Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Photocatalytic three-component radical cascade: a general route to heterocyclic-substituted alkyl sulfones

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Supporting Information

1. General experimental method (S2)
2. General experimental procedure (S3-S4)
3. Radical trapping experiment (S5-S6)
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5. Characterization data of compounds (S8-S21)
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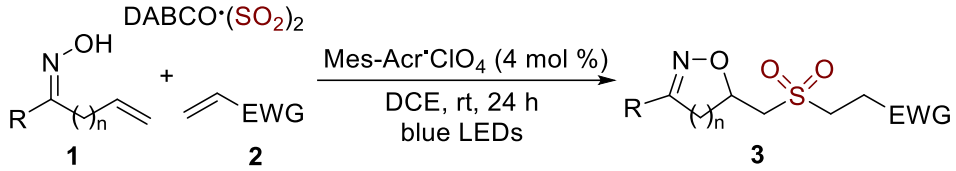
General experimental methods:

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 (ppm) 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 oxime **1**, DABSO and alkene **2**.*

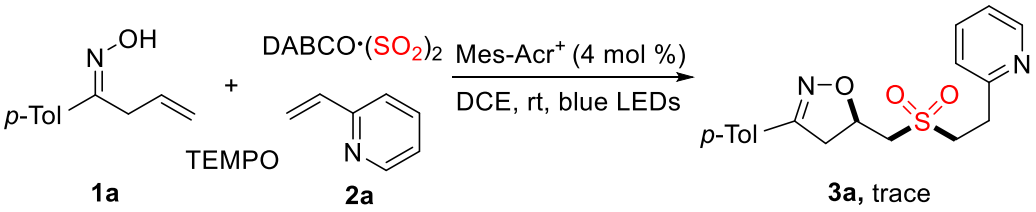


A dry tube was charged with oxime **1** (0.3 mmol), DABSO (0.2 mmol), alkene **2** (0.2 mmol) and Mes-Acr·ClO_4 (4.0 mol %), sealed with a rubber stopper, evacuated and backfilled with argon for four times before the addition of DCE (3.0 mL) *via* a syringe. The mixture was then placed around a blue LED (24 W) with a distance of 10 centimeters, and was stirred under blue light irradiation for 24 hours at room temperature. After completion of reaction as indicated by TLC, the solvent was evaporated in vacuo, and purified by flash column chromatography (EtOAc/*n*-hexane, 1:3) to provide the desired product **3**.

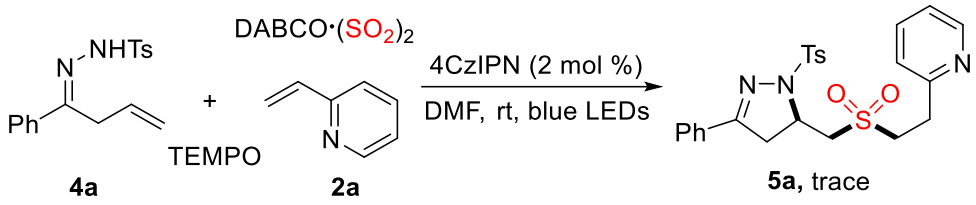
*General experimental procedure for the aminosulfonylation of β,γ-unsaturated hydrazones **4** with DABSO and alkene **2**.*

A dry tube was charged with β,γ-unsaturated hydrazones **4** (0.2 mmol), DABSO (0.2 mmol), alkene **2** (0.3 mmol) and 4CzIPN (2.0 mol %), sealed with a rubber stopper, evacuated and backfilled with argon for four times before the addition of DMF (3.0 mL) *via* a syringe. The mixture was then placed around a blue LED (24 W) with a distance of 10 centimeters, and was stirred under blue light irradiation for 24 hours at room temperature. After completion of reaction as indicated by TLC, the solvent was evaporated in *vacuo*, and purified by flash column chromatography (EtOAc/*n*-hexane, 1:2) to provide the desired product **5**.

Radical trapping experiment



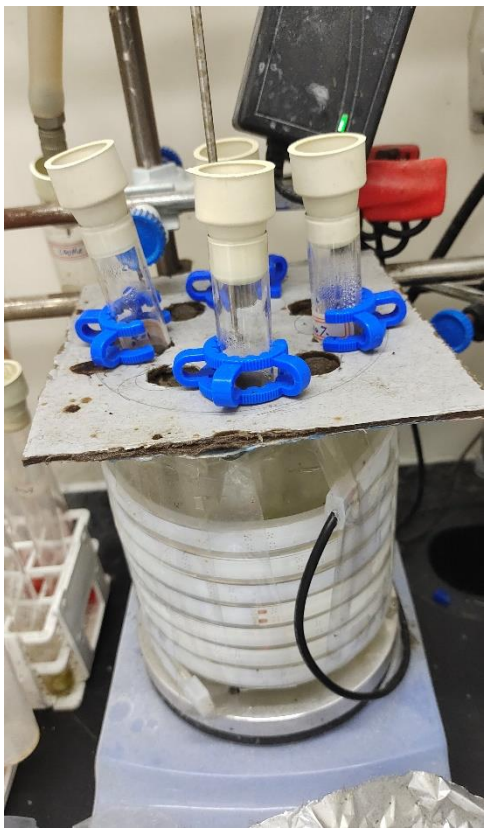
A dry tube was charged with (*E*)-1-(*p*-tolyl)but-3-en-1-one oxime **1a** (0.3 mmol), DABSO (0.2 mmol), 2-vinylpyridine **2a** (0.2 mmol), Mes-Acr$^+$ (4.0 mol %) and TEMPO (0.4 mmol), sealed with a rubber stopper, evacuated and backfilled with argon for four times before the addition of DCE (3.0 mL) *via* a syringe. The mixture was then placed around a blue LED (24 W) with a distance of 10 centimeters, and was stirred under blue light irradiation for 24 hours at room temperature. After completion of reaction as indicated by TLC, only a trace of the desired product **3a** was detected.

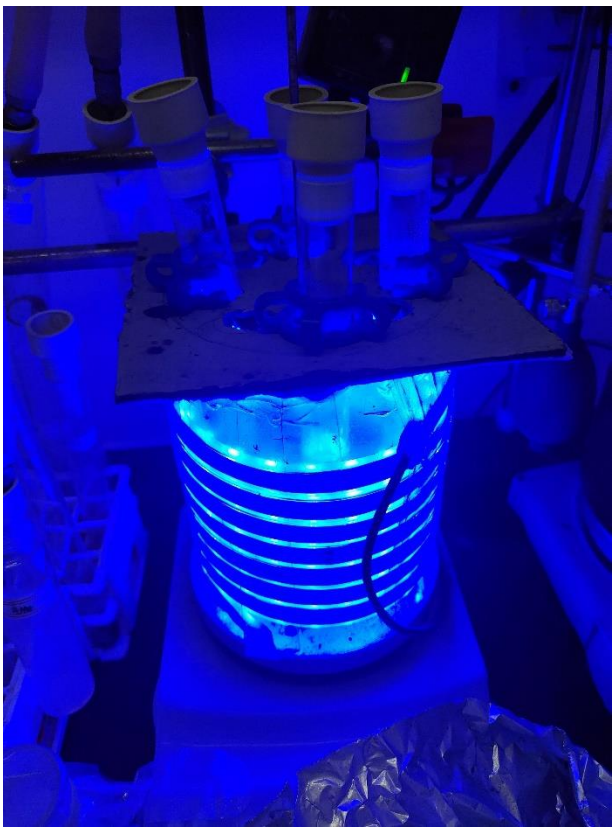


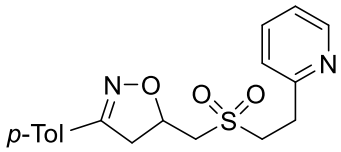
4a **2a** **5a**, trace

A dry tube was charged with (*E*)-4-methyl-*N*'-(1-phenylbut-3-en-1-ylidene)benzenesulfonohydrazide **4a** (0.2 mmol), DABSO (0.2 mmol), 2-vinylpyridine **2a** (0.3 mmol), 4CzIPN (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 DMF (3.0 mL) *via* a syringe. The mixture was then placed around a blue LED (24 W) with a distance of 10 centimeters, and was stirred under blue light irradiation for 24 hours at room temperature. After completion of reaction as indicated by TLC, only a trace of the desired product **5a** was detected.

Devices for the photocatalytic reactions

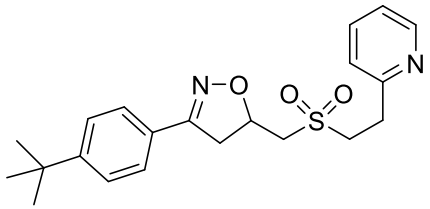






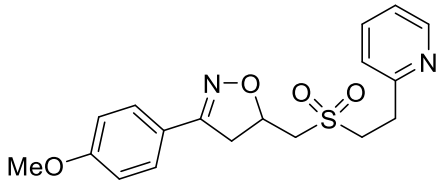
5-(((2-(Pyridin-2-yl)ethyl)sulfonyl)methyl)-3-(*p*-tolyl)-4,5-dihydroisoxazole (**3a**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.53 (d, *J* = 4.3 Hz, 1H), 7.63 (td, *J* = 7.7, 1.8 Hz, 1H), 7.54 (d, *J* = 8.2 Hz, 2H), 7.25 (d, *J* = 7.9 Hz, 1H), 7.22 (d, *J* = 8.0 Hz, 2H), 7.17 (dd, *J* = 7.2, 5.1 Hz, 1H), 5.25 (dq, *J* = 10.5, 6.8 Hz, 1H), 3.70 (td, *J* = 7.1, 2.0 Hz, 2H), 3.62 (dd, *J* = 17.0, 10.4 Hz, 1H), 3.49 (dd, *J* = 14.4, 6.9 Hz, 1H), 3.38 – 3.27 (m, 3H), 3.14 (dd, *J* = 14.4, 5.7 Hz, 1H), 2.38 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 157.0, 156.9, 149.5, 141.0, 136.8, 129.5, 126.7, 125.7, 123.3, 122.0, 74.6, 57.3, 53.6, 40.5, 29.9, 21.4; HRMS calcd for $C_{18}H_{20}N_2NaO_3S^+$ (M+Na^+): 367.1087, found: 367.1095.



3-(4-(*tert*-Butyl)phenyl)-5-(((2-(pyridin-2-yl)ethyl)sulfonyl)methyl)-4,5-dihydroisoxazole (**3b**)

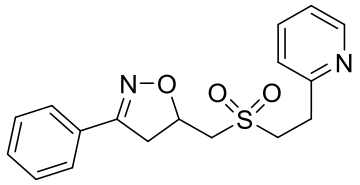
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.53 (d, *J* = 4.2 Hz, 1H), 7.66 – 7.58 (m, 3H), 7.44 (d, *J* = 8.4 Hz, 2H), 7.25 (d, *J* = 7.8 Hz, 1H), 7.19 – 7.15 (m, 1H), 5.30 – 5.21 (m, 1H), 3.72 – 3.59 (m, 3H), 3.49 (dd, *J* = 14.4, 6.9 Hz, 1H), 3.39 – 3.29 (m, 3H), 3.14 (dd, *J* = 14.4, 5.7 Hz, 1H), 1.33 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 157.0, 156.8, 154.1, 149.5, 136.8, 126.6, 125.8, 125.7, 123.3, 122.0, 74.6, 57.3, 53.6, 40.5, 34.9, 31.1, 29.9; HRMS calcd for $C_{21}H_{26}N_2NaO_3S^+$ (M+Na^+): 409.1556, found: 409.1563.



3-(4-Methoxyphenyl)-5-(((2-(pyridin-2-yl)ethyl)sulfonyl)methyl)-4,5-dihydroisoxazole (**3c**)

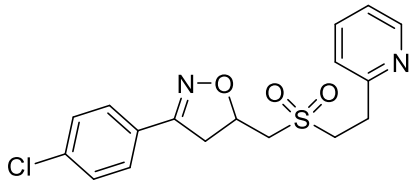
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.53 (d, *J* = 4.4 Hz, 1H), 7.66 – 7.61 (m, 1H), 7.59 (d, *J* = 8.8 Hz, 2H), 7.25 (d, *J* = 7.8 Hz, 1H), 7.16 (dd, *J* = 7.2, 5.1 Hz, 1H), 6.92 (d, *J* = 8.8 Hz,

2H), 5.23 (dq, *J* = 10.5, 6.7 Hz, 1H), 3.84 (s, 3H), 3.72 – 3.67 (m, 2H), 3.60 (dd, *J* = 16.9, 10.4 Hz, 1H), 3.49 (dd, *J* = 14.4, 6.9 Hz, 1H), 3.37 – 3.26 (m, 3H), 3.14 (dd, *J* = 14.4, 5.7 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 161.4, 157.0, 156.5, 149.5, 136.7, 128.4, 123.3, 122.0, 121.0, 114.2, 74.5, 57.2, 55.3, 53.6, 40.6, 29.9; HRMS calcd for $C_{18}H_{20}N_2NaO_4S^+$ ($M+Na^+$): 383.1036, found: 383.1041.



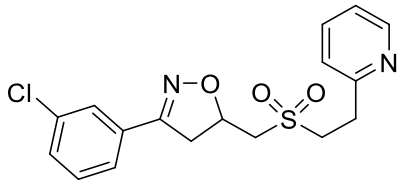
3-Phenyl-5-(((2-(pyridin-2-yl)ethyl)sulfonyl)methyl)-4,5-dihydroisoxazole (**3d**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.53 (d, *J* = 4.3 Hz, 1H), 7.68 – 7.61 (m, 3H), 7.42 (q, *J* = 5.2 Hz, 3H), 7.25 (d, *J* = 8.5 Hz, 1H), 7.17 (dd, *J* = 6.9, 5.3 Hz, 1H), 5.28 (dq, *J* = 12.9, 6.6 Hz, 1H), 3.75 – 3.61 (m, 3H), 3.50 (dd, *J* = 14.4, 6.8 Hz, 1H), 3.40 – 3.30 (m, 3H), 3.16 (dd, *J* = 14.4, 5.8 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 156.9, 149.5, 136.8, 130.6, 128.8, 128.6, 126.8, 123.4, 122.1, 74.8, 57.3, 53.6, 40.4, 29.9; HRMS calcd for $C_{17}H_{18}N_2NaO_3S^+$ ($M+Na^+$): 353.0930, found: 353.0935.



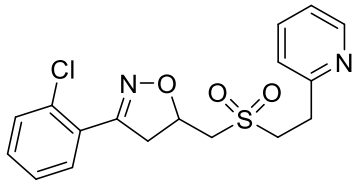
3-(4-Chlorophenyl)-5-(((2-(pyridin-2-yl)ethyl)sulfonyl)methyl)-4,5-dihydroisoxazole (**3e**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.54 (d, *J* = 4.3 Hz, 1H), 7.64 (td, *J* = 7.7, 1.8 Hz, 1H), 7.59 (d, *J* = 8.6 Hz, 2H), 7.39 (d, *J* = 8.6 Hz, 2H), 7.25 (d, *J* = 7.9 Hz, 1H), 7.18 (dd, *J* = 7.0, 5.2 Hz, 1H), 5.28 (dq, *J* = 10.6, 6.6 Hz, 1H), 3.70 (td, *J* = 7.3, 3.4 Hz, 2H), 3.61 (dd, *J* = 17.0, 10.5 Hz, 1H), 3.49 (dd, *J* = 14.4, 6.5 Hz, 1H), 3.39 – 3.30 (m, 3H), 3.16 (dd, *J* = 14.4, 6.2 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 156.9, 156.1, 149.5, 136.8, 136.6, 129.1, 128.0, 127.1, 123.4, 122.1, 75.0, 57.1, 53.6, 40.2, 29.9; HRMS calcd for $C_{17}H_{17}ClN_2NaO_3S^+$ ($M+Na^+$): 387.0541, found: 387.0548.



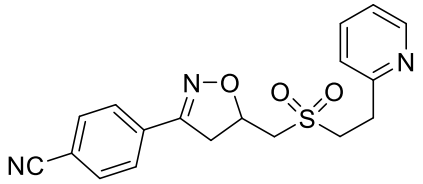
3-(3-Chlorophenyl)-5-(((2-(pyridin-2-yl)ethyl)sulfonyl)methyl)-4,5-dihydroisoxazole (**3f**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.54 (d, *J* = 4.1 Hz, 1H), 7.64 (ddd, *J* = 9.5, 5.6, 1.8 Hz, 2H), 7.55 – 7.52 (m, 1H), 7.43 – 7.33 (m, 2H), 7.25 (d, *J* = 7.8 Hz, 1H), 7.17 (dd, *J* = 7.0, 5.2 Hz, 1H), 5.29 (dq, *J* = 10.6, 6.6 Hz, 1H), 3.73 – 3.58 (m, 3H), 3.49 (dd, *J* = 14.4, 6.6 Hz, 1H), 3.38 – 3.30 (m, 3H), 3.17 (dd, *J* = 14.4, 6.1 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 156.9, 156.0, 149.5, 136.8, 134.9, 130.5, 130.3, 130.1, 126.8, 124.9, 123.3, 122.1, 75.1, 57.1, 53.6, 40.1, 29.9; HRMS calcd for $C_{17}H_{17}ClN_2NaO_3S^+$ ($M+Na^+$): 387.0541, found: 387.0551.



3-(2-Chlorophenyl)-5-(((2-(pyridin-2-yl)ethyl)sulfonyl)methyl)-4,5-dihydroisoxazole (**3g**)

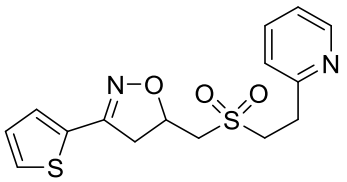
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.54 (s, 1H), 7.68 – 7.62 (m, 2H), 7.53 (d, *J* = 7.6 Hz, 1H), 7.38 (dt, *J* = 15.6, 4.8 Hz, 2H), 7.19 (s, 2H), 5.33 – 5.25 (m, 1H), 3.74 – 3.57 (m, 3H), 3.50 (dd, *J* = 14.4, 6.6 Hz, 1H), 3.39 – 3.29 (m, 3H), 3.18 (dd, *J* = 14.4, 6.0 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 156.8, 156.0, 149.4, 136.9, 134.8, 130.5, 130.3, 130.1, 126.8, 124.9, 123.4, 122.1, 75.1, 57.1, 53.6, 40.1, 29.9; HRMS calcd for $C_{17}H_{17}ClN_2NaO_3S^+$ ($M+Na^+$): 387.0541, found: 387.0548.



4-(5-(((2-(Pyridin-2-yl)ethyl)sulfonyl)methyl)-4,5-dihydroisoxazol-3-yl)benzonitrile (**3h**)

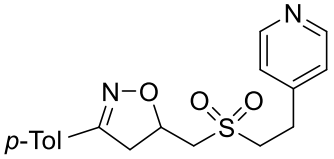
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.54 (d, *J* = 4.3 Hz, 1H), 7.77 (d, *J* = 8.5 Hz, 2H),

7.71 (d, *J* = 8.5 Hz, 2H), 7.65 (td, *J* = 7.7, 1.7 Hz, 1H), 7.25 (d, *J* = 7.8 Hz, 1H), 7.19 (dd, *J* = 6.9, 5.3 Hz, 1H), 5.38 – 5.30 (m, 1H), 3.74 – 3.61 (m, 3H), 3.51 (dd, *J* = 14.3, 6.2 Hz, 1H), 3.42 – 3.34 (m, 3H), 3.20 (dd, *J* = 14.3, 6.5 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 156.7, 155.8, 149.5, 136.8, 132.9, 132.6, 127.3, 123.4, 122.2, 118.1, 113.9, 75.6, 56.9, 53.6, 39.7, 29.9; HRMS calcd for $C_{18}H_{17}N_3NaO_3S^+$ ($M+Na^+$): 378.0883, found: 378.0890.



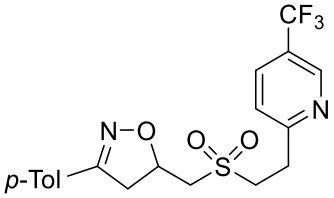
5-(((2-(Pyridin-2-yl)ethyl)sulfonyl)methyl)-3-(thiophen-2-yl)-4,5-dihydroisoxazole (**3i**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.53 (d, *J* = 4.2 Hz, 1H), 7.64 (td, *J* = 7.7, 1.6 Hz, 1H), 7.43 (d, *J* = 4.5 Hz, 1H), 7.24 (t, *J* = 5.5 Hz, 2H), 7.17 (dd, *J* = 7.1, 5.2 Hz, 1H), 7.08 (dd, *J* = 4.9, 3.8 Hz, 1H), 5.30 – 5.22 (m, 1H), 3.72 – 3.61 (m, 3H), 3.50 (dd, *J* = 14.4, 6.9 Hz, 1H), 3.37 – 3.31 (m, 3H), 3.16 (dd, *J* = 14.4, 5.7 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 156.9, 152.7, 149.4, 136.8, 130.8, 129.2, 128.9, 127.5, 123.3, 122.1, 75.0, 57.0, 53.6, 41.1, 29.8; HRMS calcd for $C_{15}H_{16}N_2NaO_3S_2^+$ ($M+Na^+$): 359.0495, found: 359.0495.



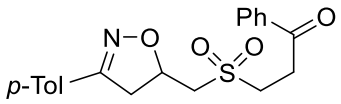
5-(((2-(Pyridin-4-yl)ethyl)sulfonyl)methyl)-3-(*p*-tolyl)-4,5-dihydroisoxazole (**3j**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.56 (dd, *J* = 4.4, 1.4 Hz, 2H), 7.55 (d, *J* = 8.1 Hz, 2H), 7.23 (d, *J* = 7.2 Hz, 4H), 5.31 – 5.23 (m, 1H), 3.65 (dd, *J* = 16.9, 10.5 Hz, 1H), 3.55 – 3.42 (m, 3H), 3.27 – 3.12 (m, 4H), 2.39 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 157.0, 150.2, 146.5, 141.3, 129.6, 126.8, 125.4, 123.8, 74.8, 57.6, 54.7, 40.6, 27.3, 21.5; HRMS calcd for $C_{18}H_{20}N_2NaO_3S^+$ ($M+Na^+$): 367.1087, found: 367.1095.



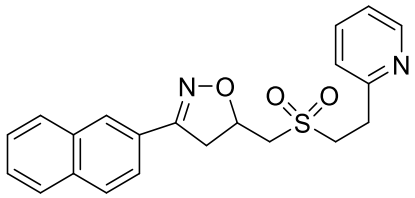
3-(*p*-Tolyl)-5-(((2-(5-(trifluoromethyl)pyridin-2-yl)ethyl)sulfonyl)methyl)-4,5-dihydrois oxazole (**3k**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.80 (s, 1H), 7.88 (dd, *J* = 8.1, 1.8 Hz, 1H), 7.55 (d, *J* = 8.1 Hz, 2H), 7.40 (d, *J* = 8.1 Hz, 1H), 7.23 (d, *J* = 8.0 Hz, 2H), 5.31 – 5.23 (m, 1H), 3.77 – 3.72 (m, 2H), 3.64 (dd, *J* = 16.9, 10.5 Hz, 1H), 3.54 (dd, *J* = 14.6, 7.6 Hz, 1H), 3.46 – 3.42 (m, 2H), 3.29 (dd, *J* = 16.9, 6.8 Hz, 1H), 3.19 (dd, *J* = 14.6, 4.7 Hz, 1H), 2.39 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 161.1, 156.9, 146.4 (q, *J* = 4.0 Hz), 141.1, 133.8 (q, *J* = 3.3 Hz), 129.6, 126.8, 125.6, 123.5 (q, *J* = 272.4 Hz), 123.1, 74.7, 57.6, 53.1, 40.6, 29.8, 21.5; HRMS calcd for $C_{19}H_{19}F_3N_2NaO_3S^+$ ($M+Na^+$): 435.0961, found: 435.0970.



1-Phenyl-3-(((3-(*p*-tolyl)-4,5-dihydroisoxazol-5-yl)methyl)sulfonyl)propan-1-one (**3l**)

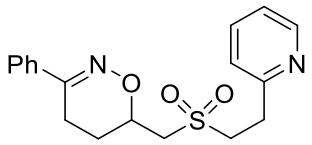
^{1}H NMR (400 MHz, DMSO) δ (ppm) 8.03 (dd, *J* = 8.3, 1.1 Hz, 2H), 7.70 – 7.65 (m, 1H), 7.58 – 7.53 (m, 4H), 7.28 (d, *J* = 8.0 Hz, 2H), 5.18 – 5.10 (m, 1H), 3.86 (dd, *J* = 14.7, 7.6 Hz, 1H), 3.68 (dd, *J* = 17.1, 10.6 Hz, 1H), 3.61 – 3.54 (m, 4H), 3.37 – 3.28 (m, 1H), 2.51 (dt, *J* = 3.5, 1.7 Hz, 1H), 2.35 (s, 3H); ^{13}C NMR (101 MHz, DMSO) δ (ppm) 196.7, 157.4, 140.6, 136.4, 134.0, 129.8, 129.2, 128.5, 127.1, 126.6, 75.2, 56.6, 48.0 (dt, *J* = 42.4, 21.1 Hz), 31.4, 21.4; HRMS calcd for $C_{20}H_{21}NNaO_4S^+$ ($M+Na^+$): 394.1083, found: 394.1089.



3-(naphthalen-2-yl)-5-(((2-(pyridin-2-yl)ethyl)sulfonyl)methyl)-4,5-dihydroisoxazole (**3m**)

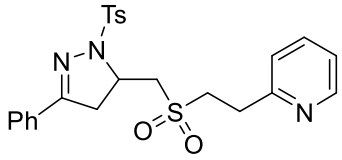
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.53 (d, *J* = 4.1 Hz, 1H), 7.94 – 7.89 (m, 2H), 7.86 – 7.83 (m, 3H), 7.63 (td, *J* = 7.7, 1.8 Hz, 1H), 7.56 – 7.50 (m, 2H), 7.25 (d, *J* = 7.8 Hz, 1H), 7.16 (dd, *J* = 7.1, 5.3 Hz, 1H), 5.31 (dq, *J* = 10.5, 6.4 Hz, 1H), 3.77 – 3.68 (m, 3H), 3.53 (dd, *J* = 14.4, 6.7 Hz, 1H), 3.45 (dd, *J* = 16.9, 7.0 Hz, 1H), 3.37 (t, *J* = 7.8 Hz, 2H), 3.19 (dd, *J* = 14.4, 6.0 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 157.1, 157.0, 149.5,

136.8, 134.2, 132.9, 128.7, 128.4, 127.8, 127.4, 126.8, 126.1, 123.3, 123.3, 122.1, 74.9, 57.3, 53.7, 40.4, 29.9; HRMS calcd for $C_{21}H_{20}N_2NaO_3S^+$ ($M+Na^+$): 403.1087, found: 403.1095.



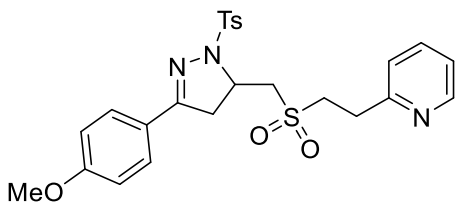
3-Phenyl-6-(((2-(pyridin-2-yl)ethyl)sulfonyl)methyl)-5,6-dihydro-4*H*-1,2-oxazine (**3n**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.54 (d, *J* = 4.1 Hz, 1H), 7.81 (d, *J* = 7.1 Hz, 2H), 7.62 (td, *J* = 7.7, 1.8 Hz, 1H), 7.46 – 7.42 (m, 1H), 7.39 – 7.35 (m, 2H), 7.22 (d, *J* = 7.8 Hz, 1H), 7.17 (dd, *J* = 7.1, 5.3 Hz, 1H), 4.76 – 4.67 (m, 1H), 3.98 – 3.90 (m, 1H), 3.85 – 3.77 (m, 1H), 3.47 – 3.34 (m, 3H), 3.18 – 3.06 (m, 2H), 2.99 – 2.89 (m, 1H), 2.51 – 2.40 (m, 1H), 1.85 – 1.75 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 174.2, 157.7, 149.5, 136.6, 133.7, 130.9, 128.5, 127.9, 123.3, 121.9, 67.4, 58.8, 53.5, 35.1, 30.4, 29.1; HRMS calcd for $C_{18}H_{20}N_2NaO_3S^+$ ($M+Na^+$): 367.1087, found: 367.1094.



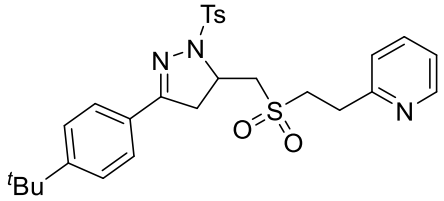
2-(2-(((3-Phenyl-1-tosyl-4,5-dihydro-1*H*-pyrazol-5-yl)methyl)sulfonyl)ethyl)pyridine (**5a**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.56 (s, 1H), 7.80 (d, *J* = 7.5 Hz, 2H), 7.64 (d, *J* = 6.9 Hz, 3H), 7.42 – 7.18 (m, 7H), 4.18 (d, *J* = 11.9 Hz, 2H), 3.73 – 3.63 (m, 2H), 3.41 (t, *J* = 9.8 Hz, 4H), 3.29 – 3.22 (m, 1H), 2.37 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) (ppm) 158.3, 156.6, 149.4, 144.8, 136.7, 130.8, 130.4, 123.0, 129.6, 128.8, 128.5, 126.8, 123.3, 122.0, 57.4, 56.0, 53.3, 39.8, 29.9, 21.5; HRMS calcd for $C_{24}H_{25}N_3NaO_4S_2^+$ ($M+Na^+$): 506.1179, found: 506.1188.



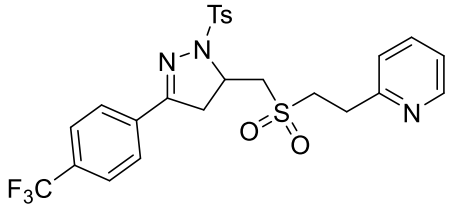
2-(2-(((3-(4-Methoxyphenyl)-1-tosyl-4,5-dihydro-1*H*-pyrazol-5-yl)methyl)sulfonyl)ethyl)pyridine (**5b**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.57 (d, *J* = 4.1 Hz, 1H), 7.80 (d, *J* = 8.3 Hz, 2H), 7.66 (td, *J* = 7.7, 1.8 Hz, 1H), 7.61 – 7.58 (m, 2H), 7.29 (d, *J* = 8.2 Hz, 3H), 7.20 (dd, *J* = 7.1, 5.2 Hz, 1H), 6.87 (d, *J* = 8.9 Hz, 2H), 4.20 – 4.10 (m, 2H), 3.82 (s, 3H), 3.68 (dd, *J* = 9.0, 6.6 Hz, 2H), 3.43 – 3.33 (m, 4H), 3.21 (dd, *J* = 17.6, 10.2 Hz, 1H), 2.38 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 161.7, 158.1, 156.7, 149.5, 144.8, 136.8, 130.4, 129.7, 128.9, 128.6, 123.4, 122.6, 122.1, 114.0, 57.6, 55.9, 55.3, 53.4, 40.0, 30.0, 21.6; HRMS calcd for $C_{25}H_{27}N_3NaO_5S_2^+$ ($M+Na^+$): 536.1284, found: 536.1293.



2-(2-(((3-(4-(*tert*-Butyl)phenyl)-1-tosyl-4,5-dihydro-1*H*-pyrazol-5-yl)methyl)sulfonyl)ethyl)pyridine (**5c**)

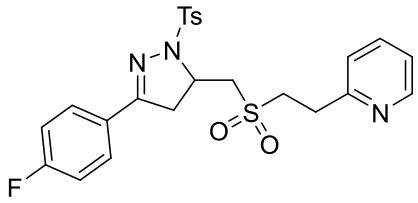
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.58 (d, *J* = 4.4 Hz, 1H), 7.80 (d, *J* = 8.3 Hz, 2H), 7.67 (td, *J* = 7.7, 1.8 Hz, 1H), 7.60 (d, *J* = 8.5 Hz, 2H), 7.40 (d, *J* = 8.5 Hz, 2H), 7.29 (d, *J* = 8.3 Hz, 3H), 7.21 (dd, *J* = 7.2, 5.1 Hz, 1H), 4.20 – 4.11 (m, 2H), 3.70 (d, *J* = 7.3 Hz, 1H), 3.67 (d, *J* = 5.8 Hz, 1H), 3.45 – 3.31 (m, 4H), 3.23 (dd, *J* = 17.7, 10.2 Hz, 1H), 2.39 (s, 3H), 1.32 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 158.3, 156.7, 154.5, 149.6, 144.9, 136.9, 130.5, 129.8, 128.9, 127.3, 126.9, 125.7, 123.4, 122.2, 57.8, 56.0, 53.5, 40.0, 34.9, 31.1, 30.1, 21.6; HRMS calcd for $C_{28}H_{33}N_3NaO_4S_2^+$ ($M+Na^+$): 540.1985, found: 540.1995.



2-(2-(((1-tosyl-3-(4-(Trifluoromethyl)phenyl)-4,5-dihydro-1*H*-pyrazol-5-yl)methyl)sulfonyl)ethyl)pyridine (**5d**)

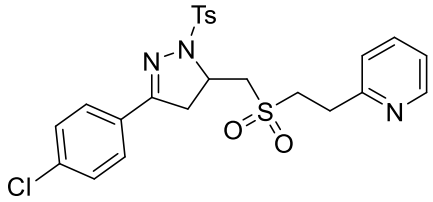
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.57 (d, *J* = 4.1 Hz, 1H), 7.78 (dd, *J* = 13.5, 8.2 Hz, 4H), 7.70 – 7.61 (m, 3H), 7.30 (dd, *J* = 11.9, 9.0 Hz, 3H), 7.21 (dd, *J* = 7.0, 5.2 Hz, 1H), 4.30 – 4.16 (m, 2H), 3.70 (dd, *J* = 8.8, 6.7 Hz, 2H), 3.50 – 3.36 (m, 4H), 3.28 (dd, *J* =

17.6, 10.3 Hz, 1H), 2.40 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 156.8 (d, *J* = 35.1 Hz), 149.5, 145.2, 136.9, 133.4, 132.4 (q, *J* = 32.8 Hz), 130.5, 129.9, 128.8, 127.2, 125.6 (q, *J* = 3.7 Hz), 123.6 (q, *J* = 271.0 Hz), 123.4, 122.2, 57.5, 56.4, 53.5, 39.7, 30.0, 21.6; HRMS calcd for $C_{25}H_{24}F_3N_3NaO_4S_2^+$ (M+Na$^+$): 552.1233, found: 552.1248.



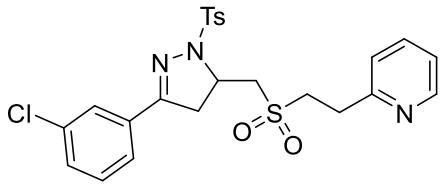
2-(2-(((3-(4-Fluorophenyl)-1-tosyl-4,5-dihydro-1*H*-pyrazol-5-yl)methyl)sulfonyl)ethyl) pyridine (**5e**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.57 (d, *J* = 4.0 Hz, 1H), 7.80 (d, *J* = 8.2 Hz, 2H), 7.69 – 7.63 (m, 3H), 7.32 – 7.27 (m, 3H), 7.22 – 7.18 (m, 1H), 7.06 (t, *J* = 8.6 Hz, 2H), 4.25 – 4.14 (m, 2H), 3.71 – 3.66 (m, 2H), 3.45 – 3.35 (m, 4H), 3.25 (dd, *J* = 17.7, 10.1 Hz, 1H), 2.39 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 164.31 (d, *J* = 252.3 Hz), 157.4, 156.7, 149.6, 145.0, 136.9, 130.5, 129.8, 129.1 (d, *J* = 8.7 Hz), 128.9, 126.45 (d, *J* = 3.4 Hz), 123.5, 122.3, 115.9 (d, *J* = 22.1 Hz), 57.6, 56.2, 53.5, 40.0, 30.1, 21.7; HRMS calcd for $C_{24}H_{24}FN_3NaO_4S_2^+$ (M+Na$^+$): 524.1084, found: 524.1096.



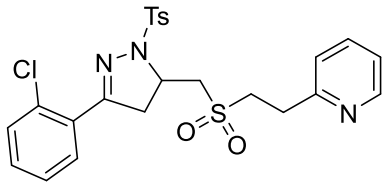
2-(2-(((3-(4-Chlorophenyl)-1-tosyl-4,5-dihydro-1*H*-pyrazol-5-yl)methyl)sulfonyl)ethyl) pyridine (**5f**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.57 (d, *J* = 4.4 Hz, 1H), 7.79 (d, *J* = 8.2 Hz, 2H), 7.67 (td, *J* = 7.7, 1.5 Hz, 1H), 7.58 (d, *J* = 8.5 Hz, 2H), 7.35 – 7.27 (m, 5H), 7.20 (dd, *J* = 7.0, 5.3 Hz, 1H), 4.25 – 4.15 (m, 2H), 3.71 – 3.66 (m, 2H), 3.44 – 3.36 (m, 4H), 3.24 (dd, *J* = 17.7, 10.1 Hz, 1H), 2.39 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 157.3, 156.6, 149.5, 145.0, 137.0, 136.9, 130.4, 129.8, 128.9, 128.8, 128.5, 128.2, 123.4, 122.2, 57.5, 56.2, 53.4, 39.8, 30.0, 21.6; HRMS calcd for $C_{24}H_{24}ClN_3NaO_4S_2^+$ (M+Na$^+$): 540.0789, found: 540.0798.



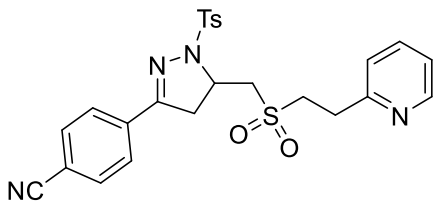
2-(2-(((3-(3-Chlorophenyl)-1-tosyl-4,5-dihydro-1*H*-pyrazol-5-yl)methyl)sulfonyl)ethyl) pyridine (**5g**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.57 (d, *J* = 4.6 Hz, 1H), 7.80 (d, *J* = 8.2 Hz, 2H), 7.69 – 7.65 (m, 2H), 7.50 (d, *J* = 7.6 Hz, 1H), 7.39 – 7.36 (m, 1H), 7.33 – 7.28 (m, 4H), 7.21 (dd, *J* = 7.2, 5.1 Hz, 1H), 4.26 – 4.15 (m, 2H), 3.69 (dd, *J* = 8.9, 6.6 Hz, 2H), 3.45 – 3.35 (m, 4H), 3.24 (dd, *J* = 17.7, 10.3 Hz, 1H), 2.40 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 157.1, 156.6, 149.5, 145.1, 136.9, 134.8, 131.8, 130.8, 130.4, 129.9, 129.8, 128.8, 126.8, 125.0, 123.4, 122.2, 57.5, 56.2, 53.5, 39.8, 30.0, 21.6; HRMS calcd for $C_{24}H_{24}ClN_3NaO_4S_2^+$ ($M+Na^+$): 540.0789, found: 540.0801.



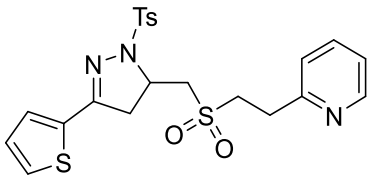
2-(2-(((3-(2-Chlorophenyl)-1-tosyl-4,5-dihydro-1*H*-pyrazol-5-yl)methyl)sulfonyl)ethyl) pyridine (**5h**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.58 (d, *J* = 4.3 Hz, 1H), 7.83 (d, *J* = 8.2 Hz, 2H), 7.67 (td, *J* = 7.7, 1.7 Hz, 1H), 7.52 (dd, *J* = 7.6, 1.4 Hz, 1H), 7.38 – 7.32 (m, 4H), 7.31 – 7.25 (m, 1H), 7.21 (dd, *J* = 7.1, 5.2 Hz, 1H), 4.25 – 4.15 (m, 2H), 3.68 (dd, *J* = 8.9, 6.7 Hz, 2H), 3.55 (dd, *J* = 18.0, 10.3 Hz, 1H), 3.46 – 3.36 (m, 4H), 2.43 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 158.6, 156.7, 149.6, 145.1, 136.9, 132.9, 131.3, 130.6, 130.5, 129.8, 129.6, 129.1, 126.9, 123.4, 122.2, 57.6, 56.6, 53.5, 42.9, 30.1, 21.7; HRMS calcd for $C_{24}H_{24}ClN_3NaO_4S_2^+$ ($M+Na^+$): 540.0789, found: 540.0796.



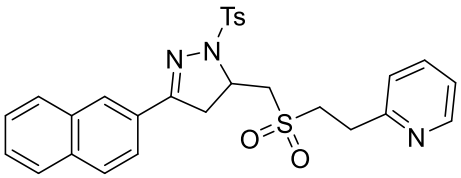
4-(5-(((2-(Pyridin-2-yl)ethyl)sulfonyl)methyl)-1-tosyl-4,5-dihydro-1*H*-pyrazol-3-yl)ben zonitrile (**5i**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.58 (d, *J* = 4.1 Hz, 1H), 7.79 (d, *J* = 8.3 Hz, 2H), 7.75 (d, *J* = 8.5 Hz, 2H), 7.70 – 7.65 (m, 3H), 7.34 – 7.27 (m, 3H), 7.22 (dd, *J* = 7.0, 5.2 Hz, 1H), 4.32 – 4.15 (m, 2H), 3.72 – 3.67 (m, 2H), 3.49 – 3.55 (m, 4H), 3.28 (dd, *J* = 17.7, 10.4 Hz, 1H), 2.41 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 156.5, 156.4, 149.6, 145.3, 136.9, 134.2, 132.4, 130.5, 129.9, 128.8, 127.3, 123.4, 122.3, 118.1, 114.1, 57.4, 56.5, 53.5, 39.5, 30.0, 21.6; HRMS calcd for $C_{25}H_{24}N_4NaO_4S_2^+$ ($M+Na^+$): 531.1131, found: 531.1142.



2-(2-(((3-(Thiophen-2-yl)-1-tosyl-4,5-dihydro-1*H*-pyrazol-5-yl)methyl)sulfonyl)ethyl)pyridine (**5j**)

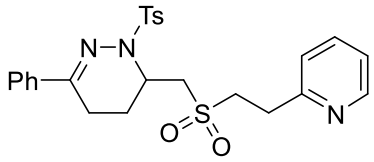
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.58 (d, *J* = 4.5 Hz, 1H), 7.79 (d, *J* = 8.2 Hz, 2H), 7.67 (td, *J* = 7.7, 1.6 Hz, 1H), 7.43 (d, *J* = 4.8 Hz, 1H), 7.32 – 7.26 (m, 3H), 7.21 (dd, *J* = 7.2, 5.1 Hz, 1H), 7.18 (d, *J* = 3.2 Hz, 1H), 7.02 (dd, *J* = 4.8, 3.9 Hz, 1H), 4.21 – 4.13 (m, 2H), 3.69 (d, *J* = 7.3 Hz, 1H), 3.67 (d, *J* = 6.1 Hz, 1H), 3.44 – 3.33 (m, 4H), 3.27 (dd, *J* = 17.5, 10.3 Hz, 1H), 2.40 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 156.6, 153.9, 149.5, 144.9, 136.9, 133.5, 130.3, 129.8, 129.7, 129.0, 127.6, 123.4, 122.2, 57.5, 56.2, 53.5, 40.6, 30.1, 21.6; HRMS calcd for $C_{22}H_{23}N_3NaO_4S_3^+$ ($M+Na^+$): 512.0743, found: 512.0753.



2-(2-(((3-(Naphthalen-2-yl)-1-tosyl-4,5-dihydro-1*H*-pyrazol-5-yl)methyl)sulfonyl)ethyl)pyridine (**5k**)

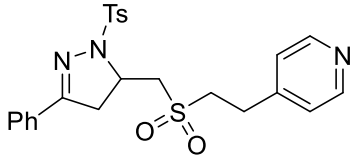
^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.06 (s, 1H), 7.78 (d, *J* = 8.1 Hz, 2H), 7.60 (d, *J* = 7.1 Hz, 2H), 7.55 (d, *J* = 7.9 Hz, 2H), 7.41 – 7.27 (m, 6H), 7.09 (t, *J* = 7.3 Hz, 1H), 4.25 – 4.13 (m, 2H), 3.61 – 3.51 (m, 3H), 3.40 – 3.26 (m, 2H), 3.01 (t, *J* = 7.4 Hz, 2H), 2.36 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 167.0, 158.8, 145.1, 137.6, 131.0, 130.3,

129.9, 129.9, 129.0, 128.8, 128.7, 127.0, 124.6, 120.0, 57.6, 56.0, 50.3, 39.9, 29.8, 21.6; HRMS calcd for $C_{28}H_{27}N_3NaO_4S_2^+$(M+$Na^+$): 556.1335, found: 556.1342.



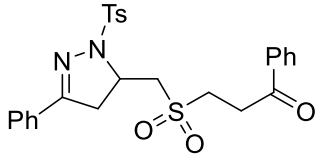
3-Phenyl-6-(((2-(pyridin-2-yl)ethyl)sulfonyl)methyl)-1-tosyl-1,4,5,6-tetrahydropyridazine (**5l**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.54 (d, *J* = 3.5 Hz, 1H), 7.87 (d, *J* = 8.2 Hz, 2H), 7.70 – 7.67 (m, 2H), 7.63 (t, *J* = 7.6 Hz, 1H), 7.39 – 7.27 (m, 6H), 7.19 – 7.14 (m, 1H), 4.97 (s, 1H), 3.68 – 3.64 (m, 2H), 3.46 (dd, *J* = 14.0, 2.0 Hz, 1H), 3.39 – 3.34 (m, 2H), 3.15 (dd, *J* = 14.0, 10.9 Hz, 1H), 2.72 – 2.43 (m, 3H), 2.41 (s, 3H), 1.77 – 1.67 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 156.8, 149.5, 148.5, 144.4, 136.9, 136.3, 135.0, 129.7, 129.6, 128.4, 128.0, 125.3, 123.5, 122.1, 53.7, 53.5, 46.5, 30.0, 21.6, 21.0, 17.9; HRMS calcd for $C_{25}H_{27}N_3NaO_4S_2^+$ (M+Na^+): 520.1335, found: 520.1346.



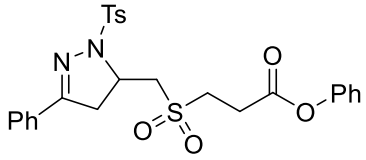
5-(*p*-Tolyl)-2-(((4-(trifluoromethyl)benzyl)sulfonyl)methyl)-3,4-dihydro-2*H*-pyrrole (**5m**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.59 (s, 2H), 7.78 (d, *J* = 8.2 Hz, 2H), 7.64 (d, *J* = 6.9 Hz, 2H), 7.44 – 7.34 (m, 3H), 7.30 (d, *J* = 8.1 Hz, 2H), 7.26 (d, *J* = 3.3 Hz, 2H), 4.22 (qd, *J* = 10.3, 2.2 Hz, 1H), 4.09 (dd, *J* = 14.0, 2.3 Hz, 1H), 3.57 (dd, *J* = 14.0, 9.7 Hz, 1H), 3.50 – 3.44 (m, 2H), 3.38 (dd, *J* = 10.5, 4.6 Hz, 2H), 3.27 – 3.20 (m, 2H), 2.39 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 158.7, 150.2, 146.3, 145.1, 131.0, 130.4, 129.9, 129.8, 128.8, 128.7, 127.0, 123.8, 57.2, 56.0, 54.8, 39.7, 27.4, 21.6; HRMS calcd for $C_{24}H_{25}N_3NaO_4S_2^+$ (M+Na^+): 506.1179, found: 506.1185.



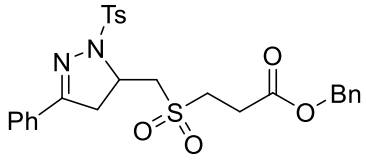
1-Phenyl-3-(((3-phenyl-1-tosyl-4,5-dihydro-1*H*-pyrazol-5-yl)methyl)sulfonyl)propan-1-one (**5n**)

^{1}H NMR (400 MHz, DMSO) δ (ppm) 8.05 (d, *J* = 7.5 Hz, 2H), 7.75 (d, *J* = 8.1 Hz, 2H), 7.70 – 7.65 (m, 3H), 7.57 (t, *J* = 7.6 Hz, 2H), 7.49 – 7.42 (m, 5H), 4.22 (q, *J* = 9.2 Hz, 1H), 4.05 – 3.92 (m, 1H), 3.69 – 3.58 (m, 4H), 3.51 (dd, *J* = 17.6, 11.0 Hz, 1H), 3.39 – 3.30 (m, 1H), 2.36 (s, 3H); ^{13}C NMR (101 MHz, DMSO) δ (ppm) 196.5, 159.9, 145.3, 136.4, 134.1, 131.4, 131.2, 130.6, 130.4, 129.3, 129.3, 128.9, 128.6, 127.4, 57.2, 56.5, 49.0, 39.9, 31.6, 21.6; HRMS calcd for $C_{26}H_{26}N_2NaO_5S_2^+$ (M+Na$^+$): 533.1175, found: 533.1186.



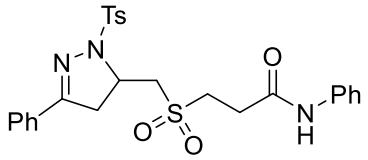
Phenyl 3-(((3-phenyl-1-tosyl-4,5-dihydro-1*H*-pyrazol-5-yl)methyl)sulfonyl)propanoate (**5o**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.80 (d, *J* = 8.2 Hz, 2H), 7.65 (d, *J* = 6.9 Hz, 2H), 7.44 – 7.35 (m, 5H), 7.30 – 7.25 (m, 3H), 7.14 (d, *J* = 7.7 Hz, 2H), 4.26 – 4.16 (m, 2H), 3.64 – 3.50 (m, 3H), 3.42 (dd, *J* = 17.6, 10.5 Hz, 1H), 3.34 – 3.26 (m, 1H), 3.21 (t, *J* = 7.3 Hz, 2H), 2.38 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 168.8, 158.4, 150.3, 145.0, 131.0, 130.5, 130.0, 129.8, 129.5, 128.9, 128.7, 127.0, 126.2, 121.3, 57.86, 56.0, 49.9, 39.9, 27.2, 21.6; HRMS calcd for $C_{26}H_{26}N_2NaO_6S_2^+$ (M+Na$^+$): 549.1124, found: 549.1132.



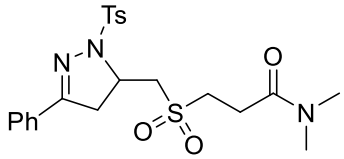
Benzyl 3-(((3-phenyl-1-tosyl-4,5-dihydro-1H-pyrazol-5-yl)methyl)sulfonyl)propanoate (**5p**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.79 (d, *J* = 8.3 Hz, 2H), 7.64 (d, *J* = 6.7 Hz, 2H), 7.43 – 7.32 (m, 8H), 7.28 (d, *J* = 8.1 Hz, 2H), 5.19 (s, 2H), 4.21 – 4.12 (m, 2H), 3.52 – 3.35 (m, 4H), 3.23 (dd, *J* = 17.7, 10.0 Hz, 1H), 2.99 (t, *J* = 7.4 Hz, 2H), 2.38 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 169.9, 158.4, 144.9, 135.1, 130.9, 130.5, 130.0, 129.8, 128.84, 128.6, 128.6, 128.5, 128.4, 127.0, 67.3, 57.8, 56.0, 49.9, 39.9, 27.1, 21.6; HRMS calcd for $C_{27}H_{28}N_2NaO_6S_2^+$ (M+Na$^+$): 563.1281, found: 563.1287.



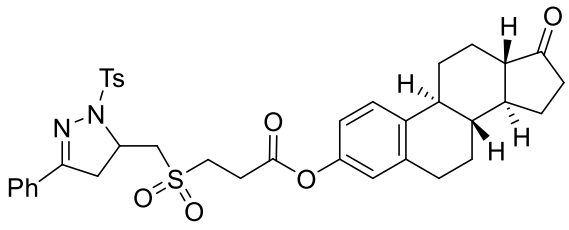
N-Phenyl-3-(((3-phenyl-1-tosyl-4,5-dihydro-1*H*-pyrazol-5-yl)methyl)sulfonyl)propanamide (**5q**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.58 (d, *J* = 4.1 Hz, 1H), 7.96 (dd, *J* = 8.7, 1.5 Hz, 1H), 7.88 – 7.78 (m, 6H), 7.67 (td, *J* = 7.7, 1.7 Hz, 1H), 7.54 – 7.46 (m, 2H), 7.29 (d, *J* = 8.1 Hz, 3H), 7.21 (dd, *J* = 7.0, 5.2 Hz, 1H), 4.28 – 4.19 (m, 2H), 3.72 (d, *J* = 7.2 Hz, 1H), 3.70 (d, *J* = 6.0 Hz, 1H), 3.56 (dd, *J* = 17.5, 10.7 Hz, 1H), 3.45 – 3.33 (m, 4H), 2.36 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 158.4, 156.7, 149.5, 144.9, 136.9, 134.3, 132.7, 130.5, 129.8, 128.9, 128.5, 128.5, 127.9, 127.7, 127.6, 127.6, 126.8, 123.4, 123.3, 122.2, 57.7, 56.2, 53.5, 39.9, 30.1, 21.6; HRMS calcd for $C_{26}H_{27}N_3NaO_5S_2^+$ ($M+Na^+$): 548.1284, found: 548.1296.



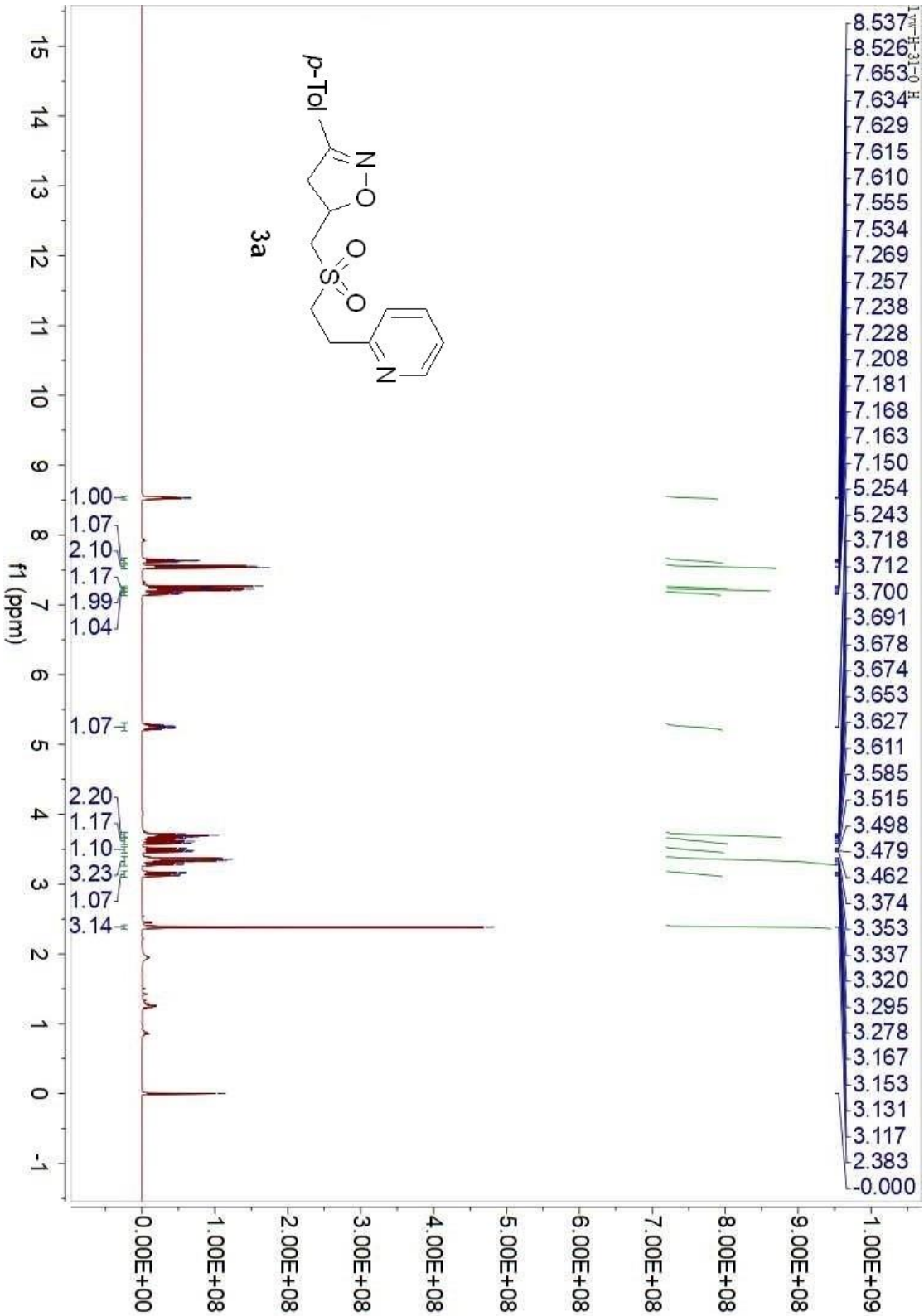
N,N-Dimethyl-3-(((3-phenyl-1-tosyl-4,5-dihydro-1*H*-pyrazol-5-yl)methyl)sulfonyl)propanamide (**5r**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.81 (d, *J* = 8.1 Hz, 2H), 7.66 (d, *J* = 6.9 Hz, 2H), 7.44 – 7.36 (m, 3H), 7.31 (d, *J* = 8.0 Hz, 2H), 4.24 – 4.15 (m, 2H), 3.54 (t, *J* = 7.4 Hz, 2H), 3.49 – 3.39 (m, 2H), 3.26 (dd, *J* = 17.7, 10.1 Hz, 1H), 3.08 (s, 3H), 3.01 (s, 3H), 2.94 (t, *J* = 7.4 Hz, 2H), 2.39 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 168.5, 158.3, 144.9, 130.9, 130.6, 130.1, 129.8, 128.9, 128.7, 127.0, 58.0, 56.1, 50.4, 40.0, 37.1, 35.8, 26.0, 21.6; HRMS calcd for $C_{22}H_{27}N_3NaO_5S_2^+$ ($M+Na^+$): 500.1284, found: 500.1299.



(8*S*,9*S*,13*S*,14*S*)-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[*a*]phenanthren-3-yl 3-(((3-phenyl-1-tosyl-4,5-dihydro-1*H*-pyrazol-5-yl)methyl)sulfonyl)propanoate (**5s**)

^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.81 (d, *J* = 8.3 Hz, 2H), 7.66 (dd, *J* = 8.1, 1.4 Hz, 2H), 7.44 – 7.35 (m, 3H), 7.30 (d, *J* = 8.3 Hz, 3H), 6.92 – 6.87 (m, 2H), 4.26 – 4.16 (m, 2H), 3.62 – 3.39 (m, 4H), 3.29 (dd, *J* = 17.7, 9.9 Hz, 1H), 3.19 (t, *J* = 7.3 Hz, 2H), 2.92 (dd, *J* = 8.5, 3.8 Hz, 2H), 2.55 – 2.40 (m, 2H), 2.39 (s, 3H), 2.32 – 2.25 (m, 1H), 2.19 – 1.94 (m, 4H), 1.63 – 1.42 (m, 6H), 0.88 – 0.83 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ (ppm) 169.1, 158.4, 148.2, 145.0, 138.2, 137.8, 131.0, 130.5, 130.0, 129.8, 128.9, 128.7, 127.0, 126.5, 121.3, 118.5, 57.9, 56.0, 50.4, 50.0, 47.9, 44.1, 39.9, 37.9, 35.8, 31.5, 29.3, 27.3, 26.3, 25.7, 21.5, 13.8; HRMS calcd for $C_{37}H_{40}N_2NaO_7S_2^+$ ($M+Na^+$): 711.2169, found: 711.2175.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O
S
O
N
3a
f1 (ppm)
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2.10
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1.99
1.04
1.07
2.20
1.17
1.10
3.23
1.07
3.14
8.537
8.526
7.653
7.634
7.629
7.615
7.610
7.555
7.534
7.269
7.257
7.238
7.228
7.208
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7.168
7.163
7.150
5.254
5.243
3.718
3.712
3.700
3.691
3.678
3.674
3.653
3.627
3.611
3.585
3.515
3.498
3.479
3.462
3.374
3.353
3.337
3.320
3.295
3.278
3.167
3.153
3.131
3.117
2.383
-0.000
0.00E+00
1.00E+08
2.00E+08
3.00E+08
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5.00E+08
6.00E+08
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8.00E+08
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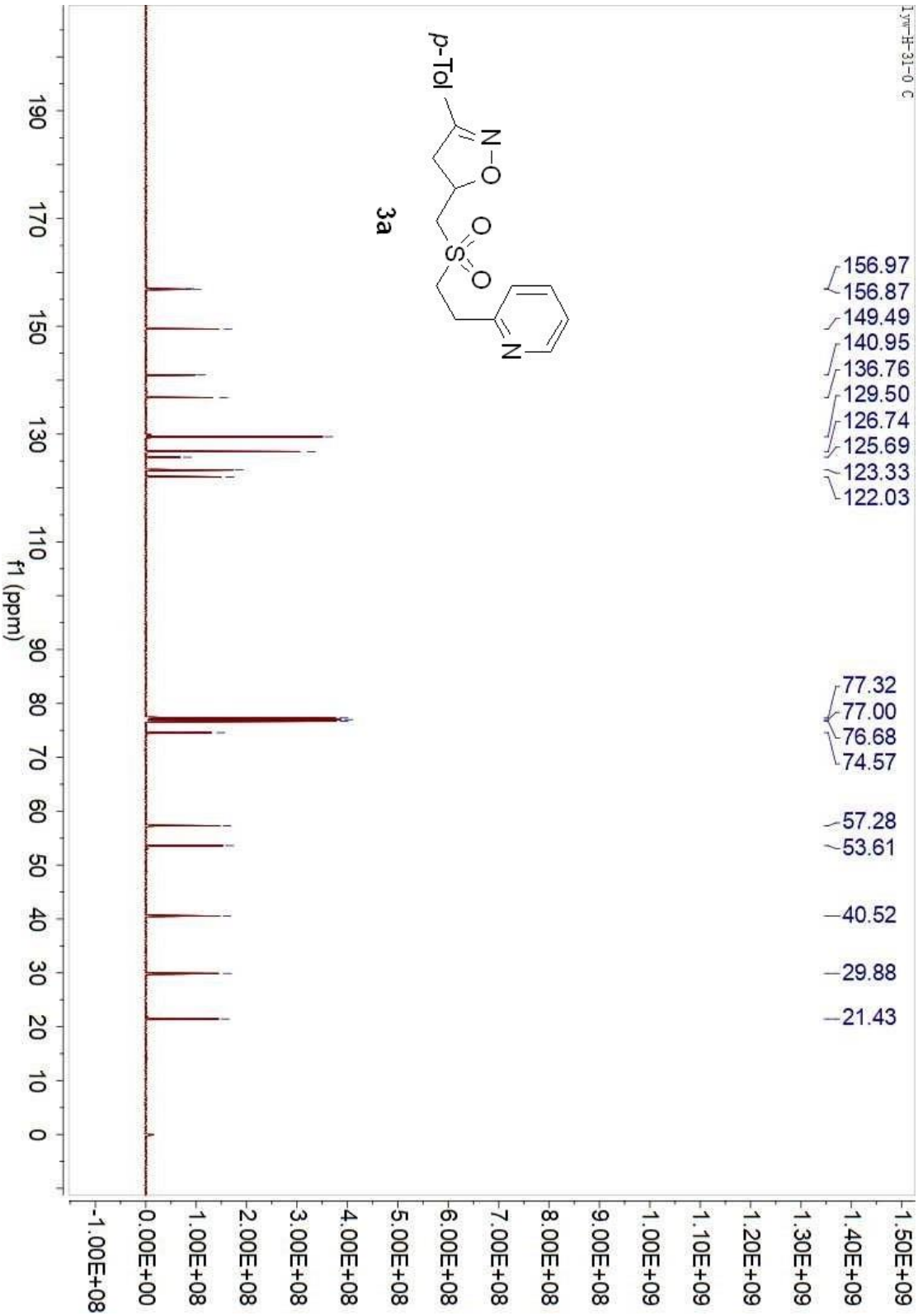
1.00E+09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156.87
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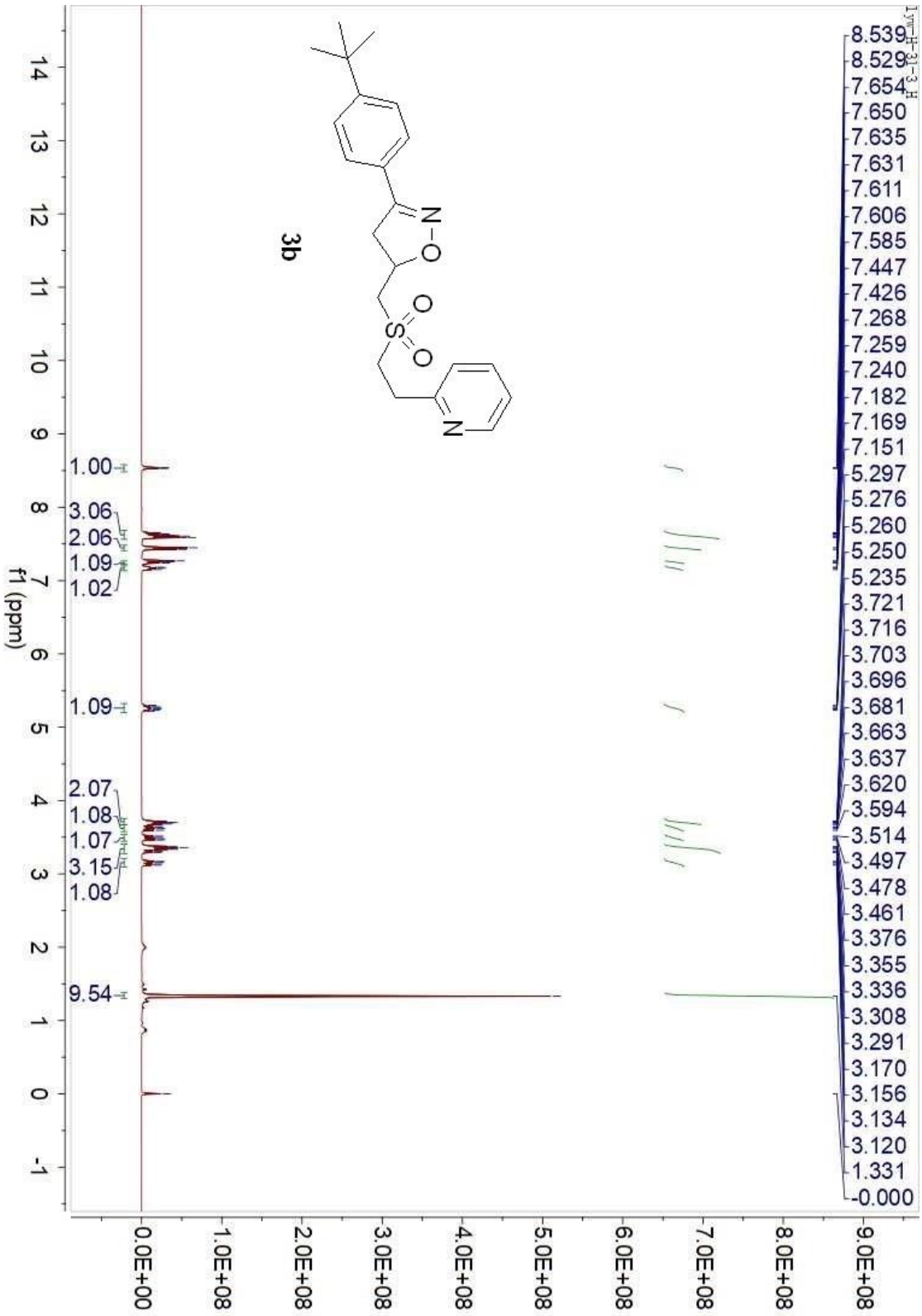
140.95
136.76
129.50
126.74
125.69
123.33
122.03
77.32
77.00
76.68
74.57
57.28
53.61
40.52
29.88
21.43
p-Tol
N
O
O
O
S
O
N
3a
f1 (ppm)


3b
f1 (ppm)
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3.06
2.06
1.09
1.02
1.09
2.07
1.08
1.07
3.15
1.08
9.54
8.539
8.529
7.654
7.650
7.635
7.631
7.611
7.606
7.585
7.447
7.426
7.268
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5.276
5.260
5.250
5.235
3.721
3.716
3.703
3.696
3.681
3.663
3.637
3.620
3.594
3.514
3.497
3.478
3.461
3.376
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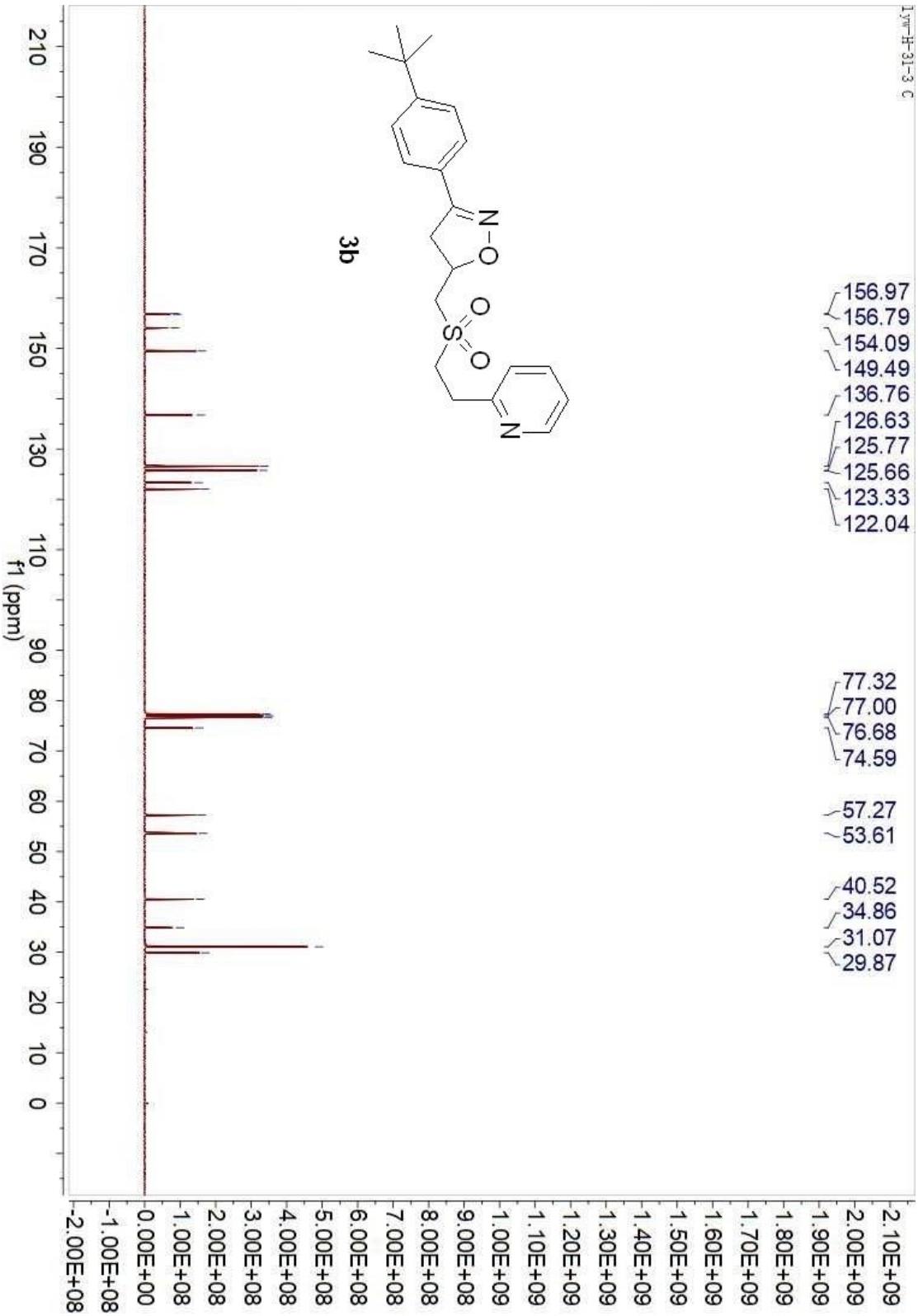
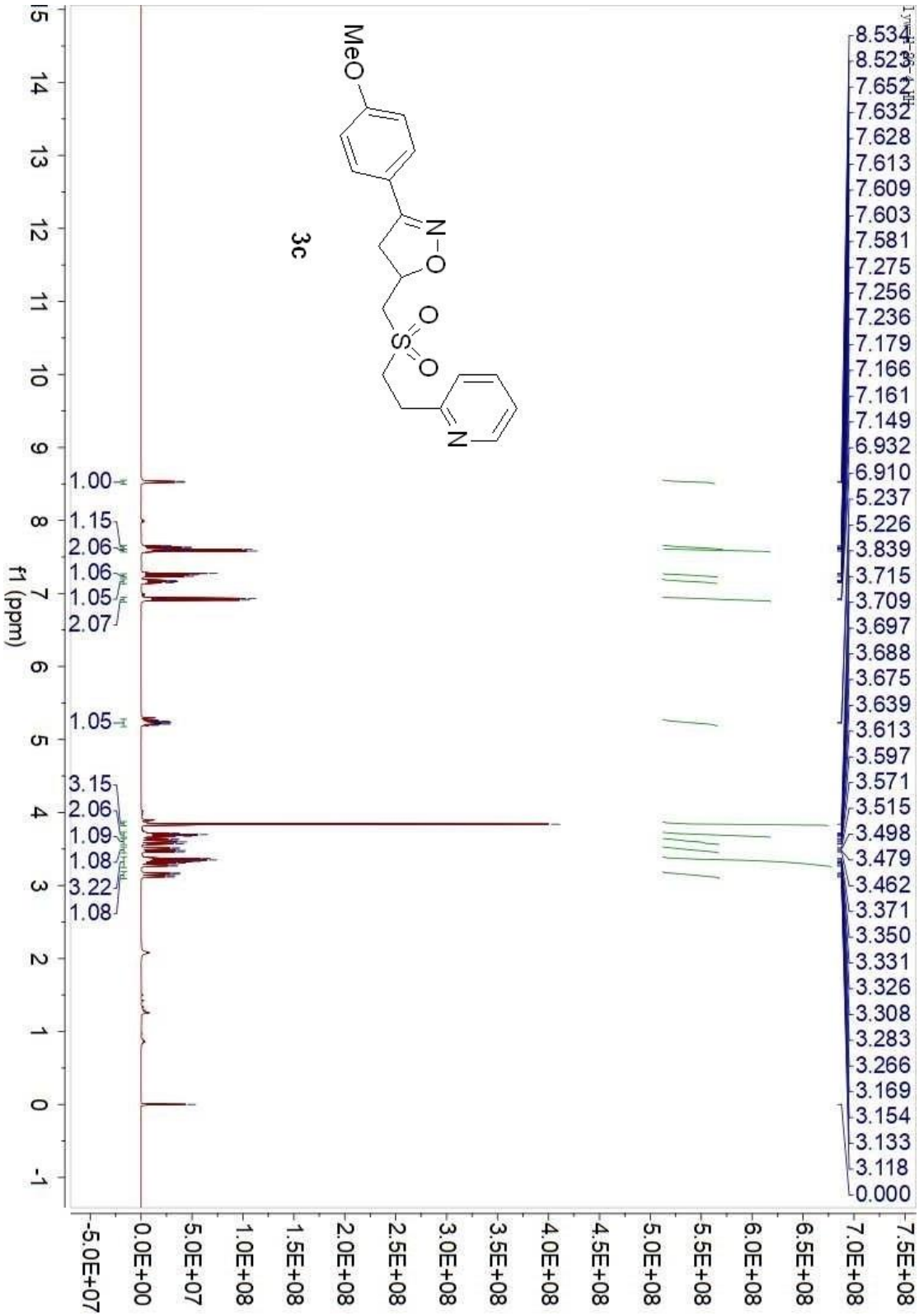
3.170
3.156
3.134
3.120
1.331
-0.000


lyw-H-31-3 C
3b
156.97
156.79
154.09
149.49
136.76
126.63
125.77
125.66
123.33
122.04
77.32
77.00
76.68
74.59
57.27
53.61
40.52
34.86
31.07
29.87
f1 (ppm)


MeO
N
O
O
S
O
N
3c
f1 (ppm)
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1.15
2.06
1.06
1.05
2.07
1.05
3.15
2.06
1.09
1.08
3.22
1.08
8.534
8.525
7.652
7.632
7.628
7.613
7.609
7.603
7.581
7.275
7.256
7.236
7.179
7.166
7.161
7.149
6.932
6.910
5.237
5.226
3.839
3.715
3.709
3.697
3.688
3.675
3.639
3.613
3.597
3.571
3.515
3.498
3.479
3.462
3.371
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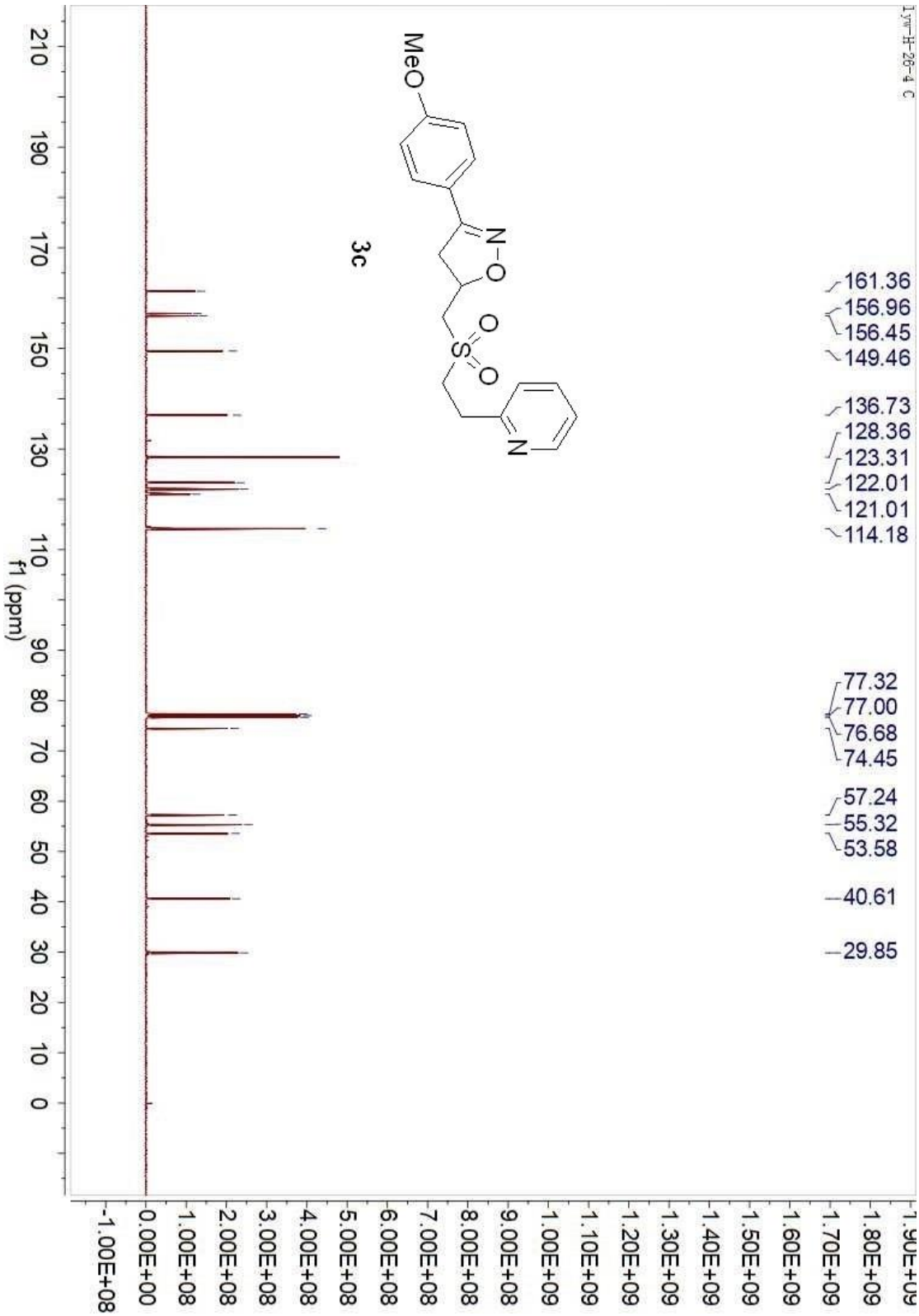
3.326
3.308
3.283
3.266
3.169
3.154
3.133
3.118
0.000


MeO
N
O
S
O
O
N
3c
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156.45
149.46
136.73
128.36
123.31
122.01
121.01
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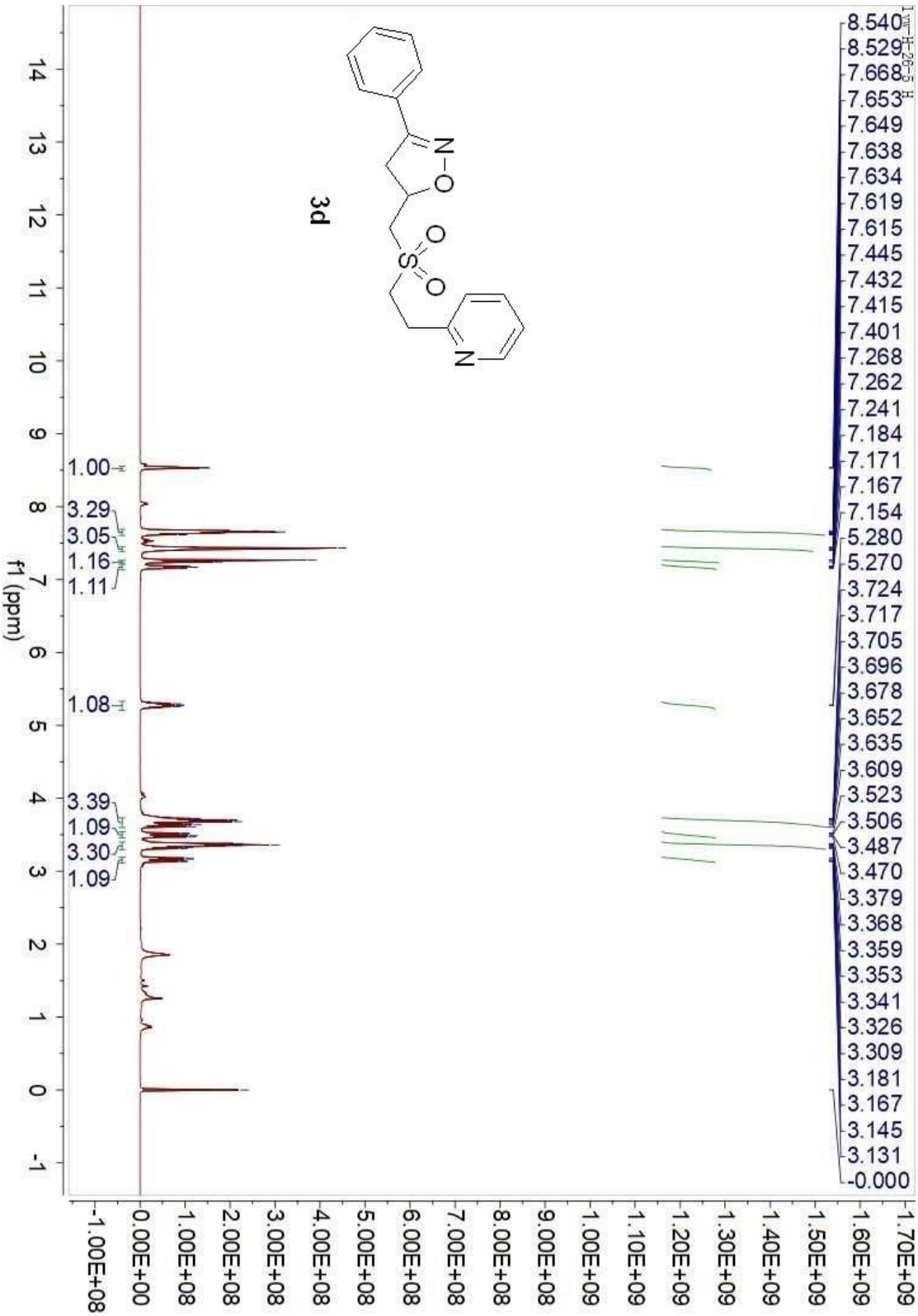
77.00
76.68
74.45
57.24
55.32
53.58
40.61
29.85
f1 (ppm)


3d
f1 (ppm)
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3.29
3.05
1.16
1.11
1.08
3.39
1.09
3.30
1.09
8.540
8.529
7.668
7.653
7.649
7.638
7.634
7.619
7.615
7.445
7.432
7.415
7.401
7.268
7.262
7.241
7.184
7.171
7.167
7.154
5.280
5.270
3.724
3.717
3.705
3.696
3.678
3.652
3.635
3.609
3.523
3.506
3.487
3.470
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3.368
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3.353
3.341
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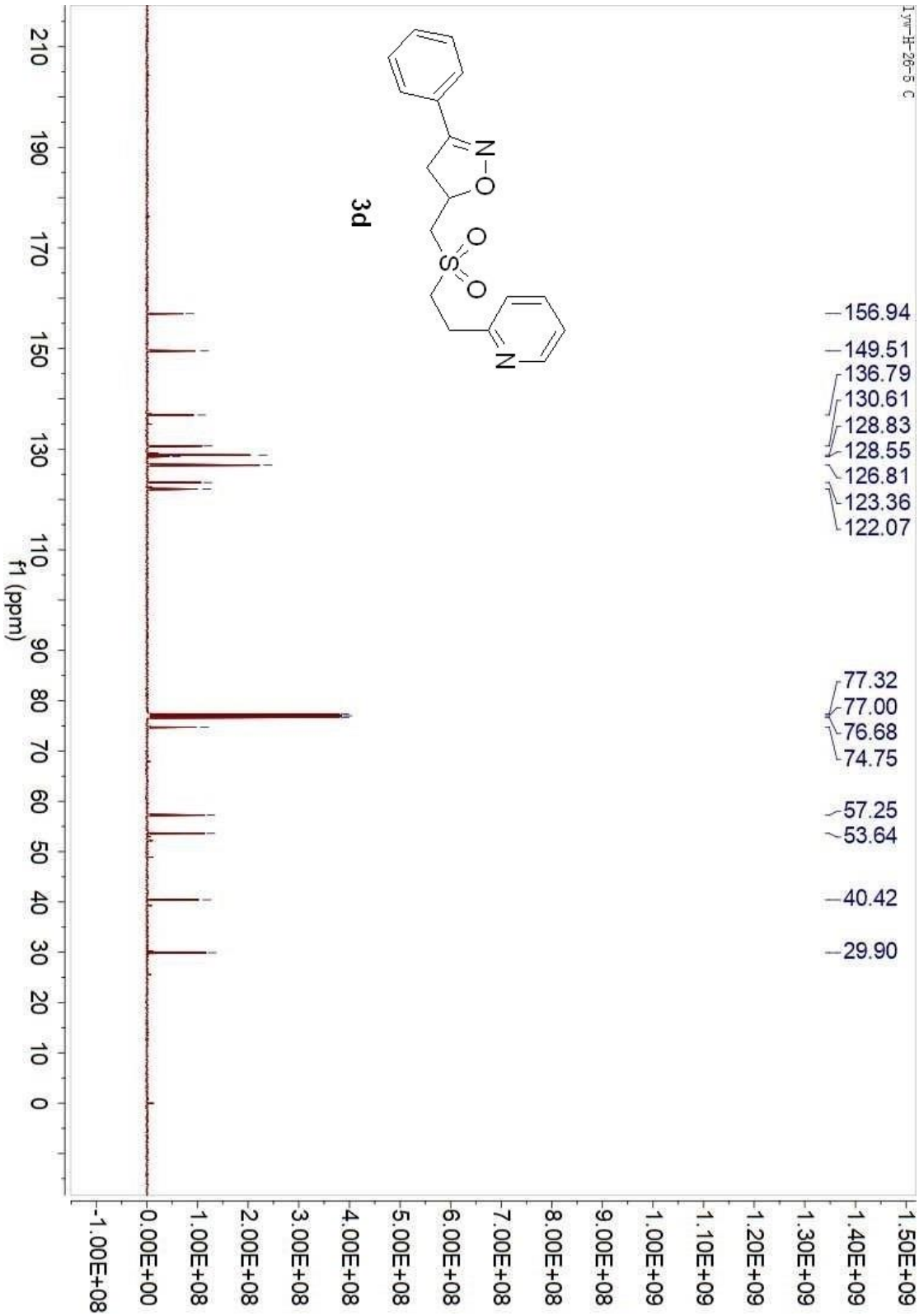
3.131
-0.000


3d
156.94
149.51
136.79
130.61
128.83
128.55
126.81
123.36
122.07
77.32
77.00
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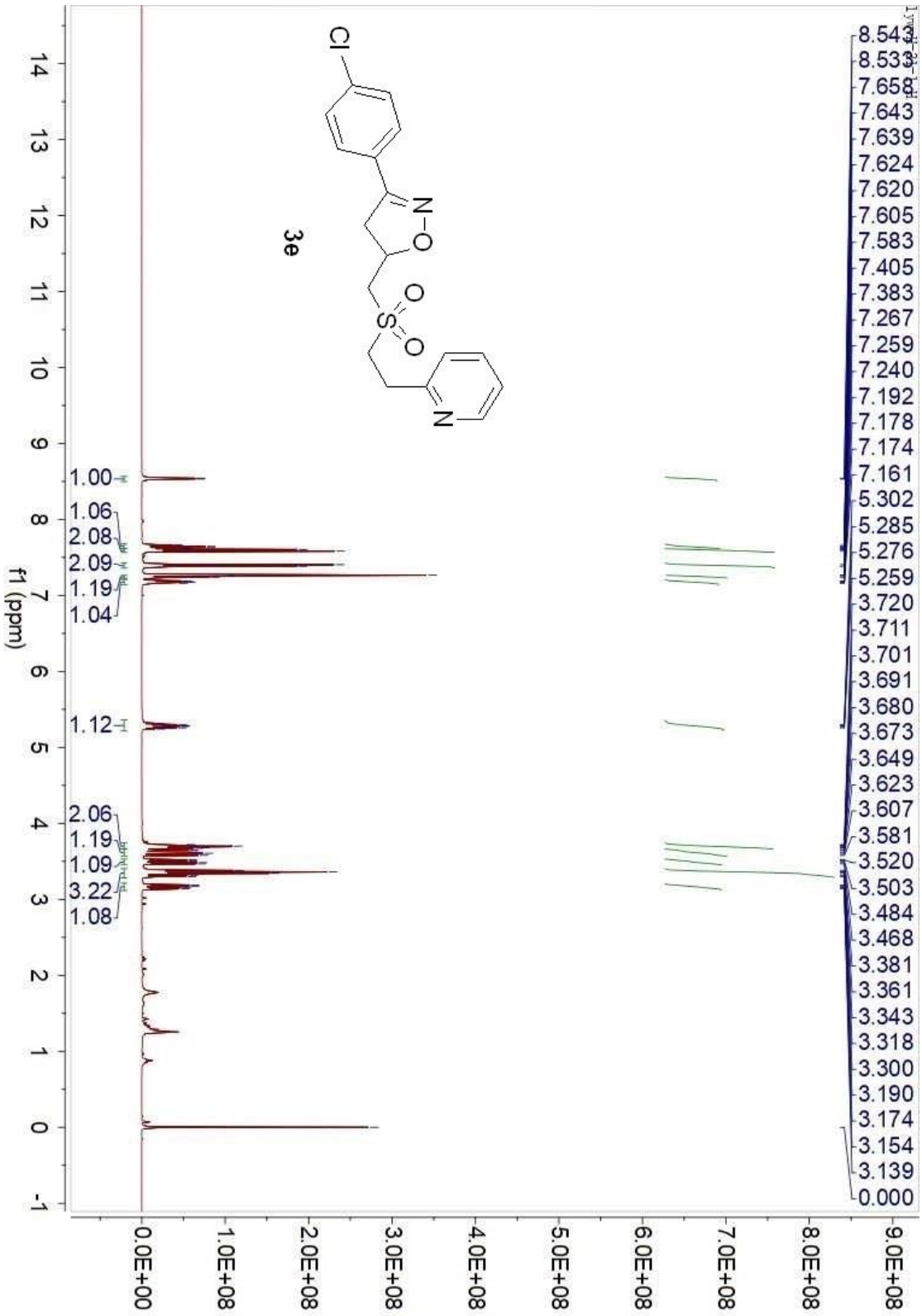
57.25
53.64
40.42
29.90
f1 (ppm)


Cl
N
O
O
S
O
N
3e
f1 (ppm)
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2.09
1.19
1.04
1.12
2.06
1.19
1.09
3.22
1.08
8.543
8.533
7.658
7.643
7.639
7.624
7.620
7.605
7.583
7.405
7.383
7.267
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7.174
7.161
5.302
5.285
5.276
5.259
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3.711
3.701
3.691
3.680
3.673
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3.623
3.607
3.581
3.520
3.503
3.484
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3.381
3.361
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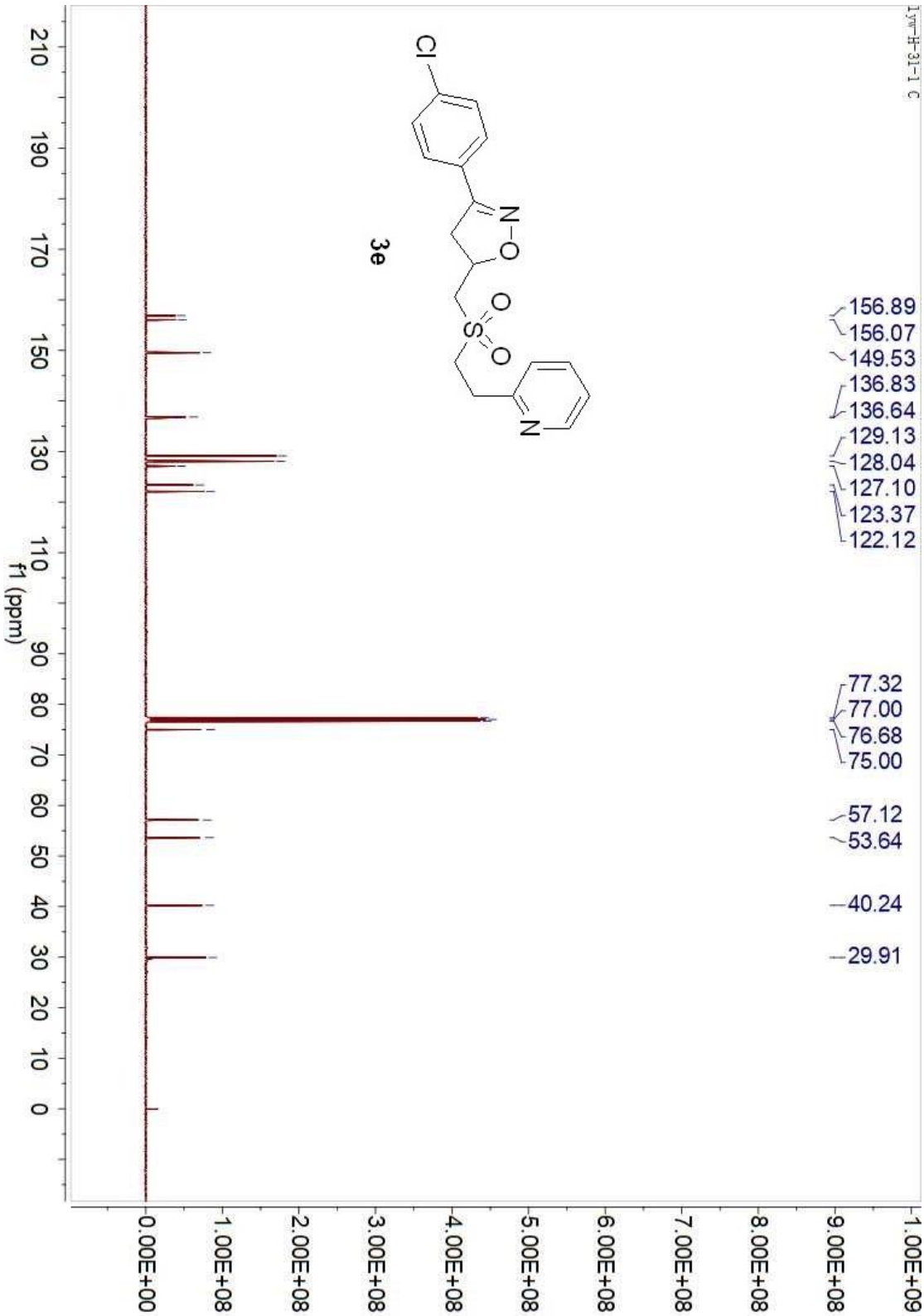
3.300
3.190
3.174
3.154
3.139
0.000


lyw-H-31-1 C
Cl
N
O
O
S
O
O
N
3e
156.89
156.07
149.53
136.83
136.64
129.13
128.04
127.10
123.37
122.12
77.32
77.00
76.68
75.00
57.12
53.64
40.24
29.91
f1 (ppm)
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
0.00E+00
1.00E+08
2.00E+08
3.00E+08
4.00E+08
5.00E+08
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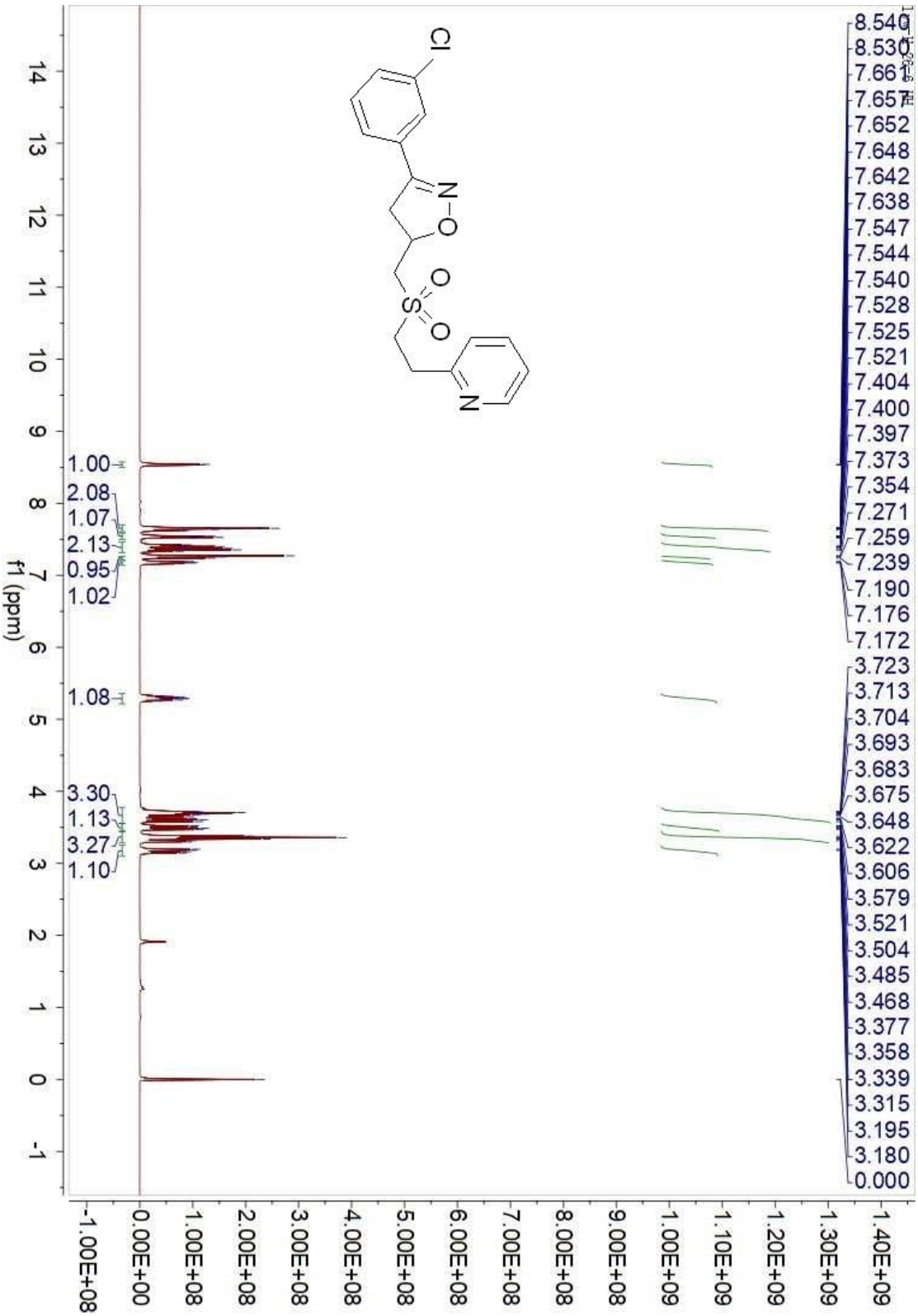
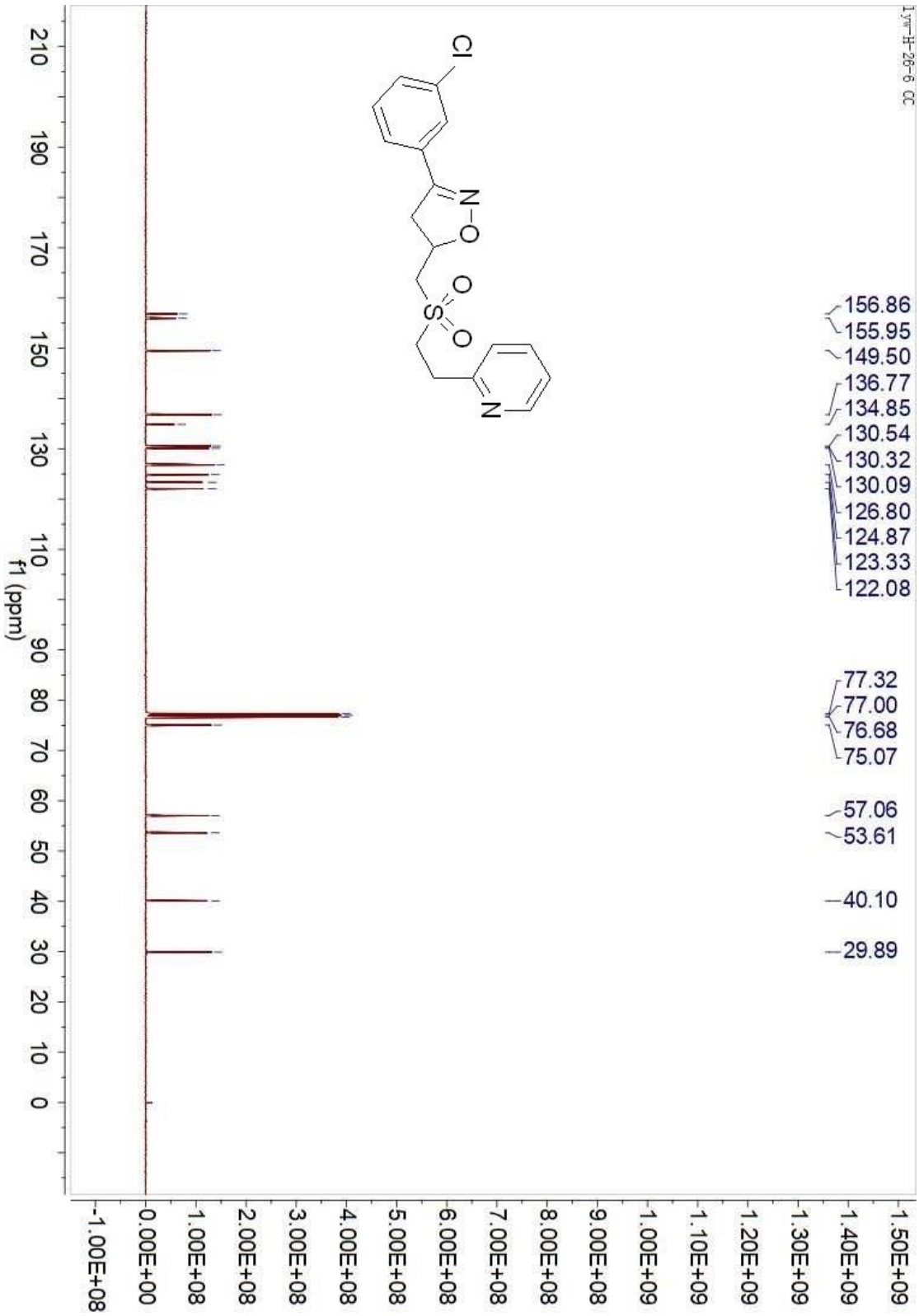
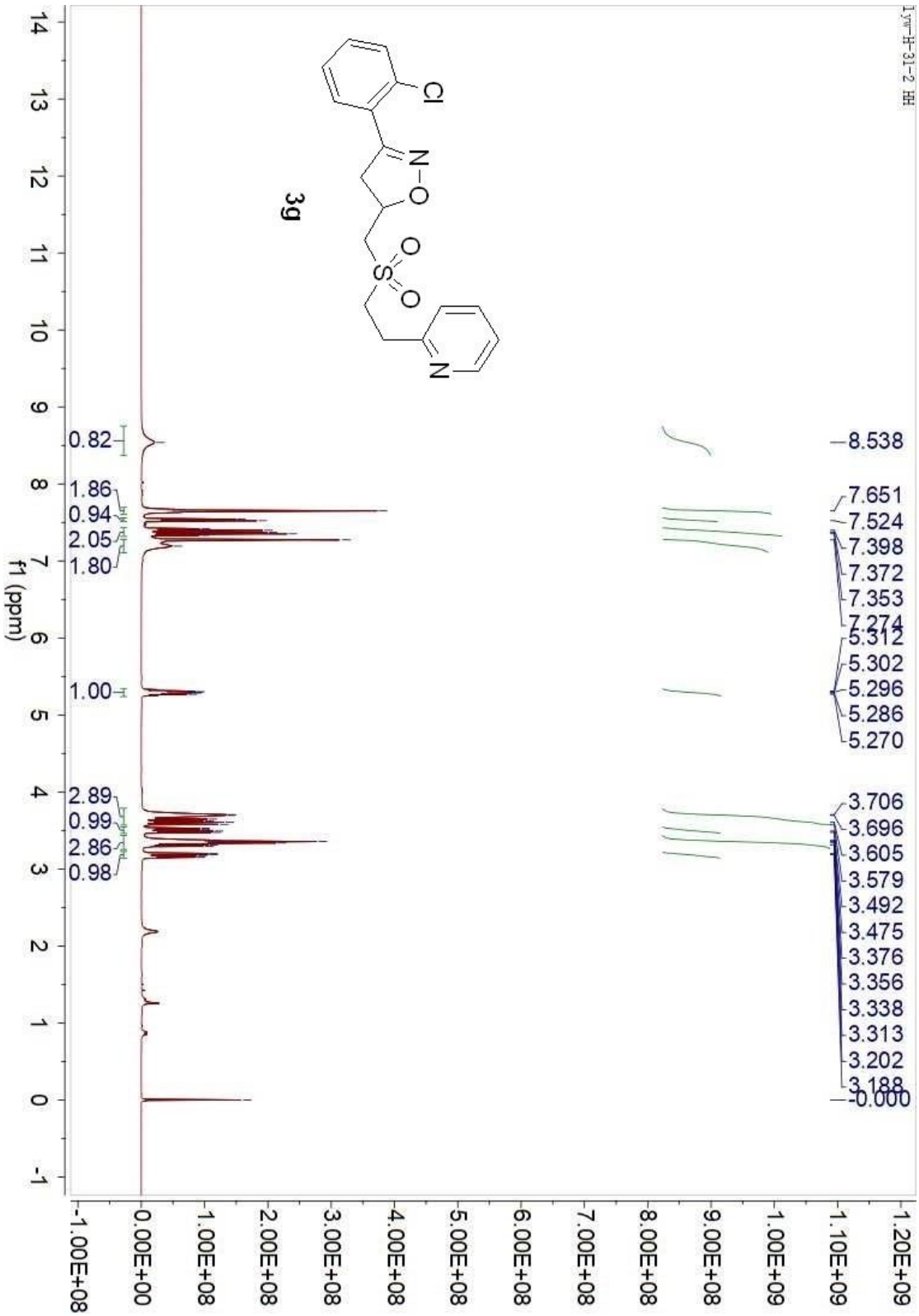
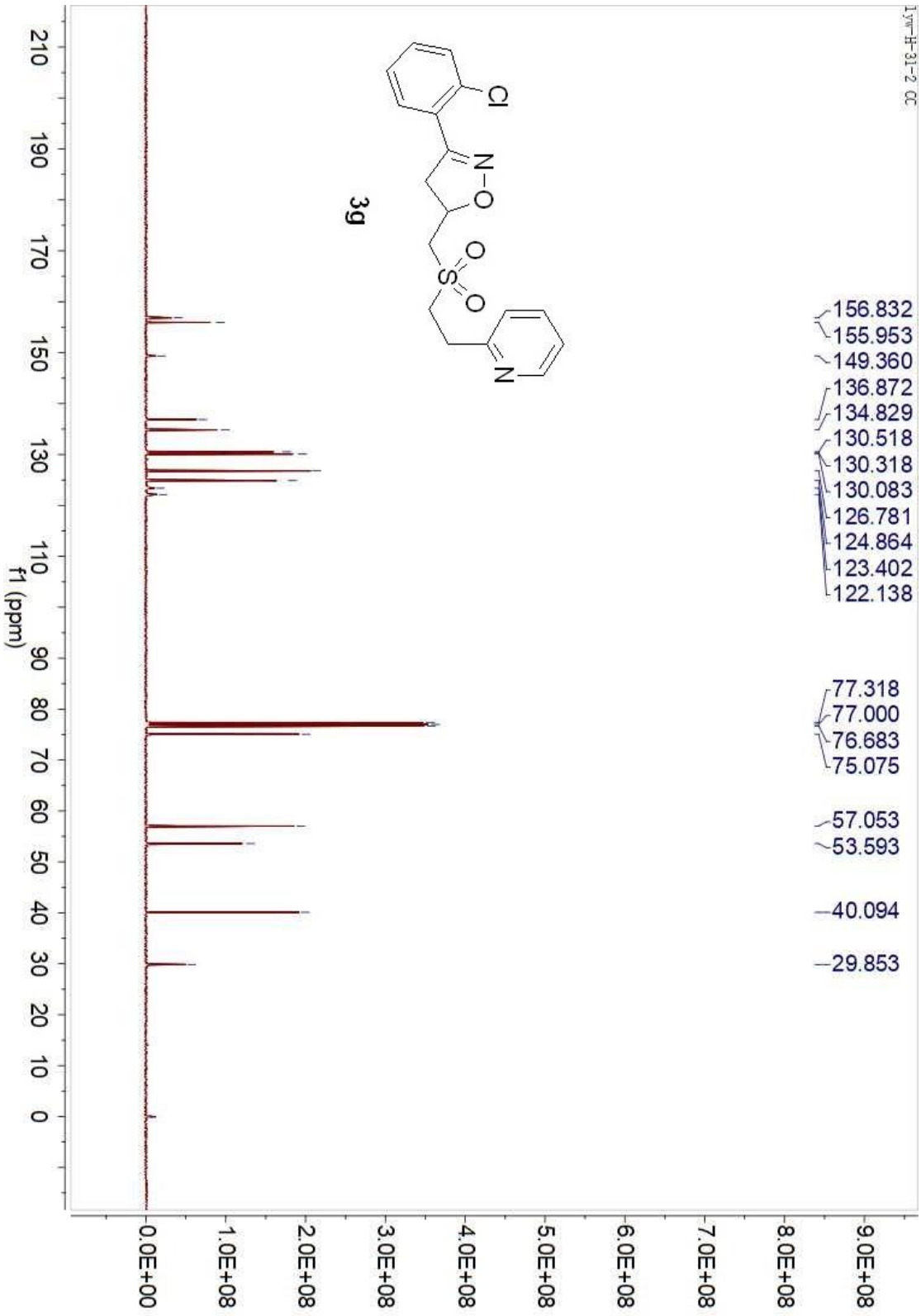
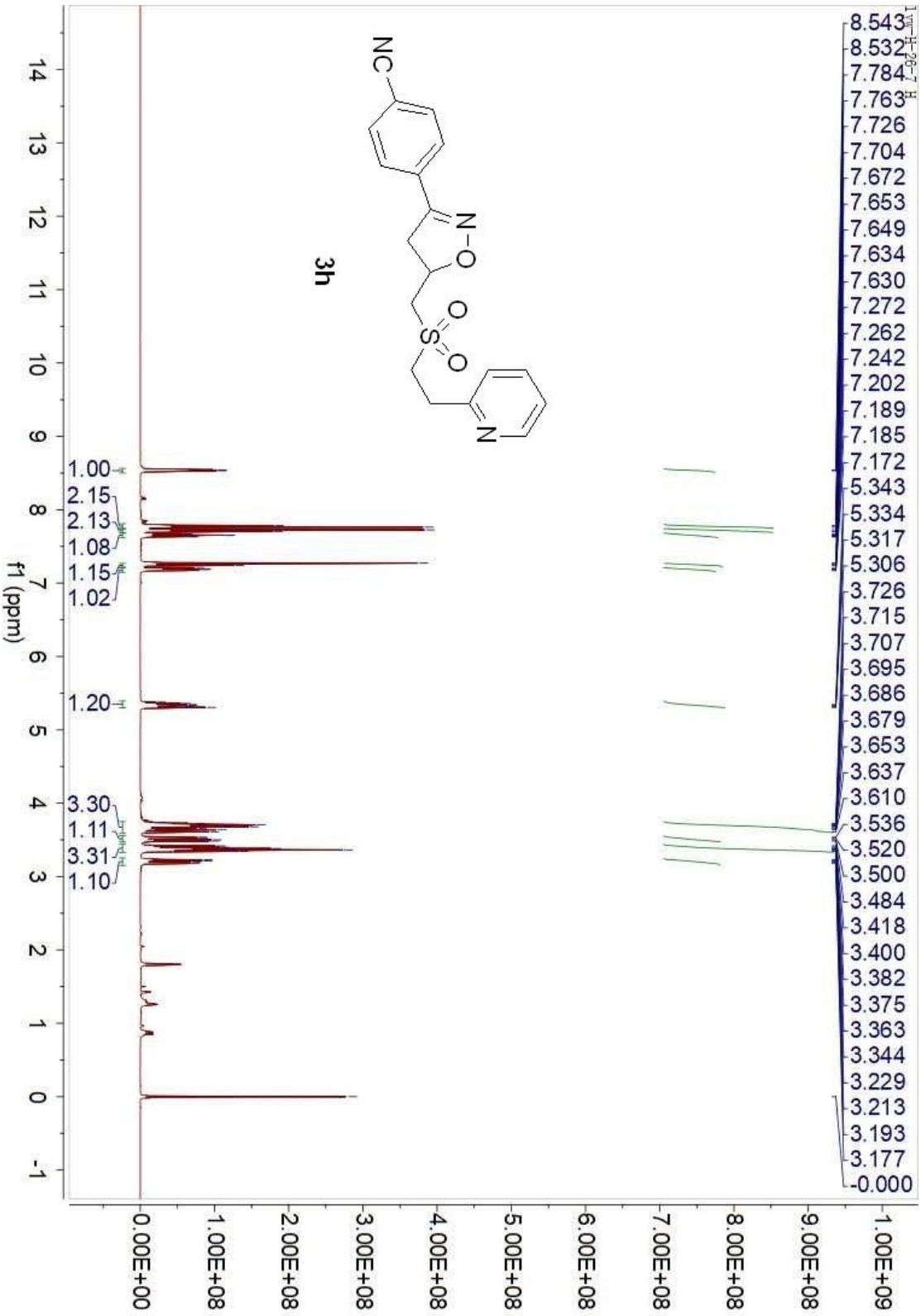
8.00E+08
9.00E+08
1.00E+09

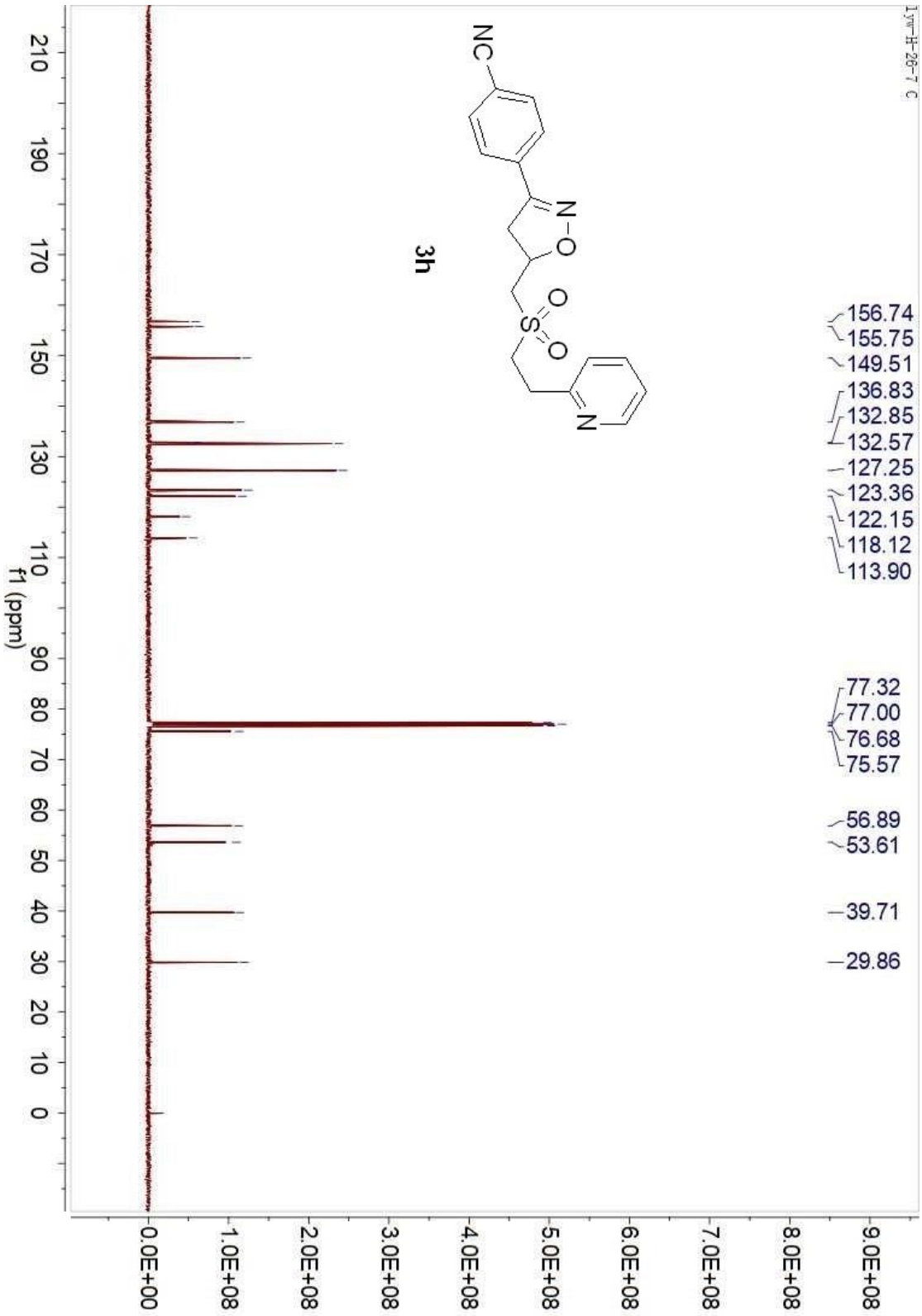

Cl
N
O
O
S
O
N
f1 (ppm)
1.00
2.08
1.07
2.13
0.95
1.02
1.08
3.30
1.13
3.27
1.10
8.540
8.530
7.667
7.657
7.652
7.648
7.642
7.638
7.547
7.544
7.540
7.528
7.525
7.521
7.404
7.400
7.397
7.373
7.354
7.271
7.259
7.239
7.190
7.176
7.172
3.723
3.713
3.704
3.693
3.683
3.675
3.648
3.622
3.606
3.579
3.521
3.504
3.485
3.468
3.377
3.358
3.339
3.315
3.195
3.180
0.000

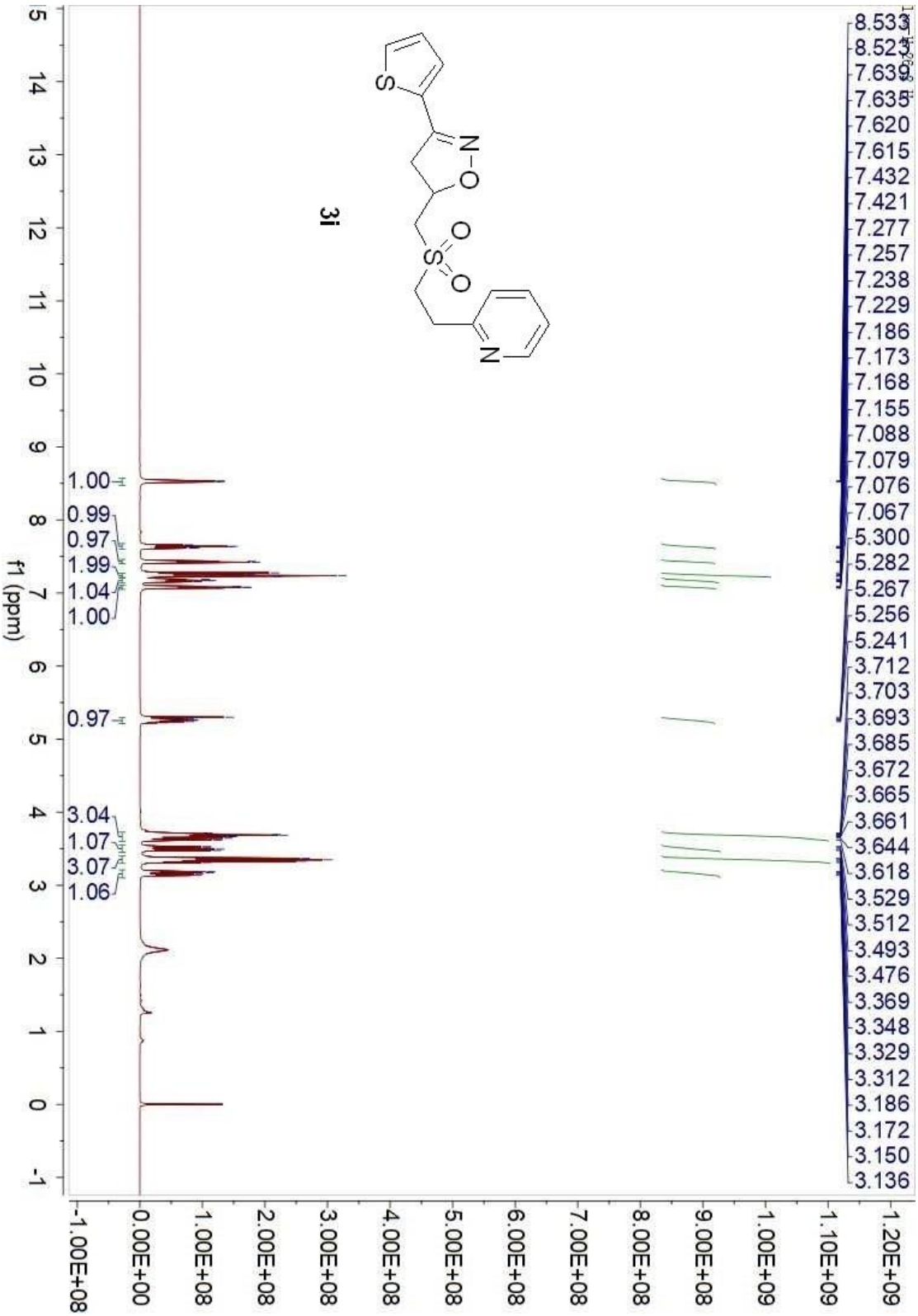

1yw-H-26-6 CC
Cl
N
O
O
S
O
O
N
156.86
155.95
149.50
136.77
134.85
130.54
130.32
130.09
126.80
124.87
123.33
122.08
77.32
77.00
76.68
75.07
57.06
53.61
40.10
29.89
f1 (ppm)

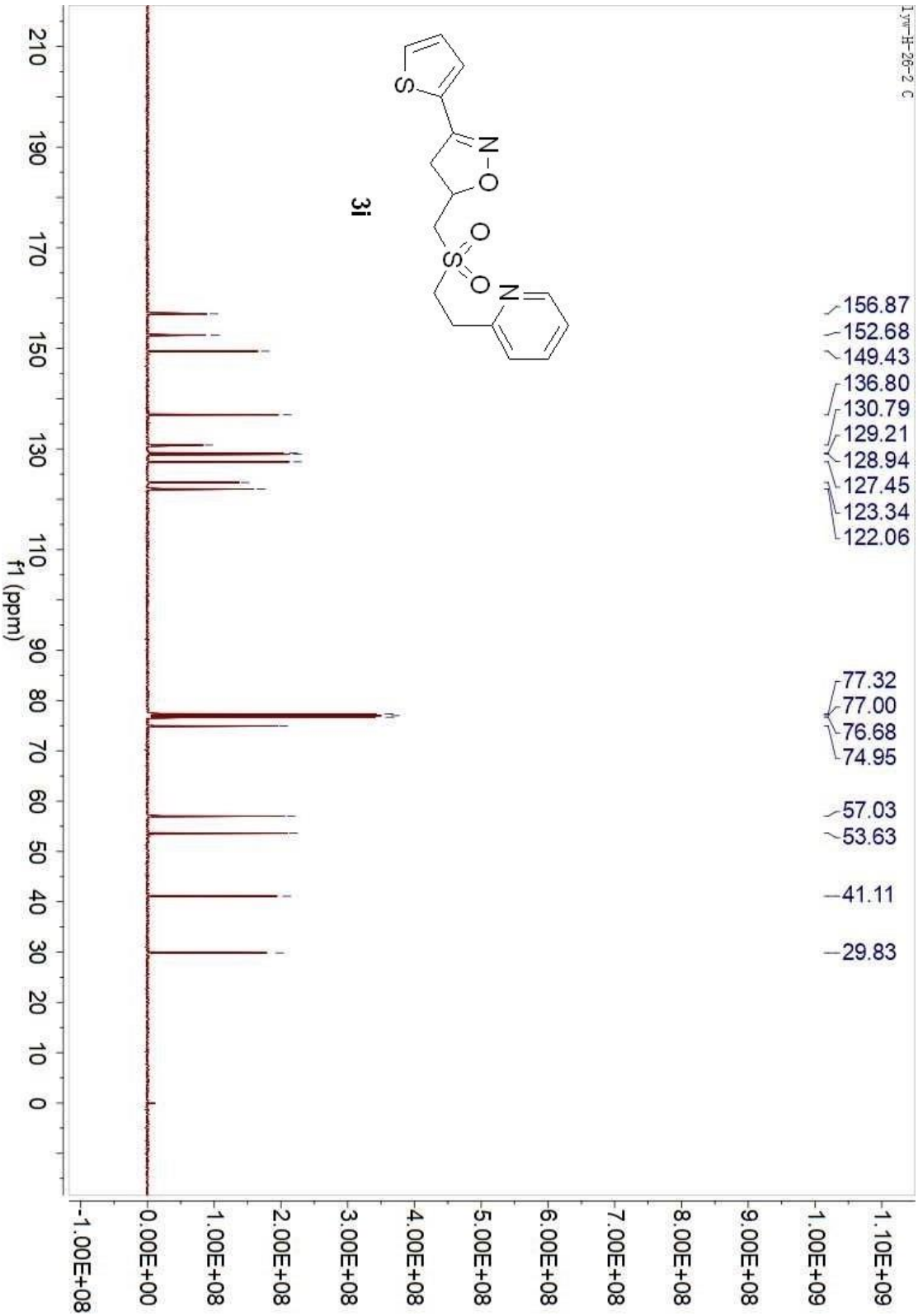

3g
Cl
N
O
O
S
O
N
f1 (ppm)
0.82
1.86
0.94
2.05
1.80
1.00
2.89
0.99
2.86
0.98
8.538
7.651
7.524
7.398
7.372
7.353
7.274
5.312
5.302
5.296
5.286
5.270
3.706
3.696
3.605
3.579
3.492
3.475
3.376
3.356
3.338
3.313
3.202
3.188
0.000

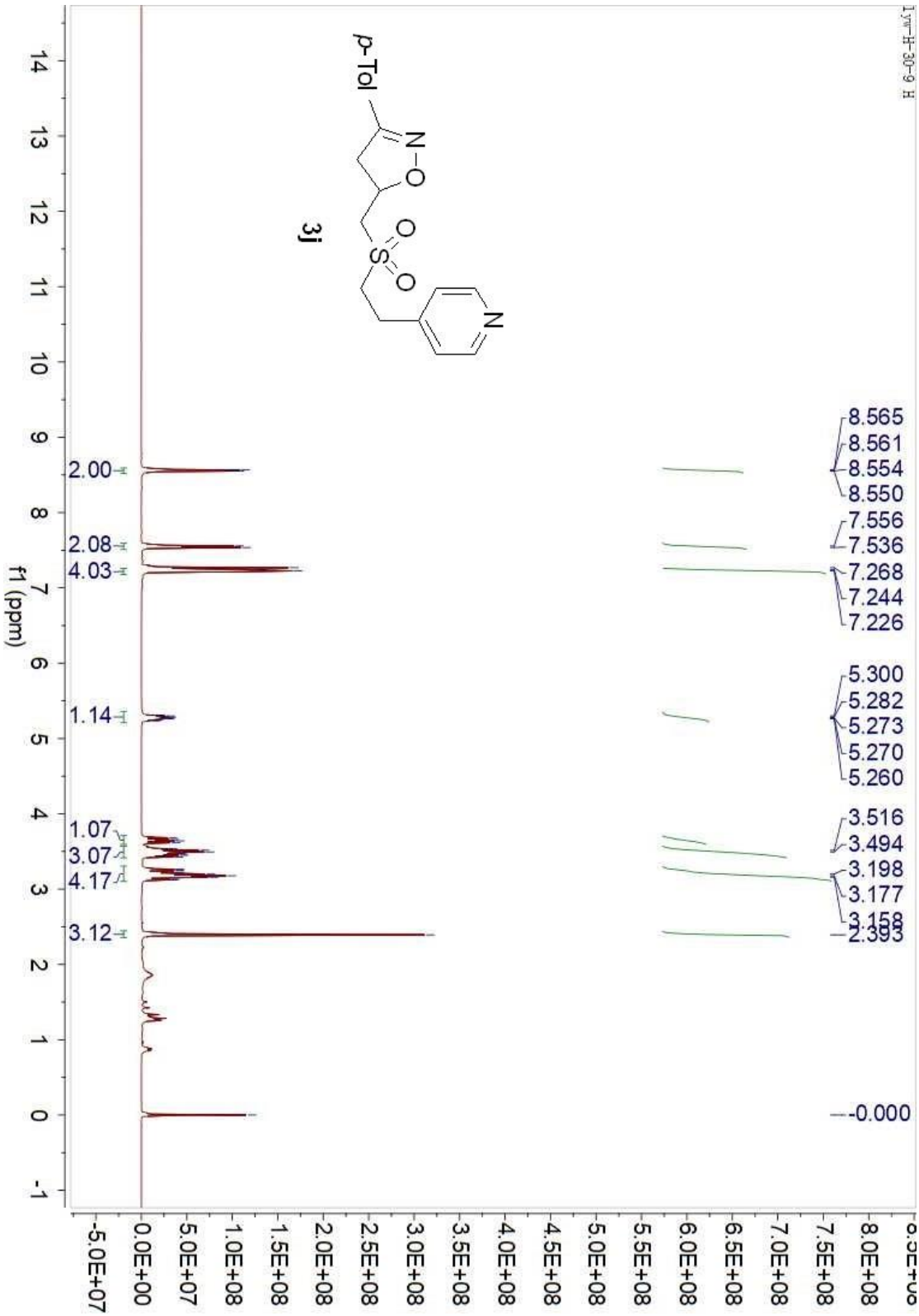

1yw-H-31-2 CC
3g
Cl
N
O
O
S
O
O
N
156.832
155.953
149.360
136.872
134.829
130.518
130.318
130.083
126.781
124.864
123.402
122.138
77.318
77.000
76.683
75.075
57.053
53.593
40.094
29.853
f1 (ppm)
0.0E+00
1.0E+08
2.0E+08
3.0E+08
4.0E+08
5.0E+08
6.0E+08
7.0E+08
8.0E+08
9.0E+08

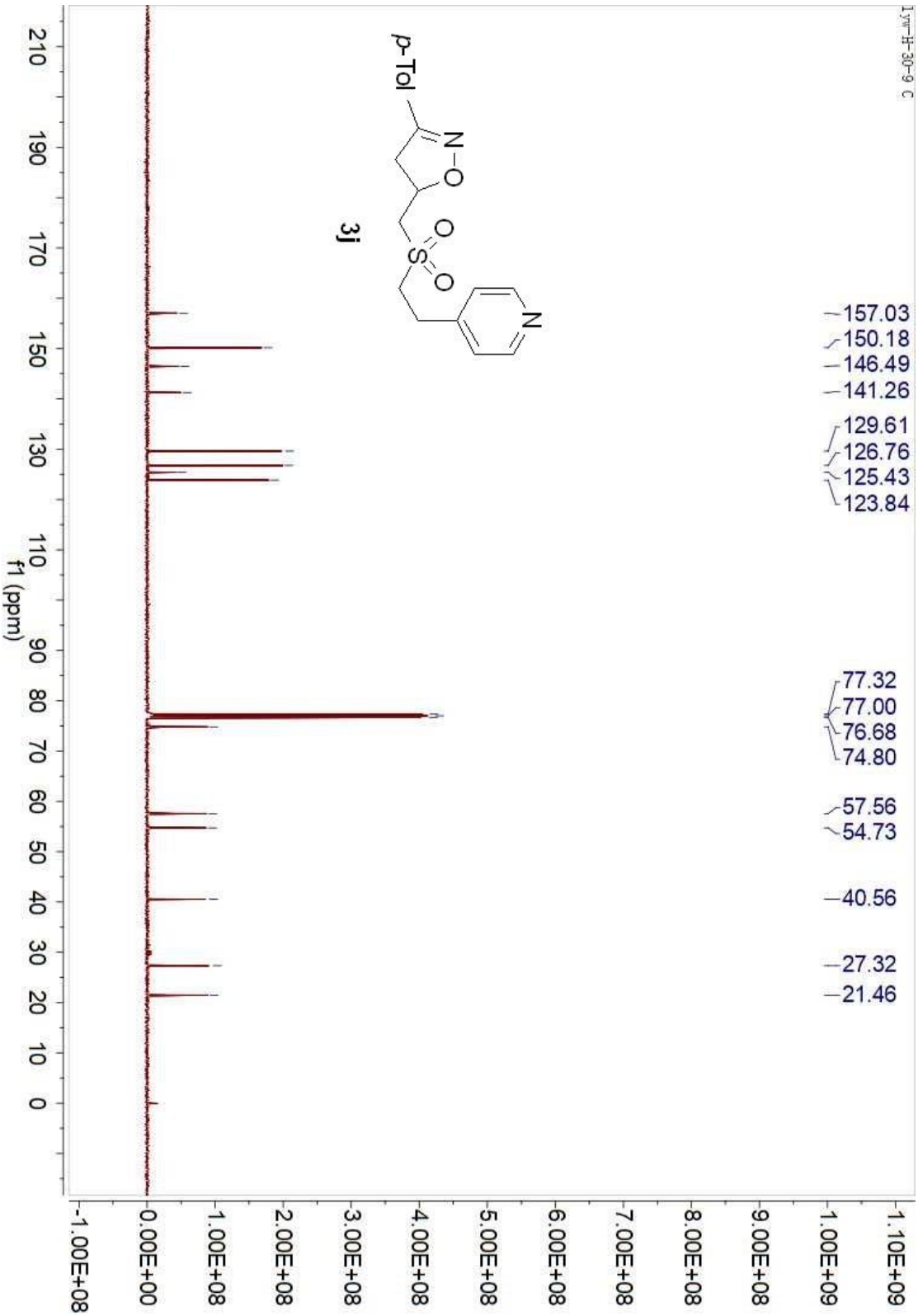

3h
NC
N
O
O
S
O
O
N
f1 (ppm)
1.00
2.15
2.13
1.08
1.15
1.02
1.20
3.30
1.11
3.31
1.10
8.543
8.532
7.784
7.763
7.726
7.704
7.672
7.653
7.649
7.634
7.630
7.272
7.262
7.242
7.202
7.189
7.185
7.172
5.343
5.334
5.317
5.306
3.726
3.715
3.707
3.695
3.686
3.679
3.653
3.637
3.610
3.536
3.520
3.500
3.484
3.418
3.400
3.382
3.375
3.363
3.344
3.229
3.213
3.193
3.177
-0.000

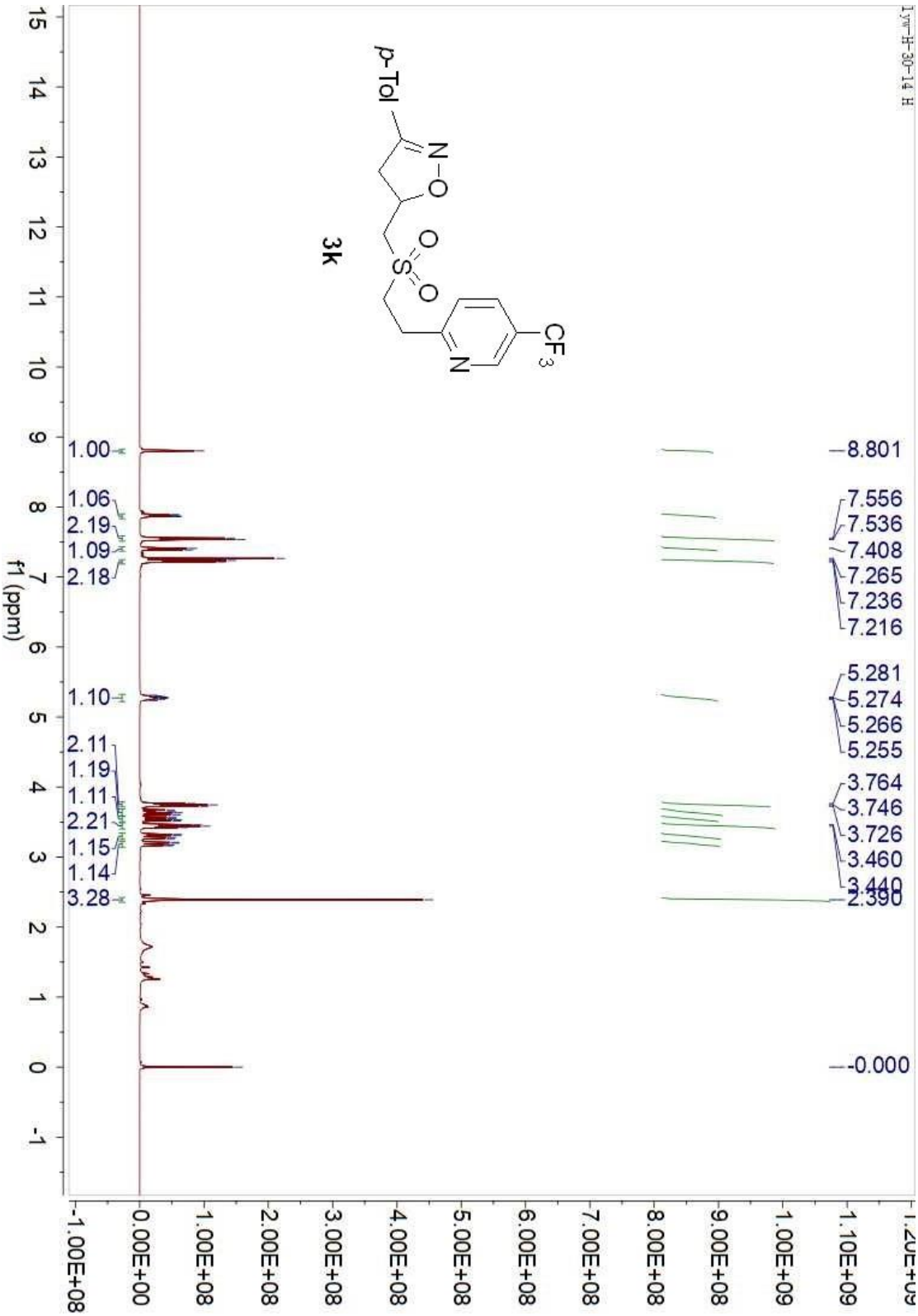

3h
156.74
155.75
149.51
136.83
132.85
132.57
127.25
123.36
122.15
118.12
113.90
77.32
77.00
76.68
75.57
56.89
53.61
39.71
29.86
f1 (ppm)

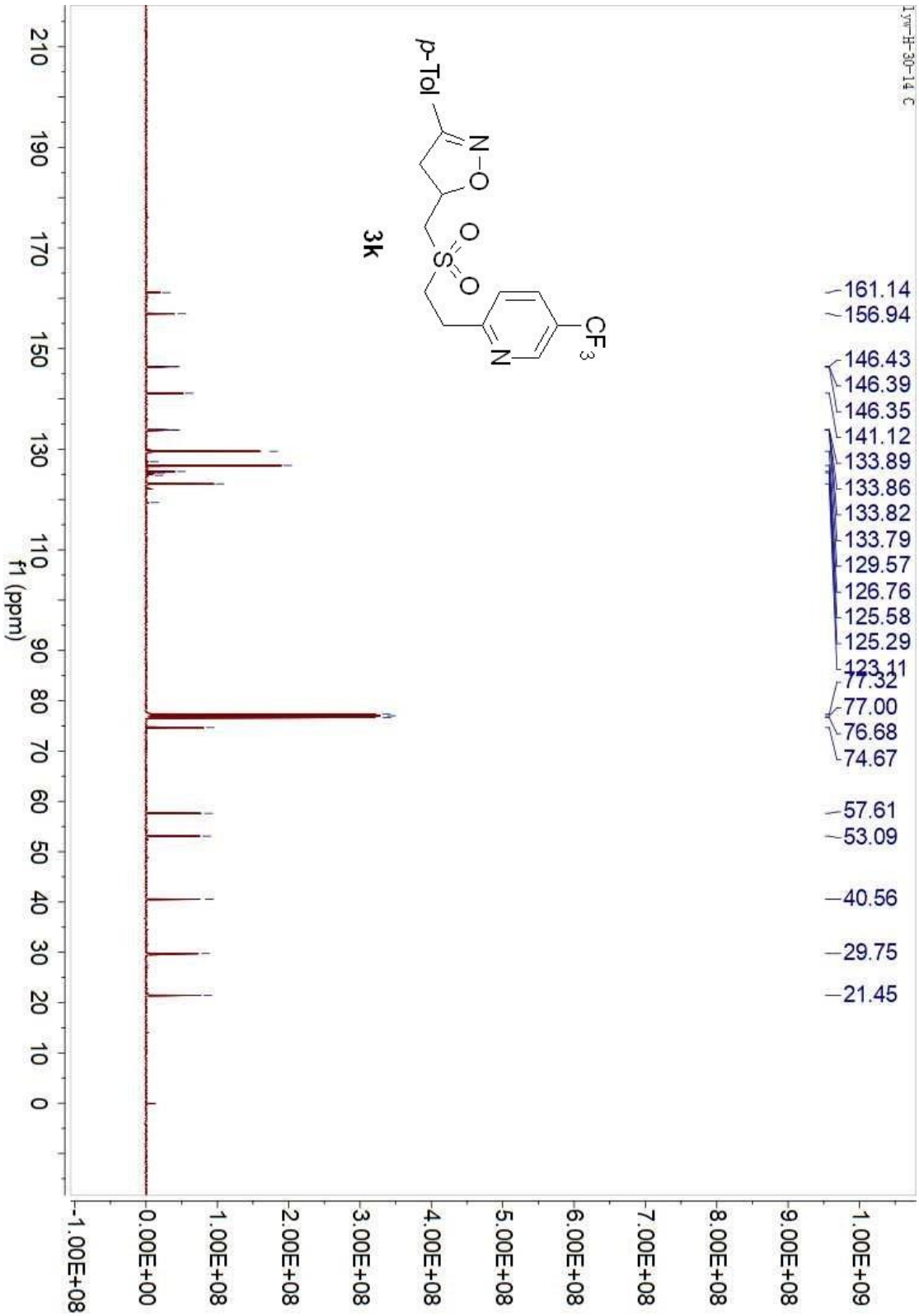

3i
f1 (ppm)
1.00
0.99
0.97
1.99
1.04
1.00
0.97
3.04
1.07
3.07
1.06
8.533
8.525
7.639
7.635
7.620
7.615
7.432
7.421
7.277
7.257
7.238
7.229
7.186
7.173
7.168
7.155
7.088
7.079
7.076
7.067
5.300
5.282
5.267
5.256
5.241
3.712
3.703
3.693
3.685
3.672
3.665
3.661
3.644
3.618
3.529
3.512
3.493
3.476
3.369
3.348
3.329
3.312
3.186
3.172
3.150
3.136

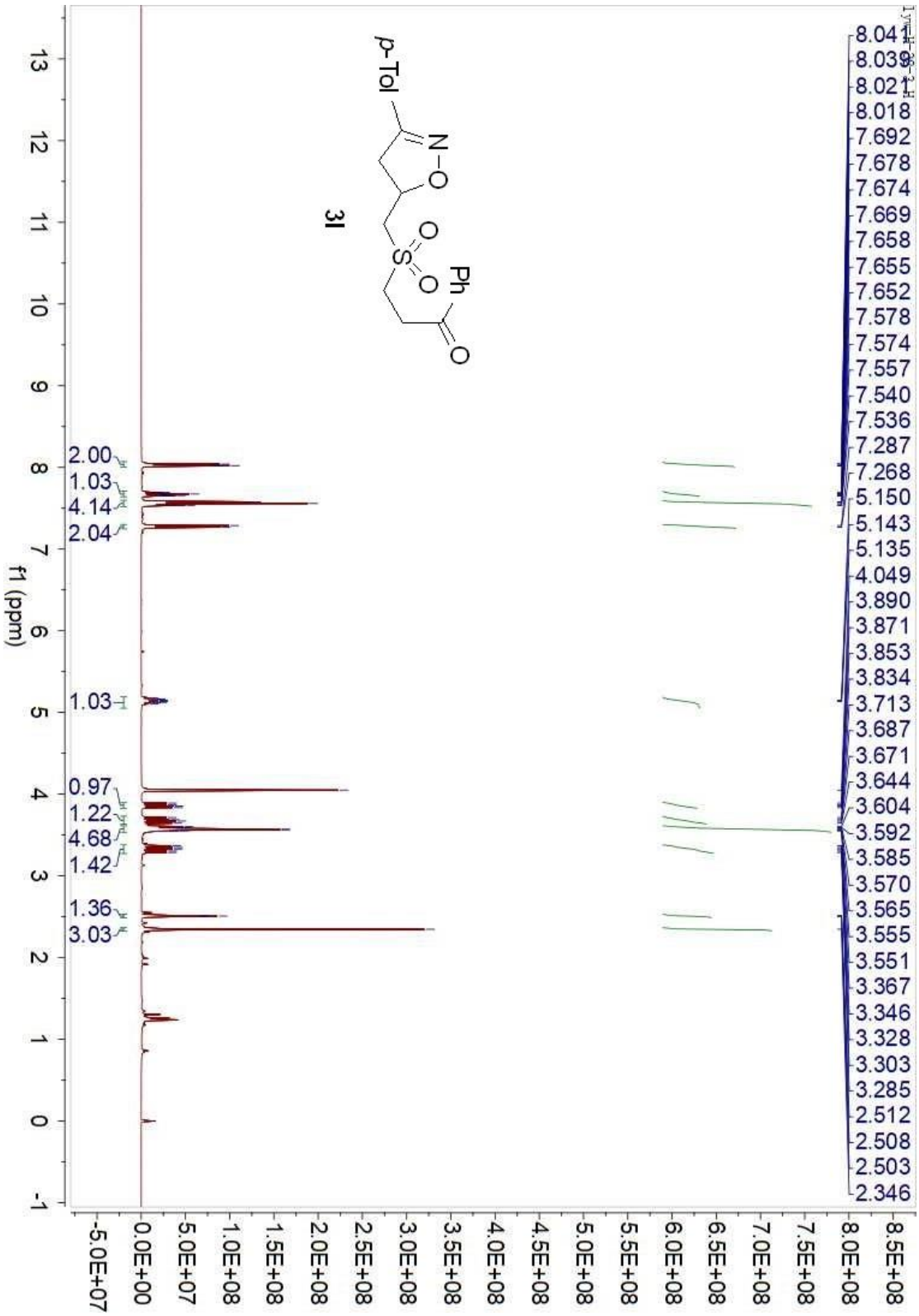

3i
156.87
152.68
149.43
136.80
130.79
129.21
128.94
127.45
123.34
122.06
77.32
77.00
76.68
74.95
57.03
53.63
41.11
29.83
f1 (ppm)

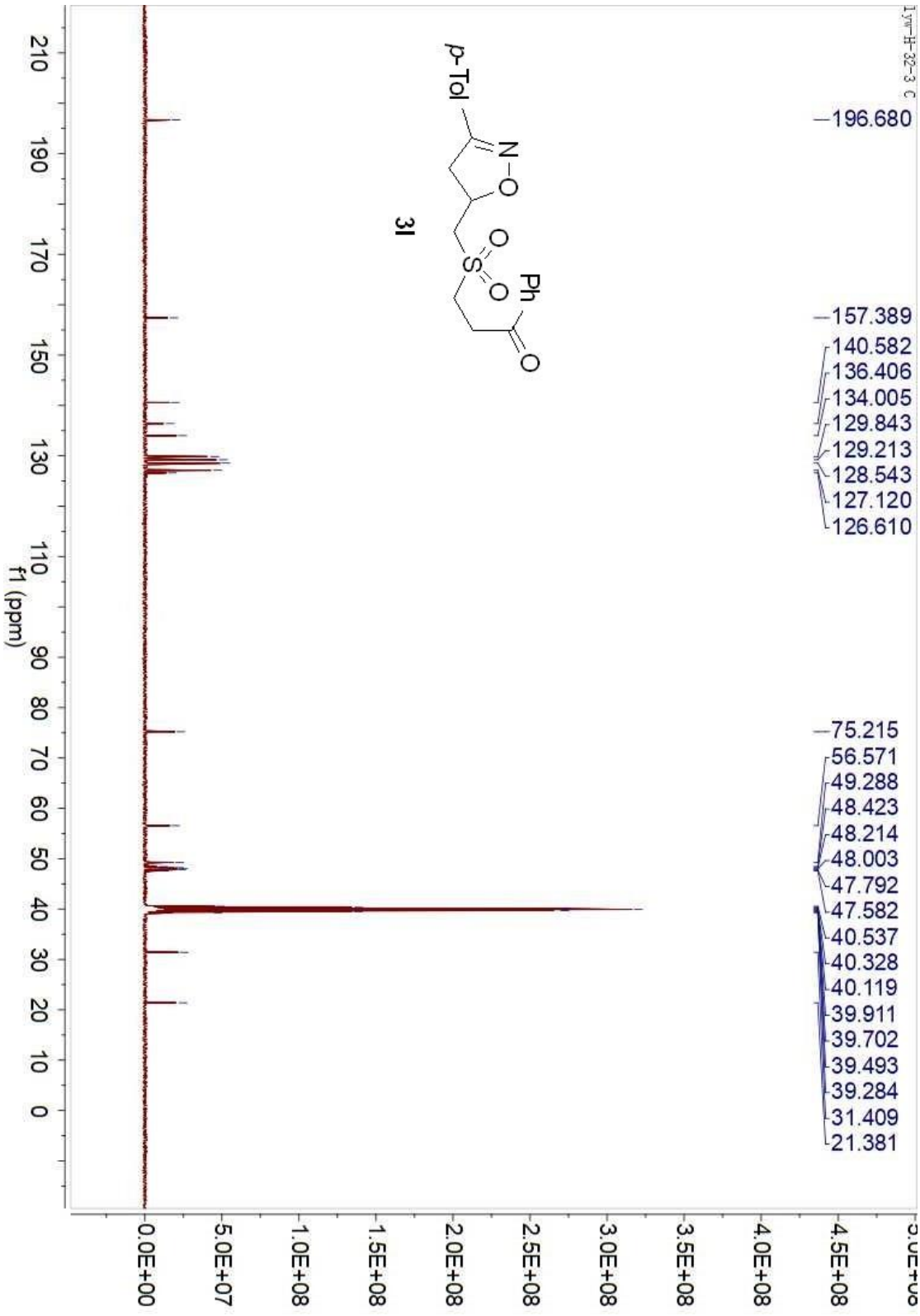

p-Tol
3j
8.565
8.561
8.554
8.550
7.556
7.536
7.268
7.244
7.226
5.300
5.282
5.273
5.270
5.260
3.516
3.494
3.198
3.177
3.158
2.393
-0.000
2.00
2.08
4.03
1.14
1.07
3.07
4.17
3.12
f1 (ppm)

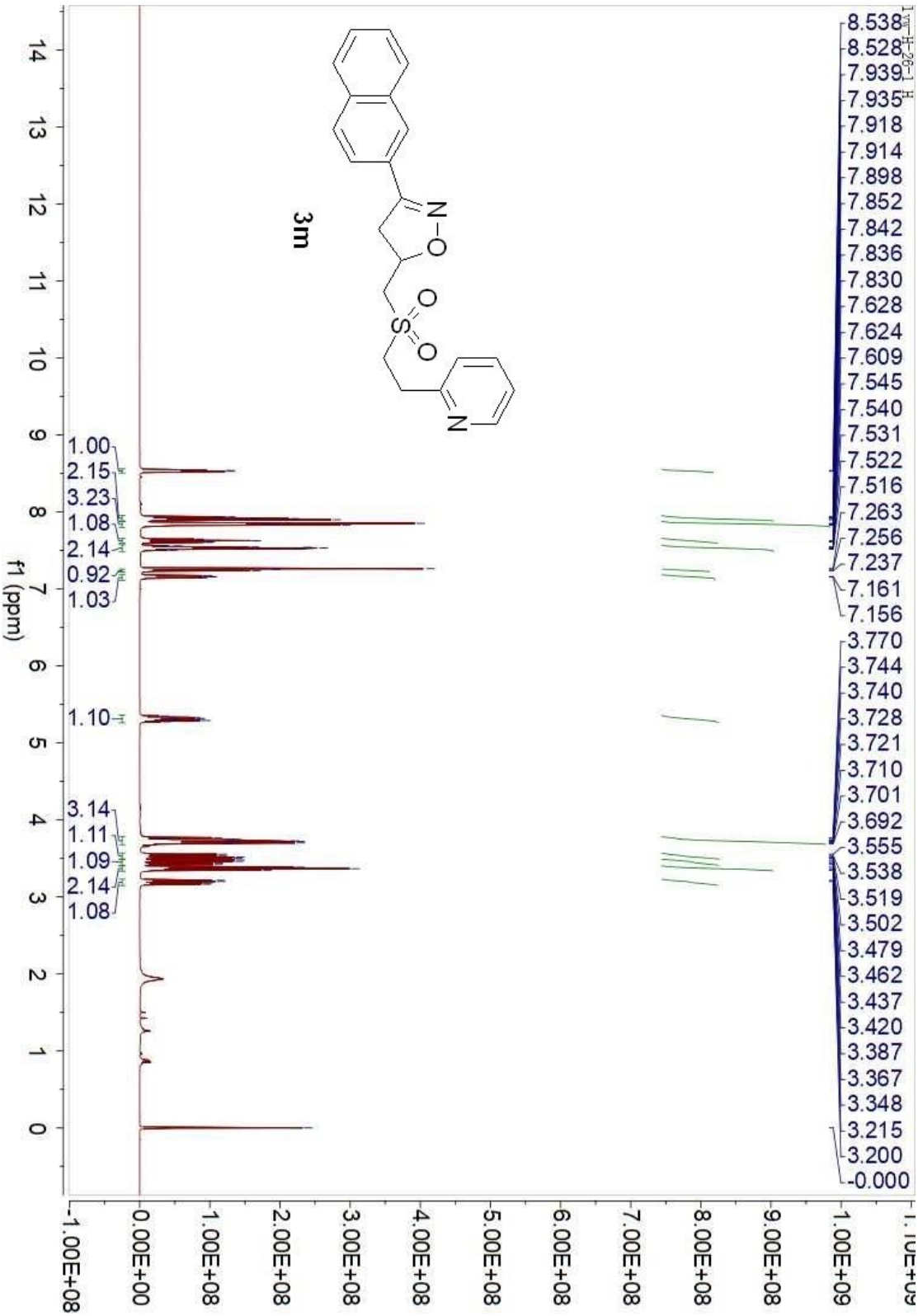

1yw-H-30-9 C
p-Tol
N
O
O
S
O
N
3j
157.03
150.18
146.49
141.26
129.61
126.76
125.43
123.84
77.32
77.00
76.68
74.80
57.56
54.73
40.56
27.32
21.46
f1 (ppm)

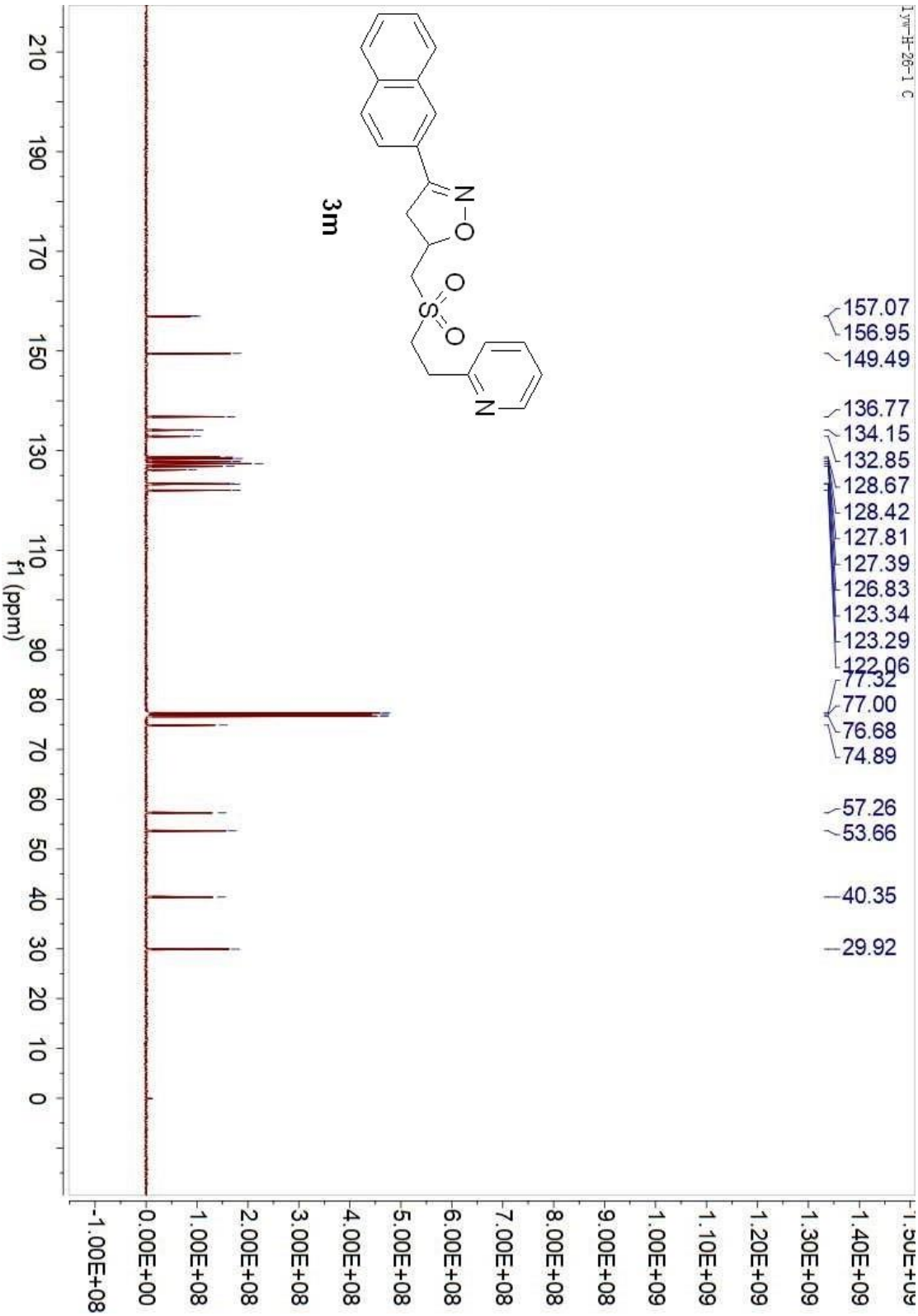

3k
p-Tol
N
O
O
S
O
O
N
CF3
f1 (ppm)
1.00
1.06
2.19
1.09
2.18
1.10
2.11
1.19
1.11
2.21
1.15
1.14
3.28
8.801
7.556
7.536
7.408
7.265
7.236
7.216
5.281
5.274
5.266
5.255
3.764
3.746
3.726
3.460
3.440
2.390
-0.000

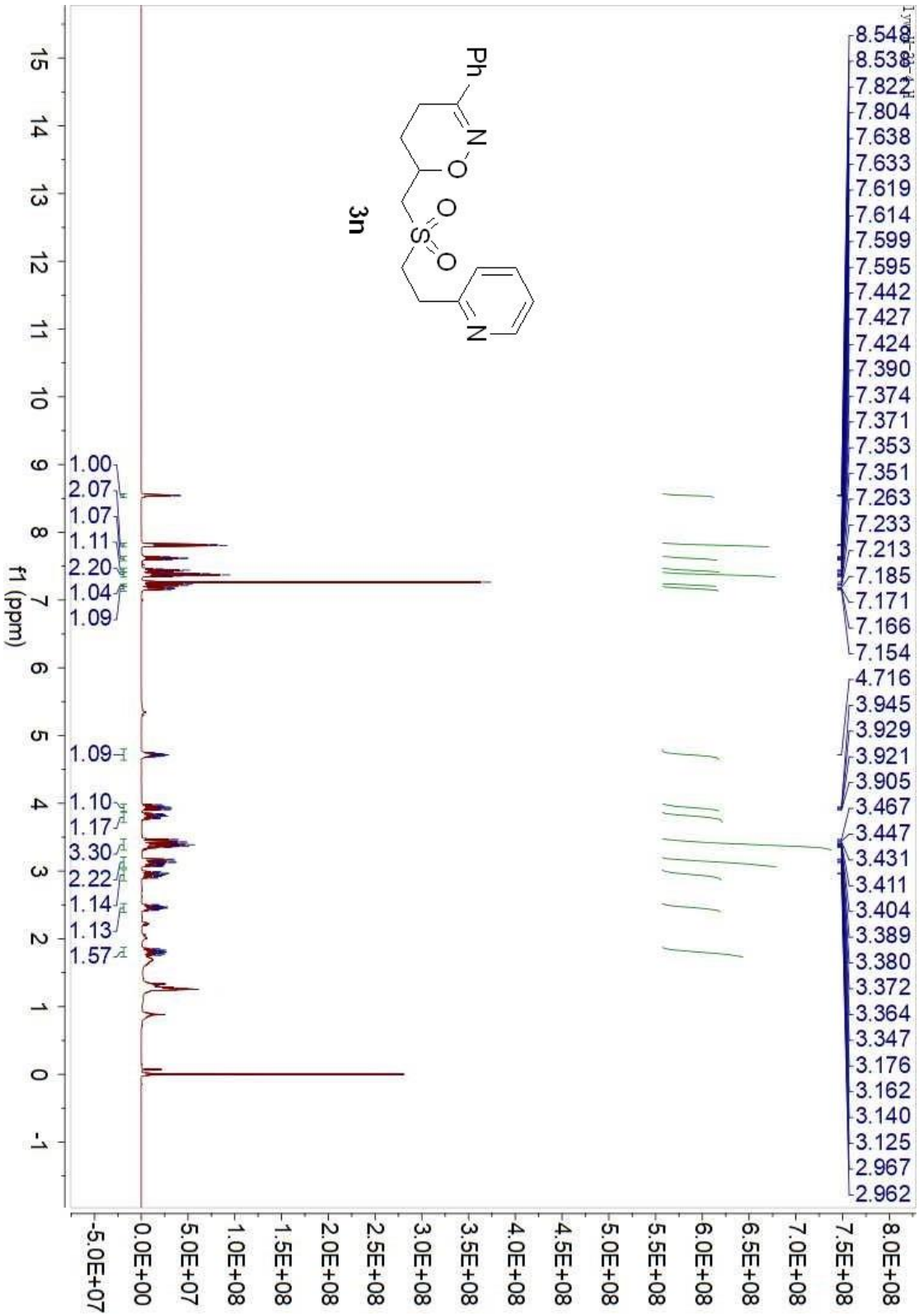

lyw-H-30-14 C
p-Tol
N
O
O
S
O
CF3
N
3k
161.14
156.94
146.43
146.39
146.35
141.12
133.89
133.86
133.82
133.79
129.57
126.76
125.58
125.29
123.11
77.32
77.00
76.68
74.67
57.61
53.09
40.56
29.75
21.45
f1 (ppm)

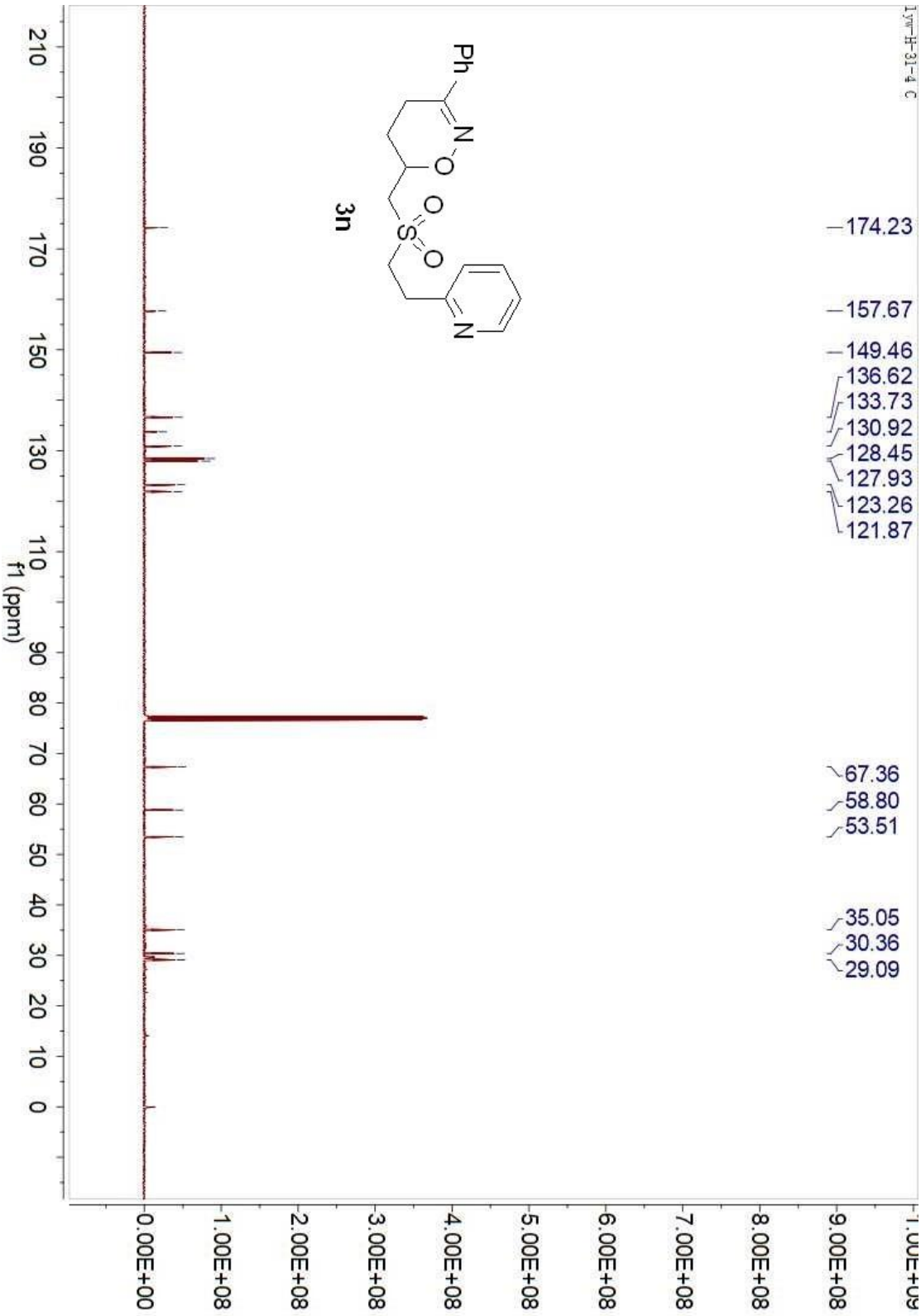

p-Tol
N–O
O
O
S
O
Ph
O
3l
f1 (ppm)
2.00
1.03
4.14
2.04
1.03
0.97
1.22
4.68
1.42
1.36
3.03
8.041
8.039
8.021
8.018
7.692
7.678
7.674
7.669
7.658
7.655
7.652
7.578
7.574
7.557
7.540
7.536
7.287
7.268
5.150
5.143
5.135
4.049
3.890
3.871
3.853
3.834
3.713
3.687
3.671
3.644
3.604
3.592
3.585
3.570
3.565
3.555
3.551
3.367
3.346
3.328
3.303
3.285
2.512
2.508
2.503
2.346

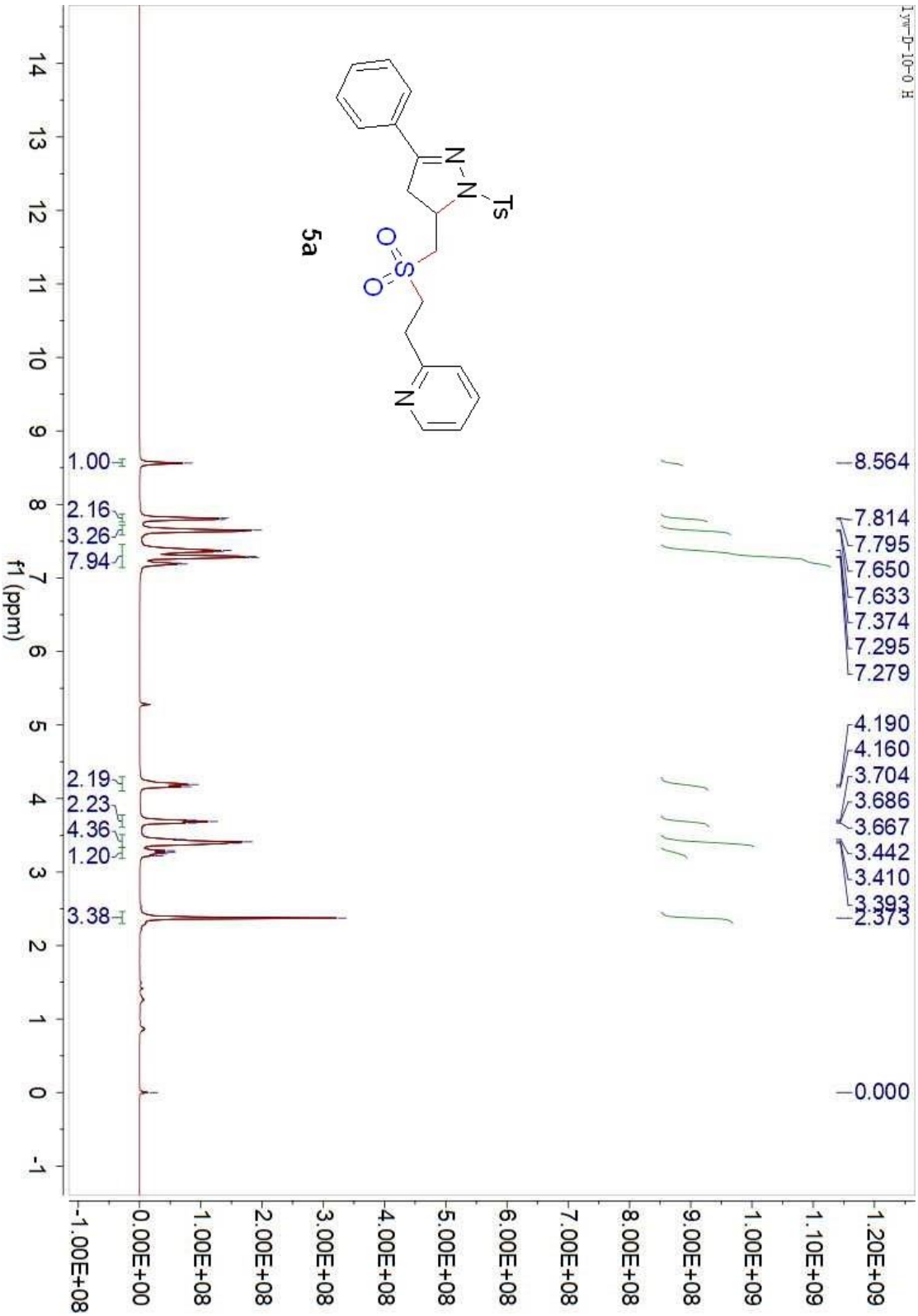

p-Tol
N
O
O
S
O
O
Ph
O
3l
196.680
157.389
140.582
136.406
134.005
129.843
129.213
128.543
127.120
126.610
75.215
56.571
49.288
48.423
48.214
48.003
47.792
47.582
40.537
40.328
40.119
39.911
39.702
39.493
39.284
31.409
21.381
f1 (ppm)

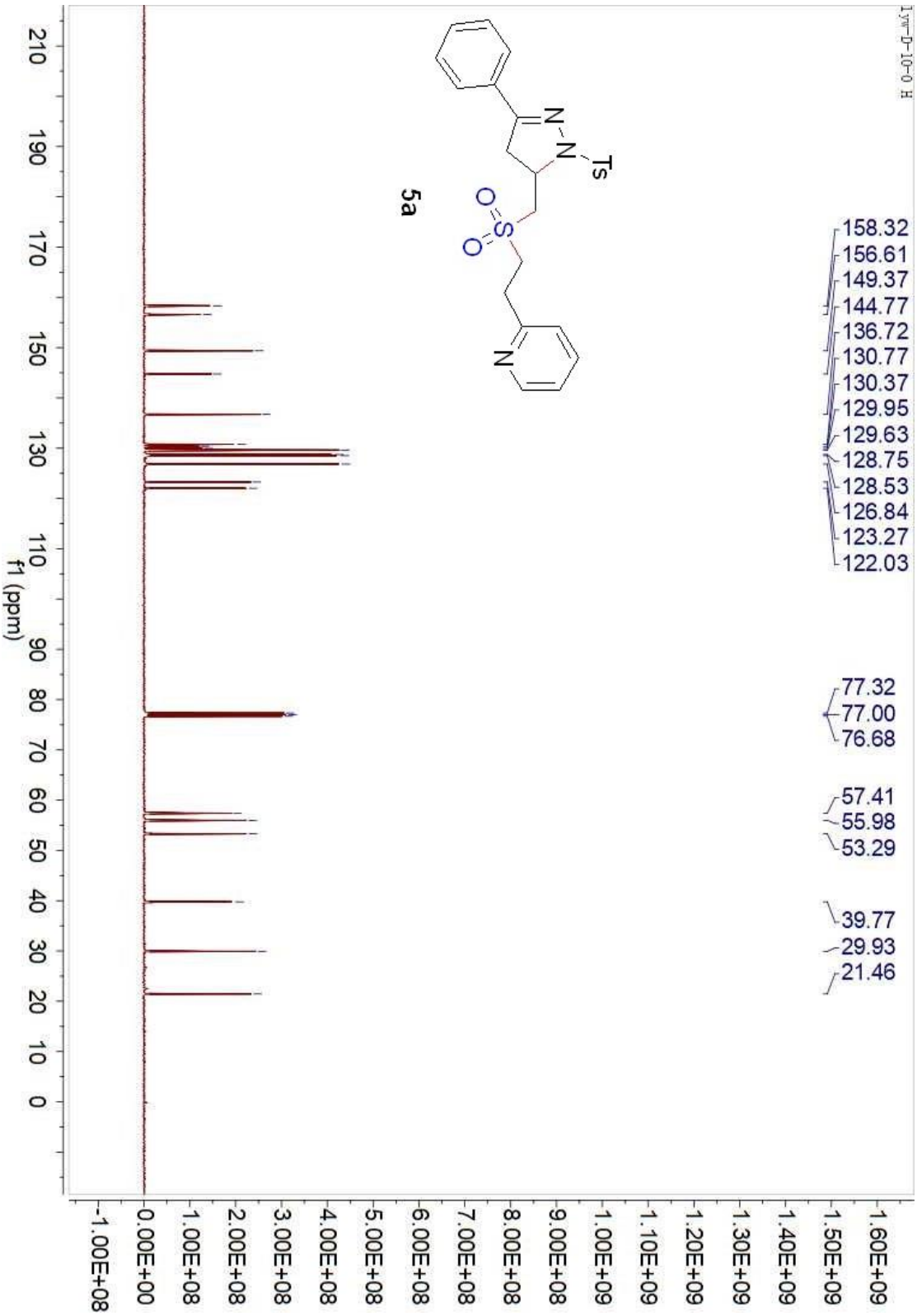

3m
f1 (ppm)
1.00
2.15
3.23
1.08
2.14
0.92
1.03
1.10
3.14
1.11
1.09
2.14
1.08
8.538
8.528
7.939
7.935
7.918
7.914
7.898
7.852
7.842
7.836
7.830
7.628
7.624
7.609
7.545
7.540
7.531
7.522
7.516
7.263
7.256
7.237
7.161
7.156
3.770
3.744
3.740
3.728
3.721
3.710
3.701
3.692
3.555
3.538
3.519
3.502
3.479
3.462
3.437
3.420
3.387
3.367
3.348
3.215
3.200
-0.000

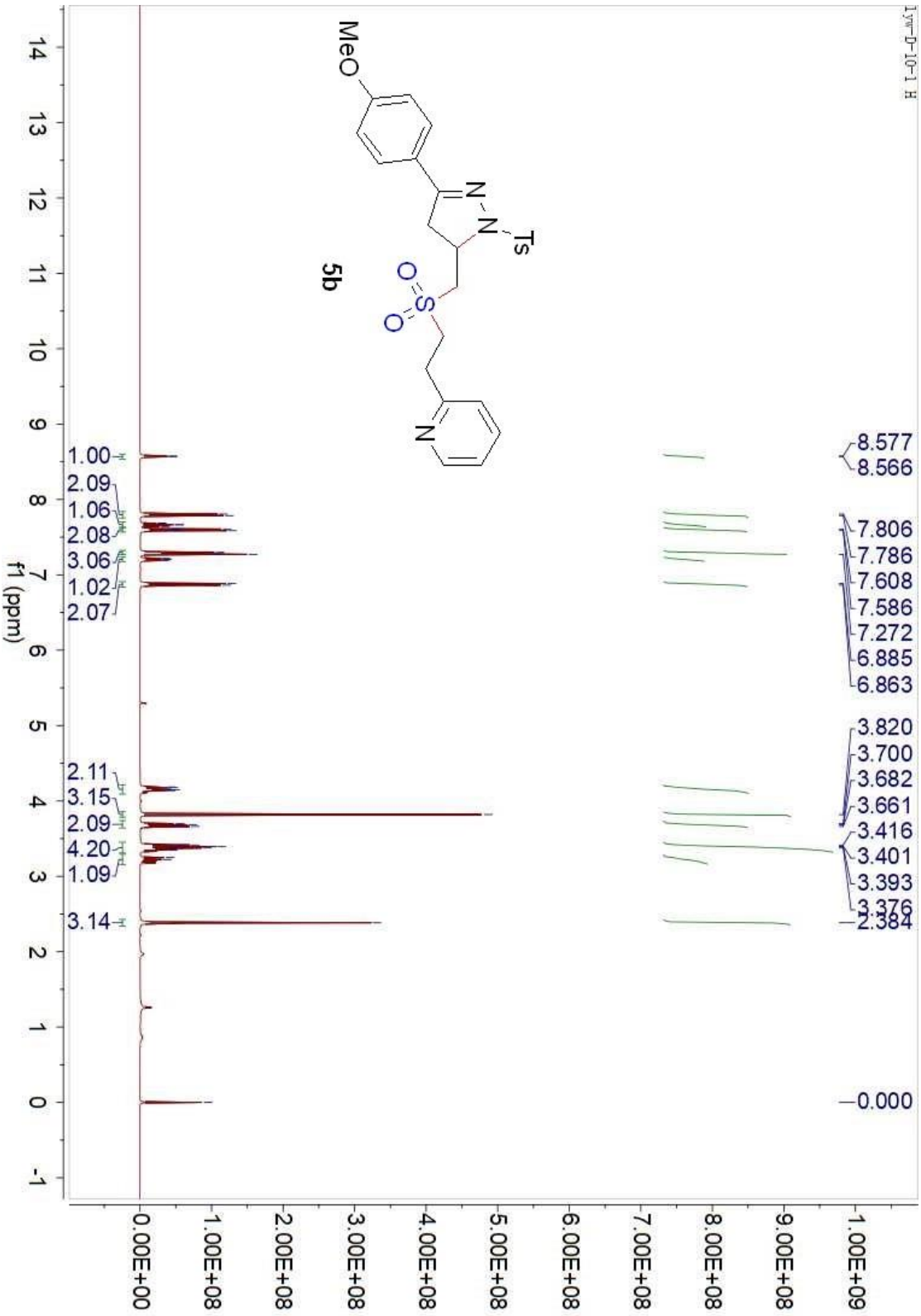

lyw-H-26-1 C
3m
157.07
156.95
149.49
136.77
134.15
132.85
128.67
128.42
127.81
127.39
126.83
123.34
123.29
122.06
77.32
77.00
76.68
74.89
57.26
53.66
40.35
29.92
f1 (ppm)

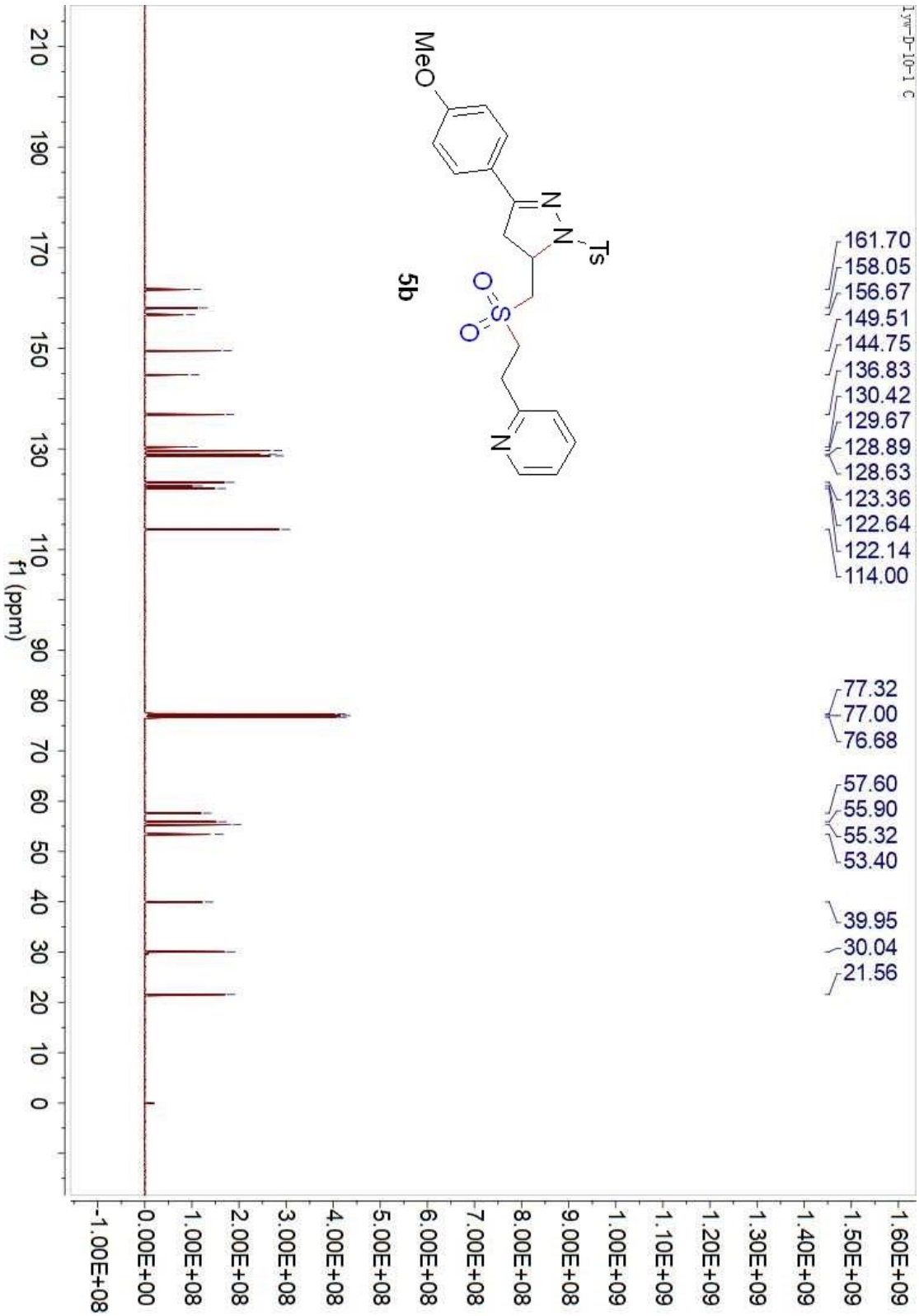

Ph
N
O
O
S
O
O
N
3n
f1 (ppm)
1.00
2.07
1.07
1.11
2.20
1.04
1.09
1.09
1.10
1.17
3.30
2.22
1.14
1.13
1.57
8.548
8.538
7.822
7.804
7.638
7.633
7.619
7.614
7.599
7.595
7.442
7.427
7.424
7.390
7.374
7.371
7.353
7.351
7.263
7.233
7.213
7.185
7.171
7.166
7.154
4.716
3.945
3.929
3.921
3.905
3.467
3.447
3.431
3.411
3.404
3.389
3.380
3.372
3.364
3.347
3.176
3.162
3.140
3.125
2.967
2.962

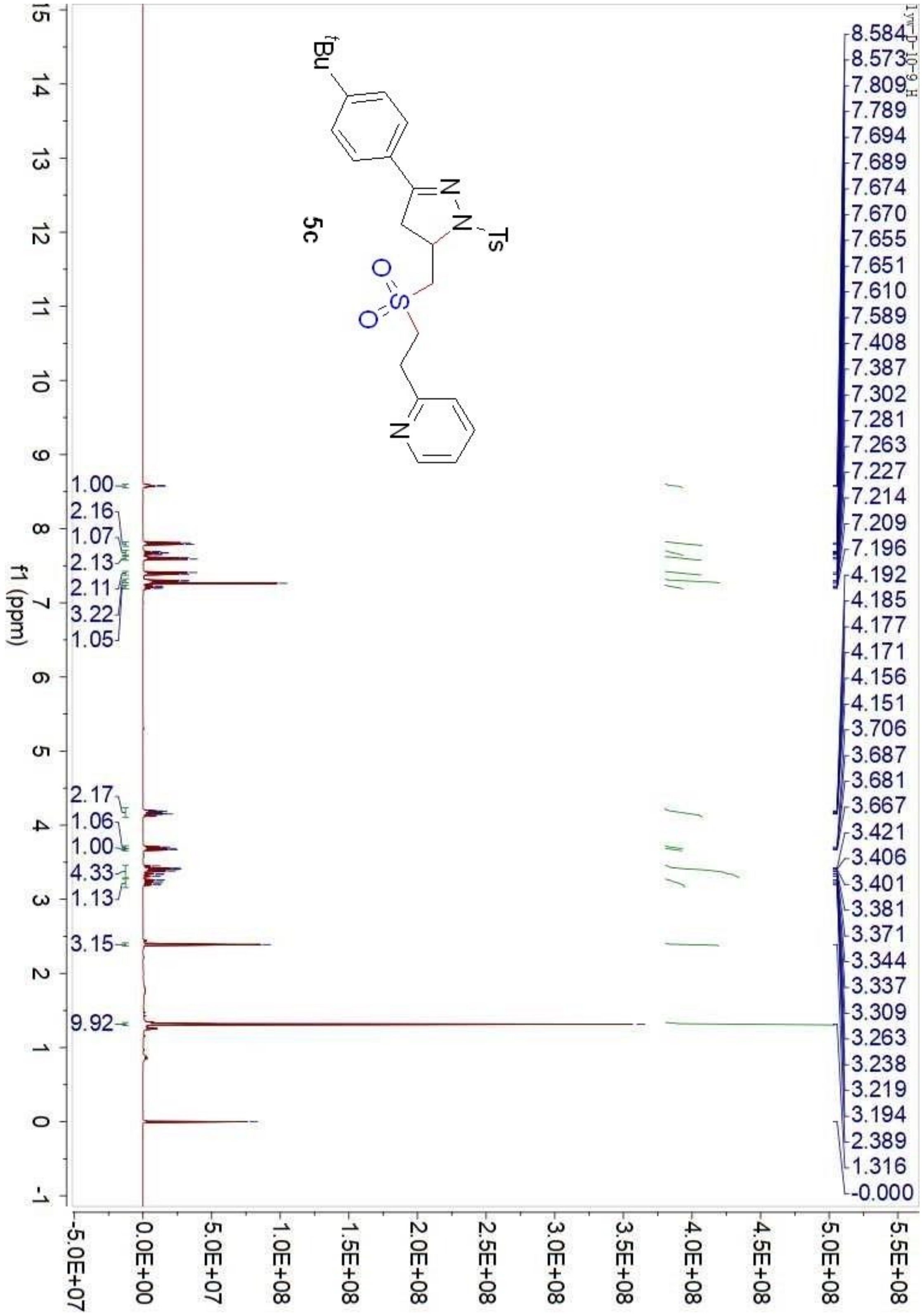

lyw-H-31-4 C
Ph
N
O
O
S
O
N
3n
174.23
157.67
149.46
136.62
133.73
130.92
128.45
127.93
123.26
121.87
67.36
58.80
53.51
35.05
30.36
29.09
f1 (ppm)


5a
Ts
1.00
2.16
3.26
7.94
2.19
2.23
4.36
1.20
3.38
8.564
7.814
7.795
7.650
7.633
7.374
7.295
7.279
4.190
4.160
3.704
3.686
3.667
3.442
3.410
3.393
2.373
0.000
f1 (ppm)

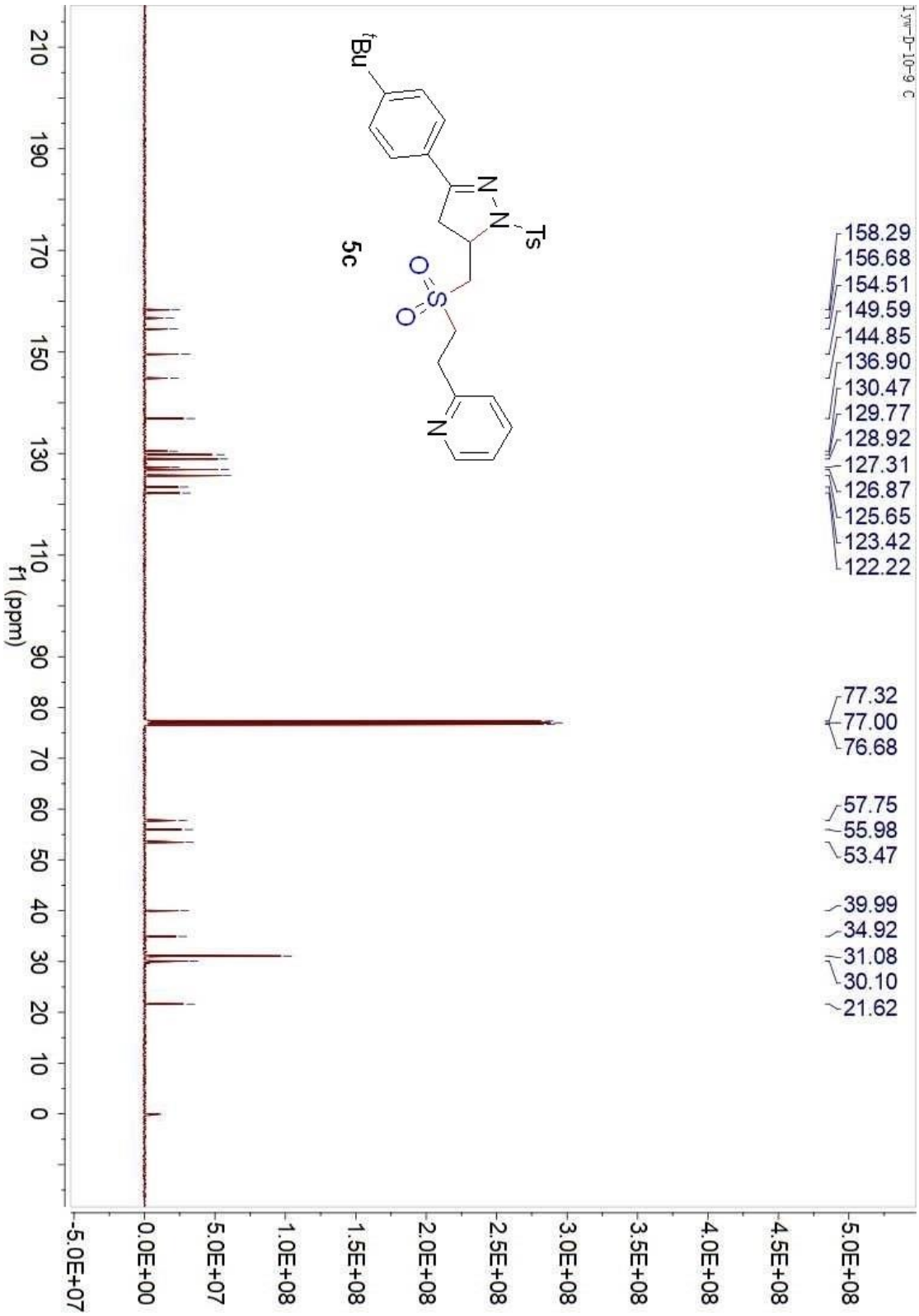

5a
Ts
158.32
156.61
149.37
144.77
136.72
130.77
130.37
129.95
129.63
128.75
128.53
126.84
123.27
122.03
77.32
77.00
76.68
57.41
55.98
53.29
39.77
29.93
21.46
f1 (ppm)

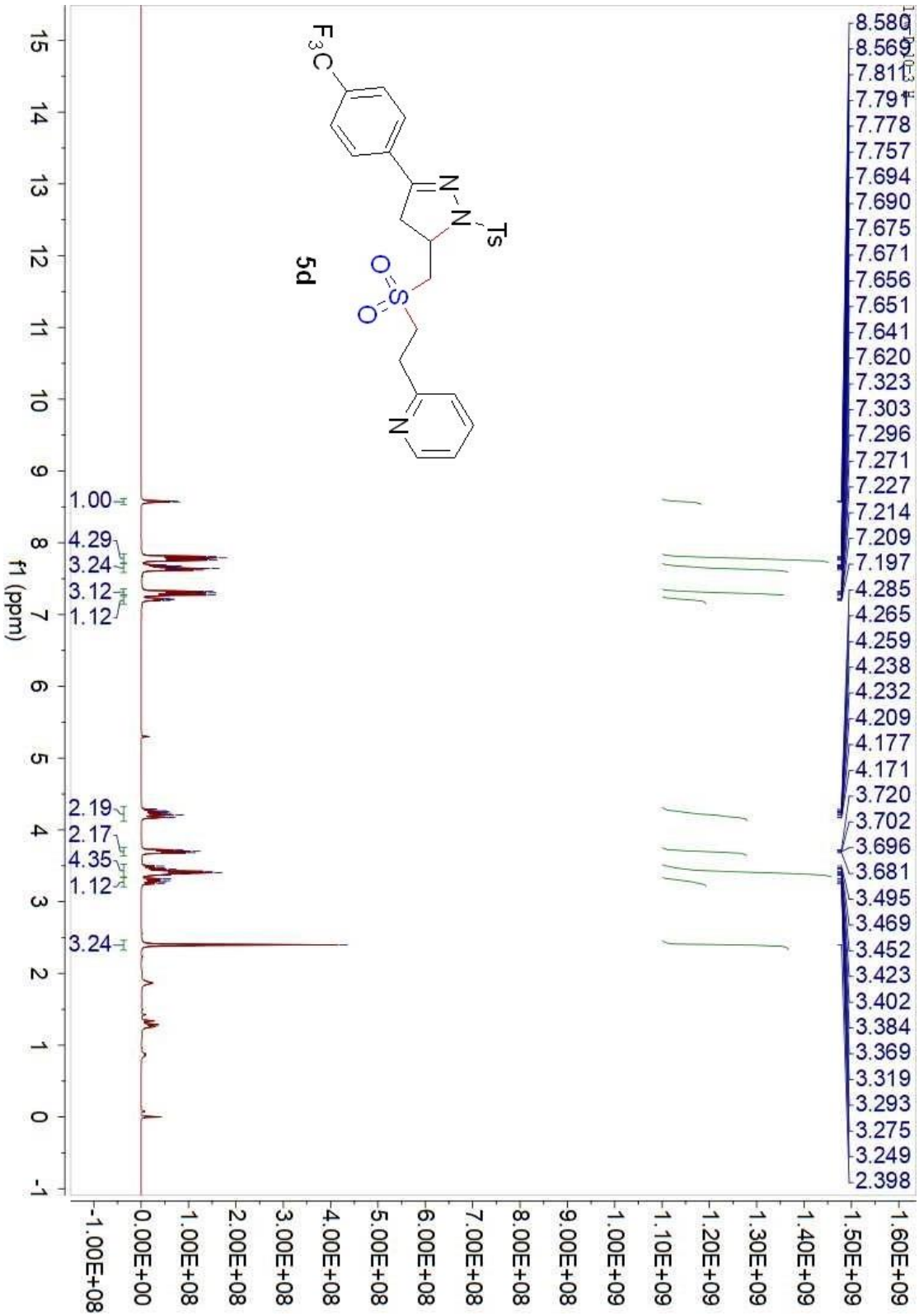

MeO
N
N
Ts
O
S
O
N
5b
lyw-D-10-1 H
8.577
8.566
7.806
7.786
7.608
7.586
7.272
6.885
6.863
3.820
3.700
3.682
3.661
3.416
3.401
3.393
3.376
2.384
0.000
1.00
2.09
1.06
2.08
3.06
1.02
2.07
2.11
3.15
2.09
4.20
1.09
3.14
f1 (ppm)

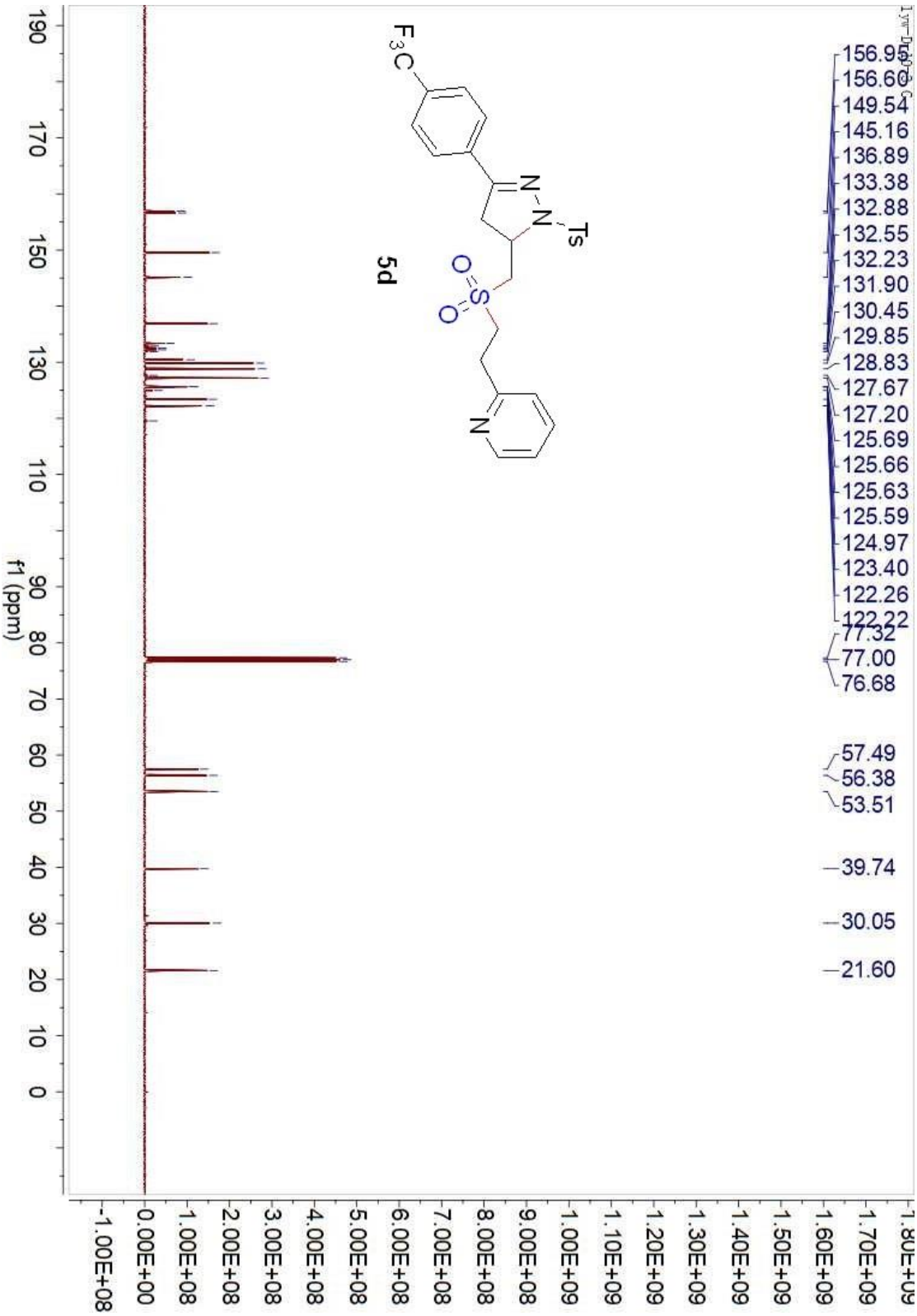

MeO
N
N
Ts
O
S
O
N
5b
161.70
158.05
156.67
149.51
144.75
136.83
130.42
129.67
128.89
128.63
123.36
122.64
122.14
114.00
77.32
77.00
76.68
57.60
55.90
55.32
53.40
39.95
30.04
21.56
f1 (ppm)

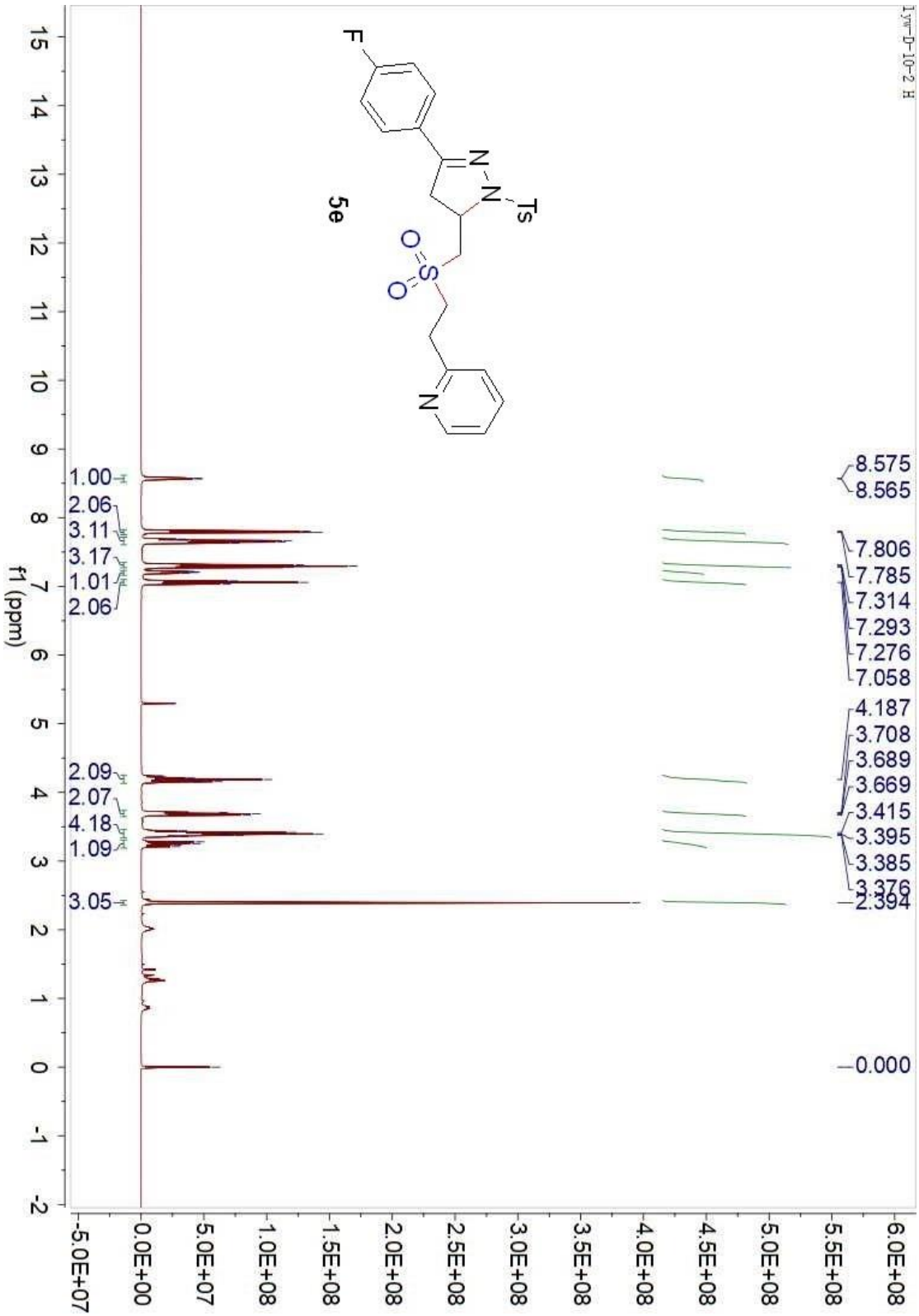


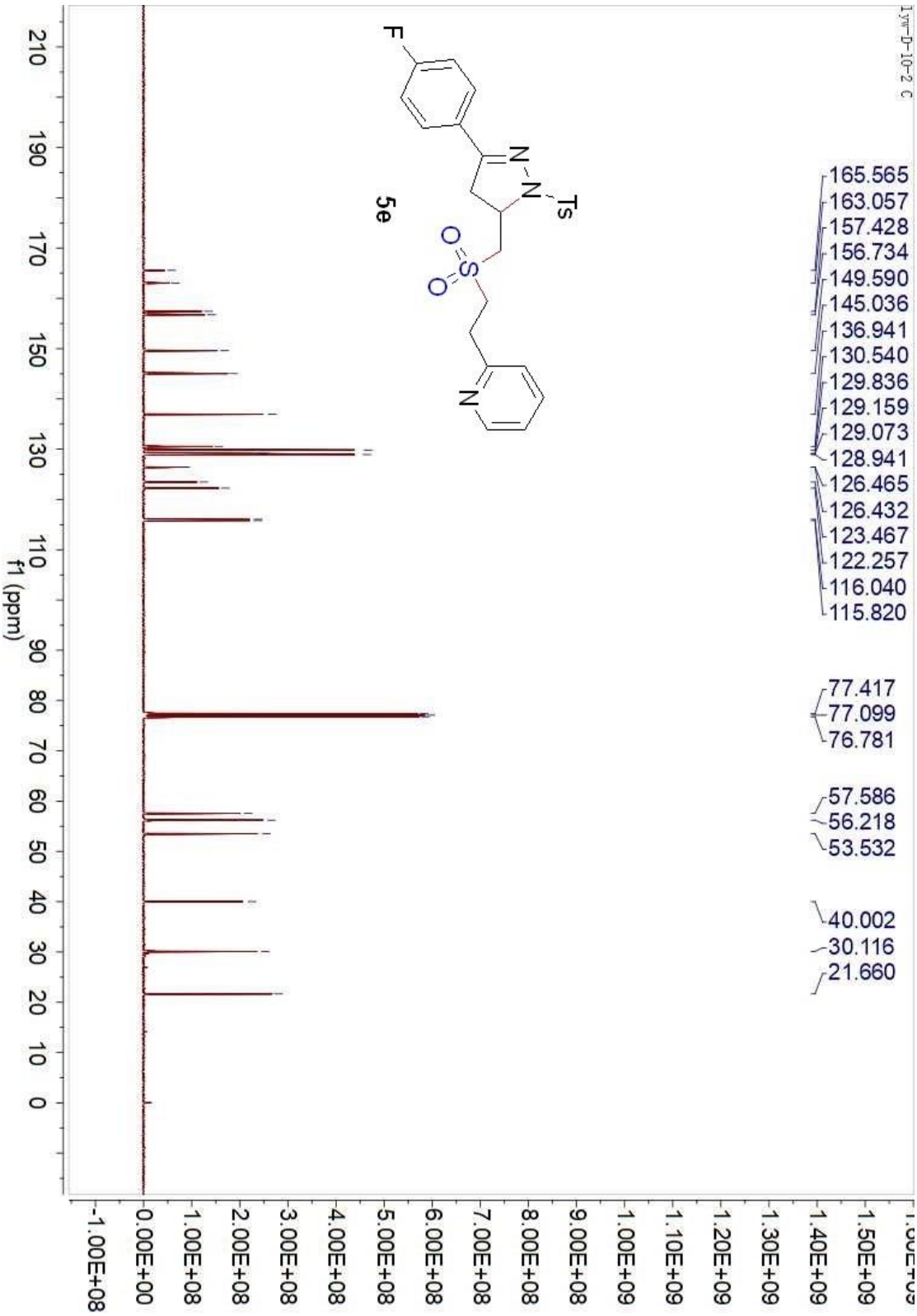
tBu
N–N
Ts
O=S=O
N
5c
f1 (ppm)
8.584
8.573
7.809
7.789
7.694
7.689
7.674
7.670
7.655
7.651
7.610
7.589
7.408
7.387
7.302
7.281
7.263
7.227
7.214
7.209
7.196
4.192
4.185
4.177
4.171
4.156
4.151
3.706
3.687
3.681
3.667
3.421
3.406
3.401
3.381
3.371
3.344
3.337
3.309
3.263
3.238
3.219
3.194
2.389
1.316
-0.000
1.00
2.16
1.07
2.13
2.11
3.22
1.05
2.17
1.06
1.00
4.33
1.13
3.15
9.92

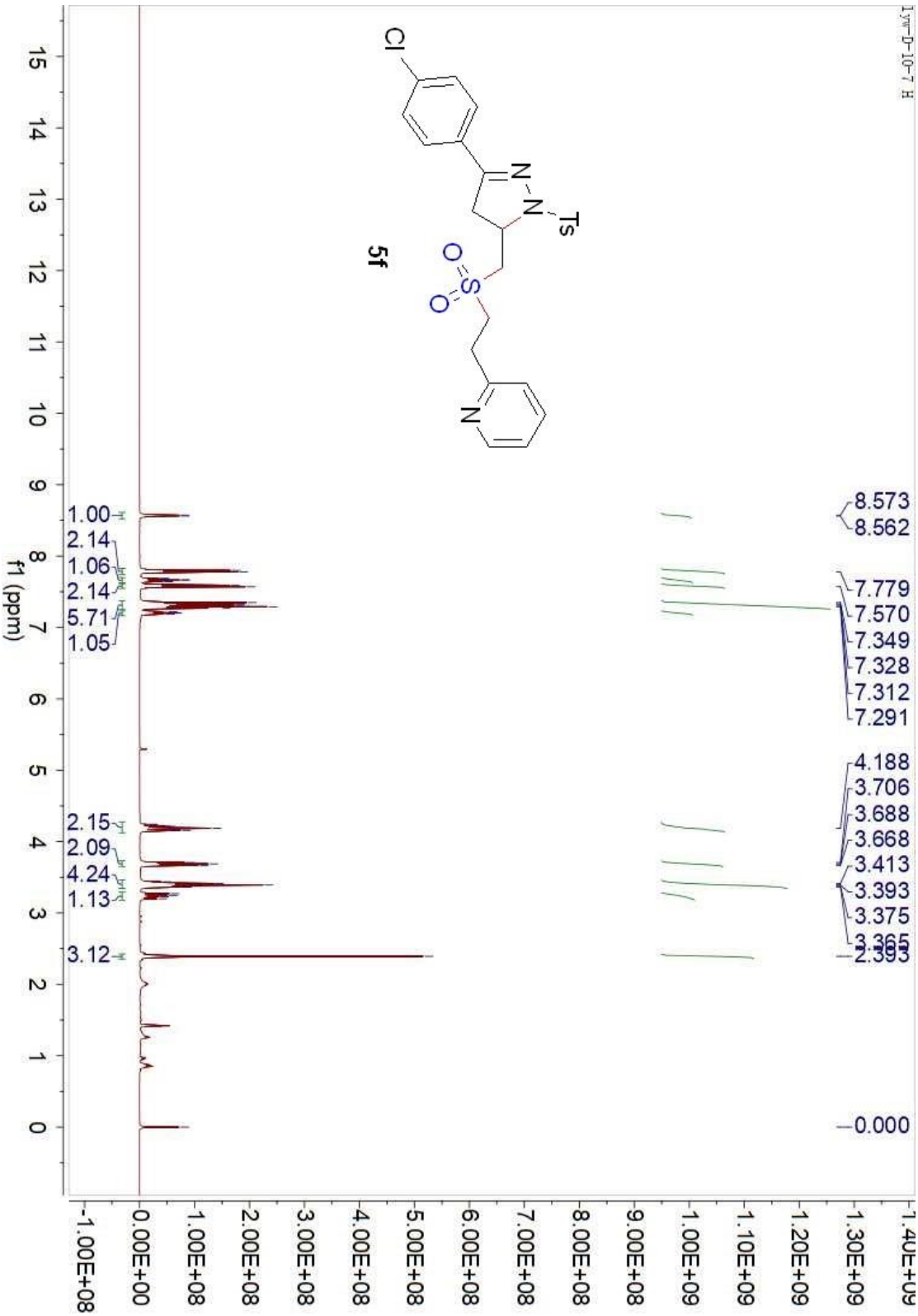

158.29
156.68
154.51
149.59
144.85
136.90
130.47
129.77
128.92
127.31
126.87
125.65
123.42
122.22
77.32
77.00
76.68
57.75
55.98
53.47
39.99
34.92
31.08
30.10
21.62
f1 (ppm)
5c

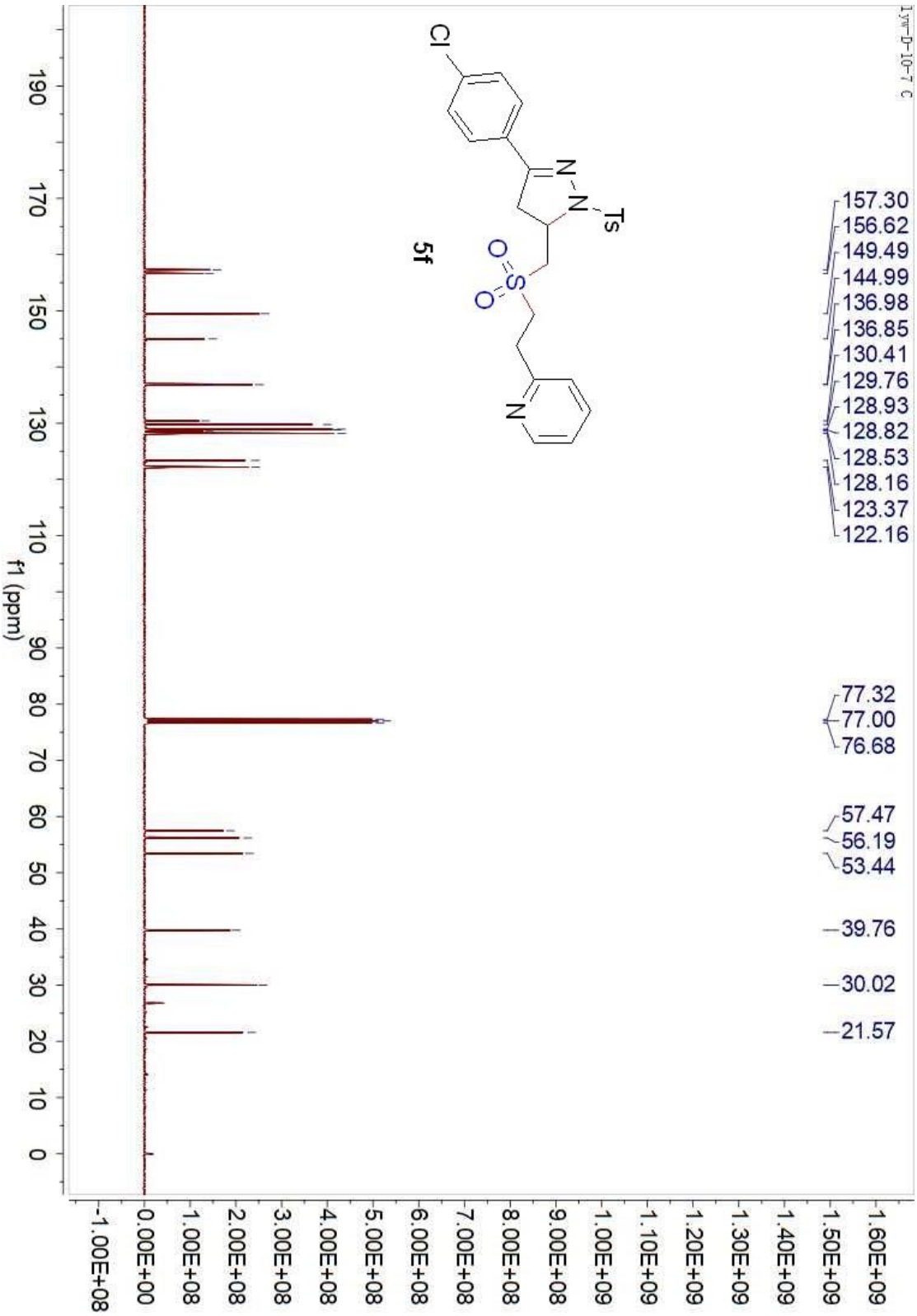

5d
Ts
1.00
4.29
3.24
3.12
1.12
2.19
2.17
4.35
1.12
3.24
f1 (ppm)

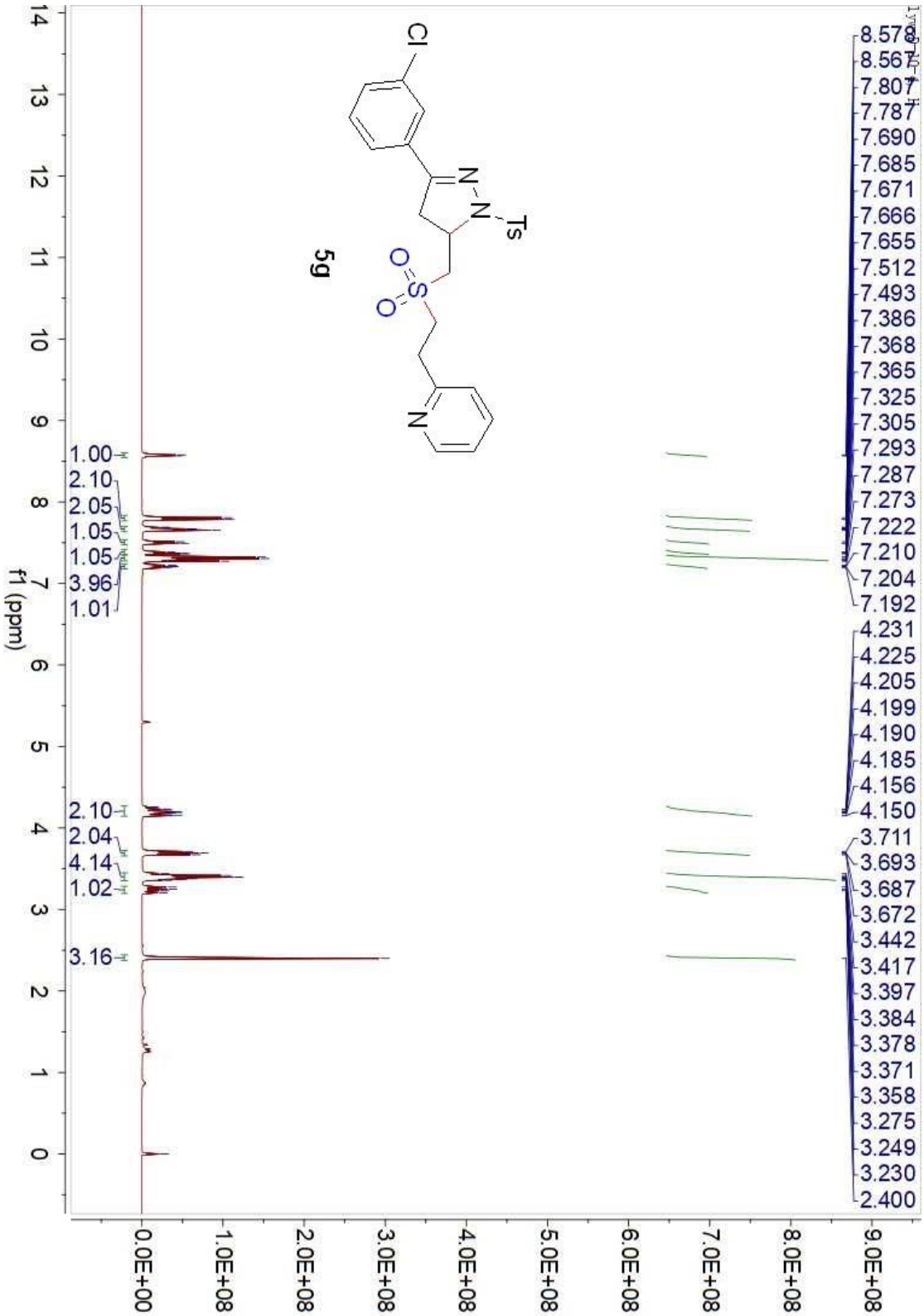

5d
156.95
156.66
149.54
145.16
136.89
133.38
132.88
132.55
132.23
131.90
130.45
129.85
128.83
127.67
127.20
125.69
125.66
125.63
125.59
124.97
123.40
122.26
122.22
77.32
77.00
76.68
57.49
56.38
53.51
39.74
30.05
21.60
f1 (ppm)

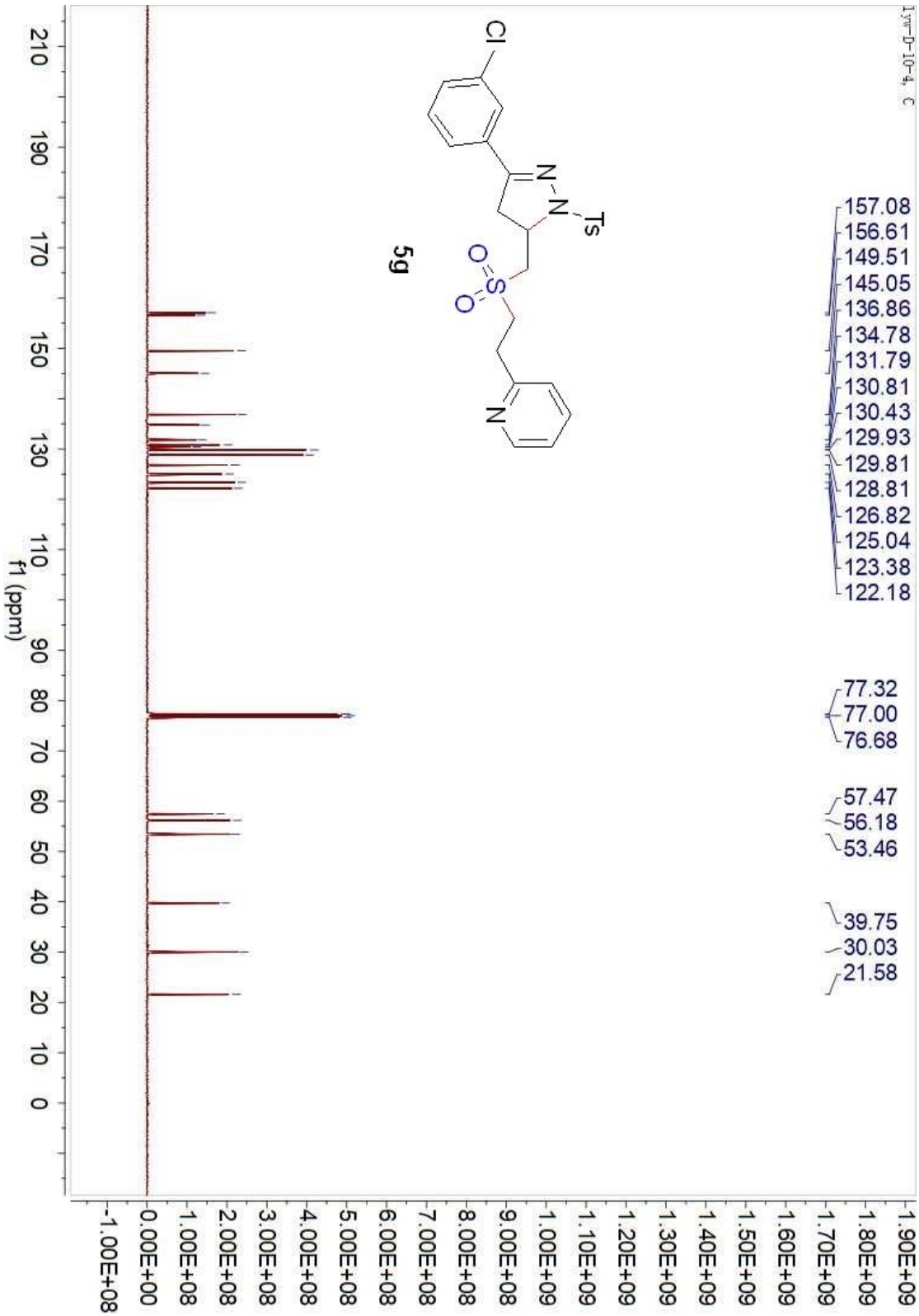

5e
F
N
N
Ts
O
S
O
N
1.00
2.06
3.11
3.17
1.01
2.06
2.09
2.07
4.18
1.09
3.05
8.575
8.565
7.806
7.785
7.314
7.293
7.276
7.058
4.187
3.708
3.689
3.669
3.415
3.395
3.385
3.376
2.394
0.000
f1 (ppm)

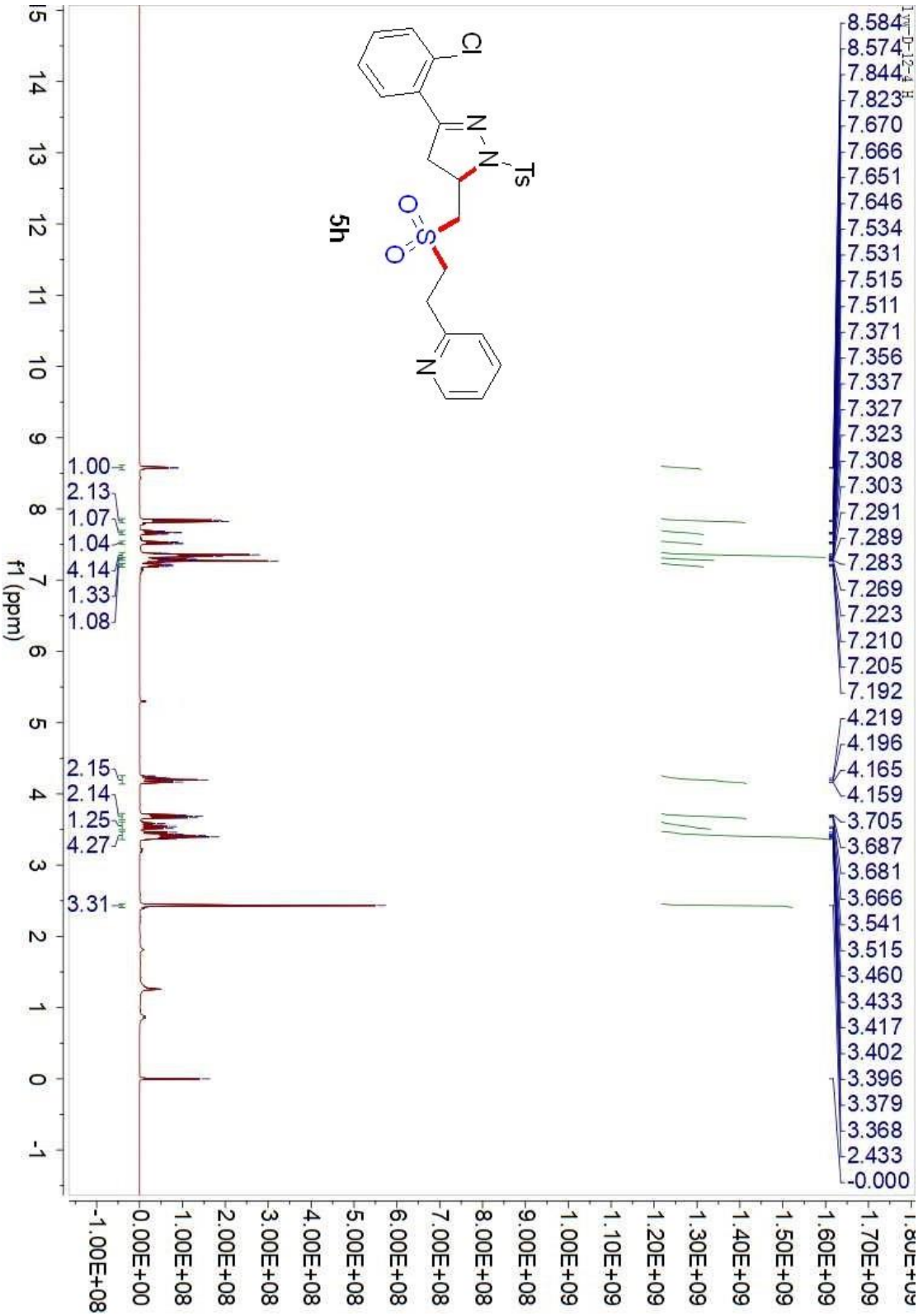

1yw-D-10-2 C
165.565
163.057
157.428
156.734
149.590
145.036
136.941
130.540
129.836
129.159
129.073
128.941
126.465
126.432
123.467
122.257
116.040
115.820
77.417
77.099
76.781
57.586
56.218
53.532
40.002
30.116
21.660
F
N
N
Ts
O
S
O
N
5e
f1 (ppm)

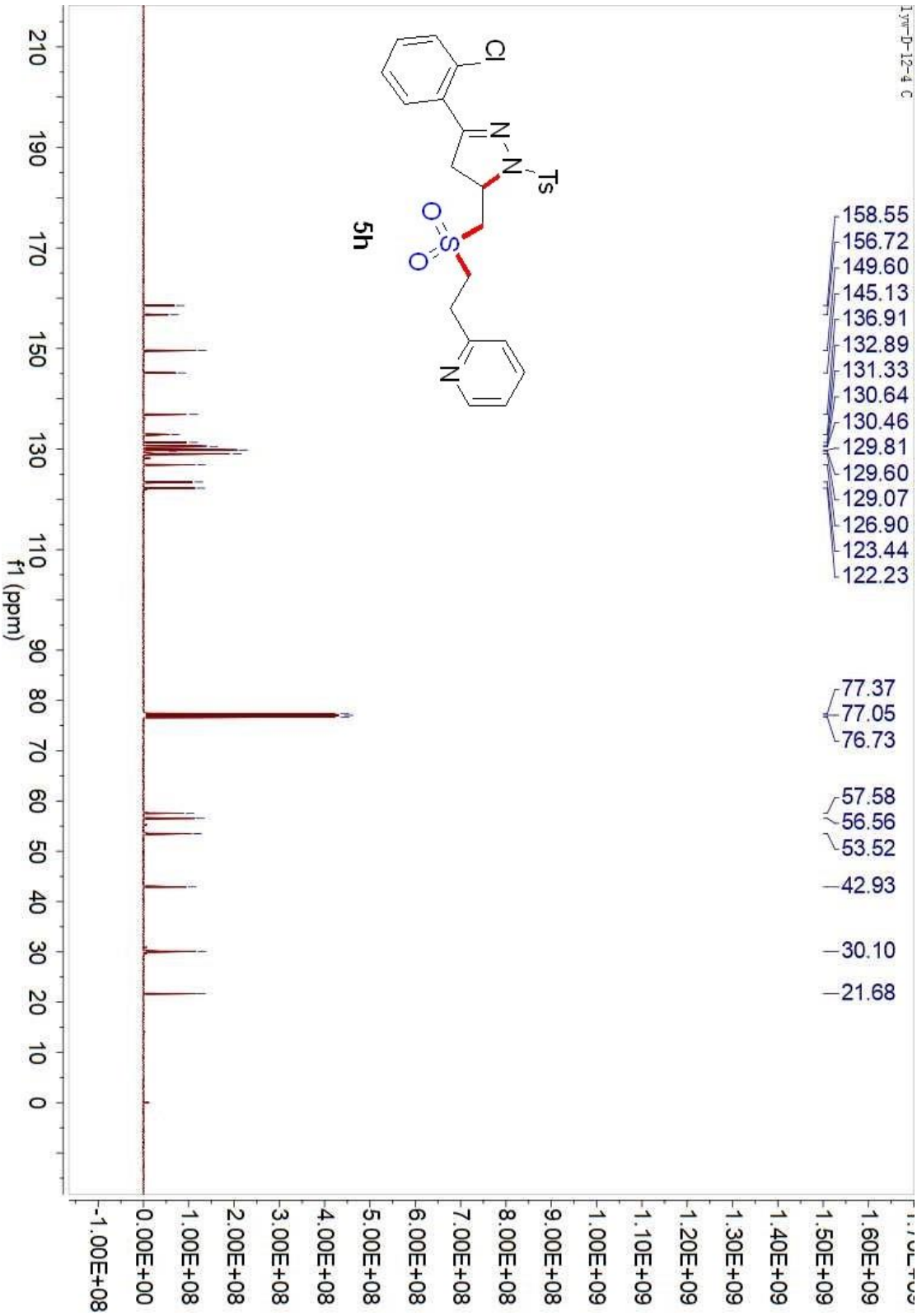

Cl
N
N
Ts
O
S
O
N
5f
8.573
8.562
7.779
7.570
7.349
7.328
7.312
7.291
4.188
3.706
3.688
3.668
3.413
3.393
3.375
2.393
0.000
1.00
2.14
1.06
2.14
5.71
1.05
2.15
2.09
4.24
1.13
3.12
f1 (ppm)

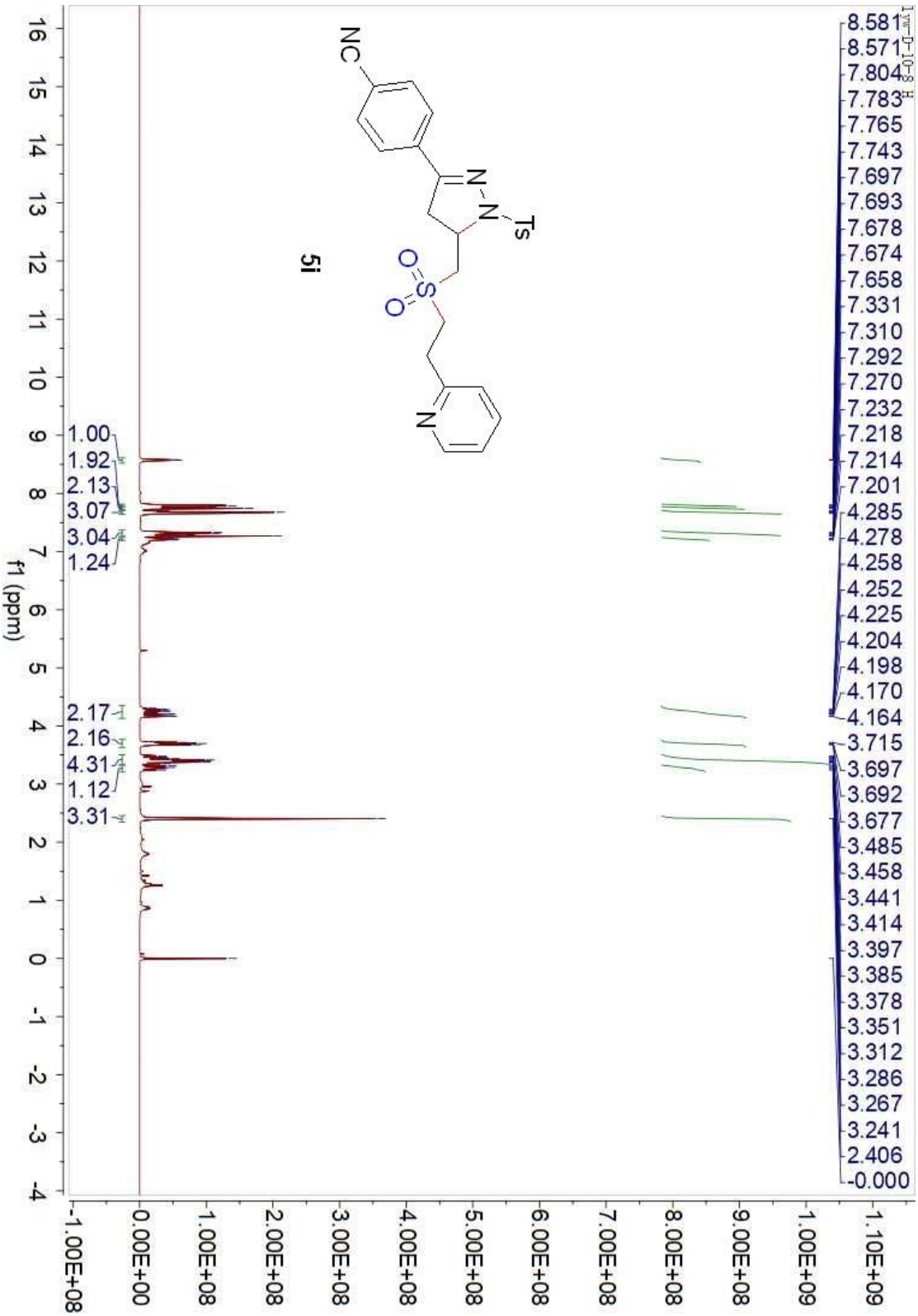

lyw-D-10-7 C
157.30
156.62
149.49
144.99
136.98
136.85
130.41
129.76
128.93
128.82
128.53
128.16
123.37
122.16
77.32
77.00
76.68
57.47
56.19
53.44
39.76
30.02
21.57
Cl
N
N
Ts
O
S
O
N
5f
f1 (ppm)

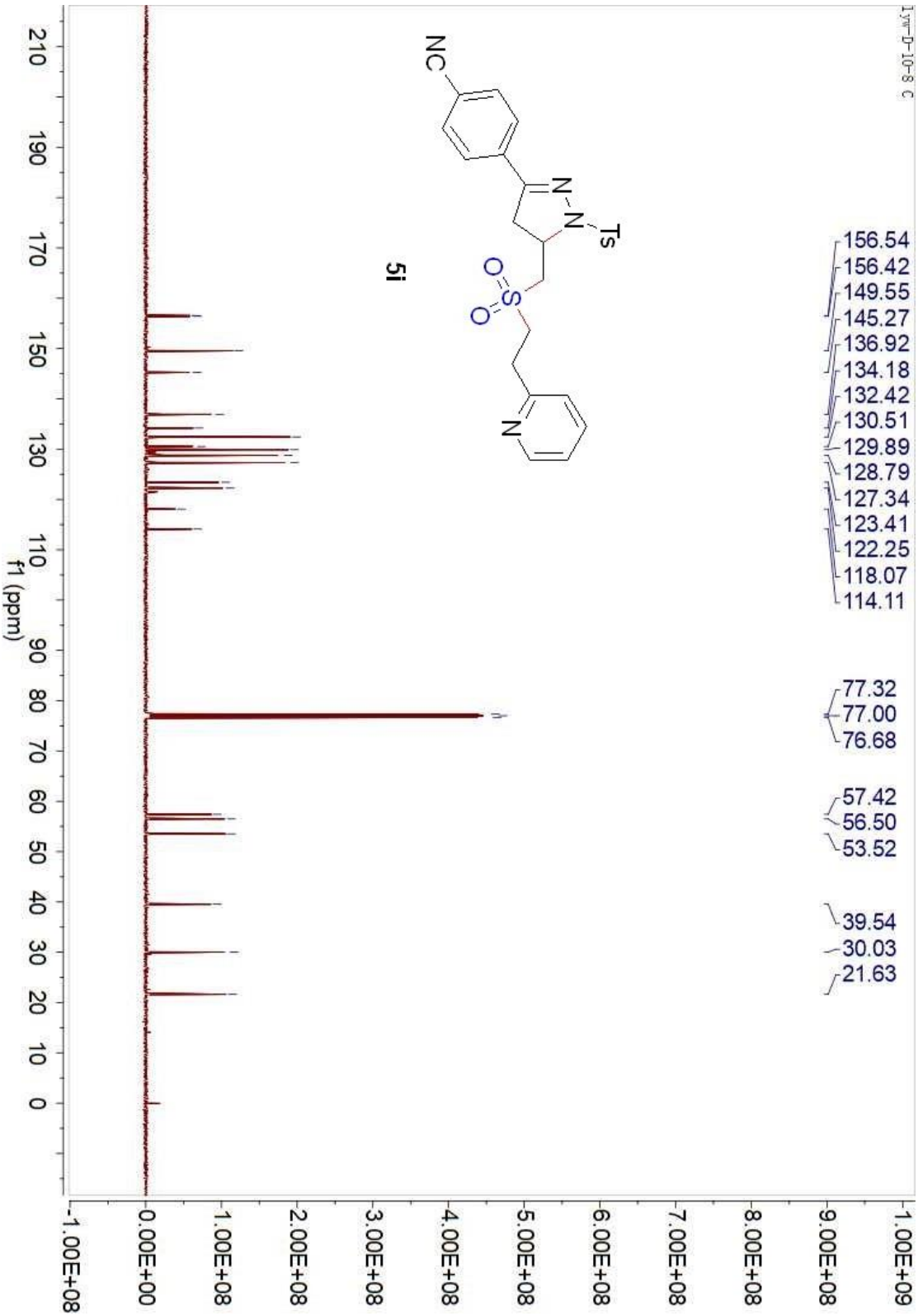

Cl
N
N
Ts
O
S
O
N
5g
f1 (ppm)
1.00
2.10
2.05
1.05
1.05
3.96
1.01
2.10
2.04
4.14
1.02
3.16
8.578
8.567
7.807
7.787
7.690
7.685
7.671
7.666
7.655
7.512
7.493
7.386
7.368
7.365
7.325
7.305
7.293
7.287
7.273
7.222
7.210
7.204
7.192
4.231
4.225
4.205
4.199
4.190
4.185
4.156
4.150
3.711
3.693
3.687
3.672
3.442
3.417
3.397
3.384
3.378
3.371
3.358
3.275
3.249
3.230
2.400

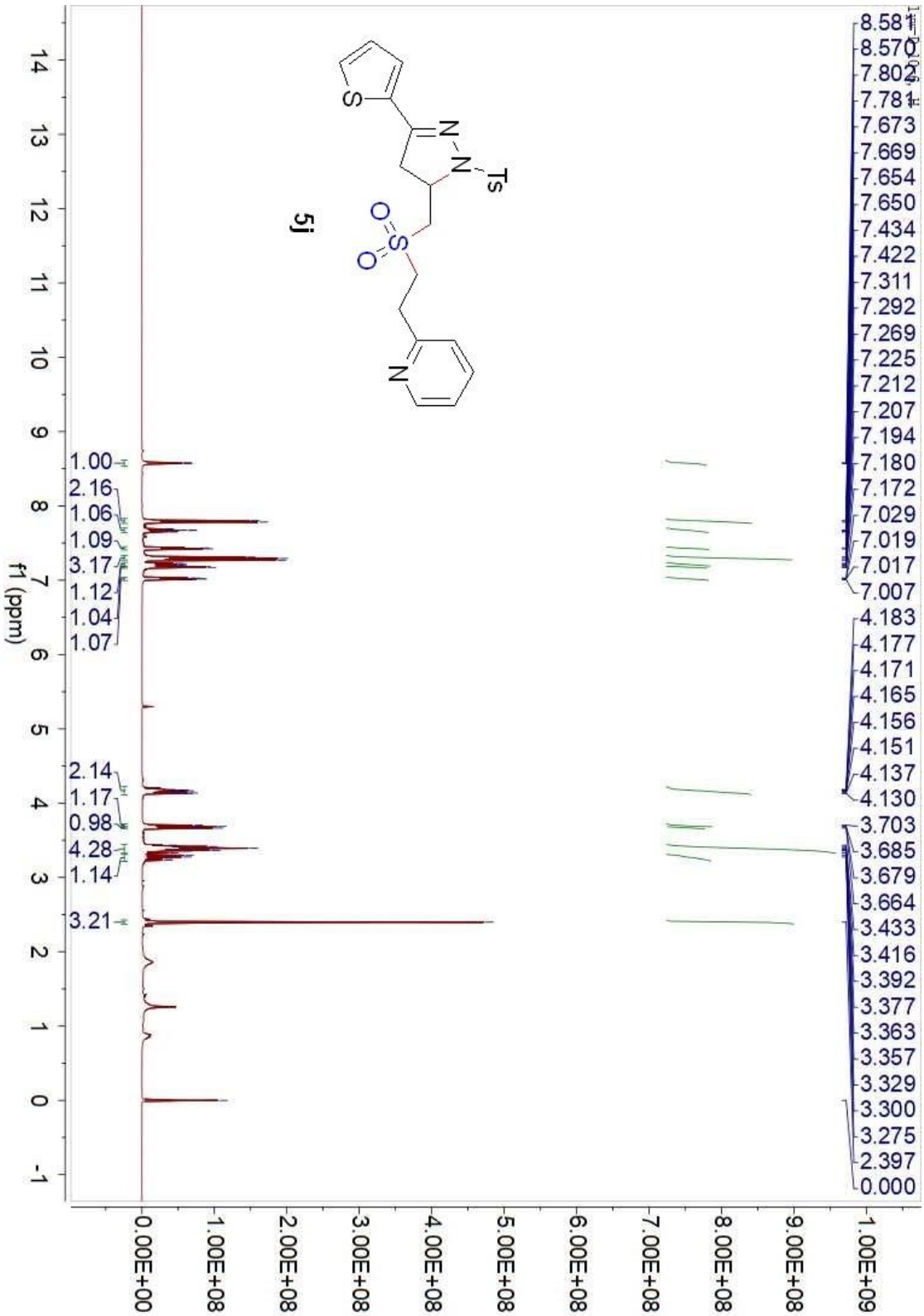

Cl
N
N
Ts
O
S
O
N
5g
157.08
156.61
149.51
145.05
136.86
134.78
131.79
130.81
130.43
129.93
129.81
128.81
126.82
125.04
123.38
122.18
77.32
77.00
76.68
57.47
56.18
53.46
39.75
30.03
21.58
f1 (ppm)

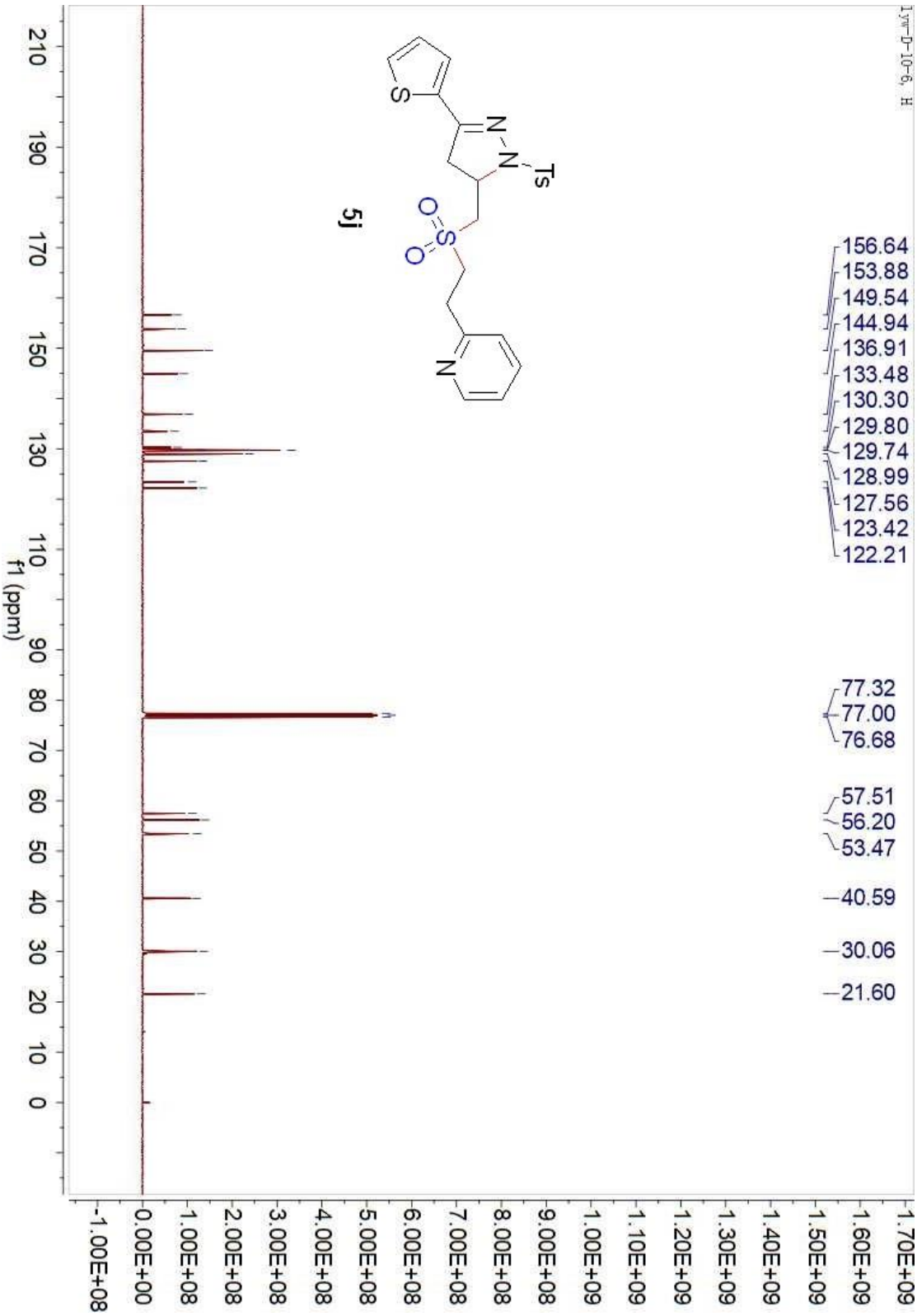

5h
Cl
N
N
Ts
O
O
S
N
f1 (ppm)
1.00
2.13
1.07
1.04
4.14
1.33
1.08
2.15
2.14
1.25
4.27
3.31
8.584
8.574
7.844
7.823
7.670
7.666
7.651
7.646
7.534
7.531
7.515
7.511
7.371
7.356
7.337
7.327
7.323
7.308
7.303
7.291
7.289
7.283
7.269
7.223
7.210
7.205
7.192
4.219
4.196
4.165
4.159
3.705
3.687
3.681
3.666
3.541
3.515
3.460
3.433
3.417
3.402
3.396
3.379
3.368
2.433
-0.000

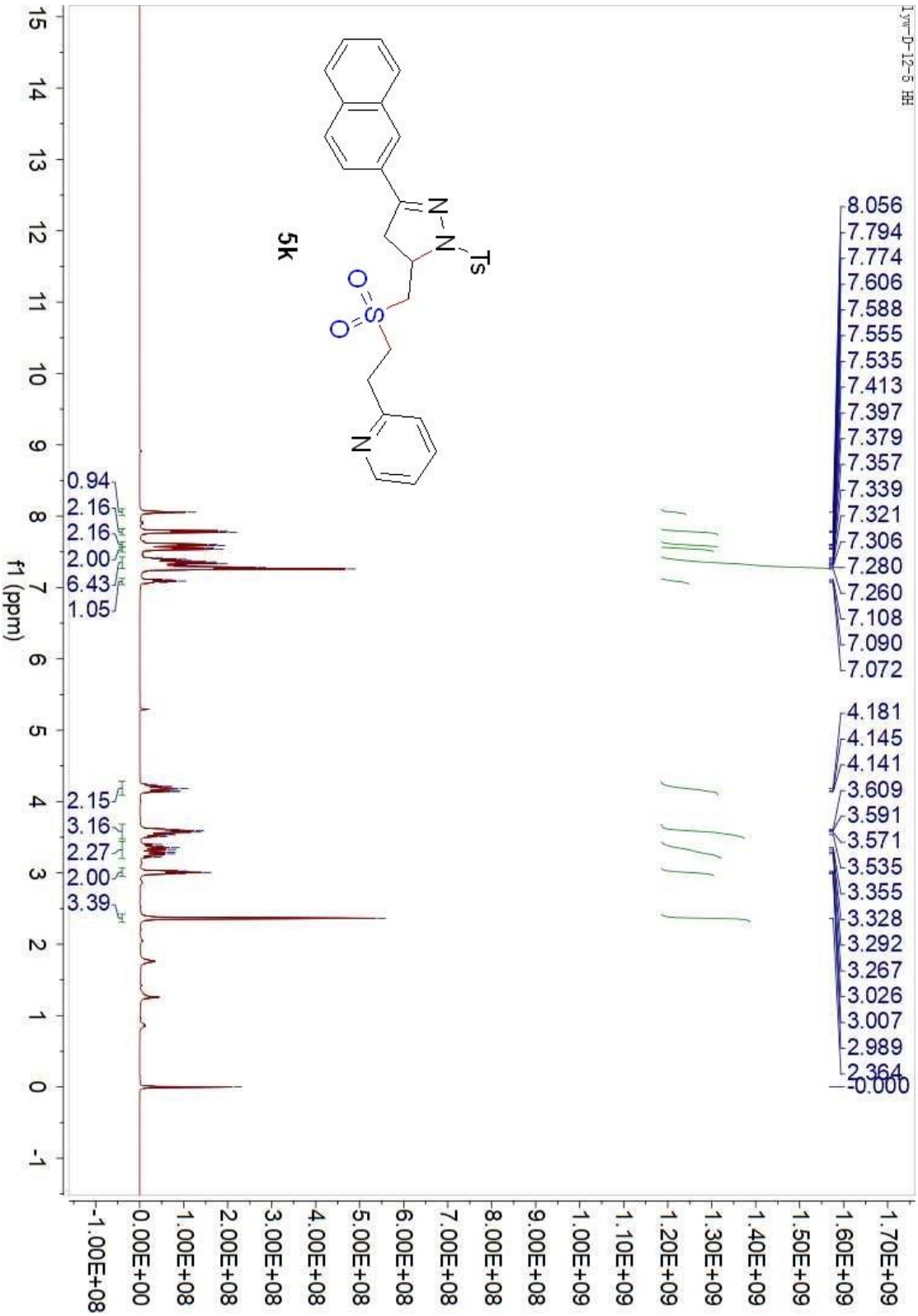

158.55
156.72
149.60
145.13
136.91
132.89
131.33
130.64
130.46
129.81
129.60
129.07
126.90
123.44
122.23
77.37
77.05
76.73
57.58
56.56
53.52
42.93
30.10
21.68
5h
Cl
N
N
Ts
O
O
S
N
f1 (ppm)

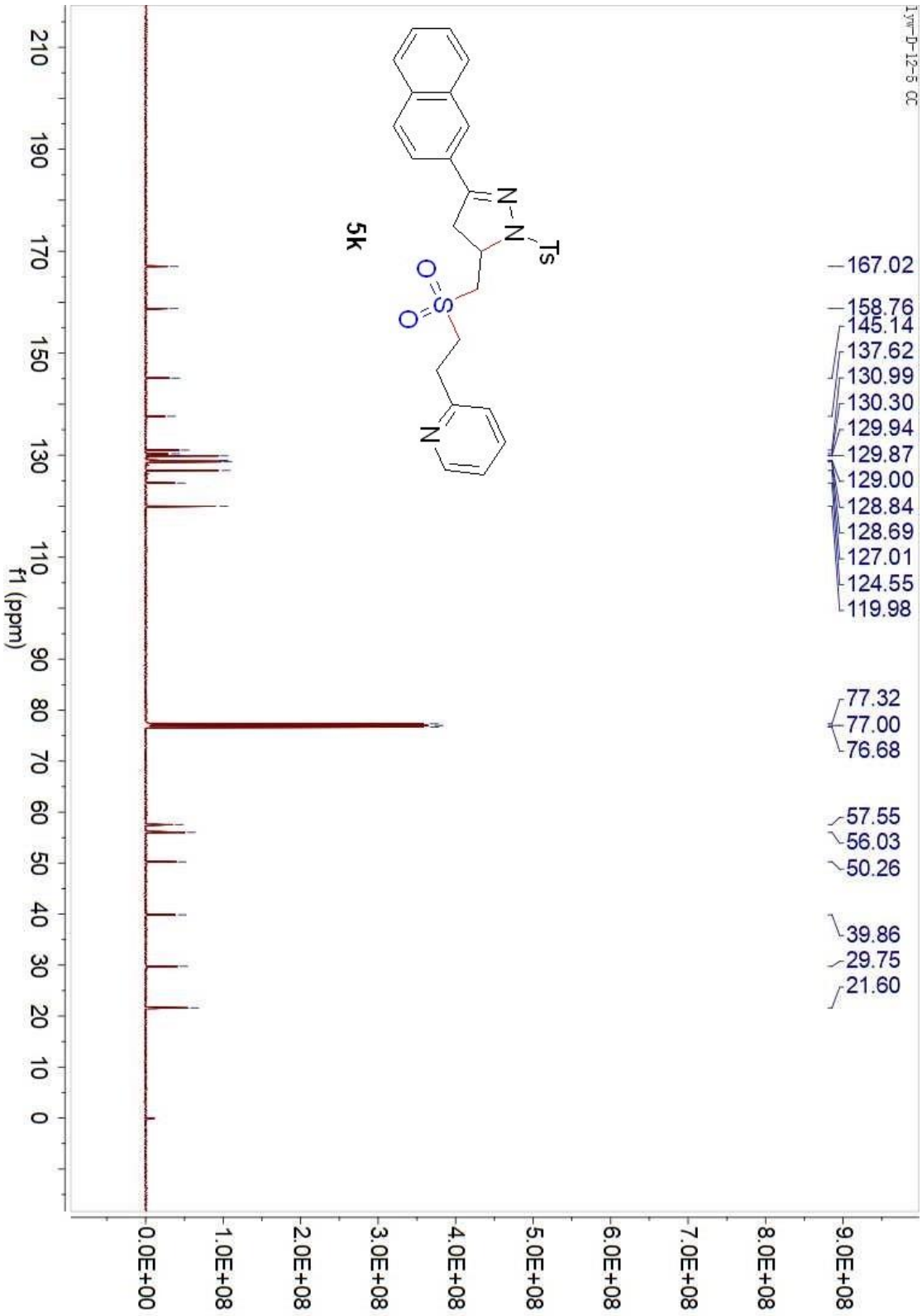

5i
NC
N
N
Ts
O
S
O
N
f1 (ppm)
1.00
1.92
2.13
3.07
3.04
1.24
2.17
2.16
4.31
1.12
3.31
8.581
8.571
7.804
7.783
7.765
7.743
7.697
7.693
7.678
7.674
7.658
7.331
7.310
7.292
7.270
7.232
7.218
7.214
7.201
4.285
4.278
4.258
4.252
4.225
4.204
4.198
4.170
4.164
3.715
3.697
3.692
3.677
3.485
3.458
3.441
3.414
3.397
3.385
3.378
3.351
3.312
3.286
3.267
3.241
2.406
-0.000

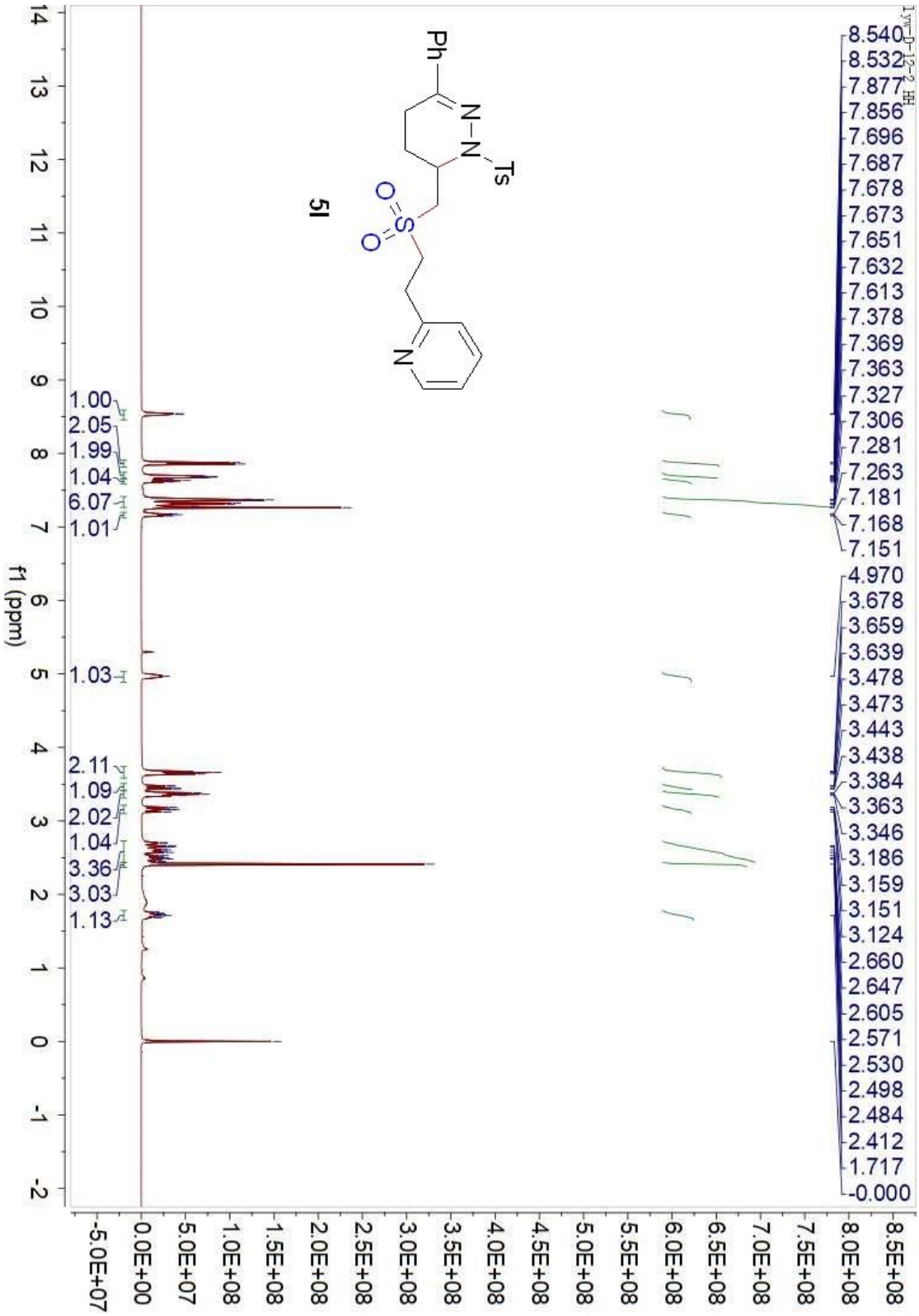

lyw-D-10-8 C
NC
N
N
Ts
O
S
O
N
5i
156.54
156.42
149.55
145.27
136.92
134.18
132.42
130.51
129.89
128.79
127.34
123.41
122.25
118.07
114.11
77.32
77.00
76.68
57.42
56.50
53.52
39.54
30.03
21.63
f1 (ppm)

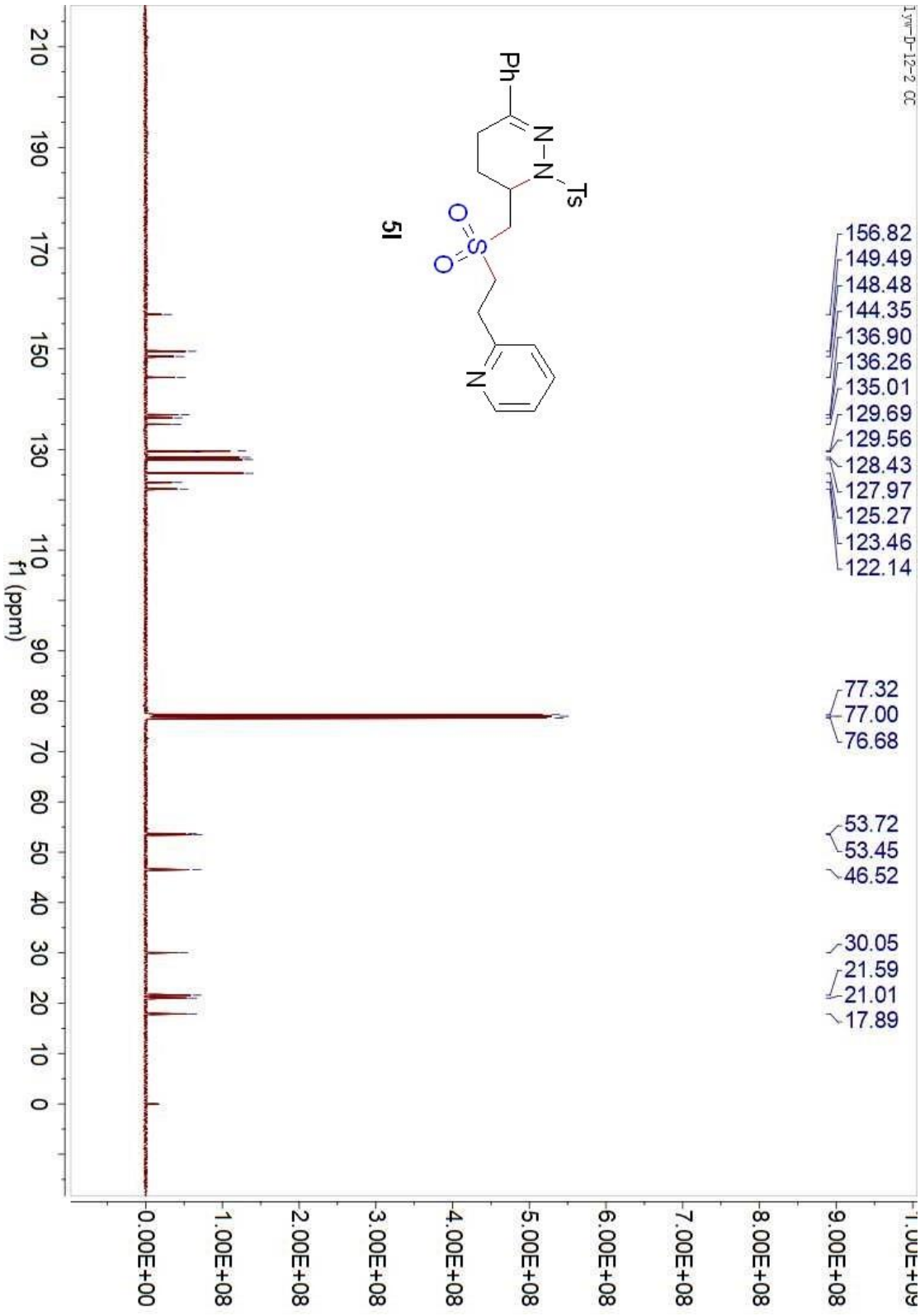

5j
f1 (ppm)
1.00
2.16
1.06
1.09
3.17
1.12
1.04
1.07
2.14
1.17
0.98
4.28
1.14
3.21
8.581
8.570
7.802
7.781
7.673
7.669
7.654
7.650
7.434
7.422
7.311
7.292
7.269
7.225
7.212
7.207
7.194
7.180
7.172
7.029
7.019
7.017
7.007
4.183
4.177
4.171
4.165
4.156
4.151
4.137
4.130
3.703
3.685
3.679
3.664
3.433
3.416
3.392
3.377
3.363
3.357
3.329
3.300
3.275
2.397
0.000

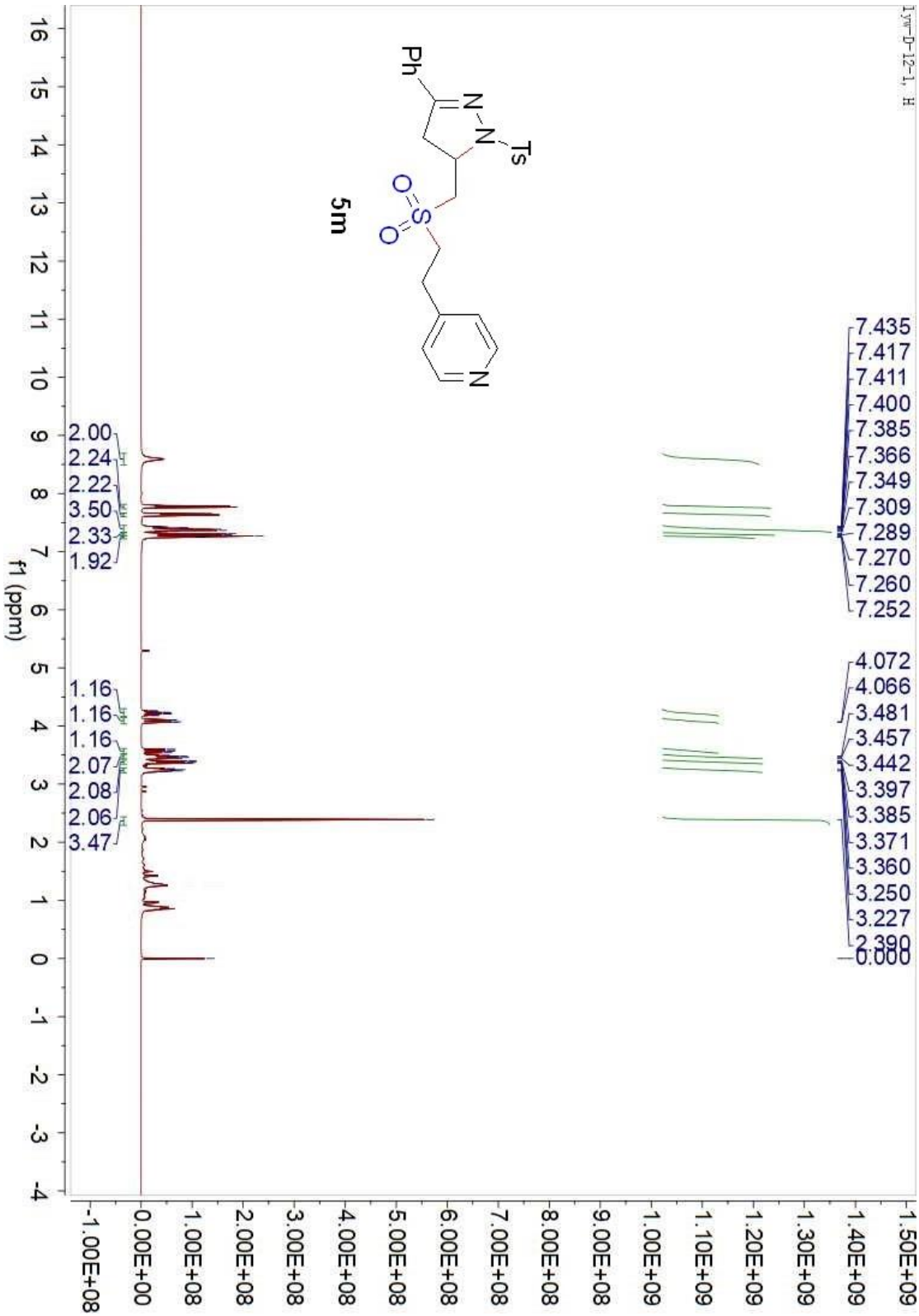

lyw-D-10-6, H
156.64
153.88
149.54
144.94
136.91
133.48
130.30
129.80
129.74
128.99
127.56
123.42
122.21
77.32
77.00
76.68
57.51
56.20
53.47
40.59
30.06
21.60
5j
Ts
f1 (ppm)

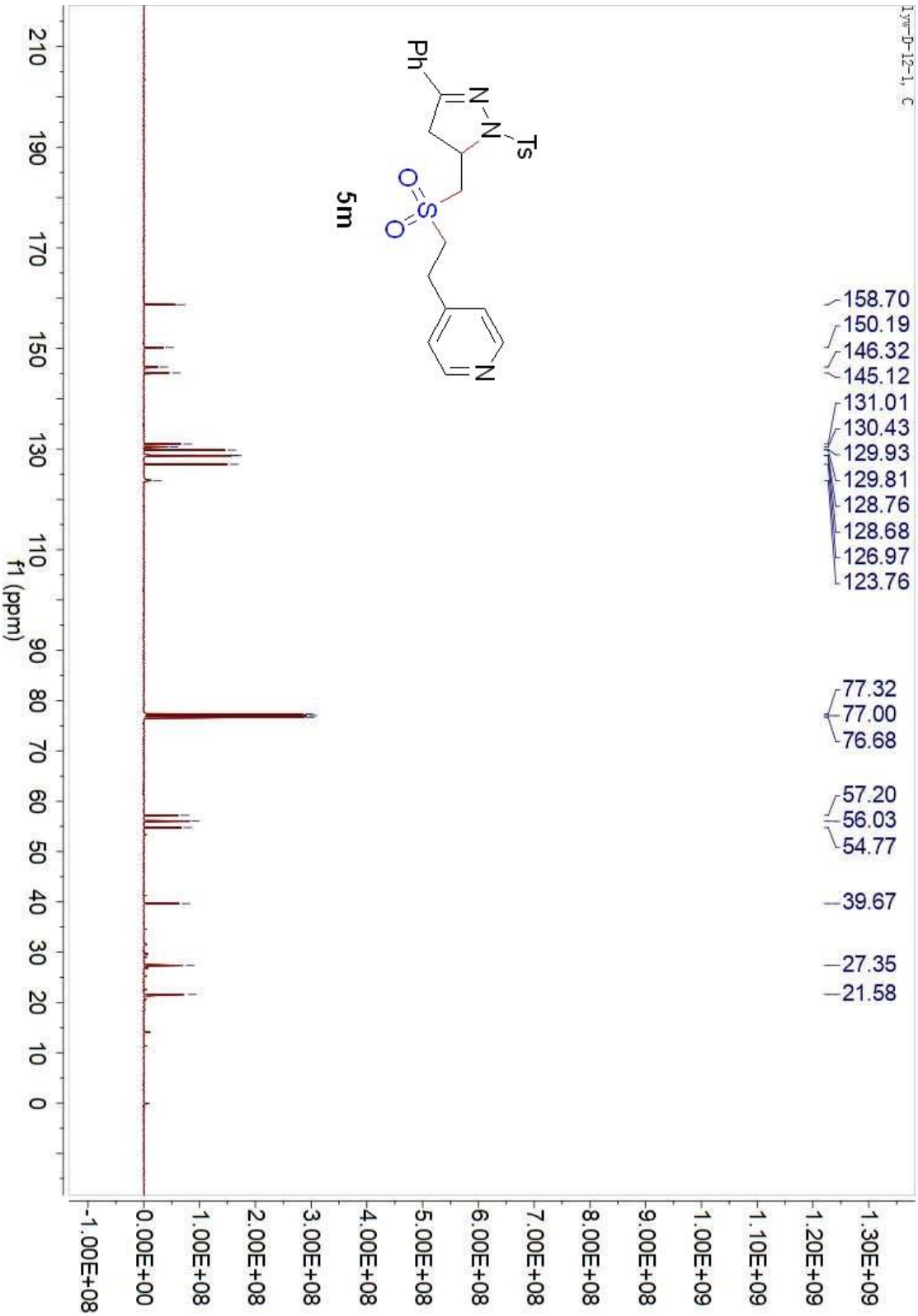

5k
Ts
N
S
O
f1 (ppm)
0.94
2.16
2.16
2.00
6.43
1.05
2.15
3.16
2.27
2.00
3.39
8.056
7.794
7.774
7.606
7.588
7.555
7.535
7.413
7.397
7.379
7.357
7.339
7.321
7.306
7.280
7.260
7.108
7.090
7.072
4.181
4.145
4.141
3.609
3.591
3.571
3.535
3.355
3.328
3.292
3.267
3.026
3.007
2.989
2.364
-0.000

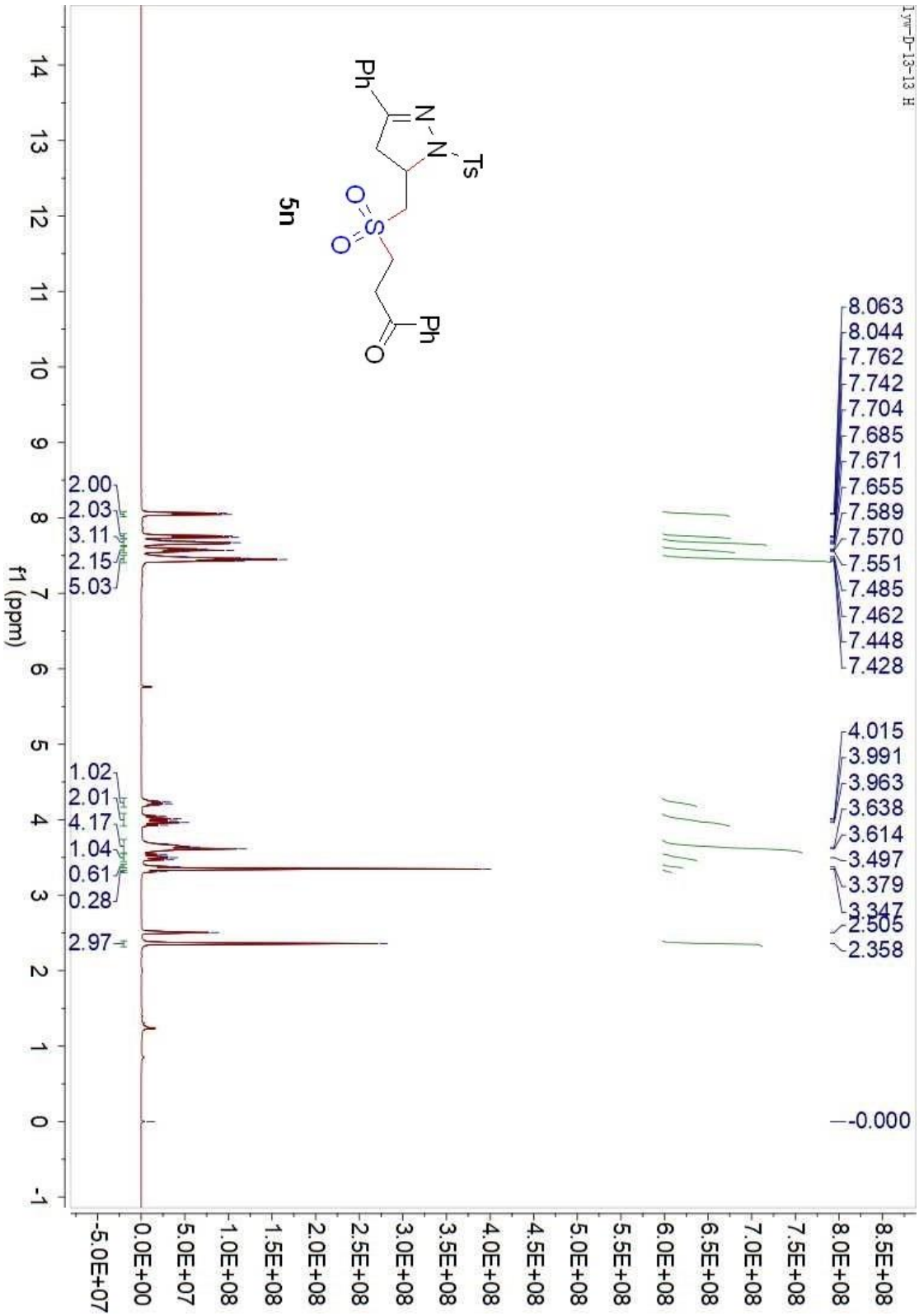

5k
Ts
167.02
158.76
145.14
137.62
130.99
130.30
129.94
129.87
129.00
128.84
128.69
127.01
124.55
119.98
77.32
77.00
76.68
57.55
56.03
50.26
39.86
29.75
21.60
f1 (ppm)

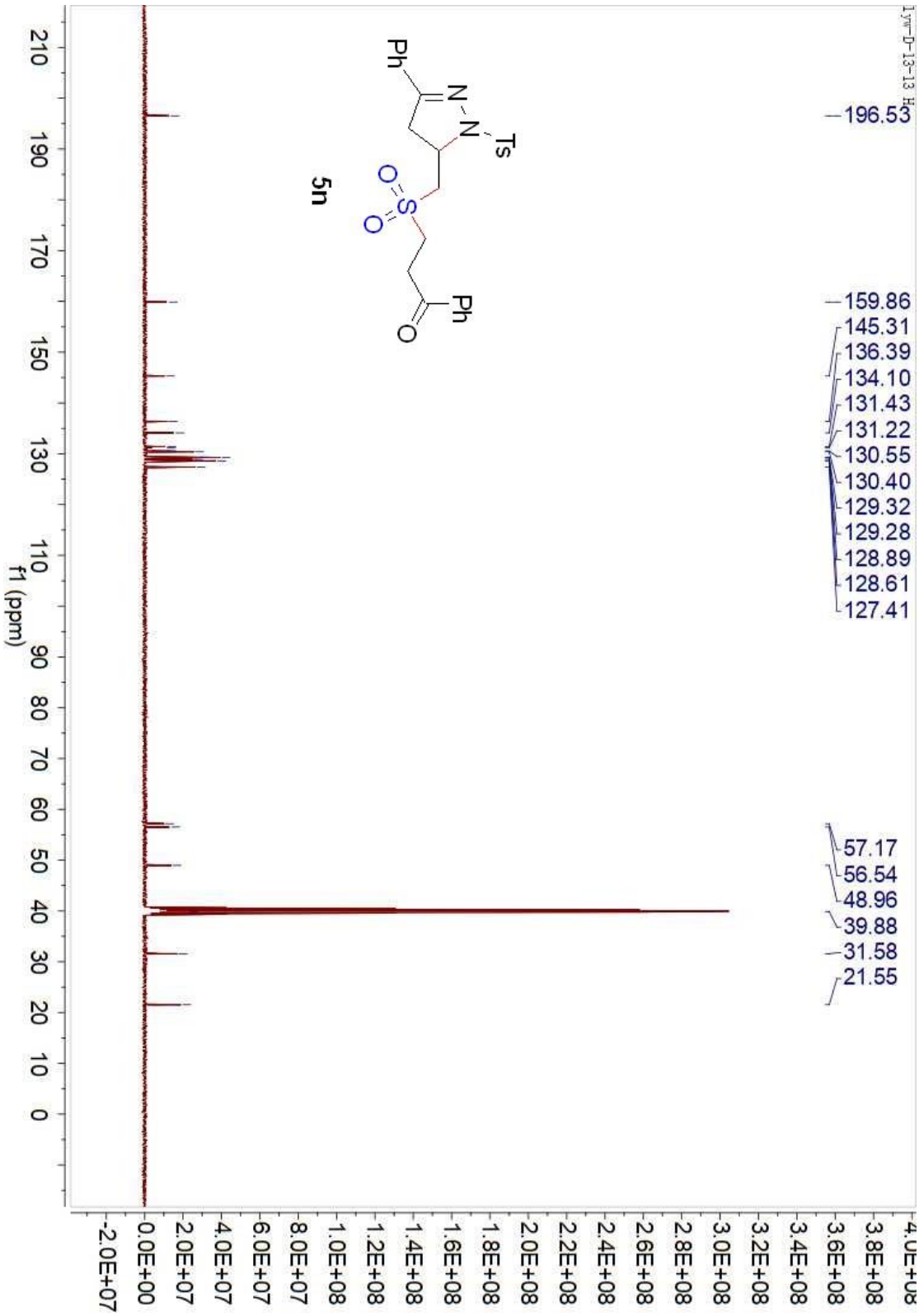

5l
Ph
N–N
Ts
O
O
S
N
f1 (ppm)
1.00
2.05
1.99
1.04
6.07
1.01
1.03
2.11
1.09
2.02
1.04
3.36
3.03
1.13
8.540
8.532
7.877
7.856
7.696
7.687
7.678
7.673
7.651
7.632
7.613
7.378
7.369
7.363
7.327
7.306
7.281
7.263
7.181
7.168
7.151
4.970
3.678
3.659
3.639
3.478
3.473
3.443
3.438
3.384
3.363
3.346
3.186
3.159
3.151
3.124
2.660
2.647
2.605
2.571
2.530
2.498
2.484
2.412
1.717
-0.000

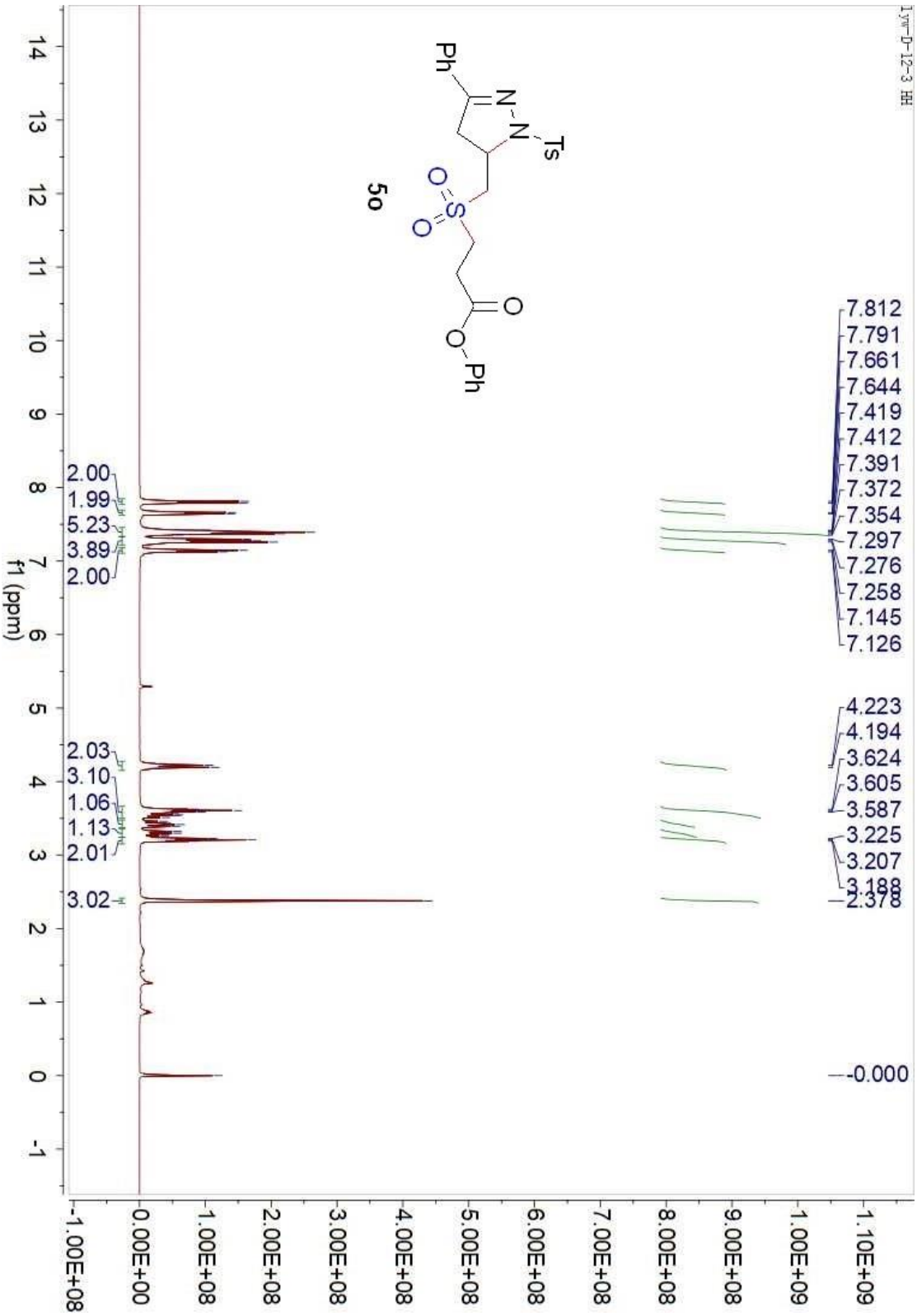

lyw-D-12-2 CC
Ph
N–N
Ts
O
O
S
N
5l
156.82
149.49
148.48
144.35
136.90
136.26
135.01
129.69
129.56
128.43
127.97
125.27
123.46
122.14
77.32
77.00
76.68
53.72
53.45
46.52
30.05
21.59
21.01
17.89
f1 (ppm)
0
10
20
30
40
50
60
70
80
90
110
130
150
170
190
210
0.00E+00
1.00E+08
2.00E+08
3.00E+08
4.00E+08
5.00E+08
6.00E+08
7.00E+08
8.00E+08
9.00E+08
1.00E+09

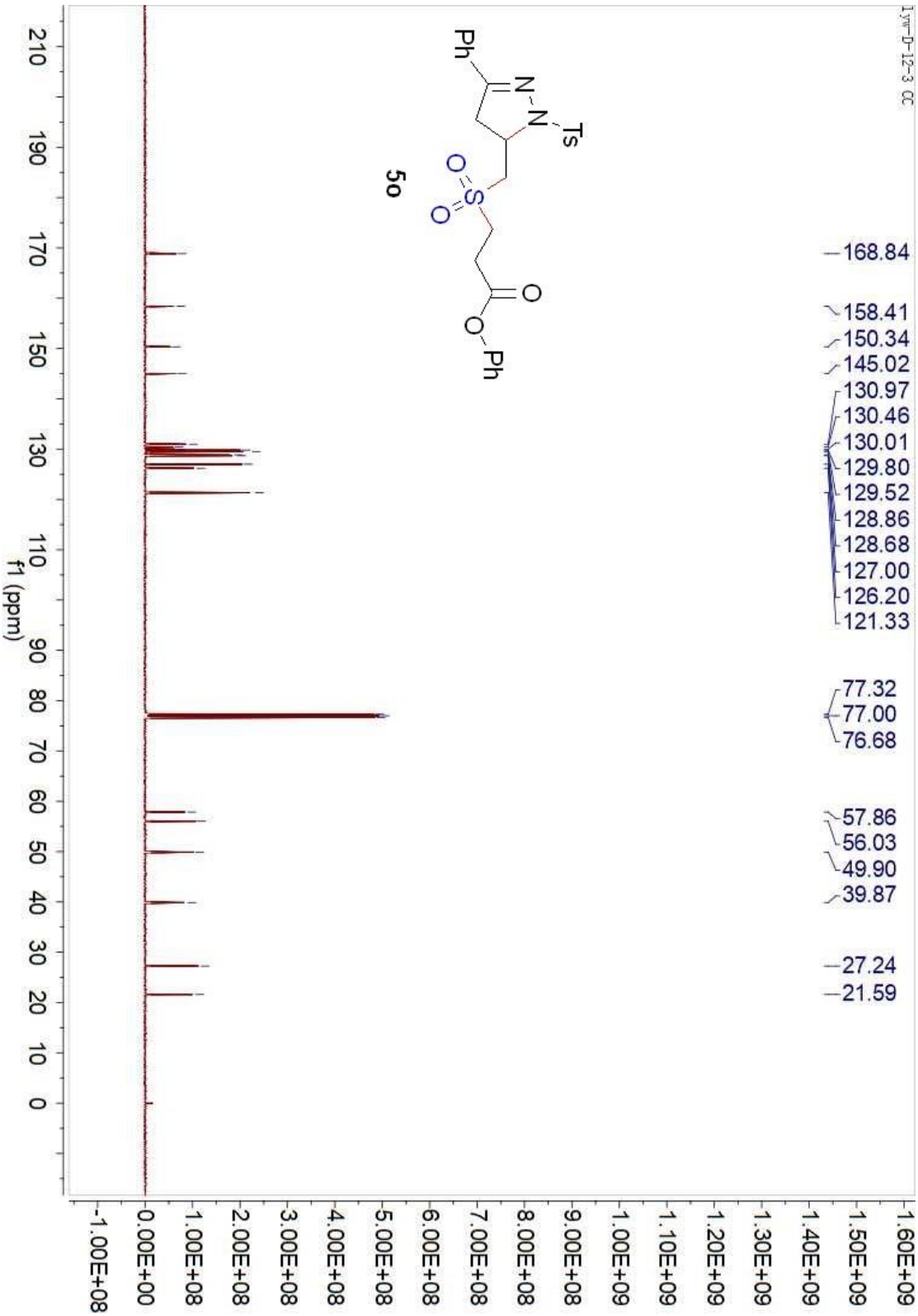

5m
Ph
N
N
Ts
O
S
O
N
f1 (ppm)
2.00
2.24
2.22
3.50
2.33
1.92
1.16
1.16
1.16
2.07
2.08
2.06
3.47
7.435
7.417
7.411
7.400
7.385
7.366
7.349
7.309
7.289
7.270
7.260
7.252
4.072
4.066
3.481
3.457
3.442
3.397
3.385
3.371
3.360
3.250
3.227
2.390
0.000

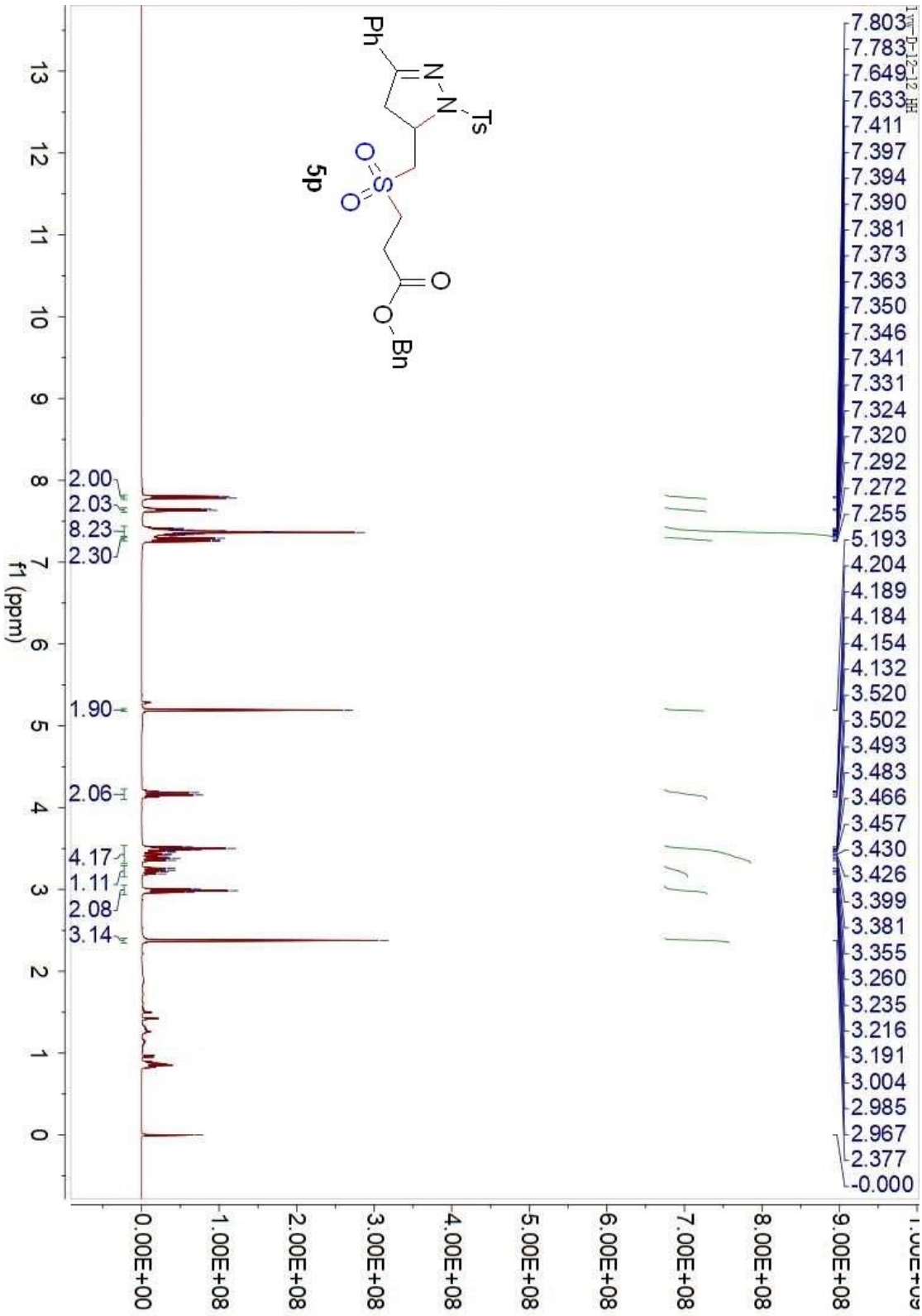

lyw-D-12-1, C
Ph
N
N
Ts
O
S
O
N
5m
158.70
150.19
146.32
145.12
131.01
130.43
129.93
129.81
128.76
128.68
126.97
123.76
77.32
77.00
76.68
57.20
56.03
54.77
39.67
27.35
21.58
f1 (ppm)

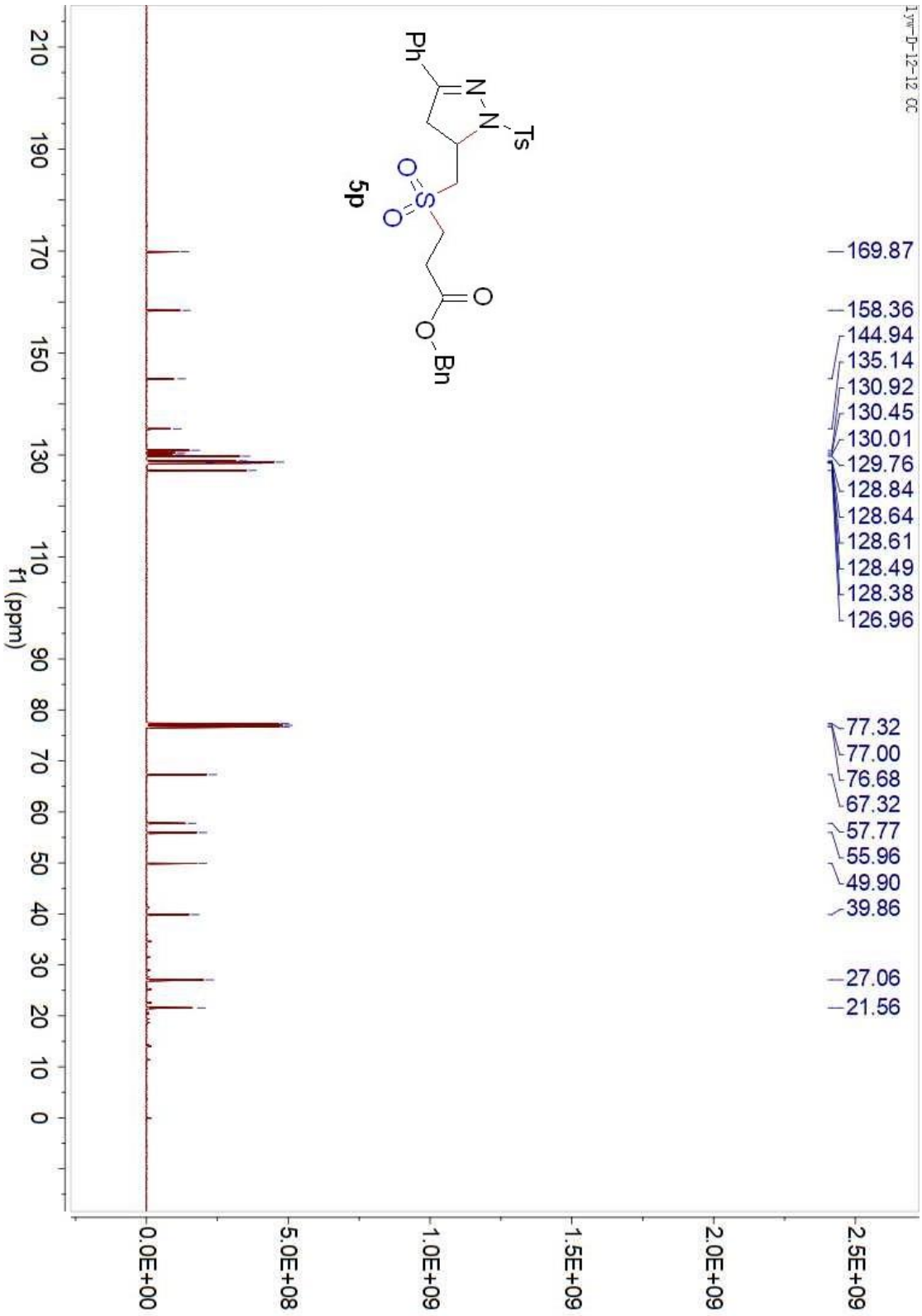

lyw-D-13-13 H
Ph
N
N
Ts
O
S
O
Ph
O
5n
8.063
8.044
7.762
7.742
7.704
7.685
7.671
7.655
7.589
7.570
7.551
7.485
7.462
7.448
7.428
4.015
3.991
3.963
3.638
3.614
3.497
3.379
3.347
2.505
2.358
-0.000
2.00
2.03
3.11
2.15
5.03
1.02
2.01
4.17
1.04
0.61
0.28
2.97
f1 (ppm)

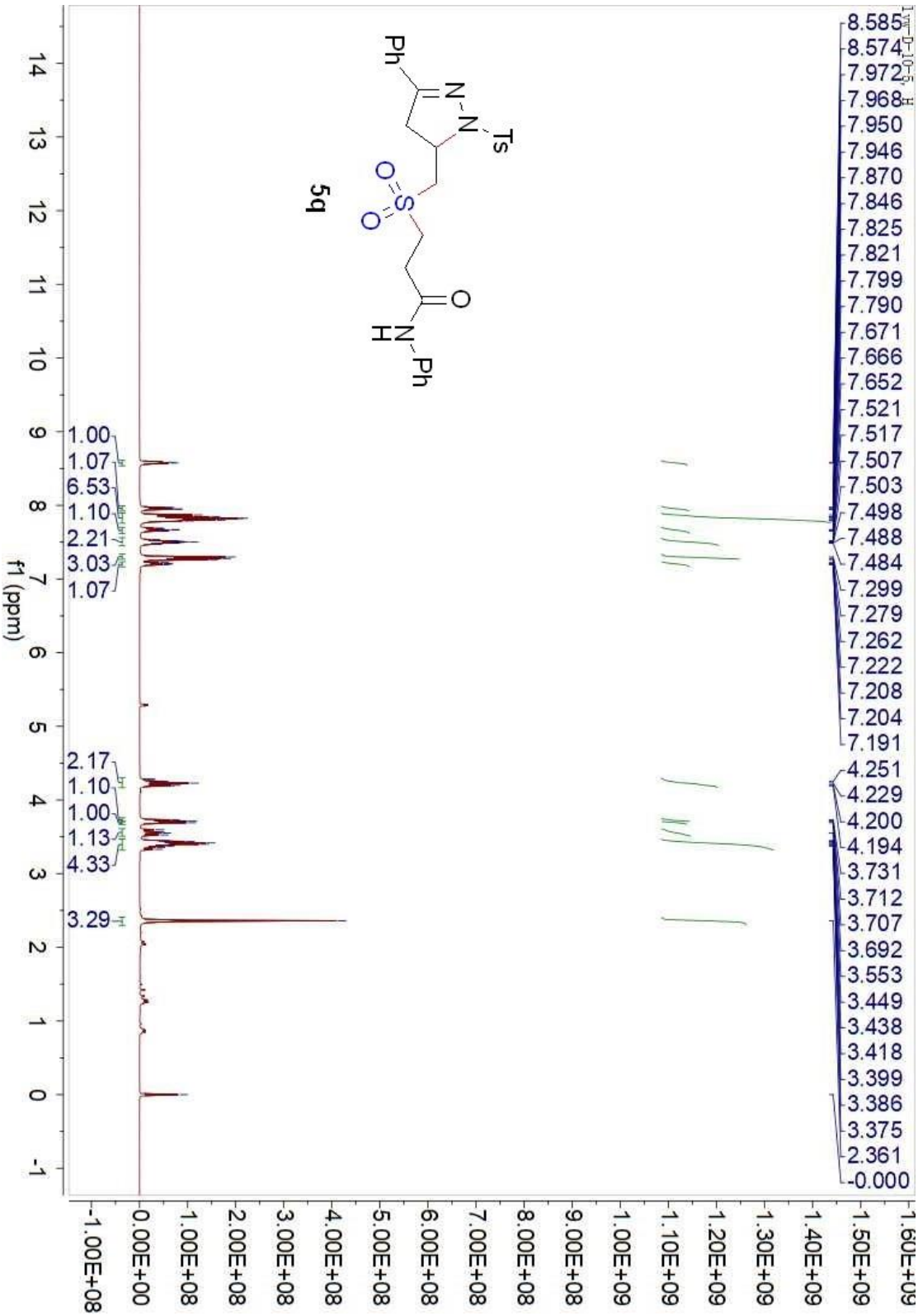

5n
Ph
N
N
Ts
O
S
O
Ph
O
196.53
159.86
145.31
136.39
134.10
131.43
131.22
130.55
130.40
129.32
129.28
128.89
128.61
127.41
57.17
56.54
48.96
39.88
31.58
21.55
f1 (ppm)

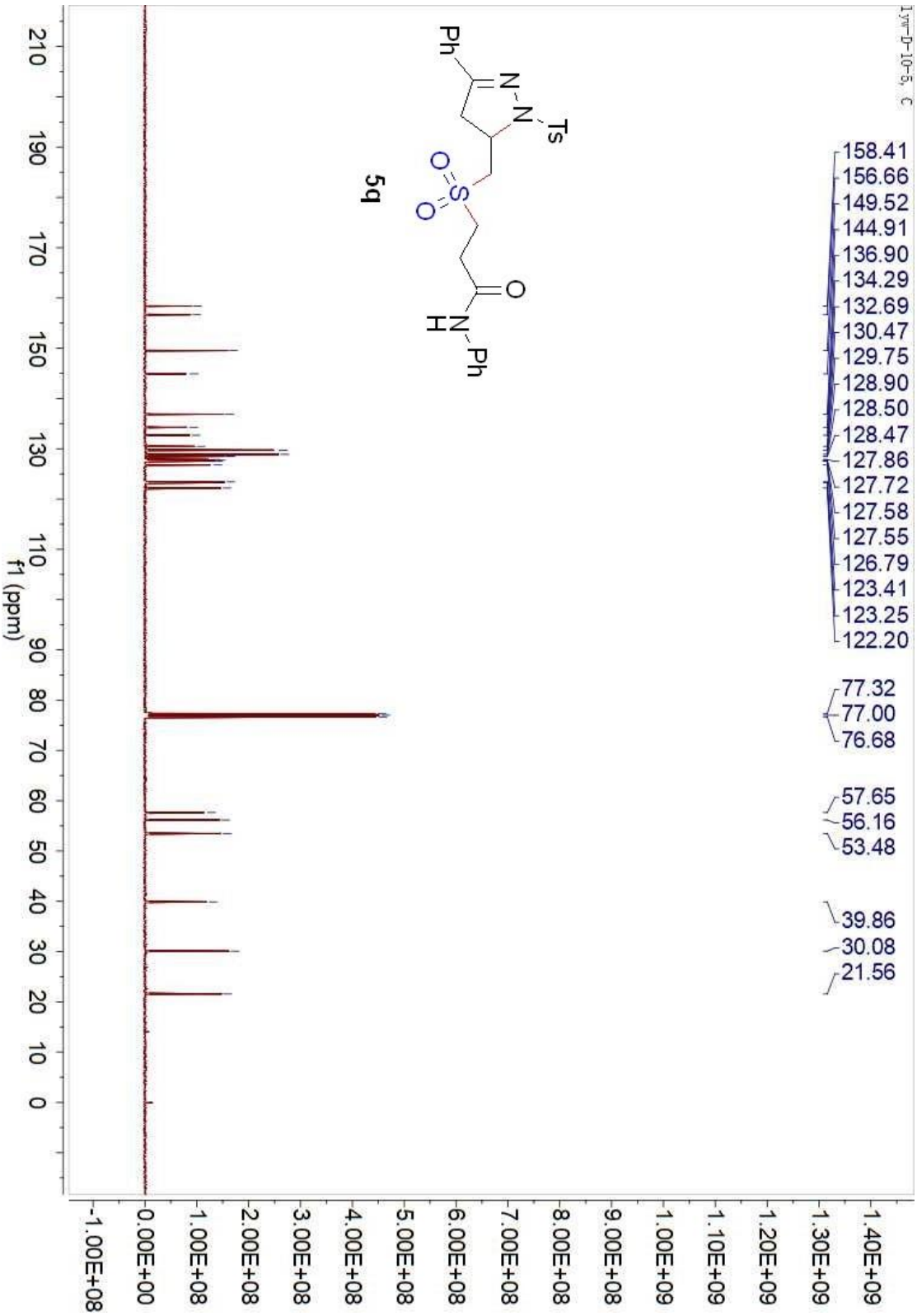

5o
Ph
N
N
Ts
O
S
O
O
O
Ph
7.812
7.791
7.661
7.644
7.419
7.412
7.391
7.372
7.354
7.297
7.276
7.258
7.145
7.126
4.223
4.194
3.624
3.605
3.587
3.225
3.207
3.188
2.378
-0.000
2.00
1.99
5.23
3.89
2.00
2.03
3.10
1.06
1.13
2.01
3.02
f1 (ppm)

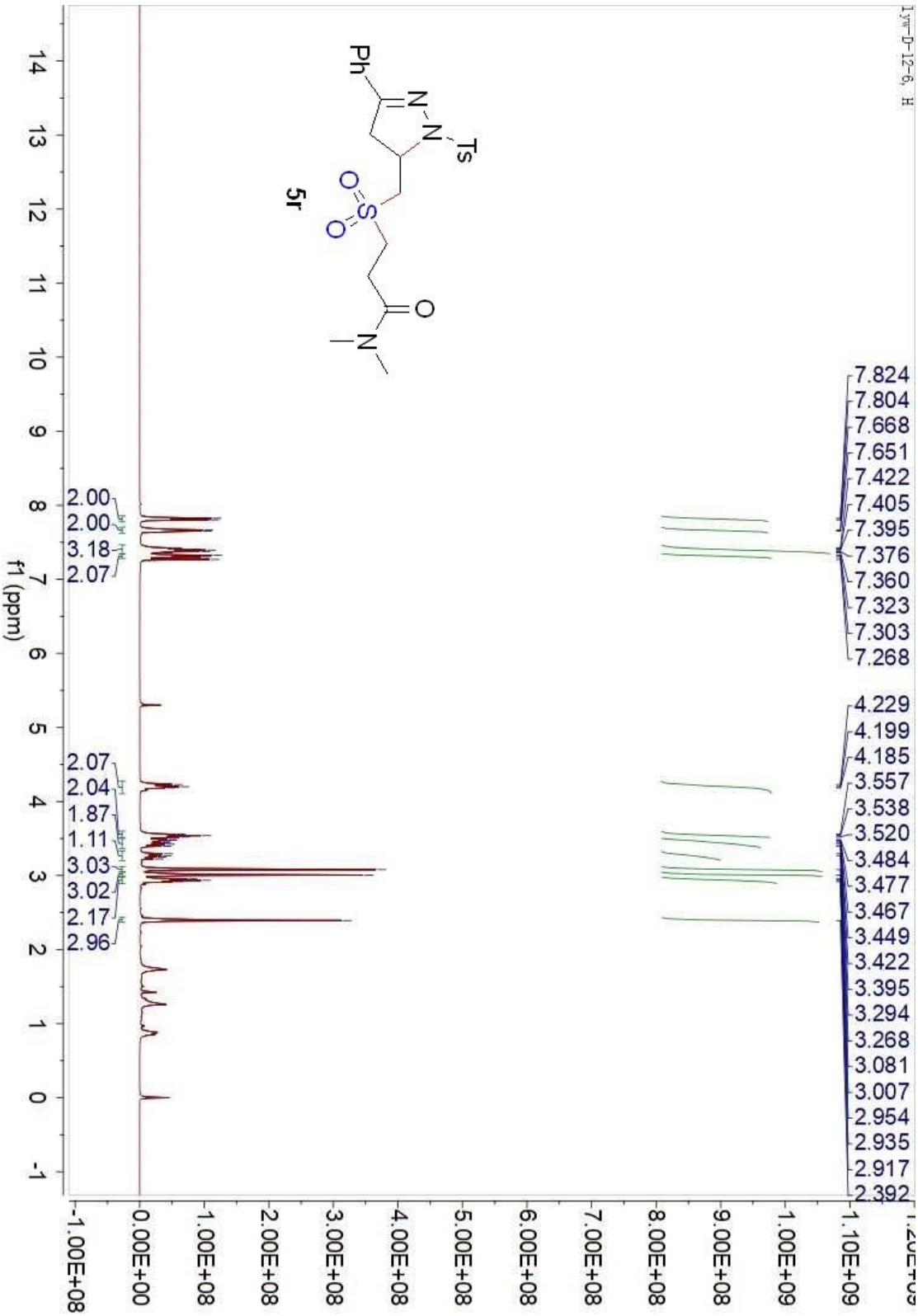

lyw-D-12-3 CC
Ph
N
N
Ts
O
S
O
O
O
O
Ph
5o
168.84
158.41
150.34
145.02
130.97
130.46
130.01
129.80
129.52
128.86
128.68
127.00
126.20
121.33
77.32
77.00
76.68
57.86
56.03
49.90
39.87
27.24
21.59
f1 (ppm)

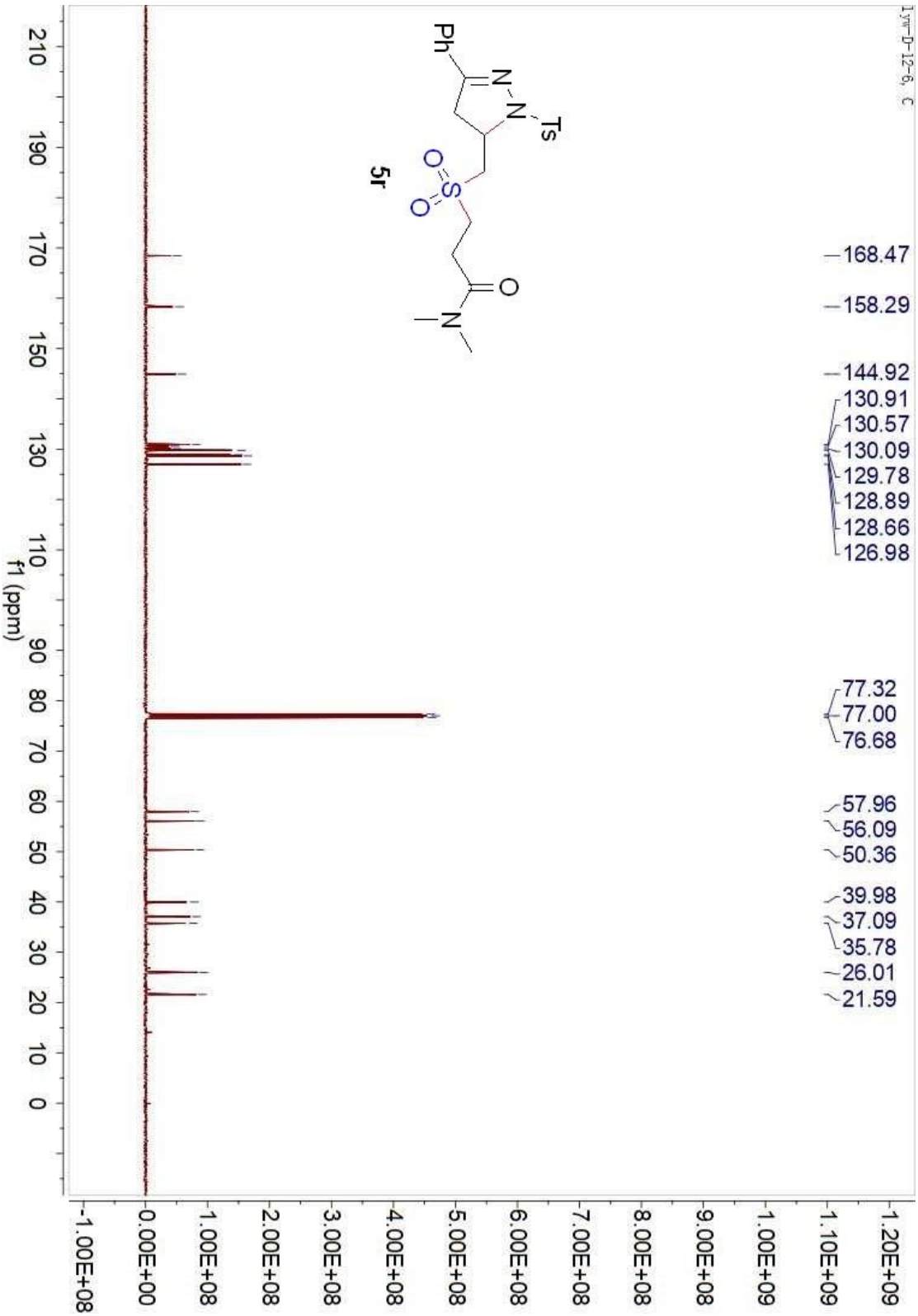

Ph
N
N
Ts
O
S
O
O
O
Bn
5p
f1 (ppm)
2.00
2.03
8.23
2.30
1.90
2.06
4.17
1.11
2.08
3.14
7.803
7.783
7.649
7.633
7.411
7.397
7.394
7.390
7.381
7.373
7.363
7.350
7.346
7.341
7.331
7.324
7.320
7.292
7.272
7.255
5.193
4.204
4.189
4.184
4.154
4.132
3.520
3.502
3.493
3.483
3.466
3.457
3.430
3.426
3.399
3.381
3.355
3.260
3.235
3.216
3.191
3.004
2.985
2.967
2.377
-0.000

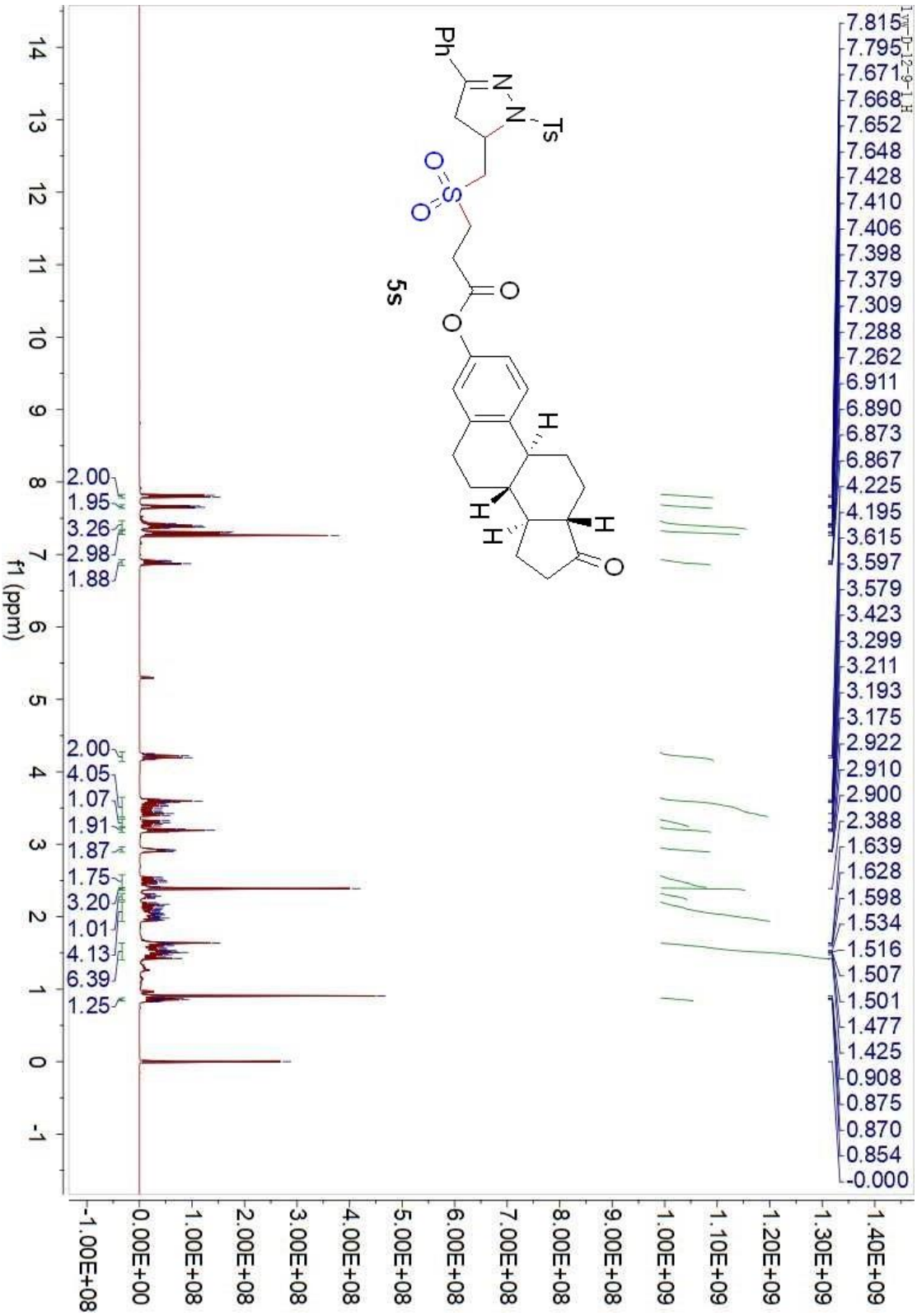

lyw-D-12-12 CC
Ph
N
N
Ts
O
S
O
O
O
Bn
5p
169.87
158.36
144.94
135.14
130.92
130.45
130.01
129.76
128.84
128.64
128.61
128.49
128.38
126.96
77.32
77.00
76.68
67.32
57.77
55.96
49.90
39.86
27.06
21.56
f1 (ppm)
0.0E+00
5.0E+08
1.0E+09
1.5E+09
2.0E+09
2.5E+09

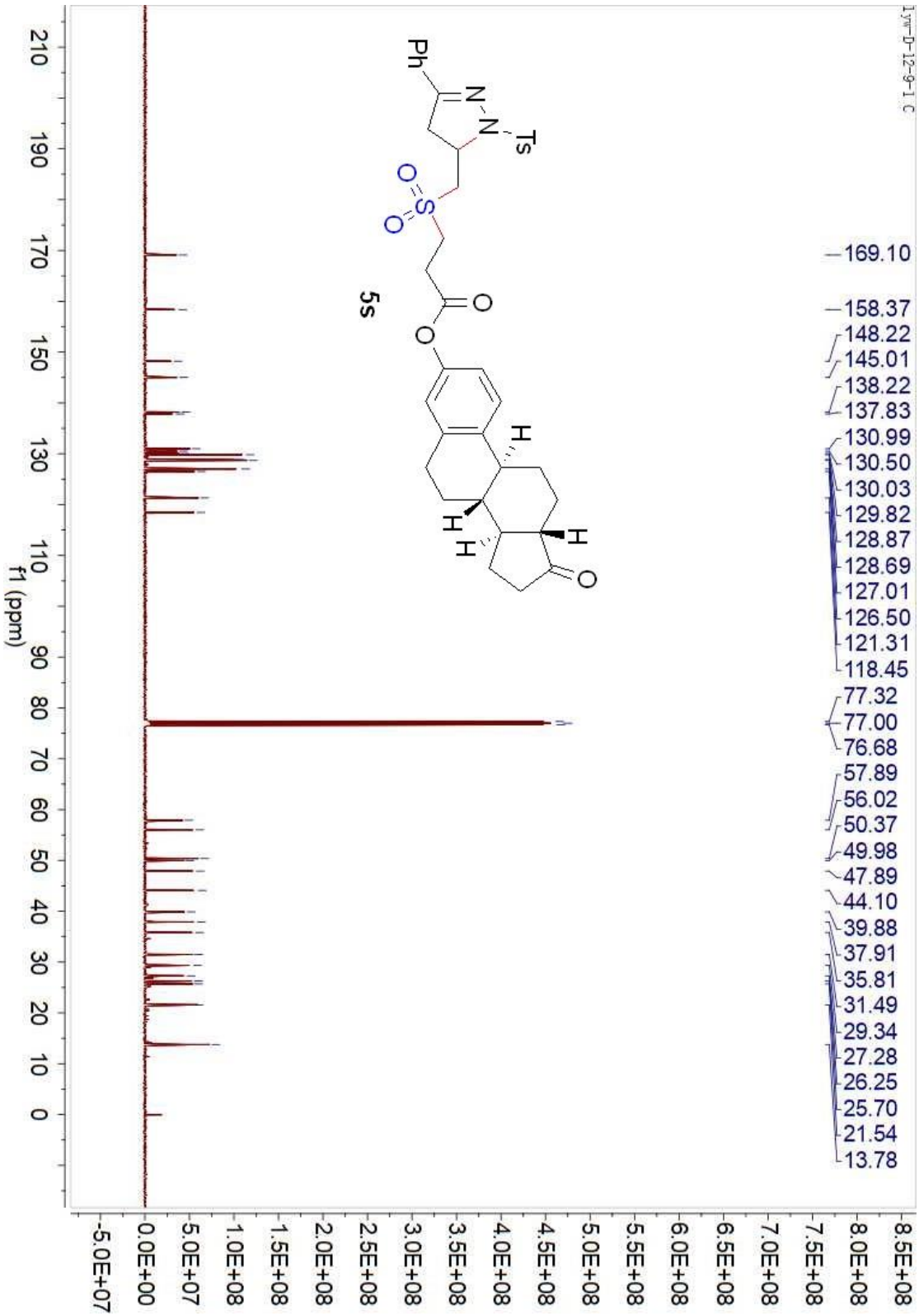

5q
Ph
N
N
Ts
O
S
O
O
N
H
Ph
f1 (ppm)
1.00
1.07
6.53
1.10
2.21
3.03
1.07
2.17
1.10
1.00
1.13
4.33
3.29
8.585
8.574
7.972
7.968
7.950
7.946
7.870
7.846
7.825
7.821
7.799
7.790
7.671
7.666
7.652
7.521
7.517
7.507
7.503
7.498
7.488
7.484
7.299
7.279
7.262
7.222
7.208
7.204
7.191
4.251
4.229
4.200
4.194
3.731
3.712
3.707
3.692
3.553
3.449
3.438
3.418
3.399
3.386
3.375
2.361
-0.000


5q
158.41
156.66
149.52
144.91
136.90
134.29
132.69
130.47
129.75
128.90
128.50
128.47
127.86
127.72
127.58
127.55
126.79
123.41
123.25
122.20
77.32
77.00
76.68
57.65
56.16
53.48
39.86
30.08
21.56
f1 (ppm)


5r
Ph
N
N
Ts
O
S
O
O
N
f1 (ppm)
2.00
2.00
3.18
2.07
2.07
2.04
1.87
1.11
3.03
3.02
2.17
2.96
7.824
7.804
7.668
7.651
7.422
7.405
7.395
7.376
7.360
7.323
7.303
7.268
4.229
4.199
4.185
3.557
3.538
3.520
3.484
3.477
3.467
3.449
3.422
3.395
3.294
3.268
3.081
3.007
2.954
2.935
2.917
2.392


5r
Ph
Ts
O
N
168.47
158.29
144.92
130.91
130.57
130.09
129.78
128.89
128.66
126.98
77.32
77.00
76.68
57.96
56.09
50.36
39.98
37.09
35.78
26.01
21.59
f1 (ppm)


Ph
N
N
Ts
O
S
O
O
O
O
H
H
H
O
5s
f1 (ppm)
2.00
1.95
3.26
2.98
1.88
2.00
4.05
1.07
1.91
1.87
1.75
3.20
1.01
4.13
6.39
1.25
7.815
7.795
7.671
7.668
7.652
7.648
7.428
7.410
7.406
7.398
7.379
7.309
7.288
7.262
6.911
6.890
6.873
6.867
4.225
4.195
3.615
3.597
3.579
3.423
3.299
3.211
3.193
3.175
2.922
2.910
2.900
2.388
1.639
1.628
1.598
1.534
1.516
1.507
1.501
1.477
1.425
0.908
0.875
0.870
0.854
-0.000


5s
Ph
N
N
Ts
O
S
O
O
O
O
H
H
H
O
169.10
158.37
148.22
145.01
138.22
137.83
130.99
130.50
130.03
129.82
128.87
128.69
127.01
126.50
121.31
118.45
77.32
77.00
76.68
57.89
56.02
50.37
49.98
47.89
44.10
39.88
37.91
35.81
31.49
29.34
27.28
26.25
25.70
21.54
13.78
f1 (ppm)