Electronic Supplementary Material (ESI) for ChemComm.

Supplementary Information

Copper-catalyzed oxidative C(sp^3)-H/N-H coupling of sulfoximines, amides with simple alkanes via radical process

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1. General Considerations

All chemicals were used as received without further purification unless stated otherwise. ^{1}H NMR and ^{13}C NMR spectra were recorded at ambient temperature on a 400 MHz spectrometer (100 MHz for ^{13}C). NMR experiments are reported in δ units, parts per million (ppm), and were referenced to $CDCl_3$ (δ 7.26 or 77.0 ppm) as the internal standard. The coupling constants *J* are given in Hz. Column chromatography was performed using EM Silica gel 60 (300-400 meshes) or neutral aluminum oxide (200-300 meshes).

2. Experimental Procedures.

Under air, a 20 mL of Schlenk tube equipped with a stir bar was charged with sulfoximines **1** (0.2 mmol), DTBP (0.8 mmol, 4eq.), $Cu(acac)_2$ (0.02 mmol, 10 mol%) and cyclohexane (2 mL). The tube was sealed with a Teflon lined cap. The reaction mixture was stirred at 115 °C for 12 h in oil bath. After the completion of the reaction (monitored by TLC), the solvent was concentrated in vacuum and the residue was purified by flash column chromatography on silica gel with petroleum ether-ethyl acetate as the eluent to give the desired product.

3. Research on the Mechanism

3.1 Free Radical Capture Experiments

Fig S1 GC spectrum of the *N*-alkylated product **3aa**

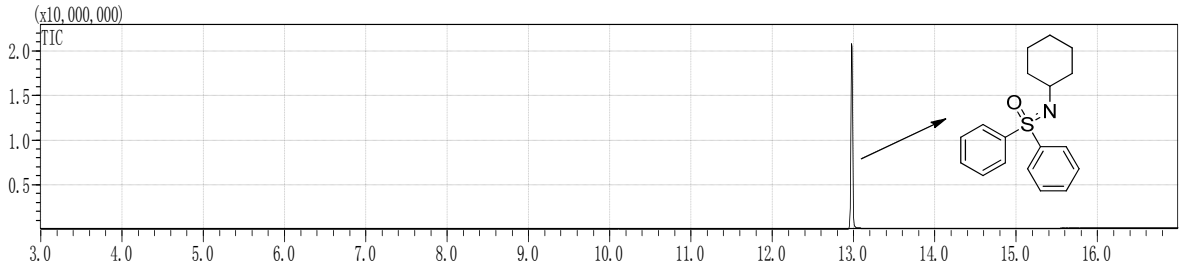


Fig S2 After adding 2.0 equiv of TEMPO to the reaction mixture

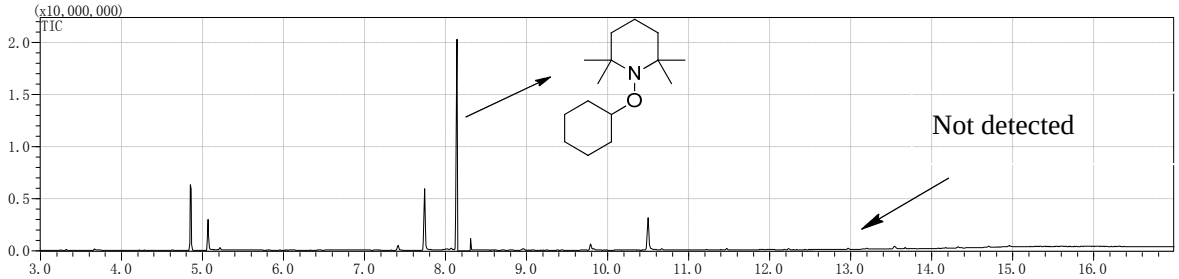
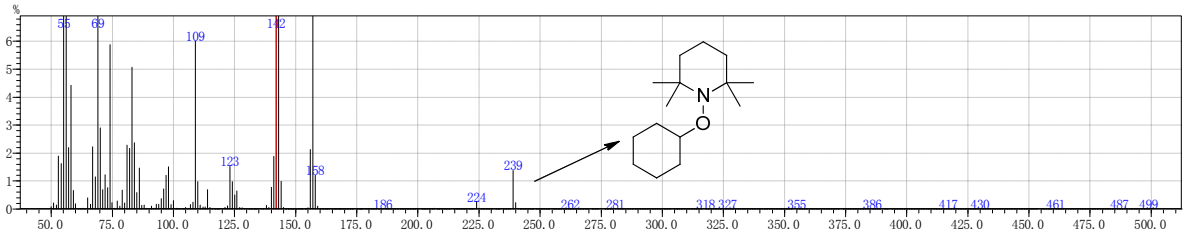
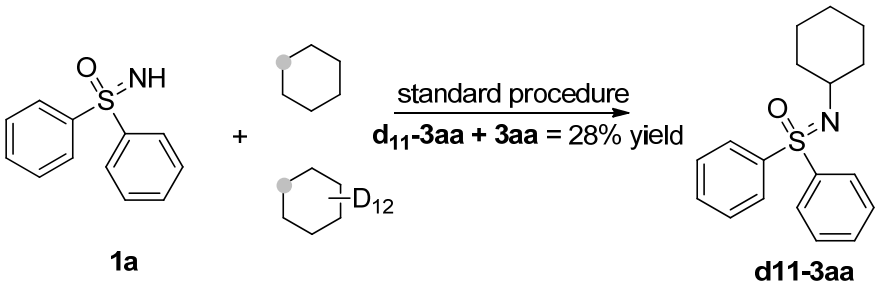


Fig S3 The MS spectrum of the adduct formed by TEMPO and cyclohexane radical



3.2 The KIE Studies on Cyclohexane

In a sealed tube, a mixture of **1a** (0.1 mmol), cyclohexane/D_{12}-cyclohexane (1: 1, 1.0 mL) was treated under standard conditions for 6 h. After that, the mixture was concentrated in vacuo and the residue was purified by flash column chromatography on silica gel with petroleum ether-ethyl acetate as eluent to give products **3aa** and **d_{11}-3aa** in 28% yield. The mixture was analyzed using ^{1}H NMR spectrometer. As shown in Scheme S1, the ratio of **3aa** and **D_{11}-3aa** is nearly 9.0: 1.



Scheme S1 KIE experiment of cyclohexane and D_{12}-cyclohexane

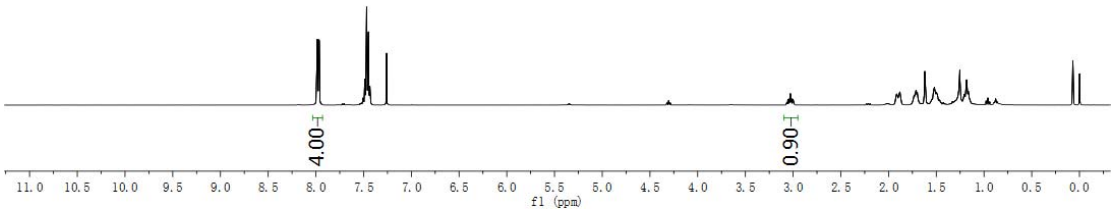
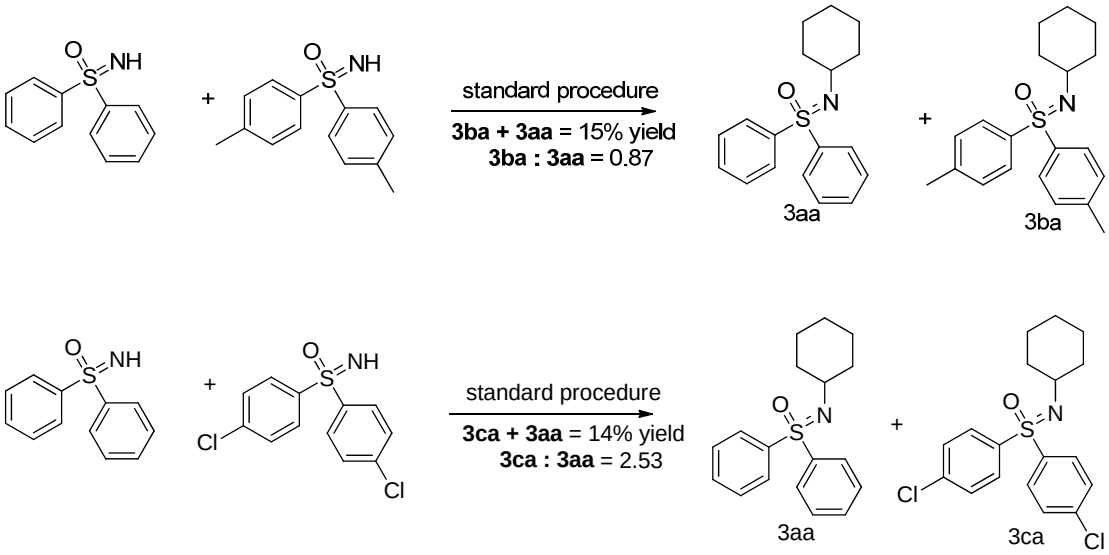


Figure S4 The ^{1}H NMR spectrum of the KIE results.

3.3 Competitive Experiments

In order to investigate deeply mechanism of the electronic effect, the competition experiments were conducted by using substrates of **3aa** and *para*-substituted **R-3aa** (1:1 molar ratio) under standard conditions with low conversion (less than 20%) for 60 min.. The ratios of *N*-alkylated **3aa** and **R-3aa** were analyzed by ^{1}H NMR or flash column chromatography. The results were listed.

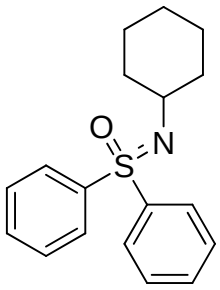
Scheme S2 Competitive experiments



The result indicated that the substrate with electron-withdrawing group was prone to promote this transformation.

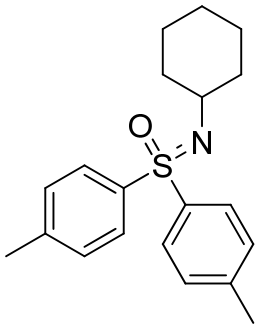
4. Characterization Data for the Products

N-(Cyclohexyl) diphenyl sulfoximine (3aa):



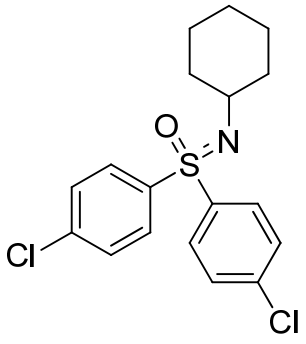
Flash column chromatography on a silica gel (ethyl acetate: petroleum ether, 1: 20) give the product (48.4 mg, 81% yield) as a white solid; m.p.: 155-157 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.16-1.20 (m, 3H), 1.50-1.52 (m, 2H), 1.69-1.73 (m, 3H), 1.88-1.91 (m, 2H), 2.99-3.06 (m, 1H), 7.42-7.48 (m, 6H), 7.76-7.98 (m, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 25.2, 25.6, 37.1, 54.0, 128.5, 129.0, 132.1, 141.6. MS (EI): 299 (M^+). HRMS (ESI) *m*/*z* calcd for $C_{18}H_{22}NOS$ $(M+H)^+$ 300.1417, found 300.1416. IR (KBr): 3060, 2930, 2852, 2359, 2332, 1448, 1246, 1136.

N-(Cyclohexyl)-4,4'-dimethyl diphenyl sulfoximine (3ba):



Flash column chromatography on a silica gel (ethyl acetate: petroleum ether, 1: 25) give the product (48.8 mg, 73% yield) as a white solid; m.p.: 93-95 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.15-1.19 (m, 3H), 1.48-1.51 (m, 3H), 1.68-1.72 (m, 2H), 1.87-1.91 (m, 2H), 2.35 (s, 6H), 2.96-3.03 (m, 1H), 7.22 (d, J = 8.2 Hz, 4H), 7.83 (d, J = 8.2 Hz, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.4, 25.3, 25.6, 37.1, 54.0, 128.4, 129.6, 138.8, 142.6. MS (EI): 327 (M^+). HRMS (ESI) *m*/*z* calcd for $C_{20}H_{26}NOS$ $(M+H)^+$ 328.1730, found 328.1733. IR (KBr): 3075, 3069, 3062, 2924, 2852, 2361, 2341, 1448, 1250 ,1136.

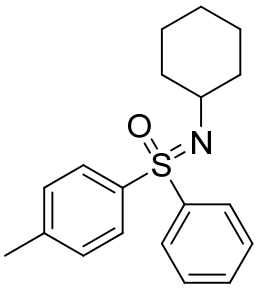
N-(Cyclohexyl)-4,4'-dicholo diphenyl sulfoximine (3ca):



Flash column chromatography on a silica gel (ethyl acetate: petroleum ether, 1: 40) give the product (60.4 mg, 85% yield) as a white solid; m.p.: 94-95 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.16-1.20 (m, 3H), 1.46-1.51 (m, 3H), 1.69-1.71 (m, 2H), 1.83-1.86 (m, 2H), 2.98-3.05 (m, 1H), 7.40-7.43 (m 4H), 7.86-7.88 (m, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 25.1, 25.5, 36.9, 54.0, 129.4, 129.9, 139.0, 139.9. MS (EI): 367 (M^+). HRMS (ESI) *m*/*z* calcd for $C_{18}H_{22}NOS$ $(M+H)^+$ 368.0637, found 368.0639. IR (KBr): 3070, 3065, 2924, 2850, 2357, 2330, 1473, 1250, 1142, 1088.

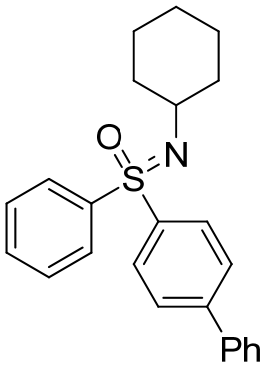
N-(Cyclohexyl)-4-methyl diphenyl sulfoximine (3da):

Flash column chromatography on a silica gel (ethyl acetate: petroleum ether, 1: 20) give the product (45.1 mg, 72% yield) as a white solid; m.p.: 110-112 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.15-1.20 (m, 3H), 1.49-1.51 (m, 3H), 1.68-1.70 (m, 2H),



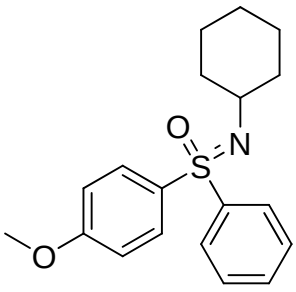
1.87-1.91 (m, 2H), 2.35 (s, 3H), 2.98-3.04 (m, 1H), 7.22-7.24 (m, 2H), 7.40-7.45 (m, 3H), 7.83-7.85 (m, 2H), 7.94-7.97 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.3, 25.2, 25.6, 37.0, 54.0, 128.3, 128.5, 128.9, 129.6, 131.9, 138.5, 141.9, 142.8. MS (EI): 313 (M^+). HRMS (ESI) *m*/*z* calcd for $C_{19}H_{24}NOS$ $(M+H)^+$ 314.1573, found 314.1574. IR (KBr): 3064, 2932, 2852, 2359, 2342, 1462, 1248, 1136.

_N_-(Cyclohexyl)-4-phenyl diphenyl sulfoximine (3ea):



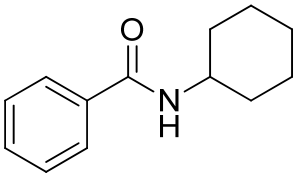
Flash column chromatography on a silica gel (ethyl acetate: petroleum ether, 1: 20) give the product (41.8 mg, 55% yield) as a white solid; m.p.: 109-111 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.18-1.23 (m, 3H), 1.50-1.57 (m, 2H), 1.72-1.75 (m, 3H), 1.91-1.95 (m, 2H), 3.04-3.11 (m, 1H), 7.36-7.50 (m, 6H), 7.55-7.57 (m, 2H), 7.65-7.67 (m, 2H), 8.01-8.04 (m, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 25.2, 25.7, 37.1, 54.1, 127.3, 127.7, 128.3, 128.5, 128.9, 129.0, 129.0, 132.1, 139.5, 140.2, 141.7, 145.1. MS (EI): 375 (M^+). HRMS (ESI) *m*/*z* calcd for $C_{24}H_{26}NOS$ $(M+H)^+$ 376.1730, found 376.1729. IR (KBr): 3067, 2930, 2855, 2361, 2348, 1466, 1250, 1146.

_N_-(Cyclohexyl)-4-methoxyl diphenyl sulfoximine (3fa):



Flash column chromatography on a silica gel (ethyl acetate: petroleum ether, 1: 20) give the product (47.4 mg, 72% yield) as a white solid; m.p.: 87-89 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.15-1.19 (m, 3H), 1.48-1.51 (m, 3H), 1.61-1.78 (m, 2H), 1.87-1.90 (m, 2H), 2.97-3.04 (m, 1H), 3.80 (s, 3H), 6.91 (d, J = 8.9 Hz, 2H), 7.41-7.45 (m, 3H), 7.82 (d, J = 8.8 Hz, 2H), 7.93-7.95 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 25.2, 25.6, 37.1, 54.0, 55.5, 114.2, 128.2, 128.9, 130.6, 131.8, 132.9, 142.2, 162.6. MS (EI): 329 (M^+). HRMS (ESI) *m*/*z* calcd for $C_{19}H_{24}NO_2S$ $(M+H)^+$ 330.1522, found 330.1523. IR (KBr): 3060, 2932, 2858, 2837, 2359, 2341, 1495, 1248, 1134.

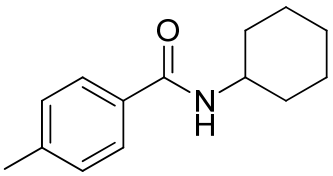
_N_-Cyclohexylbenzamide (5a): [1]



Flash column chromatography on a silica gel (ethyl acetate: petroleum ether: triethylamine, 1: 20: 0.1) give the product (36.9 mg, 91% yield) as a white solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.15-1.27 (m, 3H), 1.33-1.40 (m, 2H), 1.60-1.64 (m, 1H), 1.71-1.75 (m, 2H), 1.97-2.01 (m, 2H), 3.91-3.98 (m, 1H), 6.20 (s, 1H), 7.36-7.39 (m, 2H), 7.42-7.46 (m, 1H), 7.73-7.75 (m, 2H); ^{13}C NMR

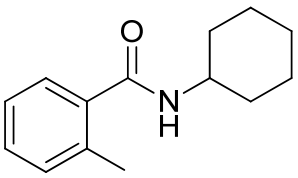
($CDCl_3$, 100 MHz) δ 24.8, 25.5, 33.1, 48.6, 126.8, 128.4, 131.1, 135.0, 166.6.

_N_-Cyclohexyl-4-methylbenzamide (5b)[1]:



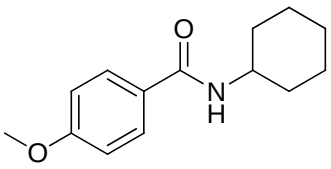
Flash column chromatography on a silica gel (ethyl acetate: petroleum ether: triethylamine, 1: 15: 0.1) give the product (38.2 mg, 88% yield) as a white solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.18-1.24 (m, 4H), 1.38-1.47 (m, 2H), 1.73-1.76 (m, 2H), 2.01-2.03 (m, 2H), 2.38 (s, 3H), 3.93-4.00 (m, 1H), 5.94 (s, 1H), 7.21 (d, J = 7.8 Hz, 2H), 7.64 (d, J = 7.9 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 21.4, 24.9, 25.6, 33.2, 48.5, 126.8, 129.1, 132.1, 141.6, 166.5.

_N_-Cyclohexyl-2-methylbenzamide (5c)[1]:



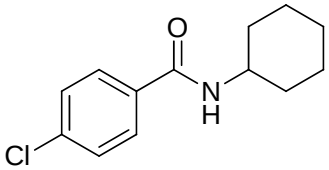
Flash column chromatography on a silica gel (ethyl acetate: petroleum ether: triethylamine, 1: 15: 0.1) give the product (32.5 mg, 75% yield) as a white solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.20-1.25 (m, 3H), 1.37-1.43 (m, 2H), 1.62-1.66 (m, 1H), 1.72-1.76 (m, 2H), 2.00-2.04 (m, 2H), 2.42 (s, 3H), 3.91-3.98 (m, 1H), 5.72 (s, 1H), 7.15-7.20 (m, 2H), 7.26-7.32 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 19.6, 24.8, 25.4, 33.1, 48.4, 125.6, 126.5, 129.5, 130.8, 135.6, 136.9, 169.2.

_N_-Cyclohexyl-4-methoxybenzamide (5d)[1]:



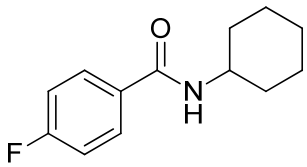
Flash column chromatography on a silica gel (ethyl acetate: petroleum ether: triethylamine, 1: 10: 0.1) give the product (43.4 mg, 93% yield) as a white solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.14-1.25 (m, 3H), 1.36-1.42 (m, 2H), 1.60-1.63 (m, 1H), 1.70-1.73 (m, 2H), 1.96-2.02 (m, 2H), 3.80 (s, 3H), 3.89-3.96 (m, 1H), 6.09 (d, J = 7.3 Hz, 1H), 6.86 (d, J = 8.8 Hz, 2H), 7.71 (d, J = 8.7 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 24.9, 25.5, 33.2, 48.5, 113.5, 127.3, 128.6, 161.8, 166.0.

4-Chloro-_N_-cyclohexylbenzamide (5e)[1]:



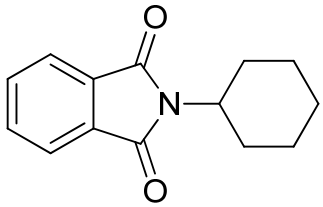
Flash column chromatography on a silica gel (ethyl acetate: petroleum ether: triethylamine, 1: 15: 0.1) give the product (45.6 mg, 96% yield) as a white solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.14-1.25 (m, 3H), 1.33-1.39 (m, 2H), 1.61-1.64 (m, 1H), 1.71-1.74 (m, 2H), 1.97-2.00 (m, 2H), 3.91-3.93 (m, 1H), 6.17 (d, J = 6.4 Hz, 1H), 7.34 (d, J = 8.3 Hz, 2H), 7.67 (d, J = 8.3 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 24.9, 25.4, 33.1, 48.5, 128.3, 128.6, 133.4, 137.3, 165.5.

***N*-Cyclohexyl-4-fluorobenzamide (5f)[1]:**



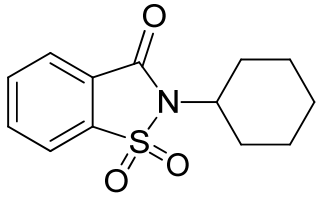
Flash column chromatography on a silica gel (ethyl acetate: petroleum ether: triethylamine, 1: 15: 0.1) give the product (40.7 mg, 92% yield) as a white solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.13-1.23 (m, 3H), 1.32-1.42 (m, 2H), 1.60-1.65 (m, 1H), 1.70-1.75 (m, 2H), 1.96-2.00 (m, 2H), 3.87-3.96 (m, 1H), 6.14 (s, 1H), 7.03-7.07 (m, 2H), 7.73-7.76 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 24.9, 25.5, 33.1, 48.8, 115.3 (J = 21.7 Hz), 129.1 (J = 9 Hz), 131.2 (J = 3.1 Hz), 164.5 (J = 249.8 Hz), 165.5.

2-Cyclohexylisoindoline-1,3-dione (5g)[1]:



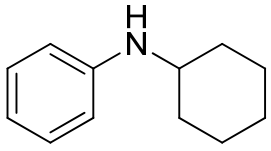
Flash column chromatography on a silica gel (ethyl acetate: petroleum ether, 1: 40) give the product (36.6 mg, 90% yield) as a white solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.26-1.40 (m, 3H), 1.66-1.72 (m, 1H), 1.82-1.86 (m, 2H), 2.13-2.23 (m, 2H), 4.04-4.12 (m, 1H), 7.65-7.68 (m, 2H), 7.77-7.79 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 25.0, 26.0, 29.8, 50.8, 122.9, 132.0, 133.7, 168.4.

2-Cyclohexylbenzo[d]isothiazol-3(2H)-one 1,1-dioxide (5h)[2]:



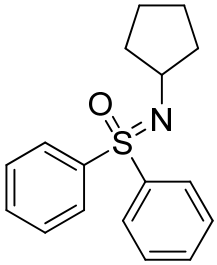
Flash column chromatography on a silica gel (ethyl acetate: petroleum ether, 1: 40) give the product (36.6 mg, 90% yield) as a white solid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.26-1.40 (m, 3H), 1.66-1.72 (m, 1H), 1.82-1.86 (m, 2H), 2.13-2.23 (m, 2H), 4.04-4.12 (m, 1H), 7.65-7.68 (m, 2H), 7.77-7.79 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 25.0, 26.0, 29.8, 50.8, 122.9, 132.0, 133.7, 168.4.

***N*-Cyclohexylaniline (5i)[3]:**



Flash column chromatography on a silica gel (ethyl acetate: petroleum ether: triethylamine, 1: 100: 0.1) give the product (14.7 mg, 42% yield) as a yellowish liquid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.12-1.15 (m, 1H), 1.22-1.28 (m, 2H), 1.35-1.43 (m, 2H), 1.64-1.68 (m, 1H), 1.75-1.76 (m, 2H), 2.05-2.09 (m, 2H), 3.23-3.30 (m, 1H), 3.52 (s, 1H), 6.59-6.61 (m, 2H), 6.65-6.69 (m, 1H), 7.15-7.19 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 25.0, 25.9, 33.5, 51.6, 113.1, 116.8, 129.2, 147.4.

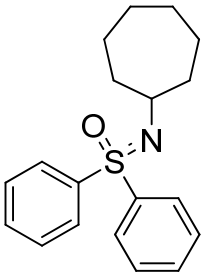
***N*-(Cyclopentyl) diphenyl sulfoximine (3ab):**



Flash column chromatography on a silica gel (ethyl acetate: petroleum ether, 1: 20) give the product (25.1 mg, 44% yield) as a white solid; m.p.: 130-133 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ

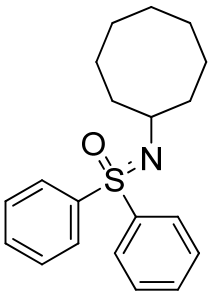
1.43-1.50 (m, 2H), 1.62-1.71 (m, 2H), 1.73-1.78 (m, 2H), 1.80-1.85 (m, 2H), 3.45-3.52 (m, 1H), 7.42-7.48 (m, 6H), 7.96-7.98 (m, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 23.6, 36.2, 56.0, 128.6, 129.0, 132.1, 141.4. MS (EI): 285 (M^+). HRMS (ESI) *m*/*z* calcd for $C_{17}H_{20}NOS$ $(M+H)^+$ 286.1260, found 286.1260. IR (KBr): 3065, 3062, 2955, 2860, 2359, 2341, 1448, 1244, 1138.

***N*-(Cycloheptyl) diphenyl sulfoximine (3ac):**



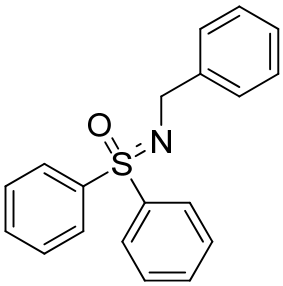
Flash column chromatography on a silica gel (ethyl acetate: petroleum ether, 1: 20) give the product (50.7 mg, 81% yield) as a white solid; m.p.: 99-101 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.32-1.38 (m, 2H), 1.51-1.54 (m, 4H), 1.66-1.72 (m, 2H), 1.74-1.81 (m, 2H), 1.89-1.95 (m, 2H), 3.20-3.27 (m, 1H), 7.42-7.47 (m, 6H), 7.95-7.98 (m, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 24.0, 28.1, 38.9, 56.2, 128.6, 128.9, 132.0, 141.5. MS (EI): 313 (M^+); HRMS (ESI) *m*/*z* calcd for $C_{19}H_{24}NOS$ $(M+H)^+$ 314.1573, found 314.1577. IR (KBr): 3068, 2935, 2854, 2359, 2341, 1446, 1240, 1132.

***N*-(Cyclooctyl) diphenyl sulfoximine (3ad):**



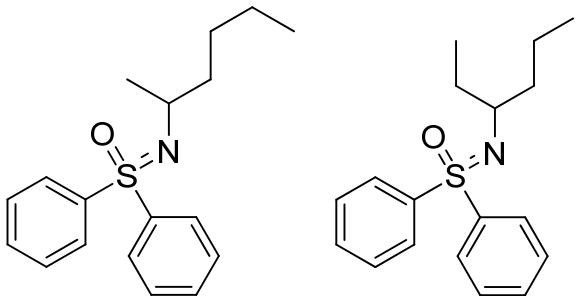
Flash column chromatography on a silica gel (ethyl acetate: petroleum ether, 1: 20) give the product (32.7 mg, 50% yield) as a colorless liquid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.34-1.43 (m, 4H), 1.47-1.51 (m, 2H), 1.54-1.61 (m, 2H), 1.73-1.80 (m, 4H), 1.84-1.92 (m, 2H), 3.24-3.30 (m, 1H), 7.42-7.49 (m, 6H), 7.95-7.98 (m, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 23.6, 25.4, 27.5, 35.8, 55.1, 128.6, 128.9, 132.0, 141.5. MS (EI): 327 (M^+); HRMS (ESI) *m*/*z* calcd for $C_{20}H_{26}NOS$ $(M+H)^+$ 328.1730, found 328.1725. IR (KBr): 3063, 2920, 2850, 2385, 1446, 1246, 1136.

***N*-(Benzyl) diphenyl sulfoximine (3ae):**



Flash column chromatography on a silica gel (ethyl acetate: petroleum ether, 1: 25) give the product (27.0 mg, 44% yield) as a yellowish solid; m.p.: 58-60 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 4.29 (s, 2H), 7.21-7.24 (m, 1H), 7.31-7.34 (m, 2H), 7.45-7.51 (m, 8H), 8.01-8.03 (m, 4H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 47.1, 126.4, 127.4, 128.2, 128.6, 129.1, 132.4, 140.7, 141.5. MS (EI): 307 (M^+); HRMS (ESI) *m*/*z* calcd for $C_{19}H_{17}NNaOS$ $(M+Na)^+$ 330.0923, found 330.0937. IR (KBr): 3273, 3071, 2918, 2850, 2361, 2341, 1446, 1227, 1130, 1095.

***N*-(2-Hexyl) diphenyl sulfoximine (3af):**



Flash column chromatography on a silica gel (ethyl acetate: petroleum ether, 1: 20) give the product (39.1 mg, 65% yield) as a colorless liquid. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 0.84-0.96 (m, 4H), 1.21-1.60 (m, 8H), 2.97-3.19 (m, 1H), 7.43-7.49 (m, 6H), 7.93-8.01 (m, 4H). MS (EI): 301 (M^+). HRMS (ESI) *m*/*z* calcd for $C_{18}H_{23}NNaOS$ $(M+Na)^+$ 324.1393, found 324.1396. IR (KBr): 3065, 2957, 2928, 2858, 2361, 2341, 1446, 1246, 1140.

5. References

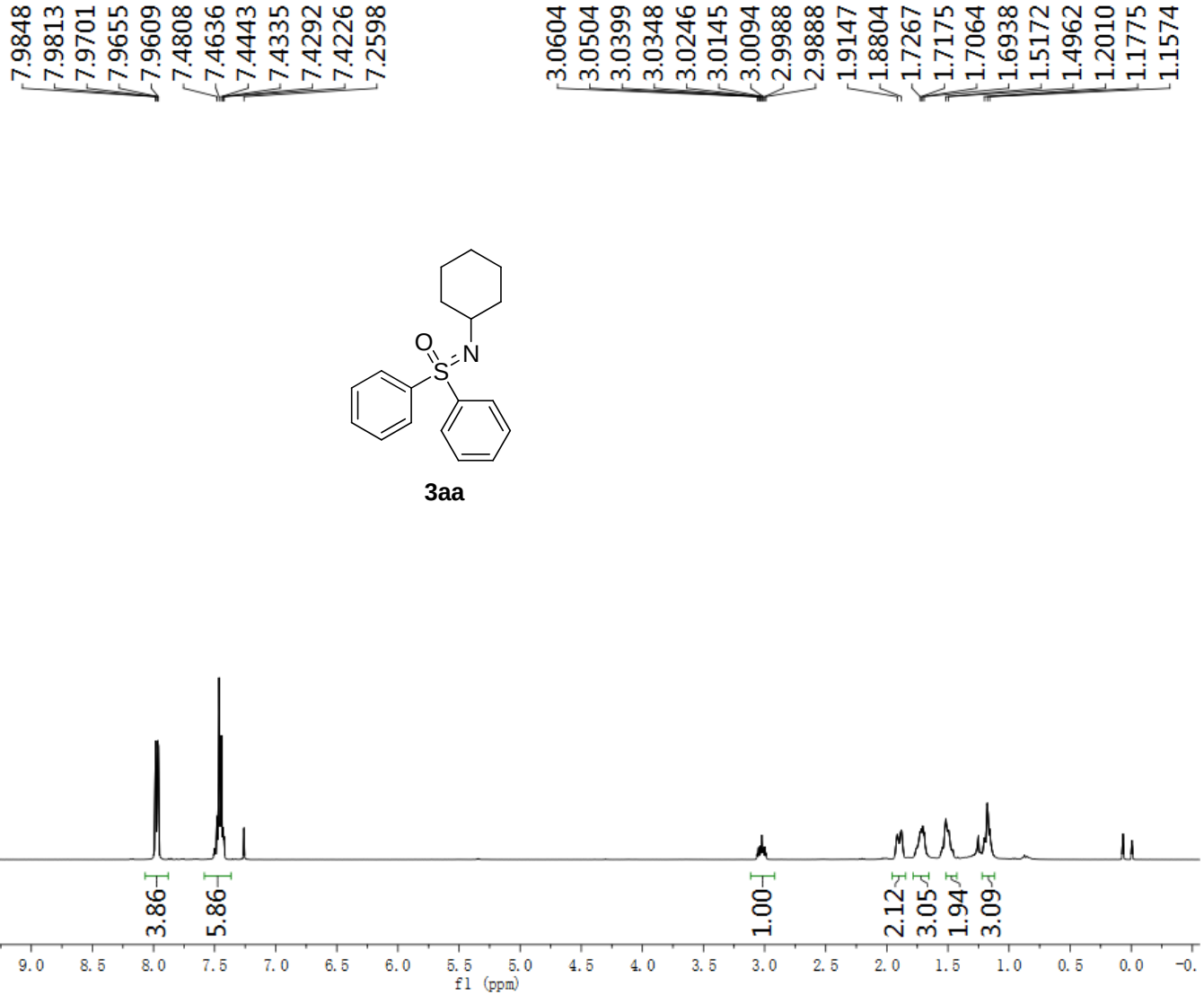
1 B. L. Tran, B. Li, M. Driess and J. F. Hartwig, *J. Am. Chem. Soc.,* 2014, **136**, 2555.

2 K. Smith, C. D. Hupp, K. L. Allen and G. A. Slough, *Organometallics,* 2005, **24**, 1747.

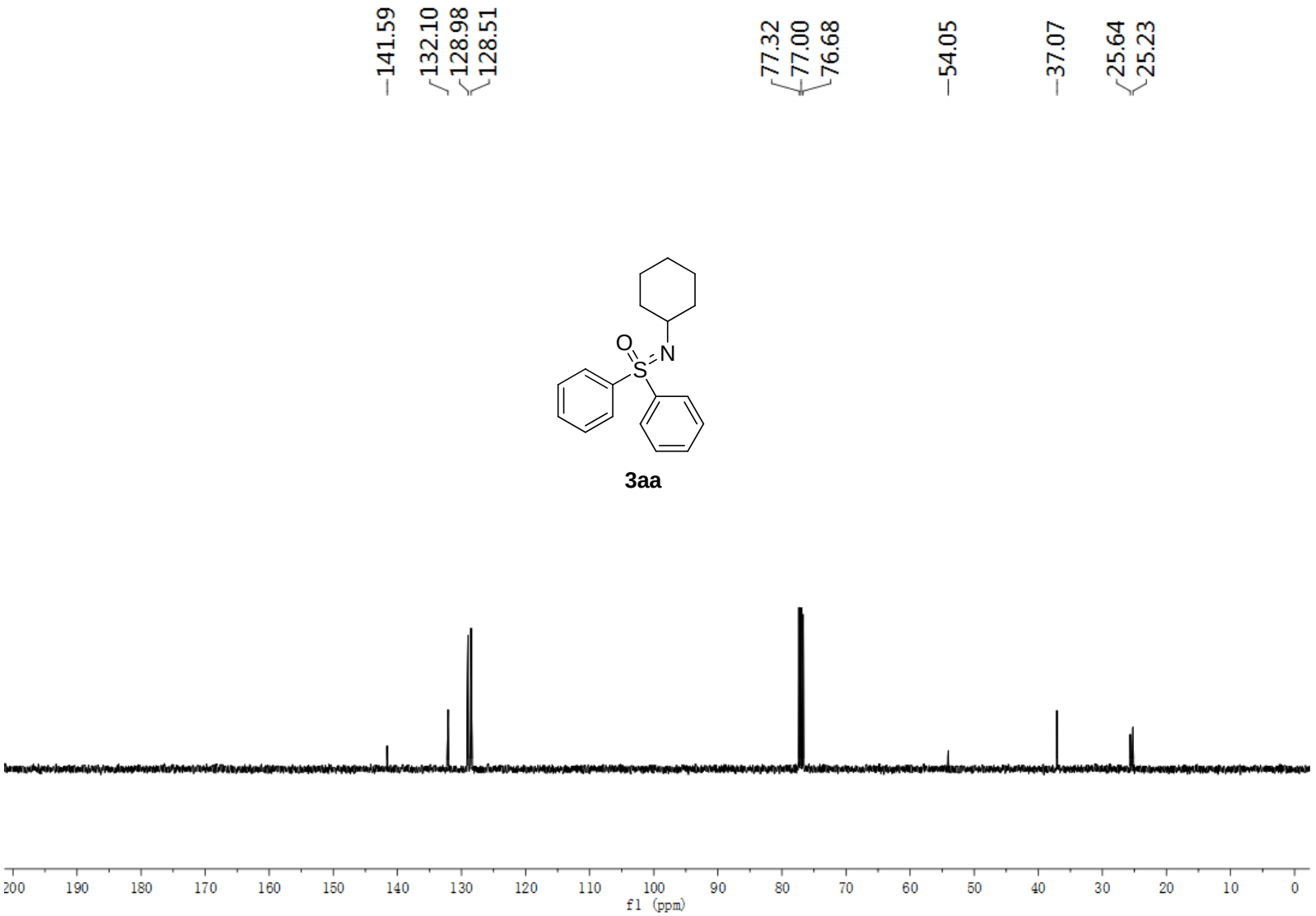
3 D. Hollmann, S. Bähn, A. Tillack and M. Beller, *Chem. Commun.,* 2008, 3199.

6. Copies of the ^{1}H NMR and ^{13}C NMR Spectra

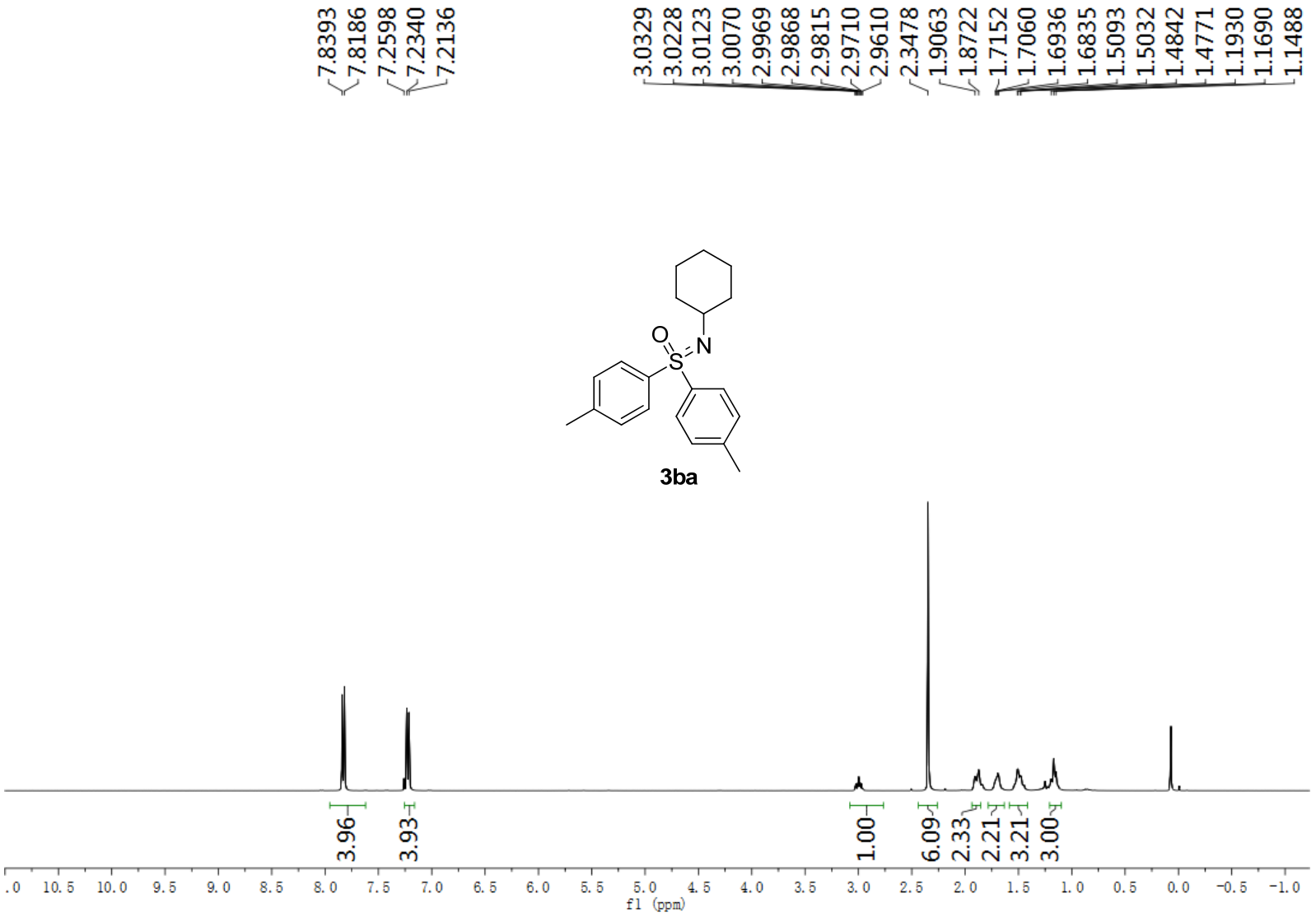
***N*-(Cyclohexyl) diphenyl sulfoximine (3aa)**

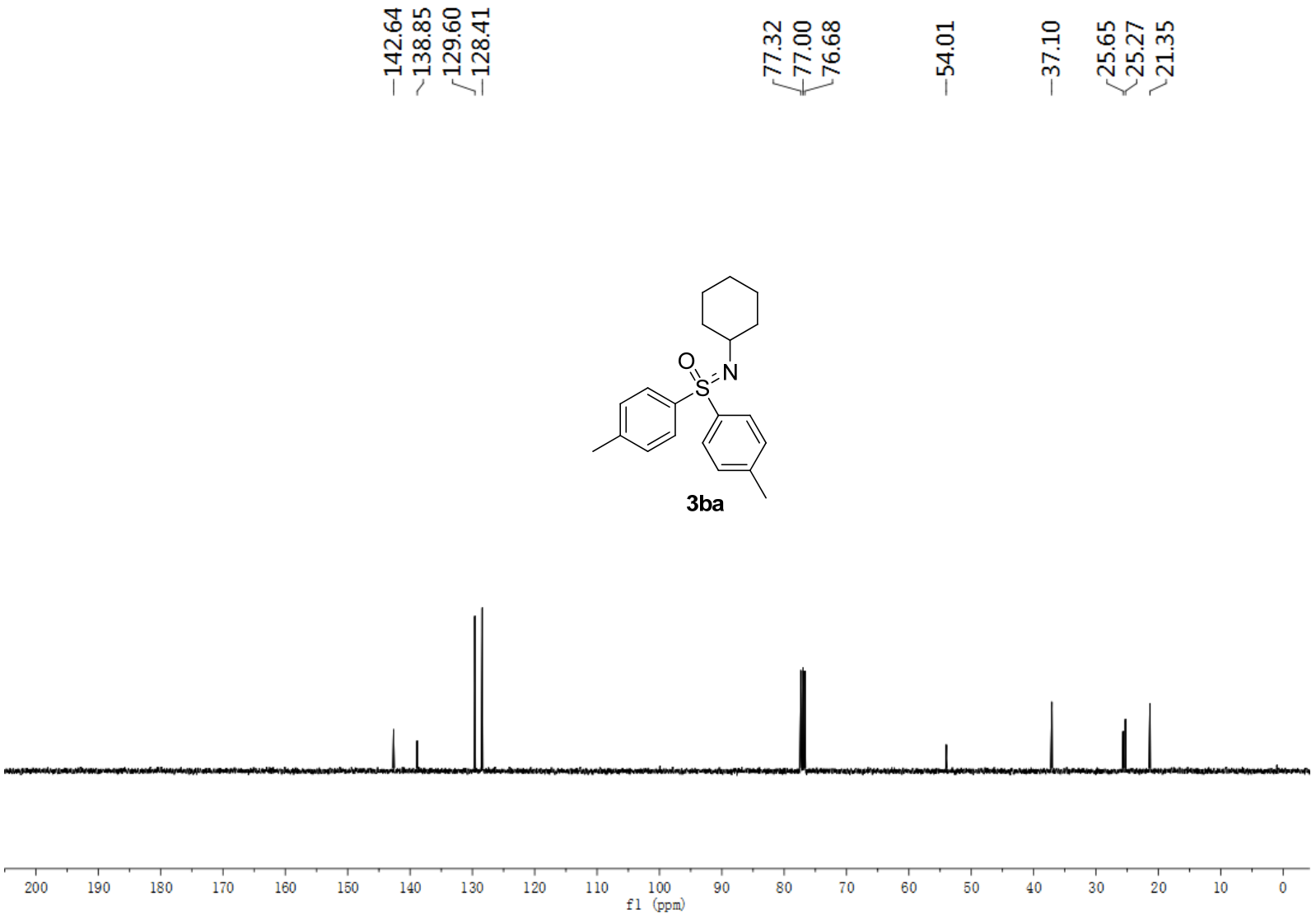


3aa

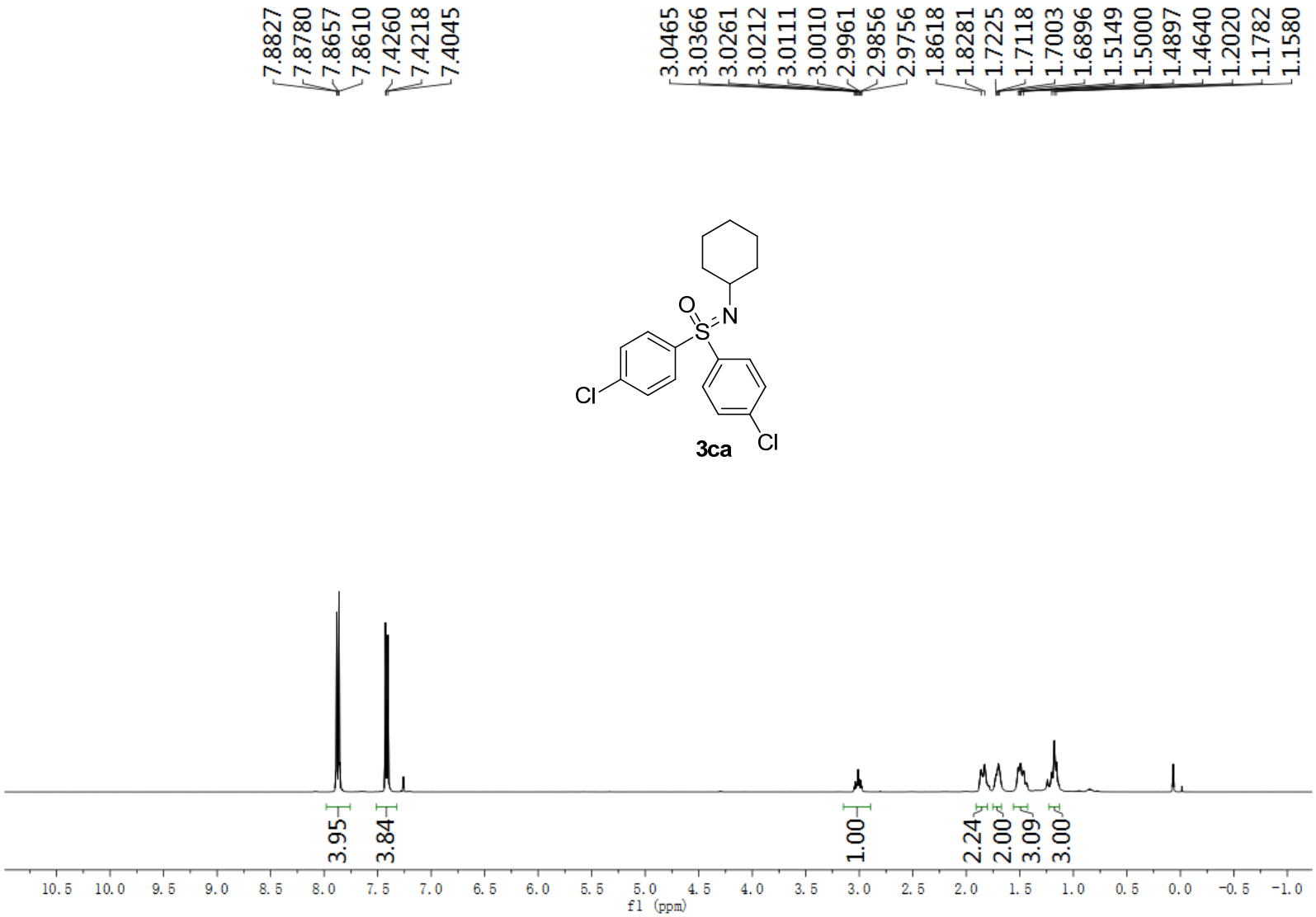

141.59
132.10
128.98
128.51
77.32
77.00
76.68
54.05
37.07
25.64
25.23
O
S
N
3aa
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

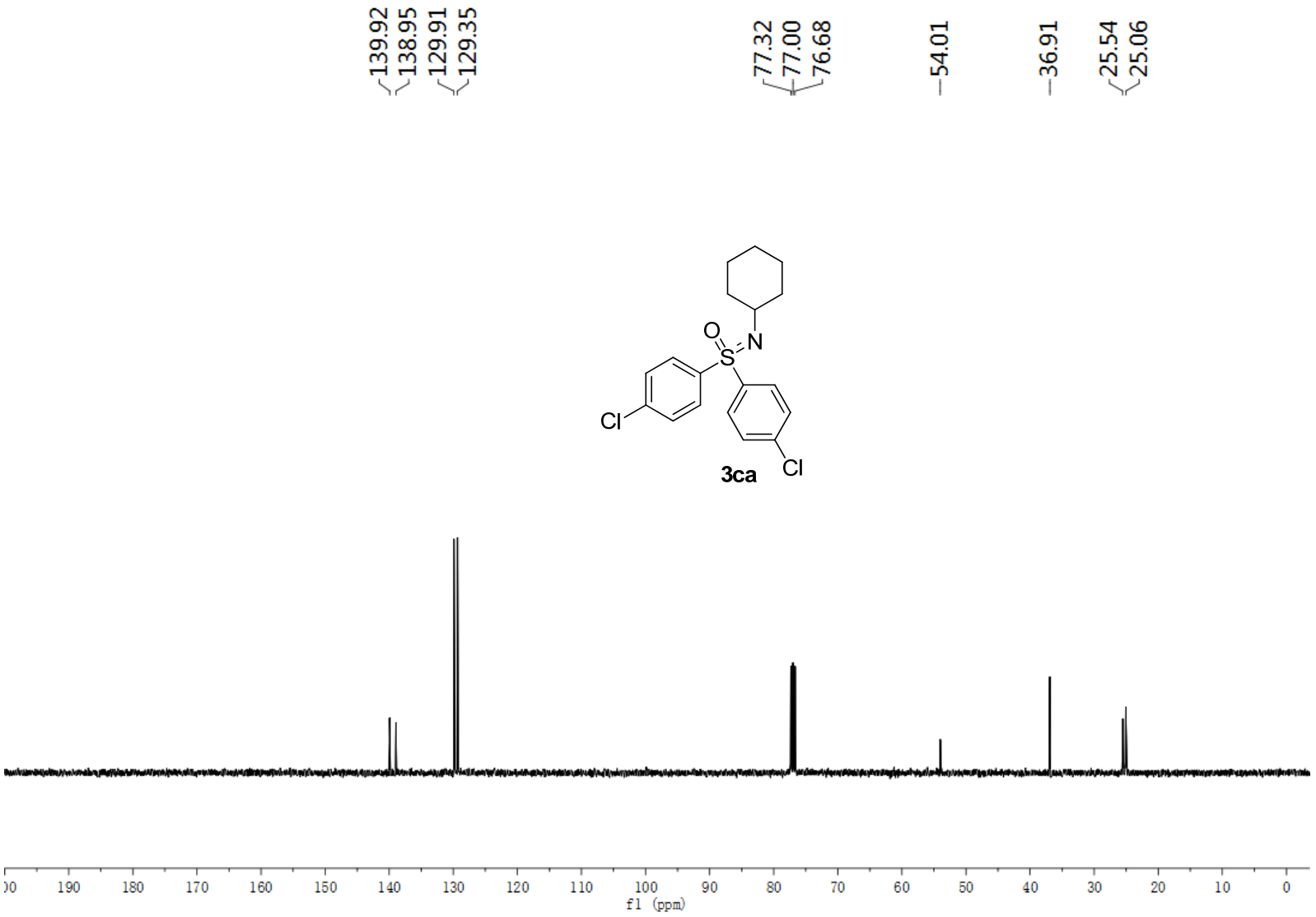
_N_-(Cyclohexyl)-4,4’-dimethyl diphenyl sulfoximine (3ba)



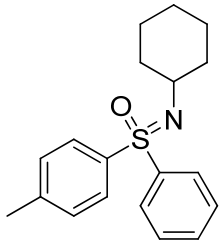

142.64
138.85
129.60
128.41
77.32
77.00
76.68
54.01
37.10
25.65
25.27
21.35
O
S
N
3ba
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

_N_-(Cyclohexyl)-4,4'-dicholo diphenyl sulfoximine (3ca)

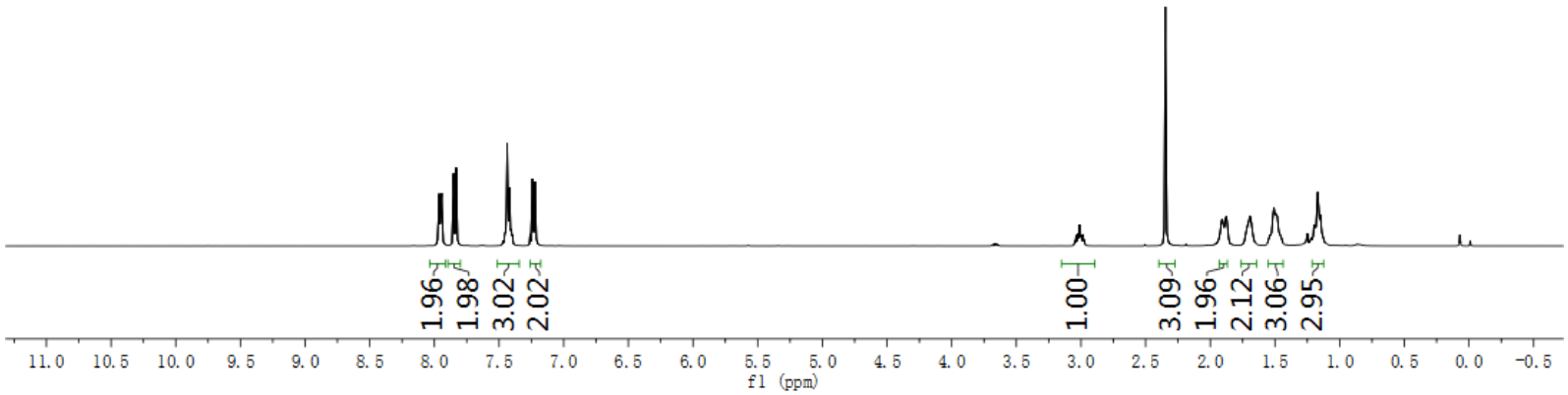


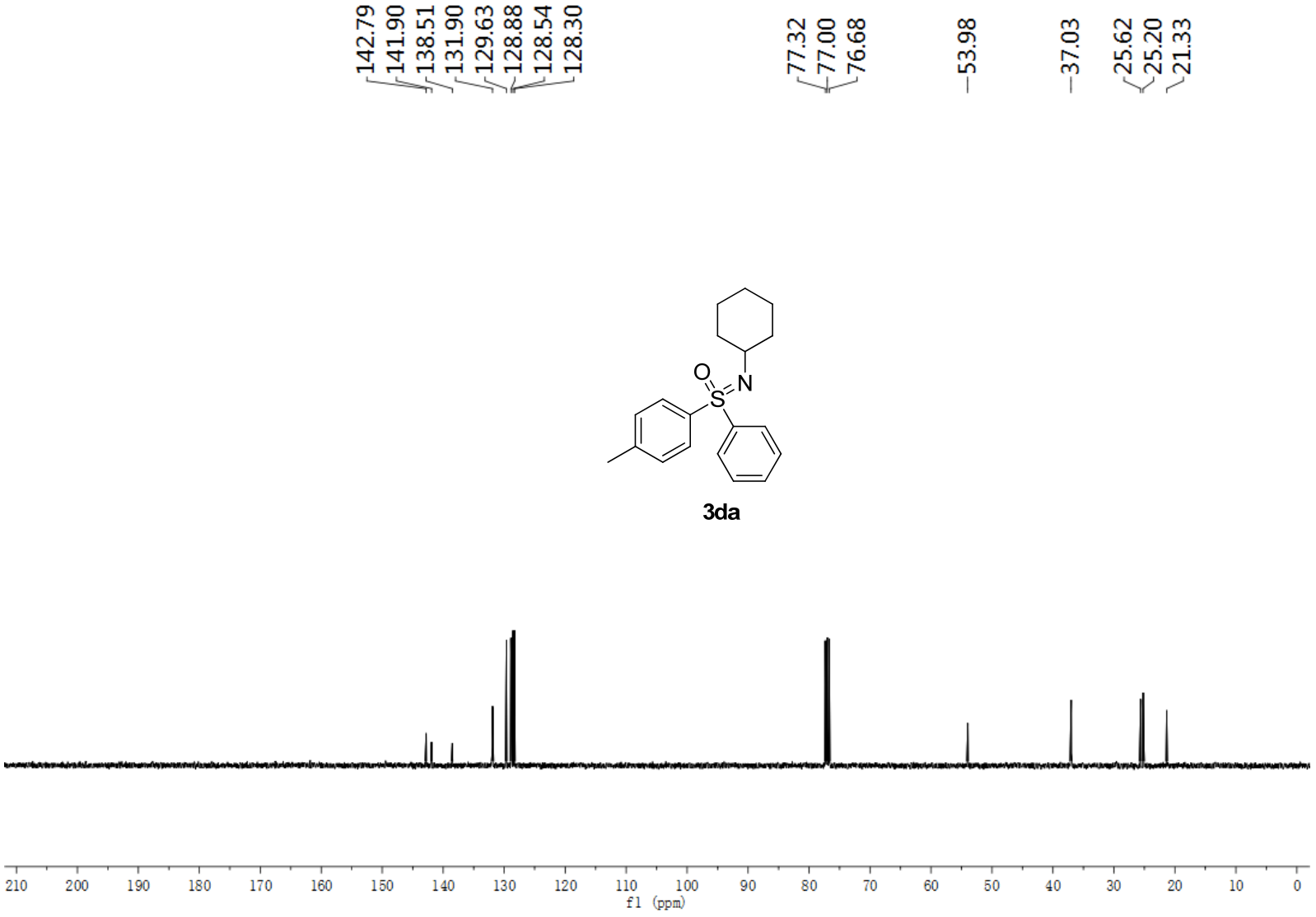

139.92
138.95
129.91
129.35
77.32
77.00
76.68
54.01
36.91
25.54
25.06
O
S
N
Cl
Cl
3ca
f1 (ppm)

_N_-(Cyclohexyl)-4-methyl diphenyl sulfoximine (3da)

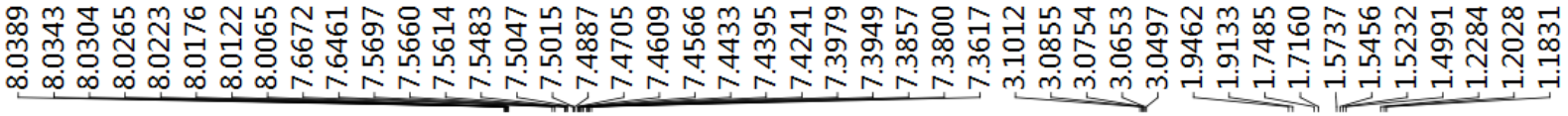


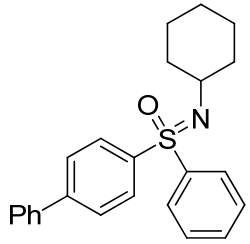
3da



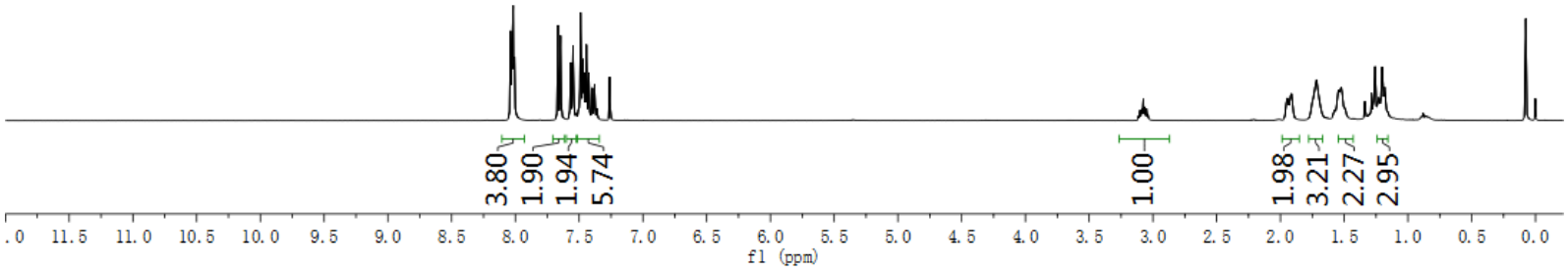

142.79
141.90
138.51
131.90
129.63
128.88
128.54
128.30
77.32
77.00
76.68
53.98
37.03
25.62
25.20
21.33
O
S
N
3da
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

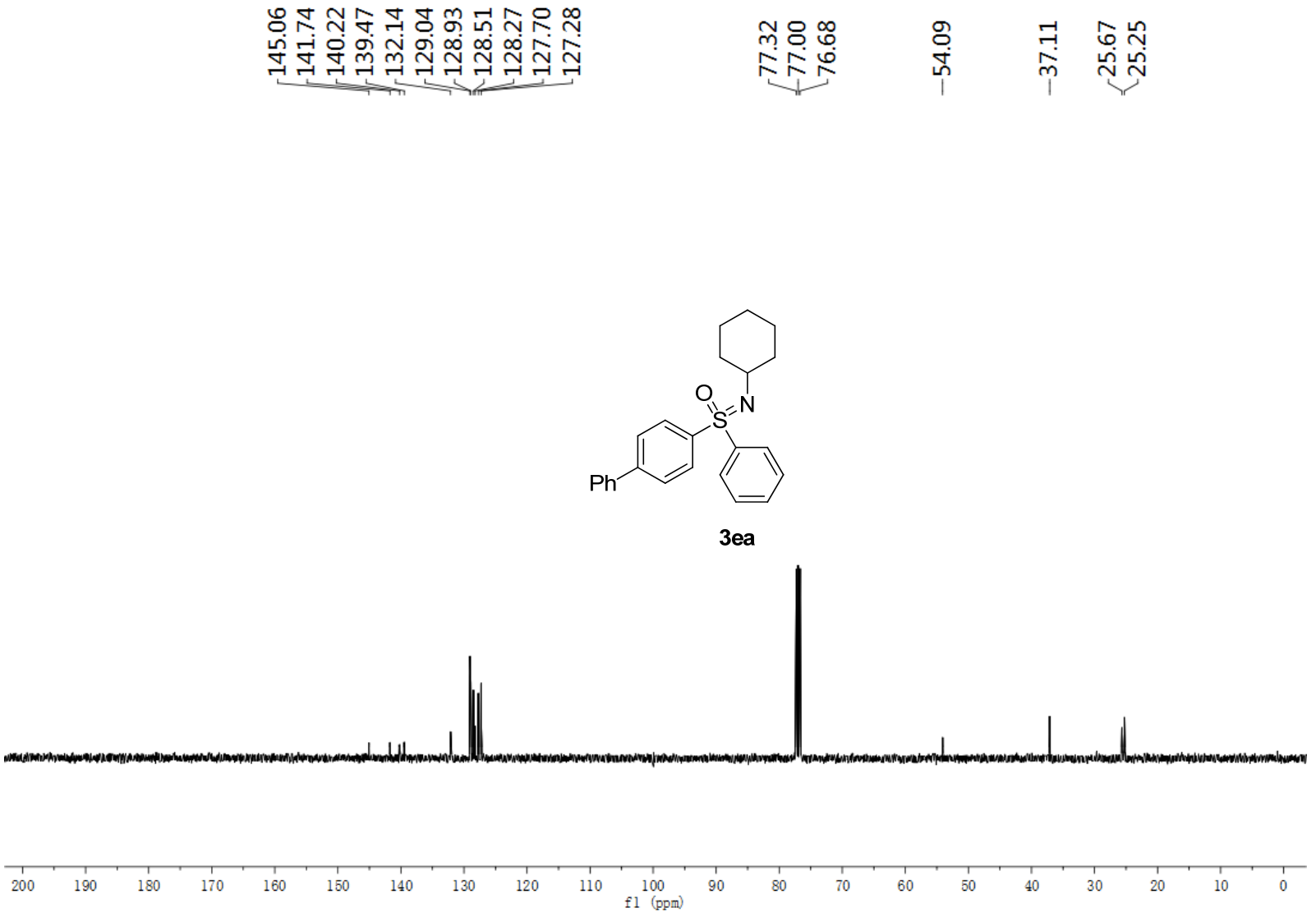
_N_-(Cyclohexyl)-4-phenyl diphenyl sulfoximine (3ea)



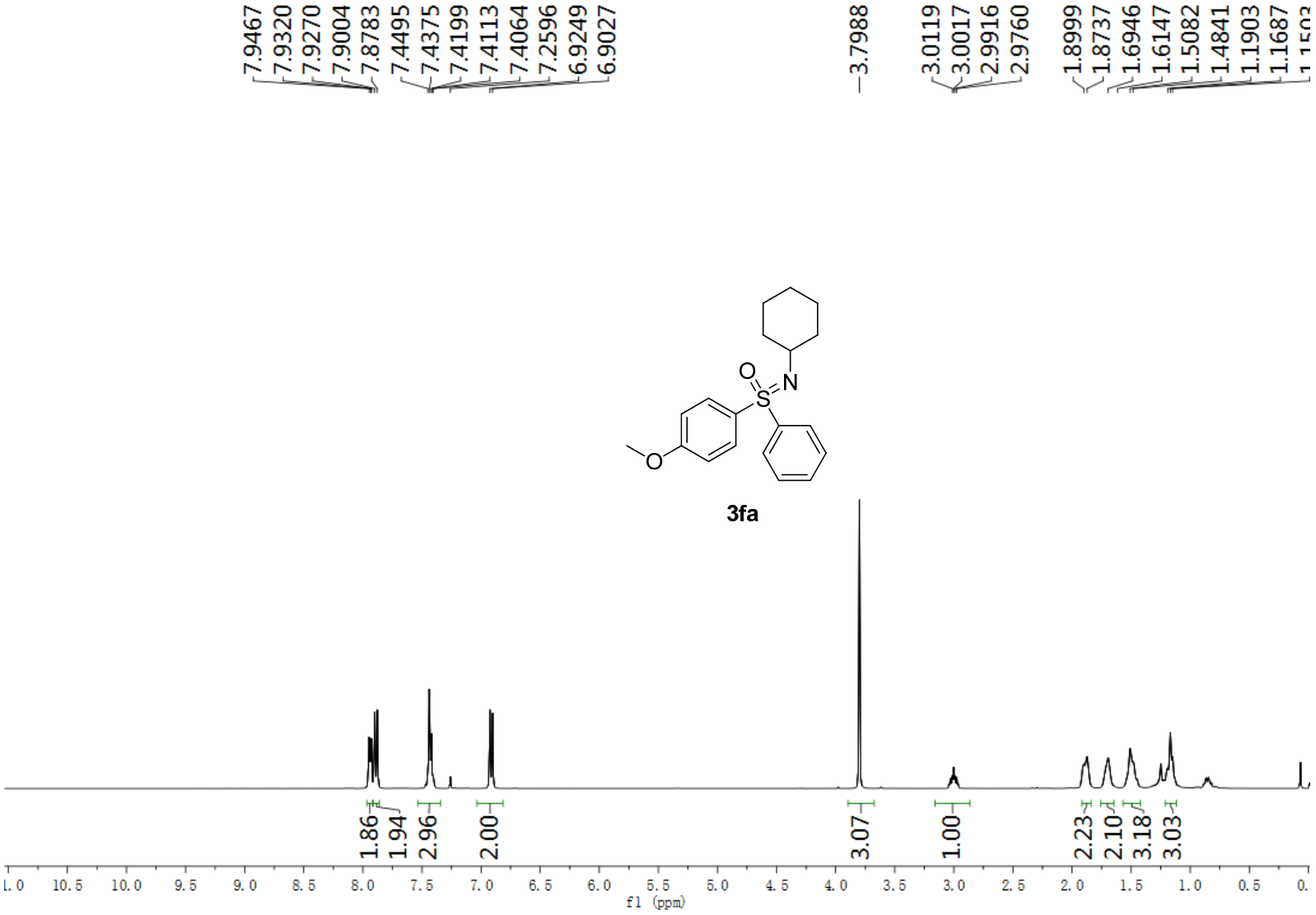


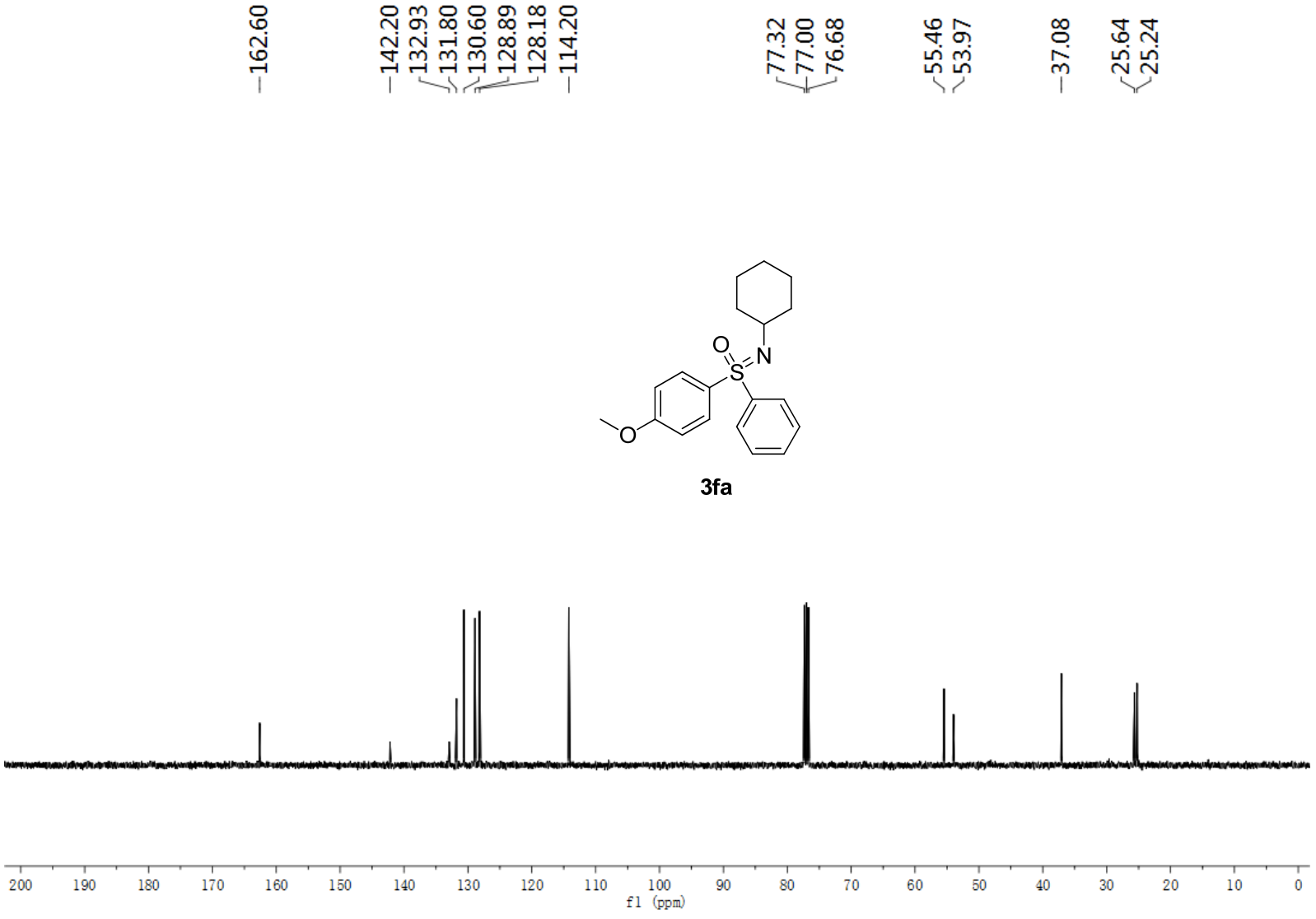
3ea




145.06
141.74
140.22
139.47
132.14
129.04
128.93
128.51
128.27
127.70
127.28
77.32
77.00
76.68
54.09
37.11
25.67
25.25
O
S
N
Ph
3ea
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

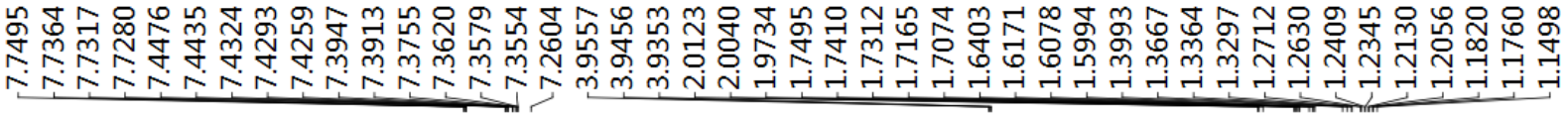
_N_-(Cyclohexyl)-4-methoxyl diphenyl sulfoximine (3fa)

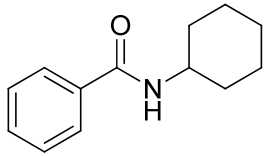



162.60
142.20
132.93
131.80
130.60
128.89
128.18
114.20
77.32
77.00
76.68
55.46
53.97
37.08
25.64
25.24
O
S
N
O
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

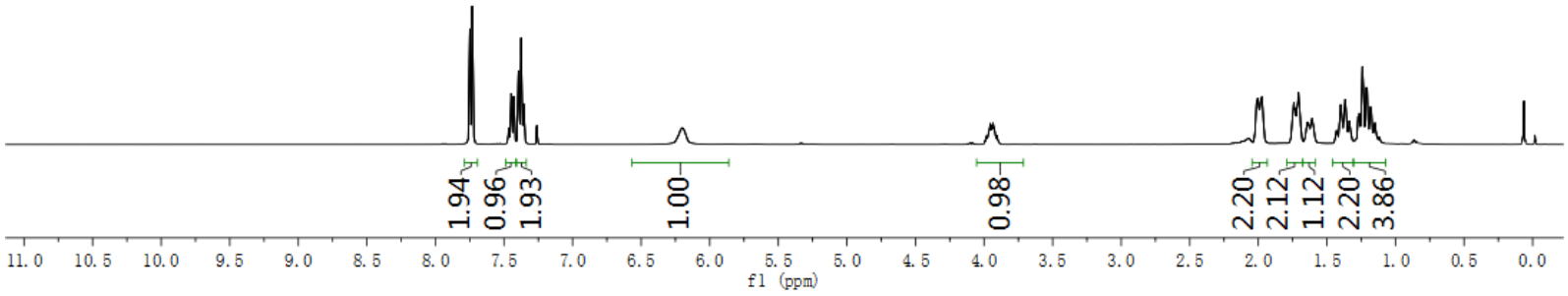
3fa

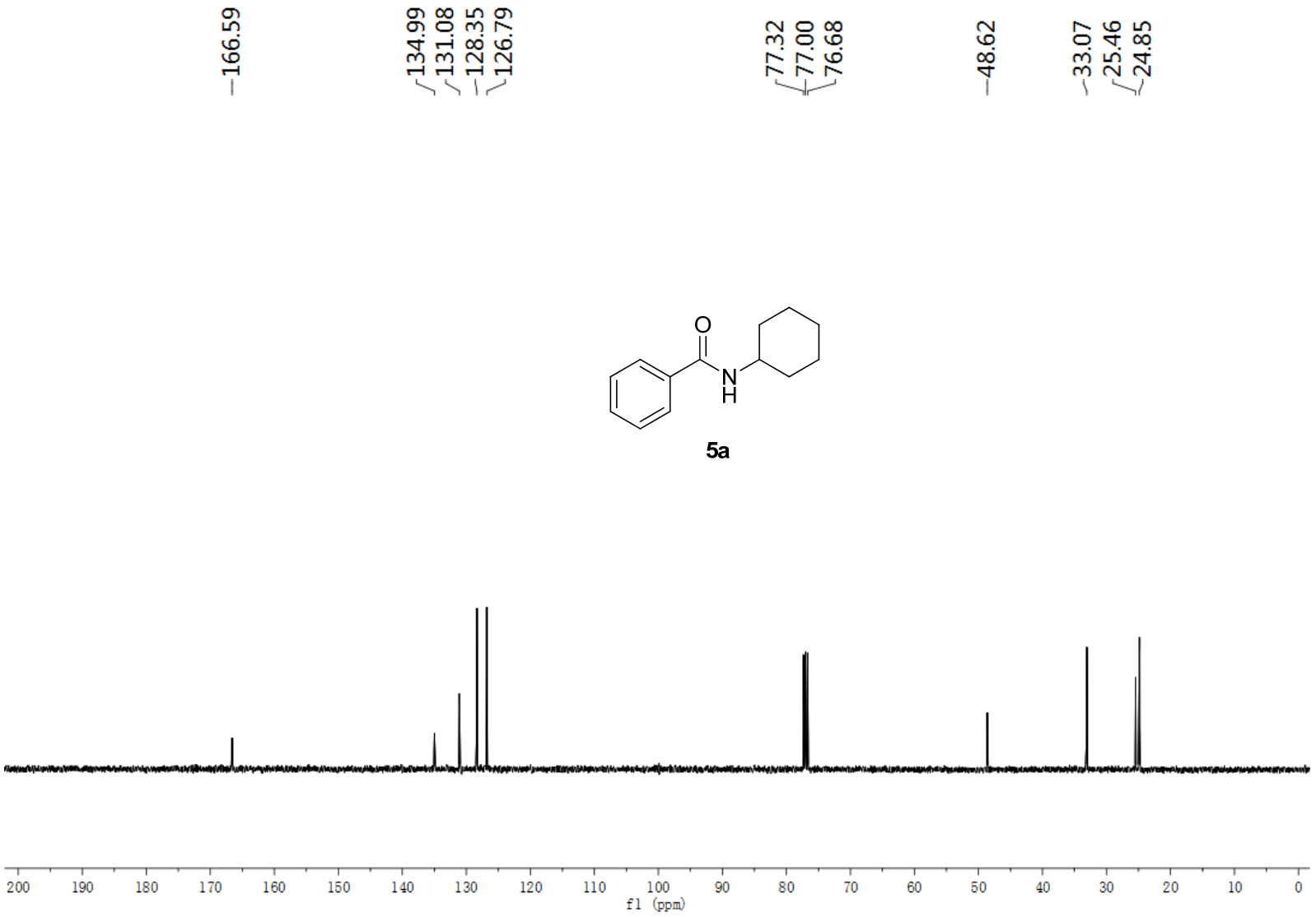
_N_-Cyclohexylbenzamide (5a)



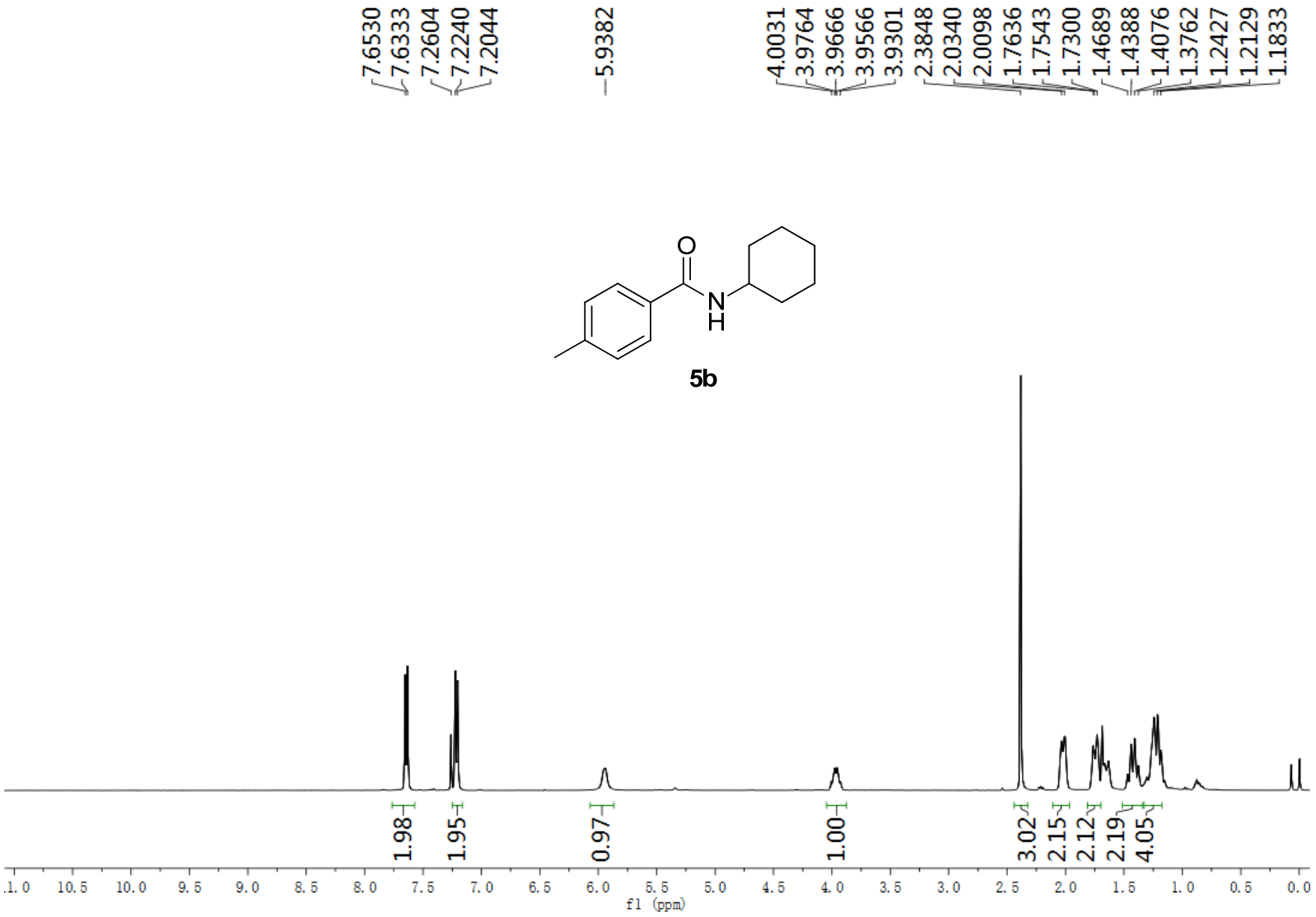


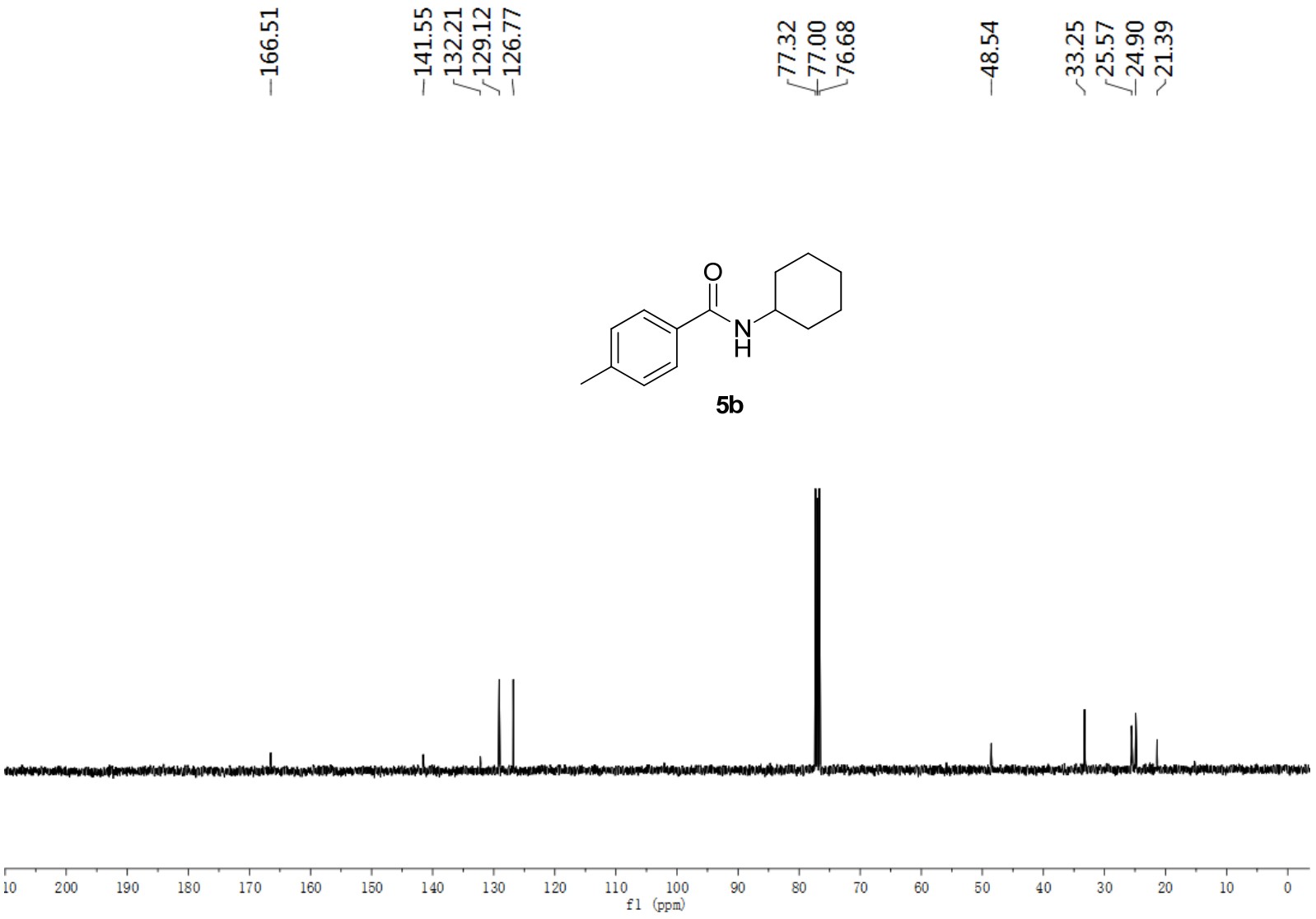
5a



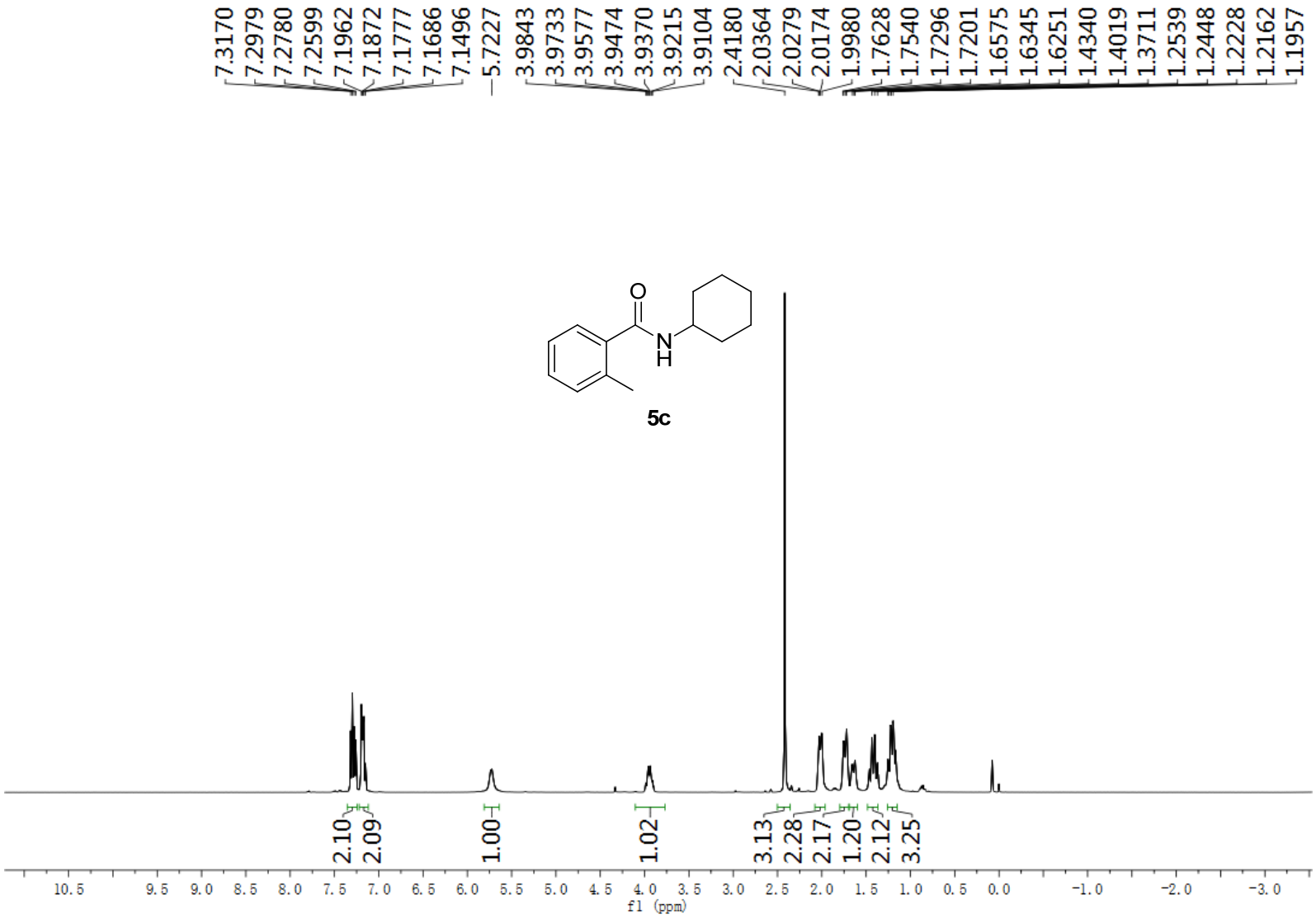

166.59
134.99
131.08
128.35
126.79
77.32
77.00
76.68
48.62
33.07
25.46
24.85
O
N
H
5a
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

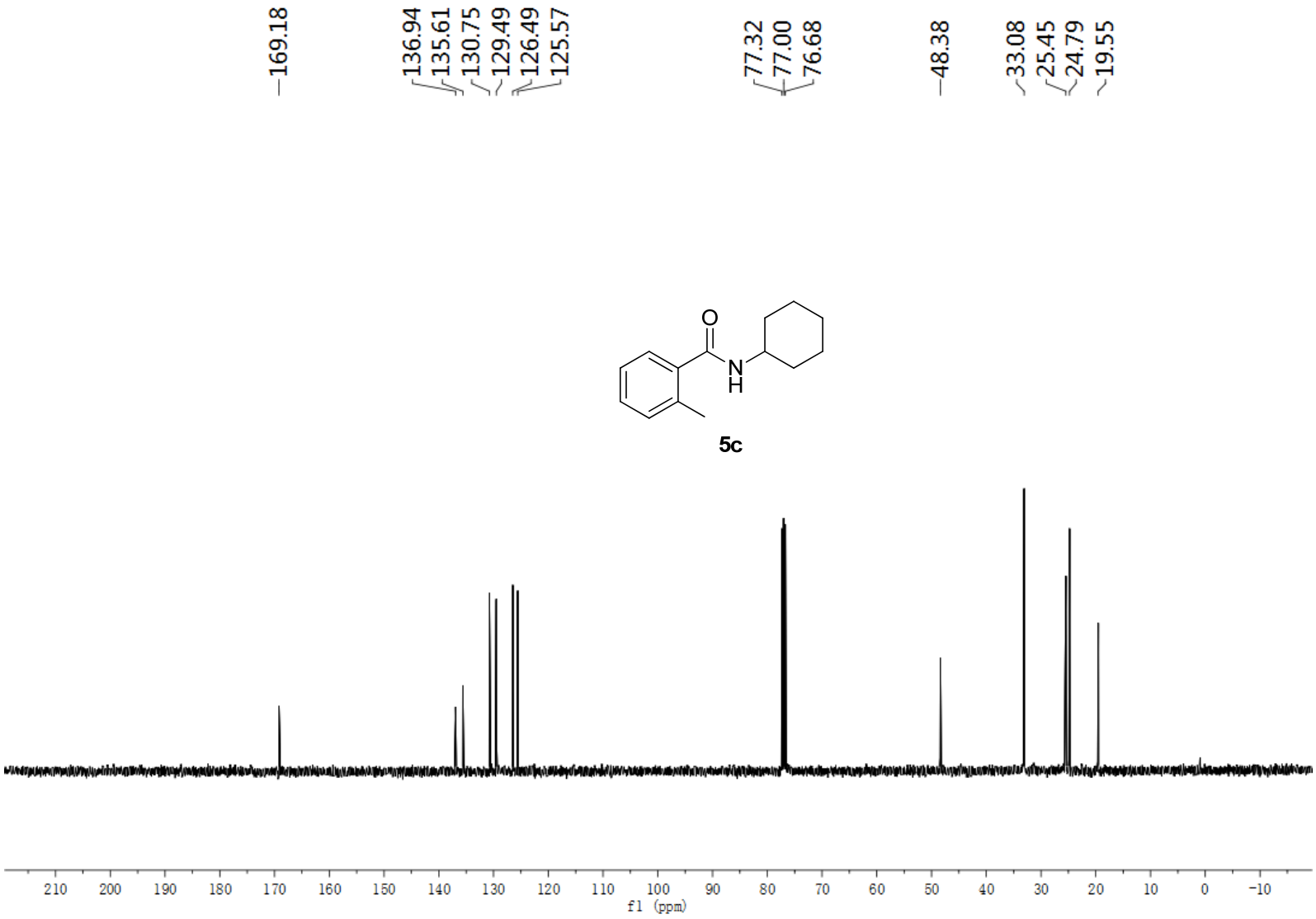
_N_-Cyclohexyl-4-methylbenzamide (5b)



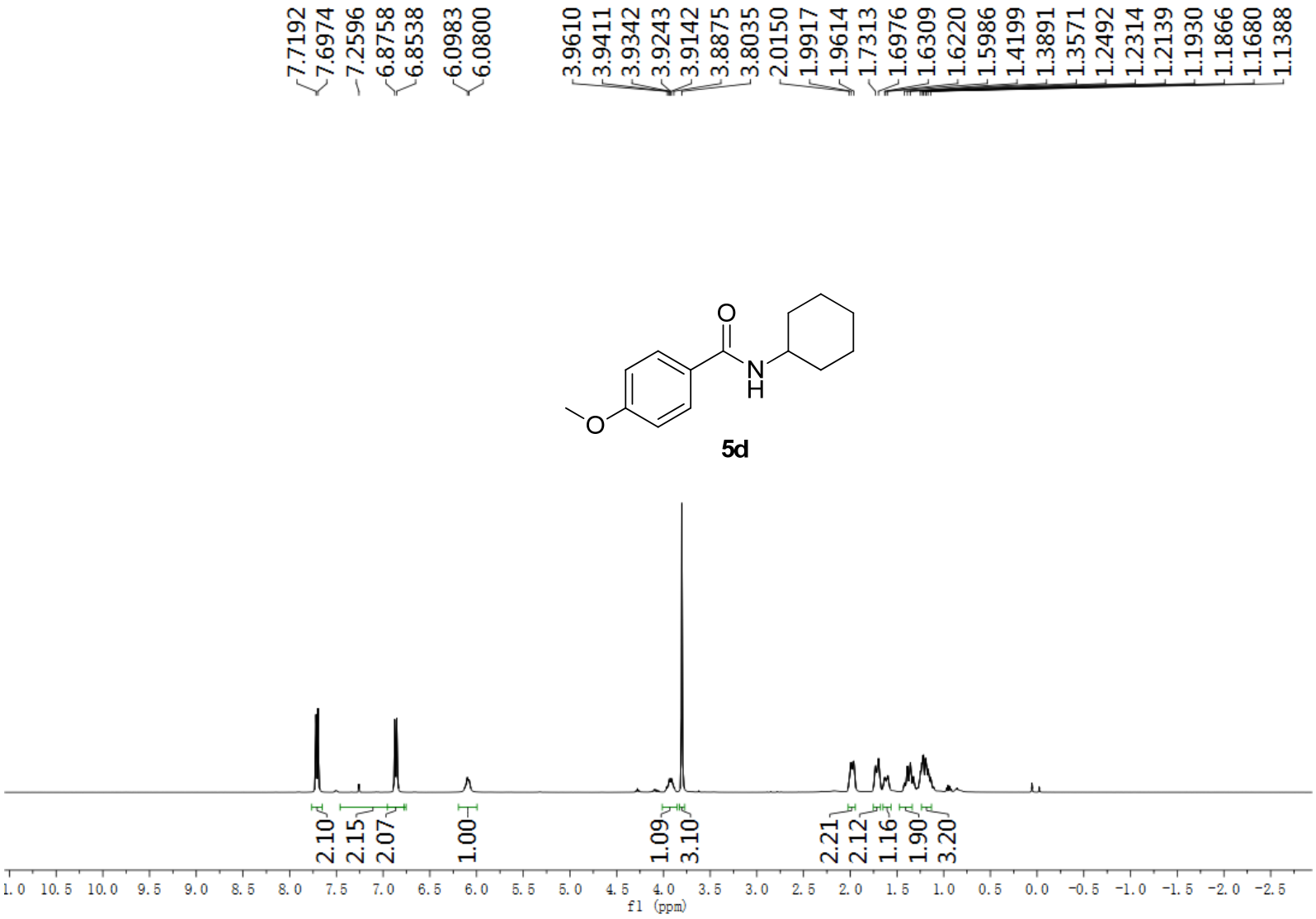

166.51
141.55
132.21
129.12
126.77
77.32
77.00
76.68
48.54
33.25
25.57
24.90
21.39
O
N
H
5b
f1 (ppm)

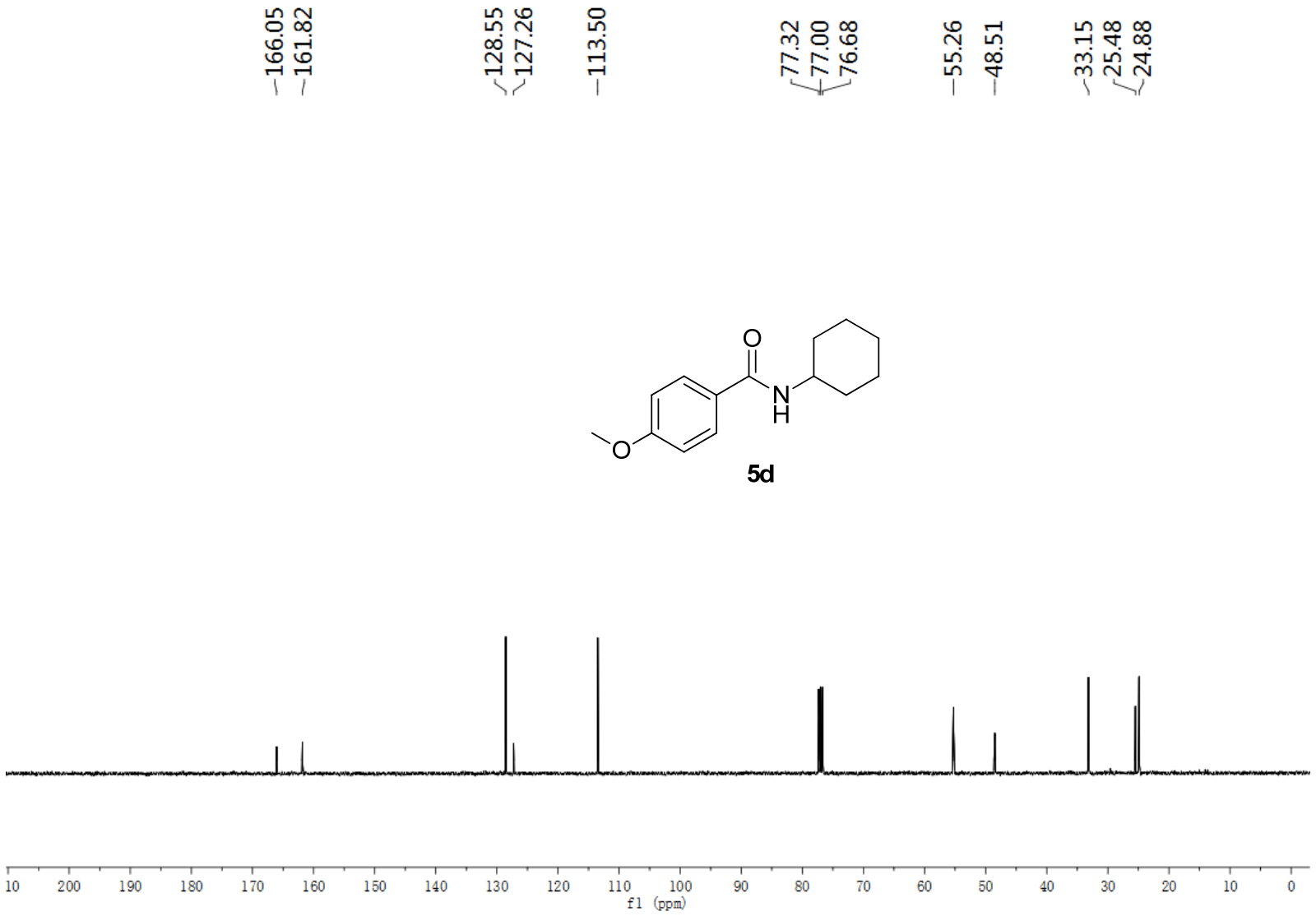
_N_-Cyclohexyl-2-methylbenzamide (5c)



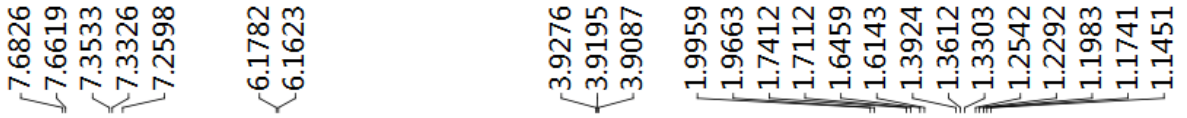

169.18
136.94
135.61
130.75
129.49
126.49
125.57
77.32
77.00
76.68
48.38
33.08
25.45
24.79
19.55
O
N
H
5c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

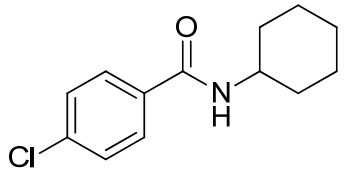
_N_-Cyclohexyl-4-methoxybenzamide (5d)



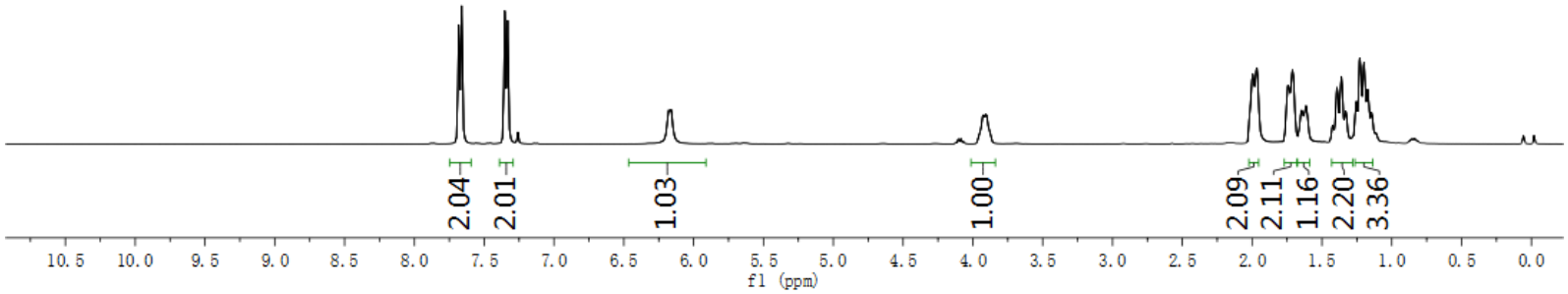

166.05
161.82
128.55
127.26
113.50
77.32
77.00
76.68
55.26
48.51
33.15
25.48
24.88
O
N
H
O
5d
10
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

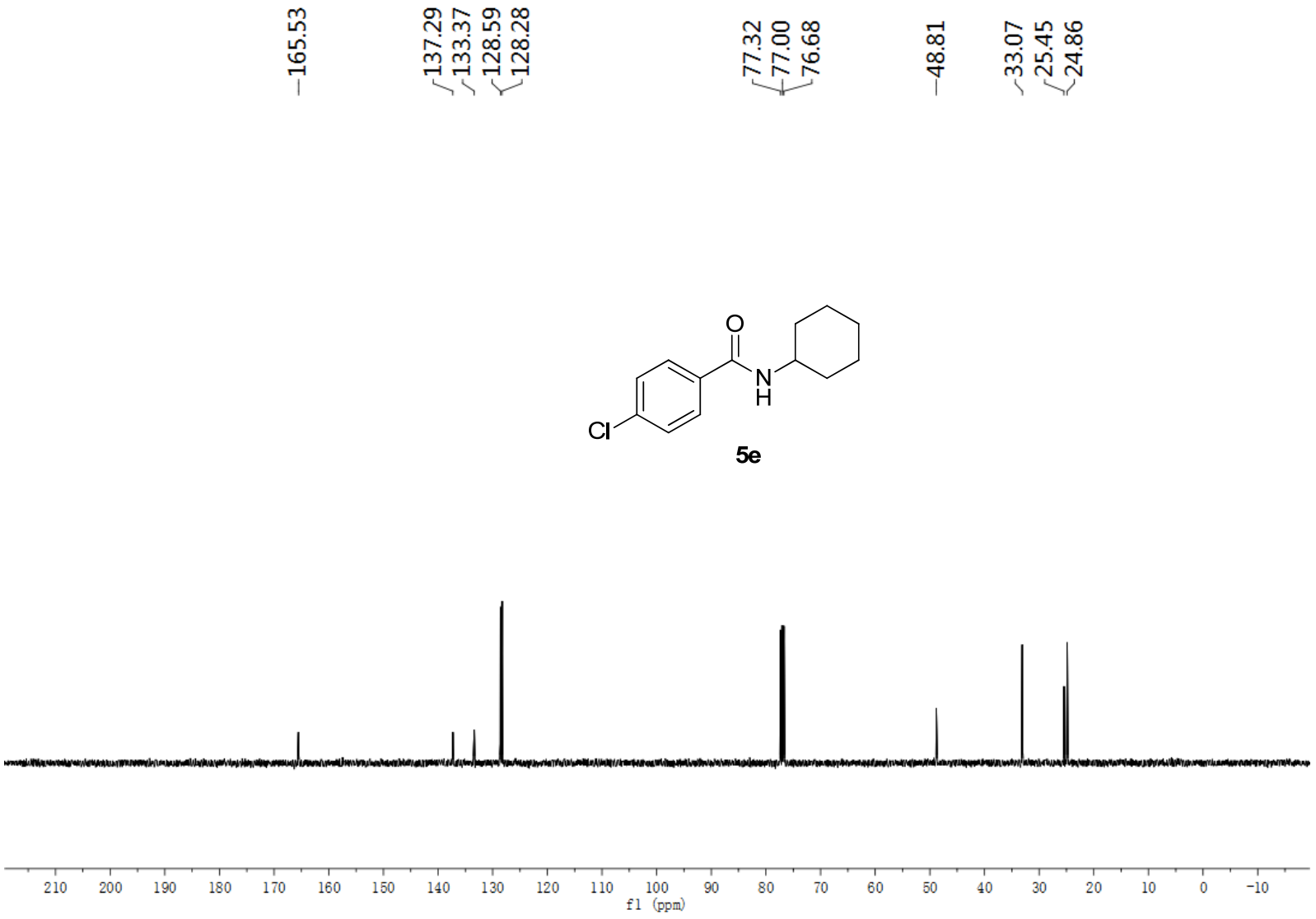
4-Chloro-*N*-cyclohexylbenzamide (5e)



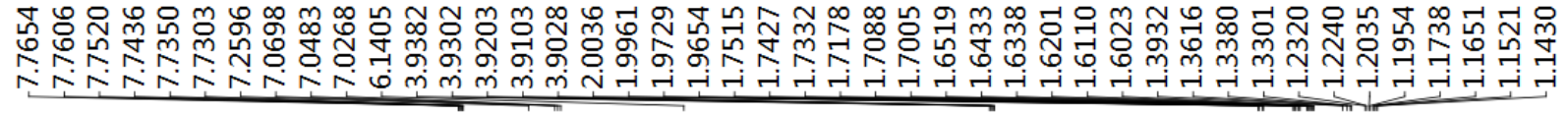


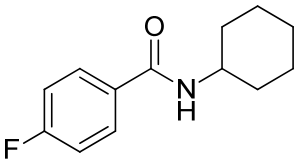
5e



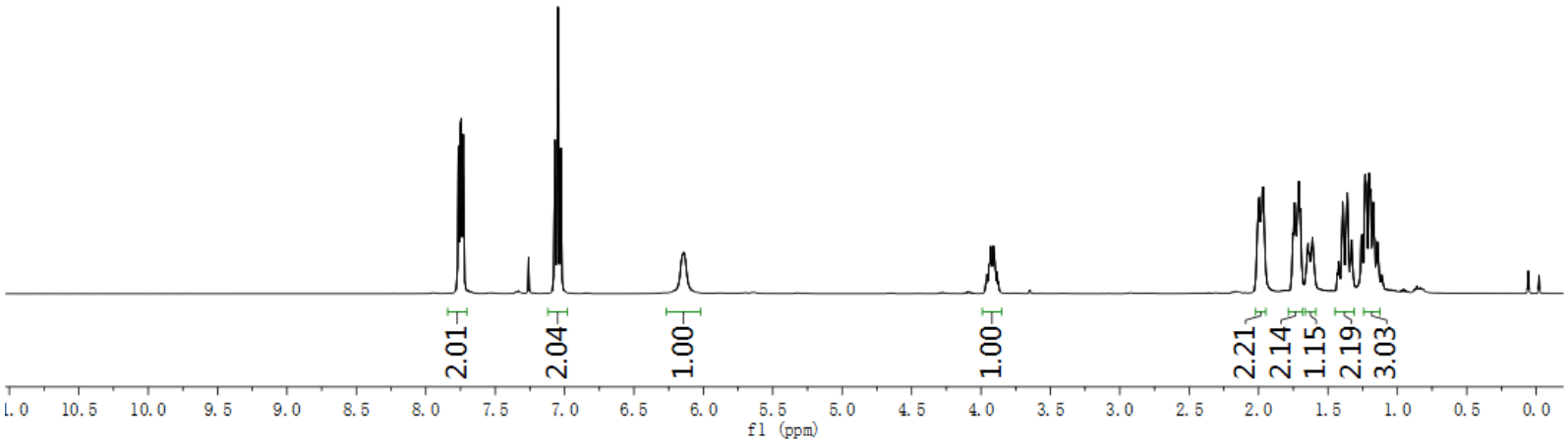

165.53
137.29
133.37
128.59
128.28
77.32
77.00
76.68
48.81
33.07
25.45
24.86
O
N
H
Cl
5e
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10
f1 (ppm)

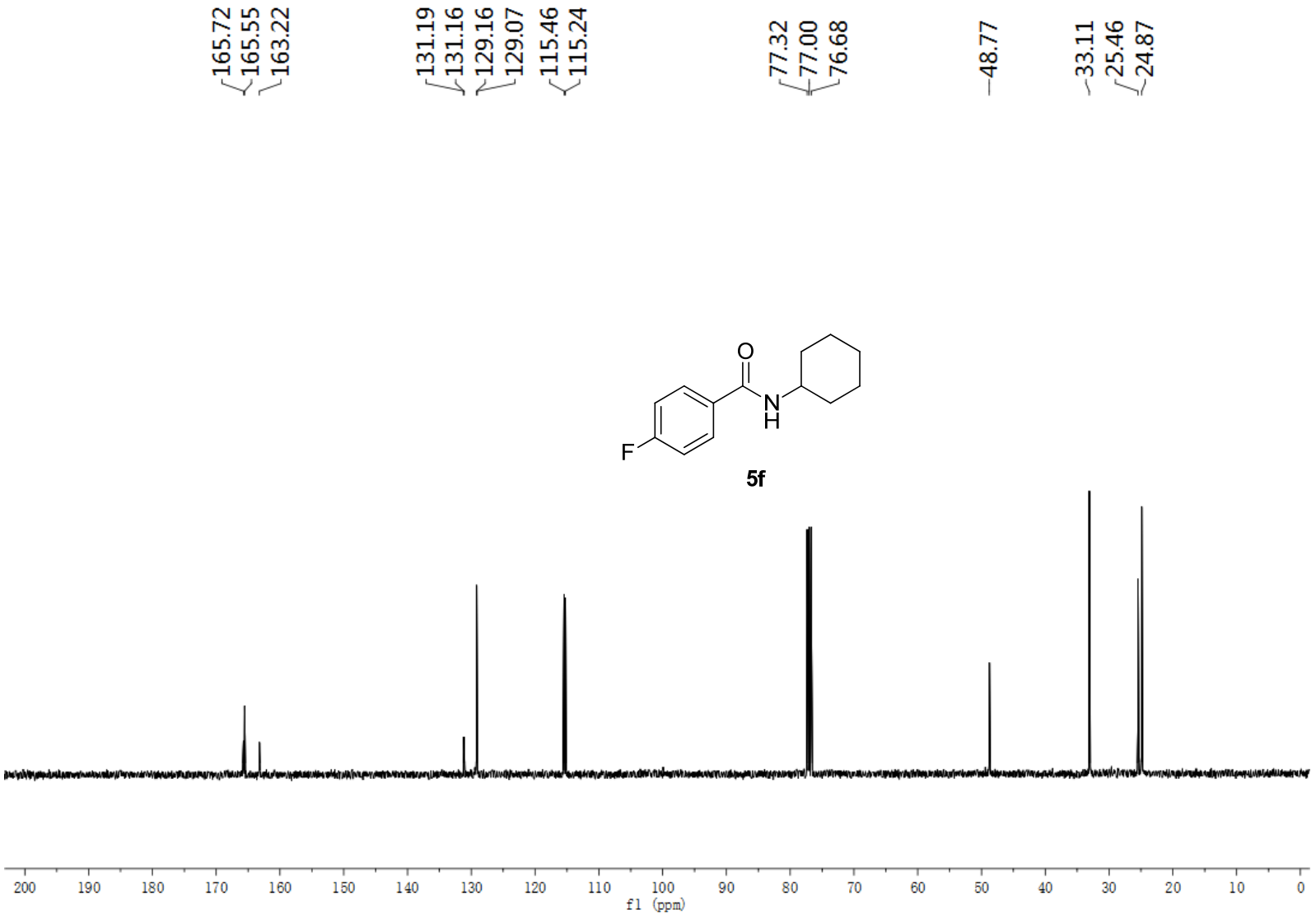
_N_-Cyclohexyl-4-fluorobenzamide (5f)



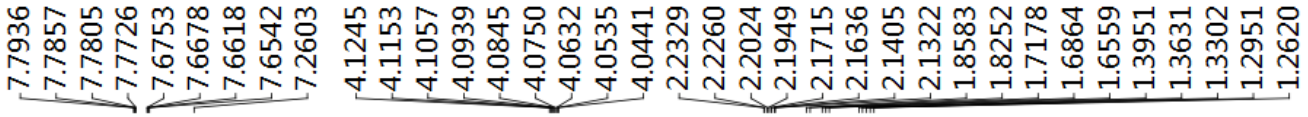


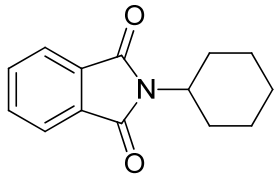
5f



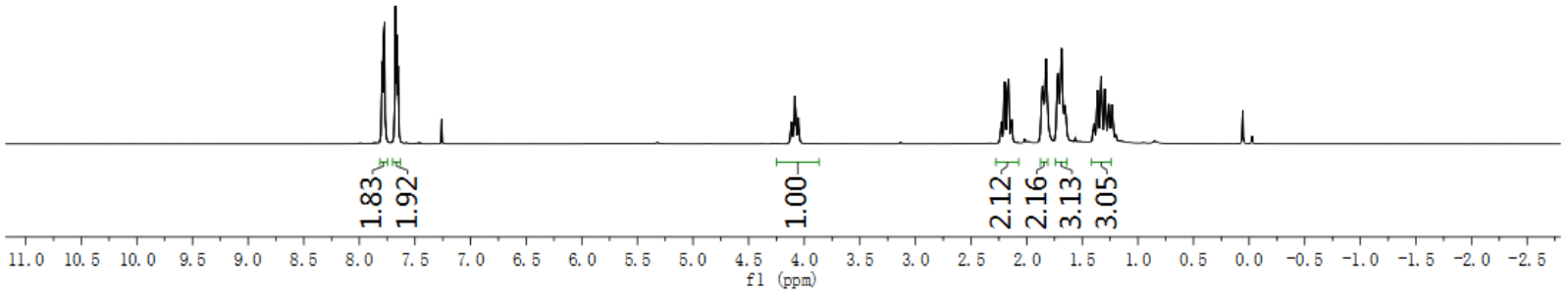

165.72
165.55
163.22
131.19
131.16
129.16
129.07
115.46
115.24
77.32
77.00
76.68
48.77
33.11
25.46
24.87
O
N
H
F
5f
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

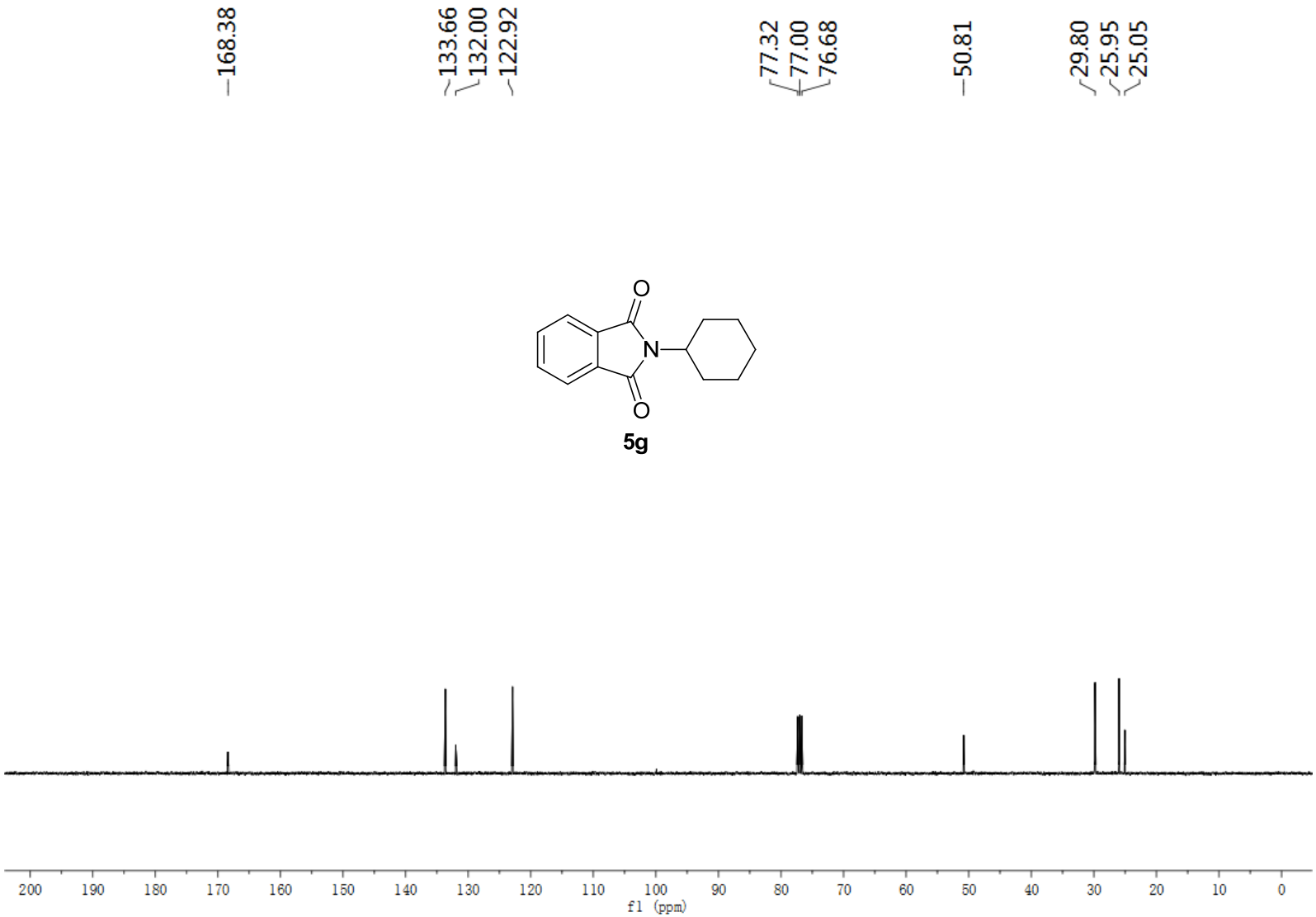
2-Cyclohexylisoindoline-1,3-dione (5g)



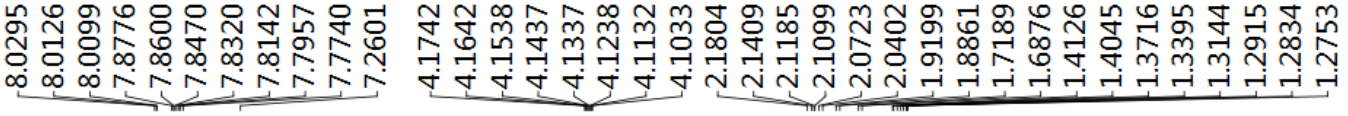


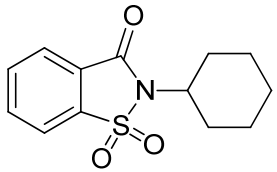
5g



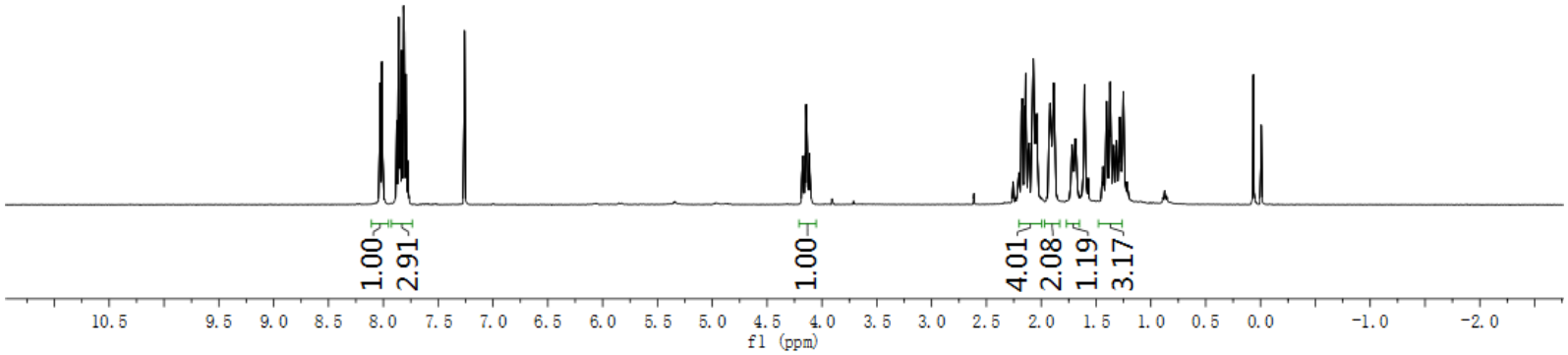

168.38
133.66
132.00
122.92
77.32
77.00
76.68
50.81
29.80
25.95
25.05
O
N
O
5g
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

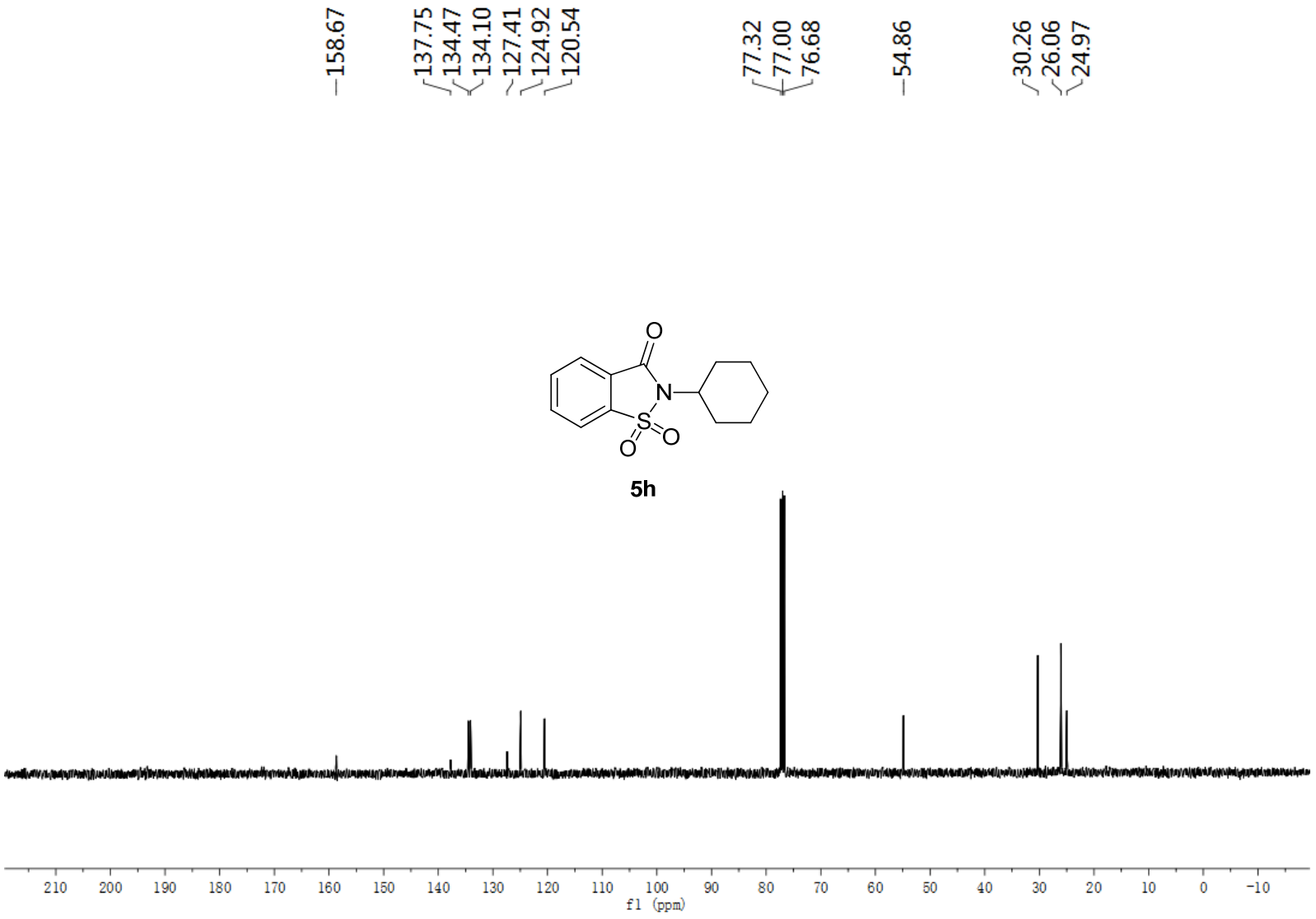
2-Cyclohexylbenzo[d]isothiazol-3(2H)-one 1,1-dioxide (5h)



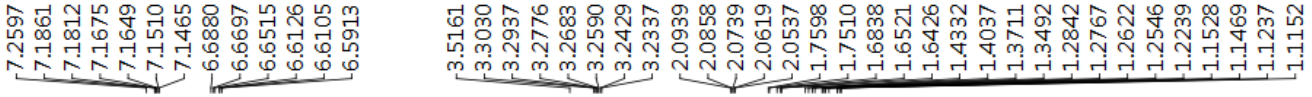


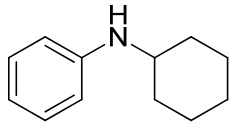
5h



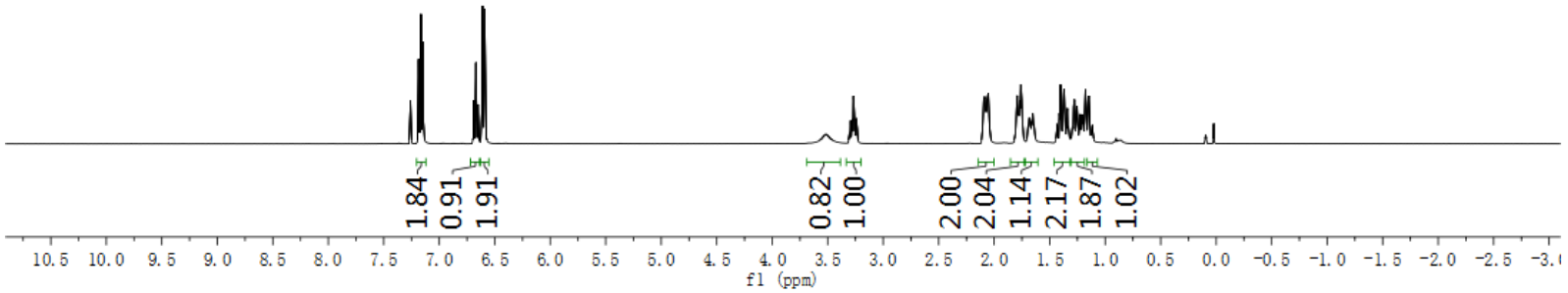

158.67
137.75
134.47
134.10
127.41
124.92
120.54
77.32
77.00
76.68
54.86
30.26
26.06
24.97
O
N
S
O
O
5h
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
−10
f1 (ppm)

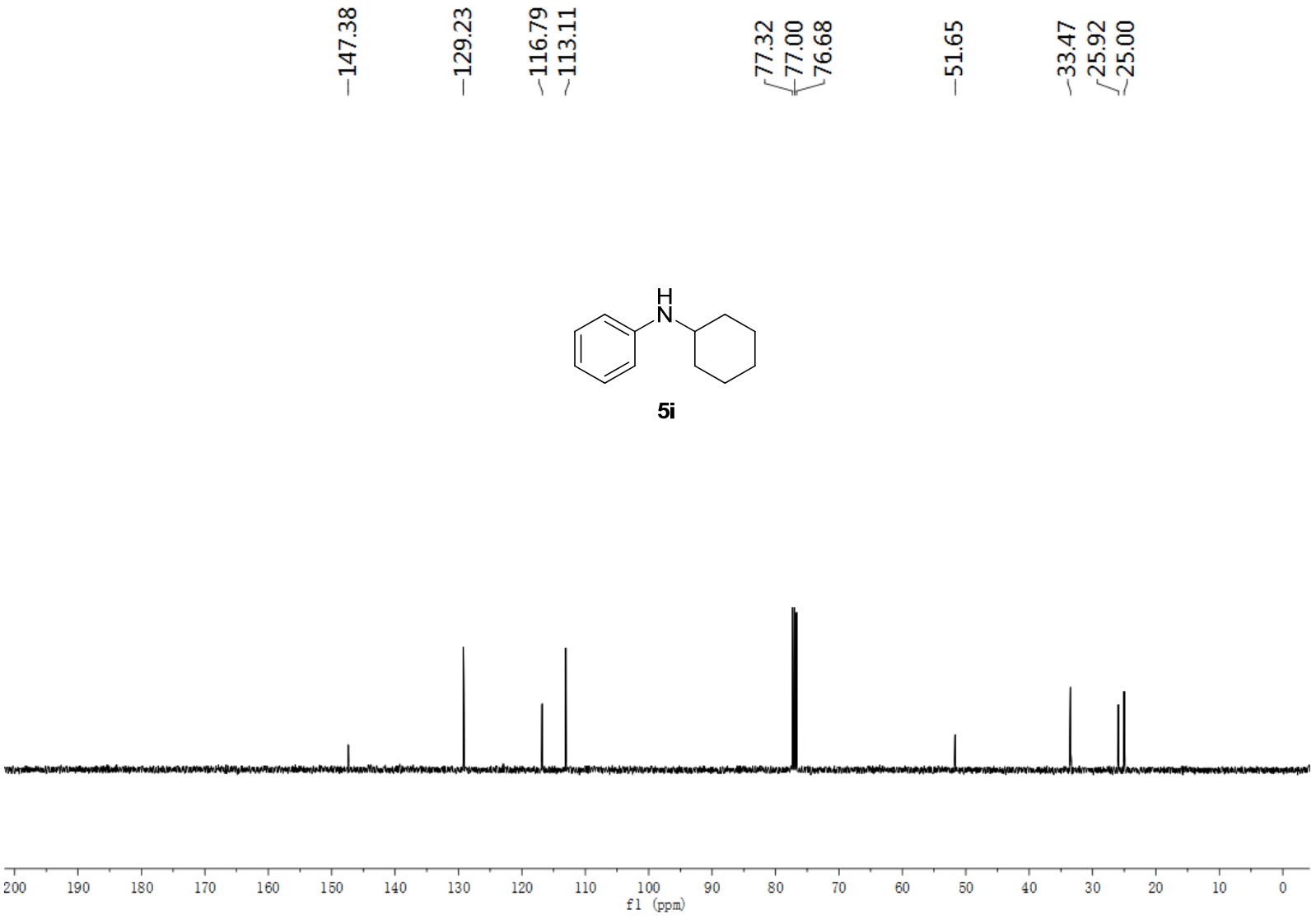
N-Cyclohexylaniline (5i)





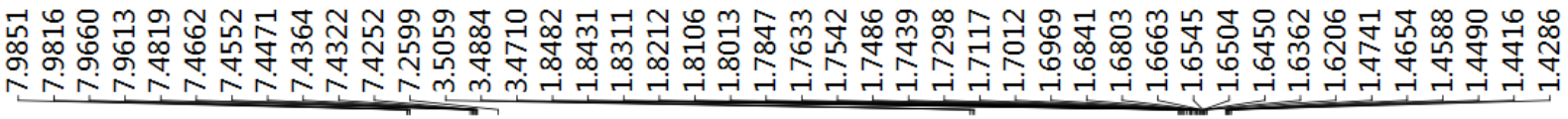
5i

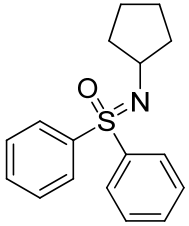



147.38
129.23
116.79
113.11
77.32
77.00
76.68
51.65
33.47
25.92
25.00
H
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

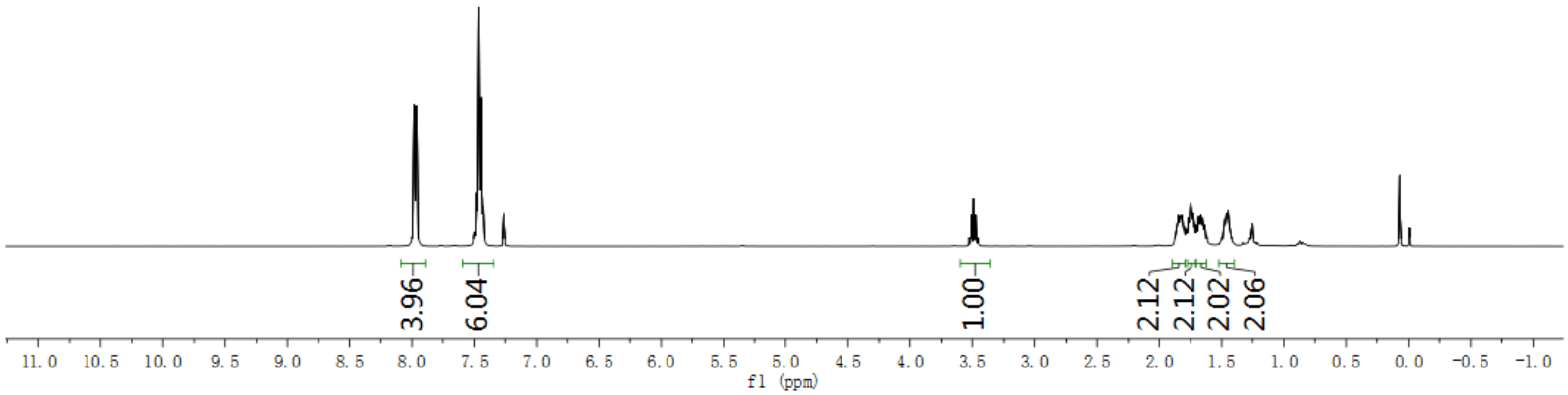
5i

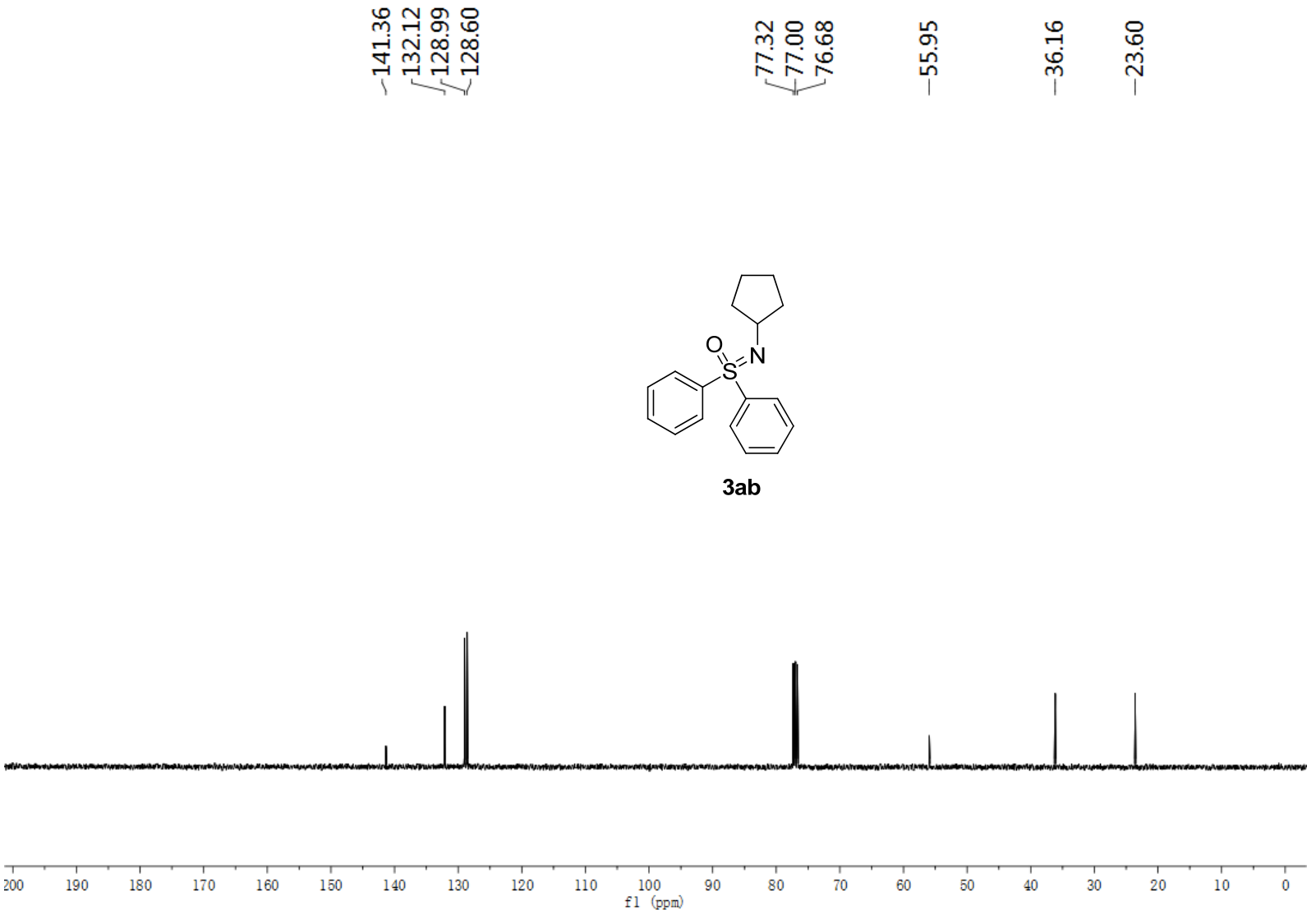
_N_-(Cyclopentyl) diphenyl sulfoximine (3ab)



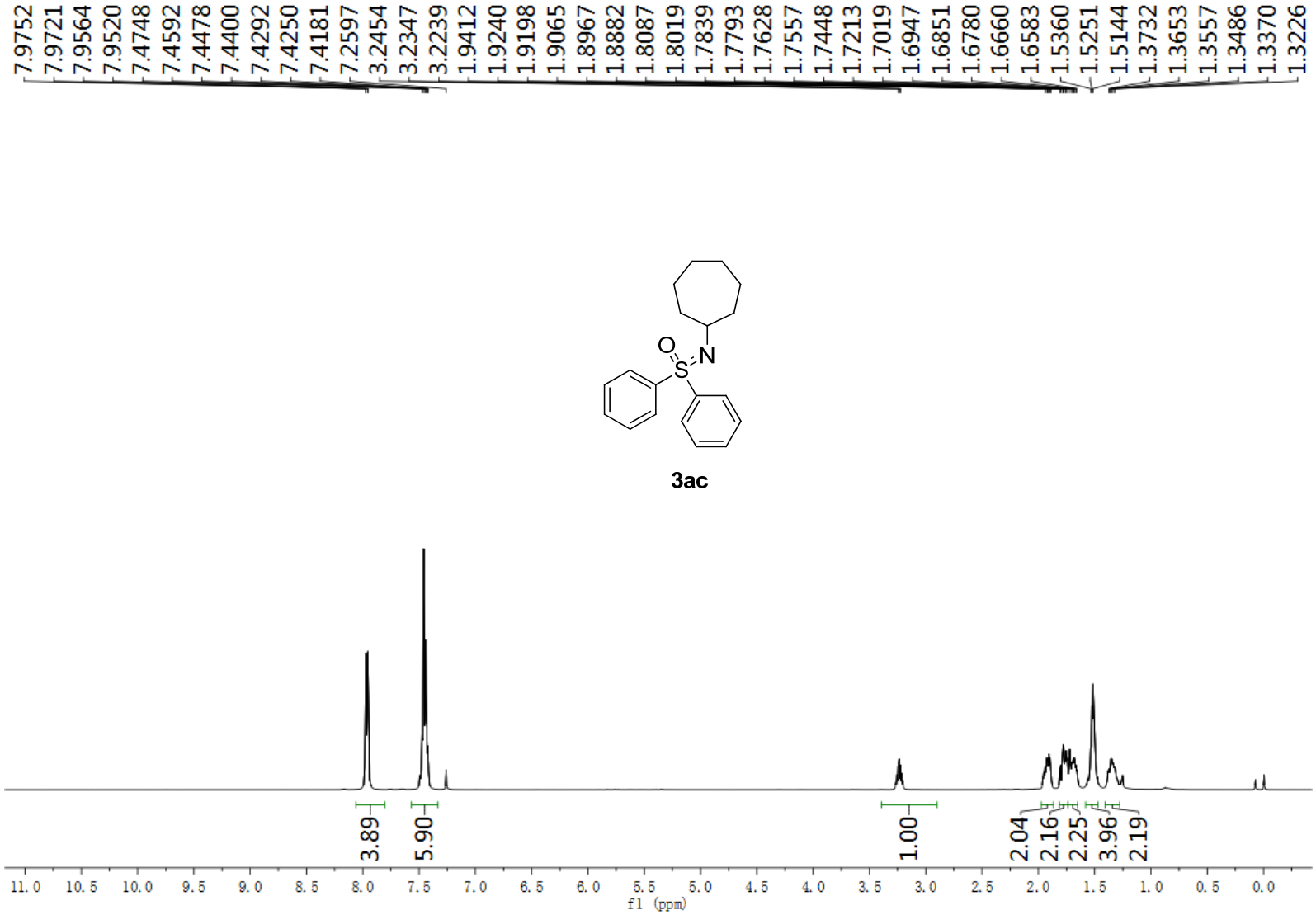


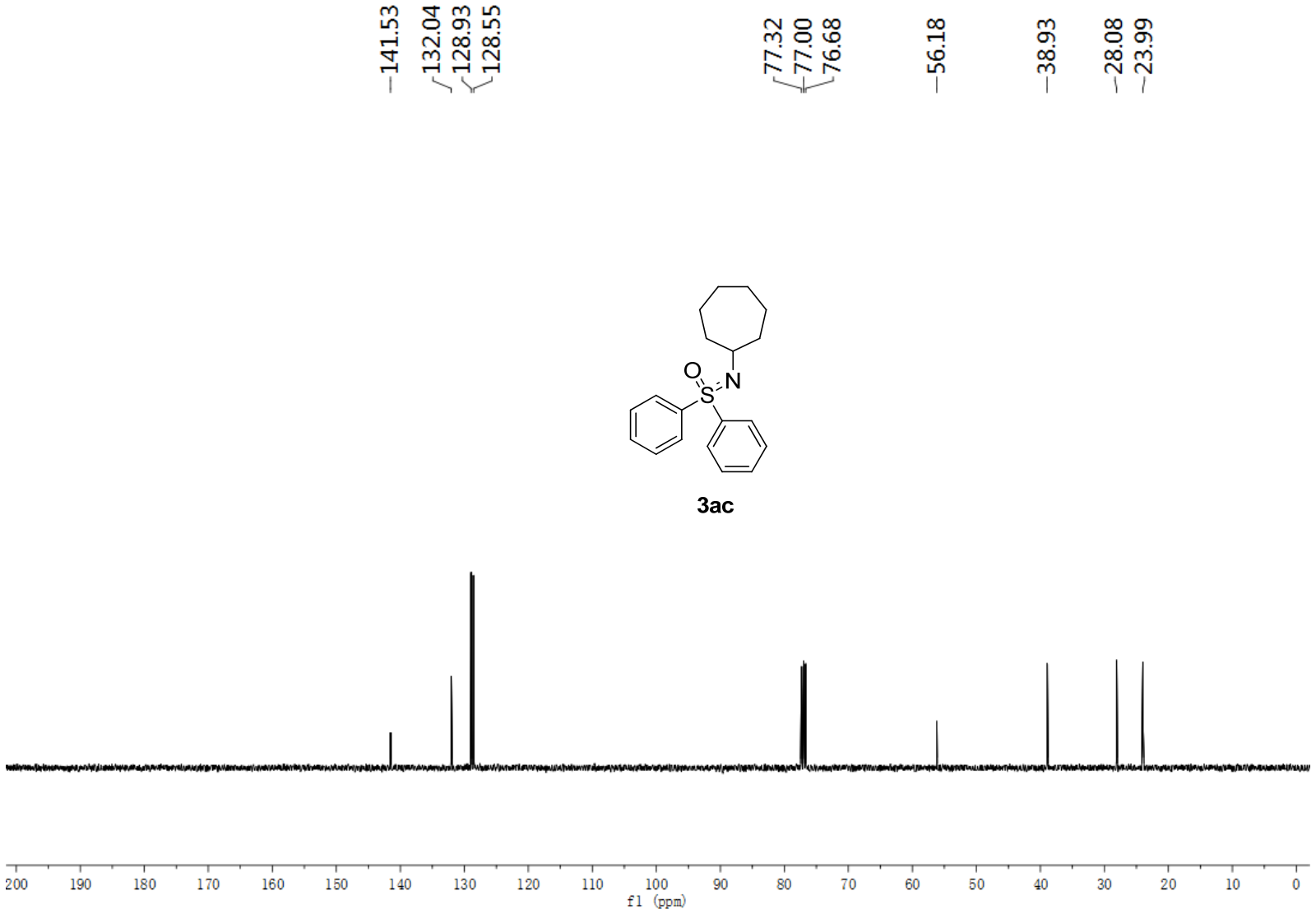
3ab




141.36
132.12
128.99
128.60
77.32
77.00
76.68
55.95
36.16
23.60
O
S
N
3ab
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

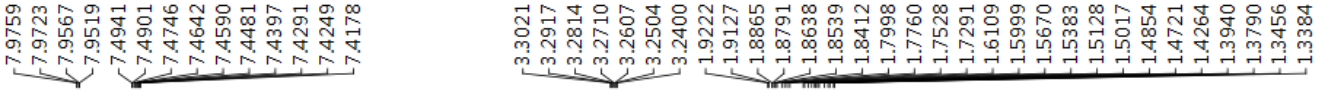
_N_-(Cycloheptyl) diphenyl sulfoximine (3ac)

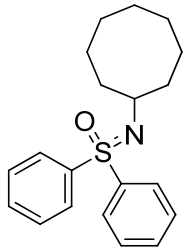



141.53
132.04
128.93
128.55
77.32
77.00
76.68
56.18
38.93
28.08
23.99
O
S
N
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

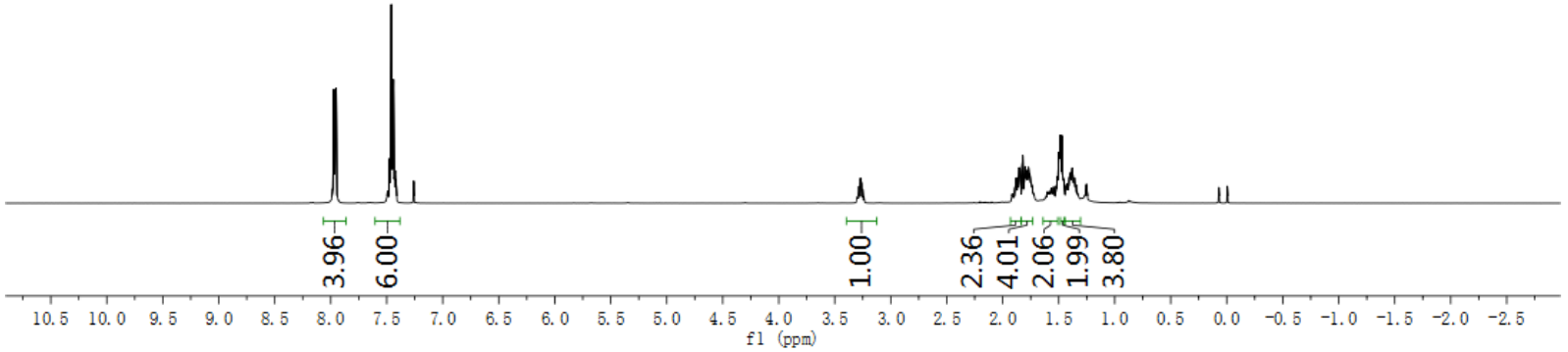
3ac

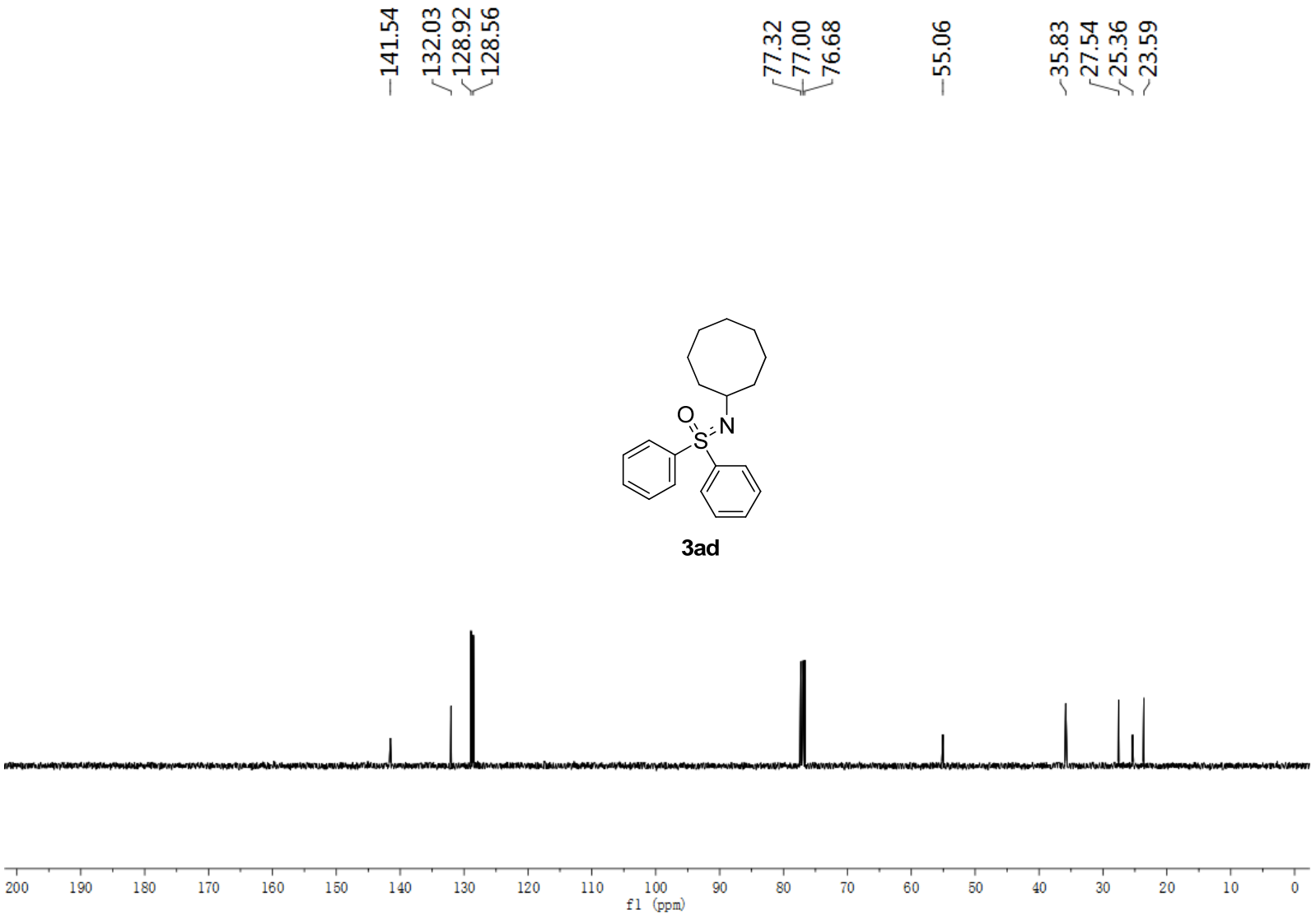
N-(Cyclooctyl) diphenyl sulfoximine (3ad)



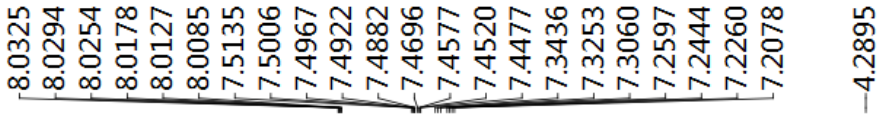


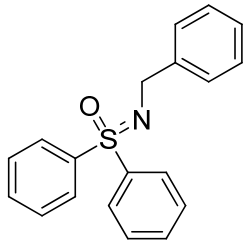
3ad



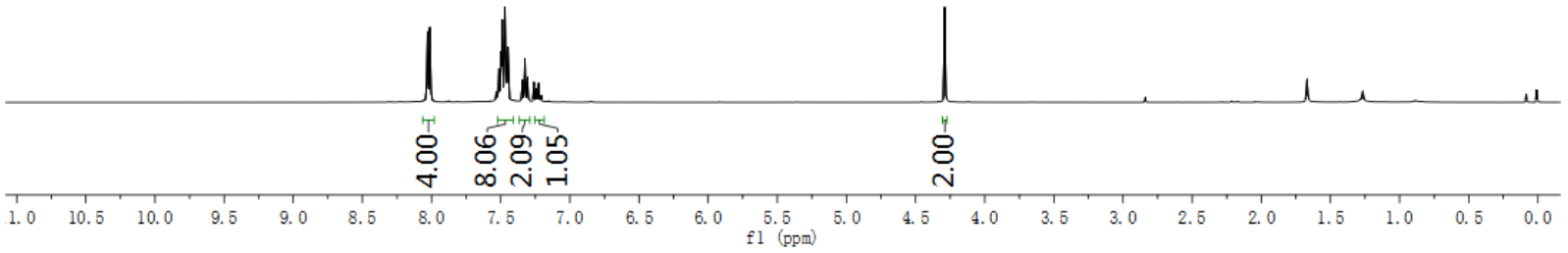

141.54
132.03
128.92
128.56
77.32
77.00
76.68
55.06
35.83
27.54
25.36
23.59
O
S
N
3ad
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

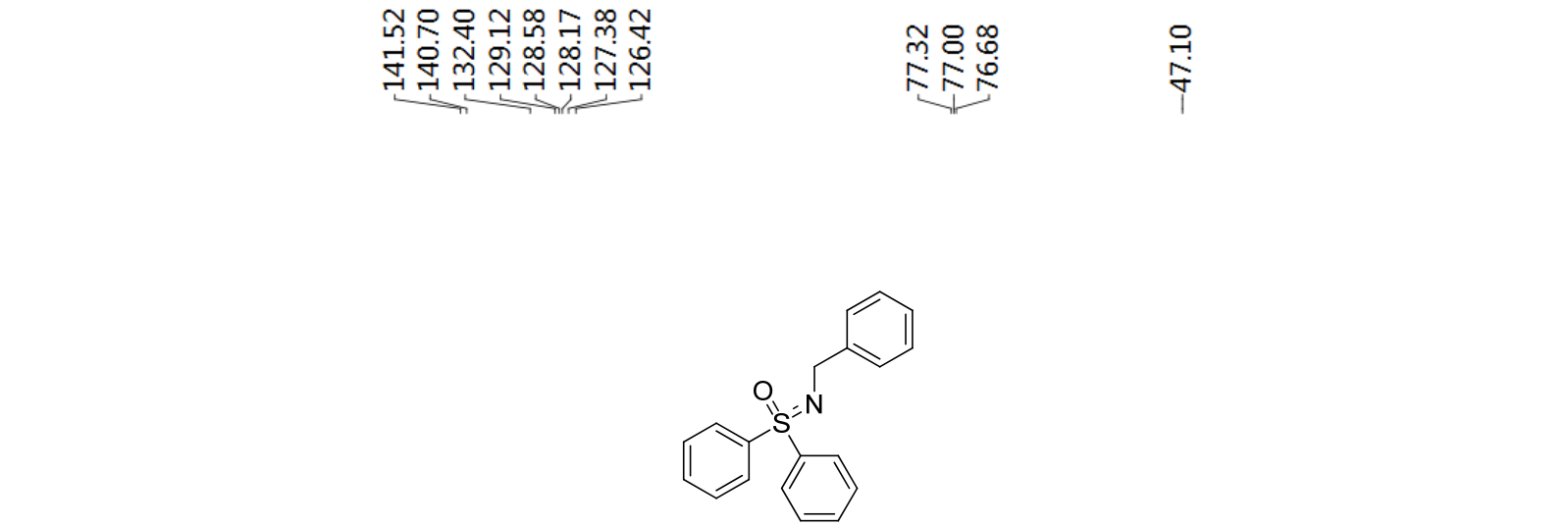
_N_-(Benzyl) diphenyl sulfoximine (3ae)



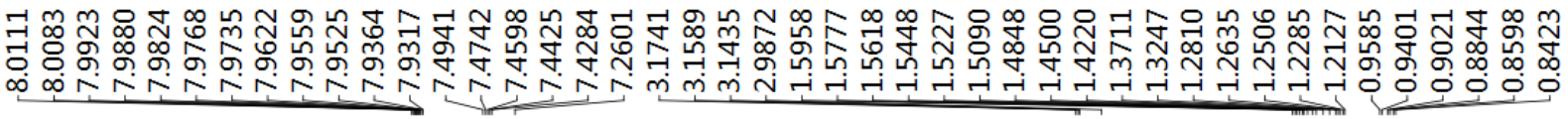


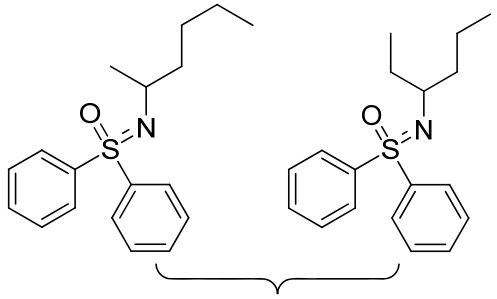
3ae




141.52
140.70
132.40
129.12
128.58
128.17
127.38
126.42
77.32
77.00
76.68
47.10
O
S
N
3ae
f1 (ppm)

_N_-(2-Hexyl) diphenyl sulfoximine (3af)





3af