Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Generation of *N*-aminosulfonamides via a photo-induced fixation of sulfur dioxide into aryl/alkyl halides

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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 spectromete 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.

Computational Details: First principle density functional theory (DFT) calculations were performed with the M06-2x/6-31+G(d,p) method.[1,2] M06-2X is by far one of the most accurate DFT functionals in predicting energy barriers.[1] To account for solvation effect, the calculations were performed with the IEFPCM solvation model[3] in the CH_3CN solution with radii and non-electrostatic terms for Truhlar and coworkers' SMD solvation model.[4] All the geometry optimizations and vibrational frequency analyses were performed with solvation effect considered. Default geometry convergence criterion of Gaussian 09[5] were used. All these calculations were performed by using the Gaussian 09 quantum software package.[5]

1. Zhao,Y. & Truhlar, D. G. Comparative DFT study of van der waals complexes: Rare-gas dimers, alkaline-earth dimers, zinc dimer, and zinc-rare-gas dimers *J. Phys. Chem*. A **110**, 5121-5129 (2006).
2. Krishnan, R., Binkley, J. S., Seeger, R. & Pople, J. A. Self-consistent molecular orbital methods. XX. A basis set for correlated wave functions. *J. Chem. Phys*. **72**, 650-654 (1980).

3. Scalmani, G. & Frisch, M. J. Continuous surface charge polarizable continuum models of solvation. I. General formalism *J. Chem. Phys.* **132**, 114110 (2010).

4. Marenich, A. V., Cramer, C. J. & Truhlar, D. G. Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. *J. Phys. Chem. B* **113**, 6378-6396 (2009).

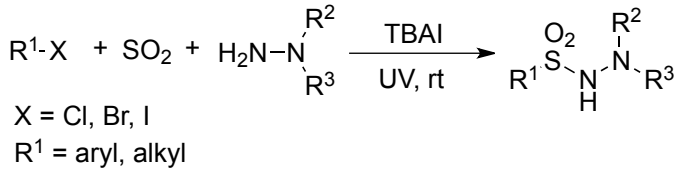
5. Gaussian 09, Revision A.02, Frisch, M. J. et al. Gaussian, Inc., Wallingford CT, **2009**.

Full citation of Gaussian 09:

Gaussian 09, Revision A.02, Frisch, M. J. et al. Gaussian, Inc., Wallingford CT, 2009.

M. J. Frisch, G. W. T., H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox; Gaussian, Inc.: Wallingford CT, 2009.

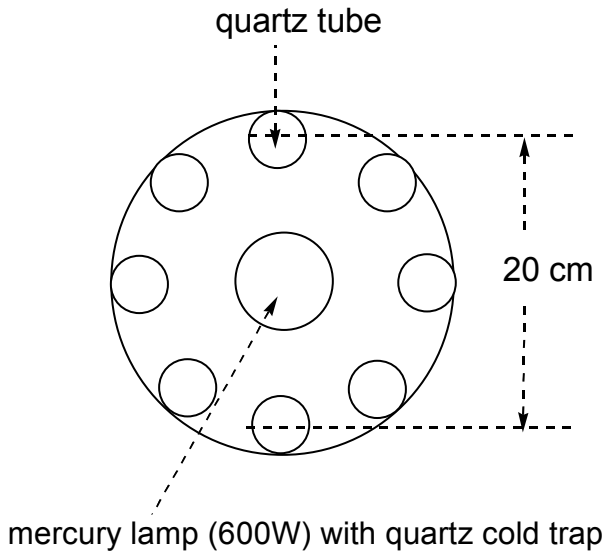
General experimental procedure for the aminosulfonylation reaction of haloalkane *with DABCO•$(SO_2)_2$ and hydrazines 2:*



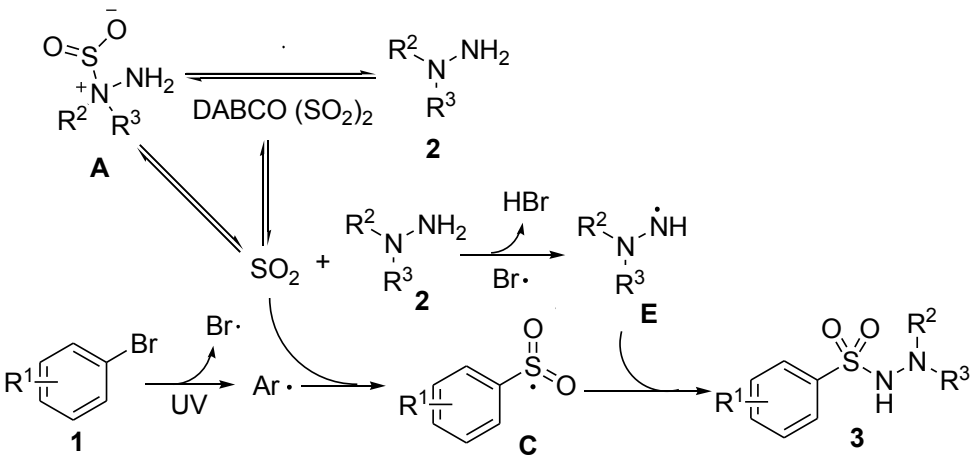
X = Cl, Br, I

R^1 = aryl, alkyl

In a quartz tube, TBAI (112 mg, 0.3 mmol) and DABCO•$(SO_2)_2$ (38.4 mg, 0.16 mmol) were added. The flask was evacuated and backfilled with N_2 three times, before a solution of aryl/alkyl halide (0.2 mmol) and hydrazine (0.3 mmol) in CH_3CN (4.0 mL) was added. The mixture, placed around the mercury lamp (purchased from Yuming, Shanghai) with a distance of 10 centimeters, was stirred under UV irradiation (0.67W cm^{-1}) for 10 hours at room temperature. After completion of reaction as indicated by TLC, the mixture was directly purified by flash column chromatograph (EtOAc/Petroleum, 1:2) to give the desired product.



Theoretical calculations:



Scheme S-1.

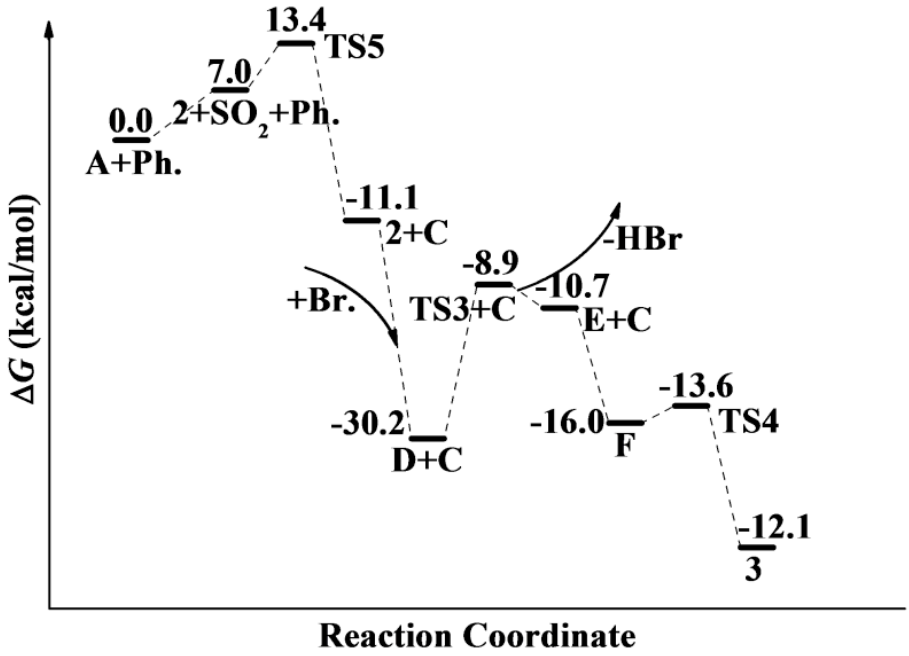
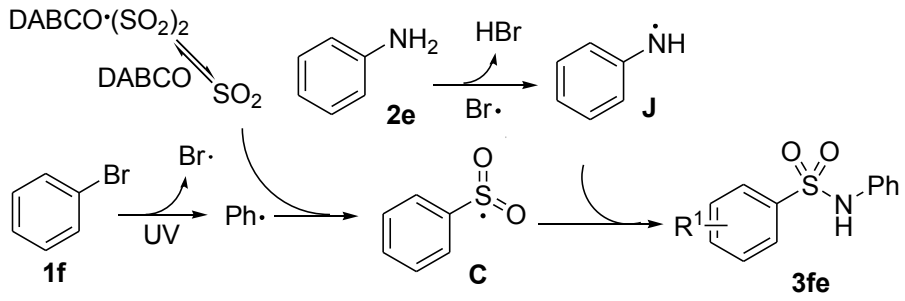


Figure S-1. Free-energy profiles in acetonitrile for the disfavored reaction pathway at 298 K calculated by the M06-2x/6-31+G(d,p) method.



Scheme S-2.

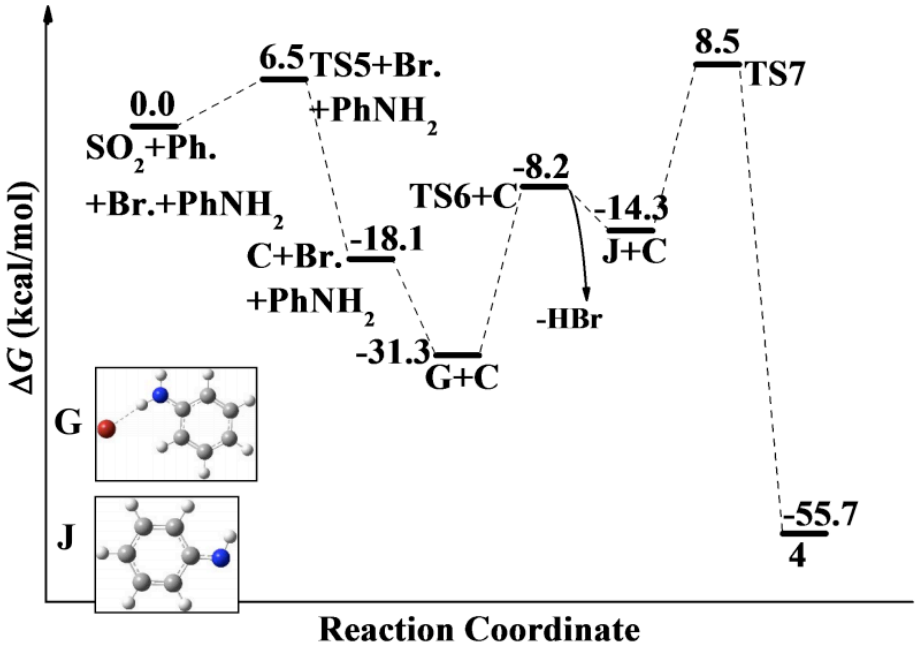


Figure S-2. Free-energy profiles in acetonitrile for the reaction of aniline at 298 K calculated by the M06-2x/6-31+G(d,p) method.

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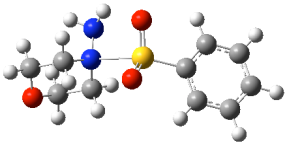

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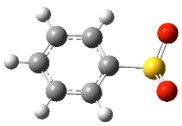

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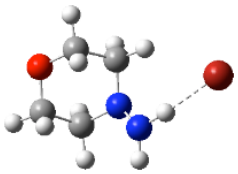

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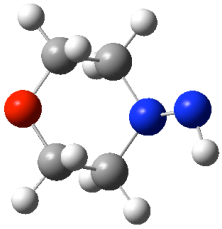

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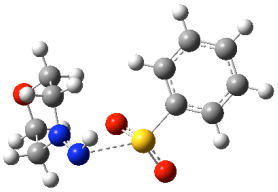

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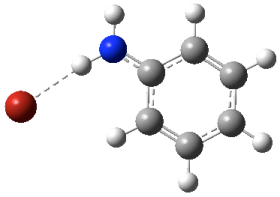

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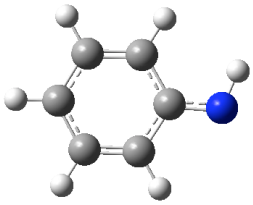

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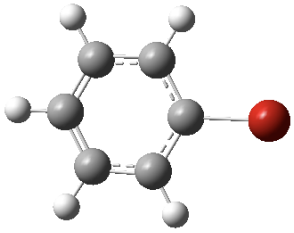

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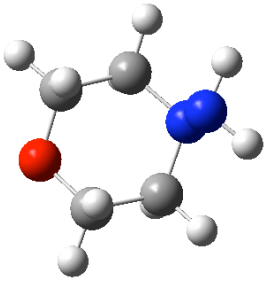

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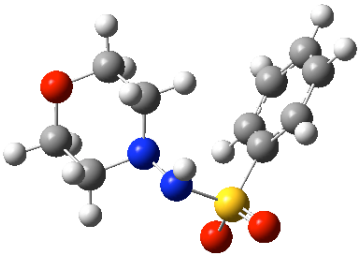

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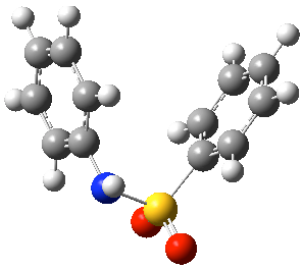

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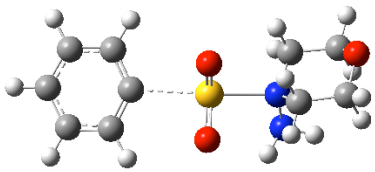
TS1



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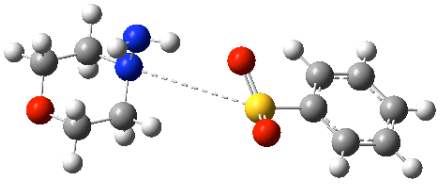
TS2



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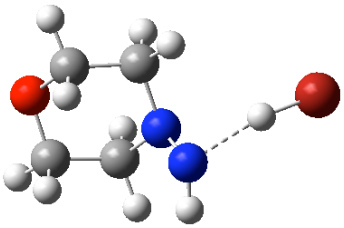
TS3



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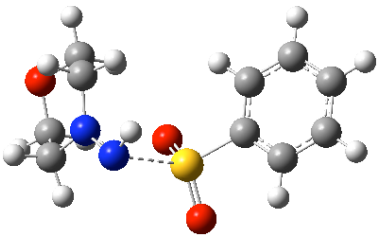
TS4



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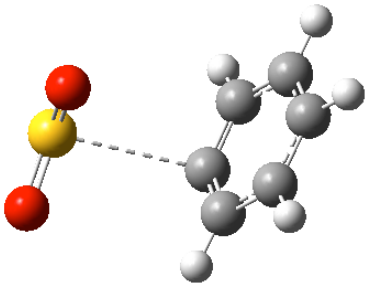
TS5



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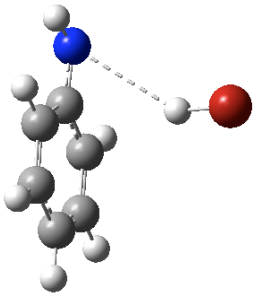
TS6



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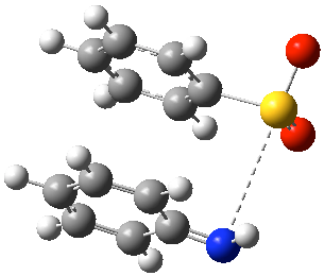
TS7



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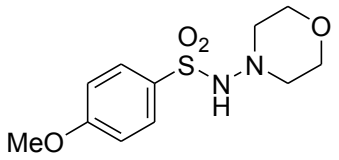
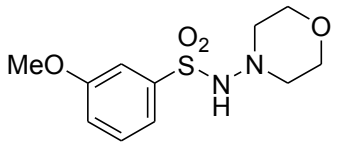


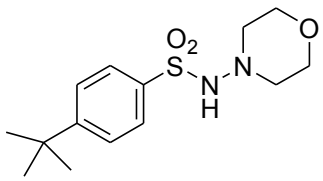
4-methoxy-*N*-morpholinobenzenesulfonamide (**3a**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 – 7.89 (m, 2H), 7.00 – 6.97 (m, 2H), 5.63 (s, 1H), 3.88 (s, 3H), 3.61 (t, *J* = 4.6 Hz, 4H), 2.62 (t, *J* = 4.6 Hz, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.3, 130.3, 130.1, 114.0, 66.7, 56.7, 55.6; HRMS (ESI) calcd for $C_{11}H_{17}N_2O_4S$: 273.0904 ($M + H^+$), found: 273.0912.



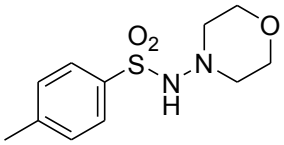
3-methoxy-*N*-morpholinobenzenesulfonamide (**3b**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 7.7 Hz, 1H), 7.50 – 7.48 (m, 1H), 7.43 (t, *J* = 8.0 Hz, 1H), 7.13 (dd, *J* = 8.2, 2.1 Hz, 1H), 5.74 (s, 1H), 3.87 (s, 3H), 3.62 (t, *J* = 4.6 Hz, 4H), 2.64 (t, *J* = 4.6 Hz, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.7, 139.8, 129.9, 120.2, 119.6, 112.6, 66.6, 56.7, 55.7; HRMS (ESI) calcd for $C_{11}H_{17}N_2O_4S$: 273.0904 ($M + H^+$), found: 273.0911.



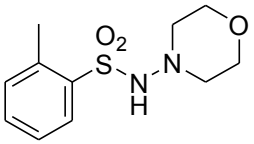
4-*tert*-butyl-*N*-morpholinobenzenesulfonamide (**3c**):

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.5 Hz, 2H), 7.52 (d, *J* = 8.5 Hz, 2H), 5.76 (s, 1H), 3.61 (t, *J* = 4.6 Hz, 4H), 2.64 (t, *J* = 4.6 Hz, 4H), 1.34 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.0, 135.6, 127.9, 125.8, 66.6, 56.7, 35.2, 31.0; HRMS (ESI) calcd for $C_{14}H_{23}N_2O_3S$: 299.1424 ($M + H^+$), found: 299.1446.



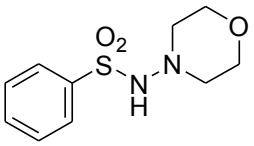
4-methyl-*N*-morpholinobenzenesulfonamide (**3d**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.2 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 5.75 (s, 1H), 3.60 (t, *J* = 4.6 Hz, 4H), 2.62 (t, *J* = 4.6 Hz, 4H), 2.44 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.0, 135.7, 129.4, 128.1, 66.6, 56.6, 21.6; HRMS (ESI) calcd for $C_{11}H_{17}N_2O_3S$: 257.0954 ($M + H^+$), found: 257.0964.



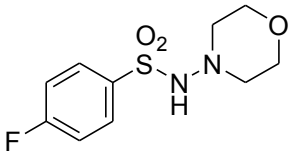
2-methyl-*N*-morpholinobenzenesulfonamide (**3e**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (dd, *J* = 7.9, 1.0 Hz, 1H), 7.48 (td, *J* = 7.5, 1.2 Hz, 1H), 7.35 (d, *J* = 7.7 Hz, 1H), 7.31 (d, *J* = 8.1 Hz, 1H), 5.75 (s, 1H), 3.57 (t, *J* = 4.6 Hz, 4H), 2.70 (s, 3H), 2.65 (t, *J* = 4.6 Hz, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.0, 136.5, 133.2, 132.3, 131.0, 126.1, 66.5, 56.7, 20.6. HRMS (ESI) calcd for $C_{11}H_{17}N_2O_3S$: 257.0954 ($M + H^+$), found: 257.0975.



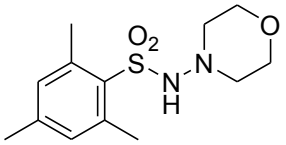
N-morpholinobenzenesulfonamide (**3f**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 – 7.97 (m, 2H), 7.63 – 7.60 (m, 1H), 7.53 (t, *J* = 7.6 Hz, 2H), 5.75 (s, 1H), 3.60 (t, *J* = 4.6 Hz, 4H), 2.62 (t, *J* = 4.6 Hz, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.6, 133.1, 128.8, 128.1, 66.6, 56.7; HRMS (ESI) calcd for $C_{10}H_{15}N_2O_3S$: 243.0698 ($M + H^+$), found: 243.0812.



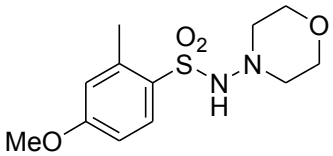
4-fluoro-*N*-morpholinobenzenesulfonamide (**3g**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (dd, *J* = 8.6, 5.1 Hz, 2H), 7.21 (t, *J* = 8.5 Hz, 2H), 5.58 (s, 1H), 3.62 (t, *J* = 4.6 Hz, 4H), 2.64 (t, *J* = 4.6 Hz, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.4 (d, *J* = 255.7 Hz), 134.6, 130.9 (d, *J* = 9.3 Hz), 116.1 (d, *J* = 22.6 Hz), 66.6, 56.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -104.30; HRMS (ESI) calcd for $C_{10}H_{14}FN_2O_3S$: 261.0704 ($M + H^+$), found: 261.0709.



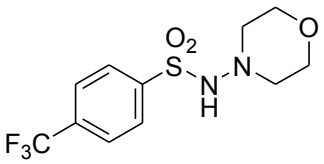
2,4,6-trimethyl-*N*-morpholinobenzenesulfonamide (**3h**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.95 (s, 2H), 5.58 (s, 1H), 3.58 (t, *J* = 4.6 Hz, 4H), 2.68 (s, 6H), 2.65 (t, *J* = 4.6 Hz, 4H), 2.31 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.7, 140.5, 132.5, 131.6, 66.8, 56.6, 23.1, 21.0; HRMS (ESI) calcd for $C_{13}H_{21}N_2O_3S$: 285.1267 ($M + H^+$), found: 285.1275.



4-methoxy-2-methyl-*N*-morpholinobenzenesulfonamide (**3i**)

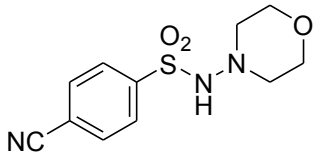
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.5 Hz, 1H), 6.82 – 6.79 (m, 2H), 5.60 (s, 1H), 3.86 (s, 3H), 3.58 (t, *J* = 4.6 Hz, 4H), 2.68 – 2.63 (m, 7H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.0, 140.3, 133.4, 128.2, 117.7, 110.7, 66.6, 56.7, 55.4, 20.9. HRMS (ESI) calcd for $C_{12}H_{18}N_2NaO_4S$: 309.0879 ($M + Na^+$), found: 309.0888.



N-morpholino-4-(trifluoromethyl)benzenesulfonamide (**3j**)

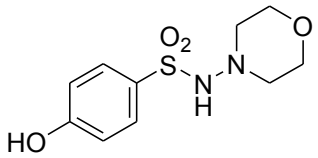
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.2 Hz, 2H), 7.81 (d, *J* = 8.3 Hz, 2H), 5.92 (s, 1H), 3.63 (t, *J* = 4.6 Hz, 4H), 2.67 (t, *J* = 4.6 Hz, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.3,

134.8 (q, *J* = 32.6 Hz), 128.6, 126.0 (d, *J* = 3.2 Hz), 123.16 (q, *J* = 273.0 Hz), 66.5, 56.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.12.



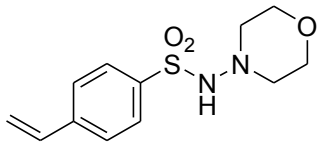
4-cyano-*N*-morpholinobenzenesulfonamide (**3k**)

^{1}H NMR (400 MHz, DMSO) δ 9.25 (s, 1H), 8.10 (d, *J* = 8.6 Hz, 2H), 8.02 (d, *J* = 8.6 Hz, 2H), 3.46 (t, *J* = 4.0 Hz, 4H), 2.49 (t, *J* = 4.0 Hz, 4H); ^{13}C NMR (101 MHz, DMSO) δ 144.0, 133.7, 128.7, 118.2, 115.8, 66.4, 56.3.



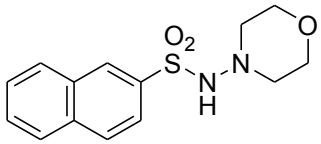
4-hydroxy-*N*-morpholinobenzenesulfonamide **(3l**)

^{1}H NMR (400 MHz, DMSO) δ 10.43 (s, 1H), 8.56 (s, 1H), 7.67 (d, *J* = 8.4 Hz, 2H), 6.90 (d, *J* = 8.4 Hz, 2H), 3.46 – 3.43 (m, 4H), 2.46 (t, *J* = 4.2 Hz, 4H); ^{13}C NMR (101 MHz, DMSO) δ 161.7, 130.3, 129.8, 115.8, 66.4, 56.3; HRMS (ESI) calcd for $C_{10}H_{15}N_2O_4S$: 259.0747 ($M + H^+$), found: 259.0765.



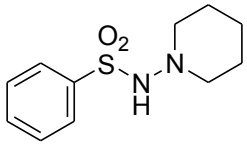
N-morpholino-4-vinylbenzenesulfonamide (**3m**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.3 Hz, 2H), 7.53 (d, *J* = 8.2 Hz, 2H), 6.76 (dd, *J* = 17.6, 10.9 Hz, 1H), 5.90 (d, *J* = 17.6 Hz, 1H), 5.65 (s, 1H), 5.45 (d, *J* = 10.9 Hz, 1H), 3.61 (t, *J* = 4.2 Hz, 4H), 2.64 (t, *J* = 4.2 Hz, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.3, 137.5, 135.4, 128.5, 126.5, 117.6, 66.7, 56.8. HRMS (ESI) calcd for $C_{12}H_{16}N_2NaO_3S$: 291.0774 ($M + Na^+$), found: 291.0769.



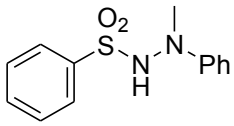
N-morpholinonaphthalene-2-sulfonamide (**3n**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56 (s, 1H), 8.00 – 7.91 (m, 4H), 7.69 – 7.60 (m, 2H), 5.78 (s, 1H), 3.58 (t, *J* = 4.6 Hz, 4H), 2.64 (t, *J* = 4.6 Hz, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 135.6, 135.0, 132.0, 129.7, 129.3, 129.0, 129.0, 127.9, 127.5, 123.1, 66.6, 56.8; HRMS (ESI) calcd for $C_{14}H_{17}N_2O_3S$: 293.0954 ($M + H^+$), found: 293.0960.



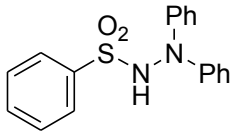
N-(piperidin-1-yl)benzenesulfonamide (**3o**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 – 7.98 (m, 2H), 7.63 – 7.59 (m, 1H), 7.55 – 7.51 (m, 2H), 5.52 (s, 1H), 2.54 (t, *J* = 4.6 Hz, 4H), 1.54 – 1.48 (m, 4H), 1.34 – 1.27 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.8, 132.9, 128.6, 128.1, 57.7, 25.6, 23.0; HRMS (ESI) calcd for $C_{11}H_{17}N_2O_2S$: 241.1005 ($M + H^+$), found: 241.1026.



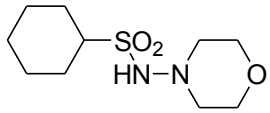
N'-methyl-*N*'-phenylbenzenesulfonohydrazide (**3p**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 7.5 Hz, 2H), 7.59 (t, *J* = 7.3 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 2H), 7.15 (t, *J* = 7.8 Hz, 2H), 6.87 – 6.81 (m, 3H), 6.32 (s, 1H), 2.96 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.6, 138.6, 133.3, 129.1, 128.9, 128.1, 120.9, 114.3, 42.7; HRMS (ESI) calcd for $C_{13}H_{15}N_2O_2S$: 263.0849 ($M + H^+$), found: 263.0849.



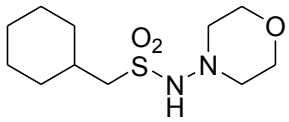
N',*N'*-diphenylbenzenesulfonohydrazide (**3q**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 – 7.74 (m, 2H), 7.44 (t, *J* = 7.5 Hz, 1H), 7.30 (t, *J* = 7.8 Hz, 2H), 7.15 (t, *J* = 7.9 Hz, 4H), 7.08 (s, 1H), 7.00 – 6.95 (m, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.8, 138.6, 133.0, 129.0, 128.7, 128.2, 124.0, 120.7; HRMS (ESI) calcd for $C_{18}H_{16}N_2NaO_2S$: 347.0825 ($M + Na^+$), found: 347.0841.



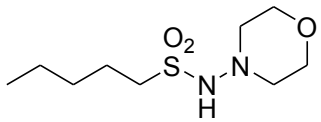
N-morpholinocyclohexanesulfonamide (**7a**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.30 (s, 1H), 3.76 (t, *J* = 4.6 Hz, 4H), 3.19 – 3.10 (m, 1H), 2.89 – 2.87 (m, 4H), 2.18 (d, *J* = 11.7 Hz, 2H), 1.93 – 1.89 (m, 2H), 1.72 (d, *J* = 11.2 Hz, 1H), 1.61 – 1.51 (m, 2H), 1.35 – 1.21 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 66.6, 58.5, 57.5, 26.2, 25.2, 25.1; HRMS (ESI) calcd for $C_{10}H_{20}N_2NaO_3S$: 271.1087 ($M + Na^+$), found: 271.1105.



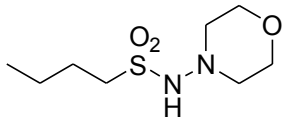
cyclohexyl-*N*-morpholinomethanesulfonamide (**7b**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.43 (s, 1H), 3.76 (t, *J* = 4.6 Hz, 4H), 3.04 (d, *J* = 6.0 Hz, 2H), 2.90 – 2.86 (m, 4H), 2.02 – 1.95 (m, 3H), 1.75 – 1.64 (m, 3H), 1.37 – 1.25 (m, 2H), 1.22 – 1.04 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 66.6, 57.4, 56.7, 33.4, 33.0, 25.8, 25.8; HRMS (ESI) calcd for $C_{11}H_{22}N_2NaO_3S$: 285.1243 ($M + Na^+$), found: 285.1249.



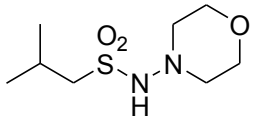
N-morpholinopentane-1-sulfonamide (**7c**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.50 (s, 1H), 3.76 (t, *J* = 4.6 Hz, 4H), 3.14 (t, *J* = 8.0 Hz, 2H), 2.90 – 2.87 (m, 4H), 1.86 – 1.79 (m, 2H), 1.44 – 1.33 (m, 4H), 0.92 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 66.6, 57.3, 50.0, 30.3, 22.9, 22.1, 13.7; HRMS (ESI) calcd for $C_9H_{20}N_2NaO_3S$: 259.1087 ($M + Na^+$), found: 259,1088.



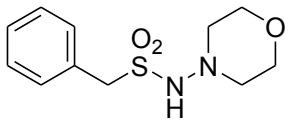
N-morpholinobutane-1-sulfonamide (**7d**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.42 (s, 1H), 3.76 (t, *J* = 4.6 Hz, 4H), 3.15 (t, *J* = 8.0 Hz, 2H), 2.90 – 2.87 (m, 4H), 1.85 – 1.76 (m, 2H), 1.52 – 1.43 (m, 2H), 0.96 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 66.6, 57.4, 49.8, 25.3, 21.6, 13.6; HRMS (ESI) calcd for $C_8H_{18}N_2NaO_3S$: 245.0930 (M + Na^+), found: 245.0932.



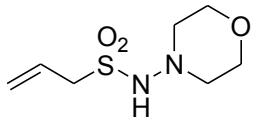
2-methyl-*N*-morpholinopropane-1-sulfonamide (**7e**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.45 (s, 1H), 3.76 (t, *J* = 4.6 Hz, 4H), 3.05 (d, *J* = 6.6 Hz, 2H), 2.90 – 2.87 (m, 4H), 2.42 – 2.34 (m, 1H), 1.12 (d, *J* = 6.7 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 66.6, 57.7, 57.4, 24.5, 22.6; HRMS (ESI) calcd for $C_8H_{18}N_2NaO_3S$: 245.0930 (M + Na^+), found: 245.0930.



N-morpholino(phenyl)methanesulfonamide (**7f**)

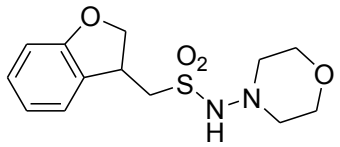
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.36 (m, 5H), 5.31 (s, 1H), 4.39 (s, 2H), 3.75 (t, *J* = 4.6 Hz, 4H), 2.85 (t, *J* = 4.6 Hz, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 130.7, 128.8, 128.7, 128.4, 66.6, 57.4, 56.3. HRMS (ESI) calcd for $C_{11}H_{16}N_2NaO_3S$: 279.0774 (M + Na^+), found: 279.0764.



N-morpholinoprop-2-ene-1-sulfonamide (**7g**)

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.96 – 5.86 (m, 1H), 5.45 – 5.38 (m, 3H), 3.90 (d, *J* = 7.1 Hz, 2H), 3.76 (t, *J* = 4.6 Hz, 4H), 2.91 – 2.88 (m, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ

125.5, 123.7, 66.6, 57.4, 54.5; HRMS (ESI) calcd for $C_7H_{14}N_2NaO_3S$: 229.0617 (M + Na^+), found: 229.0618.

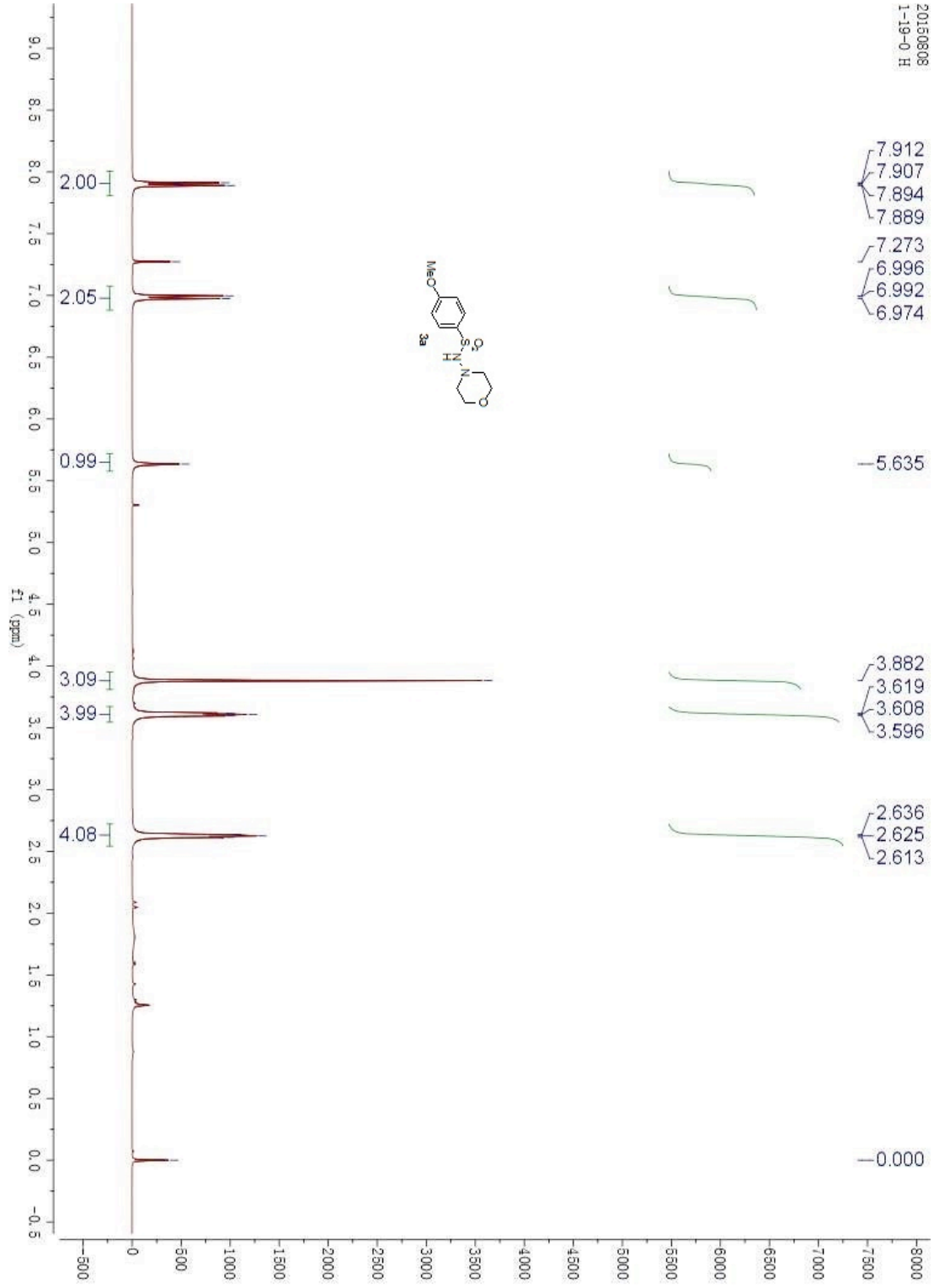


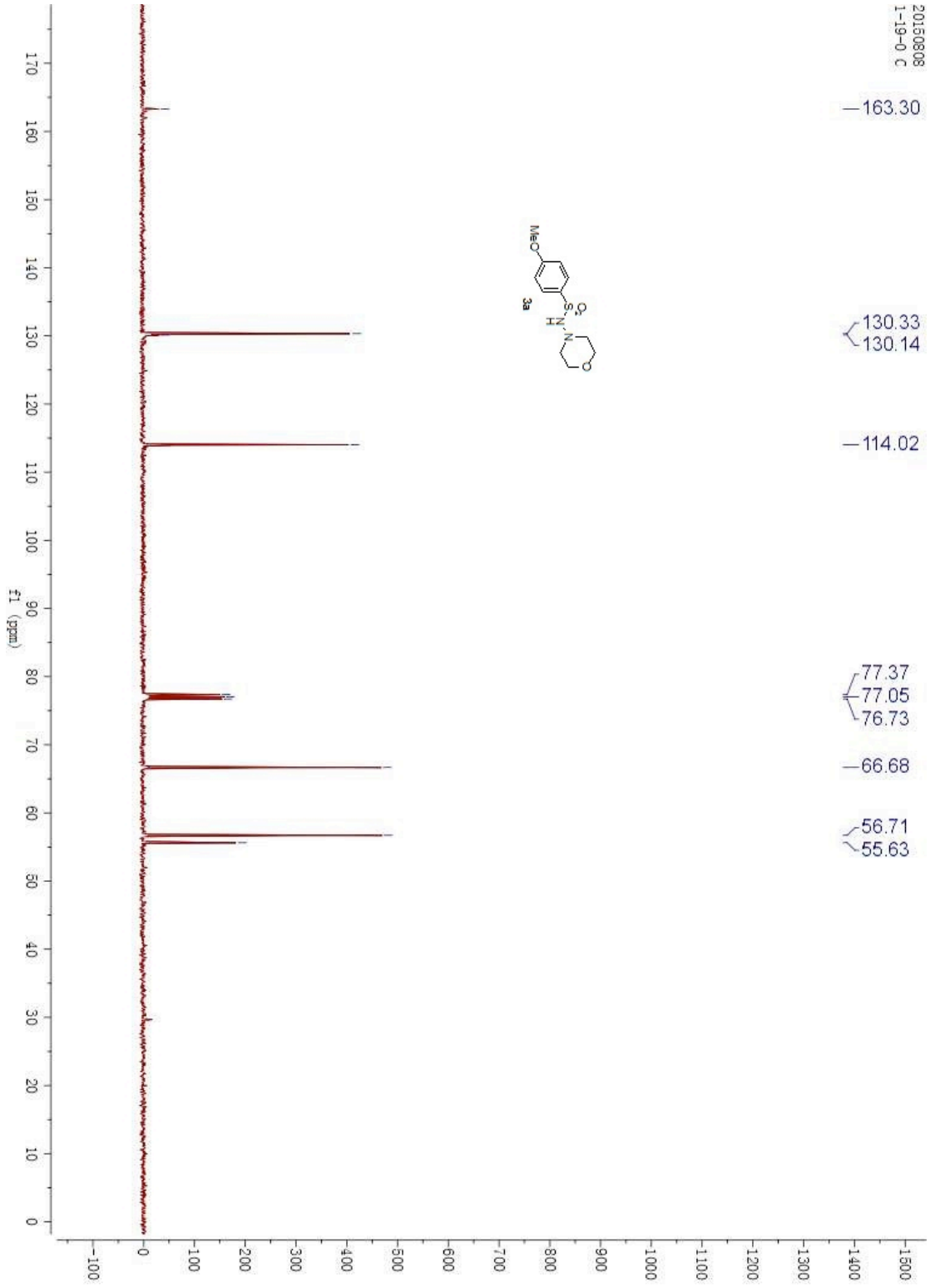
(2,3-dihydrobenzofuran-3-yl)-*N*-morpholinomethanesulfonamide (**9**)

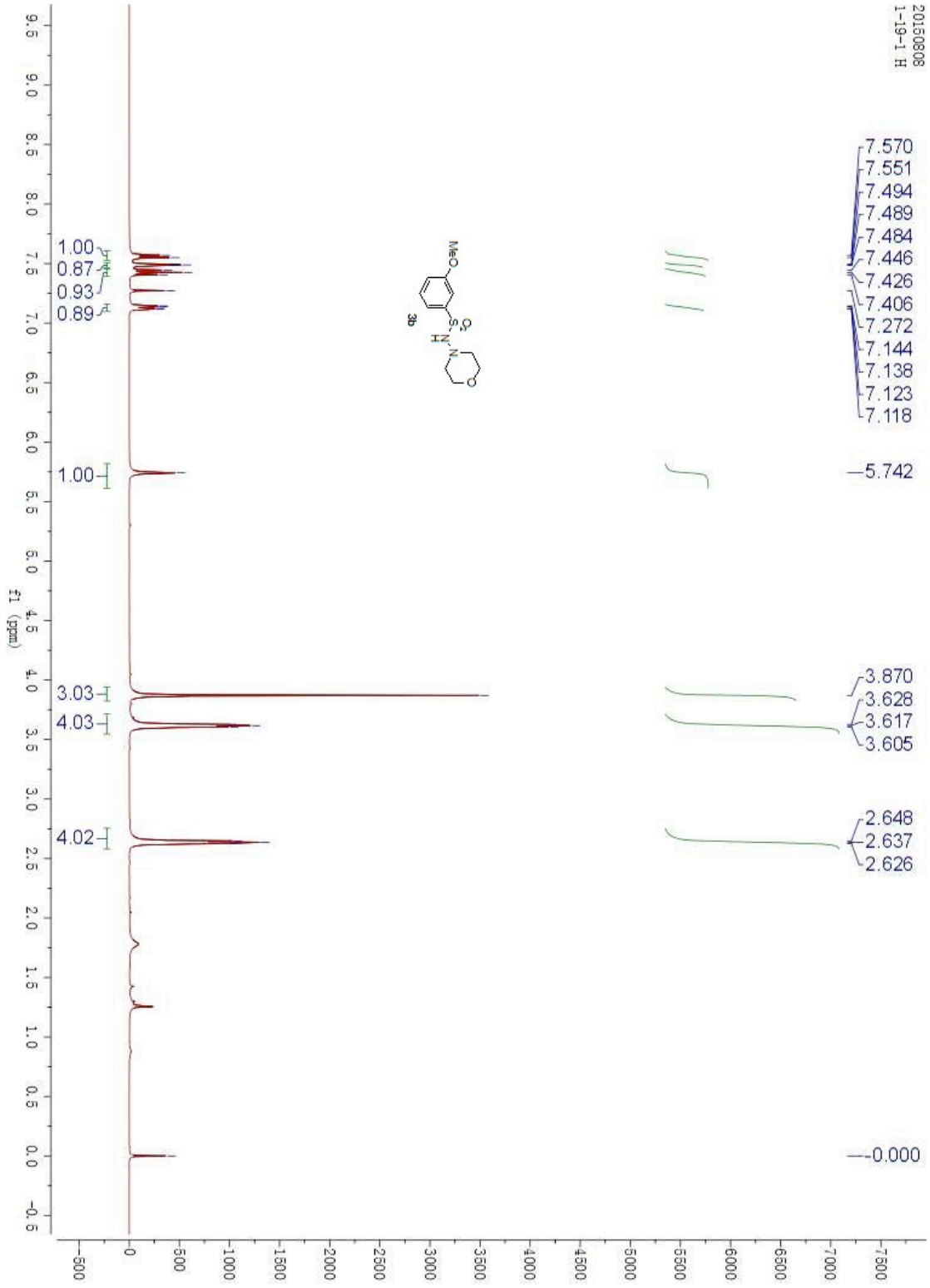
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19 (t, *J* = 7.3 Hz, 2H), 6.90 (t, *J* = 7.4 Hz, 1H), 6.84 (d, *J* = 8.3 Hz, 1H), 5.53 (s, 1H), 4.74 (t, *J* = 9.2 Hz, 1H), 4.60 (dd, *J* = 9.6, 6.1 Hz, 1H), 4.08 – 4.00 (m, 1H), 3.77 (t, *J* = 4.6 Hz, 4H), 3.60 (dd, *J* = 14.2, 3.0 Hz, 1H), 3.33 (dd, *J* = 14.1, 10.8 Hz, 1H), 2.94 – 2.86 (m, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.7, 129.4, 127.0, 124.2, 120.9, 110.1, 75.9, 66.5, 57.4, 54.2, 37.4; HRMS (ESI) calcd for $C_{13}H_{19}N_2O_4S$: 299.1060 (M + H^+), found: 299.1092.

References：

1. Nguyen, B., Emmet, E. J. & Willis, M. C. Palladium-catalyzed aminosulfonylation of aryl halides. *J. Am. Chem. Soc.* **132**, 16372-16373 (2010).
2. Ye, S. & Wu, J. A palladium-catalyzed three-component coupling of arylboronic acids, sulfur dioxide and hydrazines. *Chem. Commun*. **48**, 7753-7755 (2012).
3. Ye, S. & Wu, J. A palladium-catalyzed reaction of aryl halides, potassium metabisulfite, and hydrazines. *Chem. Commun*. **48**, 10037-10039 (2012).
4. Zheng, D. An, Y., Li, Z. & Wu, J. Metal-free aminosulfonylation of aryldiazonium tetrafluoroborates with $DABCO^{\cdot}(SO_2)_2$ and Hydrazines *Angew. Chem. Int. Ed*. **53**, 2451-2454 (2014).


20160808
1-19-0 H
7.912
7.907
7.894
7.889
7.273
6.996
6.992
6.974
5.635
3.882
3.619
3.608
3.596
2.636
2.625
2.613
0.000
2.00
2.05
0.99
3.09
3.99
4.08
MeO
3a
f1 (ppm)


20150808
1-19-0 C
163.30
130.33
130.14
114.02
77.37
77.05
76.73
66.68
56.71
55.63
MeO
3a
f1 (ppm)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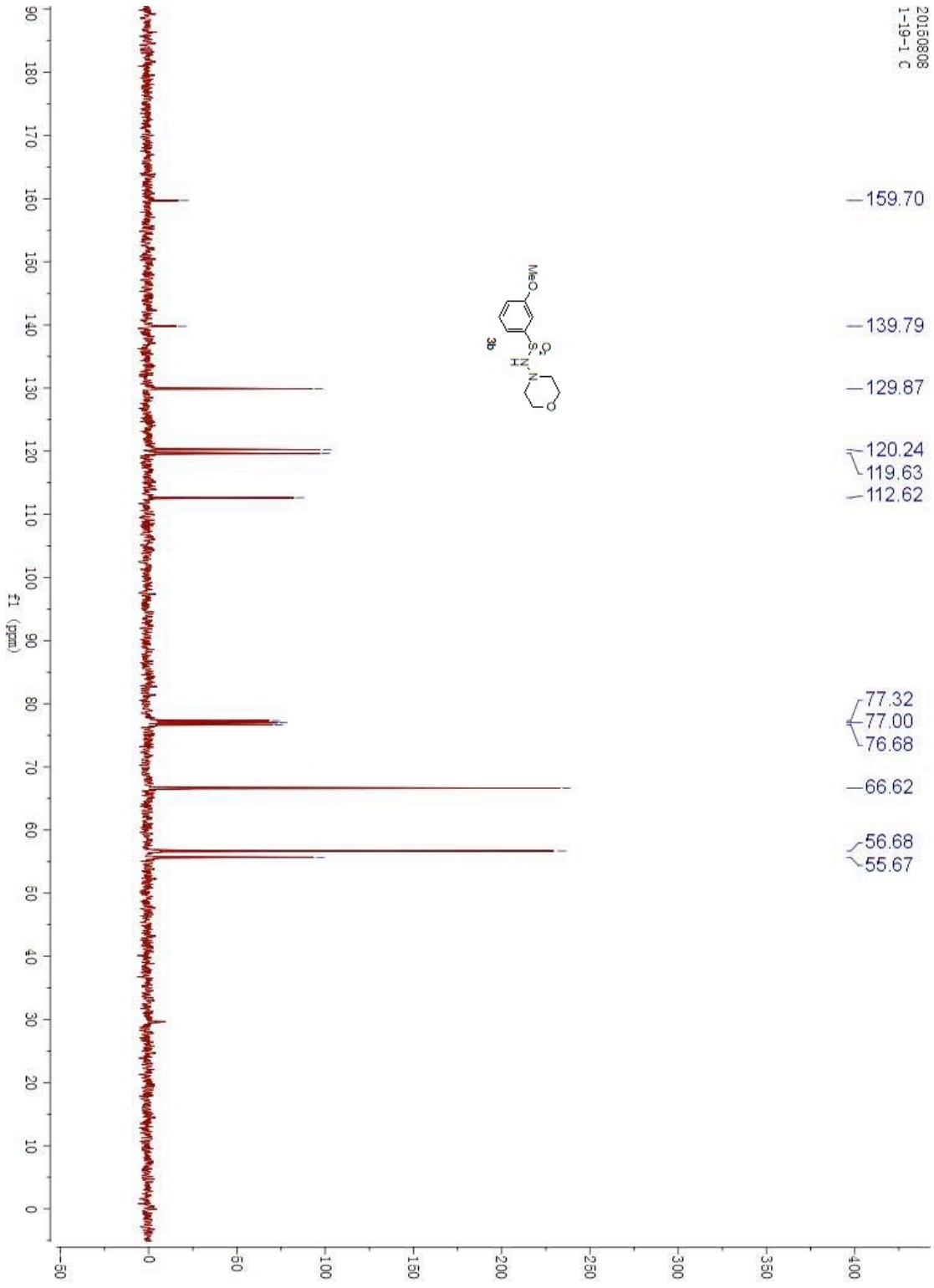
1-19-1 H
7.570
7.551
7.494
7.489
7.484
7.446
7.426
7.406
7.272
7.144
7.138
7.123
7.118
5.742
3.870
3.628
3.617
3.605
2.648
2.637
2.626
0.000
1.00
0.87
0.93
0.89
1.00
3.03
4.03
4.02
MeO
3b
f1 (ppm)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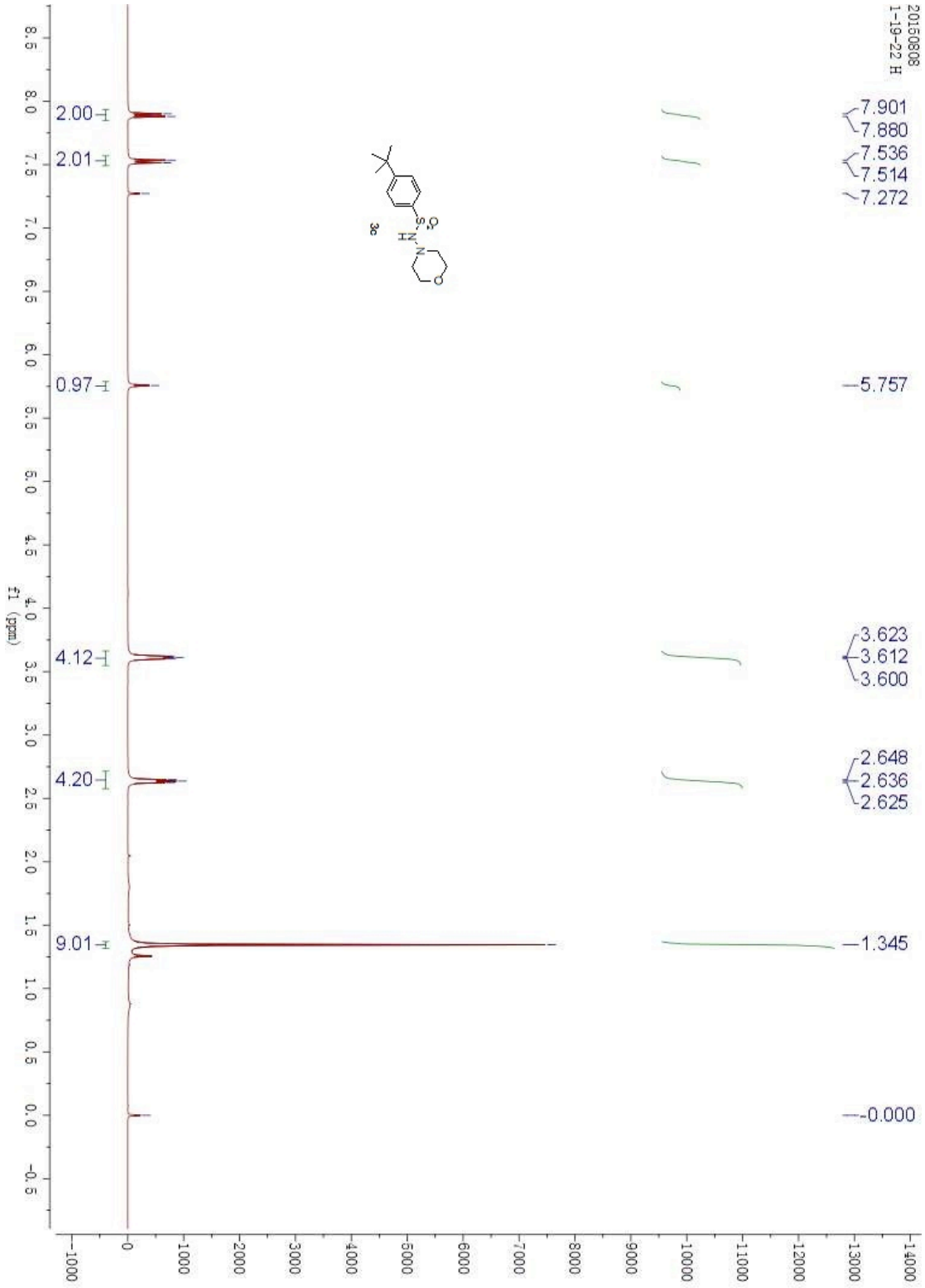
1-19-1 C
159.70
139.79
129.87
120.24
119.63
112.62
77.32
77.00
76.68
66.62
56.68
55.67
MeO
3b
f1 (ppm)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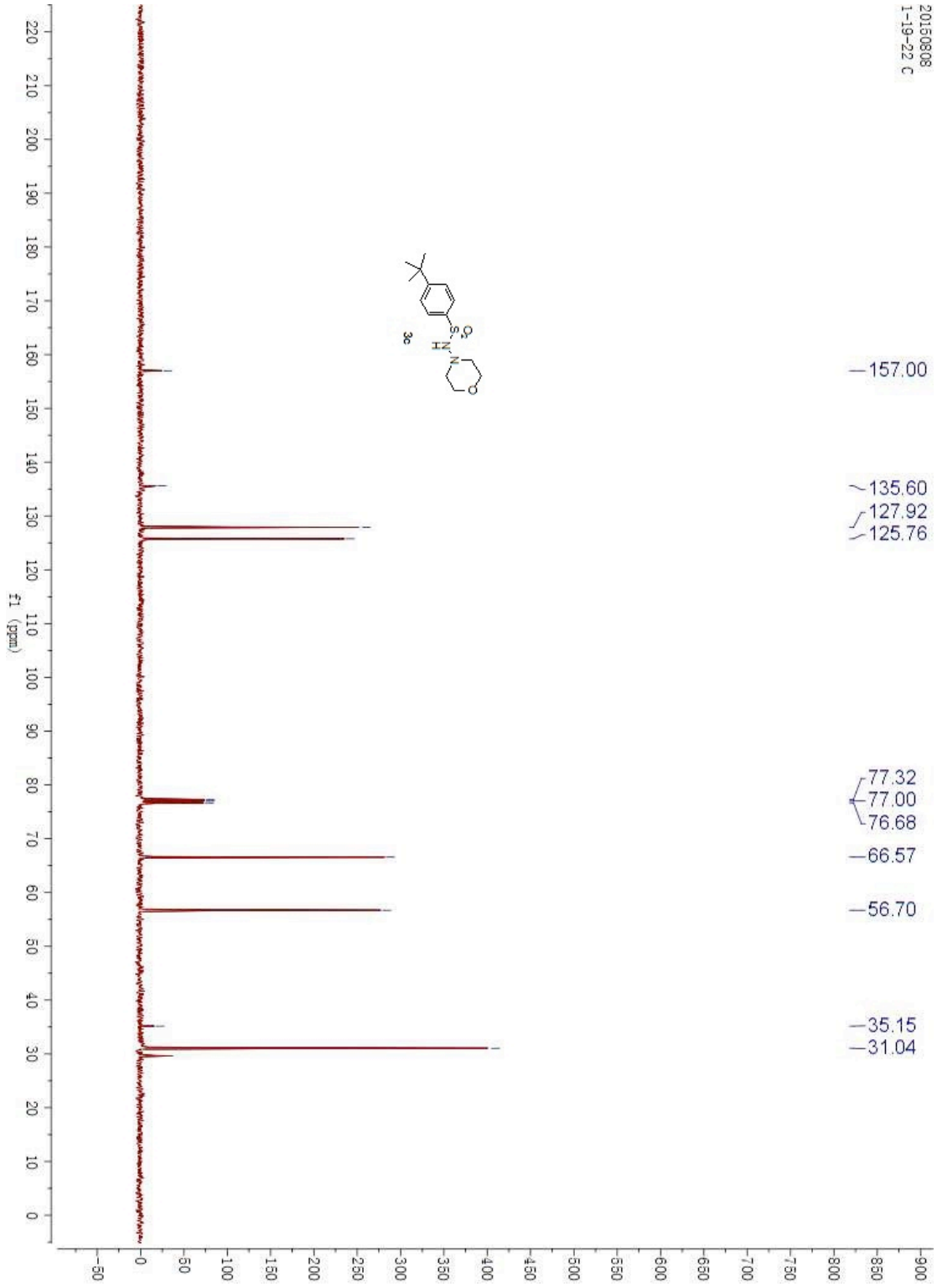
1-19-22 H
7.901
7.880
7.536
7.514
7.272
5.757
3.623
3.612
3.600
2.648
2.636
2.625
1.345
0.000
2.00
2.01
0.97
4.12
4.20
9.01
3e
f1 (ppm)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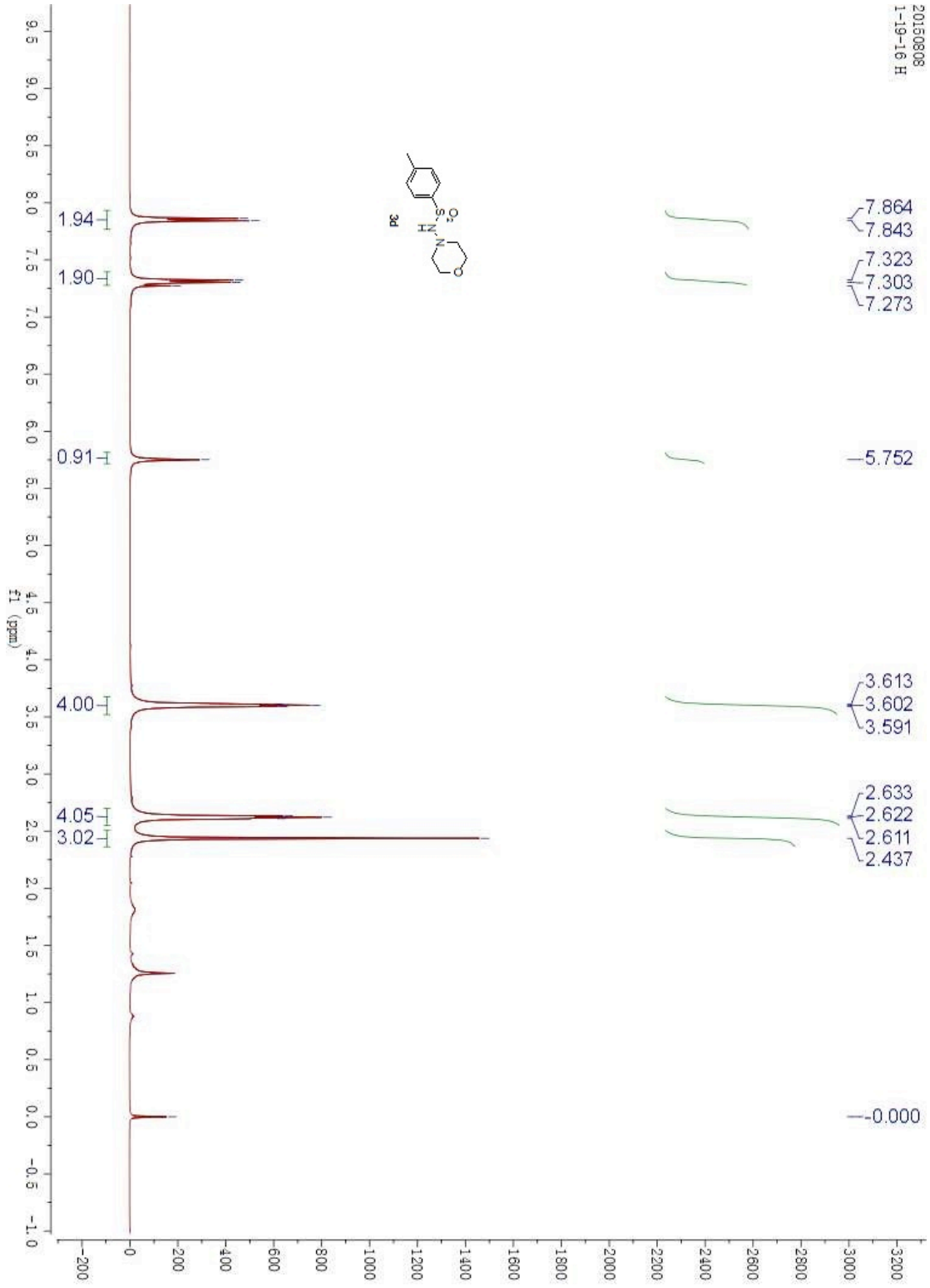
1-19-22 C
3e
157.00
135.60
127.92
125.76
77.32
77.00
76.68
66.57
56.70
35.15
31.04
f1 (ppm)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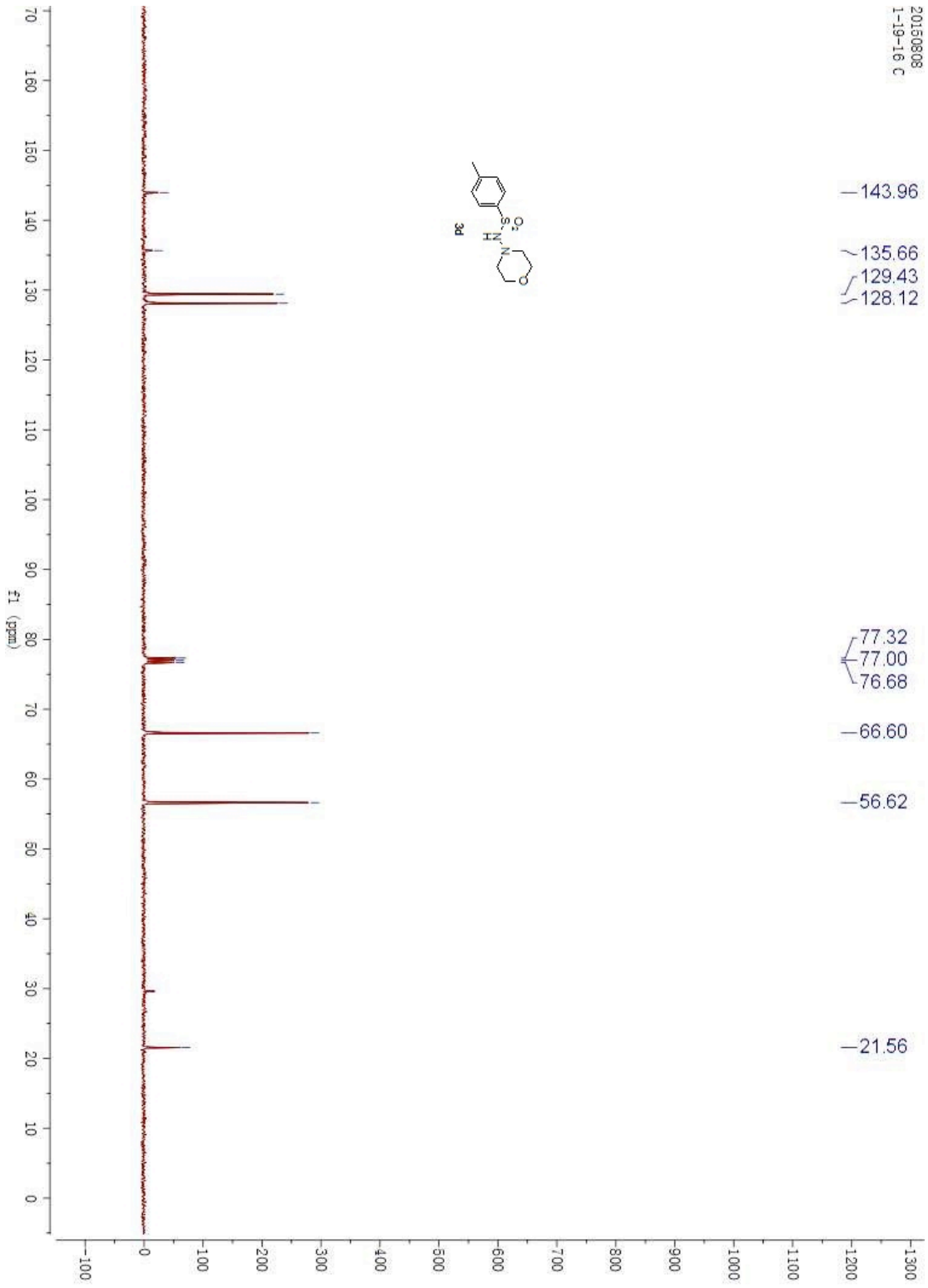
7.843
7.323
7.303
7.273
5.752
3.613
3.602
3.591
2.633
2.622
2.611
2.437
0.000
1.94
1.90
0.91
4.00
4.05
3.02
f1 (ppm)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1-19-16 C
3d
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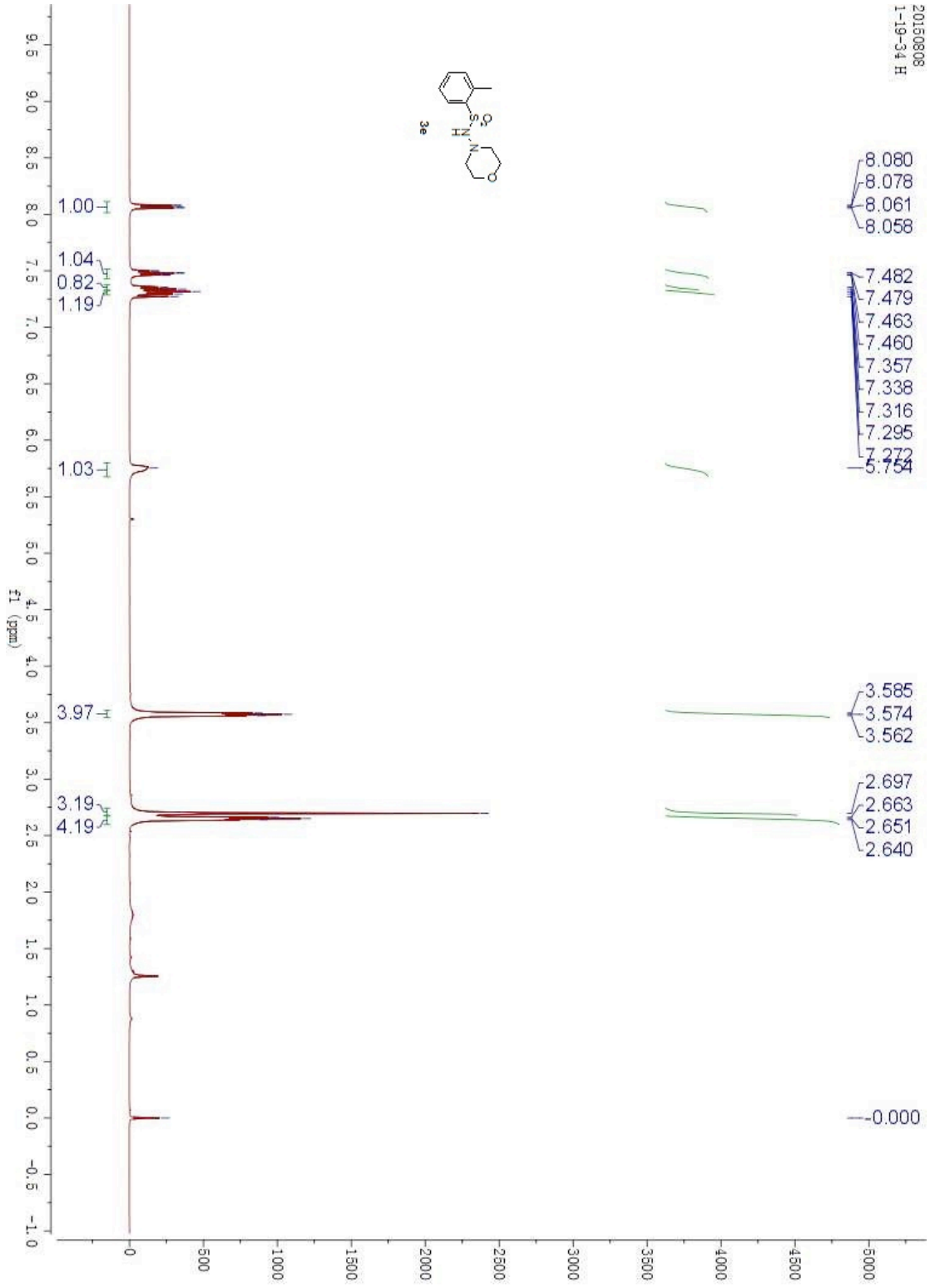
135.66
129.43
128.12
77.32
77.00
76.68
66.60
56.62
21.56
f1 (ppm)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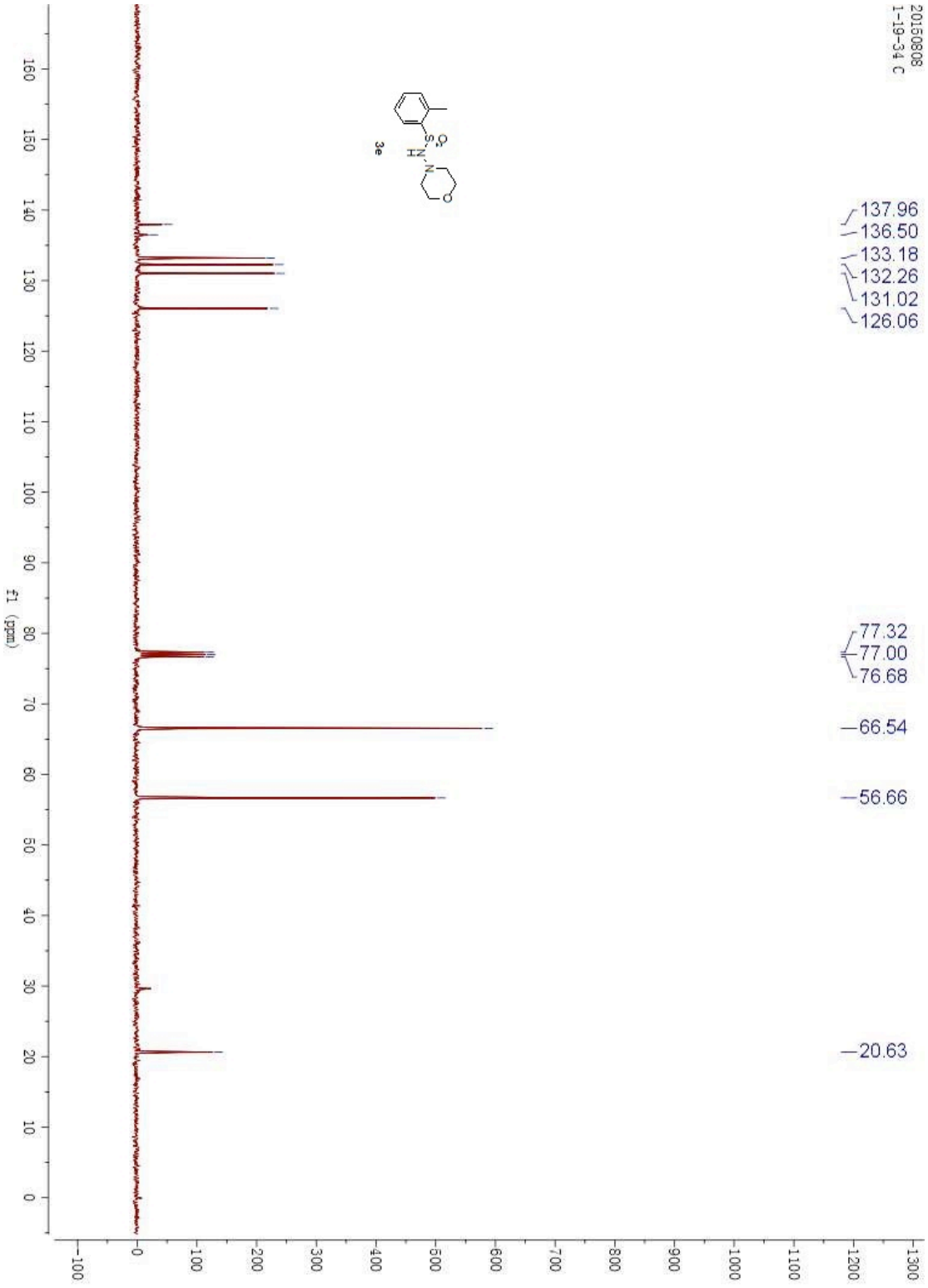
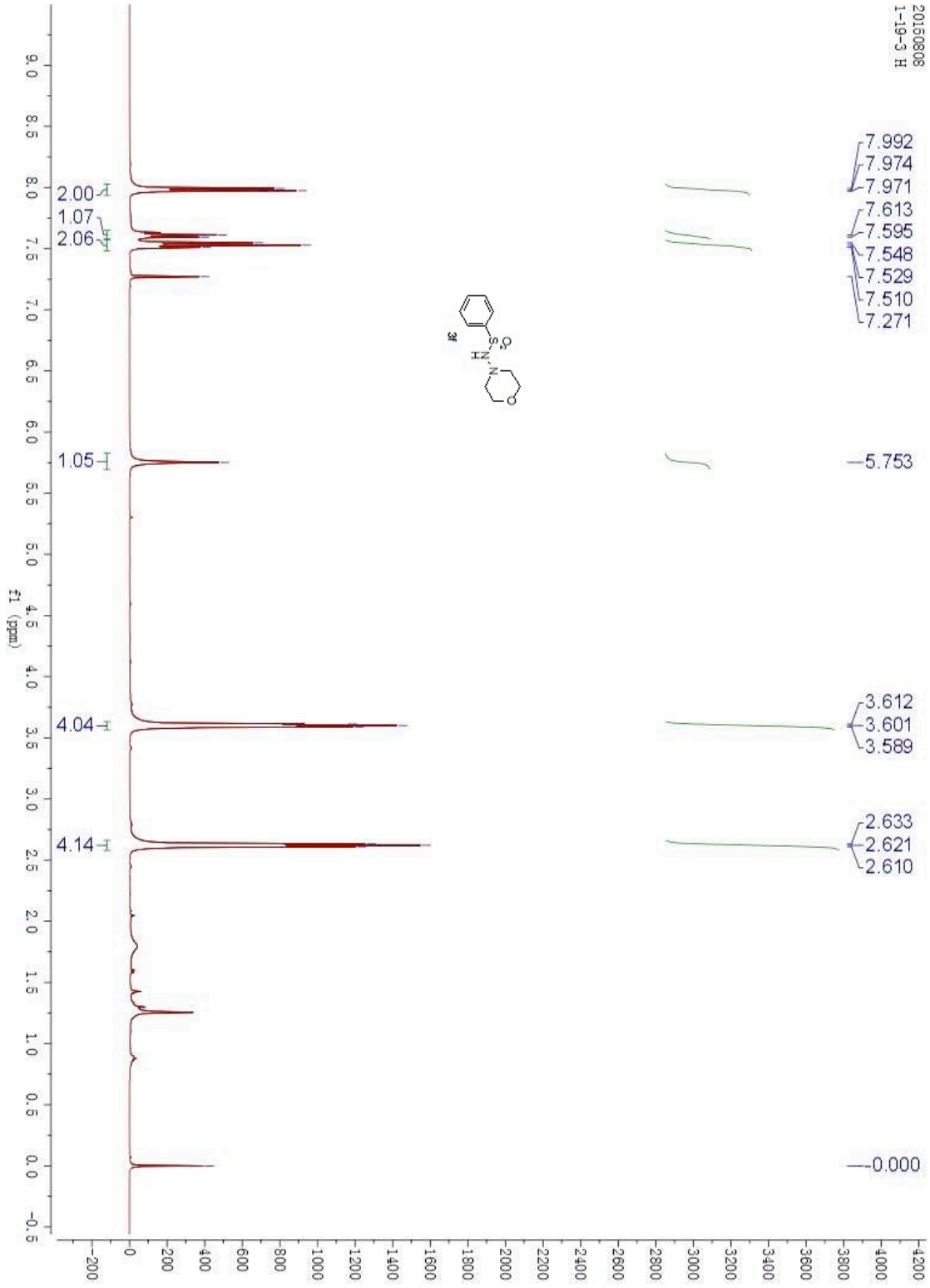
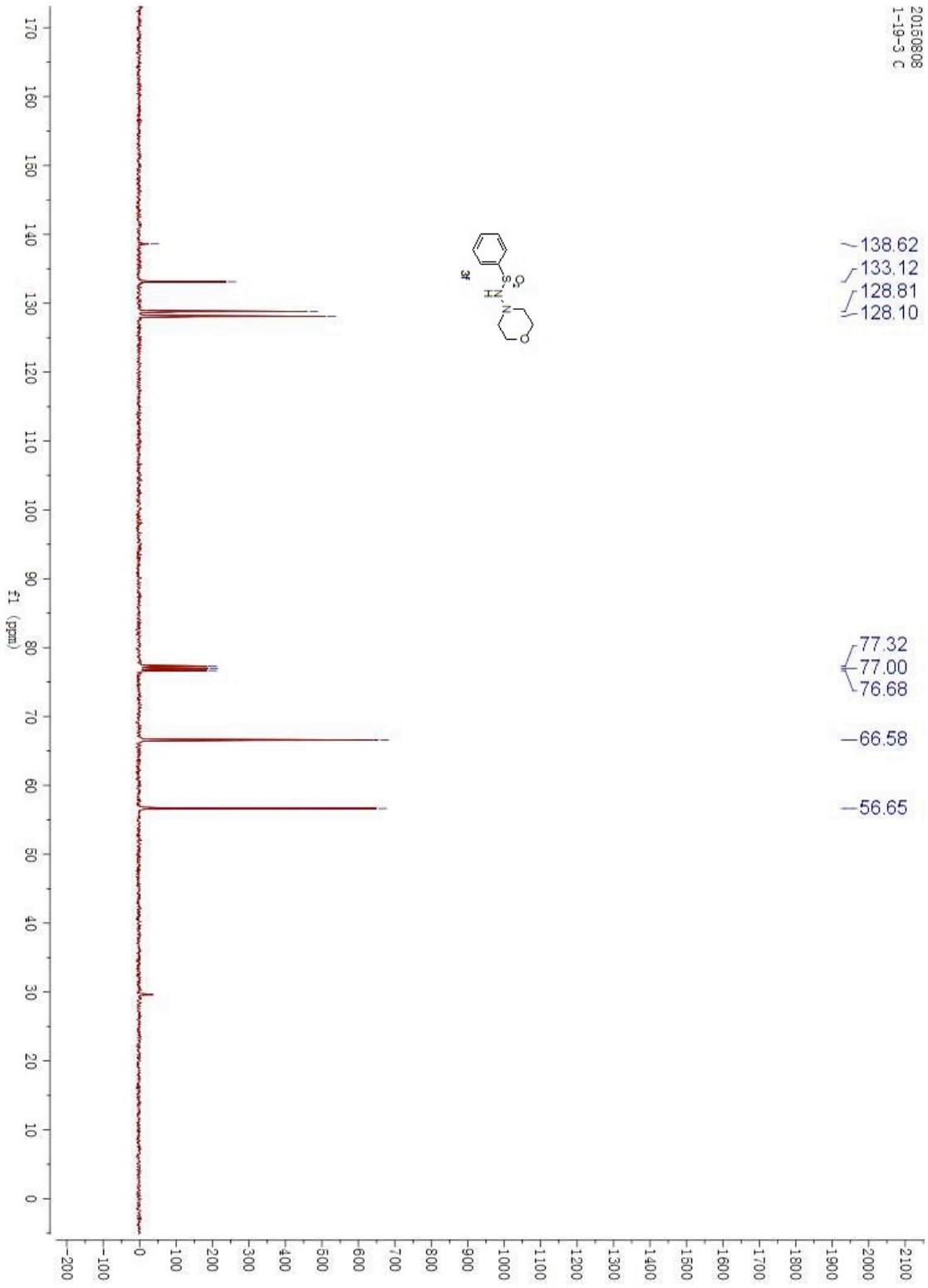
1-19-34 H
3e
8.080
8.078
8.061
8.058
7.482
7.479
7.463
7.460
7.357
7.338
7.316
7.295
7.272
5.754
3.585
3.574
3.562
2.697
2.663
2.651
2.640
0.000
1.00
1.04
0.82
1.19
1.03
3.97
3.19
4.19
f1 (ppm)


20150808
1-19-34 C
137.96
136.50
133.18
132.26
131.02
126.06
77.32
77.00
76.68
66.54
56.66
20.63
3e
f1 (ppm)


20150808
1-19-3 H
7.992
7.974
7.971
7.613
7.595
7.548
7.529
7.510
7.271
5.753
3.612
3.601
3.589
2.633
2.621
2.610
0.000
2.00
1.07
2.06
1.05
4.04
4.14
3f
f1 (ppm)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1-19-3 C
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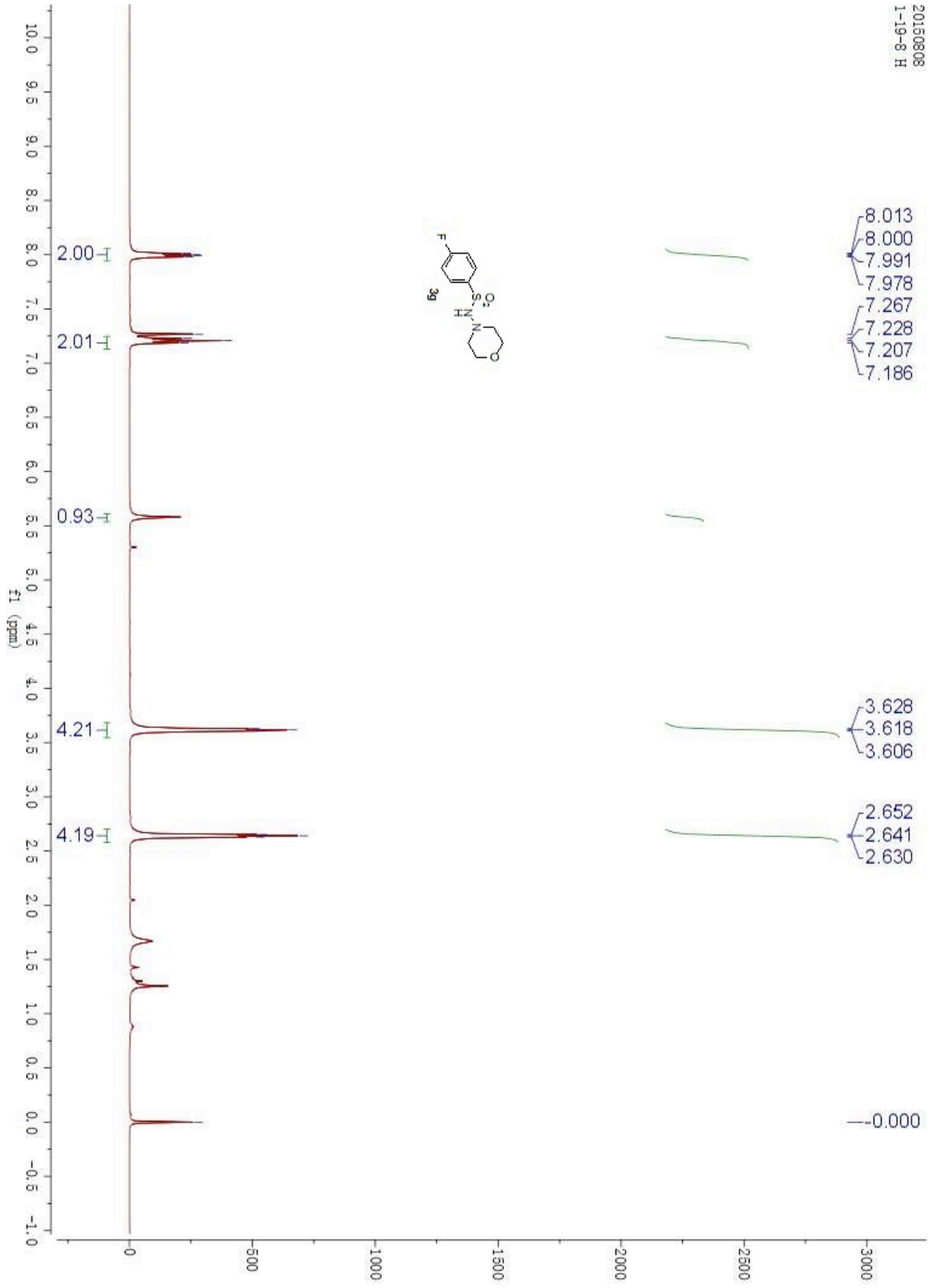
128.81
128.10
77.32
77.00
76.68
66.58
56.65
f1 (ppm)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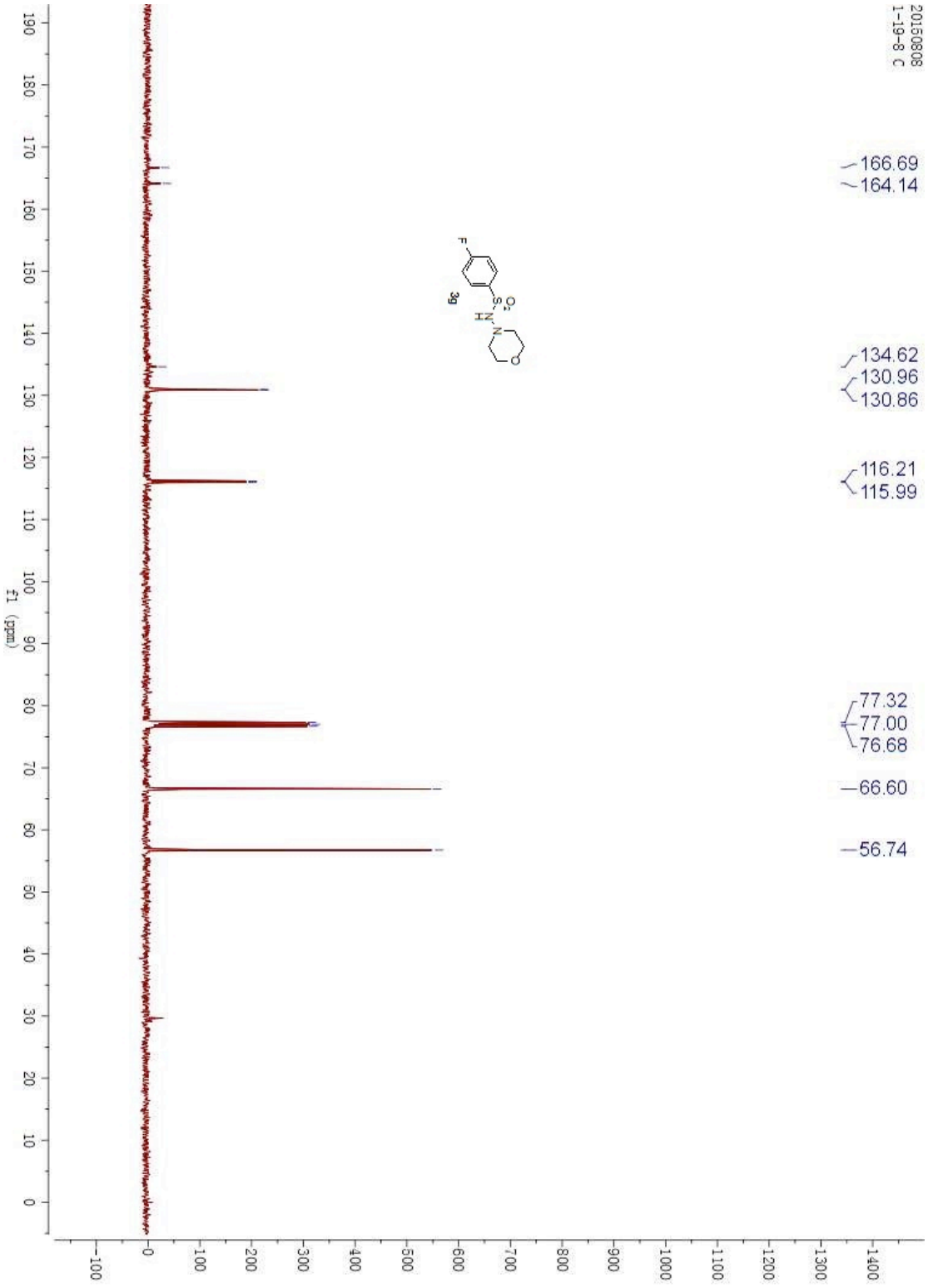
8.000
7.991
7.978
7.267
7.228
7.207
7.186
3.628
3.618
3.606
2.652
2.641
2.630
-0.000
2.00
2.01
0.93
4.21
4.19
3g
f1 (ppm)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1-19-8 C
166.69
164.14
134.62
130.96
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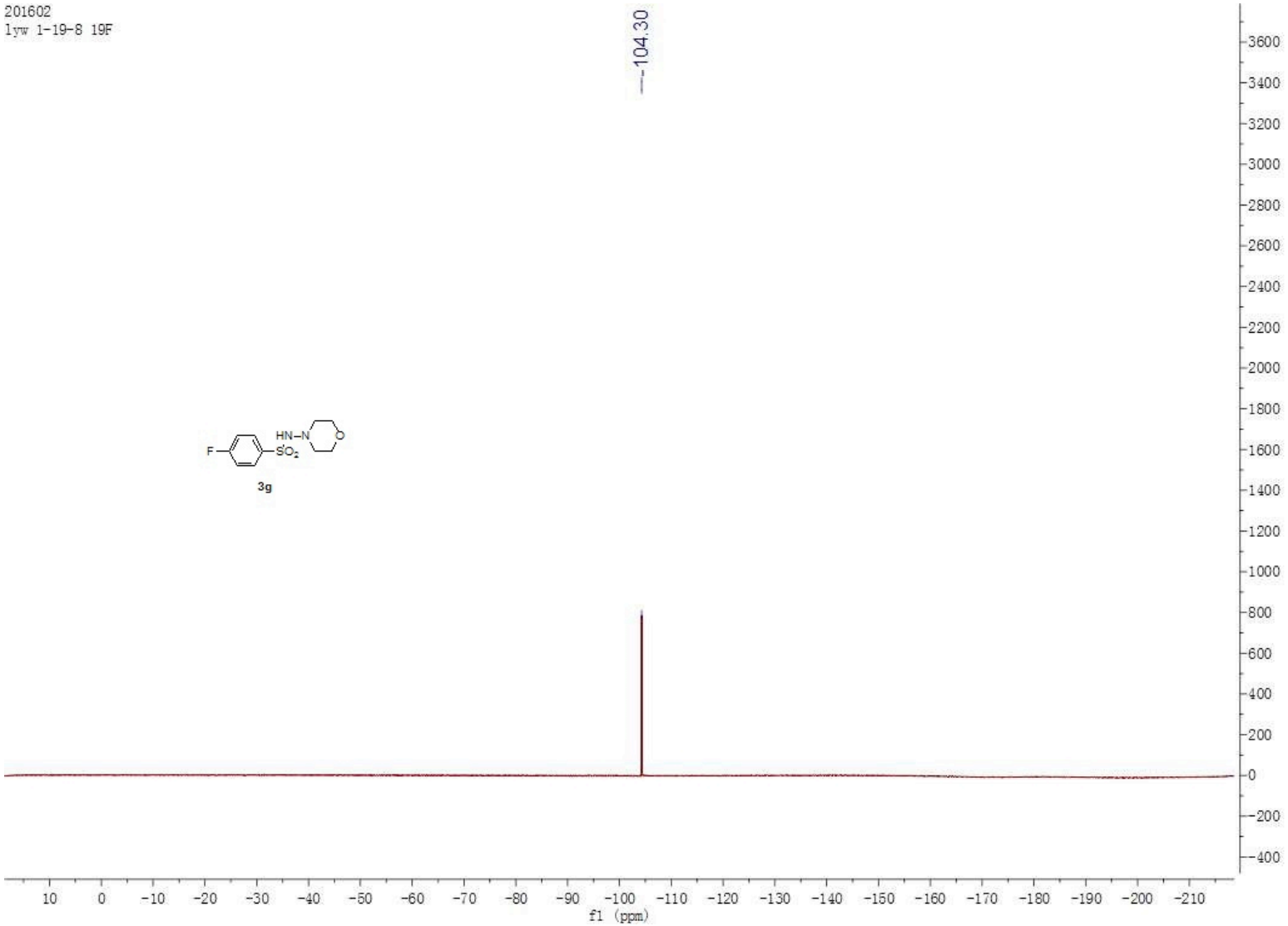
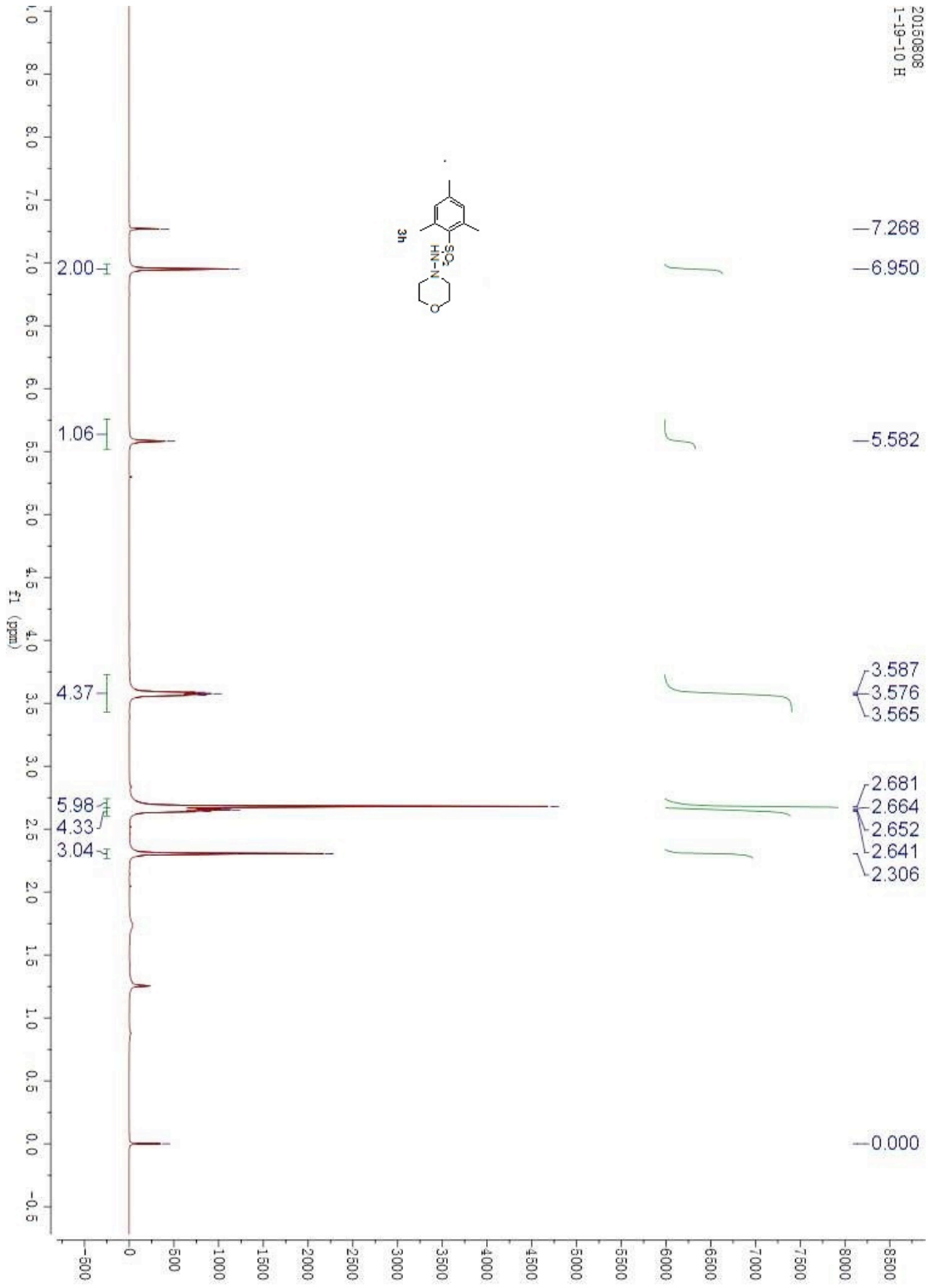
116.21
115.99
77.32
77.00
76.68
66.60
56.74
3g
f1 (ppm)


201602
lyw 1-19-8 19F
-104.30
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
-400
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)
F
HN
N
O
SO2
3g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3h
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5.582
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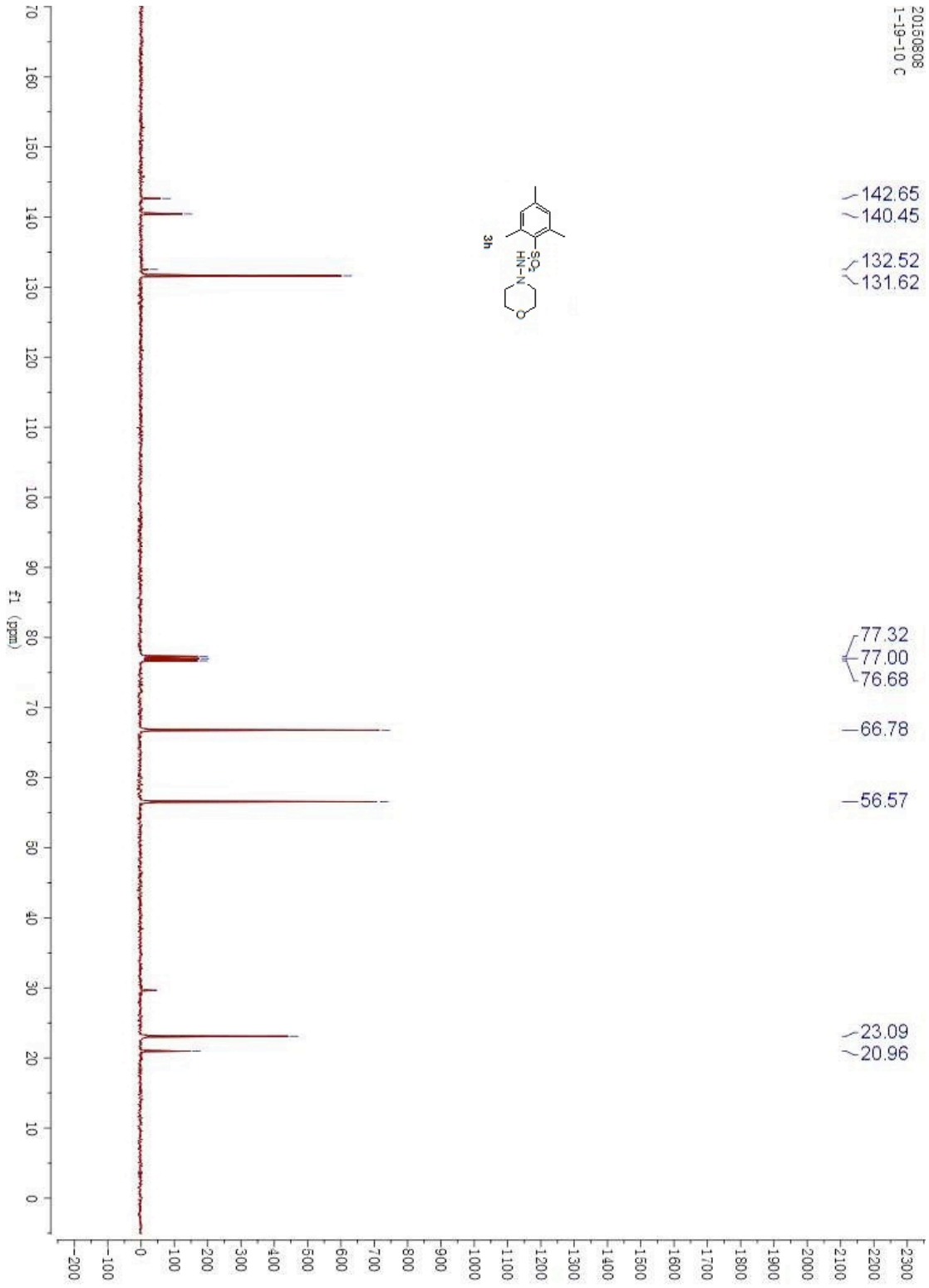
3.576
3.565
2.681
2.664
2.652
2.641
2.306
0.000
2.00
1.06
4.37
5.98
4.33
3.04
f1 (ppm)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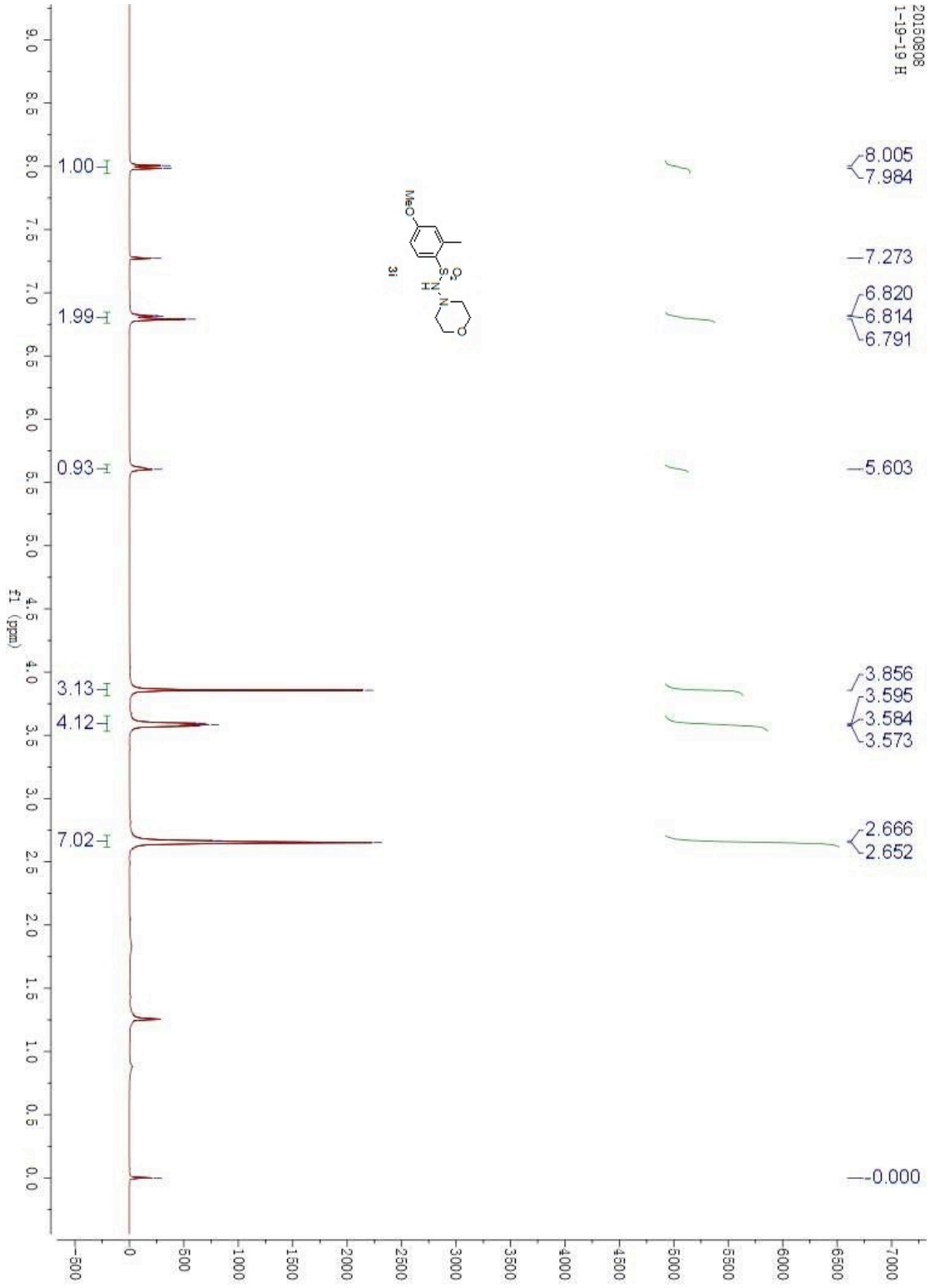
131.62
77.32
77.00
76.68
66.78
56.57
23.09
20.96
f1 (ppm)
3h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6.814
6.791
5.603
3.856
3.595
3.584
3.573
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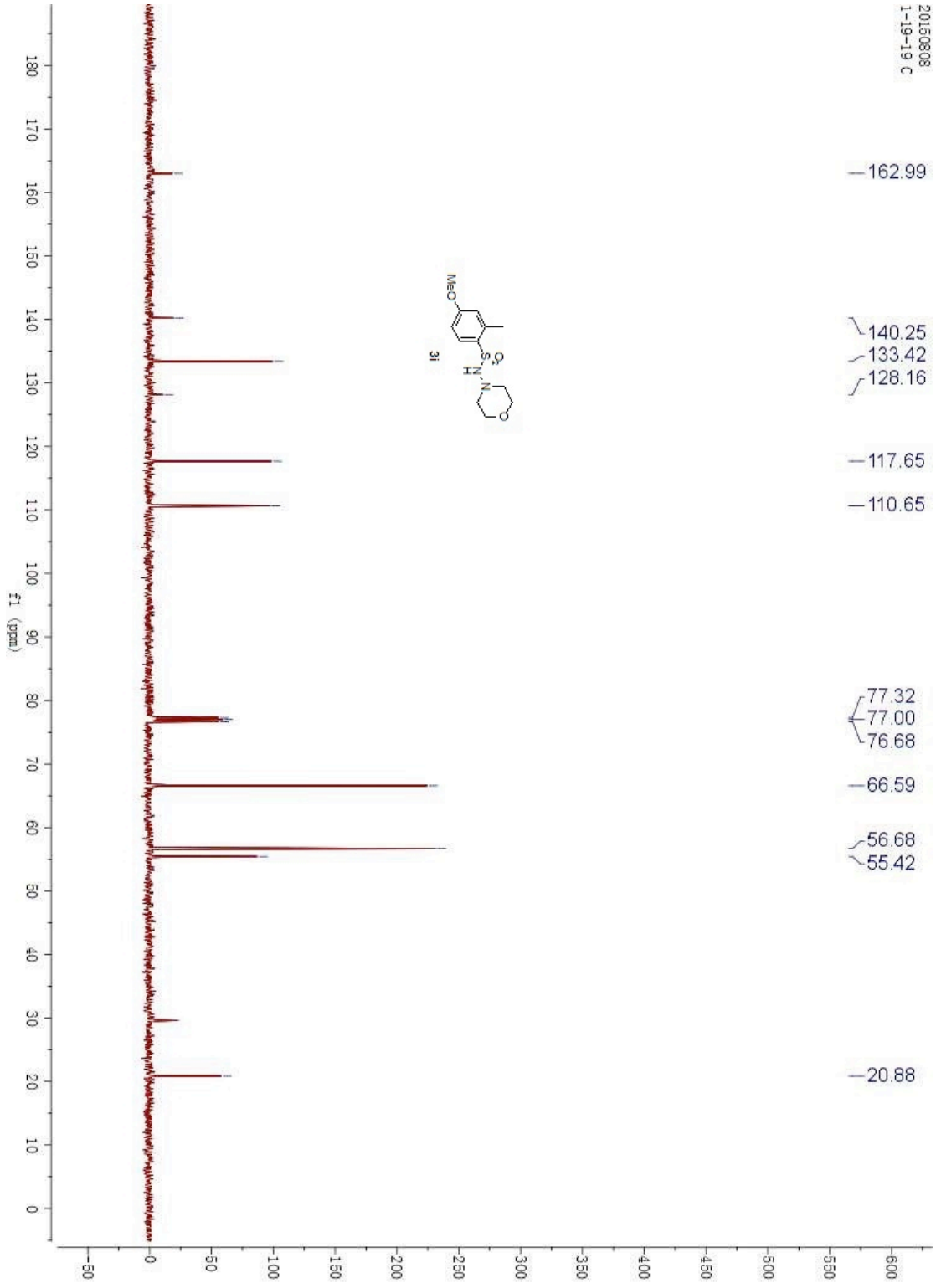
1.00
1.99
0.93
3.13
4.12
7.02
MeO
3i
f1 (ppm)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133.42
128.16
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77.00
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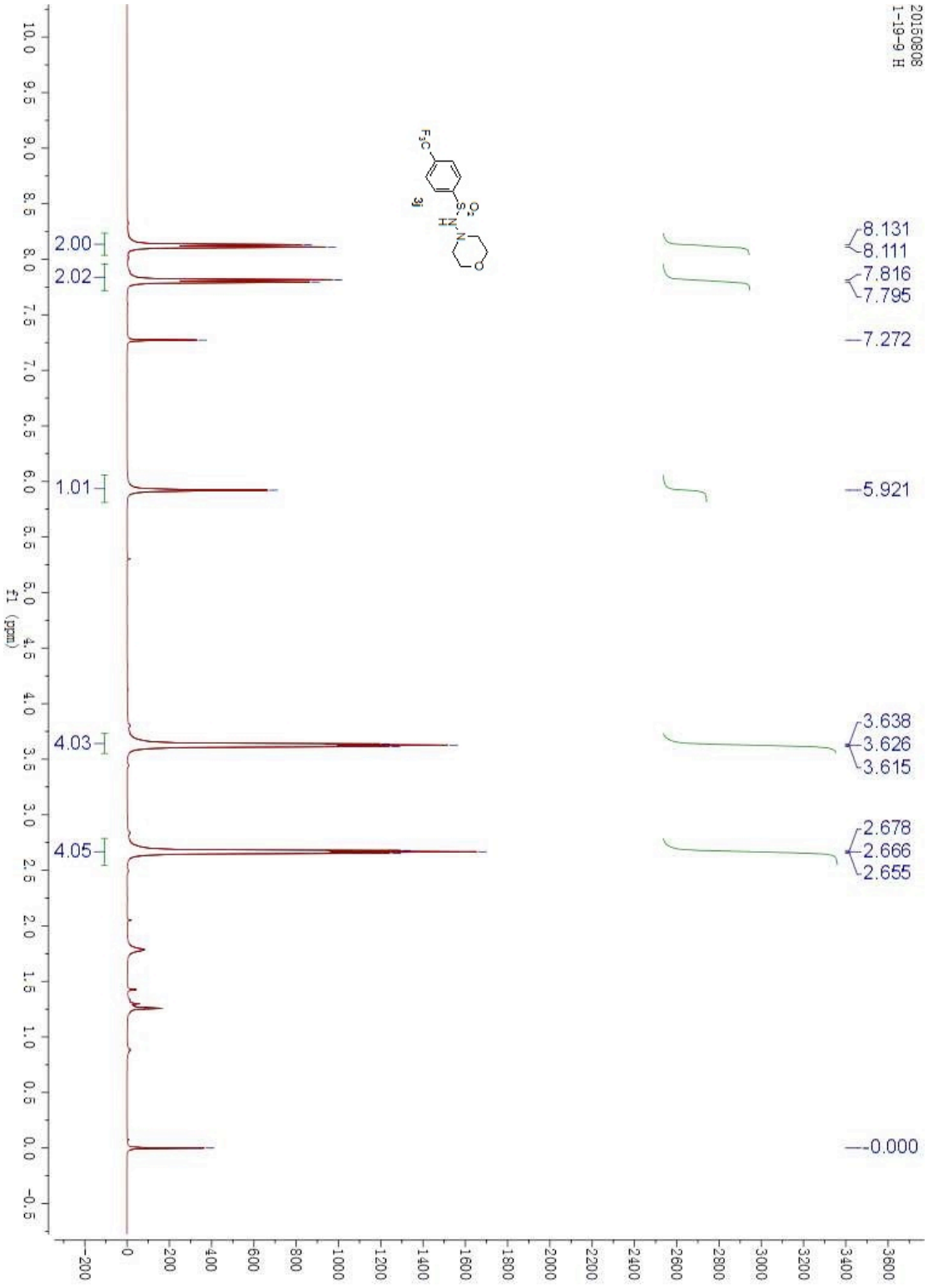
56.68
55.42
20.88
MeO
3i
f1 (ppm)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1-19-9 H
3j
8.131
8.111
7.816
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7.272
5.921
3.638
3.626
3.615
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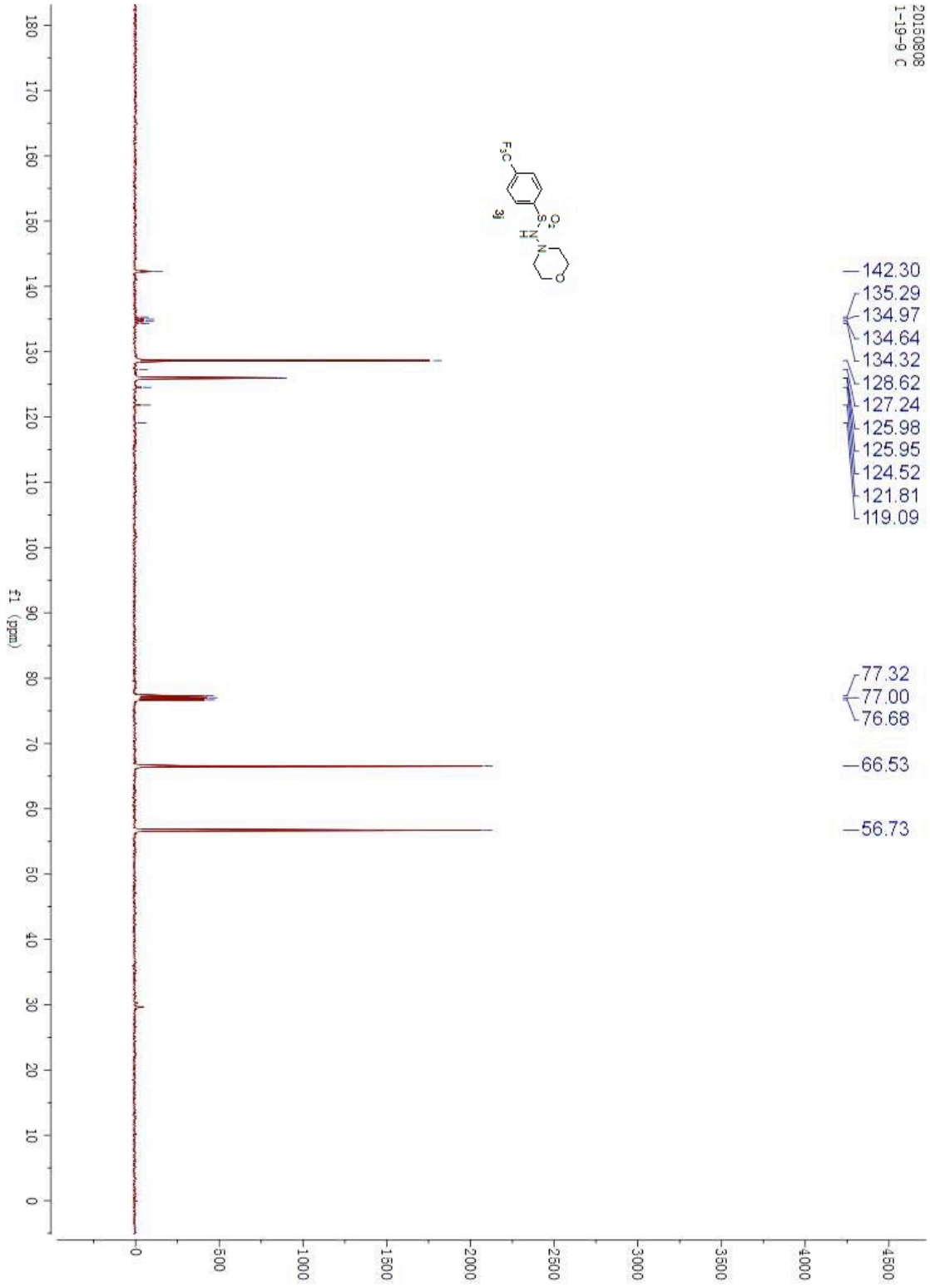
2.666
2.655
0.000
2.00
2.02
1.01
4.03
4.05
f1 (ppm)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135.29
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134.32
128.62
127.24
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125.95
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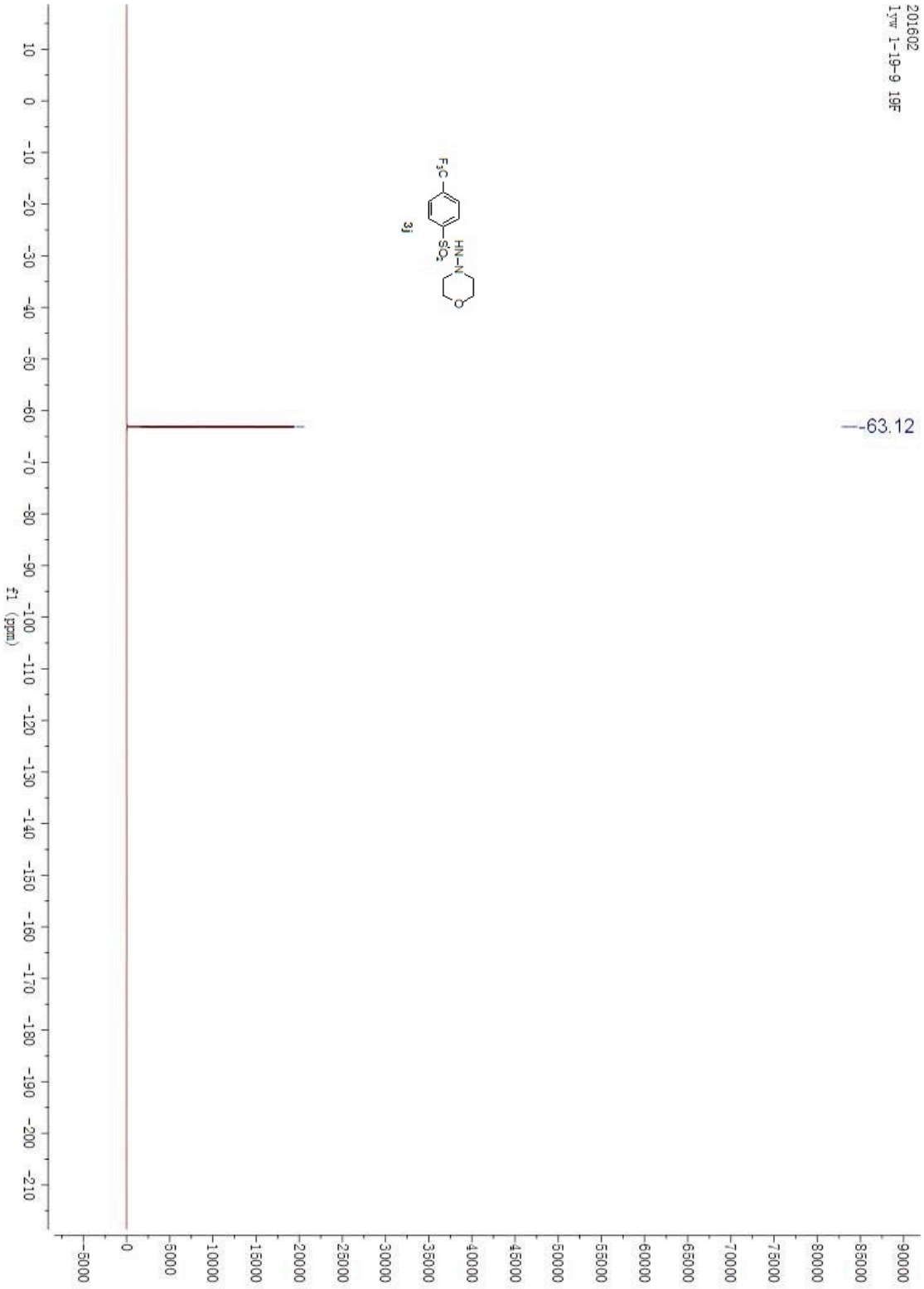
77.00
76.68
66.53
56.73
f1 (ppm)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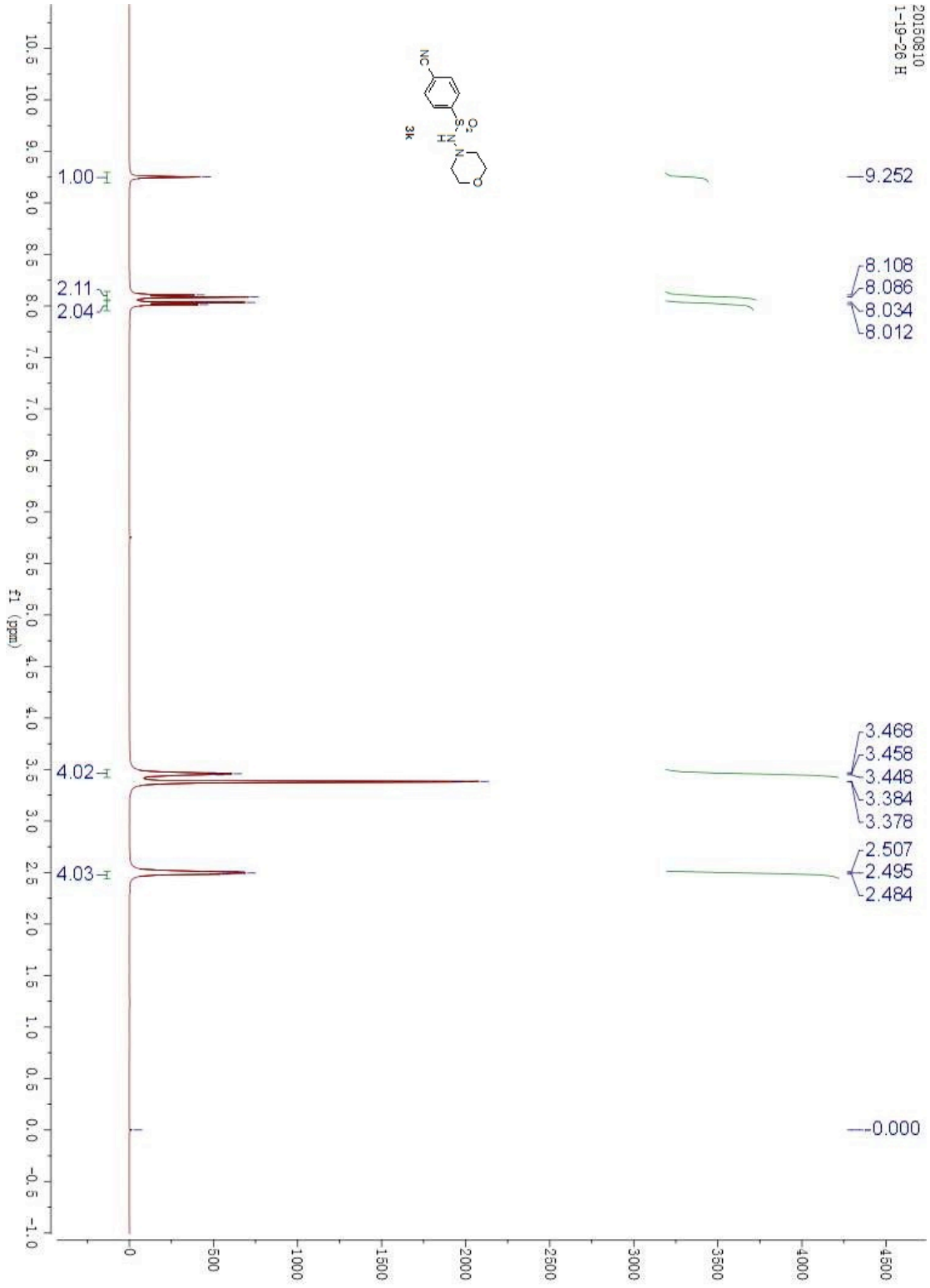
lyw 1-19-9 19F
-63.12
3j
F3C
SO2
HN-N
O
f1 (ppm)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1-19-26 H
3k
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2.11
2.04
4.02
4.03
9.252
8.108
8.086
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2.507
2.495
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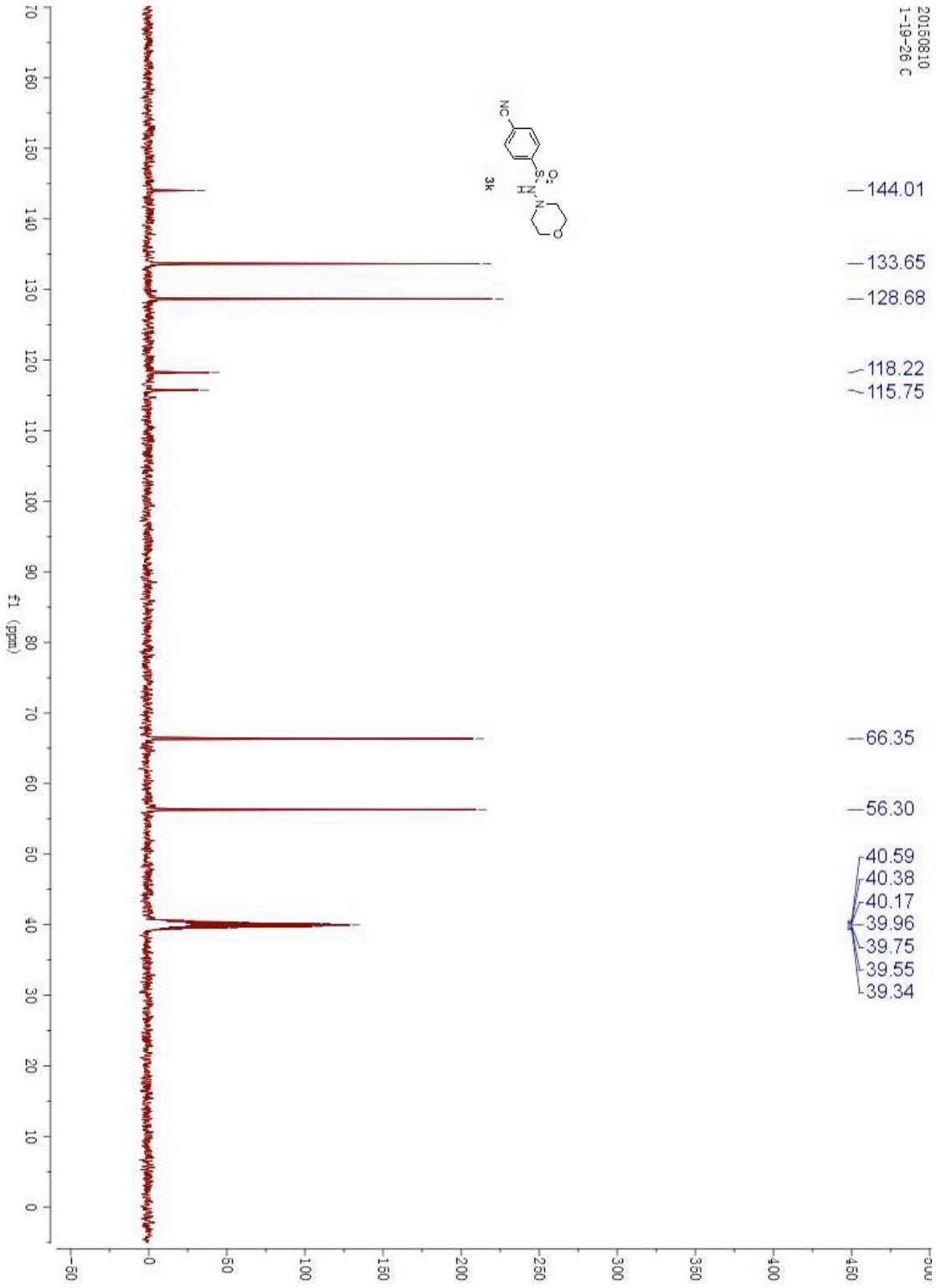
0.000
f1 (ppm)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1-19-26 C
3k
144.01
133.65
128.68
118.22
115.75
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56.30
40.59
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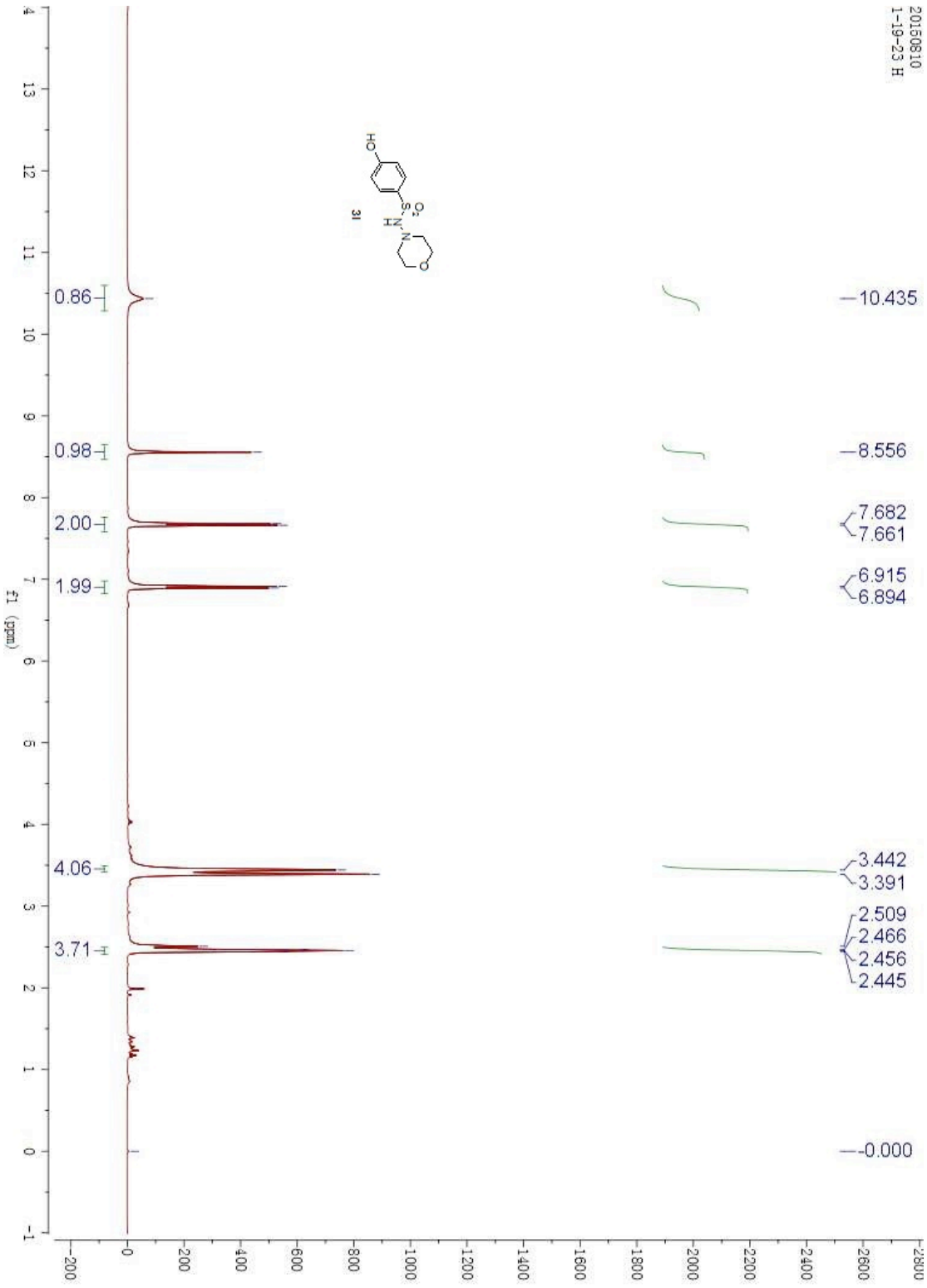
39.96
39.75
39.55
39.34
f1 (ppm)


20150810
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3l
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0.98
2.00
1.99
4.06
3.71
10.435
8.556
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7.661
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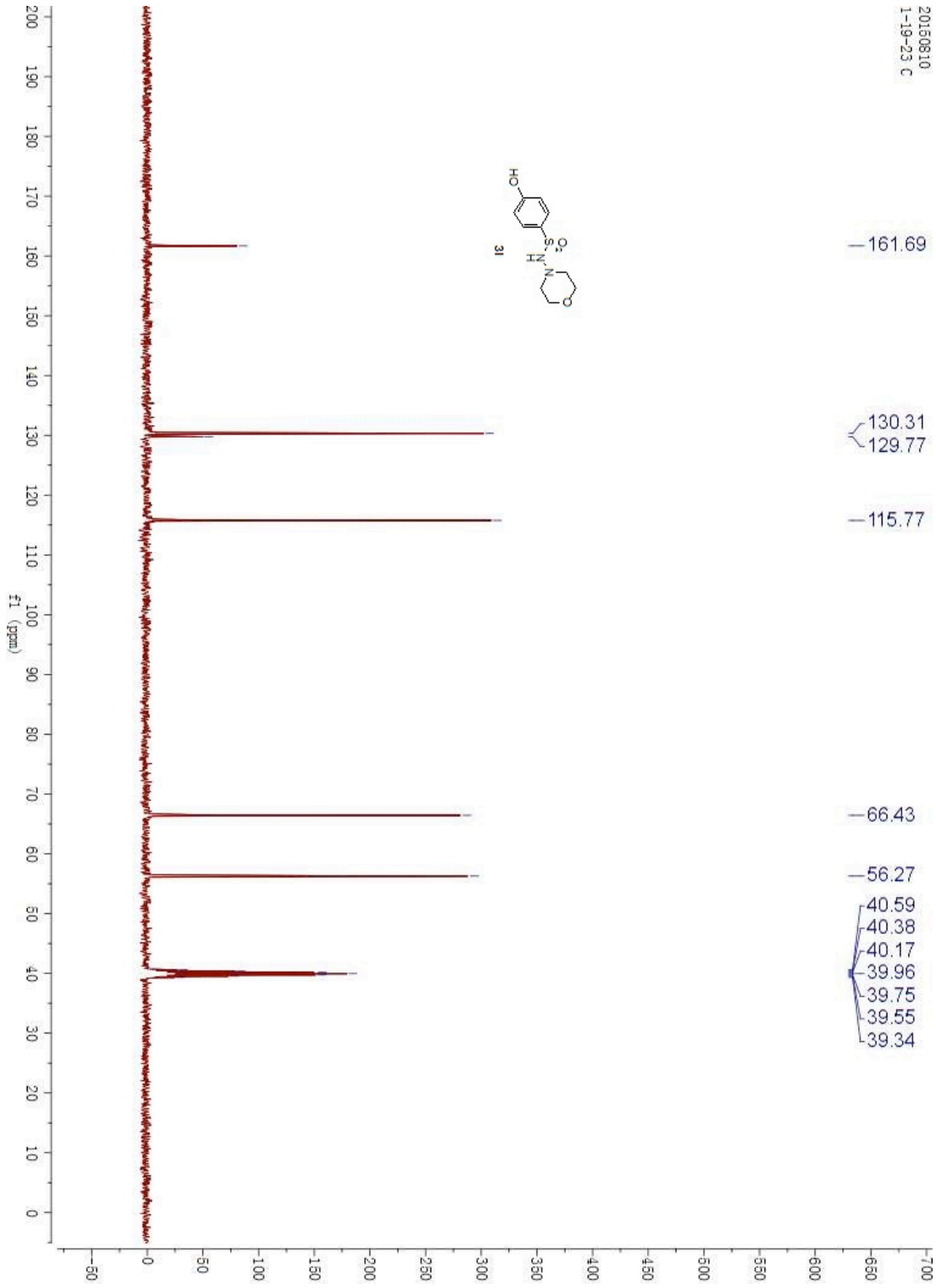
6.894
3.442
3.391
2.509
2.466
2.456
2.445
-0.000
f1 (ppm)


20150810
1-19-23 C
3l
161.69
130.31
129.77
115.77
66.43
56.27
40.59
40.38
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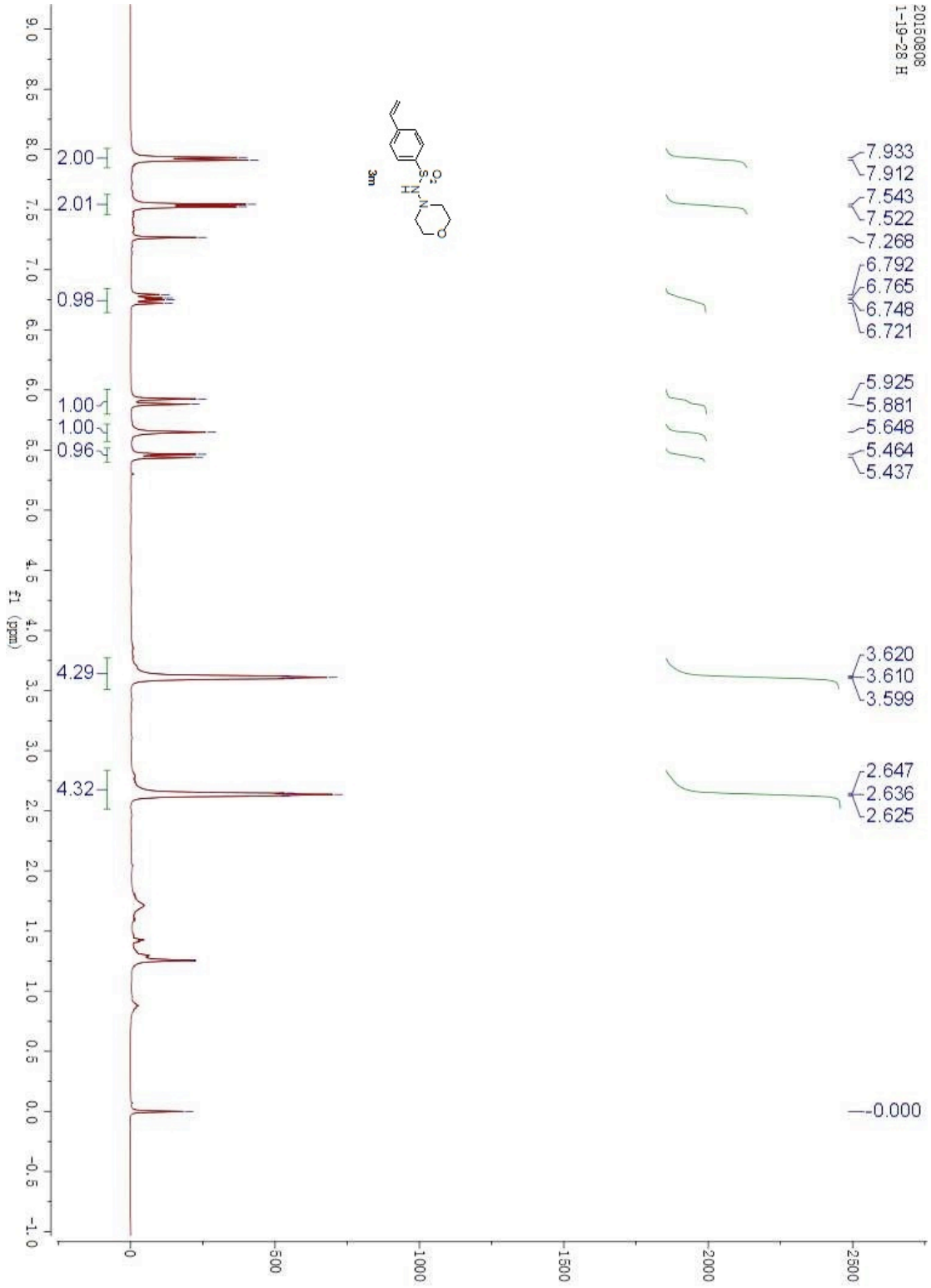
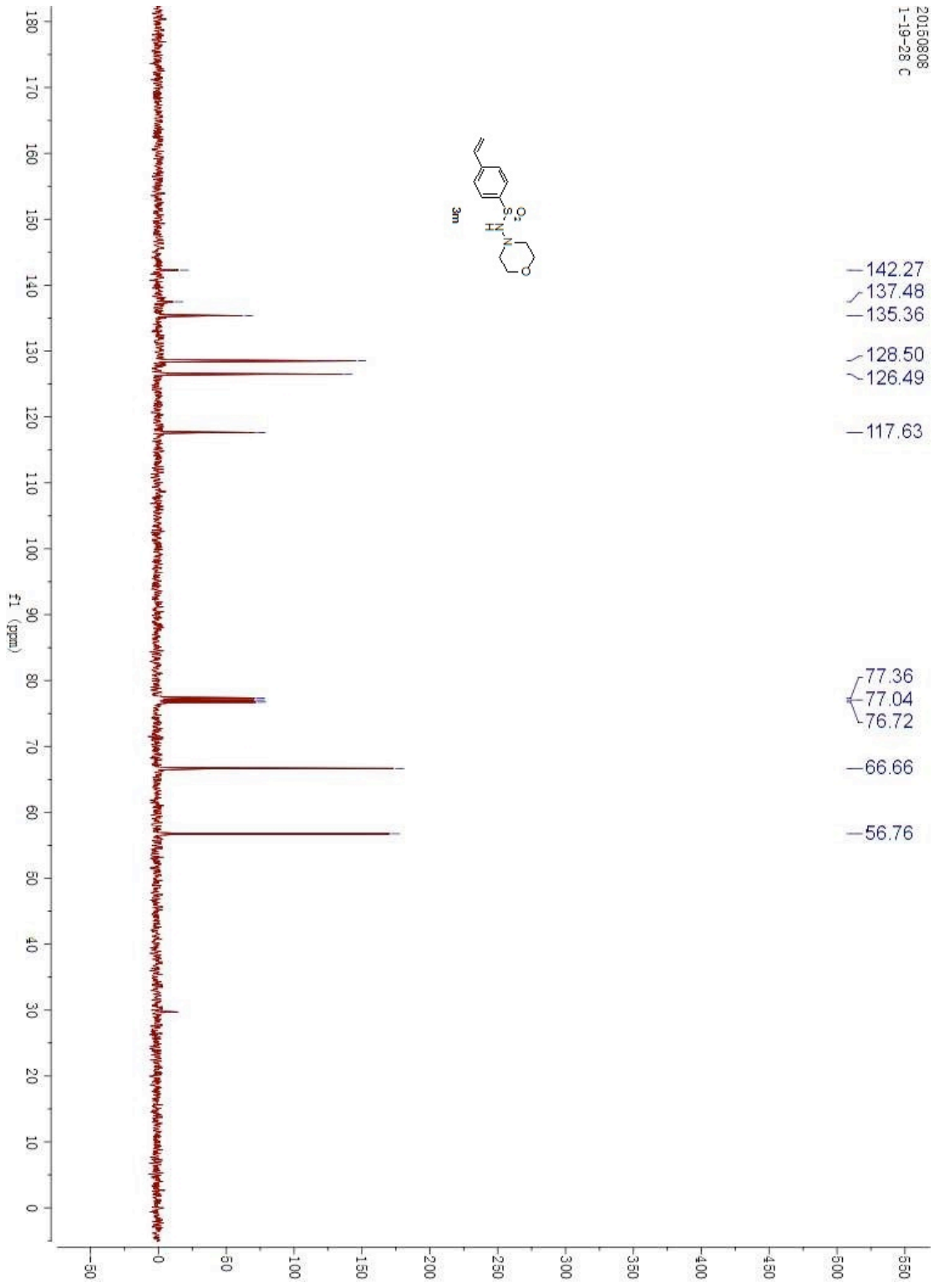
39.96
39.75
39.55
39.34
f1 (ppm)


20150808
1-19-28 H
3am
7.933
7.912
7.543
7.522
7.268
6.792
6.765
6.748
6.721
5.925
5.881
5.648
5.464
5.437
3.620
3.610
3.599
2.647
2.636
2.625
0.000
2.00
2.01
0.98
1.00
1.00
0.96
4.29
4.32
f1 (ppm)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1-19-28 C
3m
142.27
137.48
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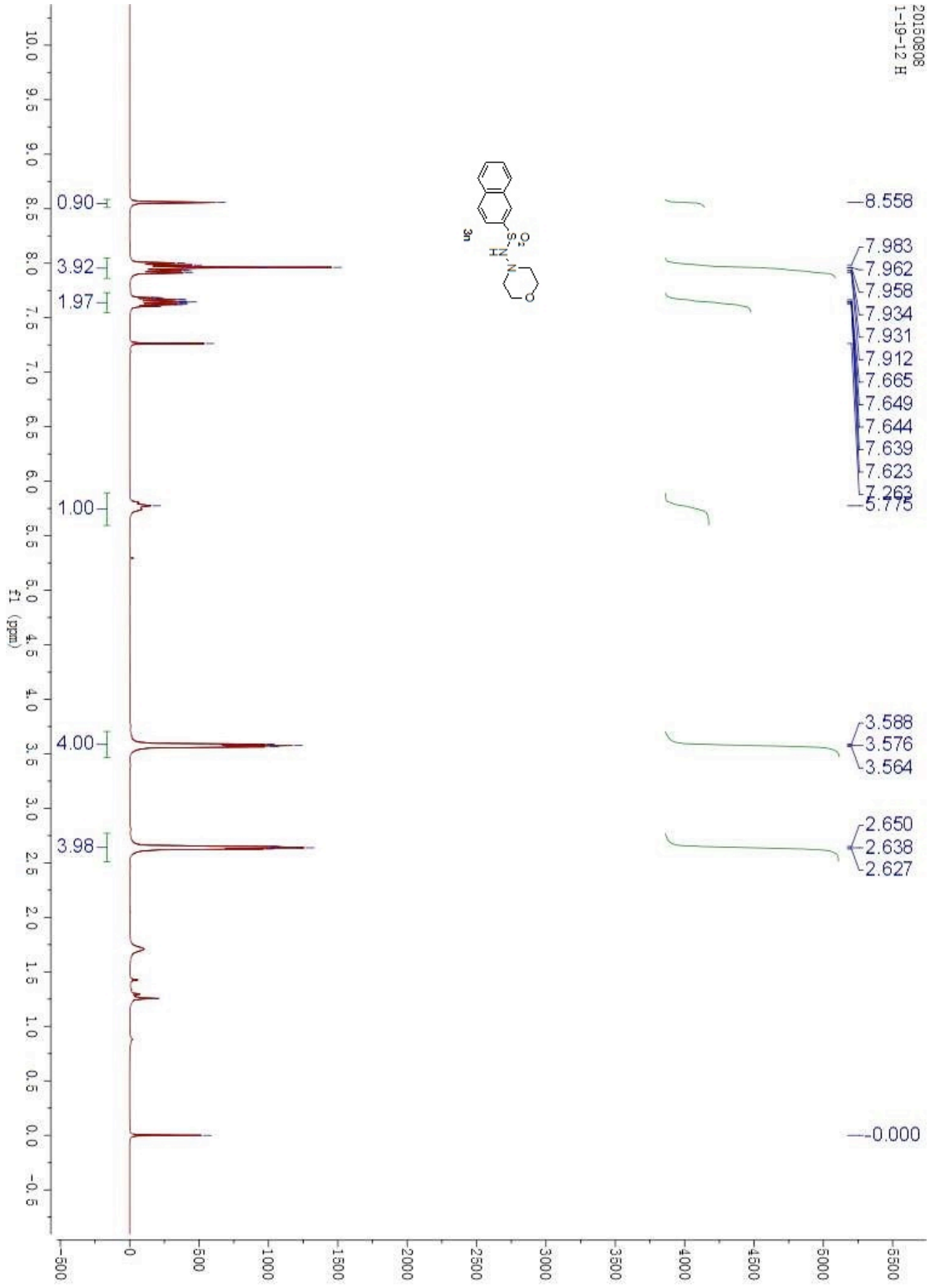
117.63
77.36
77.04
76.72
66.66
56.76
f1 (ppm)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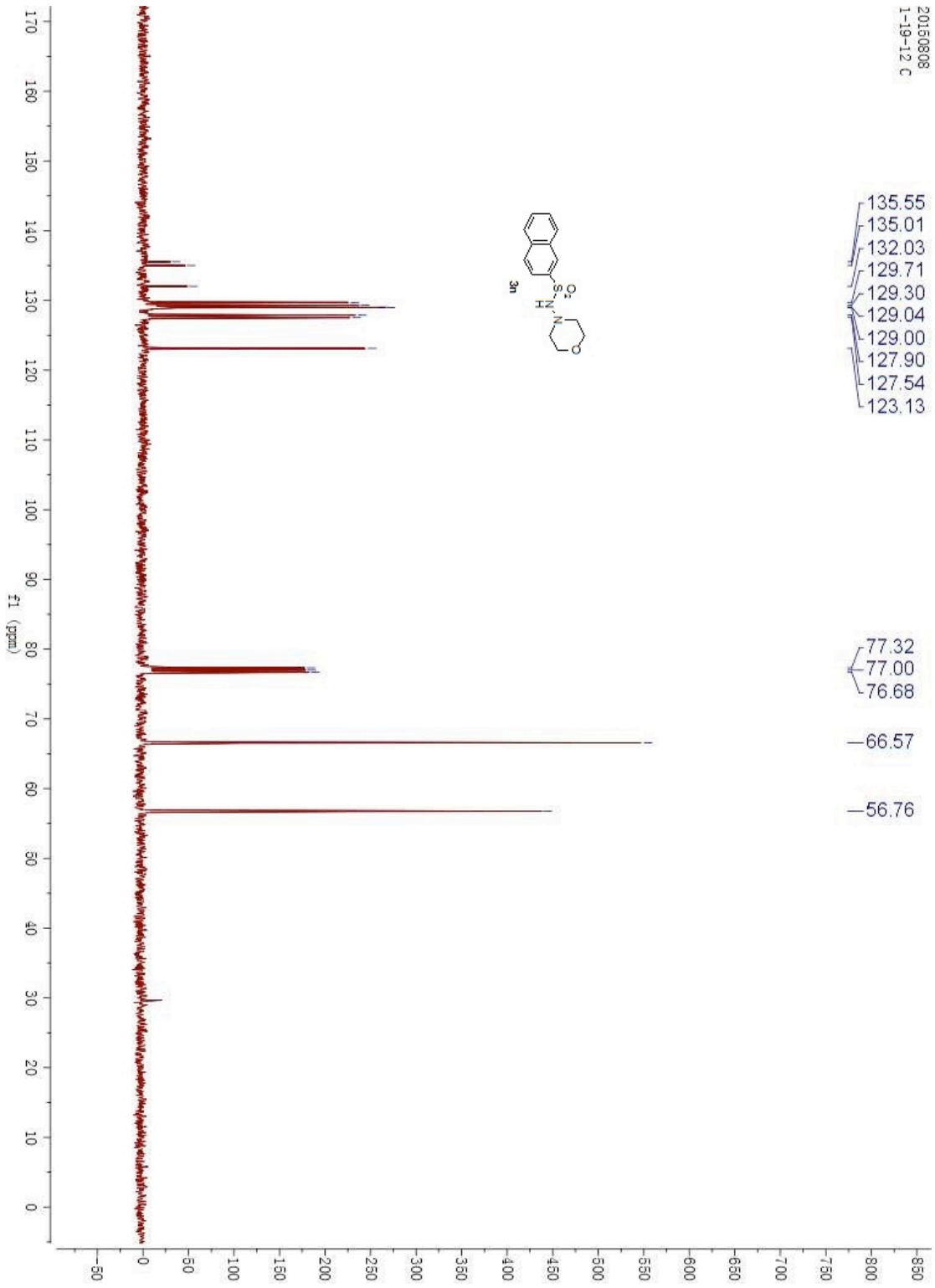
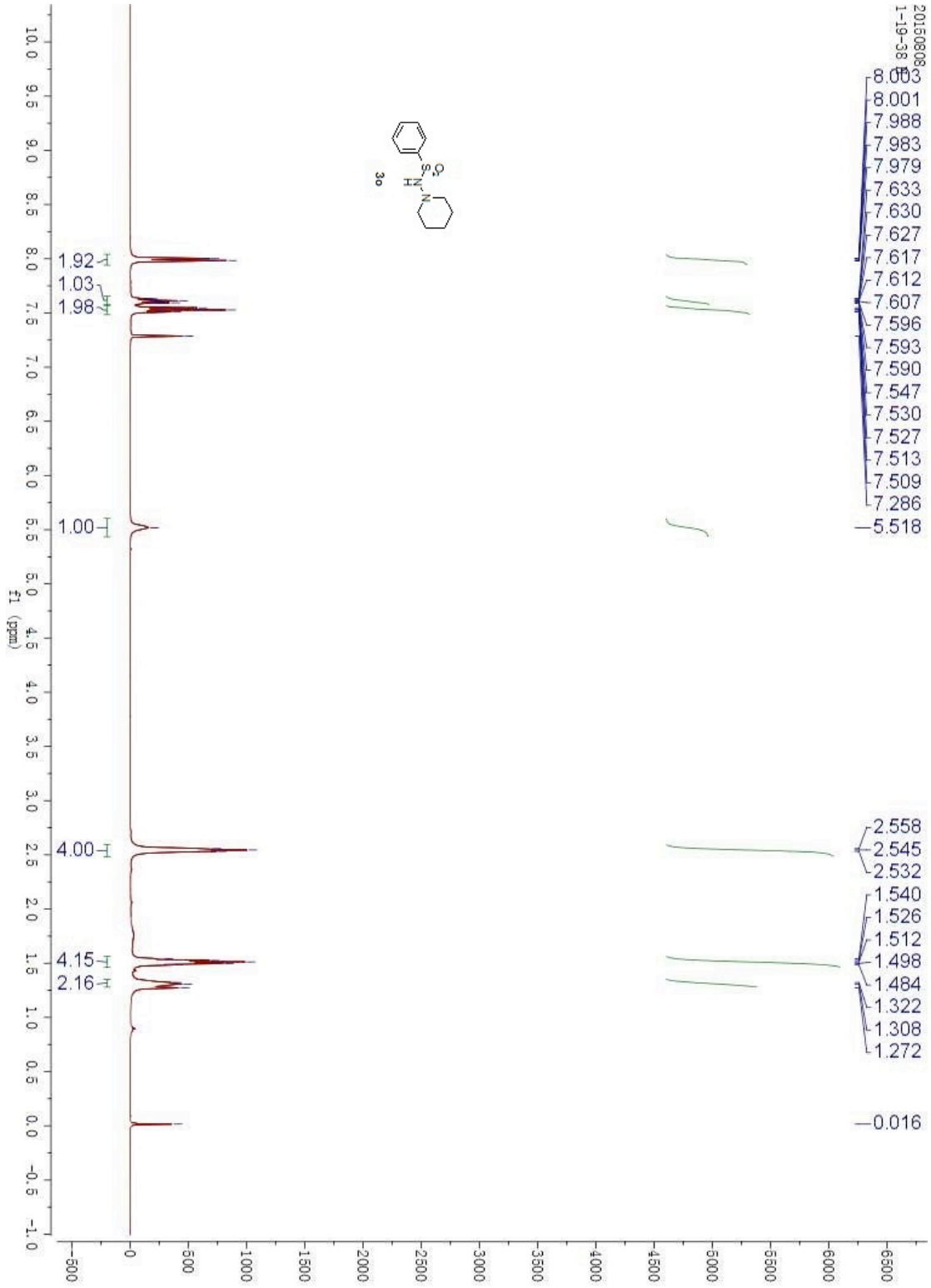
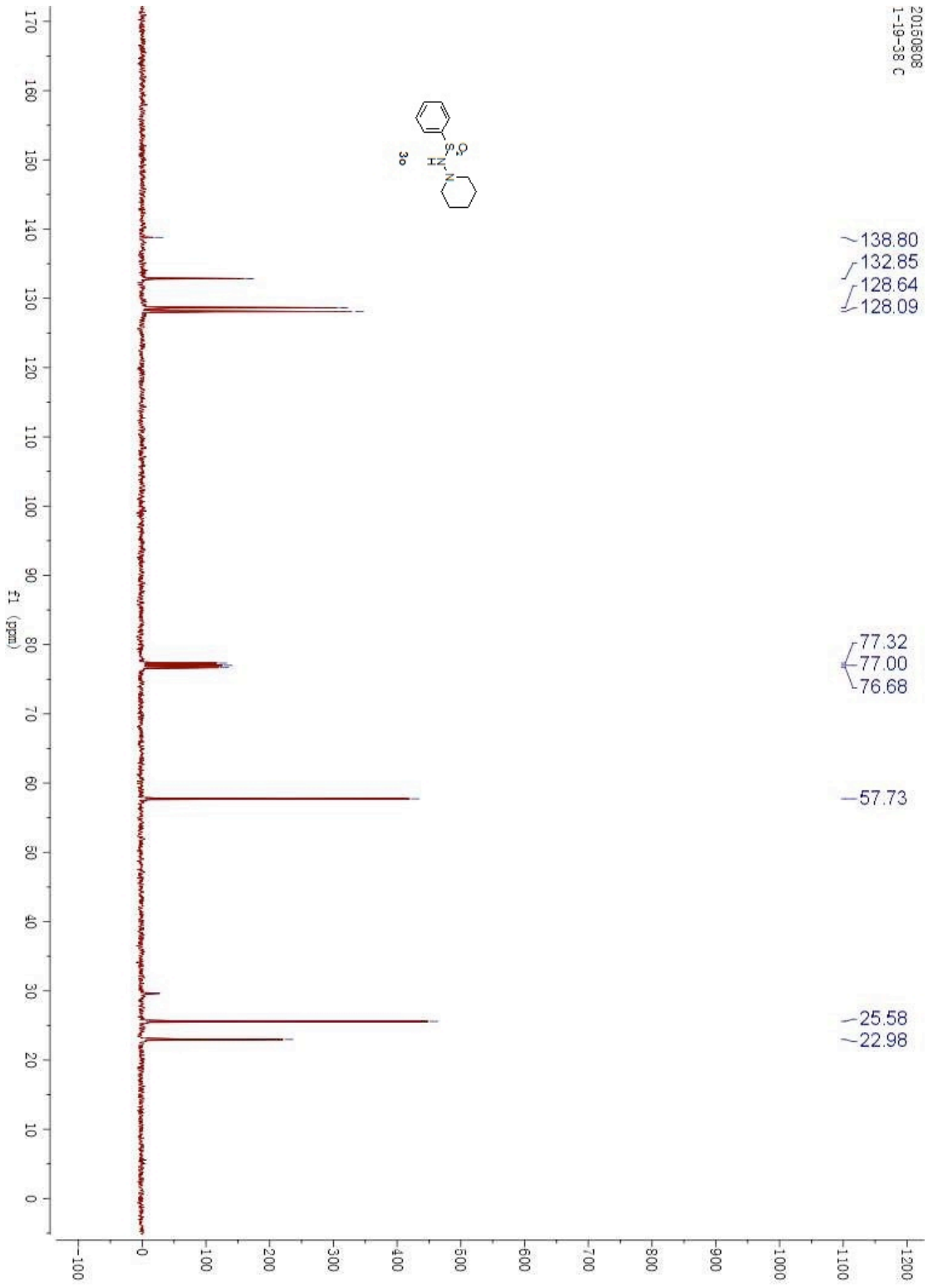
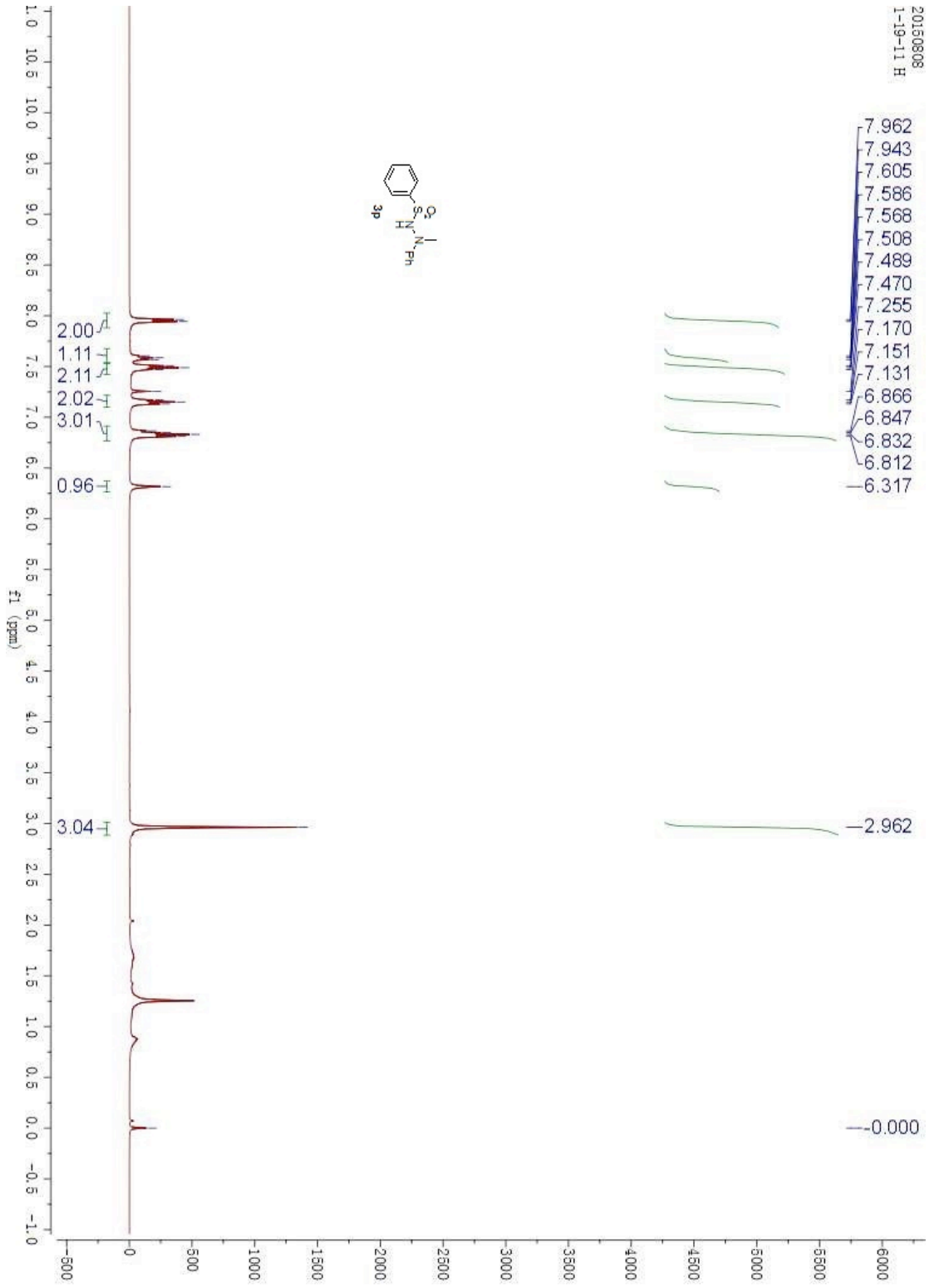
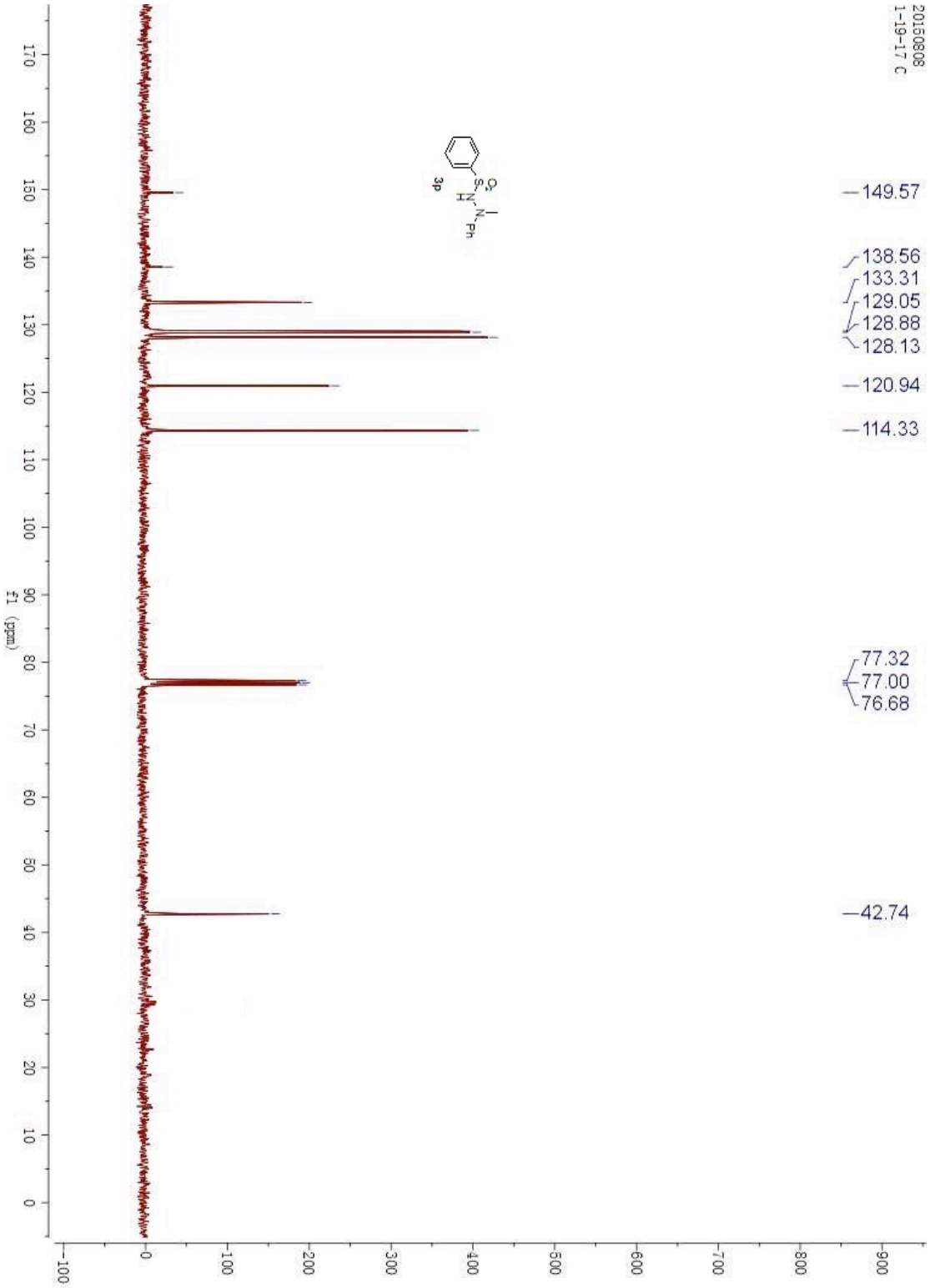
1-19-12 H
8.558
7.983
7.962
7.958
7.934
7.931
7.912
7.665
7.649
7.644
7.639
7.623
7.263
5.775
3.588
3.576
3.564
2.650
2.638
2.627
0.000
0.90
3.92
1.97
1.00
4.00
3.98
f1 (ppm)

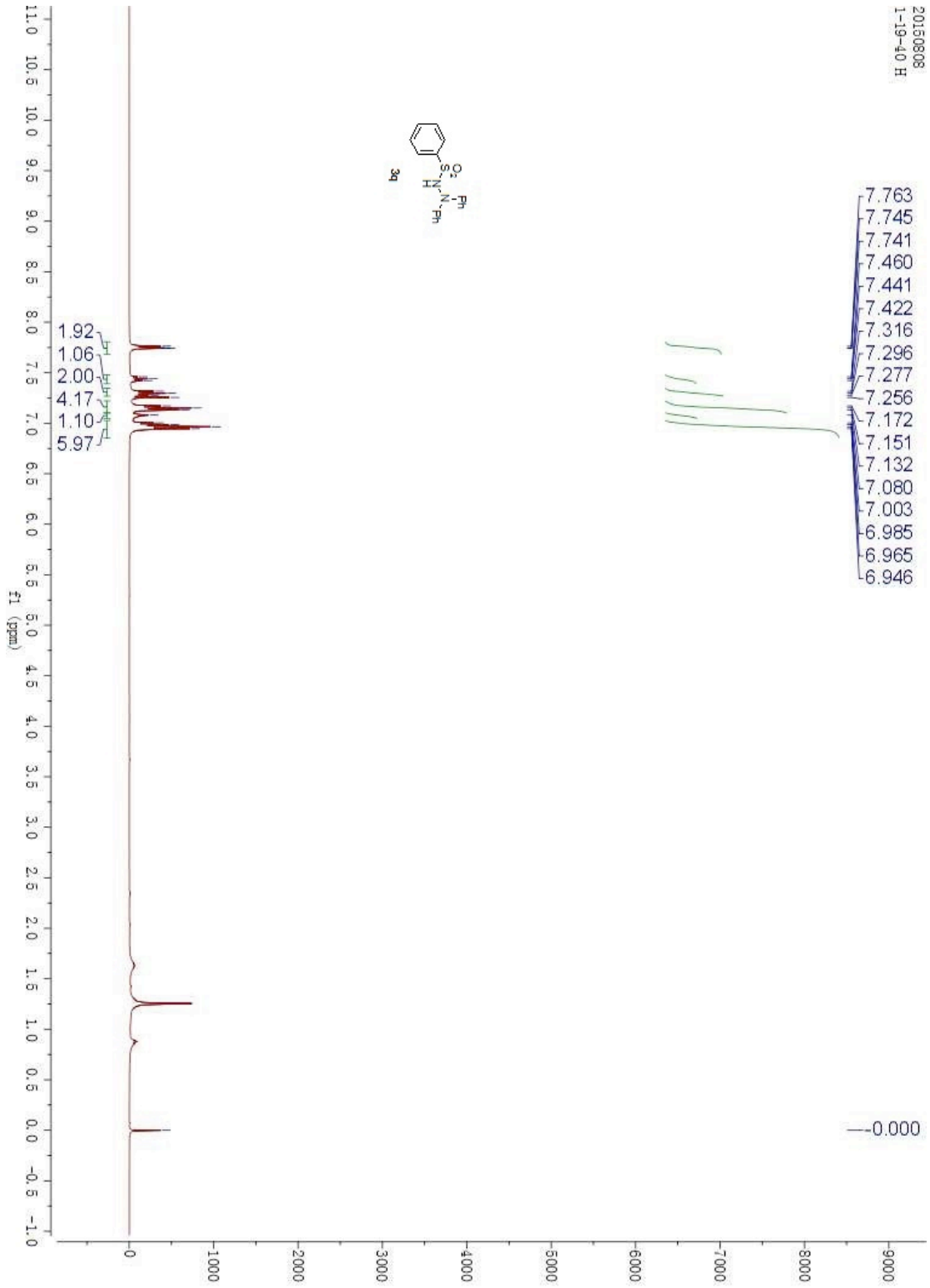

20150808
1-19-12 C
135.55
135.01
132.03
129.71
129.30
129.04
129.00
127.90
127.54
123.13
77.32
77.00
76.68
66.57
56.76
3n
f1 (ppm)

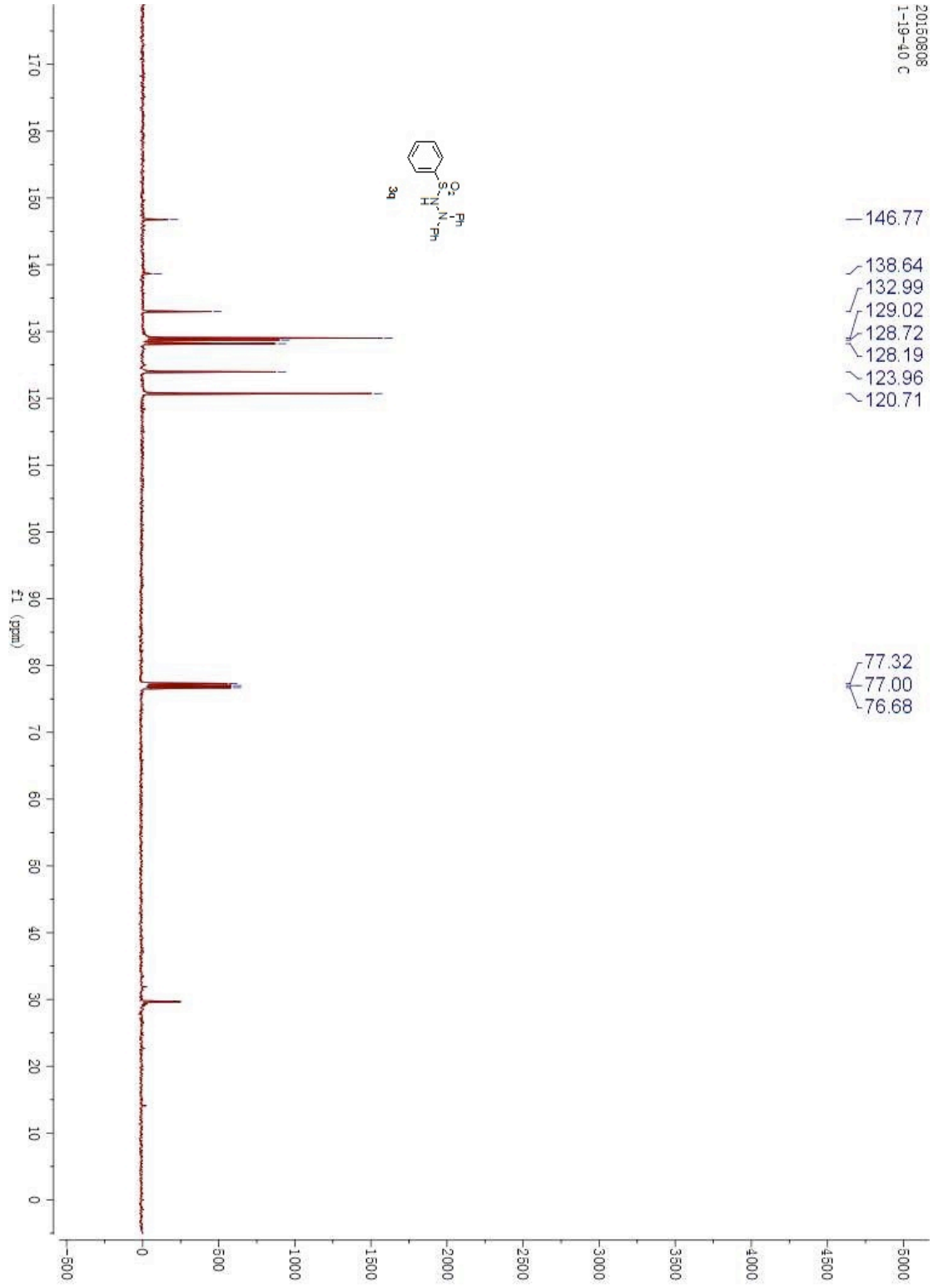

20150808
1-19-3B
3o
8.003
8.001
7.988
7.983
7.979
7.633
7.630
7.627
7.617
7.612
7.607
7.596
7.593
7.590
7.547
7.530
7.527
7.513
7.509
7.286
5.518
2.558
2.545
2.532
1.540
1.526
1.512
1.498
1.484
1.322
1.308
1.272
0.016
1.92
1.03
1.98
1.00
4.00
4.15
2.16
f1 (ppm)

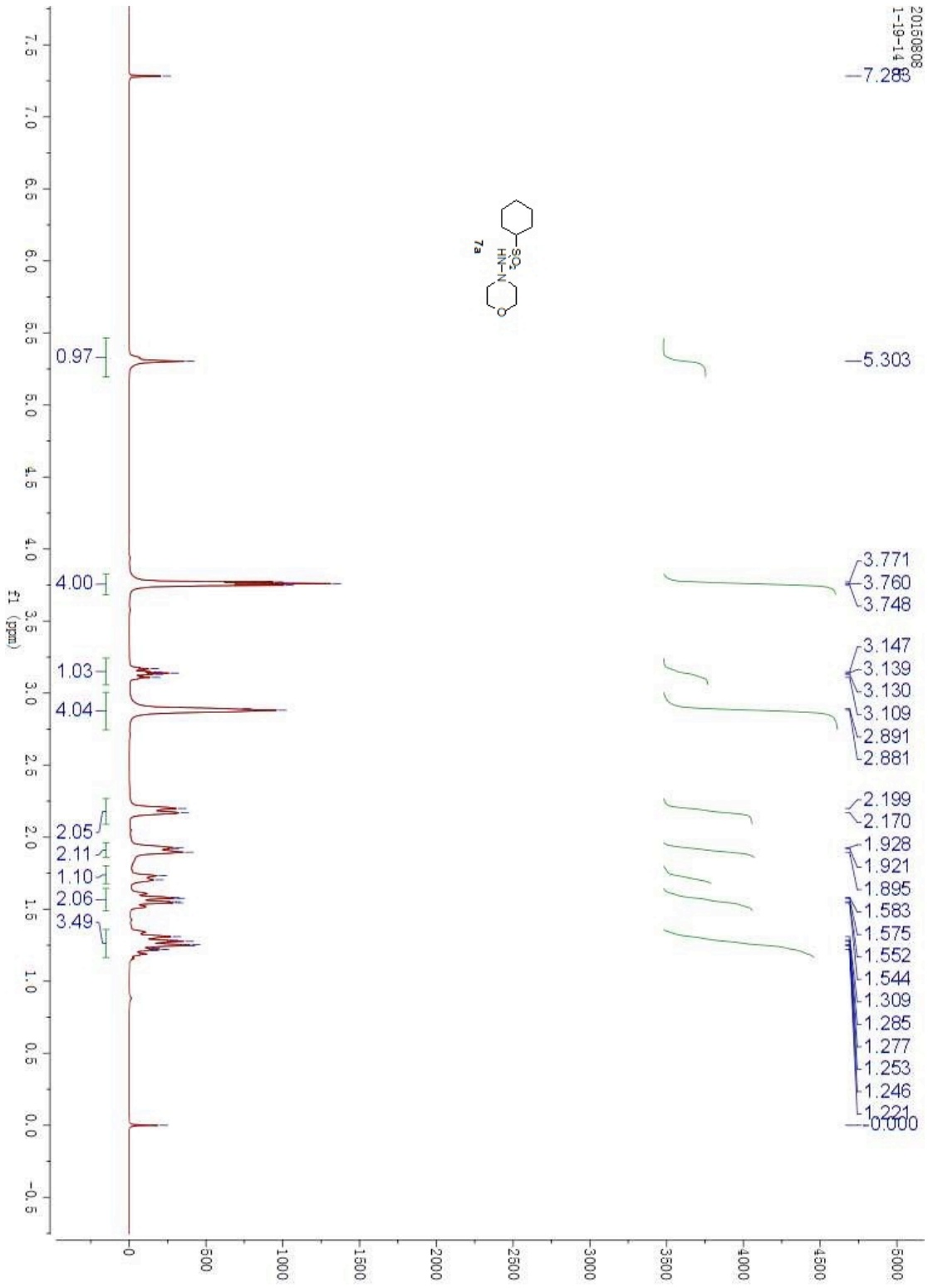

20150808
1-19-3B C
3o
138.80
132.85
128.64
128.09
77.32
77.00
76.68
57.73
25.58
22.98
f1 (ppm)

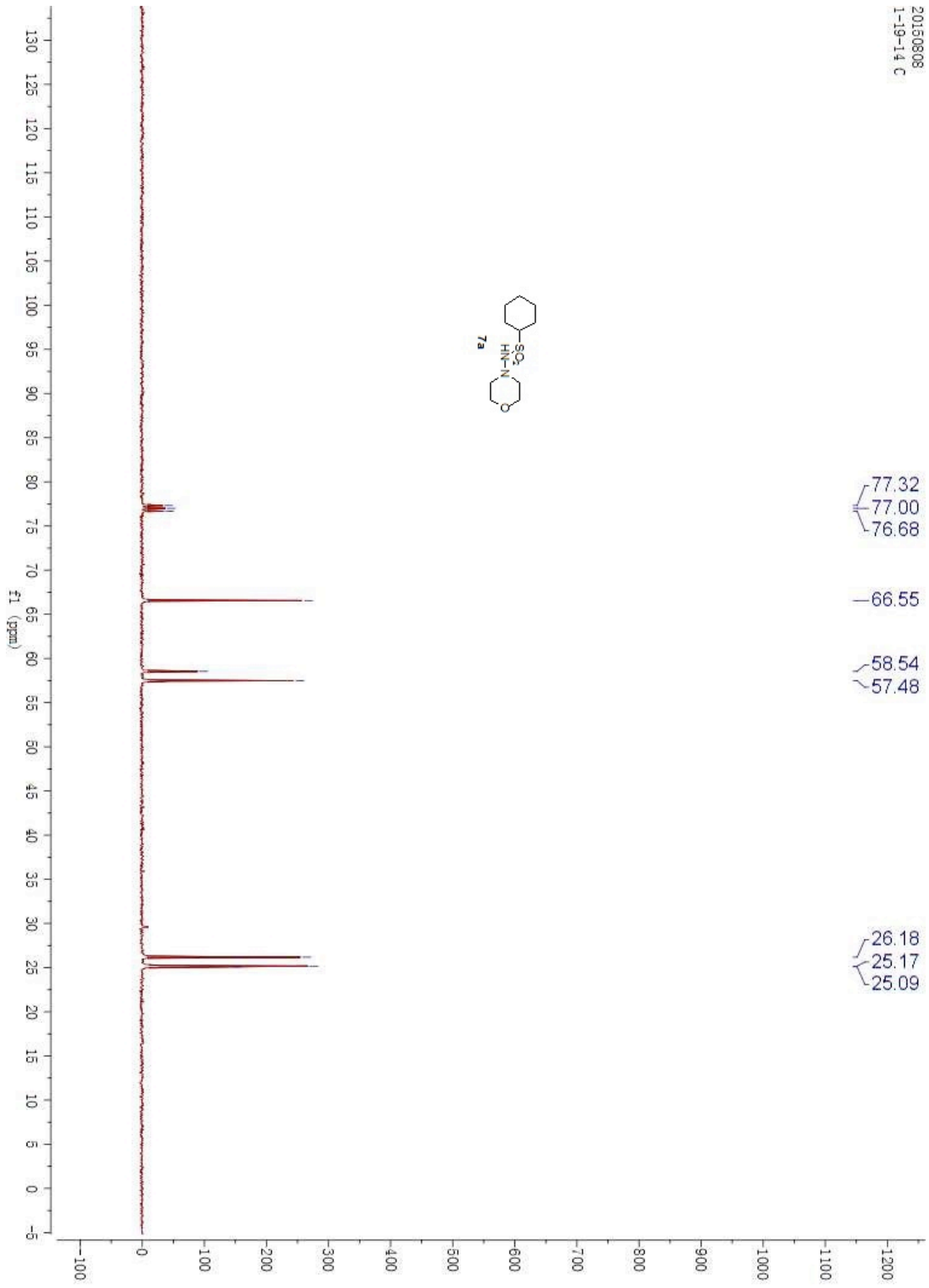

20150808
1-19-11 H
7.962
7.943
7.605
7.586
7.568
7.508
7.489
7.470
7.255
7.170
7.151
7.131
6.866
6.847
6.832
6.812
6.317
2.962
0.000
2.00
1.11
2.11
2.02
3.01
0.96
3.04
3p
f1 (ppm)

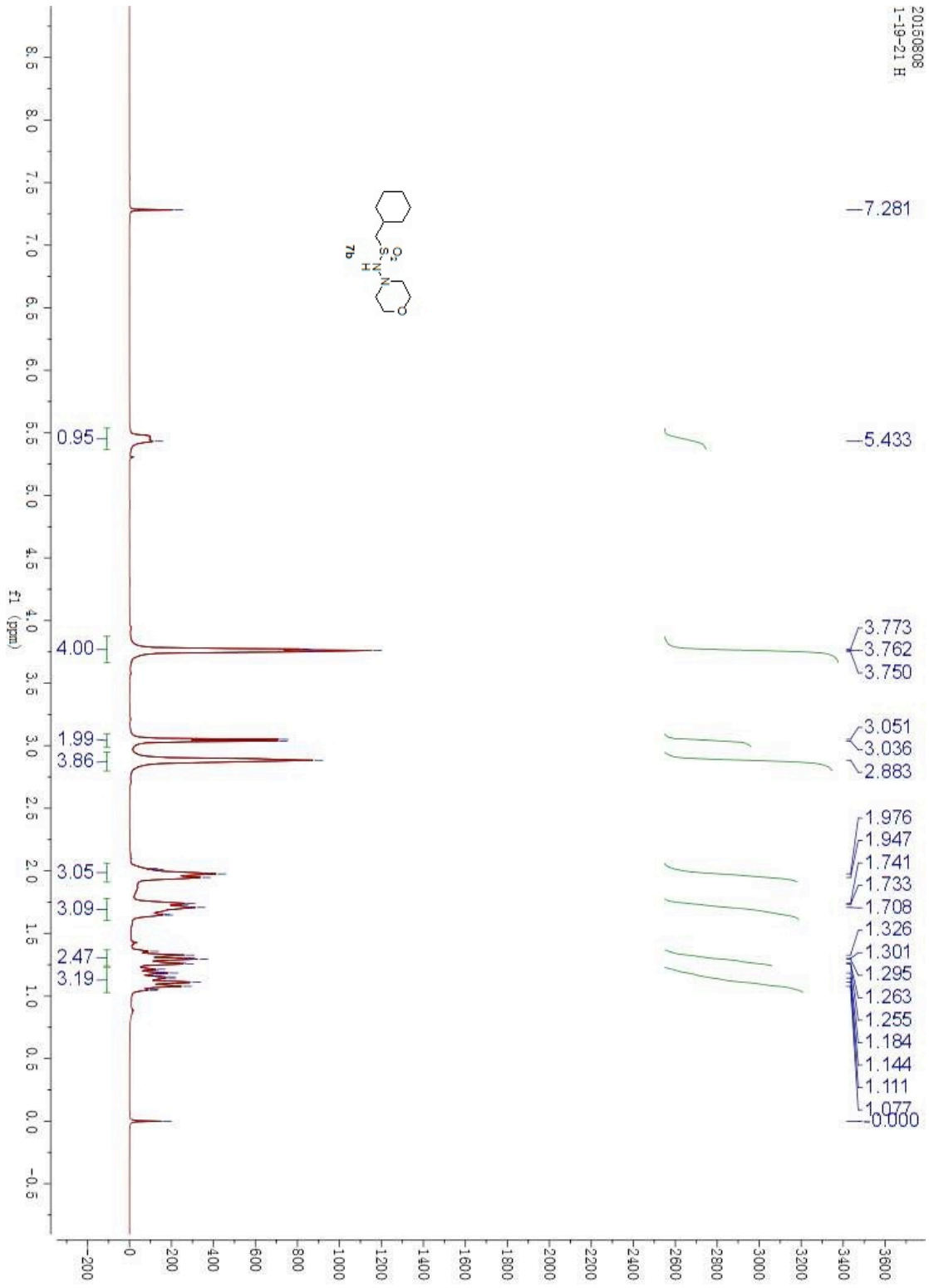

20150808
1-19-17 C
3p
149.57
138.56
133.31
129.05
128.88
128.13
120.94
114.33
77.32
77.00
76.68
42.74
f1 (ppm)

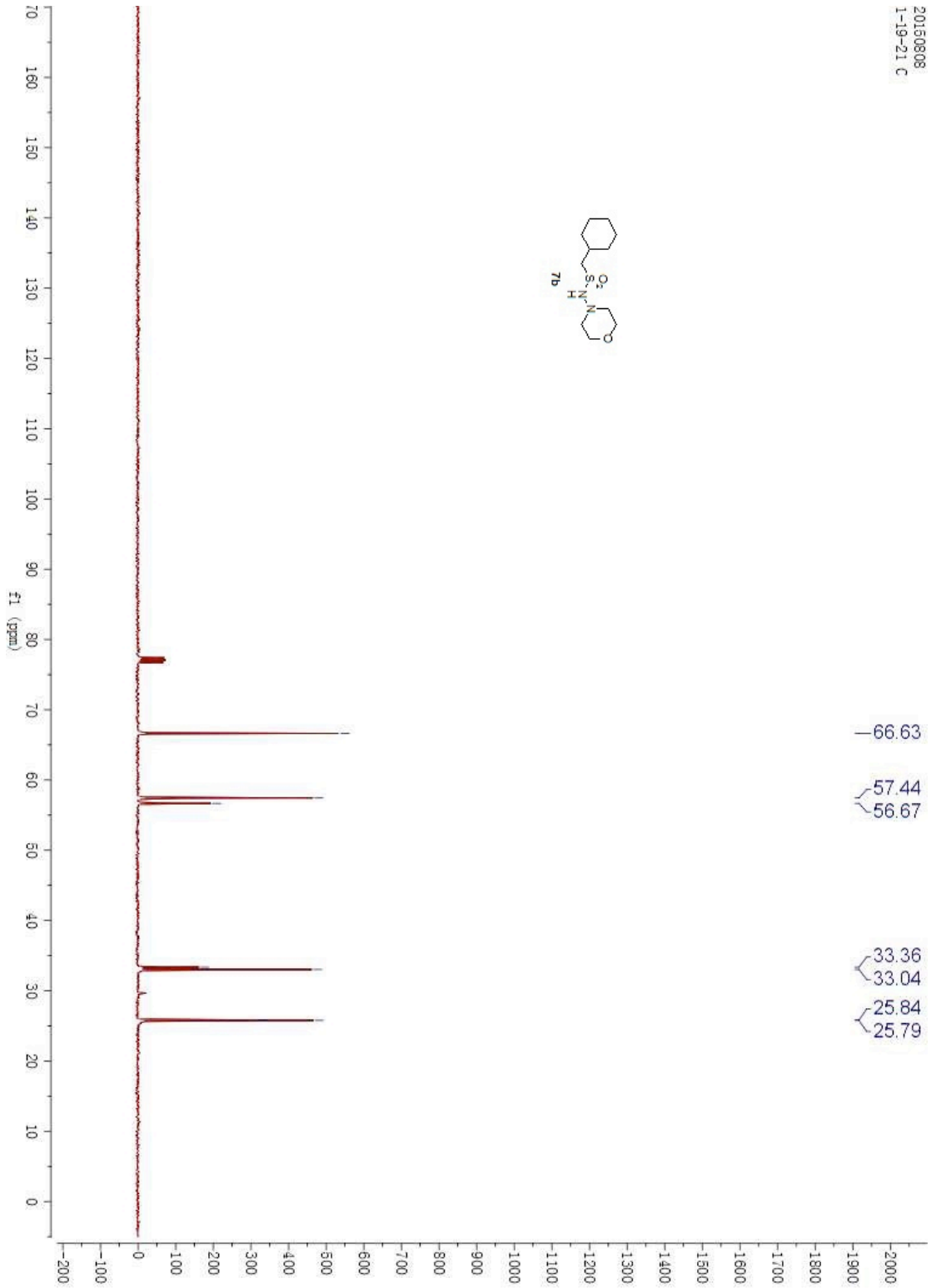

20150808
1-19-40 H
3aa
1.92
1.06
2.00
4.17
1.10
5.97
7.763
7.745
7.741
7.460
7.441
7.422
7.316
7.296
7.277
7.256
7.172
7.151
7.132
7.080
7.003
6.985
6.965
6.946
-0.000
f1 (ppm)

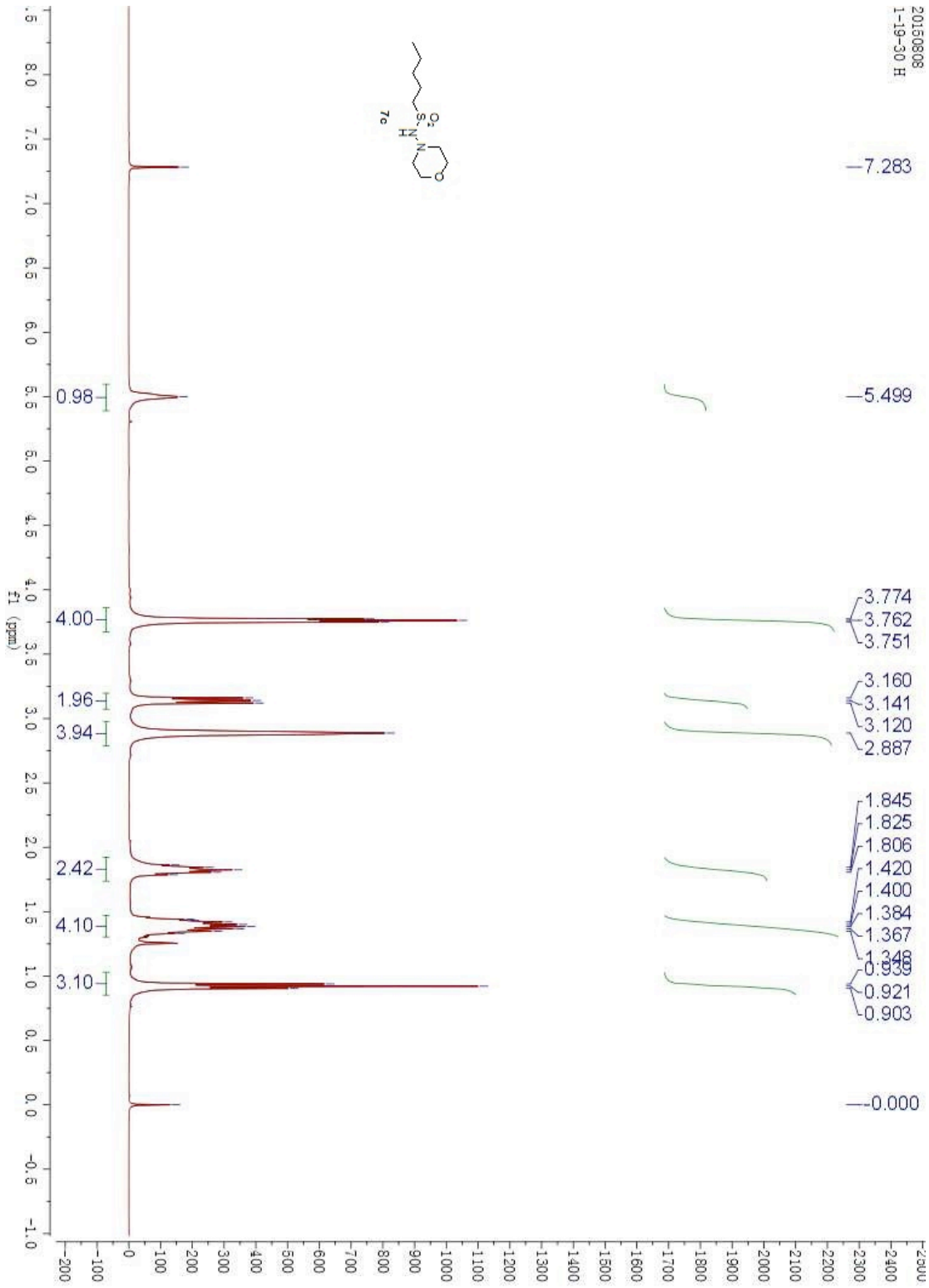

20150808
1-19-40 C
3aj
146.77
138.64
132.99
129.02
128.72
128.19
123.96
120.71
77.32
77.00
76.68
f1 (ppm)

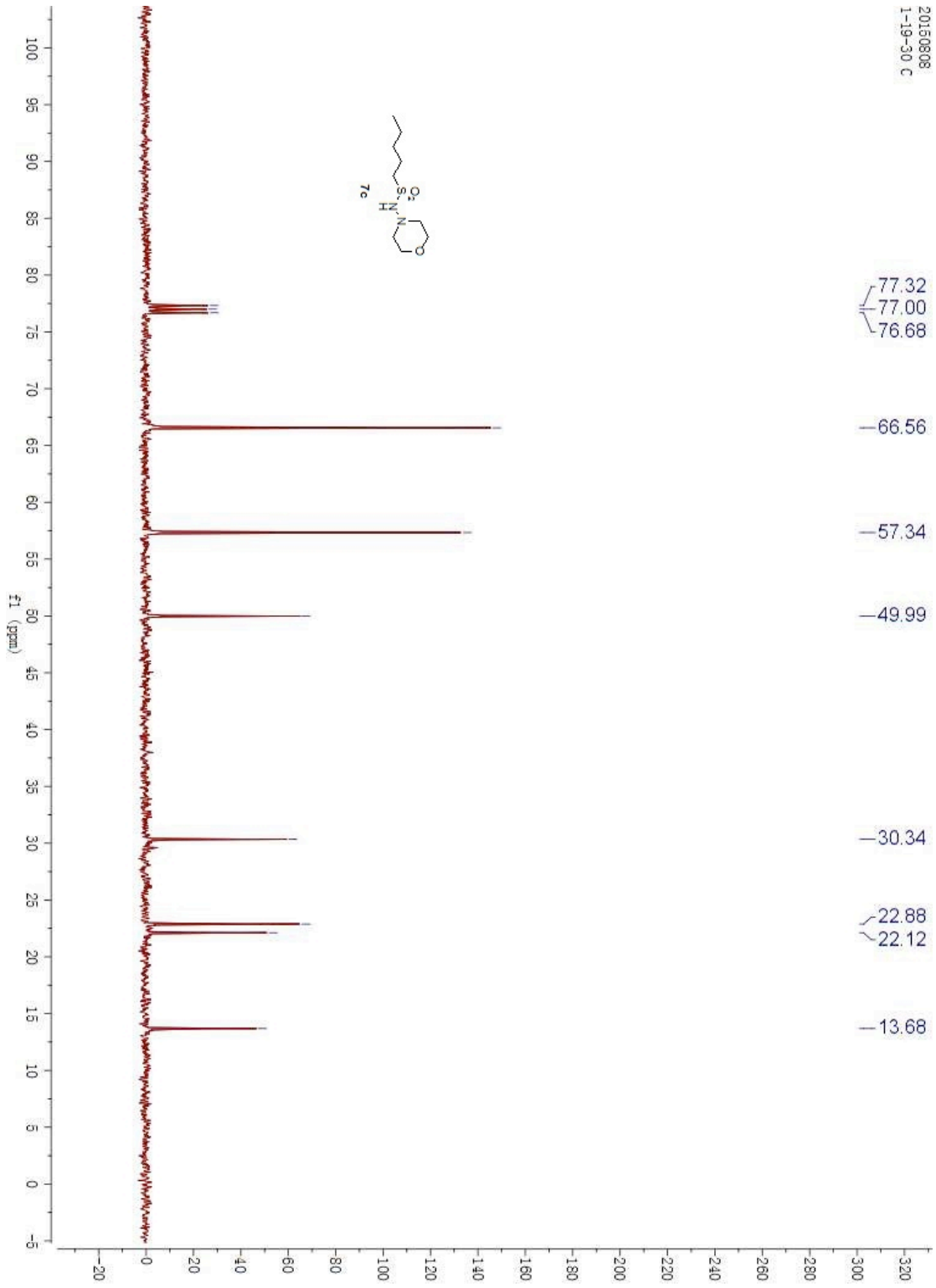

20150808
1-19-14
7.283
5.303
3.771
3.760
3.748
3.147
3.139
3.130
3.109
2.891
2.881
2.199
2.170
1.928
1.921
1.895
1.583
1.575
1.552
1.544
1.309
1.285
1.277
1.253
1.246
1.221
0.000
0.97
4.00
1.03
4.04
2.05
2.11
1.10
2.06
3.49
f1 (ppm)
7a

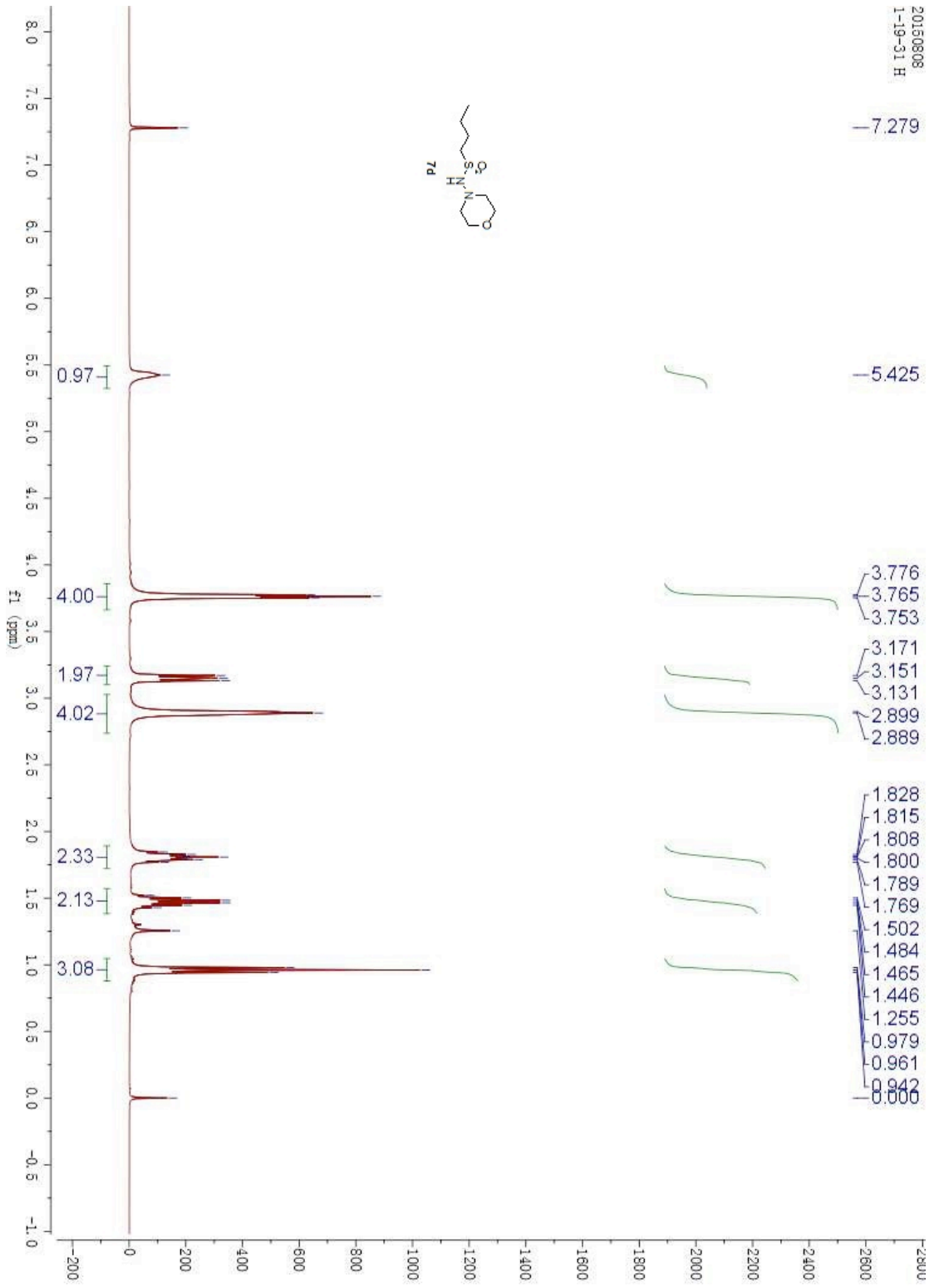

20150808
1-19-14 C
7a
77.32
77.00
76.68
66.55
58.54
57.48
26.18
25.17
25.09
f1 (ppm)

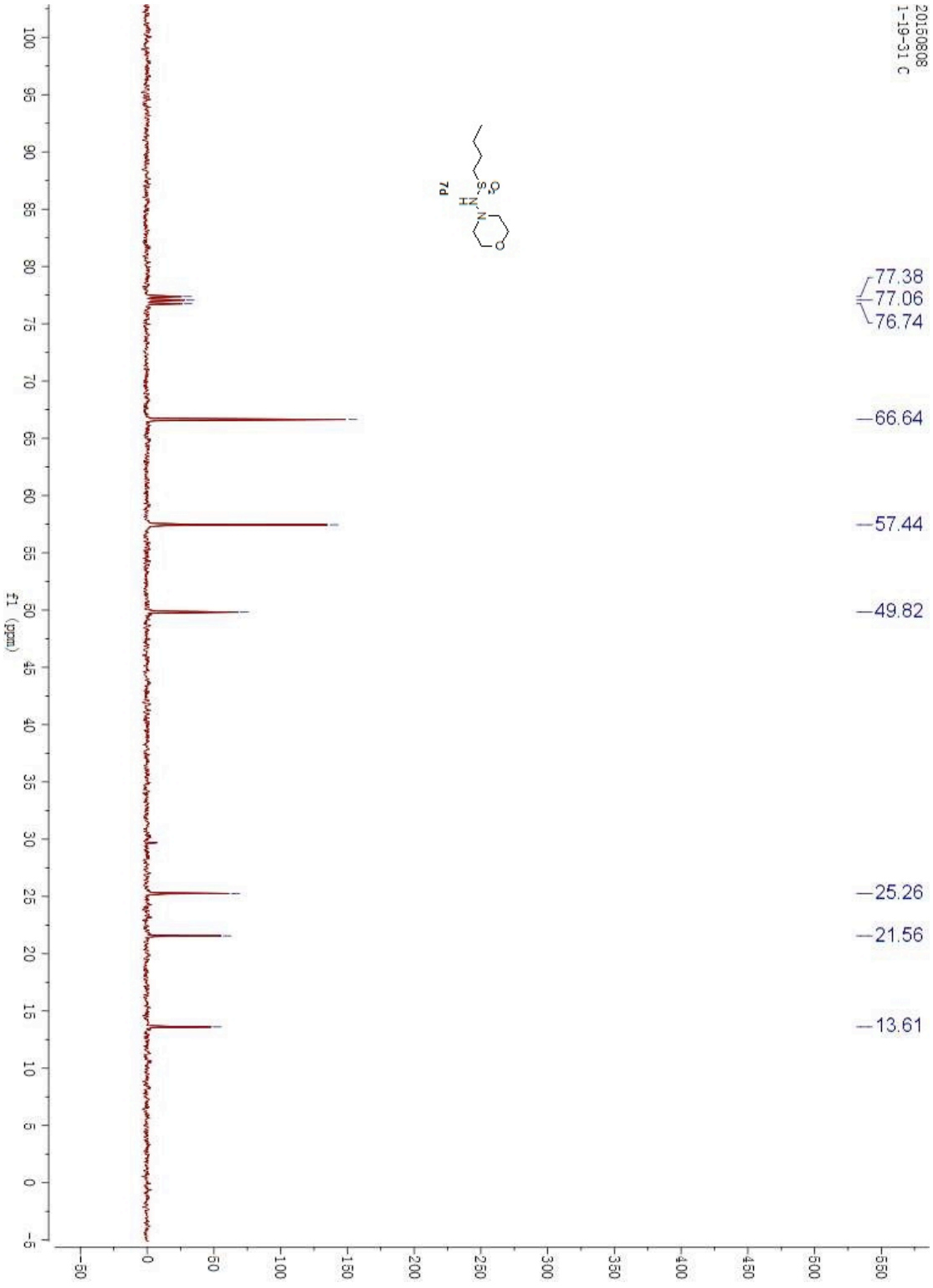

20150808
1-19-21 H
7b
7.281
5.433
3.773
3.762
3.750
3.051
3.036
2.883
1.976
1.947
1.741
1.733
1.708
1.326
1.301
1.295
1.263
1.255
1.184
1.144
1.111
1.077
0.000
0.95
4.00
1.99
3.86
3.05
3.09
2.47
3.19
f1 (ppm)

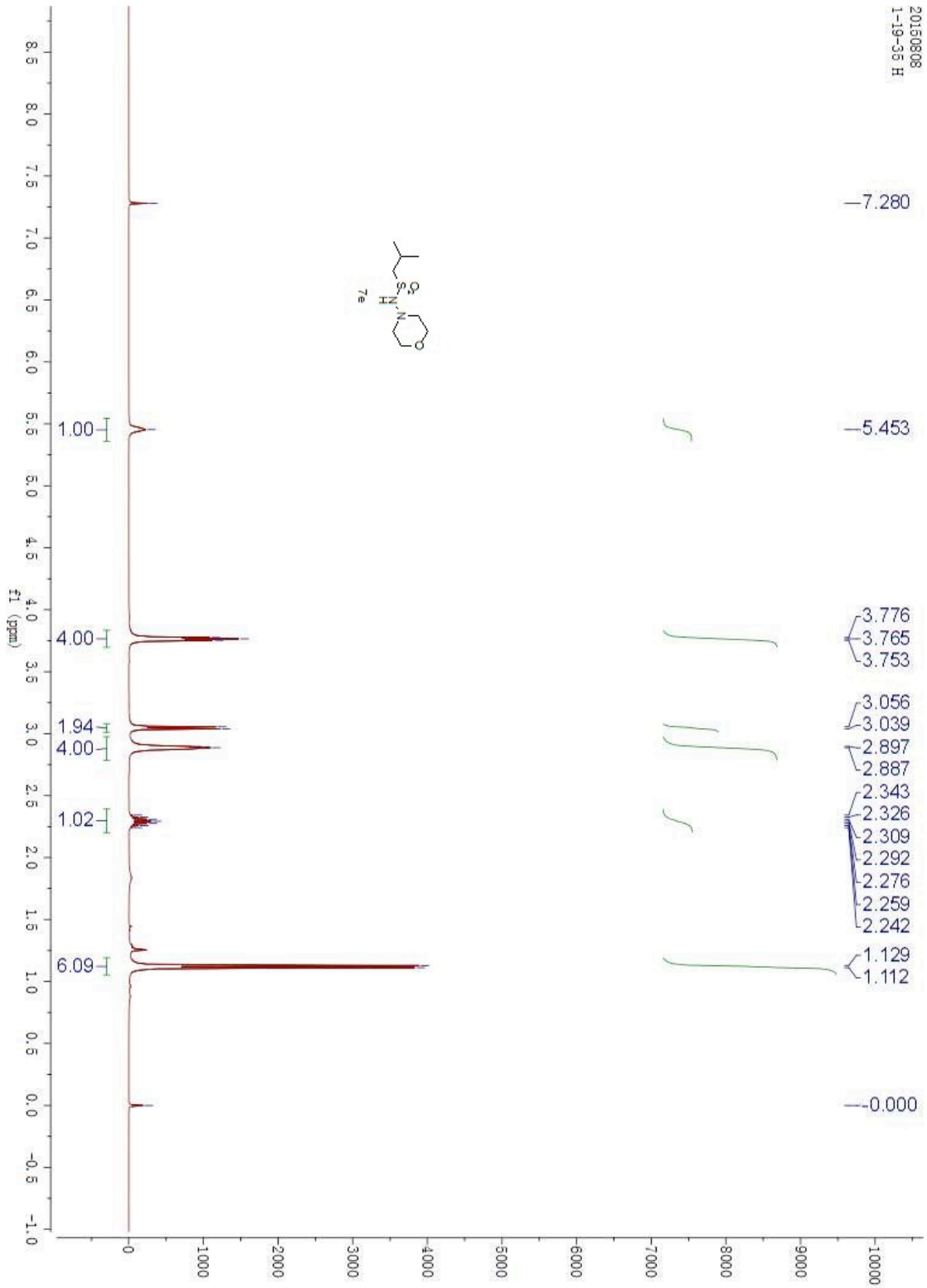

20150808
1-19-21 C
7b
66.63
57.44
56.67
33.36
33.04
25.84
25.79
f1 (ppm)

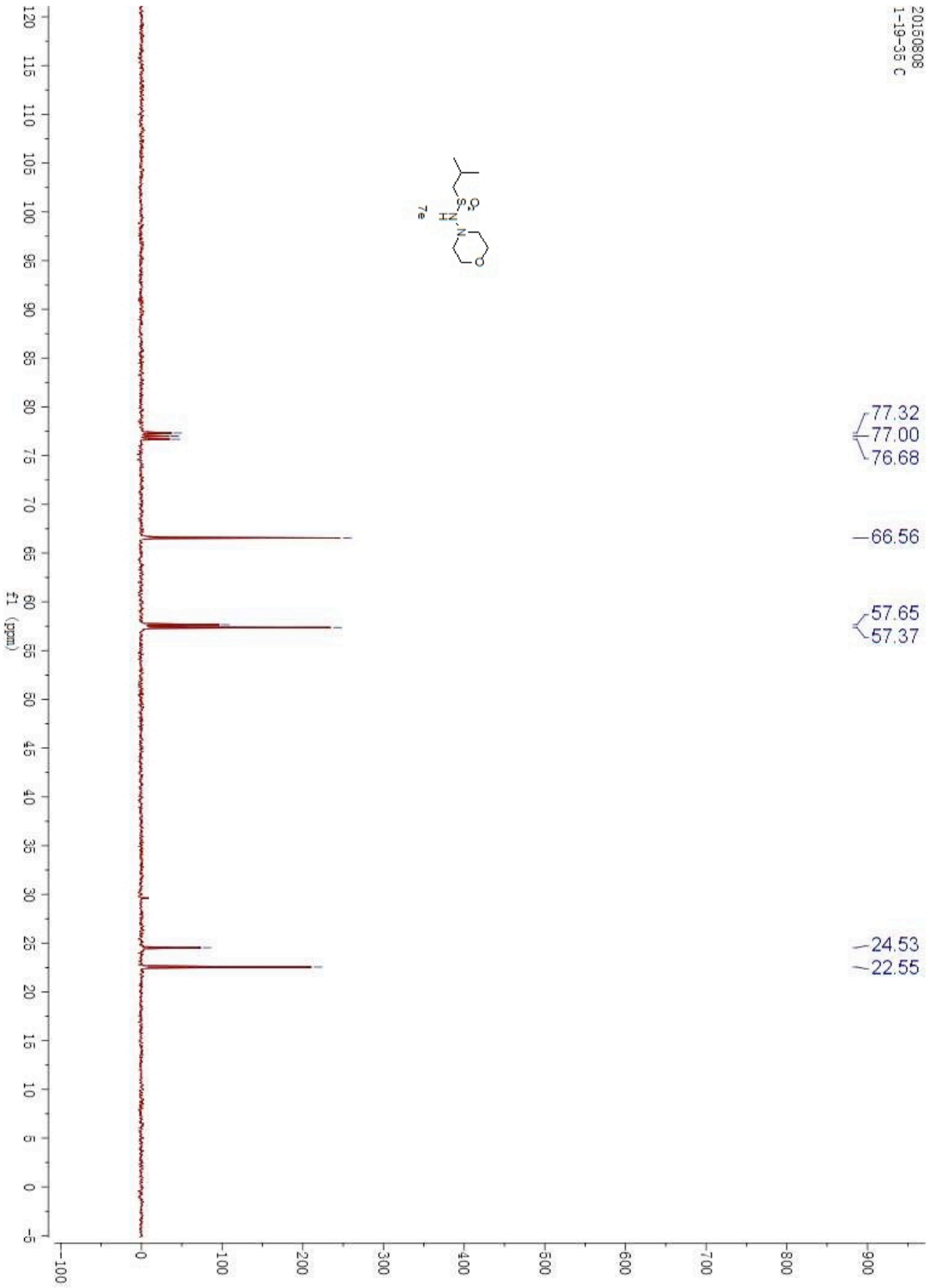

20150808
1-19-30 H
7e
7.283
5.499
3.774
3.762
3.751
3.160
3.141
3.120
2.887
1.845
1.825
1.806
1.420
1.400
1.384
1.367
1.348
0.939
0.921
0.903
0.000
0.98
4.00
1.96
3.94
2.42
4.10
3.10
f1 (ppm)

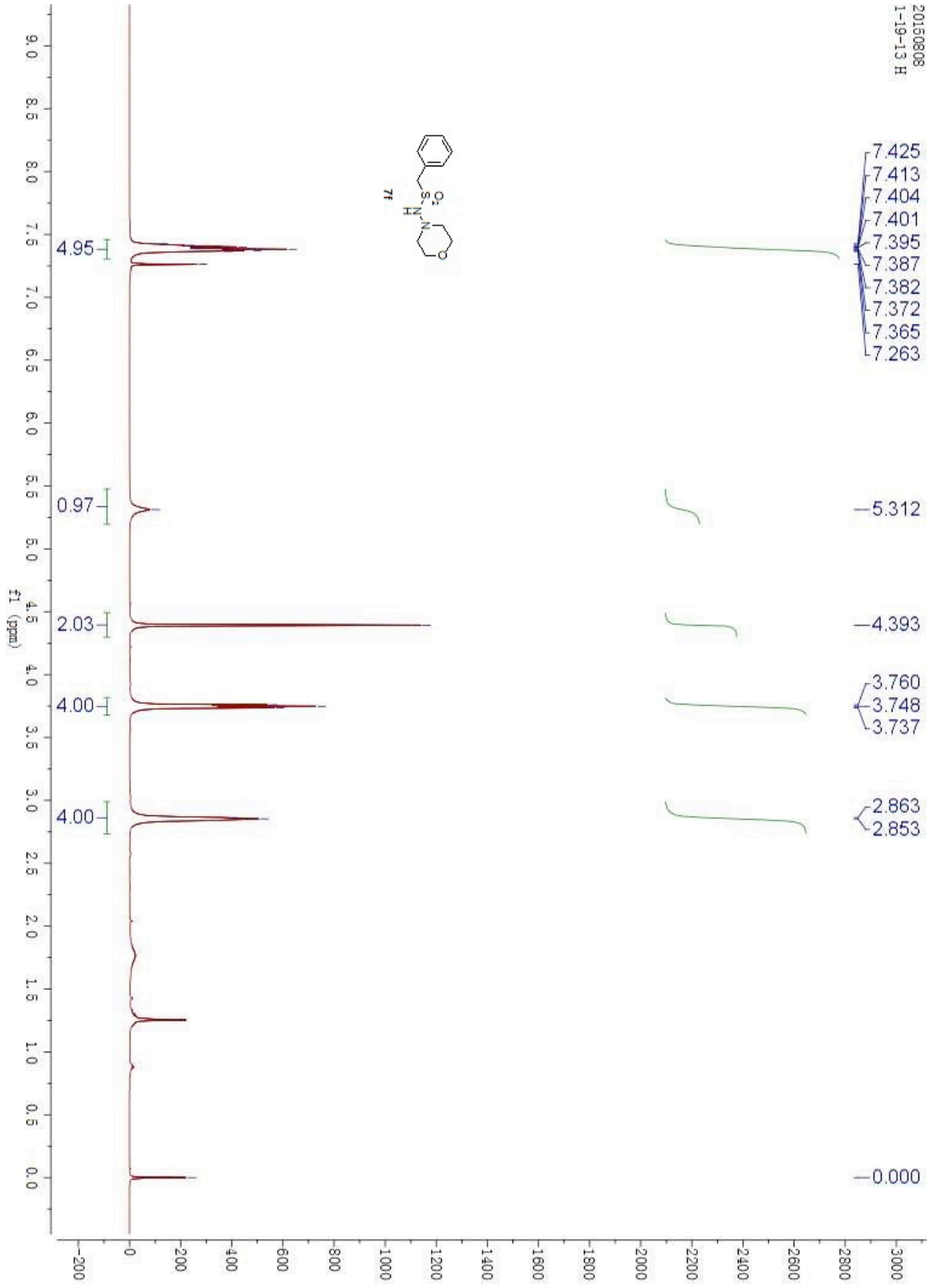

20150808
1-19-30 C
77.32
77.00
76.68
66.56
57.34
49.99
30.34
22.88
22.12
13.68
f1 (ppm)

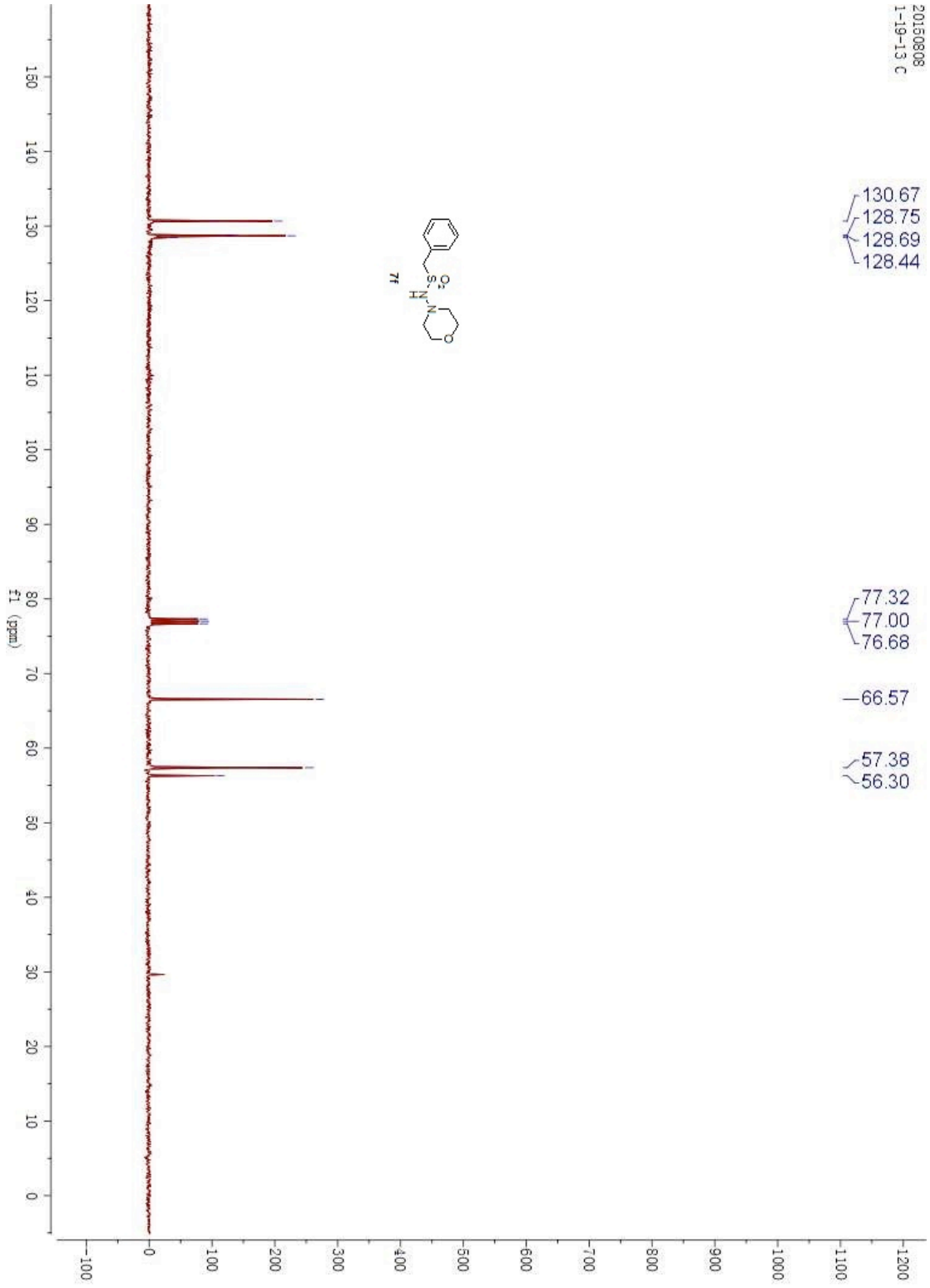

20150808
1-19-31 H
7.279
5.425
3.776
3.765
3.753
3.171
3.151
3.131
2.899
2.889
1.828
1.815
1.808
1.800
1.789
1.769
1.502
1.484
1.465
1.446
1.255
0.979
0.961
0.942
0.000
0.97
4.00
1.97
4.02
2.33
2.13
3.08
f1 (ppm)

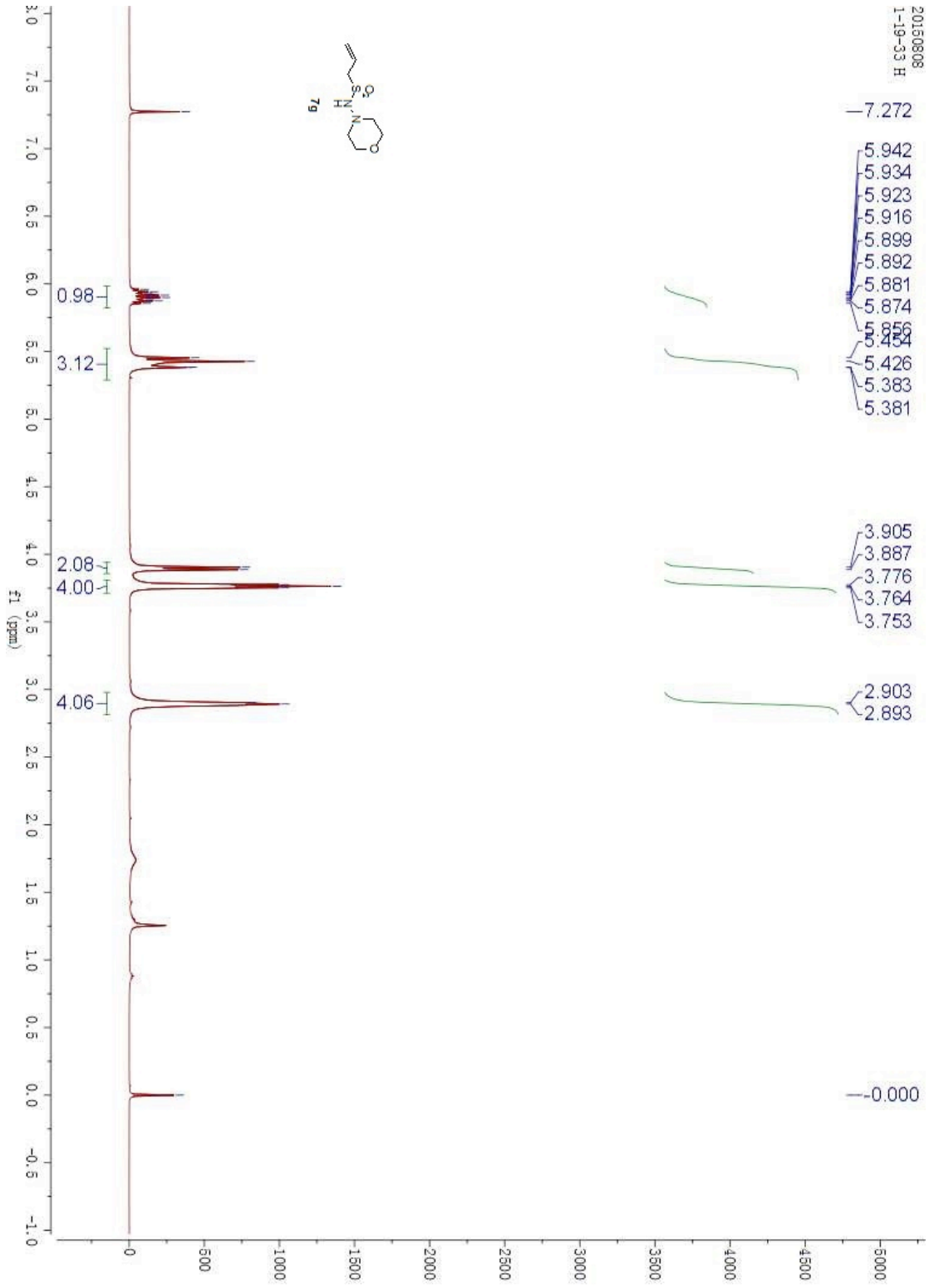

20150808
1-19-31 C
7d
77.38
77.06
76.74
66.64
57.44
49.82
25.26
21.56
13.61
f1 (ppm)

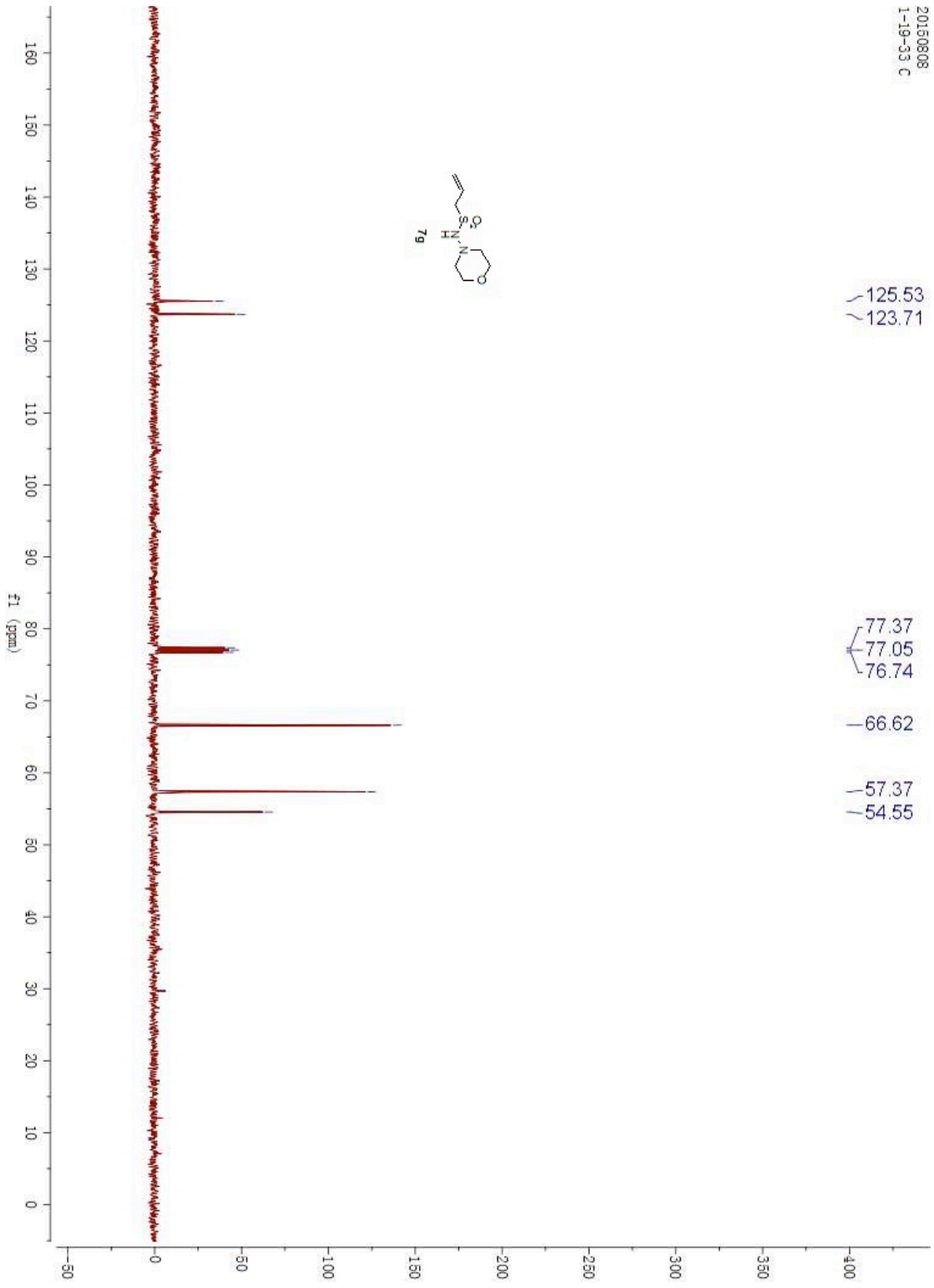

20150808
1-19-35 H
7.280
5.453
3.776
3.765
3.753
3.056
3.039
2.897
2.887
2.343
2.326
2.309
2.292
2.276
2.259
2.242
1.129
1.112
0.000
1.00
4.00
1.94
4.00
1.02
6.09
f1 (ppm)

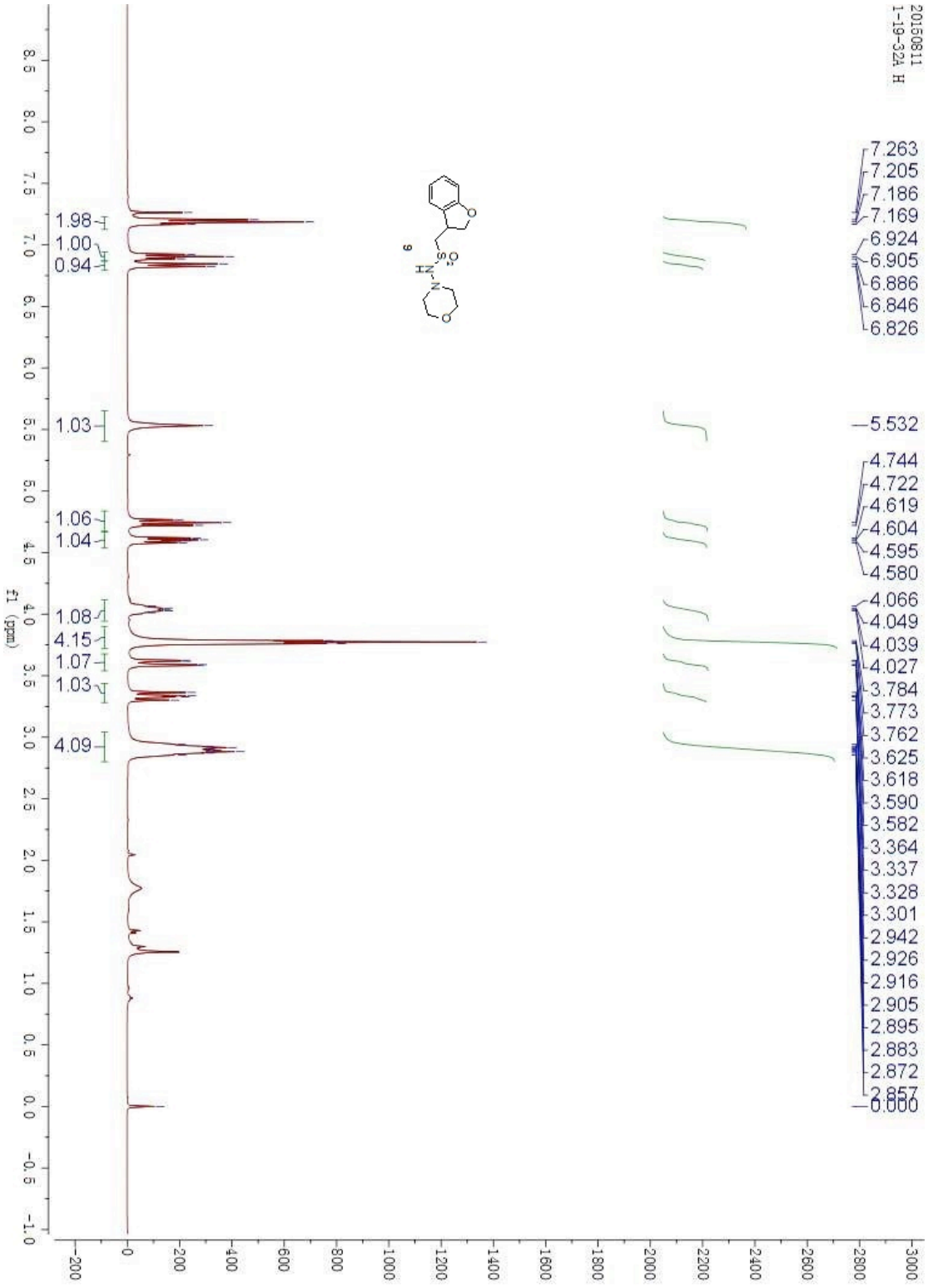

20150808
1-19-3S C
77.32
77.00
76.68
66.56
57.65
57.37
24.53
22.55
f1 (ppm)
7e

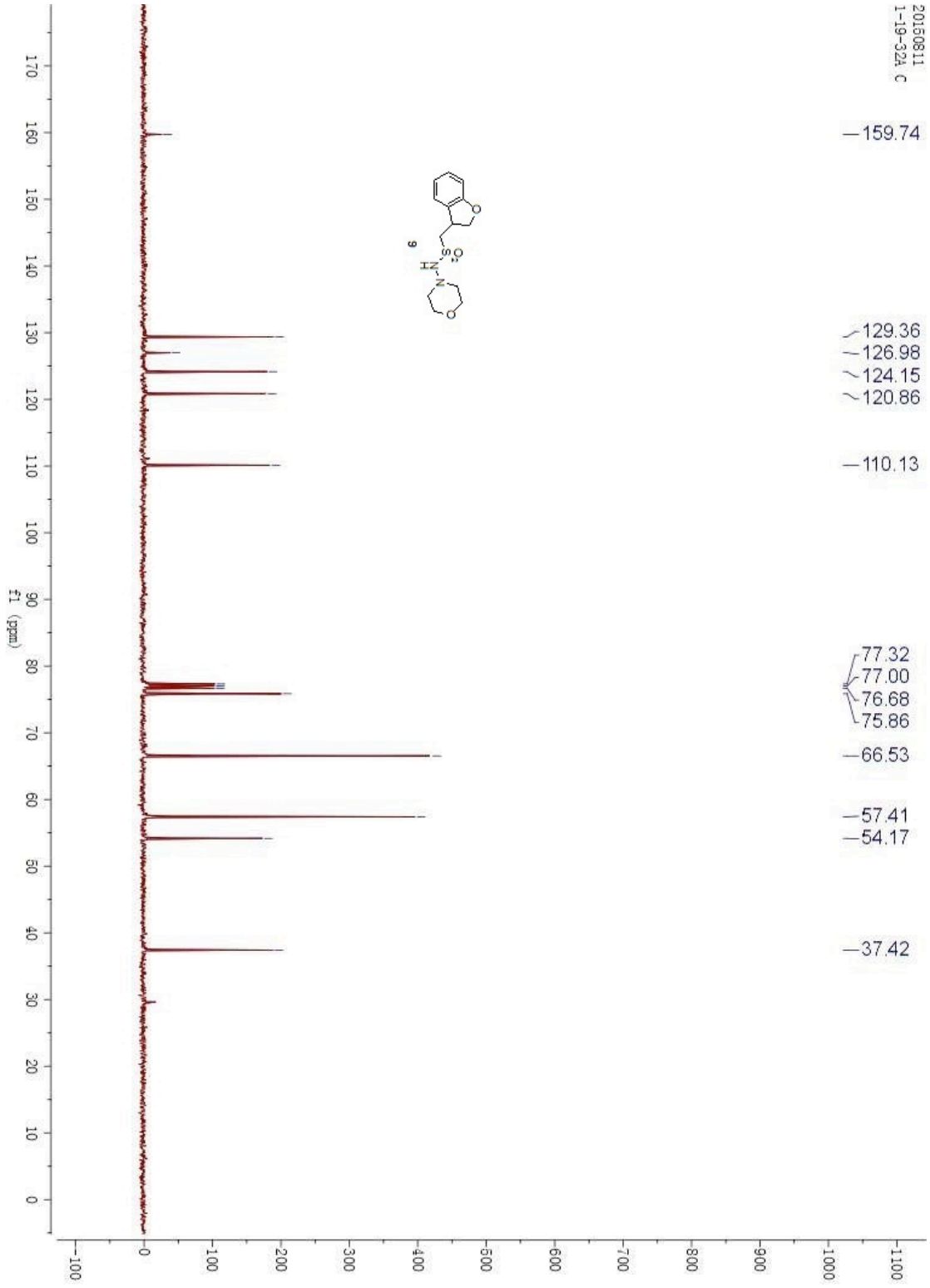

20150808
1-19-13 H
7.425
7.413
7.404
7.401
7.395
7.387
7.382
7.372
7.365
7.263
5.312
4.393
3.760
3.748
3.737
2.863
2.853
0.000
4.95
0.97
2.03
4.00
4.00
f1 (ppm)


20150808
1-19-13 C
130.67
128.75
128.69
128.44
77.32
77.00
76.68
66.57
57.38
56.30
7f
f1 (ppm)


20150808
1-19-33 H
7.272
5.942
5.934
5.923
5.916
5.899
5.892
5.881
5.874
5.856
5.454
5.426
5.383
5.381
3.905
3.887
3.776
3.764
3.753
2.903
2.893
-0.000
0.98
3.12
2.08
4.00
4.06
f1 (ppm)


20150808
1-19-33 C
7g
125.53
123.71
77.37
77.05
76.74
66.62
57.37
54.55
f1 (ppm)


20150811
1-19-32A H
7.263
7.205
7.186
7.169
6.924
6.905
6.886
6.846
6.826
5.532
4.744
4.722
4.619
4.604
4.595
4.580
4.066
4.049
4.039
4.027
3.784
3.773
3.762
3.625
3.618
3.590
3.582
3.364
3.337
3.328
3.301
2.942
2.926
2.916
2.905
2.895
2.883
2.872
2.857
0.000
1.98
1.00
0.94
1.03
1.06
1.04
1.08
4.15
1.07
1.03
4.09
f1 (ppm)


20150811
1-19-32A C
159.74
129.36
126.98
124.15
120.86
110.13
77.32
77.00
76.68
75.86
66.53
57.41
54.17
37.42
f1 (ppm)