Electronic Supplementary Material (ESI) for Chemical Communications

A Palladium-Catalyzed Three-Component Coupling of Arylboronic Acids, Sulfur Dioxide, and Hydrazines

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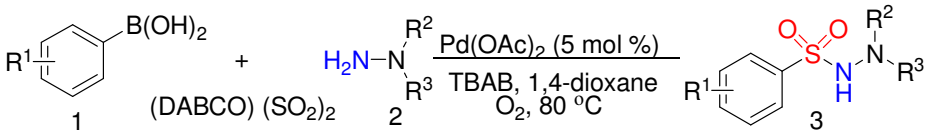
Supporting Information

General experimental methods:

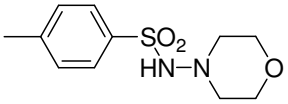
Unless otherwise stated, all commercial reagents were used as received. All solvents were dried and distilled according to standard procedures. Flash column chromatography was performed using silica gel (60-Å pore size, 32–63μm, standard grade). Analytical thin–layer chromatography was performed using 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 palladium-catalyzed three-component reaction of arylboronic acids **1**, DABCO-bis(sulfur dioxide), with amines **2**.*



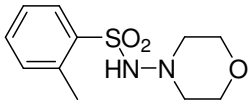
Hydrazine **2** (0.5 mmol) in 1,4-dioxane (2.0 mL) was added to a mixture of arylboronic acids **1** (1.0 mmol), DABCO·$(SO_2)_2$ (1.0 mmol)[1], $Pd(OAc)_2$ (0.025 mmol), and TBAB (0.75 mmol) under a balloon of O_2. The reaction was stirred at 80 °C for 12 hours. After completion of the reaction as indicated by TLC, the residue was purified directly by flash chromatography on silica gel to afford aryl *N*-aminosulfonamides **3**.

[1] Santos, P. S.; Mello, M. T. S. *J. Mol. Struct.* **1988**, *178*, 121-133.



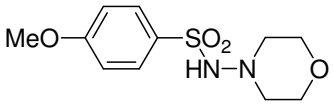
4-Methyl-*N*-morpholinobenzenesulfonamide (**3a**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.43 (s, 3H), 2.62 (d, J = 3.2 Hz, 4H), 3.59 (d, J = 3.2 Hz, 4H), 5.97 (s, 1H), 7.31 (d, J = 7.8 Hz, 2H), 7.85 (d, J = 7.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.5, 56.5, 66.5, 128.0, 129.4, 135.5, 143.9; HRMS (ESI) calcd for $C_{11}H_{17}N_2O_3S$: 257.0954 ($M + H^+$), found: 257.0964.



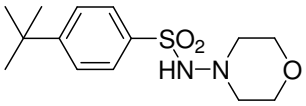
2-Methyl-*N*-morpholinobenzenesulfonamide (**3b**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.64 (s, 4H), 2.69 (s, 3H), 3.56 (s, 4H), 5.98 (s, 1H), 7.29-7.35 (m, 2H), 7.46 (d, J = 7.3 Hz, 1H), 8.06 (d, J = 7.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.6, 56.5, 66.5, 126.0, 130.9, 132.2, 133.1, 136.4, 137.8; HRMS (ESI) calcd for $C_{11}H_{17}N_2O_3S$: 257.0954 ($M + H^+$), found: 257.0975.



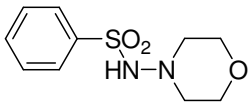
4-Methoxy-*N*-morpholinobenzenesulfonamide (**3c**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.63 (s, 4H), 3.60 (s, 4H), 3.88 (s, 3H), 5.78 (s, 1H), 6.98 (d, J = 7.3 Hz, 2H), 7.90 (d, J = 7.3 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.5, 56.5, 66.6, 113.9, 130.0, 130.2, 163.2; HRMS (ESI) calcd for $C_{11}H_{17}N_2O_4S$: 273.0904 ($M + H^+$), found: 273.0912.



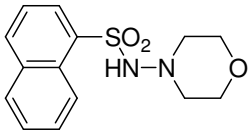
4-(*tert*-Butyl)-*N*-morpholinobenzenesulfonamide (**3d**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.35 (s, 9H), 2.64 (s, 4H), 3.61 (s, 4H), 6.00 (s, 1H), 7.52 (d, J = 7.3 Hz, 2H), 7.90 (d, J = 7.3 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 31.0, 35.1, 56.5, 66.5, 125.7, 127.8, 135.5, 156.9; HRMS (ESI) calcd for $C_{14}H_{23}N_2O_3S$: 299.1424 ($M + H^+$), found: 299.1446.



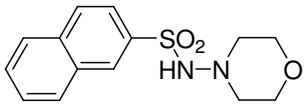
N-Morpholinobenzenesulfonamide (**3e**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.62 (d, J = 3.6 Hz, 4H), 3.59 (d, J = 3.2 Hz, 4H), 5.87 (s, 1H), 7.53 (t, J = 7.3 Hz, 2H), 7.62 (t, J = 7.3 Hz, 1H), 7.98 (d, J = 7.3 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 56.5, 66.5, 128.0, 128.8, 133.1, 138.5; HRMS (ESI) calcd for $C_{10}H_{15}N_2O_3S$: 243.0798 ($M + H^+$), found: 243.0812.



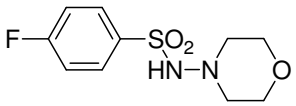
N-Morpholinonaphthalene-1-sulfonamide (**3f**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.53 (d, J = 2.7 Hz, 4H), 3.46 (d, J = 2.7 Hz, 4H), 6.04 (s, 1H), 7.55-7.61 (m, 2H), 7.67 (t, J = 7.8 Hz, 1H), 7.93 (d, J = 7.8 Hz, 1H), 8.09 (d, J = 7.8 Hz, 1H), 8.39 (d, J = 7.3 Hz, 1H), 8.80 (d, J = 8.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 56.6, 66.4, 124.1, 125.0, 126.8, 128.1, 128.4, 128.8, 131.3, 133.4, 133.9, 134.7; HRMS (ESI) calcd for $C_{14}H_{17}N_2O_3S$: 293.0954 ($M + H^+$), found: 293.0956.



N-Morpholinonaphthalene-2-sulfonamide (**3g**)

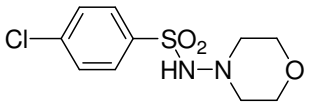
^{1}H NMR (400 MHz, $CDCl_3$) δ 2.64 (d, J = 3.2 Hz, 4H), 3.57 (d, J = 3.2 Hz, 4H), 6.03 (s, 1H), 7.60-7.68 (m, 2H), 7.91-7.99 (m, 4H), 8.57 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 56.6, 66.5, 123.1, 127.5, 127.8, 128.9, 129.0, 129.2, 129.6, 131.9, 134.9, 135.4; HRMS (ESI) calcd for $C_{14}H_{17}N_2O_3S$: 293.0954 ($M + H^+$), found: 293.0960.



4-Fluoro-*N*-morpholinobenzenesulfonamide (**3h**)

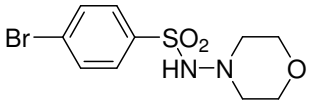
^{1}H NMR (400 MHz, $CDCl_3$) δ 2.64 (s, 4H), 3.62 (s, 4H), 5.53 (s, 1H), 7.21 (t, J = 7.8 Hz, 2H), 7.99 (d, J = 5.5 Hz, 2H); ^{13}C NMR (100 MHz, CD_3OD) δ 56.3, 66.4, 116.7 (d, J_F = 22.9 Hz), 131.1 (d, J_F = 9.5 Hz), 136.1, 164.9 (d, J_F = 250.7 Hz); HRMS (ESI)

calcd for $C_{10}H_{14}FN_2O_3S$: 261.0704 ($M + H^+$), found: 261.0709.



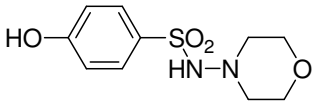
4-Chloro-*N*-morpholinobenzenesulfonamide (**3i**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.65 (s, 4H), 3.62 (s, 4H), 5.68 (s, 1H), 7.51 (d, J = 7.3 Hz, 2H), 7.92 (d, J = 7.3 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 56.7, 66.6, 129.1, 129.5, 137.0, 139.7; HRMS (ESI) calcd for $C_{10}H_{14}ClN_2O_3S$: 277.0408 ($M + H^+$), found: 277.0425.



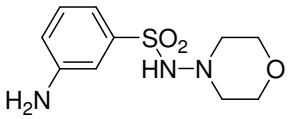
4-Bromo-*N*-morpholinobenzenesulfonamide (**3j**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.64 (d, J = 3.2 Hz, 4H), 3.62 (d, J = 2.8 Hz, 4H), 5.72 (s, 1H), 7.67 (d, J = 7.3 Hz, 2H), 7.84 (d, J = 7.3 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 56.7, 66.6, 128.3, 129.2, 132.1, 137.6; HRMS (ESI) calcd for $C_{10}H_{14}BrN_2O_3S$: 320.9903 ($M + H^+$), found: 320.9912.



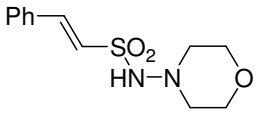
4-Hydroxy-*N*-morpholinobenzenesulfonamide (**3k**)

^{1}H NMR (400 MHz, CD_3OD) δ 2.54 (s, 4H), 3.55 (s, 4H), 4.89 (br, 2H), 6.90 (d, J = 7.8 Hz, 2H), 7.75 (d, J = 7.8 Hz, 2H); ^{13}C NMR (100 MHz, CD_3OD) δ 56.0, 66.5, 115.0, 129.1, 130.1, 161.9; HRMS (ESI) calcd for $C_{10}H_{15}N_2O_4S$: 259.0747 ($M + H^+$), found: 259.0765.



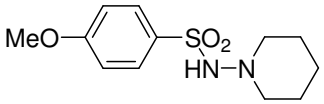
3-Amino-*N*-morpholinobenzenesulfonamide (**3l**)

^{1}H NMR (400 MHz, CD_3OD) δ 2.56 (s, 4H), 3.56 (s, 4H), 4.88 (s, 3H), 6.88 (d, J = 7.3 Hz, 1H), 7.14 (d, J = 6.8 Hz, 1H), 7.21-7.25 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 56.7, 66.6, 113.7, 117.6, 119.2, 129.7, 139.4, 147.0; HRMS (ESI) calcd for $C_{10}H_{16}N_3O_3S$: 258.0907 ($M + H^+$), found: 258.0918.



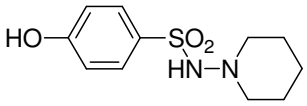
(*E*)-*N*-Morpholino-2-phenylethenesulfonamide (**3m**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.88 (s, 4H), 3.72 (s, 4H), 5.72 (s, 1H), 6.83 (d, J = 15.6 Hz, 1H), 7.43-7.50 (m, 5H), 7.60 (d, J = 15.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 57.3, 66.5, 123.4, 128.3, 129.1, 131.1, 132.4, 143.7; HRMS (ESI) calcd for $C_{12}H_{17}N_2O_3S$: 269.0954 (M + H^+), found: 269.0965.



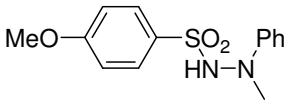
4-Methoxy-*N*-(piperidin-1-yl)benzenesulfonamide (**3n**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.29 (s, 2H), 1.49 (d, J = 4.1 Hz, 4H), 2.53 (s, 4H), 3.88 (s, 3H), 5.58 (s, 1H), 6.97 (d, J = 7.8 Hz, 2H), 7.90 (d, J = 7.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 22.9, 25.5, 55.5, 57.6, 113.7, 130.2, 130.3, 162.9; HRMS (ESI) calcd for $C_{12}H_{19}N_2O_3S$: 271.1111 (M + H^+), found: 271.1124.



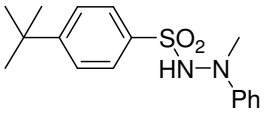
4-Hydroxy-*N*-(piperidin-1-yl)benzenesulfonamide (**3o**)

^{1}H NMR (400 MHz, CD_3OD) δ 1.27 (s, 2H), 1.45 (d, J = 5.0 Hz, 4H), 2.49 (s, 4H), 4.90 (br, 2H), 6.90 (d, J = 7.8 Hz, 2H), 7.74 (d, J = 7.8 Hz, 2H); ^{13}C NMR (100 MHz, CD_3OD) δ 23.0, 25.6, 56.9, 114.9, 129.3, 130.1, 161.7; HRMS (ESI) calcd for $C_{11}H_{17}N_2O_3S$: 257.0954 (M + H^+), found: 257.0968.



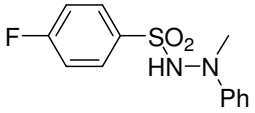
4-Methoxy-*N*'-methyl-*N*'-phenylbenzenesulfonohydrazide (**3p**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.93 (s, 3H), 3.84 (s, 3H), 6.31 (s ,1H), 6.85-6.87 (m, 3H), 6.94 (d, J = 7.3 Hz, 2H), 7.17 (t, J = 7.3 Hz, 2H), 7.87 (d, J = 7.3 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 42.4, 55.6, 114.2, 114.3, 120.8, 128.8, 129.8, 130.3, 149.7, 163.4; HRMS (ESI) calcd for $C_{14}H_{17}N_2O_3S$: 293.0954 (M + H^+), found: 293.0964.



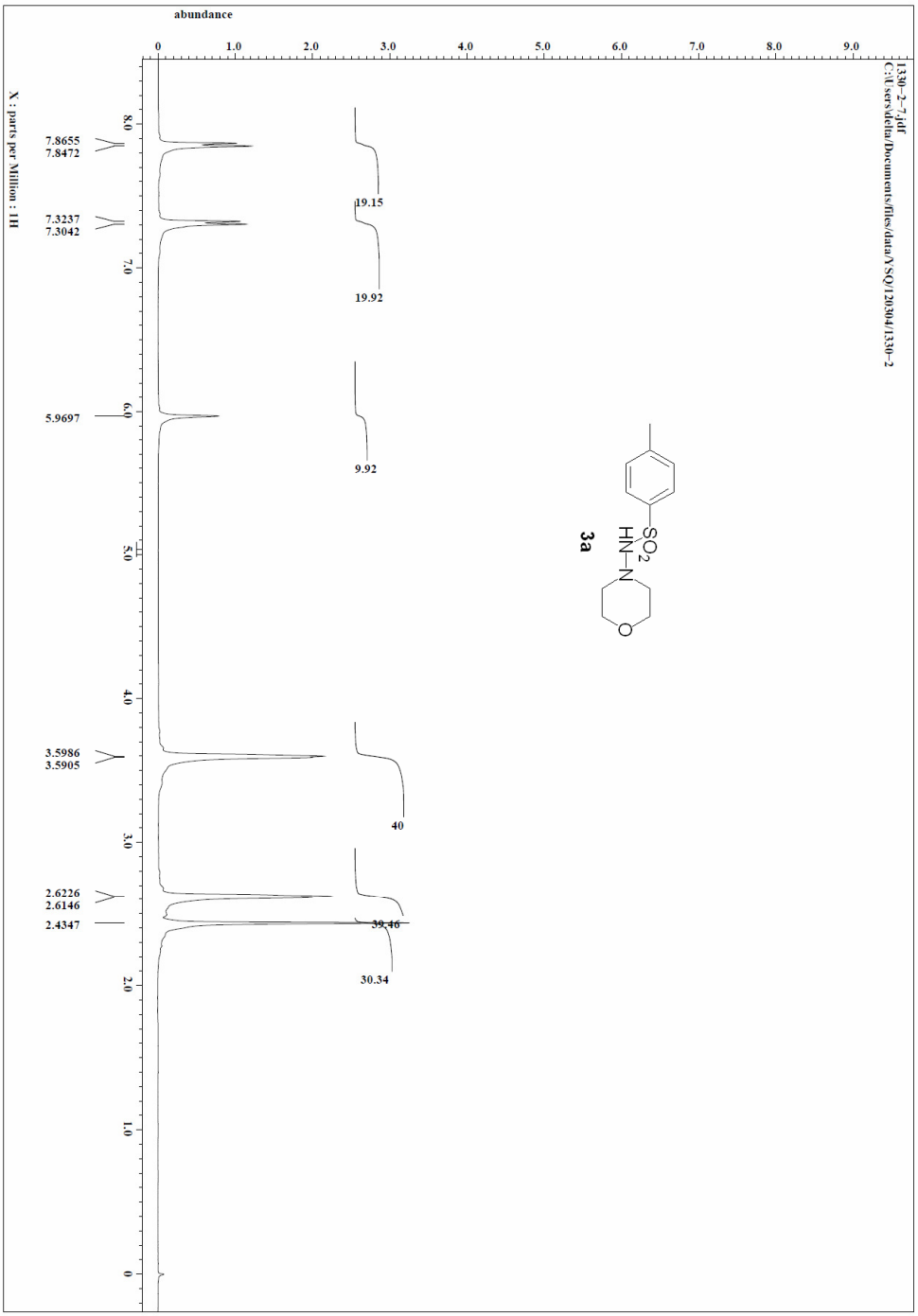
4-(*tert*-Butyl)-*N*'-methyl-*N*'-phenylbenzenesulfonohydrazide (**3q**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.31 (s, 9H), 2.93 (s, 3H), 6.50 (s, 1H), 6.80-6.84 (m, 3H), 7.12 (t, J = 7.3 Hz, 2H), 7.46 (d, J = 8.3 Hz, 2H), 7.85 (d, J = 7.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 30.9, 35.1, 42.4, 114.3, 120.7, 126.0, 127.9, 128.7, 135.4, 149.6, 157.2; HRMS (ESI) calcd for $C_{17}H_{23}N_2O_2S$: 319.1475 ($M + H^+$), found: 319.1487.



4-Fluoro-*N*'-methyl-*N*'-phenylbenzenesulfonohydrazide (**3r**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.97 (s, 3H), 6.46 (s, 1H), 6.81-6.88 (m, 3H), 7.12-7.17 (m, 4H), 7.94 (t, J = 6.9 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 42.8, 114.3, 116.3 (d, J_F = 22.9 Hz), 121.0, 128.9, 130.9 (d, J_F = 9.5 Hz), 134.4, 149.4, 165.4 (d, J_F= 254.6 Hz); HRMS (ESI) calcd for $C_{13}H_{14}FN_2O_2S$: 281.0755 ($M + H^+$), found: 281.0764.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X : parts per Million : 1H
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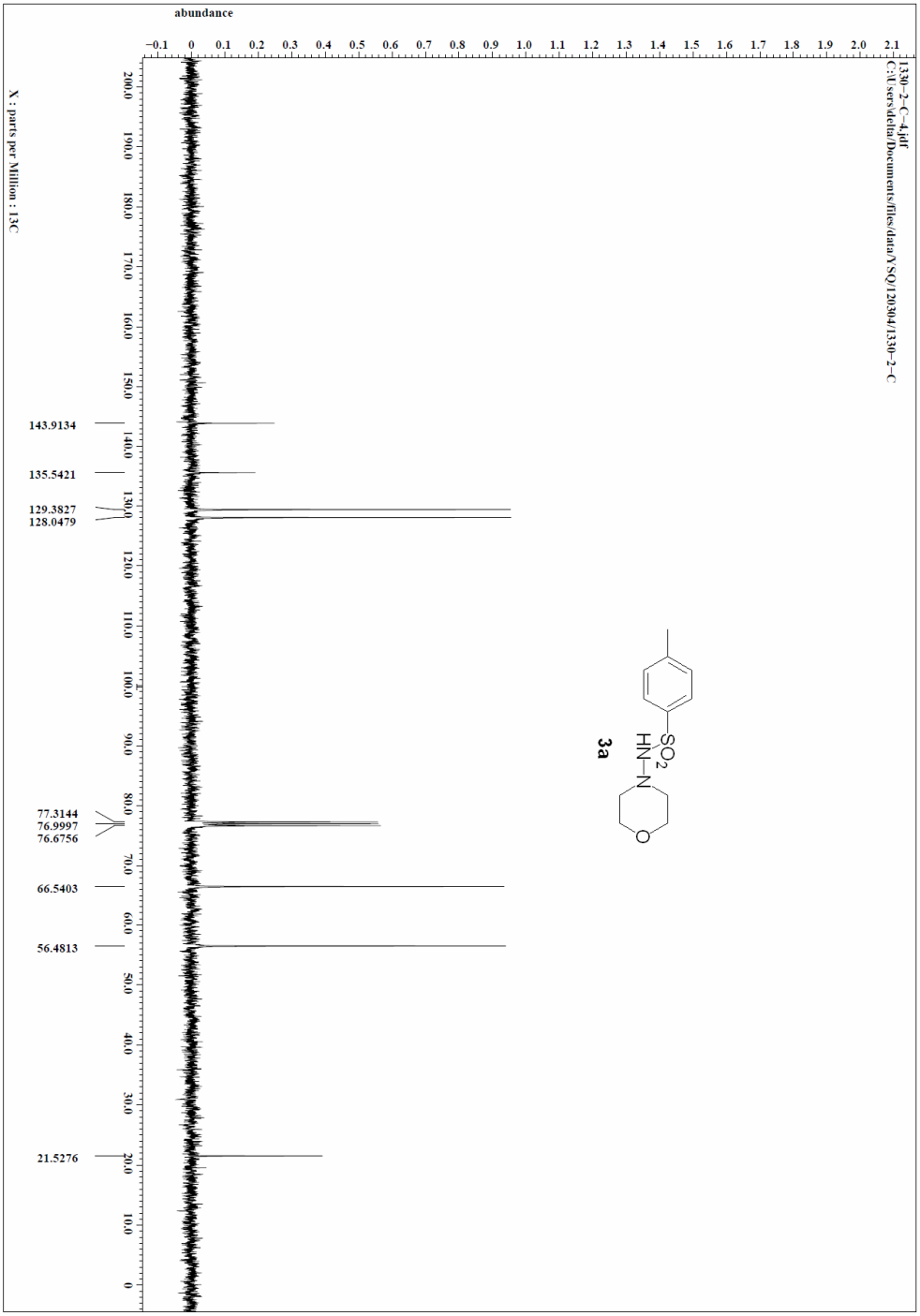
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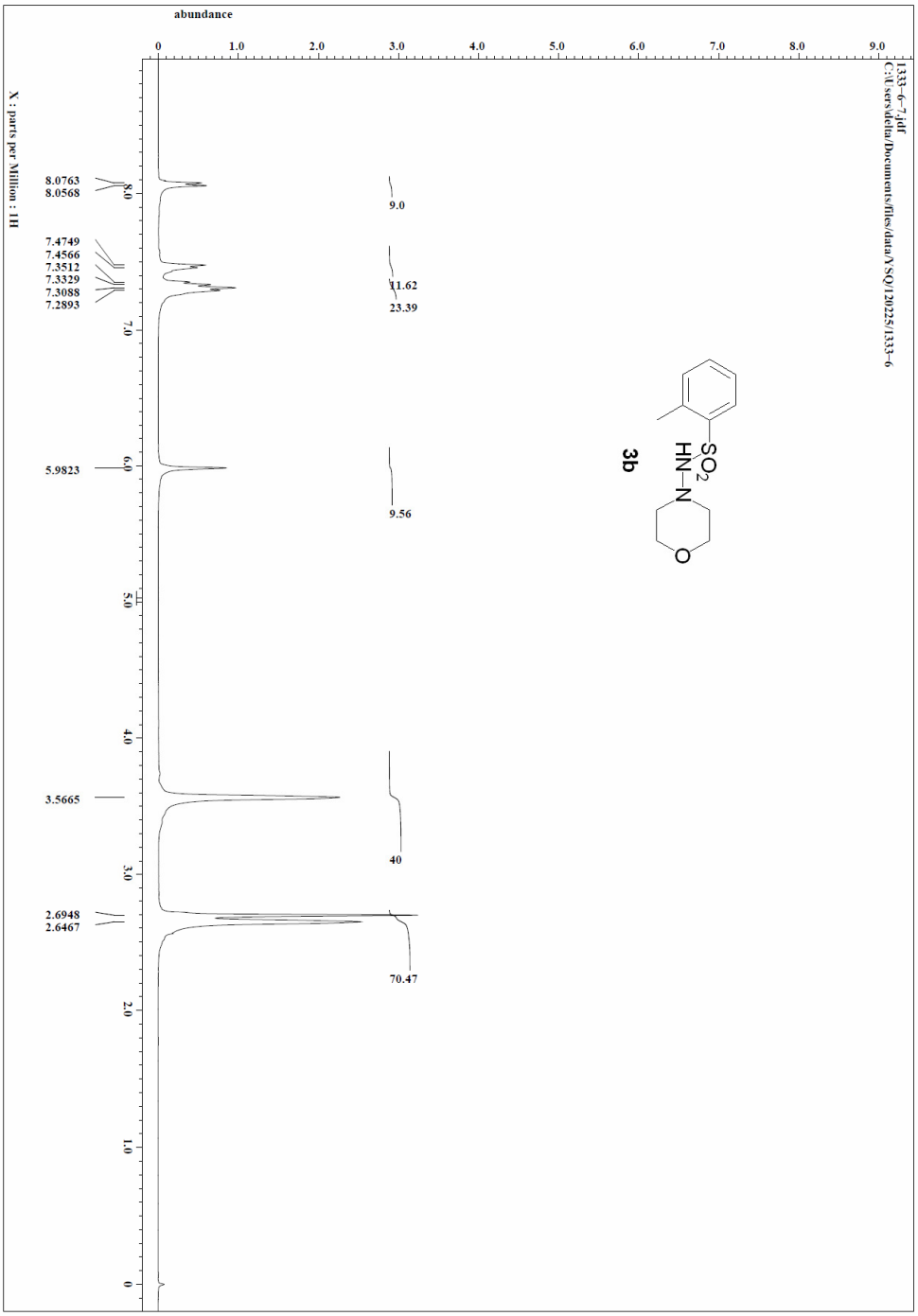
abundance
X : parts per Million : 1H
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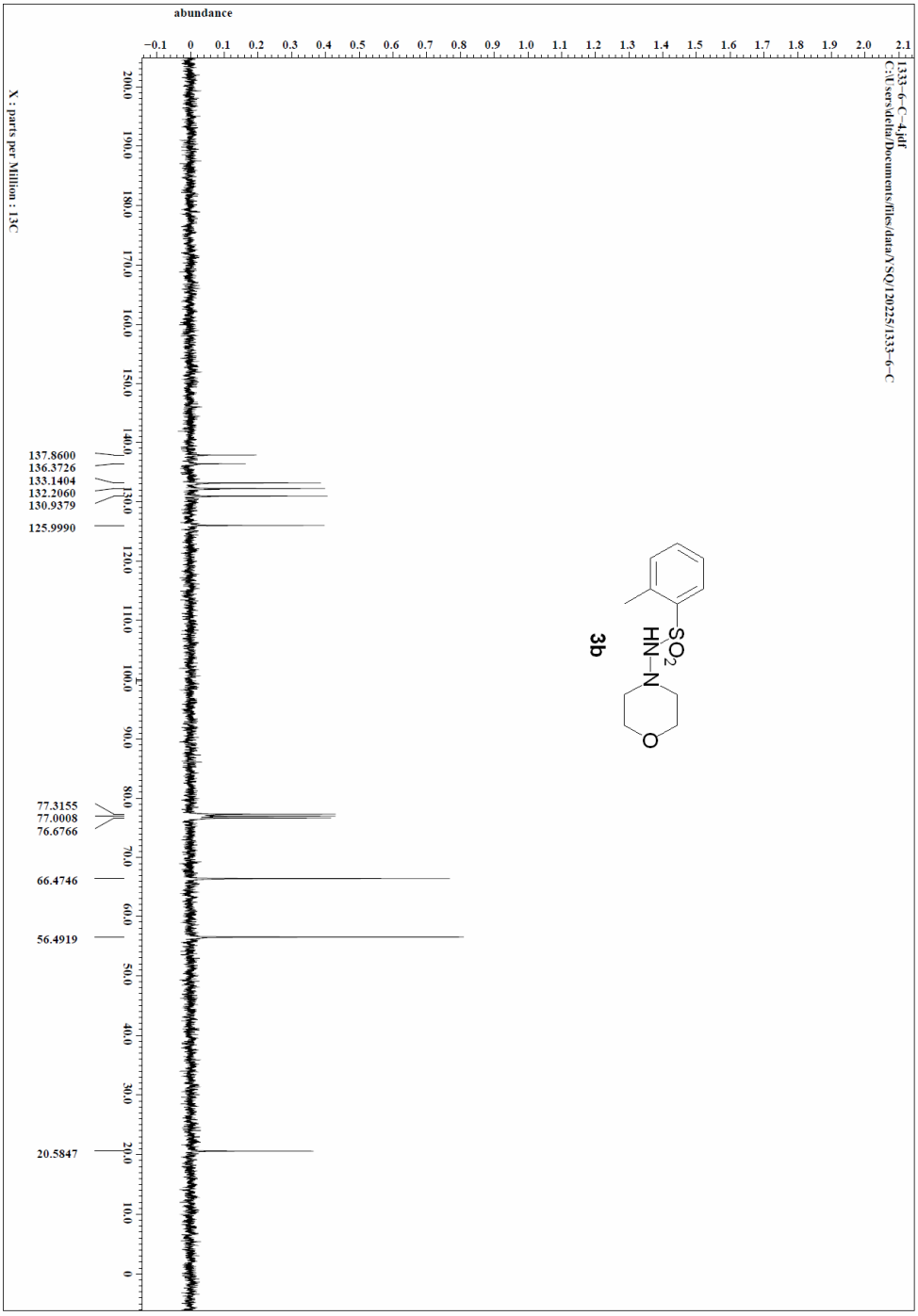
3b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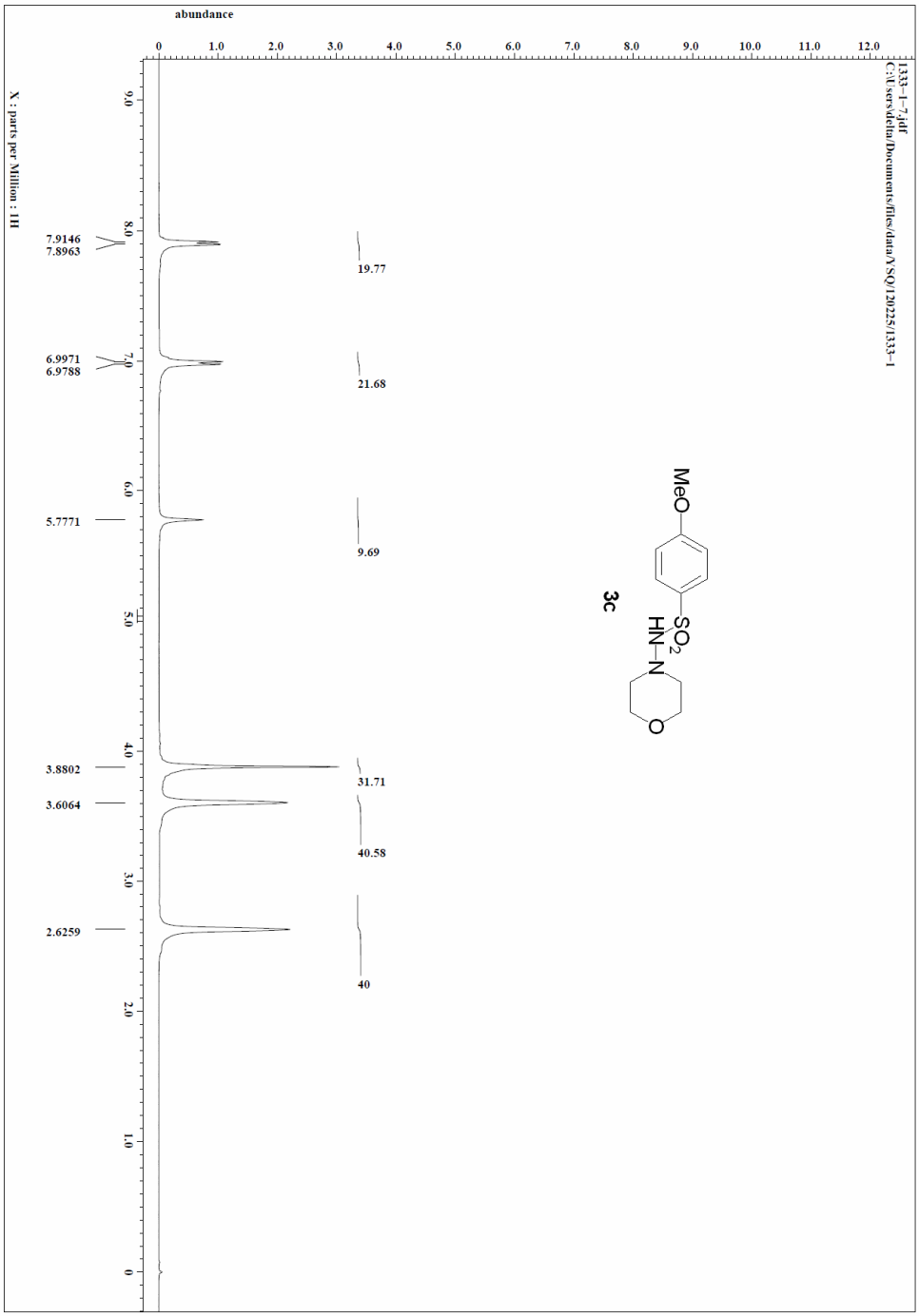
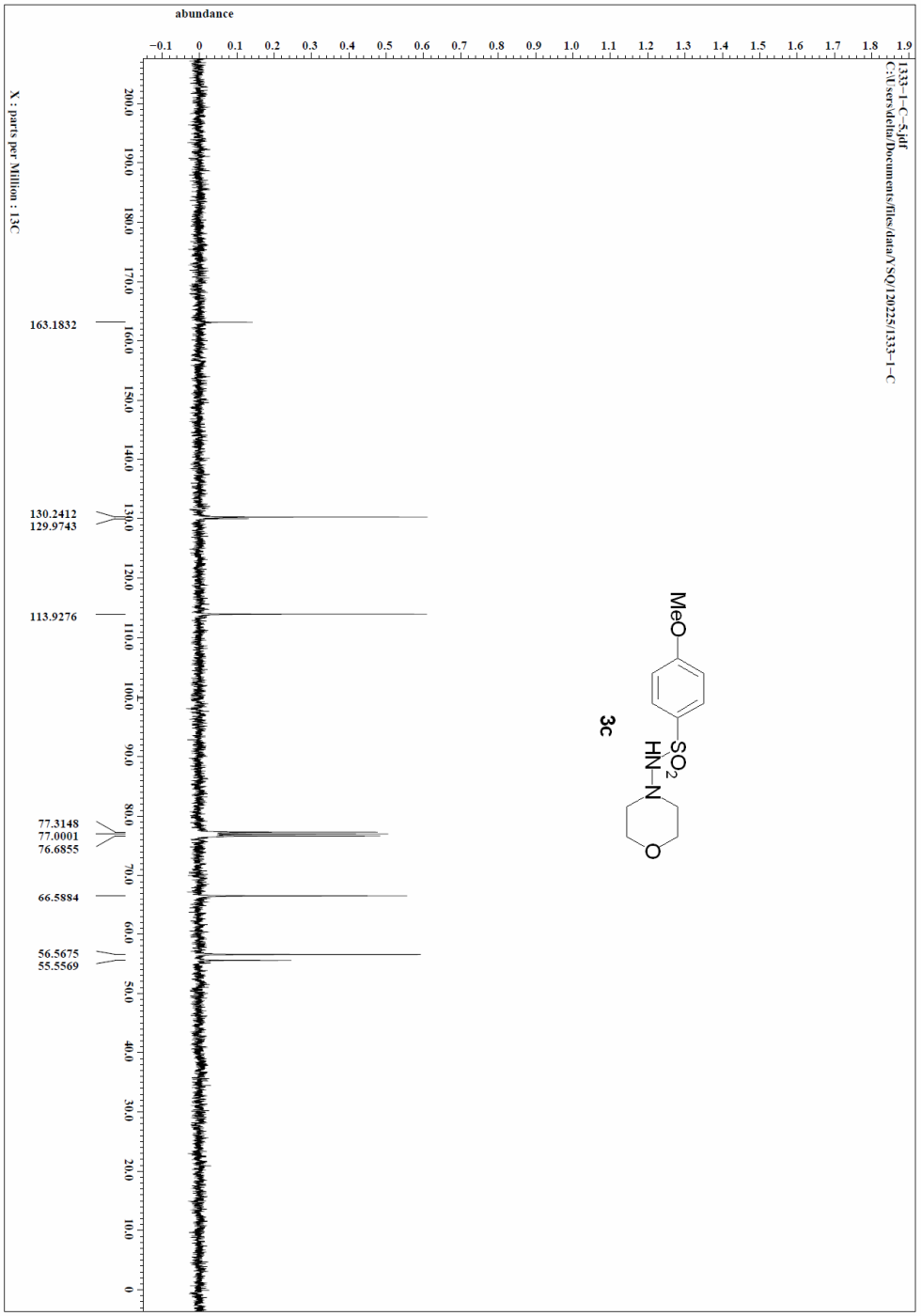
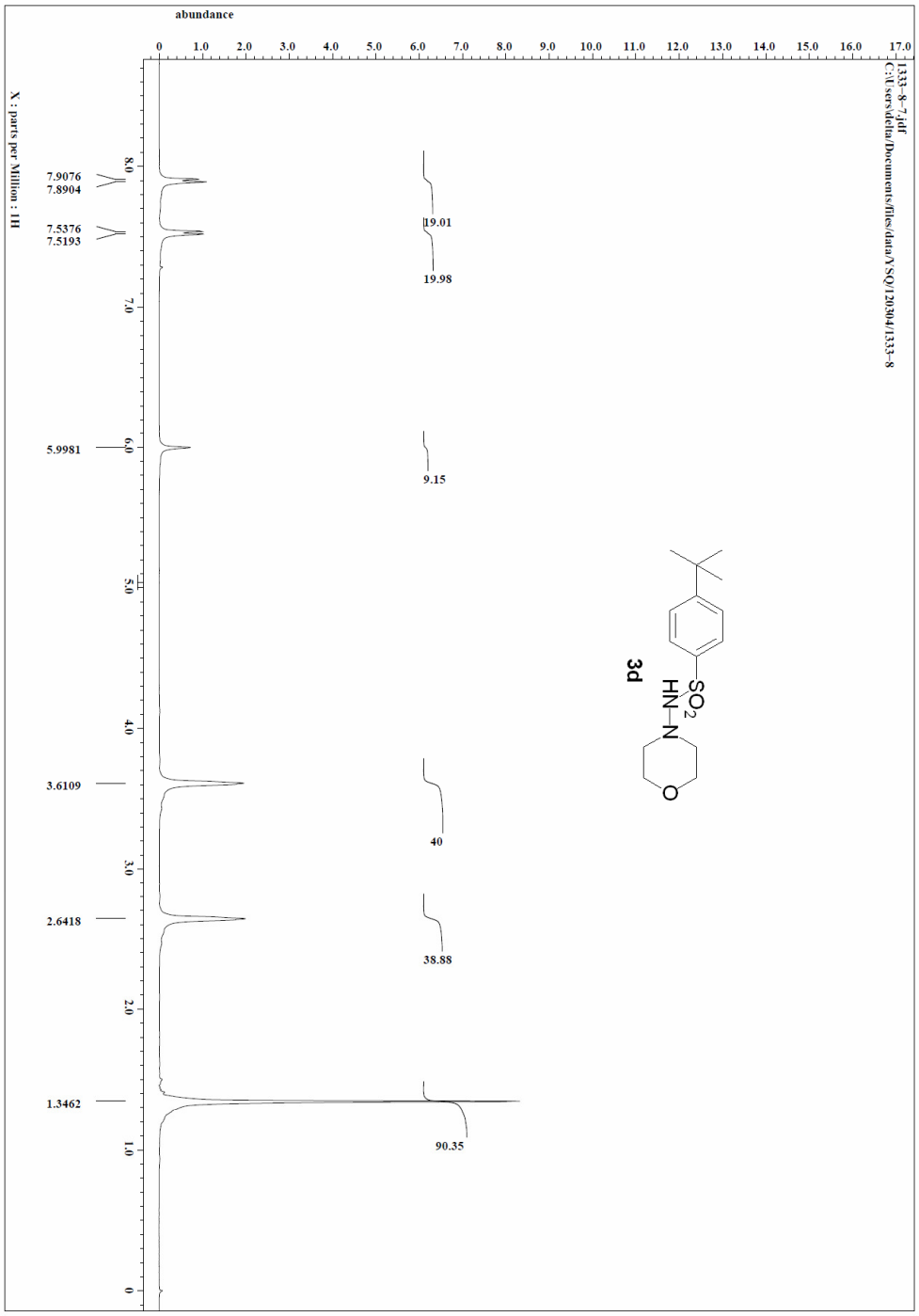
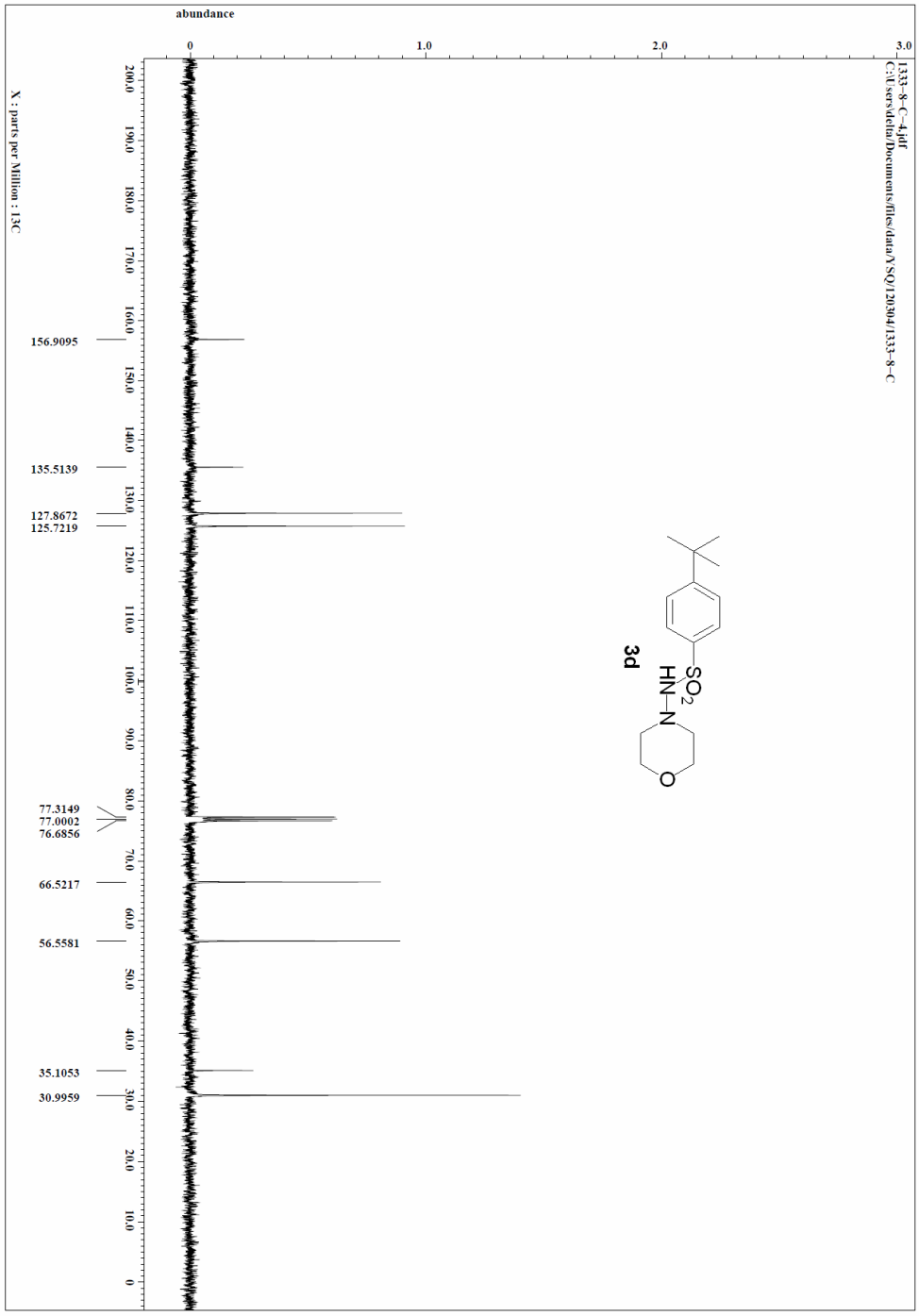
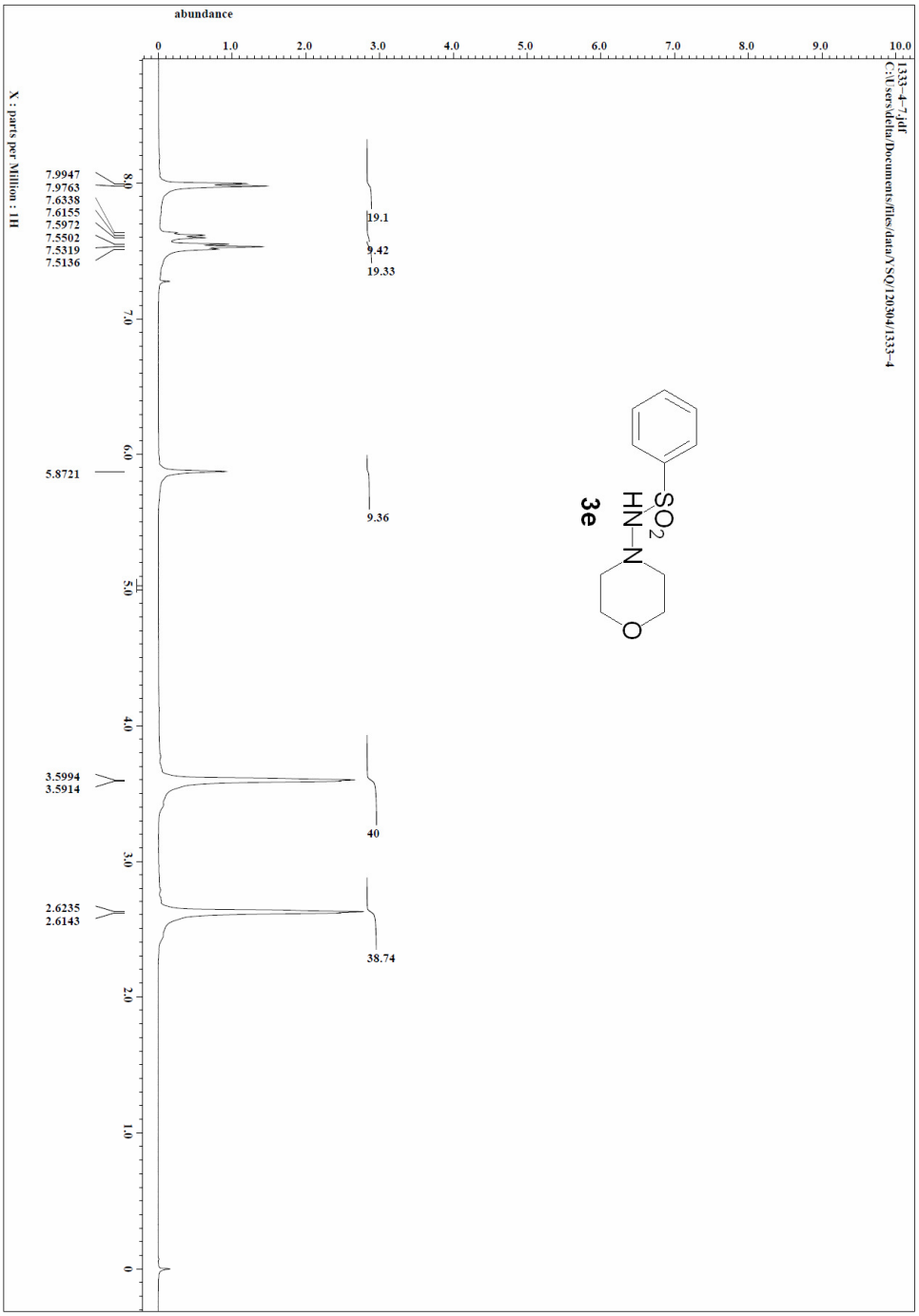
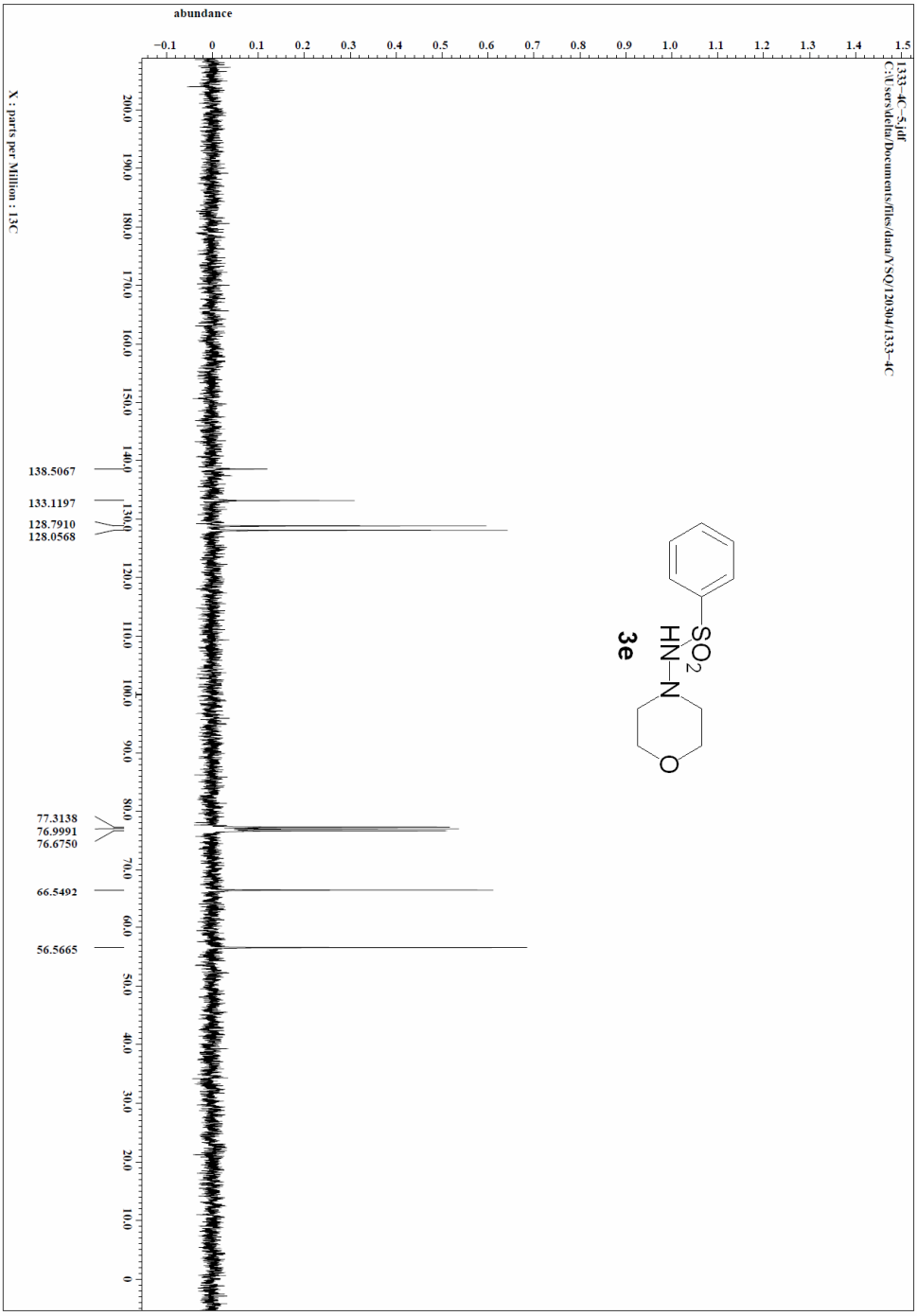

abundance
1333-1-7.jdf
C:\Users\dell\Documents\files\data\XSQ\120225\1333-1
X : parts per Million : 1H
7.9146
7.8963
6.9971
6.9788
5.7771
3.8802
3.6064
2.6259
19.77
21.68
9.69
31.71
40.58
40
MeO
SO2
HN
N
O
3c

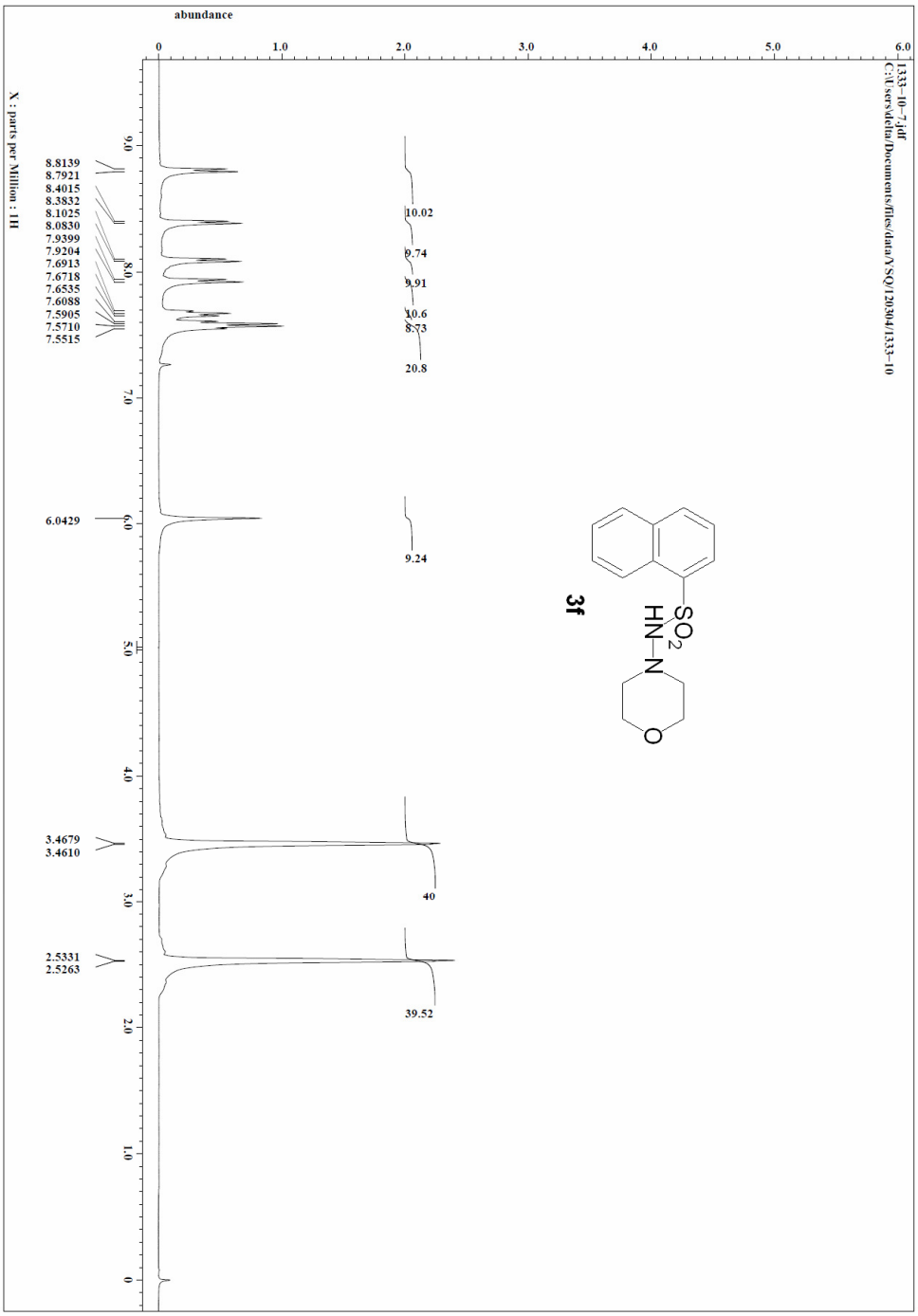

abundance
X : parts per Million : 13C
163.1832
130.2412
129.9743
113.9276
77.3148
77.0001
76.6855
66.5884
56.5675
55.5569
MeO
SO2
HN
N
O
3c

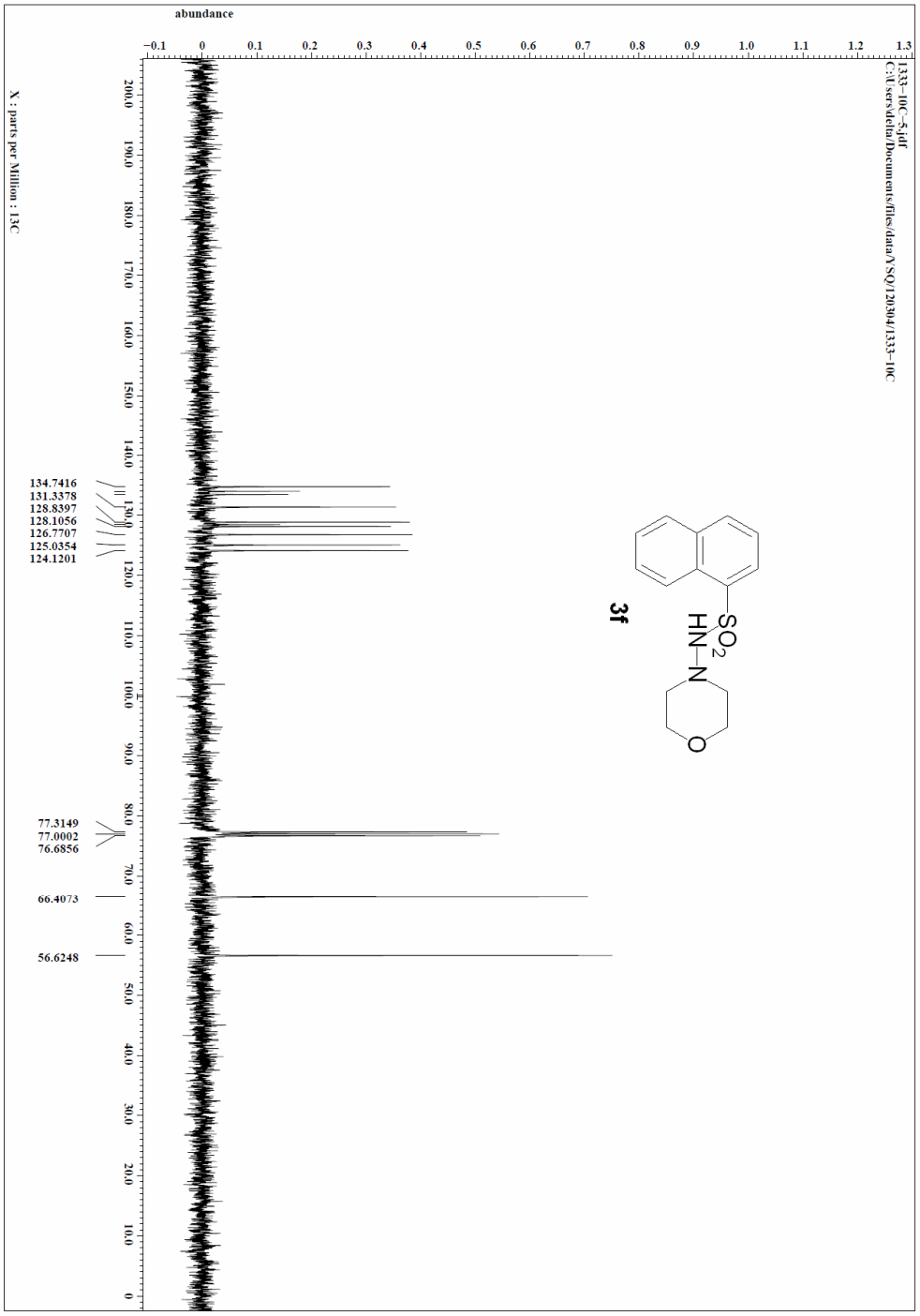

abundance
X : parts per Million : 1H
C:\Users\delta\Documents\files\data\YSQ\120304\1333-8
1333-8--7.jdf
7.9076
7.8904
7.5376
7.5193
5.9981
3.6109
2.6418
1.3462
19.01
19.98
9.15
40
38.88
90.35
3d

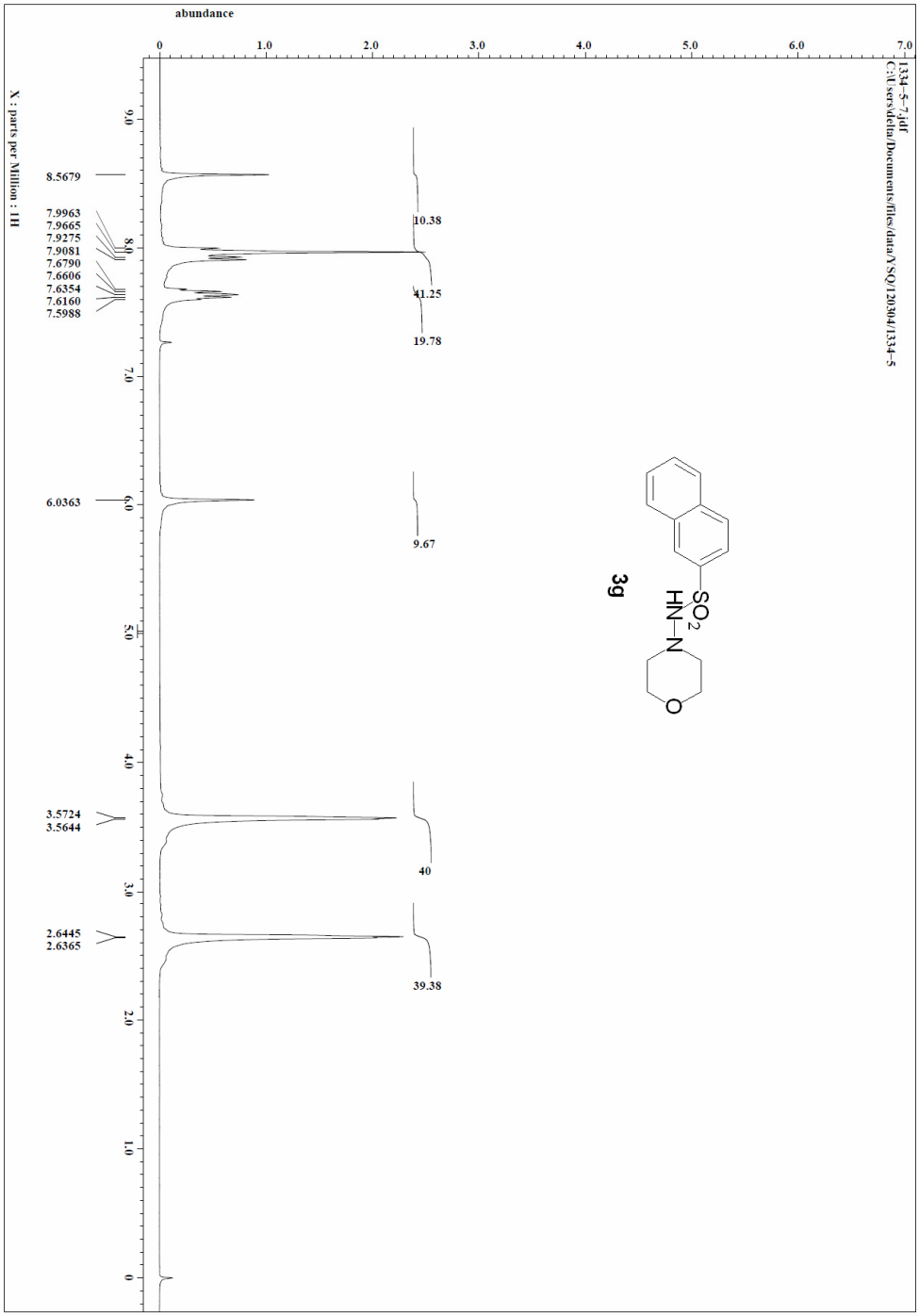

abundance
0
1.0
2.0
3.0
1333-8-C-4.jdf
C:\Users\delia\Documents\files\data\YSQ\120304\1333-8-C
X : parts per Million : 13C
156.9095
135.5139
127.8672
125.7219
77.3149
77.0002
76.6856
66.5217
56.5581
35.1053
30.9959
3d
SO2
HN
N
O

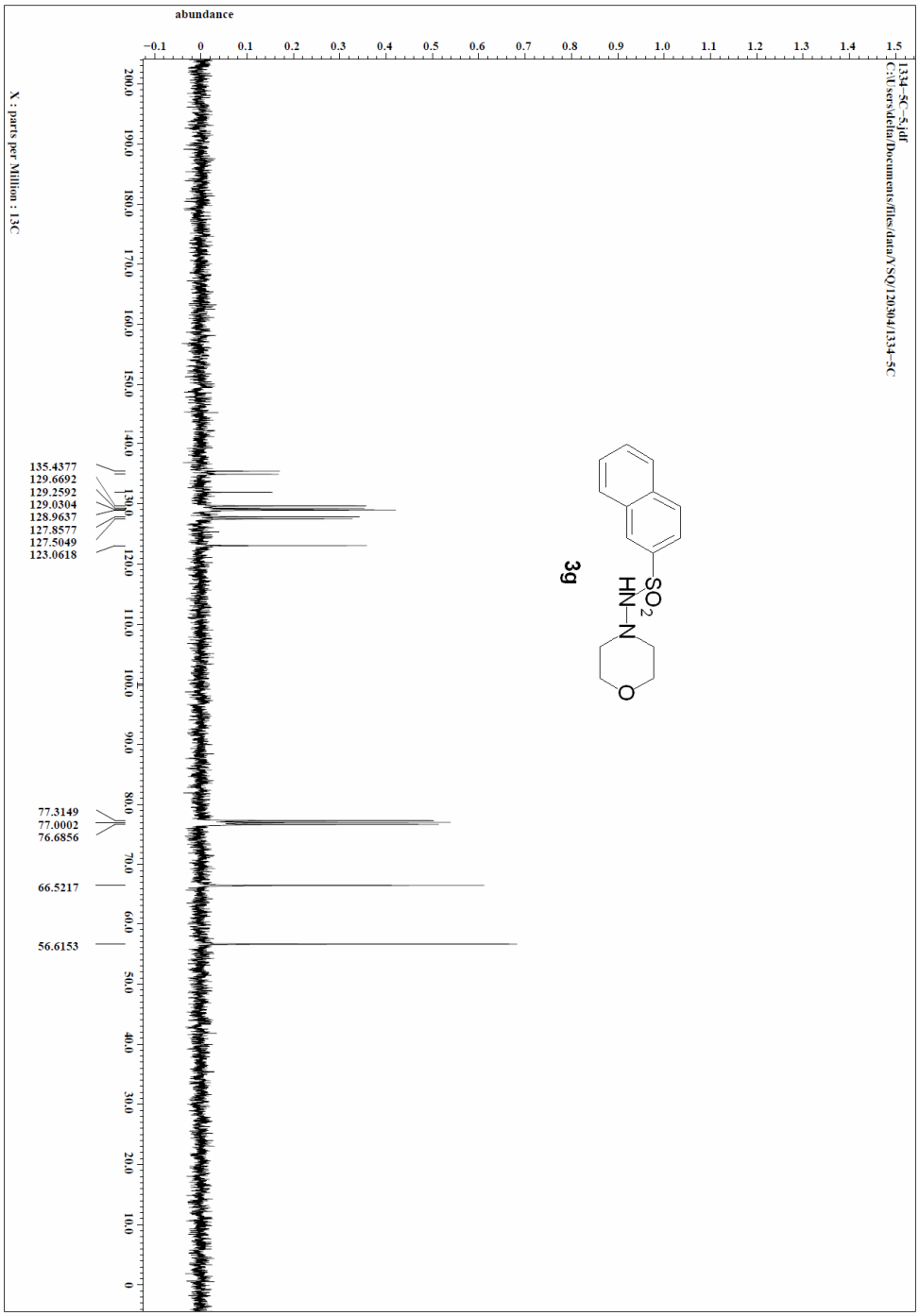

abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
1333--4--7.jdf
C:\Users\delta\Documents\files\data\YSQ\20304\1333--4
X : parts per Million : 1H
7.9947
7.9763
7.6338
7.6155
7.5972
7.5502
7.5319
7.5136
5.8721
3.5994
3.5914
2.6235
2.6143
19.1
9.42
19.33
9.36
40
38.74
3e
SO2
HN
N
O

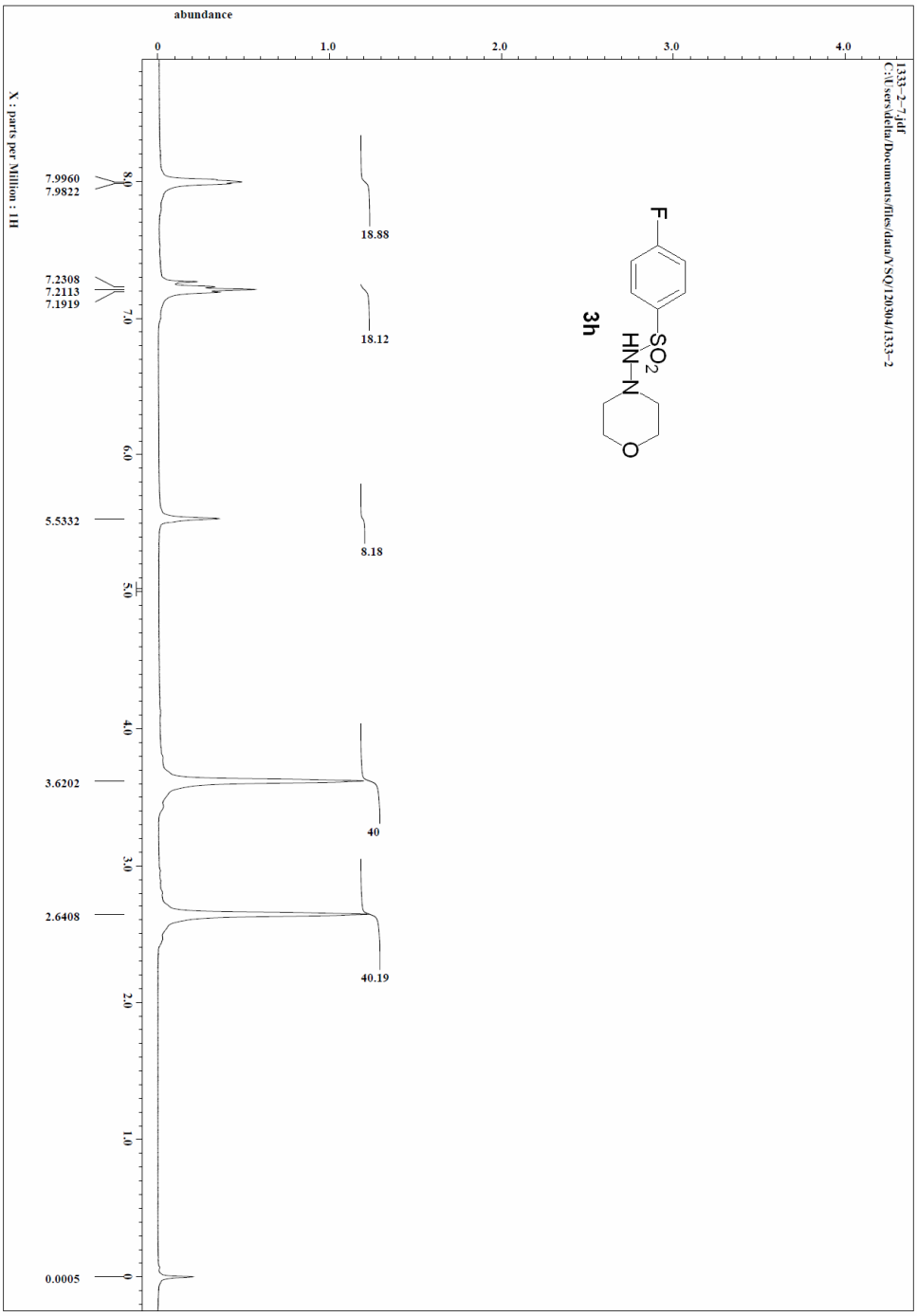

abundance
X : parts per Million : 13C
138.5067
133.1197
128.7910
128.0568
77.3138
76.9991
76.6750
66.5492
56.5665
3e

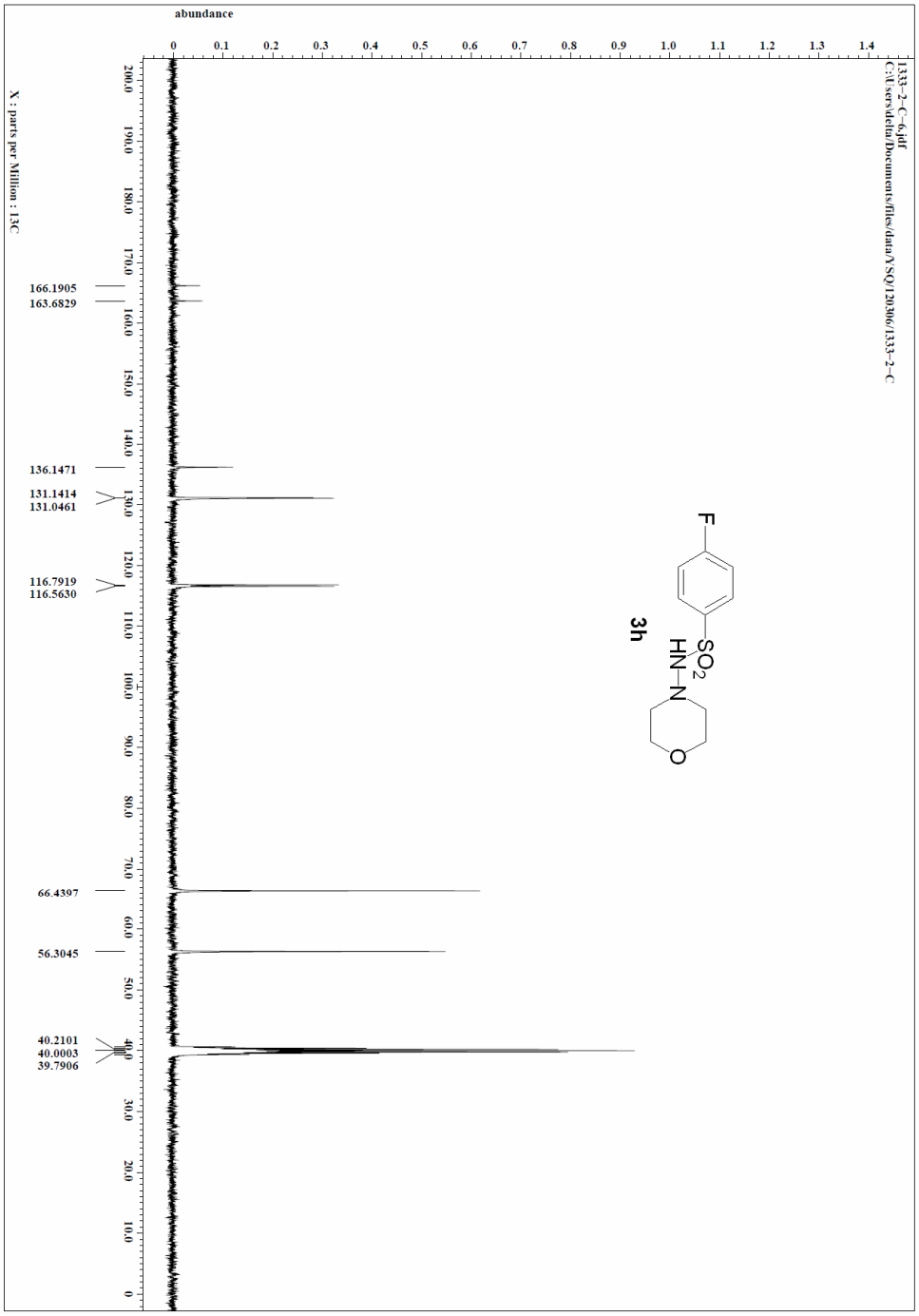

abundance
X : parts per Million : 1H
C:\Users\delta\Documents\files\data\YSQ\120304\1333-10
1333-10-7.jdf
8.8139
8.7921
8.4015
8.3832
8.1025
8.0830
7.9399
7.9204
7.6913
7.6718
7.6535
7.6088
7.5905
7.5710
7.5515
6.0429
3.4679
3.4610
2.5331
2.5263
10.02
9.74
9.91
10.6
8.73
20.8
9.24
40
39.52
3f
SO2
HN
N
O

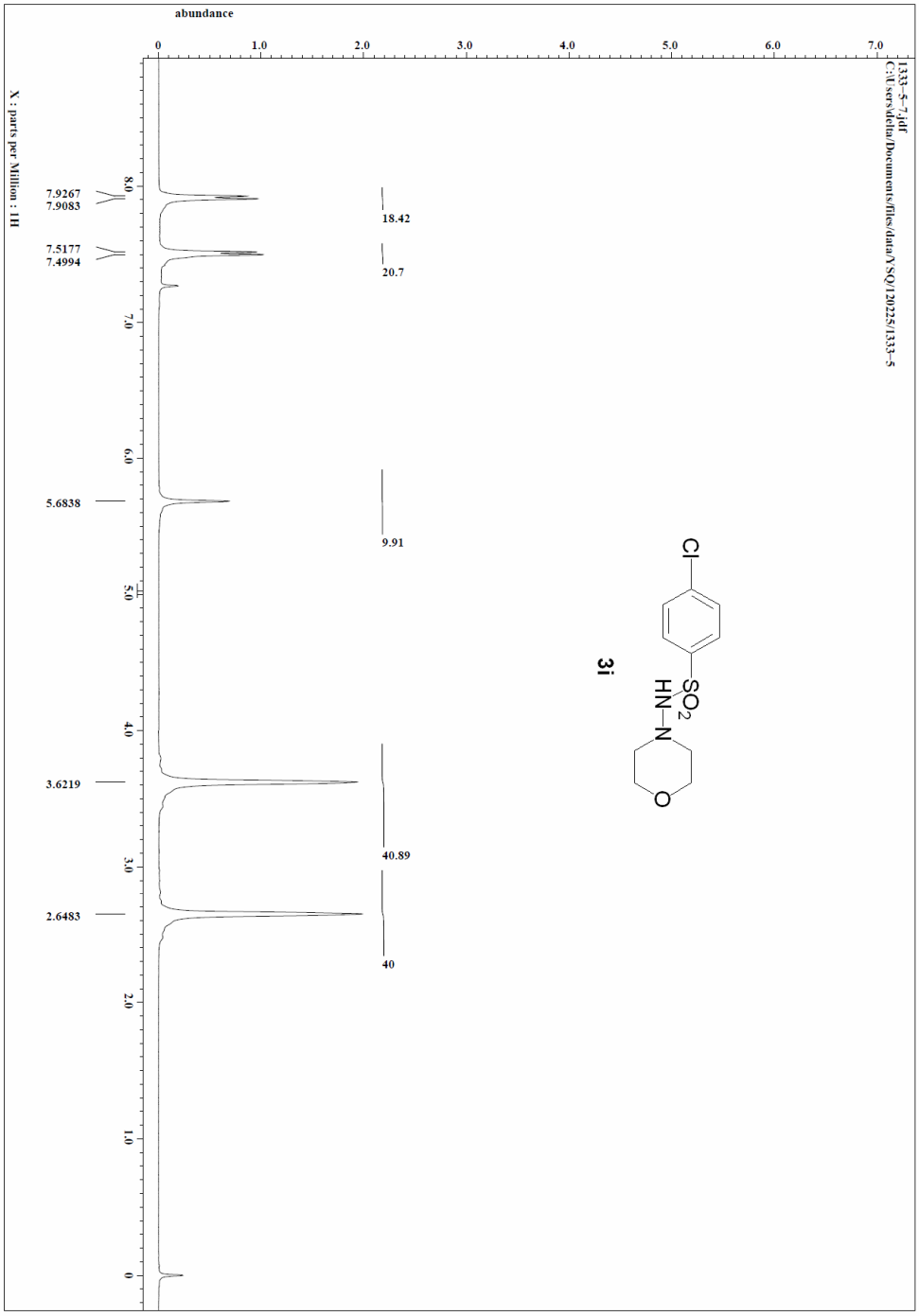

abundance
X : parts per Million : 13C
134.7416
131.3378
128.8397
128.1056
126.7707
125.0354
124.1201
77.3149
77.0002
76.6856
66.4073
56.6248
3f

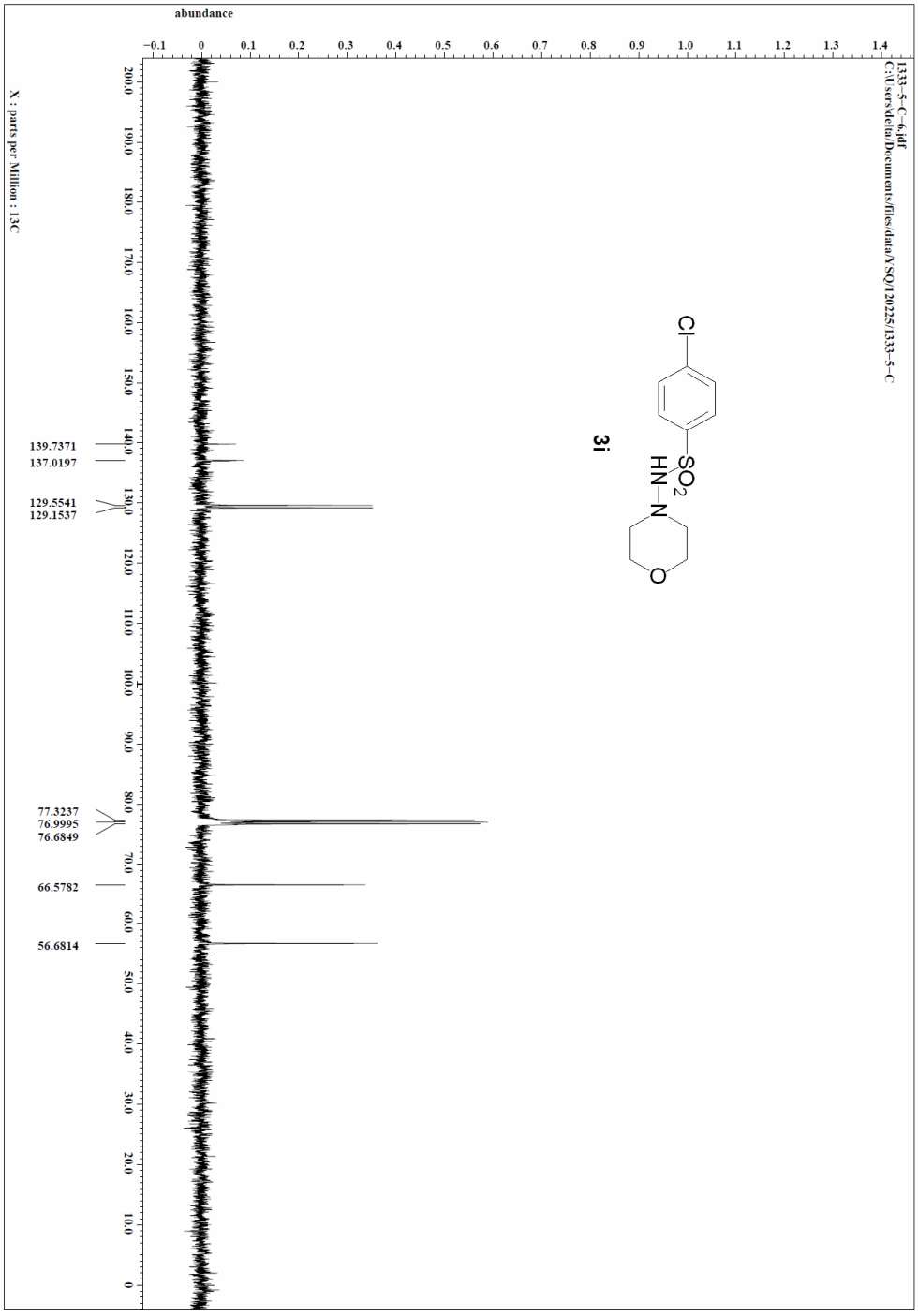

abundance
X : parts per Million : 1H
1334-5-7.jdf
C:\Users\delta\Documents\files\data\VSQ\120304\1334-5
8.5679
7.9963
7.9665
7.9275
7.9081
7.6790
7.6606
7.6354
7.6160
7.5988
6.0363
3.5724
3.5644
2.6445
2.6365
10.38
11.25
19.78
9.67
40
39.38
3g
SO2
HN
N
O

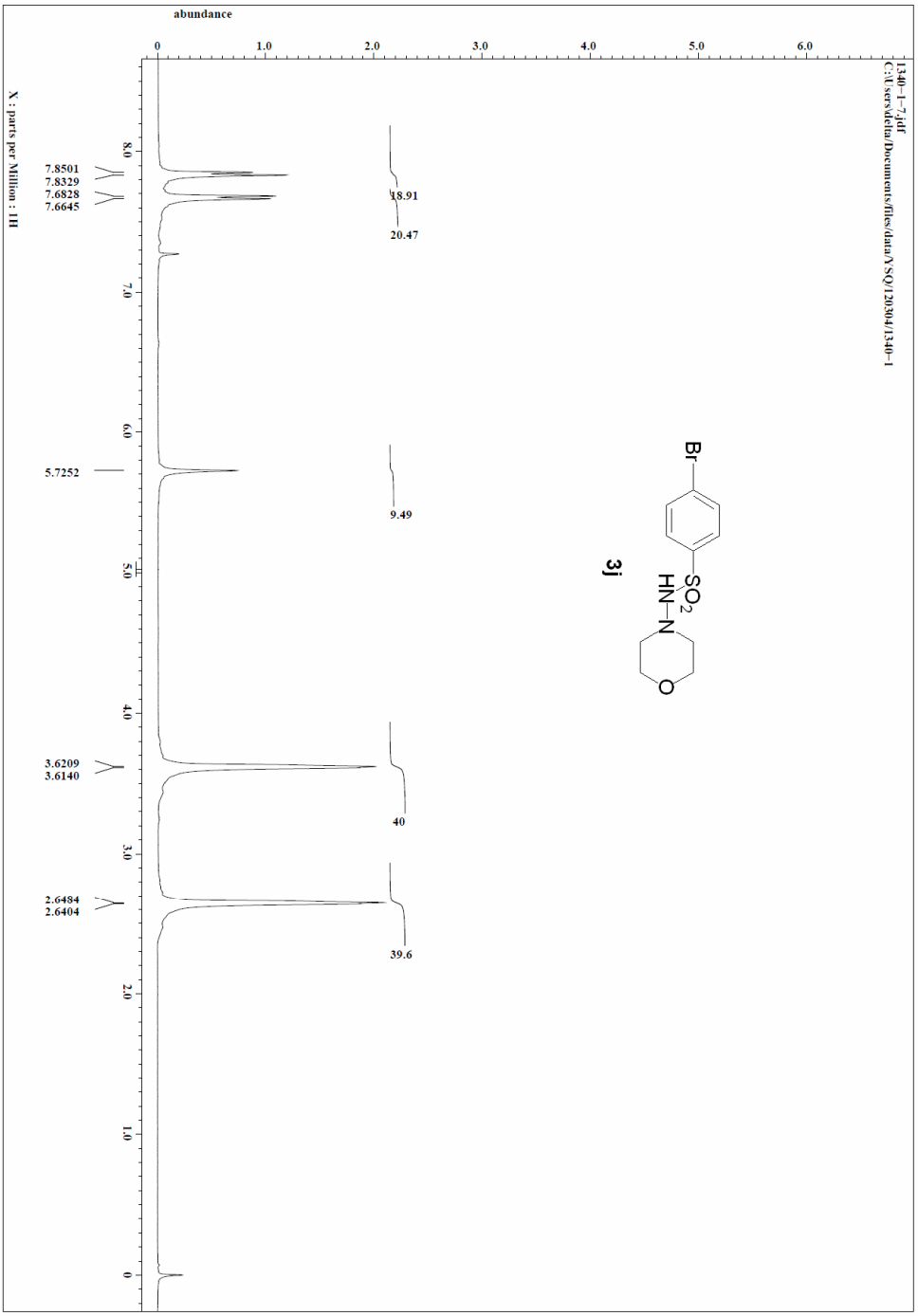

abundance
X : parts per Million : 13C
135.4377
129.6692
129.2592
129.0304
128.9637
127.8577
127.5049
123.0618
77.3149
77.0002
76.6856
66.5217
56.6153
3g
SO2
HN
N
O

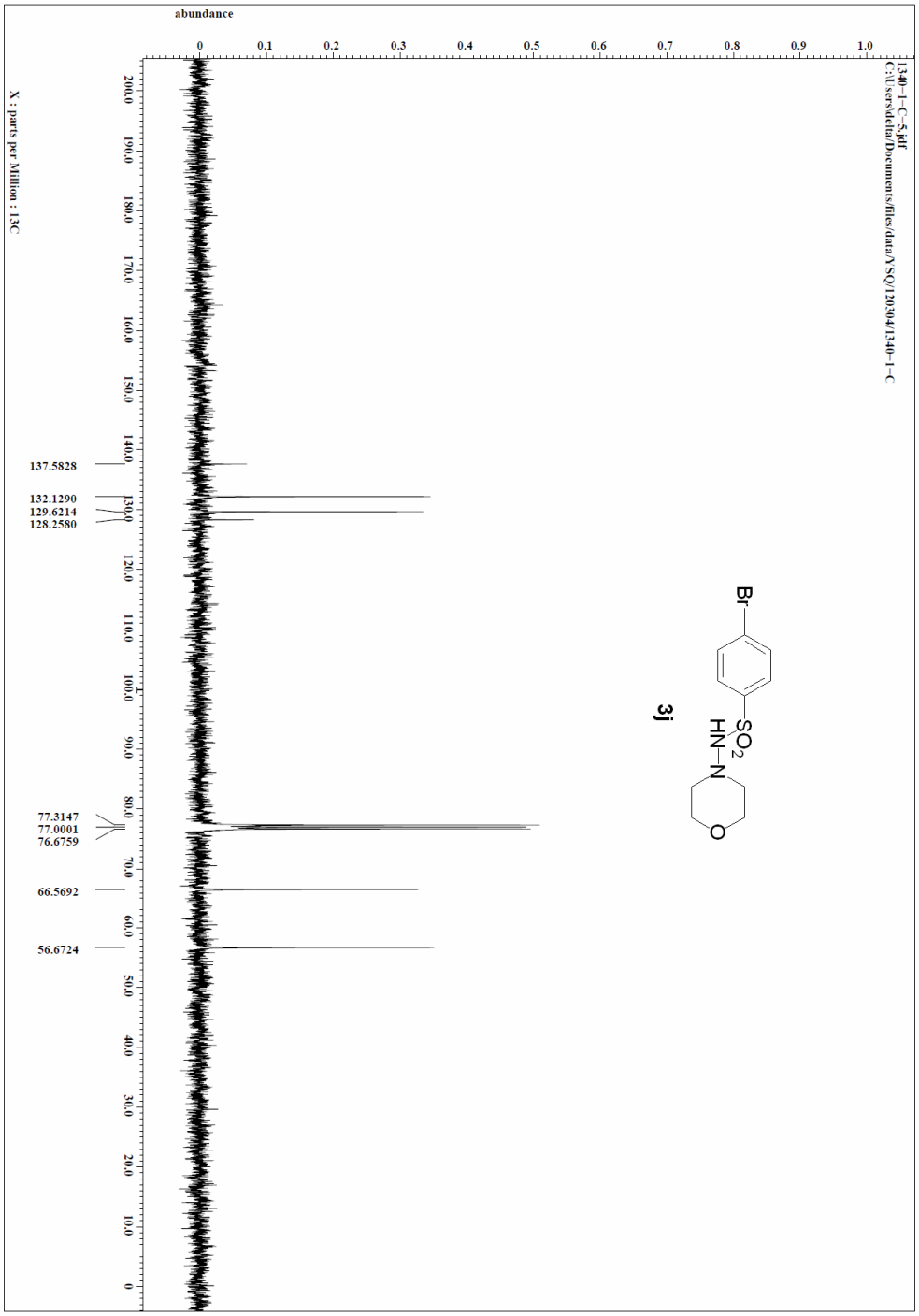

abundance
0
1.0
2.0
3.0
4.0
1333-2-7.jdf
C:\Users\delta\Documents\files\data\YSQ\120304\1333-2
X : parts per Million : 1H
7.9960
7.9822
7.2308
7.2113
7.1919
5.5332
3.6202
2.6408
0.0005
18.88
18.12
8.18
40
40.19
F
SO2
HN
N
O
3h

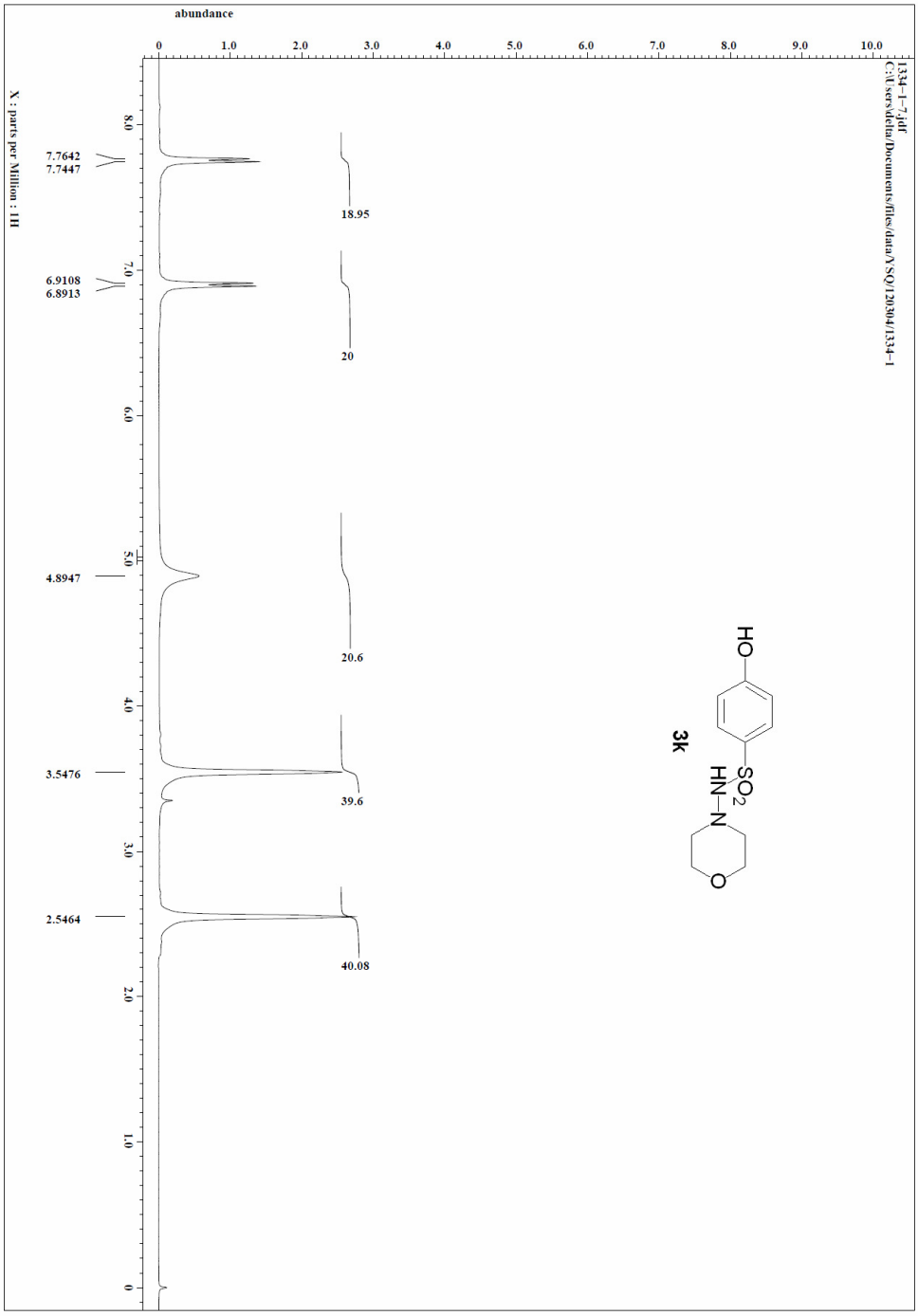

abundance
X : parts per Million : 13C
C:\Users\delta\Documents\files\data\YSQ\120306\1333-2-C
166.1905
163.6829
136.1471
131.1414
131.0461
116.7919
116.5630
66.4397
56.3045
40.2101
40.0003
39.7906
F
SO2
HN
N
O
3h

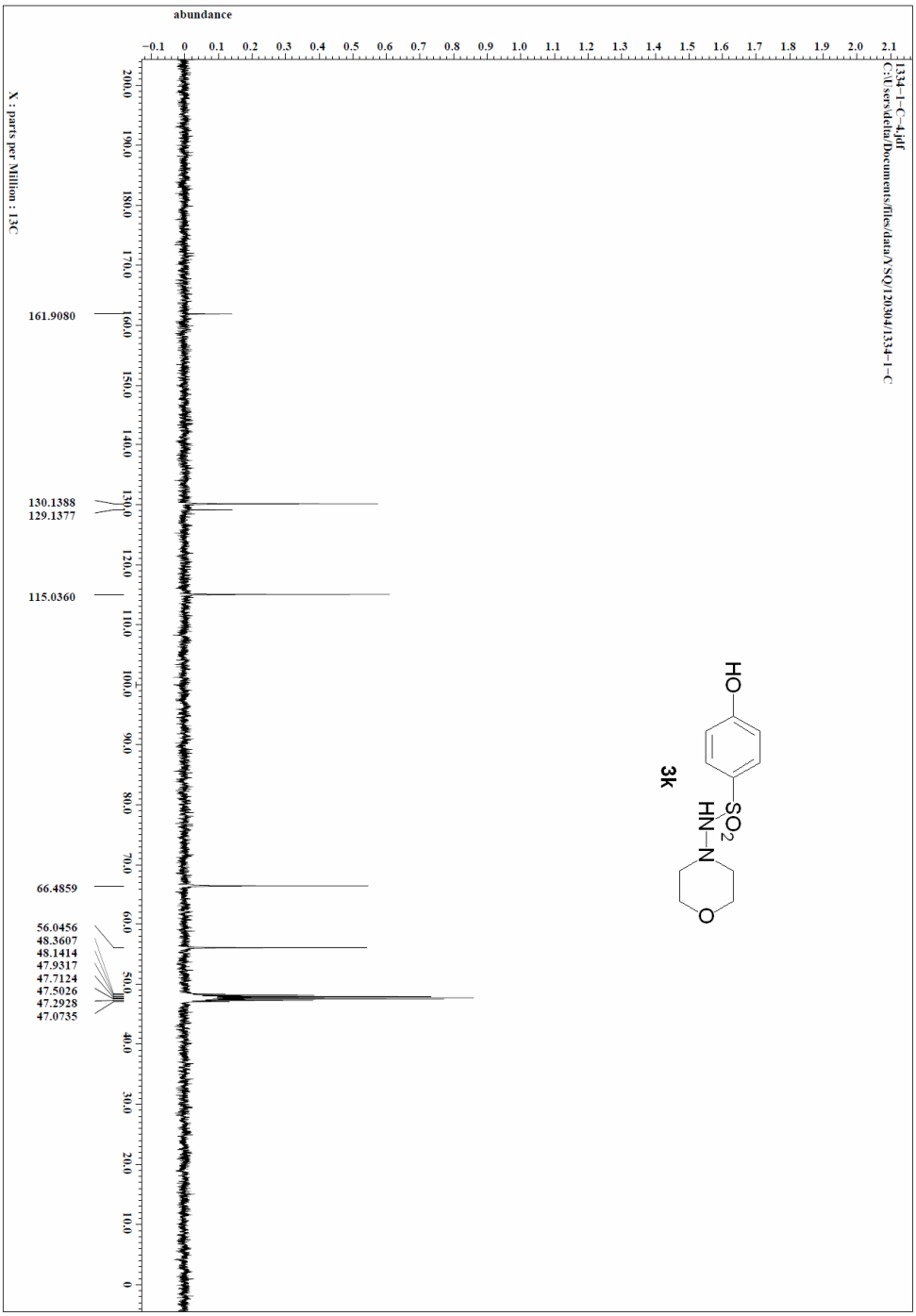

abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
1333--5--7.jdf
C:\Users\delta\Documents\files\data\YSQ\120225\1333--5
X : parts per Million : 1H
7.9267
7.9083
7.5177
7.4994
5.6838
3.6219
2.6483
18.42
20.7
9.91
40.89
40
3i
Cl
SO2
HN
N
O

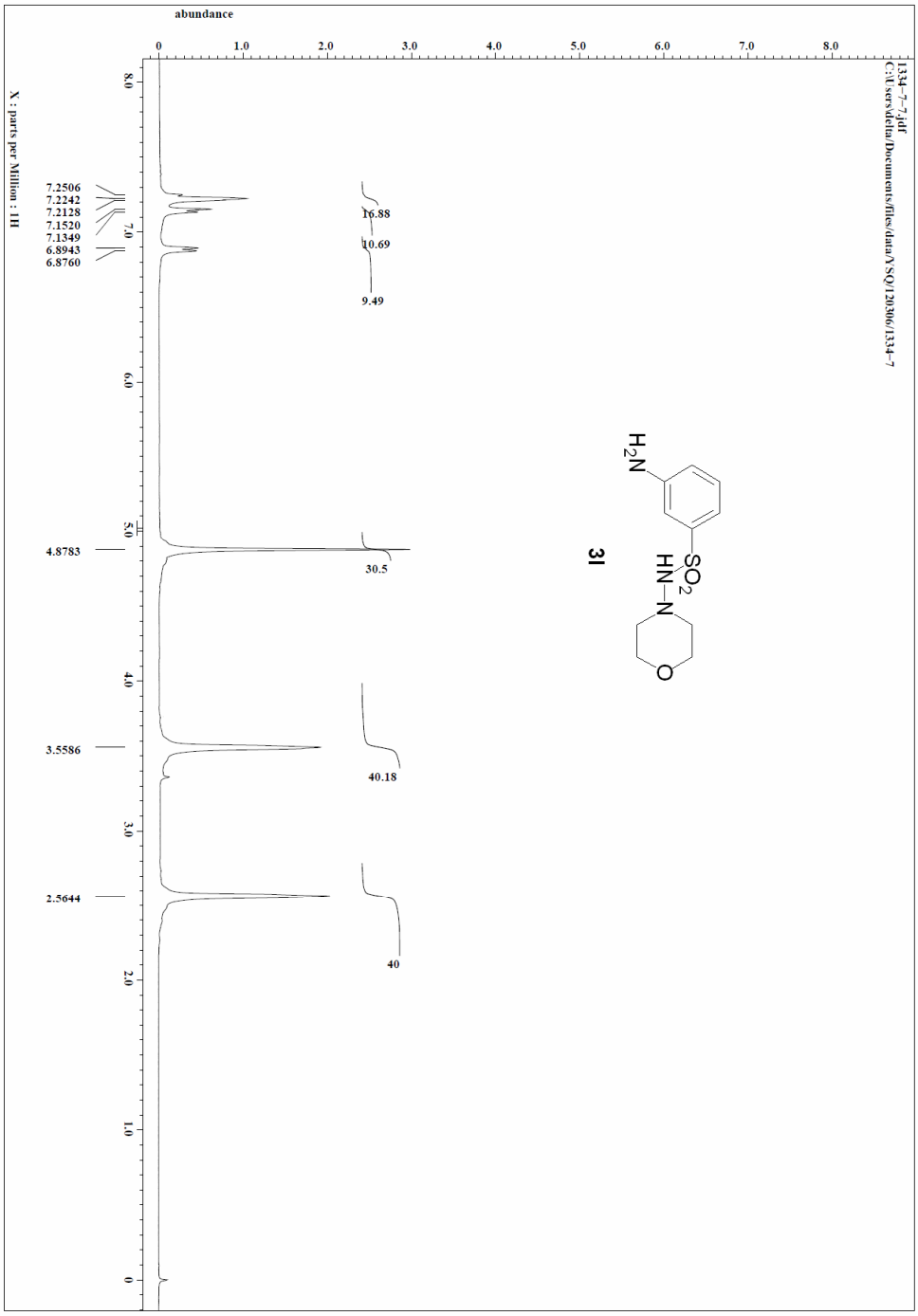

abundance
X : parts per Million : 13C
1333-5-C-6.jdf
C:\Users\delia\Documents\files\data\YSQ\120225\1333-5-C
139.7371
137.0197
129.5541
129.1537
77.3237
76.9995
76.6849
66.5782
56.6814
3i
Cl
SO2
HN
N
O

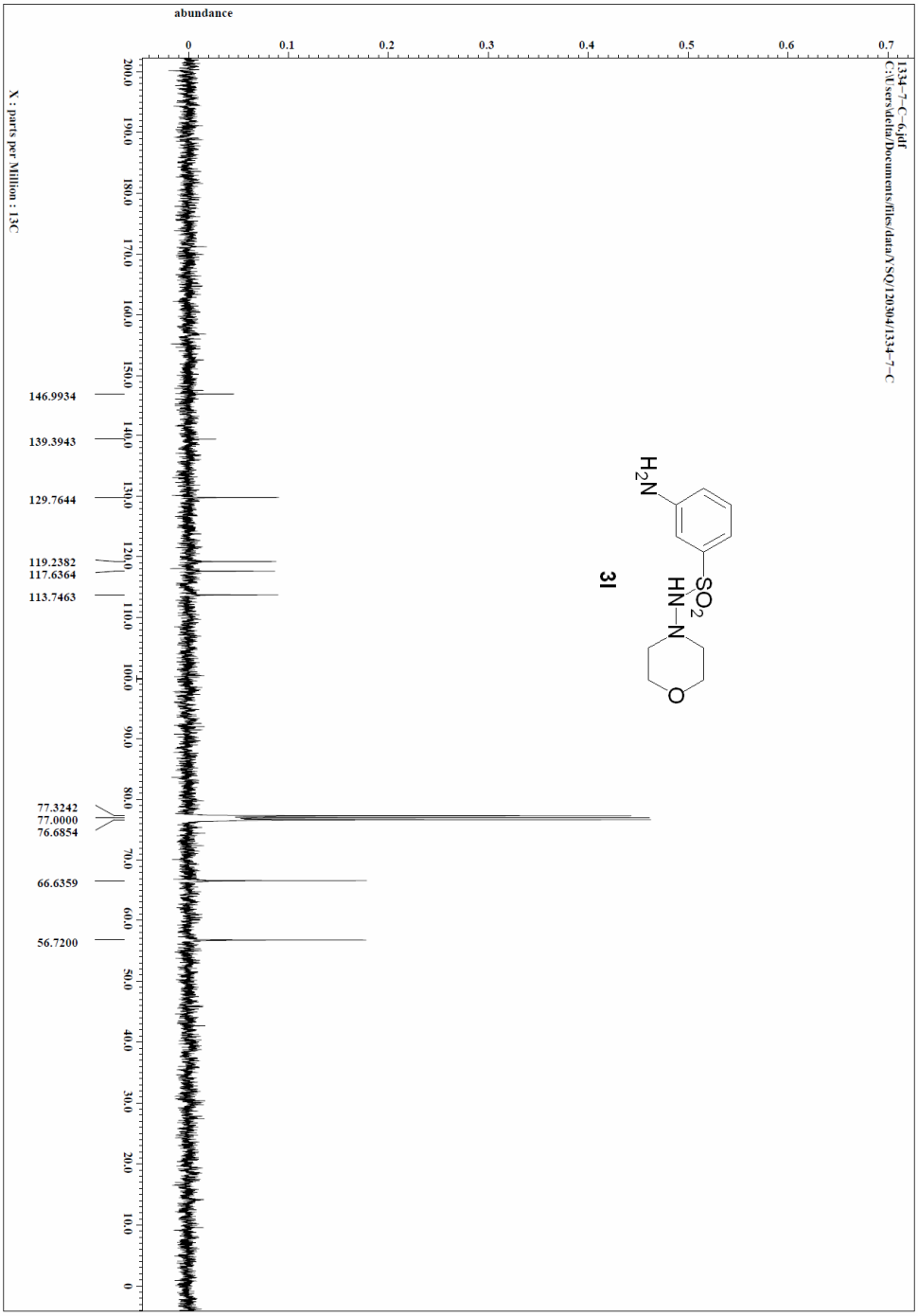

abundance
X : parts per Million : 1H
C:\Users\delia\Documents\files\data\YSQ\120304\1340-1
1340-1-7.jdf
7.8501
7.8329
7.6828
7.6645
5.7252
3.6209
3.6140
2.6484
2.6404
18.91
20.47
9.49
40
39.6
3j
Br
SO2
HN
N
O

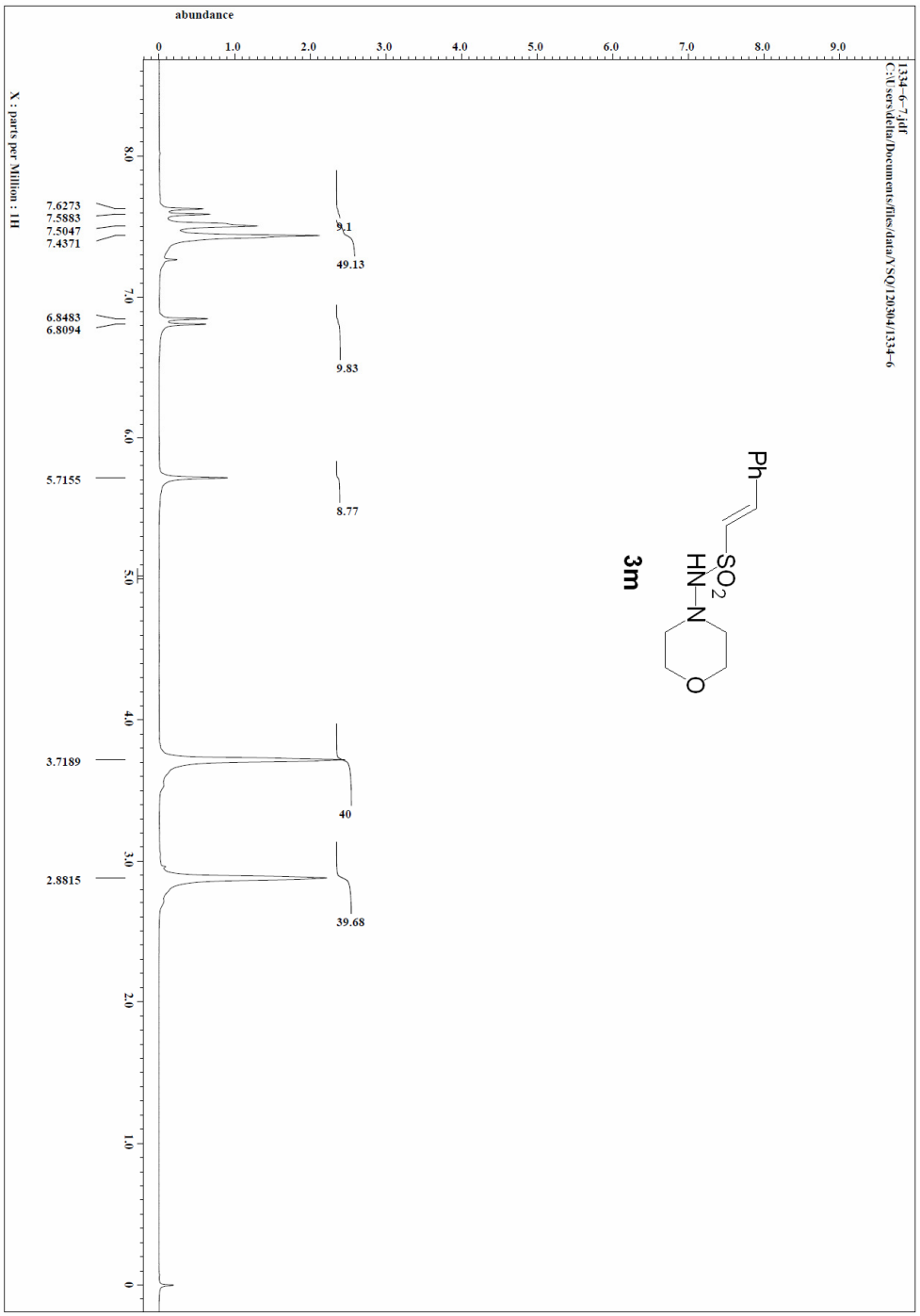

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1340-1-C-5.jdf
C:\Users\delta\Documents\files\data\YSQ\120304\1340-1-C
X : parts per Million : 13C
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
137.5828
132.1290
129.6214
128.2580
77.3147
77.0001
76.6759
66.5692
56.6724
3j
Br
SO2
HN
N
O

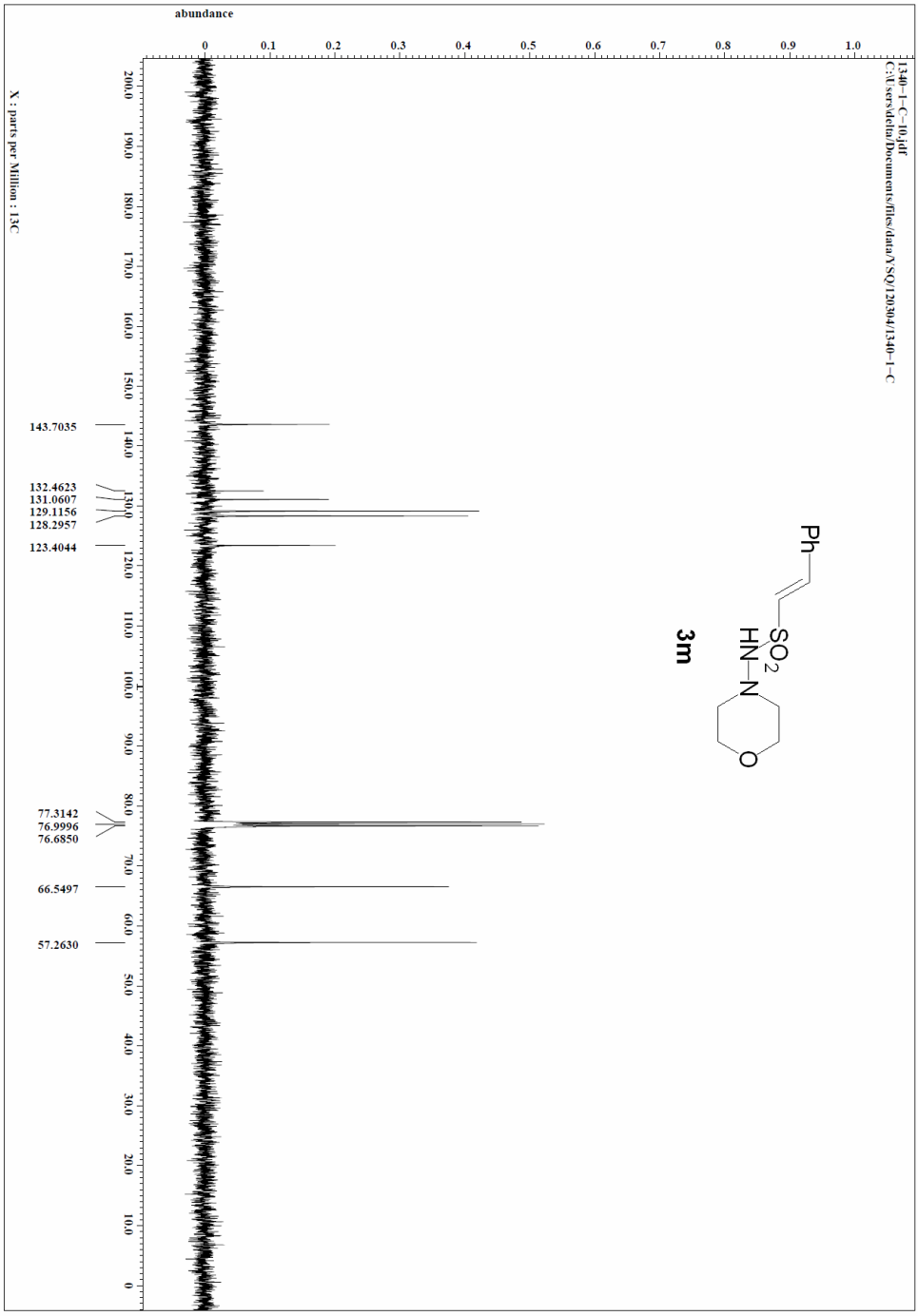

abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
1334-1-7.jdf
C:\Users\delta\Documents\files\data\YSQ\120304\1334-1
X : parts per Million : 1H
7.7642
7.7447
6.9108
6.8913
4.8947
3.5476
2.5464
18.95
20
20.6
39.6
40.08
HO
SO2
HN
N
O
3k

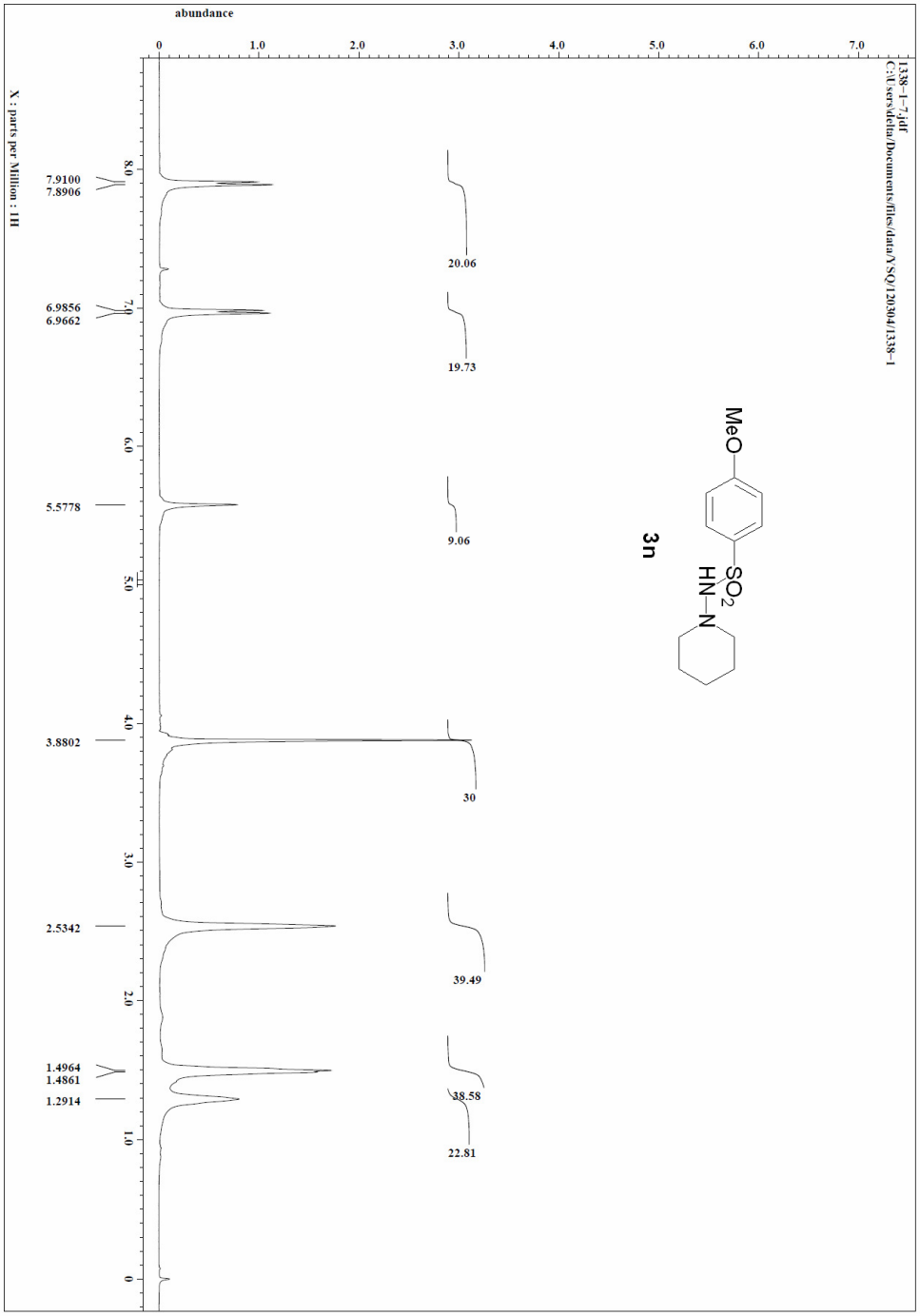

abundance
X : parts per Million : 13C
C:\Users\delta\Documents\files\data\YSQ\120304\1334-1-C
1334-1-C-4.jdf
161.9080
130.1388
129.1377
115.0360
66.4859
56.0456
48.3607
48.1414
47.9317
47.7124
47.5026
47.2928
47.0735
HO
SO2
HN
N
O
3k

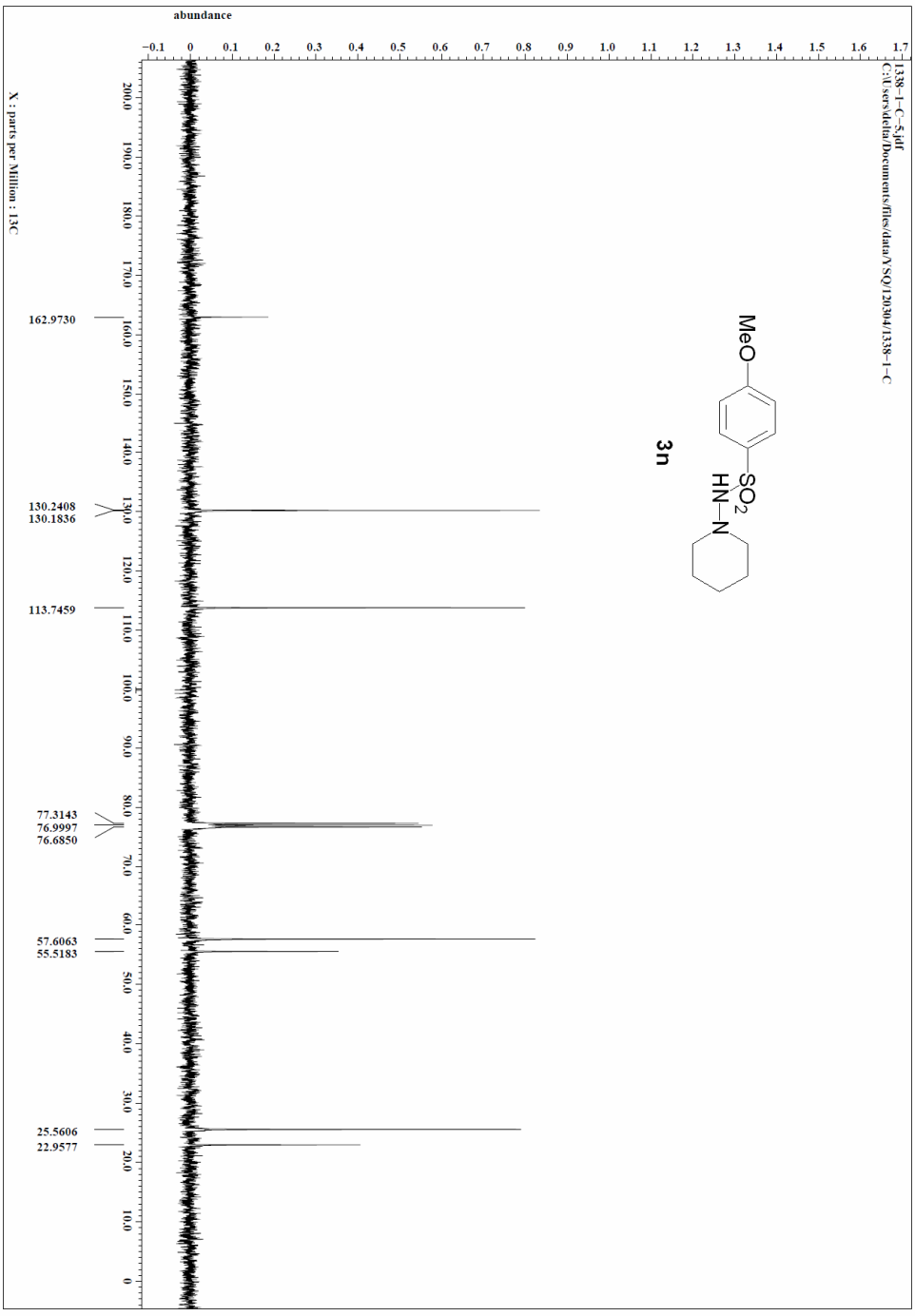

abundance
X : parts per Million : 1H
C:\Users\delta\Documents\files\data\YSQ\120306\1334-7
1334-7-7.jdf
7.2506
7.2242
7.2128
7.1520
7.1349
6.8943
6.8760
4.8783
3.5586
2.5644
16.88
10.69
9.49
30.5
40.18
40
3l
H2N
SO2
HN
N
O

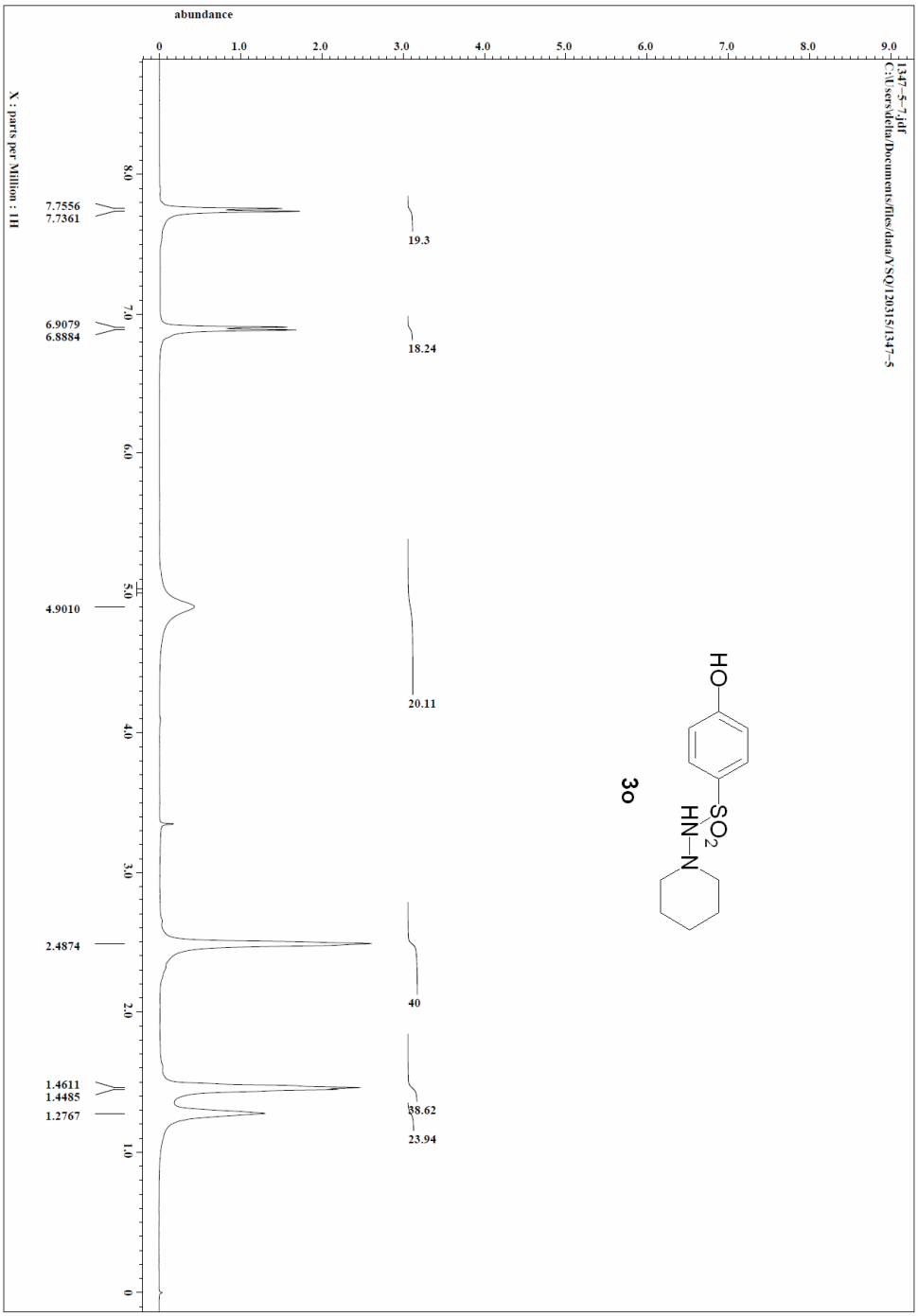

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
1334-7-C--6.jdf
C:\Users\delta\Documents\files\data\YSQ\120304\1334-7-C
X : parts per Million : 13C
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
146.9934
139.3943
129.7644
119.2382
117.6364
113.7463
77.3242
77.0000
76.6854
66.6359
56.7200
H2N
SO2
HN
N
O
3l

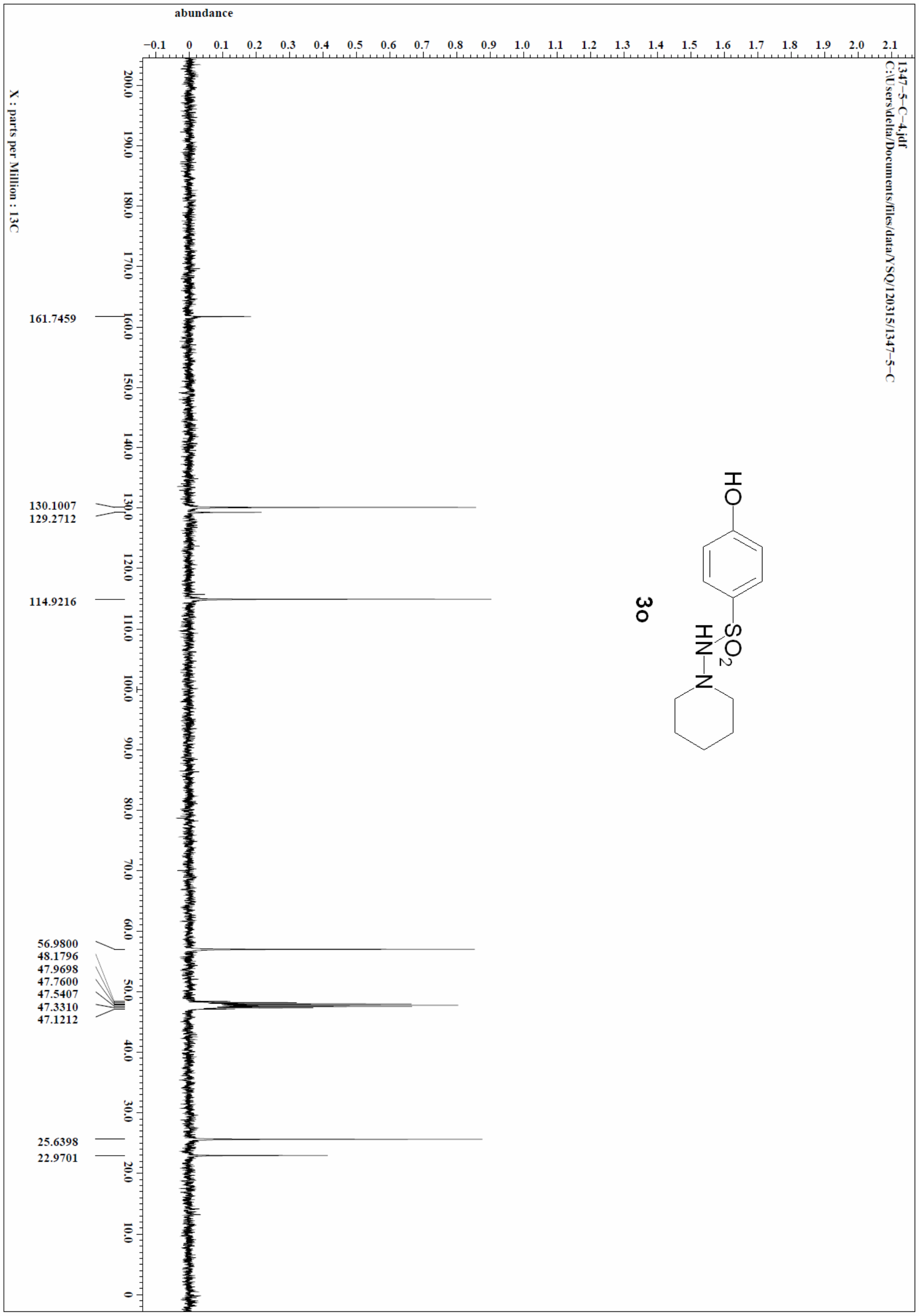

abundance
X : parts per Million : 1H
7.6273
7.5883
7.5047
7.4371
6.8483
6.8094
5.7155
3.7189
2.8815
9.1
49.13
9.83
8.77
40
39.68
Ph
SO2
HN
N
O
3m

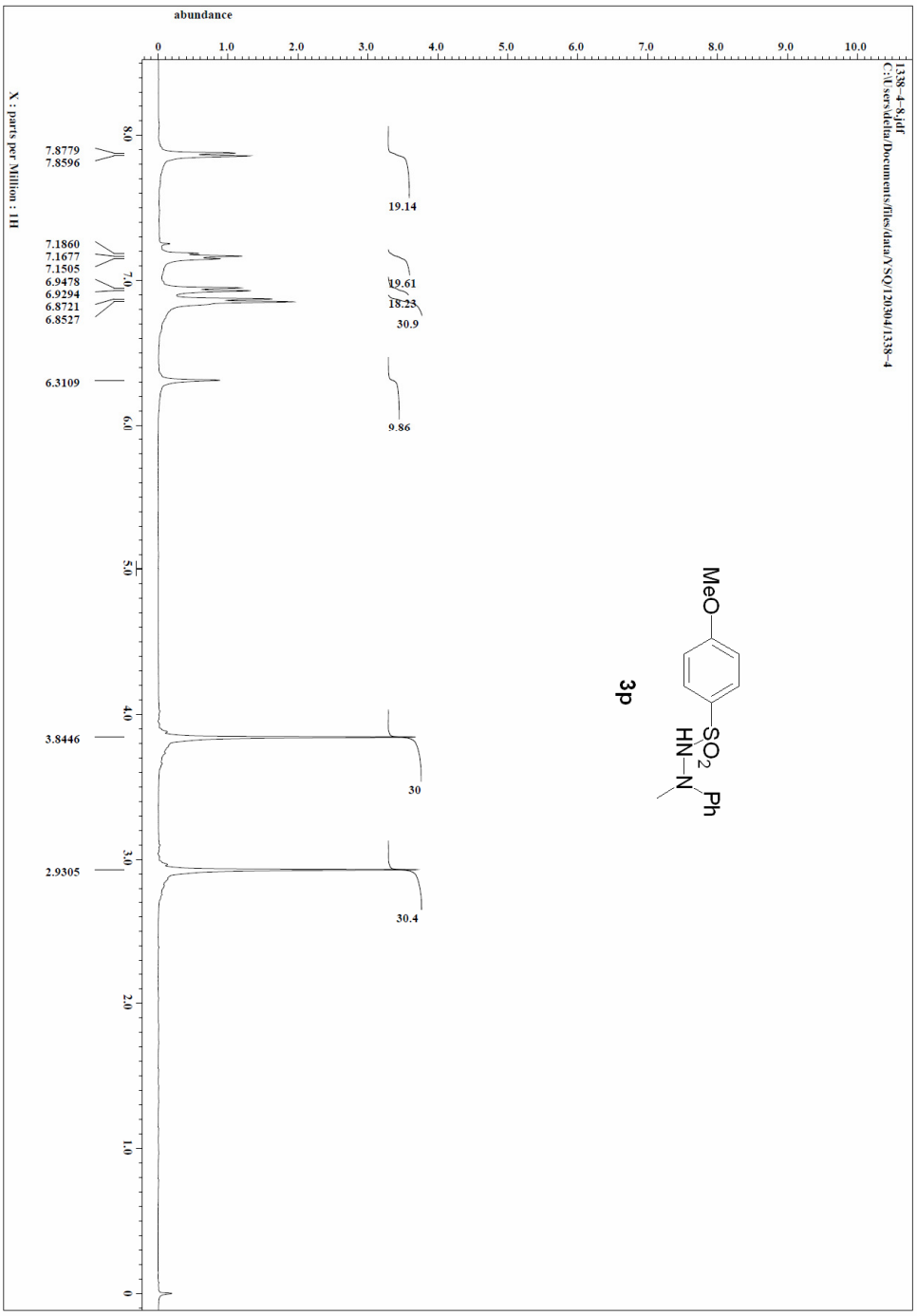

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1340-1-C-10.jdf
C:\Users\delta\Documents\files\data\YSQ\120304\1340-1-C
X : parts per Million : 13C
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
143.7035
132.4623
131.0607
129.1156
128.2957
123.4044
77.3142
76.9996
76.6850
66.5497
57.2630
Ph
SO2
HN
N
O
3m

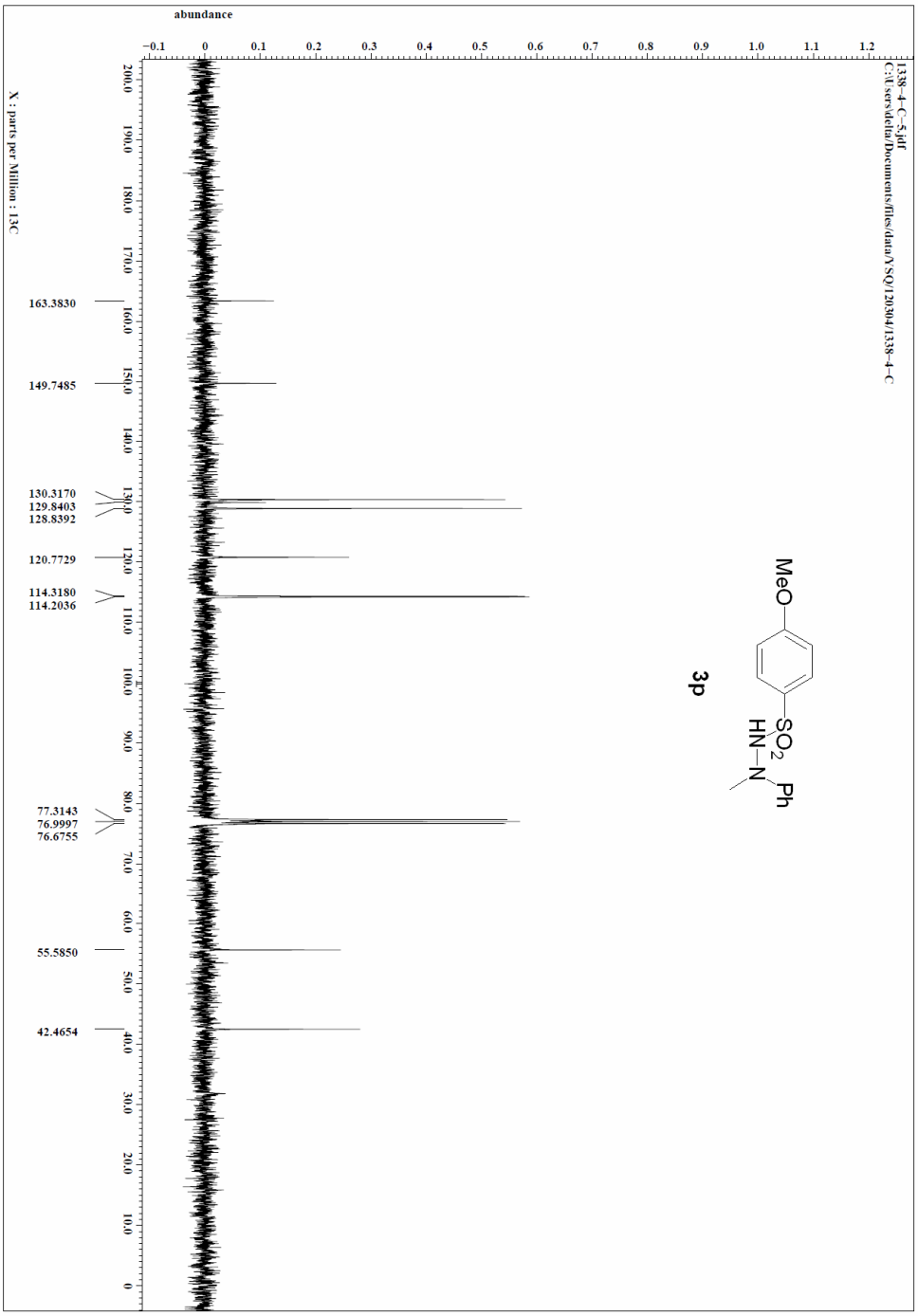

abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
1338-1-7.jdf
C:\Users\della\Documents\files\data\YSQ\120304\1338-1
X : parts per Million : 1H
7.9100
7.8906
6.9856
6.9662
5.5778
3.8802
2.5342
1.4964
1.4861
1.2914
20.06
19.73
9.06
30
39.49
38.58
22.81
MeO
SO2
HN
N
3n

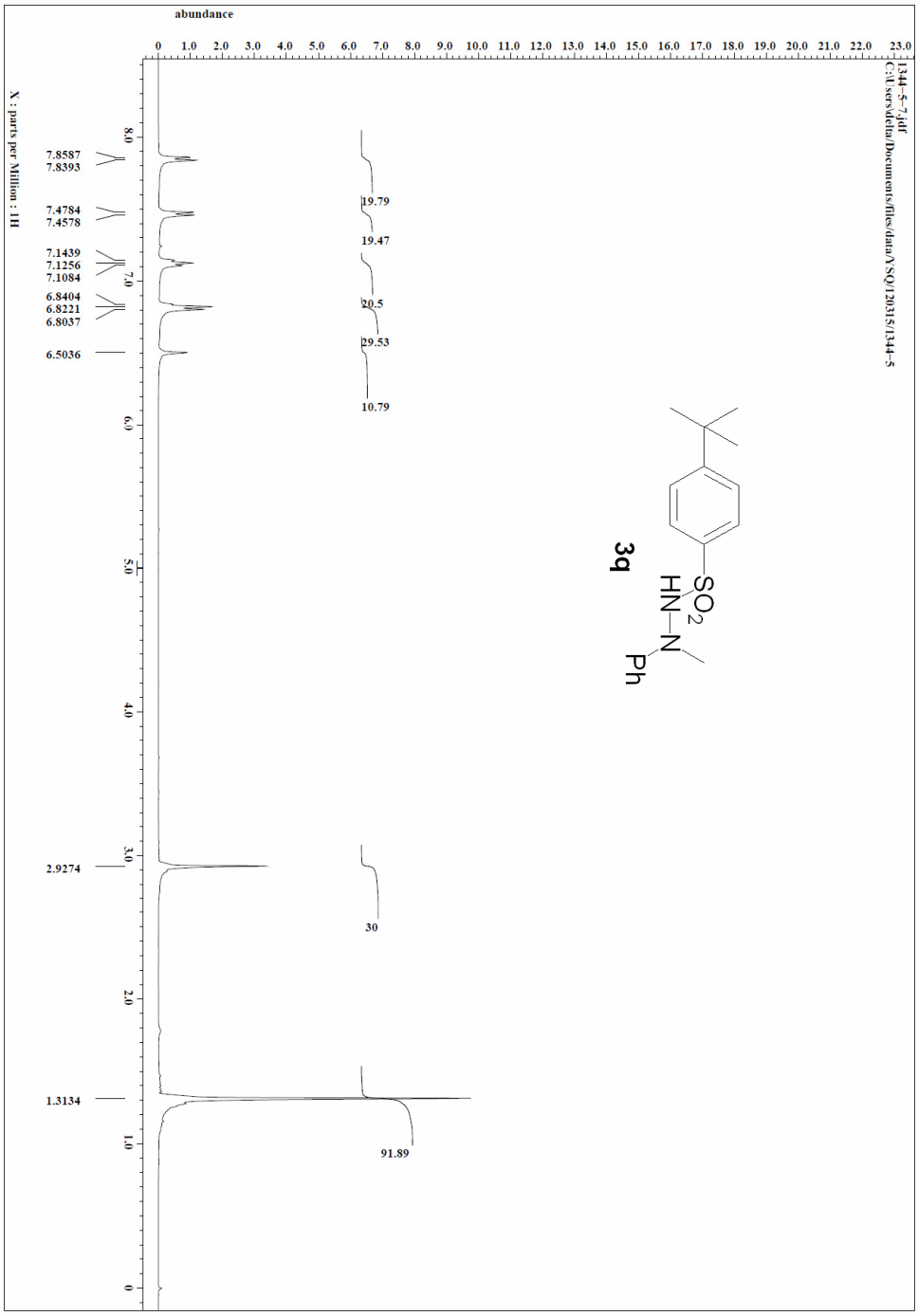

abundance
X : parts per Million : 13C
C:\Users\delia\Documents\files\data\SQ\120304\1338-1-C
1338-1-C-5.jdf
162.9730
130.2408
130.1836
113.7459
77.3143
76.9997
76.6850
57.6063
55.5183
25.5606
22.9577
MeO
SO2
HN
N
3n

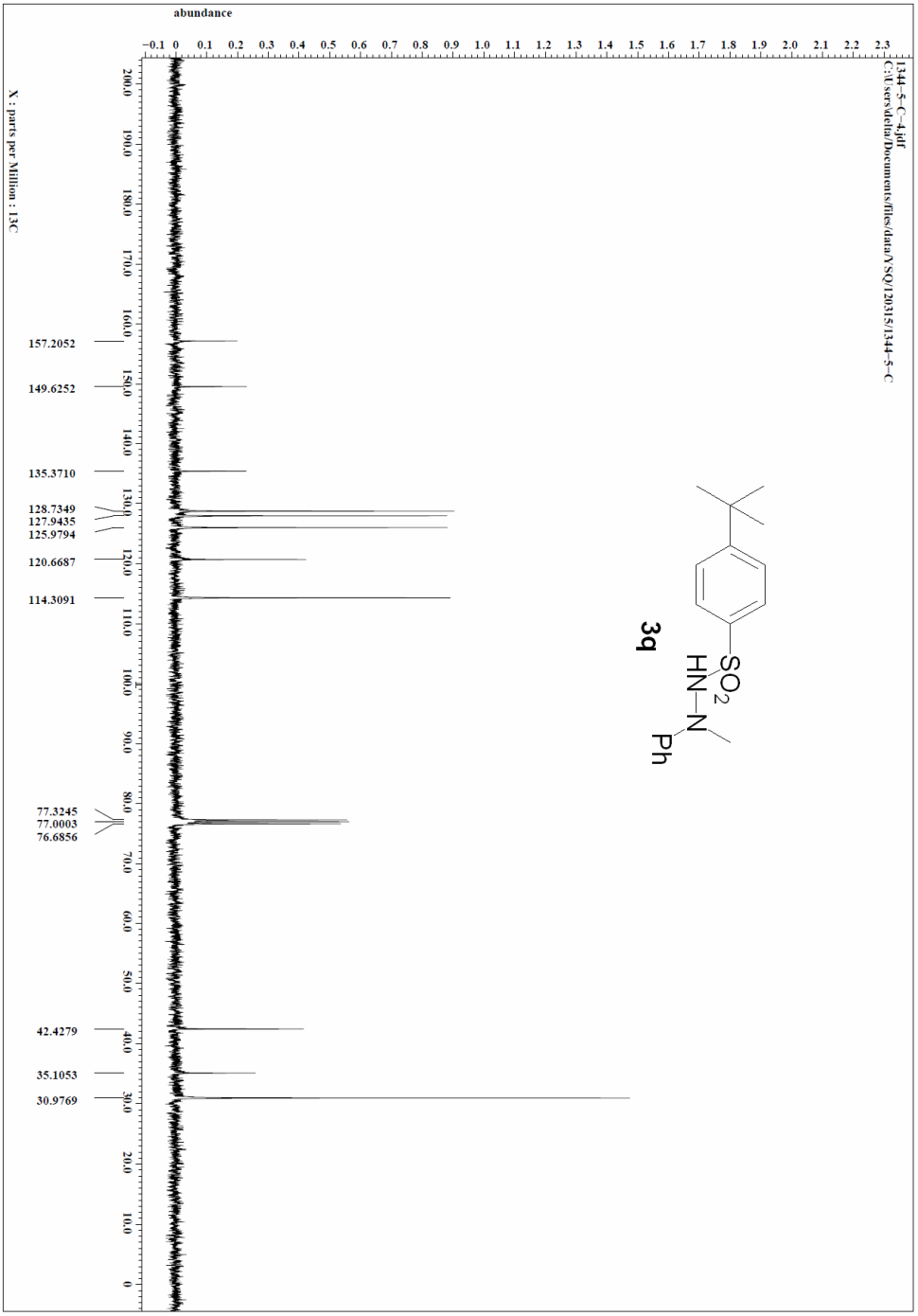

abundance
X : parts per Million : 1H
C:\Users\delia\Documents\files\data\YSQ\120315\1347-5
1347-5-7.jdf
7.7556
7.7361
6.9079
6.8884
4.9010
2.4874
1.4611
1.4485
1.2767
19.3
18.24
20.11
40
38.62
23.94
3o
HO
SO2
HN
N

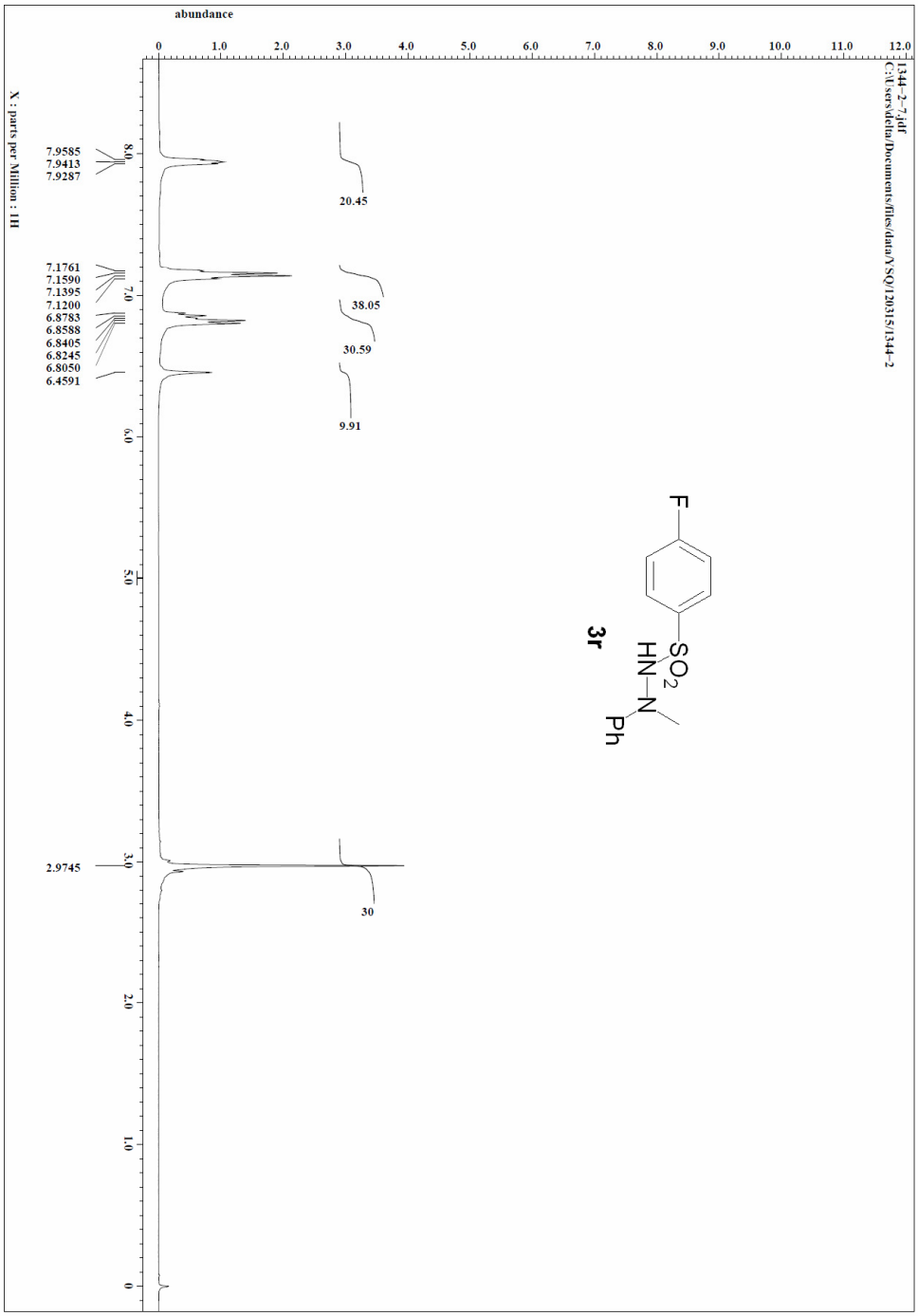

abundance
X : parts per Million : 13C
1347−5−C−4.jdf
3o
161.7459
130.1007
129.2712
114.9216
56.9800
48.1796
47.9698
47.7600
47.5407
47.3310
47.1212
25.6398
22.9701

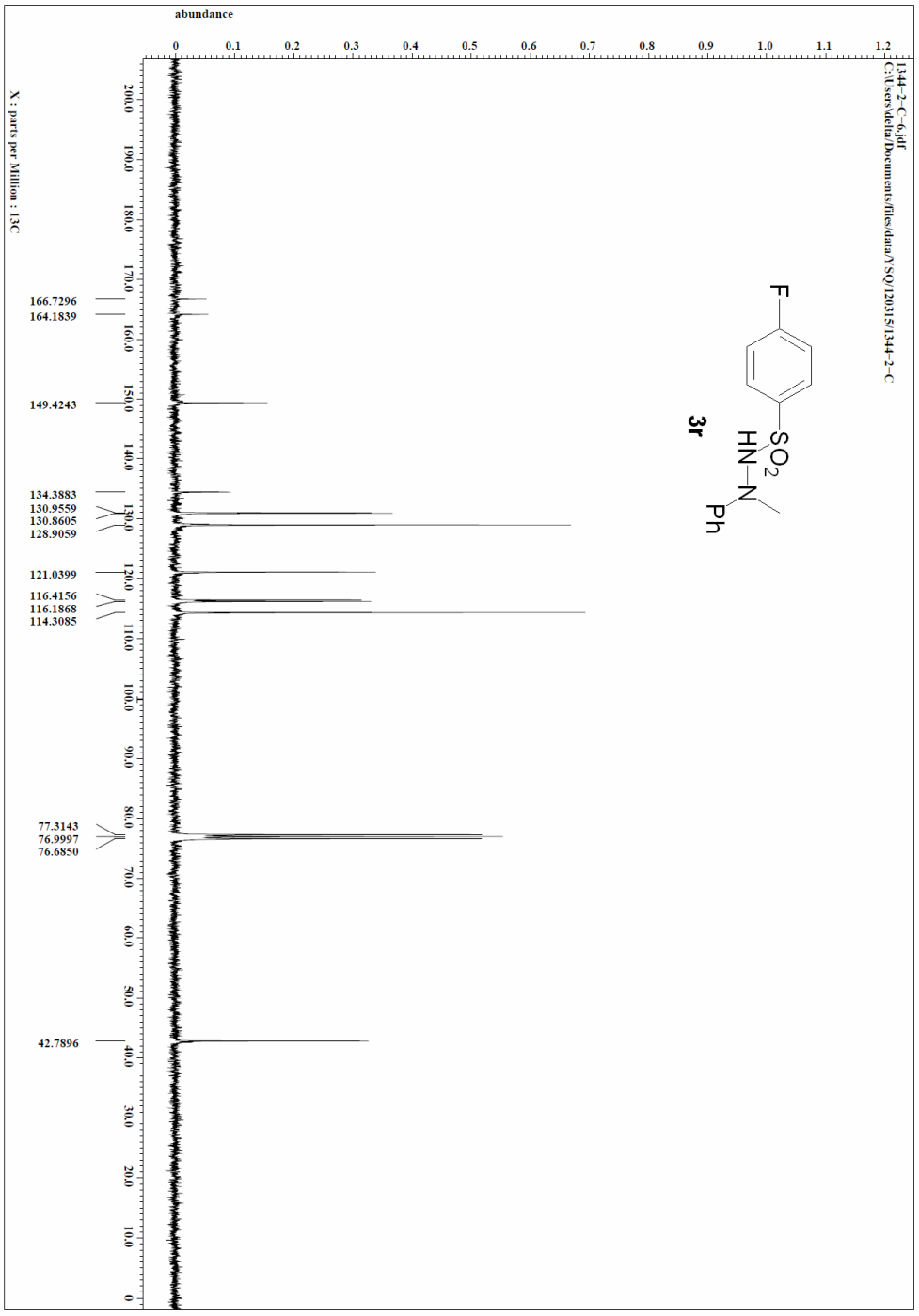

abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
1338--4--8.idf
C:\Users\dela\Documents\files\data\TSQ\120304\1338--4
X : parts per Million : 1H
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.8779
7.8596
7.1860
7.1677
7.1505
6.9478
6.9294
6.8721
6.8527
6.3109
3.8446
2.9305
19.14
19.61
18.23
30.9
9.86
30
30.4
MeO
SO2
HN
N
Ph
3p


abundance
X : parts per Million : 13C
163.3830
149.7485
130.3170
129.8403
128.8392
120.7729
114.3180
114.2036
77.3143
76.9997
76.6755
55.5850
42.4654
MeO
SO2
HN
N
Ph
3p


abundance
X : parts per Million : 1H
C:\Users\delta\Documents\files\data\YSQ\120315\1344-5
1344-5-7.jdf
7.8587
7.8393
7.4784
7.4578
7.1439
7.1256
7.1084
6.8404
6.8221
6.8037
6.5036
2.9274
1.3134
19.79
19.47
20.5
29.53
10.79
30
91.89
3q
SO2
HN
N
Ph


abundance
X : parts per Million : 13C
157.2052
149.6252
135.3710
128.7349
127.9435
125.9794
120.6687
114.3091
77.3245
77.0003
76.6856
42.4279
35.1053
30.9769
3q
SO2
HN
N
Ph


abundance
X : parts per Million : 1H
C:\Users\delta\Documents\files\data\YSQ\120315\1344-2_7.jdf
1344-2--7.jdf
7.9585
7.9413
7.9287
7.1761
7.1590
7.1395
7.1200
6.8783
6.8588
6.8405
6.8245
6.8050
6.4591
2.9745
20.45
38.05
30.59
9.91
30
F
SO2
HN
N
Ph
3r


abundance
X : parts per Million : 13C
1344-2-C-6.jdf
C:\Users\dell\Documents\files\data\YSQ\120315\1344-2-C
166.7296
164.1839
149.4243
134.3883
130.9559
130.8605
128.9059
121.0399
116.4156
116.1868
114.3085
77.3143
76.9997
76.6850
42.7896
F
SO2
HN
N
Ph
3r