Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Synthesis of N-indolated Amino Acids or Peptides from 2-Alkynylanilines via A Dearomatization Process

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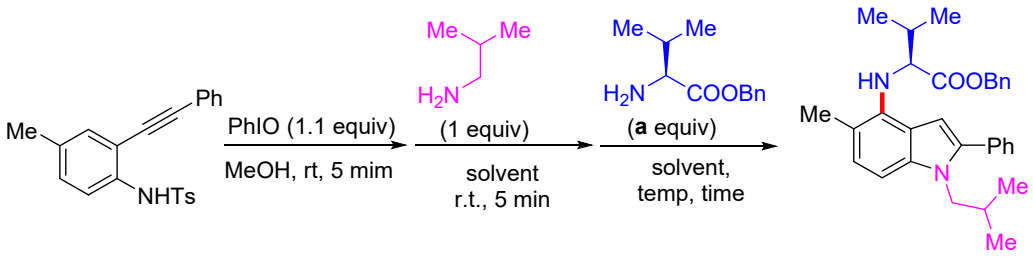
Content

1. General Information

All reactions were performed in Schlenk tubes under nitrogen atmosphere. Flash column chromatography was performed using silica gel (60-Å pore size, 32–63 μm, standard grade). Analytical thin–layer chromatography was performed using glass plates pre-coated with 0.25 mm 230–400 mesh silica gel impregnated with a fluorescent indicator (254 nm). Thin layer chromatography plates were visualized by exposure to ultraviolet light. Organic solutions were concentrated on rotary evaporators at ~20 Torr (house vacuum) at 35–40 °C. Commercial reagents and solvents were used as received. Nuclear magnetic resonance (NMR) spectra are recorded in parts per million from internal tetramethylsilane on the δ scale.

2. Evaluation of Conditions

Table S1. Evaluation of bases, solvents and temperatures for the first catalysis cycle

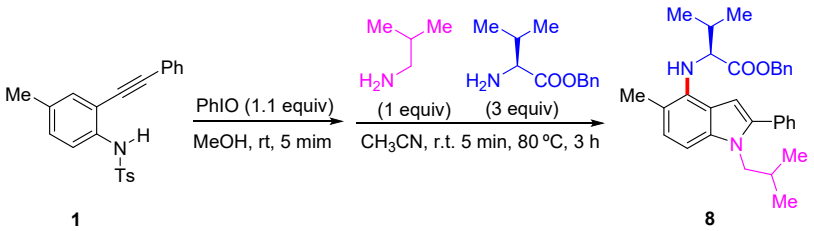


1 **8**

entry	**a**	solvent	Temperature (°C)	Time (h)	yield (%)
1	**3.0**	**MeCN**	**80**	**3**	**78**
2	3.0	MeCN	80	1	69
3	3.0	MeCN	80	6	77
4	3.0	MeCN	50	3	39
5	3.0	MeCN	25	3	0
6	1.2	DCE	80	1	32
7	2.0	DCE	80	1	44
8	3.0	DCE	80	1	65
9	3.0	DMF	80	3	68
10	3.0	toluene	80	3	47
11	3.0	1,4-dioxane	80	3	42

3. Representative Procedure and Spectral Data of Products

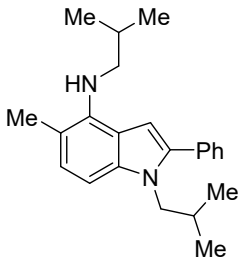
3.1 Representative Procedure



1 **8**

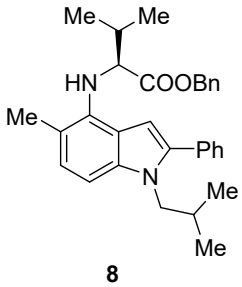
To a solution of 4-methyl-2-(2-phenylethynyl)benzenamine **1** (0.1 mmol) in MeOH (2.0 mL) was added PhIO (0.11 mmol) at 25 °C. After 5 min, the reaction mixture was concentrated *in vacuo*. The resulting crude product was mixed with a solution of 2-methylpropan-1-amine (0.1 mmol) in MeCN (2.0 mL), and the resulting mixture was stirred at 25 °C for another 5 min. After the substrates were completely consumed (monitored by TLC analysis), benzyl L-valinate (0.3 mmol) was added and the reaction mixture was warmed to 80 °C and stirred for 3 h. The mixture was then concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel (petroleum ether/ethyl acetate = 10/1) to furnish the desired compound **8**.

3.2 Spectral Data of Products



7

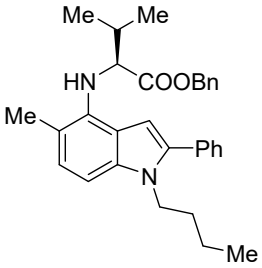
N,1-diisobutyl-5-methyl-2-phenyl-1H-indol-4-amine (22 mg, 67 %): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 – 7.34 (m, 5H), 6.95 (d, J = 8.2 Hz, 1H), 6.78 (d, J = 8.2 Hz, 1H), 6.59 (s, 1H), 3.95 (d, J = 7.5 Hz, 2H), 3.34 (d, J = 6.7 Hz, 2H), 2.31 (s, 3H), 2.03 (hept, J = 7.1 Hz, 1H), 1.92 (hept, J = 6.7 Hz, 1H), 1.01 (d, J = 6.6 Hz, 6H), 0.63 (d, J = 6.7 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.8, 139.4, 138.5, 133.9, 129.5, 128.3, 127.5, 124.9, 118.5, 113.0, 101.5, 101.0, 55.5, 51.2, 29.4, 28.6, 20.5, 20.1, 17.6; HRMS m/z calcd for $C_{23}H_{31}N_2$ ($[M+H]^+$): 335.2482, found 335.2490.



8

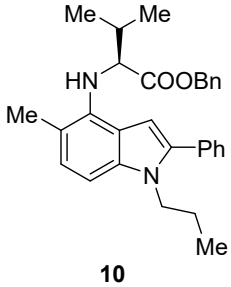
Benzyl (1-isobutyl-5-methyl-2-phenyl-1H-indol-4-yl)-L-valinate (37 mg, 78 %): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.34 (m, 5H), 7.27 – 7.22 (m, 3H), 7.19 – 7.15 (m, 2H),

6.95 (d, J = 8.3 Hz, 1H), 6.84 (d, J = 8.2 Hz, 1H), 6.49 (s, 1H), 5.07 – 5.00 (m, 2H), 4.41 (d, J = 5.9 Hz, 1H), 4.16 (s, 1H), 3.94 (d, J = 7.5 Hz, 2H), 2.36 (s, 3H), 2.25 – 2.13 (m, 1H), 2.00 (hept, J = 6.9 Hz, 1H), 1.12 (d, J = 6.9 Hz, 3H), 1.05 (d, J = 6.8 Hz, 3H), 0.62 – 0.60 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ174.4, 140.1, 138.3, 137.8, 135.6, 133.8, 129.5, 128.4, 128.3, 128.2, 128.1, 127.5, 125.0, 119.2, 115.1, 103.0, 100.3, 66.4, 64.7, 51.2, 32.5, 28.7, 20.0, 19.0, 18.8, 17.4; HRMS m/z calcd for $C_{31}H_{37}N_2O_2$ ($[M+H]^+$): 469.2850, found 469.2843.



9

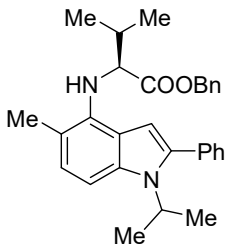
Benzyl (1-butyl-5-methyl-2-phenyl-1H-indol-4-yl)-L-valinate (33 mg, 70 %): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.38 (m, 5H), 7.27 – 7.25 (m, 3H), 7.19 – 7.17 (m, 2H), 6.96 (dd, J = 8.4, 2.5 Hz, 1H), 6.85 (dd, J = 8.5, 2.5 Hz, 1H), 6.49 (d, J = 2.8 Hz, 1H), 5.09 – 5.01 (m, 2H), 4.42 (d, J = 4.8 Hz, 1H), 4.19 (s, 1H), 4.07 (t, J = 6.9 Hz, 2H), 2.36 (s, 3H), 2.23 – 2.15 (m, 1H), 1.64 (p, J = 8.0 Hz, 2H), 1.17 – 1.11 (m, 5H), 1.05 (d, J = 6.7 Hz, 3H), 0.78 (t, J = 6.3 Hz, 3H). ^{13}C NMR (100 MHz, CDCl3) δ 174.4, 139.7, 138.0, 137.9, 135.6, 133.5, 129.4, 128.4, 128.2, 128.1, 127.6, 125.1, 119.2, 115.1, 102.5, 100.1, 66.2, 64.7, 43.8, 32.5, 31.9, 20.0, 19.0, 18.8, 17.4, 13.6. HRMS m/z calcd for $C_{31}H_{37}N_2O_2$ ($[M+H]^+$): 469.2850, found 469.2836.



10

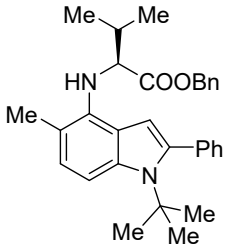
Benzyl (5-methyl-2-phenyl-1-propyl-1H-indol-4-yl)-L-valinate (35 mg, 76 %): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.37 (m, 5H), 7.27 – 7.24 (m, 3H), 7.19 – 7.17 (m, 2H), 6.96 (dd, J = 8.4, 2.3 Hz, 1H), 6.85 (dd, J = 8.4, 2.4 Hz, 1H), 6.50 (d, J = 2.4 Hz, 1H), 5.09 – 5.01 (m, 2H), 4.42 (d, J = 5.4 Hz, 1H), 4.19 – 4.02 (m, 3H), 2.36 (s, 3H), 2.20 – 2.17 (m, 1H), 1.69 (h, J = 7.7 Hz, 2H), 1.12 (d, J = 6.6 Hz, 3H), 1.05 (d, J = 6.4 Hz, 3H),

0.74 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, CDCl3) δ 174.4, 139.8, 138.1, 137.9, 135.6, 133.5, 129.3, 128.4, 128.2, 128.1, 127.6, 125.1, 119.2, 115.1, 102.5, 100.1, 66.5, 64.7, 45.6, 32.5, 23.2, 19.0, 18.8, 17.4, 11.3. HRMS m/z calcd for $C_{31}H_{39}N_2O_2Si$ ([M+H]$^+$): 455.2693, found 455.2670.



11

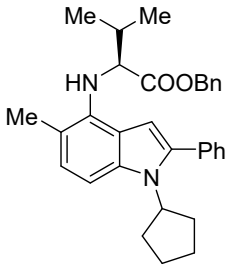
Benzyl (1-isopropyl-5-methyl-2-phenyl-1H-indol-4-yl)-L-valinate (28 mg, 61 %): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.39 (m, 5H), 7.27 – 7.25 (m, 3H), 7.19 – 7.17 (m, 2H), 7.08 (dd, J = 8.6, 2.5 Hz, 1H), 6.91 (dd, J = 8.5, 2.5 Hz, 1H), 6.43 (d, J = 2.6 Hz, 1H), 5.09 – 5.01 (m, 2H), 4.62 (hept, J = 8.9 Hz, 1H), 4.37 (dd, J = 5.9, 2.6 Hz, 1H), 4.14 (s, 1H), 2.35 (s, 3H), 2.18 (q, J = 6.7, 6.1 Hz, 1H), 1.59 (d, J = 6.8 Hz, 3H), 1.55 (d, J = 5.3 Hz, 3H), 1.12 (d, J = 6.4 Hz, 3H), 1.05 (d, J = 6.3 Hz, 3H). ^{13}C NMR (100 MHz, CDCl3) δ 174.5, 139.8, 138.0, 136.0, 135.6, 134.0, 129.6, 128.4, 128.3, 128.2, 128.1, 127.6, 124.6, 120.4, 115.2, 105.1, 100.1, 66.4, 64.8, 47.8, 32.5, 21.5, 21.4, 19.0, 18.8, 17.3. HRMS m/z calcd for $C_{30}H_{35}N_2O_2$ ([M+H]$^+$): 455.2693, found 455.2683.



12

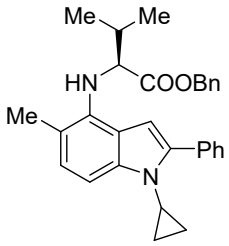
Benzyl (1-(tert-butyl)-5-methyl-2-phenyl-1H-indol-4-yl)-L-valinate (25 mg, 53 %): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.38 (m, 2H), 7.34 – 7.32 (m, 3H), 7.28 – 7.25 (m, 3H), 7.20 (dd, J = 8.6, 0.8 Hz, 1H), 7.16 – 7.14 (m, 2H), 6.90 (d, J = 8.6 Hz, 1H), 6.27 (d, J = 0.8 Hz, 1H), 5.06 – 5.00 (m, 2H), 4.28 (d, J = 6.1 Hz, 1H), 4.08 (s, 1H), 2.35 (s, 3H), 2.19 – 2.10 (m, 1H), 1.56 (s, 9H), 1.09 (d, J = 6.8 Hz, 3H), 1.02 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, CDCl3) δ 174.5, 140.3, 138.4, 137.9, 137.6, 135.6, 130.2, 128.4, 128.2, 128.1, 127.3, 124.1, 120.9, 115.5,

108.1, 103.8, 66.4, 65.0, 58.6, 32.4, 32.0, 19.0, 18.8, 17.2; HRMS m/z calcd for $C_{31}H_{37}N_2O_2$ ($[M+H]^+$): 469.2850, found 469.2865.



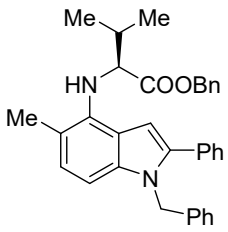
13

Benzyl (1-cyclopentyl-5-methyl-2-phenyl-1H-indol-4-yl)-L-valinate (36 mg, 76 %): yellow solid, m.p. 109-110 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.38 (m, 5H), 7.27 – 7.25 (m, 3H), 7.19 – 7.17 (m, 2H), 6.95 (dd, J = 8.5, 2.4 Hz, 1H), 6.90 (dd, J = 8.5, 2.5 Hz, 1H), 6.43 (d, J = 2.6 Hz, 1H), 5.09 – 5.01 (m, 2H), 4.75 (h, J = 9.0, 8.3 Hz, 1H), 4.38 (d, J = 4.2 Hz, 1H), 4.13 (s, 1H), 2.41 – 2.32 (m, 5H), 2.23 – 2.14 (m, 1H), 2.00 – 1.93 (m, 4H), 1.65 – 1.64 (m, 2H), 1.12 (d, J = 6.5 Hz, 3H), 1.05 (d, J = 6.4 Hz, 3H). ^{13}C NMR (100 MHz, CDCl3) δ 174.5, 140.5, 138.2, 135.6, 135.5, 133.9, 129.5, 128.4, 128.3, 128.2, 128.1, 127.6, 124.6, 120.3, 115.2, 104.7, 99.8, 66.5, 64.8, 57.0, 32.5, 29.9, 29.8, 25.3, 19.0, 18.8, 17.4. HRMS m/z calcd for $C_{32}H_{37}N_2O_2$ ($[M+H]^+$): 481.2850, found 481.2833.



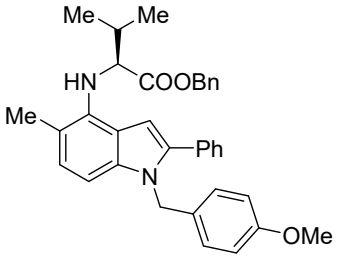
14

Benzyl (1-cyclopropyl-5-methyl-2-phenyl-1H-indol-4-yl)-L-valinate (28 mg, 62 %): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 – 7.57 (m, 2H), 7.40 (t, J = 7.4 Hz, 2H), 7.33 (t, J = 7.3 Hz, 1H), 7.26 (s, 3H), 7.21 – 7.15 (m, 2H), 7.07 (d, J = 8.0 Hz, 1H), 6.97 (d, J = 8.3 Hz, 1H), 6.51 (s, 1H), 5.07 (d, J = 12.3 Hz, 1H), 5.02 (d, J = 12.3 Hz, 1H), 4.39 (d, J = 6.0 Hz, 1H), 4.14 (s, 1H), 3.37 (tt, J = 7.0, 3.7 Hz, 1H), 2.35 (s, 3H), 2.23 – 2.15 (m, 1H), 1.12 (d, J = 6.9 Hz, 3H), 1.05 (d, J = 6.8 Hz, 3H), 0.94 – 0.89 (m, 2H), 0.64 – 0.60 (m, 2H). ^{13}C NMR (100 MHz, CDCl3) δ 174.4, 140.0, 139.5, 137.9, 135.6, 133.6, 128.7, 128.4, 128.2, 128.1, 127.1, 125.2, 118.7, 115.3, 103.4, 99.9, 66.5, 64.7, 32.4, 26.0, 19.0, 18.8, 17.5, 9.0. HRMS m/z calcd for $C_{30}H_{33}N_2O_2$ ($[M+H]^+$): 453.2537, found 453.2521.



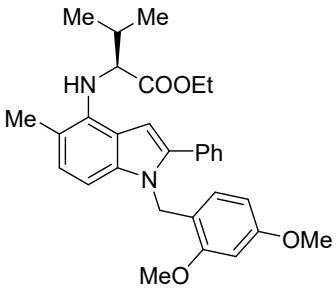
15

Benzyl (1-benzyl-5-methyl-2-phenyl-1H-indol-4-yl)-L-valinate (39 mg, 78 %): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.32 (m, 5H), 7.28 – 7.17 (m, 8H), 7.02 – 7.00 (m, 2H), 6.88 (d, J = 8.3 Hz, 1H), 6.65 – 6.63 (m, 2H), 5.29 (s, 2H), 5.08 (s, 2H), 4.46 (d, J = 5.9 Hz, 1H), 4.20 (s, 1H), 2.34 (s, 3H), 2.28 – 2.17 (m, 1H), 1.15 (d, J = 6.9 Hz, 3H), 1.08 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.4, 140.1, 138.3, 137.8, 135.6, 133.8, 129.5, 128.4, 128.3, 128.2, 128.1, 127.5, 125.0, 119.2, 115.1, 103.0, 100.3, 66.4, 64.7, 51.2, 32.5, 28.7, 20.0, 19.0, 18.8, 17.4; HRMS m/z calcd for $C_{34}H_{35}N_2O_2$([M+H]$^+$): 503.2693, found 503.2679.



16

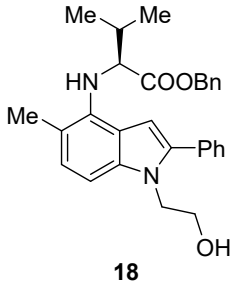
Benzyl (1-(4-methoxybenzyl)-5-methyl-2-phenyl-1H-indol-4-yl)-L-valinate (35 mg, 66 %): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.34 (m, 5H), 7.26 – 7.25 (m, 3H), 7.20 – 7.18 (m, 2H), 6.92 (d, J = 7.9 Hz, 2H), 6.88 (d, J = 8.3 Hz, 1H), 6.77 (d, J = 8.0 Hz, 2H), 6.66 (d, J = 8.2 Hz, 1H), 6.62 (s, 1H), 5.23 (s, 2H), 5.07 (s, 2H), 4.45 (d, J = 4.3 Hz, 1H), 4.16 (s, 1H), 3.75 (s, 3H), 2.34 (s, 3H), 2.22 (h, J = 5.9 Hz, 1H), 1.15 (d, J = 6.6 Hz, 3H), 1.08 (d, J = 6.4 Hz, 3H). ^{13}C NMR (100 MHz, CDCl3) δ 174.4, 158.6, 140.1, 138.7, 137.9, 135.6, 132.9, 130.4, 129.1, 128.4, 128.2, 128.1, 127.7, 127.1, 125.5, 119.2, 115.4, 114.0, 103.0, 100.3, 66.5, 64.8, 55.2, 47.2, 32.5, 19.0, 18.8, 17.5. HRMS m/z calcd for $C_{35}H_{37}N_2O_3$ ([M+H]$^+$): 533.2799, found 533.2781.



17

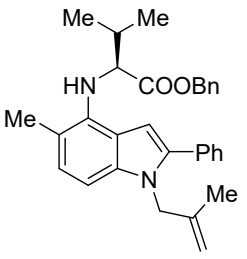
Ethyl (1-(2,4-dimethoxybenzyl)-5-methyl-2-phenyl-1H-indol-4-yl)-L-valinate (36 mg, 72 %): yellow solid, m.p. 79-80 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.41 (m, 2H), 7.38 – 7.31 (m, 3H), 6.87 (d, J = 8.2 Hz, 1H), 6.65 (s, 1H), 6.62 (d, J = 8.3 Hz,

1H), 6.49 (d, *J* = 8.3 Hz, 1H), 6.46 (d, *J* = 2.4 Hz, 1H), 5.20 (s, 2H), 4.42 (d, *J* = 5.7 Hz, 1H), 4.22 – 4.08 (m, 3H), 3.80 (s, 3H), 3.75 (s, 3H), 2.38 (s, 3H), 2.27 – 2.19 (m, 1H), 1.22 – 1.16 (m, 6H), 1.11 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, CDCl3) δ 174.4, 159.8, 157.0, 140.2, 138.8, 138.0, 133.0, 128.8, 128.4, 127.6, 127.3, 125.4, 119.1, 118.9, 115.2, 103.9, 102.9, 100.1, 98.2, 64.6, 60.6, 55.3, 55.2, 42.8, 32.5, 18.9, 17.5, 14.2. HRMS m/z calcd for $C_{31}H_{37}N_2O_4$ ([M+H]$^+$): 501.2748, found 501.2756.



18

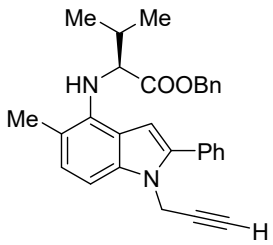
Benzyl (1-(2-hydroxyethyl)-5-methyl-2-phenyl-1H-indol-4-yl)-L-valinate (35 mg, 76 %): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 – 7.46 (m, 2H), 7.44 – 7.34 (m, 3H), 7.27 – 7.23 (m, 3H), 7.19 – 7.16 (m, 2H), 6.96 (d, *J* = 8.3 Hz, 1H), 6.87 (d, *J* = 8.3 Hz, 1H), 6.53 (s, 1H), 5.07 – 4.99 (m, 2H), 4.40 (d, *J* = 6.0 Hz, 1H), 4.23 – 4.20 (m, 3H), 3.75 (t, *J* = 5.9 Hz, 2H), 2.35 (s, 3H), 2.18 (h, *J* = 6.6 Hz, 1H), 1.62 (s, 1H), 1.12 (d, *J* = 6.8 Hz, 3H), 1.05 (d, *J* = 6.7 Hz, 3H); ^{13}C NMR (100 MHz, CDCl3) δ 174.4, 140.0, 138.2, 137.9, 135.5, 132.9, 129.6, 128.5, 128.4, 128.2, 128.1, 127.8, 125.5, 119.2, 115.5, 102.4, 100.8, 66.5, 64.7, 61.4, 45.9, 32.4, 19.0, 18.8, 17.4; HRMS m/z calcd for $C_{29}H_{33}N_2O_3$ ([M+H]$^+$): 457.2486, found 457.2473.



19

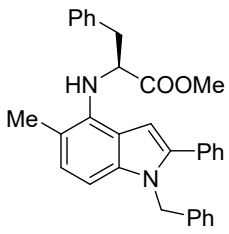
Benzyl (5-methyl-1-(2-methylallyl)-2-phenyl-1H-indol-4-yl)-L-valinate (32 mg, 69 %): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 – 7.46 (m, 2H), 7.42 – 7.33 (m, 3H), 7.27 – 7.23 (m, 3H), 7.18 – 7.16 (m, 2H), 6.94 (d, *J* = 8.2 Hz, 1H), 6.74 (d, *J* = 8.2 Hz, 1H), 6.58 (s, 1H), 5.09 – 5.02 (m, 2H), 4.87 (t, *J* = 1.5 Hz, 1H), 4.54 (t, *J* = 1.4 Hz, 1H), 4.52 (s, 2H), 4.43 (d, *J* = 6.0 Hz, 1H), 4.19 (s, 1H), 2.35 (s, 3H), 2.21 (h, *J* = 6.7 Hz, 1H), 1.67 (s, 3H), 1.14 (d, *J* = 6.9 Hz, 3H), 1.07 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz,

CDCl3) δ 174.4, 141.2, 140.0, 138.7, 137.8, 135.5, 133.0, 128.8, 128.4, 128.4, 128.2, 128.1, 127.7, 125.4, 119.1, 115.3, 111.3, 102.9, 100.0, 66.4, 64.8, 49.9, 32.5, 20.1, 19.0, 18.8, 17.5; HRMS m/z calcd for $C_{31}H_{35}N_2O_2$ ([M+H]$^+$): 467.2693, found 467.2699.



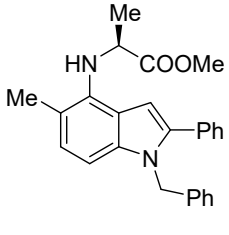
20

Benzyl (5-methyl-2-phenyl-1-(prop-2-yn-1-yl)-1H-indol-4-yl)-L-valinate (29 mg, 65 %): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 – 7.55 (m, 2H), 7.48 – 7.44 (m, 2H), 7.41 – 7.37 (m, 1H), 7.28 – 7.24 (m, 3H), 7.20 – 7.17 (m, 2H), 7.02 (d, J = 8.3 Hz, 1H), 6.97 (dd, J = 8.2, 0.8 Hz, 1H), 6.57 (d, J = 0.8 Hz, 1H), 5.09 – 5.02 (m, 2H), 4.75 – 4.74 (m, 2H), 4.41 (d, J = 5.9 Hz, 1H), 4.18 (s, 1H), 2.36 (s, 3H), 2.35 (t, J = 2.7 Hz, 1H), 2.24 – 2.15 (m, 1H), 1.12 (d, J = 6.9 Hz, 3H), 1.06 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, CDCl3) δ 174.3, 139.2, 138.3, 138.1, 135.5, 132.4, 129.1, 128.7, 128.4, 128.2, 128.1, 127.9, 125.8, 119.1, 115.9, 102.2, 100.6, 79.1, 72.5, 66.5, 64.7, 34.2, 32.4, 19.0, 18.8, 17.5; HRMS m/z calcd for $C_{30}H_{31}N_2O_2$ ([M+H]$^+$): 451.2380, found 451.2365



21

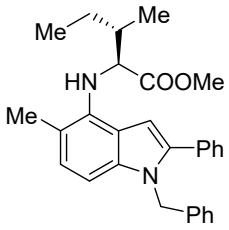
Methyl 2-((1-benzyl-5-methyl-2-phenyl-1H-indol-4-yl)amino) -3-phenylpropanoate (30 mg, 63 %): brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38-7.15 (m, 13 H), 7.00 (d, J = 7.0 Hz, 2 H), 6.87 (d, J = 8.2 Hz, 1 H), 6.63 (d, J = 8.2 Hz, 1 H), 6.38 (s, 1 H), 5.28 (s, 2 H), 4.80 (t, J = 6.2 Hz, 1 H), 4.21 (s, 1 H), 3.62 (s, 3 H), 3.21-3.16 (m, 2 H), 2.28 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.7, 140.4, 138.7, 138.4, 137.5, 137.1, 132.8, 129.6, 129.1, 128.7, 128.5, 128.4, 127.8, 127.1, 126.9, 126.0, 125.6, 119.7, 116.0, 103.3, 100.2, 60.9, 51.9, 47.9, 40.7, 17.4; HRMS m/z calcd for $C_{32}H_{31}N_2O_2$ ([M+H]$^+$): 475.2386, found 475.2375.



22

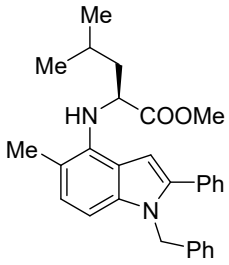
Methyl 2-((1-benzyl-5-methyl-2-phenyl-1H-indol-4-yl)amino)

propanoate (31 mg, 78 %): brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44-7.34 (m, 5 H), 7.28-7.22 (m, 3 H), 7.04-7.00 (m, 2 H), 6.99 (d, J = 7.7 Hz, 1 H), 6.66 (d, J = 7.8 Hz, 1 H), 6.61 (s, 1 H), 5.29 (s, 2 H), 4.65-4.60 (m, 1 H), 4.23 (s, 1 H), 3.70 (s, 3 H), 2.37 (s, 3 H), 1.54 (d, J = 6.0 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.0, 140.5, 138.6, 138.4, 137.7, 132.9, 129.1, 128.7, 128.5, 127.9, 127.1, 126.0, 125.5, 119.8, 116.0, 103.3, 100.2, 55.0, 52.1, 47.8, 20.6, 17.5; HRMS m/z calcd for $C_{26}H_{27}N_2O_2$ ($[M+H]^+$): 399.2073, found 399.2066.



23

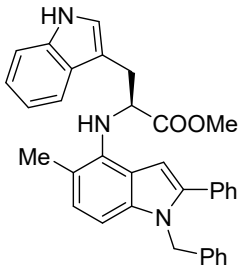
Methyl 2-((1-benzyl-5-methyl-2-phenyl-1H-indol-4-yl)amino)-3-methylpentanoate (24 mg, 55 %): brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45-7.15 (m, 8 H), 7.04-7.00 (m, 2 H), 6.88 (d, J = 8.3 Hz, 1 H), 6.68-6.60 (m, 2 H), 5.29 (s, 2 H), 4.49 (d, J = 5.8 Hz, 1 H), 4.24 (s, 1 H), 3.66 (s, 3 H), 2.37 (s, 3 H), 1.99-1.97 (m, 1 H), 1.92-1.85 (m, 1 H), 1.42-1.30 (m, 1 H), 1.05-0.98 (m, 6 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.9, 140.2, 138.7, 138.4, 138.0, 129.1, 128.7, 128.5, 127.8, 127.0, 126.0, 125.6, 119.4, 115.5, 103.0, 100.3, 63.7, 51.6, 47.8, 39.4, 25.9, 17.5, 15.4, 12.0; HRMS m/z calcd for $C_{29}H_{33}N_2O_2$ ($[M+H]^+$): 441.2542, found 441.2534.



24

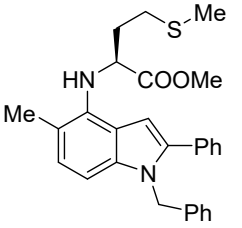
Methyl 2-((1-benzyl-5-methyl-2-phenyl-1H-indol-4-yl)amino)-4-methylpentanoate (35 mg, 80 %): brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42-7.12 (m, 8 H), 7.01-6.98 (m, 2 H), 6.88 (d, J = 8.3 Hz, 1 H), 6.70-6.60 (m, 2 H), 5.29 (s, 2 H), 4.60 (t, J = 7.1 Hz, 1 H), 3.65 (s, 3 H), 2.36 (s, 3 H), 1.98-1.92 (m, 1 H), 1.98-1.92 (m, 1 H), 1.80-1.72 (m, 2 H), 1.04-0.96 (m, 6 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.9, 140.4, 138.7, 138.4, 137.8, 133.0, 129.1, 128.7, 128.6, 127.8, 127.1, 126.0, 125.5, 120.7, 116.4, 103.2, 100.2, 58.2, 52.2, 51.9, 47.9, 44.1, 25.1, 22.9, 22.8, 17.7, 17.6;

HRMS m/z calcd for $C_{29}H_{33}N_2O_2$ ([M+H]$^+$): 441.2542, found 441.2529.



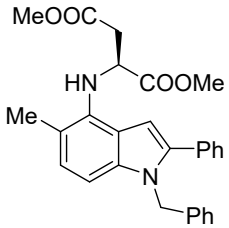
25

Methyl 2-((1-benzyl-5-methyl-2-phenyl-1H-indol-4-yl)amino) -3-(1H-indol-3-yl)propanoate (38 mg, 73 %); brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (s, 1 H), 7.61 (d, J = 7.8 Hz, 1 H), 7.35-7.12 (m, 10 H), 7.10-6.98 (m, 4 H), 6.86 (d, J = 8.3 Hz, 1 H), 6.62 (d, J = 8.2 Hz, 1 H), 6.41 (s, 1 H), 5.27 (s, 2 H), 4.92 (t, J = 5.9 Hz, 1 H), 3.58 (s, 3 H), 3.39 (dd, J = 14.3, 5.9 Hz, 2 H), 2.27 (s, 3 H);; ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.2, 140.3, 138.8, 137.8, 136.1, 132.7, 129.0, 128.7, 128.5, 127.7, 127.1, 126.0, 125.6, 123.2, 122.1, 119.5, 119.4, 118.8, 115.7, 111.2, 111.0, 103.0, 100.3, 60.1, 52.0, 47.9, 30.2, 17.4; HRMS m/z calcd for $C_{34}H_{32}N_3O_2$ ([M+H]$^+$): 514.2495, found 514.2480.



26

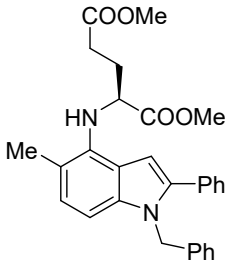
Methyl 2-((1-benzyl-5-methyl-2-phenyl-1H-indol-4-yl) amino)- 4-(methylthio)butanoate (34 mg, 73 %): brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48-7.23 (m, 8 H), 7.01 (d, J = 6.7 Hz, 2 H), 6.89 (d, J = 8.1 Hz, 1 H), 6.71-6.63 (m, 2 H), 5.29 (s, 2 H), 4.75-4.70 (m, 1 H), 4.19 (s, 1 H), 3.68 (s, 3 H), 2.78-2.72 (m, 2 H), 2.38 (s, 3 H), 2.25-2.15 (m, 2 H), 2.09 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.1, 140.5, 138.7, 138.4, 137.6, 132.8, 129.1, 128.7, 128.6, 127.9, 127.1, 126.0, 125.6, 119.7, 116.0, 103.5, 100.2, 58.4, 52.2, 47.9, 33.9, 30.4, 17.5, 15.5; HRMS m/z calcd for $C_{28}H_{31}N_2O_2S$ ([M+H]$^+$): 459.2106, found 459.2106.



27

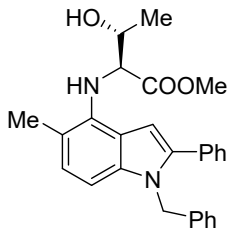
Dimethyl 2-((1-benzyl-5-methyl-2-phenyl-1H-indol-4-yl)amino) pentanedioate (32 mg, 70 %): brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48-7.15 (m, 8 H), 7.01-6.98 (m, 2 H), 6.89 (d, J = 8.2 Hz, 1 H), 6.70-6.66 (m, 2 H), 5.30 (s, 2 H), 4.89 (t, J =

5.6 Hz, 1 H), 4.47 (s, 1 H), 3.72 (s, 3 H), 3.71 (s, 3 H), 2.98 (d, *J* = 4.7 Hz, 2 H), 2.37 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.7, 171.4, 140.7, 138.6, 138.3, 137.1, 132.8, 129.1, 128.7, 128.6, 127.9, 127.1, 126.0, 125.5, 120.0, 116.7, 103.9, 100.0, 56.3, 52.4, 51.9, 47.9, 38.5, 17.3; HRMS m/z calcd for $C_{28}H_{29}N_2O_4$ ($[M+H]^+$): 457.2127, found 457.2122.



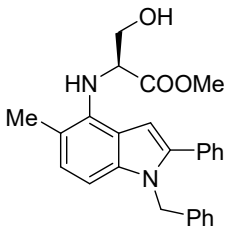
28

Dimethyl 2-((1-benzyl-5-methyl-2-phenyl-1H-indol-4-yl)amino) pentanedioate (33 mg, 71 %): brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48-7.40 (m, 2 H), 7.39-7.32 (m, 3 H), 7.23-7.15 (m, 3 H), 7.03-6.98 (m, 2 H), 6.88 (d, *J* = 6.5 Hz, 1 H), 6.66 (d, *J* = 8.2 Hz, 1 H), 6.58 (s, 1 H), 5.29 (s, 2 H), 4.62 (t, *J* = 7.1 Hz, 1 H), 4.18 (s, 1 H), 3.67 (s, 3 H), 3.65 (s, 3 H), 2.68-2.59 (m, 2 H), 2.37 (s, 3 H), 2.25-2.12 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.9, 173.5, 140.5, 138.6, 138.3, 137.5, 132.8, 129.1, 128.7, 128.5, 127.9, 127.1, 126.0, 125.6, 119.6, 116.1, 103.5, 100.1, 58.6, 52.1, 51.7, 47.9, 30.3, 29.4, 17.5; HRMS m/z calcd for $C_{29}H_{31}N_2O_4$ ($[M+H]^+$): 471.2284, found 471.2275.



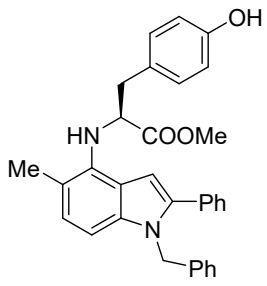
29

Methyl 2-((1-benzyl-5-methyl-2-phenyl-1H-indol-4-yl)amino) -3-hydroxybutanoate (24 mg, 55 %): brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44-7.23 (m, 8 H), 7.01 (d, *J* = 6.0 Hz, 2 H), 6.89 (d, *J* = 7.8 Hz, 1 H), 6.75-6.68 (m, 2 H), 5.29 (s, 2 H), 4.38-4.36 (m, 1 H), 4.11-4.00 (m, 1 H), 3.67 (s, 3 H), 2.39 (s, 3 H), 1.39-1.35 (m, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.3, 140.8, 138.6, 138.3, 137.5, 132.7, 129.2, 128.8, 128.6, 128.0, 127.2, 126.0, 125.5, 120.1, 116.7, 104.3, 100.1, 68.9, 66.1, 52.2, 47.9, 19.3, 17.3; HRMS m/z calcd for $C_{27}H_{29}N_2O_3$ ($[M+H]^+$): 429.2178, found 429.2173.



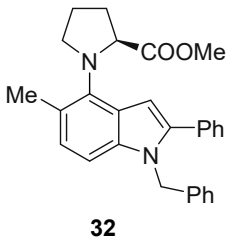
30

Methyl 2-((1-benzyl-5-methyl-2-phenyl-1H-indol-4-yl) amino)- 3-hydroxypropanoate (24 mg, 58 %): brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45-7.18 (m, 8 H), 7.02 (d, J = 7.0 Hz, 2 H), 6.91 (d, J = 8.2 Hz, 1 H), 6.73-6.68 (m, 2 H), 5.30 (s, 2 H), 4.69 (t, J = 5.0 Hz, 1 H), 4.08-4.00 (m, 1 H), 3.91-3.83 (m, 1 H), 3.74 (s, 3 H), 2.42 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.6, 140.8, 138.5, 138.2, 137.4, 132.7, 129.2, 128.7, 128.6, 128.0, 127.1, 126.0, 125.5, 120.0, 116.8, 110.0, 104.1, 100.0, 63.9, 61.4, 52.4, 47.9, 17.3; HRMS m/z calcd for $C_{26}H_{27}N_2O_3$ ($[M+H]^+$): 415.2022, found 415.2016.



31

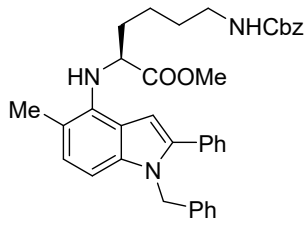
Methyl 2-((1-benzyl-5-methyl-2-phenyl-1H-indol-4-yl)amino) -3-(4-hydroxyphenyl)propanoate (36 mg, 73 %): brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42-7.19 (m, 8 H), 7.07 (d, J = 8.3 Hz, 2 H), 7.00 (d, J = 7.1 Hz, 2 H), 6.87 (d, J = 8.2 Hz, 1 H), 6.72 (d, J = 8.3 Hz, 2 H), 6.63 (d, J = 8.2 Hz, 1 H), 6.38 (s, 1 H), 5.28 (s, 2 H), 4.75 (t, J = 6.1 Hz, 1 H), 3.63 (s, 3 H), 3.13-3.10 (m, 2 H), 2.28 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.9, 154.7, 140.4, 138.7, 138.4, 137.5, 132.8, 130.7, 129.1, 128.9, 128.7, 128.5, 127.8, 127.1, 126.0, 125.6, 119.6, 115.9, 115.4, 103.3, 100.2, 61.0, 52.0, 47.8, 39.7, 17.4; HRMS m/z calcd for $C_{32}H_{31}N_2O_3$ ($[M+H]^+$): 491.2335, found 491.2324.



32

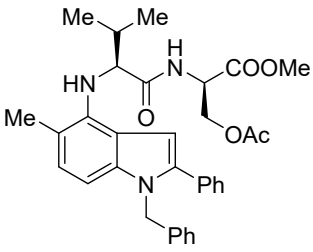
Methyl (1-benzyl-5-methyl-2-phenyl-1H-indol-4-yl)-L-prolinate (17 mg, 40 %): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ7.44 – 7.41 (m, 2H), 7.39 – 7.34 (m, 3H), 7.28 – 7.24 (m, 3H), 7.07 – 7.04 (m, 2H), 6.98 (d, J = 8.3 Hz, 1H), 6.91 (d, J = 8.3 Hz, 1H), 6.51 (s, 1H), 5.31 (s, 2H), 4.56 (dd, J = 9.0, 3.3 Hz, 1H), 3.65 – 3.56 (m, 4H), 3.33 (td, J = 8.3, 6.6 Hz, 1H), 2.44 (s, 3H), 2.30 – 2.02 (m, 4H); ^{13}C NMR (100 MHz, CDCl3) δ 175.8, 140.9, 138.9,

138.3, 138.3, 132.7, 129.1, 128.7, 128.6, 128.5, 128.0, 127.1, 126.0, 125.0, 124.9, 107.9, 100.1, 63.6, 53.4, 51.5, 47.8, 31.0, 26.0, 17.7. HRMS m/z calcd for $C_{28}H_{29}N_2O_2$ ($[M+H]^+$): 425.2224, found 425.2235.



33

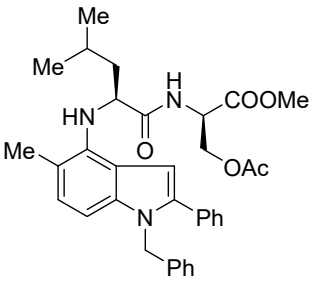
Methyl 2-((1-benzyl-5-methyl-2-phenyl-1H-indol-4-yl)amino)-6-(((benzyloxy)carbonyl)amino)hexanoate (46 mg, 78 %): brown oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52-7.20 (m, 13 H), 7.00 (d, J = 7.0 Hz, 2 H), 6.88 (d, J = 8.2 Hz, 1 H), 6.65 (d, J = 8.2 Hz, 1 H), 6.59 (s, 1 H), 5.28 (s, 2 H), 5.07 (s, 2 H), 4.74 (s, 1 H), 4.58 (t, J = 6.1 Hz, 1 H), 3.67 (s, 3 H), 3.20-3.13 (m, 2 H), 2.36 (s, 3 H), 1.90-1.80 (m, 2 H), 1.54-1.50 (m, 4 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.3, 156.4, 140.5, 138.7, 138.4, 137.7, 136.7, 132.8, 129.1, 128.7, 128.6, 128.1, 127.9, 127.1, 126.0, 125.6, 119.6, 115.8, 103.3, 100.2, 66.6, 59.3, 52.1, 47.8, 40.8, 34.1, 29.8, 22.8, 17.5; HRMS m/z calcd for $C_{37}H_{40}N_3O_4$ ($[M+H]^+$): 590.3019, found 590.3017.



40

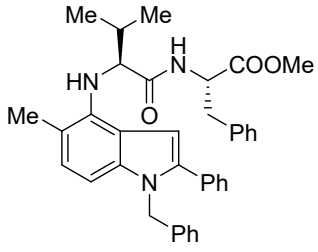
Methyl O-acetyl-N-((1-benzyl-5-methyl-2-phenyl-1H-indol-4-yl)-L-valyl)-D-serinate (28 mg, 51 %): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, J = 8.4 Hz, 1H), 7.41 – 7.30 (m, 5H), 7.31 – 7.19 (m, 3H), 7.03 (s, 2H), 6.90 (d, J = 8.2 Hz, 1H), 6.63 (d, J = 8.2 Hz, 1H), 6.47 (s, 1H), 5.28 (s, 2H), 4.95 (dt, J = 8.4, 4.2 Hz, 1H), 4.41 – 4.37 (m, 2H), 4.32 (dd, J = 11.3, 3.8 Hz, 1H), 4.10 (s, 1H), 3.74 (s, 3H), 2.66 – 2.58 (m, 1H), 2.38 (s, 3H), 1.63 (s, 3H), 1.10 (d, J = 7.0 Hz, 3H), 1.05 (d, J = 7.0 Hz, 3H). ^{13}C NMR (100 MHz, CDCl3) δ 174.1, 170.4, 169.8, 140.4, 138.9, 138.7, 138.2, 132.5, 129.1, 128.7, 128.5, 127.9, 127.1, 126.0, 125.4, 117.9, 113.0, 102.5, 100.0, 66.0, 63.6, 52.7, 51.4, 47.8, 31.5, 20.1, 19.7, 17.6, 16.7. HRMS m/z calcd for $C_{33}H_{38}N_3O_5$ ($[M+H]^+$): 556.2806,

found 556.2823.



41

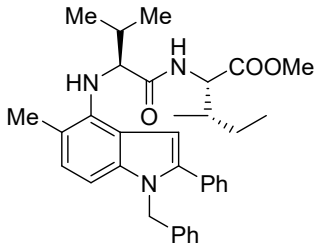
Methyl O-acetyl-N-((1-benzyl-5-methyl-2-phenyl-1H-indol-4-yl)-L-leucyl)-D-serinate (30 mg, 52 %): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, J = 8.4 Hz, 1H), 7.38 – 7.32 (m, 5H), 7.29 – 7.22 (m, 3H), 7.03 (d, J = 7.0 Hz, 2H), 6.90 (d, J = 8.2 Hz, 1H), 6.62 (d, J = 8.2 Hz, 1H), 6.51 (s, 1H), 5.28 (s, 2H), 4.92 (dt, J = 8.3, 4.0 Hz, 1H), 4.47 (d, J = 9.5 Hz, 1H), 4.36 (dd, J = 11.3, 4.3 Hz, 1H), 4.29 (dd, J = 11.3, 3.8 Hz, 1H), 3.87 (s, 1H), 3.75 (s, 3H), 2.34 (s, 3H), 2.03 – 1.96 (m, 1H), 1.90 – 1.83 (m, 1H), 1.75 – 1.68 (m, 1H), 1.60 (s, 3H), 0.99 (d, J = 6.5 Hz, 3H), 0.86 (d, J = 6.4 Hz, 3H). ^{13}C NMR (100 MHz, CDCl3) δ 175.1, 170.4, 169.9, 140.5, 139.0, 138.2, 138.1, 132.5, 129.0, 128.7, 128.5, 127.9, 127.1, 126.0, 125.4, 117.6, 112.9, 102.4, 99.9, 63.7, 59.6, 52.8, 51.4, 47.8, 43.8, 25.2, 23.4, 21.6, 20.1, 17.7. HRMS m/z calcd for $C_{34}H_{40}N_3O_5$ ($[M+H]^+$): 570.2962, found 570.2964.



42

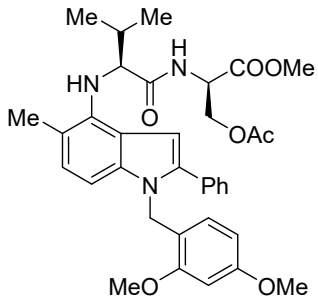
Methyl (1-benzyl-5-methyl-2-phenyl-1H-indol-4-yl)-L-valyl-L-phenylalaninate (28 mg, 48 %): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 – 7.40 (m, 3H), 7.37 – 7.31 (m, 3H), 7.28 – 7.22 (m, 3H), 7.21 – 7.16 (m, 3H), 7.05 – 7.03 (m, 2H), 7.00 – 6.98 (m, 2H), 6.89 (d, J = 8.3 Hz, 1H), 6.66 (d, J = 8.2 Hz, 1H), 6.54 (s, 1H), 5.32 – 5.26 (m, 2H), 4.95 (td, J = 8.1, 5.4 Hz, 1H), 4.18 (d, J = 4.3 Hz, 1H), 3.94 (s, 1H), 3.48 (s, 3H), 3.12 (dd, J = 13.9, 5.5 Hz, 1H), 2.97 (dd, J = 13.9, 7.8 Hz, 1H), 2.46 (pd, J = 7.0, 4.4 Hz, 1H), 2.34 (s, 3H), 0.93 (d, J = 6.9 Hz, 3H), 0.85 (d, J = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, CDCl3) δ 173.7, 171.6, 140.3, 138.9, 138.2, 136.1, 132.6, 129.1, 128.7, 128.5, 128.5, 127.8, 127.1, 126.9, 126.0, 125.5, 118.9, 113.9, 103.0, 100.5, 66.6, 52.9, 52.0, 47.9, 37.9, 31.4, 19.5, 17.5, 16.9; HRMS m/z calcd for

$C_{37}H_{40}N_3O_3$ ([M+H]$^+$): 574.3064, found 574.3077.



43

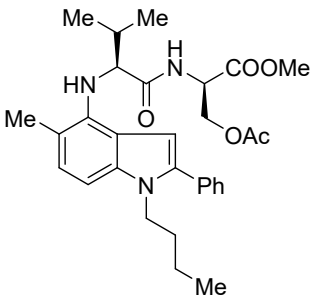
Methyl (1-benzyl-5-methyl-2-phenyl-1H-indol-4-yl)-L-valyl-L-isoleucinate (25 mg, 46 %): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, J = 8.9 Hz, 1H), 7.43 – 7.40 (m, 2H), 7.37 – 7.31 (m, 3H), 7.29 – 7.20 (m, 3H), 7.05 – 7.03 (m, 2H), 6.89 (d, J = 8.3 Hz, 1H), 6.65 (d, J = 8.3 Hz, 1H), 6.54 (s, 1H), 5.30 (s, 2H), 4.60 (dd, J = 9.0, 5.3 Hz, 1H), 4.24 (s, 1H), 4.02 (s, 1H), 3.49 (s, 3H), 2.58 (qd, J = 6.9, 4.2 Hz, 1H), 2.37 (s, 3H), 1.93 – 1.83 (m, 1H), 1.40 – 1.30 (m, 1H), 1.11 (d, J = 6.9 Hz, 3H), 1.07 – 1.00 (m, 4H), 0.86 (t, J = 7.4 Hz, 3H), 0.82 (d, J = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, CDCl3) δ 173.8, 172.0, 140.3, 139.0, 138.8, 138.3, 132.6, 129.1, 128.7, 128.5, 127.8, 127.1, 126.0, 125.5, 118.9, 114.0, 103.0, 100.4, 66.9, 56.5, 51.7, 47.8, 37.3, 31.4, 25.0, 19.6, 17.6, 17.2, 15.5, 11.4. HRMS m/z calcd for $C_{34}H_{42}N_3O_3$ ([M+H]$^+$): 540.3221, found 540.3228.



44

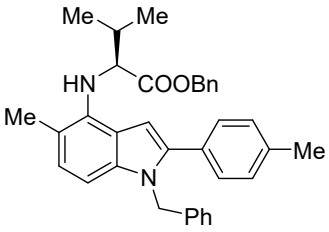
Methyl O-acetyl-N-((1-(2,4-dimethoxybenzyl)-5-methyl-2-phenyl-1H-indol-4-yl)-L-valyl)-D-serinate (34 mg, 56 %): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, J = 8.4 Hz, 1H), 7.38 – 7.29 (m, 5H), 6.90 (d, J = 8.3 Hz, 1H), 6.63 (d, J = 8.2 Hz, 1H), 6.54 (d, J = 8.4 Hz, 1H), 6.48 – 6.46 (m, 2H), 6.30 (dd, J = 8.4, 2.4 Hz, 1H), 5.18 (s, 2H), 4.95 (dt, J = 8.4, 4.2 Hz, 1H), 4.42 – 4.38 (m, 2H), 4.33 (dd, J = 11.3, 3.8 Hz, 1H), 4.08 (s, 1H), 3.81 (s, 3H), 3.76 (s, 3H), 3.75 (s, 4H), 2.67 – 2.59 (m, 1H), 2.38 (s, 3H), 1.65 (s, 3H), 1.10 (d, J = 7.0 Hz, 3H), 1.06 (d, J = 7.0 Hz, 3H). ^{13}C NMR (100 MHz, CDCl3) δ 174.2, 170.4, 169.9, 159.9, 157.0, 140.5, 139.0, 138.6, 132.6, 128.8, 128.5, 127.7, 127.2, 125.3, 118.7, 117.9, 112.8, 103.9, 102.6, 99.7, 98.2, 66.0, 63.6, 55.3, 55.2, 52.7, 51.4, 42.9, 31.5, 20.1, 19.7, 17.6, 16.7. HRMS

m/z calcd for $C_{35}H_{42}N_3O_7$ ([M+H]$^+$): 616.3017, found 616.3024.



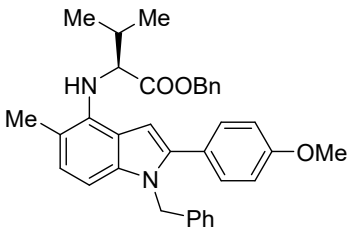
45

Methyl O-acetyl-N-((1-butyl-5-methyl-2-phenyl-1H-indol-4-yl)-L-valyl)-D-serinate (27 mg, 51 %): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, J = 8.5 Hz, 1H), 7.45 – 7.34 (m, 5H), 6.98 (d, J = 8.3 Hz, 1H), 6.84 (d, J = 8.2 Hz, 1H), 6.32 (s, 1H), 4.93 (dt, J = 8.4, 4.1 Hz, 1H), 4.38 – 4.34 (m, 2H), 4.28 (dd, J = 11.3, 3.7 Hz, 1H), 4.09 – 4.02 (m, 3H), 3.74 (s, 3H), 2.65 – 2.55 (m, 1H), 2.40 (s, 3H), 1.68 – 1.60 (m, 5H), 1.18 (h, J = 7.5 Hz, 2H), 1.08 (d, J = 7.0 Hz, 3H), 1.03 (d, J = 7.0 Hz, 3H), 0.79 (t, J = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, CDCl3) δ 174.1, 170.4, 169.9, 140.0, 138.7, 138.2, 133.1, 129.4, 128.4, 127.8, 125.0, 117.8, 112.4, 102.0, 99.6, 65.9, 63.6, 52.7, 51.3, 43.8, 31.9, 31.5, 20.1, 20.0, 19.7, 17.6, 16.6, 13.6. HRMS m/z calcd for $C_{30}H_{40}N_3O_5$ ([M+H]$^+$): 522.2962, found 522.2959.



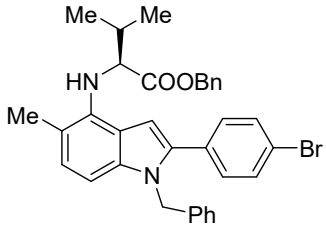
46

Benzyl (1-benzyl-5-methyl-2-(p-tolyl)-1H-indol-4-yl)-L-valinate (40 mg, 78 %): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 – 7.21 (m, 6H), 7.20 – 7.14 (m, 6H), 7.02 – 6.99 (m, 2H), 6.86 (d, J = 8.3 Hz, 1H), 6.63 (dd, J = 8.2, 0.8 Hz, 1H), 6.61 (d, J = 0.8 Hz, 1H), 5.27 (s, 2H), 5.10 – 5.04 (m, 2H), 4.46 (d, J = 6.0 Hz, 1H), 2.36 (s, 3H), 2.34 (s, 3H), 2.22 (dq, J = 13.5, 6.5 Hz, 1H), 1.15 (d, J = 6.9 Hz, 3H), 1.08 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, CDCl3) δ 174.4, 140.2, 138.6, 138.4, 137.8, 137.6, 135.6, 129.9, 129.2, 129.0, 128.6, 128.4, 128.2, 128.1, 126.9, 125.9, 125.4, 119.2, 115.5, 102.9, 100.0, 66.5, 64.8, 47.7, 32.5, 21.2, 19.0, 18.9, 18.8, 17.4. HRMS m/z calcd for $C_{35}H_{37}N_2O_2$ ([M+H]$^+$): 517.2850, found 517.2847.



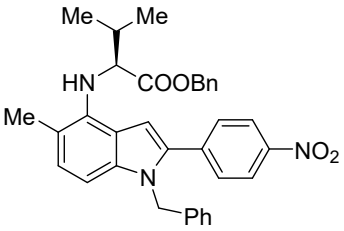
47

Benzyl (1-benzyl-2-(4-methoxyphenyl)-5-methyl-1H-indol-4-yl)-L-valinate (40 mg, 75 %): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.28 (m, 2H), 7.27 – 7.17 (m, 8H), 7.01 – 6.99 (m, 2H), 6.89 – 6.85 (m, 3H), 6.63 (dd, J = 8.2, 0.8 Hz, 1H), 6.57 (d, J = 0.9 Hz, 1H), 5.26 (s, 2H), 5.07 – 5.07 (m, 2H), 4.45 (d, J = 6.0 Hz, 1H), 4.18 (s, 1H), 3.80 (s, 3H), 2.34 (s, 3H), 2.26 – 2.17 (m, 1H), 1.15 (d, J = 6.9 Hz, 3H), 1.08 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, CDCl3) δ 174.4, 159.4, 140.0, 138.5, 138.5, 137.8, 135.6, 130.4, 128.6, 128.4, 128.2, 128.1, 127.0, 126.0, 125.3, 119.3, 115.5, 113.9, 66.5, 64.8, 55.3, 47.7, 32.5, 19.0, 18.9, 17.5. HRMS m/z calcd for $C_{35}H_{37}N_2O_3$ ($[M+H]^+$): 533.2799, found 533.2806.



48

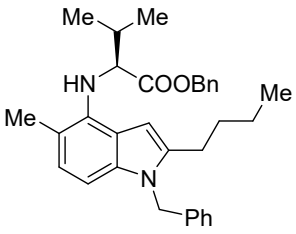
Benzyl (1-benzyl-2-(4-bromophenyl)-5-methyl-1H-indol-4-yl)-L-valinate (46 mg, 79 %): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.44 (m, 2H), 7.27 – 7.17 (m, 10H), 6.98 (dd, J = 7.9, 1.6 Hz, 2H), 6.89 (d, J = 8.3 Hz, 1H), 6.65 – 6.63 (m, 2H), 5.25 (s, 2H), 5.07 (s, 2H), 4.43 (d, J = 6.0 Hz, 1H), 2.34 (s, 3H), 2.26 – 2.18 (m, 1H), 1.15 (d, J = 6.9 Hz, 3H), 1.08 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, CDCl3) δ 174.3, 138.9, 138.8, 138.1, 138.0, 135.5, 131.6, 130.5, 128.7, 128.4, 128.2, 128.1, 127.1, 125.9, 125.8, 122.0, 119.0, 115.6, 102.8, 100.7, 66.5, 64.8, 47.7, 32.5, 19.0, 18.8, 17.5. HRMS m/z calcd for $C_{34}H_{34}BrN_2O_2$ ($[M+H]^+$): 581.1798, found 581.1786.



49

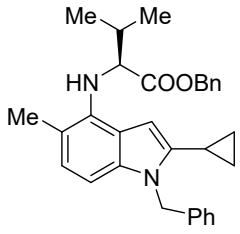
Benzyl (1-benzyl-5-methyl-2-(4-nitrophenyl)-1H-indol-4-yl)-L-valinate (36 mg, 66 %): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, J = 8.8 Hz, 2H), 7.49 (d, J = 8.8 Hz, 2H), 7.31 – 7.25 (m, 6H), 7.20 – 7.18 (m, 2H), 7.03 – 7.00 (m, 2H), 6.96 (d, J = 8.3 Hz, 1H), 6.79 (d, J = 0.8 Hz, 1H), 6.68 (dd, J = 8.3, 0.8 Hz, 1H),

5.30 (s, 2H), 5.09 (d, *J* = 1.3 Hz, 2H), 4.42 (d, *J* = 6.0 Hz, 1H), 4.24 (s, 1H), 2.35 (s, 3H), 2.29 – 2.19 (m, 1H), 1.17 (d, *J* = 6.8 Hz, 3H), 1.10 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, CDCl3) *δ* 174.2, 146.8, 139.9, 139.2, 138.4, 137.6, 137.5, 135.5, 129.0, 128.9, 128.5, 128.2, 127.4, 127.1, 125.8, 123.9, 119.0, 115.9, 103.0, 102.8, 66.6, 65.0, 48.1, 32.6, 19.0, 18.8, 17.5. HRMS m/z calcd for $C_{34}H_{34}N_3O_4$ ([M+H]$^+$): 548.2544, found 548.2539.



50

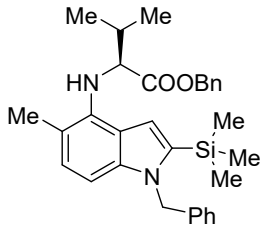
Benzyl (1-benzyl-2-butyl-5-methyl-1H-indol-4-yl)-L-valinate (37 mg, 77 %): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.29 – 7.26 (m, 3H), 7.23 – 7.16 (m, 5H), 6.92 (dd, *J* = 7.8, 1.7 Hz, 2H), 6.82 (d, *J* = 8.2 Hz, 1H), 6.65 (d, *J* = 8.2 Hz, 1H), 6.30 (s, 1H), 5.23 (s, 2H), 5.10 – 5.03 (m, 2H), 4.40 (d, *J* = 5.9 Hz, 1H), 2.62 – 2.58 (m, 2H), 2.32 (s, 3H), 2.26 – 2.17 (m, 1H), 1.65 – 1.57 (m, 2H), 1.37 (h, *J* = 7.4 Hz, 2H), 1.15 (d, *J* = 6.9 Hz, 3H), 1.08 (d, *J* = 6.8 Hz, 3H), 0.88 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, CDCl3) *δ* 174.5, 139.5, 138.2, 137.7, 137.2, 135.7, 128.6, 128.4, 128.2, 128.1, 127.0, 125.9, 124.1, 119.1, 115.2, 102.1, 97.2, 66.4, 64.7, 46.38, 32.5, 30.6, 26.4, 22.5, 19.0, 18.9, 17.5, 13.8. HRMS m/z calcd for $C_{32}H_{39}N_2O_2$ ([M+H]$^+$): 483.3006, found 483.3017.



51

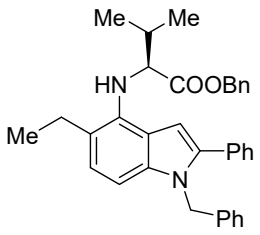
Benzyl (1-benzyl-2-cyclopropyl-5-methyl-1H-indol-4-yl)-L-valinate (36 mg, 77 %): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) *δ* 7.30 – 7.27 (m, 3H), 7.26 – 7.17 (m, 5H), 7.01 – 6.98 (m, 2H), 6.83 (d, *J* = 8.2 Hz, 1H), 6.66 (dd, *J* = 8.2, 0.7 Hz, 1H), 6.17 (d, *J* = 0.9 Hz, 1H), 5.39 (s, 2H), 5.10 – 5.03 (m, 2H), 4.36 (d, *J* = 5.9 Hz, 1H), 4.12 (s, 1H), 2.31 (s, 3H), 2.24 – 2.16 (m, 1H), 1.71 (ttd, *J* = 8.2, 5.2, 1.0 Hz, 1H), 1.14 (d, *J* = 6.9 Hz, 3H), 1.07 (d, *J* = 6.8 Hz, 3H), 0.90 – 0.79 (m, 2H), 0.69 – 0.61 (m, 2H). ^{13}C NMR (100 MHz, CDCl3) *δ* 174.5, 141.3, 138.4, 137.9, 137.5, 135.6, 128.6,

128.5, 128.2, 128.1, 127.0, 126.1, 124.6, 118.7, 115.1, 101.9, 96.1, 66.4, 64.7, 46.7, 32.5, 19.0, 18.8, 17.5, 7.4, 6.6, 6.3. HRMS m/z calcd for $C_{31}H_{35}N_2O_2$ ($[M+H]^+$): 467.2693, found 467.2689.



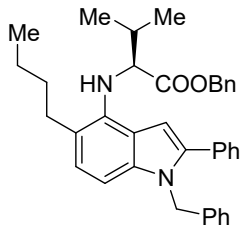
52

Benzyl (1-benzyl-5-methyl-2-(trimethylsilyl)-1H-indol-4-yl)-L-valinate (27 mg, 54 %): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.28 (m, 3H), 7.24 – 7.17 (m, 5H), 6.88 – 6.86 (m, 2H), 6.84 (d, J = 8.3 Hz, 1H), 6.75 (s, 1H), 6.57 (d, J = 8.2 Hz, 1H), 5.38 (s, 2H), 5.13 (d, J = 12.3 Hz, 1H), 5.06 (d, J = 12.3 Hz, 1H), 4.46 (s, 1H), 4.23 (s, 1H), 2.31 (s, 3H), 2.25 (td, J = 7.0, 5.9 Hz, 1H), 1.16 (d, J = 6.9 Hz, 3H), 1.09 (d, J = 6.8 Hz, 3H), 0.22 (s, 9H). ^{13}C NMR (100 MHz, CDCl3) δ 174.4, 140.7, 139.2, 138.4, 138.0, 135.6, 128.5, 128.3, 128.2, 127.0, 126.0, 125.7, 119.7, 114.4, 110.0, 102.2, 66.5, 64.8, 49.9, 32.6, 19.0, 18.8, 17.3, -0.4. HRMS m/z calcd for $C_{31}H_{39}N_2O_2Si$ ($[M+H]^+$): 499.2775, found 499.2770.



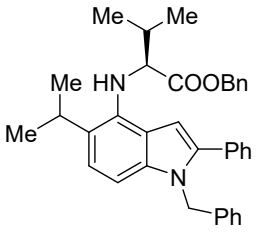
53

Benzyl (1-benzyl-5-ethyl-2-phenyl-1H-indol-4-yl)-L-valinate (40 mg, 78 %): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.31 (m, 5H), 7.27 – 7.16 (m, 8H), 7.04 – 7.01 (m, 2H), 6.91 (d, J = 8.3 Hz, 1H), 6.69 (dd, J = 8.3, 0.8 Hz, 1H), 6.66 (d, J = 0.8 Hz, 1H), 5.28 (s, 2H), 5.10 – 5.03 (m, 2H), 4.48 (d, J = 6.0 Hz, 1H), 2.79 (dq, J = 15.0, 7.5 Hz, 1H), 2.68 (dq, J = 15.0, 7.6 Hz, 1H), 2.23 (dq, J = 13.6, 6.8 Hz, 1H), 1.24 (t, J = 7.6 Hz, 3H), 1.16 (d, J = 6.9 Hz, 3H), 1.08 (d, J = 6.7 Hz, 3H); ^{13}C NMR (100 MHz, CDCl3) δ 174.4, 140.1, 138.6, 138.4, 137.3, 135.5, 132.8, 129.1, 128.6, 128.5, 128.4, 128.2, 128.1, 127.7, 127.0, 126.0, 123.9, 121.9, 119.3, 103.2, 100.7, 66.5, 65.0, 47.8, 32.6, 24.0, 19.0, 18.9, 14.8. HRMS m/z calcd for $C_{35}H_{37}N_2O_2$ ($[M+H]^+$): 517.2850, found 517.2862.



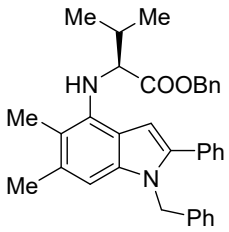
54

Benzyl (1-benzyl-5-butyl-2-phenyl-1H-indol-4-yl)-L-valinate (38 mg, 70 %): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.32 (m, 5H), 7.29 – 7.16 (m, 8H), 7.04 – 7.02 (m, 2H), 6.88 (d, J = 8.2 Hz, 1H), 6.68 – 6.65 (m, 2H), 5.28 (s, 2H), 5.07 (s, 2H), 4.48 (d, J = 6.0 Hz, 1H), 4.31 (s, 1H), 2.80 (dt, J = 15.0, 7.7 Hz, 1H), 2.60 (dt, J = 14.2, 7.9 Hz, 1H), 2.23 (dq, J = 14.0, 7.0 Hz, 1H), 1.63 – 1.55 (m, 2H), 1.40 (h, J = 7.3 Hz, 2H), 1.16 (d, J = 6.9 Hz, 3H), 1.08 (d, J = 6.8 Hz, 3H), 0.94 (t, J = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, CDCl3) δ 174.3, 140.1, 138.6, 138.4, 137.4, 135.6, 132.9, 129.1, 128.6, 128.5, 128.4, 128.2, 128.1, 127.7, 127.0, 126.0, 124.9, 120.7, 119.3, 103.1, 100.7, 66.5, 65.0, 47.8, 32.7, 32.6, 30.9, 22.8, 19.0, 18.9, 14.1. HRMS m/z calcd for $C_{37}H_{41}N_2O_2$ ([M+H]$^+$): 545.3163, found 545.3169.



55

Benzyl (1-benzyl-5-isopropyl-2-phenyl-1H-indol-4-yl)-L-valinate (29 mg, 55 %): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 – 7.32 (m, 5H), 7.28 – 7.21 (m, 6H), 7.16 – 7.14 (m, 2H), 7.05 – 7.03 (m, 2H), 7.00 (d, J = 8.5 Hz, 1H), 6.76 (dd, J = 8.5, 0.8 Hz, 1H), 6.65 (d, J = 0.8 Hz, 1H), 5.28 (d, J = 1.4 Hz, 2H), 5.10 – 5.03 (m, 2H), 4.41 (d, J = 6.2 Hz, 1H), 4.36 (s, 1H), 3.33 (hept, J = 6.8 Hz, 1H), 2.27 – 2.18 (m, 1H), 1.27 – 1.23 (m, 6H), 1.18 (d, J = 6.9 Hz, 3H), 1.08 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, CDCl3) δ 174.4, 140.2, 138.4, 138.1, 136.4, 135.6, 132.9, 129.1, 128.7, 128.5, 128.4, 128.1, 127.7, 127.2, 127.0, 126.0, 120.5, 120.0, 103.9, 100.9, 66.4, 65.6, 47.8, 32.6, 26.9, 24.0, 23.8, 19.1, 19.0. HRMS m/z calcd for $C_{36}H_{39}N_2O_2$ ([M+H]$^+$): 531.3006, found 531.2997.



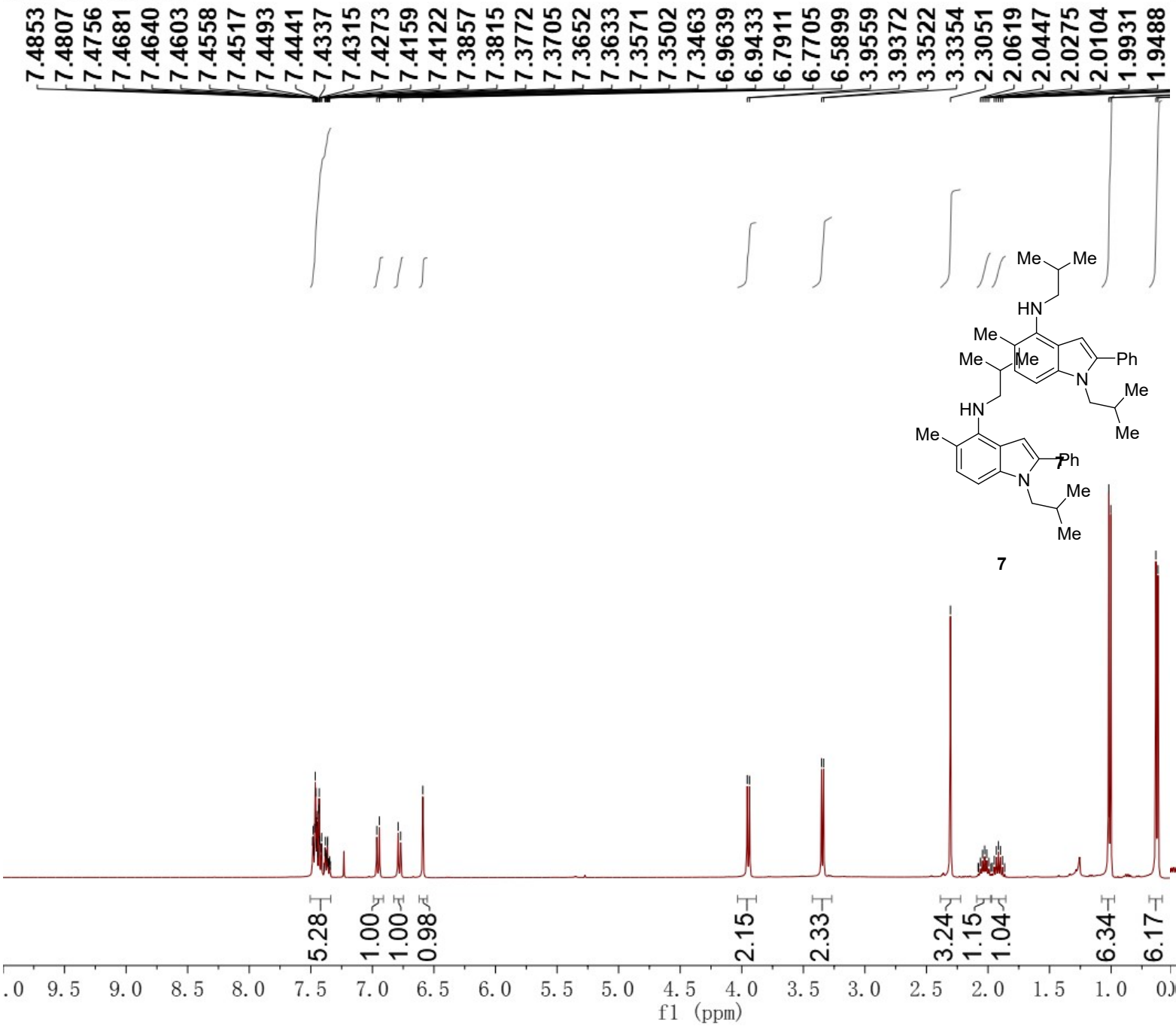
56

Benzyl (1-benzyl-5,6-dimethyl-2-phenyl-1H-indol-4-yl)-L-

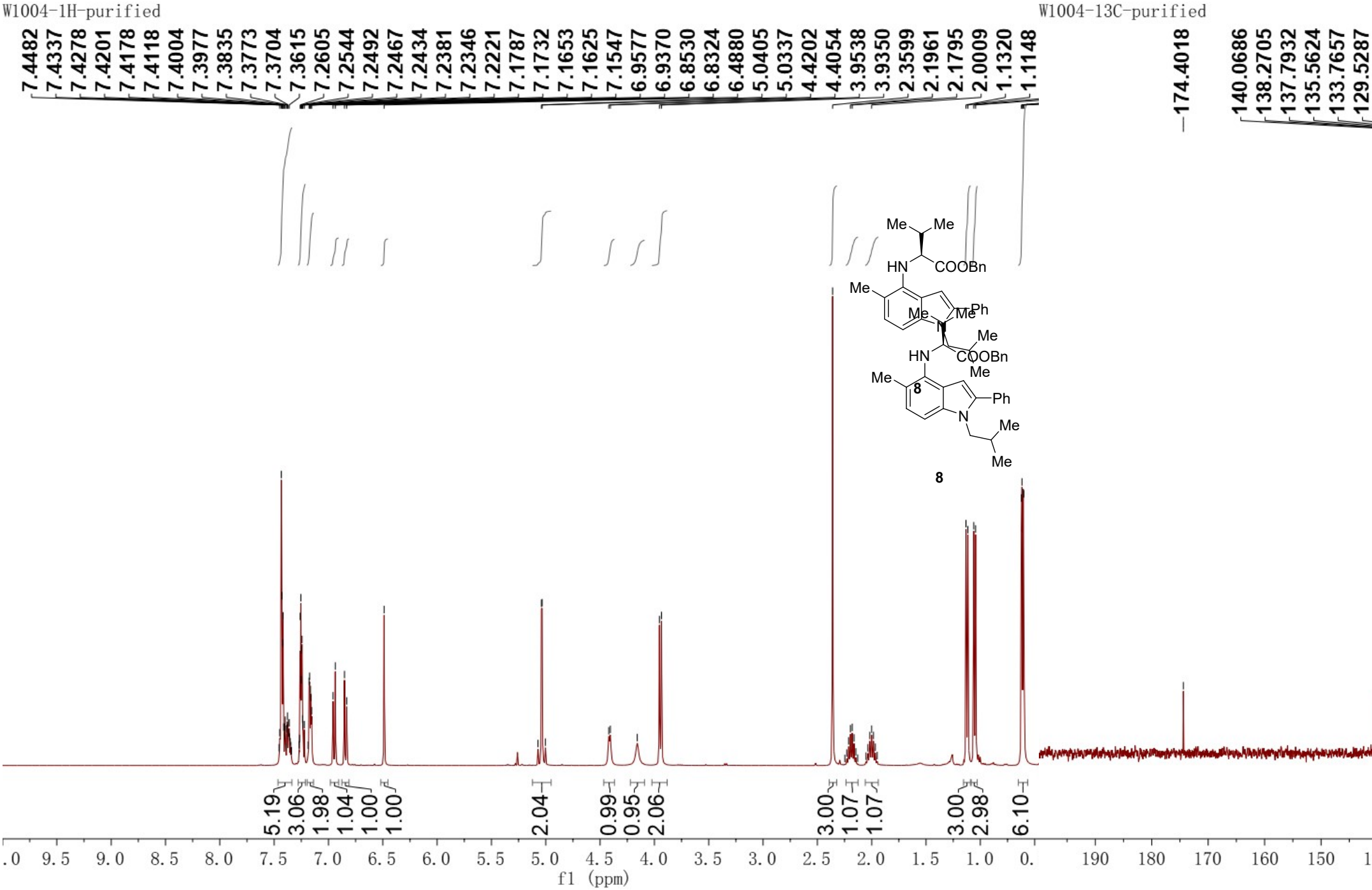
valinate (41 mg, 80 %): yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.29 (m, 5H), 7.28 – 7.21 (m, 6H), 7.17 – 7.14 (m, 2H), 7.02 (dd, J = 8.0, 1.6 Hz, 2H), 6.61 – 6.60 (m, 2H), 5.27 (s, 2H), 5.06 (s, 2H), 4.37 (d, J = 6.2 Hz, 1H), 4.23 (s, 1H), 2.29 (s, 3H), 2.26 – 2.19 (m, 4H), 1.17 (d, J = 6.8 Hz, 3H), 1.08 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, CDCl3) δ 174.5, 139.4, 138.5, 137.9, 137.8, 135.6, 132.9, 132.1, 129.0, 128.6, 128.4, 128.4, 128.1, 128.1, 127.5, 126.9, 125.9, 118.2, 115.5, 104.7, 100.4, 66.4, 65.3, 47.6, 32.5, 22.0, 19.0, 19.0, 13.1. HRMS m/z calcd for $C_{35}H_{37}N_2O_2$ ($[M+H]^+$): 517.2850, found 517.2854.

W1041-1H-purified

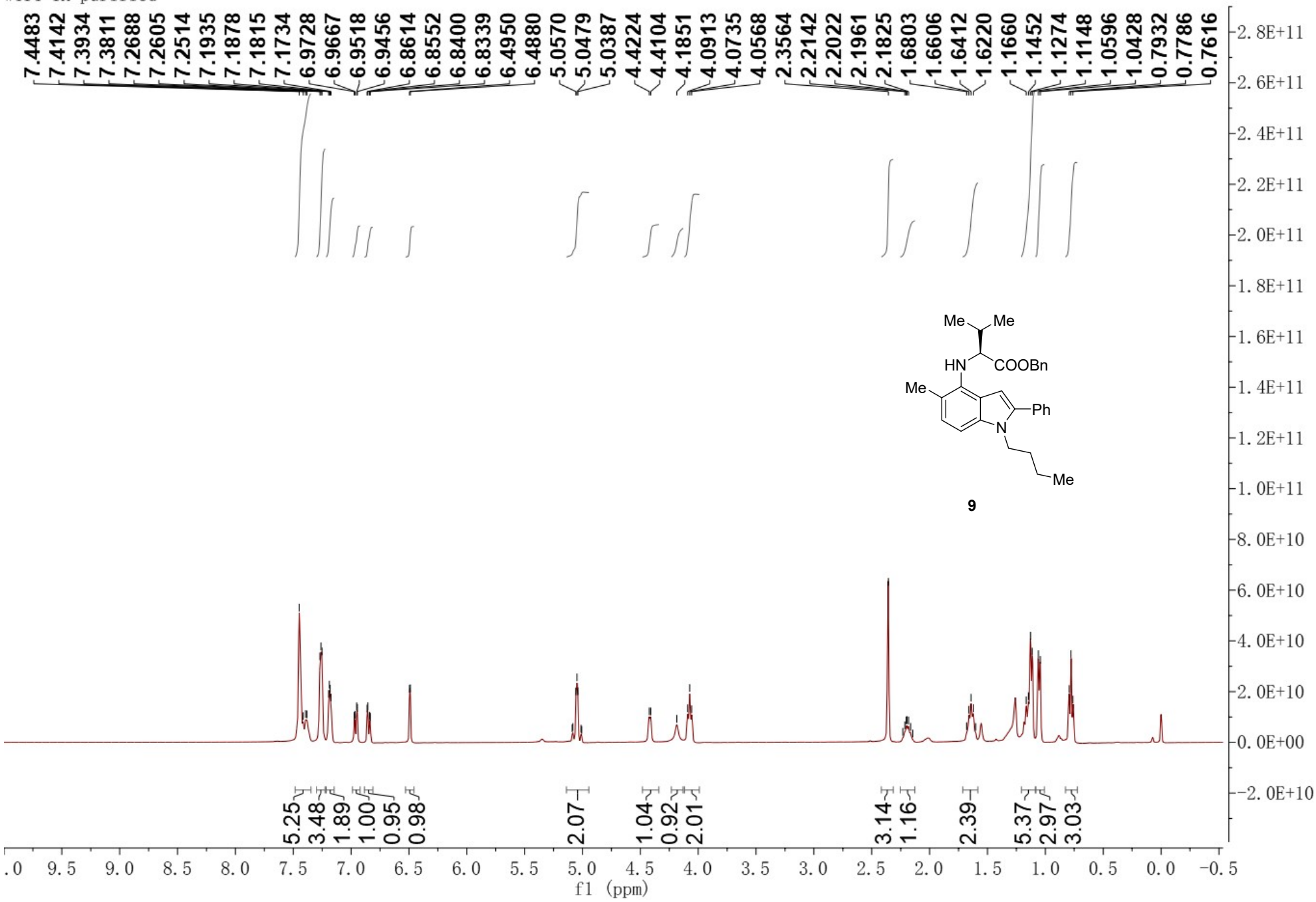
W1041-13C-purified



7

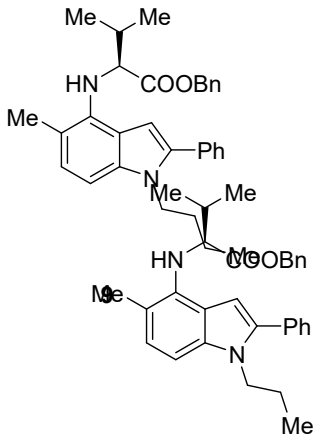

W1004-1H-purified
W1004-13C-purified
7.4482
7.4337
7.4278
7.4201
7.4178
7.4118
7.4004
7.3977
7.3835
7.3773
7.3704
7.3615
7.2605
7.2544
7.2492
7.2467
7.2434
7.2381
7.2346
7.2221
7.1787
7.1732
7.1653
7.1625
7.1547
6.9577
6.9370
6.8530
6.8324
6.4880
5.0405
5.0337
4.4202
4.4054
3.9538
3.9350
2.3599
2.1961
2.1795
2.0009
1.1320
1.1148
174.4018
140.0686
138.2705
137.7932
135.5624
133.7657
129.5287
Me
Me
HN
COOBn
Me
Me
Me
Ph
N
Me
HN
COOBn
Me
Me
Ph
N
Me
Me
8
8
5.19
3.06
1.98
1.04
1.00
1.00
2.04
0.99
0.95
2.06
3.00
1.07
1.07
3.00
2.98
6.10
f1 (ppm)

W414-1H-purified

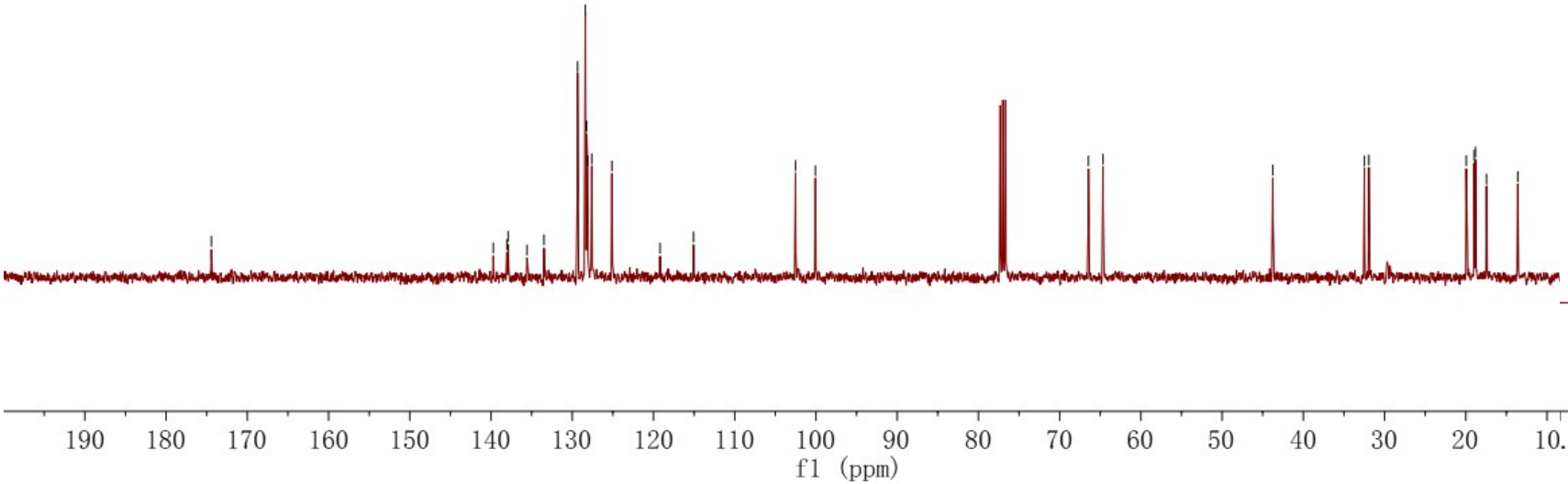


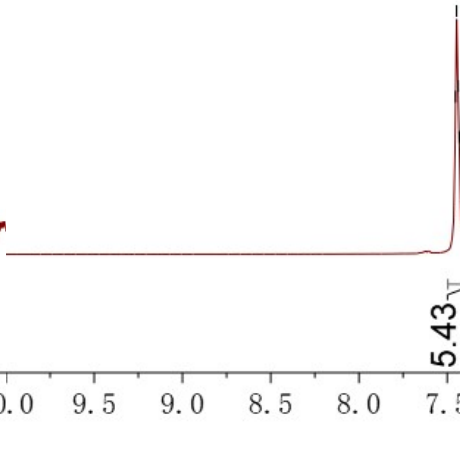
W414-13C-purified

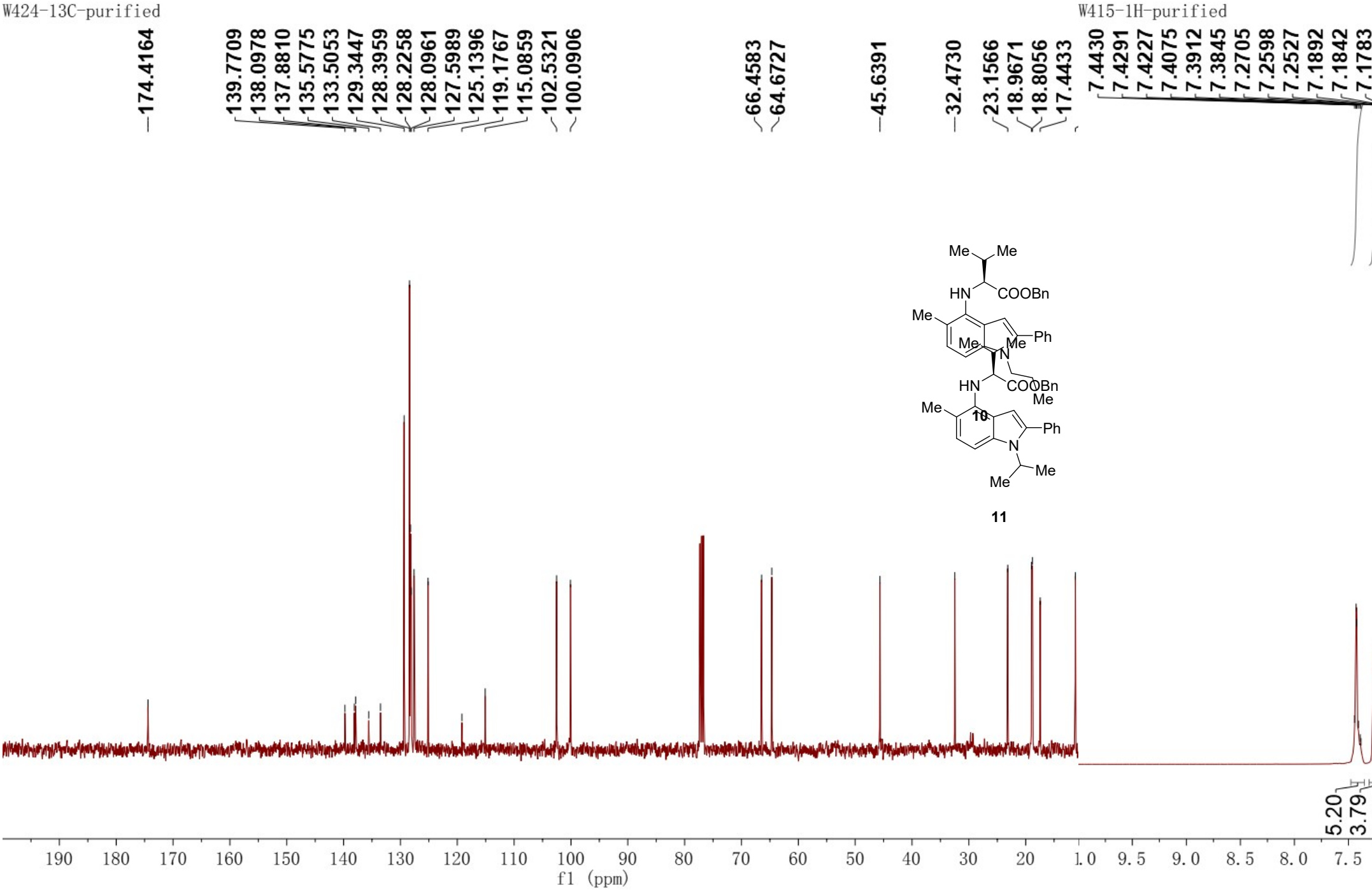
W424-1H-purified

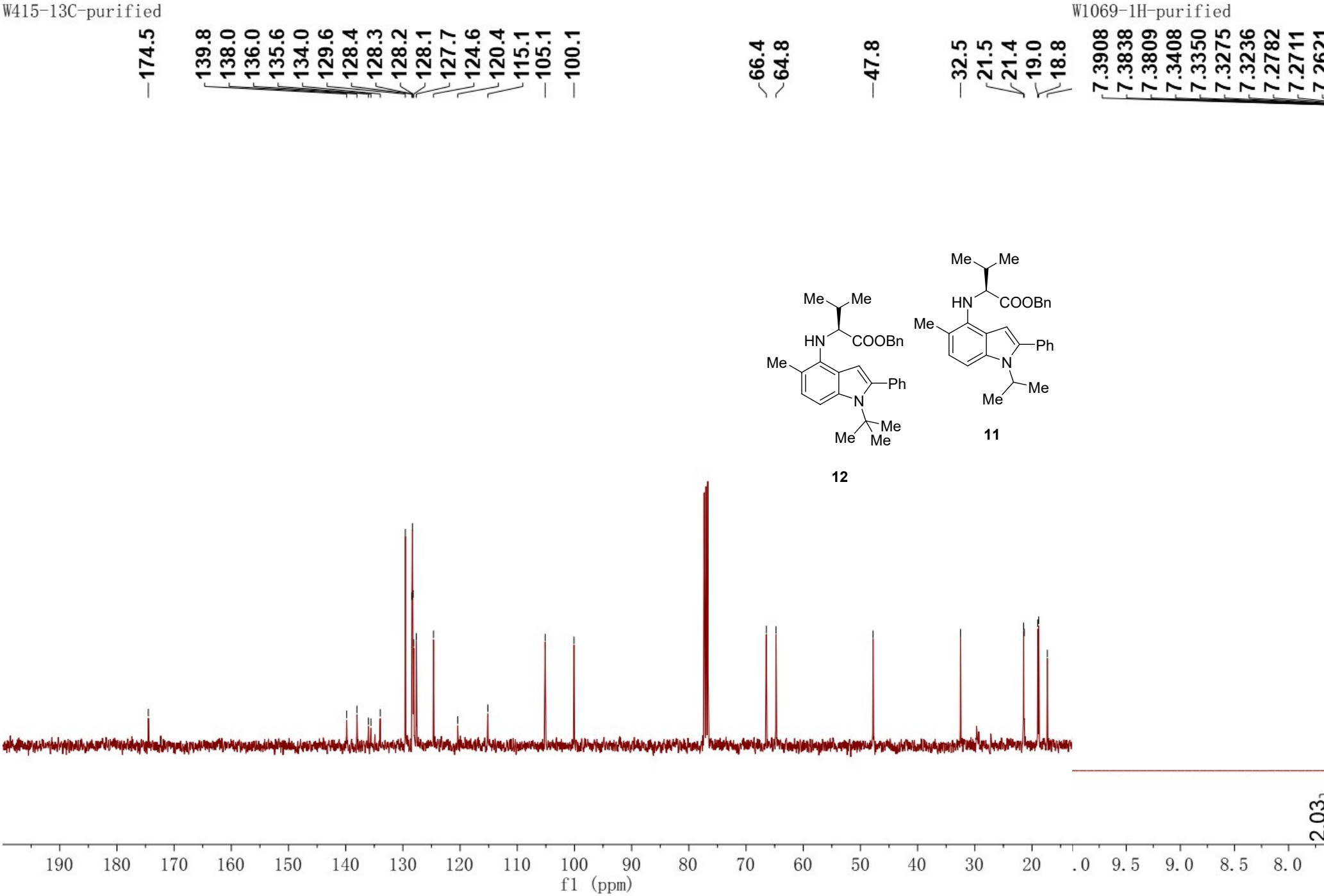


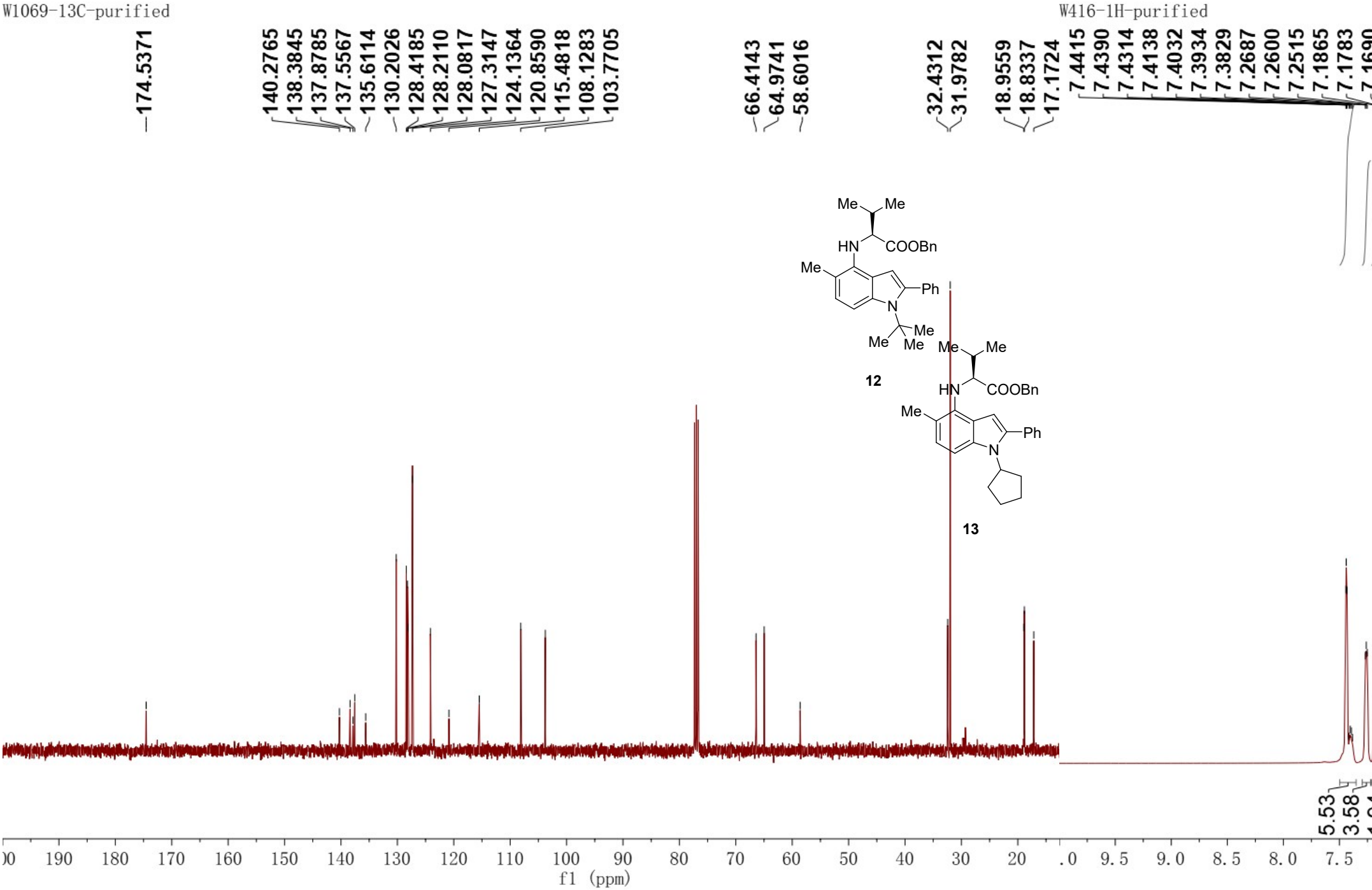
10

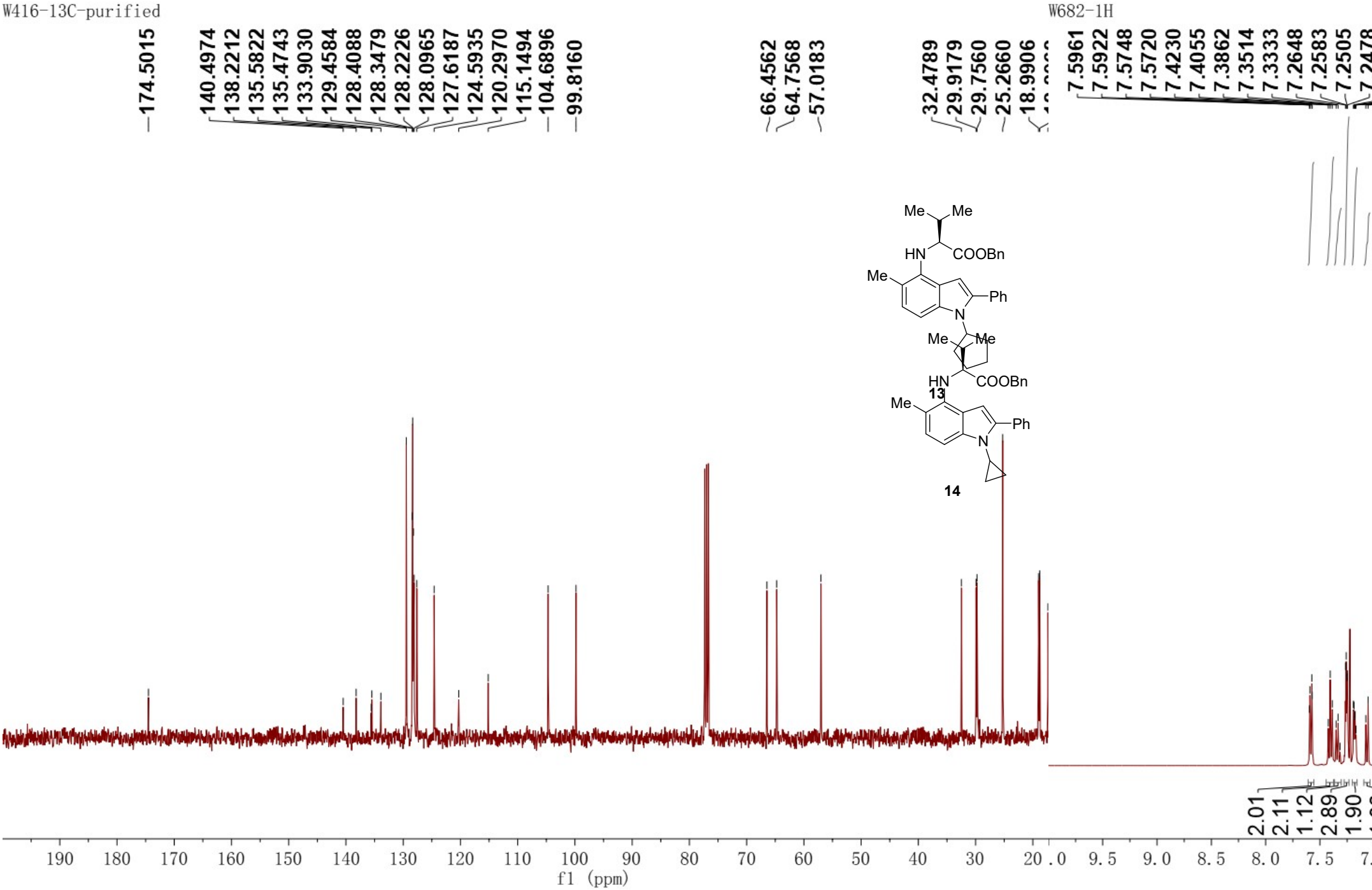





W424-13C-purified
W415-1H-purified
174.4164
139.7709
138.0978
137.8810
135.5775
133.5053
129.3447
128.3959
128.2258
128.0961
127.5989
125.1396
119.1767
115.0859
102.5321
100.0906
66.4583
64.6727
45.6391
32.4730
23.1566
18.9671
18.8056
17.4433
7.4430
7.4291
7.4227
7.4075
7.3912
7.3845
7.2705
7.2598
7.2527
7.1892
7.1842
7.1783
Me
Me
HN
COOBn
Me
Me
Me
Ph
N
HN
COOBn
Me
Me
Ph
N
Me
Me
10
11
5.20
3.79
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
9.5
9.0
8.5
8.0
7.5
f1 (ppm)

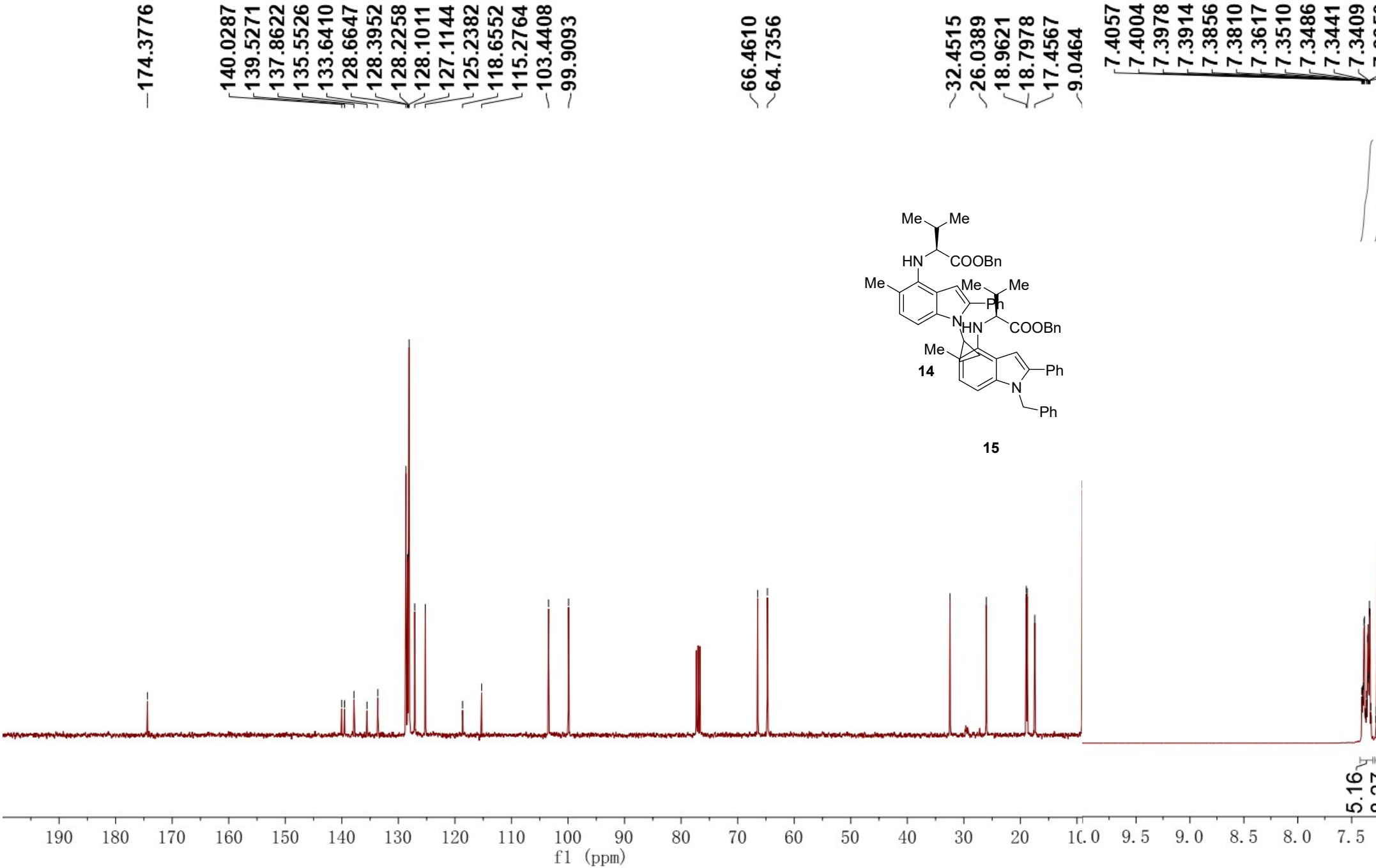

W415-13C-purified
174.5
139.8
138.0
136.0
135.6
134.0
129.6
128.4
128.3
128.2
128.1
127.7
124.6
120.4
115.1
105.1
100.1
66.4
64.8
47.8
32.5
21.5
21.4
19.0
18.8
W1069-1H-purified
7.3908
7.3838
7.3809
7.3408
7.3350
7.3275
7.3236
7.2782
7.2711
7.2621
7.2541
7.2115
Me
Me
HN
COOBn
Me
Ph
N
Me
Me
Me
12
11
2.03
3.01
3.31
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
.0
9.5
9.0
8.5
8.0
7.5
f1 (ppm)


W1069-13C-purified
W416-1H-purified
174.5371
140.2765
138.3845
137.8785
137.5567
135.6114
130.2026
128.4185
128.2110
128.0817
127.3147
124.1364
120.8590
115.4818
108.1283
103.7705
66.4143
64.9741
58.6016
32.4312
31.9782
18.9559
18.8337
17.1724
7.4415
7.4390
7.4314
7.4138
7.4032
7.3934
7.3829
7.2687
7.2600
7.2515
7.1865
7.1783
Me
Me
HN
COOBn
Me
Ph
N
Me
Me
Me
12
Me
Me
HN
COOBn
Me
Ph
N
13
5.53
3.58
f1 (ppm)


W416-13C-purified
W682-1H
174.5015
140.4974
138.2212
135.5822
135.4743
133.9030
129.4584
128.4088
128.3479
128.2226
128.0965
127.6187
124.5935
120.2970
115.1494
104.6896
99.8160
66.4562
64.7568
57.0183
32.4789
29.9179
29.7560
25.2660
18.9906
7.5961
7.5922
7.5748
7.5720
7.4230
7.4055
7.3862
7.3514
7.3333
7.2648
7.2583
7.2505
Me
Me
HN
COOBn
Me
Ph
N
Me
Me
HN
COOBn
13
Me
Ph
N
14
2.01
2.11
1.12
2.89
1.90
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
.0
9.5
9.0
8.5
8.0
7.5
f1 (ppm)

W682-13C

W1005-1H-purified



W1005-13C-purified

174.4176
140.1399
138.7072
138.3395
137.9106
135.5521
132.8251
129.0564
128.6357
128.4739
128.4360
128.1846
128.1067
127.7392
126.9833
125.9394
125.5803
119.1786
115.5015
102.9379
100.3721

66.4923
64.7858

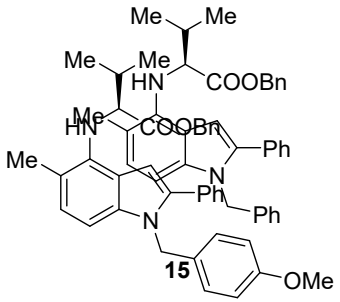
47.7586

32.5076

18.9987
18.8351
17.4510

W425-1H-purified

7.3923
7.3859
7.3639
7.3593
7.3540
7.3425
7.3367
7.2603
7.2532
7.2470
7.1963



16

5.27
3.43

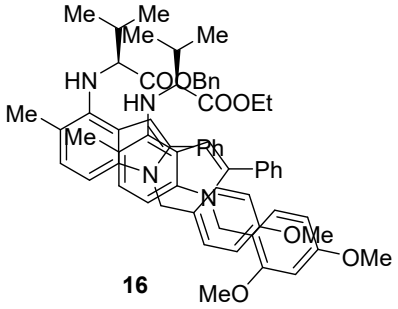
f1 (ppm)

W425-13C-purified

174.4243
158.5560
140.0829
138.6663
137.8938
135.5695
132.9051
130.3644
129.0763
128.4528
128.1813
128.0975
127.7193
127.1228
125.5388
119.2020
115.4520
114.0105
102.9807
100.3190
66.4791
64.7861
55.1968
47.2025
32.5100
19.0045
18.8392
17.4577

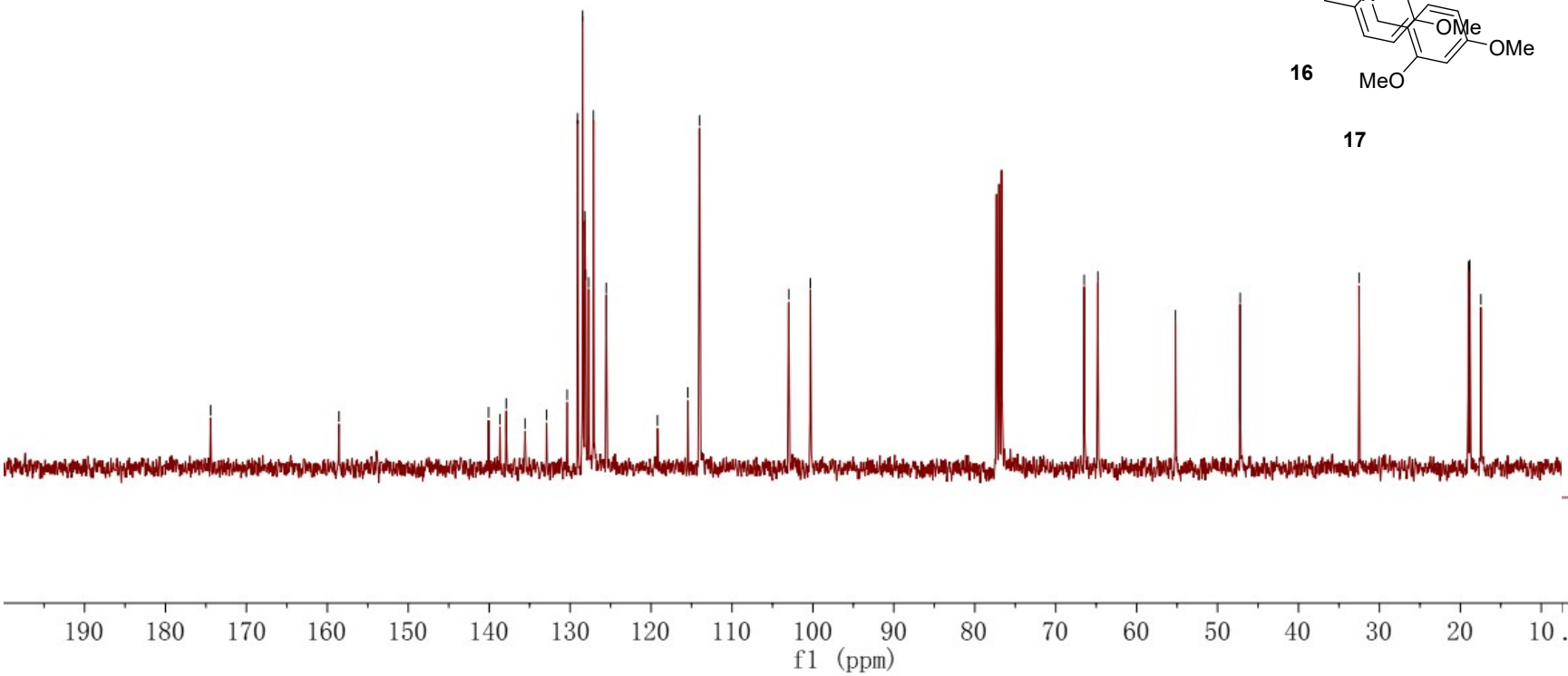
SM-1

7.4392
7.4347
7.4298
7.4228
7.4186
7.4149
7.3750
7.3693
7.3553
7.3531
7.3491



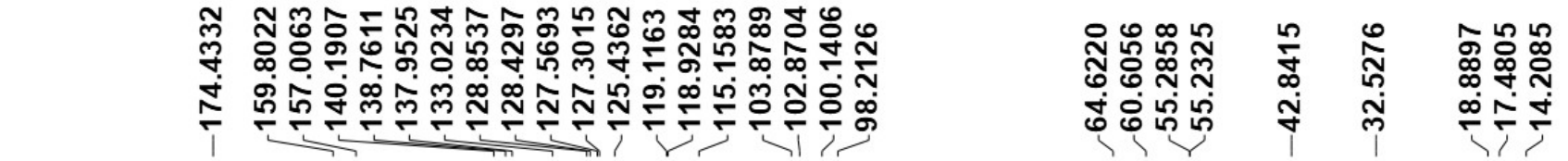
16

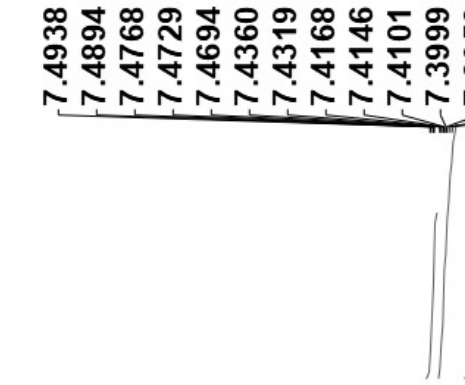
17

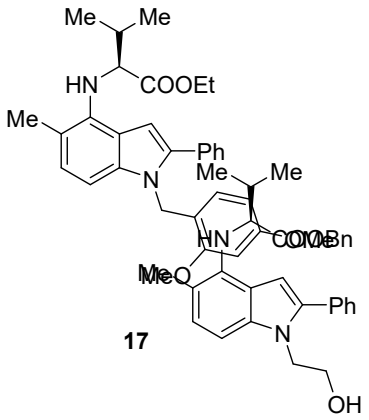


Dmb-13C

W1062

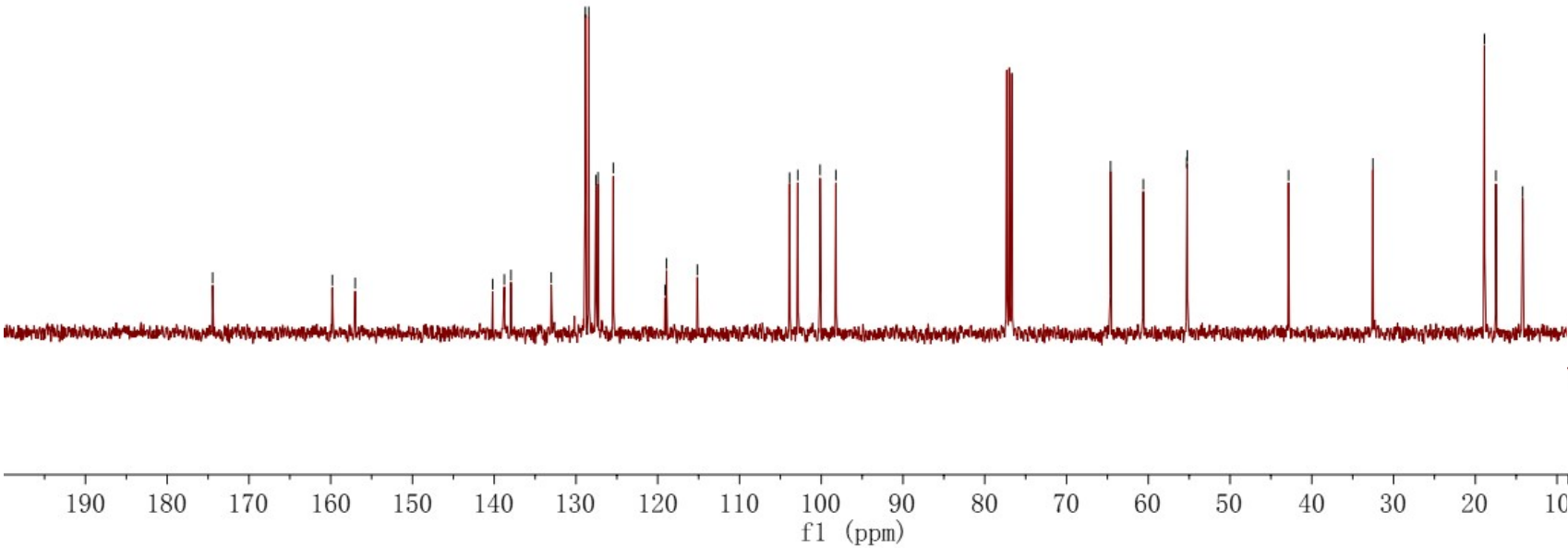


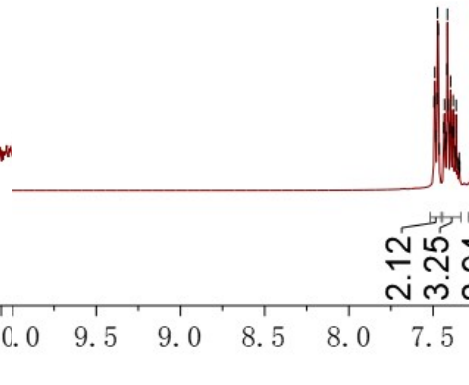


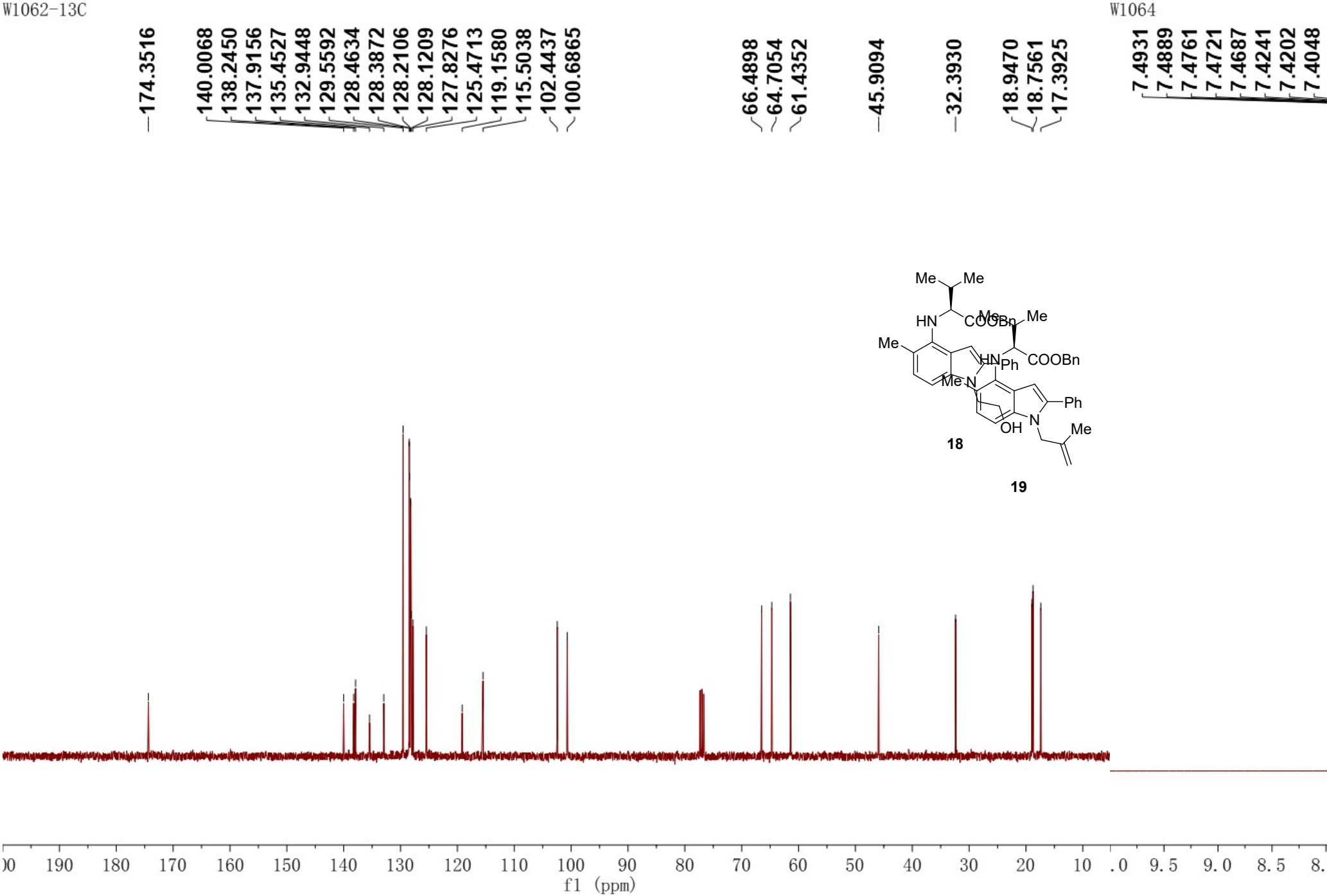


17

18

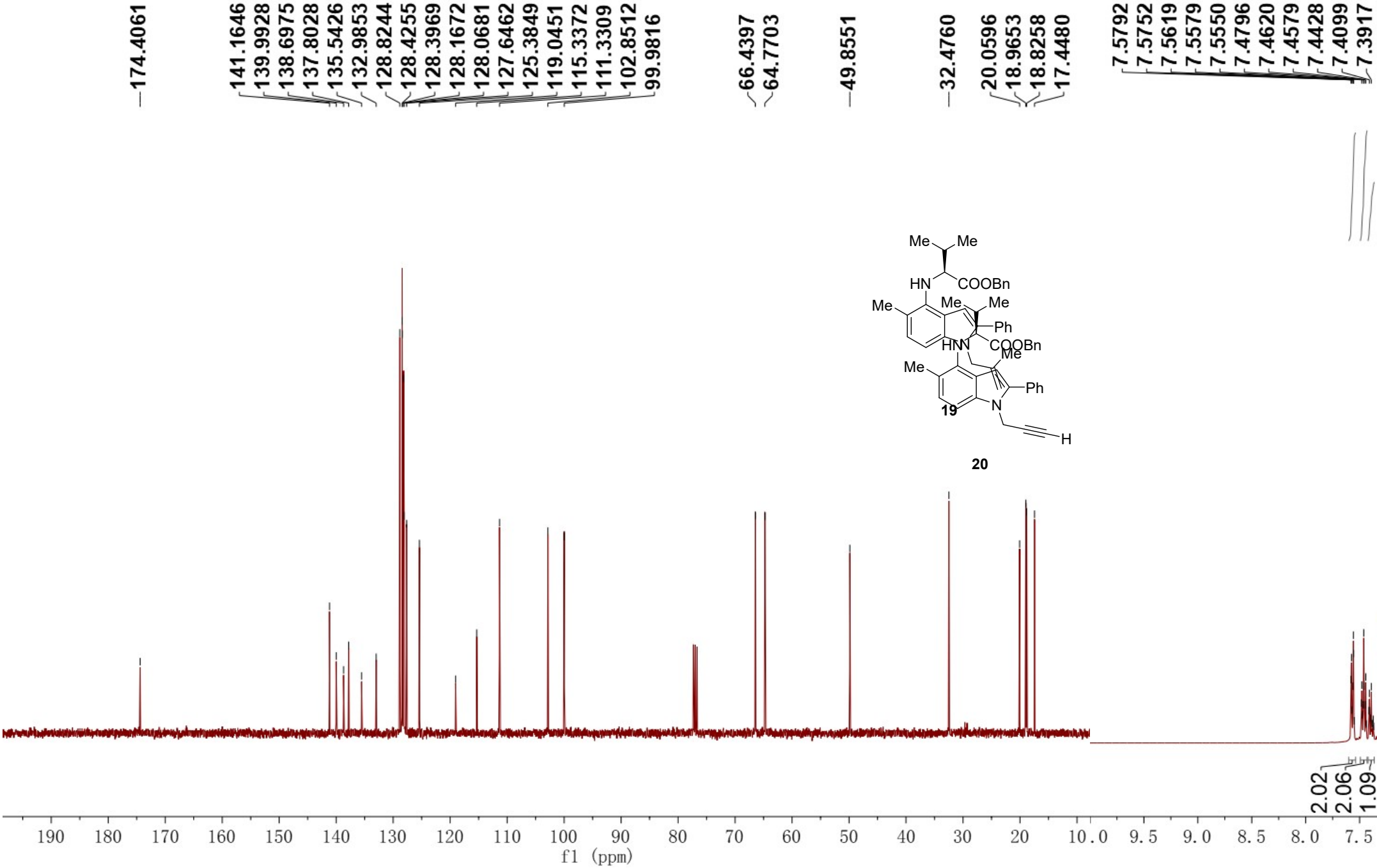


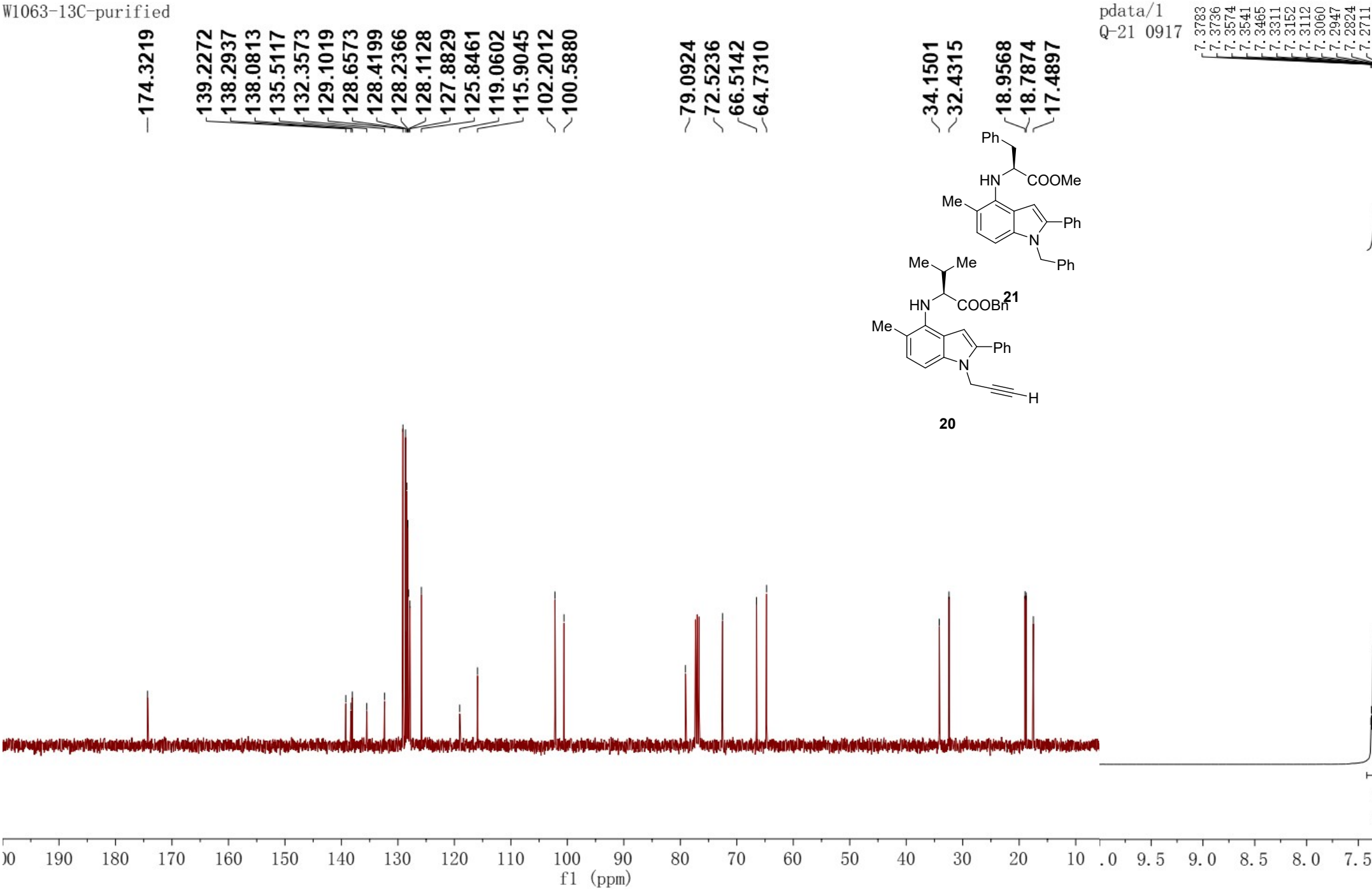


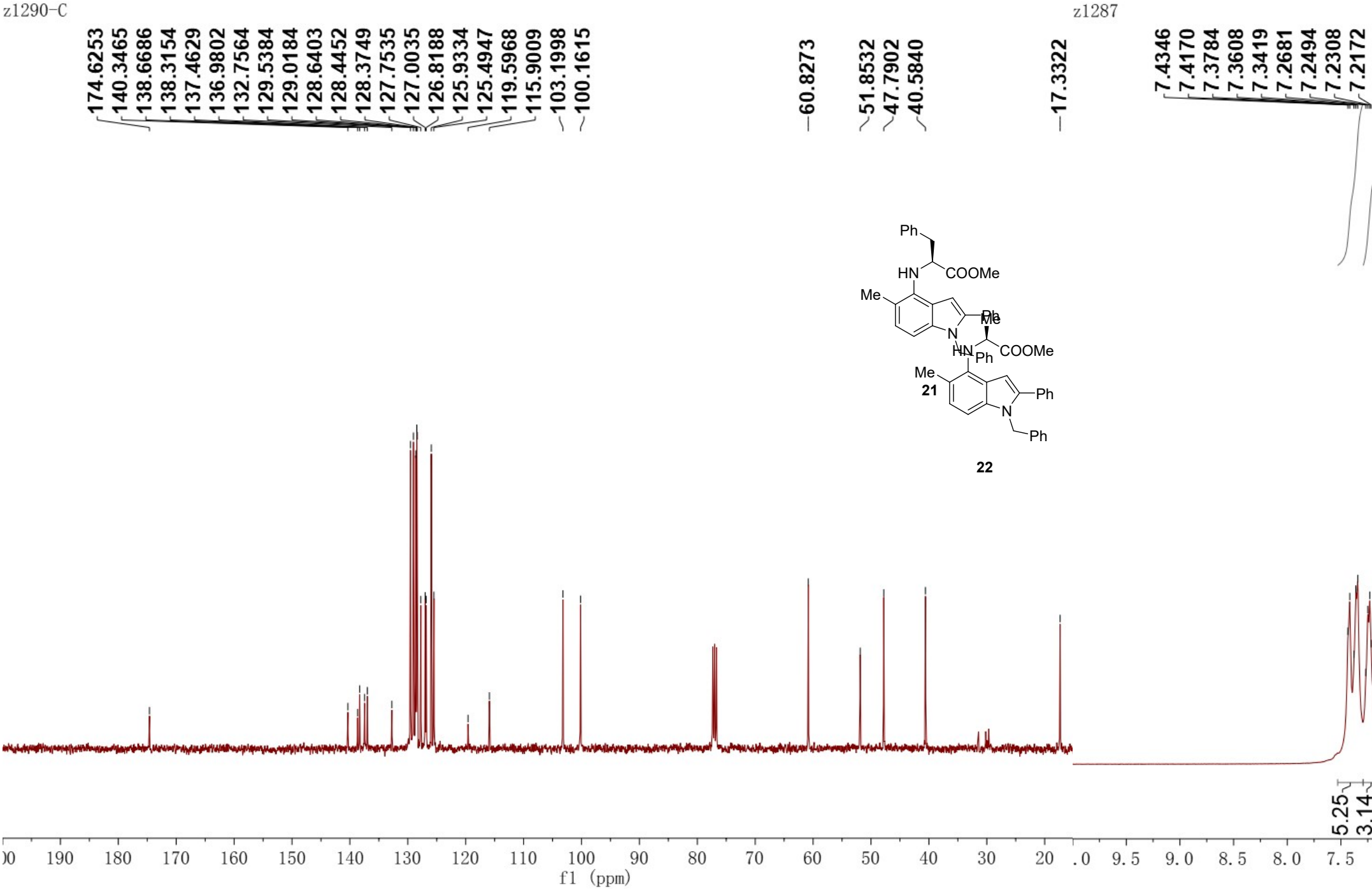

W1062-13C
174.3516
140.0068
138.2450
137.9156
135.4527
132.9448
129.5592
128.4634
128.3872
128.2106
128.1209
127.8276
125.4713
119.1580
115.5038
102.4437
100.6865
66.4898
64.7054
61.4352
45.9094
32.3930
18.9470
18.7561
17.3925
W1064
7.4931
7.4889
7.4761
7.4721
7.4687
7.4241
7.4202
7.4048
7.4027
7.3984
Me
Me
HN
COOBn
Me
Me
HN
Ph
COOBn
Me
N
Ph
OH
N
Me
18
19
2.01
f1 (ppm)

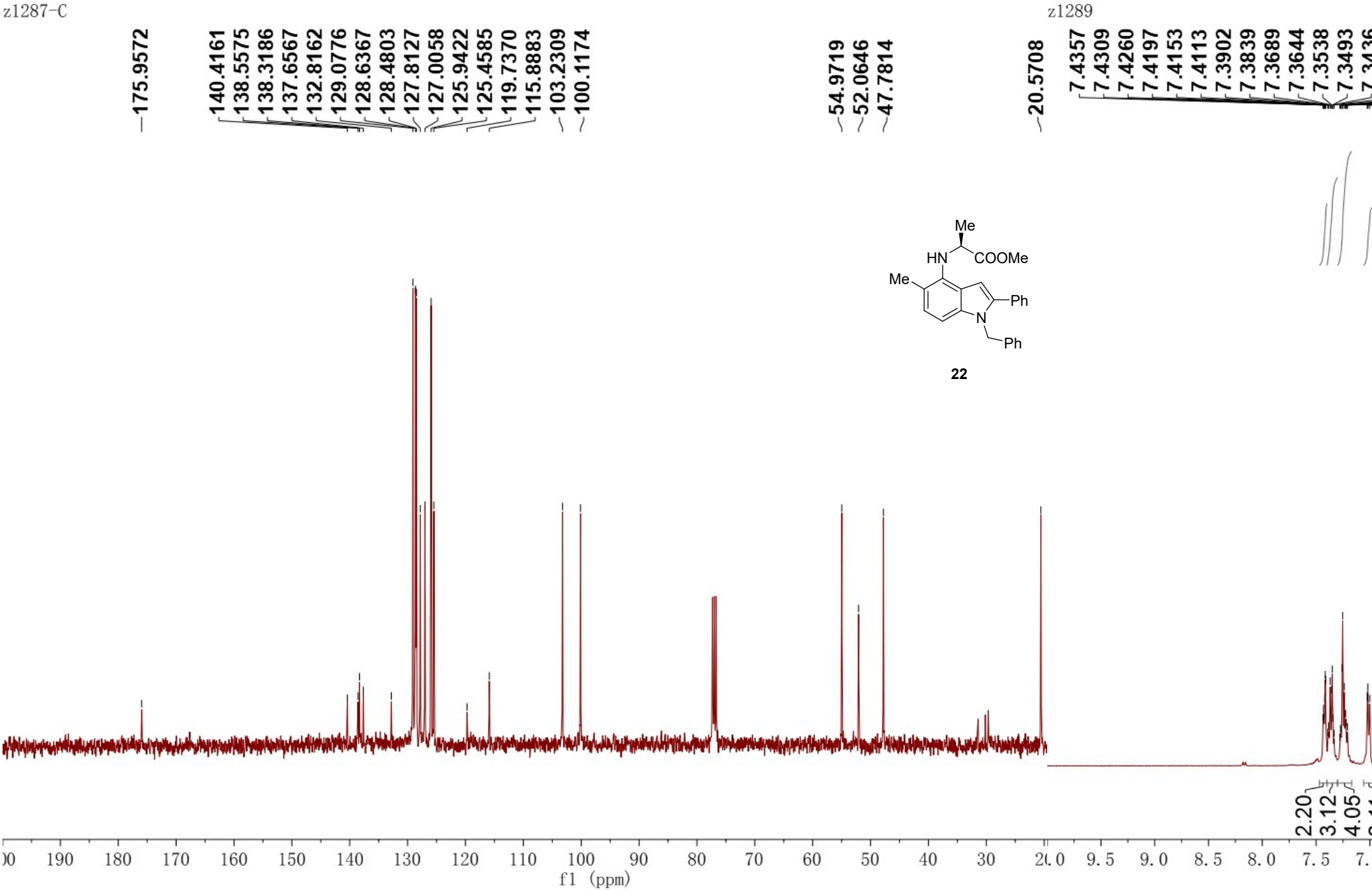
W1064-13C

W1063-2

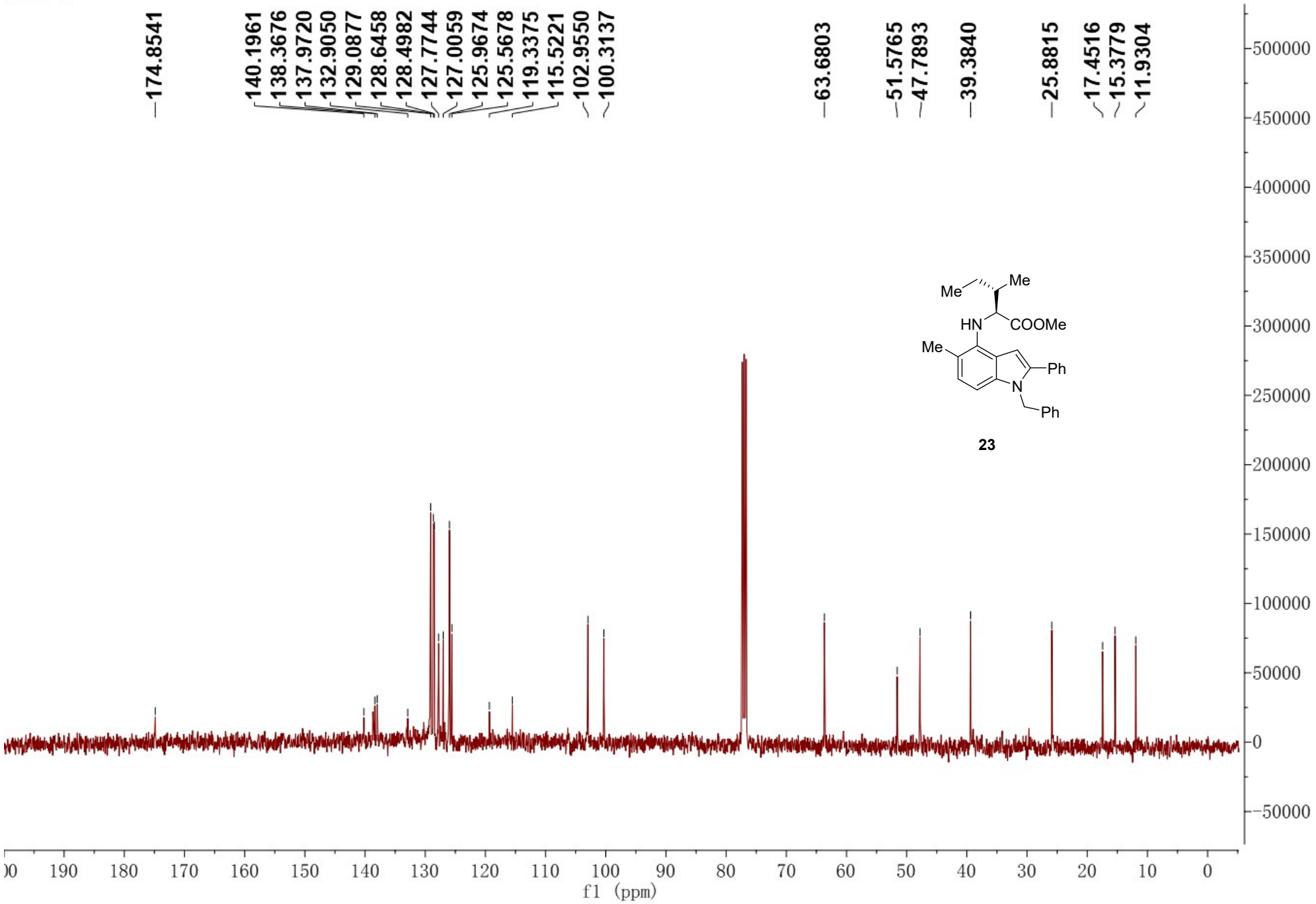



W1063-13C-purified
pdata/1
Q-21 0917
174.3219
139.2272
138.2937
138.0813
135.5117
132.3573
129.1019
128.6573
128.4199
128.2366
128.1128
127.8829
125.8461
119.0602
115.9045
102.2012
100.5880
79.0924
72.5236
66.5142
64.7310
34.1501
32.4315
18.9568
18.7874
17.4897
7.3783
7.3736
7.3574
7.3541
7.3465
7.3311
7.3152
7.3112
7.3060
7.2947
7.2824
7.2711
Ph
HN
COOMe
Me
Ph
N
Ph
Me
Me
HN
COOBn
21
Me
Ph
N
H
20
f1 (ppm)

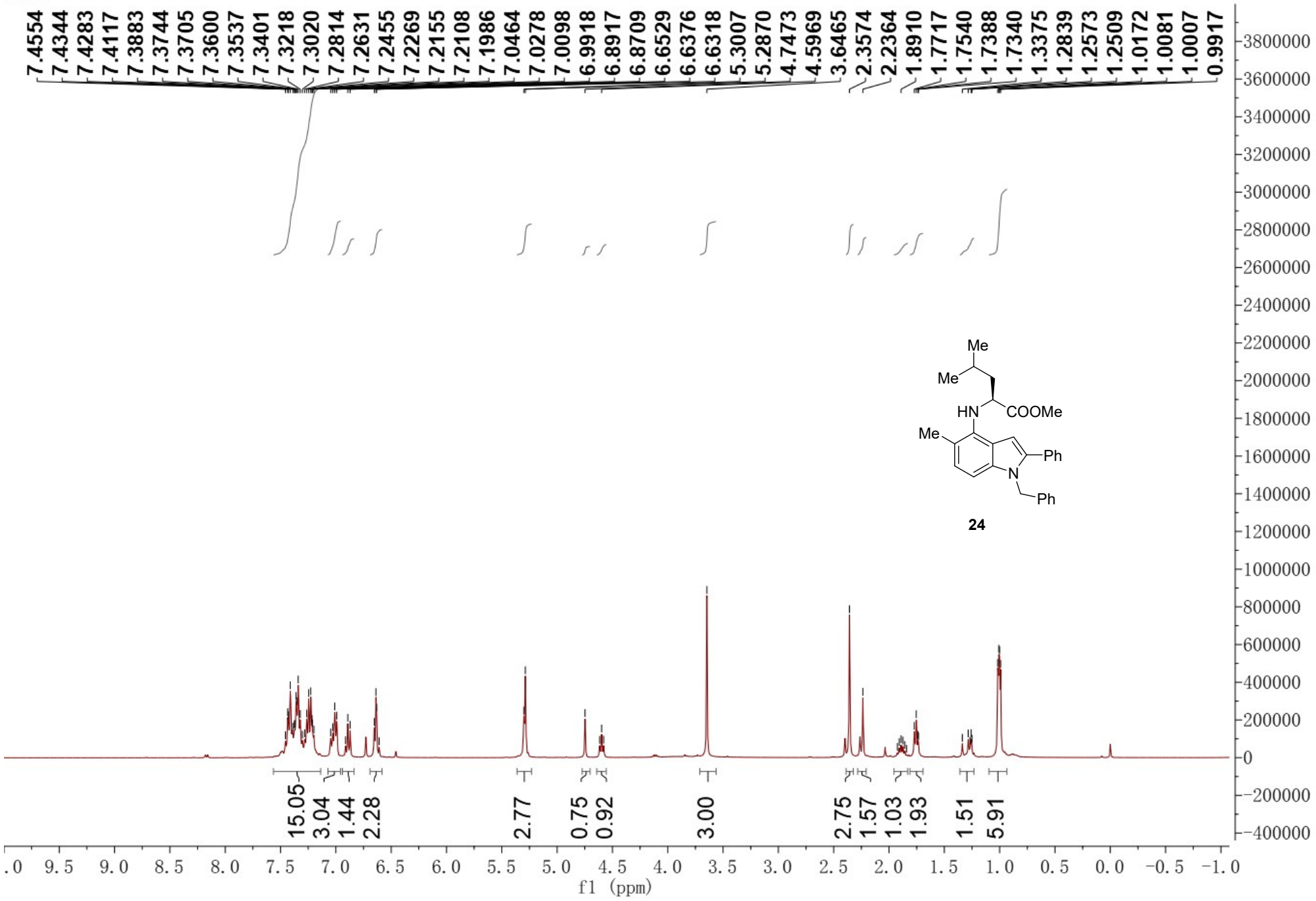

z1290-C
174.6253
140.3465
138.6686
138.3154
137.4629
136.9802
132.7564
129.5384
129.0184
128.6403
128.4452
128.3749
127.7535
127.0035
126.8188
125.9334
125.4947
119.5968
115.9009
103.1998
100.1615
60.8273
51.8532
47.7902
40.5840
17.3322
z1287
7.4346
7.4170
7.3784
7.3608
7.3419
7.2681
7.2494
7.2308
7.2172
Ph
HN
COOMe
Me
N
Ph
Me
HN
Ph
COOMe
Me
21
Ph
N
Ph
22
5.25
3.14
f1 (ppm)


z1287-C
175.9572
140.4161
138.5575
138.3186
137.6567
132.8162
129.0776
128.6367
128.4803
127.8127
127.0058
125.9422
125.4585
119.7370
115.8883
103.2309
100.1174
54.9719
52.0646
47.7814
20.5708
z1289
7.4357
7.4309
7.4260
7.4197
7.4153
7.4113
7.3902
7.3839
7.3689
7.3644
7.3538
7.3493
Me
HN
COOMe
Me
Ph
N
Ph
22
2.20
3.12
4.05
f1 (ppm)

z1289-C


174.8541
140.1961
138.3676
137.9720
132.9050
129.0877
128.6458
128.4982
127.7744
127.0059
125.9674
125.5678
119.3375
115.5221
102.9550
100.3137
63.6803
51.5765
47.7893
39.3840
25.8815
17.4516
15.3779
11.9304
Me
Me
HN
COOMe
Me
Ph
N
Ph
23
f1 (ppm)

z1288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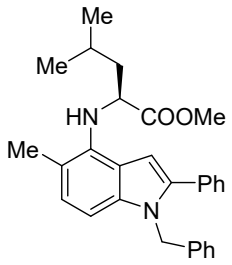
7.4283
7.4117
7.3883
7.3744
7.3705
7.3600
7.3537
7.3401
7.3218
7.3020
7.2814
7.2631
7.2455
7.2269
7.2155
7.2108
7.1986
7.0464
7.0278
7.0098
6.9918
6.8917
6.8709
6.6529
6.6376
6.6318
5.3007
5.2870
4.7473
4.5969
3.6465
2.3574
2.2364
1.8910
1.7717
1.7540
1.7388
1.7340
1.3375
1.2839
1.2573
1.2509
1.0172
1.0081
1.0007
0.9917
15.05
3.04
1.44
2.28
2.77
0.75
0.92
3.00
2.75
1.57
1.03
1.93
1.51
5.91
f1 (ppm)

Me
Me
HN
COOMe
Me
Ph
N
Ph

24

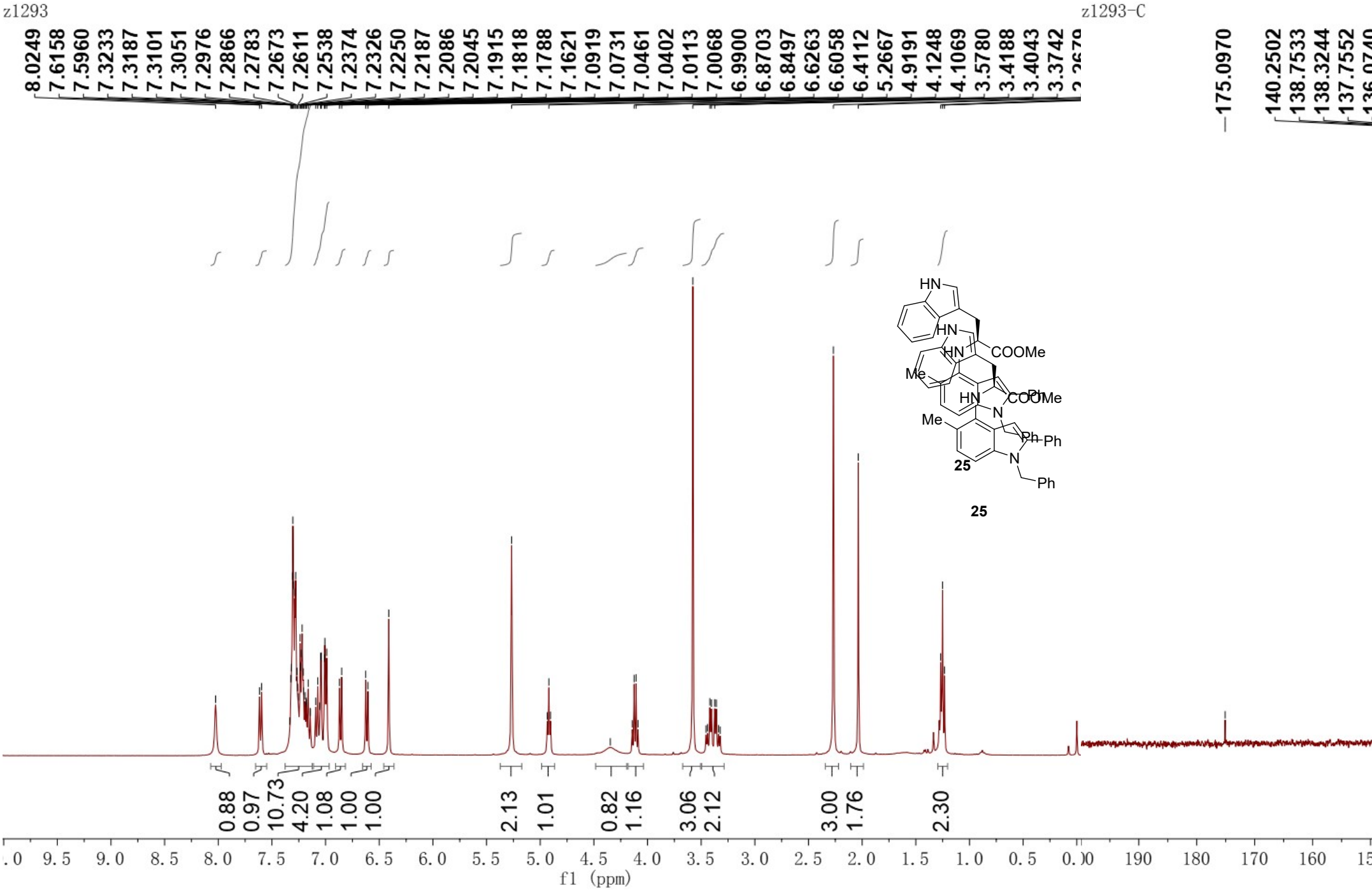
z1288-C

175.8211
140.2930
139.6402
138.9868
138.6629
138.3537
137.7719
132.8844
130.2441
129.0495
129.0151
128.6279
128.4857
127.7913
127.7574
127.7024
127.4367
127.2153
126.9905
126.7726
125.9434
125.5058
125.4332
120.5992
119.5459
116.3510
115.7129
114.0179
113.5424
103.1747
101.9713
100.9613
100.1676
58.1415
52.1208
51.8046
47.7863
43.9847
25.0547
22.8252
22.7204
17.5832
17.4846

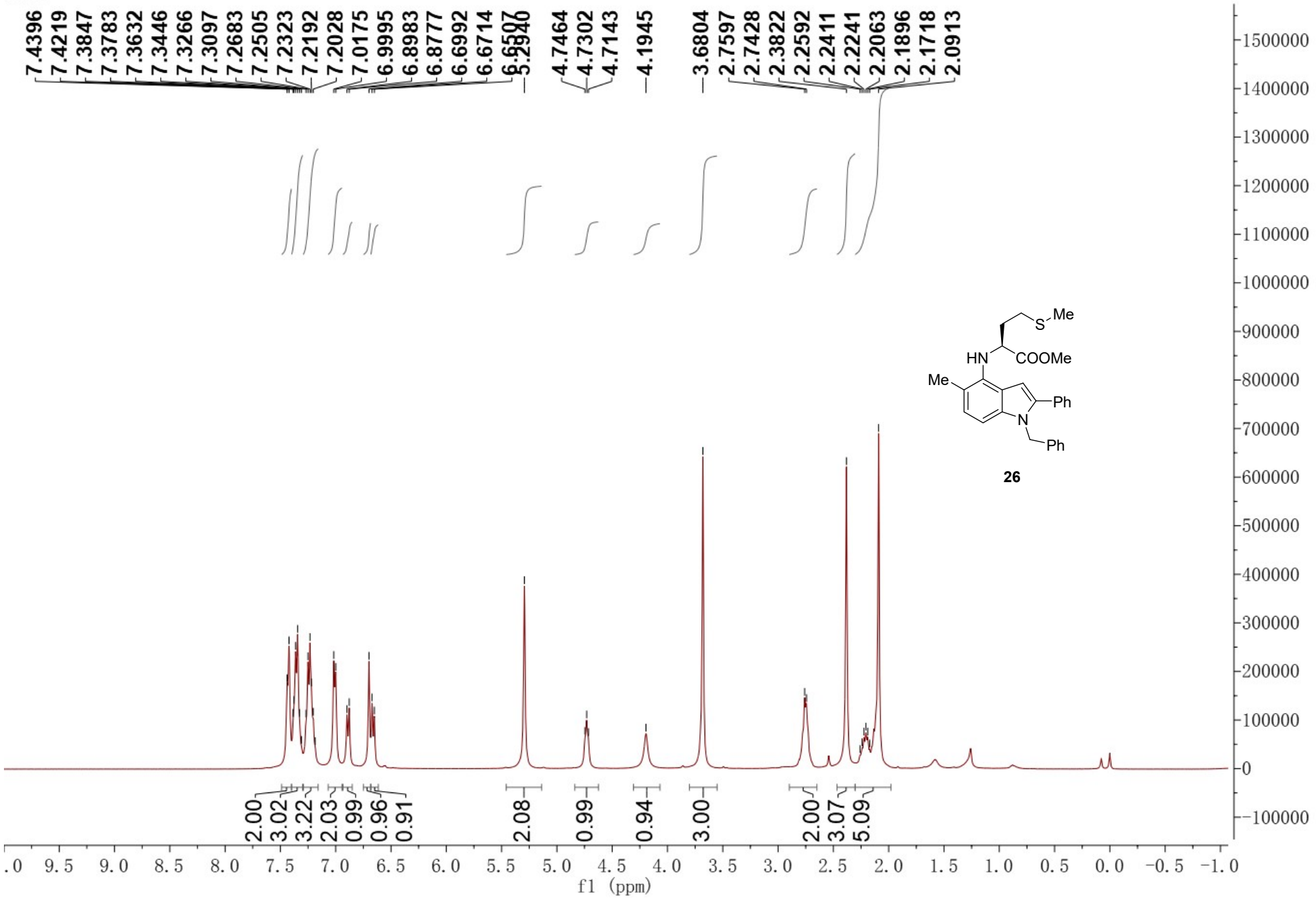


24

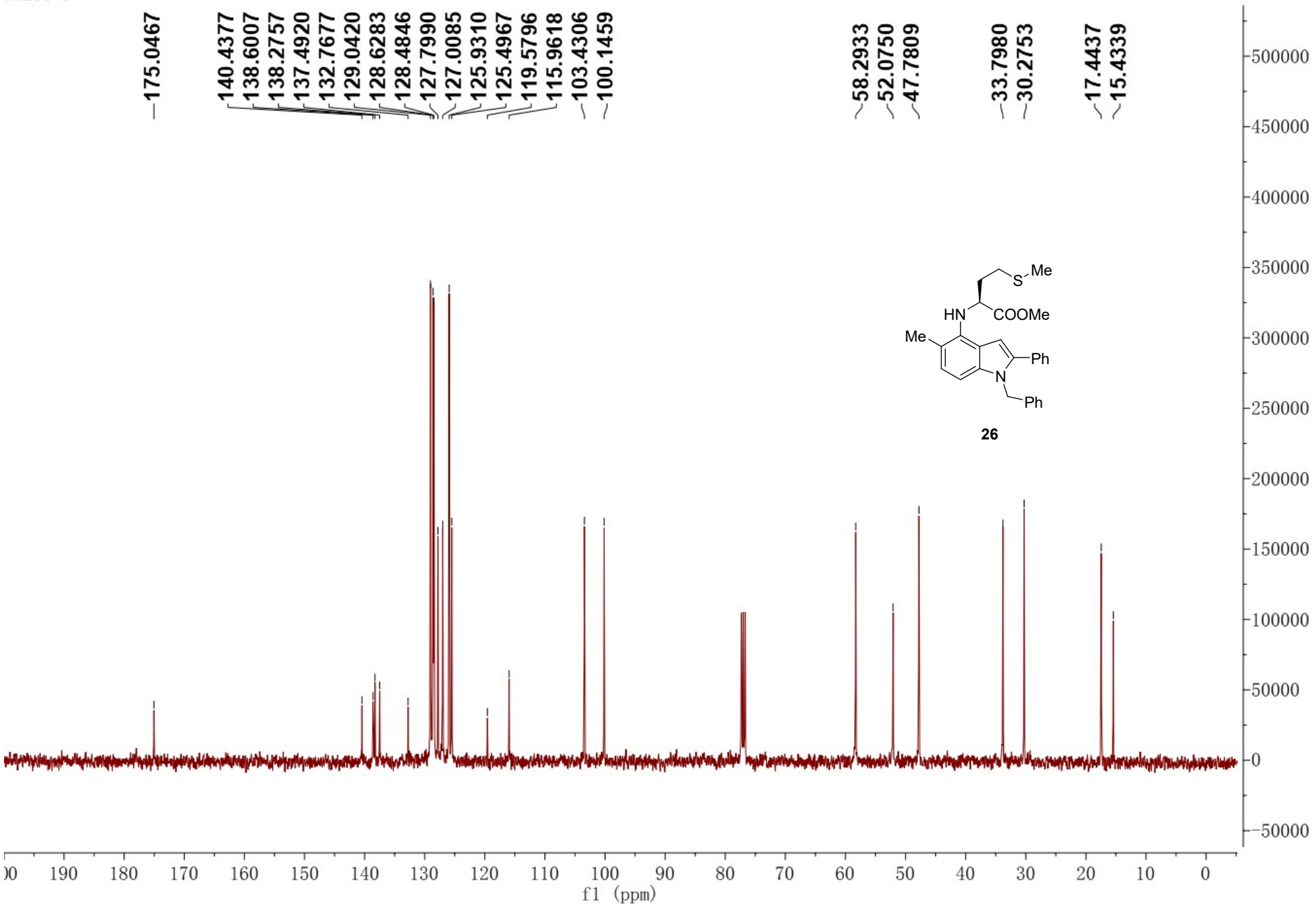
f1 (ppm)

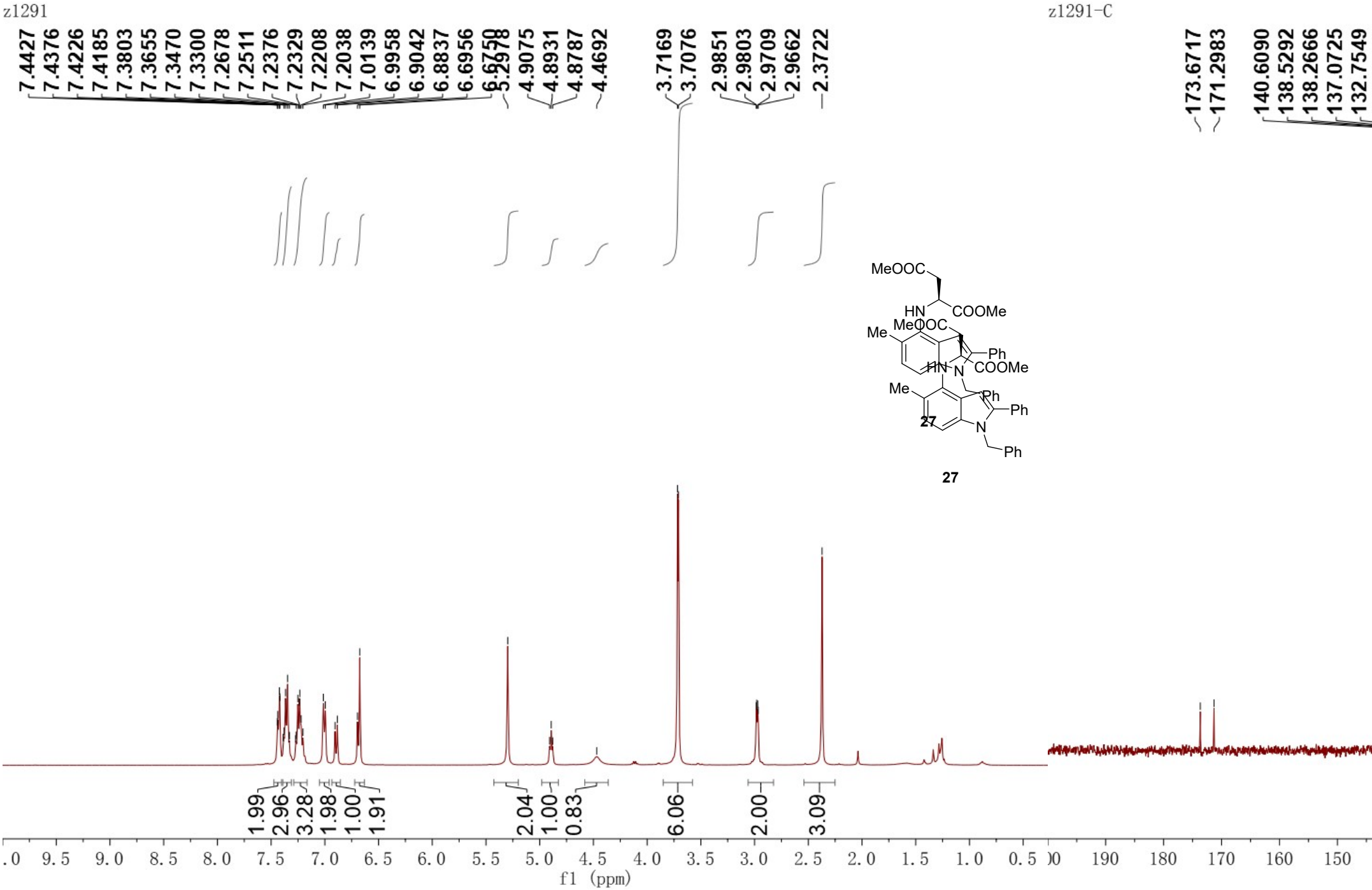

z1293
z1293-C
8.0249
7.6158
7.5960
7.3233
7.3187
7.3101
7.3051
7.2976
7.2866
7.2783
7.2673
7.2611
7.2538
7.2374
7.2326
7.2250
7.2187
7.2086
7.2045
7.1915
7.1818
7.1788
7.1621
7.0919
7.0731
7.0461
7.0402
7.0113
7.0068
6.9900
6.8703
6.8497
6.6263
6.6058
6.4112
5.2667
4.9191
4.1248
4.1069
3.5780
3.4188
3.4043
3.3742
175.0970
140.2502
138.7533
138.3244
137.7552
HN
HN
HN
COOMe
Me
HN
COOMe
Ph
N
Me
Ph
Ph
N
Ph
25
0.88
0.97
10.73
4.20
1.08
1.00
1.00
2.13
1.01
0.82
1.16
3.06
2.12
3.00
1.76
2.30
f1 (ppm)

25

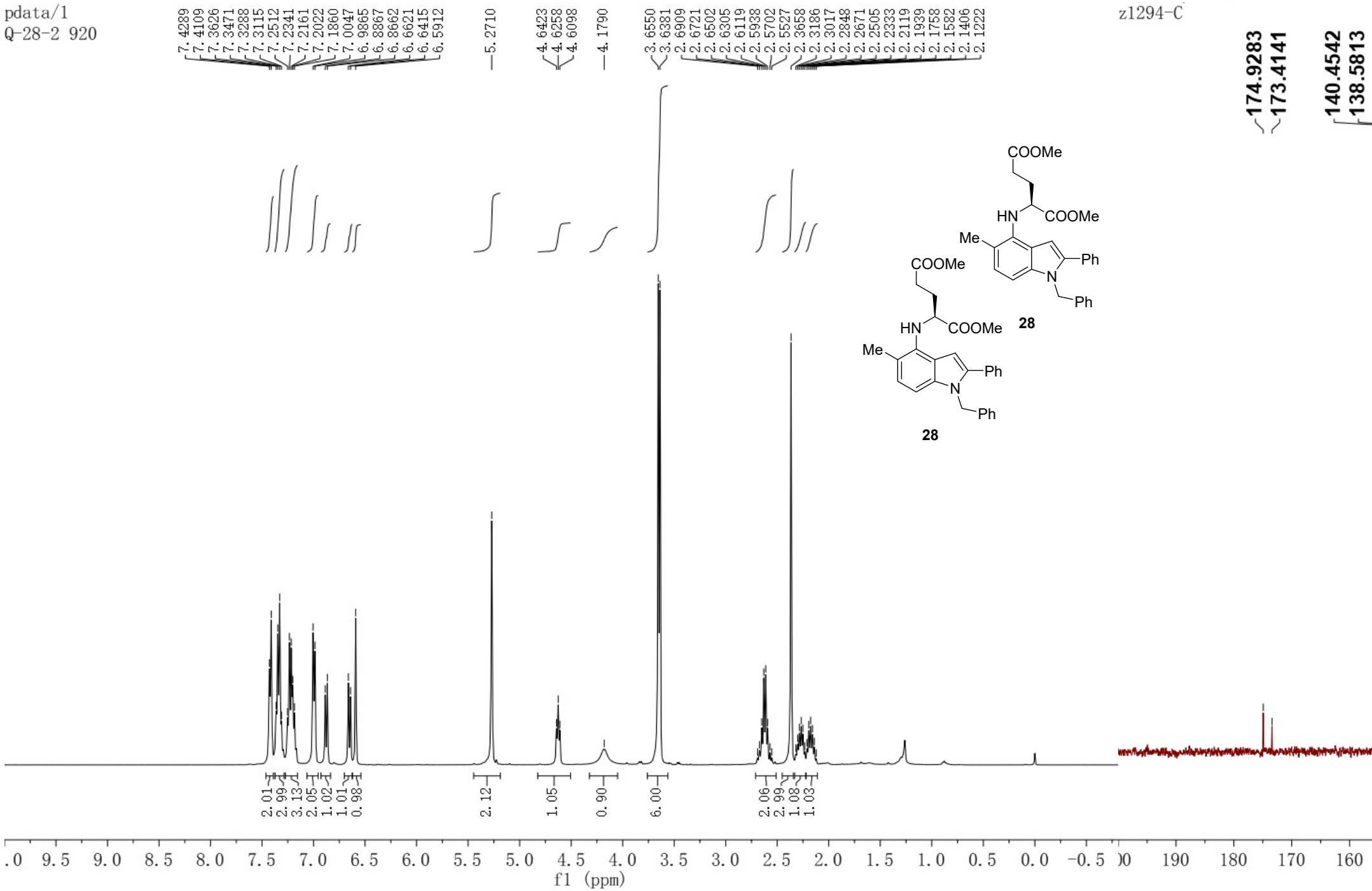

z1281
7.4396
7.4219
7.3847
7.3783
7.3632
7.3446
7.3266
7.3097
7.2683
7.2505
7.2323
7.2192
7.2028
7.0175
6.9995
6.8983
6.8777
6.6992
6.6714
6.6507
5.2940
4.7464
4.7302
4.7143
4.1945
3.6804
2.7597
2.7428
2.3822
2.2592
2.2411
2.2241
2.2063
2.1896
2.1718
2.0913
S
Me
HN
COOMe
Me
Ph
N
Ph
26
2.00
3.02
3.22
2.03
0.99
0.96
0.91
2.08
0.99
0.94
3.00
2.00
3.07
5.09
f1 (ppm)

z1281-C

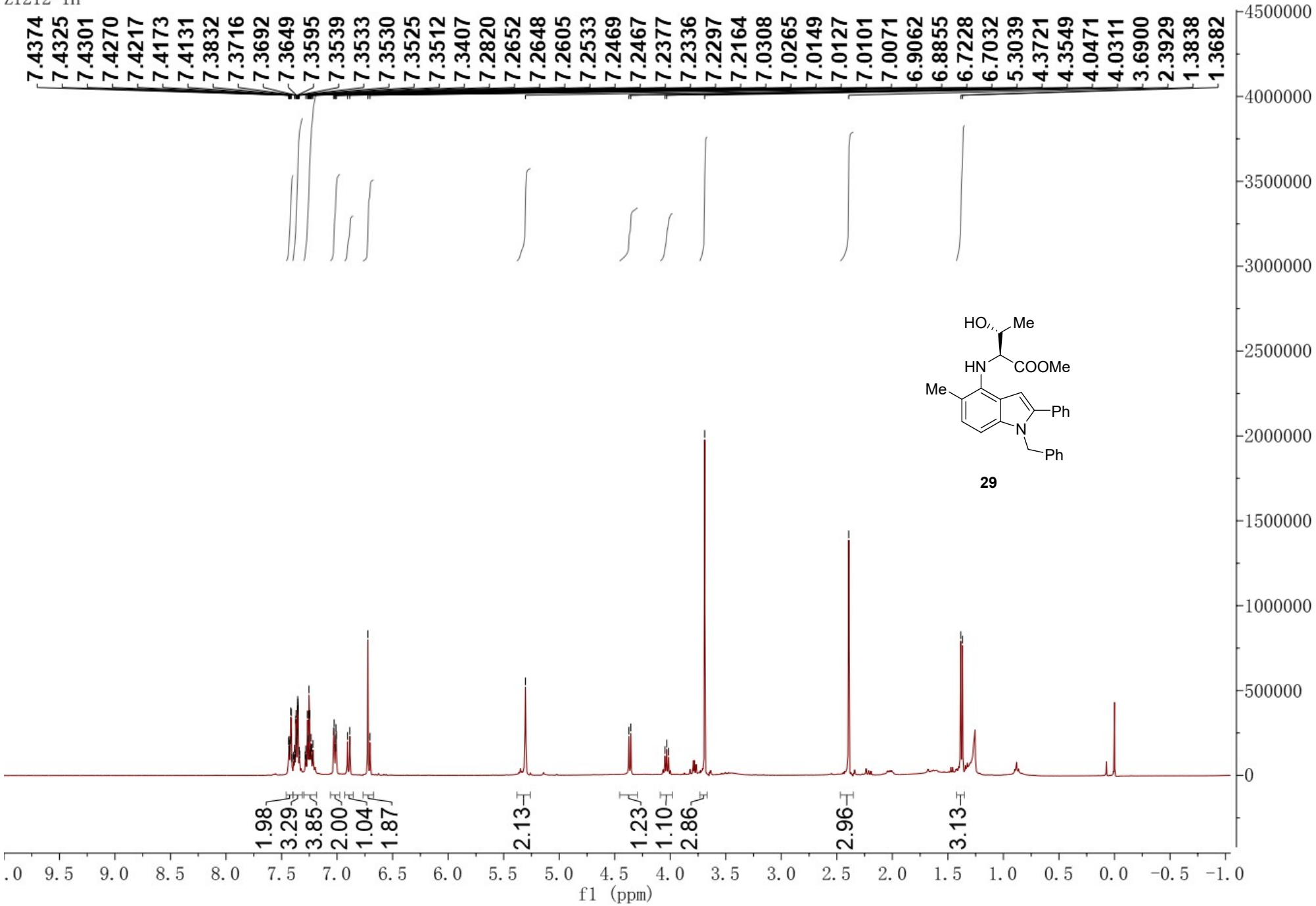

175.0467
140.4377
138.6007
138.2757
137.4920
132.7677
129.0420
128.6283
128.4846
127.7990
127.0085
125.9310
125.4967
119.5796
115.9618
103.4306
100.1459
58.2933
52.0750
47.7809
33.7980
30.2753
17.4437
15.4339
S
Me
HN
COOMe
Me
Ph
N
Ph
26
f1 (ppm)


z1291
z1291-C
7.4427
7.4376
7.4226
7.4185
7.3803
7.3655
7.3470
7.3300
7.2678
7.2511
7.2376
7.2329
7.2208
7.2038
7.0139
6.9958
6.9042
6.8837
6.6956
4.9075
4.8931
4.8787
4.4692
3.7169
3.7076
2.9851
2.9803
2.9709
2.9662
2.3722
173.6717
171.2983
140.6090
138.5292
138.2666
137.0725
132.7549
MeOOC
HN
COOMe
Me
MeOOC
Ph
HN
N
COOMe
Me
Ph
Ph
N
Ph
27
1.99
2.96
3.28
1.98
1.00
1.91
2.04
1.00
0.83
6.06
2.00
3.09
f1 (ppm)

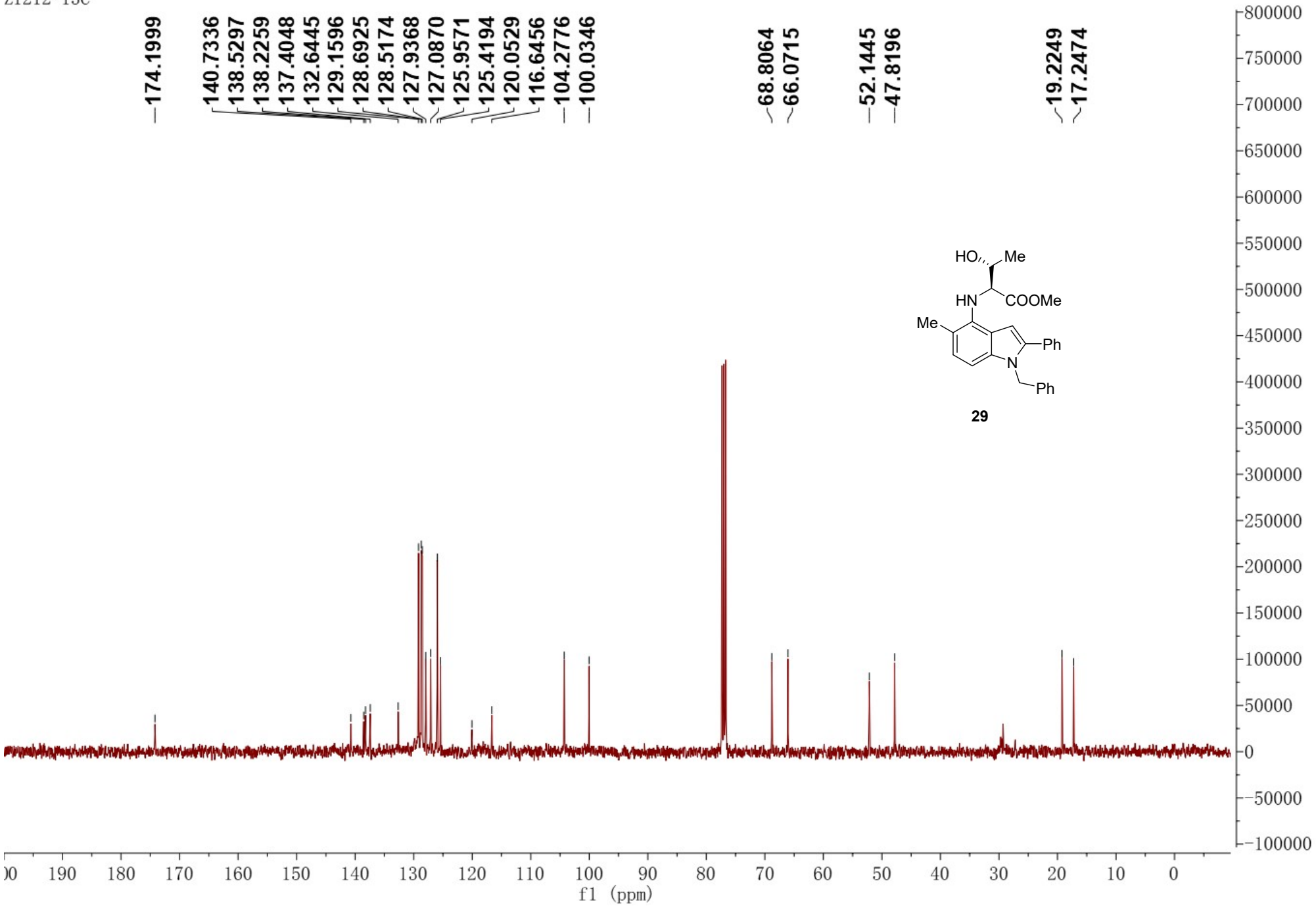
27

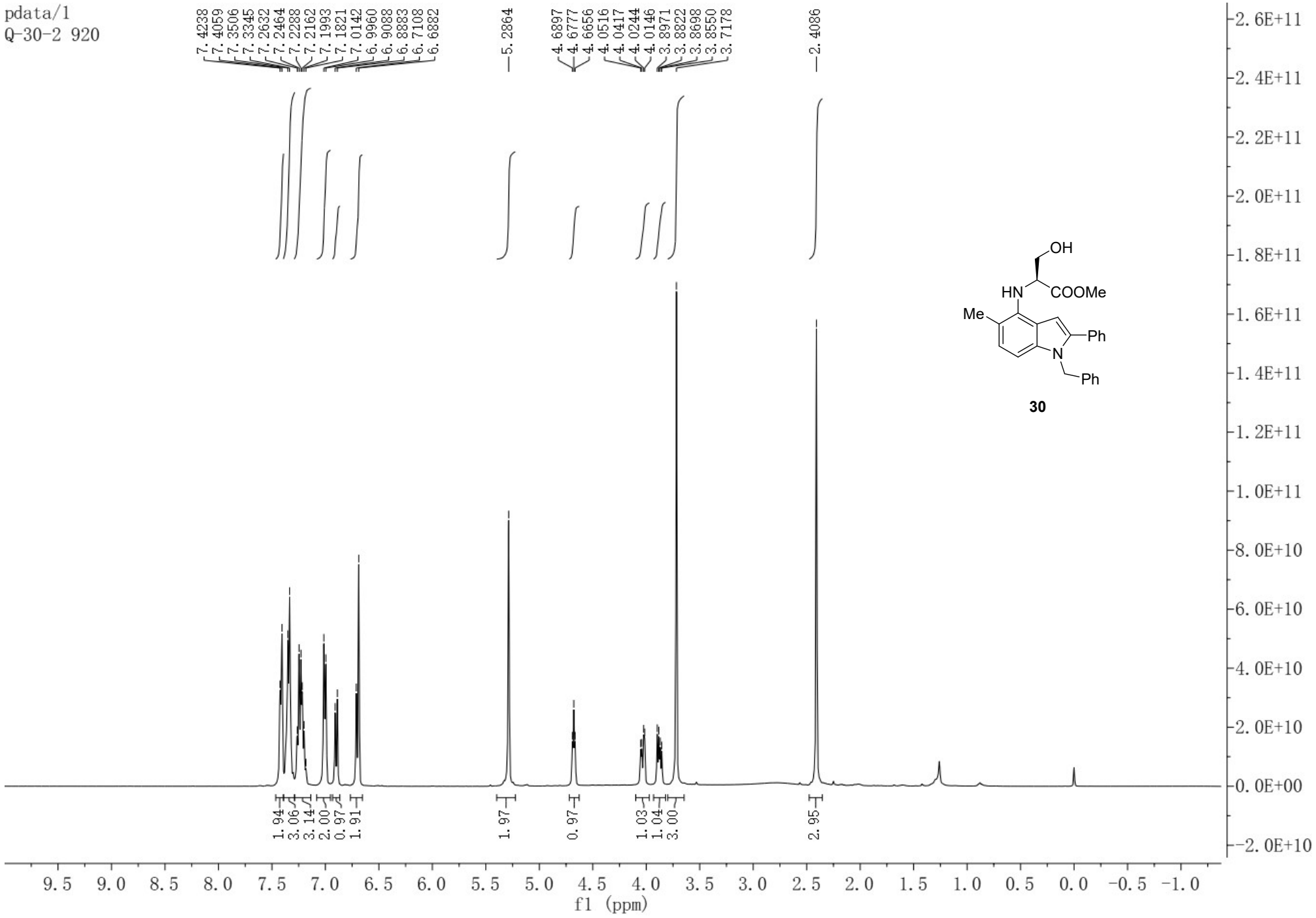

pdata/1
Q-28-2 920
z1294-C
7.4289
7.4109
7.3626
7.3471
7.3288
7.3115
7.2512
7.2341
7.2161
7.2022
7.1860
7.0047
6.9865
6.8867
6.8662
6.6621
6.6415
6.5912
5.2710
4.6423
4.6258
4.6098
4.1790
3.6550
3.6381
2.6909
2.6721
2.6502
2.6305
2.6119
2.5938
2.5702
2.5527
2.3658
2.3186
2.3017
2.2848
2.2671
2.2505
2.2333
2.2119
2.1939
2.1758
2.1582
2.1406
2.1222
174.9283
173.4141
140.4542
138.5813
COOMe
HN
COOMe
Me
Ph
N
Ph
28
2.01
2.99
3.13
2.05
1.02
1.01
0.98
2.12
1.05
0.90
6.00
2.06
2.99
1.08
1.03
f1 (ppm)

Z1212-1H

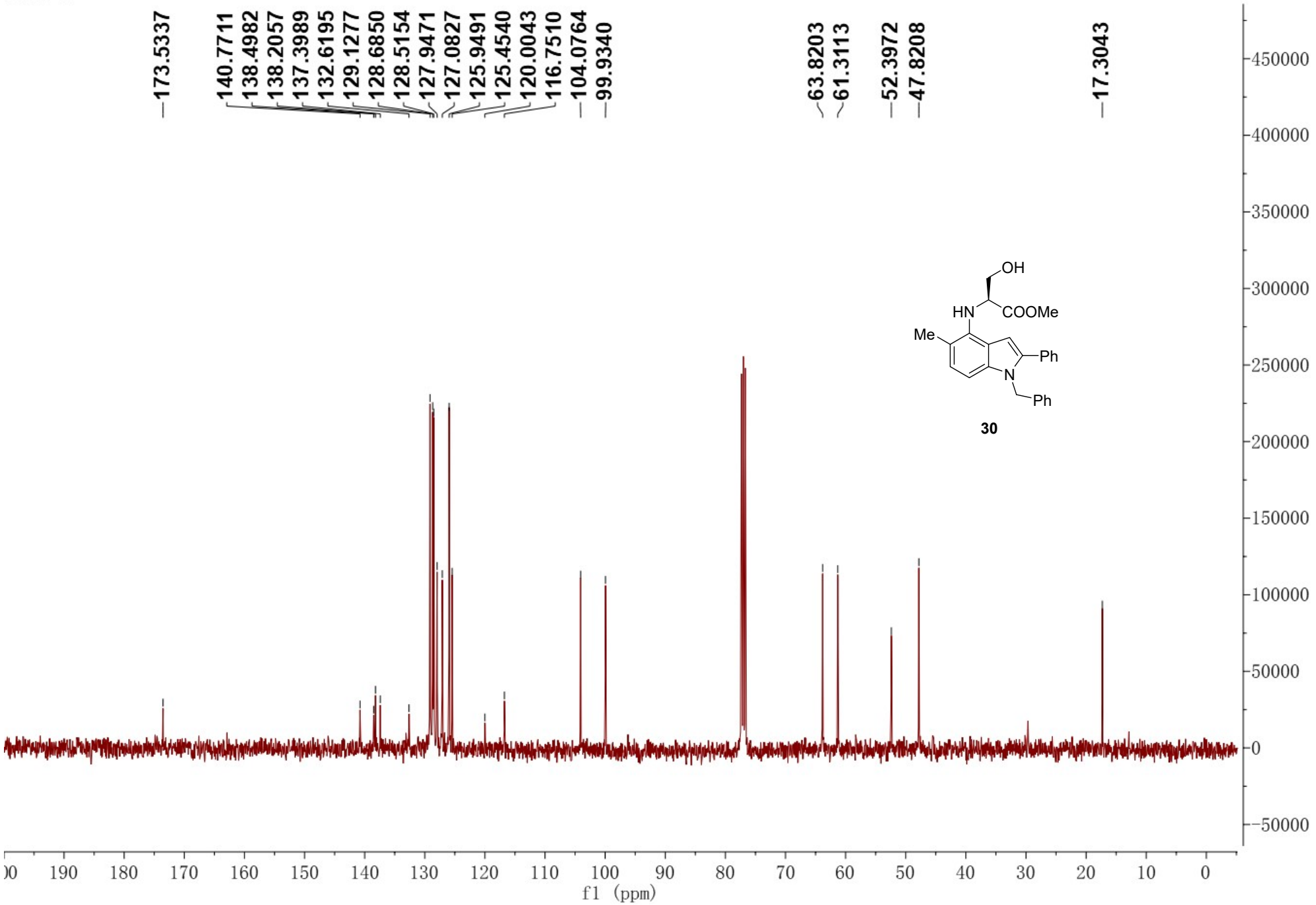

7.4374
7.4325
7.4301
7.4270
7.4217
7.4173
7.4131
7.3832
7.3716
7.3692
7.3649
7.3595
7.3539
7.3533
7.3530
7.3525
7.3512
7.3407
7.2820
7.2652
7.2648
7.2605
7.2533
7.2469
7.2467
7.2377
7.2336
7.2297
7.2164
7.0308
7.0265
7.0149
7.0127
7.0101
7.0071
6.9062
6.8855
6.7228
6.7032
5.3039
4.3721
4.3549
4.0471
4.0311
3.6900
2.3929
1.3838
1.3682
HO
Me
HN
COOMe
Me
Ph
N
Ph
29
1.98
3.29
3.85
2.00
1.04
1.87
2.13
1.23
1.10
2.86
2.96
3.13
f1 (ppm)

Z1212-13C

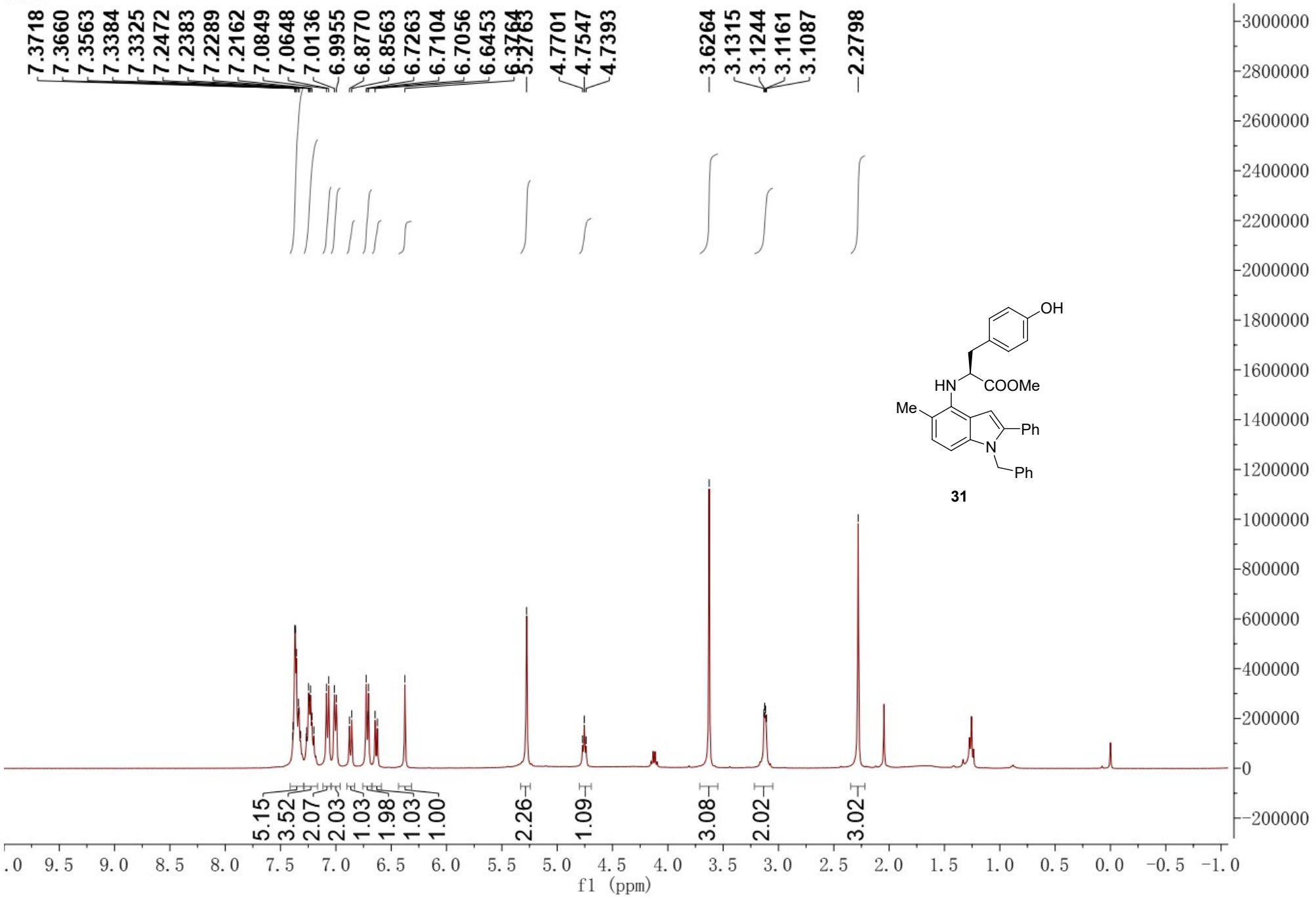

174.1999
140.7336
138.5297
138.2259
137.4048
132.6445
129.1596
128.6925
128.5174
127.9368
127.0870
125.9571
125.4194
120.0529
116.6456
104.2776
100.0346
68.8064
66.0715
52.1445
47.8196
19.2249
17.2474
HO
Me
HN
COOMe
Me
Ph
N
Ph
29
f1 (ppm)


pdata/1
Q-30-2 920
7.4238
7.4059
7.3506
7.3345
7.2632
7.2464
7.2288
7.2162
7.1993
7.1821
7.0142
6.9960
6.9088
6.8883
6.7108
6.6882
5.2864
4.6897
4.6777
4.6656
4.0516
4.0417
4.0244
4.0146
3.8971
3.8822
3.8698
3.8550
3.7178
2.4086
OH
HN
COOMe
Me
Ph
N
Ph
30
1.94
3.06
3.14
2.00
0.97
1.91
1.97
0.97
1.03
1.04
3.00
2.95
2.6E+11
2.4E+11
2.2E+11
2.0E+11
1.8E+11
1.6E+11
1.4E+11
1.2E+11
1.0E+11
8.0E+10
6.0E+10
4.0E+10
2.0E+10
0.0E+00
-2.0E+10
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

z1285-C


173.5337
140.7711
138.4982
138.2057
137.3989
132.6195
129.1277
128.6850
128.5154
127.9471
127.0827
125.9491
125.4540
120.0043
116.7510
104.0764
99.9340
63.8203
61.3113
52.3972
47.8208
17.3043
OH
HN
COOMe
Me
Ph
N
Ph
30
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
−50000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

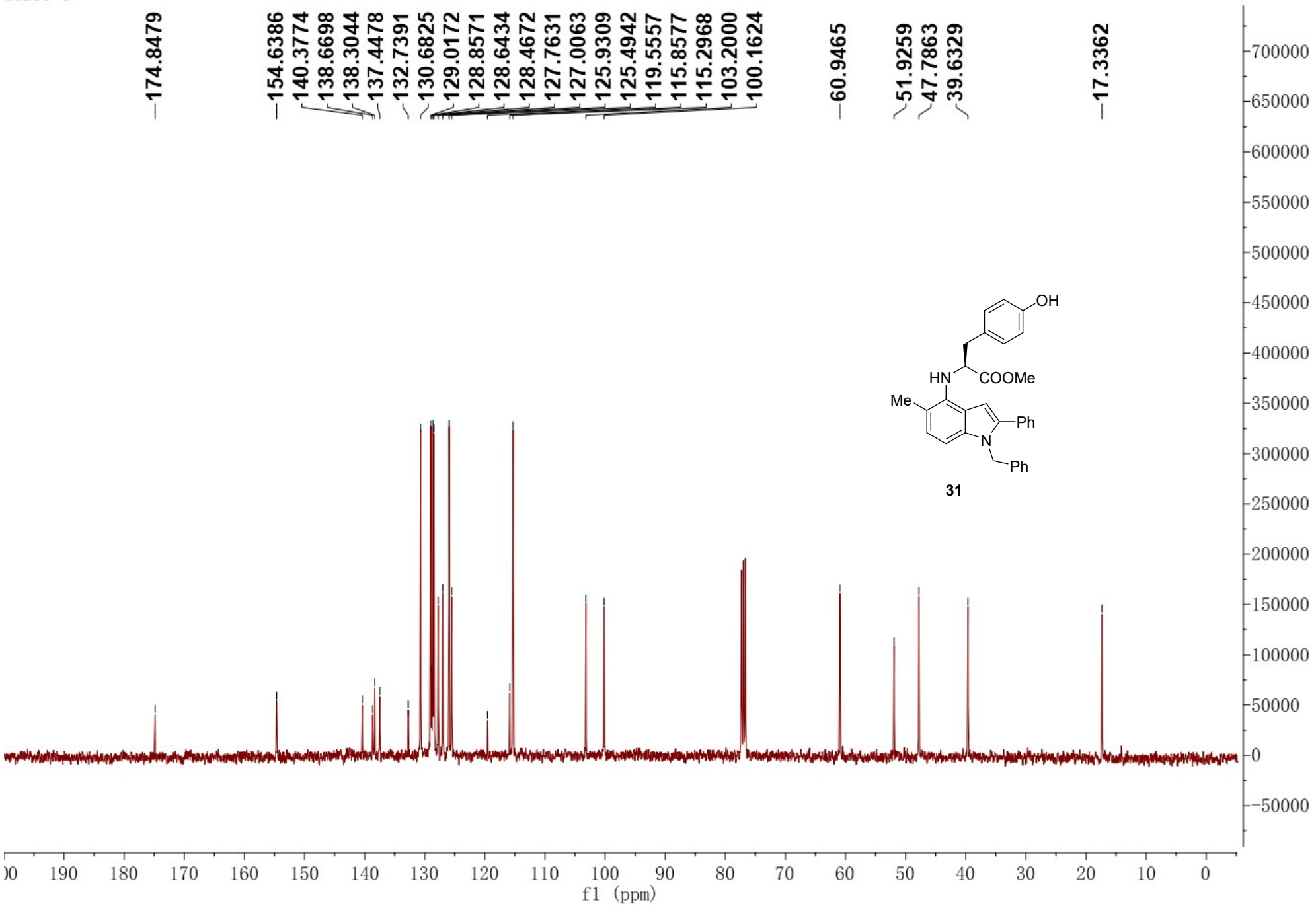
z1283

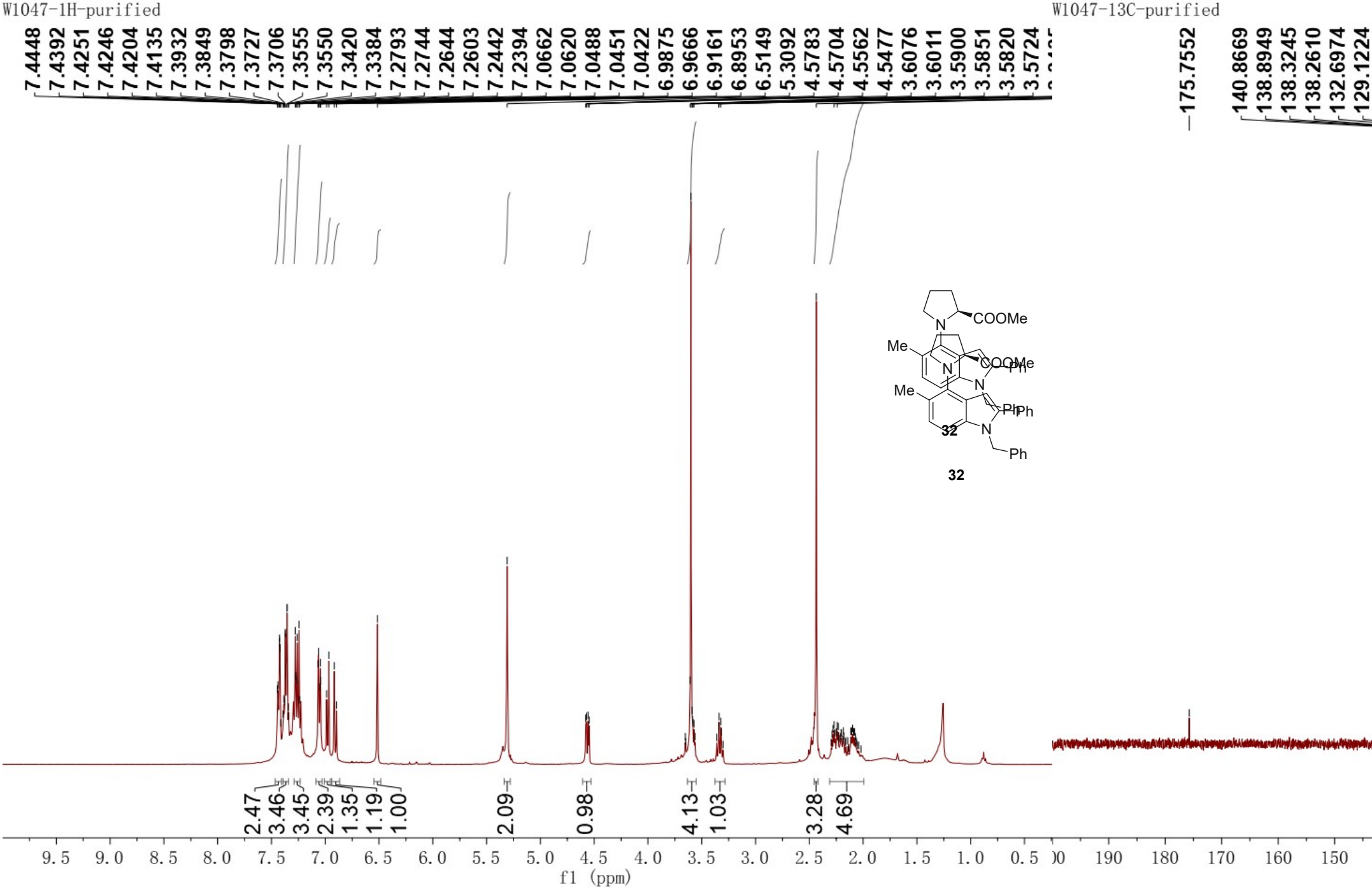

7.3718
7.3660
7.3563
7.3384
7.3325
7.2472
7.2383
7.2289
7.2162
7.0849
7.0648
7.0136
6.9955
6.8770
6.8563
6.7263
6.7104
6.7056
6.6453
5.2763
4.7701
4.7547
4.7393
3.6264
3.1315
3.1244
3.1161
3.1087
2.2798
5.15
3.52
2.07
2.03
1.03
1.98
1.03
1.00
2.26
1.09
3.08
2.02
3.02
f1 (ppm)

OH
HN
COOMe
Me
Ph
N
Ph

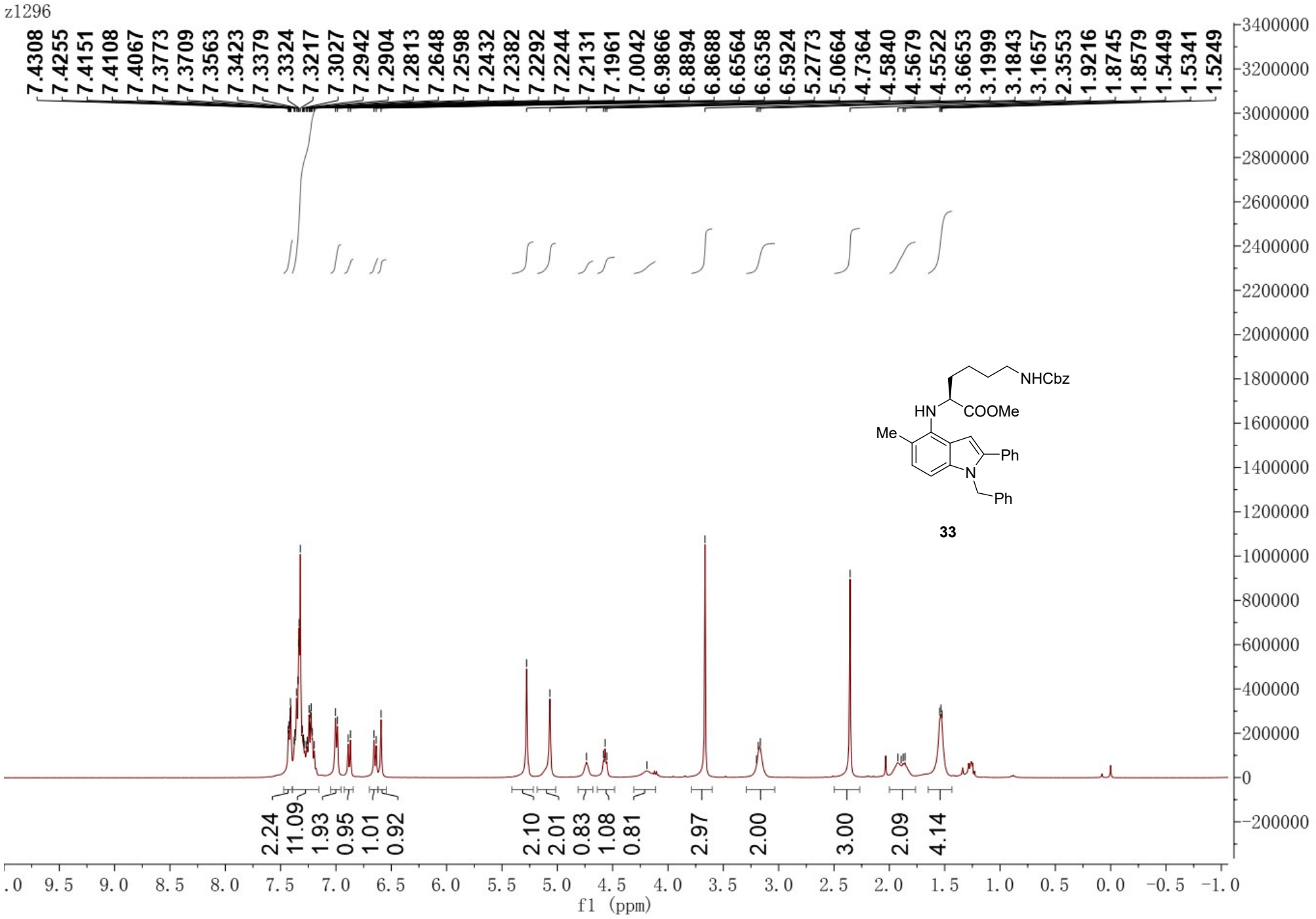
31

z1283-C

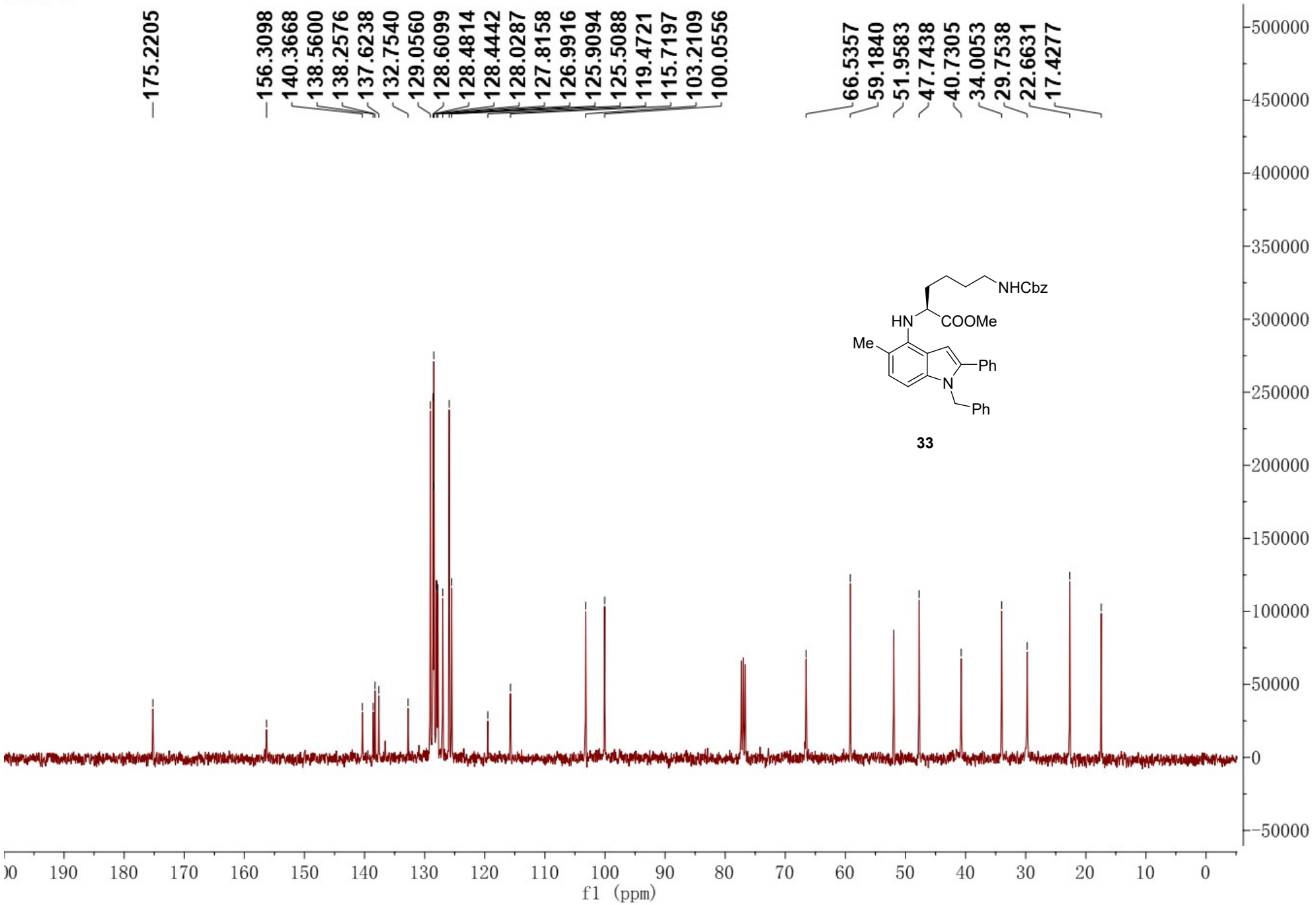

174.8479
154.6386
140.3774
138.6698
138.3044
137.4478
132.7391
130.6825
129.0172
128.8571
128.6434
128.4672
127.7631
127.0063
125.9309
125.4942
119.5557
115.8577
115.2968
103.2000
100.1624
60.9465
51.9259
47.7863
39.6329
17.3362
OH
HN
COOMe
Me
Ph
N
Ph
31
f1 (ppm)


W1047-1H-purified
W1047-13C-purified
7.4448
7.4392
7.4251
7.4246
7.4204
7.4135
7.3932
7.3849
7.3798
7.3727
7.3706
7.3555
7.3550
7.3420
7.3384
7.2793
7.2744
7.2644
7.2603
7.2442
7.2394
7.0662
7.0620
7.0488
7.0451
7.0422
6.9875
6.9666
6.9161
6.8953
6.5149
5.3092
4.5783
4.5704
4.5562
4.5477
3.6076
3.6011
3.5900
3.5851
3.5820
3.5724
175.7552
140.8669
138.8949
138.3245
138.2610
132.6974
129.1224
COOMe
Me
N
COOMe
Ph
Me
Ph
Ph
32
Ph
2.47
3.46
3.45
2.39
1.35
1.19
1.00
2.09
0.98
4.13
1.03
3.28
4.69
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
190
180
170
160
150
f1 (ppm)

32


z1296
7.4308
7.4255
7.4151
7.4108
7.4067
7.3773
7.3709
7.3563
7.3423
7.3379
7.3324
7.3217
7.3027
7.2942
7.2904
7.2813
7.2648
7.2598
7.2432
7.2382
7.2292
7.2244
7.2131
7.1961
7.0042
6.9866
6.8894
6.8688
6.6564
6.6358
6.5924
5.2773
5.0664
4.7364
4.5840
4.5679
4.5522
3.6653
3.1999
3.1843
3.1657
2.3553
1.9216
1.8745
1.8579
1.5449
1.5341
1.5249
NHCbz
HN
COOMe
Me
Ph
N
Ph
33
2.24
11.09
1.93
0.95
1.01
0.92
2.10
2.01
0.83
1.08
0.81
2.97
2.00
3.00
2.09
4.14
f1 (ppm)

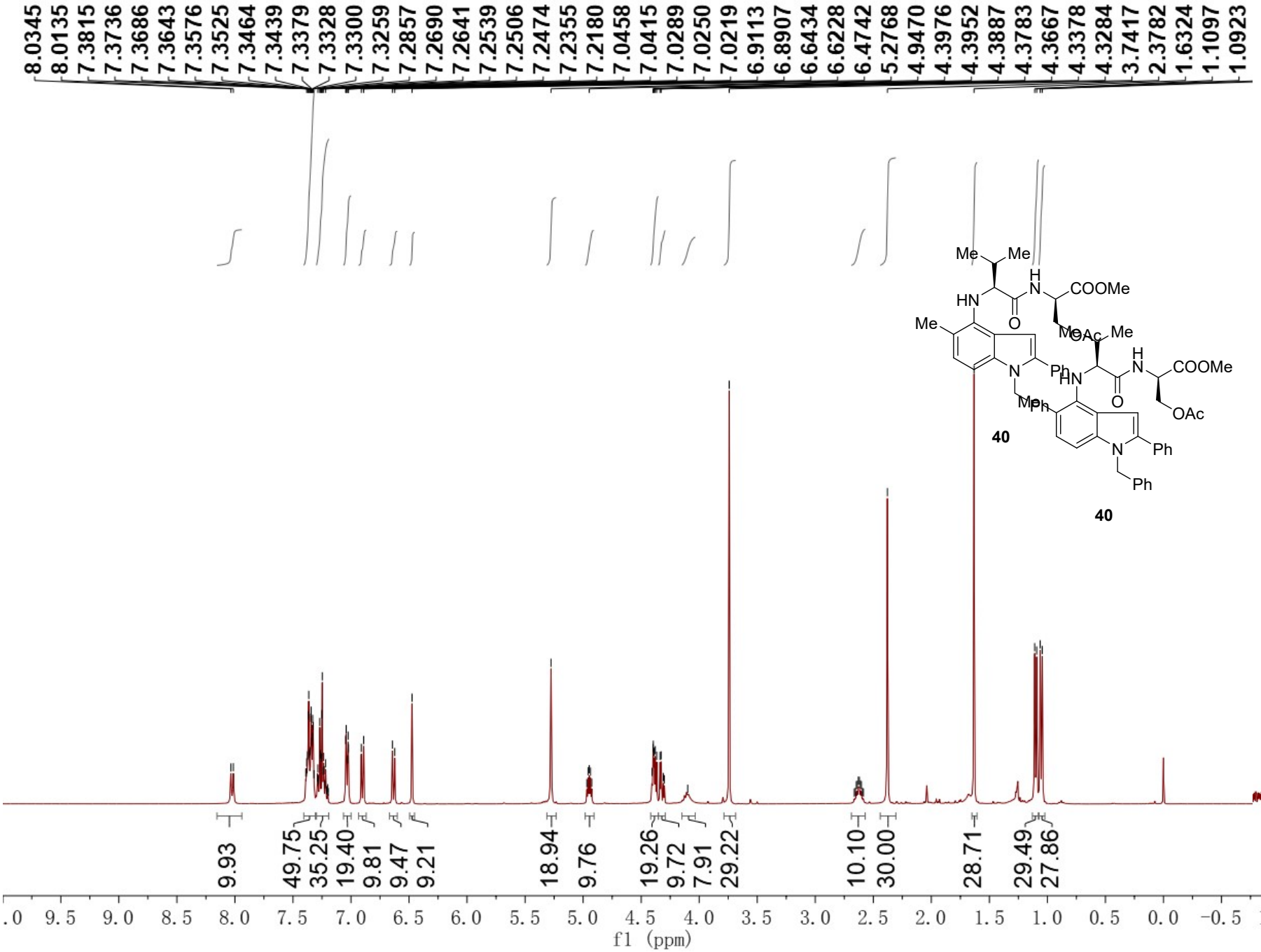
z1296-C


175.2205
156.3098
140.3668
138.5600
138.2576
137.6238
132.7540
129.0560
128.6099
128.4814
128.4442
128.0287
127.8158
126.9916
125.9094
125.5088
119.4721
115.7197
103.2109
100.0556
66.5357
59.1840
51.9583
47.7438
40.7305
34.0053
29.7538
22.6631
17.4277
NHCbz
HN
COOMe
Me
Ph
N
Ph
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
-50000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

33

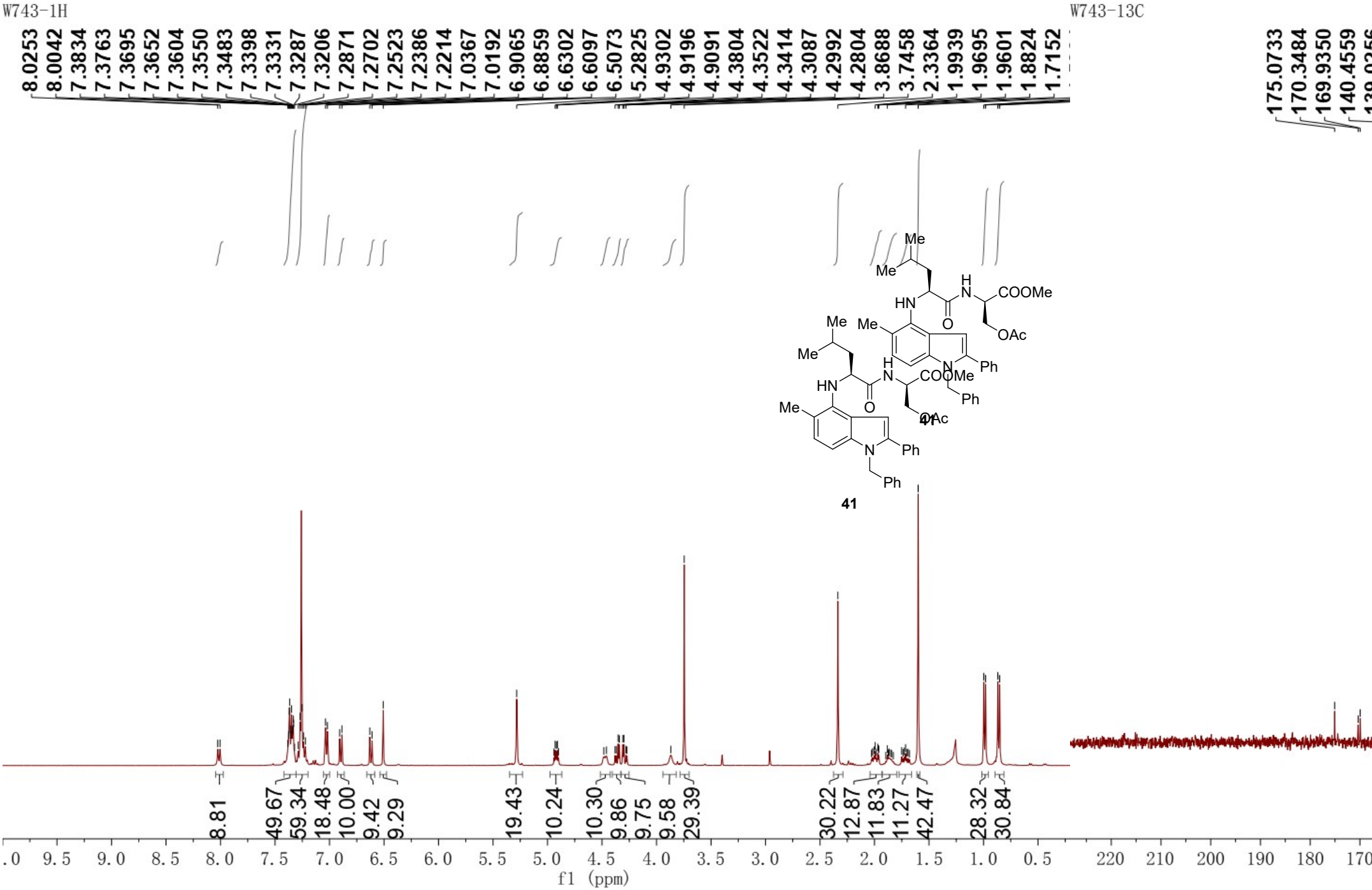
W730-1H-purified

W730-13C-purified



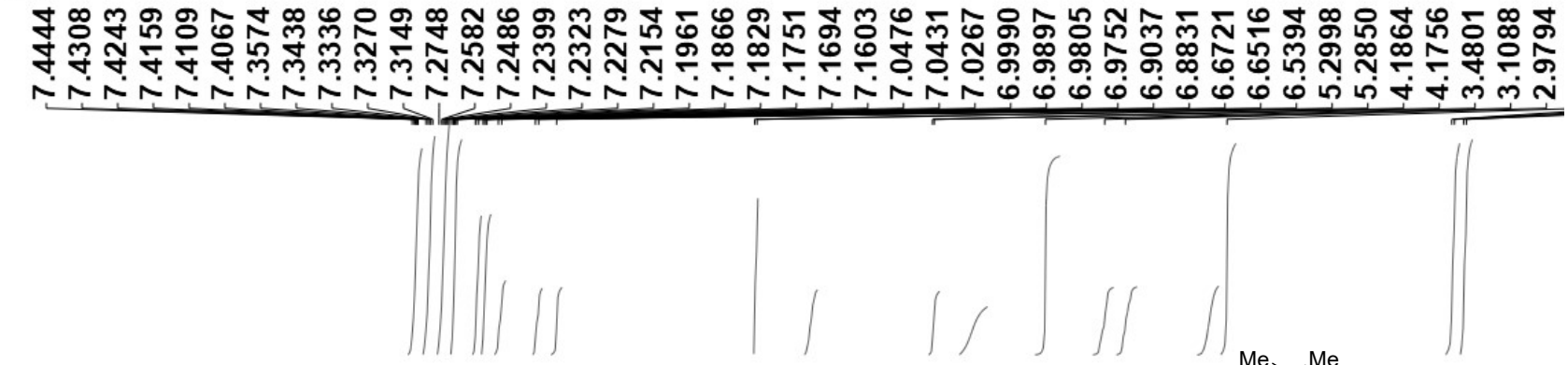
40

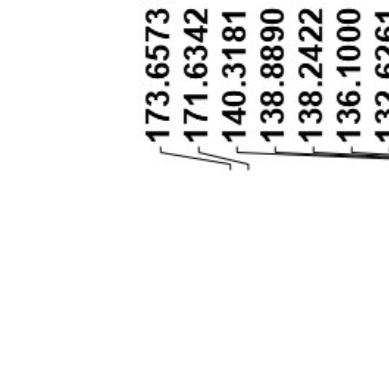
40

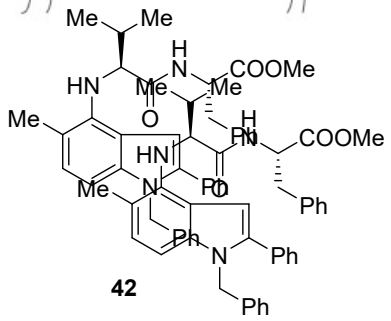

W743-1H
W743-13C
8.0253
8.0042
7.3834
7.3763
7.3695
7.3652
7.3604
7.3550
7.3483
7.3398
7.3331
7.3287
7.3206
7.2871
7.2702
7.2523
7.2386
7.2214
7.0367
7.0192
6.9065
6.8859
6.6302
6.6097
6.5073
5.2825
4.9302
4.9196
4.9091
4.3804
4.3522
4.3414
4.3087
4.2992
4.2804
3.8688
3.7458
2.3364
1.9939
1.9695
1.9601
1.8824
1.7152
175.0733
170.3484
169.9350
140.4559
Me
Me
HN
H
N
COOMe
O
OAc
Me
Me
Me
N
Ph
HN
H
N
COOMe
Ph
O
Me
OAc
N
Ph
Ph
41
8.81
49.67
59.34
18.48
10.00
9.42
9.29
19.43
10.24
10.30
9.86
9.75
9.58
29.39
30.22
12.87
11.83
11.27
42.47
28.32
30.84
f1 (ppm)

W983

W983-13C-purified

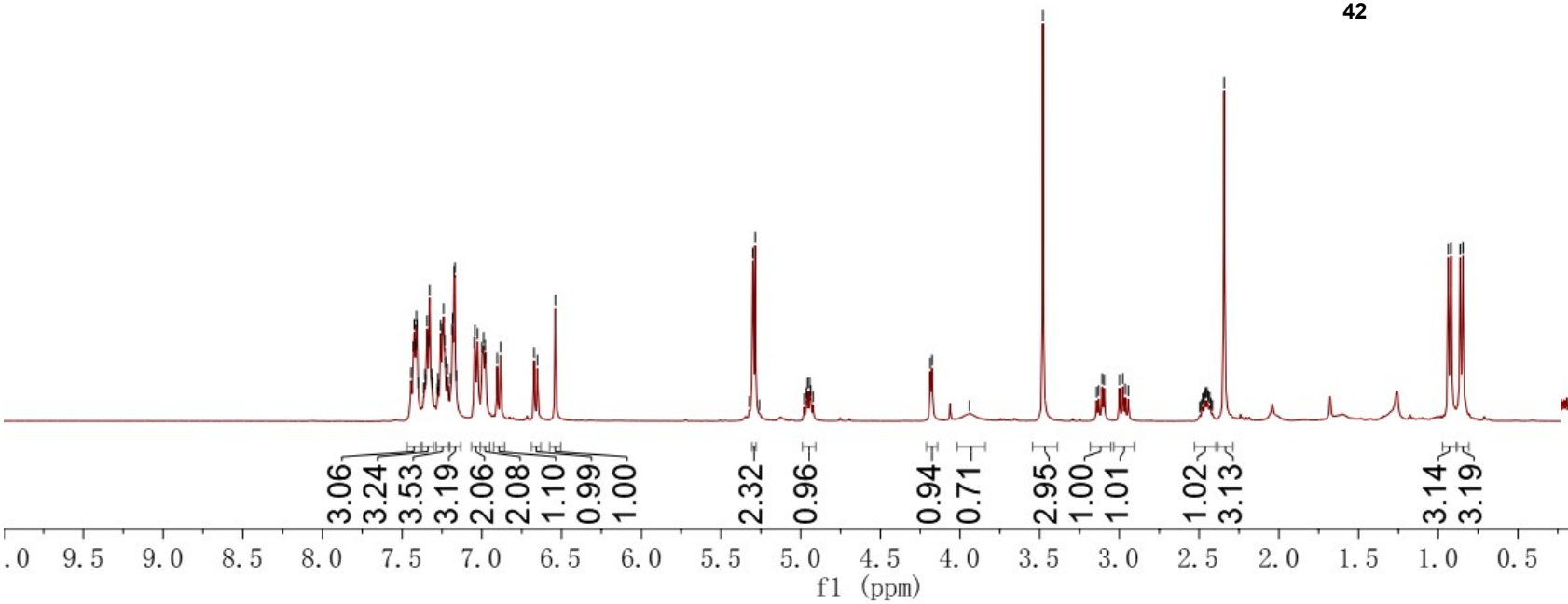


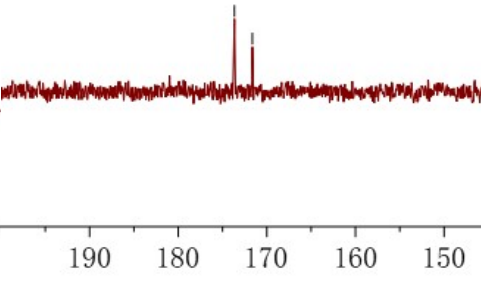




42

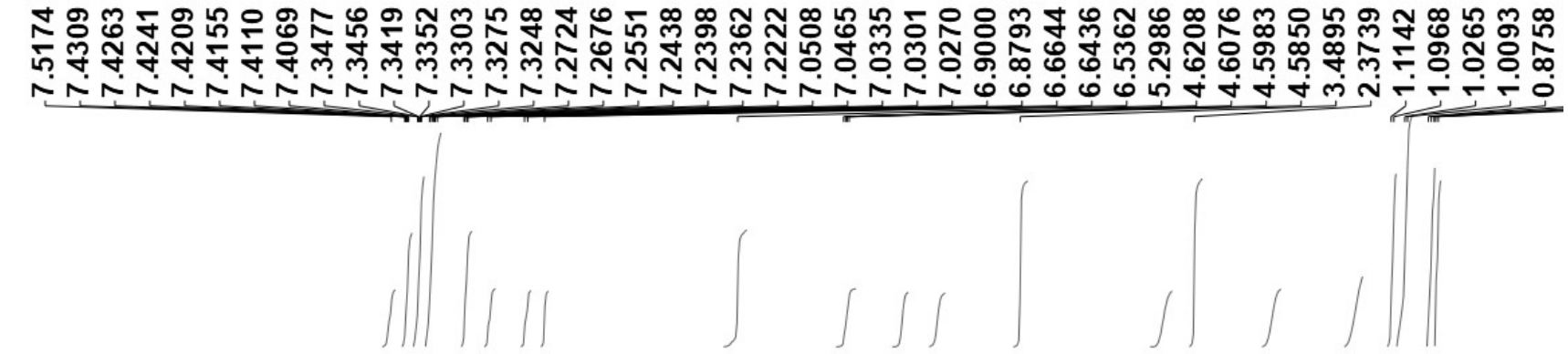
42

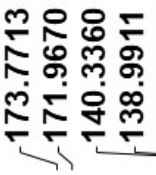


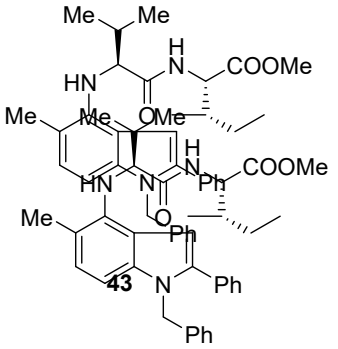


W992-1H-purified

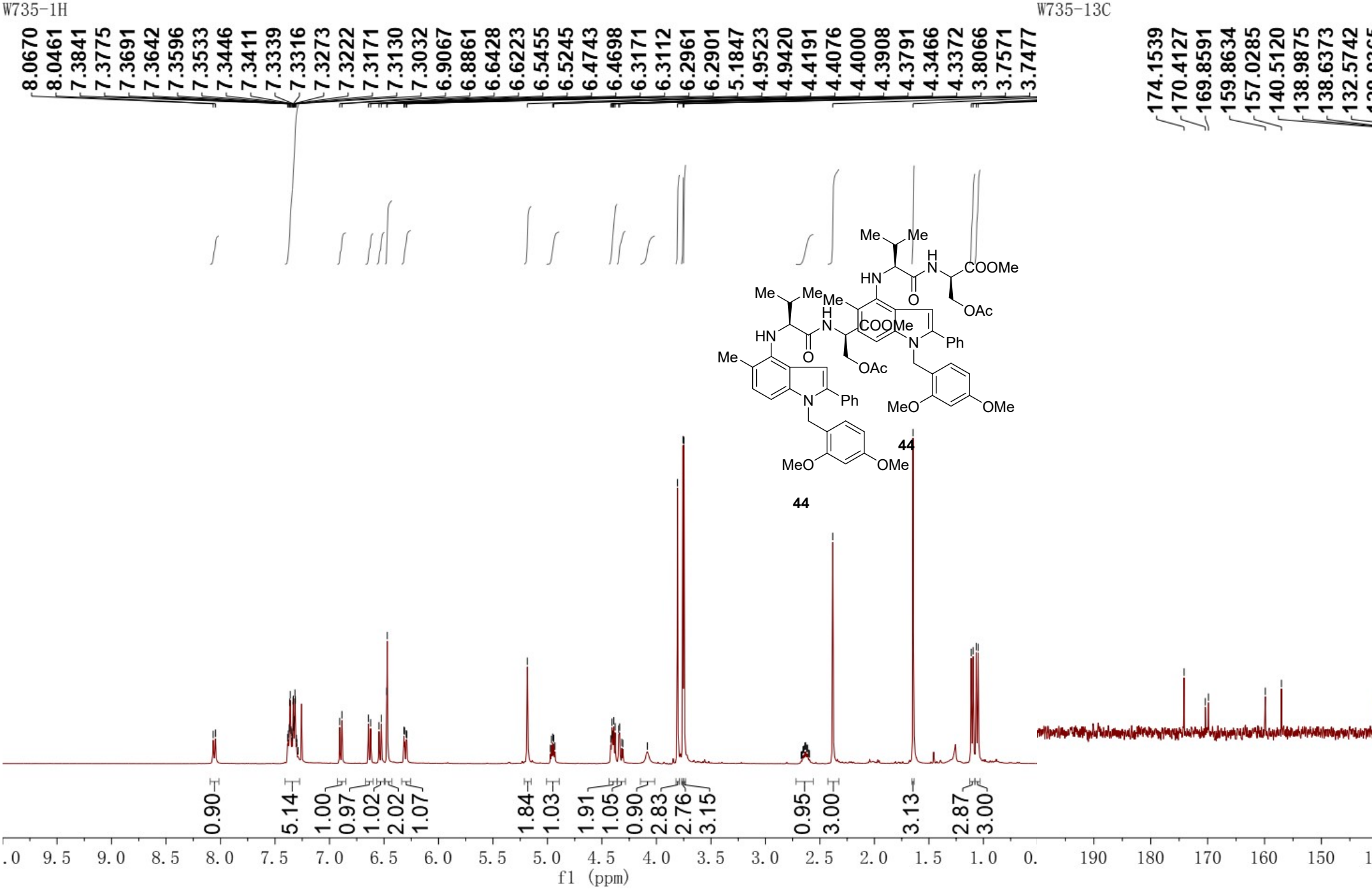
W992-13C-purified

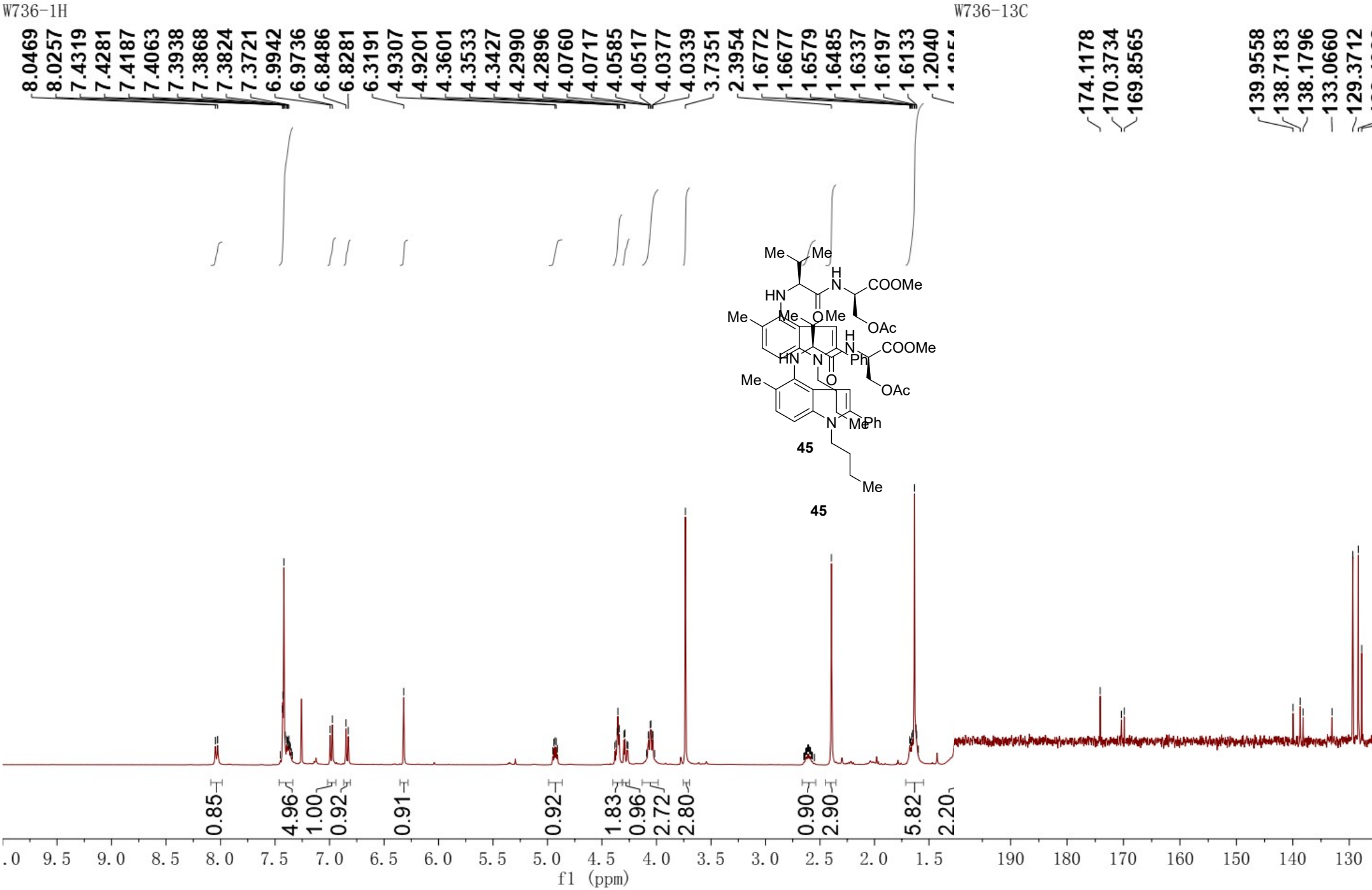


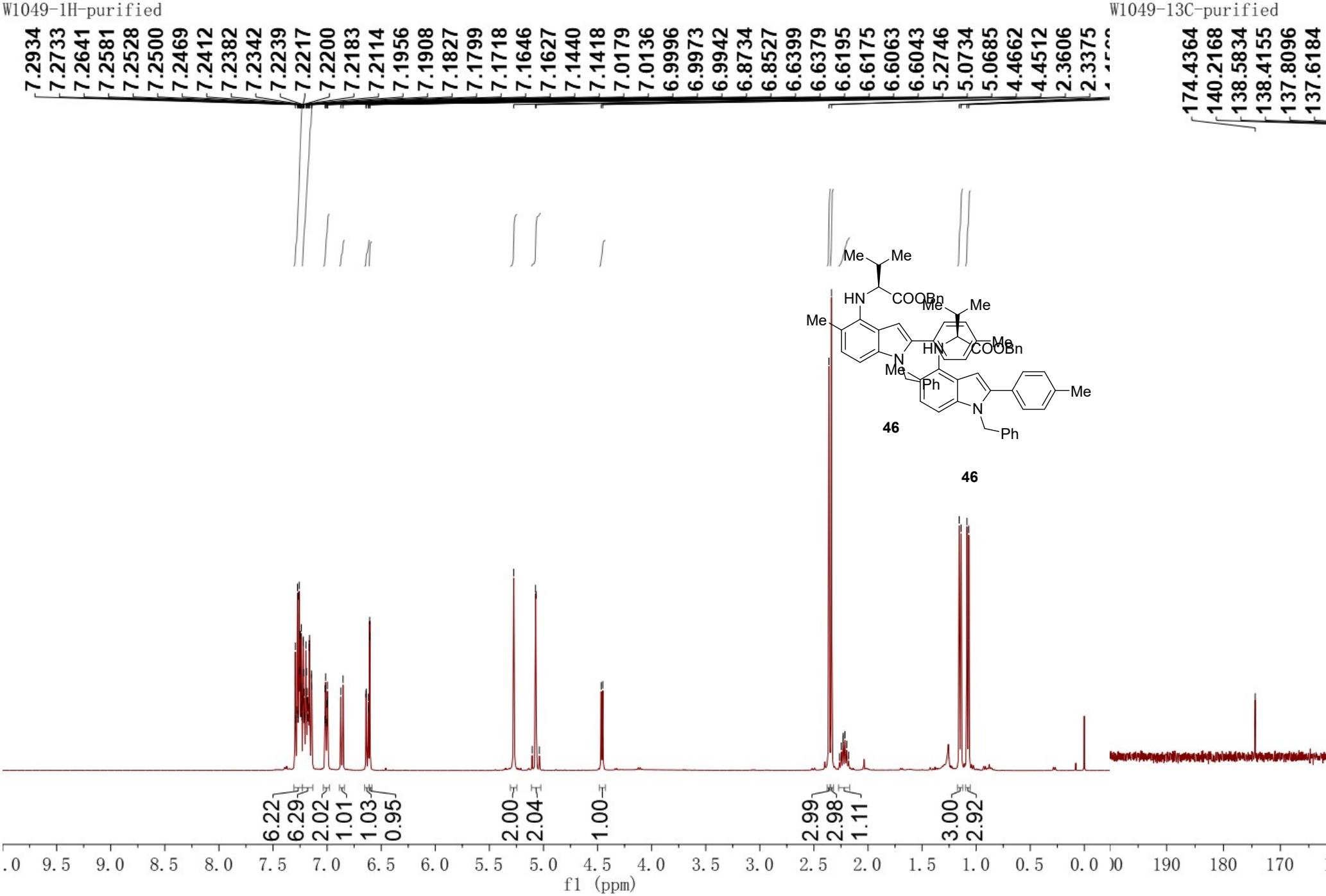


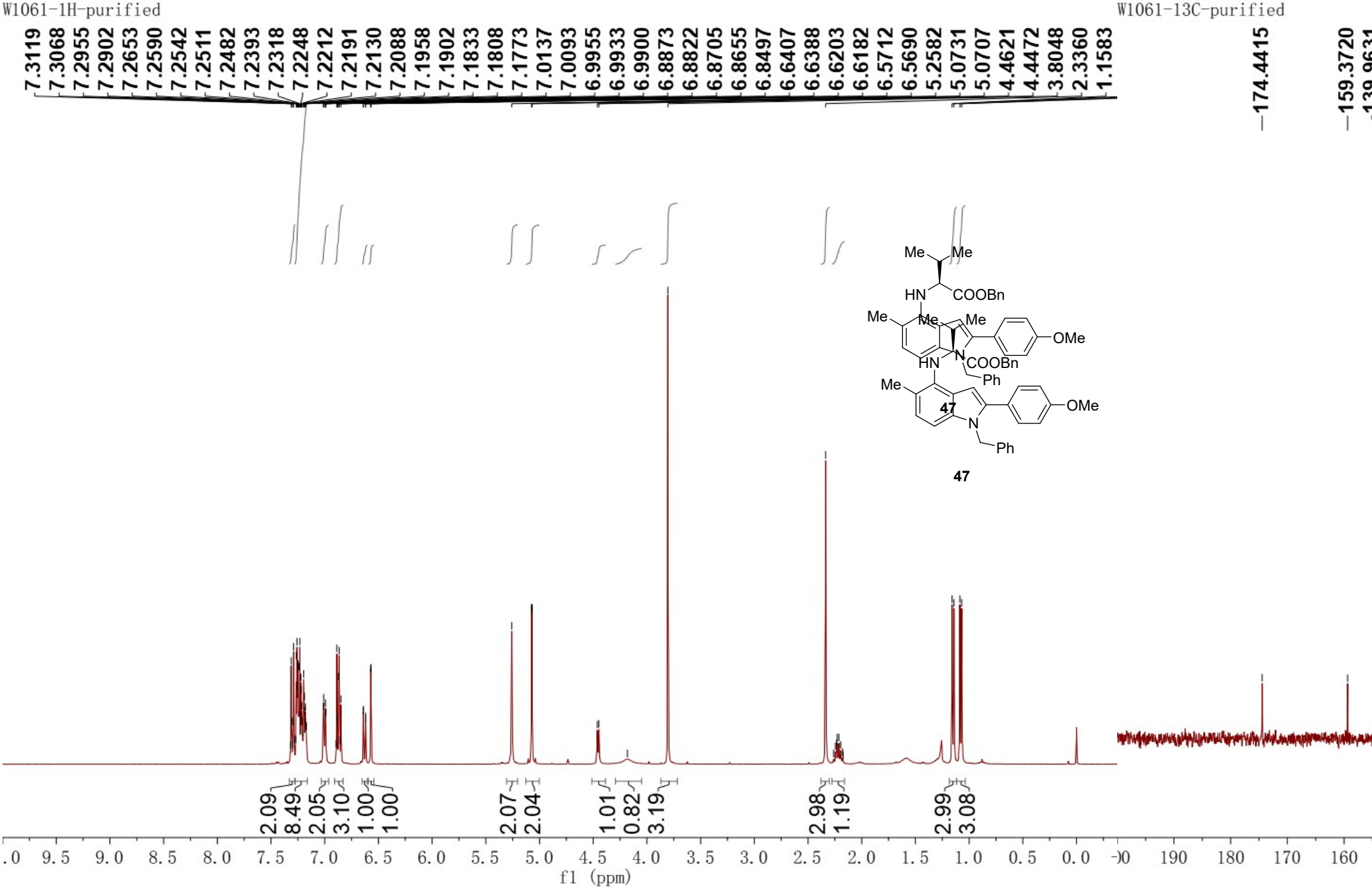


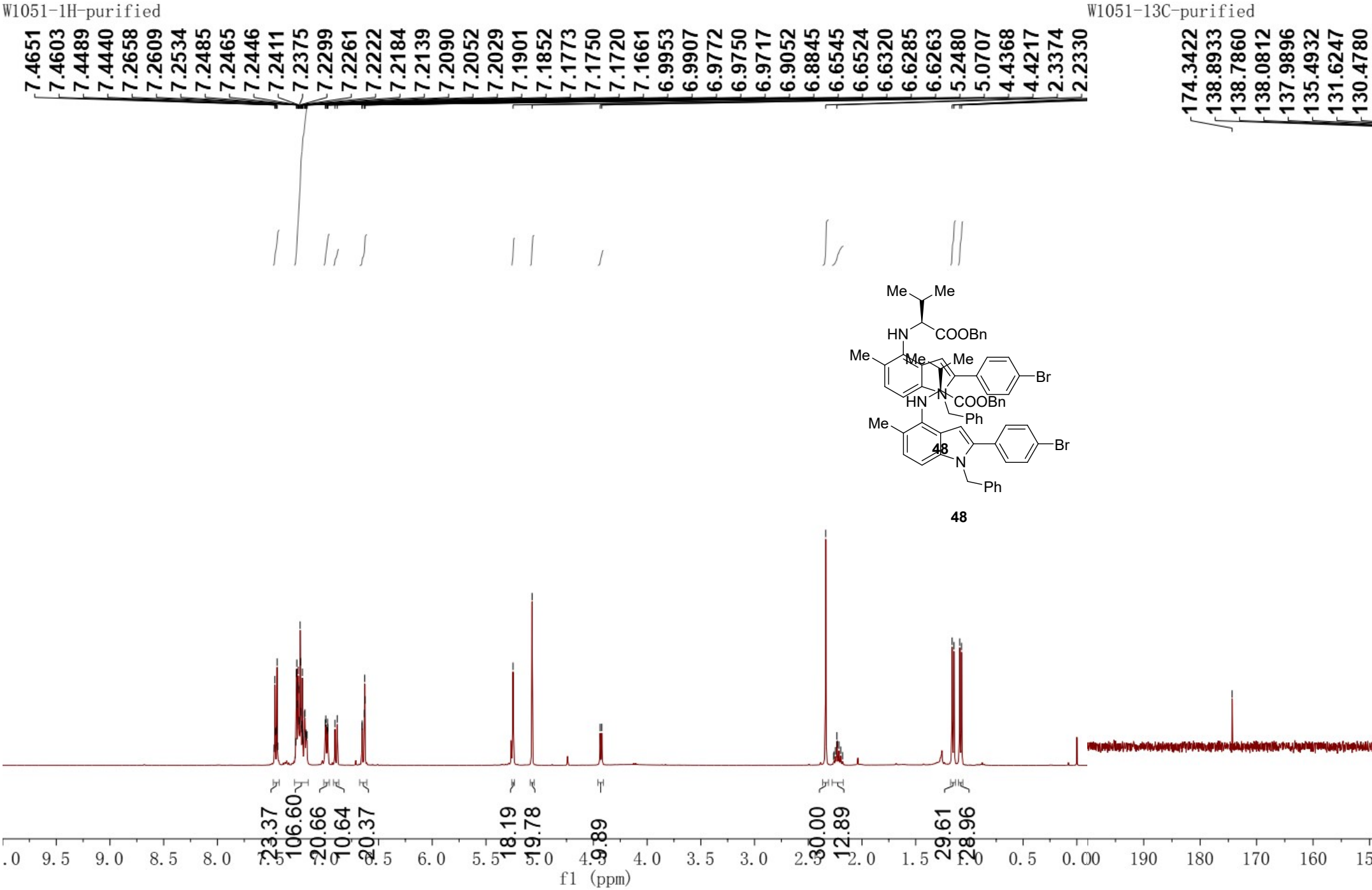
43


W735-1H
W735-13C
8.0670
8.0461
7.3841
7.3775
7.3691
7.3642
7.3596
7.3533
7.3446
7.3411
7.3339
7.3316
7.3273
7.3222
7.3171
7.3130
7.3032
6.9067
6.8861
6.6428
6.6223
6.5455
6.5245
6.4743
6.4698
6.3171
6.3112
6.2961
6.2901
5.1847
4.9523
4.9420
4.4191
4.4076
4.4000
4.3908
4.3791
4.3466
4.3372
3.8066
3.7571
3.7477
174.1539
170.4127
169.8591
159.8634
157.0285
140.5120
138.9875
138.6373
132.5742
Me
Me
HN
H
N
COOMe
O
OAc
Ph
MeO
OMe
44
0.90
5.14
1.00
0.97
1.02
2.02
1.07
1.84
1.03
1.91
1.05
0.90
2.83
2.76
3.15
0.95
3.00
3.13
2.87
3.00
f1 (ppm)

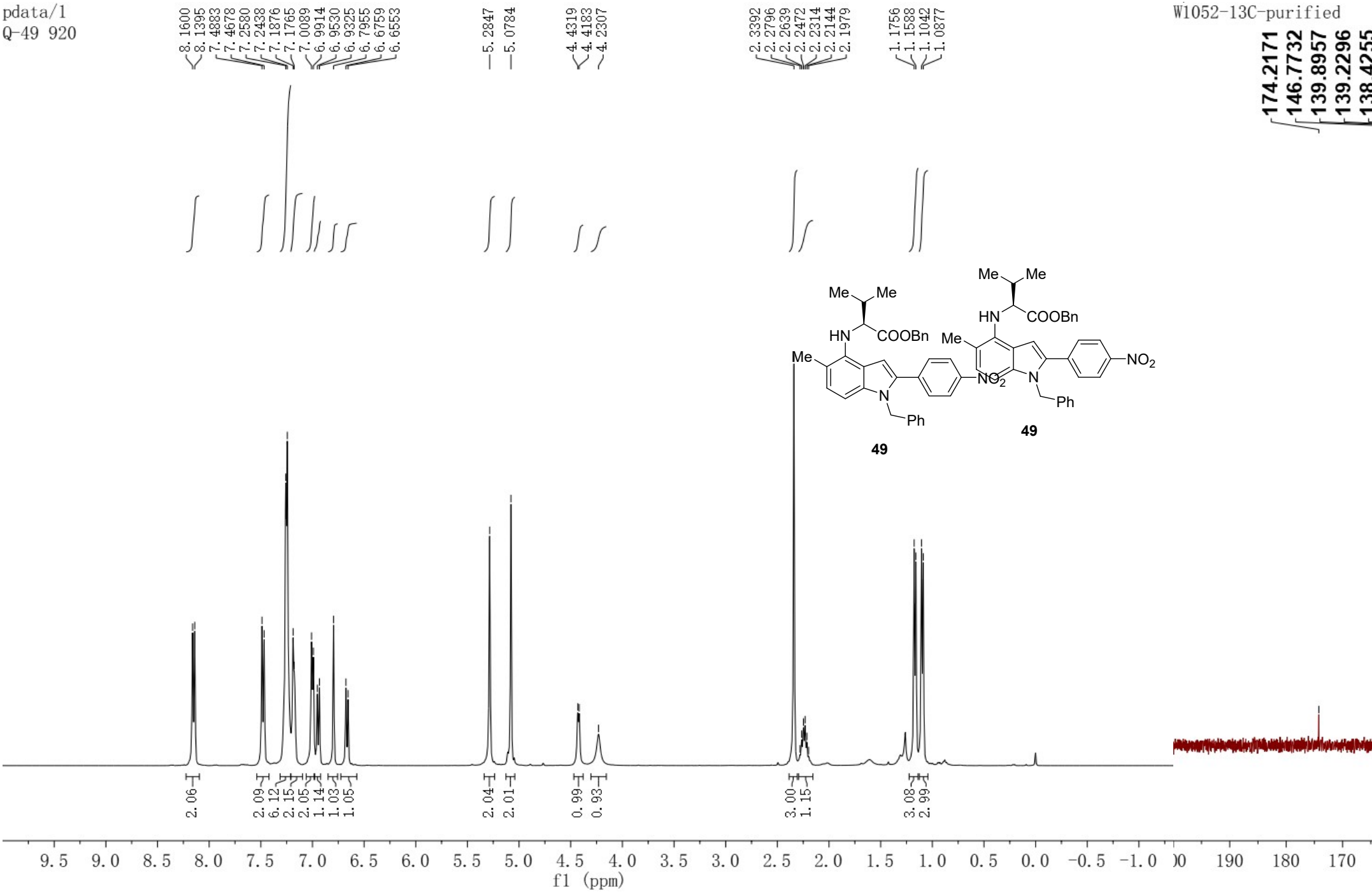

W736-1H
W736-13C
8.0469
8.0257
7.4319
7.4281
7.4187
7.4063
7.3938
7.3868
7.3824
7.3721
6.9942
6.9736
6.8486
6.8281
6.3191
4.9307
4.9201
4.3601
4.3533
4.3427
4.2990
4.2896
4.0760
4.0717
4.0585
4.0517
4.0377
4.0339
3.7351
2.3954
1.6772
1.6677
1.6579
1.6485
1.6337
1.6197
1.6133
1.2040
174.1178
170.3734
169.8565
139.9558
138.7183
138.1796
133.0660
129.3712
45
0.85
4.96
1.00
0.92
0.91
0.92
1.83
0.96
2.72
2.80
0.90
2.90
5.82
2.20
f1 (ppm)


W1049-1H-purified
W1049-13C-purified
7.2934
7.2733
7.2641
7.2581
7.2528
7.2500
7.2469
7.2412
7.2382
7.2342
7.2239
7.2217
7.2200
7.2183
7.2114
7.1956
7.1908
7.1827
7.1799
7.1718
7.1646
7.1627
7.1440
7.1418
7.0179
7.0136
6.9996
6.9973
6.9942
6.8734
6.8527
6.6399
6.6379
6.6195
6.6175
6.6063
6.6043
5.2746
5.0734
5.0685
4.4662
4.4512
2.3606
2.3375
174.4364
140.2168
138.5834
138.4155
137.8096
137.6184
135.5658
129.8914
Me
Me
HN
COOBn
Me
Me
Me
HN
COOBn
Me
N
Me
Ph
Me
N
Ph
46
46
6.22
6.29
2.02
1.01
1.03
0.95
2.00
2.04
1.00
2.99
2.98
1.11
3.00
2.92
f1 (ppm)


W1061-1H-purified
W1061-13C-purified
7.3119
7.3068
7.2955
7.2902
7.2653
7.2590
7.2542
7.2511
7.2482
7.2393
7.2318
7.2248
7.2212
7.2191
7.2130
7.2088
7.1958
7.1902
7.1833
7.1808
7.1773
7.0137
7.0093
6.9955
6.9933
6.9900
6.8873
6.8822
6.8705
6.8655
6.8497
6.6407
6.6388
6.6203
6.6182
6.5712
6.5690
5.2582
5.0731
5.0707
4.4621
4.4472
3.8048
2.3360
1.1583
174.4415
159.3720
Me
Me
HN
COOBn
Me
Me
Me
OMe
HN
N
COOBn
Ph
Me
47
OMe
N
Ph
47
2.09
8.49
2.05
3.10
1.00
1.00
2.07
2.04
1.01
0.82
3.19
2.98
1.19
2.99
3.08
f1 (ppm)

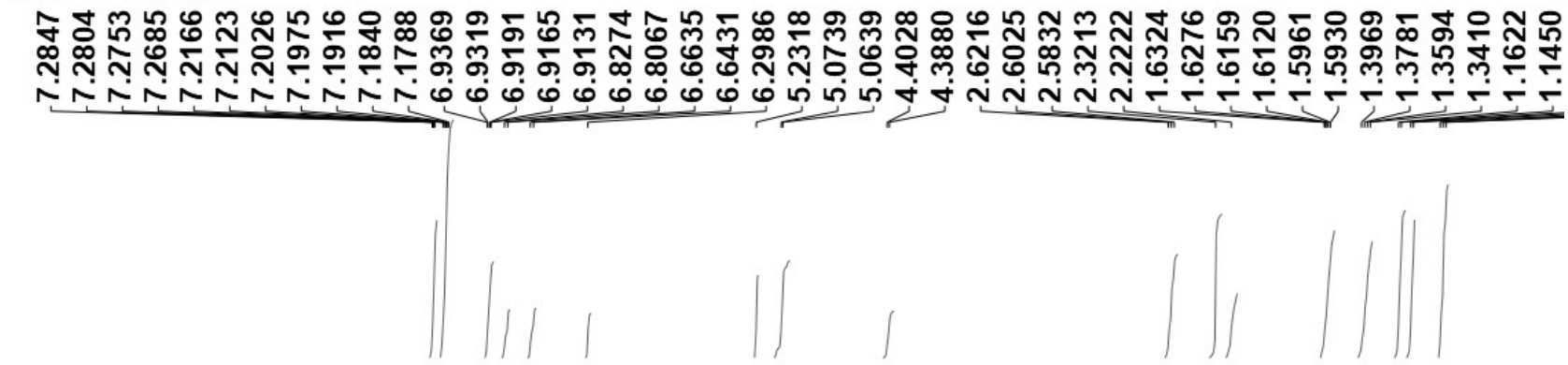

W1051-1H-purified
W1051-13C-purified
7.4651
7.4603
7.4489
7.4440
7.2658
7.2609
7.2534
7.2485
7.2465
7.2446
7.2411
7.2375
7.2299
7.2261
7.2222
7.2184
7.2139
7.2090
7.2052
7.2029
7.1901
7.1852
7.1773
7.1750
7.1720
7.1661
6.9953
6.9907
6.9772
6.9750
6.9717
6.9052
6.8845
6.6545
6.6524
6.6320
6.6285
6.6263
5.2480
5.0707
4.4368
4.4217
2.3374
2.2330
174.3422
138.8933
138.7860
138.0812
137.9896
135.4932
131.6247
130.4780
Me
Me
HN
COOBn
Me
Me
Me
Br
N
HN
COOBn
Ph
Me
Br
N
Ph
48
23.37
106.60
20.66
10.64
20.37
18.19
19.78
9.89
30.00
12.89
29.61
28.96
f1 (ppm)

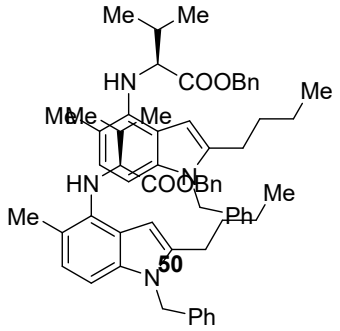
48


pdata/1
Q-49 920
W1052-13C-purified
8.1600
8.1395
7.4883
7.4678
7.2580
7.2438
7.1876
7.1765
7.0089
6.9914
6.9530
6.9325
6.7955
6.6759
6.6553
5.2847
5.0784
4.4319
4.4183
4.2307
2.3392
2.2796
2.2639
2.2472
2.2314
2.2144
2.1979
1.1756
1.1588
1.1042
1.0877
174.2171
146.7732
139.8957
139.2296
138.4255
Me
Me
HN
COOBn
Me
N
Ph
NO2
49
2.06
2.09
6.12
2.15
2.05
1.14
1.03
1.05
2.04
2.01
0.99
0.93
3.00
1.15
3.08
2.99
f1 (ppm)

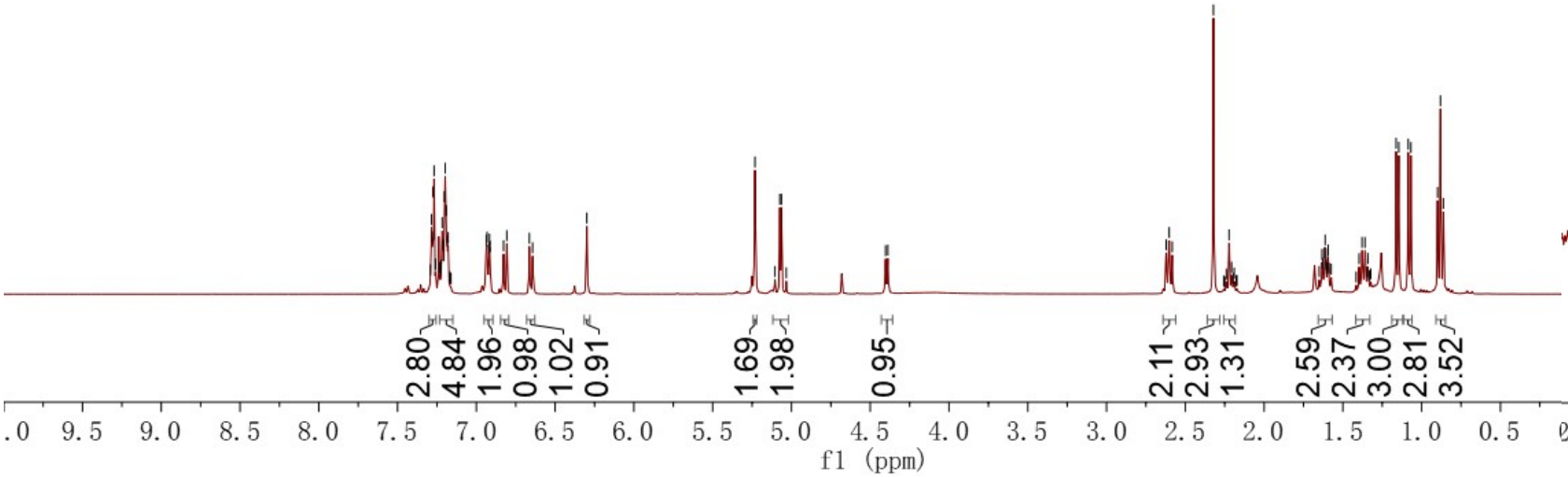
W1053-1H-purified

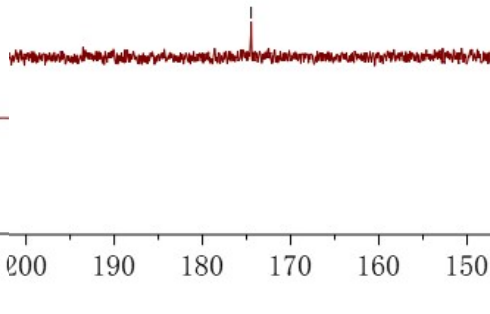
W1053-13C-purified

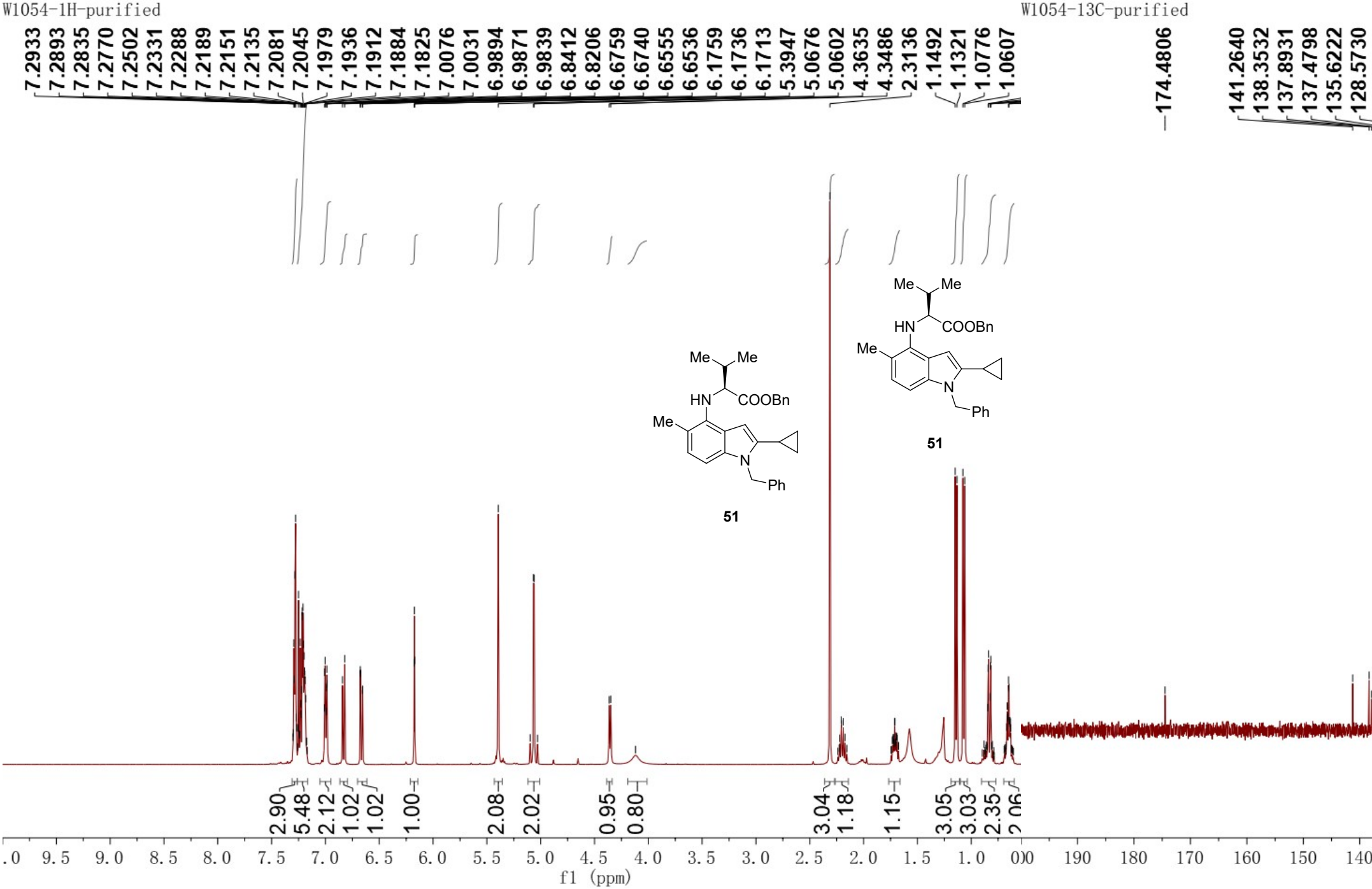


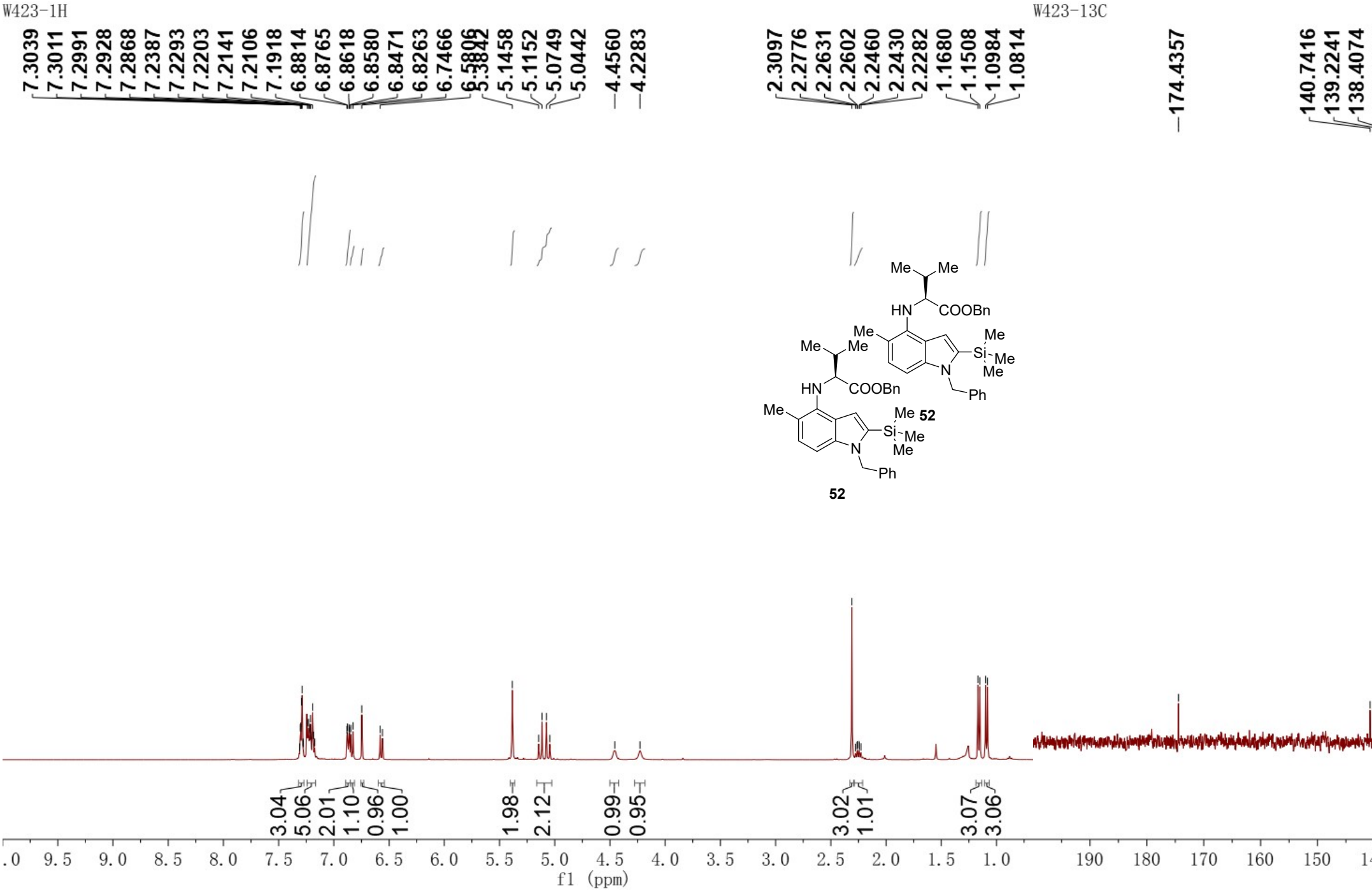


50



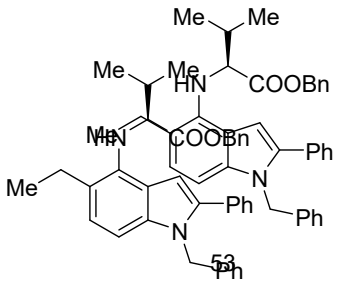



W1054-1H-purified
W1054-13C-purified
7.2933
7.2893
7.2835
7.2770
7.2502
7.2331
7.2288
7.2189
7.2151
7.2135
7.2081
7.2045
7.1979
7.1936
7.1912
7.1884
7.1825
7.0076
7.0031
6.9894
6.9871
6.9839
6.8412
6.8206
6.6759
6.6740
6.6555
6.6536
6.1759
6.1736
6.1713
5.3947
5.0676
5.0602
4.3635
4.3486
2.3136
1.1492
1.1321
1.0776
1.0607
174.4806
141.2640
138.3532
137.8931
137.4798
135.6222
128.5730
Me
Me
HN
COOBn
Me
N
Ph
51
Me
Me
HN
COOBn
Me
N
Ph
51
2.90
5.48
2.12
1.02
1.02
1.00
2.08
2.02
0.95
0.80
3.04
1.18
1.15
3.05
3.03
2.35
f1 (ppm)


W423-1H
7.3039
7.3011
7.2991
7.2928
7.2868
7.2387
7.2293
7.2203
7.2141
7.2106
7.1918
6.8814
6.8765
6.8618
6.8580
6.8471
6.8263
6.7466
5.1458
5.1152
5.0749
5.0442
4.4560
4.2283
W423-13C
2.3097
2.2776
2.2631
2.2602
2.2460
2.2430
2.2282
1.1680
1.1508
1.0984
1.0814
174.4357
140.7416
139.2241
138.4074
Me
Me
HN
COOBn
Me
Me
Me
Si
Me
Me
N
Ph
HN
COOBn
Me
Me
52
Si
Me
Me
N
Ph
52
3.04
5.06
2.01
1.10
0.96
1.00
1.98
2.12
0.99
0.95
3.02
1.01
3.07
3.06
f1 (ppm)

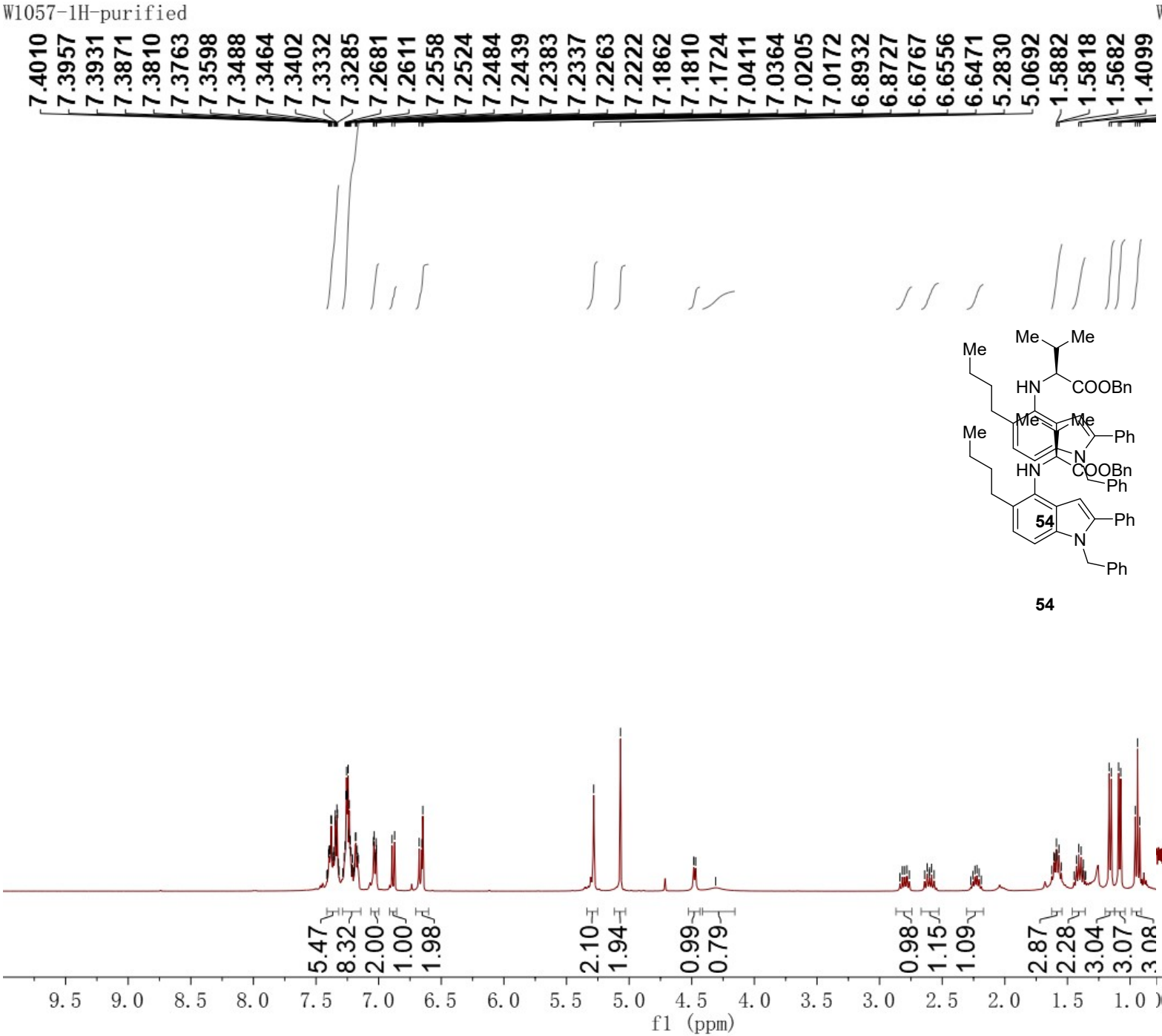
W1056-1H-purified

W1056-13C-purified



53

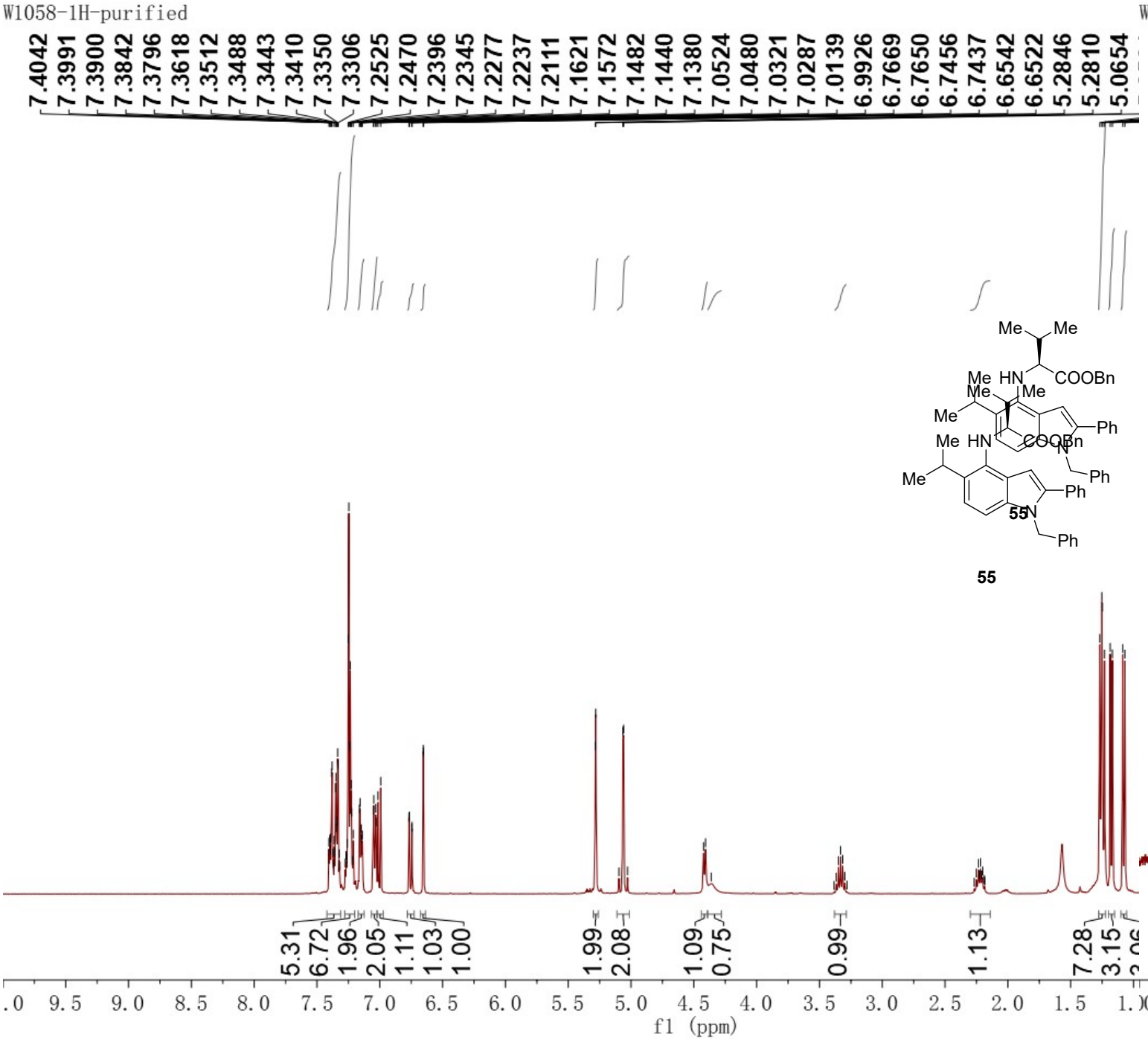
f1 (ppm)


W1057-1H-purified
7.4010
7.3957
7.3931
7.3871
7.3810
7.3763
7.3598
7.3488
7.3464
7.3402
7.3332
7.3285
7.2681
7.2611
7.2558
7.2524
7.2484
7.2439
7.2383
7.2337
7.2263
7.2222
7.1862
7.1810
7.1724
7.0411
7.0364
7.0205
7.0172
6.8932
6.8727
6.6767
6.6556
6.6471
5.2830
5.0692
1.5882
1.5818
1.5682
1.4099
5.47
8.32
2.00
1.00
1.98
2.10
1.94
0.99
0.79
0.98
1.15
1.09
2.87
2.28
3.04
3.07
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)

Me
Me
Me
HN
COOBn
Me
Me
Ph
Me
N
HN
COOBn
Ph
54
Ph
N
Ph

54


W1057-13C-purified
174.3179
140.0706
138.5742
138.3832
137.4032
135.5573
132.8641
129.0619
128.6411
128.4722
128.4270
128.1683
128.0826
190
180
170
160
150
140


W1058-1H-purified
7.4042
7.3991
7.3900
7.3842
7.3796
7.3618
7.3512
7.3488
7.3443
7.3410
7.3350
7.3306
7.2525
7.2470
7.2396
7.2345
7.2277
7.2237
7.2111
7.1621
7.1572
7.1482
7.1440
7.1380
7.0524
7.0480
7.0321
7.0287
7.0139
6.9926
6.7669
6.7650
6.7456
6.7437
6.6542
6.6522
5.2846
5.2810
5.0654
5.31
6.72
1.96
2.05
1.11
1.03
1.00
1.99
2.08
1.09
0.75
0.99
1.13
7.28
3.15
f1 (ppm)

Me
Me
Me HN
COOBn
Me
Me
Me
Ph
Me HN
COOBn
N
Ph
Me
Ph
55
N
Ph

55

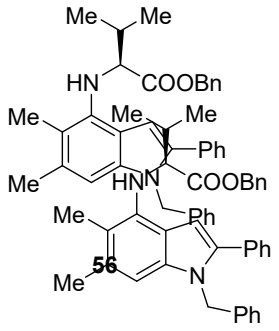

W1058-13C-purified
174.3990
140.2101
138.4223
138.0970
136.4204
135.6249
132.9129
129.0938
128.6500
128.4754
128.4315
128.0708
127.7348
190
180
170
160
150
140

W1059-1H-purified

7.3817 7.3767 7.3743 7.3664 7.3616 7.3572 7.3381 7.3267 7.3243 7.3200 7.3146 7.3095 7.3062 7.3039 7.2567 7.2503 7.2452 7.2377 7.2323 7.2230 7.2197 7.2086 7.2065 7.1685 7.1636 7.1563 7.1533 7.1501 7.1445 7.0308 7.0264 7.0104 7.0071 6.6117 6.6096 6.6014 5.2669 5.0566 4.3814 4.3660 2.2890 2.2434

W1059-13C-purified

174.5086 139.3980 138.5391 137.9340 137.7885 135.5827 132.9427 132.0606 128.9556 128.6414 128.4210



56

5.31 6.33 1.98 2.05 2.02 2.00 1.94 1.03 0.80 2.97 4.22 2.99 2.92

f1 (ppm)