Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Regio- and Stereo-Selective Synthesis of β-Phenylthio Enamides via Intramolecular 1,2-Thiol Migration

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1 General Information

All reagents used in the experiments were obtained from commercial sources and used without further purification. Thin layer chromatography (TLC) employed glass 0.25 mm silica gel plates. All NMR spectra were recorded on Bruker AVANCE 400 for ^{1}H and ^{13}C NMR in $CDCl_3$. The NMR chemical shift was reported in ppm relative to 7.26 / 77.23 ppm of $CDCl_3$ as the standards of ^{1}H and ^{13}C NMR, respectively. The HRMS of products were tested on electrospray ionization quadrupole time-of-flight (ESI-Q-TOF) mass spectrometer. IR was tested on Bruker ALPHA. Besides, melting point was tested on micro melting point apparatus.

2 Experimental details for Single crystals A (3d)

Pure **3d** was carefully dissolved in dichloromethane to form a saturated solution, then and *n*-hexane was slowly added dropwise, and the solvent was slowly evaporated at room temperature until the crystals were precipitated.

A suitable crystal was selected and detected on a Bruker D8 VENTURE diffractometer. The crystal was kept at 193.00 K during data collection. Using Olex2, the structure was solved with the SHELXT structure solution program using Intrinsic Phasing and refined with the SHELXL refinement package using Least Squares minimisation.

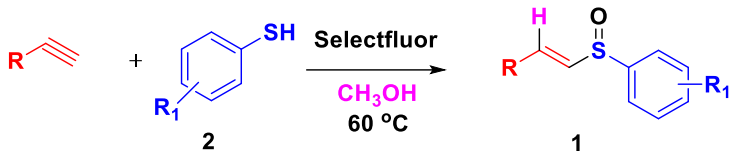
Table 1 Crystal data and structure refinement for A.

Identification code	A
Empirical formula	$C_{16}H_{13}Cl_2NOS$
Formula weight	338.23
Temperature/K	193.00
Crystal system	monoclinic
Space group	C2/c
a/Å	14.980(3)
b/Å	20.733(3)
c/Å	20.244(3)
α/°	90
β/°	98.28(5)
γ/°	90
Volume/Å^3	6222.0(19)
Z	16
ρ_{calc}g/cm^3	1.444
μ/mm^{-1}	0.548
F(000)	2784.0
Crystal size/mm^3	0.15 × 0.12 × 0.1
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.732 to 56.048
Index ranges	-19 ≤ h ≤ 18, -27 ≤ k ≤ 25, -23 ≤ l ≤ 26
Reflections collected	23013
Independent reflections	7235 [R_{int} = 0.1163, R_{sigma} = 0.1243]
Data/restraints/parameters	7235/0/381
Goodness-of-fit on F^2	1.030
Final R indexes [I>=2σ (I)]	R_1 = 0.0969, wR_2 = 0.2476
Final R indexes [all data]	R_1 = 0.1776, wR_2 = 0.3043
Largest diff. peak/hole / e Å^{-3}	0.67/-0.49

3 General procedure and characterization for vinyl sulfoxides 1

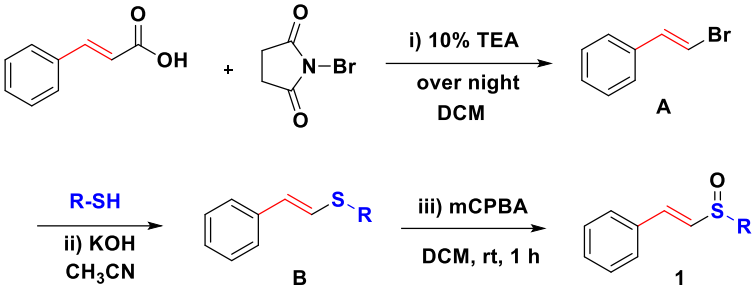
Unless noted otherwise, the vinyl sulfoxides **1** were synthesized and confirmed by **GP 1** according to our previous report.[1]

General Procedure 1 (GP 1):



The mixture of alkyne (0.5 mmol), Selectfluor (1.5 equiv), thiophenol **2** (0.8 mmol) and methanol (4 mL) was stirred at 60°C in heating mantle under air for 12 h. After completion of reaction (monitored by TLC), the mixture was washed with water and extracted with ethyl acetate then dried over Na_2SO_4. The organic layer was then evaporated under reduced pressure and the residue was separated by column chromatography on silica gel (200-300) with petroleum ether/ethyl acetate (5:1) to get the desired product **1**.

General Procedure 2 (GP 2):



i) According to the literature[2]: To a solution of cinnamic acid (1.48 g, 10.0 mmol) in methylene chloride triethylamine (0.10 mL, 0.5 mmol) was added at room temperature and stirred for five minutes. N-bromosuccinimide (2.13 g, 12.0 mmol) was added in one portion and stirred over night.The solvent was removed under reduced pressure. The crude was purified by flash column chromatography (silica gel, hexanes) to afford 0.97 g of colorless oil **A** in 58% yield.

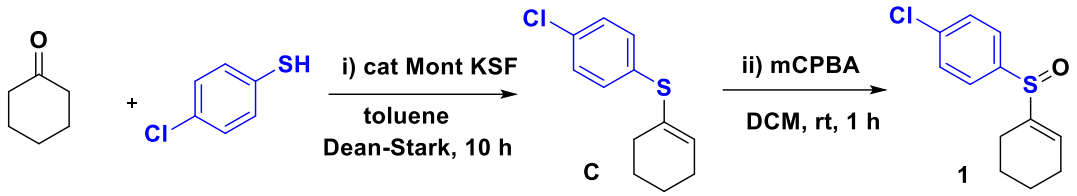
ii) According to the literature[3]: A 4 mL vial sealed equipped with a magnetic stirrer bar was charged with KOH (56.0 mg, 1.0 mmol) and vinyl bromide (0.6 mmol) in dioxane (0.25 mL). The aliphatic thiol (0.5 mmol) was added via syringe, and the vial was sealed with a cap containing a PTFE septum and the reaction vessel was heated at 110 °C in an oil bath. After stirring at this temperature for 12 h, the heterogeneous mixture was cooled to room temperature and diluted with ethyl acetate (20 mL). The resulting solution was directly filtered then washed with ethyl acetate (20 mL) and concentrated to give the crude material which was then purified by column chromatography (SiO2, hexane) to afford the vinyl thioether **B**.

Noting: **B** could smoothly undergo the next oxidation reaction by *m*-CPBA without column chromatography.

iii) According to our previous report[4]: *m*-CPBA (2.0 equiv) was slowly added to the vinyl thioether organic phase (DCM as the solvent) in a new reaction vessel and stirred at ambient temperature for 1 h. After completion of the reaction (monitored by TLC), the mixture was washed with water and extracted with ethyl

acetate and then dried over Na_2SO_4. The organic layer was then evaporated under reduced pressure, and the residue was separated by column chromatography on a silica gel (200-300) with petroleum ether/ethyl acetate (2:1 to 1:1) to get the desired product **1**.

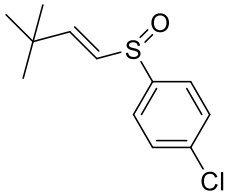
General Procedure 3 (GP 3):



i) According to the literature[5]: To a solution of cyclohexanone (1.11 g, 11.3 mmol) in toluene (20 mL) was added a slurry of montmorillonite KSF (1.0 g) in 5 mL of toluene. An additional 5 mL of toluene was used to wash any remaining montmorillonite KSF into the reaction flask. Thiophenol (1.18g, 10.7 mmol) was added, and the mixture was heated at reflux

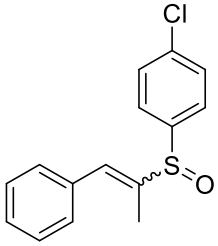
for 10 h with magnetic stirring. Water formed during the reaction was removed with a Dean-Stark trap. After being cooled to ambient temperature, the mixture was filtered to remove the montmorillonite KSF and the filter cake washed with hexanes. The solution was concentrated in vacuo to remove the toluene. The residue **C** was a pale yellow oil, which was used directly without further purification.

ii) According to our previous report[4]: *m*-CPBA (2.0 equiv) was slowly added to organic phase containing **C** (DCM as the solvent) in a new reaction vessel and stirred at ambient temperature for 1 h. After completion of the reaction (monitored by TLC), the mixture was washed with water and extracted with ethyl acetate and then dried over Na_2SO_4. The organic layer was then evaporated under reduced pressure, and the residue was separated by column chromatography on a silica gel (200-300) with petroleum ether/ethyl acetate (2:1 to 1:1) to get the desired product **1**.



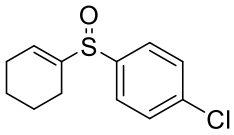
(E)-1-chloro-4-((3,3-dimethylbut-1-en-1-yl)sulfinyl)benzene

Eluent in chromatography: petroleum ether/ethyl acetate 5:1, **1i** was isolated as a yellow oily liquid by **GP1** (90.7 mg, 75%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.52 (d, *J* = 10.8 Hz, 2H), 7.47 (d, *J* = 8.0 Hz, 2H), 6.60 (d, *J* = 15.6 Hz, 1H), 6.09 (d, *J* = 15.2 Hz, 1H), 1.07 (s, 9H).



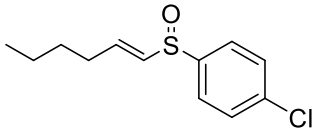
1-chloro-4-((1-phenylprop-1-en-2-yl)sulfinyl)benzene[6]

Eluent in chromatography: petroleum ether/ethyl acetate 5:1, **1u** was isolated as a colorless oily liquid by **GP1** (63.5 mg, 46%, *E*/*Z*=1.3); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.60-7.03 (m, 11H), 1.90 (s, 3H, *E*), 1.88 (s, 3H, *Z*).



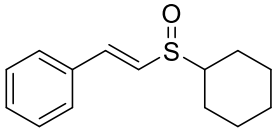
1-chloro-4-(cyclohex-1-en-1-ylsulfinyl)benzene[7]

Eluent in chromatography: petroleum ether/ethyl acetate 2:1, **1v** was isolated as a yellow solid by **GP3**;^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.52 (d, *J* = 8.8 Hz, 2H), 7.46 (d, *J* = 8.8 Hz, 2H), 6.71 (t, *J* = 3.6 Hz, 1H), 2.26-2.17 (m, 3H), 1.65-1.46 (m, 5H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 143.8, 141.5, 136.9, 135.3, 129.5, 126.3, 26.0, 22.2, 21.9, 19.4; IR (KBr): ν_{max} 3073, 2918, 1572, 1471, 1241, 1080, 823, 739, 556.



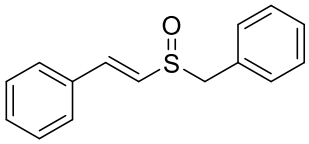
(E)-1-chloro-4-(hex-1-en-1-ylsulfinyl)benzene[8]

Eluent in chromatography: petroleum ether/ethyl acetate 2:1, **1w** was isolated as a yellow oily liquid (Noting: mixed with 1-chloro-4-(hex-1-en-2-ylsulfinyl)benzene **1w'**, the ratio of **1w/1w'** = 6.9:1) by **GP2**; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.54 (d, *J* = 8.8 Hz, 2H), 7.47 (d, *J* = 8.8 Hz, 2H), 6.66-6.58 (m, 1H), 6.20 (d, *J* = 15.2 Hz, 1H), 2.25-2.19 (m, 2H), 1.47-1.29 (m, 4H), 0.89 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 143.1, 142.4, 137.2, 135.0, 129.7, 126.1, 32.0, 30.3, 22.3, 14.0; IR (KBr): ν_{max} 2957, 2911, 1474, 1050, 823, 741.



(E)-(2-(cyclohexylsulfinyl)vinyl)benzene[9]

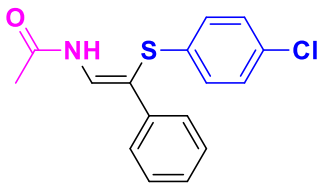
Eluent in chromatography: petroleum ether/ethyl acetate 2:1, **1x** was isolated as a pale yellow solid by **GP2**; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.49-7.47 (m, 2H), 7.39-7.34 (m, 3H), 7.22 (d, *J* = 15.6 Hz, 1H), 6.82 (d, *J* = 15.6 Hz, 1H), 2.74-2.66 (m, 1H), 2.09-1.86 (m, 4H), 1.71-1.68 (m, 1H), 1.52-1.22 (m, 5H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 138.2, 134.1, 129.8, 129.1, 128.5, 127.8, 61.2, 26.3, 25.7, 25.5, 24.9; IR (KBr): ν_{max} 2930, 2854, 1711, 1446, 1044, 744.



(E)-(2-(benzylsulfinyl)vinyl)benzene[10]

Eluent in chromatography: petroleum ether/ethyl acetate 2:1, **1y** was isolated as a yellow solid by **GP2**; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.38-7.28 (m, 10H), 7.12 (d, *J* = 15.6 Hz, 1H), 6.76 (d, *J* = 15.6 Hz, 1H), 4.16-4.04 (m, 2H); IR (KBr): ν_{max} 2962, 2914, 1704, 1038, 961, 698.

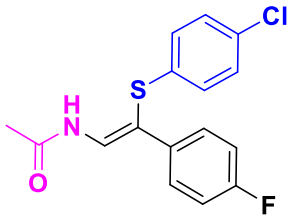
4 Characterization of products



(*Z*)-N-(2-((4-chlorophenyl)thio)-2-phenylvinyl)acetamide (3a)

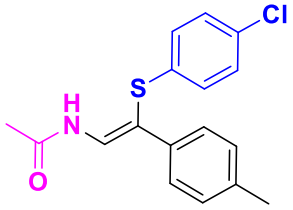
Eluent in chromatography: petroleum ether/ethyl acetate 5:1, **3a** was isolated as a pale yellow oily liquid (47.9

mg, 79%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.17 (br.d, *J* = 11.2 Hz, 1H), 7.95 (d, *J* = 11.6 Hz, 1H), 7.57 (d, *J* = 8.0 Hz, 2H) 7.30-7.20 (m, 3H), 7.17 (d, *J* = 8.0 Hz, 2H), 7.09 (d, *J* = 8.0 Hz, 2H), 2.15 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.8, 137.4, 133.2, 132.0, 130.1, 129.5, 128.8, 128.2, 127.8, 126.5, 111.6, 23.8; IR (KBr): ν_{max} 3061, 2924, 1676, 1620, 1468, 1241, 1092, 1011, 904, 814, 761, 694, 574, 485; HRMS(ESI, *m/z*) calcd. for $C_{16}H_{15}ClNOS^+$ $[M+H]^+$ 304.0557, found 304.0561.



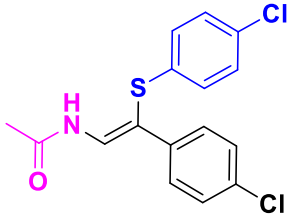
(*Z*)-N-(2-((4-chlorophenyl)thio)-2-(4-fluorophenyl)vinyl)acetamide (3b)

Eluent in chromatography: petroleum ether/ethyl acetate 5:1, **3b** was isolated as a yellow solid (m.p. 125-126ºC) (45.6 mg, 71%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.13 (br.d, *J* = 10.8 Hz, 1H), 7.85 (d, *J* = 10.8 Hz, 1H), 7.53-7.50 (m, 2H), 7.18 (d, *J* = 8.0 Hz, 2H), 7.07 (d, *J* = 8.0 Hz, 2H), 6.96 (t, *J* = 10.8 Hz, 2H), 2.15 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.8, 162.5 (d, *J* = 246 Hz), 133.5 (d, *J* = 3.1 Hz), 132.8, 132.2, 129.8, 129.5, 128.4, 128.2 (d, *J* = 8.0 Hz), 115.8 (d, *J* = 21.6 Hz), 110.9, 23.8; ^{19}F NMR (Chloroform-*d*) δ -114.4; IR (KBr): ν_{max} 3160, 1710, 1623, 1401, 1272, 1222, 1161, 1090, 1008, 821, 640; HRMS(ESI, *m/z*) calcd. for $C_{16}H_{13}ClFNNaOS^+$ $[M+Na]^+$ 344.0283, found 344.0286.



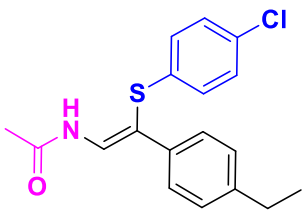
(*Z*)-N-(2-((4-chlorophenyl)thio)-2-(p-tolyl)vinyl)acetamide (3c)

Eluent in chromatography: petroleum ether/ethyl acetate 5:1, **3c** was isolated as a white solid (m.p. 112-113ºC) (40.6 mg, 64%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.14 (br.d, *J* = 11.2 Hz, 1H), 7.90 (d, *J* = 11.2 Hz, 1H), 7.46 (d, *J* = 7.2 Hz, 2H), 7.07-7.07 (m, 6H), 2.30 (s, 3H), 2.14 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.7, 137.7, 134.4, 133.4, 131.9, 129.5, 129.4, 129.3, 128.2, 126.4, 111.7, 23.8, 21.3; IR (KBr): ν_{max} 3144, 1711, 1631, 1476, 1452, 1399, 1298, 1211, 1091, 647; HRMS(ESI, *m/z*) calcd. for $C_{17}H_{16}ClNNaOS^+$ $[M+Na]^+$ 340.0533, found 340.0542.



(*Z*)-N-(2-(4-chlorophenyl)-2-((4-chlorophenyl)thio)vinyl)acetamide (3d)

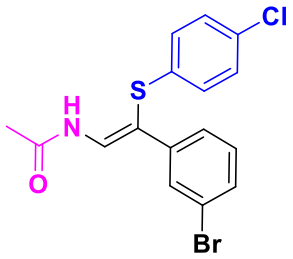
Eluent in chromatography: petroleum ether/ethyl acetate 5:1, **3d** was isolated as a pale yellow solid (m.p. 132-133ºC) (38.4 mg, 57%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.16 (br.d, *J* = 10.0 Hz, 1H), 7.92 (d, *J* = 10.0 Hz, 1H), 7.50 (d, *J* = 6.4 Hz, 2H), 7.26-7.18 (m, 4H), 7.07 (d, *J* = 6.4 Hz, 2H), 2.16 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.8, 135.9, 133.5, 132.8, 132.3, 130.3, 129.6, 129.0, 128.4, 127.7, 110.7, 23.8; IR (KBr): ν_{max} 3161, 1681, 1624, 1472, 1400, 1293, 1229, 1091, 729; HRMS(ESI, *m/z*) calcd. for $C_{16}H_{13}Cl_2NNaOS^+$ $[M+Na]^+$ 359.9987, found 359.9994.



(*Z*)-N-(2-((4-chlorophenyl)thio)-2-(4-ethylphenyl)vinyl)acetamide (3e)

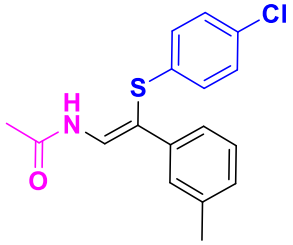
Eluent in chromatography: petroleum ether/ethyl acetate 5:1, **3e** was isolated a yellow oily liquid (31.1 mg, 47%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.13 (br.d, *J* = 10.8 Hz, 1H), 7.92 (d, *J* = 10.8 Hz, 1H), 7.48 (d, *J* = 8.0 Hz, 2H), 7.18-7.08 (m, 6H), 2.60 (q, *J* = 7.2 Hz, 2H), 2.14 (s, 3H), 1.20 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR

(100 MHz, Chloroform-*d*) δ 167.7, 144.0, 134.7, 133.4, 131.9, 129.5, 129.4, 128.4, 128.1, 126.4, 111.6, 28.6, 23.8, 15.6; IR (KBr): ν_{max} 3149, 1630, 1400, 1090, 656, 577; HRMS(ESI, *m/z*) calcd. for $C_{18}H_{18}ClNNaOS^+$ $[M+Na]^+$ 354.0690, found 354.0693.



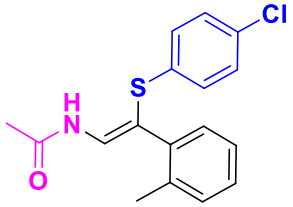
(*Z*)-N-(2-(3-bromophenyl)-2-((4-chlorophenyl)thio)vinyl)acetamide (3f)

Eluent in chromatography: petroleum ether/ethyl acetate 5:1, **3f** was isolated as a pale yellow solid (m.p. 82-83°C) (46.5 mg, 61%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.16 (br.d, *J* = 10.8 Hz, 1H), 7.93 (d, *J* = 10.8 Hz, 1H), 7.72 (s, 1H), 7.49 (d, *J* = 7.6 Hz, 1H), 7.33 (d, *J* = 7.6 Hz, 1H), 7.20-7.06 (m, 5H), 2.16 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.8, 139.7, 132.7, 132.3, 131.0, 130.7, 130.3, 129.6, 129.3, 128.3, 125.1, 123.1, 110.3, 23.8; IR (KBr): ν_{max} 3120, 2050, 1630, 1475, 1401, 1244, 1093, 597; HRMS(ESI, *m/z*) calcd. for $C_{16}H_{13}BrClNNaOS^+$ $[M+Na]^+$ 403.9482, found 403.9488.



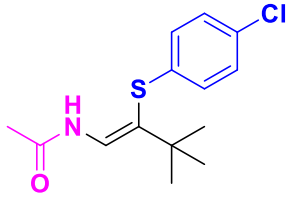
(*Z*)-N-(2-((4-chlorophenyl)thio)-2-(m-tolyl)vinyl)acetamide (3g)

Eluent in chromatography: petroleum ether/ethyl acetate 5:1, **3g** was isolated as a pale yellow solid (m.p. 56-57°C) (43.8 mg, 69%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.15 (br.d, *J* = 10.8 Hz, 1H), 7.93 (d, *J* = 10.8 Hz, 1H), 7.39-7.36 (m, 2H), 7.18-7.16 (m, 3H), 7.10-7.03 (m, 3H), 2.32 (s, 3H), 2.14 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.8, 138.5, 137.3, 133.4, 131.9, 129.9, 129.5, 128.7, 128.6, 128.1, 127.0, 123.8, 111.7, 23.8, 21.7; IR (KBr): ν_{max} 3141, 1626, 1624, 1473, 1402, 1238, 1187, 1091, 699; HRMS(ESI, *m/z*) calcd. for $C_{17}H_{16}ClNNaOS^+$ $[M+Na]^+$ 340.0533, found 340.0540.



(*Z*)-N-(2-((4-chlorophenyl)thio)-2-(o-tolyl)vinyl)acetamide (3h)

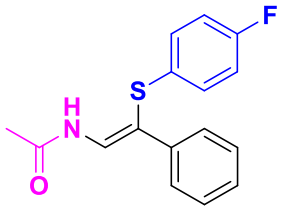
Eluent in chromatography: petroleum ether/ethyl acetate 5:1, **3h** was isolated as a yellow solid (m.p. 78-79°C) (15.8 mg, 25%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.06 (br.d, *J* = 10.8 Hz, 1H), 7.42 (d, *J* = 10.8 Hz, 1H), 7.20-7.00 (m, 8H), 2.35 (s, 3H), 2.15 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.7, 137.5, 136.8, 132.9, 132.3, 131.0, 130.8, 130.5, 130.5, 129.3, 128.1, 125.8, 112.3, 23.8, 20.7; IR (KBr): ν_{max} 3151, 2065, 1630, 1474, 1400, 1183, 1090, 1008, 606; HRMS(ESI, *m/z*) calcd. for $C_{17}H_{16}ClNNaOS^+$ $[M+Na]^+$ 340.0533, found 340.0538.



(*Z*)-N-(2-((4-chlorophenyl)thio)-3,3-dimethylbut-1-en-1-yl)acetamide (3i)

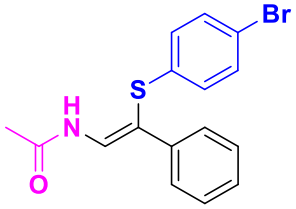
Eluent in chromatography: petroleum ether/ethyl acetate 5:1, **3i** was isolated as a colorless oily liquid (14.2 mg, 25%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.79 (br.d, *J* = 10.0 Hz, 1H), 7.53 (d, *J* = 10.8 Hz, 1H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.06 (d, *J* = 8.0 Hz, 2H), 2.00 (s, 3H), 1.15 (s, 9H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.9, 134.3, 131.3, 129.4, 128.2, 127.2, 121.5, 38.0, 29.6, 23.7; IR (KBr): ν_{max} 2970, 2056, 1632, 1474,

1400, 1296, 1239, 1172, 1092, 1011, 814, 592; HRMS(ESI, *m/z*) calcd. for $C_{14}H_{18}ClNNaOS^+$ $[M+Na]^+$ 306.0690, found 306.0694.



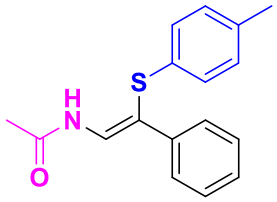
(*Z*)-N-(2-((4-fluorophenyl)thio)-2-phenylvinyl)acetamide (3j)

Eluent in chromatography: petroleum ether/ethyl acetate 5:1, **3j** was isolated as a pale brown solid (m.p. 125-126ºC) (36.7 mg, 64%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.13 (br.d, *J* = 10.8 Hz, 1H), 7.83 (d, *J* = 10.8 Hz, 1H), 7.49 (d, *J* = 8.0 Hz, 2H), 7.22-7.05 (m, 5H), 6.83 (t, *J* = 8.0 Hz, 2H), 2.07 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.8, 161.6 (d, *J* = 244 Hz), 137.5, 129.6, 129.5, 129.2 (d, *J* = 7.9 Hz), 128.8, 127.7, 126.6, 116.5 (d, *J* = 22.1 Hz), 112.6, 23.8; ^{19}F NMR (Chloroform-*d*) δ -116.1; IR (KBr): ν_{max} 3154, 2055, 1630, 1488, 1401, 1244, 1085, 755, 628; HRMS(ESI, *m/z*) calcd. for $C_{16}H_{14}FNNaOS^+$ $[M+Na]^+$ 310.0672, found 310.0679.



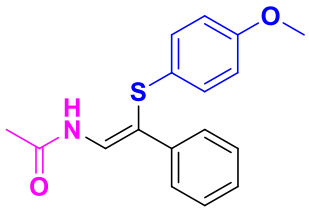
(*Z*)-N-(2-((4-bromophenyl)thio)-2-phenylvinyl)acetamide (3k)

Eluent in chromatography: petroleum ether/ethyl acetate 5:1, **3k** was isolated as a brown solid (m.p. 135-136ºC) (40.9 mg, 59%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.16 (br.d, *J* = 11.2 Hz, 1H), 7.95 (d, *J* = 11.2 Hz, 1H), 7.57 (d, *J* = 8.0 Hz, 2H), 7.32-7.20 (m, 5H), 7.03 (d, *J* = 8.0 Hz, 2H), 2.14 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.8, 137.3, 133.9, 132.4, 130.1, 128.8, 128.5, 127.8, 126.5, 119.8, 111.5, 23.8; IR (KBr): ν_{max} 3182, 2066, 1629, 1469, 1401, 1082, 1052, 586; HRMS(ESI, *m/z*) calcd. for $C_{16}H_{14}BrNNaOS^+$ $[M+Na]^+$ 369.9872, found 369.9875.



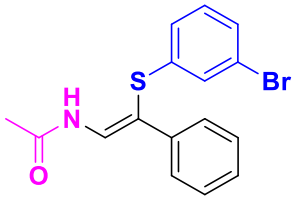
(*Z*)-N-(2-phenyl-2-(p-tolylthio)vinyl)acetamide (3l)

Eluent in chromatography: petroleum ether/ethyl acetate 5:1, **3l** was isolated as a yellow solid (m.p. 103-104ºC) (39.6 mg, 70%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.23 (br.d, *J* = 10.8 Hz, 1H), 7.92 (d, *J* = 10.8 Hz, 1H), 7.60 (d, *J* = 8.0 Hz, 2H), 7.29-7.18 (m, 3H), 7.08 (d, *J* = 8.0 Hz, 2H), 7.02 (d, *J* = 8.0 Hz, 2H), 6.78 (d, *J* = 8.0 Hz, 1H), 2.26 (s, 3H), 2.13 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.8, 137.9, 136.1, 131.0, 130.1, 129.5, 128.7, 127.5, 127.2, 126.6, 112.6, 23.8, 21.1; IR (KBr): ν_{max} 3154, 2059, 1620, 1417, 1400, 1244, 1088, 769, 761, 600; HRMS(ESI, *m/z*) calcd. for $C_{17}H_{17}NNaOS^+$ $[M+Na]^+$ 306.0923, found 306.0931.



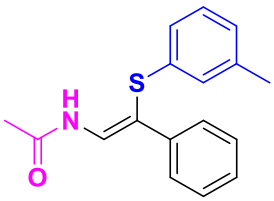
(*Z*)-N-(2-((4-methoxyphenyl)thio)-2-phenylvinyl)acetamide (3m)

Eluent in chromatography: petroleum ether/ethyl acetate 5:1, **3m** was isolated as a yellow oily liquid (22.7 mg, 38%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.25 (br.d, *J* = 10.8 Hz, 1H), 7.84 (d, *J* = 10.8 Hz, 1H), 7.57 (d, *J* = 8.0 Hz, 2H), 7.28-7.17 (m, 3H), 7.12 (d, *J* = 8.0 Hz, 2H), 6.75 (d, *J* = 8.0 Hz, 2H), 3.73 (s, 3H), 2.14 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.8, 158.6, 137.8, 129.6, 128.7, 128.6, 127.5, 126.8, 124.9, 115.1, 113.9, 55.5, 23.8; IR (KBr): ν_{max} 3053, 2042, 1631, 1402, 1247, 1226, 1085, 590; HRMS(ESI, *m/z*) calcd. for $C_{17}H_{17}NNaO_2S^+$ $[M+Na]^+$ 322.0872, found 322.0884.



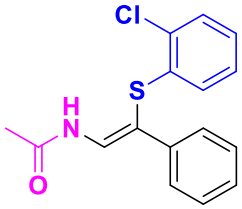
(*Z*)-N-(2-((3-bromophenyl)thio)-2-phenylvinyl)acetamide (3o)

Eluent in chromatography: petroleum ether/ethyl acetate 5:1, **3o** was isolated as a brown solid (m.p. 127-128ºC) (52.1 mg, 75%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.09 (br.d, *J* = 11.2 Hz, 1H), 7.90 (d, *J* = 11.2 Hz, 1H), 7.50 (d, *J* = 8.0 Hz, 2H), 7.24-7.15 (m, 5H), 7.02-6.97 (m, 2H), 2.07 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.9, 137.4, 137.2, 130.7, 130.5, 129.3, 129.1, 128.9, 127.8, 126.5, 125.2, 123.3, 111.0, 23.8; IR (KBr): ν_{max} 3155, 1629, 1455, 1400, 1233, 1081, 761, 691; HRMS(ESI, *m/z*) calcd. for $C_{16}H_{14}BrNNaOS^{+}$ $[M+Na]^{+}$ 369.9872, found 369.9872.



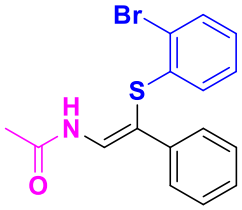
(*Z*)-N-(2-phenyl-2-(m-tolylthio)vinyl)acetamide (3p)

Eluent in chromatography: petroleum ether/ethyl acetate 5:1, **3p** was isolated as a yellow solid (m.p. 85-86ºC) (38.5 mg, 68%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.21 (br.d, *J* = 10.8 Hz, 1H), 7.96 (d, *J* = 10.8 Hz, 1H), 7.60 (d, *J* = 8.0 Hz, 2H), 7.30-7.19 (m, 3H), 7.10 (t, *J* = 8.0 Hz, 2H), 7.00-6.91 (m, 3H), 2.26 (s, 3H), 2.13 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.8, 139.2, 137.9, 134.5, 129.8, 129.2, 128.7, 127.6, 127.4, 127.0, 126.5, 123.8, 112.0, 23.8, 21.6; IR (KBr): ν_{max} 3160, 1620, 1466, 1401, 1230, 1079, 757, 687; HRMS(ESI, *m/z*) calcd. for $C_{17}H_{17}NNaOS^{+}$ $[M+Na]^{+}$ 306.0923, found 306.0930.



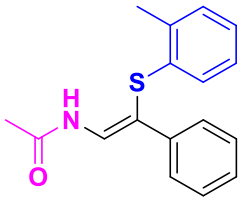
(*Z*)-N-(2-((2-chlorophenyl)thio)-2-phenylvinyl)acetamide (3q)

Eluent in chromatography: petroleum ether/ethyl acetate 5:1, **3q** was isolated as a yellow solid (m.p. 142-143ºC) (37.0 mg, 61%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.18 (br.d, *J* = 10.8 Hz, 1H), 8.03 (d, *J* = 10.8 Hz, 1H), 7.61 (d, *J* = 8.0 Hz, 2H), 7.36-7.21 (m, 4H), 7.06-6.98 (m, 3H), 2.14 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.9, 137.4, 134.0, 132.0, 130.9, 129.9, 128.9, 127.8, 127.6, 127.3, 126.9, 126.4, 110.5, 23.8; IR (KBr): ν_{max} 3155, 2043, 1625, 1400, 1241, 1096, 999, 600; HRMS(ESI, *m/z*) calcd. for $C_{16}H_{14}ClNNaOS^{+}$ $[M+Na]^{+}$ 326.0377, found 326.0386.



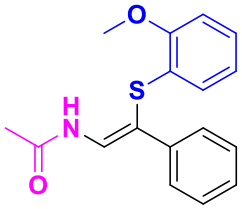
(*Z*)-N-(2-((2-bromophenyl)thio)-2-phenylvinyl)acetamide (3r)

Eluent in chromatography: petroleum ether/ethyl acetate 5:1, **3r** was isolated as a brown solid (m.p. 124-125ºC) (52.0 mg, 75%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.11 (br.d, *J* = 10.8 Hz, 1H), 7.97 (d, *J* = 10.8 Hz, 1H), 7.53 (d, *J* = 8.0 Hz, 2H), 7.44 (d, *J* = 8.0 Hz, 1H), 7.23-7.15 (m, 3H), 7.02 (t, *J* = 8.0 Hz, 1H), 6.89 (t, *J* = 8.0 Hz, 2H), 2.06 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.9, 137.3, 136.0, 133.2, 130.8, 128.9, 128.2, 127.8, 127.2, 127.0, 126.3, 121.6, 111.1, 23.8; IR (KBr): ν_{max} 3119, 2060, 1639, 1401, 1103, 597; HRMS(ESI, *m/z*) calcd. for $C_{16}H_{14}BrNNaOS^{+}$ $[M+Na]^{+}$ 369.9872, found 369.9879.



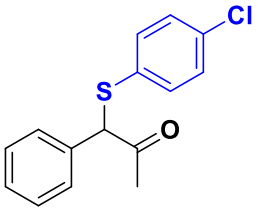
(*Z*)-N-(2-phenyl-2-(o-tolylthio)vinyl)acetamide (3s)

Eluent in chromatography: petroleum ether/ethyl acetate 5:1, **3s** was isolated as a yellow solid (m.p. 85-86ºC) (36.2 mg, 64%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.17 (br.d, *J* = 10.8 Hz, 1H), 8.00 (d, *J* = 10.8 Hz, 1H), 7.59 (d, *J* = 8.0 Hz, 2H), 7.30-7.19 (m, 3H), 7.15 (d, *J* = 8.0 Hz, 1H), 7.05-6.95 (m, 3H), 2.45 (s, 3H), 2.13 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.8, 137.8, 135.7, 133.7, 130.5, 130.1, 128.7, 127.6, 126.9, 126.5, 125.9, 125.8, 111.5, 23.8, 20.3; IR (KBr): ν_{max} 3122, 2042, 1629, 1400, 1087, 601; HRMS(ESI, *m/z*) calcd. for $C_{17}H_{17}NNaOS^{+}$ $[M+Na]^{+}$ 306.0923, found 306.0931.



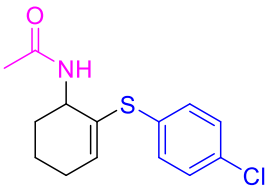
(*Z*)-N-(2-((2-methoxyphenyl)thio)-2-phenylvinyl)acetamide (3t)

Eluent in chromatography: petroleum ether/ethyl acetate 5:1, **3t** was isolated as a yellow solid (m.p. 105-106ºC) (31.1 mg, 52%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.28 (br.d, *J* = 10.8 Hz, 1H), 7.97 (d, *J* = 10.8 Hz, 1H), 7.62 (d, *J* = 8.0 Hz, 2H), 7.30-7.19 (m, 3H), 7.12 (t, *J* = 8.0 Hz, 1H), 6.96 (d, *J* = 8.0 Hz, 1H), 6.86 (d, *J* = 8.0 Hz, 1H), 6.78 (d, *J* = 8.0 Hz, 1H), 3.94 (s, 3H), 2.11 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.8, 156.4, 138.0, 130.3, 128.7, 127.6, 127.5, 127.1, 126.5, 123.0, 121.7, 111.1, 110.7, 56.1, 23.8; IR (KBr): ν_{max} 3034, 2035, 1629, 1400, 1240, 1193, 1076, 602; HRMS(ESI, *m/z*) calcd. for $C_{17}H_{17}NNaO_2S^{+}$ $[M+Na]^{+}$ 322.0872, found 322.0881.



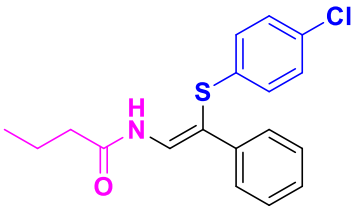
1-((4-chlorophenyl)thio)-1-phenylpropan-2-one (3u')[11]

Eluent in chromatography: petroleum ether/ethyl acetate 10:1, **3u'** was isolated as a yellow oily liquid (19.3 mg, 35%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.28 (br.d, *J* = 10.8 Hz, 1H), 7.97 (d, *J* = 10.8 Hz, 1H), 7.62 (d, *J* = 8.0 Hz, 2H), 7.32-7.19 (m, 9H), 4.94 (s, 1H), 2.18 (s, 3H). The analytic data is in accordance with literature.



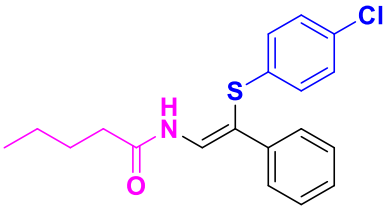
N-(2-((4-chlorophenyl)thio)cyclohex-2-en-1-yl)acetamide (3v)

Eluent in chromatography: petroleum ether/ethyl acetate 2:1, **3v** was isolated as a yellow oily liquid (39.9 mg, 71%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.26-7.24 (m, 4H), 6.22 (t, *J* = 3.6 Hz, 1H), 5.58 (br.d, *J* = 80 Hz, 1H), 4.42-4.38 (m, 1H), 2.19-2.15 (m, 2H),1.90 (s, 3H), 1.83-1.72 (m, 2H), 1.70-1.65 (m, 1H), 1.59-1.49 (m, 1H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 169.5, 137.6, 133.5, 132.8, 132.6, 132.4, 129.5, 47.0, 30.3, 27.0, 23.5, 18.0; IR (KBr): ν_{max} 3258, 1901, 1641, 1548, 1474, 1092, 1012, 818, 495.



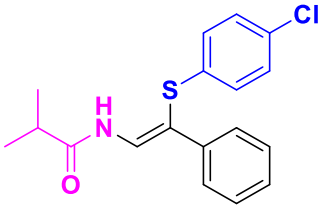
(*Z*)-N-(2-((4-chlorophenyl)thio)-2-phenylvinyl)butyramide (4a)

Eluent in chromatography: petroleum ether/ethyl acetate 5:1, **4a** was isolated as a pale yellow solid (m.p. 66-67°C) (47.0 mg, 71%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.13 (br.d, *J* = 10.8 Hz, 1H), 7.96 (d, *J* = 10.8 Hz, 1H), 7.57 (d, *J* = 8.0 Hz, 2H), 7.30-7.21 (m, 3H), 7.17 (d, *J* = 8.0 Hz, 2H), 7.09 (d, *J* = 8.0 Hz, 2H), 2.31 (t, *J* = 7.2 Hz, 2H), 1.72-1.67 (m, 2H), 0.96 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.7, 137.5, 133.3, 132.0, 130.0, 129.5, 128.8, 128.2, 127.7, 126.5, 111.5, 38.8, 18.9, 13.9; IR (KBr): ν_{max} 3155, 2054, 1621, 1474, 1401, 1204, 1093, 1011, 805, 759, 695; HRMS(ESI, *m/z*) calcd. for $C_{18}H_{18}ClNNaOS^+$ $[M+Na]^+$ 354.0690, found 354.0698.



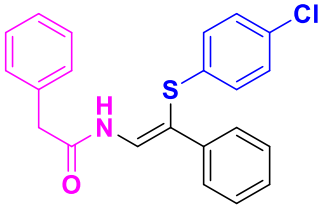
(*Z*)-N-(2-((4-chlorophenyl)thio)-2-phenylvinyl)pentanamide (4b)

Eluent in chromatography: petroleum ether/ethyl acetate 5:1, **4b** was isolated as a pale yellow solid (m.p. 80-81°C) (32.5 mg, 47%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.12 (br.d, *J* = 10.8 Hz, 1H), 7.95 (d, *J* = 10.8 Hz, 1H), 7.57 (d, *J* = 8.0 Hz, 2H), 7.30-7.21 (m, 3H), 7.17 (d, *J* = 8.0 Hz, 2H), 7.09 (d, *J* = 8.0 Hz, 2H), 2.32 (t, *J* = 7.2 Hz, 2H), 1.67-1.60 (m, 2H), 1.39-1.32 (m, 2H), 0.91 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 170.9, 137.5, 133.3, 132.0, 130.0, 129.5, 128.8, 128.2, 127.7, 126.5, 111.5, 36.7, 27.5, 22.5, 14.0; IR (KBr): ν_{max} 3191, 2055, 1633, 1470, 1401, 1195, 1091, 594; HRMS(ESI, *m/z*) calcd. for $C_{19}H_{20}ClNNaOS^+$ $[M+Na]^+$ 368.0846, found 368.0850.



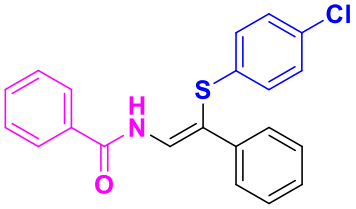
(*Z*)-N-(2-((4-chlorophenyl)thio)-2-phenylvinyl)isobutyramide (4c)

Eluent in chromatography: petroleum ether/ethyl acetate 5:1, **4c** was isolated as a pale yellow solid (m.p. 73-74°C) (25.8 mg, 39%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.17 (br.d, *J* = 10.8 Hz, 1H), 7.94 (d, *J* = 10.8 Hz, 1H), 7.57 (d, *J* = 8.0 Hz, 2H), 7.30-7.21 (m, 3H), 7.17 (d, *J* = 8.0 Hz, 2H), 7.10 (d, *J* = 8.0 Hz, 2H), 2.53-2.43 (m,1H), 1.20-1.18 (d, *J* = 8.0 Hz, 6H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 174.6, 137.6, 133.3, 132.0, 130.1, 129.5, 128.8, 128.3, 127.7, 126.5, 111.8, 36.0, 19.5; IR (KBr): ν_{max} 3096, 2077, 1632, 1401, 1200, 1090, 688, 589; HRMS(ESI, *m/z*) calcd. for $C_{18}H_{18}ClNNaOS^+$ $[M+Na]^+$ 354.0690, found 354.0697.



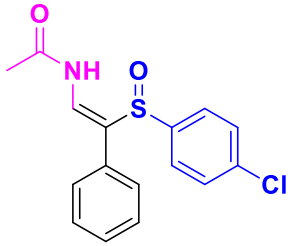
(*Z*)-N-(2-((4-chlorophenyl)thio)-2-phenylvinyl)-2-phenylacetamide (4d)

Eluent in chromatography: petroleum ether/ethyl acetate 5:1, **4d** was isolated as a pale yellow oily liquid (15.9 mg, 21%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.10 (br.d, *J* = 10.8 Hz, 1H), 7.88 (d, *J* = 11.2 Hz, 1H), 7.53 (d, *J* = 8.0 Hz, 2H), 7.36-7.09 (m, 10H), 6.92 (d, *J* = 8.0 Hz, 2H), 3.68 (s, 2H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 168.6, 137.6, 133.5, 133.1, 131.9, 129.6, 129.5, 129.4, 129.3, 128.8, 128.2, 128.0, 127.8, 126.5, 112.8, 44.0; IR (KBr): ν_{max} 3075, 2056, 1625, 1460, 1401, 1091, 1049, 815, 758, 696; HRMS(ESI, *m/z*) calcd. for $C_{22}H_{18}ClNNaOS^+$ $[M+Na]^+$ 402.0690, found 402.0697.



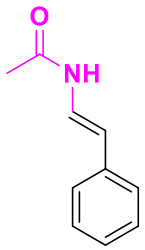
(*Z*)-N-(2-((4-chlorophenyl)thio)-2-phenylvinyl)benzamide (4e)

Eluent in chromatography: petroleum ether/ethyl acetate 5:1, **4e** was isolated as a brown solid (m.p. 105-106ºC) (25.6 mg, 35%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.05 (br.d, *J* = 10.8 Hz, 1H), 8.26 (d, *J* = 11.2 Hz, 1H), 7.90 (d, *J* = 8.0 Hz, 2H), 7.73 (d, *J* = 8.0 Hz, 2H), 7.66 (t, *J* = 8.0 Hz, 1H), 7.57 (t, *J* = 8.0 Hz, 2H), 7.41 (t, *J* = 8.0 Hz, 2H), 7.35-7.24 (m, 5H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 164.4, 137.4, 133.1, 133.0, 132.8, 132.2, 130.2, 129.5, 129.1, 128.9, 128.5, 127.9, 127.5, 126.6, 113.2; IR (KBr): ν_{max} 3016, 2053, 1634, 1401, 1086, 699, 579; HRMS(ESI, *m/z*) calcd. for $C_{21}H_{16}ClNNaOS^+$ $[M+Na]^+$ 388.0533, found 388.0538.



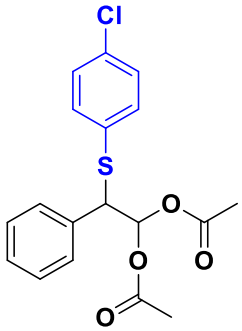
(*Z*)-N-(2-((4-chlorophenyl)sulfinyl)-2-phenylvinyl)acetamide (5a)

Eluent in chromatography: petroleum ether/ethyl acetate 5:1, **5a** was isolated as a pale yellow solid (52.3 mg, 82%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 10.95 (br.d, *J* = 10.0 Hz, 1H), 7.59 (d, *J* = 10.4 Hz, 1H), 7.44-7.23 (m, 9H), 2.16 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.9, 141.4, 138.0, 133.1, 130.1, 129.8, 129.3, 128.7, 128.0, 126.6, 119.8, 23.8; IR (KBr): ν_{max} 3050, 2924, 2358, 1707, 1631, 1474, 1369, 1242, 1089, 1010, 821, 763, 698, 597; HRMS(ESI, *m/z*) calcd. for $C_{16}H_{15}ClNO_2S^+$ $[M+H]^+$ 320.0507, found 320.0491.



(E)-N-styrylacetamide (5b)[12]

Eluent in chromatography: petroleum ether/ethyl acetate 2:1, **5b** was isolated as a light yellow solid (36.2 mg, 75%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.71 (br.d, *J* = 4.8 Hz, 1H), 7.52-7.48 (m, 1H), 7.31-7.25 (m, 4H), 7.19-7.15 (m, 1H), 6.10 (d, *J* = 14.4 Hz, 1H), 2.11 (s, 3H); ^{13}C NMR (100 MHz, Chloroform-*d*) δ 167.8, 136.2, 128.9, 126.8, 125.7, 122.9, 112.7, 23.5.



2-((4-chlorophenyl)thio)-2-phenylethane-1,1-diyl diacetate (6)[13]

Eluent in chromatography: petroleum ether/ethyl acetate 10:1, **6** was isolated as an oily liquid (40.8 mg, 56%); ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.32-7.20 (m, 9H), 7.14 (d, *J* = 5.6 Hz, 1H), 4.47 (d, *J* = 5.6 Hz, 1H), 1.99 (s, 3H), 1.97 (s, 3H). The analytic data is in accordance with literature.

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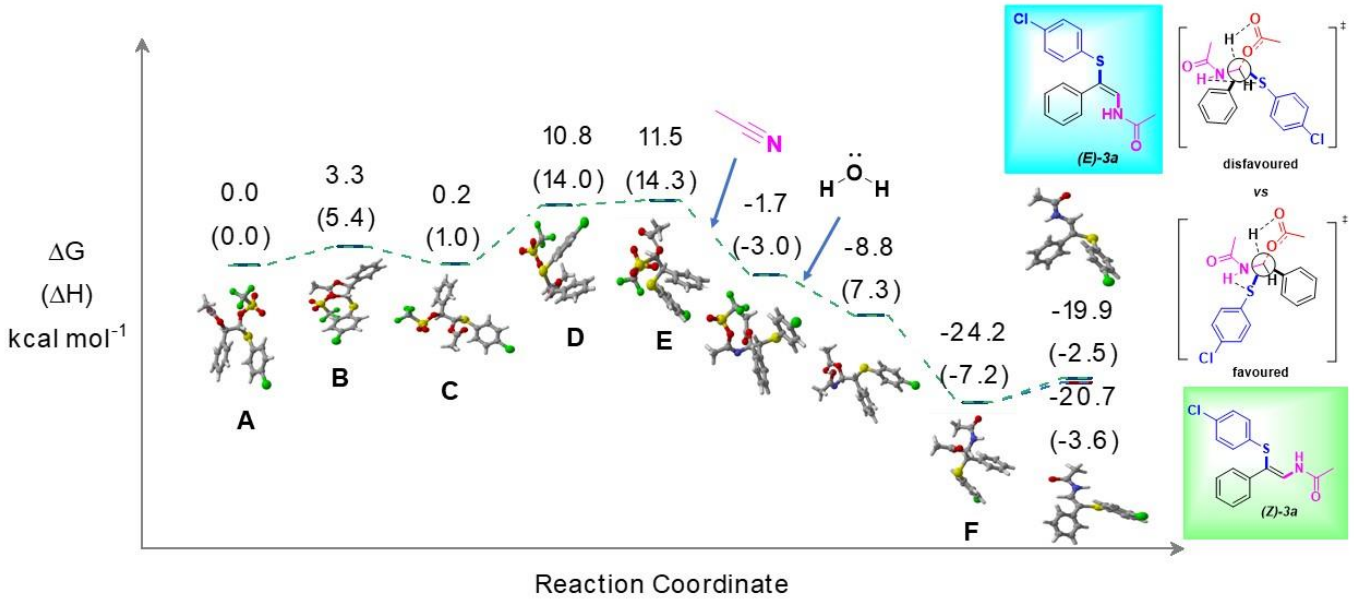
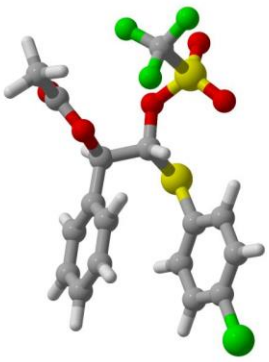
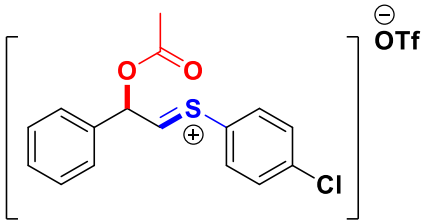
5 Density functional theory (DFT) calculations

All geometry optimizations and frequency calculations were conducted in Gaussian 09 package with the B3LYP functional and 6-311G (d, p) basis set level. The unit of the energies was kcal mol^{-1} and the 3D pictures were drawn by using CYLview 20 software(CYLview20; Legault, C. Y., Université de Sherbrooke, 2020. http://www.cylview.org).The acetonitrile solvent corrections were included into all calculations using the SMD solvation model. The Gibbs free energies and Thermal Enthalpies of the organics were calculated. The Grimme's D3BJ dispersion correction was considered in the electronic energy calculations.







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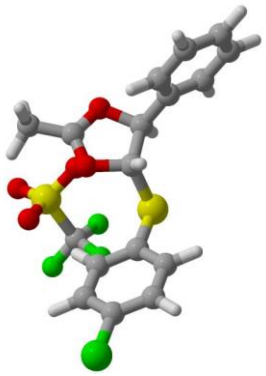

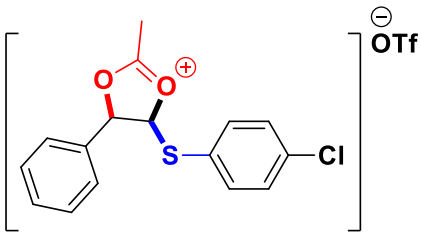

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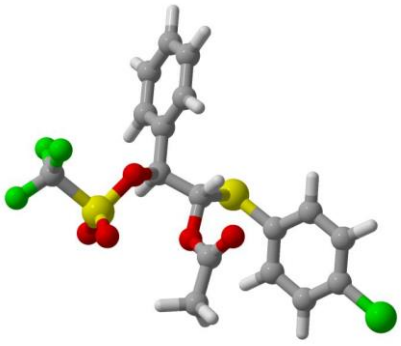

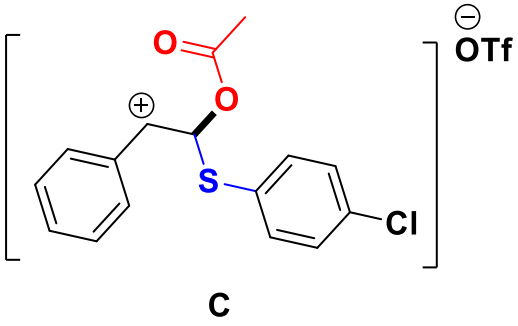

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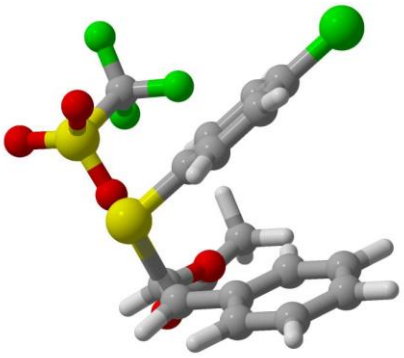

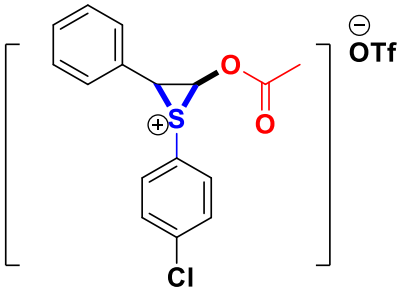

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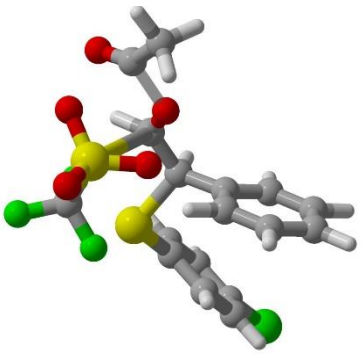

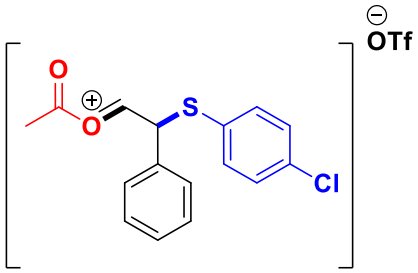

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H 4.89352800 1.99116600 2.32781100
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H -2.48237300 2.11915900 1.20626300
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H 0.38204700 2.76800700 -2.79122600
H -2.99306800 3.94460200 -0.39546500

H -1.55825100 4.27215800 -2.39980600
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H -3.13873300 -1.92962400 2.19731800
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O 3.25529200 0.91389800 -1.08788300
S 4.05645200 -0.31733400 -0.87951500
O 4.95248200 -0.69094300 -1.99112300
O 4.63286400 -0.44237900 0.48308400
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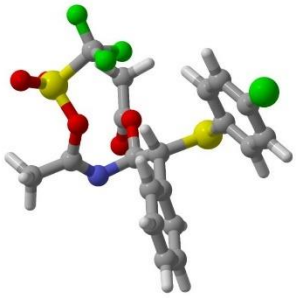

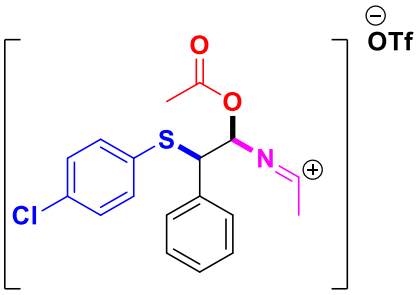

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H -1.62695100 -4.48292900 -2.24420400
H -3.36211700 -4.69461800 -1.85710300
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C -1.06631200 -1.50668900 0.32352300
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H 2.25733200 -0.99313600 -1.76807000
C 2.46673800 -4.13994500 0.47835800
H 0.77783700 -3.32503100 1.52441400
C 3.39054500 -3.96361900 -0.55660800
H 4.02921100 -2.68152000 -2.16832200
H 2.52089800 -5.02035700 1.11175100
H 4.16439500 -4.70573400 -0.72817300
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C 2.18129600 1.88412400 0.12283800
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H 1.20978000 2.27205000 -0.16273900
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H 3.27282000 3.29218600 -1.09366200
Cl 6.04217700 2.66801100 -0.68550400
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H -2.57309900 -1.79048500 2.61112200
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S -3.76666700 1.75282700 -0.34669300
O -4.05119400 0.86166600 -1.45853900
O -4.64243100 2.86557100 -0.01645300
C -2.04039500 2.50344500 -0.58005500
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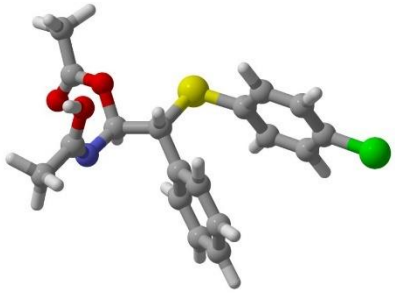

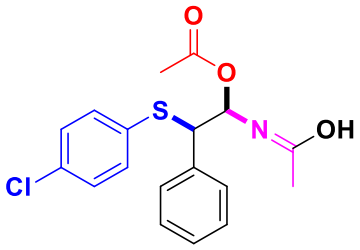

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H 0.53760200 -0.37856800 -1.36233100
S 0.02529500 -1.56477100 0.68534200
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C -2.25007000 -1.63597500 -0.90075300
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C -3.58397600 -1.35892200 -1.19566800
H -1.63333600 -2.14150500 -1.63633800
C -4.36185200 -0.70874000 -0.23929900
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H -4.00940200 -1.64593800 -2.15050100

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C -0.30448300 2.94036500 1.65629600
H 1.00885500 1.27955700 2.02364700
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H -2.12041100 3.41387900 -1.18079300
H -0.11722900 3.39286600 2.62563700
H -1.69890900 4.46590000 1.03419900
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N 2.86281000 -1.36254500 -0.69480700
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O 3.21318500 -2.14951900 1.44233900
H 3.62884700 -2.91719500 1.86849600
C 3.95780600 -3.50937900 -0.42264200
H 3.99870500 -3.48988000 -1.51121700
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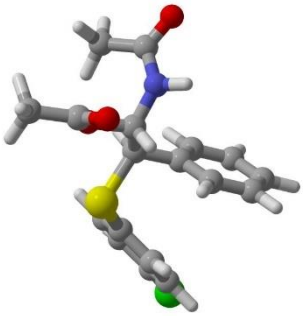

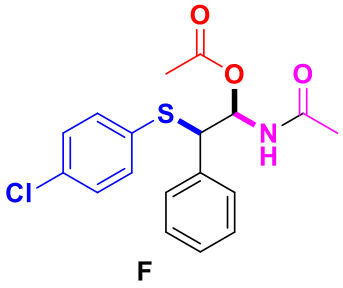

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C 2.20546600 -0.13721000 -0.05498800
H 2.48350200 0.05496700 0.98416800
C 0.68654800 -0.12679100 -0.25786000
H 0.50060400 -0.32666500 -1.31523900
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C -2.25380500 -1.65624000 -0.94923500
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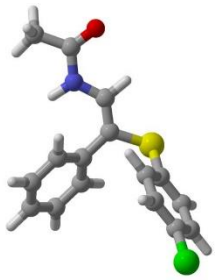

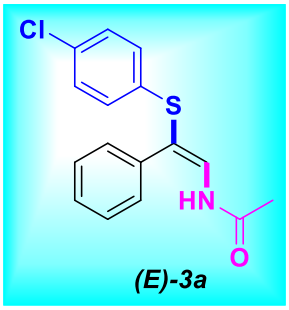

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H 1.54436500 -0.93162300 -1.64925900
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H 0.38903900 -1.60425800 2.43662800
C 0.60398100 -3.82508700 -0.13276600
H 1.20240000 -3.32503900 -2.14361600
H 0.03108800 -3.99817000 1.93950400
H 0.44015600 -4.87567000 -0.35221800
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C -3.89215200 0.71987500 0.85590100
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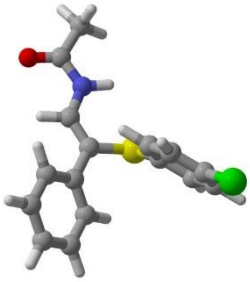

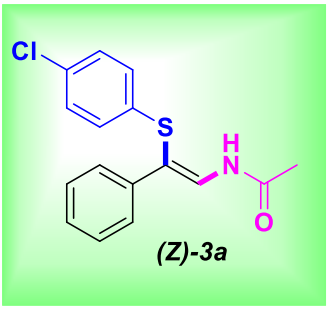

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H 6.12487700 1.35693100 1.38219000
H 4.73580400 0.42321100 1.99174500
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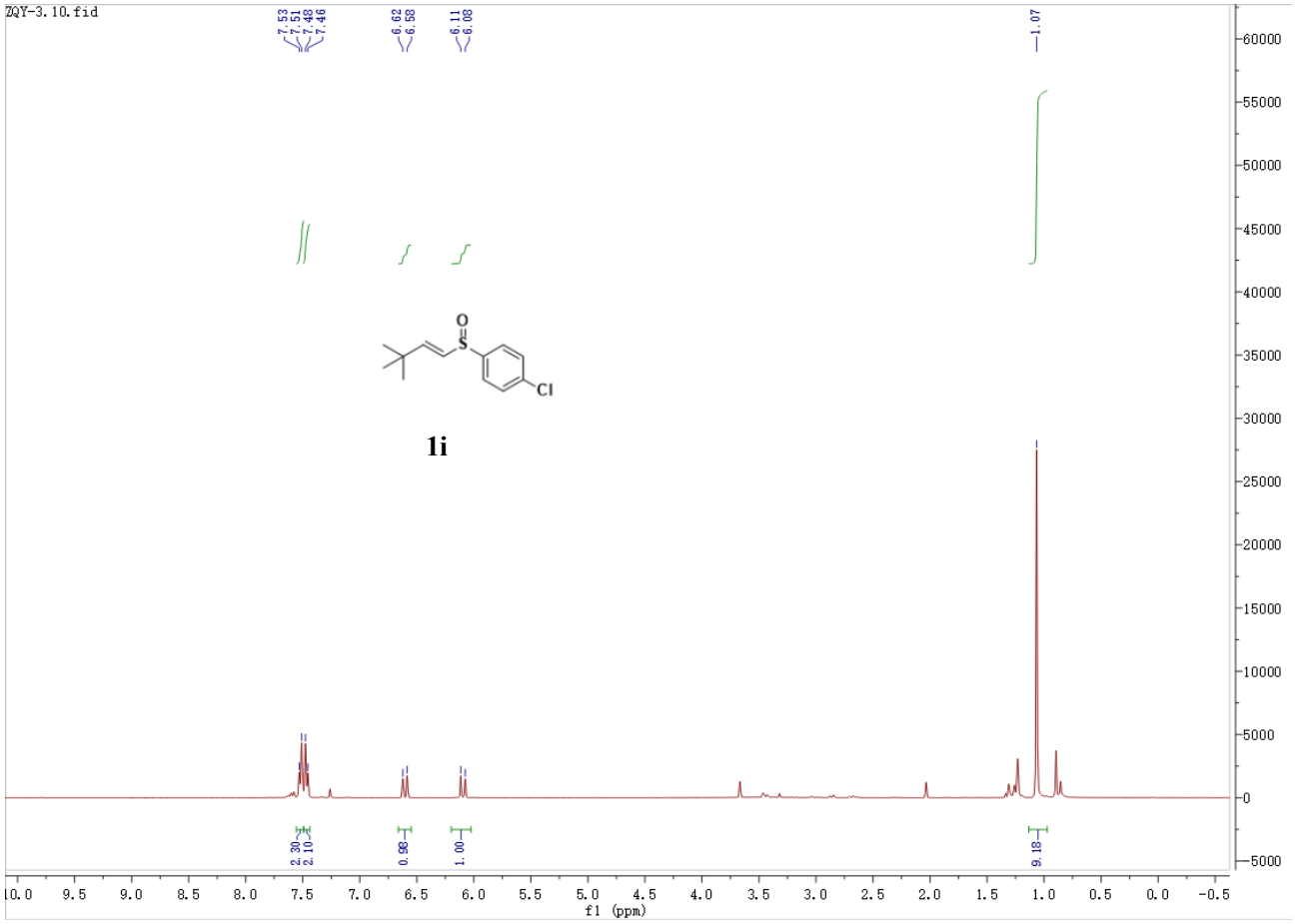
6 NMR Spectra of Compounds



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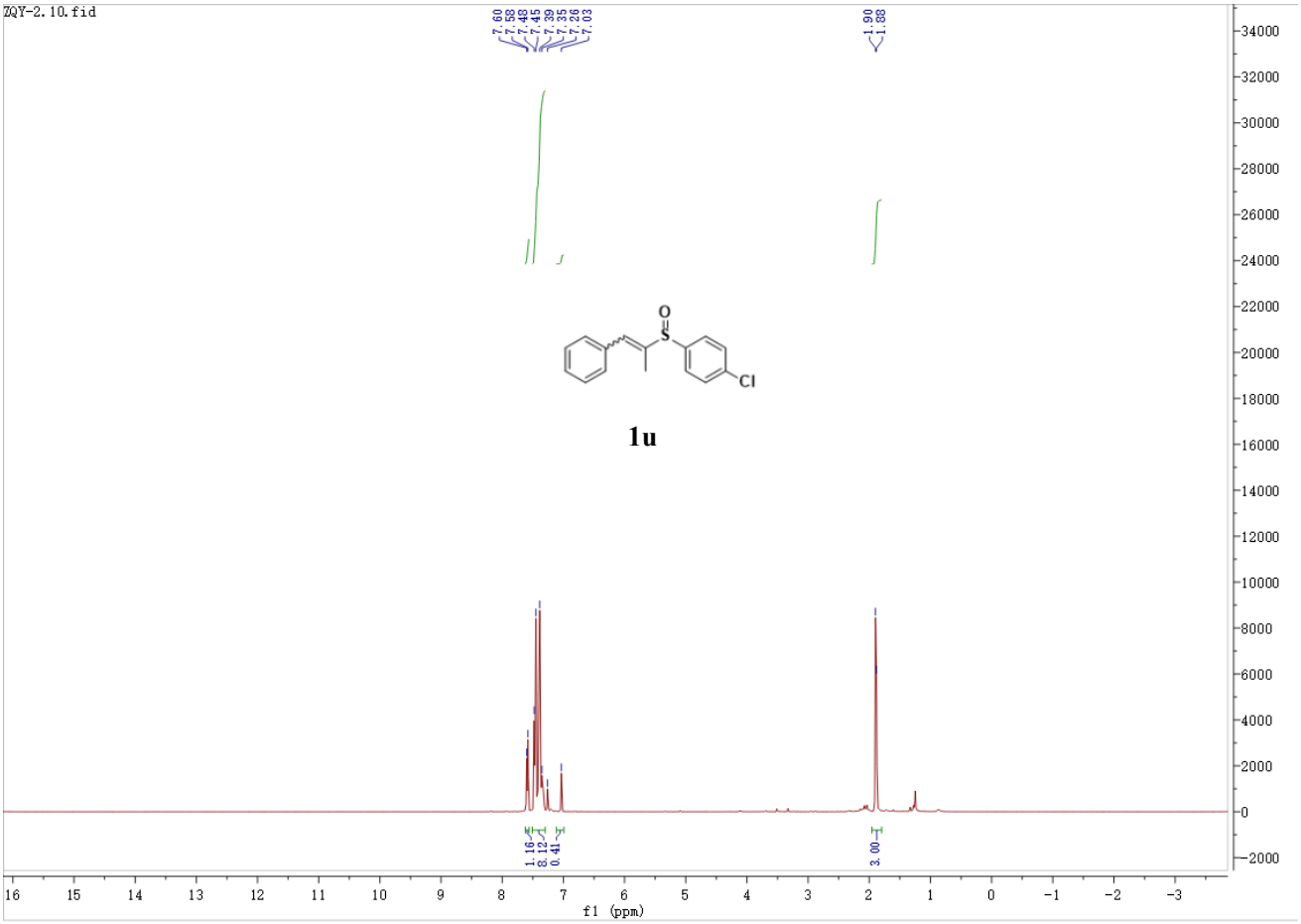

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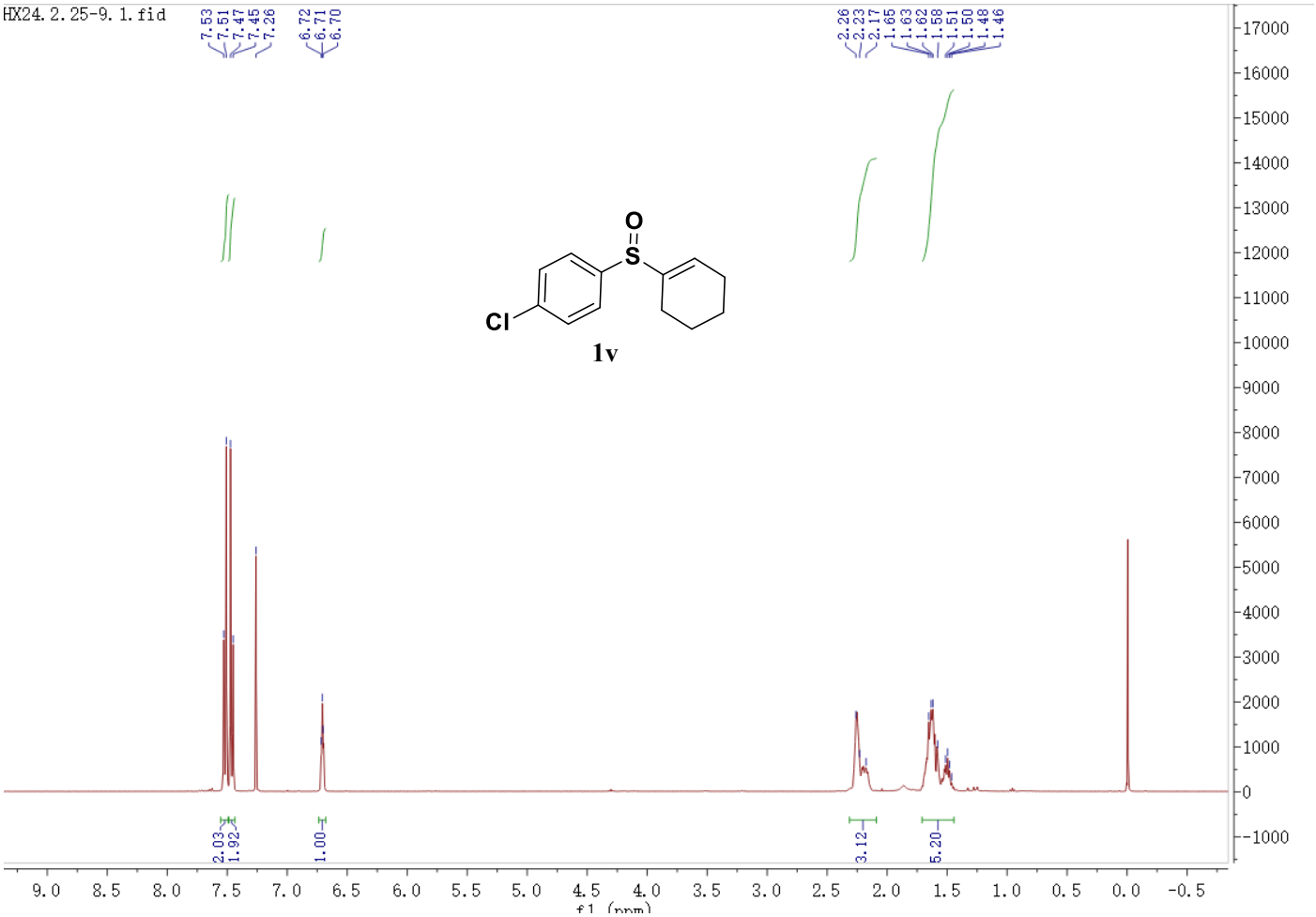
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6.70
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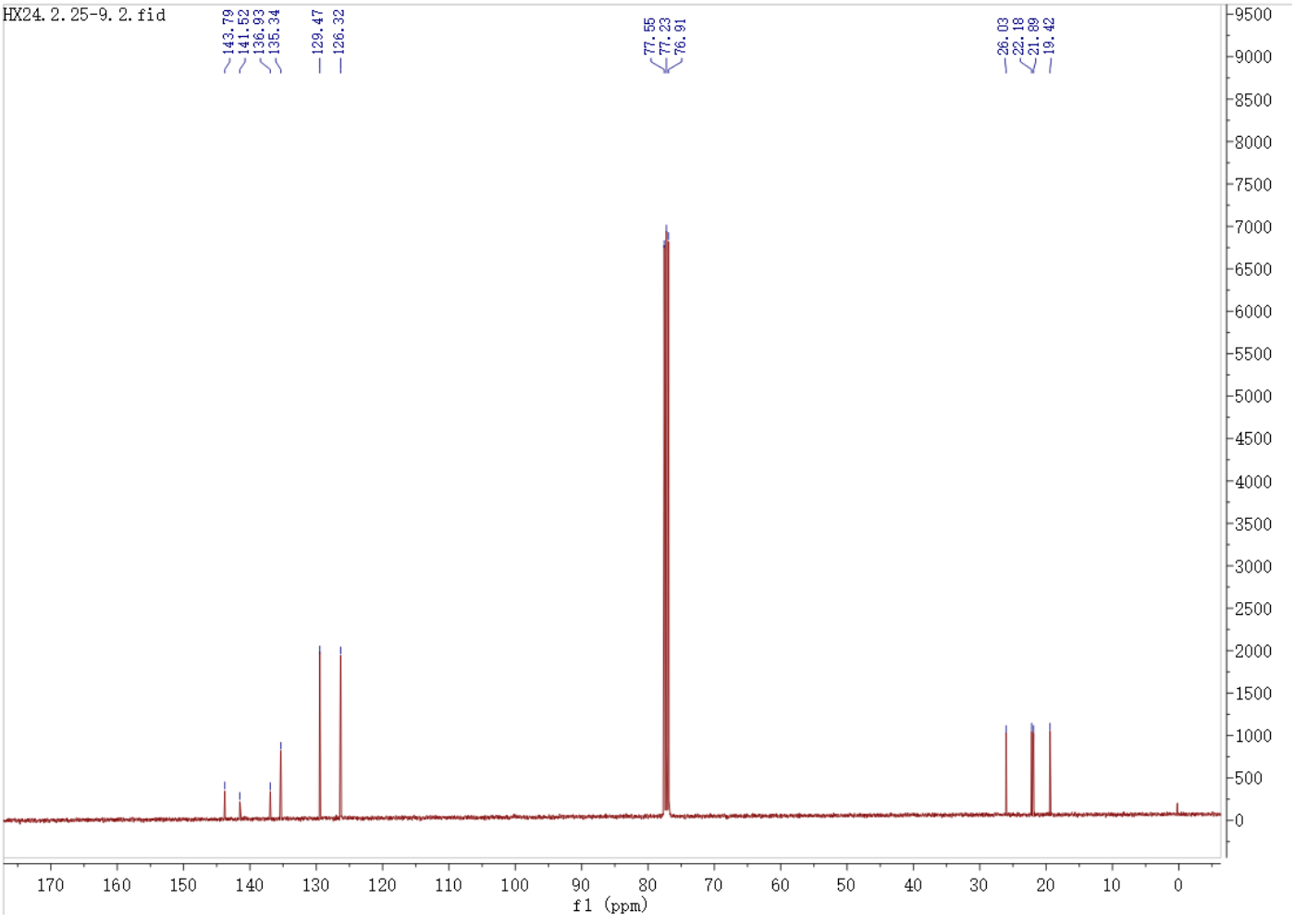
2.23
2.17
1.65
1.63
1.62
1.58
1.51
1.50
1.48
1.46
O
S
Cl
1v
2.03
1.92
1.00
3.12
5.20
f1 (ppm)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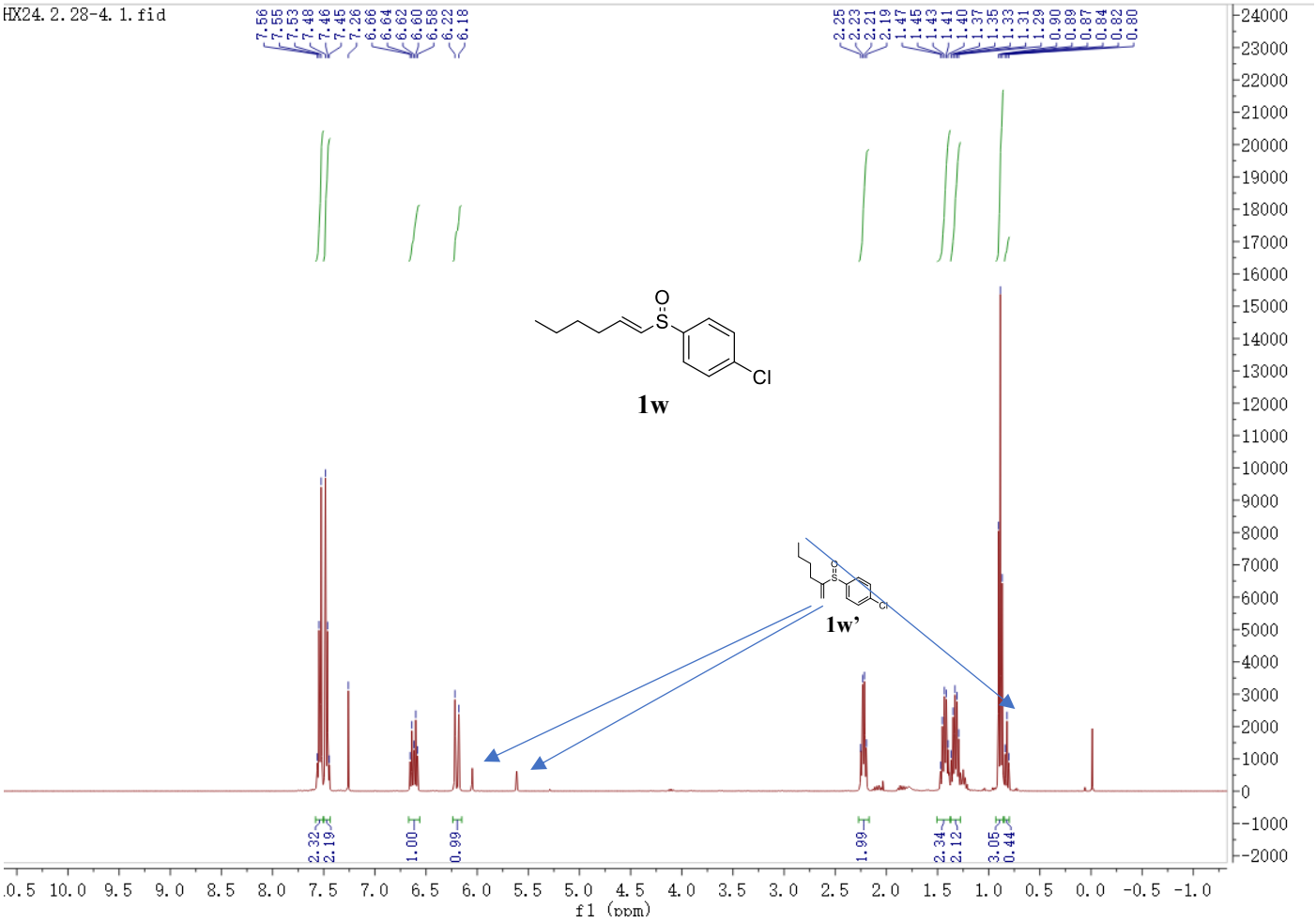
21.89
19.42
f1 (ppm)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1.41
1.40
1.37
1.35
1.33
1.31
1.29
0.90
0.89
0.87
0.84
0.82
0.80
O
S
Cl
1w
1w'
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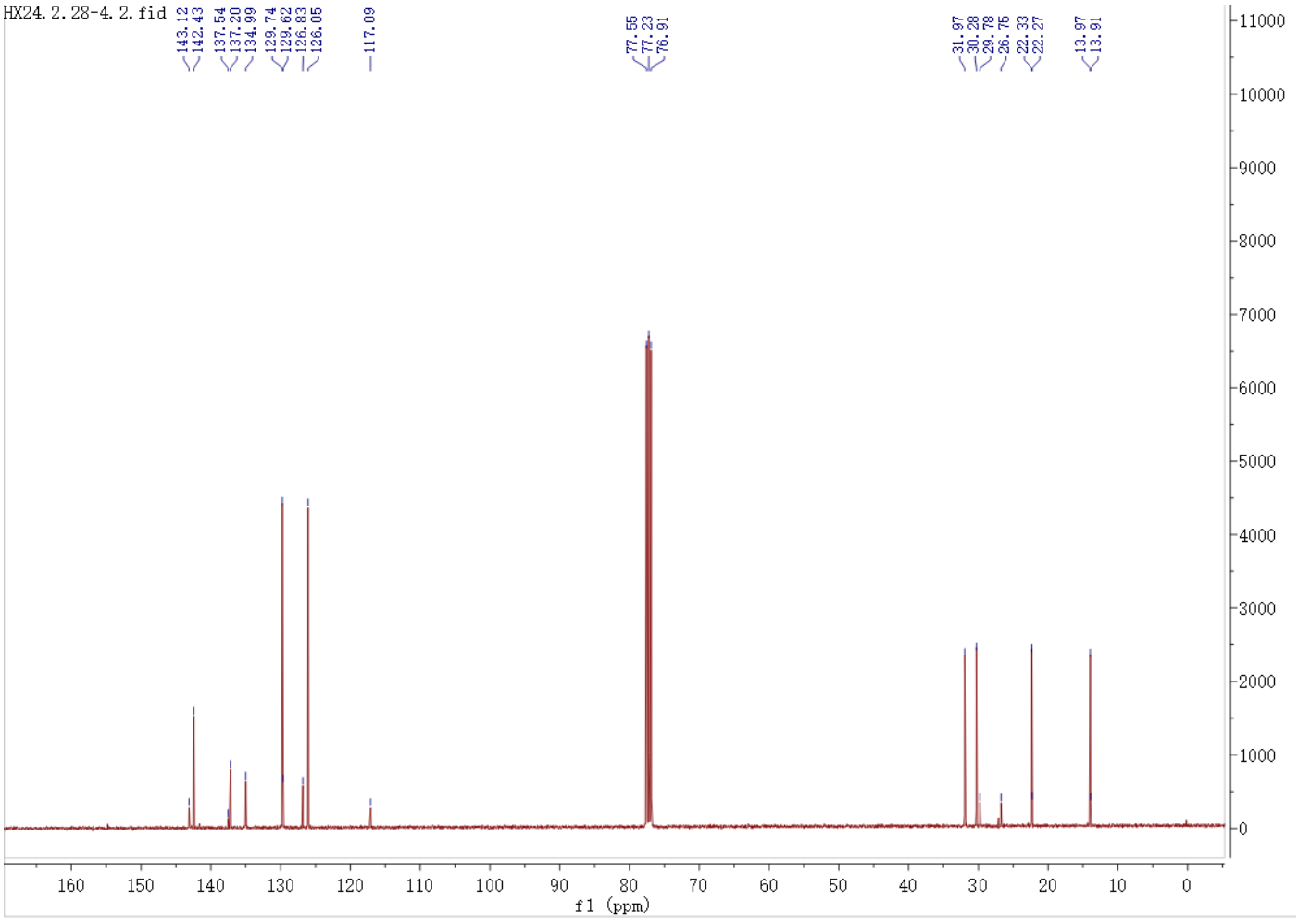
0.99
1.99
2.34
2.12
3.05
0.44
f1 (ppm)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129.62
126.83
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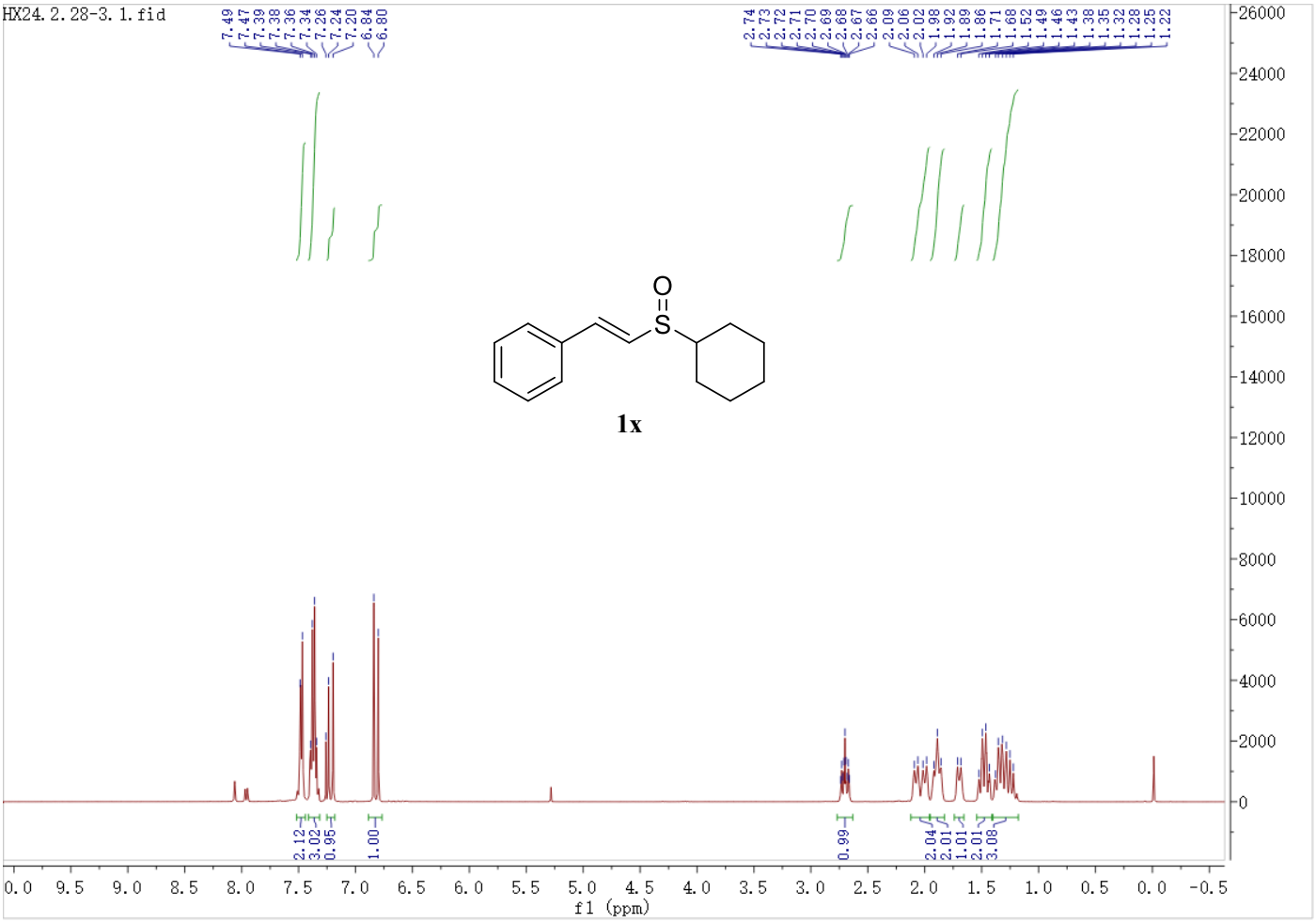
26.75
22.33
22.27
13.97
13.91
f1 (ppm)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7.36
7.34
7.26
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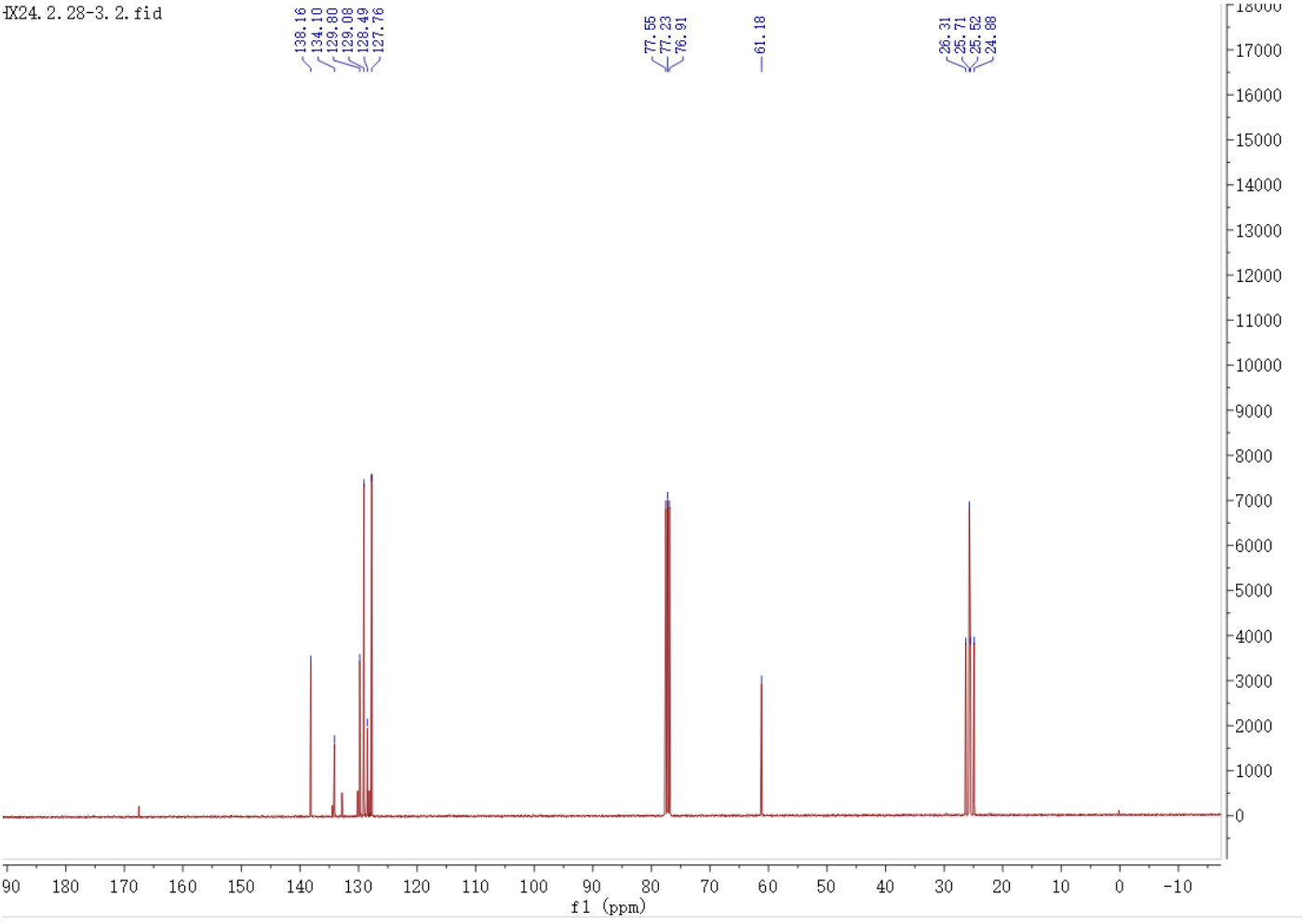
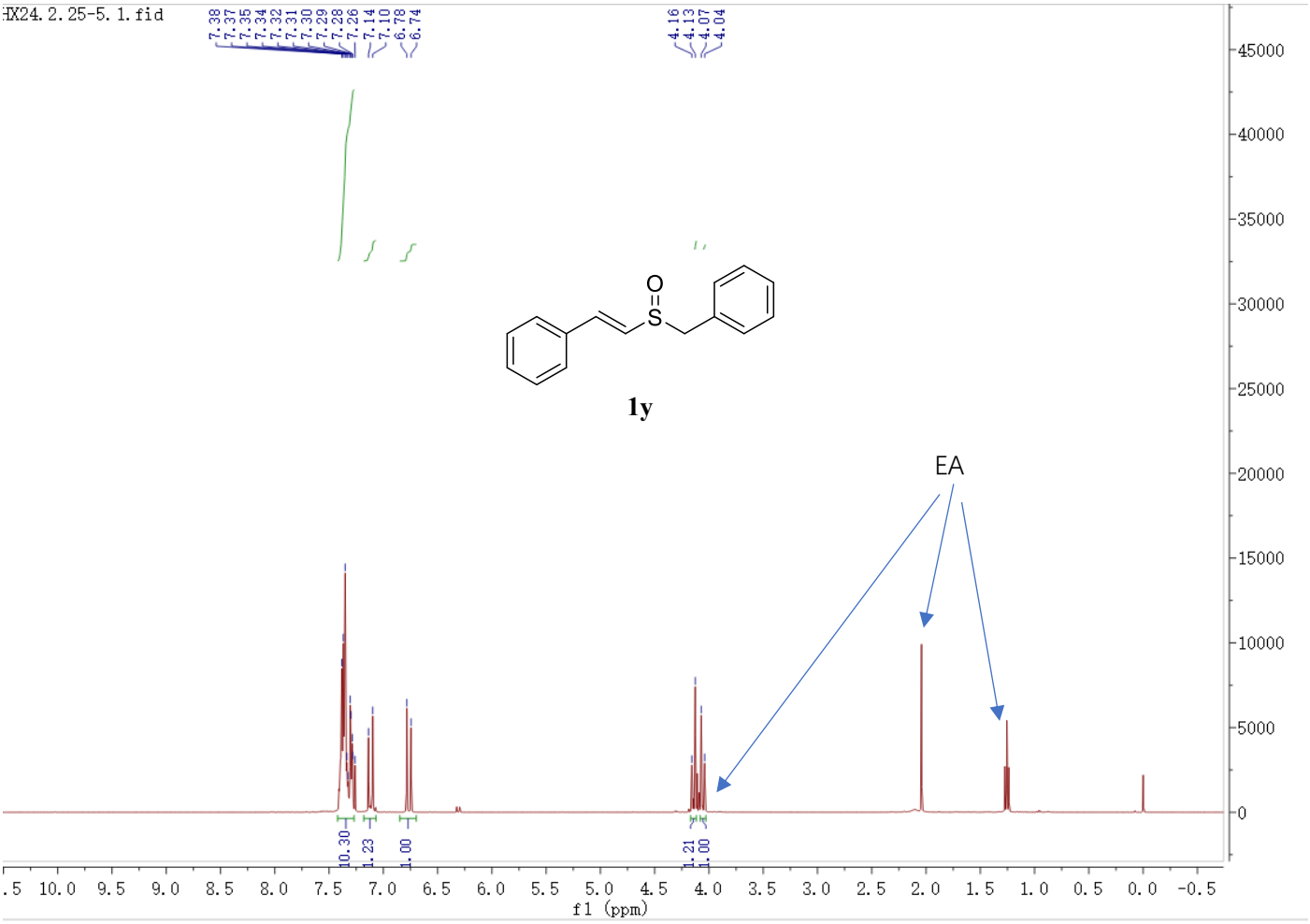
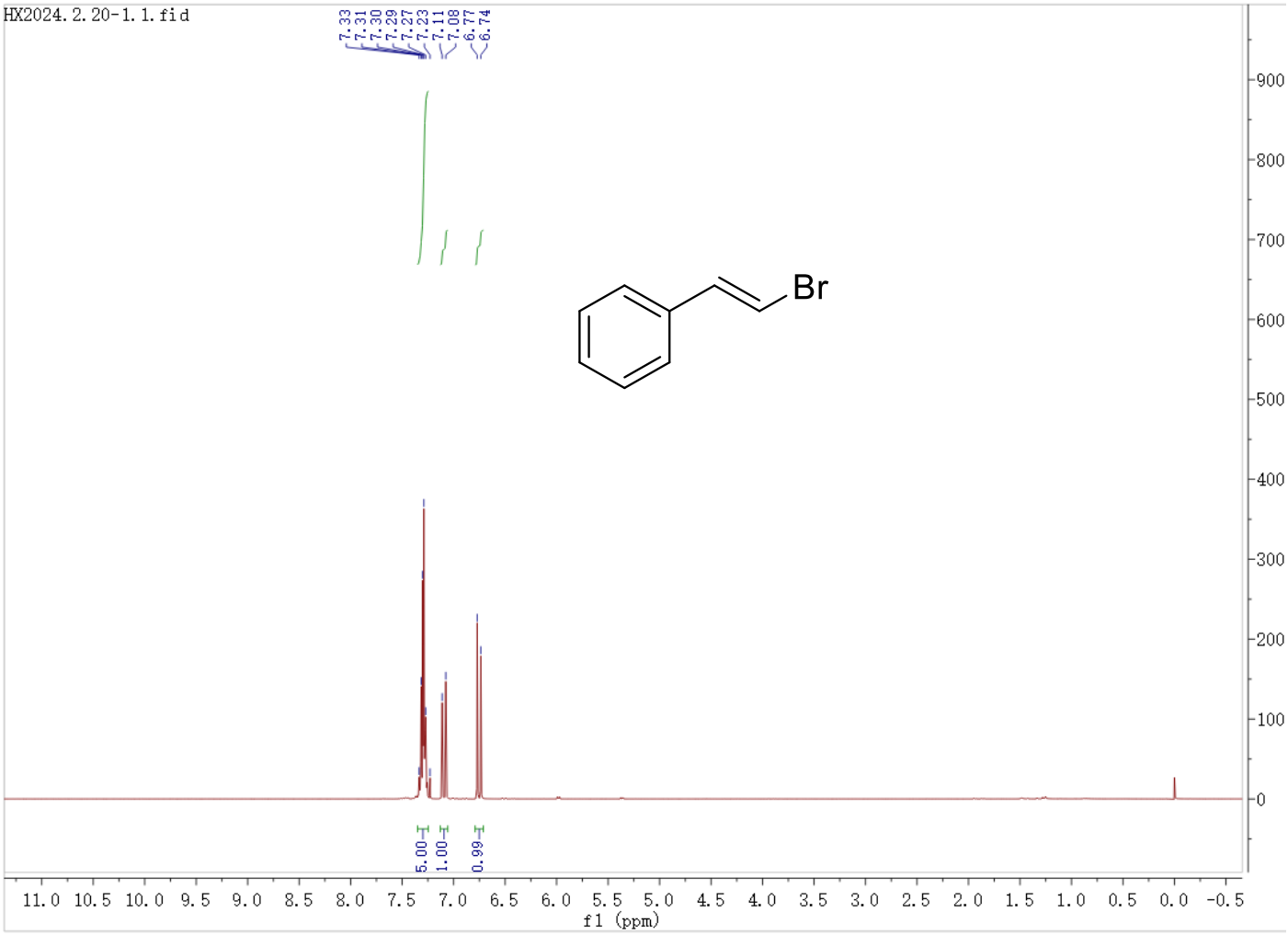
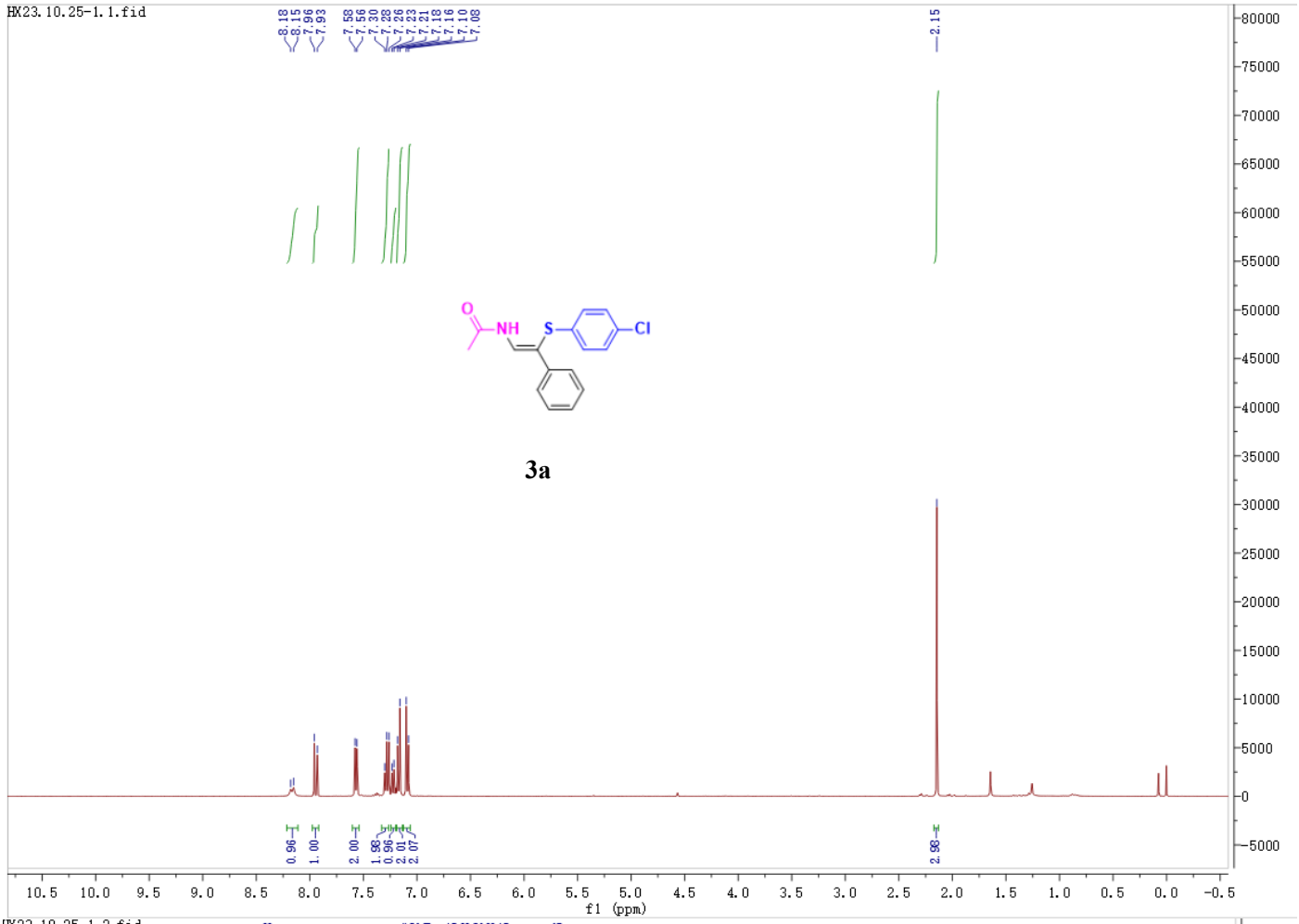
6.80
2.74
2.73
2.72
2.71
2.70
2.69
2.68
2.67
2.66
2.09
2.06
2.02
1.98
1.92
1.89
1.86
1.71
1.68
1.52
1.49
1.46
1.43
1.38
1.35
1.32
1.28
1.25
1.22
O
S
2.12
3.02
0.95
1.00
0.99
2.04
2.01
1.01
2.01
3.08
f1 (ppm)

1x

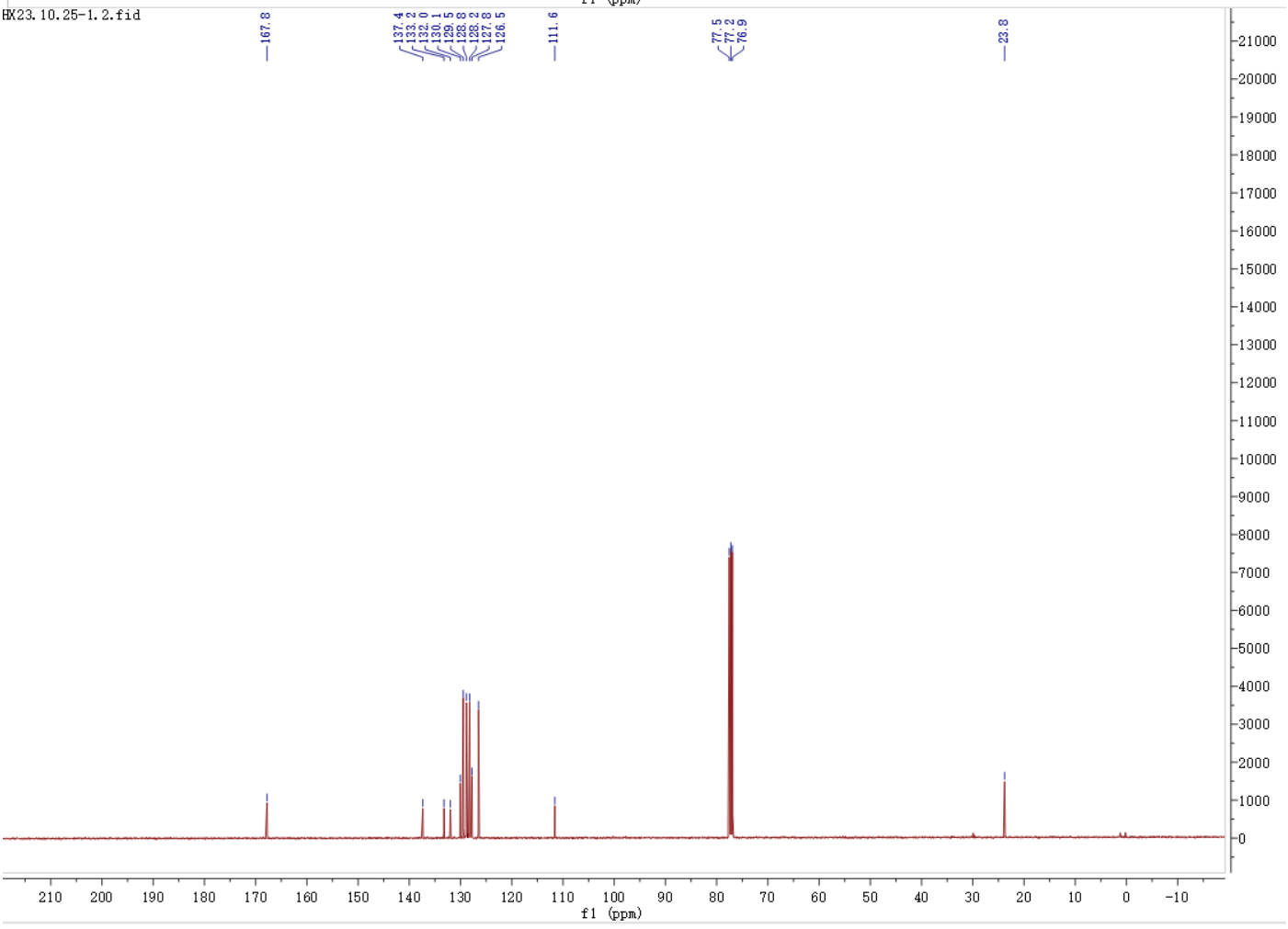

HX24.2.28-3.2.fid
138.16
134.10
129.80
129.08
128.49
127.76
77.55
77.23
76.91
61.18
26.31
25.71
25.52
24.88
f1 (ppm)

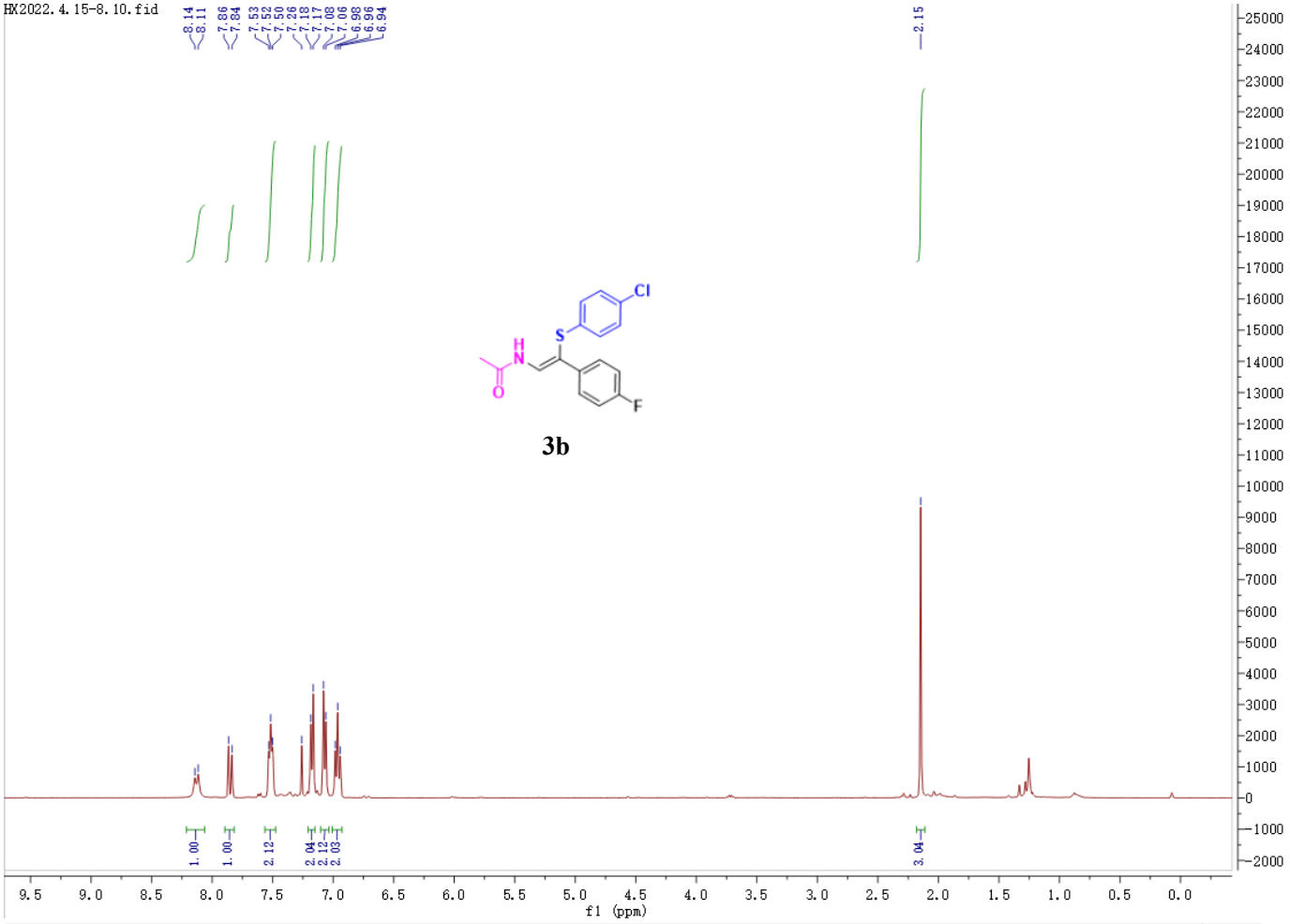

HX24.2.25-5.1.fid
7.38
7.37
7.35
7.34
7.32
7.31
7.30
7.29
7.28
7.26
7.14
7.10
6.78
6.74
4.16
4.13
4.07
4.04
O
S
1y
EA
10.30
1.23
1.00
1.21
1.00
f1 (ppm)


HX2024.2.20-1.1.fid
7.33
7.31
7.30
7.29
7.27
7.23
7.11
7.08
6.77
6.74
Br
5.00
1.00
0.99
f1 (ppm)

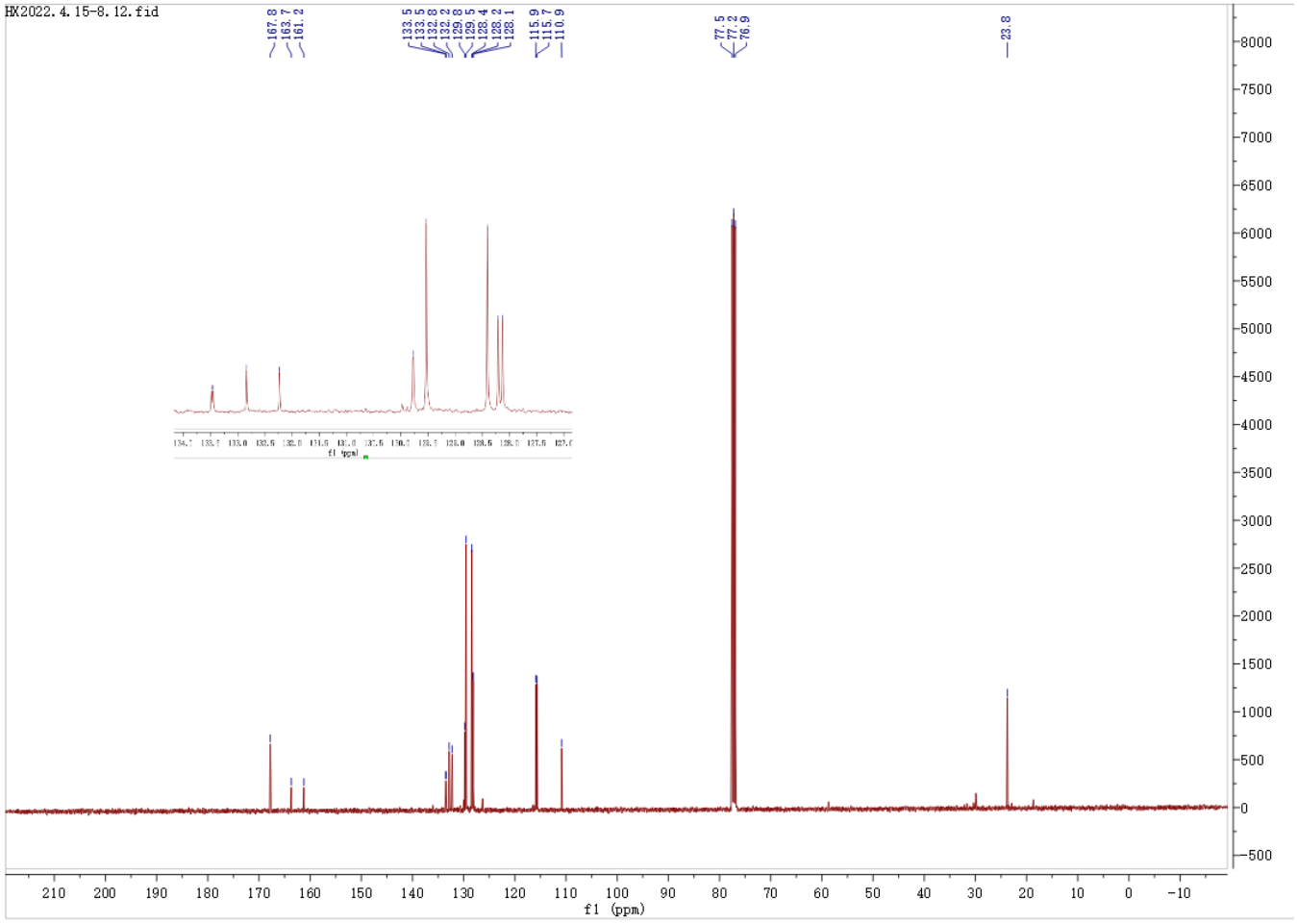

HX23.10.25-1.1.fid
8.18
8.15
7.96
7.93
7.58
7.56
7.30
7.28
7.26
7.23
7.21
7.18
7.16
7.10
7.08
2.15
O
NH
S
Cl
0.96
1.00
2.00
1.98
0.96
2.01
2.07
2.98
f1 (ppm)

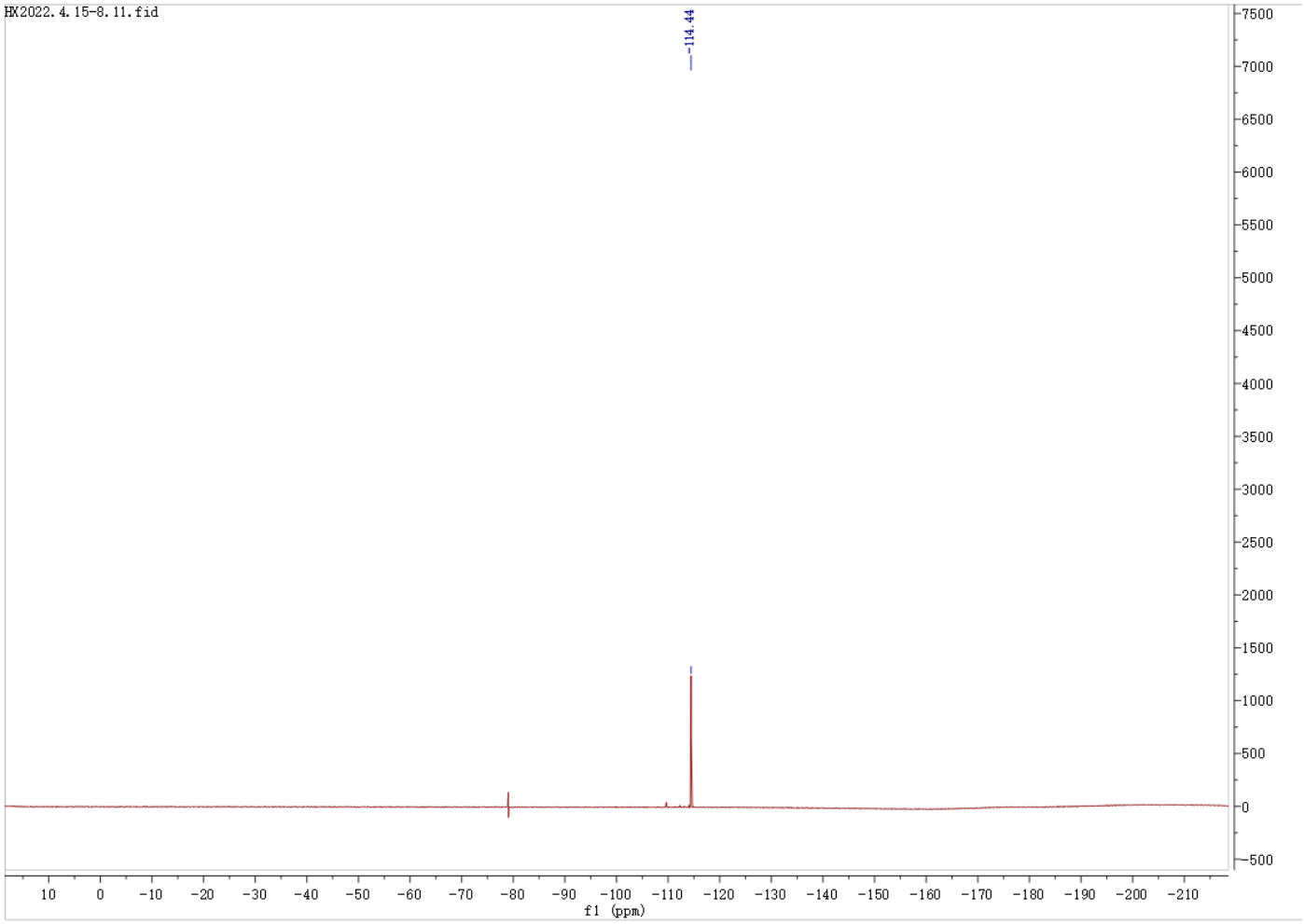
3a

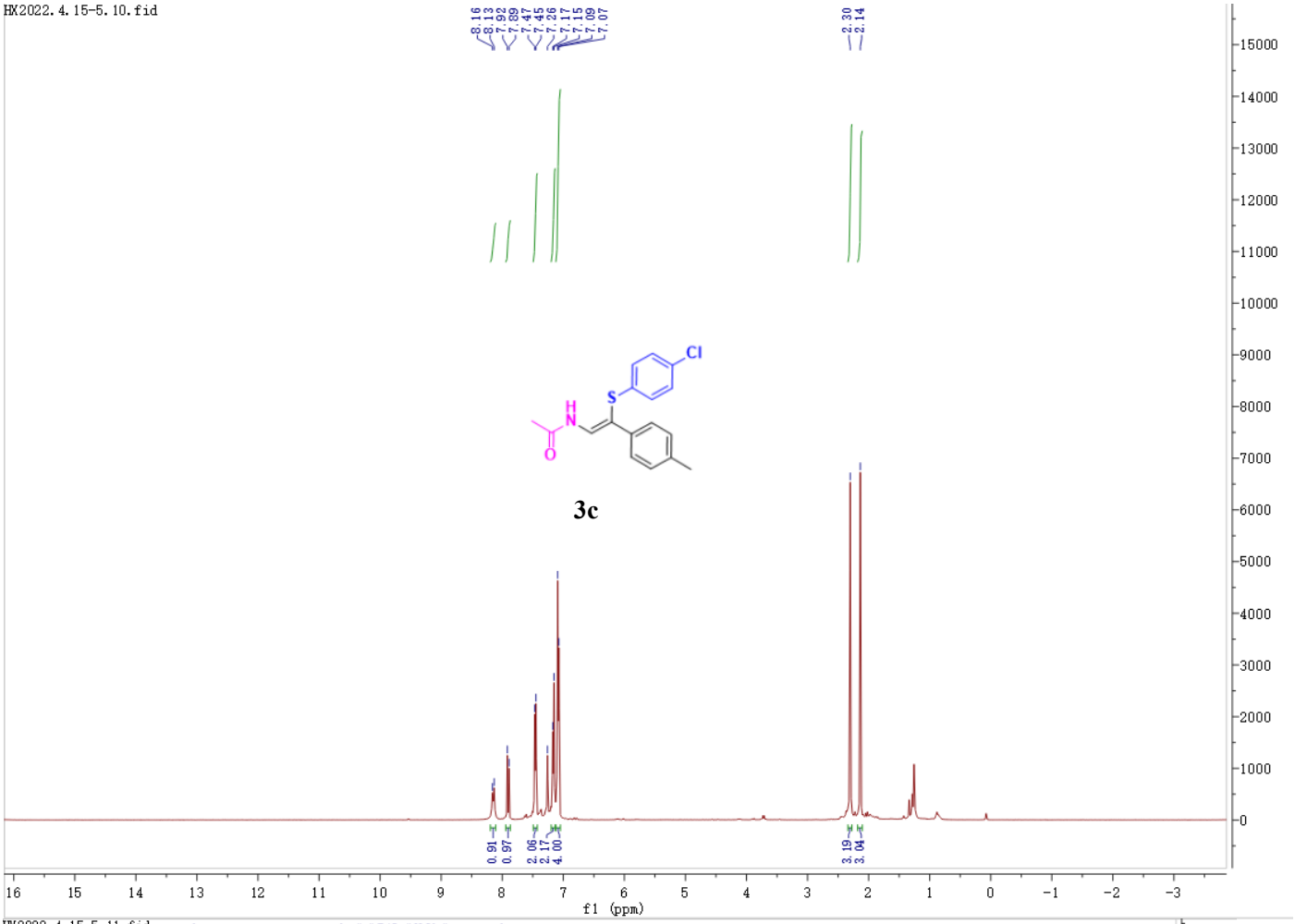

HX23.10.25-1.2.fid
167.8
137.4
133.2
132.0
130.1
129.5
128.8
128.2
127.8
126.5
111.6
77.5
77.2
76.9
23.8
f1 (ppm)


HX2022.4.15-8.10.fid
8.14
8.11
7.86
7.84
7.53
7.52
7.50
7.26
7.18
7.17
7.08
7.06
6.98
6.96
6.94
2.15
Cl
S
H
N
O
F
1.00
1.00
2.12
2.04
2.13
2.03
3.04
f1 (ppm)

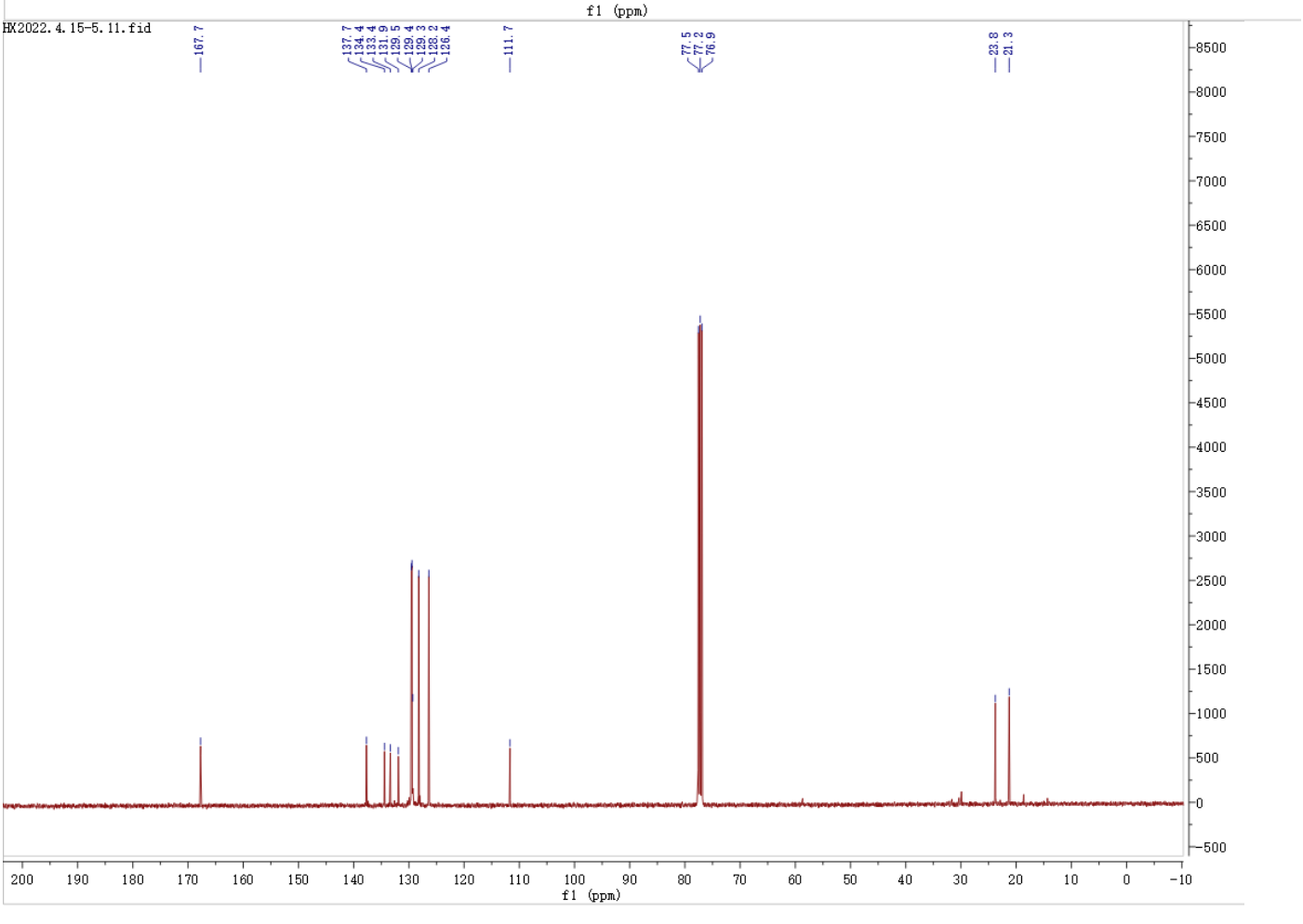
3b

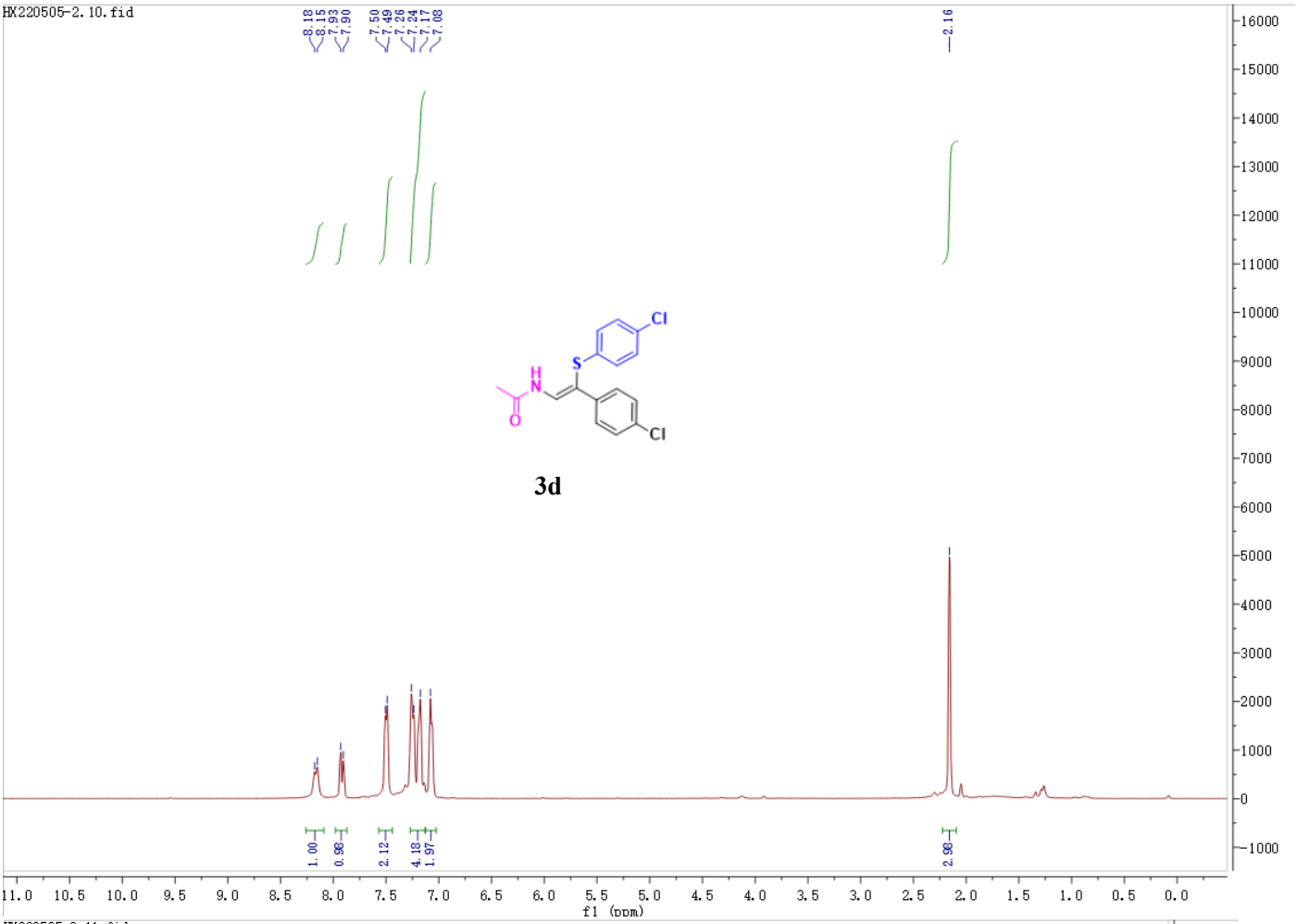

HX2022.4.15-8.12.fid
167.8
163.7
161.2
133.5
133.5
132.8
132.2
129.8
129.5
128.4
128.2
128.1
115.9
115.7
110.9
77.5
77.2
76.9
23.8
f1 (ppm)


HX2022.4.15-8.11.fid
-114.44
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

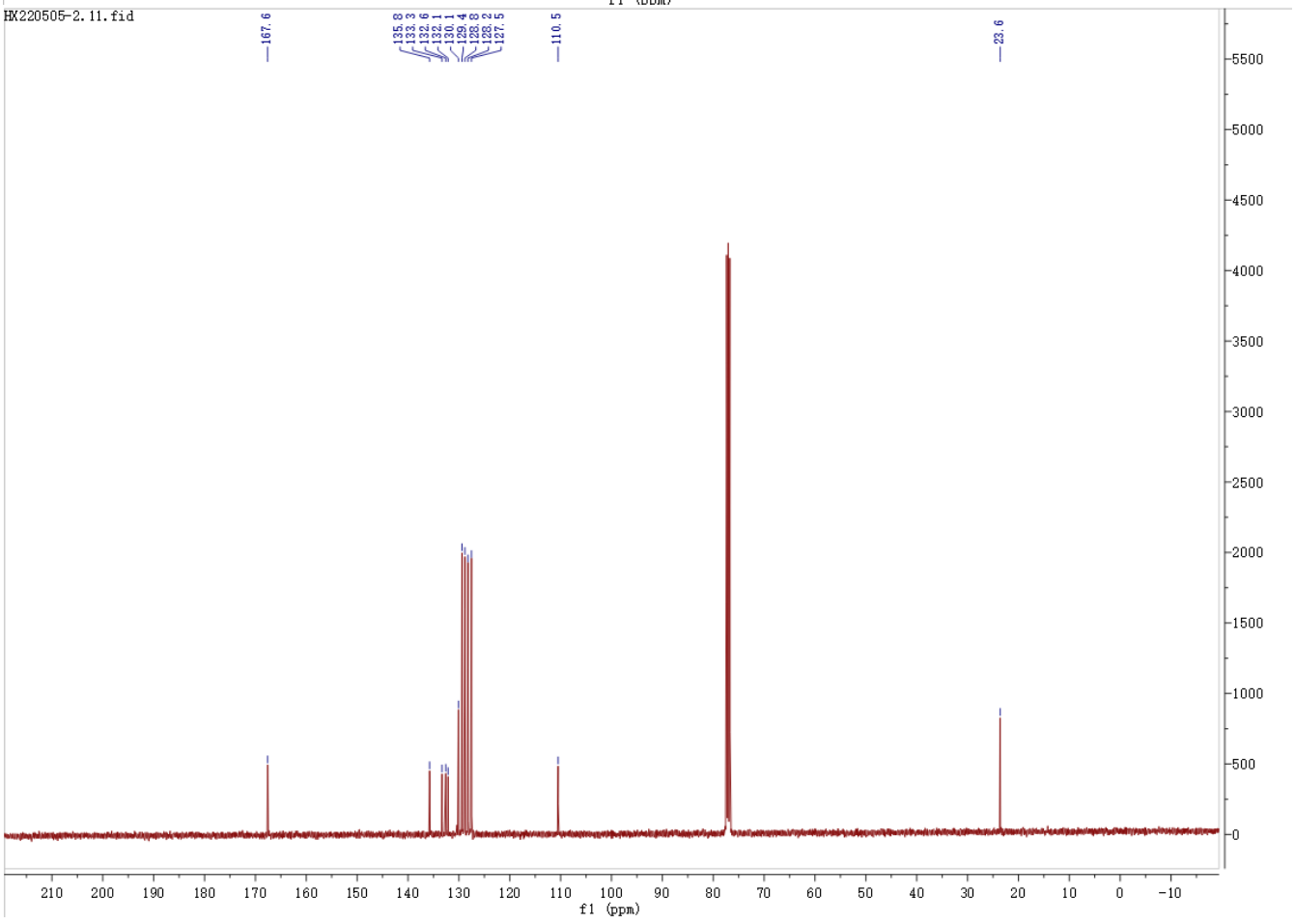

HX2022.4.15-5.10.fid
8.16
8.13
7.92
7.89
7.47
7.45
7.26
7.17
7.15
7.09
7.07
2.30
2.14
Cl
S
H
N
O
0.91
0.97
2.06
2.17
4.00
3.19
3.04
f1 (ppm)

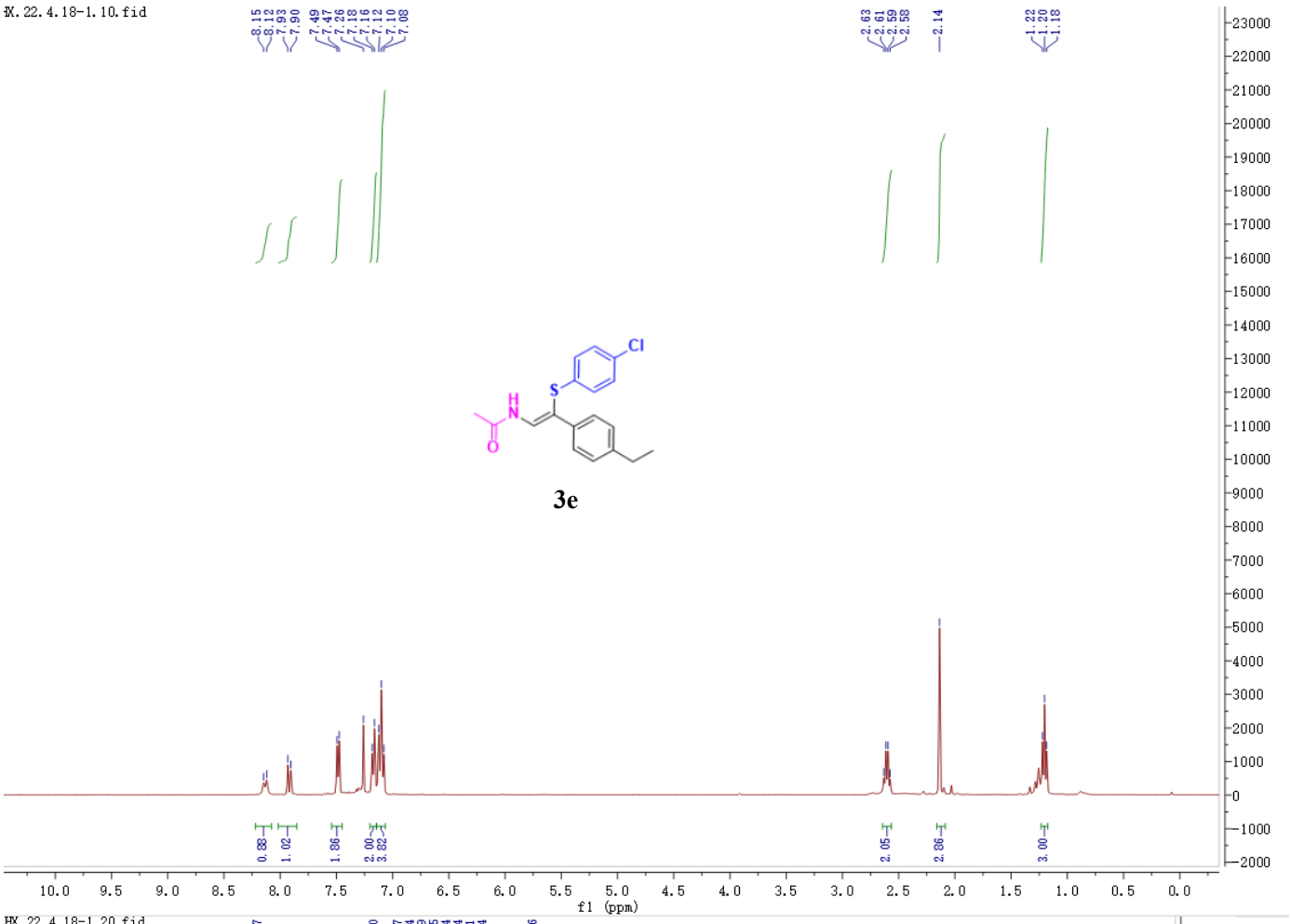
3c


HX2022.4.15-5.11.fid
167.7
137.7
134.4
133.4
131.9
130.5
129.4
128.3
128.2
126.4
111.7
77.5
77.2
76.9
23.8
21.3
f1 (ppm)

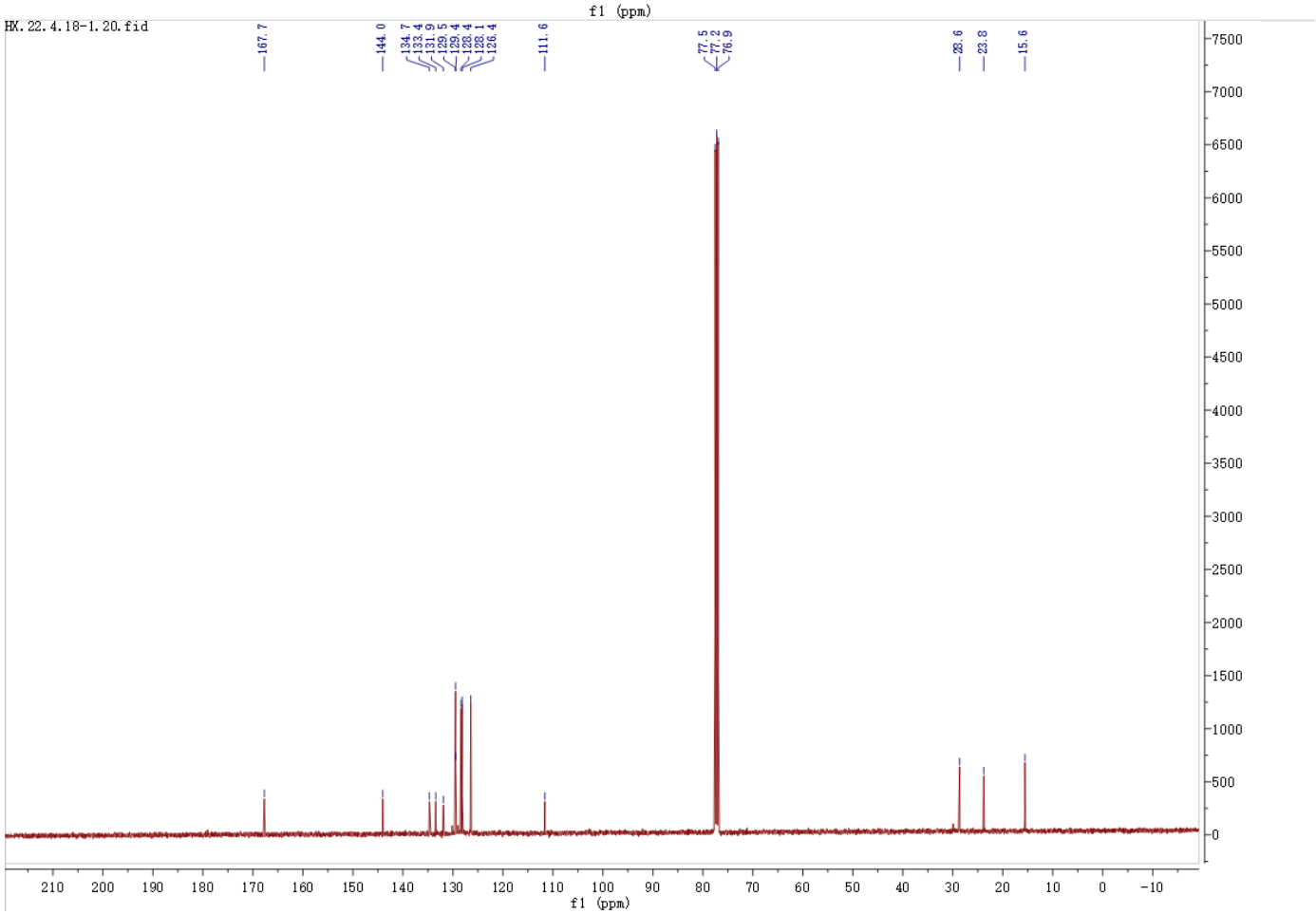

HX220505-2.10.fid
8.18
8.15
7.93
7.90
7.50
7.49
7.26
7.24
7.17
7.08
2.16
Cl
S
H
N
O
Cl
1.00
0.98
2.12
4.18
1.97
2.98
f1 (ppm)

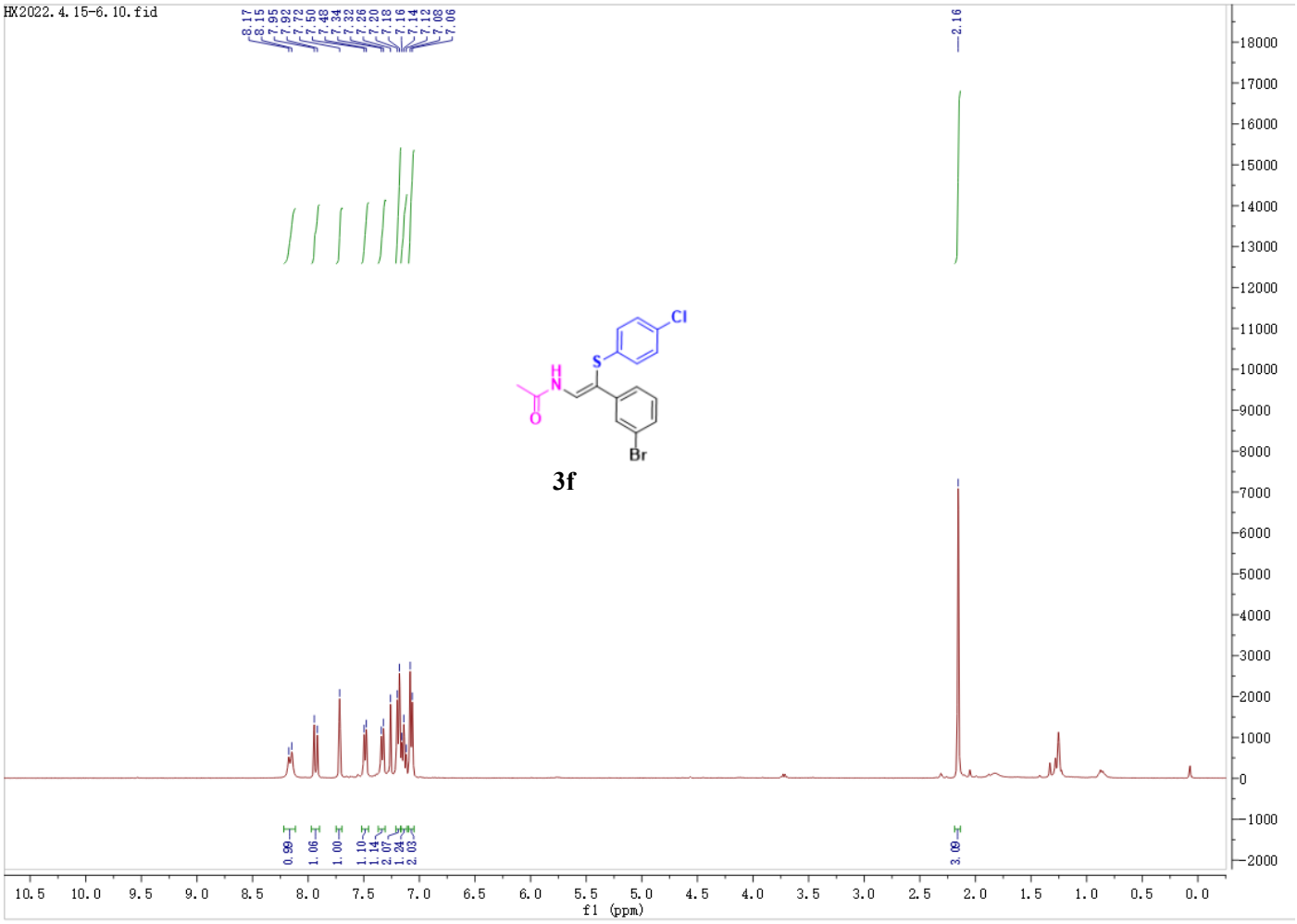
3d


HX220505-2.11.fid
167.6
135.8
133.3
132.6
132.1
130.1
129.4
128.8
128.2
127.5
110.5
23.6
f1 (ppm)

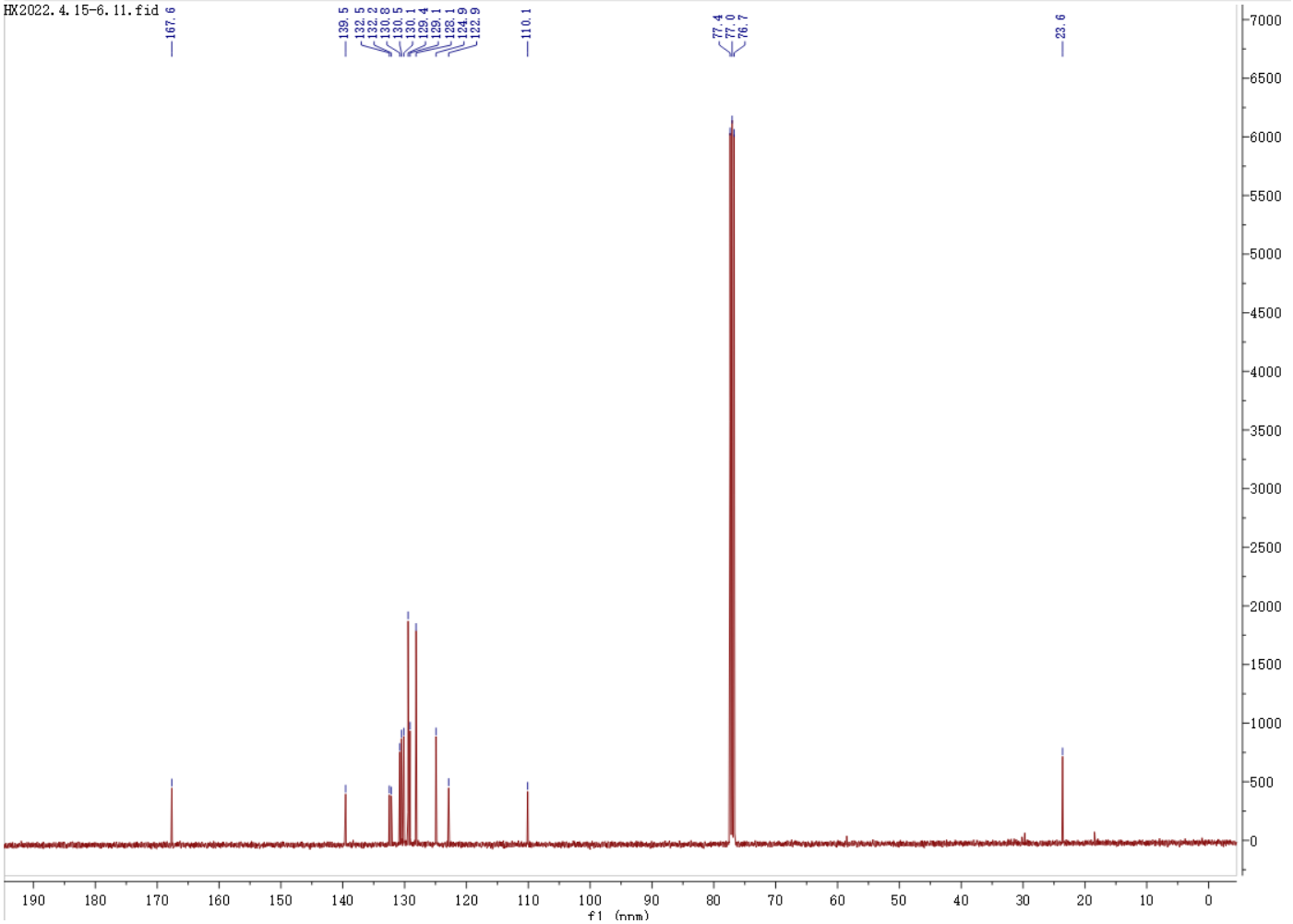

HX.22.4.18-1.10.fid
8.15
8.12
7.93
7.90
7.49
7.47
7.26
7.18
7.16
7.12
7.10
7.08
2.63
2.61
2.59
2.58
2.14
1.22
1.20
1.18
Cl
S
H
N
O
0.88
1.02
1.86
2.00
3.82
2.05
2.86
3.00
f1 (ppm)

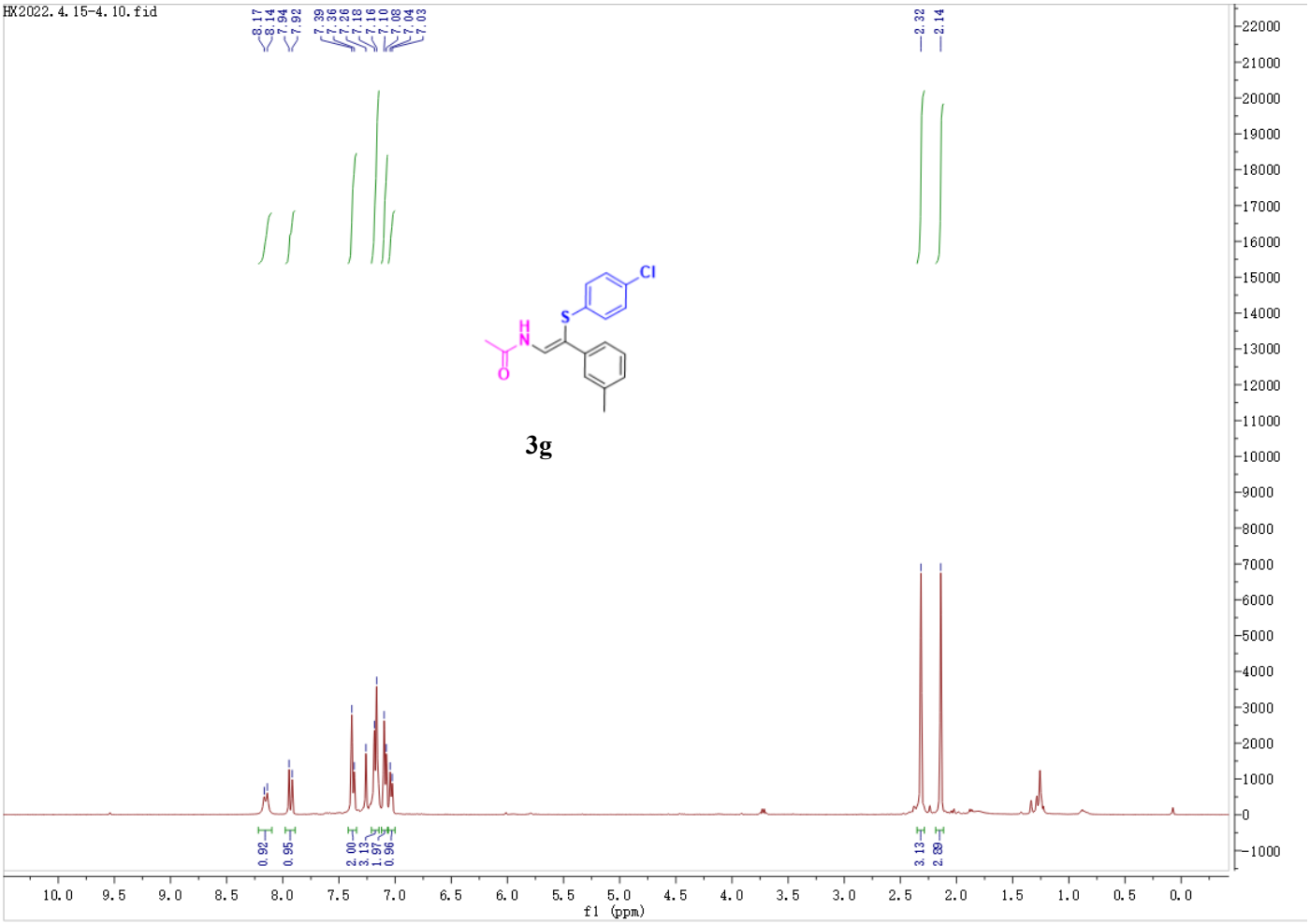
3e


HX.22.4.18-1.20.fid
167.7
144.0
134.7
133.4
131.9
129.5
129.4
128.4
128.1
126.4
111.6
77.5
77.2
76.9
28.6
23.8
15.6
f1 (ppm)

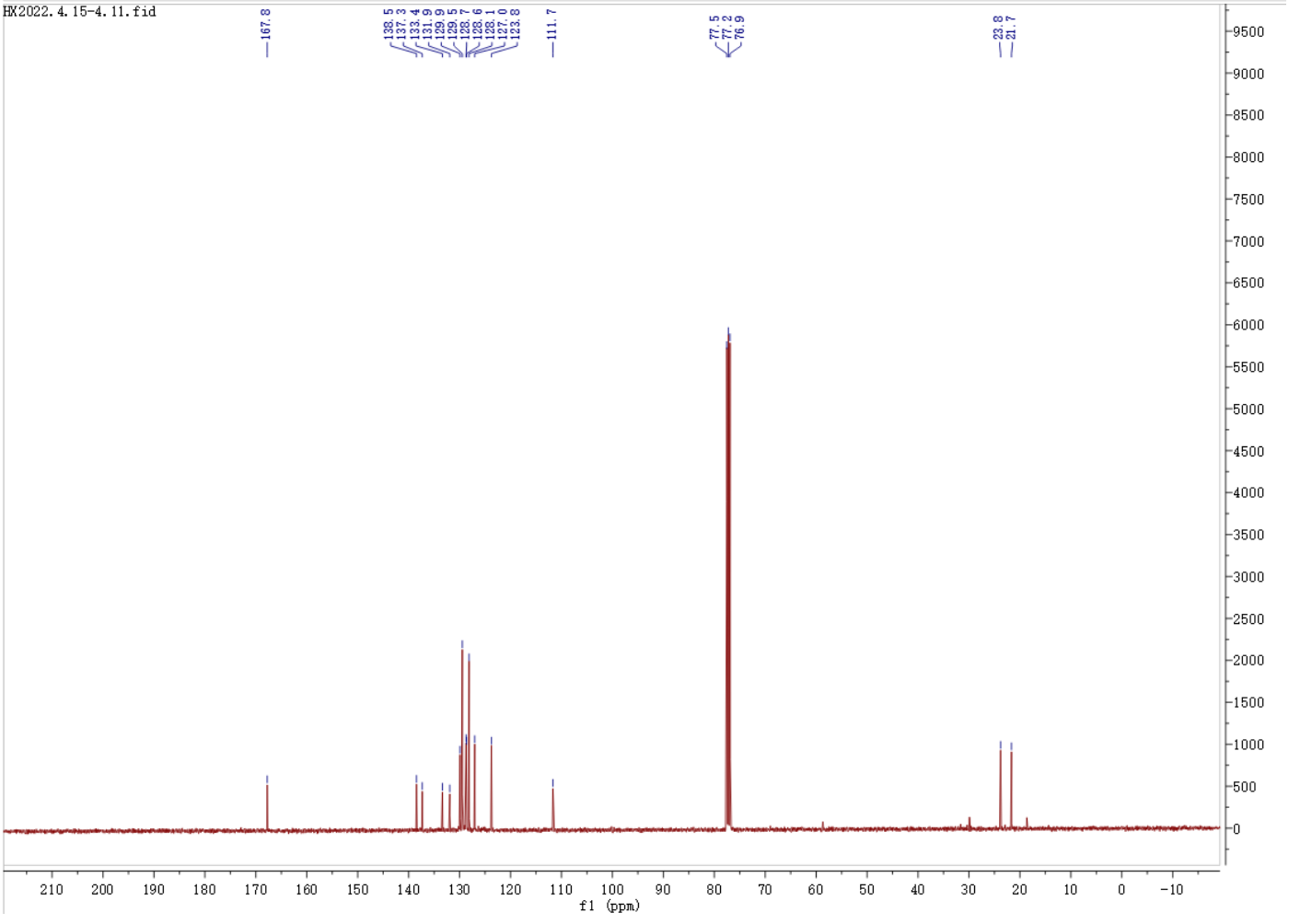

HX2022.4.15-6.10.fid
8.17
8.15
7.95
7.92
7.72
7.50
7.48
7.34
7.32
7.26
7.20
7.18
7.16
7.14
7.12
7.08
7.06
2.16
Cl
S
H
N
O
Br
0.99
1.06
1.00
1.10
1.14
2.07
1.24
2.03
3.09
f1 (ppm)

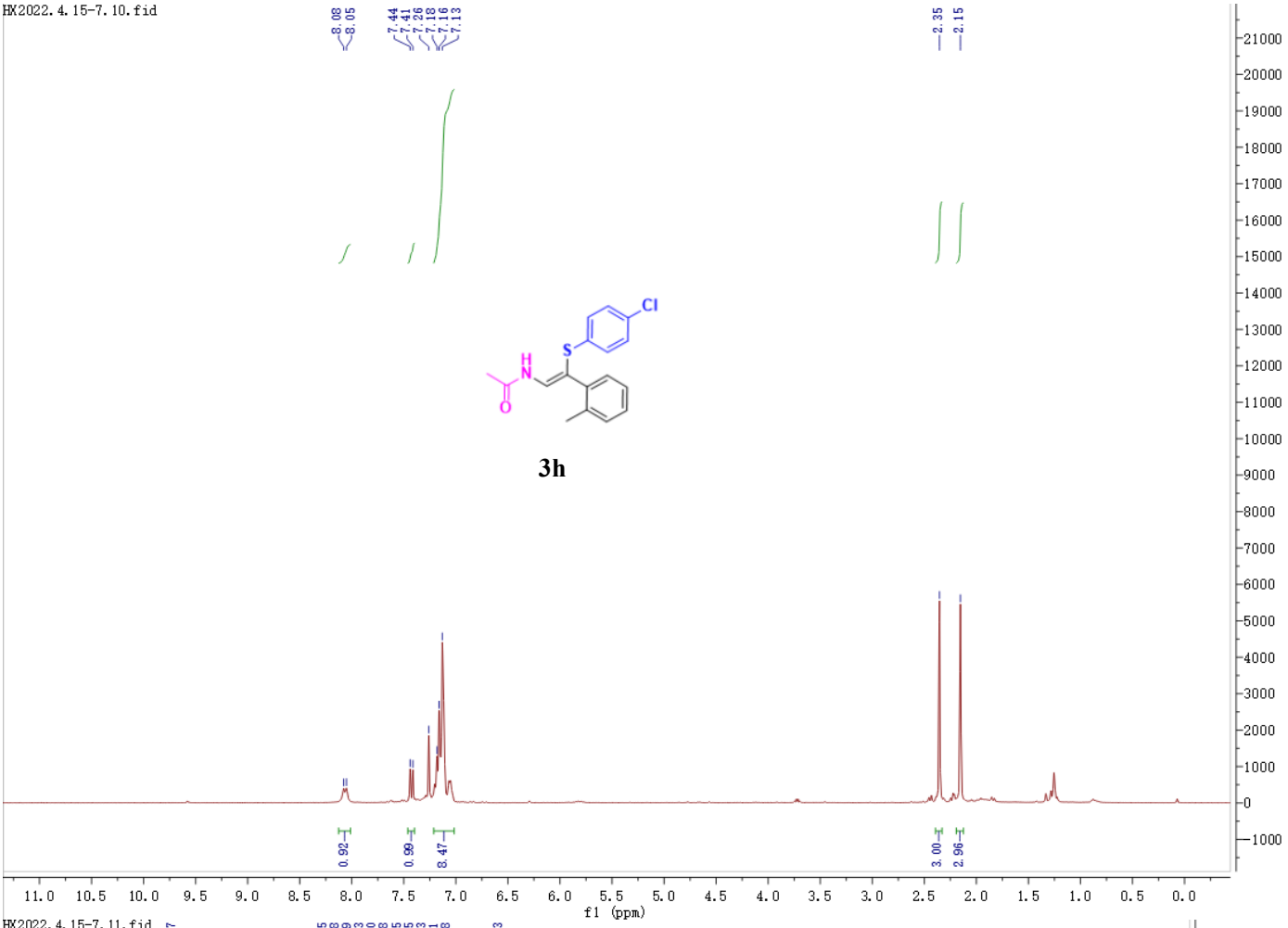
3f


HX2022.4.15-6.11.fid
167.6
139.5
132.5
132.2
130.8
130.5
130.1
129.4
129.1
128.1
124.9
122.9
110.1
77.4
77.0
76.7
23.6
f1 (ppm)

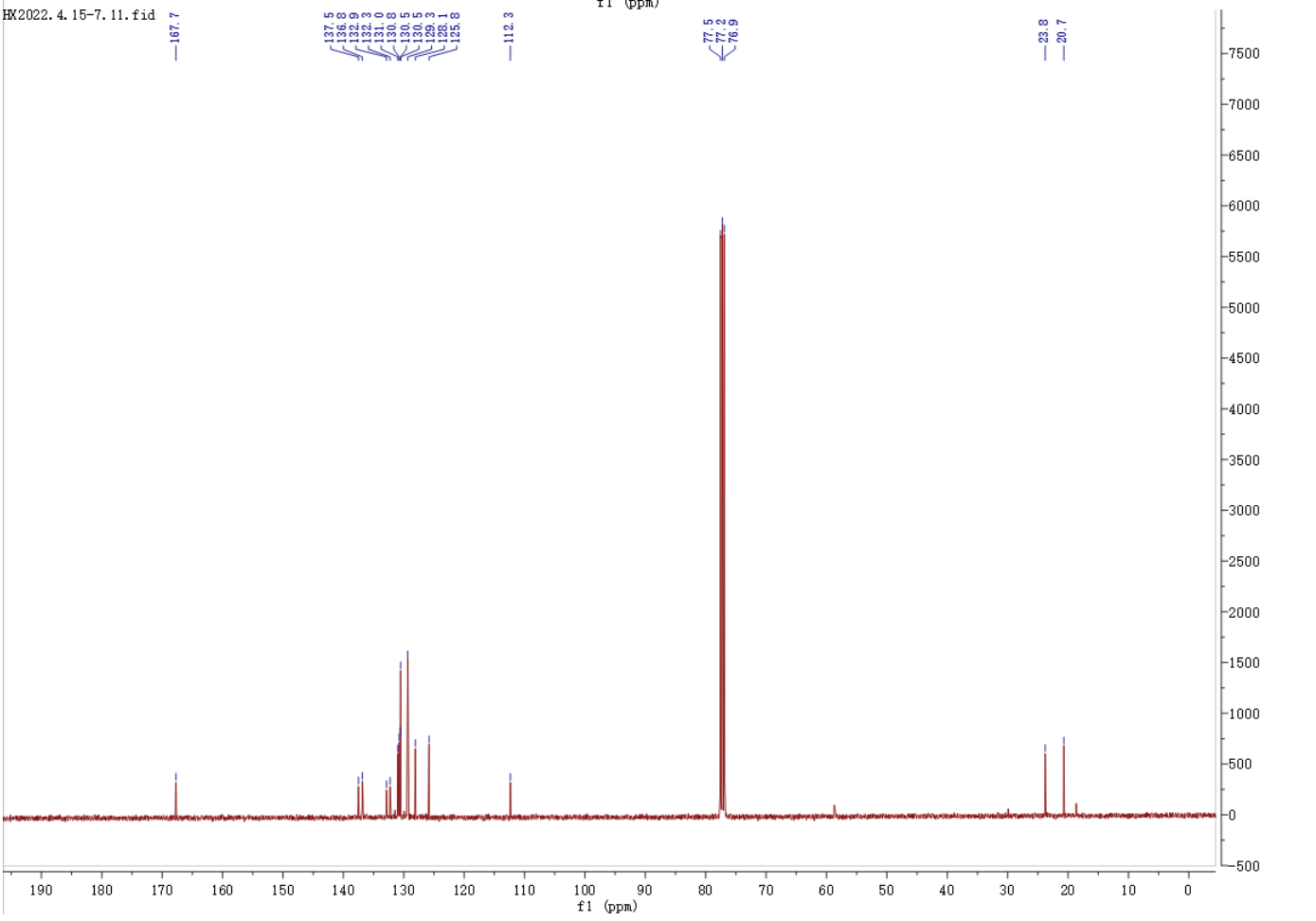

HX2022.4.15-4.10.fid
8.17
8.14
7.94
7.92
7.39
7.36
7.26
7.18
7.16
7.10
7.08
7.04
7.03
2.32
2.14
Cl
S
H
N
O
0.92
0.95
2.00
3.13
1.97
0.96
3.13
2.89
f1 (ppm)

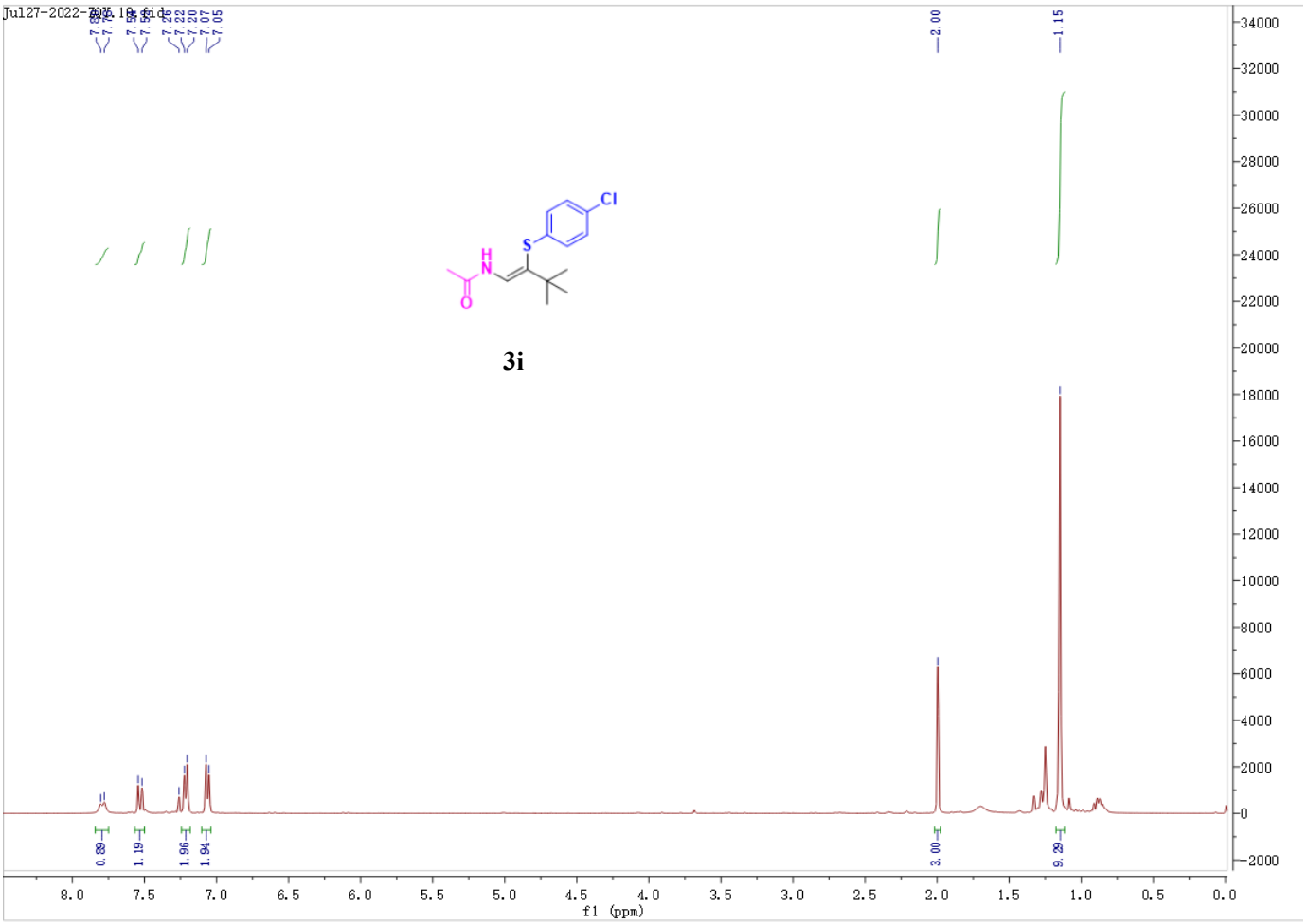
3g


HX2022.4.15-4.11.fid
167.8
138.5
137.3
133.4
131.9
129.5
128.7
128.6
128.1
127.0
123.8
111.7
77.5
77.2
76.9
23.8
21.7
f1 (ppm)

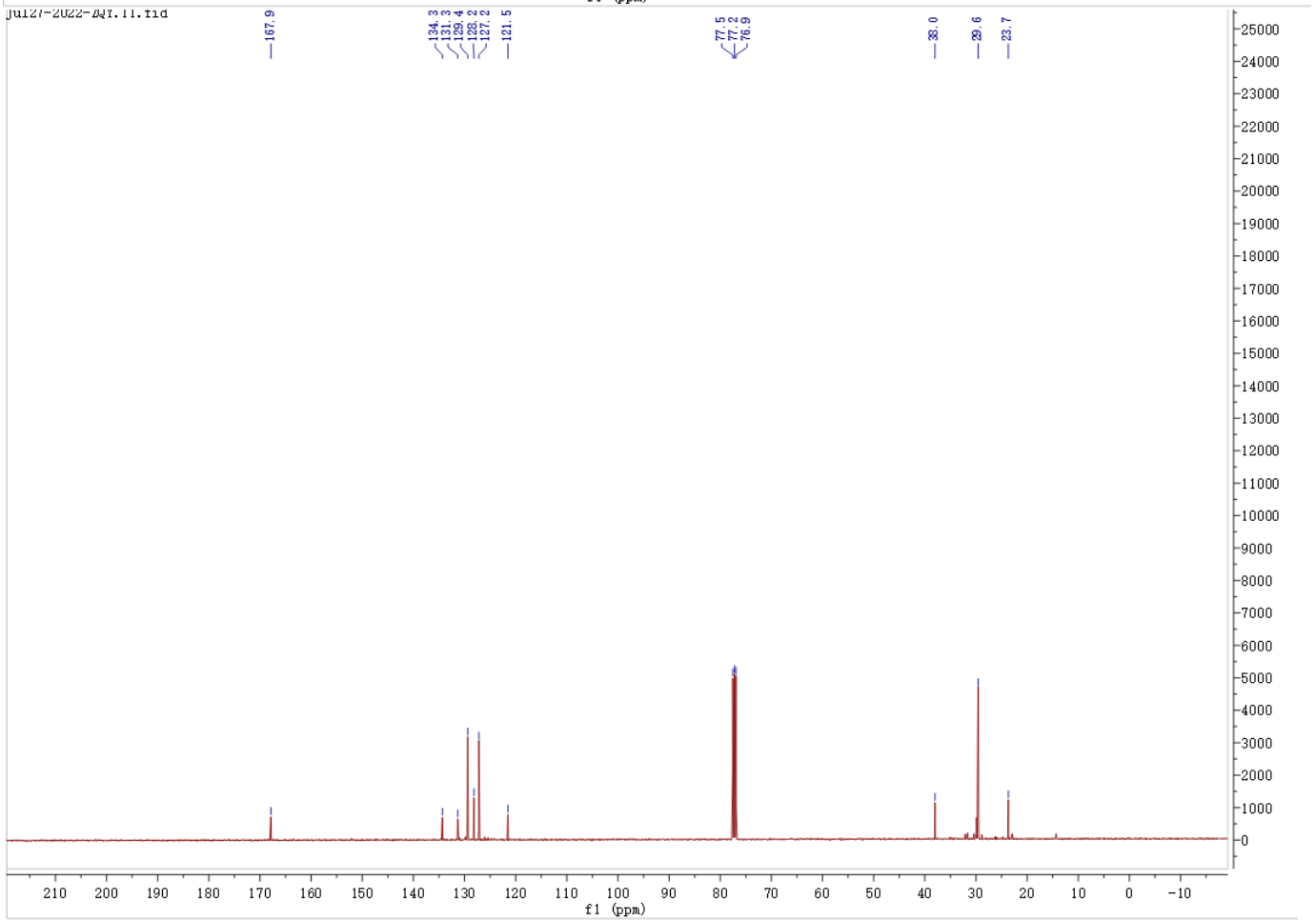

HX2022.4.15-7.10.fid
8.08
8.05
7.44
7.41
7.26
7.18
7.16
7.13
2.35
2.15
Cl
S
H
N
O
0.92
0.99
8.47
3.00
2.96
f1 (ppm)

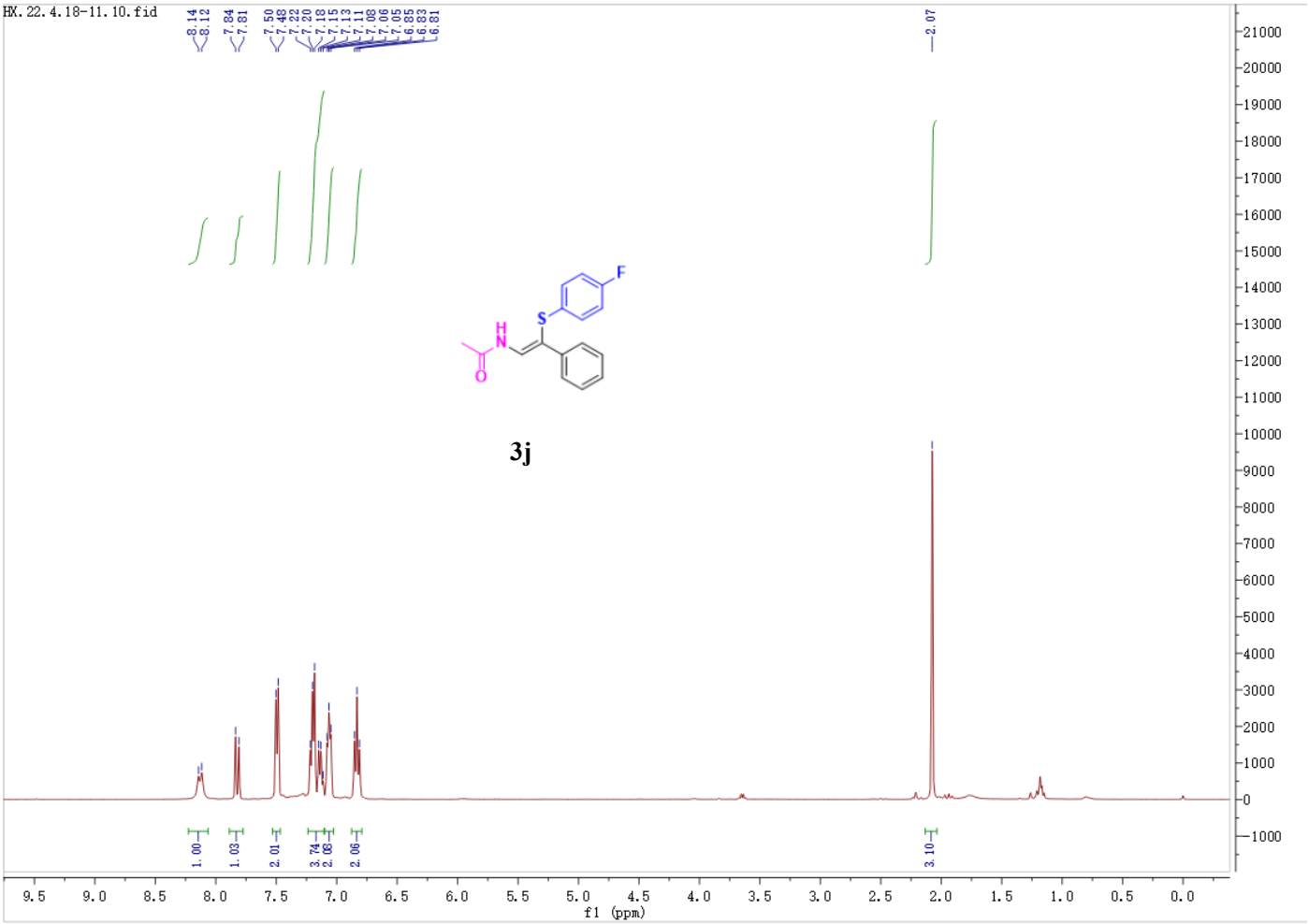
3h


HX2022.4.15-7.11.fid
167.7
137.5
136.8
132.9
132.3
131.0
130.8
130.5
130.5
129.3
128.1
125.8
112.3
77.5
77.2
76.9
23.8
20.7
f1 (ppm)

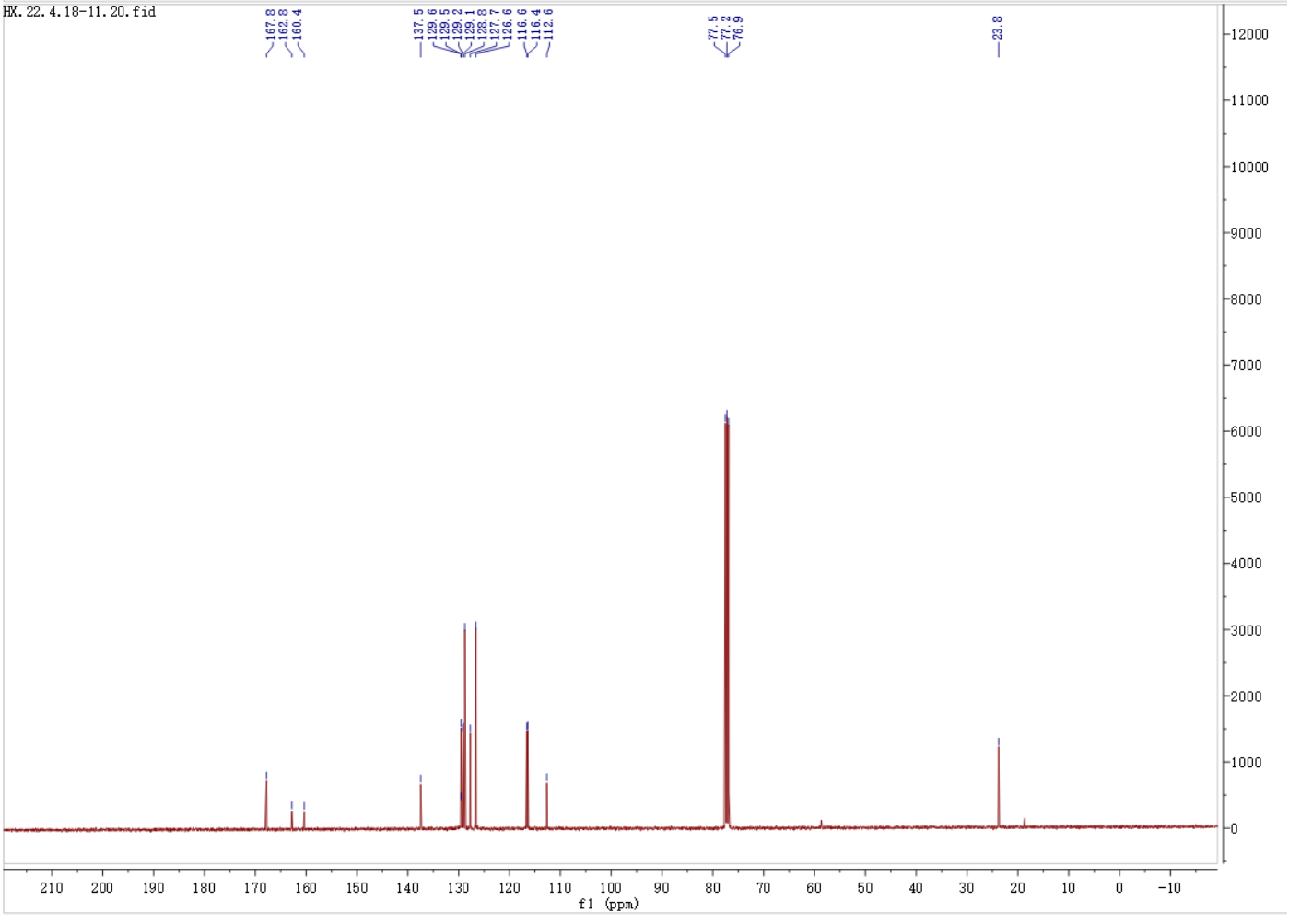

Jul27-2022-ZQX.19.fid
7.69
7.67
7.59
7.57
7.26
7.22
7.20
7.07
7.05
2.00
1.15
Cl
S
H
N
O
0.89
1.19
1.96
1.94
3.00
9.29
f1 (ppm)

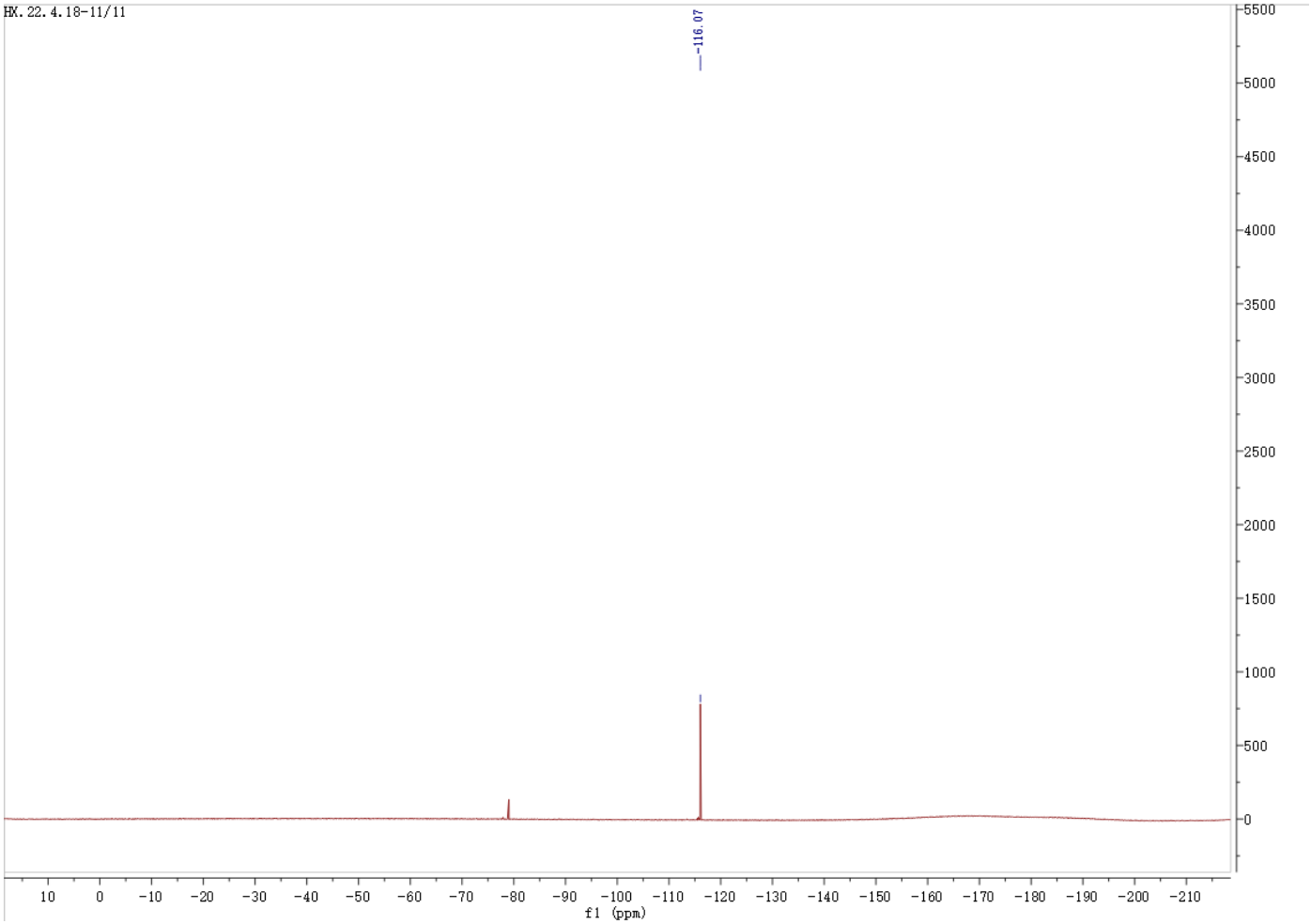
3i

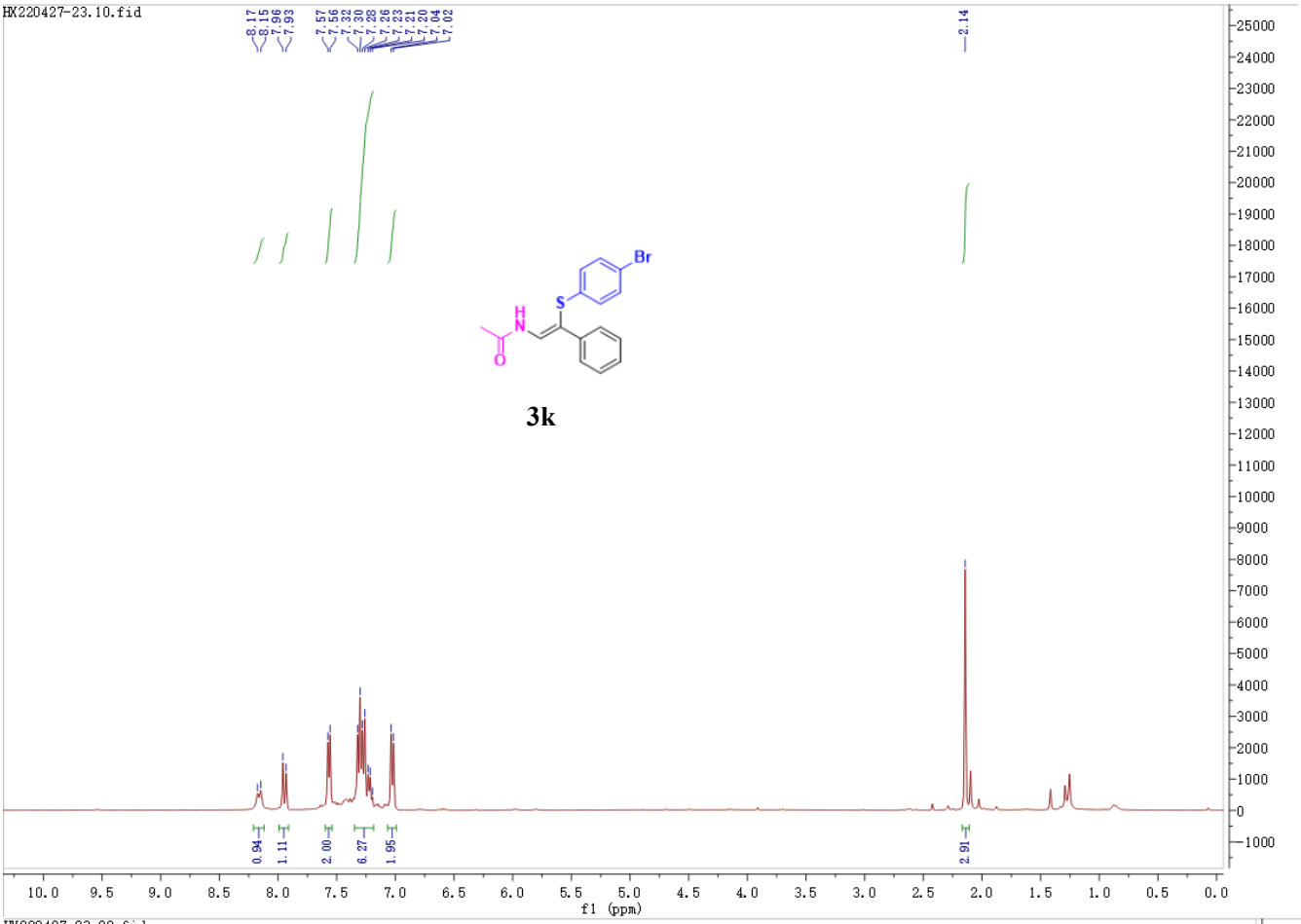

Jul27-2022-ZQX.11.fid
167.9
134.3
131.3
129.4
128.2
127.2
121.5
77.5
77.2
76.9
38.0
29.6
23.7
f1 (ppm)


HX.22.4.18-11.10.fid
8.14
8.12
7.84
7.81
7.50
7.48
7.22
7.20
7.18
7.15
7.13
7.11
7.08
7.06
7.05
6.85
6.83
6.81
2.07
F
S
H
N
O
1.00
1.03
2.01
3.74
2.08
2.06
3.10
f1 (ppm)

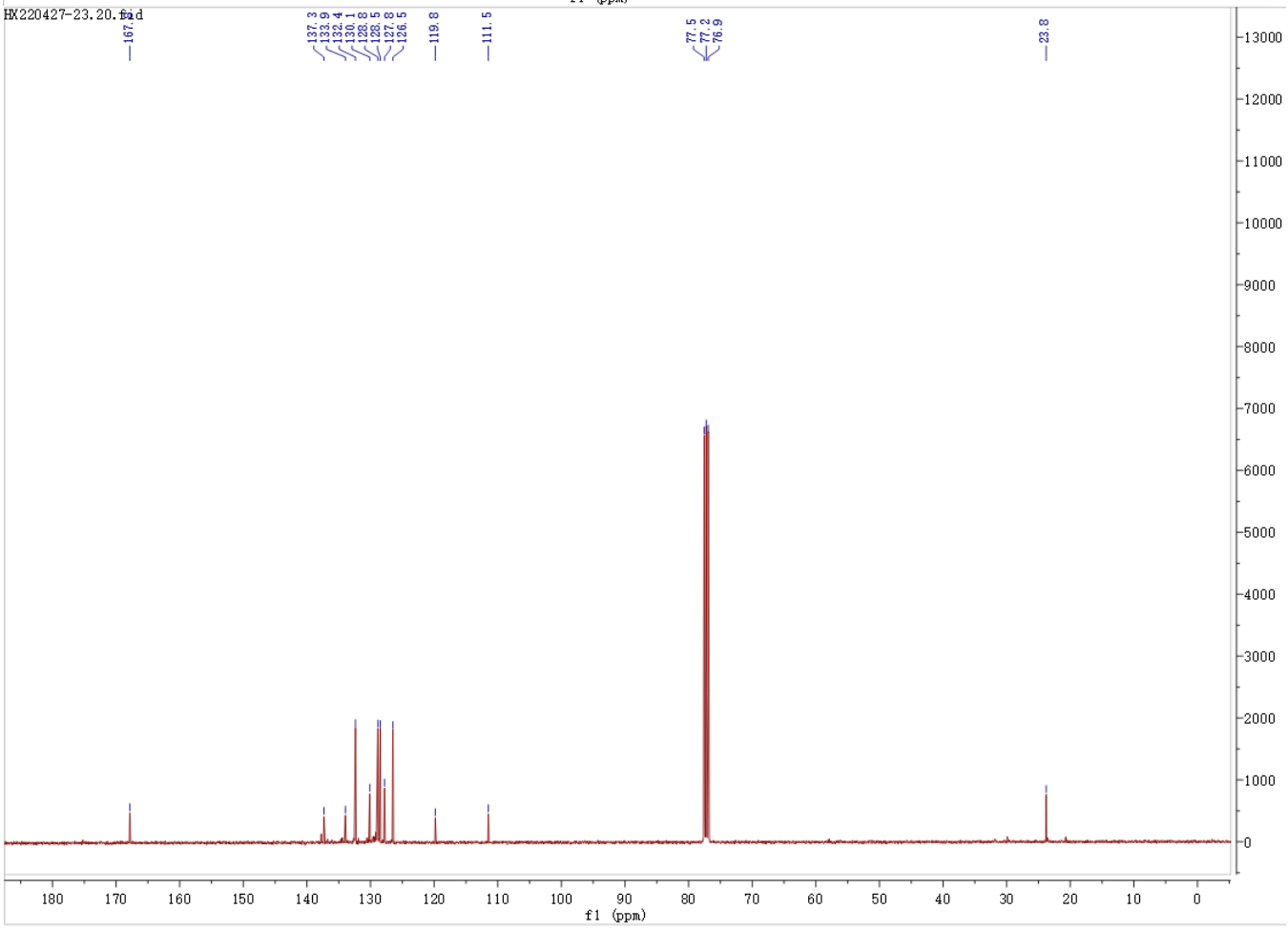
3j

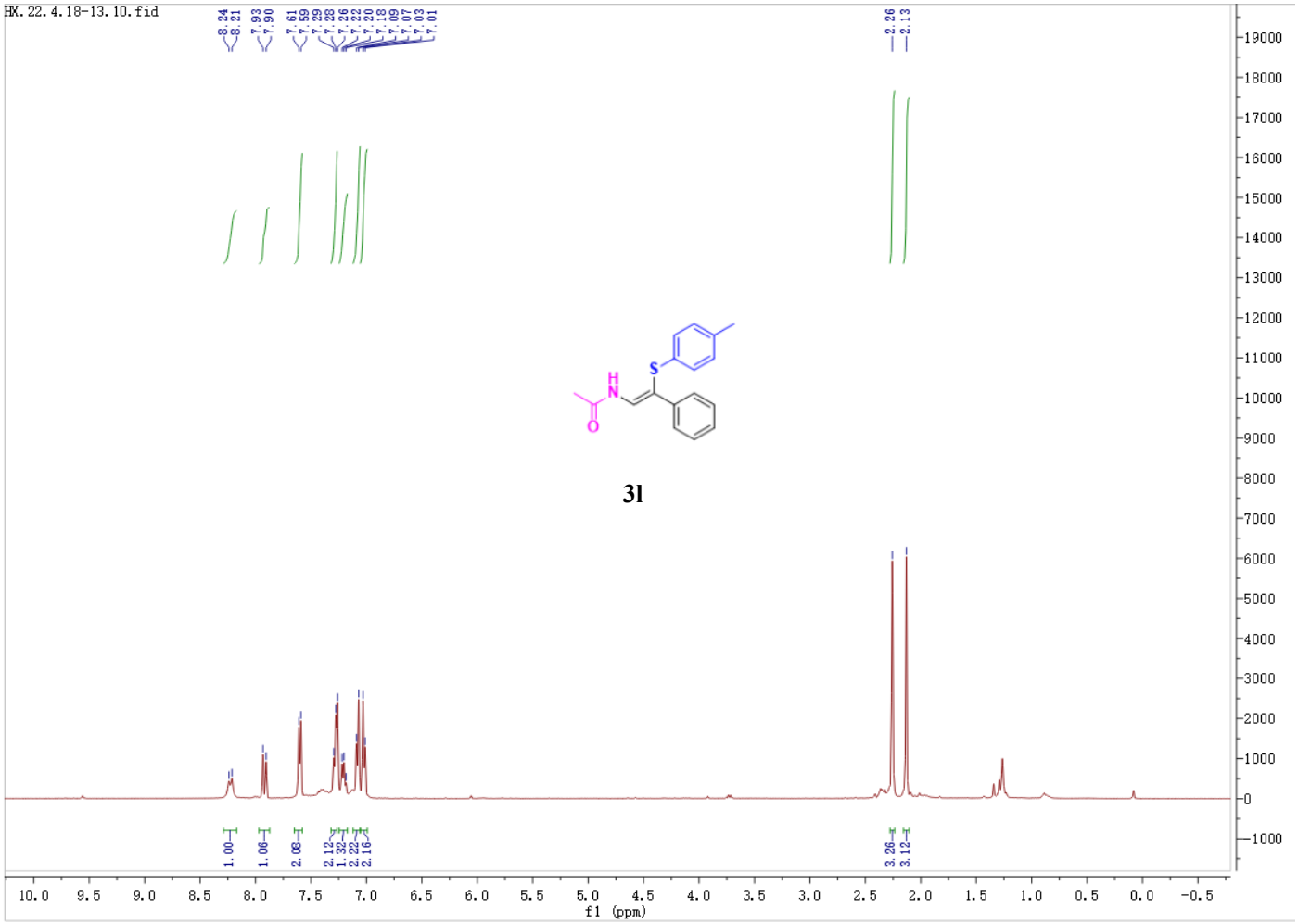

HX.22.4.18-11.20.fid
167.8
162.8
160.4
137.5
129.6
129.5
129.2
129.1
128.8
127.7
126.6
116.6
116.4
112.6
77.5
77.2
76.9
23.8
f1 (ppm)


HX.22.4.18-11/11
-116.07
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

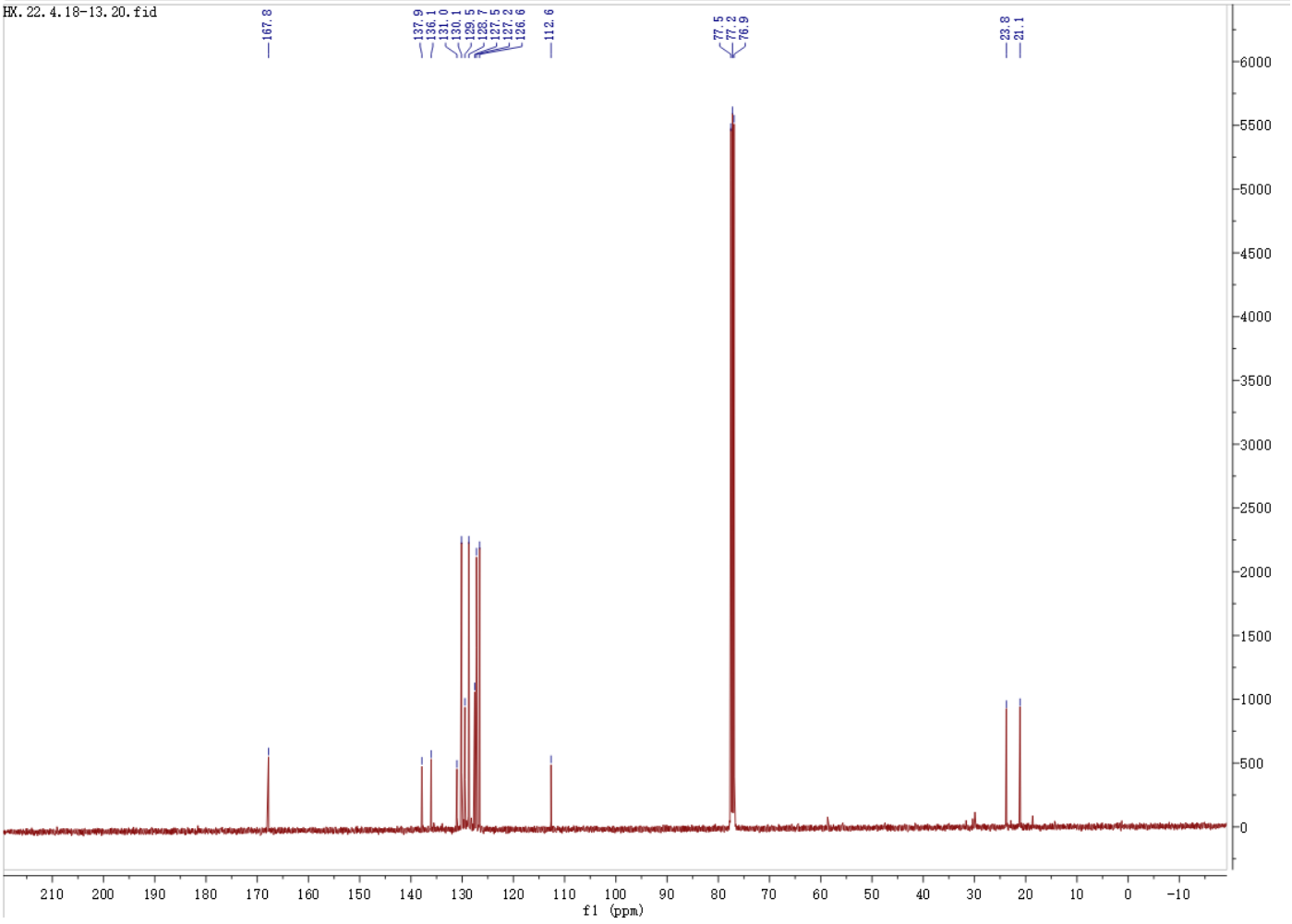

HX220427-23.10.fid
8.17
8.15
7.96
7.93
7.57
7.56
7.32
7.30
7.28
7.26
7.23
7.21
7.20
7.04
7.02
2.14
Br
S
H
N
O
0.94
1.11
2.00
6.27
1.95
2.91
f1 (ppm)

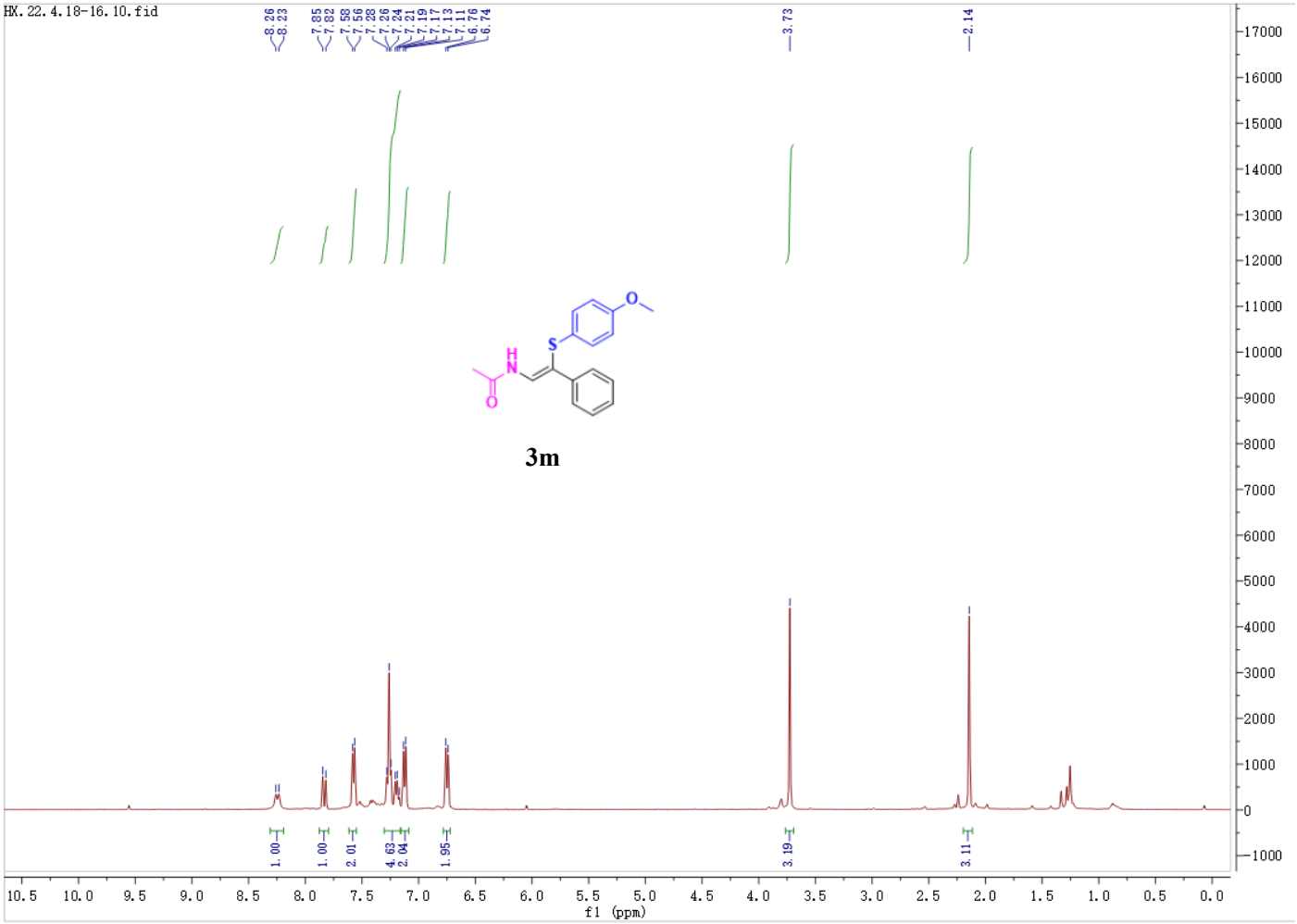
3k


HX220427-23.20.fid
167.2
137.3
133.9
133.4
130.1
128.8
128.5
127.8
126.5
119.8
111.5
77.5
77.2
76.9
23.8
f1 (ppm)

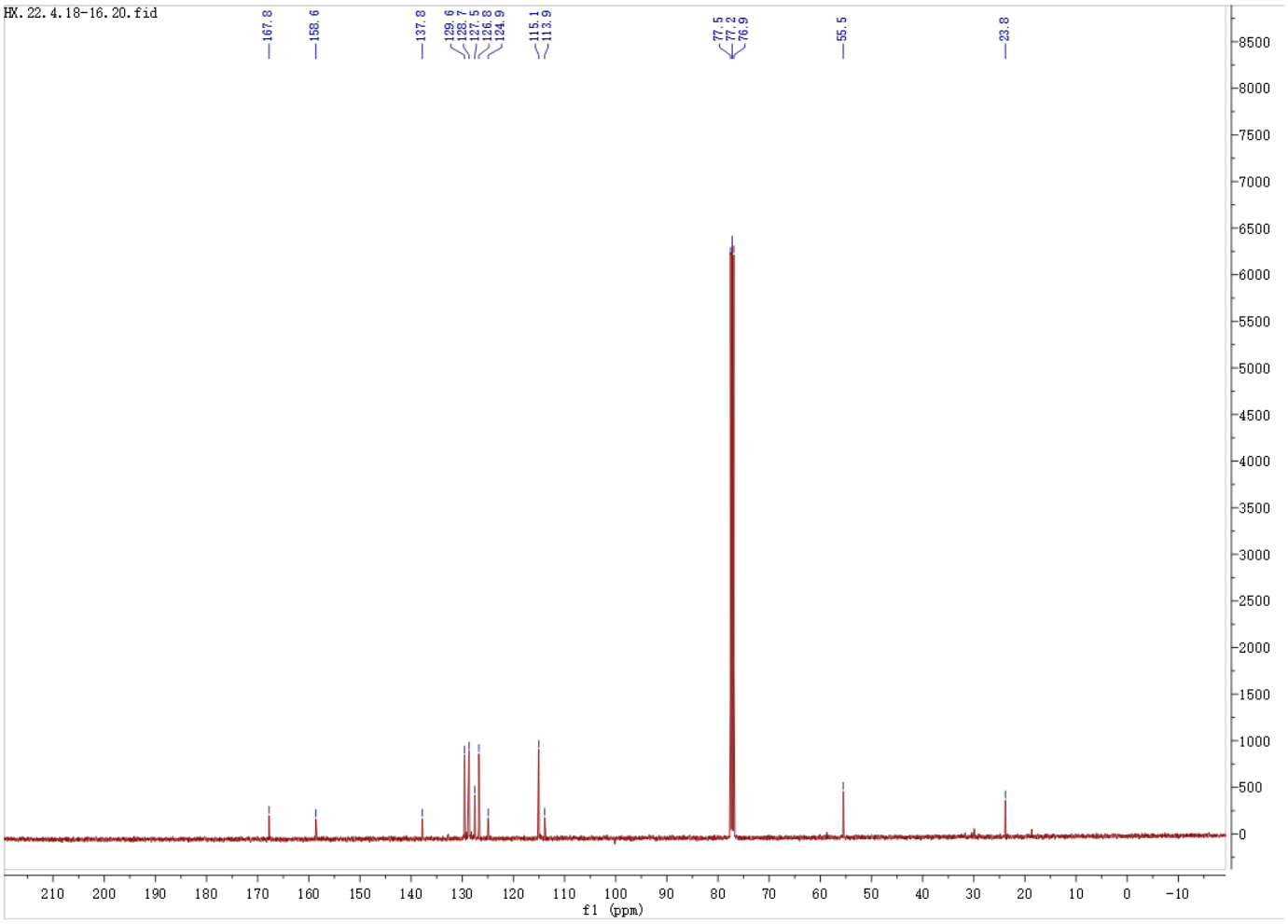

HX.22.4.18-13.10.fid
8.24
8.21
7.93
7.90
7.61
7.59
7.29
7.28
7.26
7.22
7.20
7.18
7.09
7.07
7.03
7.01
2.26
2.13
1.00
1.06
2.08
2.12
1.32
2.22
2.16
3.26
3.12
f1 (ppm)

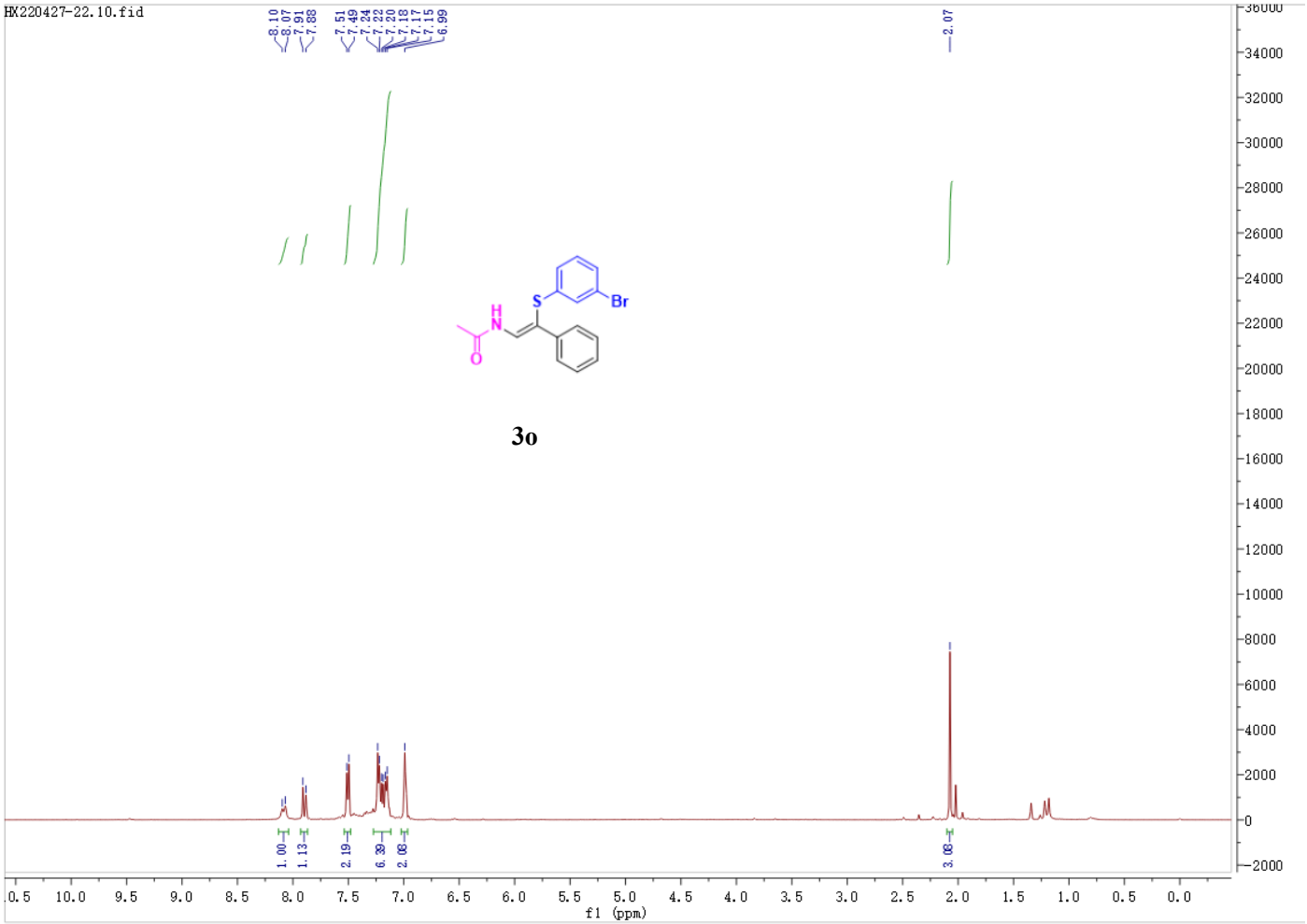
31


HX.22.4.18-13.20.fid
167.8
137.9
136.1
131.0
130.1
129.5
128.7
127.5
127.2
126.6
112.6
77.5
77.2
76.9
23.8
21.1
f1 (ppm)

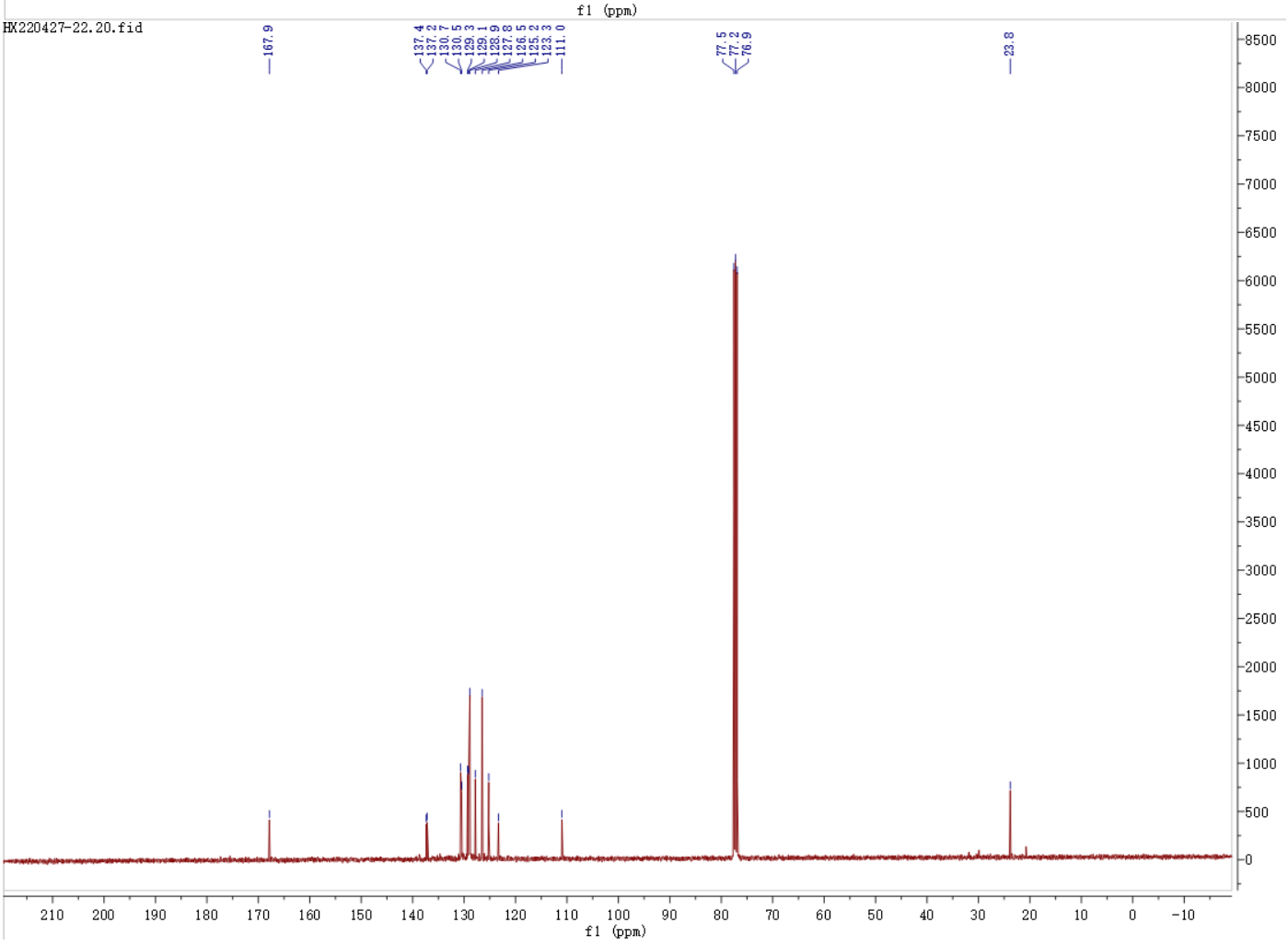

HX.22.4.18-16.10.fid
8.26
8.23
7.85
7.82
7.58
7.56
7.28
7.26
7.24
7.21
7.19
7.17
7.13
7.11
6.76
6.74
3.73
2.14
1.00
1.00
2.01
4.63
2.04
1.95
3.19
3.11
f1 (ppm)

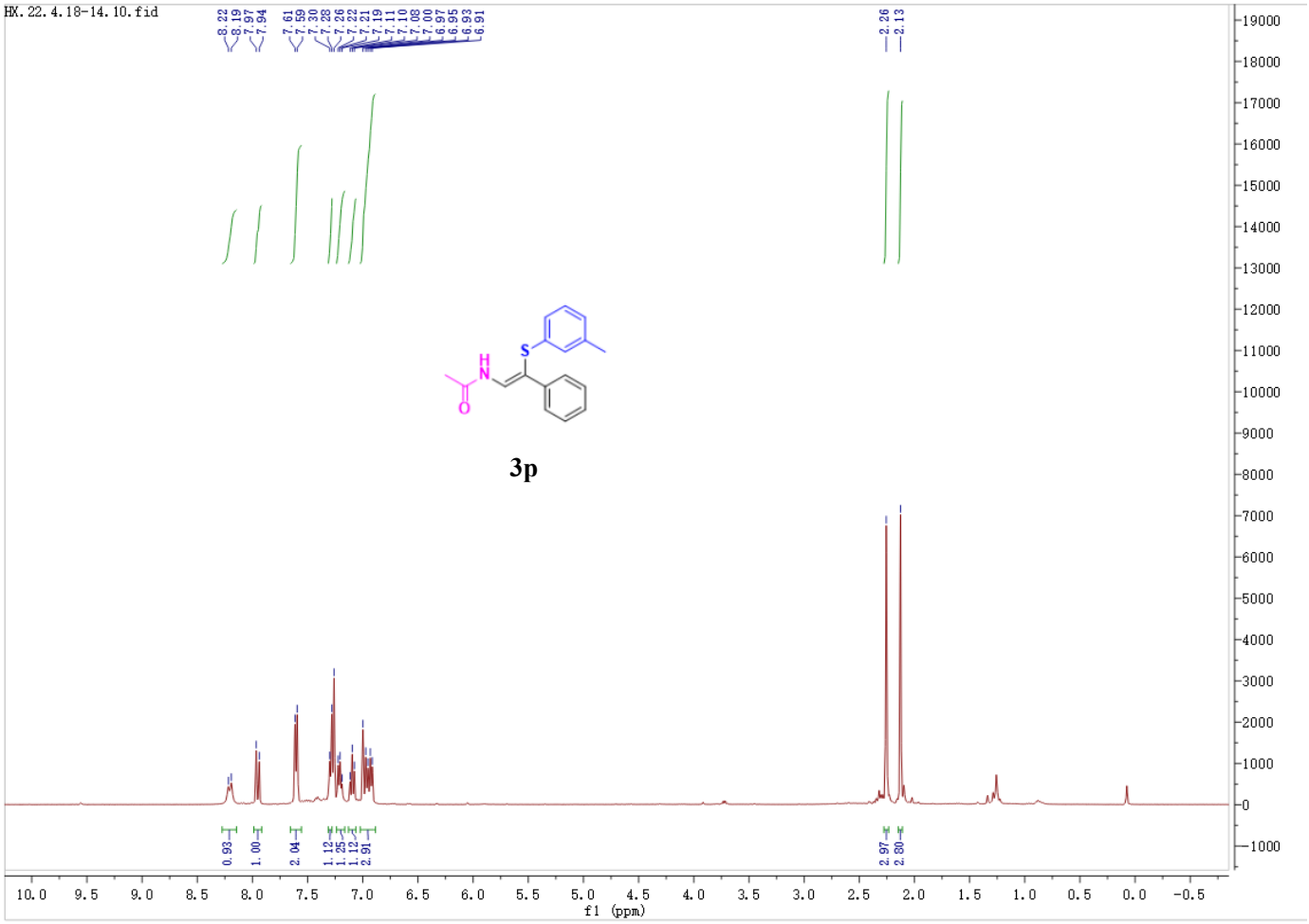
3m


HX.22.4.18-16.20.fid
167.8
158.6
137.8
129.6
128.7
127.5
126.8
124.9
115.1
113.9
77.5
77.2
76.9
55.5
23.8
f1 (ppm)

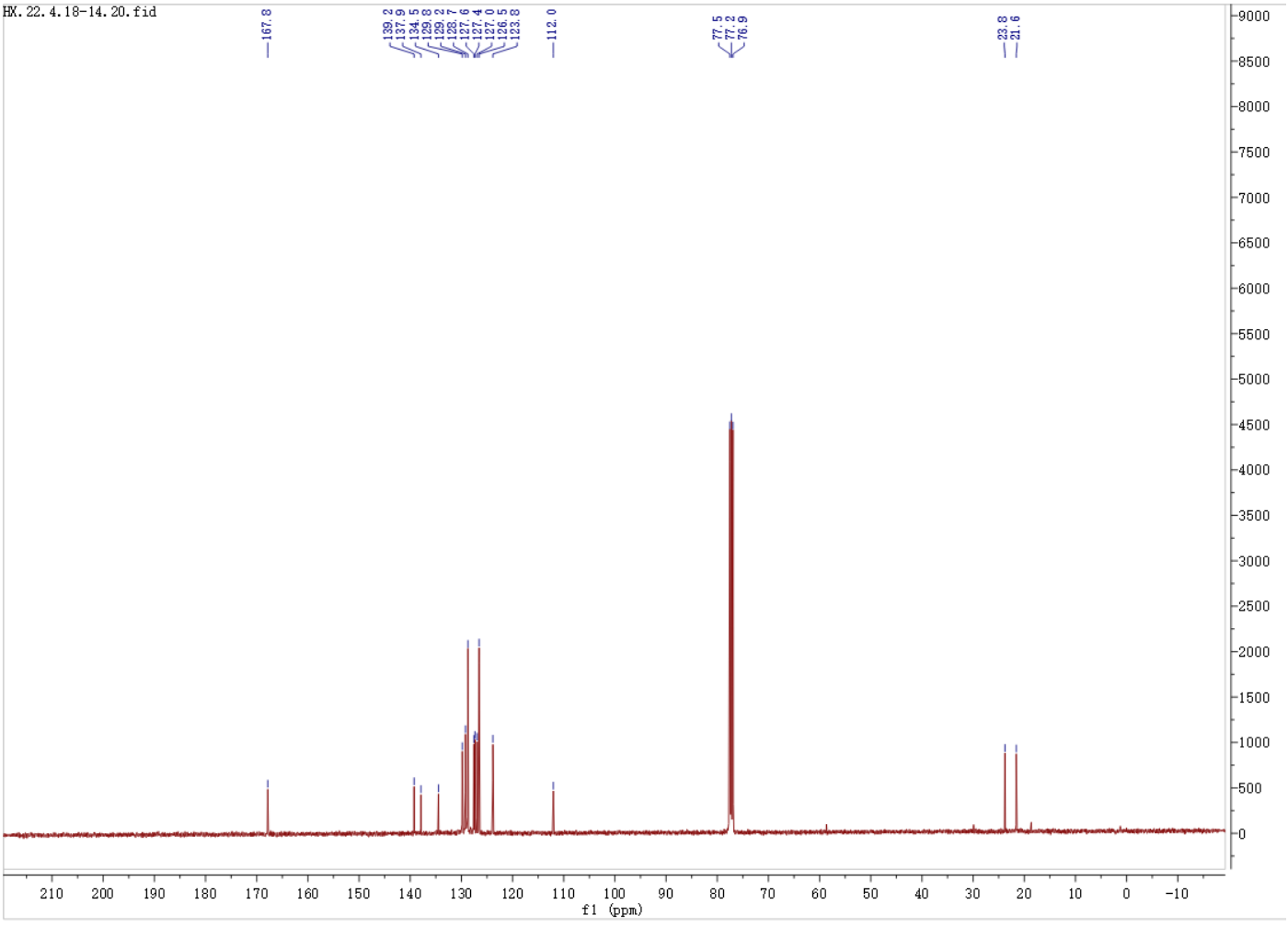

HX220427-22.10.fid
8.10
8.07
7.91
7.88
7.51
7.49
7.24
7.22
7.20
7.18
7.17
7.15
6.99
2.07
1.00
1.13
2.19
6.39
2.08
3.08
f1 (ppm)

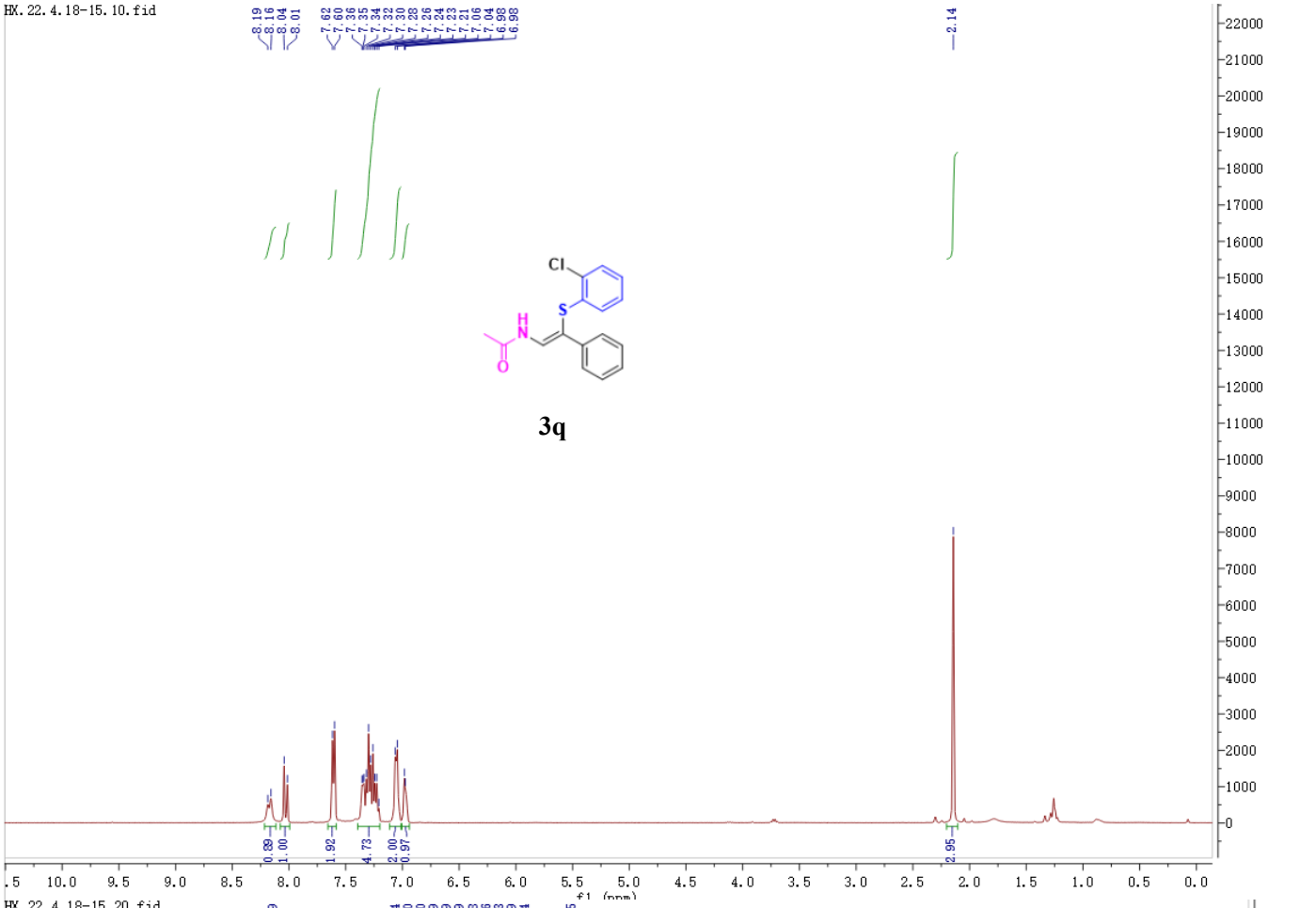
3o


HX220427-22.20.fid
167.9
137.4
137.2
130.7
130.5
129.3
129.1
128.9
127.8
126.5
125.2
123.3
111.0
77.5
77.2
76.9
23.8
f1 (ppm)

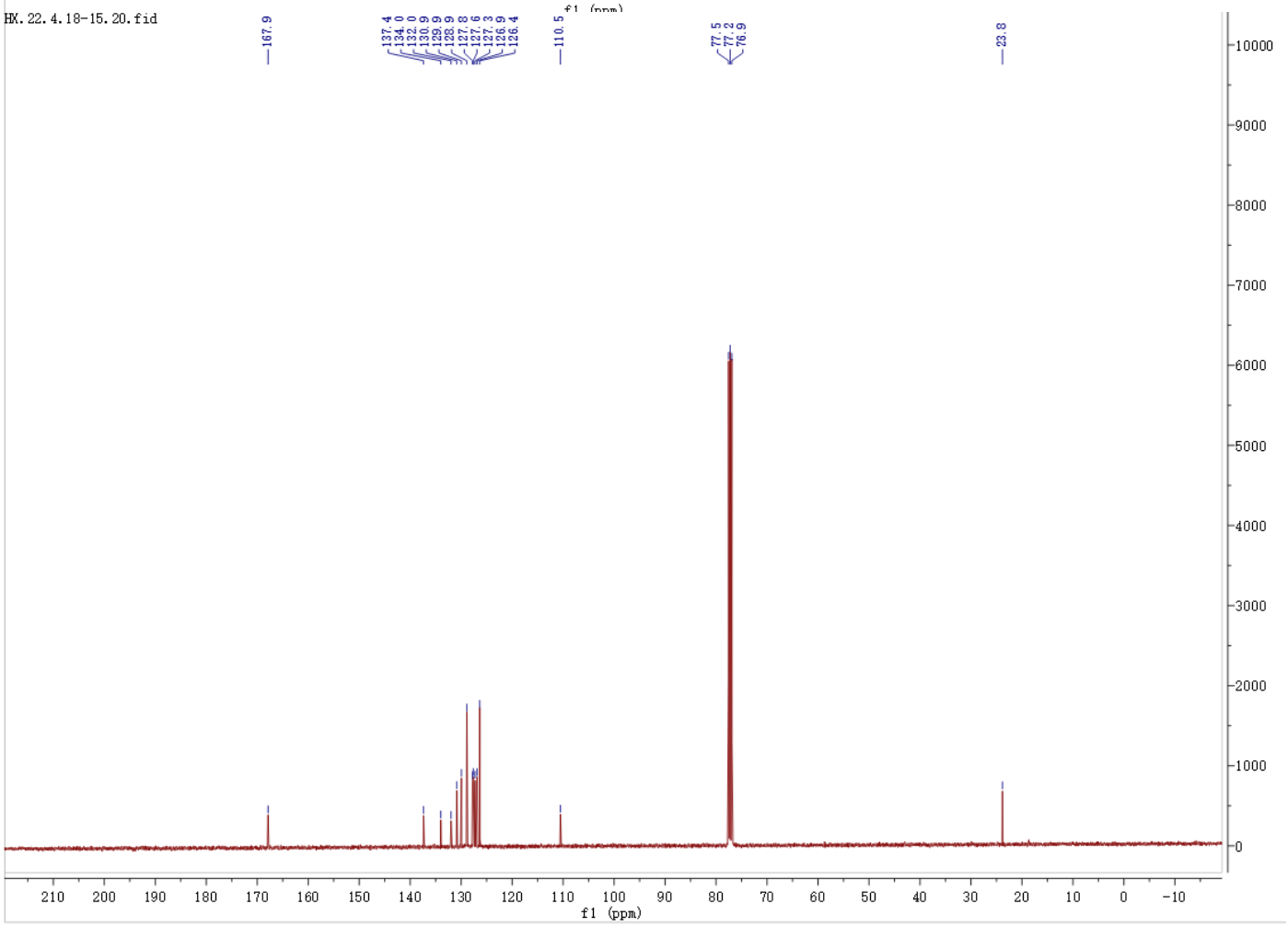

HX.22.4.18-14.10.fid
8.22
8.19
7.97
7.94
7.61
7.59
7.30
7.28
7.26
7.22
7.21
7.19
7.11
7.10
7.08
7.00
6.97
6.95
6.93
6.91
2.26
2.13
0.93
1.00
2.04
1.12
1.25
1.12
2.91
2.97
2.80
f1 (ppm)

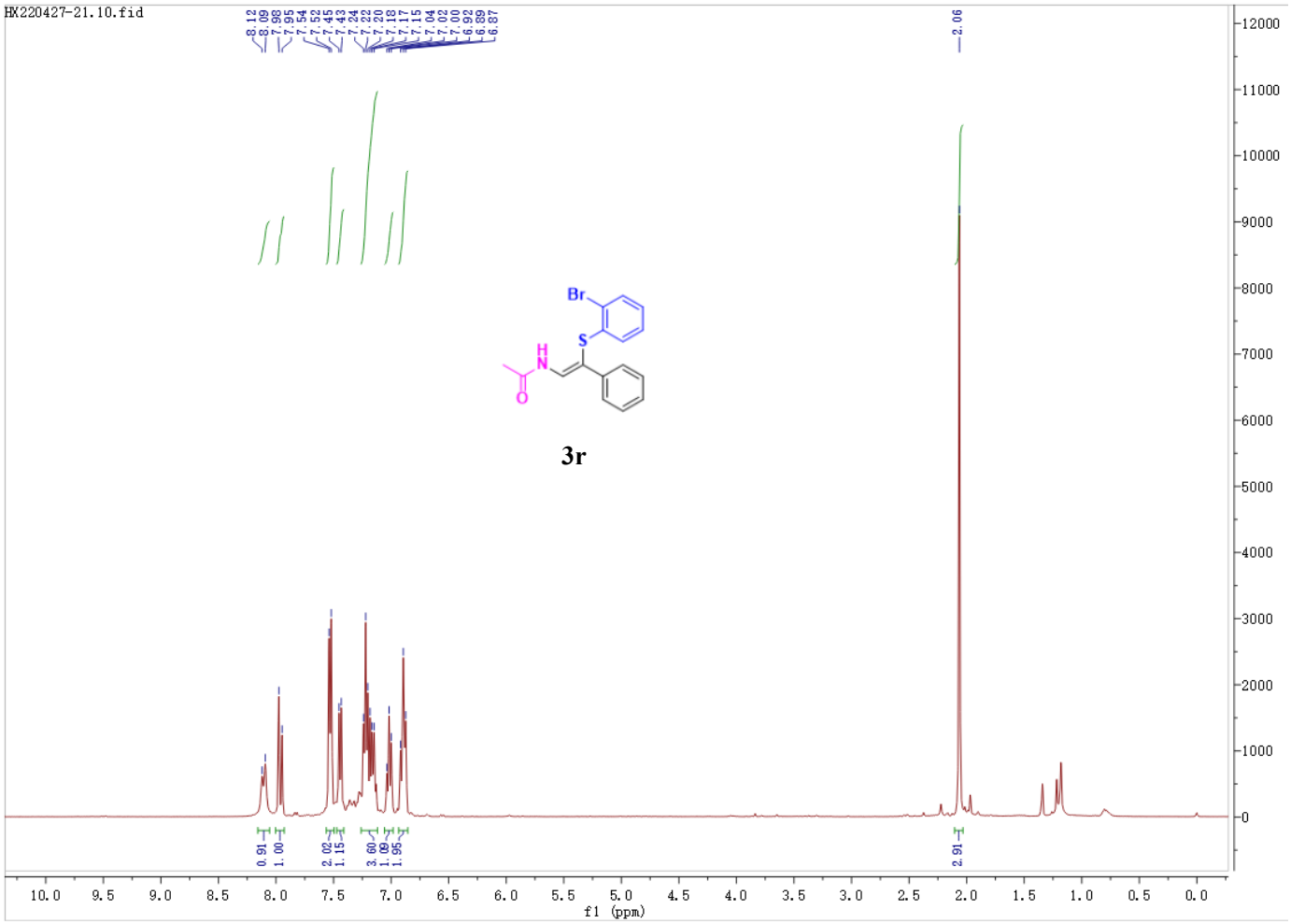
3p


HX.22.4.18-14.20.fid
167.8
139.2
137.9
134.5
129.8
129.3
128.7
127.6
127.4
127.0
126.5
123.8
112.0
77.5
77.2
76.9
23.8
21.6
f1 (ppm)

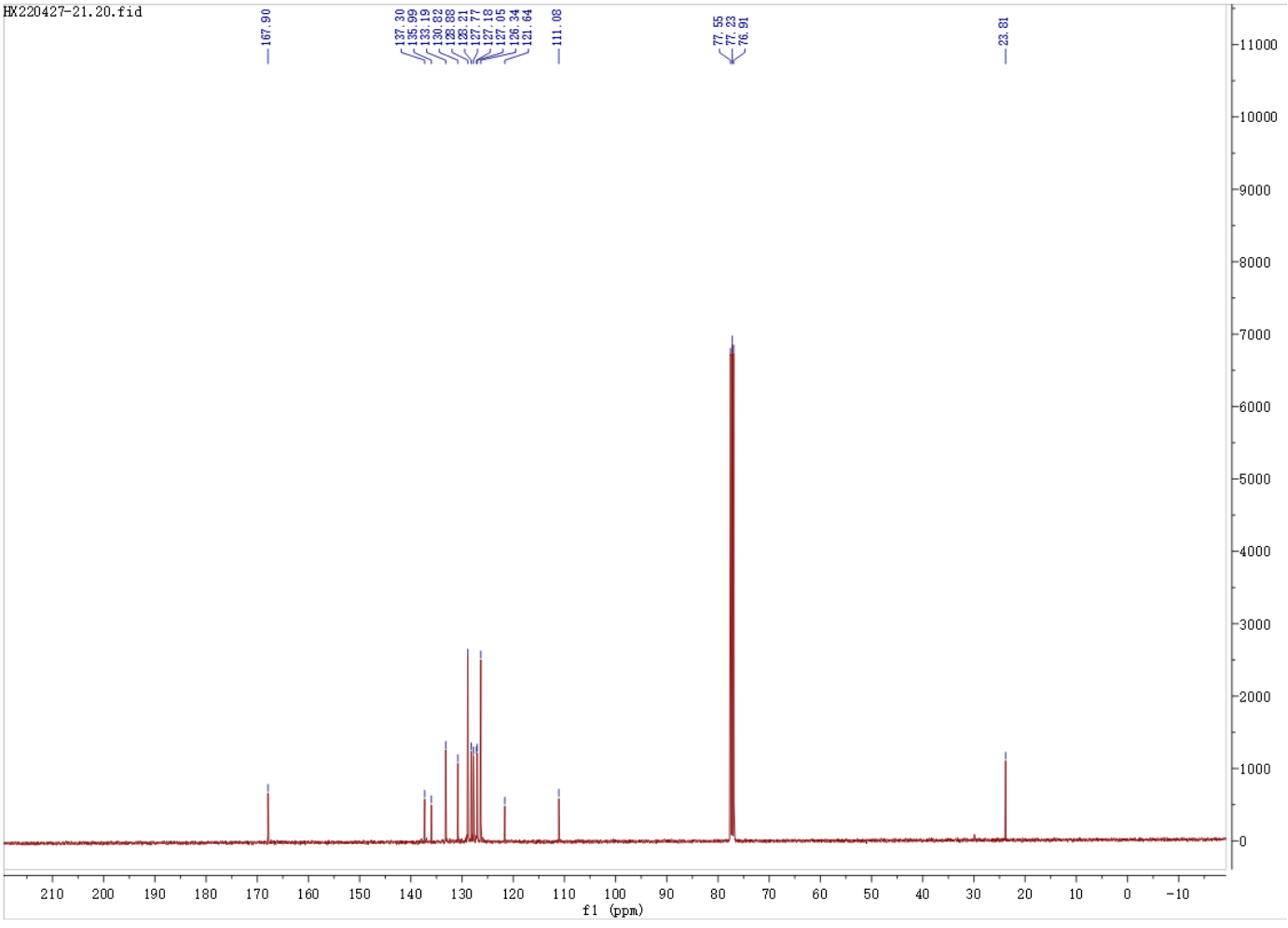

HX.22.4.18-15.10.fid
8.19
8.16
8.04
8.01
7.62
7.60
7.36
7.35
7.34
7.32
7.30
7.28
7.26
7.24
7.23
7.21
7.16
7.04
6.98
6.98
2.14
Cl
S
H
N
O
0.89
1.00
1.92
4.73
2.00
0.97
2.95
f1 (ppm)

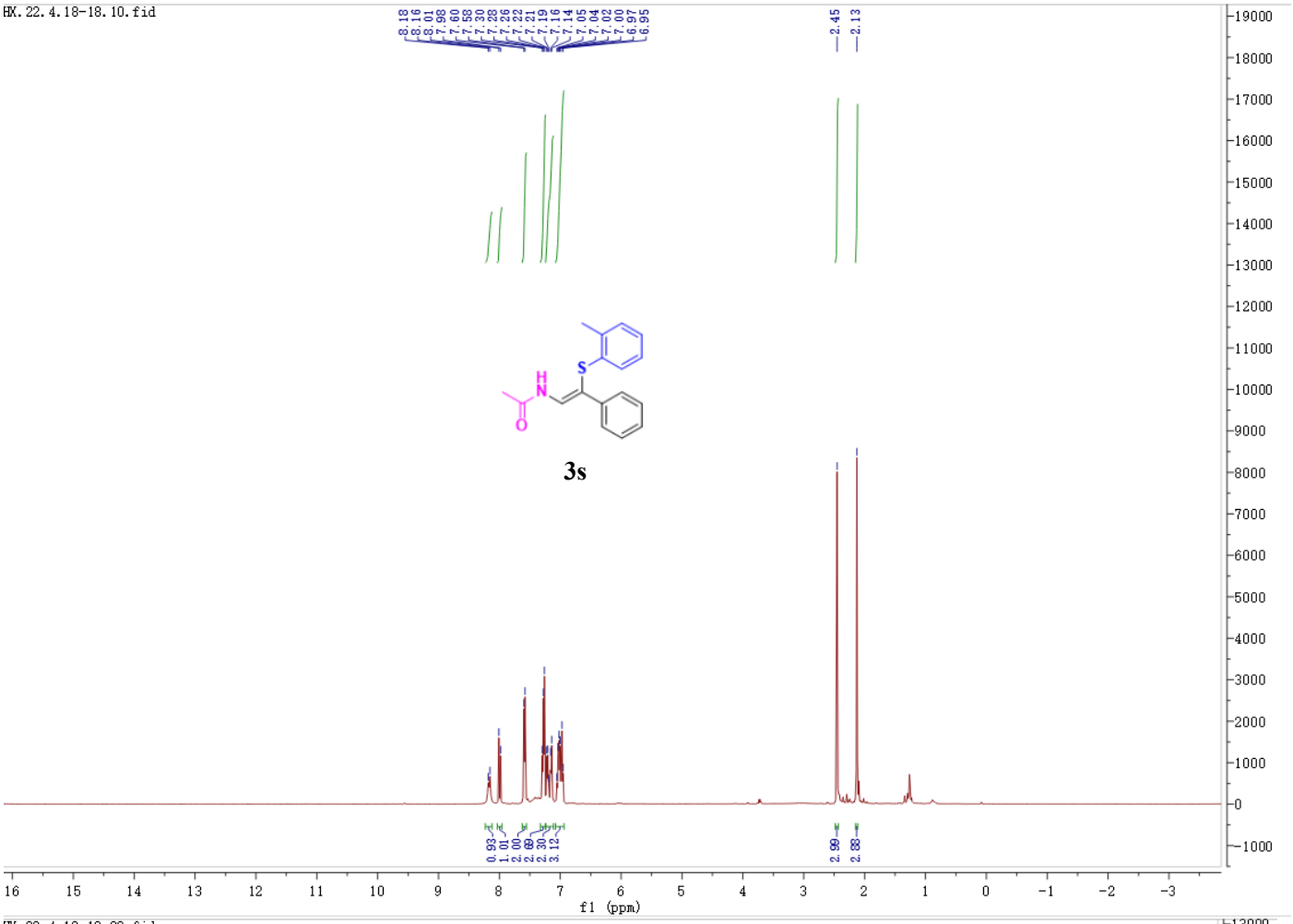
3q


HX.22.4.18-15.20.fid
167.9
137.4
134.0
132.0
130.9
129.9
128.9
127.8
127.6
127.3
126.9
126.4
110.5
77.5
77.2
76.9
23.8
f1 (ppm)

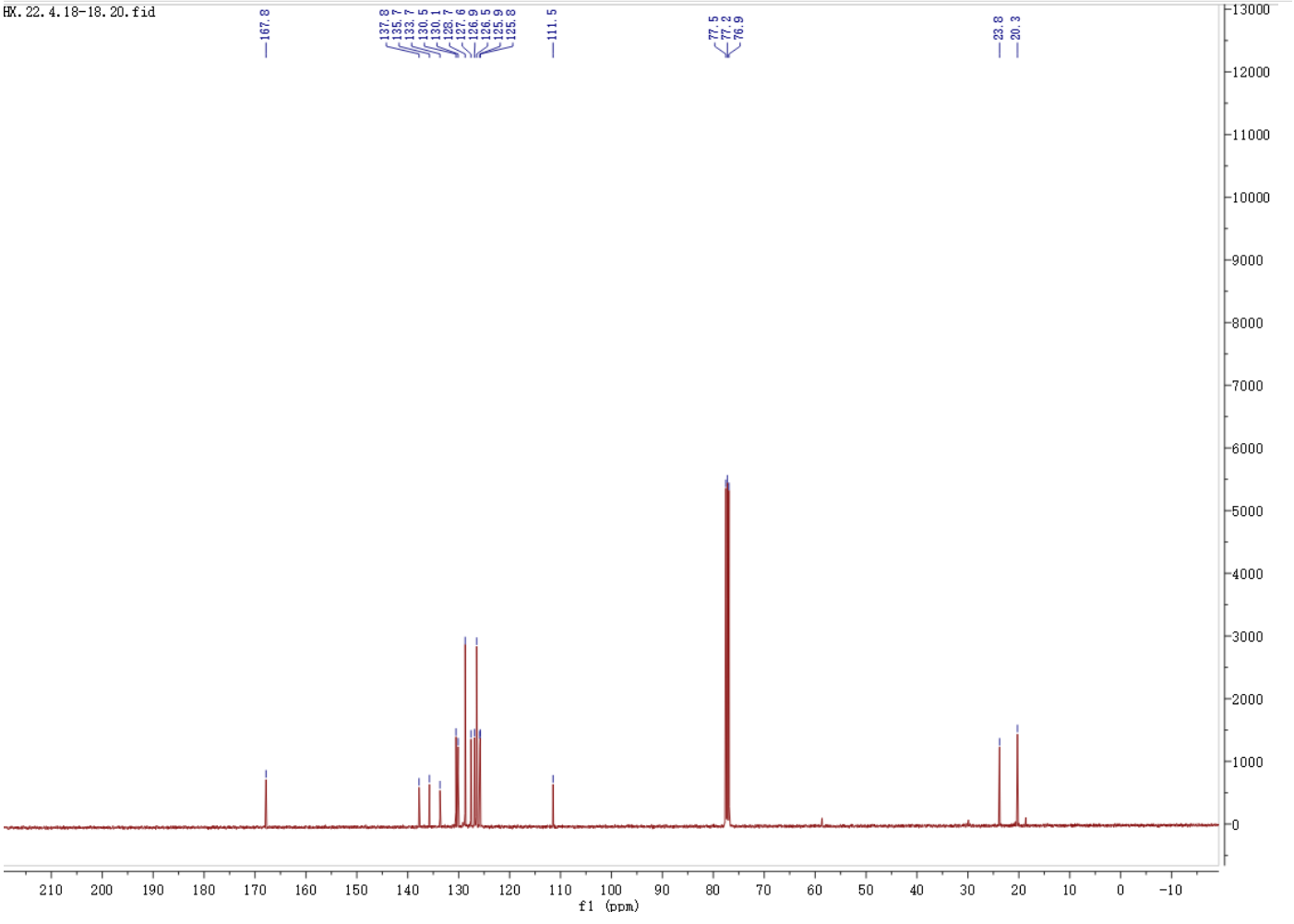

HX220427-21.10.fid
8.12
8.09
7.98
7.95
7.54
7.52
7.45
7.43
7.24
7.22
7.20
7.18
7.17
7.15
7.04
7.02
7.00
6.92
6.89
6.87
2.06
Br
S
H
N
O
0.91
1.00
2.02
1.15
3.60
1.09
1.95
2.91
f1 (ppm)

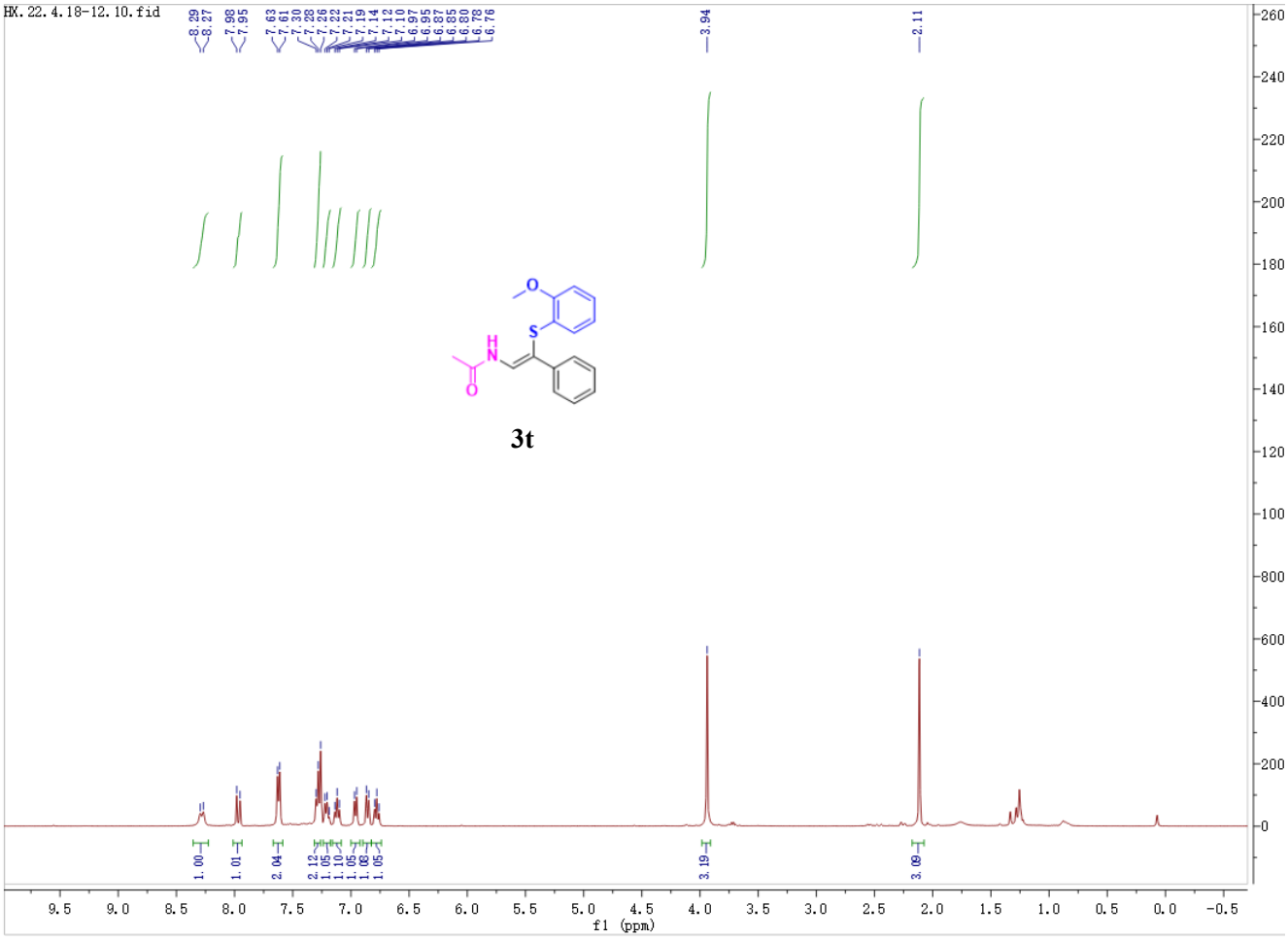
3r


HX220427-21.20.fid
167.90
137.30
135.99
133.19
130.82
128.88
128.21
127.77
127.18
127.05
126.34
121.64
111.08
77.55
77.23
76.91
23.81
f1 (ppm)

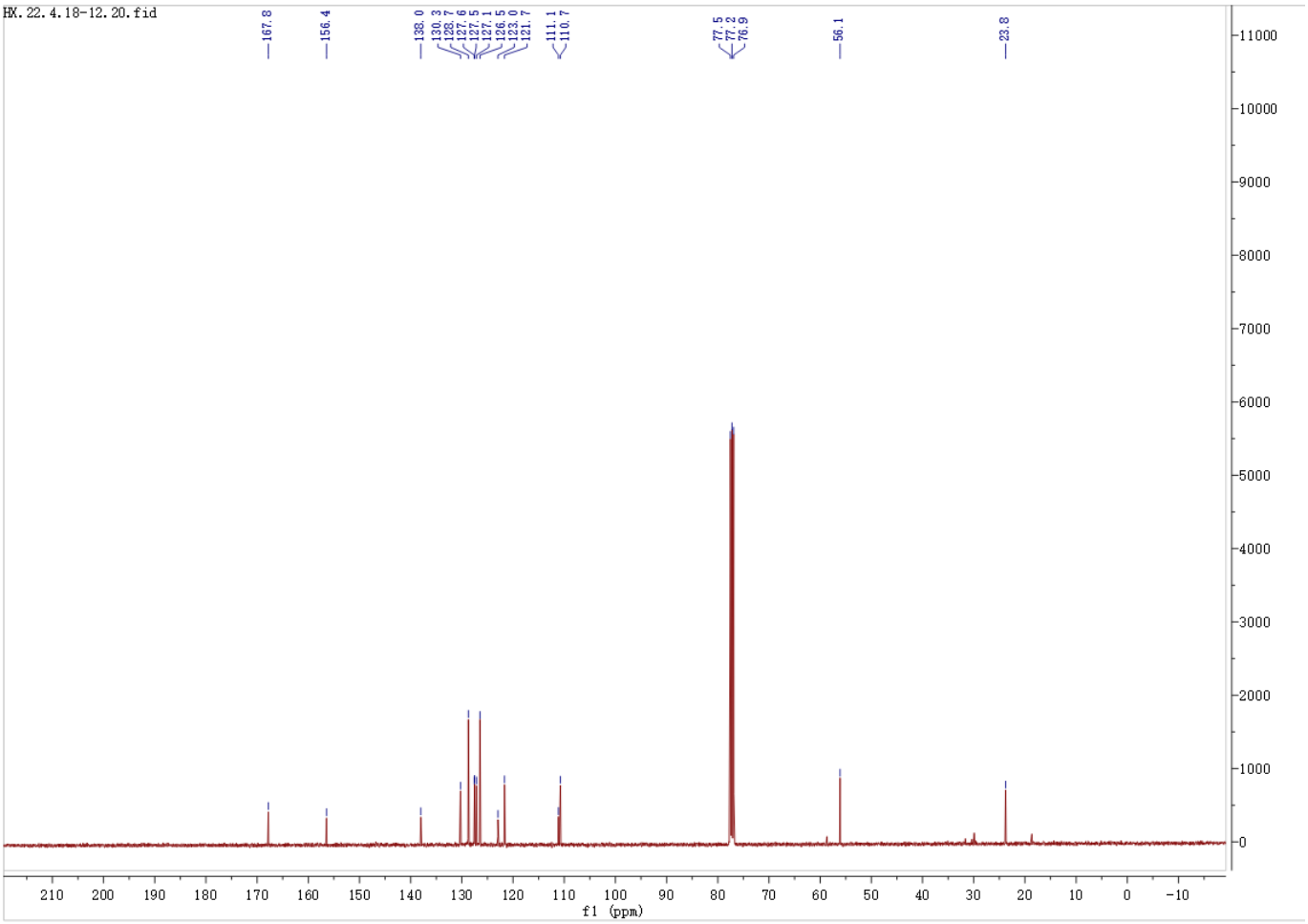

HX.22.4.18-18.10.fid
8.18
8.16
8.01
7.98
7.60
7.58
7.30
7.28
7.26
7.22
7.21
7.19
7.16
7.14
7.05
7.04
7.02
7.00
6.97
6.95
2.45
2.13
0.93
1.01
2.00
2.09
2.30
3.12
2.99
2.88
f1 (ppm)

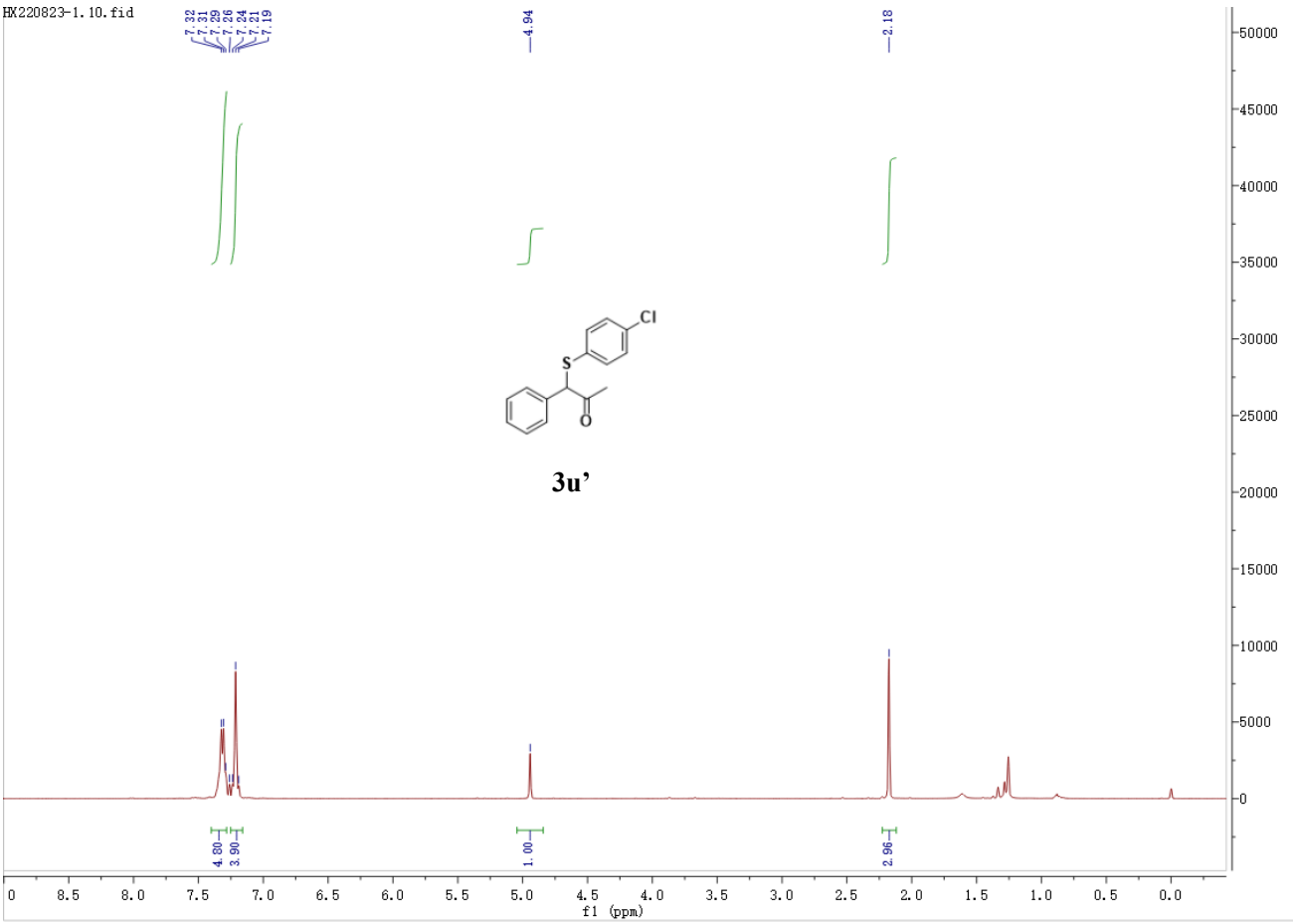
3s


HX.22.4.18-18.20.fid
167.8
137.8
135.7
133.7
130.5
130.1
128.7
127.6
126.9
126.5
125.9
125.8
111.5
77.5
77.2
76.9
23.8
20.3
f1 (ppm)

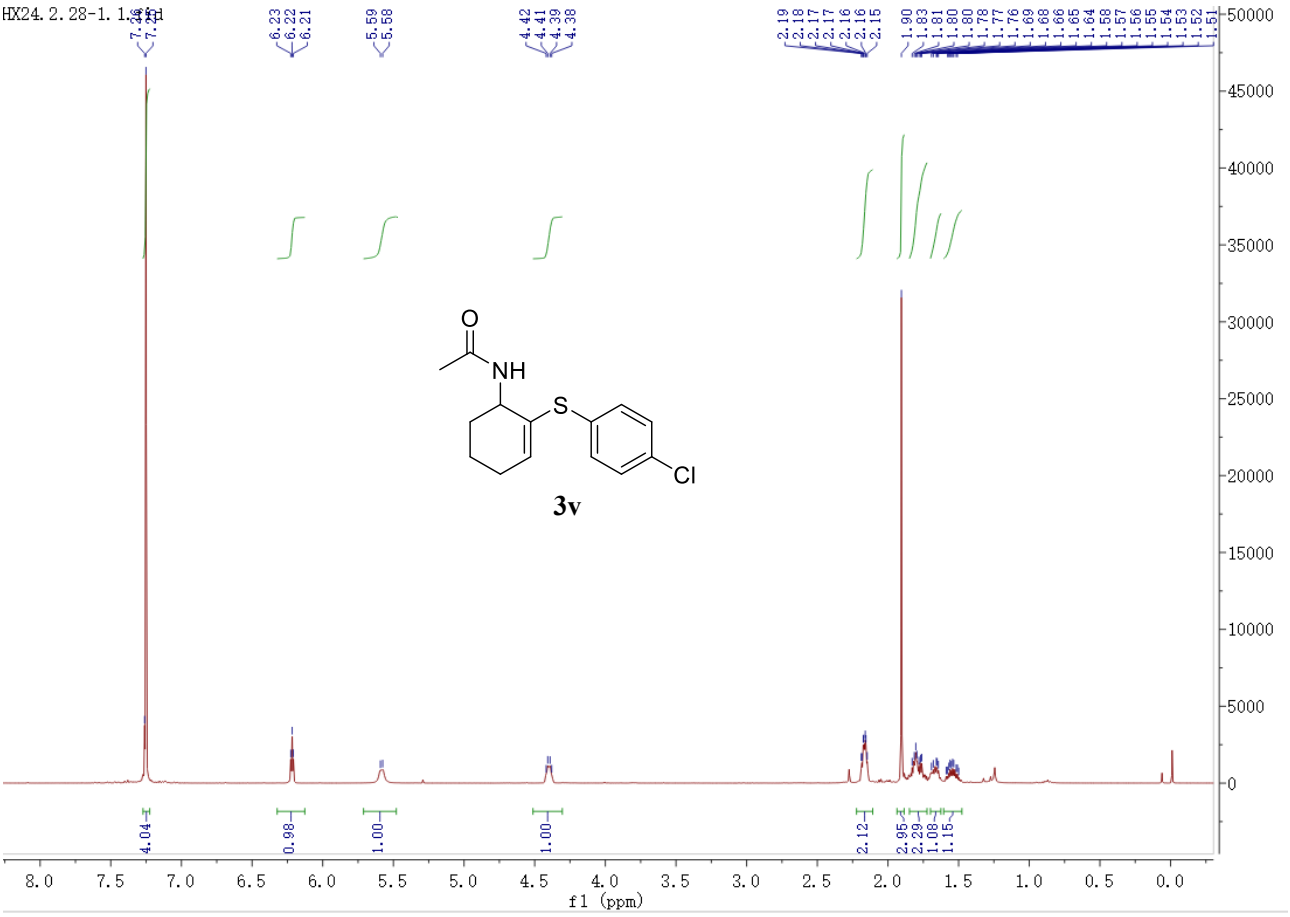

HX.22.4.18-12.10.fid
8.29
8.27
7.98
7.95
7.63
7.61
7.30
7.28
7.26
7.22
7.21
7.19
7.14
7.12
7.10
6.97
6.95
6.87
6.85
6.80
6.78
6.76
3.94
2.11
1.00
1.01
2.04
2.12
1.05
1.05
1.08
1.05
3.19
3.09
f1 (ppm)

3t

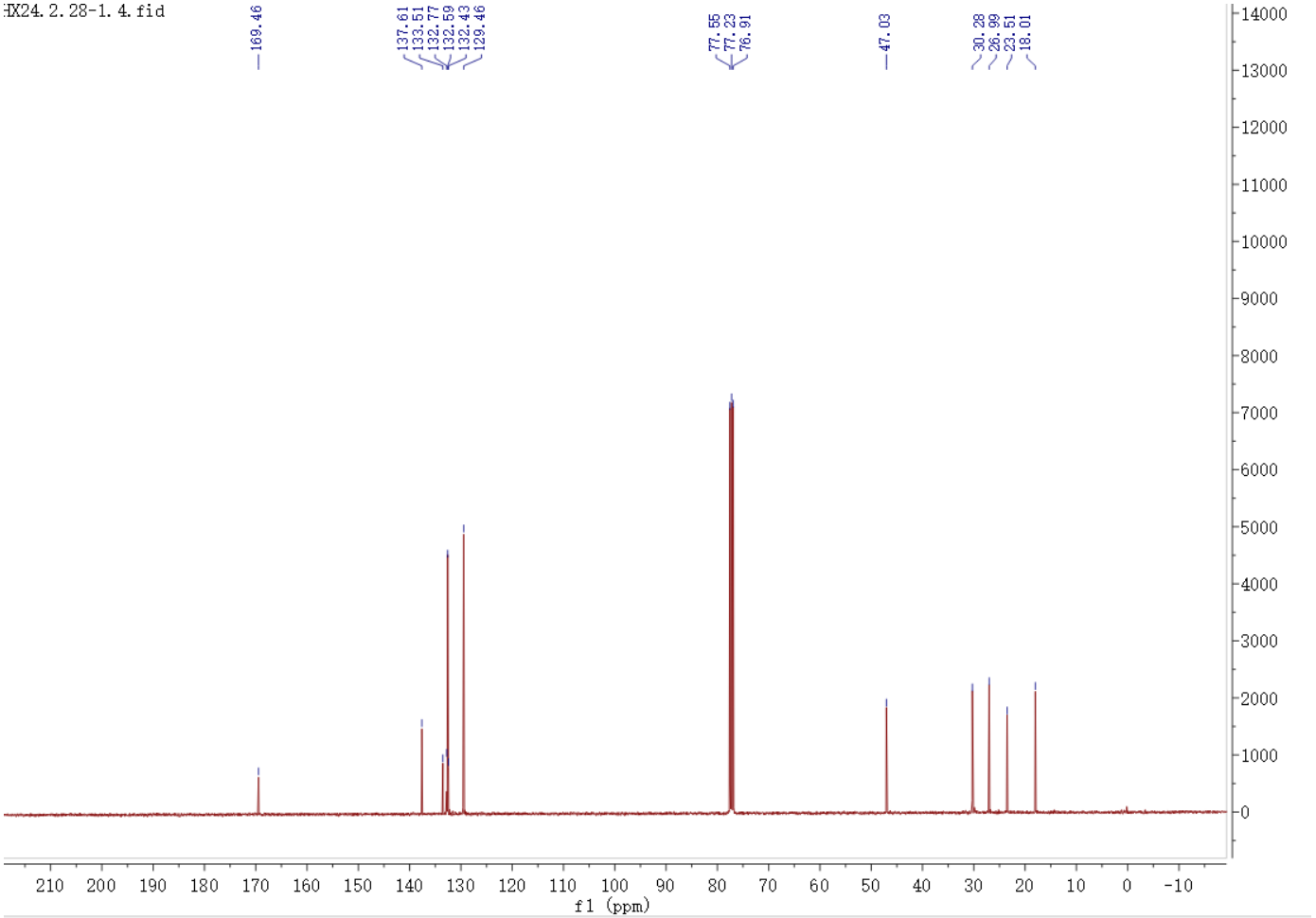

HX.22.4.18-12.20.fid
167.8
156.4
138.0
130.3
128.7
127.6
127.5
127.1
126.5
123.0
121.7
111.1
110.7
77.5
77.2
76.9
56.1
23.8
f1 (ppm)

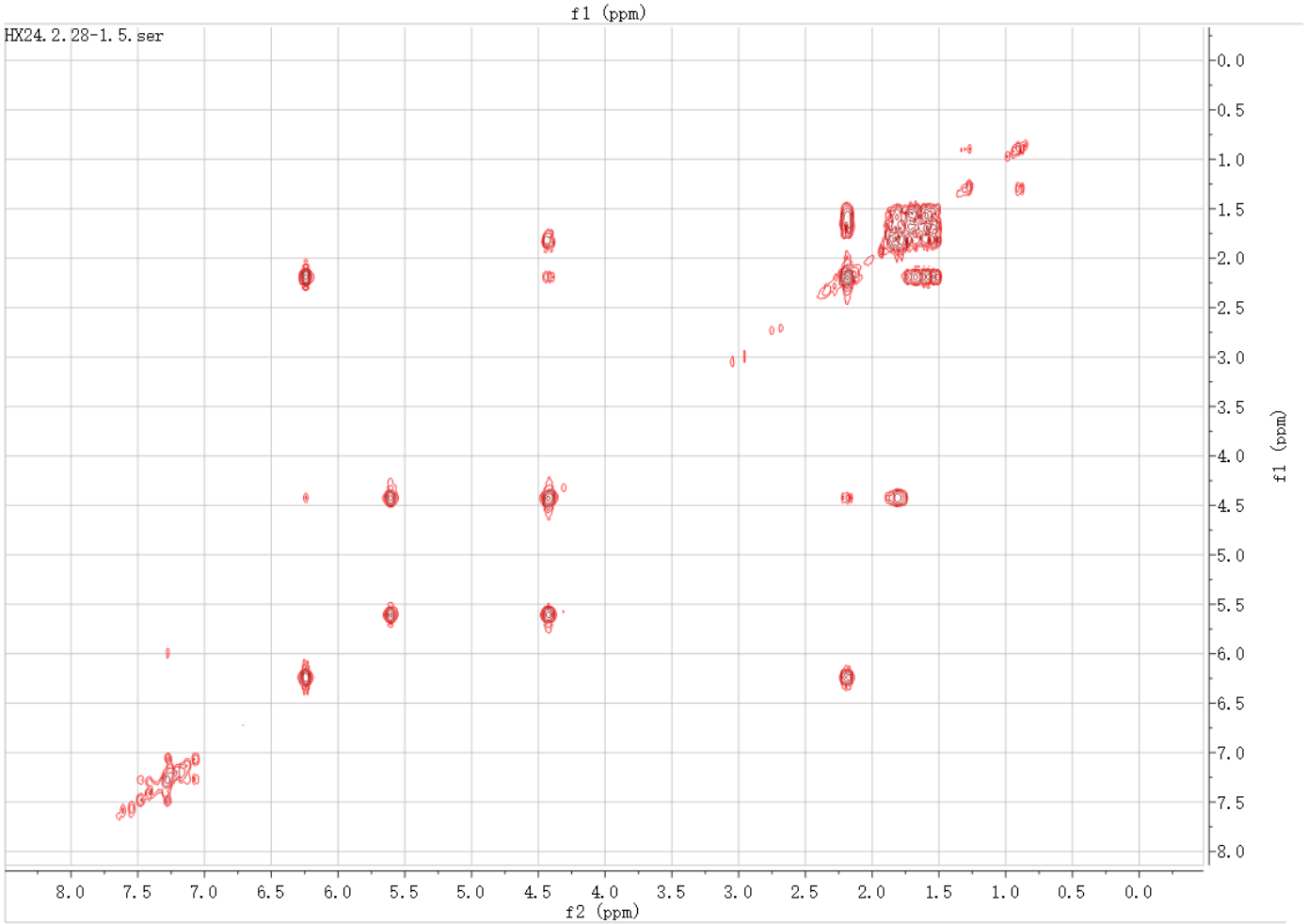

HX220823-1.10.fid
7.32
7.31
7.29
7.26
7.24
7.21
7.19
4.94
2.18
Cl
S
O
4.80
3.90
1.00
2.96
f1 (ppm)

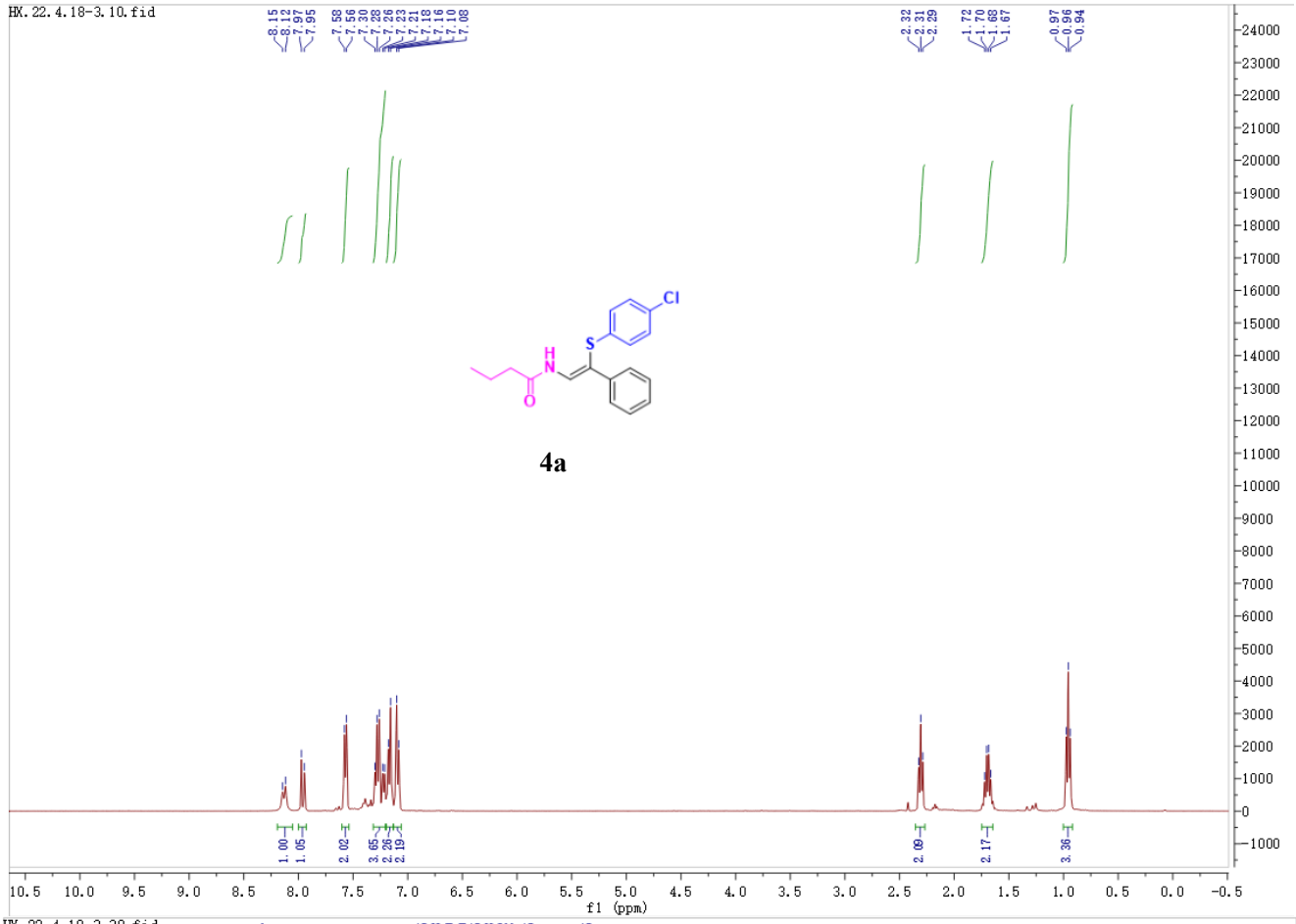
3u'


HX24.2.28-1.1.fid
6.23
6.22
6.21
5.59
5.58
4.42
4.41
4.39
4.38
2.19
2.18
2.17
2.16
2.15
1.90
1.83
1.81
1.80
1.78
1.77
1.76
1.69
1.68
1.66
1.65
1.64
1.58
1.57
1.56
1.55
1.54
1.53
1.52
1.51
O
NH
S
Cl
4.04
0.98
1.00
1.00
2.12
2.95
2.29
1.08
1.15
f1 (ppm)

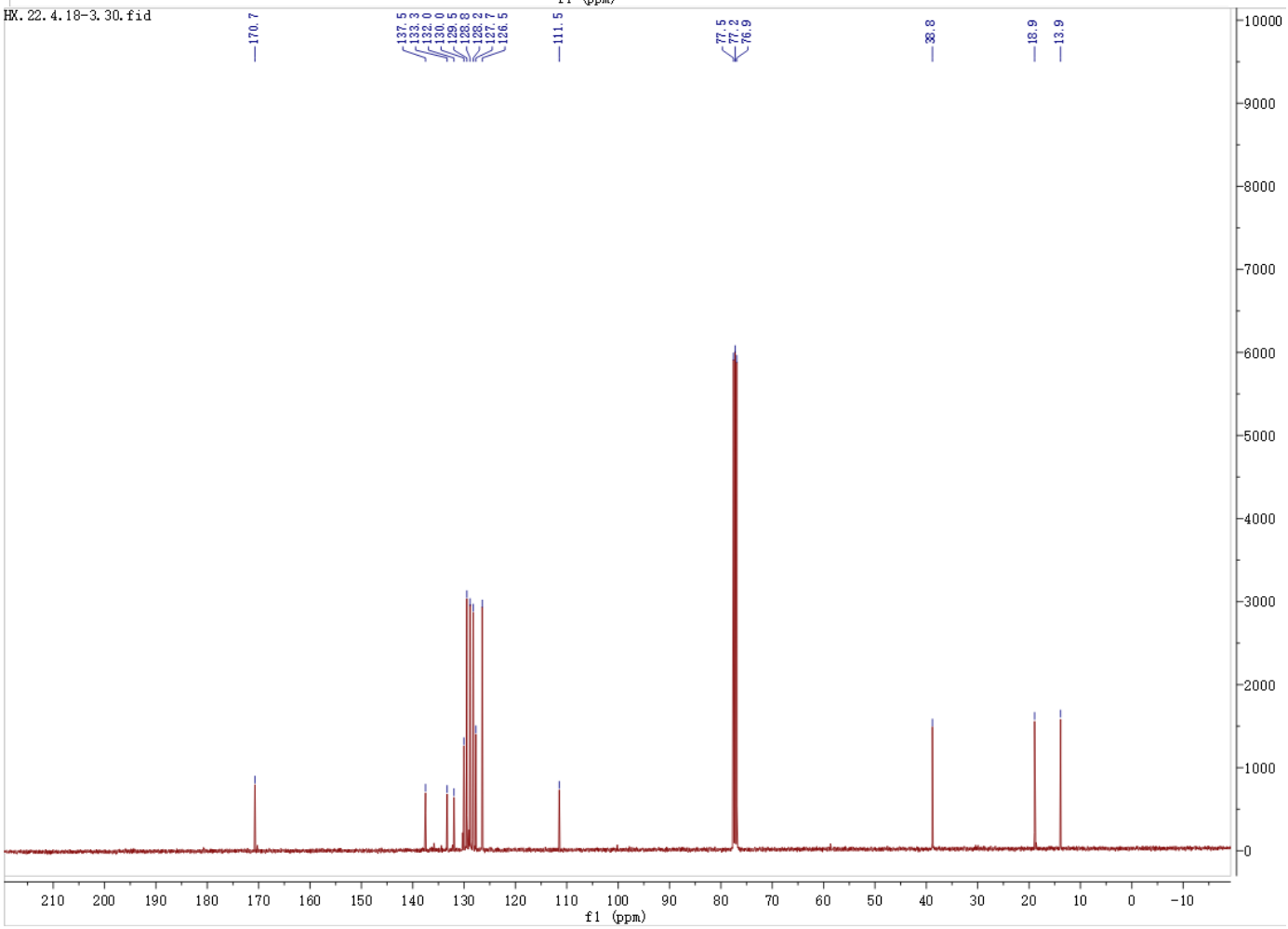
3v

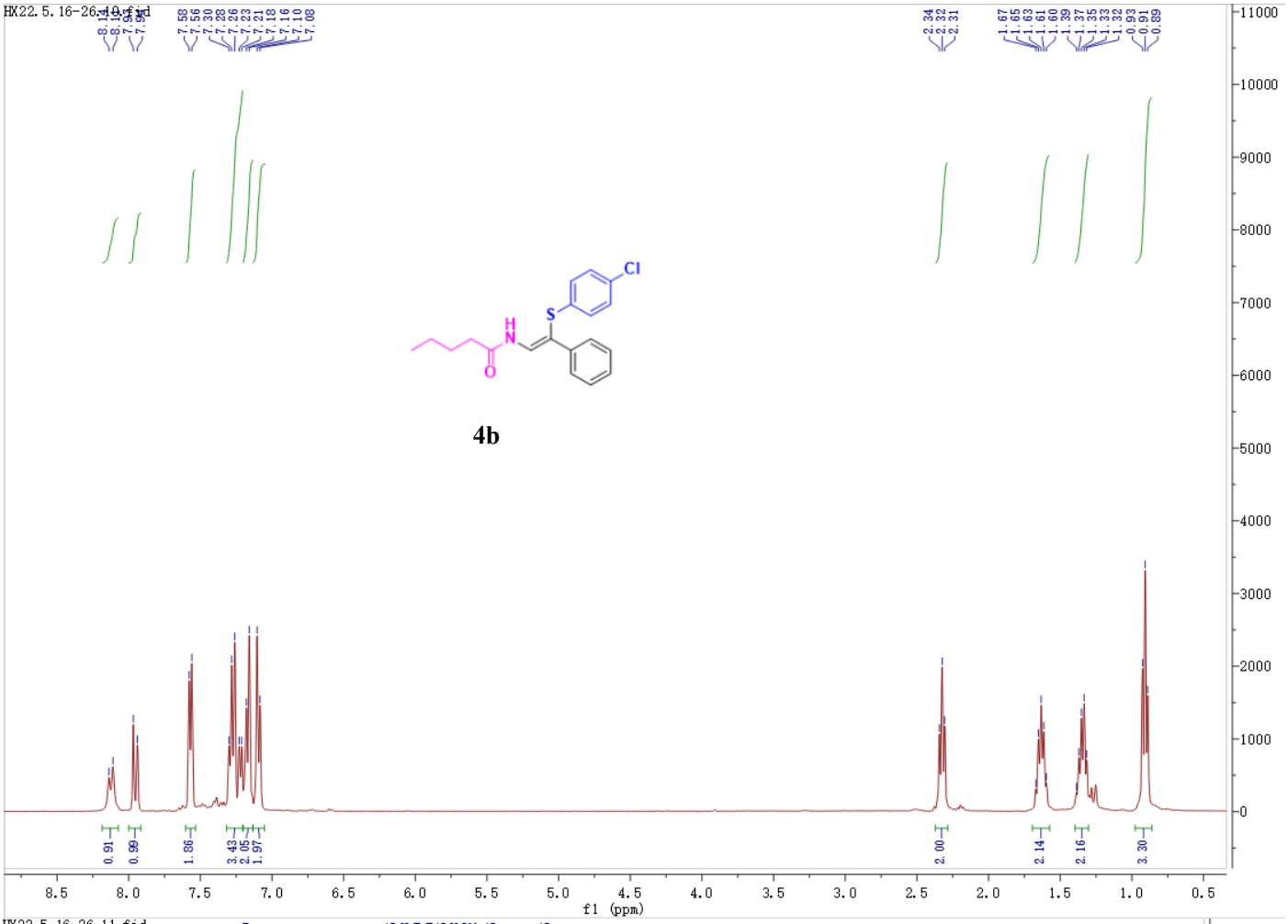

HX24.2.28-1.4.fid
169.46
137.61
133.51
132.77
132.59
132.43
129.46
77.55
77.23
76.91
47.03
30.28
26.99
23.51
18.01
f1 (ppm)


HX24.2.28-1.5.ser
f2 (ppm)
f1 (ppm)

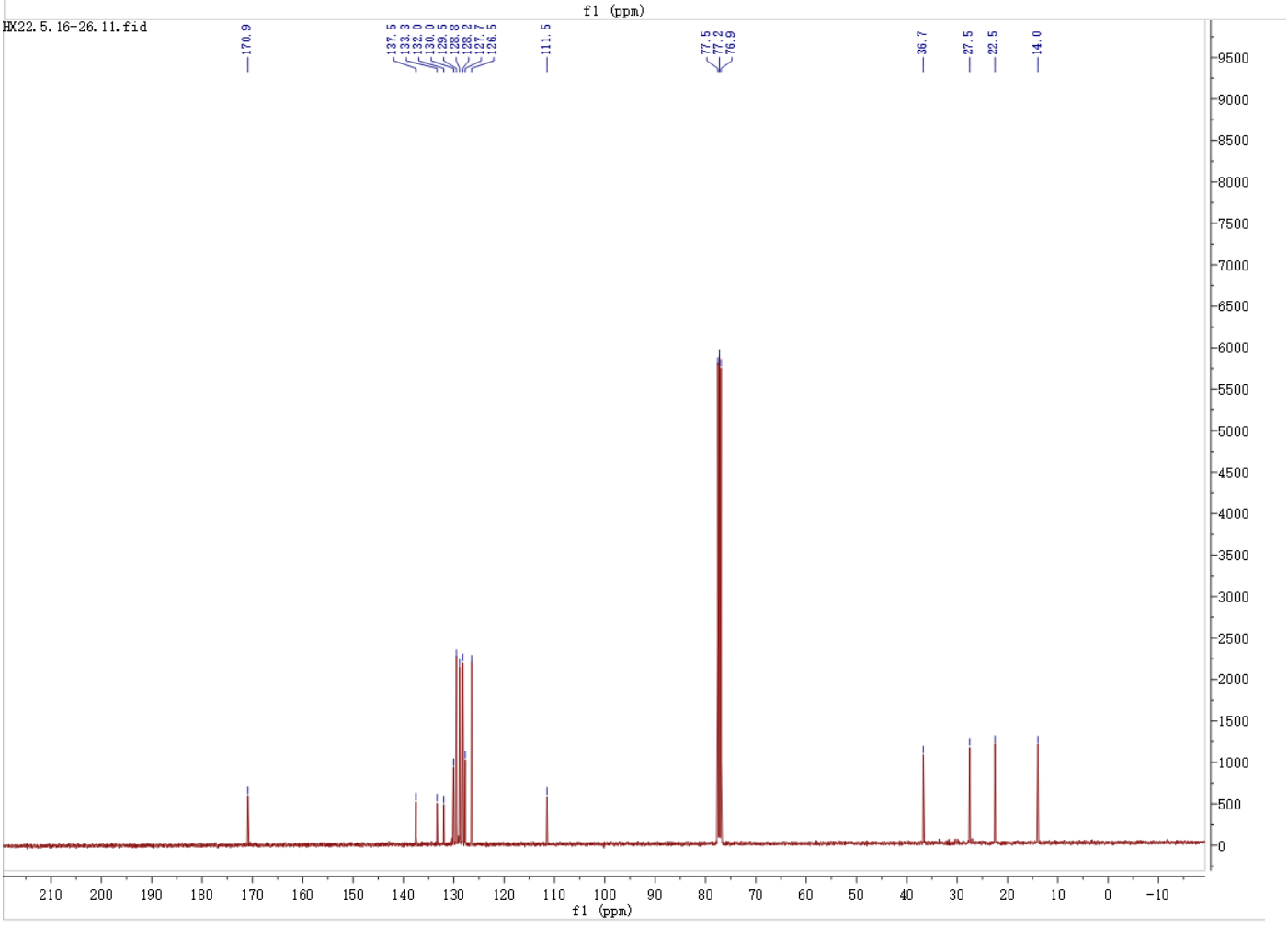

HX.22.4.18-3.10.fid
8.15
8.12
7.97
7.95
7.58
7.56
7.30
7.28
7.26
7.23
7.21
7.18
7.16
7.10
7.08
2.32
2.31
2.29
1.72
1.70
1.68
1.67
0.97
0.96
0.94
Cl
S
H
N
O
1.00
1.05
2.02
3.65
2.26
2.19
2.09
2.17
3.36
f1 (ppm)

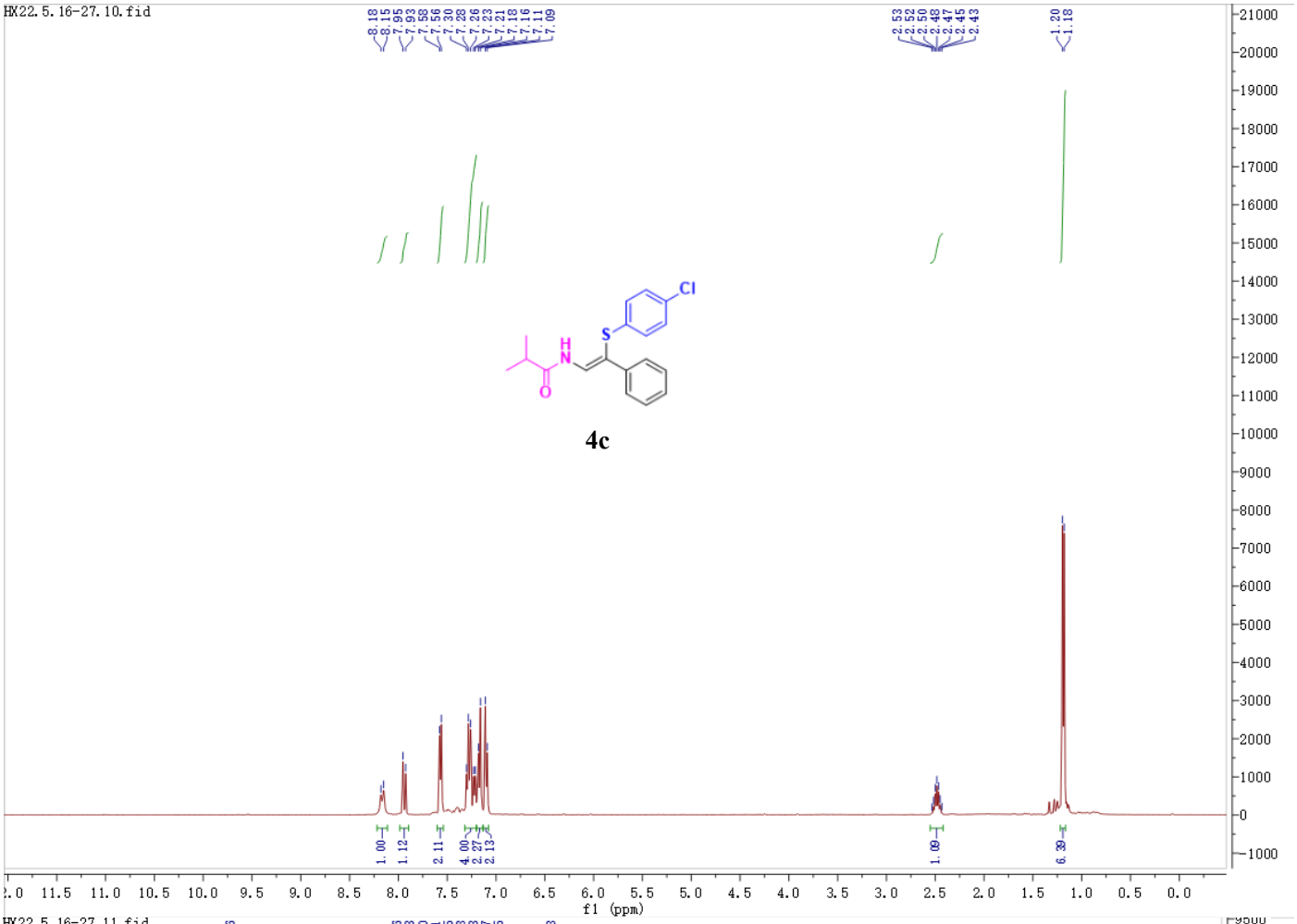
4a


HX.22.4.18-3.30.fid
170.7
137.5
133.3
132.0
130.0
129.5
128.8
128.2
127.7
126.5
111.5
77.5
77.2
76.9
38.8
18.9
13.9
f1 (ppm)

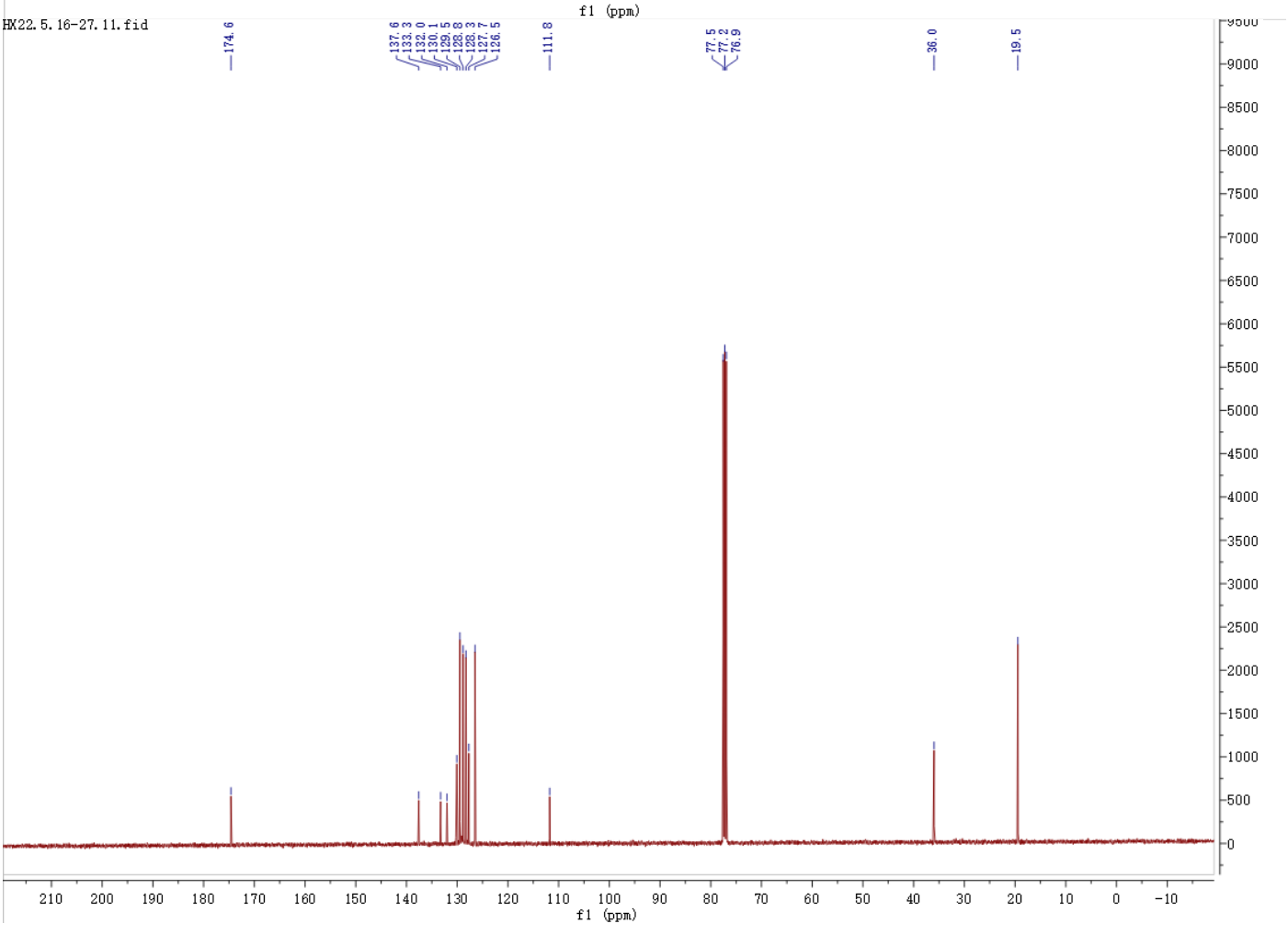

HX22.5.16-26.10.fid
8.15
8.13
7.96
7.94
7.58
7.56
7.30
7.28
7.26
7.23
7.21
7.18
7.16
7.10
7.08
2.34
2.32
2.31
1.67
1.65
1.63
1.61
1.60
1.39
1.37
1.35
1.33
1.32
0.93
0.91
0.89
Cl
S
H
N
O
0.91
0.99
1.86
3.43
2.05
1.97
2.00
2.14
2.16
3.30
f1 (ppm)

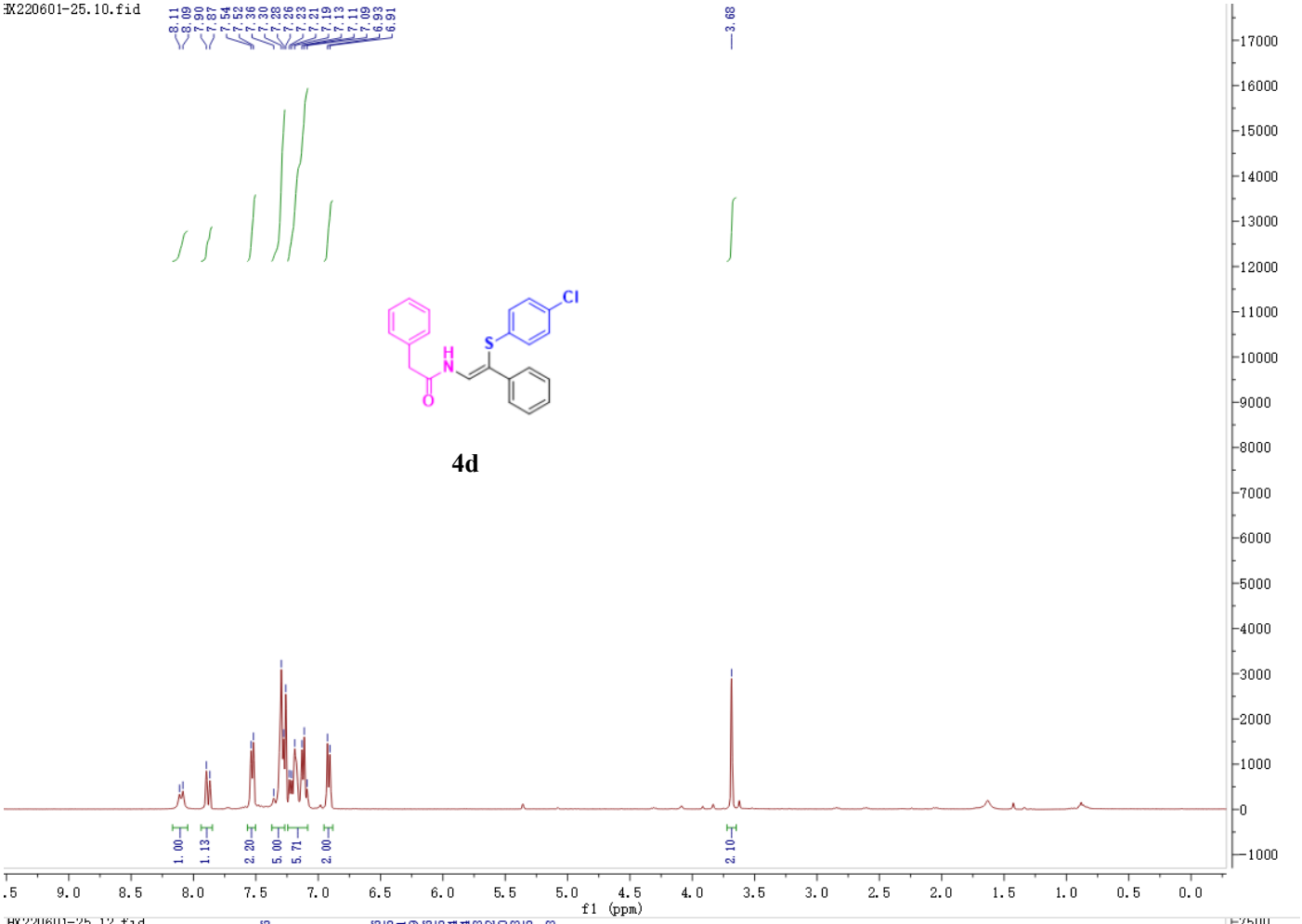
4b


HX22.5.16-26.11.fid
170.9
137.5
133.3
132.0
130.0
129.5
128.8
128.2
127.7
126.5
111.5
77.5
77.2
76.9
36.7
27.5
22.5
14.0
f1 (ppm)

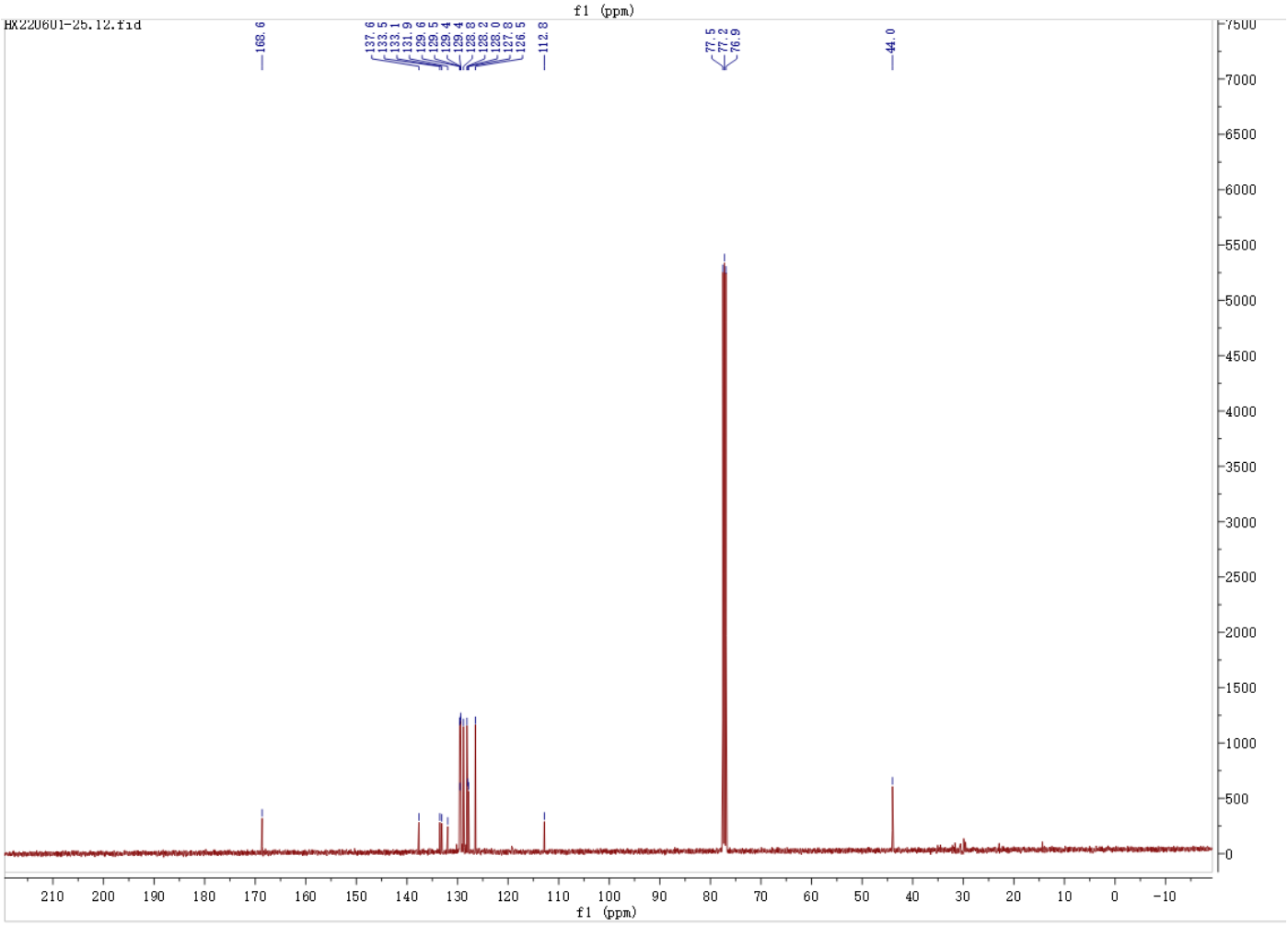

HX22.5.16-27.10.fid
8.18
8.15
7.95
7.93
7.58
7.56
7.30
7.28
7.26
7.23
7.21
7.18
7.16
7.11
7.09
2.53
2.52
2.50
2.48
2.47
2.45
2.43
1.20
1.18
Cl
S
H
N
O
1.00
1.12
2.11
4.00
2.27
2.13
1.09
6.39
f1 (ppm)

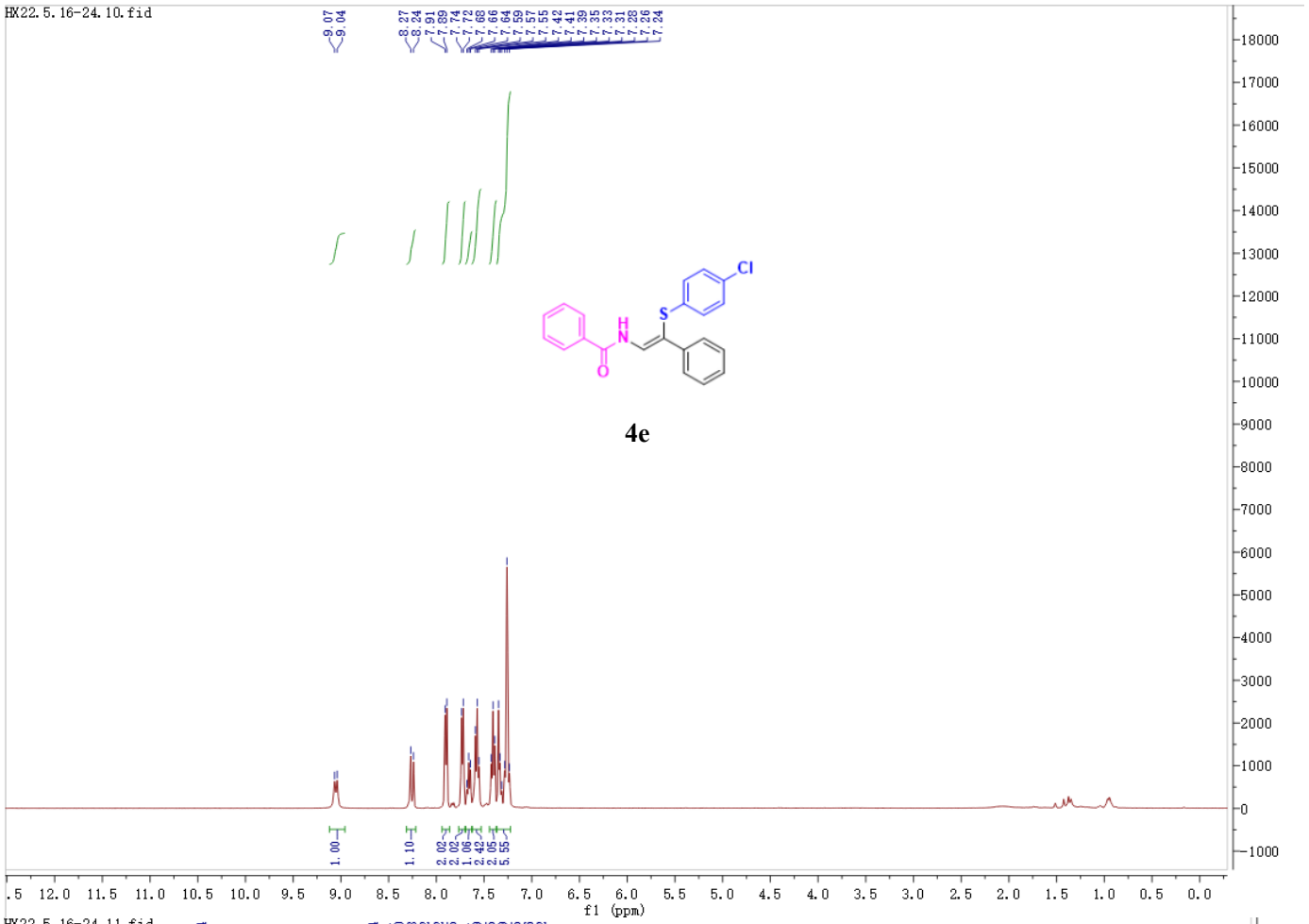
4c


HX22.5.16-27.11.fid
174.6
137.6
133.3
132.0
130.1
129.5
128.8
128.3
127.7
126.5
111.8
77.5
77.2
76.9
36.0
19.5
f1 (ppm)

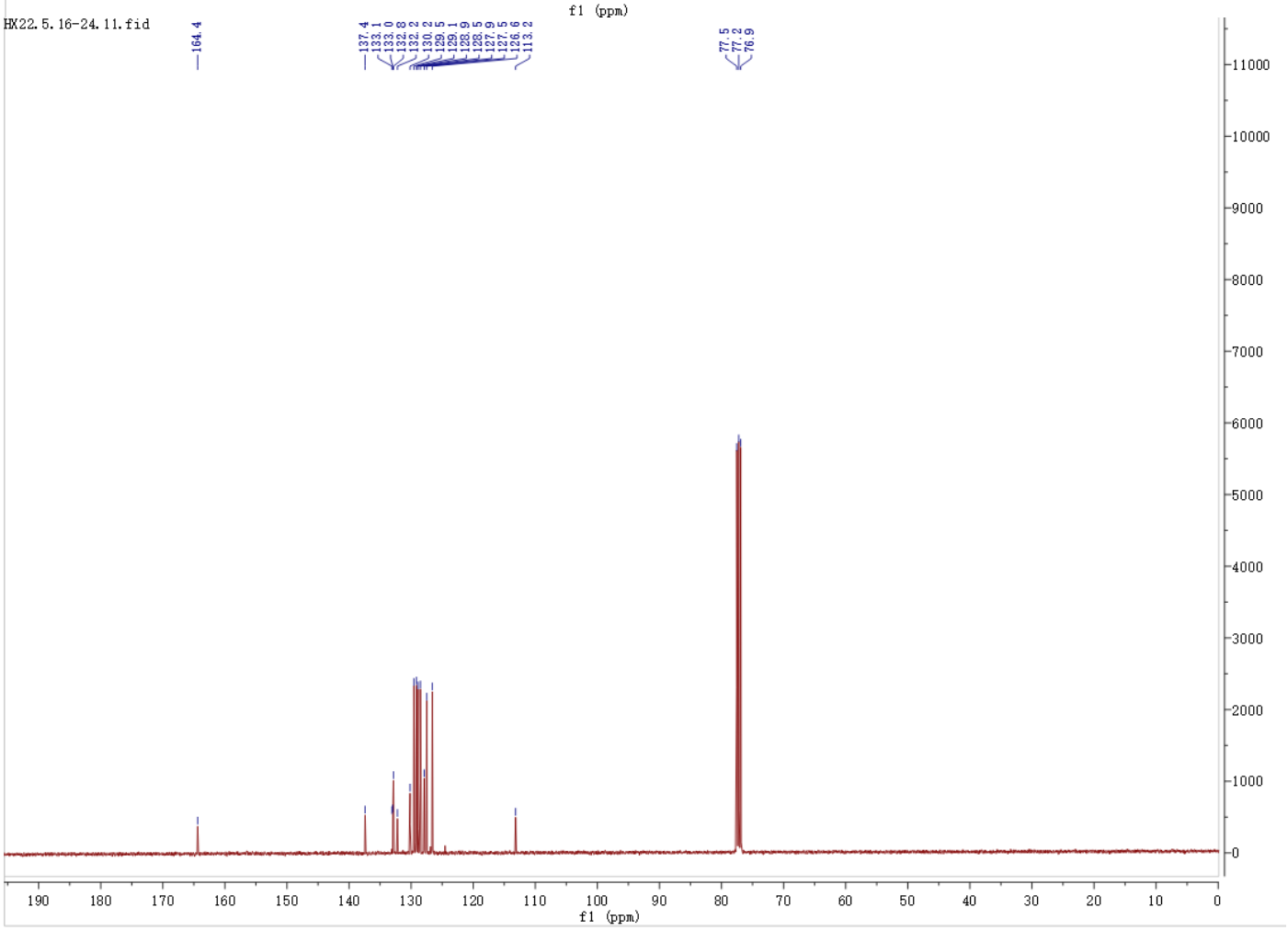

HX220601-25.10.fid
8.11
8.09
7.90
7.87
7.54
7.52
7.36
7.30
7.28
7.26
7.23
7.21
7.19
7.13
7.11
7.09
6.93
6.91
3.68
Cl
S
H
N
O
1.00
1.13
2.20
5.00
5.71
2.00
2.10
f1 (ppm)

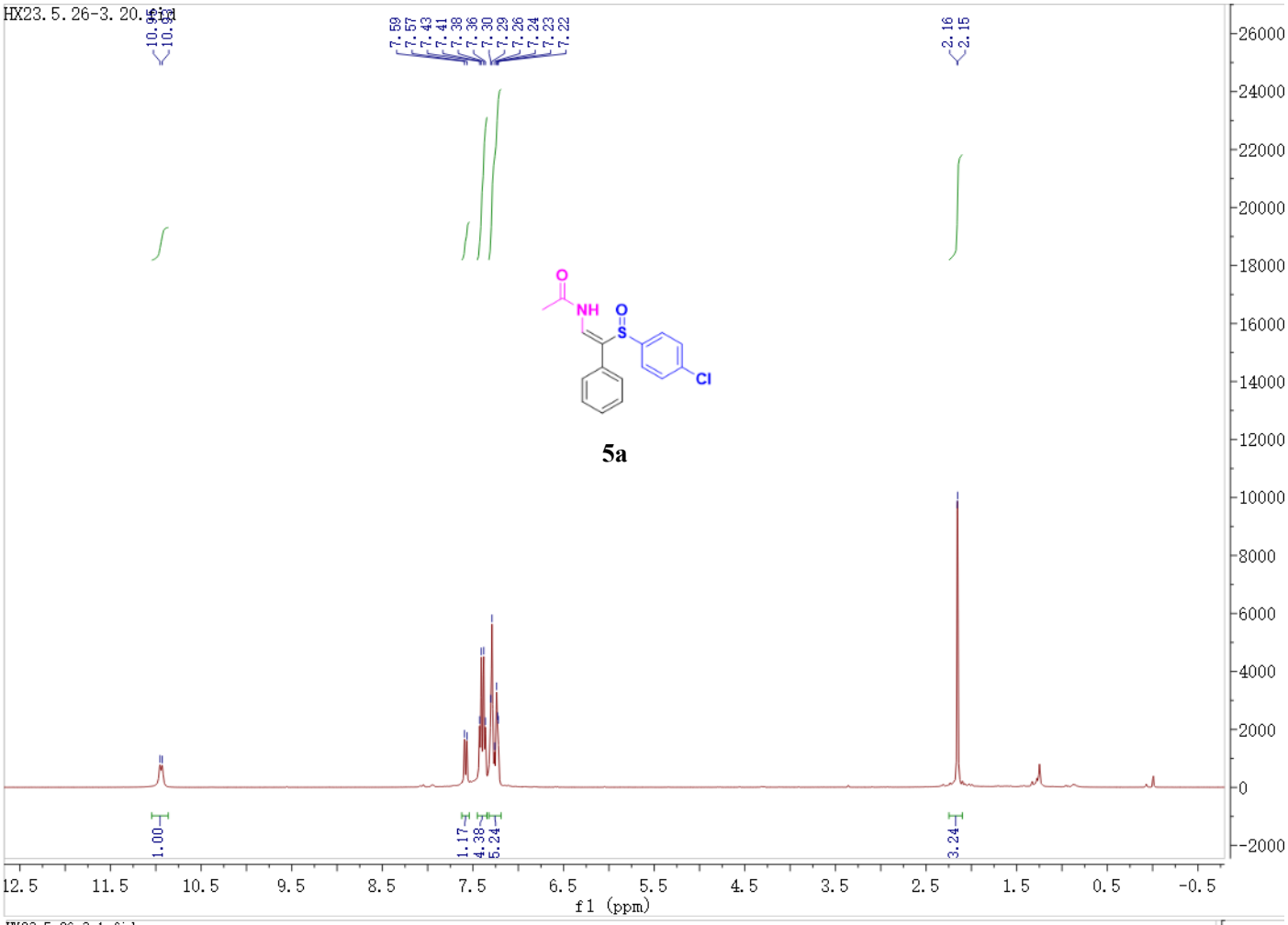
4d


HX220601-25.12.fid
168.6
137.6
133.5
133.1
131.9
129.6
129.5
129.4
128.8
128.2
128.0
127.8
126.5
112.8
77.5
77.2
76.9
44.0
f1 (ppm)

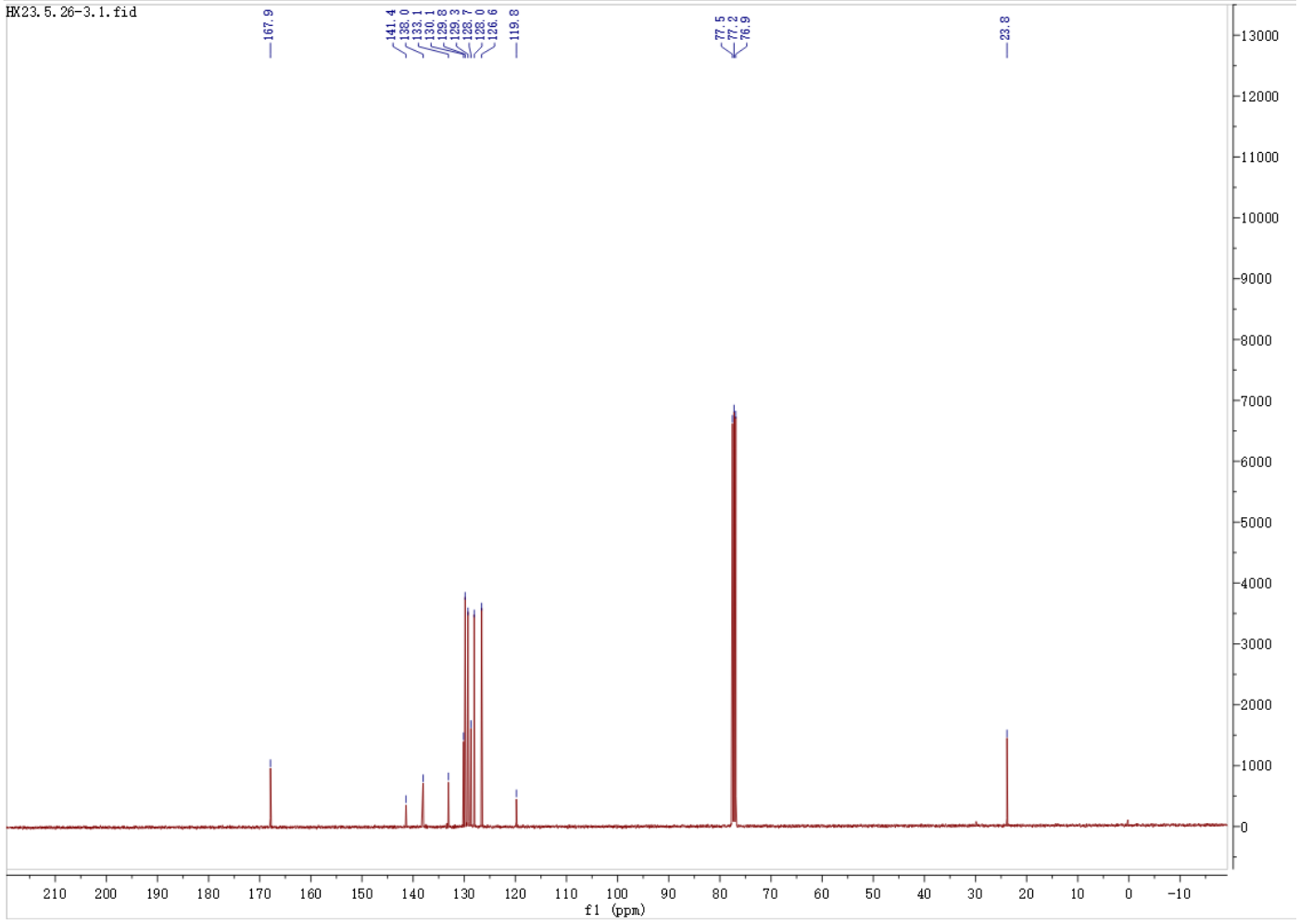

HX22.5.16-24.10.fid
9.07
9.04
8.27
8.24
7.91
7.89
7.74
7.72
7.68
7.66
7.64
7.59
7.57
7.55
7.42
7.41
7.39
7.35
7.33
7.31
7.28
7.26
7.24
Cl
S
H
N
O
1.00
1.10
2.02
2.02
1.49
2.05
2.55
f1 (ppm)

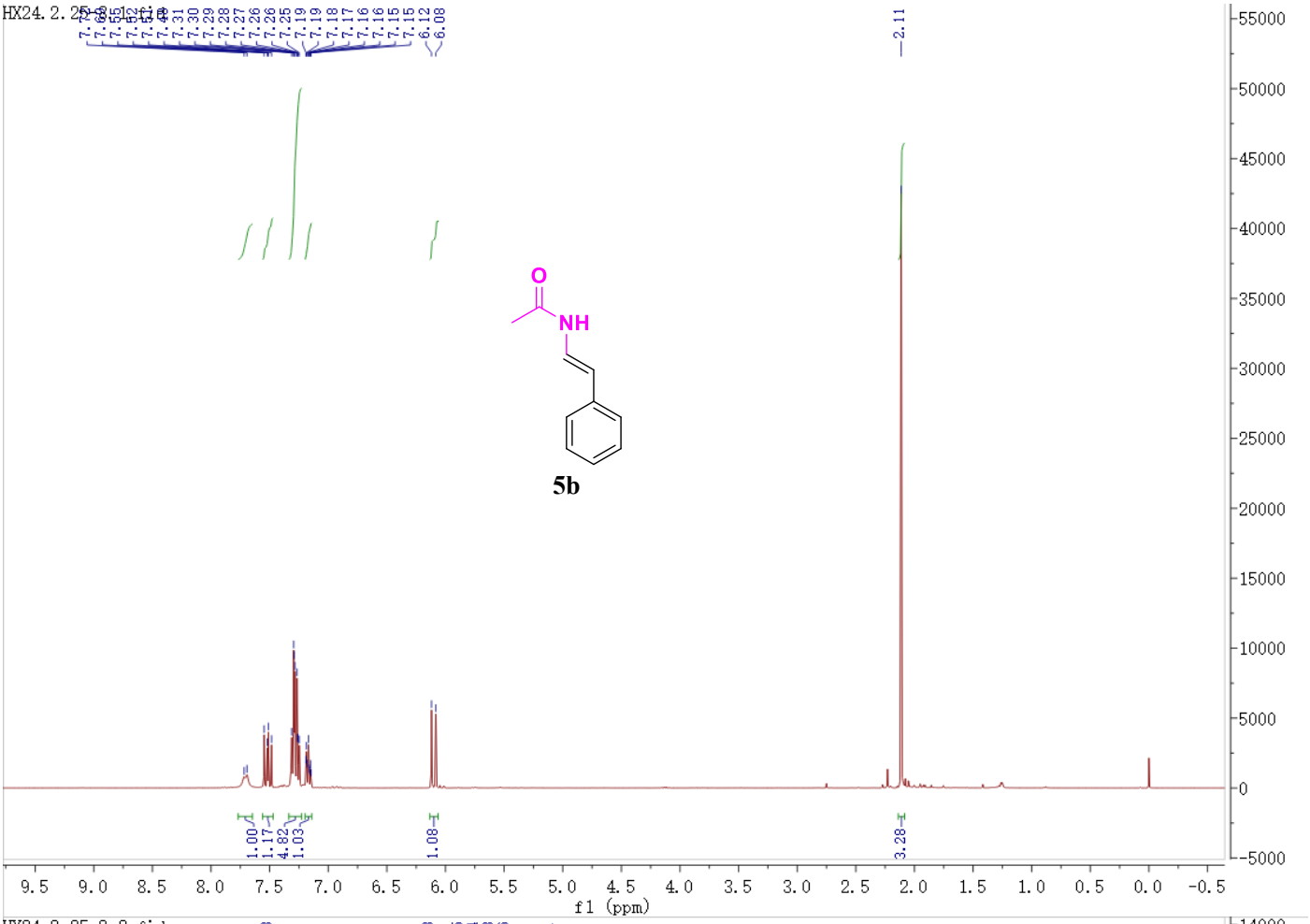
4e


HX22.5.16-24.11.fid
164.4
137.4
133.1
133.0
132.8
132.2
130.2
129.5
129.1
128.9
128.5
127.9
127.5
126.6
113.2
77.5
77.2
76.9
f1 (ppm)

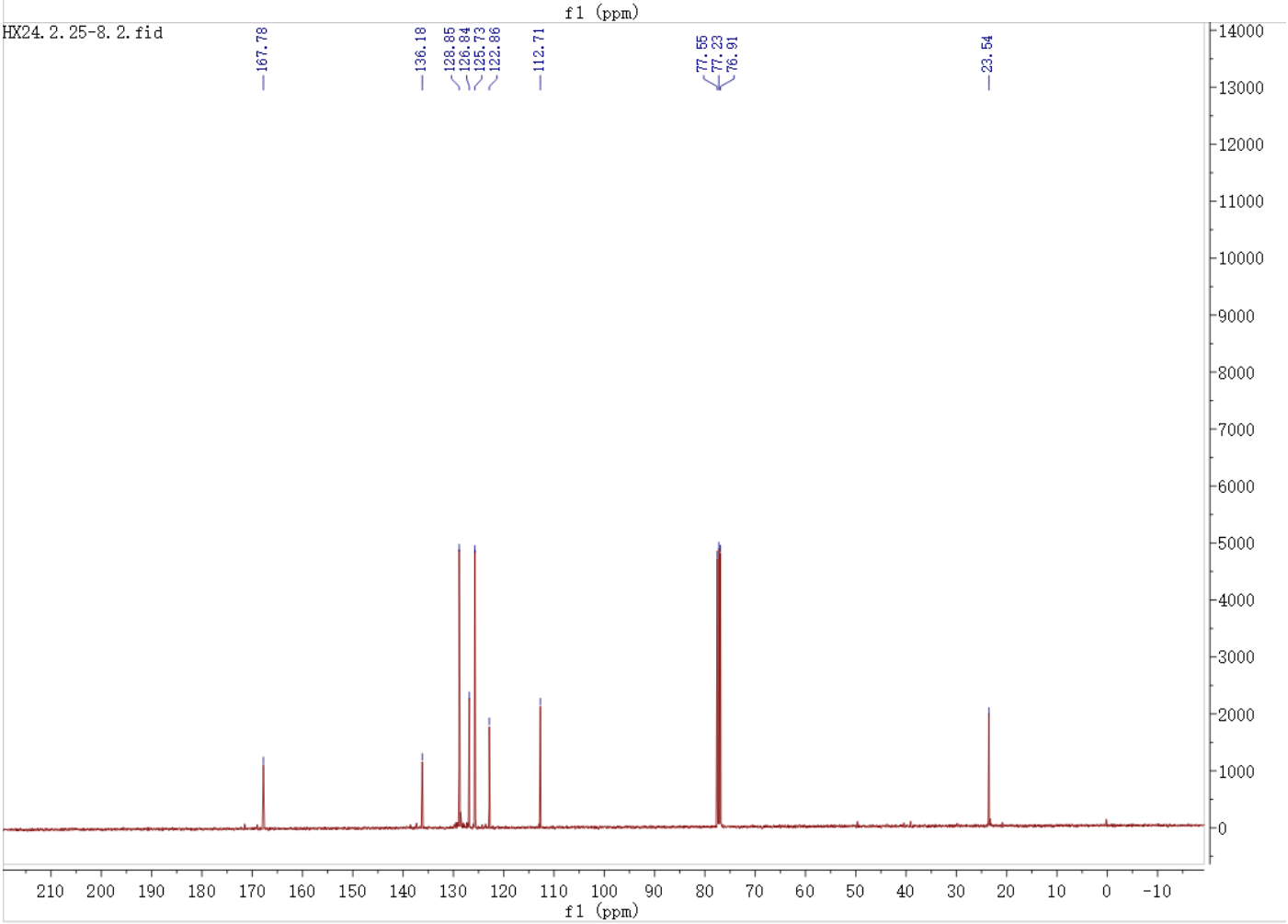

HX23.5.26-3.20.fid
10.93
10.91
7.59
7.57
7.43
7.41
7.38
7.36
7.30
7.29
7.26
7.24
7.23
7.22
2.16
2.15
O
NH
O
S
Cl
1.00
1.17
4.38
5.24
3.24
f1 (ppm)

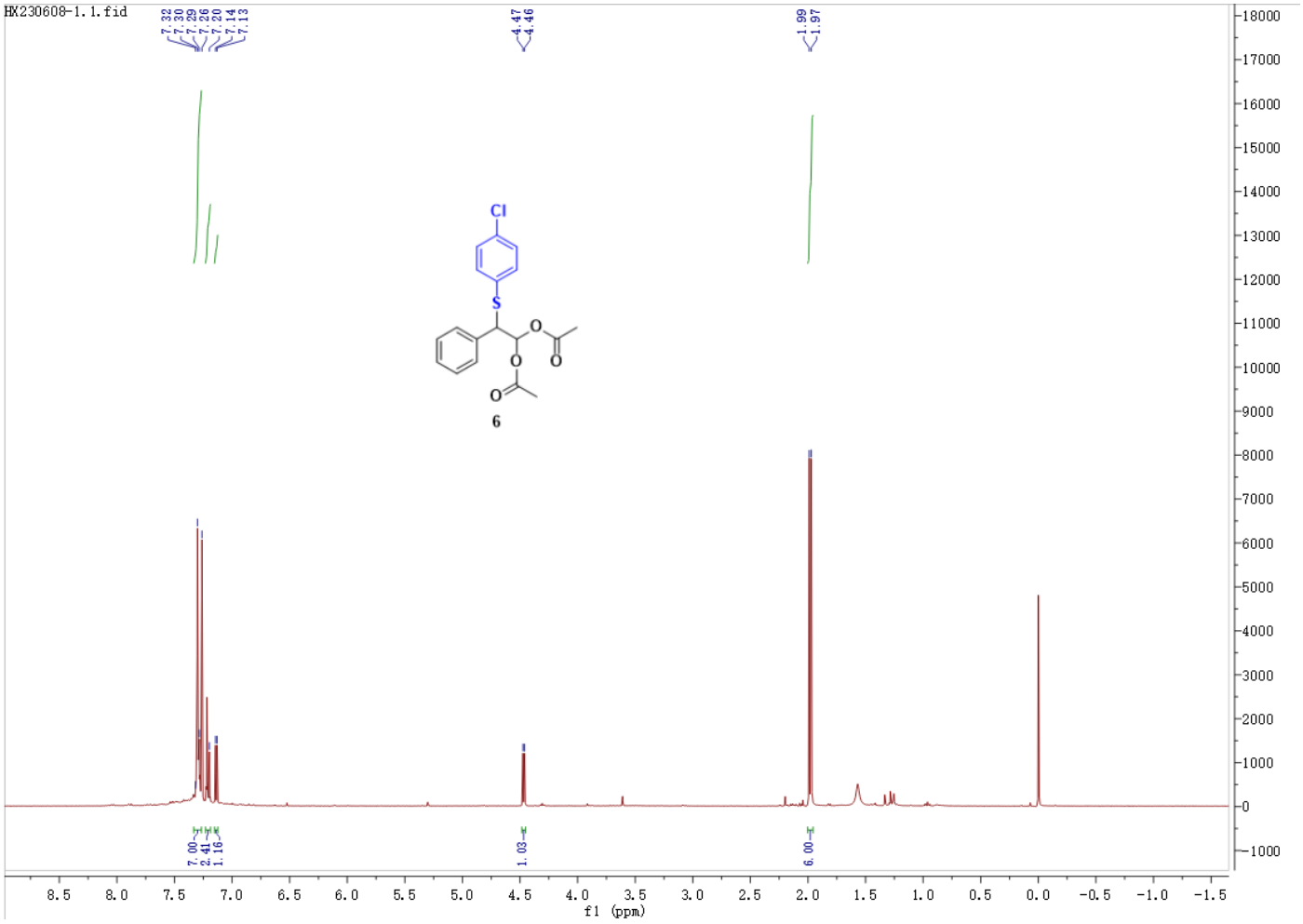
5a


HX23.5.26-3.1.fid
167.9
141.4
138.0
133.1
130.1
129.8
129.3
128.7
128.0
126.6
119.8
77.5
77.2
76.9
23.8
f1 (ppm)


HX24.2.25-8.fid
7.68
7.55
7.52
7.48
7.31
7.30
7.29
7.28
7.27
7.26
7.25
7.19
7.18
7.17
7.16
7.15
6.12
6.08
2.11
O
NH
1.00
1.17
4.82
1.03
1.08
3.28
f1 (ppm)

5b


HX24.2.25-8.2.fid
167.78
136.18
128.85
126.84
125.73
122.86
112.71
77.55
77.23
76.91
23.54
f1 (ppm)


HX230608-1.1.fid
7.32
7.30
7.29
7.26
7.20
7.14
7.13
4.47
4.46
1.99
1.97
Cl
S
O
O
O
O
6
7.00
2.41
1.16
1.03
6.00
f1 (ppm)