-Supporting information-

Eco-friendly synthesis of pyridines *via* rhodium-catalyzed cyclization of diyne with oxime

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Table of Contents

1. Experimental

1.1 General

All reactions and manipulations were carried out under a dry argon atmosphere either using an inert atmosphere glove-box or standard Schlenk techniques. Diynes were prepared according to the published procedure.[1-5] Oximes were obtained from the corresponding aldehyde and hydroxylamine[6-8]. Unless otherwise noted, commercial reagents were purchased from Aldrich, Alfa Aesar, J&K and used without purification. Anhydrous EtOH was distilled over $MgSO_4$ and I_2 before use. Column chromatography was performed on silica gel (300–400 mesh). ^1H, ^{13}C NMR and ^{19}F NMR were recorded on a 500 or 400 MHz Bruker NMR spectrometer in $CDCl_3$ using tetramethylsilane (TMS) as the internal standard. HRMS data were obtained with Micromass HPLC–Q–TOF mass spectrometer.

2. General procedure for [2 + 2 + 2] cycloaddition

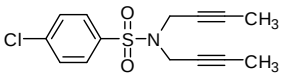
2.1 General procedure for [2 + 2 + 2] cycloaddition of diynes 1a-1m and oxime 2a-2o.

$Rh(NBD)_2BF_4$ (9.3 mg, 0.025 mmol) and MeO-Biphep (14.6 mg, 0.025 mmol) were dissolved in EtOH (6 mL) in the presence of 4Å MS, and the mixture was stirred at room temperature for 5 min. Oxime was added and the resulting mixture was stirred at 80 °C for 30 min. To this solution was added diyne (0.25mmol). Then the mixture was stirred at 80 °C for 48 h. 4Å MS was filtered off and the filtrate was evaporated. The oily residue was purified by column chromatography on silica gel with Petroleum ether/ethyl acetate (polarity from 4:1 to 1:2) to afford **3aa-3ma, 4ab-4an.**

3. Characterization of materials and products.

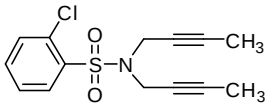
3.1 Characterization of materials 1b-1m

3.1.1 N,N-di(but-2-ynyl)-4-chlorobenzenesulfonamide 1b. White solid, mp = 52-54 °C. (eluent petroleum ether/ethyl acetate = 4:1) ^1H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 7.5 Hz, 2H), 7.47 (d, *J* = 7.5 Hz, 2H), 4.07 (s, 4H), 1.65 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.3, 137.2, 129.6, 129.0, 82.1, 71.5, 36.9, 3.5.



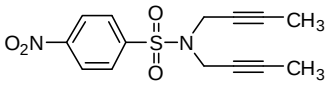
HRMS Calculated for $C_{18}H_{19}ClN_2O_4S$ $[M+Na]^+$ 318.0331, found 318.0330.

3.1.2 N,N-di(but-2-ynyl)-2-chlorobenzenesulfonamide 1c. White solid, mp = 44-45 °C. (eluent petroleum ether/ethyl acetate = 4:1) ^1H NMR (400 MHz, $CDCl_3$) δ 8.08 (dd, *J* = 7.7, 1.0 Hz, 1H), 7.51 – 7.45 (m, 2H), 7.41 – 7.36 (m, 1H), 4.19 (d, *J* = 2.2 Hz, 4H), 1.69 (t, *J* = 2.2 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.5, 133.7, 132.7, 132.2, 131.9, 127.0, 81.3, 72.2, 36.9, 3.6.



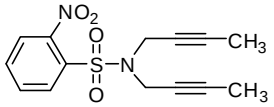
HRMS Calculated for $C_{18}H_{19}ClN_2O_4S$ $[M+Na]^+$ 318.0331, found 318.0334.

3.1.3 N,N-di(but-2-ynyl)-4-nitrobenzenesulfonamide 1d. White solid, mp = 109-110 °C. (eluent petroleum ether/ethyl acetate = 4:1) ^1H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, *J* = 8.2 Hz, 2H), 8.04 (d, *J* = 8.2 Hz, 2H), 4.13 (s, 4H), 1.65 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.2, 144.7, 129.4, 123.9, 82.5, 71.2, 37.1, 3.5.



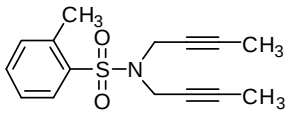
HRMS Calculated for $C_{18}H_{19}ClN_2O_4S$ $[M+Na]^+$ 329.0572, found 329.0575.

3.1.4 N,N-di(but-2-ynyl)-2-nitrobenzenesulfonamide 1e. White solid, mp = 114-116 °C. (eluent petroleum ether/ethyl acetate = 4:1) ^1H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 7.0 Hz, 1H), 7.69 (m, *J* = 14.6, 7.3 Hz, 3H), 4.22 (s, 4H), 1.71 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 133.8, 132.8, 131.6, 131.4, 129.1, 124.2, 82.0, 71.9, 37.1, 3.6.



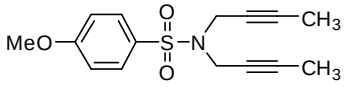
HRMS Calculated for $C_{18}H_{19}ClN_2O_4S$ $[M+Na]^+$ 329.0572, found 329.0574.

3.1.5 N,N-di(but-2-ynyl)-2-methylbenzenesulfonamide 1f. White solid, mp = 28-30 °C. (eluent petroleum ether/ethyl acetate = 4:1) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 5.2 Hz, 1H), 7.33 (m, *J* = 55.7 Hz, 3H), 4.06 (s, 4H), 2.58 (s, 3H), 1.70 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.2, 137.4, 132.9, 132.7, 123.0, 126.1, 81.4, 72.3, 36.1, 20.5, 3.6.

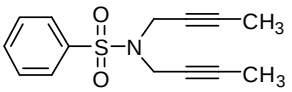


HRMS Calculated for $C_{18}H_{19}ClN_2O_4S$ $[M+Na]^+$ 298.0878, found 298.0880.

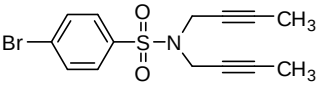
3.1.6 N,N-di(but-2-ynyl)-4-methoxybenzenesulfonamide 1g. White solid, mp = 50-52 °C. (eluent petroleum ether/ethyl acetate = 4:1) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.6 Hz, 2H), 6.96 (d, *J* = 8.6 Hz, 2H), 4.05 (s, 4H), 3.86 (s, 3H), 1.65 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.1, 130.3, 130.2, 113.9, 81.8, 71.8, 55.8, 36.8, 3.6. HRMS Calculated for $C_{18}H_{19}ClN_2O_4S$ $[M+Na]^+$ 314.0827, found 314.0824.



3.1.7 N,N-di(but-2-ynyl)benzenesulfonamide 1h. White solid, mp = 62-63 °C. (eluent petroleum ether/ethyl acetate = 4:1) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, 2H), 7.53 (m, *J* = 20.7, 6.1 Hz, 3H), 4.08 (s, 4H), 1.62 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 138.7, 138.6, 132.8, 128.8, 128.1, 81.9, 71.6, 36.8, 3.5. HRMS Calculated for $C_{18}H_{19}ClN_2O_4S$ $[M+Na]^+$ 284.0721, found 284.0726.

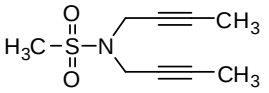


3.1.8 4-bromo-N,N-di(but-2-ynyl)benzenesulfonamide 1i. White solid, mp = 70-72 °C. (eluent petroleum ether/ethyl acetate = 4:1)^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 – 7.64 (m, 4H), 4.07 (d, *J* = 2.2 Hz, 4H), 1.66 (d, *J* = 5.9 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.7, 132.0, 129.7, 127.8, 82.1, 71.5, 36.9, 3.5.



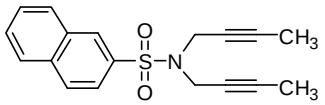
HRMS Calculated for $C_{18}H_{19}ClN_2O_4S$ $[M+Na]^+$ 361.9826, found 361.9823.

3.1.9 N,N-di(but-2-ynyl)methanesulfonamide 1j. White solid, mp = 38-40 °C. (eluent petroleum ether/ethyl acetate = 4:1)^{1}H NMR (400 MHz, $CDCl_3$) δ 4.09 (s, 4H), 2.93 (s, 3H), 1.83 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 82.2, 72.3, 38.4, 36.9, 3.6.



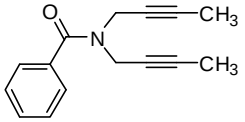
HRMS Calculated for $C_{18}H_{19}ClN_2O_4S$ $[M+Na]^+$ 222.0565, found 222.0568.

3.1.10 N,N-di(but-2-ynyl)naphthalene-2-sulfonamide 1k. White solid, mp = 71-73 °C. (eluent petroleum ether/ethyl acetate = 4:1) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (s, 1H), 7.97 (m, 3H), 7.81 (d, *J* = 8.6 Hz, 1H), 7.67 – 7.55 (m, 2H), 4.14 (s, 4H), 1.48 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 135.6, 135.6, 132.3, 129.6, 129.4, 128.9, 128.8, 127.9, 127.5, 123.4, 82.0, 71.7, 36.9, 3.4.



HRMS Calculated for $C_{18}H_{19}ClN_2O_4S$ $[M+Na]^+$ 334.0878, found 334.0876.

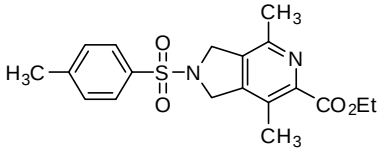
3.1.11 N,N-di(but-2-ynyl)benzamide 1m. White solid, mp = 41-42 °C. (eluent petroleum ether/ethyl acetate = 4:1) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (s, 2H), 7.40 (s, 3H), 4.24 (d, *J* = 126.3 Hz, 4H), 1.82 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.8, 135.3, 130.2, 128.5, 127.3, 73.7, 38.7, 34.0, 3.7.



HRMS Calculated for $C_{18}H_{19}ClN_2O_4S$ $[M+Na]^+$ 248.1051, found 248.1049.

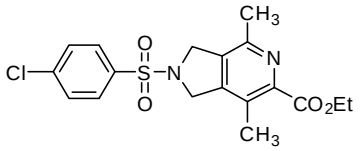
3.2 Characterization of products 3aa-3na and 4ab-4an.

3.2.1 ethyl 4,7-dimethyl-2-tosyl-2,3-dihydro-1H-pyrrolo[3,4-c]pyridine-6-carboxylate 3aa. White solid (93% isolated yield), eluent petroleum ether/ethyl acetate = 2:1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7. 81 – 7.76 (m, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 4.62 (d, *J* = 3.4 Hz, 4H), 4.42 (q, *J* = 7.1 Hz, 2H), 2.43 (d, *J* = 4.7 Hz, 6H), 2.33 (s, 3H), 1.40 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.3,



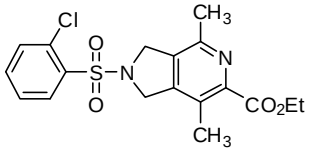
149.9, 147.6, 146.6, 144.2, 133.7, 132.8, 130.1, 127.5, 126.5, 61.8, 53.4, 52.9, 21.7, 21.6, 15.4, 14.3.

3.2.2 ethyl 2-(4-chlorophenylsulfonyl)-4,7-dimethyl-2,3-dihydro-1H-pyrrolo [3,4-c]pyridine-6-carboxylate 3ba. White solid (83% isolated yield), mp = 192-193 °C. (eluent petroleum ether/ethyl acetate = 2:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (t, *J* = 6.8 Hz, 2H), 7.53 (t, *J* = 6.8 Hz, 2H), 4.62 (s, 4H), 4.43 (m, 2H), 2.43 (s, 3H), 2.34 (d, *J* = 4.6 Hz, 3H), 1.40 (m, *J* = 11.8, 6.7 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ =^{13}C NMR (101 MHz, $CDCl_3$) δ 167.1, 150.1, 147.8, 146.4, 135.3, 132.6, 129.9, 128.9, 126.8, 122.1, 62.0, 53.5, 53.0, 21.9, 15.6, 14.4.



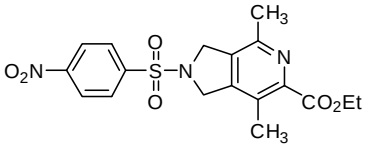
HRMS Calculated for $C_{18}H_{19}ClN_2O_4S$ $[M+Na]^+$ 417.0652, found 417.0657.

3.2.3 ethyl 2-(2-chlorophenylsulfonyl)-4,7-dimethyl-2,3-dihydro-1H-pyrrolo [3,4-c]pyridine-6-carboxylate 3ca. White solid (92% isolated yield), mp = 93-95 °C. (eluent petroleum ether/ethyl acetate = 2:1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.17 – 8.15 (m, 1H), 7.56 – 7.51 (m, 2H), 7.45 (m, *J* = 8.0, 6.6, 2.2 Hz, 1H), 4.80 (s, 4H), 4.44 (q, *J* = 7.1 Hz, 2H), 2.46 (s, 3H), 2.36 (s, 3H), 1.41 (t, *J* = 8.9, 5.3 Hz, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.3, 150.0, 148.9, 147.6, 146.5, 136.4, 134.0, 132.7, 132.3, 132.0, 127.2, 126.5, 61.8, 53.5, 52.9, 21.7, 15.4, 14.3.



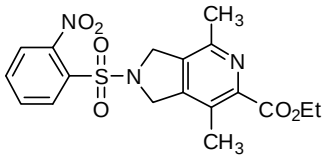
HRMS Calculated for $C_{18}H_{19}ClN_2O_4S$ $[M+Na]^+$ 417.0652, found 417.0659.

3.2.4 ethyl 4,7-dimethyl-2-(4-nitrophenylsulfonyl)-2,3-dihydro-1H-pyrrolo [3,4-c]pyridine-6-carboxylate 3da. White solid (60% isolated yield), mp = 185-187 °C. (eluent petroleum ether/ethyl acetate = 2:1).^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (d, *J* = 8.6 Hz, 2H), 8.10 (d, *J* = 8.3 Hz, 2H), 4.69 (s, 4H), 4.43 (q, *J* = 6.9 Hz, 2H), 2.41 (s, 6H), 1.41 (t, *J* = 6.7 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.2, 150.6, 150.1, 148.0, 146.0, 143.0, 132.2, 128.6, 126.6, 124.8, 62.0, 53.6, 53.1, 21.8, 15.5, 14.3.



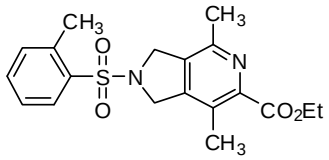
HRMS Calculated for $C_{18}H_{19}N_3O_6S$ $[M+Na]^+$ 428.0892, found 428.0889.

3.2.5 ethyl 4,7-dimethyl-2-(2-nitrophenylsulfonyl)-2,3-dihydro-1H-pyrrolo [3,4-c]pyridine-6-carboxylate 3ea. White solid (66% isolated yield), mp = 110-112 °C. (eluent petroleum ether/ethyl acetate = 2:1).^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (s, 1H), 7.71 (m, *J* = 26.5 Hz, 3H), 4.84 (s, 4H), 4.45 (q, *J* = 7.0 Hz, 2H), 2.43 (s, 6H), 1.42 (t, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.4, 150.1, 147.8, 146.3, 146.2, 134.2, 132.5, 132.0, 131.9, 130.9, 126.7, 124.5, 61.9, 53.7, 53.1, 21.8, 15.6, 14.4.



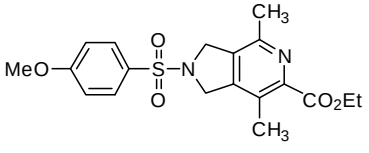
HRMS Calculated for $C_{18}H_{19}N_3O_6S$ $[M+Na]^+$ 428.0892, found 428.0898.

3.2.6 ethyl 4,7-dimethyl-2-(o-tolylsulfonyl)-2,3-dihydro-1H-pyrrolo[3,4-c]pyridine-6-carboxylate 3fa. White solid (81% isolated yield), mp = 117-119 °C. (eluent petroleum ether/ethyl acetate = 2:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 7.9 Hz, 1H), 7.50 (m, 1H), 7.36 (m, *J* = 7.2 Hz, 2H), 4.70 (s, 4H), 4.45 (q, *J* = 7.0 Hz, 2H), 2.68 (s, 3H), 2.46 (s, 3H), 2.36 (s, 3H), 1.42 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) 166.4, 150.2, 147.7, 146.7, 138.2, 136.7, 133.3, 133.1, 133.0, 129.5, 126.8, 126.5, 62.0, 53.2, 52.6, 21.9, 20.7, 15.6, 14.4.



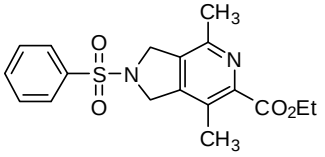
HRMS Calculated for $C_{19}H_{22}N_2O_4S$ $[M+Na]^+$ 397.1198, found 397.1192.

3.2.7 ethyl 2-(4-methoxyphenylsulfonyl)-4,7-dimethyl-2,3-dihydro-1H-pyrrolo [3,4-c]pyridine-6-carboxylate 3ga. White solid (80% isolated yield), mp = 168-170 °C. (eluent petroleum ether/ethyl acetate = 2:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 8.8 Hz, 2H),



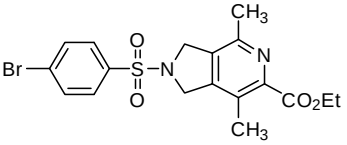
6.98 (d, *J* = 8.8 Hz, 2H), 4.57 (d, *J* = 1.8 Hz, 4H), 4.39 (q, *J* = 7.1 Hz, 2H), 3.82 (s, 3H), 2.40 (s, 3H), 2.31 (s, 3H), 1.36 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.4, 163.4, 150.0, 147.5, 146.7, 133.0, 129.7, 128.2, 126.6, 114.7, 61.9, 55.8, 53.5, 52.9, 21.8, 15.6, 14.4.
HRMS Calculated for $C_{19}H_{22}N_2O_5S$ $[M+Na]^+$ 413.1147, found 413.1151.

3.2.8 ethyl 4,7-dimethyl-2-(phenylsulfonyl)-2,3-dihydro-1H-pyrrolo [3,4-c]pyridine-6-carboxylate 3ha. White solid (81% isolated yield), mp = 175-177 °C. (eluent petroleum ether/ethyl acetate = 2:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 7.4 Hz, 2H), 7.56 (m, *J* = 7.1 Hz, 3H), 4.63 (s, 4H), 4.41 (q, *J* = 7.1 Hz, 2H), 2.43 (s, 3H), 2.33 (s, 3H), 1.39 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.4, 150.1, 147.6, 146.6, 136.7, 133.4, 132.8, 129.6, 127.5, 126.7, 62.0, 53.5, 53.0, 21.9, 15.6, 14.4.



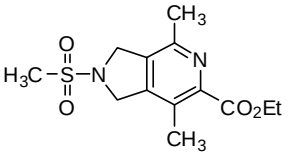
HRMS Calculated for $C_{18}H_{20}N_2O_4S$ $[M+Na]^+$ 383.1041, found 383.1049.

3.2.9 ethyl 2-(4-bromophenylsulfonyl)-4,7-dimethyl-2,3-dihydro-1H-pyrrolo [3,4-c]pyridine-6-carboxylate 3ia. White solid, mp = 193-195 °C. (eluent petroleum ether/ethyl acetate = 2:1). White solid (78% isolated yield). Petroleum ether/ethyl acetate = 2:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 – 7.75 (m, 2H), 7.70 – 7.68 (m, 2H), 4.62 (d, *J* = 2.5 Hz, 4H), 4.42 (q, *J* = 7.1 Hz, 2H), 2.43 (s, 3H), 2.34 (s, 3H), 1.40 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.3, 150.1, 147.8, 146.4, 135.9, 132.9, 132.6, 129.0, 128.5, 126.7, 62.0, 53.5, 53.0, 21.9, 15.6, 14.4.



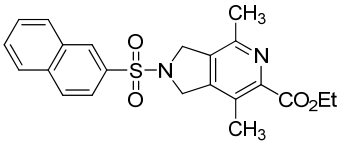
HRMS Calculated for $C_{18}H_{19}BrN_2O_4S$ $[M+Na]^+$ 461.0147, found 461.0142.

3.2.10 ethyl 4,7-dimethyl-2-(methylsulfonyl)-2,3-dihydro-1H-pyrrolo [3,4-c]pyridine-6-carboxylate 3ja. White solid (72% isolated yield), mp = 163-165 °C. (eluent petroleum ether/ethyl acetate = 2:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.70 (s, 4H), 4.64 – 4.33 (q, 2H), 2.92 (s, 3H), 2.42 (s, 6H), 1.41 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.4, 150.2, 147.8, 146.7, 132.9, 126.8, 62.0, 53.5, 53.0, 36.0, 21.9, 15.6, 14.4.



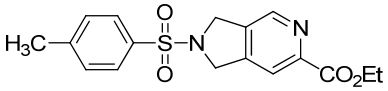
HRMS Calculated for $C_{13}H_{18}N_2O_4S$ $[M+Na]^+$ 321.0885, found 321.0883.

3.2.11 ethyl 4,7-dimethyl-2-(naphthalen-2-ylsulfonyl)-2,3-dihydro-1H-pyrrolo[3,4-c] pyridine -6-carboxylate 3ka. White solid (79% isolated yield), mp = 159-161 °C. (eluent petroleum ether/ethyl acetate = 2:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (s, 1H), 7.97 (m, *J* = 8.6, 4.7 Hz, 2H), 7.85 (m, *J* = 8.6 Hz, 2H), 7.67 – 7.55 (m, 2H), 4.66 (s, 4H), 4.38 (q, *J* = 7.1 Hz, 2H), 2.39 (s, 3H), 2.30 (s, 3H), 1.36 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.31, 150.01, 147.50, 146.59, 135.12, 133.76, 132.84, 132.33, 129.92, 129.40, 129.14, 128.96, 128.06, 127.87, 126.69, 122.64, 61.90, 53.58, 53.01, 21.81, 15.60, 14.36.

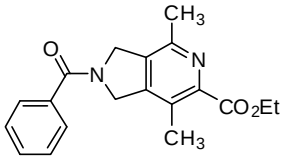


HRMS Calculated for $C_{22}H_{22}N_2O_4S$ $[M+Na]^+$ 433.1198, found 433.1191.

3.2.12 ethyl 2-tosyl-2,3-dihydro-1H-pyrrolo[3,4-c]pyridine-6-carboxylate 3la. White solid (73% isolated yield), eluent petroleum ether/ethyl acetate = 2:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (s, 1H), 7.99 (s, 1H), 7.77 (d, J = 8.1 Hz, 2H), 7.34 (d, J = 8.0 Hz, 2H), 4.70 (d, J = 13.1 Hz, 4H), 4.46 (q, J = 7.1 Hz, 2H), 2.41 (s, 3H), 1.43 (t, J = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$)δ 164.82, 147.85, 147.10, 144.40, 144.37, 136.21, 133.43, 130.19, 127.65, 119.58, 62.32, 53.31, 51.91, 21.67, 14.42.

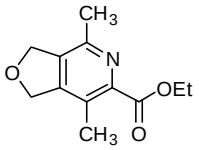


3.2.13 ethyl 2-benzoyl-4,7-dimethyl-2,3-dihydro-1H-pyrrolo [3,4-c]pyridine-6-carboxylate 3ma. White solid (75% isolated yield), mp = 139-141 °C. (eluent petroleum ether/ethyl acetate = 2:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (s, 2H), 7.49 (m, *J* = 6.0 Hz, 3H), 5.03



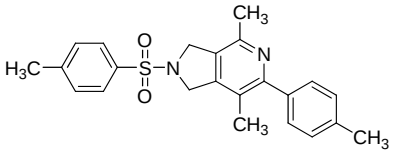
(s, 2H), 4.78 (d, *J* = 5.7 Hz, 2H), 4.46 (m, 2H), 2.51 (d, *J* = 38.1 Hz, 3H), 2.36 (d, *J* = 38.5 Hz, 3H), 1.43 (m, *J* = 11.0, 6.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ = 172.4, 158.3, 136.0, 134.0, 133.4, 133.3, 130.6, 128.9, 127.1, 110.1, 62.0, 54.4, (d, *J* = 57.3 Hz), 52.2 (d, *J* = 62.0 Hz), 21.8, 15.7, 14.4.
HRMS Calculated for $C_{19}H_{20}N_2O_3$ $[M+Na]^+$ 347.1372, found 347.1369.

3.2.14 ethyl 4,7-dimethyl-1,3-dihydrofuro[3,4-c]pyridine-6-carboxylate 3na. White solid (69% isolated yield) , eluent petroleum ether/ethyl acetate = 2:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.14 (dd, *J* = 6.6, 2.0 Hz, 4H), 4.46 (q, *J* = 7.1 Hz, 2H), 2.47 (s, 3H), 2.38 (s, 3H), 1.43 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.6, 149.6, 148.7, 147.1, 135.4, 125.6, 73.3, 73.0, 61.7, 21.9, 15.8, 14.3.

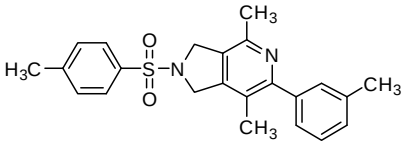


HRMS Calculated for $C_{12}H_{15}NO_3$ 221.1052，found 221.1055

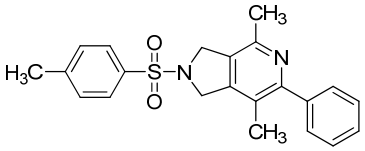
3.2.15 4,7-dimethyl-6-p-tolyl-2-tosyl-2,3-dihydro-1H-pyrrolo[3,4-c] pyridine 4ab. White solid (31% isolated yield), eluent petroleum ether/ethyl acetate = 4:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 8.2 Hz, 2H), 7.35 (d, *J* = 8.1 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 7.22 (d, *J* = 7.9 Hz, 2H), 4.69-4.58 (m, 4H), 2.42 (d, *J* = 3.0 Hz, 6H), 2.38 (s, 3H), 2.14 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.9, 149.3, 145.7, 143.9, 140.9, 137.8, 133.9, 130.0, 128.92, 128.91, 128.8, 127.5, 122.8, 53.5, 52.8, 21.7, 21.5, 21.2, 16.0. HRMS Calculated for $C_{23}H_{24}N_2O_2S$ 392.1558,found 392.1565



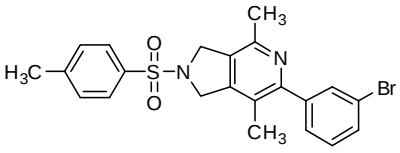
3.2.16 4,7-dimethyl-6-m-tolyl-2-tosyl-2,3-dihydro-1H-pyrrolo[3,4-c]pyridine 4ac. White solid (37% isolated yield), eluent petroleum ether/ethyl acetate = 4:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 8.3 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 7.28 (d, *J* = 7.4 Hz, 1H), 7.22 (s, 1H), 7.17 (d, *J* = 7.7 Hz, 2H), 4.67-4.59 (m, 4H), 2.43 (s, 6H), 2.38 (s, 3H), 2.13 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.1, 149.3, 145.7, 143.9, 139.8, 138.0, 133.9, 130.0, 129.7, 128.9, 128.7, 128.0, 127.5, 126.0, 122.9, 53.5, 52.8, 21.7, 21.5, 21.5, 16.0.
HRMS Calculated for $C_{23}H_{24}N_2O_2S$ 392.1558,found 392.1571



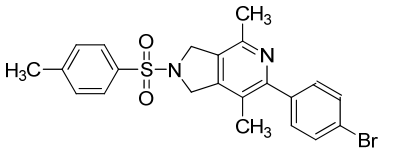
3.2.17 4,7-dimethyl-6-phenyl-2-tosyl-2,3-dihydro-1H-pyrrolo[3,4-c]pyridine 4ad. White solid (60% isolated yield), eluent petroleum ether/ethyl acetate = 4:1. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.81 (d, *J* = 8.3 Hz, 2H), 7.44 – 7.34 (m, 7H), 4.64 (dd, *J* = 15.6, 1.9 Hz, 4H), 2.43 (s, 6H), 2.14 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.9, 149.4, 145.8, 144.0, 139.8, 133.9, 130.0, 129.1, 129.0, 128.3, 128.0, 127.6, 122.9, 53.5, 52.8, 21.7, 21.6, 16.0.



3.2.18 6-(3-bromophenyl)-4,7-dimethyl-2-tosyl-2,3-dihydro-1H-pyrrolo[3,4-c]pyridine 4ae. White solid (64% isolated yield), eluent petroleum ether/ethyl acetate = 4:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 8.3 Hz, 2H), 7.52-7.57 (m, 2H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.27- 7.32 (m, 2H), 4.63 (dd, *J* = 11.1, 1.8 Hz, 4H), 2.42 (d, *J* = 3.8 Hz, 6H), 2.13 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.6, 149.7, 146.0, 144.0, 138.75, 135.8, 133.81, 131.4, 130.7, 130.0, 129.4, 127.5, 122.9, 122.3, 120.7, 53.5, 52.7, 21.7, 21.5, 15.9.
HRMS Calculated for $C_{22}H_{21}BrN_2O_2S$ 456.0507, found 456.0517

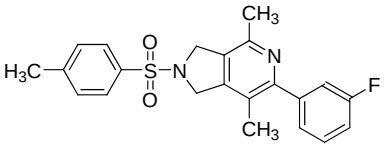


3.2.19 6-(4-bromophenyl)-4,7-dimethyl-2-tosyl-2,3-dihydro-1H-pyrrolo[3,4-c]pyridine 4af. White solid (50% isolated yield), eluent petroleum ether/ethyl acetate = 4:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 8.2 Hz, 2H), 7.56 (t, *J* = 1.6 Hz, 1H), 7.53-7.47 (m, 1H), 7.39-7.29 (m, 4H), 4.67-4.60 (m, 4H), 2.42 (d, *J* = 1.5 Hz,



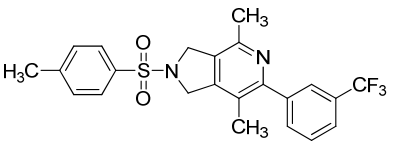
6H), 2.13 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.2, 149.6, 146.0, 144.0, 141.8, 133.8, 132.1, 131.1, 130.0, 129.7, 127.5, 123.1, 122.4, 53.5, 52.7, 21.6, 21.5, 15.9.
HRMS Calculated for $C_{22}H_{21}BrN_2O_2S$ 456.0507, found 456.0519

3.2.20 6-(3-fluorophenyl)-4,7-dimethyl-2-tosyl-2,3-dihydro-1H-pyrrolo[3,4-c]pyridine 4ag. White solid (31% isolated yield), eluent petroleum ether/ethyl acetate = 4:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 8.2 Hz, 2H), 7.38 (dd, *J* = 14.3, 7.9 Hz, 3H), 7.18 (d, *J* = 7.7 Hz, 1H), 7.13 (d, *J* = 9.6 Hz, 1H), 7.08 (dd, *J* = 8.5, 1.7 Hz, 1H), 4.64 (d, *J* = 13.0 Hz, 4H), 2.43 (s, 6H), 2.14 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.7, 149.6, 146.1, 144.0, 133.8, 129.9, 129.7 (d, *J* = 13.9 Hz), 128.8 (d, *J* = 248.2 Hz), 124.8 (d, *J* = 2.7 Hz), 123.0, 116.2 (d, *J* = 22.1 Hz), 115.1, 114.9, 53.5, 52.7, 21.6, 21.5, 15.9. ^{19}F NMR (376 MHz, $CDCl_3$) δ -113.09.



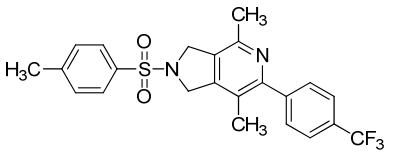
HRMS Calculated for $C_{22}H_{21}FN_2O_2S$ 396.1308,found 396.1319

3.2.21 4,7-dimethyl-2-tosyl-6-(3-(trifluoromethyl)phenyl)-2,3-dihydro-1H-pyrrolo[3,4-c] pyridine 4ah. White solid (38% isolated yield), eluent petroleum ether/ethyl acetate = 2:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.2 Hz, 2H), 7.69 (s, 1H), 7.62 (t, *J* = 7.9 Hz, 2H), 7.54 (t, *J* = 7.7 Hz, 1H), 7.36 (d, *J* = 8.1 Hz, 2H), 4.70 -4.60 (m, 4H), 2.43 (s, 6H), 2.14 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.2, 149.8, 146.1, 144.0, 140.6, 133.8, 132.4, 130.7 (d, *J* = 32.3 Hz), 128.8 (d, *J* = 249.6 Hz), 129.8, 128.7, 126.0 (q, *J* = 3.7 Hz), 125.4, 124.8 (q, *J* = 3.6 Hz), 123.1, 122.7, 53.5, 52.7, 21.7, 21.5, 15.9.^{19}F NMR (376 MHz, $CDCl_3$) δ -62.6.

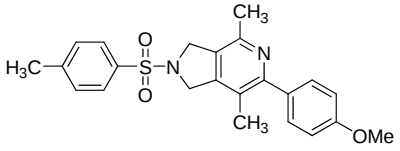


HRMS Calculated for $C_{23}H_{21}F_3N_2O_2S$ 446.1276, found 446.1294

3.2.22 4,7-dimethyl-2-tosyl-6-(4-(trifluoromethyl)phenyl)-2,3-dihydro-1H-pyrrolo[3,4-c] pyridine 4ai. White solid (44% isolated yield), eluent petroleum ether/ethyl acetate = 2:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.3 Hz, 2H), 7.68 (d, *J* = 8.2 Hz, 2H), 7.54 (d, *J* = 8.0 Hz, 2H), 7.36 (d, *J* = 8.0 Hz, 2H), 4.64 (dd, *J* = 11.0, 1.7 Hz, 4H), 2.43 (s, 6H), 2.14 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.3, 156.3, 149.8, 146.1, 144.0, 143.4, 133.8, 129.8, 129.5, 128.8 (d, *J* = 247.9 Hz), 125.3 (dd, *J* = 7.2, 3.4 Hz), 123.1, 121.3, 120.0, 53.5, 52.7, 21.7, 21.5, 15.8. ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.64 HRMS Calculated for $C_{23}H_{21}F_3N_2O_2S$ 446.1276, found 446.1284

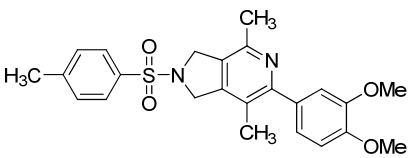


3.2.23 6-(4-methoxyphenyl)-4,7-dimethyl-2-tosyl-2,3-dihydro-1H-pyrrolo[3,4-c]pyridine 4aj. White solid (25% isolated yield), eluent petroleum ether/ethyl acetate = 4:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 8.2 Hz, 2H), 7.42-7.31 (m, 4H), 6.99 – 6.90 (m, 2H), 4.69-4.56 (m, 4H), 3.84 (d, *J* = 3.4 Hz, 3H), 2.42 (d, *J* = 3.7 Hz, 6H), 2.15 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.5, 157.5, 149.5, 145.8, 144.0, 133.8, 132.2, 130.3, 130.0, 128.7, 127.5, 122.8, 113.7, 55.4, 53.5, 52.7, 21.6, 21.5, 16.1.



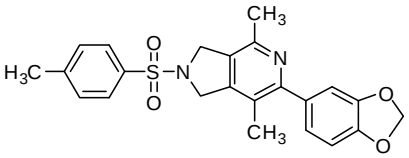
HRMS Calculated for $C_{23}H_{24}N_2O_3S$ 408.1508,found 408.1518

3.2.24 6-(3,4-dimethoxyphenyl)-4,7-dimethyl-2-tosyl-2,3-dihydro-1H-pyrrolo[3,4-c]pyridine 4ak. White solid (26% isolated yield), eluent petroleum ether/ethyl acetate = 4:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J*=8.2 Hz, 2H), 7.36 (d, *J*=8.1 Hz, 2H), 7.00-6.88 (m, 3H), 4.63 (d, *J* = 13.1 Hz, 4H), 3.90 (d, *J* = 7.1 Hz, 6H), 2.43 (s, 6H), 2.16 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.5, 149.3, 149.1, 148.9, 143.9, 141.2, 133.8, 130.0, 128.8, 127.6, 122.8, 121.7, 118.0, 112.5, 110.9, 56.0, 55.9, 53.5, 52.8, 21.7, 21.53, 16.1.



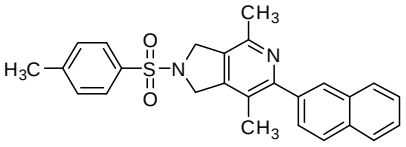
HRMS Calculated for $C_{24}H_{26}N_2O_4S$ 438.1613,found 438.1625.

3.2.25 6-(benzo[d][1,3]dioxol-5-yl)-4,7-dimethyl-2-tosyl-2,3-dihydro-1H-pyrrolo[3,4-c] pyridine 4al. White solid (29% isolated yield), eluent petroleum ether/ethyl acetate = 4:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 8.2 Hz, 2H), 7.35 (d, *J* = 8.1 Hz, 2H), 6.87 (dd, *J*=11.7, 10.3 Hz, 3H), 5.98 (s, 2H), 4.62 (d, *J*=13.9 Hz, 4H), 2.42 (d, *J*=6.9 Hz, 6H), 2.15 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.3, 149.3, 147.6, 147.5, 145.9, 144.0, 133.8, 130.0, 128.9, 127.5, 122.9, 122.8, 112.2, 109.7, 108.1, 101.1, 53.5, 52.7, 21.7, 21.5, 16.1.



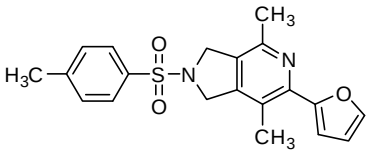
HRMS Calculated for $C_{23}H_{22}N_2O_4S$ 422.1300, found 422.1304.

3.2.26 4,7-dimethyl-6-(naphthalen-2-yl)-2-tosyl-2,3-dihydro-1H-pyrrolo[3,4-c]pyridine 4am. White solid (26% isolated yield), eluent petroleum ether/ethyl acetate = 4:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (dt, *J* = 11.7, 9.7 Hz, 6H), 7.54 (dd, *J* = 8.4, 1.3 Hz, 1H), 7.49 (dd, *J* = 6.3, 3.2 Hz, 2H), 7.36 (d, *J* = 8.2 Hz, 2H), 4.72-4.60 (m, 4H), 2.45 (d, *J* = 9.0 Hz, 6H), 2.19 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.8, 149.5, 145.9, 144.0, 137.2, 133.9, 133.1, 132.9, 130.0, 129.1, 128.3, 128.3, 127.9, 127.7, 127.6, 126.9, 126.3, 126.2, 123.2, 53.5, 52.8, 21.8, 21.6, 16.1.



HRMS Calculated for $C_{26}H_{24}N_2O_2S$ 428.1558, found 428.1565.

3.2.27 6-(furan-2-yl)-4,7-dimethyl-2-tosyl-2,3-dihydro-1H-pyrrolo[3,4-c]pyridine 4an. White solid (15% isolated yield), eluent petroleum ether/ethyl acetate = 4:1. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 8.3 Hz, 2H), 7.55 (d, *J* = 1.1 Hz, 1H), 7.34 (d, *J* = 8.1 Hz, 2H), 6.85 (d, *J* = 3.0 Hz, 1H), 6.51 (dd, *J* = 3.4, 1.8 Hz, 1H), 4.62 (s, 4H), 2.42 (s, 6H), 2.35 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.2, 149.6, 147.0, 146.2, 144.0, 143.0, 133.8, 130.0, 128.9, 127.5, 122.1, 111.4, 111.3, 53.6, 52.8, 21.8, 21.5, 16.0.



HRMS Calculated for $C_{20}H_{20}N_2O_3S$ 368.1195,found 368.1202.

4. References

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(5) Y. Yamamoto, K. Kinpara, R. Ogawa, H. Nishiyama, Itoh. K, *Chem. Eur. J.* **2006**, *12*, 5618.
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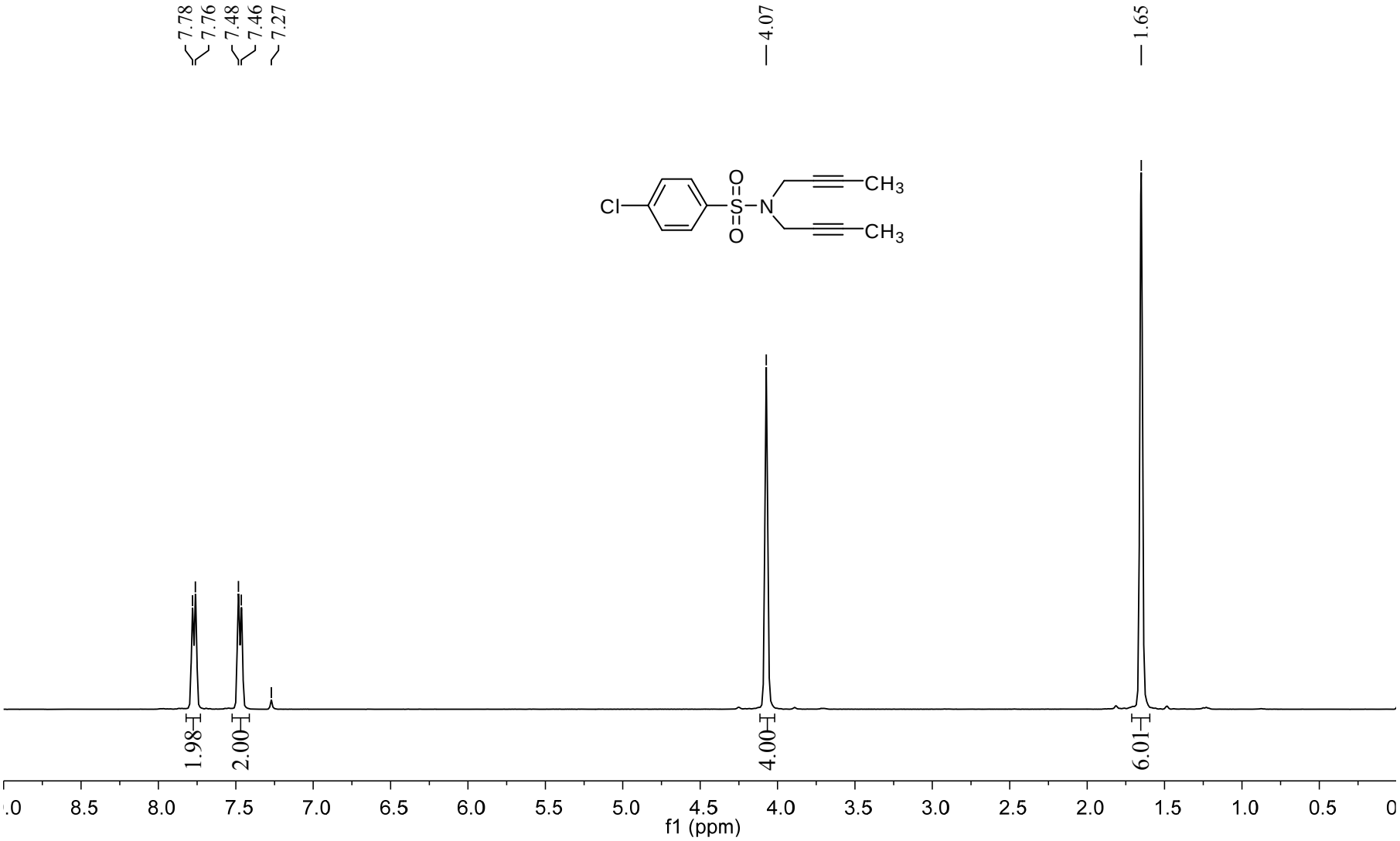
(8) H. Sharghi, M. H. Sarvari, *Synlett* **2001**, *1*, 99..

5. Copy of NMR (^{1}H, ^{13}C, ^{19}F) Spectra

6. Copy of HRMS Spectra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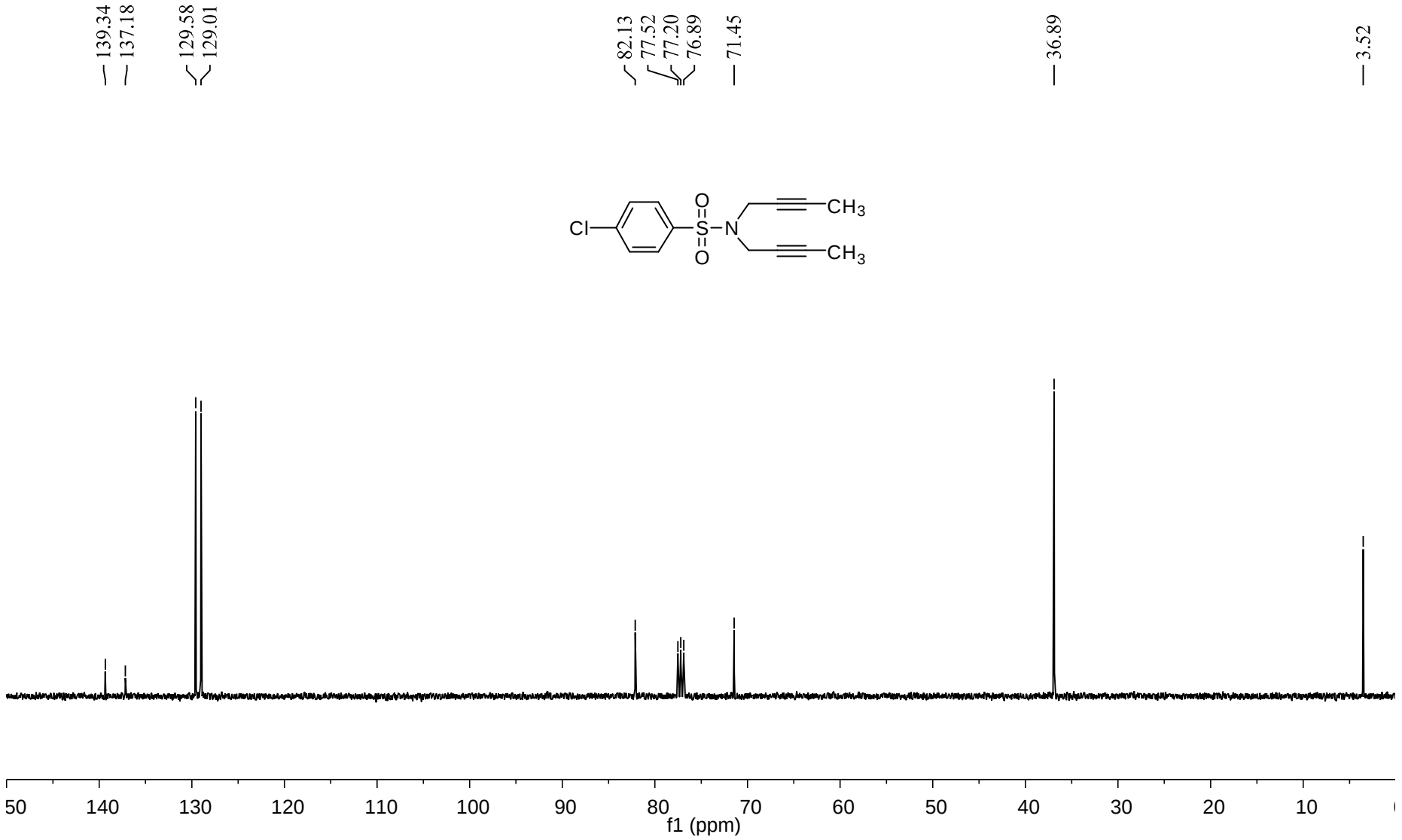
6.01
f1 (ppm)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S
O
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30
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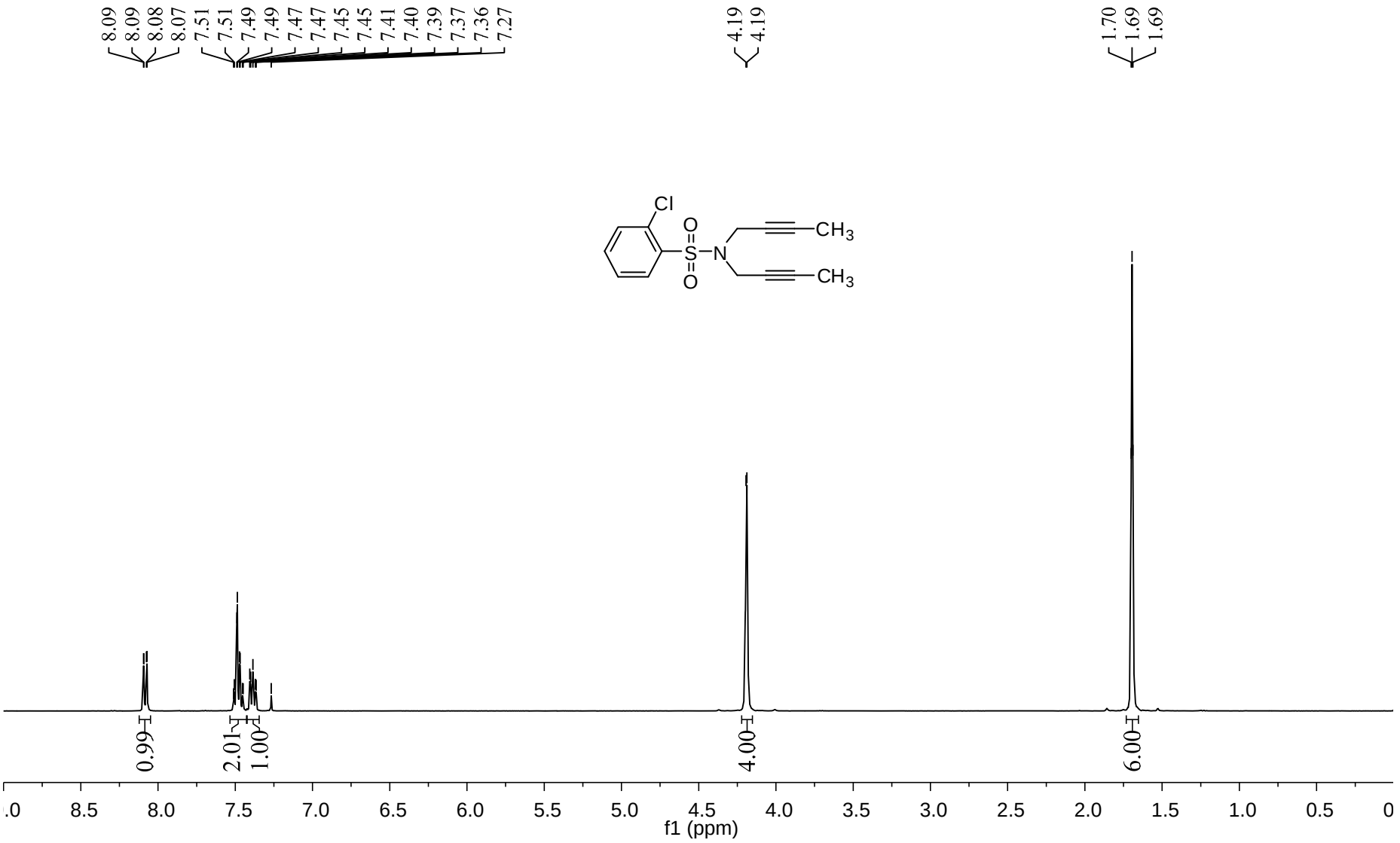
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7.45
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7.36
7.27
4.19
4.19
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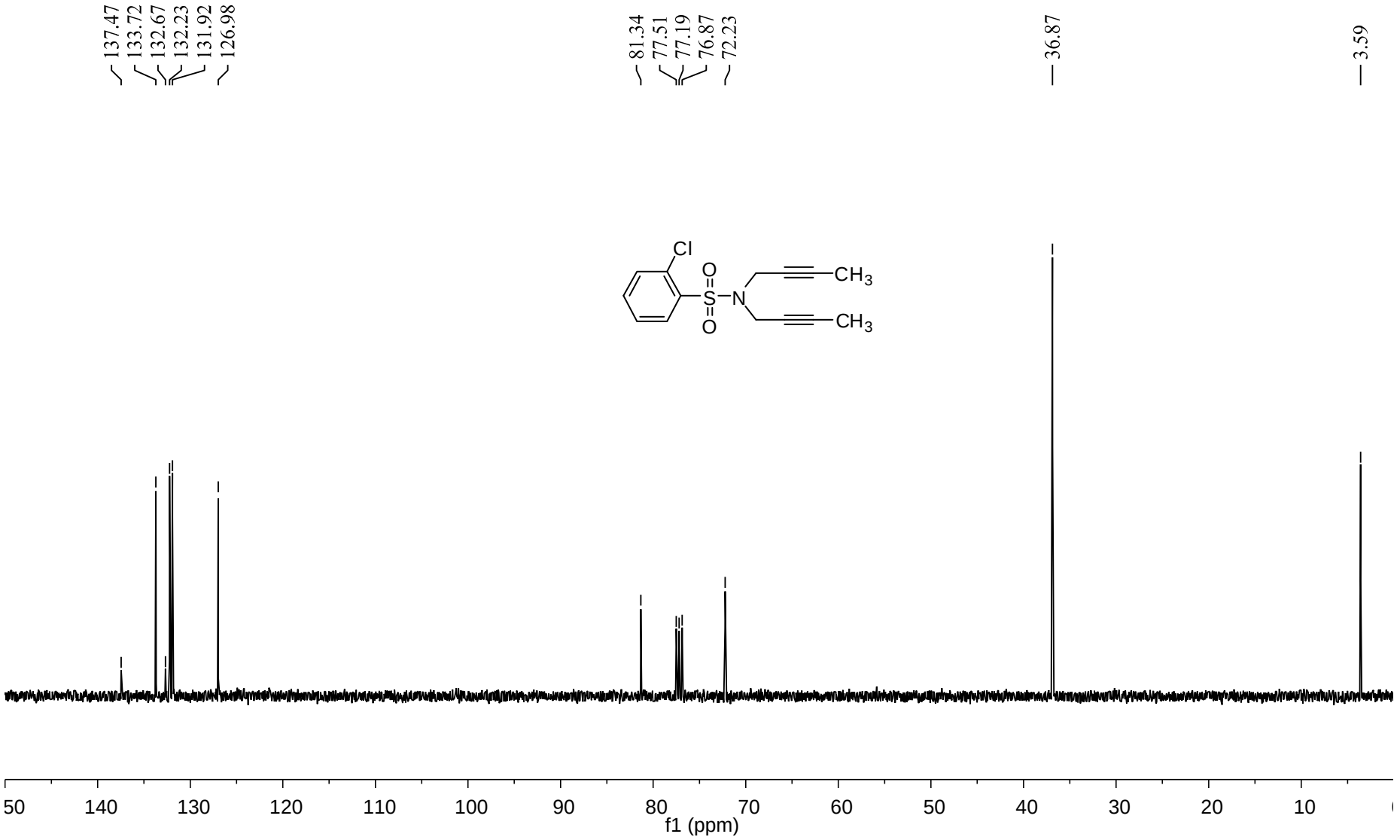
6.00
f1 (ppm)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20
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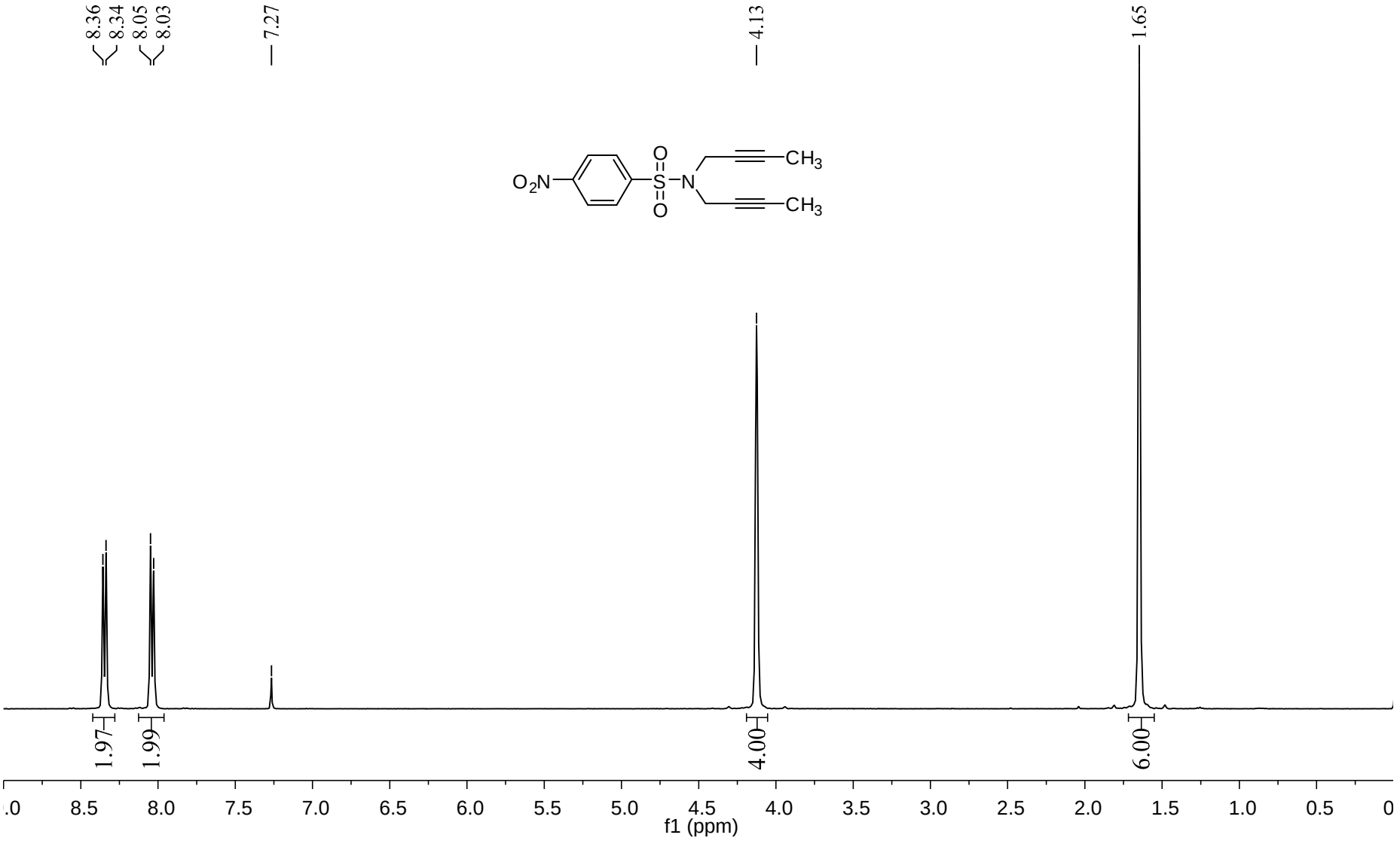
f1 (ppm)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O
S
O
N
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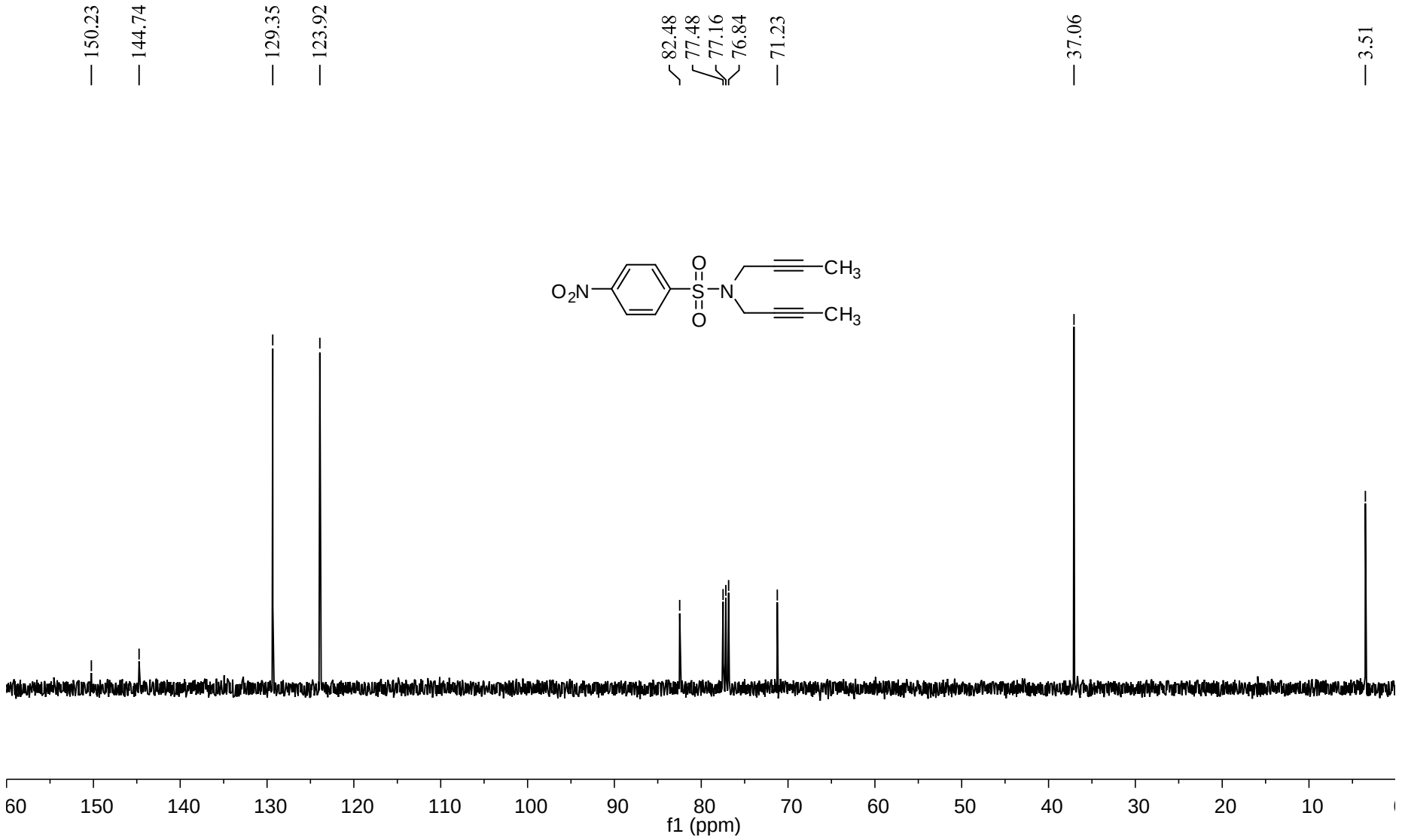
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N
O
O
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60
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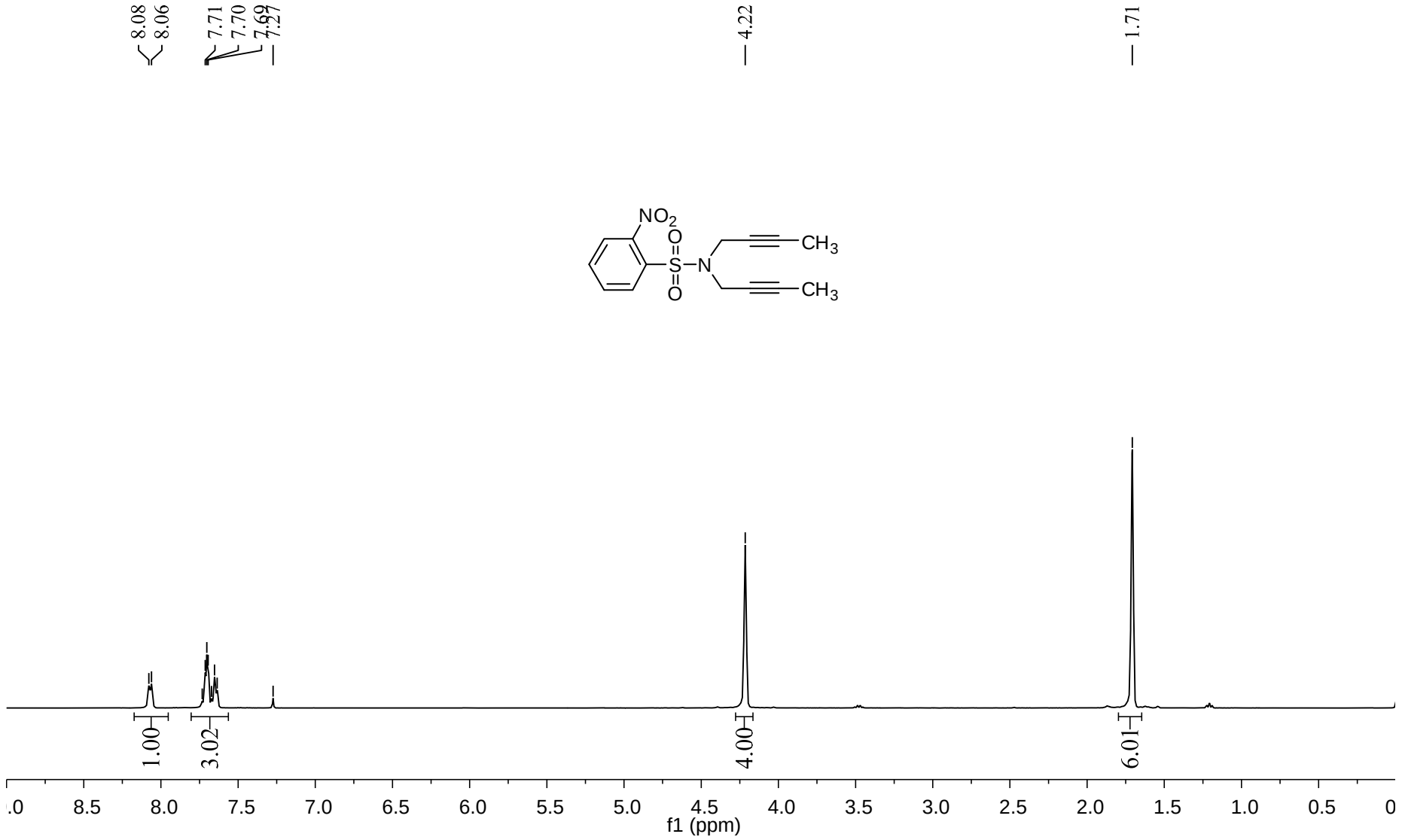
f1 (ppm)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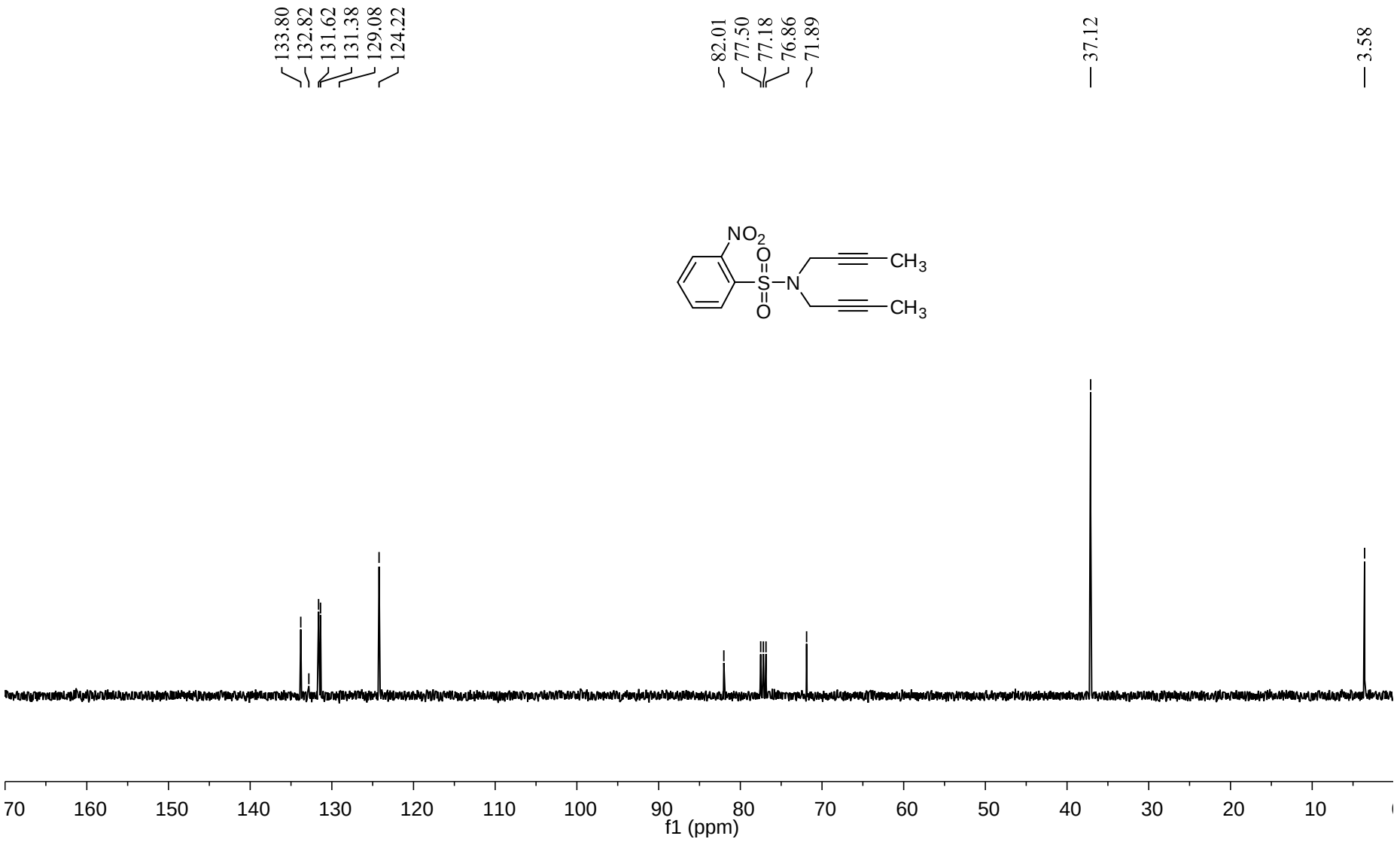
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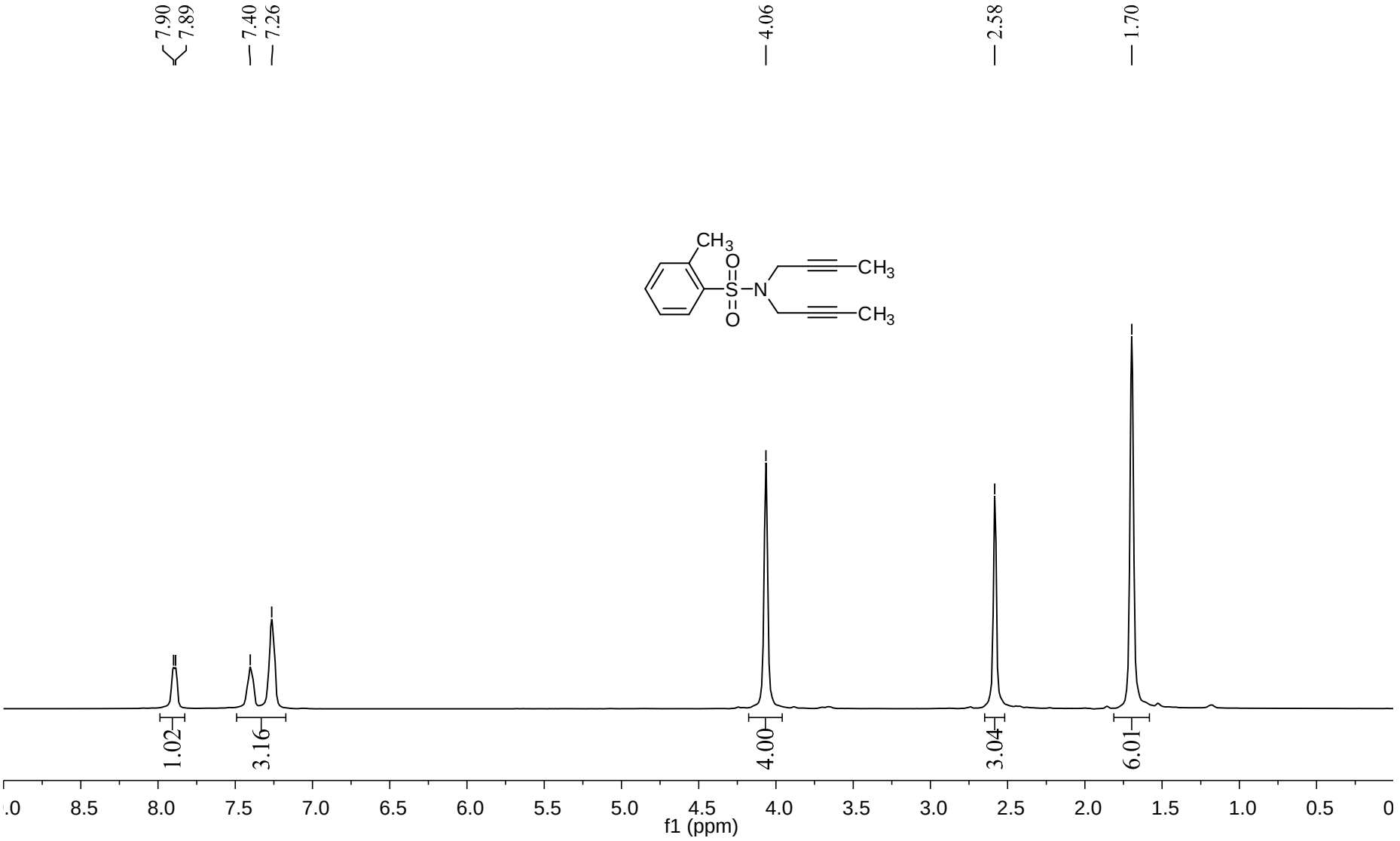
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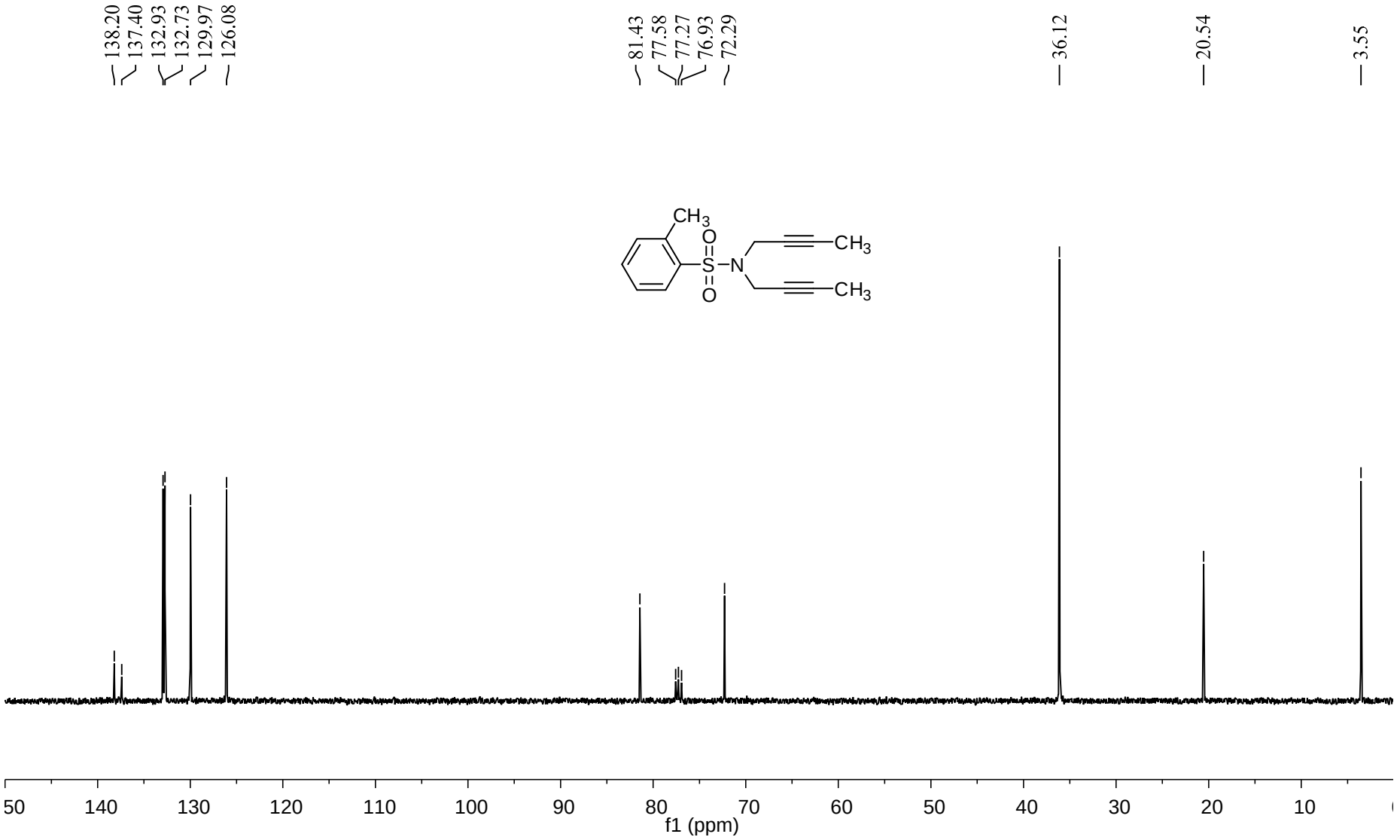
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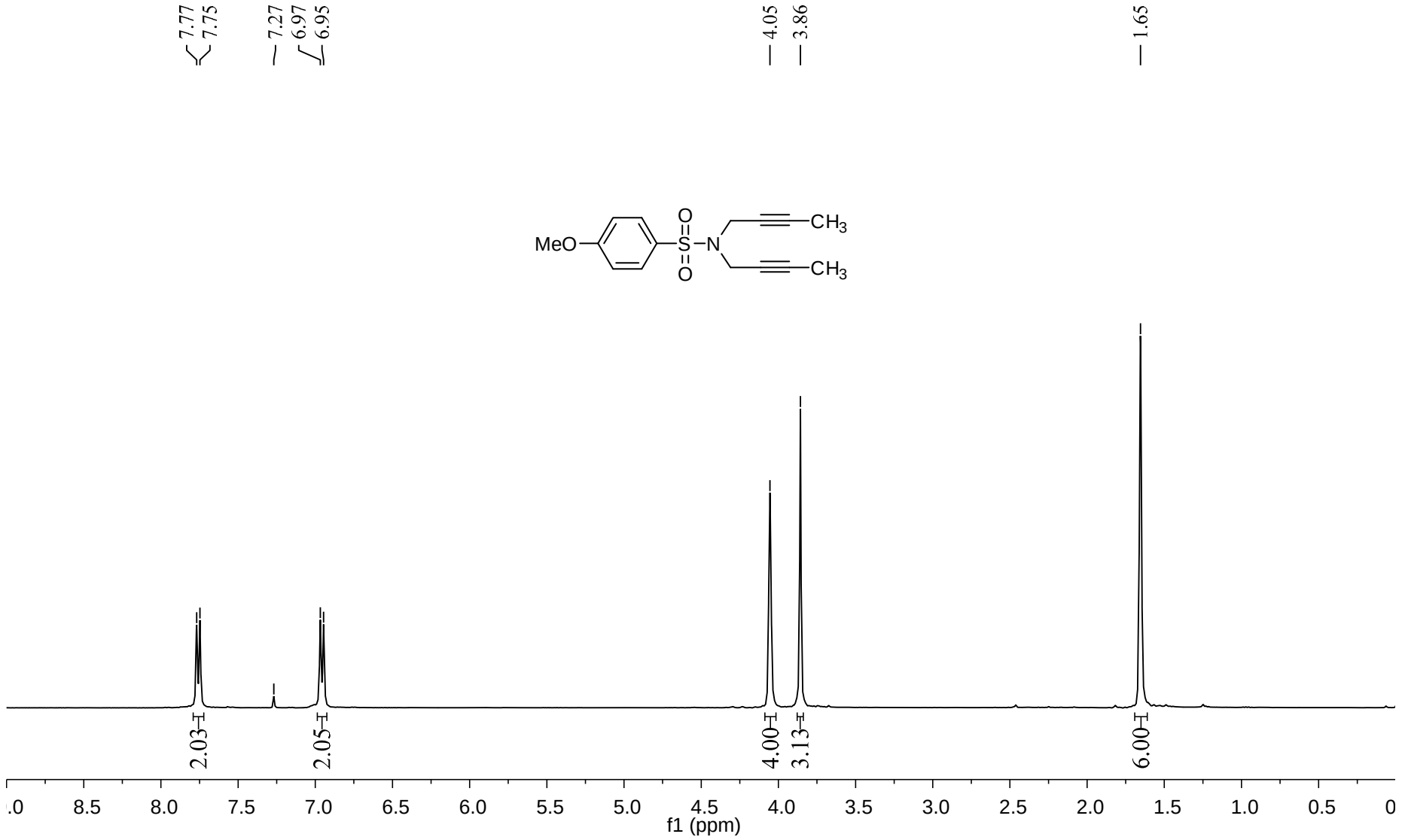
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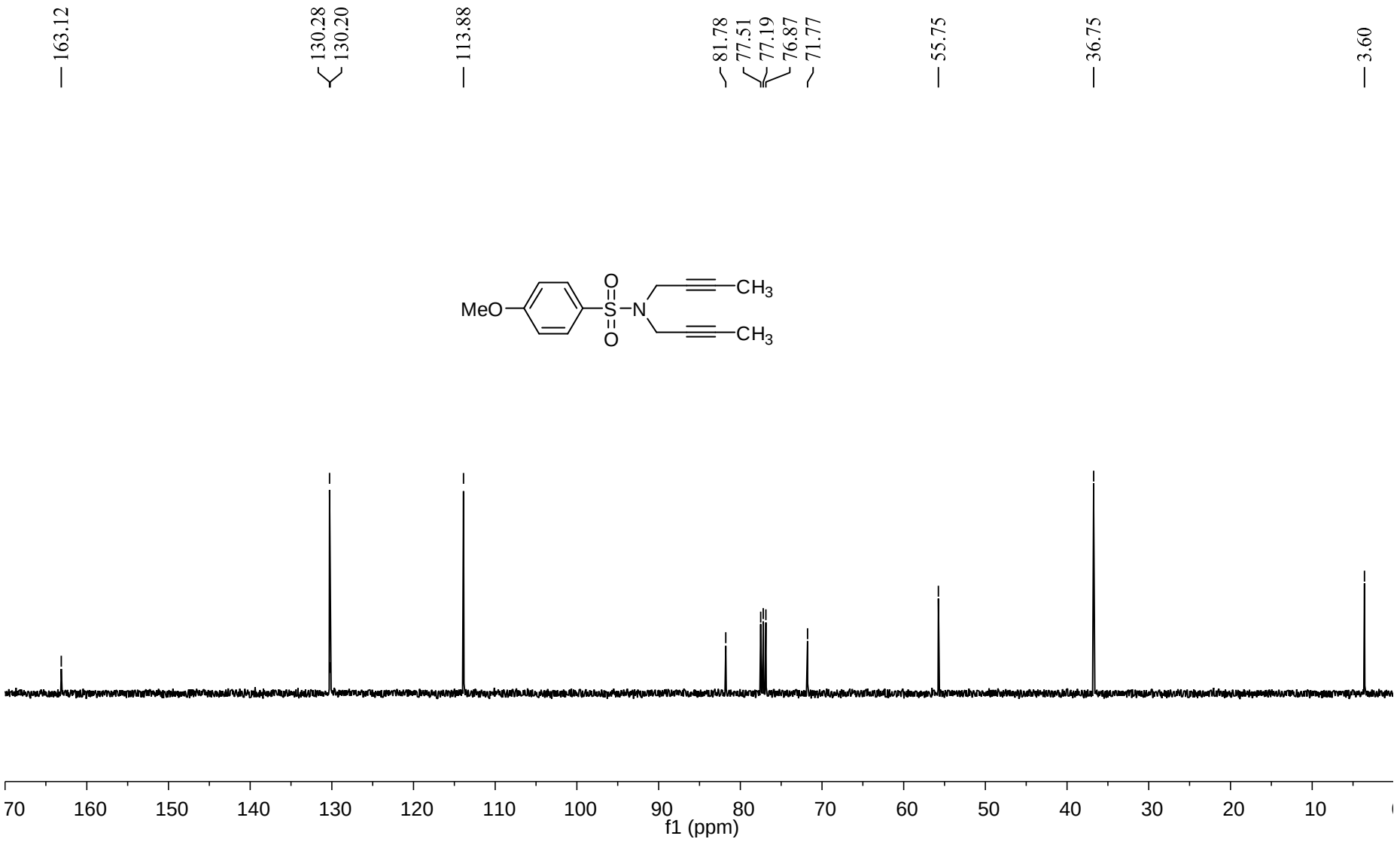
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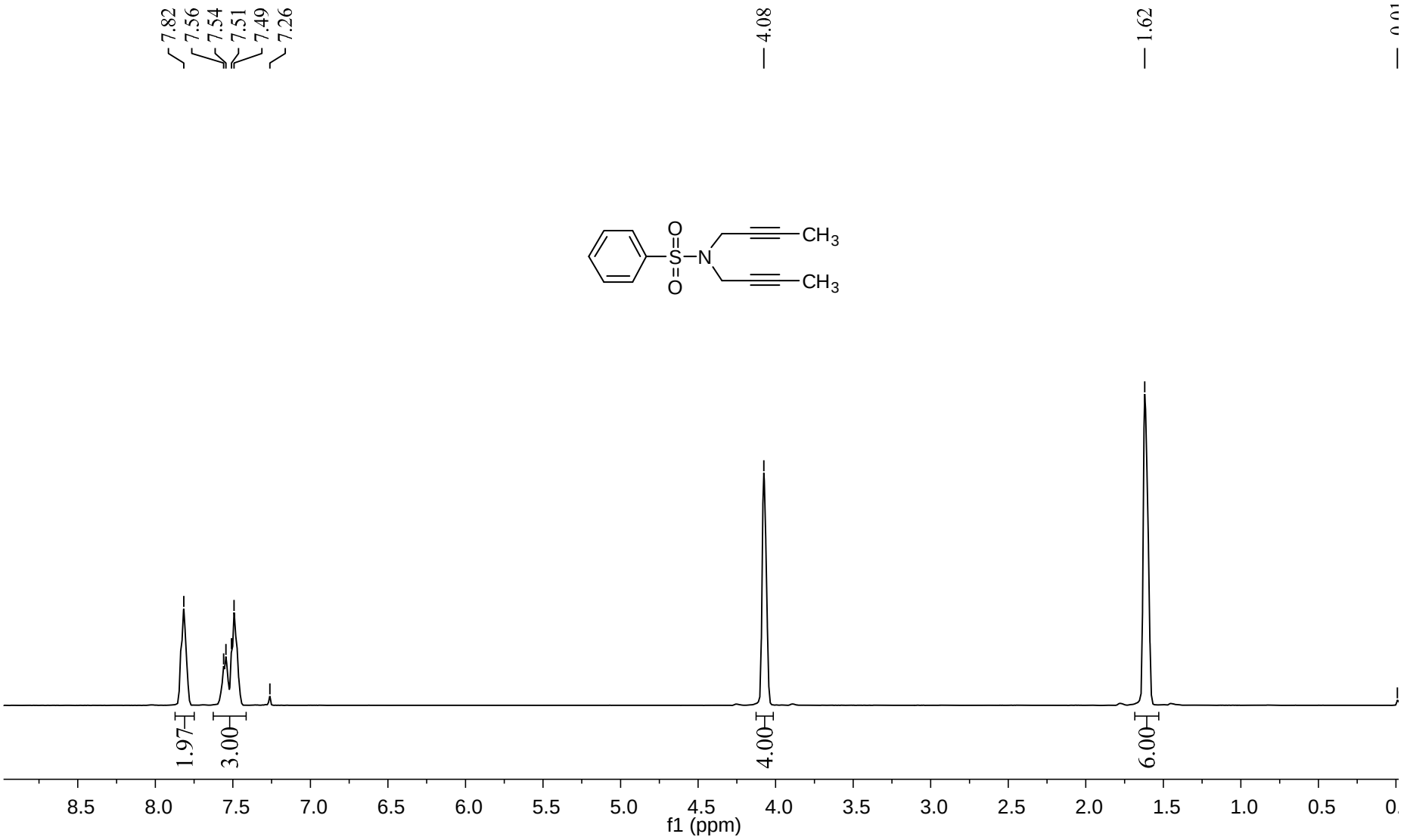
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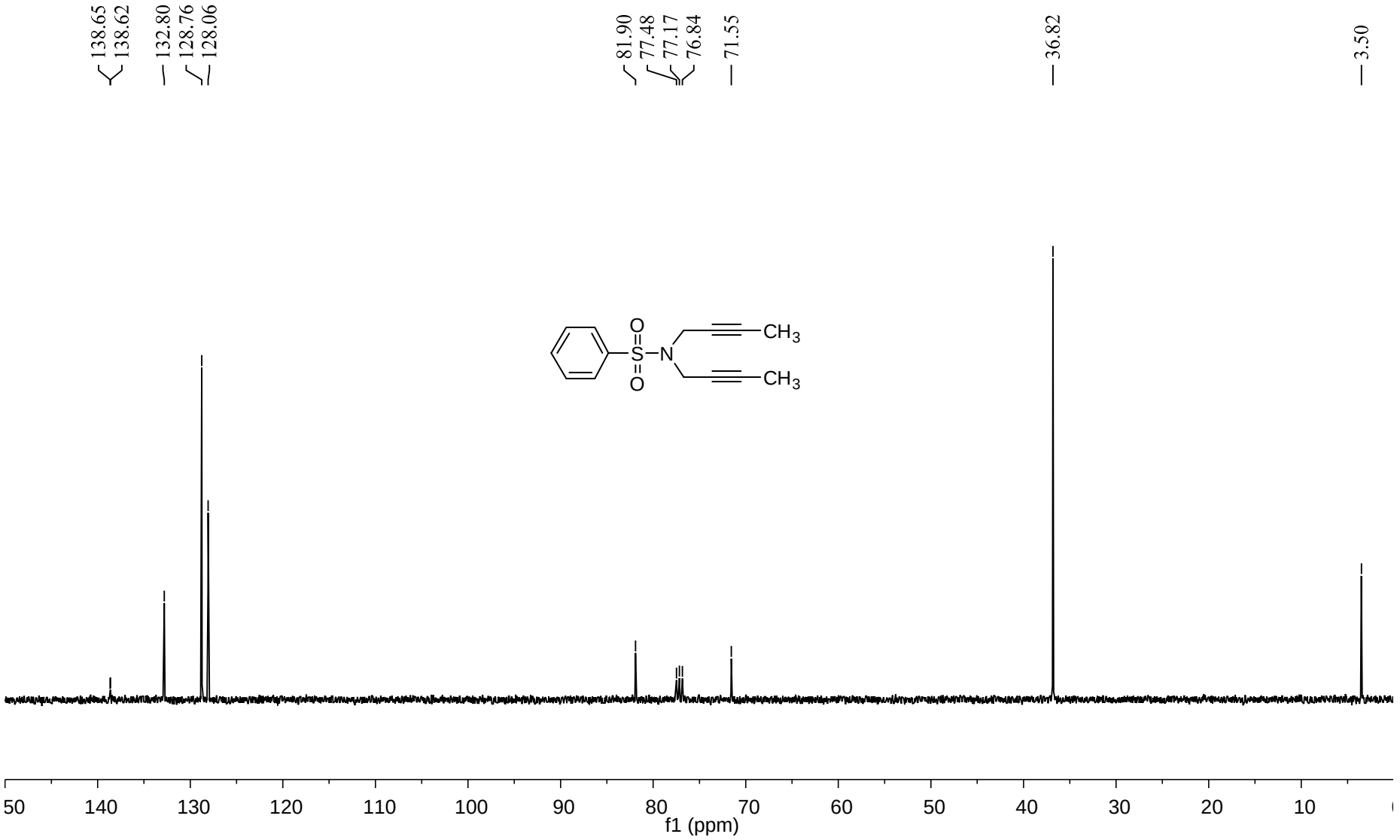
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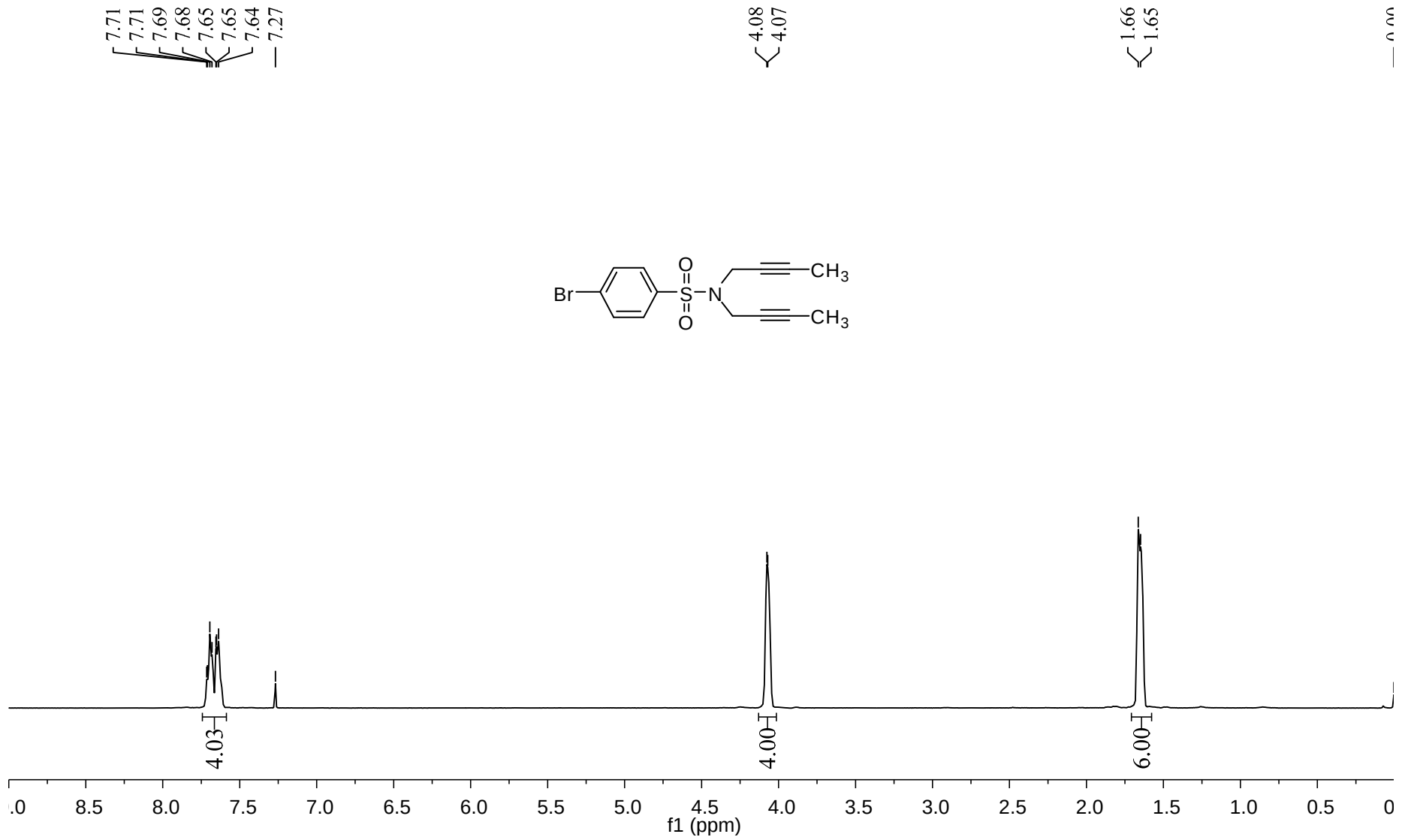
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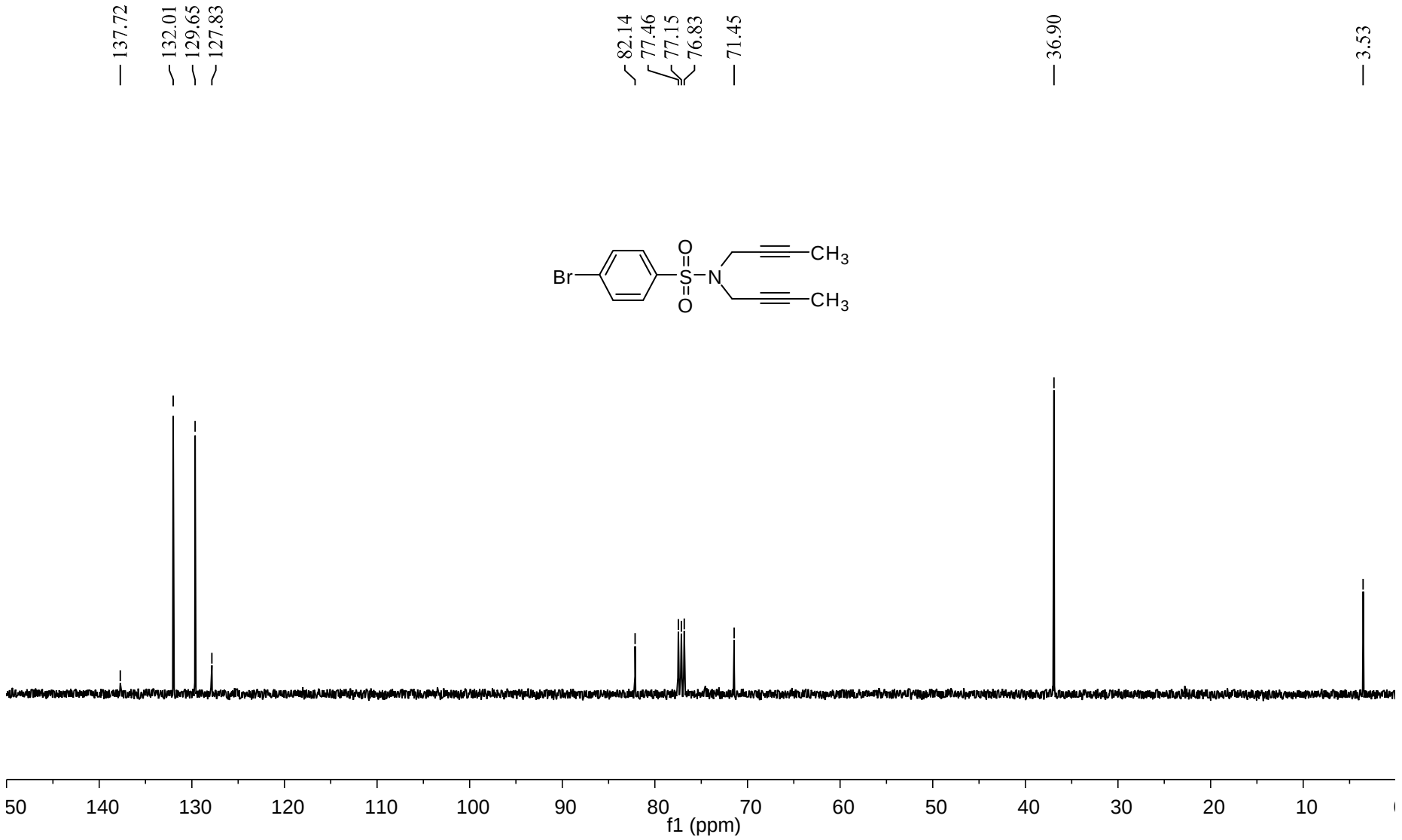
f1 (ppm)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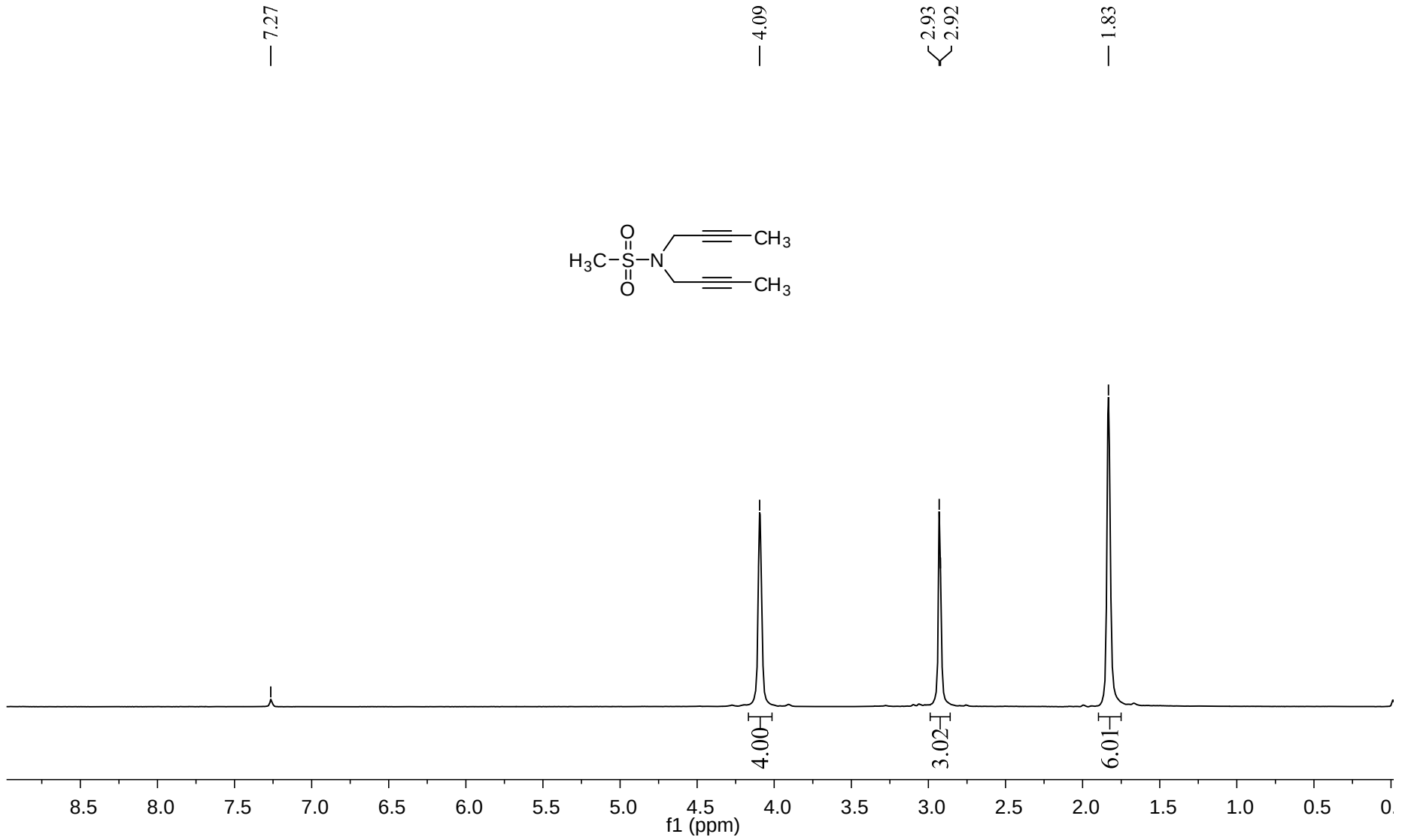
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8.0
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6.5
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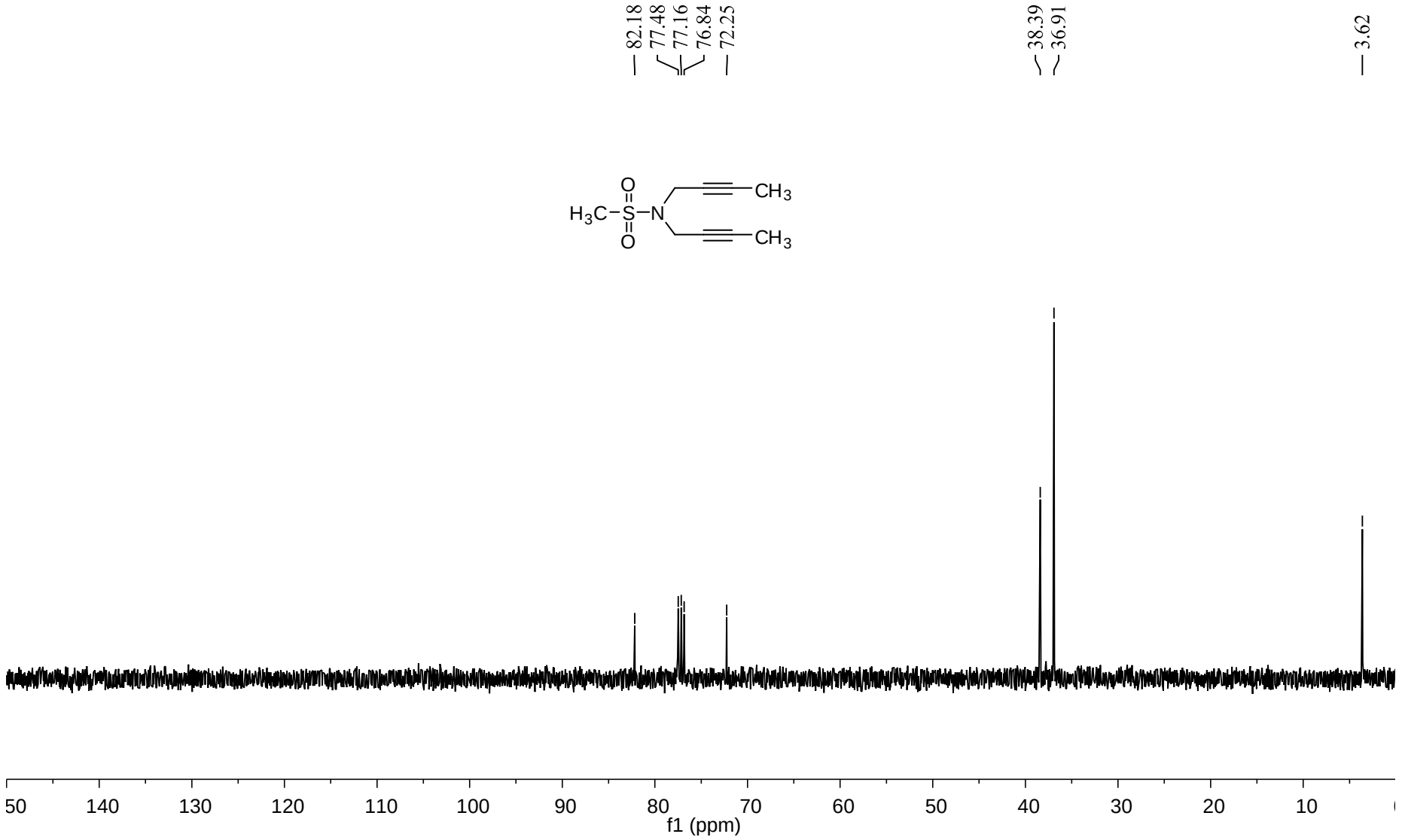
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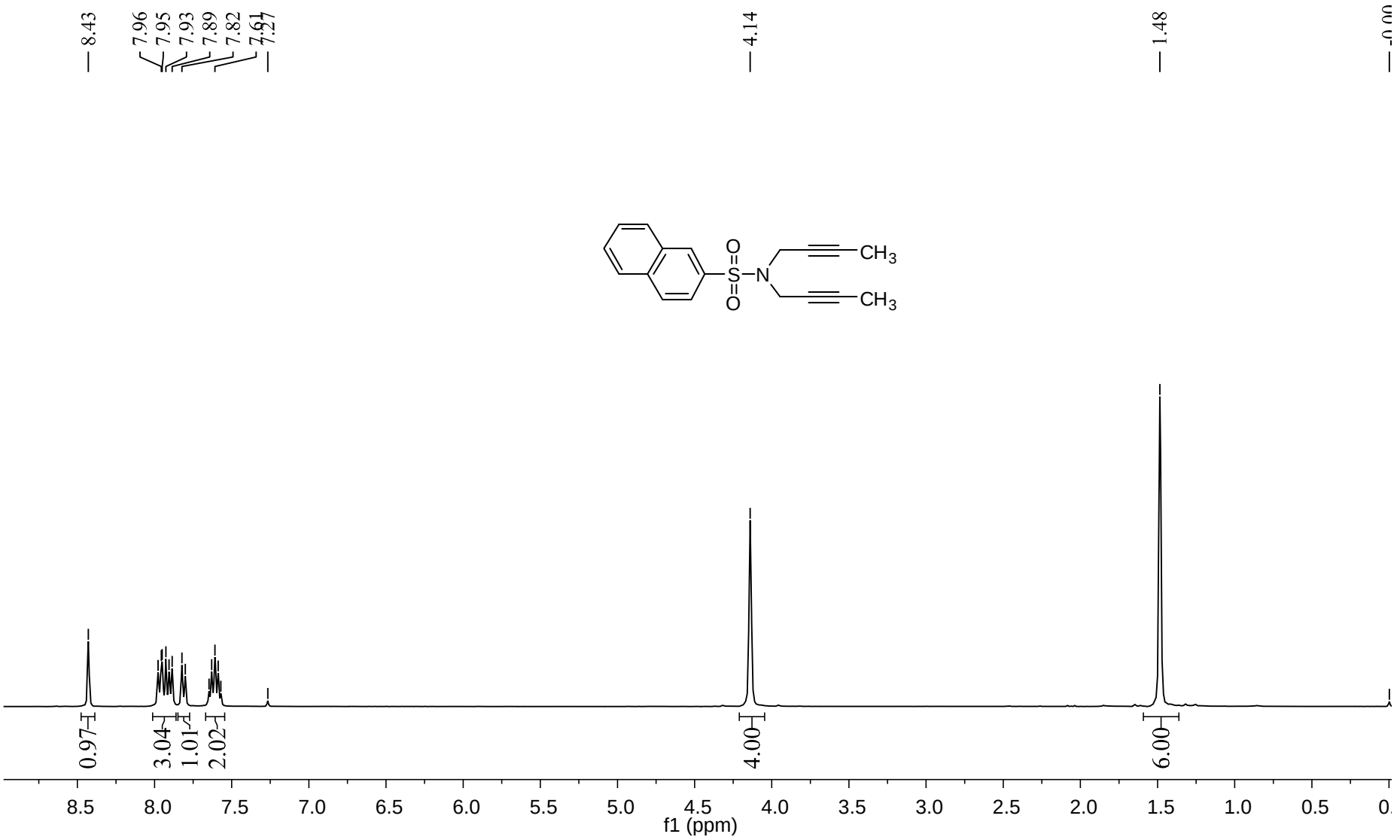
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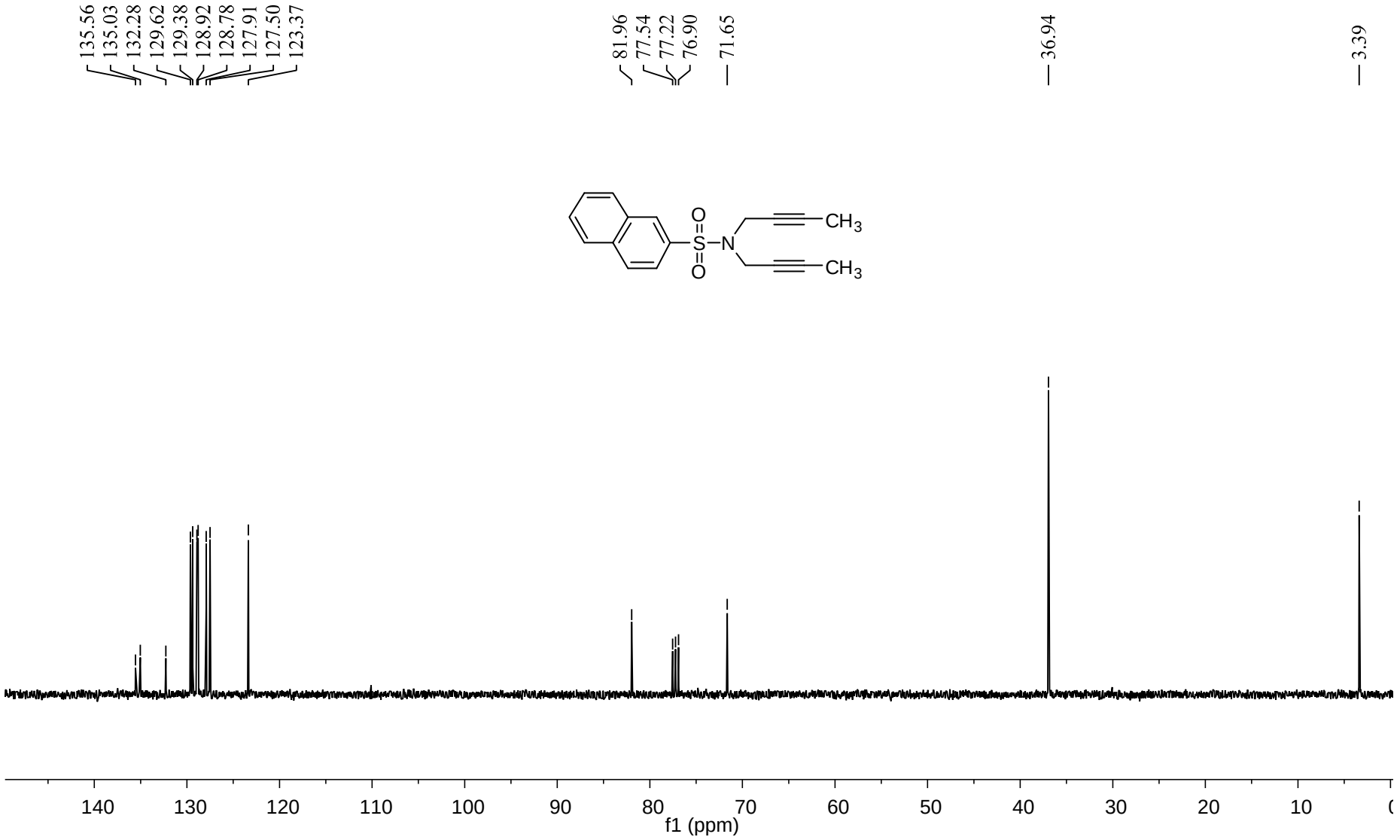
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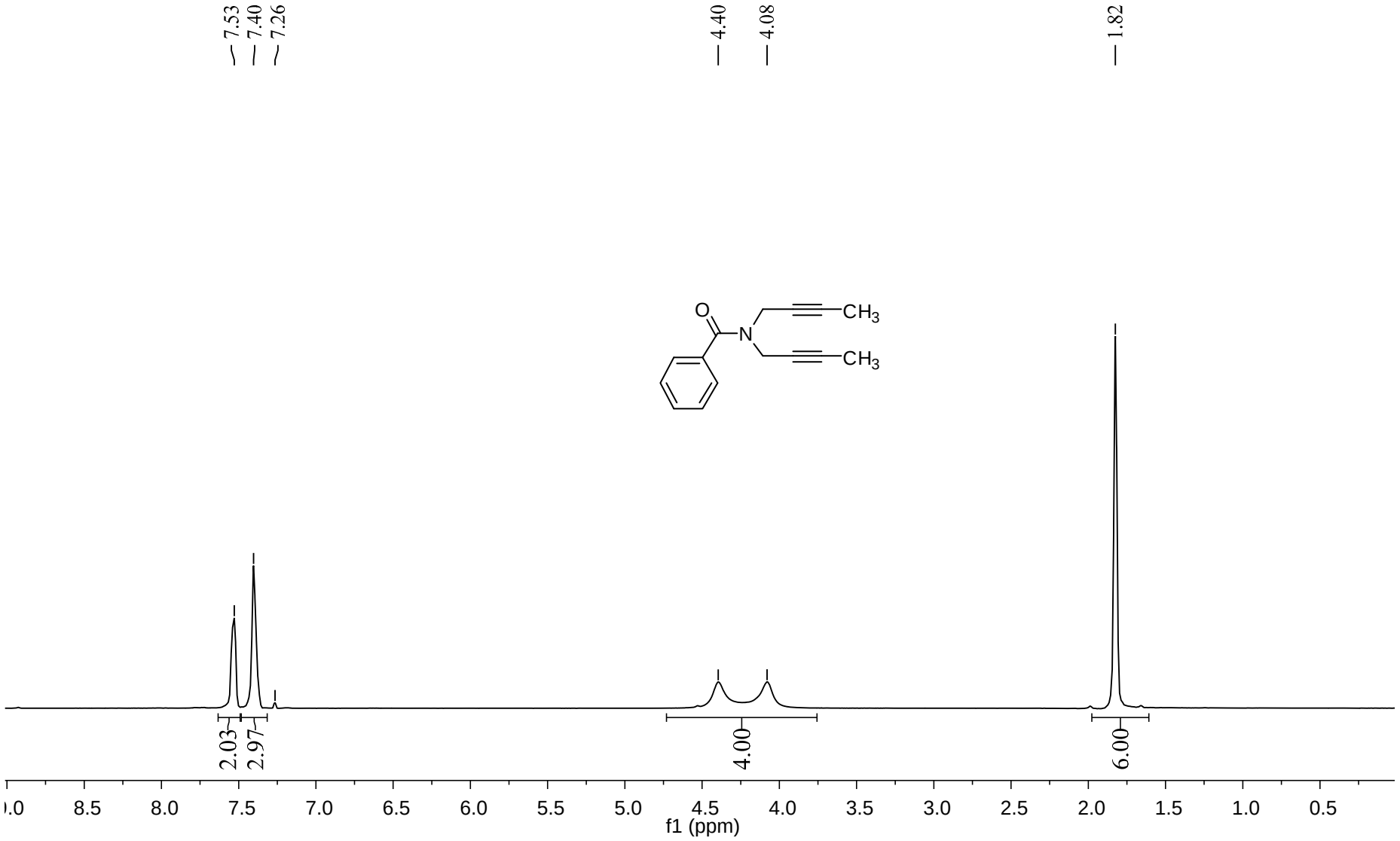
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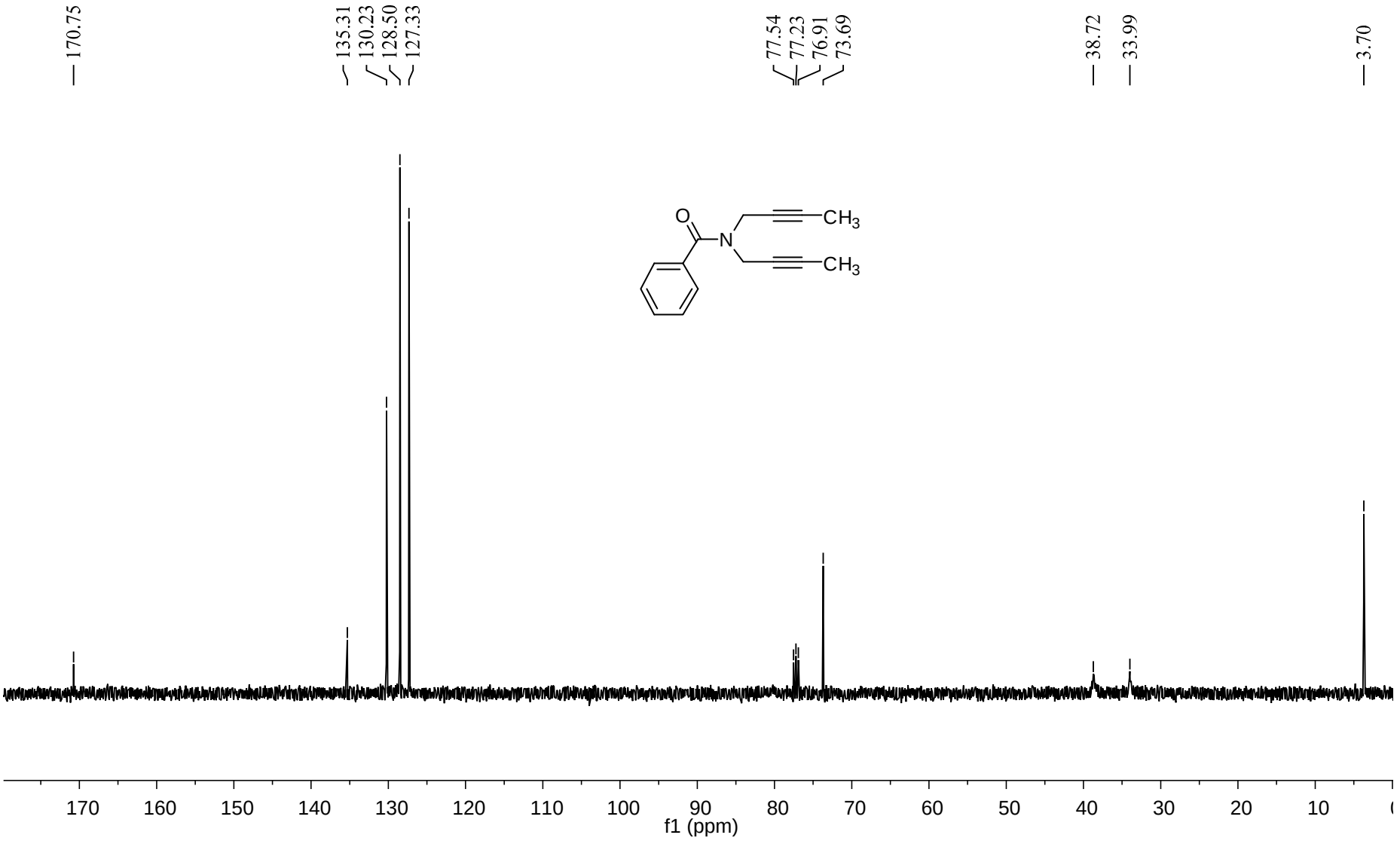
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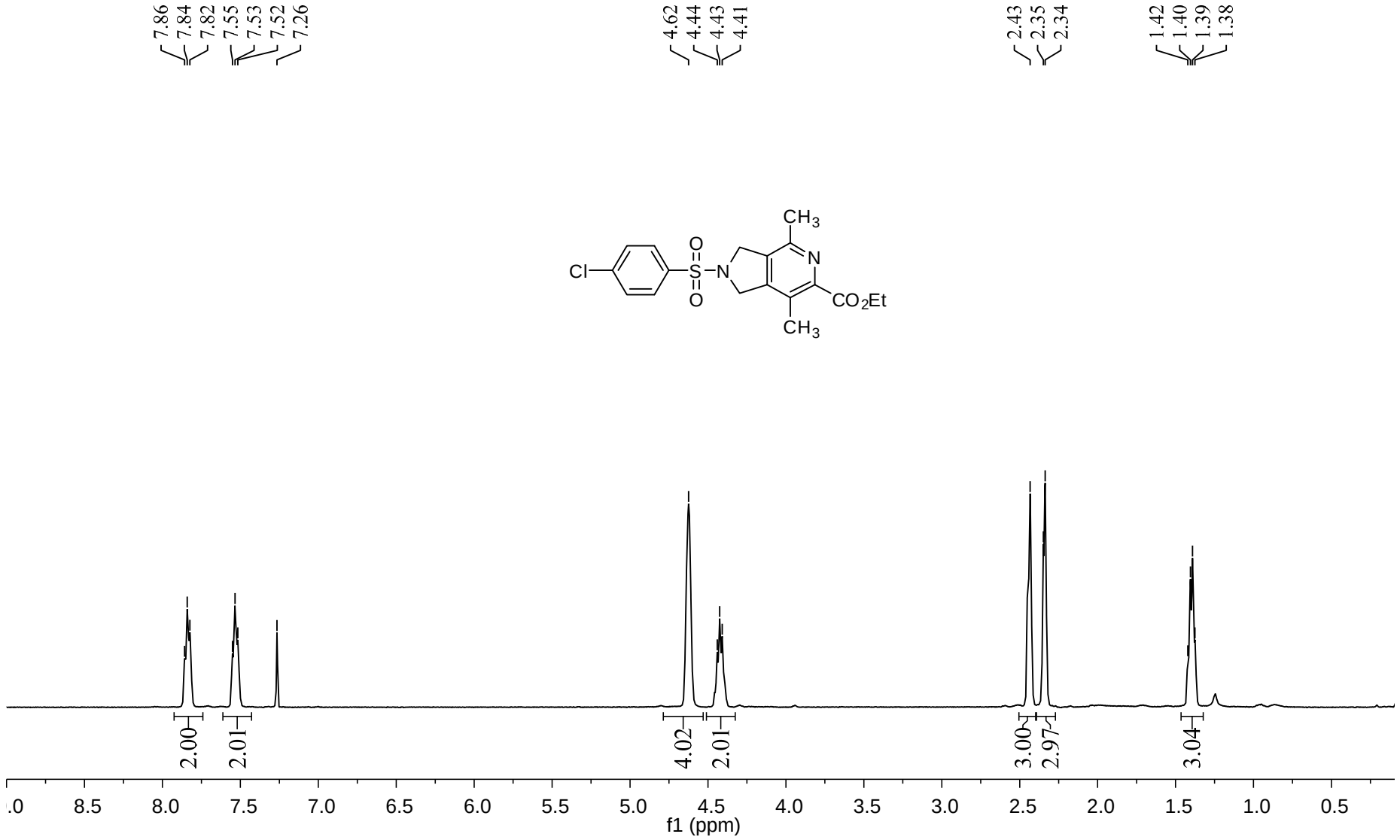
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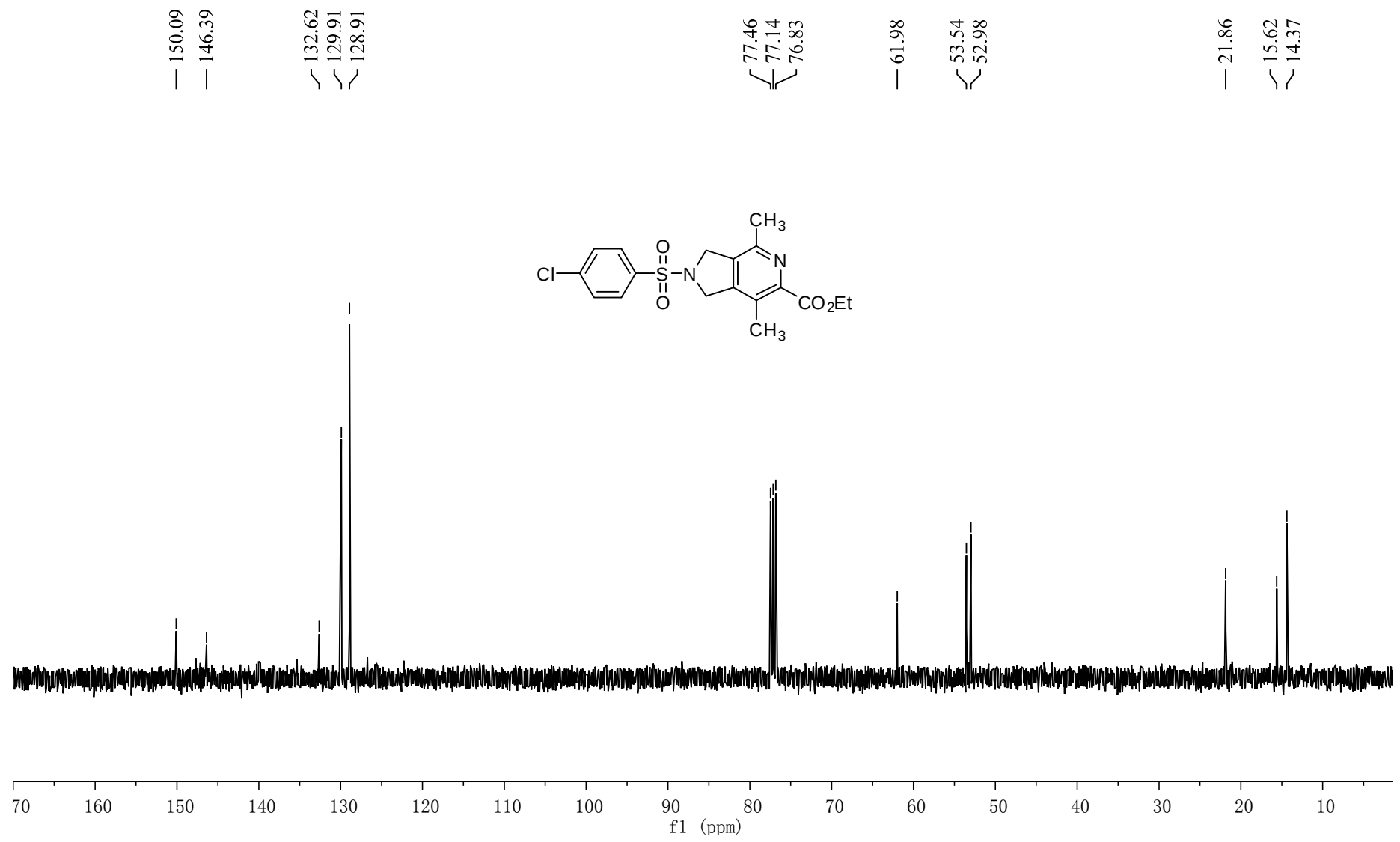
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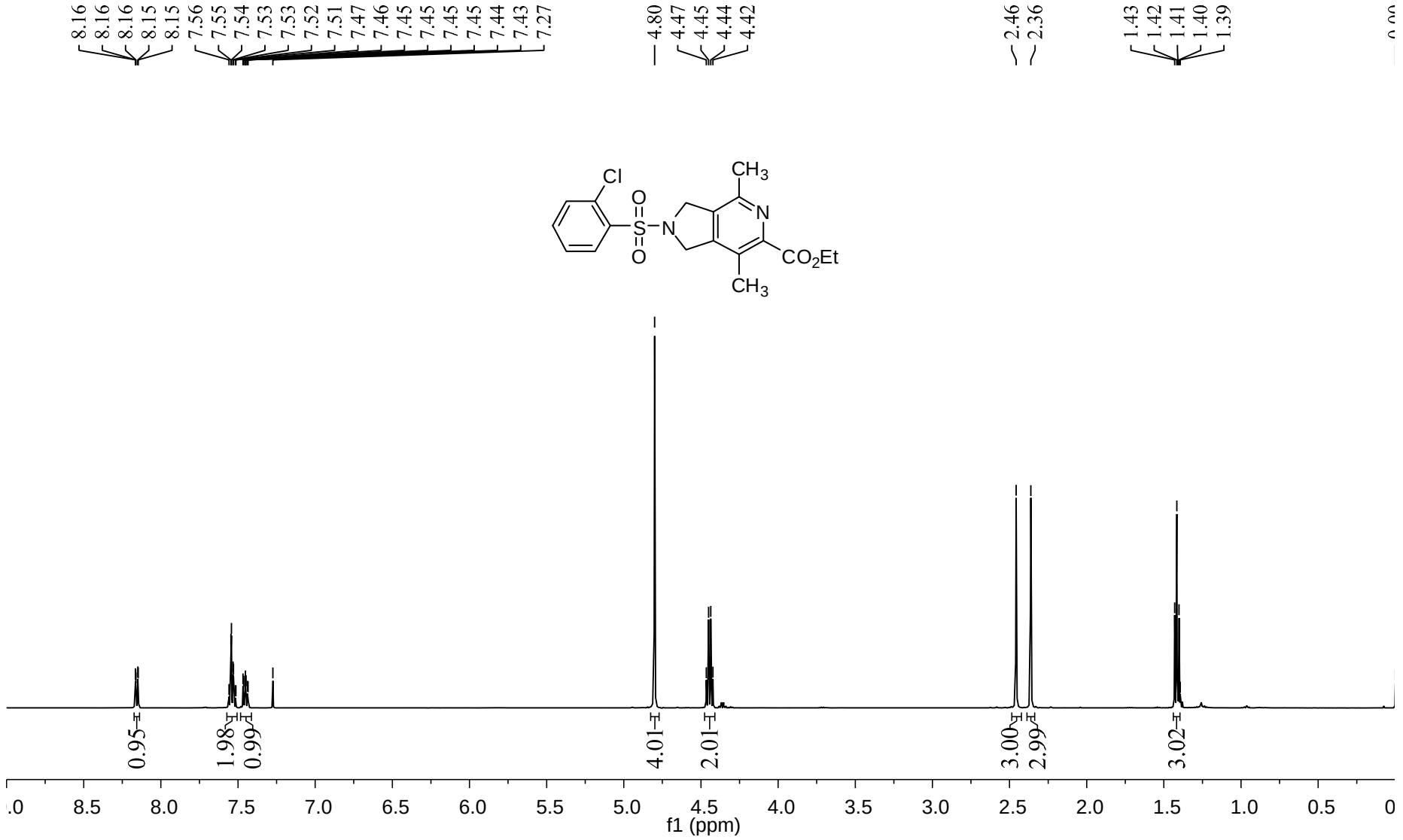
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1.43
1.42
1.41
1.40
1.39
Cl
O
S
O
N
CH3
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CO2Et
CH3
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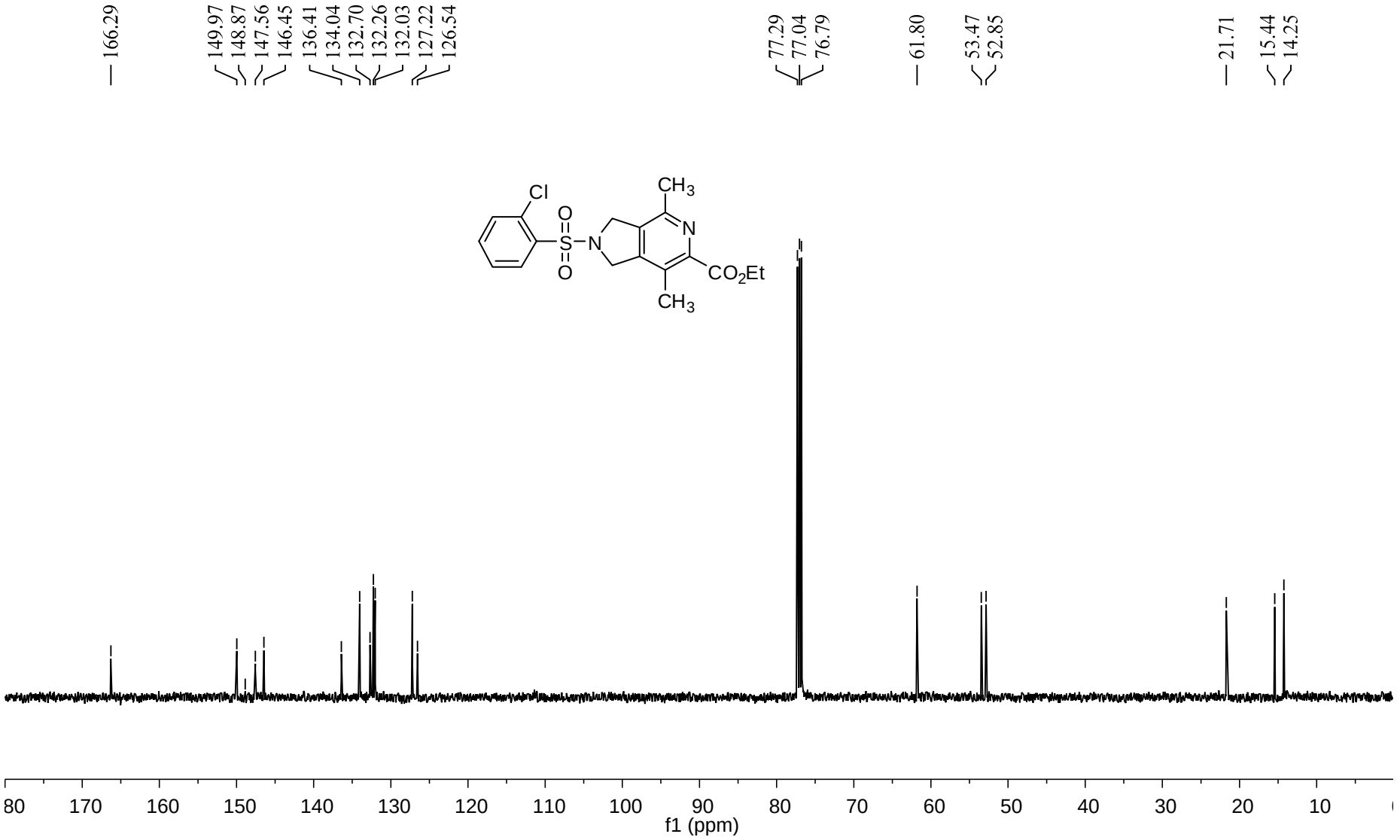
2.01
3.00
2.99
3.02
f1 (ppm)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132.70
132.26
132.03
127.22
126.54
77.29
77.04
76.79
61.80
53.47
52.85
21.71
15.44
14.25
Cl
O
S
O
N
CH3
N
CO2Et
CH3
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140
130
120
110
100
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80
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60
50
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20
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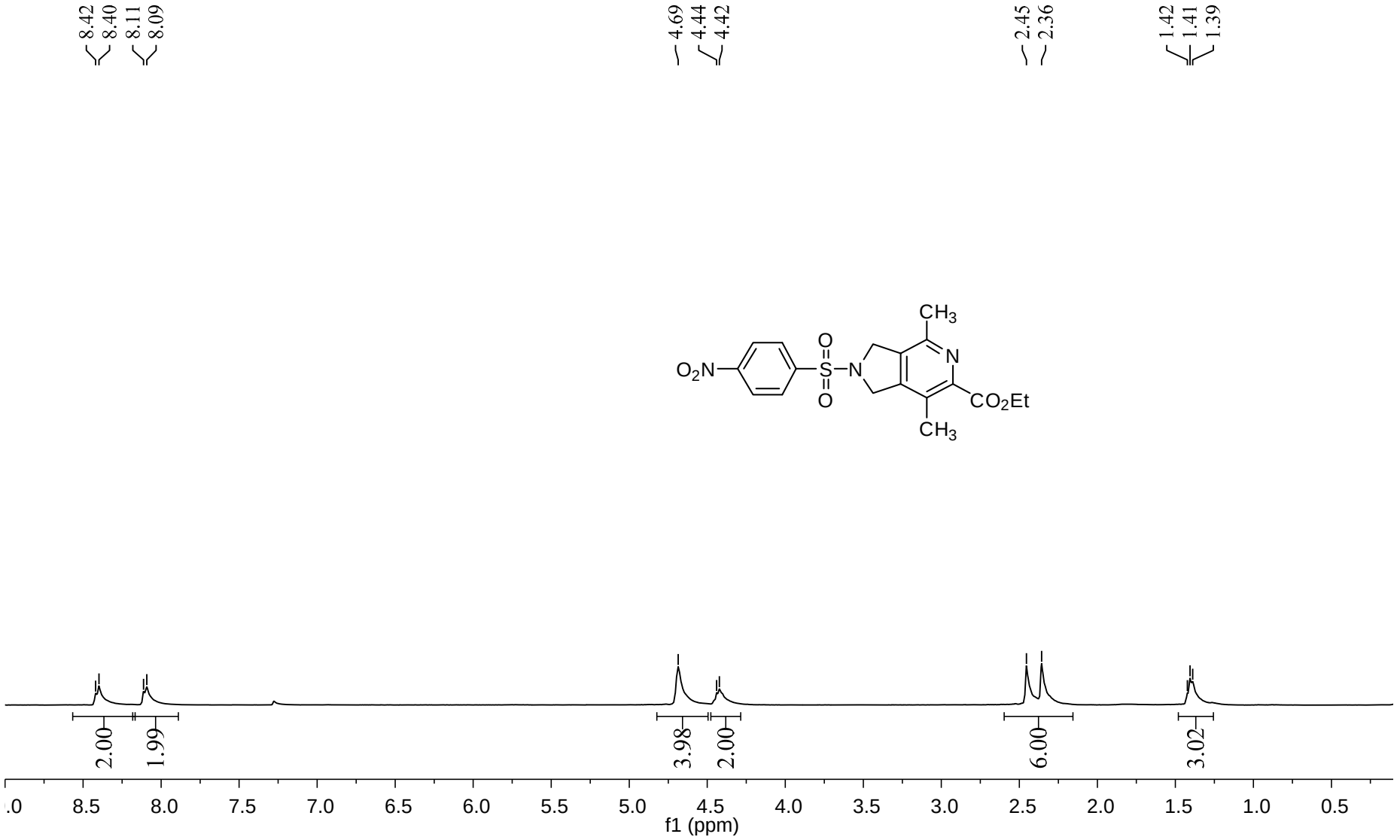
f1 (ppm)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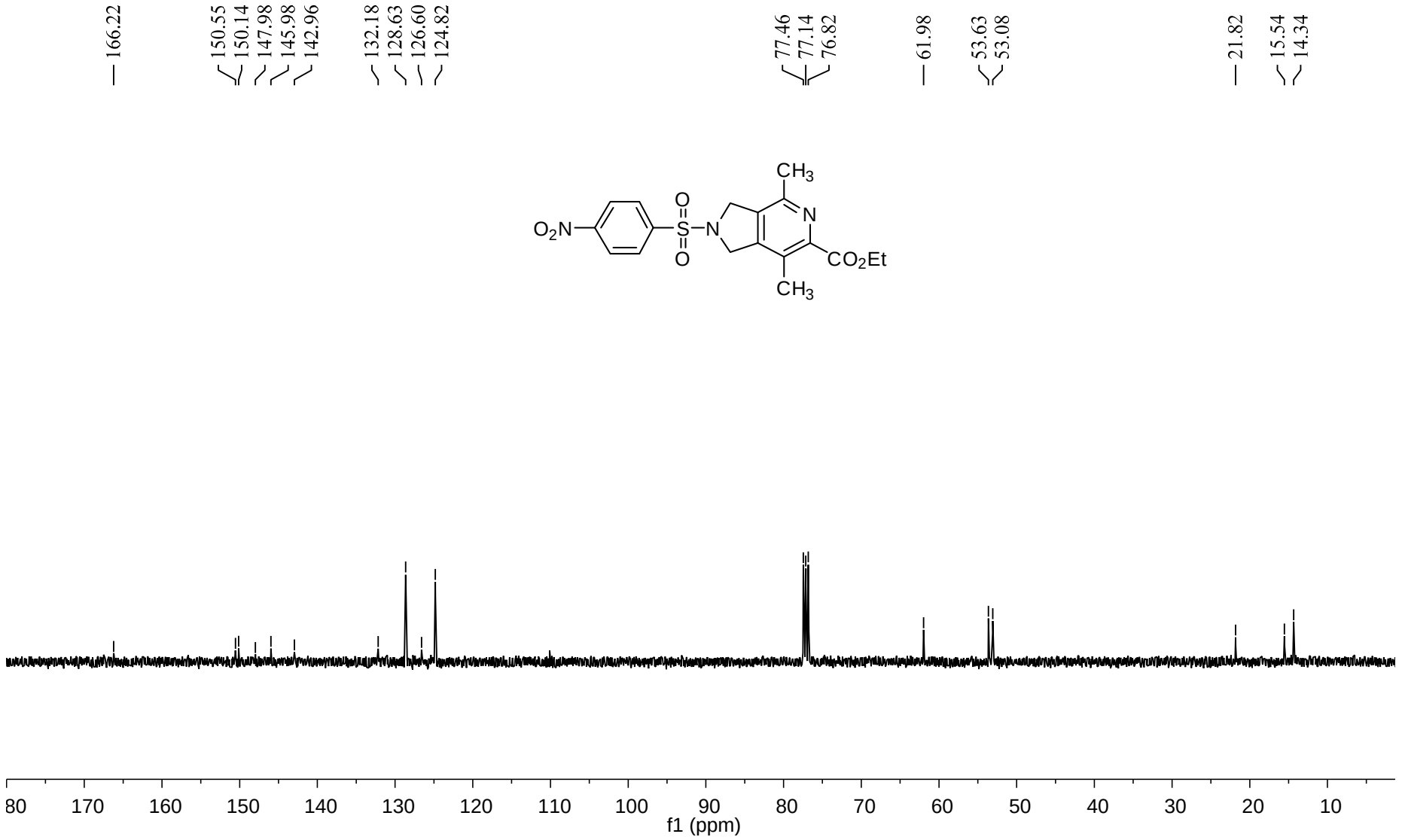
4.44
4.42
2.45
2.36
1.42
1.41
1.39
CH3
O
S
O
O2N
N
N
CO2Et
CH3
2.00
1.99
3.98
2.00
6.00
3.02
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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132.18
128.63
126.60
124.82
77.46
77.14
76.82
61.98
53.63
53.08
21.82
15.54
14.34
CH3
O2N
S
O
O
N
N
CO2Et
CH3
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140
130
120
110
100
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80
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60
50
40
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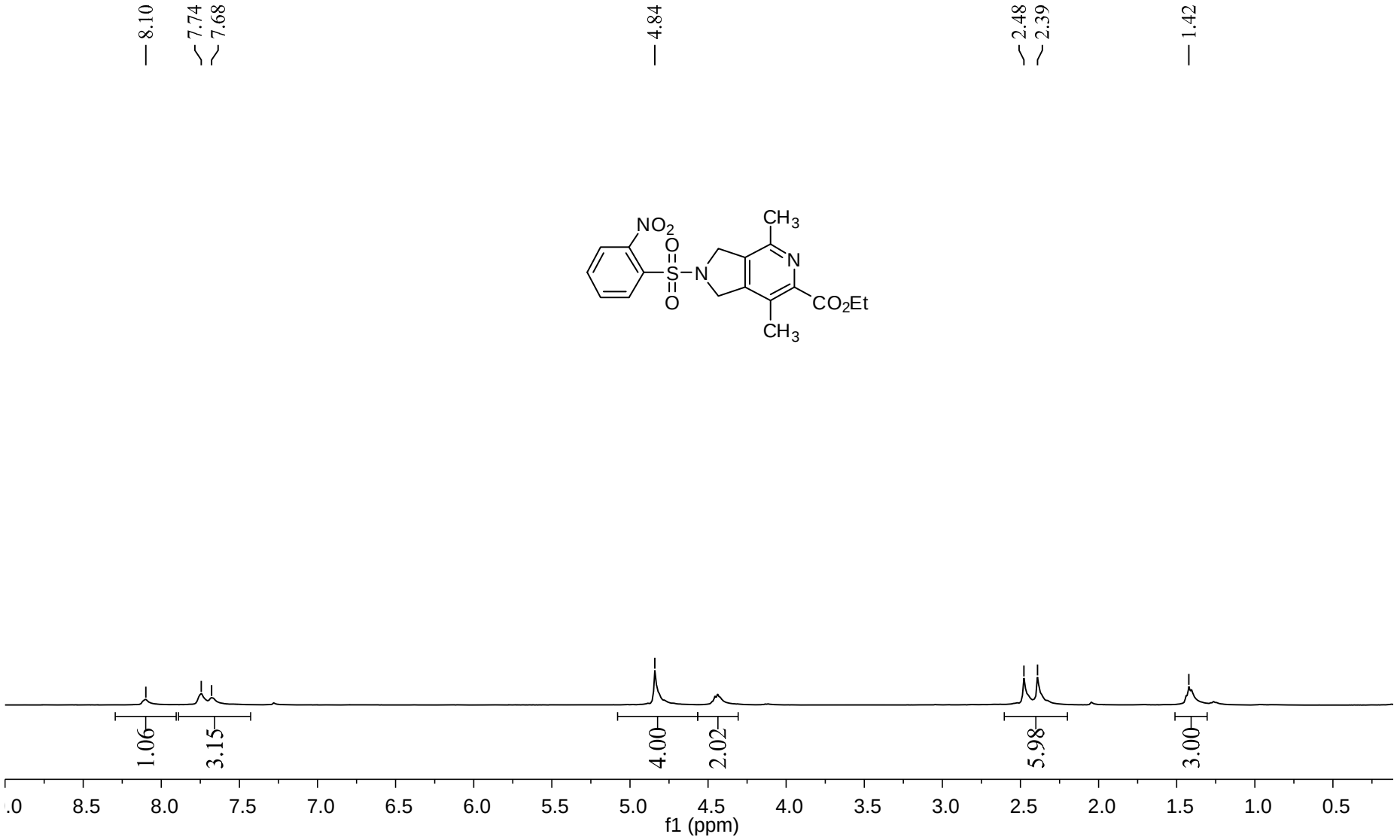
20
10
f1 (ppm)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7.74
7.68
4.84
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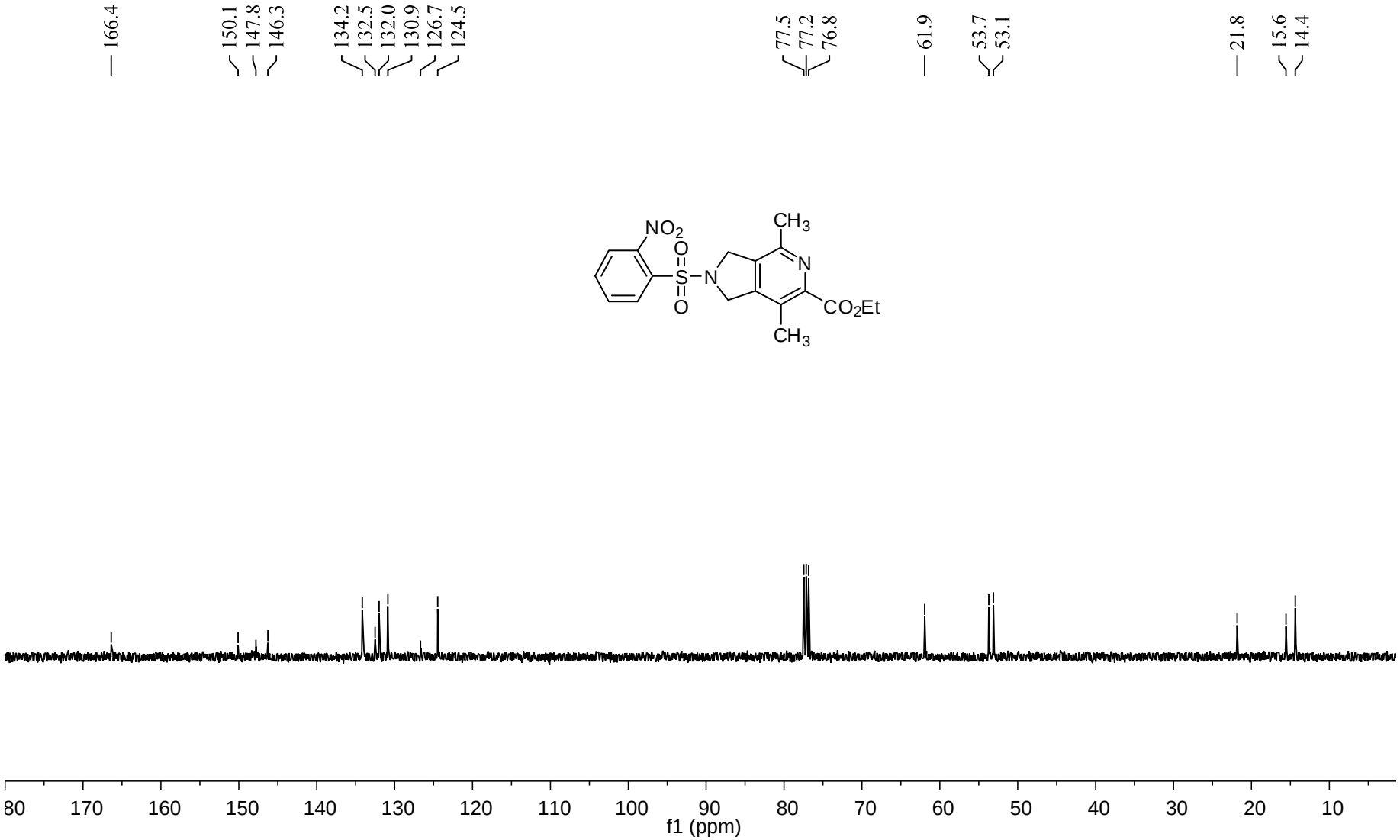
2.39
1.42
NO2
O
S
O
N
CH3
N
CO2Et
CH3
1.06
3.15
4.00
2.02
5.98
3.00
f1 (ppm)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147.8
146.3
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130.9
126.7
124.5
77.5
77.2
76.8
61.9
53.7
53.1
21.8
15.6
14.4
NO2
O
S
O
N
CH3
N
CO2Et
CH3
80
170
160
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140
130
120
110
100
90
80
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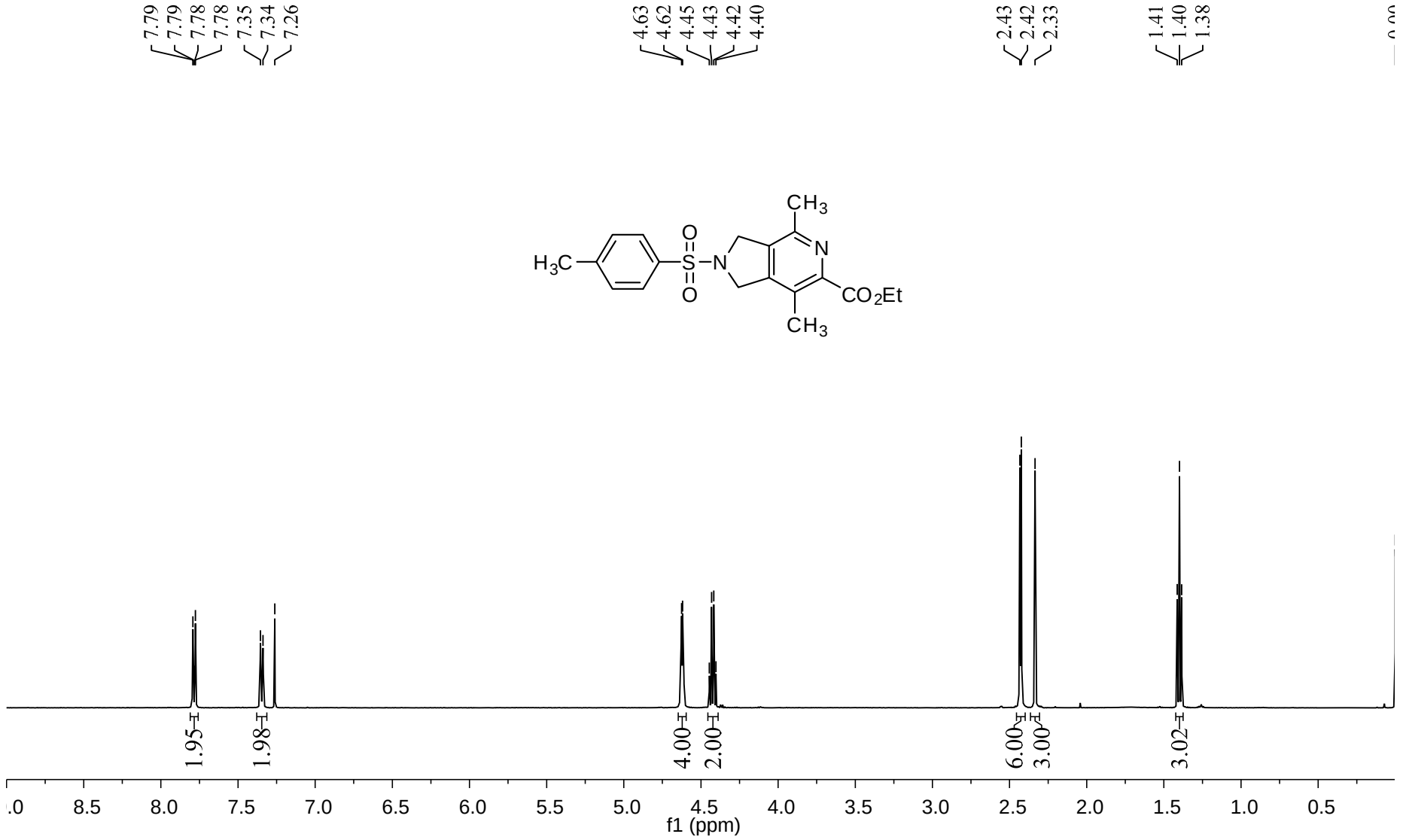
60
50
40
30
20
10
f1 (ppm)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7.34
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4.63
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4.45
4.43
4.42
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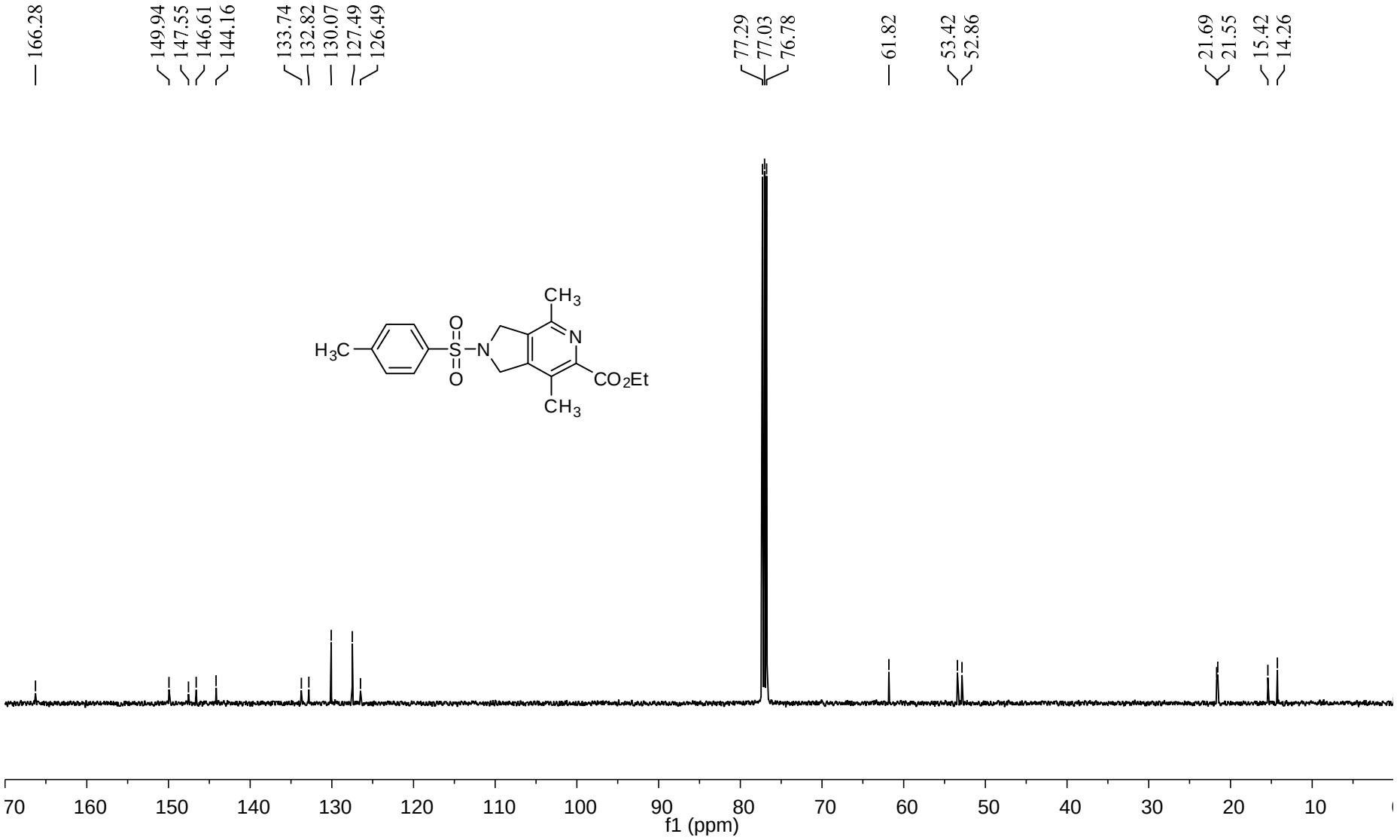
2.43
2.42
2.33
1.41
1.40
1.38
CH3
H3C
S
O
O
N
N
CO2Et
CH3
1.95
1.98
4.00
2.00
6.00
3.00
3.02
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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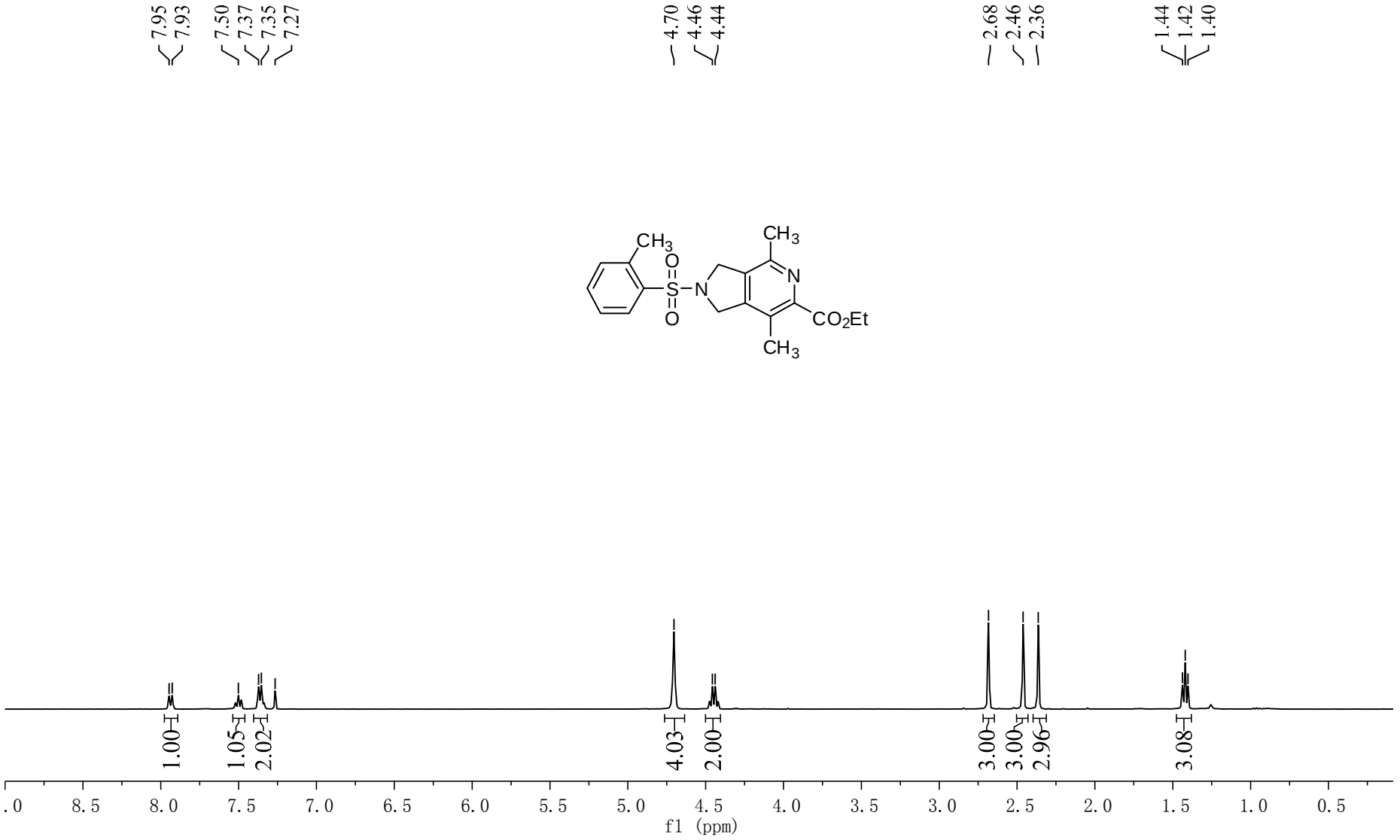
130.07
127.49
126.49
77.29
77.03
76.78
61.82
53.42
52.86
21.69
21.55
15.42
14.26
CH3
H3C
O
S
O
N
N
CO2Et
CH3
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.50
7.37
7.35
7.27
4.70
4.46
4.44
2.68
2.46
2.36
1.44
1.42
1.40
CH3
O
S
O
N
CH3
N
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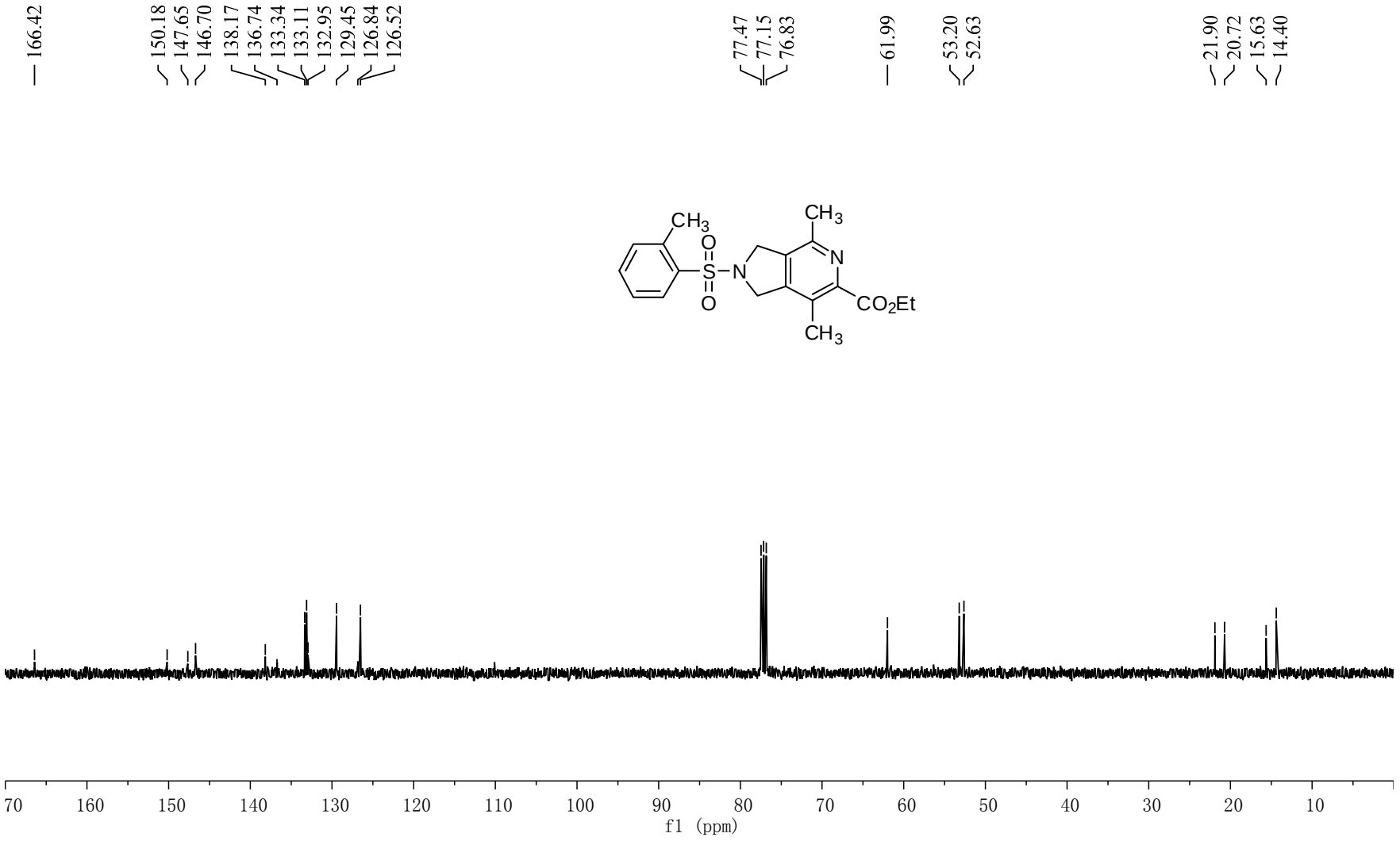
2.00
3.00
3.00
2.96
3.08
f1 (ppm)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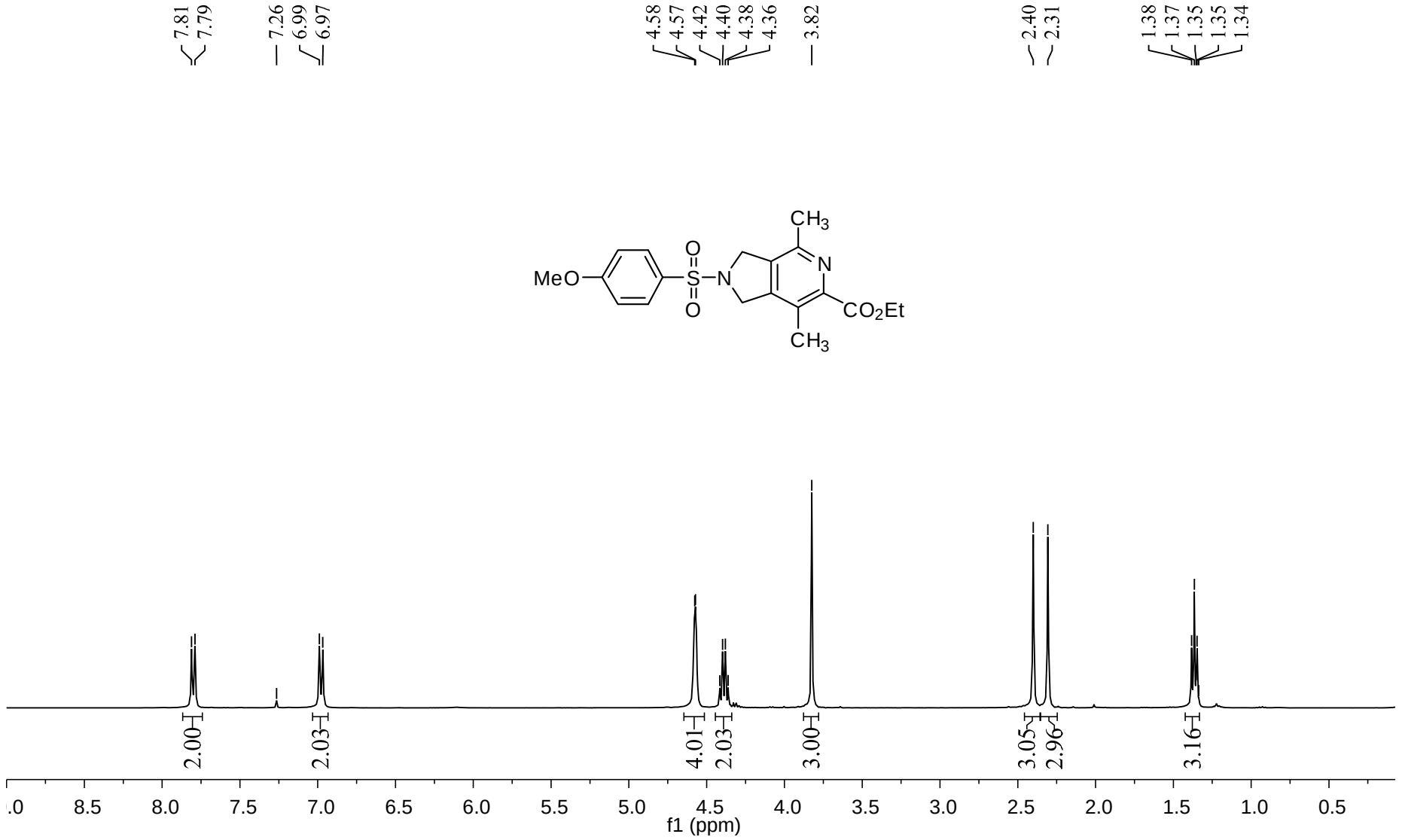
133.34
133.11
132.95
129.45
126.84
126.52
77.47
77.15
76.83
61.99
53.20
52.63
21.90
20.72
15.63
14.40
CH3
O
S
O
N
CH3
N
CO2Et
CH3
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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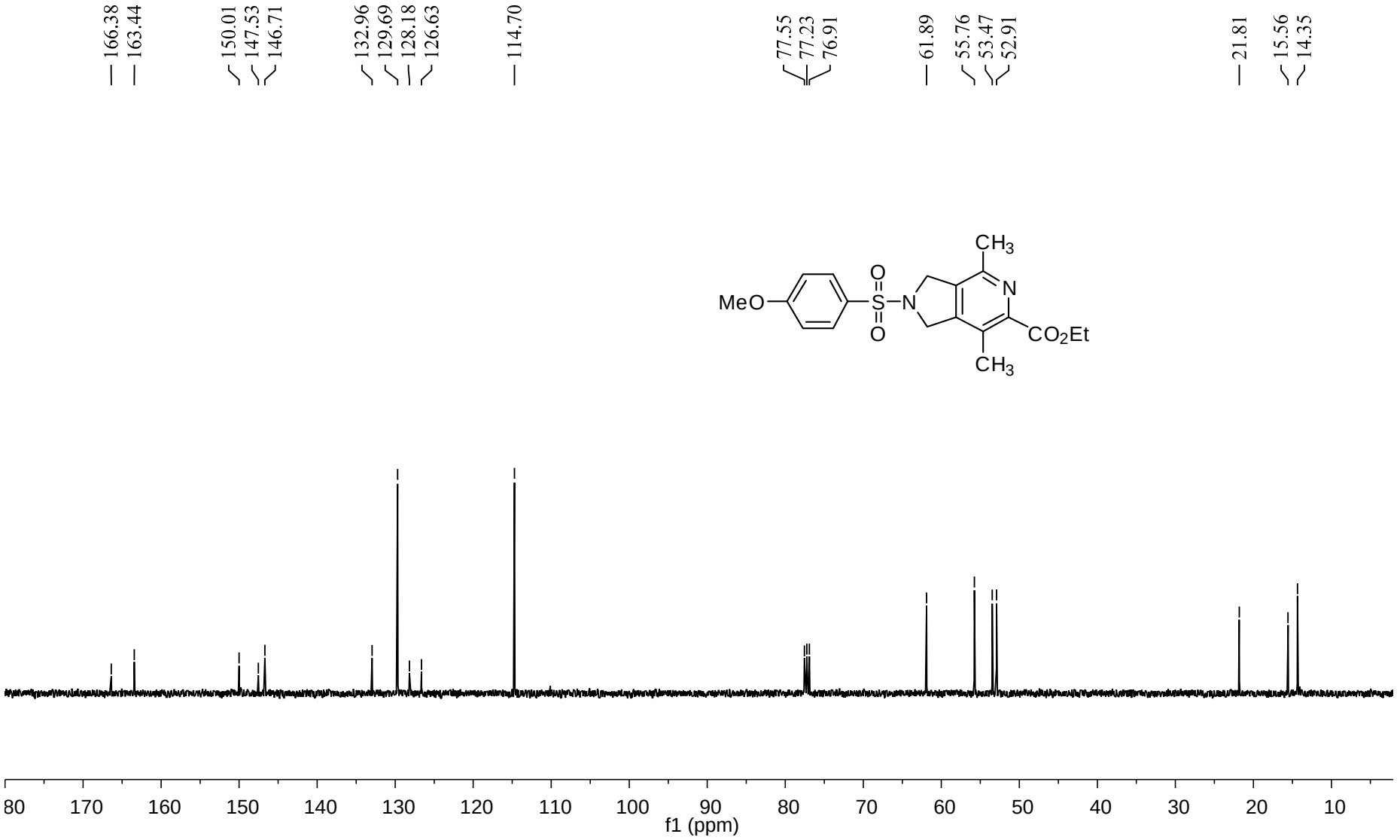
7.79
7.26
6.99
6.97
4.58
4.57
4.42
4.40
4.38
4.36
3.82
2.40
2.31
1.38
1.37
1.35
1.35
1.34
CH3
MeO
O
S
O
N
N
CO2Et
CH3
2.00
2.03
4.01
2.03
3.00
3.05
2.96
3.16
f1 (ppm)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129.69
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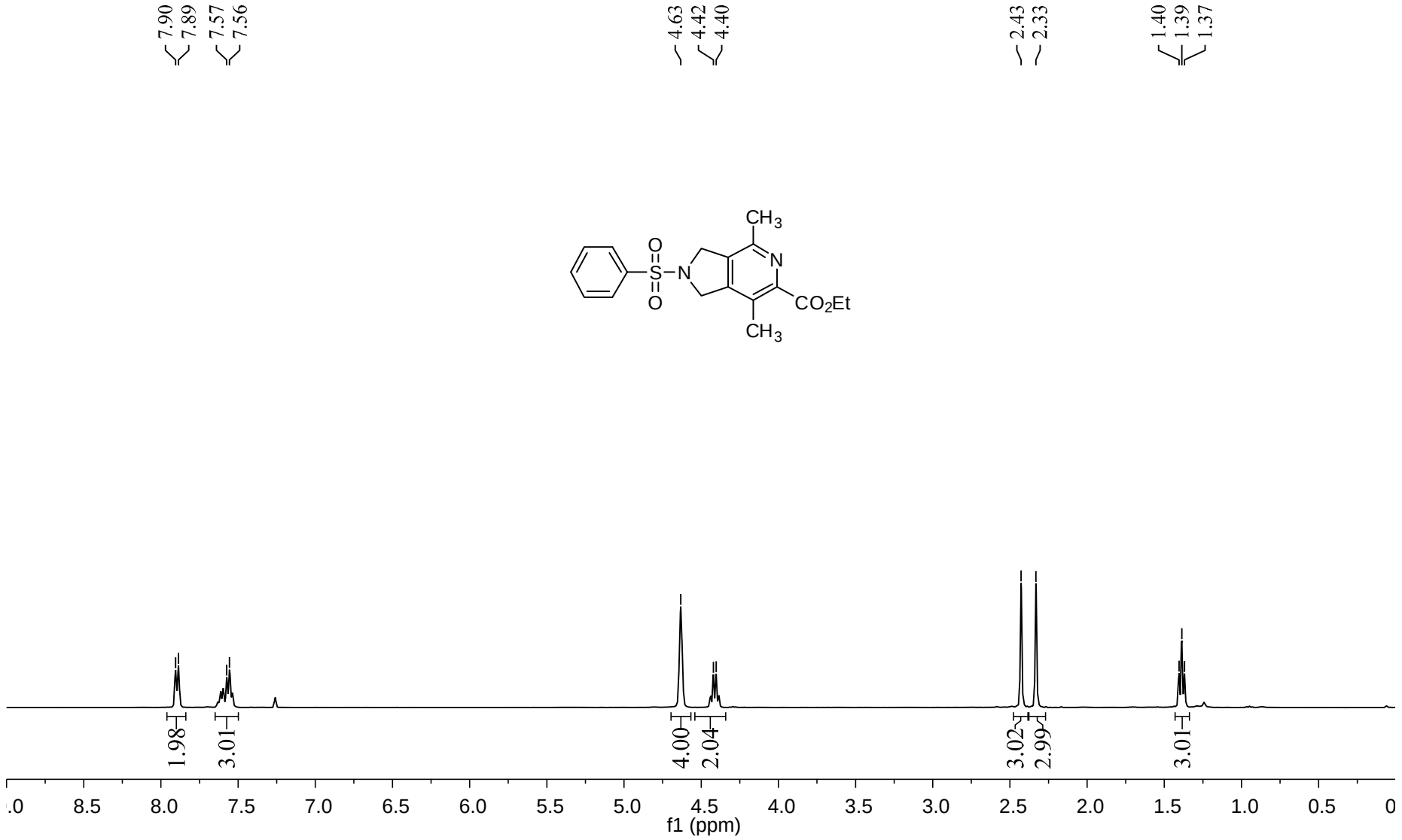
114.70
77.55
77.23
76.91
61.89
55.76
53.47
52.91
21.81
15.56
14.35
CH3
MeO
O
S
O
N
N
CO2Et
CH3
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.89
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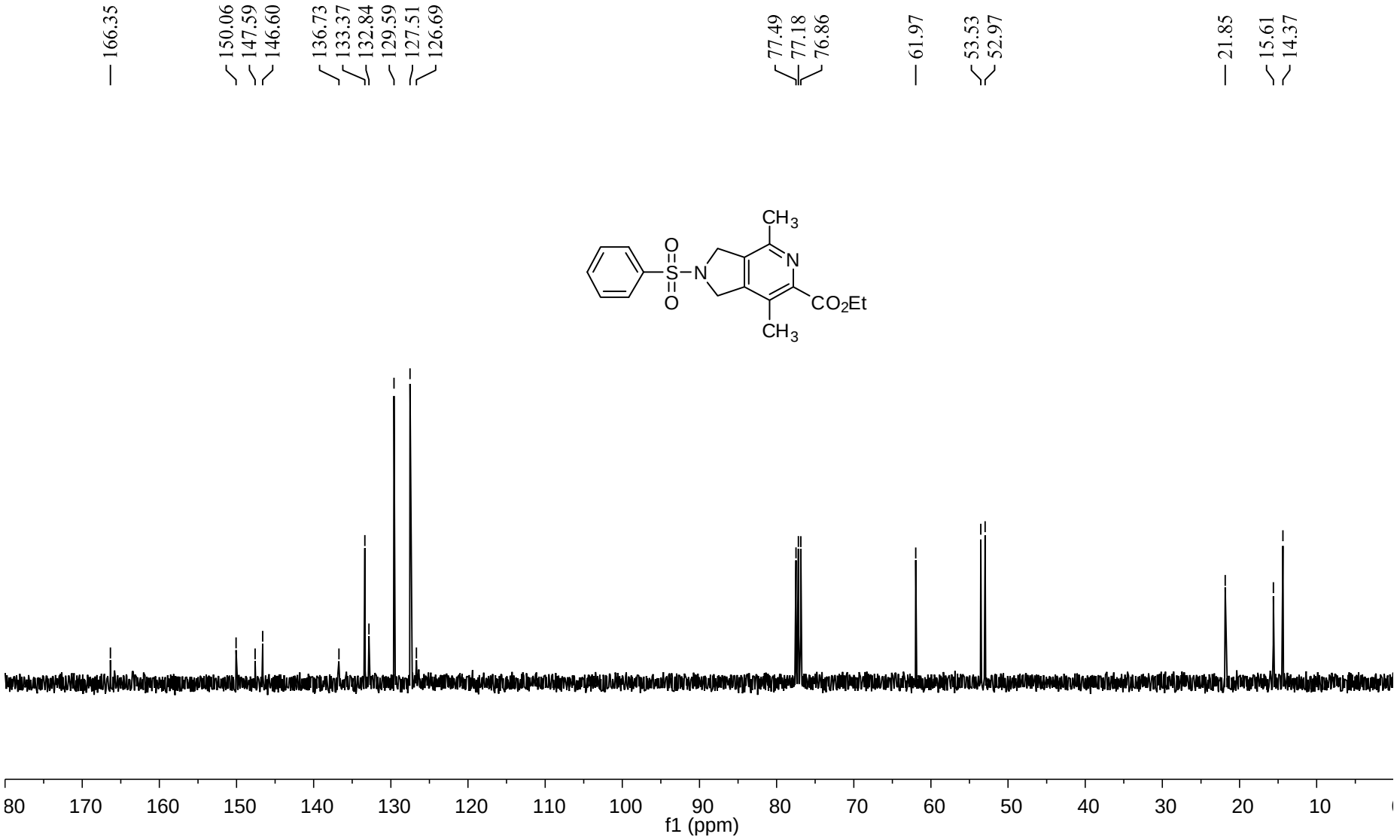
7.56
4.63
4.42
4.40
2.43
2.33
1.40
1.39
1.37
CH3
O
S
O
N
N
CO2Et
CH3
1.98
3.01
4.00
2.04
3.02
2.99
3.01
f1 (ppm)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129.59
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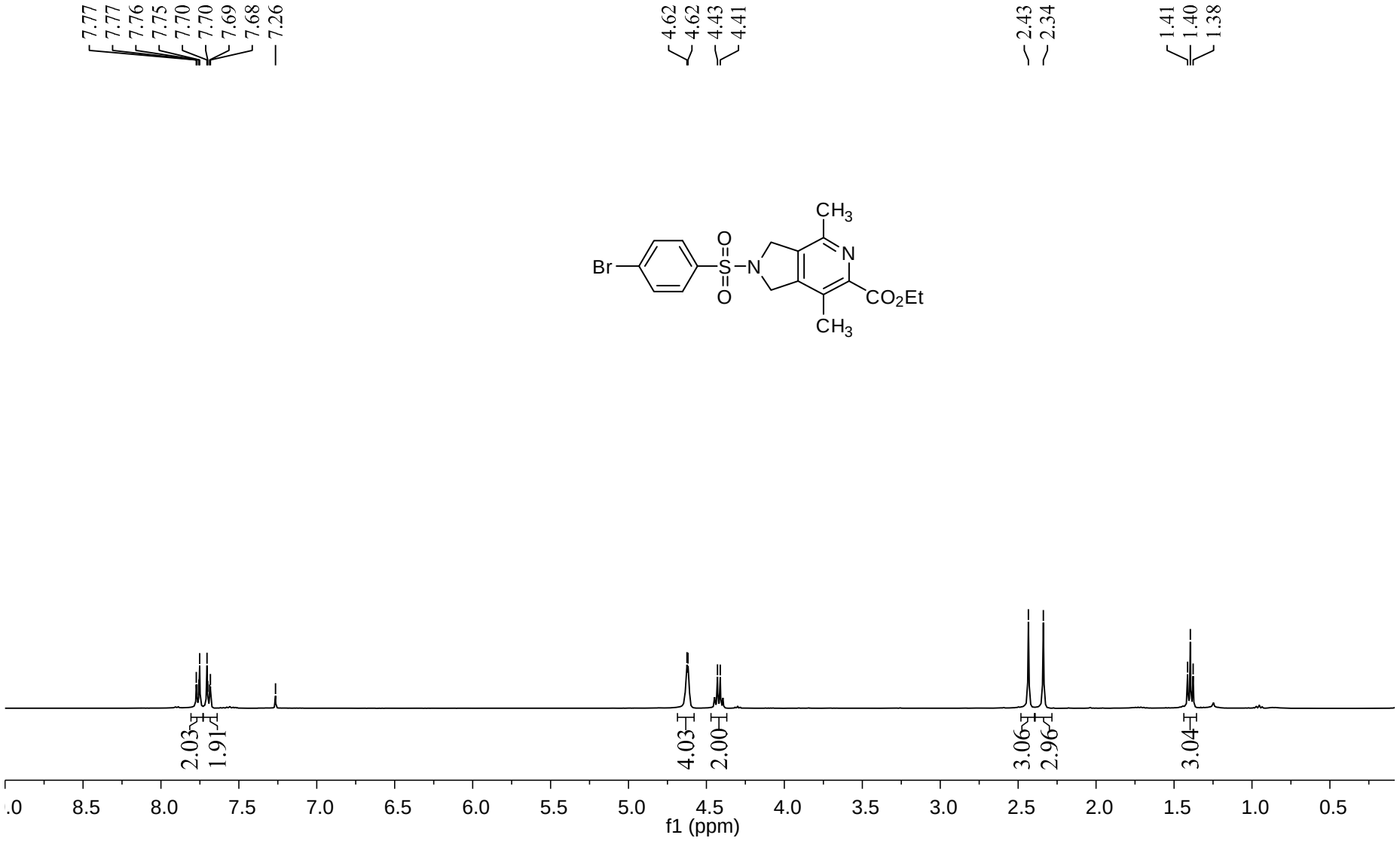
126.69
77.49
77.18
76.86
61.97
53.53
52.97
21.85
15.61
14.37
CH3
O
S
O
N
N
CO2Et
CH3
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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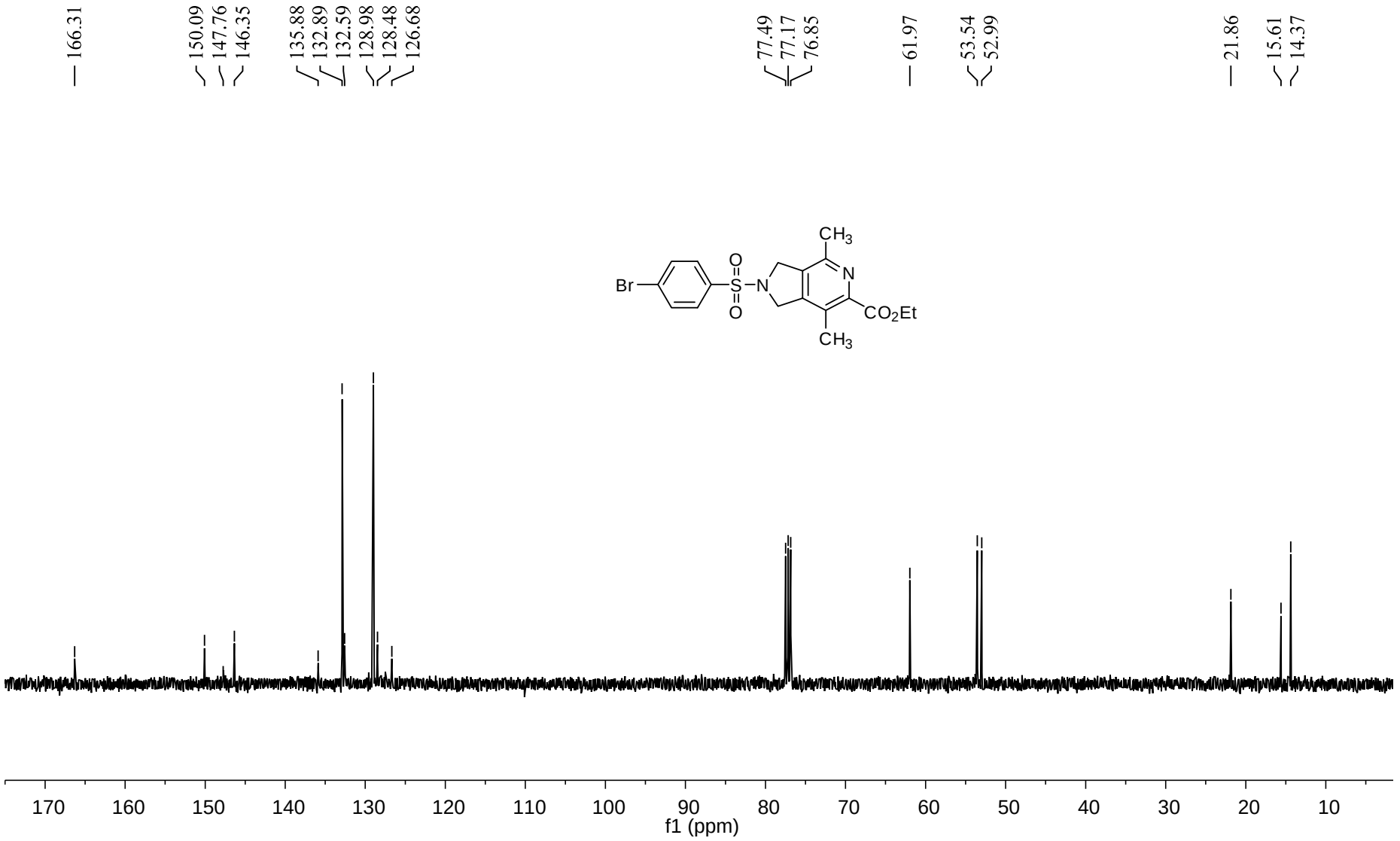
7.69
7.68
7.26
4.62
4.62
4.43
4.41
2.43
2.34
1.41
1.40
1.38
CH3
O
S
O
N
Br
N
CO2Et
CH3
2.03
1.91
4.03
2.00
3.06
2.96
3.04
f1 (ppm)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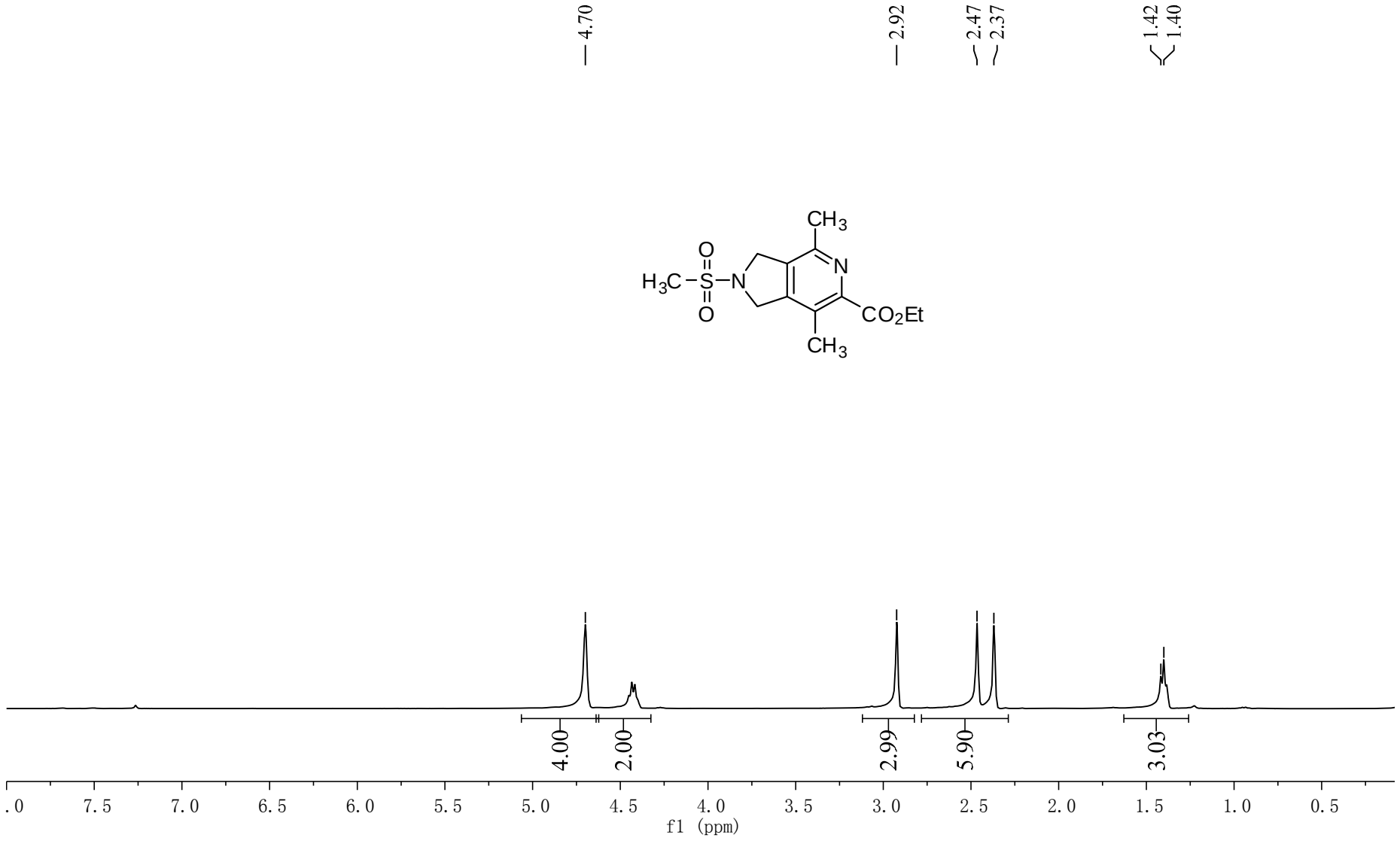
132.59
128.98
128.48
126.68
77.49
77.17
76.85
61.97
53.54
52.99
21.86
15.61
14.37
CH3
Br
S
O
O
N
N
CO2Et
CH3
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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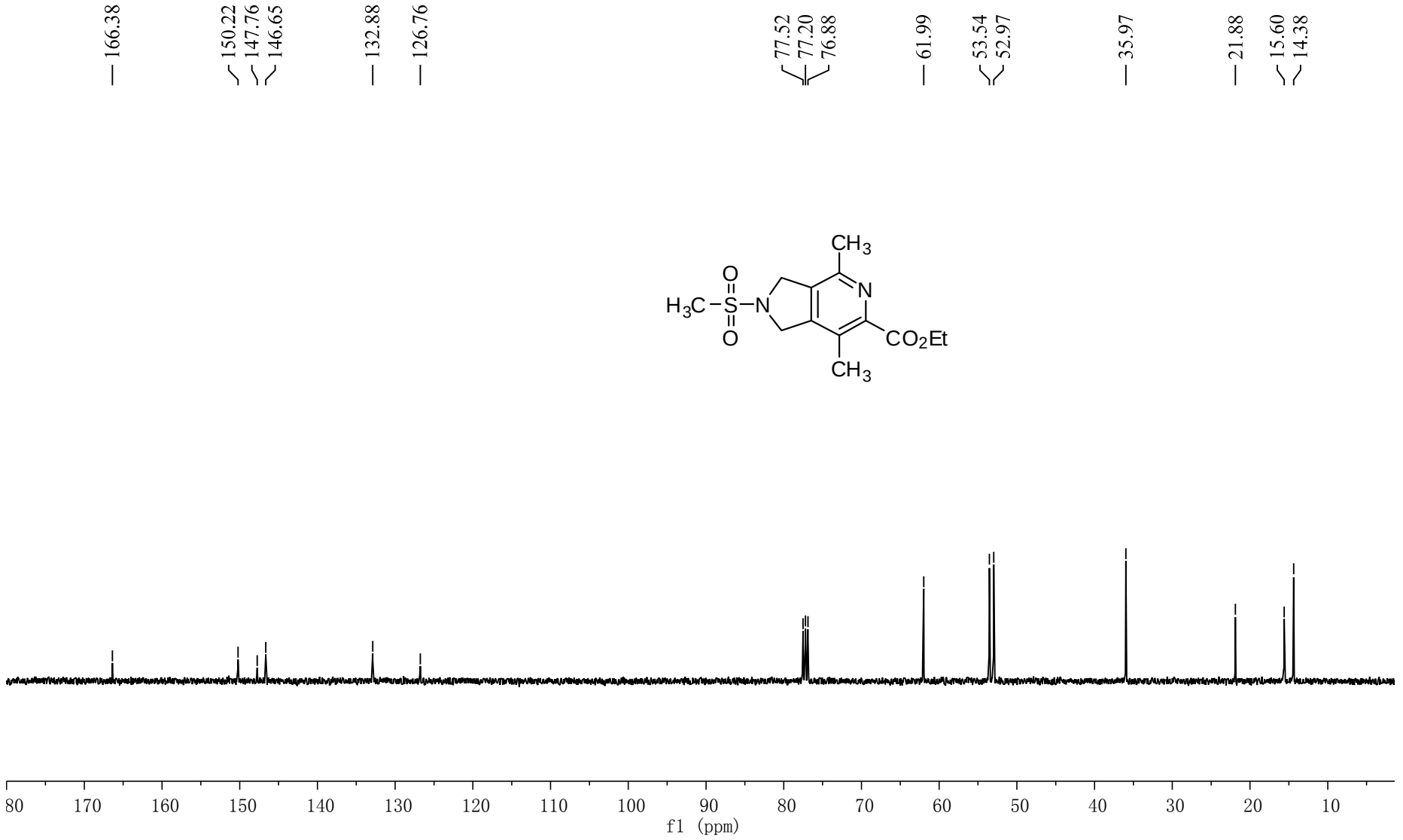
2.92
2.47
2.37
1.42
1.40
CH3
O
H3C–S–N
O
N
CO2Et
CH3
4.00
2.00
2.99
5.90
3.03
.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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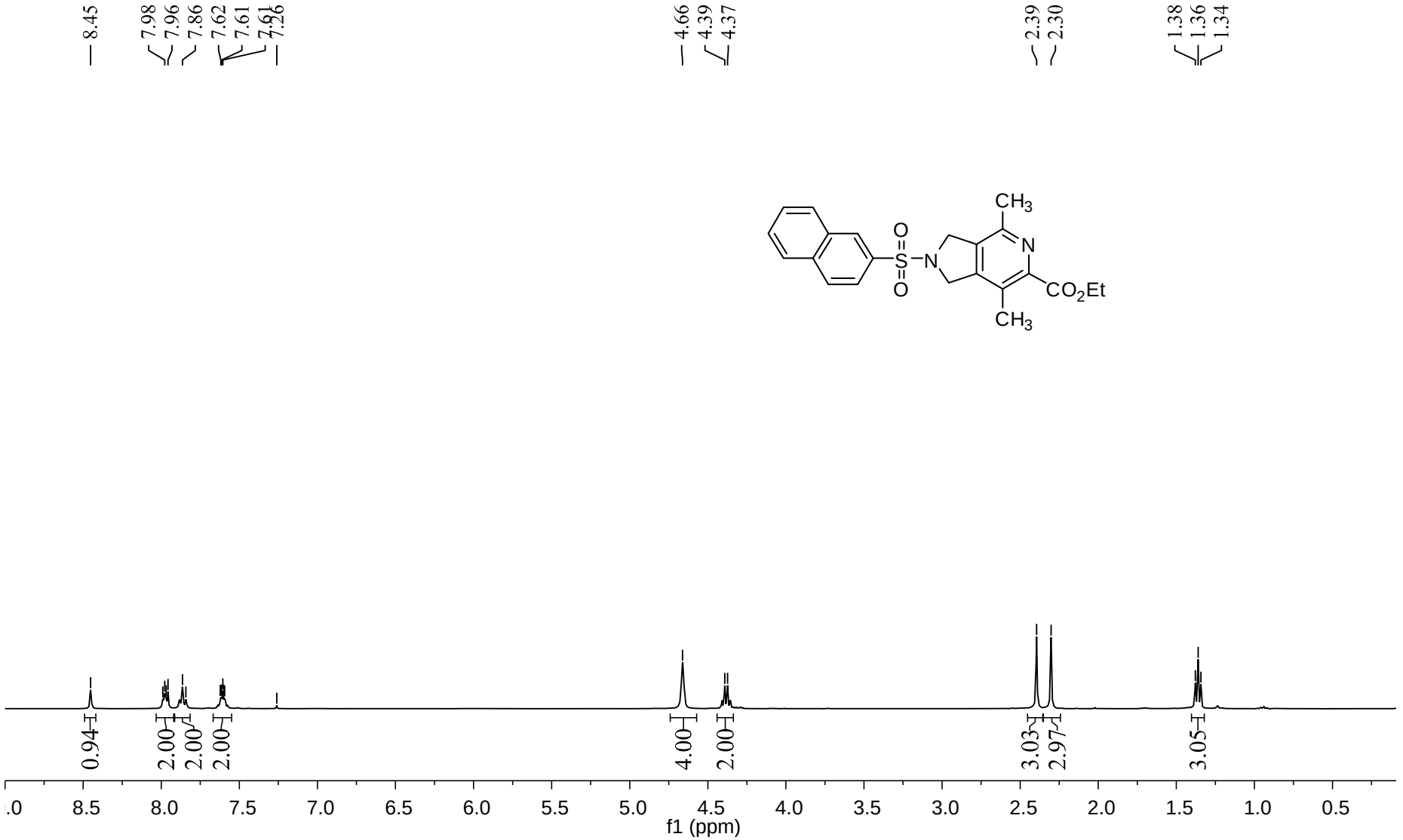
76.88
61.99
53.54
52.97
35.97
21.88
15.60
14.38
CH3
O
H3C−S−N
O
N
CO2Et
CH3
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.86
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7.61
7.26
4.66
4.39
4.37
2.39
2.30
1.38
1.36
1.34
CH3
O
S
O
N
N
CO2Et
CH3
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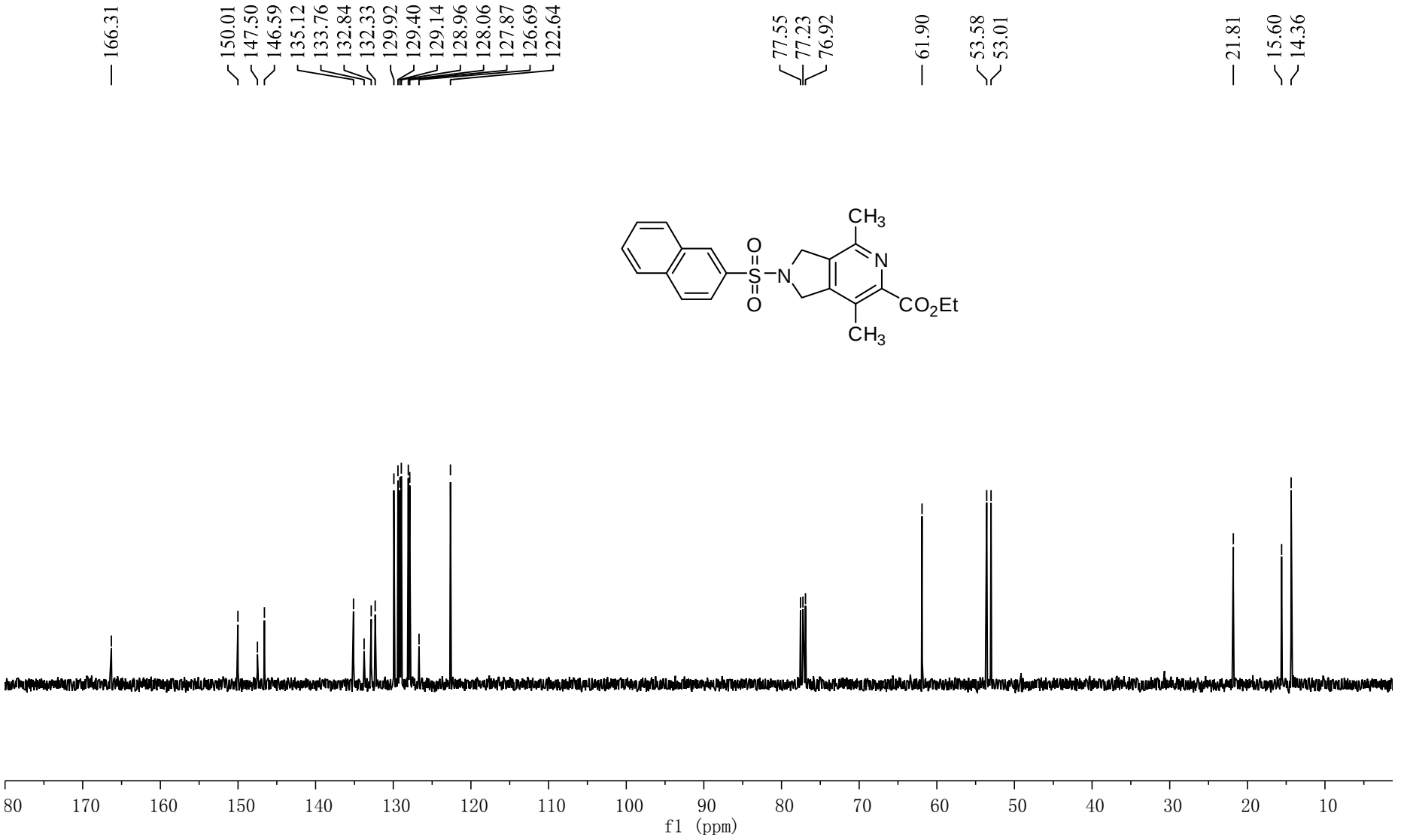
2.00
2.00
2.00
4.00
2.00
3.03
2.97
3.05
f1 (ppm)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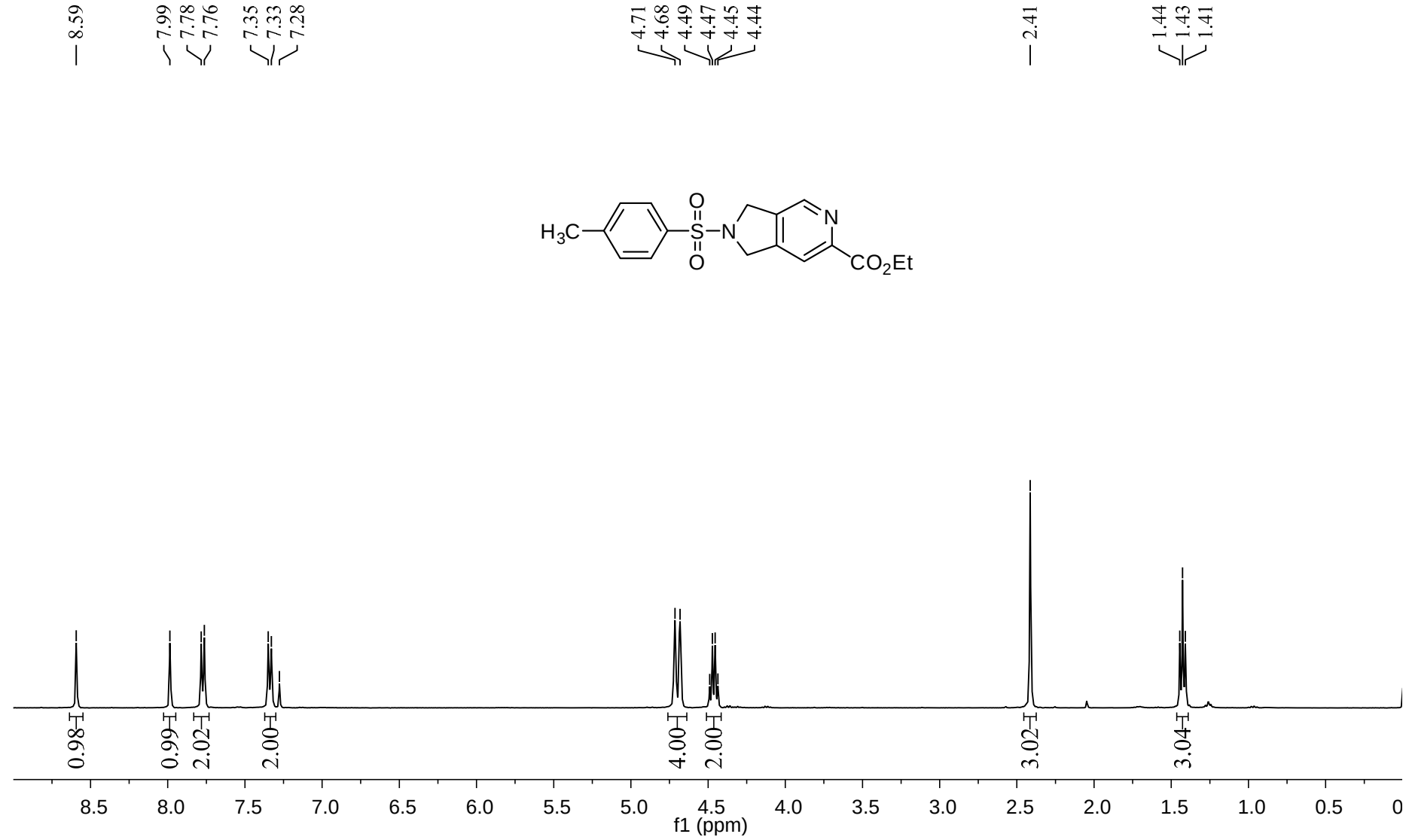
133.76
132.84
132.33
129.92
129.40
129.14
128.96
128.06
127.87
126.69
122.64
77.55
77.23
76.92
61.90
53.58
53.01
21.81
15.60
14.36
CH3
N
O
S
O
N
CO2Et
CH3
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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7.76
7.35
7.33
7.28
4.71
4.68
4.49
4.47
4.45
4.44
2.41
1.44
1.43
1.41
H3C
O
S
O
N
N
CO2Et
0.98
0.99
2.02
2.00
4.00
2.00
3.02
3.04
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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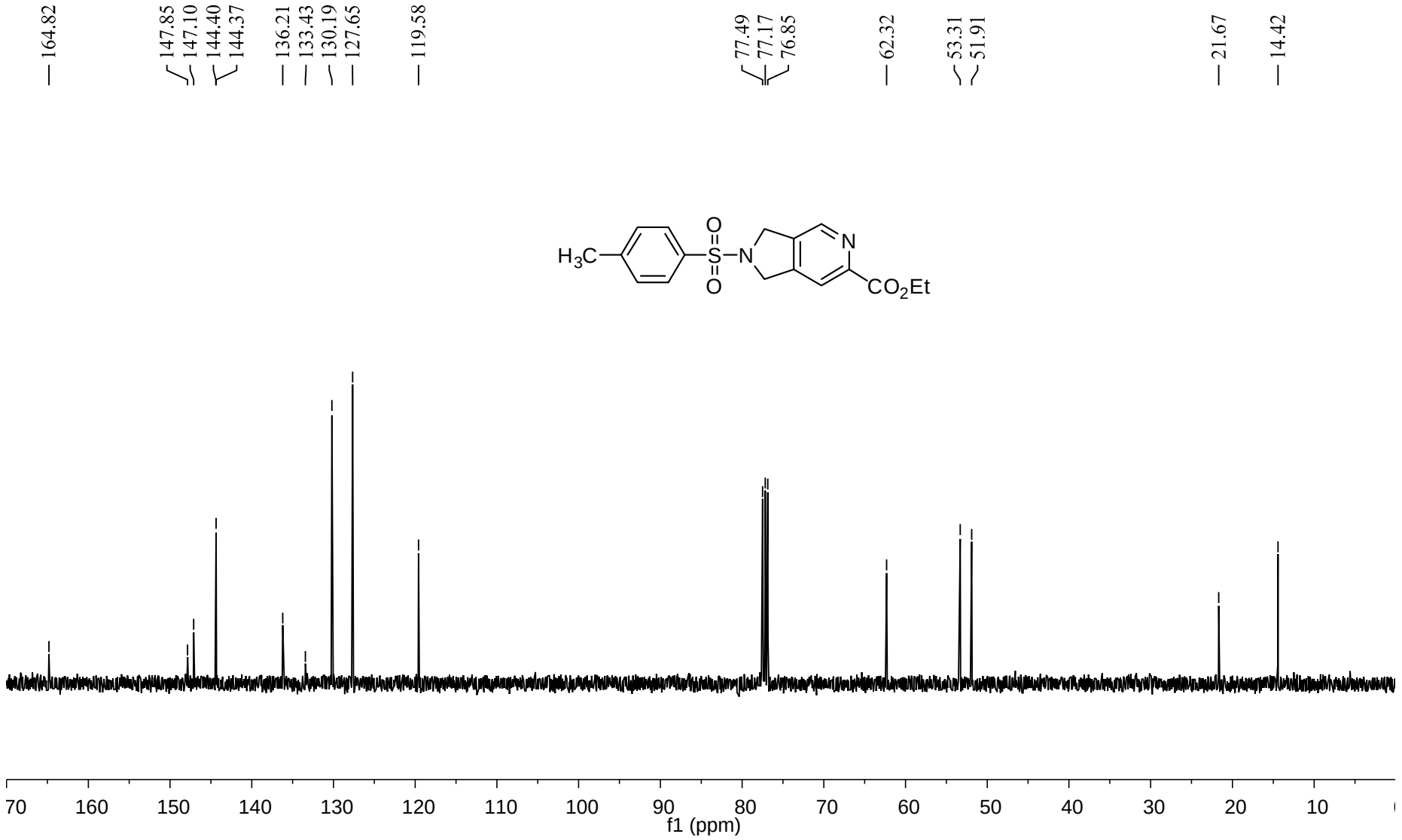
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0
f1 (ppm)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119.58
77.49
77.17
76.85
62.32
53.31
51.91
21.67
14.42
H3C
S
O
O
N
N
CO2Et
70
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150
140
130
120
110
100
90
80
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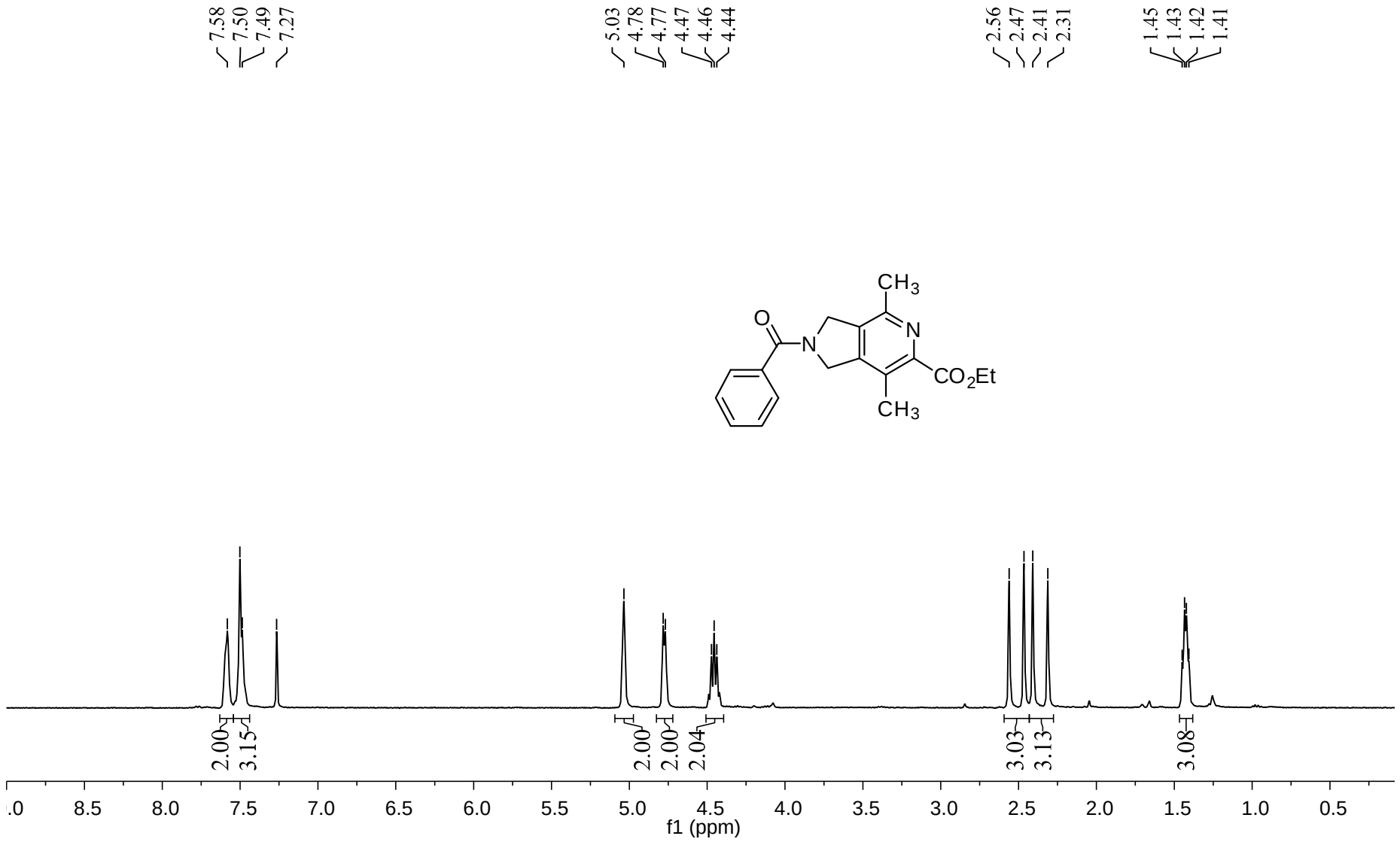
60
50
40
30
20
10
f1 (ppm)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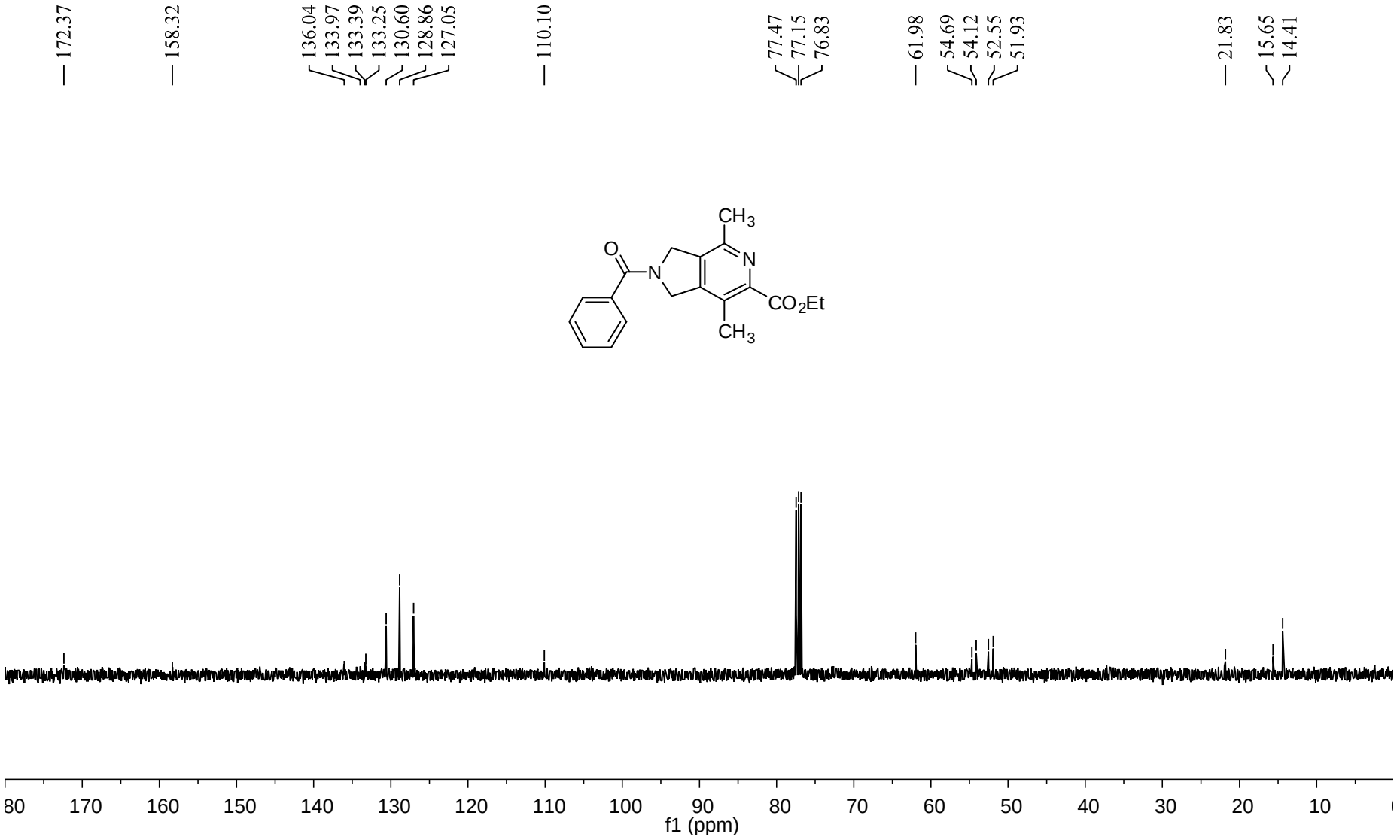
4.47
4.46
4.44
2.56
2.47
2.41
2.31
1.45
1.43
1.42
1.41
CH3
O
N
N
CO2Et
CH3
2.00
3.15
2.00
2.00
2.04
3.03
3.13
3.08
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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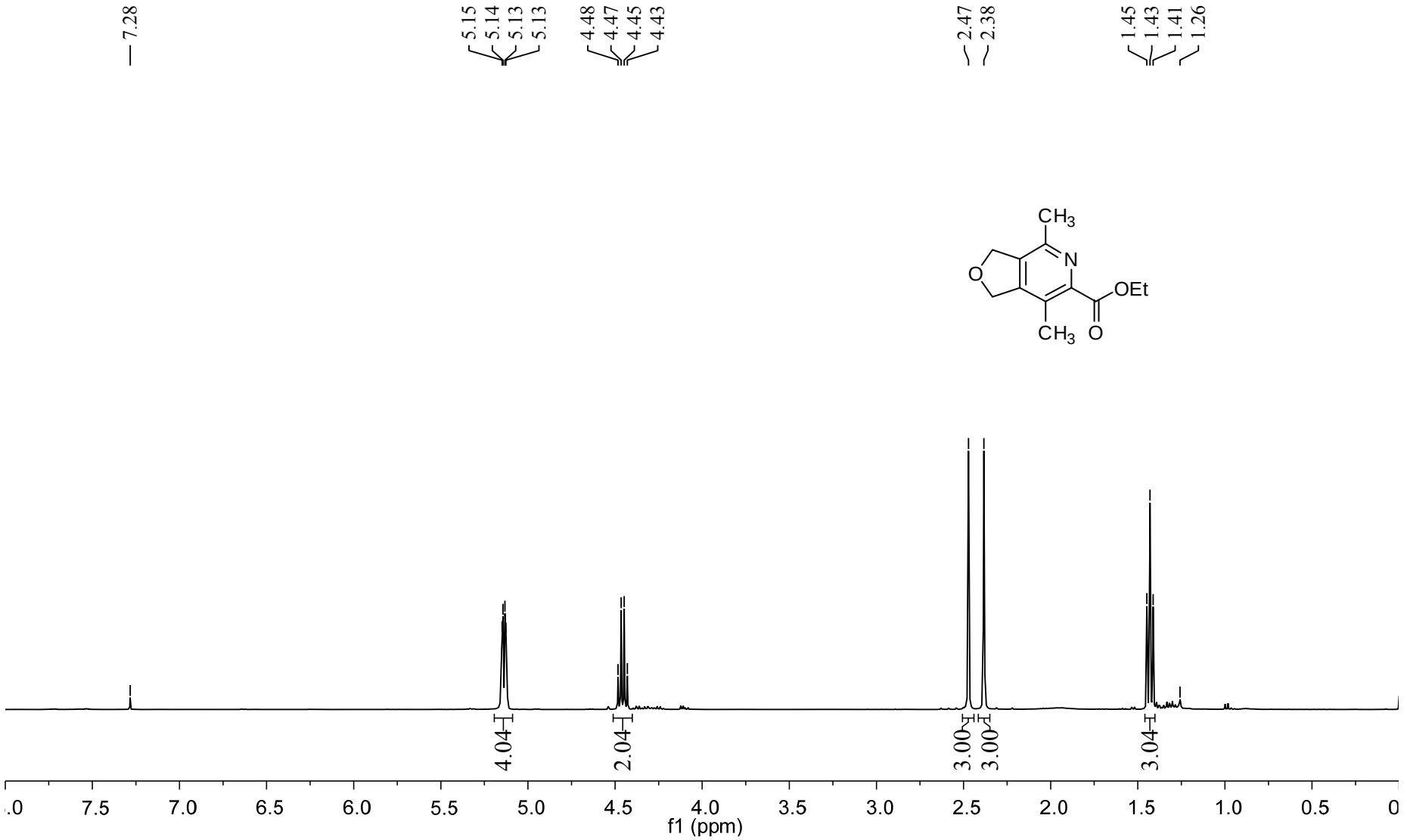
133.25
130.60
128.86
127.05
110.10
77.47
77.15
76.83
61.98
54.69
54.12
52.55
51.93
21.83
15.65
14.41
CH3
O
N
N
CO2Et
CH3
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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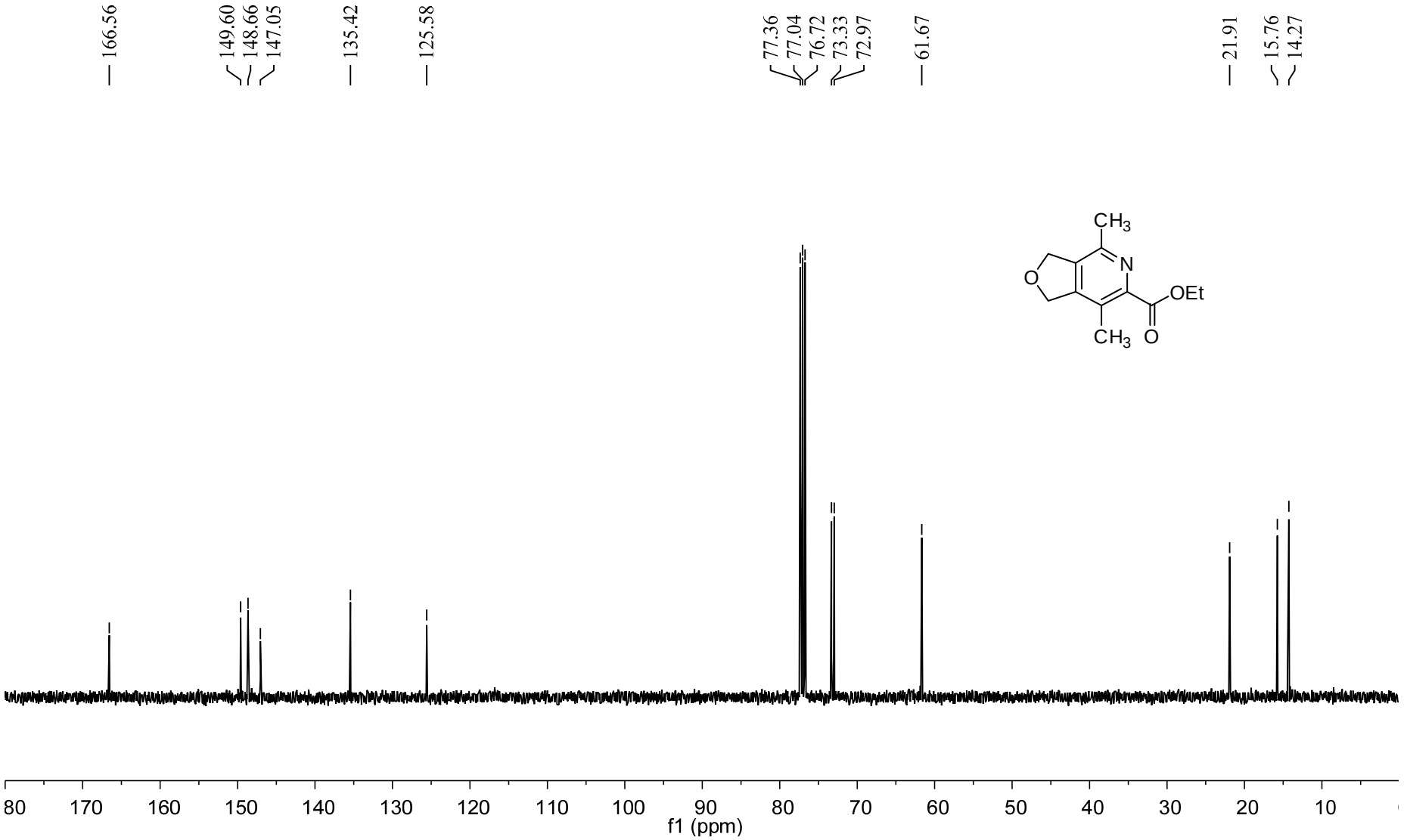
5.13
4.48
4.47
4.45
4.43
2.47
2.38
1.45
1.43
1.41
1.26
CH3
N
O
OEt
CH3
O
4.04
2.04
3.00
3.00
3.04
f1 (ppm)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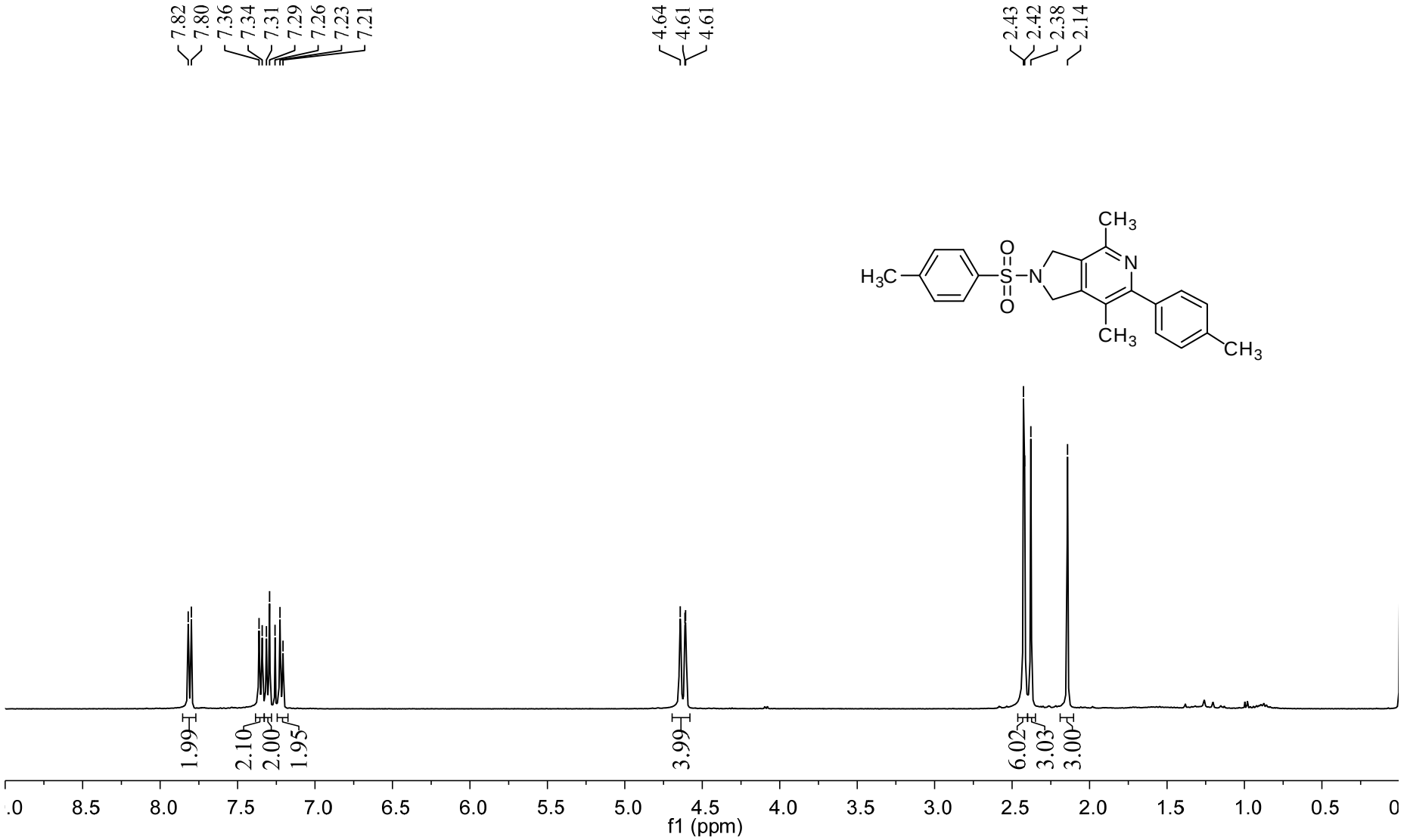
125.58
77.36
77.04
76.72
73.33
72.97
61.67
21.91
15.76
14.27
CH3
N
O
OEt
CH3
O
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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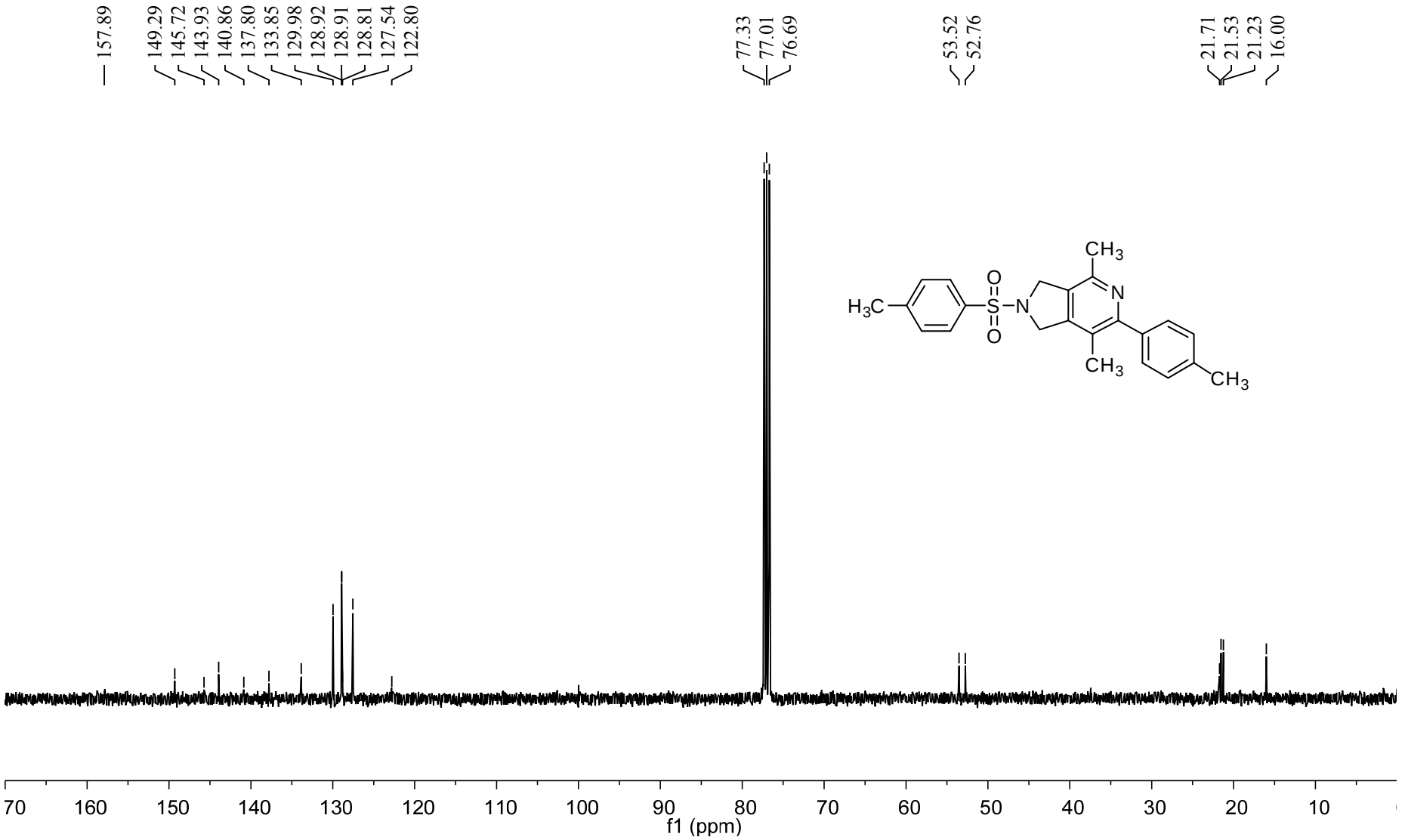
7.34
7.31
7.29
7.26
7.23
7.21
4.64
4.61
4.61
2.43
2.42
2.38
2.14
CH3
H3C
S
O
O
N
N
CH3
CH3
1.99
2.10
2.00
1.95
3.99
6.02
3.03
3.00
f1 (ppm)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128.81
127.54
122.80
77.33
77.01
76.69
53.52
52.76
21.71
21.53
21.23
16.00
CH3
H3C
O
S
O
N
N
CH3
CH3
CH3
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140
130
120
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100
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80
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60
50
40
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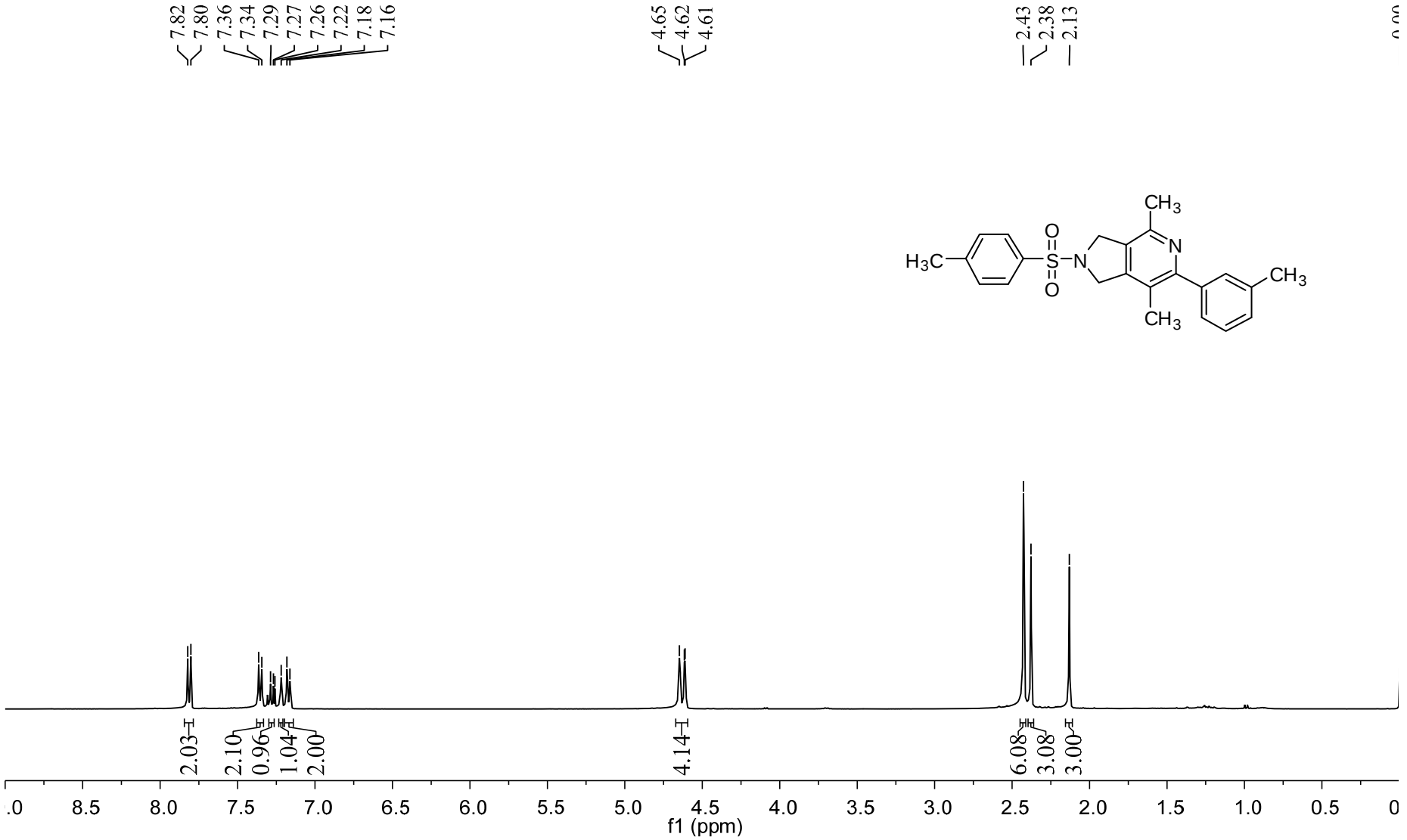
20
10
f1 (ppm)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7.22
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4.62
4.61
2.43
2.38
2.13
CH3
H3C
S
O
O
N
CH3
CH3
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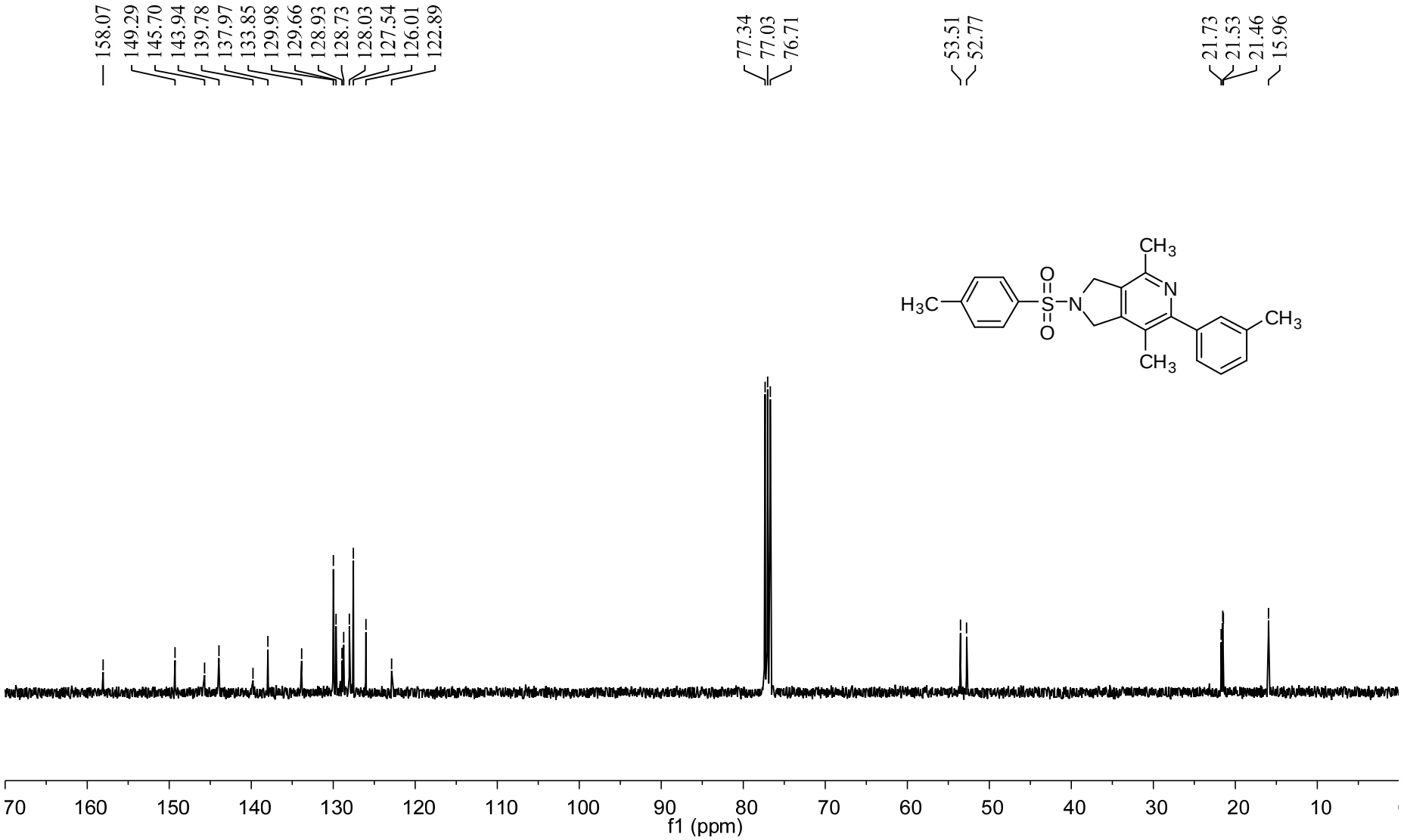
2.10
0.96
1.04
2.00
4.14
6.08
3.08
3.00
f1 (ppm)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127.54
126.01
122.89
77.34
77.03
76.71
53.51
52.77
21.73
21.53
21.46
15.96
CH3
H3C
O
S
O
N
N
CH3
CH3
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120
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100
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80
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60
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20
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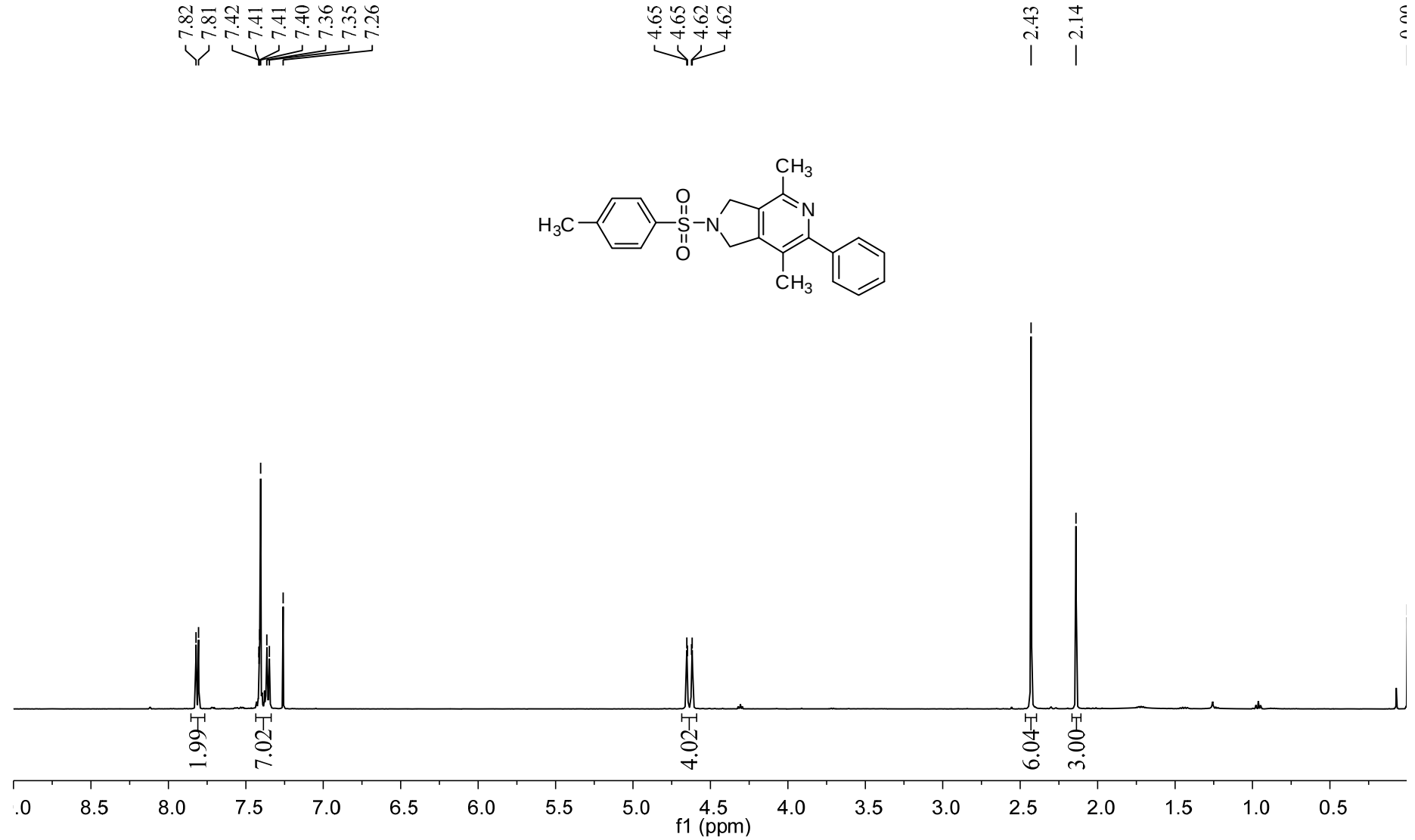
f1 (ppm)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7.35
7.26
4.65
4.65
4.62
4.62
2.43
2.14
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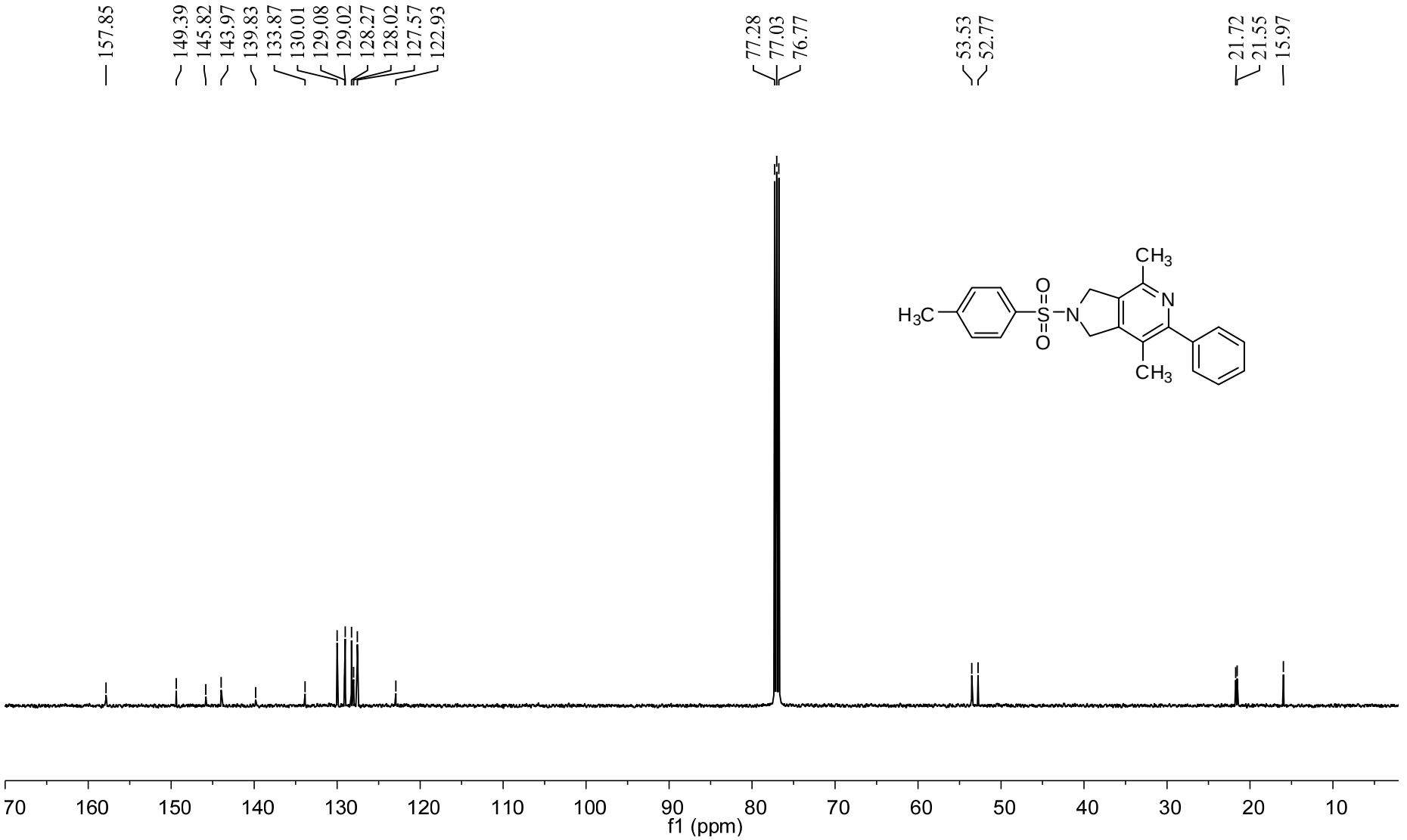
S
O
N
H3C
N
CH3
1.99
7.02
4.02
6.04
3.00
f1 (ppm)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129.08
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128.27
128.02
127.57
122.93
77.28
77.03
76.77
53.53
52.77
21.72
21.55
15.97
CH3
H3C
O
S
O
N
N
CH3
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130
120
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100
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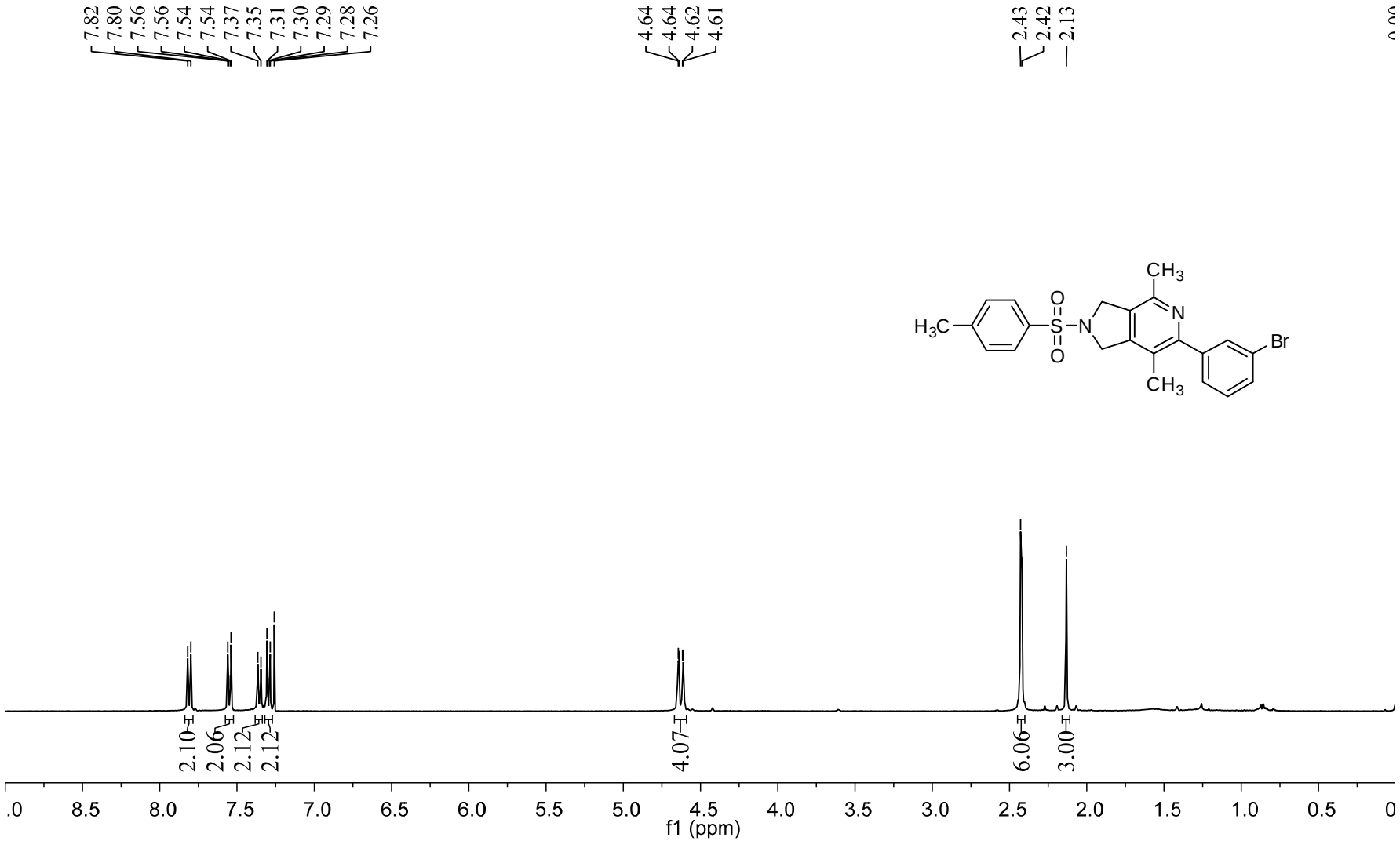
80
70
60
50
40
30
20
10
f1 (ppm)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7.35
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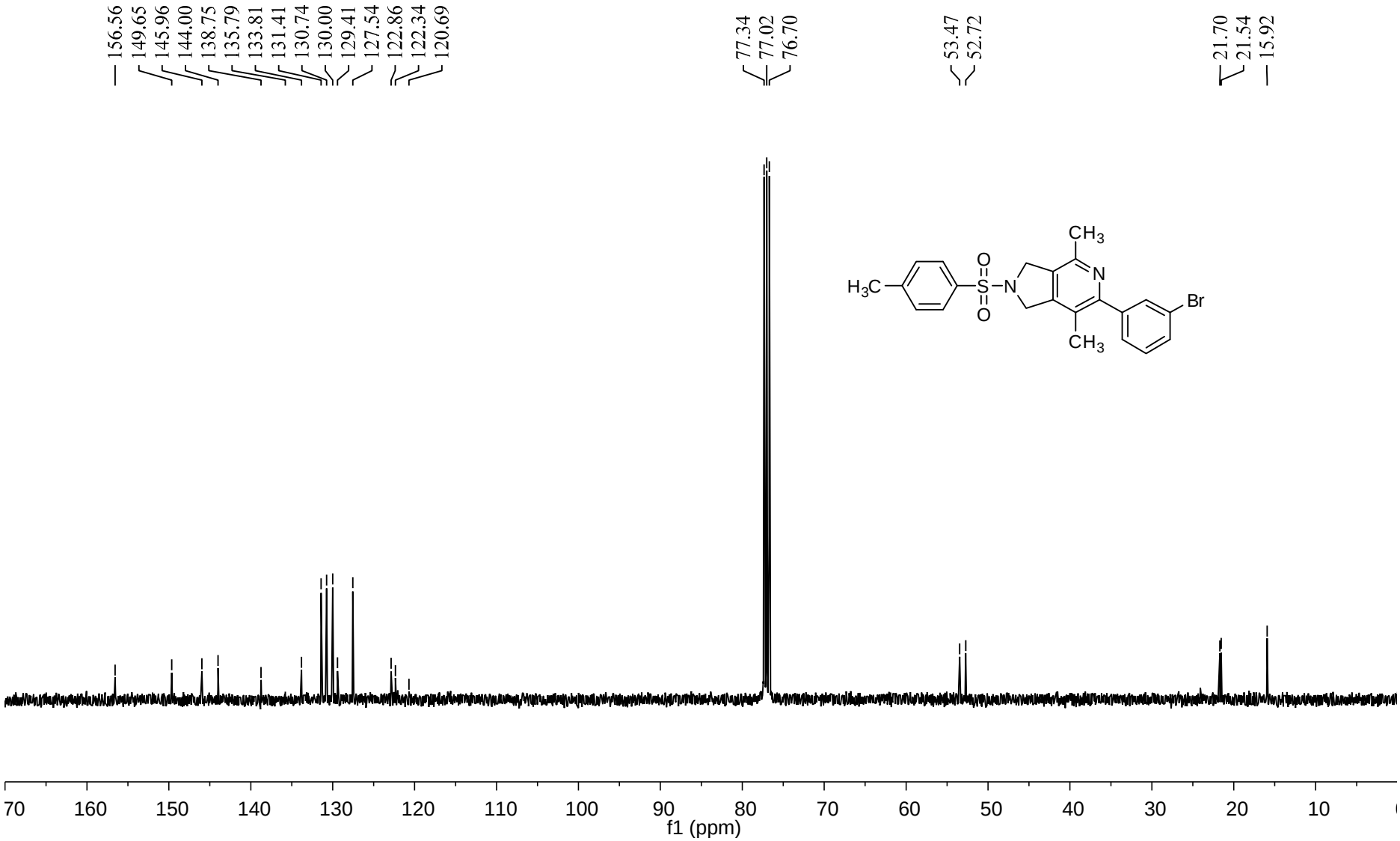
7.30
7.29
7.28
7.26
4.64
4.64
4.62
4.61
2.43
2.42
2.13
CH3
H3C
S
O
O
N
N
CH3
Br
2.10
2.06
2.12
2.12
4.07
6.06
3.00
f1 (ppm)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122.86
122.34
120.69
77.34
77.02
76.70
53.47
52.72
21.70
21.54
15.92
CH3
H3C
S
O
O
N
N
CH3
Br
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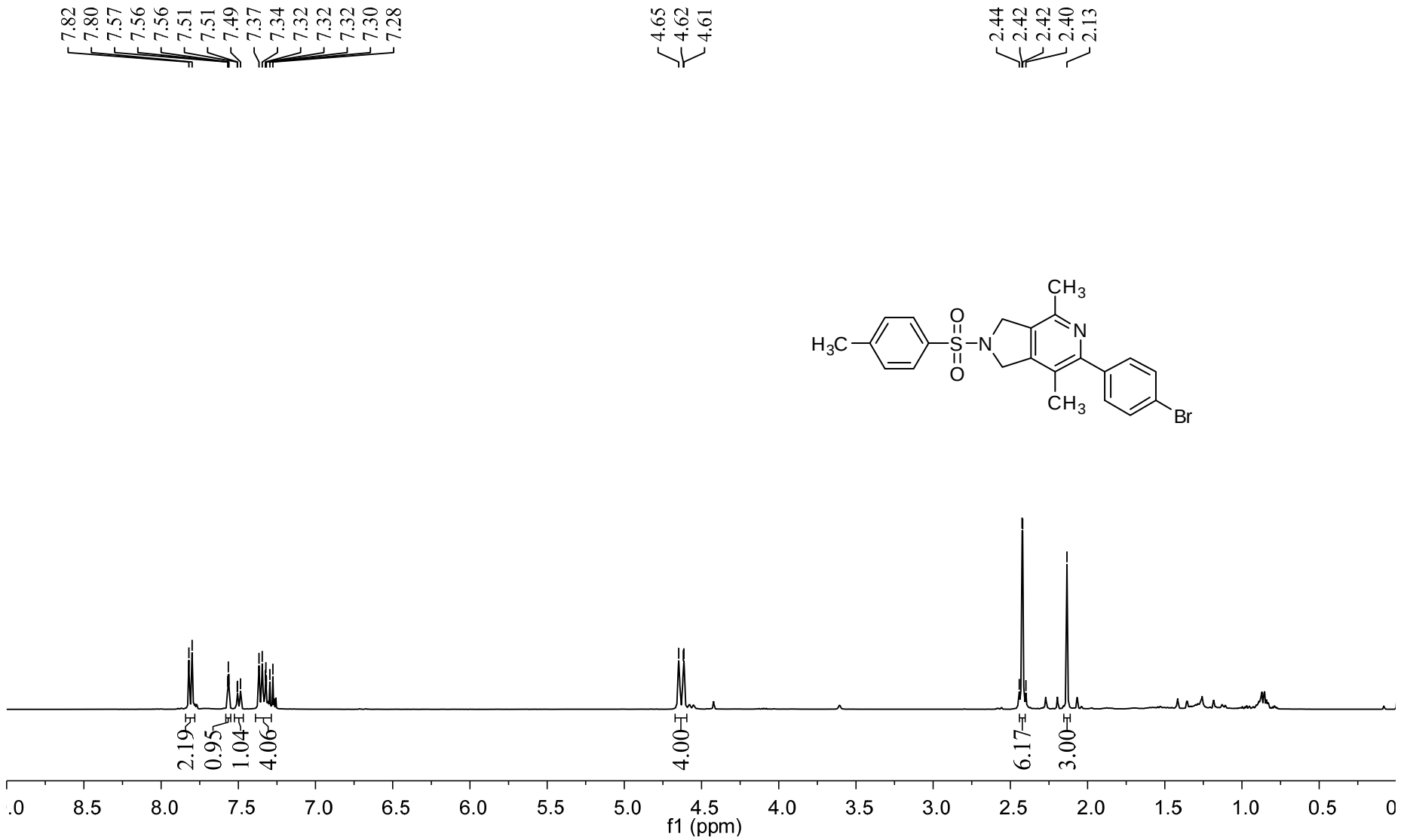
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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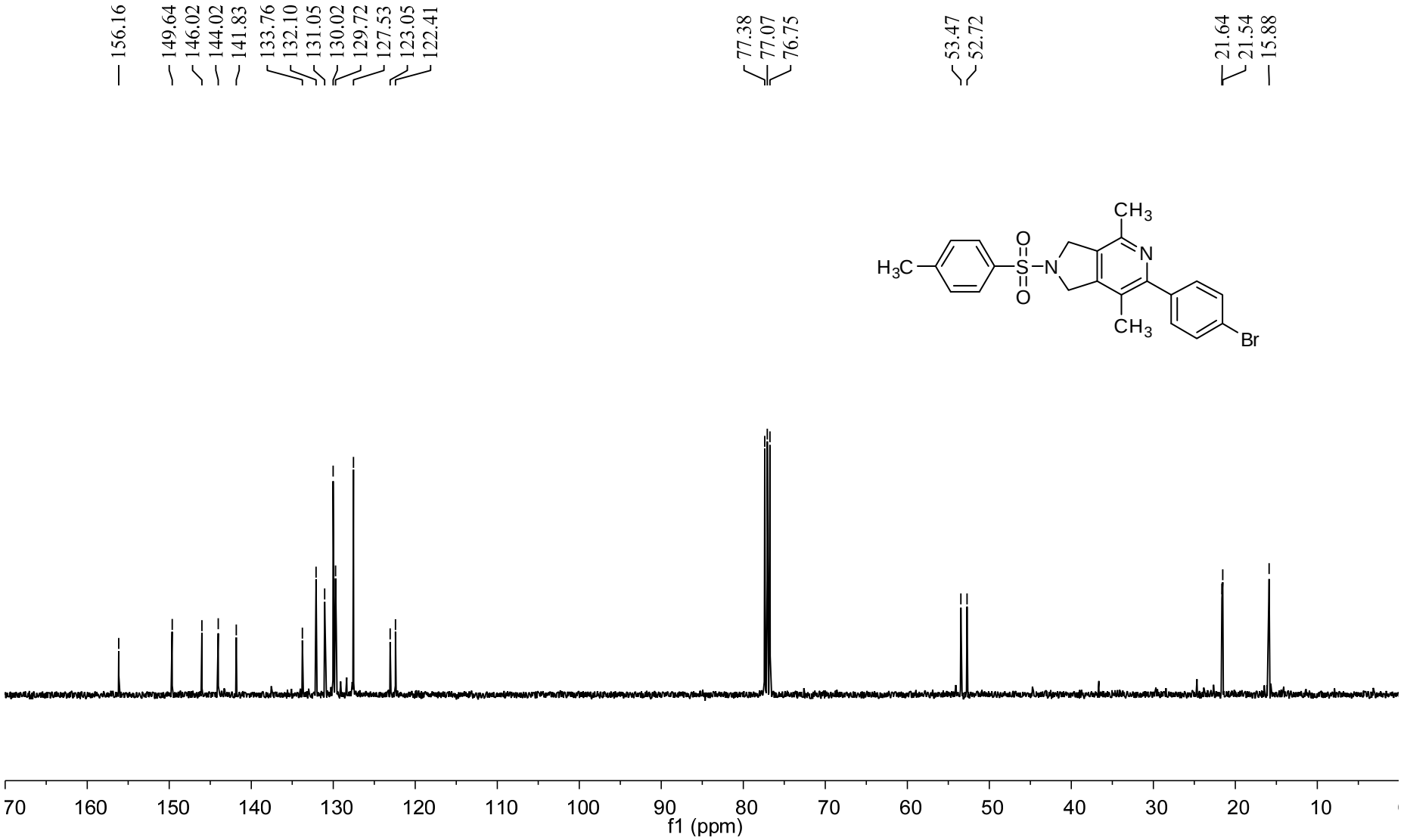
7.49
7.37
7.34
7.32
7.32
7.32
7.30
7.28
4.65
4.62
4.61
2.44
2.42
2.42
2.40
2.13
CH3
H3C
S
O
O
N
N
CH3
Br
2.19
0.95
1.04
4.06
4.00
6.17
3.00
f1 (ppm)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144.02
141.83
133.76
132.10
131.05
130.02
129.72
127.53
123.05
122.41
77.38
77.07
76.75
53.47
52.72
21.64
21.54
15.88
CH3
H3C
S
O
O
N
N
CH3
Br
70
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140
130
120
110
100
90
80
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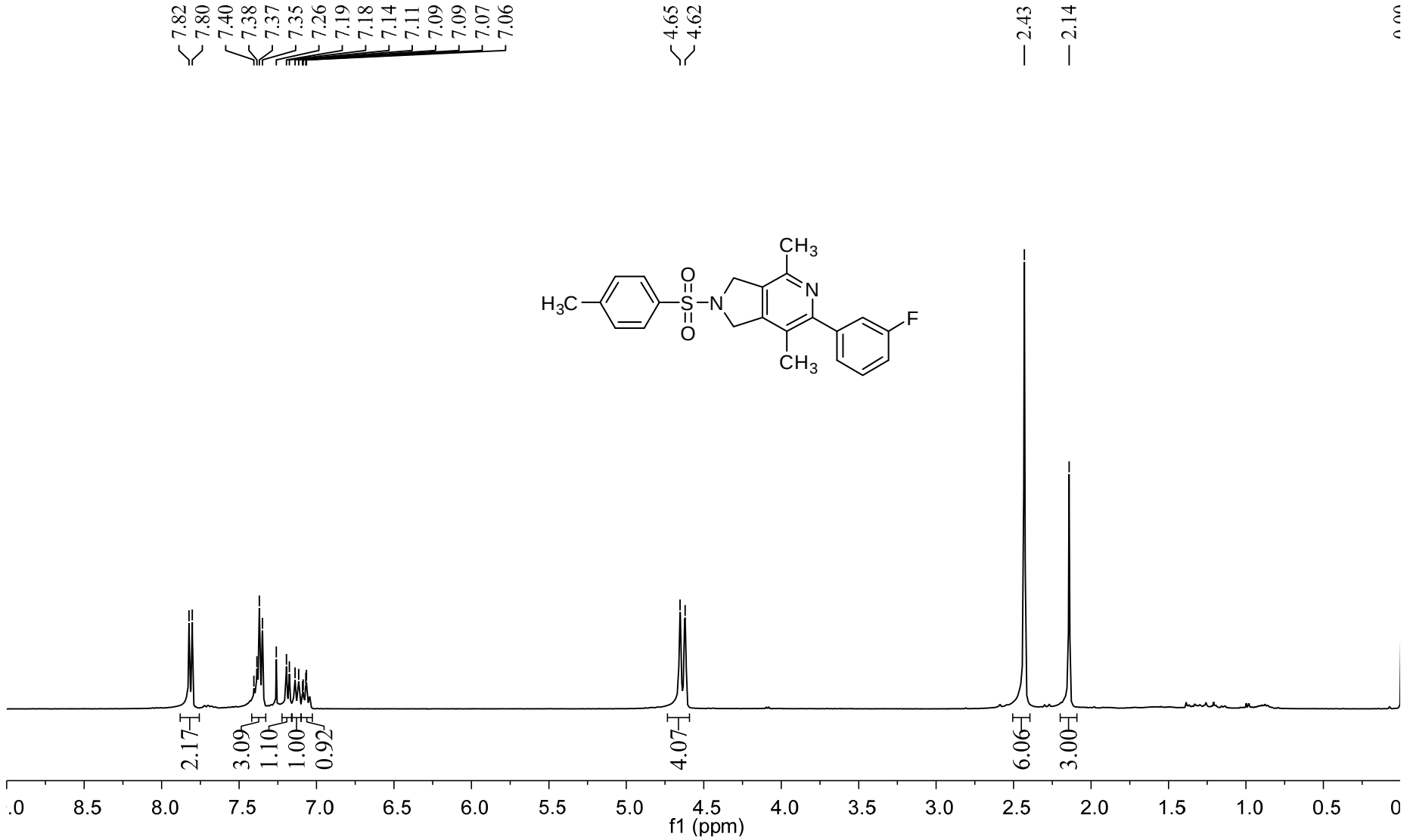
60
50
40
30
20
10
f1 (ppm)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7.80
7.40
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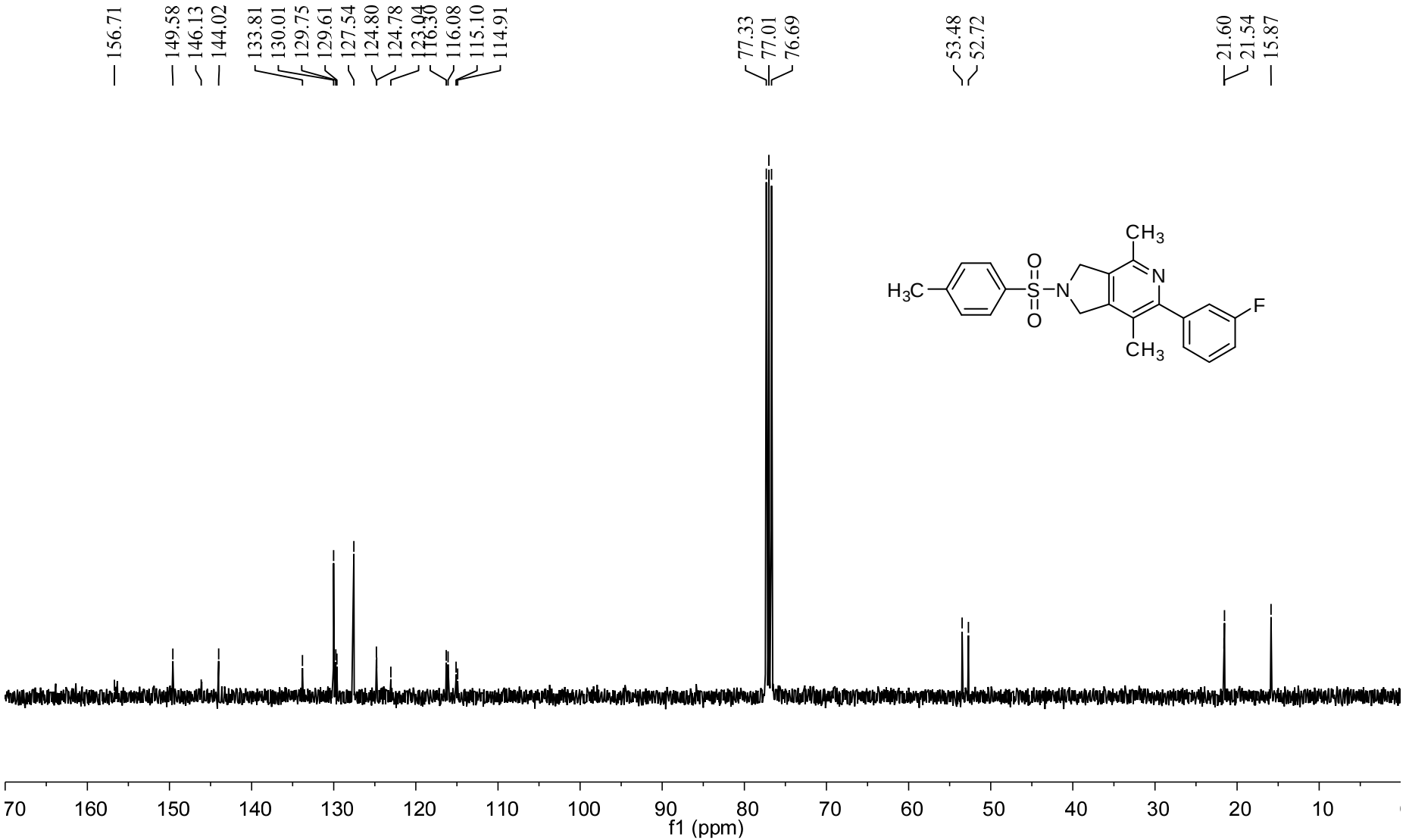
7.35
7.26
7.19
7.18
7.14
7.11
7.09
7.09
7.07
7.06
4.65
4.62
2.43
2.14
CH3
H3C
S
O
O
N
N
F
CH3
2.17
3.09
1.10
1.00
0.92
4.07
6.06
3.00
f1 (ppm)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129.61
127.54
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124.78
123.04
116.30
116.08
115.10
114.91
77.33
77.01
76.69
53.48
52.72
21.60
21.54
15.87
CH3
H3C
S
O
O
N
N
CH3
F
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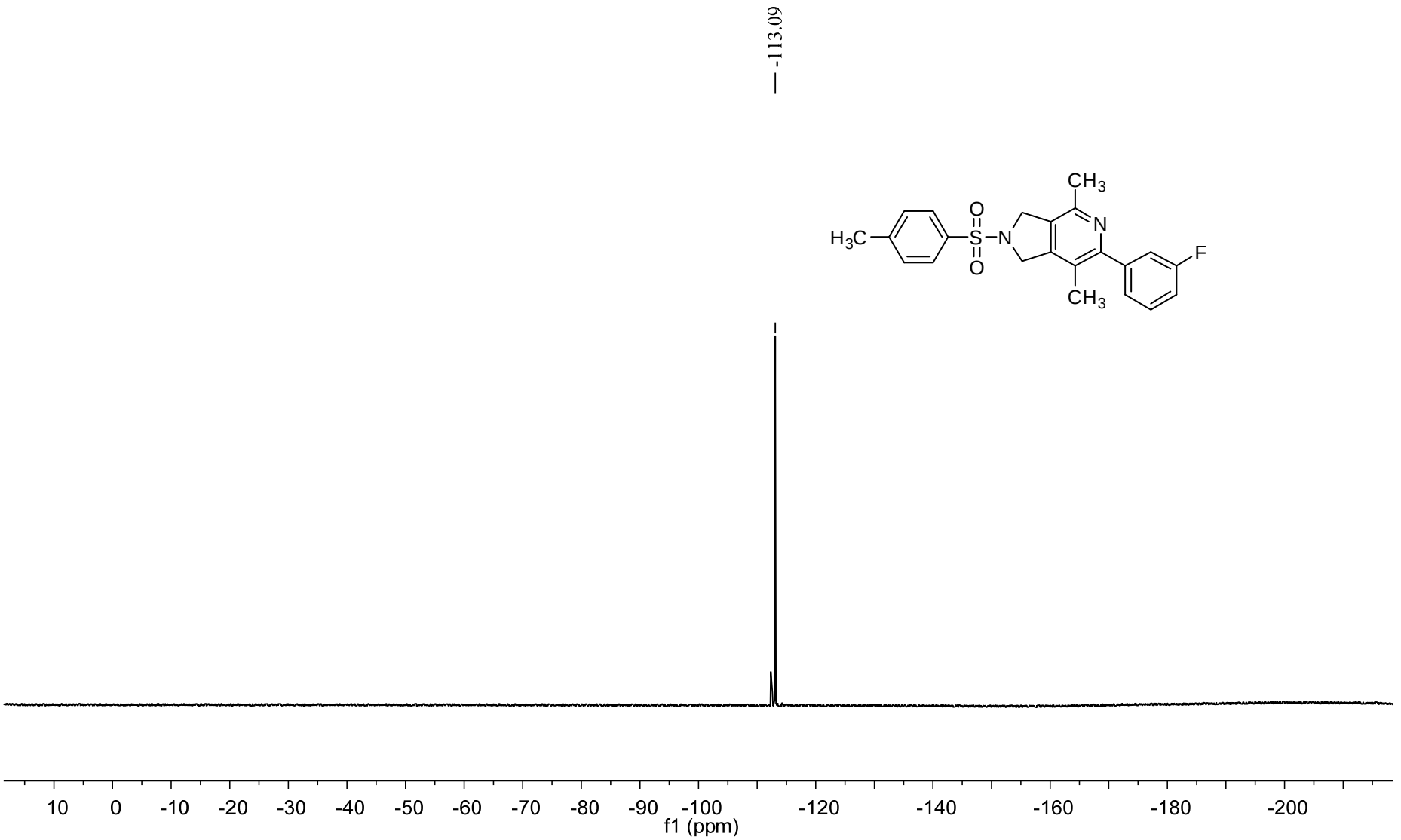
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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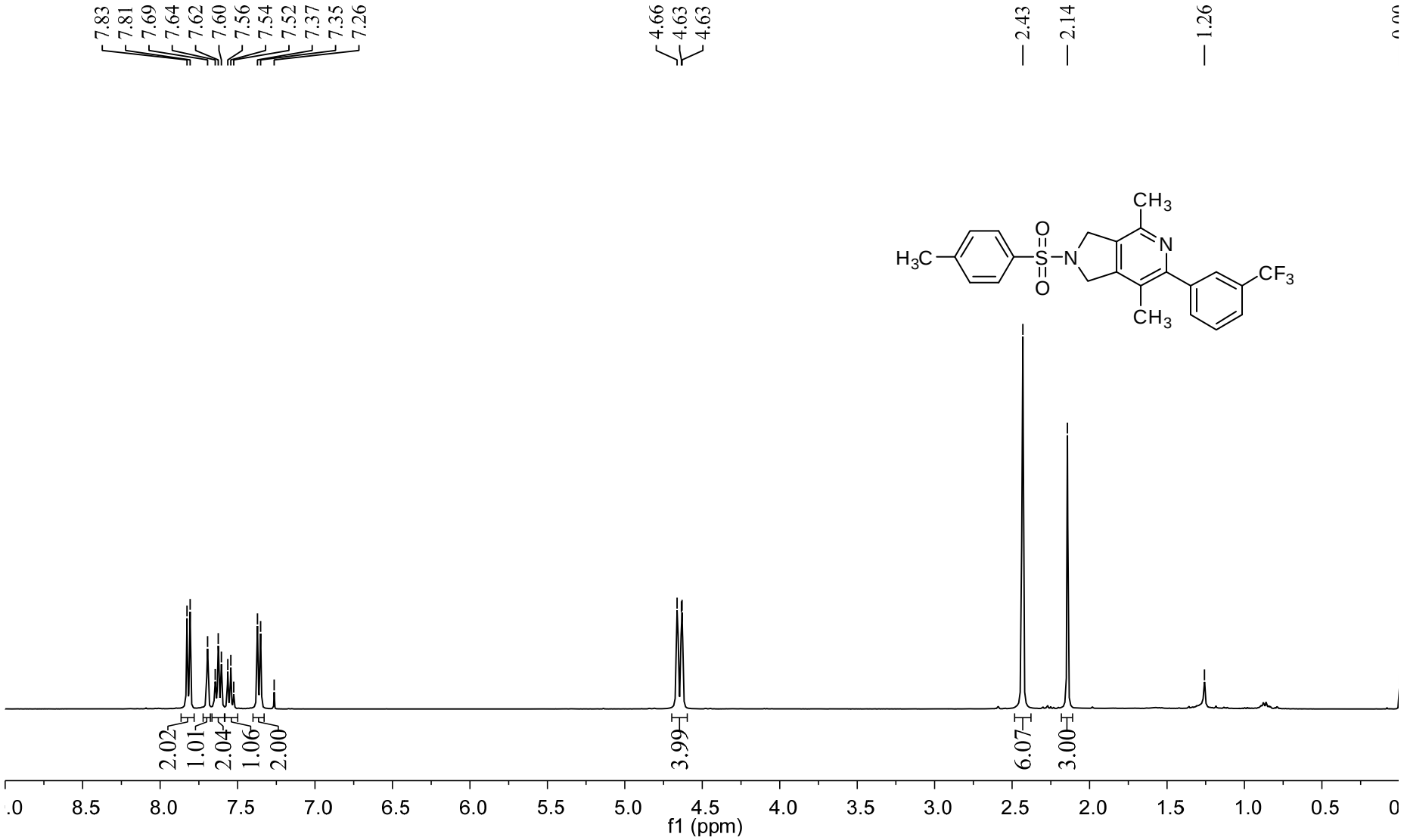
H3C
O
S
O
N
N
F
CH3
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)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7.62
7.60
7.56
7.54
7.52
7.37
7.35
7.26
4.66
4.63
4.63
2.43
2.14
1.26
CH3
H3C
S
O
O
N
N
CF3
CH3
2.02
1.01
2.04
1.06
2.00
3.99
6.07
3.00
8.5
8.0
7.5
7.0
6.5
6.0
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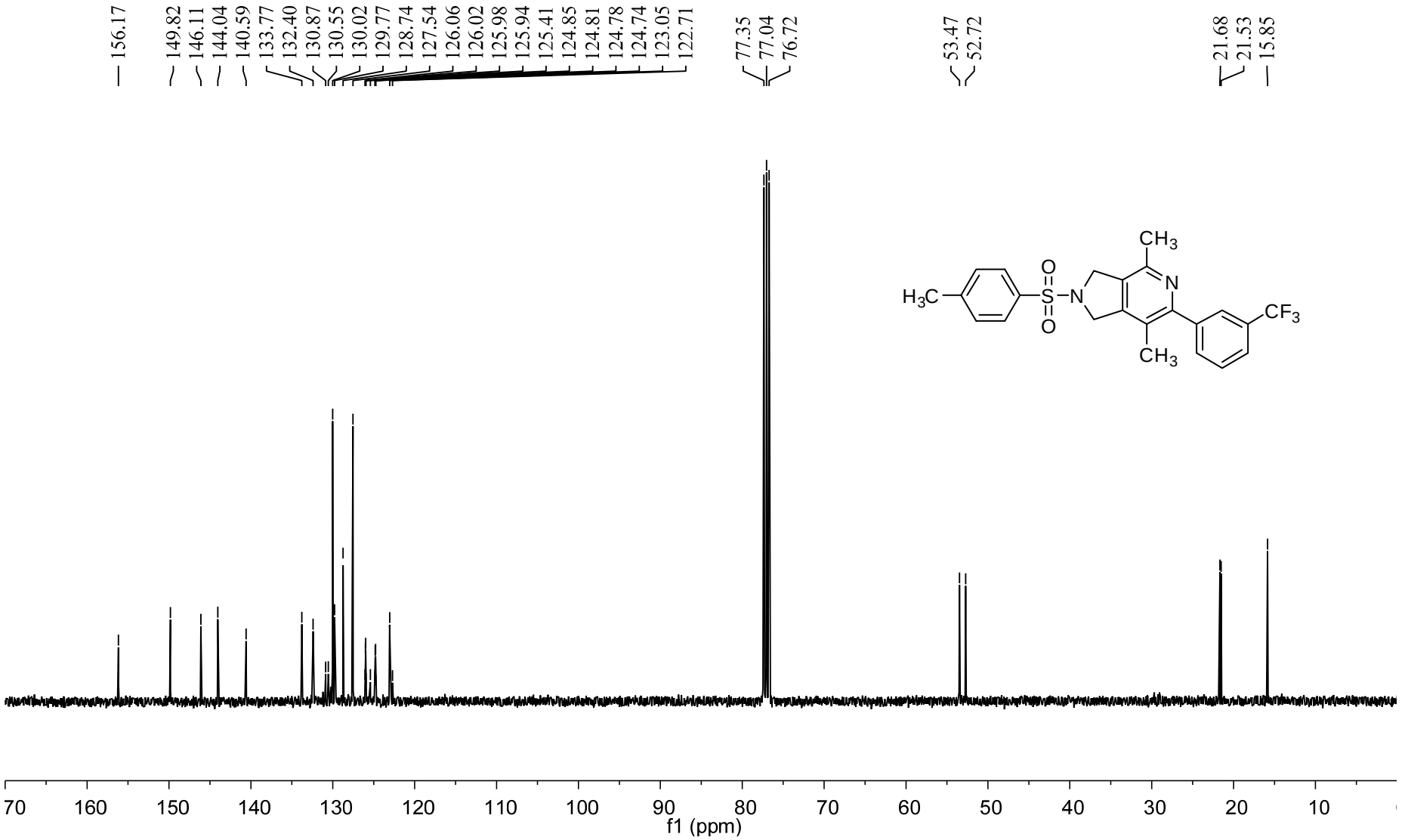
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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130.02
129.77
128.74
127.54
126.06
126.02
125.98
125.94
125.41
124.85
124.81
124.78
124.74
123.05
122.71
77.35
77.04
76.72
53.47
52.72
21.68
21.53
15.85
CH3
H3C
S
O
O
N
N
CH3
CF3
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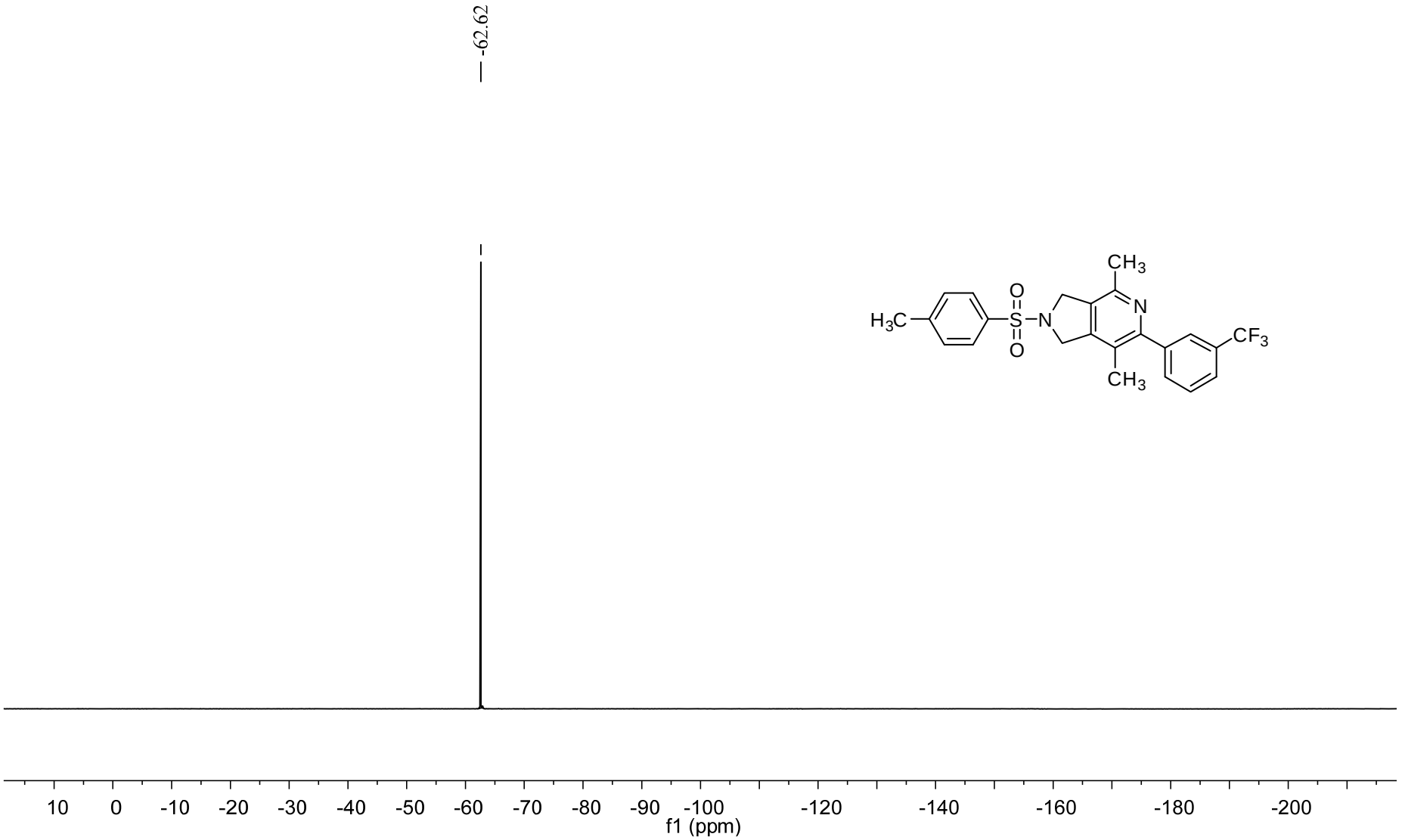
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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H3C
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N
N
O
CF3
CH3
10
0
-10
-20
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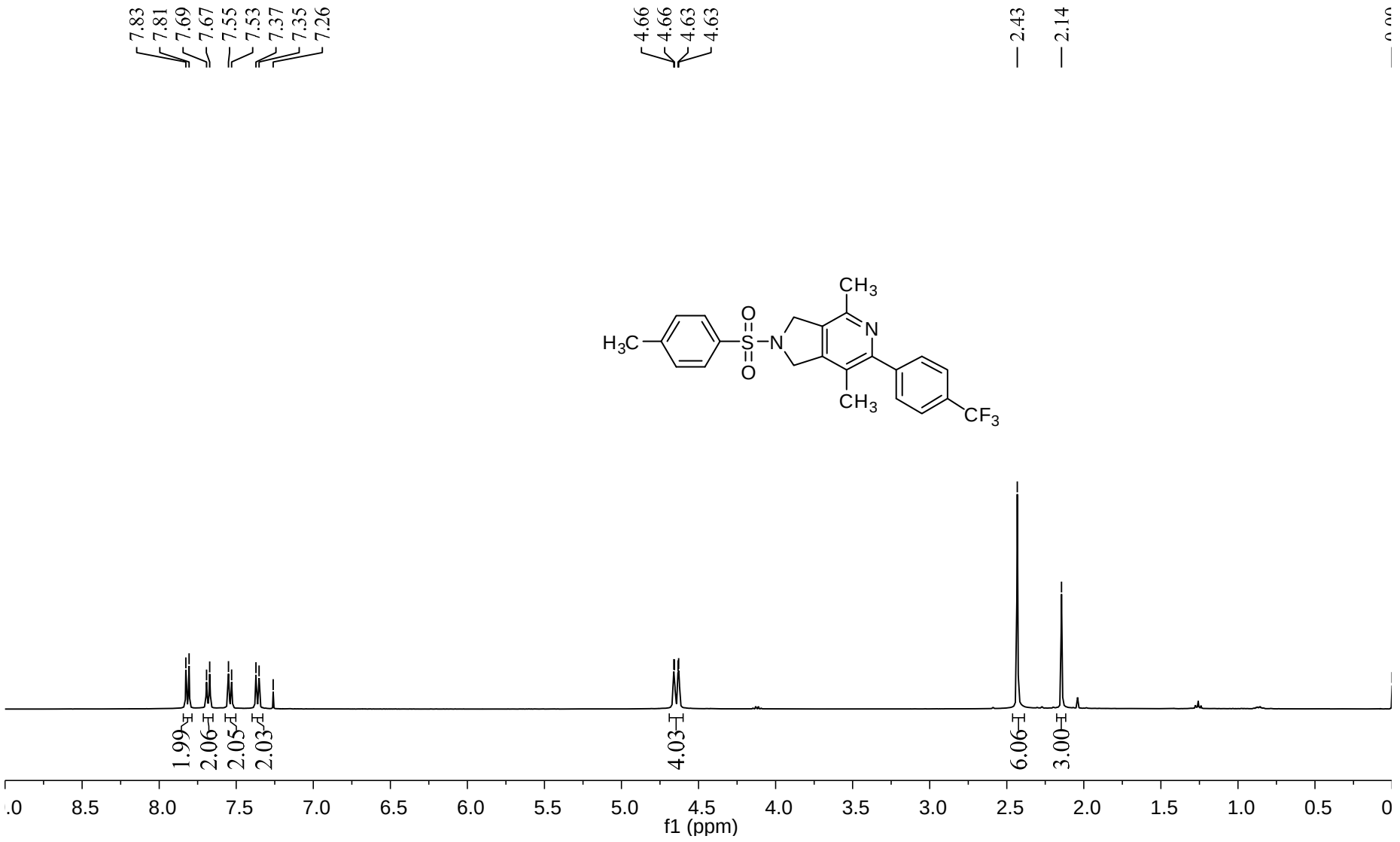
-60
-70
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)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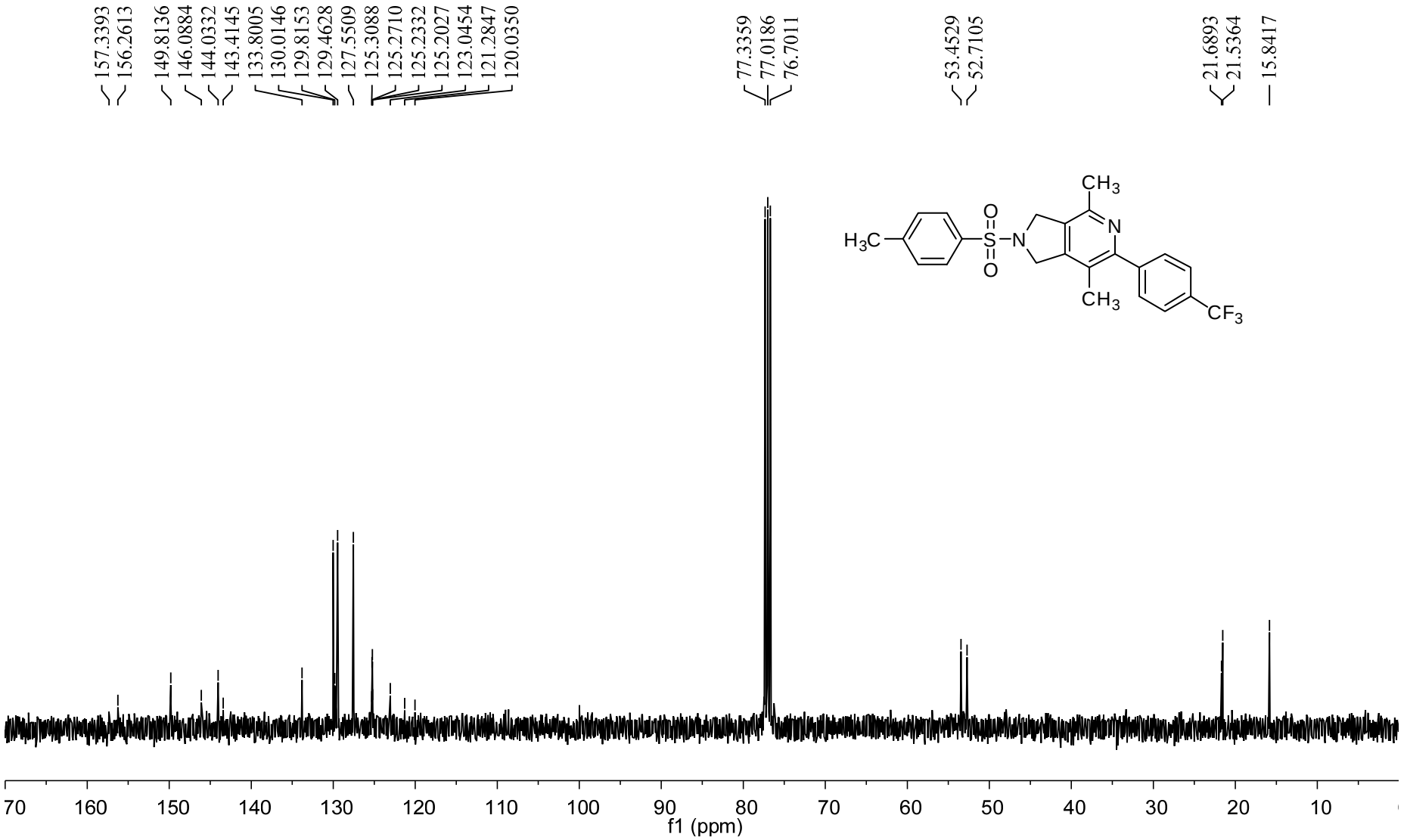
7.37
7.35
7.26
4.66
4.66
4.63
4.63
2.43
2.14
CH3
H3C
S
O
O
N
N
CH3
CF3
1.99
2.06
2.05
2.03
4.03
6.06
3.00
f1 (ppm)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129.4628
127.5509
125.3088
125.2710
125.2332
125.2027
123.0454
121.2847
120.0350
77.3359
77.0186
76.7011
53.4529
52.7105
21.6893
21.5364
15.8417
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O
N
N
CH3
CF3
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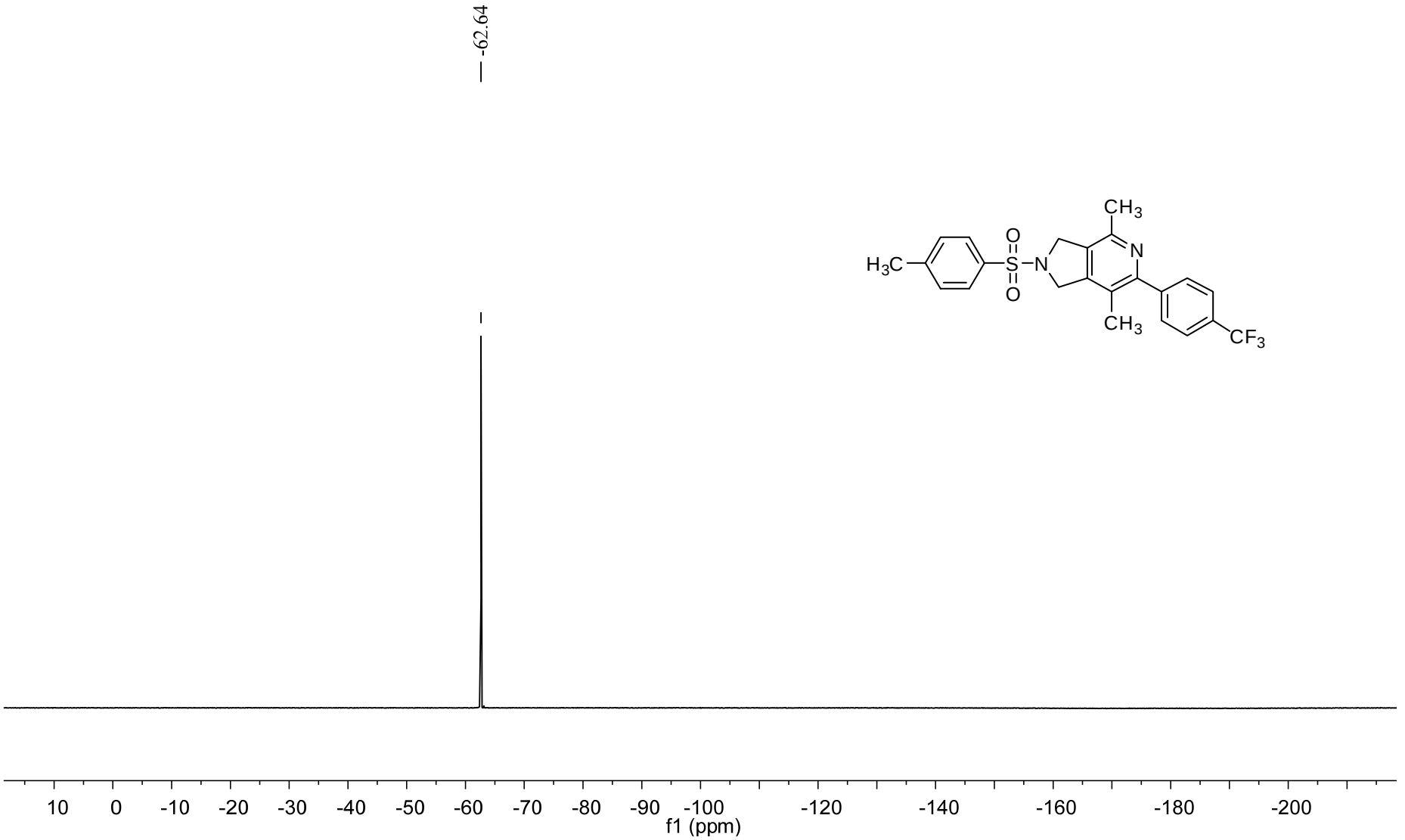
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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CF3
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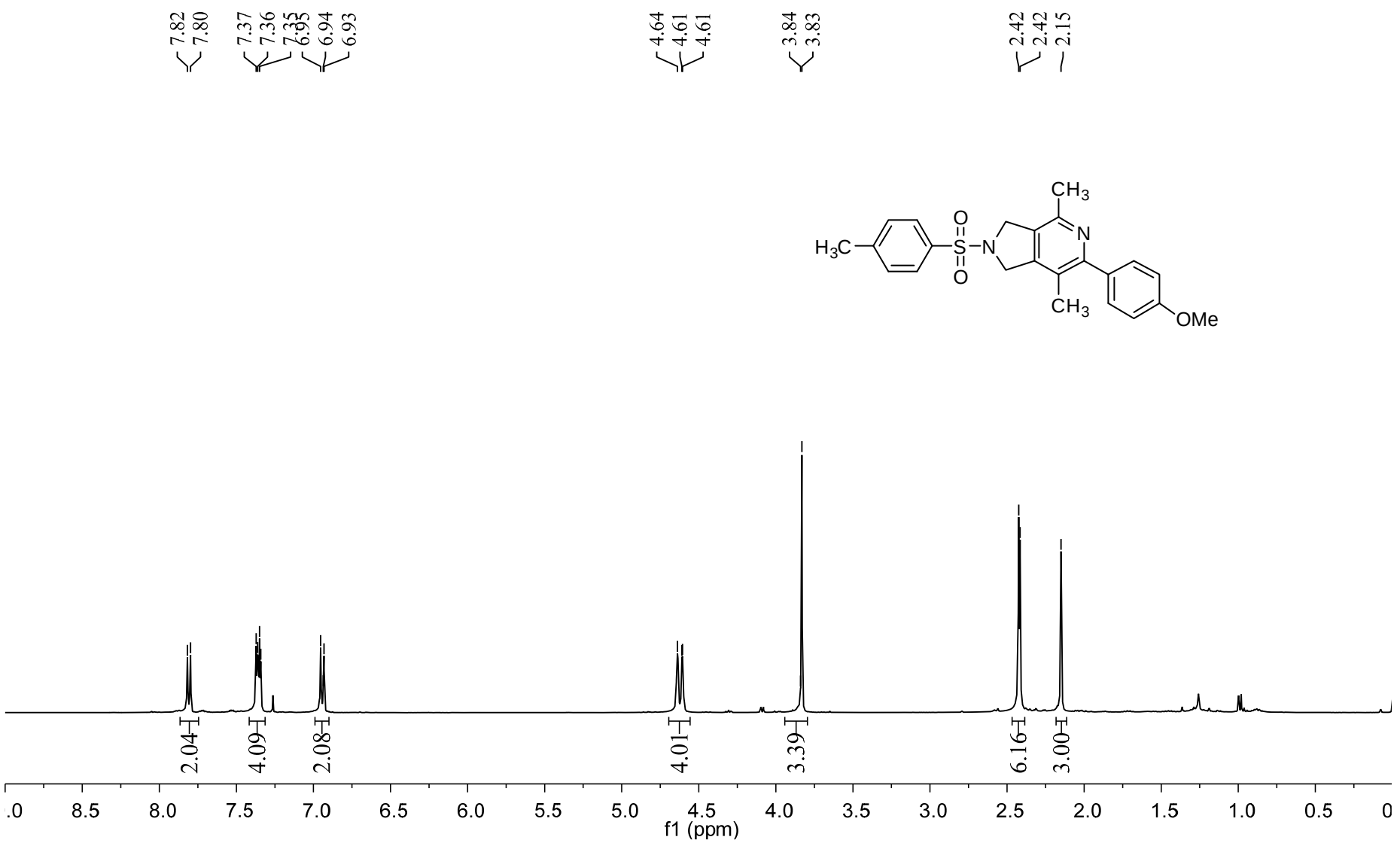
-80
-90
-100
-120
-140
-160
-180
-200
f1 (ppm)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4.61
3.84
3.83
2.42
2.42
2.15
CH3
O
S
N
O
H3C
N
CH3
OMe
2.04
4.09
2.08
4.01
3.39
6.16
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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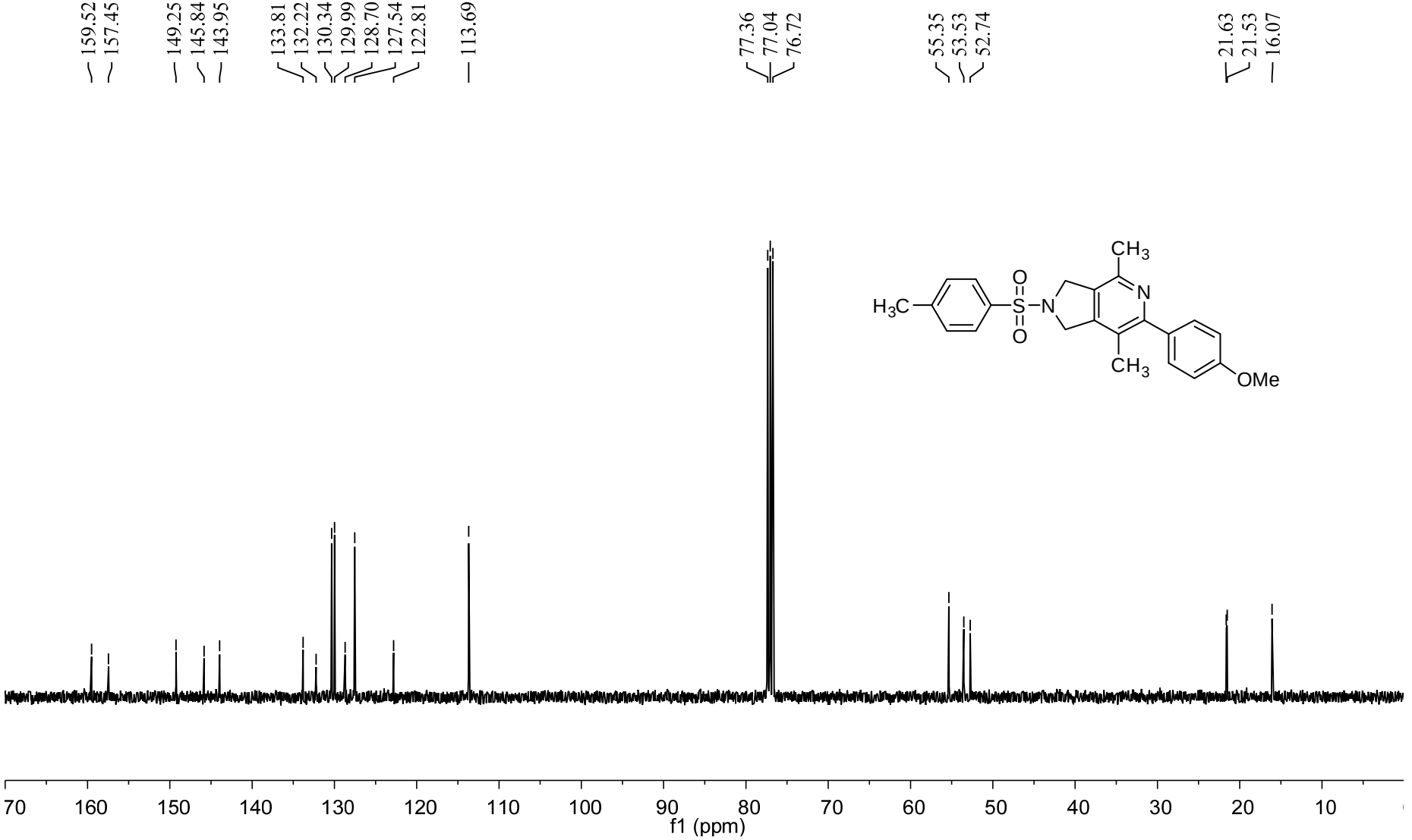
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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130.34
129.99
128.70
127.54
122.81
113.69
77.36
77.04
76.72
55.35
53.53
52.74
21.63
21.53
16.07
CH3
N
H3C
S
O
O
N
CH3
OMe
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140
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120
110
100
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80
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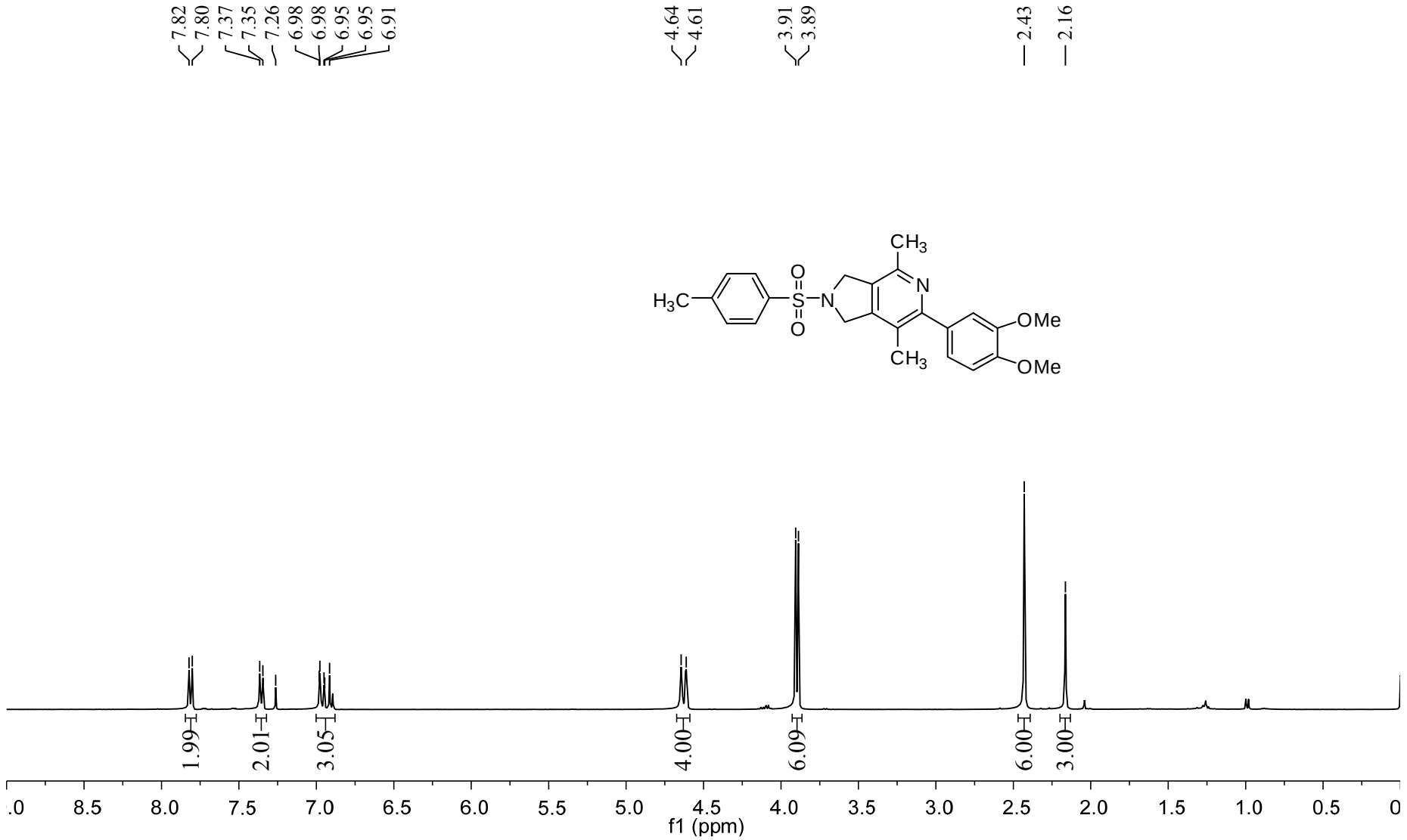
60
50
40
30
20
10
f1 (ppm)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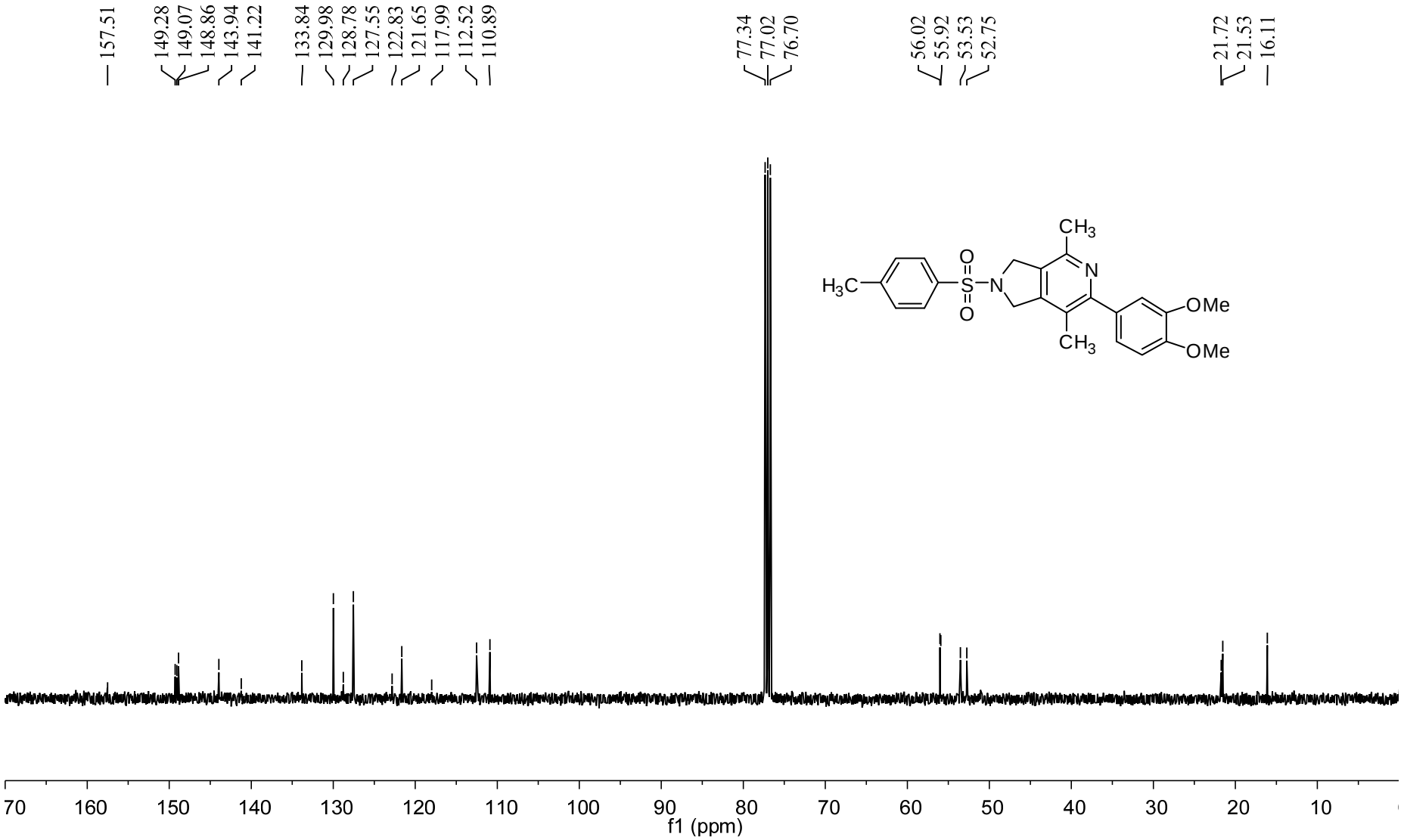
6.98
6.95
6.95
6.91
4.64
4.61
3.91
3.89
2.43
2.16
CH3
O
S
O
N
H3C
N
OMe
OMe
CH3
1.99
2.01
3.05
4.00
6.09
6.00
3.00
f1 (ppm)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129.98
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127.55
122.83
121.65
117.99
112.52
110.89
77.34
77.02
76.70
56.02
55.92
53.53
52.75
21.72
21.53
16.11
CH3
O
S
N
O
H3C
N
CH3
OMe
OMe
70
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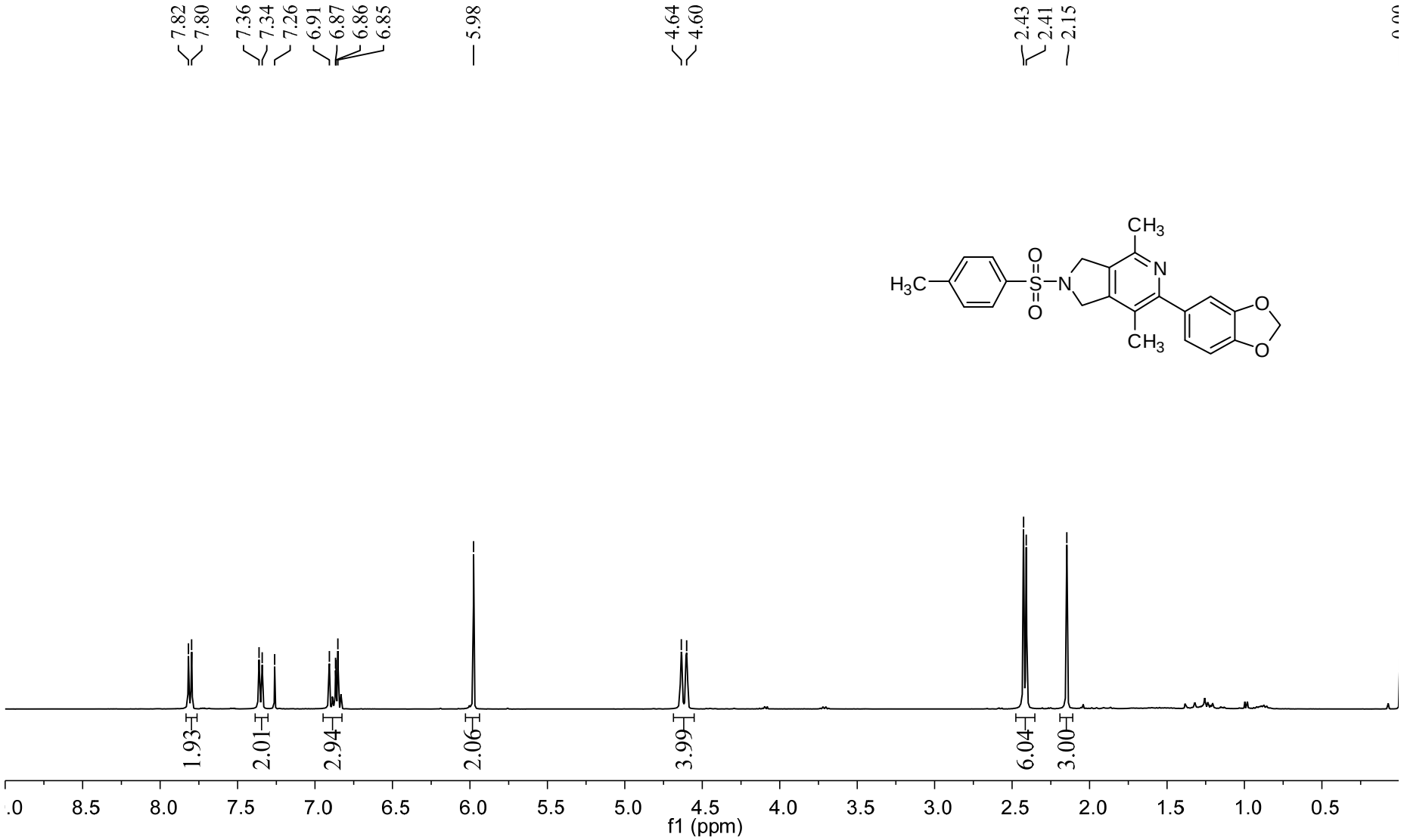
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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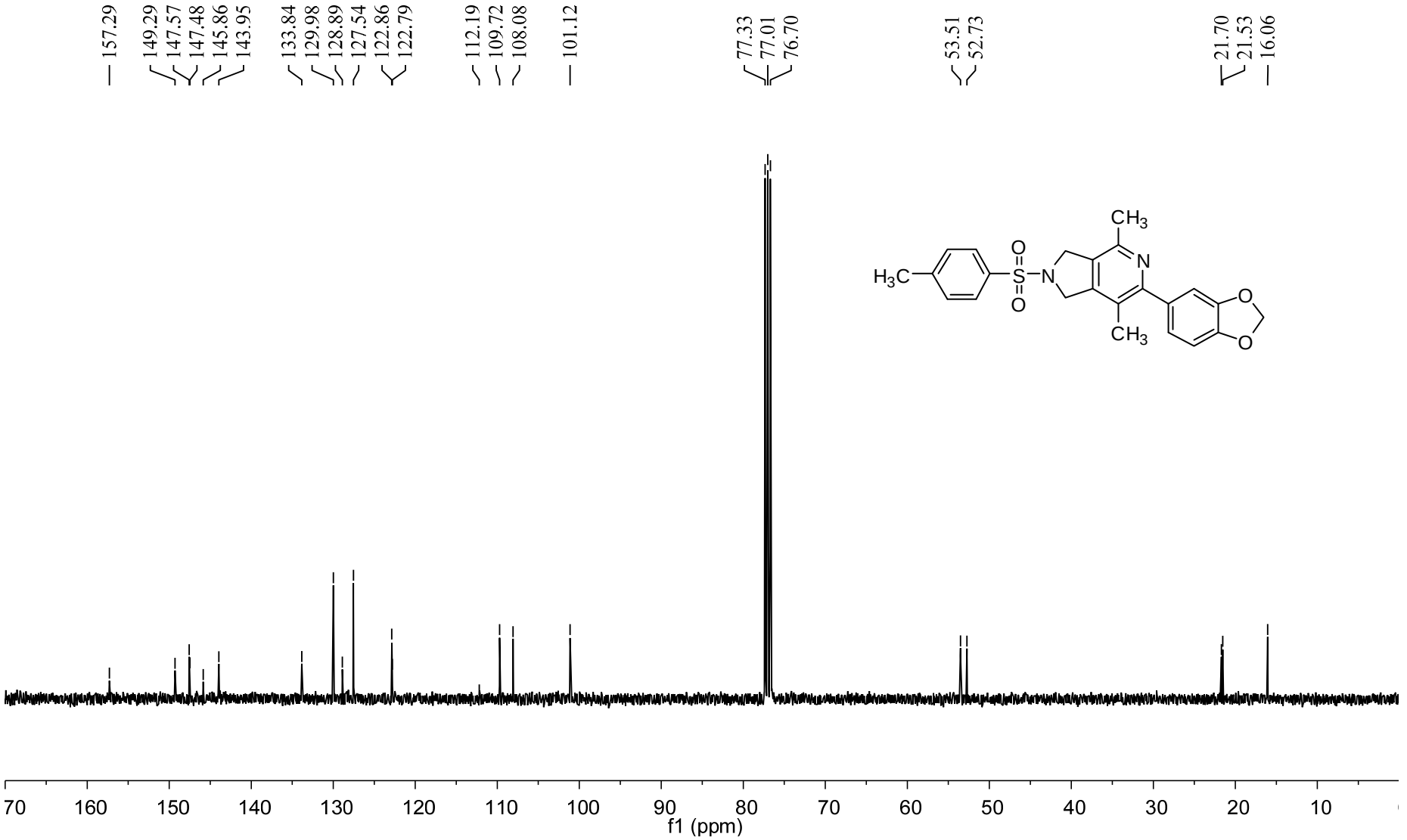
4.64
4.60
2.43
2.41
2.15
CH3
H3C
S
O
O
N
N
CH3
O
O
1.93
2.01
2.94
2.06
3.99
6.04
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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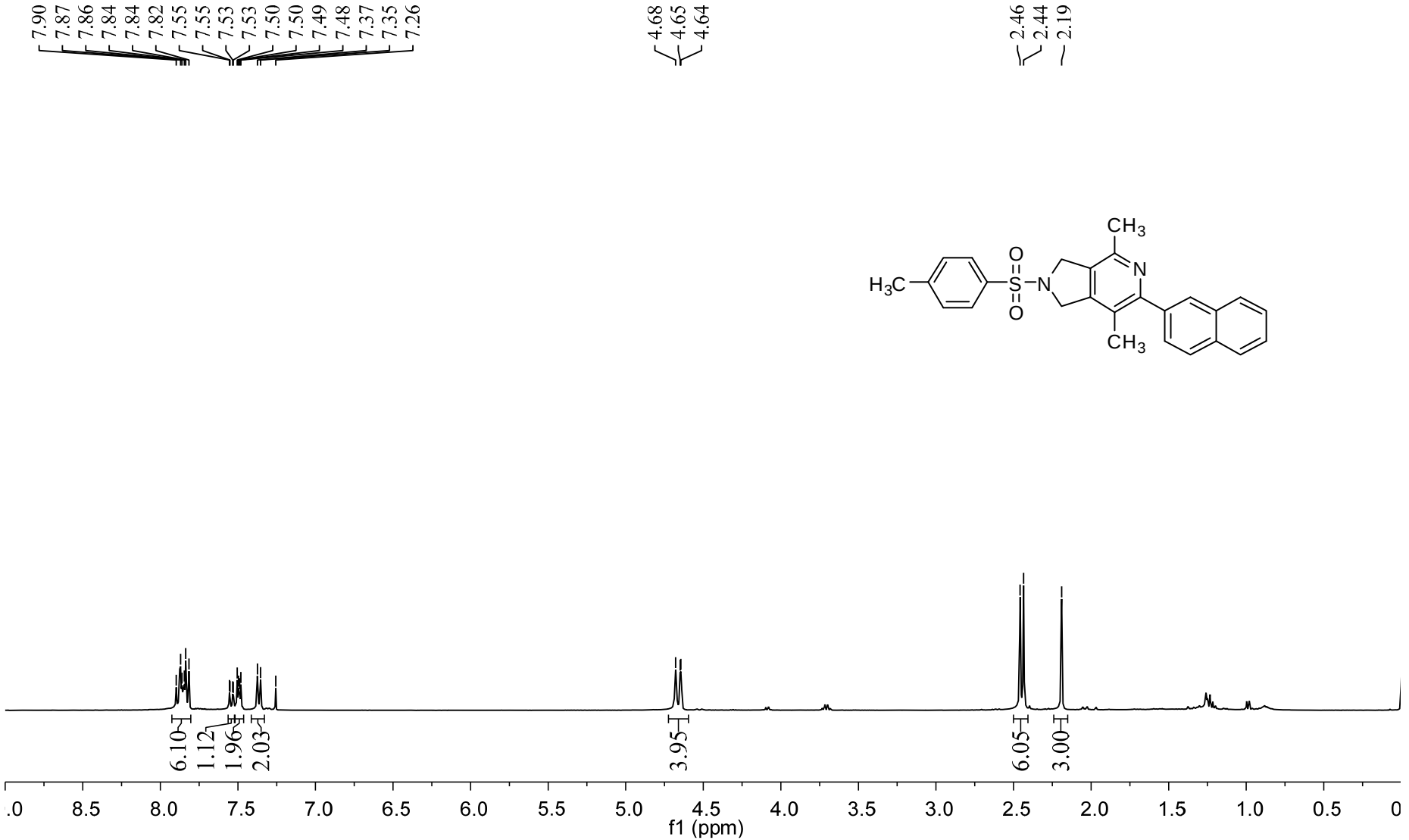
129.98
128.89
127.54
122.86
122.79
112.19
109.72
108.08
101.12
77.33
77.01
76.70
53.51
52.73
21.70
21.53
16.06
CH3
H3C
S
O
O
N
N
CH3
O
O
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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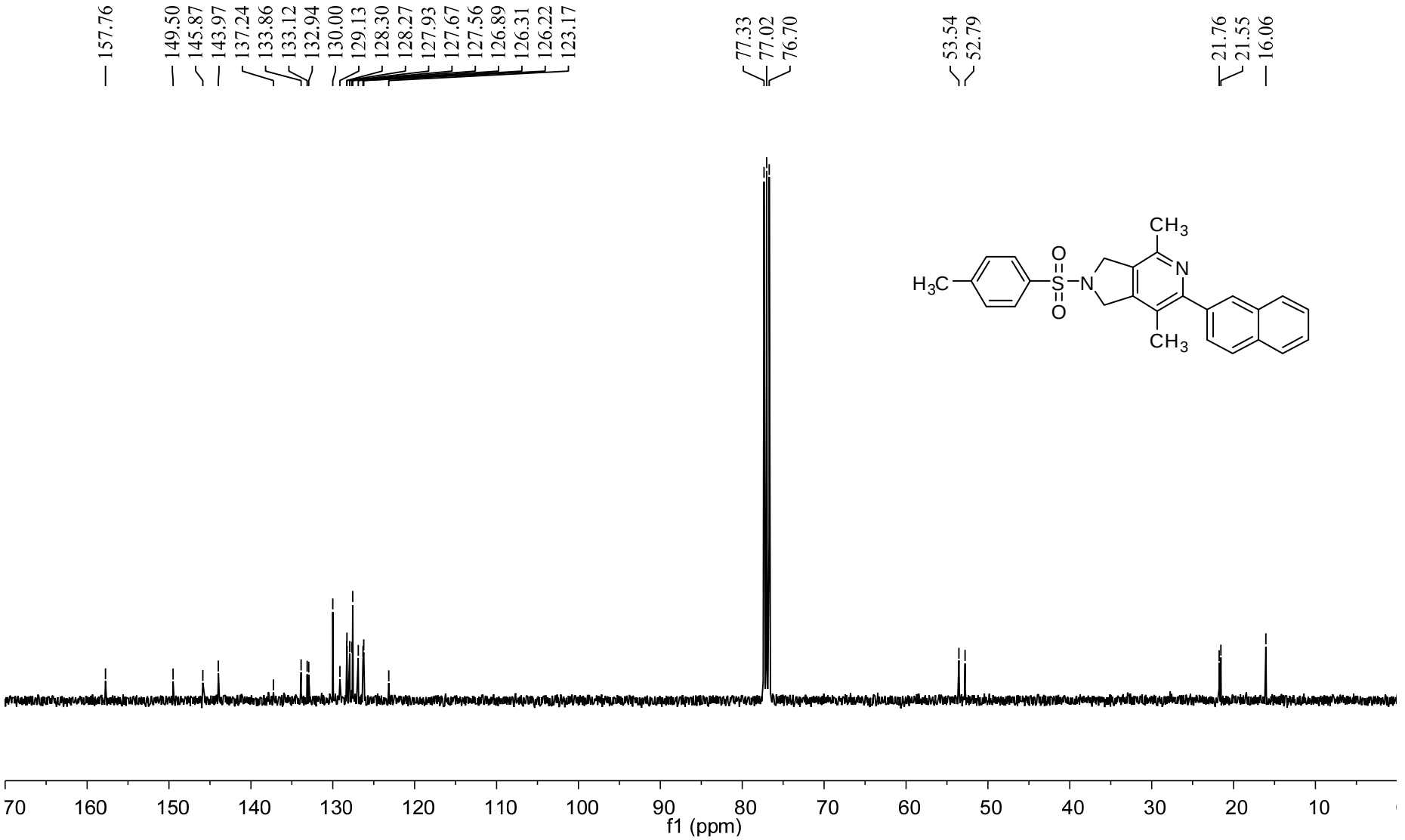
7.55
7.55
7.53
7.53
7.50
7.50
7.49
7.48
7.37
7.35
7.26
4.68
4.65
4.64
2.46
2.44
2.19
CH3
H3C
O
S
O
N
N
CH3
6.10
1.12
1.96
2.03
3.95
6.05
3.00
f1 (ppm)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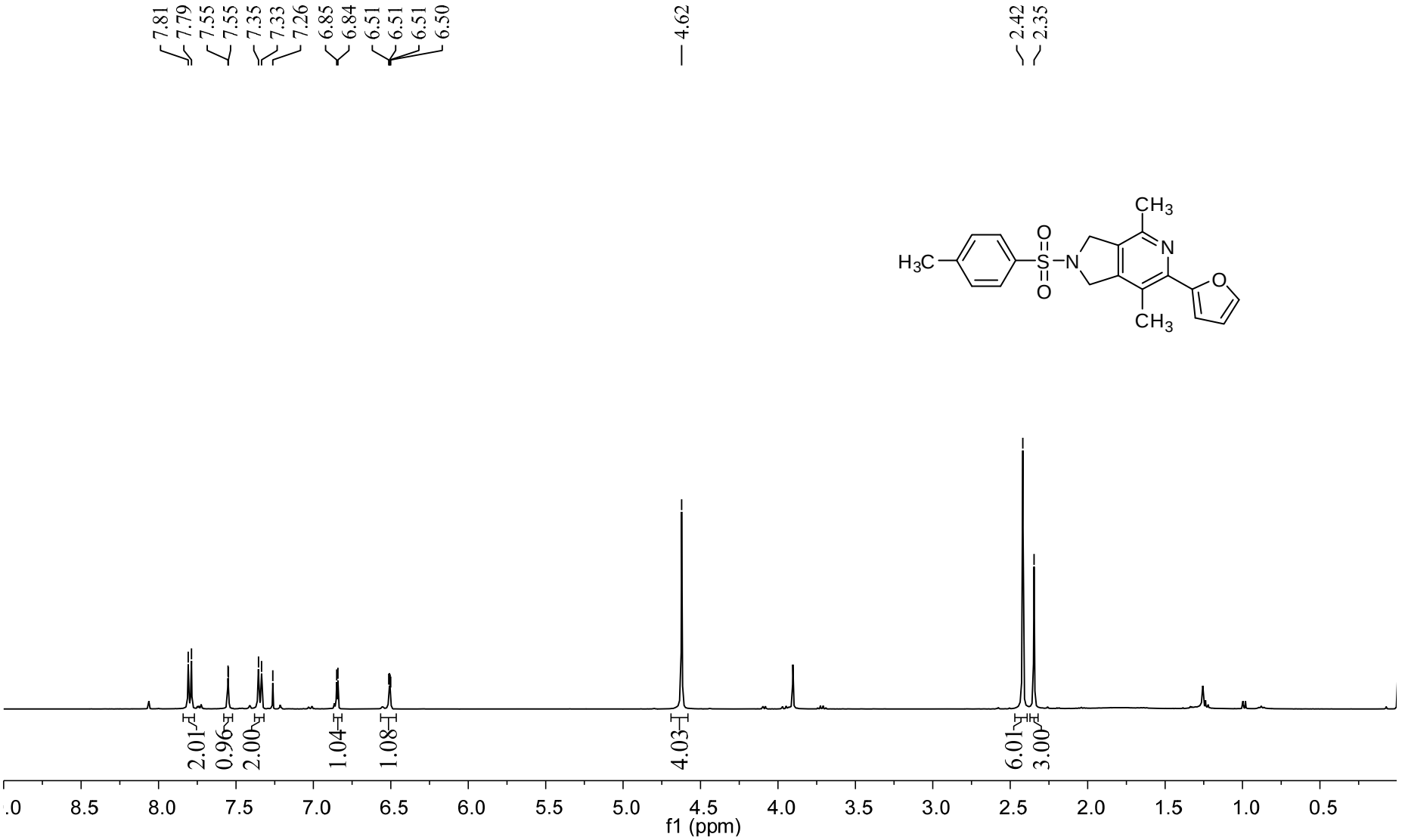
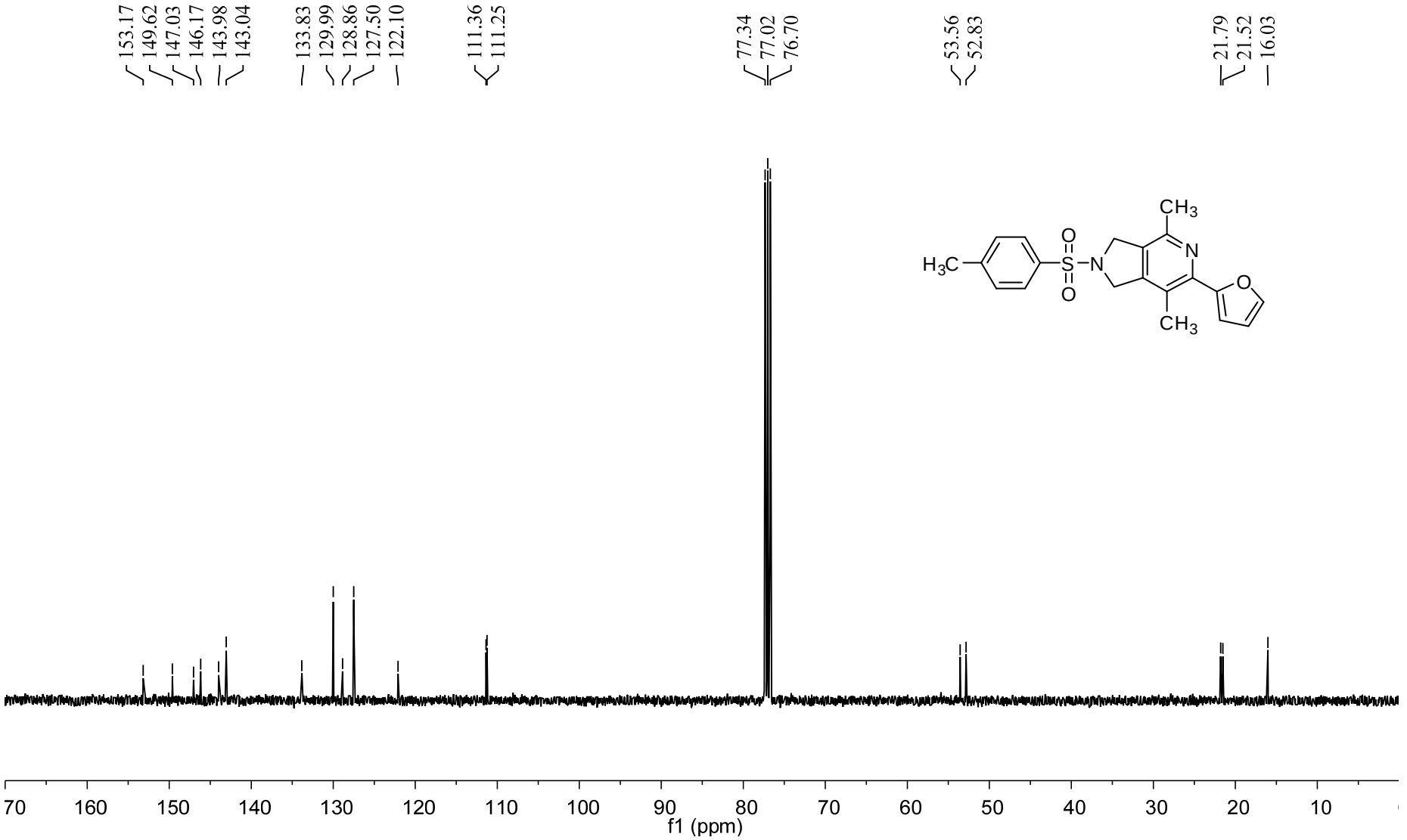
128.30
128.27
127.93
127.67
127.56
126.89
126.31
126.22
123.17
77.33
77.02
76.70
53.54
52.79
21.76
21.55
16.06
CH3
H3C
S
O
O
N
N
CH3
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

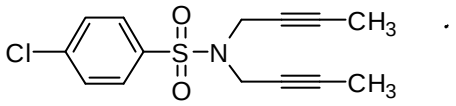

7.81
7.79
7.55
7.55
7.35
7.33
7.26
6.85
6.84
6.51
6.51
6.51
6.50
4.62
2.42
2.35
CH3
N
O
H3C
S
O
O
N
CH3
2.01
0.96
2.00
1.04
1.08
4.03
6.01
3.00
f1 (ppm)


153.17
149.62
147.03
146.17
143.98
143.04
133.83
129.99
128.86
127.50
122.10
111.36
111.25
77.34
77.02
76.70
53.56
52.83
21.79
21.52
16.03
CH3
H3C
S
O
O
N
N
O
CH3
70
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

Elemental Composition Report

Single Mass Analysis (displaying only valid results)

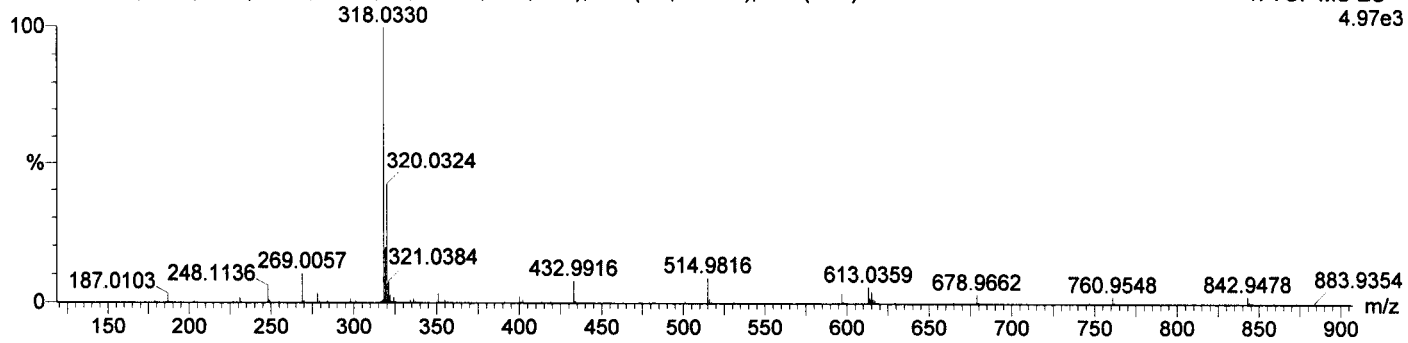
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None



Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-150 N: 1-1 O: 2-2 Na: 1-1 S: 1-1 Cl: 1-1

XFF-B-44
12052719 12 (0.223) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x1.00); Cm (8:13)

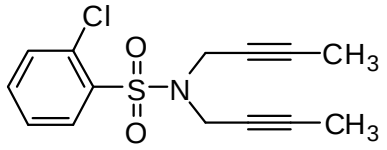
12:34:07
1: TOF MS ES+
4.97e3



Minimum:				-200.0		
Maximum:		5.0	5.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
318.0330	318.0331	-0.1	-0.3	7.5	13.7	C14 H14 N O2 Na S Cl

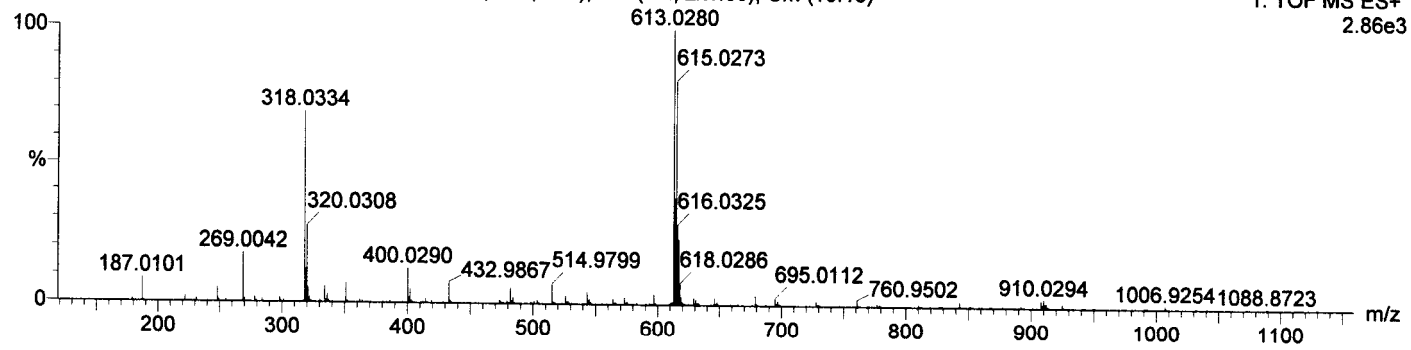
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None



Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-150 N: 1-1 O: 2-2 Na: 1-1 S: 1-1 Cl: 1-1
XFF-B-43
12052718 12 (0.223) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x1.00); Cm (10:15)

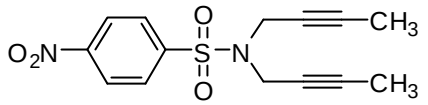
12:30:00
1: TOF MS ES+
2.86e3



Minimum:				-200.0		
Maximum:		5.0	5.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
318.0334	318.0331	0.3	0.9	7.5	0.3	C14 H14 N O2 Na S Cl

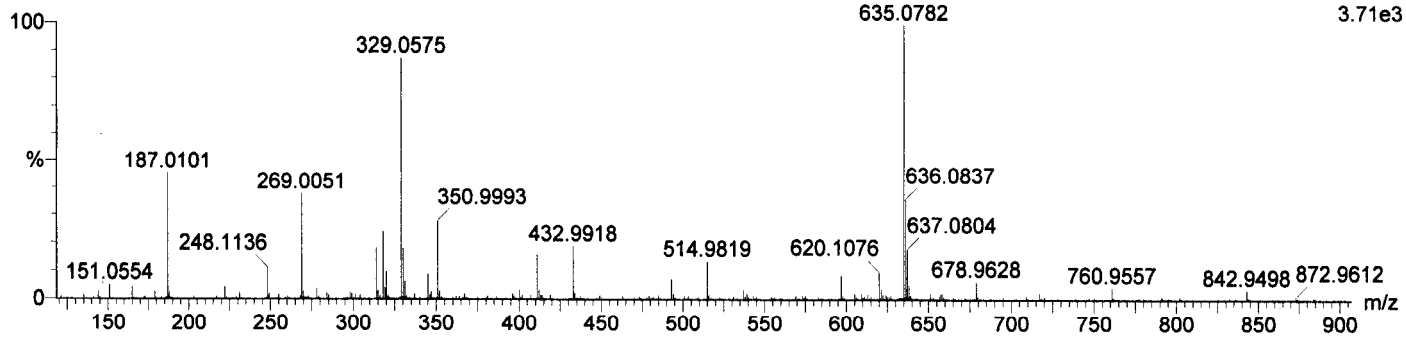
Single Mass Analysis (displaying only valid results)

Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None



Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-150 N: 2-2 O: 4-4 Na: 1-1 S: 1-1

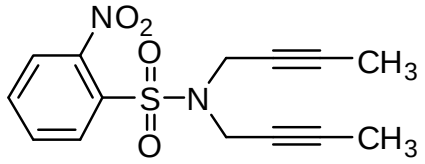
XFF-B-46
12052721 26 (0.486) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x1.00); Cm (21:34)
12:44:33
1: TOF MS ES+
3.71e3



Minimum:				-200.0		
Maximum:		5.0	5.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
329.0575	329.0572	0.3	0.9	8.5	8.1	C14 H14 N2 O4 Na S

Elemental Composition Report

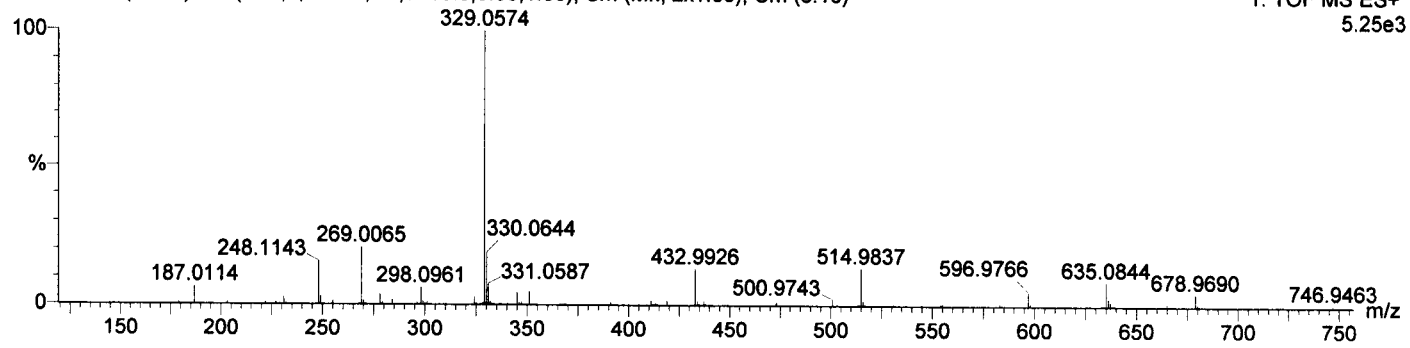
Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None



Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-150 N: 2-2 O: 4-4 Na: 1-1 S: 1-1

XFF-B-40
12052715 8 (0.149) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x1.00); Cm (8:16)

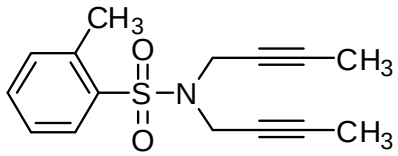
12:06:28
1: TOF MS ES+
5.25e3



Minimum:				-200.0		
Maximum:		5.0	5.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
329.0574	329.0572	0.2	0.6	8.5	5.4	C14 H14 N2 O4 Na S

Elemental Composition Report

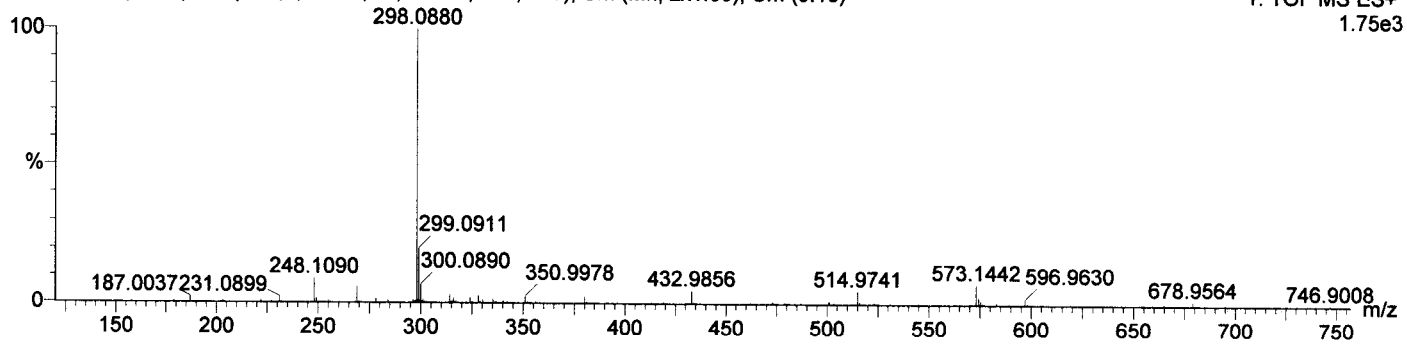
Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None



Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-150 N: 1-1 O: 2-2 Na: 1-1 S: 1-1

XFF-B-39
12052714 9 (0.168) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x1.00); Cm (9:15)

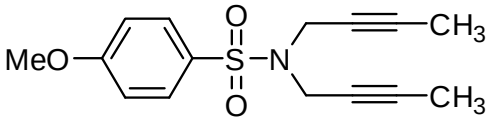
12:01:16
1: TOF MS ES+
1.75e3



Minimum:				-200.0		
Maximum:		5.0	5.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
298.0880	298.0878	0.2	0.7	7.5	1.3	C15 H17 N O2 Na S

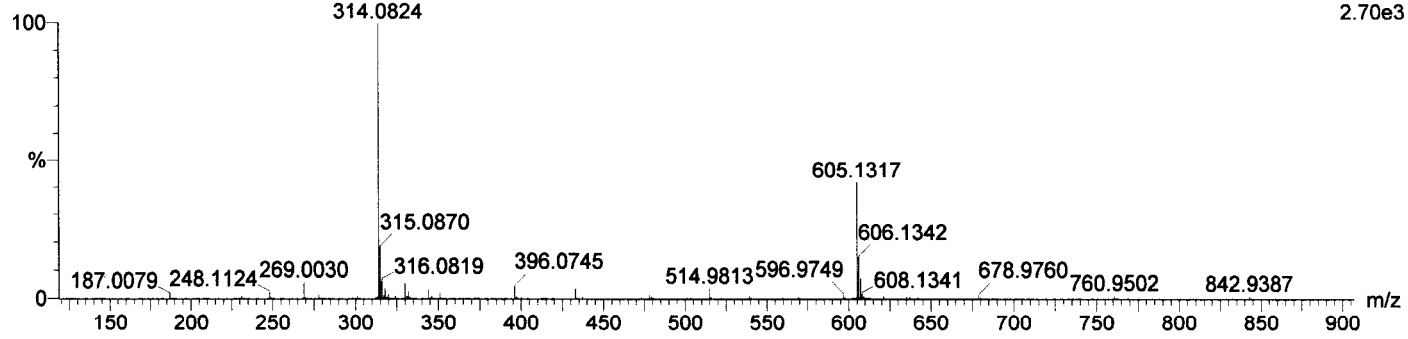
Elemental Composition Report

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None



Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-150 N: 1-1 O: 3-3 Na: 1-1 S: 1-1

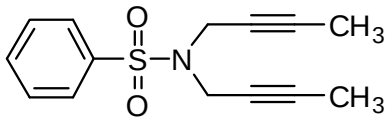
XFF-B-45 12:39:57
12052720 37 (0.689) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x1.00); Cm (27:37) 1: TOF MS ES+
2.70e3



Minimum:				-200.0		
Maximum:		5.0	5.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
314.0824	314.0827	-0.3	-1.0	7.5	0.4	C15 H17 N O3 Na S

Elemental Composition Report

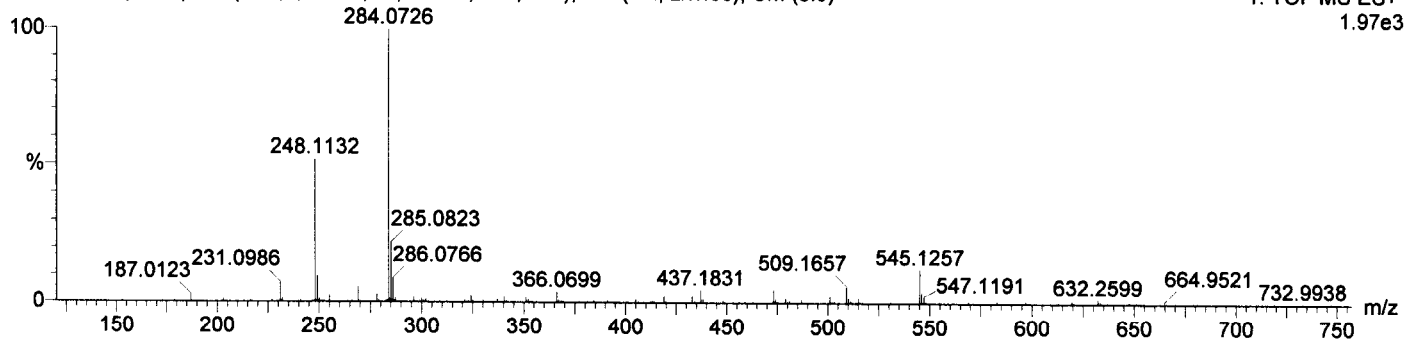
Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None



Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-150 N: 1-1 O: 2-2 Na: 1-1 S: 1-1

XFF-B-37
12052712 8 (0.149) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x1.00); Cm (8:9)

11:52:23
1: TOF MS ES+
1.97e3

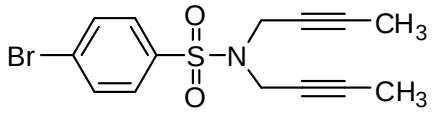


Minimum:				-200.0		
Maximum:		5.0	5.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
284.0726	284.0721	0.5	1.8	7.5	16.2	C14 H15 N O2 Na S

Elemental Composition Report

Single Mass Analysis (displaying only valid results)

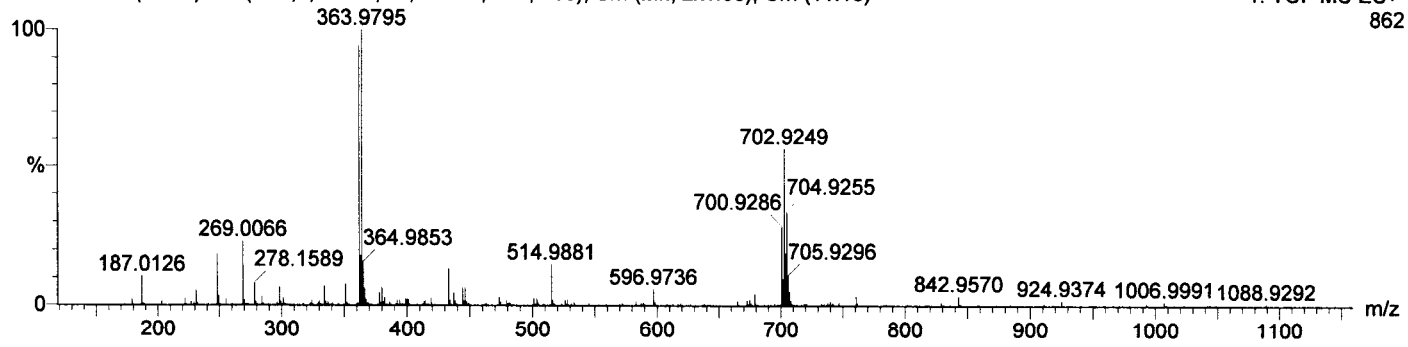
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None



Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-150 N: 1-1 O: 2-2 Na: 1-1 S: 1-1 Br: 1-1

XFF-B-42
12052717 11 (0.204) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x1.00); Cm (11:13)

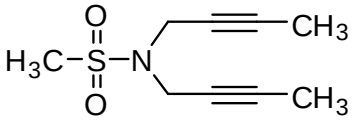
12:22:03
1: TOF MS ES+
862



Minimum:				-200.0		
Maximum:		5.0	5.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
361.9823	361.9826	-0.3	-0.8	7.5	1.0	C14 H14 N O2 Na S Br

Elemental Composition Report

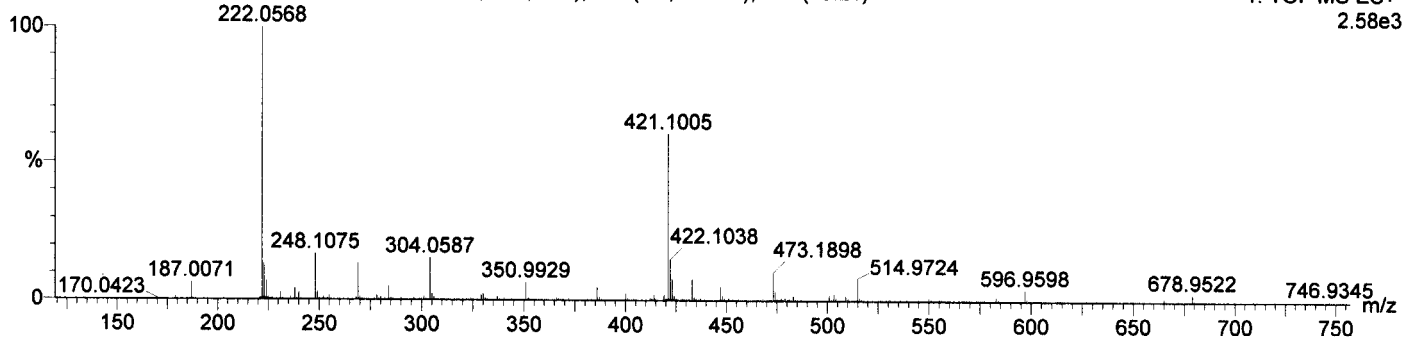
Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None



Monoisotopic Mass, Even Electron Ions
11 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-150 N: 1-1 O: 2-2 Na: 1-1 S: 1-1

XFF-B-38
12052713 21 (0.391) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x1.00); Cm (16:21)

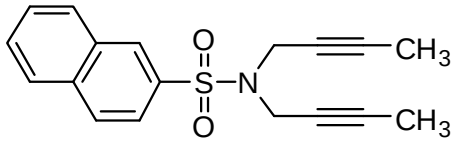
11:57:12
1: TOF MS ES+
2.58e3



Minimum:				-200.0		
Maximum:		5.0	5.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
222.0568	222.0565	0.3	1.4	3.5	7.4	C9 H13 N O2 Na S

Elemental Composition Report

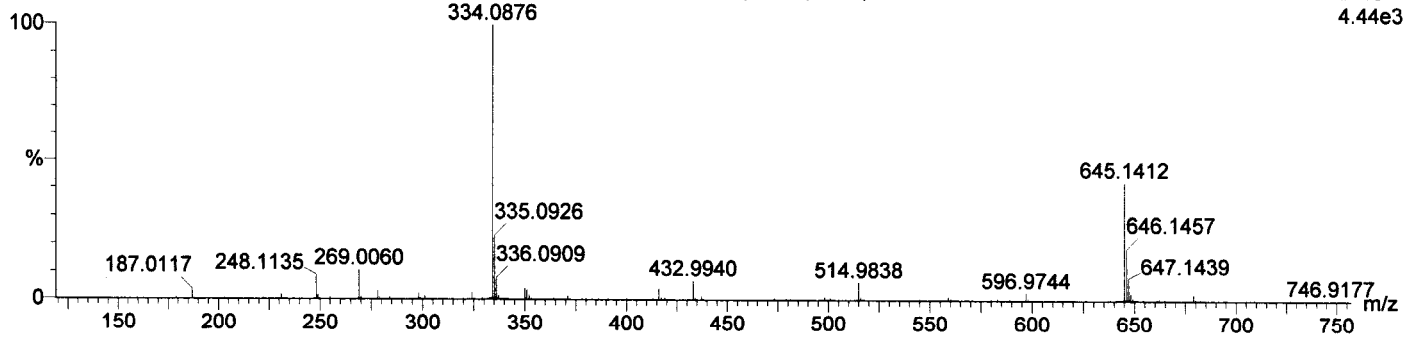
Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None



Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-150 N: 1-1 O: 2-2 Na: 1-1 S: 1-1

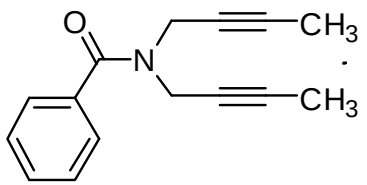
XFF-B-41
12052716 12 (0.223) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x1.00); Cm (12:20)

12:12:25
1: TOF MS ES+
4.44e3



Minimum:				-200.0		
Maximum:		5.0	5.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
334.0876	334.0878	-0.2	-0.6	10.5	3.2	C18 H17 N O2 Na S

Elemental Composition Report

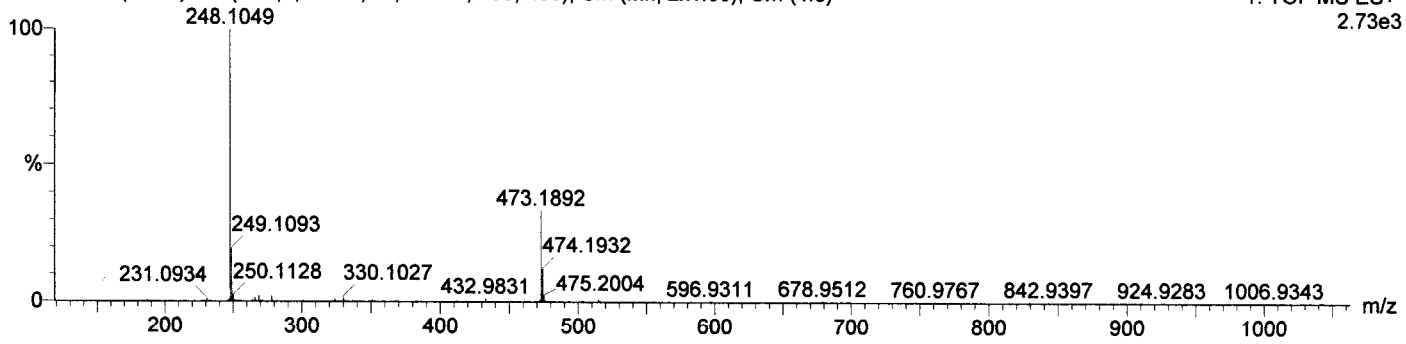


Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-150 N: 1-1 O: 1-1 Na: 1-1

XFF-B-36
12052711 7 (0.130) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x1.00); Cm (4:8)

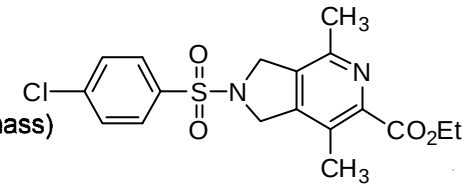
11:46:52
1: TOF MS ES+
2.73e3



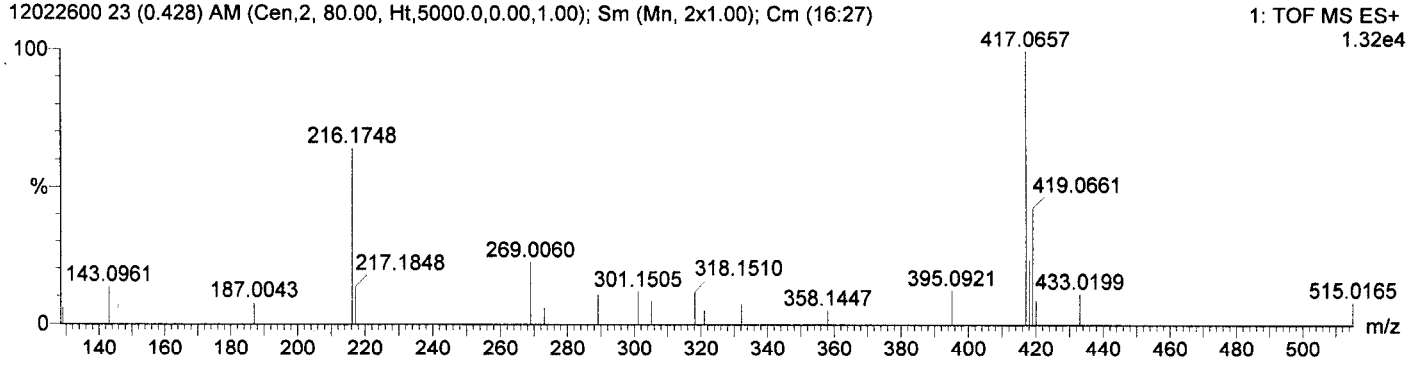
Minimum:				-200.0		
Maximum:		5.0	5.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
248.1049	248.1051	-0.2	-0.8	8.5	5.2	C15 H15 N O Na

Single Mass Analysis (displaying only valid results)

Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

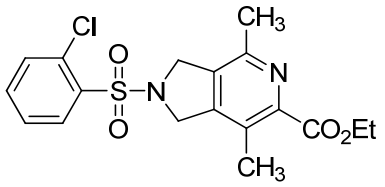


Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-150 N: 2-2 O: 4-4 Na: 1-1 S: 1-1 Cl: 1-1
XFF-B-1
12022600 23 (0.428) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x1.00); Cm (16:27)



Minimum:				-200.0		
Maximum:		5.0	5.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
417.0657	417.0652	0.5	1.2	9.5	16.7	C18 H19 N2 O4 Na S Cl

Elemental Composition Report

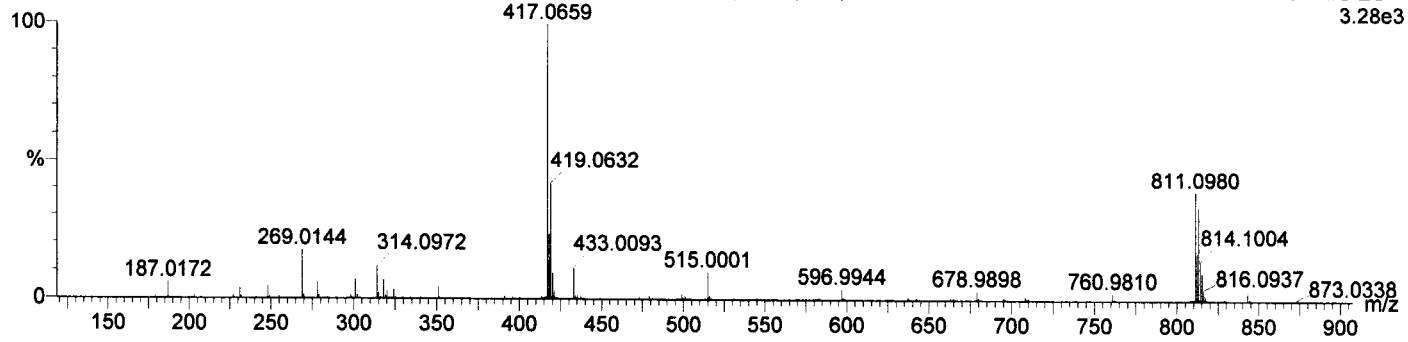


Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-150 N: 2-2 O: 4-4 Na: 1-1 S: 1-1 Cl: 1-1

XFF-B-47
12052722 7 (0.130) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x1.00); Cm (6:13)

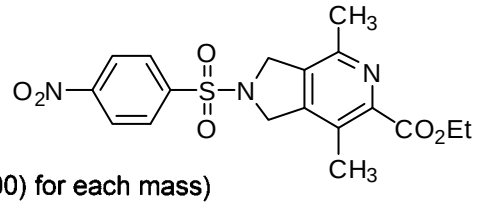
12:50:54
1: TOF MS ES+
3.28e3



Minimum:				-200.0		
Maximum:		5.0	5.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
417.0659	417.0652	0.7	1.7	9.5	2.1	C18 H19 N2 O4 Na S Cl

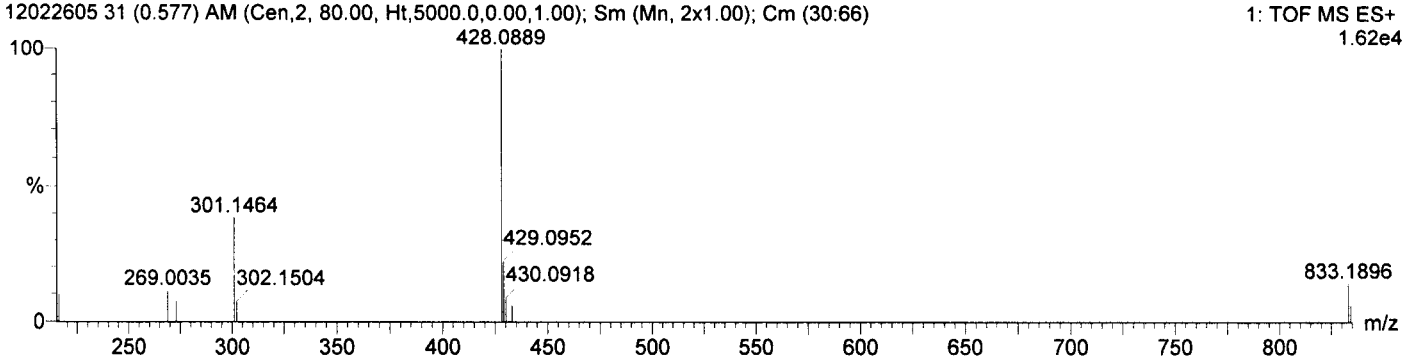
Single Mass Analysis (displaying only valid results)

Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None



Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-150 N: 3-3 O: 6-6 Na: 1-1 S: 1-1

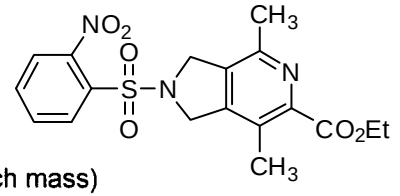
XFF-B-6
12022605 31 (0.577) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x1.00); Cm (30:66)



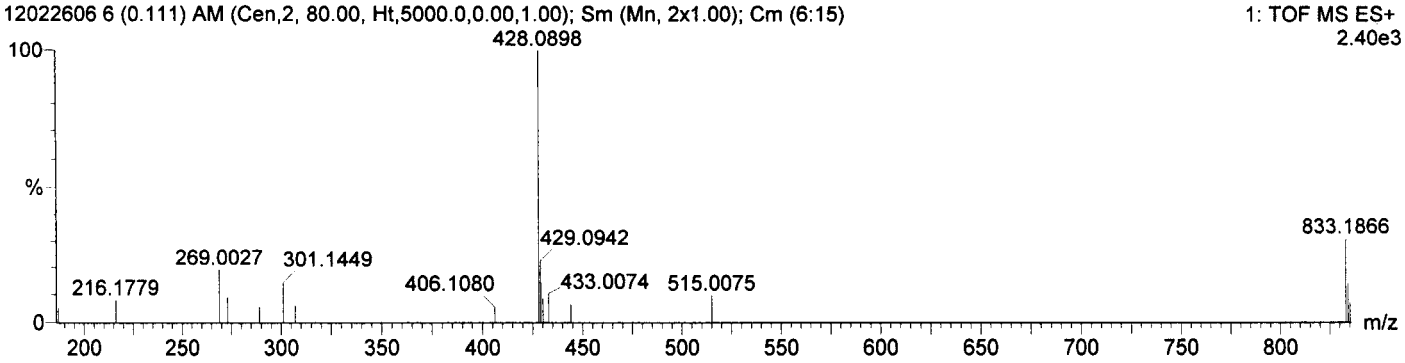
Minimum:				-200.0		
Maximum:		5.0	5.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
428.0889	428.0892	-0.3	-0.7	10.5	1.9	C18 H19 N3 O6 Na S

Single Mass Analysis (displaying only valid results)

Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

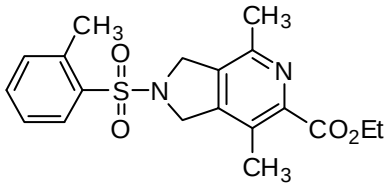


Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-150 N: 3-3 O: 6-6 Na: 1-1 S: 1-1
XFF-B-7
12022606 6 (0.111) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x1.00); Cm (6:15)



Minimum:				-200.0		
Maximum:		5.0	5.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
428.0898	428.0892	0.6	1.4	10.5	0.5	C18 H19 N3 O6 Na S

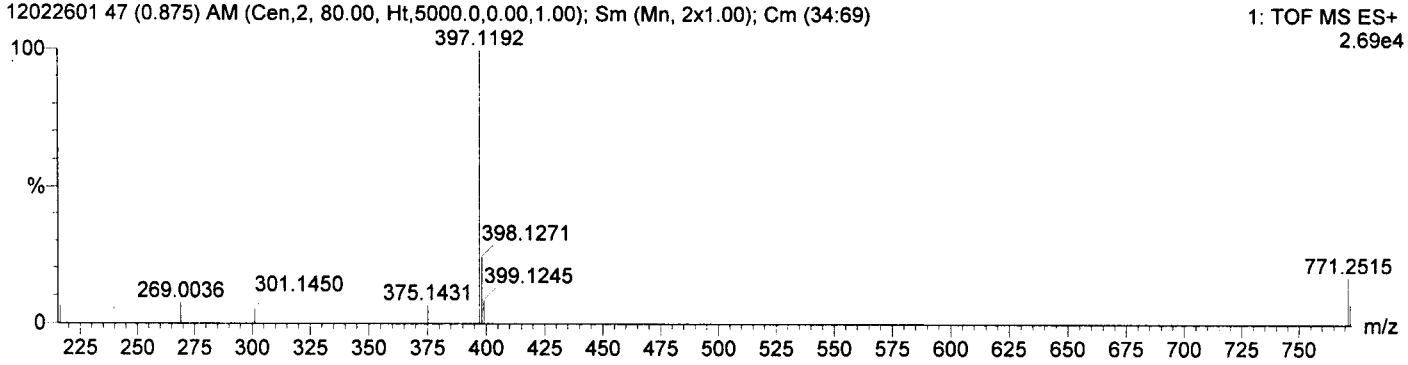
Elemental Composition Report **Page 1**



Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

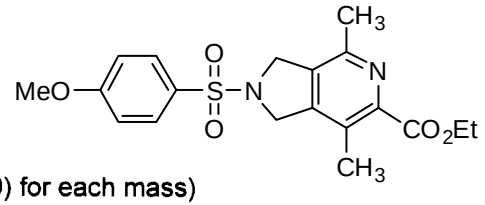
Monoisotopic Mass, Even Electron Ions
12 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-150 N: 2-2 O: 4-4 Na: 1-1 S: 1-1

XFF-B-2
12022601 47 (0.875) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x1.00); Cm (34:69)

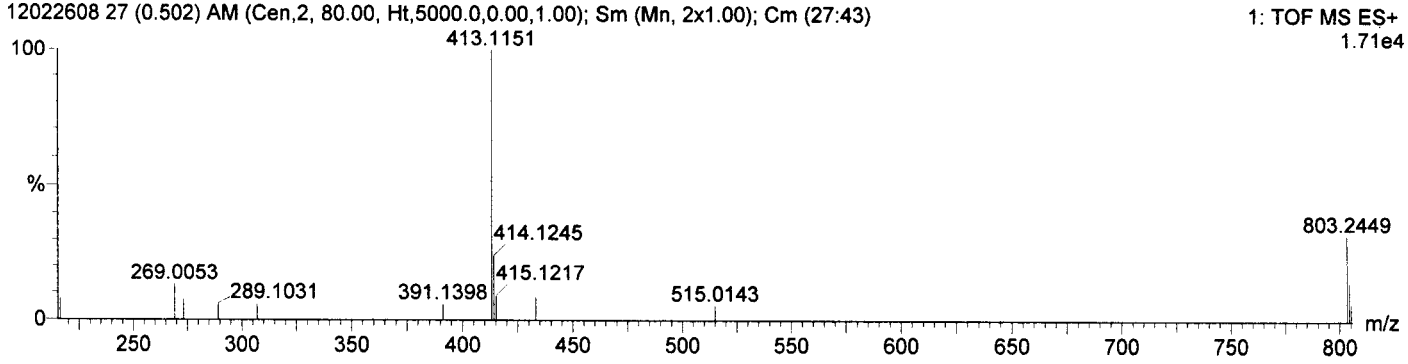


Minimum:				-200.0		
Maximum:		5.0	5.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
397.1192	397.1198	-0.6	-1.5	9.5	10.9	C19 H22 N2 O4 Na S

Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

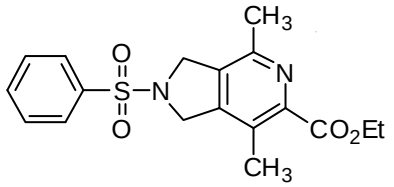


Monoisotopic Mass, Even Electron Ions
12 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-150 N: 2-2 O: 5-5 Na: 1-1 S: 1-1
XFF-B-9
12022608 27 (0.502) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x1.00); Cm (27:43)



Minimum:				-200.0		
Maximum:		5.0	5.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
413.1151	413.1147	0.4	1.0	9.5	10.2	C19 H22 N2 O5 Na S

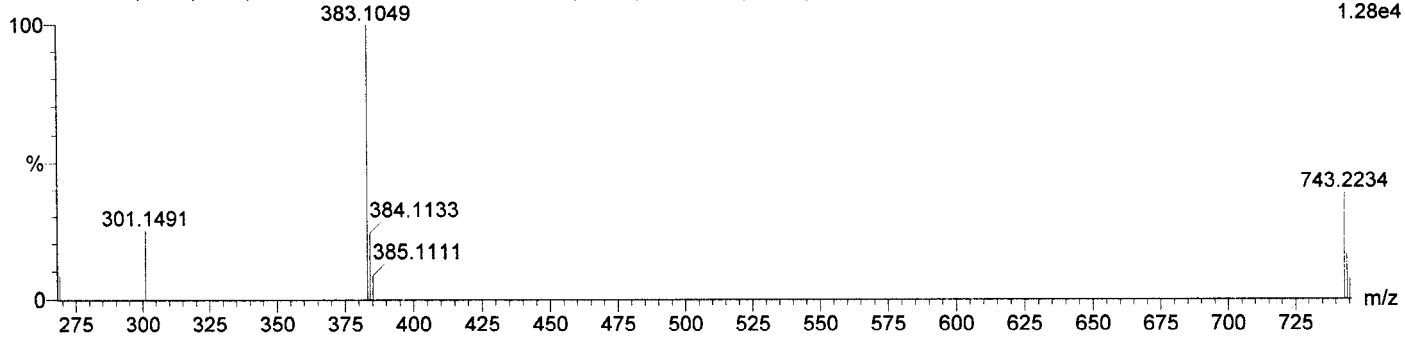
Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None



Monoisotopic Mass, Even Electron Ions
12 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-150 N: 2-2 O: 4-4 Na: 1-1 S: 1-1

XFF-B-4
12022603 12 (0.224) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x1.00); Cm (9:21)

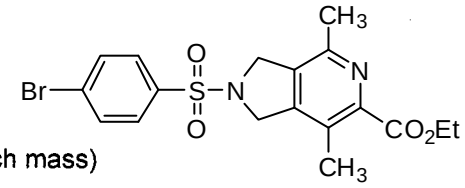
1: TOF MS ES+
1.28e4



Minimum:				-200.0		
Maximum:		5.0	5.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
383.1049	383.1041	0.8	2.1	9.5	12.8	C18 H20 N2 O4 Na S

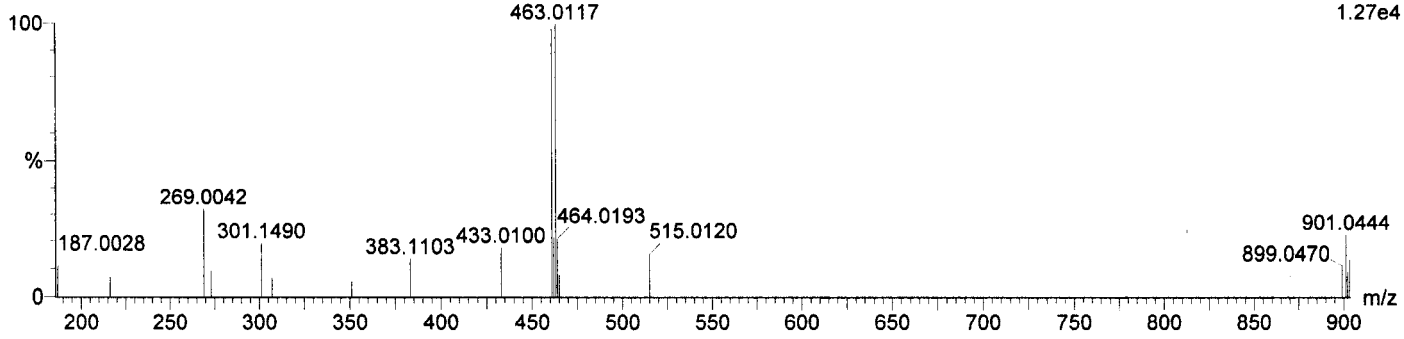
Single Mass Analysis (displaying only valid results)

Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None



Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-150 N: 2-2 O: 4-4 Na: 1-1 S: 1-1 Br: 1-1

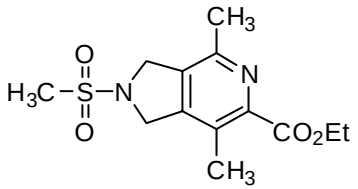
XFF-B-11
12022610 13 (0.243) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x1.00); Cm (5:19)
1: TOF MS ES+
1.27e4



Minimum:				-200.0		
Maximum:		5.0	5.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
461.0142	461.0147	-0.5	-1.1	9.5	3.4	C18 H19 N2 O4 Na S Br

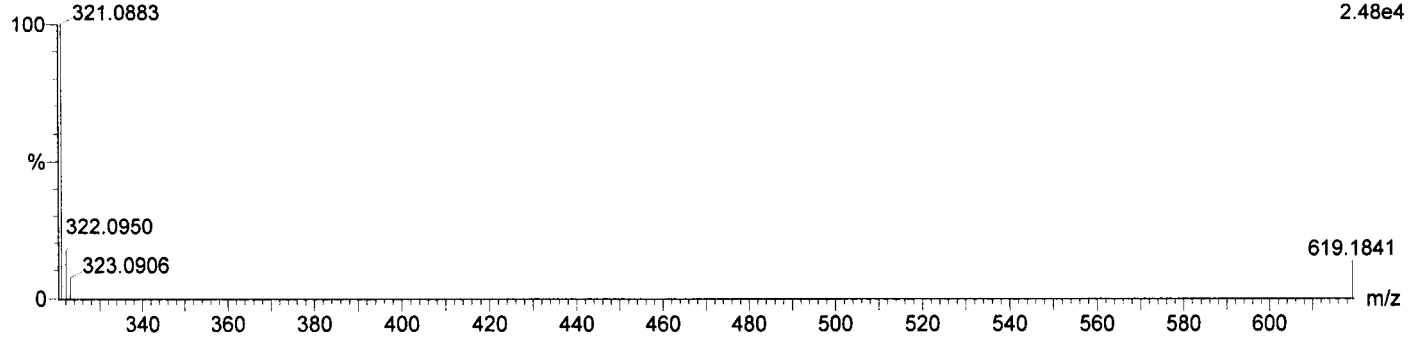
Single Mass Analysis (displaying only valid results)

Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None



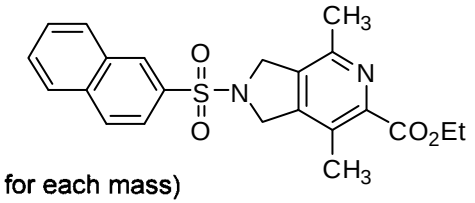
Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-150 N: 2-2 O: 4-4 Na: 1-1 S: 1-1

XFF-B-5
12022604 55 (1.024) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x1.00); Cm (23:59) 1: TOF MS ES+
2.48e4

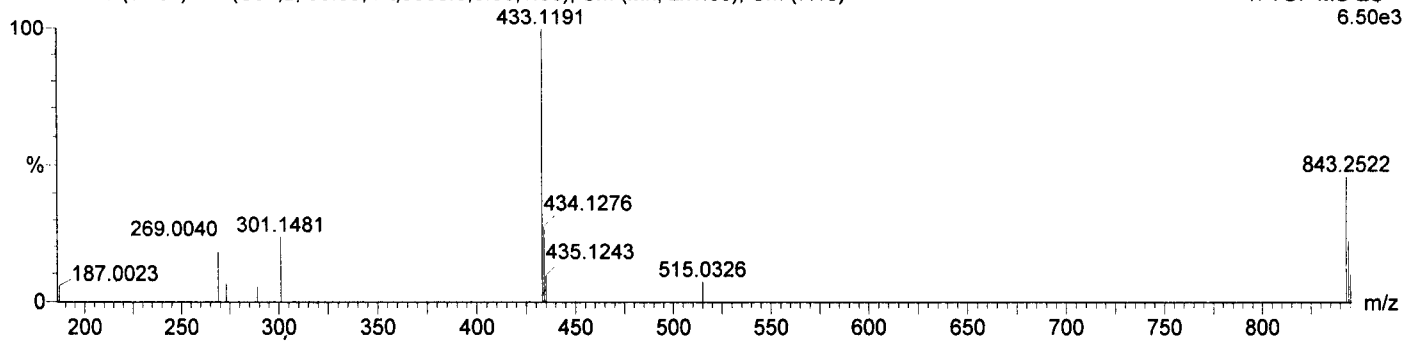


Minimum:				-200.0		
Maximum:		5.0	5.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
321.0883	321.0885	-0.2	-0.6	5.5	13.6	C13 H18 N2 O4 Na S

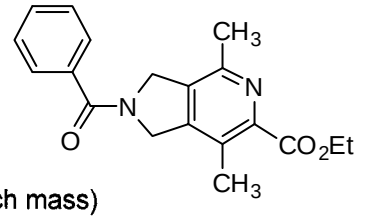
Single Mass Analysis (displaying only valid results)
Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None



Monoisotopic Mass, Even Electron Ions
12 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-150 N: 2-2 O: 4-4 Na: 1-1 S: 1-1
XFF-B-8
12022607 9 (0.167) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x1.00); Cm (7:15) 1: TOF MS ES+ 6.50e3



Minimum:				-200.0		
Maximum:		5.0	5.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
433.1191	433.1198	-0.7	-1.6	12.5	2.9	C22 H22 N2 O4 Na S

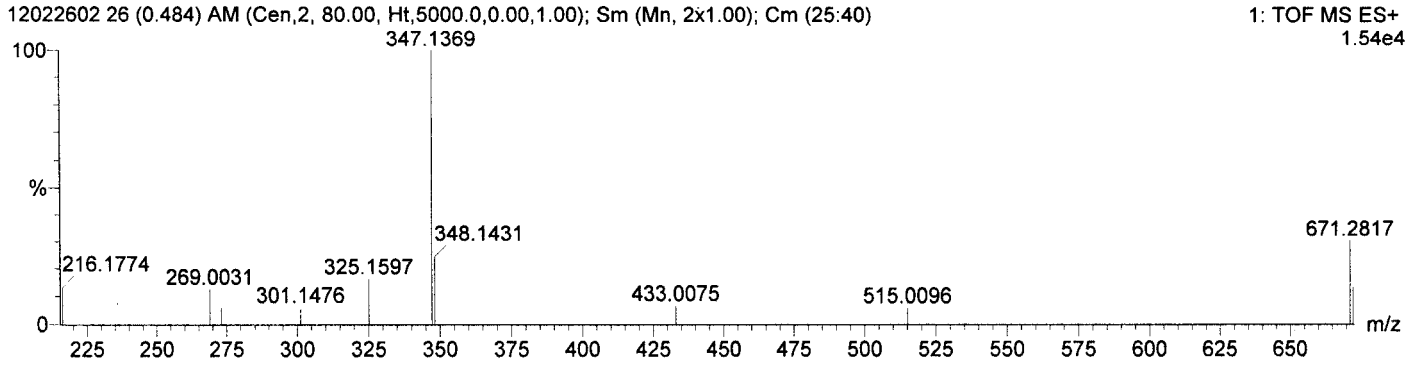


Single Mass Analysis (displaying only valid results)

Tolerance = 5.0 PPM / DBE: min = -200.0, max = 200.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
12 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-150 N: 2-2 O: 3-3 Na: 1-1

XFF-B-3
12022602 26 (0.484) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x1.00); Cm (25:40)



Minimum:				-200.0		
Maximum:		5.0	5.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
347.1369	347.1372	-0.3	-0.9	10.5	2781763.3	C19 H20 N2 O3 Na