Electronic Supplementary Material (ESI) for Chemical Communications

A palladium-catalyzed reaction of aryl halides, potassium metabisulfite, and hydrazines

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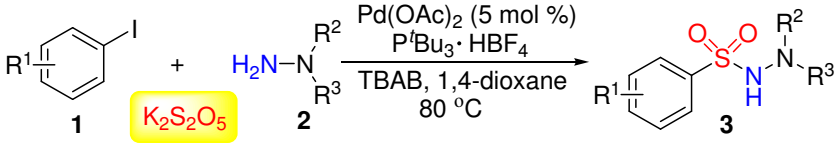
Supporting Information

General experimental methods:

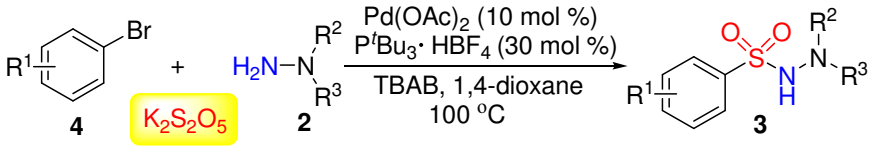
Unless otherwise stated, all commercial reagents were used as received. All solvents were dried and distilled according to standard procedures. Flash column chromatography was performed using silica gel (60-Å pore size, 32–63μm, standard grade). Analytical thin–layer chromatography was performed using 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 aryl iodide **1**, potassium metabisulfite, with hydrazines **2***

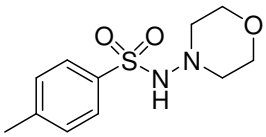


Hydrzine **2** (0.6 mmol) was added to a mixture of aryl iodide **1** (0.5 mmol), potassium metabisulfite (0.5 mmol), $Pd(OAc)_2$ (5 mol %), $P^tBu_3{\cdot}HBF_4$ (10 mol %), HBF_4 (20 mol %), and TBAB (0.75 mmol) in 1,4-dioxane (2.0 mL). The reaction was stirred at 80 °C for 12 hours. After completion of the reaction as indicated by TLC, the residue was purified directly by flash chromatography on silica gel to afford aryl *N*-aminosulfonamides **3**.

*General experimental procedure for the palladium-catalyzed three-component reaction of aryl bromide **4**, potassium metabisulfite, with hydrazines **2***

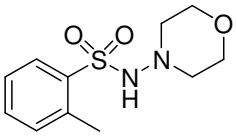


Hydrzine **2** (0.75 mmol) was added to a mixture of aryl bromide **4** (0.5 mmol), potassium metabisulfite (1.0 mmol), $Pd(OAc)_2$ (10 mol %), $P^tBu_3{\cdot}HBF_4$ (30 mol %) and TBAB (0.75 mmol) in 1,4-dioxane (2.0 mL). The reaction was stirred at 100 °C for 12 hours. After completion of the reaction as indicated by TLC, the residue was purified directly by flash chromatography on silica gel to afford aryl *N*-aminosulfonamides **3**.



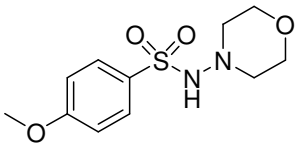
4-Methyl-*N*-morpholinobenzenesulfonamide (**3a**)[1]

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.43 (s, 3H), 2.63 (t, J = 4.1 Hz, 4H), 3.59 (d, J = 4.4 Hz, 4H), 6.21 (s, 1H), 7.31 (d, J = 8.2Hz, 2H), 7.86 (d, J = 8.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.4, 56.3, 66.5, 128.0, 129.3, 135.5, 143.8.



2-Methyl-*N*-morpholinobenzenesulfonamide (**3b**)[1]

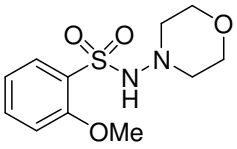
^{1}H NMR (400 MHz, $CDCl_3$) δ 2.65 (t, J = 4.6 Hz, 4H), 2.70 (s, 3H), 3.57 (t, J = 4.1 Hz, 4H), 5.98 (s, 1H), 7.29-7.35 (m, 2H), 7.47 (t, J = 7.8 Hz, 1H), 8.07 (d, J = 7.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 20.6, 56.5, 66.5, 126.0, 130.9, 132.2, 133.1, 136.4, 137.9.



4-Methoxy-*N*-morpholinobenzenesulfonamide (**3c**)[1]

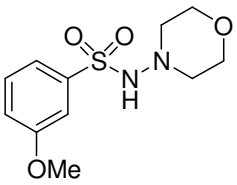
^{1}H NMR (400 MHz, $CDCl_3$) δ 2.62 (t, J = 4.6 Hz, 4H), 3.61 (t, J = 4.1 Hz, 4H), 3.88 (s, 3H), 5.68 (s, 1H), 6.98 (d, J = 9.2 Hz, 2H), 7.90 (d, J = 9.2 Hz, 2H); ^{13}C NMR

(100 MHz, $CDCl_3$) δ 55.6, 56.6, 66.6, 113.9, 130.0, 130.3, 163.2.



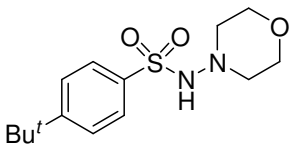
2-Methoxy-*N*-morpholinobenzenesulfonamide (**3d**)[1]

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.67 (t, J = 4.6 Hz, 4H), 3.56 (t, J = 4.1 Hz, 4H), 4.00 (s, 3H), 6.19 (s, 1H), 7.04 (d, J = 8.2 Hz, 1H), 7.10 (t, J = 7.8 Hz, 1H), 7.58 (t, J = 7.3 Hz, 1H), 8.00 (d, J = 7.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 56.2, 56.3, 66.3, 112.0, 120.6, 126.7, 131.7, 135.0, 156.1.



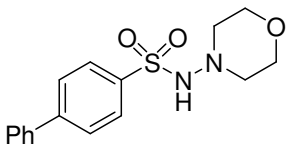
3-Methoxy-*N*-morpholinobenzenesulfonamide (**3e**)[1]

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.64 (t, J = 4.1 Hz, 4H), 3.60 (d, J = 4.1Hz, 4H), 3.86 (s, 3H), 6.19 (s, 1H), 7.13 (d, J = 7.8 Hz, 1H), 7.42 (t, J = 8.2 Hz, 1H), 7.50 (s, 1H), 7.56 (d, J = 7.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 55.6, 56.4, 66.5, 112.5, 119.5, 120.1, 129.8, 139.7, 159.6.



4-(*tert*-Butyl)-*N*-morpholinobenzenesulfonamide (**3f**)[1]

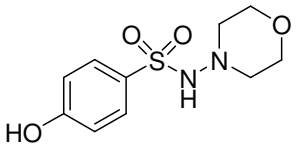
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.34 (s, 9H), 2.64 (s, 4H), 3.61 (s, 4H), 6.25 (s, 1H), 7.53 (d, J = 8.3 Hz, 2H), 7.90 (d, J = 8.3 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 30.9, 35.0, 56.4, 66.4, 125.6, 127.8, 135.5, 156.8.



N-Morpholino-[1,1'-biphenyl]-4-sulfonamide (**3g**)[1]

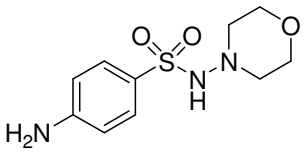
^{1}H NMR (400 MHz, $CDCl_3$) δ 2.67 (t, J = 4.6 Hz, 4H), 3.62 (t, J = 4.6 Hz, 4H), 5.89 (s, 1H), 7.40-7.50 (m, 3H), 7.62 (d, J = 7.3 Hz, 2H), 7.74 (d, J = 7.8 Hz, 2H), 8.04 (d,

J = 8.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 56.7, 66.6, 127.2, 127.3, 128.5, 128.6, 129.0, 137.2, 139.0, 145.9.



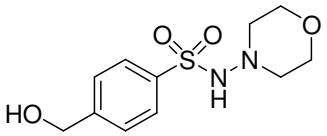
4-Hydroxy-*N*-morpholinobenzenesulfonamide (**3h**)[1]

^{1}H NMR (400 MHz, CD_3OD) δ 2.55 (t, *J* = 4.56, 4H), 3.55 (t, *J* = 4.1 Hz, 4H), 4.88 (br, 2H), 6.91 (d, *J* = 8.7 Hz, 2H), 7.76 (d, *J* = 8.7 Hz, 2H); ^{13}C NMR (100 MHz, CD_3OD) δ 56.0, 66.5, 115.1, 129.1, 130.1, 161.9.



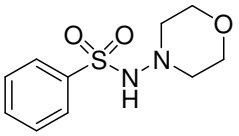
4-Amino-*N*-morpholinobenzenesulfonamide (**3i**)[2]

^{1}H NMR (400 MHz, CD_3OD) δ 2.55 (t, *J* = 4.6 Hz, 4H), 3.55 (t, *J* = 4.2 Hz, 4H), 4.83 (s, 3H), 6.69 (d, *J* = 8.2 Hz, 2H), 7.58 (d, *J* = 8.2 Hz, 2H); ^{13}C NMR (100 MHz, CD_3OD) δ 56.0, 66.5, 112.8, 124.6, 129.8, 153.2.



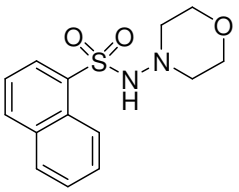
4-(Hydroxymethyl)-*N*-morpholinobenzenesulfonamide (**3j**)

^{1}H NMR (400 MHz, CD_3OD) δ 2.55 (t, *J* = 4.6 Hz, 4H), 3.53 (d, *J* = 4.1 Hz, 4H), 4.69 (s, 2H), 4.86 (s, 2H), 7.55 (d, *J* = 7.8 Hz, 2H), 7.90 (d, *J* = 7.8 Hz, 2H); ^{13}C NMR (100 MHz, CD_3OD) δ 56.0, 62.9, 66.4, 126.5, 127.9, 138.0, 147.3. HRMS (ESI) calcd for $C_{11}H_{16}N_2NaO_4S$: 295.0723 ($M + Na^+$), found: 295.0712.



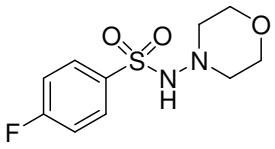
N-Morpholinobenzenesulfonamide (**3k**)[1]

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.62 (t, *J* = 4.1 Hz, 4H), 3.59 (t, *J* = 4.1 Hz, 4H), 6.11 (s, 1H), 7.53 (t, *J* = 7.3 Hz, 2H), 7.61 (t, *J* = 7.3 Hz, 1H), 7.98 (d, *J* = 7.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 56.4, 66.5, 128.0, 128.7, 133.0, 138.5.



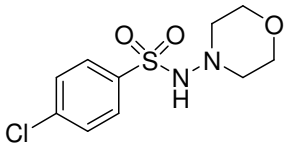
N-Morpholinonaphthalene-1-sulfonamide (**3l**)[1]

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.53 (t, J = 4.6 Hz, 4H), 3.46 (t, J = 4.1 Hz, 4H), 6.12 (s, 1H), 7.54-7.60 (m, 2H), 7.66 (t, J = 7.3 Hz, 1H), 7.92 (d, J = 8.2 Hz, 1H), 8.08 (d, J = 7.8 Hz, 1H), 8.39 (d, J = 7.3 Hz, 1H), 8.81 (d, J = 8.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 56.6, 66.4, 124.1, 125.0, 126.7, 128.1, 128.4, 128.8, 131.3, 133.5, 133.9, 134.7.



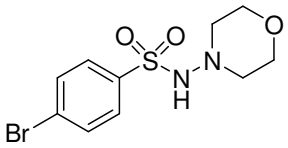
4-Fluoro-*N*-morpholinobenzenesulfonamide (**3m**)[3]

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.64 (t, J = 4.6 Hz, 4H), 3.62 (t, J = 4.6 Hz, 4H), 5.57 (s, 1H), 7.21 (t, J = 8.7 Hz, 2H), 8.00 (dd, J = 5.0, 8.7 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 56.7, 66.6, 116.1 (d, J_{CF} = 22.9 Hz), 130.9 (d, J_{CF} = 9.5 Hz), 134.6, 165.4 (d, J_{CF} = 254.6 Hz).



4-Chloro-*N*-morpholinobenzenesulfonamide (**3n**)[3]

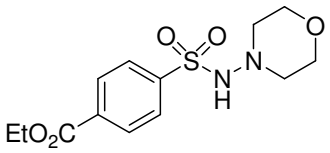
^{1}H NMR (400 MHz, $CDCl_3$) δ 2.65 (t, J = 4.6 Hz, 4H), 3.62 (t, J = 4.1 Hz, 4H), 5.74 (s, 1H), 7.51 (d, J = 8.7 Hz, 2H), 7.91 (d, J = 8.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 56.6, 66.6, 129.1, 129.6, 137.0, 139.7.



4-Bromo-*N*-morpholinobenzenesulfonamide (**3o**)[3]

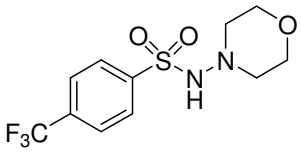
^{1}H NMR (400 MHz, $CDCl_3$) δ 2.65 (t, J = 4.6 Hz, 4H), 3.61 (t, J = 4.6 Hz, 4H), 5.99 (s, 1H), 7.67 (d, J = 8.7 Hz, 2H), 7.84 (d, J = 8.3 Hz, 2H); ^{13}C NMR (100 MHz,

$CDCl_3$) δ 56.5, 66.5, 128.2, 129.6, 132.1, 137.6.



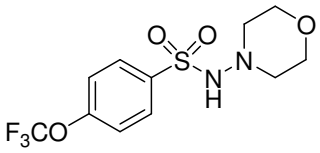
Ethyl 4-(*N*-morpholinosulfamoyl)benzoate (**3p**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.43 (t, J = 7.3 Hz, 3H), 2.66 (s, 4H), 3.61 (s, 4H), 4.43 (q, J = 6.8 Hz, 2H), 6.14 (s, 1H), 8.06 (d, J = 7.8 Hz, 2H), 8.19 (d, J = 7.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 14.2, 56.5, 61.7, 66.5, 128.0, 129.9, 134.5, 142.4, 165.1. HRMS (ESI) calcd for $C_{13}H_{18}N_2NaO_5S$: 337.0829 ($M + Na^+$), found: 337.0846.



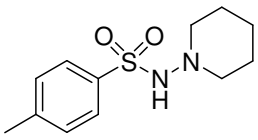
N-Morpholino-4-(trifluoromethyl)benzenesulfonamide (**3q**)[1]

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.67 (s, 4H), 3.63 (s, 4H), 5.86 (s, 1H), 7.80 (d, J = 7.8 Hz, 2H), 8.12 (d, J = 7.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 56.7, 66.5, 123.1 (q, J_{CF} = 271.7 Hz), 125.9 (d, J_{CF} = 3.8 Hz), 128.6, 134.8 (q, J_{CF} = 32.4 Hz), 142.2.



N-Morpholino-4-(trifluoromethoxy)benzenesulfonamide (**3r**)

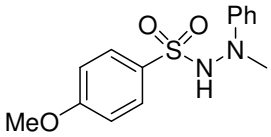
^{1}H NMR (400 MHz, $CDCl_3$) δ 2.66 (s, 4H), 3.62 (s, 4H), 6.07 (s, 1H), 7.36 (d, J = 8.2 Hz, 2H), 8.04 (d, J = 8.7 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 56.6, 66.5, 120.1 (d, J_{CF} = 257.4 Hz), 120.5, 130.3, 136.8, 152.4. HRMS (ESI) calcd for $C_{11}H_{14}F_3N_2O_4S$: 327.0621 ($M + H^+$), found: 327.0623.



4-Methyl-*N*-(piperidin-1-yl)benzenesulfonamide (**3s**)[1]

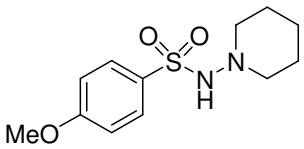
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.28 (s, 2H), 1.46-1.50 (m, 4H), 2.43 (s ,3H), 2.52-2.54 (m, 4H), 5.77 (s ,1H), 7.30 (d, J = 7.8 Hz, 2H), 7.85 (d, J = 8.2 Hz, 2H); ^{13}C NMR

(100 MHz, $CDCl_3$) δ 21.5, 22.9, 25.5, 57.5, 128.0, 129.2, 135.8, 143.5.



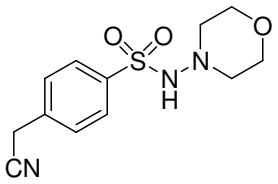
4-Methoxy-*N*′-methyl-*N*′-phenylbenzenesulfonohydrazide (**3t**)[3]

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.9 (s, 3H), 3.8 (s, 3H), 6.42 (s, 1H), 6.82-6.87 (m, 3H), 6.92 (d, J = 8.7 Hz, 2H), 7.15 (t, J = 8.2 Hz, 2H), 7.85 (d, J = 8.7 Hz, 2H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 42.4, 55.5, 114.2, 114.3, 120.7, 128.8, 129.4, 129.9, 130.3, 149.8, 163.3.



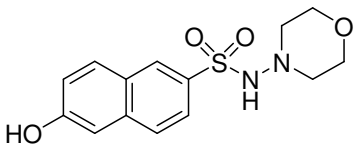
4-Methoxy-*N*-(piperidin-1-yl)benzenesulfonamide (**3u**)[3]

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.26-1.29 (m, 2H), 1.46-1.51 (m, 4H), 2.52-2.53 (m, 4H), 3.87 (s, 3H), 5.58 (s, 1H), 6.97 (d, J = 8.7 Hz, 2H), 7.89 (d, J = 8.7 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 22.9, 25.6, 55.5, 57.6, 113.7, 130.2, 130.3, 163.0.



4-(Cyanomethyl)-*N*-morpholinobenzenesulfonamide (**3v**)

^{1}H NMR (400 MHz, DMSO-d_6) δ 3.00 (t, J = 4.1 Hz, 4H), 3.96 (s, 4H), 4.70 (s, 2H), 8.09 (d, J = 7.8 Hz, 2H), 8.40 (d, J = 8.2 Hz, 2H), 9.45 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 22.9, 56.3, 66.4, 119.1, 128.6, 129.1, 136.9, 139.4. HRMS (ESI) calcd for $C_{12}H_{15}N_3NaO_3S$: 304.0726 ($M + Na^+$), found: 304.0728.



6-Hydroxy-*N*-morpholinonaphthalene-2-sulfonamide (**3w**)

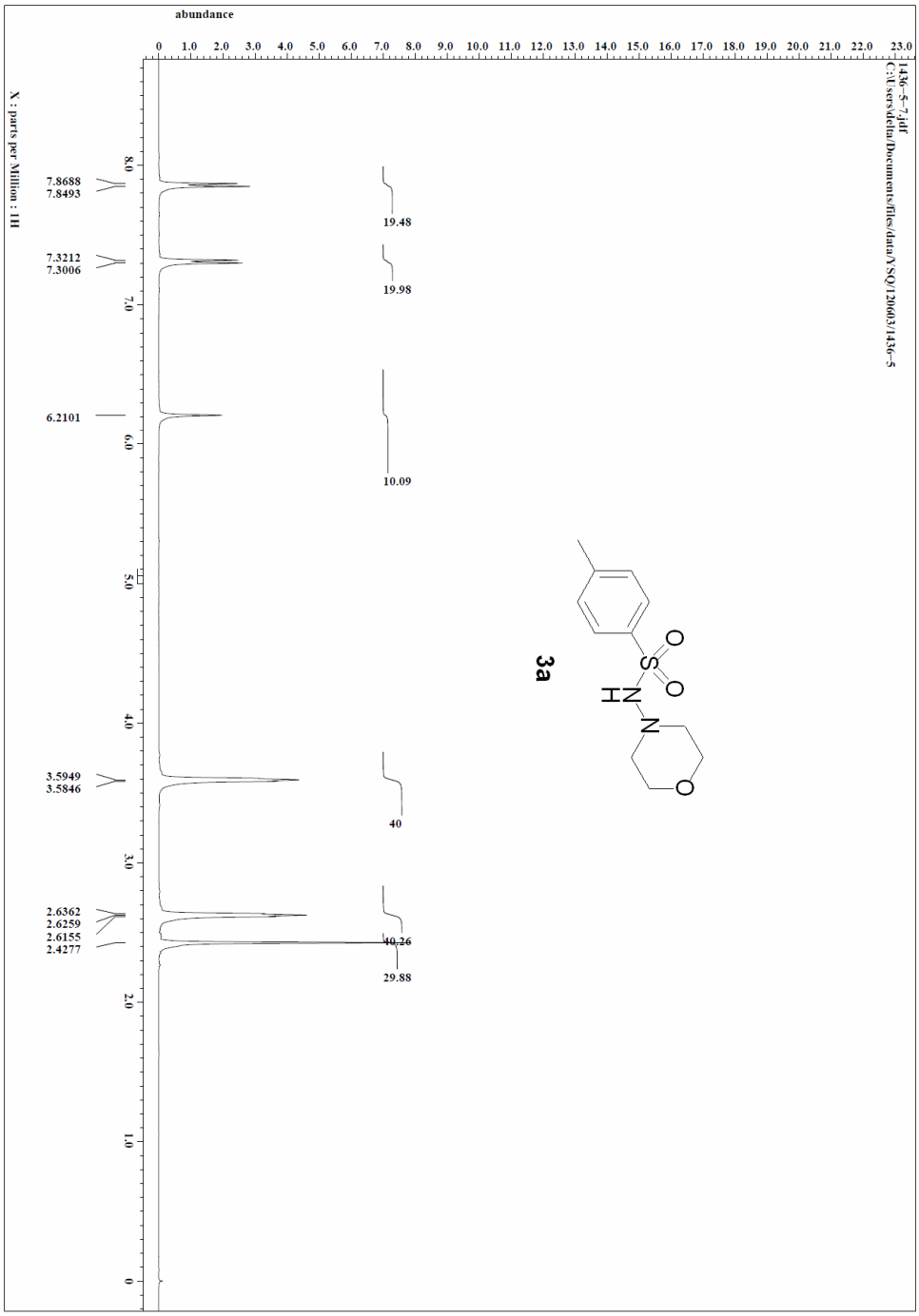
^{1}H NMR (400 MHz, CD_3OD) δ 2.55 (t, J = 4.6 Hz, 4H), 3.50 (t, J = 4.1 Hz, 4H), 4.88 (br, 2H), 7.20-7.23 (m, 2H), 7.77-7.80 (m, 2H), 7.90 (d, J = 8.2 Hz, 1H), 8.38 (s, 1H);

^{13}C NMR (100 MHz, CD_3OD) δ 56.1, 66.4, 108.8, 119.8, 123.3, 126.7, 126.8, 129.2, 130.7, 132.9, 137.1, 158.2. HRMS (ESI) calcd for $C_{14}H_{16}N_2NaO_4S$: 331.0723 (M + Na^+), found: 331.0705.

[1] B. Nguyen, E. J. Emmett, M. C. Willis, *J. Am. Chem. Soc.* **2010**, *132*, 16372.

[2] E. J. Emmett, C. S. Richards-Taylor, B. Nguyen, A. Garcia-Rubia, B. R. Hayter, M. C. Willis, *Org. Biomol. Chem.* **2012**, *10*, 4007.

[3] S. Ye, J. Wu, *Chem. Commun.* **2012**, DOI:10.1039/C2CC33725H.


abundance
X : parts per Million : 1H
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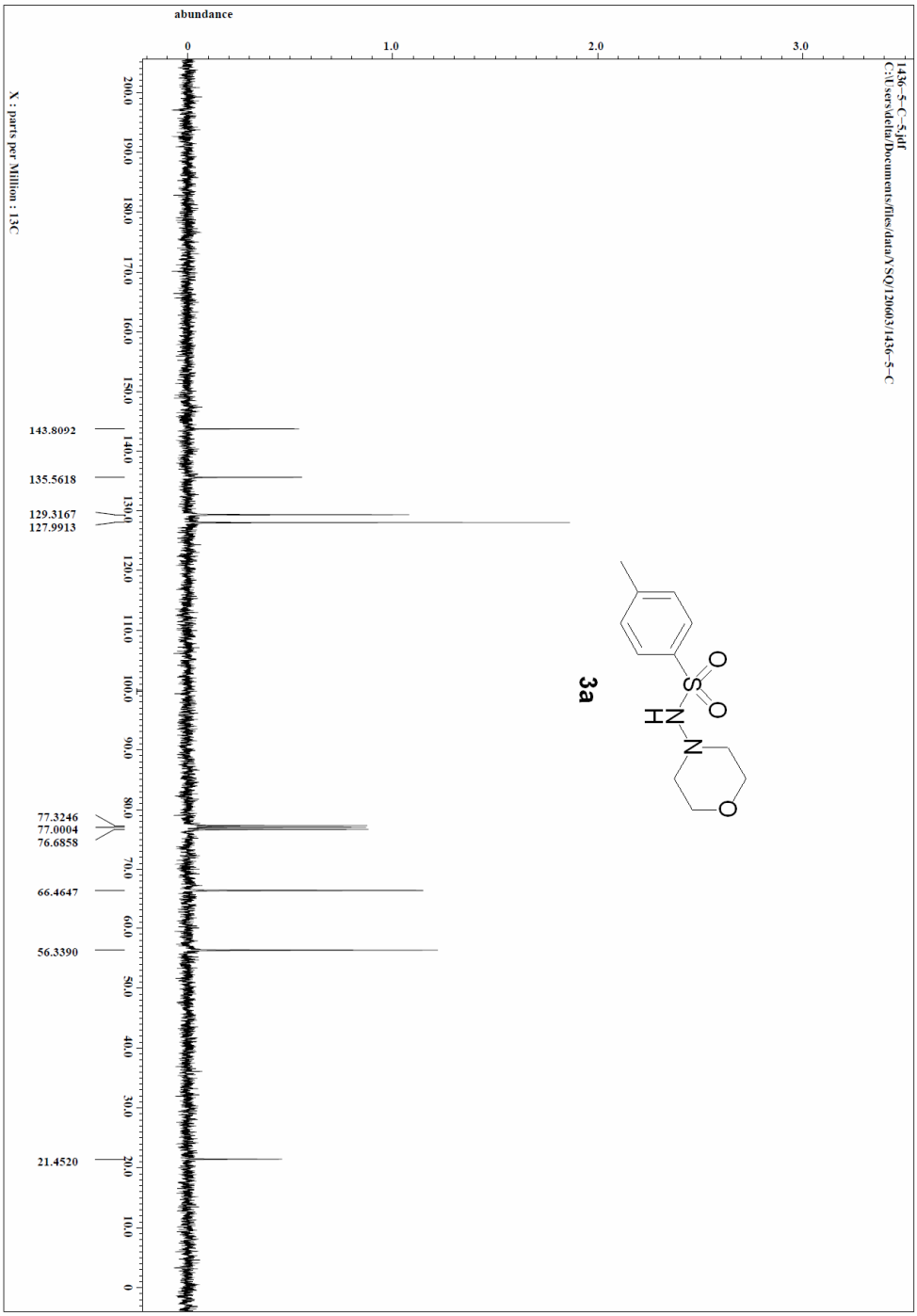
7.3212
7.3006
6.2101
3.5949
3.5846
2.6362
2.6259
2.6155
2.4277
19.48
19.98
10.09
40
40.26
29.88
3a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2.0
3.0
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X : parts per Million : 13C
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180.0
170.0
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
143.8092
135.5618
129.3167
127.9913
77.3246
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76.6858
66.4647
56.3390
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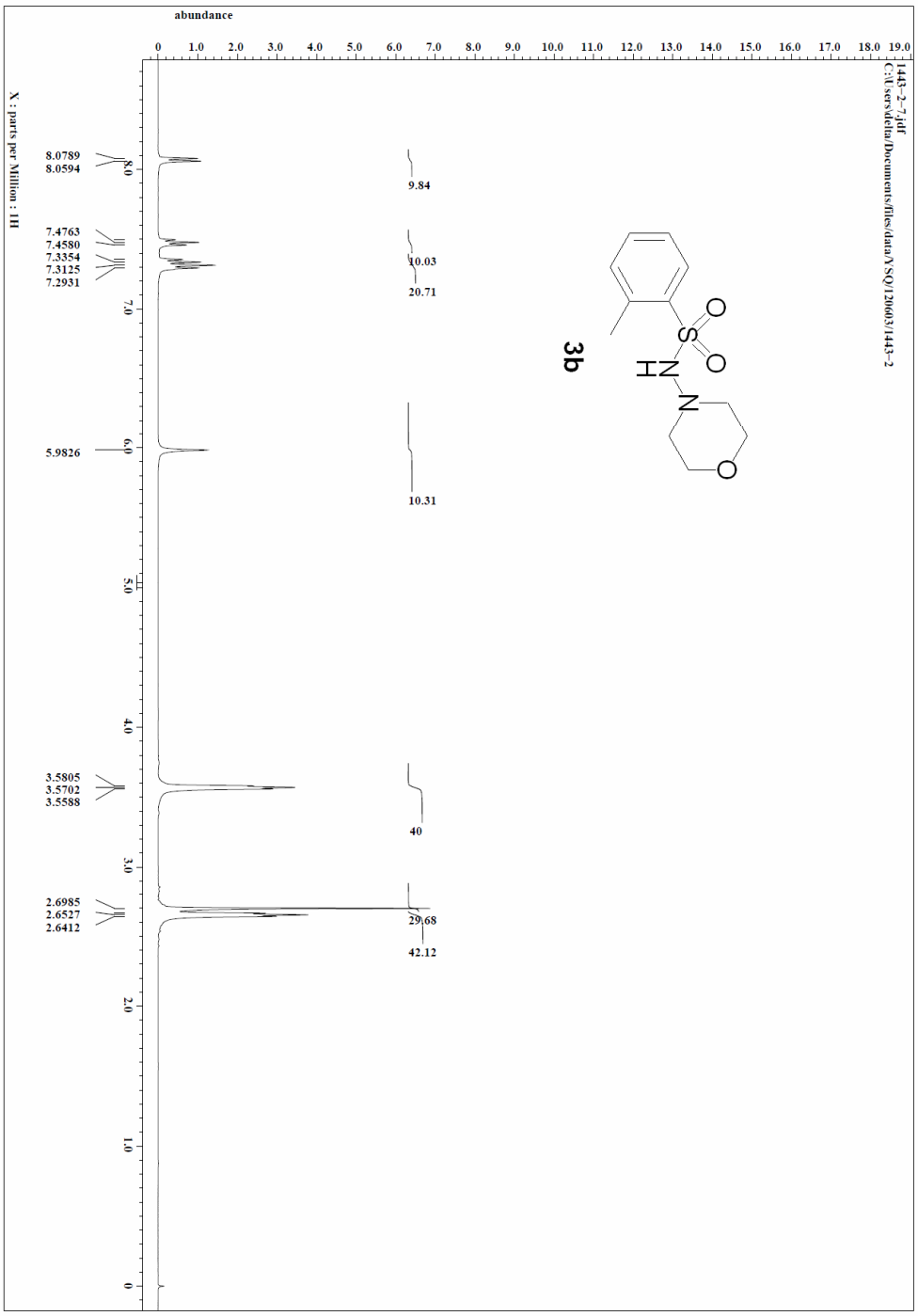
3a
O
S
O
HN
N
O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X : parts per Million : 1H
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7.4763
7.4580
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7.3125
7.2931
5.9826
3.5805
3.5702
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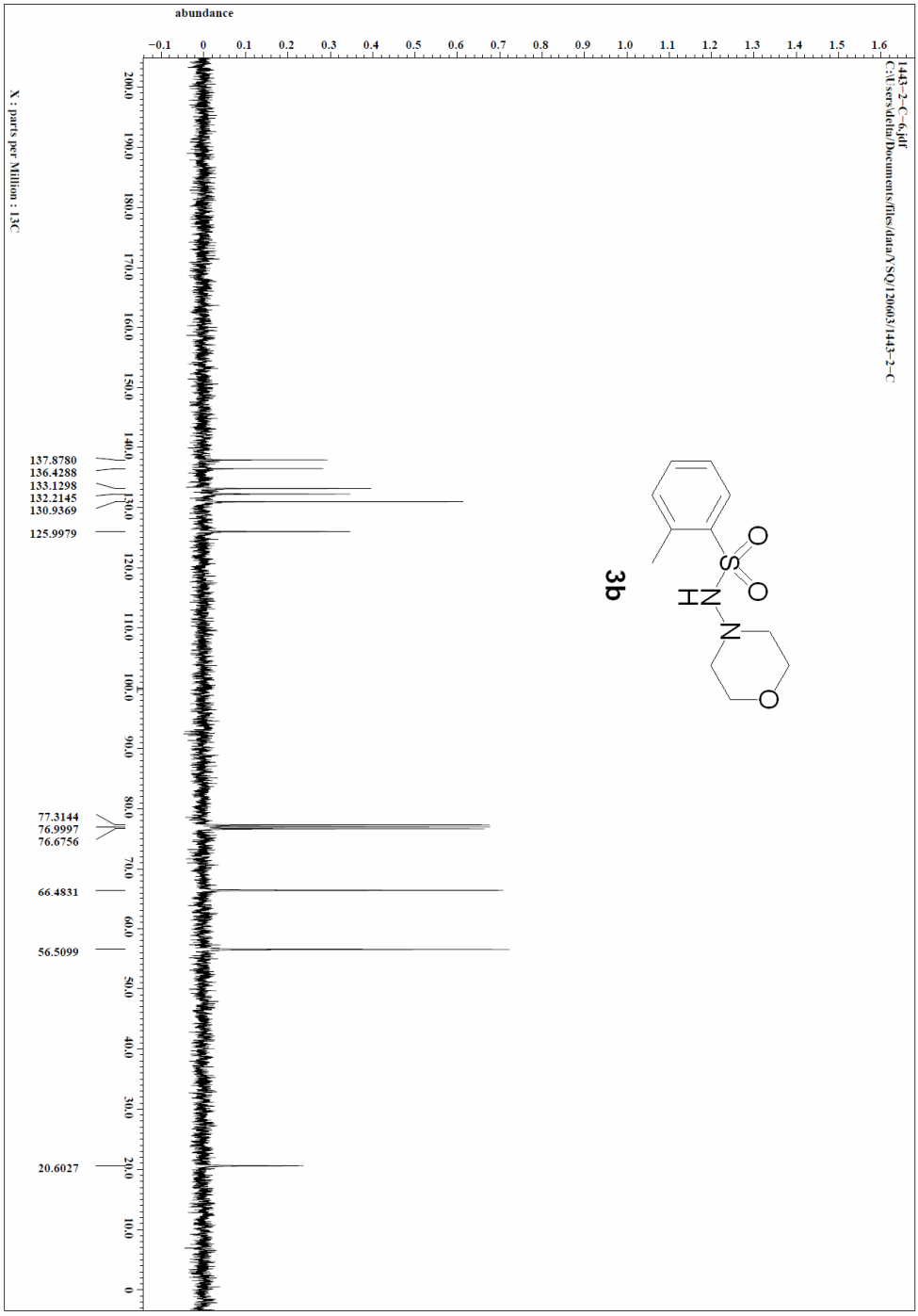
2.6527
2.6412
9.84
10.03
20.71
10.31
40
29.68
42.12
3b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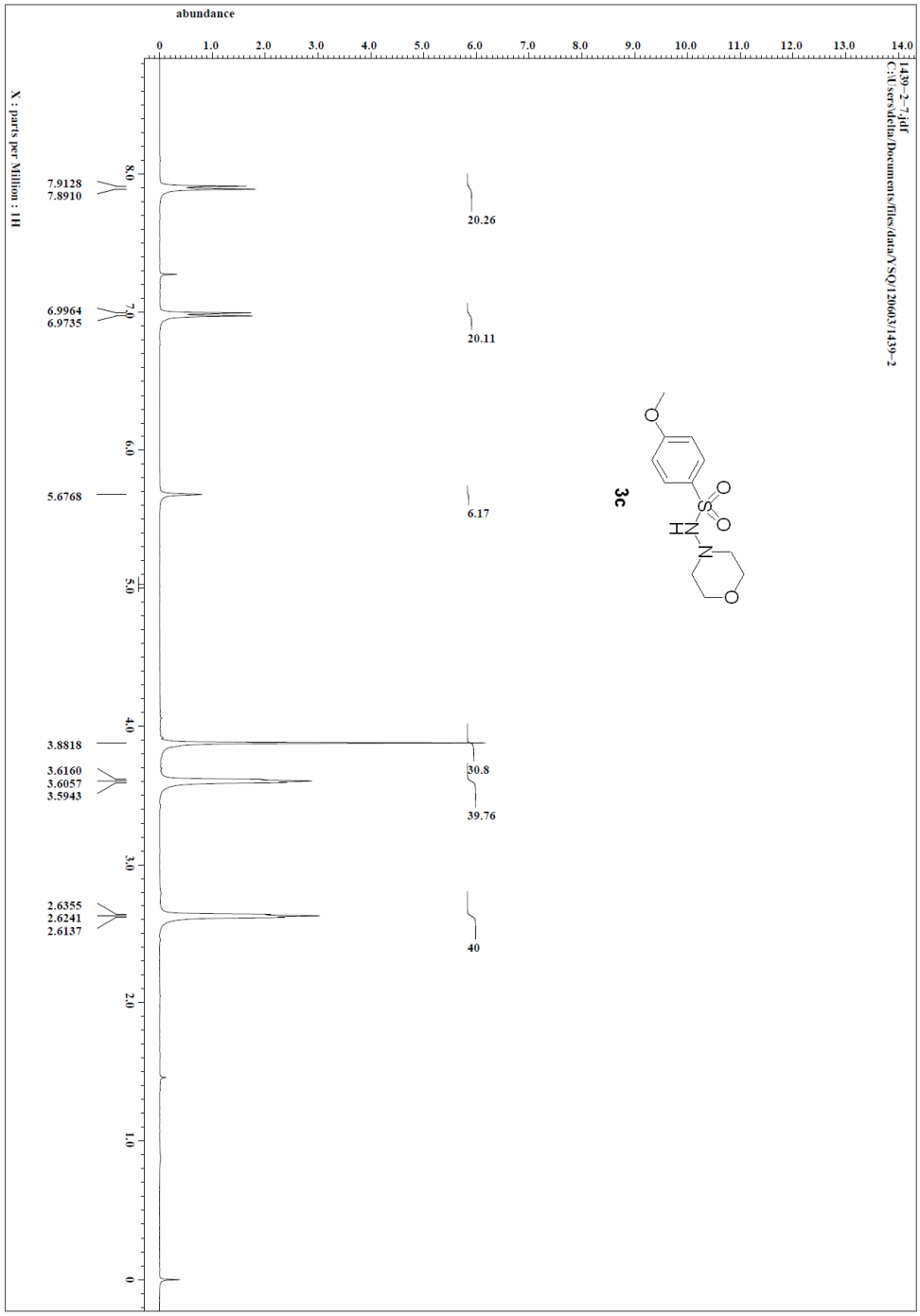
76.9997
76.6756
66.4831
56.5099
20.6027
3b
O
S
O
HN
N
O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X : parts per Million : 1H
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6.9964
6.9735
5.6768
3.8818
3.6160
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2.6241
2.6137
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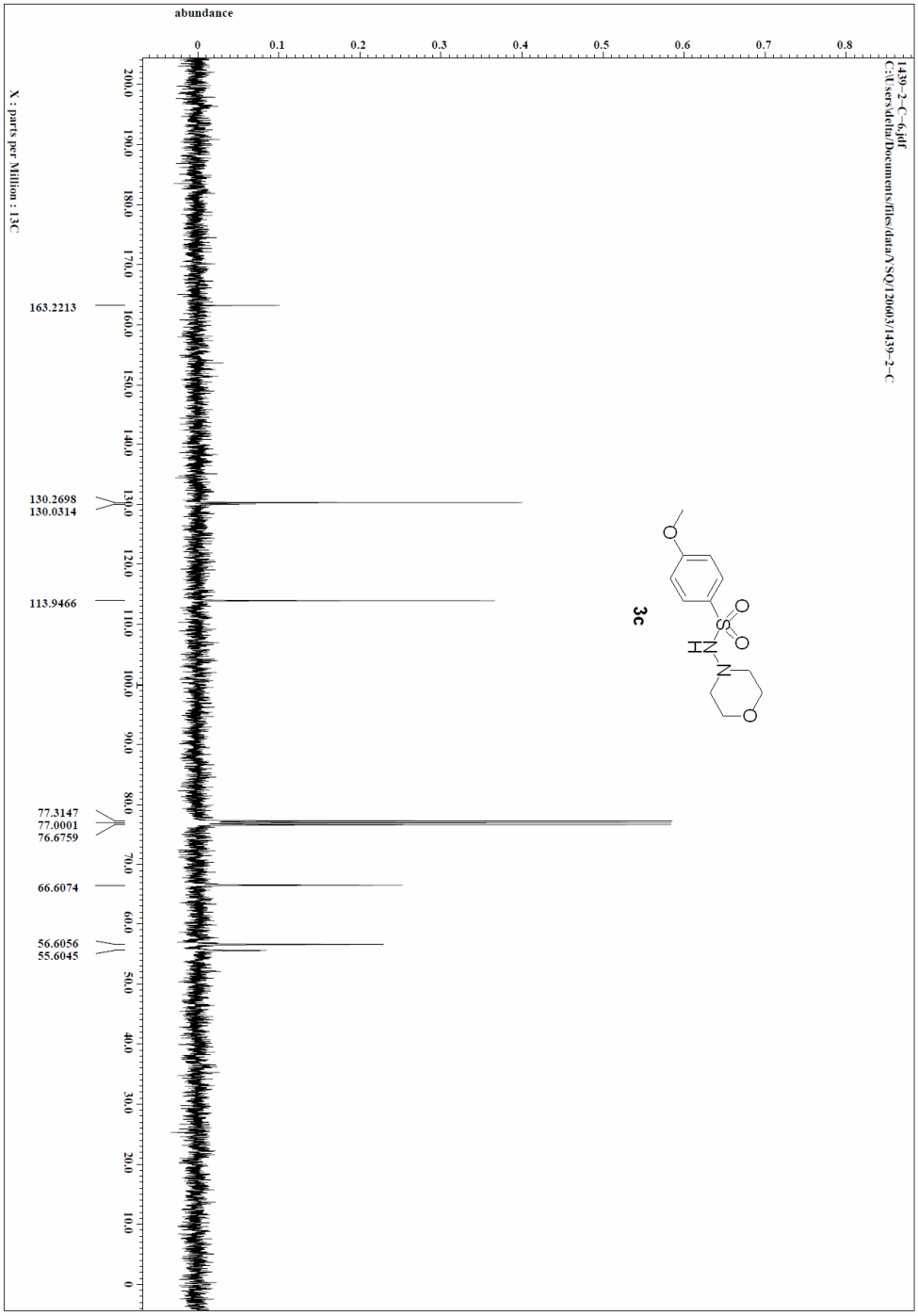
20.11
6.17
30.8
39.76
40
3c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0.3
0.4
0.5
0.6
0.7
0.8
X : parts per Million : 13C
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190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
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60.0
50.0
40.0
30.0
20.0
10.0
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130.2698
130.0314
113.9466
77.3147
77.0001
76.6759
66.6074
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55.6045
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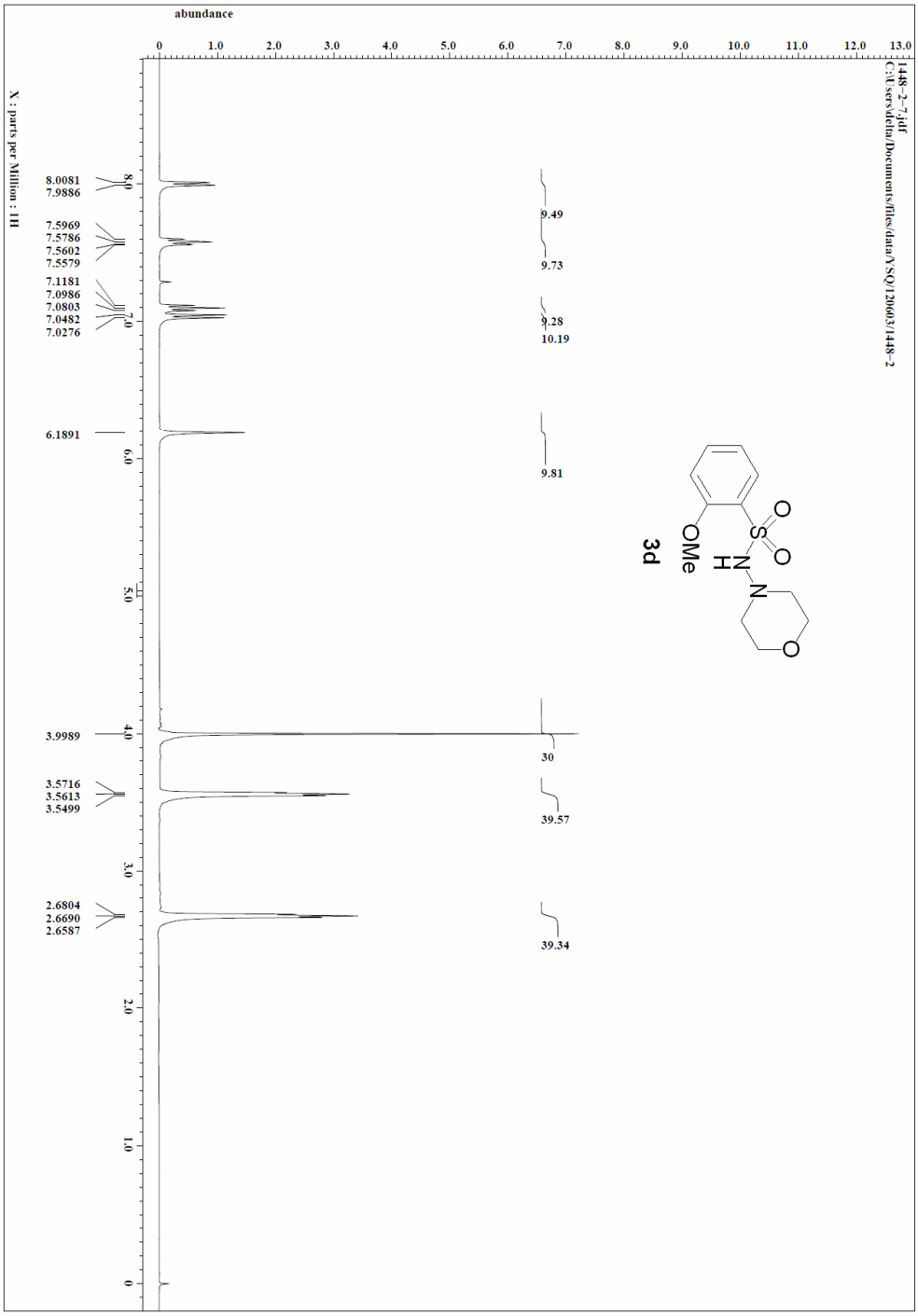
3c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X : parts per Million : 1H
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1448-2-7.jdf
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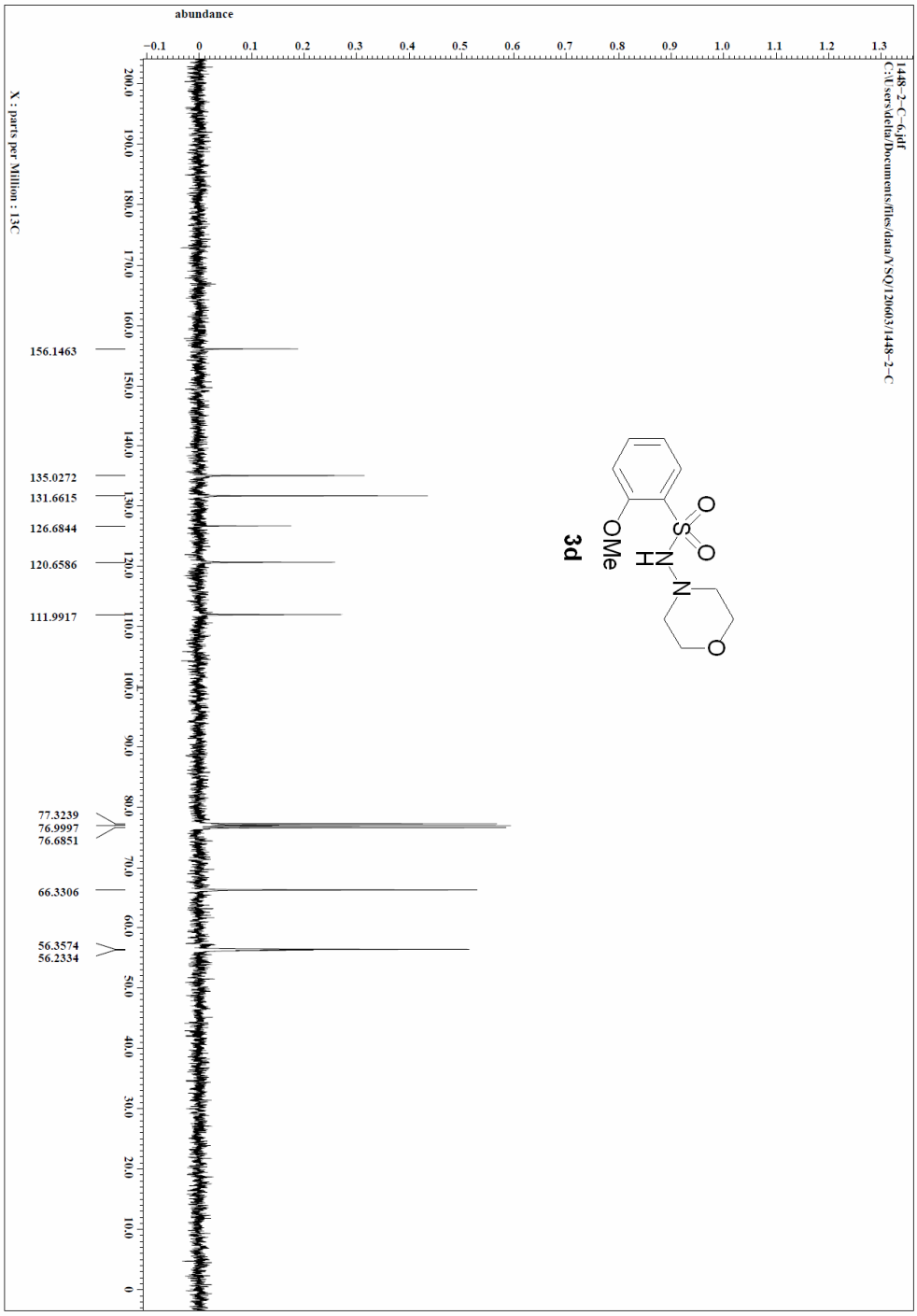
7.5579
7.1181
7.0986
7.0803
7.0482
7.0276
6.1891
3.9989
3.5716
3.5613
3.5499
2.6804
2.6690
2.6587
9.49
9.73
9.28
10.19
9.81
30
39.57
39.34
OMe
3d


abundance
X : parts per Million : 13C
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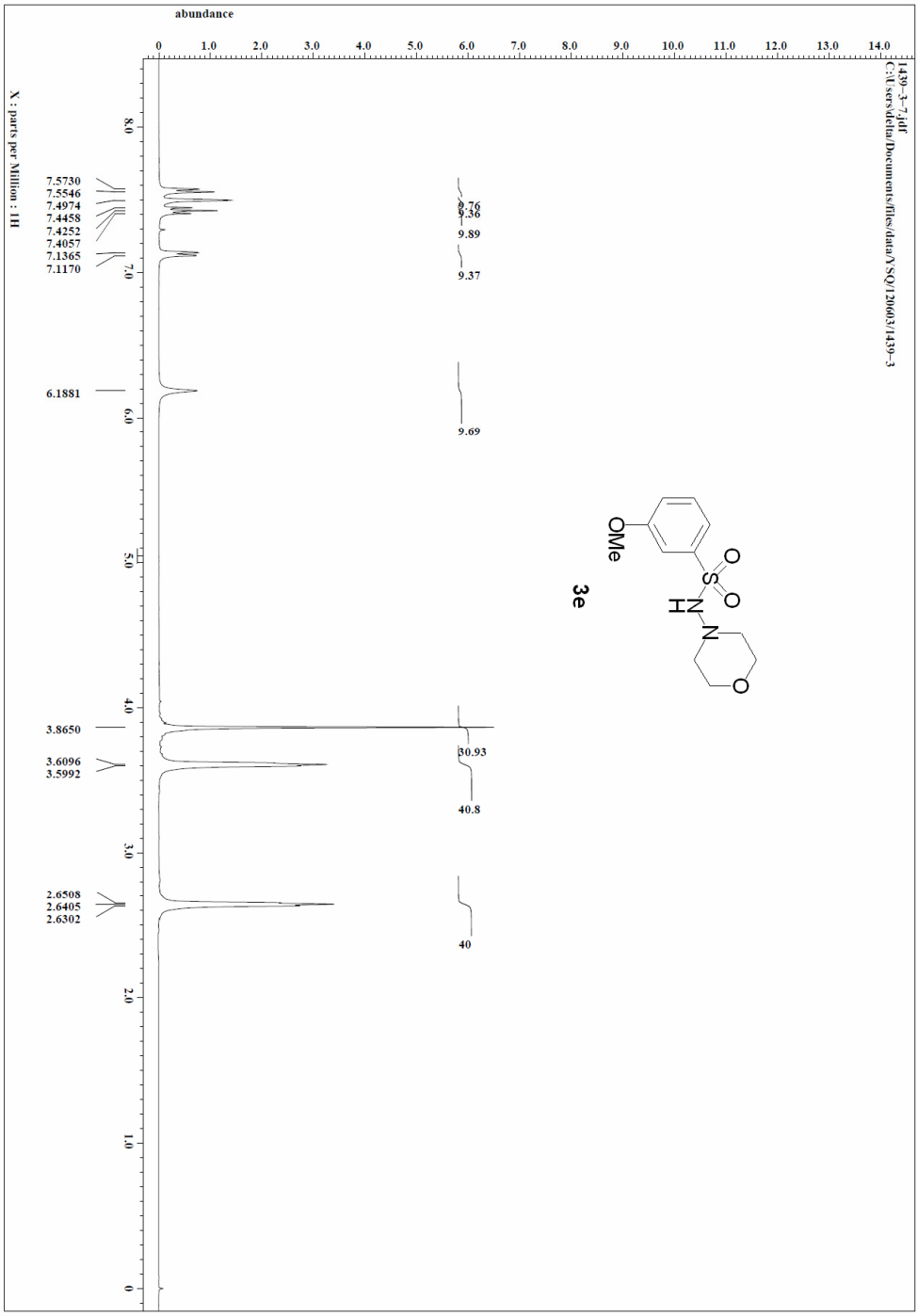
131.6615
126.6844
120.6586
111.9917
77.3239
76.9997
76.6851
66.3306
56.3574
56.2334
OMe
S
O
O
H
N
N
O
3d


abundance
X : parts per Million : 1H
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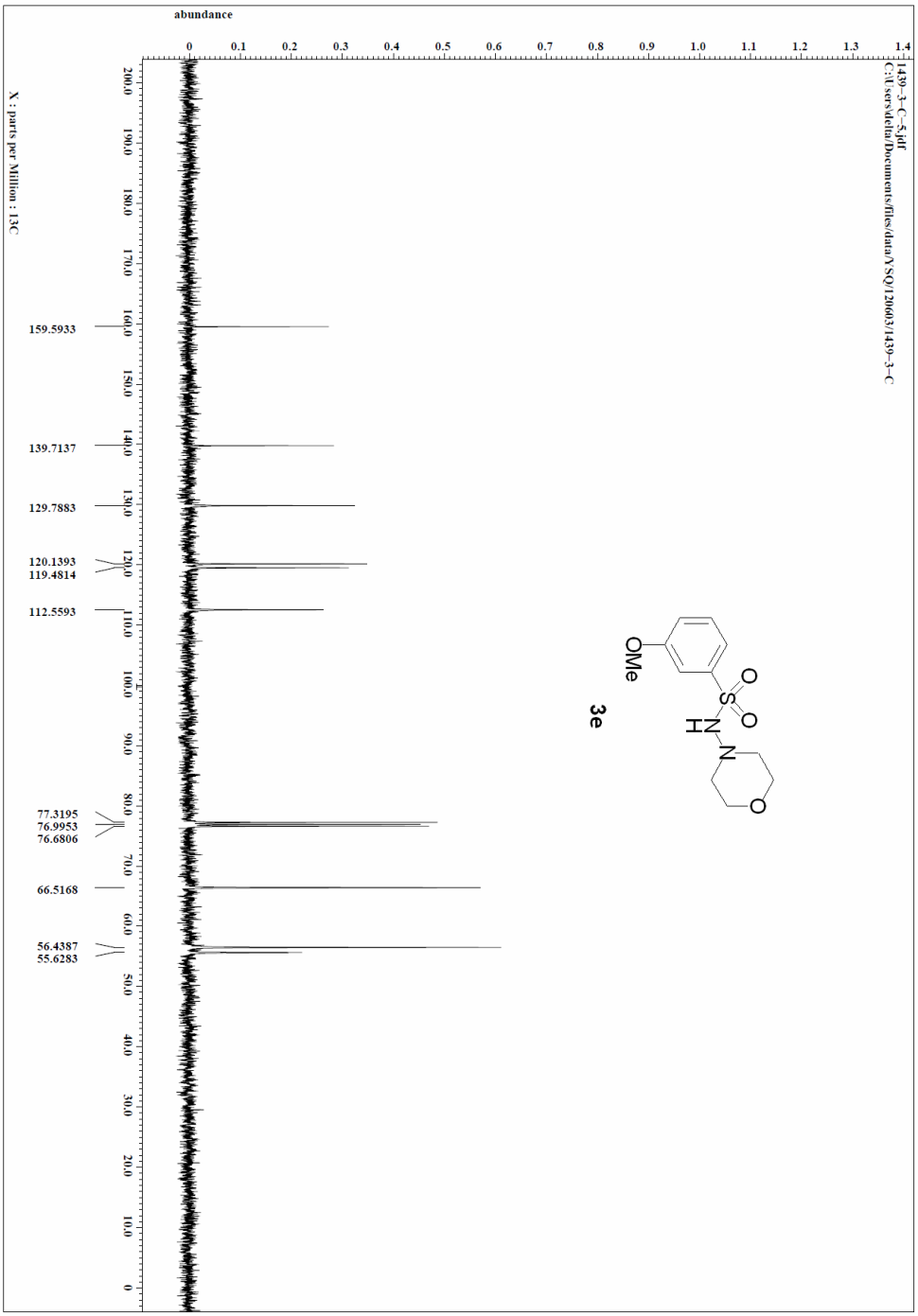
7.4974
7.4458
7.4252
7.4057
7.1365
7.1170
6.1881
3.8650
3.6096
3.5992
2.6508
2.6405
2.6302
9.76
9.36
9.89
9.37
9.69
30.93
40.8
40
OMe
O
S
O
HN
N
O
3e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X : parts per Million : 13C
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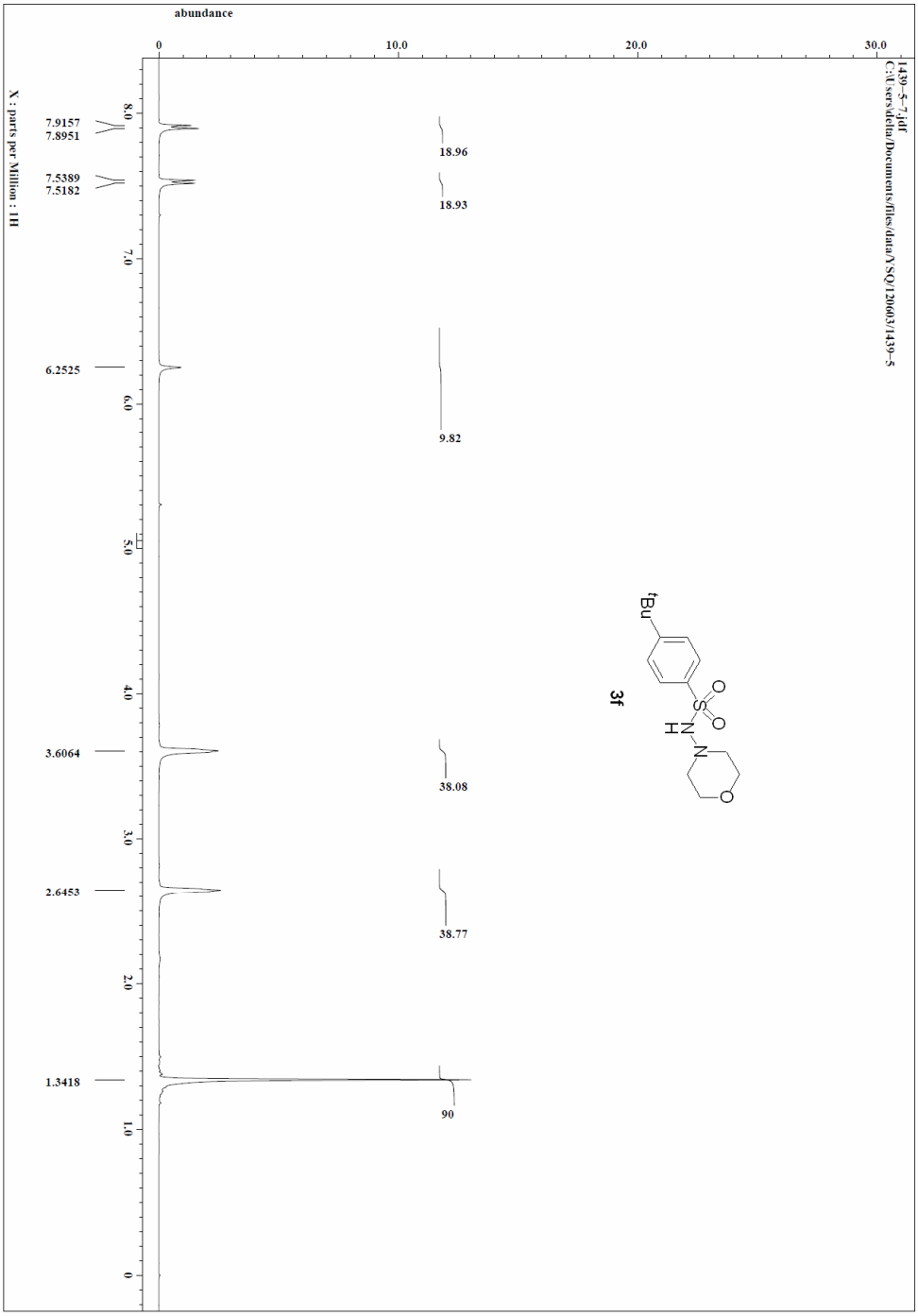
112.5593
77.3195
76.9953
76.6806
66.5168
56.4387
55.6283
OMe
3e


abundance
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20.0
30.0
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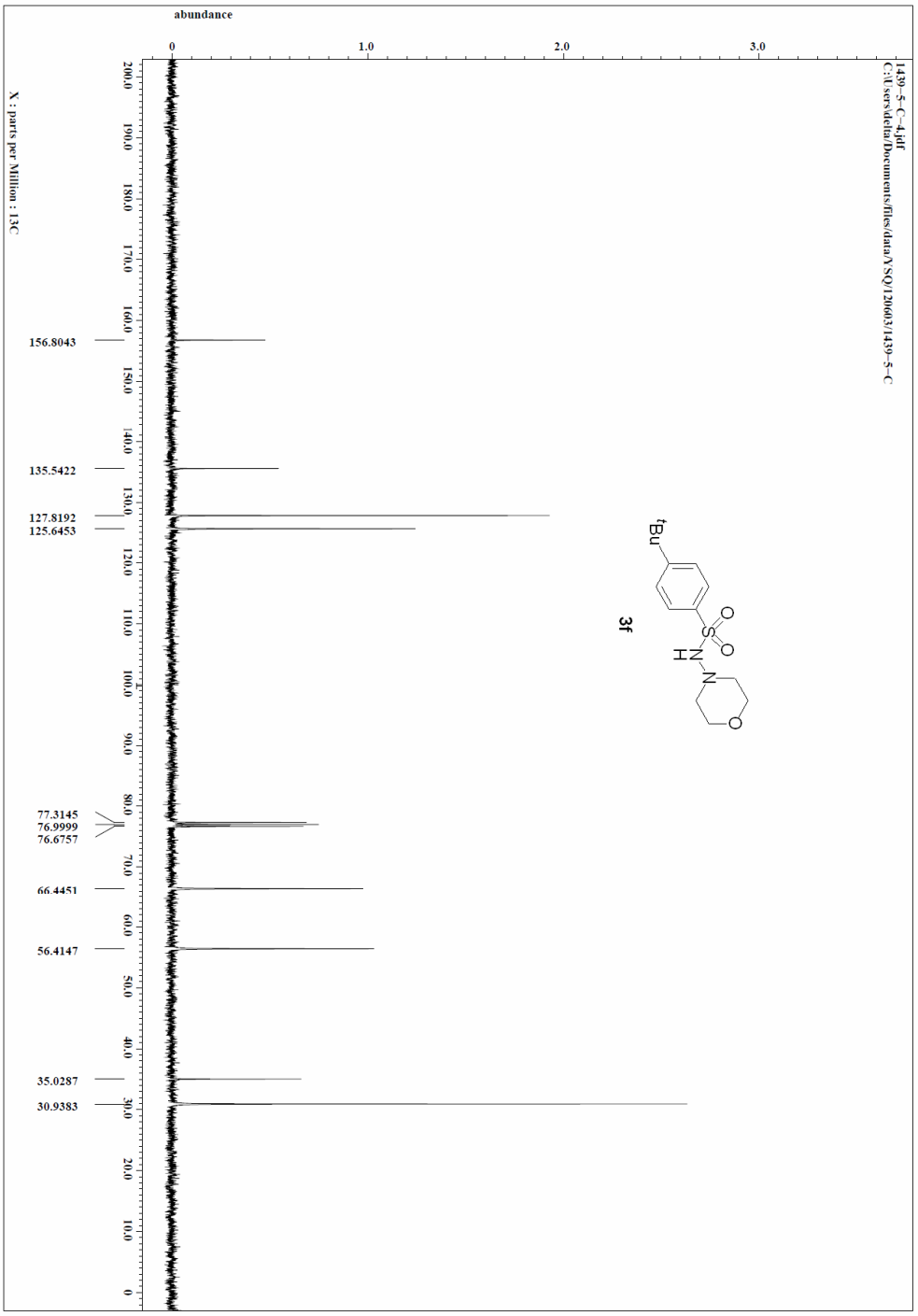
7.5389
7.5182
6.2525
3.6064
2.6453
1.3418
18.96
18.93
9.82
38.08
38.77
90
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
tBu
S
O
O
N
H
N
O
3f


abundance
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1.0
2.0
3.0
1439-5-C-4.jdf
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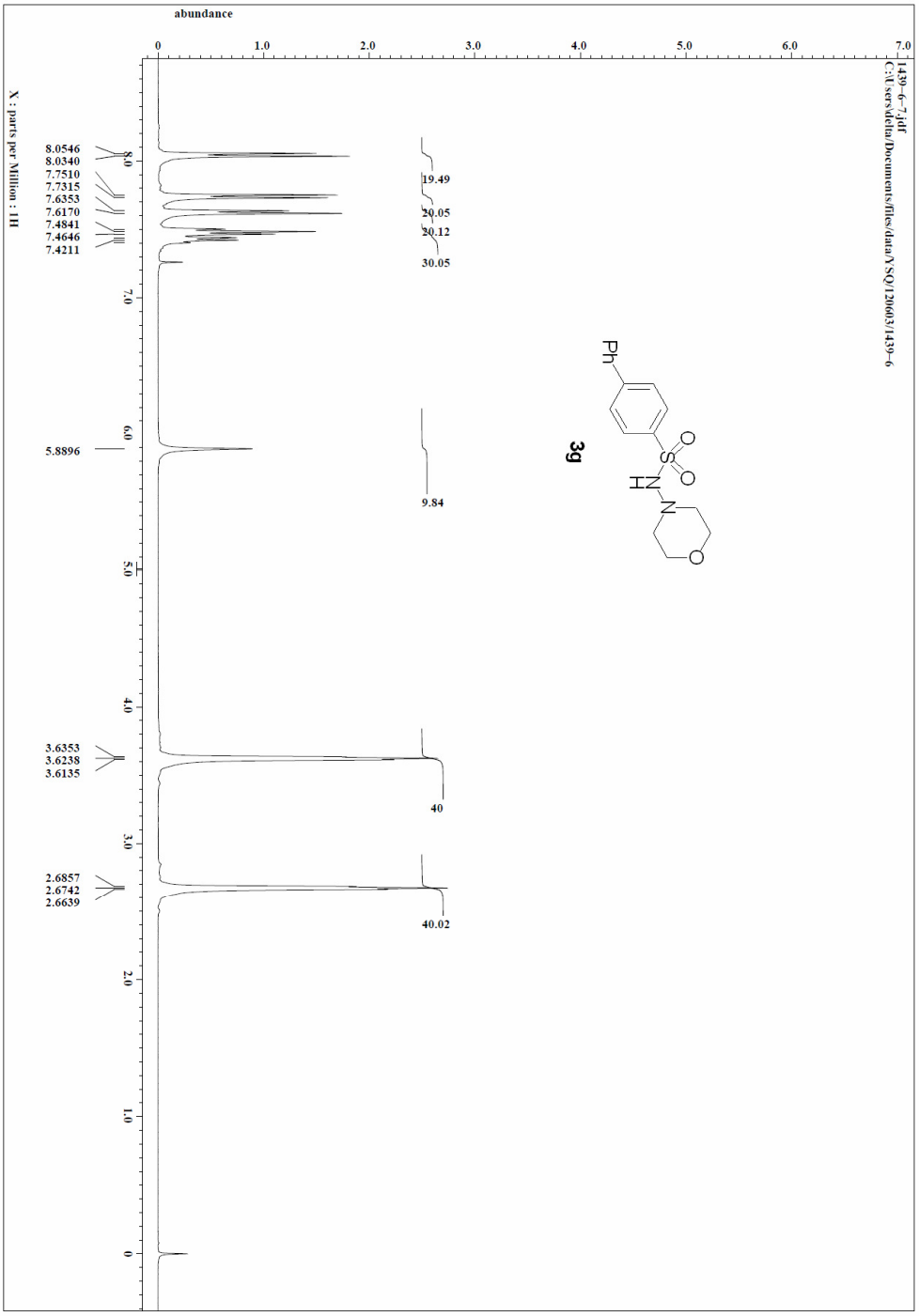
125.6453
77.3145
76.9999
76.6757
66.4451
56.4147
35.0287
30.9383
tBu
3f


abundance
X : parts per Million : 1H
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1439-6-7.jdf
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7.7510
7.7315
7.6353
7.6170
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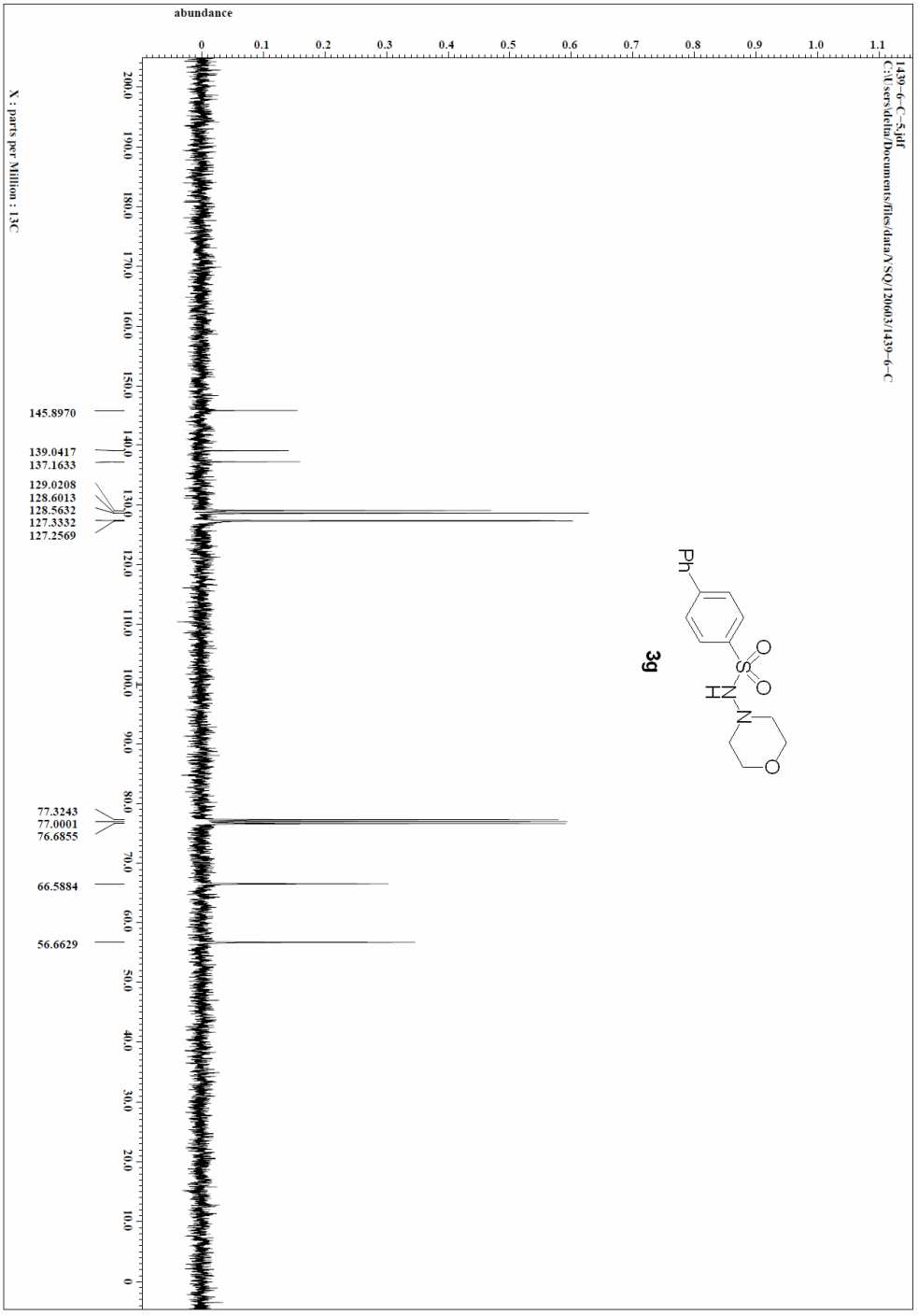
5.8896
3.6353
3.6238
3.6135
2.6857
2.6742
2.6639
19.49
20.05
20.12
30.05
9.84
40
40.02
3g
Ph
S
O
O
HN
N
O


abundance
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0.6
0.7
0.8
0.9
1.0
1.1
1439-6-C-5.jdf
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X : parts per Million : 13C
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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
145.8970
139.0417
137.1633
129.0208
128.6013
128.5632
127.3332
127.2569
77.3243
77.0001
76.6855
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Ph
S
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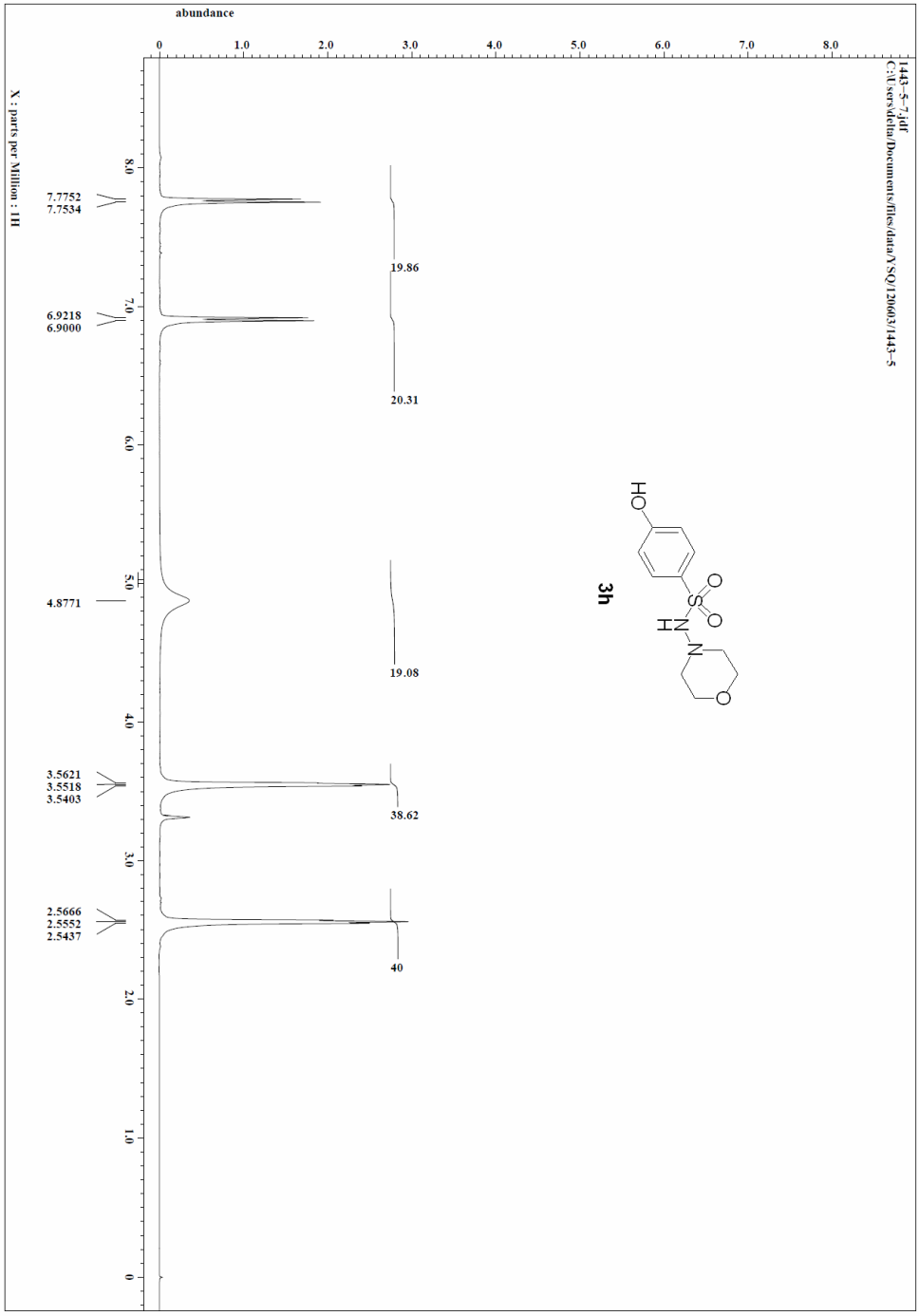
O
HN
N
O
3g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6.0
7.0
8.0
1443–5–7.jdf
C:\Users\delta\Documents\files\data\YSQ\120603\1443–5
X : parts per Million : 1H
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6.9000
4.8771
3.5621
3.5518
3.5403
2.5666
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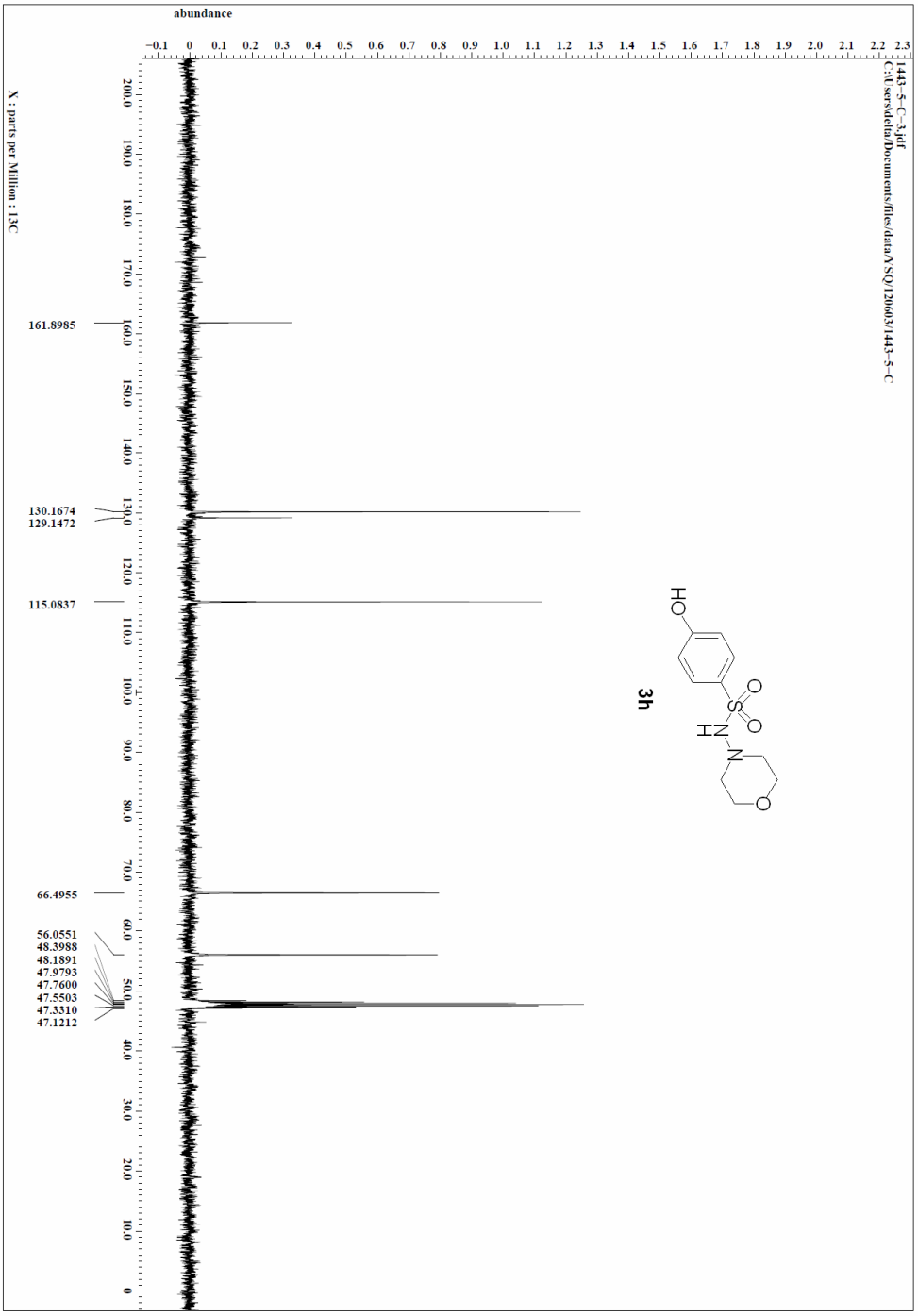
2.5437
19.86
20.31
19.08
38.62
40
3h
HO
S
O
O
HN
N
O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X : parts per Million : 13C
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48.1891
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47.5503
47.3310
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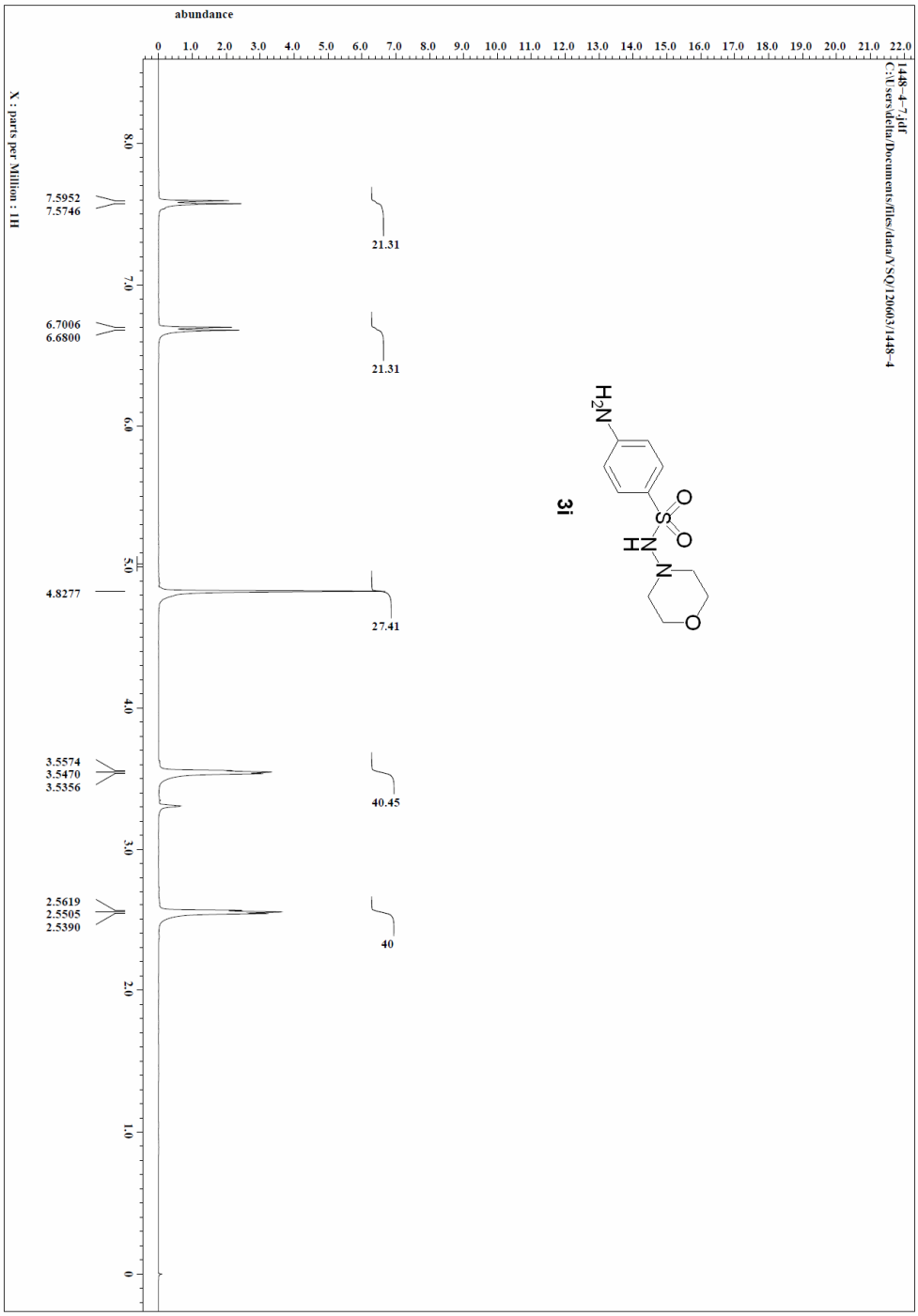
3h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X : parts per Million : 1H
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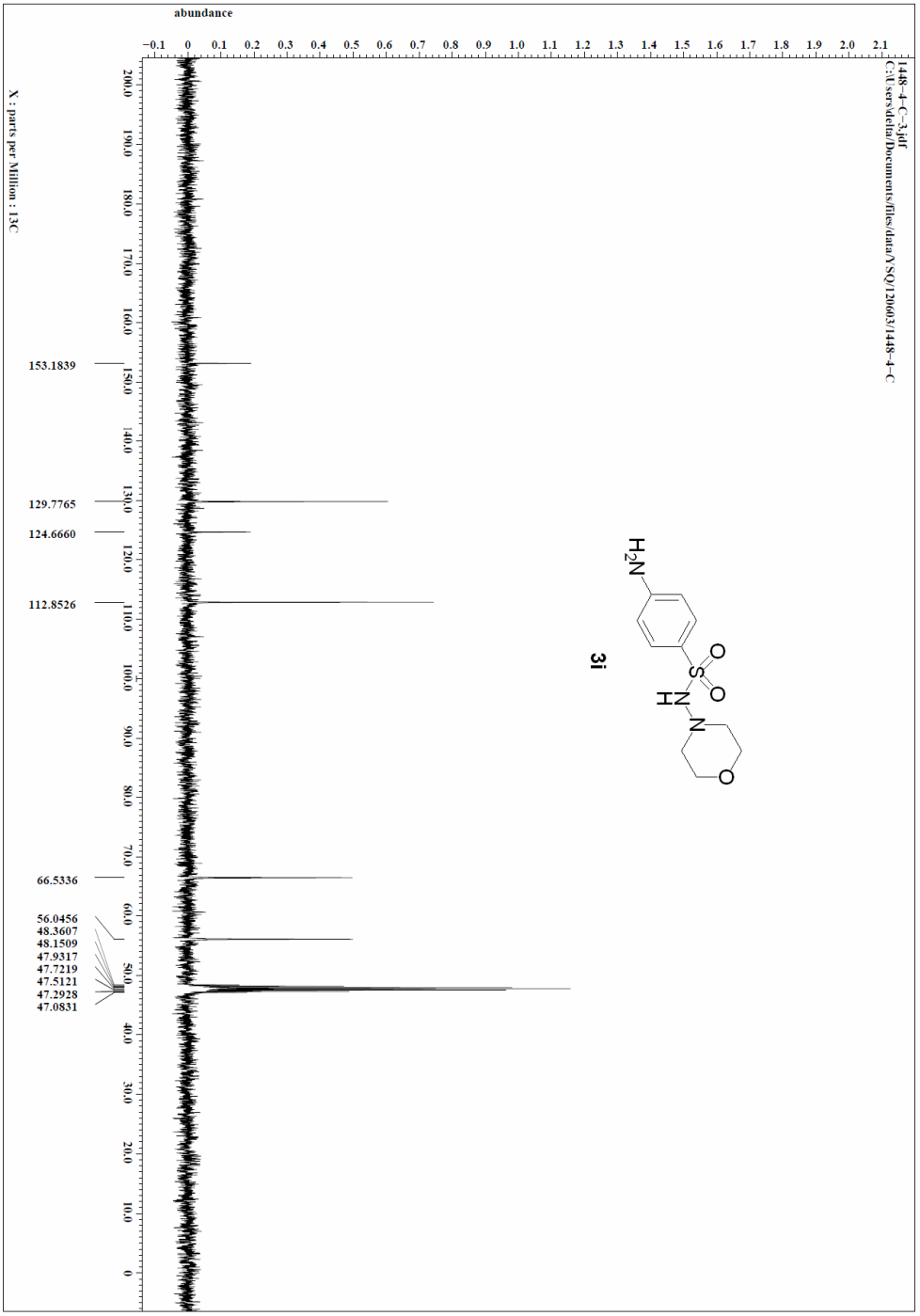
21.31
27.41
40.45
40
3i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X : parts per Million : 13C
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48.3607
48.1509
47.9317
47.7219
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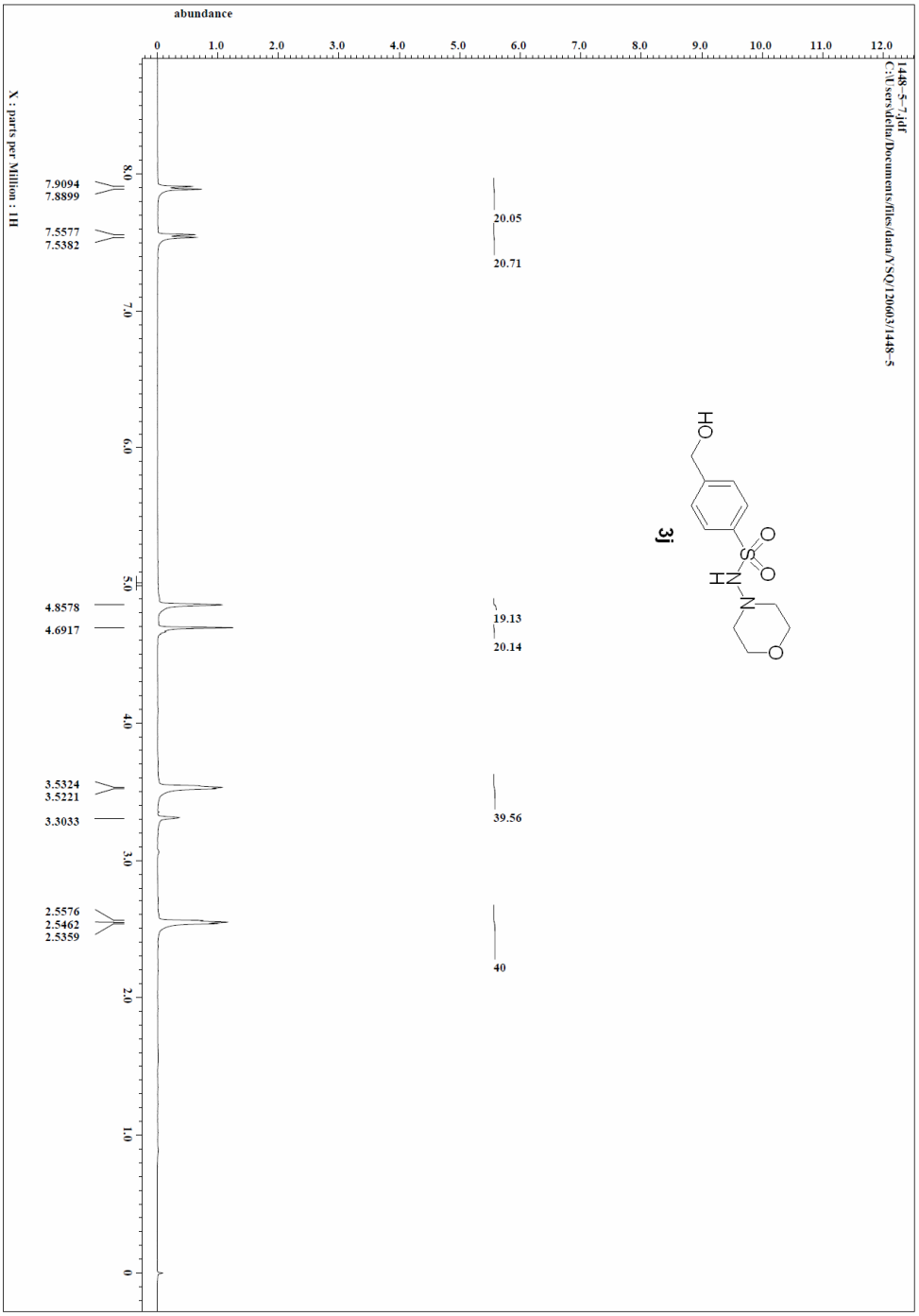
C:\U sers\delta\Documents\files\data\YSQ\120603\1448-4-C
3i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X : parts per Million : 1H
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19.13
20.14
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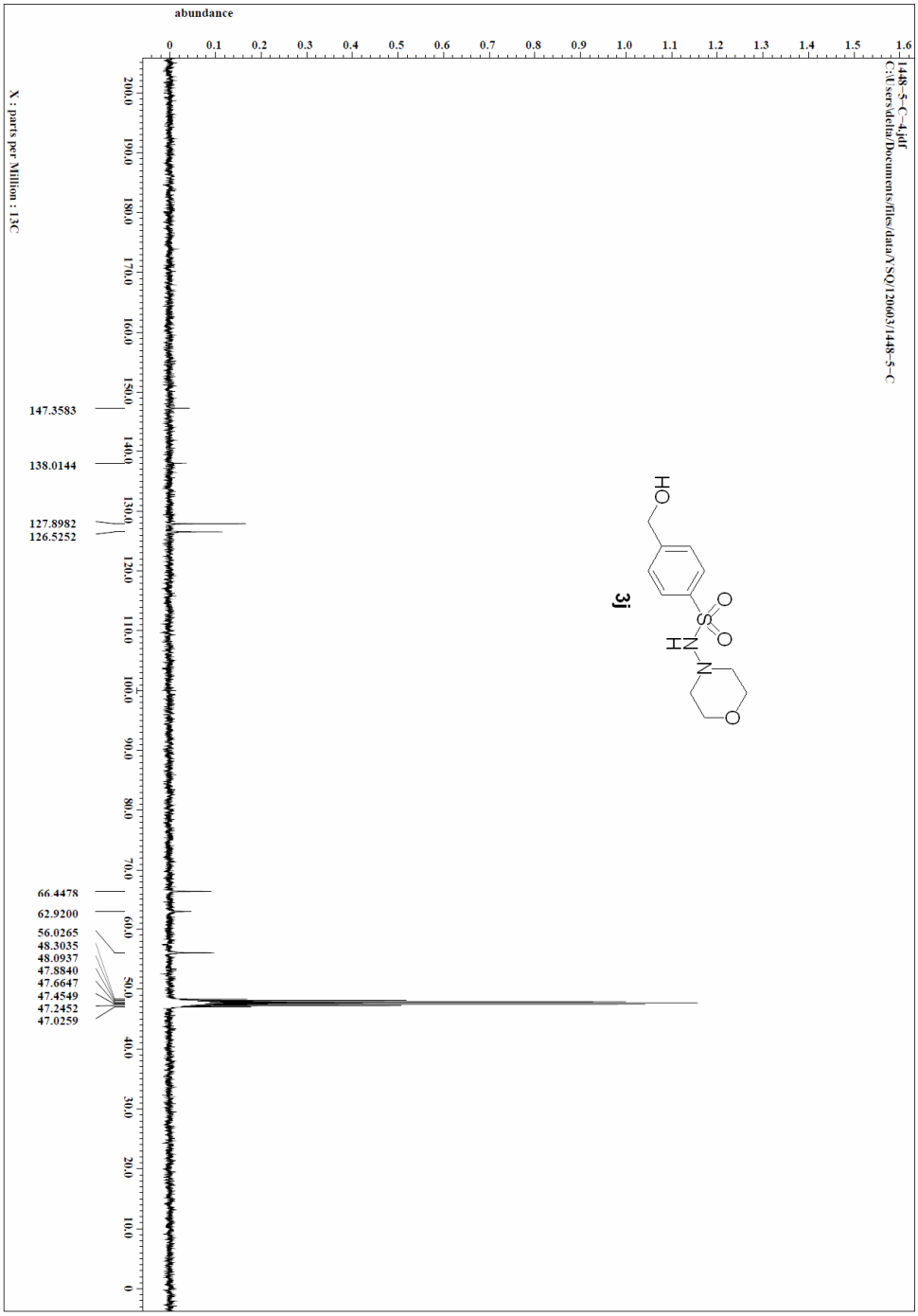
40
3j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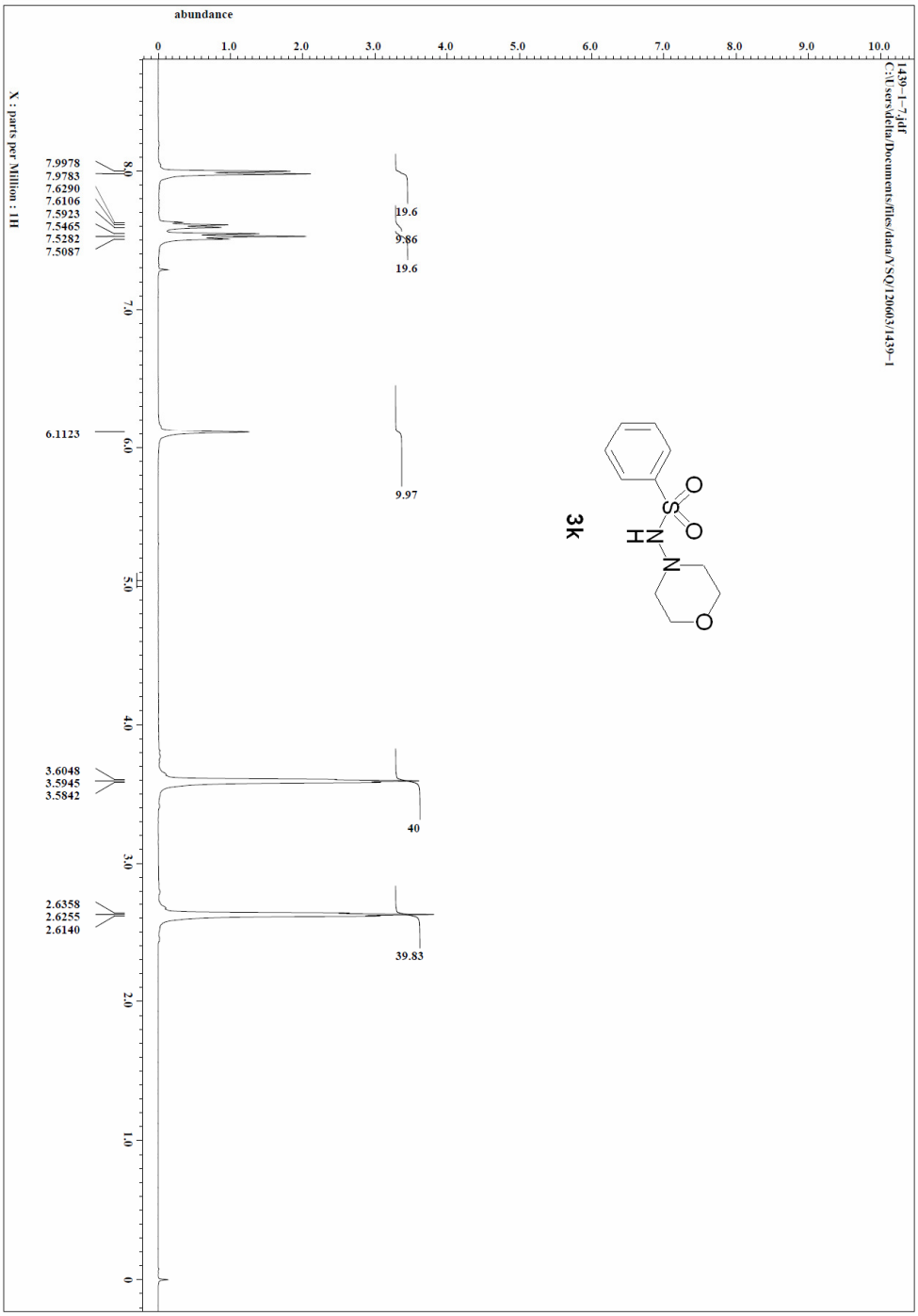
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X : parts per Million : 1H
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7.5282
7.5087
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3.6048
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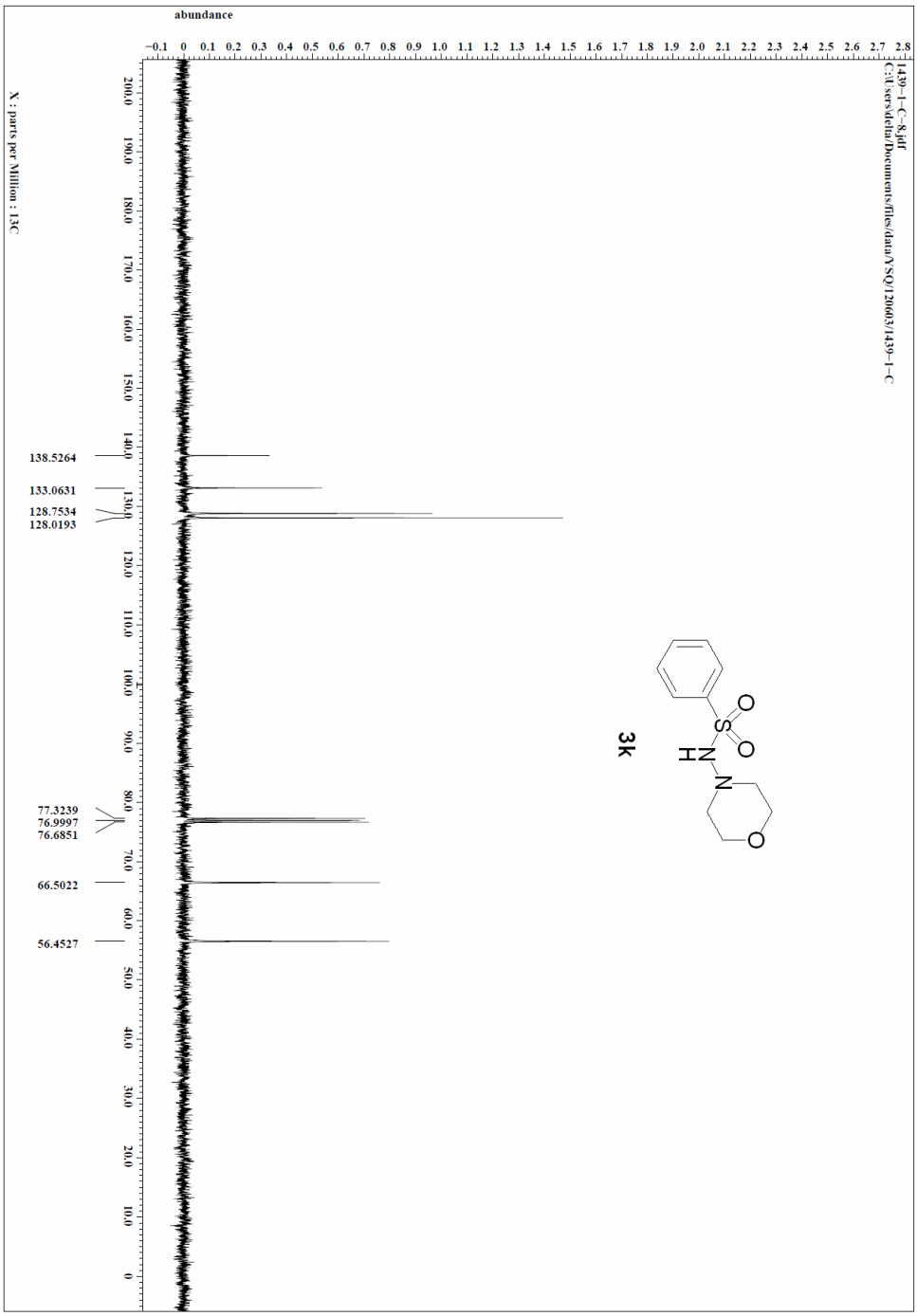
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76.6851
66.5022
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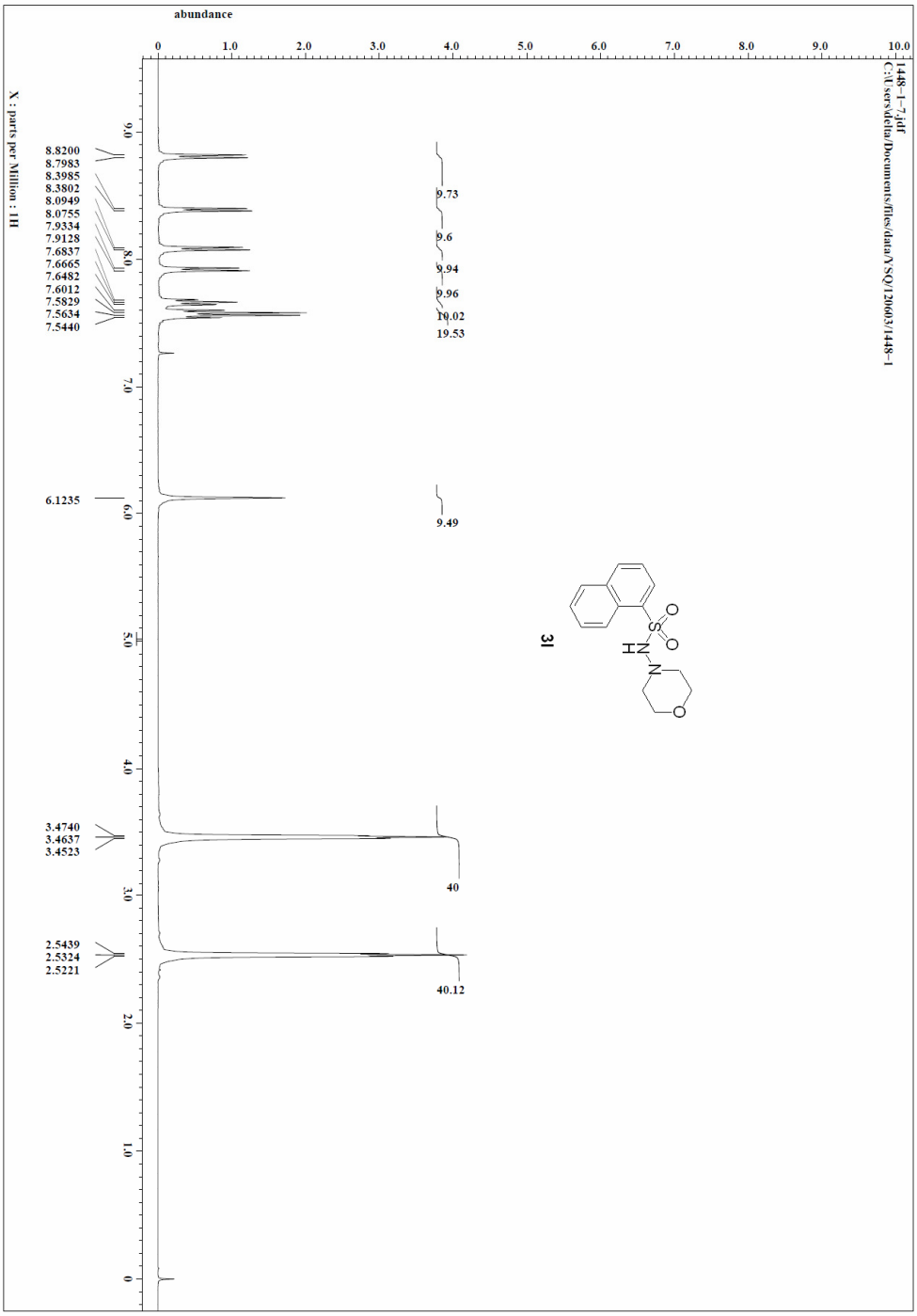
3k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1448-1-7.jdf
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7.9128
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7.6482
7.6012
7.5829
7.5634
7.5440
6.1235
3.4740
3.4637
3.4523
2.5439
2.5324
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9.73
9.6
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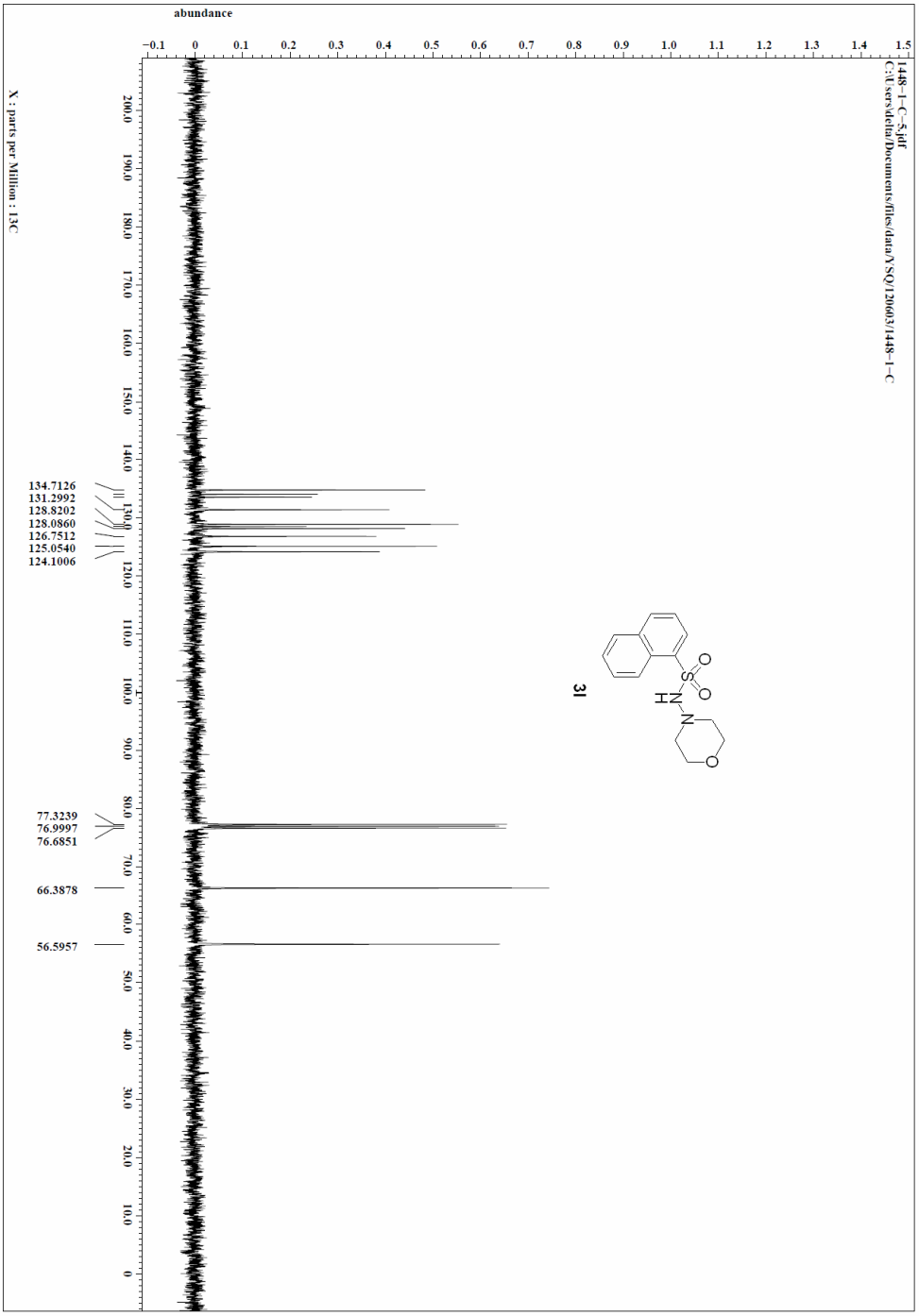
9.96
10.02
19.53
9.49
40
40.12
3l


abundance
X : parts per Million : 13C
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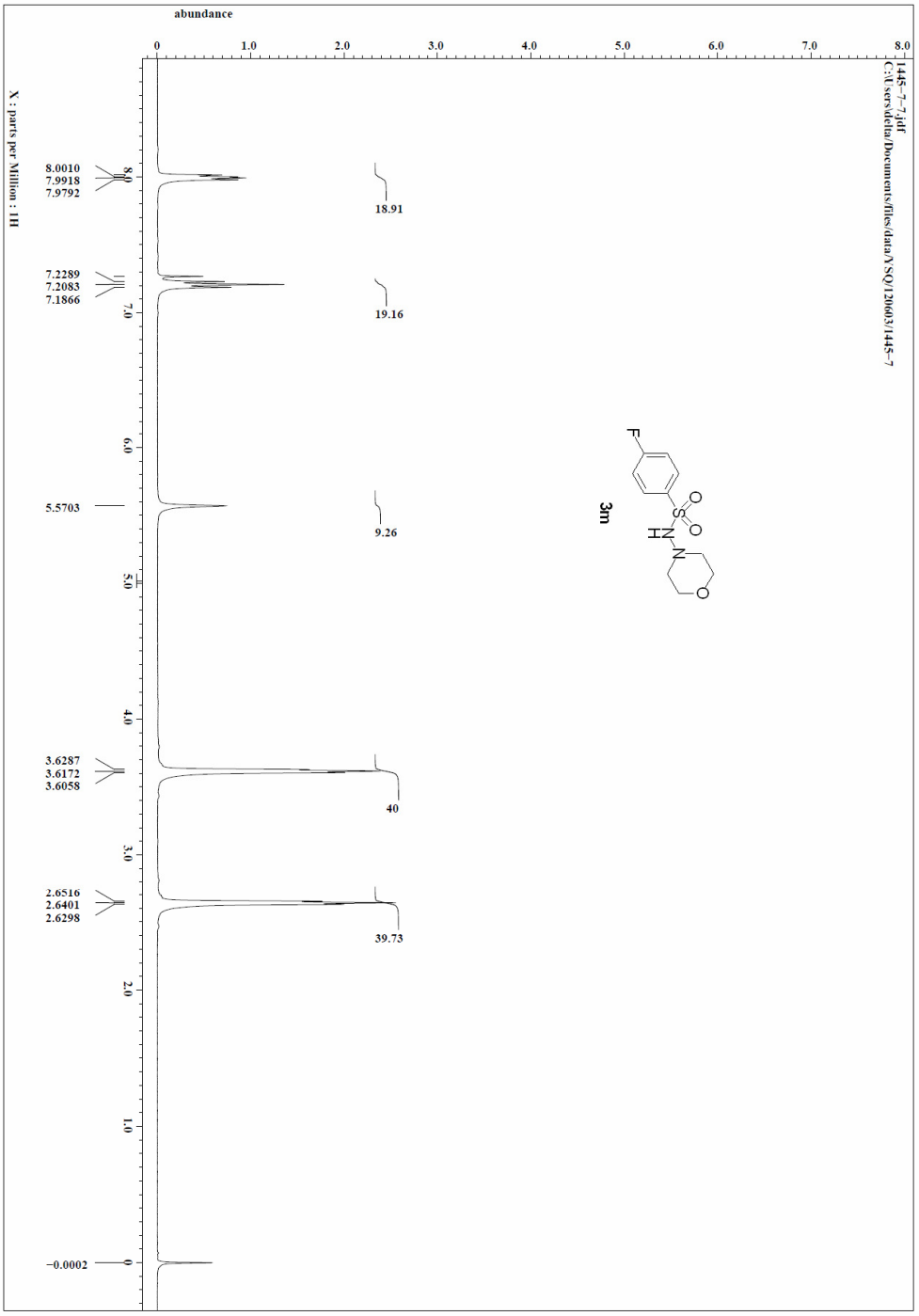
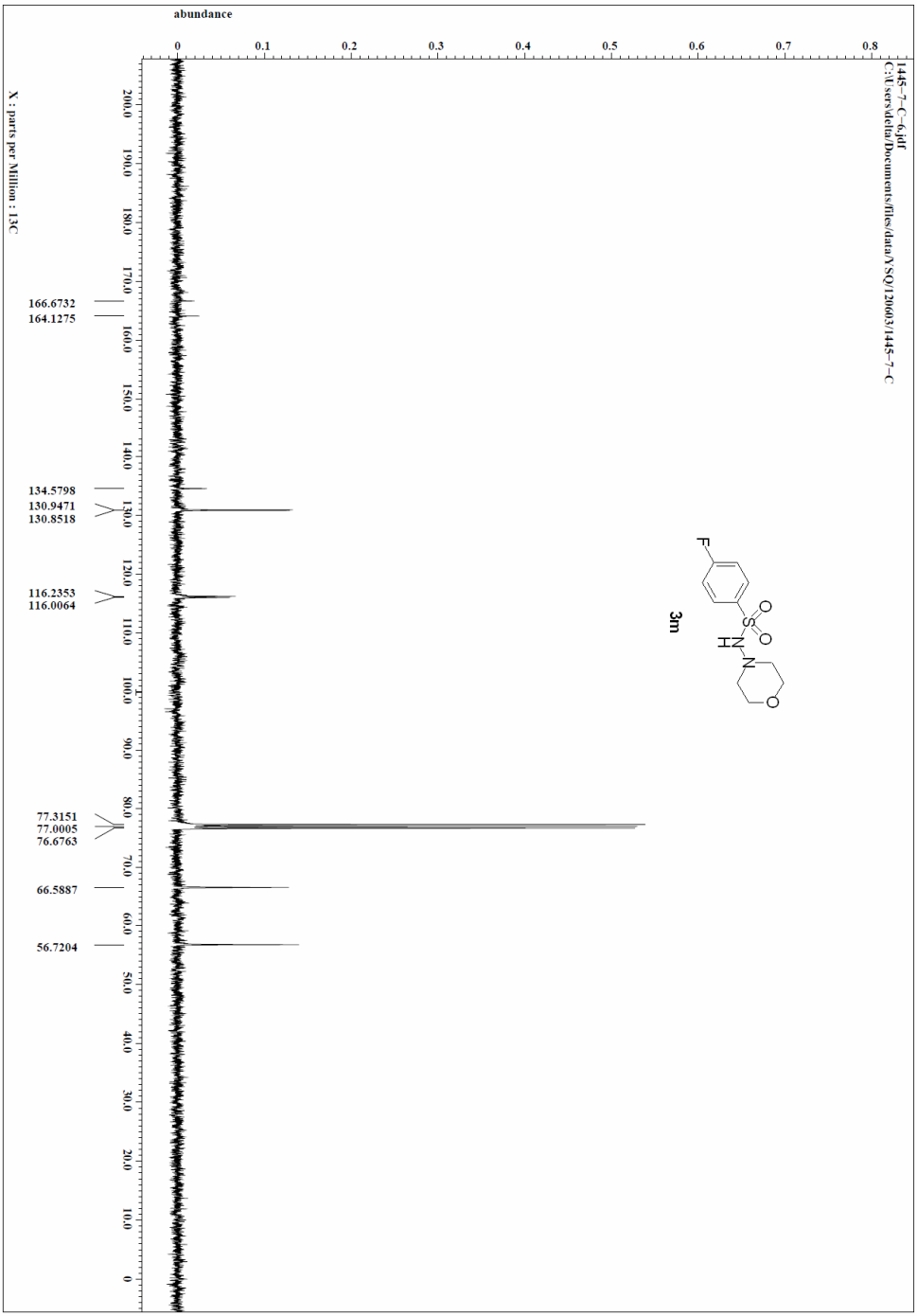
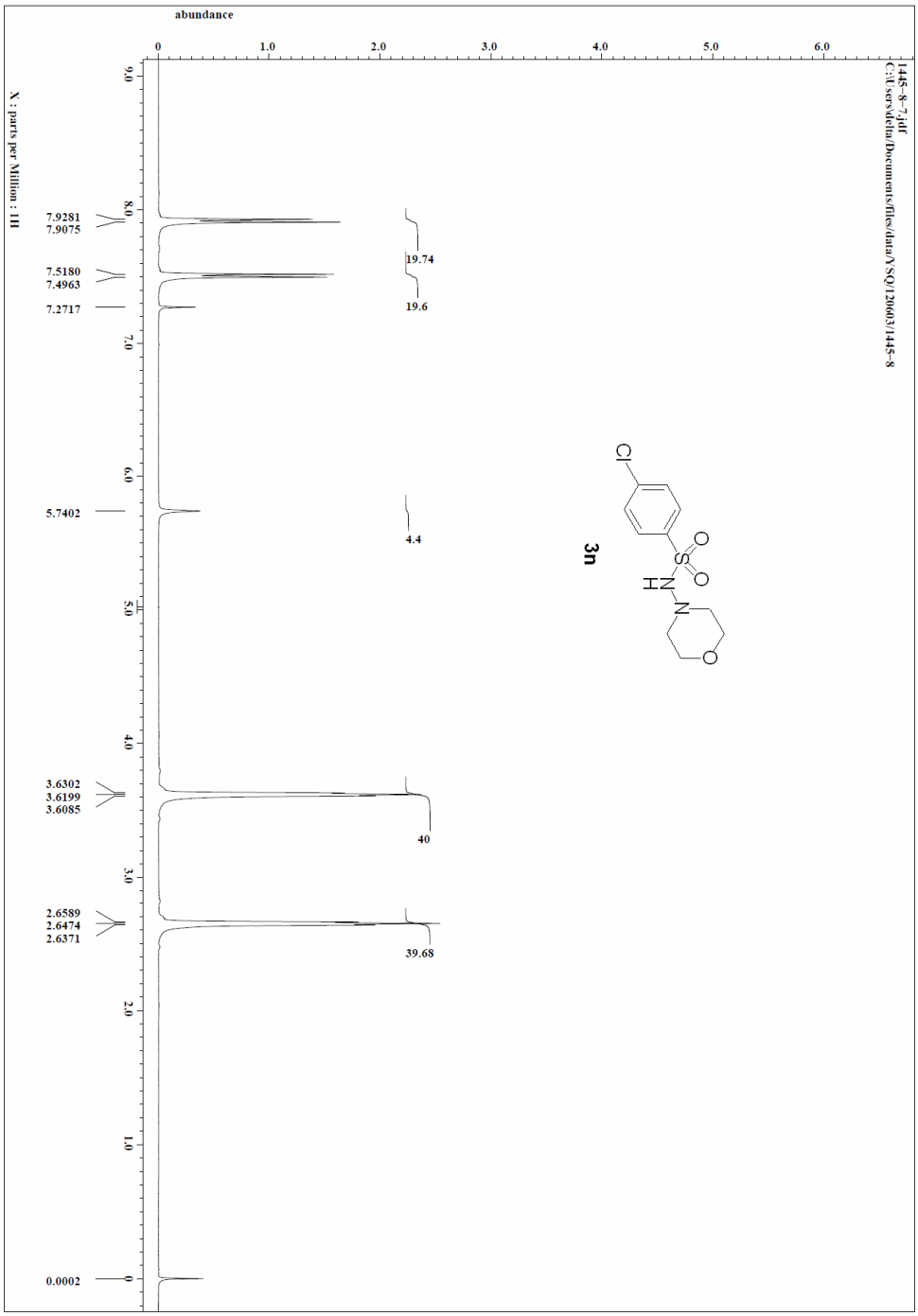
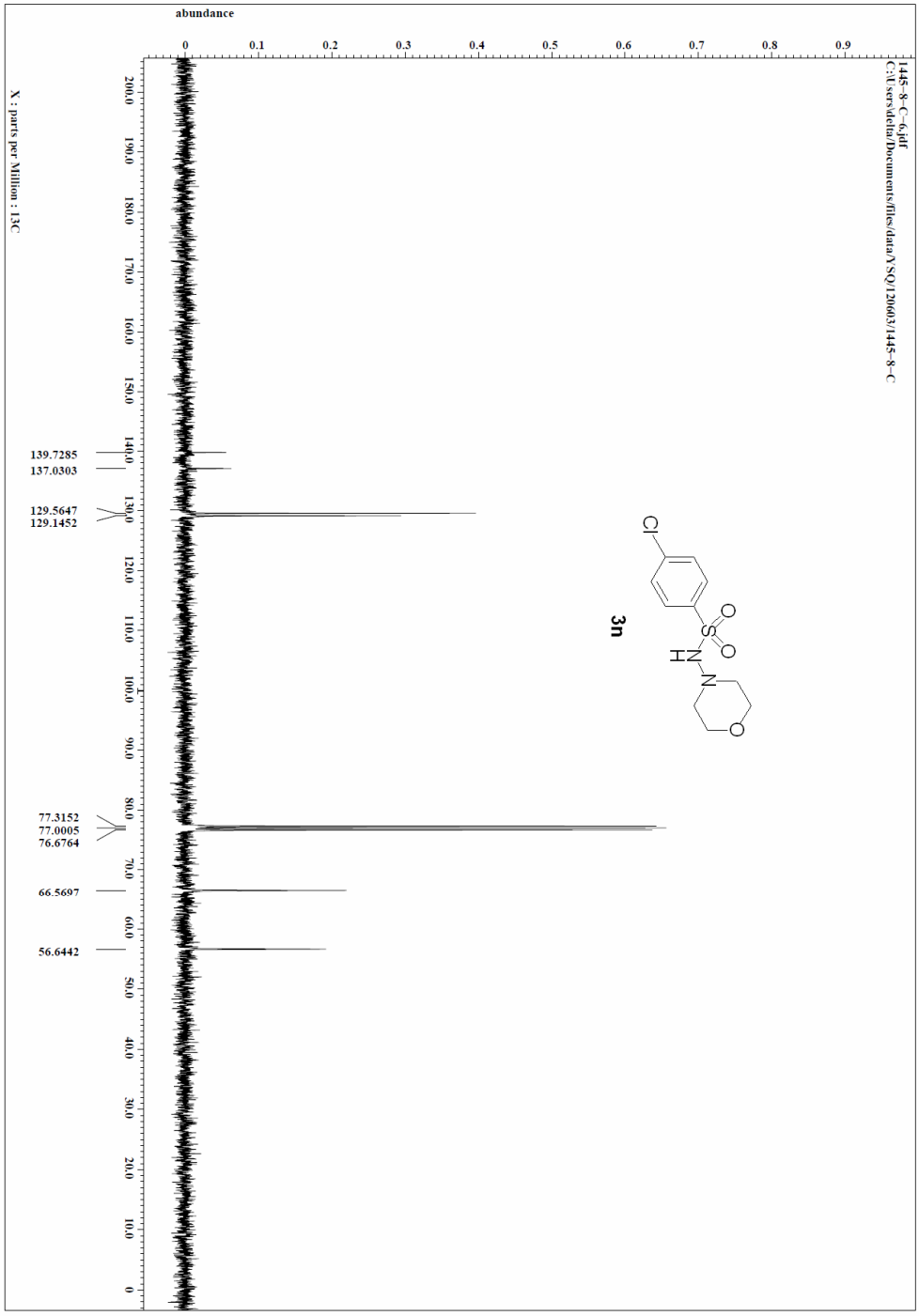
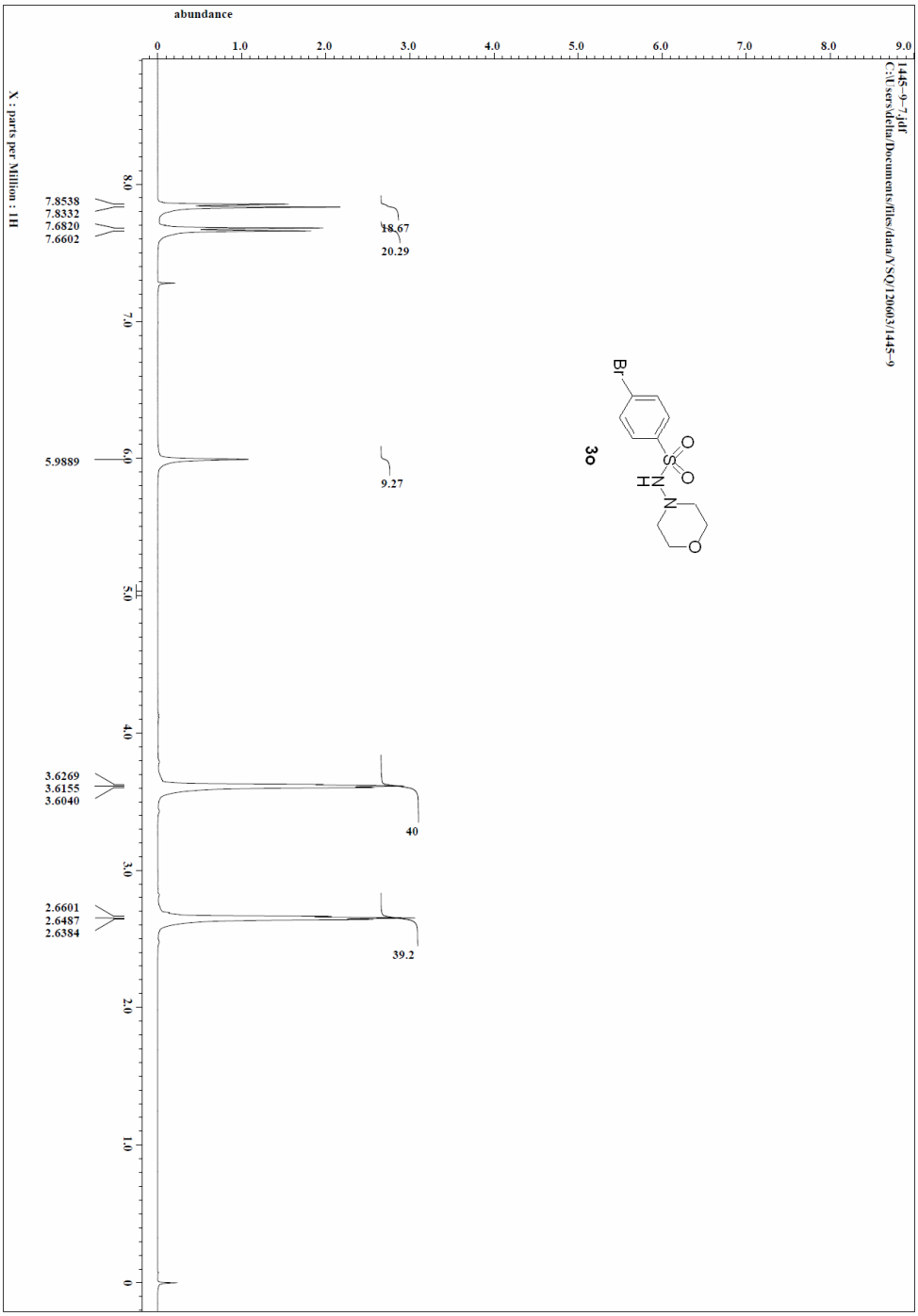
128.8202
128.0860
126.7512
125.0540
124.1006
77.3239
76.9997
76.6851
66.3878
56.5957
31

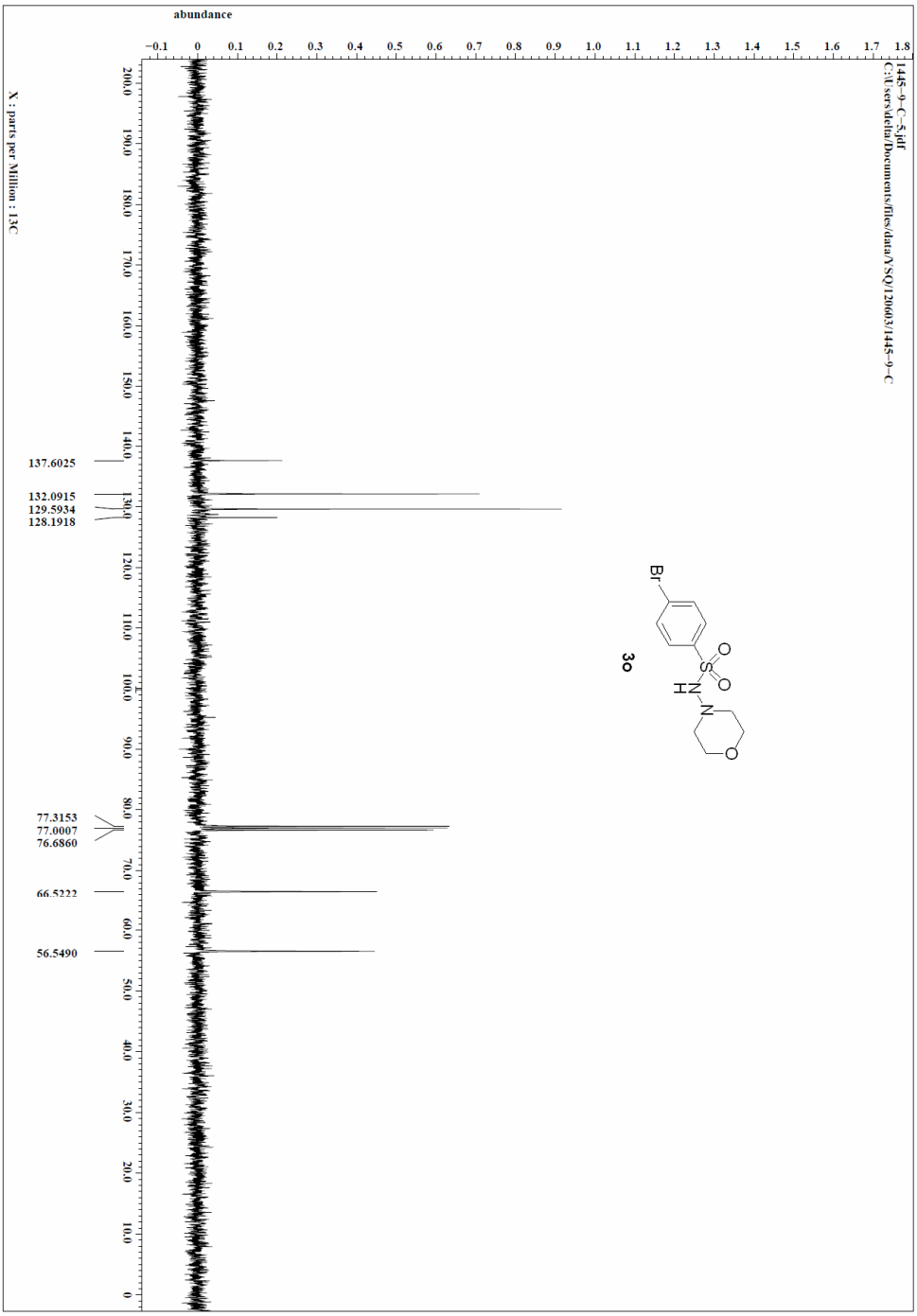

abundance
X : parts per Million : 1H
8.0010
7.9918
7.9792
7.2289
7.2083
7.1866
5.5703
3.6287
3.6172
3.6058
2.6516
2.6401
2.6298
−0.0002
18.91
19.16
9.26
40
39.73
3m
1445-7-7.jdf
C:\Users\delta\Documents\files\data\YSQ\120603\1445-7

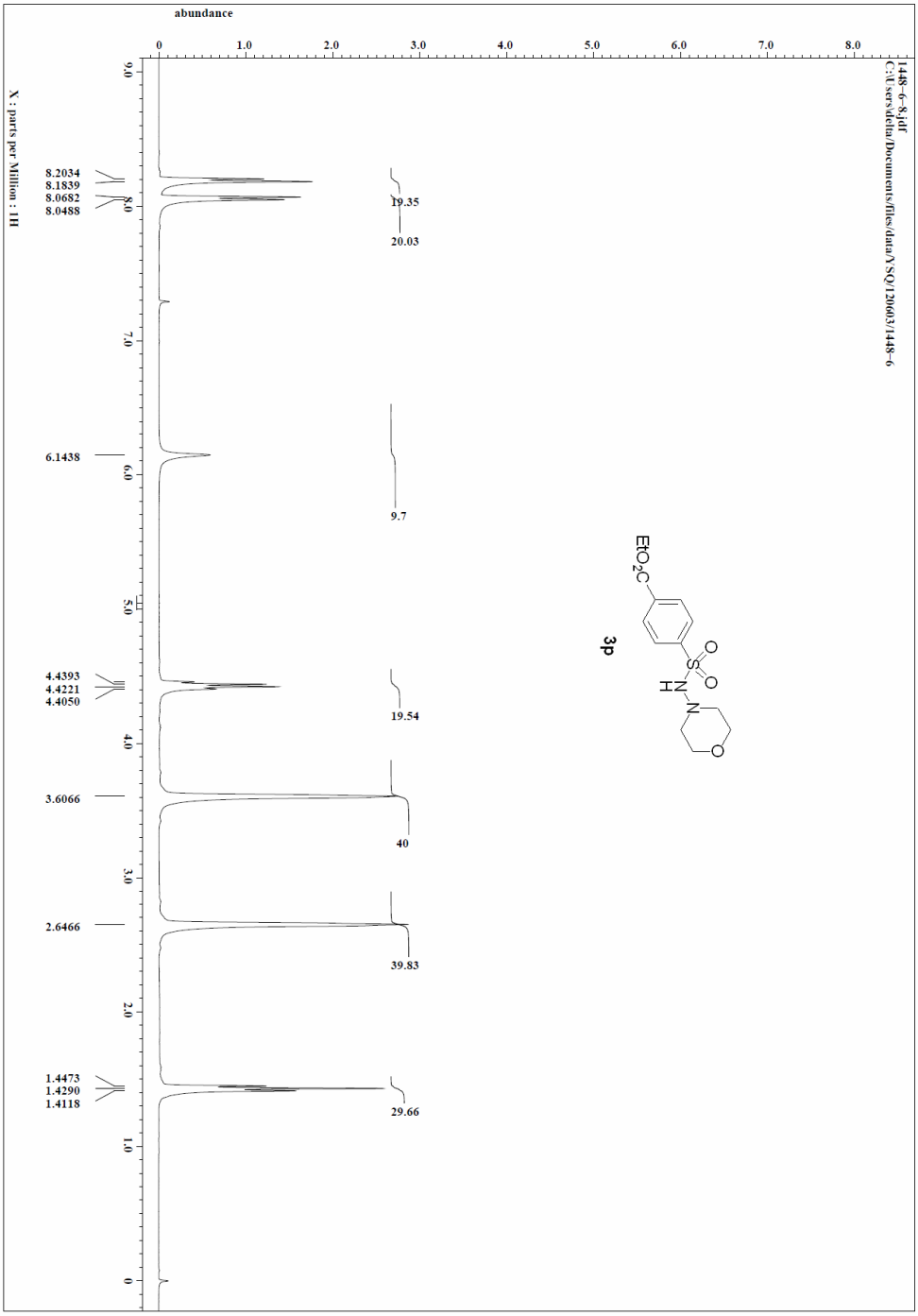

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
1445-7-C-6.jdf
C:\Users\delta\Documents\files\data\XSQ\120603\1445-7-C
X : parts per Million : 13C
166.6732
164.1275
134.5798
130.9471
130.8518
116.2353
116.0064
77.3151
77.0005
76.6763
66.5887
56.7204
3m
F
S
O
O
HN
N
O

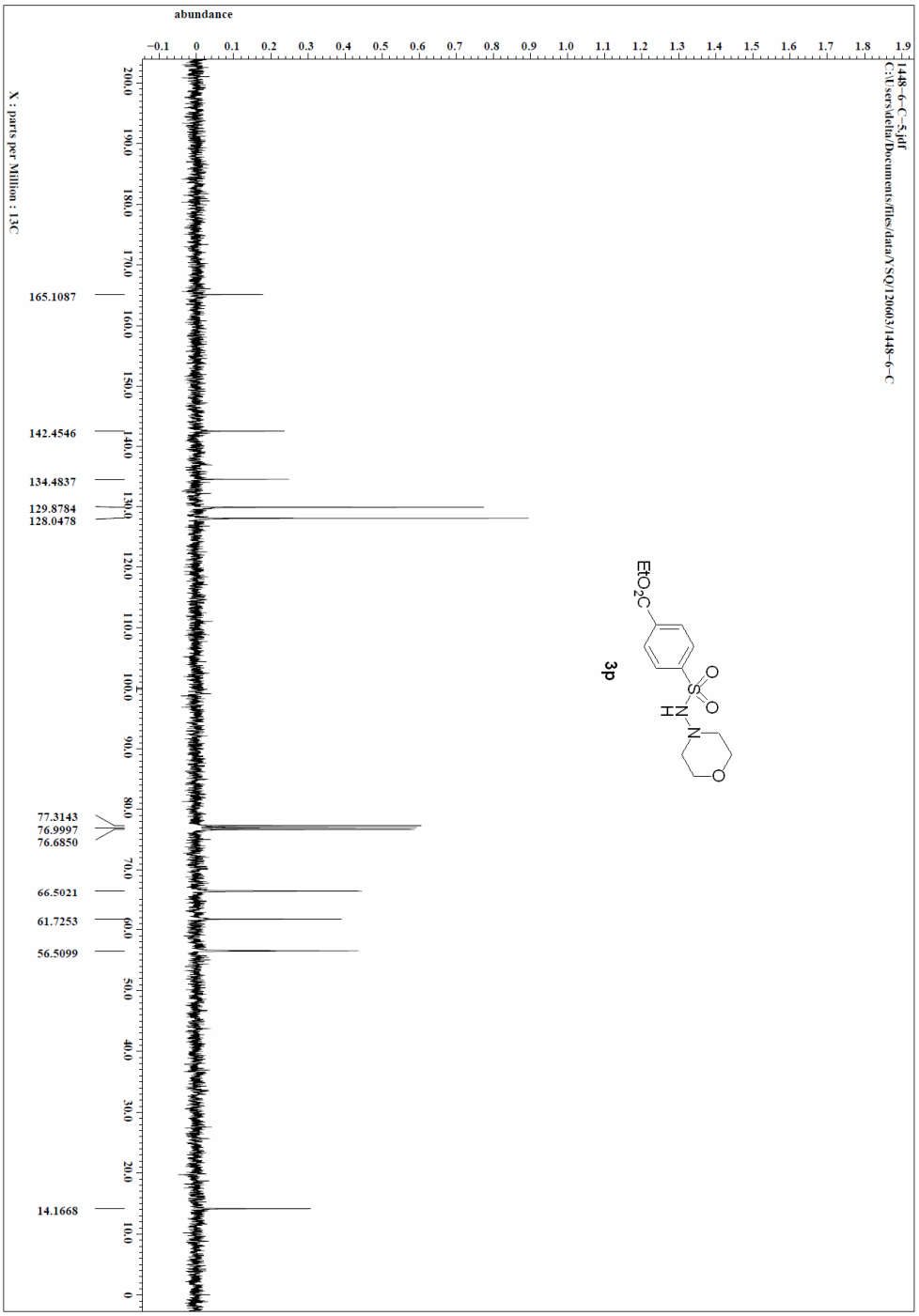

abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
C:\Users\delta\Documents\files\data\YSQ\120603\1445-8
X : parts per Million : 1H
7.9281
7.9075
7.5180
7.4963
7.2717
5.7402
3.6302
3.6199
3.6085
2.6589
2.6474
2.6371
0.0002
19.74
19.6
4.4
40
39.68
3n
Cl
O
S
O
HN
N
O

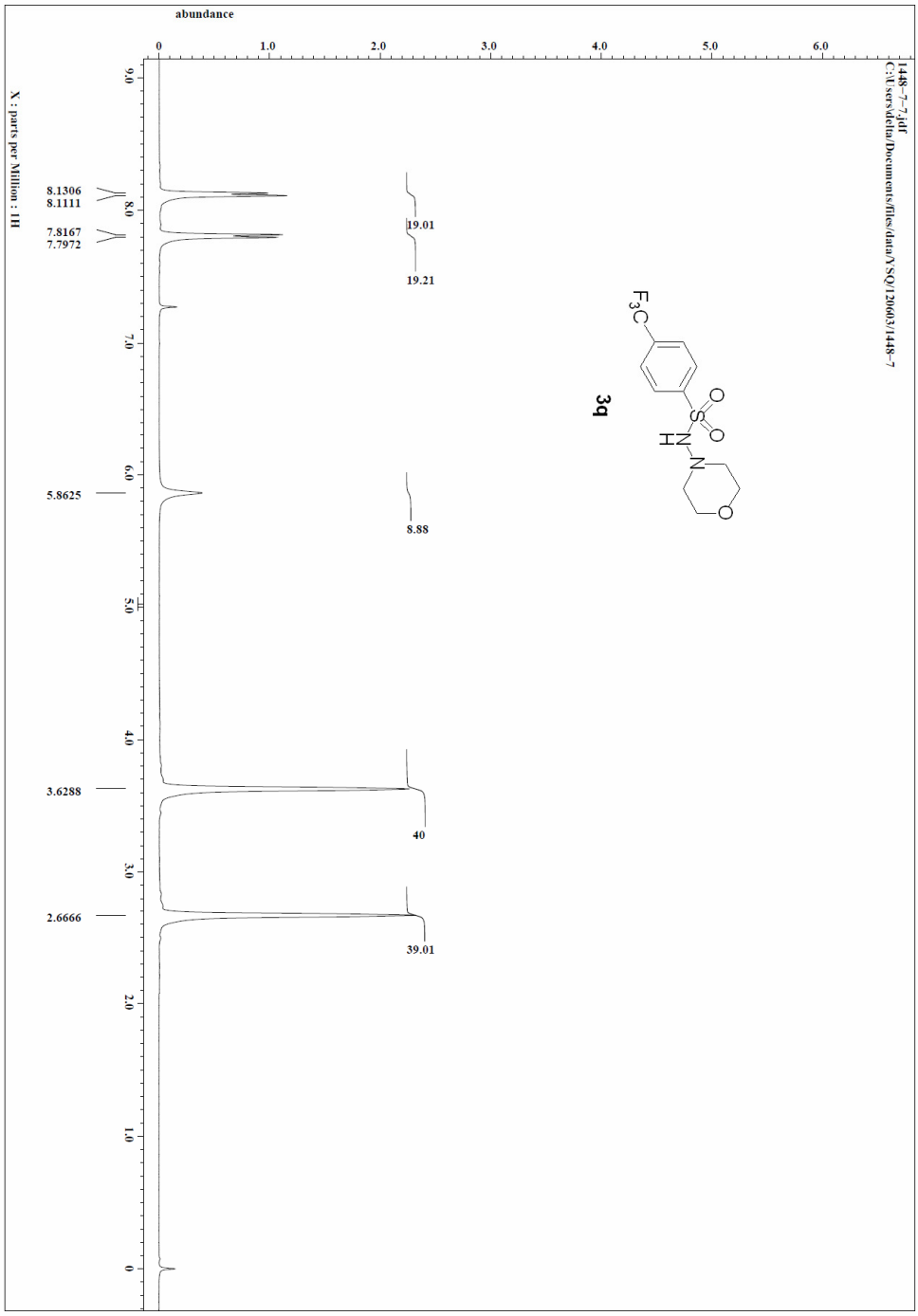

abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1445-8-C-6.jdf
C:\Users\delta\Documents\fils\data\YSQ\120603\1445-8-C
X : parts per Million : 13C
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
139.7285
137.0303
129.5647
129.1452
77.3152
77.0005
76.6764
66.5697
56.6442
3n
Cl
O
S
O
HN
N
O

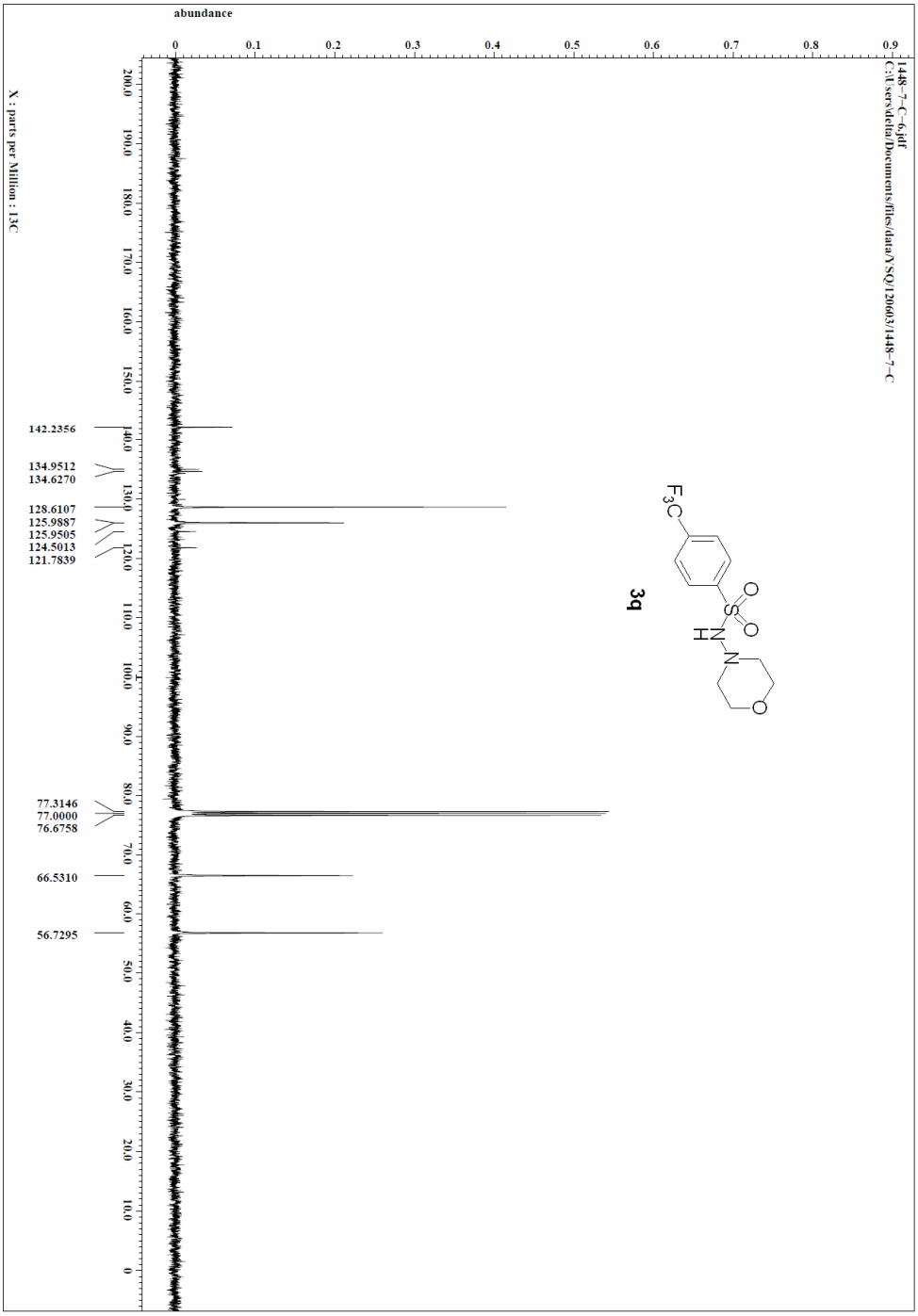

abundance
X : parts per Million : 1H
C:\Users\delta\Documents\files\data\YSQ\120603\1445-9
1445-9-7.jdf
7.8538
7.8332
7.6820
7.6602
5.9889
3.6269
3.6155
3.6040
2.6601
2.6487
2.6384
18.67
20.29
9.27
40
39.2
Br
O
S
O
HN
N
O
3o

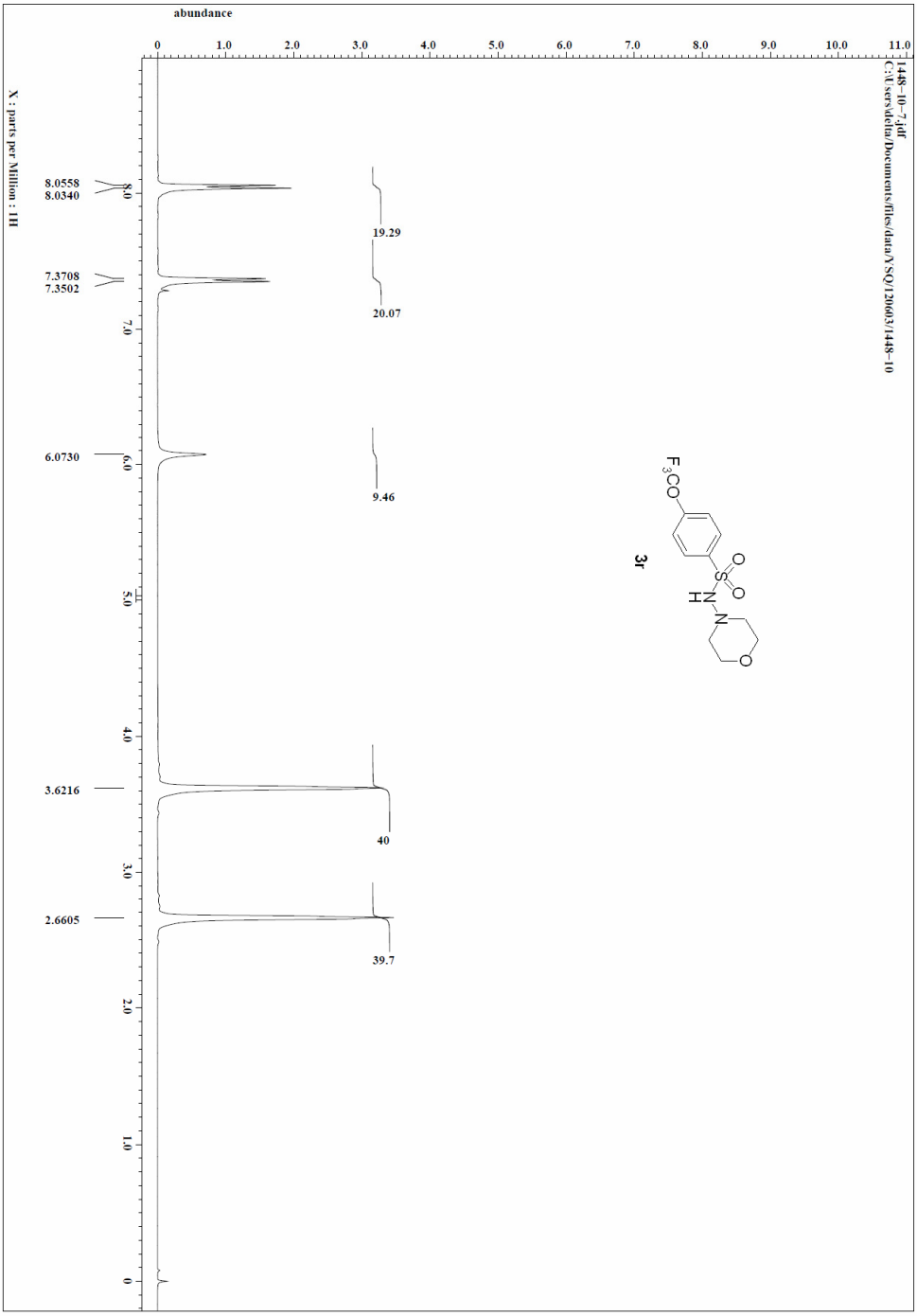

abundance
X : parts per Million : 13C
137.6025
132.0915
129.5934
128.1918
77.3153
77.0007
76.6860
66.5222
56.5490
Br
O
S
O
N
H
N
O
3o

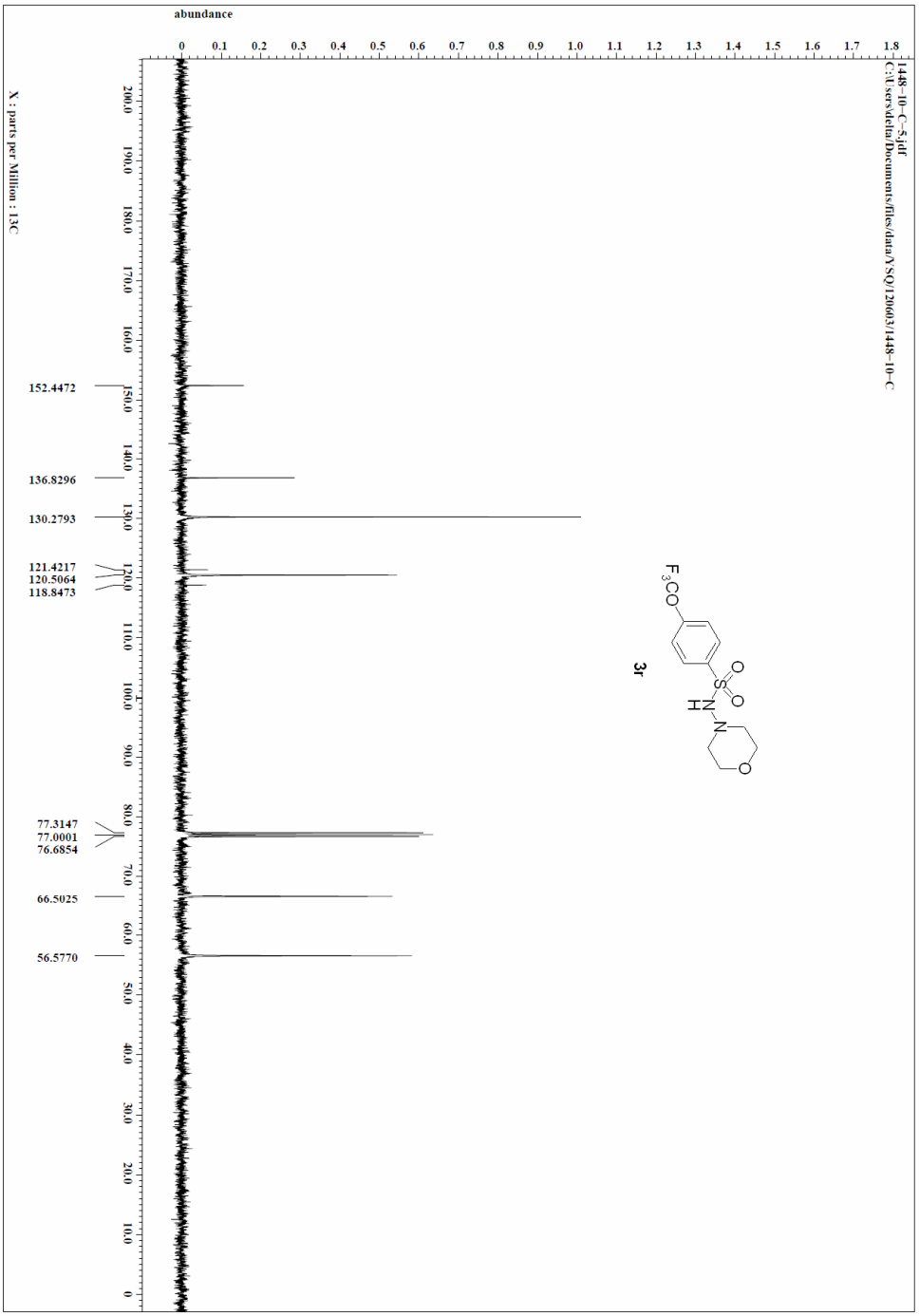

abundance
X : parts per Million : 1H
1448-6-8.jdf
C:\Users\delia\Documents\files\data\YSQ\120603\1448-6
8.2034
8.1839
8.0682
8.0488
6.1438
4.4393
4.4221
4.4050
3.6066
2.6466
1.4473
1.4290
1.4118
19.35
20.03
9.7
19.54
40
39.83
29.66
3p

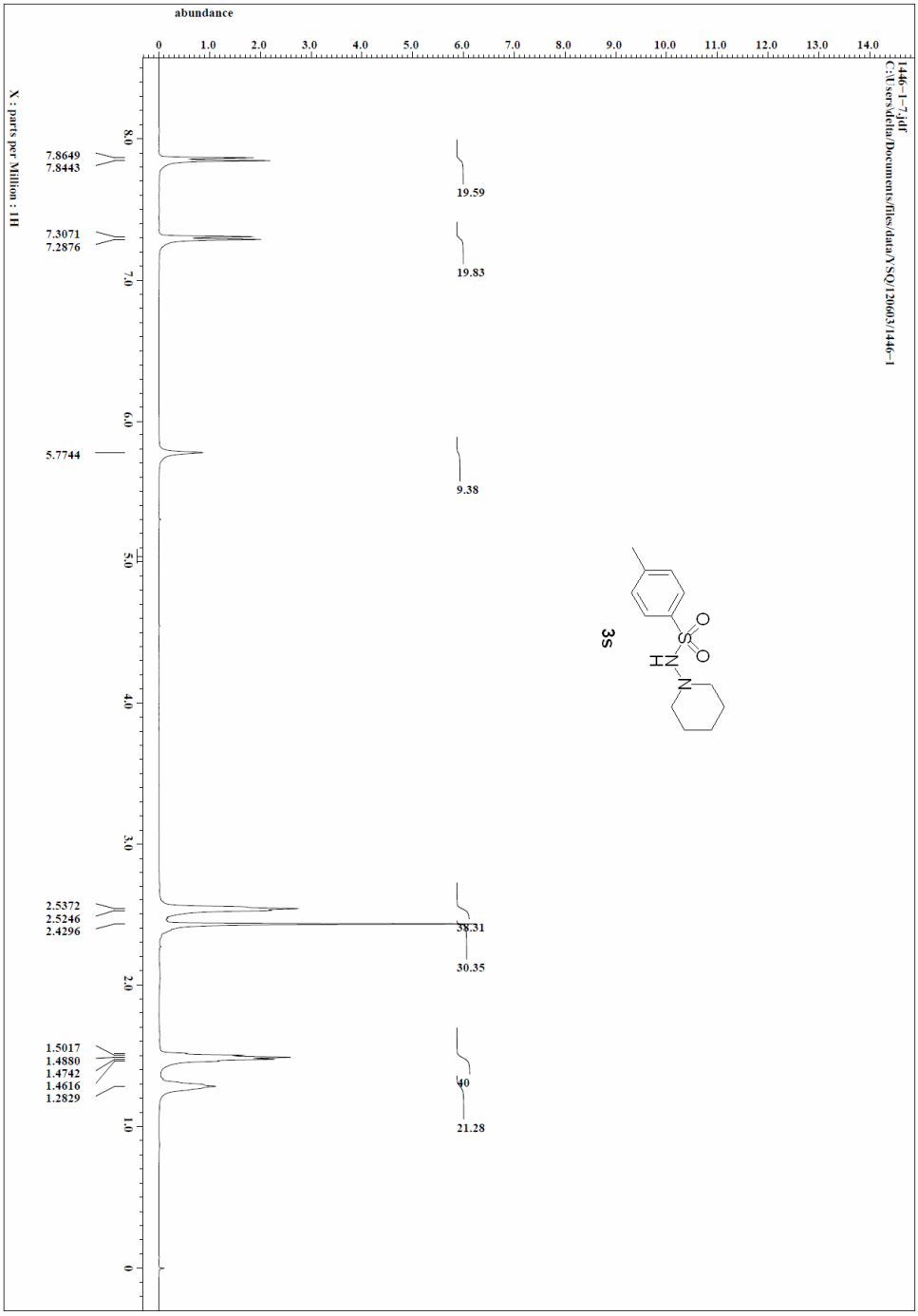

abundance
X : parts per Million : 13C
C:\Users\delta\Documents\files\data\NSQ\120603\1448-6-C
1448-6-C-5.jdf
165.1087
142.4546
134.4837
129.8784
128.0478
77.3143
76.9997
76.6850
66.5021
61.7253
56.5099
14.1668
EtO2C
3p

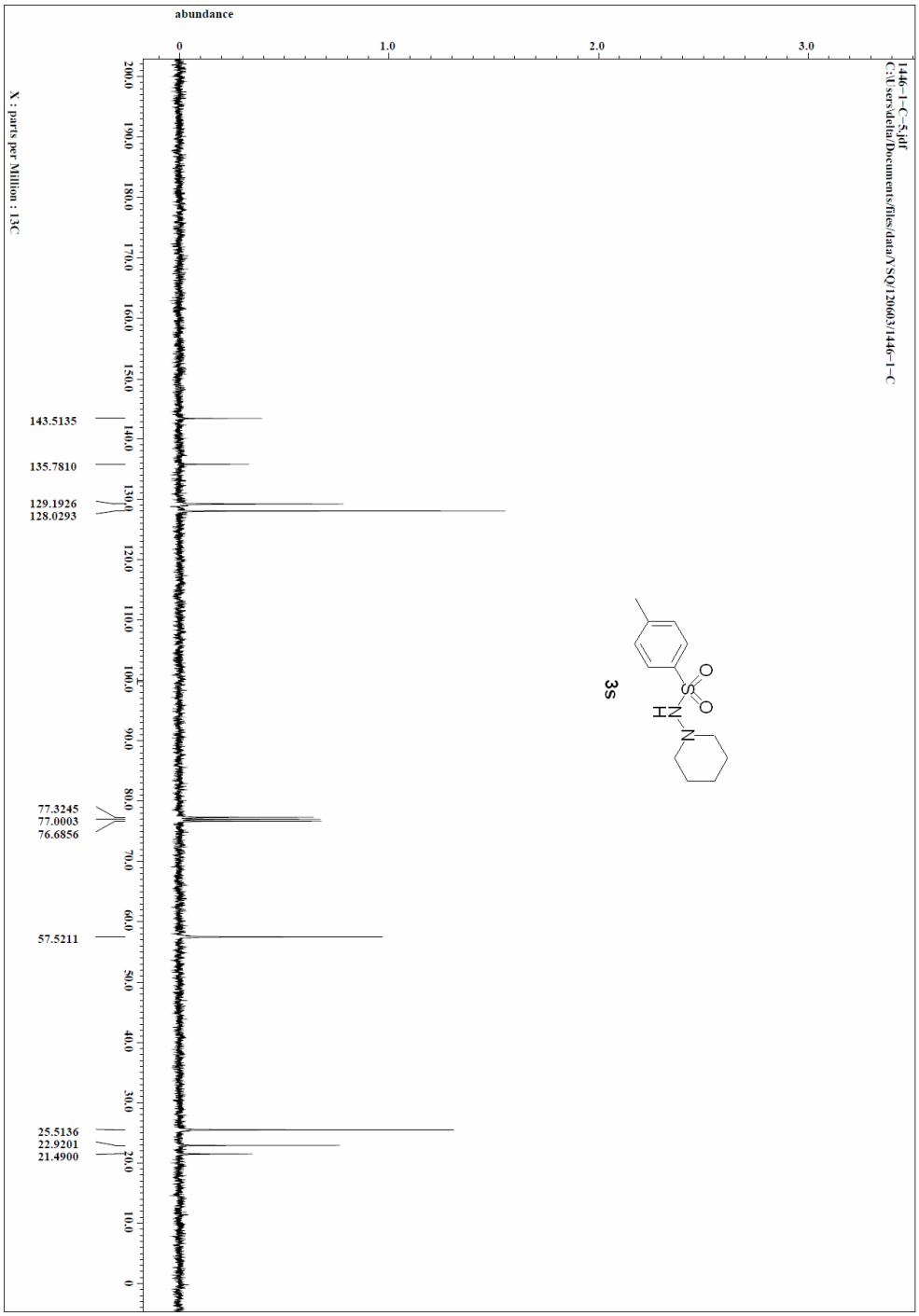

abundance
X : parts per Million : 1H
C:\Users\delta\Documents\files\data\YSQ\12060\1448-7
1448--7--7.jdf
8.1306
8.1111
7.8167
7.7972
5.8625
3.6288
2.6666
19.01
19.21
8.88
40
39.01
3q

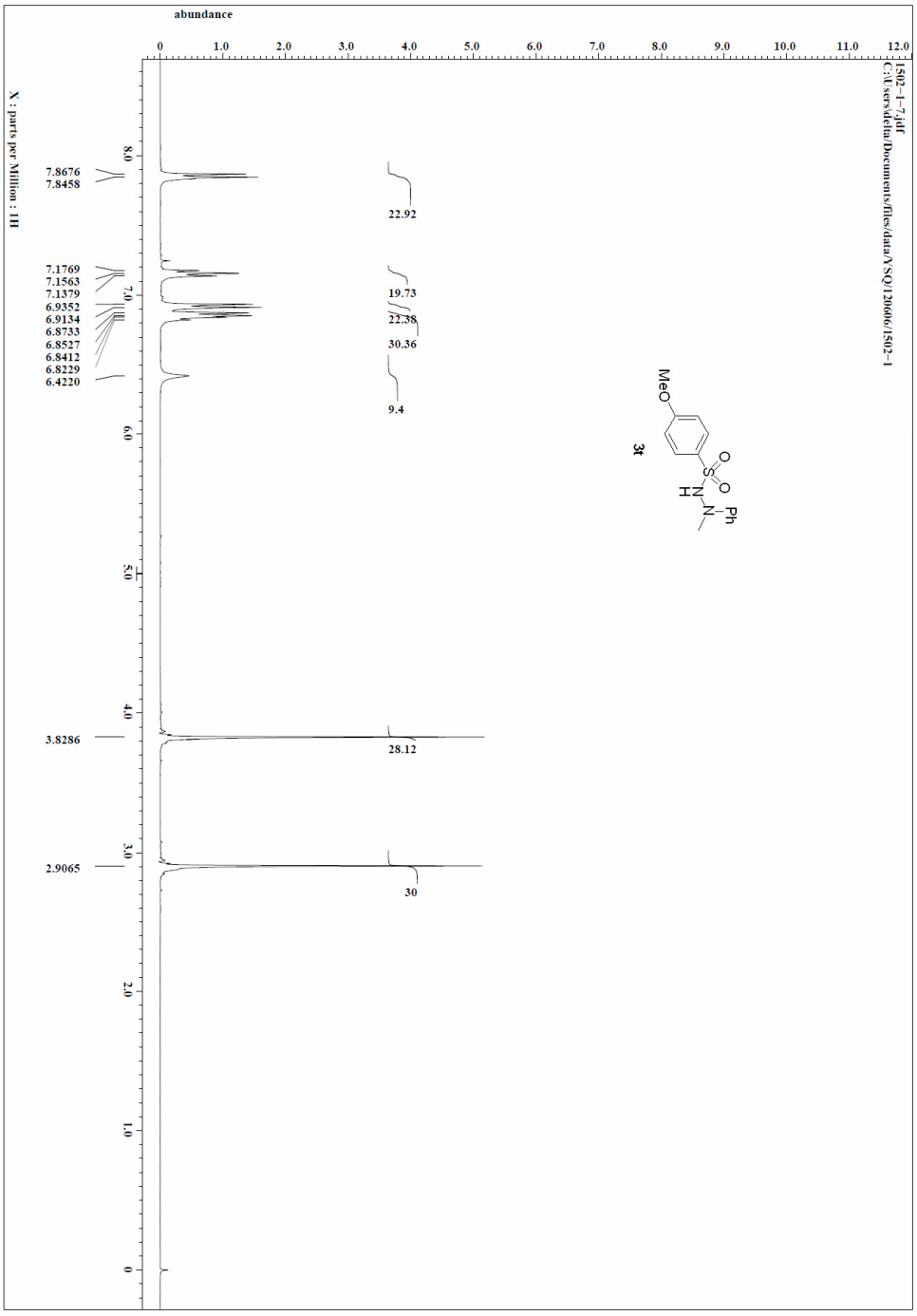

abundance
X : parts per Million : 13C
142.2356
134.9512
134.6270
128.6107
125.9887
125.9505
124.5013
121.7839
77.3146
77.0000
76.6758
66.5310
56.7295
3q

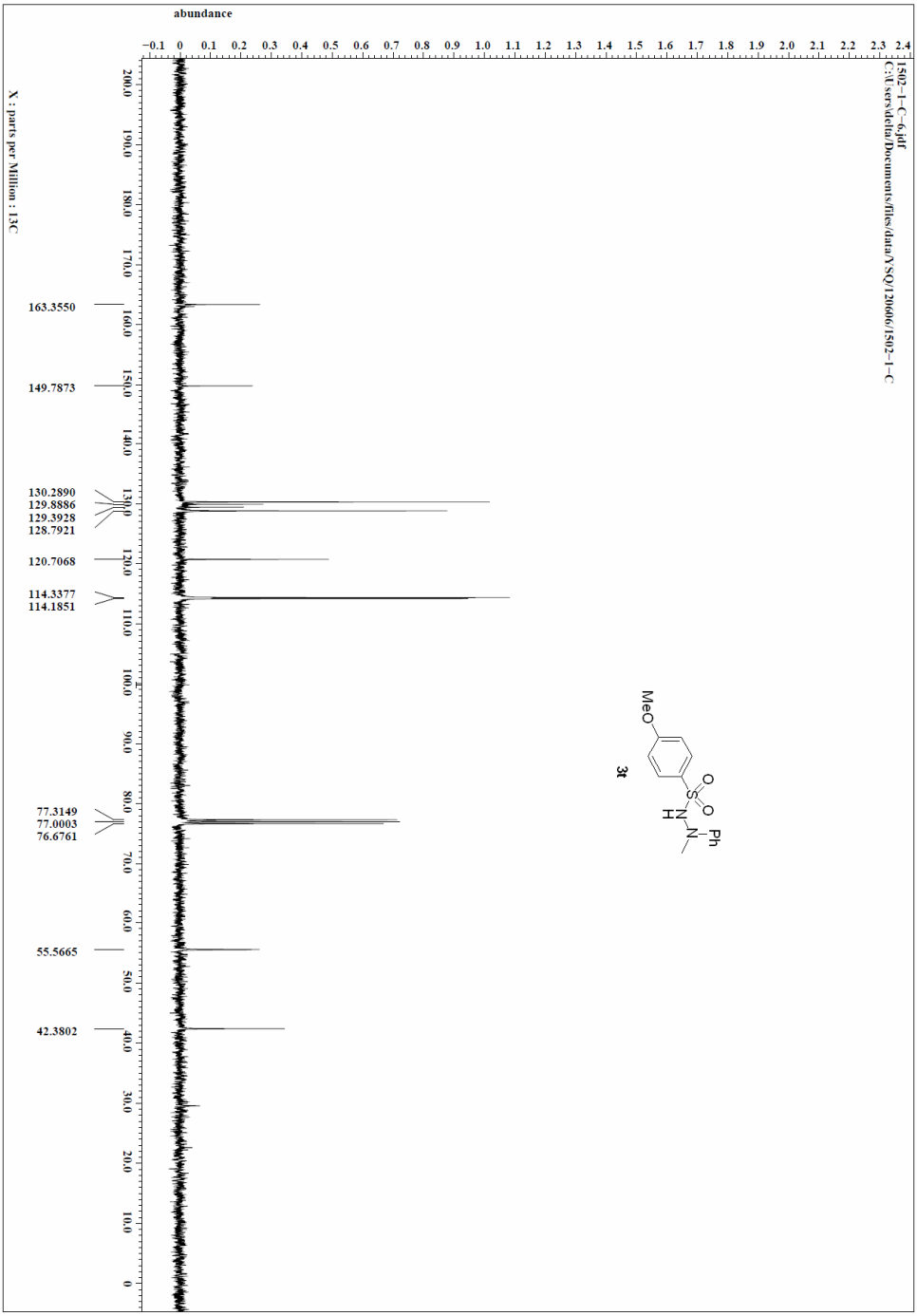

abundance
X : parts per Million : 1H
C:\Users\delia\Documents\files\data\YSQ\120603\1448-10_7.jdf
1448-10-7.jdf
8.0558
8.0340
7.3708
7.3502
6.0730
3.6216
2.6605
19.29
20.07
9.46
40
39.7
3r

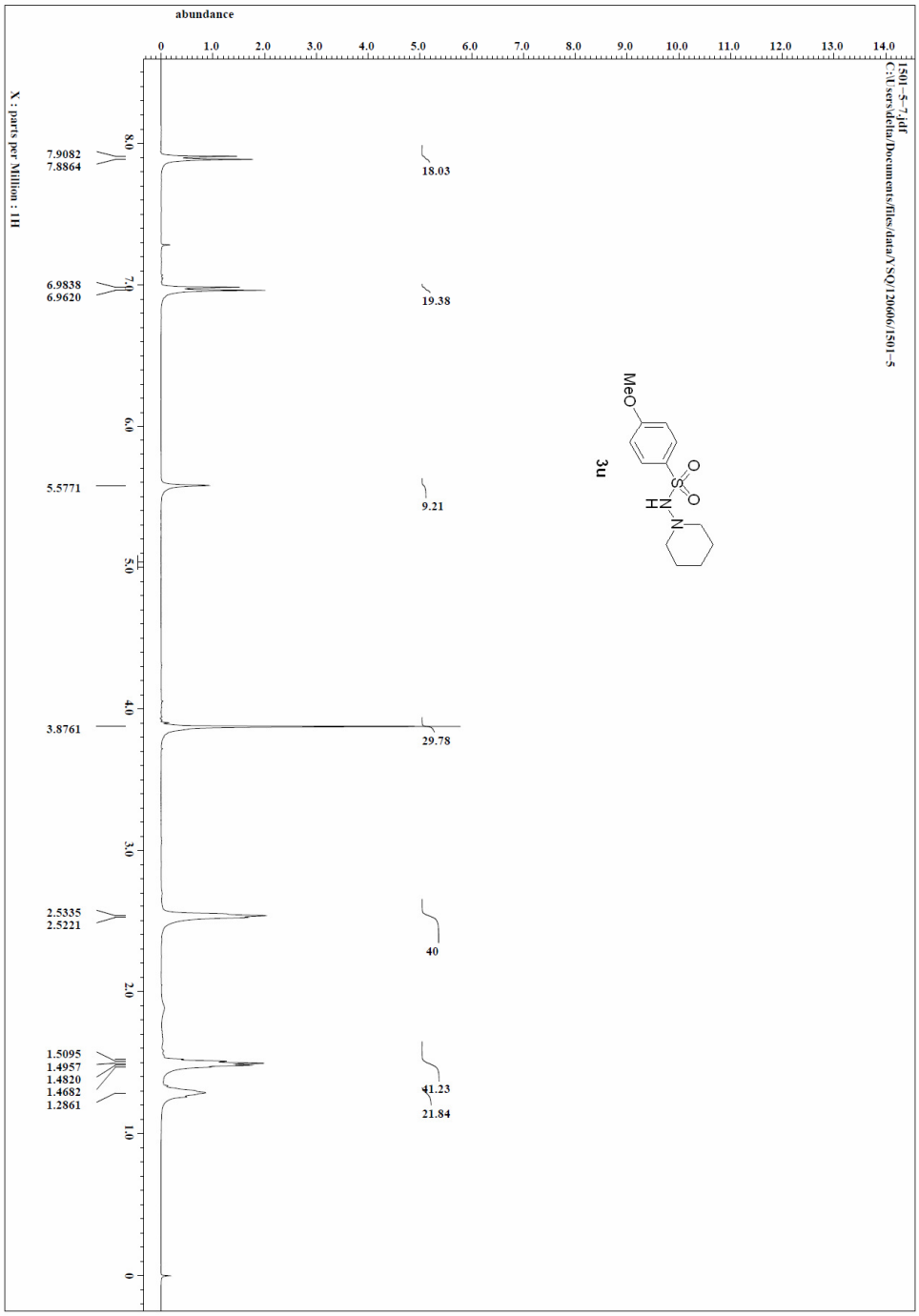

abundance
X : parts per Million : 13C
1448-10-C--5.jdf
C:\Users\delia\Documents\files\data\YSQ\120603\1448-10-C
152.4472
136.8296
130.2793
121.4217
120.5064
118.8473
77.3147
77.0001
76.6854
66.5025
56.5770
3r

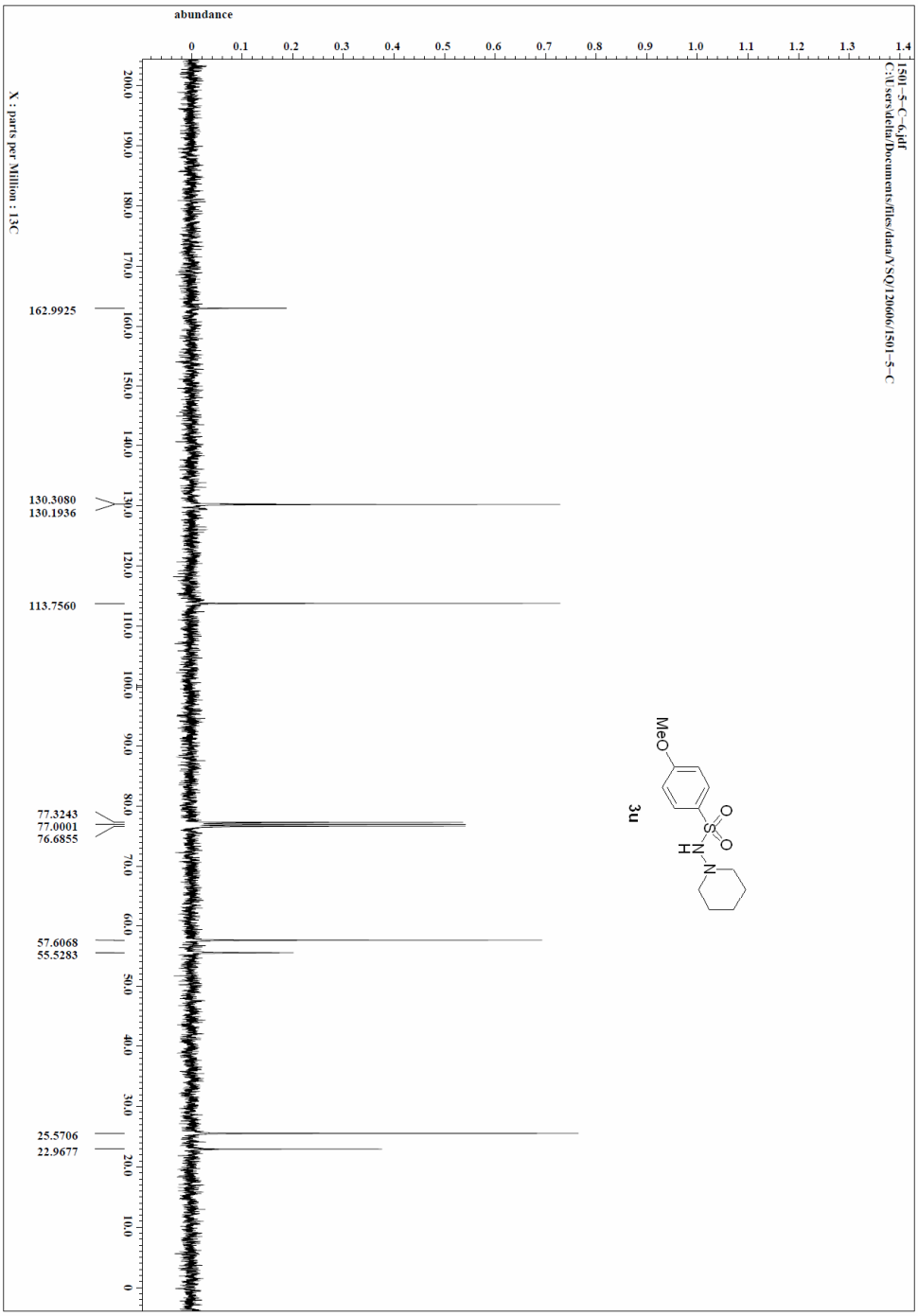

abundance
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0
1446-1-7.jdf
C:\Users\delta\Documents\files\data\YSQ\120603\1446-1
X : parts per Million : 1H
7.8649
7.8443
7.3071
7.2876
5.7744
2.5372
2.5246
2.4296
1.5017
1.4880
1.4742
1.4616
1.2829
19.59
19.83
9.38
38.31
30.35
40
21.28
3s

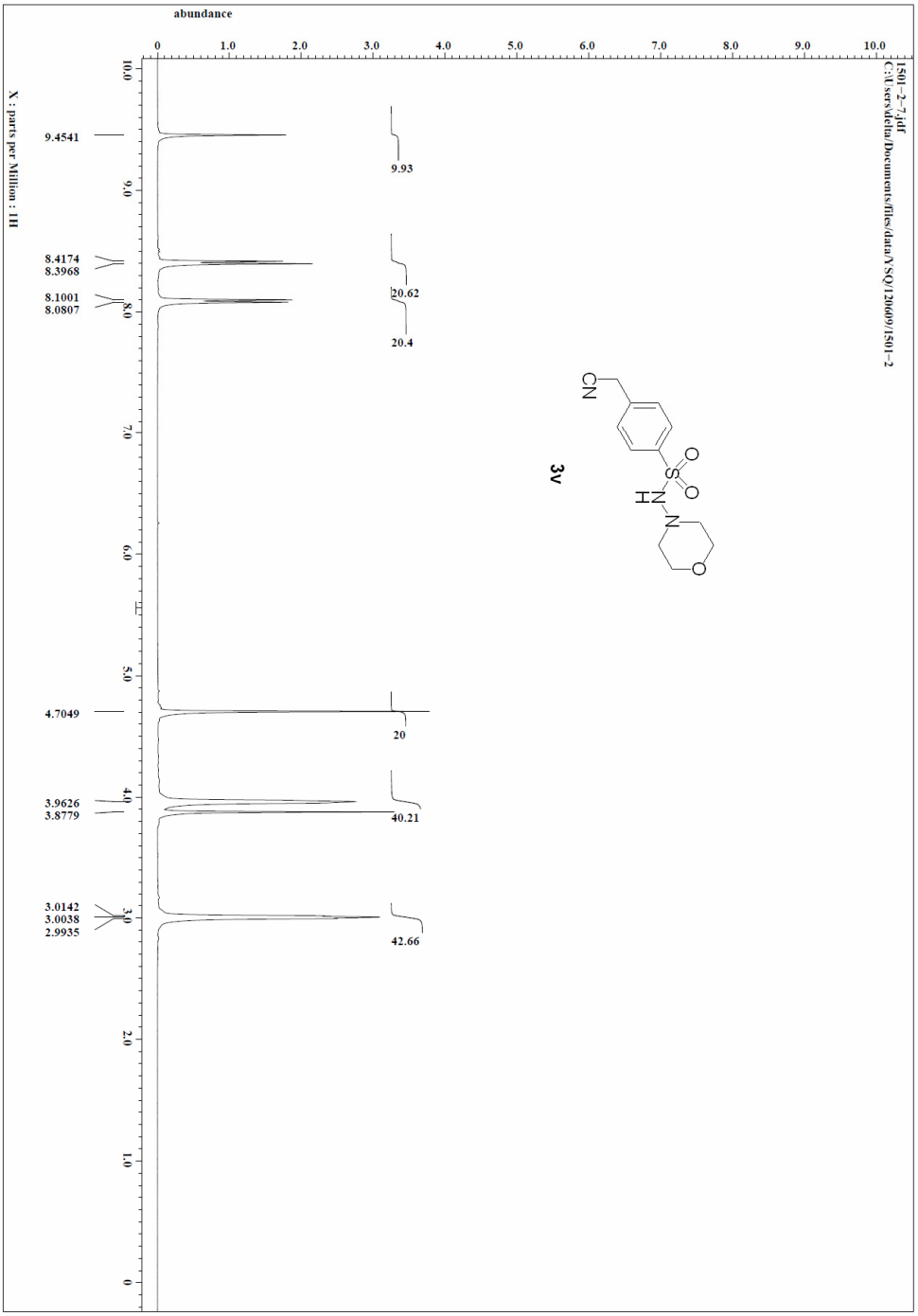

abundance
0
1.0
2.0
3.0
1446-1-C-5.jdf
C:\Users\delta\Documents\files\data\YSQ\120603\1446-1-C
X : parts per Million : 13C
143.5135
135.7810
129.1926
128.0293
77.3245
77.0003
76.6856
57.5211
25.5136
22.9201
21.4900
3s

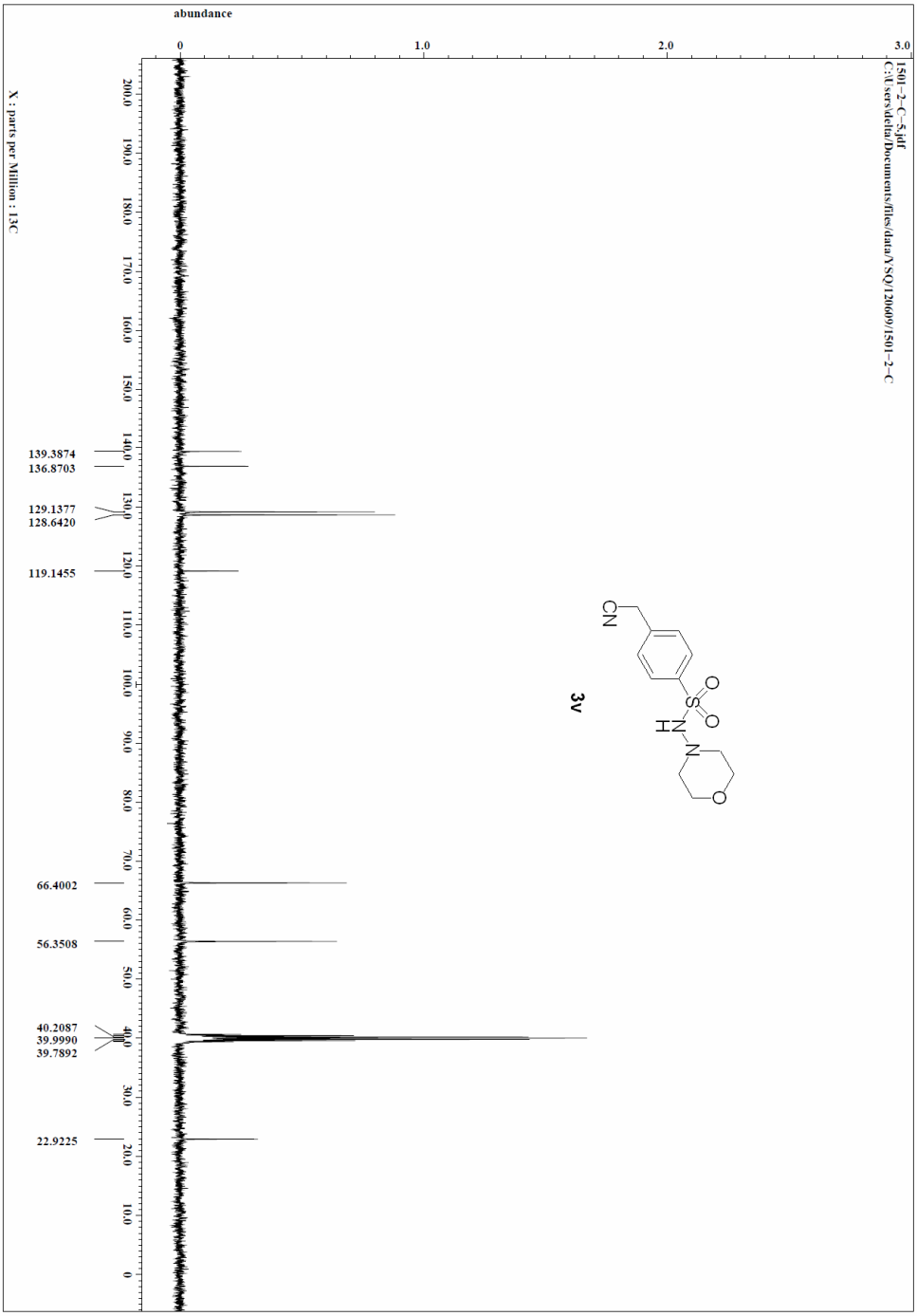

abundance
X : parts per Million : 1H
C:\Users\delta\Documents\files\data\YSQ\120606\1502-1
1502-1-7.jdf
7.8676
7.8458
7.1769
7.1563
7.1379
6.9352
6.9134
6.8733
6.8527
6.8412
6.8229
6.4220
3.8286
2.9065
22.92
19.73
22.38
30.36
9.4
28.12
30
MeO
3t
Ph

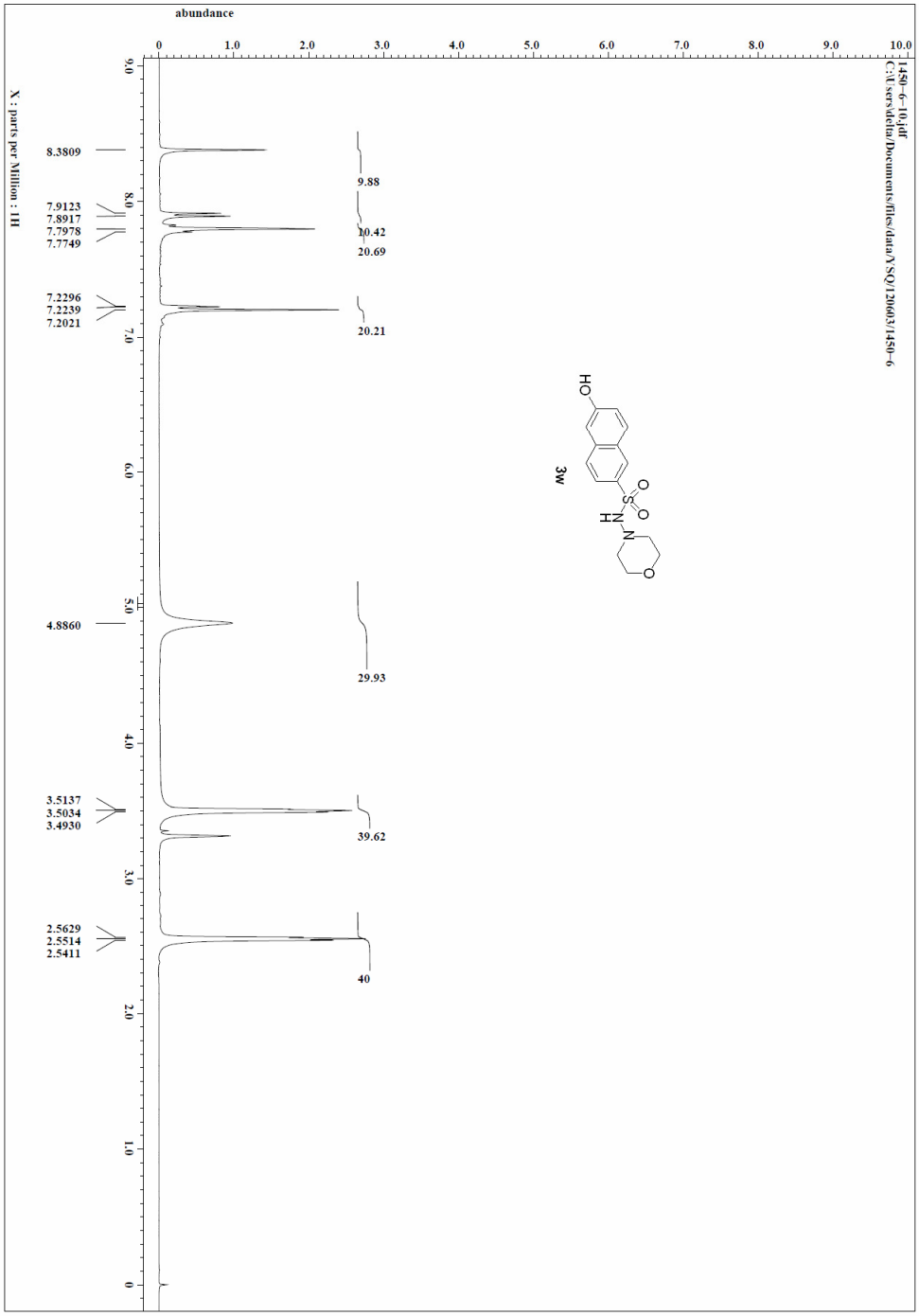

abundance
X : parts per Million : 13C
C:\Users\delta\Documents\files\data\YSQ\120606\1502-1-C
1502-1-C-6.jdf
163.3550
149.7873
130.2890
129.8886
129.3928
128.7921
120.7068
114.3377
114.1851
77.3149
77.0003
76.6761
55.5665
42.3802
MeO
3t
O
S
O
N
H
N
Ph

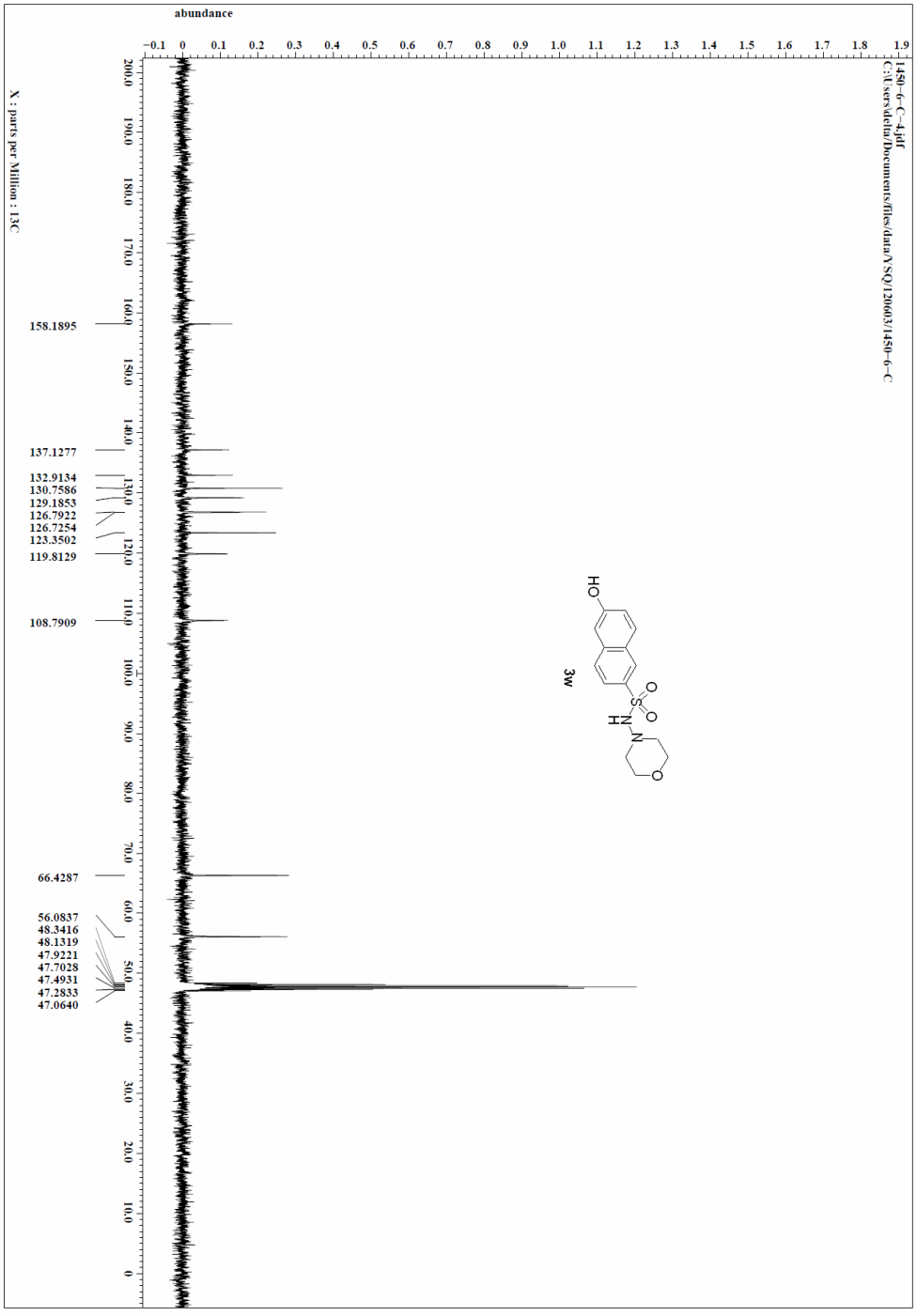

abundance
X : parts per Million : 1H
1501 -5- 7.jdf
C:\Users\dela\Documents\files\data\YSQ\120606\1501 -5
7.9082
7.8864
6.9838
6.9620
5.5771
3.8761
2.5335
2.5221
1.5095
1.4957
1.4820
1.4682
1.2861
18.03
19.38
9.21
29.78
40
41.23
21.84
MeO
3u


abundance
X : parts per Million : 13C
C:\Users\delta\Documents\files\data\YSQ\120606\1501-5-C
1501-5-C-6.jdf
162.9925
130.3080
130.1936
113.7560
77.3243
77.0001
76.6855
57.6068
55.5283
25.5706
22.9677
MeO
3u


abundance
X : parts per Million : 1H
C:\Users\delta\Documents\files\data\NSQ\120609\1501-2
1501-2-7.jdf
9.4541
8.4174
8.3968
8.1001
8.0807
4.7049
3.9626
3.8779
3.0142
3.0038
2.9935
9.93
20.62
20.4
20
40.21
42.66
3v
CN
O
S
O
HN
N
O


abundance
0
1.0
2.0
3.0
1501-2-C--5.jdf
C:\it-serv\delta\Documents\files\data\VSQ\120609\1501-2-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
139.3874
136.8703
129.1377
128.6420
119.1455
66.4002
56.3508
40.2087
39.9990
39.7892
22.9225
3v
CN
O
S
O
HN
N
O


abundance
X : parts per Million : 1H
C:\Users\defia\Documents\files\data\YSQ\120603\1450-6
1450-6-10.jdf
8.3809
7.9123
7.8917
7.7978
7.7749
7.2296
7.2239
7.2021
4.8860
3.5137
3.5034
3.4930
2.5629
2.5514
2.5411
9.88
10.42
20.69
20.21
29.93
39.62
40
3w


abundance
X : parts per Million : 13C
158.1895
137.1277
132.9134
130.7586
129.1853
126.7922
126.7254
123.3502
119.8129
108.7909
66.4287
56.0837
48.3416
48.1319
47.9221
47.7028
47.4931
47.2833
47.0640
1450-6-C--4.jdf
C:\Users\delta\Documents\files\data\YSQ\120603\1450-6-C
3w
OH
O
S
O
H
N
N
O