Electronic Supplementary Material (ESI) for ChemComm.

Aminosulfonylation of aromatic amines, sulfur dioxide and hydrazines

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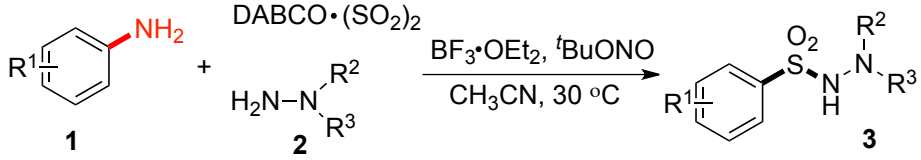
Supporting Information

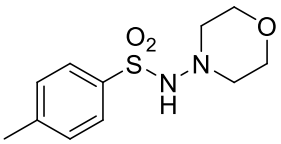
General experimental methods:

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.

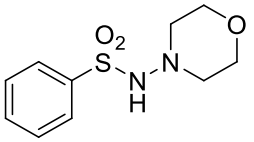
*General experimental procedure for the aminosulfonylation reaction of anilines **1** with DABCO•$(SO_2)_2$ and hydrazines **2**:*



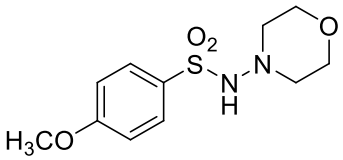
^{t}BuONO (0.54 mmol) was added to a solution of aniline **1** (0.45 mmol) and $BF_3{\cdot}OEt_2$ (0.54 mmol) in CH_3CN (1.0 mL) dropwisely at 0 °C. After 5 min, the solution was slowly added into a mixture of DABCO•$(SO_2)_2$ (0.18 mmol) and hydrazine **2** (0.30 mmol) in CH_3CN (3.0 mL) at 30 °C. The mixture was stirred at 30 °C for another 10 minutes. The solvent was then evaporated and the residue was purified directly by flash column chromatograph (EtOAc/*n*-hexane, 1:2) to give the desired product **3**.



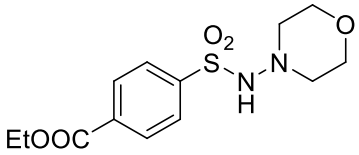
4-Methyl-*N*-morpholinobenzenesulfonamide (**3a**)[1]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.4 Hz, 2H), 7.32 (d, *J* = 8.4 Hz, 2H), 5.75 (s, 1H), 3.61 (t, *J* = 4.4 Hz, 4H), 2.63 (t, *J* = 4.4 Hz, 4H), 2.44 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.0, 135.7, 129.4, 128.1, 66.5, 56.6, 21.6; HRMS (ESI) calcd for $C_{11}H_{17}N_2O_3S$: 257.0954 (M + H+), found: 257.0964.



N-Morpholinobenzenesulfonamide (**3b**)[1]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.0 Hz, 2H), 7.57 (t, *J* = 7.6 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 2H), 5.97 (s, 1H), 3.55 (t, *J* = 4.4 Hz, 4H), 2.58 (t, *J* = 4.4 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.5, 133.0, 128.7, 128.0, 66.5, 56.5; HRMS (ESI) calcd for $C_{10}H_{15}N_2O_3S$: 243.0798 (M + H^+), found: 243.0812.

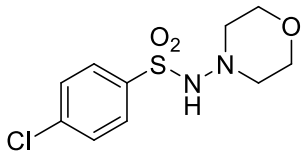


4-Methoxy-*N*-morpholinobenzenesulfonamide (**3c**)[1]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.8 Hz, 2H), 6.99 (d, *J* = 8.8 Hz, 2H), 5.67 (s, 1H), 3.88 (s, 3H), 3.61 (t, *J* = 4.4 Hz, 4H), 2.63 (t, *J* = 4.4 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.2, 130.3, 130.1, 114.0, 66.6, 56.9, 55.6; HRMS (ESI) calcd for $C_{11}H_{17}N_2O_4S$: 273.0904 (M + H^+), found: 273.0912.

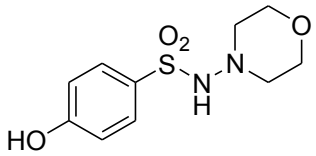


Ethyl 4-(*N*-morpholinosulfamoyl)benzoate (**3d**)[1]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (d, *J* = 8.4 Hz, 2H), 8.05 (t, *J* = 8.4 Hz, 2H), 6.00 (s, 1H), 4.43 (q, *J* = 7.2 Hz, 2H), 3.60 (t, *J* = 4.4 Hz, 4H), 2.64 (t, *J* = 4.4 Hz, 4H), 1.42 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.1, 142.5, 134.6, 129.9, 128.1, 66.6, 61.8, 56.6, 14.2; HRMS

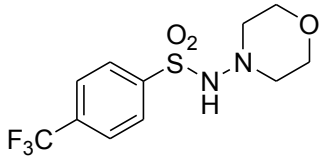
(ESI) calcd for $C_{13}H_{18}N_2O_5S$: 337.0829 (M + Na^+), found: 337.0846.



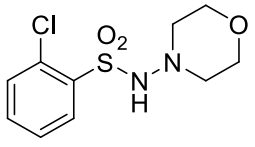
4-Chloro-*N*-morpholinobenzenesulfonamide (**3e**)[1]: ^1H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.8 Hz, 2H), 7.51 (d, *J* = 8.8 Hz, 2H), 5.74 (s, 1H), 3.63 (t, *J* = 4.4 Hz, 4H), 2.66 (t, *J* = 4.4 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.7, 137.1, 129.6, 129.1, 66.6, 56.7; HRMS (ESI) calcd for $C_{10}H_{14}ClN_2O_3S$: 277.0408 (M + H^+), found: 277.0425.



4-Hydroxy-*N*-morpholinobenzenesulfonamide (**3f**)[2]: ^1H NMR (400 MHz, CD_3OD) δ 2.57 (t, *J* = 4.4 Hz, 4H), 3.57 (t, *J* = 4.4 Hz, 4H), 4.89 (br, 2H), 6.92 (d, *J* = 8.8 Hz, 2H), 7.78 (d, *J* = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, CD_3OD) δ 55.9, 66.4, 114.9, 129.1, 130.1, 161.8; HRMS (ESI) calcd for $C_{10}H_{15}N_2O_4S$: 259.0747 (M + H^+), found: 259.0765.

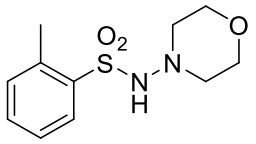


N-Morpholino-4-(trifluoromethyl)benzenesulfonamide (**3g**)[2]: ^1H NMR (400 MHz, $CDCl_3$) 8.14 (d, *J* = 8.0, 2H), 7.82 (d, *J* = 8.4, 2H), 5.81 (s, 1H), 3.65 (t, *J* = 4.4 Hz, 4H), 2.68 (t, *J* = 4.4 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) 142.3, 134.9 (q, *J* = 33.4), 128.6, 126.0 (d, *J* = 3.1), 124.5, 66.5, 56.8.

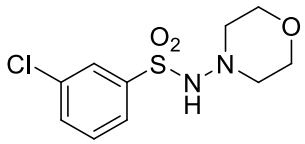


2-Chloro-*N*-morpholinobenzenesulfonamide (**3h**)[1]: ^1H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, *J* = 8.0 Hz, 1H), 7.51-7.56 (m, 2H), 7.45 (t, *J* = 7.2 Hz, 1H), 6.13 (s, 1H), 3.56 (t, *J* = 4.4 Hz, 4H), 2.70 (t, *J* = 4.4 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.3, 134.2, 133.0, 131.6, 131.5, 127.1, 66.4, 56.6; HRMS (ESI) calcd for $C_{10}H_{13}ClN_2O_3S$:

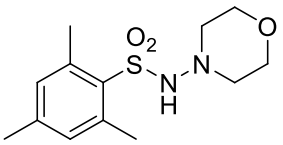
277.0414 (M + H^+), found: 277.0404.



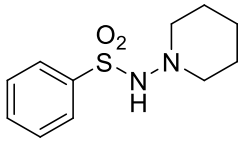
2-Methyl-*N*-morpholinobenzenesulfonamide (**3i**)[1]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 8.0 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 1H), 7.30-7.36 (m, 2H), 5.71 (s, 1H), 3.58 (t, *J* = 4.4 Hz, 4H), 2.70 (s, 3H), 2.66 (t, *J* = 4.4 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.0, 136.5, 133.2, 132.3, 131.0, 126.1, 66.6, 56.7, 20.6; HRMS (ESI) calcd for $C_{11}H_{17}N_2O_3S$: 257.0954 (M + H^+), found: 257.0975.



3-Chloro-*N*-morpholinobenzenesulfonamide (**3j**)[1]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (s, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.48 (t, *J* = 8.0 Hz, 1H), 6.09 (s, 1H), 3.62 (t, *J* = 4.4 Hz, 4H), 2.65 (t, *J* = 4.4 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.3, 135.0, 133.2, 130.1, 128.1, 126.2, 66.5, 56.5; HRMS (ESI) calcd for $C_{10}H_{13}ClN_2O_3S$: 277.0414 (M + H^+), found: 277.0420.

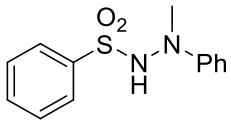


2,4,6-Trimethyl-*N*-morpholinobenzenesulfonamide (**3k**)[1]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.95 (s, 2H), 5.65 (s, 1H), 3.57 (t, *J* = 4.4 Hz, 4H), 2.68 (s, 6H), 2.65 (t, *J* = 4.4 Hz, 4H), 2.30 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.6, 140.4, 132.5, 131.6, 66.8, 56.5, 23.1, 21.0; HRMS (ESI) calcd for $C_{13}H_{20}N_2O_3S$: 285.1273 (M + H^+), found: 285.1275.

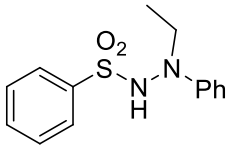


N-(Piperidin-1-yl)benzenesulfonamide (**3l**)[1]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96-7.98 (m, 2H), 7.59 (t, *J* = 7.2 Hz, 1H), 7.49-7.53 (m, 2H), 5.54 (s, 1H), 2.52 (t, *J* = 5.2 Hz, 4H), 1.46-1.52 (m, 4H), 1.25-1.32 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ

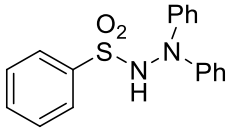
138.8, 132.8, 128.6, 128.1, 57.7, 25.6, 23.0; HRMS (ESI) calcd for $C_{11}H_{16}N_2O_2S$: 241.1011 (M + H^+), found: 241.1026.



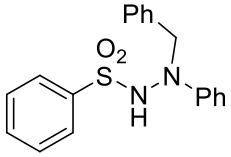
N'-Methyl-*N*'-phenylbenzenesulfonohydrazide (**3m**)[1]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.4 Hz, 2H), 7.57 (t, *J* = 8.4 Hz, 1H), 7.47 (t, *J* = 8.4 Hz, 2H), 7.14 (t, *J* = 7.6 Hz, 2H), 6.80-6.86 (m, 3H), 6.44 (s, 1H), 2.93 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.6, 138.6, 133.3, 129.1, 128.9, 128.1, 120.9, 114.4, 42.7; HRMS (ESI) calcd for $C_{13}H_{14}N_2O_2S$: 263.0854 (M + H^+), found: 263.0849.



N'-Ethyl-*N*'-phenylbenzenesulfonohydrazide (**3n**)[1]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 7.2 Hz, 2H), 7.57 (t, *J* = 7.6 Hz, 1H), 7.47 (d, *J* = 8.0 Hz, 2H), 7.14-7.18 (m, 2H), 6.82-6.86 (m, 3H), 6.74 (s, 1H), 3.44 (s, 2H), 1.03 (t, *J* = 7.2Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.7, 138.7, 133.2, 128.9, 128.1, 120.8, 115.1, 49.2, 9.5; HRMS (ESI) calcd for $C_{14}H_{16}N_2O_2S$: 299.0825 (M + Na^+), found: 299.0839.

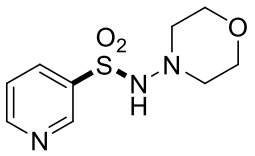


N',*N'*-Diphenylbenzenesulfonohydrazide (**3o**)[1]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 7.2 Hz, 2H), 7.45 (t, *J* = 7.6 Hz, 1H), 7.27-7.33 (m, 3H), 7.14-7.18 (m, 4H), 6.97-7.02 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.7, 138.5, 133.0, 129.0, 128.7, 128.2, 123.9, 120.7; HRMS (ESI) calcd for $C_{18}H_{16}N_2O_2S$: 347.0825 (M + Na^+), found: 347.0841.

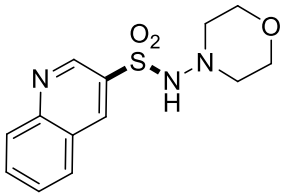


N'-Benzyl-*N*'-phenylbenzenesulfonohydrazide (**3p**)[1]: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 7.6 Hz, 2H), 7.56 (t, *J* = 7.6 Hz, 1H), 7.46 (d, *J* = 7.6 Hz, 2H), 7.26 (s, 3H),

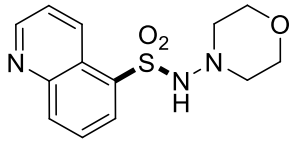
7.16 (t, *J* = 8.0 Hz, 2H), 7.05 (s, 2H), 6.91 (d, *J* = 8.0 Hz, 2H), 6.86 (t, *J* = 7.2 Hz, 1H), 6.42 (s, 1H), 4.56 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.6, 138.8, 134.5, 133.3, 129.0, 128.8, 128.3, 128.1, 128.0, 121.0, 115.3, 58.2; HRMS (ESI) calcd for $C_{19}H_{18}N_2O_2S$: 361.0981 (M + Na^+), found: 361.1003.



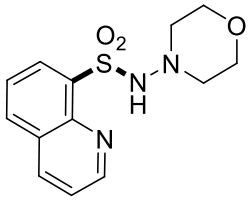
N-Morpholinopyridine-3-sulfonamide (**5c**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.17 (s, 1H), 8.83 (d, *J* = 3.6 Hz, 1H), 8.26 (dt, ^1J = 2.0 Hz, ^2J = 8.0 Hz, 1H), 7.49 (dd, ^1J = 4.8 Hz, ^2J = 8.0 Hz, 1H), 5.78 (s, 1H), 3.62 (t, *J* = 4.8 Hz, 4H), 2.67 (t, *J* = 4.8 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.5, 148.9, 135.7, 135.3, 123.5, 66.5, 56.8; HRMS (ESI) calcd for $C_9H_{13}N_3O_3S$: 266.0570 (M + Na^+), found: 266.0567.



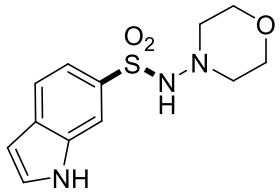
N-Morpholinoquinoline-3-sulfonamide (**5d**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.36 (s, 1H), 8.81 (s, 1H), 8.19 (d, *J* = 8.8 Hz, 1H), 7.98 (d, *J* = 8.0 Hz, 1H), 7.90 (t, *J* = 8.4 Hz, 1H), 7.69 (t, *J* = 7.2 Hz, 1H), 6.25 (s, 1H), 3.59 (t, *J* = 4.8 Hz, 4H), 2.69 (t, *J* = 4.4 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.2, 147.4, 137.4, 132.7, 131.8, 129.5, 129.1, 128.3, 126.2, 66.5, 56.7; HRMS (ESI) calcd for $C_{13}H_{15}N_3O_3S$: 316.0726 (M + Na^+), found: 316.0724.



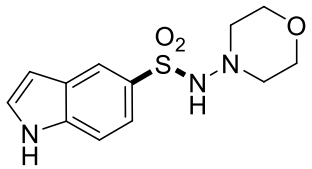
N-Morpholinoquinoline-5-sulfonamide (**5e**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.22 (d, *J* = 8.8 Hz, 1H), 9.00 (d, *J* = 4.0 Hz, 1H), 8.36-8.41 (m, 2H), 7.81 (t, *J* =8.0 Hz, 1H), 7.57 (q, *J* = 4.4 Hz, 1H), 6.09 (s, 1H), 3.47 (t, *J* = 4.4 Hz, 4H), 2.55 (t, *J* = 4.4 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.1, 148.2, 136.0, 134.1, 131.2, 129.2, 127.9, 127.8, 122.4, 66.4, 56.8; HRMS (ESI) calcd for $C_{13}H_{15}N_3O_3S$: 316.0726 (M + Na^+), found: 316.0724.



N-Morpholinoquinoline-8-sulfonamide (**5f**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.05 (d, *J* = 4.4 Hz, 1H), 8.53 (d, *J* = 7.6 Hz, 1H), 8.29 (d, *J* = 8.4 Hz, 1H), 8.08 (d, *J* = 8.4 Hz, 1H), 7.68 (t, *J* = 7.6 Hz, 1H), 7.57 (q, *J* = 4.0 Hz, 1H), 7.30 (s, 1H), 3.49 (t, *J* = 4.4 Hz, 4H), 2.57 (t, *J* = 4.4 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.2, 143.2, 137.2, 135.7, 133.8, 132.6 128.8, 125.8, 122.4, 66.3, 56.5; HRMS (ESI) calcd for $C_{13}H_{15}N_3O_3S$: 316.0726 ($M + Na^+$), found: 316.0730.



N-Morpholino-1*H*-indole-6-sulfonamide (**5g**): ^{1}H NMR (400 MHz, CD_3OD) δ 8.03 (s, 1H), 7.69 (d, *J* = 8.4 Hz, 1H), 7.55 (d, *J* = 8.4 Hz, 1H), 7.49 (d, *J* = 3.2 Hz, 1H), 6.56 (d, *J* = 3.2 Hz, 1H), 3.49 (t, *J* = 4.4 Hz, 4H), 2.50 (t, *J* = 4.4 Hz, 4H); ^{13}C NMR (100 MHz, CD_3OD) δ 134.7, 131.3, 131.0, 128.6, 120.0, 117.7, 112.2, 101.6, 66.4, 55.9; HRMS (ESI) calcd for $C_{12}H_{15}N_3O_3S$: 304.0726 ($M + Na^+$), found: 304.0732.

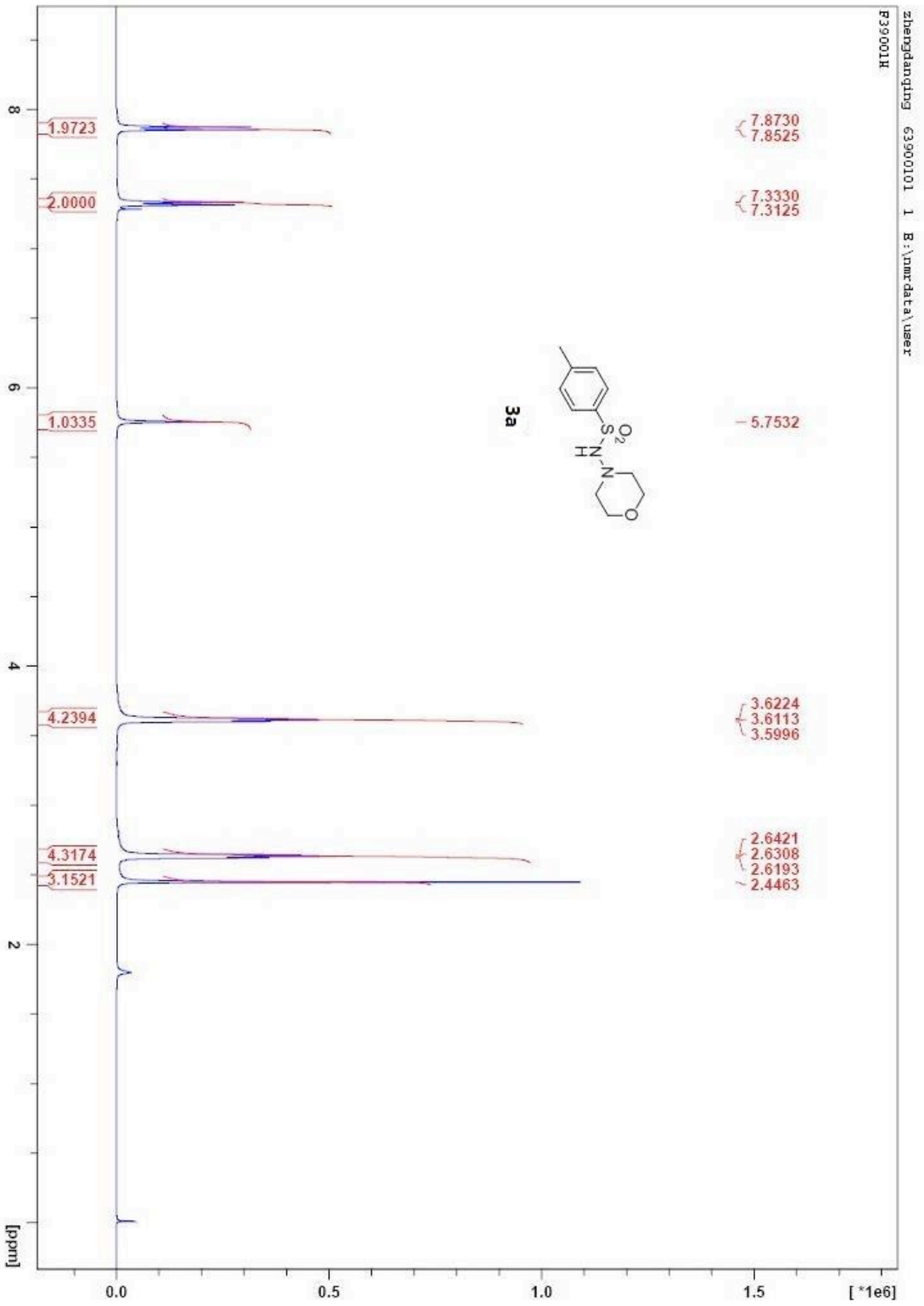


N-Morpholino-1*H*-indole-5-sulfonamide (**5h**): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.80 (s, 1H), 8.31 (s, 1H), 7.75 (d, *J* = 8.4 Hz, 1H), 7.47 (d, *J* = 8.8 Hz, 1H), 7.34 (t, *J* = 2.4 Hz, 1H), 6.66 (d, *J* = 2.0 Hz, 1H), 5.51 (s, 1H), 3.55 (t, *J* = 4.4 Hz, 4H), 2.57 (t, *J* = 4.4 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.5, 129.4, 127.2, 126.6, 122.4, 121.2, 111.4, 104.0, 66.6, 56.7; HRMS (ESI) calcd for $C_{12}H_{15}N_3O_3S$: 304.0726 ($M + Na^+$), found: 304.0711.

References:

1. Zheng, D.; An, Y.; Li, Z.; Wu, J. *Angw. Chem. Int. Ed.* **2014**, *53*, 2451.

2. Ye, S.; Wu, J. *Chem. Commun.* **2012**, *48*, 10037.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1.0335
4.2394
4.3174
3.1521
7.8730
7.8525
7.3330
7.3125
5.7532
3.6224
3.6113
3.5996
2.6421
2.6308
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8
6
4
2
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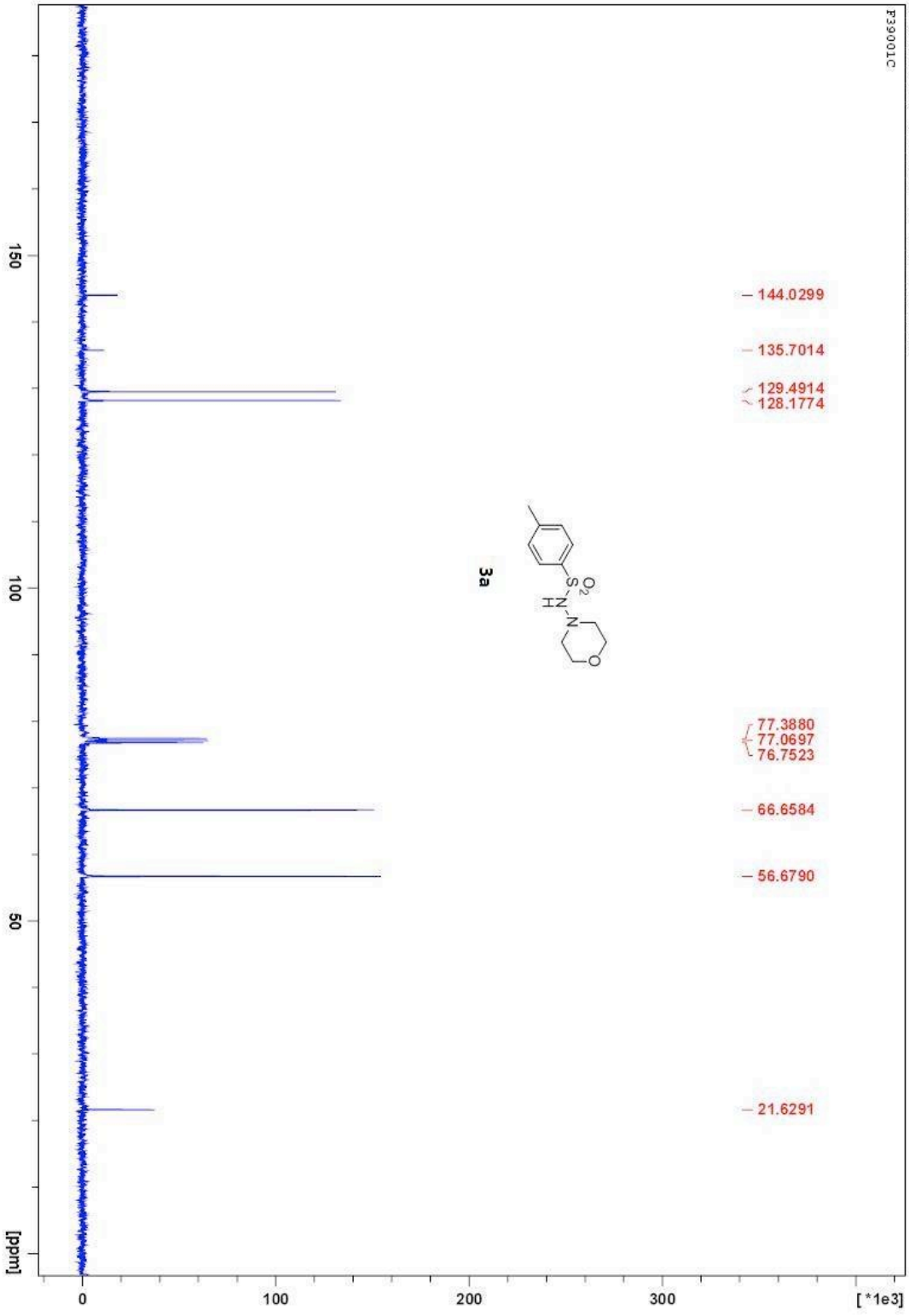
0.0
0.5
1.0
1.5
[*1e6]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129.4914
128.1774
77.3880
77.0697
76.7523
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56.6790
21.6291
3a
[ppm]
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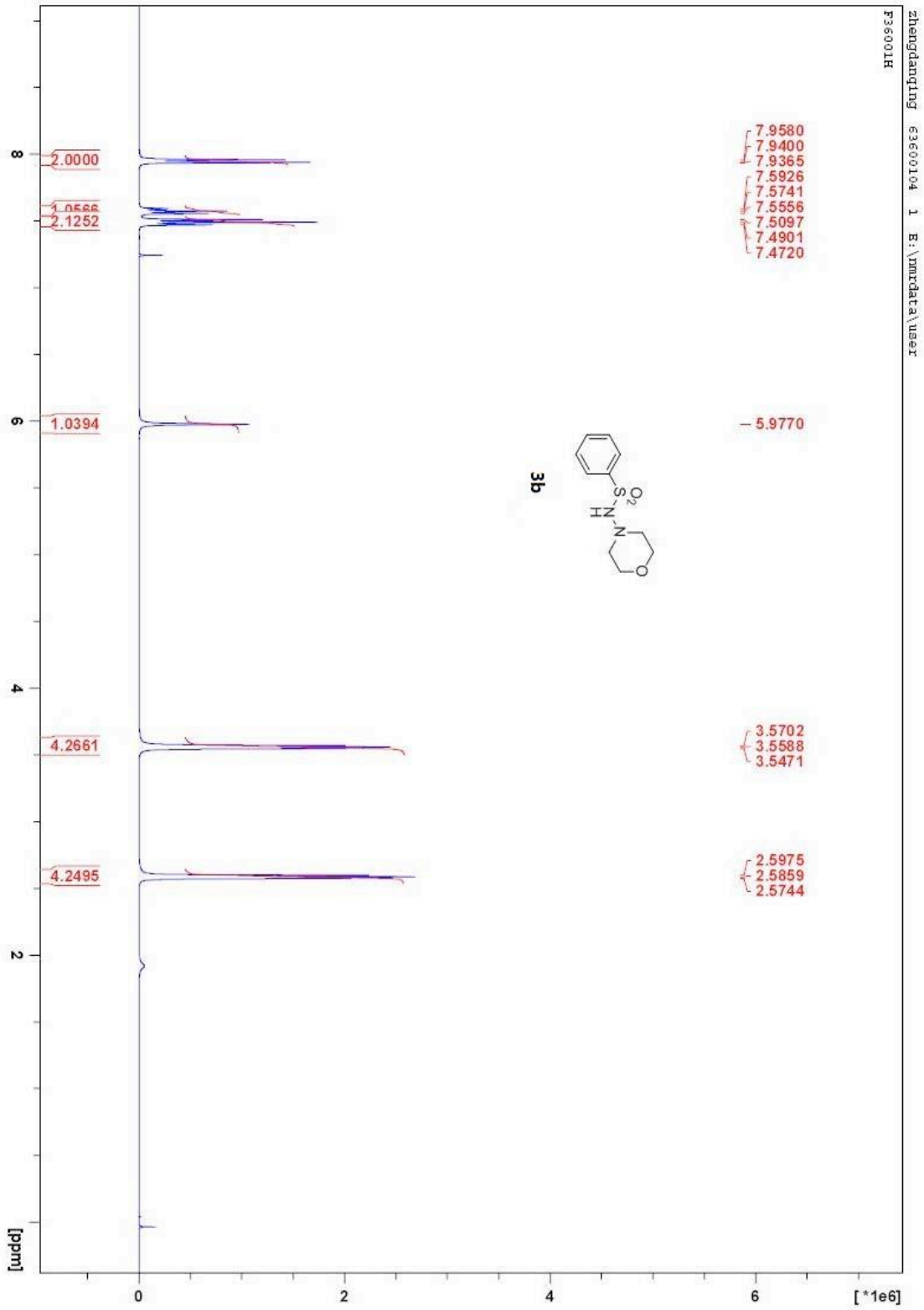
100
50
0
100
200
300
[*1e3]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7.5926
7.5741
7.5556
7.5097
7.4901
7.4720
5.9770
3.5702
3.5588
3.5471
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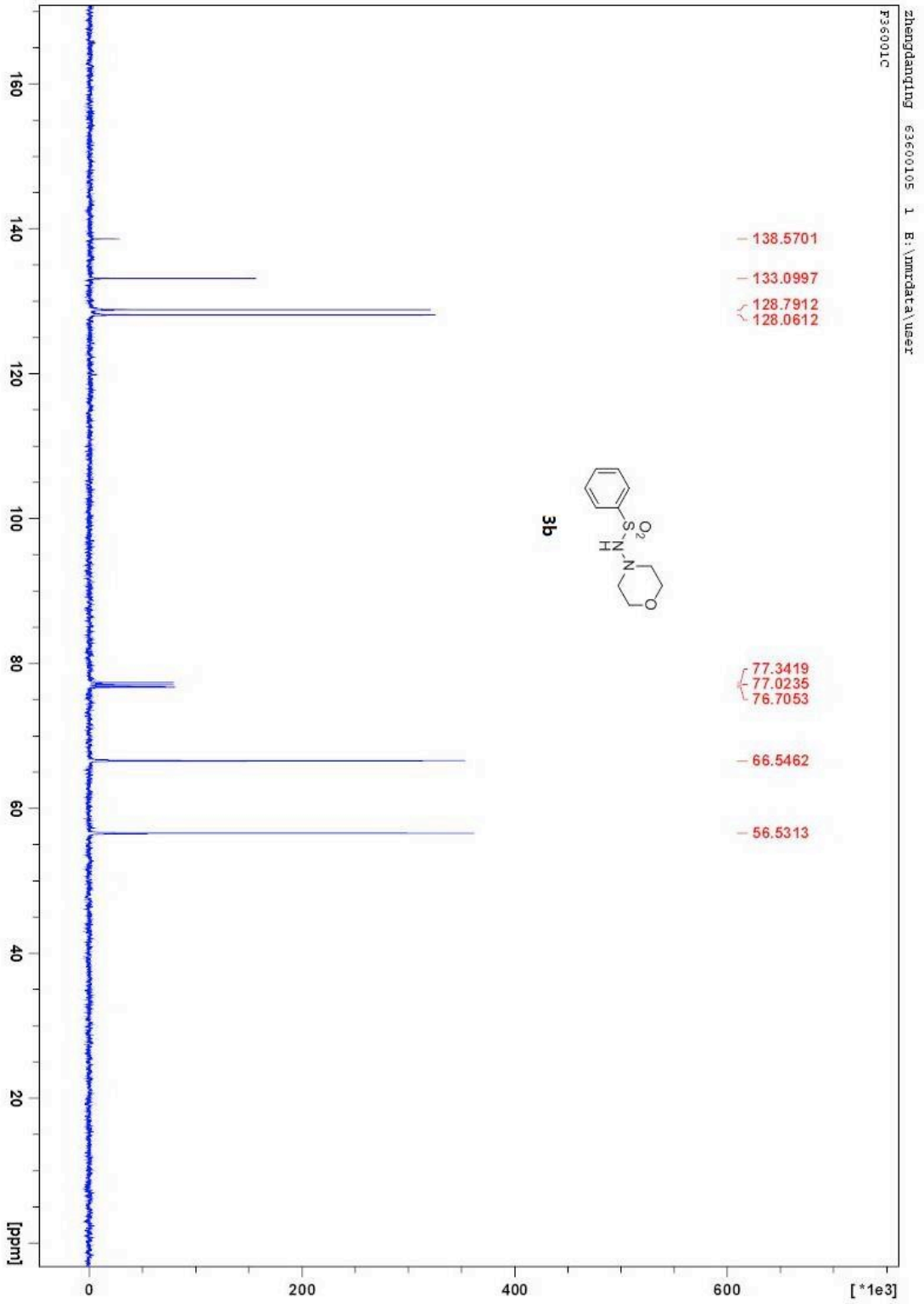
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3b
O2
S
N
H
N
O
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400
600
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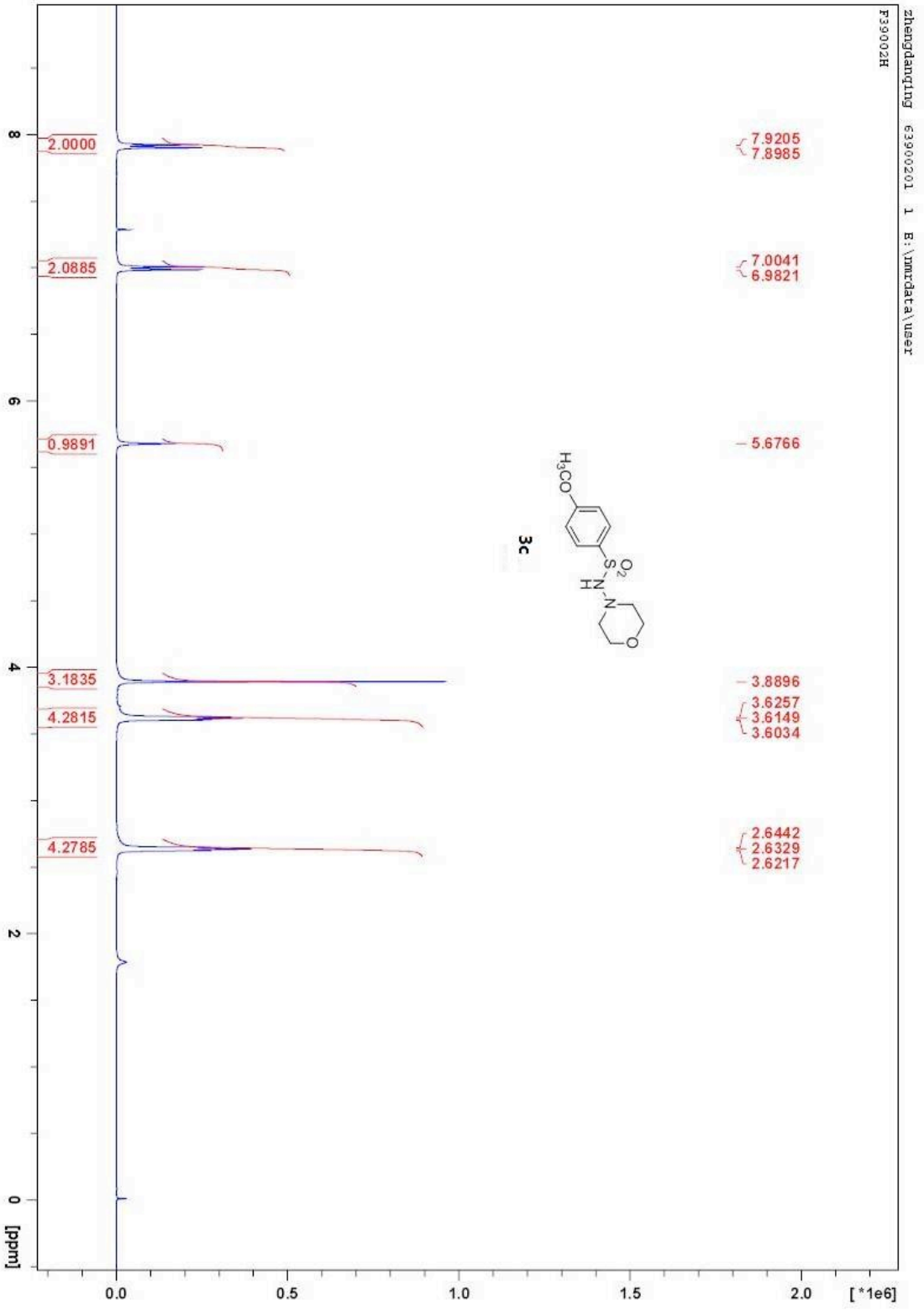
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4.2785
7.9205
7.8985
7.0041
6.9821
5.6766
3.8896
3.6257
3.6149
3.6034
2.6442
2.6329
2.6217
3c
H3CO
O2
S
N
H
N
O
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6
4
2
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2.0
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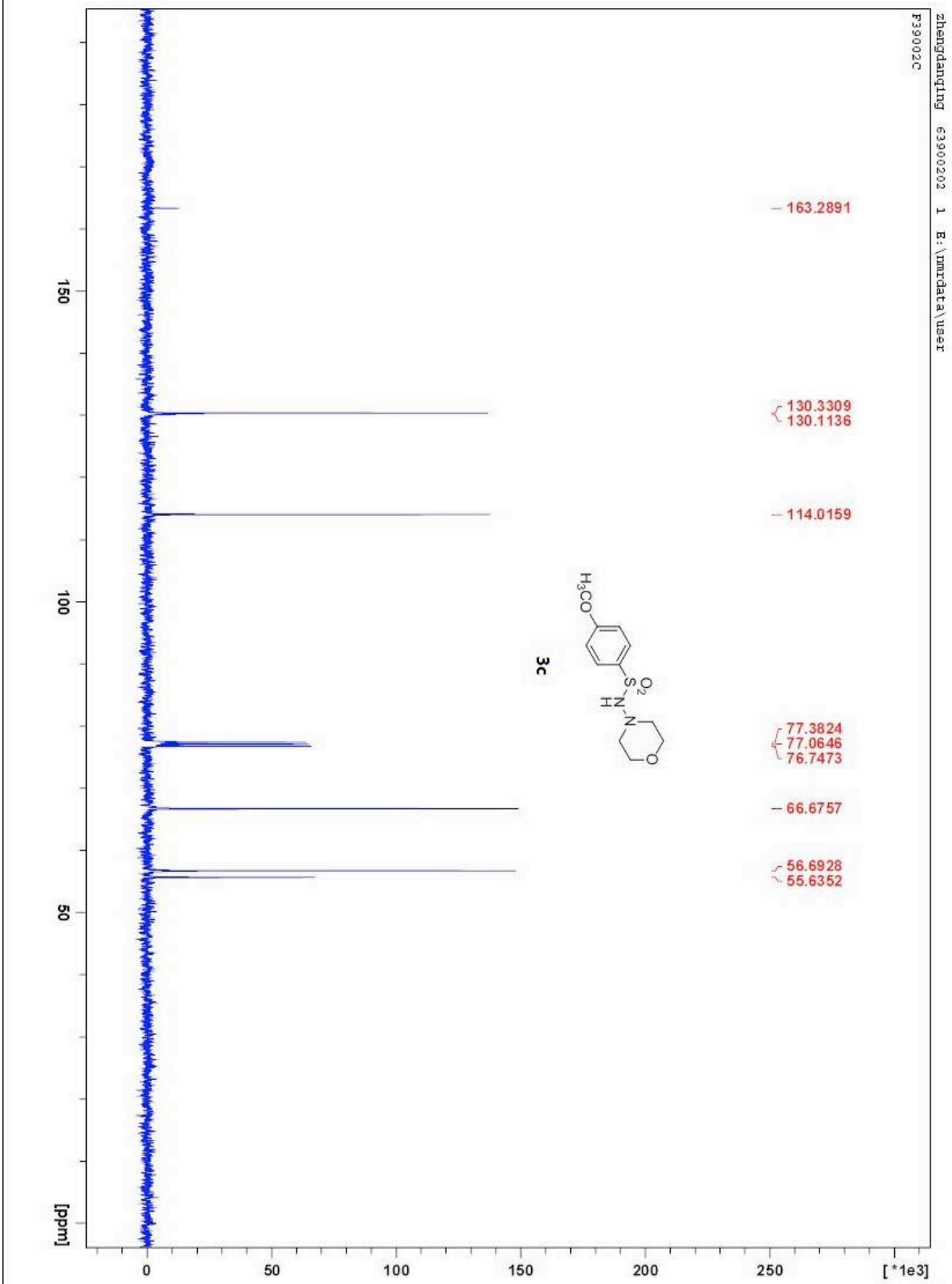
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55.6352
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O2
S
N
H
N
O
[ppm]
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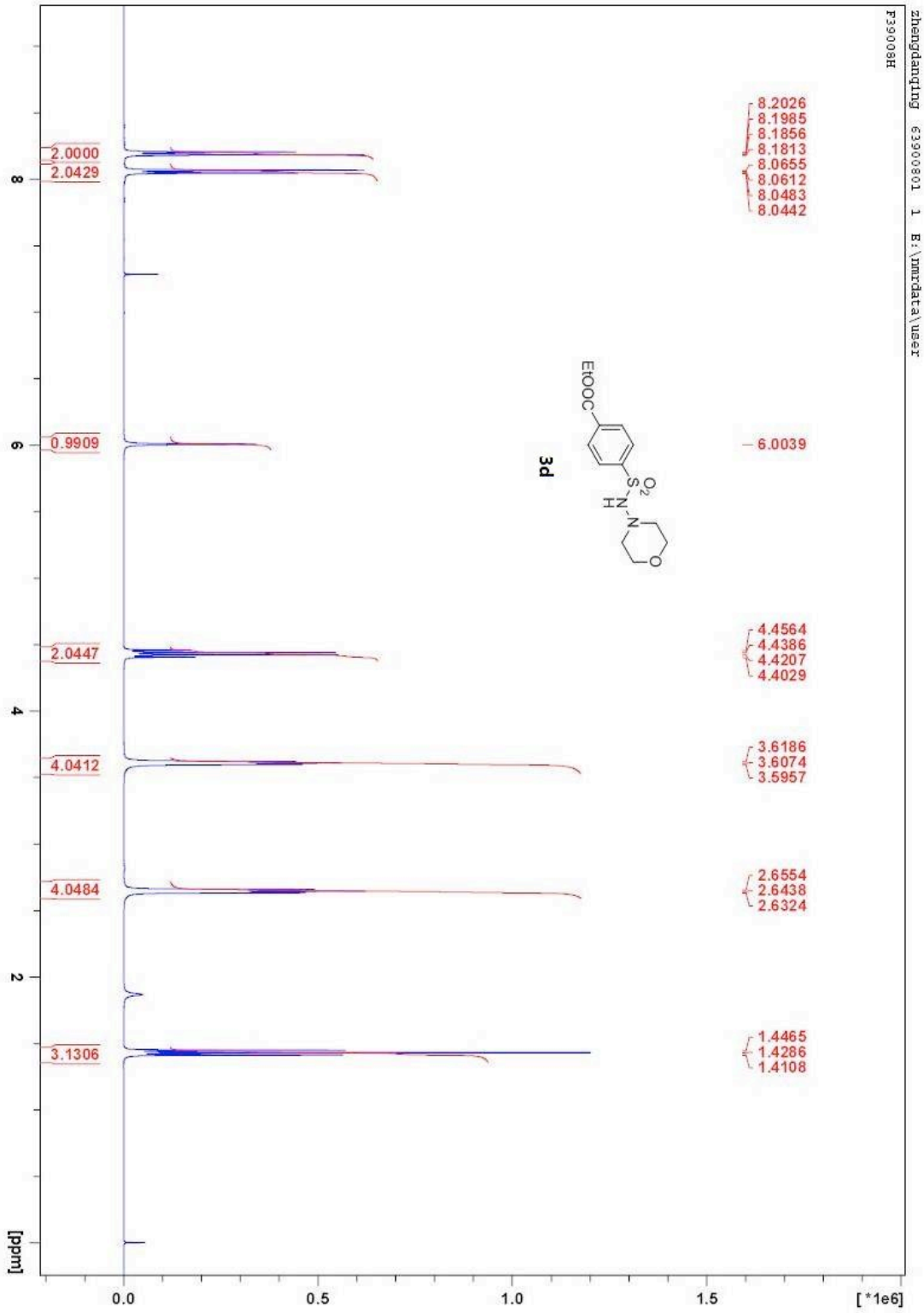
100
150
200
250
[*1e3]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8.0442
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4.4029
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3.6074
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2.6324
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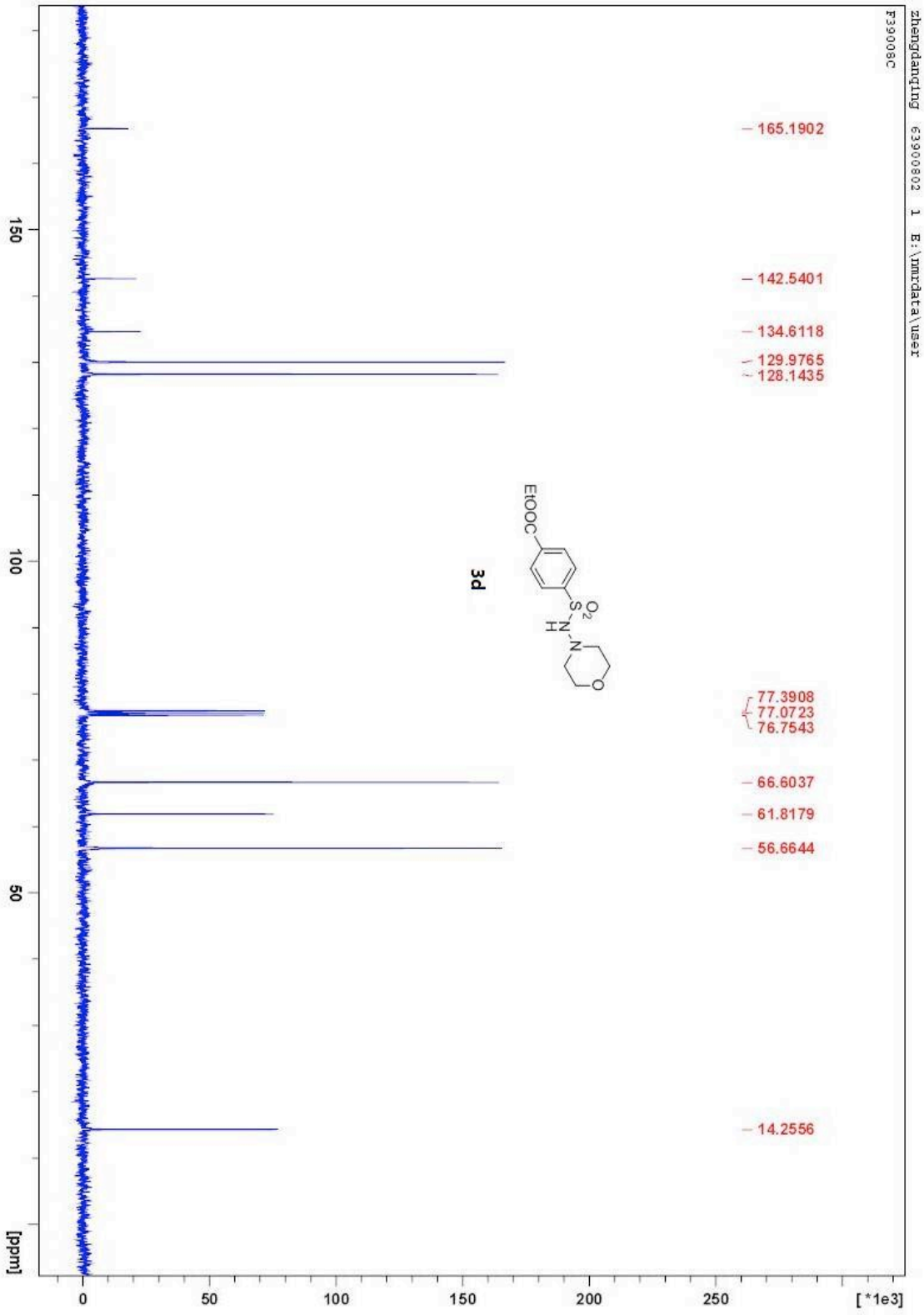
3d
[ppm]
[*1e6]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61.8179
56.6644
14.2556
3d
EtOOC
O2
S
N
H
N
O
[ppm]
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100
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100
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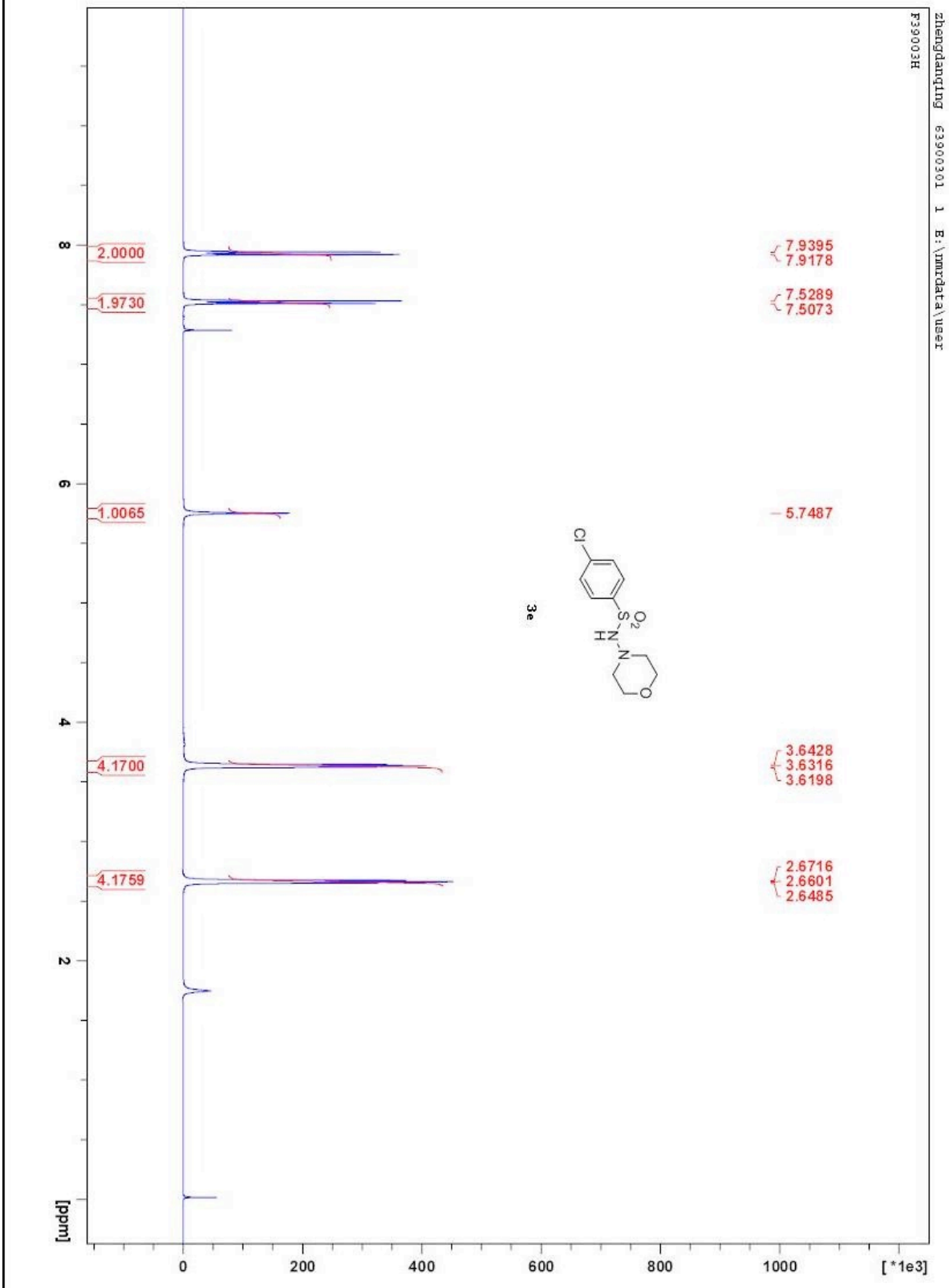
250
[*1e3]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3.6316
3.6198
2.6716
2.6601
2.6485
3e
Cl
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S
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H
N
O
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6
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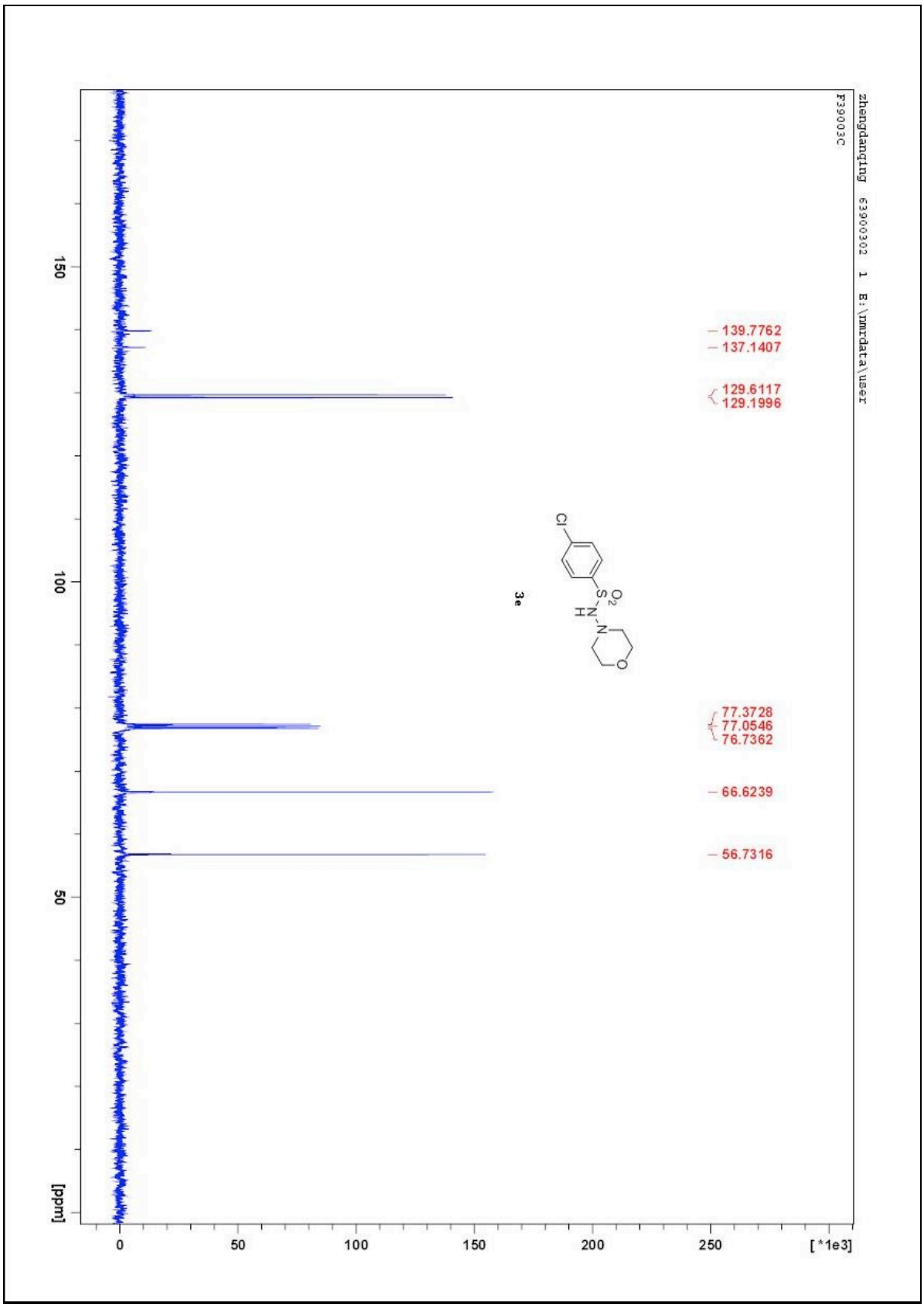
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H
N
O
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[ppm]
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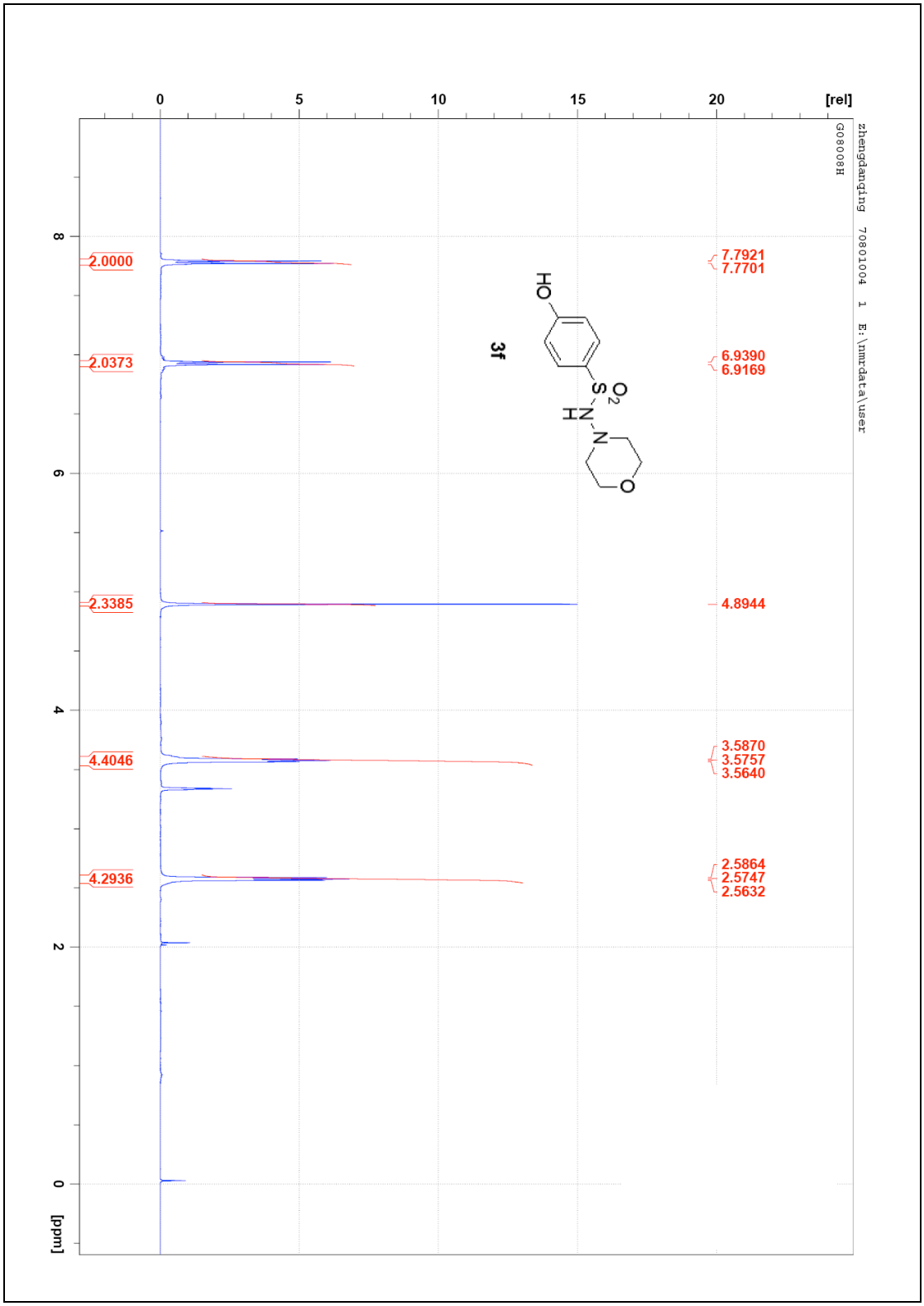
[*1e3]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7.7701
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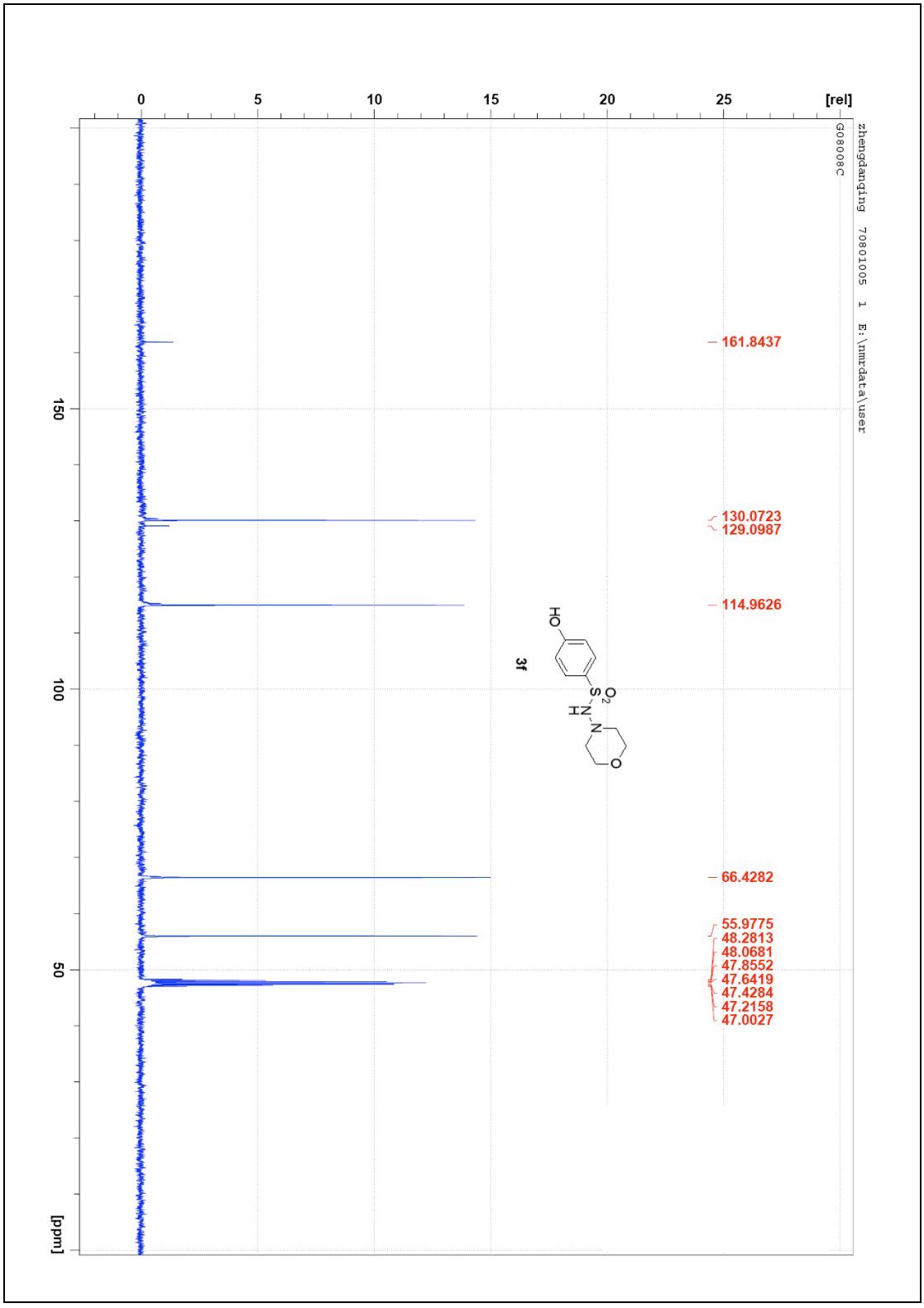
HO
O2
S
N
H
N
O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O2
S
H
N
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O
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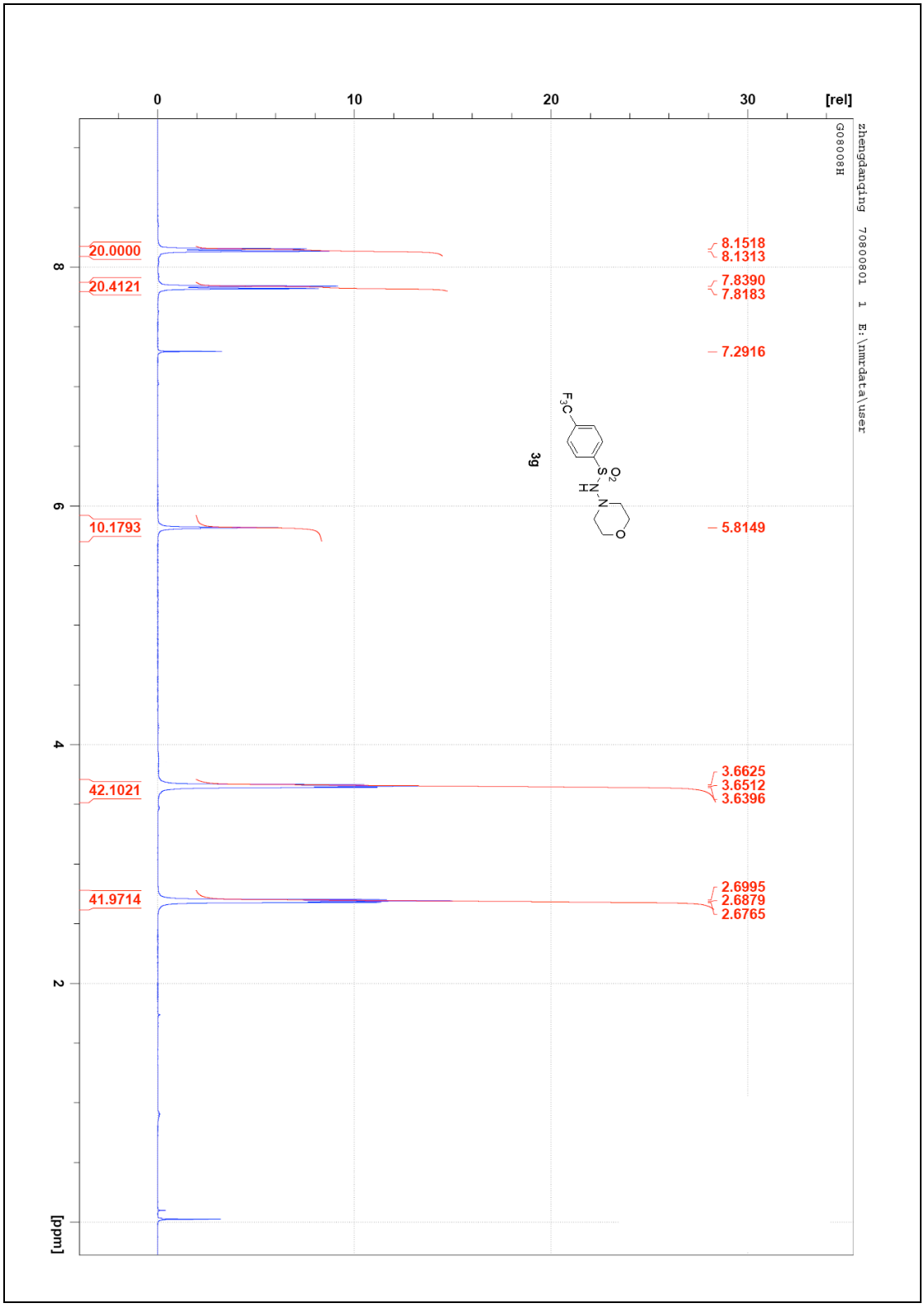
G08008C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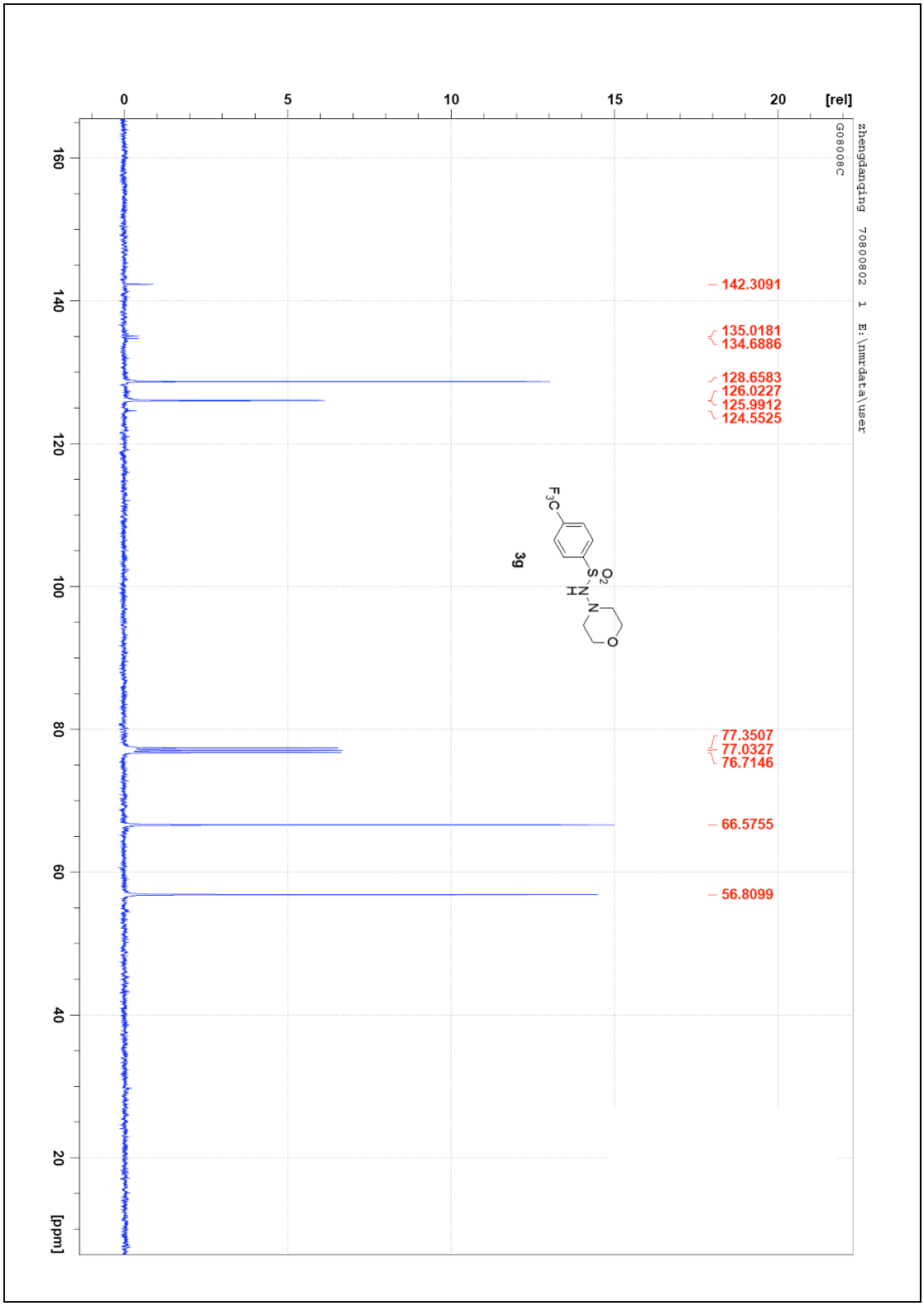
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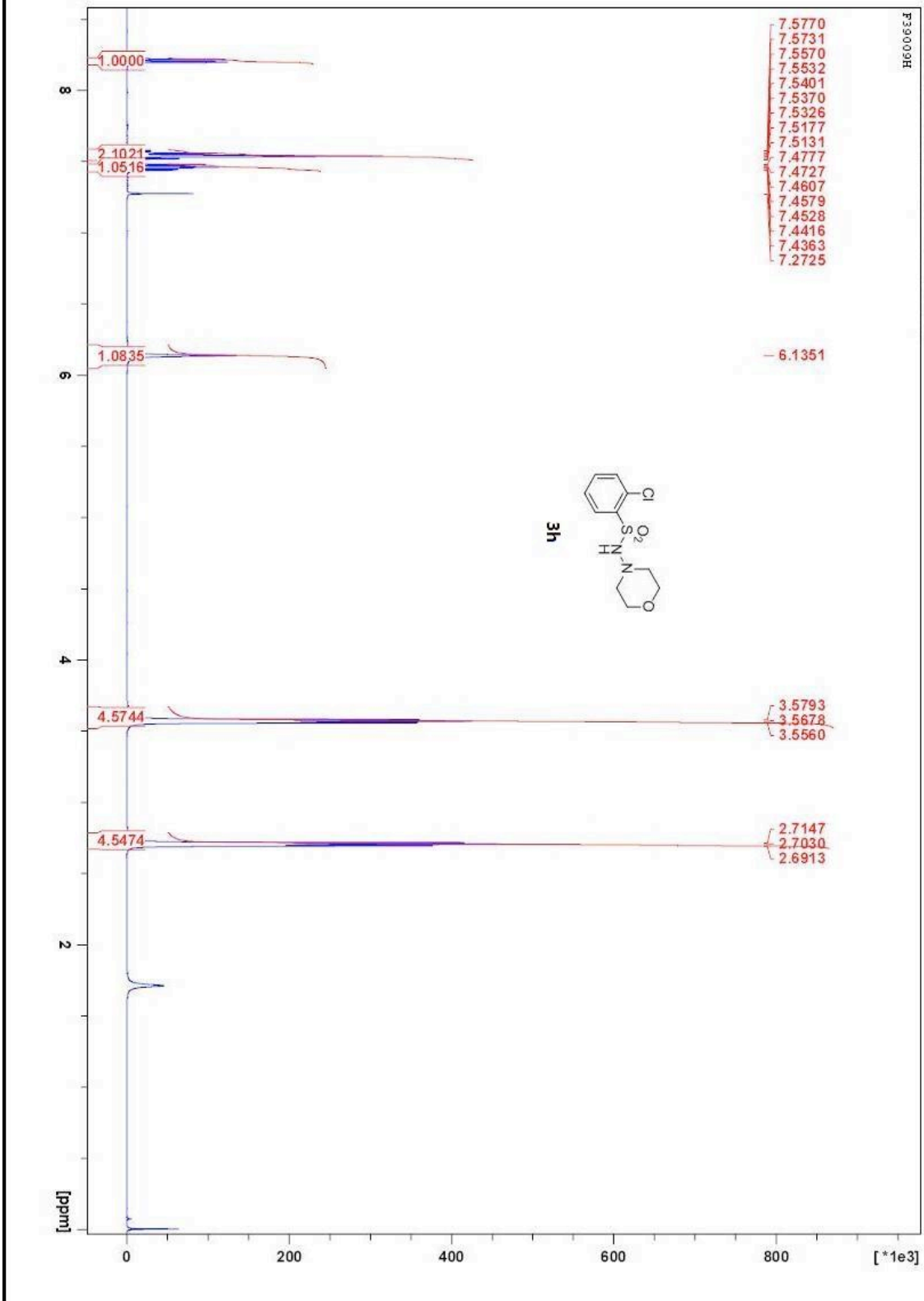
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Cl
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H
N
O
8
6
4
2
[ppm]
0
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400
600
800
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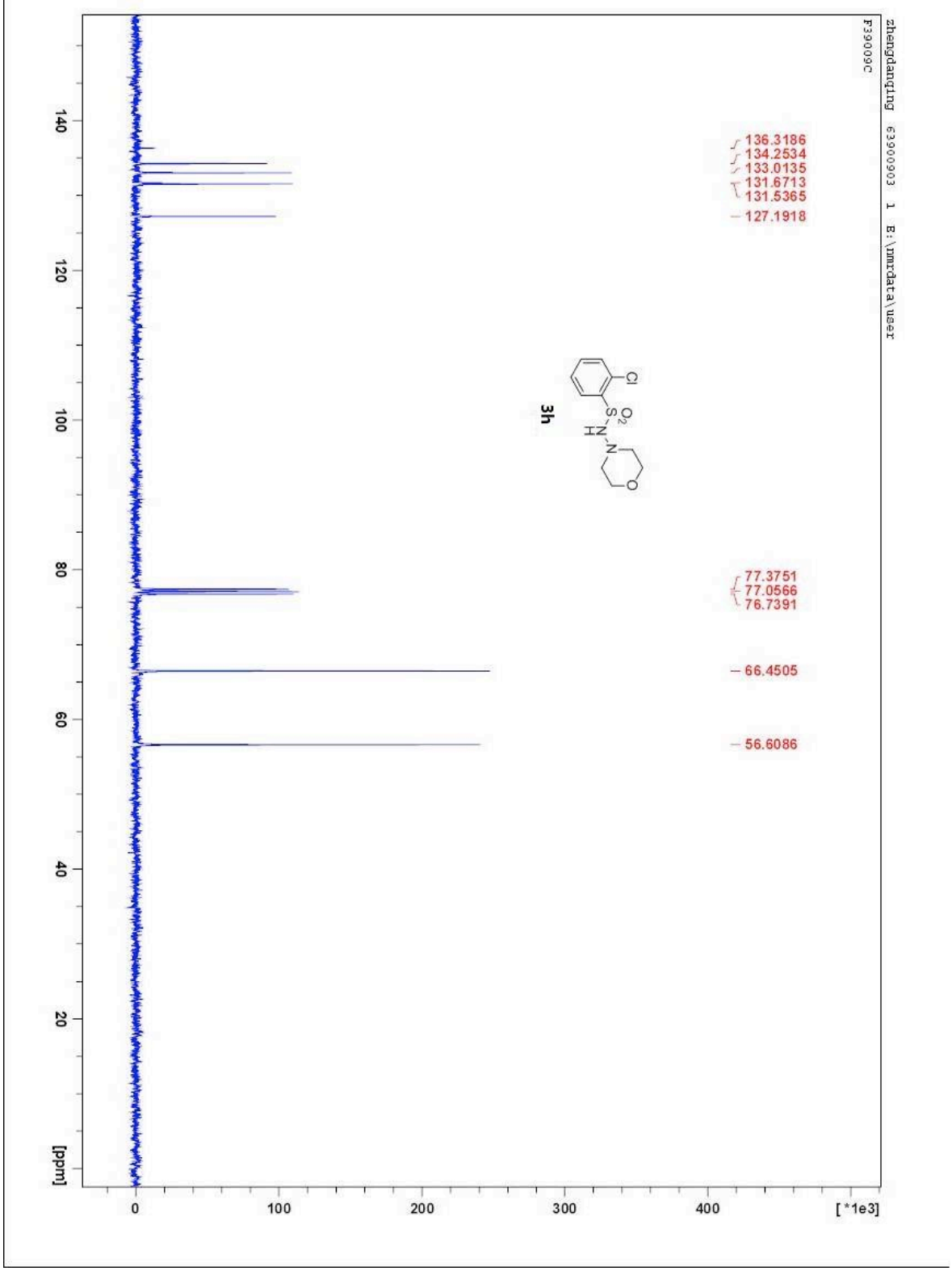
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O2
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N
N
O
[ppm]
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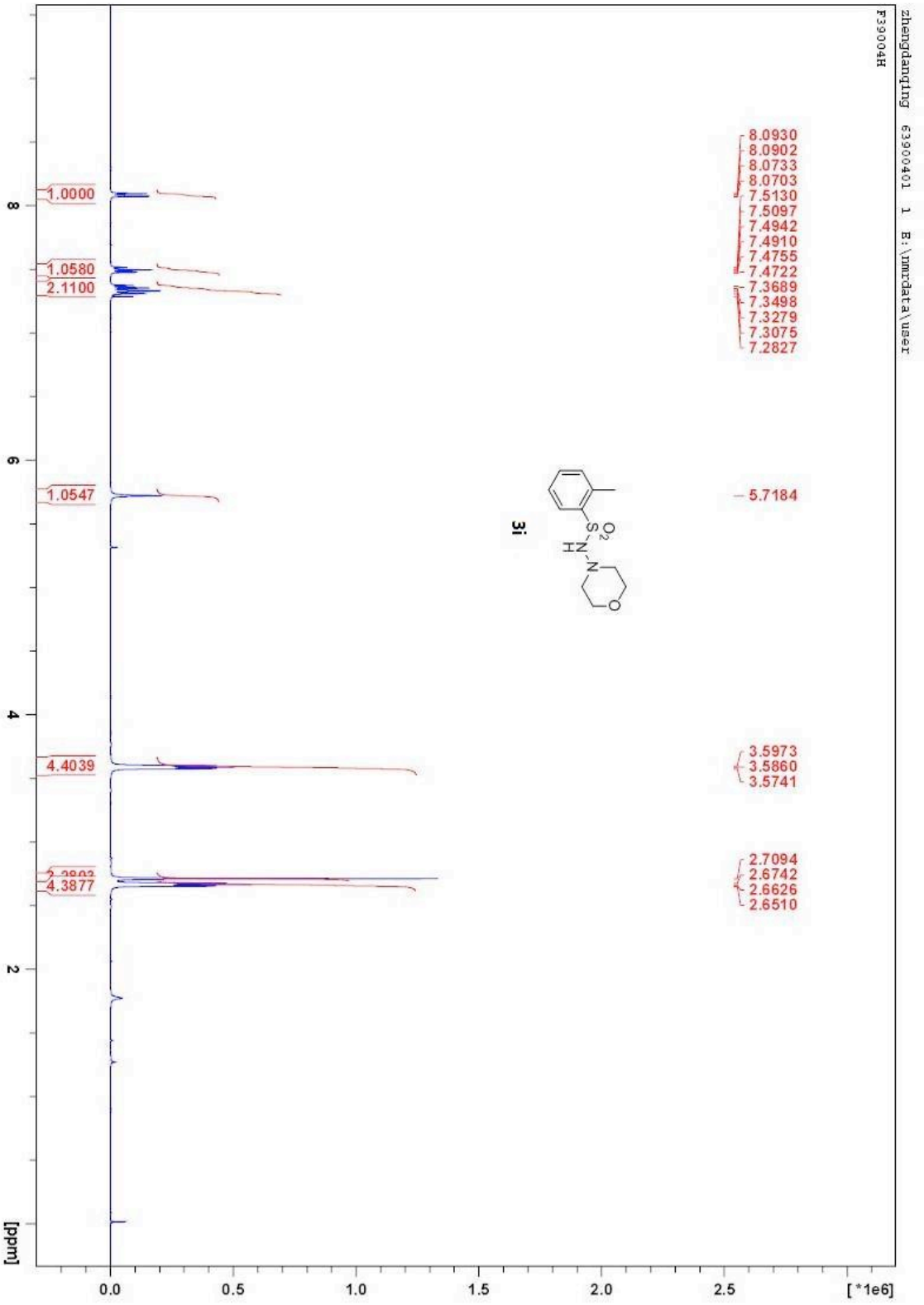
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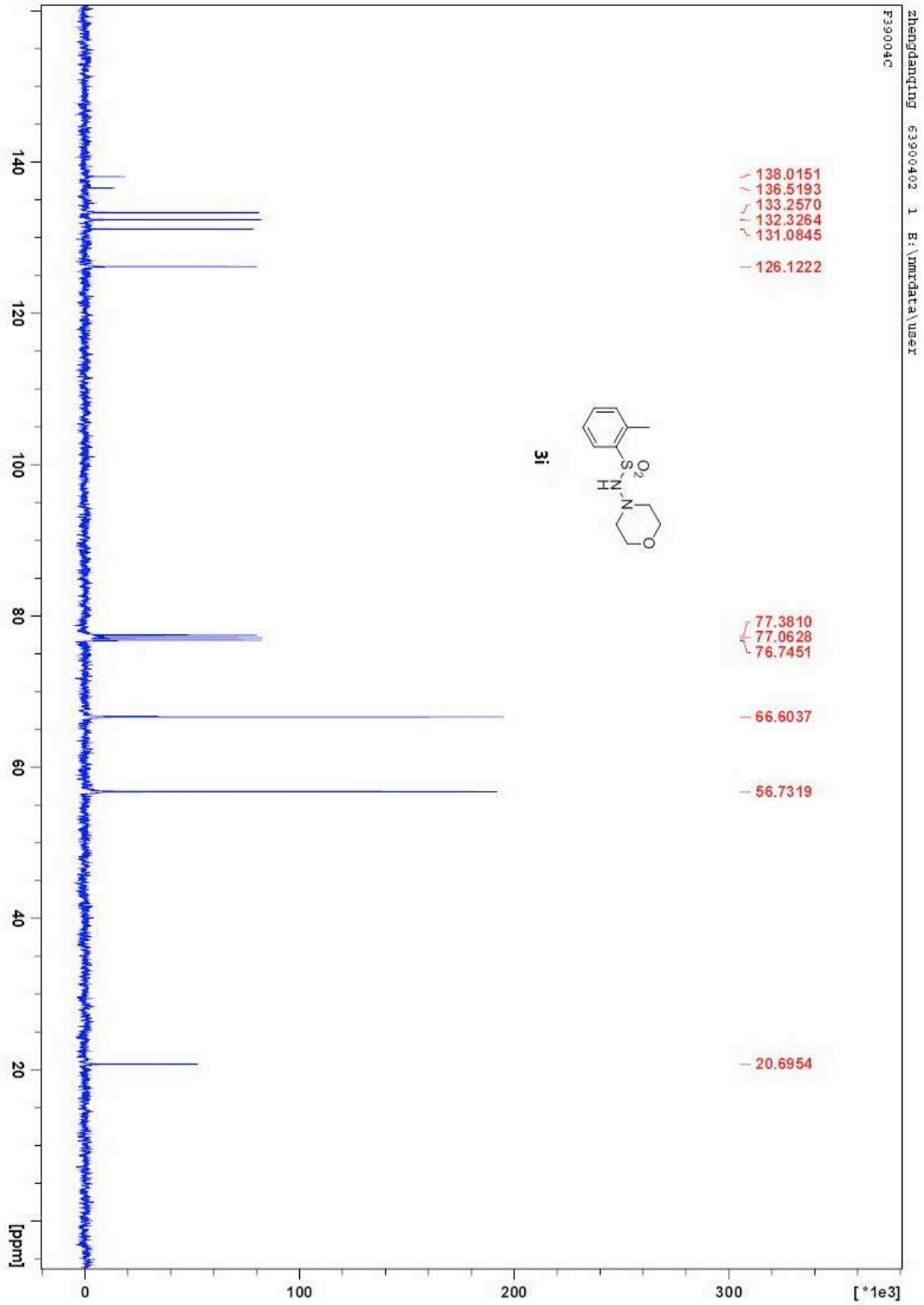
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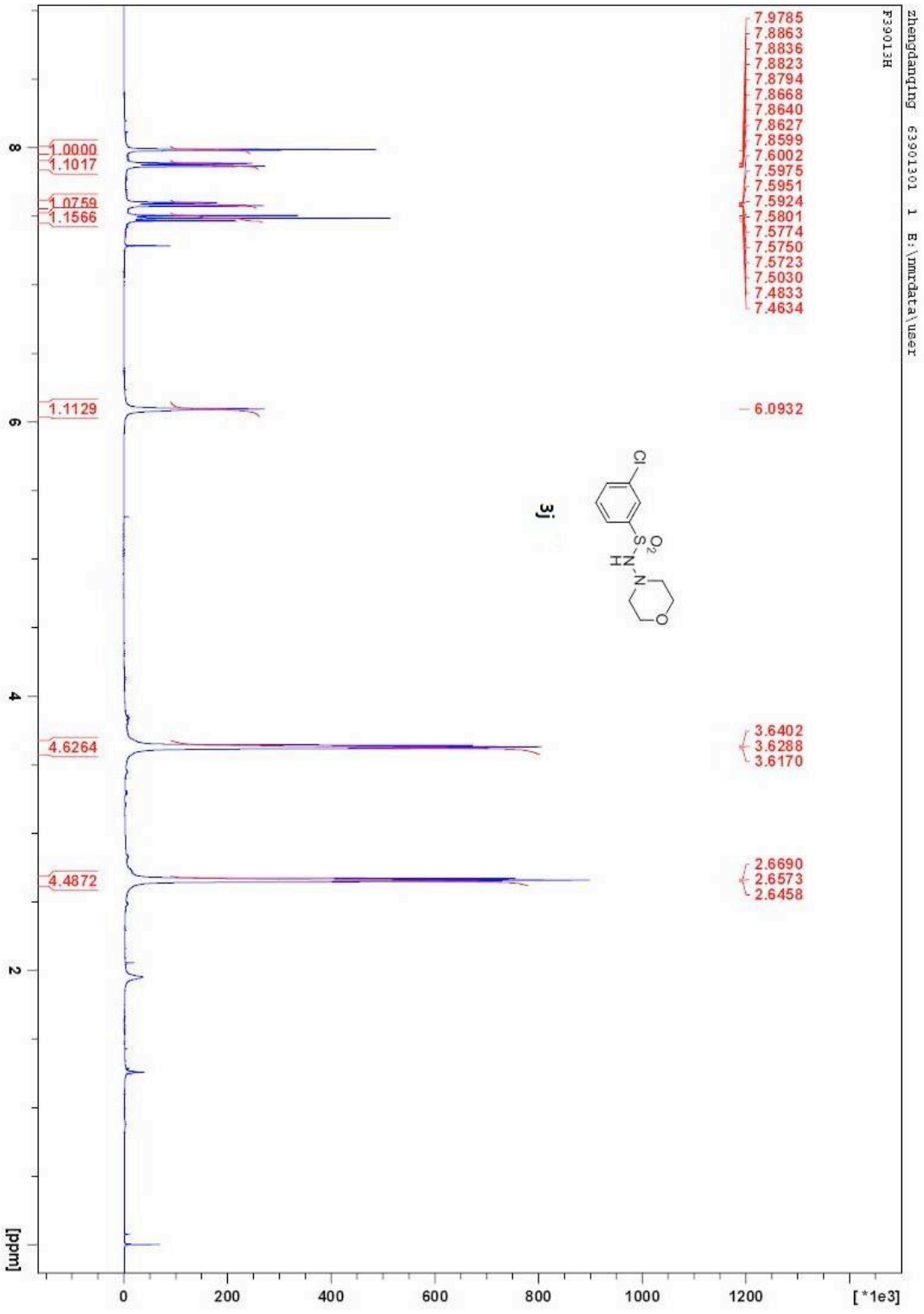
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3j
Cl
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O
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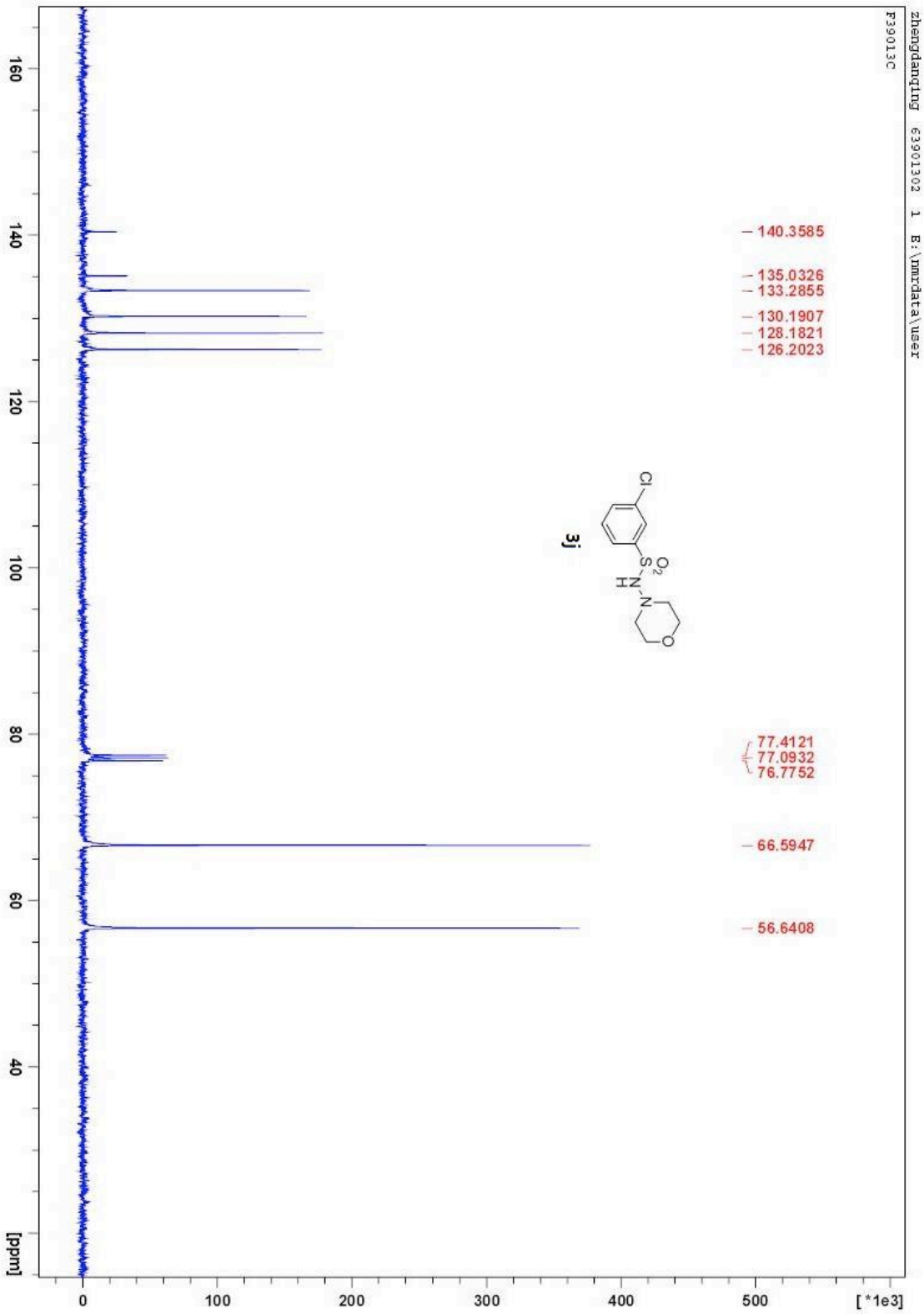
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3j
Cl
O2
S
N
H
N
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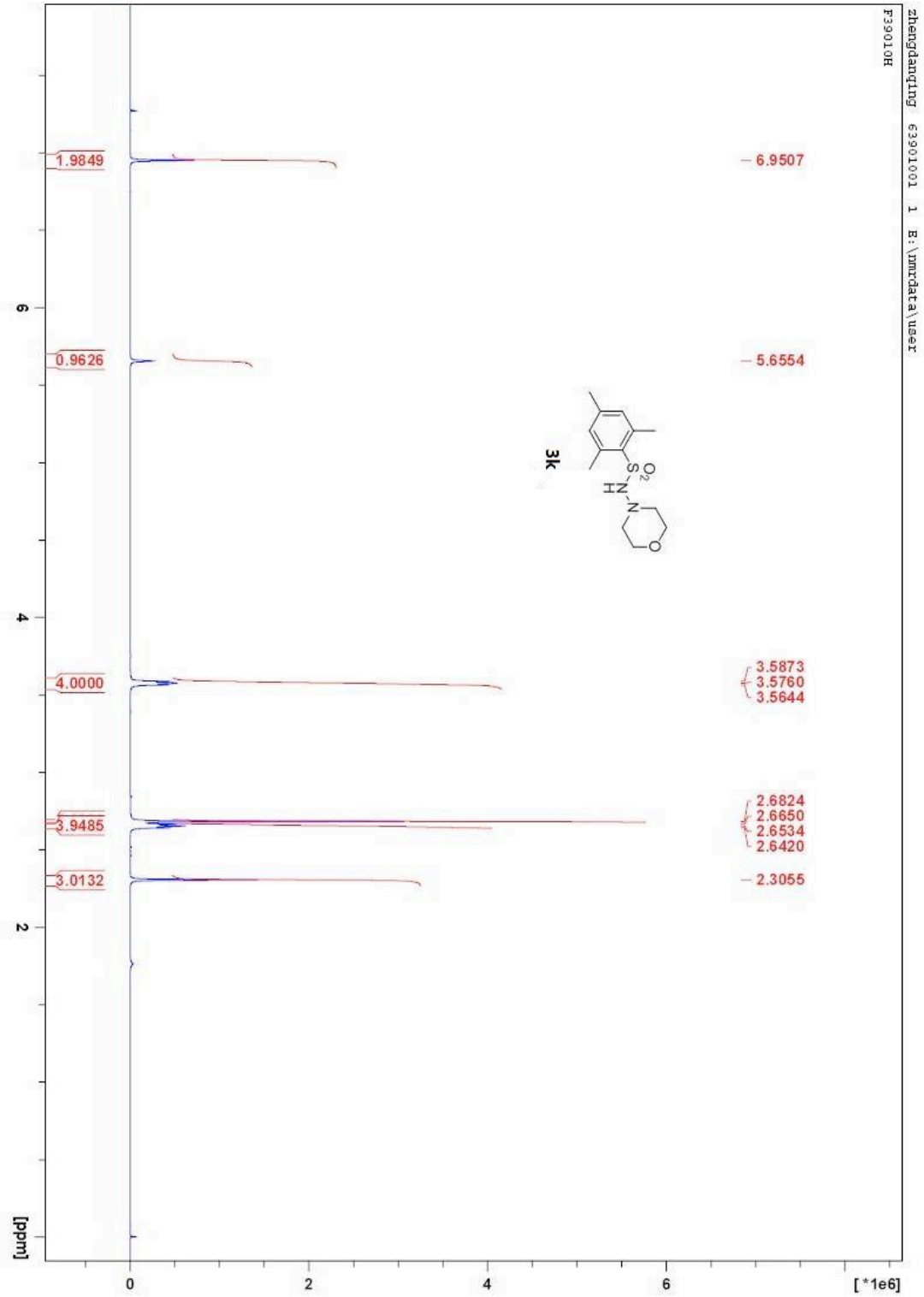
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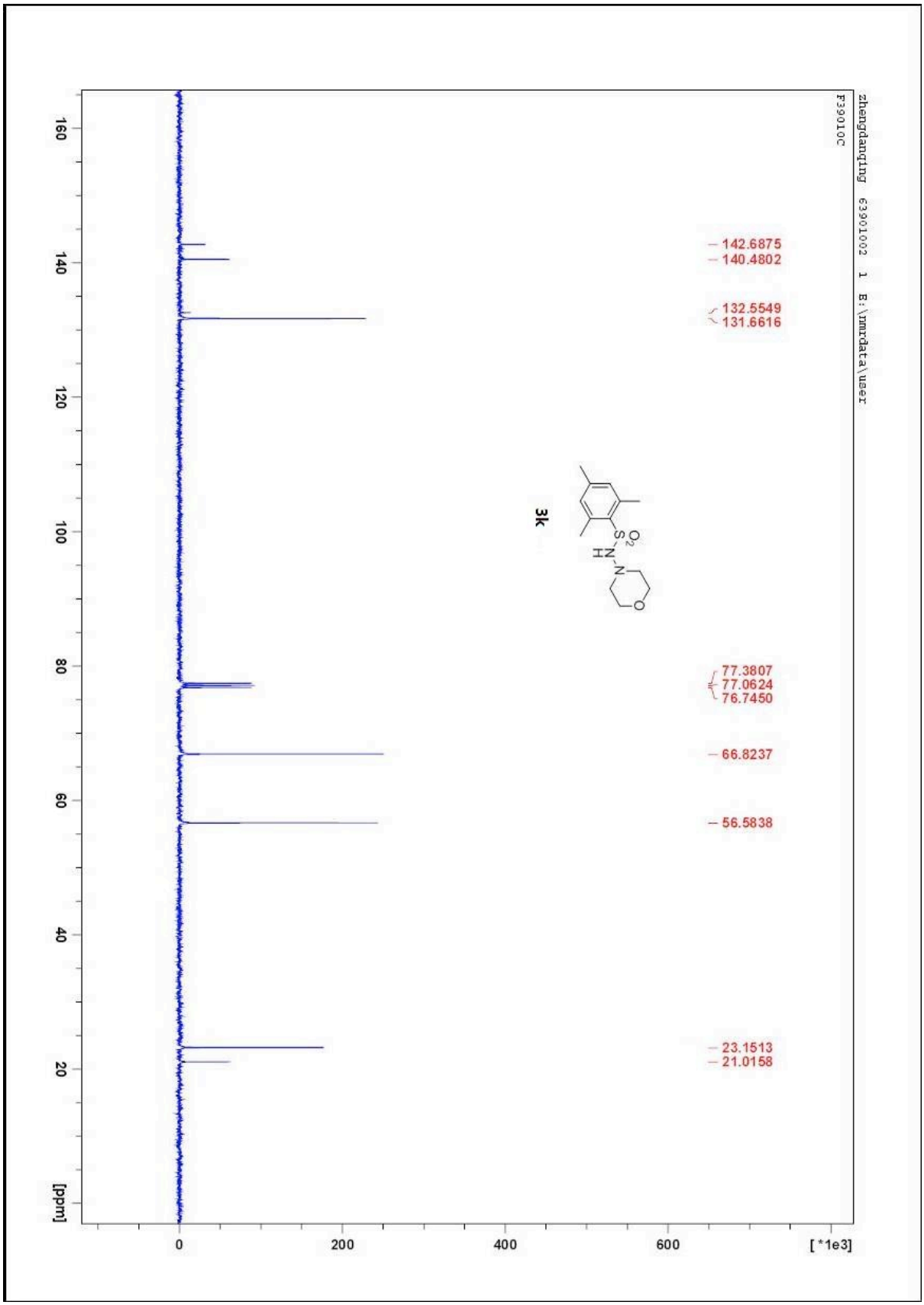
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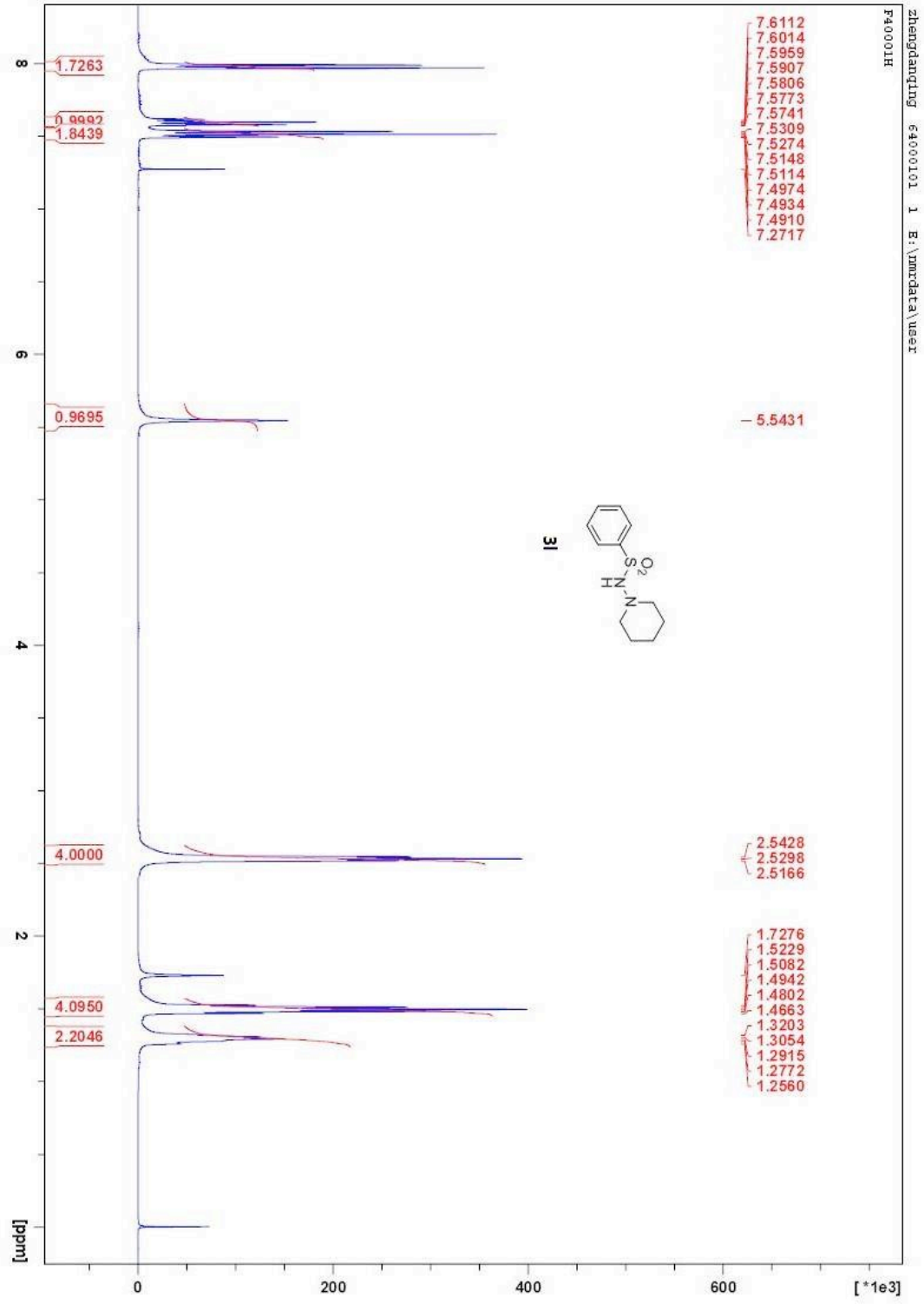
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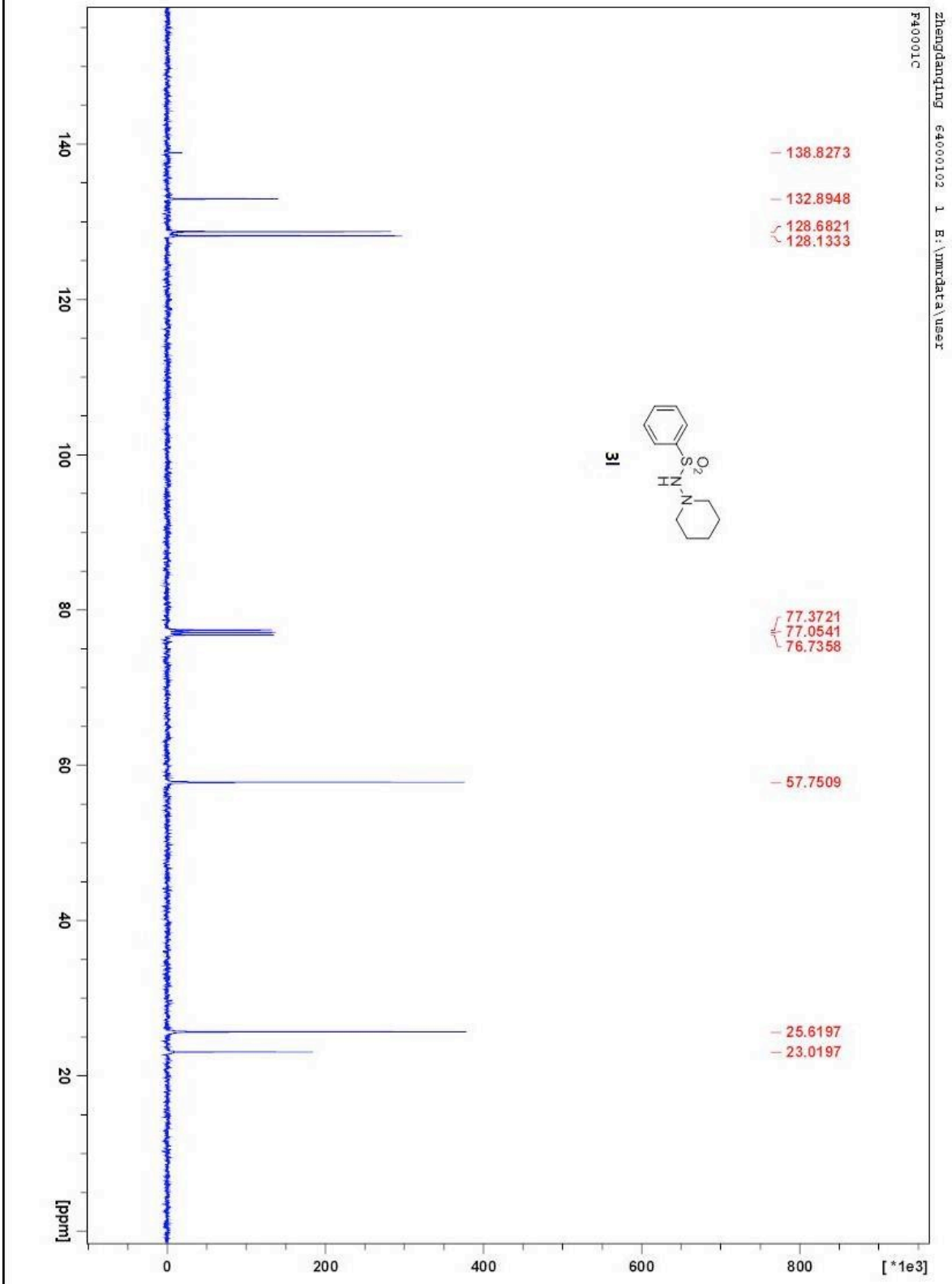
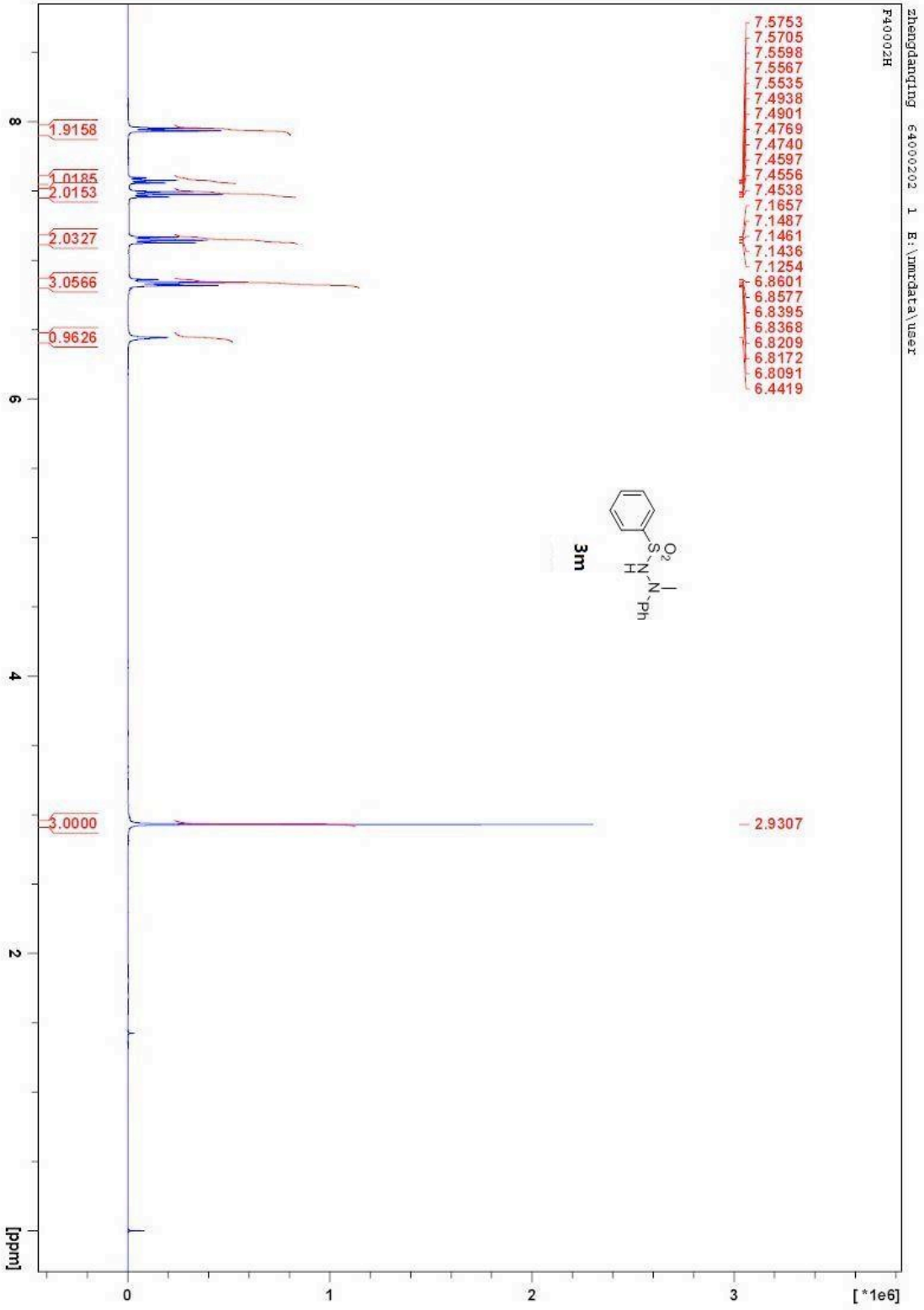
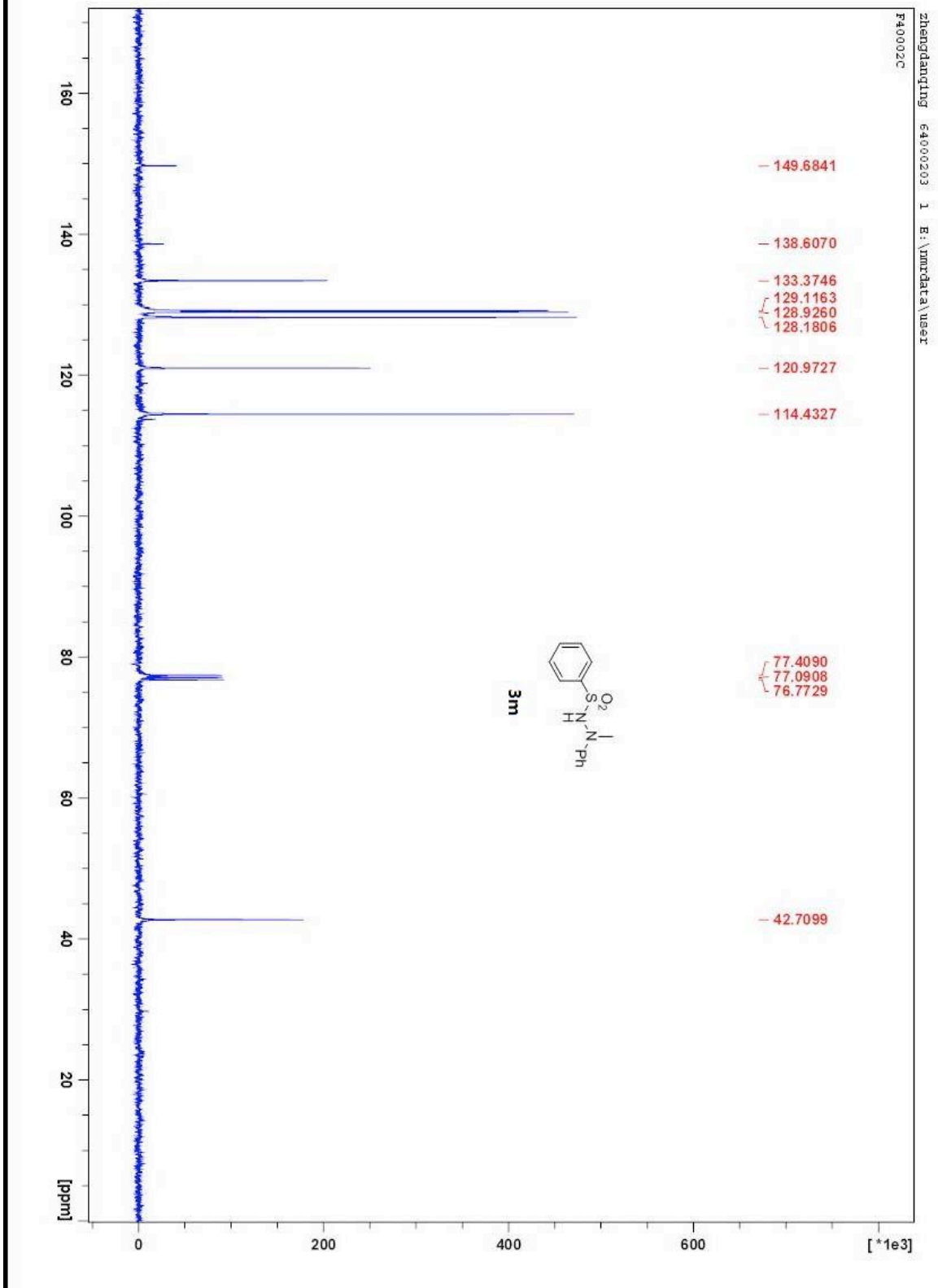
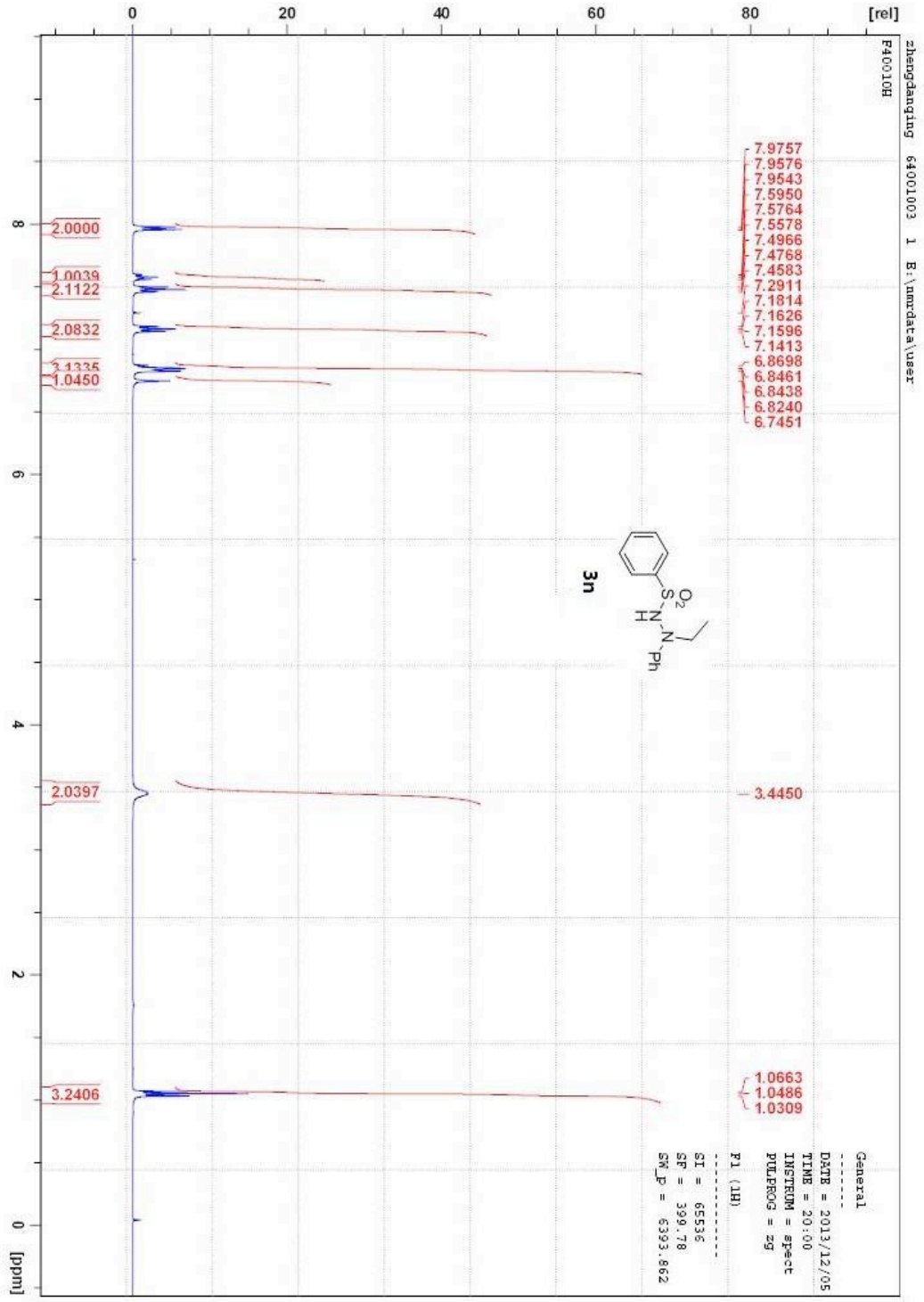
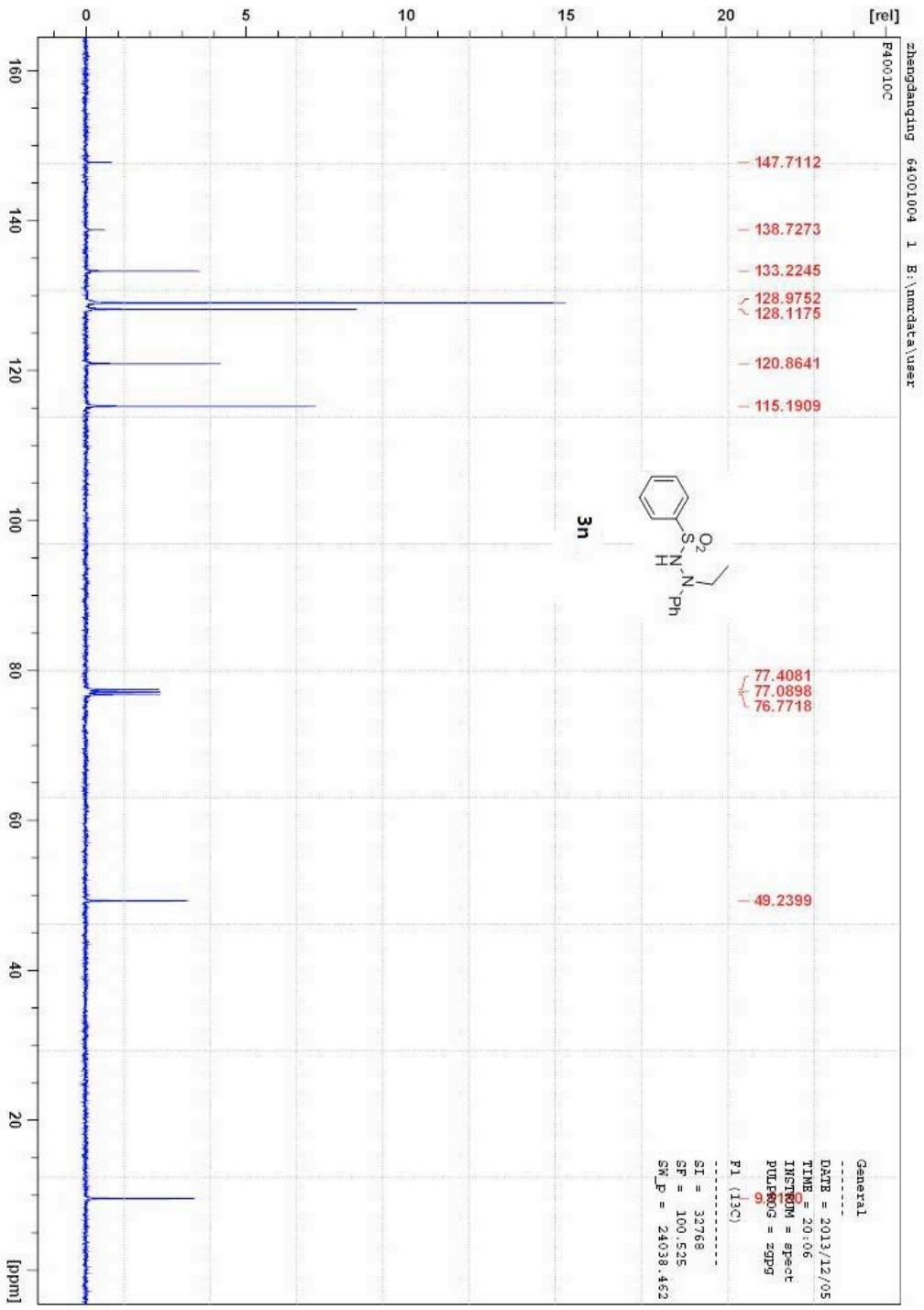
[ppm]
[*1e3]

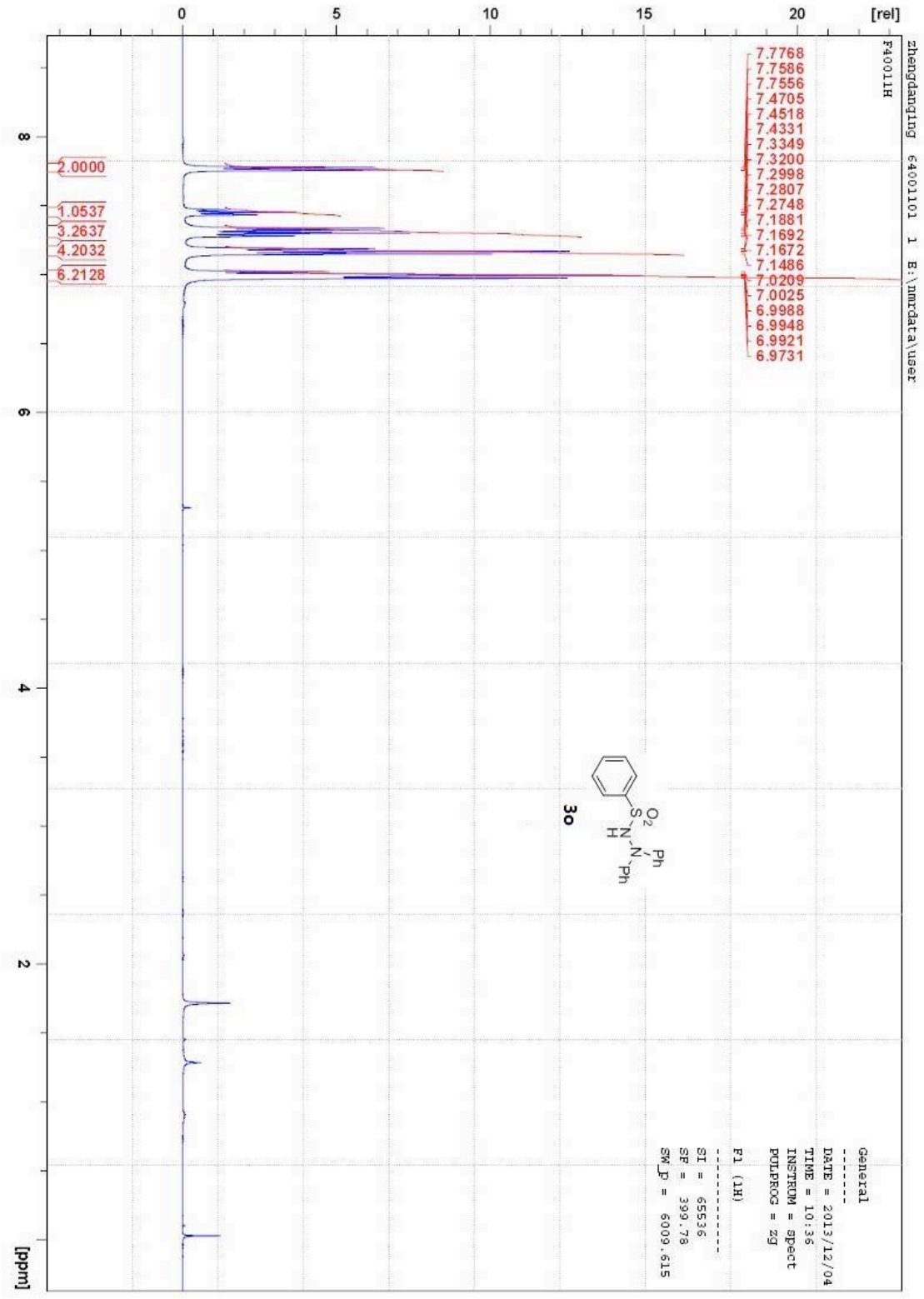

zhengdanqing 64000102 1 E:\nmrdata\user
F4000IC
138.8273
132.8948
128.6821
128.1333
77.3721
77.0541
76.7358
57.7509
25.6197
23.0197
3l
[ppm]
[*1e3]

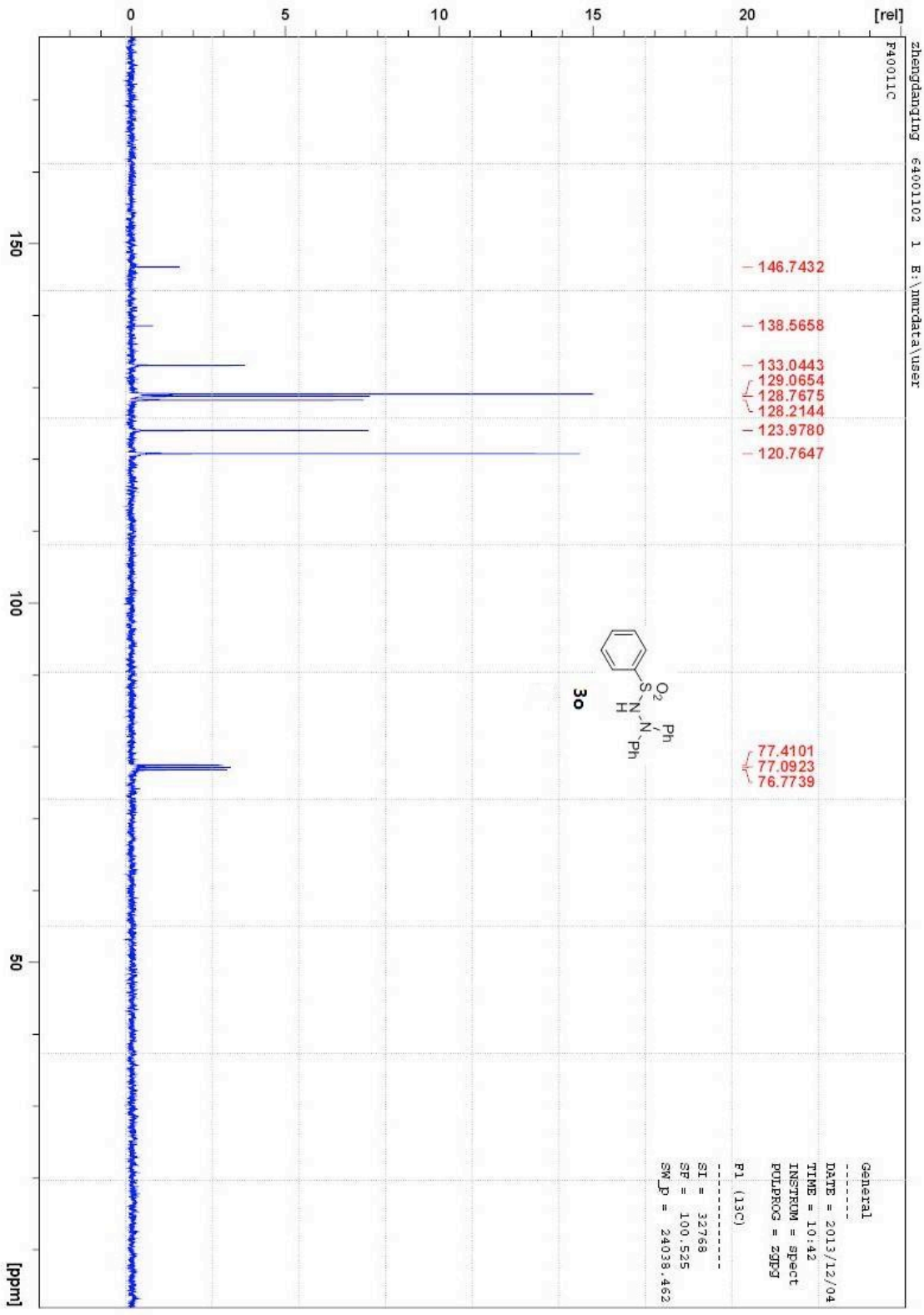

zhengdanqing 64000202 1 E:\nmrdata\wer
F40002H
7.5753
7.5705
7.5598
7.5567
7.5535
7.4938
7.4901
7.4769
7.4740
7.4597
7.4556
7.4538
7.1657
7.1487
7.1461
7.1436
7.1254
6.8601
6.8577
6.8395
6.8368
6.8209
6.8172
6.8091
6.4419
1.9158
1.0185
2.0153
2.0327
3.0566
0.9626
3.0000
2.9307
3m
[ppm]
[*1e6]


zhengdanqing 64000203 1 E:\nmrdata\user
F40002C
149.6841
138.6070
133.3746
129.1163
128.9260
128.1806
120.9727
114.4327
77.4090
77.0908
76.7729
42.7099
3m
O2
S
N
H
N
Ph
[ppm]
0
200
400
600
[*1e3]


zhengdanqing 64001003 1 B:\nmrdata\user
F400108H
7.9757
7.9576
7.9543
7.5950
7.5764
7.5578
7.4966
7.4768
7.4583
7.2911
7.1814
7.1626
7.1596
7.1413
6.8698
6.8461
6.8438
6.8240
6.7451
3.4450
1.0663
1.0486
1.0309
2.0000
1.0039
2.1122
2.0832
2.1335
1.0450
2.0397
3.2406
3n
General
DATE = 2013/12/05
TIME = 20:00
INSTRUM = spect
PULPROG = zg
F1 (1H)
SI = 65536
SF = 399.78
SW_P = 6393.862
[rel]
[ppm]


147.7112
138.7273
133.2245
128.9752
128.1175
120.8641
115.1909
77.4081
77.0898
76.7718
49.2239
3n
zhengdanqing 64001004 1 B:\nmrdata\user
F400106
General
DATE = 2013/12/05
TIME = 20:06
INSTRUM = spect
PULPROG = zgpg
F1 (13C)
SI = 32768
SF = 100.525
SW_p = 24038.462
[rel]
[ppm]


zhengdanqing 64001101 1 E:\nmrdata\user
F4001IH
[rel]
[ppm]
7.7768
7.7586
7.7556
7.4705
7.4518
7.4331
7.3349
7.3200
7.2998
7.2807
7.2748
7.1881
7.1692
7.1672
7.1486
7.0209
7.0025
6.9988
6.9948
6.9921
6.9731
2.0000
1.0537
3.2637
4.2032
6.2128
3o
General
DATE = 2013/12/04
TIME = 10:36
INSTRUM = spect
PULPROG = zg
F1 (1H)
SI = 65536
SF = 399.78
SW_p = 6009.615


zhengdanqing 64001102 1 E:\nmrdata\user
F4001IC
[rel]
0
5
10
15
20
150
100
50
[ppm]
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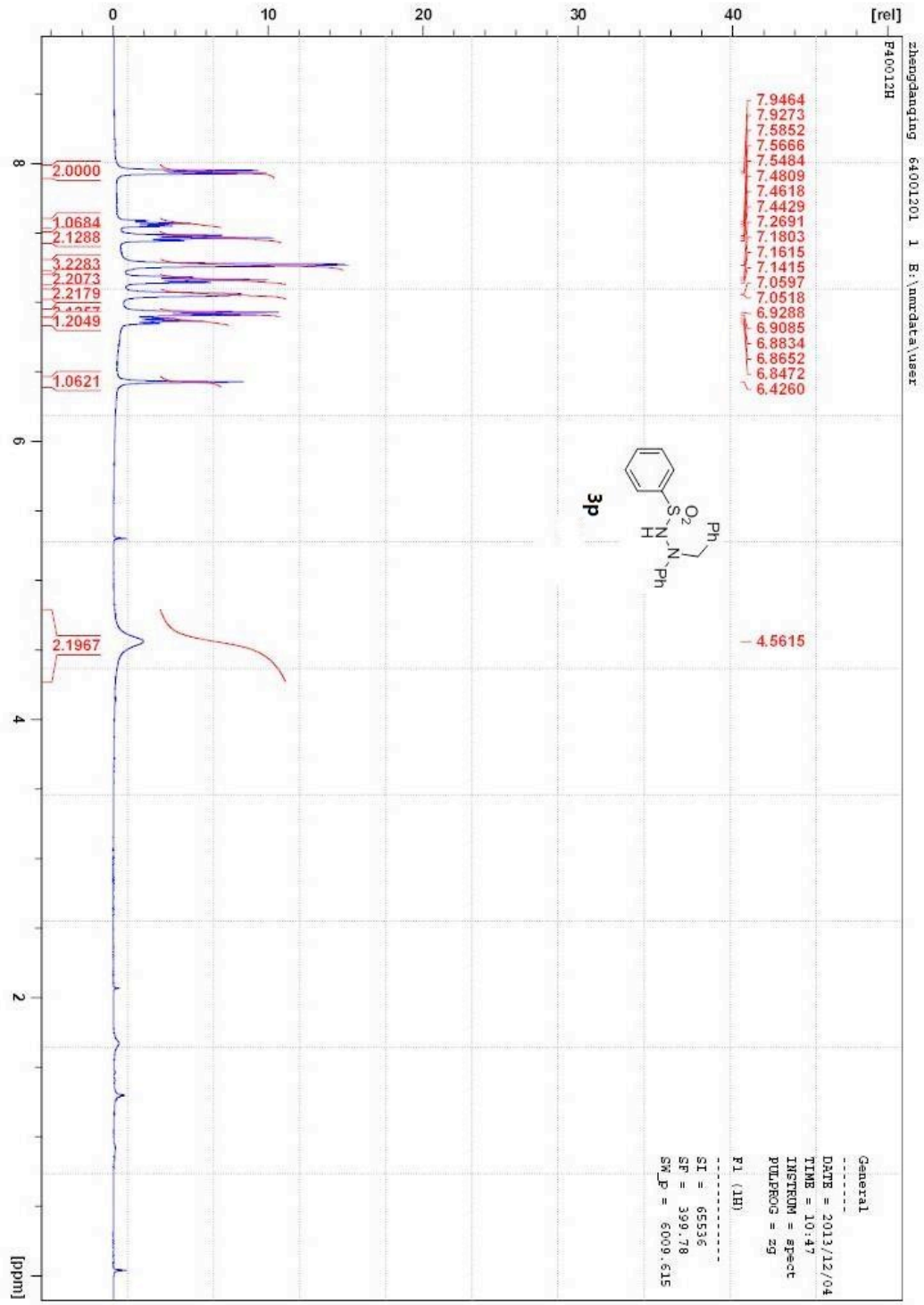
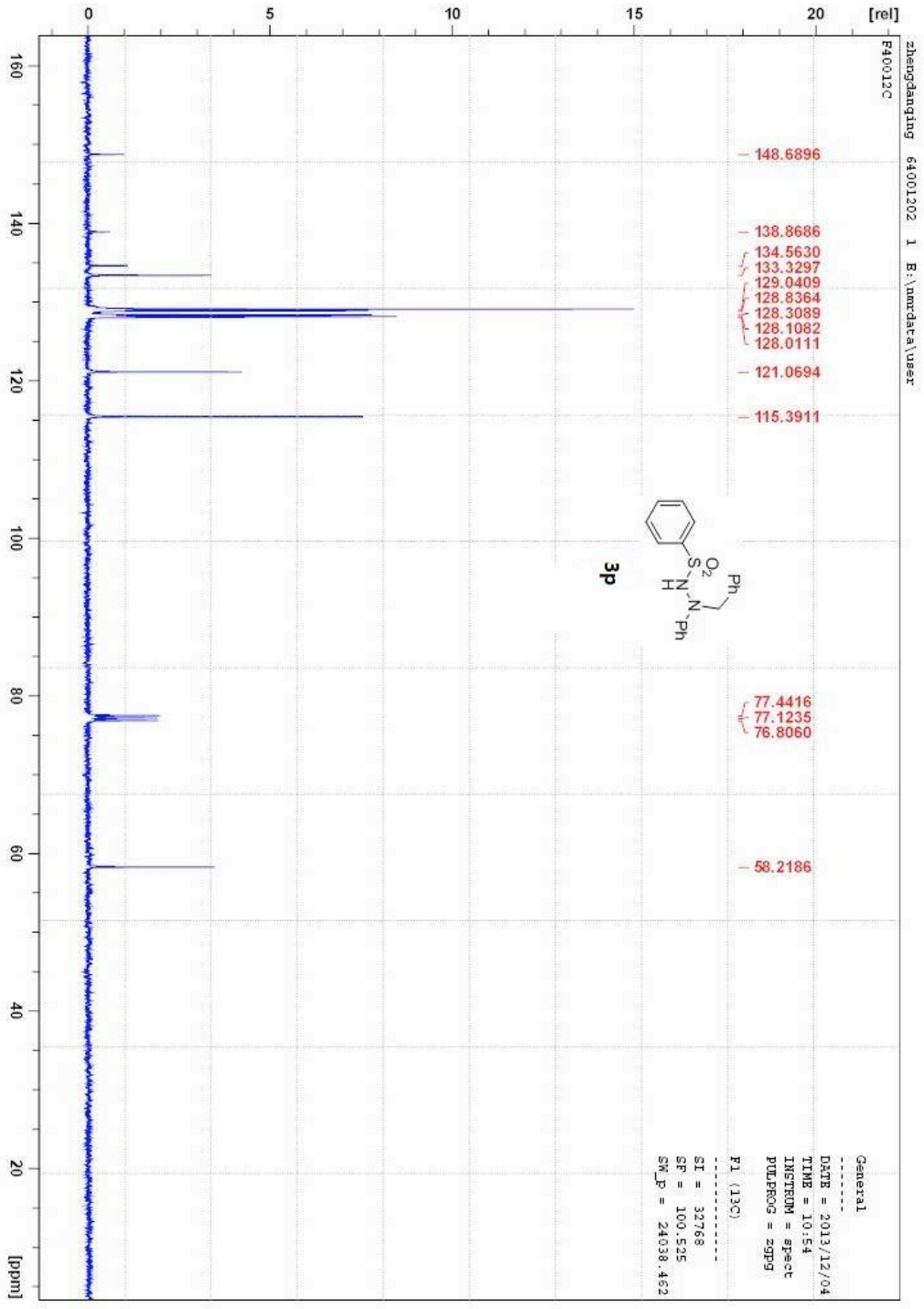
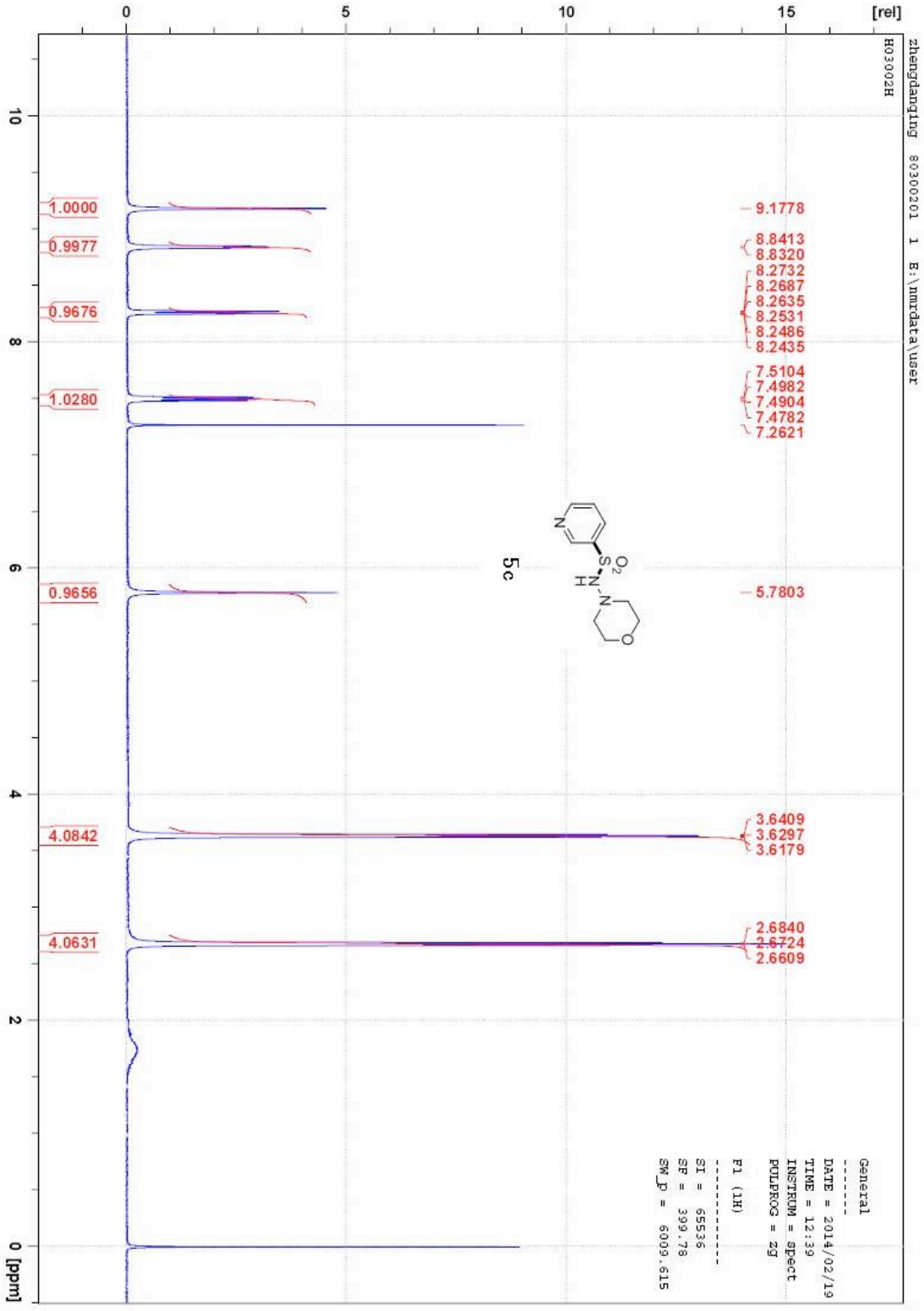
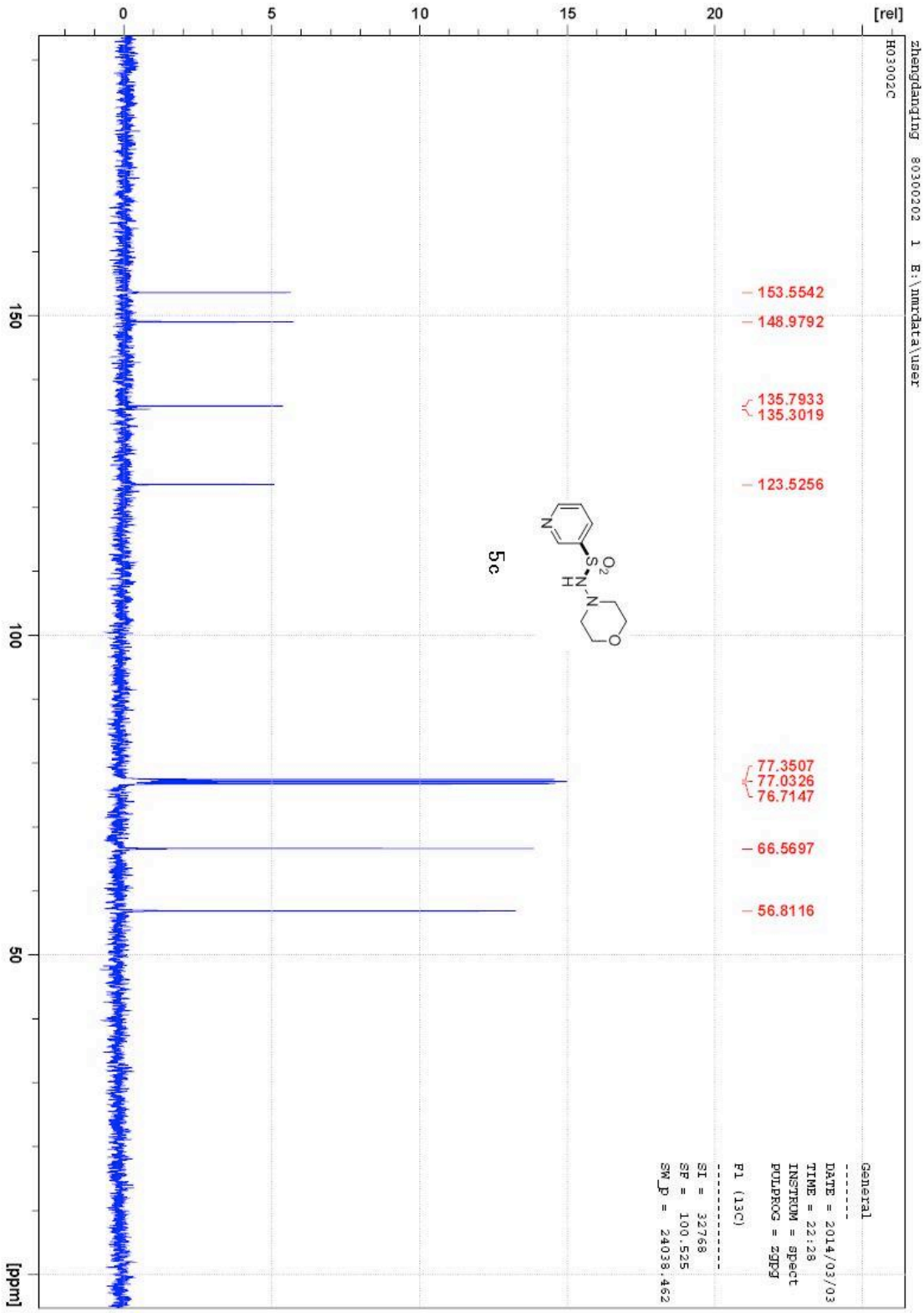
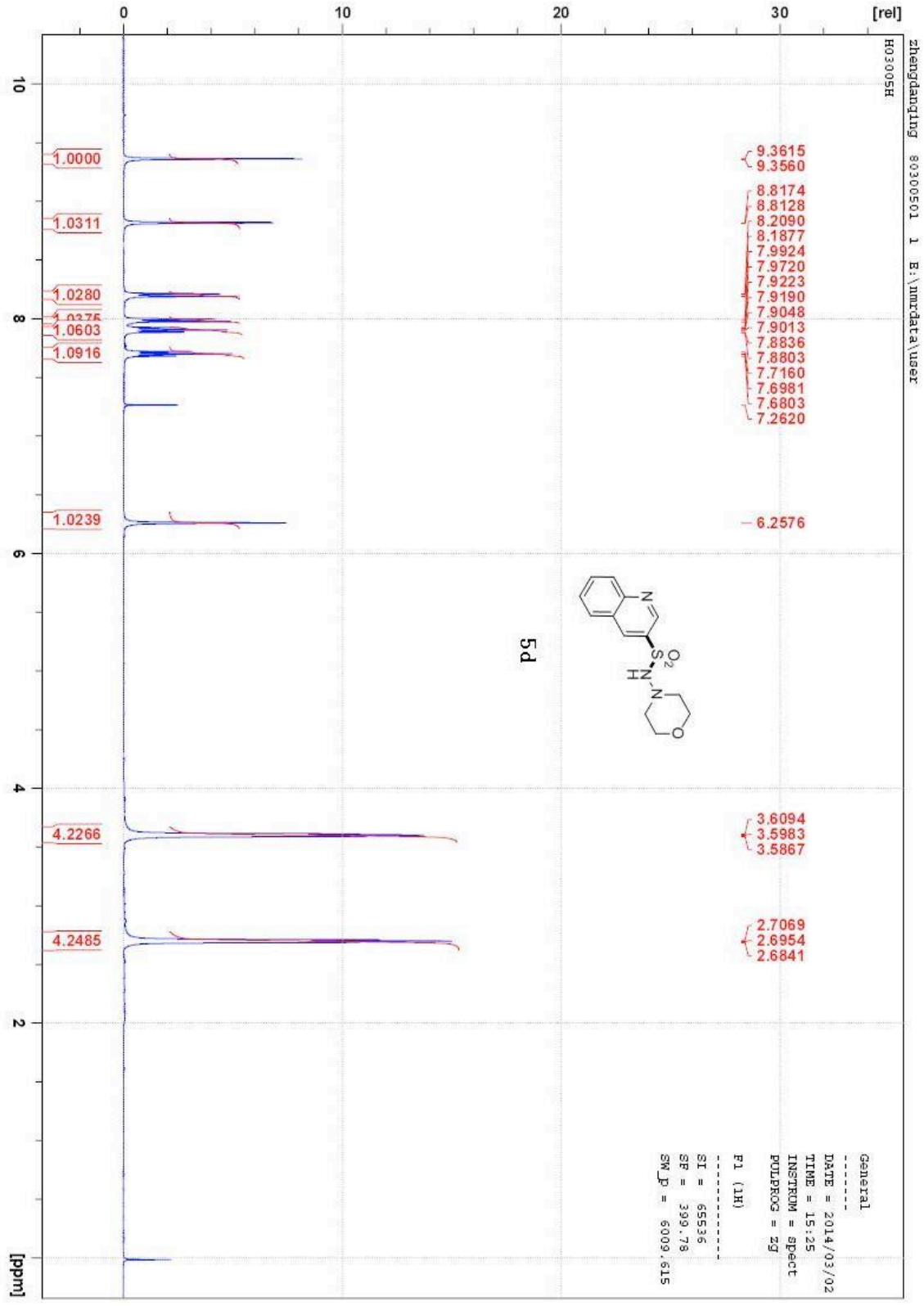
128.7675
128.2144
123.9780
120.7647
77.4101
77.0923
76.7739
3o
O2
S
N
H
N
Ph
Ph
General
DATE = 2013/12/04
TIME = 10:42
INSTRUM = spect
POLPROG = zgpg
F1 (13C)
SI = 32768
SF = 100.525
SW_p = 24038.462

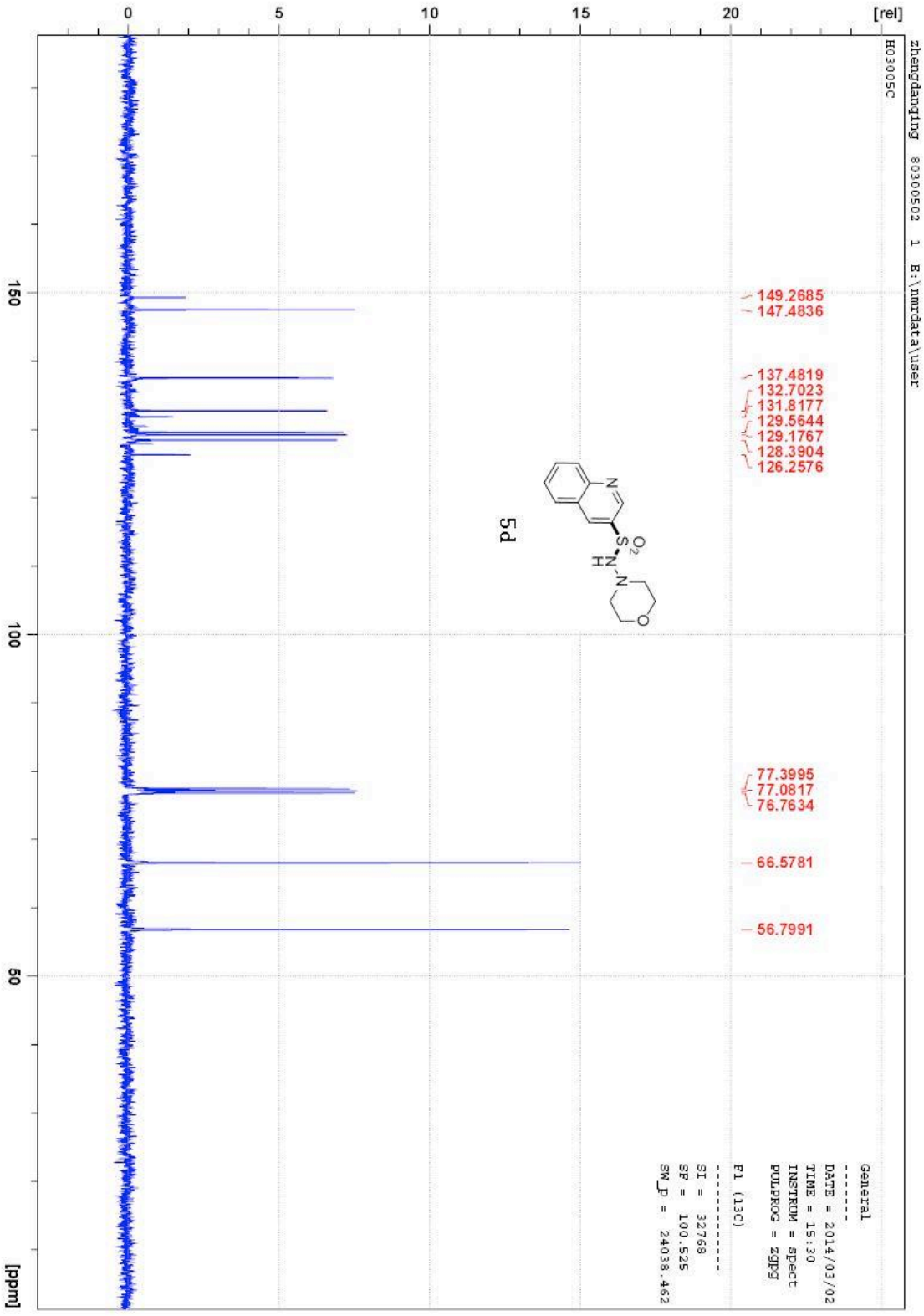

zhengdanqing 64001201 1 B:\nmrdata\user
P40012H
7.9464
7.9273
7.5852
7.5666
7.5484
7.4809
7.4618
7.4429
7.2691
7.1803
7.1615
7.1415
7.0597
7.0518
6.9288
6.9085
6.8834
6.8652
6.8472
6.4260
4.5615
2.0000
1.0684
2.1288
2.2283
2.2073
2.2179
1.2049
1.0621
2.1967
3p
Ph
O2
S
N
H
N
Ph
General
DATE = 2013/12/04
TIME = 10:47
INSTRUM = spect
PULPROG = zg
F1 (1H)
SI = 65536
SF = 399.78
SW_P = 6009.615
[rel]
[ppm]

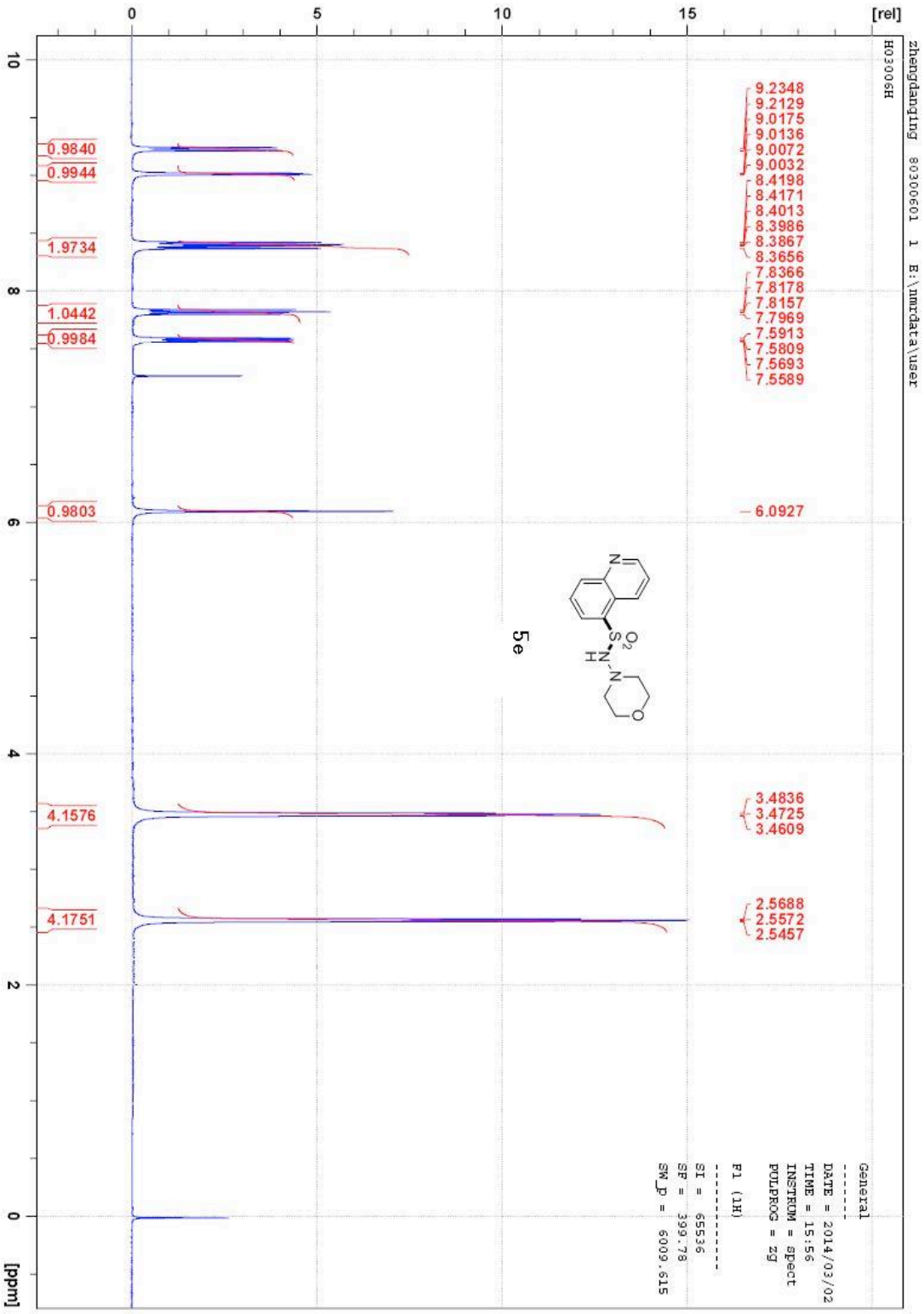

zhengdanqing 64001202 1 E:\nmrdata\user
F400120C
148.6896
138.8686
134.5630
133.3297
129.0409
128.8364
128.3089
128.1082
128.0111
121.0694
115.3911
77.4416
77.1235
76.8060
58.2186
3p
General
DATE = 2013/12/04
TIME = 10:54
INSTRUM = spect
PULPROG = zgpg
F1 (13C)
SI = 32768
SF = 100.525
SW_p = 24038.462
[rel]
[ppm]

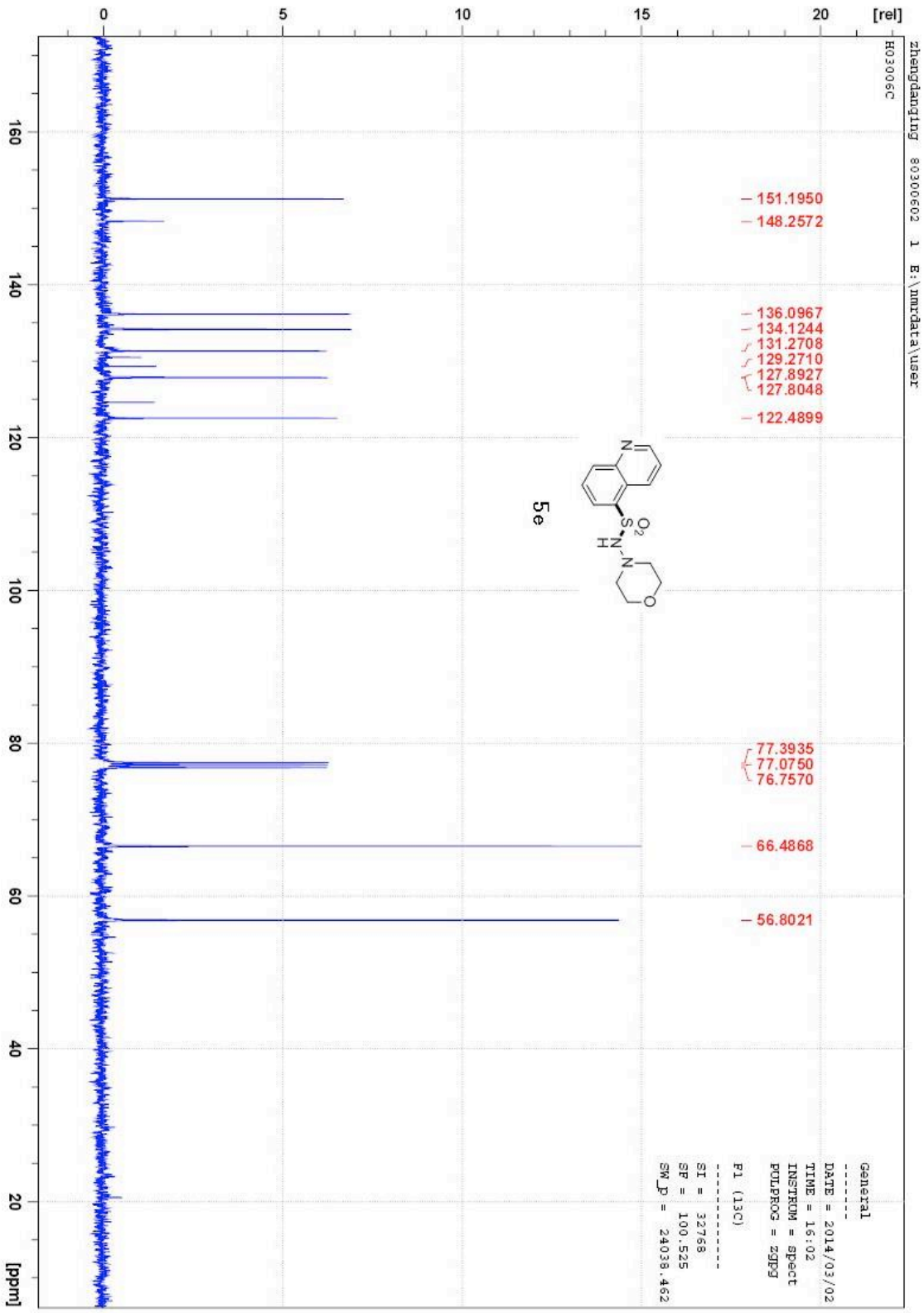

zhengdanqing 80300201 1 B:\nmrdata\user
HO3002H
[rel]
0
5
10
15
[ppm]
0
2
4
6
8
10
1.0000
0.9977
0.9676
1.0280
0.9656
4.0842
4.0631
9.1778
8.8413
8.8320
8.2732
8.2687
8.2635
8.2531
8.2486
8.2435
7.5104
7.4982
7.4904
7.4782
7.2621
5.7803
3.6409
3.6297
3.6179
2.6840
2.6724
2.6609
5c
General
DATE = 2014/02/19
TIME = 12:39
INSTRUM = spect
PULPROG = zg
F1 (1H)
SI = 65536
SF = 399.78
SW_p = 6009.615

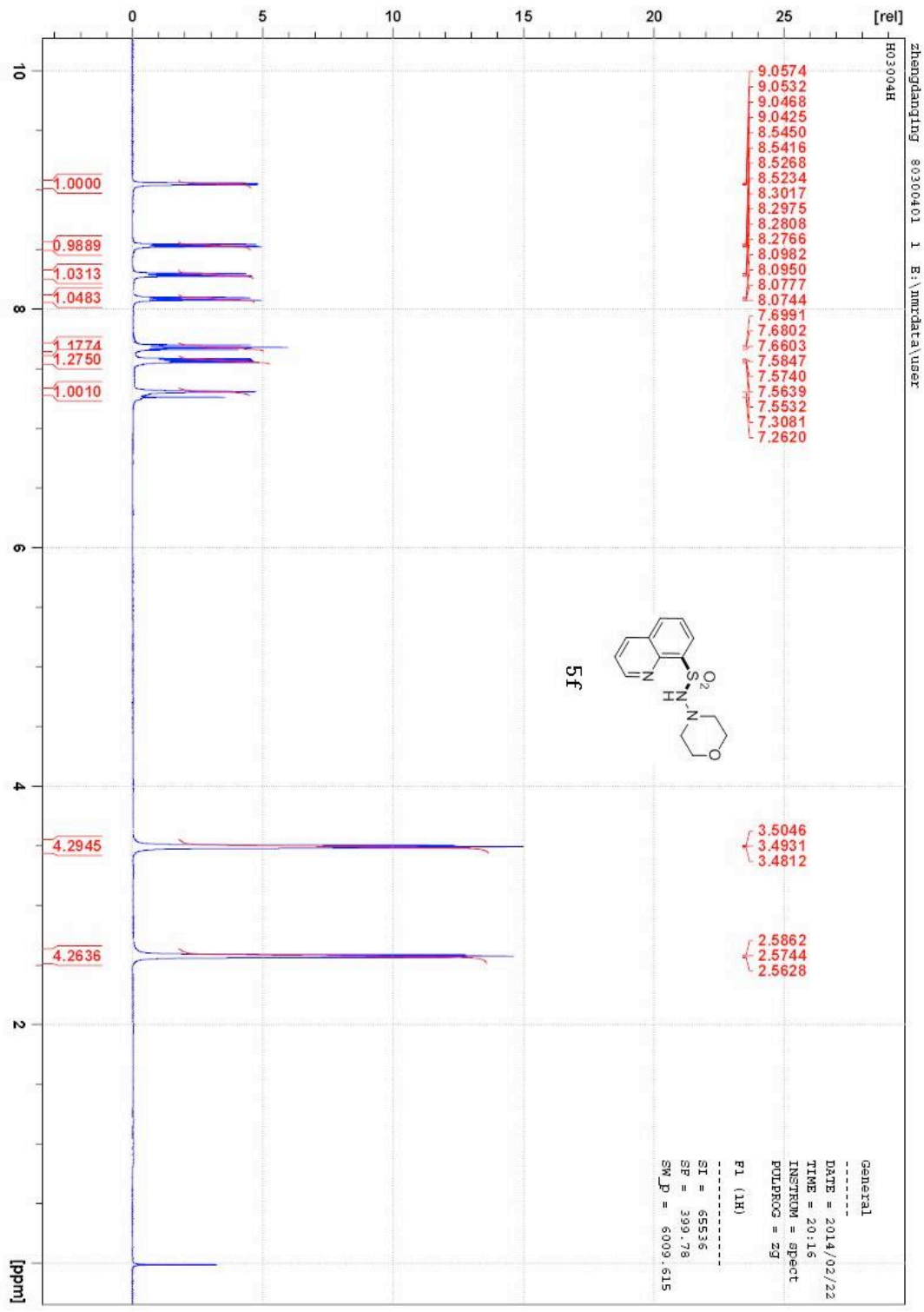

zhengdanqing 80300202 1 E:\nmrdata\user
H03002C
General
DATE = 2014/03/03
TIME = 22:28
INSTRUM = spect
PULPROG = zgpg
F1 (13C)
SI = 32768
SF = 100.525
SW_p = 24038.462
153.5542
148.9792
135.7933
135.3019
123.5256
77.3507
77.0326
76.7147
66.5697
56.8116
5c
[rel]
[ppm]

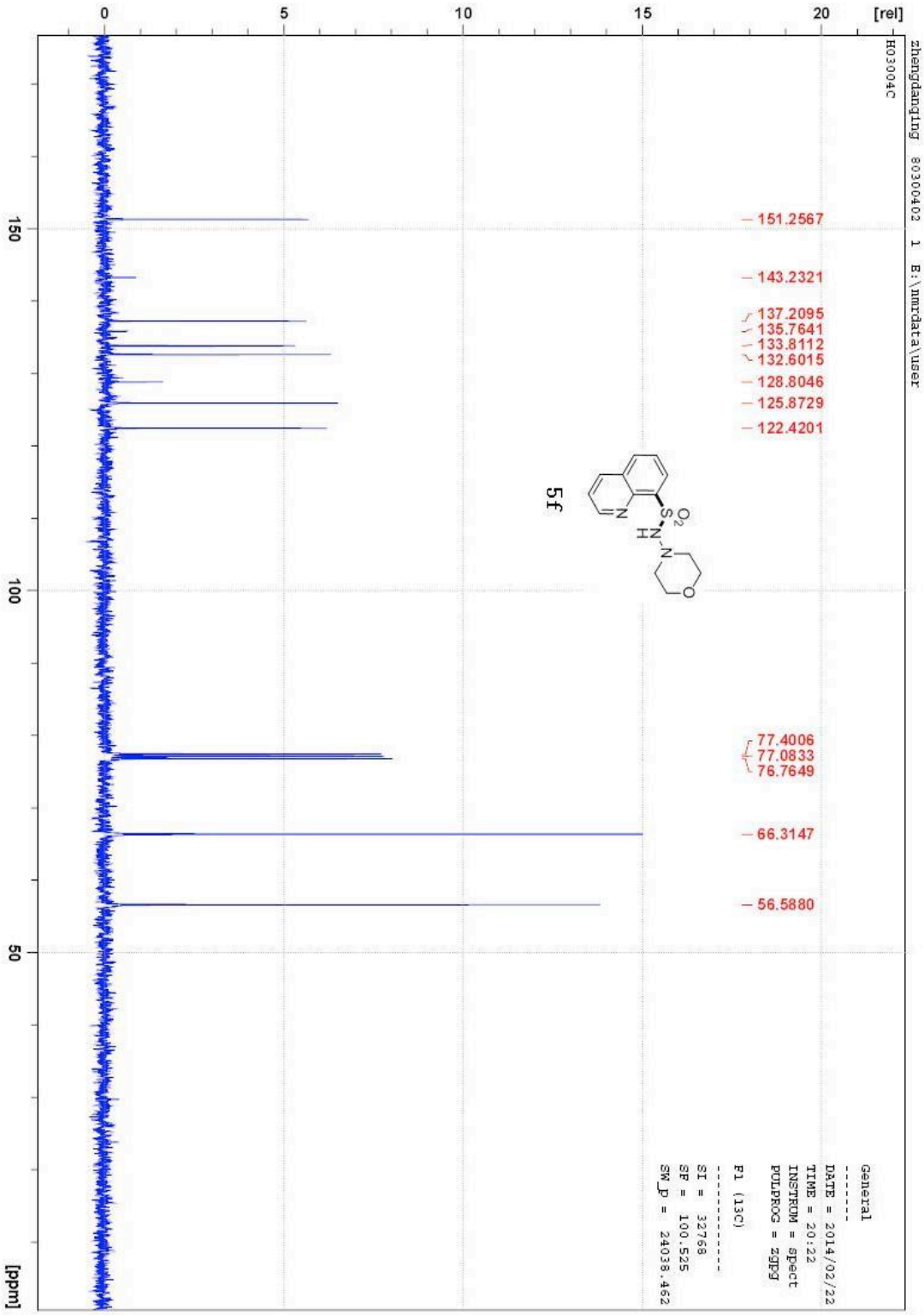

zhengdanqing 80300501 1 E:\nmrdata\user
H0300501
General
DATE = 2014/03/02
TIME = 15:25
INSTRUM = spect
PULPROG = zg
F1 (1H)
SI = 65536
SF = 399.78
SW_p = 6009.615
9.3615
9.3560
8.8174
8.8128
8.2090
8.1877
7.9924
7.9720
7.9223
7.9190
7.9048
7.9013
7.8836
7.8803
7.7160
7.6981
7.6803
7.2620
6.2576
3.6094
3.5983
3.5867
2.7069
2.6954
2.6841
1.0000
1.0311
1.0280
1.0603
1.0916
1.0239
4.2266
4.2485
5d
[rel]
[ppm]

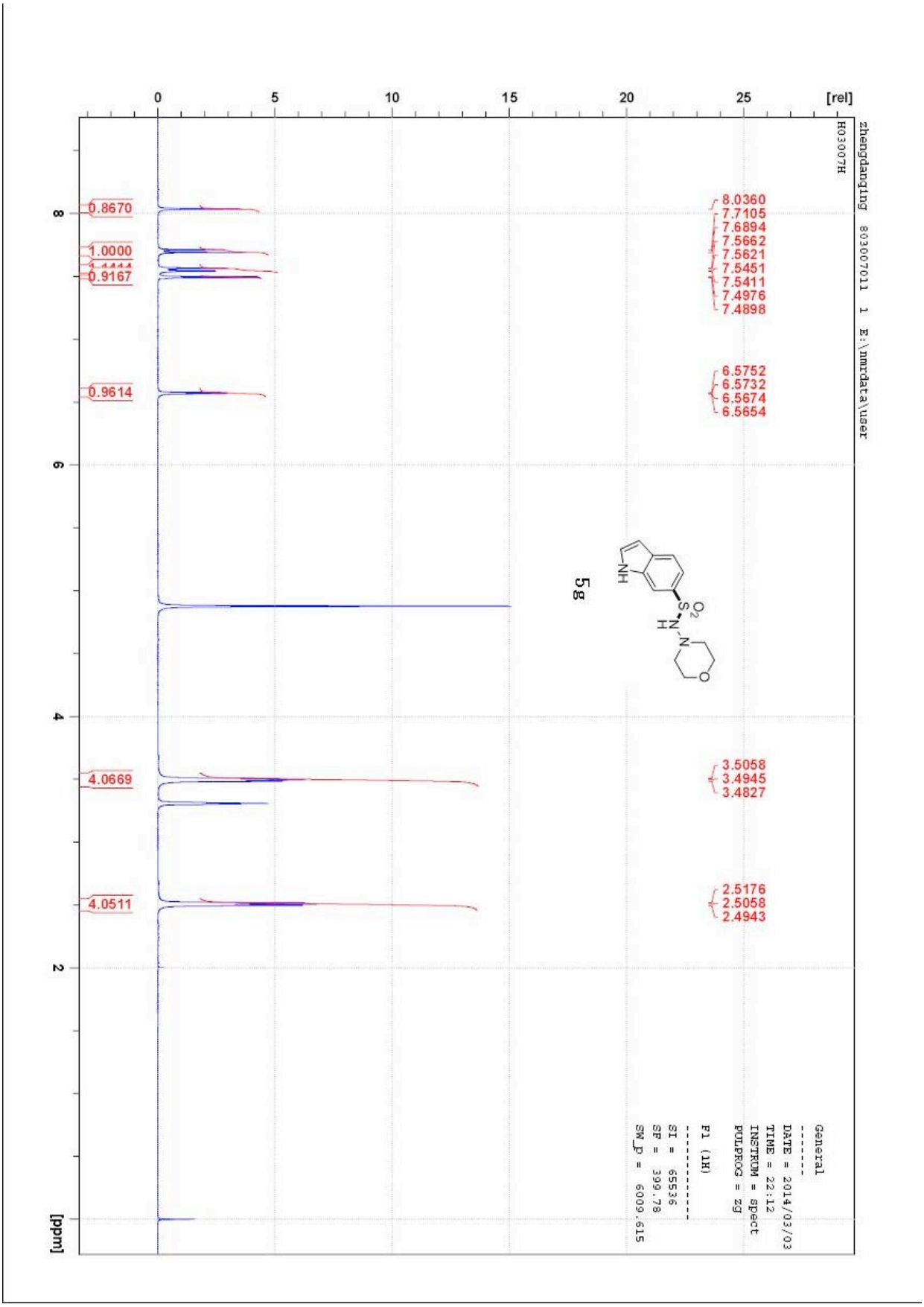

zhengdanqing 80300502 1 B:\nmrdata\user
H03005C
[rel]
0
5
10
15
20
[ppm]
150
100
50
149.2685
147.4836
137.4819
132.7023
131.8177
129.5644
129.1767
128.3904
126.2576
77.3995
77.0817
76.7634
66.5781
56.7991
5d
General
DATE = 2014/03/02
TIME = 15:30
INSTRUM = spect
PULPROG = zgpg
F1 (13C)
SI = 32768
SF = 100.525
SW_p = 24038.462

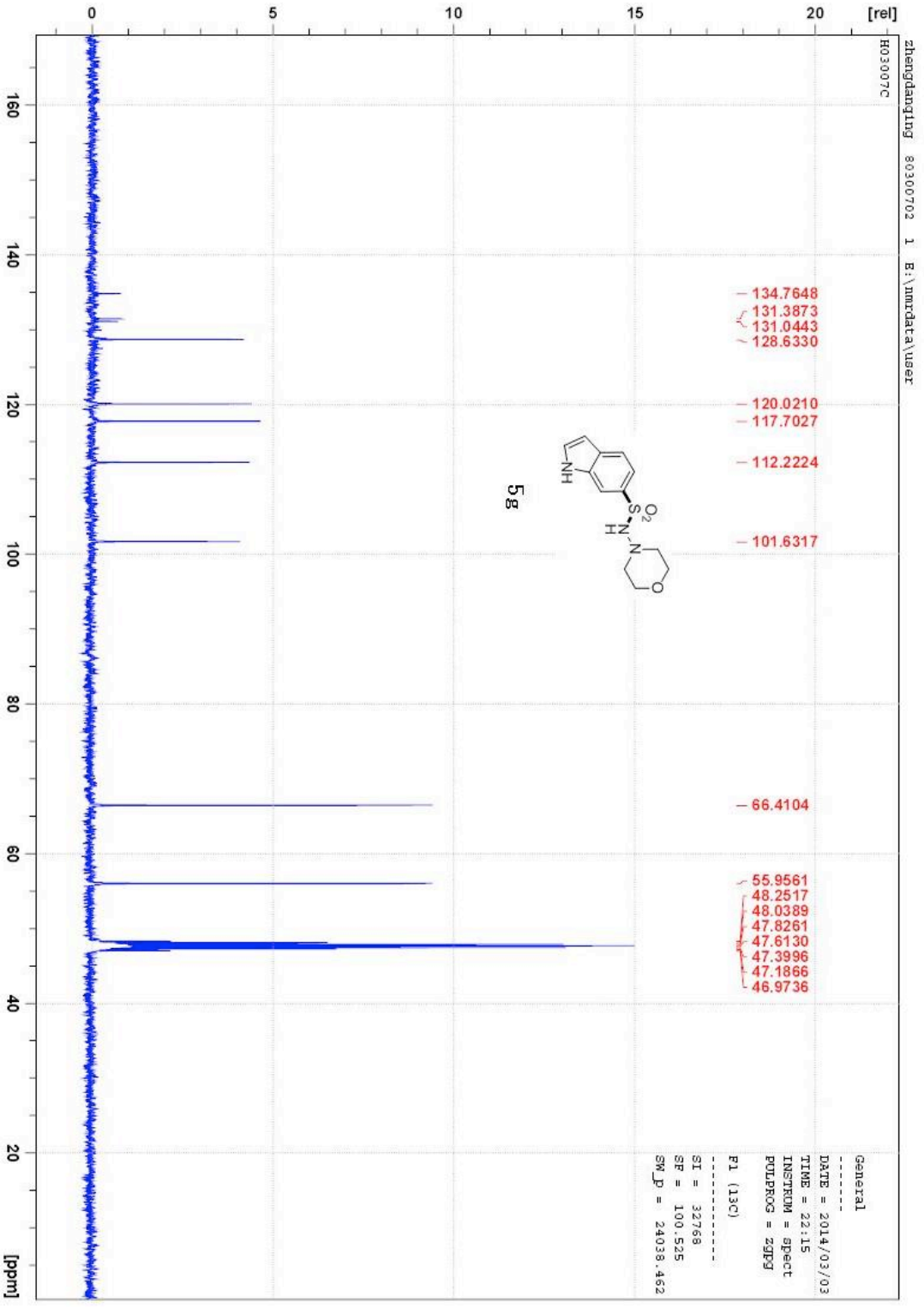

zhengdangting 80300601 1 E:\nmrdata\user
H03006H
9.2348
9.2129
9.0175
9.0136
9.0072
9.0032
8.4198
8.4171
8.4013
8.3986
8.3867
8.3656
7.8366
7.8178
7.8157
7.7969
7.5913
7.5809
7.5693
7.5589
6.0927
3.4836
3.4725
3.4609
2.5688
2.5572
2.5457
0.9840
0.9944
1.9734
1.0442
0.9984
0.9803
4.1576
4.1751
5e
General
DATE = 2014/03/02
TIME = 15:56
INSTRUM = spect
PULPROG = zg
F1 (1H)
SI = 65536
SF = 399.78
SW_p = 6009.615
[rel]
[ppm]

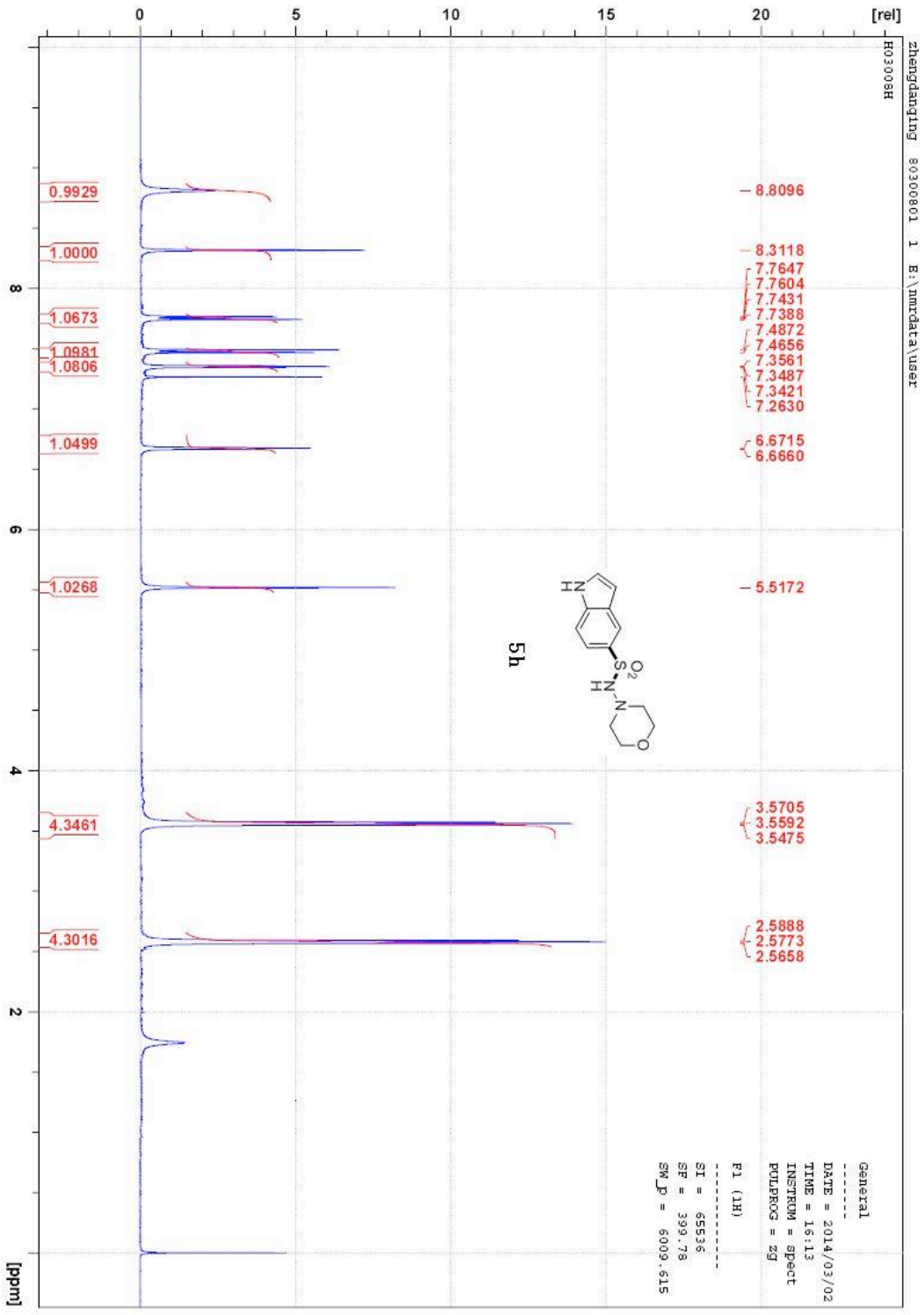

151.1950
148.2572
136.0967
134.1244
131.2708
129.2710
127.8927
127.8048
122.4899
77.3935
77.0750
76.7570
66.4868
56.8801
5e
zhengdanqing 80300602 1 E:\nmrdata\user
H03006C
[rel]
[ppm]


zhengdanqing 80300401 1 E:\nmrdata\user
H03004H
9.0574
9.0532
9.0468
9.0425
8.5450
8.5416
8.5268
8.5234
8.3017
8.2975
8.2808
8.2766
8.0982
8.0950
8.0777
8.0744
7.6991
7.6802
7.6603
7.5847
7.5740
7.5639
7.5532
7.3081
7.2620
1.0000
0.9889
1.0313
1.0483
1.1774
1.2750
1.0010
4.2945
4.2636
3.5046
3.4931
3.4812
2.5862
2.5744
2.5628
5f
General
DATE = 2014/02/22
TIME = 20:16
INSTRUM = spect
PULPROG = zg
F1 (1H)
SI = 65536
SF = 399.78
SWp = 6009.615
[rel]
[ppm]


zhengdanqing 80300402 1 E:\nmrdata\user
H03004C
[rel]
0
5
10
15
20
[ppm]
150
100
50
151.2567
143.2321
137.2095
135.7641
133.8112
132.6015
128.8046
125.8729
122.4201
77.4006
77.0833
76.7649
66.3147
56.5880
5f
General
DATE = 2014/02/22
TIME = 20:22
INSTRUM = spect
PULPROG = zgpg
F1 (13C)
SI = 32768
SF = 100.525
SW_p = 24038.462


zhengdangting 803007011 1 E:\nmrdata\user
H03007H
0.8670
1.0000
0.9167
0.9614
4.0669
4.0511
8.0360
7.7105
7.6894
7.5662
7.5621
7.5451
7.5411
7.4976
7.4898
6.5752
6.5732
6.5674
6.5654
3.5058
3.4945
3.4827
2.5176
2.5058
2.4943
5g
General
DATE = 2014/03/03
TIME = 22:12
INSTRUM = spect
PULPROG = zg
F1 (1H)
SI = 65536
SF = 399.78
SW_p = 6009.615
[rel]
[ppm]


zhengdangting 80300702 1 B:\nmrdata\user
H03007C
134.7648
131.3873
131.0443
128.6330
120.0210
117.7027
112.2224
101.6317
66.4104
55.9561
48.2517
48.0389
47.8261
47.6130
47.3996
47.1866
46.9736
5g
General
DATE = 2014/03/03
TIME = 22:15
INSTRUM = spect
PULPROG = zgpg
F1 (13C)
SI = 32768
SF = 100.525
SW_p = 24038.462
[rel]
[ppm]


zhengdanqing 80300801 1 E:\nmrdata\user
HO3008H
[rel]
[ppm]
0.9929
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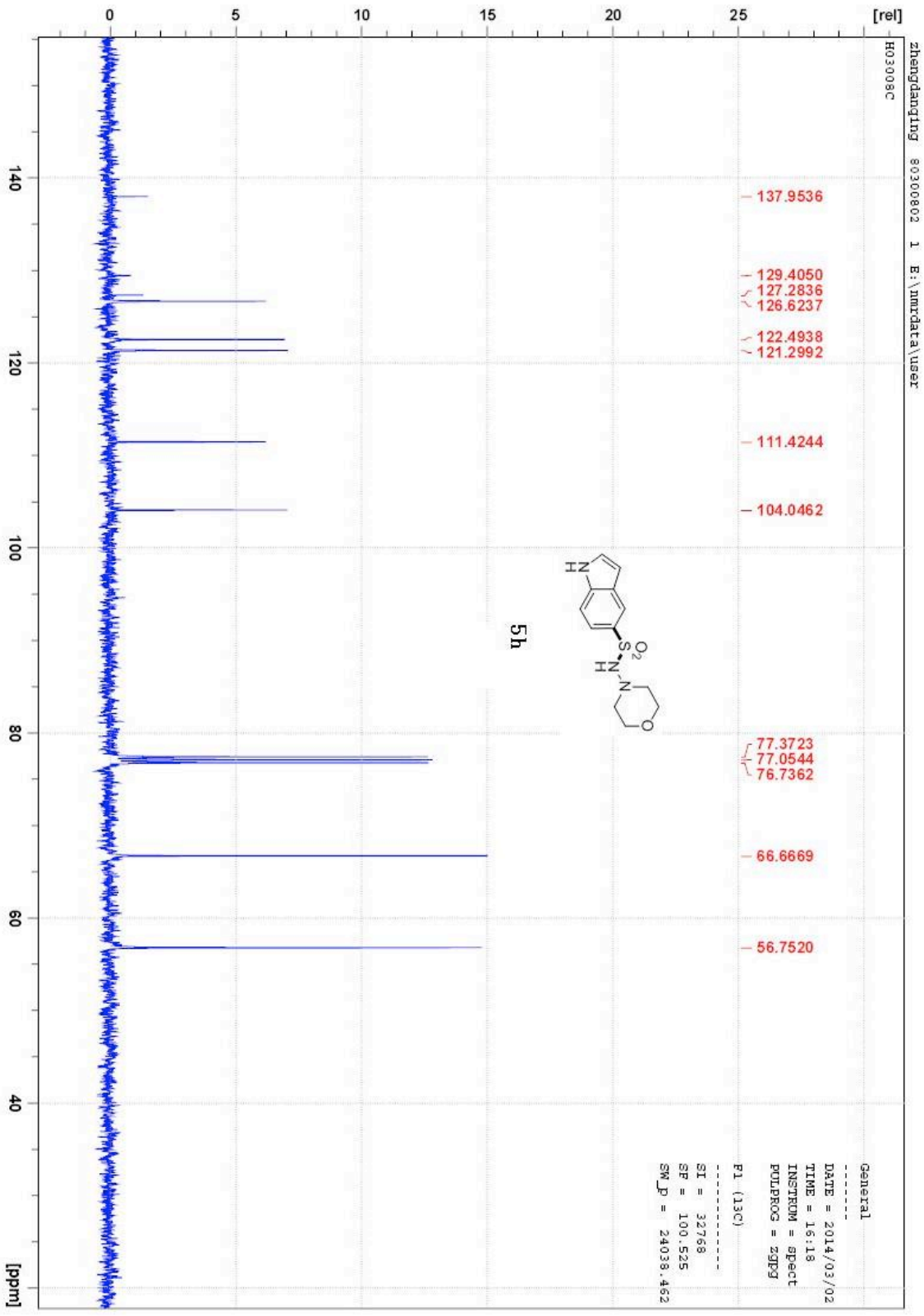
1.0673
1.0981
1.0806
1.0499
1.0268
4.3461
4.3016
8.8096
8.3118
7.7647
7.7604
7.7431
7.7388
7.4872
7.4656
7.3561
7.3487
7.3421
7.2630
6.6715
6.6660
5.5172
3.5705
3.5592
3.5475
2.5888
2.5773
2.5658
5h
General
DATE = 2014/03/02
TIME = 16:13
INSTRUM = spect
PULPROG = zg
F1 (1H)
SI = 65536
SF = 399.78
SW_p = 6009.615


zhengdanqing 80300802 1 E:\nmrdata\user
H03008C
General
DATE = 2014/03/02
TIME = 16:18
INSTRUM = spect
PULPROG = zgpg
F1 (13C)
SI = 32768
SF = 100.525
SW_p = 24038.462
137.9536
129.4050
127.2836
126.6237
122.4938
121.2992
111.4244
104.0462
77.3723
77.0544
76.7362
66.6669
56.7520
5h
[rel]
[ppm]