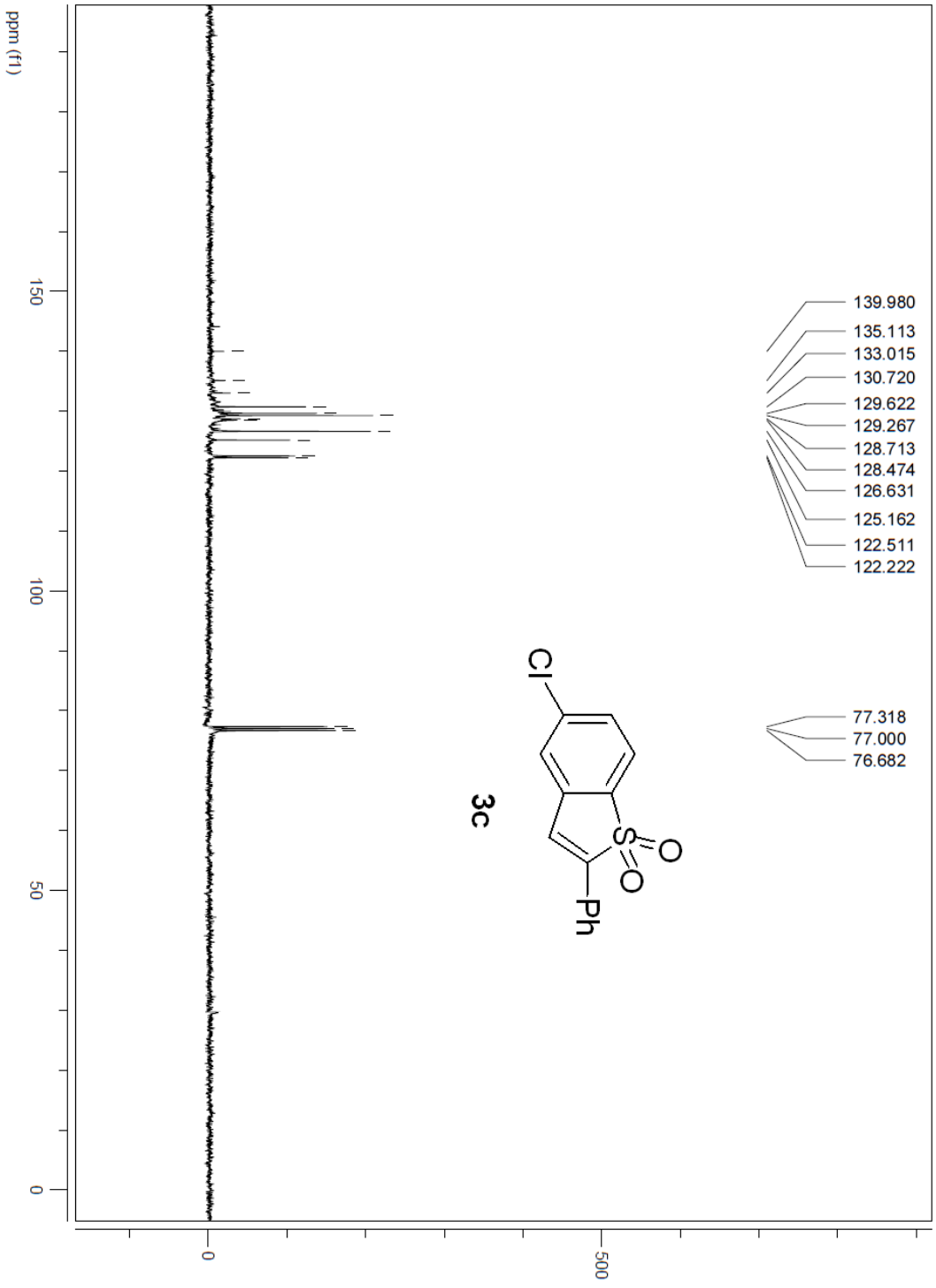
20
30
40
[rel]


20140724 521180601 1 E:\nmrdata\user\panxiaolin
52-118h
7.8298
7.8197
7.8111
7.8063
7.6989
7.6789
7.4830
7.4750
7.4701
7.3857
7.3823
7.2294
2.0005
1.0000
1.0006
1.0022
1.0392
Cl
O
S
O
Ph
3c
General
DATE = 2014/07/24
TIME = 11:01
INSTRUM = spect
PULPROG = zg
F1 (1H)
SI = 65536
SF = 399.78
SW_p = 6009.615
10
8
6
4
2
[ppm]


ppm (f1)
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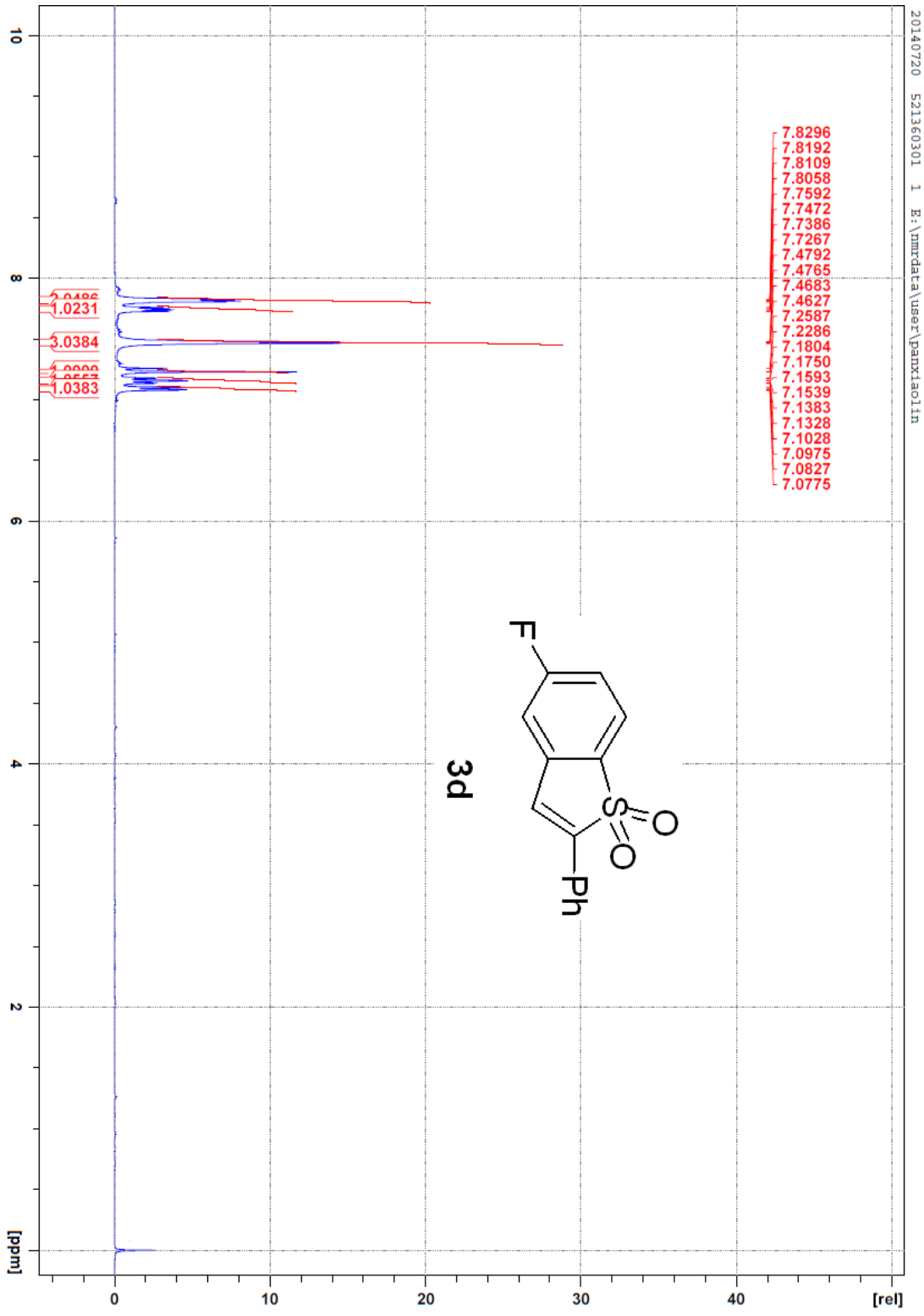
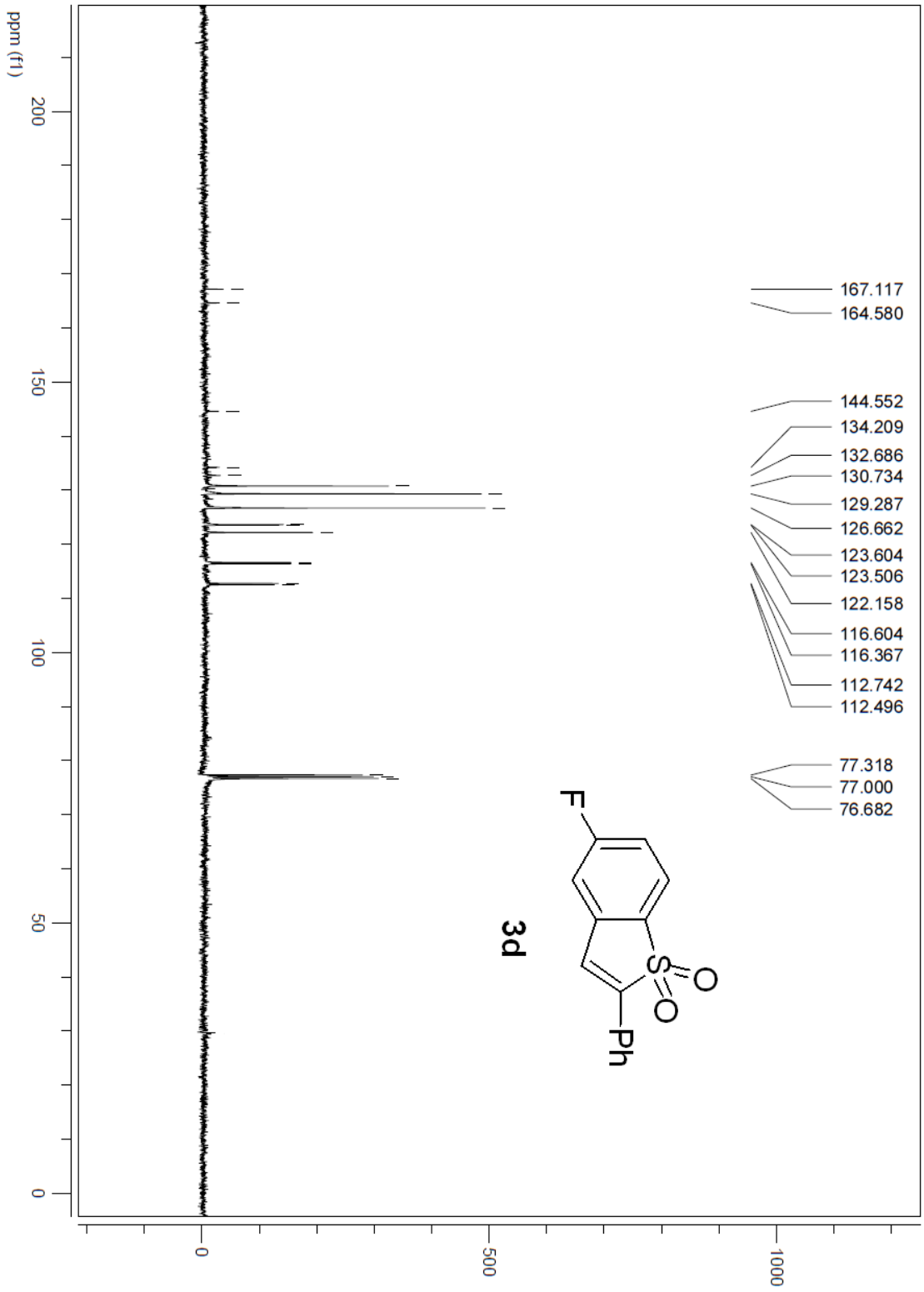
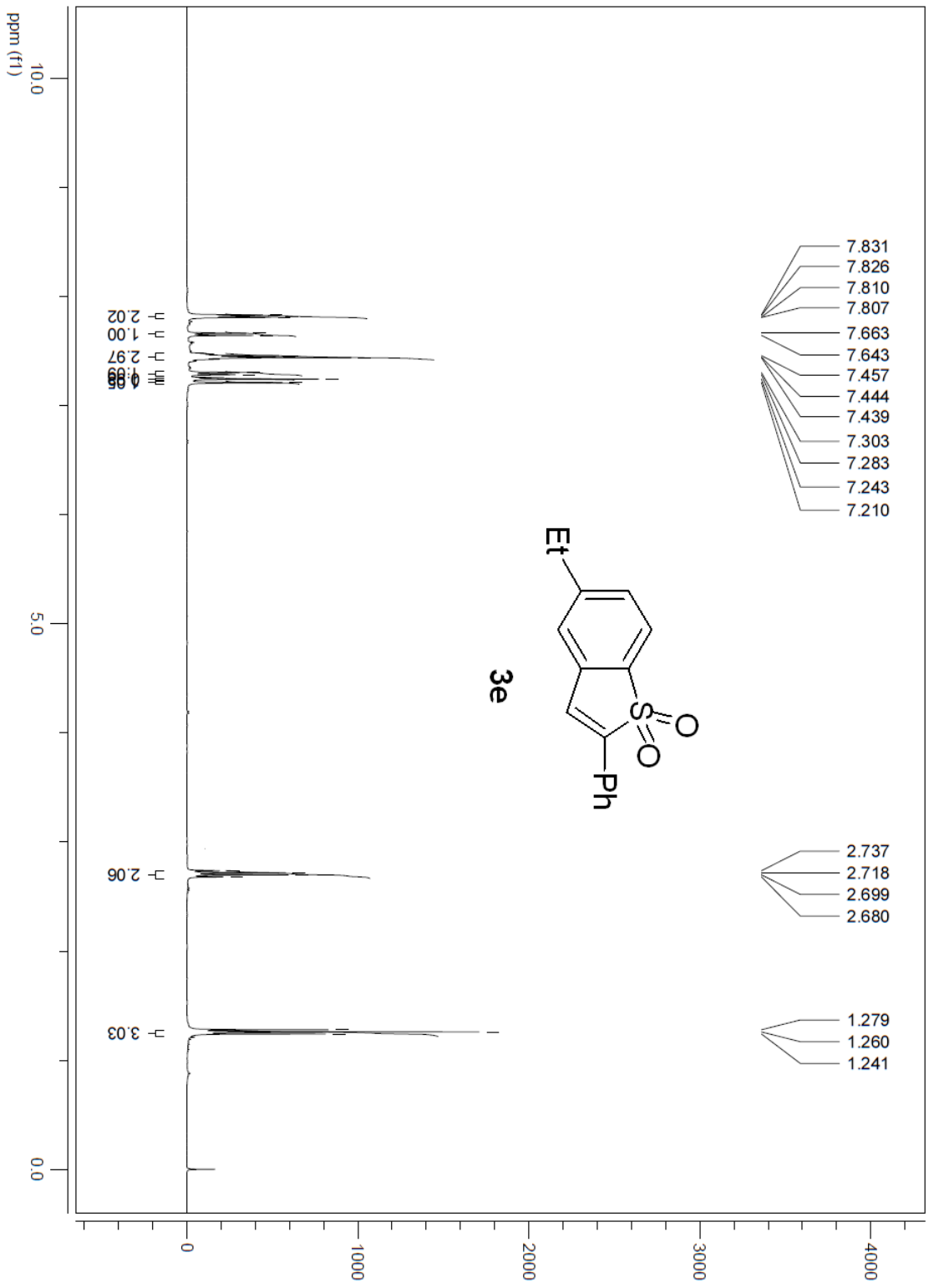
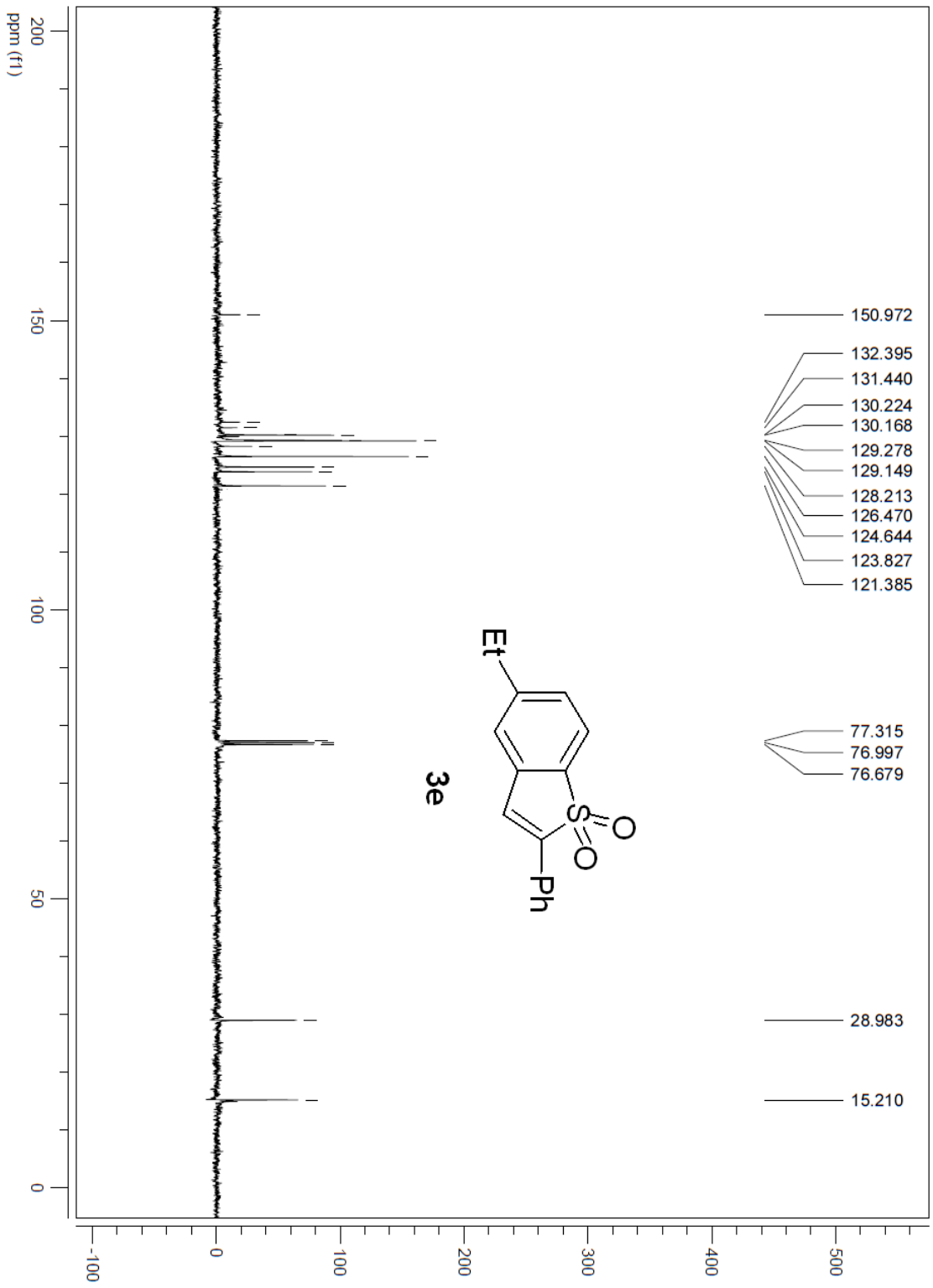
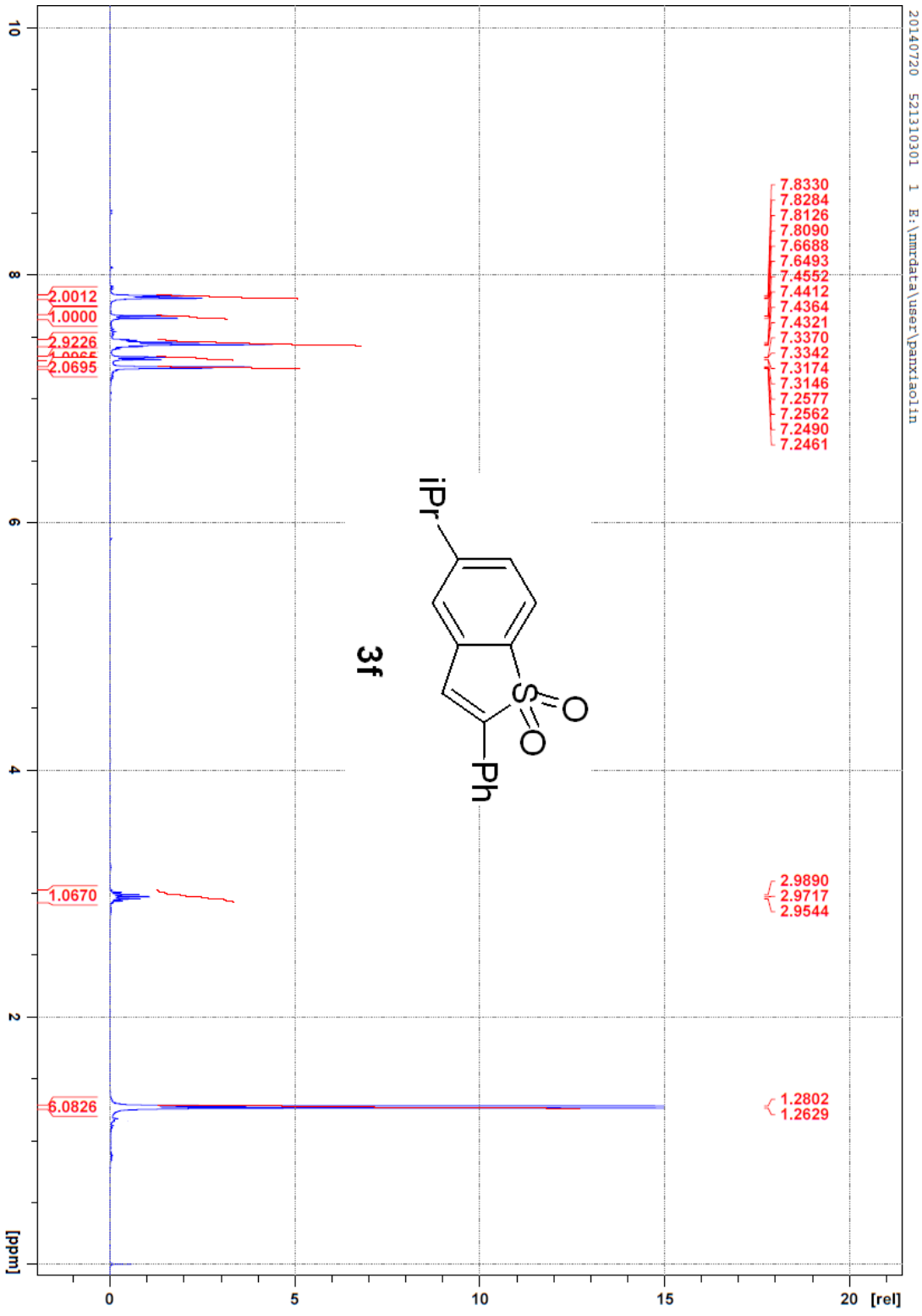
50
0
0
500
139.980
135.113
133.015
130.720
129.622
129.267
128.713
128.474
126.631
125.162
122.511
122.222
77.318
77.000
76.682
Cl
S
O
O
Ph
3c

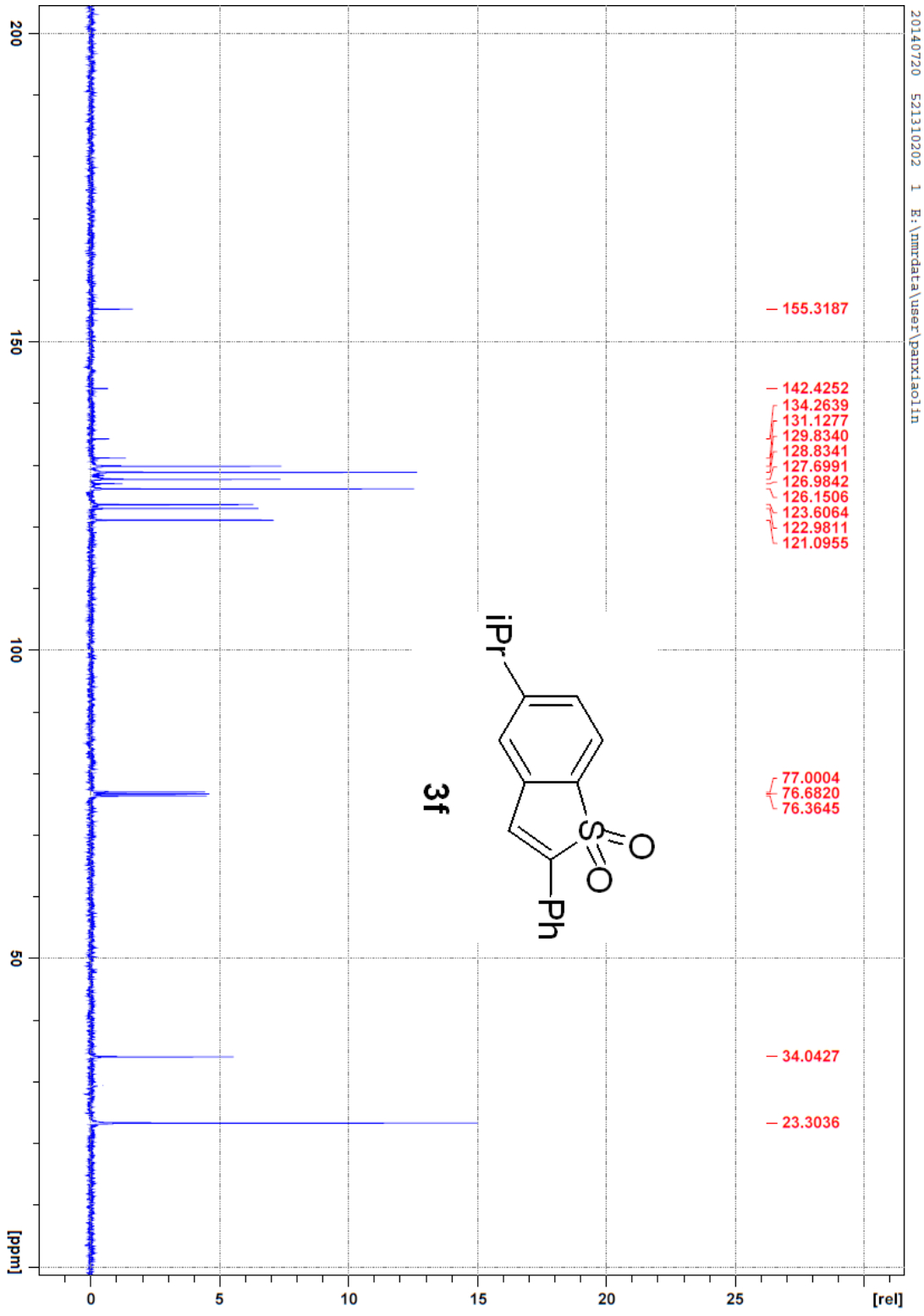

20140720 521360301 1 E:\nmrdata\user\panxiaolin
7.8296
7.8192
7.8109
7.8058
7.7592
7.7472
7.7386
7.7267
7.4792
7.4765
7.4683
7.4627
7.2587
7.2286
7.1804
7.1750
7.1593
7.1539
7.1383
7.1328
7.1028
7.0975
7.0827
7.0775
1.0231
3.0384
1.0383
3d
F
S
O
O
Ph
[ppm]
[rel]

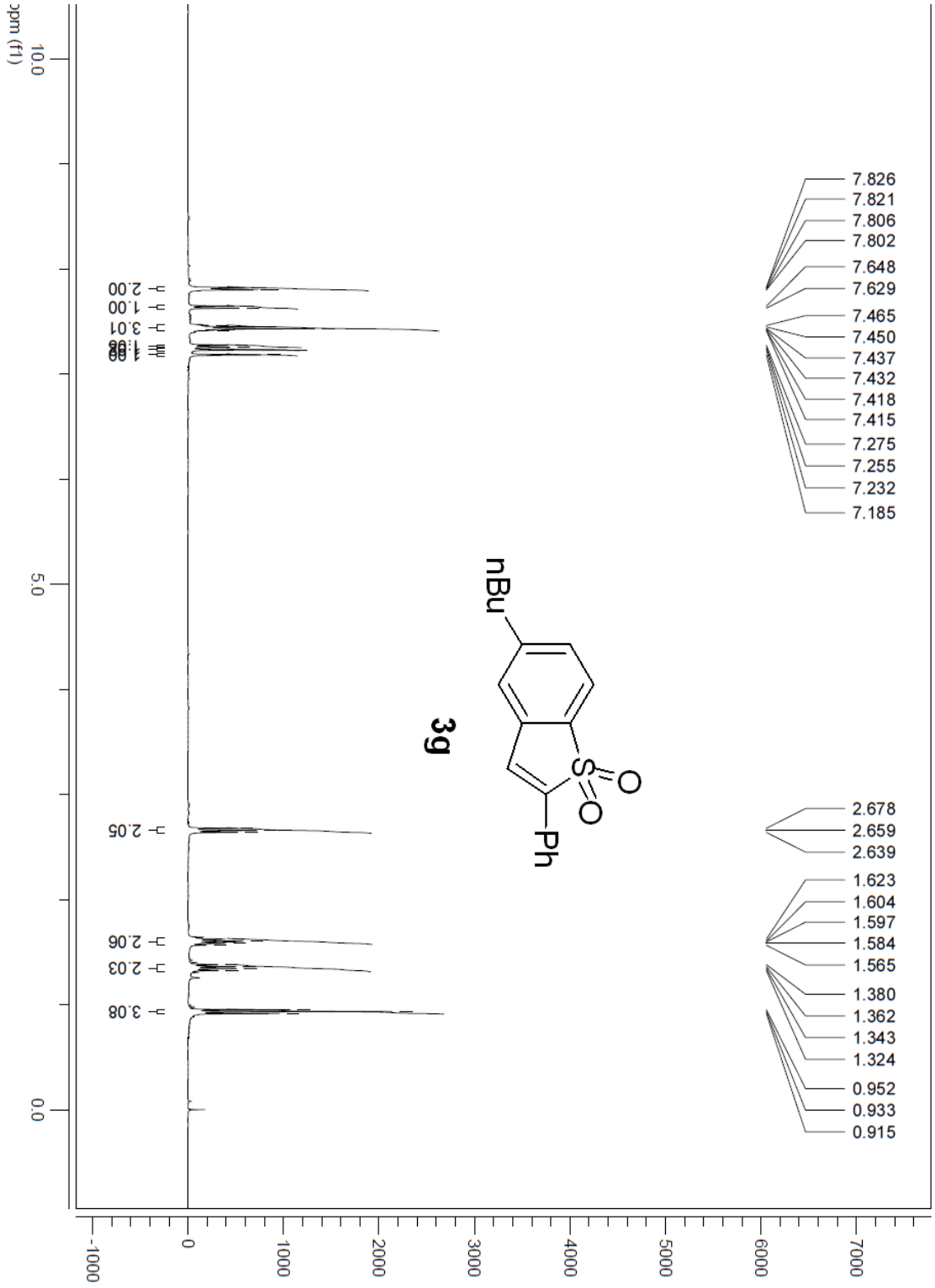

ppm (f1)
200
150
100
50
0
0
500
1000
167.117
164.580
144.552
134.209
132.686
130.734
129.287
126.662
123.604
123.506
122.158
116.604
116.367
112.742
112.496
77.318
77.000
76.682
F
S
O
O
Ph
3d

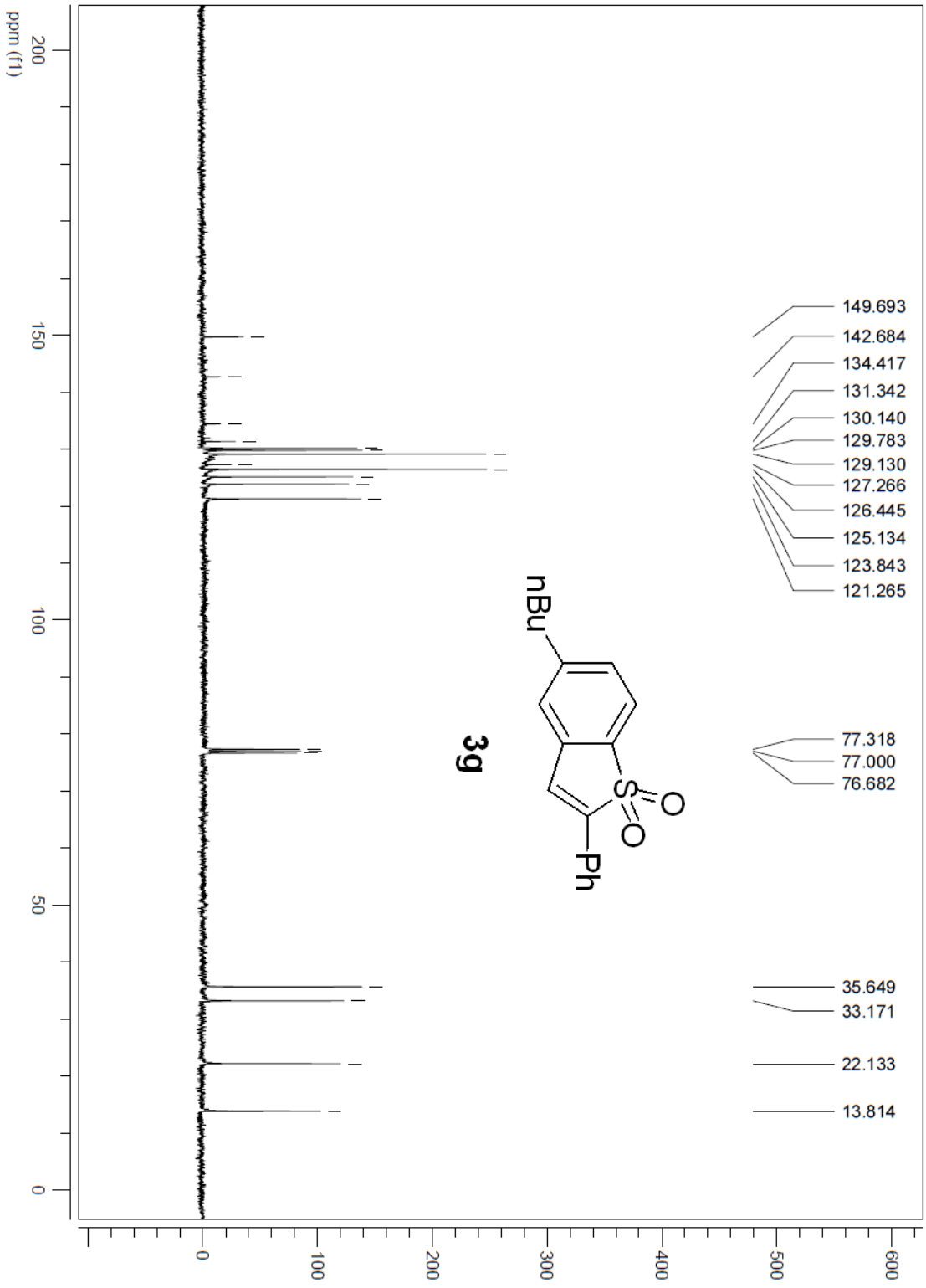

ppm (f1)
10.0
5.0
0.0
0
1000
2000
3000
4000
2.02
1.00
2.97
2.06
3.03
7.831
7.826
7.810
7.807
7.663
7.643
7.457
7.444
7.439
7.303
7.283
7.243
7.210
2.737
2.718
2.699
2.680
1.279
1.260
1.241
Et
S
O
O
Ph
3e

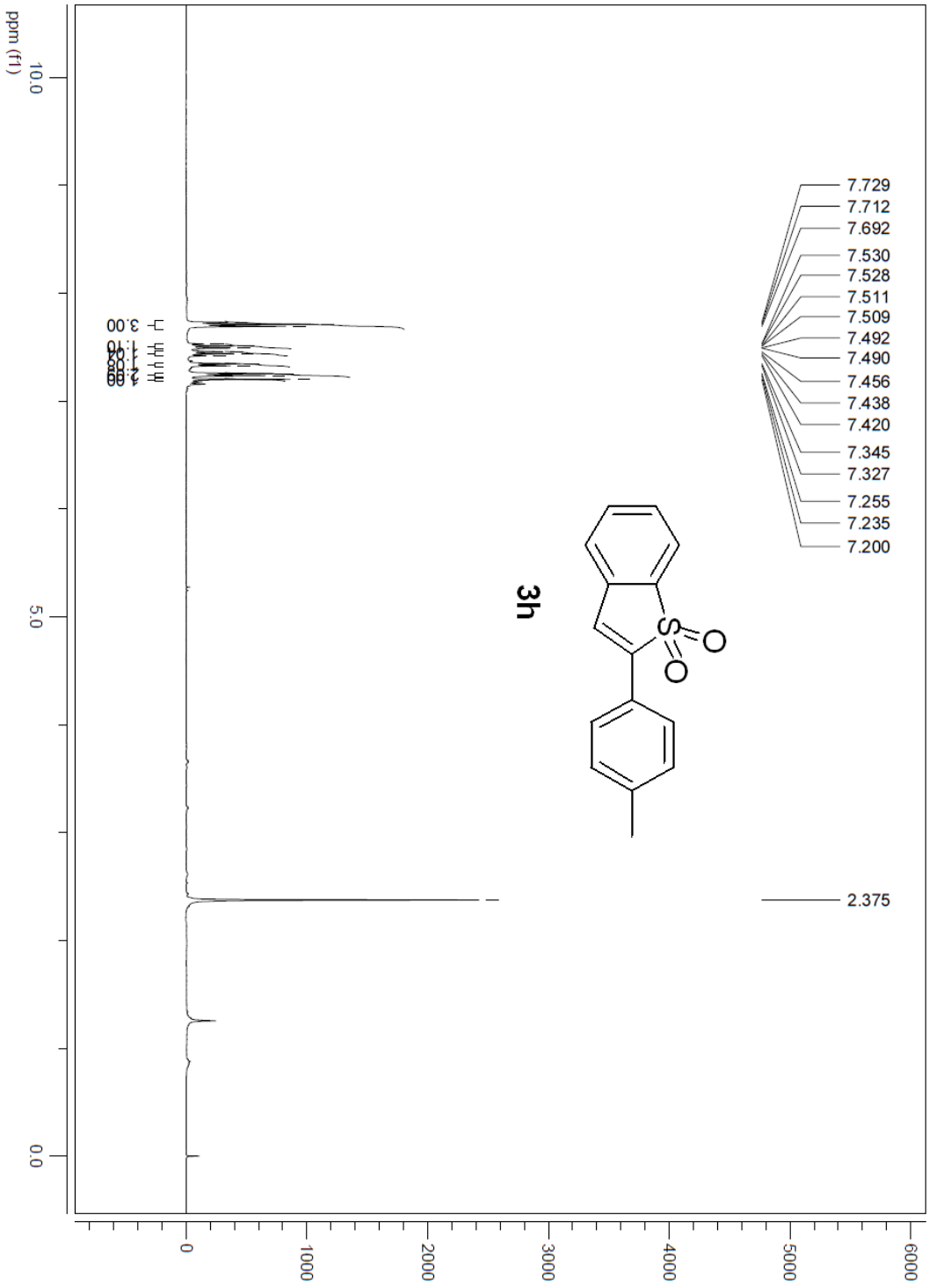

ppm (f1)
200
150
100
50
0
-100
0
100
200
300
400
500
150.972
132.395
131.440
130.224
130.168
129.278
129.149
128.213
126.470
124.644
123.827
121.385
77.315
76.997
76.679
28.983
15.210
Et
Ph
O
S
O
3e

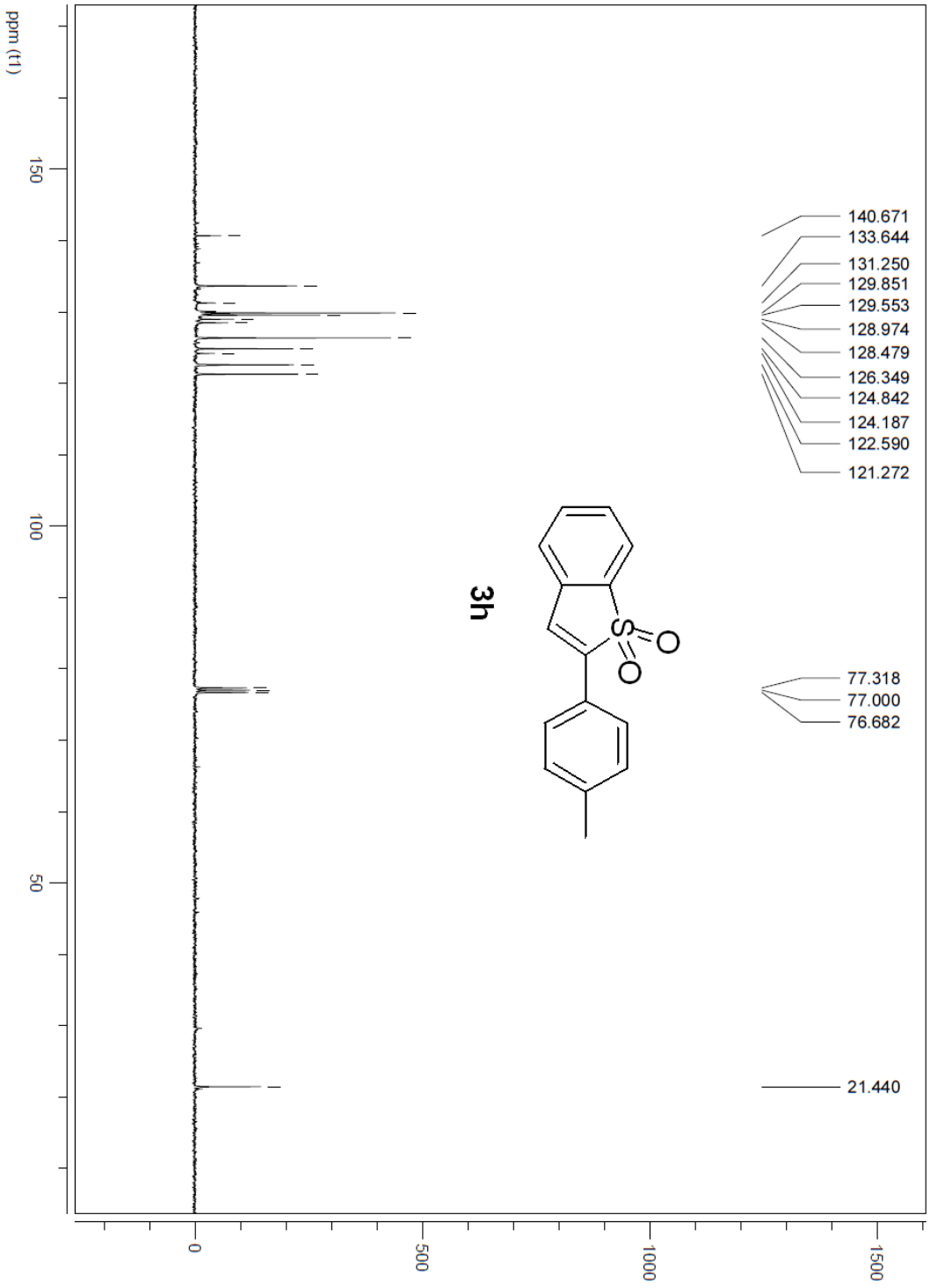

20140720 521310301 1 E:\nmrdata\user\panxiaolin
7.8330
7.8284
7.8126
7.8090
7.6688
7.6493
7.4552
7.4412
7.4364
7.4321
7.3370
7.3342
7.3174
7.3146
7.2577
7.2562
7.2490
7.2461
2.0012
1.0000
2.9226
2.0695
1.0670
6.0826
2.9890
2.9717
2.9544
1.2802
1.2629
iPr
Ph
S
O
O
3f
[ppm]
[rel]

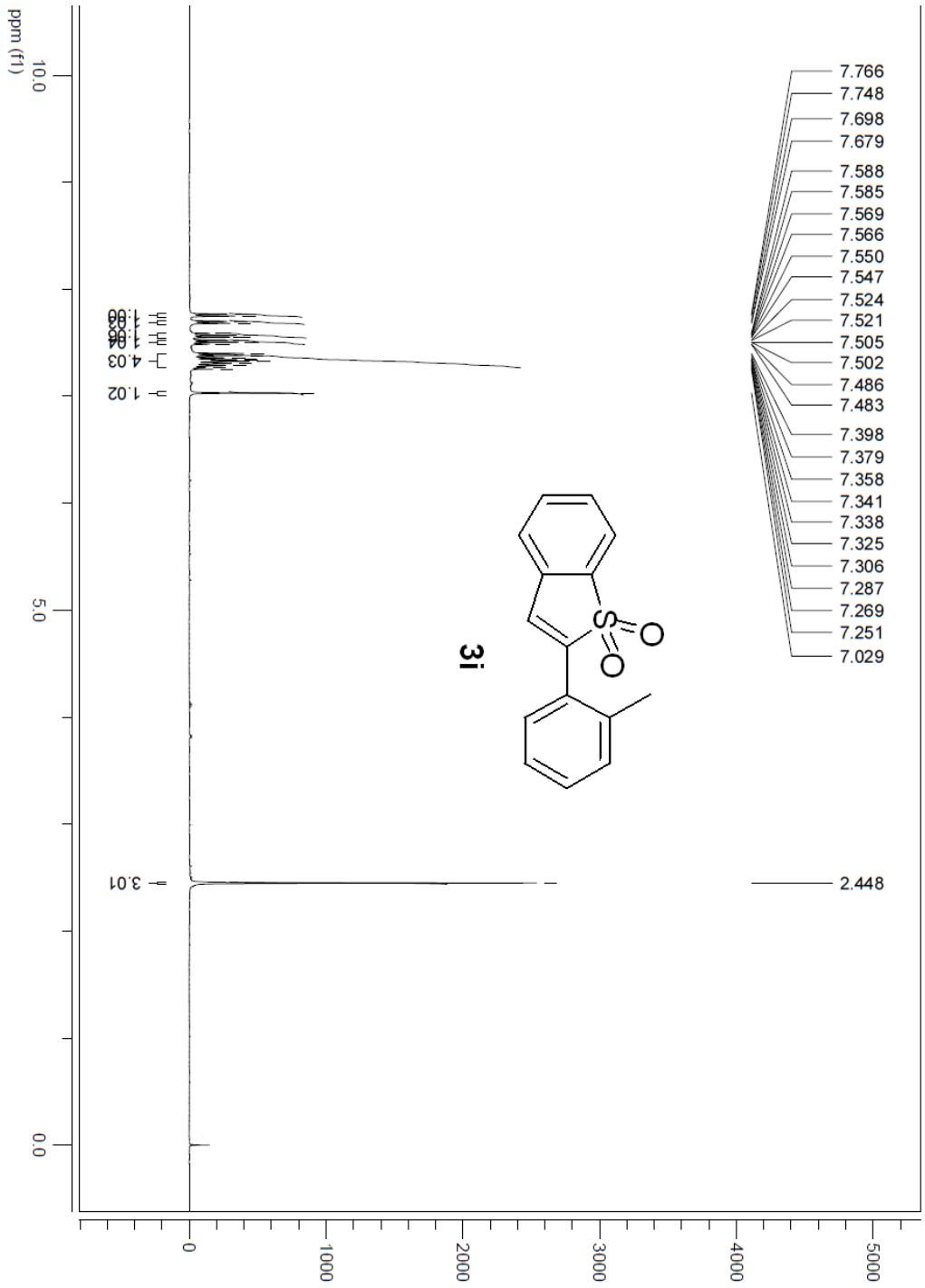

20140720 521310202 1 E:\nmrdata\user\panxiaolin
155.3187
142.4252
134.2639
131.1277
129.8340
128.8341
127.6991
126.9842
126.1506
123.6064
122.9811
121.0955
77.0004
76.6820
76.3645
34.0427
23.3036
iPr
Ph
O
O
S
3f
[ppm]
[rel]
200
150
100
50
0
5
10
15
20
25


7.826
7.821
7.806
7.802
7.648
7.629
7.465
7.450
7.437
7.432
7.418
7.415
7.275
7.255
7.232
7.185
2.678
2.659
2.639
1.623
1.604
1.597
1.584
1.565
1.380
1.362
1.343
1.324
0.952
0.933
0.915
nBu
Ph
O
O
S
3g


ppm (f1)
200
150
100
50
0
0
100
200
300
400
500
600
149.693
142.684
134.417
131.342
130.140
129.783
129.130
127.266
126.445
125.134
123.843
121.265
77.318
77.000
76.682
35.649
33.171
22.133
13.814
nBu
Ph
O
O
S
3g


ppm (f1)
10.0
5.0
0.0
0
1000
2000
3000
4000
5000
6000
3.00
7.729
7.712
7.692
7.530
7.528
7.511
7.509
7.492
7.490
7.456
7.438
7.420
7.345
7.327
7.255
7.235
7.200
2.375
3h
S
O
O


ppm (t1)
150
100
50
0
500
1000
1500
140.671
133.644
131.250
129.851
129.553
128.974
128.479
126.349
124.842
124.187
122.590
121.272
77.318
77.000
76.682
21.440
3h
S
O
O


ppm (f1)
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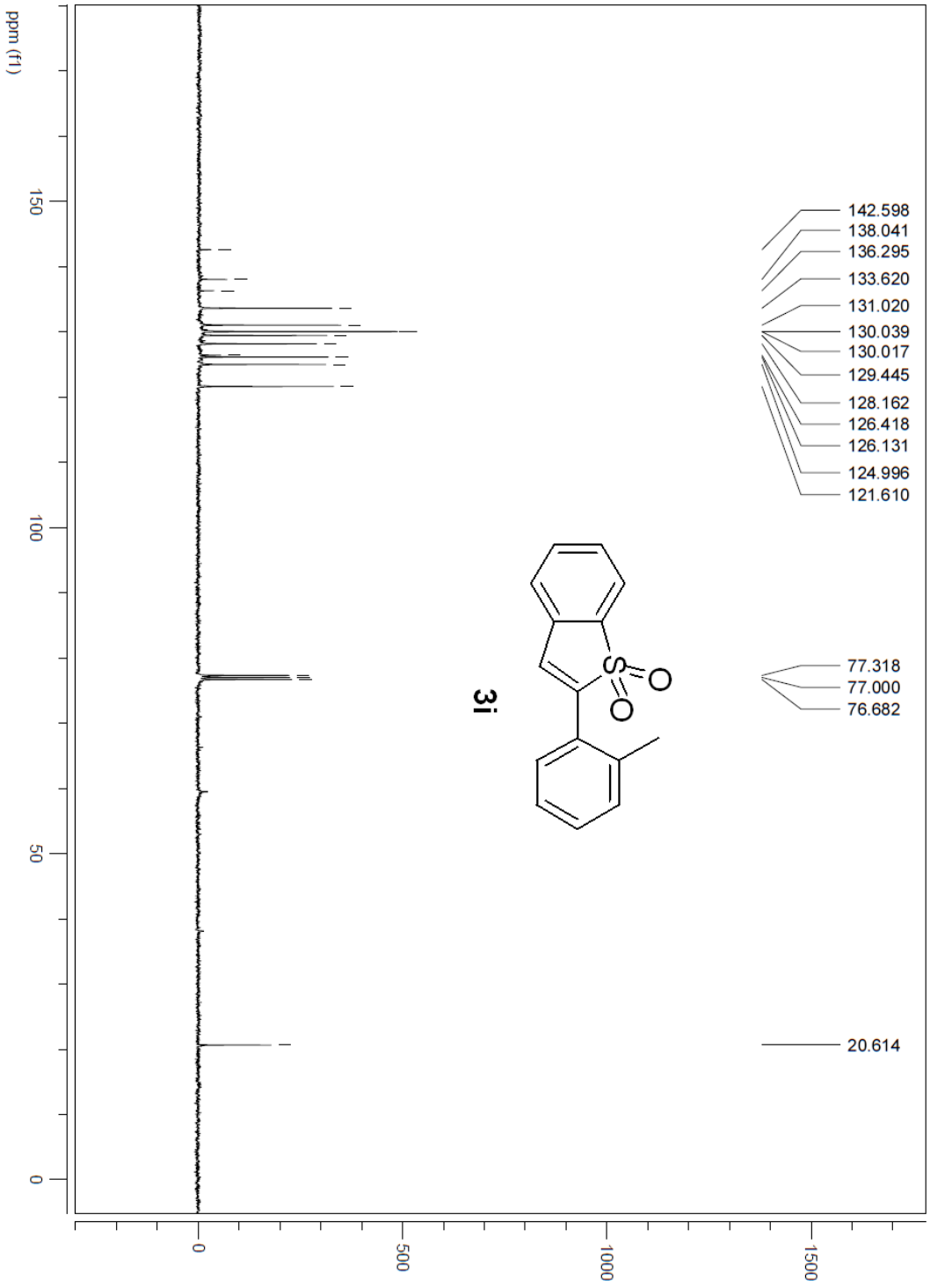
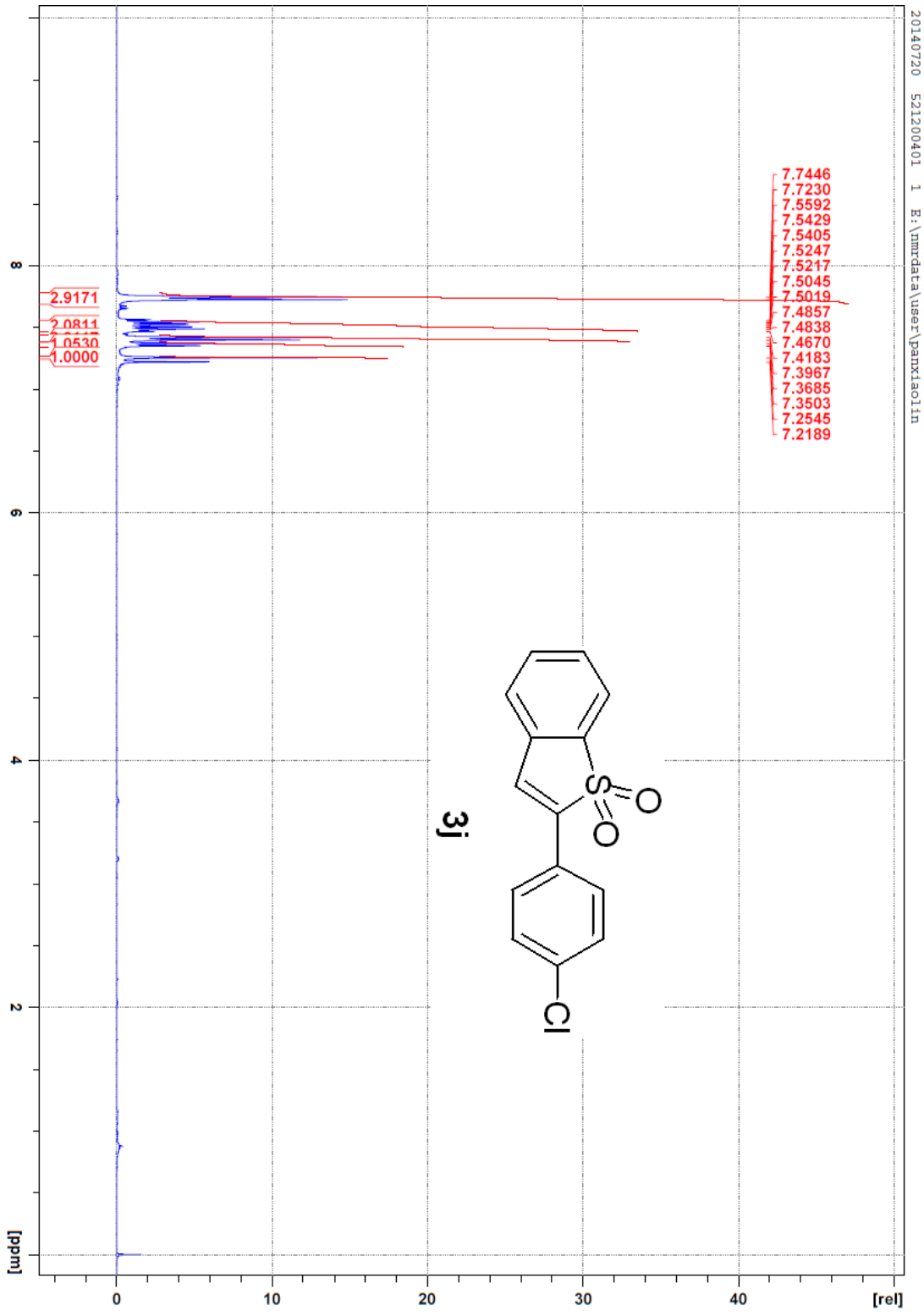
5.0
0.0
0
1000
2000
3000
4000
5000
7.766
7.748
7.698
7.679
7.588
7.585
7.569
7.566
7.550
7.547
7.524
7.521
7.505
7.502
7.486
7.483
7.398
7.379
7.358
7.341
7.338
7.325
7.306
7.287
7.269
7.251
7.029
2.448
3.01
1.02
4.03
3i
S
O
O


ppm (f1)
150
100
50
0
0
500
1000
1500
142.598
138.041
136.295
133.620
131.020
130.039
130.017
129.445
128.162
126.418
126.131
124.996
121.610
77.318
77.000
76.682
20.614
3i
S
O
O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7.7230
7.5592
7.5429
7.5405
7.5247
7.5217
7.5045
7.5019
7.4857
7.4838
7.4670
7.4183
7.3967
7.3685
7.3503
7.2545
7.2189
2.9171
2.0811
1.0530
1.0000
3j
S
O
O
Cl
8
6
4
2
[ppm]
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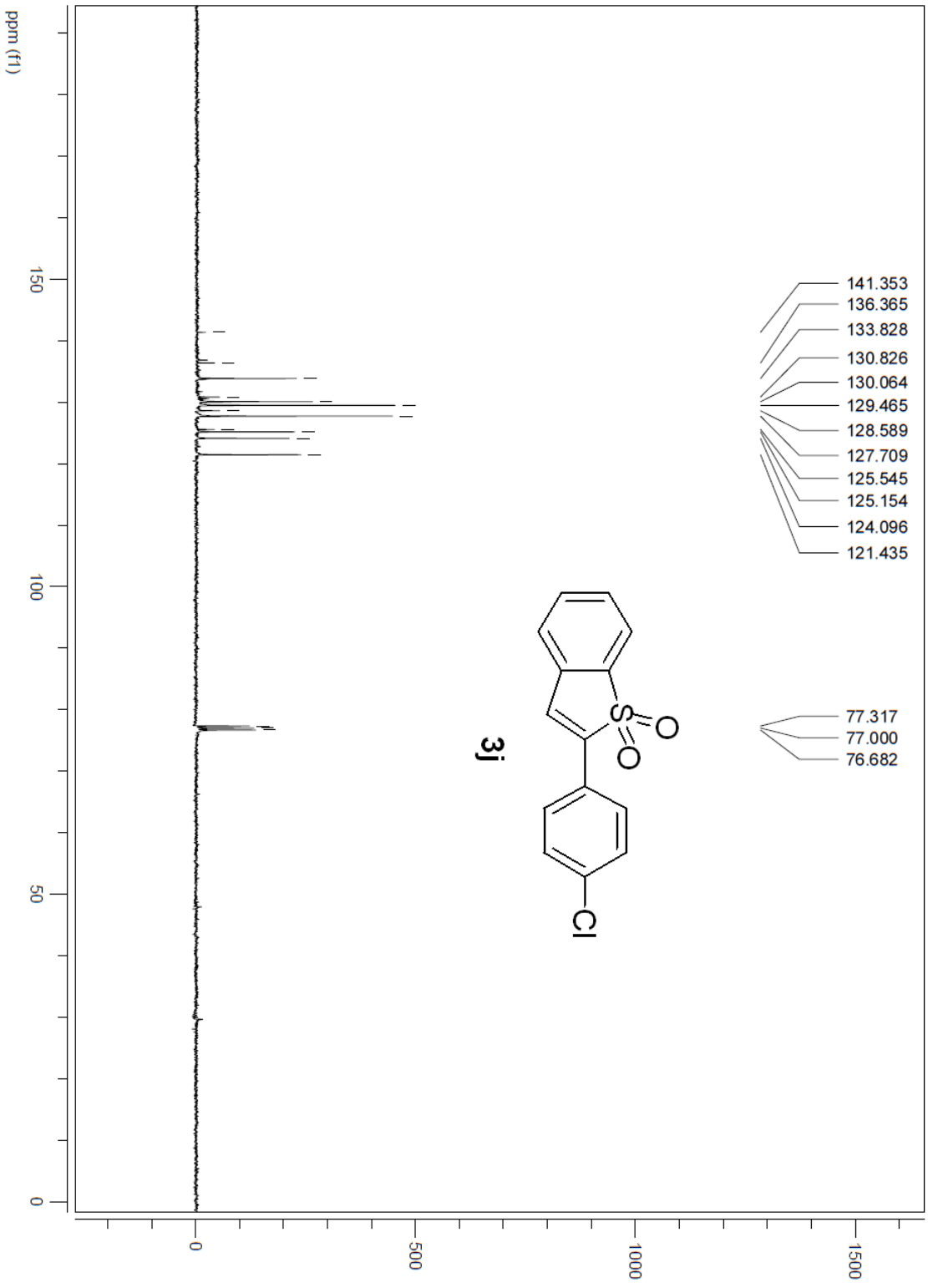
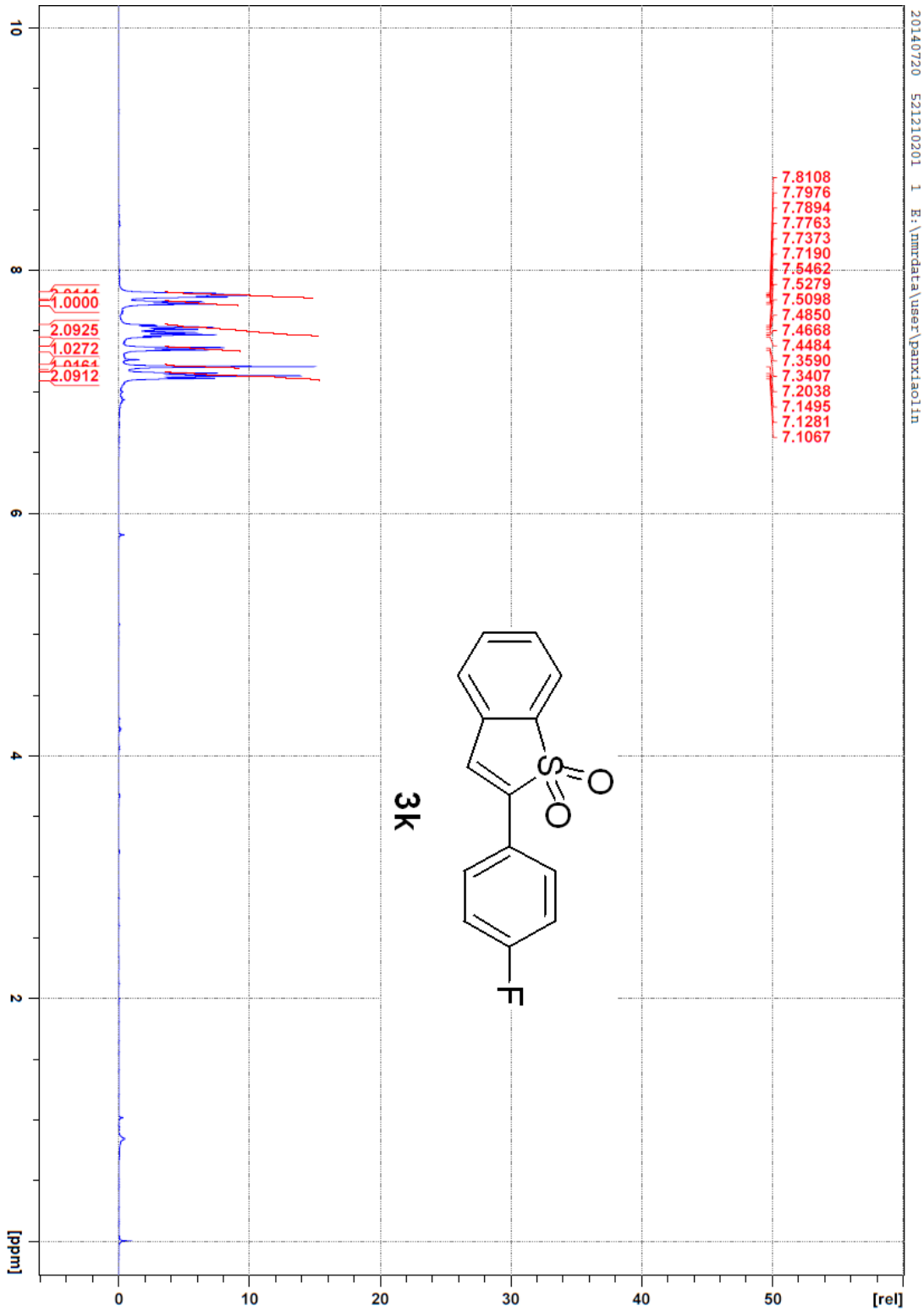
10
20
30
40
[rel]


ppm (f1)
150
100
50
0
0
500
1000
1500
141.353
136.365
133.828
130.826
130.064
129.465
128.589
127.709
125.545
125.154
124.096
121.435
77.317
77.000
76.682
3j
S
O
O
Cl


20140720 521210201 1 E:\nmrdata\user\panxiaolin
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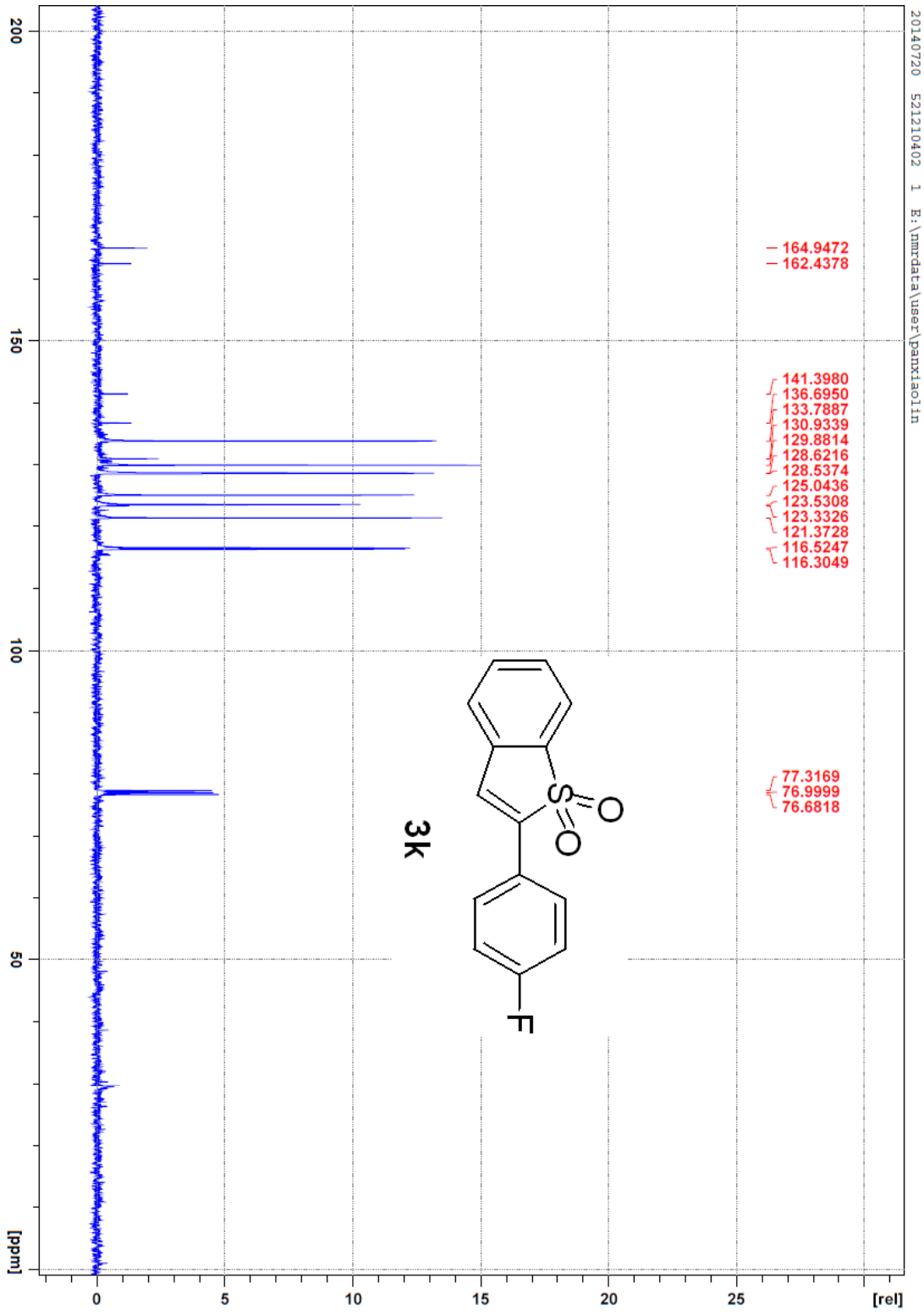
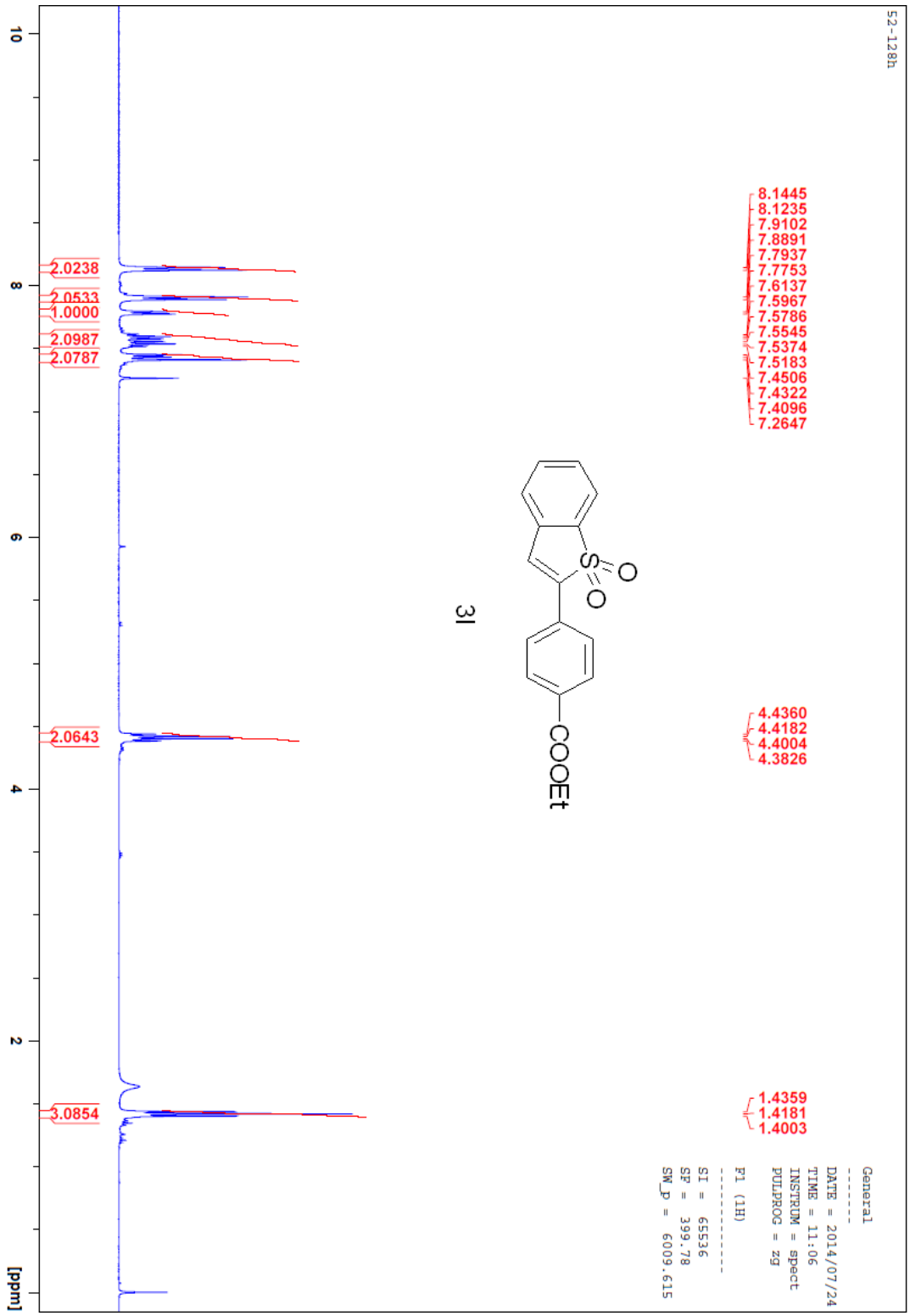
7.7976
7.7894
7.7763
7.7373
7.7190
7.5462
7.5279
7.5098
7.4850
7.4668
7.4484
7.3590
7.3407
7.2038
7.1495
7.1281
7.1067
1.0000
2.0925
1.0272
2.0912
3k
S
O
O
F
[ppm]
[rel]


20140720 521210402 1 E:\nmrdata\user\panxiaolin
164.9472
162.4378
141.3980
136.6950
133.7887
130.9339
129.8814
128.6216
128.5374
125.0436
123.5308
123.3326
121.3728
116.5247
116.3049
77.3169
76.9999
76.6818
3k
O
S
O
F
200
150
100
50
[ppm]
0
5
10
15
20
25
[rel]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52-128h
General
DATE = 2014/07/24
TIME = 11:06
INSTRUM = spect
PULPROG = zg
F1 (1H)
SI = 65536
SF = 399.78
SW_p = 6009.615
8.1445
8.1235
7.9102
7.8891
7.7937
7.7753
7.6137
7.5967
7.5786
7.5545
7.5374
7.5183
7.4506
7.4322
7.4096
7.2647
4.4360
4.4182
4.4004
4.3826
1.4359
1.4181
1.4003
2.0238
2.0533
1.0000
2.0987
2.0787
2.0643
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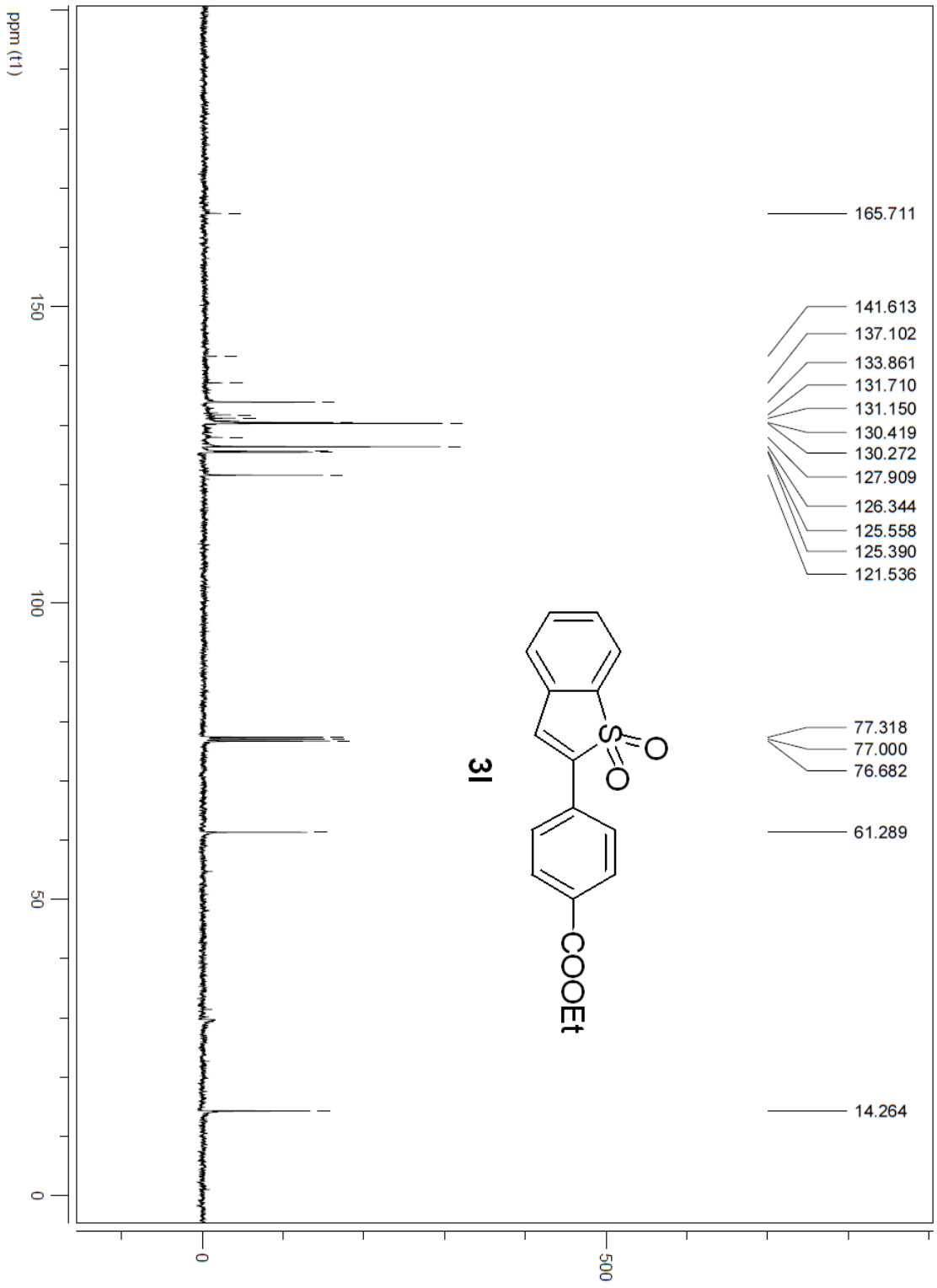
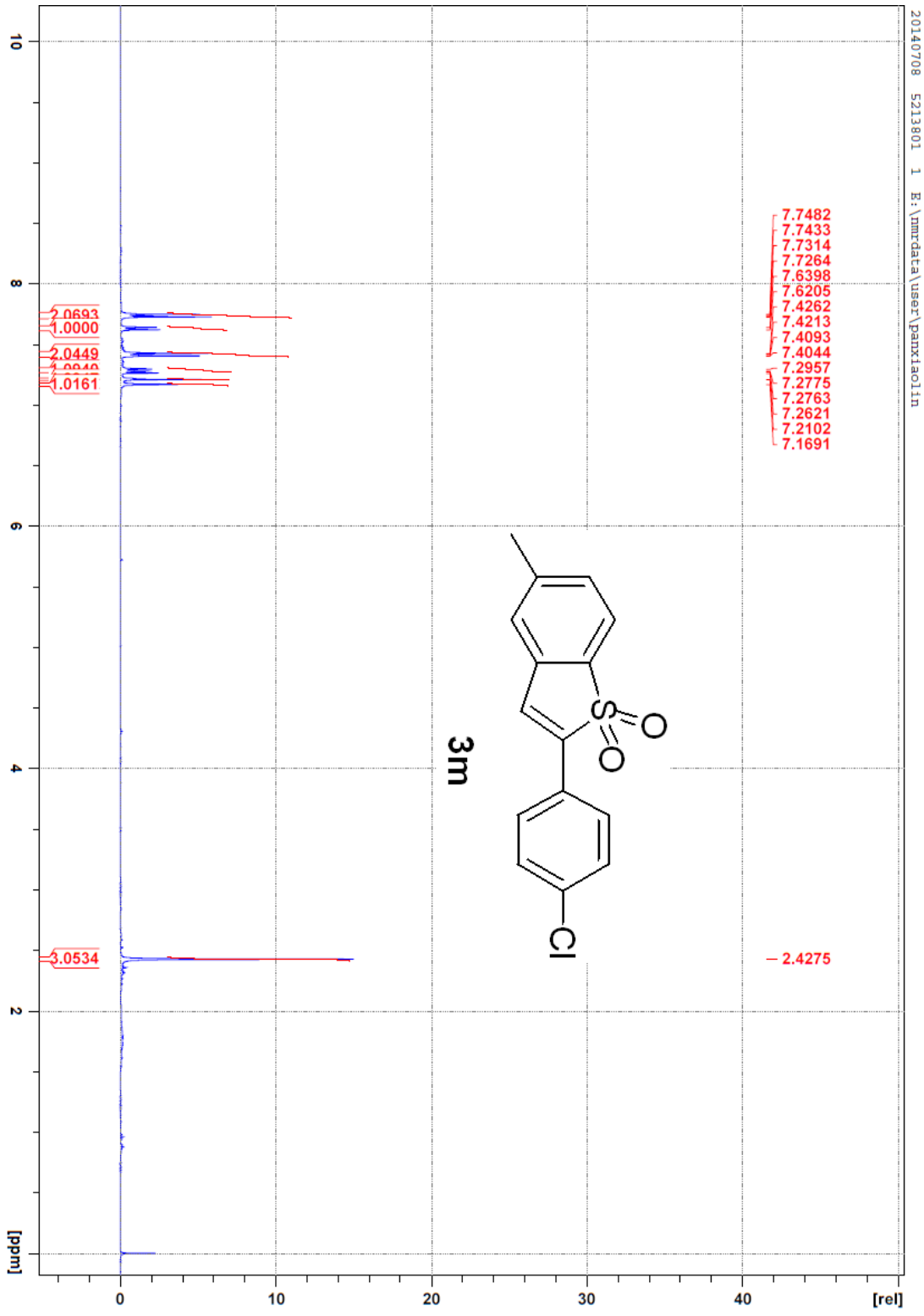
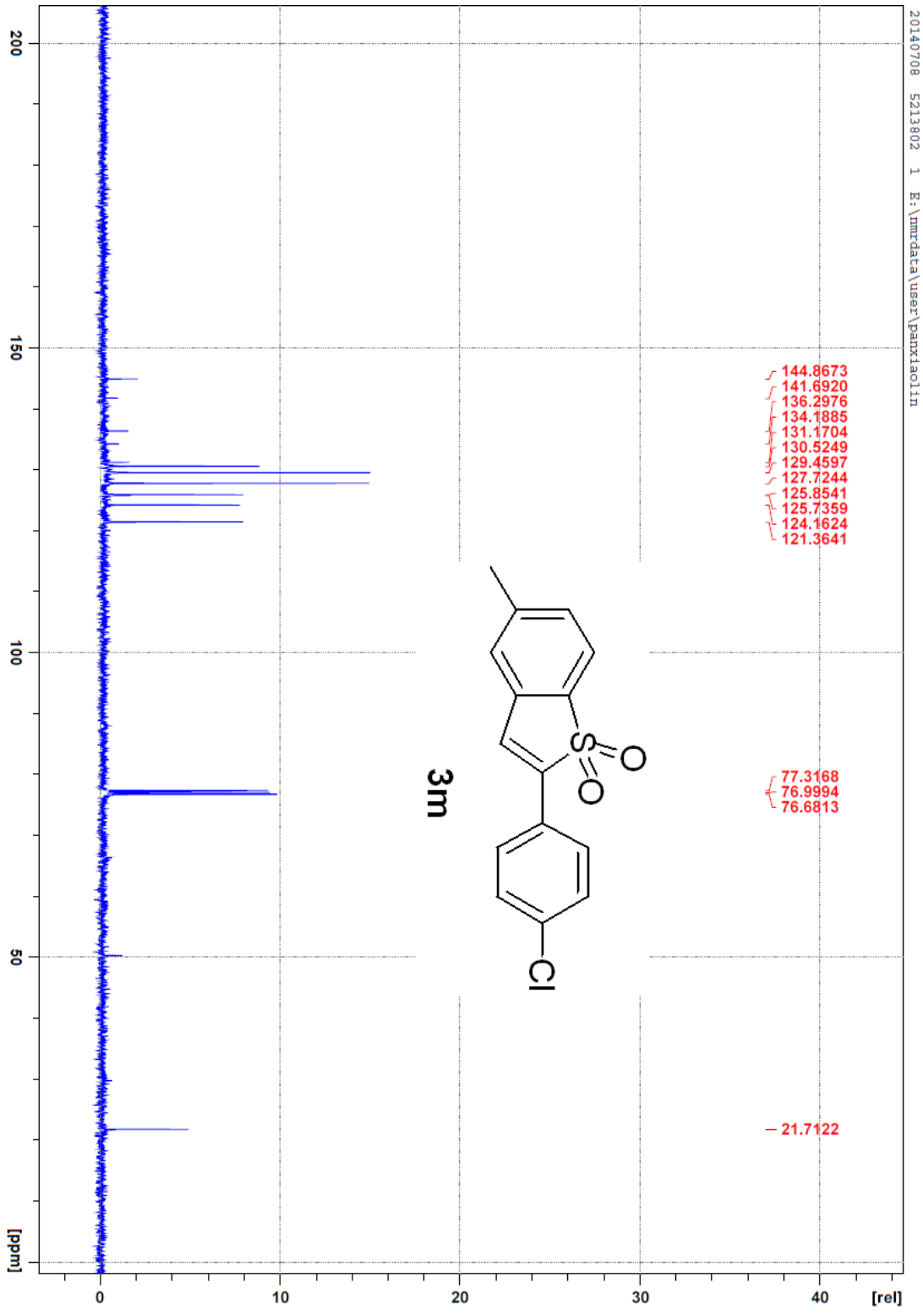
3l
COOEt
[ppm]


ppm (t1)
150
100
50
0
0
500
165.711
141.613
137.102
133.861
131.710
131.150
130.419
130.272
127.909
126.344
125.558
125.390
121.536
77.318
77.000
76.682
61.289
14.264
3l
S
O
O
COOEt


20140708 5213801 1 E:\nmrdata\user\panxiaolin
7.7482
7.7433
7.7314
7.7264
7.6398
7.6205
7.4262
7.4213
7.4093
7.4044
7.2957
7.2775
7.2763
7.2621
7.2102
7.1691
2.0693
1.0000
2.0449
1.0161
3.0534
2.4275
3m
O
S
O
Cl
[ppm]
[rel]


20140708 5213802 1 E:\nmrdata\user\panxiaolin
144.8673
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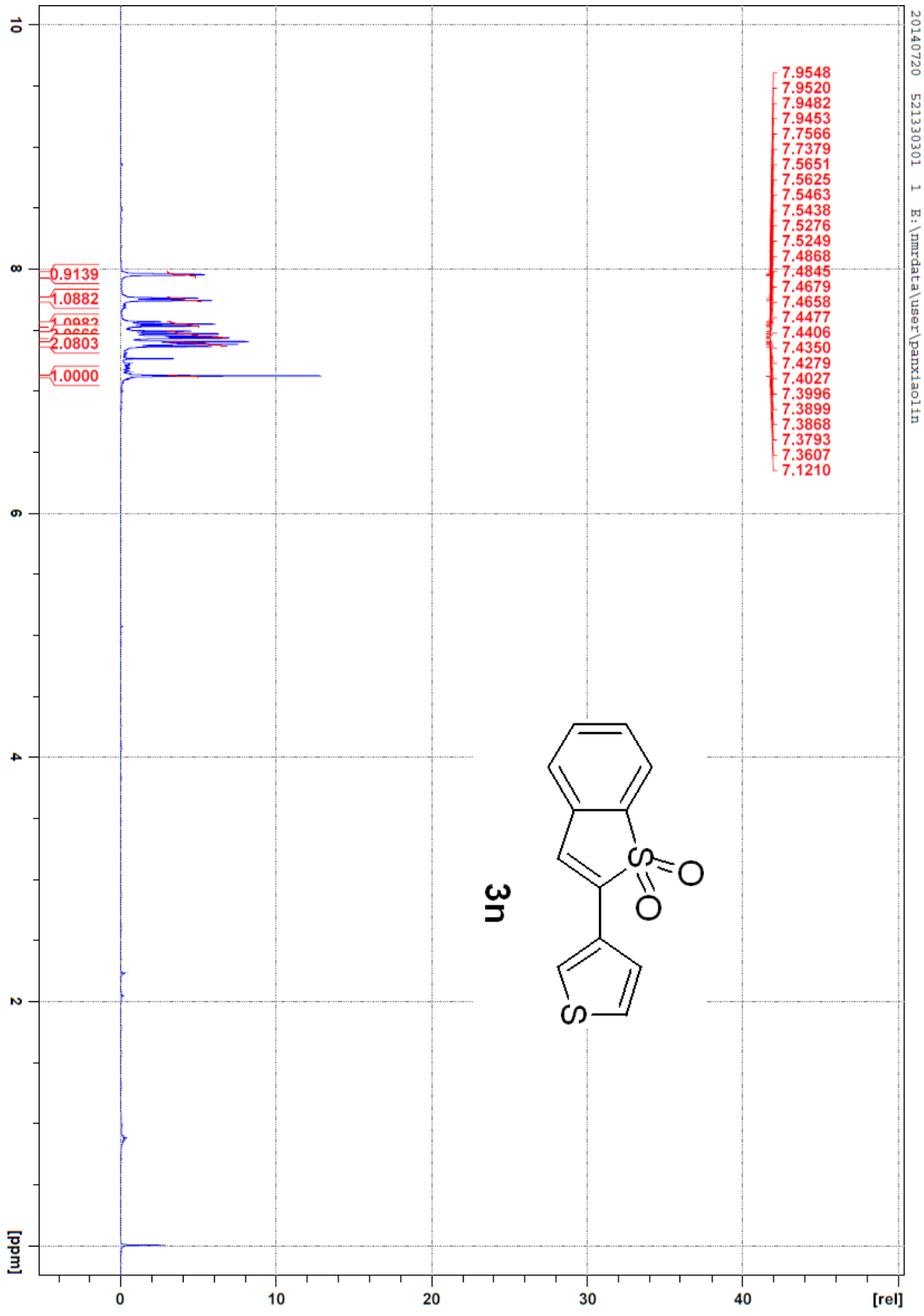
136.2976
134.1885
131.1704
130.5249
129.4597
127.7244
125.8541
125.7359
124.1624
121.3641
77.3168
76.9994
76.6813
21.7122
3m
O
O
S
Cl
200
150
100
50
[ppm]
0
10
20
30
40
[rel]


20140720 521330301 1 E:\nmrdata\user\panxiaolin
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7.9520
7.9482
7.9453
7.7566
7.7379
7.5651
7.5625
7.5463
7.5438
7.5276
7.5249
7.4868
7.4845
7.4679
7.4658
7.4477
7.4406
7.4350
7.4279
7.4027
7.3996
7.3899
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7.3793
7.3607
7.1210
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1.0882
2.0803
1.0000
3n
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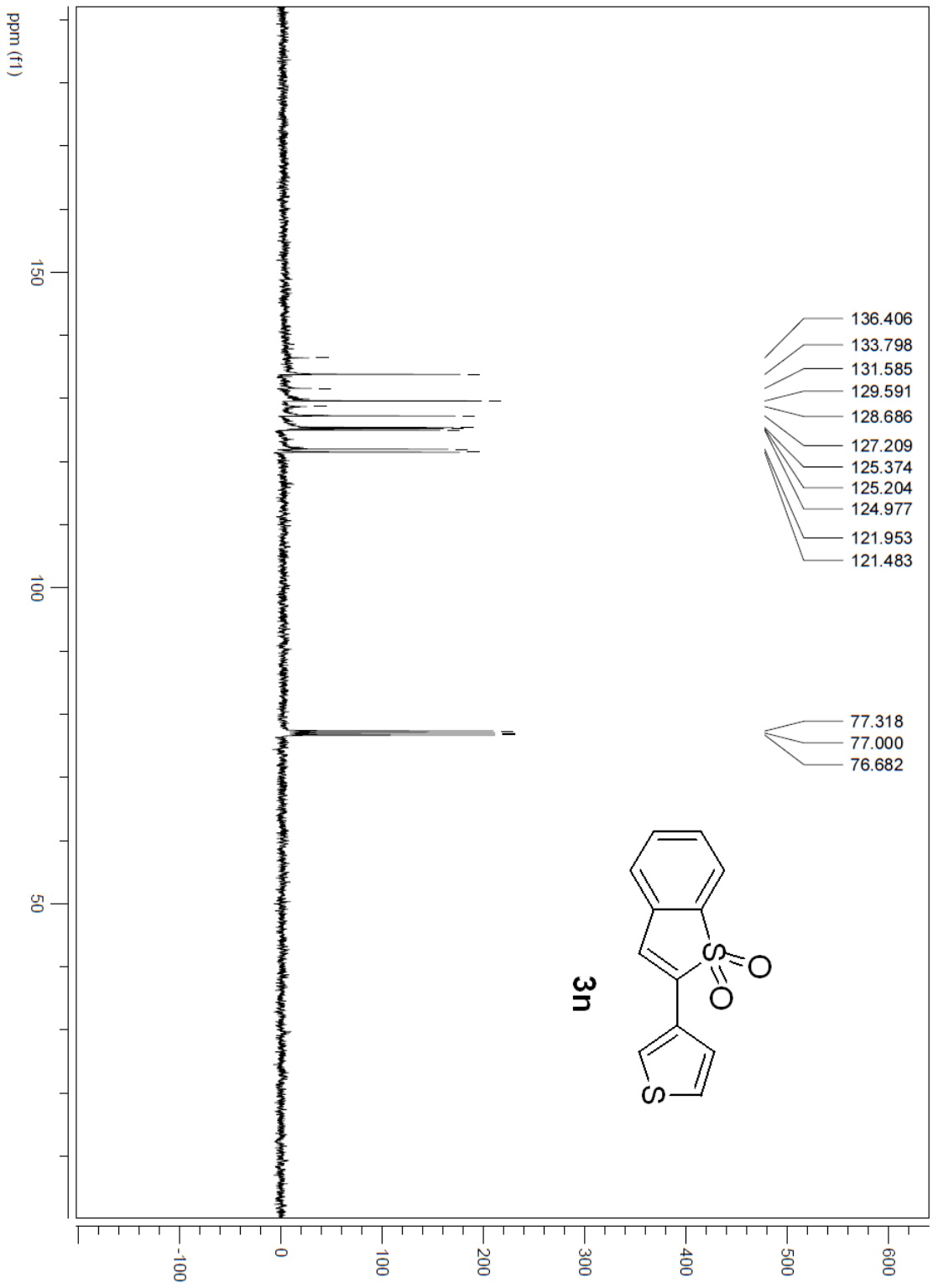
[rel]


ppm (f1)
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100
50
-100
0
100
200
300
400
500
600
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133.798
131.585
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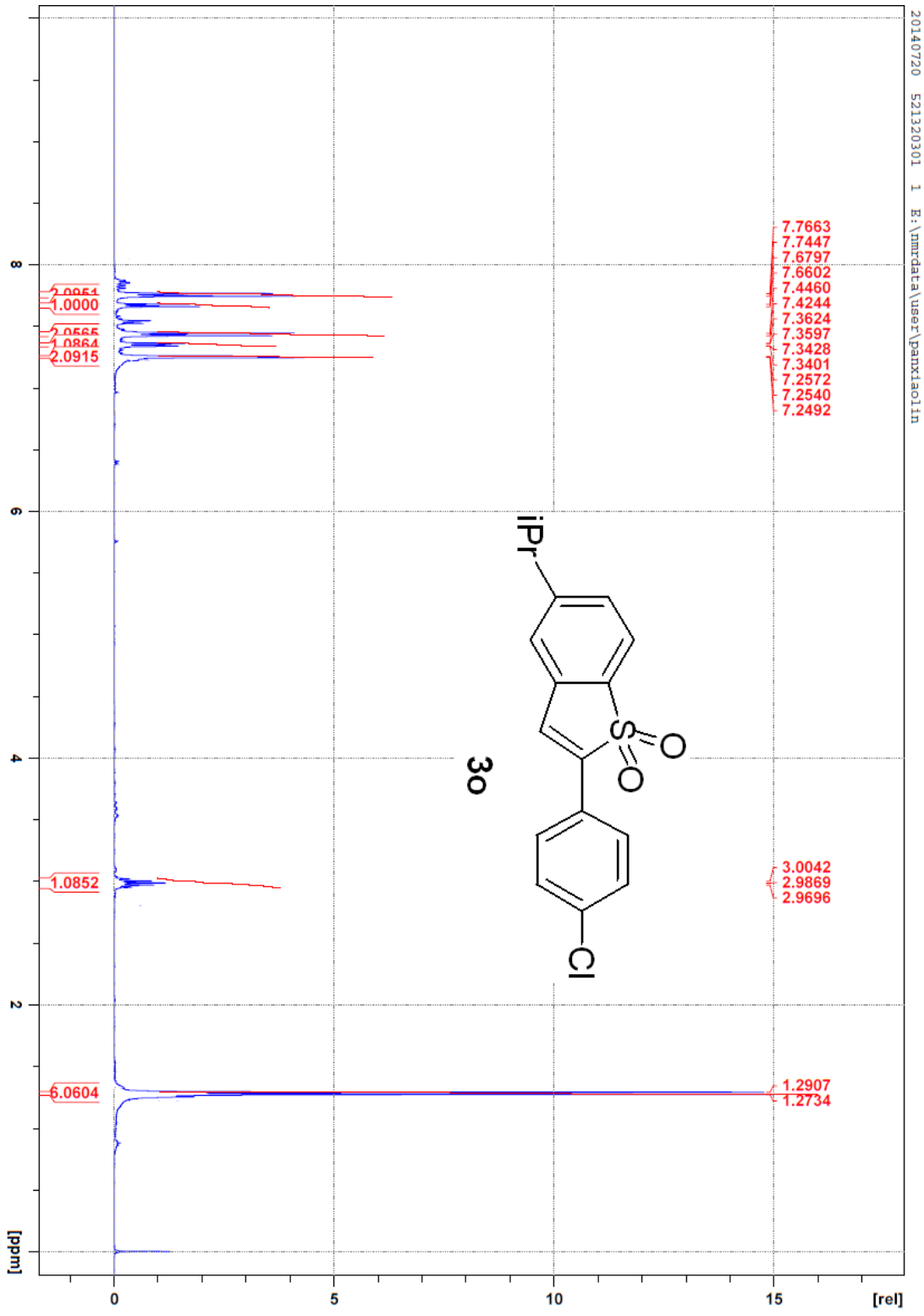
128.686
127.209
125.374
125.204
124.977
121.953
121.483
77.318
77.000
76.682
3n
S
O
O
S


20140720 521320301 1 E:\nmrdata\user\panxiaolin
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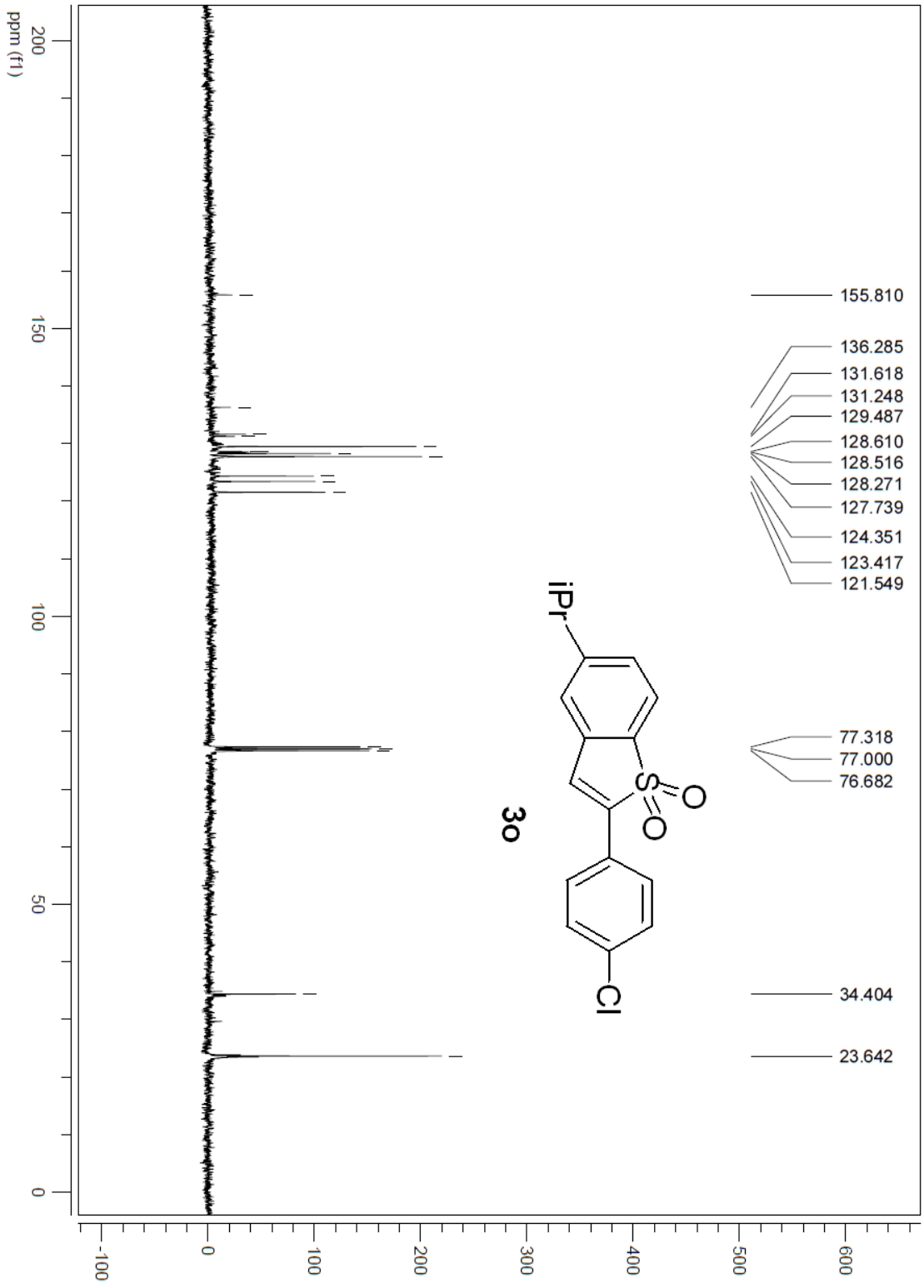
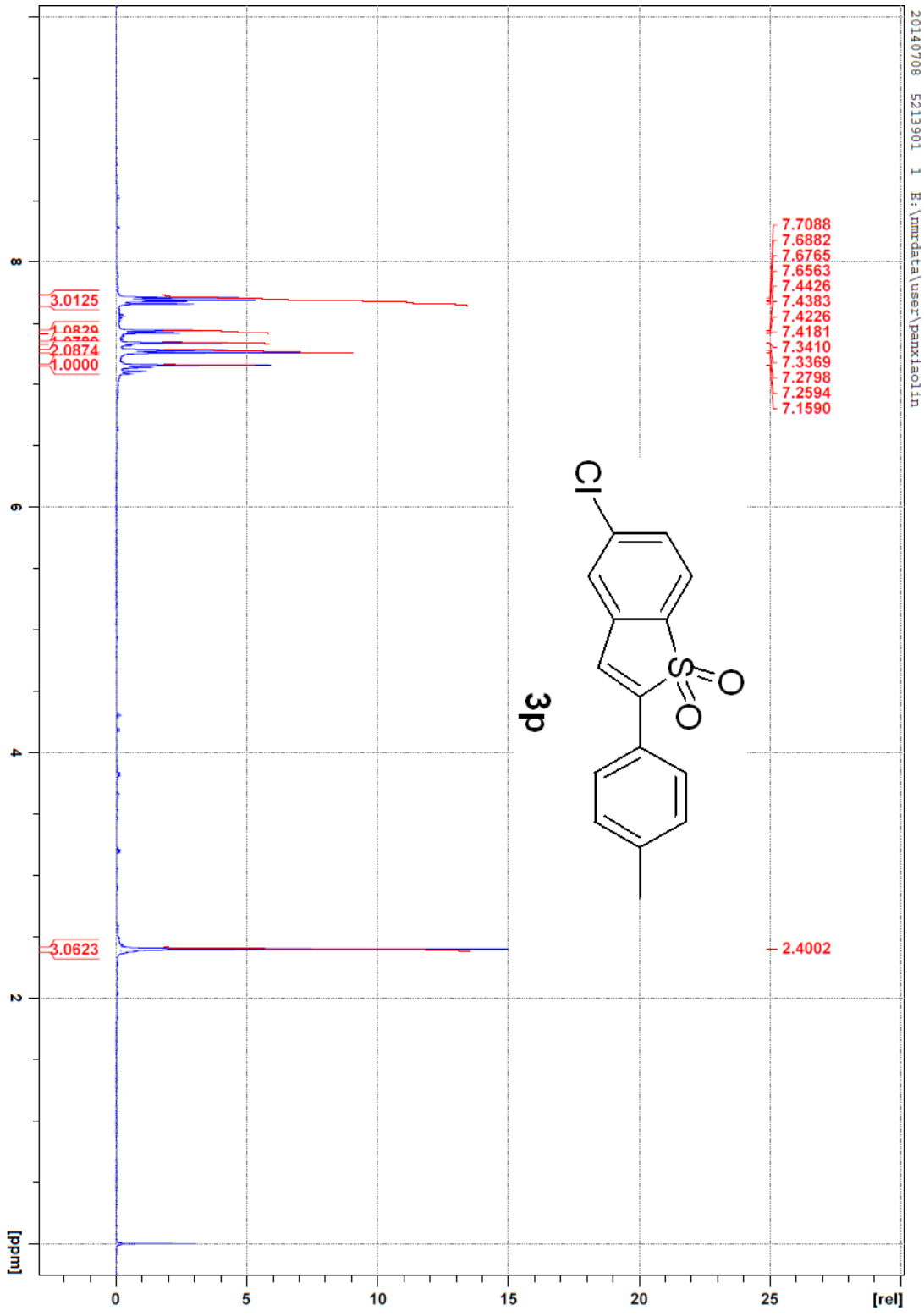
7.7447
7.6797
7.6602
7.4460
7.4244
7.3624
7.3597
7.3428
7.3401
7.2572
7.2540
7.2492
1.0000
2.0915
1.0852
6.0604
3.0042
2.9869
2.9696
1.2907
1.2734
iPr
S
O
O
Cl
3o
[ppm]
[rel]
0
5
10
15
2
4
6
8


155.810
136.285
131.618
131.248
129.487
128.610
128.516
128.271
127.739
124.351
123.417
121.549
77.318
77.000
76.682
34.404
23.642
iPr
S
O
O
Cl
3o
ppm (f1)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7.4226
7.4181
7.3410
7.3369
7.2798
7.2594
7.1590
3.0125
2.0874
1.0000
3.0623
2.4002
Cl
S
O
O
3p
[ppm]
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10
15
20
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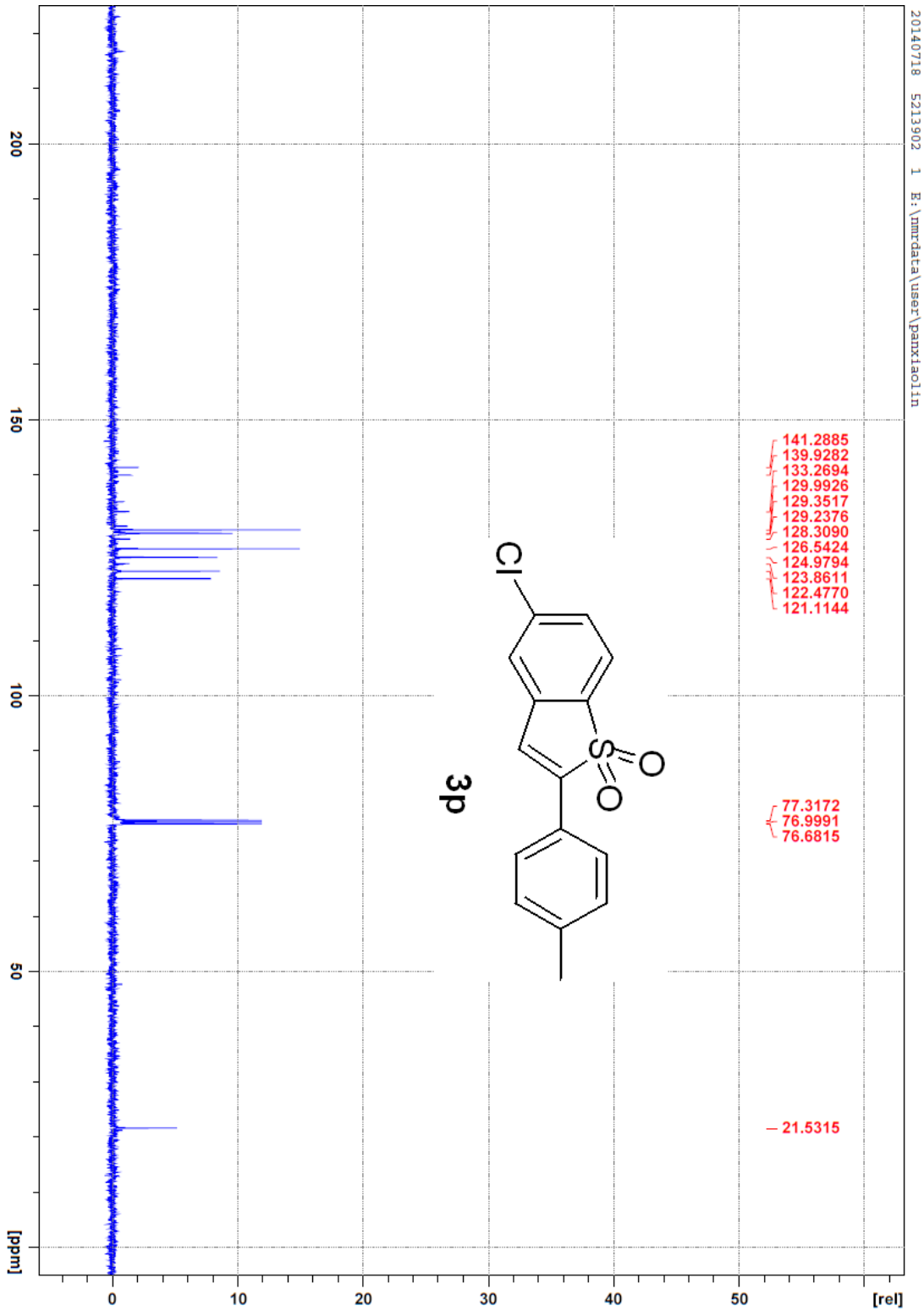
2
4
6
8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129.2376
128.3090
126.5424
124.9794
123.8611
122.4770
121.1144
77.3172
76.9991
76.6815
21.5315
Cl
S
O
O
3p
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150
100
50
[ppm]
0
10
20
30
40
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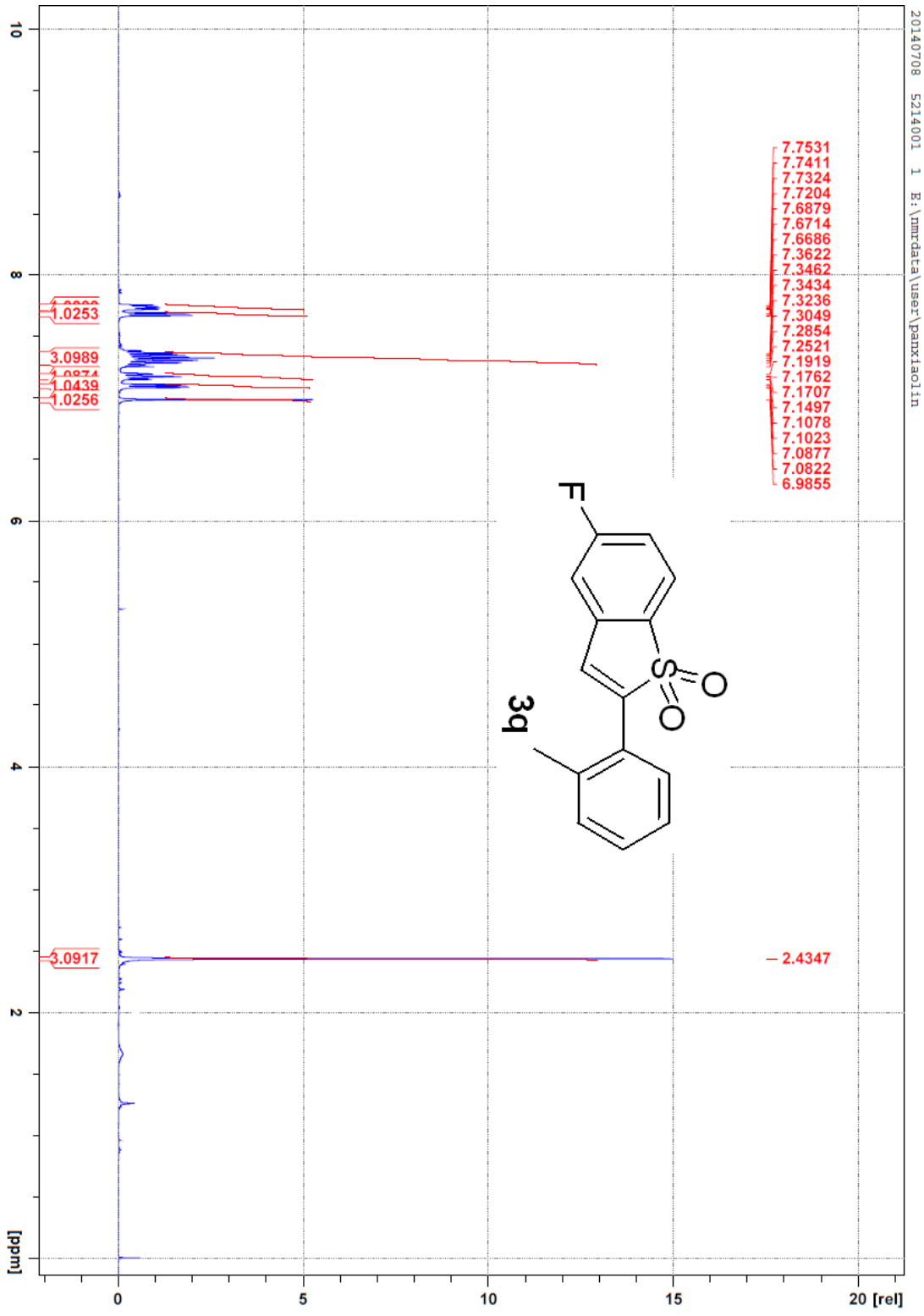
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7.6686
7.3622
7.3462
7.3434
7.3236
7.3049
7.2854
7.2521
7.1919
7.1762
7.1707
7.1497
7.1078
7.1023
7.0877
7.0822
6.9855
1.0253
3.0989
1.0439
1.0256
3.0917
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F
S
O
O
3q
10
8
6
4
2
[ppm]
0
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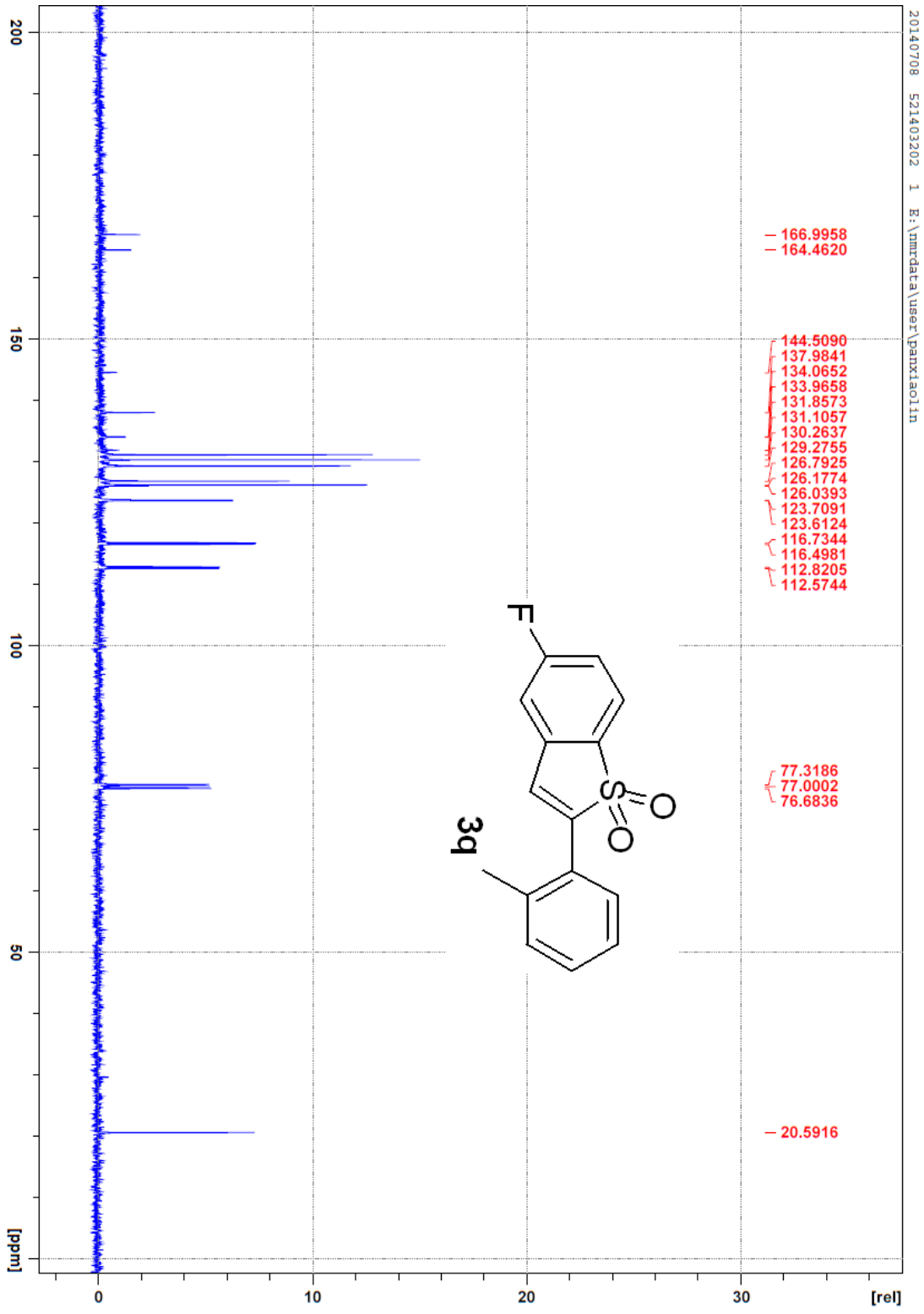
10
15
20 [rel]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123.7091
123.6124
116.7344
116.4981
112.8205
112.5744
77.3186
77.0002
76.6836
20.5916
F
S
O
O
3q
200
150
100
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20
30
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