Electronic Supplementary Material (ESI) for ChemComm.

Thiourea dioxide as the source of sulfonyl group: Photoredox generation of sulfones and sulfonamides from heteroaryl/aryl halides

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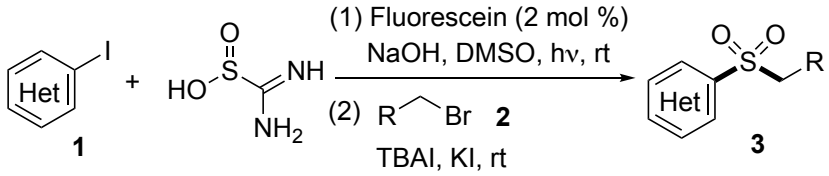
Supporting Information

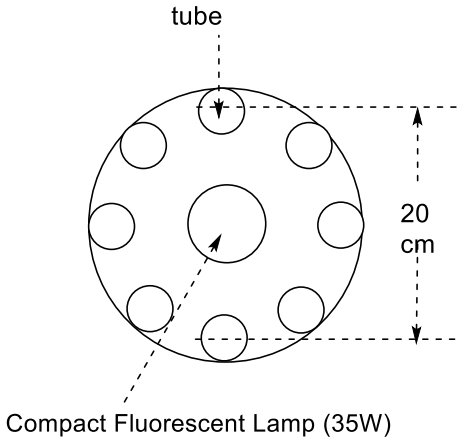
General experimental methods:

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 NMR、^{19}F NRM and ^{13}C NMR spectra were recorded in $CDCl_3$ on a Bruker DRX - 400 spectrometer operating at 400 MHz、376 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.

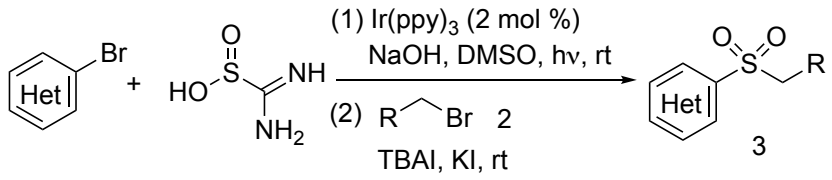
*General experimental procedure for the visible-light-induced sulfonylation of heteroaryl/aryl iodides **1** with thiourea dioxide and alkyl halides **2**.*



A dry tube was charged with heteroaryl/aryl iodide (**1**, 0.2 mmol), thiourea dioxide (0.4 mmol), NaOH (0.8 mmol) and fluorescein (2.0 mol %), sealed with a rubber stopper, evacuated and backfilled with argon for four times before the addition of DMSO (3.0 mL) via a syringe. The mixture was stirred and irradiated with a commercially available 35 W CFL for 16 h. Subsequently, TBAI (0.02 mmol, 7.4 mg), KI (0.24 mmol, 40.0 mg) and alkyl halide **2** (0.4 mmol) were added to the reaction before the tube was evacuated and backfilled with argon three times and stirred at room temperature for another 12 h. After completion of the reaction as indicated by TLC, the mixture was quenched with saturated brine. The mixture was extracted with ethyl acetate (20 mL) for three times. The organic phases were combined and dried over anhydrous Na_2SO_4. The solvent was evaporated *in vacuo*, and purified by flash column chromatography (EtOAc/*n*-hexane, 1:4) to give the desired product **3**.

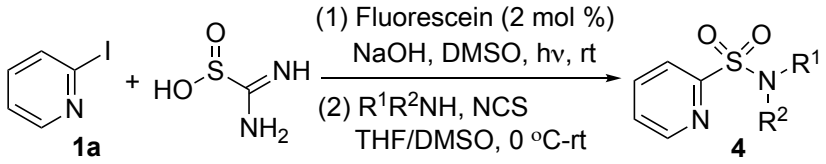


General experimental procedure for the visible-light-induced sulfonylation of heteroaryl/aryl bromides with thiourea dioxide and alkyl halides ***2***.



A dry tube was charged with heteroaryl/aryl bromide (0.2 mmol), thiourea dioxide (0.4 mmol), NaOH (0.8 mmol) and $Ir(ppy)_3$ (2.0 mol %), sealed with a rubber stopper, evacuated and backfilled with argon for four times before the addition of DMSO (3.0 mL) via a syringe. The mixture was stirred and irradiated with a commercially available 15 W Blue LED for 16 h. Subsequently, TBAI (0.02 mmol, 7.4 mg), KI (0.24 mmol, 40.0 mg) and alkyl halide **2** (0.4 mmol) were added to the reaction before the tube was evacuated and backfilled with argon three times and stirred at room temperature for another 12 h. After completion of the reaction as indicated by TLC, the mixture was quenched with saturated brine. The mixture was extracted with ethyl acetate (20 mL) for three times. The organic phases were combined and dried over anhydrous Na_2SO_4. The solvent was evaporated *in vacuo*, and purified by flash column chromatography (EtOAc/*n*-hexane, 1:4) to give the desired product **3**.

*General experimental procedure for the aminosulfonylation of 2-iodopyridine **1a***

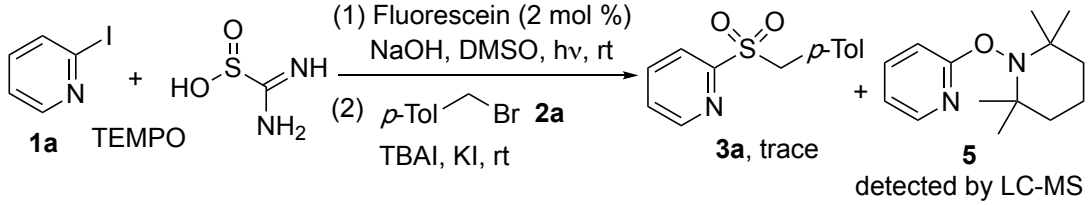


A dry tube was charged with 2-iodopyridine **1a** (0.2 mmol), thiourea dioxide (0.4 mmol), NaOH (0.8 mmol), fluorescein (2.0 mol %), sealed with a rubber stopper, evacuated and backfilled with argon for four times before the addition of DMSO (3.0 mL) via a syringe. The mixture was stirred and irradiated with a commercially available 35 W CFL for 16 h. Subsequently, THF (8 mL) and amine (0.4 mmol) were added to the mixture via a syringe, followed by dropwise addition of *N*-chlorosuccinimide (0.3 mmol, dissolved in THF) at 0 °C in 30 minutes. The reaction mixture was warmed to room temperature and stirred for 2 hours. After completion of the reaction as indicated by TLC, the mixture was quenched with saturated brine. The mixture was extracted with ethyl acetate (20 mL) for three times. The organic phases were combined and dried over anhydrous Na_2SO_4. The solvent was evaporated *in vacuo*, and purified by flash column chromatography (EtOAc/*n*-hexane, 1:4) to give the desired product **4**.

A typical example for the gram-scale experiment

A dry falsk was charged with thiourea dioxide (1.05 g), NaOH (0.78 g), fluorescein (2 mol %), sealed with a rubber stopper, evacuated and backfilled with argon for four times before the addition of DMSO (15 mL) and 2-iodopyridine **1a** (1.0 g) via syringe. Then the mixture was stirred and irradiated with a commercially available 100 W CFL for 24 h. Subsequently, TBAI (0.18 g), KI (0.97 g) and 4-methylbenzyl bromide **2a** (1.8 g) were added to the reaction before the falsk was evacuated and backfilled with argon three times and stirred at room temperature for another 12h. After completion of the reaction as indicated by TLC, the mixture was quenched with brine. The mixture was extracted with ethyl acetate for three times. The organic phases were combined and dried over anhydrous Na_2SO_4. The solvent was evaporated in vacuo, and purified by flash column chromatography (EtOAc/n-hexane, 1:4) to give the desired product **3a** (0.94 g, 78%).

Radical trapping experiment



A dry tube was charged with thiourea dioxide (0.4 mmol), NaOH (0.8 mmol), fluorescein (2.0 mol %) and TEMPO (0.4 mmol), sealed with a rubber stopper, evacuated and backfilled with argon for four times before the addition of DMSO (3.0 mL) via a syringe. Subsequently, 2-iodopyridine **1a** (0.2 mmol) was added to the solution, then the mixture was stirred and irradiated with a commercially available 35 W CFL for 16 h. Subsequently, TBAI (0.02 mmol, 7.4 mg), KI (0.24 mmol, 40.0 mg) and 1-(bromomethyl)-4-methylbenzene **2a** (0.4 mmol) were added to the reaction before the tube was evacuated and backfilled with argon three times and stirred at room temperature for another 12h. After completion of the reaction as indicated by TLC, only a trace of the desired product **3a** was detected. The mixture was analyzed by LC-MS, and product **5** was detected [HRMS calcd for $C_{14}H_{23}N_2O$ ($M+H^+$): 235.1805, found: 235.1811].

EPR experiments.

1) Procedure for EPR investigation of Fluorescein and NaOH in DMSO.

A dry tube was charged with Fluorescein (0.0002 mmol, 1.3 mg) and NaOH (0.8 mmol, 32.0 mg), sealed with a rubber stopper, evacuated and backfilled with argon for four times before the addition of DMSO (3.0 mL) via a syringe. Then 5,5-dimethyl-1-pyrroline *N*-oxide (11.3 mg, 0.1 mmol) was added. The mixture was stirred and irradiated with a commercially available 35 W CFL for 15 min. Subsequently, the solution sample was taken out into a small tube, and then analyzed by EPR. As shown in Figure S1, no obvious signal was observed.

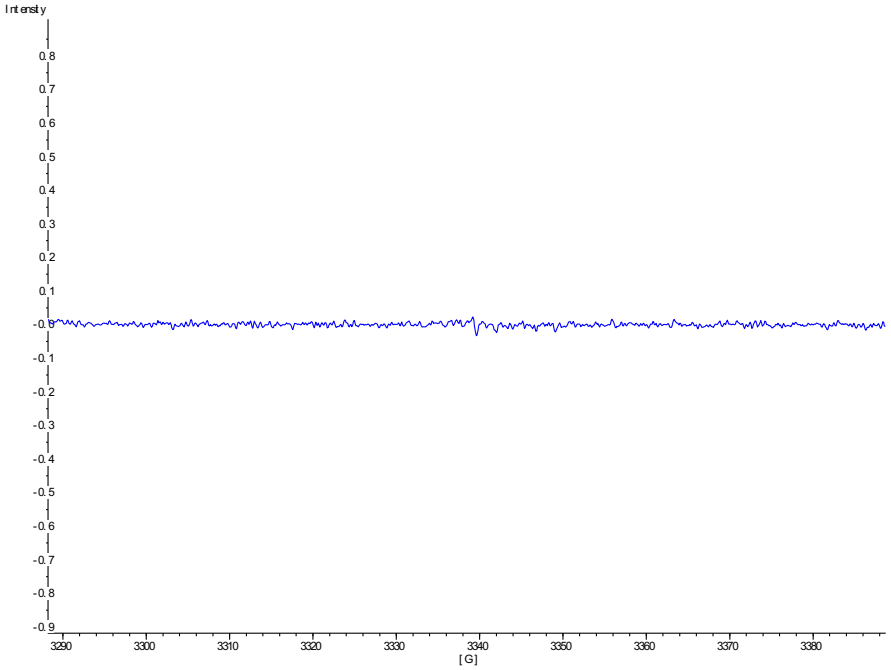


Figure S1. *EPR Investigation of Fluorescein and NaOH in DMSO.*

2) Procedure for EPR investigation of thiourea dioxide and NaOH in DMSO.

A dry tube was charged with thiourea dioxide (0.4 mmol, 43.2 mg) and NaOH (0.8 mmol, 32.0 mg), sealed with a rubber stopper, evacuated and backfilled with argon for four times before the addition of DMSO (3.0 mL) via a syringe. Then 5,5-dimethyl-1-pyrroline *N*-oxide (11.3 mg, 0.1 mmol) was added. The mixture was stirred and irradiated with a commercially available 35 W CFL for 15 min.

Subsequently, the solution sample was taken out into a small tube, and then analyzed by EPR. As shown in Figure S2, no obvious signal was observed.

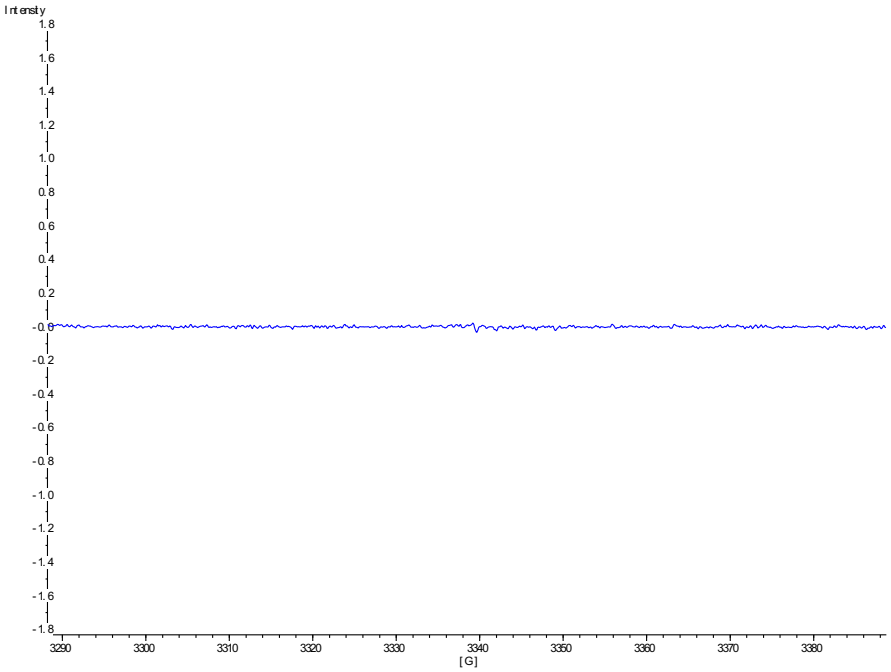


Figure S2. *EPR Investigation of Thiourea dioxide and NaOH in DMSO.*

3) Procedure for EPR investigation of Fluorescein, thiourea dioxide and NaOH in DMSO.

A dry tube was charged with Fluorescein (0.0002 mmol, 1.3 mg), thiourea dioxide (0.4 mmol, 43.2 mg) and NaOH (0.8 mmol, 32.0 mg), sealed with a rubber stopper, evacuated and backfilled with argon for four times before the addition of DMSO (3.0 mL) via a syringe. Then 5,5-dimethyl-1-pyrroline *N*-oxide (11.3 mg, 0.1 mmol) was added. The mixture was stirred and irradiated with a commercially available 35 W CFL for 15 min. Subsequently, the solution sample was taken out into a small tube, and then analyzed by EPR. As shown in Figure S3, a distinct signal of a trapped radical was observed.

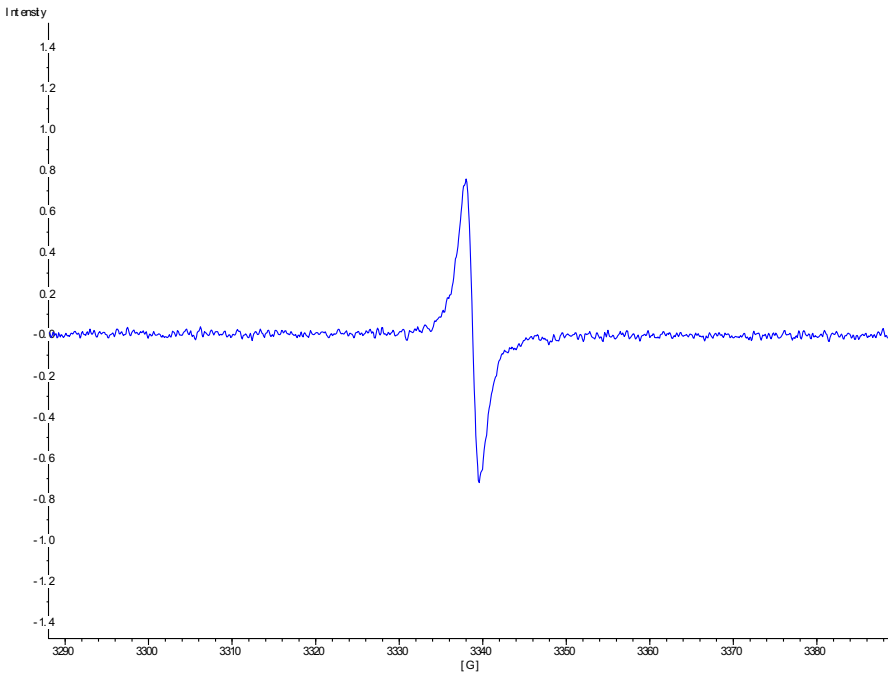


Figure S3. *EPR Investigation of Fluorescein, Thiourea dioxide and NaOH in DMSO.*

4) Procedure for EPR investigation of 2-Iodopyridine, thiourea dioxide and NaOH in DMSO.

A dry tube was charged with thiourea dioxide (0.4 mmol, 43.2 mg) and NaOH (0.8 mmol, 32.0 mg), sealed with a rubber stopper, evacuated and backfilled with argon for four times before the addition of DMSO (3.0 mL) via a syringe. Then 2-iodopyridine (**1a**) (0.2 mmol) and 5,5-dimethyl-1-pyrroline *N*-oxide (11.3 mg, 0.1 mmol) were added. The mixture was stirred and irradiated with a commercially available 35 W CFL for 15 min. Subsequently, the solution sample was taken out into a small tube, and then analyzed by EPR. As shown in Figure S4, a distinct signal of a trapped radical was observed.

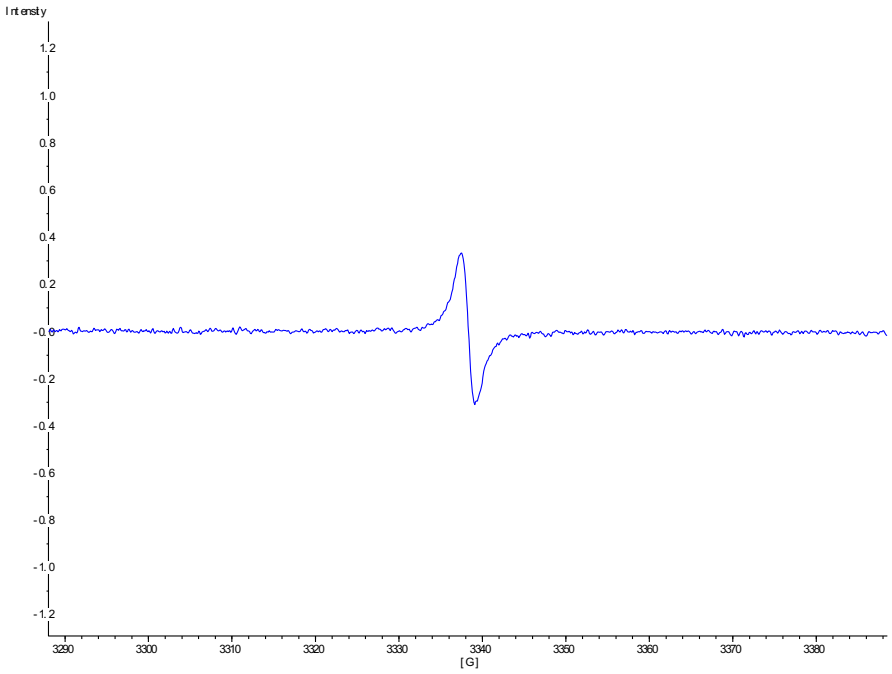


Figure S4. *EPR Investigation of 2-Iodopyridine, Thiourea dioxide and NaOH in DMSO.*

5) Procedure for EPR investigation of Fluorescein, 2-iodopyridine, thiourea dioxide and NaOH in DMSO.

A dry tube was charged with Fluorescein (0.0002 mmol, 1.3 mg), thiourea dioxide (0.4 mmol, 43.2 mg) and NaOH (0.8 mmol, 32.0 mg), sealed with a rubber stopper, evacuated and backfilled with argon for four times before the addition of DMSO (3.0 mL) via a syringe. Then 2-iodopyridine (**1a**) (0.2 mmol) and 5,5-dimethyl-1-pyrroline *N*-oxide (11.3 mg, 0.1 mmol) were added. The mixture was stirred and irradiated with a commercially available 35 W CFL for 15 min. Subsequently, the solution sample was taken out into a small tube, and then analyzed by EPR. As shown in Figure S5, a distinct signal of a trapped radical was observed.

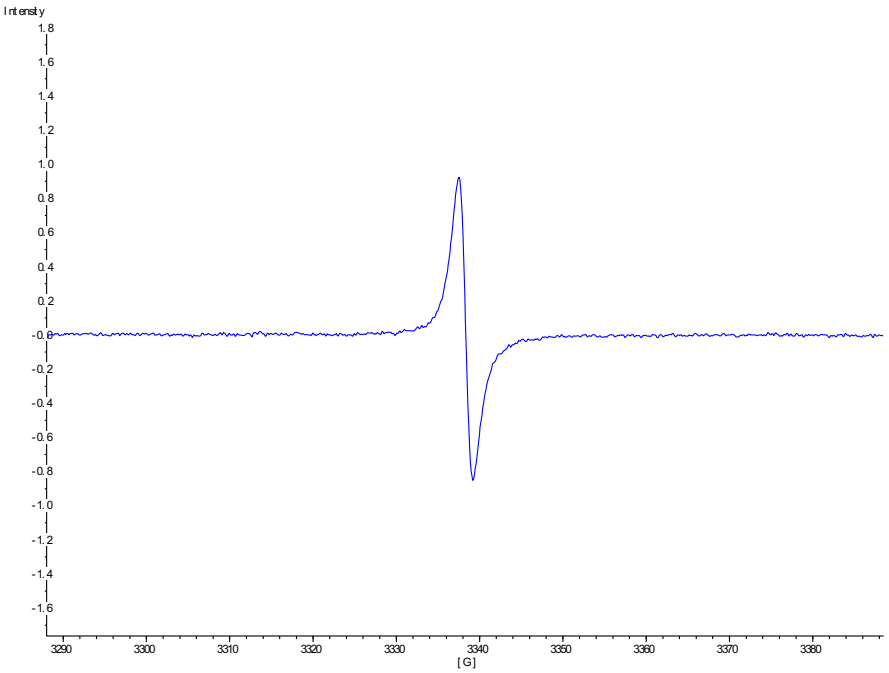


Figure S5. *EPR Investigation of Fluorescein, 2-Iodopyridine, Thiourea dioxide and NaOH in DMSO.*

6) Procedure for EPR investigation of Fluorescein, 2-iodopyridine, and NaOH in DMSO.

A dry tube was charged with Fluorescein (0.0002 mmol, 1.3 mg) and NaOH (0.8 mmol, 32.0 mg), sealed with a rubber stopper, evacuated and backfilled with argon for four times before the addition of DMSO (3.0 mL) via a syringe. Then 2-iodopyridine (**1a**) (0.2 mmol) and 5,5-dimethyl-1-pyrroline *N*-oxide (11.3 mg, 0.1 mmol) were added. The mixture was stirred and irradiated with a commercially available 35 W CFL for 15 min. Subsequently, the solution sample was taken out into a small tube, and then analyzed by EPR. As shown in Figure S6, no obvious signal was observed.

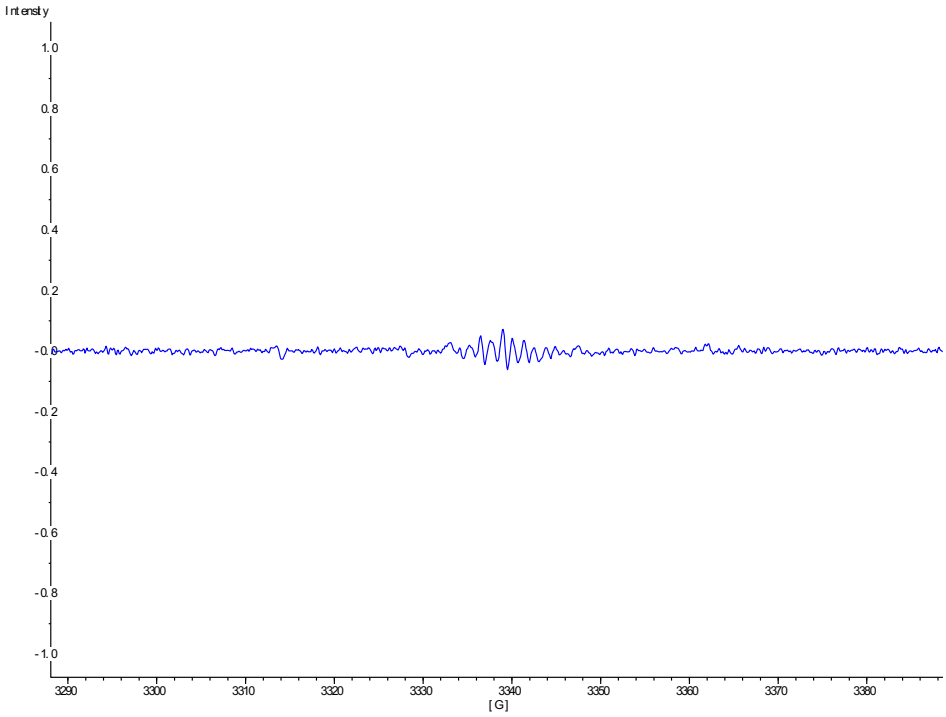
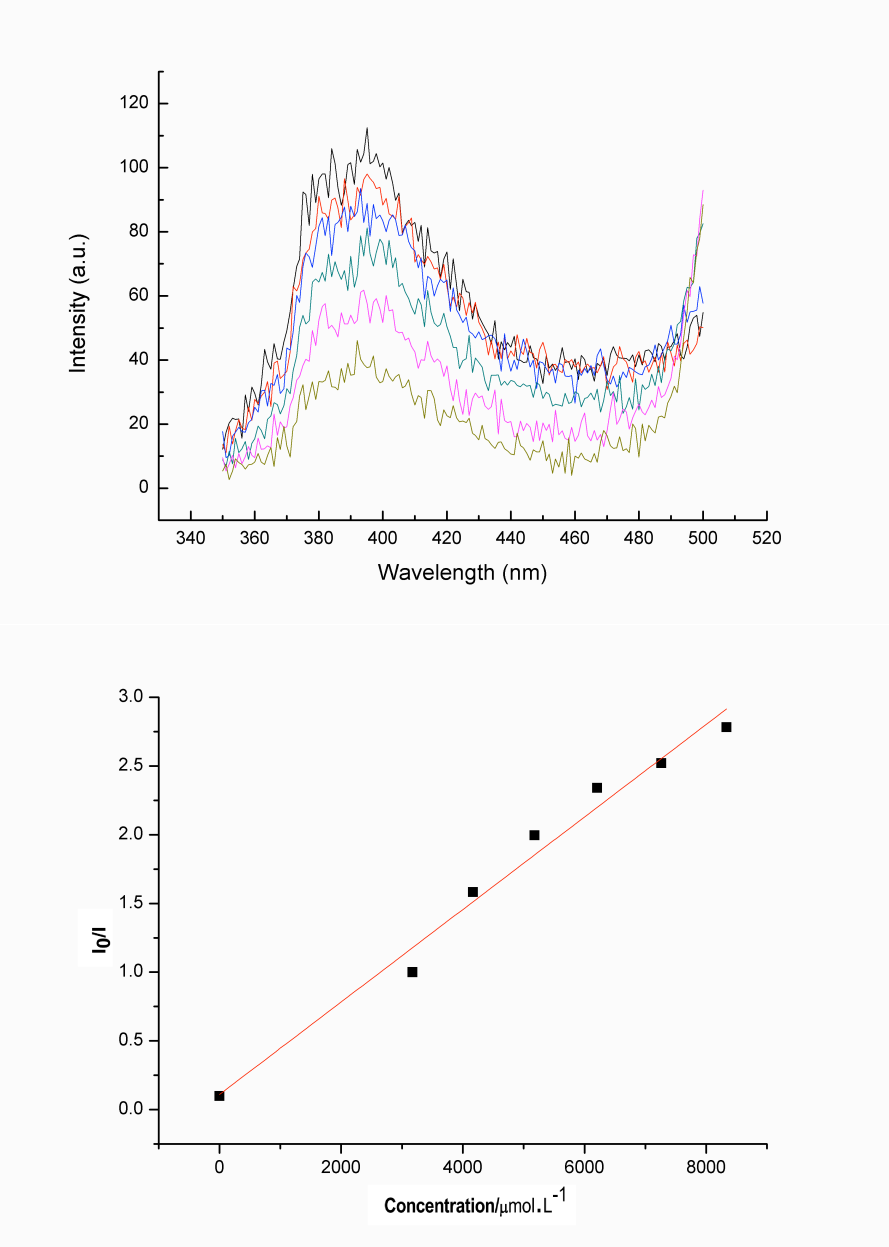


Figure S6. *EPR Investigation of Fluorescein, 2-Iodopyridine and NaOH in DMSO.*

All the results of Electron Paramagnetic Resonance (EPR) experiments shown above indicated that the excited state of fluorescein or 2-iodopyridine could react with sulfur dioxide anion **A** to afford the sulfur dioxide radical anion **B**.

Fluorescence quenching experiments

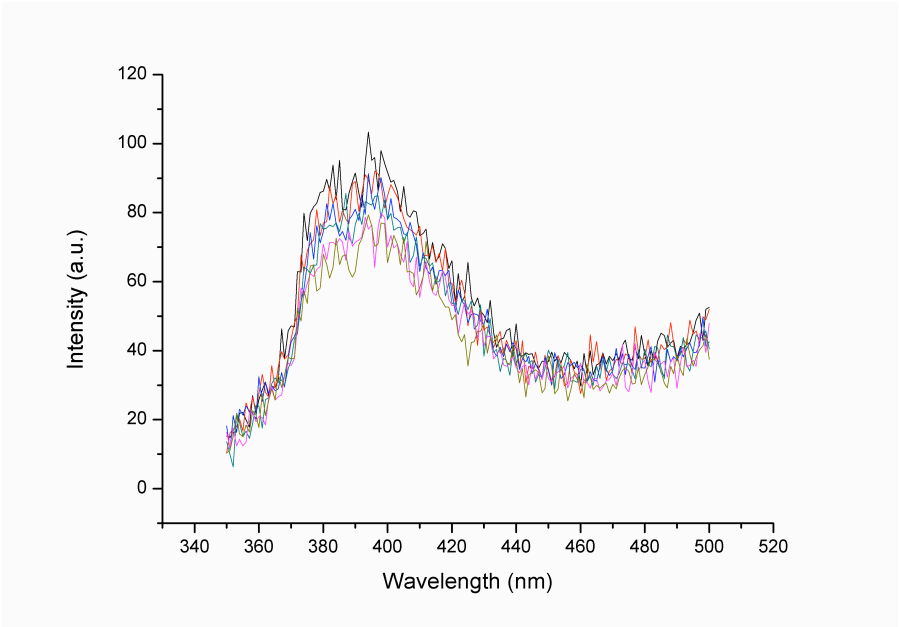
1) Luminescence quenching by thiourea dioxide and NaOH (1:2)



Fluorescence spectra were collected on Cary Eclipse Fluorescence Spectrophotometer. The solvent DMSO was degassed with a stream of Ar for 30 min. The fluorescein solutions were excited at 280 nm and the emission intensity at 380 - 400 nm was observed. In a typical experiment, the emission spectrum of a 8.3×10^{-3} M solution of fluorescein in DMSO was collected. Then, appropriate amount of quencher was added to the measured solution in a quartz cuvette and the emission spectrum of the sample was collected. I_0 and I represent the intensities of the

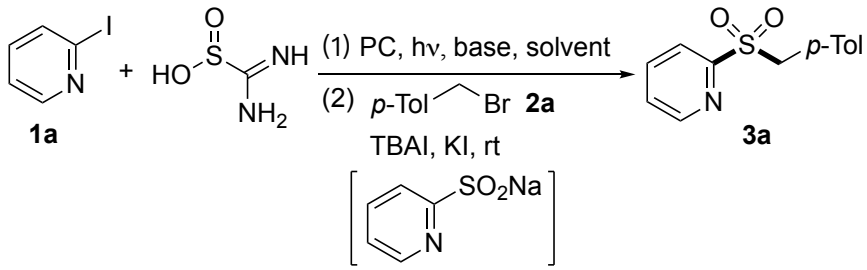
emission in the absence and presence of the quencher within the wavelength range of 380-400 nm. It supports our hypothesis on the initiation of this visible-light-induced sulfonylation reaction through reductive quenching of the excited state of the photocatalyst by sulfur dioxide anion, which is generated from the reaction of thiourea dioxide and NaOH.

*2) Luminescence quenching by 2-iodopyridine (**1a**)*



As shown above, the intensities of fluorescence emission were hardly changed with the concentration of 2-iodopyridine. It would support our hypothesis that the excited state of the photocatalyst could not be quenched by the 2-iodopyridine (**1a**).

Table S1. Optimization of reaction conditions[a]



Entry	[PC]	Base	Solvent	Yield (%)[b]
1	/	NaOH	DMF	trace
2	/	NaOH	CH_3CN	n.d.
3	/	NaOH	DCE	n.d.
4	/	NaOH	DMA	trace
5	/	NaOH	THF	n.d.
6	/	NaOH	DMSO	42
7[c]	/	NaOH	DMSO	7
8	$Ir(ppy)_3$	NaOH	DMSO	80
9	Eosin Y	NaOH	DMSO	39
10	$Ru(bpy)_3Cl_2$	NaOH	DMSO	trace
11	Rhodamin B	NaOH	DMSO	62
12	Rhodamin 6G	NaOH	DMSO	78
13	Fluorescein	NaOH	DMSO	81
14	Fluorescein	Na_2CO_3	DMSO	trace
15	Fluorescein	Cs_2CO_3	DMSO	trace
16	Fluorescein	LiO^tBu	DMSO	79
17	Fluorescein	NaO^tBu	DMSO	76
18[d]	Fluorescein	NaOH	DMSO	57
19[e]	Fluorescein	NaOH	DMSO	81

[a]Reaction conditions: photocatalyst (2 mol %), 2-iodopyridine **1a** (0.2 mmol), thiourea dioxide (0.4 mmol), base (0.8 mmol) and solvent (3.0 mL), stirred under argon with irradiation by CFL (35 W) at room temperature for 16 h, then TBAI (0.02 mmol), KI (0.24 mmol) and 1-(bromomethyl)-4-methylbenzene **2a** (0.4 mmol) were added in the cooled solution, and the mixture was stirred at room temperature for another 12 h. [b] Isolated yield based on 2-iodopyridine **1a.** [c] The reaction was performed at 50 °C. [d] In the presence of thiourea dioxide (0.3 mmol) and NaOH (0.6 mmol). [e] In the presence of thiourea dioxide (0.5 mmol) and NaOH (1.0 mmol).

DFT calculations

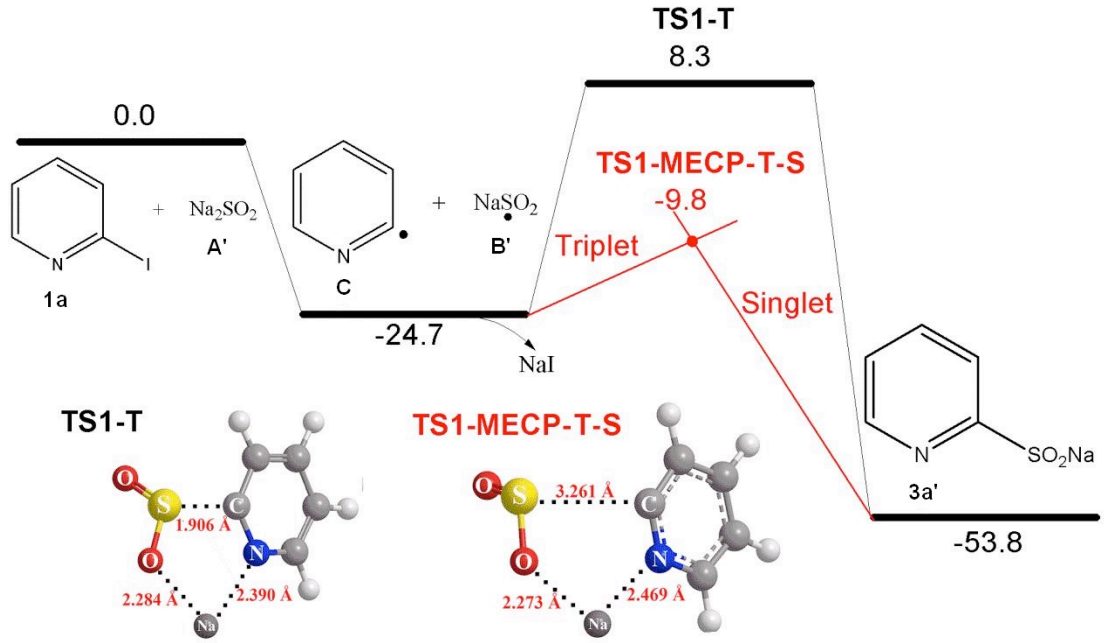


Figure S7. Free energy reaction profile (kcal/mol) in DMSO from reactants **1a** and Na_2SO_2 to sodium pyridine-2-sulfinate **3a'**, calculated at the B3LYP/6-31+G(d,p) with LANL2DZ (for I) level.

To shed light on the reaction mechanism especially on the formation of key intermediate sodium pyridine-2-sulfinate, B3LYP density functional theory (DFT) calculations were performed with the Gaussian09 software package.[S1] The free energy reaction profile is shown in Figue L1. The presence of Na_2SO_2 promotes the homolytic dissociation of Iodopyridine **1a** and subsequently single electron transfer from Na_2SO_2 to **1a** leads to the formation of radicals pyridine **C** and $NaSO_2$ **B'** and NaI. This is an exothermic process and the exothermicity is 24.7 kcal/mol. Then sodium pyridine-2-sulfinate **3a'** can be generated via spin inversion through the minimum energy crossing point (MECP), that is radicals pyridine **C** and $NaSO_2$ **B'** cross the triplet–singlet potential energy surface and then crosses over **TS1-MECP-T-S** (-9.8 kcal/mol), leading to sodium pyridine-2-sulfinate **3a'** (red line). This is the favored pathway. Another pathway via the triplet transition state **TS1-T** (8.3 kcal/mol) was also found to generate **3a'**, which is less favorable. The exothermicity of the overall reaction is 53.8 kcal/mol, which means that the whole process is thermodynamically beneficial. In addition, the attempt to locate the stationary point of negative radical iodopyridine is failed, as well as the direct nucleophilic substitution.

Computational details

The B3LYP density functional theory calculations were performed with the Gaussian09 package using 6-31+G(d,p) basis set for C, H, O, N, S and Na.[2-3] For I, we used the Lanl2DZ pseudo potential with the associated double-z basis set.[4] Structures were optimized with Truhlar and coworkers' SMD solvation model[5] in dimethylsulfoxide solution. The geometry optimizations were performed without symmetry constraints, and the nature of the extrema was checked by analytical frequency calculations. The intrinsic reaction coordinate (IRC)[6] pathways have been traced to verify two desired minima connected by the transition states.

In this study, for the reaction is a two-state reaction,[7] the minimum energy crossing point (MECP) between potential energy surface (PES) of different spin states must be located to calculate the reaction barrier. In the present work, the MECPs were located with the code developed by Harvey and co-workers[8] at B3LYP/6-31+g(d,p) (Lanl2DZ for I element) level in dimethylsulfoxide solution.

Table S2. Coordinate data sets and absolute energies for DFT optimized complexes at B3LYP/6-31+G(d,p) (Lanl2DZ for I element).

A -259.035324 a.u.

C	-3.32639700	-0.06089200	-0.00007300
C	-2.54859900	-1.21556400	-0.00014600
N	-1.20206300	-1.19086200	0.00014000
C	-0.62152700	-0.01123800	0.00049800
C	-1.28391100	1.21724200	0.00050700
C	-2.67834400	1.17656800	-0.00052400
I	1.55795000	-0.00426000	-0.00006300
H	-4.40901200	-0.13052500	-0.00028100
H	-3.00638600	-2.20164300	0.00053100
H	-0.74272800	2.15538900	0.00090300
H	-3.24609100	2.10189300	-0.00034200

Na_2SO_2 -873.387217 a.u.

S	-0.977331	0.640894	0.268966
O	-0.501373	1.072893	-1.234891
O	-0.610135	-0.985278	0.388358
Na	-0.391417	-1.072892	-1.868422
Na	0.977330	-0.604794	1.868422

B -247.580936 a.u.

C	-0.031800	0.974704	-0.171233
C	1.254770	0.529023	0.106423
N	1.494353	-0.777868	0.390416
C	0.485142	-1.592572	0.400036
C	-0.845304	-1.285737	0.142104
C	-1.093911	0.059179	-0.157665
H	-0.201592	2.021706	-0.400036
H	2.111025	1.196527	0.104004
H	-1.642351	-2.021706	0.163282
H	-2.111025	0.375449	-0.379769

Radical NaSO2 -711.034489 a.u.

S	-0.056573	-0.225694	-1.396890
O	-0.195227	1.215169	-0.837291
O	0.195227	-1.215168	-0.228934
Na	-0.099101	0.481260	1.396890

NaI -173.846548 a.u.

Na	-1.459642	-0.375889	0.306055
I	1.459642	0.375888	-0.306055

TS1-T -958.562712 a.u.

C	2.89729600	0.29644700	0.35860900
C	1.88509100	1.24543200	0.29915300
N	0.64088700	1.00697800	-0.15996800
C	0.35554900	-0.28294300	-0.53456100
C	1.32489500	-1.33117200	-0.48580700
C	2.59988100	-1.02947800	-0.07123000
S	-1.42511800	-0.86200100	-0.17681500
O	-1.75775900	-1.88502600	0.90093100
O	-2.29402400	0.38749100	-0.18551800
Na	-1.27638500	2.42012400	0.03483700
H	3.88407300	0.56749000	0.71821400
H	2.07845500	2.27159900	0.61252400
H	1.05507400	-2.33608900	-0.80209200

H	3.37629600	-1.79064800	-0.08330800

TS1-MECP-T-S -958.591616 a.u.

6	3.10813360	0.34292449	0.27627177
6	2.02641804	1.21501178	0.33243809
7	0.78512936	0.82359813	-0.05626115
6	0.62777559	-0.39589462	-0.48612386
6	1.62645114	-1.36261661	-0.59024612
6	2.90609893	-0.96343913	-0.19236583
16	-2.56752586	-0.96251945	-0.16092505
8	-2.55606126	-1.71333080	1.17831452
8	-2.76290230	0.56276322	0.01757338
11	-1.23323726	2.24406522	0.02409751
1	4.08969030	0.67749209	0.59460291
1	2.13126716	2.23545283	0.68859431
1	1.42573037	-2.36355640	-0.95561459
1	3.73724304	-1.66174285	-0.24538664

C -958.661687 a.u.

C	3.17045500	0.34940500	0.36728800
C	2.65238000	-0.94739000	0.34788400
N	1.37839500	-1.22743200	0.03645900
C	0.58314700	-0.19715000	-0.26532700
C	0.99838500	1.13296900	-0.29385600
C	2.32534200	1.40990700	0.03810800
H	4.21093600	0.51693700	0.62687400
H	3.28674400	-1.79793600	0.59066500
H	0.29220500	1.90801600	-0.57108500
H	2.69494500	2.43186200	0.03552000
S	-1.15892400	-0.66998000	-0.67595600
O	-1.78817100	0.70134400	-1.01755100
O	-1.70731900	-1.12402300	0.69859100
Na	-2.90955800	0.83161900	1.02410900

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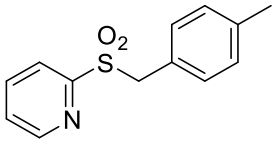
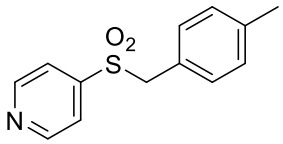


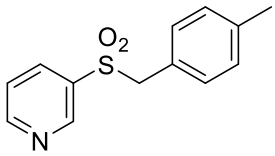
2-((4-Methylbenzyl)sulfonyl)pyridine (**3a**)

Yield: 40.1 mg (81%); White solid, m.p. 91-93 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.80 (dt, *J* = 4.7, 1.3 Hz, 1H), 7.83 – 7.81 (m, 2H), 7.52 (ddd, *J* = 5.9, 4.7, 2.9 Hz, 1H), 7.08 – 7.03 (m, 4H), 4.60 (s, 2H), 2.28 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 156.3, 150.1, 138.6, 137.8, 130.8, 129.3, 127.3, 124.2, 123.1, 58.0, 21.1; HRMS calcd for $C_{13}H_{14}NO_2S$ ($M+H^+$): 248.0740, found: 248.0738; IR (KBr): 3441, 2929, 1574, 1424, 1307, 1113, 1044 cm^{-1}.



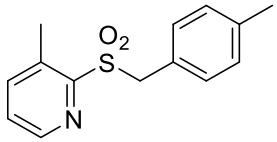
4-((4-Methylbenzyl)sulfonyl)pyridine (**3b**)

Yield: 37.1 mg (75%); White solid, m.p. 138-140 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.79 (dd, *J* = 4.4, 1.6 Hz, 2H), 7.48 (dd, *J* = 4.4, 1.6 Hz, 2H), 7.09 (d, *J* = 7.9 Hz, 2H), 6.98 (d, *J* = 8.0 Hz, 2H), 4.31 (s, 2H), 2.33 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 150.9, 139.3, 130.7, 130.6, 129.7, 129.6, 121.8, 62.2, 21.2; HRMS calcd for $C_{13}H_{14}NO_2S$ ($M+H^+$): 248.0740, found: 248.0738; IR (KBr): 3441, 2920, 1629, 1455, 1324, 1155 cm^{-1}.



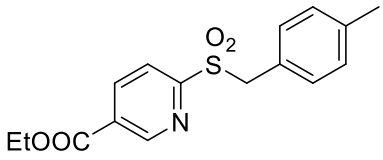
3-((4-Methylbenzyl)sulfonyl)pyridine (**3c**)

Yield: 9.9 mg (20%); White solid, m.p. 139-141 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.82 – 8.78 (m, 1H), 7.86 (ddd, *J* = 8.0, 2.2, 1.7 Hz, 1H), 7.38 (ddd, *J* = 8.0, 4.9, 0.8 Hz, 1H), 7.09 (d, *J* = 7.9 Hz, 2H), 6.97 (d, *J* = 8.0 Hz, 2H), 4.33 (s, 2H), 2.33 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 154.1, 149.5, 139.2, 136.4, 134.2, 130.6, 129.5, 124.2, 123.4, 62.9, 21.2; HRMS calcd for $C_{13}H_{14}NO_2S$ ($M+H^+$): 248.0740, found: 248.0737; IR (KBr): 3443, 2920, 1442, 1316, 1162, 1095 cm^{-1}.



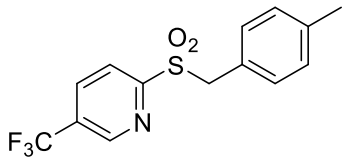
3-Methyl-2-((4-methylbenzyl)sulfonyl)pyridine (**3d**)

Yield: 29.7 mg (57%); White solid, m.p. 102-104 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.52 (dd, *J* = 4.6, 0.9 Hz, 1H), 7.59 (dd, *J* = 7.8, 0.8 Hz, 1H), 7.38 (dd, *J* = 7.8, 4.6 Hz, 1H), 7.22 (d, *J* = 8.0 Hz, 2H), 7.11 (d, *J* = 7.9 Hz, 2H), 4.75 (s, 2H), 2.51 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 146.1, 141.2, 138.6, 134.3, 131.3, 130.7, 129.3, 126.8, 124.4, 58.0, 21.2, 18.2; HRMS calcd for $C_{14}H_{16}NO_2S$ ($M+H^+$): 262.0896, found: 262.0897; IR (KBr): 3419, 1512, 1412, 1303, 1120 cm^{-1}.



Ethyl 6-((4-methylbenzyl)sulfonyl)nicotinate (**3e**)

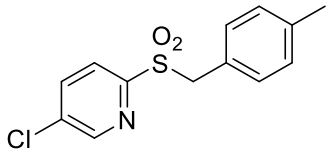
Yield: 48.4 mg (76%); White solid, m.p. 92-94 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 9.83 – 9.18 (m, 1H), 8.41 (dd, *J* = 8.1, 2.0 Hz, 1H), 7.88 (dt, *J* = 8.0, 4.0 Hz, 1H), 7.09 – 7.03 (m, 4H), 4.64 (s, 2H), 4.46 (q, *J* = 7.1 Hz, 2H), 2.28 (s, 3H), 1.44 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 163.8, 159.6, 151.0, 139.0, 138.9, 130.9, 129.5, 129.4, 123.9, 122.6, 62.3, 57.9, 21.2, 14.2; HRMS calcd for $C_{16}H_{18}NO_4S$ ($M+H^+$): 320.0951, found: 320.0948; IR (KBr): 3436, 2922, 1717, 1581, 1316, 1160, 1113 cm^{-1}.



2-((4-Methylbenzyl)sulfonyl)-5-(trifluoromethyl)pyridine (**3f**)

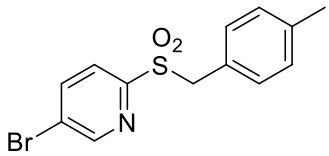
Yield: 47.2 mg (75%); White solid, m.p. 143-145 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 9.04 (s, 1H), 8.08 (dd, *J* = 8.2, 1.6 Hz, 1H), 7.96 (d, *J* = 8.1 Hz, 1H), 7.10 – 7.05 (m, 4H), 4.65 (s, 2H), 2.29 (s, 3H); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -62.60 (s); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 159.7, 147.0 (q, *J* = 3.9 Hz), 139.0, 135.4 (q, *J* = 3.5 Hz), 130.8, 130.0, 129.5, 123.5, 122.8, 122.4 (q, *J* = 273.5 Hz), 57.9, 21.1; HRMS calcd for

$C_{14}H_{13}F_3NO_2S$ ($M+H^+$): 316.0614, found: 316.0613; IR (KBr): 3441, 2936, 1508, 1317, 1105 cm^{-1}.



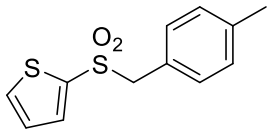
5-Chloro-2-((4-methylbenzyl)sulfonyl)pyridine (**3g**)

Yield: 30.8 mg (55%); White solid, m.p. 108-110 °C; ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.73 (d, *J* = 1.7 Hz, 1H), 7.79 (dd, *J* = 8.3, 2.2 Hz, 1H), 7.74 (dd, *J* = 8.3, 0.5 Hz, 1H), 7.08 – 7.04 (m, 4H), 4.58 (s, 2H), 2.29 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 154.2, 149.1, 138.8, 137.4, 136.2, 130.7, 129.4, 124.1, 123.9, 58.1, 21.1; HRMS calcd for $C_{13}H_{13}ClNO_2S$ ($M+H^+$): 282.0350, found: 282.0349; IR (KBr): 3440, 3051, 2922, 1511, 1365, 1317, 1105 cm^{-1}.



5-Bromo-2-((4-methylbenzyl)sulfonyl)pyridine (**3h**)

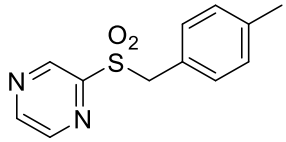
Yield: 33.1 mg (51%); White solid, m.p. 122-124 °C; ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.84 (dd, *J* = 2.2, 0.5 Hz, 1H), 7.95 (dd, *J* = 8.3, 2.2 Hz, 1H), 7.68 (dd, *J* = 8.3, 0.6 Hz, 1H), 7.09 – 7.04 (m, 4H), 4.58 (s, 2H), 2.29 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 154.7, 151.2, 140.4, 138.8, 130.7, 129.4, 125.2, 124.4, 123.8, 58.1, 21.1; HRMS calcd for $C_{13}H_{13}BrNO_2S$ ($M+H^+$): 325.9845, found: 325.9844; IR (KBr): 3453, 2919, 1445, 1316, 1162, 1094 cm^{-1}.



2-((4-Methylbenzyl)sulfonyl)thiophene (**3i**)

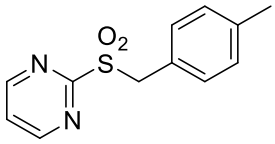
Yield: 14.6 mg (29%); White solid, m.p. 131-133 °C; ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.65 (dd, *J* = 5.0, 1.3 Hz, 1H), 7.36 (dd, *J* = 3.8, 1.3 Hz, 1H), 7.10 (d, *J* = 7.9 Hz, 2H), 7.07 – 7.02 (m, 3H), 4.36 (s, 2H), 2.33 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 138.9, 138.7, 134.8, 134.2, 130.6, 129.4, 127.6, 125.1, 63.8, 21.2; HRMS calcd for

$C_{12}H_{13}O_2S_2$ ($M+H^+$): 253.0351, found: 253.0346; IR (KBr): 3442, 2922, 1402, 1313, 1153, 1129, 1016 cm^{-1}.



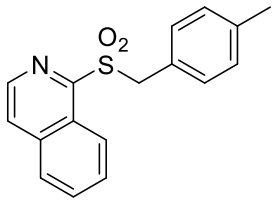
2-((4-Methylbenzyl)sulfonyl)pyrazine (**3j**)

Yield: 39.6 mg (80%); White solid, m.p. 137-139 °C; ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.95 (d, *J* = 1.3 Hz, 1H), 8.81 (d, *J* = 2.4 Hz, 1H), 8.76 (dd, *J* = 2.3, 1.5 Hz, 1H), 7.09 – 7.04 (m, 4H), 4.60 (s, 2H), 2.29 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 152.1, 148.2, 144.3, 144.0, 139.1, 130.7, 129.6, 123.4, 58.6, 21.1; HRMS calcd for $C_{12}H_{13}N_2O_2S$ ($M+H^+$): 249.0692, found: 249.0691; IR (KBr): 3443, 2922, 1317, 1116, 1016 cm^{-1}.



2-((4-Methylbenzyl)sulfonyl)pyrimidine (**3k**)

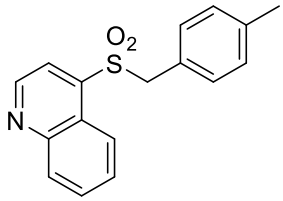
Yield: 38.7 mg (78%); White solid, m.p. 105-107 °C; ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.92 (d, *J* = 4.9 Hz, 2H), 7.53 (t, *J* = 4.9 Hz, 1H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.10 (d, *J* = 7.9 Hz, 2H), 4.74 (s, 2H), 2.30 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 165.3, 158.5, 138.9, 131.0, 129.4, 123.7, 123.2, 57.4, 21.1; HRMS calcd for $C_{12}H_{13}N_2O_2S$ ($M+H^+$): 249.0692, found: 249.0693; IR (KBr): 3447, 2921, 1565, 1384, 1329, 1124 cm^{-1}.



1-((4-Methylbenzyl)sulfonyl)isoquinoline (**3l**)

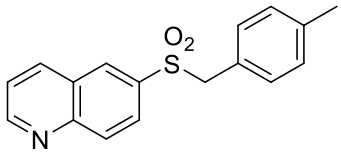
Yield: 39.2 mg (66%); White solid, m.p. 115-117 °C; ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.30 (dd, *J* = 8.4, 3.6 Hz, 2H), 7.92 – 7.86 (m, 3H), 7.72 (t, *J* = 7.5 Hz, 1H), 7.11 (d, *J* = 8.0 Hz, 2H), 7.02 (d, *J* = 7.9 Hz, 2H), 4.76 (s, 2H), 2.26 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ(ppm) 156.3, 147.1, 138.6, 138.4, 131.2, 131.0, 130.1, 129.4, 129.3, 129.1,

127.9, 124.2, 118.0, 57.9, 21.1; HRMS calcd for $C_{17}H_{16}NO_2S$ ($M+H^+$): 298.0896, found: 298.0895; IR (KBr): 3441, 2920, 1631, 1314, 1166, 1123 cm^{-1}.



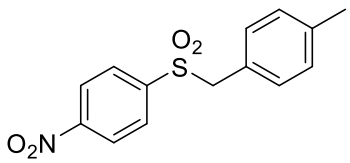
4-((4-Methylbenzyl)sulfonyl)quinoline (**3m**)

Yield: 43.3 mg (73%); White solid, m.p. 165-167 °C; ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.97 (d, *J* = 4.4 Hz, 1H), 8.67 (dd, *J* = 8.6, 0.6 Hz, 1H), 8.31 – 8.22 (m, 1H), 7.88 – 7.84 (m, 1H), 7.75 – 7.70 (m, 2H), 6.97 (d, *J* = 7.9 Hz, 2H), 6.83 (d, *J* = 8.0 Hz, 2H), 4.49 (s, 2H), 2.26 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 149.5, 149.2, 141.7, 139.2, 130.8, 130.5, 130.4, 129.4, 129.1, 124.1, 123.9, 123.1, 62.4, 21.1; HRMS calcd for $C_{17}H_{16}NO_2S$ ($M+H^+$): 298.0896, found: 298.0886; IR (KBr): 3448, 2988, 1625, 1310, 1147, 1110 cm^{-1}.



6-((4-Methylbenzyl)sulfonyl)quinoline (**3n**)

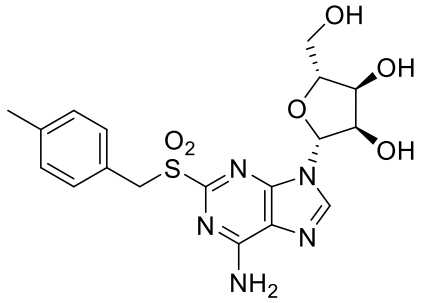
Yield: 18.4 mg (31%); White solid, m.p. 175-177 °C; ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 9.07 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.22 – 8.14 (m, 3H), 7.84 (dd, *J* = 8.9, 2.0 Hz, 1H), 7.53 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.04 (d, *J* = 7.9 Hz, 2H), 6.97 (d, *J* = 8.0 Hz, 2H), 4.37 (s, 2H), 2.30 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 153.5, 149.8, 138.9, 137.3, 135.9, 130.8, 130.7, 130.7, 129.4, 127.1, 124.8, 122.6, 62.7, 21.2; HRMS calcd for $C_{17}H_{16}NO_2S$ ($M+H^+$): 298.0896, found: 298.0894; IR (KBr): 3440, 2983, 1615, 1311, 1141, 1119 cm^{-1}.



1-Methyl-4-(((4-nitrophenyl)sulfonyl)methyl)benzene (**3o**)

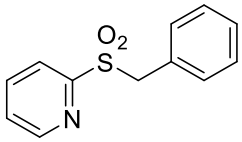
Yield: 10.0 mg (17%); White solid, m.p. 173-175 °C; ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.28 (d, *J* = 8.8 Hz, 2H), 7.80 (d, *J* = 8.8 Hz, 2H), 7.09 (d, *J* = 7.9 Hz, 2H), 6.96 (d, *J* = 8.0

Hz, 2H), 4.34 (s, 2H), 2.34 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 150.7, 143.4, 139.4, 130.6, 130.2, 129.6, 124.0, 123.9, 62.5, 21.2; HRMS calcd for $C_{14}H_{14}NO_4S$ ($M+H^+$): 292.0638, found: 292.0636; IR (KBr): 3445, 3214, 1759, 1577, 1335, 1151, 1056 cm^{-1}.



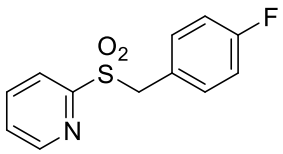
(2R,3R,4S,5R)-2-(6-Amino-2-((4-methylbenzyl)sulfonyl)-9*H*-purin-9-yl)-5-(hydroxymethyl)tetrahydrofuran-3,4-diol (**3p**)

Yield: 48.6 mg (56%); White solid, m.p. 276-278 °C; ^{1}H NMR (400 MHz, DMSO) δ (ppm) 8.61 (s, 1H), 8.11 (s, 2H), 7.26 (d, *J* = 7.5 Hz, 2H), 7.13 (d, *J* = 7.5 Hz, 2H), 5.95 (d, *J* = 5.6 Hz, 1H), 5.55 (d, *J* = 5.8 Hz, 1H), 5.28 (d, *J* = 4.4 Hz, 1H), 5.02 (t, *J* = 4.9 Hz, 1H), 4.87 – 4.77 (m, 2H), 4.61 – 4.56 (m, 1H), 4.18 (d, *J* = 3.3 Hz, 1H), 3.98 (s, 1H), 3.70 – 3.66 (m, 1H), 3.59 – 3.56 (m, 1H), 2.26 (s, 3H); ^{13}C NMR (101 MHz, DMSO) δ (ppm) 159.1, 156.7, 149.2, 142.3, 138.2, 131.8, 129.4, 125.5, 120.4, 87.7, 86.3, 74.4, 70.9, 61.8, 56.6, 21.3; HRMS calcd for $C_{18}H_{22}N_5O_6S$ ($M+H^+$):436.1285, found: 436.1289; IR (KBr): 3357, 3204, 1645, 1595, 1228, 1085 cm^{-1}.



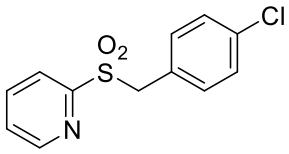
2-(Benzylsulfonyl)pyridine (**3aa**)[1]

Yield: 31.7 mg (68%); White solid, m.p. 104-106 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.82 – 8.80 (m, 1H), 7.85 – 7.78 (m, 2H), 7.52 (ddd, *J* = 6.7, 4.7, 2.2 Hz, 1H), 7.30 – 7.22 (m, 3H), 7.18 (dd, *J* = 7.9, 1.6 Hz, 2H), 4.64 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 156.3, 150.1, 137.8, 130.9, 128.7, 128.6, 127.4, 123.1, 58.3; IR (KBr): 3450, 3075, 2929, 1579, 1455, 1322, 1257 cm^{-1}.



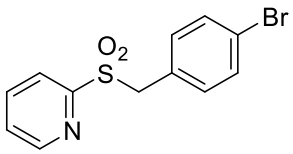
2-((4-Fluorobenzyl)sulfonyl)pyridine (**3ab**)

Yield: 36.6 mg (73%); White solid, m.p. 76-78 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.81 – 8.79 (m, 1H), 7.89 – 7.81 (m, 2H), 7.54 (ddd, *J* = 6.7, 4.7, 1.9 Hz, 1H), 7.21 – 7.16 (m, 2H), 6.98 – 6.91 (m, 2H), 4.62 (s, 2H); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -112.48 (dq, *J* = 8.6, 5.3 Hz); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 163.0 (d, *J* = 248.6 Hz), 156.2, 150.2, 138.0, 132.7 (d, *J* = 8.5 Hz), 127.5, 123.2 (d, *J* = 3.3 Hz), 123.0, 115.7 (d, *J* = 21.8 Hz), 57.4; HRMS calcd for $C_{12}H_{11}FNO_2S$ ($M+H^+$): 252.0489, found: 252.0486; IR (KBr): 3443, 2922, 1327, 1136, 1073, 1014 cm^{-1}.



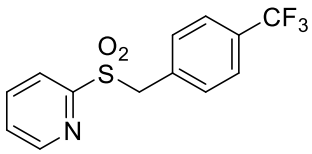
2-((4-Chlorobenzyl)sulfonyl)pyridine (**3ac**)

Yield: 39.5 mg (74%); White solid, m.p. 74-76 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.81 – 8.79 (m, 1H), 7.89 – 7.82 (m, 2H), 7.54 (ddd, *J* = 6.7, 4.7, 1.9 Hz, 1H), 7.25 – 7.21 (m, 2H), 7.16 – 7.12 (m, 2H), 4.62 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 156.1, 150.2, 138.0, 135.0, 132.2, 128.9, 127.5, 125.9, 123.0, 57.4; HRMS calcd for $C_{12}H_{11}ClNO_2S$ ($M+H^+$): 268.0194, found: 268.0193; IR (KBr): 3443, 2981, 1576, 1491, 1314, 1163, 1135 cm^{-1}.



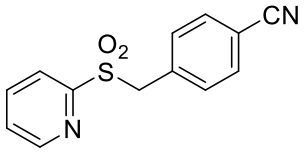
2-((4-Bromobenzyl)sulfonyl)pyridine (**3ad**)

Yield: 45.8 mg (74%); White solid, m.p. 76-78 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.83 – 8.81 (m, 1H), 7.91 – 7.84 (m, 2H), 7.56 (ddd, *J* = 6.7, 4.7, 1.9 Hz, 1H), 7.43 – 7.39 (m, 2H), 7.12 – 7.08 (m, 2H), 4.62 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 156.1, 150.2, 138.1, 132.5, 131.9, 127.5, 126.4, 123.2, 123.0, 57.5; HRMS calcd for $C_{12}H_{11}BrNO_2S$ ($M+H^+$): 311.9688, found: 311.9687; IR (KBr): 3453, 1488, 1319, 1165, 1110, 1014 cm^{-1}.



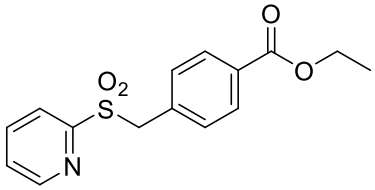
2-((4-(trifluoromethyl)benzyl)sulfonyl)pyridine (**3ae**)[2]

Yield: 40.9 mg (68%); White solid, m.p. 86-88 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.81 (dd, *J* = 3.4, 2.3 Hz, 1H), 7.91 – 7.84 (m, 2H), 7.58 – 7.52 (m, 3H), 7.36 (d, *J* = 8.1 Hz, 2H), 4.72 (s, 2H); ^{19}F NMR (376 MHz, $CDCl_3$) δ (ppm) -62.82 (s); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 156.1, 150.2, 138.2, 131.4, 131.1, 130.7, 127.7, 125.6 (q, *J* = 3.8 Hz), 123.8 (q, *J* = 271.0 Hz), 122.9, 57.6; IR (KBr): 3442, 2927, 1575, 1513, 1307, 1162, 1113 cm^{-1}.



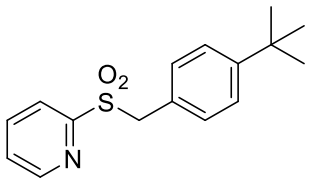
4-((Pyridin-2-ylsulfonyl)methyl)benzonitrile (**3af**)

Yield: 33.5 mg (65%); White solid, m.p. 153-155 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.82 – 8.80 (m, 1H), 7.92 – 7.85 (m, 2H), 7.59 – 7.55 (m, 3H), 7.37 (d, *J* = 8.3 Hz, 2H), 4.71 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 156.1, 150.2, 138.2, 132.8, 132.3, 131.8, 127.8, 122.9, 118.2, 112.8, 57.7; HRMS calcd for $C_{13}H_{11}N_2O_2S$ ($M+H^+$): 259.0536, found: 259.0535; IR (KBr): 3441, 2924, 2233, 1312, 1164, 1108 cm^{-1}.



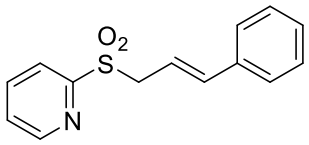
Ethyl 4-((pyridin-2-ylsulfonyl)methyl)benzoate (**3ag**)

Yield: 43.3 mg (71%); White solid, m.p. 105-107 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.82 (d, *J* = 3.9 Hz, 1H), 7.94 (d, *J* = 7.9 Hz, 2H), 7.88 – 7.80 (m, 2H), 7.59 – 7.52 (m, 1H), 7.29 (d, *J* = 8.0 Hz, 2H), 4.73 (s, 2H), 4.36 (q, *J* = 7.1 Hz, 2H), 1.38 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 165.9, 156.0, 150.1, 138.0, 132.2, 130.9, 130.7, 129.7, 127.5, 123.0, 61.1, 57.9, 14.2; HRMS calcd for $C_{15}H_{16}NO_4S$ ($M+H^+$): 306.0795, found: 306.0794; IR (KBr): 3436, 2979, 1710, 1453, 1281, 1111, 1024 cm^{-1}.



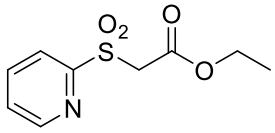
2-((4-(*tert*-Butyl)benzyl)sulfonyl)pyridine (**3ah**)

Yield: 42.2 mg (73%); White solid, m.p. 130-132 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.83 (dt, *J* = 4.7, 1.4 Hz, 1H), 7.89 – 7.85 (m, 2H), 7.55 (ddd, *J* = 6.3, 4.7, 2.7 Hz, 1H), 7.32 – 7.29 (m, 2H), 7.17 – 7.14 (m, 2H), 4.63 (s, 2H), 1.29 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 156.6, 151.8), 150.1, 137.8, 130.7, 127.3, 125.6, 124.0, 123.0, 57.9, 34.5, 31.1; HRMS calcd for $C_{16}H_{20}NO_2S$ ($M+H^+$): 290.1209, found: 290.1205; IR: (KBr) 3424, 2957, 1450, 1313, 1166, 1109 cm^{-1}.



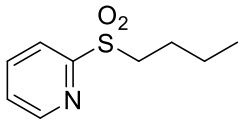
2-(cinnamylsulfonyl)pyridine (**3ai**)[3]

Yield: 42.4 mg (82%); White solid, m.p. 78-80 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.79 – 8.77 (m, 1H), 8.03 (dt, *J* = 7.8, 0.9 Hz, 1H), 7.91 (td, *J* = 7.8, 1.7 Hz, 1H), 7.53 (ddd, *J* = 7.6, 4.7, 1.1 Hz, 1H), 7.30 – 7.21 (m, 5H), 6.48 (d, *J* = 15.8 Hz, 1H), 6.14 – 6.06 (m, 1H), 4.29 (dd, *J* = 7.6, 1.1 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 156.6, 150.2, 139.5, 138.0, 135.6, 128.5, 128.5, 127.4, 126.6, 122.8, 114.4, 56.1; HRMS calcd for $C_{14}H_{14}NO_2S$ ($M+H^+$): 260.0740, found: 260.0734; IR (KBr): 3441, 3055, 2919, 1428, 1318, 1166, 1111, 1082 cm^{-1}.



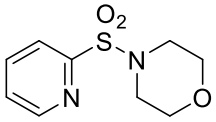
Ethyl 2-(pyridin-2-ylsulfonyl)acetate (**3aj**)[1]

Yield: 34.8 mg (76%); Colourless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.78 – 8.76 (m, 1H), 8.11 (d, *J* = 7.9 Hz, 1H), 8.00 (td, *J* = 7.8, 1.7 Hz, 1H), 7.60 (ddd, *J* = 7.6, 4.7, 1.1 Hz, 1H), 4.49 (s, 2H), 4.13 (q, *J* = 7.1 Hz, 2H), 1.16 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 162.4, 156.6, 150.2, 138.2, 127.6, 122.4, 62.3, 56.0, 13.8; IR (KBr): 3447, 2982, 1715, 1442, 1267, 1111 cm^{-1}.



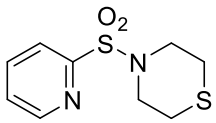
2-(Butylsulfonyl)pyridine (**3ak**)

Yield: 28.2 mg (71%); Colourless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.77 – 8.75 (m, 1H), 8.10 (dt, *J* = 7.8, 1.0 Hz, 1H), 7.98 (td, *J* = 7.8, 1.7 Hz, 1H), 7.57 (ddd, *J* = 7.7, 4.7, 1.2 Hz, 1H), 3.42 – 3.38 (m, 2H), 1.78 – 1.68 (m, 2H), 1.50 – 1.39 (m, 2H), 0.92 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 157.3, 150.2, 138.1, 127.3, 122.1, 51.6, 24.0, 21.5, 13.4; HRMS calcd for $C_9H_{14}NO_2S$ ($M+H^+$): 200.0740, found: 200.0738; IR (KBr): 2961, 2874, 1578, 1428, 1233, 784 cm^{-1}.



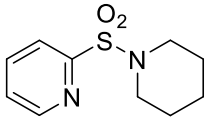
4-(Pyridin-2-ylsulfonyl)morpholine (**4a**)

Yield: 33.3 mg (73%); White solid, m.p. 75-77 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.75 (d, *J* = 4.6 Hz, 1H), 7.98 – 7.93 (m, 2H), 7.56 – 7.51 (m, 1H), 3.76 (t, *J* = 4.8 Hz, 4H), 3.35 (t, *J* = 4.8 Hz, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 156.1, 150.1, 138.0, 126.8, 123.2, 66.4, 46.6; HRMS calcd for $C_9H_{13}N_2O_3S$ ($M+H^+$): 229.0641, found: 229.0641; IR (KBr): 3440, 2865, 1578, 1256, 1176, 954 cm^{-1}.



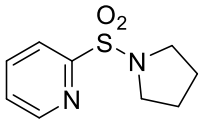
4-(Pyridin-2-ylsulfonyl)thiomorpholine (**4b**)

Yield: 36.6 mg (75%); Colourless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.73 (d, *J* = 4.7 Hz, 1H), 7.96 – 7.90 (m, 2H), 7.54 – 7.50 (m, 1H), 3.65 (t, *J* = 5.0 Hz, 4H), 2.72 (t, *J* = 5.2 Hz, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 156.9, 150.1, 138.0, 126.7, 122.7, 48.5, 27.4; HRMS calcd for $C_9H_{13}N_2O_2S_2$ ($M+H^+$): 245.0413, found: 245.0414; IR (KBr): 3482, 2975, 2733, 1617, 1444, 1323, 1113 cm^{-1}.



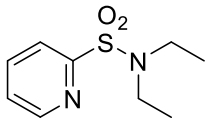
2-(Piperidin-1-ylsulfonyl)pyridine (**4c**)[4]

Yield: 34.3 mg (76%); White solid, m.p. 50-52 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.73 (d, *J* = 4.4 Hz, 1H), 7.96 – 7.89 (m, 2H), 7.52 – 7.47 (m, 1H), 3.29 (t, *J* = 5.0 Hz, 4H), 1.66 – 1.62 (m, 4H), 1.54 – 1.47 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 156.7, 149.9, 137.7, 126.3, 122.9, 47.4, 25.4, 23.6; IR (KBr): 3480, 2983, 2750, 1613, 1451, 1332, 1221, 1099 cm^{-1}.



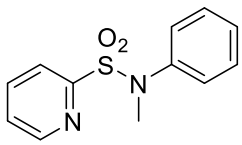
2-(Pyrrolidin-1-ylsulfonyl)pyridine (**4d**)

Yield: 27.5 mg (65%); Yellow liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.70 (d, *J* = 4.7 Hz, 1H), 8.00 – 7.96 (m, 1H), 7.91 (td, *J* = 7.7, 1.7 Hz, 1H), 7.50 (ddd, *J* = 7.5, 4.7, 1.2 Hz, 1H), 3.52 – 3.48 (m, 4H), 1.87 – 1.83 (m, 4H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 156.9, 145.0, 137.7, 126.4, 122.9, 48.6, 25.6; HRMS calcd for $C_9H_{13}N_2O_2S$ ($M+H^+$): 213.0692, found: 213.0697; IR (KBr): 2977, 2904, 1576, 1344, 1172 cm^{-1}.



N,N-Diethylpyridine-2-sulfonamide (**4e**)

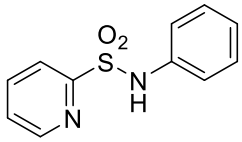
Yield: 20.5 mg (48%); Yellow liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.68 (ddd, *J* = 4.7, 1.6, 0.8 Hz, 1H), 7.96 (dt, *J* = 7.9, 1.0 Hz, 1H), 7.87 (td, *J* = 7.7, 1.7 Hz, 1H), 7.45 (ddd, *J* = 7.6, 4.7, 1.2 Hz, 1H), 3.41 (q, *J* = 7.2 Hz, 4H), 1.15 (t, *J* = 7.2 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 158.7, 149.9, 137.7, 126.2, 122.2, 42.8, 14.4; HRMS calcd for $C_9H_{15}N_2O_2S$ ($M+H^+$): 215.0849, found: 215.0849. IR (KBr): 2976, 2937, 1577, 1333, 1172 cm^{-1}.



N-methyl-*N*-phenylpyridine-2-sulfonamide (**4f**)

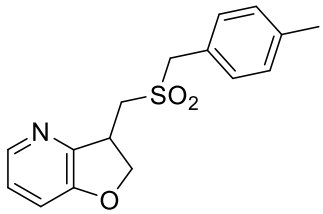
Yield: 17.8 mg (36%); White solid, m.p. 116-118 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.75 (d, *J* = 4.4 Hz, 1H), 7.80 (t, *J* = 7.7 Hz, 1H), 7.71 (d, *J* = 7.8 Hz, 1H), 7.50 – 7.46 (m,

1H), 7.30 – 7.18 (m, 5H), 3.50 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 156.9, 149.9, 141.2, 137.6, 129.0, 127.4, 127.0, 126.6, 123.2, 40.0; HRMS calcd for $C_{12}H_{13}N_2O_2S$ ($M+H^+$): 249.0692, found: 249.0694; IR (KBr): 3421, 2905, 1641, 1575, 1418, 1166 cm^{-1}.



N-phenylpyridine-2-sulfonamide (**4g**)[5]

Yield: 16.3 mg (35%); White solid, m.p. 143-146 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.74 (s, 1H), 7.92 – 7.80 (m, 3H), 7.46 (s, 1H), 7.27 – 7.18 (m, 4H), 7.09 (s, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 156.1, 150.1, 138.0, 136.0, 129.2, 127.0, 125.7, 123.1, 122.6; IR (KBr): 3426, 2888, 1632, 1572, 1456, 1112 cm^{-1}.



3-(((4-Methylbenzyl)sulfonyl)methyl)-2,3-dihydrofuro[3,2-b]pyridine (**7**)

Yield: 39.9 mg (66%); White solid, m.p. 128-130 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.04 (dd, *J* = 4.3, 1.9 Hz, 1H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.21 (d, *J* = 7.9 Hz, 2H), 7.08 – 7.02 (m, 2H), 4.90 (t, *J* = 9.7 Hz, 1H), 4.51 (dd, *J* = 10.0, 8.0 Hz, 1H), 4.35 – 4.24 (m, 2H), 4.13 – 4.05 (m, 1H), 3.70 (dd, *J* = 13.8, 2.6 Hz, 1H), 3.00 (dd, *J* = 13.7, 11.5 Hz, 1H), 2.36 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 153.6, 149.6, 142.0, 139.3, 130.5, 129.9, 124.4, 123.4, 116.5, 75.8, 60.5, 53.6, 36.4, 21.2; HRMS calcd for $C_{16}H_{18}NO_3S$ ($M+H^+$): 304.1002, found: 304.1000; IR (KBr): 3440, 2918, 1431, 1305, 1124 cm^{-1}.

References

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[2] P. D. Legarda, A. García-Rubia, R. G. Arrayás, J. C. Carretero, *Adv. Synth. Catal.* **2016**, *358*, 1065.

[3] P. H. Bos, A. J. Minnaard, B. L. Feringa, *Org. Lett.* **2008**, *10*, 4219.

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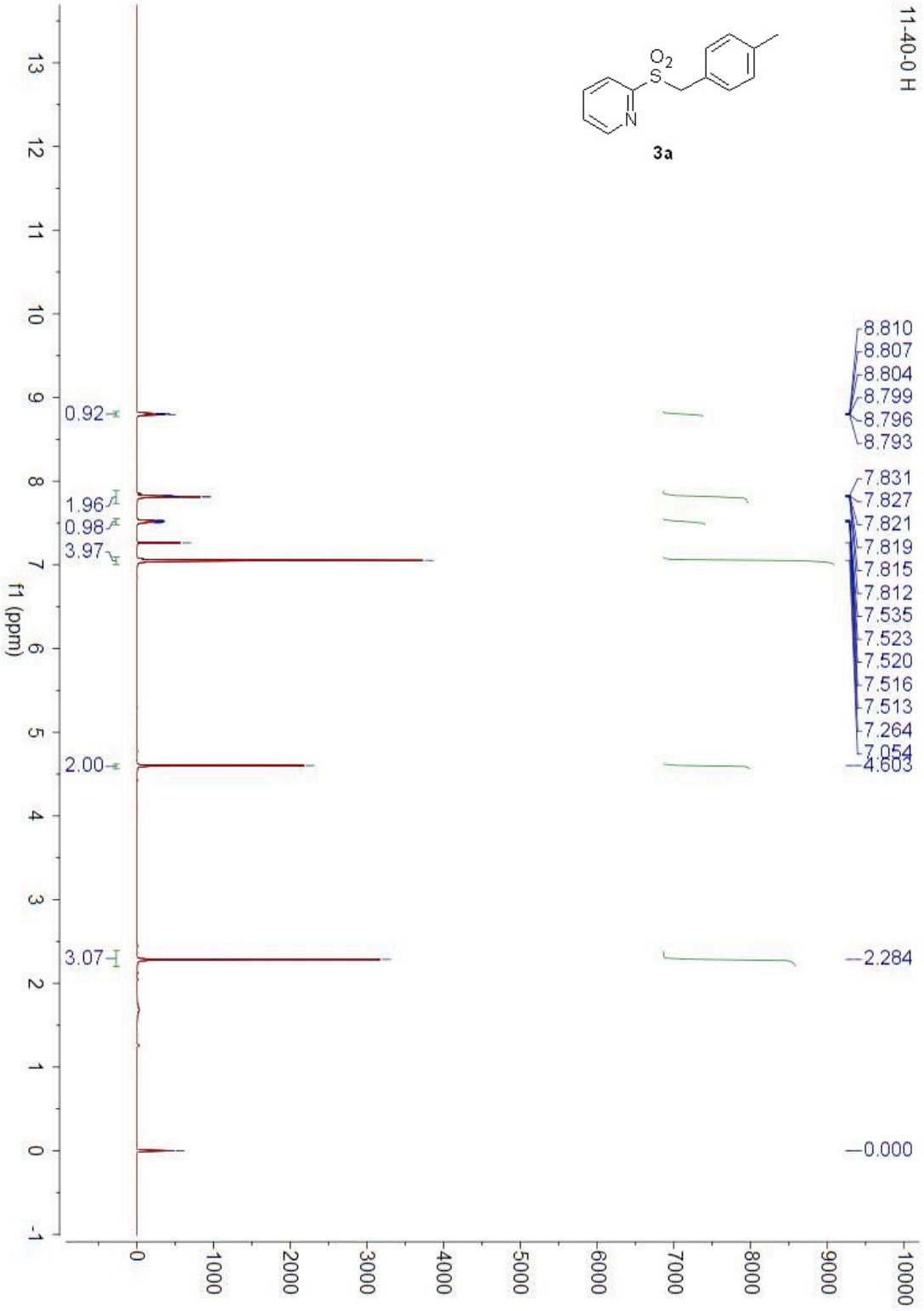
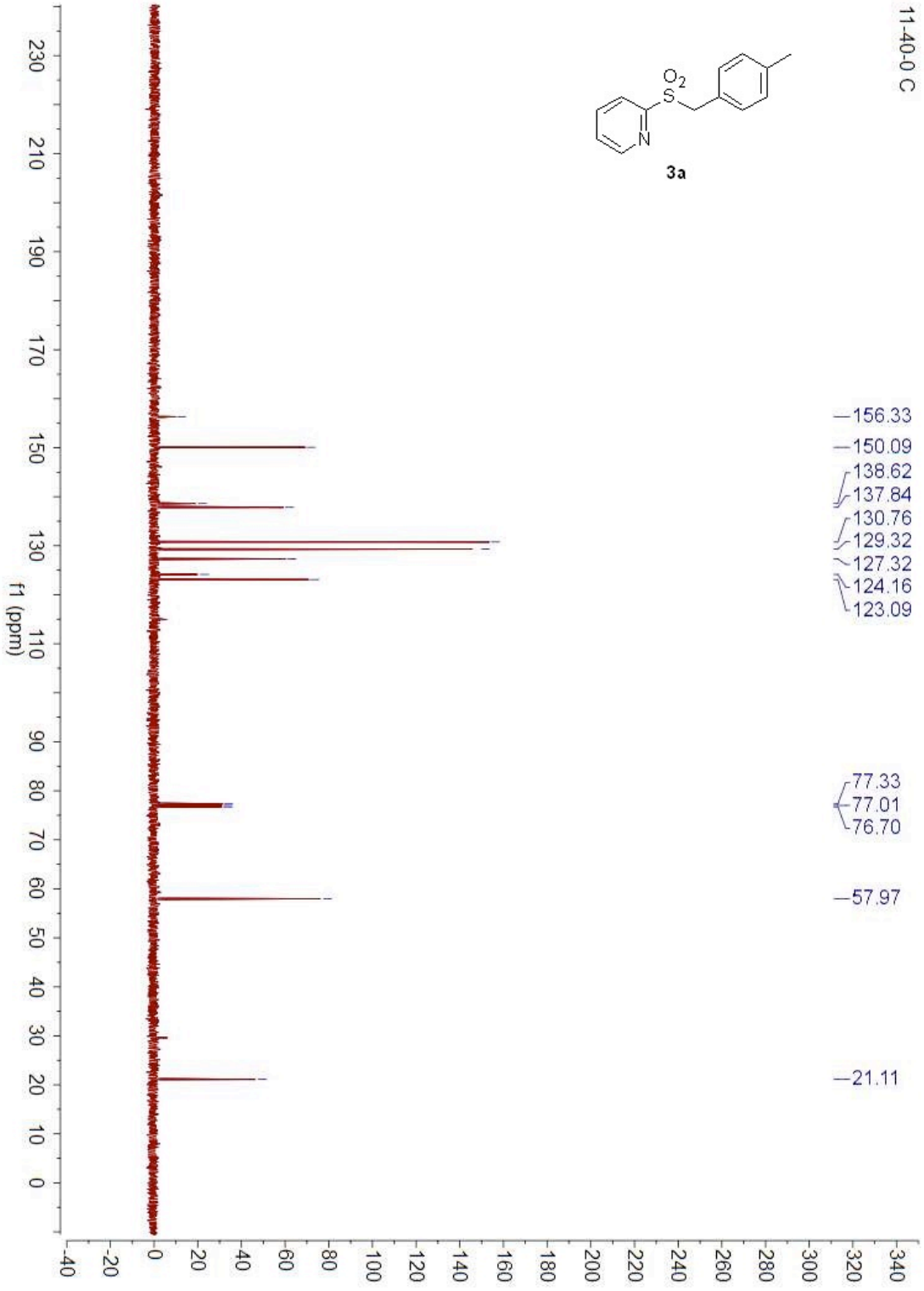
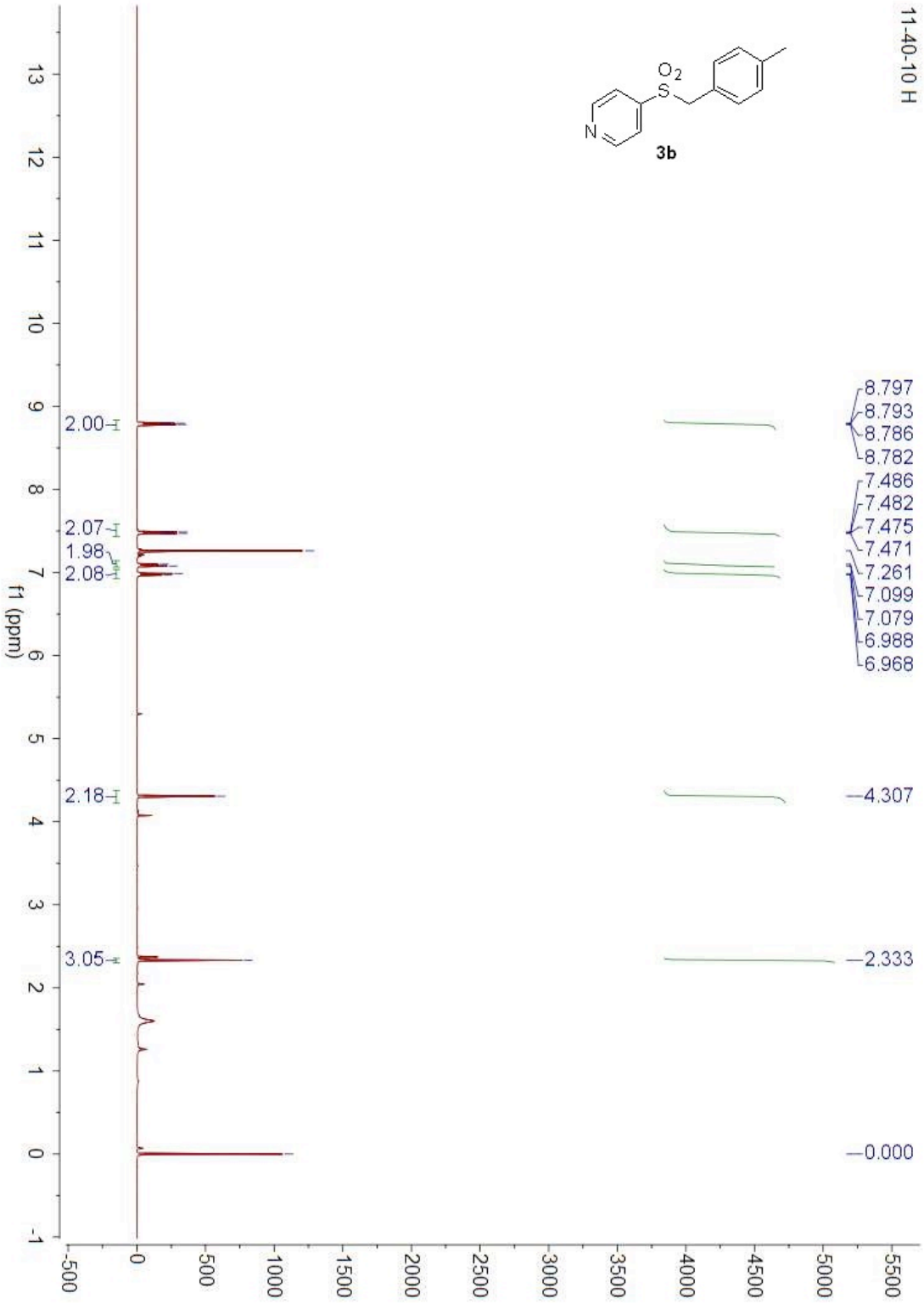
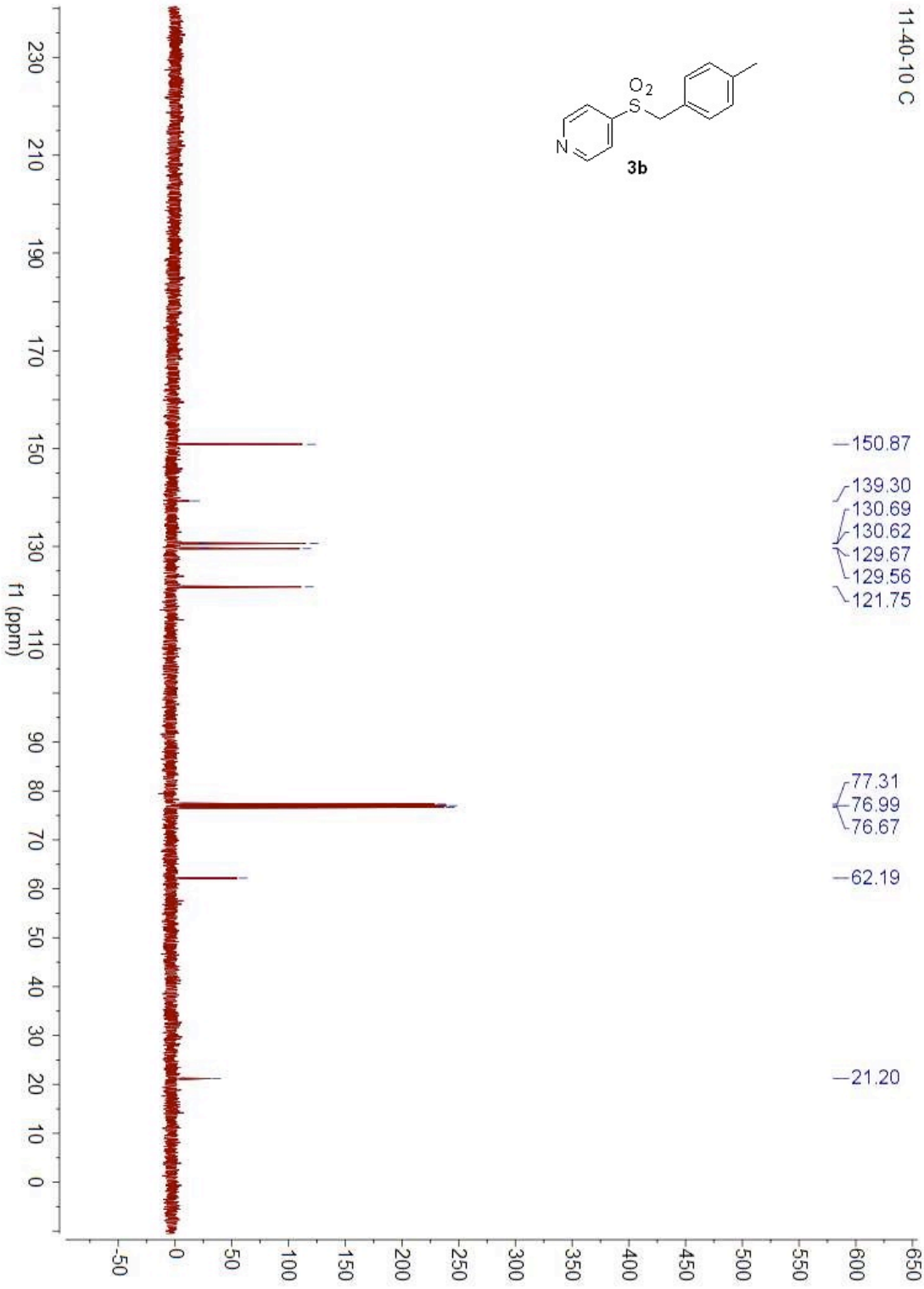

11-40-0 H
3a
8.810
8.807
8.804
8.799
8.796
8.793
7.831
7.827
7.821
7.819
7.815
7.812
7.535
7.523
7.520
7.516
7.513
7.264
7.054
4.603
2.284
0.000
0.92
1.96
0.98
3.97
2.00
3.07
f1 (ppm)


11-40-0 C
3a
156.33
150.09
138.62
137.84
130.76
129.32
127.32
124.16
123.09
77.33
77.01
76.70
57.97
21.11
f1 (ppm)


11-40-10 H
3b
8.797
8.793
8.786
8.782
7.486
7.482
7.475
7.471
7.261
7.099
7.079
6.988
6.968
4.307
2.333
0.000
2.00
2.07
1.98
2.08
2.18
3.05
f1 (ppm)


11-40-10 C
O2
S
N
3b
150.87
139.30
130.69
130.62
129.67
129.56
121.75
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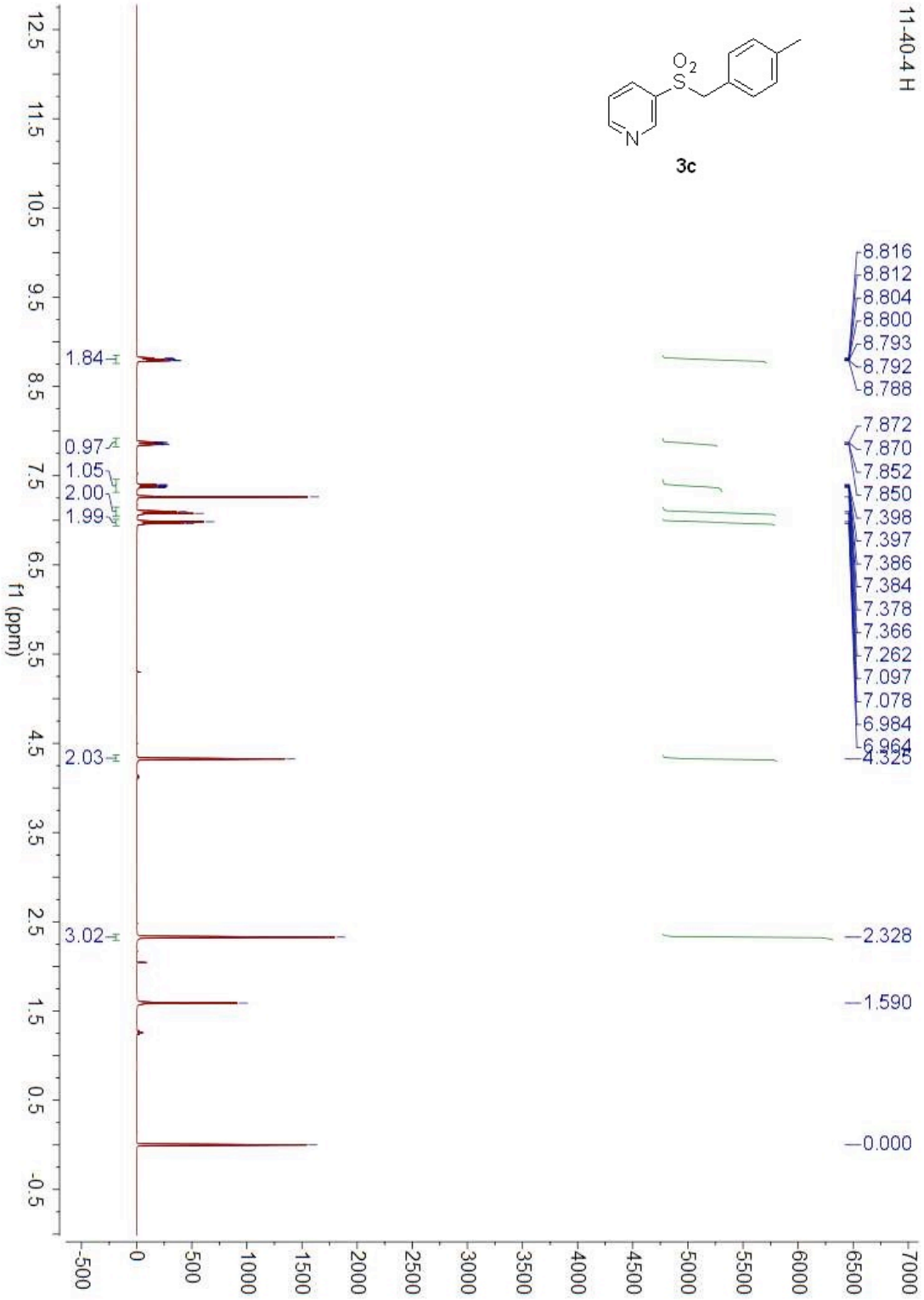
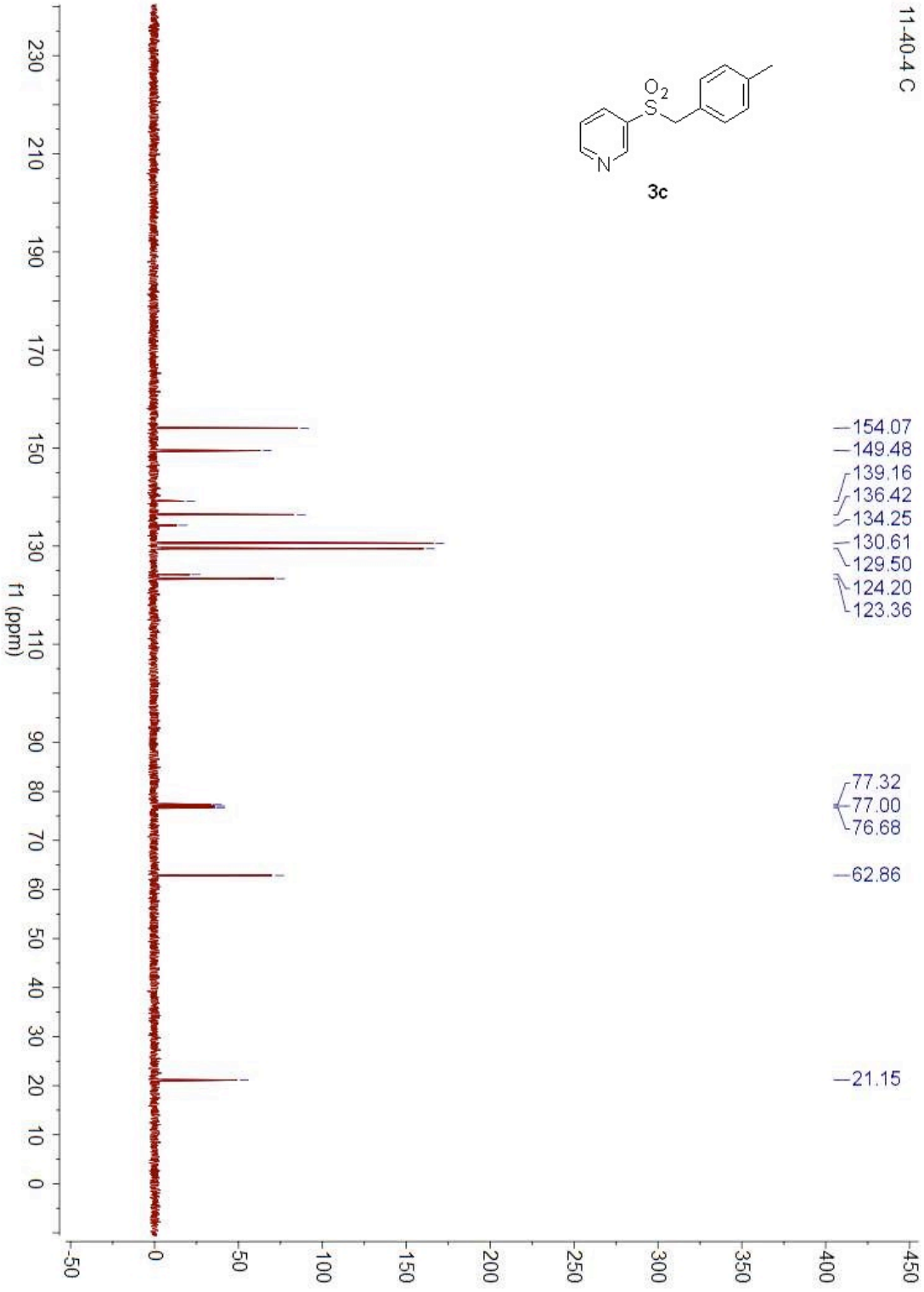
76.99
76.67
62.19
21.20
f1 (ppm)


11-40-4 H
3c
8.816
8.812
8.804
8.800
8.793
8.792
8.788
7.872
7.870
7.852
7.850
7.398
7.397
7.386
7.384
7.378
7.366
7.262
7.097
7.078
6.984
6.964
4.325
2.328
1.590
0.000
1.84
0.97
1.05
2.00
1.99
2.03
3.02
f1 (ppm)


11-40-4 C
3c
154.07
149.48
139.16
136.42
134.25
130.61
129.50
124.20
123.36
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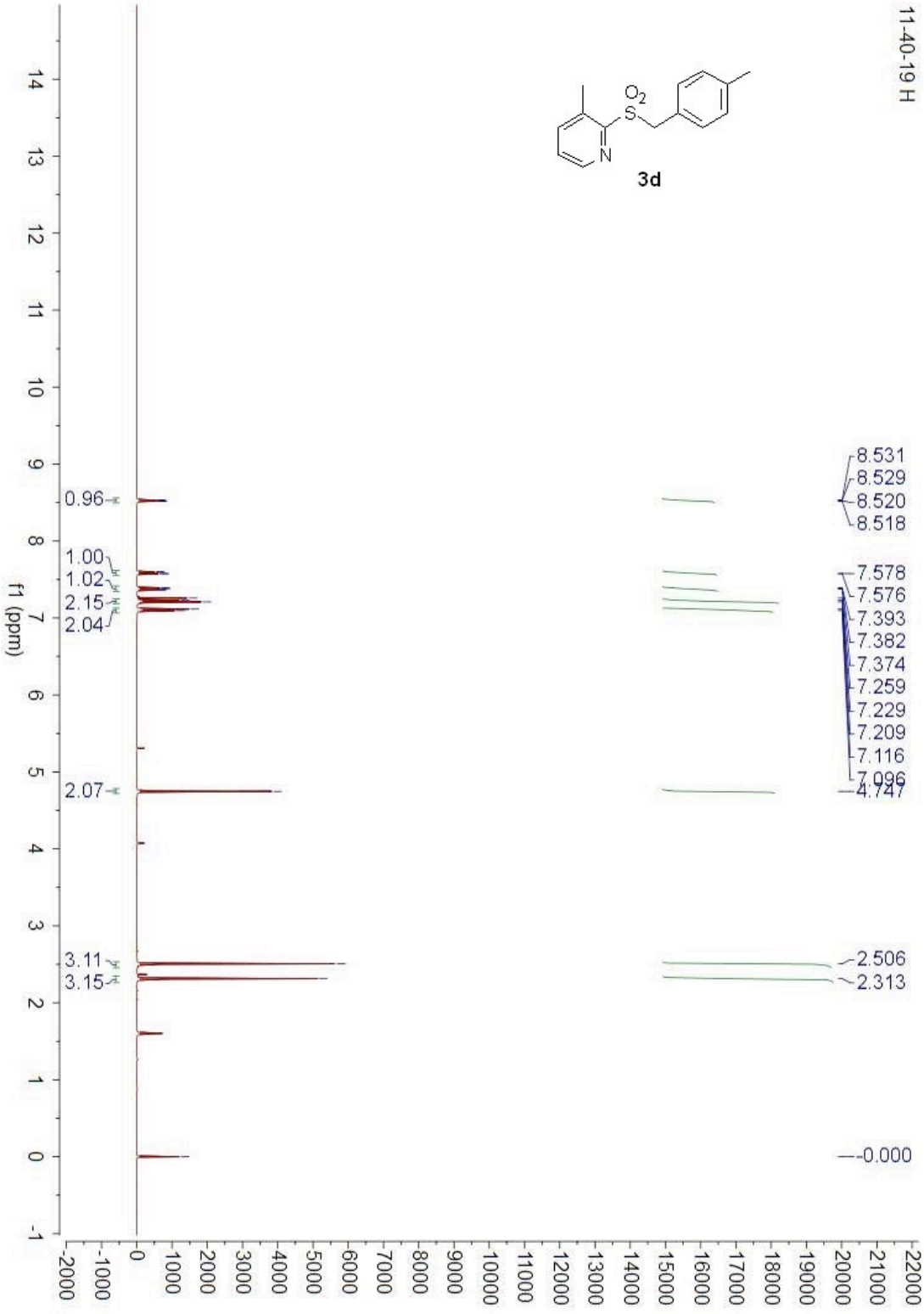
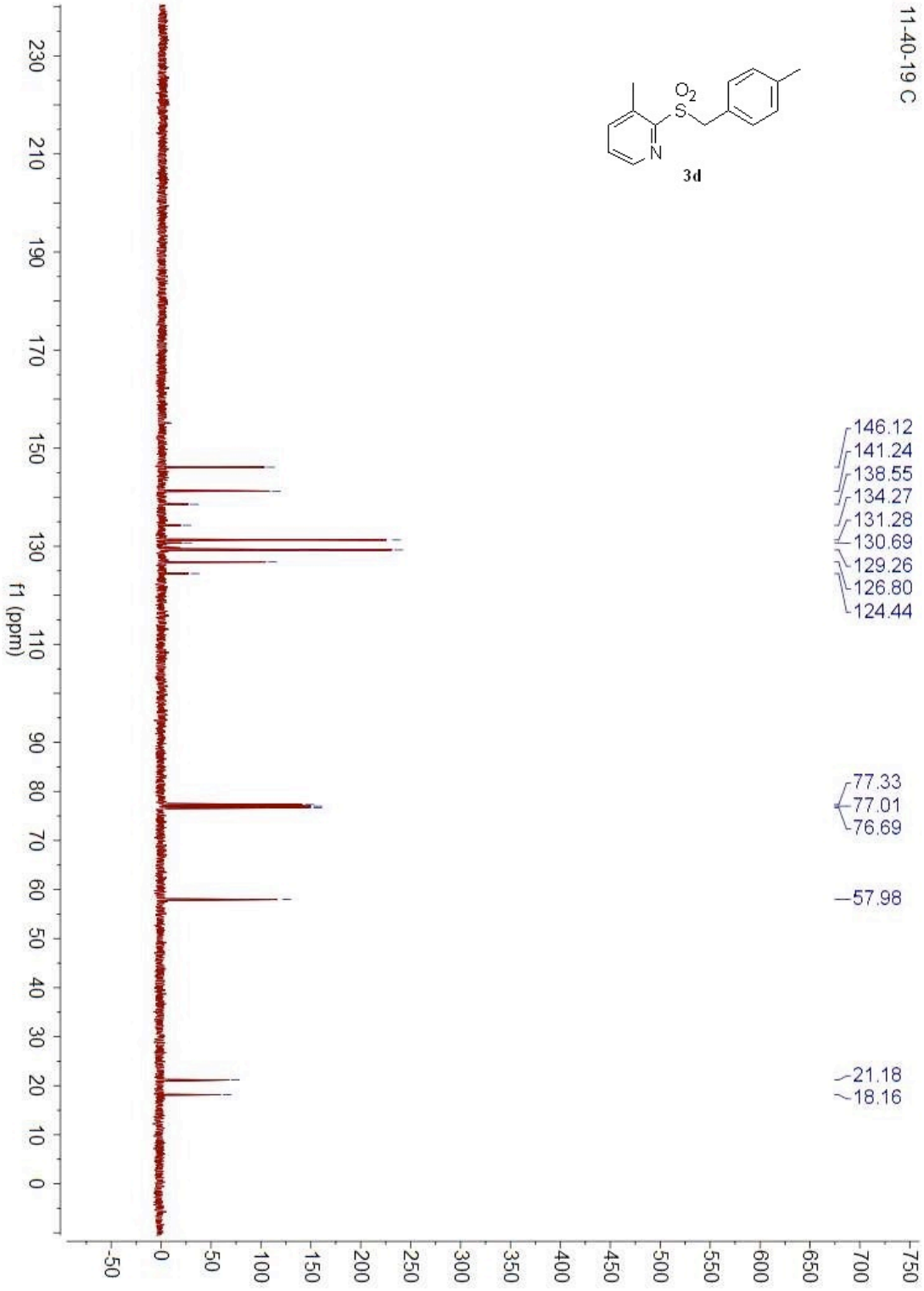
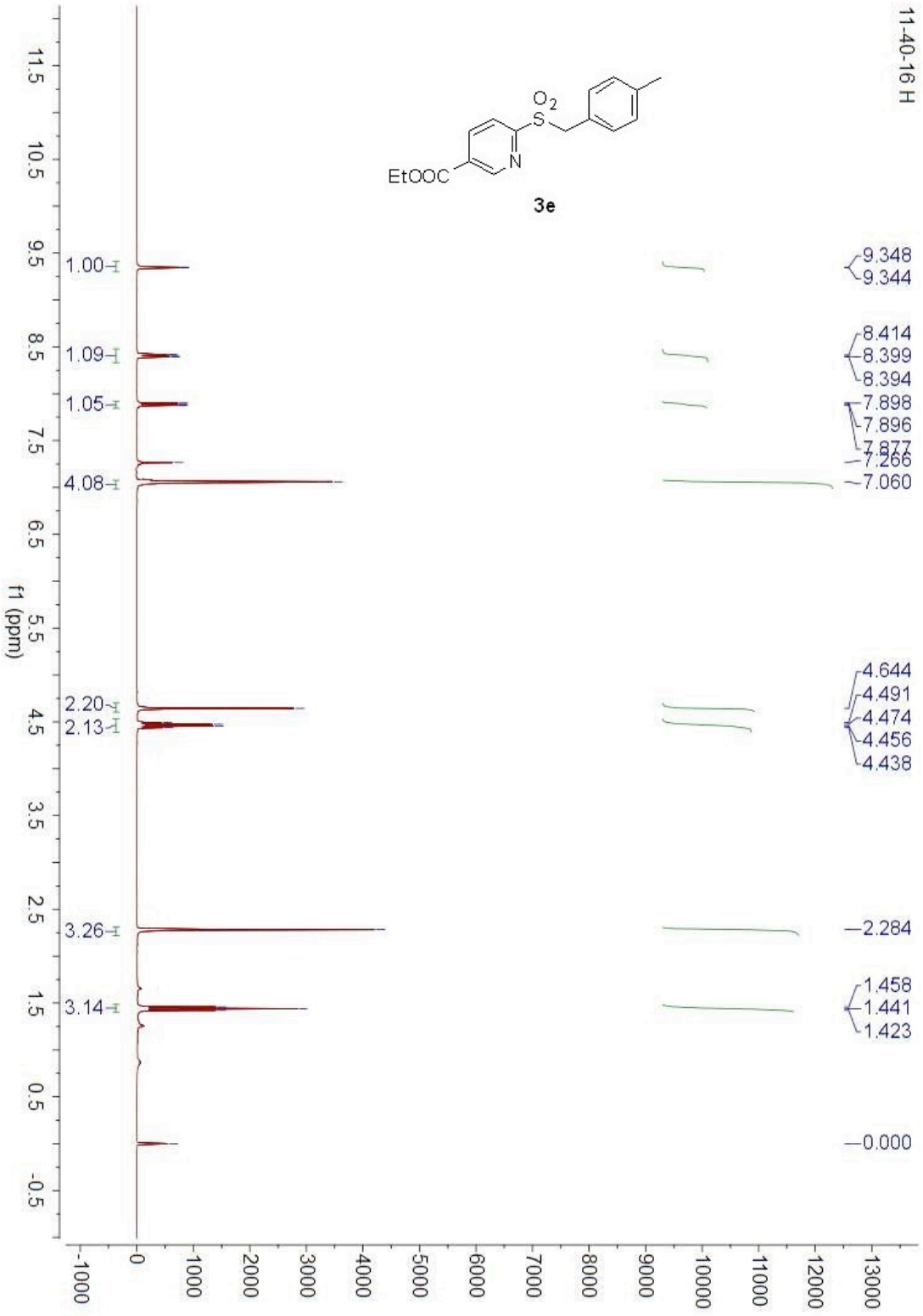
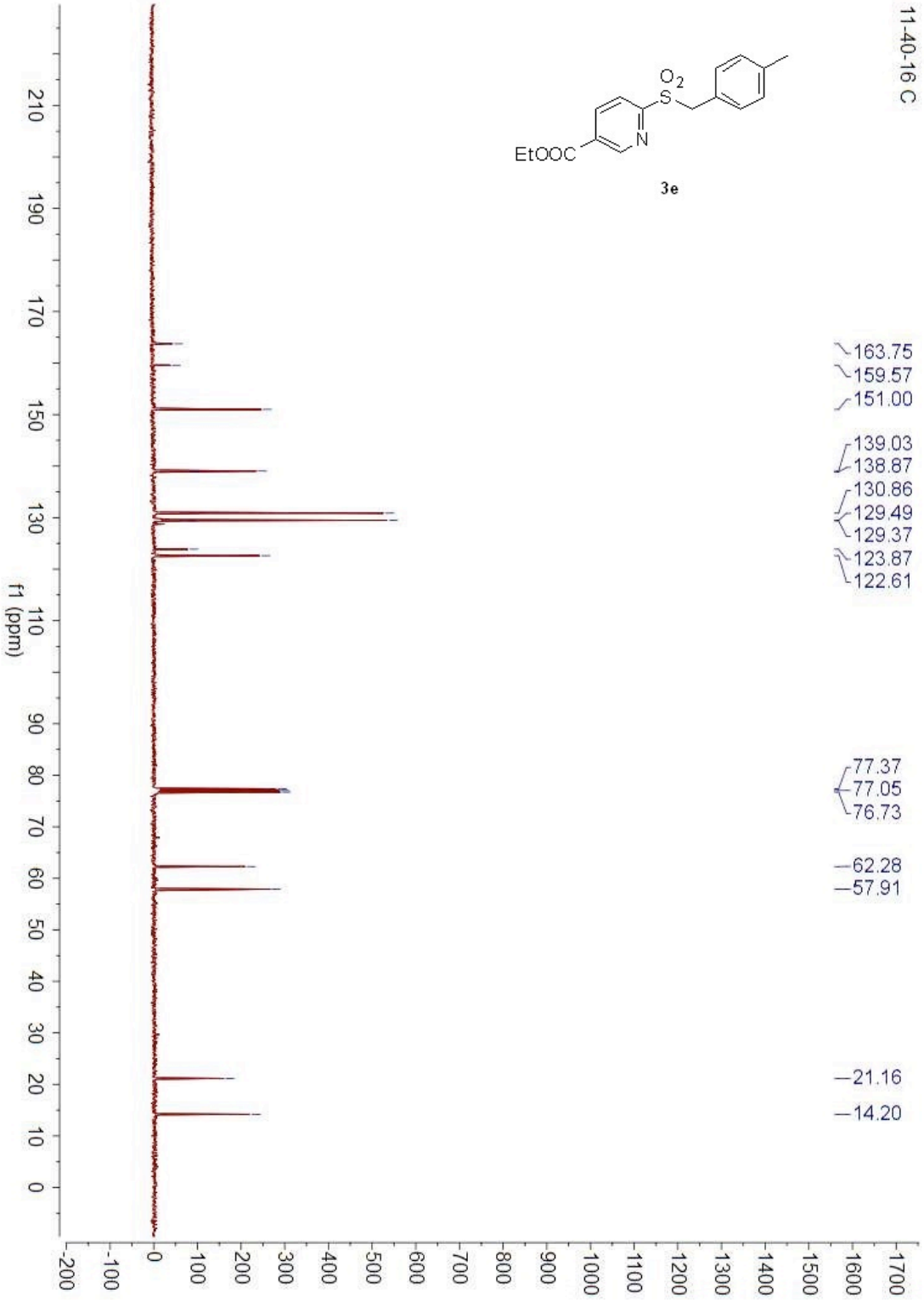
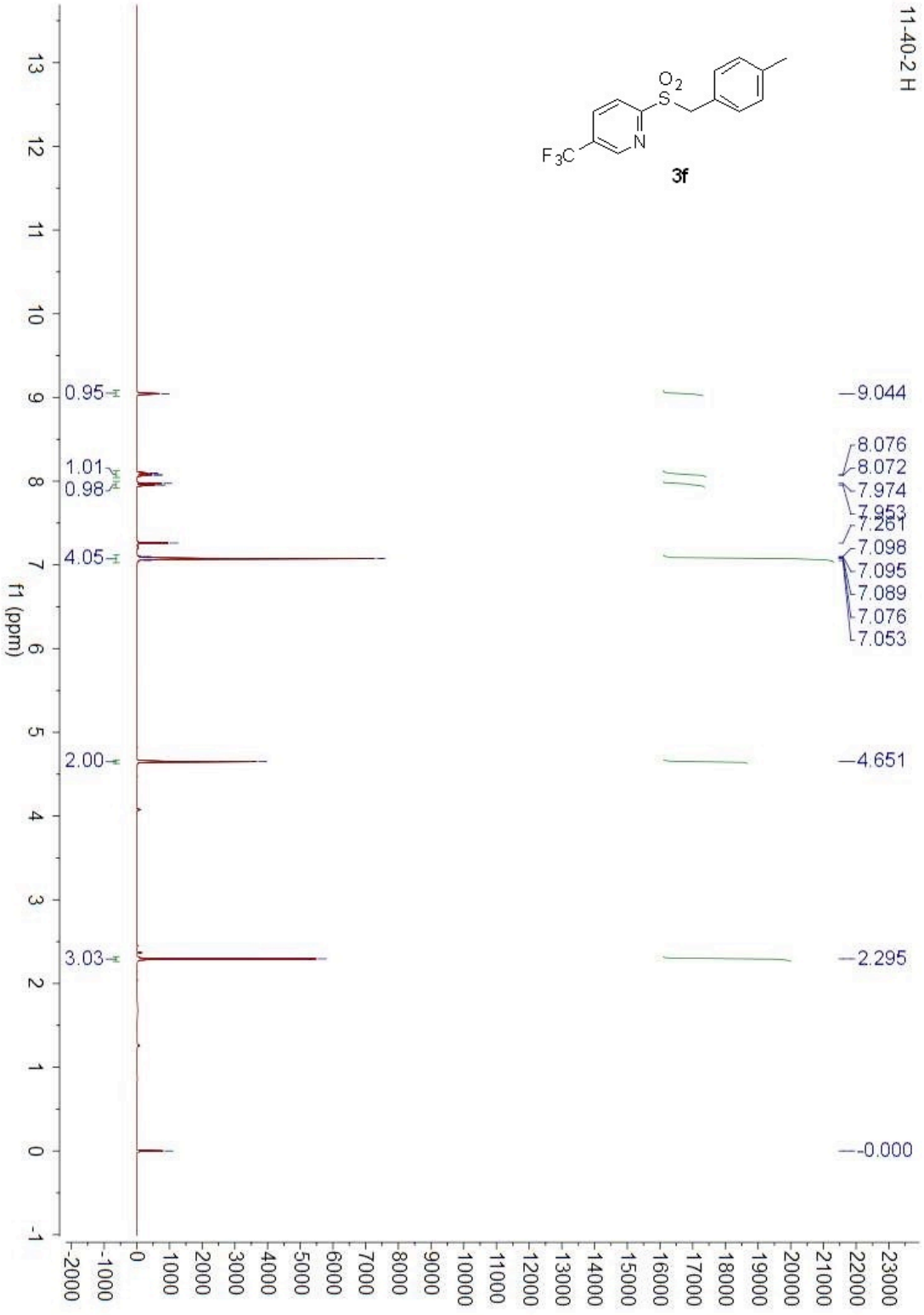
77.00
76.68
62.86
21.15
f1 (ppm)

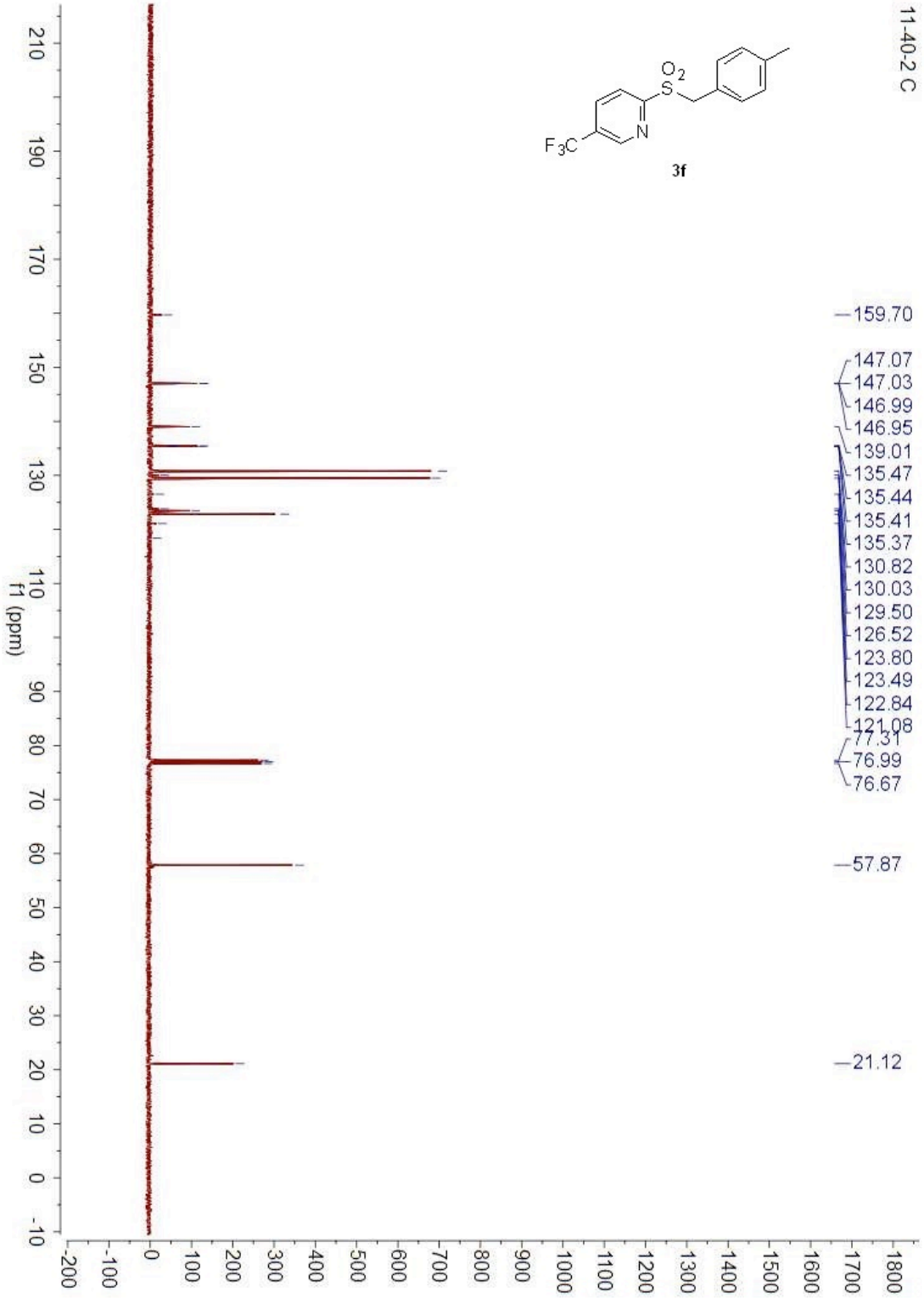

11-40-19 H
3d
f1 (ppm)
0.96
1.00
1.02
2.15
2.04
2.07
3.11
3.15
8.531
8.529
8.520
8.518
7.578
7.576
7.393
7.382
7.374
7.259
7.229
7.209
7.116
7.096
4.747
2.506
2.313
0.000

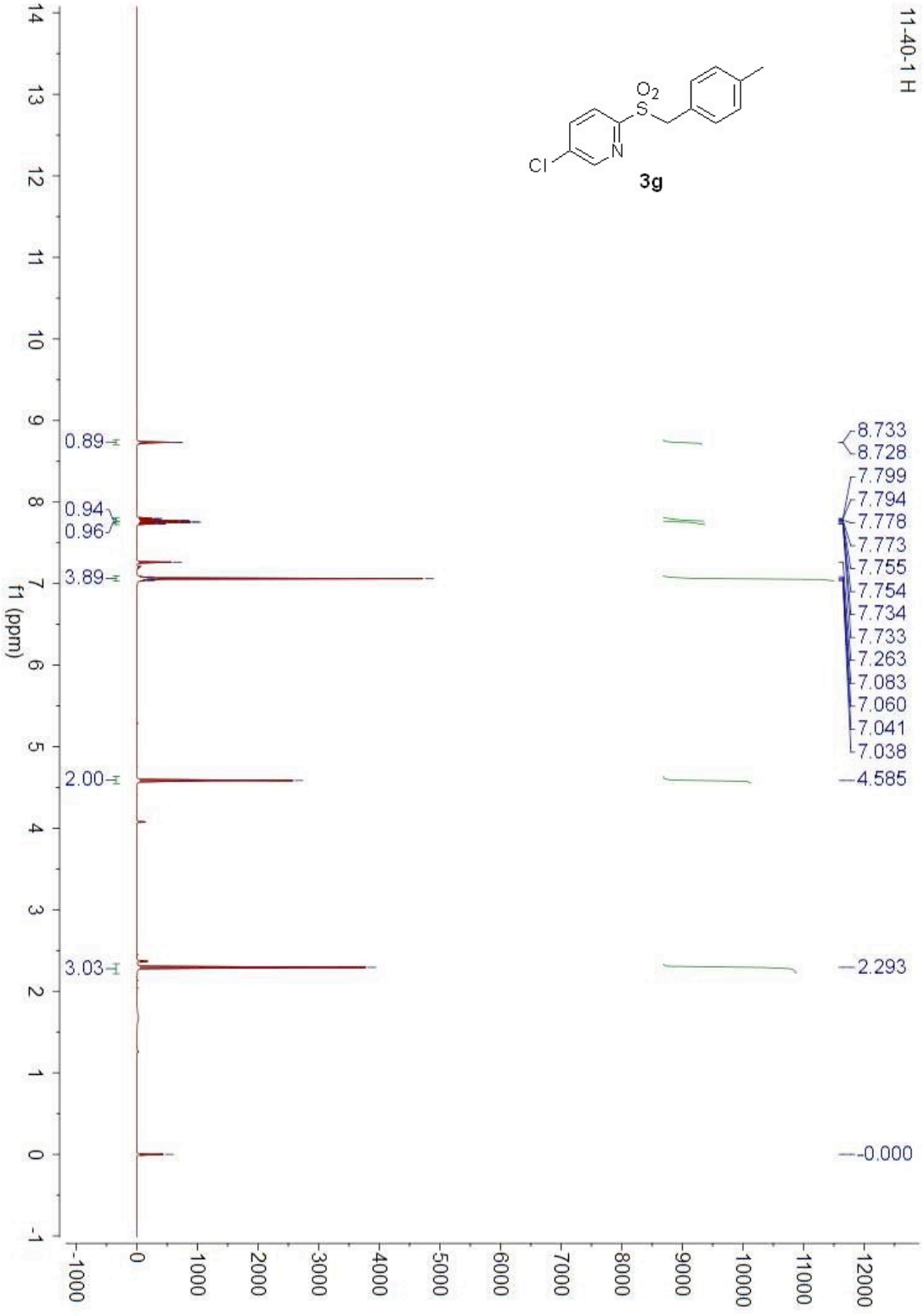

11-40-19 C
3d
146.12
141.24
138.55
134.27
131.28
130.69
129.26
126.80
124.44
77.33
77.01
76.69
57.98
21.18
18.16
f1 (ppm)


11-40-16 H
O2
S
N
EtOOC
3e
1.00
1.09
1.05
4.08
2.20
2.13
3.26
3.14
9.348
9.344
8.414
8.399
8.394
7.898
7.896
7.877
7.266
7.060
4.644
4.491
4.474
4.456
4.438
2.284
1.458
1.441
1.423
0.000
f1 (ppm)


11-40-16 C
O2
S
N
EtOOC
3e
163.75
159.57
151.00
139.03
138.87
130.86
129.49
129.37
123.87
122.61
77.37
77.05
76.73
62.28
57.91
21.16
14.20
f1 (ppm)


11-40-2 H
3f
f1 (ppm)
0.95
1.01
0.98
4.05
2.00
3.03
9.044
8.076
8.072
7.974
7.953
7.261
7.098
7.095
7.089
7.076
7.053
4.651
2.295
0.000


11-40-2 C
3f
159.70
147.07
147.03
146.99
146.95
139.01
135.47
135.44
135.41
135.37
130.82
130.03
129.50
126.52
123.80
123.49
122.84
121.08
77.31
76.99
76.67
57.87
21.12
f1 (ppm)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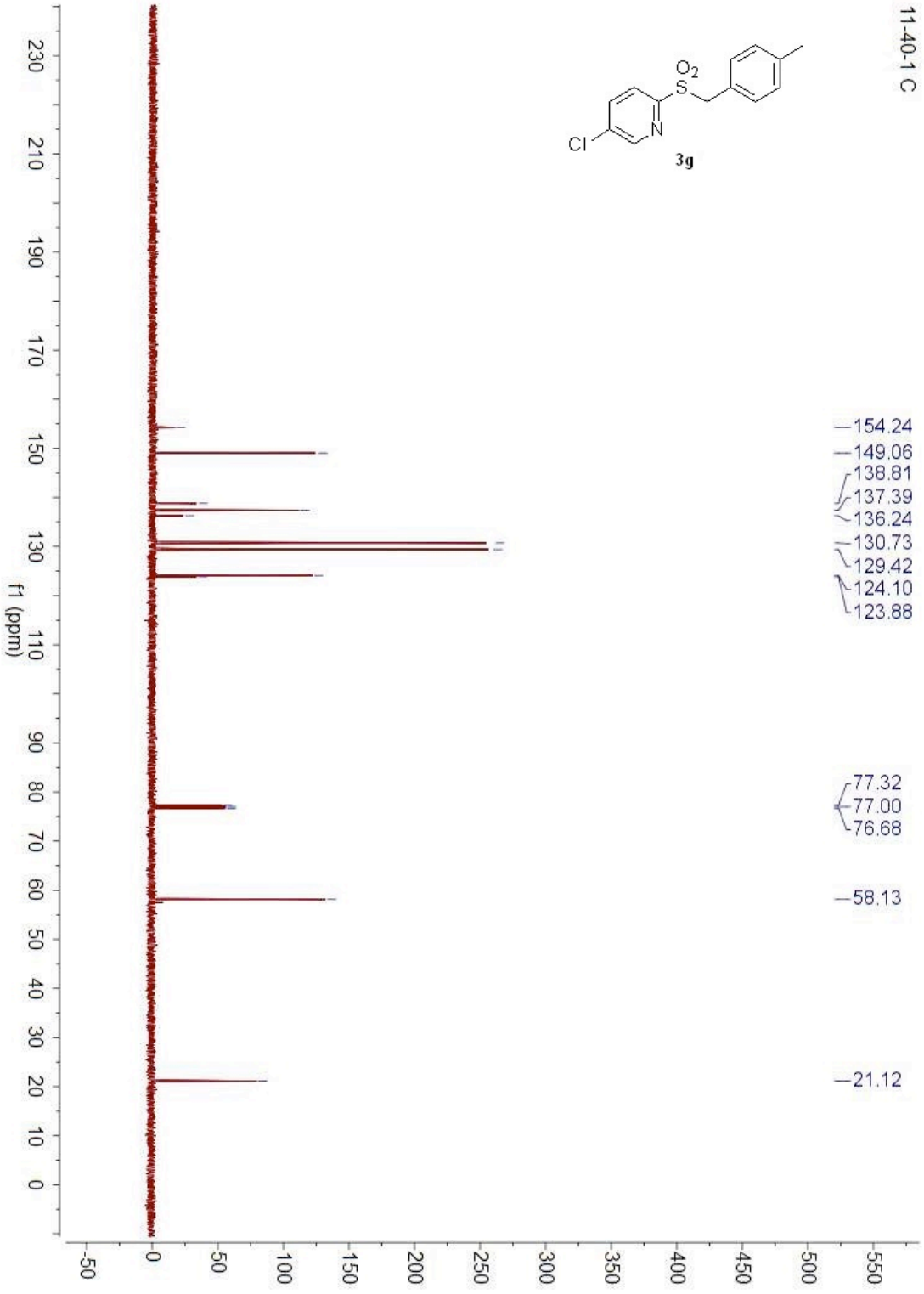
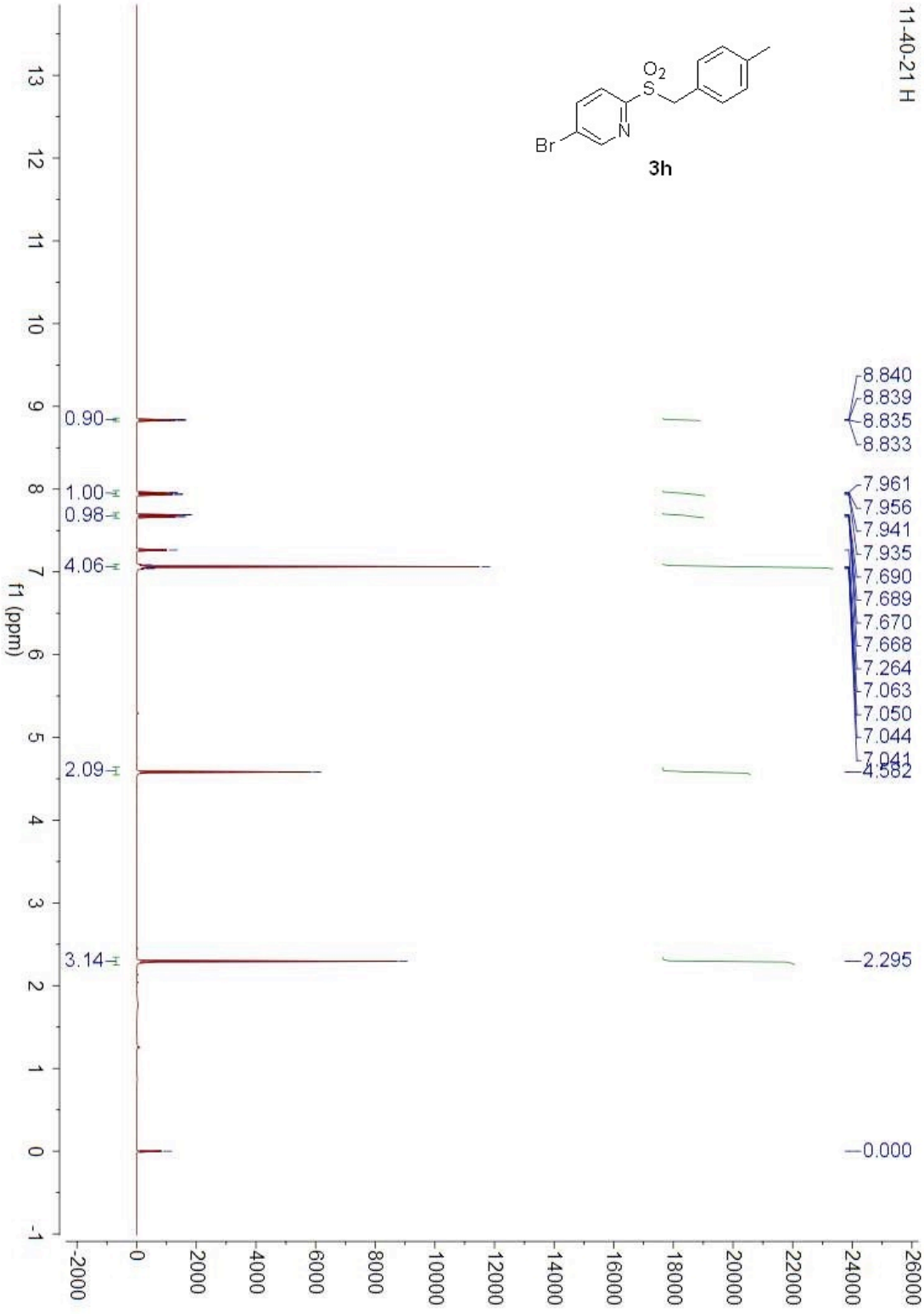
3g
f1 (ppm)
0.89
0.94
0.96
3.89
2.00
3.03
8.733
8.728
7.799
7.794
7.778
7.773
7.755
7.754
7.734
7.733
7.263
7.083
7.060
7.041
7.038
4.585
2.293
0.000


11-40-1 C
O2
S
N
Cl
3g
154.24
149.06
138.81
137.39
136.24
130.73
129.42
124.10
123.88
77.32
77.00
76.68
58.13
21.12
f1 (ppm)


11-40-21 H
3h
Br
O2
S
N
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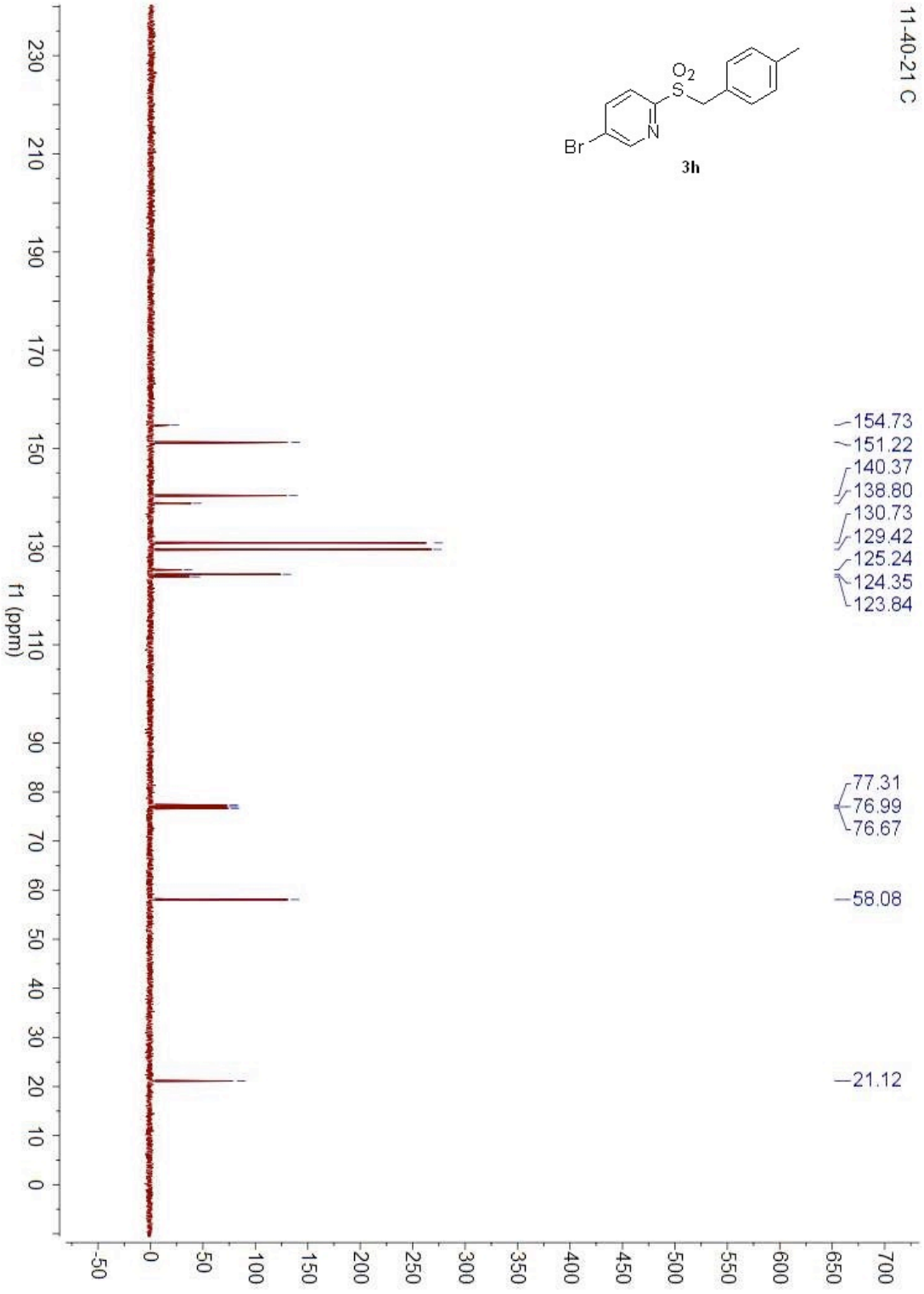
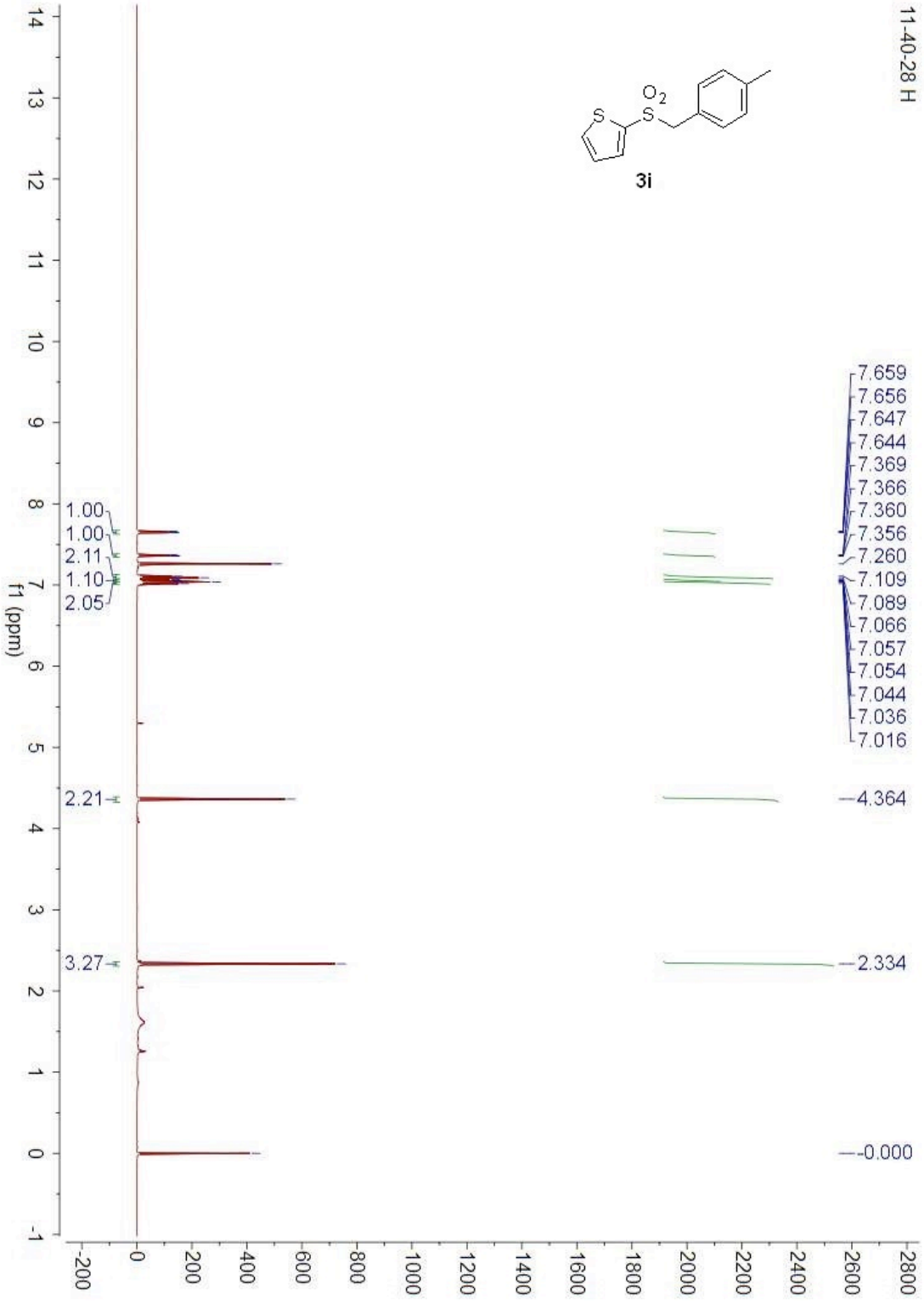
8.839
8.835
8.833
7.961
7.956
7.941
7.935
7.690
7.689
7.670
7.668
7.264
7.063
7.050
7.044
7.041
4.582
2.295
0.000
0.90
1.00
0.98
4.06
2.09
3.14
f1 (ppm)


11-40-21 C
O2
S
N
Br
3h
154.73
151.22
140.37
138.80
130.73
129.42
125.24
124.35
123.84
77.31
76.99
76.67
58.08
21.12
f1 (ppm)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3i
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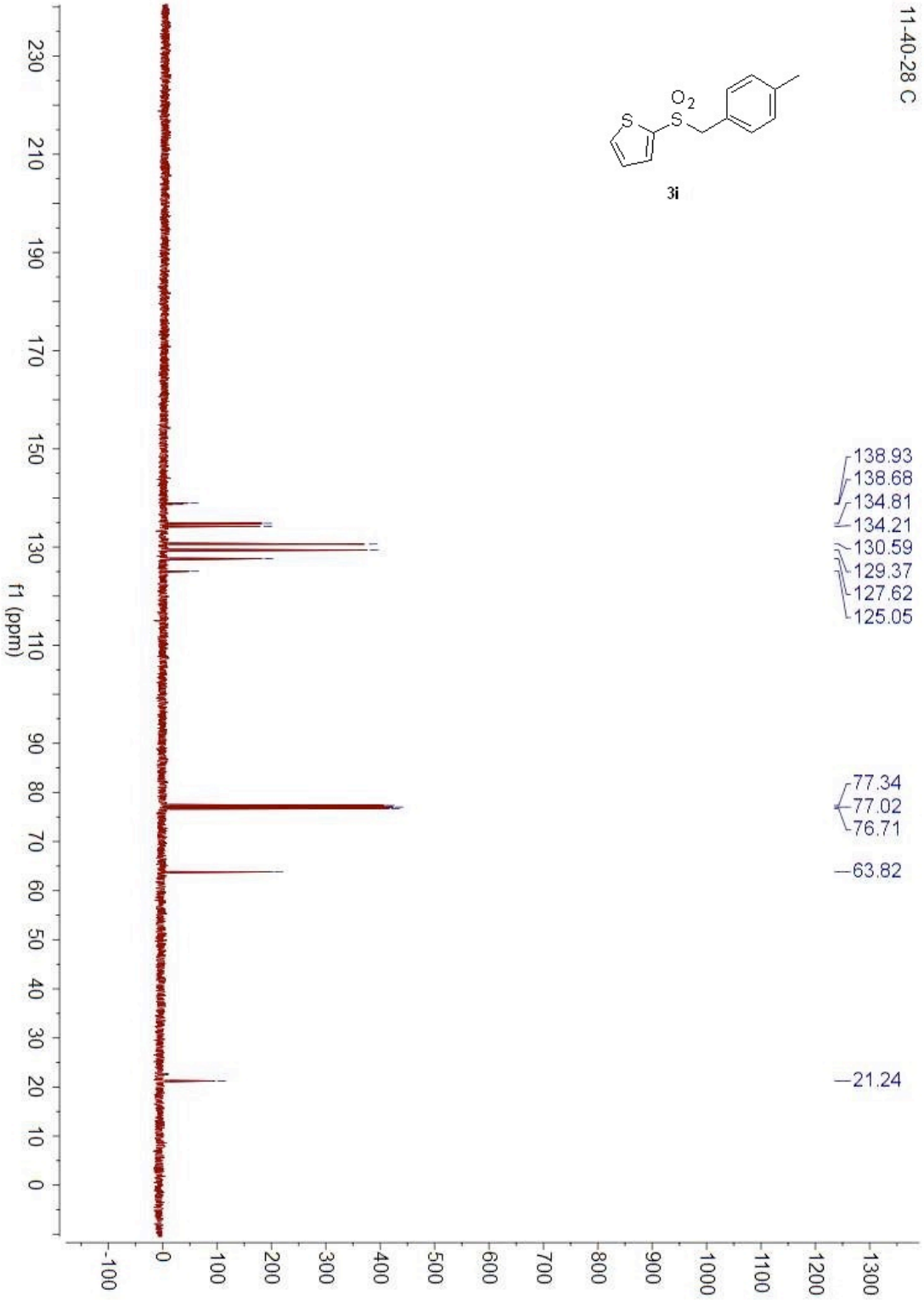
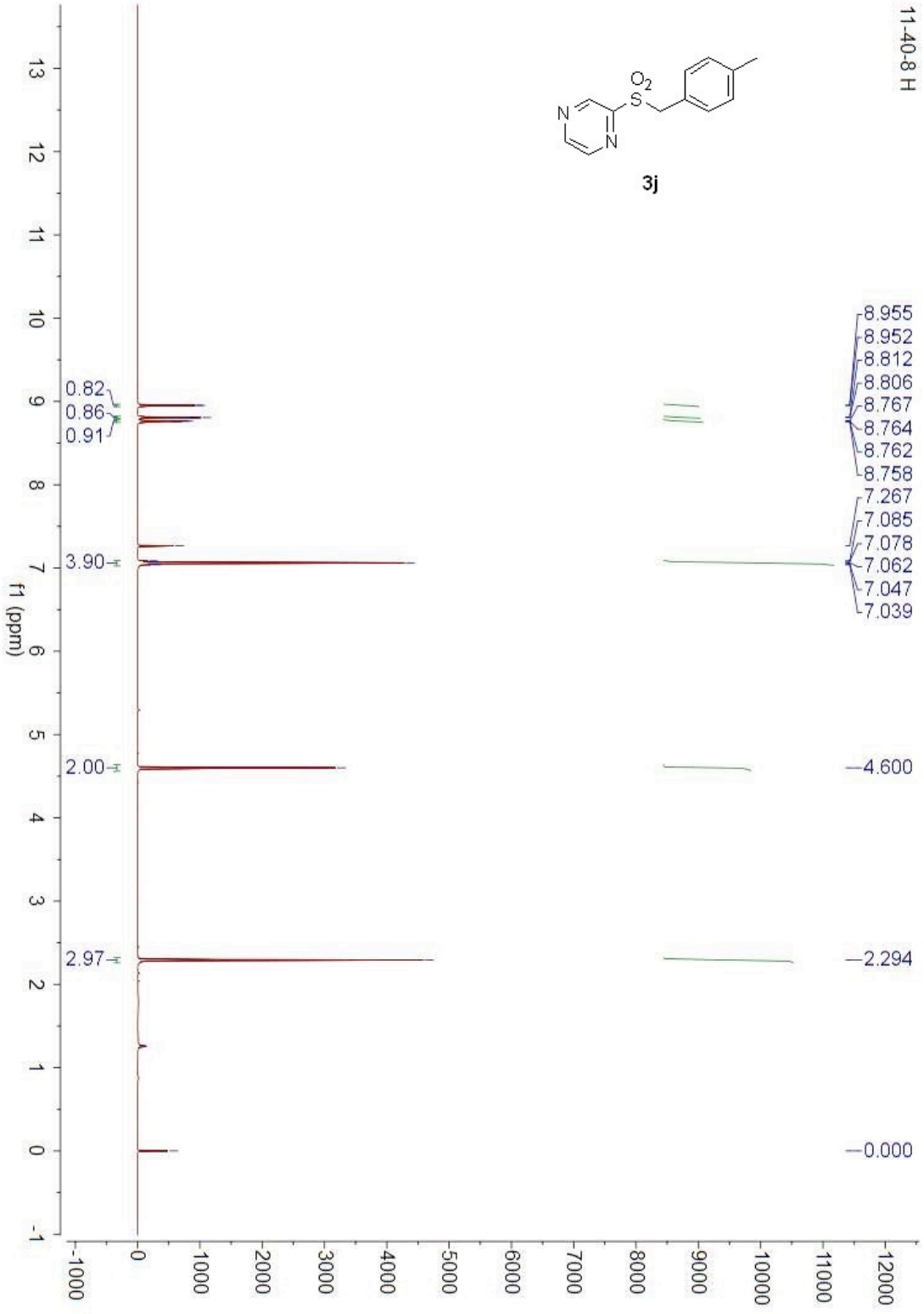
7.647
7.644
7.369
7.366
7.360
7.356
7.260
7.109
7.089
7.066
7.057
7.054
7.044
7.036
7.016
4.364
2.334
0.000
1.00
1.00
2.11
1.10
2.05
2.21
3.27
f1 (ppm)


11-40-28 C
O2
S
S
3i
138.93
138.68
134.81
134.21
130.59
129.37
127.62
125.05
77.34
77.02
76.71
63.82
21.24
f1 (ppm)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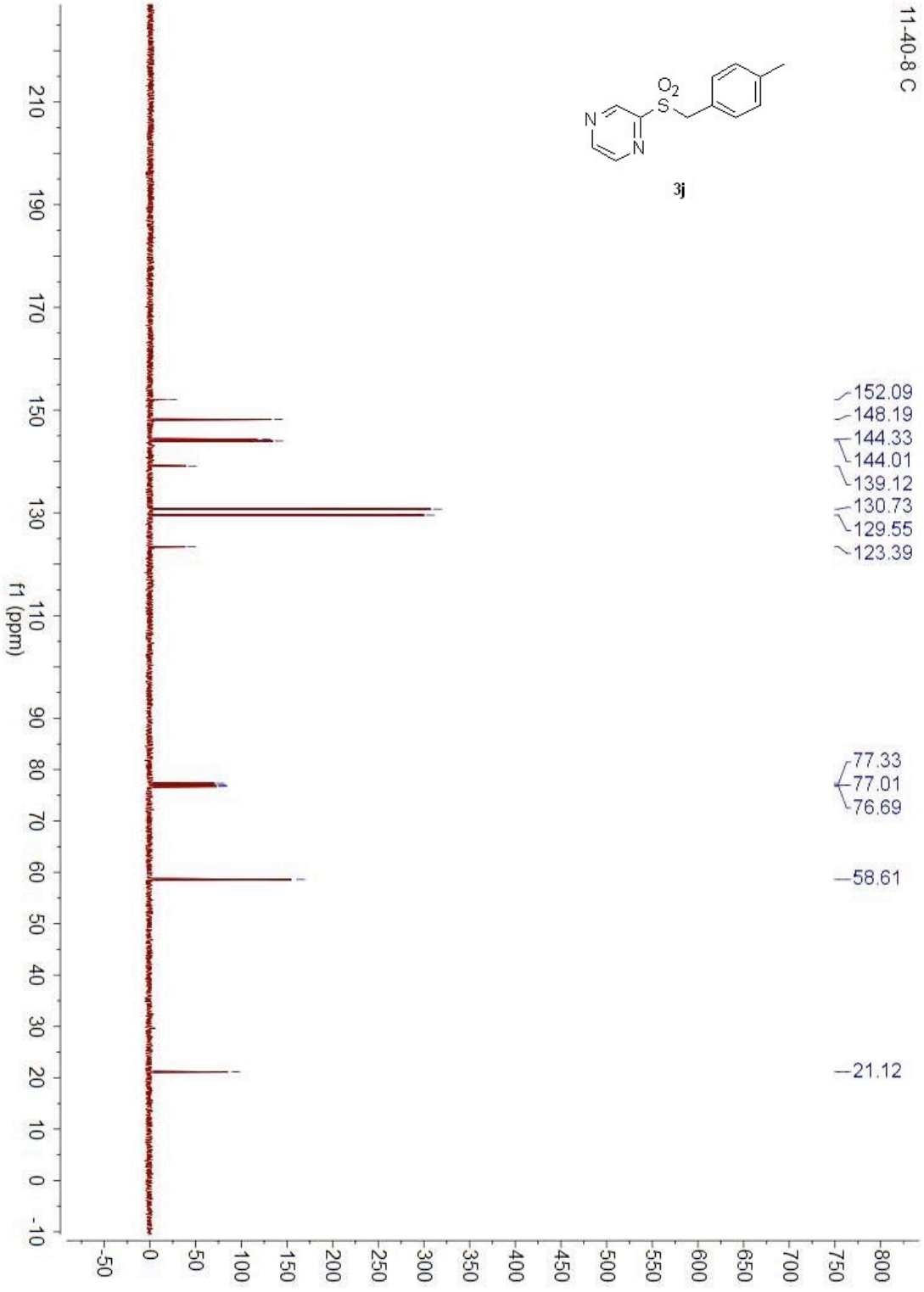
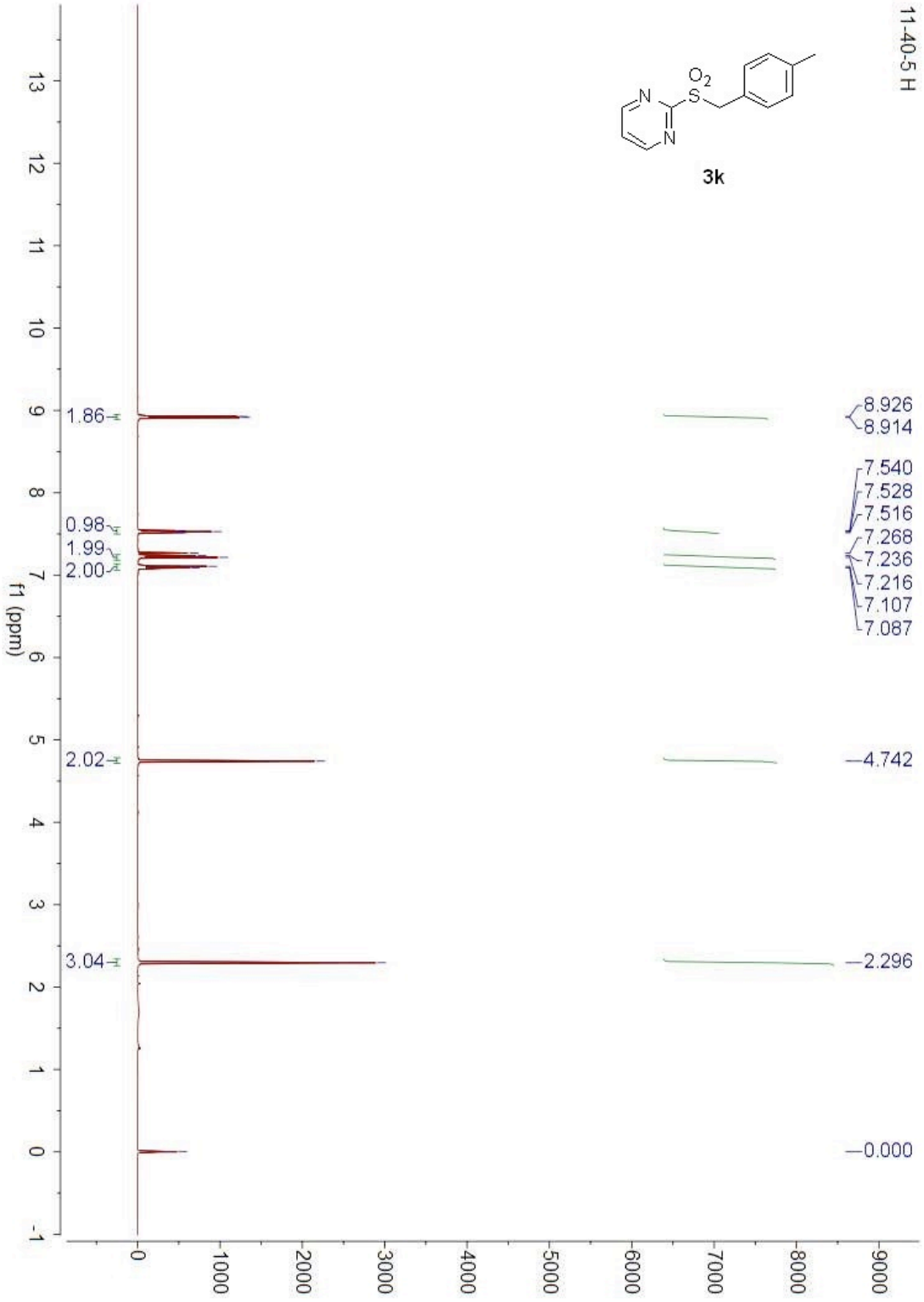
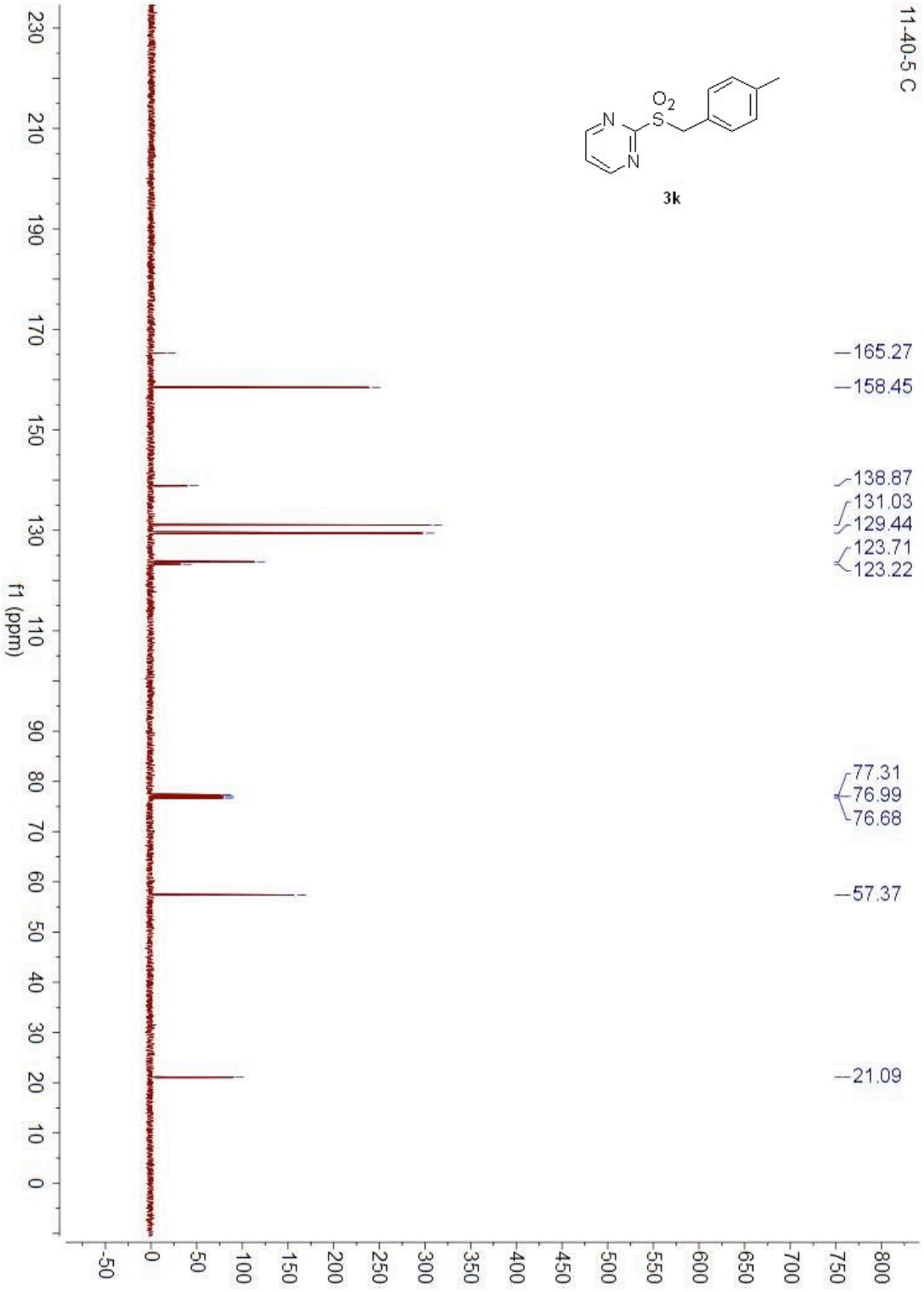
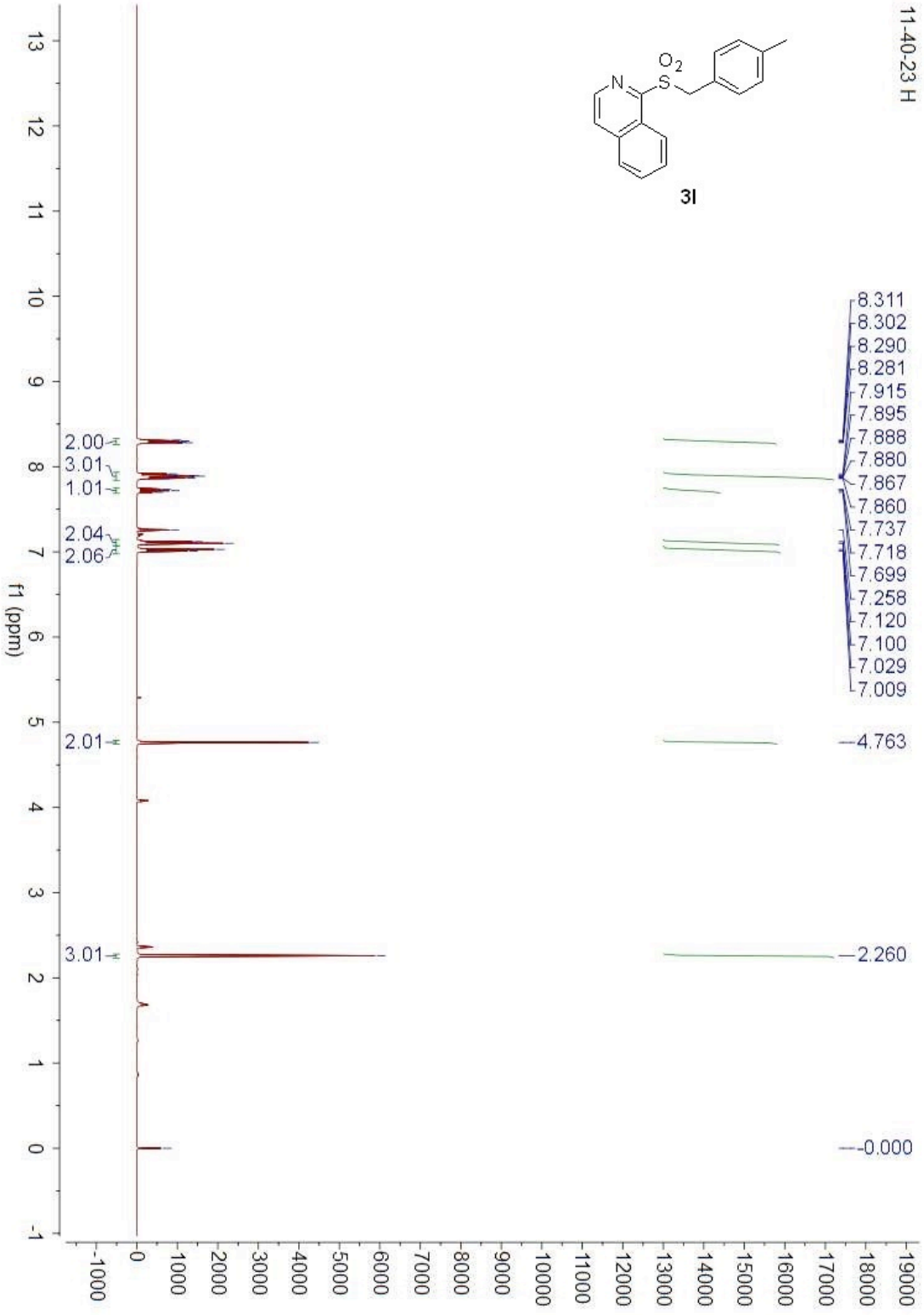
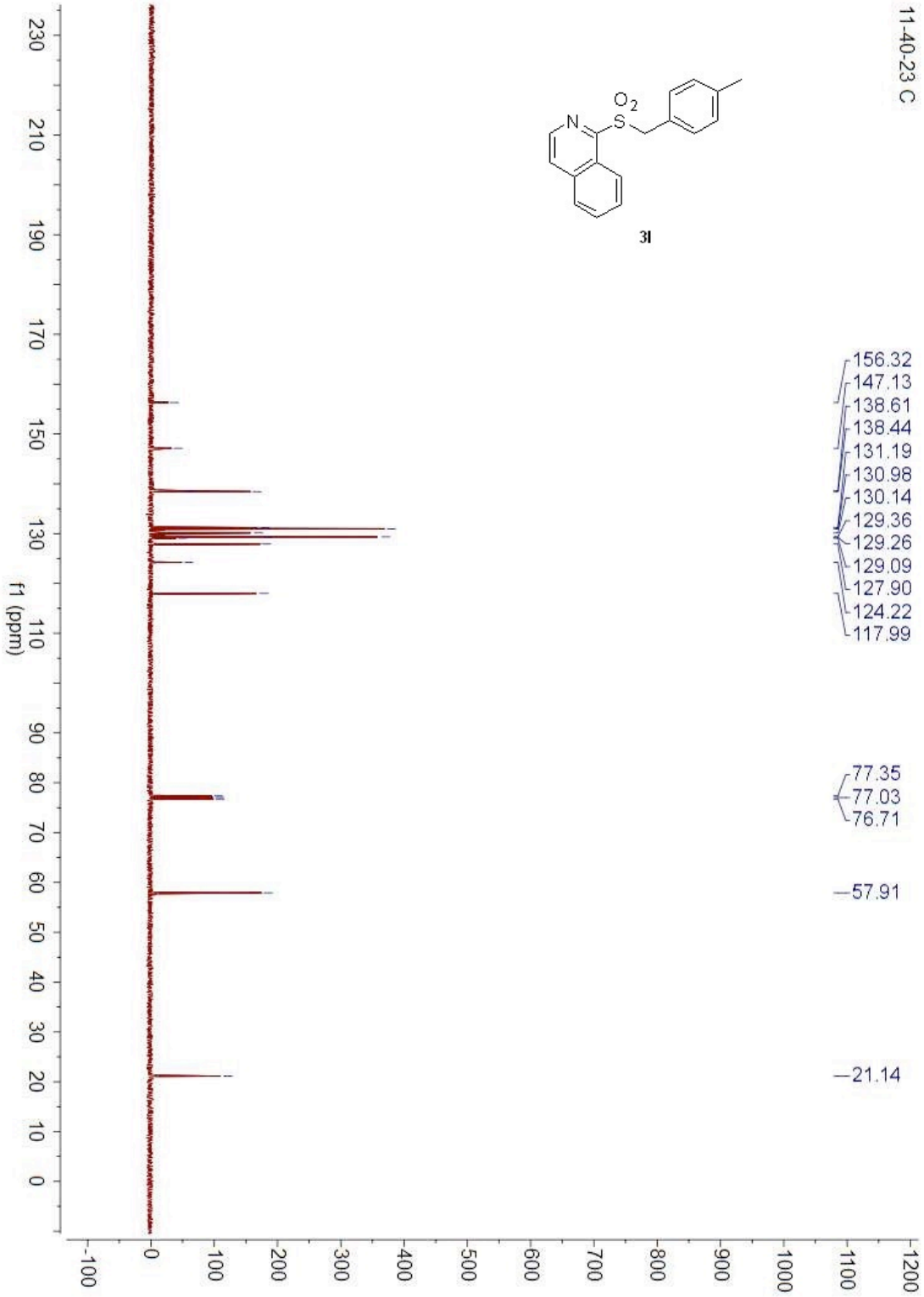
3j
8.955
8.952
8.812
8.806
8.767
8.764
8.762
8.758
7.267
7.085
7.078
7.062
7.047
7.039
4.600
2.294
0.000
0.82
0.86
0.91
3.90
2.00
2.97
f1 (ppm)

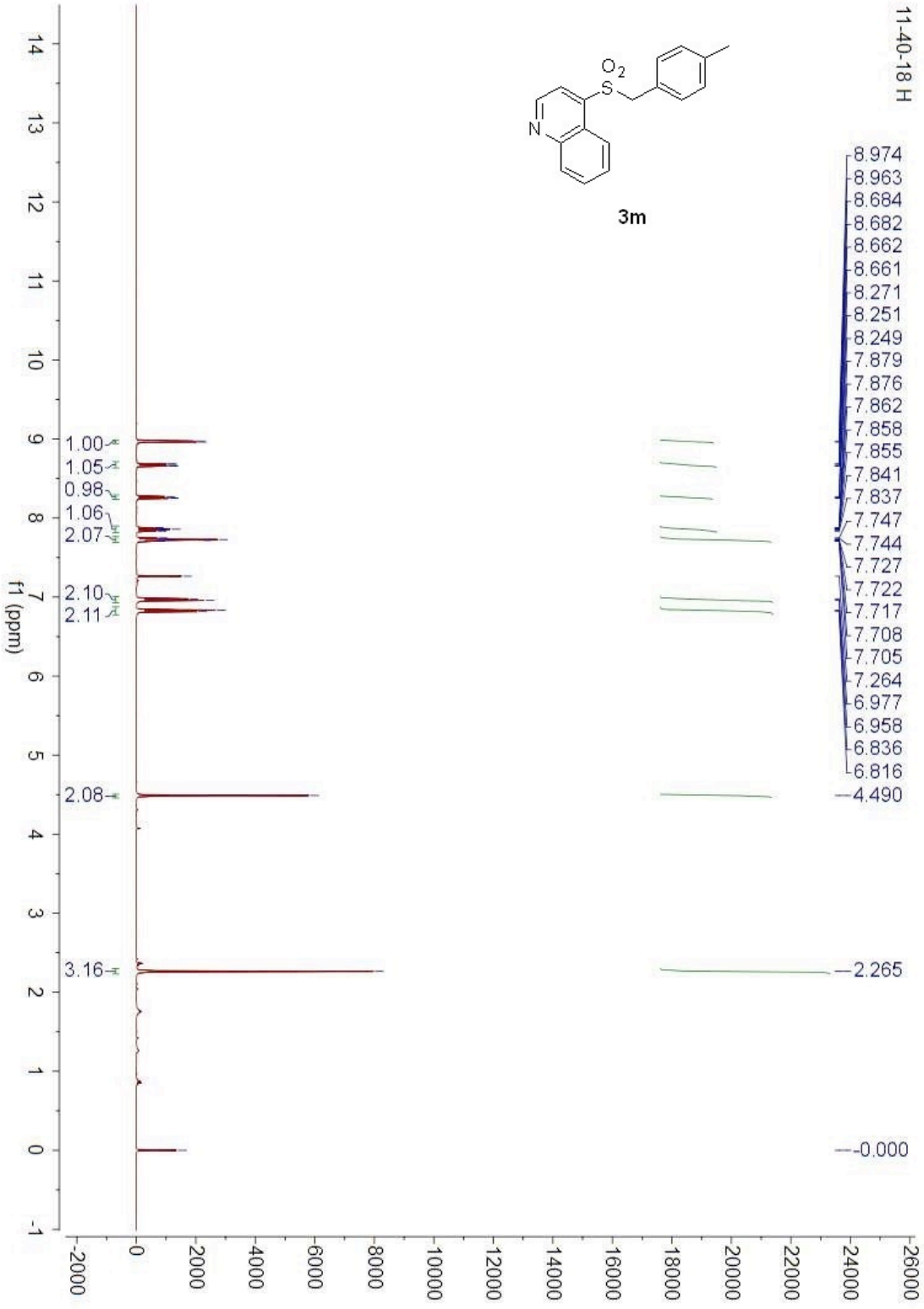

11-40-8 C
3j
152.09
148.19
144.33
144.01
139.12
130.73
129.55
123.39
77.33
77.01
76.69
58.61
21.12
f1 (ppm)

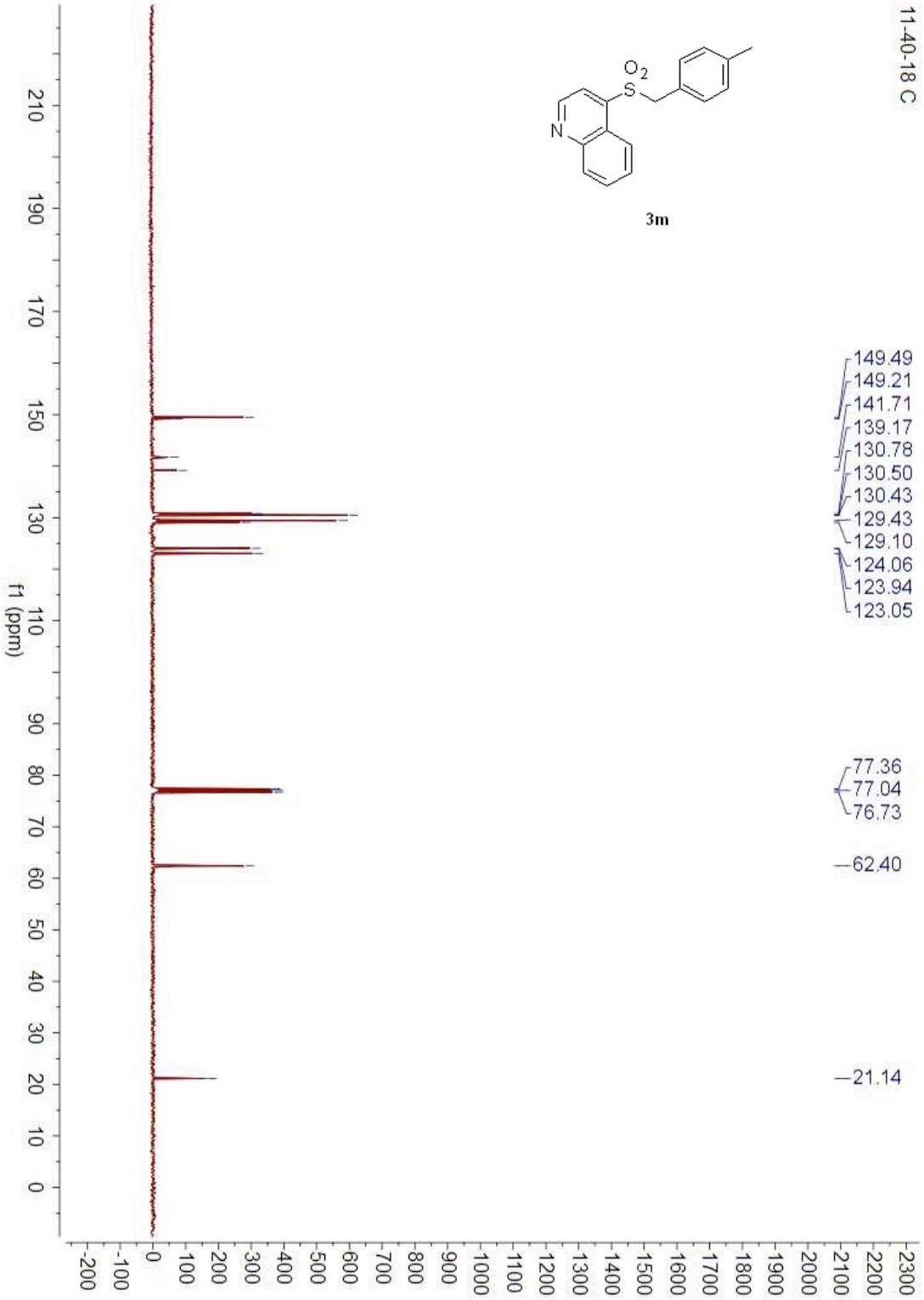

11-40-5 H
3k
1.86
0.98
1.99
2.00
2.02
3.04
8.926
8.914
7.540
7.528
7.516
7.268
7.236
7.216
7.107
7.087
4.742
2.296
0.000
f1 (ppm)

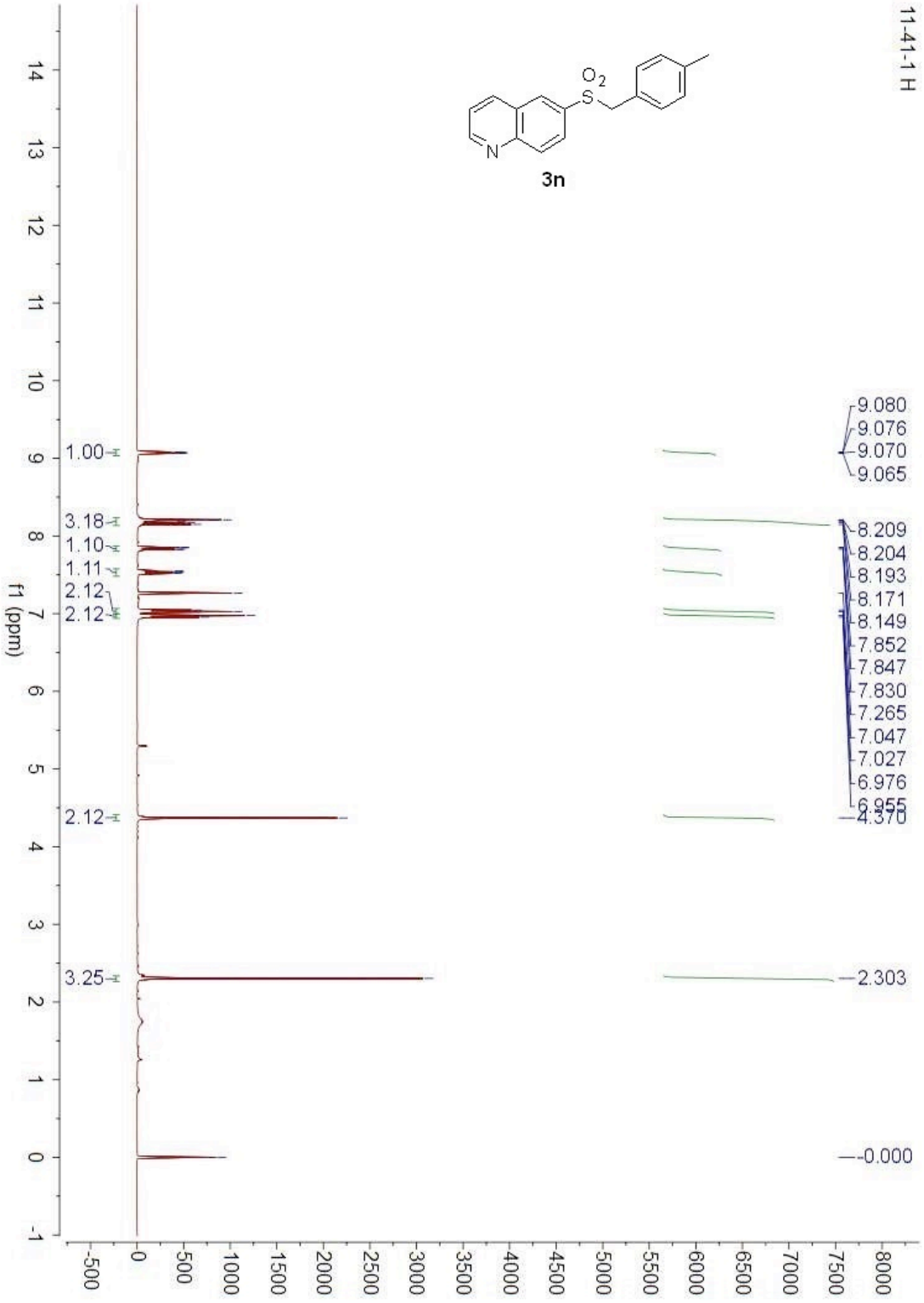

11-40-5 C
3k
165.27
158.45
138.87
131.03
129.44
123.71
123.22
77.31
76.99
76.68
57.37
21.09
f1 (ppm)

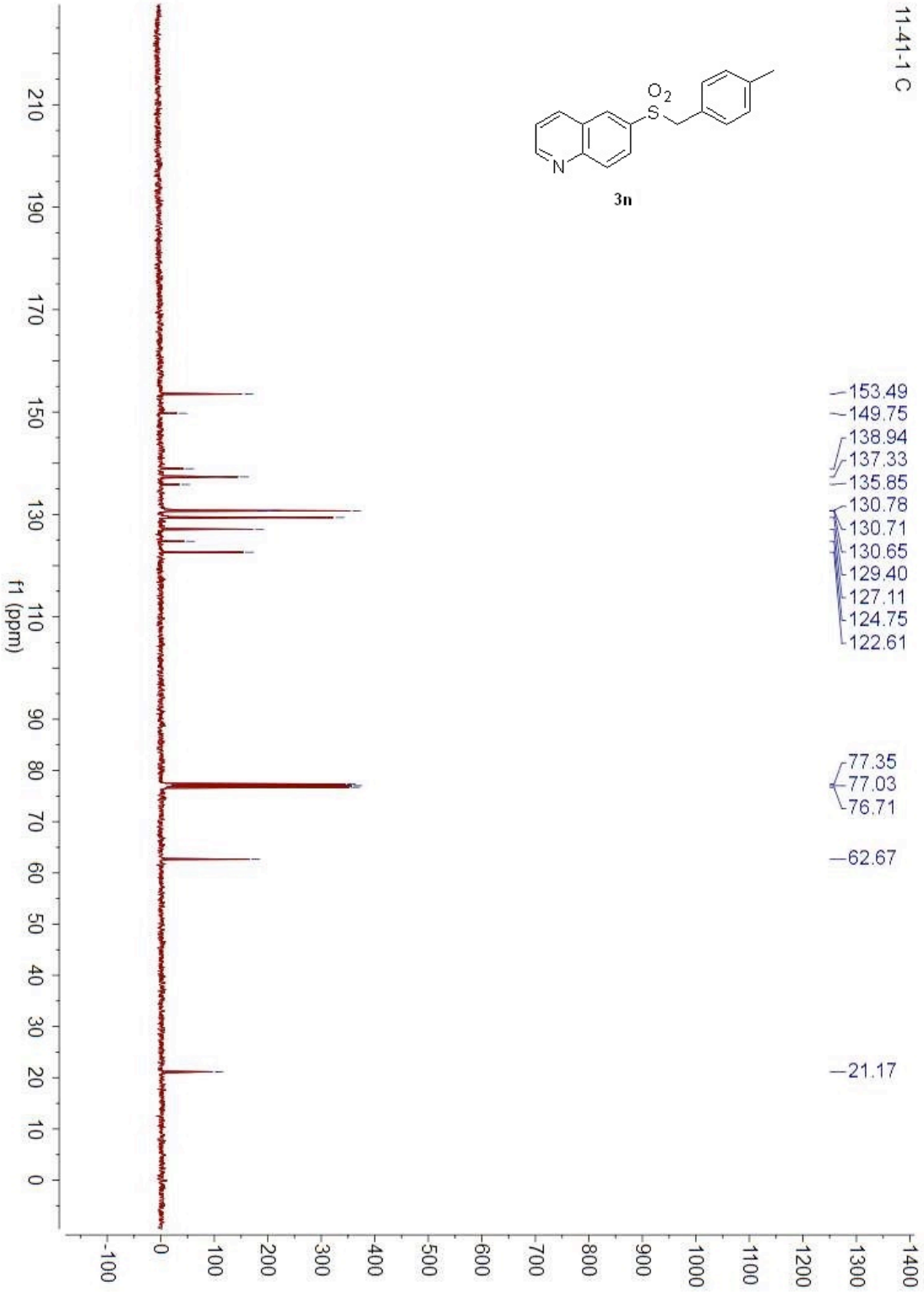

11-40-23 H
3l
8.311
8.302
8.290
8.281
7.915
7.895
7.888
7.880
7.867
7.860
7.737
7.718
7.699
7.258
7.120
7.100
7.029
7.009
4.763
2.260
0.000
2.00
3.01
1.01
2.04
2.06
2.01
3.01
f1 (ppm)

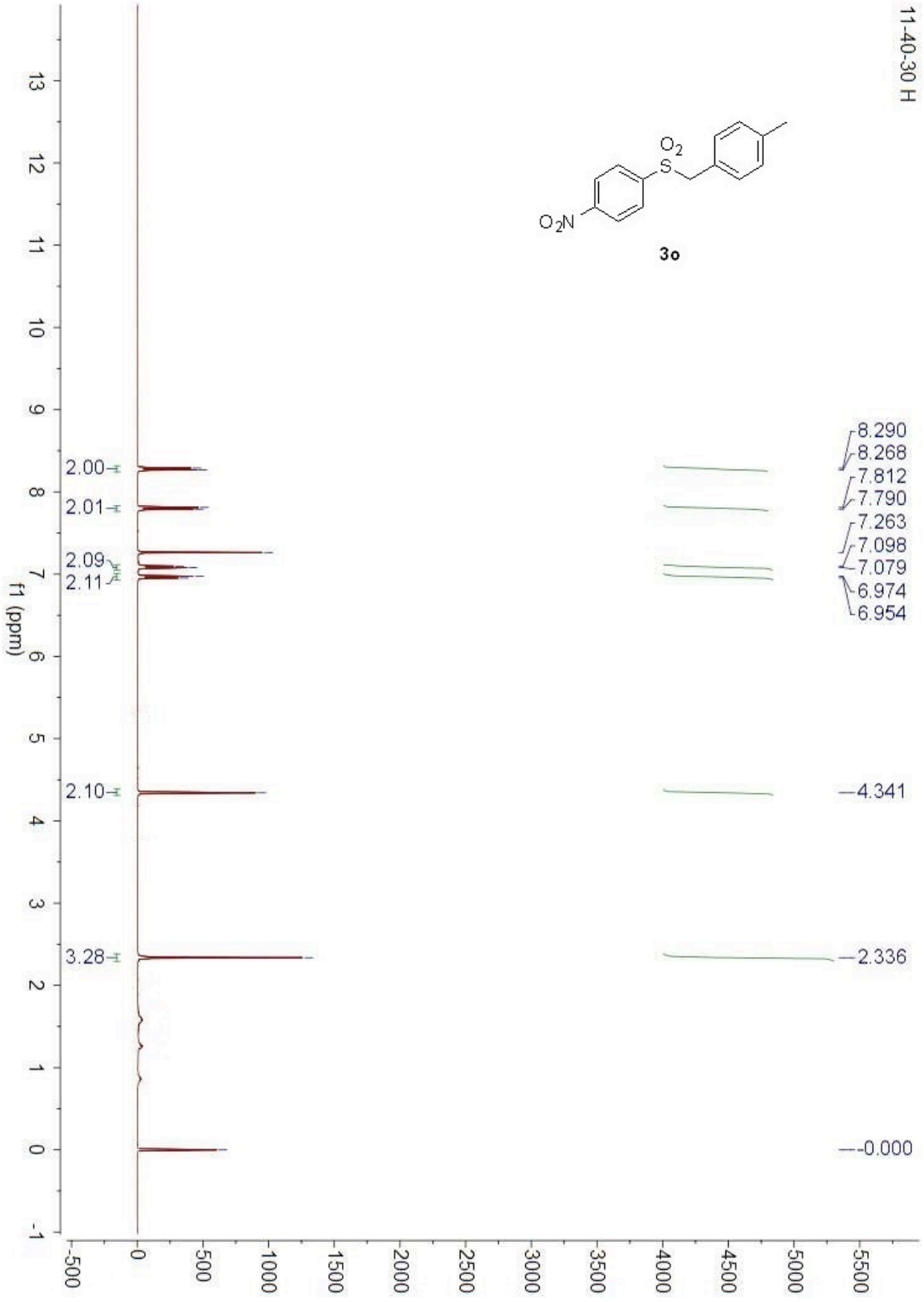

11-40-23 C
O2
N
S
3l
156.32
147.13
138.61
138.44
131.19
130.98
130.14
129.36
129.26
129.09
127.90
124.22
117.99
77.35
77.03
76.71
57.91
21.14
f1 (ppm)

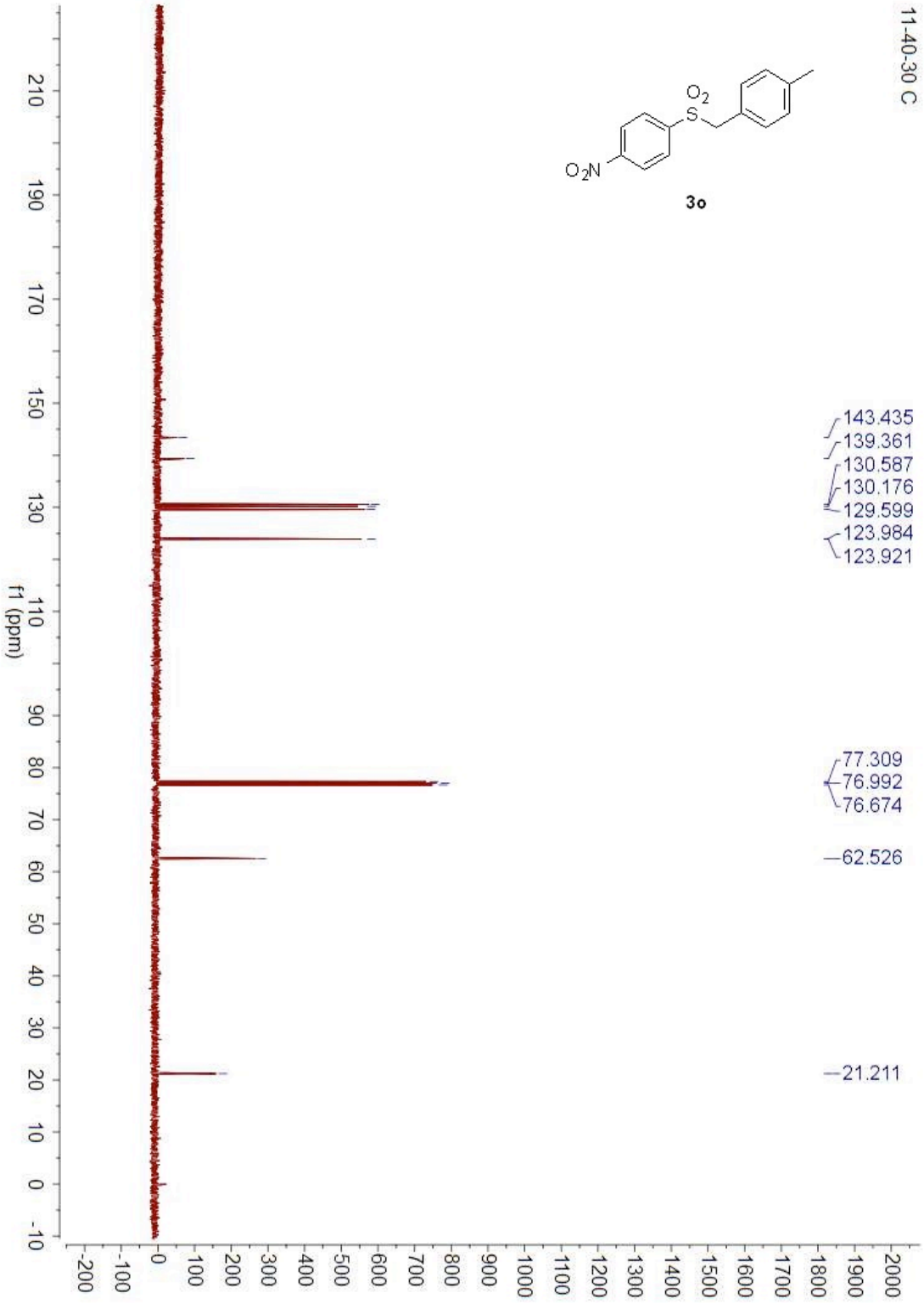

11-40-18 H
3m
8.974
8.963
8.684
8.682
8.662
8.661
8.271
8.251
8.249
7.879
7.876
7.862
7.858
7.855
7.841
7.837
7.747
7.744
7.727
7.722
7.717
7.708
7.705
7.264
6.977
6.958
6.836
6.816
4.490
2.265
0.000
1.00
1.05
0.98
1.06
2.07
2.10
2.11
2.08
3.16
f1 (ppm)

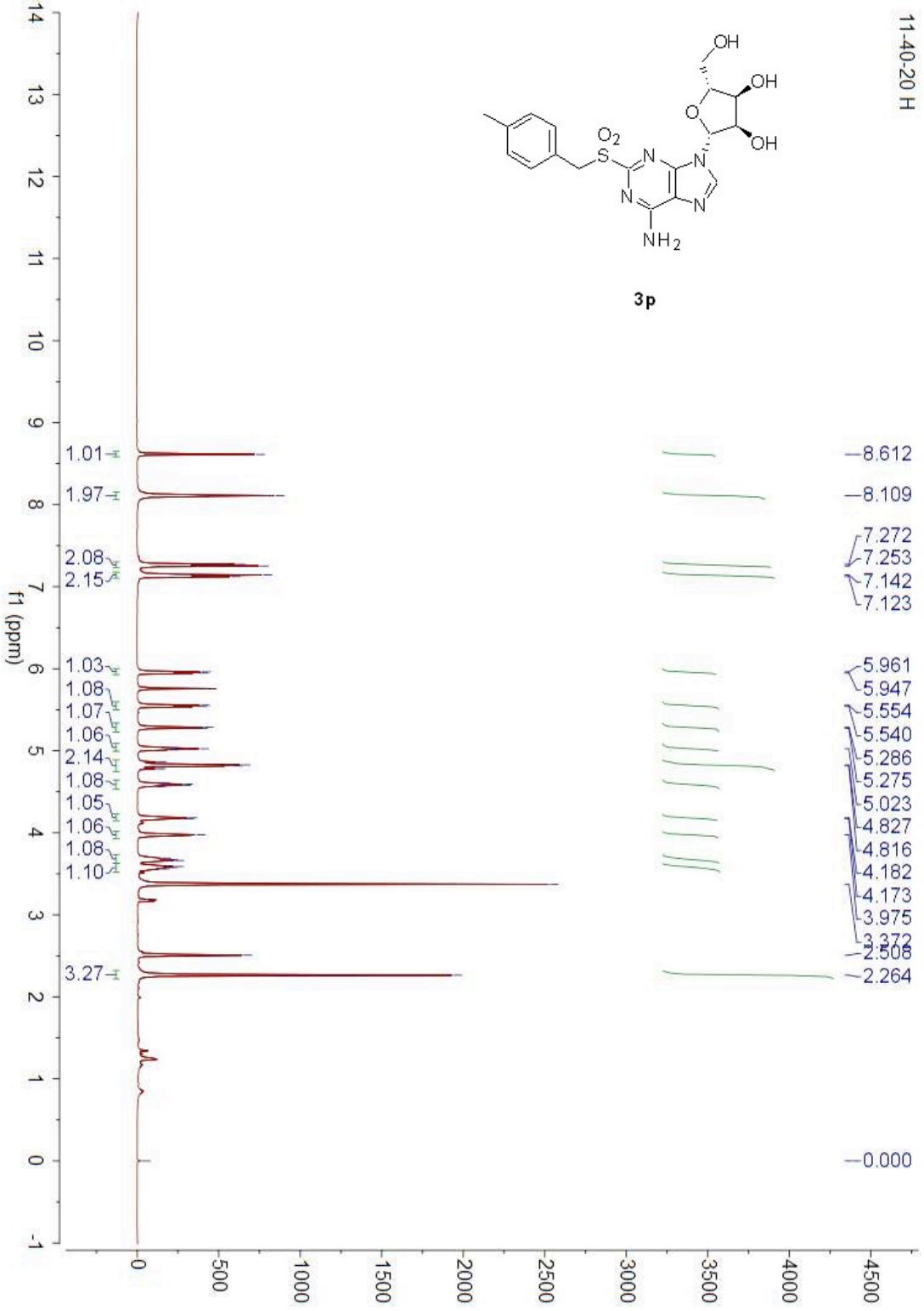

11-40-18 C
O2
S
N
3m
149.49
149.21
141.71
139.17
130.78
130.50
130.43
129.43
129.10
124.06
123.94
123.05
77.36
77.04
76.73
62.40
21.14
f1 (ppm)

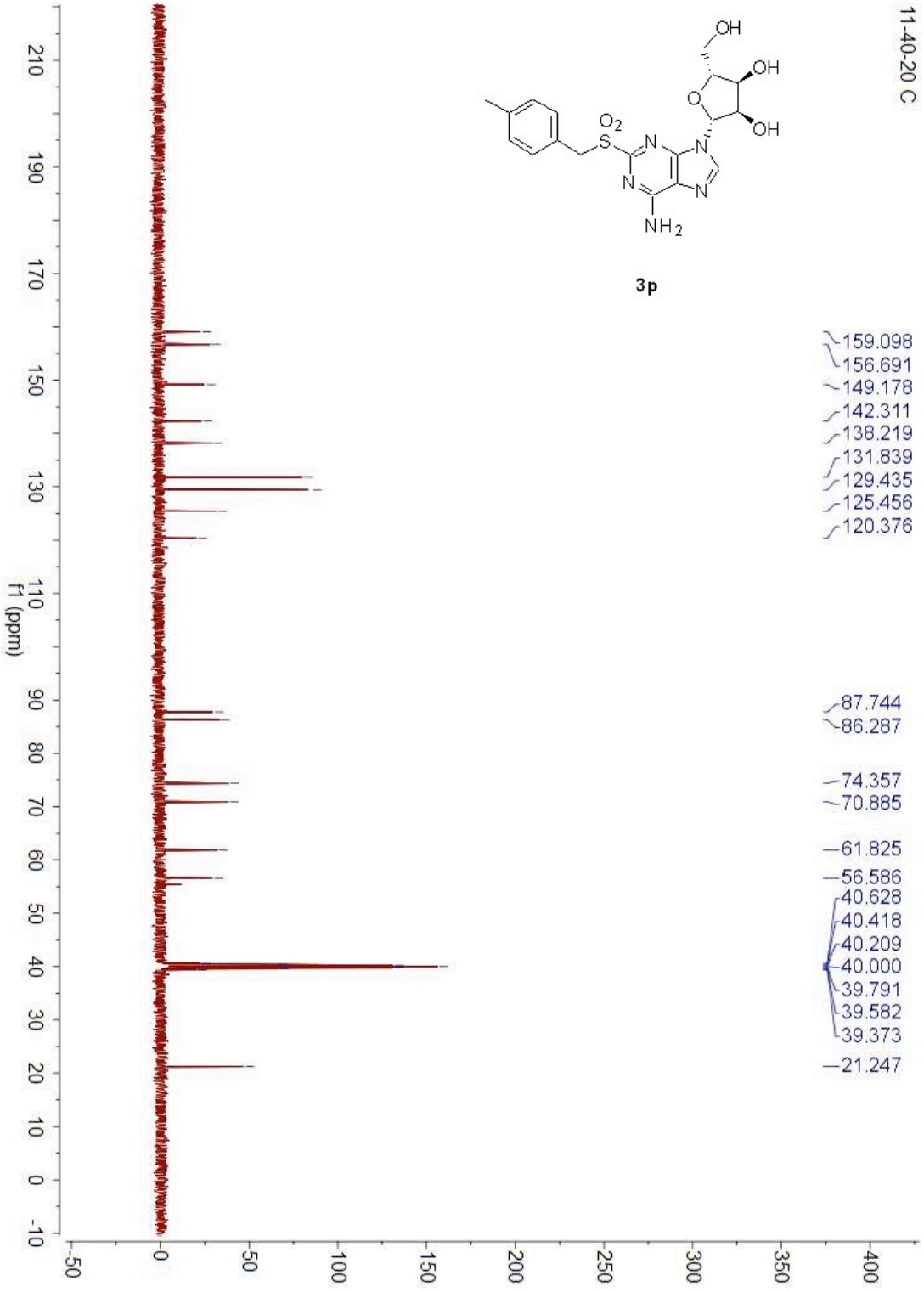

11-41-1 H
3n
O2
S
N
f1 (ppm)
1.00
3.18
1.10
1.11
2.12
2.12
2.12
3.25
9.080
9.076
9.070
9.065
8.209
8.204
8.193
8.171
8.149
7.852
7.847
7.830
7.265
7.047
7.027
6.976
6.955
4.370
2.303
0.000

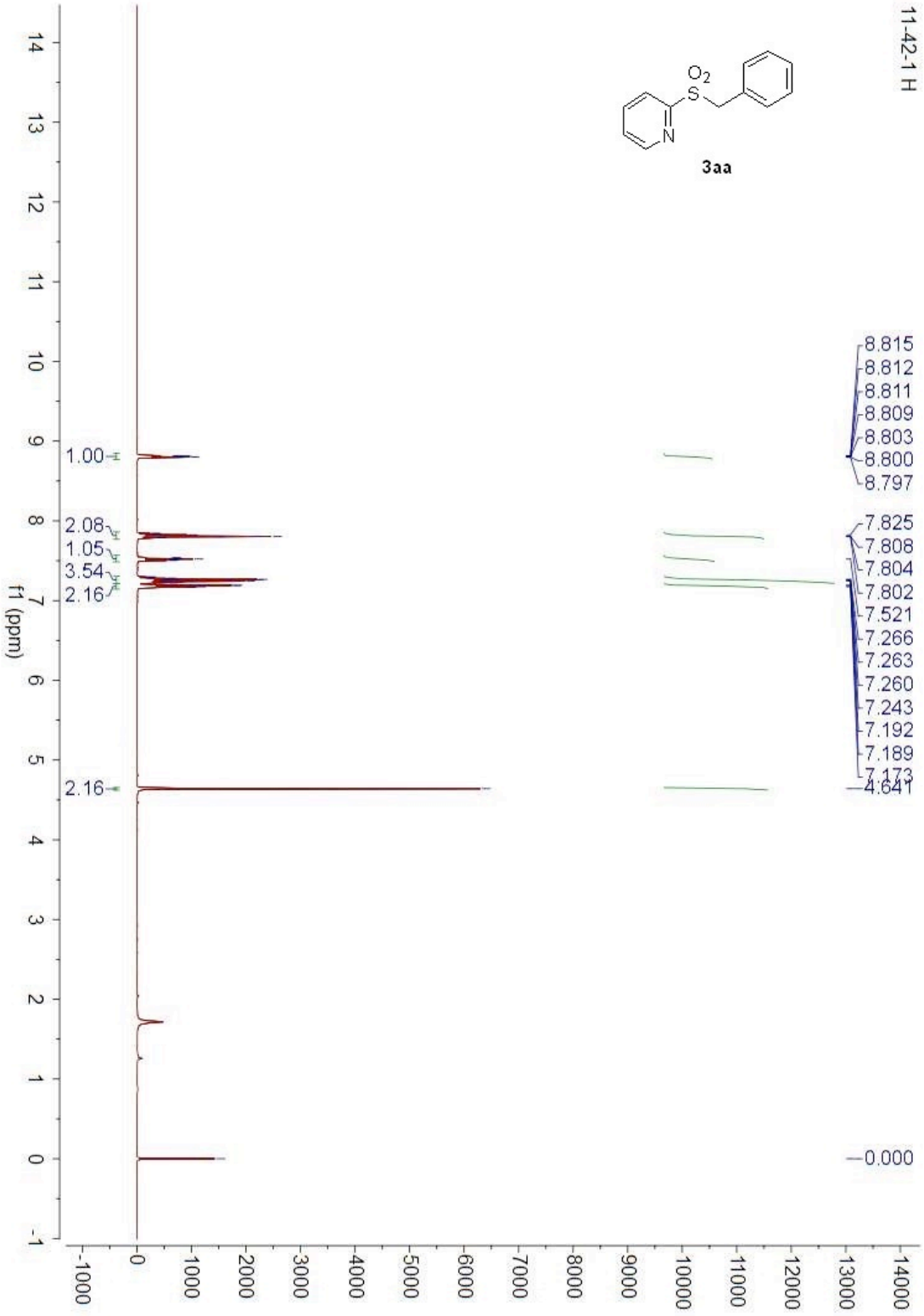

11-41-1 C
3n
153.49
149.75
138.94
137.33
135.85
130.78
130.71
130.65
129.40
127.11
124.75
122.61
77.35
77.03
76.71
62.67
21.17
f1 (ppm)

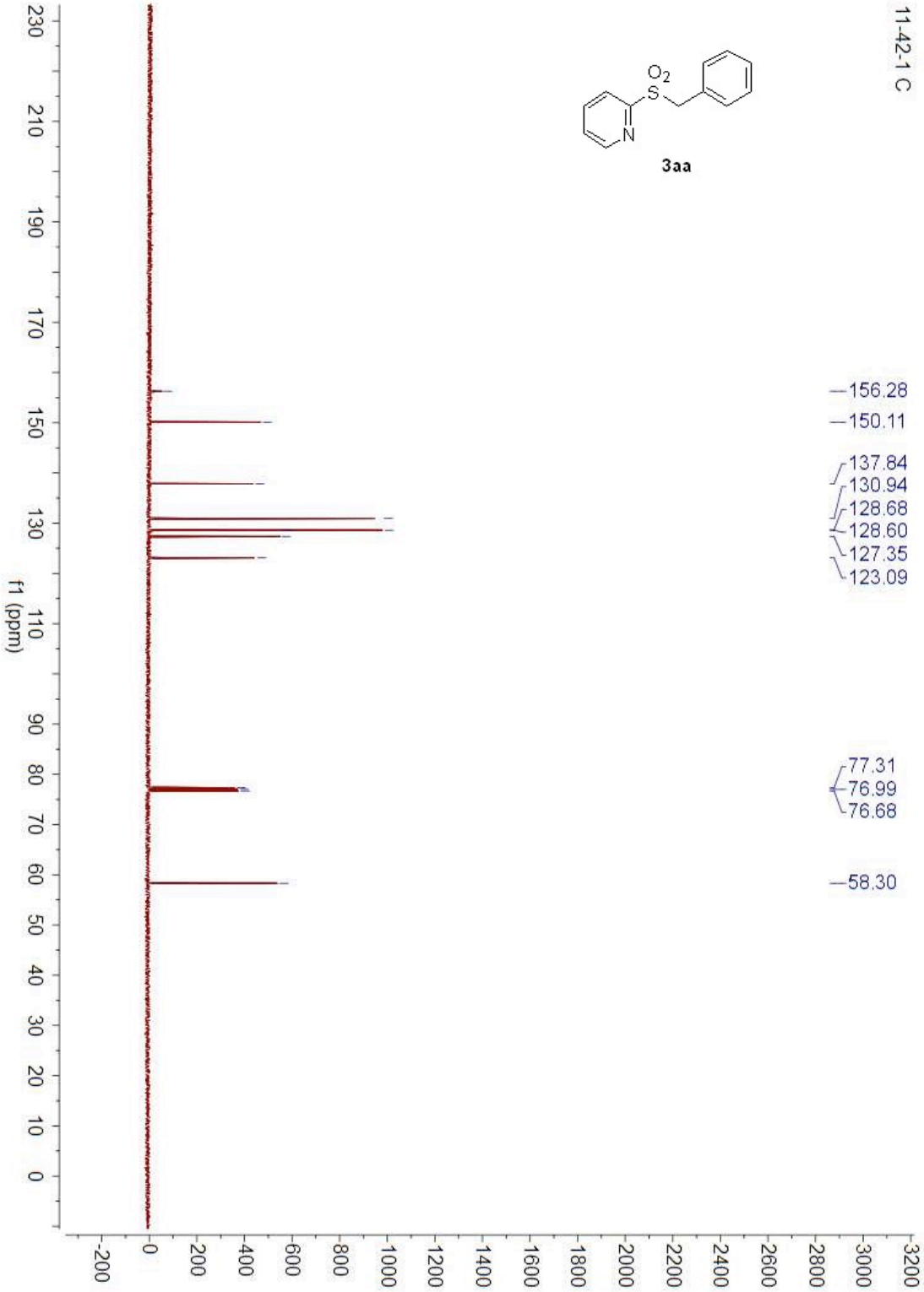

11-40-30 H
3o
8.290
8.268
7.812
7.790
7.263
7.098
7.079
6.974
6.954
4.341
2.336
0.000
2.00
2.01
2.09
2.11
2.10
3.28
f1 (ppm)

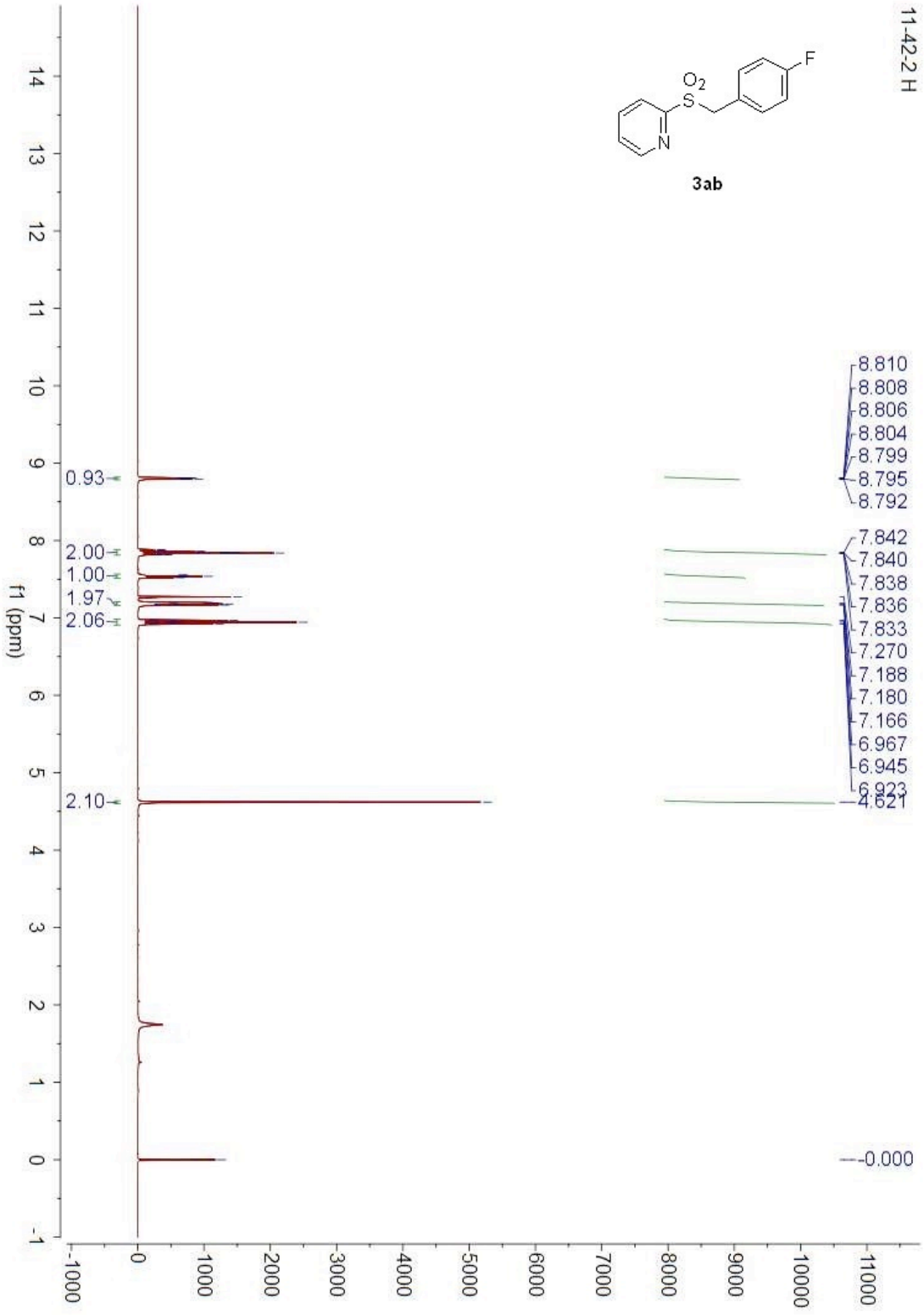

11-40-30 C
O2
S
O2N
3o
143.435
139.361
130.587
130.176
129.599
123.984
123.921
77.309
76.992
76.674
62.526
21.211
f1 (ppm)

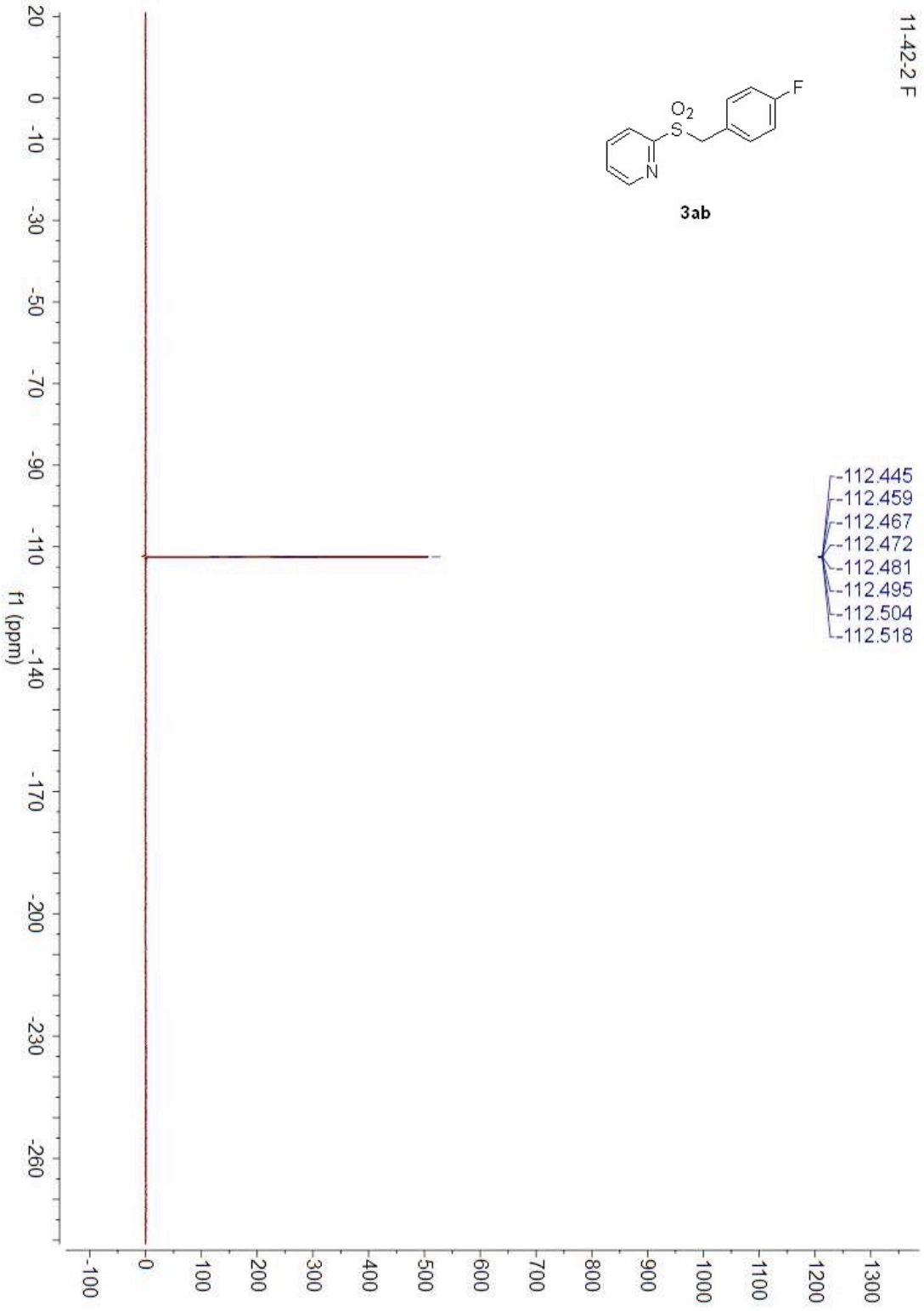

11-40-20 H
OH
OH
OH
O
O2
S
N
N
N
N
NH2
3p
f1 (ppm)
1.01
1.97
2.08
2.15
1.03
1.08
1.07
1.06
2.14
1.08
1.05
1.06
1.08
1.10
3.27
8.612
8.109
7.272
7.253
7.142
7.123
5.961
5.947
5.554
5.540
5.286
5.275
5.023
4.827
4.816
4.182
4.173
3.975
3.372
2.508
2.264
0.000

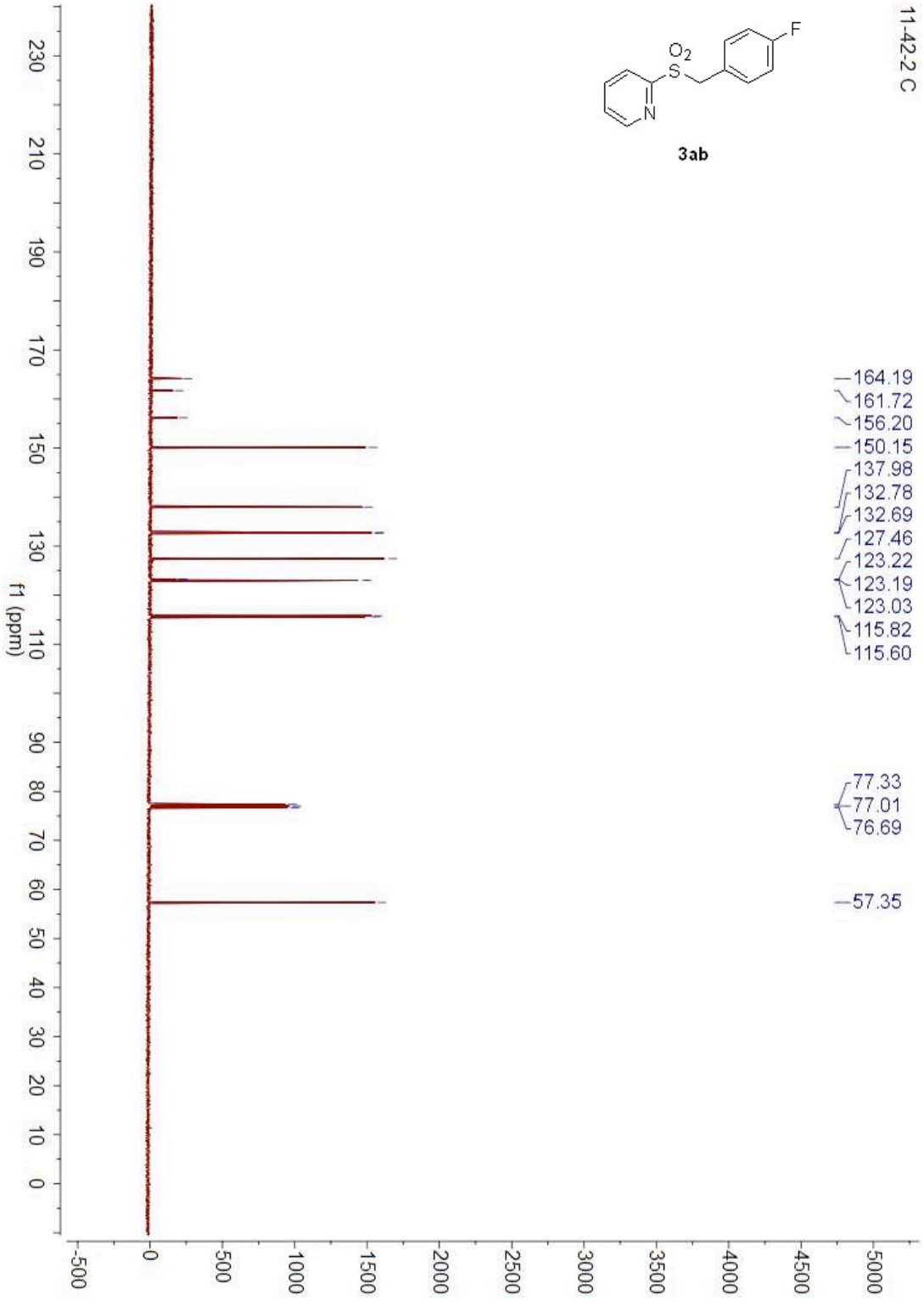

11-40-20 C
OH
OH
OH
O
O2
S
N
N
N
N
NH2
3p
159.098
156.691
149.178
142.311
138.219
131.839
129.435
125.456
120.376
87.744
86.287
74.357
70.885
61.825
56.586
40.628
40.418
40.209
40.000
39.791
39.582
39.373
21.247
f1 (ppm)

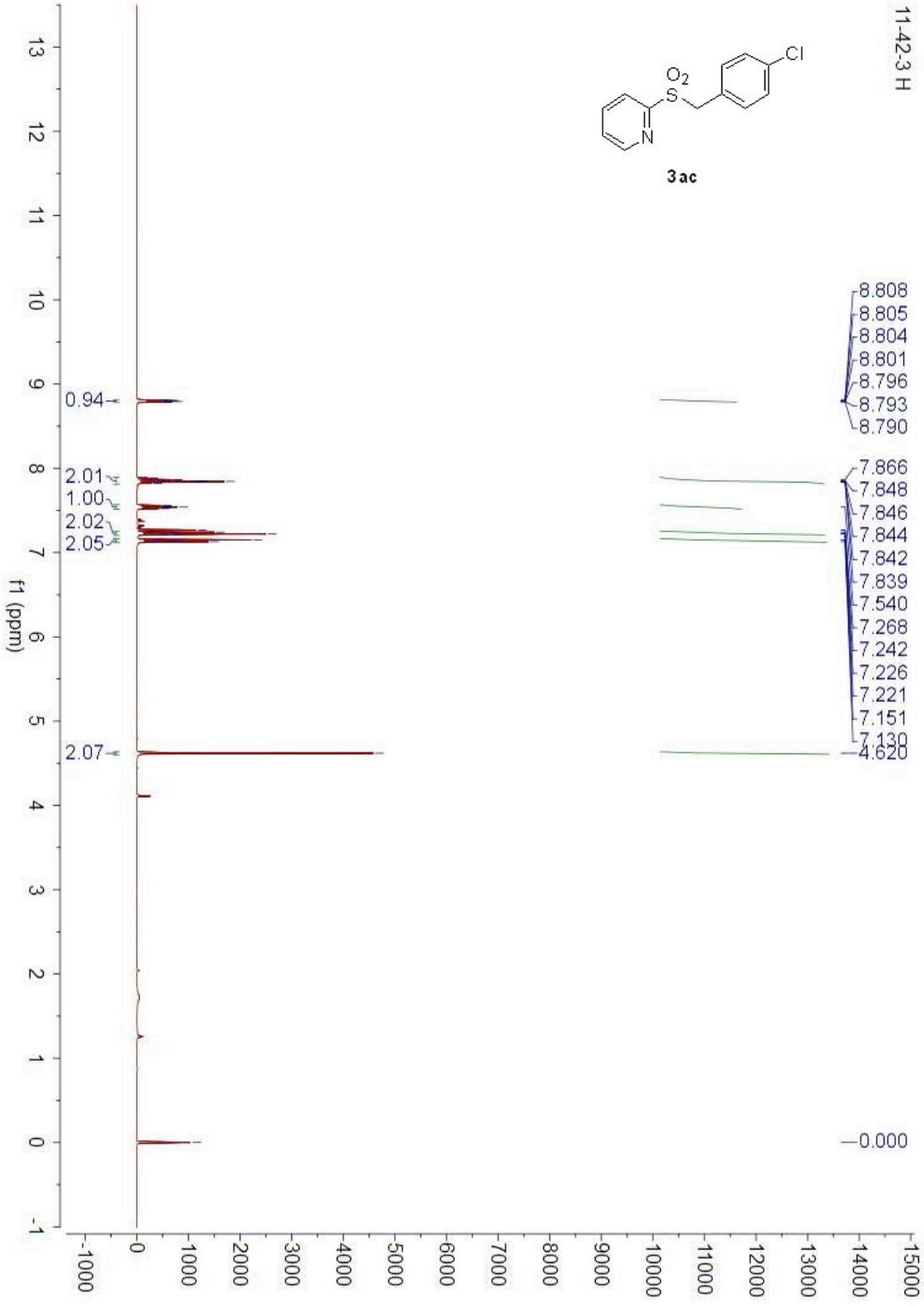

11-42-1 H
3aa
8.815
8.812
8.811
8.809
8.803
8.800
8.797
7.825
7.808
7.804
7.802
7.521
7.266
7.263
7.260
7.243
7.192
7.189
7.173
4.641
0.000
1.00
2.08
1.05
3.54
2.16
2.16
f1 (ppm)

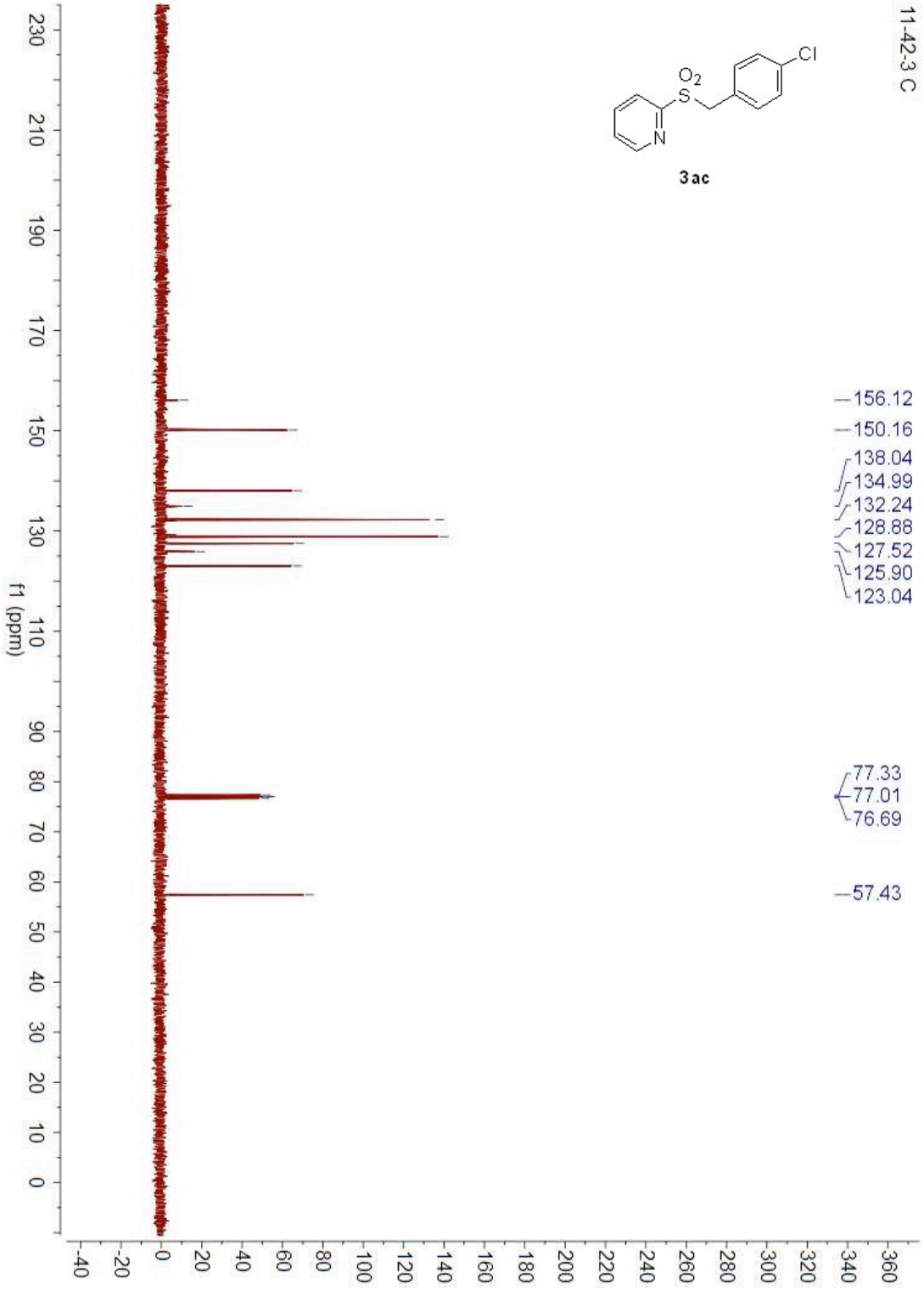

11-42-1 C
O2
S
N
3aa
156.28
150.11
137.84
130.94
128.68
128.60
127.35
123.09
77.31
76.99
76.68
58.30
f1 (ppm)

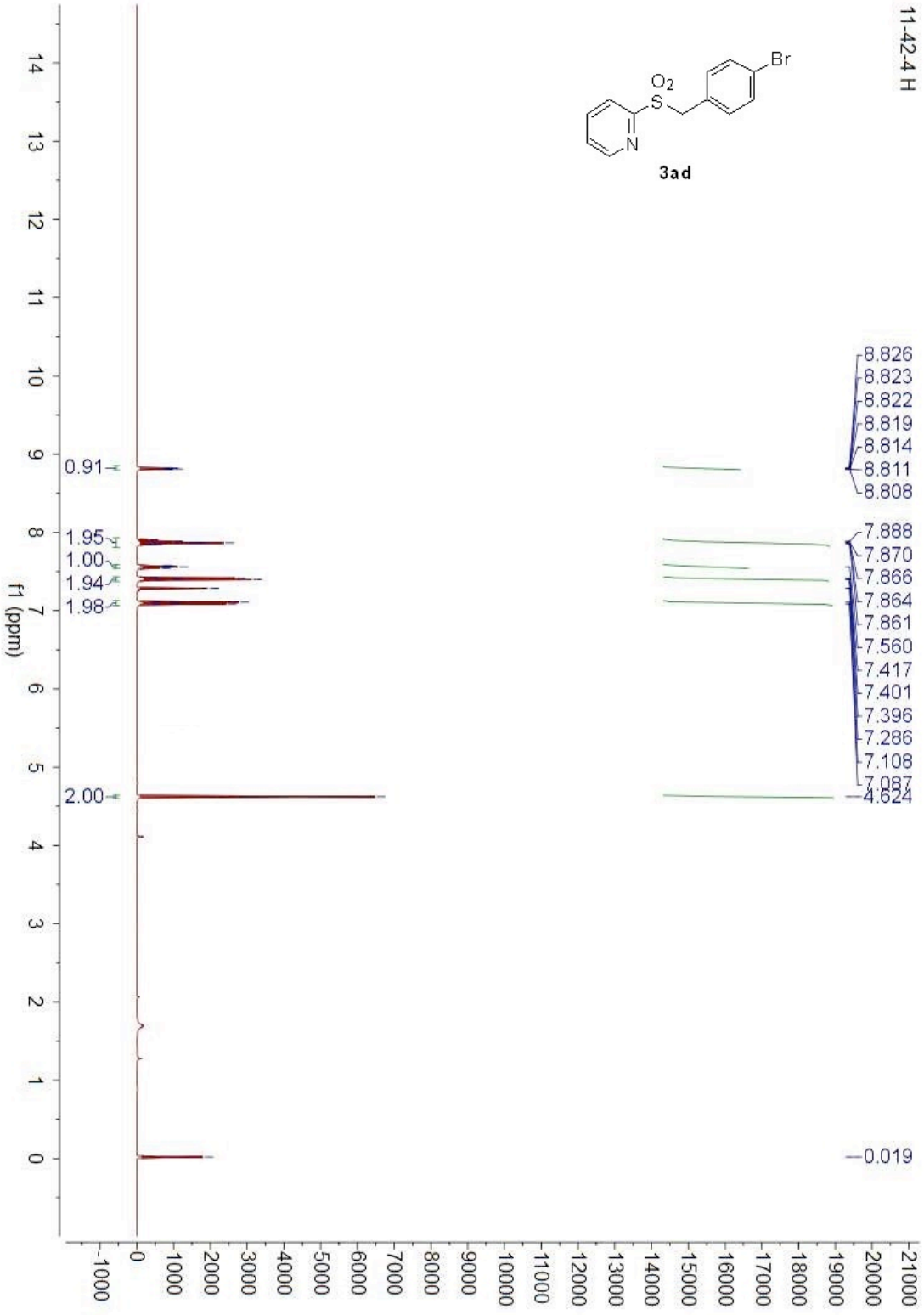

11-42-2 H
3ab
f1 (ppm)
0.93
2.00
1.00
1.97
2.06
2.10
8.810
8.808
8.806
8.804
8.799
8.795
8.792
7.842
7.840
7.838
7.836
7.833
7.270
7.188
7.180
7.166
6.967
6.945
6.923
4.621
0.000

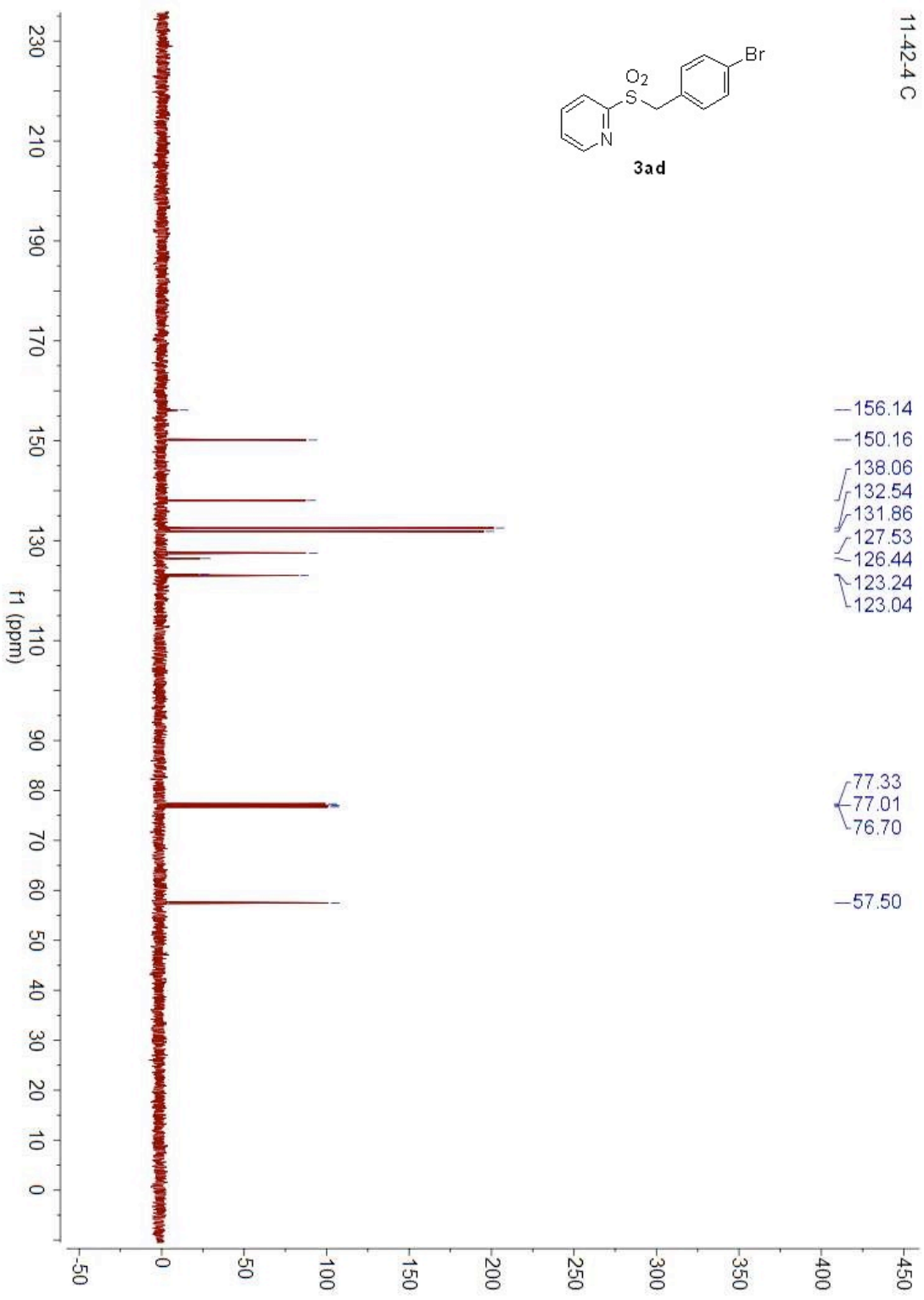

11-42-2 F
3ab
-112.445
-112.459
-112.467
-112.472
-112.481
-112.495
-112.504
-112.518
f1 (ppm)

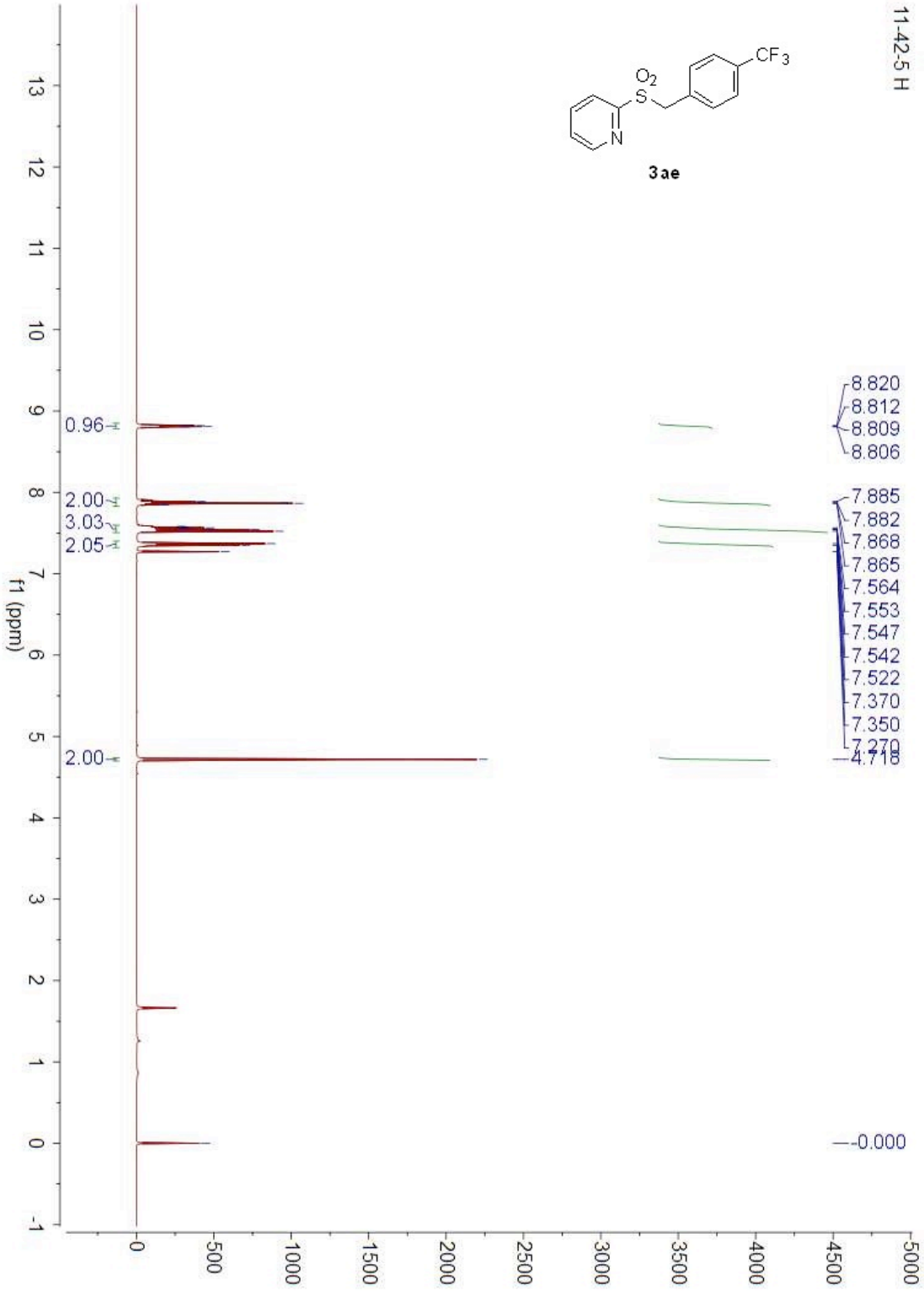

11-42-2 C
3ab
F
O2
S
N
164.19
161.72
156.20
150.15
137.98
132.78
132.69
127.46
123.22
123.19
123.03
115.82
115.60
77.33
77.01
76.69
57.35
f1 (ppm)

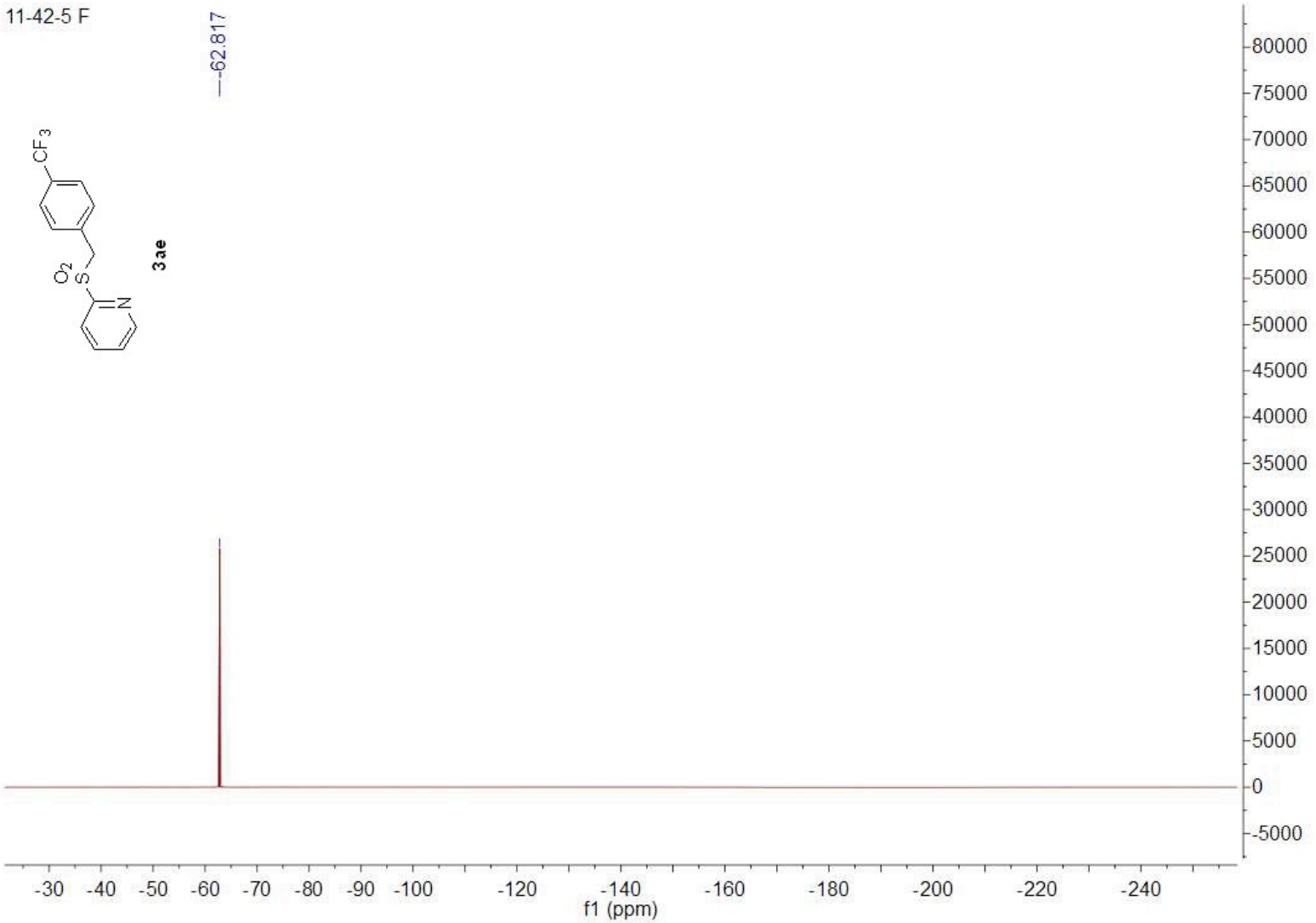

11-42-3 H
3ac
Cl
O2
S
N
8.808
8.805
8.804
8.801
8.796
8.793
8.790
7.866
7.848
7.846
7.844
7.842
7.839
7.540
7.268
7.242
7.226
7.221
7.151
7.130
4.620
0.000
0.94
2.01
1.00
2.02
2.05
2.07
f1 (ppm)

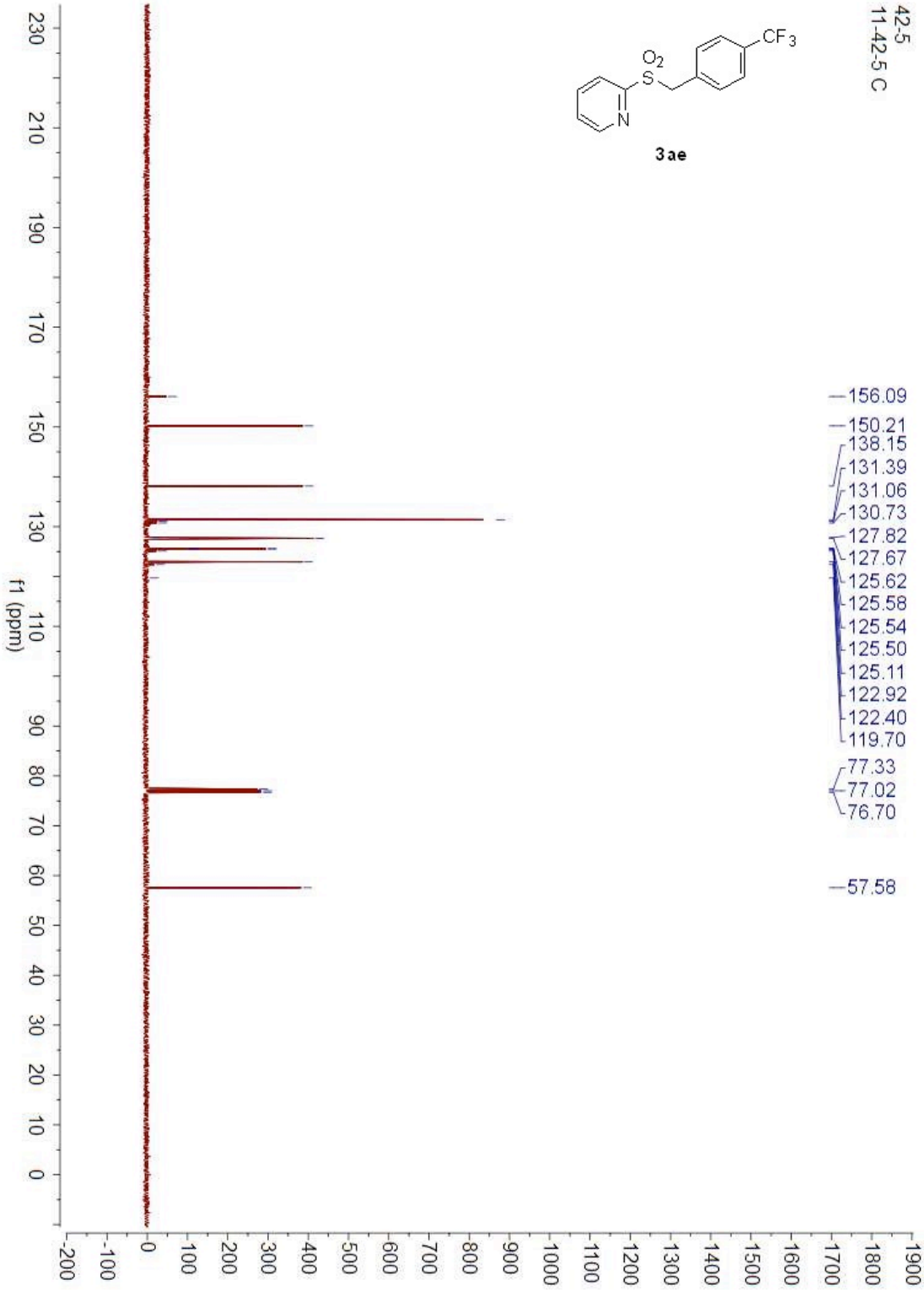

11-42-3 C
Cl
O2
S
N
3ac
156.12
150.16
138.04
134.99
132.24
128.88
127.52
125.90
123.04
77.33
77.01
76.69
57.43
f1 (ppm)

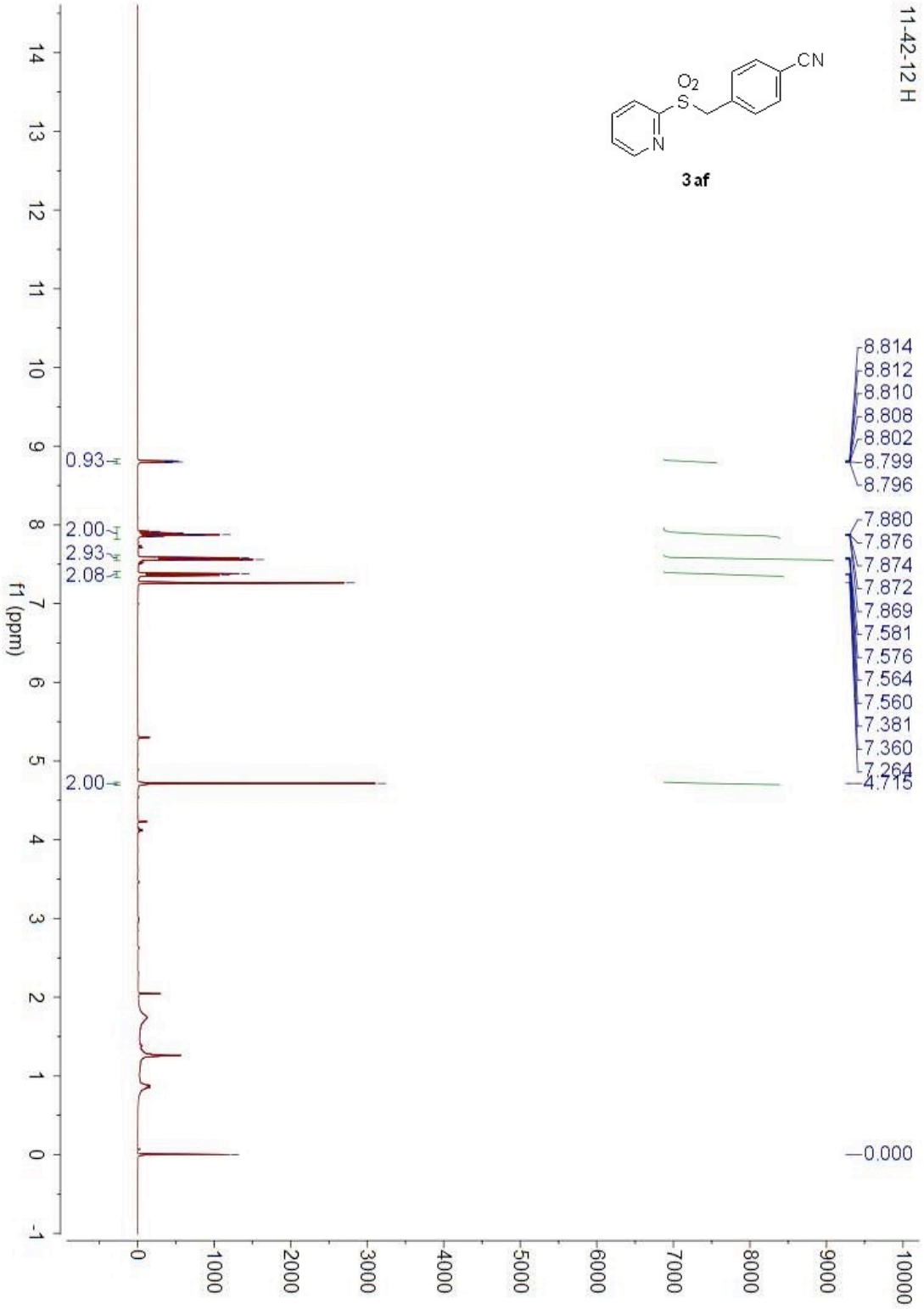

11-42-4 H
Br
O2
S
N
3ad
8.826
8.823
8.822
8.819
8.814
8.811
8.808
7.888
7.870
7.866
7.864
7.861
7.560
7.417
7.401
7.396
7.286
7.108
7.087
4.624
0.019
0.91
1.95
1.00
1.94
1.98
2.00
f1 (ppm)

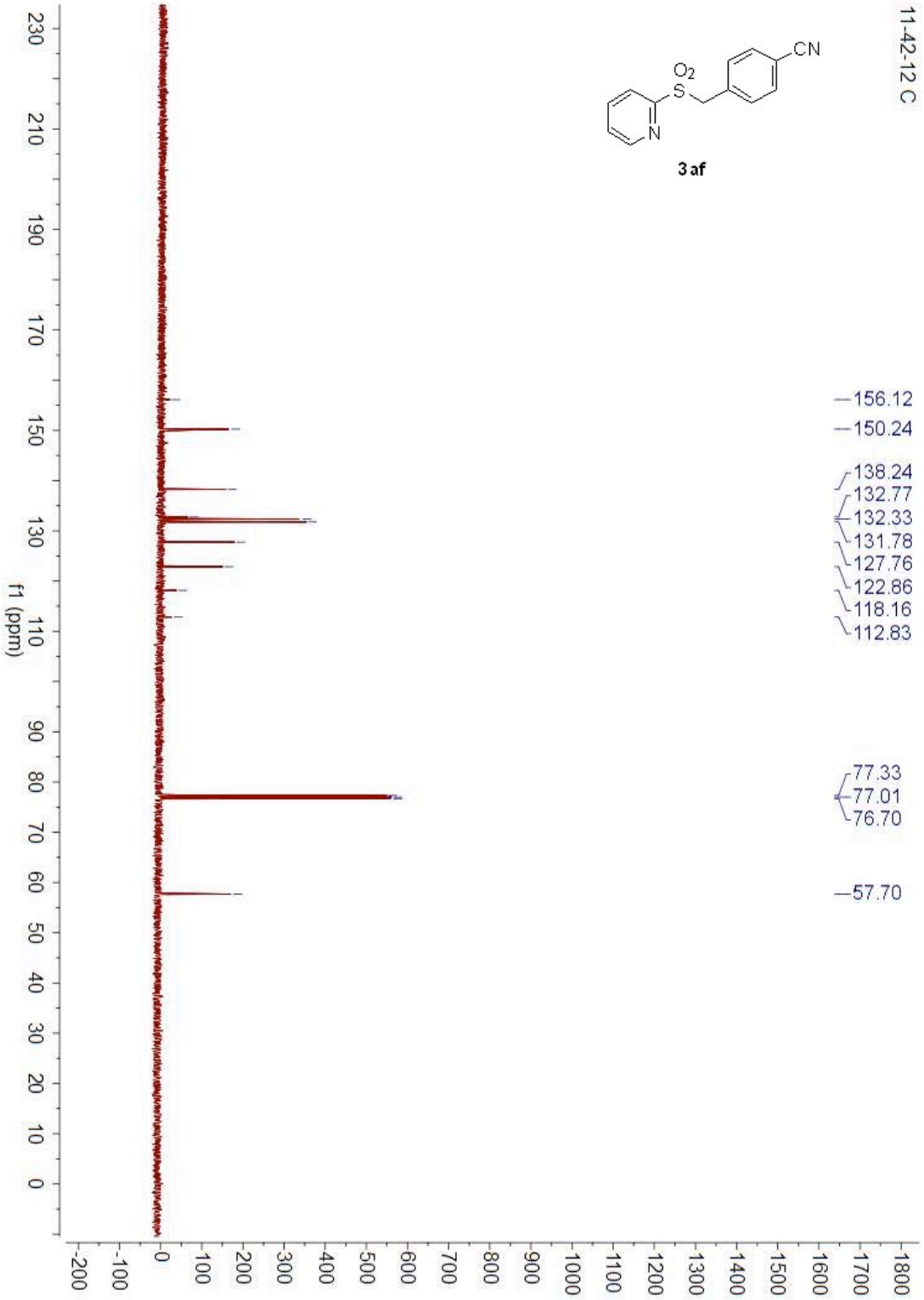

11-42-4 C
Br
O2
S
N
3ad
156.14
150.16
138.06
132.54
131.86
127.53
126.44
123.24
123.04
77.33
77.01
76.70
57.50
f1 (ppm)

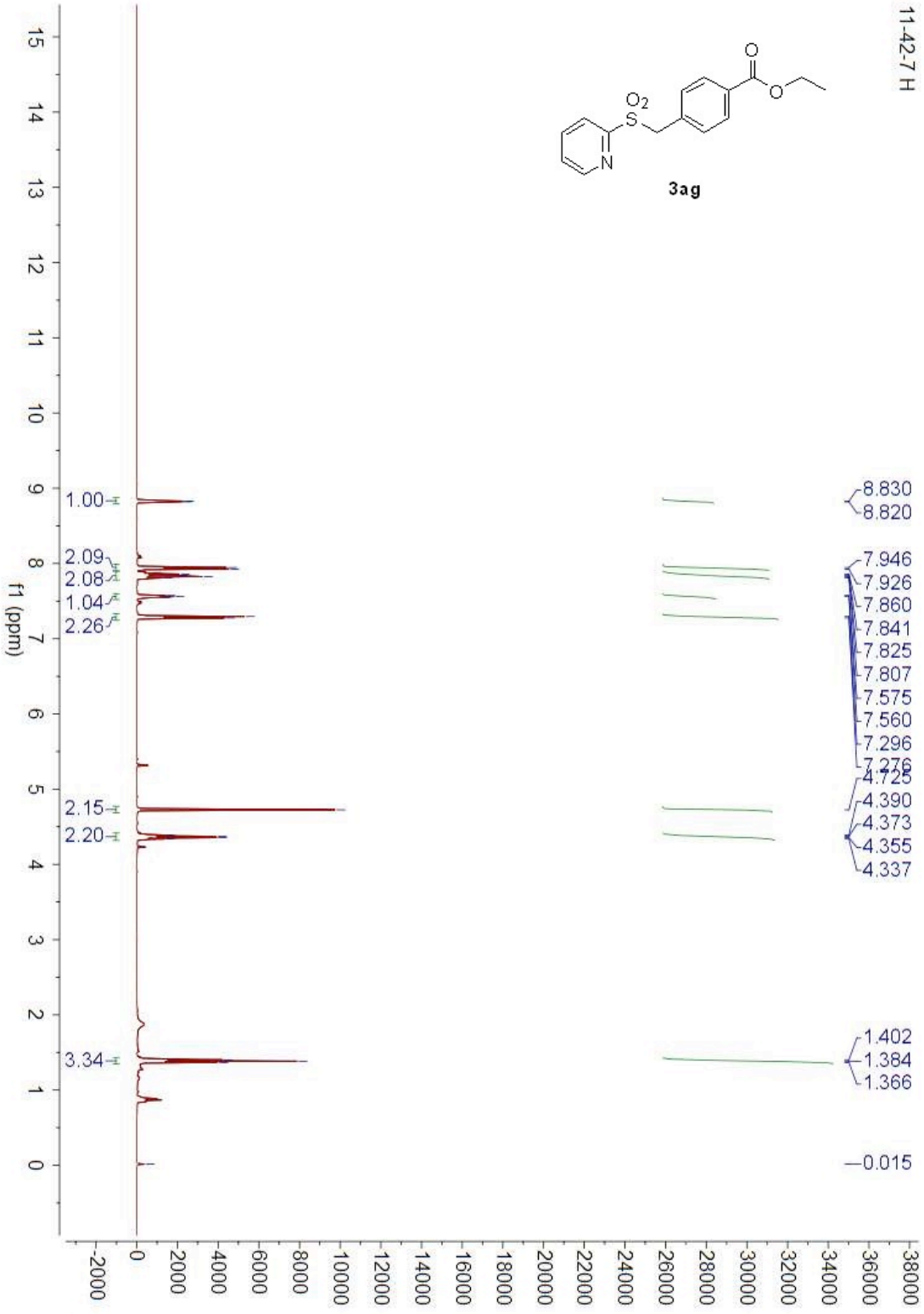

11-42-5 H
3ae
8.820
8.812
8.809
8.806
7.885
7.882
7.868
7.865
7.564
7.553
7.547
7.542
7.522
7.370
7.350
7.270
4.718
0.000
0.96
2.00
3.03
2.05
2.00
f1 (ppm)

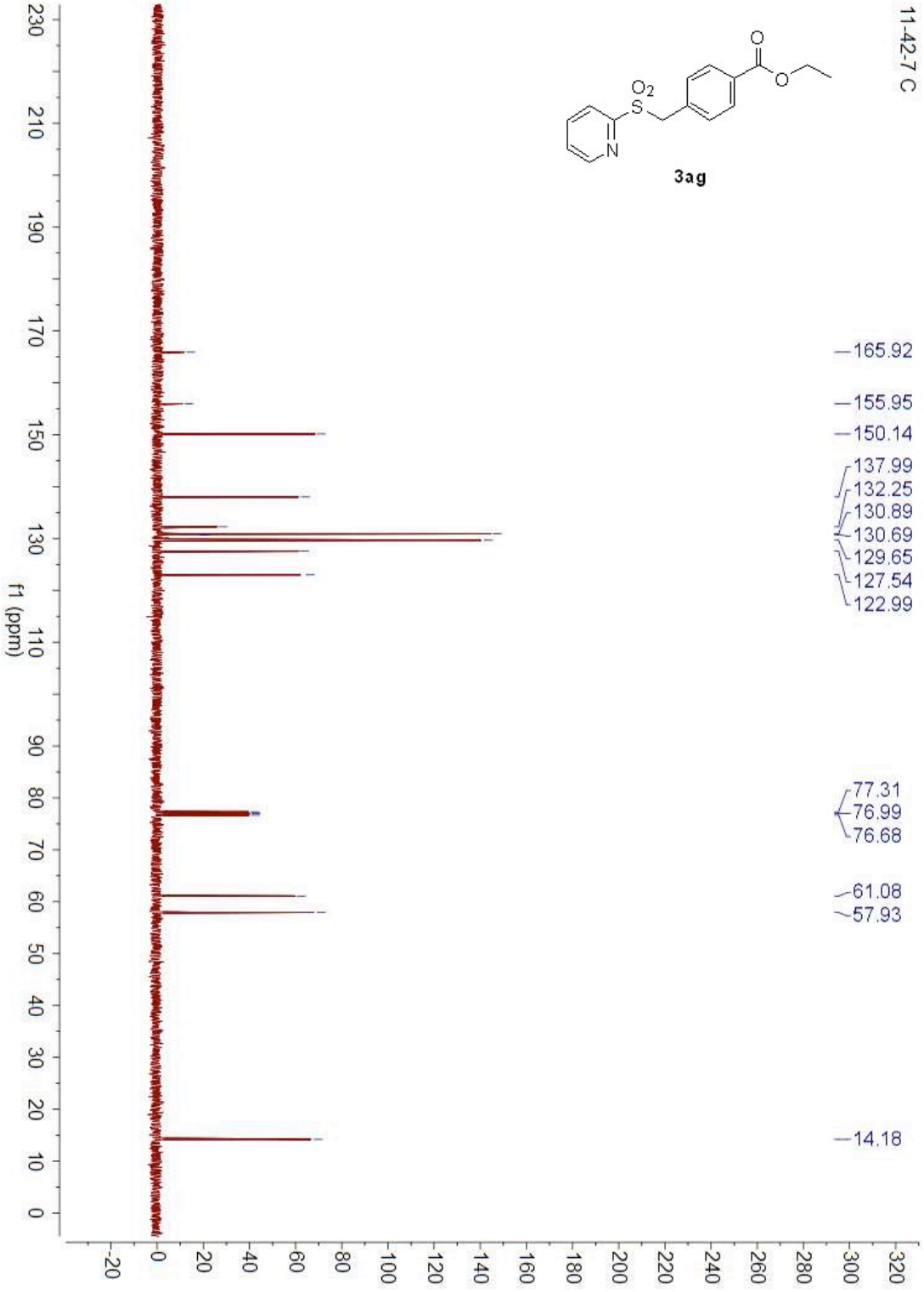

11-42-5 F
-62.817
3ae
CF3
O2
S
N
80000
75000
70000
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
-30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200 -220 -240
f1 (ppm)

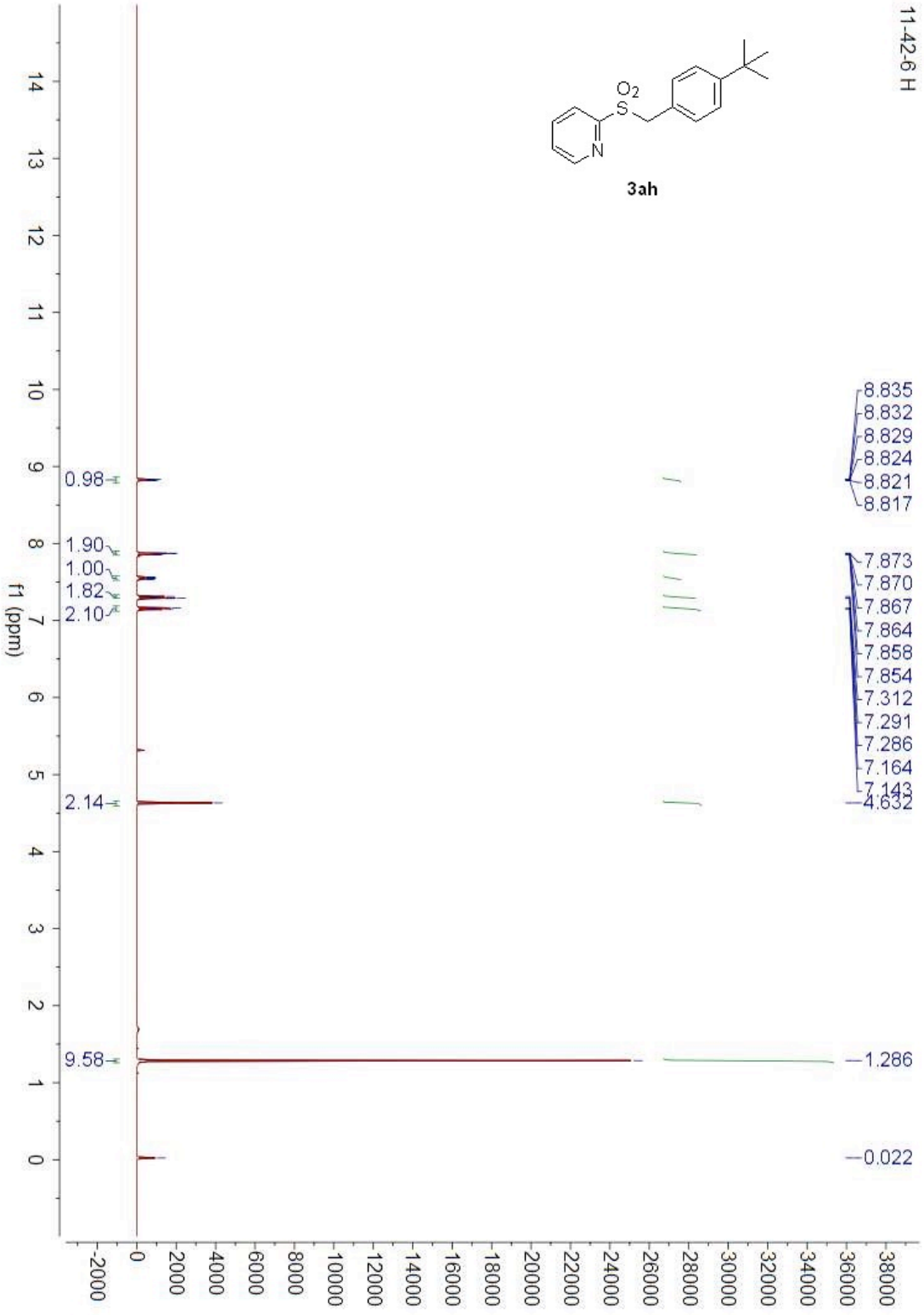

42-5
11-42-5 C
3ae
156.09
150.21
138.15
131.39
131.06
130.73
127.82
127.67
125.62
125.58
125.54
125.50
125.11
122.92
122.40
119.70
77.33
77.02
76.70
57.58
f1 (ppm)

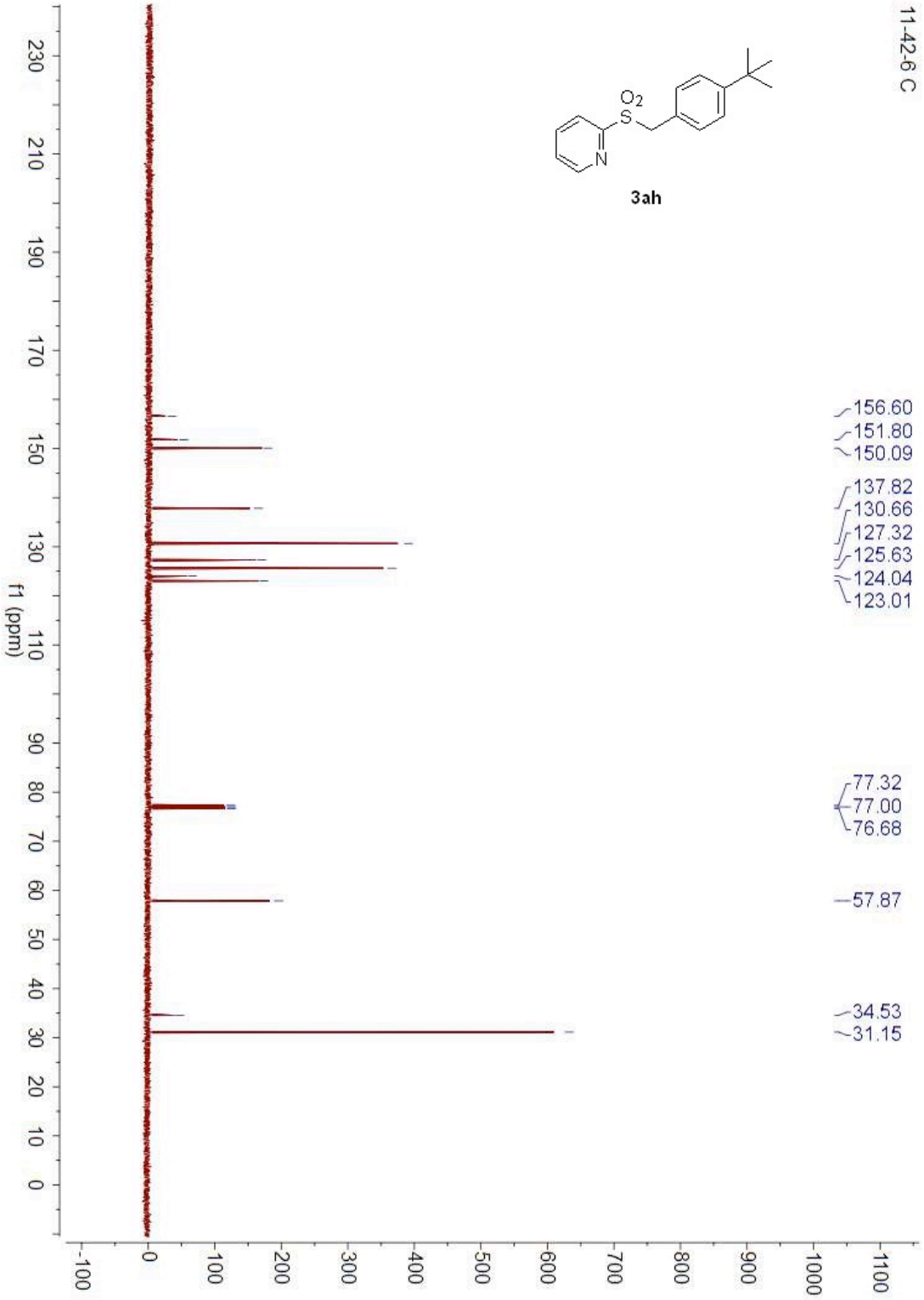

11-42-12 H
3af
8.814
8.812
8.810
8.808
8.802
8.799
8.796
7.880
7.876
7.874
7.872
7.869
7.581
7.576
7.564
7.560
7.381
7.360
7.264
4.715
0.000
0.93
2.00
2.93
2.08
2.00
f1 (ppm)

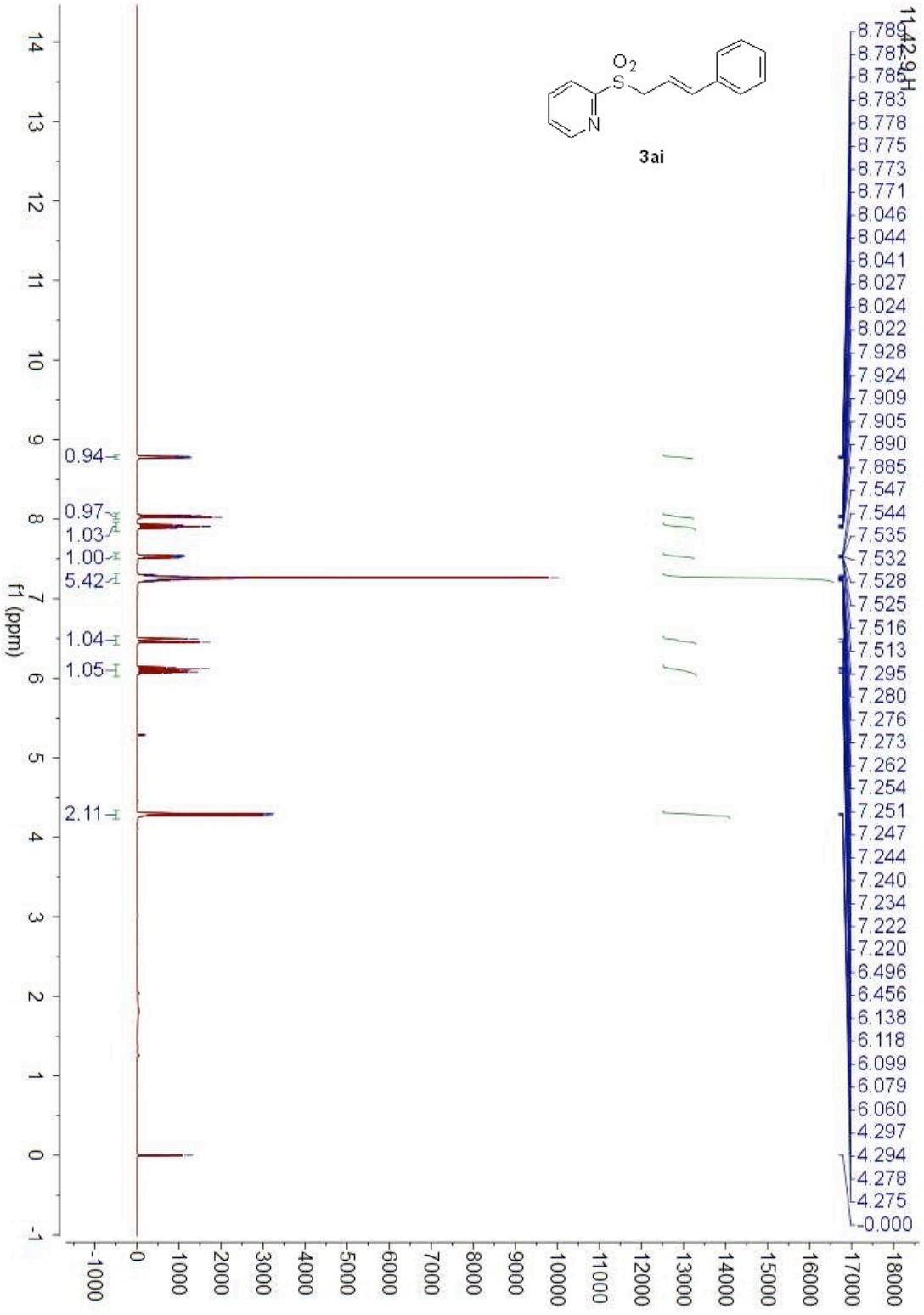

11-42-12 C
CN
O2
S
N
3af
156.12
150.24
138.24
132.77
132.33
131.78
127.76
122.86
118.16
112.83
77.33
77.01
76.70
57.70
f1 (ppm)

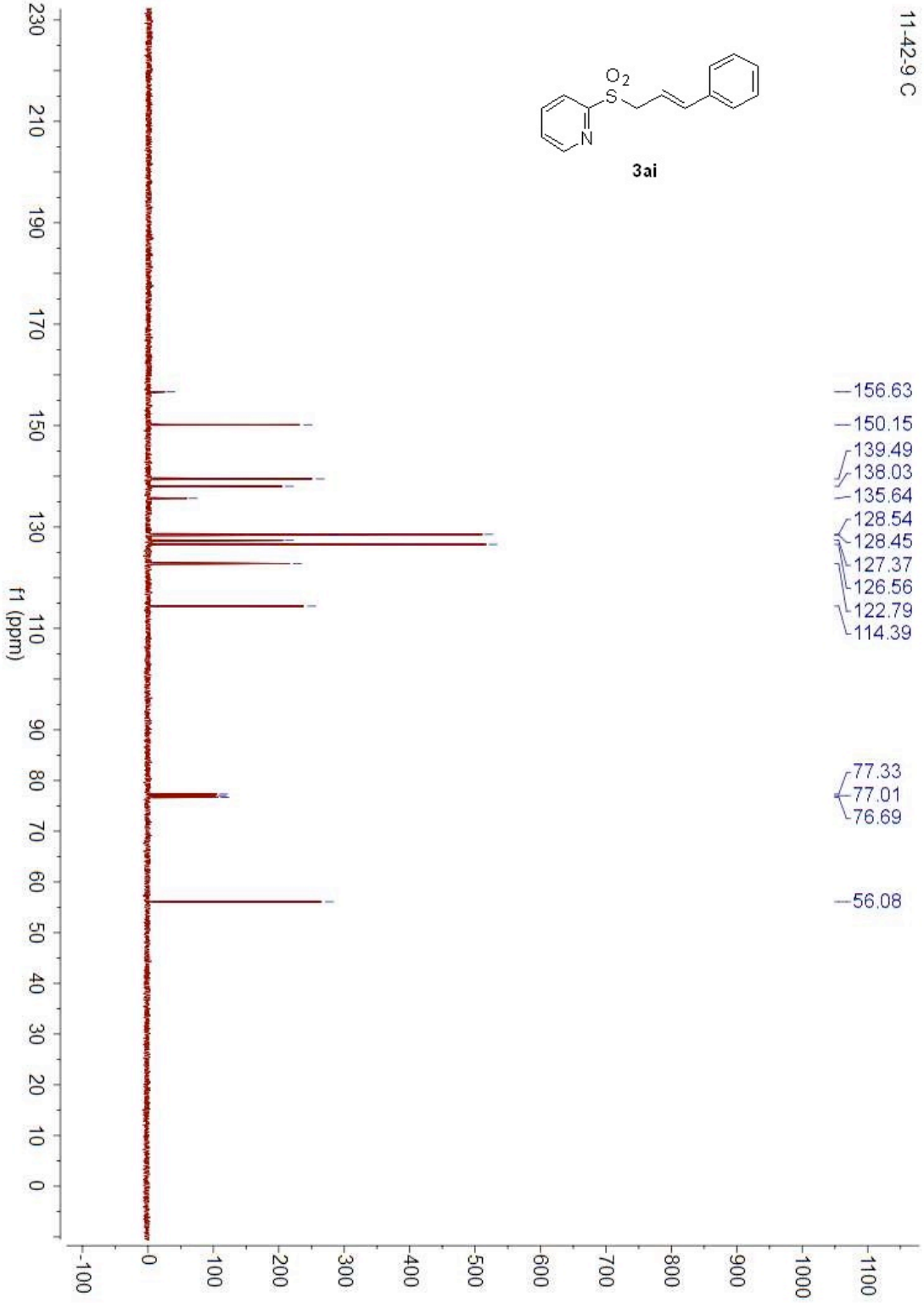

11-42-7 H
3ag
f1 (ppm)
1.00
2.09
2.08
1.04
2.26
2.15
2.20
3.34
8.830
8.820
7.946
7.926
7.860
7.841
7.825
7.807
7.575
7.560
7.296
7.276
4.725
4.390
4.373
4.355
4.337
1.402
1.384
1.366
0.015

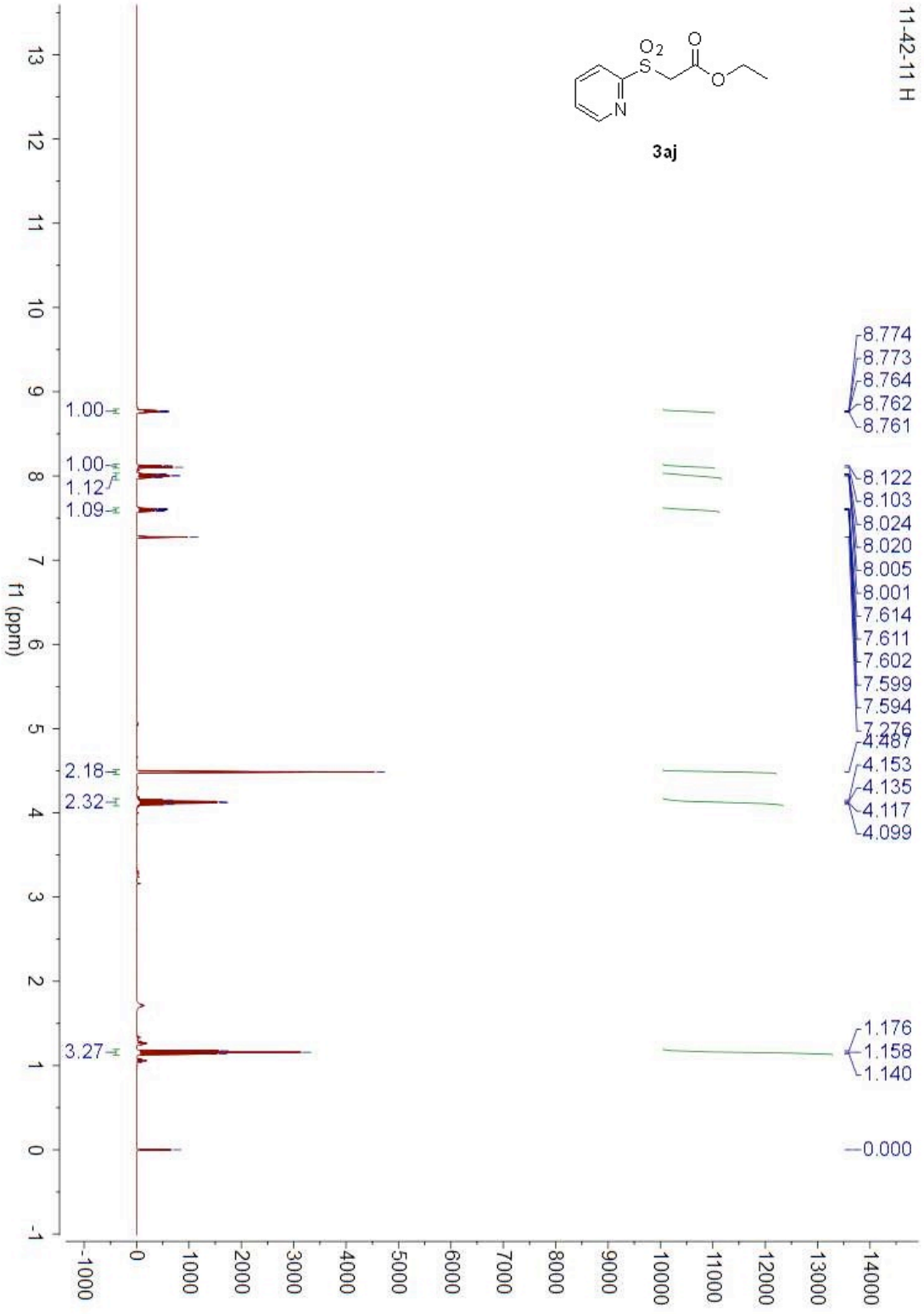

11-42-7 C
3ag
165.92
155.95
150.14
137.99
132.25
130.89
130.69
129.65
127.54
122.99
77.31
76.99
76.68
61.08
57.93
14.18
f1 (ppm)

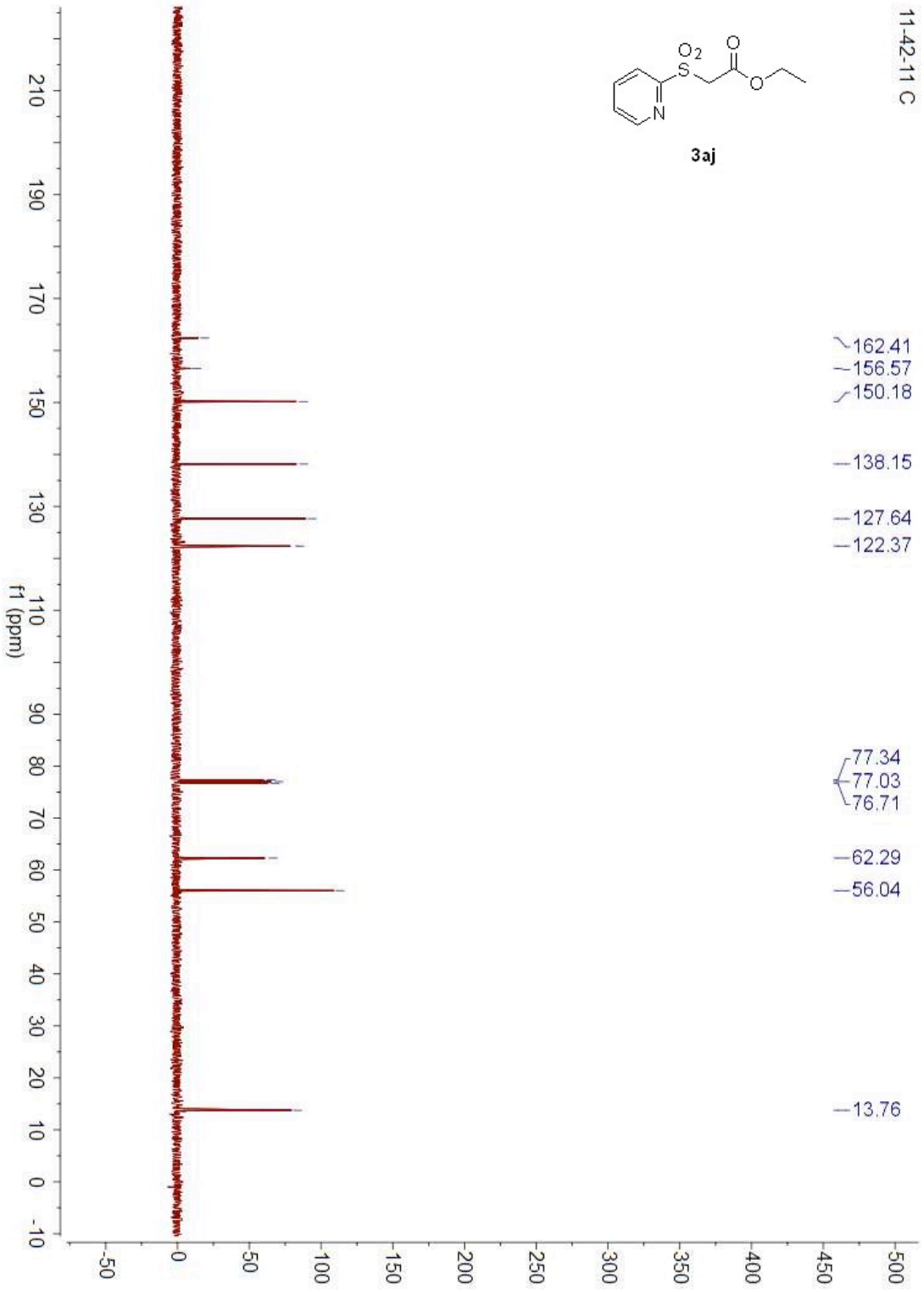

11-42-6 H
3ah
8.835
8.832
8.829
8.824
8.821
8.817
7.873
7.870
7.867
7.864
7.858
7.854
7.312
7.291
7.286
7.164
7.143
4.632
1.286
0.022
0.98
1.90
1.00
1.82
2.10
2.14
9.58
f1 (ppm)

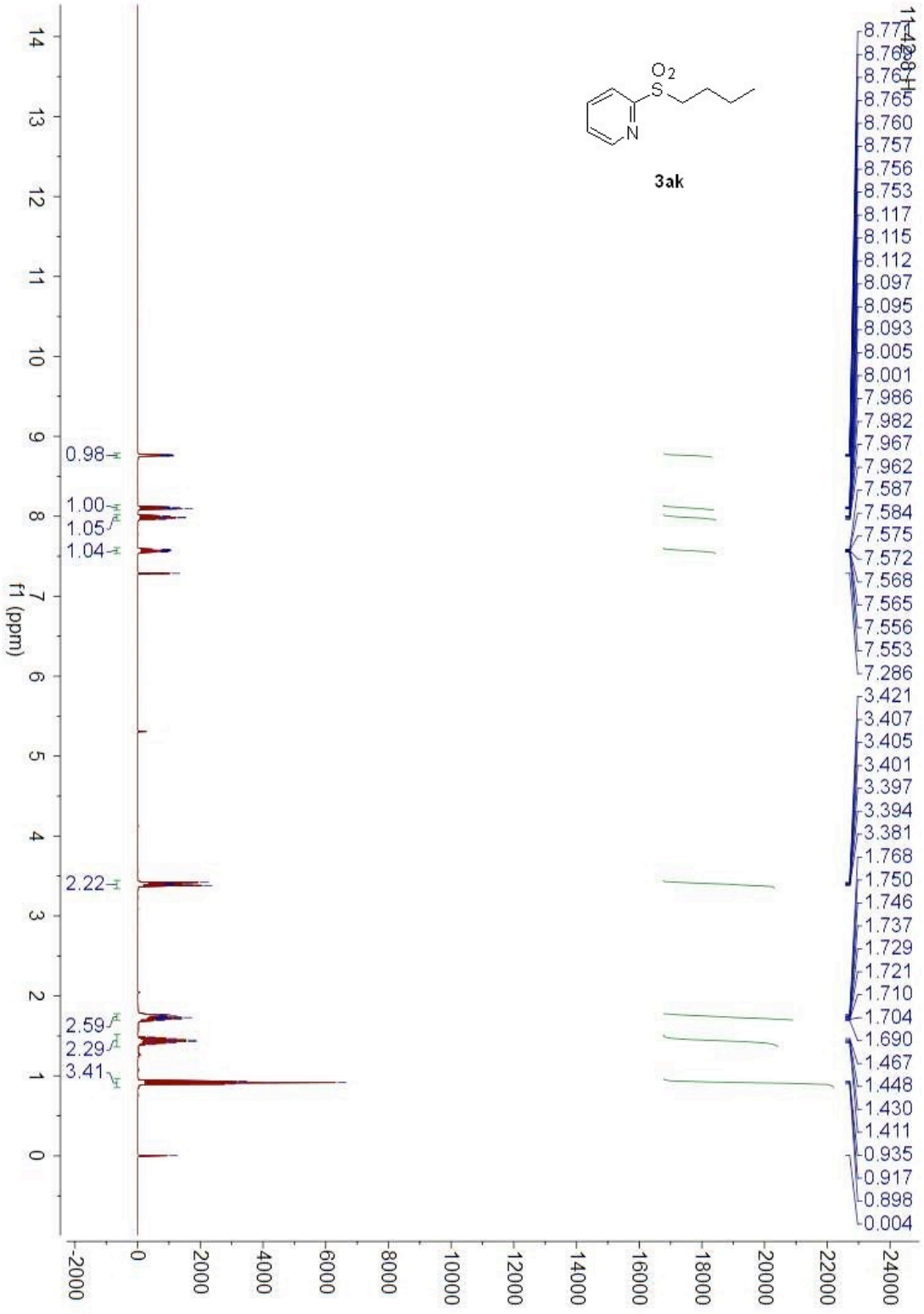

11-42-6 C
O2
S
N
3ah
156.60
151.80
150.09
137.82
130.66
127.32
125.63
124.04
123.01
77.32
77.00
76.68
57.87
34.53
31.15
f1 (ppm)

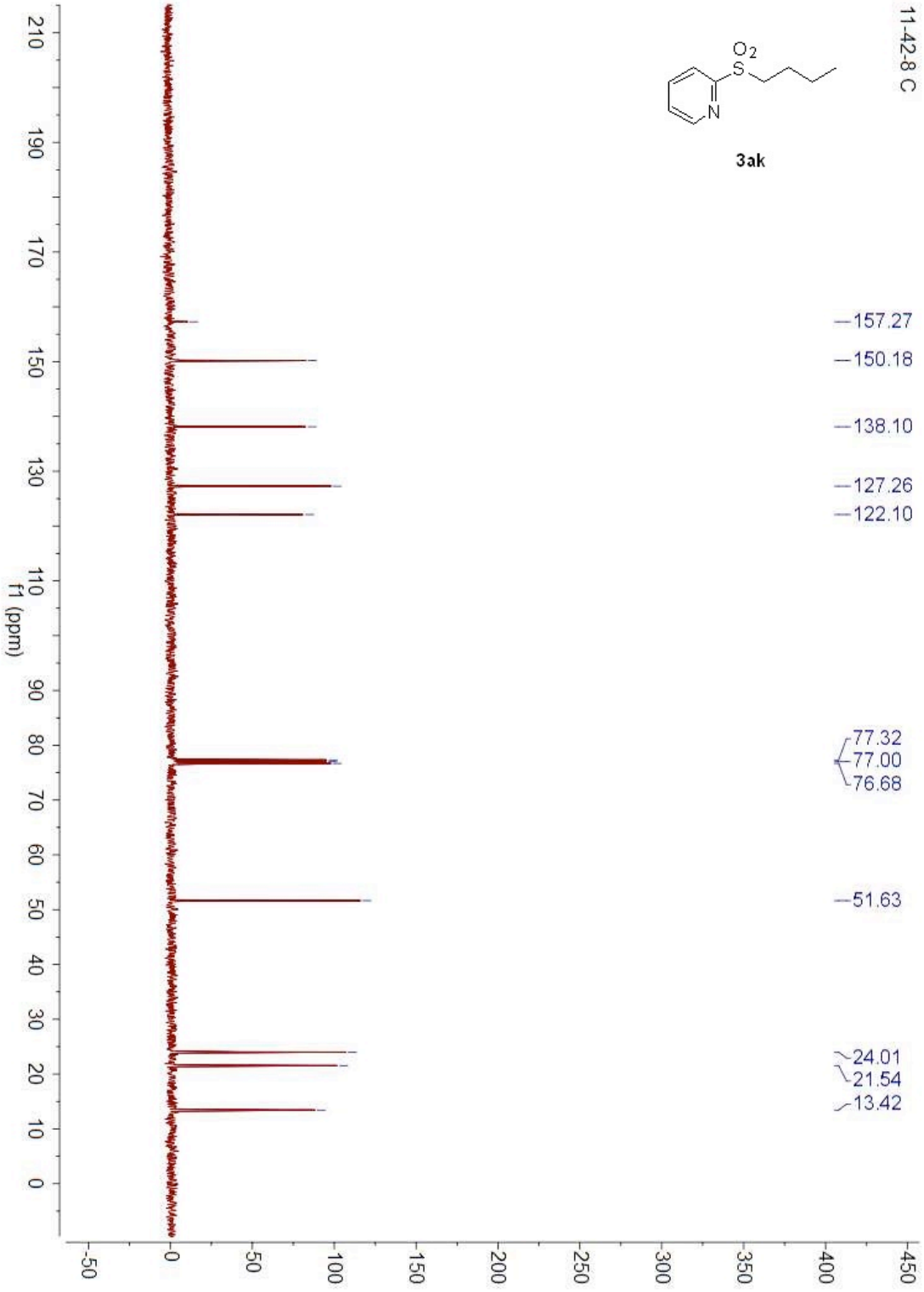

3ai
f1 (ppm)
0.94
0.97
1.03
1.00
5.42
1.04
1.05
2.11
11.42
8.786
8.781
8.785
8.783
8.778
8.775
8.773
8.771
8.046
8.044
8.041
8.027
8.024
8.022
7.928
7.924
7.909
7.905
7.890
7.885
7.547
7.544
7.535
7.532
7.528
7.525
7.516
7.513
7.295
7.280
7.276
7.273
7.262
7.254
7.251
7.247
7.244
7.240
7.234
7.222
7.220
6.496
6.456
6.138
6.118
6.099
6.079
6.060
4.297
4.294
4.278
4.275
-0.000

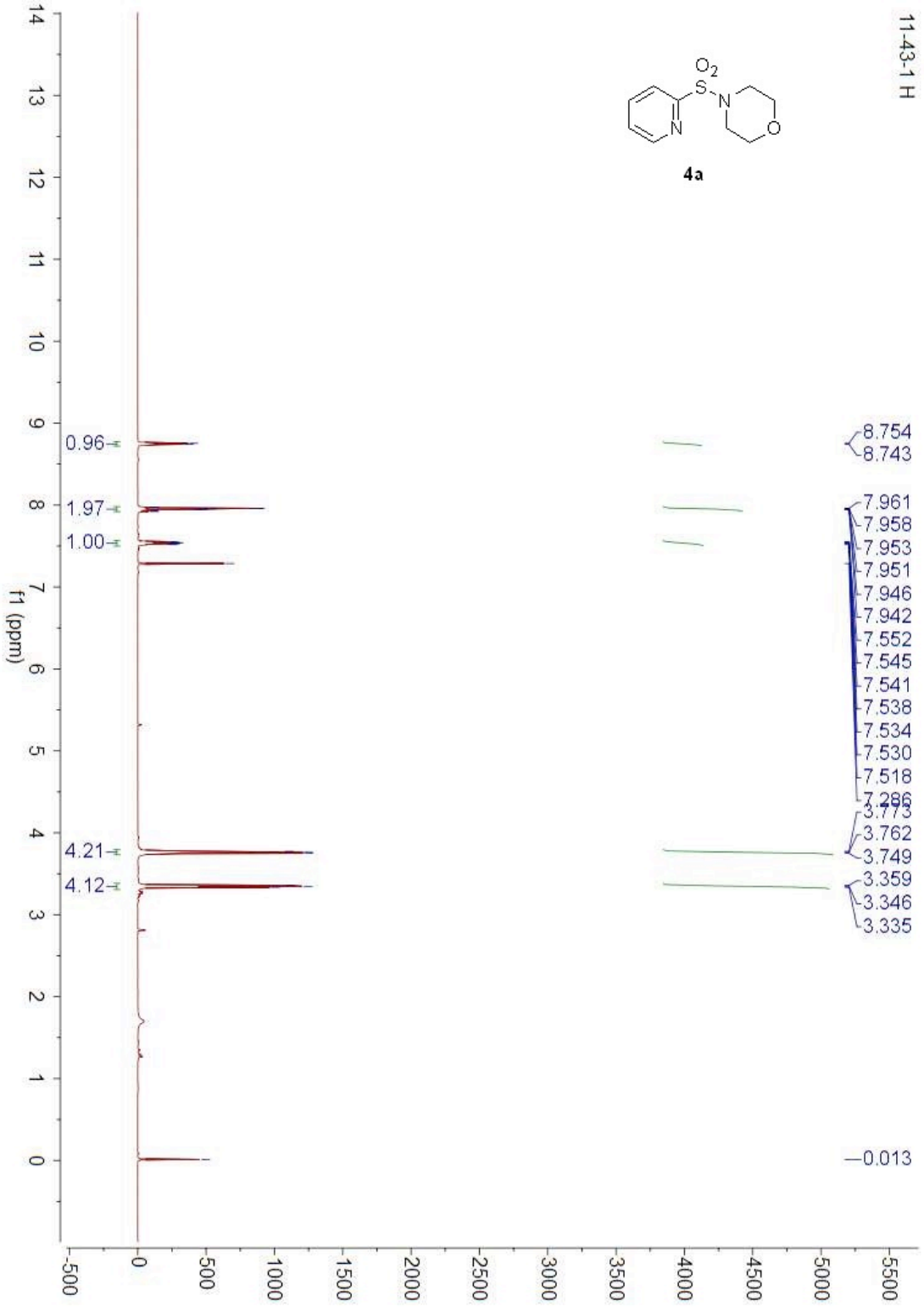

11-42-9 C
3ai
156.63
150.15
139.49
138.03
135.64
128.54
128.45
127.37
126.56
122.79
114.39
77.33
77.01
76.69
56.08
f1 (ppm)

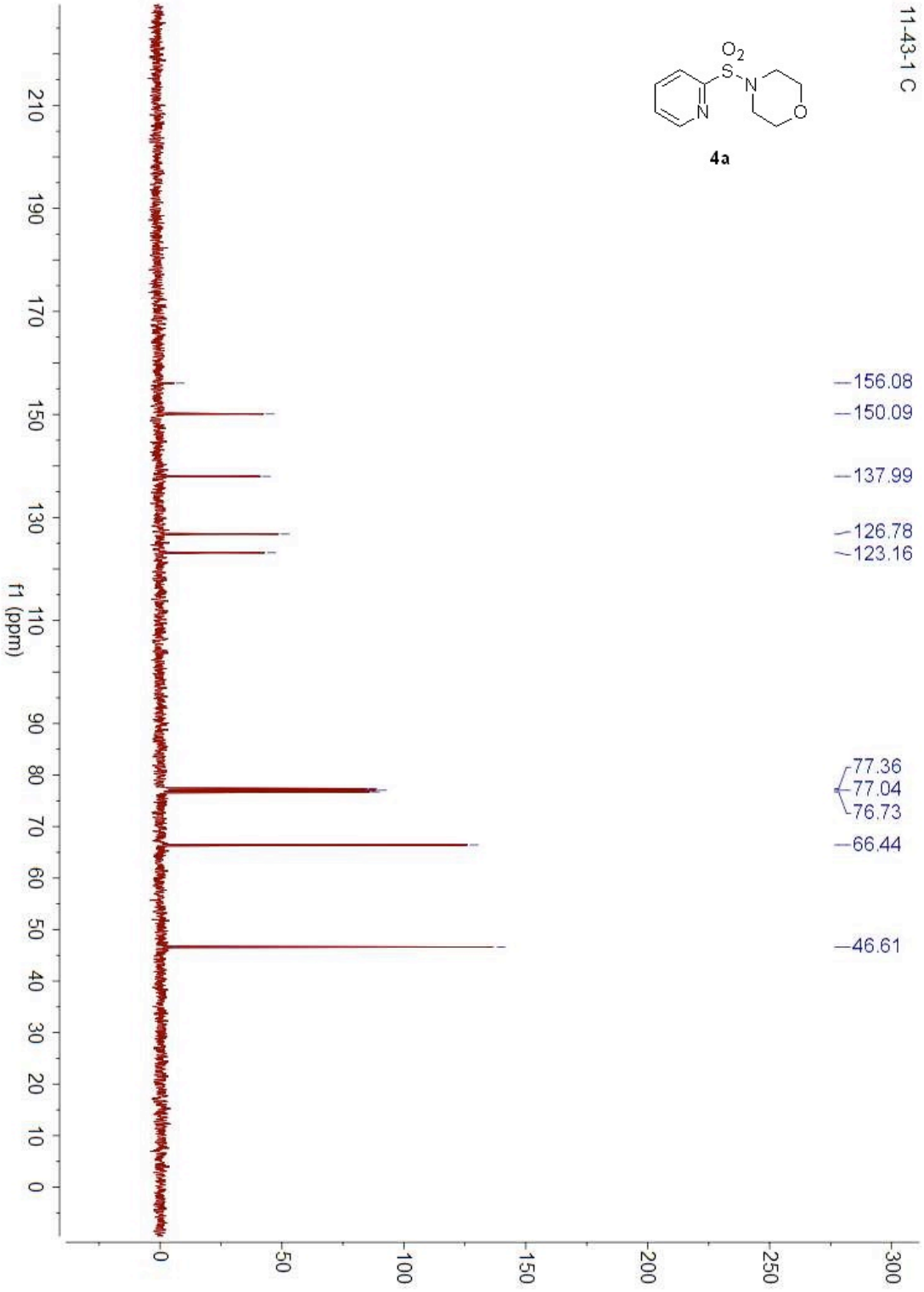

11-42-11 H
3aj
f1 (ppm)
1.00
1.00
1.12
1.09
2.18
2.32
3.27
8.774
8.773
8.764
8.762
8.761
8.122
8.103
8.024
8.020
8.005
8.001
7.614
7.611
7.602
7.599
7.594
4.487
4.153
4.135
4.117
4.099
1.176
1.158
1.140
0.000

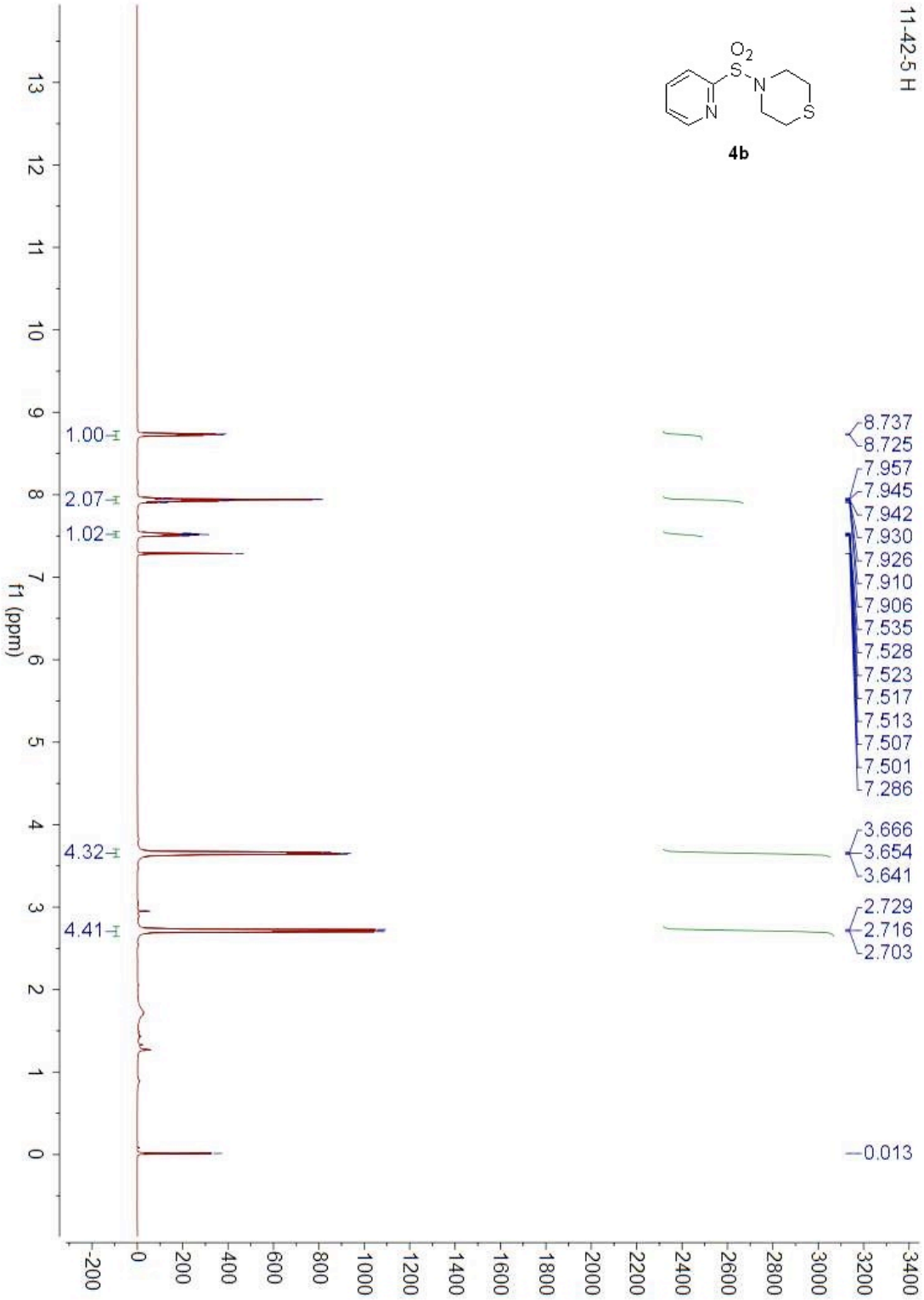

11-42-11 C
3aj
162.41
156.57
150.18
138.15
127.64
122.37
77.34
77.03
76.71
62.29
56.04
13.76
f1 (ppm)

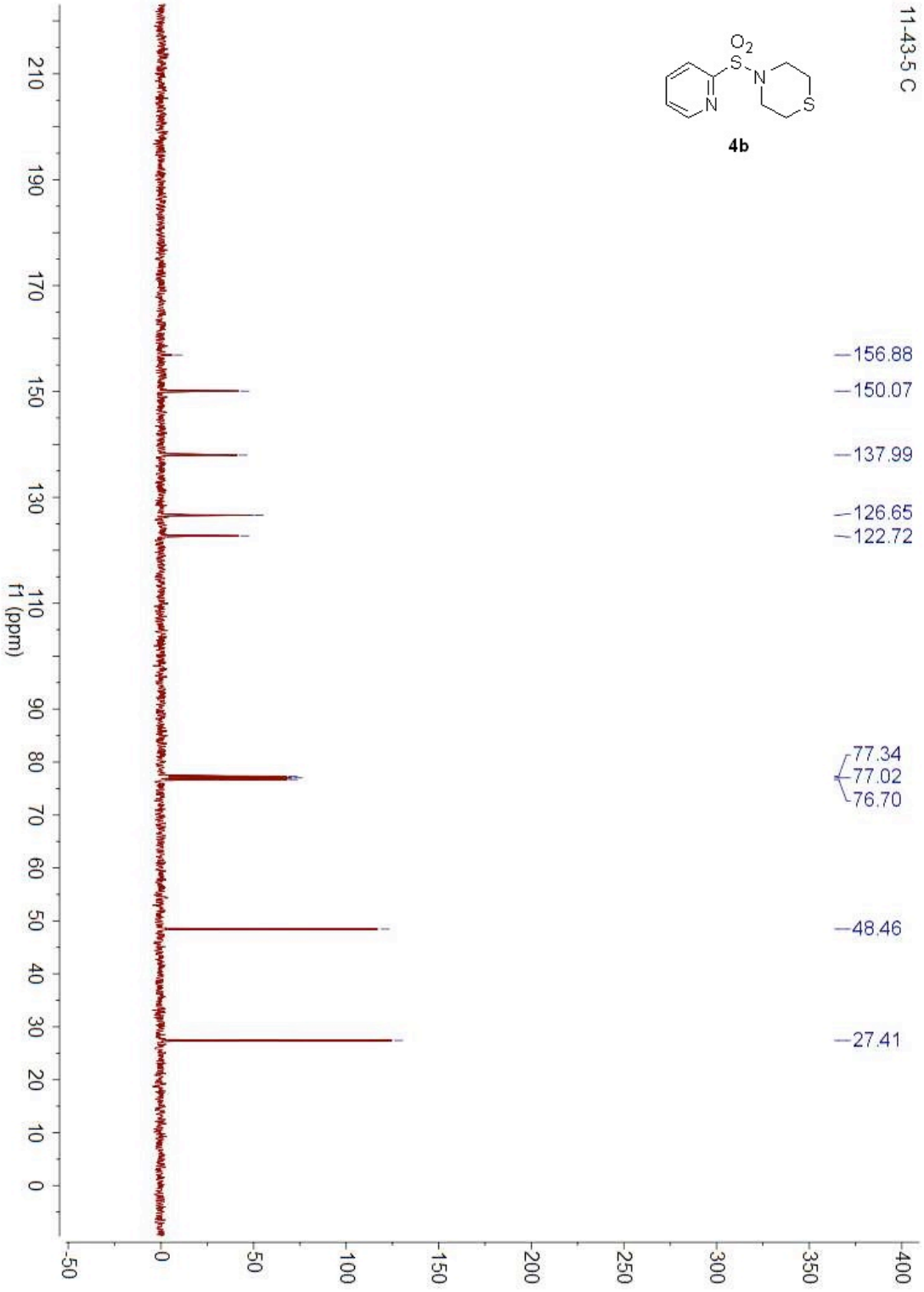

3ak
f1 (ppm)
0.98
1.00
1.05
1.04
2.22
2.59
2.29
3.41
8.771
8.768
8.765
8.760
8.757
8.756
8.753
8.117
8.115
8.112
8.097
8.095
8.093
8.005
8.001
7.986
7.982
7.967
7.962
7.587
7.584
7.575
7.572
7.568
7.565
7.556
7.553
7.286
3.421
3.407
3.405
3.401
3.397
3.394
3.381
1.768
1.750
1.746
1.737
1.729
1.721
1.710
1.704
1.690
1.467
1.448
1.430
1.411
0.935
0.917
0.898
0.004

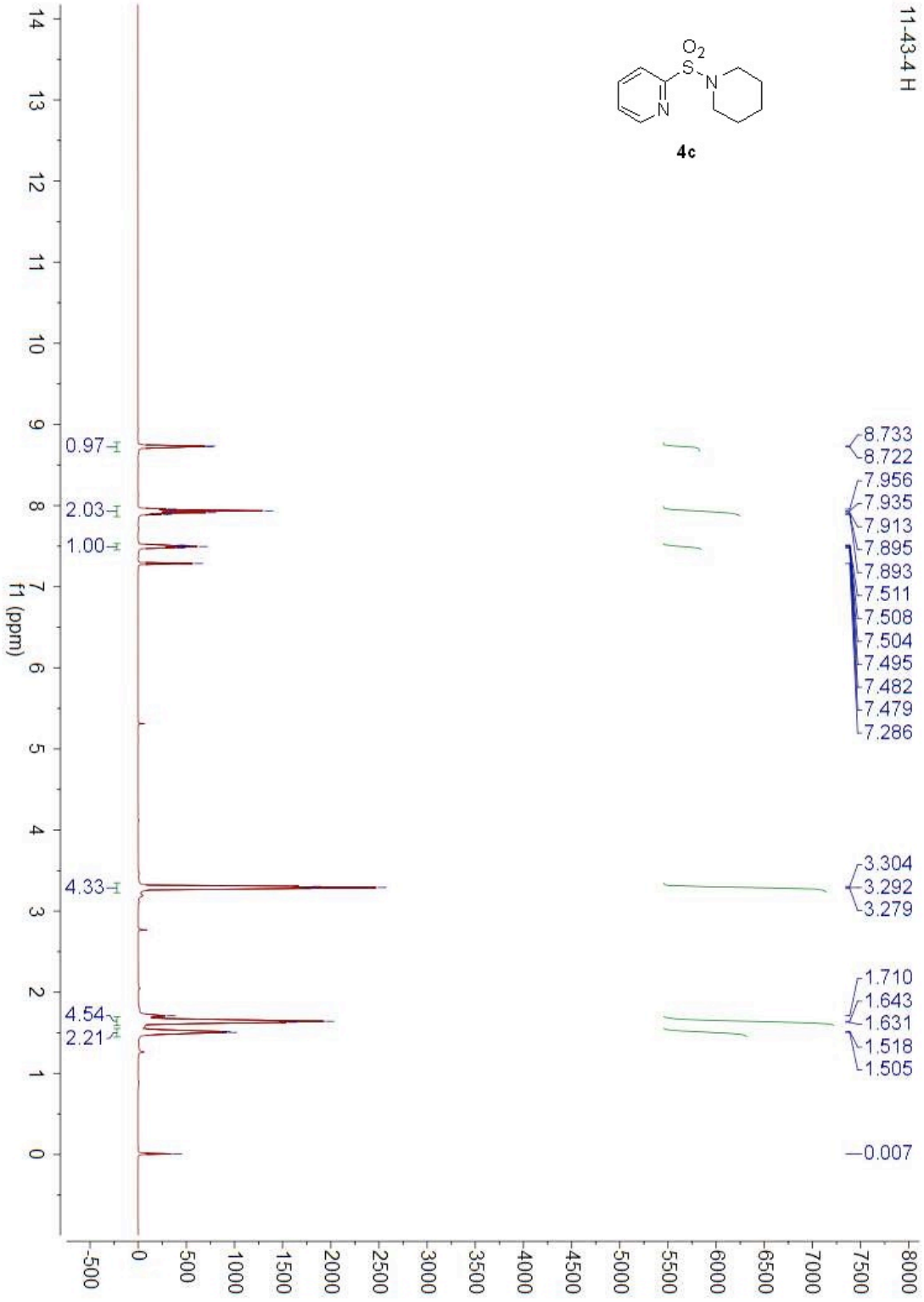

11-42-8 C
O2
S
N
3ak
157.27
150.18
138.10
127.26
122.10
77.32
77.00
76.68
51.63
24.01
21.54
13.42
f1 (ppm)

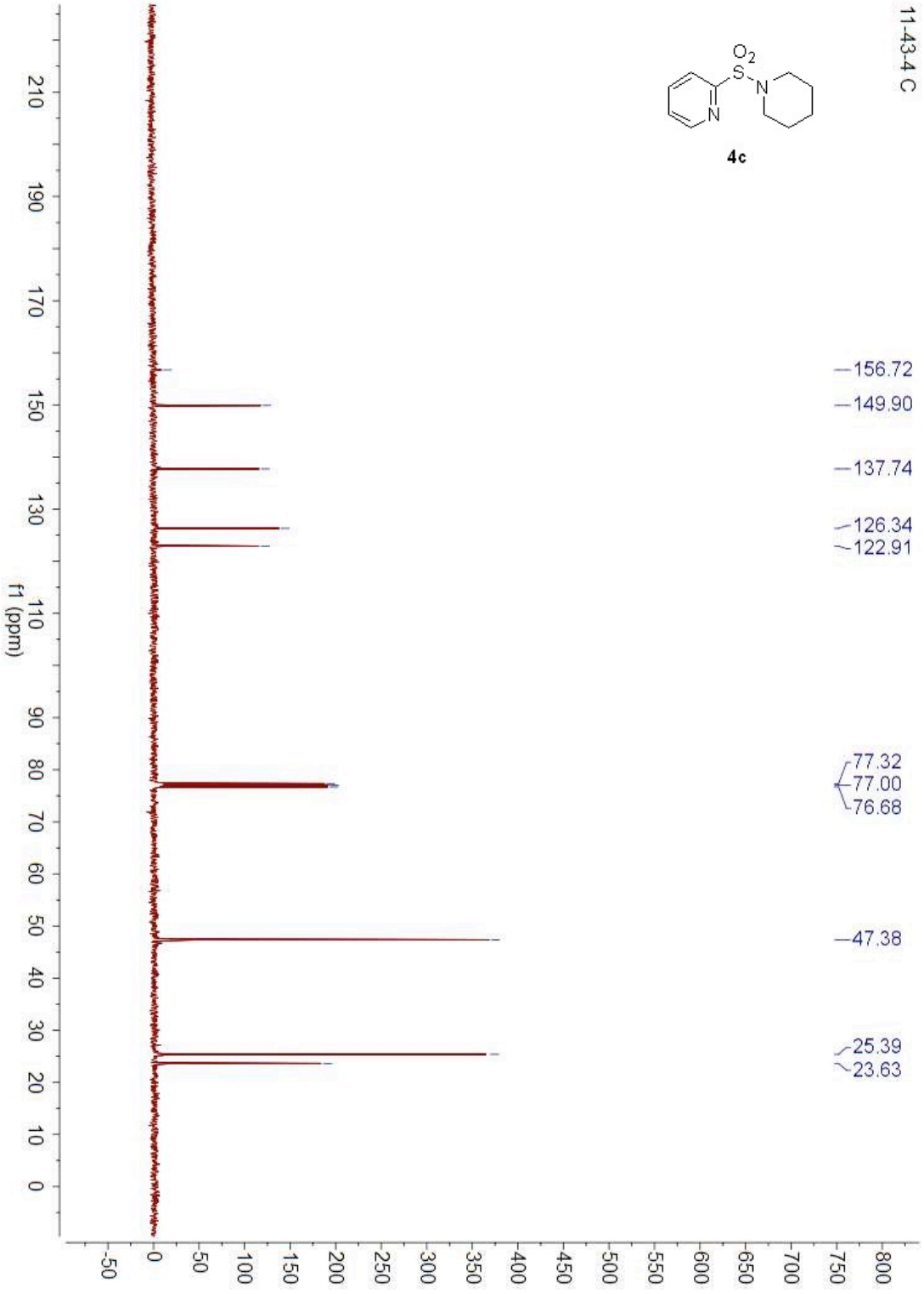

11-43-1 H
4a
f1 (ppm)
0.96
1.97
1.00
4.21
4.12
8.754
8.743
7.961
7.958
7.953
7.951
7.946
7.942
7.552
7.545
7.541
7.538
7.534
7.530
7.518
3.773
3.762
3.749
3.359
3.346
3.335
0.013

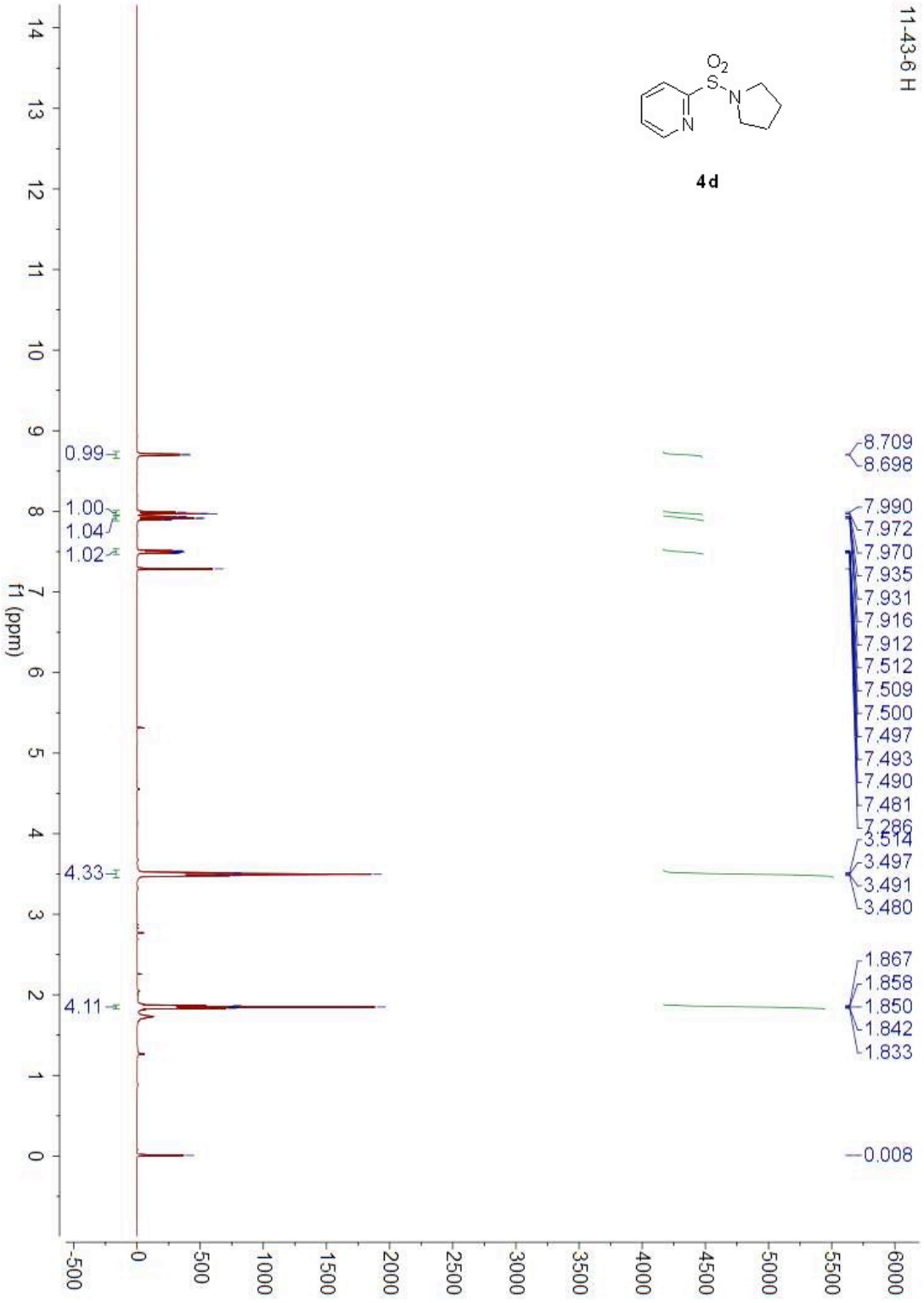

11-43-1 C
4a
156.08
150.09
137.99
126.78
123.16
77.36
77.04
76.73
66.44
46.61
f1 (ppm)

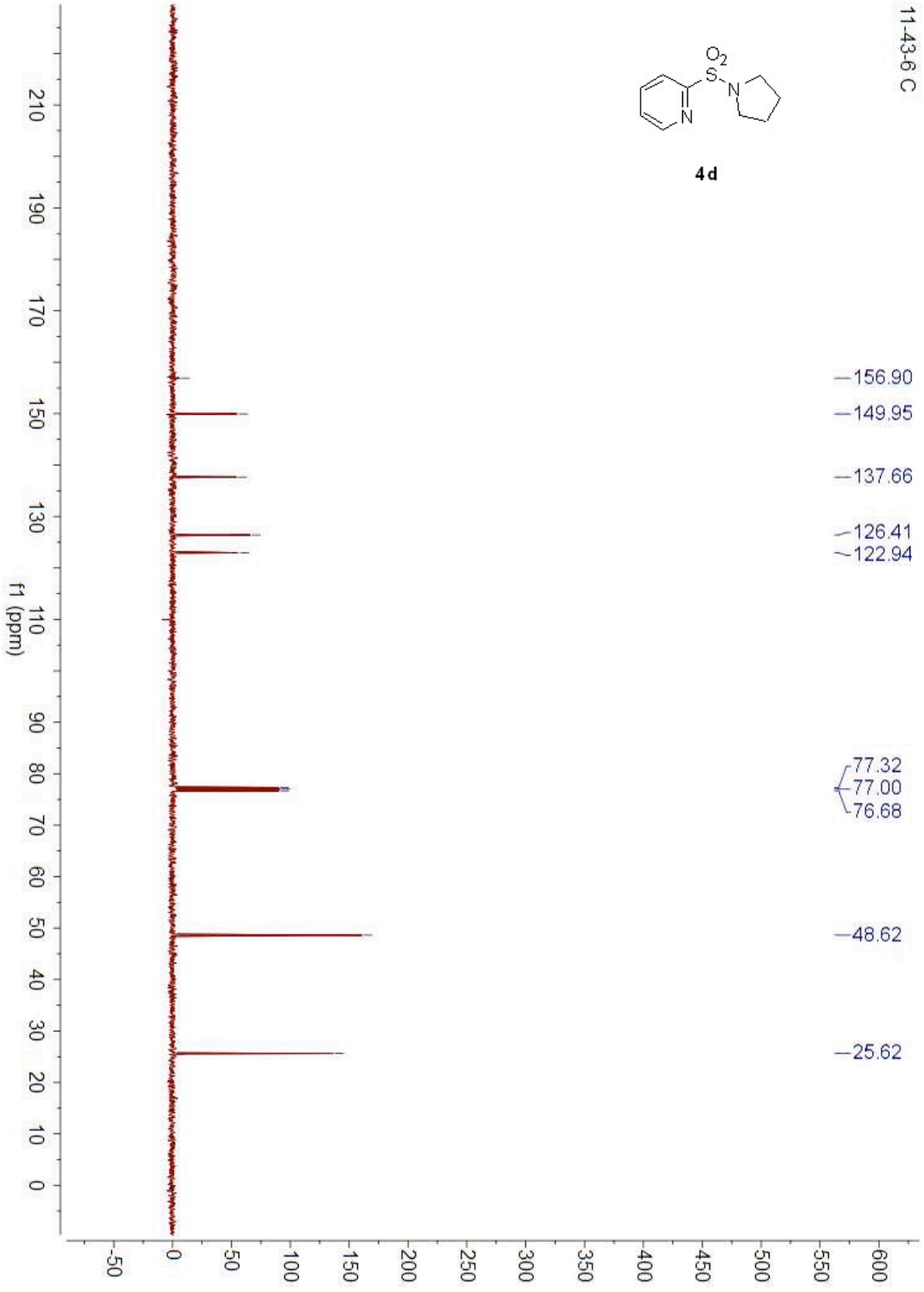

11-42-5 H
4b
f1 (ppm)
1.00
2.07
1.02
4.32
4.41
8.737
8.725
7.957
7.945
7.942
7.930
7.926
7.910
7.906
7.535
7.528
7.523
7.517
7.513
7.507
7.501
7.286
3.666
3.654
3.641
2.729
2.716
2.703
0.013

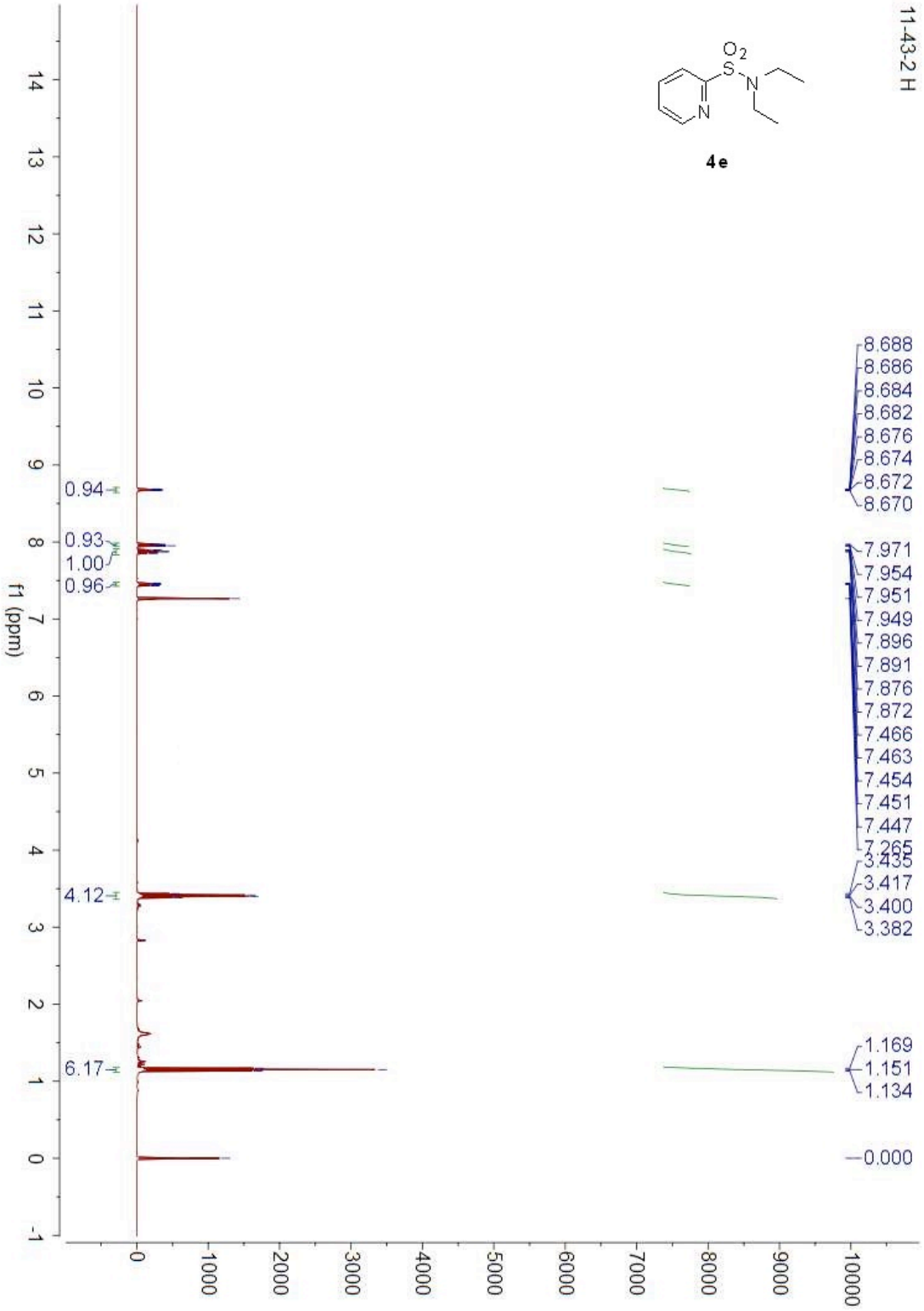

11-43-5 C
4b
156.88
150.07
137.99
126.65
122.72
77.34
77.02
76.70
48.46
27.41
f1 (ppm)

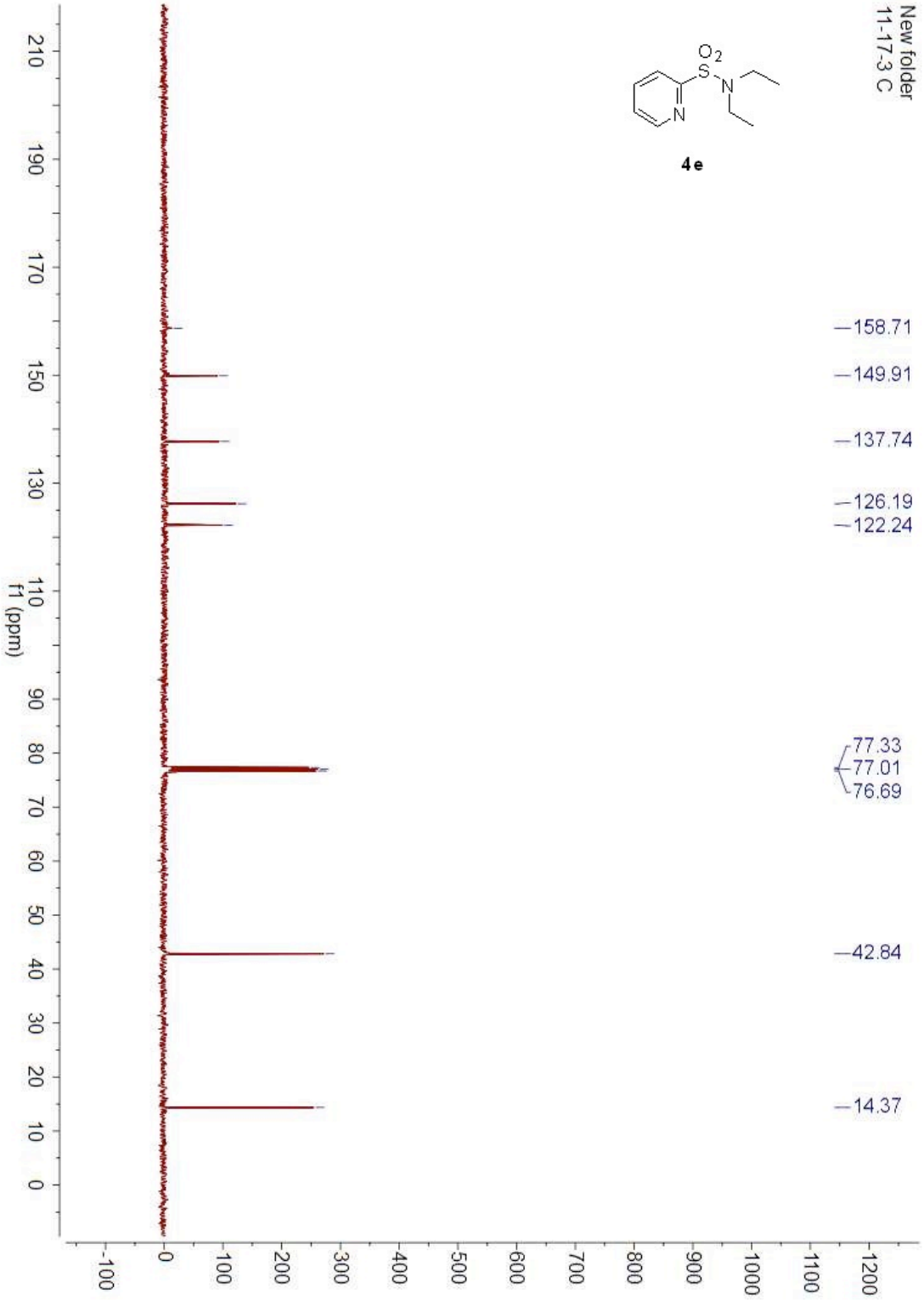

11-43-4 H
4c
f1 (ppm)
0.97
2.03
1.00
4.33
4.54
2.21
8.733
8.722
7.956
7.935
7.913
7.895
7.893
7.511
7.508
7.504
7.495
7.482
7.479
7.286
3.304
3.292
3.279
1.710
1.643
1.631
1.518
1.505
0.007

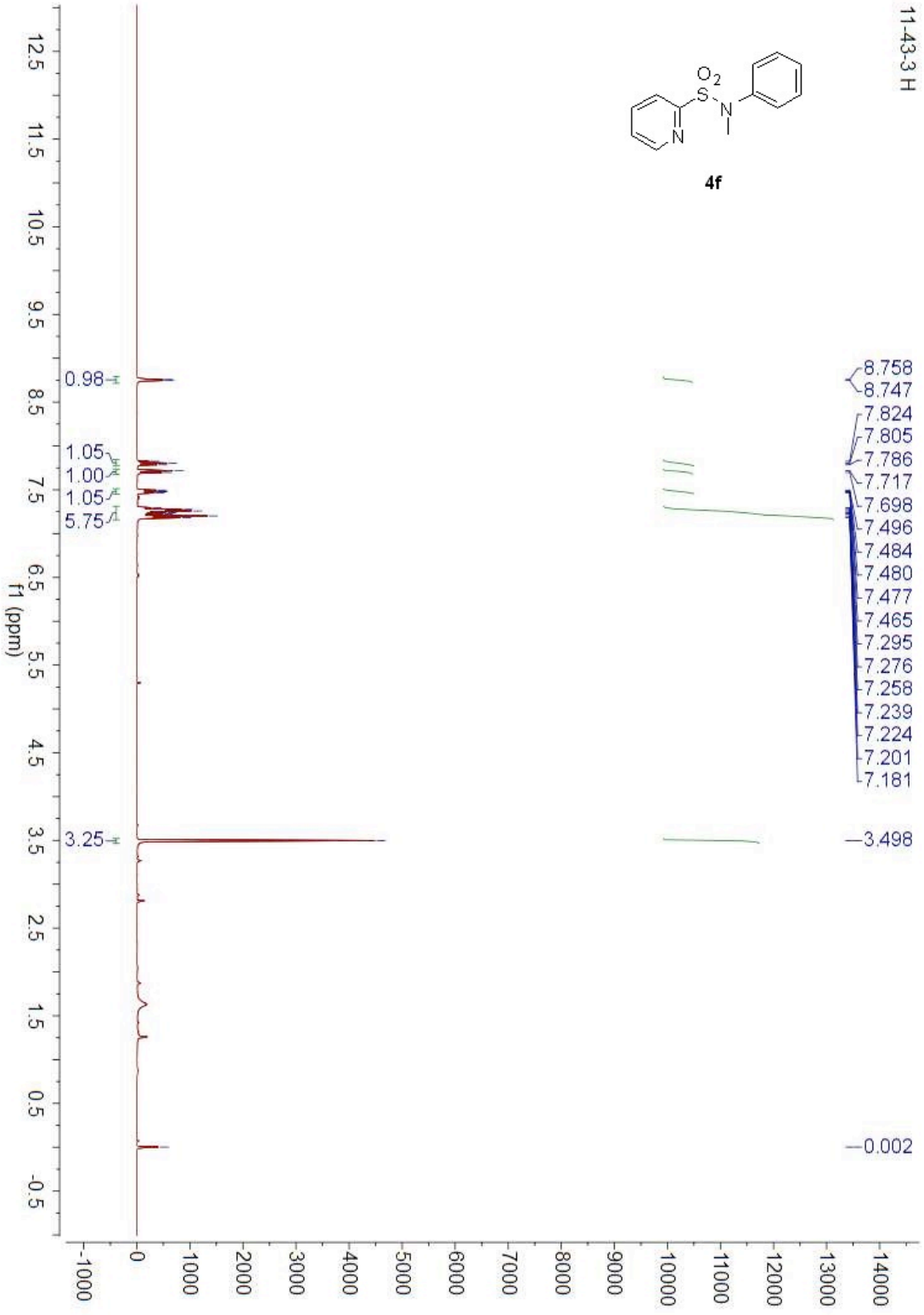

11-43-4 C
4c
156.72
149.90
137.74
126.34
122.91
77.32
77.00
76.68
47.38
25.39
23.63
f1 (ppm)

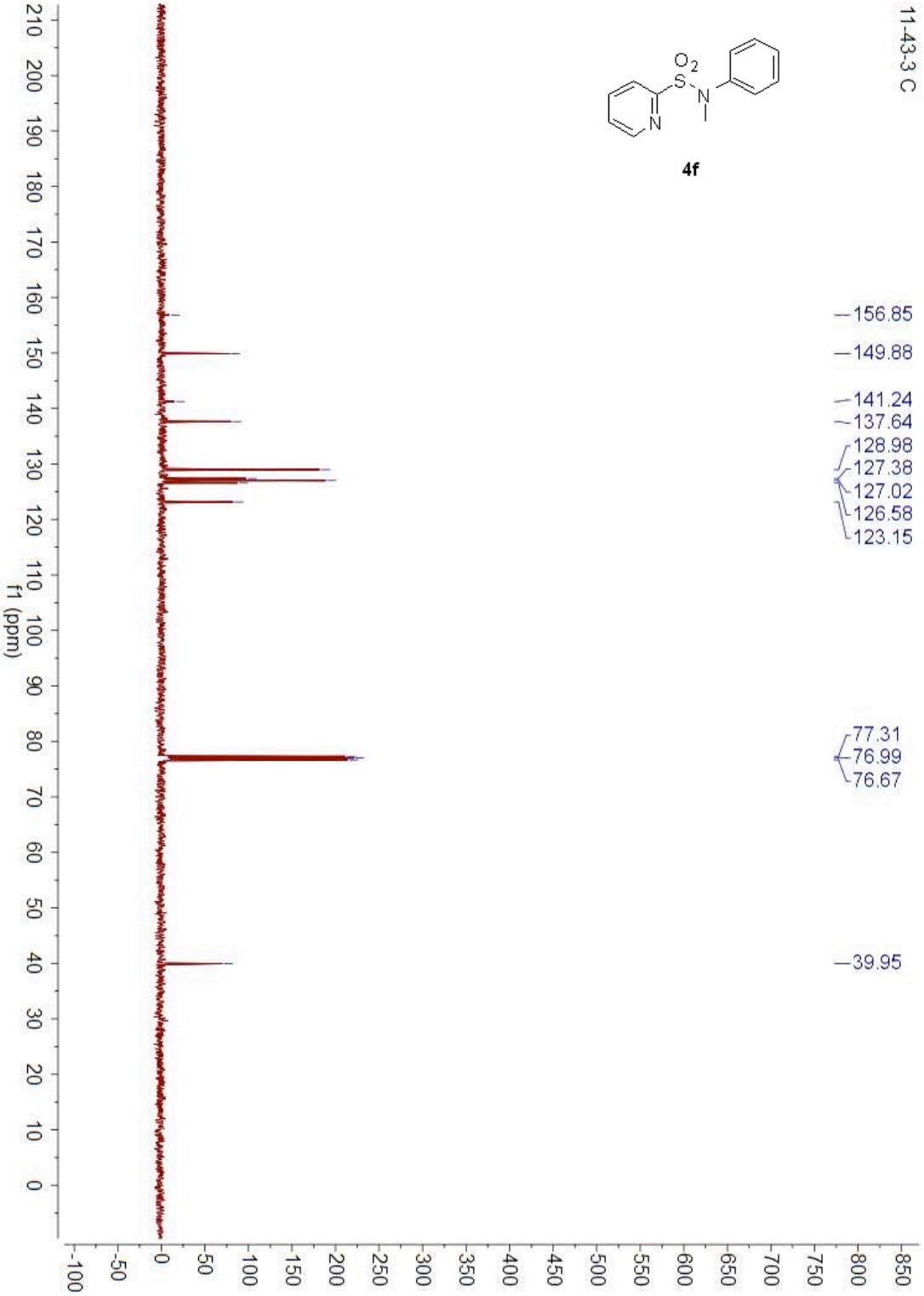

11-43-6 H
4d
f1 (ppm)
0.99
1.00
1.04
1.02
4.33
4.11
8.709
8.698
7.990
7.972
7.970
7.935
7.931
7.916
7.912
7.512
7.509
7.500
7.497
7.493
7.490
7.481
7.286
3.514
3.497
3.491
3.480
1.867
1.858
1.850
1.842
1.833
0.008

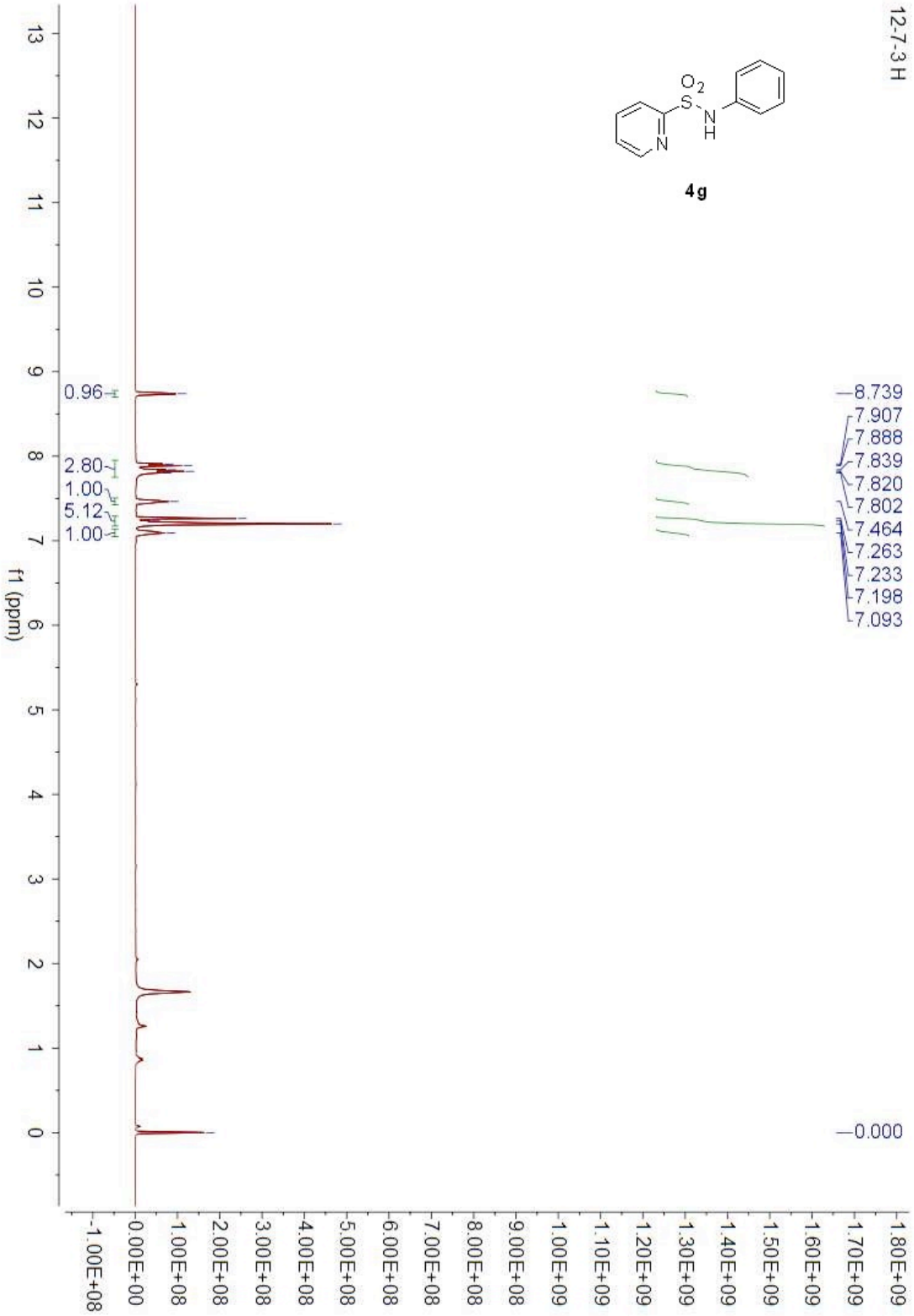

11-43-6 C
4d
156.90
149.95
137.66
126.41
122.94
77.32
77.00
76.68
48.62
25.62
f1 (ppm)

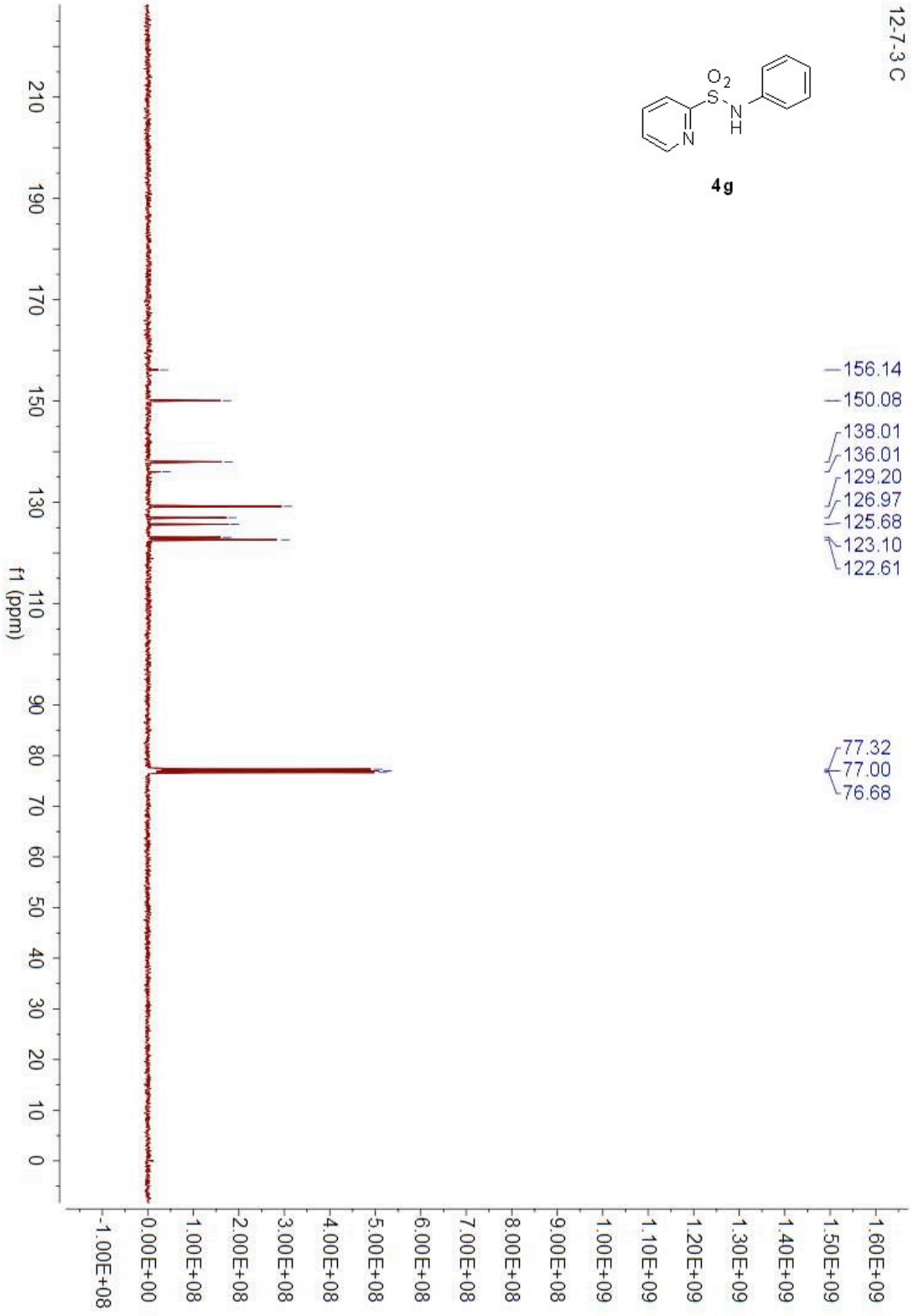

11-43-2 H
4e
f1 (ppm)
0.94
0.93
1.00
0.96
4.12
6.17
8.688
8.686
8.684
8.682
8.676
8.674
8.672
8.670
7.971
7.954
7.951
7.949
7.896
7.891
7.876
7.872
7.466
7.463
7.454
7.451
7.447
7.265
3.435
3.417
3.400
3.382
1.169
1.151
1.134
0.000

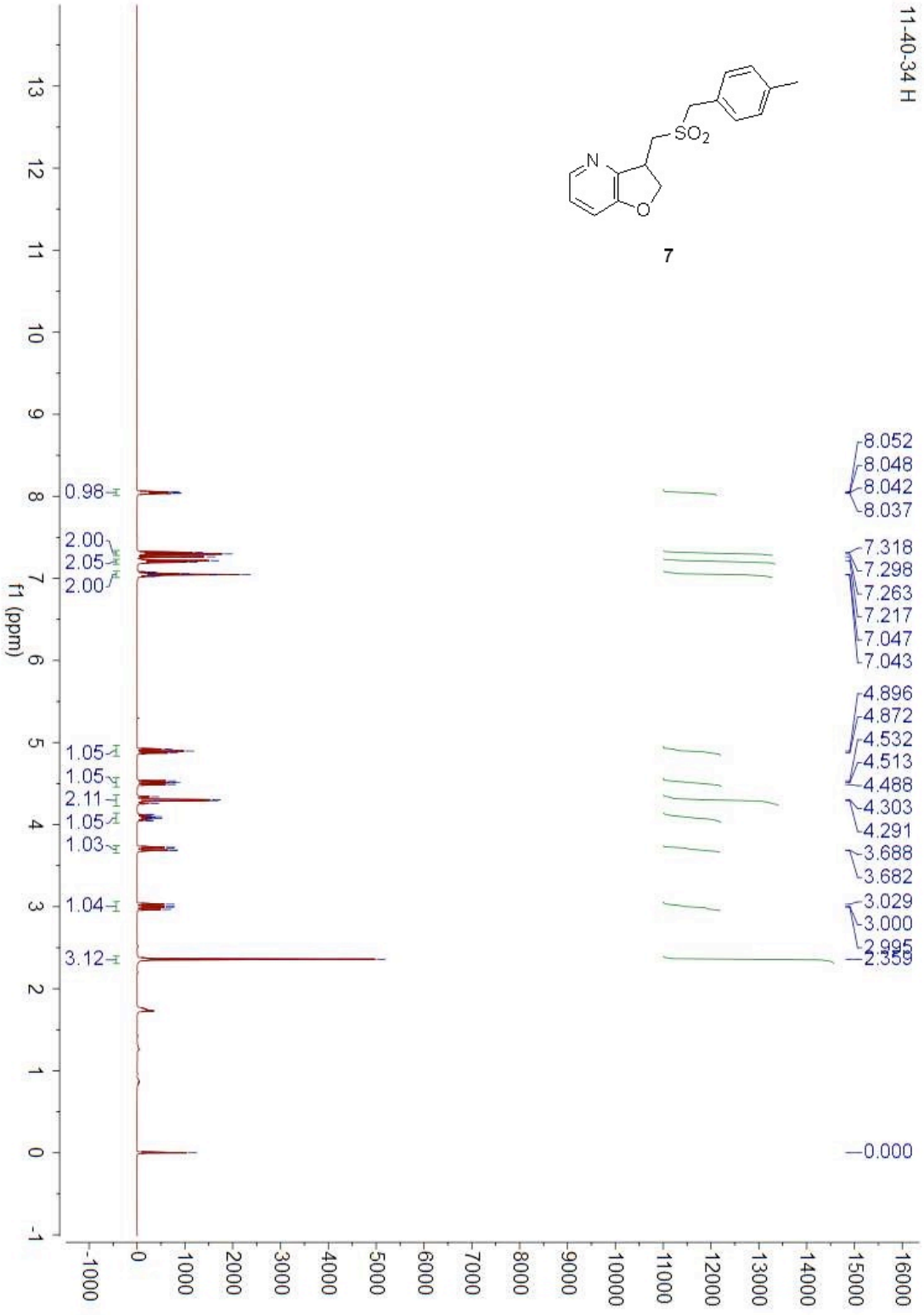

New folder
11-17-3 C
4e
158.71
149.91
137.74
126.19
122.24
77.33
77.01
76.69
42.84
14.37
f1 (ppm)

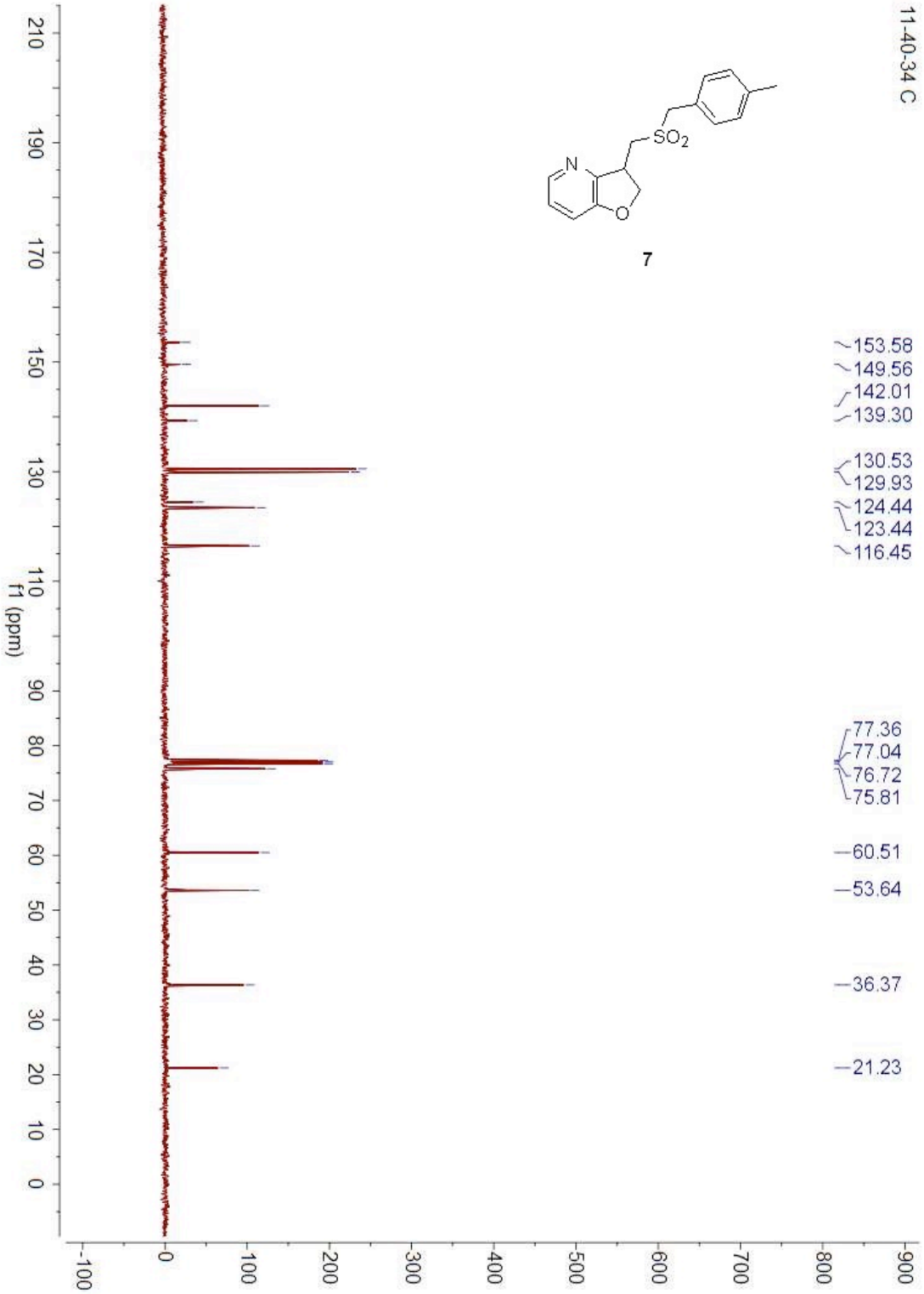

11-43-3 H
4f
8.758
8.747
7.824
7.805
7.786
7.717
7.698
7.496
7.484
7.480
7.477
7.465
7.295
7.276
7.258
7.239
7.224
7.201
7.181
3.498
0.002
0.98
1.05
1.00
1.05
5.75
3.25
f1 (ppm)


11-43-3 C
4f
156.85
149.88
141.24
137.64
128.98
127.38
127.02
126.58
123.15
77.31
76.99
76.67
39.95
f1 (ppm)


12-7-3 H
4g
8.739
7.907
7.888
7.839
7.820
7.802
7.464
7.263
7.233
7.198
7.093
0.000
0.96
2.80
1.00
5.12
1.00
f1 (ppm)


12-7-3 C
4g
156.14
150.08
138.01
136.01
129.20
126.97
125.68
123.10
122.61
77.32
77.00
76.68
f1 (ppm)


11-40-34 H
7
f1 (ppm)
8.052
8.048
8.042
8.037
7.318
7.298
7.263
7.217
7.047
7.043
4.896
4.872
4.532
4.513
4.488
4.303
4.291
3.688
3.682
3.029
3.000
2.995
2.359
0.000
0.98
2.00
2.05
2.00
1.05
1.05
2.11
1.05
1.03
1.04
3.12


11-40-34 C
SO2
N
O
7
153.58
149.56
142.01
139.30
130.53
129.93
124.44
123.44
116.45
77.36
77.04
76.72
75.81
60.51
53.64
36.37
21.23
f1 (ppm)