

Supporting Information

**Transition-metal-free oxidative cyclization of *N*-propargyl ynamides:
stereospecific construction of linear polycyclic *N*-heterocycles**

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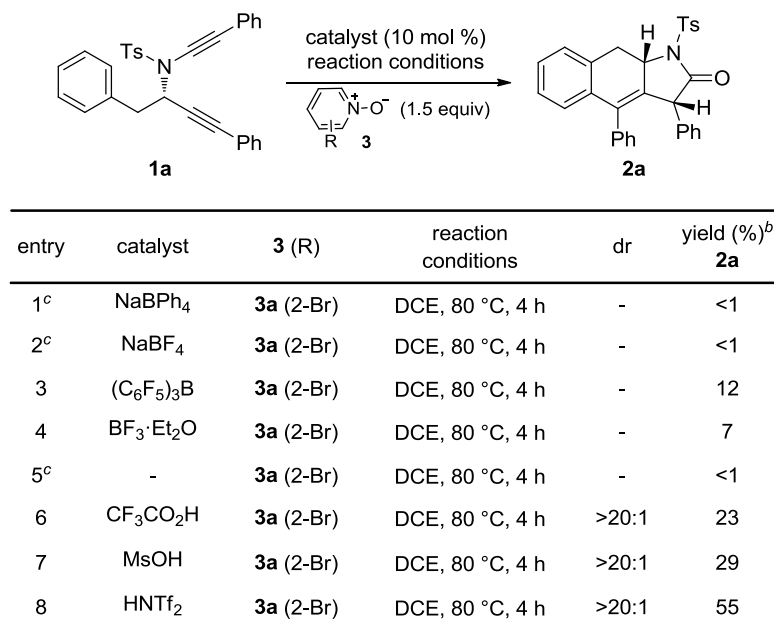
General Information. Ethyl acetate (ACS grade), hexanes (ACS grade), anhydrous 1,2-dichloroethane (ACS grade) and chlorobenzene (ACS grade) were obtained commercially and used without further purification. Methylene chloride, tetrahydrofuran and diethyl ether were purified according to standard methods unless otherwise noted. Commercially available reagents were used without further purification. Reactions were monitored by thin layer chromatography (TLC) using silicycle pre-coated silica gel plates. Flash column chromatography was performed over silica gel (300-400 mesh). Infrared spectra were recorded on a Nicolet AVATER FTIR330 spectrometer as thin film and are reported in reciprocal centimeter (cm^{-1}). Mass spectra were recorded with Agilent 6224 TOF LC/MS using electron spray ionization.

^1H NMR spectra were recorded on a Bruker AV-400 spectrometer and a Bruker AV-500 spectrometer in chloroform- d_3 . Chemical shifts are reported in ppm with the internal TMS signal at 0.0 ppm as a standard. The data is being reported as (s = singlet, d = doublet, t = triplet, m = multiplet or unresolved, brs = broad singlet, coupling constant(s) in Hz, integration).

^{13}C NMR spectra were recorded on a Bruker AV-400 spectrometer and a Bruker AV-500 spectrometer in chloroform- d_3 . Chemical shifts are reported in ppm with the internal chloroform signal at 77.0 ppm as a standard.

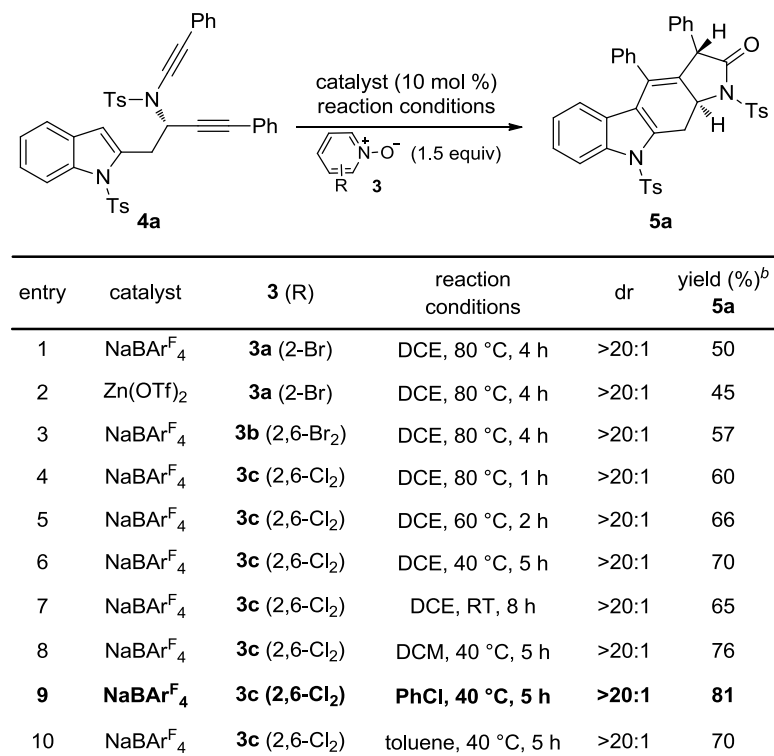
More Reaction Condition, Scope and Mechanism Studies

1. Other reaction condition studies on the oxidative cyclization of **1a**.^a



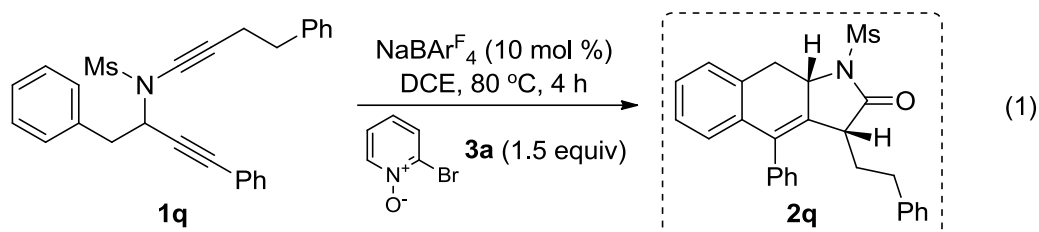
^aReaction conditions: [**1a**] = 0.05 M. ^bMeasured by ¹H NMR using diethyl phthalate as the internal standard. ^c>95% of **1a** remained unreacted.

2. Reaction condition studies on the oxidative cyclization of **4a**.^a

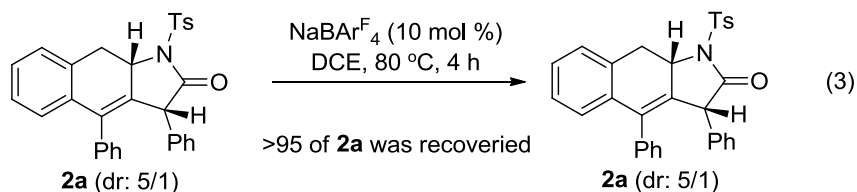
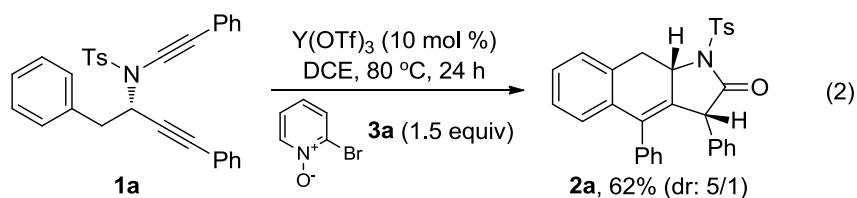


^aReaction conditions: [**4a**] = 0.05 M. ^bMeasured by ¹H NMR using diethyl phthalate as the internal standard.

1. Attempts to extend the reaction to alkyl-substituted ynamide **1q** only gave a complicated mixture of products, and no desired tricyclic *N*-heterocycle **2q** was obtained (eq 1).



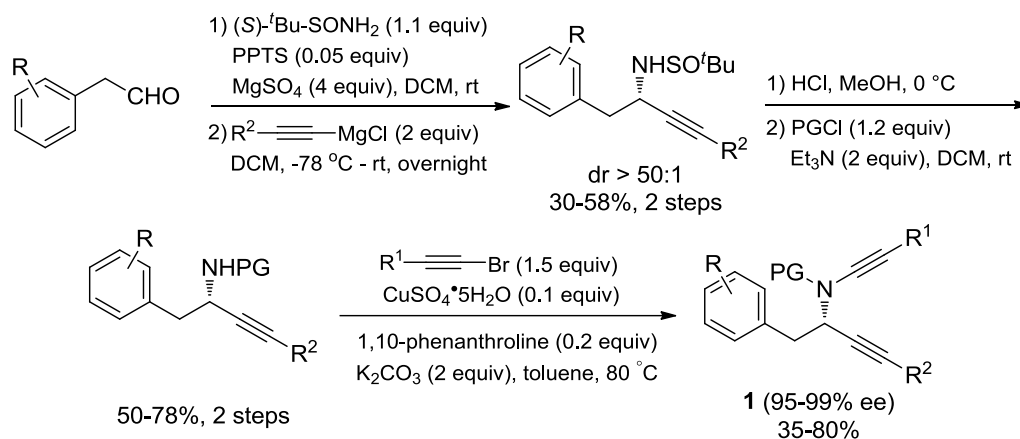
2. It should be mentioned that dr did not change by prolonging the reaction time from 4 h (Table 1, entry 7) to 24 h (eq 2). In addition, it was found that dr remained the same under the relevant reaction conditions (eq 3).



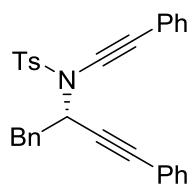
- a) 2-bromopyridine *N*-oxide **3a** (0.5-1.5 equiv)
- b) 2-bromopyridine (0.5-1.5 equiv)
- c) 2-bromopyridine *N*-oxide **3a** (0.5-1.5 equiv), without NaBARF₄

3. Of note, we also tried various NaBARF₄ prepared by ourselves and ordered from different chemical suppliers, but found that the reaction gave the same results.

Compounds **1a-1o** were prepared according to the following procedures.^{1,2}



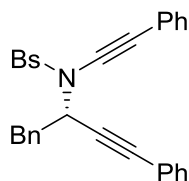
(S)-N-(1,4-diphenylbut-3-yn-2-yl)-4-methyl-N-(phenylethynyl)benzenesulfonamide (1a)



1a

Yellow solid (mp 119-121 °C). $[\alpha]_D^{20} = -30.2^\circ$ ($c = 1.0$, $CHCl_3$). 99% ee (determined by HPLC: Chiralcel AS-H Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; $t_R = 34.95$ min (minor), 16.47 min (major)). 1H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, $J = 8.0$ Hz, 2H), 7.41 – 7.39 (m, 2H), 7.38 – 7.15 (m, 13H), 7.08 (d, $J = 7.2$ Hz, 2H), 5.13 (t, $J = 7.6$ Hz, 1H), 3.34 – 3.14 (m, 2H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.6, 136.0, 134.5, 131.6, 131.5, 129.5, 129.4, 128.5, 128.4, 128.3, 128.1, 128.0, 127.9, 127.1, 122.9, 122.1, 86.7, 84.6, 79.8, 73.6, 54.8, 41.0, 21.5; IR (neat): 2925, 2237, 2235, 1597, 1491, 1369, 1139, 756, 691, 598, 589; HRESIMS Calcd for $[C_{31}H_{25}NNaO_2S]^+$ ($M + Na^+$) 498.1498, found 498.1495.

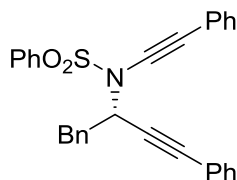
(S)-4-bromo-N-(1,4-diphenylbut-3-yn-2-yl)-N-(phenylethynyl)benzenesulfonamide (1b)



1b

Yellow solid (mp 121-123 °C). $[\alpha]_D^{20} = -47.5^\circ$ ($c = 1.0$, CHCl_3). 99% ee (determined by HPLC: Chiralcel AS-H Column, 20/80 *i*-PrOH/hexane, 1.5 mL/min, 254 nm, 25 °C; $t_R = 20.43$ min (minor), 6.77 min (major)). ^1H NMR (400 MHz, CDCl_3) δ 7.74 (d, $J = 8.4$ Hz, 2H), 7.55 (d, $J = 12.4$ Hz, 2H), 7.47 – 7.40 (m, 2H), 7.37 – 7.21 (m, 11H), 7.10 (d, $J = 6.4$ Hz, 2H), 5.13 (t, $J = 7.6$ Hz, 1H), 3.38 – 3.12 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 136.4, 135.8, 132.1, 131.8, 131.5, 129.5(3), 129.5(0), 128.9, 128.7, 128.5, 128.4, 128.3, 128.2, 127.2, 122.5, 121.8, 87.0, 84.3, 79.2, 73.9, 55.1, 40.9; IR (neat): 2925, 2237, 1597, 1491, 1443, 1369, 1169, 1090, 756, 691, 663, 598; HRESIMS Calcd for $[\text{C}_{30}\text{H}_{22}\text{BrNNaO}_2\text{S}]^+$ ($\text{M} + \text{Na}^+$) 562.0447, found 562.0447.

(S)-N-(1,4-diphenylbut-3-yn-2-yl)-N-(phenylethynyl)benzenesulfonamide (1c)

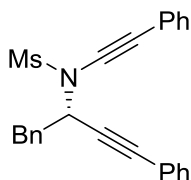


1c

White solid (mp 116-118 °C). $[\alpha]_D^{20} = +54.3^\circ$ ($c = 1.0$, CHCl_3). 96% ee (determined by HPLC: Chiralcel AS-H Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; $t_R = 25.69$ min (minor), 11.46 min (major)). ^1H NMR (500 MHz, CDCl_3) δ 7.95 – 7.87 (m, 2H), 7.56 – 7.48 (m, 1H), 7.47 – 7.37 (m, 4H), 7.35 – 7.20 (m, 9H), 7.19 – 7.16 (m, 2H), 7.10 (d, $J = 7.0$ Hz, 2H), 5.17 (t, $J = 7.5$ Hz, 1H), 3.34 – 3.17 (m, 2H); ^{13}C NMR (125 MHz, CDCl_3) δ 137.3, 135.9, 133.5, 131.6, 131.5, 129.5, 128.8, 128.4(9), 128.4(5), 128.3, 128.0(5), 128.0(3), 128.0(1), 127.1, 122.6, 121.9, 86.8, 84.4, 79.5, 73.6, 54.8, 41.0; IR (neat): 2925, 2237, 1597, 1491, 1442, 1369, 1169, 1090, 756, 691, 598; HRESIMS Calcd for $[\text{C}_{30}\text{H}_{23}\text{NNaO}_2\text{S}]^+$ ($\text{M} + \text{Na}^+$) 484.1342, found

484.1344.

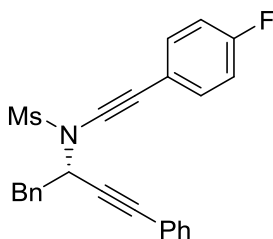
(S)-N-(1,4-diphenylbut-3-yn-2-yl)-N-(phenylethynyl)methanesulfonamide (1d)



1d

Yellow solid (mp 112-114 °C). $[\alpha]_D^{20} = +90.8^\circ$ ($c = 1.0$, CHCl_3). 98% ee (determined by HPLC: Chiralcel IA Column, 2/98 *i*-PrOH/hexane, 0.8 mL/min, 254 nm, 25 °C; $t_R = 22.59$ min (minor), 19.67 min (major)). ^1H NMR (400 MHz, CDCl_3) δ 7.56 – 7.46 (m, 2H), 7.45 – 7.39 (m, 2H), 7.39 – 7.25 (m, 11H), 5.13 (dd, $J = 8.0, 6.8$ Hz, 1H), 3.45 – 3.19 (m, 2H), 2.95 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 136.0, 131.8, 129.6, 128.9, 128.6, 128.3(8), 128.3(5), 128.2, 127.4, 122.5, 121.9, 86.9, 84.9, 78.8, 74.1, 54.8, 40.8, 38.4; IR (neat): 2925, 2237, 1597, 1491, 1443, 1369, 1169, 1090, 756, 691, 598; HRESIMS Calcd for $[\text{C}_{25}\text{H}_{21}\text{NNaO}_2\text{S}]^+$ ($\text{M} + \text{Na}^+$) 422.1185, found 422.1184.

(S)-N-(1,4-diphenylbut-3-yn-2-yl)-N-((4-fluorophenyl)ethynyl)methanesulfonamide (1e)

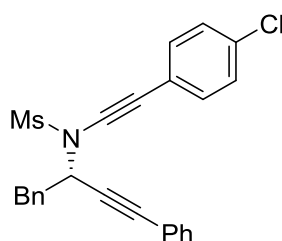


1e

White solid (mp 111-113 °C). $[\alpha]_D^{20} = +109.9^\circ$ ($c = 1.0$, CHCl_3). 98% ee (determined by HPLC: Chiralcel IA Column, 2/98 *i*-PrOH/hexane, 0.8 mL/min, 254 nm, 25 °C; $t_R = 18.86$ min (minor), 16.62 min (major)). ^1H NMR (400 MHz, CDCl_3) δ 7.51 – 7.44 (m, 2H), 7.43 – 7.39 (m, 2H), 7.38 – 7.24 (m, 8H), 7.07 – 6.98 (m, 2H), 5.13 (dd, $J =$

8.4, 7.2 Hz, 1H), 3.40 – 3.22 (m, 2H), 2.93 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 162.5 (d, $J = 248.1$ Hz), 135.9, 133.9 (d, $J = 8.3$ Hz), 131.7, 129.5, 128.9, 128.6, 128.4, 127.4, 121.8, 118.5 (d, $J = 3.4$ Hz), 115.6 (d, $J = 22.0$ Hz), 87.0, 84.8, 78.5, 73.0, 54.8, 40.8, 38.4; IR (neat): 2928, 2239, 1508, 1490, 1362, 1167, 1093, 756, 692; HRESIMS Calcd for $[\text{C}_{25}\text{H}_{20}\text{FNNaO}_2\text{S}]^+$ ($\text{M} + \text{Na}^+$) 440.1091, found 440.1092.

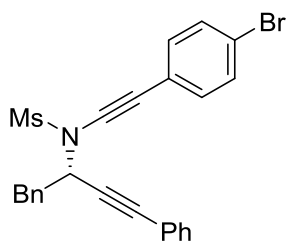
(S)-N-((4-chlorophenyl)ethynyl)-N-(1,4-diphenylbut-3-yn-2-yl)methanesulfonamide (1f)



1f

White solid (mp 112-113 °C). $[\alpha]_{\text{D}}^{20} = +102.1$ °(c = 1.0, CHCl_3). 98% ee (determined by HPLC: Chiralcel IA Column, 2/98 *i*-PrOH/hexane, 0.8 mL/min, 254 nm, 25 °C; $t_{\text{R}} = 20.35$ min (minor), 18.10 min (major)). ^1H NMR (400 MHz, CDCl_3) δ 7.46 – 7.38 (m, 4H), 7.37 – 7.28 (m, 10H), 5.13 (dd, $J = 8.4, 7.2$ Hz, 1H), 3.40 – 3.25 (m, 2H), 2.93 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 135.9, 134.2, 132.9, 131.7, 129.5, 128.9, 128.7, 128.6, 128.4, 127.4, 121.8, 121.0, 87.1, 84.8, 79.9, 73.1, 54.8, 40.9, 38.6; IR (neat): 2926, 2237, 1558, 1490, 1362, 1166, 1098, 758, 692; HRESIMS Calcd for $[\text{C}_{25}\text{H}_{20}\text{ClNNaO}_2\text{S}]^+$ ($\text{M} + \text{Na}^+$) 456.0795, found 456.0799.

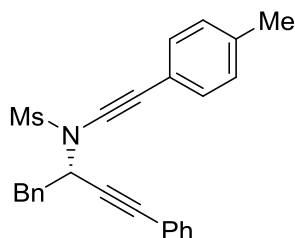
(S)-N-((4-bromophenyl)ethynyl)-N-(1,4-diphenylbut-3-yn-2-yl)methanesulfonamide (1g)



1g

Yellow solid (mp 110-112 °C). $[\alpha]_D^{20} = +114.4^\circ$ ($c = 1.0$, CHCl_3). 98% ee (determined by HPLC: Chiralcel IA Column, 2/98 *i*-PrOH/hexane, 0.8 mL/min, 254 nm, 25 °C; $t_R = 21.25$ min (minor), 18.85 min (major)). ^1H NMR (400 MHz, CDCl_3) δ 7.48 – 7.38 (m, 4H), 7.37 – 7.26 (m, 10H), 5.13 (t, $J = 7.2$ Hz, 1H), 3.38 – 3.25 (m, 2H), 2.92 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 135.9, 133.0, 131.7, 131.6, 129.5, 128.9, 128.6, 128.4, 127.4, 122.3, 121.8, 121.5, 87.1, 84.7, 80.1, 73.2, 54.8, 40.9, 38.6; IR (neat): 2929, 2237, 1489, 1364, 1167, 1100, 758, 691, 517; HRESIMS Calcd for $[\text{C}_{25}\text{H}_{20}\text{BrNNaO}_2\text{S}]^+$ ($M + \text{Na}^+$) 500.0290, found 500.0292.

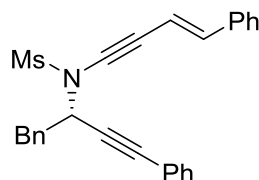
(S)-N-(1,4-diphenylbut-3-yn-2-yl)-N-(p-tolylethynyl)methanesulfonamide (1h)



1h

White solid (mp 113-115 °C). $[\alpha]_D^{20} = +108.8^\circ$ ($c = 1.0$, CHCl_3). 99% ee (determined by HPLC: Chiralcel IA Column, 2/98 *i*-PrOH/hexane, 0.8 mL/min, 254 nm, 25 °C; $t_R = 23.01$ min (minor), 20.07 min (major)). ^1H NMR (400 MHz, CDCl_3) δ 7.47 – 7.26 (m, 12H), 7.14 (d, $J = 7.6$ Hz, 2H), 5.12 (dd, $J = 8.8, 6.8$ Hz, 1H), 3.40 – 3.25 (m, 2H), 2.94 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 138.5, 136.1, 131.9, 131.8, 129.6, 129.1, 128.8, 128.6, 128.4, 127.3, 122.0, 119.4, 86.9, 85.0, 78.2, 74.1, 54.8, 40.8, 38.3, 21.4; IR (neat): 2926, 2235, 1490, 1361, 1166, 1101, 816, 756, 691, 516; HRESIMS Calcd for $[\text{C}_{26}\text{H}_{23}\text{NNaO}_2\text{S}]^+$ ($M + \text{Na}^+$) 436.1342, found 436.1344.

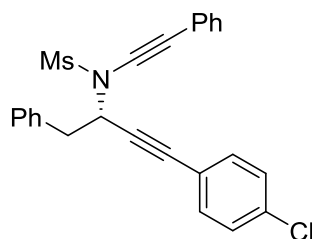
(*S,E*)-*N*-(1,4-diphenylbut-3-yn-2-yl)-*N*-(4-phenylbut-3-en-1-yn-1-yl)methanesulfonamide (1i**)**



1i

White solid (mp 106-108 °C). $[\alpha]_D^{20} = +74.5^\circ$ (c = 1.0, CHCl₃). 97% ee (determined by HPLC: Chiralcel IC Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; t_R = 12.75 min (minor), 16.52 min (major)). ¹H NMR (400 MHz, CDCl₃) δ 7.45 – 7.25 (m, 15H), 6.97 (d, J = 16.0 Hz, 1H), 6.36 (d, J = 16.4 Hz, 1H), 5.11 (dd, J = 8.4, 6.8 Hz, 1H), 3.36 – 3.24 (m, 2H), 2.92 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 140.6, 136.2, 136.0, 131.8, 129.5, 128.9, 128.7, 128.6, 128.5, 128.4, 127.3, 126.1, 121.9, 107.3, 86.9, 84.9, 80.7, 73.7, 54.8, 40.8, 38.4; IR (neat): 2927, 2219, 1490, 1362, 1165, 956, 750, 691; HRESIMS Calcd for [C₂₇H₂₃NNaO₂S]⁺ (M + Na⁺) 448.1342, found 448.1342.

(*S*)-*N*-(4-(4-chlorophenyl)-1-phenylbut-3-yn-2-yl)-*N*-(phenylethynyl)methanesulfonamide (1j**)**

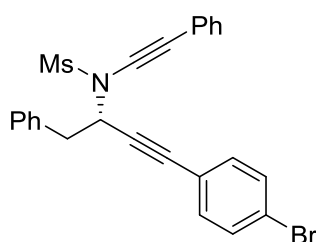


1j

Yellow solid (mp 114-116 °C). $[\alpha]_D^{20} = +101.3^\circ$ (c = 1.0, CHCl₃). 96% ee (determined by HPLC: Chiralcel IC Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; t_R = 10.47 min (minor), 13.51min (major)). ¹H NMR (400 MHz, CDCl₃) δ 7.54 – 7.45 (m, 2H), 7.36 – 7.26 (m, 12H), 5.13 (dd, J = 8.4, 6.8 Hz, 1H), 3.40 – 3.25 (m, 2H),

2.87 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 135.9, 135.0, 133.0, 131.7, 129.5, 128.7, 128.6, 128.4, 128.3, 127.4, 122.4, 120.3, 86.0, 85.7, 78.7, 74.2, 54.7, 40.7, 38.4; IR (neat): 2929, 2237, 1489, 1362, 1166, 1092, 1015, 755, 692; HRESIMS Calcd for $[\text{C}_{25}\text{H}_{20}\text{ClNNaO}_2\text{S}]^+$ ($\text{M} + \text{Na}^+$) 456.0795, found 456.0797.

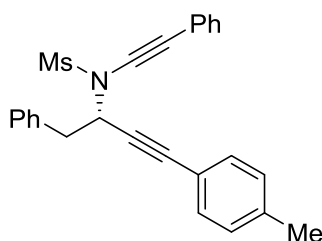
(S)-N-(4-(4-bromophenyl)-1-phenylbut-3-yn-2-yl)-N-(phenylethynyl)methanesulfonamide (1k)



1k

Yellow solid (mp 115-117 °C). $[\alpha]_{\text{D}}^{20} = +95.8^\circ$ ($c = 1.0$, CHCl_3). 97% ee (determined by HPLC: Chiralcel IC Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; $t_{\text{R}} = 10.85$ min (minor), 14.07 min (major)). ^1H NMR (400 MHz, CDCl_3) δ 7.53 – 7.48 (m, 2H), 7.45 – 7.39 (m, 2H), 7.37 – 7.28 (m, 10H), 5.14 (dd, $J = 8.0, 6.8$ Hz, 1H), 3.40 – 3.25 (m, 2H), 2.93 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 136.0, 133.1, 131.7, 129.5, 128.8, 128.6, 128.3(4), 128.3(1), 128.2, 127.3, 122.5, 121.8, 86.9, 84.9, 78.9, 74.1, 54.8, 40.8, 38.4; IR (neat): 2929, 2236, 1598, 1490, 1362, 1323, 1166, 963, 755, 691; HRESIMS Calcd for $[\text{C}_{25}\text{H}_{20}\text{BrNNaO}_2\text{S}]^+$ ($\text{M} + \text{Na}^+$) 500.0290, found 500.0291.

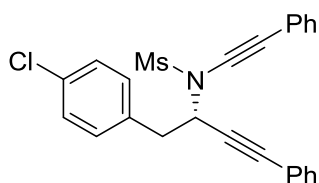
(S)-N-(1-phenyl-4-(*p*-tolyl)but-3-yn-2-yl)-N-(phenylethynyl)methanesulfonamide (1l)



1l

White solid (mp 113-115 °C). $[\alpha]_D^{20} = +112.3^\circ$ (c = 1.0, CHCl₃). 99% ee (determined by HPLC: Chiralcel IC Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; t_R = 11.67 min (minor), 16.25 min (major)). ¹H NMR (400 MHz, CDCl₃) δ 7.51 – 7.48 (m, 2H), 7.38 – 7.26 (m, 10H), 7.12 (d, *J* = 7.6 Hz, 2H), 5.12 (dd, *J* = 8.4, 6.8 Hz, 1H), 3.40 – 3.25 (m, 2H), 2.95 (s, 3H), 2.34 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 139.1, 136.1, 131.7, 131.6, 129.5, 129.1, 128.6, 128.3, 128.2, 127.3, 122.5, 118.8, 87.1, 84.2, 78.9, 74.0, 54.9, 40.8, 38.3, 21.5; IR (neat): 2927, 2236, 1509, 1362, 1166, 1104, 963, 754, 692, 558; HRESIMS Calcd for [C₂₆H₂₃NNaO₂S]⁺ (M + Na⁺) 436.1342, found 436.1342.

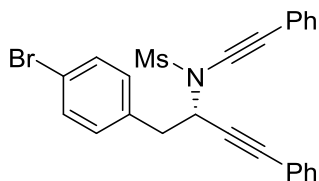
(S)-N-(1-(4-chlorophenyl)-4-phenylbut-3-yn-2-yl)-N-(phenylethynyl)methanesulfonamide (1m)



1m

White solid (mp 116-118 °C). $[\alpha]_D^{20} = +95.3^\circ$ (c = 1.0, CHCl₃). 95% ee (determined by HPLC: Chiralcel IA Column, 2/98 *i*-PrOH/hexane, 0.8 mL/min, 254 nm, 25 °C; t_R = 24.65 min (minor), 18.24 min (major)). ¹H NMR (400 MHz, CDCl₃) δ 7.51 – 7.46 (m, 2H), 7.42 – 7.38 (m, 2H), 7.37 – 7.26 (m, 10H), 5.09 (t, *J* = 7.2 Hz, 1H), 3.36 – 3.24 (m, 2H), 3.08 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 134.3, 133.2, 131.7(3), 131.7(1), 130.9, 129.0, 128.7, 128.4(2), 128.3(5), 128.3(0), 122.3, 121.6, 87.4, 84.4, 78.8, 74.1, 54.5, 40.2, 38.4; IR (neat): 2928, 2237, 1491, 1455, 1362, 1163, 1094, 1016, 756, 691; HRESIMS Calcd for [C₂₅H₂₀ClNNaO₂S]⁺ (M + Na⁺) 456.0795, found 456.0794.

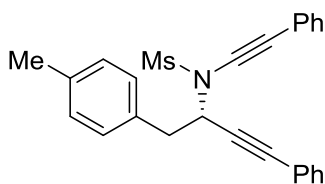
(S)-N-(1-(4-bromophenyl)-4-phenylbut-3-yn-2-yl)-N-(phenylethynyl)methanesulfonamide (1n)



1n

Yellow solid (mp 117-119 °C). $[\alpha]_D^{20} = +95.6^\circ$ (c = 1.0, CHCl₃). 99% ee (determined by HPLC: Chiralcel IA Column, 2/98 *i*-PrOH/hexane, 0.8 mL/min, 254 nm, 25 °C; t_R 25.46 = min (minor), 19.77 min (major)). ¹H NMR (400 MHz, CDCl₃) δ 7.50 – 7.44 (m, 4H), 7.43 – 7.38 (m, 2H), 7.37 – 7.29 (m, 6H), 7.23 (d, J = 7.2 Hz, 2H), 5.09 (dd, J = 8.0, 7.2 Hz, 1H), 3.35 – 3.21 (m, 2H), 3.09 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 134.9, 131.8, 131.7(4), 131.7(0), 131.2, 129.0, 128.5, 128.4, 128.3, 122.3, 121.7, 121.4, 87.5, 84.4, 78.8, 74.2, 54.4, 40.3, 38.5; IR (neat): 2929, 2360, 2237, 1489, 1363, 1167, 1012, 757, 691; HRESIMS Calcd for [C₂₅H₂₀BrNNaO₂S]⁺ (M + Na⁺) 500.0290, found 500.0290.

(S)-N-(4-phenyl-1-(*p*-tolyl)but-3-yn-2-yl)-N-(phenylethynyl)methanesulfonamide (1o)

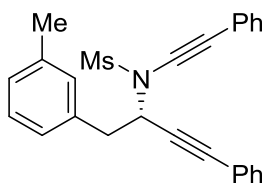


1o

White solid (mp 114-116 °C). $[\alpha]_D^{20} = +105.1^\circ$ (c = 1.0, CHCl₃). 95% ee (determined by HPLC: Chiralcel IC Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; t_R = 10.94 min (minor), 13.19 min (major)). ¹H NMR (500 MHz, CDCl₃) δ 7.51 – 7.47 (m, 2H), 7.44 – 7.39 (m, 2H), 7.35 – 7.28 (m, 6H), 7.25 (d, J = 8.0 Hz, 2H), 7.14 (d, J = 7.5 Hz, 2H), 5.10 (dd, J = 8.5, 6.5 Hz, 1H), 3.34 – 3.22 (m, 2H), 2.94 (s, 3H), 2.32 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 136.9, 132.8, 131.6(9), 131.6(7), 129.3, 129.2, 128.8, 128.3(2), 128.2(8), 128.1(5), 122.4, 121.8, 86.8, 84.9, 78.9, 73.9, 54.8, 40.4,

38.3, 21.0; IR (neat): 2927, 2236, 1490, 1443, 1363, 1166, 963, 757, 691; HRESIMS Calcd for $[C_{26}H_{23}NNaO_2S]^+$ ($M + Na^+$) 436.1342, found 436.1338.

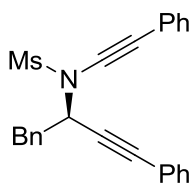
(S)-N-(4-phenyl-1-(*m*-tolyl)but-3-yn-2-yl)-N-(phenylethynyl)methanesulfonamide (1p)



1p

Pale yellow oil: $[\alpha]_D^{20} = +114.9^\circ$ ($c = 1.0$, $CHCl_3$); 95% ee (determined by HPLC: Chiralcel IA Column, 2/98 *i*-PrOH/hexane, 0.8 mL/min, 254 nm, 25 °C; $t_R = 14.79$ min (major), 17.41 min (minor)); 1H NMR (500 MHz, $CDCl_3$) δ 7.58 – 7.52 (m, 2H), 7.46 (d, $J = 7.5$ Hz, 2H), 7.40 – 7.32 (m, 6H), 7.28 (d, $J = 8.5$ Hz, 1H), 7.22 (d, $J = 8.5$ Hz, 2H), 7.13 (d, $J = 7.5$ Hz, 1H), 5.17 (t, $J = 8.0$ Hz, 1H), 3.40 – 3.26 (m, 2H), 2.99 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 137.9, 135.7, 131.5, 130.1, 128.7, 128.3, 128.2(2), 128.2(0), 128.1, 127.9, 126.4, 122.3, 121.7, 86.8, 84.9, 78.9, 73.9, 54.7, 40.6, 38.2, 21.2; IR (neat): 3022, 2925, 2236, 1490, 1442, 1361, 1165, 963, 948, 756, 690, 561; HRESIMS Calcd for $[C_{26}H_{23}NNaO_2S]^+$ ($M + Na^+$) 436.1342, found 436.1346.

(R)-N-(1,4-diphenylbut-3-yn-2-yl)-N-(phenylethynyl)methanesulfonamide (1d')

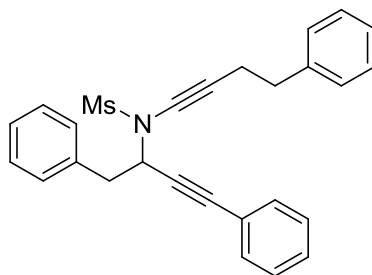


1d'

$[\alpha]_D^{20} = -131.5^\circ$ ($c = 1.0$, $CHCl_3$). 98% ee (determined by HPLC: Chiralcel IA Column, 2/98 *i*-PrOH/hexane, 0.8 mL/min, 254 nm, 25 °C; $t_R = 19.71$ min (minor),

22.40 min (major)).

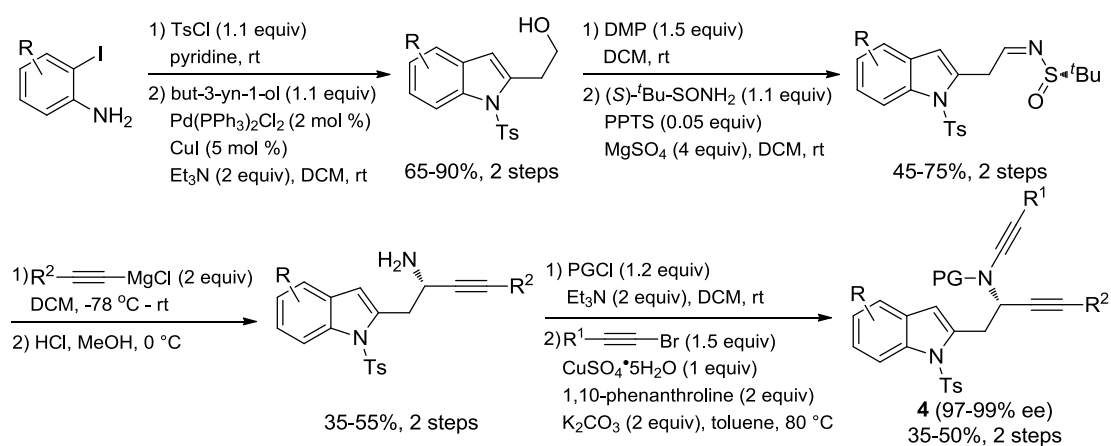
***N*-(1,4-diphenylbut-3-yn-2-yl)-*N*-(4-phenylbut-1-yn-1-yl)methanesulfonamide (1q)**



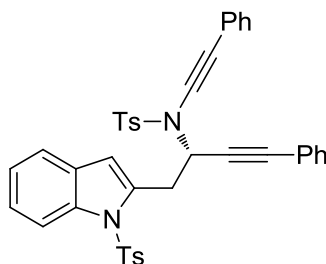
1q

^1H NMR (400 MHz, CDCl_3) δ 7.44 – 7.39 (m, 2H), 7.38 – 7.25 (m, 12H), 7.21 – 7.17 (m, 1H), 5.00 (t, $J = 7.6$ Hz, 1H), 3.20 – 3.08 (m, 2H), 2.93 (t, $J = 7.2$ Hz, 2H), 2.82 – 2.72 (m, 5H); ^{13}C NMR (100 MHz, CDCl_3) δ 140.4, 136.1, 131.7, 129.5, 128.8, 128.5(4), 128.5(0), 128.4, 127.2, 126.3, 122.0, 86.6, 85.2, 73.1, 70.6, 54.2, 40.4, 37.7, 35.1, 20.5; HRESIMS Calcd for $[\text{C}_{27}\text{H}_{25}\text{NNaO}_2\text{S}]^+$ ($\text{M} + \text{Na}^+$) 450.1498, found 450.1499.

Compounds **4a-4l** were prepared according to the following procedures.¹⁻³



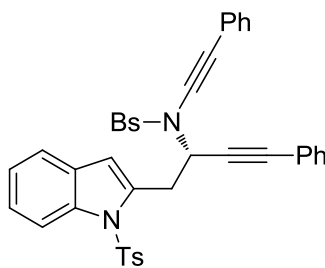
(*S*)-4-methyl-*N*-(4-phenyl-1-(1-tosyl-1*H*-indol-2-yl)but-3-yn-2-yl)-*N*-(phenylethynyl)benzenesulfonamide (4a)



4a

Yellow solid (mp 94-96 °C). $[\alpha]_D^{20} = -24.5^\circ$ ($c = 1.0$, CHCl_3). 99% ee (determined by HPLC: Chiralcel IC Column, 10/90 *i*-PrOH/hexane, 1.5 mL/min, 210 nm, 25 °C; $t_R = 17.45$ min (minor), 26.37 min (major)). ^1H NMR (500 MHz, CDCl_3) δ 8.12 (d, $J = 8.5$ Hz, 1H), 7.78 (d, $J = 8.5$ Hz, 2H), 7.62 (d, $J = 8.5$ Hz, 2H), 7.49 – 7.43 (m, 2H), 7.40 (d, $J = 7.5$ Hz, 1H), 7.35 – 7.30 (m, 3H), 7.29 – 7.26 (m, 2H), 7.25 – 7.19 (m, 3H), 7.16 – 7.08 (m, 6H), 6.67 (s, 1H), 5.53 (dd, $J = 9.0, 8.5$ Hz, 1H), 3.72 – 3.62 (m, 2H), 2.27 (s, 3H), 2.24 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 144.8, 144.6, 137.2, 135.7, 135.0, 134.4, 131.7, 131.5, 129.9, 129.5, 129.4, 128.5, 128.3, 128.0(4), 127.9(8), 127.9(5), 126.3, 124.5, 123.6, 122.9, 122.0, 120.7, 114.8, 112.5, 86.4, 84.4, 79.6, 73.8, 52.9, 34.3, 21.5(2), 21.4(9); IR (neat): 2924, 2234(s), 1596, 1451, 1366, 1171, 1090, 755, 592; HRESIMS Calcd for $[\text{C}_{40}\text{H}_{32}\text{N}_2\text{NaO}_4\text{S}_2]^+$ ($\text{M} + \text{Na}^+$) 691.1696, found 691.1709.

(S)-4-bromo-N-(4-phenyl-1-(1-tosyl-1H-indol-2-yl)but-3-yn-2-yl)-N-(phenylethynyl)benzenesulfonamide (4b)

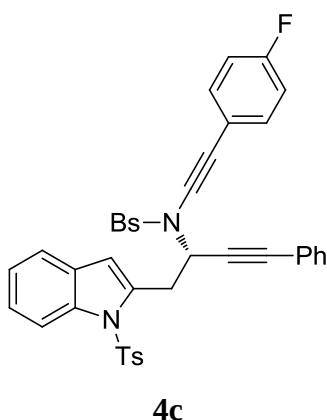


4b

Yellow solid (mp 95-97 °C). $[\alpha]_D^{20} = -20.3^\circ$ ($c = 1.0$, CHCl_3). 99% ee (determined by HPLC: Chiralcel IC Column, 8/92 *i*-PrOH/hexane, 1.5 mL/min, 210 nm, 25 °C; $t_R =$

16.71 min (minor), 24.63 min (major)). ^1H NMR (500 MHz, CDCl_3) δ 8.13 (m, 1H), 7.72 (d, J = 8.5 Hz, 2H), 7.62 (d, J = 8.5 Hz, 2H), 7.48 – 7.44 (m, 2H), 7.43 – 7.37 (m, 3H), 7.36 – 7.31 (m, 3H), 7.31 – 7.20 (m, 5H), 7.18 – 7.14 (m, 2H), 7.10 (d, J = 8.0 Hz, 2H), 6.63 (s, 1H), 5.57 (t, J = 7.4 Hz, 1H), 3.67 (d, J = 7.4 Hz, 2H), 2.27 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 144.9, 137.1, 136.3, 135.6, 134.7, 132.0, 131.6(9), 131.6(5), 129.9, 129.3(2), 129.3(0), 128.9, 128.7, 128.4, 128.2, 126.2, 124.7, 123.8, 122.5, 121.7, 120.7, 114.9, 112.8, 86.8, 84.1, 79.0, 74.0, 53.2, 34.4, 21.5; IR (neat): 2924, 2235(s), 1573, 1451, 1369, 1174, 1089, 755, 580; HRESIMS Calcd for $[\text{C}_{39}\text{H}_{29}\text{BrN}_2\text{NaO}_4\text{S}_2]^+$ ($\text{M} + \text{Na}^+$) 755.0644, found 755.0665.

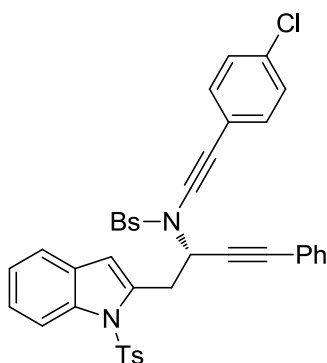
(S)-4-bromo-*N*-((4-fluorophenyl)ethynyl)-*N*-(4-phenyl-1-(1-tosyl-1*H*-indol-2-yl)but-3-yn-2-yl)benzenesulfonamide (4c)



Yellow solid (mp 96-98 °C). $[\alpha]_{\text{D}}^{20}$ = -32.3 °(c = 1.0, CHCl_3). 98% ee (determined by HPLC: Chiralcel IC Column, 10/90 *i*-PrOH/hexane, 1.5 mL/min, 210 nm, 25 °C; t_{R} = 13.43 min (minor), 19.49 min (major)). ^1H NMR (500 MHz, CDCl_3) δ 8.12 (d, J = 8.5 Hz, 1H), 7.72 (d, J = 9.0 Hz, 2H), 7.62 (d, J = 8.5 Hz, 2H), 7.46 – 7.38 (m, 5H), 7.34 – 7.21 (m, 5H), 7.19 – 7.10 (m, 4H), 7.06 – 7.01 (m, 2H), 6.62 (s, 1H), 5.56 (t, J = 7.5 Hz, 1H), 3.66 (d, J = 7.0 Hz, 2H), 2.29 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 162.6 (d, J = 247.5 Hz), 144.9, 137.2, 136.3, 135.6, 134.7, 133.8 (d, J = 7.5 Hz), 132.1, 131.7, 129.9, 129.3, 129.0, 128.7, 128.3, 126.3, 124.8, 123.9, 121.7, 120.7, 118.5 (d, J = 3.8 Hz), 115.7 (d, J = 21.3 Hz), 114.9, 112.8, 86.8, 84.1, 78.7, 72.9, 53.3, 34.5, 21.5;

IR (neat): 2925, 2237(s), 1599, 1509, 1369, 1175, 1090, 752,578; HRESIMS Calcd for $[\text{C}_{39}\text{H}_{28}\text{BrFN}_2\text{NaO}_4\text{S}_2]^+$ ($\text{M} + \text{Na}^+$) 773.0550, found 773.0568.

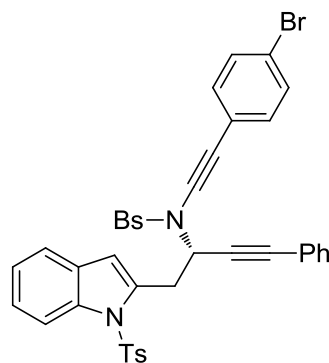
(S)-4-bromo-N-((4-chlorophenyl)ethynyl)-N-(4-phenyl-1-(1-tosyl-1*H*-indol-2-yl)but-3-yn-2-yl)benzenesulfonamide (4d)



4d

Yellow solid (mp 95-97 °C). $[\alpha]_{\text{D}}^{20} = -36.7^\circ$ ($c = 1.0$, CHCl_3). 98% ee (determined by HPLC: Chiralcel IC Column, 10/90 *i*-PrOH/hexane, 1.5 mL/min, 210 nm, 25 °C; $t_{\text{R}} = 14.03$ min (minor), 22.80 min (major)). ^1H NMR (500 MHz, CDCl_3) δ 8.12 (d, $J = 8.5$ Hz, 1H), 7.71 (d, $J = 9.0$ Hz, 2H), 7.61 (d, $J = 8.5$ Hz, 2H), 7.43 – 7.35 (m, 5H), 7.33 – 7.19 (m, 7H), 7.18 – 7.14 (m, 2H), 7.11 (d, $J = 8.0$ Hz, 2H), 6.61 (s, 1H), 5.56 (t, $J = 7.5$ Hz, 1H), 3.66 (d, $J = 7.0$ Hz, 2H), 2.28 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 144.9, 137.1, 136.3, 135.6, 134.6, 134.2, 132.8, 132.1, 131.7, 129.9, 129.3, 129.2, 129.0, 128.8, 128.7, 128.3, 126.2, 124.8, 123.9, 121.7, 121.0, 120.7, 114.9, 112.8, 86.9, 84.0, 80.0, 73.1, 53.3, 34.5, 21.5; IR (neat): 2924, 2236(s), 1573, 1451, 1369, 1174, 1089, 743, 575; HRESIMS Calcd for $[\text{C}_{39}\text{H}_{28}\text{BrClN}_2\text{NaO}_4\text{S}_2]^+$ ($\text{M} + \text{Na}^+$) 789.0255, found 789.0275.

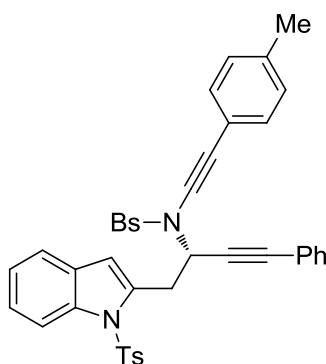
(S)-4-bromo-N-((4-bromophenyl)ethynyl)-N-(4-phenyl-1-(1-tosyl-1*H*-indol-2-yl)but-3-yn-2-yl)benzenesulfonamide (4e)



4e

Yellow solid (mp 94-96 °C). $[\alpha]_D^{20} = -38.3^\circ$ ($c = 1.0$, CHCl_3). 97% ee (determined by HPLC: Chiralcel IC Column, 8/92 *i*-PrOH/hexane, 1.5 mL/min, 210 nm, 25 °C; $t_R = 18.32$ min (minor), 27.15 min (major)). ^1H NMR (500 MHz, CDCl_3) δ 8.12 (d, $J = 8.5$ Hz, 1H), 7.70 (d, $J = 8.5$ Hz, 2H), 7.61 (d, $J = 8.0$ Hz, 2H), 7.46 (d, $J = 8.0$ Hz, 2H), 7.43 – 7.36 (m, 3H), 7.35 – 7.22 (m, 7H), 7.16 (d, $J = 8.0$ Hz, 2H), 7.11 (d, $J = 8.1$ Hz, 2H), 6.61 (s, 1H), 5.56 (t, $J = 7.3$ Hz, 1H), 3.66 (d, $J = 7.5$ Hz, 2H), 2.28 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 145.0, 137.1, 136.3, 135.6, 134.6, 133.0, 132.1, 131.6(8), 131.6(5), 129.9, 129.2(7), 129.2(5), 129.1, 128.8, 128.3, 126.2, 124.8, 123.9, 122.4, 121.6, 121.4, 120.7, 114.9, 112.8, 86.9, 84.0, 80.2, 73.2, 53.3, 34.5, 21.5; IR (neat): 2923, 2234(s), 1595, 1451, 1367, 1173, 1088, 742, 582; HRESIMS Calcd for $[\text{C}_{39}\text{H}_{28}\text{Br}_2\text{N}_2\text{NaO}_4\text{S}_2]^+$ ($\text{M} + \text{Na}^+$) 832.9749, found 832.9782.

(S)-4-bromo-N-(4-phenyl-1-(1-tosyl-1H-indol-2-yl)but-3-yn-2-yl)-N-(p-tolyethynyl)benzenesulfonamide (4f)

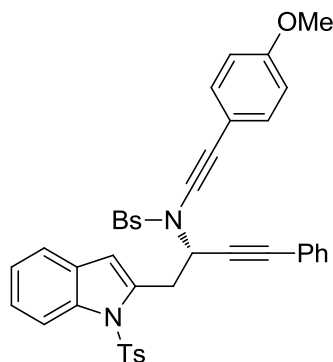


4f

Yellow solid (mp 100-102 °C). $[\alpha]_D^{20} = -14.5^\circ$ ($c = 1.0$, CHCl_3). 98% ee (determined

by HPLC: Chiralcel IC Column, 10/90 *i*-PrOH/hexane, 1.5 mL/min, 210 nm, 25 °C; t_R = 17.83 min (minor), 25.88 min (major)). ^1H NMR (500 MHz, CDCl_3) δ 8.13 (d, J = 8.0 Hz, 1H), 7.72 (d, J = 8.5 Hz, 2H), 7.62 (d, J = 8.5 Hz, 2H), 7.44 – 7.34 (m, 5H), 7.33 – 7.20 (m, 5H), 7.19 – 7.13 (m, 4H), 7.11 (d, J = 8.5 Hz, 2H), 6.63 (s, 1H), 5.56 (t, J = 7.5 Hz, 1H), 3.67 – 3.65 (m, 2H), 2.37 (s, 3H), 2.28 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 144.9, 138.5, 137.1, 136.3, 135.7, 134.8, 132.0, 131.8, 131.7, 129.9, 129.3, 129.2, 128.9, 128.7, 128.2, 126.3, 124.7, 123.8, 121.8, 120.7, 119.3, 114.9, 112.8, 86.7, 84.2, 78.3, 74.0, 53.2, 34.4, 21.5, 21.4; IR (neat): 2923, 2234(s), 1573, 1451, 1368, 1174, 1088, 749, 581; HRESIMS Calcd for $[\text{C}_{40}\text{H}_{31}\text{BrN}_2\text{NaO}_4\text{S}_2]^+$ ($\text{M} + \text{Na}^+$) 769.0801, found 769.0822.

(S)-4-bromo-N-((4-methoxyphenyl)ethynyl)-N-(4-phenyl-1-(1-tosyl-1*H*-indol-2-yl)but-3-yn-2-yl)benzenesulfonamide (4g)

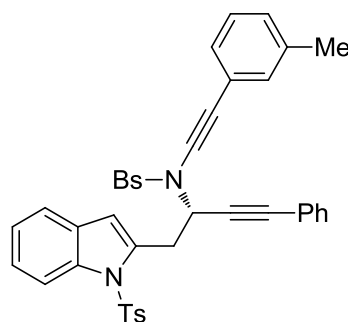


4g

Yellow solid (mp 98-100 °C). $[\alpha]_D^{20}$ = -55.6 ° (c = 1.0, CHCl_3). 97% ee (determined by HPLC: Chiralcel IC Column, 15/85 *i*-PrOH/hexane, 1.5 mL/min, 210 nm, 25 °C; t_R = 18.61 min (minor), 26.33 min (major)). ^1H NMR (500 MHz, CDCl_3) δ 8.13 (d, J = 8.0 Hz, 1H), 7.73 (d, J = 8.5 Hz, 2H), 7.62 (d, J = 8.5 Hz, 2H), 7.48 – 7.35 (m, 6H), 7.35 – 7.19 (m, 4H), 7.18 – 7.08 (m, 4H), 6.87 (d, J = 9.0 Hz, 2H), 6.63 (s, 1H), 5.55 (dd, J = 8.0, 6.5 Hz, 1H), 3.83 (s, 3H), 3.69 – 3.60 (m, 2H), 2.29 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 159.9, 144.9, 137.1, 136.4, 135.7, 134.8, 133.8, 132.0, 131.7, 129.9, 129.4, 128.8, 128.6, 128.2, 126.3, 124.7, 123.8, 121.8, 120.7, 114.9, 114.3, 114.1, 112.7, 86.7, 84.2, 77.6, 73.7, 55.4, 53.3, 34.4, 21.5; IR (neat): 2923, 2234(s),

1573, 1451, 1368, 1174, 1088, 749, 581; HRESIMS Calcd for $[\text{C}_{40}\text{H}_{31}\text{BrN}_2\text{NaO}_5\text{S}_2]^+$ (M + Na⁺) 785.0750, found 785.0765.

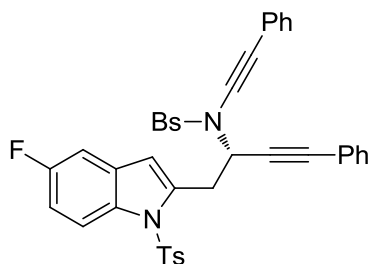
(S)-4-bromo-N-(4-phenyl-1-(1-tosyl-1H-indol-2-yl)but-3-yn-2-yl)-N-(m-tolylethynyl)benzenesulfonamide (4h)



4h

Yellow solid (mp 93-95 °C). $[\alpha]_{\text{D}}^{20} = -31.6^\circ$ (c = 1.0, CHCl_3). 99% ee (determined by HPLC: Chiralcel IC Column, 8/92 *i*-PrOH/hexane, 1.5 mL/min, 210 nm, 25 °C; $t_{\text{R}} = 20.77$ min (minor), 30.23 min (major)). ^1H NMR (500 MHz, CDCl_3) δ 8.13 (d, $J = 8.5$ Hz, 1H), 7.72 (d, $J = 9.0$ Hz, 2H), 7.62 (d, $J = 8.5$ Hz, 2H), 7.43 – 7.36 (m, 3H), 7.35 – 7.20 (m, 8H), 7.19 – 7.12 (m, 3H), 7.10 (d, $J = 8.5$ Hz, 2H), 6.63 (s, 1H), 5.56 (t, $J = 7.5$ Hz, 1H), 3.67 (d, $J = 7.5$ Hz, 2H), 2.33 (s, 3H), 2.28 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 144.9, 138.1, 137.1, 136.4, 135.6, 134.7, 132.2, 132.0, 131.7, 129.9, 129.3(4), 129.3(1), 129.1, 128.9, 128.6(9), 128.6(7), 128.3, 128.2, 126.3, 124.7, 123.8, 122.3, 121.8, 120.7, 114.9, 112.8, 86.8, 84.2, 78.7, 74.2, 53.2, 34.4, 21.5, 21.2; IR (neat): 2922, 2234(s), 1596, 1451, 1366, 1180, 1075, 755, 581; HRESIMS Calcd for $[\text{C}_{40}\text{H}_{31}\text{BrN}_2\text{NaO}_4\text{S}_2]^+$ (M + Na⁺) 769.0801, found 769.0828.

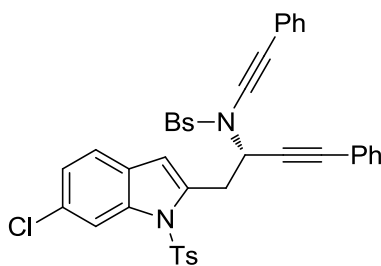
(S)-4-bromo-N-(1-(5-fluoro-1-tosyl-1H-indol-2-yl)-4-phenylbut-3-yn-2-yl)-N-(phenylethynyl)benzenesulfonamide (4i)



4i

White solid (mp 93-95 °C). $[\alpha]_D^{20} = -34.6^\circ$ (c = 1.0, CHCl₃). 98% ee (determined by HPLC: Chiralcel IC Column, 10/90 *i*-PrOH/hexane, 1.5 mL/min, 210 nm, 25 °C; t_R = 13.30 min (minor), 17.90 min (major)). ¹H NMR (500 MHz, CDCl₃) δ 8.10 – 8.05 (m, 1H), 7.75 (d, *J* = 8.5 Hz, 2H), 7.60 (d, *J* = 8.0 Hz, 2H), 7.48 – 7.42 (m, 4H), 7.36 – 7.26 (m, 6H), 7.18 – 7.10 (m, 4H), 7.08 – 7.00 (m, 2H), 6.60 (s, 1H), 5.55 (dd, *J* = 8.5, 6.5 Hz, 1H), 3.67 – 3.64 (m, 2H), 2.29 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 159.8 (d, *J* = 238.8 Hz), 145.2, 136.6, 136.3, 135.4, 133.4, 132.1, 131.7 (d, *J* = 2.5 Hz), 130.4 (d, *J* = 10.0 Hz), 123.0, 129.3, 129.0, 128.8, 128.4, 128.3(0), 128.2(7), 126.2, 122.4, 121.6, 116.0 (d, *J* = 8.8 Hz), 112.7, 112.5(0), 112.4(7) (d, *J* = 3.8 Hz), 106.3 (d, *J* = 23.8 Hz), 86.9, 83.9, 79.0, 74.1, 53.2, 34.5, 21.5; IR (neat): 2922, 2235(s), 1597, 1468, 1369, 1172, 1089, 756, 577; HRESIMS Calcd for [C₃₉H₂₈BrFN₂NaO₄S₂]⁺ (M + Na⁺) 773.0550, found 773.0572.

(S)-4-bromo-N-(1-(6-chloro-1-tosyl-1H-indol-2-yl)-4-phenylbut-3-yn-2-yl)-N-(phenylethynyl)benzenesulfonamide (4j)

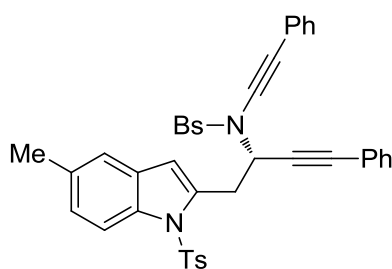


4j

White solid (mp 91-93 °C). $[\alpha]_D^{20} = -32.5^\circ$ (c = 1.0, CHCl₃). 98% ee (determined by HPLC: Chiralcel IC Column, 10/90 *i*-PrOH/hexane, 1.5 mL/min, 210 nm, 25 °C; t_R =

10.07 min (minor), 14.55 min (major)). ^1H NMR (500 MHz, CDCl_3) δ 8.17 (d, $J = 1.5$ Hz, 1H), 7.75 (d, $J = 8.5$ Hz, 2H), 7.62 (d, $J = 8.5$ Hz, 2H), 7.49 – 7.42 (m, 4H), 7.37 – 7.26 (m, 7H), 7.23 – 7.20 (m, 1H), 7.18 – 7.10 (m, 4H), 6.62 (s, 1H), 5.52 (dd, $J = 8.5, 6.5$ Hz, 1H), 3.66 – 3.61 (m, 2H), 2.30 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 145.3, 137.4, 136.3, 135.4(1), 135.3(9), 132.1, 131.6(8), 131.6(5), 130.7, 130.1, 129.3, 129.0, 128.7, 128.4, 128.2(9), 128.2(7), 127.8, 126.3, 124.5, 122.4, 121.6, 121.4, 115.0, 112.1, 86.9, 83.9, 78.9, 74.1, 53.1, 34.3, 21.5; IR (neat): 2918, 2232(s), 1595, 1366, 1168, 1087, 756, 611, 573; HRESIMS Calcd for $[\text{C}_{39}\text{H}_{28}\text{BrClN}_2\text{NaO}_4\text{S}_2]^+$ ($\text{M} + \text{Na}^+$) 789.0255, found 789.0261.

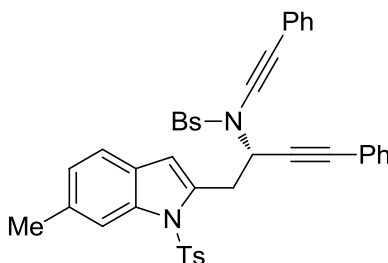
(S)-4-bromo-N-(1-(5-methyl-1-tosyl-1*H*-indol-2-yl)-4-phenylbut-3-yn-2-yl)-N-(phenylethynyl)benzenesulfonamide (4k)



4k

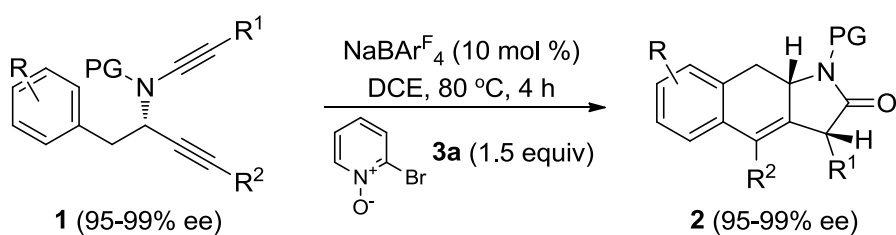
Yellow solid (mp 94-98 °C). $[\alpha]_{\text{D}}^{20} = -8.2^\circ$ ($c = 1.0$, CHCl_3). 99% ee (determined by HPLC: Chiralcel IC Column, 15/85 *i*-PrOH/hexane, 1.5 mL/min, 210 nm, 25 °C; $t_{\text{R}} = 14.12$ min (minor), 20.94 min (major)). ^1H NMR (500 MHz, CDCl_3) δ 8.00 (d, $J = 8.5$ Hz, 1H), 7.69 (d, $J = 8.5$ Hz, 2H), 7.60 (d, $J = 8.5$ Hz, 2H), 7.49 – 7.43 (m, 2H), 7.39 – 7.31 (m, 5H), 7.31 – 7.24 (m, 3H), 7.18 (d, $J = 7.0$ Hz, 2H), 7.16 – 7.06 (m, 4H), 6.52 (s, 1H), 5.59 (t, $J = 7.5$ Hz, 1H), 3.65 (d, $J = 7.5$ Hz, 2H), 2.39 (s, 3H), 2.26 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 144.8, 136.4, 135.6, 135.4, 134.7, 133.4, 131.9, 131.7, 131.6, 129.8, 129.6, 129.2, 128.8, 128.6, 128.4, 128.2, 126.2, 126.1, 122.5, 121.8, 120.6, 114.5, 112.7, 86.6, 84.3, 79.0, 74.0, 53.3, 34.5, 21.5, 21.2; IR (neat): 2922, 2236(s), 1574, 1391, 1368, 1172, 1090, 756, 577; HRESIMS Calcd for $[\text{C}_{40}\text{H}_{31}\text{BrN}_2\text{NaO}_4\text{S}_2]^+$ ($\text{M} + \text{Na}^+$) 769.0801, found 769.0823.

(S)-4-bromo-N-(1-(6-methyl-1-tosyl-1*H*-indol-2-yl)-4-phenylbut-3-yn-2-yl)-*N*-(phenylethynyl)benzenesulfonamide (4l)



4l

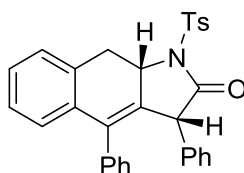
Yellow solid (mp 95-97 °C). $[\alpha]_D^{20} = -12.5^\circ$ ($c = 1.0$, CHCl_3). 99% ee (determined by HPLC: Chiralcel IC Column, 10/90 *i*-PrOH/hexane, 1.5 mL/min, 210 nm, 25 °C; $t_R = 11.66$ min (minor), 20.48 min (major)). ^1H NMR (500 MHz, CDCl_3) δ 7.94 (s, 1H), 7.71 (d, $J = 8.5$ Hz, 2H), 7.60 (d, $J = 8.0$ Hz, 2H), 7.48 – 7.43 (m, 2H), 7.41 – 7.37 (m, 2H), 7.36 – 7.24 (m, 7H), 7.20 – 7.16 (m, 2H), 7.11 (d, $J = 8.5$ Hz, 2H), 7.08 – 7.03 (m, 1H), 6.57 (s, 1H), 5.54 (t, $J = 7.5$ Hz, 1H), 3.62 (d, $J = 7.5$ Hz, 2H), 2.50 (s, 3H), 2.28 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 144.8, 137.6, 136.4, 135.8, 134.8, 133.9, 132.0, 131.7(2), 131.6(9), 129.9, 129.3, 128.8, 128.7, 128.4, 128.1(9), 128.1(8), 127.0, 126.2, 125.4, 122.5, 121.8, 120.2, 115.0, 112.8, 86.7, 84.3, 79.1, 74.0, 53.3, 34.5, 22.1, 21.5; IR (neat): 2924, 2236(s), 1573, 1367, 1173, 1089, 756, 579; HRESIMS Calcd for $[\text{C}_{40}\text{H}_{31}\text{BrN}_2\text{NaO}_4\text{S}_2]^+$ ($M + \text{Na}^+$) 769.0801, found 769.0827.



General procedure for the synthesis of linear tricyclic *N*-heterocycles 2:

NaBAR^F₄ (0.02 mmol, 17.8 mg) was added to a mixture of the *N*-propargyl ynamide **1** (0.20 mmol) and 2-bromopyridine *N*-oxide **3a** (52.2 mg, 0.30 mmol) in DCE (4.0 mL) at room temperature. Then, the reaction mixture was stirred at 80 °C and the progress of the reaction was monitored by TLC. The reaction typically took 4 h. Upon completion, the mixture was concentrated and the residue was purified by chromatography on silica gel (eluent: hexanes/ethyl acetate) to afford the desired tricyclic *N*-heterocycle **2**.

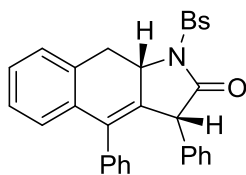
(3*R*,9*aS*)-3,4-diphenyl-1-tosyl-1,3,9,9*a*-tetrahydro-2*H*-benzo[*f*]indol-2-one (**2a**)



2a

Compound **2a** was prepared in 80% yield (78.6 mg) according to the general procedure. White solid (mp 168–170 °C). $[\alpha]_{\text{D}}^{20} = -14.6^\circ$ ($c = 1.0$, CHCl₃). 98% ee (determined by HPLC: Chiralcel AD-H Column, 5/95 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; $t_{\text{R}} = 29.54$ min (minor), 22.77 min (major)). ¹H NMR (500 MHz, CDCl₃) δ 7.84 (d, $J = 8.0$ Hz, 2H), 7.37 (d, $J = 7.5$ Hz, 1H), 7.31 – 7.07 (m, 11H), 6.94 – 6.70 (m, 4H), 5.26 – 5.21 (m, 1H), 4.01 (s, 1H), 3.91 (dd, $J = 14.5, 6.0$ Hz, 1H), 3.15 (t, $J = 14.5$ Hz, 1H), 2.38 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 172.9, 145.1, 138.1, 137.2, 136.4, 135.4, 135.0, 132.9, 129.8, 129.4, 128.9, 128.6, 128.2, 128.1, 128.0, 127.5, 127.4, 127.2, 126.5, 60.8, 52.5, 36.4, 21.6; IR (neat): 3061, 3029, 1743(s), 1367, 1171, 702, 664, 593, 560; HRESIMS Calcd for [C₃₁H₂₅NNaO₃S]⁺ (M + Na⁺) 514.1447, found 514.1449.

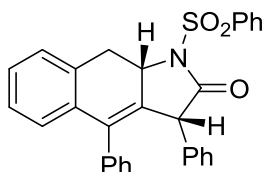
(3*R*,9*aS*)-1-((4-bromophenyl)sulfonyl)-3,4-diphenyl-1,3,9,9*a*-tetrahydro-2*H*-benzo[*f*]indol-2-one (**2b**)



2b

Compound **2b** was prepared in 75% yield (83.3 mg) according to the general procedure. White solid (mp 171–172 °C). $[\alpha]_D^{20} = -12.8^\circ$ ($c = 1.0$, CHCl_3). 98% ee (determined by HPLC: Chiralcel AS-H Column, 10/90 *i*-PrOH/hexane, 1.5 mL/min, 254 nm, 25 °C; $t_R = 16.61$ min (minor), 25.89 min (major)). ^1H NMR (400 MHz, CDCl_3) δ 7.77 (d, $J = 8.4$ Hz, 2H), 7.50 (d, $J = 8.8$ Hz, 2H), 7.42 – 7.10 (m, 9H), 7.05 – 6.73 (m, 5H), 5.20 (dd, $J = 14.0, 5.2$ Hz, 1H), 4.03 (s, 1H), 3.87 (dd, $J = 14.4, 6.0$ Hz, 1H), 3.16 (t, $J = 14.4$ Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 172.8, 137.6, 137.5, 136.7, 136.3, 135.3, 132.8, 132.1, 129.4, 129.2, 129.0, 128.6, 128.2(2), 128.1(7), 128.1, 127.7, 127.5, 127.1, 126.6, 60.9, 52.4, 36.4; IR (neat): 3060, 3027, 1744(s), 1371, 1174, 732, 701, 605; HRESIMS Calcd for $[\text{C}_{30}\text{H}_{22}\text{BrNNaO}_3\text{S}]^+$ ($\text{M} + \text{Na}^+$) 578.0396, found 578.0399.

(3R,9aS)-3,4-diphenyl-1-(phenylsulfonyl)-1,3,9,9a-tetrahydro-2H-benzo[f]indol-2-one (2c)

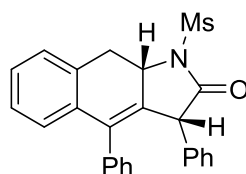


2c

Compound **2c** was prepared in 83% yield (79.2 mg) according to the general procedure. White solid (mp 169–171 °C). $[\alpha]_D^{20} = -27.7^\circ$ ($c = 1.0$, CHCl_3). 96% ee (determined by HPLC: Chiralcel AD-H Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; $t_R = 20.32$ min (minor), 13.86 min (major)). ^1H NMR (500 MHz, CDCl_3) δ 7.97 (d, $J = 9.0$ Hz, 2H), 7.59 – 7.53 (m, 1H), 7.46 – 7.34 (m, 3H), 7.33 –

7.03 (m, 9H), 6.93 – 6.66 (m, 4H), 5.25 (dd, $J = 14.0, 5.5$ Hz, 1H), 4.02 (s, 1H), 3.92 (dd, $J = 14.0, 6.0$ Hz, 1H), 3.16 (t, $J = 14.0$ Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 172.8, 138.1, 137.9, 137.3, 136.4, 135.4, 133.9, 132.9, 129.7, 128.9, 128.8, 128.6, 128.2, 128.1, 128.0(0), 127.9(8), 127.6, 127.5, 127.2, 126.5, 60.9, 52.5, 36.4; IR (neat): 2925, 1744(s), 1364, 1174, 719, 686, 596, 583; HRESIMS Calcd for $[\text{C}_{30}\text{H}_{23}\text{NNaO}_3\text{S}]^+$ ($\text{M} + \text{Na}^+$) 500.1291, found 500.1292.

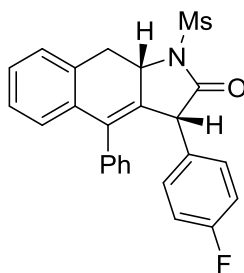
(3R,9aS)-1-(methylsulfonyl)-3,4-diphenyl-1,3,9,9a-tetrahydro-2H-benzo[*f*]indol-2-one (2d)



2d

Compound **2d** was prepared in 84% yield (69.8 mg) according to the general procedure. White solid (mp 165–167 °C). $[\alpha]_{\text{D}}^{20} = -23.6^\circ$ ($c = 1.0$, CHCl_3). 98% ee (determined by HPLC: Chiralcel AD-H Column, 10/90 *i*-PrOH/hexane, 0.8 mL/min, 254 nm, 25 °C; $t_{\text{R}} = 12.95$ min (minor), 28.91 min (major)). ^1H NMR (500 MHz, CDCl_3) δ 7.37 – 7.26 (m, 6H), 7.25 – 7.20 (m, 2H), 7.19 – 7.10 (m, 4H), 6.81 (d, $J = 7.5$ Hz, 2H), 5.27 – 5.21 (m, 1H), 4.14 (s, 1H), 3.82 (dd, $J = 14.0, 5.5$ Hz, 1H), 3.26 (s, 3H), 3.15 (t, $J = 14.5$ Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 174.0, 138.7, 137.5, 136.3, 135.4, 132.7, 129.6, 129.2, 128.5, 128.2(3), 128.1(8), 128.1, 128.0, 127.5, 127.3, 126.6, 60.5, 52.6, 41.6, 36.1; IR (neat): 2927, 3028, 1742(s), 1494, 1358, 1167, 1129, 969, 728, 700, 540; HRESIMS Calcd for $[\text{C}_{25}\text{H}_{21}\text{NNaO}_3\text{S}]^+$ ($\text{M} + \text{Na}^+$) 438.1134, found 438.1135.

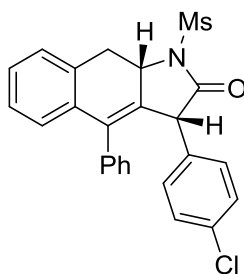
(3R,9aS)-3-(4-fluorophenyl)-1-(methylsulfonyl)-4-phenyl-1,3,9,9a-tetrahydro-2H-benzo[*f*]indol-2-one (2e)



2e

Compound **2e** was prepared in 76% yield (65.8 mg) according to the general procedure. White solid (mp 164–165 °C). $[\alpha]_D^{20} = -27.1^\circ$ ($c = 1.0$, CHCl_3). 98% ee (determined by HPLC: Chiralcel AD-H Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; $t_R = 9.91$ min (minor), 15.01 min (major)). ^1H NMR (400 MHz, CDCl_3) δ 7.38 – 7.28 (m, 3H), 7.26 – 7.21 (m, 2H), 7.20 – 7.08 (m, 4H), 7.06 – 6.98 (m, 2H), 6.89 – 6.79 (m, 2H), 5.26 – 5.19 (m, 1H), 4.13 (s, 1H), 3.82 (dd, $J = 14.4$, 5.6 Hz, 1H), 3.28 (s, 3H), 3.14 (t, $J = 14.0$ Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 173.8, 162.3 (d, $J = 245.8$ Hz), 137.8, 136.3, 135.2, 134.3 (d, $J = 3.3$ Hz), 132.6, 129.2, 129.0, 128.9 (d, $J = 8.3$ Hz), 128.6, 128.3, 128.2, 127.6, 126.6, 116.2 (d, $J = 21.6$ Hz), 60.3, 51.8, 41.8, 36.0; IR (neat): 2926, 2854, 1734(s), 1507, 1360, 1167, 971, 772, 750, 729; HRESIMS Calcd for $[\text{C}_{25}\text{H}_{20}\text{FNNaO}_3\text{S}]^+$ ($\text{M} + \text{Na}^+$) 456.1040, found 456.1040.

(3R,9aS)-3-(4-chlorophenyl)-1-(methylsulfonyl)-4-phenyl-1,3,9,9a-tetrahydro-2H-benzo[f]indol-2-one (2f)

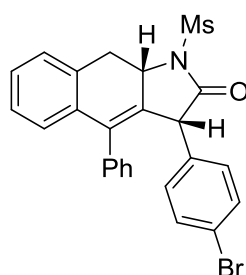


2f

Compound **2f** was prepared in 72% yield (64.7 mg) according to the general procedure. White solid (mp 163–165 °C). $[\alpha]_D^{20} = -50.1^\circ$ ($c = 1.0$, CHCl_3). 98% ee

(determined by HPLC: Chiralcel AD-H Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; t_R = 10.13 min (minor), 14.41 min (major)). ^1H NMR (400 MHz, CDCl_3) δ 7.35 – 7.13 (m, 9H), 7.08 (d, J = 8.4 Hz, 2H), 6.89 – 6.71 (m, 2H), 5.22 (dd, J = 14.0, 5.6 Hz, 1H), 4.12 (s, 1H), 3.82 (dd, J = 14.4, 6.0 Hz, 1H), 3.28 (s, 3H), 3.14 (t, J = 14.4 Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 173.6, 138.0, 137.0, 136.2, 135.2, 134.0, 132.6, 129.4, 128.9, 128.6(2), 128.5(9), 128.4, 128.2, 127.6, 126.6, 60.3, 51.9, 41.8, 36.0; IR (neat): 2926, 2237, 1748(s), 1558, 1490, 1456, 1362, 1166, 1098, 828, 758, 692; HRESIMS Calcd for $[\text{C}_{25}\text{H}_{20}\text{ClNNaO}_3\text{S}]^+$ ($\text{M} + \text{Na}^+$) 472.0745, found 472.0747.

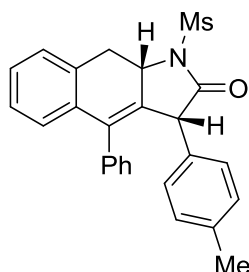
(3*R*,9*aS*)-3-(4-bromophenyl)-1-(methylsulfonyl)-4-phenyl-1,3,9,9*a*-tetrahydro-2*H*-benzo[*f*]indol-2-one (2g)



2g

Compound **2g** was prepared in 75% yield (74.0 mg) according to the general procedure. White solid (mp 168–169 °C). $[\alpha]_D^{20}$ = -79.8 ° (c = 1.0, CHCl_3). 97% ee (determined by HPLC: Chiralcel AD-H Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; t_R = 11.97 min (minor), 15.91 min (major)). ^1H NMR (500 MHz, CDCl_3) δ 7.46 (d, J = 8.5 Hz, 2H), 7.36 – 7.22 (m, 5H), 7.21 – 7.18 (m, 2H), 7.03 (d, J = 8.5 Hz, 2H), 6.87 – 6.76 (m, 2H), 5.25 – 5.18 (m, 1H), 4.10 (s, 1H), 3.82 (dd, J = 14.5, 6.0 Hz, 1H), 3.28 (s, 3H), 3.14 (t, J = 14.0 Hz, 1H); ^{13}C NMR (125 MHz, CDCl_3) δ 173.5, 138.1, 137.5, 136.2, 135.2, 132.6, 132.4, 128.9, 128.8, 128.6, 128.4, 128.2, 127.7, 127.6, 126.7, 122.1, 60.3, 52.0, 41.8, 36.0; IR (neat): 2927, 1740(s), 1486, 1359, 1167, 1129, 969, 729, 537, 509; HRESIMS Calcd for $[\text{C}_{25}\text{H}_{20}\text{BrNNaO}_3\text{S}]^+$ ($\text{M} + \text{Na}^+$) 516.0239, found 516.0242.

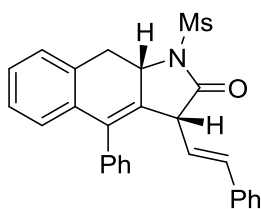
(3*R*,9*aS*)-1-(methylsulfonyl)-4-phenyl-3-(*p*-tolyl)-1,3,9,9*a*-tetrahydro-2*H*-benzo[*f*]indol-2-one (2h)



2h

Compound **2h** was prepared in 74% yield (63.5 mg) according to the general procedure. White solid (mp 161–163 °C). $[\alpha]_D^{20} = -37.2^\circ$ ($c = 1.0$, CHCl_3). 98% ee (determined by HPLC: Chiralcel AD-H Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; $t_R = 9.09$ min (minor), 14.49 min (major)). ^1H NMR (500 MHz, CDCl_3) δ 7.33 – 7.18 (m, 5H), 7.17 – 7.09 (m, 4H), 7.03 (d, $J = 8.0$ Hz, 2H), 6.88 – 6.75 (m, 2H), 5.23 (dd, $J = 14.0, 6.0$ Hz, 1H), 4.10 (s, 1H), 3.81 (dd, $J = 14.0, 5.5$ Hz, 1H), 3.25 (s, 3H), 3.14 (t, $J = 15.0$ Hz, 1H), 2.34 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 174.2, 137.7, 137.3, 136.4, 135.6, 135.4, 132.7, 129.9, 129.7, 128.5, 128.2, 128.1, 128.0, 127.5, 127.0, 126.6, 60.5, 52.3, 41.6, 36.1, 21.1; IR (neat): 2926, 1741(s), 1358, 1166, 1129, 969, 744, 540, 510; HRESIMS Calcd for $[\text{C}_{26}\text{H}_{23}\text{NNaO}_3\text{S}]^+$ ($\text{M} + \text{Na}^+$) 452.1291, found 452.1292.

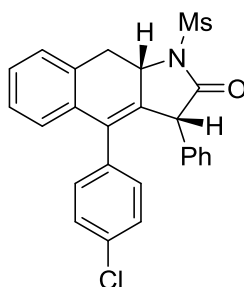
(3*R*,9*aS*)-1-(methylsulfonyl)-4-phenyl-3-((*E*)-styryl)-1,3,9,9*a*-tetrahydro-2*H*-benzo[*f*]indol-2-one (2i)



2i

Compound **2i** was prepared in 61% yield (53.8 mg) according to the general procedure. White solid (mp 165–167 °C). $[\alpha]_D^{20} = +61.4^\circ$ (c = 1.0, CHCl₃). 97% ee (determined by HPLC: Chiralcel AD-H Column, 10/90 *i*-PrOH/hexane, 1.5 mL/min, 254 nm, 25 °C; t_R = 21.15 min (minor), 11.21 min (major)). ¹H NMR (400 MHz, CDCl₃) δ 7.95 (d, J = 16.4 Hz, 1H), 7.53 (d, J = 7.6 Hz, 2H), 7.43 – 7.36 (m, 2H), 7.35 – 7.15 (m, 6H), 7.15 – 7.05 (m, 4H), 5.57 (s, 1H), 4.90 (dd, J = 10.8, 6.4 Hz, 1H), 4.04 (dd, J = 15.6, 6.4 Hz, 1H), 3.40 (s, 3H), 2.88 (dd, J = 15.2, 10.8 Hz, 1H); ¹³C NMR (125 MHz, CDCl₃) δ 168.8, 157.4, 142.5, 136.9, 135.2, 135.1, 132.5, 130.1, 129.2, 129.1, 128.8, 128.6, 128.4, 127.8, 127.6, 127.5, 126.9, 124.1, 115.3, 56.4, 45.5, 42.0, 37.9; IR (neat): 2924, 2853, 1716(s), 1653, 1558, 1506, 1456, 1354, 1170, 1121, 968, 749; HRESIMS Calcd for [C₂₇H₂₃NNaO₃S]⁺ (M + Na⁺) 464.1291, found 464.1296.

(3*R*,9*aS*)-4-(4-chlorophenyl)-1-(methylsulfonyl)-3-phenyl-1,3,9,9*a*-tetrahydro-2*H*-benzo[*f*]indol-2-one (2j)

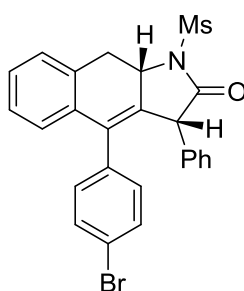


2j

Compound **2j** was prepared in 76% yield (68.2 mg) according to the general procedure. White solid (mp 169–170 °C). $[\alpha]_D^{20} = -84.8^\circ$ (c = 1.0, CHCl₃). 96% ee (determined by HPLC: Chiralcel AD-H Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; t_R = 9.91 min (minor), 17.59 min (major)). ¹H NMR (400 MHz, CDCl₃) δ 7.40 – 7.07 (m, 11H), 6.77 (d, J = 7.6 Hz, 2H), 5.23 (dd, J = 14.0, 5.6 Hz, 1H), 4.11 (s, 1H), 3.82 (dd, J = 14.4, 2.0 Hz, 1H), 3.26 (s, 3H), 3.13 (t, J = 14.4 Hz, 1H); ¹³C NMR (125 MHz, CDCl₃) δ 173.7, 138.6, 136.4, 135.0, 134.8, 134.1, 132.7,

130.2, 129.4, 128.7, 128.6, 128.4, 128.1, 127.6, 127.2, 126.4, 60.5, 52.6, 41.6, 36.0; IR (neat): 2925, 2853, 1734(s), 1653, 1558, 1506, 1490, 1456, 1361, 1167, 1131, 971, 765, 743; HRESIMS Calcd for $[C_{25}H_{20}ClNNaO_3S]^+$ ($M + Na^+$) 472.0745, found 472.0747.

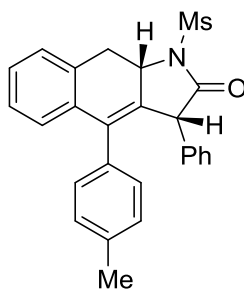
(3*R*,9*aS*)-4-(4-bromophenyl)-1-(methylsulfonyl)-3-phenyl-1,3,9,9*a*-tetrahydro-2*H*-benzo[*f*]indol-2-one (2k)



2k

Compound **2k** was prepared in 74% yield (73.0 mg) according to the general procedure. White solid (mp 171–173 °C). $[\alpha]_D^{20} = -85.9^\circ$ ($c = 1.0$, $CHCl_3$). 96% ee (determined by HPLC: Chiralcel AD-H Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; $t_R = 10.44$ min (minor), 19.39 min (major)). 1H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.20 (m, 7H), 7.18 – 7.07 (m, 4H), 6.81 (d, $J = 7.6$ Hz, 2H), 5.24 (dd, $J = 14.0, 6.0$ Hz, 1H), 4.14 (s, 1H), 3.82 (dd, $J = 14.4, 6.0$ Hz, 1H), 3.26 (s, 3H), 3.15 (t, $J = 14.0$ Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 174.0, 138.7, 137.5, 136.4, 135.4, 132.7, 129.6, 129.3, 128.6, 128.2(3), 128.1(9), 128.0(9), 127.9(6), 127.5, 127.3, 126.6, 60.5, 52.6, 41.6, 36.1; IR (neat): 3027, 2926, 1741(s), 1506, 1455, 1358, 1167, 1129, 969, 727, 700, 668, 540; HRESIMS Calcd for $[C_{25}H_{20}BrNNaO_3S]^+$ ($M + Na^+$) 516.0239, found 516.0240.

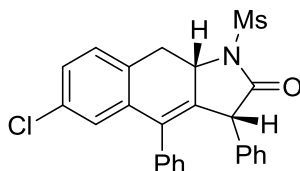
(3*R*,9*aS*)-1-(methylsulfonyl)-3-phenyl-4-(*p*-tolyl)-1,3,9,9*a*-tetrahydro-2*H*-benzo[*f*]indol-2-one (2l)



2l

Compound **2l** was prepared in 79% yield (67.8 mg) according to the general procedure. White solid (mp 170–172 °C). $[\alpha]_D^{20} = -60.2^\circ$ ($c = 1.0$, CHCl_3). 99% ee (determined by HPLC: Chiralcel AD-H Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; $t_R = 8.81$ min (minor), 13.93 min (major)). ^1H NMR (400 MHz, CDCl_3) δ 7.38 – 7.28 (m, 4H), 7.25 – 7.20 (m, 2H), 7.19 – 7.12 (m, 3H), 7.10 – 6.93 (m, 2H), 6.83 (d, $J = 7.6$ Hz, 2H), 5.23 (dd, $J = 14.0, 6.0$ Hz, 1H), 4.15 (s, 1H), 3.80 (dd, $J = 14.4, 6.0$ Hz, 1H), 3.24 (s, 3H), 3.13 (t, $J = 14.0$ Hz, 1H), 2.33 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 174.1, 138.8, 137.9, 137.5, 135.5, 133.4, 132.7, 129.2(4), 129.1(9), 128.9, 128.5, 128.1, 127.9, 127.5, 127.3, 126.7, 60.6, 52.7, 41.6, 36.1, 21.2; IR (neat): 2926, 2855, 1742(s), 1455, 1359, 1167, 1130, 970, 772, 732, 669, 513; HRESIMS Calcd for $[\text{C}_{26}\text{H}_{23}\text{NNaO}_3\text{S}]^+$ ($\text{M} + \text{Na}^+$) 452.1291, found 452.1293.

(3R,9aS)-6-chloro-1-(methylsulfonyl)-3,4-diphenyl-1,3,9,9a-tetrahydro-2H-benzo[f]indol-2-one (2m)

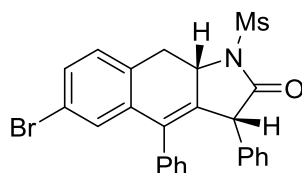


2m

Compound **2m** was prepared in 78% yield (70.0 mg) according to the general procedure. White solid (mp 172–174 °C). $[\alpha]_D^{20} = -51.5^\circ$ ($c = 1.0$, CHCl_3). 95% ee (determined by HPLC: Chiralcel AD-H Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; $t_R = 7.89$ min (minor), 18.79 min (major)). ^1H NMR (400 MHz,

CDCl₃) δ 7.45 – 7.20 (m, 9H), 7.12 (d, J = 7.6 Hz, 2H), 6.93 – 6.73 (m, 2H), 5.21 (dd, J = 14.0, 5.6 Hz, 1H), 4.13 (s, 1H), 3.81 (dd, J = 14.4, 6.0 Hz, 1H), 3.26 (s, 3H), 3.09 (t, J = 14.0 Hz, 1H); ¹³C NMR (125 MHz, CDCl₃) δ 173.7, 138.4, 137.0, 136.7, 135.6, 133.4, 131.6, 131.1, 131.0(3), 130.9(5), 129.7, 129.3, 128.4, 128.1, 128.0, 127.2, 126.5, 60.3, 52.6, 41.6, 35.4; IR (neat): 2926, 2854, 1734(s), 1653, 1558, 1507, 1457, 1361, 1266, 1167, 969, 748, 703, 551; HRESIMS Calcd for [C₂₅H₂₀ClNNaO₃S]⁺ (M + Na⁺) 472.0745, found 472.0743.

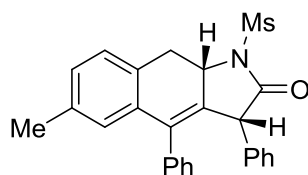
(3R,9aS)-6-bromo-1-(methylsulfonyl)-3,4-diphenyl-1,3,9,9a-tetrahydro-2H-benzof[*f*]indol-2-one (2n)



2n

Compound **2n** was prepared in 80% yield (78.9 mg) according to the general procedure. White solid (mp 175–177 °C). [α]_D²⁰ = -52.3 ° (c = 1.0, CHCl₃). 98% ee (determined by HPLC: Chiralcel AD-H Column, 10/90 i-PrOH/hexane, 1.5 mL/min, 254 nm, 25 °C; t_R = 8.03 min (minor), 18.95 min (major)). ¹H NMR (500 MHz, CDCl₃) δ 7.43 – 7.27 (m, 6H), 7.25 – 7.16 (m, 2H), 7.15 – 7.04 (m, 3H), 6.95 – 6.82 (m, 2H), 5.26 – 5.14 (m, 1H), 4.13 (s, 1H), 3.80 (dd, J = 14.0, 5.5 Hz, 1H), 3.26 (s, 3H), 3.06 (t, J = 14.0 Hz, 1H); ¹³C NMR (125 MHz, CDCl₃) δ 173.7, 138.4, 137.3, 136.6, 135.5, 131.5, 131.1, 131.0, 130.0, 129.4, 129.3, 128.5, 128.4, 128.1, 127.2, 121.4, 60.2, 52.6, 41.6, 35.5; IR (neat): 3028, 2928, 1740(s), 1494, 1477, 1358, 1167, 1132, 971, 731, 701, 547; HRESIMS Calcd for [C₂₅H₂₀BrNNaO₃S]⁺ (M + Na⁺) 516.0239, found 516.0240.

(3R,9aS)-6-methyl-1-(methylsulfonyl)-3,4-diphenyl-1,3,9,9a-tetrahydro-2H-benzof[*f*]indol-2-one (2o)

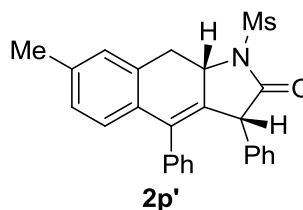
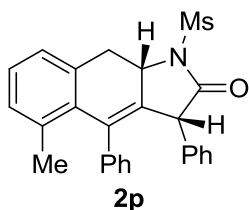


2o

Compound **2o** was prepared in 82% yield (70.4 mg) according to the general procedure. White solid (mp 174–176 °C). $[\alpha]_D^{20} = -55.7^\circ$ ($c = 1.0$, CHCl_3). 96% ee (determined by HPLC: Chiralcel AD-H Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; $t_R = 10.02$ min (minor), 20.23 min (major)). ^1H NMR (500 MHz, CDCl_3) δ 7.45 – 7.26 (m, 5H), 7.24 – 7.20 (m, 1H), 7.17 – 7.07 (m, 3H), 7.06 – 7.03 (m, 2H), 6.83 – 6.61 (m, 2H), 5.24 – 5.18 (m, 1H), 4.12 (s, 1H), 3.78 (dd, $J = 14.0$, 5.5 Hz, 1H), 3.25 (s, 3H), 3.09 (t, $J = 14.0$ Hz, 1H), 2.20 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 174.0, 138.7, 137.6, 137.2, 136.4, 135.2, 129.6(2), 129.5(7), 129.2, 128.8, 128.4, 128.0, 127.9, 127.3, 127.2, 60.7, 52.7, 41.6, 35.7, 21.1; IR (neat): 3027, 2926, 1741(s), 1493, 1358, 1169, 1129, 1147, 972, 730, 702, 551, 519; HRESIMS Calcd for $[\text{C}_{26}\text{H}_{23}\text{NNaO}_3\text{S}]^+$ ($M + \text{Na}^+$) 452.1291, found 452.1292.

(3R,9aS)-5-methyl-1-(methylsulfonyl)-3,4-diphenyl-9,9a-dihydro-1H-benzo[*f*]indol-2(3H)-one (2p)

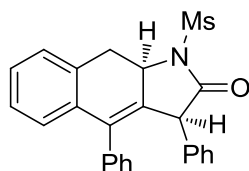
(3R,9aS)-7-methyl-1-(methylsulfonyl)-3,4-diphenyl-9,9a-dihydro-1H-benzo[*f*]indol-2(3H)-one (2p')



Compounds **2p** and **2p'** were prepared in 74% yield (63.5 mg; **2p/2p'** = 1/1, determined by ^1H NMR integration of crude mixture; unseparated mixtures) according to the general procedure. White solid (mp 111–114 °C). $[\alpha]_D^{20} = -55.5^\circ$ ($c =$

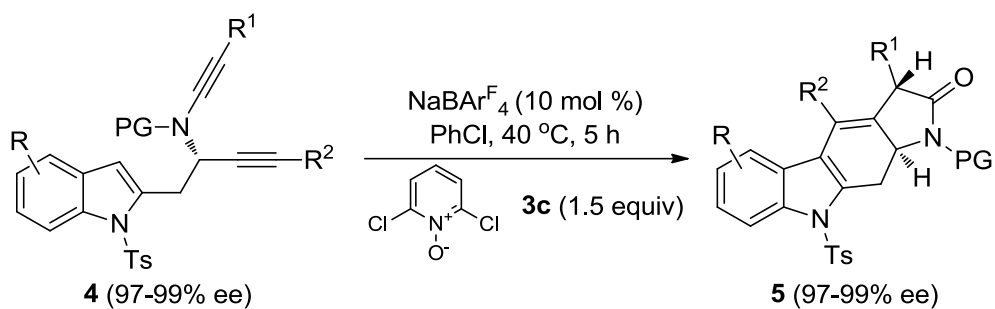
1.0, CHCl₃); 95% ee (determined by HPLC: Chiralcel IA Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 240 nm, 25 °C; *t*_R = 10.68 min (minor), 21.45 min (major), *t*_R = 11.53 min (minor), 29.17 min (major)). ¹H NMR (500 MHz, CDCl₃) δ 7.43 – 7.27 (m, 5H), 7.25 – 7.12 (m, 4H), 7.04 – 6.90 (m, 3H), 6.73 – 6.67 (m, 1H), 5.22 (dd, *J* = 14.0, 6.0 Hz, 0.4H), 5.10 (dd, *J* = 14.0, 5.0 Hz, 0.6H), 4.17 – 4.10 (m, 1H), 3.77 (dd, *J* = 14.0, 6.0 Hz, 0.4H), 3.72 (dd, *J* = 14.0, 5.0 Hz, 0.6H), 3.25 (s, 1.2H), 3.24 (s, 1.8H), 3.12 (dd, *J* = 14.0 Hz, 0.4H), 3.04 (dd, *J* = 14.0 Hz, 0.6H), 2.35 (s, 1.2H), 1.62 (s, 1.8H); ¹³C NMR (125 MHz, CDCl₃) δ 174.1, 173.5, 140.0, 139.4, 138.8, 138.3, 137.5, 136.5, 136.0, 134.1, 134.0, 132.7, 132.2, 131.5, 129.4(4), 129.4(1), 129.2, 128.5, 128.0(4), 128.0(0), 127.9, 127.6, 127.3(1), 127.3(0), 126.5, 126.3, 60.6, 60.4, 52.9, 52.6, 41.6, 38.0, 36.1, 22.2, 21.2; IR (neat): 2925, 1738, 1493, 1452, 1356, 1167, 1131, 970, 704, 585; HRESIMS Calcd for [C₂₆H₂₃NNaO₃S]⁺ (*M* + Na⁺) 452.1291, found 452.1293.

(3*S*,9*aR*)-1-(methylsulfonyl)-3,4-diphenyl-9,9a-dihydro-1*H*-benzo[*f*]indol-2(3*H*)-one (2*d'*)



2*d'*

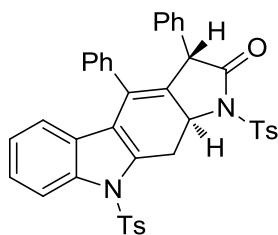
Compound **2*d'*** was prepared in 83% yield (69.0 mg) according to the general procedure. [α]_D²⁰ = +38.7 °(c = 1.0, CHCl₃). 97% ee (determined by HPLC: Chiralcel AD-H Column, 10/90 *i*-PrOH/hexane, 0.8 mL/min, 254 nm, 25 °C; *t*_R = 28.41 min (minor), 13.13 min (major)).



General procedure for the synthesis of linear tetracyclic *N*-heterocycles **5**:

NaBARF₄ (0.02 mmol, 17.8 mg) was added to a mixture of the indolyl *N*-propargyl ynamide **4** (0.20 mmol) and 2,6-dichloropyridine *N*-oxide **3c** (49.2 mg, 0.30 mmol) in PhCl (4.0 mL) at room temperature. Then, the reaction mixture was stirred at 40 °C and the progress of the reaction was monitored by TLC. The reaction typically took 5 h. Upon completion, the mixture was concentrated and the residue was purified by chromatography on silica gel (eluent: hexanes/ethyl acetate) to afford the desired tetracyclic *N*-heterocycle **5**.

(3*S*,10*aS*)-3,4-diphenyl-1,9-ditosyl-3,9,10,10*a*-tetrahydropyrrolo[2,3-*b*]carbazol-2(1*H*)-one (**5a**)

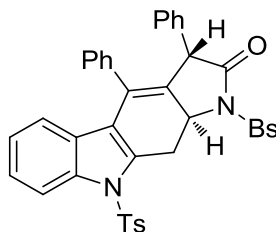


5a

Compound **5a** was prepared in 78% yield (106.7 mg) according to the general procedure. White solid (mp 142-144 °C). [α]_D²⁰ = +24.5 ° (c = 1.0, CHCl₃). 99% ee (determined by HPLC: Chiralcel AD-H Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; t_R = 12.02 min (minor), 21.36 min (major)). ¹H NMR (600 MHz, CDCl₃) δ 8.28 (d, *J* = 8.4 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 2H), 7.92 (d, *J* = 8.4 Hz, 2H), 7.35 (d, *J* = 7.8 Hz, 2H), 7.31 – 7.07 (m, 11H), 7.04 – 7.00 (m, 2H), 6.95 – 6.91 (m,

1H), 6.31 (d, $J = 7.8$ Hz, 1H), 5.20 – 5.15 (m, 1H), 4.79 (dd, $J = 16.4, 7.2$ Hz, 1H), 4.07 (s, 1H), 3.07 (t, $J = 15.6$ Hz, 1H), 2.43 (s, 3H), 2.42 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3) δ 172.6, 145.5, 145.3, 139.1, 136.9, 135.6, 135.4, 135.3, 133.0, 132.6, 130.3, 129.6, 129.1, 128.4, 128.1, 127.7, 127.3, 126.7, 126.5, 125.7, 124.3, 123.4, 120.1, 118.7, 114.5, 61.1, 52.1, 29.5, 21.7; IR (neat): 2924, 1746(s), 1372, 1189, 1172, 1088, 664, 579; HRESIMS Calcd for $[\text{C}_{40}\text{H}_{32}\text{N}_2\text{NaO}_5\text{S}_2]^+$ ($\text{M} + \text{Na}^+$) 707.1645, found 707.1659.

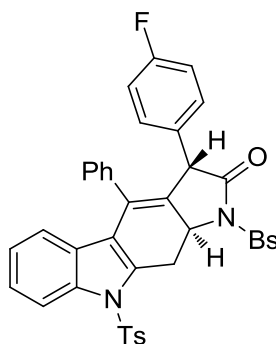
(3*S*,10*aS*)-1-((4-bromophenyl)sulfonyl)-3,4-diphenyl-9-tosyl-3,9,10,10*a*-tetrahydropyrrolo[2,3-*b*]carbazol-2(1*H*)-one (5b)



5b

Compound **5b** was prepared in 81% yield (121.4 mg) according to the general procedure. White solid (mp 144-146 °C). $[\alpha]_{\text{D}}^{20} = -13.3^\circ$ ($c = 1.0$, CHCl_3). 98% ee (determined by HPLC: Chiralcel AD-H Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; $t_{\text{R}} = 12.27$ min (minor), 24.69 min (major)). ^1H NMR (500 MHz, CDCl_3) δ 8.28 (d, $J = 8.5$ Hz, 1H), 7.92 – 7.85 (m, 4H), 7.59 (d, $J = 9.0$ Hz, 2H), 7.34 (d, $J = 8.1$ Hz, 2H), 7.31 – 7.10 (m, 9H), 7.02 (d, $J = 7.0$ Hz, 2H), 6.97 – 6.91 (m, 1H), 6.32 (d, $J = 8.0$ Hz, 1H), 5.20 – 5.14 (m, 1H), 4.77 (dd, $J = 16.0, 7.0$ Hz, 1H), 4.09 (s, 1H), 3.09 (t, $J = 16.0$ Hz, 1H), 2.43 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 172.6, 145.5, 138.5, 137.0, 136.9, 135.4(3), 135.4(0), 132.9, 132.8, 132.3, 130.3, 129.6, 129.5, 129.2, 128.6, 128.5, 128.2, 127.9, 127.2, 126.7, 126.4, 125.0, 124.4, 123.5, 120.1, 118.7, 114.5, 61.2, 52.0, 29.6, 21.7; IR (neat): 2924, 1747(s), 1374, 1174, 1152, 1088, 742, 577; HRESIMS Calcd for $[\text{C}_{39}\text{H}_{29}\text{BrN}_2\text{NaO}_5\text{S}_2]^+$ ($\text{M} + \text{Na}^+$) 771.0593, found 771.0615.

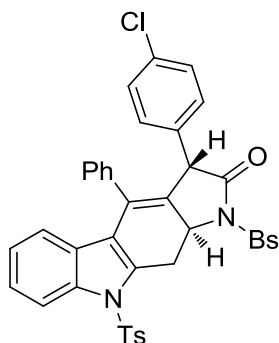
(3*S*,10*aS*)-1-((4-bromophenyl)sulfonyl)-3-(4-fluorophenyl)-4-phenyl-9-tosyl-3,9,10,10*a*-tetrahydropyrrolo[2,3-*b*]carbazol-2(1*H*)-one (5c)



5c

Compound **5c** was prepared in 67% yield (102.6 mg) according to the general procedure. White solid (mp 147-149 °C). $[\alpha]_D^{20} = -18.6^\circ$ ($c = 1.0$, CHCl_3). 98% ee (determined by HPLC: Chiralcel AD-H Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; $t_R = 13.64$ min (minor), 19.94 min (major)). ^1H NMR (500 MHz, CDCl_3) δ 8.27 (d, $J = 8.5$ Hz, 1H), 7.95 – 7.87 (m, 4H), 7.64 (d, $J = 9.0$ Hz, 2H), 7.39 – 7.12 (m, 8H), 7.05 – 6.99 (m, 2H), 6.98 – 6.92 (m, 3H), 6.32 (d, $J = 8.0$ Hz, 1H), 5.16 (dd, $J = 15.2, 7.5$ Hz, 1H), 4.77 (dd, $J = 16.5, 7.0$ Hz, 1H), 4.07 (s, 1H), 3.07 (t, $J = 16.0$ Hz, 1H), 2.43 (s, 3H); ^{13}C NMR (212.5 MHz, CDCl_3) δ 172.4, 162.4 (d, $J = 247.1$ Hz), 145.6, 137.0, 136.9, 135.4, 134.4, 133.3, 132.8, 132.4, 130.3, 129.7, 129.5, 128.9 (d, $J = 8.5$ Hz), 128.6, 128.5, 128.2, 126.7, 126.3, 124.5 (d, $J = 3.2$ Hz), 123.5, 120.0, 118.6, 116.2 (d, $J = 21.3$ Hz), 114.5, 60.9, 51.2, 29.5, 21.7; IR (neat): 2923, 1746(s), 1373, 1174, 1153, 1088, 742, 577; HRESIMS Calcd for $[\text{C}_{39}\text{H}_{28}\text{BrFN}_2\text{NaO}_5\text{S}_2]^+$ ($M + \text{Na}^+$) 789.0499, found 789.0528.

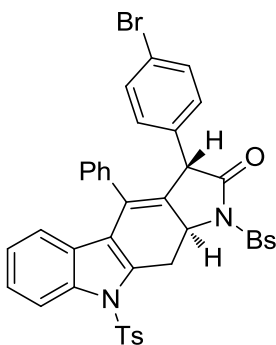
(3*S*,10*aS*)-1-((4-bromophenyl)sulfonyl)-3-(4-chlorophenyl)-4-phenyl-9-tosyl-3,9,10,10*a*-tetrahydropyrrolo[2,3-*b*]carbazol-2(1*H*)-one (5d)



5d

Compound **5d** was prepared in 67% yield (104.8 mg) according to the general procedure. White solid (mp 149-151 °C). $[\alpha]_D^{20} = -15.3^\circ$ ($c = 1.0$, CHCl_3). 98% ee (determined by HPLC: Chiralcel AD-H Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; $t_R = 13.17$ min (minor), 19.08 min (major)). ^1H NMR (500 MHz, CDCl_3) δ 8.27 (d, $J = 8.5$ Hz, 1H), 7.89 (d, $J = 8.5$ Hz, 4H), 7.65 – 7.60 (m, 2H), 7.38 – 7.11 (m, 10H), 7.00 – 6.91 (m, 3H), 6.32 (d, $J = 7.5$ Hz, 1H), 5.15 (ddd, $J = 15.0, 7.0, 1.5$ Hz, 1H), 4.76 (dd, $J = 16.5, 7.0$ Hz, 1H), 4.06 (s, 1H), 3.07 (t, $J = 15.5$ Hz, 1H), 2.42 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 172.2, 145.6, 136.9(4), 136.9(0), 136.8(7), 135.4(0), 135.3(5), 134.1, 133.5, 132.8, 132.3, 130.3, 129.7, 129.5, 129.4, 128.6(1), 128.5(5), 128.5, 128.3, 126.7, 126.3, 124.5, 124.2, 123.6, 120.1, 118.5, 114.5, 60.9, 51.3, 29.5, 21.7; IR (neat): 2924, 1746(s), 1374, 1174, 1152, 1088, 742, 579; HRESIMS Calcd for $[\text{C}_{39}\text{H}_{28}\text{BrClN}_2\text{NaO}_5\text{S}_2]^+$ ($\text{M} + \text{Na}^+$) 805.0204, found 805.0203.

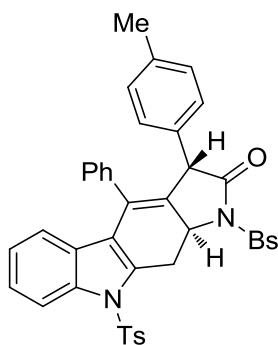
(3*S*,10*aS*)-3-(4-bromophenyl)-1-((4-bromophenyl)sulfonyl)-4-phenyl-9-tosyl-3,9,10,10*a*-tetrahydropyrrolo[2,3-*b*]carbazol-2(1*H*)-one (5e)



5e

Compound **5e** was prepared in 75% yield (123.8 mg) according to the general procedure (Table 2, entry 1). White solid (mp 144-146 °C). $[\alpha]_D^{20} = -18.8^\circ$ (c = 1.0, CHCl₃). 97% ee (determined by HPLC: Chiralcel AD-H Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; t_R = 14.54 min (minor), 20.57 min (major)). ¹H NMR (500 MHz, CDCl₃) δ 8.27 (d, J = 8.5 Hz, 1H), 7.95 – 7.83 (m, 4H), 7.63 (d, J = 9.0 Hz, 2H), 7.39 (d, J = 8.4 Hz, 2H), 7.36 – 7.27 (m, 4H), 7.25 – 7.09 (m, 3H), 6.99 – 6.88 (m, 3H), 6.86 – 6.70 (m, 1H), 6.32 (d, J = 8.0 Hz, 1H), 5.15 (dd, J = 15.1, 7.0 Hz, 1H), 4.76 (dd, J = 16.0, 7.0 Hz, 1H), 4.04 (s, 1H), 3.07 (t, J = 16.0 Hz, 1H), 2.43 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 172.1, 145.6, 137.4, 136.9, 135.4(1), 135.3(5), 133.5, 132.8, 132.4, 132.3, 130.3, 129.8, 129.5, 128.9, 128.6, 128.5, 128.3, 126.7, 126.3, 124.5, 124.1, 123.6, 122.2, 120.1, 118.5, 114.5, 61.0, 51.4, 29.5, 21.7; IR (neat): 2924, 1746(s), 1374, 1174, 1151, 1088, 742, 577; HRESIMS Calcd for [C₃₉H₂₈Br₂N₂NaO₅S₂]⁺ (M + Na⁺) 848.9699, found 848.9728.

(3*S*,10*aS*)-1-((4-bromophenyl)sulfonyl)-4-phenyl-3-(*p*-tolyl)-9-tosyl-3,9,10*a*-tetrahydropyrrolo[2,3-*b*]carbazol-2(1*H*)-one (5f)

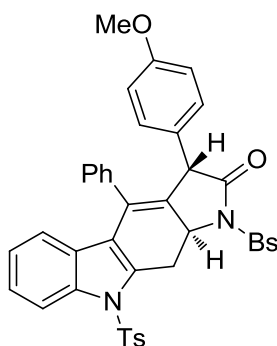


5f

Compound **5f** was prepared in 65% yield (99.1 mg) according to the general procedure. White solid (mp 139-141 °C). $[\alpha]_D^{20} = +28.5^\circ$ (c = 1.0, CHCl₃). 98% ee (determined by HPLC: Chiralcel AD-H Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; t_R = 11.55 min (minor), 18.13 min (major)). ¹H NMR (500 MHz, CDCl₃) δ 8.28 (d, J = 8.5 Hz, 1H), 7.89 (d, J = 8.0 Hz, 2H), 7.85 (d, J = 8.5 Hz, 2H),

7.57 (d, $J = 8.5$ Hz, 2H), 7.34 (d, $J = 8.0$ Hz, 2H), 7.31 – 7.22 (m, 3H), 7.21 – 7.05 (m, 3H), 7.03 (d, $J = 8.0$ Hz, 2H), 6.95 (t, $J = 7.5$ Hz, 1H), 6.89 (d, $J = 8.0$ Hz, 2H), 6.34 (d, $J = 8.0$ Hz, 1H), 5.14 (dd, $J = 15.0, 7.0$ Hz, 1H), 4.75 (dd, $J = 16.5, 7.5$ Hz, 1H), 4.05 (s, 1H), 3.08 (t, $J = 16.0$ Hz, 1H), 2.42 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 172.7, 145.5, 137.8, 136.8(9), 136.8(7), 135.5(0), 135.4(6), 135.2, 132.9, 132.7, 132.2, 130.3, 129.9, 129.4, 128.6, 128.4, 128.1, 127.0, 126.7, 126.4, 125.1, 124.4, 123.5, 120.1, 118.7, 114.5, 61.1, 51.6, 29.6, 21.7, 21.1; IR (neat): 2919, 1746(s), 1372, 1180, 1075, 742, 577; HRESIMS Calcd for $[\text{C}_{40}\text{H}_{31}\text{BrN}_2\text{NaO}_5\text{S}_2]^+$ (M + Na^+) 785.0750, found 785.0773.

(3*S*,10*aS*)-1-((4-bromophenyl)sulfonyl)-3-(4-methoxyphenyl)-4-phenyl-9-tosyl-3,9,10,10a-tetrahydropyrrolo[2,3-*b*]carbazol-2(1*H*)-one (5g)

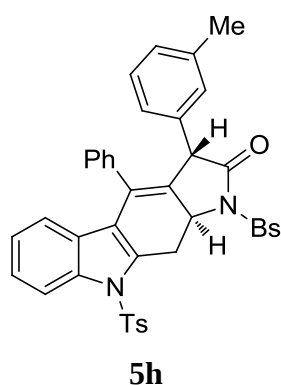


5g

Compound **5g** was prepared in 68% yield (105.8 mg) according to the general procedure. White solid (mp 146-148 °C). $[\alpha]_{\text{D}}^{20} = -15.3^\circ$ ($c = 1.0$, CHCl_3). 97% ee (determined by HPLC: Chiralcel AD-H Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; $t_{\text{R}} = 19.96$ min (minor), 24.32 min (major)). ^1H NMR (500 MHz, CDCl_3) δ 8.27 (d, $J = 8.5$ Hz, 1H), 7.91 – 7.85 (m, 4H), 7.60 (d, $J = 9.0$ Hz, 2H), 7.34 (d, $J = 8.0$ Hz, 2H), 7.32 – 7.24 (m, 3H), 7.21 – 7.07 (m, 3H), 6.97 – 6.90 (m, 3H), 6.77 (d, $J = 9.0$ Hz, 2H), 6.33 (d, $J = 8.0$ Hz, 1H), 5.14 (dd, $J = 15.5, 7.5$ Hz, 1H), 4.75 (dd, $J = 16.5, 7.5$ Hz, 1H), 4.03 (s, 1H), 3.81 (s, 3H), 3.07 (t, $J = 15.5$ Hz, 1H), 2.42 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 172.8, 159.3, 145.5, 137.0, 136.9, 135.5, 135.4, 132.8, 132.7, 132.2, 130.5, 130.3, 129.5, 129.4, 128.6, 128.4, 128.3, 128.2,

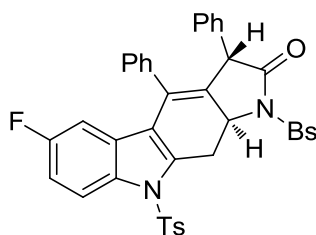
126.7, 126.4, 125.2, 124.4, 123.5, 120.1, 118.7, 114.6, 114.5, 61.1, 55.3, 51.1, 29.6, 21.7; IR (neat): 2925, 1746(s), 1373, 1256, 1174, 1088, 748, 577; HRESIMS Calcd for $[\text{C}_{40}\text{H}_{31}\text{BrN}_2\text{NaO}_6\text{S}_2]^+$ ($\text{M} + \text{Na}^+$) 801.0699, found 801.0700.

(3*S*,10*aS*)-1-((4-bromophenyl)sulfonyl)-4-phenyl-3-(*m*-tolyl)-9-tosyl-3,9,10,10a-tetrahydropyrrolo[2,3-*b*]carbazol-2(1*H*)-one (5h)



Compound **5h** was prepared in 73% yield (111.3 mg) according to the general procedure. White solid (mp 141-143 °C). $[\alpha]_{\text{D}}^{20} = +24.5^\circ$ ($c = 1.0$, CHCl_3). 99% ee (determined by HPLC: Chiralcel AD -H Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; $t_{\text{R}} = 11.18$ min (minor), 18.44 min (major)). ^1H NMR (500 MHz, CDCl_3) δ 8.27 (d, $J = 8.5$ Hz, 1H), 7.92 – 7.84 (m, 4H), 7.59 (d, $J = 8.5$ Hz, 2H), 7.34 (d, $J = 8.5$ Hz, 2H), 7.32 – 7.04 (m, 7H), 6.97 – 6.91 (m, 1H), 6.85 – 6.68 (m, 3H), 6.33 (d, $J = 8.0$ Hz, 1H), 5.16 (dd, $J = 15.0, 7.0$ Hz, 1H), 4.76 (dd, $J = 16.5, 7.0$ Hz, 1H), 4.05 (s, 1H), 3.09 (t, $J = 16.0$ Hz, 1H), 2.42 (s, 3H), 2.26 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 172.8, 145.5, 138.9, 138.4, 136.9(4), 136.8(9), 135.5, 132.9, 132.7, 132.2, 130.3, 129.5, 129.0, 128.7, 128.4, 128.1, 127.8, 126.7, 126.4, 125.1, 124.4, 124.2, 123.5, 120.1, 118.7, 114.5, 61.2, 51.9, 29.6, 21.7, 21.4; IR (neat): 2922, 1748(s), 1374, 1174, 1152, 1088, 745, 577; HRESIMS Calcd for $[\text{C}_{40}\text{H}_{31}\text{BrN}_2\text{NaO}_5\text{S}_2]^+$ ($\text{M} + \text{Na}^+$) 785.0750, found 785.0749.

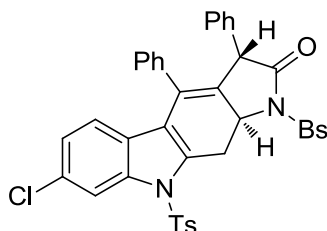
(3*S*,10*aS*)-1-((4-bromophenyl)sulfonyl)-6-fluoro-3,4-diphenyl-9-tosyl-3,9,10,10a-tetrahydropyrrolo[2,3-*b*]carbazol-2(1*H*)-one (5i)



5i

Compound **5i** was prepared in 80% yield (122.6 mg) according to the general procedure. White solid (mp 140-142 °C). $[\alpha]_D^{20} = +12.5^\circ$ (c = 1.0, CHCl₃). 98% ee (determined by HPLC: Chiralcel AD-H Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; t_R = 13.51 min (minor), 18.73 min (major)). ¹H NMR (500 MHz, CDCl₃) δ 8.25 – 8.18 (m, 1H), 7.92 – 7.84 (m, 4H), 7.59 (d, J = 8.5 Hz, 2H), 7.36 (d, J = 8.0 Hz, 2H), 7.33 – 7.11 (m, 8H), 7.02 – 6.94 (m, 3H), 6.00 – 5.88 (m, 1H), 5.15 (ddd, J = 15.5, 7.0, 1.5 Hz, 1H), 4.75 (dd, J = 16.5, 7.5 Hz, 1H), 4.08 (s, 1H), 3.08 (t, J = 16.0 Hz, 1H), 2.44 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ 172.5, 159.3 (d, J = 238.8 Hz), 145.7, 138.4, 136.9, 135.2, 134.9, 134.5, 133.2, 132.5, 132.3, 130.4, 129.6, 129.5, 129.2, 128.7, 128.3, 128.0, 127.5, 127.4 (d, J = 10.0 Hz), 126.7, 125.2, 118.5 (d, J = 3.8 Hz), 115.6 (d, J = 8.8 Hz), 112.3 (d, J = 25.0 Hz), 105.8 (d, J = 25.0 Hz), 61.0, 51.9, 29.7, 21.7; IR (neat): 2922, 1747(s), 1375, 1175, 1122, 1087, 742, 563; HRESIMS Calcd for [C₃₉H₂₈BrFN₂NaO₅S₂]⁺ (M + Na⁺) 789.0499, found 789.0506.

(3S,10aS)-1-((4-bromophenyl)sulfonyl)-7-chloro-3,4-diphenyl-9-tosyl-3,9,10,10a-tetrahydropyrrolo[2,3-b]carbazol-2(1H)-one (5j)

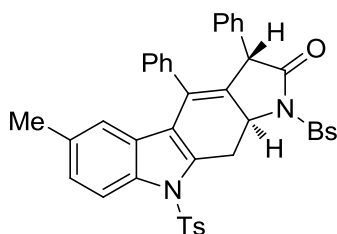


5j

Compound **5j** was prepared in 75% yield (117.6 mg) according to the general procedure. White solid (mp 145-147 °C). $[\alpha]_D^{20} = +14.5^\circ$ (c = 1.0, CHCl₃). 97% ee

(determined by HPLC: Chiralcel AD-H Column, 15/85 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; t_R = 7.26 min (minor), 13.35 min (major)). ^1H NMR (500 MHz, CDCl_3) δ 8.30 (d, J = 2.0 Hz, 1H), 7.90 (d, J = 8.5 Hz, 2H), 7.86 (d, J = 8.5 Hz, 2H), 7.59 (d, J = 9.0 Hz, 2H), 7.38 (d, J = 8.5 Hz, 2H), 7.31 – 7.10 (m, 8H), 6.99 (d, J = 7.0 Hz, 2H), 6.95 – 6.90 (m, 1H), 6.21 (d, J = 8.5 Hz, 1H), 5.15 (ddd, J = 15.5, 7.5, 1.5 Hz, 1H), 4.72 (dd, J = 16.5, 7.0 Hz, 1H), 4.08 (s, 1H), 3.07 (t, J = 15.5 Hz, 1H), 2.45 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 172.5, 145.9, 138.4, 137.2, 136.9, 135.1(9), 135.1(7), 133.4, 132.5, 132.3, 130.5, 129.6, 129.5, 129.2, 128.6, 128.3, 128.0, 127.2, 126.8, 125.4, 124.9, 124.2, 120.8, 118.3, 114.6, 61.0, 51.9, 29.6, 21.7; IR (neat): 2924, 1747(s), 1375, 1172, 1088, 912, 743, 585; HRESIMS Calcd for $[\text{C}_{39}\text{H}_{28}\text{BrClN}_2\text{NaO}_5\text{S}_2]^+$ ($M + \text{Na}^+$) 805.0204, found 805.0210.

(3*S*,10*aS*)-1-((4-bromophenyl)sulfonyl)-6-methyl-3,4-diphenyl-9-tosyl-3,9,10,10a-tetrahydropyrrolo[2,3-*b*]carbazol-2(1*H*)-one (5k)

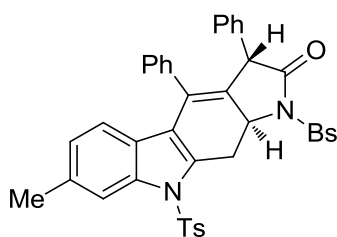


5k

Compound **5k** was prepared in 70% yield (106.9 mg) according to the general procedure. White solid (mp 143-145 °C). $[\alpha]_D^{20}$ = +15.4 °(c = 1.0, CHCl_3). 98% ee (determined by HPLC: Chiralcel AD-H Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; t_R = 12.27 min (minor), 20.51 min (major)). ^1H NMR (500 MHz, CDCl_3) δ 8.14 (d, J = 8.5 Hz, 1H), 7.91 – 7.83 (m, 4H), 7.59 (d, J = 8.5 Hz, 2H), 7.33 (d, J = 8.0 Hz, 2H), 7.31 – 7.20 (m, 6H), 7.21 – 7.11 (m, 2H), 7.10 – 6.99 (m, 3H), 6.07 (s, 1H), 5.15 (dd, J = 15.0, 7.0 Hz, 1H), 4.74 (dd, J = 16.5, 7.0 Hz, 1H), 4.09 (s, 1H), 3.05 (t, J = 16.0 Hz, 1H), 2.42 (s, 3H), 2.11 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ 172.6, 145.4, 138.6, 137.0, 135.5, 135.4, 135.2, 133.1, 133.0, 132.9, 132.3, 130.2, 129.5(2), 129.4(7), 129.2, 128.6, 128.4, 128.1, 127.9, 127.2, 126.7, 126.6, 125.8,

124.8, 120.0, 118.5, 114.2, 61.2, 52.0, 29.6, 21.7, 21.2; IR (neat): 2922, 1747(s), 1374, 1174, 1133, 1087, 742, 575; HRESIMS Calcd for $[C_{40}H_{31}BrN_2NaO_5S_2]^+$ ($M + Na^+$) 785.0750, found 785.0755.

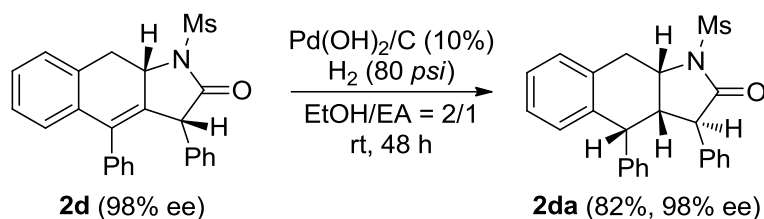
(3*S*,10*aS*)-1-((4-bromophenyl)sulfonyl)-7-methyl-3,4-diphenyl-9-tosyl-3,9,10,10a-tetrahydropyrrolo[2,3-*b*]carbazol-2(1*H*)-one (5l)



5l

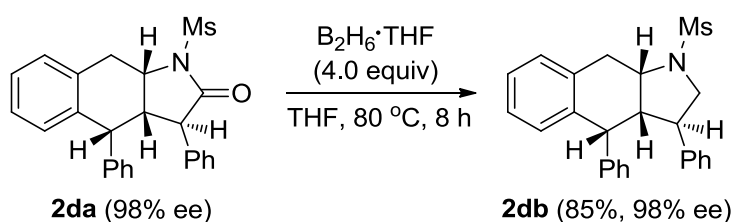
Compound **5l** was prepared in 69% yield (105.2 mg) according to the general procedure. White solid (mp 139-141 °C). $[\alpha]_D^{20} = +13.5^\circ$ ($c = 1.0$, $CHCl_3$). 99% ee (determined by HPLC: Chiralcel AD-H Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; $t_R = 10.54$ min (minor), 19.83 min (major)). 1H NMR (500 MHz, $CDCl_3$) δ 8.09 (s, 1H), 7.92 – 7.84 (m, 4H), 7.58 (d, $J = 9.0$ Hz, 2H), 7.34 (d, $J = 8.0$ Hz, 2H), 7.30 – 7.09 (m, 7H), 7.06 – 6.99 (m, 2H), 6.83 – 6.71 (m, 2H), 6.19 (d, $J = 8.0$ Hz, 1H), 5.16 (ddd, $J = 15.0, 7.0, 1.5$ Hz, 1H), 4.72 (dd, $J = 16.5, 7.0$ Hz, 1H), 4.08 (s, 1H), 3.05 (t, $J = 16.0$ Hz, 1H), 2.44 (s, 3H), 2.43 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 172.7, 145.4, 138.6, 137.4, 137.0, 135.5(4), 135.5(0), 134.6, 132.9, 132.3, 132.1, 130.2, 129.5(1), 129.4(5), 129.2, 128.6, 128.4, 128.1, 127.9, 127.2, 126.6, 125.0, 124.8, 124.2, 119.6, 118.7, 114.6, 61.2, 52.0, 29.6, 21.9, 21.7; IR (neat): 2922, 1747(s), 1373, 1173, 1143, 1088, 743, 579; HRESIMS Calcd for $[C_{40}H_{31}BrN_2NaO_5S_2]^+$ ($M + Na^+$) 785.0750, found 785.0759.

(3*R*,3*aS*,4*R*,9*aS*)-1-(methylsulfonyl)-3,4-diphenyl-3*a*,4,9,9*a*-tetrahydro-1*H*-benzo[*f*]indol-2(3*H*)-one (2da)



Compound **2da** was prepared in 82% yield (68.4 mg; 0.2 mmol scale) according to the known procedure.⁴ White solid (mp 125-127 °C). $[\alpha]_D^{20} = -43.5^\circ$ (c = 1.0, CHCl₃). 98% ee (determined by HPLC: Chiralcel AD-H Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; t_R = 40.33 min (minor), 32.23 min (major)). ¹H NMR (400 MHz, CDCl₃) δ 7.33 – 7.17 (m, 6H), 7.15 – 7.05 (m, 4H), 7.00 – 6.90 (m, 2H), 6.88 – 6.79 (m, 2H), 4.86 (dt, J = 8.4, 6.0 Hz, 1H), 4.45 (d, J = 6.8 Hz, 1H), 3.66 – 3.58 (m, 1H), 3.55 (d, J = 9.6 Hz, 1H), 3.33 (dd, J = 5.2, 2.0 Hz, 2H), 3.28 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 174.2, 139.1, 138.3, 137.3, 134.0, 129.9, 129.1, 128.6, 128.3, 128.1, 127.6, 127.5, 127.2, 127.0, 57.9, 51.3, 46.9, 43.0, 41.9, 34.1; IR (neat): 2927, 2828, 1742 (s), 1495, 1358, 1167, 1129, 969, 728, 701, 545; HRESIMS Calcd for [C₂₅H₂₃NNaO₃S]⁺ (M + Na⁺) 440.1291, found 440.1292.

(3R,3aS,4R,9aS)-1-(methylsulfonyl)-3,4-diphenyl-2,3,3a,4,9,9a-hexahydro-1H-benzof[3,4-b]indole (2db)

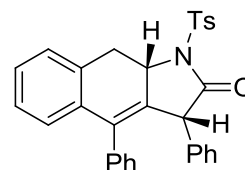
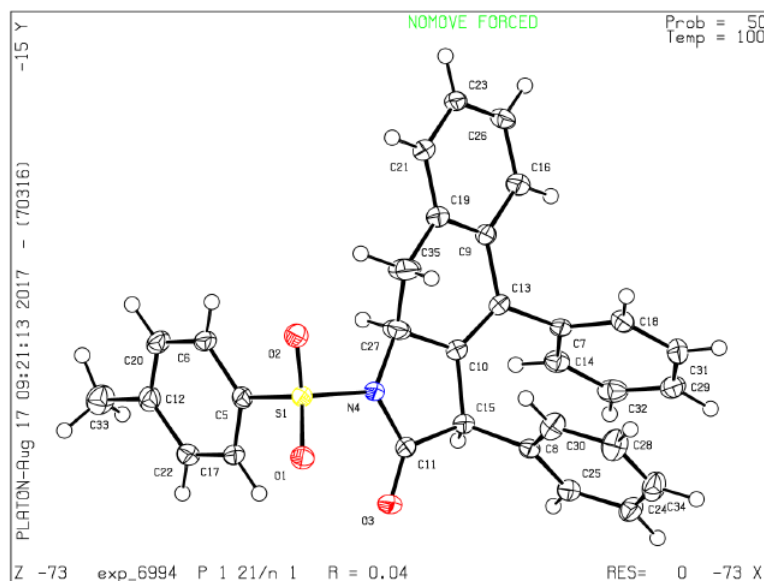


Compound **2db** was prepared in 85% yield (34.3 mg; 0.1 mmol scale) according to the known procedure.⁵ White solid (mp 117-120 °C). $[\alpha]_D^{20} = -44.4^\circ$ (c = 1.0, CHCl₃); 98% ee (determined by HPLC: Chiralcel AD-H Column, 10/90 *i*-PrOH/hexane, 1.0 mL/min, 254 nm, 25 °C; t_R = 12.81 min (major), 15.29 min (minor)). ¹H NMR (400 MHz, CDCl₃) δ 7.28 (d, J = 6.8 Hz, 1H), 7.24 – 7.18 (m, 1H), 7.17 – 7.10 (m, 4H), 7.08 – 6.96 (m, 4H), 6.87 – 6.83 (m, 2H), 6.82 – 6.75 (m, 2H), 4.40 (d, J = 8.4 Hz, 1H), 4.34 – 4.25 (m, 1H), 3.57 – 3.48 (m, 1H), 3.46 – 3.37 (m, 1H), 3.29 – 3.16 (m,

3H), 3.06 (t, $J = 9.2$ Hz, 1H), 2.89 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3) δ 140.0, 139.8, 139.3, 135.3, 129.9, 129.0, 128.4(2), 128.4(0), 127.8, 127.3, 127.0, 126.7(4), 126.7(1), 126.4, 60.5, 56.6, 47.3, 46.5, 45.8, 35.8, 35.6; IR (neat): 3026, 2924, 2852, 1494, 1452, 1333, 1149, 1029, 962, 742, 698, 564; HRESIMS Calcd for $[\text{C}_{25}\text{H}_{25}\text{NNaO}_2\text{S}]^+$ ($\text{M} + \text{Na}^+$) 426.1498, found 426.1501.

(3*R*,9*aS*)-3,4-diphenyl-1-tosyl-9,9a-dihydro-1*H*-benzo[*f*]indol-2(3*H*)-one (2a).

CCDC Number = 1569444



Bond precision: C-C = 0.0030 Å

Wavelength=1.54184

Cell: a=11.7246 (4)

b=12.2563 (6)

c=16.5665 (7)

alpha=90

beta=98.550 (4)

gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	2354.15 (17)	2354.15 (18)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C ₃₁ H ₂₅ N O ₃ S	C ₃₁ H ₂₅ N O ₃ S
Sum formula	C ₃₁ H ₂₅ N O ₃ S	C ₃₁ H ₂₅ N O ₃ S
Mr	491.58	491.58
Dx, g cm ⁻³	1.387	1.387
Z	4	4
Mu (mm ⁻¹)	1.505	1.505
F ₀₀₀	1032.0	1032.0
F ₀₀₀ '	1036.16	
h,k,l _{max}	13,14,19	13,14,19
N _{ref}	4009	3942
T _{min} ,T _{max}	0.693,0.822	0.754,1.000
T _{min} '	0.571	

Correction method= # Reported T Limits: T_{min}=0.754 T_{max}=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.983

Theta(max)= 64.995

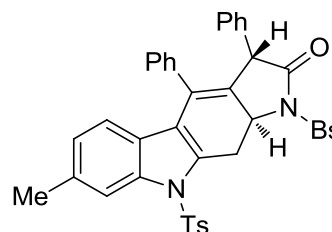
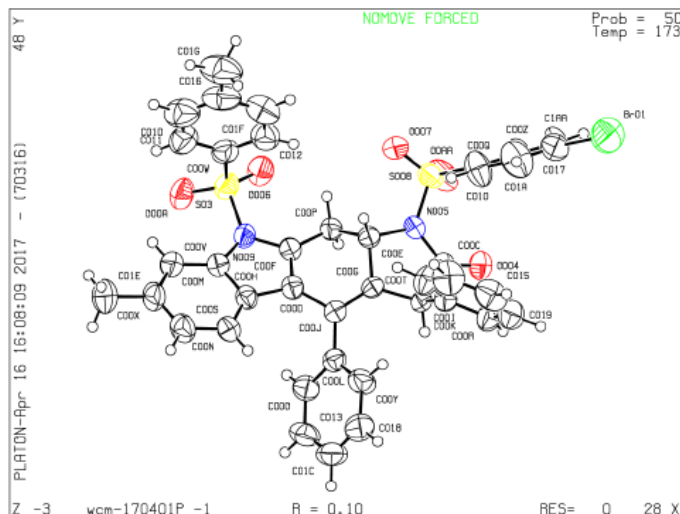
R(reflections)= 0.0430 (3487)

wR2(reflections)= 0.1149 (3942)

S = 1.035

N_{par}= 326

(3*S*,10*aS*)-1-((4-bromophenyl)sulfonyl)-7-methyl-3,4-diphenyl-9-tosyl-3,9,10,10*a*-tetrahydropyrrolo[2,3-*b*]carbazol-2(1*H*)-one (5l). CCDC Number = 1569442



Bond precision: C-C = 0.0125 Å

Wavelength=1.54184

Cell: a=10.1352 (5) b=13.2429 (7) c=16.5954 (8)
 alpha=110.962 (5) beta=96.295 (4) gamma=91.276 (4)
 Temperature: 173 K

	Calculated	Reported
Volume	2062.93 (19)	2062.93 (19)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C40 H31 Br N2 O5 S2 [+ solvent]	C40 H31 Br N2 O5 S2
Sum formula	C40 H31 Br N2 O5 S2 [+ solvent]	C40 H31 Br N2 O5 S2
Mr	763.69	763.70
Dx, g cm ⁻³	1.230	1.229
Z	2	2
Mu (mm ⁻¹)	2.639	2.639
F000	784.0	784.0
F000'	785.96	
h,k,lmax	11,15,18	11,15,18
Nref	6349	6019
Tmin, Tmax		0.389, 1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.389 Tmax=1.000
 AbsCorr = MULTI-SCAN

Data completeness= 0.948

Theta(max)= 61.160

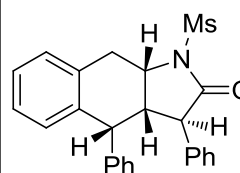
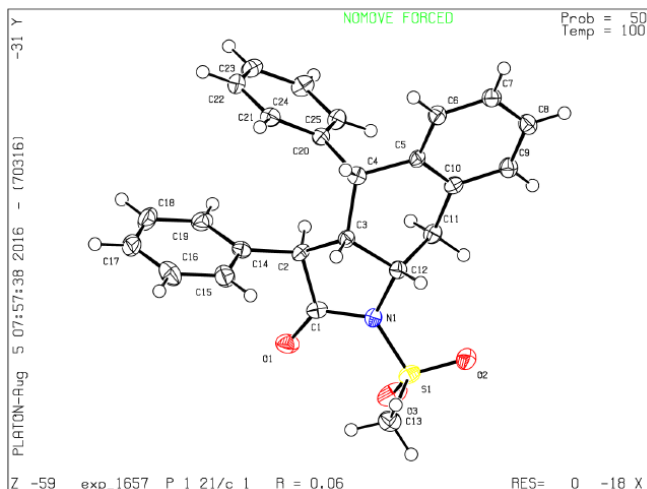
R(reflections)= 0.0992 (3620)

wR2(reflections)= 0.2740 (6019)

S = 1.076

Npar= 453

(3*R*,3*aS*,4*R*,9*aS*)-1-(methylsulfonyl)-3,4-diphenyl-3*a*,4,9,9*a*-tetrahydro-1*H*-benzo[*f*]indol-2(3*H*)-one (2*da*). CCDC Number = 1569443



Bond precision: C-C = 0.0050 Å

Wavelength=1.54184

Cell: a=18.5095 (15)

b=10.9007 (8)

c=10.3745 (8)

alpha=90

beta=103.857 (8)

gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	2032.3 (3)	2032.3 (3)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C25 H23 N O3 S	C25 H23 N O3 S
Sum formula	C25 H23 N O3 S	C25 H23 N O3 S
Mr	417.50	417.50
Dx, g cm ⁻³	1.365	1.365
Z	4	4
Mu (mm ⁻¹)	1.637	1.637
F000	880.0	880.0
F000'	883.75	
h,k,lmax	21,12,12	21,12,12
Nref	3540	3416
Tmin,Tmax	0.745,0.849	0.878,1.000
Tmin'	0.721	

Correction method= # Reported T Limits: Tmin=0.878 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 0.965

Theta(max)= 65.949

R(reflections)= 0.0583 (2384)

wR2(reflections)= 0.1675 (3416)

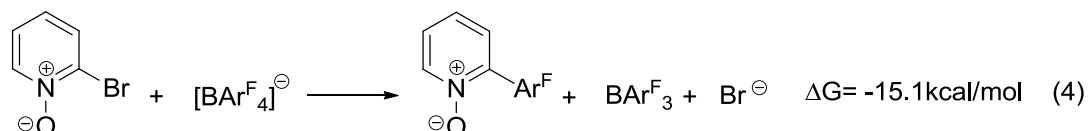
S = 1.028

Npar= 272

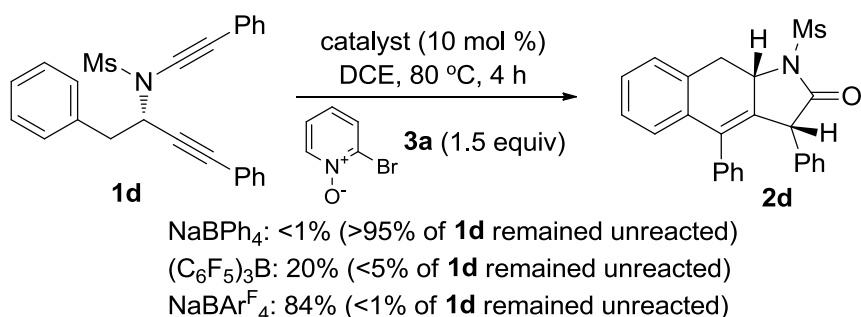
Computational Details

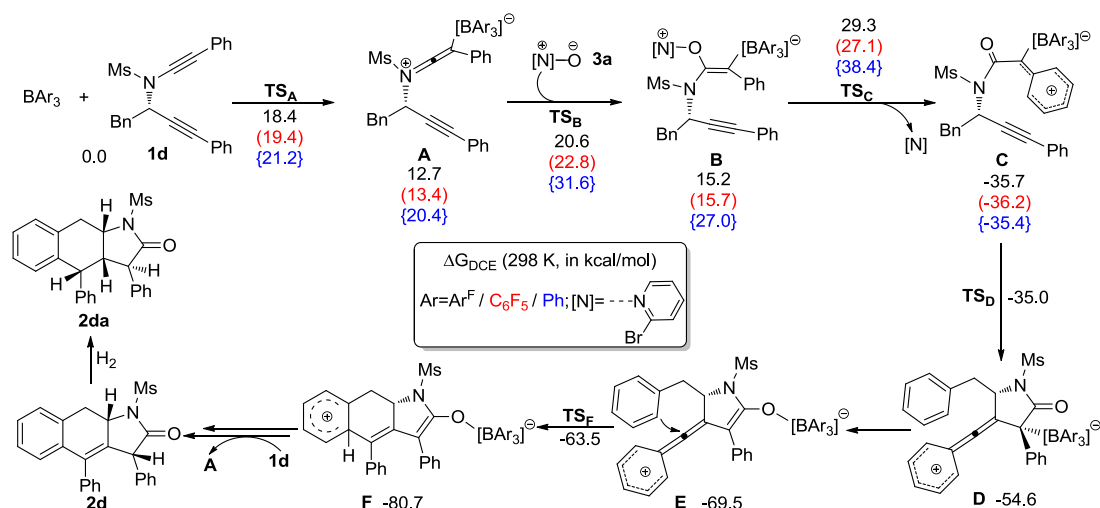
All density functional theory (DFT) calculations were carried out with the Gaussian 09 programs.⁶ The meta-hybrid GGA functional, M06,⁷ was used in combination with the 6-31G(d, p) basis set⁸ for C, H, B, N, O, F, S and Br. Vibrational analyses were performed to confirm each stationary point to be either a local minimum or a transition state (TS). The connection between each transition state and its neighboring reactant and product were verified by intrinsic reaction coordinate (IRC)⁹ calculations. Solvent effects of solvents, i.e., DCE (dielectric constant $\epsilon = 10.125$) and PhCl ($\epsilon = 5.6968$), were taken in account by using the SMD-flavor¹⁰ of self-consistent reaction field (SCRF) theory.

Cleavage of C-X (X=Br, Cl) in the halogen-substituted *N*-oxide likely facilitates the release of BAr^{F}_3 from $\text{NaBAr}^{\text{F}}_4$ with concomitant precipitation of NaX ($\text{Na}^+ + \text{Br}^- = \text{NaBr(s)}\downarrow$) from the organic solution, as shown in eq. 4. Hence, the thus-released BAr^{F}_3 can be the catalytically active Lewis acid in the concerned reactions.



1. Theoretical study on catalytic efficiencies of $\text{NaBAr}^{\text{F}}_4/(\text{C}_6\text{F}_5)_3\text{B}/\text{NaBPh}_4$ catalysts





Scheme S1. Plausible mechanism for the NaBAR^F₄/(C₆F₅)₃B/NaBPh₄-catalyzed oxidative polycyclization of N-propargyl ynamide **1d**. Relative free energies (ΔG_{DCE}) of key intermediates and transition states were computed at the SMD-M06/6-31G(d,p) level of theory in DCE at 298 K. Data for Ar=C₆F₅ (i.e., (C₆F₅)₃B as catalyst) and Ar=Ph (i.e., NaBPh₄ as catalyst) were given in parentheses and braces, respectively.

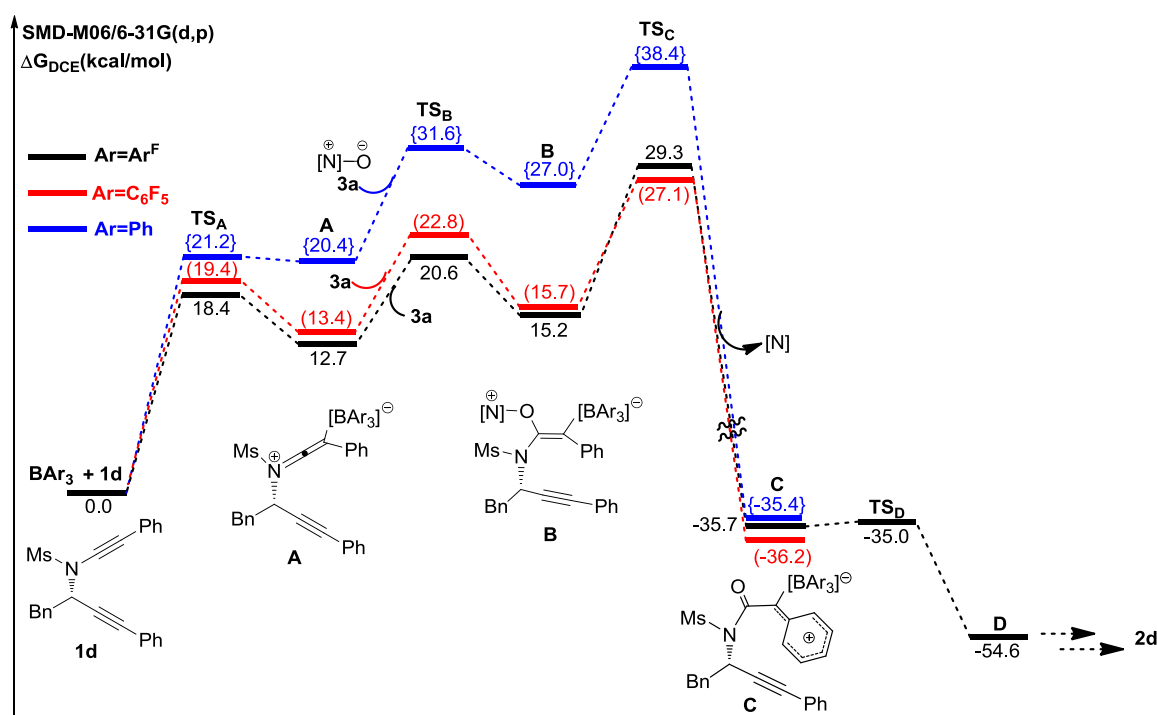
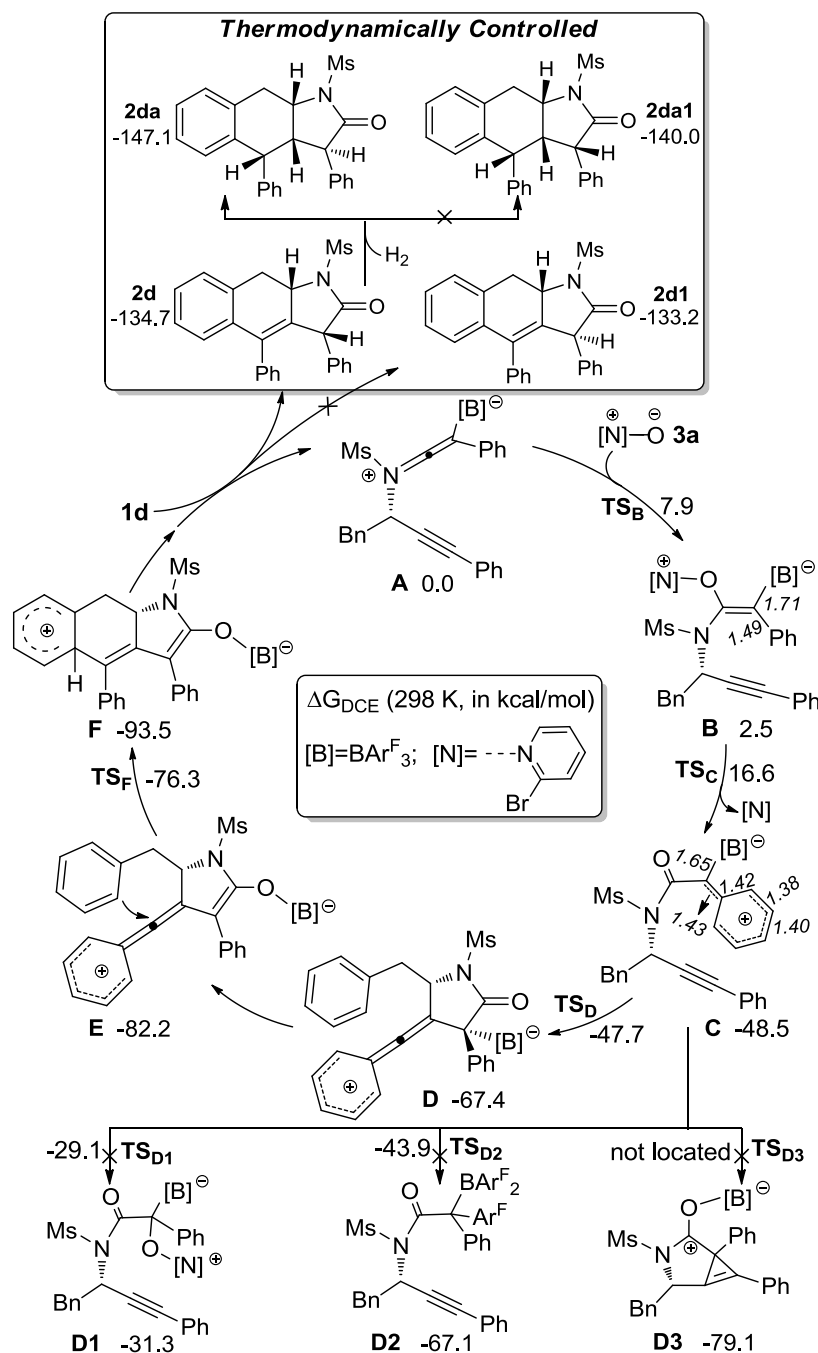


Figure S1. Free energy profiles for NaBAR^F₄/(C₆F₅)₃B/NaBPh₄-catalyzed formation of **2d** (NaBAR^F₄ catalysis (Ar=Ar^F), black line; (C₆F₅)₃B catalysis (Ar=C₆F₅), red line; NaBPh₄ catalysis (Ar=Ph), blue line). Data for (C₆F₅)₃B catalysis (Ar=C₆F₅) and

NaBPh₄ catalysis (Ar=Ph) were given in parentheses and braces, respectively.

As shown in **Scheme S1 and Figure S1**, ligation of *N*-propargyl ynamide **1d** to the catalytically active species BAr₃, which initiates the concerned process, is also the rate-limiting step. In the case of Ar=Ar^F (i.e., NaBAr^F₄ as catalyst), the activation energy of this step is 18.4 kcal/mol, 1.0 kcal/mol lower than that in the case of Ar=C₆F₅ (i.e., (C₆F₅)₃B as catalyst). This accounts for the higher efficiency of the NaBAr^F₄ catalyst than (C₆F₅)₃B catalyst in the synthesis of **2d**. On the other hand, in the case of Ar=Ph (i.e., NaBPh₄ as catalyst), the process has to surmount an overall activation barrier amounting up to 38.4 kcal/mol (via **TSc**). Hence, NaBPh₄ shows almost no catalytic efficiency in the synthesis of **2d**.

2. Plausible mechanism for the NaBAr^F₄-catalyzed oxidative polycyclization of *N*-propargyl ynamide **1d**

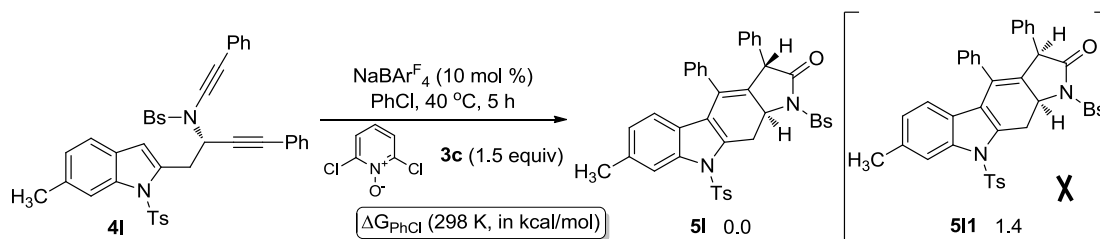


Scheme S2. Plausible mechanism for the $\text{NaBAr}^{\text{F}}_4$ -catalyzed oxidative polycyclization of *N*-propargyl ynamide **1d**. Relative free energies (ΔG_{DCE}) of key intermediates and transition states were computed at the SMD-M06/6-31G(d,p) level of theory in DCE at 298 K. Key bond lengths were shown in italic (unit: Å).

A plausible mechanism for the $\text{NaBAr}^{\text{F}}_4$ -catalyzed oxidative polycyclization of *N*-propargyl ynamide **1d** is illustrated in Scheme S2. Initially, nucleophilic attack of *N*-oxide **3a** on the BAr^{F}_3 -ligated ynamide **A** forms the vinyl borate intermediate **B**.

N-O bond cleavage gives rise to the phenyl-stabilized carbocation **C**. Then, an intramolecular cyclization (via **TS_D**), overoxidation (via **TS_{D1}**), Ar^F migration (via **TS_{D2}**), and cyclopropanation (Although the **TS_{D3}** is not located, we suspect that the energy barrier of cyclopropanation is higher than that of intramolecular cyclization due to the large steric repulsion between the phenyl group on α -carbon and the phenyl group on alkynyl) within the intermediate **C** occur competitively to afford the enylium-cationic intermediate **D**, **D₁**, **D₂**, and **D₃** respectively. Obviously, the intramolecular cyclization to furnish the intermediate **D** is kinetically the most favorable (only requiring an energy barrier of 0.8 kcal/mol, nearly barrierless), thus predicting good chemoselectivity. Upon intramolecular migration of BAr^F₃, **D** isomerizes into **E**, followed by a second cyclization to afford intermediate **F**. The latter undergoes sequentially deprotonation-aromatization, protonation, and substrate exchange, leading eventually to the thermodynamically favoured **2d**, but not **2d1**. Likewise, further hydrogenation of **2d** affords the thermodynamically favoured **2da**, but not **2da1**.

3. Construction of linear tetracyclic *N*-heterocycles **5l**



Scheme S3. The reaction for NaBARF₄-catalyzed oxidative polycyclization of indolyl *N*-propargyl ynamide **4l**. Relative free energies (ΔG_{PhCl}) of **5l** and another isomer **5l1** were computed at the SMD-M06/6-31G(d,p) level of theory in PhCl at 298 K. It clearly shows that the formation of tetracyclic *N*-heterocycle **5l**, but not **5l1**, is thermodynamically controlled.

Reference:

1. a) Y.-F. Yu, C. Shu, T.-D. Tan, L. Li, S. Rafique, L.-W. Ye, *Org. Lett.* **2016**, *18*, 5178; b) C. Shu, L. Li, C.-H. Shen, P.-P. Ruan, C.-Y. Liu, L.-W. Ye, *Chem. Eur. J.*

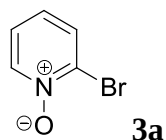
- 2016**, 22, 2282; c) Y.-F. Yu, C. Shu, B. Zhou, J.-Q. Li, J.-M. Zhou, L.-W. Ye, *Chem. Commun.* **2015**, 51, 2126; d) C. Shu, M.-Q. Liu, S.-S. Wang, L. Li, L.-W. Ye, *J. Org. Chem.* **2013**, 78, 3292.
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Molecular Geometries and Energies

Cartesian Coordinates and Energies in Hartree

NaBAr^F₄ as catalyst



Number of imaginary frequencies: 0

O	-2.74775900	1.13127200	-0.42017700
C	-0.62813300	1.87082600	-0.87074200
C	-2.48624500	3.01477700	-1.73395400
C	0.22647600	2.76710500	-1.47035200
H	-0.31501900	1.02525800	-0.26863600
C	-1.65589800	3.93480100	-2.35069900
C	-0.27985300	3.82165500	-2.22558300
H	1.29518100	2.62753900	-1.33736200
H	-2.11003500	4.73657400	-2.92545700
H	0.37881700	4.53881300	-2.70474700
N	-1.99154300	1.97327000	-0.98709000
Br	-4.34839000	3.11882500	-1.86559100

Energy (0K) = -2893.8798597

Energy (0K) + ZPE = -2893.797170

Enthalpy (298K) = -2893.789799

Free Energy (298K) = -2893.829097

[BAr^F₄]⁻

Number of imaginary frequencies: 0

B	-0.00294500	-0.00041800	-0.00499800
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C	-1.30275000	0.93040200	0.35418200
C	-1.97861600	0.72529100	1.57186700
C	-1.87207200	1.86799200	-0.50818800
C	-3.12437100	1.43092900	1.91045600
H	-1.59527300	-0.01726500	2.27204800
C	-3.02943800	2.58067500	-0.17493400
H	-1.41208400	2.06134900	-1.47834900
C	-3.66537300	2.37521600	1.03667600
H	-4.56290300	2.92834200	1.30285400
C	-0.61962500	-1.51208300	-0.14901900
C	-0.40089700	-2.54147900	0.76746900
C	-1.52214400	-1.79830600	-1.19066100
C	-1.02409000	-3.78862000	0.65150700
H	0.27035000	-2.37900000	1.61174300
C	-2.13457600	-3.03703700	-1.31829600
H	-1.75740900	-1.02054700	-1.91721500
C	-1.88928400	-4.05444500	-0.39522800
H	-2.37376300	-5.02240000	-0.49720300
C	0.75828500	0.49506900	-1.37009600
C	1.06577600	-0.33342700	-2.44994800
C	1.23991300	1.81529900	-1.45171300
C	1.79049600	0.12263300	-3.55668700
H	0.73902100	-1.37421800	-2.44130500
C	1.95493200	2.27522700	-2.54875500
H	1.05351000	2.50051800	-0.62468400
C	2.23829300	1.43035200	-3.62254100
H	2.79901100	1.78896700	-4.48258300
C	1.15457300	0.08618500	1.15375500
C	1.16661800	1.02099300	2.18984600
C	2.28222000	-0.75216300	1.06960200

C	2.22459400	1.11003900	3.10070900
H	0.33198400	1.71489300	2.30012800
C	3.33090900	-0.67454600	1.97534700
H	2.34169900	-1.48233400	0.26202200
C	3.31419900	0.26167200	3.01006500
H	4.13710400	0.32608900	3.71828600
C	-0.72041000	-4.82135100	1.68764000
C	-3.06254600	-3.34284900	-2.44913700
C	-3.83176500	1.20675900	3.20782300
C	-3.56149900	3.55498500	-1.17452200
C	2.45085100	3.68311500	-2.62501400
C	2.05597100	-0.83989900	-4.66785000
C	2.13880600	2.14163300	4.17794100
C	4.52197700	-1.57158100	1.87327500
F	-2.55484800	-4.28930300	-3.25742200
F	-3.32908200	-2.27835000	-3.21205800
F	-4.23877400	-3.82093600	-2.01055800
F	-1.42405400	-5.94811400	1.52682900
F	0.57823600	-5.16464500	1.67823400
F	-0.97832100	-4.36834800	2.92495800
F	1.97606900	3.37413600	3.67161800
F	1.08752900	1.92741800	4.98599500
F	3.22842900	2.17650500	4.95354600
F	5.65692900	-0.86801200	1.72083500
F	4.44745400	-2.42508400	0.84751200
F	4.68661900	-2.30688500	2.98637100
F	-4.61200800	4.24923900	-0.72146700
F	-3.95239700	2.94168300	-2.30380000
F	-2.62677800	4.44731200	-1.53930300
F	-5.09825500	0.80037300	3.01519800

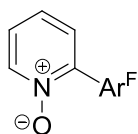
F	-3.91012800	2.33784600	3.92895800
F	-3.23818600	0.28969000	3.97744100
F	1.94851100	4.32649500	-3.69260000
F	3.78727300	3.73118200	-2.75730500
F	2.13634200	4.40790900	-1.54702900
F	2.76704700	-0.30113500	-5.66535600
F	0.91414900	-1.30164500	-5.20351700
F	2.73137300	-1.91854300	-4.23994000

Energy (0K) = -3646.366217

Energy (0K) + ZPE = -3645.959627

Enthalpy (298K) = -3645.909235

Free Energy (298K) = -3646.053081



Number of imaginary frequencies: 0

O	2.31067800	1.17519400	-0.84204600
C	3.91929500	-0.21248400	-0.02226300
C	1.63015000	-0.67961800	0.37581300
C	4.30836900	-1.33569500	0.67125000
C	2.01384200	-1.81450200	1.08596600
C	3.34573900	-2.16175100	1.24259700
H	5.36942700	-1.54900600	0.76112200
H	1.23245600	-2.41783100	1.54072600
H	3.62524500	-3.04720000	1.80488200
N	2.60417300	0.12737400	-0.17719600
C	0.21398300	-0.31647600	0.19877400
C	-0.23422200	1.00725900	0.27316200
C	-0.72890700	-1.32880100	0.00769200

C	-1.59003600	1.29249200	0.17669300
H	0.48333900	1.81056700	0.40665800
C	-2.08344500	-1.02719700	-0.09596700
H	-0.40497300	-2.36468100	-0.08001000
C	-2.52888500	0.28448200	-0.01338900
H	-3.58516500	0.52020600	-0.09708800
C	-3.03906900	-2.15696500	-0.32275100
C	-2.01116100	2.72807400	0.23862400
F	-4.31308100	-1.75660900	-0.34526600
F	-2.93012400	-3.09098300	0.63375100
F	-2.79439200	-2.77667800	-1.48653800
F	-3.33496400	2.86678200	0.36153800
F	-1.44400900	3.36531200	1.27207700
F	-1.64295300	3.39304000	-0.86604100
H	4.60042200	0.48481400	-0.49678300

Energy (0K) = -1227.9884474

Energy (0K) + ZPE = -1227.804312

Enthalpy (298K) = -1227.786513

Free Energy (298K) = -1227.851501

BAr₃ (Ar=Ar^F)

Number of imaginary frequencies: 0

B	-0.01688600	-0.01829600	0.09810600
C	-0.96995600	1.21887900	0.03606600
C	-2.20916300	1.14993700	-0.62511900
C	-0.62166500	2.43848900	0.62858800
C	-3.04486700	2.25469400	-0.69825500
H	-2.51232300	0.22087500	-1.10365800
C	-1.47593200	3.53864200	0.57768200
H	0.32883100	2.53479900	1.15321500

C	-2.68755700	3.45782300	-0.09092300
H	-3.35050200	4.31853400	-0.14423600
C	1.53256600	0.19010200	0.12783500
C	2.13663900	1.24755000	-0.56231100
C	2.37108800	-0.67869100	0.84809200
C	3.51955300	1.42271600	-0.55034900
H	1.52015000	1.94010600	-1.13548400
C	3.74365400	-0.48351600	0.88287100
H	1.93786100	-1.50838800	1.40242100
C	4.33055900	0.56566000	0.17692700
H	5.40871200	0.70750900	0.19857500
C	-0.60605200	-1.46635200	0.12058800
C	-1.82809200	-1.75486000	0.74584700
C	0.06944200	-2.53140300	-0.49261400
C	-2.34051100	-3.04816000	0.76744800
H	-2.38366700	-0.95824100	1.24071400
C	-0.45720500	-3.81844400	-0.49086600
H	1.01960300	-2.35233600	-0.99554300
C	-1.66403400	-4.08921500	0.14293300
H	-2.06729400	-5.09733100	0.15052500
C	-3.64688600	-3.28022800	1.46162400
C	0.30272900	-4.89468000	-1.20189400
C	4.64415700	-1.37902500	1.67561700
C	4.09659000	2.56634200	-1.32590700
C	-1.02806600	4.80724200	1.23557600
C	-4.34906100	2.20467400	-1.43212200
F	-4.01309000	-4.56421400	1.45378800
F	-4.63573700	-2.57952600	0.88756000
F	-3.59660900	-2.88639900	2.74178400
F	-0.23264100	-6.10494200	-1.02545500

F	0.34923700	-4.66622300	-2.52263400
F	1.57449300	-4.95323600	-0.78327400
F	5.30007900	-0.69333900	2.62308700
F	5.58027400	-1.94226800	0.89849400
F	3.98296200	-2.36616400	2.28455400
F	3.76542300	2.49252900	-2.62273000
F	5.42910900	2.61498800	-1.25602700
F	3.62956100	3.74120700	-0.88048300
F	-0.73098800	4.60727200	2.52721000
F	-1.95072000	5.77086500	1.18144500
F	0.08438100	5.28438100	0.65891800
F	-5.37769900	2.49734500	-0.62343800
F	-4.59190300	1.00649100	-1.96795700
F	-4.38045100	3.10317500	-2.42729700

Energy (0K) = -2740.8853313

Energy (0K) + ZPE = -2740.578445

Enthalpy (298K) = -2740.540592

Free Energy (298K) = -2740.655204

Br⁻

Number of imaginary frequencies: 0

Br	0.00000000	0.00000000	0.00000000
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Energy (0K) = -2571.3834097

Energy (0K) + ZPE = -2571.383410

Enthalpy (298K) = -2571.381049

Free Energy (298K) = -2571.399585

1d

Number of imaginary frequencies: 0

C	0.71495600	2.06071400	1.57711500
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C	1.88211800	2.28966800	1.81391400
C	3.25394000	2.55554600	2.10355500
C	4.14189700	1.50015100	2.35758200
C	3.72467300	3.87685100	2.13106500
C	5.47584400	1.76674200	2.63622600
H	3.77337000	0.47669500	2.33491900
C	5.06074000	4.13317200	2.41005200
H	3.03155000	4.69207900	1.93073500
C	5.93787600	3.08081600	2.66347000
H	6.15964400	0.94446400	2.83335800
H	5.41943600	5.15958700	2.42999900
H	6.98345100	3.28536400	2.88207900
N	-1.25869800	3.08757900	0.60728900
C	-0.60032800	3.64644400	-0.42931100
C	0.03297700	4.10915400	-1.35610000
C	0.79774900	4.64700300	-2.43272700
C	2.19460200	4.50570400	-2.43500500
C	0.17266200	5.31811300	-3.49451000
C	2.94559900	5.01974400	-3.48356100
H	2.67517500	3.98811700	-1.60652900
C	0.93352400	5.84177400	-4.53160800
H	-0.90979300	5.42428100	-3.49232300
C	2.31847700	5.69133200	-4.53110500
H	4.02668200	4.90140000	-3.48087500
H	0.44197500	6.36474900	-5.34878200
H	2.91009000	6.09787200	-5.34817000
S	-2.07359000	4.17870900	1.65210800
O	-2.80473200	3.34728800	2.59600500
O	-2.77032800	5.11443600	0.78691800
C	-0.76801800	5.02848400	2.49934700

H	-1.23017500	5.79607500	3.12682200
H	-0.11005700	5.49027300	1.75716000
H	-0.22047100	4.30916000	3.11475800
C	-0.83836500	0.69291700	0.19392500
H	-0.26621700	0.93821000	-0.71032900
H	-1.90013200	0.64748900	-0.07883800
C	-0.37767900	-0.61366200	0.77446900
C	-1.21440700	-1.33497000	1.63028100
C	0.89970500	-1.11012800	0.50578000
C	-0.78506500	-2.52700300	2.20432000
H	-2.21428600	-0.95513900	1.84225900
C	1.33219600	-2.30316000	1.07781900
H	1.55917200	-0.54971400	-0.15705700
C	0.49067900	-3.01412300	1.92926500
H	-1.44895300	-3.07991100	2.86557300
H	2.32890400	-2.67924700	0.85620200
H	0.82705600	-3.94758300	2.37532000
C	-0.67911500	1.84510600	1.19693200
H	-1.29177400	1.62083500	2.08129700

Energy (0K) = -1567.6681343

Energy (0K) + ZPE = -1567.274869

Enthalpy (298K) = -1567.247779

Free Energy (298K) = -1567.334385

TS_A

Number of imaginary frequencies: 1

C	-0.02194100	-2.26825700	2.04471800
C	0.67921200	-2.75607500	2.90467700
C	1.50342100	-3.34818100	3.90767800
C	1.67198900	-4.74057200	3.93791300

C	2.14872200	-2.55011600	4.86277300
C	2.47457500	-5.31962400	4.91184000
H	1.16580700	-5.35457500	3.19534800
C	2.94750000	-3.13967100	5.83373300
H	2.01701500	-1.47020700	4.83348100
C	3.11193300	-4.52278000	5.86037800
H	2.60212700	-6.39929700	4.93219800
H	3.44434600	-2.51682700	6.57374800
H	3.73843400	-4.98083700	6.62214900
N	-0.94774500	-0.26020700	1.00350900
C	-0.68949400	0.49696700	-0.02189400
C	-0.55784600	1.16756200	-1.06721400
C	0.51068800	1.73150300	-1.88117900
C	0.69287400	3.10923200	-2.04240200
C	1.36082100	0.84311600	-2.55731500
C	1.70375400	3.58459400	-2.87159400
H	0.04881100	3.80837200	-1.51540400
C	2.36383100	1.32816200	-3.38697100
H	1.20826400	-0.22976200	-2.45037600
C	2.53638700	2.70026700	-3.55115000
H	1.83700200	4.65788000	-2.98707300
H	3.00942200	0.62854600	-3.91283700
H	3.31813500	3.07849700	-4.20552300
S	-1.51207800	0.52940300	2.48097600
O	-2.31843600	-0.46778100	3.15694000
O	-2.06946200	1.79950600	2.05537200
C	-0.00202400	0.82603600	3.34964500
H	-0.26720600	1.35468300	4.27040700
H	0.63634700	1.45197200	2.72029800
H	0.46958100	-0.13434500	3.57371700

C	-0.29098200	-2.20772600	-0.40733900
H	0.75977500	-1.89163600	-0.46060300
H	-0.83395400	-1.67610200	-1.19904600
C	-0.42981500	-3.68684600	-0.63703200
C	-1.50527800	-4.16206900	-1.38972500
C	0.49363600	-4.60264000	-0.12661100
C	-1.66711500	-5.52325200	-1.62347300
H	-2.22194300	-3.44955100	-1.79761900
C	0.33188800	-5.96616100	-0.35349000
H	1.34518800	-4.24225000	0.45009600
C	-0.74875100	-6.42978200	-1.10070600
H	-2.50837100	-5.87022300	-2.22033200
H	1.05779800	-6.66974700	0.04926200
H	-0.86992900	-7.49570700	-1.28098000
C	-0.85097400	-1.76886000	0.95699000
H	-1.87462500	-2.15146300	1.07700800
B	-2.61929600	1.35505900	-1.89030300
C	-3.65675200	0.78611000	-0.81232100
C	-3.71515500	-0.56644900	-0.42968300
C	-4.63970100	1.61945000	-0.26670800
C	-4.68414900	-1.04392200	0.44480200
H	-2.99775900	-1.27402300	-0.84358500
C	-5.60848100	1.14676000	0.61864200
H	-4.67433500	2.67175000	-0.54288300
C	-5.63691100	-0.18630800	0.98924700
H	-6.38836900	-0.56417700	1.67777000
C	-2.53624900	2.94414900	-1.97023300
C	-2.63299400	3.64438200	-3.17361100
C	-2.39786700	3.71181700	-0.79864200
C	-2.57943300	5.03995300	-3.21498400

H	-2.76201300	3.10421800	-4.11118000
C	-2.33981000	5.09688100	-0.84002100
H	-2.31785400	3.21122500	0.16611600
C	-2.42815500	5.77893800	-2.05395800
H	-2.38101900	6.86435300	-2.08538100
C	-2.41697000	0.49324000	-3.22361800
C	-1.44082500	0.80965700	-4.18695400
C	-3.23056600	-0.60912900	-3.51768500
C	-1.26416300	0.04621600	-5.33509200
H	-0.79627300	1.67428400	-4.04672600
C	-3.05929200	-1.37257700	-4.67216000
H	-4.04017800	-0.88434900	-2.84403400
C	-2.06545900	-1.06292400	-5.58750400
H	-1.92529500	-1.66008000	-6.48433300
C	-3.96478100	-2.54495100	-4.88524100
C	-0.14117800	0.36499500	-6.27150100
C	-2.67005000	5.70564600	-4.55193400
C	-2.22838300	5.89385000	0.42118400
C	-6.60578000	2.12515600	1.15512100
C	-4.73125000	-2.48059900	0.86174900
F	-0.41735400	0.00782400	-7.53192700
F	0.15945500	1.66837100	-6.28285500
F	0.97978200	-0.29024900	-5.92423700
F	-3.76523000	-3.14129400	-6.06360300
F	-5.25611900	-2.18983400	-4.82987500
F	-3.79174200	-3.48099800	-3.93481600
F	-1.62904600	5.37872800	-5.33332100
F	-3.77299300	5.32760800	-5.21435700
F	-2.69505200	7.03873900	-4.46422000
F	-1.38613500	6.92834900	0.28059400

F	-3.41243900	6.41455800	0.77905400
F	-1.79287600	5.16333700	1.45194700
F	-5.97023400	-2.98138300	0.77150100
F	-4.34821100	-2.63495500	2.13754600
F	-3.93250400	-3.25839600	0.12039000
F	-7.51837900	1.55180100	1.94523100
F	-7.26735300	2.74262800	0.16505500
F	-6.00998000	3.09023800	1.86999800

Energy (0K) = -4308.5606161

Energy (0K) + ZPE = -4307.856010

Enthalpy (298K) = -4307.792558

Free Energy (298K) = -4307.960283

A

Number of imaginary frequencies: 0

C	0.05402700	1.75328400	1.46061100
C	1.26308600	1.79073600	1.54506200
C	2.68600900	1.82549300	1.62900500
C	3.42057100	0.63263600	1.68426100
C	3.35719600	3.05746600	1.62262500
C	4.80730200	0.67637900	1.73451600
H	2.89184400	-0.31850600	1.68408800
C	4.74457900	3.08982200	1.66816900
H	2.77919100	3.97955500	1.56787500
C	5.47067400	1.90199400	1.72489700
H	5.37481400	-0.25014000	1.77668000
H	5.26125100	4.04693400	1.65355600
H	6.55713400	1.93159200	1.75962300
N	-1.71565300	3.24741500	0.89863200
C	-1.38711600	3.78898000	-0.20437900

C	-0.99505900	4.40211000	-1.26560700
C	0.47602500	4.68550900	-1.26543000
C	0.97332200	5.96461700	-1.00167400
C	1.35159100	3.64525100	-1.59072400
C	2.34228400	6.20117900	-1.09623000
H	0.29175700	6.77334200	-0.74135600
C	2.71664400	3.89379000	-1.68550700
H	0.95250800	2.65277700	-1.79557100
C	3.21369200	5.17239400	-1.44527000
H	2.72724800	7.19891600	-0.89877900
H	3.39322000	3.08347200	-1.94765000
H	4.28174900	5.36384900	-1.51902200
S	-2.18981700	4.36132700	2.24914700
O	-2.47202200	3.47676800	3.36066500
O	-3.19963100	5.23294700	1.68497600
C	-0.67231200	5.23331100	2.49083400
H	-0.84624900	5.94819800	3.30148800
H	-0.41412400	5.75839900	1.56551800
H	0.09784100	4.50780800	2.77001200
C	-1.85761200	0.89583500	0.09555700
H	-1.33935400	1.18284100	-0.82930900
H	-2.92884500	1.08247700	-0.03793600
C	-1.60864300	-0.55112300	0.40961900
C	-2.56114500	-1.28967400	1.11491900
C	-0.41780200	-1.17038300	0.02303700
C	-2.32528400	-2.62378200	1.43254100
H	-3.49696600	-0.81181200	1.40547800
C	-0.18002800	-2.50391900	0.34046000
H	0.32414400	-0.60024000	-0.53657800
C	-1.13356900	-3.23247100	1.04733600

H	-3.07672400	-3.19098400	1.97745000
H	0.74924600	-2.97695300	0.03001600
H	-0.95019600	-4.27626600	1.29266800
C	-1.38123600	1.80478800	1.23069000
H	-1.94848000	1.57563500	2.14208300
B	-2.06266900	4.91659500	-2.51267800
C	-3.50651500	4.22189800	-2.23812800
C	-3.62249700	2.82120500	-2.21050000
C	-4.68636100	4.94102400	-2.04048500
C	-4.83617200	2.18441200	-1.98489000
H	-2.73833500	2.21060900	-2.39261300
C	-5.91013800	4.30573000	-1.81195400
H	-4.66648200	6.03077000	-2.06516000
C	-5.99833100	2.92451200	-1.77405800
H	-6.94814400	2.42697400	-1.59352300
C	-2.07560300	6.52818900	-2.27286300
C	-1.70906200	7.47024200	-3.23810200
C	-2.43448000	7.03780800	-1.01749000
C	-1.67649000	8.83691100	-2.95572300
H	-1.42839500	7.14154500	-4.23884100
C	-2.39093800	8.39654800	-0.72774100
H	-2.75173700	6.35290300	-0.23050800
C	-2.00389500	9.31743000	-1.69453600
H	-1.96121200	10.37870700	-1.46975200
C	-1.40927300	4.48121800	-3.93902900
C	-0.11707200	4.87934000	-4.31872400
C	-2.11313600	3.72683000	-4.88498500
C	0.44051200	4.52349300	-5.54353300
H	0.48327000	5.49505500	-3.64873300
C	-1.56344800	3.37833700	-6.11850400

H	-3.12927700	3.39871900	-4.66786800
C	-0.27510300	3.76437900	-6.46096600
H	0.15936200	3.49030500	-7.41749200
C	-2.38720100	2.53945800	-7.04268700
C	1.82182500	5.00714200	-5.85052500
C	-1.27377200	9.77105200	-4.05233800
C	-2.74244600	8.81631000	0.66315700
C	-7.11988300	5.16194200	-1.60945400
C	-4.93539000	0.69326500	-1.92015400
F	-3.62034400	3.04198000	-7.20231300
F	-1.84513800	2.42402000	-8.25992900
F	-2.54695300	1.29455100	-6.56359600
F	1.86904500	6.34682700	-5.92086300
F	2.29036000	4.53486000	-7.01056800
F	2.69557200	4.65078600	-4.89508000
F	-1.20397500	11.04380600	-3.64758000
F	-2.13824900	9.72770300	-5.07755200
F	-0.07285300	9.45002400	-4.55789800
F	-4.00687200	8.50157300	0.97455300
F	-2.59844300	10.13029500	0.86108500
F	-1.96433000	8.19187500	1.56699100
F	-5.95046900	0.22650200	-2.65802300
F	-5.16417500	0.27695300	-0.65896500
F	-3.82277400	0.07744500	-2.33406600
F	-8.23332800	4.44620200	-1.41782700
F	-7.33826400	5.96144700	-2.66476200
F	-6.97912500	5.96941100	-0.54755000

Energy (0K) = -4308.56676

Energy (0K) + ZPE = -4307.863748

Enthalpy (298K) = -4307.799614

Free Energy (298K) = -4307.969303

TS_B

Number of imaginary frequencies: 1

C	0.13924800	1.22344500	1.57047800
C	0.87350700	0.84219500	2.45644600
C	1.74932200	0.47134200	3.51966500
C	1.48277800	-0.64961900	4.31861900
C	2.88170400	1.25790500	3.78208600
C	2.33911200	-0.97489800	5.36229500
H	0.60278000	-1.25419300	4.11158100
C	3.72883200	0.92700900	4.83108300
H	3.08280300	2.12274300	3.15204000
C	3.45936100	-0.18819100	5.62191200
H	2.12865300	-1.84531300	5.97917400
H	4.60390000	1.54002700	5.03354000
H	4.12419000	-0.44514700	6.44329100
N	-0.85489300	3.19694400	0.54950200
C	-0.32583700	3.99518900	-0.35357200
C	-0.44434100	4.57724800	-1.51939700
C	0.73073900	4.99052900	-2.33017700
C	1.10250200	6.32050100	-2.55686700
C	1.43066500	3.97668800	-2.99687500
C	2.15142500	6.62103800	-3.42057600
H	0.57886500	7.12849700	-2.05242000
C	2.46268500	4.28260200	-3.87784900
H	1.14069300	2.93850000	-2.84359800
C	2.83002200	5.60723600	-4.09149300
H	2.43476400	7.66096000	-3.57051300
H	2.98394300	3.47812200	-4.39243100

H	3.63905800	5.84927600	-4.77685000
S	-1.45757300	3.91968900	2.02464700
O	-2.49734500	3.02028900	2.49073100
O	-1.74859300	5.29881100	1.65862600
C	-0.11261600	3.95958200	3.18688600
H	-0.38804600	4.72990400	3.91363500
H	0.80018500	4.23385900	2.65111200
H	-0.01700300	2.98564800	3.66770000
C	-0.11435600	1.29064300	-0.88232500
H	0.92172200	1.65720500	-0.92161400
H	-0.67303900	1.80264900	-1.67486100
C	-0.17329300	-0.19182400	-1.12563900
C	-1.21164000	-0.72641600	-1.89211200
C	0.80177100	-1.05337200	-0.61683100
C	-1.28429300	-2.09441500	-2.13479700
H	-1.96438900	-0.05726800	-2.30986200
C	0.73026300	-2.42214100	-0.85600300
H	1.62547800	-0.64266300	-0.03445900
C	-0.31450800	-2.94640600	-1.61303600
H	-2.09690100	-2.49346200	-2.73813800
H	1.49708100	-3.08157500	-0.45499800
H	-0.36763700	-4.01606800	-1.80367200
C	-0.70415900	1.69456400	0.48039800
H	-1.71470400	1.27599500	0.58491300
B	-2.02610300	4.89149600	-2.18265400
C	-3.25039500	4.32688600	-1.26154900
C	-3.41744500	2.96209500	-0.96291500
C	-4.24021500	5.17439500	-0.75527000
C	-4.47831100	2.48702600	-0.20204900
H	-2.70104300	2.23973000	-1.34874300

C	-5.30909100	4.70613800	0.01327300
H	-4.19121700	6.24393500	-0.95656700
C	-5.43649500	3.36005000	0.30671300
H	-6.26017400	2.98837300	0.91103900
C	-2.04539800	6.52523200	-2.18247200
C	-2.37766400	7.30507200	-3.28918300
C	-1.71902300	7.22266600	-1.00490500
C	-2.34532500	8.70325300	-3.24375800
H	-2.66051600	6.82473100	-4.22618800
C	-1.67345700	8.60792600	-0.95915100
H	-1.48714000	6.65937700	-0.10284800
C	-1.97785500	9.37011500	-2.08750600
H	-1.93268200	10.45595100	-2.05487700
C	-2.02880300	4.24523100	-3.68824500
C	-1.16483900	4.72339400	-4.69409500
C	-2.85290400	3.18250200	-4.06607700
C	-1.10104600	4.14951100	-5.95572600
H	-0.51574700	5.57115200	-4.49127600
C	-2.79607200	2.60077200	-5.33643900
H	-3.57936500	2.78013700	-3.36162800
C	-1.91320800	3.06859400	-6.29365600
H	-1.85818000	2.61408300	-7.28002600
C	1.50847800	6.42111500	0.67724000
C	2.17687900	7.61937000	0.55652100
C	3.46894600	7.63581000	0.03975000
C	4.06599200	6.43884900	-0.33007400
C	3.36459000	5.25384400	-0.19188200
N	2.09340600	5.25679100	0.29281500
H	4.01165400	8.56973100	-0.06827500
H	0.49734300	6.31835800	1.06507400

H	1.67412500	8.53038900	0.86487100
H	5.07734000	6.40706500	-0.72312900
O	1.43936900	4.12426100	0.41586600
Br	4.11730200	3.60110200	-0.60407300
C	-2.69206400	9.45299400	-4.49035400
C	-1.24996700	9.32730500	0.27972900
C	-0.14322300	4.65496500	-6.98584200
C	-3.69324700	1.43861400	-5.61379500
C	-4.61575400	1.03984300	0.14465000
C	-6.30340300	5.70272700	0.51613800
F	-2.65137500	10.77972800	-4.32714700
F	-3.92272300	9.14413700	-4.92533300
F	-1.85171000	9.15274700	-5.49381800
F	-0.12904200	10.04560200	0.06510200
F	-2.17497200	10.19853800	0.70197900
F	-0.98694500	8.49973400	1.29987200
F	-0.77463900	5.03896400	-8.10693100
F	0.72491700	3.69808600	-7.35604500
F	0.57853900	5.69719600	-6.56189800
F	-3.61906100	1.01504500	-6.87980500
F	-4.97842500	1.73188400	-5.36659200
F	-3.39280300	0.38764500	-4.82962000
F	-6.88483100	6.37239900	-0.49185300
F	-5.72499800	6.62848600	1.29686800
F	-7.28437300	5.14145200	1.23158200
F	-5.83057100	0.56629200	-0.17189500
F	-4.45998800	0.83001800	1.46047600
F	-3.71624000	0.26543800	-0.48019000

Energy (0K) = -7202.4634466

Energy (0K) + ZPE = -7201.675234

Enthalpy (298K) = -7201.604553

Free Energy (298K) = -7201.785823

B

Number of imaginary frequencies: 0

C	1.18995300	-2.88769600	2.80120600
C	1.98349300	-3.28469300	3.62788800
C	2.92144200	-3.67513200	4.62995700
C	2.87456400	-4.95083400	5.21016200
C	3.89761800	-2.75892500	5.05148600
C	3.78864500	-5.29723800	6.19686100
H	2.11788300	-5.65879300	4.87960600
C	4.80436400	-3.11325700	6.04132100
H	3.93332200	-1.77359300	4.58961400
C	4.75120000	-4.38139200	6.61620000
H	3.74753600	-6.28767800	6.64397900
H	5.55632400	-2.39802700	6.36646900
H	5.46182900	-4.65671700	7.39196400
N	0.14116900	-0.88629500	1.84948900
C	0.90707900	-0.06643600	1.02890100
C	0.61995400	0.45238900	-0.17209400
C	1.77260200	0.90143100	-1.01067500
C	2.12037600	2.23827800	-1.24941800
C	2.48857500	-0.09551700	-1.68907800
C	3.13569400	2.55952900	-2.14545000
H	1.60241200	3.04067400	-0.72848900
C	3.49050500	0.22731300	-2.59850300
H	2.22716900	-1.14018700	-1.52621700
C	3.81598300	1.55866500	-2.83491300
H	3.38833000	3.60486000	-2.31195500

H	4.01182200	-0.56814900	-3.12694400
H	4.59649000	1.81591700	-3.54733200
S	-0.50489200	-0.21035300	3.26434400
O	-1.65300300	-1.02277800	3.63467800
O	-0.65170800	1.21521200	2.96970000
C	0.69882700	-0.31647400	4.57336400
H	0.31950400	0.33361000	5.36797900
H	1.66445300	0.04894300	4.21363300
H	0.77343500	-1.34607700	4.92466400
C	0.82239700	-2.78166900	0.37419100
H	1.87816300	-2.48133800	0.31291400
H	0.28293100	-2.21115200	-0.39102000
C	0.66780700	-4.25009800	0.08895200
C	-0.39767500	-4.68305000	-0.70305300
C	1.57080400	-5.19793200	0.57771800
C	-0.57165200	-6.03233300	-0.99175200
H	-1.09749300	-3.94702300	-1.09788200
C	1.39847900	-6.54942600	0.29355000
H	2.41652200	-4.87051500	1.18113700
C	0.32604500	-6.97041300	-0.48925300
H	-1.40620400	-6.34591000	-1.61596400
H	2.10945200	-7.27668800	0.68034400
H	0.19554800	-8.02699000	-0.71335100
C	0.29286700	-2.37721700	1.76573500
H	-0.71240000	-2.80219200	1.90338100
B	-0.93121600	0.67719400	-0.84619800
C	-2.18923900	0.15261500	0.07452400
C	-2.41815000	-1.20527200	0.36975200
C	-3.16206200	1.03057600	0.56297500
C	-3.52154200	-1.64226200	1.09135300

H	-1.71671800	-1.95721200	0.01433000
C	-4.26648400	0.60309800	1.30526800
H	-3.07664900	2.09796300	0.36567500
C	-4.46008100	-0.73773400	1.58116200
H	-5.31683300	-1.08030600	2.15581300
C	-1.00907000	2.31526000	-0.94756800
C	-1.28083500	3.05019000	-2.10038700
C	-0.76652200	3.06444500	0.21756500
C	-1.25869500	4.45031600	-2.10801500
H	-1.50493800	2.53499400	-3.03503500
C	-0.72756700	4.44964600	0.21370100
H	-0.60864800	2.53564500	1.15518800
C	-0.96239600	5.16628400	-0.96028000
H	-0.92067500	6.25266500	-0.96839600
C	-0.95103100	-0.02417500	-2.33912400
C	-0.08141700	0.41025700	-3.35981700
C	-1.79430100	-1.08011700	-2.69832000
C	-0.01738000	-0.20030300	-4.60558200
H	0.56986300	1.26167600	-3.18696500
C	-1.74074000	-1.69885700	-3.95159900
H	-2.53685600	-1.44848200	-1.99180400
C	-0.84082300	-1.27936200	-4.91685000
H	-0.78838300	-1.76463500	-5.88830800
C	2.28232800	2.29705900	2.05015500
C	2.96300400	3.49377300	2.03666900
C	4.27881200	3.52828700	1.58218300
C	4.89879700	2.35600600	1.17189700
C	4.18945000	1.16878900	1.19111600
N	2.89822100	1.17957500	1.60141300
H	4.83025400	4.46322900	1.56305200

H	1.25933100	2.16970000	2.40437000
H	2.45893100	4.38726900	2.38908600
H	5.93076900	2.34696300	0.83662400
O	2.24951500	-0.01695800	1.64168600
Br	4.96814600	-0.45509400	0.73388200
C	-1.53926300	5.14939700	-3.39933900
C	-0.36355500	5.20769600	1.44671700
C	0.99786200	0.24190300	-5.61023800
C	-2.66750800	-2.84234500	-4.20869100
C	-3.72401900	-3.08451400	1.42413600
C	-5.23338900	1.63623400	1.78402700
F	-1.51052800	6.48208500	-3.28548200
F	-2.74464900	4.81969700	-3.88763800
F	-0.64608700	4.81569100	-4.34527200
F	0.79790600	5.87463400	1.28054100
F	-1.27918300	6.12812700	1.77271100
F	-0.19816500	4.41357300	2.51441700
F	0.49221000	0.28359800	-6.85214100
F	2.04162500	-0.60644200	-5.65779800
F	1.49902200	1.45364100	-5.34393100
F	-2.61425800	-3.27941100	-5.47153500
F	-3.94335000	-2.51658200	-3.95368900
F	-2.38811600	-3.89631900	-3.41902000
F	-5.77097800	2.32388200	0.76260700
F	-4.63982500	2.54498700	2.57423500
F	-6.24919000	1.11372300	2.48113400
F	-4.97706700	-3.48365300	1.14985600
F	-3.53158000	-3.32712300	2.73038300
F	-2.89712500	-3.89793800	0.75400600

Energy (0K) = -7202.4755344

Energy (0K) + ZPE = -7201.683858

Enthalpy (298K) = -7201.613466

Free Energy (298K) = -7201.794477

TS_C

Number of imaginary frequencies: 1

C	0.30268500	-2.18038300	2.06346700
C	1.16330700	-2.56750900	2.82499800
C	2.17483900	-3.00543400	3.73077200
C	2.43757200	-4.37396800	3.89112500
C	2.91724500	-2.06745500	4.46287000
C	3.42717900	-4.79172000	4.77154900
H	1.85784000	-5.09673400	3.31992200
C	3.90365500	-2.49530400	5.34173000
H	2.70969000	-1.00686500	4.33065000
C	4.16048900	-3.85584900	5.49766900
H	3.62709800	-5.85391100	4.89227500
H	4.47613600	-1.76401700	5.90763200
H	4.93405600	-4.18785700	6.18623200
N	-0.88689700	-0.29598600	0.99775100
C	-0.06019300	0.41485400	0.09252200
C	-0.51669100	1.11784700	-1.02648200
C	0.61869400	1.60442200	-1.85695200
C	0.98142000	2.95077300	-1.97754900
C	1.35271100	0.64625600	-2.57527400
C	2.02754400	3.32700000	-2.81774800
H	0.46387800	3.71180000	-1.40006800
C	2.37042900	1.02895300	-3.43666700
H	1.08323100	-0.40567600	-2.48523800
C	2.71071000	2.37423800	-3.56445200

H	2.29838400	4.37787200	-2.89138600
H	2.90295900	0.27121300	-4.00661600
H	3.51251100	2.67498700	-4.23476000
S	-1.63600000	0.48035100	2.28835600
O	-2.80248100	-0.30903600	2.65412100
O	-1.76914200	1.87740300	1.88044800
C	-0.50695300	0.44727100	3.66353900
H	-0.94131000	1.09934800	4.42770700
H	0.46876600	0.83015600	3.34958700
H	-0.41904400	-0.57449400	4.03858900
C	-0.34449000	-2.35863300	-0.30094800
H	0.72142200	-2.18140400	-0.49556500
H	-0.91257100	-1.82223100	-1.07273000
C	-0.66820200	-3.82275300	-0.37979000
C	-1.90791700	-4.21570100	-0.88616200
C	0.22267300	-4.80380600	0.06068200
C	-2.26693500	-5.55807100	-0.93557000
H	-2.59536800	-3.45288200	-1.25020500
C	-0.13105000	-6.14948300	0.00934500
H	1.20113600	-4.50950200	0.43983300
C	-1.37720500	-6.52956100	-0.48363700
H	-3.24106400	-5.84063100	-1.33024900
H	0.57208200	-6.90515100	0.35397700
H	-1.65089800	-7.58170700	-0.52132300
C	-0.70283700	-1.77082300	1.08371900
H	-1.68362300	-2.16618500	1.38409100
B	-2.05005600	1.37560500	-1.62694100
C	-3.34422200	0.85726600	-0.75326300
C	-3.58467200	-0.48168100	-0.40894100
C	-4.37716900	1.74056900	-0.40450100

C	-4.76984900	-0.91146800	0.18350000
H	-2.83067400	-1.23943600	-0.61518600
C	-5.54726900	1.32704700	0.22907500
H	-4.28593700	2.80100400	-0.63231100
C	-5.76792800	-0.01027900	0.52309000
H	-6.68773700	-0.33941700	0.99634200
C	-2.18570600	2.99989600	-1.80040200
C	-2.68632100	3.63541300	-2.93971300
C	-1.87886700	3.83316600	-0.71674000
C	-2.83834500	5.02216100	-3.00450300
H	-2.97505800	3.04264300	-3.80849000
C	-2.00640500	5.21652200	-0.78471300
H	-1.53859700	3.38607000	0.21930900
C	-2.48432500	5.83324500	-1.93442100
H	-2.58365800	6.91278000	-1.99136500
C	-1.96887900	0.59825500	-3.09670900
C	-1.20461200	1.12052400	-4.15549900
C	-2.54238900	-0.65602600	-3.33162300
C	-0.99783400	0.42147300	-5.33946300
H	-0.73673100	2.09748300	-4.05294300
C	-2.32917300	-1.37023100	-4.51132800
H	-3.18964000	-1.10978600	-2.58672100
C	-1.54180100	-0.84561200	-5.52514400
H	-1.35617000	-1.40207400	-6.44163700
C	1.41105600	2.67961900	1.26781700
C	2.09512300	3.85050100	1.55116100
C	3.47322900	3.87657900	1.35369400
C	4.13722100	2.74515600	0.89526000
C	3.39377000	1.59820700	0.64648100
N	2.08822700	1.61366100	0.86618800

H	4.03562500	4.78519000	1.54876500
H	0.32238500	2.57458700	1.34875700
H	1.54830800	4.71974200	1.89975300
H	5.20862000	2.74239600	0.71941200
O	1.22986500	0.23356500	0.25813300
Br	4.19751300	0.02691600	0.01385600
C	-2.85788700	-2.76329100	-4.64609400
C	-0.08344000	0.95707400	-6.39454000
C	-3.38226900	5.61405200	-4.26580300
C	-1.56197500	6.00716200	0.40088900
C	-6.55279100	2.37094500	0.59298600
C	-4.94521400	-2.37267000	0.43137200
F	-3.21471000	-3.05077600	-5.90447800
F	-3.92318500	-2.99162500	-3.86762100
F	-1.92748500	-3.66977100	-4.29578000
F	-0.57481600	0.76366700	-7.62700000
F	1.10831700	0.33289000	-6.36277500
F	0.16099000	2.26441400	-6.26365400
F	-4.60298000	5.13574900	-4.55052200
F	-2.60788400	5.32299500	-5.32286200
F	-3.48492900	6.94653600	-4.20884000
F	-1.71236100	7.32430300	0.24314000
F	-2.21839000	5.65868700	1.51538900
F	-0.25310700	5.78644800	0.65505900
F	-7.69664700	1.85128200	1.05467100
F	-6.86700300	3.14840700	-0.45538100
F	-6.08435000	3.19684900	1.54283700
F	-3.96952200	-2.87676000	1.20492200
F	-6.10607800	-2.66761400	1.02339100
F	-4.90854800	-3.07075000	-0.72180400

Energy (0K) = -7202.4544928

Energy (0K) + ZPE = -7201.663507

Enthalpy (298K) = -7201.593694

Free Energy (298K) = -7201.771993

[N]

Number of imaginary frequencies: 0

C	-0.66222800	1.87527400	-0.87516100
C	-2.44633000	2.98590800	-1.71231100
C	0.22819700	2.76167500	-1.46655300
H	-0.29992700	1.03962600	-0.27749400
C	-1.66377200	3.93956000	-2.35394500
C	-0.28718400	3.81245400	-2.21943400
H	1.29860500	2.63017700	-1.33902700
H	-2.11410100	4.74241600	-2.92931800
H	0.37369000	4.53012700	-2.69924400
N	-1.99191000	1.98240500	-0.99440100
Br	-4.34968200	3.12982000	-1.87332600

Energy (0K) = -2818.7547599

Energy (0K) + ZPE = -2818.676382

Enthalpy (298K) = -2818.669819

Free Energy (298K) = -2818.707215

C

Number of imaginary frequencies: 0

C	-0.19565600	-0.30061600	1.70039400
C	0.17587500	-1.72145400	2.00906800
N	1.45963500	-2.18583800	2.10923000
B	-0.69270300	-0.02251300	0.14972400
S	1.67330200	-3.89619800	2.41641000

O	3.10666300	-4.03675500	2.62990000
O	1.02066400	-4.63943700	1.35522700
C	2.69930100	-1.41333600	1.84262100
C	2.46796000	0.01103400	2.02637500
C	2.48477000	1.20727200	2.24443700
C	2.42549200	2.59461700	2.54060800
C	3.01071400	3.53464400	1.67854500
C	1.77549300	3.02737500	3.70795400
C	2.93394700	4.88669600	1.97983500
H	3.52434400	3.18775800	0.78390900
C	1.69367400	4.38307800	3.99275000
H	1.34409100	2.28932100	4.38133500
C	2.27261900	5.31217100	3.13102600
H	3.38320800	5.61287800	1.30734800
H	1.17876000	4.71460200	4.89165500
H	2.21068900	6.37396300	3.35788000
C	3.29270000	-1.74250500	0.46025700
H	2.54985400	-1.50061300	-0.30747300
H	3.47755000	-2.82392700	0.42718600
C	4.56680800	-0.98533200	0.22556300
C	5.72223100	-1.30944300	0.94120300
C	4.60421700	0.08265600	-0.67286400
C	6.89165900	-0.57701800	0.76503300
H	5.70003500	-2.14995700	1.63636700
C	5.77391400	0.81628500	-0.85302000
H	3.70919900	0.32542100	-1.24802200
C	6.91860800	0.48952500	-0.13096800
H	7.78568900	-0.84070400	1.32623700
H	5.79173000	1.64287100	-1.56008000
H	7.83348300	1.06121000	-0.27066200

C	-0.55217600	0.45762300	2.85832600
C	-0.35235900	-0.06765600	4.16560100
C	-1.19189800	1.71664600	2.74146500
C	-0.82080000	0.60125700	5.27673800
H	0.15743300	-1.01996500	4.29968800
C	-1.66834800	2.37781300	3.85985300
H	-1.32228000	2.15683800	1.75876900
C	-1.49347600	1.81843400	5.12388600
H	-0.67738700	0.17858400	6.26713600
H	-2.17383500	3.33289500	3.74861700
H	-1.87545100	2.33514800	6.00118300
O	-0.80514500	-2.43289700	2.18962900
C	0.85096600	-4.14301900	3.96265900
C	-0.51914200	1.53127100	-0.36660600
C	0.74752600	2.08937800	-0.61755600
C	-1.61146600	2.30715100	-0.76897000
C	0.90101600	3.26483900	-1.34689900
H	1.64305500	1.55620700	-0.29701100
C	-1.46273600	3.52514100	-1.43180400
H	-2.62587800	1.95590600	-0.58492100
C	-0.20582900	4.00424100	-1.75725800
H	-0.08253400	4.91884700	-2.33137400
C	-2.31109600	-0.39122700	0.12213800
C	-2.87792600	-0.52694200	-1.15436100
C	-3.19964400	-0.45438200	1.19619800
C	-4.24729700	-0.66825200	-1.34701000
H	-2.23568200	-0.48444800	-2.03491400
C	-4.57362000	-0.61634200	1.00707000
H	-2.84477300	-0.37069900	2.22217800
C	-5.11781400	-0.71717600	-0.26422500

H	-6.18827000	-0.82583200	-0.40754000
C	0.04629400	-1.05429800	-0.91233600
C	0.93868500	-0.63880100	-1.90782500
C	-0.24174900	-2.43117000	-0.89567400
C	1.56463100	-1.53287300	-2.77279800
H	1.17728200	0.41273000	-2.02831500
C	0.37060700	-3.32876400	-1.76446200
H	-0.97848400	-2.81848400	-0.19605400
C	1.29867100	-2.89216300	-2.70427800
H	1.79059900	-3.59477600	-3.37549800
H	1.31046900	-3.48522200	4.70489300
H	1.02921400	-5.19050700	4.22635500
H	-0.21594600	-3.95087800	3.84347500
H	3.42024400	-1.73112700	2.60878600
C	-5.43930700	-0.67315200	2.22444200
C	-4.75332300	-0.69728600	-2.75406100
C	-2.70484500	4.26368100	-1.81610800
C	2.24843800	3.73436100	-1.79631200
C	0.03435300	-4.78744400	-1.75099300
C	2.60525800	-1.05733600	-3.73539500
F	-6.74326100	-0.70084000	1.93198700
F	-5.23325600	0.38717900	3.02323200
F	-5.17732300	-1.75840400	2.96955600
F	-6.06745400	-0.93397700	-2.82754000
F	-4.52579000	0.47284800	-3.37363400
F	-4.13740200	-1.63744400	-3.48500400
F	-0.83387400	-5.11829400	-0.79528400
F	-0.50594000	-5.16659300	-2.92394000
F	1.12931100	-5.54389500	-1.58542800
F	2.35007000	-1.45071500	-4.99053400

F	2.72631100	0.27660600	-3.75338800
F	3.81276500	-1.55488100	-3.41902500
F	-2.45834500	5.32502500	-2.59012900
F	-3.36558400	4.70634400	-0.73389100
F	-3.56077800	3.47276700	-2.48144700
F	2.24361300	4.03832300	-3.10172200
F	2.64919500	4.84428100	-1.15620000
F	3.20170900	2.80848500	-1.61516200

Energy (0K) = -4383.7823945

Energy (0K) + ZPE = -4383.070257

Enthalpy (298K) = -4383.006801

Free Energy (298K) = -4383.168437

TS_D

Number of imaginary frequencies: 1

C	-0.14869900	-0.28890000	1.61498800
C	0.07748000	-1.74986800	1.92069200
N	1.34979700	-2.25596400	1.97905900
B	-0.69869500	-0.01692000	0.05769600
S	1.58553300	-3.94291900	2.30909800
O	3.01898600	-4.05685400	2.53856000
O	0.95211400	-4.71075300	1.25359600
C	2.53563600	-1.41526300	1.73802300
C	2.09566700	-0.01468500	1.78433700
C	2.28548600	1.18191400	2.00241400
C	2.30773600	2.54258300	2.35468400
C	2.87905100	3.50922100	1.50595500
C	1.74593100	2.92838700	3.58836700
C	2.87127600	4.84040000	1.88500800
H	3.33206600	3.18944200	0.57019700

C	1.72515000	4.26754500	3.94462200
H	1.33668300	2.16614600	4.24796600
C	2.28706900	5.21902000	3.09557000
H	3.31682300	5.59185300	1.23925500
H	1.27855800	4.57010000	4.88842100
H	2.27772700	6.26813400	3.38135400
C	3.25275100	-1.75596100	0.42107900
H	2.55996400	-1.58414700	-0.40688200
H	3.49984600	-2.82436200	0.44489900
C	4.49832100	-0.93722700	0.24497600
C	5.62416900	-1.18938300	1.03356900
C	4.54273100	0.10518500	-0.68376800
C	6.77031400	-0.41266800	0.89953700
H	5.59973300	-2.01182200	1.74976800
C	5.68941300	0.88382000	-0.82042700
H	3.67533200	0.29536600	-1.31847500
C	6.80419800	0.62730300	-0.02701100
H	7.64217000	-0.62363500	1.51512400
H	5.71360600	1.68901800	-1.55170300
H	7.70126000	1.23314200	-0.13391800
C	-0.58145600	0.45786900	2.78454700
C	-0.43718800	-0.08572900	4.08349900
C	-1.19149000	1.72284500	2.66258800
C	-0.93443100	0.57578500	5.19084500
H	0.05858700	-1.04580800	4.22059400
C	-1.70026700	2.37827300	3.77488100
H	-1.28668000	2.17767300	1.68217900
C	-1.58139000	1.80462300	5.03686600
H	-0.82800200	0.13477500	6.17841300
H	-2.18739400	3.34227100	3.65444500

H	-1.98666000	2.31532800	5.90715000
O	-0.92131500	-2.42549500	2.11286300
C	0.74726100	-4.18237400	3.84716000
C	-0.53284800	1.53264500	-0.47976500
C	0.72277000	2.08410000	-0.79141100
C	-1.63471500	2.32278800	-0.82805000
C	0.85482600	3.26382600	-1.51761300
H	1.62626900	1.54616200	-0.50999000
C	-1.50634400	3.54272100	-1.49223200
H	-2.64296100	1.98262300	-0.59508100
C	-0.26223500	4.01467200	-1.87395500
H	-0.15770700	4.93239700	-2.44705200
C	-2.31718000	-0.37796600	0.05914300
C	-2.91386600	-0.48569800	-1.20698200
C	-3.18511100	-0.47788900	1.14829400
C	-4.28563700	-0.63847900	-1.37514400
H	-2.29150000	-0.41777900	-2.10047000
C	-4.56169300	-0.64583500	0.98481500
H	-2.80588800	-0.42853200	2.16728500
C	-5.13308400	-0.72059100	-0.27635700
H	-6.20505400	-0.83680000	-0.40036500
C	0.01205700	-1.06847400	-1.00768800
C	0.91280800	-0.68231100	-2.00747100
C	-0.30342200	-2.43968500	-0.98143000
C	1.52433100	-1.59648000	-2.86152400
H	1.17015400	0.36210400	-2.14569600
C	0.28912900	-3.35673100	-1.84383100
H	-1.04482900	-2.81014000	-0.27725500
C	1.22978700	-2.94925600	-2.78412200
H	1.70796800	-3.66845500	-3.44761500

H	1.19629400	-3.51951700	4.59135800
H	0.92234300	-5.22826700	4.11896200
H	-0.31856000	-3.99146100	3.71444800
H	3.23263700	-1.57570900	2.57268600
C	-5.39886500	-0.73989100	2.21956200
C	-4.81930800	-0.65090900	-2.77160000
C	-2.75780900	4.29397000	-1.81562500
C	2.18739900	3.73016200	-2.01127200
C	-0.08828700	-4.80501800	-1.82716900
C	2.58455900	-1.14802700	-3.81472800
F	-6.70924400	-0.77497000	1.95651300
F	-5.18635500	0.30402800	3.03810400
F	-5.10955000	-1.83892100	2.93392700
F	-6.13450900	-0.88947800	-2.82291700
F	-4.60680900	0.52624400	-3.38334400
F	-4.21640300	-1.58149300	-3.52607800
F	-0.94571900	-5.11344900	-0.85446400
F	-0.66373500	-5.16539000	-2.98941000
F	0.98735000	-5.59386600	-1.68736900
F	2.34945800	-1.56264800	-5.06672700
F	2.71726500	0.18443000	-3.85464500
F	3.78258200	-1.64810500	-3.46650400
F	-2.53551000	5.36370100	-2.58582500
F	-3.37070300	4.72755800	-0.70208000
F	-3.64630200	3.51822000	-2.45524300
F	2.14861800	4.01398200	-3.32014000
F	2.59967500	4.85139800	-1.39737100
F	3.15027200	2.81115700	-1.83850600

Energy (0K) = -4383.7801657

Energy (0K) + ZPE = -4383.068918

Enthalpy (298K) = -4383.006027

Free Energy (298K) = -4383.167177

D

Number of imaginary frequencies: 0

C	-0.17932700	0.00484800	-1.63977000
C	1.11249100	-0.46012600	-2.28369500
N	1.12618400	-1.85215600	-2.37572100
B	0.25566800	0.55462700	-0.01301800
S	2.37173700	-2.67893000	-3.20500200
O	1.87614100	-4.04188400	-3.34584500
O	3.62526000	-2.42114400	-2.52208600
C	-0.14670400	-2.49562300	-2.06083800
C	-0.99349100	-1.28873100	-1.66630200
C	-2.27349500	-1.35819400	-1.51689300
C	-3.62997900	-1.23557000	-1.65989600
C	-4.50751200	-1.46095800	-0.56591000
C	-4.14975200	-0.82011800	-2.92193300
C	-5.86212900	-1.26864100	-0.72715600
H	-4.08270100	-1.77808200	0.37948000
C	-5.50513200	-0.62336600	-3.06084000
H	-3.45756500	-0.64812200	-3.74312300
C	-6.35295600	-0.84926600	-1.96815800
H	-6.54166900	-1.43081100	0.10472100
H	-5.91851700	-0.29315000	-4.00905800
H	-7.42223600	-0.69073500	-2.08867000
C	-0.07450300	-3.57453200	-0.97538800
H	0.43512300	-3.17604600	-0.08978600
H	0.54408500	-4.38661600	-1.37771100
C	-1.44754100	-4.07321900	-0.63613000

C	-2.22616100	-4.70913600	-1.61300300
C	-1.98877400	-3.89168700	0.64094500
C	-3.51916700	-5.13070900	-1.32656300
H	-1.80520100	-4.88161400	-2.60363100
C	-3.28085000	-4.31975100	0.93162100
H	-1.38381400	-3.41456800	1.41302700
C	-4.05210300	-4.93175700	-0.05479700
H	-4.11142300	-5.62118900	-2.09573800
H	-3.69132500	-4.16922800	1.92765900
H	-5.06374100	-5.26136100	0.17114600
C	-0.89520000	1.00303400	-2.55301000
C	-0.66877200	0.96950500	-3.93614300
C	-1.85606000	1.89626100	-2.07276500
C	-1.33772200	1.83205500	-4.79826400
H	0.05493900	0.27134400	-4.35570400
C	-2.52910000	2.75901700	-2.93356400
H	-2.08135600	1.92905700	-1.01169700
C	-2.26802300	2.73876700	-4.29910900
H	-1.12826600	1.79273800	-5.86503100
H	-3.25968500	3.45462700	-2.52607900
H	-2.78697300	3.41980400	-4.96961800
O	2.01756300	0.24357600	-2.68149900
C	2.37834700	-1.90702700	-4.79670000
C	-1.07723100	0.83125500	0.92134900
C	-1.88589800	-0.17639900	1.47830600
C	-1.41138900	2.13575400	1.32289000
C	-2.84888200	0.08598900	2.45593900
H	-1.73947700	-1.21519500	1.18754700
C	-2.43026600	2.41339100	2.22998500
H	-0.85808700	2.98151800	0.91546400

C	-3.14066400	1.38918900	2.83832600
H	-3.88692500	1.59736600	3.59922700
C	1.12616200	1.94649400	-0.08984100
C	1.73190200	2.37840100	1.10630100
C	1.29770600	2.78803100	-1.18997200
C	2.43744500	3.57005400	1.19599500
H	1.63780100	1.76117300	1.99939600
C	2.00621700	3.99064700	-1.10628900
H	0.87775800	2.51724300	-2.15510700
C	2.58160000	4.39872000	0.08405500
H	3.13333100	5.33310100	0.15466700
C	1.26051400	-0.57148400	0.67686500
C	0.91277800	-1.45905300	1.70071500
C	2.60514000	-0.64759700	0.25827200
C	1.80436100	-2.40312100	2.21680700
H	-0.07802800	-1.43633600	2.14333600
C	3.50040600	-1.57488400	0.77301800
H	2.97268600	0.04252300	-0.49744700
C	3.10513600	-2.48433500	1.75067900
H	3.80294400	-3.21996700	2.14444200
H	1.39776400	-2.05962800	-5.25702000
H	3.15433300	-2.40946800	-5.38225200
H	2.61212300	-0.84690600	-4.67613800
H	-0.57263100	-2.93383200	-2.97496700
C	1.29704200	-3.42444700	3.18158900
C	4.93453300	-1.59532400	0.34595100
C	2.16171100	4.80058500	-2.35261500
C	3.03490800	4.03461300	2.48447000
C	-2.71562600	3.84617200	2.54857200
C	-3.53910500	-1.04779500	3.14869500

F	2.25880000	-3.91008200	3.97427600
F	0.77125700	-4.47819200	2.52519500
F	0.32568800	-2.95087100	3.97352800
F	5.33773600	-2.83086200	0.01647200
F	5.73911200	-1.19998200	1.35155200
F	5.18793700	-0.79625500	-0.69058000
F	4.32622500	4.37326900	2.33775600
F	2.97523900	3.11485200	3.45246000
F	2.41225100	5.13295500	2.94563500
F	3.00499100	4.21673500	-3.21983500
F	0.99682500	4.94540100	-3.00381800
F	2.63618200	6.02934600	-2.11488000
F	-2.72853200	-2.10878800	3.29233900
F	-4.62751000	-1.49112500	2.48418800
F	-3.96427700	-0.70797600	4.36871900
F	-3.65376600	3.98769400	3.49106000
F	-3.14265500	4.51153500	1.46253100
F	-1.62057500	4.49032700	2.97678800

Energy (0K) = -4383.8105876

Energy (0K) + ZPE = -4383.098549

Enthalpy (298K) = -4383.035533

Free Energy (298K) = -4383.198532

TS_{D1}

Number of imaginary frequencies: 1

C	-1.39874400	0.39954400	0.76341800
C	-0.50023200	0.10634100	1.97674400
N	0.88847600	-0.04620200	1.85833800
B	-1.81791400	-1.00488600	-0.15944300
S	1.60143800	-0.66098100	3.35764800

O	3.04025000	-0.64755700	3.10237400
O	0.97970700	-1.92421200	3.71306700
C	1.88726500	0.12307800	0.76139600
C	1.76479900	1.37488900	0.02490700
C	1.82984800	2.47825800	-0.47626800
C	1.87766300	3.82256500	-0.95795000
C	1.41418700	4.16940700	-2.23396700
C	2.34551000	4.83127200	-0.10017100
C	1.41519600	5.49843500	-2.63850400
H	1.03351900	3.39614400	-2.89426500
C	2.33999900	6.15777400	-0.51101000
H	2.69958400	4.55996800	0.89242500
C	1.87415400	6.49479400	-1.78000500
H	1.05075400	5.75836400	-3.62974900
H	2.70113500	6.93185700	0.16228400
H	1.87007600	7.53422200	-2.10003000
C	2.07936700	-1.15410200	-0.06743800
H	1.22914700	-1.31021100	-0.73636000
H	2.09086800	-1.99537600	0.64104600
C	3.36186400	-1.13107400	-0.85314200
C	4.59466500	-1.06819800	-0.19424300
C	3.34915300	-1.18852500	-2.24624400
C	5.78306700	-1.04941700	-0.91499200
H	4.62027200	-1.04788900	0.89574000
C	4.53773400	-1.16954800	-2.97173600
H	2.39330500	-1.25379800	-2.76568900
C	5.75810100	-1.09689000	-2.30763500
H	6.73406000	-1.00401400	-0.38816400
H	4.50719800	-1.21288400	-4.05863900
H	6.68809700	-1.08253000	-2.87194500

C	-1.37026200	1.80100300	0.35279100
C	-0.94579700	2.79127900	1.26858800
C	-1.89167300	2.23951300	-0.87979100
C	-1.04046700	4.13873000	0.96584000
H	-0.55312700	2.49643400	2.24172000
C	-1.95673500	3.59014400	-1.19609300
H	-2.25161200	1.51915900	-1.60520200
C	-1.54291100	4.54351100	-0.27175400
H	-0.71395900	4.87945100	1.69181400
H	-2.34927000	3.89479300	-2.16337000
H	-1.59647600	5.60219800	-0.51659800
O	-0.96864200	-0.02978600	3.08932900
C	1.30499600	0.59530500	4.58065200
C	-1.11210400	-1.07384400	-1.64744200
C	-0.32159700	-0.12303000	-2.29265500
C	-1.45054000	-2.20737400	-2.41664200
C	0.09039700	-0.27790200	-3.62332900
H	0.00075100	0.77612700	-1.76649400
C	-1.02587200	-2.37637000	-3.72459100
H	-2.08501600	-2.97488800	-1.97519200
C	-0.24996900	-1.40247200	-4.35189100
H	0.06536700	-1.52439500	-5.38482200
C	-3.44223800	-1.02583600	-0.50701000
C	-4.41636100	-1.63657000	0.29507400
C	-3.93621200	-0.40058300	-1.65738500
C	-5.77766100	-1.56164700	0.00719500
H	-4.12299300	-2.18695400	1.18623800
C	-5.29829400	-0.27769300	-1.92799200
H	-3.24685100	0.03626200	-2.37914000
C	-6.24509500	-0.85222700	-1.09371000

H	-7.30751700	-0.75463300	-1.29571600
C	-1.39208100	-2.31508100	0.74434800
C	-0.48611600	-3.28439200	0.30573400
C	-1.88454800	-2.50380700	2.04942600
C	-0.09686000	-4.36745800	1.09676900
H	-0.04040500	-3.20652600	-0.68528300
C	-1.47873700	-3.56098800	2.85271900
H	-2.55739100	-1.76907900	2.48352000
C	-0.58550400	-4.51851200	2.38268600
H	-0.26072500	-5.33988900	3.01576200
H	1.46652200	1.57225700	4.11544800
H	2.05939100	0.42223700	5.35435000
H	0.29591900	0.49920600	4.97630000
H	2.82774400	0.24880900	1.31324600
O	-3.10194800	0.53704400	1.83304300
C	-4.42692800	2.02409000	0.67512100
C	-3.77580700	2.50754500	2.88759700
C	-5.11101800	3.21579900	0.58359500
H	-4.38978800	1.28569900	-0.11580400
C	-4.46231500	3.70591600	2.83419600
C	-5.12118800	4.08024700	1.66989900
H	-5.62501800	3.44585200	-0.34485100
H	-4.47144800	4.33897200	3.71579600
H	-5.65210600	5.02626000	1.62724100
N	-3.75038500	1.67189800	1.80208000
Br	-2.94034300	1.95984100	4.45596100
C	0.91332100	-5.30872300	0.52951200
C	-1.95148800	-3.66341000	4.26604700
C	-1.37200100	-3.60203000	-4.50866000
C	0.86233600	0.83143500	-4.25951100

C	-6.72583000	-2.27056200	0.92199800
C	-5.68420500	0.60704000	-3.06574700
F	-2.89907900	-4.60838700	4.41306600
F	-2.47141800	-2.51815100	4.71939200
F	-0.95490300	-4.00213800	5.09739500
F	1.18439000	-6.33666700	1.34078400
F	2.07943100	-4.68568200	0.28035400
F	0.51100800	-5.82436900	-0.64297300
F	-6.59051600	-3.60275800	0.83289200
F	-8.00669900	-1.98671300	0.65976400
F	-6.50516200	-1.95491200	2.20714200
F	-7.00003300	0.63557600	-3.28794600
F	-5.08839400	0.25208800	-4.21184300
F	-5.29714300	1.87821300	-2.81988500
F	-0.29169600	-4.37243800	-4.71576200
F	-1.84870200	-3.29005700	-5.72399500
F	-2.28953500	-4.36392200	-3.90704900
F	1.35030600	0.50708200	-5.45972700
F	0.08452100	1.92009900	-4.43220300
F	1.89757200	1.22674000	-3.50510000

Energy (0K) = -7277.6509743

Energy (0K) + ZPE = -7276.857058

Enthalpy (298K) = -7276.785924

Free Energy (298K) = -7276.966695

D1

Number of imaginary frequencies: 0

C	-0.35567200	0.80804900	0.80336200
C	0.64454100	0.49699100	1.95251600
N	2.03842000	0.40259400	1.81239500

B	-0.64769500	-0.61906900	-0.20966100
S	2.77771900	-0.21549100	3.30339300
O	4.21657700	-0.12977500	3.05574300
O	2.22419200	-1.51823700	3.63234200
C	3.03378800	0.56184400	0.71209300
C	2.94339300	1.81073300	-0.03503500
C	3.07276000	2.89857100	-0.55776900
C	3.20225900	4.22786500	-1.06581600
C	2.80261500	4.56721000	-2.36528700
C	3.69627000	5.23146100	-0.21711000
C	2.89614400	5.88202200	-2.80329600
H	2.39322200	3.80019500	-3.01539100
C	3.78055600	6.54493700	-0.66025900
H	3.99967100	4.96764300	0.79416200
C	3.38212900	6.87364800	-1.95408800
H	2.58195600	6.13533100	-3.81333500
H	4.16032200	7.31517000	0.00726200
H	3.44984000	7.90251300	-2.30026200
C	3.22373200	-0.72641800	-0.10052600
H	2.37624700	-0.88528500	-0.77142500
H	3.22148000	-1.55790000	0.61925700
C	4.51149400	-0.73557300	-0.87840500
C	5.74223400	-0.64773900	-0.21822800
C	4.50535900	-0.85746000	-2.26764900
C	6.93349700	-0.66235500	-0.93442500
H	5.76539700	-0.58101400	0.86984500
C	5.69663600	-0.87202300	-2.98871200
H	3.55139600	-0.94128000	-2.78808700
C	6.91437300	-0.77060700	-2.32380900
H	7.88246200	-0.59503400	-0.40620200

H	5.67031000	-0.96344700	-4.07277100
H	7.84672200	-0.78090100	-2.88436400
C	-0.16781800	2.21865300	0.30246800
C	0.26571300	3.20041000	1.20905200
C	-0.59106500	2.64454000	-0.96113600
C	0.27926800	4.54626600	0.86714900
H	0.58684500	2.91132200	2.21111200
C	-0.56126100	3.99081100	-1.31621100
H	-0.96297400	1.92199200	-1.68054400
C	-0.13537000	4.94677400	-0.40094900
H	0.62115300	5.28337900	1.59034000
H	-0.88540600	4.28957100	-2.31066100
H	-0.11363800	5.99927600	-0.67615000
O	0.22004200	0.29840000	3.07589700
C	2.43544200	0.99657800	4.56054500
C	0.05830000	-0.67885100	-1.69489800
C	0.87761800	0.25331500	-2.33259600
C	-0.29717100	-1.80213900	-2.47316400
C	1.29105800	0.09569600	-3.66334500
H	1.21993100	1.13806800	-1.79541500
C	0.13104000	-1.97764000	-3.77882100
H	-0.94677600	-2.56081300	-2.03822700
C	0.92872800	-1.01732500	-4.39904700
H	1.24612300	-1.14171700	-5.43107400
C	-2.27122500	-0.67898100	-0.55929400
C	-3.23124600	-1.31396000	0.24119400
C	-2.78235500	-0.05398600	-1.70535000
C	-4.59454600	-1.27286200	-0.04557100
H	-2.92342600	-1.86129500	1.12982500
C	-4.14695100	0.02506600	-1.97985700

H	-2.10232400	0.41733700	-2.41571300
C	-5.07839900	-0.57977700	-1.14860600
H	-6.14217300	-0.51679200	-1.35647900
C	-0.19460000	-1.93253500	0.68151400
C	0.72791700	-2.87835300	0.22511200
C	-0.66998700	-2.15087500	1.98884100
C	1.15657500	-3.95581500	1.00313900
H	1.15844700	-2.78324000	-0.77101400
C	-0.22793100	-3.20301200	2.77928700
H	-1.35839900	-1.44089400	2.43842200
C	0.68843600	-4.13009800	2.29377000
H	1.04493000	-4.94516700	2.91770700
H	2.54369100	1.99093700	4.11751700
H	3.21029900	0.84218300	5.31784000
H	1.43889600	0.84331500	4.96886700
H	3.97332900	0.68564400	1.26540100
O	-1.70306600	0.84472900	1.63963700
C	-3.12408700	2.33846800	0.56812600
C	-2.56204100	2.69007200	2.83396500
C	-3.91568800	3.46410300	0.55158200
H	-3.01309800	1.67045400	-0.27616200
C	-3.35251100	3.82595400	2.85085700
C	-4.01763200	4.23341000	1.70291200
H	-4.44057900	3.71454800	-0.36457800
H	-3.44214400	4.37916300	3.77980300
H	-4.62970700	5.12998200	1.72192800
N	-2.43594000	1.97864800	1.67797800
Br	-1.75045600	2.11542000	4.40041500
C	2.18867400	-4.86224100	0.41852200
C	-0.68999500	-3.33274800	4.19367900

C	-0.23206700	-3.19450400	-4.56822300
C	2.09245800	1.18614900	-4.29581200
C	-5.52449200	-2.01096400	0.86497200
C	-4.56866700	0.89213400	-3.11920900
F	-1.60319500	-4.31191500	4.33686600
F	-1.24920400	-2.21040800	4.65878800
F	0.32088300	-3.64294600	5.01872500
F	2.49469800	-5.89056800	1.21697400
F	3.33511500	-4.20381600	0.16741400
F	1.79247700	-5.37708300	-0.75643900
F	-5.36563300	-3.33893200	0.75754300
F	-6.81166600	-1.74652700	0.61398500
F	-5.30148400	-1.70754400	2.15286700
F	-5.87510200	0.81341300	-3.38404900
F	-3.90956800	0.60441000	-4.24854600
F	-4.29914900	2.18725200	-2.84622500
F	0.84029000	-3.97164100	-4.79227800
F	-0.71828800	-2.87027600	-5.77697800
F	-1.14958200	-3.95473400	-3.96410500
F	2.57561000	0.84966000	-5.49545500
F	1.34346900	2.29419900	-4.47223800
F	3.13539700	1.55540400	-3.54032900

Energy (0K) = -7277.655922

Energy (0K) + ZPE = -7276.859908

Enthalpy (298K) = -7276.788804

Free Energy (298K) = -7276.970135

TS_{D2}

Number of imaginary frequencies: 1

C	-1.39896500	-0.18659200	0.98548100
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C	-0.68550100	-1.44192500	1.41161800
N	0.60655000	-1.87177800	1.22227600
B	-2.18555200	-0.23058400	-0.35398400
S	0.88423300	-3.52016500	1.81492500
O	2.30328800	-3.75945000	1.59644700
O	-0.08709300	-4.39426000	1.18750600
C	1.87083700	-1.09509300	1.00658300
C	1.73768900	0.34557800	1.15283100
C	1.86811200	1.54573800	1.26710900
C	2.01206500	2.95958000	1.38834600
C	3.18825800	3.57356500	0.93038200
C	0.99552300	3.74422500	1.95279100
C	3.34265000	4.94871700	1.04216200
H	3.97448700	2.95971000	0.49410500
C	1.16096000	5.11976900	2.05704800
H	0.07945000	3.26911700	2.30204400
C	2.33135400	5.72433000	1.60571300
H	4.25694100	5.41814500	0.68661200
H	0.36534700	5.72388000	2.48700500
H	2.45461600	6.80153600	1.68974100
C	2.56573600	-1.45924300	-0.31999200
H	2.02453900	-0.99644000	-1.14669500
H	2.51136100	-2.54461000	-0.44716200
C	3.99957400	-1.00918900	-0.32316900
C	4.97531100	-1.76593500	0.33156800
C	4.37659400	0.18069500	-0.94893400
C	6.30007200	-1.34168800	0.35907300
H	4.68716100	-2.69809800	0.81790500
C	5.70213400	0.60607800	-0.92573300
H	3.62023800	0.77734000	-1.45871100

C	6.66671500	-0.15396500	-0.26968400
H	7.05037300	-1.94250200	0.86873600
H	5.98159100	1.53162000	-1.42542200
H	7.70321000	0.17565600	-0.25269900
C	-1.54964400	0.74420500	2.11651200
C	-0.69650800	0.62718700	3.23471100
C	-2.55814600	1.72629400	2.17297400
C	-0.83348900	1.44922300	4.34064400
H	0.08852400	-0.12615500	3.25067200
C	-2.68377800	2.56205700	3.27412700
H	-3.26580900	1.83139500	1.35764100
C	-1.82425300	2.42861900	4.36072900
H	-0.16188900	1.33006300	5.18658200
H	-3.47116400	3.31115000	3.28812700
H	-1.92996800	3.08024600	5.22458600
O	-1.49550300	-2.13574600	2.01917000
C	0.63818700	-3.38584300	3.56478800
C	-0.89133800	0.84789400	-0.78825500
C	0.03151200	0.38233500	-1.73436900
C	-0.99331000	2.22951200	-0.59492300
C	0.77220000	1.27524500	-2.50314400
H	0.12802100	-0.68504900	-1.91703900
C	-0.26310800	3.11748400	-1.37245200
H	-1.67007000	2.63557100	0.15260200
C	0.62684000	2.64759400	-2.33197900
H	1.19109400	3.34495500	-2.94836300
C	-3.65602500	0.41732500	-0.42758800
C	-4.05281300	1.48534300	-1.23290900
C	-4.65413300	-0.22568400	0.31701900
C	-5.38120900	1.91186500	-1.26812300

H	-3.31876200	2.01548800	-1.84184400
C	-5.97779500	0.19825800	0.28045200
H	-4.38250400	-1.07340600	0.95081400
C	-6.35634500	1.27772800	-0.51091300
H	-7.38850900	1.61241800	-0.53543500
C	-2.19459600	-1.53859100	-1.31118200
C	-2.39153700	-1.32382700	-2.68830500
C	-2.17113300	-2.86939600	-0.88642600
C	-2.51912700	-2.37314200	-3.58471000
H	-2.44815300	-0.30518400	-3.07205200
C	-2.30515000	-3.92827100	-1.79007700
H	-2.06760500	-3.11701400	0.16651700
C	-2.46866000	-3.69434100	-3.14398000
H	-2.57047400	-4.51571900	-3.84926700
H	1.32908500	-2.62554300	3.94246000
H	0.90138800	-4.36486500	3.97796600
H	-0.40146300	-3.13678400	3.77686100
H	2.53841300	-1.42500100	1.81836000
C	-2.20604200	-5.33476500	-1.28706500
C	-2.68842000	-2.13548200	-5.05145300
C	-6.97993800	-0.54147600	1.10961400
C	-5.71720200	3.08260900	-2.13708400
C	-0.47993400	4.59685500	-1.26560300
C	1.65913800	0.79491500	-3.61256400
F	-8.21114500	-0.03072000	1.01127500
F	-6.64698500	-0.52974100	2.40938700
F	-7.05450400	-1.83146300	0.75126200
F	-7.01420900	3.40204100	-2.10124200
F	-5.02868900	4.17534500	-1.77009800
F	-5.39968600	2.85056500	-3.41931800

F	1.97418800	-0.49849500	-3.49617500
F	1.06959800	0.95417500	-4.80427400
F	2.80651200	1.48649400	-3.65773500
F	-1.19294500	5.04694800	-2.30938900
F	-1.14378300	4.94091200	-0.15929600
F	0.67568200	5.26919600	-1.27333700
F	-2.82626500	-6.20498400	-2.09828700
F	-2.74641500	-5.47566900	-0.07158600
F	-0.93004600	-5.73396700	-1.19899000
F	-3.71633600	-2.83974700	-5.54842900
F	-1.60028700	-2.52215100	-5.73721200
F	-2.90515400	-0.85104100	-5.34963200

Energy (0K) = -4383.7662101

Energy (0K) + ZPE = -4383.058244

Enthalpy (298K) = -4382.994210

Free Energy (298K) = -4383.161210

D2

Number of imaginary frequencies: 0

C	-0.13691800	-0.17272800	1.31006300
C	0.46938900	-1.48779900	1.81408500
N	1.80212900	-1.88130800	1.75829300
B	-1.39364400	-0.65006900	0.37555800
S	2.06791700	-3.54443200	2.27863500
O	3.51153400	-3.73290100	2.20326400
O	1.20618600	-4.41264900	1.49635400
C	3.06971700	-1.09857300	1.58993300
C	2.94562000	0.32483000	1.85673000
C	3.02799000	1.51796500	2.05459400
C	3.06478600	2.93293800	2.22801200

C	3.98898200	3.70162800	1.50386900
C	2.15156700	3.56870800	3.08322800
C	4.00099300	5.08334500	1.64283000
H	4.68847900	3.20207300	0.83542600
C	2.16828200	4.95148200	3.20878800
H	1.43544900	2.96616300	3.64126600
C	3.09025800	5.71036000	2.49083500
H	4.71919800	5.67524900	1.08020600
H	1.45589100	5.43952100	3.87003600
H	3.09878300	6.79313300	2.59202300
C	3.75695000	-1.38682500	0.23885300
H	3.13720200	-1.01769200	-0.58177600
H	3.83272400	-2.47499600	0.13734400
C	5.12033400	-0.76295200	0.16483200
C	6.20355600	-1.35231200	0.82090300
C	5.32152300	0.42692800	-0.53777700
C	7.46400300	-0.76437600	0.77406100
H	6.04924400	-2.28472000	1.36510700
C	6.58179100	1.01598200	-0.58934100
H	4.47606200	0.89115300	-1.04941400
C	7.65566300	0.42109100	0.06846400
H	8.30066200	-1.23599300	1.28528500
H	6.72562100	1.94019900	-1.14562800
H	8.64174600	0.87860000	0.02733800
C	-0.48213100	0.62802300	2.58353500
C	0.17639200	0.35018100	3.79058300
C	-1.41825900	1.67009000	2.60116900
C	-0.09348200	1.06215600	4.95434100
H	0.91737900	-0.44437000	3.85110300
C	-1.68714300	2.39043100	3.76210600

H	-1.95227200	1.94691800	1.69919500
C	-1.03052700	2.08962900	4.94892400
H	0.43799600	0.80700100	5.86834800
H	-2.42279700	3.19085600	3.72842700
H	-1.24609200	2.64696700	5.85743200
O	-0.34268600	-2.24513200	2.33319000
C	1.64043500	-3.55154800	3.99896200
C	0.53675100	0.64188400	0.20436700
C	1.00782900	-0.00359900	-0.94269400
C	0.53521400	2.04302400	0.20438300
C	1.46690300	0.71919700	-2.03891500
H	1.02164000	-1.08832400	-0.99726200
C	1.01027900	2.75686400	-0.88539100
H	0.18079500	2.59118000	1.07106500
C	1.47255900	2.10570200	-2.02586800
H	1.81962000	2.67087500	-2.88918800
C	-2.67814200	0.23737100	0.21573700
C	-2.74905100	1.36006000	-0.61467700
C	-3.82559300	-0.12847500	0.92654100
C	-3.91660900	2.11368100	-0.69529400
H	-1.87907700	1.67266400	-1.19345400
C	-4.98960100	0.62941000	0.83831200
H	-3.80752900	-1.00784200	1.57264800
C	-5.04538000	1.76118400	0.03323100
H	-5.95281400	2.35377700	-0.02706000
C	-1.34368500	-1.88969100	-0.60901600
C	-1.48461200	-1.58849700	-1.97744900
C	-1.16572400	-3.23342200	-0.26248200
C	-1.35850400	-2.56935500	-2.94955100
H	-1.66286600	-0.56104700	-2.29032600

C	-1.11560700	-4.22548300	-1.24139000
H	-1.05826700	-3.51614100	0.77925500
C	-1.17916100	-3.90181300	-2.58819900
H	-1.09919900	-4.67320600	-3.35209700
H	2.23909700	-2.78050200	4.49353700
H	1.93117600	-4.53975600	4.36948000
H	0.57156500	-3.38139600	4.12187900
H	3.74185200	-1.49572200	2.36542100
C	-0.91370000	-5.66046700	-0.85862800
C	-1.38466000	-2.24043700	-4.41018500
C	-6.17616900	0.19331900	1.64143900
C	-3.90906300	3.31123800	-1.59339700
C	0.99088800	4.25594700	-0.88855300
C	1.87352900	0.00580700	-3.29114300
F	-7.25079100	0.95738900	1.42886500
F	-5.91647700	0.22624700	2.95649100
F	-6.51968700	-1.06963100	1.35390400
F	-5.02096100	4.04264000	-1.48813400
F	-2.87154900	4.11624400	-1.32000800
F	-3.78363800	2.95577600	-2.88032000
F	2.07714300	-1.30037900	-3.09333900
F	0.92414700	0.11988700	-4.23115100
F	2.99656000	0.51774600	-3.80735100
F	0.15354800	4.72369600	-1.82560400
F	0.60717300	4.76972200	0.28175200
F	2.19888800	4.75826800	-1.17544000
F	-1.60092800	-6.48417000	-1.66494000
F	-1.30542900	-5.91471500	0.39214400
F	0.37279900	-6.02060400	-0.95684100
F	-2.32585100	-2.94458600	-5.05603700

F	-0.21491800	-2.55105300	-4.98949500
F	-1.62009000	-0.94845300	-4.64873700

Energy (0K) = -4383.8107718

Energy (0K) + ZPE = -4383.099150

Enthalpy (298K) = -4383.035927

Free Energy (298K) = -4383.198134

D3

Number of imaginary frequencies: 0

C	0.38907300	0.41101500	0.70861500
C	0.02496800	-0.88425600	1.40262700
N	0.83166500	-1.01289400	2.49422200
B	-1.66384300	-2.12121400	-0.16591900
S	0.52491900	-2.19869200	3.74427400
O	1.27912700	-3.39334800	3.40836400
O	-0.91515900	-2.25805900	3.91784000
C	2.06843100	-0.13832000	2.47140600
C	1.81788800	0.56281500	1.19923200
C	1.65544600	0.44746500	-0.09408300
C	2.17839000	0.37587700	-1.43501400
C	3.53963800	0.10301500	-1.63739400
C	1.34112100	0.58414200	-2.53920100
C	4.04367000	0.00936700	-2.92597600
H	4.18540100	-0.03408500	-0.77169200
C	1.85290900	0.49424400	-3.82718000
H	0.29387600	0.83503700	-2.38097500
C	3.19988600	0.19815800	-4.02140700
H	5.09732100	-0.21010400	-3.08079500
H	1.19627000	0.64747500	-4.67989400
H	3.59706600	0.11889600	-5.03087500

C	3.33759100	-0.99139600	2.44198300
H	3.27107800	-1.66669900	1.57909300
H	3.37147800	-1.63203400	3.33313700
C	4.59110500	-0.16350100	2.37038200
C	4.83296800	0.86497400	3.28612000
C	5.55837500	-0.44443300	1.40296300
C	6.00752300	1.60718400	3.22191400
H	4.10265900	1.08317700	4.06577800
C	6.73585700	0.29582700	1.33898200
H	5.38609900	-1.26081000	0.70132600
C	6.96081100	1.32703600	2.24569900
H	6.18067300	2.40518400	3.94062500
H	7.47875200	0.06454500	0.57891300
H	7.87848900	1.90872200	2.19679800
C	-0.60410600	1.52106100	0.80992300
C	-1.65553500	1.47775100	1.73071200
C	-0.45642000	2.65417700	0.00582500
C	-2.55521300	2.53474200	1.82376300
H	-1.79049100	0.61185300	2.38016700
C	-1.34906500	3.71407000	0.10826900
H	0.35969800	2.70030200	-0.71442300
C	-2.40653200	3.65584700	1.01206600
H	-3.37907900	2.47623000	2.53179500
H	-1.23071000	4.58106400	-0.53829300
H	-3.11594900	4.47773000	1.07872000
O	-0.86592100	-1.73265800	1.18166300
C	1.20306600	-1.37892100	5.15624400
C	-2.72628500	-0.93723700	-0.44169100
C	-2.50095600	0.10521200	-1.34777400
C	-3.90175000	-0.87160100	0.31210200

C	-3.40112300	1.15547200	-1.49716200
H	-1.59502700	0.10075300	-1.95061700
C	-4.80520000	0.18075600	0.17148300
H	-4.11806900	-1.65454600	1.04041700
C	-4.56504000	1.20288900	-0.73653500
H	-5.26720400	2.02513000	-0.84828500
C	-2.37074000	-3.52378500	0.21761200
C	-3.08634000	-4.22346500	-0.76157000
C	-2.28770000	-4.11849600	1.47778600
C	-3.67210100	-5.45886500	-0.49847300
H	-3.18564300	-3.80066400	-1.76376100
C	-2.87639400	-5.35447800	1.74364300
H	-1.75831500	-3.61489800	2.28358700
C	-3.57226700	-6.04254200	0.76064400
H	-4.02533700	-7.00784800	0.96340200
C	-0.53263700	-2.38827100	-1.28914800
C	0.74996500	-2.83592200	-0.94820700
C	-0.80606700	-2.27485000	-2.65729800
C	1.71815100	-3.10176300	-1.91445200
H	1.02079300	-2.98519700	0.10030700
C	0.16112800	-2.53725600	-3.62444300
H	-1.79335700	-1.95345100	-2.99008800
C	1.43827400	-2.94643400	-3.26558000
H	2.19917400	-3.12539500	-4.01908800
H	2.29050000	-1.29222000	5.09921800
H	0.93151400	-2.01924700	6.00205000
H	0.71722100	-0.40504600	5.26098000
H	2.03378900	0.52467000	3.34507000
C	3.06752300	-3.55649300	-1.45953800
C	-0.20421900	-2.32770400	-5.05885900

C	-4.40334400	-6.14399500	-1.60804400
C	-2.72834600	-5.89963300	3.12771900
C	-5.99559000	0.22351900	1.07458900
C	-3.17240400	2.22017900	-2.52289300
F	-3.24625700	-7.12483400	3.26544400
F	-3.32932800	-5.11235100	4.03499600
F	-1.43800100	-5.96960600	3.49178800
F	-4.87819600	-7.34280200	-1.25299900
F	-3.61331300	-6.33209400	-2.67719400
F	-5.44791500	-5.41751900	-2.03694400
F	-0.79053500	-1.13250000	-5.24230600
F	-1.08135700	-3.24668500	-5.48877200
F	0.85425800	-2.37617300	-5.87407100
F	3.96501900	-3.59452200	-2.44802400
F	3.56536300	-2.74002900	-0.50987700
F	3.02214000	-4.77870800	-0.91259000
F	-6.90306000	1.12877300	0.69254300
F	-5.63994300	0.53329700	2.33442000
F	-6.61692000	-0.96198400	1.14046100
F	-3.88405800	1.98775300	-3.63832700
F	-1.88915100	2.30987800	-2.89641200
F	-3.54399600	3.43155000	-2.08473900

Energy (0K) = -4383.8298559

Energy (0K) + ZPE = -4383.117940

Enthalpy (298K) = -4383.055112

Free Energy (298K) = -4383.217231

E

Number of imaginary frequencies: 0

C	-1.72504700	0.44726500	-1.37196700
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C	-0.62584600	-0.38117700	-1.34179900
N	-1.01199100	-1.74363800	-1.30549900
B	1.45297100	0.13618400	0.00996700
S	-0.08741700	-2.96489000	-2.04843700
O	-1.00472700	-4.08999000	-2.18124600
O	1.15209700	-3.12668200	-1.31189800
C	-2.47765600	-1.83459800	-1.37471700
C	-2.90682600	-0.37594500	-1.27911000
C	-4.13435300	0.02285200	-1.03447500
C	-5.36823000	0.62762000	-1.13014000
C	-6.05612500	1.05796900	0.03850500
C	-5.97609700	0.80878000	-2.40574900
C	-7.28545400	1.67728200	-0.07501100
H	-5.58387900	0.91831300	1.00728200
C	-7.21490100	1.40427300	-2.49908200
H	-5.44443300	0.46462300	-3.28974800
C	-7.86102000	1.84216900	-1.33631000
H	-7.80664900	2.02689500	0.81143600
H	-7.68634600	1.54347200	-3.46778000
H	-8.83424400	2.32068600	-1.41910000
C	-3.07672900	-2.69821800	-0.27001200
H	-2.63239600	-2.39193300	0.68770500
H	-2.77186900	-3.73634000	-0.45505500
C	-4.56952700	-2.56122300	-0.23077200
C	-5.22195600	-2.19477800	0.95242100
C	-5.33916600	-2.77033200	-1.38659300
C	-6.59635800	-2.00043700	0.97170100
C	-6.71505700	-2.57447500	-1.36945500
H	-4.85135900	-3.08744800	-2.30810800
C	-7.34502300	-2.17453400	-0.19375700

H	-7.08882900	-1.70029600	1.89414200
H	-7.29557000	-2.72886300	-2.27610200
H	-8.41932700	-2.00390700	-0.18039800
C	-1.70501900	1.91793400	-1.34306300
C	-1.11531800	2.63693600	-2.38731800
C	-2.27392000	2.62069700	-0.27350300
C	-1.08085600	4.02699600	-2.35740900
H	-0.68002800	2.09603200	-3.22687400
C	-2.22552800	4.01022100	-0.23735300
H	-2.74445100	2.06800900	0.54051000
C	-1.62560000	4.71610600	-1.27765200
H	-0.61563300	4.57333200	-3.17465300
H	-2.65633500	4.54284500	0.60776600
H	-1.58289500	5.80276700	-1.24732400
O	0.62369200	-0.05748800	-1.33283300
C	0.26585600	-2.32997400	-3.66576400
C	0.54531200	-0.49825600	1.19421300
C	0.59924400	-1.85656100	1.51680600
C	-0.49150600	0.24132000	1.77679800
C	-0.33572800	-2.44779300	2.36465400
H	1.36109700	-2.48318500	1.05563800
C	-1.42516100	-0.34271500	2.62953100
H	-0.58792700	1.30211200	1.54351800
C	-1.36222800	-1.70063200	2.92763400
H	-2.10067300	-2.16753400	3.57484300
C	1.74134800	1.72160900	0.18777700
C	1.98543700	2.28158400	1.44752200
C	1.86152200	2.57202400	-0.91649600
C	2.30318900	3.62866700	1.60079600
H	1.92296900	1.65478000	2.33617400

C	2.17399200	3.92036900	-0.76705400
H	1.70194200	2.16703100	-1.91412400
C	2.39397900	4.46395200	0.49364500
H	2.63436700	5.52016300	0.60868000
C	2.86592300	-0.60573900	-0.24399200
C	3.72409100	-0.95068000	0.80440500
C	3.32002700	-0.88368400	-1.53565100
C	4.95489300	-1.56646000	0.57493300
H	3.42844000	-0.74663300	1.83560500
C	4.53694000	-1.51603600	-1.76919900
H	2.69548000	-0.61832500	-2.38813600
C	5.37184900	-1.86847700	-0.71573800
H	6.31981300	-2.36533100	-0.89716700
H	-0.68181200	-2.12997500	-4.17508900
H	0.82832500	-3.10290100	-4.19783600
H	0.86327900	-1.42006200	-3.57615200
H	-2.78246000	-2.20770700	-2.36407000
H	-4.63236900	-2.03251300	1.85359400
C	4.89741600	-1.82589500	-3.18497300
C	5.79541200	-1.92379100	1.75766800
C	2.28800300	4.83352700	-1.94485700
C	2.55795000	4.22505800	2.94774200
C	-0.30773000	-3.93279800	2.51240700
C	-2.58916400	0.46072200	3.10604800
F	5.19324000	-2.83720300	2.53705800
F	6.98710600	-2.42657800	1.41603500
F	6.02619500	-0.85853500	2.54190200
F	6.04891700	-2.49659400	-3.29657600
F	5.01509800	-0.71132400	-3.92570300
F	3.94757200	-2.56869400	-3.78156400

F	1.98738200	4.23272900	-3.10210100
F	1.47191000	5.89626900	-1.82839000
F	3.52866100	5.33100300	-2.07038600
F	1.72067900	5.24337200	3.20669400
F	2.42161800	3.34239200	3.94202800
F	3.79880100	4.73194500	3.03585800
F	-3.61851600	0.37087500	2.22927200
F	-3.06336500	0.04306800	4.28418000
F	-2.31110800	1.76320200	3.21949600
F	-0.74302900	-4.52643300	1.38429700
F	-1.08571900	-4.37417400	3.50803900
F	0.92675000	-4.39995200	2.73415300

Energy (0K) = -4383.8386975

Energy (0K) + ZPE = -4383.125124

Enthalpy (298K) = -4383.062760

Free Energy (298K) = -4383.222229

TS_F

Number of imaginary frequencies: 1

C	-1.70857700	0.20585300	-1.18574300
C	-0.57918400	-0.58368900	-1.29097700
N	-0.92149300	-1.95878300	-1.32133600
B	1.45301400	0.08421700	0.02748800
S	0.03004300	-3.10339400	-2.14975200
O	-0.86989000	-4.22708700	-2.37812000
O	1.26378800	-3.30575700	-1.41366700
C	-2.37926400	-2.06075700	-1.38185900
C	-2.82676900	-0.68033000	-1.00486700
C	-4.00863000	-0.35762200	-0.44963800
C	-4.94184100	0.69639700	-0.64316700

C	-5.56812900	1.32179300	0.45585900
C	-5.13354600	1.22063800	-1.93843400
C	-6.32819500	2.45918900	0.26567000
H	-5.41058200	0.91490200	1.45215700
C	-5.89638000	2.36450700	-2.12149700
H	-4.65002100	0.72994500	-2.78107400
C	-6.48927100	2.98094200	-1.02238600
H	-6.79229100	2.95476700	1.11422000
H	-6.02839100	2.77853200	-3.11763300
H	-7.08513900	3.87921500	-1.16633400
C	-3.04692300	-3.10192700	-0.48819900
H	-2.63429700	-3.01693700	0.52419800
H	-2.84743400	-4.10443400	-0.87965800
C	-4.49886400	-2.77103600	-0.49965800
C	-5.03322800	-2.01900100	0.57151000
C	-5.32428400	-3.09087100	-1.59194200
C	-6.41748900	-1.73207900	0.60325900
C	-6.65632700	-2.72808600	-1.58225300
H	-4.90449100	-3.64474600	-2.43027200
C	-7.20974800	-2.05885600	-0.47160600
H	-6.84004800	-1.23305700	1.47160000
H	-7.29116000	-2.98176300	-2.42765400
H	-8.27064200	-1.82208800	-0.46256100
C	-1.75048200	1.67714600	-1.14532300
C	-1.37021400	2.40176200	-2.28019500
C	-2.22576300	2.37481500	-0.02823200
C	-1.45569300	3.78929100	-2.29835000
H	-1.01270300	1.86259900	-3.15713100
C	-2.29941800	3.76360900	-0.04256100
H	-2.54655100	1.82617000	0.85690600

C	-1.91426600	4.47457000	-1.17674500
H	-1.16635800	4.33867300	-3.19128800
H	-2.66294000	4.29181700	0.83647900
H	-1.97250800	5.56083400	-1.18746800
O	0.66476000	-0.23976100	-1.32080400
C	0.38786400	-2.32770000	-3.70335900
C	0.58400500	-0.60047900	1.21657500
C	0.67045000	-1.97371000	1.45971900
C	-0.43597800	0.08885600	1.88479800
C	-0.23060300	-2.63070300	2.29869500
H	1.42766500	-2.56356200	0.94245000
C	-1.32941000	-0.55771400	2.73336200
H	-0.55432000	1.15842900	1.72062100
C	-1.24298700	-1.93271400	2.94173600
H	-1.94803100	-2.44005700	3.59679100
C	1.61615300	1.69150600	0.12773200
C	1.79611500	2.34815500	1.35068800
C	1.67836700	2.47903800	-1.02700700
C	1.98595100	3.72696600	1.41927400
H	1.77742400	1.77512000	2.27661000
C	1.86628900	3.85609000	-0.96223200
H	1.56368700	2.00445300	-2.00013500
C	2.01359600	4.49660900	0.26311500
H	2.14888600	5.57602800	0.31466100
C	2.91608500	-0.57479500	-0.16524300
C	3.78519300	-0.75489700	0.91562900
C	3.39344700	-0.96396400	-1.41772000
C	5.05238900	-1.31278800	0.75304500
H	3.46723500	-0.46807300	1.92030800
C	4.64740100	-1.54449100	-1.58156300

H	2.75790200	-0.83940200	-2.29269500
C	5.49707900	-1.72604200	-0.49765000
H	6.47566100	-2.18107900	-0.61950300
H	-0.55552600	-2.15702700	-4.23071900
H	1.02202300	-3.01760300	-4.26783200
H	0.91278500	-1.38583200	-3.52399100
H	-2.69985800	-2.22821400	-2.42503700
H	-4.43483900	-1.89069400	1.46965600
C	5.03248700	-1.97008900	-2.95980200
C	5.89978800	-1.50114300	1.96929400
C	1.92974500	4.69528400	-2.19706300
C	2.13127800	4.43174900	2.72974700
C	-0.12399600	-4.11716000	2.40556900
C	-2.43303700	0.19021500	3.40701100
F	5.36367700	-2.39996800	2.81134600
F	7.13583300	-1.92406300	1.68106400
F	6.02404700	-0.36205500	2.66874800
F	6.17181000	-2.66867000	-2.99391000
F	5.19143800	-0.91724100	-3.78029900
F	4.07859100	-2.73495200	-3.51875800
F	1.63424900	4.00979500	-3.30752200
F	1.07930900	5.73443300	-2.13527000
F	3.15109000	5.22469100	-2.37486100
F	1.11263400	5.28124100	2.94619000
F	2.17115900	3.59414400	3.77080400
F	3.25013200	5.17210700	2.77533000
F	-3.63268700	-0.08161700	2.84529100
F	-2.54882000	-0.13987900	4.69955300
F	-2.27968300	1.51677500	3.34403500
F	-0.42833900	-4.70818000	1.23561700

F	-0.94485900	-4.63397300	3.32715800
F	1.11921900	-4.50985200	2.71336500

Energy (0K) = -4383.82855

Energy (0K) + ZPE = -4383.115634

Enthalpy (298K) = -4383.054014

Free Energy (298K) = -4383.212700

F

Number of imaginary frequencies: 0

C	-1.94186900	0.25893200	-1.35773000
C	-0.79976000	-0.50409000	-1.29814800
N	-1.10403900	-1.88831600	-1.16363700
B	1.28730600	0.06951400	0.00172100
S	-0.15288600	-3.07591000	-1.92295900
O	-1.00268600	-4.26160900	-1.96419900
O	1.13937400	-3.14413800	-1.26557500
C	-2.56191100	-2.03419200	-1.25333300
C	-3.07991800	-0.61242400	-1.20631500
C	-4.39539700	-0.37651500	-0.95755300
C	-5.01987900	0.96072300	-0.98934900
C	-5.71818600	1.47525200	0.11216300
C	-4.92764700	1.74791900	-2.14431300
C	-6.27488900	2.74901300	0.06855300
H	-5.79223500	0.88741900	1.02708900
C	-5.48077900	3.02269200	-2.18751600
H	-4.40320700	1.35089600	-3.01212200
C	-6.15385100	3.52937400	-1.07881800
H	-6.79791900	3.13789600	0.93979000
H	-5.39004900	3.62049000	-3.09198700
H	-6.58706500	4.52658400	-1.10962300

C	-3.15331900	-2.85698700	-0.12135400
H	-2.88573700	-2.36948500	0.83322000
H	-2.76392000	-3.88006300	-0.10399800
C	-4.62807800	-2.84289800	-0.30449400
C	-5.26850400	-1.53943600	-0.54319200
C	-5.39985800	-3.98424600	-0.25106900
C	-6.67994800	-1.57163000	-0.93963500
C	-6.76473500	-3.92832200	-0.53542900
H	-4.92731800	-4.93753400	-0.02818000
C	-7.40699100	-2.72870100	-0.88242400
H	-7.15500000	-0.62464700	-1.18809100
H	-7.34636100	-4.84677800	-0.49916400
H	-8.46615000	-2.72761500	-1.12009000
C	-1.89580400	1.73377900	-1.32414500
C	-1.40723600	2.44750200	-2.42213200
C	-2.31360600	2.44504700	-0.19267500
C	-1.33929900	3.83706000	-2.39388200
H	-1.07894400	1.90058500	-3.30579800
C	-2.23300900	3.83223200	-0.15660500
H	-2.71264600	1.90057900	0.66245900
C	-1.74555200	4.53239500	-1.25832600
H	-0.95556100	4.37729700	-3.25635200
H	-2.54931300	4.36885800	0.73557800
H	-1.67432300	5.61746900	-1.22871800
O	0.43538400	-0.11767400	-1.30911500
C	0.06856500	-2.47456400	-3.57913100
C	0.48033700	-0.67290400	1.20035100
C	0.71955200	-2.00365900	1.55446000
C	-0.64475500	-0.06723200	1.77543500
C	-0.12733800	-2.70025600	2.41497500

H	1.55990900	-2.53080300	1.10653800
C	-1.49043800	-0.75558700	2.64407100
H	-0.88704900	0.96408000	1.51721000
C	-1.24509700	-2.08682300	2.96610900
H	-1.91167000	-2.63283900	3.62863300
C	1.46806200	1.66908700	0.22327900
C	1.62415700	2.23681800	1.49208400
C	1.58265700	2.53117600	-0.87437400
C	1.85653900	3.60095800	1.65907900
H	1.55835900	1.60449000	2.37661900
C	1.82298800	3.89201500	-0.71250800
H	1.46924500	2.12248100	-1.87731600
C	1.95600000	4.44251200	0.55823700
H	2.13492100	5.50936800	0.68448100
C	2.74565500	-0.54943900	-0.32505300
C	3.69239400	-0.78389300	0.67640300
C	3.14832000	-0.82263200	-1.63445800
C	4.95834500	-1.29497300	0.38802600
H	3.43875900	-0.57729700	1.71852000
C	4.40585900	-1.34066400	-1.92762500
H	2.45088900	-0.64615900	-2.45204200
C	5.32904800	-1.58791400	-0.91898400
H	6.30700600	-2.00060400	-1.14595300
H	-0.91620900	-2.34528700	-4.03897100
H	0.64555100	-3.22875200	-4.12257300
H	0.61331000	-1.52692000	-3.55062100
H	-2.83430800	-2.48883900	-2.22057400
H	-5.50156000	-1.34153600	0.55378600
C	4.71321100	-1.63888800	-3.35795700
C	5.88770300	-1.55616100	1.52825700

C	1.97006700	4.80831600	-1.88479300
C	1.98242900	4.21265300	3.01684400
C	0.10472800	-4.16256200	2.60785700
C	-2.74544400	-0.10961400	3.13167000
F	5.39127300	-2.48160800	2.36603300
F	7.08965000	-1.99098900	1.13323100
F	6.09051400	-0.45403900	2.26855700
F	5.91137700	-2.20781600	-3.52918900
F	4.69298700	-0.52768800	-4.11255600
F	3.79972500	-2.46797300	-3.89470500
F	1.71135200	4.21030500	-3.05298300
F	1.15097400	5.87058700	-1.79550300
F	3.21495900	5.30721500	-1.96682700
F	0.98119100	5.07452600	3.26471900
F	1.97085300	3.30609900	3.99955400
F	3.11886900	4.91742400	3.14192600
F	-3.77083300	-0.33099600	2.27472100
F	-3.14314900	-0.58219400	4.31842300
F	-2.63509100	1.21802700	3.24543100
F	-0.28815200	-4.85268700	1.52024100
F	-0.57306300	-4.66409600	3.64875000
F	1.39710600	-4.45516900	2.79690500

Energy (0K) = -4383.8572147

Energy (0K) + ZPE = -4383.144210

Enthalpy (298K) = -4383.082604

Free Energy (298K) = -4383.240150

2d

Number of imaginary frequencies: 0

S	3.80494900	3.40139300	16.83125500
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O	4.47865600	4.38717400	16.00262900
O	2.81628700	3.83095000	17.81119300
O	4.83274100	1.51793100	14.69406500
N	2.97353300	2.31317300	15.81487900
C	5.00299100	2.38111700	17.63871500
C	-0.19415600	-0.37629400	13.49112900
C	2.69076200	0.59932500	12.78725600
C	-1.06354400	1.37855700	15.13930700
C	1.31821600	0.96921400	14.90187600
C	3.64207800	1.48764200	14.91838200
C	0.06586600	0.65422900	14.52539800
C	0.14359400	-1.71307300	13.71776500
H	0.56902300	-1.99973200	14.67890800
C	2.62569200	0.53594900	14.29689600
H	2.91958000	-0.47476500	14.62248600
C	-2.37042900	0.88424700	15.09594600
H	-2.56264300	-0.07307500	14.61423800
C	-0.75786500	-0.01716300	12.26169000
H	-1.02717300	1.02350100	12.08341700
C	-0.81623000	2.61609900	15.77053000
C	-1.87457900	3.32121300	16.33214700
H	-1.67524100	4.27662200	16.81637100
C	-3.17347500	2.81906400	16.28434700
H	-3.98920100	3.38044600	16.73439700
C	3.01968900	-0.46615800	10.64284600
H	3.24157700	-1.36053200	10.06443300
C	2.98887200	-0.53343400	12.03360200
H	3.18088300	-1.47839300	12.54112300
C	-3.41961600	1.59663100	15.66740200
H	-4.42965000	1.19470400	15.63078300

C	1.54642600	1.99376500	15.99029700
H	1.39332800	1.55026900	16.98892000
C	2.48483700	1.88066100	10.74642600
H	2.29259400	2.82820400	10.24758600
C	-0.59353500	-2.29934500	11.49759700
H	-0.74359400	-3.04531500	10.72014600
C	2.44264000	1.80896100	12.13350800
H	2.20751200	2.69802900	12.72118100
C	-0.94331600	-0.96989500	11.26708500
H	-1.36413600	-0.67486700	10.30820700
C	-0.05853900	-2.67097800	12.72723800
H	0.20523300	-3.70928200	12.91717300
C	2.76992200	0.74048100	9.99678600
H	2.79553500	0.79443500	8.91071000
C	0.58889800	3.15440800	15.79680100
H	0.82513400	3.64313100	14.83601500
H	0.70127600	3.90267300	16.58723900
H	5.52983800	3.02674300	18.34800000
H	4.47709300	1.58268700	18.16905600
H	5.69366700	1.98267100	16.89311900

Energy (0K) = -1643.0187482

Energy (0K) + ZPE = -1642.616035

Enthalpy (298K) = -1642.590597

Free Energy (298K) = -1642.670855

2d1

Number of imaginary frequencies: 0

C	-0.23859500	-0.10758000	1.00160400
C	1.06321100	0.67590600	1.09985300
N	0.81494700	1.98795800	0.69311400

S	1.95608600	3.22048500	0.98435600
O	1.26596700	4.46242400	0.66425400
O	3.19001800	2.87671100	0.30054200
C	-0.60887100	2.27803300	0.43833100
C	-1.20830800	0.89251500	0.44246500
C	-2.42762300	0.67327500	-0.07295300
C	-3.03412900	-0.68230200	-0.02552700
C	-2.78449300	-1.60516300	-1.04464300
C	-3.83041700	-1.06239400	1.05905600
C	-3.30992500	-2.89223800	-0.97243700
H	-2.16519400	-1.31026000	-1.89108500
C	-4.35926700	-2.34767200	1.12835000
H	-4.01720400	-0.34555700	1.85849800
C	-4.09634300	-3.26548300	0.11452200
H	-3.10371200	-3.60616700	-1.76692500
H	-4.96977500	-2.63489000	1.98177400
H	-4.50460500	-4.27217400	0.17145600
C	-0.92153800	2.96356500	-0.87665400
H	-0.41332700	2.41173800	-1.68489900
H	-0.54727400	3.99164700	-0.88994300
C	-2.41293900	2.93644700	-1.09290400
C	-3.14697500	1.79609600	-0.70099600
C	-3.07325300	3.99436500	-1.70712000
C	-4.52200100	1.75020600	-0.94608500
C	-4.44655900	3.94323700	-1.93860200
H	-2.50015600	4.87093800	-2.00725400
C	-5.17062200	2.81854200	-1.55696100
H	-5.08788100	0.86822400	-0.65028700
H	-4.94761500	4.78185700	-2.41699700
H	-6.24251900	2.77046800	-1.73513200

C	-0.61886000	-0.68541400	2.34799300
C	-0.87316800	0.16468500	3.42757400
C	-0.75352200	-2.06189400	2.51791500
C	-1.26808100	-0.35462400	4.65481100
H	-0.76836000	1.24383800	3.30345500
C	-1.15027700	-2.58326200	3.74688300
H	-0.56153800	-2.72686200	1.67635300
C	-1.41140900	-1.73172600	4.81581000
H	-1.46737600	0.31612400	5.48762600
H	-1.25927000	-3.65901500	3.86628000
H	-1.72668100	-2.13843000	5.77406400
O	2.12798100	0.26254000	1.50228800
C	2.19343800	3.14298000	2.73619800
H	1.23313900	3.33580000	3.22340700
H	2.91085100	3.92798600	2.99240300
H	2.59157900	2.16193000	3.00332000
H	-1.01221600	2.87910900	1.27336800
H	-0.07532400	-0.93777300	0.29907800

Energy (0K) = -1643.0168374

Energy (0K) + ZPE = -1642.614004

Enthalpy (298K) = -1642.588570

Free Energy (298K) = -1642.668509

H₂

Number of imaginary frequencies: 0

H	1.00550300	1.85167000	0.92207300
H	1.74698200	1.85167000	0.92207300

Energy (0K) = -1.1687374

Energy (0K) + ZPE = -1.158672

Enthalpy (298K) = -1.155368

Free Energy (298K) = -1.170156

2da

Number of imaginary frequencies: 0

C	-0.62430700	0.34802600	1.30670400
C	0.69940500	1.07985400	1.49893600
N	0.46094500	2.43165300	1.26853500
S	1.72015000	3.54527900	1.00042300
O	1.05338200	4.83298300	0.85364000
O	2.57547200	3.05844700	-0.07299600
C	-0.89191300	2.66943100	0.73023600
C	-1.65833100	1.48841500	1.34281300
C	-3.05983500	1.25833200	0.71460000
C	-3.43251000	-0.21163400	0.67640000
C	-3.12868400	-1.01629100	-0.42457700
C	-4.06268900	-0.79379200	1.77784400
C	-3.43882500	-2.37313600	-0.41959500
H	-2.64922400	-0.57251000	-1.29758600
C	-4.36731200	-2.15143400	1.78994300
H	-4.30385200	-0.17264900	2.64130800
C	-4.05576700	-2.94604900	0.68975200
H	-3.19702800	-2.98469400	-1.28660600
H	-4.85272800	-2.58948700	2.65982300
H	-4.29836200	-4.00649500	0.69428900
C	-0.89381100	2.64101300	-0.79197300
H	-0.32781300	1.75999500	-1.13562200
H	-0.36166600	3.51778500	-1.18254200
C	-2.29270400	2.60506400	-1.32894400
C	-3.29784900	1.94297100	-0.61929800
C	-2.60059800	3.23251000	-2.54107500

C	-4.59689500	1.92899500	-1.14189300
C	-3.88756100	3.19999600	-3.05708100
H	-1.80664900	3.75195600	-3.07701200
C	-4.89479200	2.54533500	-2.34846500
H	-5.38363900	1.41957000	-0.58476700
H	-4.10979600	3.69131100	-4.00189900
H	-5.91141000	2.52105600	-2.73488200
C	-0.77413200	-0.77421200	2.30012900
C	-0.96949500	-0.51190200	3.65920200
C	-0.66991800	-2.10026800	1.88077700
C	-1.09451600	-1.55504200	4.57039300
H	-1.02440300	0.51869600	4.01059700
C	-0.78956000	-3.14631400	2.79095000
H	-0.50574300	-2.31416200	0.82513400
C	-1.01052700	-2.87678200	4.13782400
H	-1.25368400	-1.33526400	5.62406000
H	-0.71540500	-4.17478500	2.44368400
H	-1.11168700	-3.69200900	4.85092400
O	1.76986200	0.59977200	1.80490500
C	2.60097800	3.49285600	2.52978200
H	1.92376100	3.78874800	3.33451700
H	3.42656600	4.20522100	2.43982600
H	2.97686600	2.47770700	2.67453900
H	-1.27119100	3.63024300	1.09545200
H	-0.57407100	-0.07972300	0.29143600
H	-1.81478000	1.72834700	2.40367000
H	-3.77061800	1.72797900	1.41129900

Energy (0K) = -1644.2345646

Energy (0K) + ZPE = -1643.807204

Enthalpy (298K) = -1643.781881

Free Energy (298K) = -1643.860831

2da1

Number of imaginary frequencies: 0

S	3.84582700	3.05368700	17.09701500
O	4.09786200	4.22458300	16.26876900
O	3.03529500	3.19215000	18.30061000
O	4.68474900	1.60872900	14.55660900
N	3.05193100	1.86115600	16.17589600
C	5.37531200	2.26209100	17.48912300
C	-0.16035100	-0.84154900	13.89206200
C	2.25969500	0.88064300	12.89325000
C	-0.98466700	1.33687000	14.99966200
C	1.40399800	0.41719700	15.41404100
C	3.57008900	1.38001300	14.97693300
C	-0.07332400	0.12531000	15.06317900
C	0.30634000	-2.14660800	14.08096000
H	0.65514800	-2.45047700	15.06886800
C	2.51595800	0.48648300	14.33093400
H	2.98829900	-0.50395600	14.28188700
C	-2.33079900	1.14807300	14.65468900
H	-2.66923200	0.15071100	14.37778600
C	-0.62257600	-0.48274200	12.62462200
H	-0.99336600	0.52508100	12.45070100
C	-0.57568300	2.61196700	15.40896800
C	-1.49930500	3.66438100	15.41487000
H	-1.16118100	4.64933900	15.73663400
C	-2.81808500	3.47144400	15.03461600
H	-3.51847500	4.30361200	15.04565900
C	2.52388800	0.32753300	10.54366200

H	2.88069600	-0.35987600	9.77954500
C	2.71928900	0.02628000	11.88713200
H	3.21840600	-0.90247500	12.16342200
C	-3.23879900	2.19637300	14.66029900
H	-4.27510700	2.01759300	14.38181500
C	1.59527900	1.65884300	16.29637700
H	1.34591700	1.42209400	17.33708500
C	1.42137500	2.36911300	11.17302700
H	0.91151900	3.29137800	10.90265300
C	-0.11436800	-2.68308300	11.76813900
H	-0.09354200	-3.39319800	10.94429000
C	1.61827000	2.06317200	12.51608800
H	1.24243100	2.74628100	13.27322900
C	-0.60083400	-1.39420000	11.57260600
H	-0.95752700	-1.08663000	10.59139100
C	0.33676100	-3.05878600	13.03099600
H	0.70848100	-4.06718600	13.20139200
C	1.86917900	1.50104500	10.18127100
H	1.71044000	1.73969200	9.13190100
C	0.83322900	2.89759800	15.84640800
H	1.39511400	3.38325500	15.03389000
H	0.82029600	3.63124600	16.66316800
H	5.94924200	2.97127200	18.09290100
H	5.16245700	1.35502300	18.05990200
H	5.89545300	2.03692700	16.55523200
H	1.72638900	-0.42335900	16.04244500
H	-0.44269800	-0.44412300	15.93303400

Energy (0K) = -1644.2230972

Energy (0K) + ZPE = -1643.795428

Enthalpy (298K) = -1643.770154

Free Energy (298K) = -1643.849575

5l

Number of imaginary frequencies: 0

Br	11.81446300	9.71040400	-2.36002900
S	1.85026900	8.44976700	3.23663600
O	6.21248500	6.81649100	-3.03111000
N	5.36228100	7.66193700	-1.04878000
O	1.45113300	9.05451500	1.97910300
O	5.13901300	9.99064300	-0.17542500
S	5.49575400	9.31619800	-1.41723800
N	2.34554900	6.84979600	2.85588600
O	0.90853700	8.32326200	4.33344000
C	5.94617900	6.68334100	-1.86029100
C	3.81602000	5.35081900	2.00758900
C	5.00255900	7.18408300	0.29409800
H	5.61496300	7.69493900	1.06031200
C	3.23424100	6.57246300	1.80996100
C	5.35690100	5.71220600	0.20493400
C	3.32767100	4.83426400	3.26369500
C	6.28692200	5.50949700	-0.94819200
H	6.14119900	4.55789600	-1.47492400
C	4.77149200	4.81636800	1.02786500
C	7.77190300	5.70691100	-0.62353700
C	4.99911300	3.35889800	0.92860300
C	2.43014900	5.78966500	3.78715500
C	3.58341800	3.67249000	4.00388500
H	4.27420200	2.92142200	3.62762700
C	3.90442600	2.48290100	0.95033900
H	2.89938400	2.88720900	1.05932200

C	3.52724700	7.39509300	0.60298500
H	3.30737300	8.45672200	0.72513500
H	2.92532500	7.03849300	-0.24913700
C	7.23881900	9.48181400	-1.68781100
C	8.69908700	5.70080900	-1.67098800
H	8.34795400	5.54156500	-2.68869900
C	2.94864800	3.49627700	5.22001600
H	3.14471800	2.59628400	5.80222100
C	8.22210600	5.93942900	0.67748300
H	7.51184000	5.94043800	1.50346200
C	1.78041700	5.60530800	5.00750800
H	1.08066400	6.34124900	5.39023400
C	3.34109400	9.20845200	3.80585700
C	2.04684200	4.44791900	5.73195300
C	6.28358500	2.82299100	0.78522400
H	7.14597900	3.48730400	0.78814300
C	7.72133200	9.61913500	-2.98356000
H	7.03193900	9.65414900	-3.82216300
C	8.08845600	9.40923400	-0.58531700
H	7.68903700	9.29473200	0.42090000
C	3.77638800	8.94639000	5.10528000
H	3.18509300	8.32211500	5.77169200
C	4.07926100	10.00839200	2.93706300
H	3.72903700	10.21215800	1.92778400
C	4.09157300	1.11241600	0.82178500
H	3.23015500	0.44832400	0.83188700
C	10.49142100	6.14898400	-0.11956500
H	11.54796800	6.32063800	0.07518700
C	5.74040100	10.30756000	4.68031800
C	9.94173400	9.62502500	-2.08621100

C	6.46987500	1.44983200	0.66108100
H	7.47622500	1.05047700	0.55628000
C	10.04720100	5.92284200	-1.42121700
H	10.75536800	5.92472500	-2.24729200
C	9.45889100	9.48374900	-0.78793500
H	10.14350700	9.42848500	0.05383200
C	9.57694400	6.15000600	0.92834700
H	9.91402300	6.32005700	1.94871400
C	5.37556100	0.59102800	0.67784200
H	5.52120900	-0.48254600	0.58147700
C	4.97323600	9.50109200	5.53059800
H	5.32474200	9.30860200	6.54283900
C	1.37530800	4.20360500	7.04991900
H	0.75607800	3.29793000	7.02078600
H	0.72948200	5.04081400	7.33446100
H	2.11065200	4.05746000	7.85131700
C	5.27908400	10.54794100	3.38313700
H	5.86639000	11.17133600	2.71045200
C	7.01657400	10.91745000	5.16700600
H	6.81305100	11.82259400	5.75376800
H	7.66776000	11.20616600	4.33573800
H	7.56689800	10.23011900	5.81886600
O	4.78361500	9.60496500	-2.64671000
C	9.09412300	9.69749100	-3.18526400
H	9.49666500	9.80705800	-4.18796600

Energy (0K) = -5394.6776428

Energy (0K) + ZPE = -5394.056408

Enthalpy (298K) = -5394.012992

Free Energy (298K) = -5394.132974

511

Number of imaginary frequencies: 0

Br	11.55163700	12.68852300	-0.12041000
S	1.97315500	8.39937700	2.56990300
O	8.11287100	7.55220600	-2.29372800
N	6.34433400	8.05564500	-0.88886700
O	1.52339000	8.69534900	1.22148100
O	5.04594900	10.19338200	-0.66917400
S	6.09811000	9.62849600	-1.50156700
N	2.79671100	6.89450600	2.48503200
O	1.02202200	8.27651800	3.65997400
C	7.40917400	7.27440400	-1.35162500
C	4.71626600	5.74222700	2.14987700
C	5.76792800	7.59295100	0.38288800
H	6.07168700	8.27216700	1.20396100
C	3.92451900	6.74446700	1.66469300
C	6.42783500	6.23737600	0.55170700
C	4.09456900	5.22691000	3.34384600
C	7.53679000	6.05620300	-0.44501800
C	5.93300500	5.35531000	1.43979300
C	7.48179200	4.77139100	-1.24148600
C	6.54748200	4.02998300	1.68725700
C	2.91460000	5.97141100	3.55233400
C	4.42586200	4.20976800	4.24835300
H	5.32693300	3.61596600	4.10510000
C	5.86829700	2.85841600	1.33785100
H	4.88854400	2.93049400	0.86675300
C	4.24938300	7.47369000	0.40258000
H	3.78024100	8.45581300	0.32880400
H	3.90846500	6.88579000	-0.46687200

C	7.61151500	10.47214800	-1.12706000
C	6.35227800	4.48214600	-2.01054900
H	5.52659300	5.19439100	-2.04234900
C	3.58674800	3.97058200	5.32166300
H	3.83257800	3.18094900	6.03112300
C	8.53312800	3.85860000	-1.20481700
H	9.41364300	4.08172100	-0.60308800
C	2.06369000	5.72166200	4.62812100
H	1.15134000	6.29066600	4.76899500
C	3.27024600	9.52165000	3.00781500
C	2.40803500	4.71385400	5.52384400
C	7.80628100	3.93590900	2.28543000
H	8.33414300	4.84755200	2.56322100
C	8.60221900	10.56061600	-2.09961400
H	8.44824800	10.11294400	-3.07673300
C	7.76738500	11.03162200	0.13962700
H	6.96918300	10.96318700	0.87755800
C	3.91976600	9.36120300	4.23411100
H	3.61005900	8.58469000	4.93125500
C	3.64506700	10.51339000	2.10937800
H	3.13875100	10.61905900	1.15362600
C	6.44298700	1.61607500	1.57856400
H	5.91098300	0.71106000	1.29368300
C	7.32386000	2.37935400	-2.67658600
H	7.26131000	1.44638000	-3.23235100
C	5.37704200	11.21442100	3.65802200
C	9.94037800	11.78165400	-0.53170000
C	8.37601600	2.69073500	2.53704100
H	9.35333900	2.62779600	3.01077800
C	6.27258200	3.29329500	-2.72475500

H	5.38836800	3.07734700	-3.32040900
C	8.94940000	11.69363300	0.44200000
H	9.09627800	12.14122300	1.42114400
C	8.45488200	2.66596700	-1.91924100
H	9.27976300	1.95786800	-1.87955700
C	7.69519000	1.52933100	2.18449200
H	8.14030500	0.55582800	2.37804000
C	4.97103000	10.20694600	4.54555500
H	5.49173500	10.09048800	5.49464000
C	1.52950200	4.40674200	6.69921500
H	1.21022600	3.35696000	6.69479800
H	0.63022900	5.03143500	6.70502800
H	2.05815900	4.57178100	7.64690400
C	4.69495400	11.36020500	2.44951200
H	4.99118900	12.14729400	1.75766800
C	6.53237200	12.09987800	4.00391000
H	6.39323500	12.57062000	4.98441100
H	6.66831300	12.89357900	3.26176200
H	7.46416700	11.52219300	4.06175300
O	5.94408400	9.53180500	-2.93921100
C	9.78252500	11.22743400	-1.79714700
H	10.56960600	11.31525500	-2.54051600
H	8.53199100	6.14112000	0.02108100

Energy (0K) = -5394.6766207

Energy (0K) + ZPE = -5394.054865

Enthalpy (298K) = -5394.011731

Free Energy (298K) = -5394.130790

B(C₆F₅)₃ as catalyst

BAr₃(Ar=C₆F₅)

Number of imaginary frequencies: 0

B	-2.31988300	4.60941300	0.60188100
C	-2.53062600	4.37561600	2.13448200
C	-2.19858900	5.33686700	3.09239800
C	-3.07369900	3.18820500	2.63151700
C	-2.39605300	5.14557400	4.45049900
C	-3.26668200	2.95503100	3.98381500
C	-2.92921700	3.94446800	4.89664300
C	-1.06024300	5.37827500	0.08334700
C	-1.11509300	6.23672900	-1.01786100
C	0.19567500	5.23527400	0.67820200
C	-0.00733200	6.91546600	-1.49910300
C	1.32794400	5.88371300	0.21211800
C	1.22173500	6.73198900	-0.88130300
C	-3.37290900	4.06737300	-0.42177700
C	-3.00113900	3.51375900	-1.64872300
C	-4.74567200	4.11588100	-0.16937100
C	-3.92025300	3.03529000	-2.56836500
C	-5.69339100	3.66787500	-1.07539600
C	-5.27495500	3.12073400	-2.27984800
F	-0.10692100	7.73239100	-2.53961200
F	-2.27075200	6.45059500	-1.64418700
F	2.29034000	7.36354700	-1.33361700
F	2.50616000	5.70387200	0.79414200
F	0.35496300	4.42422100	1.72234700
F	-1.71332000	3.40354700	-1.97136100
F	-3.52265700	2.50071500	-3.71563700
F	-6.16547200	2.67864300	-3.14994200
F	-6.98964700	3.75131500	-0.80539500
F	-5.19980300	4.63086600	0.97190000

F	-1.69557600	6.51145100	2.71781400
F	-2.08121300	6.09137700	5.32589100
F	-3.11776500	3.74560500	6.18895100
F	-3.77036800	1.80514300	4.41252200
F	-3.41211600	2.20545000	1.79922600

Energy (0K) = -2207.3163907

Energy (0K) + ZPE = -2207.159718

Enthalpy (298K) = -2207.130306

Free Energy (298K) = -2207.219959

TS_A

Number of imaginary frequencies: 1

C	-0.07807700	-2.39455000	2.03783100
C	0.68757400	-2.85070300	2.85947100
C	1.58385500	-3.40447400	3.82207300
C	1.89151600	-4.77238800	3.77821900
C	2.16577900	-2.59418700	4.80748500
C	2.76395100	-5.31687600	4.71091700
H	1.43858200	-5.39414900	3.00863700
C	3.03748200	-3.14868000	5.73534300
H	1.92907000	-1.53209500	4.83499700
C	3.33711200	-4.50842600	5.69027000
H	2.99834500	-6.37808500	4.67380900
H	3.48576600	-2.51619700	6.49789400
H	4.02060400	-4.93830300	6.41881400
N	-1.08512500	-0.42300300	1.01516700
C	-0.83996100	0.36003600	0.01262700
C	-0.70470200	1.09175000	-0.99732000
C	0.47195200	1.64356800	-1.66775200
C	0.83398700	2.99010100	-1.57000900

C	1.24513600	0.77654700	-2.45206000
C	1.93549600	3.46363700	-2.27469500
C	2.33821800	1.26156100	-3.15843400
C	2.68268400	2.60883900	-3.07982000
S	-1.64724000	0.31305100	2.53036500
O	-2.35312100	-0.75381500	3.21516000
O	-2.31727200	1.53782600	2.14320700
C	-0.12567500	0.69768700	3.34180600
H	-0.38556700	1.18007900	4.28900900
H	0.43754100	1.38504700	2.70469600
H	0.42099300	-0.23363400	3.51438900
C	-0.34836000	-2.36717200	-0.39391800
H	0.69292200	-2.02371700	-0.44857500
H	-0.90536900	-1.88808300	-1.20616500
C	-0.42772700	-3.86254100	-0.53173700
C	-1.65191300	-4.46828100	-0.82920300
C	0.69820900	-4.66530100	-0.34467900
C	-1.74539700	-5.85125000	-0.94340000
H	-2.53588000	-3.84480400	-0.96909700
C	0.60673700	-6.05012600	-0.46006600
H	1.65380100	-4.19673600	-0.10868700
C	-0.61545200	-6.64532400	-0.75948600
H	-2.70291000	-6.31129800	-1.17795500
H	1.49328200	-6.66422200	-0.31645400
H	-0.68826900	-7.72671100	-0.85147500
C	-0.93634000	-1.92636400	0.95712500
H	-1.94922600	-2.33845300	1.06894400
B	-2.77129700	1.48206500	-1.99402300
C	-3.78791400	0.99979700	-0.85392100
C	-3.82702300	-0.31514500	-0.38801900

C	-4.72141900	1.83913800	-0.23934800
C	-4.67655800	-0.78167900	0.59973600
C	-5.59572900	1.41434900	0.75528700
C	-5.57644600	0.09779900	1.18128200
C	-2.61478100	3.06203100	-2.18670100
C	-2.93918400	3.70446900	-3.38129100
C	-2.21643300	3.91676000	-1.16135500
C	-2.84278900	5.07732500	-3.56393900
C	-2.08599000	5.28884900	-1.30829000
C	-2.40594300	5.87716900	-2.52096900
C	-2.54685000	0.57194600	-3.29464500
C	-1.54068600	0.86330700	-4.22636500
C	-3.33708400	-0.52686500	-3.64621600
C	-1.24768200	0.07147600	-5.32467500
C	-3.08388500	-1.33809700	-4.74595200
C	-2.02214900	-1.04813200	-5.58412500
F	-3.86768400	-2.37844700	-5.01038900
F	-1.76634000	-1.81050200	-6.63578100
F	-4.43224600	-0.84824500	-2.95610900
F	-0.25550800	0.39387700	-6.14767000
F	-0.81762700	1.97851500	-4.11632900
F	-4.85687700	3.11712000	-0.59755100
F	-6.46368800	2.26392200	1.29317600
F	-6.40812600	-0.31637300	2.12301300
F	-4.63421400	-2.05369500	0.98539800
F	-2.99894900	-1.22719000	-0.91303600
H	0.27092200	3.66099200	-0.92689900
H	2.20992100	4.51296300	-2.19149600
H	3.53633500	2.98860800	-3.63620300
H	2.92543700	0.58224900	-3.77251700

H	0.96315000	-0.27306500	-2.52159100
F	-3.16999900	5.63075400	-4.72738200
F	-3.38497700	3.01104900	-4.43237500
F	-2.29613600	7.18765900	-2.68070000
F	-1.64438500	6.03681100	-0.30144200
F	-1.90727200	3.42244600	0.03986700

Energy (0K) = -3774.9846902

Energy (0K) + ZPE = -3774.432926

Enthalpy (298K) = -3774.377349

Free Energy (298K) = -3774.523443

A

Number of imaginary frequencies: 0

C	1.68386000	-2.70279000	2.70006600
C	2.45463000	-3.07192500	3.55899200
C	3.31846800	-3.45196200	4.62806900
C	4.36407700	-4.36337200	4.42459900
C	3.11348700	-2.89926500	5.90149500
C	5.18887200	-4.71516000	5.48487800
H	4.51446800	-4.79170500	3.43587800
C	3.94806600	-3.25226400	6.95297400
H	2.29286500	-2.19867700	6.04781600
C	4.98474100	-4.16028700	6.74647100
H	5.99606800	-5.42634900	5.32684400
H	3.78803600	-2.82123000	7.93840200
H	5.63450900	-4.43829000	7.57303100
N	0.65758400	-0.76285200	1.67156600
C	0.66205100	-0.02121300	0.64431100
C	0.63718800	0.74962400	-0.38671000
C	2.00177200	1.12105800	-0.88964100

C	2.60199800	2.34277400	-0.57944800
C	2.67076400	0.20581700	-1.70853500
C	3.84490100	2.65715900	-1.12001400
C	3.90786800	0.53323100	-2.25170700
C	4.49548000	1.76172000	-1.96361100
S	0.25900300	0.03077000	3.26863900
O	-0.28798200	-1.04496900	4.06889800
O	-0.53245800	1.18637100	2.90934300
C	1.86953700	0.52070100	3.80141800
H	1.74798300	1.00315100	4.77657100
H	2.26248100	1.23219000	3.06855900
H	2.49947000	-0.36984800	3.87870100
C	1.26323200	-2.75356000	0.27386700
H	2.27814500	-2.36640000	0.11422300
H	0.61210700	-2.33611700	-0.50158600
C	1.24285500	-4.25508300	0.20619700
C	0.02197200	-4.92905500	0.11775600
C	2.42606100	-4.99218400	0.24983600
C	-0.01279300	-6.31819600	0.06964300
H	-0.90286100	-4.35087700	0.08244200
C	2.39337400	-6.38283400	0.19648900
H	3.37866200	-4.46736400	0.31972100
C	1.17370200	-7.04784600	0.10766800
H	-0.96808000	-6.83344300	-0.00294600
H	3.32252800	-6.94803400	0.22372500
H	1.14635800	-8.13435300	0.06569400
C	0.77582800	-2.27974000	1.64710700
H	-0.24121600	-2.65136700	1.84043500
B	-0.86480300	1.22086200	-1.12332500
C	-2.08040700	0.77969500	-0.09346200

C	-2.21827600	-0.52655600	0.37823700
C	-3.00361900	1.65914100	0.47429700
C	-3.11634900	-0.94201600	1.34719900
C	-3.93429100	1.28966200	1.44263400
C	-3.98998500	-0.01589000	1.89371100
C	-0.77924400	2.85238400	-1.27751500
C	-1.19987300	3.56511800	-2.39772400
C	-0.34631200	3.65823200	-0.22891600
C	-1.15128700	4.95081000	-2.49342600
C	-0.27125800	5.04146600	-0.27996300
C	-0.68044900	5.69850200	-1.42794900
C	-0.86283900	0.45659800	-2.58131700
C	0.07667000	0.79672900	-3.56027700
C	-1.74674400	-0.54320400	-2.98595300
C	0.19881400	0.16007600	-4.78549100
C	-1.66018100	-1.21021300	-4.20462700
C	-0.67341800	-0.86656800	-5.10958700
F	-2.53359300	-2.16693300	-4.51027700
F	-0.57755000	-1.48975000	-6.27717000
F	-2.78486300	-0.91366200	-2.22869200
F	1.12837800	0.53856500	-5.65927500
F	0.90208500	1.83401400	-3.37290200
F	-3.07231500	2.94532900	0.11395700
F	-4.77768600	2.19005700	1.93827400
F	-4.87185000	-0.37764100	2.81507600
F	-3.14543800	-2.21224400	1.74491500
F	-1.43736600	-1.50570800	-0.11846900
H	2.11027600	3.04073700	0.09195000
H	4.30596700	3.61171000	-0.87678300
H	5.46285700	2.01742700	-2.38934300

H	4.41403600	-0.17765900	-2.90065000
H	2.20029400	-0.74721400	-1.94595200
F	-1.56458100	5.56799000	-3.59780900
F	-1.70392700	2.94172700	-3.46925200
F	-0.62706500	7.02215100	-1.50439600
F	0.17856100	5.73759700	0.76176500
F	0.02010800	3.10120100	0.93630600

Energy (0K) = -3774.9940666

Energy (0K) + ZPE = -3774.441621

Enthalpy (298K) = -3774.385754

Free Energy (298K) = -3774.532984

TS_B

Number of imaginary frequencies: 1

C	0.11626500	1.23950500	1.53152900
C	0.81258600	0.79908300	2.42061500
C	1.63761600	0.36012600	3.49832500
C	1.29752600	-0.77473500	4.24869800
C	2.79458900	1.08518700	3.82334700
C	2.10458500	-1.17409300	5.30560800
H	0.39982600	-1.33296500	3.99280500
C	3.59167100	0.68103000	4.88598000
H	3.05569500	1.96035500	3.23014500
C	3.24887300	-0.44749300	5.62778800
H	1.83737900	-2.05541400	5.88400300
H	4.48565300	1.24739800	5.13654400
H	3.87523600	-0.76155100	6.45958000
N	-0.87991300	3.20899500	0.46520400
C	-0.36838700	4.03246300	-0.43016300
C	-0.52156600	4.70114000	-1.55377800

C	0.70548000	5.12054700	-2.29252800
C	1.19692300	6.42790600	-2.34246600
C	1.35860400	4.12652200	-3.03006000
C	2.30771900	6.73035900	-3.12319200
C	2.45332500	4.43757200	-3.82924300
C	2.93151800	5.74291700	-3.88063500
S	-1.43250400	3.89417000	1.98044900
O	-2.43434800	2.95922700	2.46553800
O	-1.76691300	5.27121900	1.65249300
C	-0.04961200	3.94029900	3.10421600
H	-0.27435400	4.75977200	3.79364400
H	0.86133200	4.14510800	2.53650500
H	0.01958500	2.99008200	3.63392400
C	0.03282700	1.30089000	-0.90534600
H	1.05932300	1.69065100	-0.88114700
H	-0.48331100	1.75795300	-1.75510900
C	0.04250200	-0.19542600	-1.05729400
C	-1.14022300	-0.88361400	-1.34480500
C	1.22684400	-0.91868500	-0.91139600
C	-1.13398900	-2.26643100	-1.49100100
H	-2.07139200	-0.32673900	-1.45436300
C	1.23604200	-2.30262600	-1.06120900
H	2.14845000	-0.38443400	-0.67859700
C	0.05530800	-2.97940000	-1.35260900
H	-2.06037800	-2.78988500	-1.71801800
H	2.16805900	-2.85265000	-0.94931300
H	0.06022400	-4.06064600	-1.47160900
C	-0.67075700	1.71111700	0.39942900
H	-1.67210200	1.26150300	0.43416900
B	-2.08994600	5.03156700	-2.24930400

C	-3.27460800	4.49867600	-1.23553000
C	-3.41483600	3.14067700	-0.95890300
C	-4.17796500	5.29337300	-0.52912400
C	-4.32914900	2.58943000	-0.08067100
C	-5.12455600	4.78702900	0.35879900
C	-5.20251100	3.42711100	0.59302700
C	-2.20881700	6.66520300	-2.44039900
C	-2.93350400	7.25336500	-3.47519900
C	-1.70584200	7.58123500	-1.52328500
C	-3.08615500	8.62601600	-3.63247900
C	-1.82121800	8.95797200	-1.64130100
C	-2.51865300	9.49024600	-2.71247600
C	-2.11627300	4.30227400	-3.74638000
C	-1.24431700	4.71113200	-4.76273400
C	-3.00655700	3.31504000	-4.17807500
C	-1.11998700	4.09342200	-5.99896800
C	-2.92737000	2.67133800	-5.40969400
C	-1.96277800	3.04609200	-6.32601500
C	1.67066100	6.27499200	0.77623900
C	2.47138800	7.39216300	0.85976700
C	3.80111600	7.31529300	0.45759700
C	4.29715600	6.10897000	-0.01640000
C	3.46217600	5.00801200	-0.08923600
N	2.16331800	5.10350800	0.30042700
H	4.45023200	8.18349900	0.51459900
H	0.61955200	6.25355600	1.05199600
H	2.04237500	8.31337400	1.23968700
H	5.33119300	6.00455800	-0.32844400
O	1.39711200	4.03213700	0.26338200
Br	4.07131300	3.34030400	-0.65419500

F	-1.87229800	2.44371800	-7.50588500
F	-3.79946200	1.71427200	-5.72316900
F	-4.06414500	2.94143400	-3.44742000
F	-0.22283800	4.52583000	-6.88324800
F	-0.49215900	5.80862400	-4.61784500
F	-2.60946200	2.25675500	-1.57169800
F	-4.34850300	1.27576300	0.14435100
F	-6.08792300	2.93509300	1.44984000
F	-5.95563600	5.61136600	0.99456300
F	-4.21185100	6.62565200	-0.65558400
F	-3.56268700	6.50659900	-4.39237100
F	-3.78125100	9.11827700	-4.65567500
F	-2.64865200	10.80472500	-2.84880700
F	-1.28016100	9.76812200	-0.73234700
F	-1.07382400	7.15194500	-0.41811300
H	2.93947600	3.65176700	-4.40358500
H	0.98716100	3.10362600	-2.98980200
H	3.79026900	5.98919800	-4.50111900
H	2.68219200	7.75205700	-3.14213500
H	0.72716400	7.21434100	-1.76098000

Energy (0K) = -6668.8850981

Energy (0K) + ZPE = -6668.247945

Enthalpy (298K) = -6668.185312

Free Energy (298K) = -6668.347134

B

Number of imaginary frequencies: 0

C	0.85611700	-2.48794800	2.97617900
C	1.44921400	-2.90664100	3.94722700
C	2.14111600	-3.39673400	5.09503600

C	2.16807800	-4.77454400	5.35801700
C	2.80319900	-2.51421800	5.96136100
C	2.84453000	-5.25568000	6.47116800
H	1.65558500	-5.45366700	4.67947400
C	3.47542100	-3.00551400	7.07288500
H	2.78519000	-1.44610500	5.75189600
C	3.49752700	-4.37439400	7.33048900
H	2.86142000	-6.32463000	6.67039000
H	3.98525900	-2.31660500	7.74233900
H	4.02478100	-4.75512200	8.20214000
N	0.05624700	-0.62159800	1.57165800
C	0.76674000	0.03509700	0.56284700
C	0.35220600	0.58194400	-0.59688900
C	1.44154900	0.78442600	-1.60567900
C	2.25854300	1.91232000	-1.72260000
C	1.62070900	-0.26682500	-2.51533800
C	3.22197100	1.98697600	-2.72453400
C	2.57781700	-0.18738300	-3.52121100
C	3.38382800	0.94237700	-3.62923300
S	-0.59646400	0.26018200	2.85628300
O	-1.74733700	-0.49015600	3.33764400
O	-0.73513300	1.62182900	2.34754600
C	0.59382600	0.34337900	4.18761000
H	0.32022900	1.22783300	4.77121400
H	1.60502200	0.45114200	3.78432000
H	0.51831400	-0.55939900	4.79410300
C	0.97440700	-2.75499200	0.55967300
H	2.03084700	-2.47435300	0.64372600
H	0.59565900	-2.34872500	-0.38098100
C	0.84183400	-4.25357600	0.56908200

C	-0.25339100	-4.86769100	-0.04342200
C	1.80277400	-5.05633500	1.18929600
C	-0.39103000	-6.25209200	-0.02694100
H	-0.99746100	-4.25102700	-0.54320500
C	1.66762500	-6.44153200	1.20702200
H	2.66806100	-4.58723000	1.65757000
C	0.56767500	-7.04307400	0.60089900
H	-1.24831300	-6.71510500	-0.51127300
H	2.42709800	-7.05252300	1.69086700
H	0.46131900	-8.12564300	0.61194400
C	0.19395000	-2.11015000	1.73034900
H	-0.82777800	-2.52074800	1.73470000
B	-1.23861900	0.95855600	-1.03607000
C	-2.32295400	0.06045200	-0.16745300
C	-2.33311800	-1.32851100	-0.27325300
C	-3.29473600	0.54936900	0.70562200
C	-3.22760600	-2.16859000	0.36816300
C	-4.21597900	-0.25413700	1.37247300
C	-4.18468600	-1.62378600	1.20911000
C	-1.57480100	2.56936500	-0.84013500
C	-2.76430700	3.06555400	-1.37554600
C	-0.79078200	3.53903800	-0.23801300
C	-3.14651100	4.39687700	-1.33030000
C	-1.12678900	4.88695000	-0.16707600
C	-2.31472700	5.32406000	-0.72109900
C	-1.39956300	0.74820000	-2.69815100
C	-0.72440600	1.60254700	-3.57750100
C	-2.20739300	-0.17362000	-3.36693700
C	-0.72333400	1.47995700	-4.96009400
C	-2.24549300	-0.32972200	-4.74942100

C	-1.48514800	0.49310000	-5.55906200
C	2.48312500	2.04957700	1.62022400
C	3.31223800	3.13142900	1.82125500
C	4.64049100	3.06159900	1.41687700
C	5.11660100	1.89817100	0.82711400
C	4.26063400	0.83086100	0.63140300
N	2.96596800	0.94284400	1.01807800
H	5.30901400	3.90432600	1.56241400
H	1.42507200	2.05047400	1.87515500
H	2.90071800	4.01795900	2.29147100
H	6.15013100	1.80612200	0.51015600
O	2.19061400	-0.16417000	0.81196900
Br	4.84103100	-0.76386500	-0.12858000
F	-1.50523600	0.35854500	-6.88056200
F	-3.03095300	-1.25496700	-5.29967300
F	-3.05900400	-0.97532400	-2.71399000
F	-0.01056100	2.31525200	-5.71458000
F	-0.01408000	2.64368100	-3.12027700
F	-1.42866400	-1.93917600	-1.06216700
F	-3.17429700	-3.49196300	0.20338600
F	-5.04650000	-2.40791000	1.84741300
F	-5.11244400	0.29024500	2.19361800
F	-3.41647700	1.85231100	0.98570300
F	-3.64437600	2.22844100	-1.94659700
F	-4.30277500	4.79644000	-1.85721100
F	-2.65636500	6.60756800	-0.66938500
F	-0.30941300	5.75902700	0.42315000
F	0.39863900	3.23019800	0.30858400
H	2.69256800	-1.01216300	-4.22124100
H	0.97872400	-1.14488700	-2.44313400

H	4.13170700	1.01012800	-4.41618200
H	3.84383400	2.87690800	-2.80046700
H	2.11877300	2.75724900	-1.05224600

Energy (0K) = -6668.8988171

Energy (0K) + ZPE = -6668.259840

Enthalpy (298K) = -6668.197499

Free Energy (298K) = -6668.358346

TS_c

Number of imaginary frequencies: 1

C	1.00861700	-2.43770700	2.87081200
C	1.65229800	-2.80264100	3.83155900
C	2.39844600	-3.23725000	4.96788900
C	2.47452800	-4.60588100	5.26786500
C	3.06259400	-2.31278000	5.78765200
C	3.20184500	-5.03679700	6.36927700
H	1.95817000	-5.31861500	4.62787400
C	3.78614500	-2.75394300	6.88797500
H	3.00737000	-1.25171100	5.55193500
C	3.85766700	-4.11392000	7.18127200
H	3.25628000	-6.09897400	6.59617600
H	4.29819700	-2.03236000	7.52030500
H	4.42595700	-4.45456800	8.04368800
N	0.09659700	-0.65231000	1.42171600
C	0.83635700	-0.01139600	0.39447800
C	0.32986900	0.66149500	-0.73414400
C	1.41688400	0.90174700	-1.72970900
C	2.27409000	2.00421700	-1.75662000
C	1.58295600	-0.10860100	-2.68592700
C	3.25326400	2.10675900	-2.74016400

C	2.57127400	-0.00661600	-3.65761200
C	3.40629800	1.10580600	-3.69373200
S	-0.72005200	0.21330400	2.61356800
O	-1.88682200	-0.57312800	2.98783100
O	-0.85219600	1.56791500	2.08922200
C	0.33274000	0.33275500	4.04916600
H	-0.07455500	1.16031400	4.63851900
H	1.35918200	0.55373500	3.74301300
H	0.28888300	-0.59905400	4.61346000
C	1.00106800	-2.83351000	0.47062500
H	2.06328000	-2.56493800	0.49757100
H	0.59212800	-2.46897000	-0.47410700
C	0.84420300	-4.32718100	0.55588300
C	-0.29212400	-4.94479700	0.02802800
C	1.82099300	-5.12027300	1.16278100
C	-0.45609600	-6.32347200	0.11644800
H	-1.05015300	-4.33471300	-0.46022100
C	1.66043200	-6.50023700	1.25142600
H	2.71620700	-4.64701200	1.56649200
C	0.51908600	-7.10490100	0.73129200
H	-1.34664900	-6.78911700	-0.30055400
H	2.43174400	-7.10459800	1.72478300
H	0.39269400	-8.18326900	0.79902100
C	0.28006100	-2.12507900	1.64216400
H	-0.73658100	-2.54444900	1.71357200
B	-1.24537600	1.07036600	-1.16864000
C	-2.36152900	0.18694400	-0.33144300
C	-2.33938400	-1.20336000	-0.40391200
C	-3.39626600	0.67933700	0.46392500
C	-3.25141400	-2.04570000	0.20808400

C	-4.34111600	-0.12656400	1.09220600
C	-4.27211300	-1.49963000	0.96828500
C	-1.51079700	2.69441500	-0.95631200
C	-2.65013900	3.26644000	-1.52496000
C	-0.69755200	3.60295000	-0.29947000
C	-2.95615400	4.61643500	-1.46003900
C	-0.95836800	4.96601800	-0.20905100
C	-2.09800900	5.48119200	-0.79740500
C	-1.39735800	0.87399000	-2.83613300
C	-0.73829300	1.74062400	-3.71670600
C	-2.19662900	-0.05815000	-3.50248000
C	-0.76239100	1.63514800	-5.10029800
C	-2.25579400	-0.19697900	-4.88631200
C	-1.52301800	0.64694300	-5.69860600
C	2.60913800	2.02628300	1.66024100
C	3.40907800	3.11161800	1.97829500
C	4.75423200	3.07086400	1.62170200
C	5.27233800	1.95818800	0.96868100
C	4.41708700	0.90204600	0.68438800
N	3.14661600	0.98030000	1.04860700
H	5.40408500	3.91261300	1.84277500
H	1.53377000	2.00079000	1.85051200
H	2.97262700	3.96855800	2.48067100
H	6.31434300	1.90516000	0.66861200
O	2.11865500	-0.28342300	0.41908500
Br	5.01203700	-0.62007500	-0.23633600
F	-1.56479300	0.52879900	-7.02032300
F	-3.03369700	-1.12946100	-5.43336100
F	-3.01521300	-0.89297000	-2.85019800
F	-0.07154600	2.48623200	-5.85645300

F	-0.01593700	2.77315700	-3.26145800
F	-1.39810800	-1.80966800	-1.15126900
F	-3.16229700	-3.37108800	0.08003000
F	-5.15792500	-2.28404100	1.57110700
F	-5.30221100	0.41968200	1.83581300
F	-3.55418800	1.98571800	0.70376200
F	-3.55190800	2.49560200	-2.14983100
F	-4.06699900	5.09254700	-2.01813000
F	-2.37116400	6.77930900	-0.72714500
F	-0.11736900	5.77537800	0.43325600
F	0.44390000	3.20856500	0.29133400
H	2.68266000	-0.80097700	-4.39247200
H	0.91926800	-0.97311500	-2.67192000
H	4.17181000	1.19234500	-4.46142700
H	3.90094800	2.98106600	-2.75601900
H	2.16158900	2.80097800	-1.02745900

Energy (0K) = -6668.8789542

Energy (0K) + ZPE = -6668.242324

Enthalpy (298K) = -6668.179864

Free Energy (298K) = -6668.340251

C

Number of imaginary frequencies: 0

C	-0.42427000	-0.11774600	1.44066700
C	0.12430400	-1.42832000	1.94271800
N	1.31868700	-2.02246500	1.63122100
B	-1.17990000	0.02210300	-0.07205900
S	1.51040200	-3.67636400	2.20693900
O	2.86594600	-4.03847400	1.81960800
O	0.38849500	-4.45055500	1.71656700

C	2.55647000	-1.39078000	1.09372600
C	2.56087700	0.05392200	1.26340800
C	2.71406600	1.25548000	1.33448500
C	2.85154800	2.67413900	1.29419300
C	3.71432500	3.25076700	0.34887700
C	2.10116300	3.50144000	2.14268200
C	3.80985900	4.63219400	0.25020800
H	4.29703100	2.60298400	-0.30399000
C	2.20106500	4.88183800	2.03261400
H	1.45034900	3.05201500	2.88789500
C	3.05102200	5.44953900	1.08596900
H	4.47713200	5.07373700	-0.48620200
H	1.61179400	5.51777100	2.68940000
H	3.12511400	6.53111000	1.00049800
C	2.83918300	-1.83118300	-0.35739600
H	2.07501500	-1.41371800	-1.01848700
H	2.73744400	-2.92238300	-0.38427500
C	4.22802400	-1.44074300	-0.78367300
C	5.31132100	-2.24112100	-0.40836100
C	4.47716500	-0.27779700	-1.51807800
C	6.61236600	-1.88986900	-0.75352100
H	5.12576300	-3.15548700	0.15559800
C	5.77873200	0.07362800	-1.86746500
H	3.64788000	0.35963000	-1.82029300
C	6.84982300	-0.72904000	-1.48493900
H	7.44230800	-2.52729700	-0.45577300
H	5.95499800	0.97963200	-2.44420600
H	7.86588300	-0.45379600	-1.75928100
C	-0.47991300	0.85263200	2.48427300
C	0.30088100	0.69663100	3.66665000

C	-1.37745600	1.95004300	2.43306100
C	0.19952100	1.58793100	4.71289400
H	1.00131700	-0.13001500	3.75591300
C	-1.48554600	2.83235500	3.48947000
H	-2.04255600	2.07258000	1.58856700
C	-0.69642000	2.65769400	4.62724200
H	0.80784800	1.45461400	5.60242400
H	-2.19629600	3.65192300	3.43812300
H	-0.78451800	3.35443500	5.45736000
O	-0.69361200	-1.95333800	2.68417100
C	1.47881900	-3.51539400	3.96932200
C	-0.70695700	1.51078800	-0.64527300
C	0.57574300	1.69963100	-1.15081400
C	-1.49116100	2.66327700	-0.70362700
C	1.05898900	2.88742000	-1.67728000
C	-1.04088300	3.88922300	-1.17994200
C	0.24669700	4.00791400	-1.67435700
C	-2.82554600	-0.08101300	0.03691700
C	-3.55140700	0.05336000	-1.14808900
C	-3.60252800	-0.36303100	1.15418100
C	-4.92718600	-0.08312100	-1.23615200
C	-4.98559700	-0.51022300	1.11085600
C	-5.65429300	-0.37448900	-0.09177600
C	-0.79060600	-1.22384900	-1.10498900
C	-0.36512300	-1.10096100	-2.43166000
C	-1.03296400	-2.54907800	-0.73427900
C	-0.07139400	-2.18140900	-3.25576500
C	-0.74968300	-3.65962400	-1.51892300
C	-0.24936500	-3.47413600	-2.79549500
H	2.26791700	-2.81461300	4.25732300

H	1.69842700	-4.51142700	4.36703300
H	0.49364000	-3.17752500	4.29075000
H	3.37218000	-1.79271800	1.71428600
F	-2.91361400	0.35463500	-2.28607500
F	-3.05260100	-0.49612700	2.36485400
F	-5.55583800	0.06569900	-2.39918900
F	-6.97298900	-0.51140200	-0.14940100
F	-5.67037800	-0.77775800	2.21984900
F	0.35720400	-1.98117800	-4.50018200
F	-0.22630900	0.08950600	-3.02316100
F	0.02264500	-4.51213400	-3.57546500
F	-0.98999900	-4.88773500	-1.07196500
F	-1.60131700	-2.81807300	0.44431500
F	2.28446100	2.95211900	-2.18962200
F	1.41802100	0.66521100	-1.20740400
F	0.68407600	5.16405200	-2.15324800
F	-1.84660100	4.94695200	-1.18239900
F	-2.76319900	2.66943300	-0.27107400

Energy (0K) = -3850.2050851

Energy (0K) + ZPE = -3849.646634

Enthalpy (298K) = -3849.590740

Free Energy (298K) = -3849.733909

NaBPh₄ as catalyst

BAr₃ (Ar=Ph)

Number of imaginary frequencies: 0

B	-2.32681900	4.60743500	0.59440200
C	-2.53927600	4.37907000	2.12653400
C	-2.06633900	5.29834900	3.08099500
C	-3.20798300	3.23942100	2.60973100

C	-2.26124600	5.09989900	4.44340800
H	-1.54533700	6.19378100	2.74319300
C	-3.38448300	3.01926400	3.97113000
H	-3.58384300	2.50403100	1.89931900
C	-2.91563900	3.95440700	4.89084600
H	-1.89708600	5.83438700	5.15895000
H	-3.89164400	2.12087000	4.31711300
H	-3.06046000	3.79065600	5.95693000
C	-1.06174800	5.36969600	0.07992200
C	-1.11270500	6.16791900	-1.07726500
C	0.17297300	5.28827800	0.74922500
C	0.00194600	6.86205500	-1.53465900
H	-2.05336500	6.25594500	-1.61979300
C	1.30060600	5.95506200	0.28270000
H	0.25015500	4.67670900	1.64753900
C	1.21420600	6.75006100	-0.85801800
H	-0.07030300	7.48577600	-2.42333400
H	2.24748000	5.86040000	0.81051000
H	2.09183100	7.28259100	-1.21916900
C	-3.37923200	4.06957300	-0.43055300
C	-2.99082300	3.60289800	-1.69943800
C	-4.75120300	4.02842100	-0.12356500
C	-3.91777000	3.10513900	-2.60866000
H	-1.93539000	3.61995400	-1.96994500
C	-5.68888300	3.56071500	-1.03785500
H	-5.08879800	4.38606900	0.84874300
C	-5.27144900	3.08985400	-2.28056000
H	-3.58649200	2.73375400	-3.57637300
H	-6.74605600	3.55595600	-0.78023100
H	-6.00099100	2.71063900	-2.99349700

Energy (0K) = -719.2725789

Energy (0K) + ZPE = -718.996391

Enthalpy (298K) = -718.980307

Free Energy (298K) = -719.040046

TS_A

Number of imaginary frequencies: 1

C	-0.07152800	-2.28127900	2.06174000
C	0.68561300	-2.74786700	2.88543700
C	1.57408300	-3.32198000	3.84319700
C	1.49738800	-4.69346600	4.12847000
C	2.53684300	-2.53291400	4.48924600
C	2.37068200	-5.26001600	5.04721000
H	0.75103700	-5.30145300	3.62140000
C	3.40366900	-3.10914700	5.40836900
H	2.59920900	-1.47097400	4.26048500
C	3.32318900	-4.47130500	5.68892900
H	2.30763600	-6.32369800	5.26433000
H	4.14776200	-2.49250400	5.90690800
H	4.00500300	-4.91892400	6.40823100
N	-1.00274500	-0.29663400	0.99763500
C	-0.78098000	0.44415600	-0.04052600
C	-0.68183900	1.12596700	-1.09180100
C	0.46311700	1.66052700	-1.83190600
C	0.71356500	3.03098100	-1.94991000
C	1.31455700	0.74930300	-2.47259600
C	1.79758700	3.47616800	-2.70070400
H	0.06136600	3.74635800	-1.45491200
C	2.38780700	1.20373000	-3.22825500
H	1.10724500	-0.31697600	-2.39723500

C	2.63288200	2.56970600	-3.34705800
H	1.98515500	4.54462100	-2.78206200
H	3.03497800	0.48544000	-3.72679900
H	3.47309900	2.92509800	-3.93915400
S	-1.55073300	0.50372200	2.48501500
O	-2.31365900	-0.50285900	3.19758900
O	-2.14578500	1.75680400	2.06557500
C	-0.01965600	0.83531700	3.30391600
H	-0.26546500	1.36254700	4.23075400
H	0.58670200	1.47026300	2.65231600
H	0.47664000	-0.11497100	3.51630800
C	-0.39538500	-2.30662600	-0.37121800
H	0.64787700	-1.98037600	-0.47433300
H	-0.96989500	-1.84248400	-1.18299000
C	-0.50590300	-3.80378300	-0.46228500
C	-1.70550900	-4.38921800	-0.87464400
C	0.56515600	-4.63048200	-0.11661500
C	-1.83508200	-5.77301900	-0.93640100
H	-2.54239000	-3.75029800	-1.15980100
C	0.43873000	-6.01522700	-0.17868700
H	1.50456900	-4.18101400	0.20419900
C	-0.76238900	-6.58931600	-0.58681700
H	-2.77392300	-6.21440200	-1.26377400
H	1.28278600	-6.64678300	0.09037300
H	-0.86118400	-7.67140600	-0.63715000
C	-0.92622600	-1.80379300	0.98245400
H	-1.95596700	-2.16449900	1.12529100
B	-2.57792800	1.37883700	-1.91539400
C	-3.65152100	0.77795100	-0.87915100
C	-3.68177000	-0.57937100	-0.51163100

C	-4.67106800	1.57577000	-0.33563000
C	-4.63435700	-1.10597100	0.35500100
H	-2.94128900	-1.25861700	-0.93250200
C	-5.63892300	1.06529600	0.52739500
H	-4.71555900	2.63210600	-0.59603400
C	-5.62015500	-0.27761200	0.88679700
H	-4.60879200	-2.16439500	0.61355700
H	-6.40986000	1.72455700	0.92290800
H	-6.36898700	-0.67835300	1.56716900
C	-2.52011600	2.98052300	-1.96873000
C	-2.60224000	3.70142300	-3.16880300
C	-2.40837100	3.74045200	-0.78826600
C	-2.55255900	5.09464100	-3.19991400
H	-2.71034100	3.16293100	-4.10957600
C	-2.35858400	5.13005700	-0.80564300
H	-2.34711500	3.22484900	0.17099100
C	-2.42318600	5.81580600	-2.01823500
H	-2.61710900	5.61665800	-4.15326100
H	-2.26659800	5.68168700	0.12860900
H	-2.38048500	6.90306800	-2.03859500
C	-2.39914200	0.57091500	-3.29615600
C	-1.43321500	0.92021800	-4.26151300
C	-3.24166900	-0.50073200	-3.64005900
C	-1.29455000	0.23188300	-5.46259500
H	-0.76629400	1.76009700	-4.07597100
C	-3.12027500	-1.19430200	-4.84253800
H	-4.03381300	-0.79594500	-2.95481900
C	-2.13685300	-0.83675100	-5.75850400
H	-0.52678300	0.53617900	-6.17222100
H	-3.80073300	-2.01499900	-5.06348900

H	-2.03351900	-1.37670600	-6.69781600
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Energy (0K) = -2286.9337423

Energy (0K) + ZPE = -2286.263499

Enthalpy (298K) = -2286.220860

Free Energy (298K) = -2286.340612

A

Number of imaginary frequencies: 0

C	0.98064400	-1.91093500	2.23215300
C	1.75643600	-2.37383400	3.04041600
C	2.66883500	-2.94052300	3.97967800
C	2.59931000	-4.30987200	4.27662800
C	3.64861200	-2.14655300	4.59315000
C	3.49744000	-4.87007000	5.17509000
H	1.83986100	-4.92100100	3.79347500
C	4.53991900	-2.71650700	5.49256300
H	3.70544500	-1.08648500	4.35449000
C	4.46696800	-4.07666900	5.78476100
H	3.44079200	-5.93212900	5.40151600
H	5.29729200	-2.09671200	5.96647100
H	5.16800900	-4.51907400	6.48863600
N	0.01710900	0.05484700	1.16008900
C	0.15496900	0.78159800	0.11515500
C	0.19247900	1.48061500	-0.94886200
C	1.43498000	1.97140100	-1.58430900
C	1.71413500	3.33111500	-1.75055300
C	2.33406900	1.01970800	-2.08207900
C	2.87346300	3.72355400	-2.41301800
H	1.02777400	4.07988200	-1.36319100
C	3.48220400	1.42081700	-2.75426300

H	2.10374600	-0.03882700	-1.97079900
C	3.75542000	2.77564600	-2.92349400
H	3.08358200	4.78402400	-2.53391000
H	4.16430700	0.67064500	-3.14815800
H	4.65290900	3.09110200	-3.45056000
S	-0.55217100	0.86269400	2.66593000
O	-1.33181400	-0.14852000	3.35217300
O	-1.13676800	2.11379800	2.23040900
C	0.97175800	1.18290700	3.50194000
H	0.71707600	1.71593800	4.42320900
H	1.59049400	1.81110800	2.85550100
H	1.45853600	0.23012000	3.72453800
C	0.60431000	-1.97778100	-0.19284800
H	1.64779900	-1.65994800	-0.31942400
H	0.01675100	-1.52208200	-1.00022500
C	0.48494800	-3.47619800	-0.25289900
C	-0.74167600	-4.06504200	-0.57130700
C	1.57425700	-4.29965600	0.03871600
C	-0.87842400	-5.44903200	-0.59567500
H	-1.59541000	-3.42945000	-0.81043800
C	1.44000400	-5.68502400	0.01493600
H	2.53500400	-3.84775700	0.28388500
C	0.21284900	-6.26220200	-0.29980000
H	-1.83814700	-5.89401200	-0.84912100
H	2.29786200	-6.31429500	0.24218600
H	0.10771500	-7.34462100	-0.31956600
C	0.10258900	-1.45548000	1.16357400
H	-0.92363400	-1.81104500	1.33798800
B	-1.47320000	1.73822800	-1.72193900
C	-2.61705200	1.12926900	-0.74008700

C	-2.67242100	-0.23669400	-0.40736800
C	-3.63591500	1.92285400	-0.19130500
C	-3.63920200	-0.77233800	0.43887200
H	-1.94135700	-0.91827300	-0.84350200
C	-4.61771500	1.40504800	0.65224500
H	-3.66620200	2.98594600	-0.42507600
C	-4.61845400	0.05491700	0.98393900
H	-3.63053200	-1.83757800	0.66896900
H	-5.38437900	2.06532100	1.05486300
H	-5.37714500	-0.35147400	1.64990600
C	-1.49702600	3.35601700	-1.79023300
C	-1.62226700	4.06920800	-2.99017800
C	-1.39828400	4.12535900	-0.61519600
C	-1.63210300	5.46367100	-3.02610000
H	-1.71297500	3.52265900	-3.92855600
C	-1.40828300	5.51605500	-0.63592000
H	-1.30236000	3.61637200	0.34506900
C	-1.51860900	6.19494900	-1.84895300
H	-1.72912100	5.97870300	-3.98076000
H	-1.32590500	6.07383300	0.29580000
H	-1.52197100	7.28303500	-1.87318000
C	-1.34904400	0.97615900	-3.15222900
C	-0.35359100	1.29771400	-4.09688700
C	-2.26351800	-0.01334000	-3.55032200
C	-0.25962200	0.66241700	-5.33155600
H	0.37105500	2.07876800	-3.87020700
C	-2.18555500	-0.65566200	-4.78535700
H	-3.07597200	-0.28774900	-2.87958200
C	-1.17489300	-0.32714800	-5.68178100
H	0.53167500	0.94503100	-6.02428800

H	-2.92177400	-1.41455200	-5.04613700
H	-1.10521000	-0.82759700	-6.64585300
Energy (0K) = -2286.9344989			
Energy (0K) + ZPE = -2286.264166			
Enthalpy (298K) = -2286.221103			
Free Energy (298K) = -2286.341861			

TS_B

Number of imaginary frequencies: 1

C	0.13273500	1.22756800	1.54746800
C	0.91255700	0.81662900	2.37989200
C	1.83897100	0.42412200	3.39170800
C	1.73868100	-0.82149400	4.02718800
C	2.85879000	1.31284800	3.76593200
C	2.64523100	-1.16626200	5.02136800
H	0.94704500	-1.50729700	3.73431100
C	3.75735800	0.96070700	4.76390900
H	2.93244700	2.27428300	3.26036600
C	3.65241100	-0.27813700	5.39297300
H	2.56309600	-2.13348300	5.51168500
H	4.54455900	1.65378200	5.05123700
H	4.35707000	-0.55232500	6.17459700
N	-0.89106300	3.21521700	0.56949800
C	-0.32893400	4.02210300	-0.32072100
C	-0.45130600	4.59895100	-1.49269900
C	0.73839000	5.01361100	-2.27942800
C	1.11385700	6.34394200	-2.49900500
C	1.46539800	4.00103900	-2.91838200
C	2.19265300	6.64516600	-3.32501100
H	0.56848600	7.14900000	-2.01306800

C	2.52881000	4.30655800	-3.76081200
H	1.16994100	2.96295900	-2.77522500
C	2.89977300	5.63153900	-3.96670000
H	2.47737900	7.68582500	-3.46903100
H	3.07047400	3.50178900	-4.25361100
H	3.73464600	5.87393700	-4.62055300
S	-1.49099400	3.90261700	2.04670600
O	-2.50241700	2.97644900	2.52703700
O	-1.81281700	5.28408300	1.71987600
C	-0.14034100	3.94045700	3.20396500
H	-0.46431900	4.61646300	4.00112400
H	0.74836900	4.32704000	2.69961000
H	0.03141400	2.93582300	3.59285100
C	-0.20723200	1.29190300	-0.87778800
H	0.81647100	1.67785100	-0.97830300
H	-0.81214500	1.75514900	-1.66719600
C	-0.22112300	-0.20364000	-1.02645400
C	-1.41828800	-0.87400100	-1.29078900
C	0.95354800	-0.94606900	-0.89650400
C	-1.44002200	-2.25835300	-1.42364000
H	-2.33940900	-0.29966300	-1.40079400
C	0.93568700	-2.33130800	-1.03167000
H	1.88970300	-0.42715000	-0.69011600
C	-0.26163700	-2.99055600	-1.29510200
H	-2.37858900	-2.76711200	-1.63334200
H	1.86020700	-2.89623800	-0.93270600
H	-0.27737300	-4.07283500	-1.40323200
C	-0.75033200	1.71989200	0.49478300
H	-1.76157900	1.30950600	0.63065900
B	-2.03280500	4.91496300	-2.20152700

C	-3.26170100	4.36837900	-1.27524000
C	-3.43734700	3.00687100	-0.96854800
C	-4.26407400	5.21994000	-0.78564800
C	-4.50759000	2.52617400	-0.22059800
H	-2.71644800	2.28256100	-1.34642800
C	-5.34323400	4.76117200	-0.03005400
H	-4.20457600	6.28666700	-0.99729900
C	-5.47065700	3.40827900	0.26318100
H	-4.58618700	1.45894700	-0.01172400
H	-6.08952900	5.46929300	0.32818200
H	-6.30945100	3.04439800	0.85380700
C	-2.02045900	6.55304300	-2.23130300
C	-2.20394800	7.31991400	-3.38950500
C	-1.81778000	7.27736200	-1.04037300
C	-2.14523900	8.71422100	-3.37823100
H	-2.38864100	6.81797400	-4.33883800
C	-1.75391000	8.66716800	-1.01209000
H	-1.71520100	6.72609800	-0.10428600
C	-1.90511700	9.39722400	-2.19087700
H	-2.28645500	9.26735700	-4.30597800
H	-1.58728900	9.18397300	-0.06706000
H	-1.84986000	10.48425400	-2.17935500
C	-2.02832100	4.23205200	-3.69772000
C	-1.13225600	4.63813700	-4.70864900
C	-2.92708900	3.22069700	-4.07713000
C	-1.10828800	4.06244800	-5.97570500
H	-0.42733100	5.44269600	-4.50899200
C	-2.91877300	2.63203200	-5.34206900
H	-3.67357900	2.87732400	-3.36363100
C	-2.00060500	3.04416200	-6.30069600

H	-0.38851200	4.41586400	-6.71325800
H	-3.63977800	1.84968500	-5.57573900
H	-1.98579200	2.58794500	-7.28898400
C	1.45313700	6.42162200	0.69737400
C	2.13422600	7.61378700	0.59221300
C	3.44365700	7.61685600	0.12206700
C	4.04454100	6.41271000	-0.21878200
C	3.32959000	5.23411400	-0.09903500
N	2.04242800	5.25265500	0.33881800
H	3.99749200	8.54564500	0.02685100
H	0.42549500	6.33110800	1.03951600
H	1.62478800	8.52970600	0.87434700
H	5.06904100	6.37114000	-0.57481500
O	1.37642500	4.12183800	0.44667500
Br	4.08400500	3.57171000	-0.46647000

Energy (0K) = -5180.8253423

Energy (0K) + ZPE = -5180.069734

Enthalpy (298K) = -5180.020297

Free Energy (298K) = -5180.153161

B

Number of imaginary frequencies: 0

C	0.08101300	-2.29976100	2.05547600
C	0.89804000	-2.72232500	2.84593300
C	1.86092900	-3.14806300	3.80957200
C	1.87569200	-4.46836100	4.28168300
C	2.80288500	-2.22950100	4.29772700
C	2.81527800	-4.85652400	5.22812600
H	1.14664300	-5.17890000	3.89839400
C	3.73581600	-2.62596500	5.24671000

H	2.79164300	-1.20827000	3.92046100
C	3.74370400	-3.93850500	5.71391400
H	2.82210800	-5.88193600	5.59011600
H	4.46130600	-1.90853200	5.62343300
H	4.47561000	-4.24728500	6.45664500
N	-0.99719500	-0.31380200	1.08133700
C	-0.23400100	0.48423600	0.23419100
C	-0.51493000	1.01930000	-0.96434100
C	0.66885400	1.43798100	-1.77506500
C	1.04601900	2.76623100	-2.01343900
C	1.40829300	0.42252100	-2.39735000
C	2.12017500	3.06156800	-2.84846500
H	0.50079900	3.57792500	-1.53738300
C	2.47102400	0.71869500	-3.24413600
H	1.12002900	-0.61526800	-2.23644500
C	2.83305100	2.04214800	-3.47439700
H	2.39709100	4.10134600	-3.01221000
H	3.01752600	-0.09118300	-3.72325600
H	3.66534600	2.27873300	-4.13368000
S	-1.59532800	0.36928200	2.50962900
O	-2.65273600	-0.50635500	2.99076800
O	-1.85502300	1.77291200	2.19907500
C	-0.29783500	0.37112300	3.73327200
H	-0.66416800	1.00142600	4.54926300
H	0.61353700	0.79738000	3.30679600
H	-0.12359500	-0.64713300	4.08393300
C	-0.35713100	-2.26662900	-0.34693500
H	0.67138500	-1.90918600	-0.49195000
H	-0.97482100	-1.80105900	-1.12482700
C	-0.40160500	-3.76464200	-0.46561100

C	-1.61853700	-4.42387100	-0.65911100
C	0.76689000	-4.52236700	-0.37198700
C	-1.66494100	-5.81064900	-0.75774100
H	-2.53687800	-3.84044900	-0.73850800
C	0.72459000	-5.91006500	-0.47287200
H	1.71821800	-4.01284700	-0.21772900
C	-0.49253600	-6.55746000	-0.66545600
H	-2.61941800	-6.30979200	-0.91147100
H	1.64482900	-6.48624500	-0.40250900
H	-0.52860900	-7.64167600	-0.74608400
C	-0.84546800	-1.80154700	1.03752100
H	-1.84783600	-2.21855200	1.21466900
B	-2.04872300	1.30924800	-1.66435100
C	-3.32803200	0.80783700	-0.76216100
C	-3.54729500	-0.54216700	-0.43199800
C	-4.34018900	1.68403400	-0.33979800
C	-4.66015900	-0.98812500	0.27304900
H	-2.82394400	-1.28716200	-0.75781800
C	-5.46056200	1.26282600	0.37821900
H	-4.25723700	2.74463400	-0.57321100
C	-5.62878700	-0.07983800	0.69468600
H	-4.76657300	-2.04930000	0.50091600
H	-6.20849600	1.99337800	0.68498000
H	-6.50022000	-0.41551500	1.25420500
C	-2.06899500	2.95597200	-1.76063700
C	-2.24451500	3.68686900	-2.94317900
C	-1.90460400	3.72275300	-0.59001300
C	-2.20824700	5.08204500	-2.97373500
H	-2.40556800	3.15531300	-3.88080200
C	-1.86459100	5.11377600	-0.60144600

H	-1.82395000	3.20388400	0.36660900
C	-2.00221600	5.80596300	-1.80446500
H	-2.34161200	5.60380500	-3.92085100
H	-1.72909800	5.66120400	0.33138400
H	-1.96548400	6.89369800	-1.82568700
C	-2.07044700	0.59709300	-3.16036200
C	-1.18204400	0.97574100	-4.18938300
C	-2.97978100	-0.41346700	-3.51775200
C	-1.17364600	0.37803900	-5.44674000
H	-0.46956200	1.77904300	-4.01382000
C	-2.98756700	-1.02556500	-4.77199700
H	-3.72432800	-0.73937400	-2.79438700
C	-2.07570200	-0.63925100	-5.74687900
H	-0.45781000	0.71395800	-6.19642500
H	-3.71745100	-1.80618100	-4.98380200
H	-2.07350000	-1.11328500	-6.72694100
C	1.15464500	2.79411200	1.21726400
C	1.84852500	3.98130500	1.28142800
C	3.20259500	4.00097200	0.96025900
C	3.84183800	2.82231000	0.59965400
C	3.11671000	1.64577500	0.53631500
N	1.79407500	1.66964500	0.82753100
H	3.76628000	4.92786900	1.00024200
H	0.09589200	2.68026900	1.44726700
H	1.31861300	4.87816900	1.58419500
H	4.90043500	2.80040100	0.36200700
O	1.13758900	0.47893500	0.79772600
Br	3.90857400	0.01445100	0.12291700

Energy (0K) = -5180.8337558

Energy (0K) + ZPE = -5180.076398

Enthalpy (298K) = -5180.026850

Free Energy (298K) = -5180.160507

TS_C

Number of imaginary frequencies: 1

C	0.28544600	-2.16217800	2.10646100
C	1.09722900	-2.62833400	2.87770700
C	2.04519200	-3.18218800	3.78926200
C	2.19329900	-4.57455200	3.88016300
C	2.83469500	-2.34993700	4.59597700
C	3.11444400	-5.11907300	4.76469500
H	1.57810100	-5.21492800	3.25088800
C	3.75231200	-2.90434600	5.47873500
H	2.71896900	-1.27019700	4.52197700
C	3.89450800	-4.28760200	5.56540400
H	3.22408700	-6.19903200	4.83090000
H	4.36088000	-2.25392300	6.10285200
H	4.61402800	-4.71766100	6.25832700
N	-0.81218400	-0.21327800	1.04154700
C	-0.01471900	0.49483800	0.10257100
C	-0.48173700	1.12091600	-1.05863600
C	0.65809300	1.61091700	-1.88609800
C	0.93974500	2.96640100	-2.09751900
C	1.50066200	0.65774700	-2.48147000
C	2.03342200	3.35113000	-2.87111700
H	0.31045600	3.72962000	-1.64758700
C	2.57024900	1.04386100	-3.27512000
H	1.28945300	-0.40053200	-2.33511400
C	2.84681500	2.39633800	-3.46964300
H	2.23850200	4.41042500	-3.01129000

H	3.19630600	0.28392900	-3.73762800
H	3.69268900	2.70042100	-4.08221600
S	-1.41470900	0.55559600	2.40863600
O	-2.50061400	-0.26203400	2.92752800
O	-1.63617900	1.94869100	2.02997700
C	-0.13024000	0.57057200	3.64564300
H	-0.46824900	1.26594900	4.41991500
H	0.81145100	0.91727400	3.21047200
H	-0.01813500	-0.43371600	4.05714200
C	-0.27848200	-2.28301600	-0.26816500
H	0.78564000	-2.07913900	-0.44384300
H	-0.84328900	-1.77353300	-1.05918500
C	-0.53834800	-3.76264000	-0.32273700
C	-1.80923000	-4.24063900	-0.65465700
C	0.47224900	-4.68109900	-0.03093600
C	-2.06540200	-5.60747800	-0.68914200
H	-2.59989400	-3.52923200	-0.90028500
C	0.21893400	-6.04928400	-0.06411000
H	1.46758600	-4.31389100	0.21966500
C	-1.05155500	-6.51537400	-0.39189900
H	-3.05778200	-5.96533500	-0.95507300
H	1.01770900	-6.75321200	0.16070200
H	-1.25069300	-7.58442900	-0.42137100
C	-0.67396000	-1.69573200	1.10457000
H	-1.67495200	-2.07262100	1.36499300
B	-2.01807600	1.33942700	-1.67881800
C	-3.28951000	0.81363700	-0.77924200
C	-3.43827400	-0.51942500	-0.35701600
C	-4.37893000	1.64709000	-0.47510900
C	-4.55585000	-0.98876600	0.32537800

H	-2.65169800	-1.23378600	-0.58317000
C	-5.50803100	1.20143500	0.21323200
H	-4.35534500	2.69090200	-0.78486100
C	-5.60407100	-0.12283400	0.62488100
H	-4.59917800	-2.03439900	0.63201000
H	-6.31847600	1.89848800	0.42334300
H	-6.48111500	-0.47618400	1.16423800
C	-2.14632000	2.97376300	-1.85375000
C	-2.45565900	3.62621800	-3.05304300
C	-1.99743400	3.79820300	-0.72253300
C	-2.57447900	5.01471000	-3.13453800
H	-2.60733500	3.03879000	-3.95808400
C	-2.10655300	5.18419400	-0.78807900
H	-1.81304400	3.32992800	0.24537100
C	-2.38599300	5.80434200	-2.00515200
H	-2.81464400	5.48019800	-4.08969800
H	-1.97965200	5.78314100	0.11330300
H	-2.46995800	6.88773400	-2.06808400
C	-1.98495300	0.55214400	-3.15183100
C	-1.17519800	0.98220400	-4.22306100
C	-2.76609400	-0.58397600	-3.42054200
C	-1.13515900	0.32823200	-5.45111500
H	-0.54740200	1.86397000	-4.10389000
C	-2.73670600	-1.25376600	-4.64462600
H	-3.44046800	-0.96373400	-2.65597000
C	-1.91456800	-0.80470500	-5.67046400
H	-0.48846300	0.70886600	-6.24073400
H	-3.36644400	-2.13028200	-4.79146200
H	-1.88415300	-1.32274500	-6.62731300
C	1.31126500	2.87575900	1.10435100

C	1.93967900	4.08874800	1.33067500
C	3.32892100	4.13788600	1.26212300
C	4.05740400	2.98407100	0.99454000
C	3.36812000	1.79586500	0.79740100
N	2.04386000	1.79537200	0.87658000
H	3.85138700	5.07850000	1.41079000
H	0.22391500	2.74209900	1.09324200
H	1.34217900	4.97107600	1.53527200
H	5.14132100	2.99500200	0.93366300
O	1.28870600	0.38511500	0.30914300
Br	4.26377100	0.18613600	0.44648600

Energy (0K) = -5180.8149307

Energy (0K) + ZPE = -5180.059153

Enthalpy (298K) = -5180.009915

Free Energy (298K) = -5180.142378

C

Number of imaginary frequencies: 0

C	-1.12484500	0.05930400	0.69343900
C	-0.92021700	-1.34257600	1.18679600
N	0.28863800	-1.99173600	1.26289600
B	-1.69917100	0.21231400	-0.83929400
S	0.24084700	-3.65401100	1.80913500
O	1.64247500	-4.04414500	1.88507700
O	-0.66680600	-4.40574600	0.96274000
C	1.62733800	-1.49799200	0.84401500
C	1.73610500	-0.04948300	0.90001800
C	2.04732300	1.12409900	0.90035400
C	2.34888400	2.51448100	0.84971500
C	3.19888700	3.00774700	-0.15299000

C	1.76690900	3.40220500	1.76583700
C	3.45492500	4.36956100	-0.23454200
H	3.64525400	2.31096600	-0.86084400
C	2.01389600	4.76472600	1.66330300
H	1.12083900	3.01178100	2.54941000
C	2.85633300	5.25031900	0.66590100
H	4.11775000	4.74847300	-1.00888200
H	1.54983500	5.45051600	2.36850000
H	3.05062600	6.31769000	0.59105000
C	2.02132900	-2.02741300	-0.54725600
H	1.34539000	-1.58473500	-1.28553900
H	1.86407700	-3.11362700	-0.54904400
C	3.45041500	-1.70957300	-0.87533900
C	4.48744800	-2.38688500	-0.22795000
C	3.76777900	-0.72084100	-1.80836500
C	5.81532000	-2.08056300	-0.50666500
H	4.24094700	-3.16520000	0.49564700
C	5.09610300	-0.41414900	-2.09221200
H	2.96074100	-0.19353300	-2.31974800
C	6.12243000	-1.09245700	-1.43972000
H	6.61405800	-2.61663900	0.00172600
H	5.32862500	0.35493800	-2.82612000
H	7.16079100	-0.85490800	-1.66102100
C	-1.17491600	1.01911900	1.75722600
C	-0.80790200	0.65936900	3.08374900
C	-1.64295400	2.34146400	1.54255000
C	-0.91137900	1.55845200	4.12417600
H	-0.43901100	-0.34204700	3.29492600
C	-1.75765300	3.23516700	2.59319000
H	-1.93010500	2.65003300	0.54325200

C	-1.39382000	2.84849600	3.88122800
H	-0.62815400	1.26238100	5.13029300
H	-2.12910900	4.23925800	2.40863500
H	-1.48412000	3.55415700	4.70378400
O	-1.96233700	-1.86356800	1.56437800
C	-0.38504600	-3.53093100	3.45985800
C	-1.44878800	1.70059600	-1.46502900
C	-0.15703800	2.25359400	-1.49848700
C	-2.47368300	2.49126800	-2.00422500
C	0.09628400	3.52822600	-1.99530600
H	0.67666500	1.66450400	-1.11409300
C	-2.23326900	3.76536300	-2.52027400
H	-3.49583700	2.11219100	-2.00710000
C	-0.94791200	4.29601000	-2.50758000
H	1.11196400	3.92453400	-1.97580500
H	-3.05938400	4.34793400	-2.92549000
H	-0.75959800	5.29542900	-2.89532300
C	-3.34541100	-0.03048200	-0.67364900
C	-4.02997200	-0.52981100	-1.79471900
C	-4.13669300	0.36053500	0.41324300
C	-5.41895300	-0.61719000	-1.83485700
H	-3.46284300	-0.83761000	-2.67235400
C	-5.52741900	0.26776800	0.38862300
H	-3.67649200	0.74752900	1.32091200
C	-6.17899000	-0.22209000	-0.73763200
H	-5.90710300	-0.99690400	-2.73124900
H	-6.10142100	0.57738000	1.26074500
H	-7.26432600	-0.29715900	-0.76057800
C	-1.09180900	-0.95358500	-1.82827300
C	-0.34133900	-0.63957500	-2.97171100

C	-1.34973600	-2.32200800	-1.62434300
C	0.14548600	-1.61717100	-3.84116700
H	-0.12703200	0.40374000	-3.19955400
C	-0.86861800	-3.30837900	-2.48018400
H	-1.95667600	-2.63955900	-0.77666300
C	-0.11126800	-2.96143100	-3.59667400
H	0.72471000	-1.32131800	-4.71496000
H	-1.08973200	-4.35432700	-2.27216000
H	0.26567700	-3.72868100	-4.27029600
H	0.29088600	-2.89162200	4.03395900
H	-0.36809500	-4.54981500	3.85992300
H	-1.40366500	-3.14189600	3.43857700
H	2.33158700	-1.91233200	1.57907800

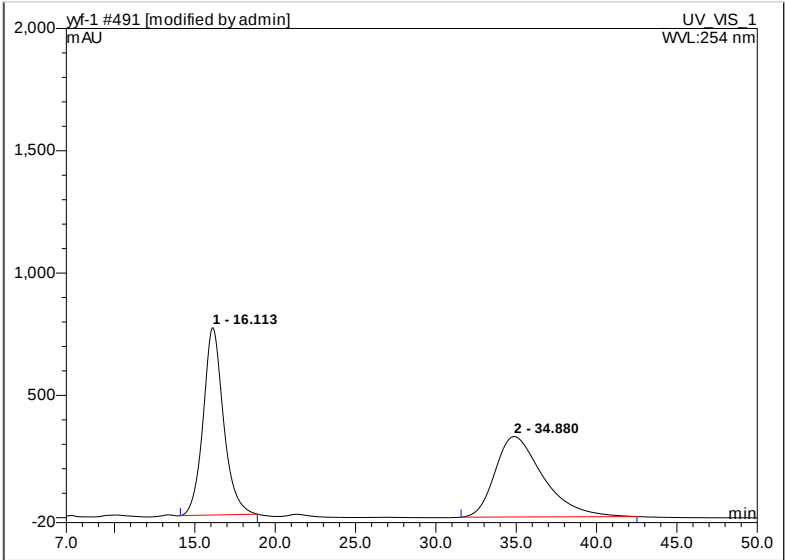
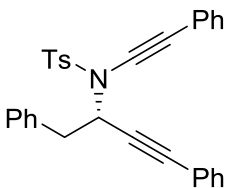
Energy (0K) = -2362.1550289

Energy (0K) + ZPE = -2361.478147

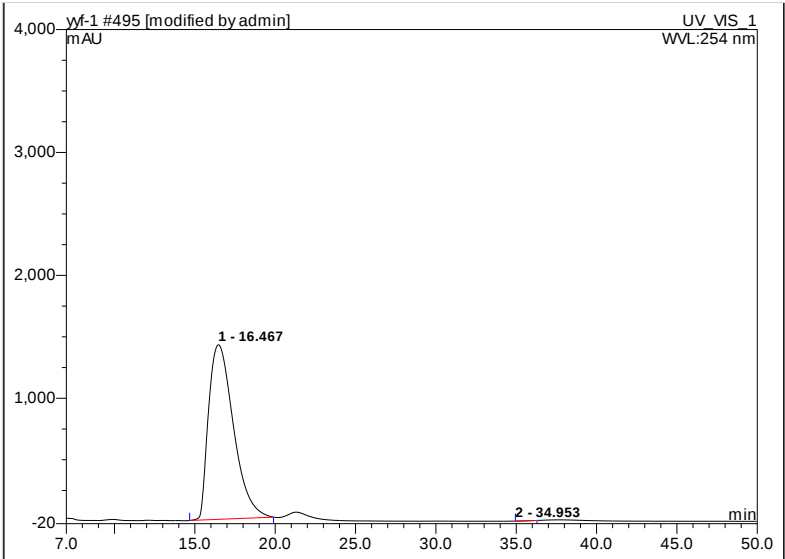
Enthalpy (298K) = -2361.434926

Free Energy (298K) = -2361.552767

Compound **1a**

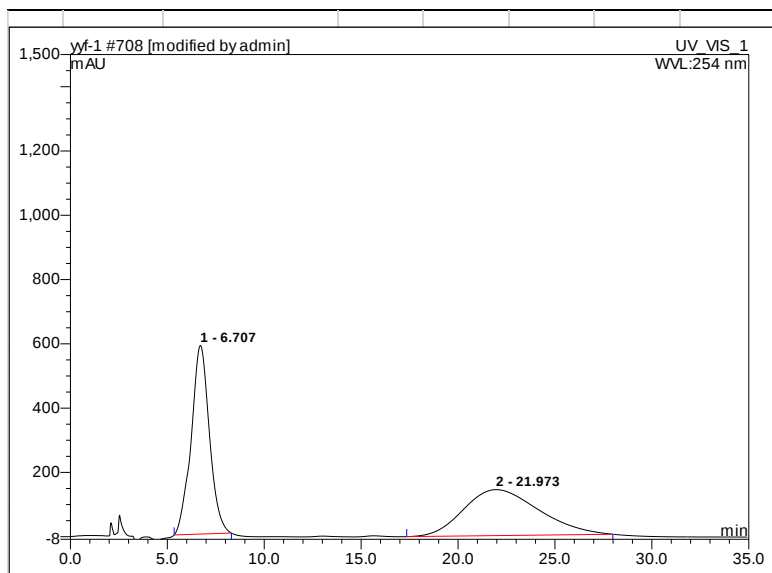
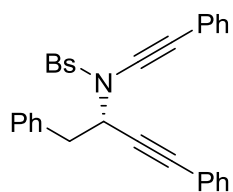


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	16.11	n.a.	765.641	1123.781	49.64	n.a.	BMB*
2	34.88	n.a.	328.661	1139.917	50.36	n.a.	BMB*
Total:			1094.302	2263.698	100.00	0.000	

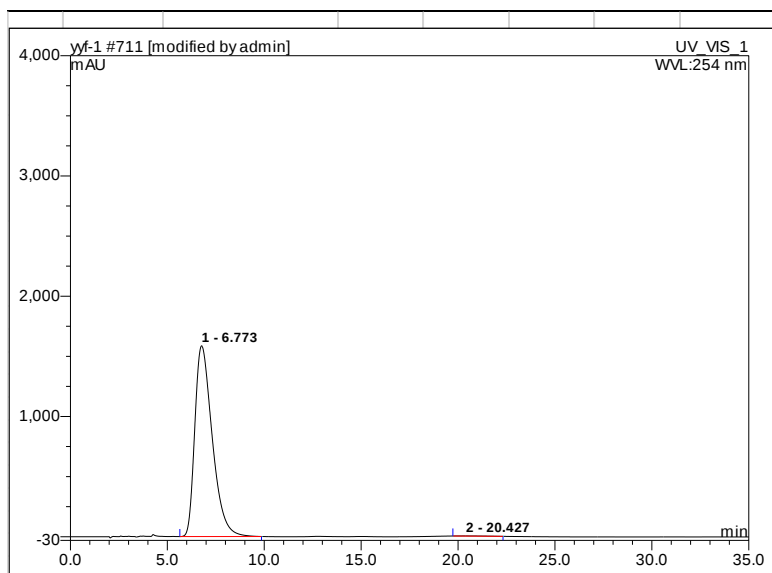


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	16.47	n.a.	1420.168	2552.524	99.98	n.a.	BMB*
2	34.95	n.a.	0.015	0.638	0.02	n.a.	BMB*
Total:			1420.183	2553.162	100.00	0.000	

Compound 1b

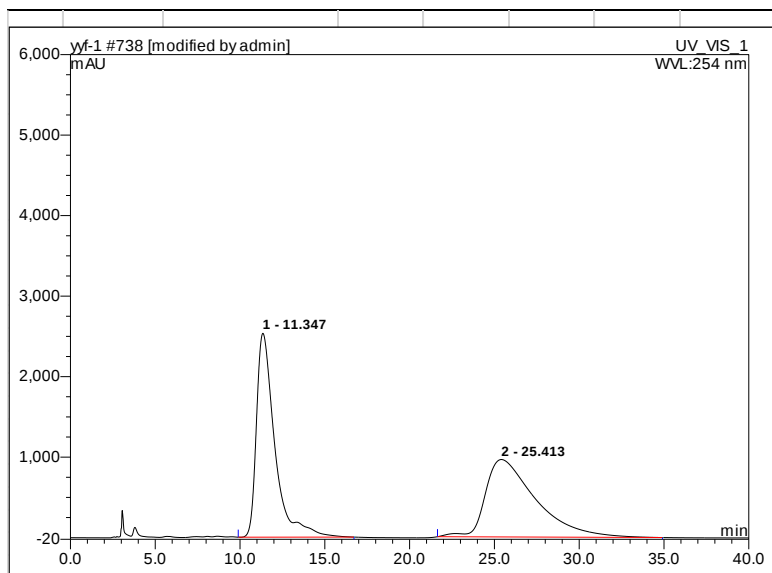
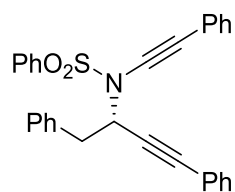


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	6.71	n.a.	586.687	640.156	49.92	n.a.	BMB*
2	21.97	n.a.	142.961	642.260	50.08	n.a.	BMB*
Total:			729.649	1282.416	100.00	0.000	

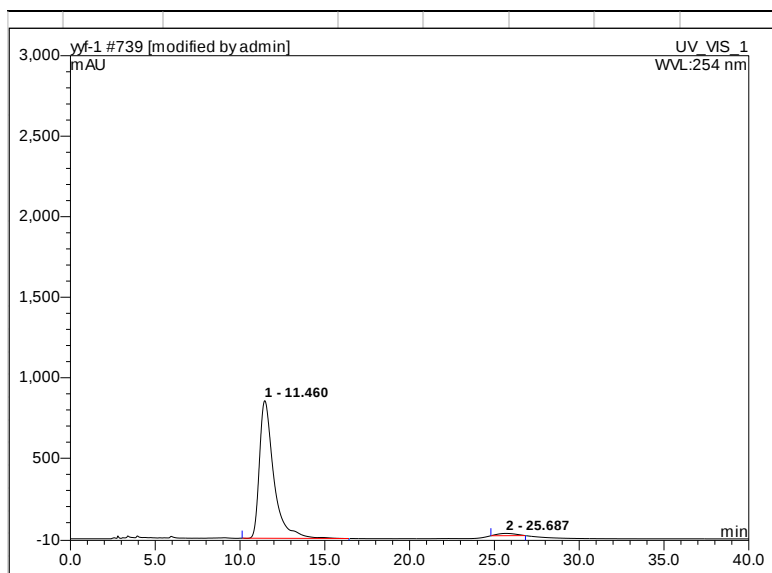


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	6.77	n.a.	1585.837	1654.646	99.84	n.a.	BMB*
2	20.43	n.a.	1.385	2.625	0.16	n.a.	BMB*
Total:			1587.222	1657.271	100.00	0.000	

Compound 1c

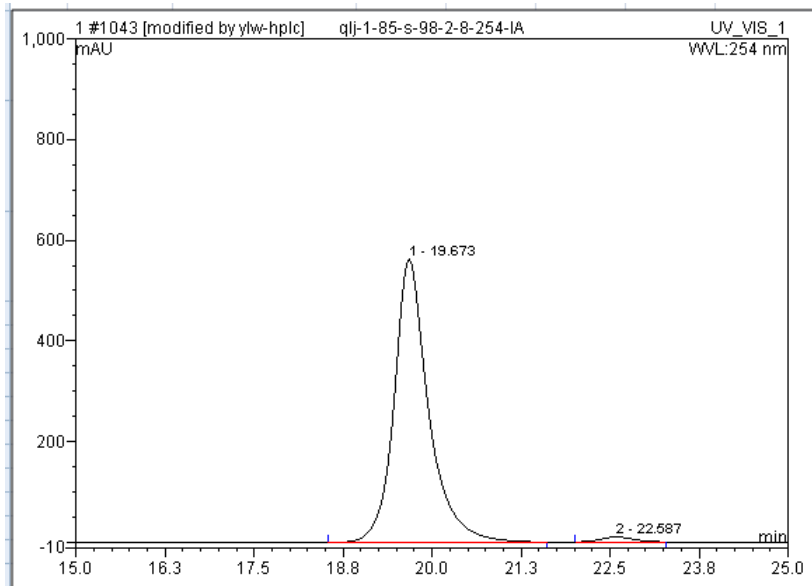
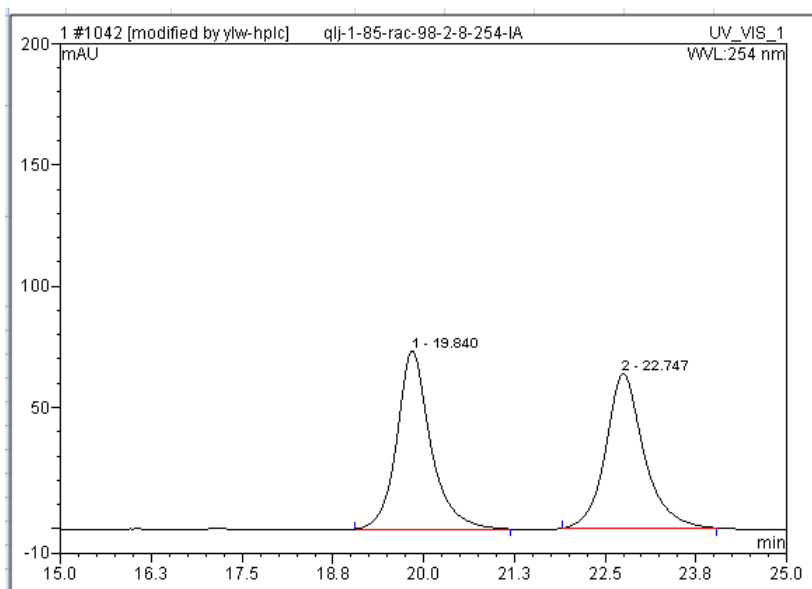
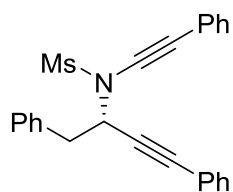


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11.35	n.a.	2531.910	3183.931	49.04	n.a.	BMB*
2	25.41	n.a.	961.530	3307.970	50.96	n.a.	BMB*
Total:			3493.441	6491.901	100.00	0.000	

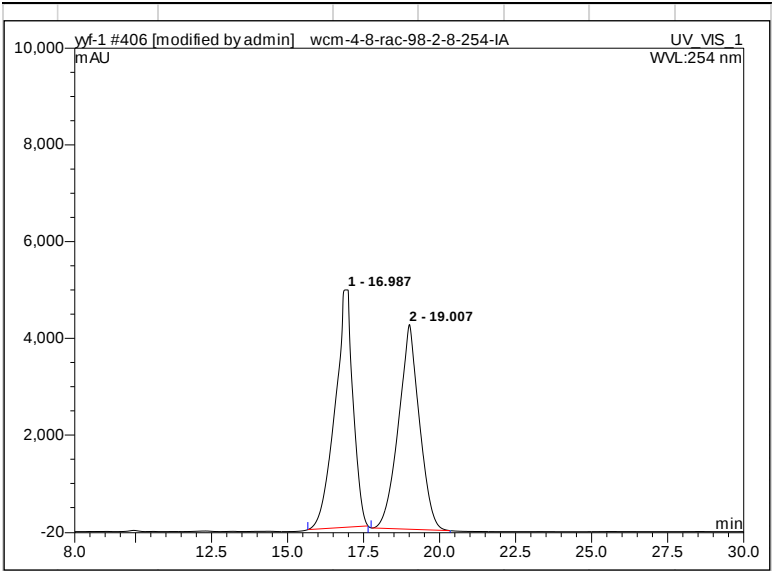
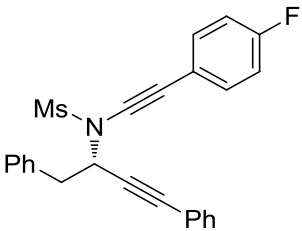


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11.46	n.a.	854.000	833.966	97.92	n.a.	BMB*
2	25.69	n.a.	14.050	17.678	2.08	n.a.	BMB*
Total:			868.050	851.644	100.00	0.000	

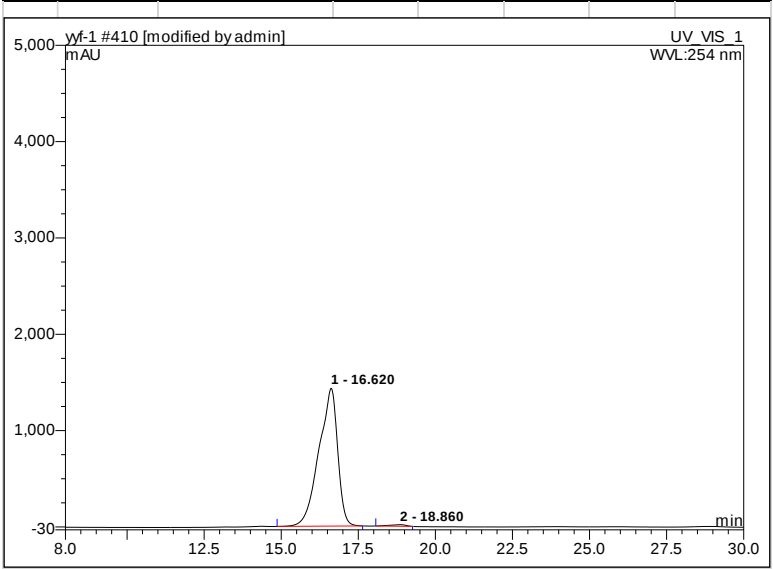
Compound **1d**



Compound **1e**

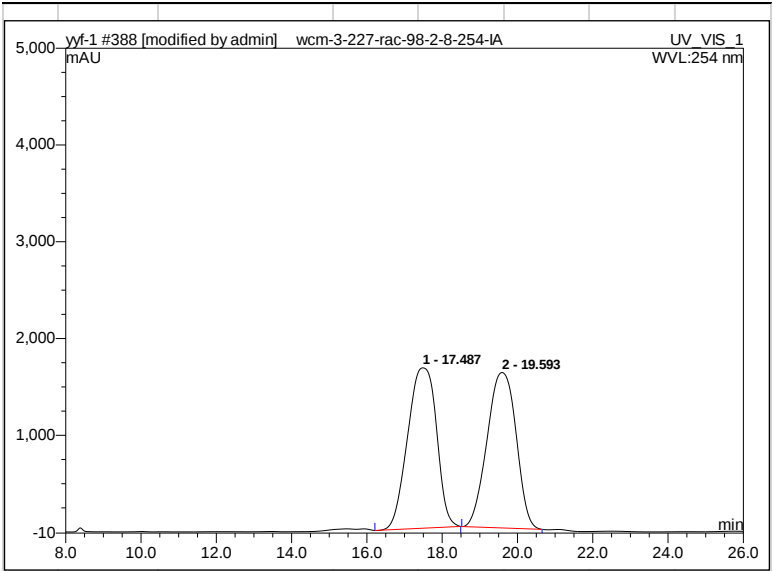
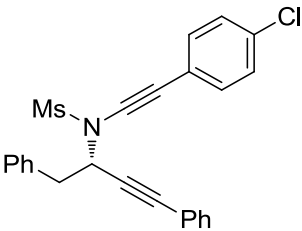


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	16.99	n.a.	4904.565	3388.893	50.13	n.a.	BMB*
2	19.01	n.a.	4232.816	3370.956	49.87	n.a.	BMB*
Total:			9137.381	6759.849	100.00	0.000	

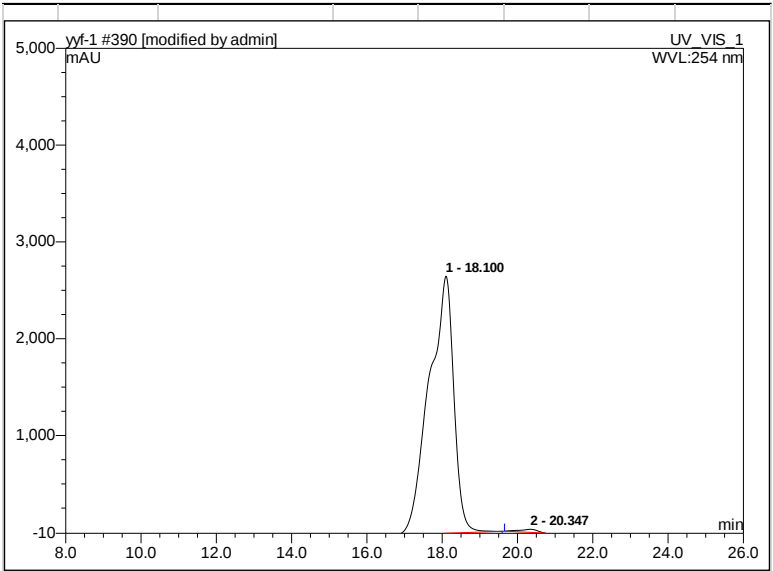


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	16.62	n.a.	1430.203	1009.349	99.05	n.a.	BMB*
2	18.86	n.a.	16.099	9.716	0.95	n.a.	BMB*
Total:			1446.302	1019.064	100.00	0.000	

Compound **1f**

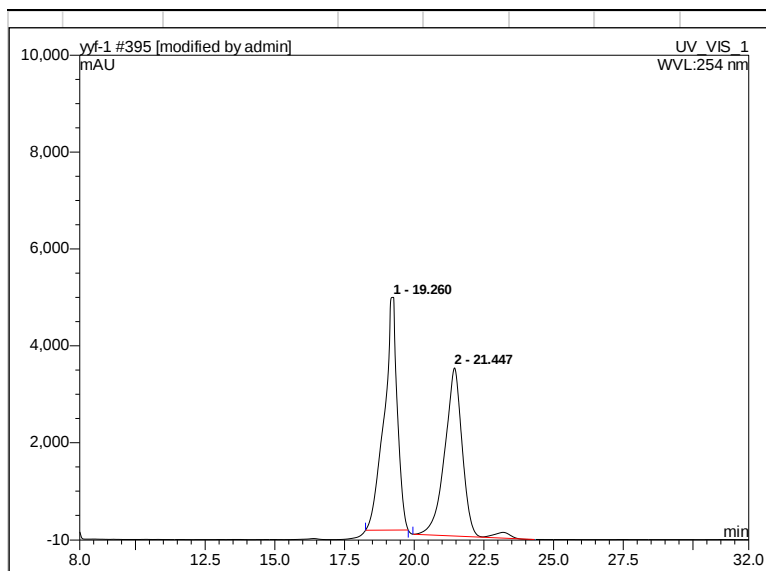
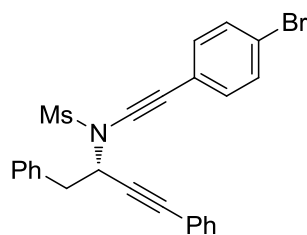


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	17.49	n.a.	1656.887	1475.734	50.68	n.a.	BMB*
2	19.59	n.a.	1605.915	1436.318	49.32	n.a.	BMB*
Total:			3262.802	2912.051	100.00	0.000	

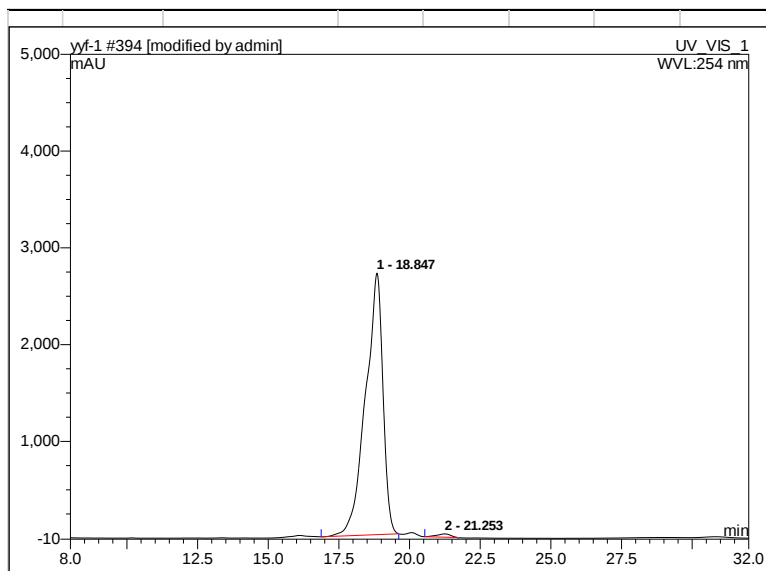


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	18.10	n.a.	2655.025	2015.856	99.14	n.a.	BMB*
2	20.35	n.a.	31.751	17.443	0.86	n.a.	BMB*
Total:			2686.777	2033.298	100.00	0.000	

Compound 1g

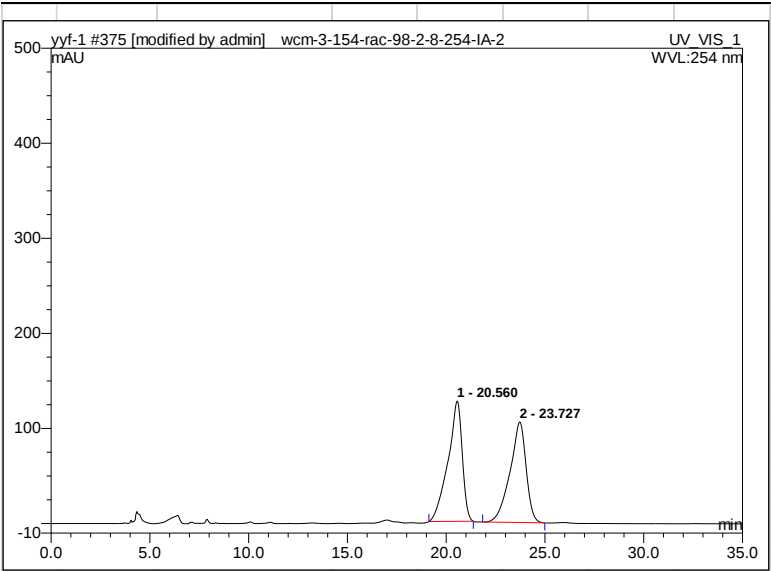
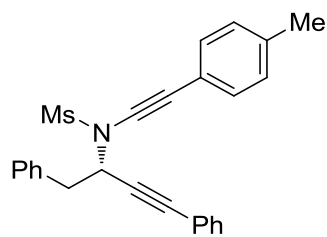


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	19.26	n.a.	4804.197	2662.777	50.86	n.a.	BMB*
2	21.45	n.a.	3470.054	2572.240	49.14	n.a.	BMB*
Total:			8274.251	5235.017	100.00	0.000	

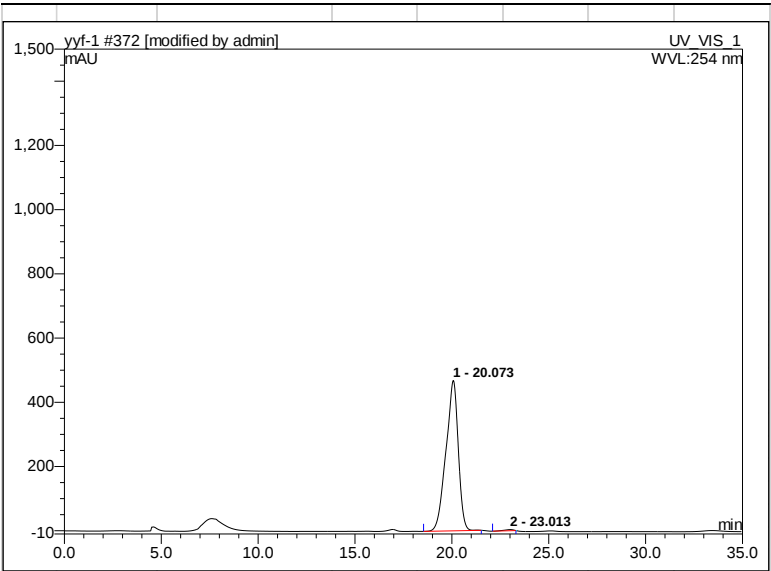


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	18.85	n.a.	2701.762	1928.096	99.01	n.a.	BMB*
2	21.25	n.a.	34.323	19.300	0.99	n.a.	BMB*
Total:			2736.085	1947.396	100.00	0.000	

Compound **1h**

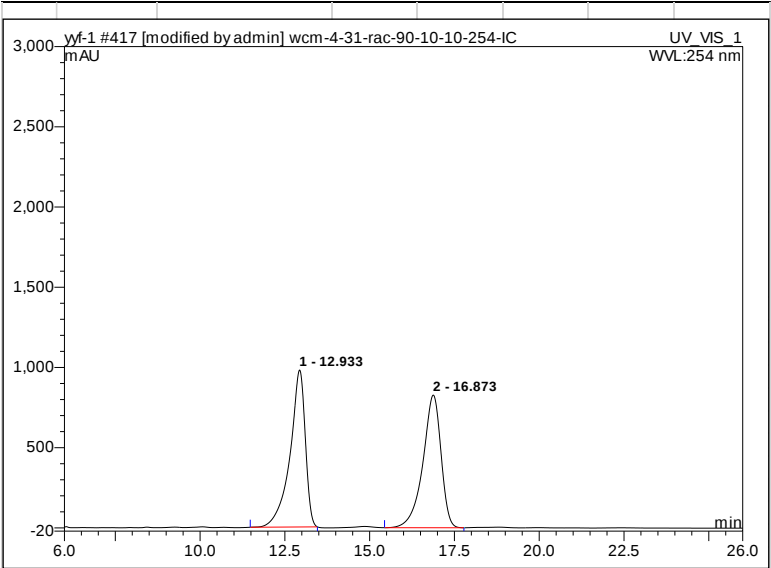
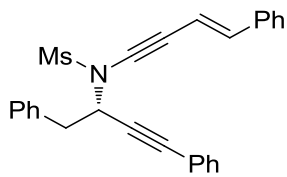


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	20.56	n.a.	126.430	105.736	51.44	n.a.	BMB*
2	23.73	n.a.	105.731	99.797	48.56	n.a.	BMB*
Total:			232.162	205.533	100.00	0.000	

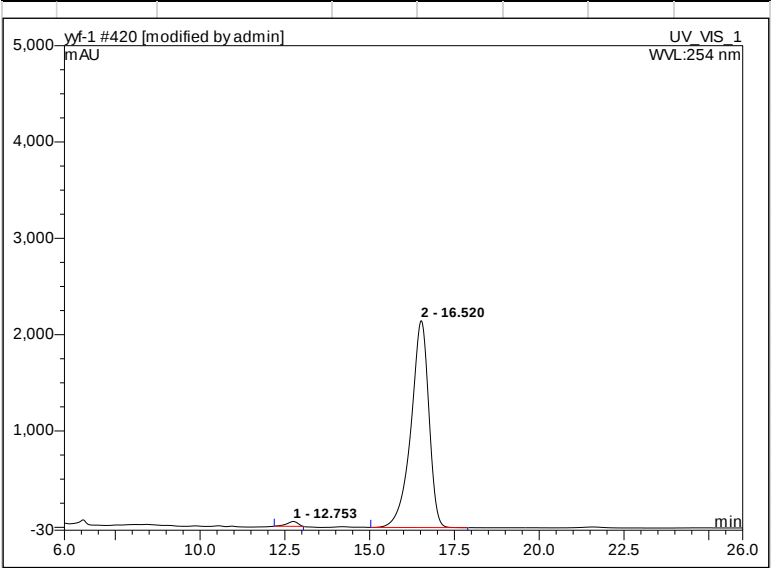


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	20.07	n.a.	468.165	344.291	99.43	n.a.	BMB*
2	23.01	n.a.	3.507	1.987	0.57	n.a.	BMB*
Total:			471.672	346.278	100.00	0.000	

Compound **1i**

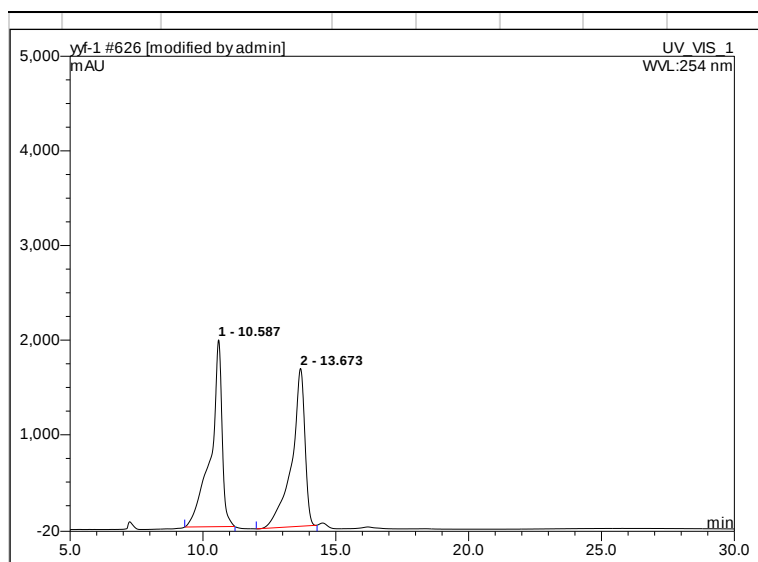
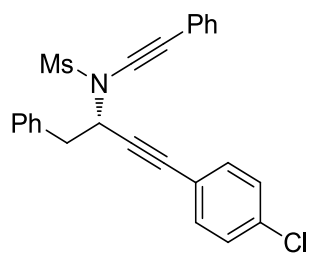


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	12.93	n.a.	978.081	509.604	49.88	n.a.	BMB*
2	16.87	n.a.	826.576	512.026	50.12	n.a.	BMB*
Total:			1804.657	1021.629	100.00	0.000	

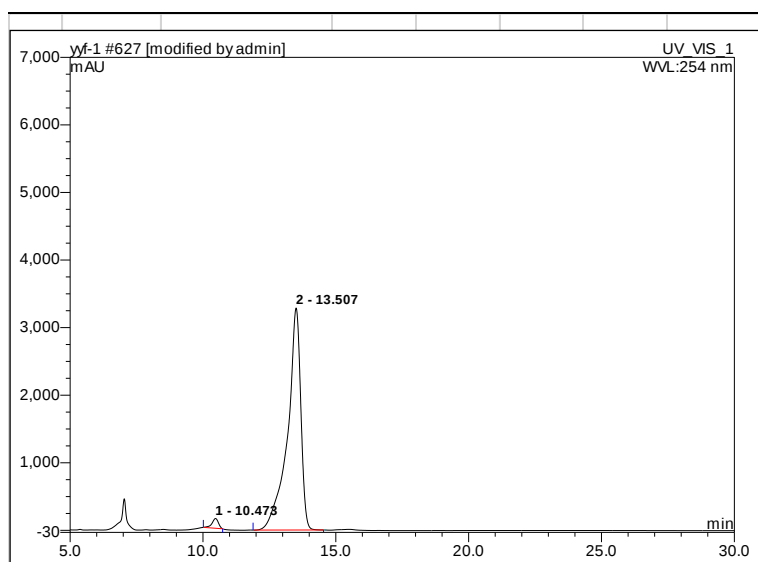


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	12.75	n.a.	50.558	19.326	1.46	n.a.	BMB*
2	16.52	n.a.	2146.795	1308.763	98.54	n.a.	BMB*
Total:			2197.352	1328.089	100.00	0.000	

Compound 1j

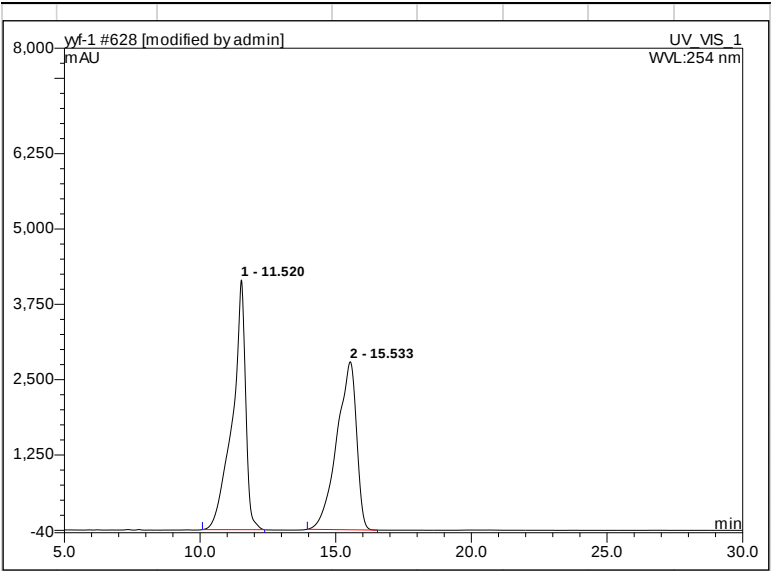
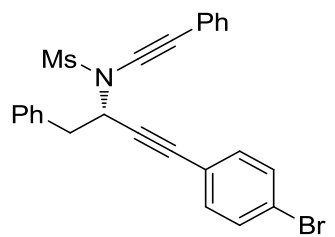


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	10.59	n.a.	1972.951	974.420	50.58	n.a.	BMB*
2	13.67	n.a.	1667.232	952.144	49.42	n.a.	BMB*
Total:			3640.183	1926.564	100.00	0.000	

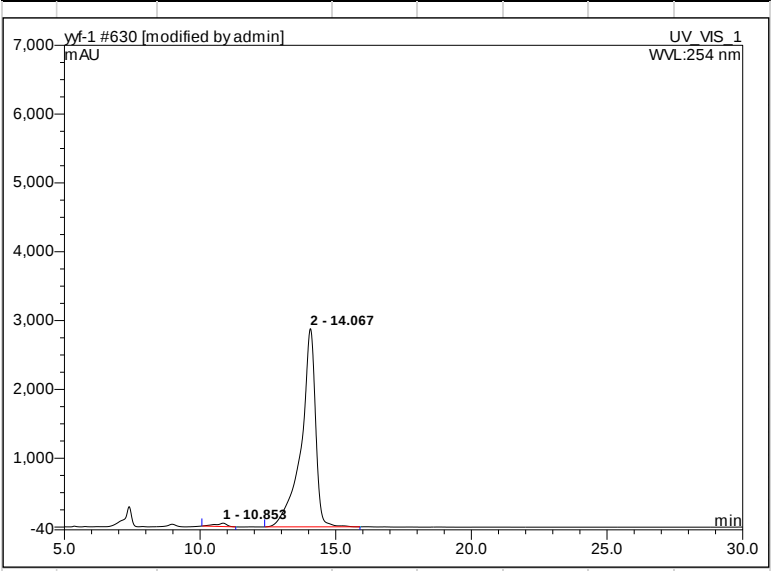


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	10.47	n.a.	144.437	40.482	2.09	n.a.	BMB*
2	13.51	n.a.	3285.320	1898.914	97.91	n.a.	BMB*
Total:			3429.758	1939.397	100.00	0.000	

Compound **1k**

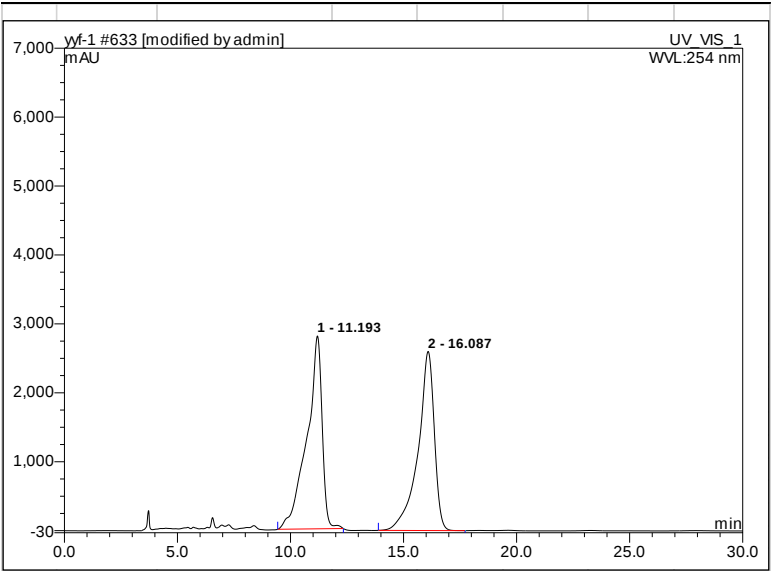
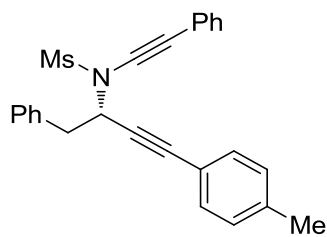


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11.52	n.a.	4142.441	2352.195	50.11	n.a.	BMB*
2	15.53	n.a.	2786.750	2341.858	49.89	n.a.	BMB*
Total:			6929.191	4694.052	100.00	0.000	

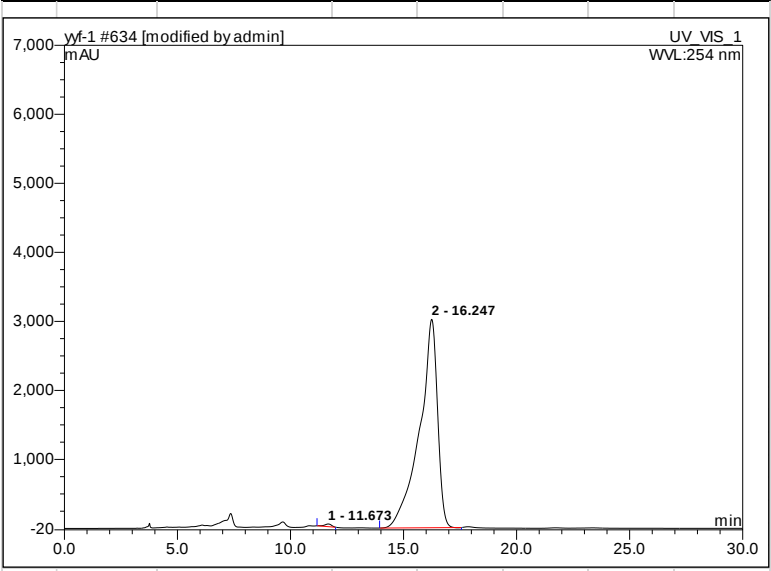


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	10.85	n.a.	49.003	24.526	1.37	n.a.	BMB*
2	14.07	n.a.	2879.864	1766.825	98.63	n.a.	BMB*
Total:			2928.868	1791.351	100.00	0.000	

Compound 11

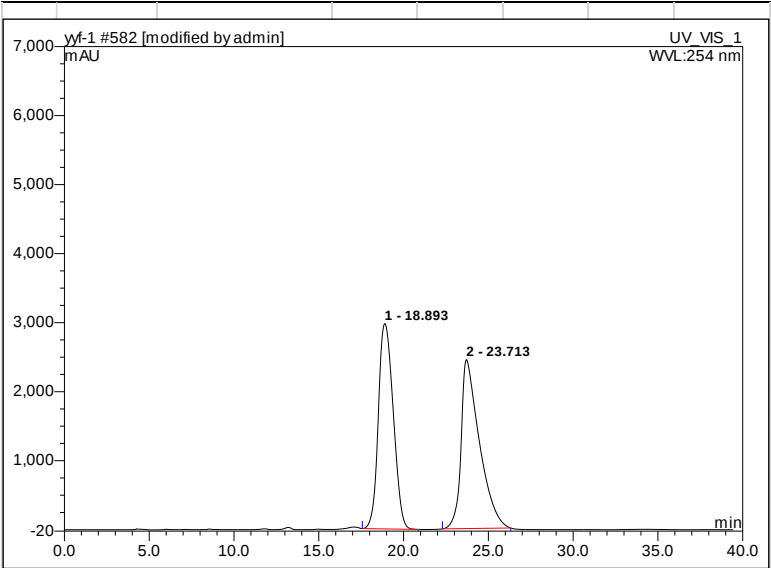
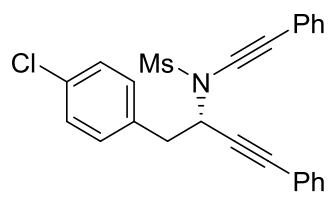


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11.19	n.a.	2797.670	2197.450	50.42	n.a.	BMB*
2	16.09	n.a.	2598.098	2161.049	49.58	n.a.	BMB*
Total:			5395.768	4358.498	100.00	0.000	

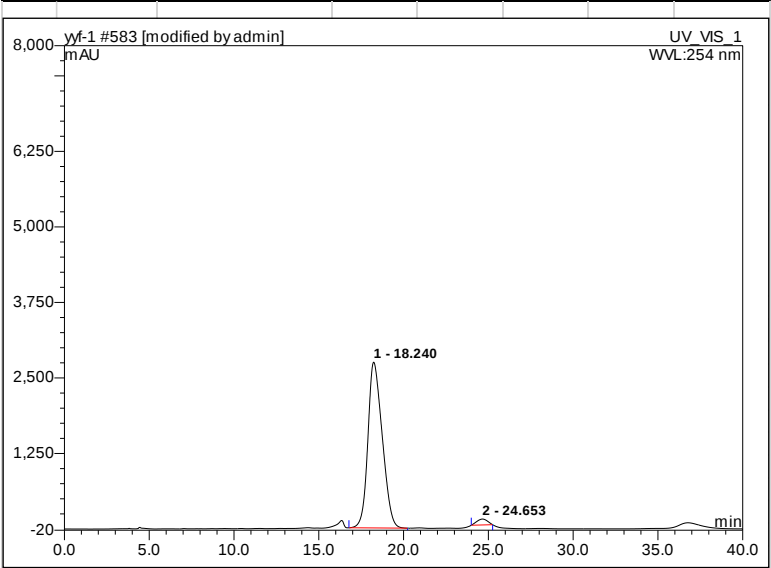


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11.67	n.a.	38.724	13.745	0.49	n.a.	BMB*
2	16.25	n.a.	3018.899	2793.151	99.51	n.a.	BMB*
Total:			3057.622	2806.896	100.00	0.000	

Compound **1m**

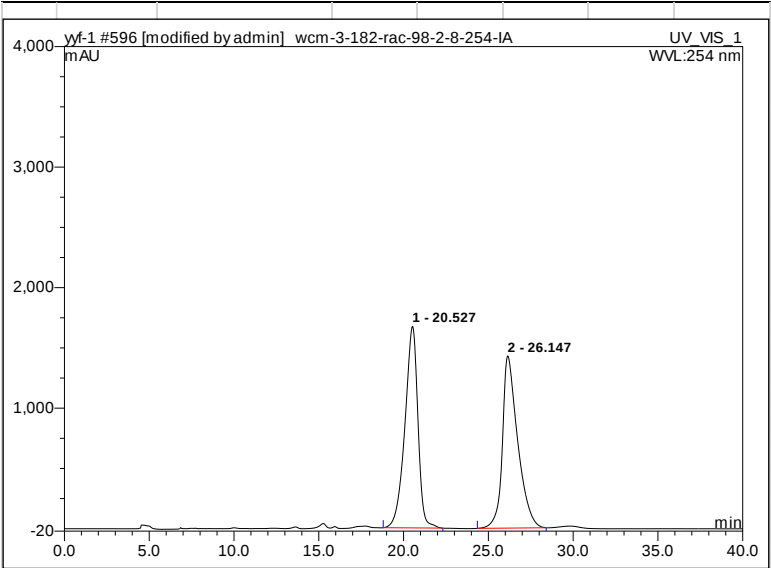
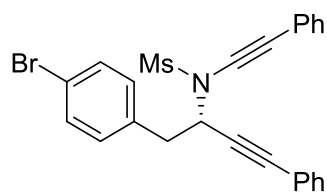


No.	Ret.Time	Peak Name	Height	Area	Rel.Area	Amount	Type
	min		mAU	mAU*min	%		
1	18.89	n.a.	2973.108	3026.939	49.66	n.a.	BMB*
2	23.71	n.a.	2446.865	3068.170	50.34	n.a.	BMB*
Total:			5419.973	6095.109	100.00	0.000	

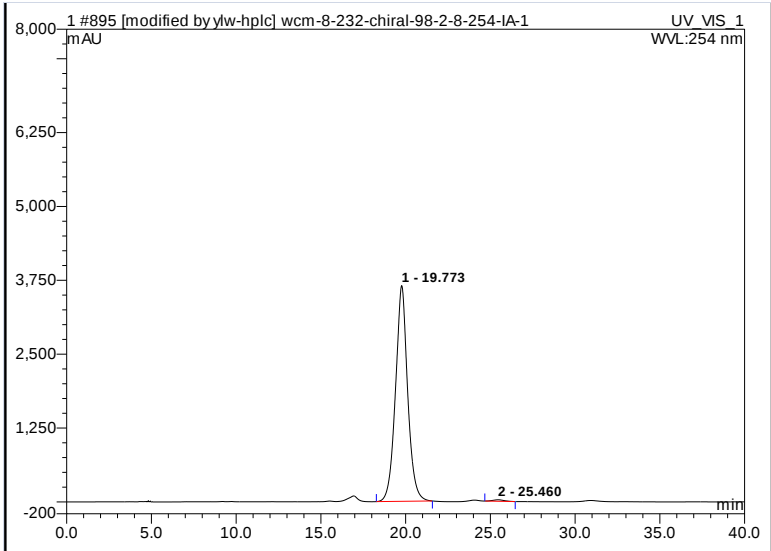


No.	Ret.Time	Peak Name	Height	Area	Rel.Area	Amount	Type
	min		mAU	mAU*min	%		
1	18.24	n.a.	2743.507	2690.338	97.41	n.a.	BMB*
2	24.65	n.a.	97.773	71.511	2.59	n.a.	BMB*
Total:			2841.280	2761.850	100.00	0.000	

Compound **1n**

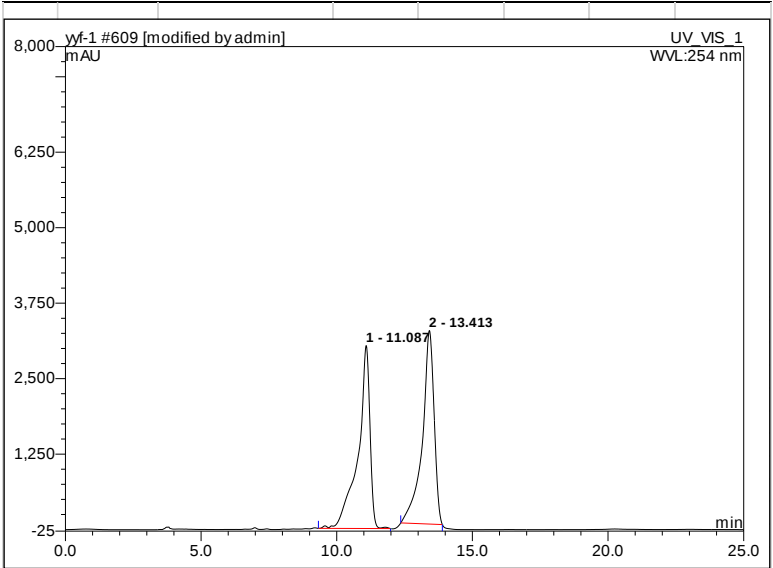
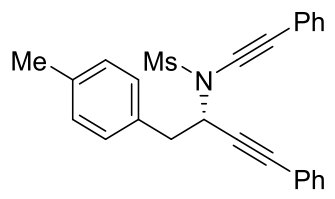


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	20.53	n.a.	1672.445	1486.837	49.93	n.a.	BMB*
2	26.15	n.a.	1428.225	1491.068	50.07	n.a.	BMB*
Total:			3100.670	2977.904	100.00	0.000	

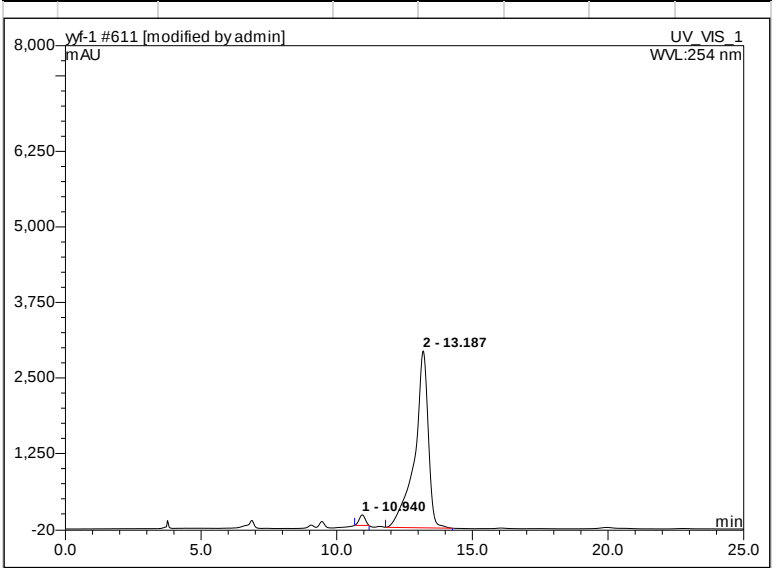


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	19.77	n.a.	3651.196	3030.971	99.37	n.a.	BMB*
2	25.46	n.a.	25.121	19.189	0.63	n.a.	BMB*
Total:			3676.317	3050.160	100.00	0.000	

Compound **1o**

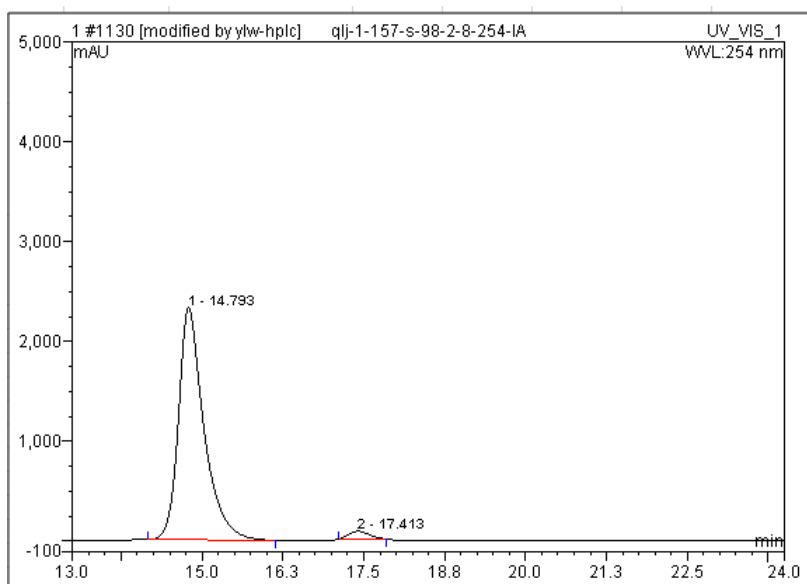
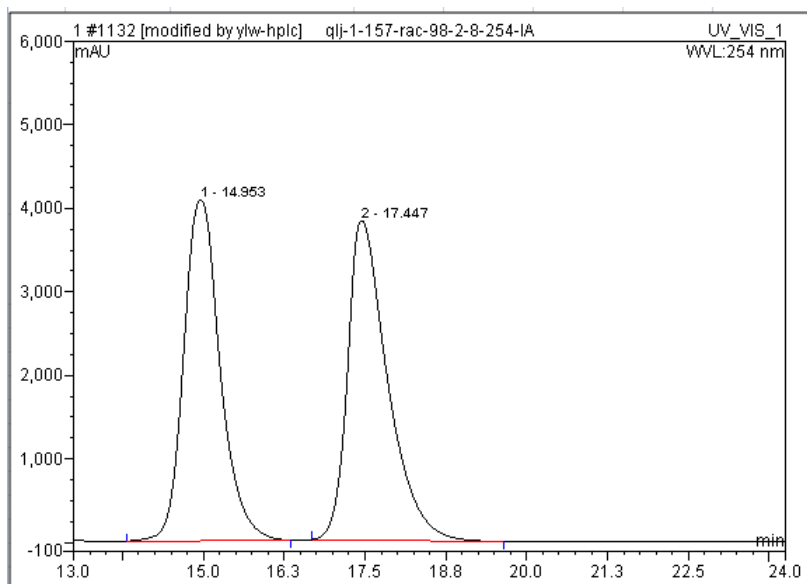
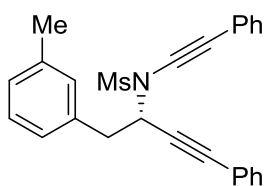


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11.09	n.a.	3028.927	1553.669	49.01	n.a.	BMB*
2	13.41	n.a.	3205.092	1616.344	50.99	n.a.	BMB*
Total:			6234.019	3170.014	100.00	0.000	

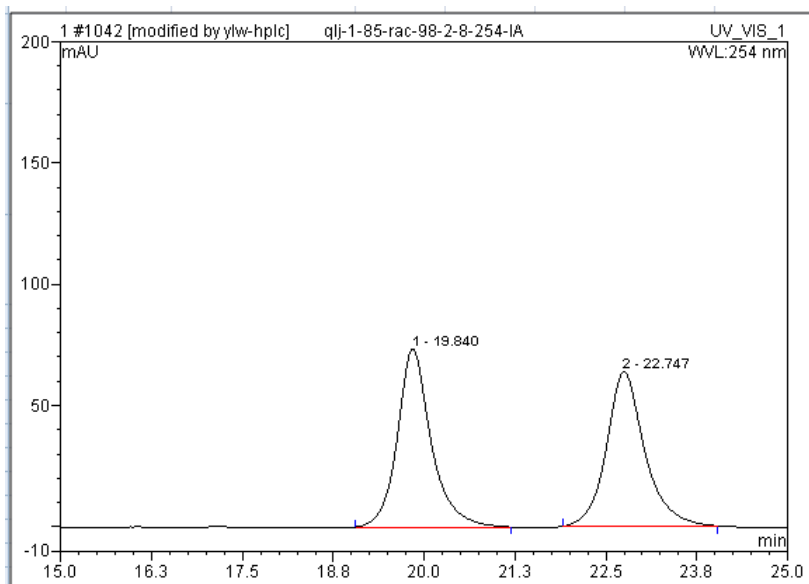
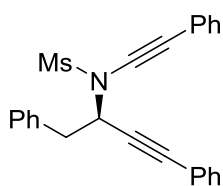


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	10.94	n.a.	173.941	45.298	2.60	n.a.	BMB*
2	13.19	n.a.	2927.979	1697.297	97.40	n.a.	BMB*
Total:			3101.919	1742.595	100.00	0.000	

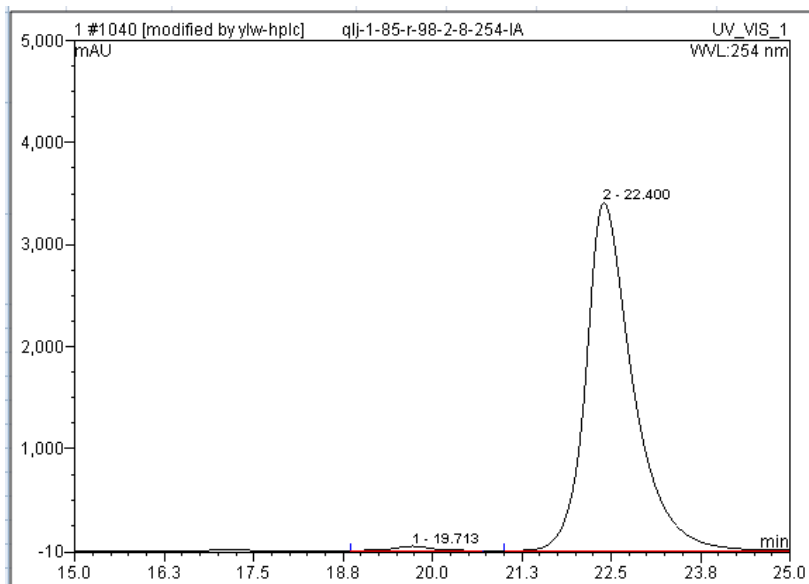
Compound 1p



Compound **1d'**

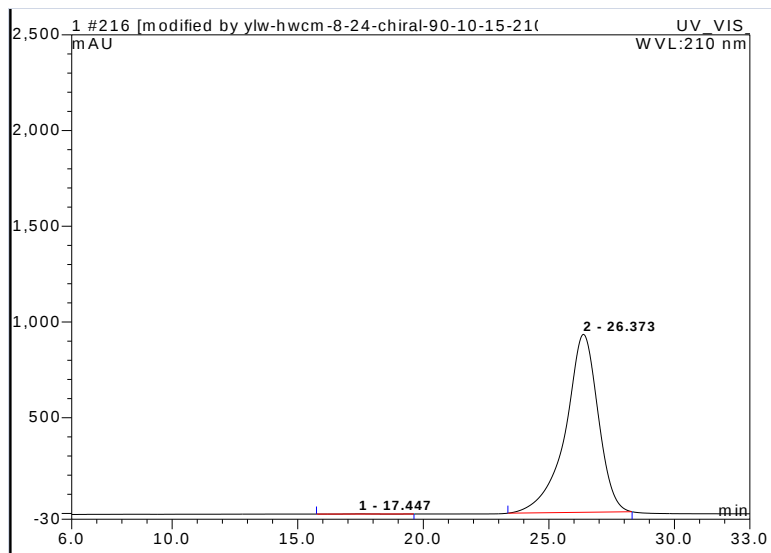
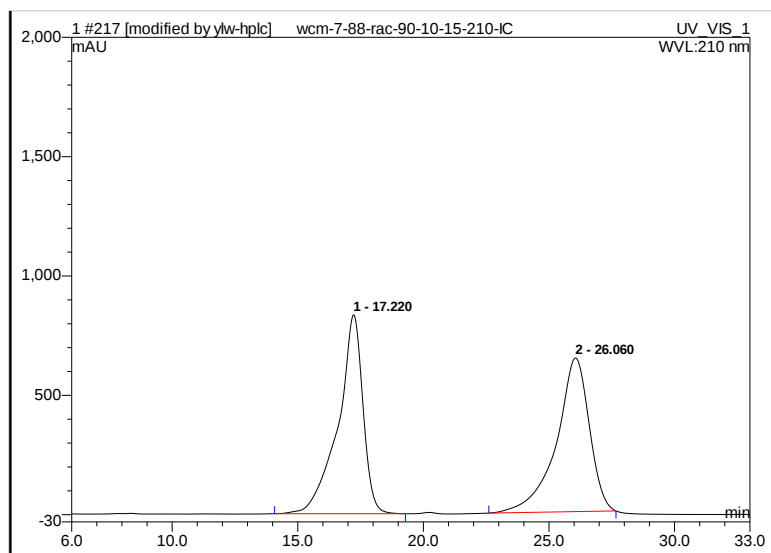
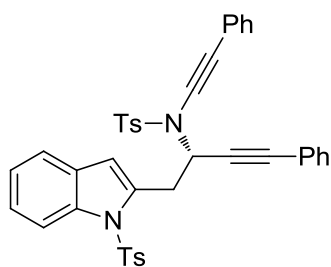


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	19.84	n.a.	73.493	39.763	50.50	n.a.	BMB*
2	22.75	n.a.	63.725	38.975	49.50	n.a.	BMB*
Total:			137.218	78.739	100.00	0.000	

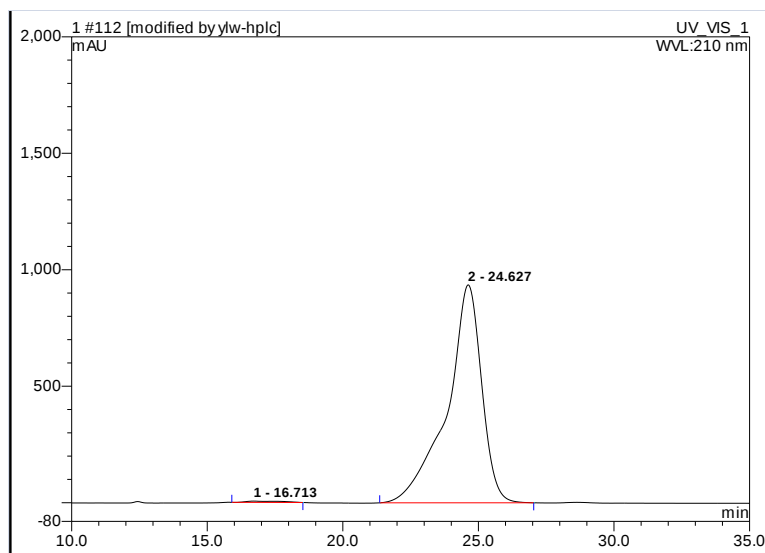
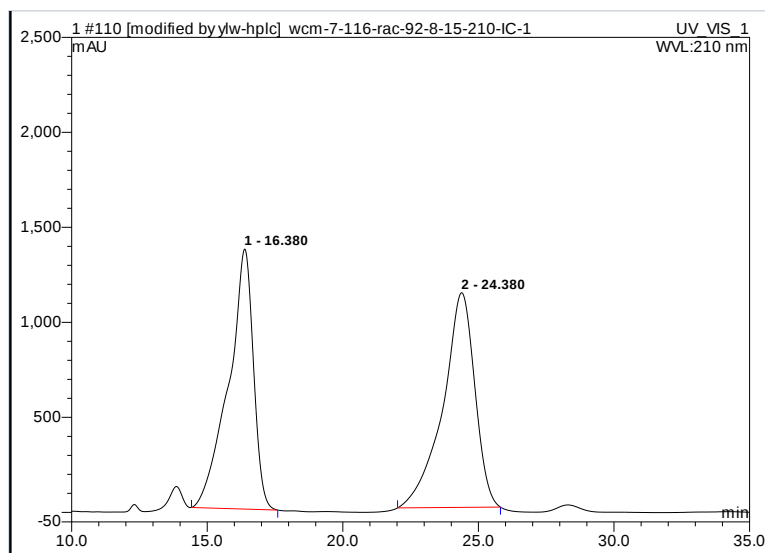
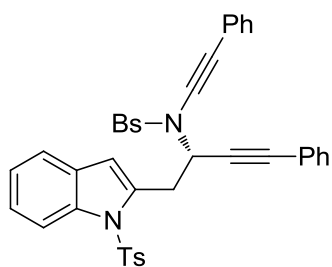


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	19.71	n.a.	43.623	25.517	0.97	n.a.	BMB*
2	22.40	n.a.	3404.237	2604.962	99.03	n.a.	BMB*
Total:			3447.860	2630.479	100.00	0.000	

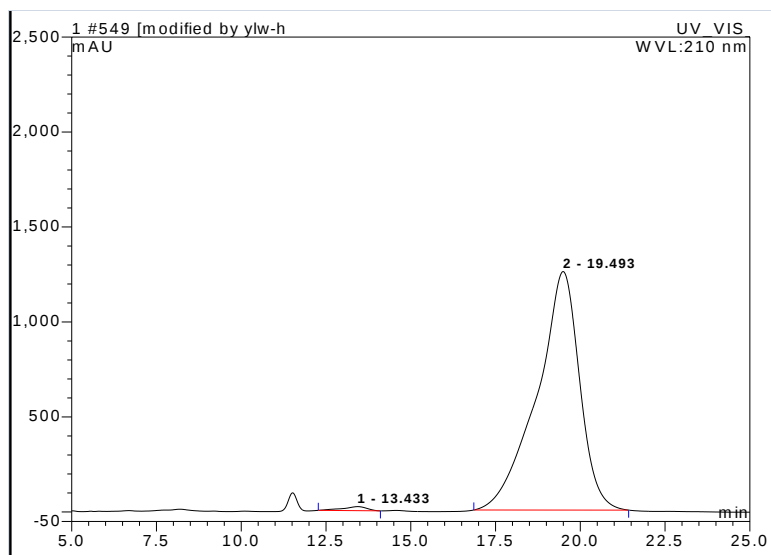
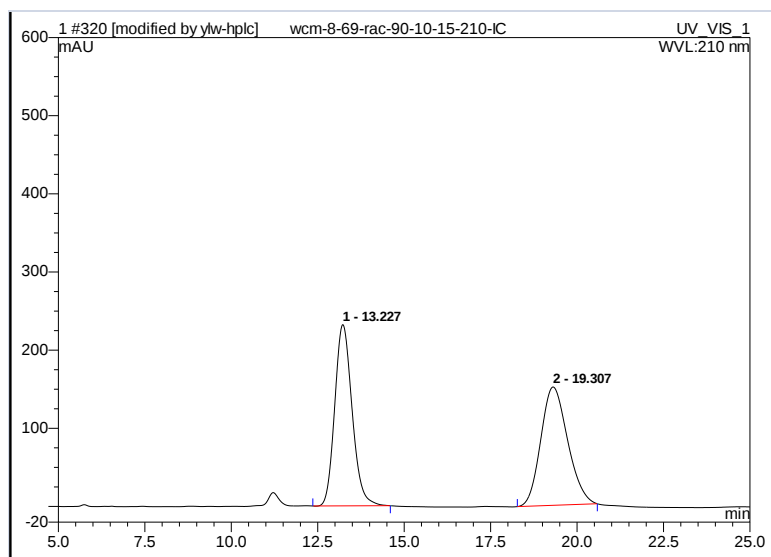
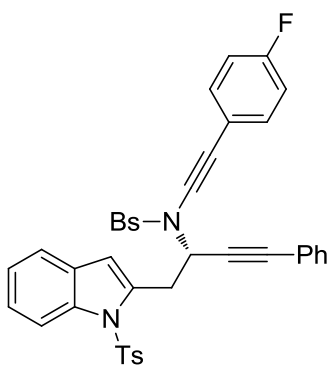
Compound 4a



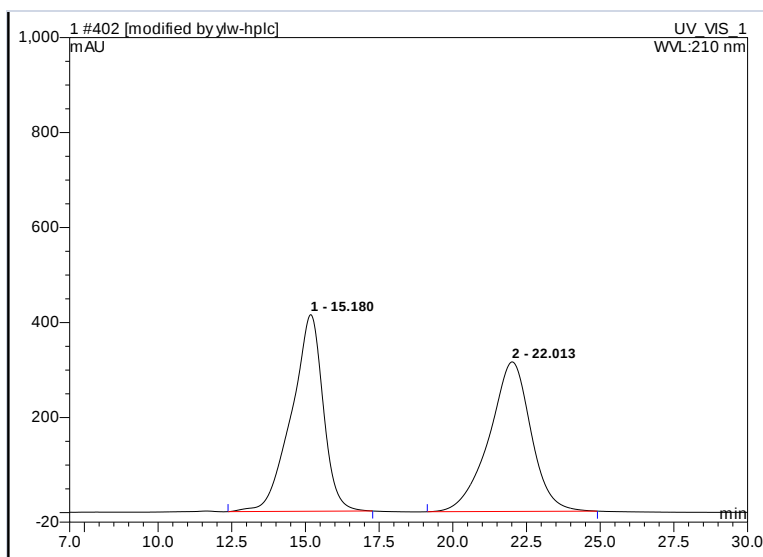
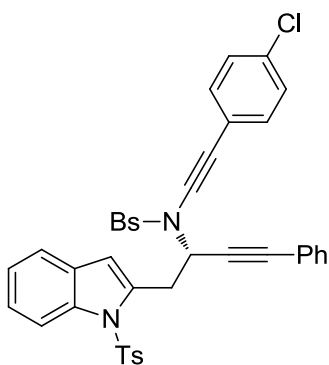
Compound 4b



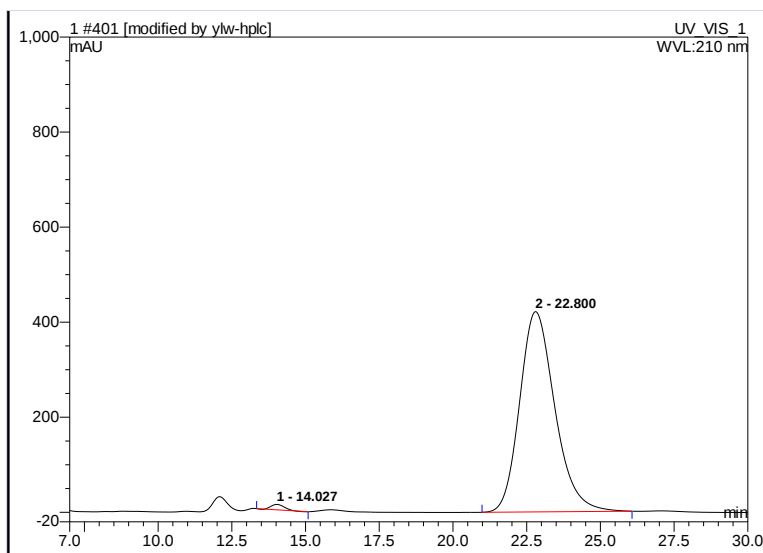
Compound 4c



Compound 4d

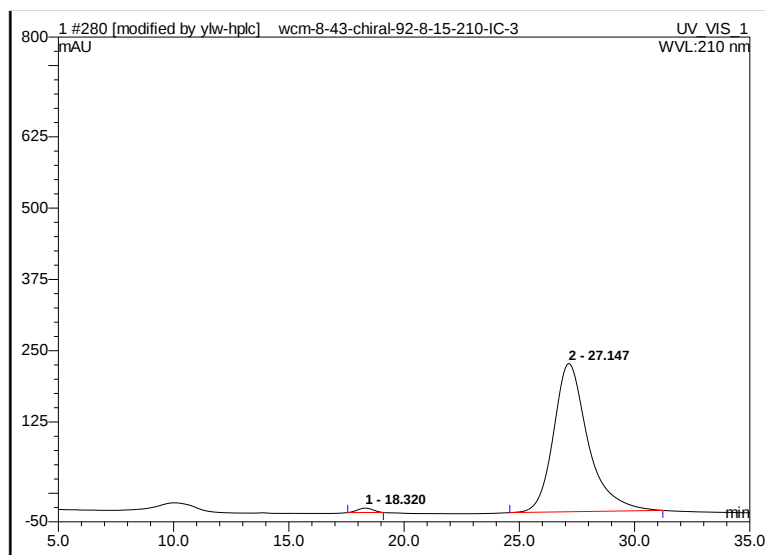
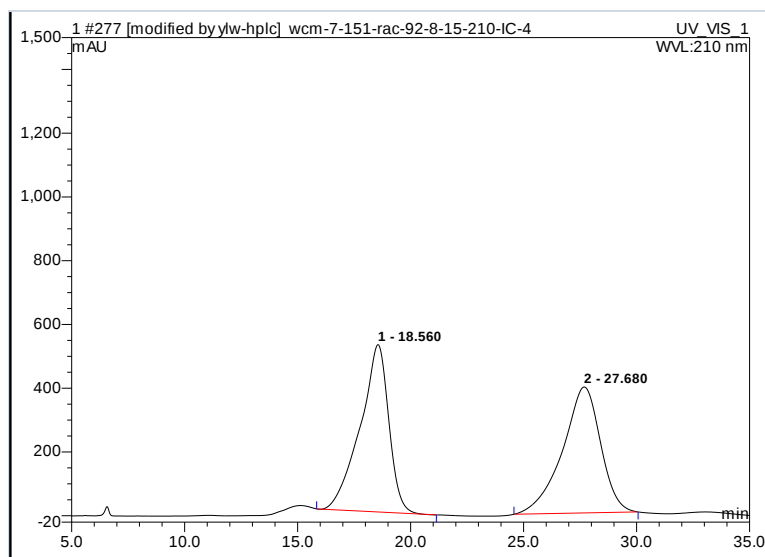
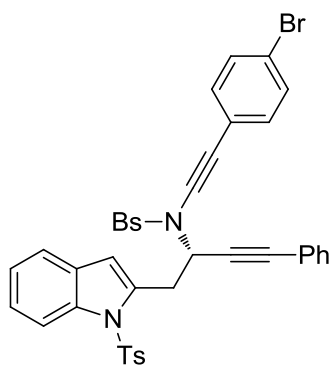


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	15.18	n.a.	413.811	515.152	49.90	n.a.	BMB*
2	22.01	n.a.	314.752	517.149	50.10	n.a.	BMB*
Total:			728.563	1032.301	100.00	0.000	

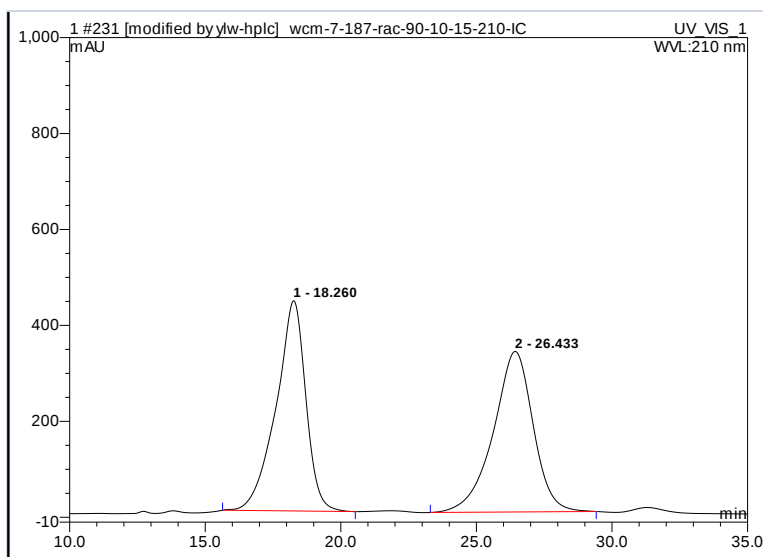
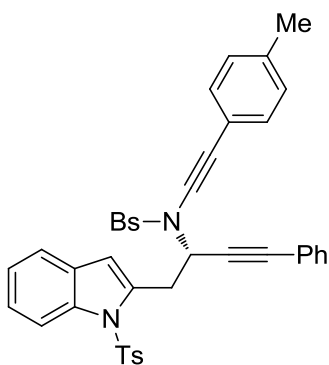


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	14.03	n.a.	11.386	5.701	0.97	n.a.	BMB*
2	22.80	n.a.	421.331	582.823	99.03	n.a.	BMB*
Total:			432.717	588.525	100.00	0.000	

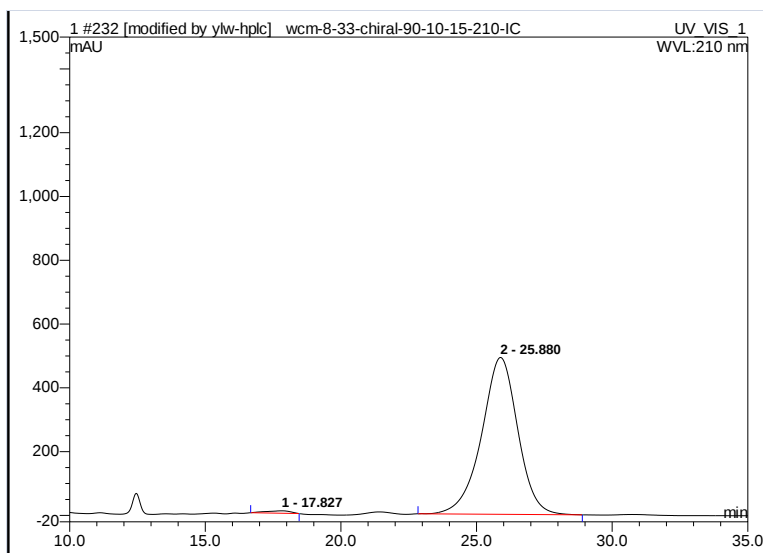
Compound 4e



Compound 4f

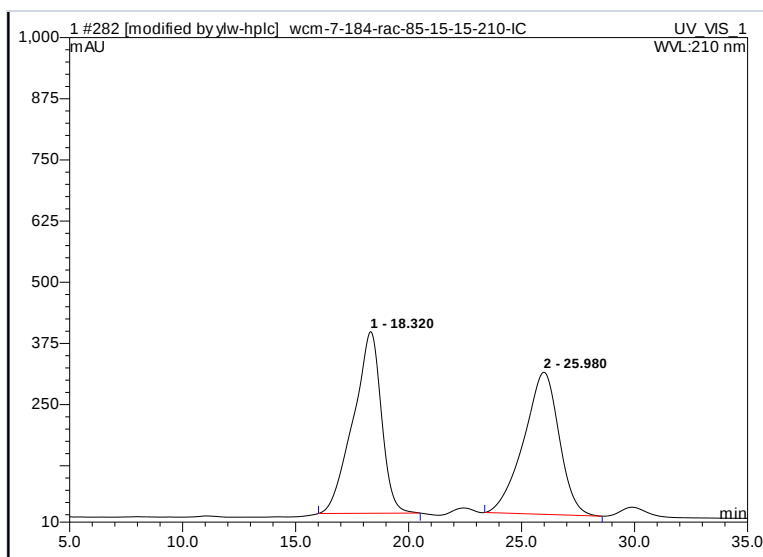
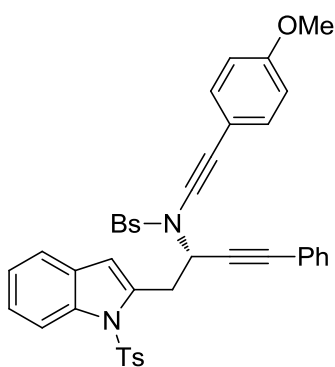


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	18.26	n.a.	438.101	558.820	49.47	n.a.	BMB*
2	26.43	n.a.	334.625	570.777	50.53	n.a.	BMB*
Total:			772.726	1129.597	100.00	0.000	

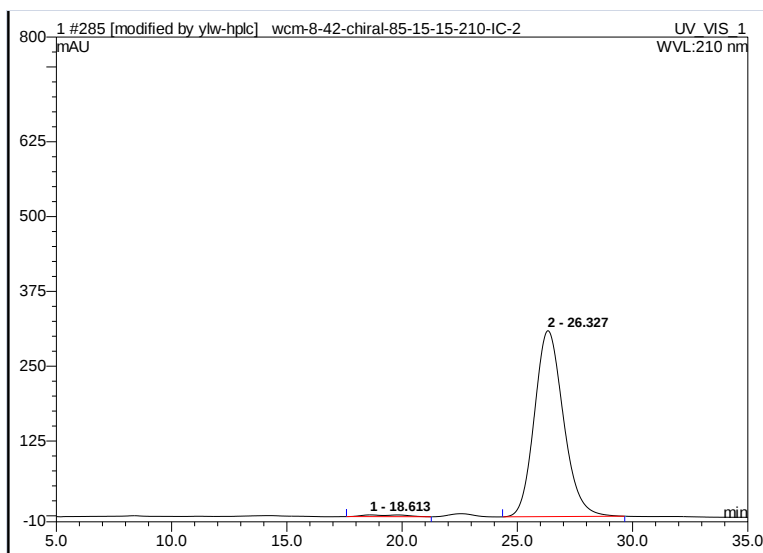


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	17.83	n.a.	7.655	7.959	1.04	n.a.	BMB*
2	25.88	n.a.	491.666	760.937	98.96	n.a.	BMB*
Total:			499.321	768.896	100.00	0.000	

Compound 4g

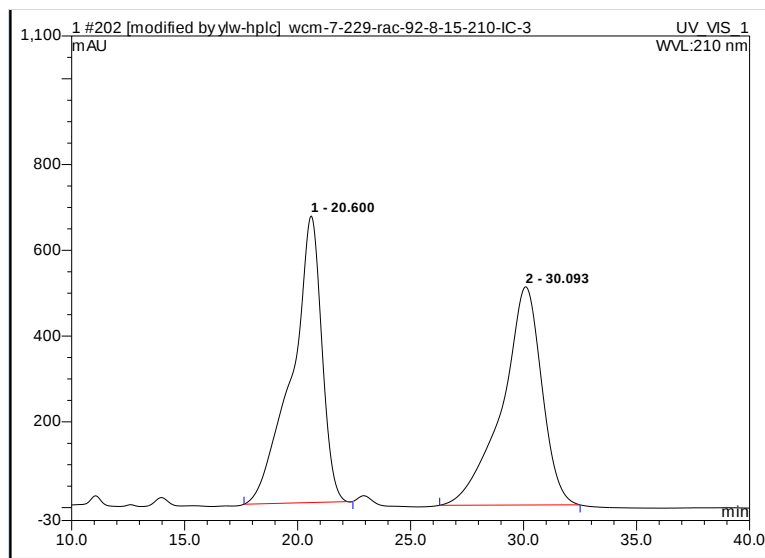
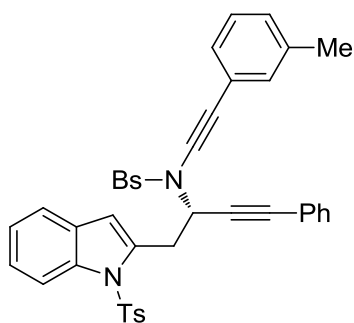


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	18.32	n.a.	370.877	535.001	50.36	n.a.	BMB*
2	25.98	n.a.	290.348	527.272	49.64	n.a.	BMB*
Total:			661.224	1062.273	100.00	0.000	

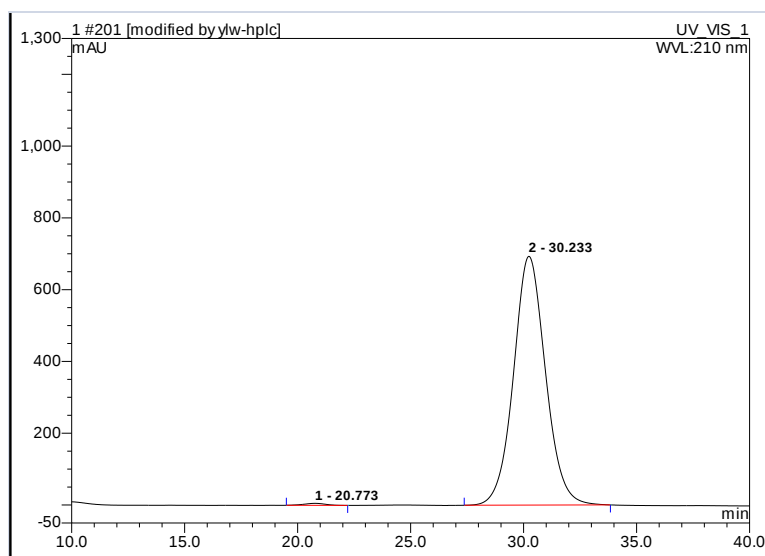


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	18.61	n.a.	2.923	6.012	1.31	n.a.	BMB*
2	26.33	n.a.	310.617	452.926	98.69	n.a.	BMB*
Total:			313.539	458.938	100.00	0.000	

Compound 4h

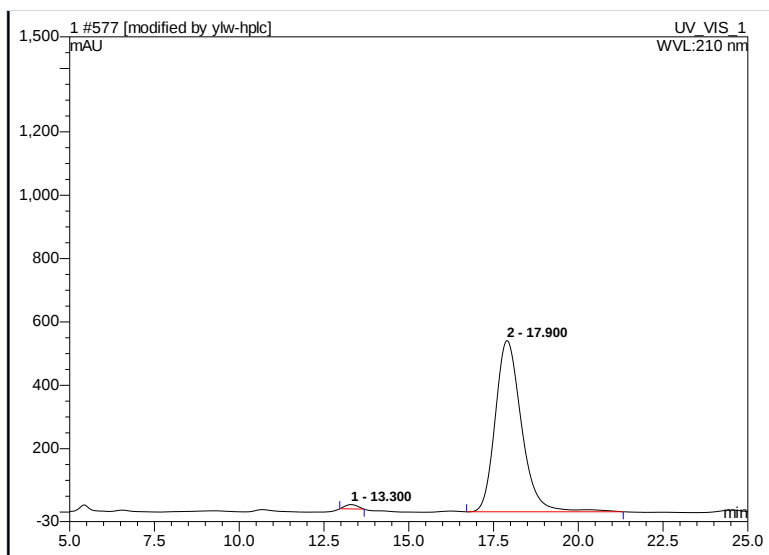
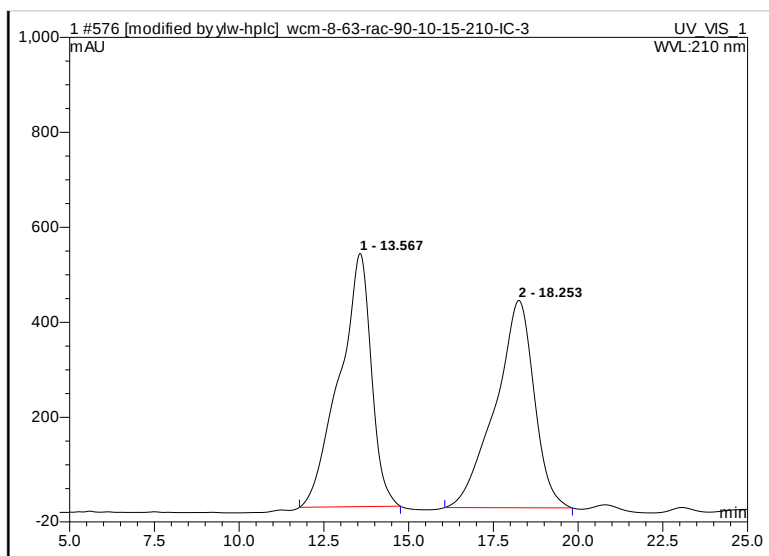
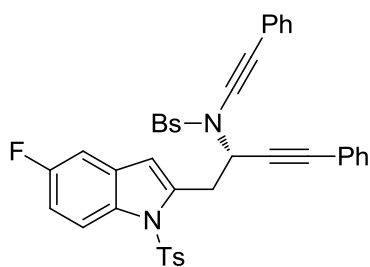


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	20.60	n.a.	667.977	1026.618	49.76	n.a.	BMB*
2	30.09	n.a.	508.822	1036.618	50.24	n.a.	BMB*
Total:			1176.799	2063.235	100.00	0.000	

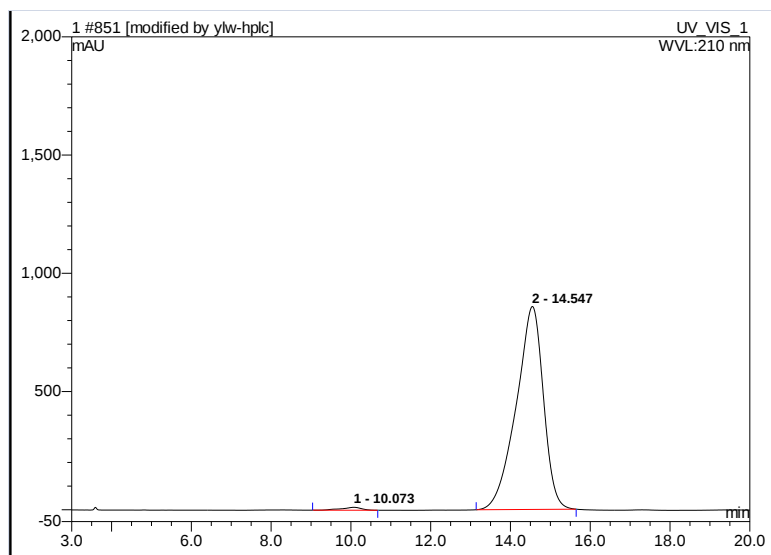
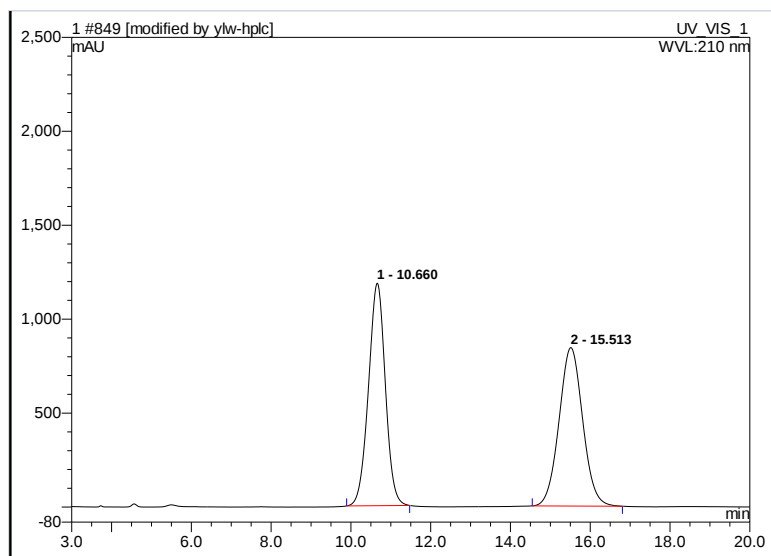
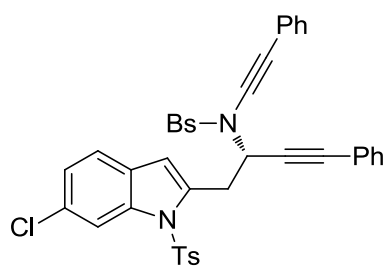


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	20.77	n.a.	5.535	6.041	0.53	n.a.	BMB*
2	30.23	n.a.	693.047	1138.397	99.47	n.a.	BMB*
Total:			698.582	1144.438	100.00	0.000	

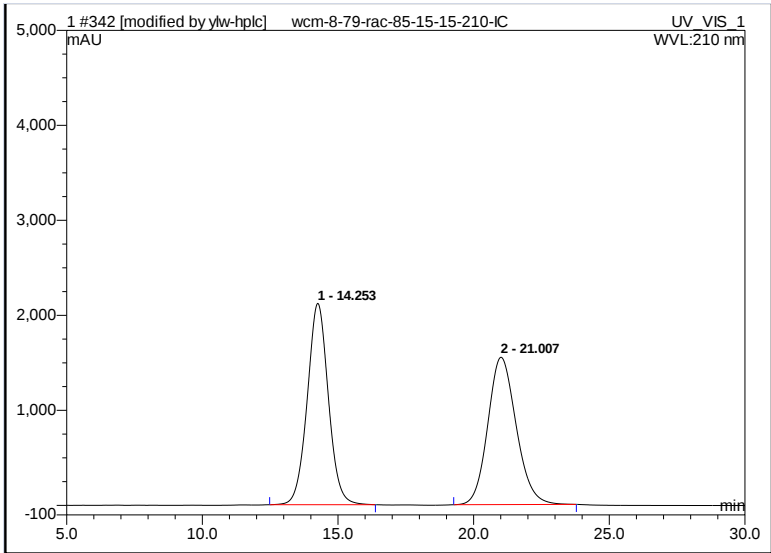
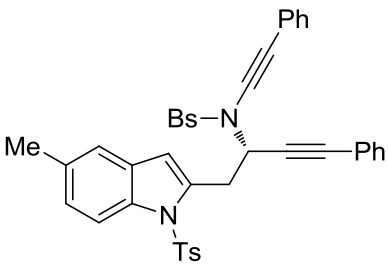
Compound 4i



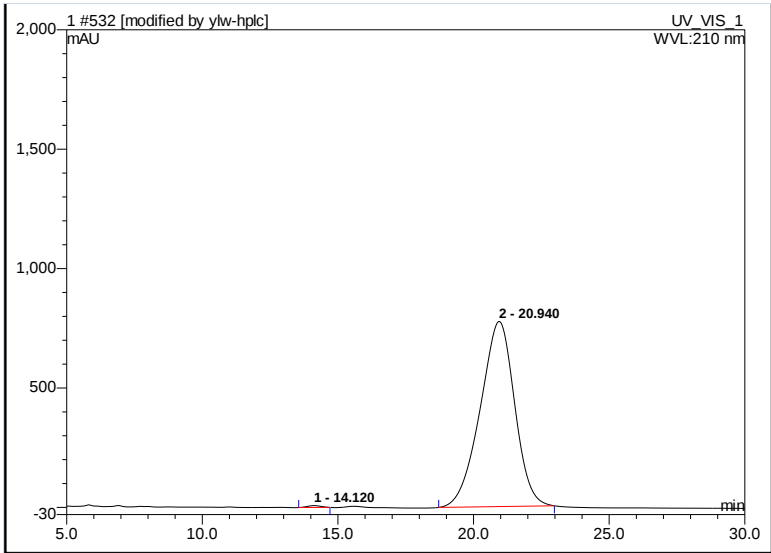
Compound 4j



Compound 4k

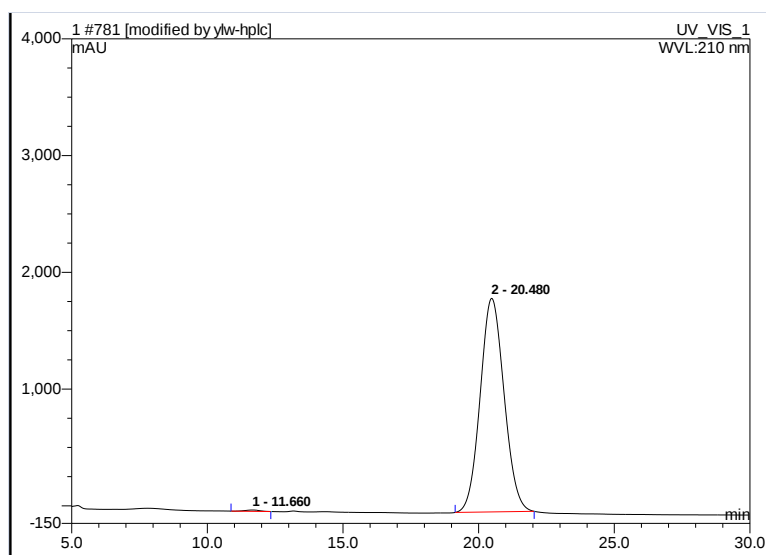
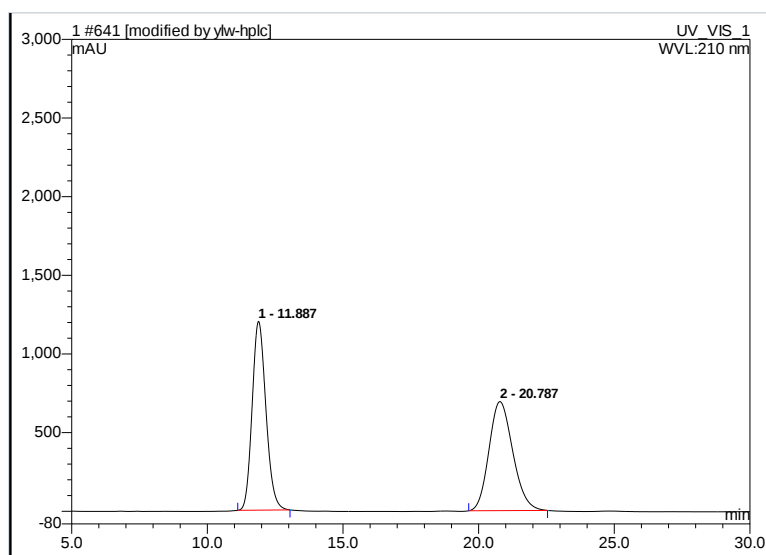
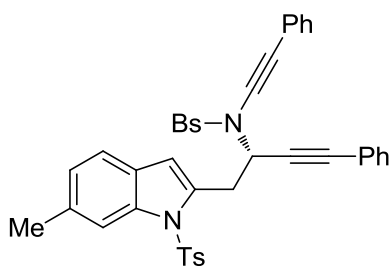


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	14.25	n.a.	2118.722	1909.458	50.38	n.a.	BMB*
2	21.01	n.a.	1550.553	1880.406	49.62	n.a.	BMB*
Total:			3669.275	3789.864	100.00	0.000	

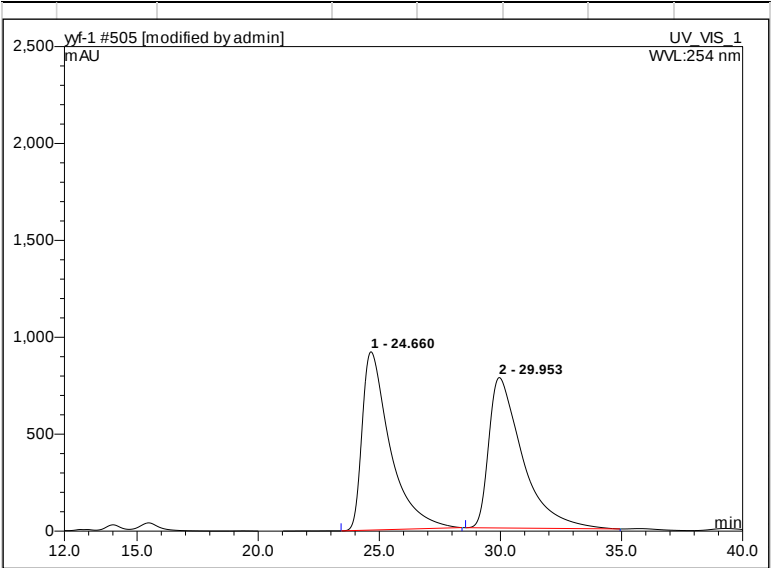
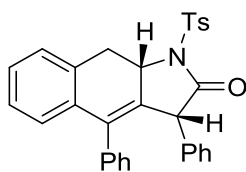


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	14.12	n.a.	7.724	4.537	0.40	n.a.	BMB*
2	20.94	n.a.	775.113	1141.154	99.60	n.a.	BMB*
Total:			782.838	1145.691	100.00	0.000	

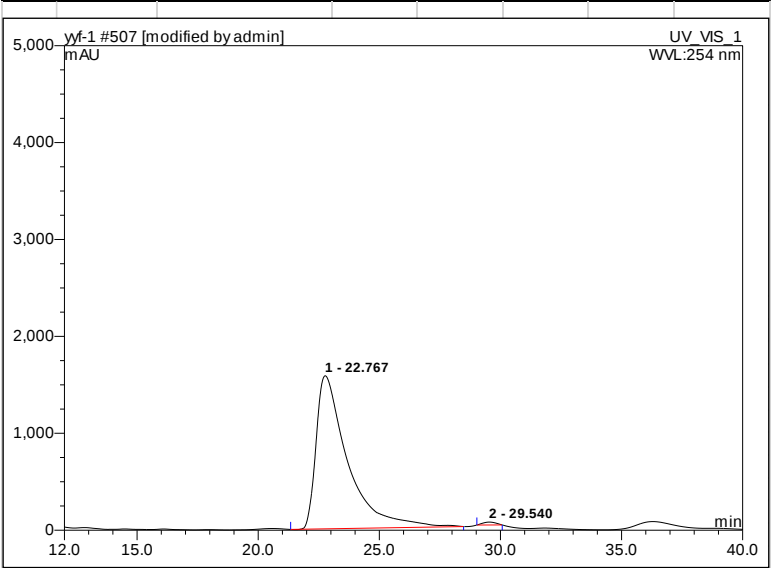
Compound 4l



Compound 2a

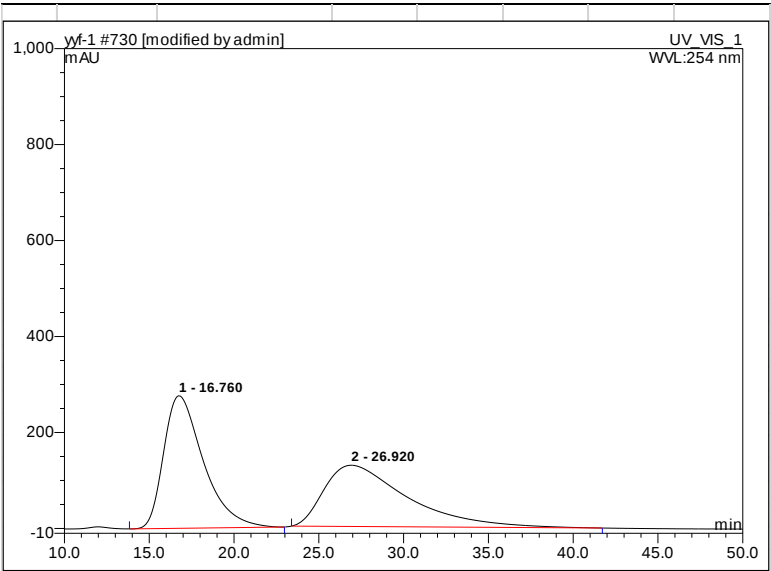
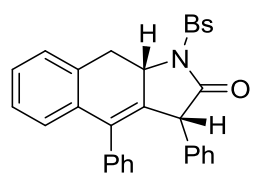


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	24.66	n.a.	919.537	1231.465	49.61	n.a.	BMB*
2	29.95	n.a.	775.851	1250.645	50.39	n.a.	BMB*
Total:			1695.388	2482.110	100.00	0.000	

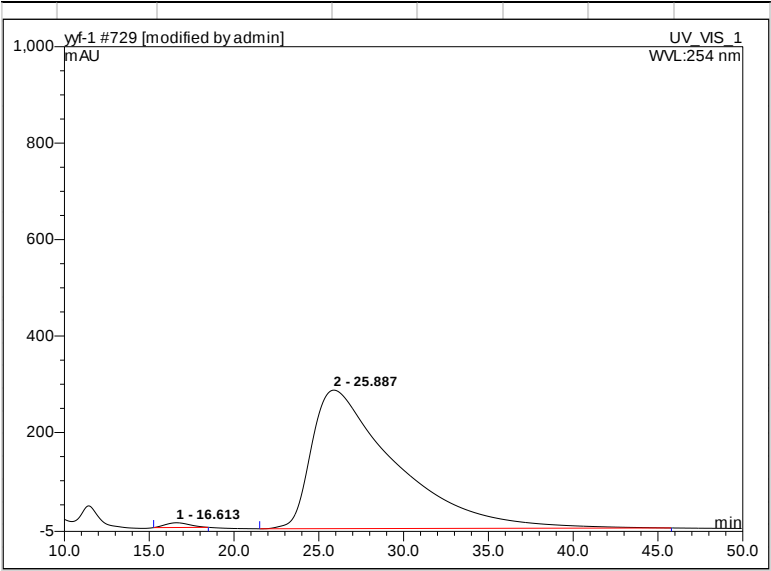


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	22.77	n.a.	1579.469	2381.697	99.21	n.a.	BMB*
2	29.54	n.a.	29.772	19.000	0.79	n.a.	BMB*
Total:			1609.240	2400.698	100.00	0.000	

Compound 2b

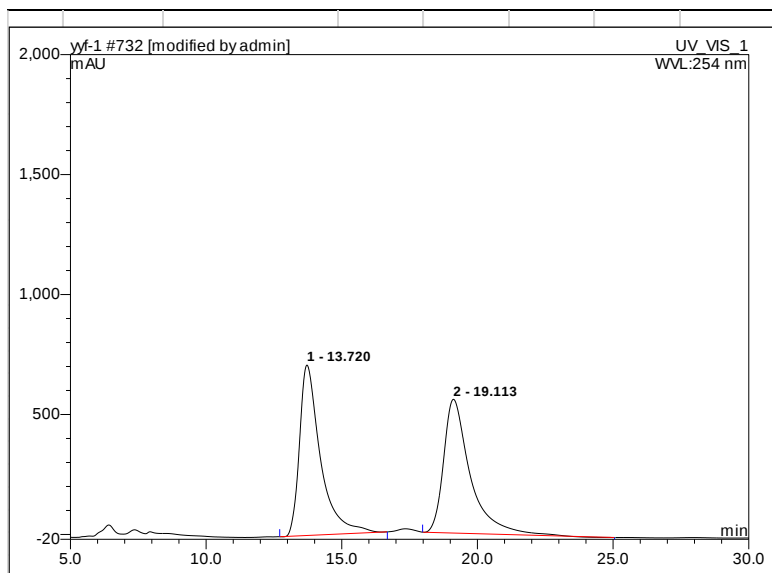
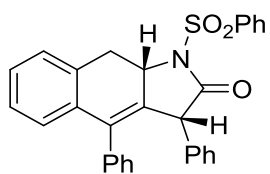


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	16.76	n.a.	276.055	749.049	50.83	n.a.	BMB*
2	26.92	n.a.	127.568	724.507	49.17	n.a.	BMB*
Total:			403.623	1473.557	100.00	0.000	

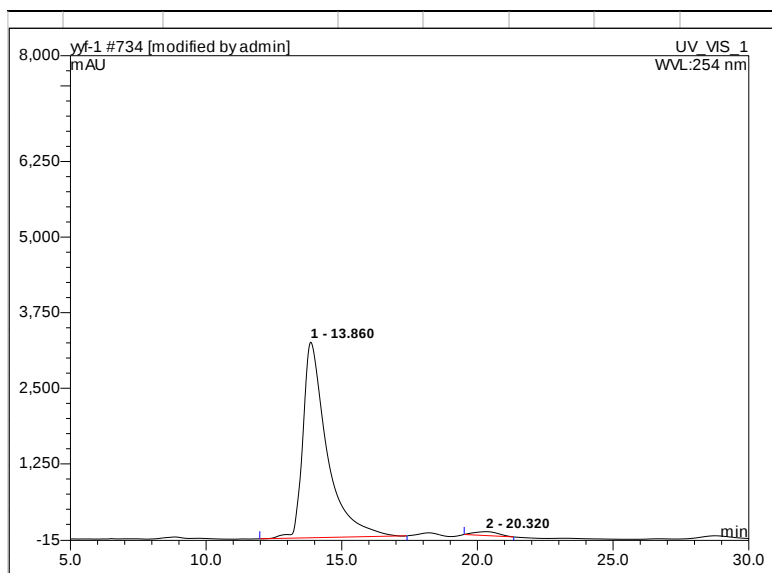


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	16.61	n.a.	9.791	16.234	0.97	n.a.	BMB*
2	25.89	n.a.	287.128	1653.261	99.03	n.a.	BMB*
Total:			296.919	1669.495	100.00	0.000	

Compound 2c

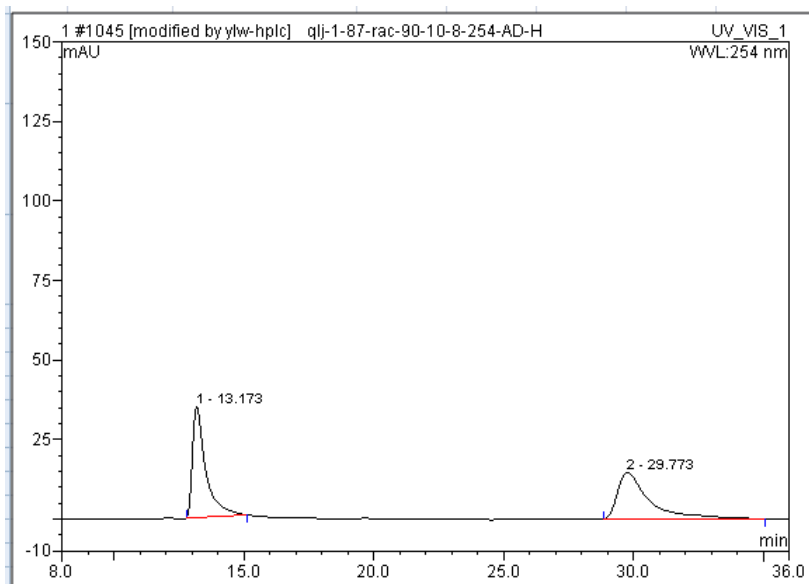
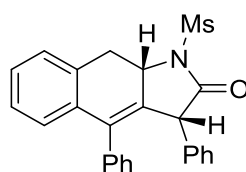


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	13.72	n.a.	709.979	635.648	50.10	n.a.	BMB*
2	19.11	n.a.	557.201	633.205	49.90	n.a.	BMB*
Total:			1267.180	1268.853	100.00	0.000	

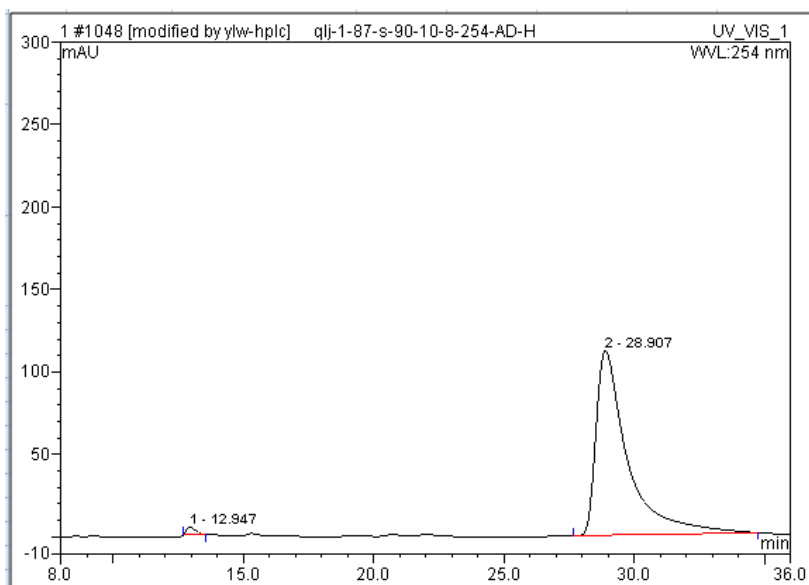


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	13.86	n.a.	3233.265	3319.049	98.05	n.a.	BMB*
2	20.32	n.a.	63.920	66.171	1.95	n.a.	BMB*
Total:			3297.185	3385.220	100.00	0.000	

Compound 2d

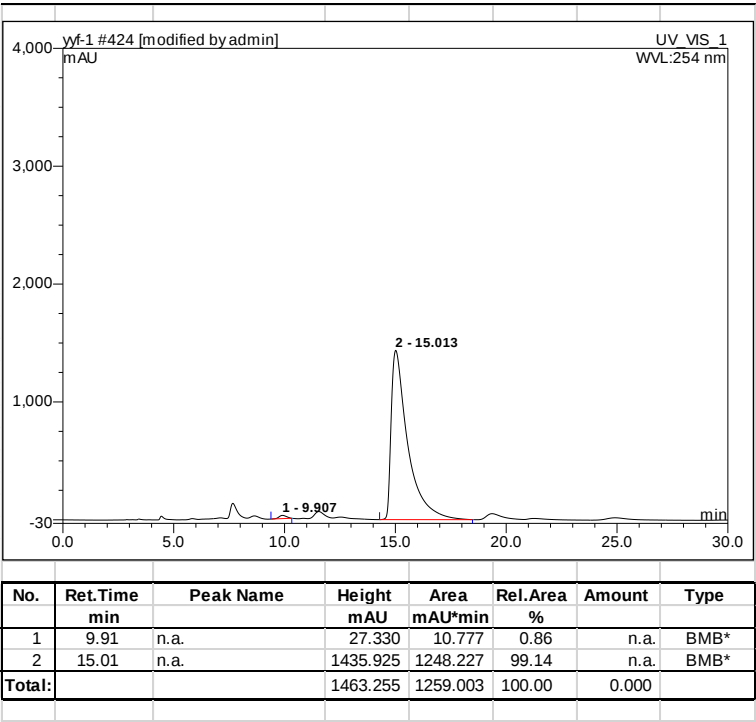
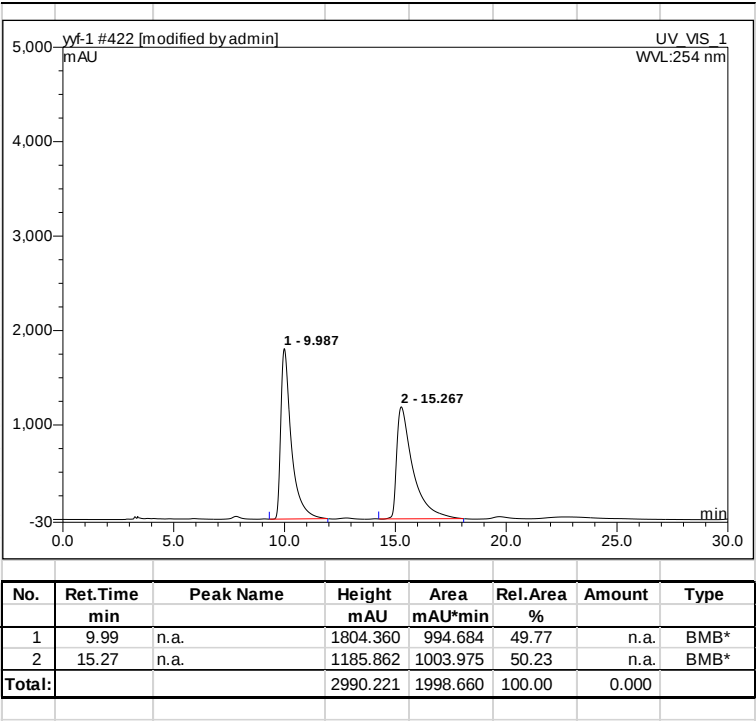
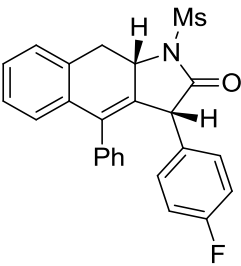


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	13.17	n.a.	34.826	20.759	50.06	n.a.	BMB*
2	29.77	n.a.	14.678	20.710	49.94	n.a.	BM *
Total:			49.504	41.469	100.00	0.000	

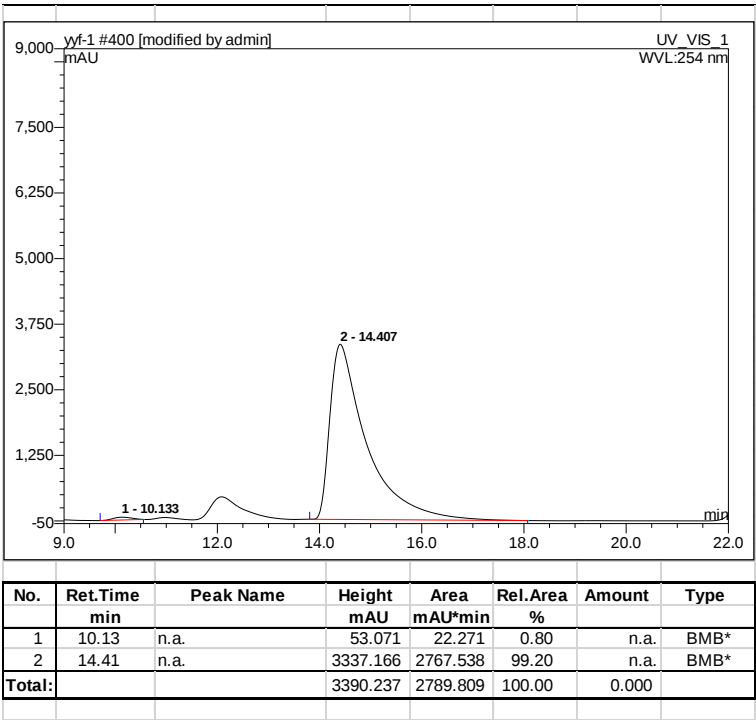
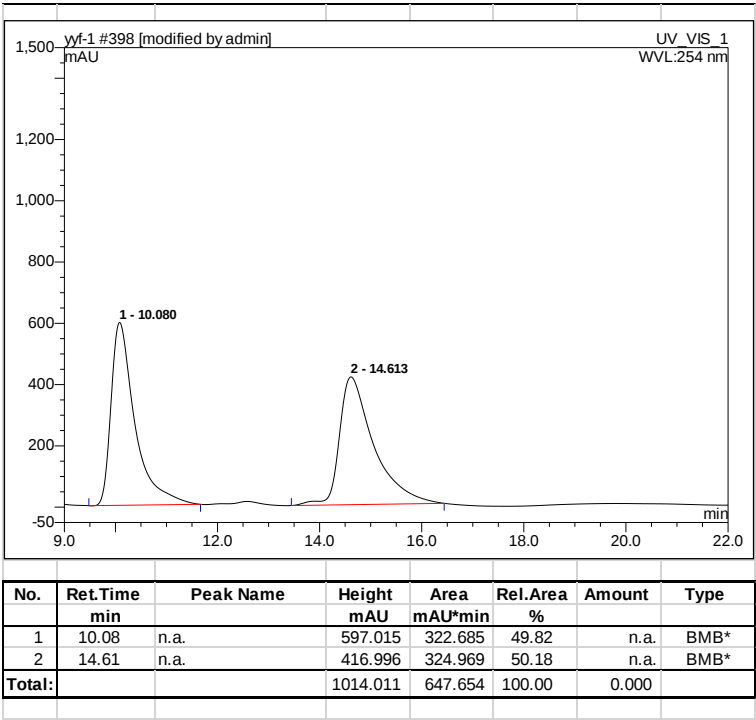
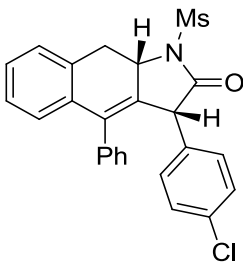


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	12.95	n.a.	4.373	1.660	1.04	n.a.	BMB*
2	28.91	n.a.	111.942	157.580	98.96	n.a.	BMB*
Total:			116.314	159.240	100.00	0.000	

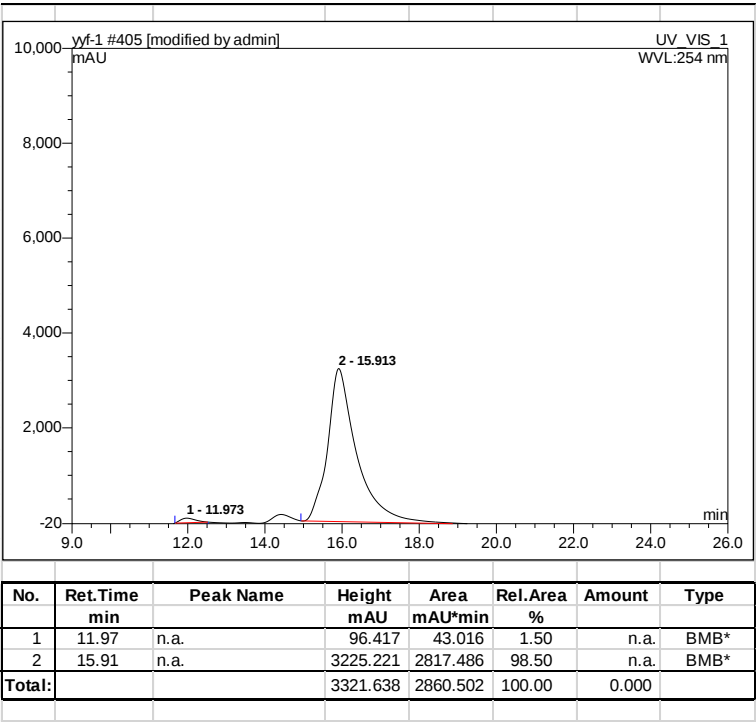
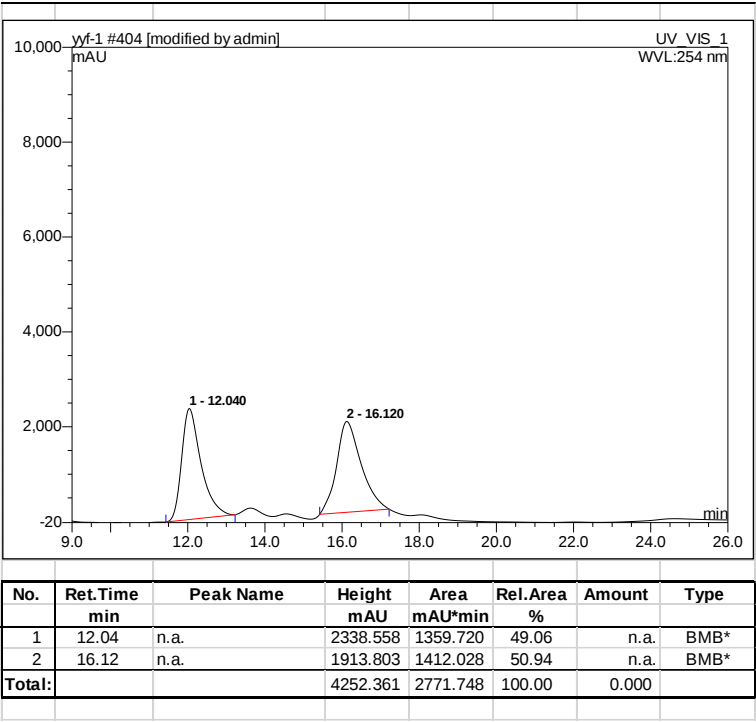
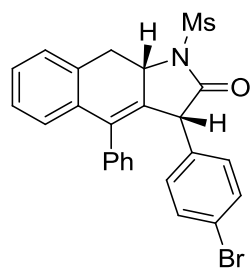
Compound 2e



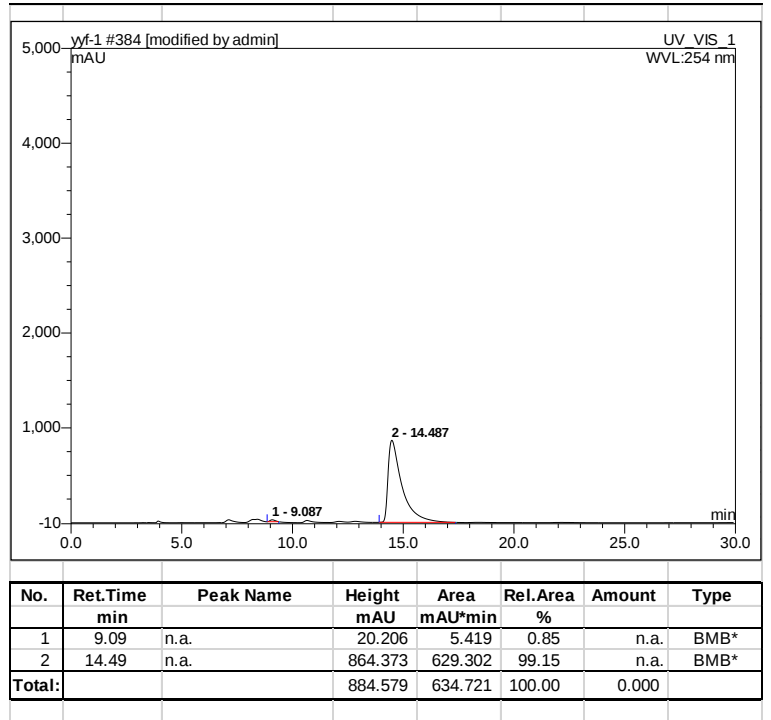
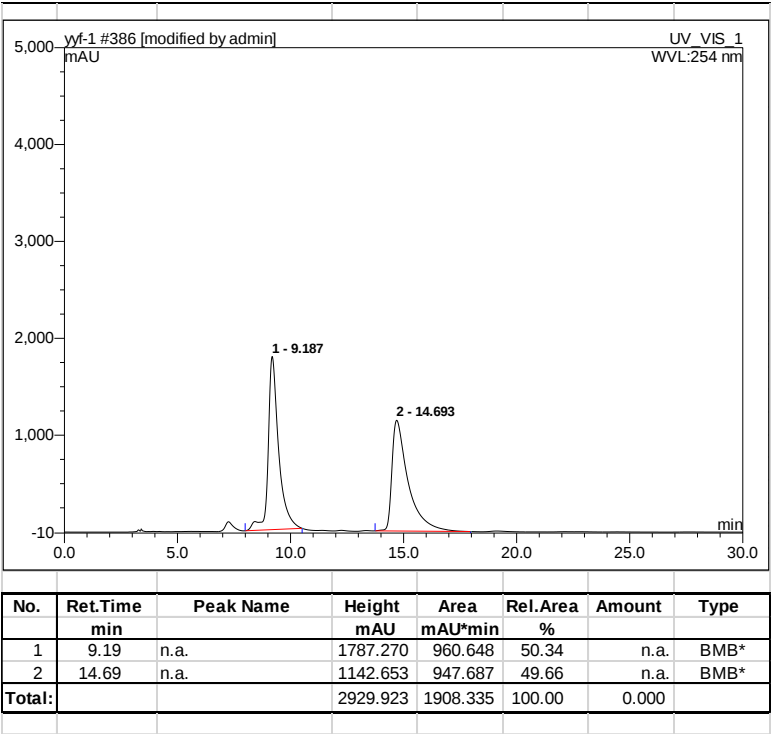
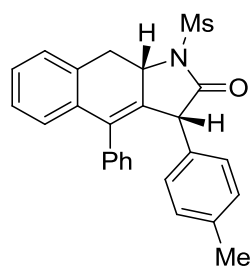
Compound 2f



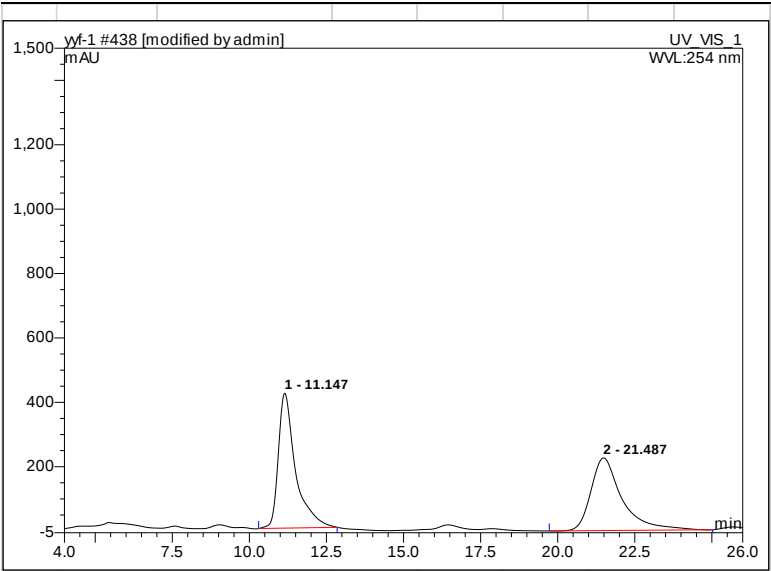
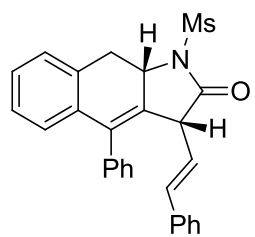
Compound 2g



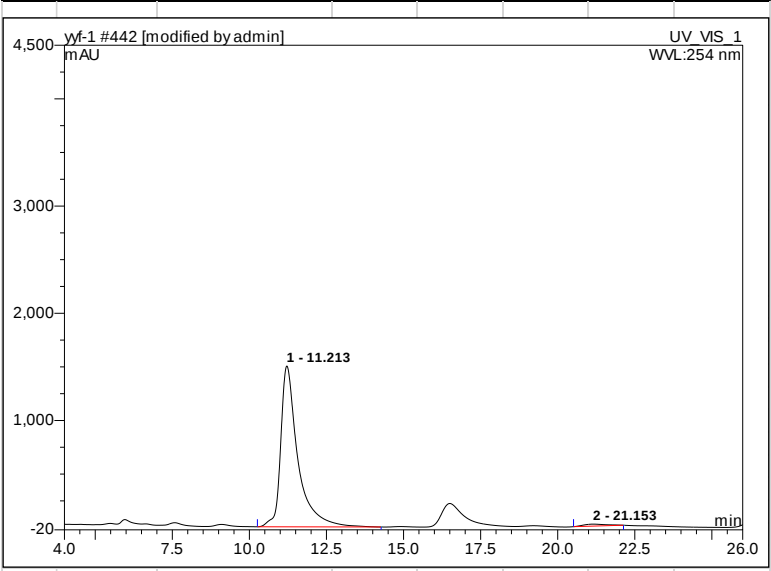
Compound 2h



Compound 2i

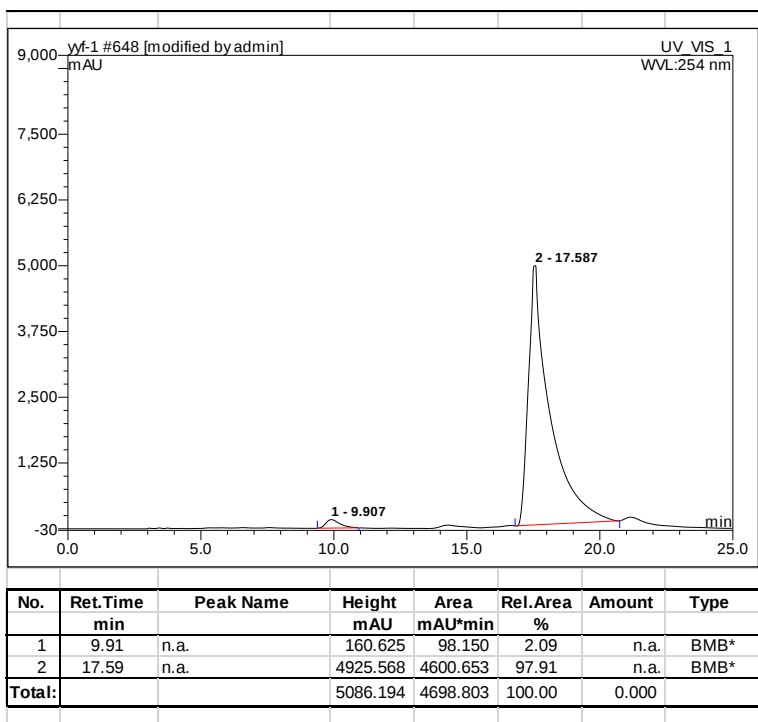
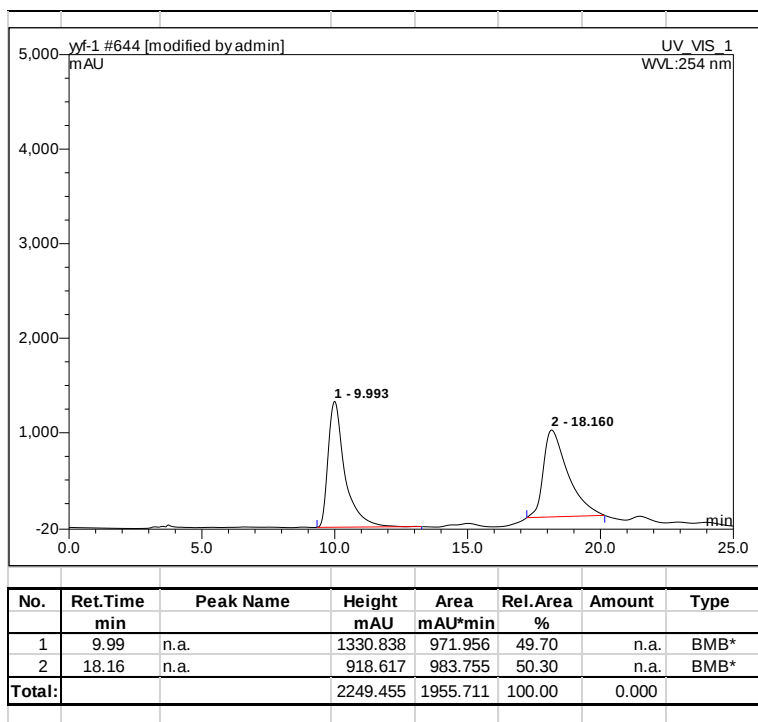
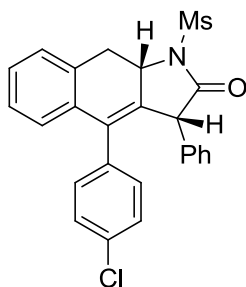


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11.15	n.a.	418.732	270.912	50.74	n.a.	BMB*
2	21.49	n.a.	225.697	263.028	49.26	n.a.	BMB*
Total:			644.428	533.940	100.00	0.000	

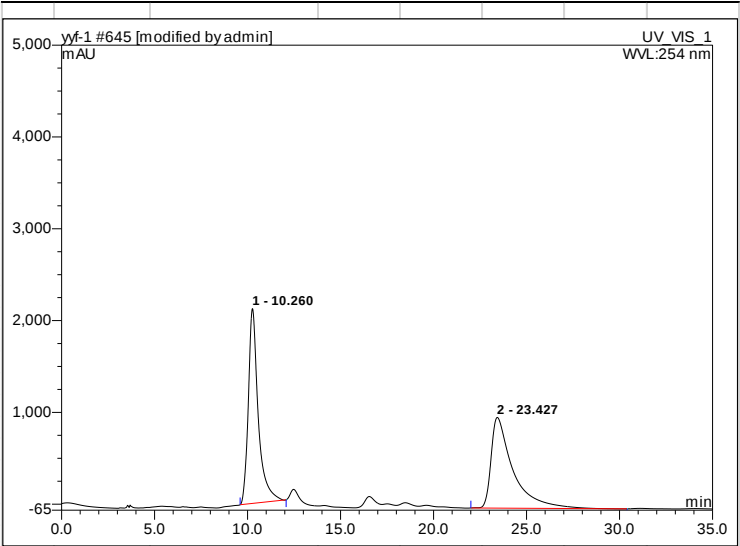
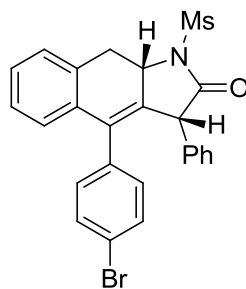


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11.21	n.a.	1499.495	968.119	98.41	n.a.	BMB*
2	21.15	n.a.	18.393	15.650	1.59	n.a.	BMB*
Total:			1517.888	983.769	100.00	0.000	

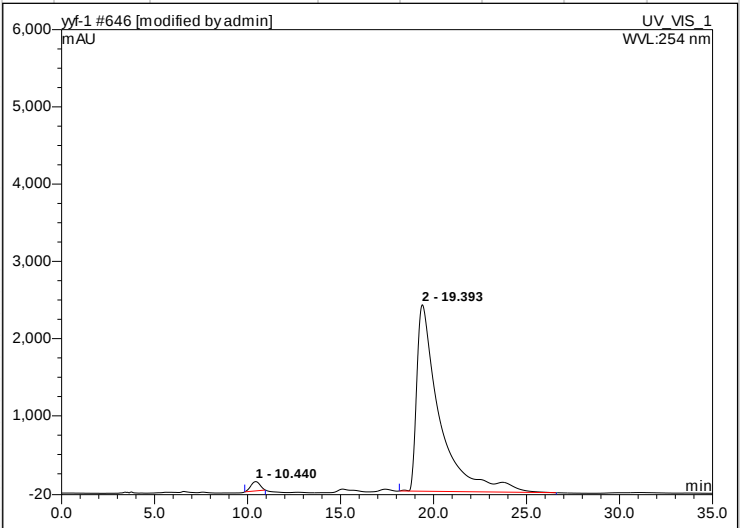
Compound 2j



Compound 2k

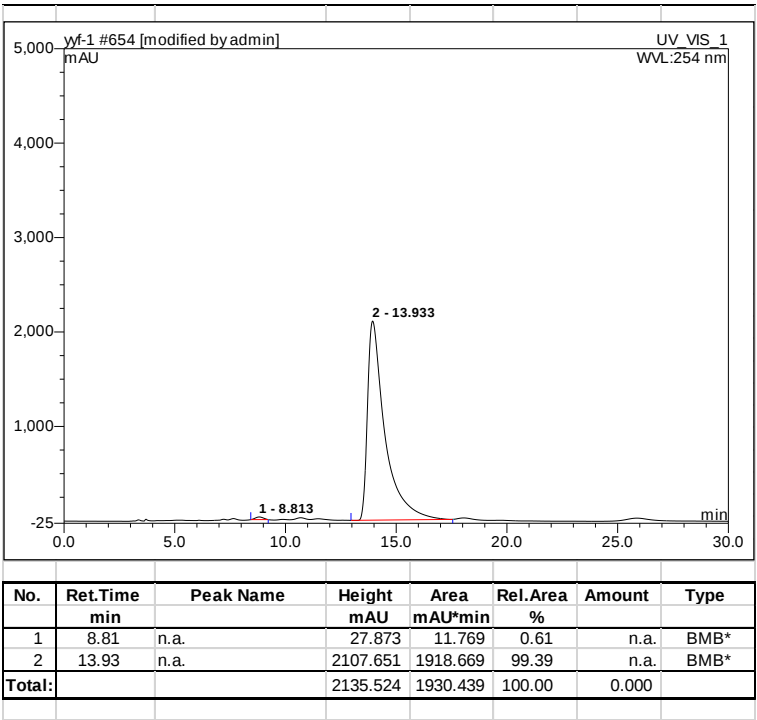
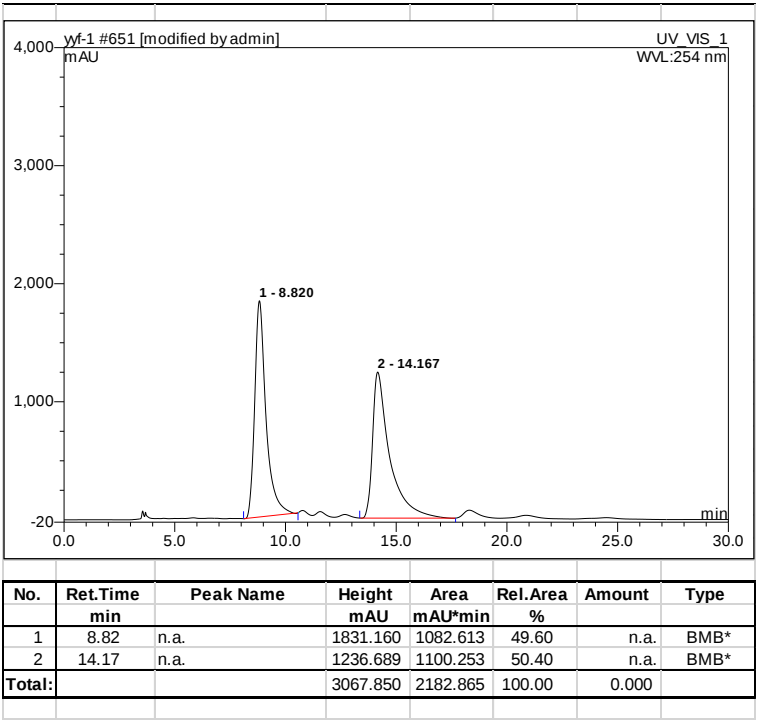
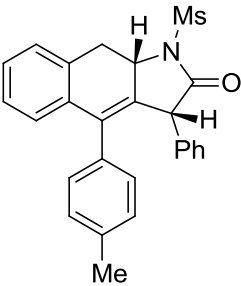


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	10.26	n.a.	2121.596	1307.919	49.42	n.a.	BMB*
2	23.43	n.a.	987.531	1338.839	50.58	n.a.	BMB*
Total:			3109.127	2646.757	100.00	0.000	

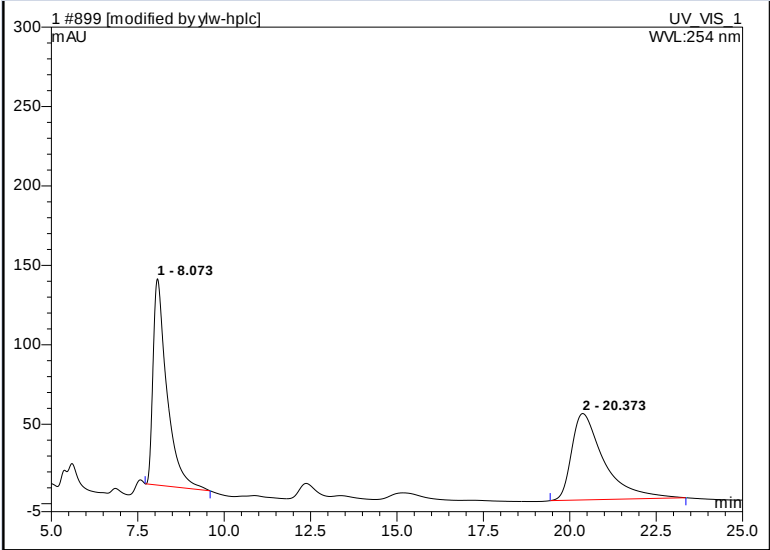
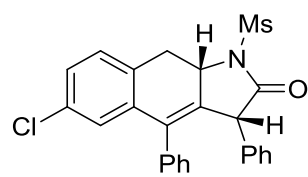


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	10.44	n.a.	119.695	68.744	1.96	n.a.	BMB*
2	19.39	n.a.	2412.764	3431.976	98.04	n.a.	BMB*
Total:			2532.459	3500.719	100.00	0.000	

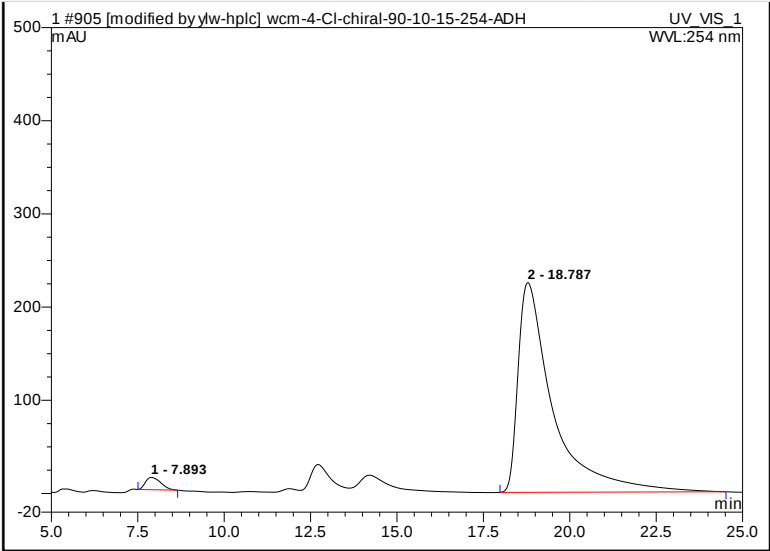
Compound 2l



Compound **2m**

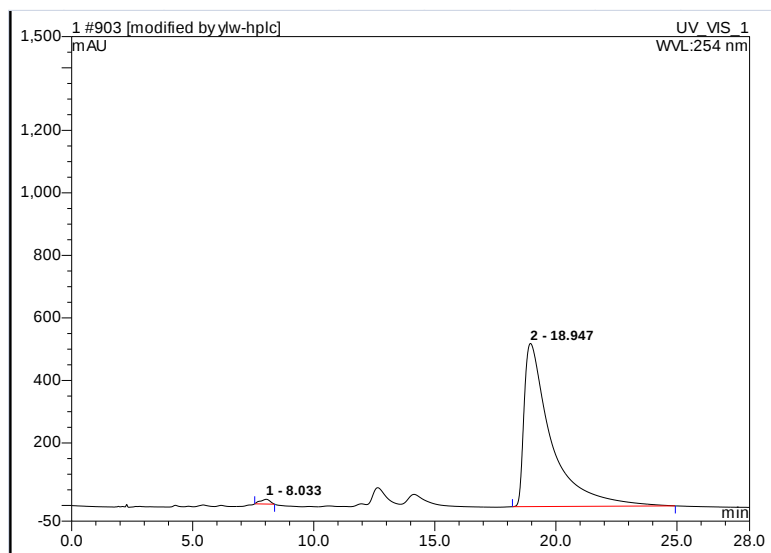
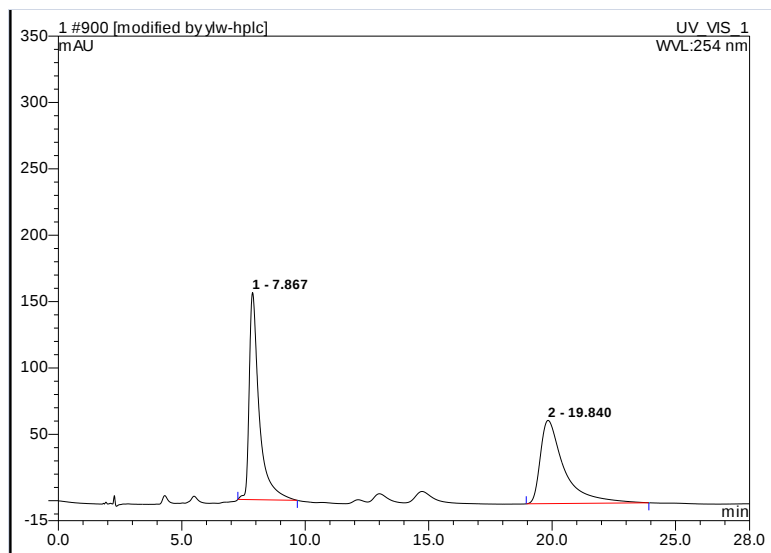
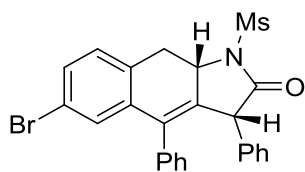


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	8.07	n.a.	129.848	60.482	50.57	n.a.	BMB*
2	20.37	n.a.	54.379	59.117	49.43	n.a.	BMB*
Total:			184.227	119.599	100.00	0.000	

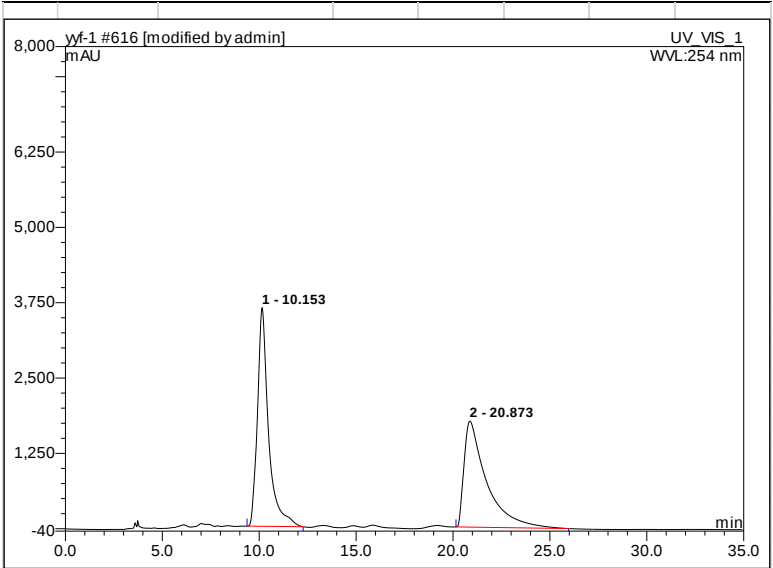
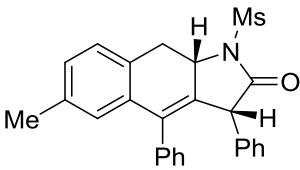


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	7.89	n.a.	13.140	6.779	2.51	n.a.	BMB*
2	18.79	n.a.	224.986	263.389	97.49	n.a.	BMB*
Total:			238.126	270.168	100.00	0.000	

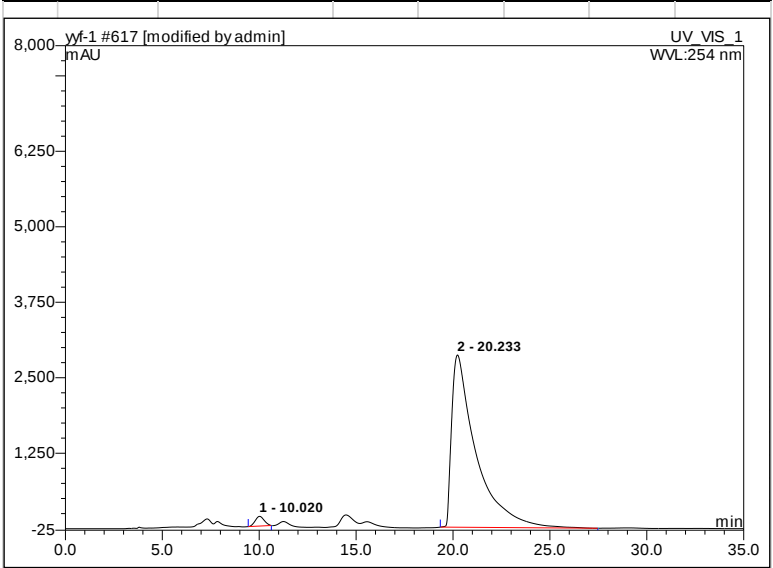
Compound 2n



Compound 2o

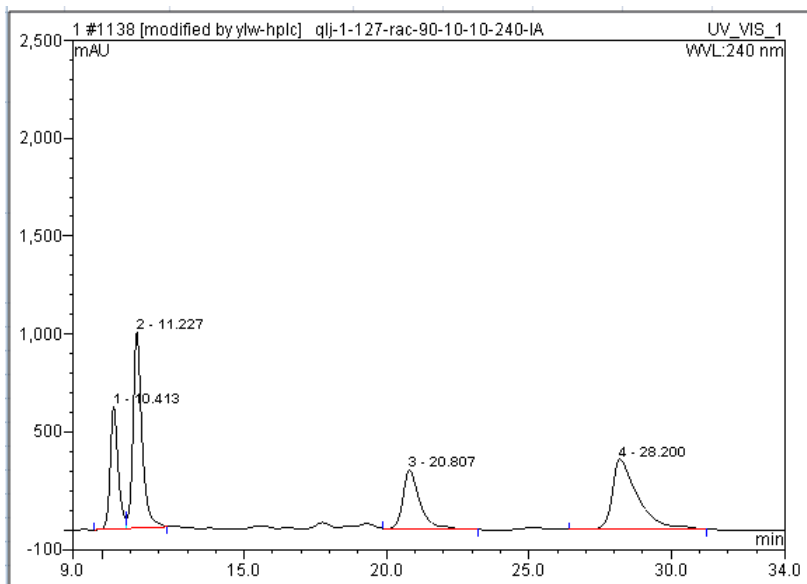
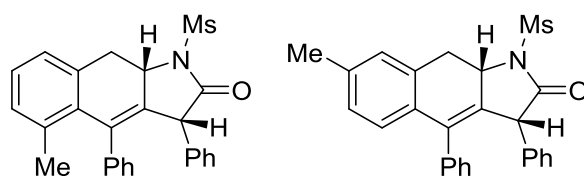


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	10.15	n.a.	3628.039	2402.307	50.46	n.a.	BMB*
2	20.87	n.a.	1757.473	2358.173	49.54	n.a.	BMB*
Total:			5385.513	4760.480	100.00	0.000	

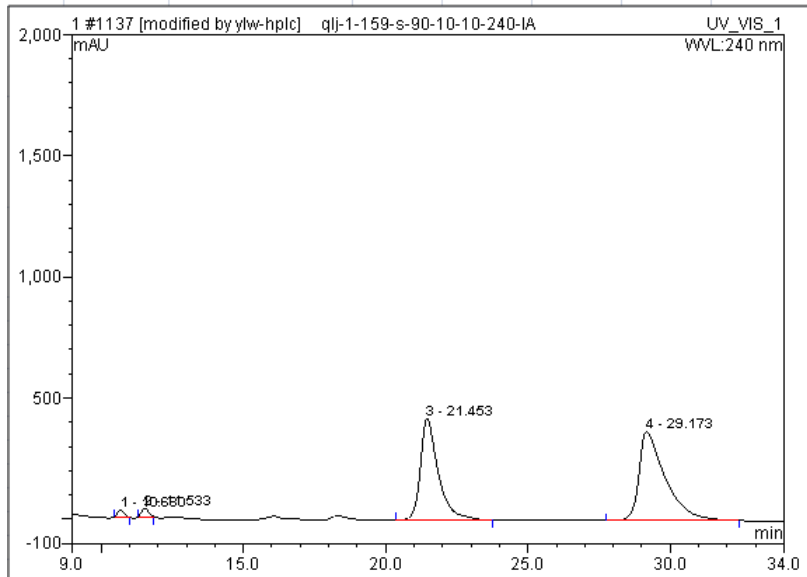


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	10.02	n.a.	160.795	86.854	2.05	n.a.	BMB*
2	20.23	n.a.	2852.688	4160.103	97.95	n.a.	BMB*
Total:			3013.483	4246.957	100.00	0.000	

Compound 2p and 2p'

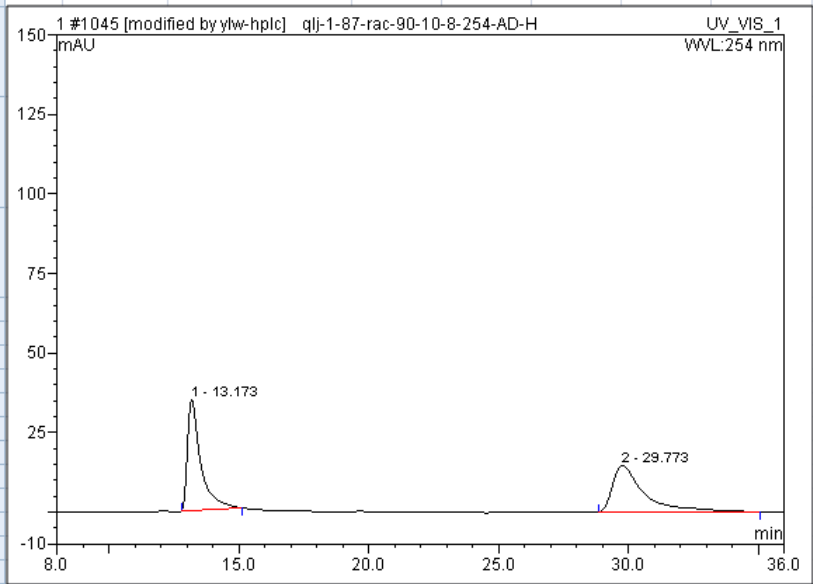
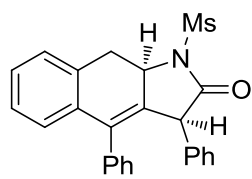


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	10.41	n.a.	621.797	201.001	17.58	n.a.	BM *
2	11.23	n.a.	999.008	365.291	31.94	n.a.	MB*
3	20.81	n.a.	299.577	206.153	18.03	n.a.	BMB*
4	28.20	n.a.	357.910	371.165	32.46	n.a.	BMB*
Total:			2278.292	1143.609	100.00	0.000	

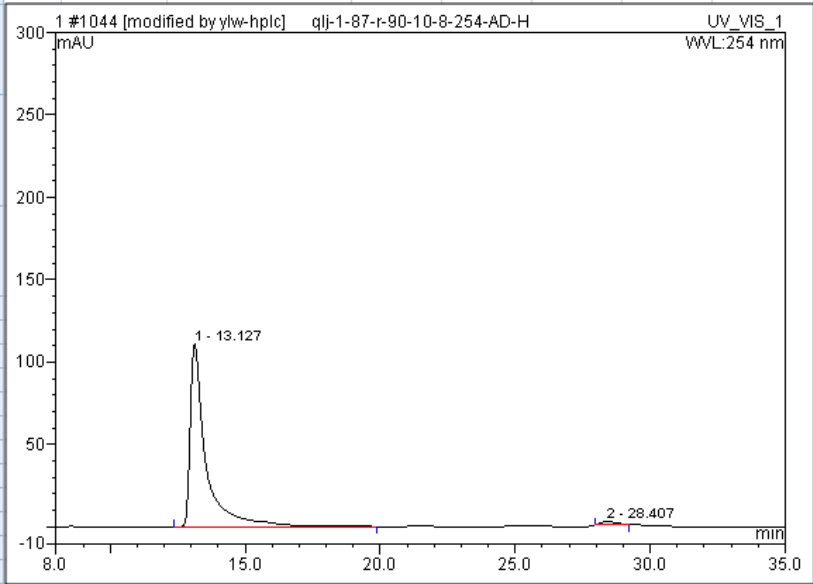


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	10.68	n.a.	29.837	7.877	1.10	n.a.	BMB*
2	11.53	n.a.	34.968	9.709	1.36	n.a.	BMB*
3	21.45	n.a.	419.229	304.759	42.56	n.a.	BMB*
4	29.17	n.a.	368.485	393.738	54.98	n.a.	BMB*
Total:			852.519	716.084	100.00	0.000	

Compound **2d'**

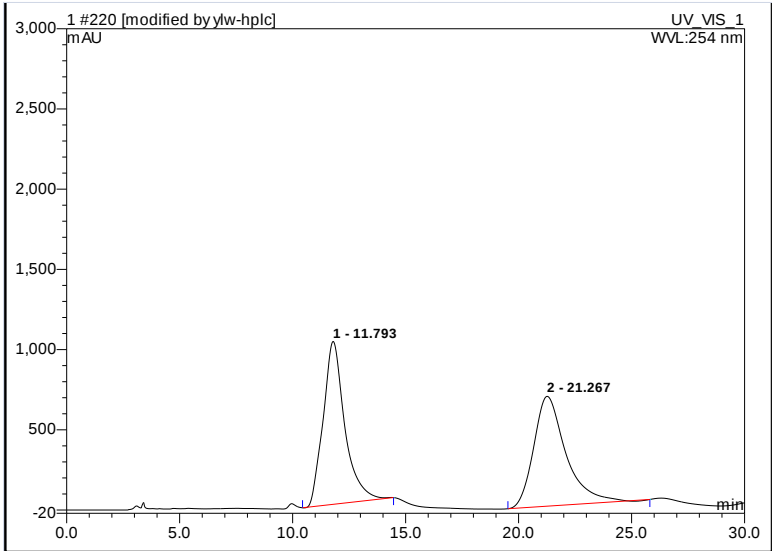
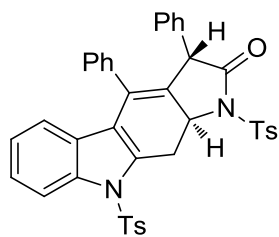


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	13.17	n.a.	34.826	20.759	50.06	n.a.	BMB*
2	29.77	n.a.	14.678	20.710	49.94	n.a.	BM *
Total:			49.504	41.469	100.00	0.000	

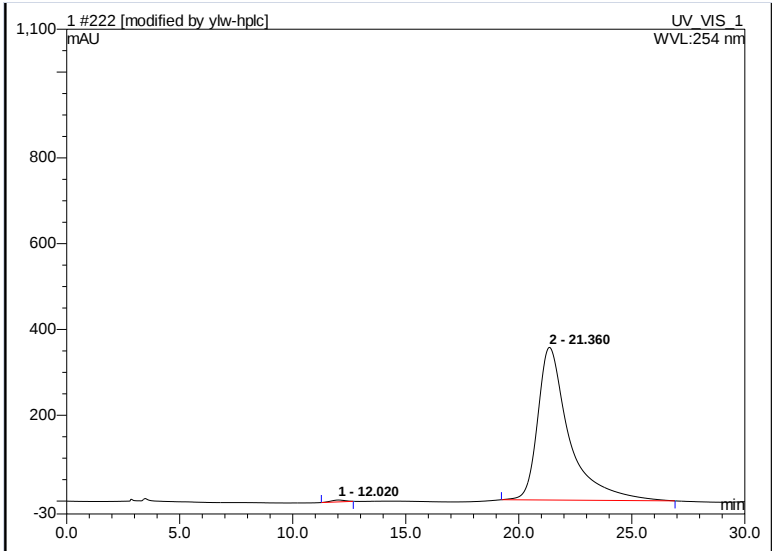


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	13.13	n.a.	110.777	74.643	98.34	n.a.	BMB*
2	28.41	n.a.	1.787	1.263	1.66	n.a.	BMB*
Total:			112.564	75.906	100.00	0.000	

Compound 5a

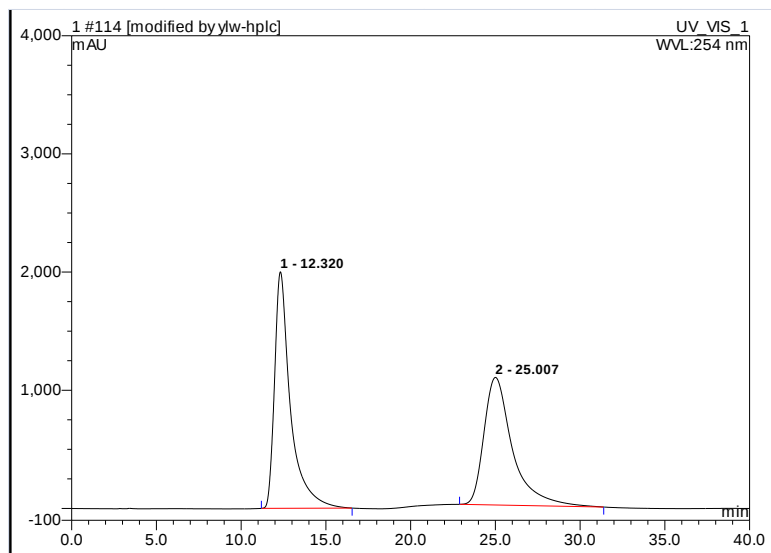
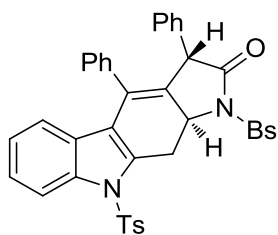


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	11.79	n.a.	1015.079	1125.295	50.00	n.a.	BMB*
2	21.27	n.a.	684.326	1125.164	50.00	n.a.	BMB*
Total:			1699.405	2250.459	100.00	0.000	

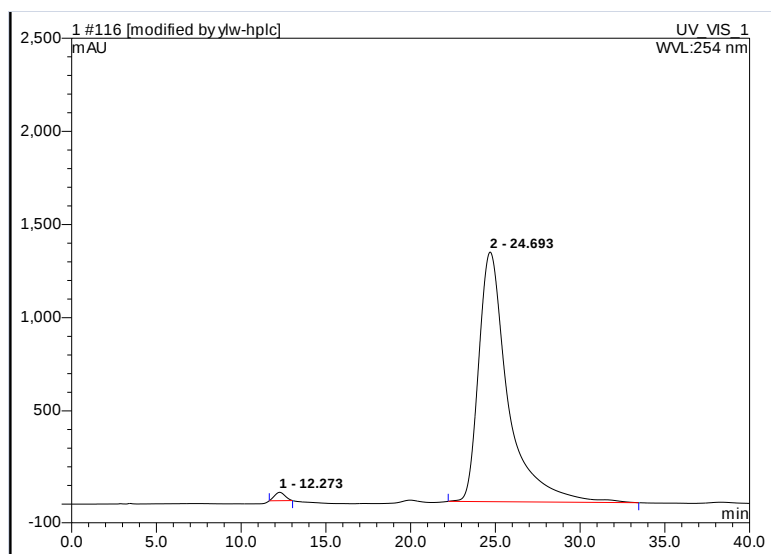


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	12.02	n.a.	4.304	3.037	0.53	n.a.	BMB*
2	21.36	n.a.	355.765	572.417	99.47	n.a.	BMB*
Total:			360.069	575.454	100.00	0.000	

Compound 5b

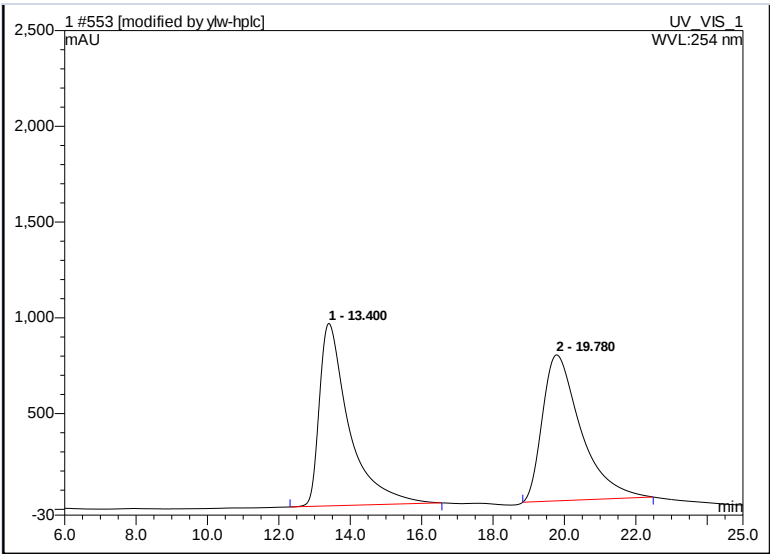
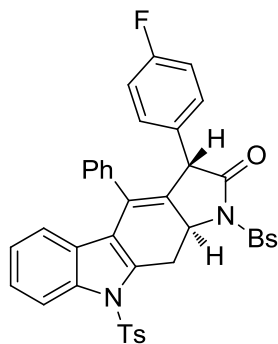


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	12.32	n.a.	2001.064	2172.633	50.76	n.a.	BMB*
2	25.01	n.a.	1079.531	2107.932	49.24	n.a.	BMB*
Total:			3080.595	4280.565	100.00	0.000	

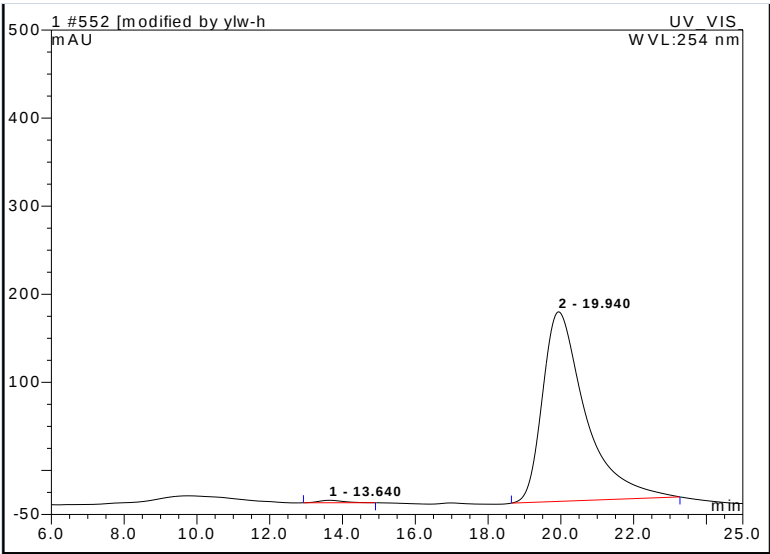


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	12.27	n.a.	44.907	31.990	1.17	n.a.	BMB*
2	24.69	n.a.	1339.056	2695.664	98.83	n.a.	BMB*
Total:			1383.963	2727.653	100.00	0.000	

Compound 5c

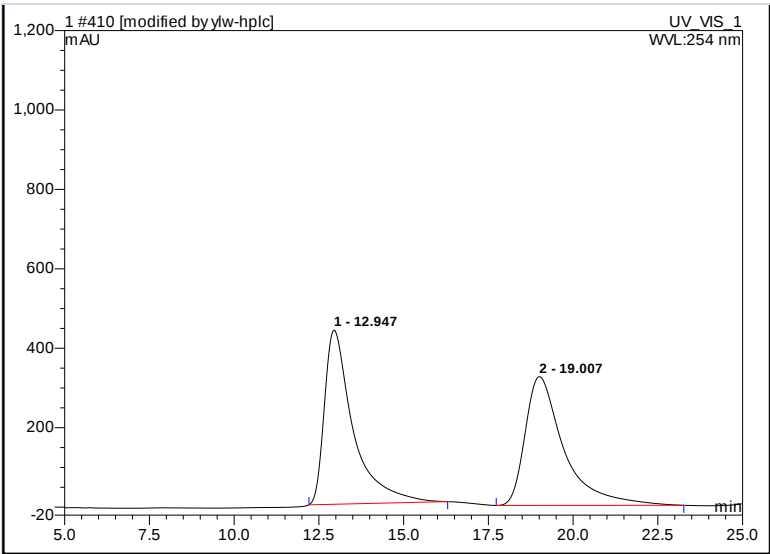
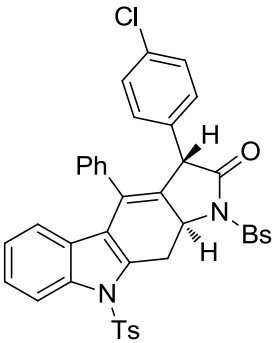


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	13.40	n.a.	952.573	913.860	49.03	n.a.	BMB*
2	19.78	n.a.	762.183	949.845	50.97	n.a.	BMB*
Total:			1714.757	1863.705	100.00	0.000	

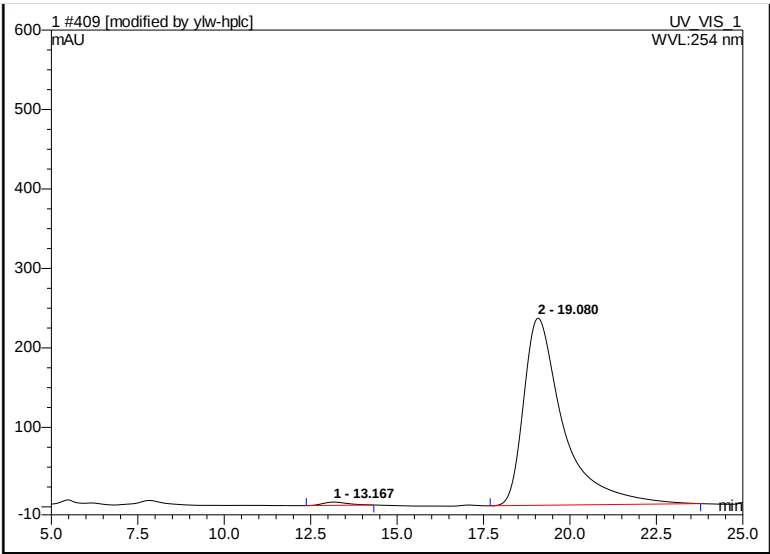


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	13.64	n.a.	2.814	2.191	0.74	n.a.	BMB*
2	19.94	n.a.	215.138	294.224	99.26	n.a.	BMB*
Total:			217.952	296.414	100.00	0.000	

Compound **5d**

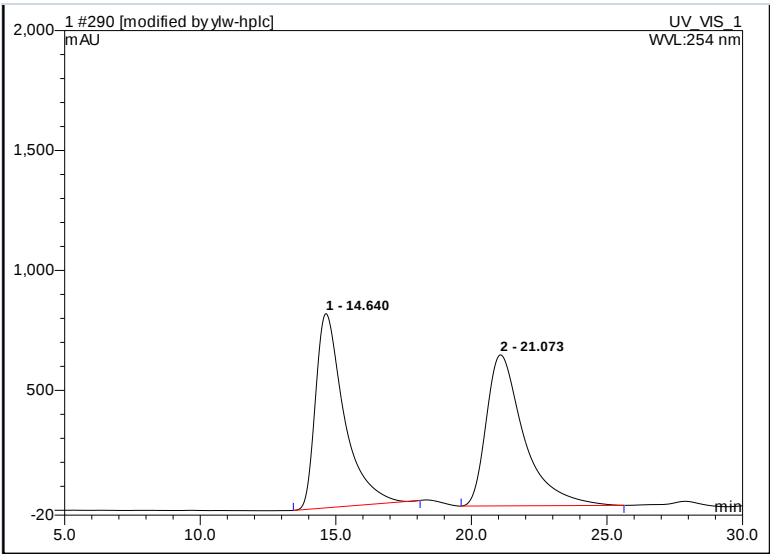
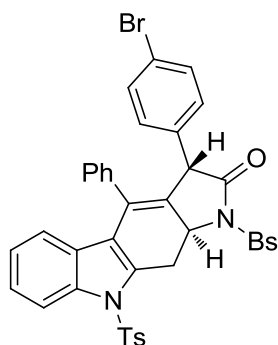


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	12.95	n.a.	438.361	430.607	50.03	n.a.	BMB*
2	19.01	n.a.	324.173	430.132	49.97	n.a.	BMB*
Total:			762.534	860.738	100.00	0.000	

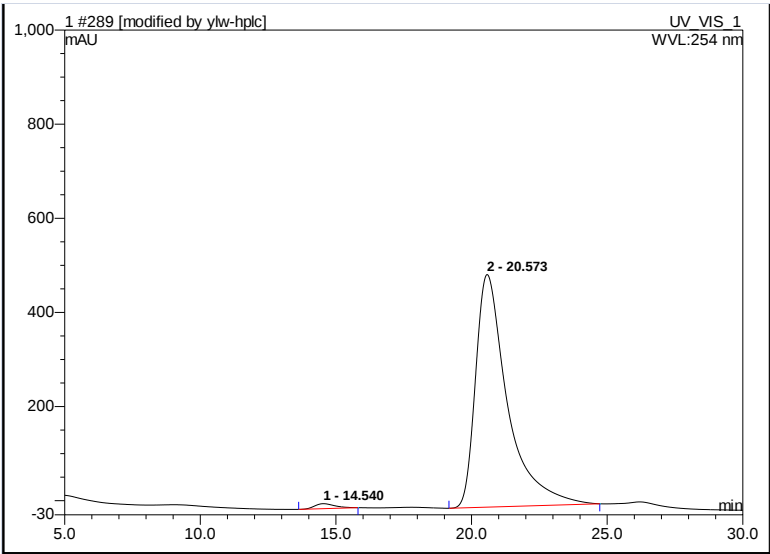


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	13.17	n.a.	4.111	3.423	1.08	n.a.	BMB*
2	19.08	n.a.	235.400	313.739	98.92	n.a.	BMB*
Total:			239.511	317.162	100.00	0.000	

Compound 5e

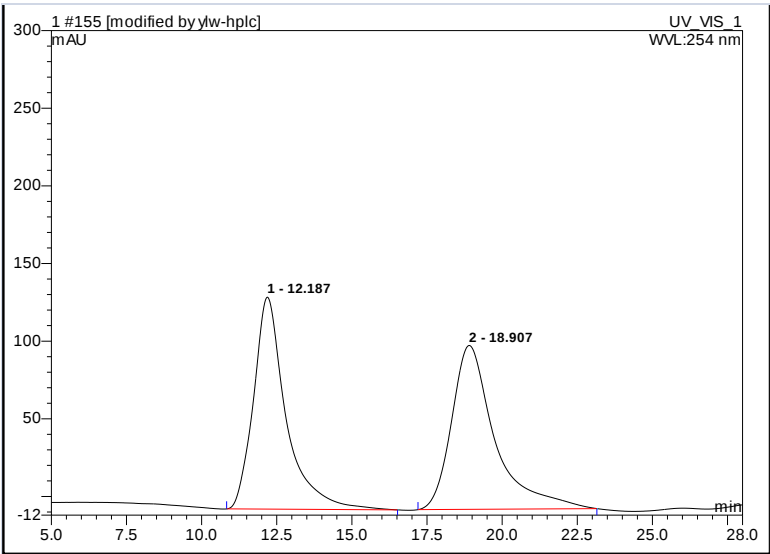
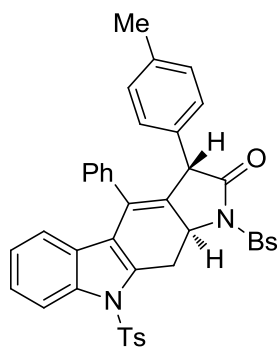


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	14.64	n.a.	809.397	988.972	49.42	n.a.	BMB*
2	21.07	n.a.	629.575	1012.097	50.58	n.a.	BMB*
Total:			1438.971	2001.069	100.00	0.000	

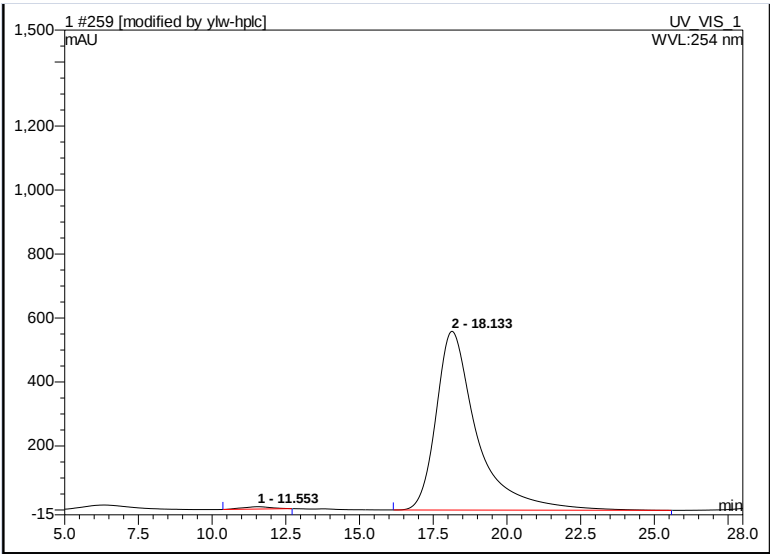


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	14.54	n.a.	10.614	9.175	1.34	n.a.	BMB*
2	20.57	n.a.	494.154	673.377	98.66	n.a.	BMB*
Total:			504.768	682.552	100.00	0.000	

Compound **5f**

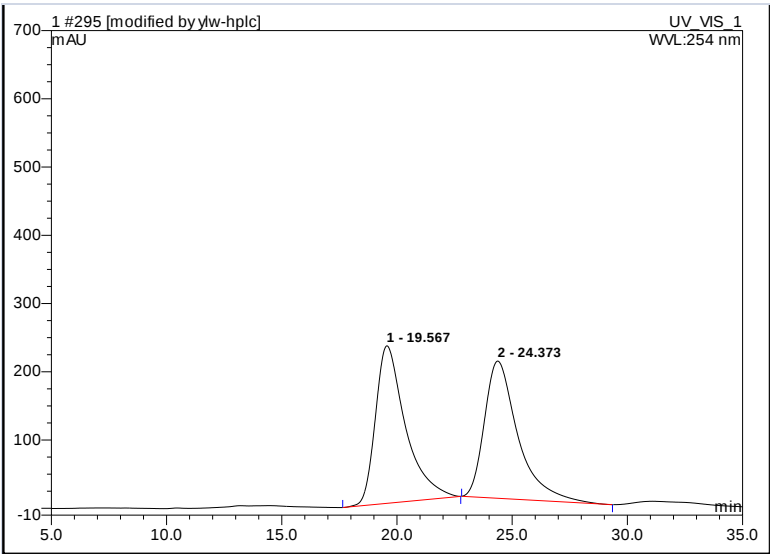
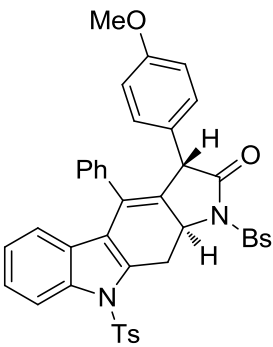


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	12.19	n.a.	136.473	171.269	49.34	n.a.	BMB*
2	18.91	n.a.	105.506	175.834	50.66	n.a.	BMB*
Total:			241.979	347.103	100.00	0.000	

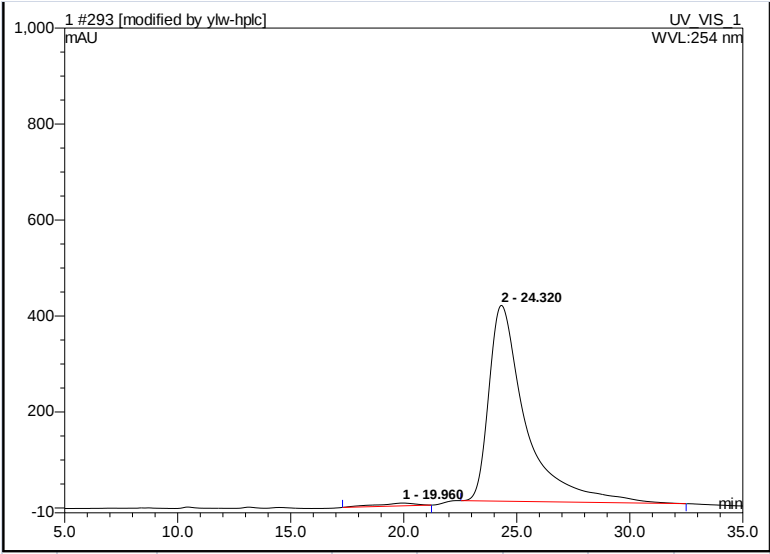


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	11.55	n.a.	7.342	8.235	0.91	n.a.	BMB*
2	18.13	n.a.	558.464	898.615	99.09	n.a.	BMB
Total:			565.806	906.850	100.00	0.000	

Compound 5g

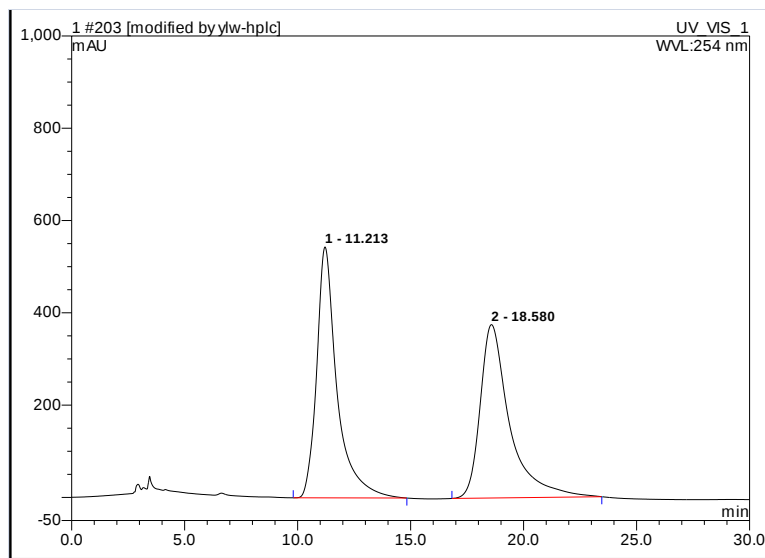
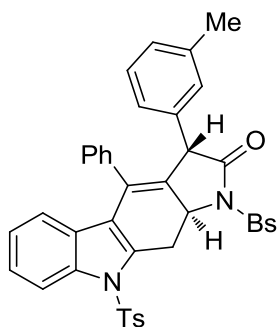


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	19.57	n.a.	230.764	349.570	50.77	n.a.	BMB*
2	24.37	n.a.	201.011	339.018	49.23	n.a.	BMB*
Total:			431.775	688.588	100.00	0.000	

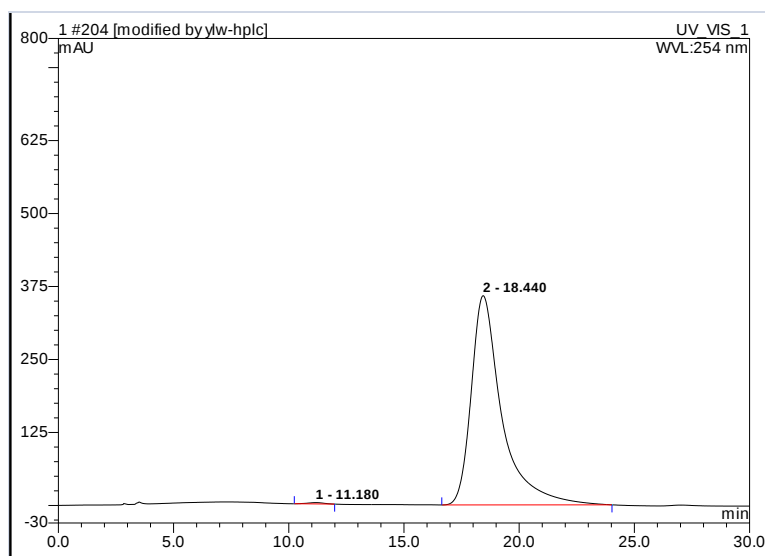


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	19.96	n.a.	5.747	11.776	1.50	n.a.	BMB*
2	24.32	n.a.	407.866	772.411	98.50	n.a.	BMB*
Total:			413.613	784.187	100.00	0.000	

Compound 5h

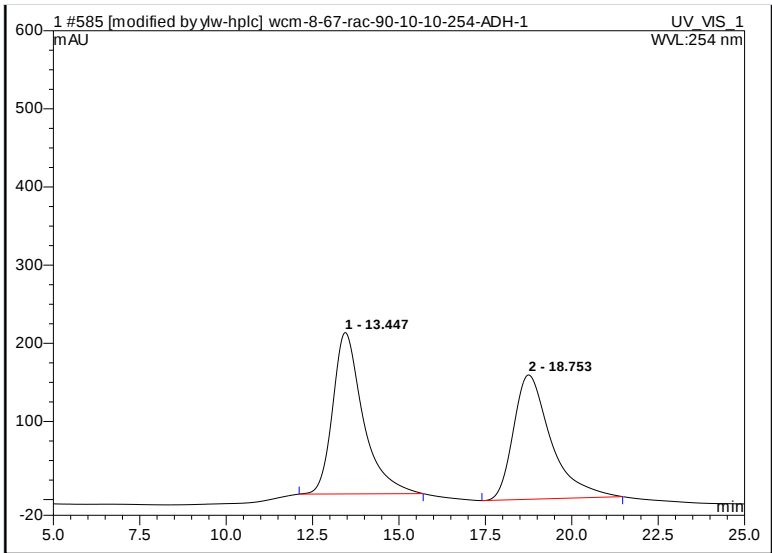
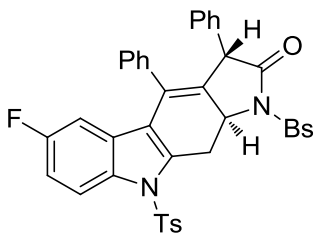


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	11.21	n.a.	543.544	567.355	50.04	n.a.	BMB*
2	18.58	n.a.	375.642	566.514	49.96	n.a.	BMB*
Total:			919.185	1133.869	100.00	0.000	

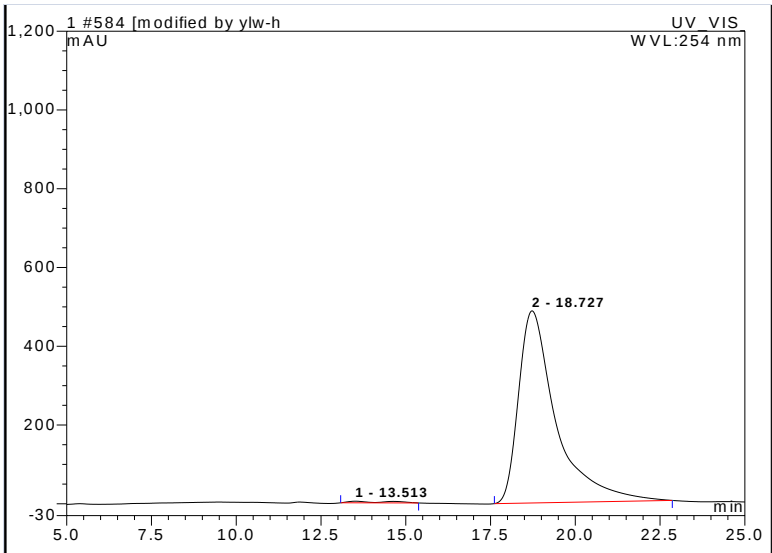


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	11.18	n.a.	2.264	1.865	0.34	n.a.	BMB*
2	18.44	n.a.	358.358	552.771	99.66	n.a.	BMB*
Total:			360.622	554.636	100.00	0.000	

Compound 5i

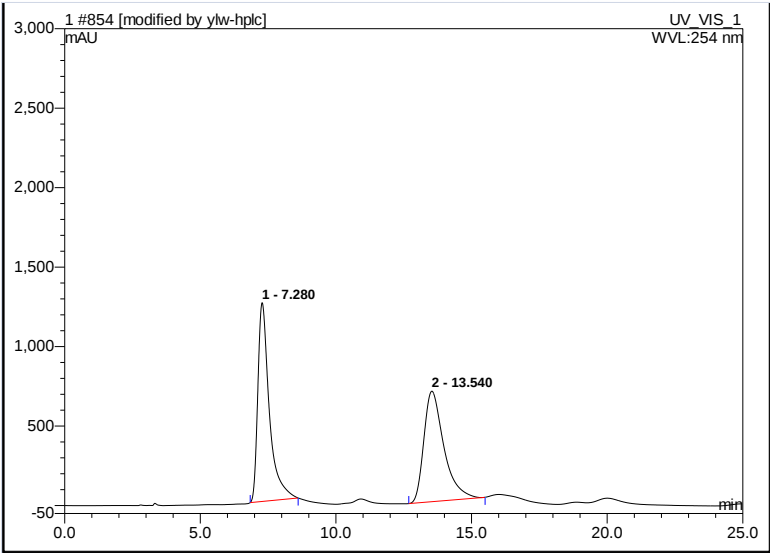
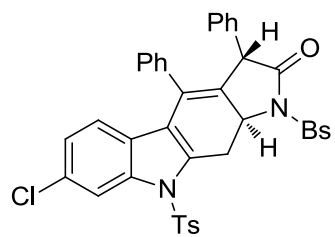


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	13.45	n.a.	206.433	210.538	51.20	n.a.	BMB*
2	18.75	n.a.	159.092	200.709	48.80	n.a.	BMB*
Total:			365.525	411.247	100.00	0.000	

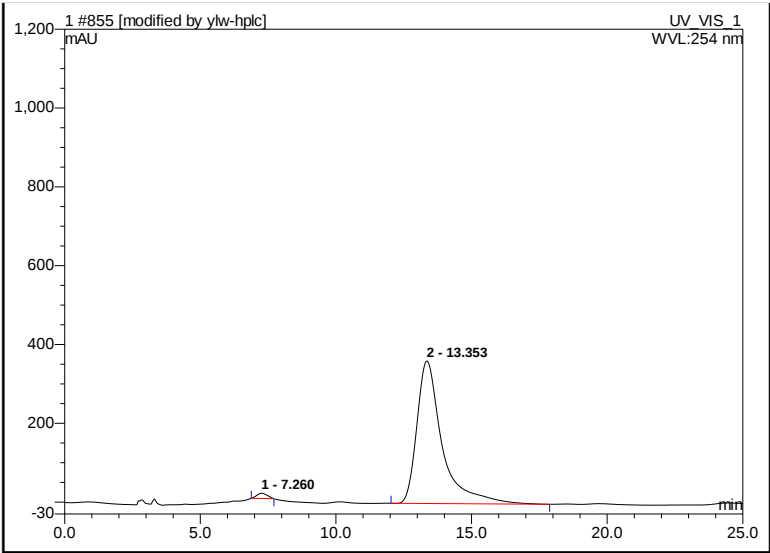


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	13.51	n.a.	4.071	5.330	0.84	n.a.	BMB*
2	18.73	n.a.	487.668	627.370	99.16	n.a.	BMB*
Total:			491.739	632.700	100.00	0.000	

Compound 5j

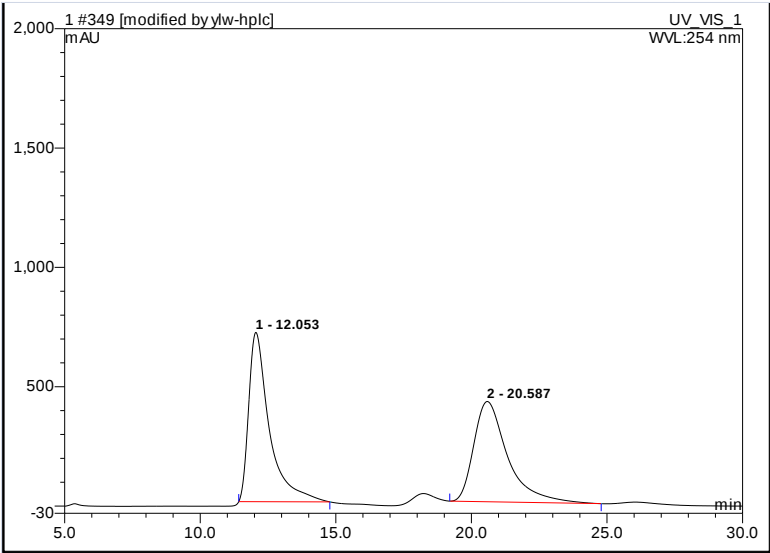
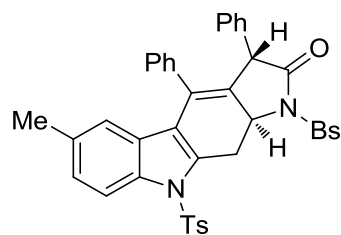


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	7.28	n.a.	1250.526	614.676	50.84	n.a.	BMB*
2	13.54	n.a.	695.278	594.280	49.16	n.a.	BMB*
Total:			1945.803	1208.956	100.00	0.000	

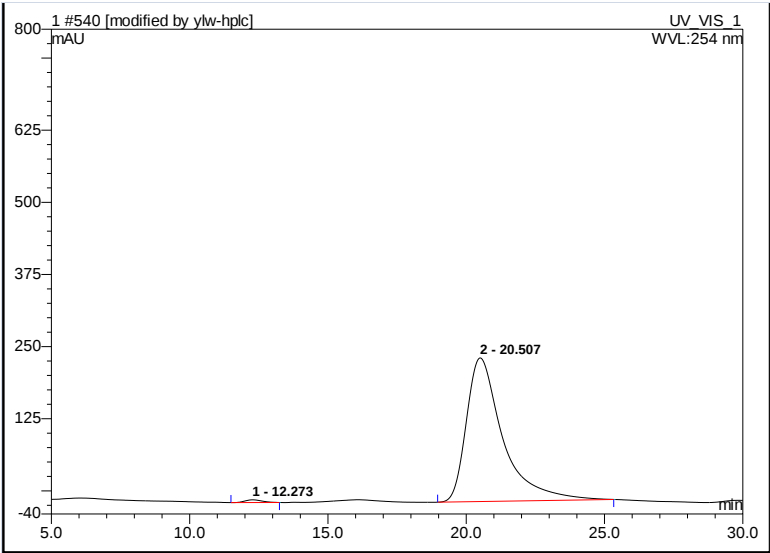


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	7.26	n.a.	13.266	5.962	1.50	n.a.	BMB*
2	13.35	n.a.	361.580	391.063	98.50	n.a.	BMB*
Total:			374.846	397.025	100.00	0.000	

Compound **5k**

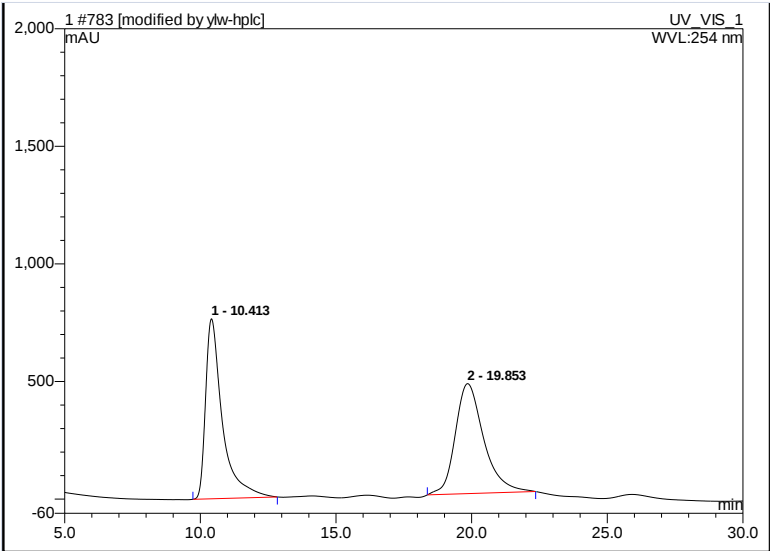
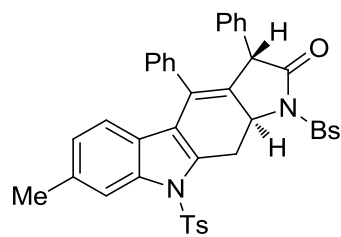


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	12.05	n.a.	709.135	626.880	50.79	n.a.	BMB*
2	20.59	n.a.	419.935	607.456	49.21	n.a.	BMB*
Total:			1129.070	1234.336	100.00	0.000	

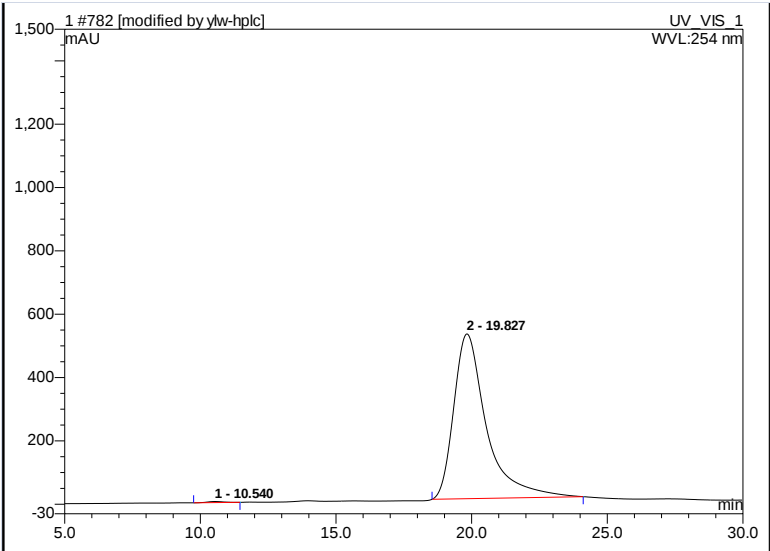


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	12.27	n.a.	4.736	3.359	0.88	n.a.	BMB*
2	20.51	n.a.	248.839	379.570	99.12	n.a.	BMB*
Total:			253.575	382.929	100.00	0.000	

Compound 51

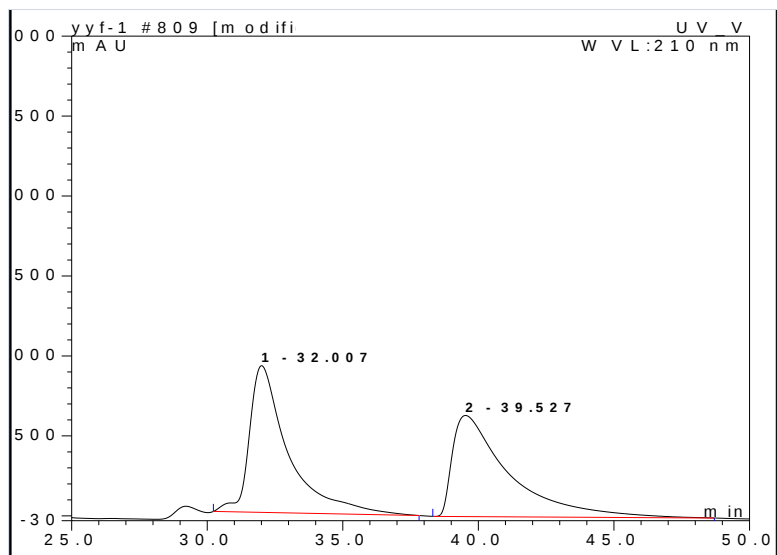
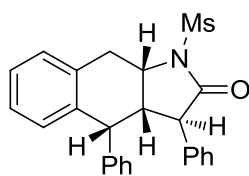


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	10.41	n.a.	765.085	547.806	49.07	n.a.	BMB*
2	19.85	n.a.	467.609	568.594	50.93	n.a.	BMB*
Total:			1232.695	1116.400	100.00	0.000	

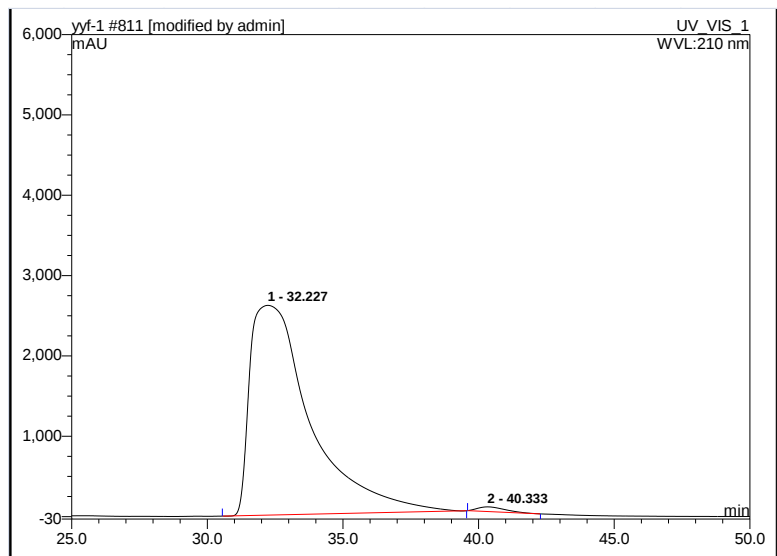


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	10.54	n.a.	3.394	2.254	0.31	n.a.	BMB*
2	19.83	n.a.	520.196	725.746	99.69	n.a.	BMB*
Total:			523.590	728.001	100.00	0.000	

Compound **2da**

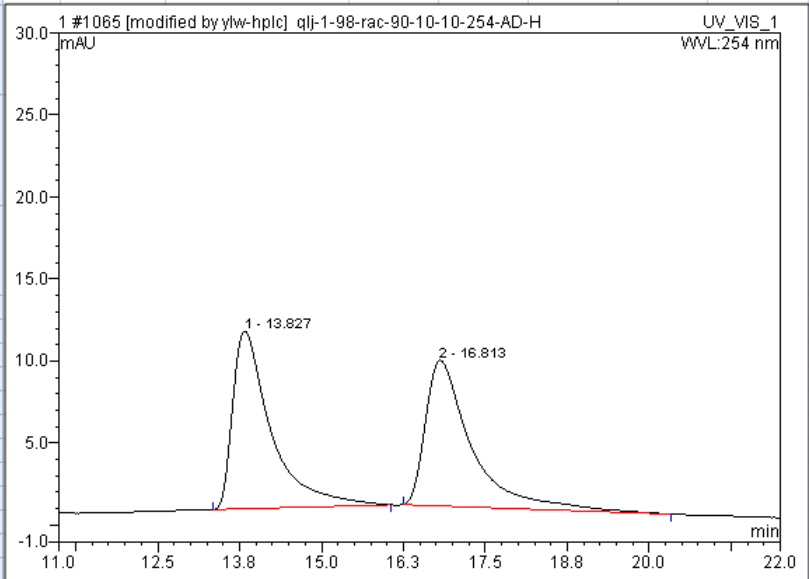
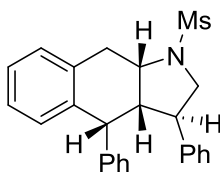


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	32.01	n.a.	917.458	1528.460	50.11	n.a.	BMB*
2	39.53	n.a.	632.122	1521.462	49.89	n.a.	BMB*
Total:			1549.580	3049.922	100.00	0.000	

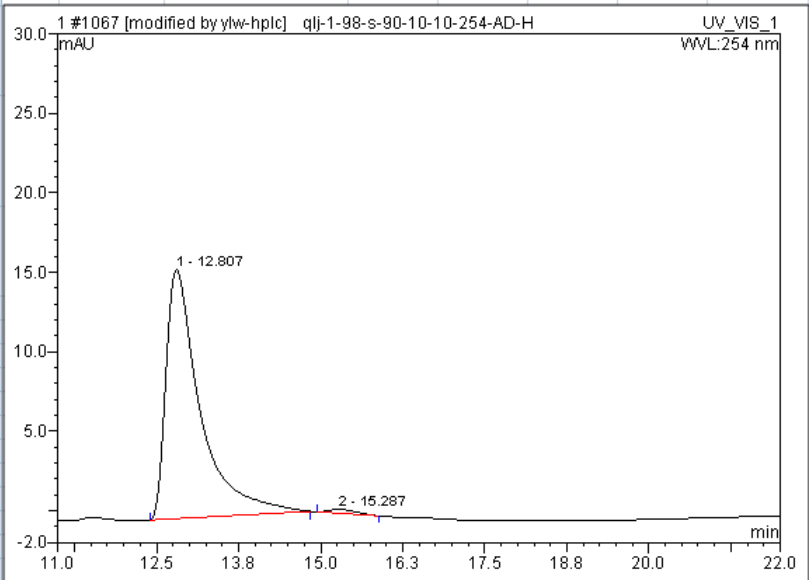


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	32.23	n.a.	2610.943	6777.531	98.99	n.a.	BMB*
2	40.33	n.a.	57.911	68.851	1.01	n.a.	BMB*
Total:			2668.854	6846.382	100.00	0.000	

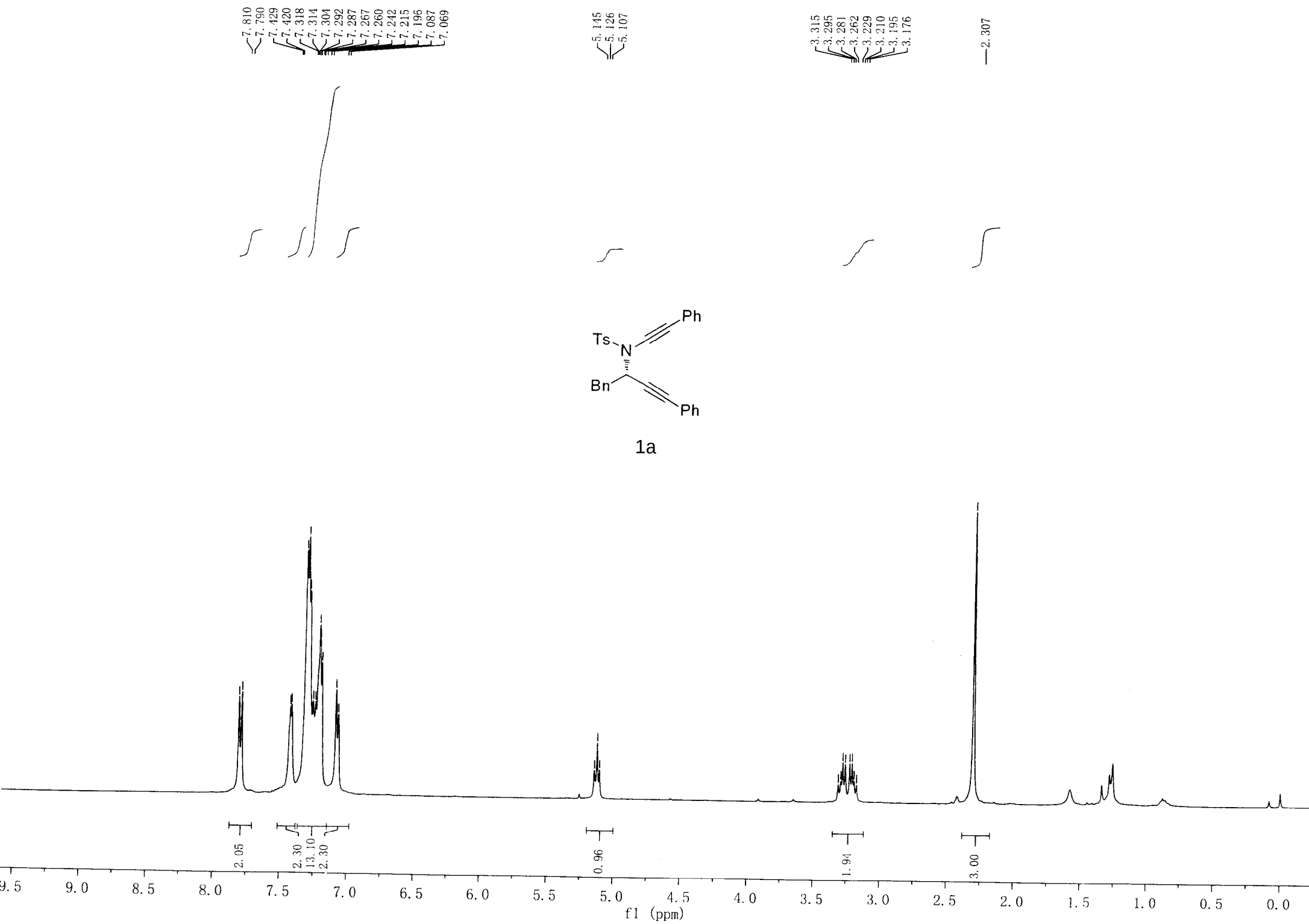
Compound **2db**

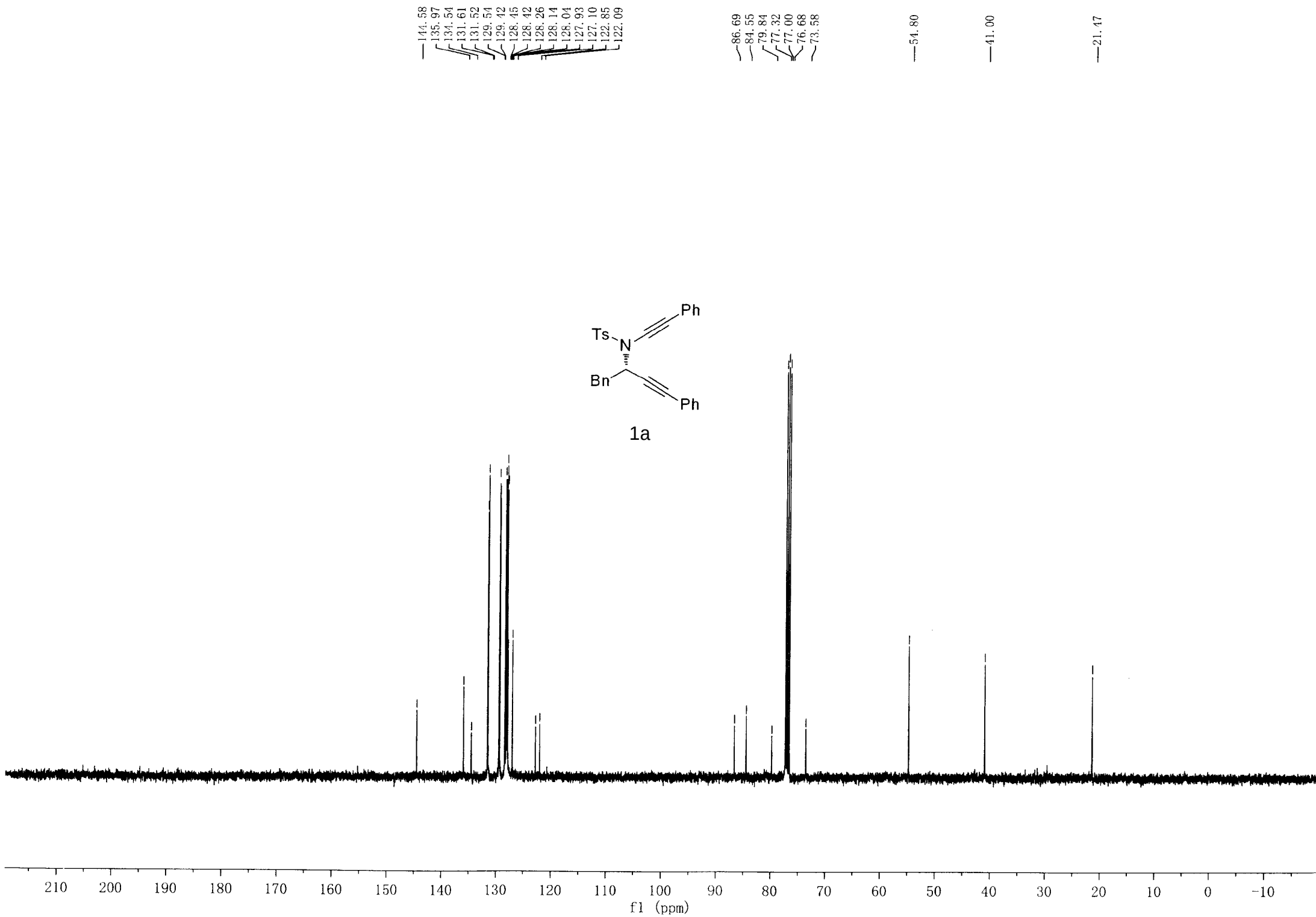


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	13.83	n.a.	10.832	7.350	50.40	n.a.	BMB*
2	16.81	n.a.	8.873	7.232	49.60	n.a.	BMB*
Total:			19.704	14.582	100.00	0.000	



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount n.a.	Type
1	12.81	n.a.	15.674	9.484	98.77	n.a.	BMB*
2	15.29	n.a.	0.248	0.118	1.23	n.a.	BMB*
Total:			15.922	9.602	100.00	0.000	

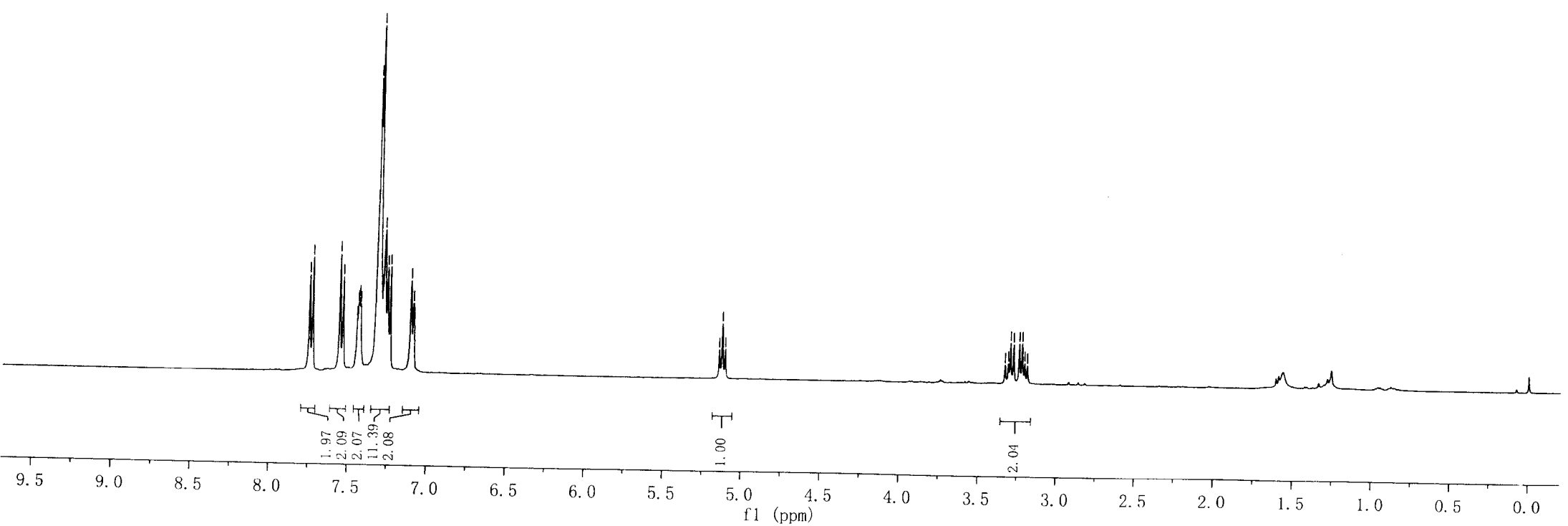
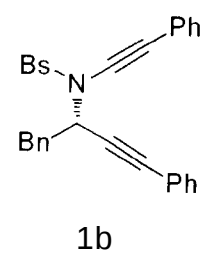


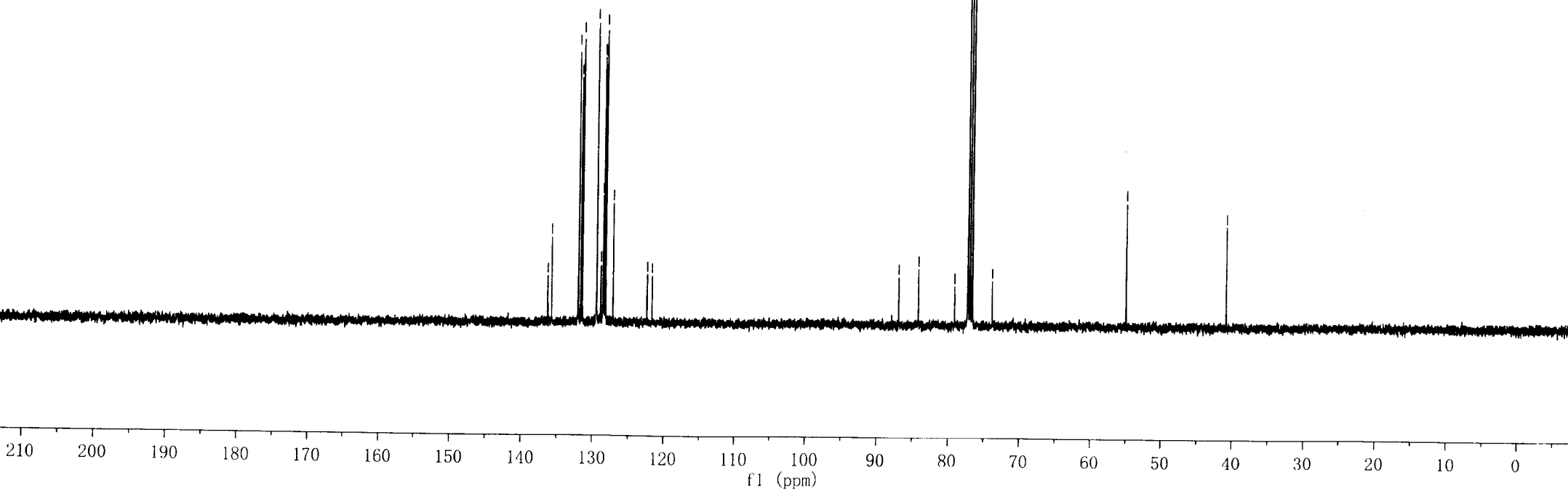
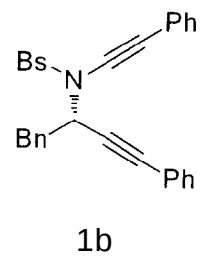
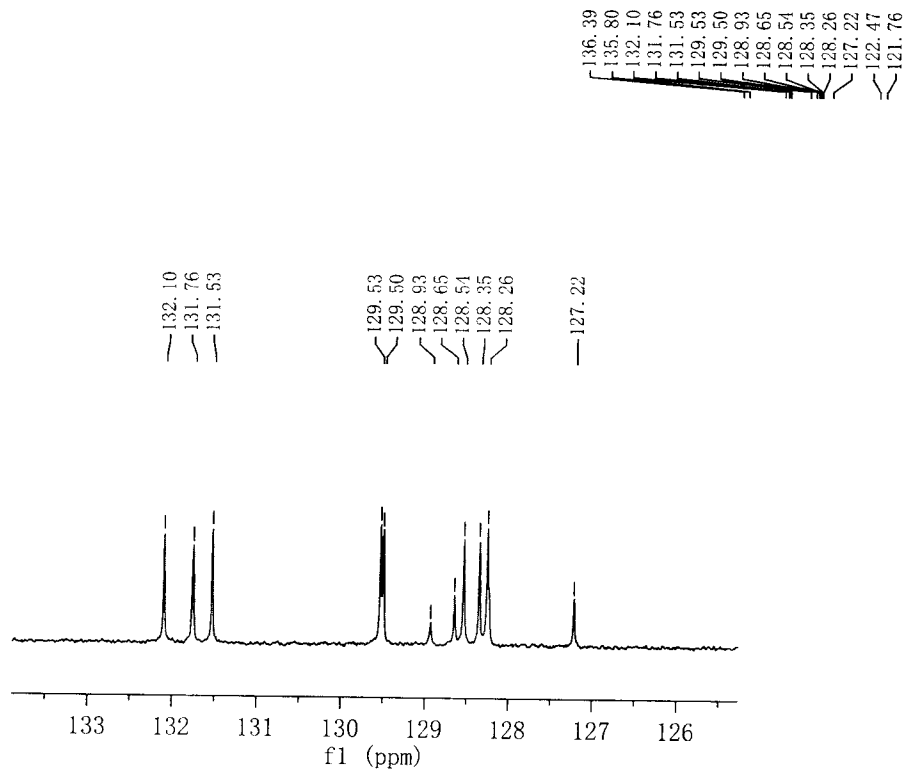


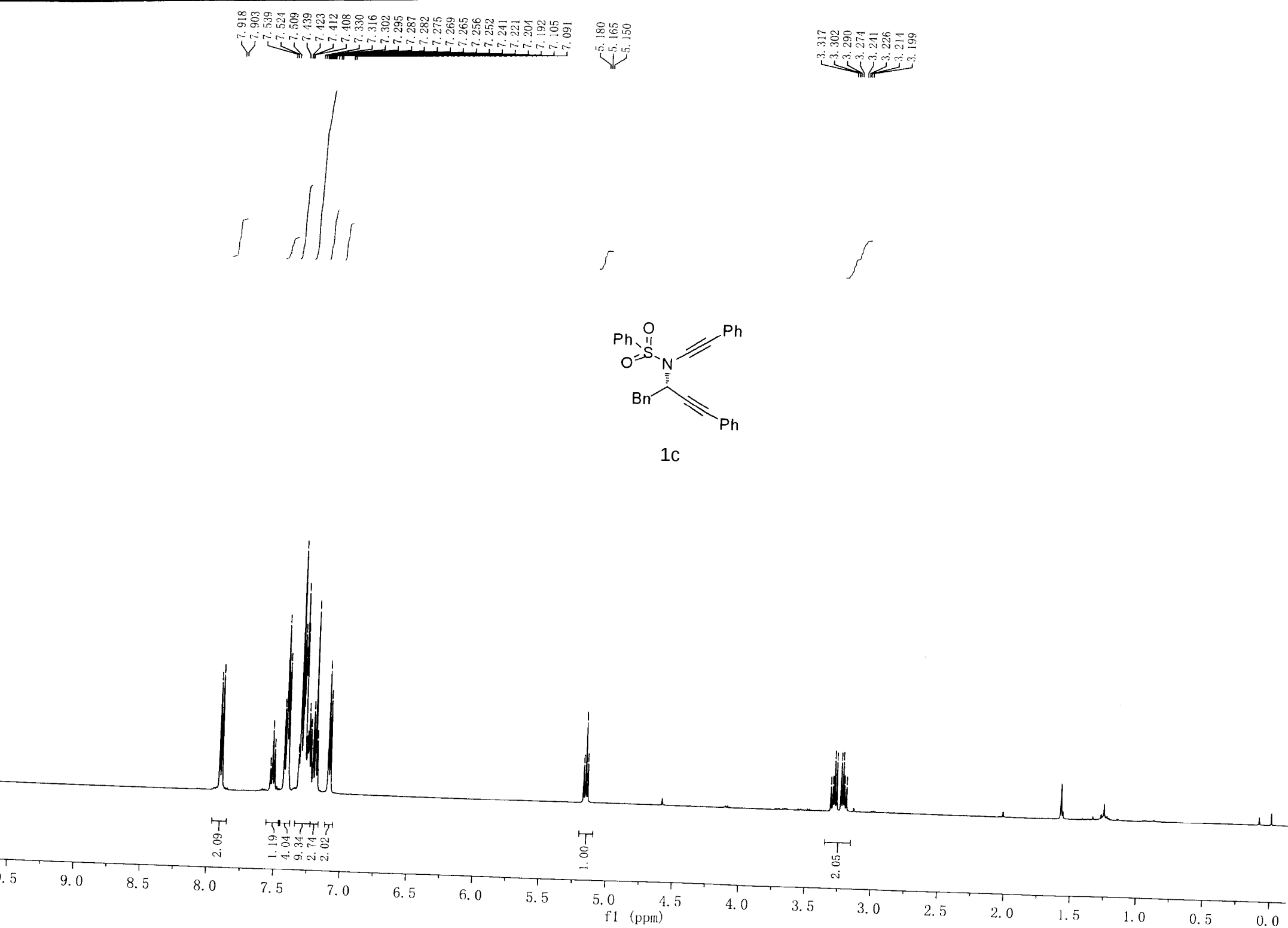
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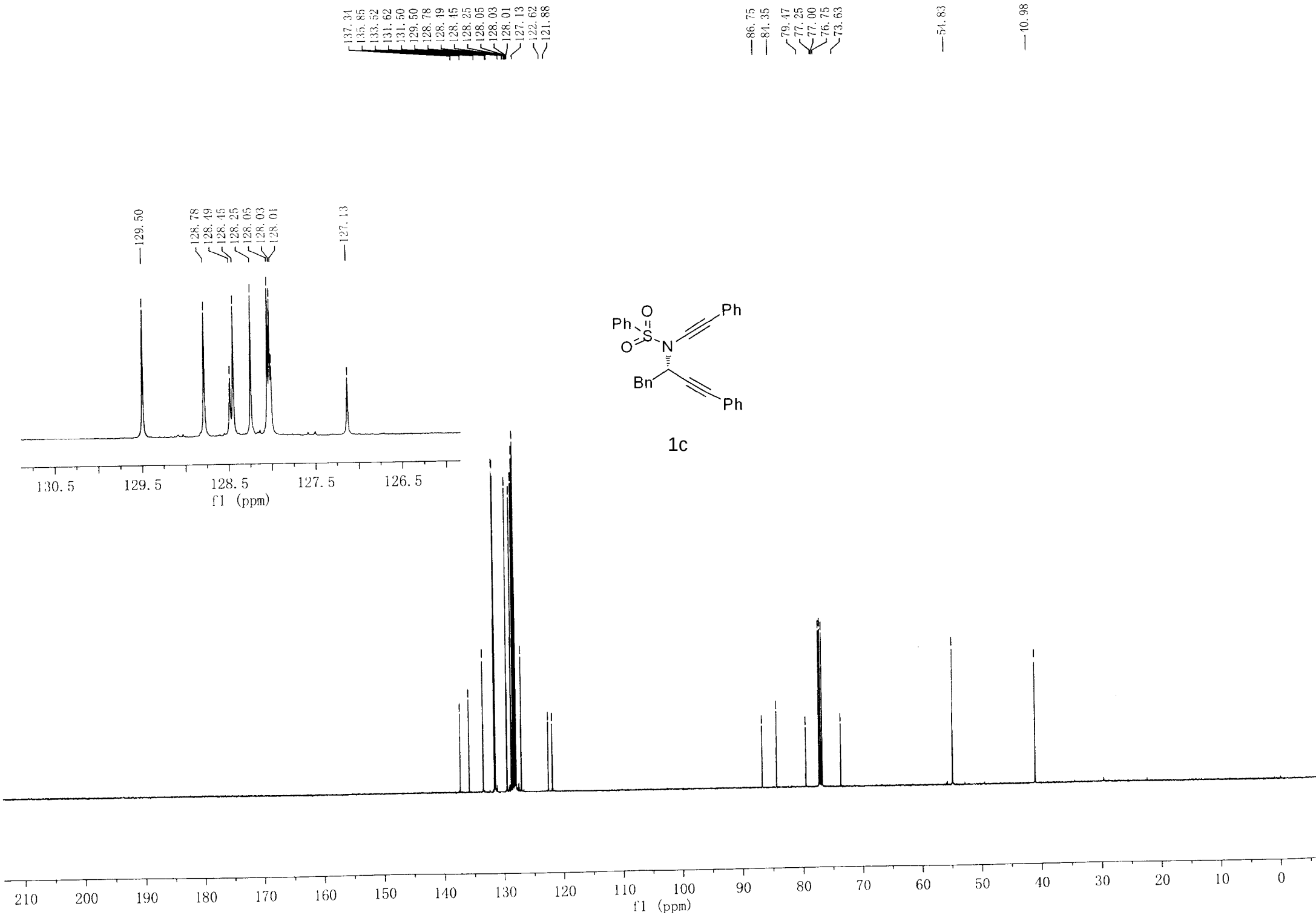
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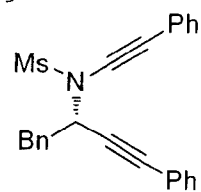




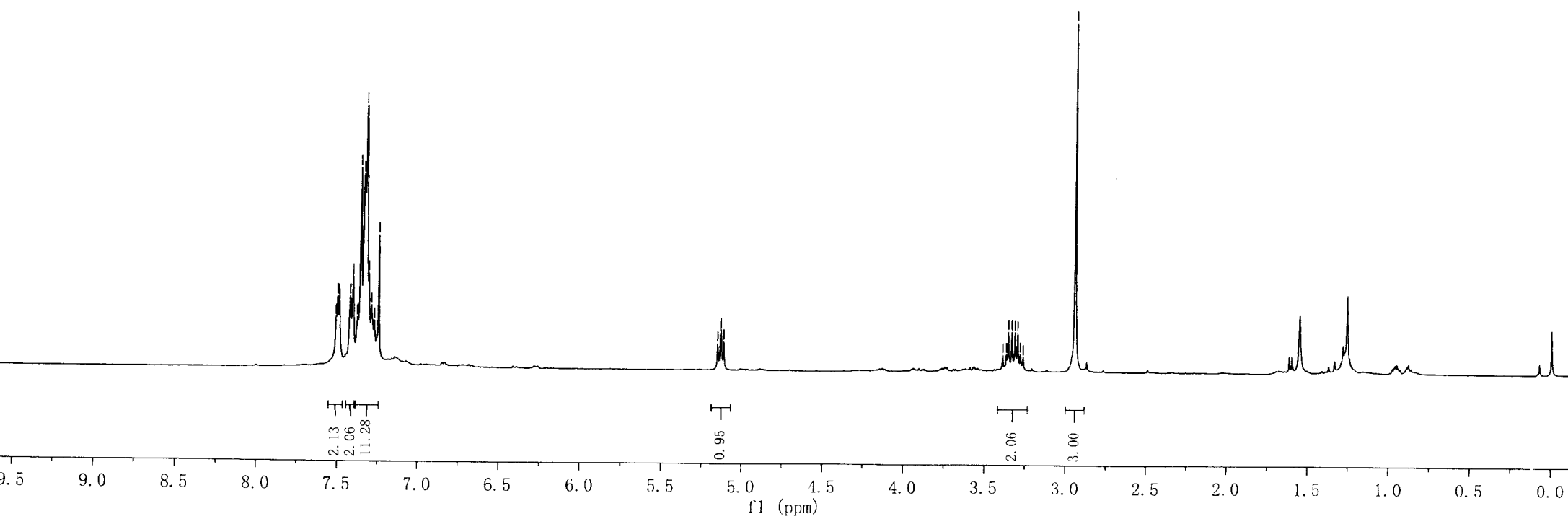
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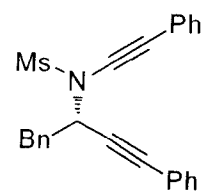
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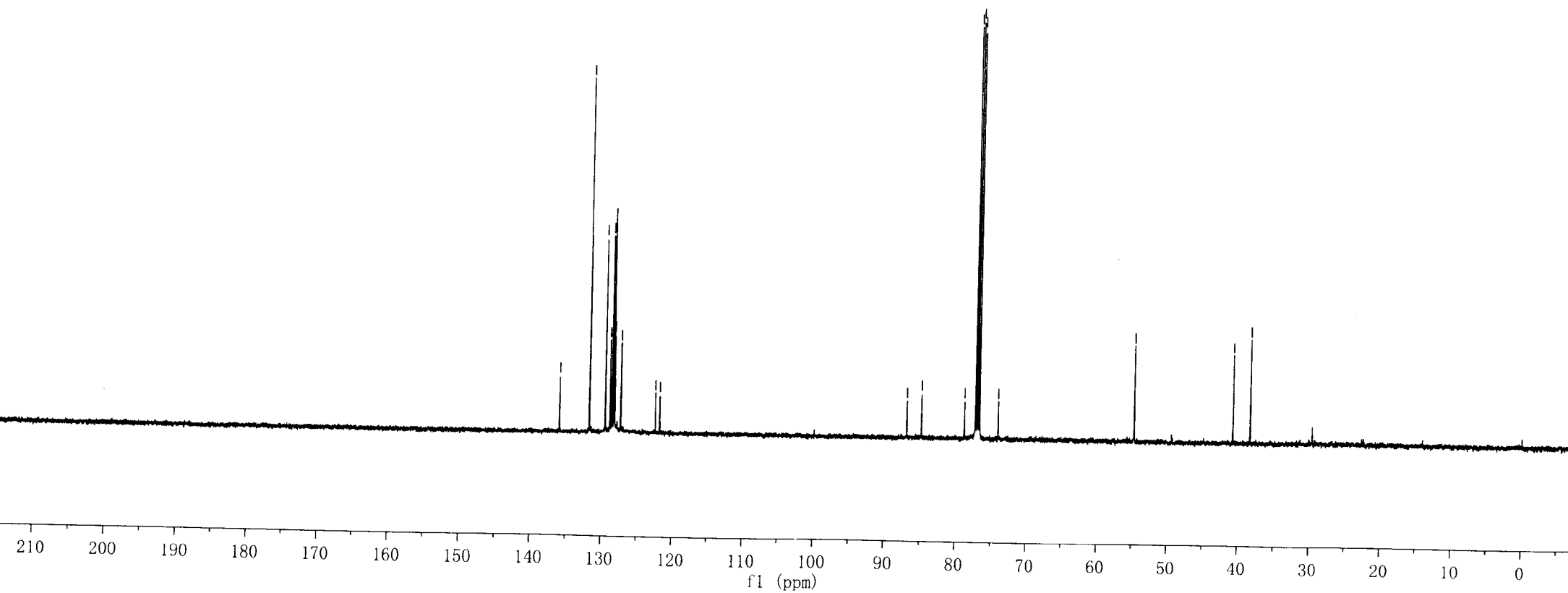


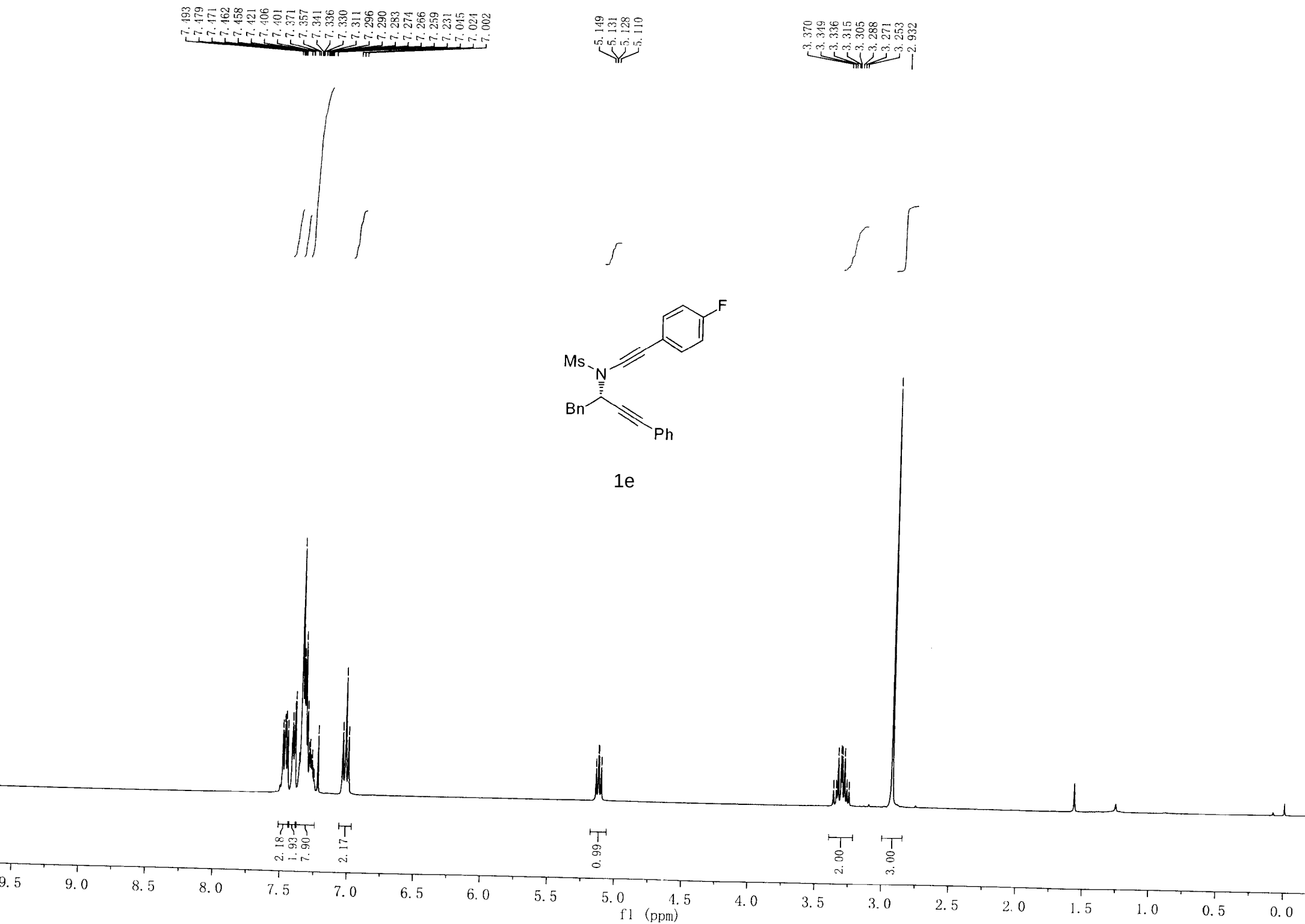
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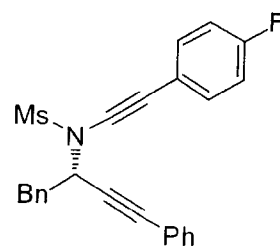
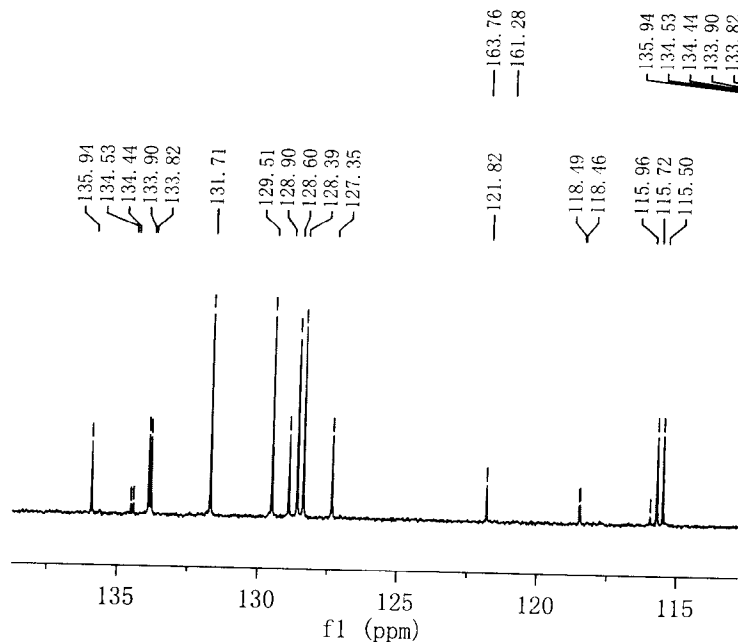




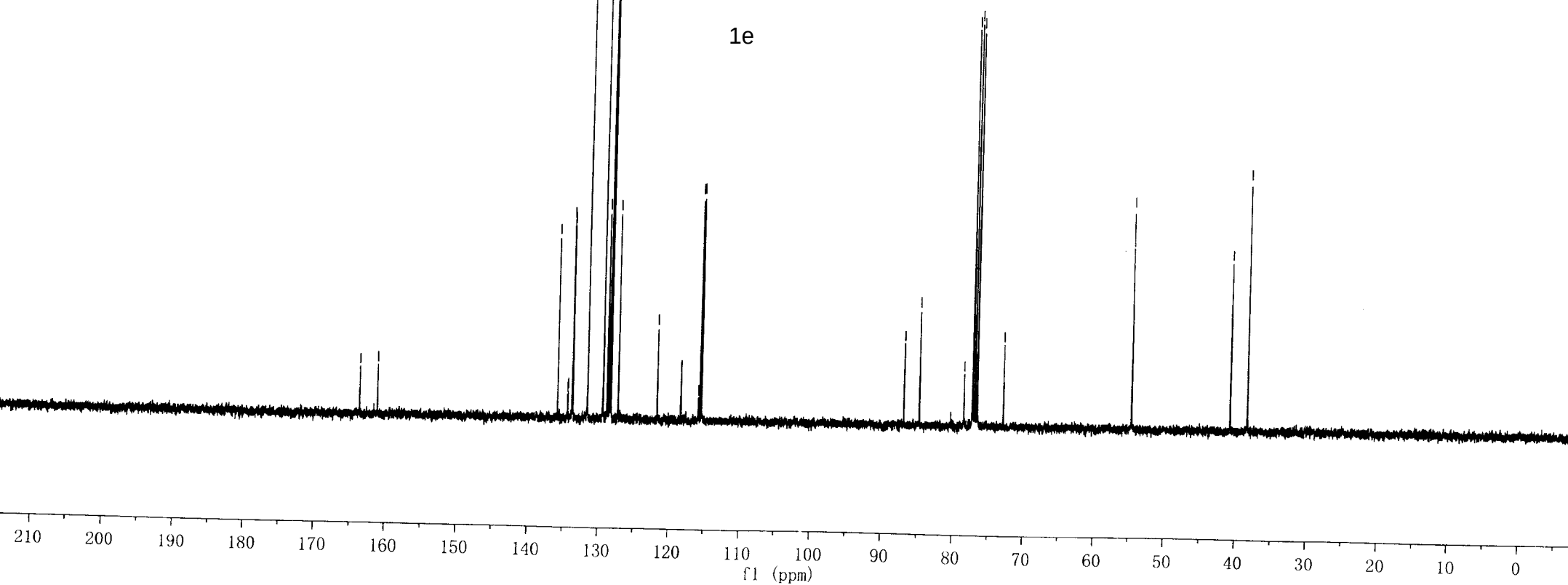
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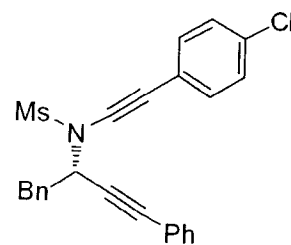
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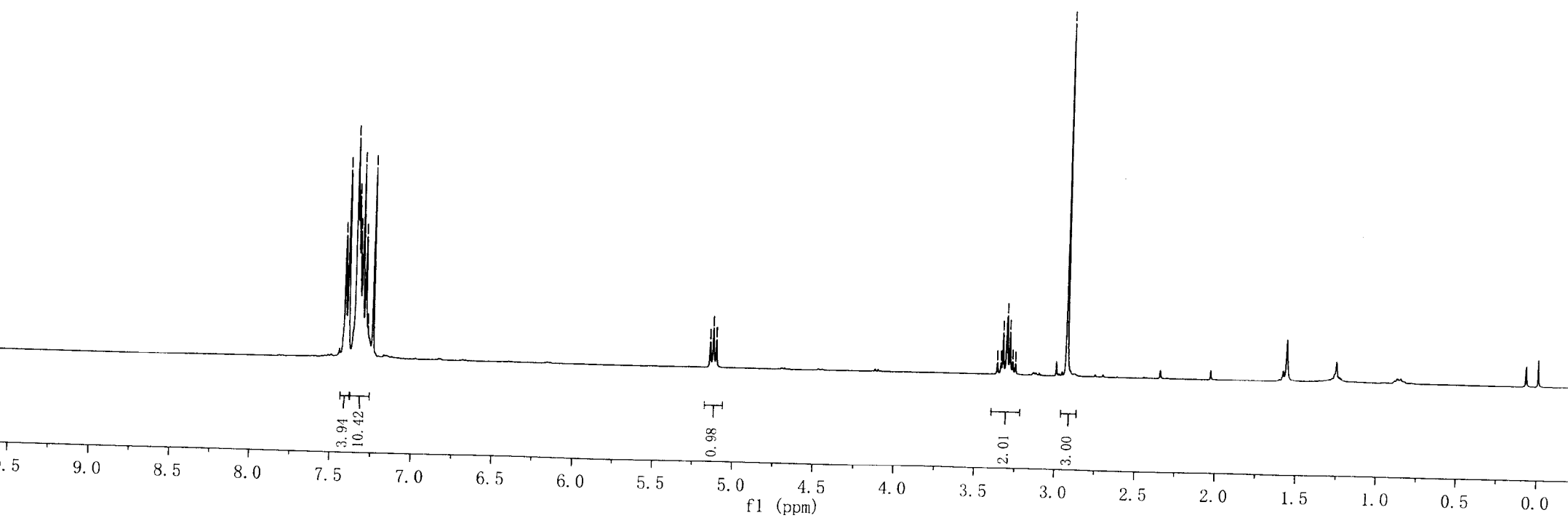
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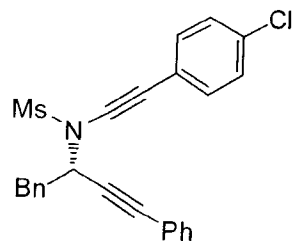
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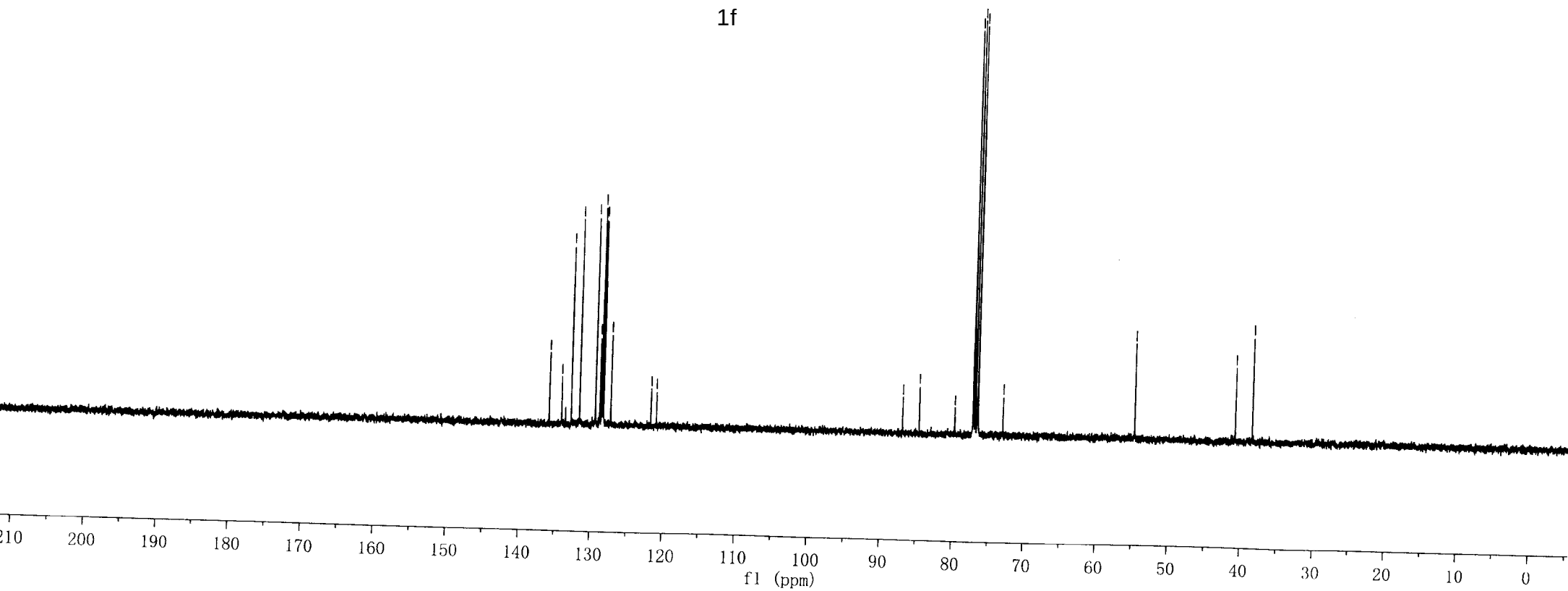


1f





1f



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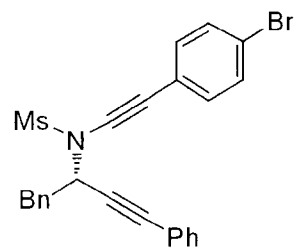
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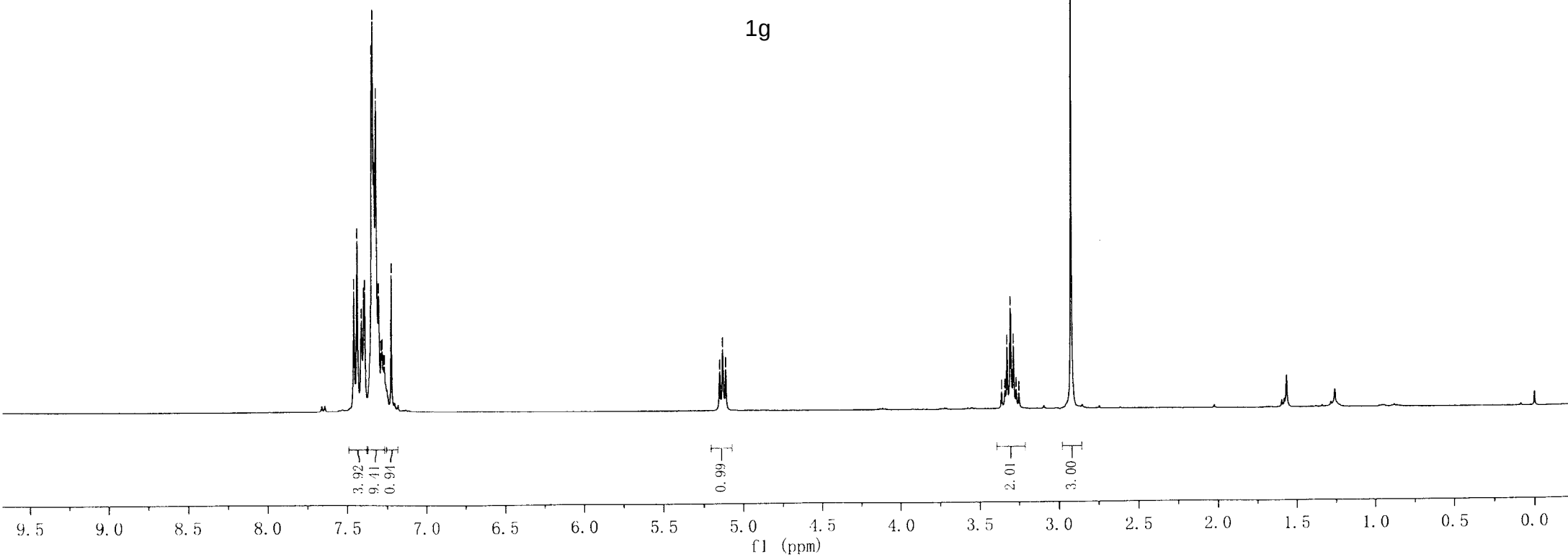
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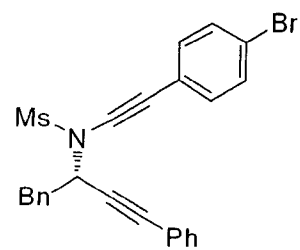


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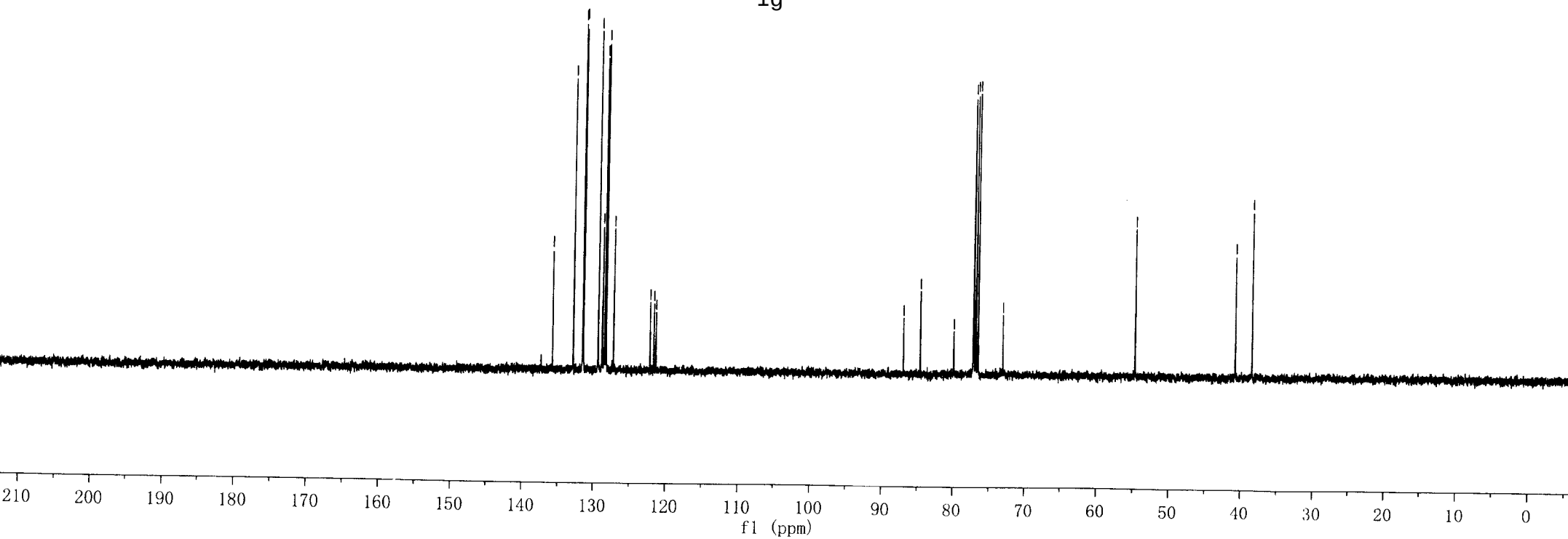
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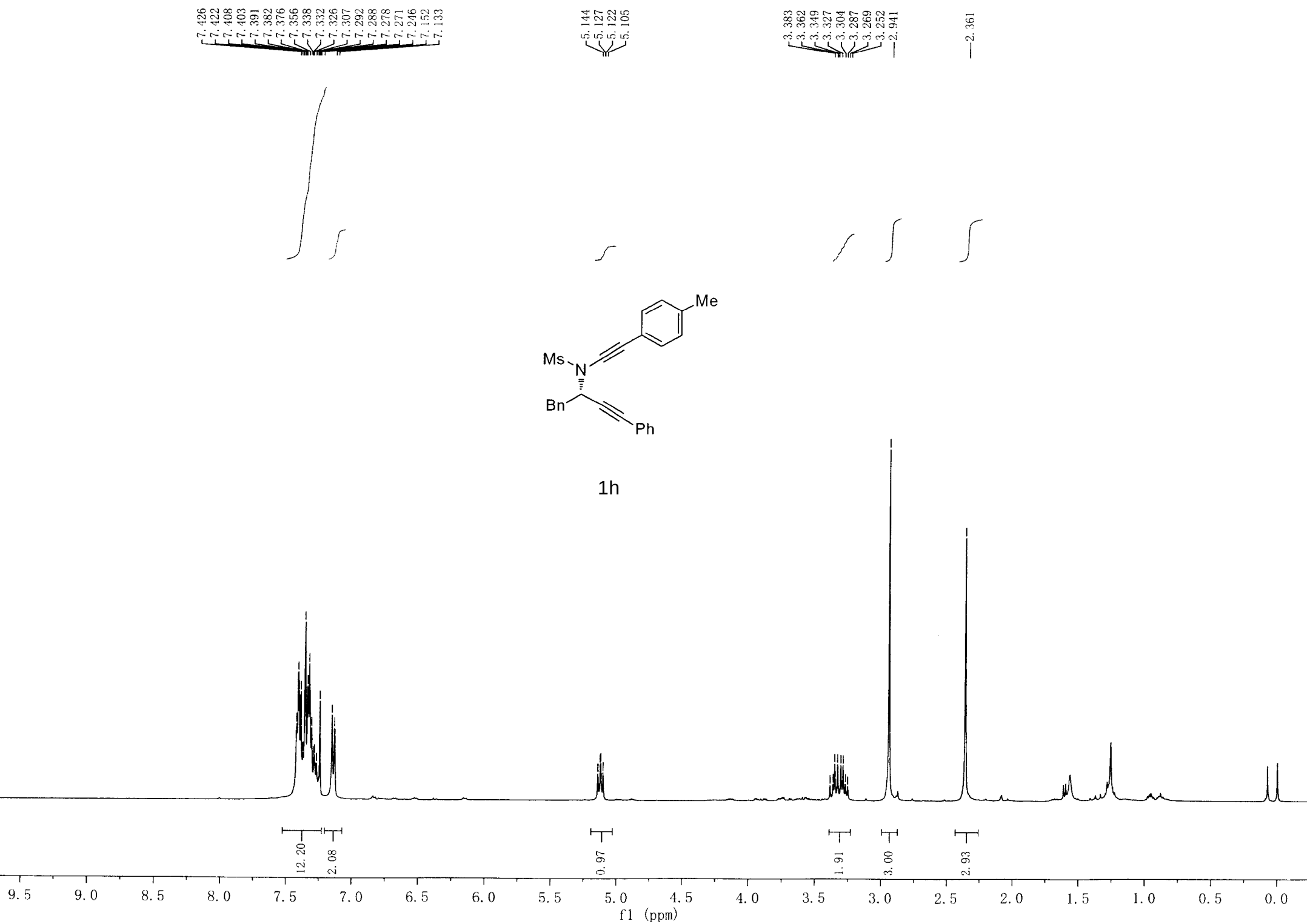
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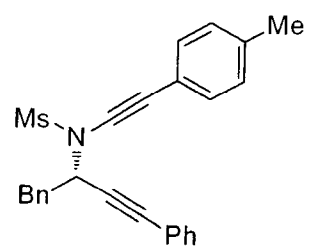
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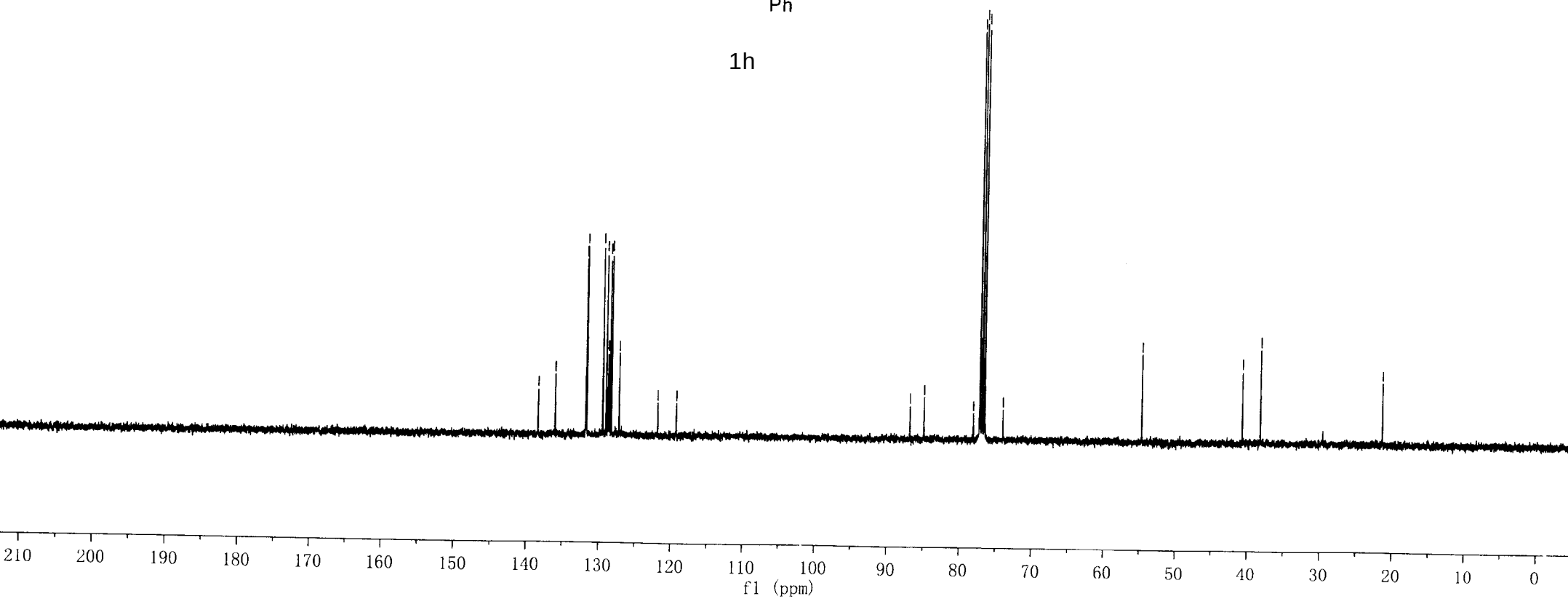
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1h

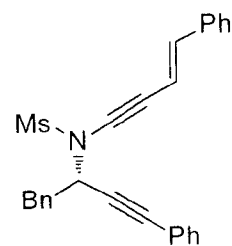


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7.423
7.418
7.403
7.384
7.372
7.359
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7.344
7.333
7.314
7.296
7.292
7.275
7.268
7.261
7.234
6.994
6.954

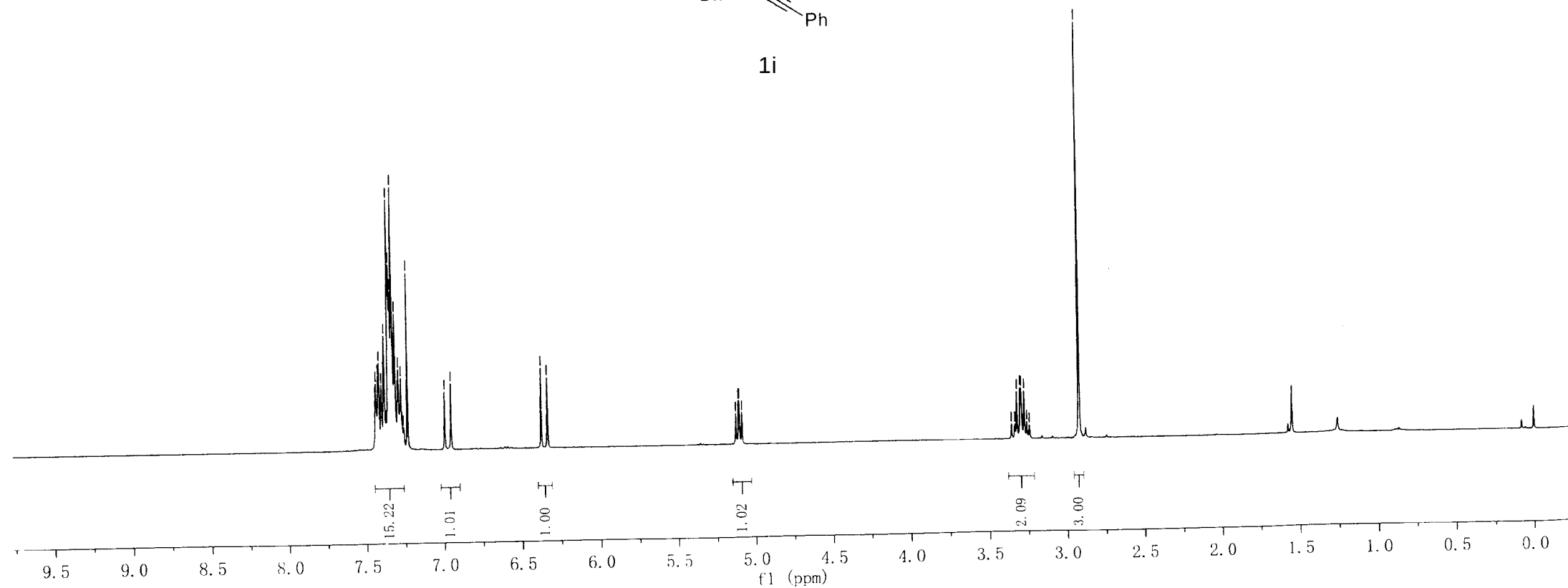
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6.335

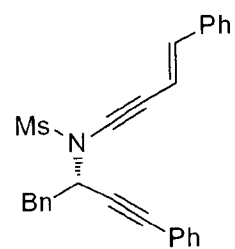
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5.105
5.087

3.356
3.334
3.321
3.300
3.293
3.275
3.258
3.241
2.921

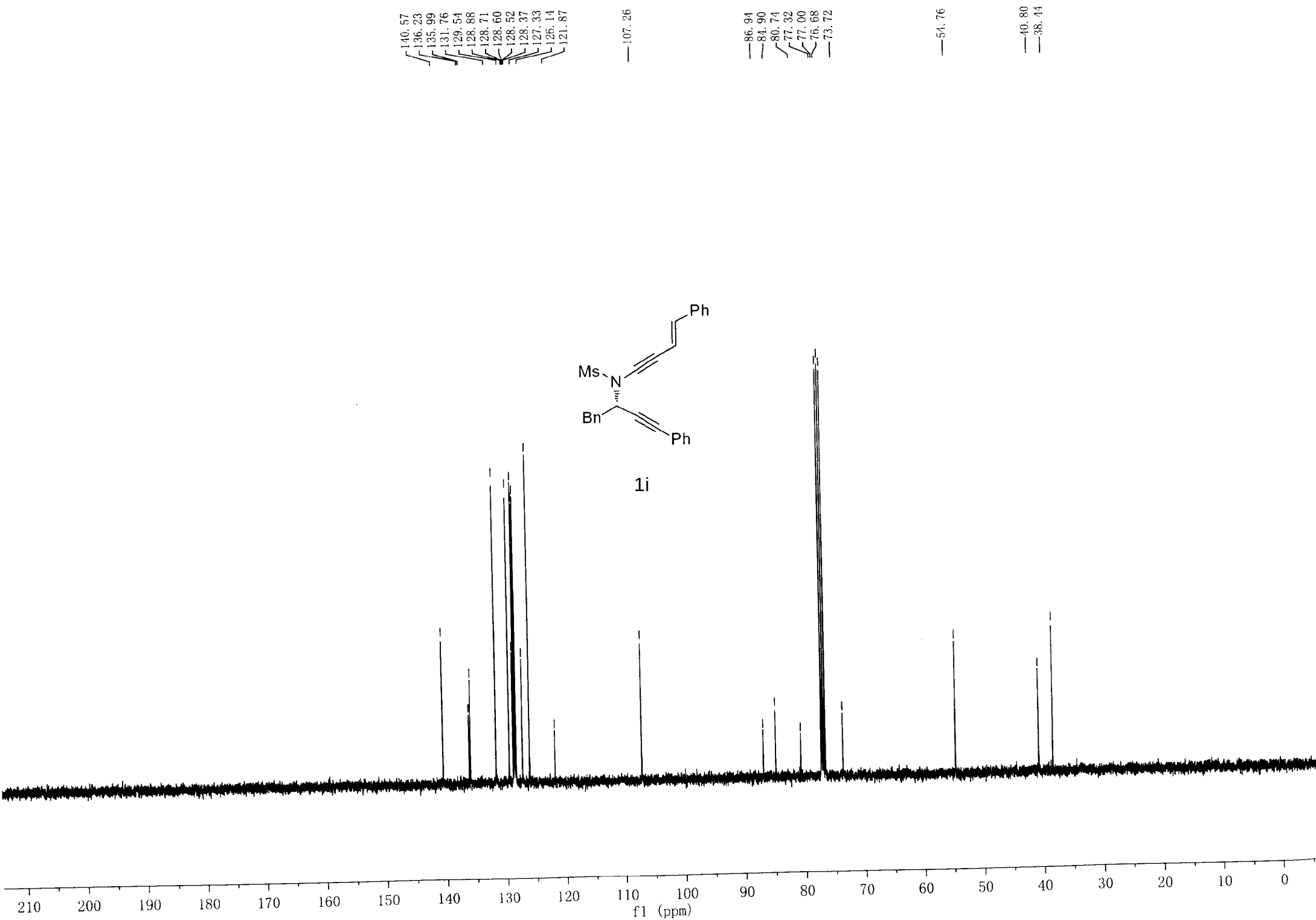


1i





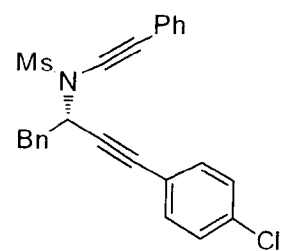
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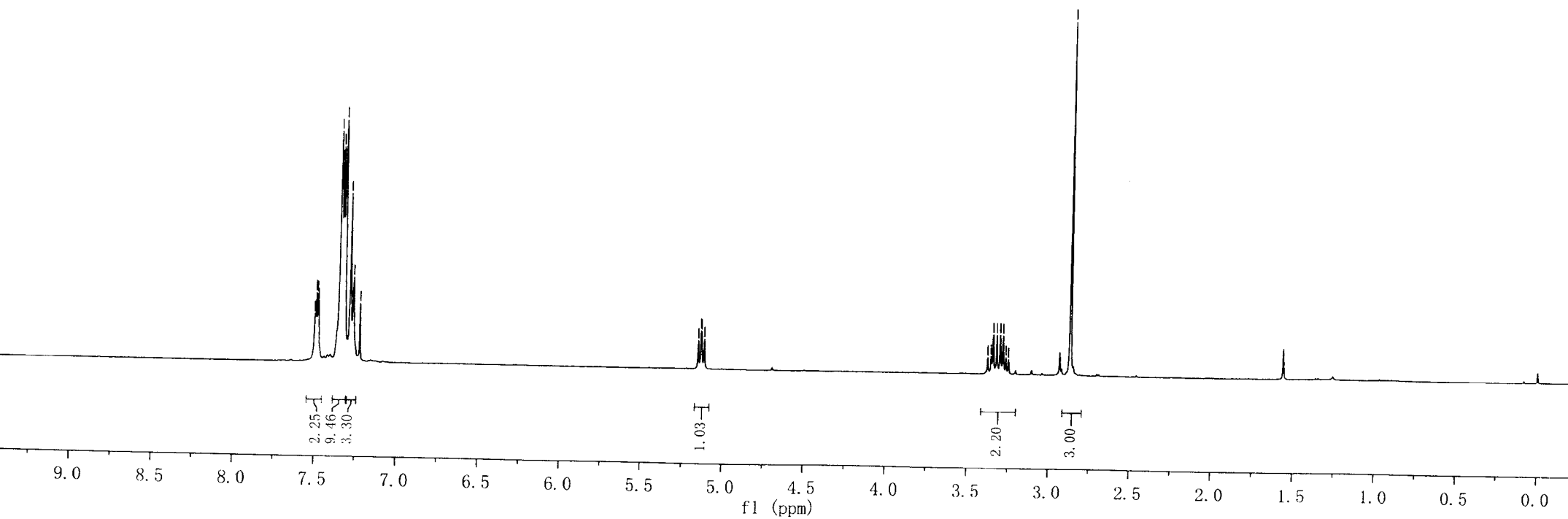
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7.487
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7.347
7.338
7.325
7.288
7.271
7.267
7.226

5.153
5.136
5.132
5.115

3.380
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3.346
3.324
3.302
3.285
3.267
3.250
2.871



1j

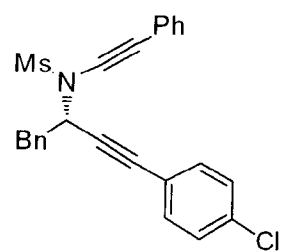


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128.62
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128.26
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122.40
120.32

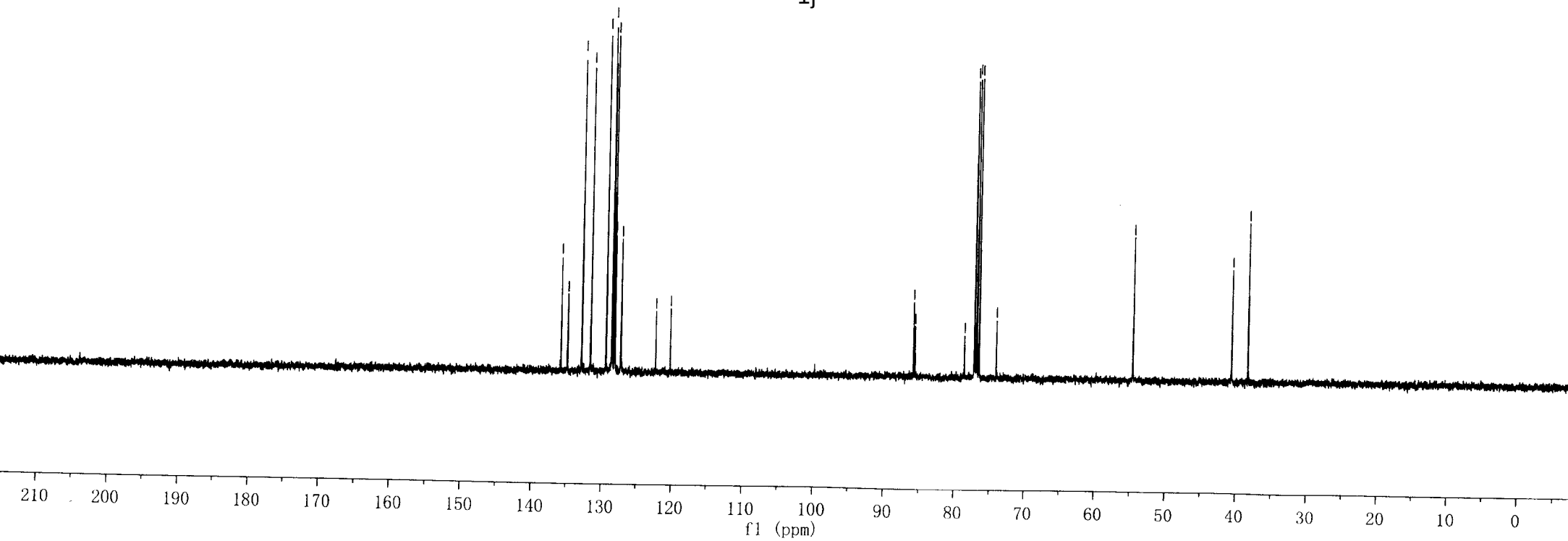
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76.68
74.19

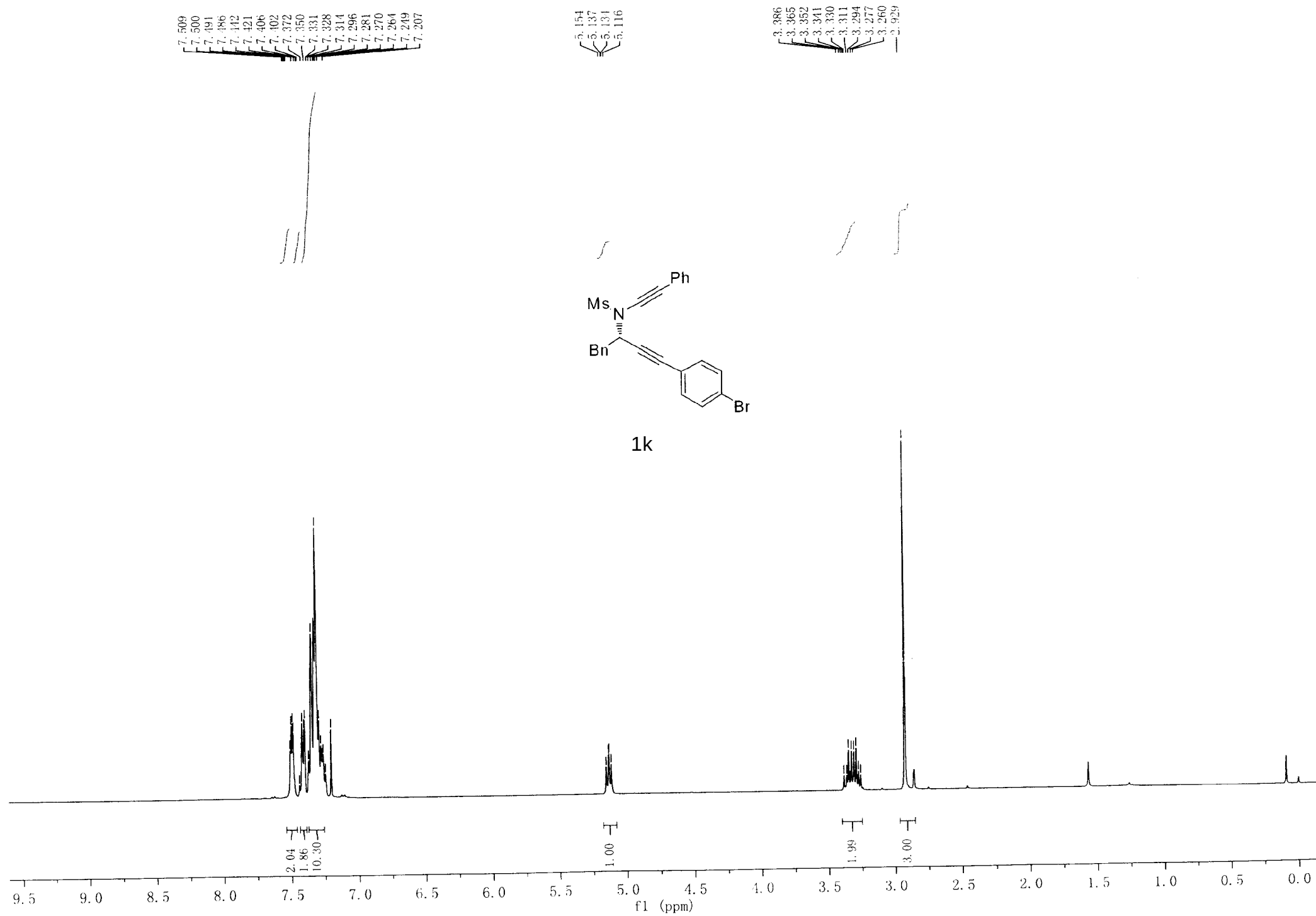
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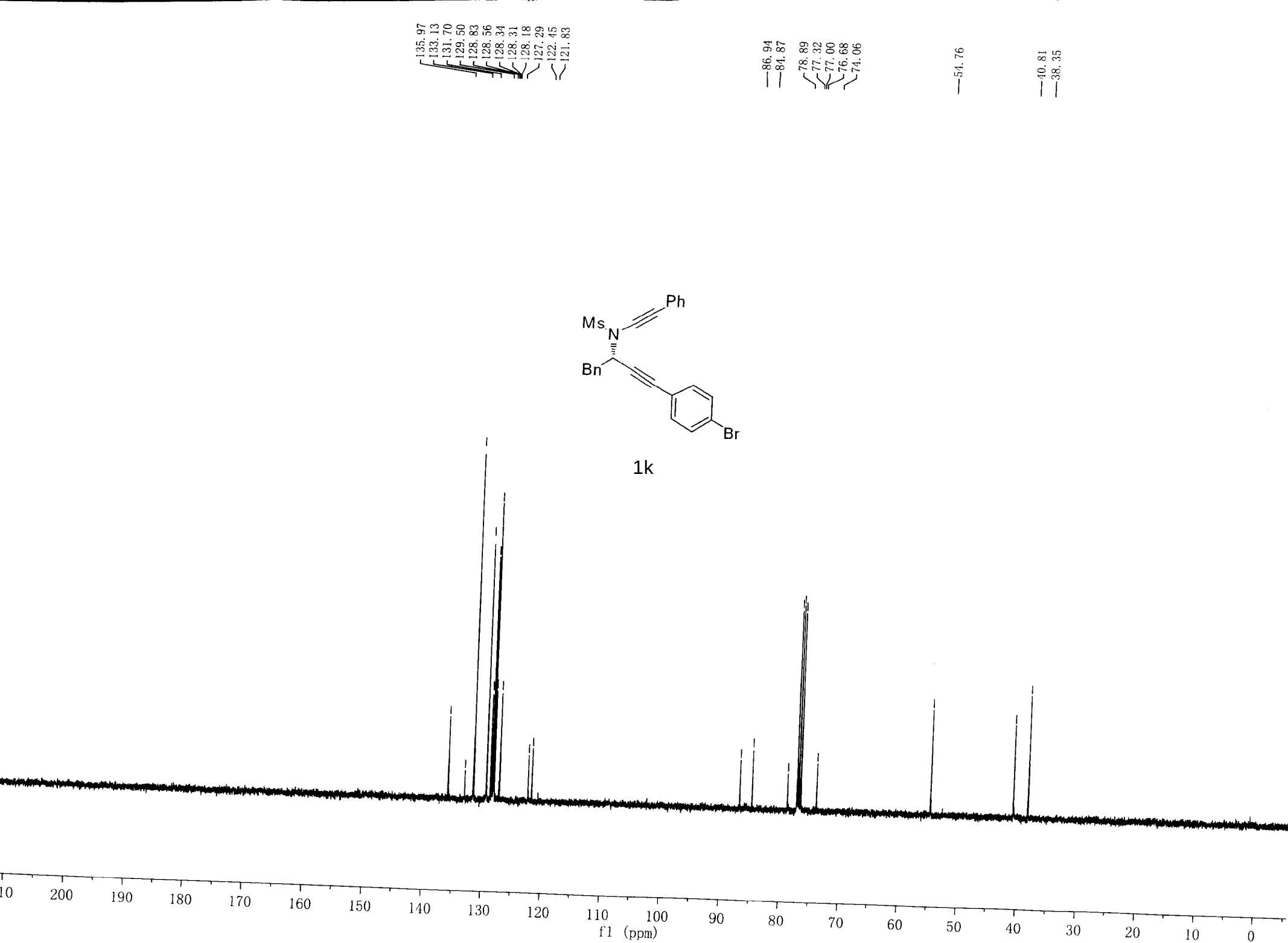
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38.43

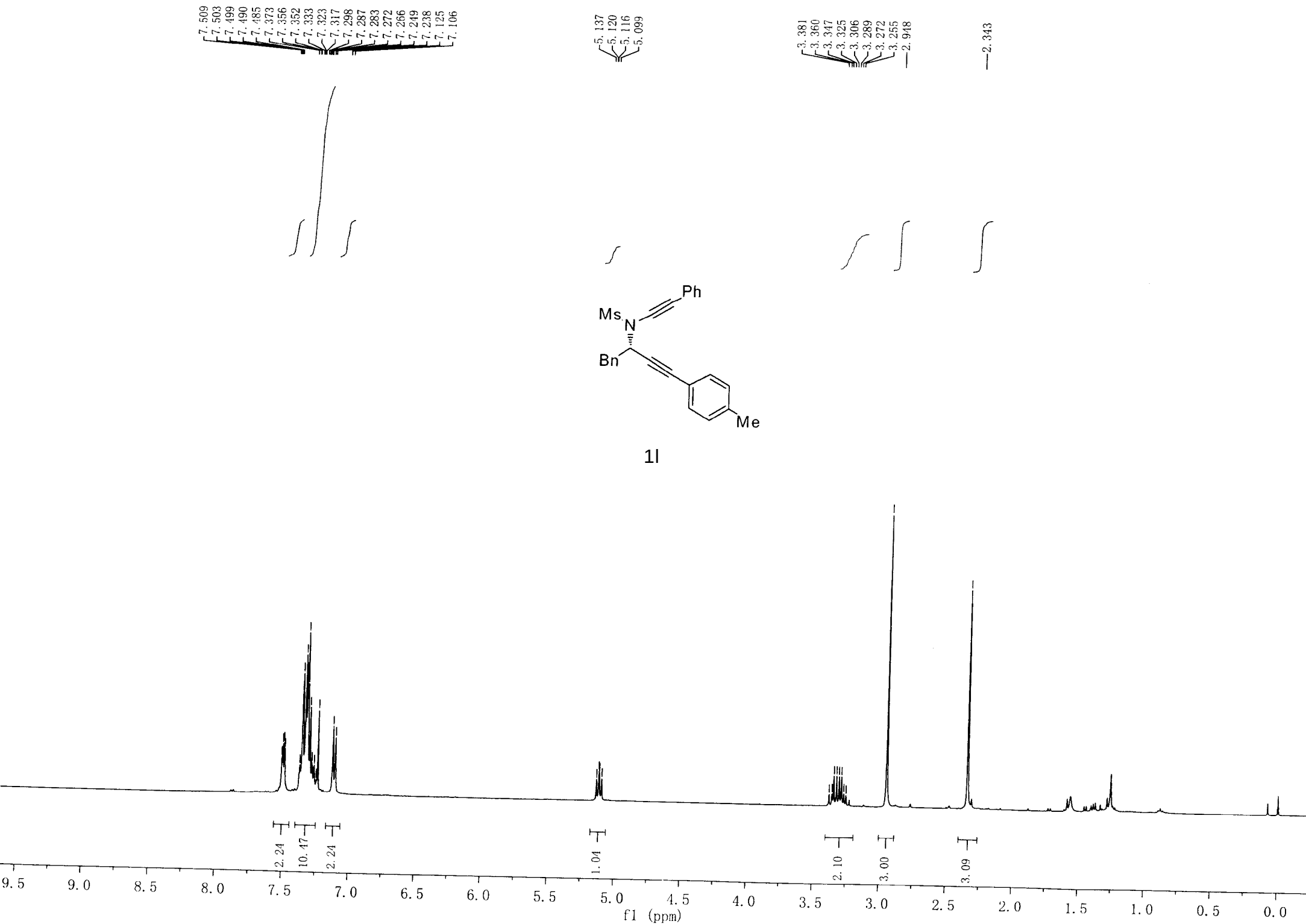


1j









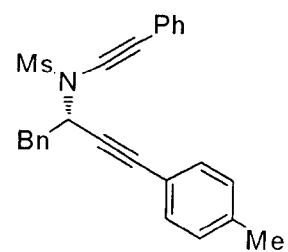
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128.19
127.29
125.48
118.76

87.11
84.15
78.90
77.25
77.00
76.75
74.00

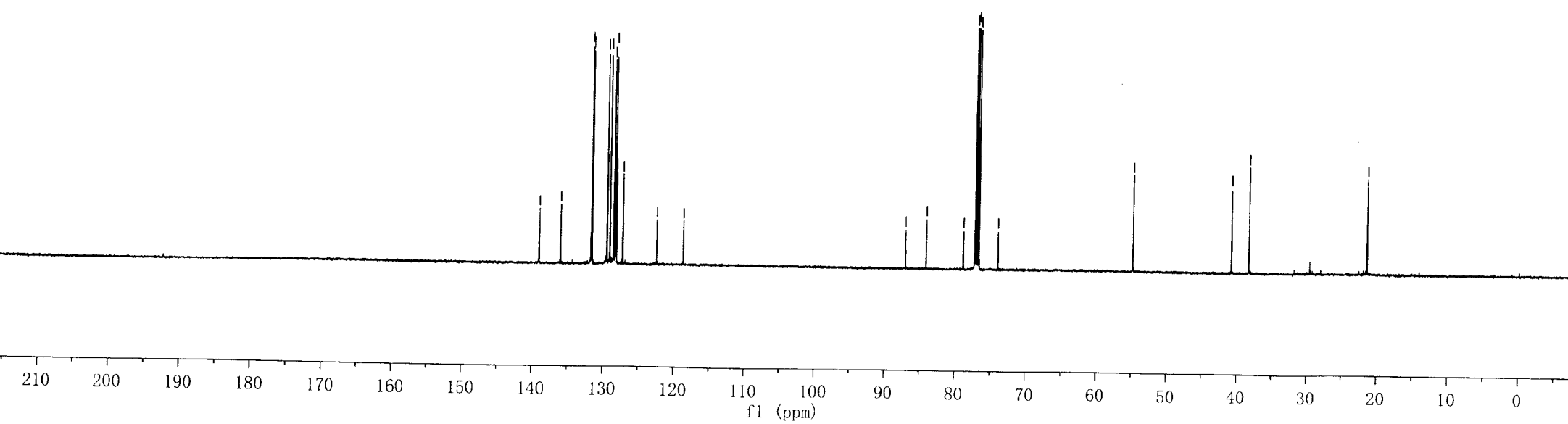
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40.84
38.33

21.47



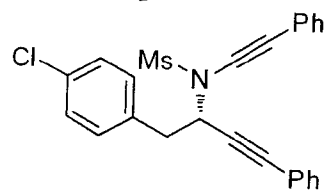
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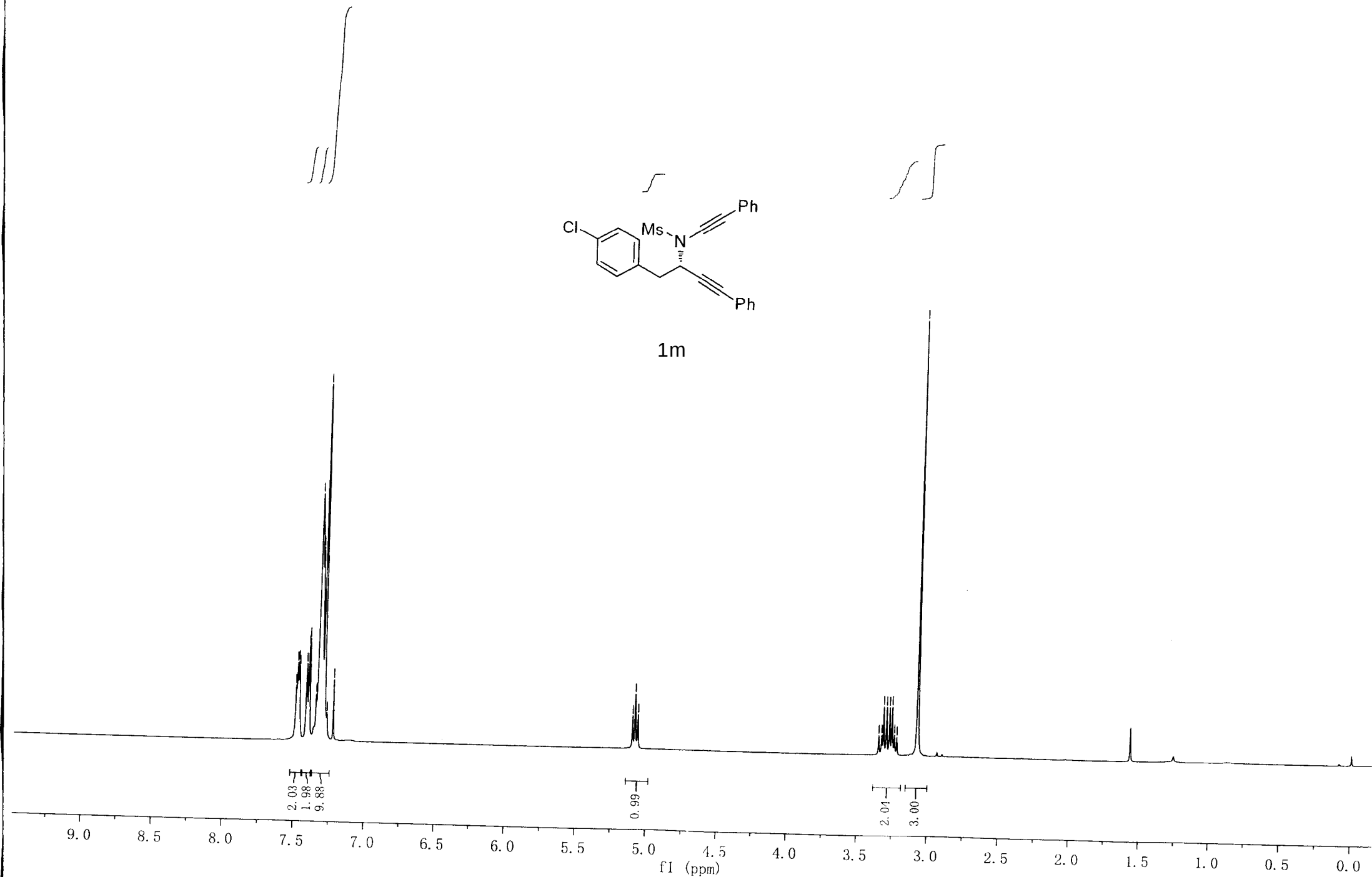
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7.470
7.419
7.404
7.400
7.350
7.332
7.318
7.297
7.273
7.228

5.104
5.086
5.066

3.353
3.332
3.318
3.298
3.276
3.258
3.241
3.224
3.079



1m

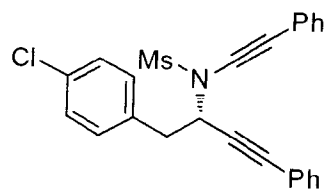


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122.29
121.64

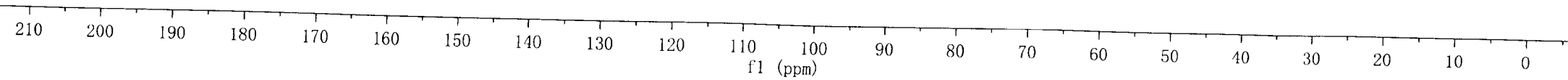
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74.13

54.46

40.17
38.40



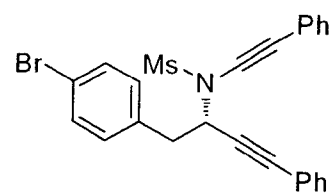
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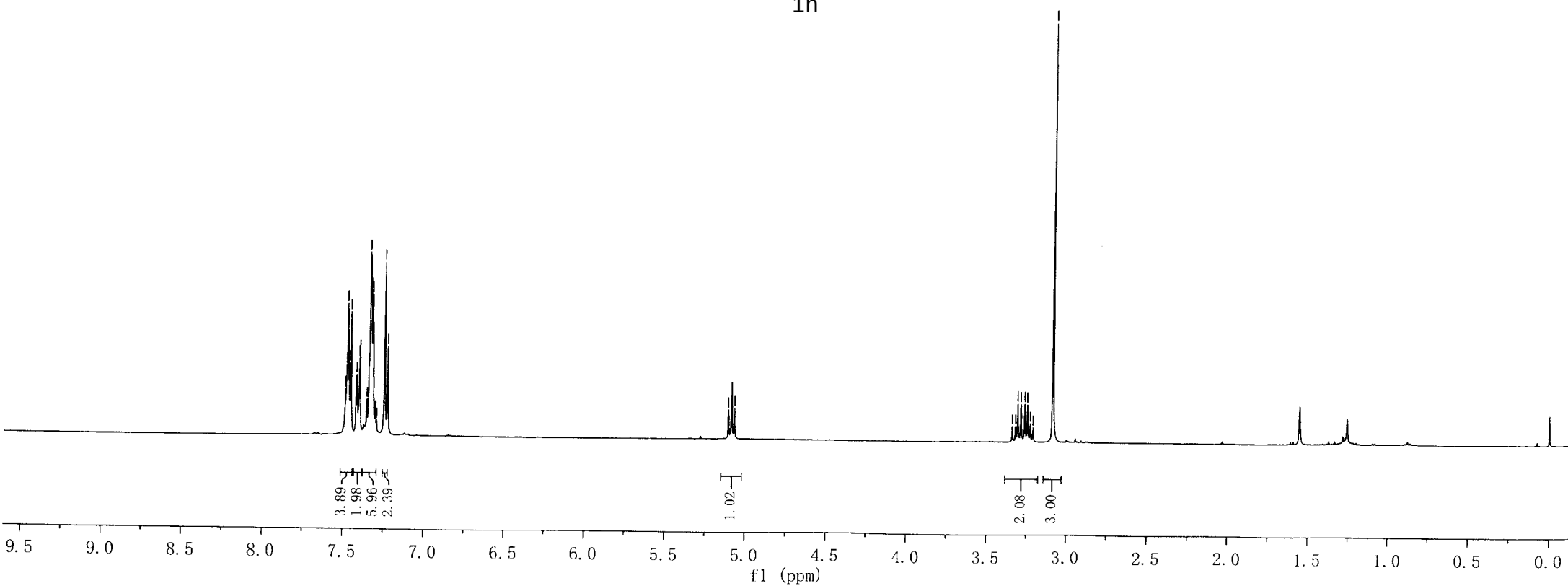
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7.454
7.422
7.418
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7.330
7.322
7.318
7.305
7.301
7.295
7.244
7.226

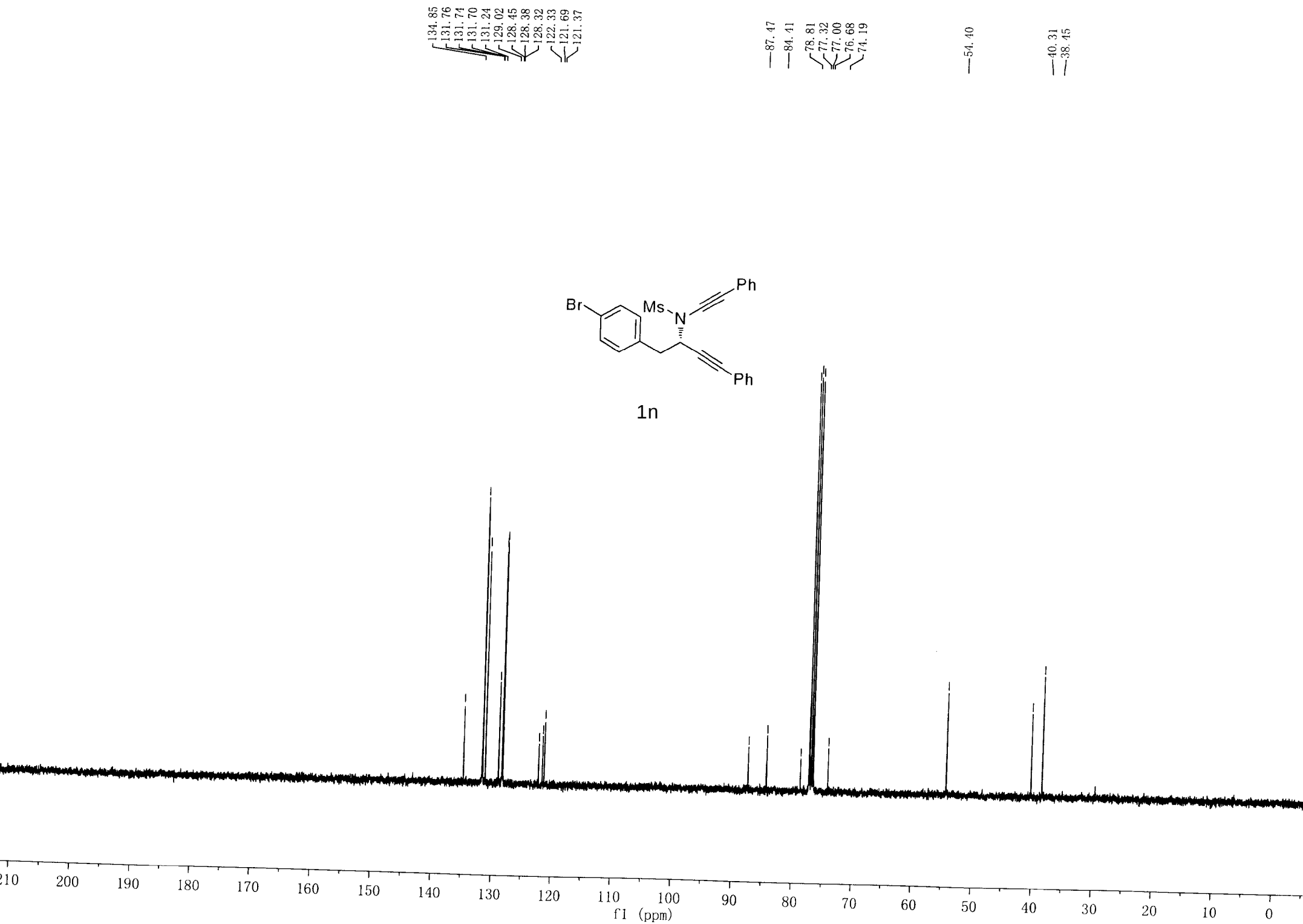
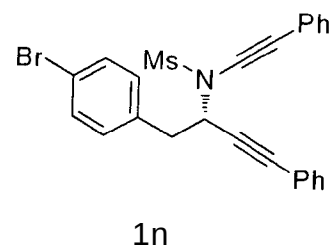
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5.087
5.085
5.067

3.341
3.320
3.306
3.286
3.263
3.245
3.229
3.211
3.087



1n



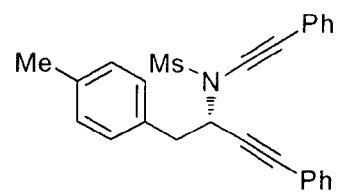


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7.484
7.432
7.427
7.424
7.416
7.412
7.408
7.342
7.339
7.331
7.327
7.323
7.320
7.313
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7.304
7.301
7.297
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7.285
7.280
7.256
7.240
7.200
7.144
7.129

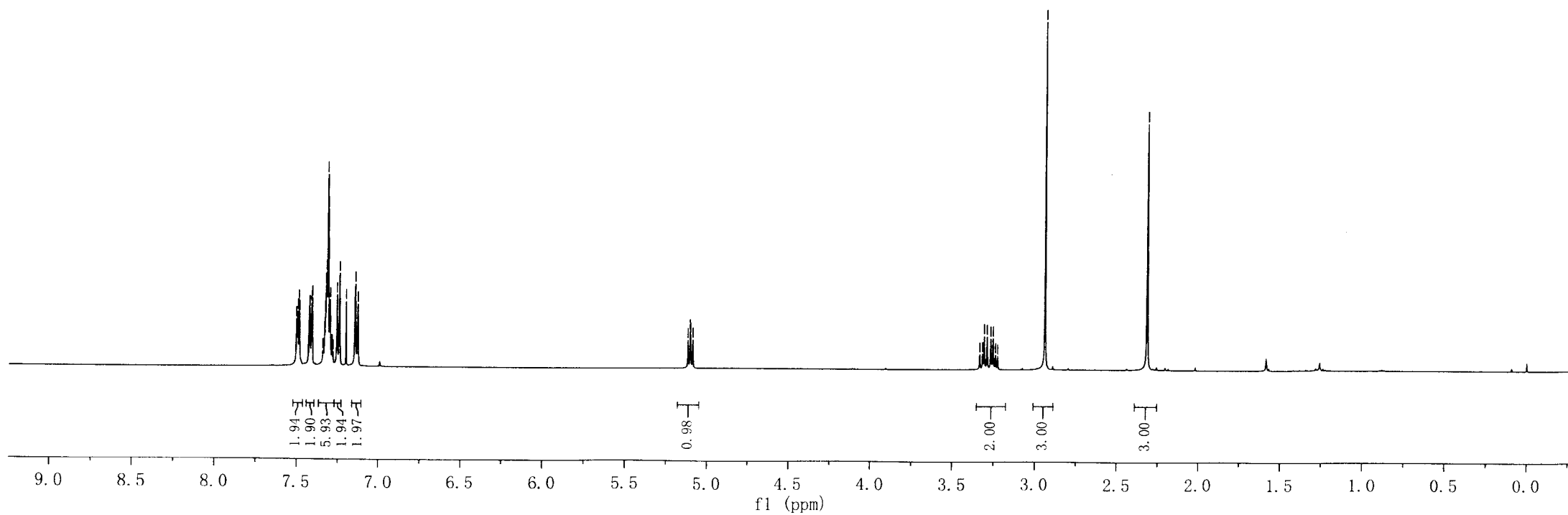
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5.086

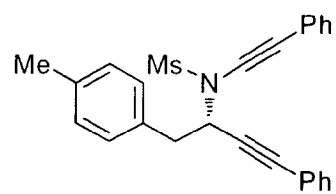
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3.291
3.268
3.255
3.241
3.227
2.939

2.315

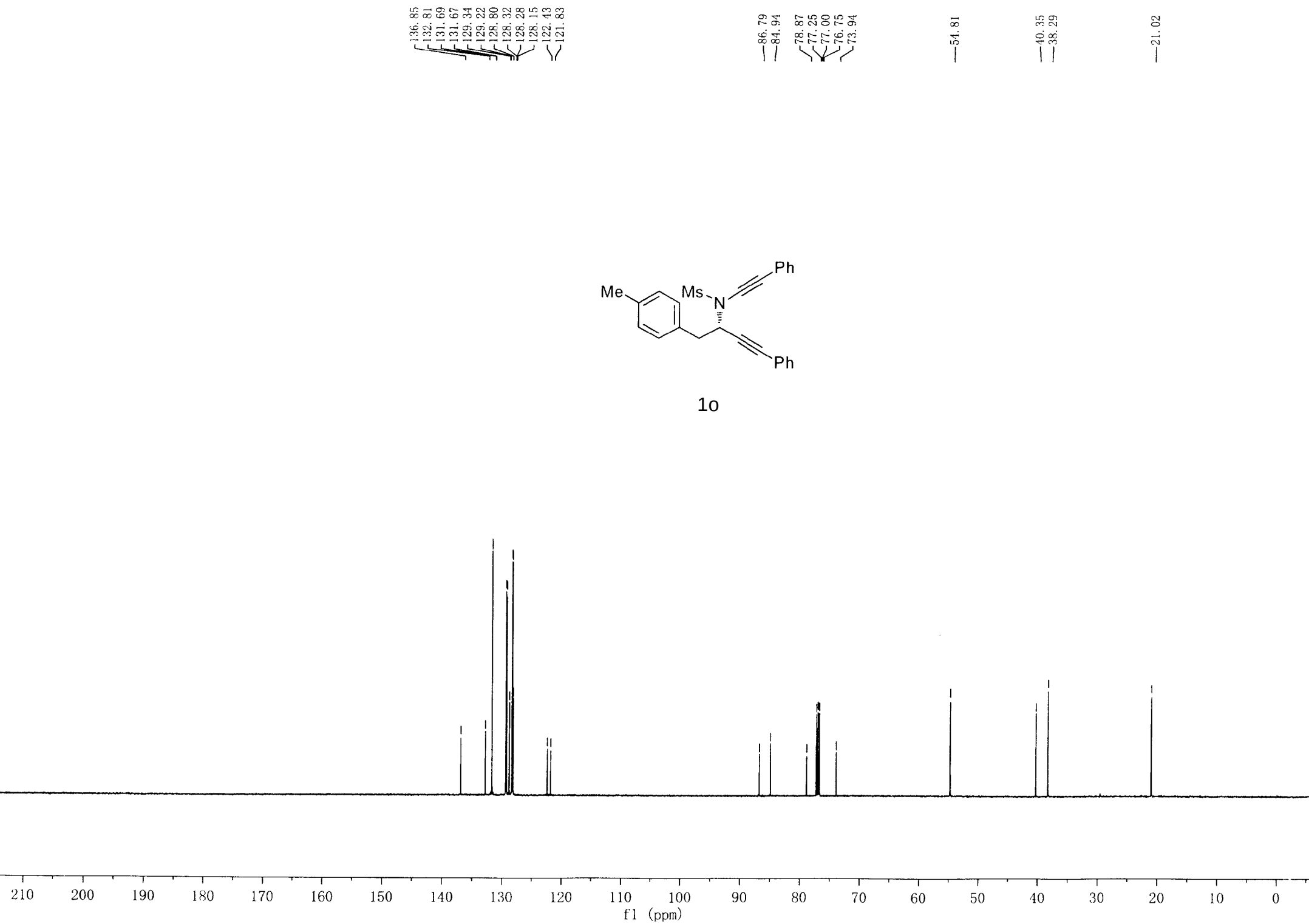


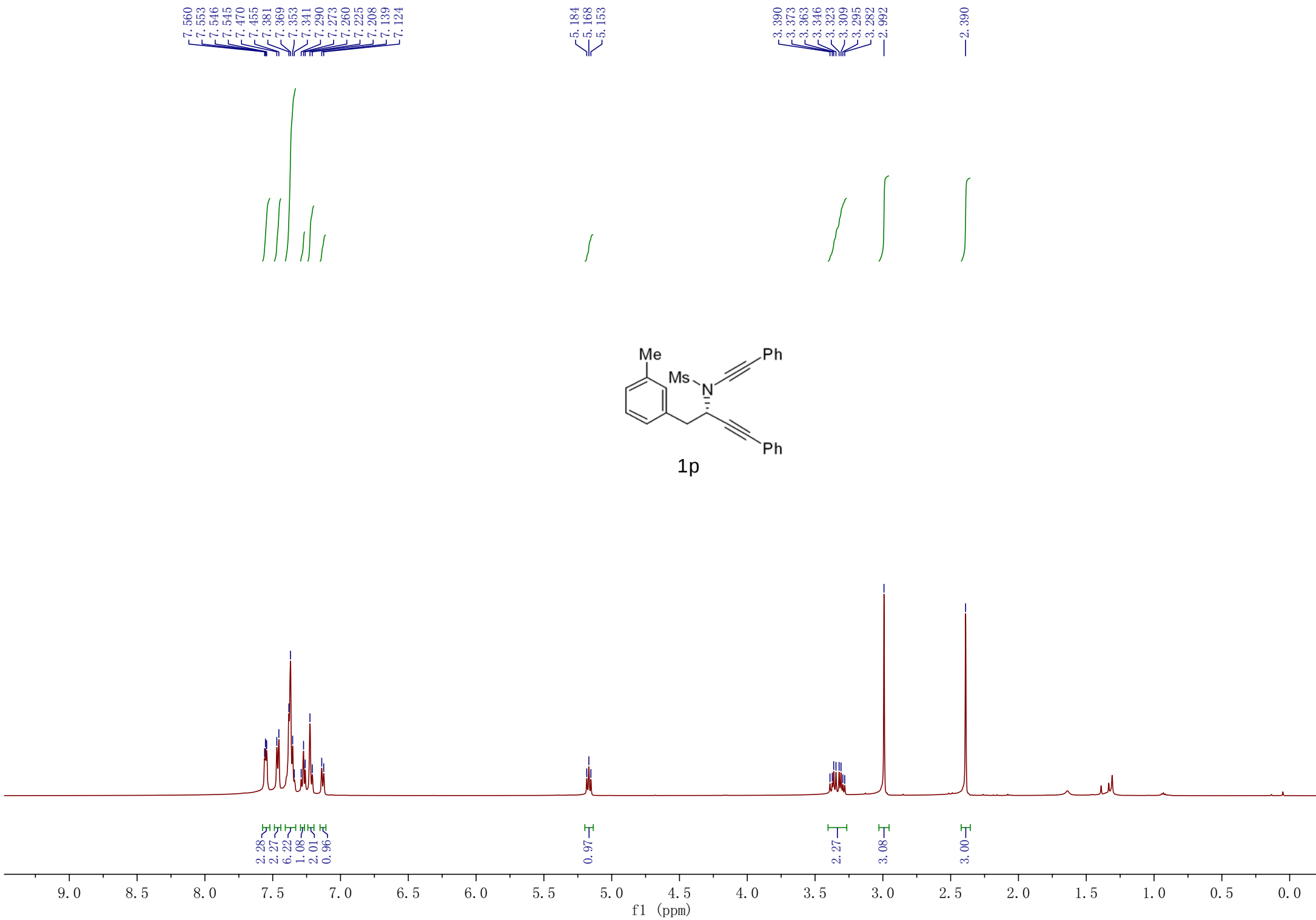
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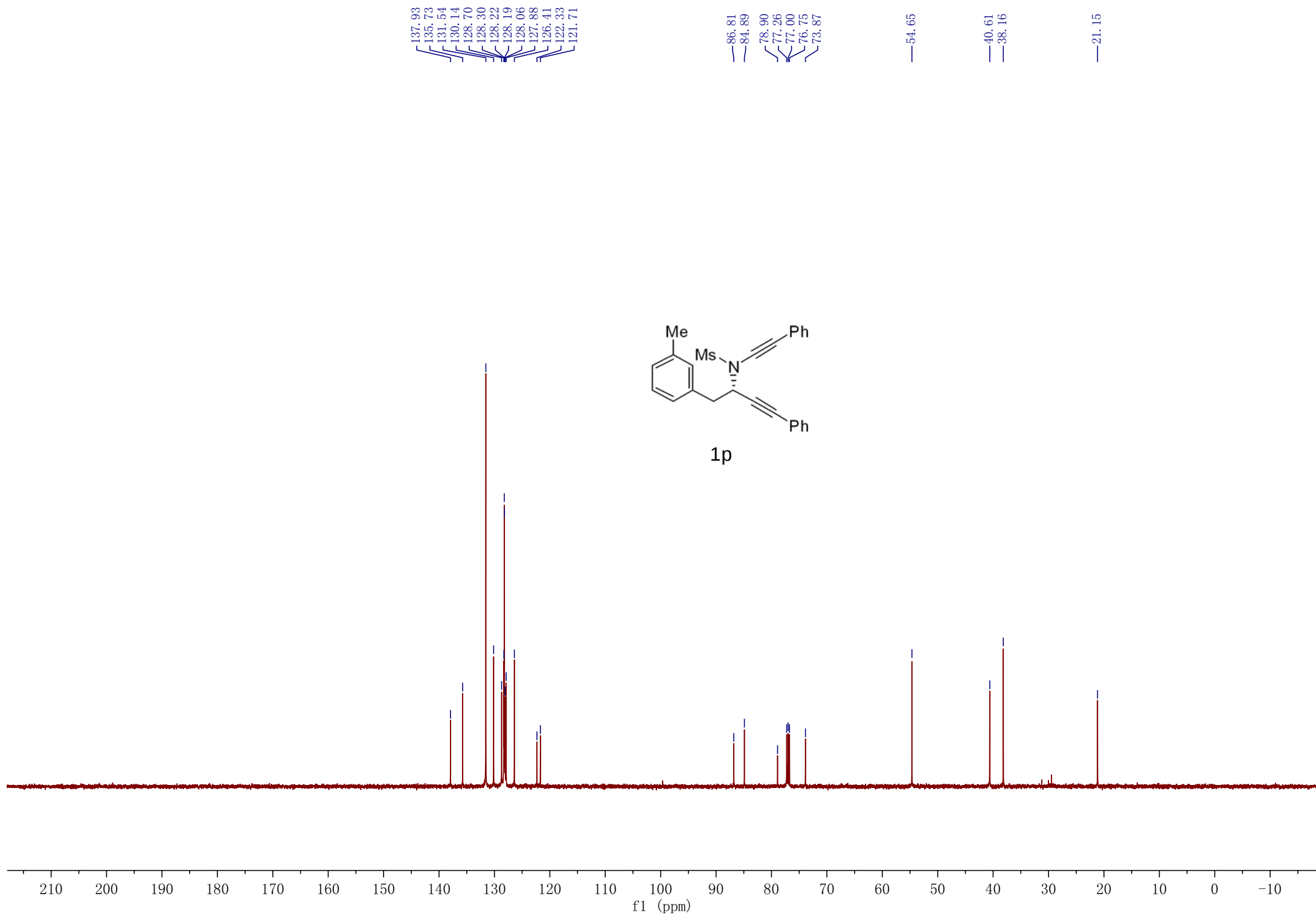


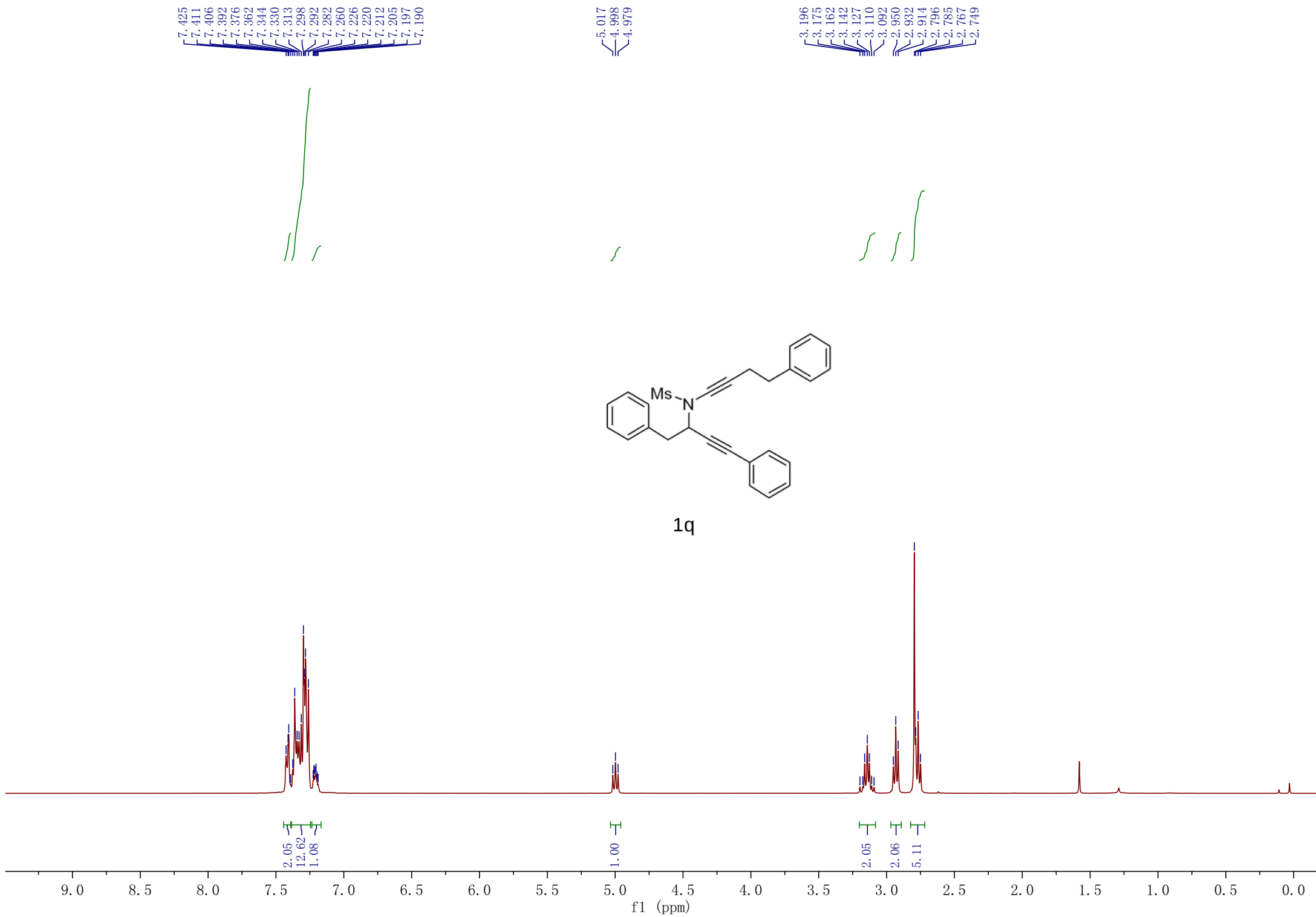


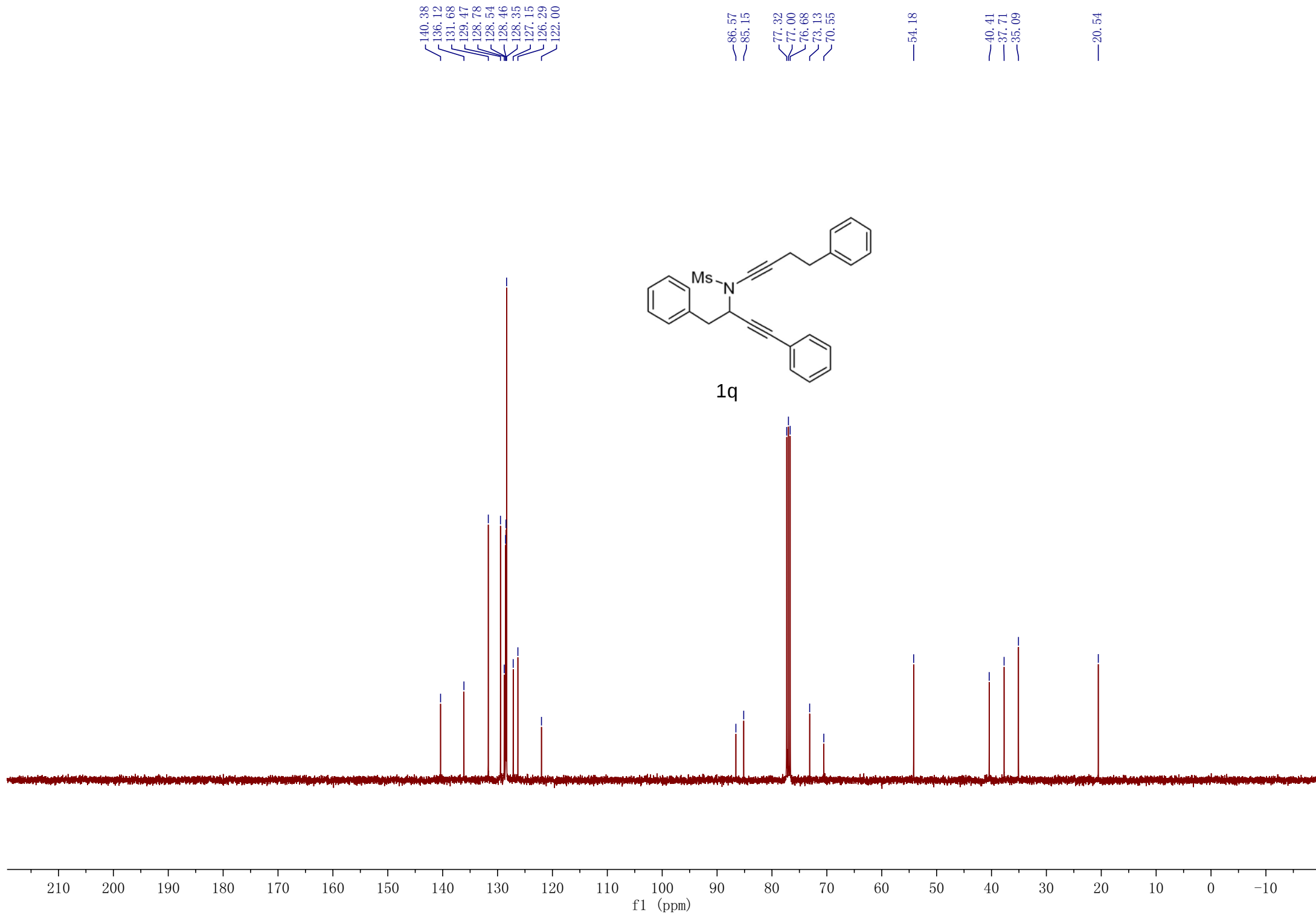
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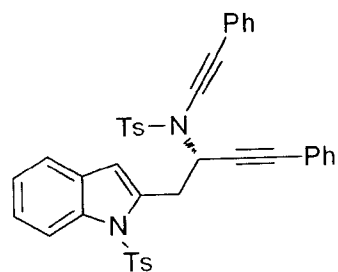
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8.112
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7.772
7.632
7.615
7.329
7.325
7.319
7.315
7.251
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7.140
7.098
7.081
7.068

5.544
5.533
5.527
5.515

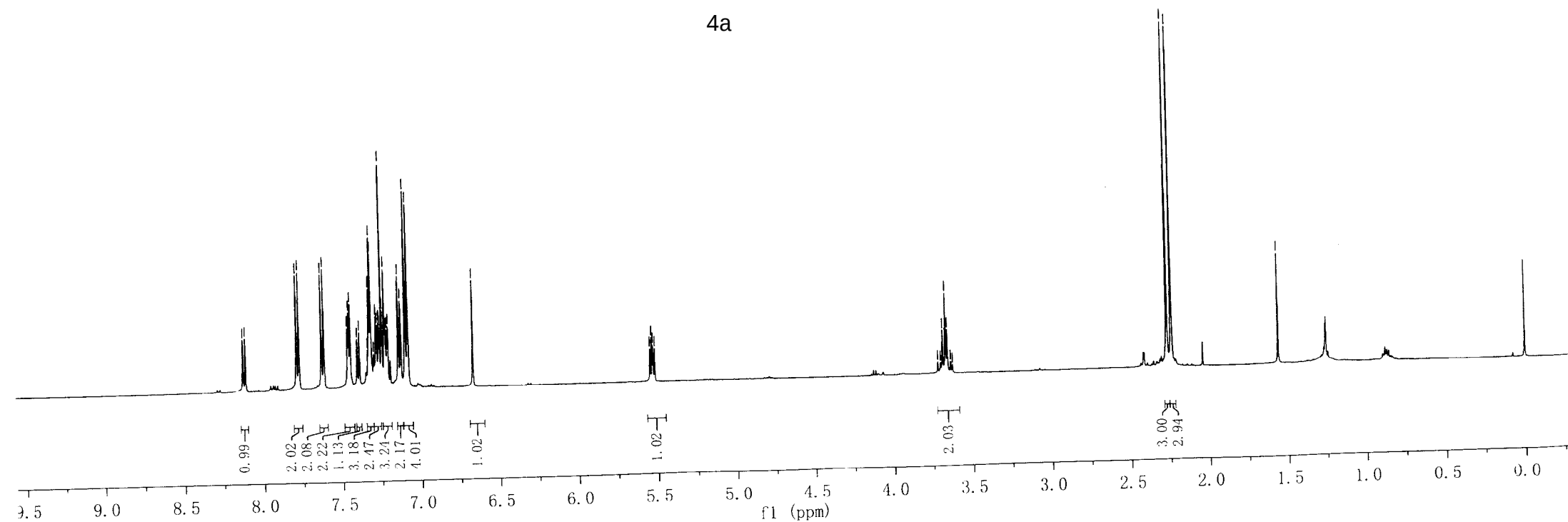
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3.668
3.656
3.636
3.625

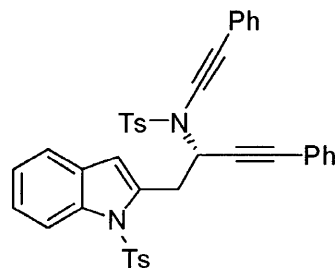
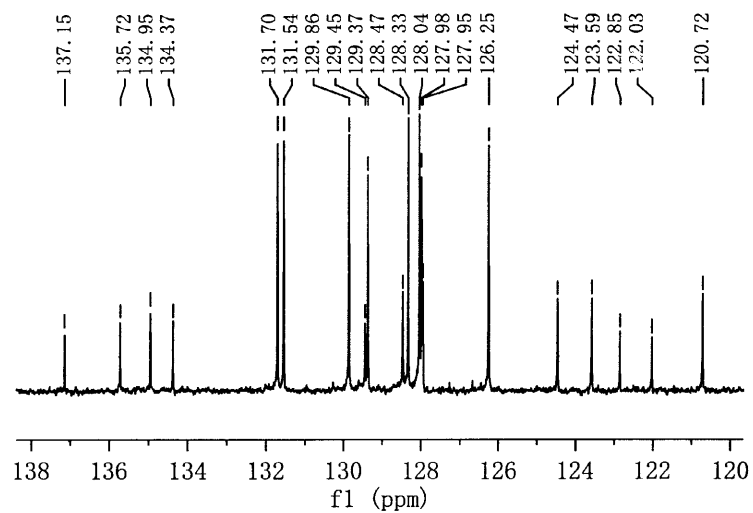
2.269
2.240

1.561



4a





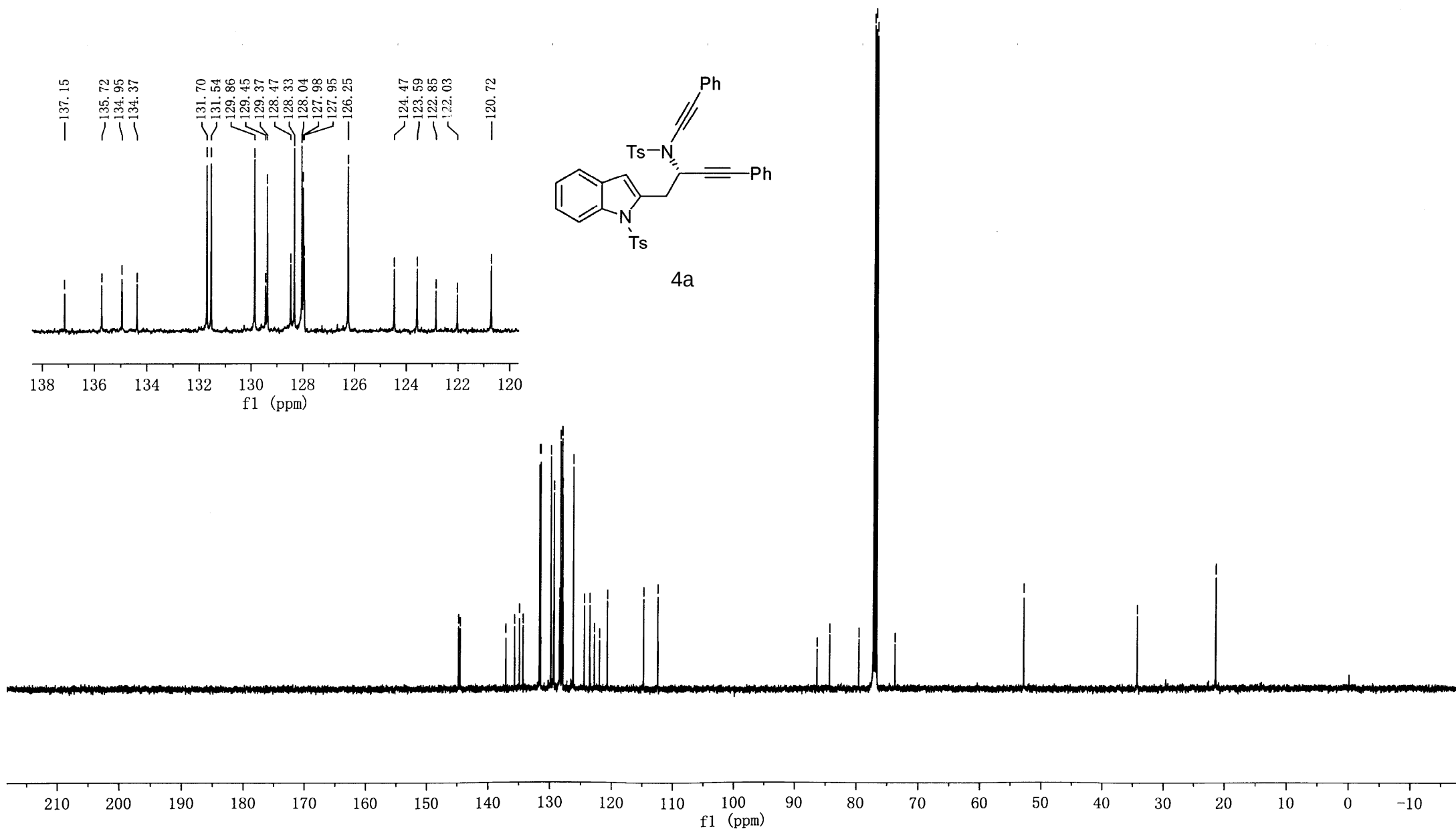
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131.54
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129.37
128.47
128.33
128.04
127.98
127.95
126.25
120.72
112.48

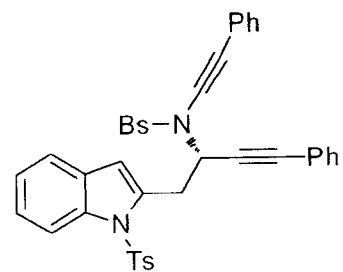
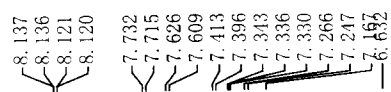
86.40
84.38
79.63
77.25
77.00
76.75
73.75

52.89

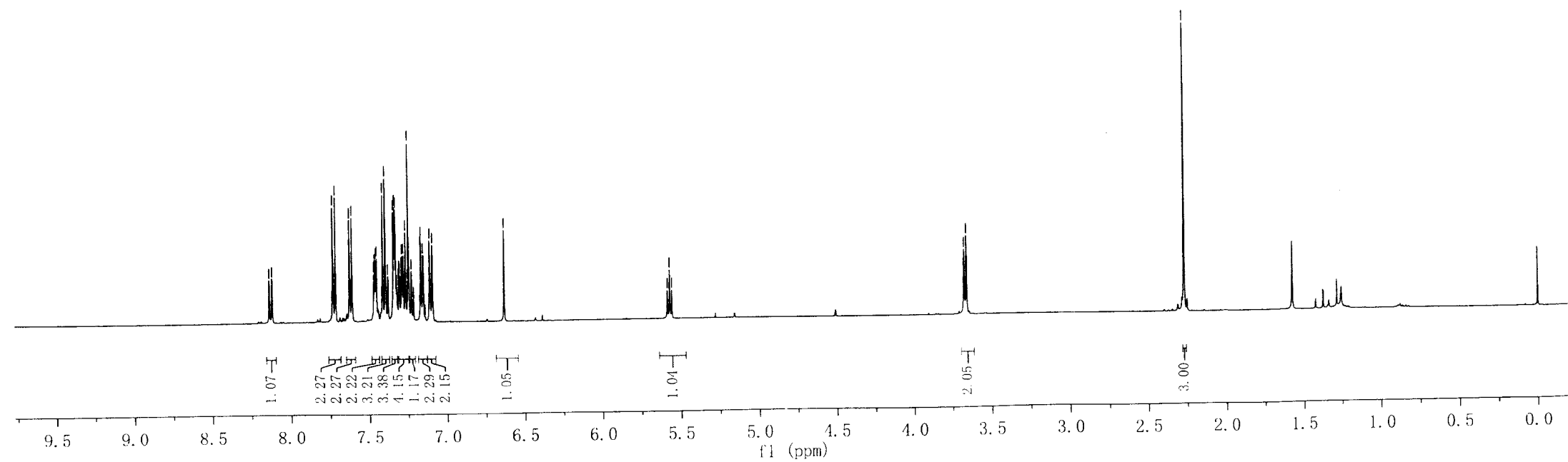
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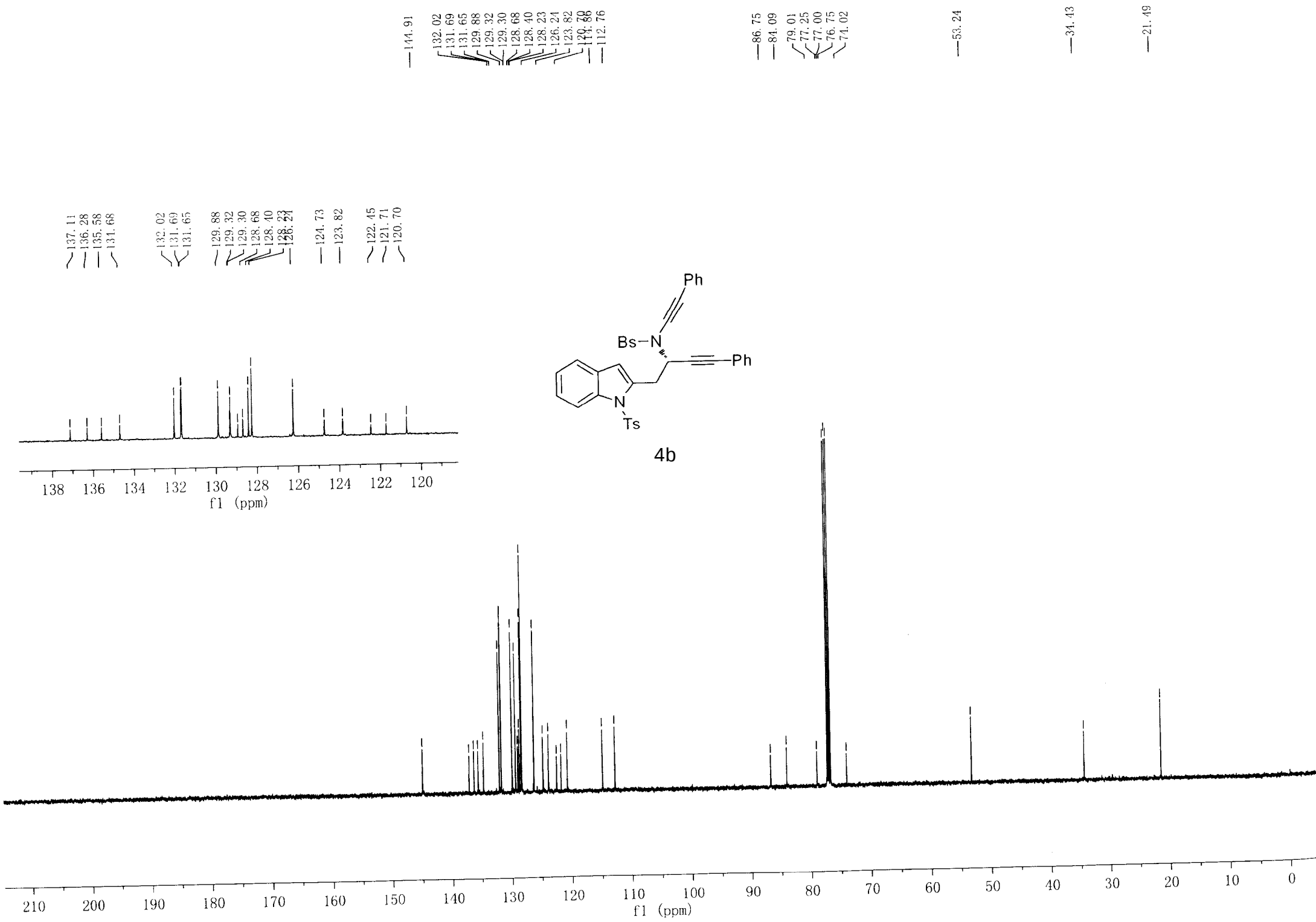
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21.49

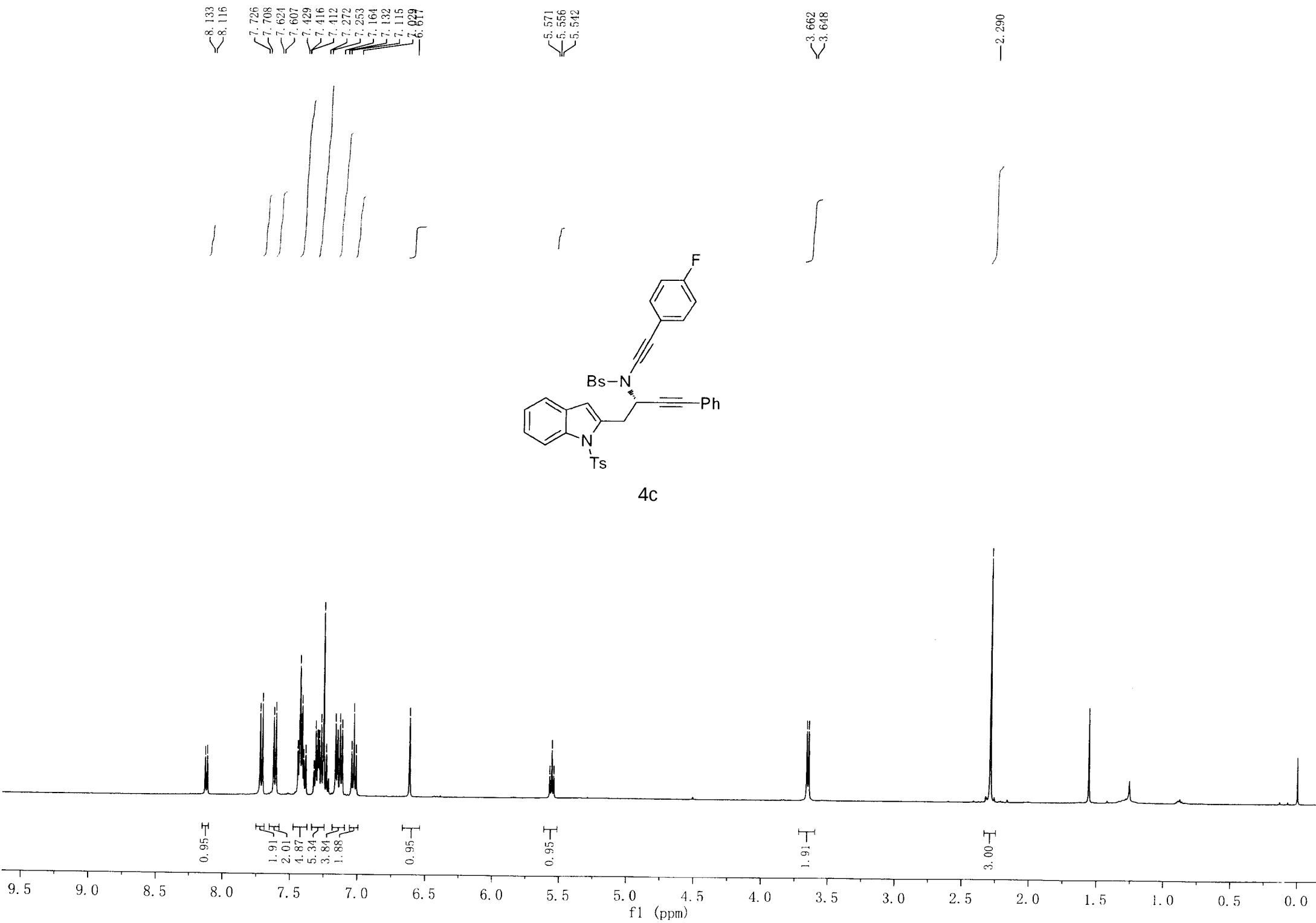


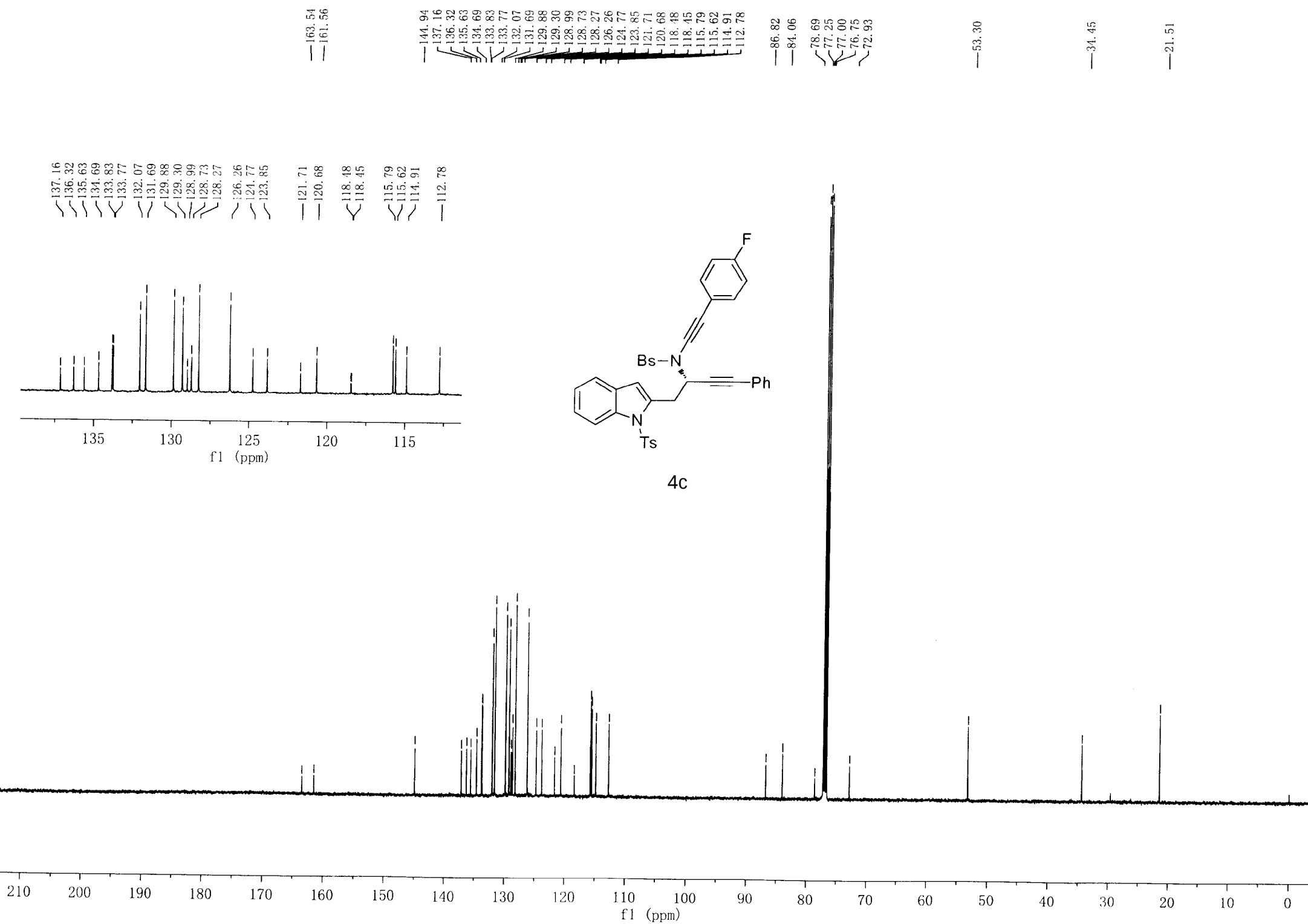


4b







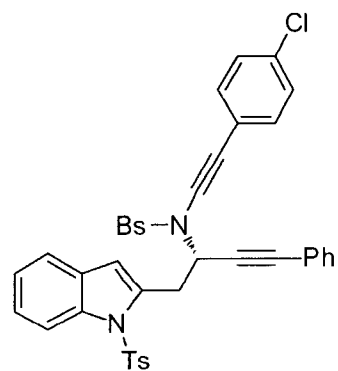


8.131
8.114
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7.698
7.619
7.602
7.419
7.402
7.377
7.360
7.308
7.292
7.217
7.164
7.123
6.609

5.578
5.563
5.548

3.665
3.651

2.281



4d

1.04

2.01

2.11

5.22

5.98

1.19

2.35

2.16

1.00

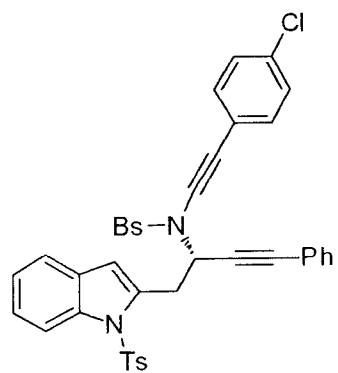
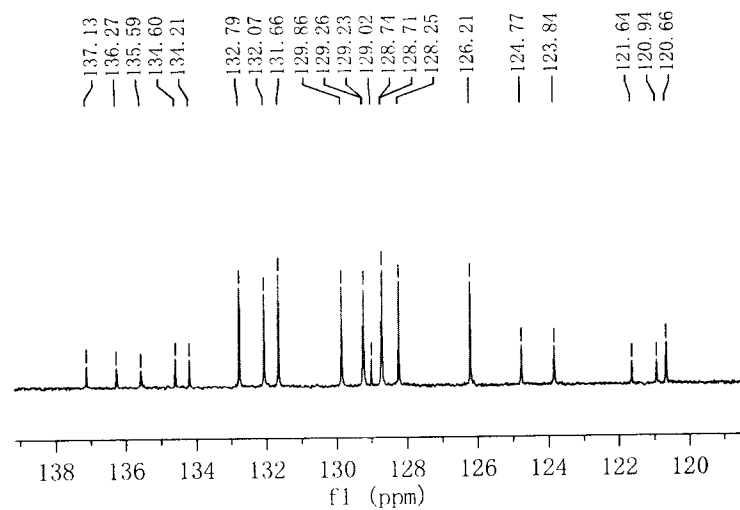
1.01

2.03

3.00

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

f1 (ppm)



4d

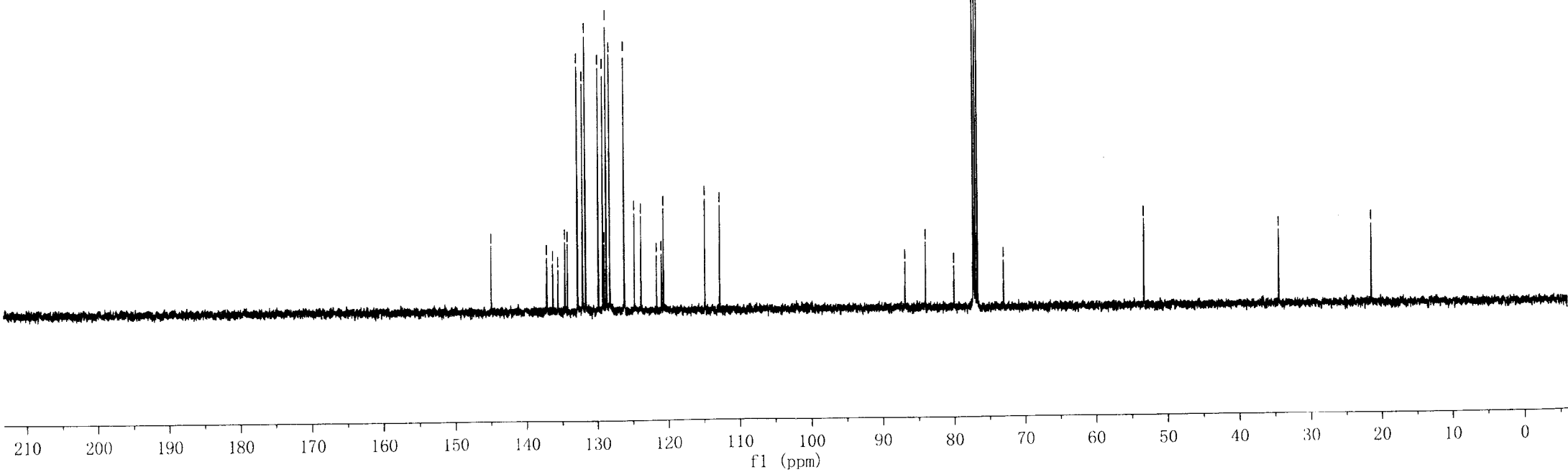
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86.86, 84.00, 80.02, 77.32, 77.00, 76.68, 73.05

53.31

34.47

21.46

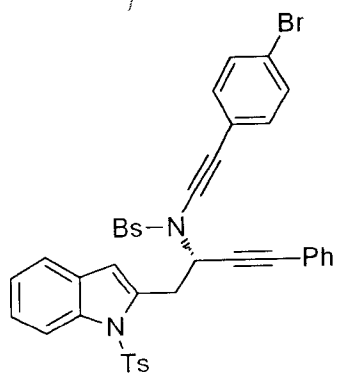


8.130
8.113
7.713
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7.466
7.450
7.418
7.401
7.307
7.292
7.248
7.165
6.663

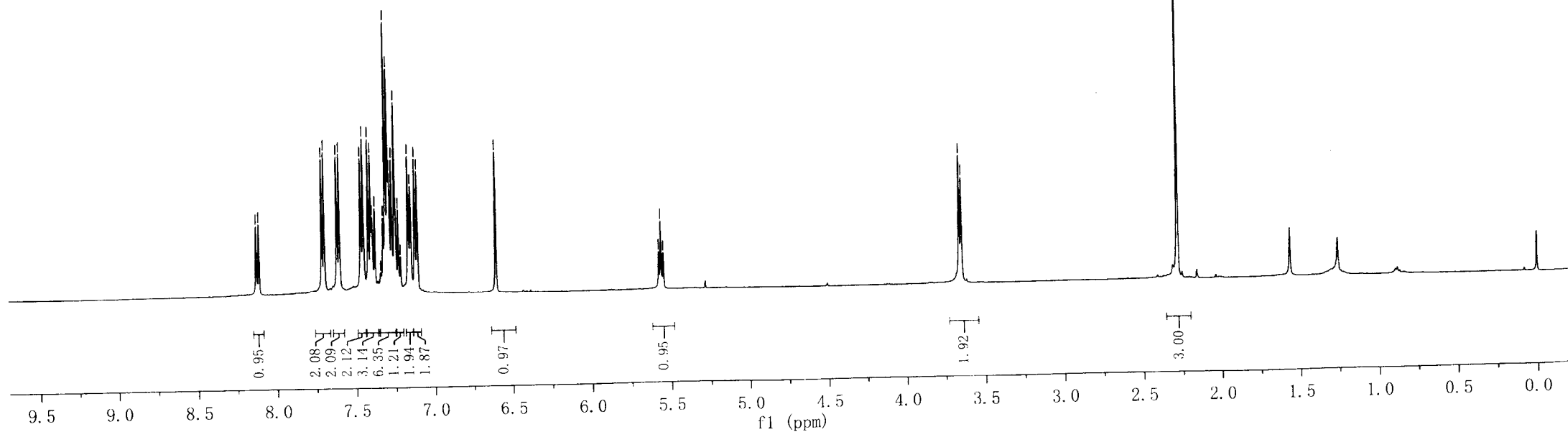
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5.561
5.546

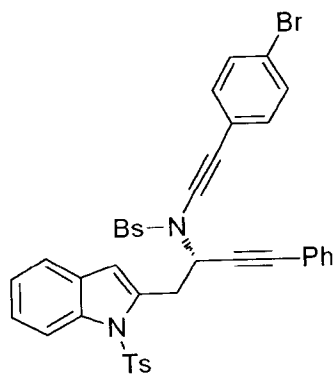
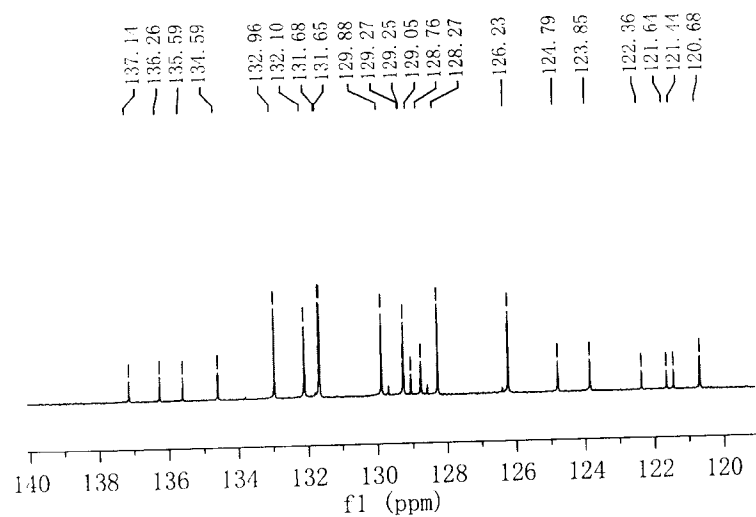
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3.648

2.283



4e





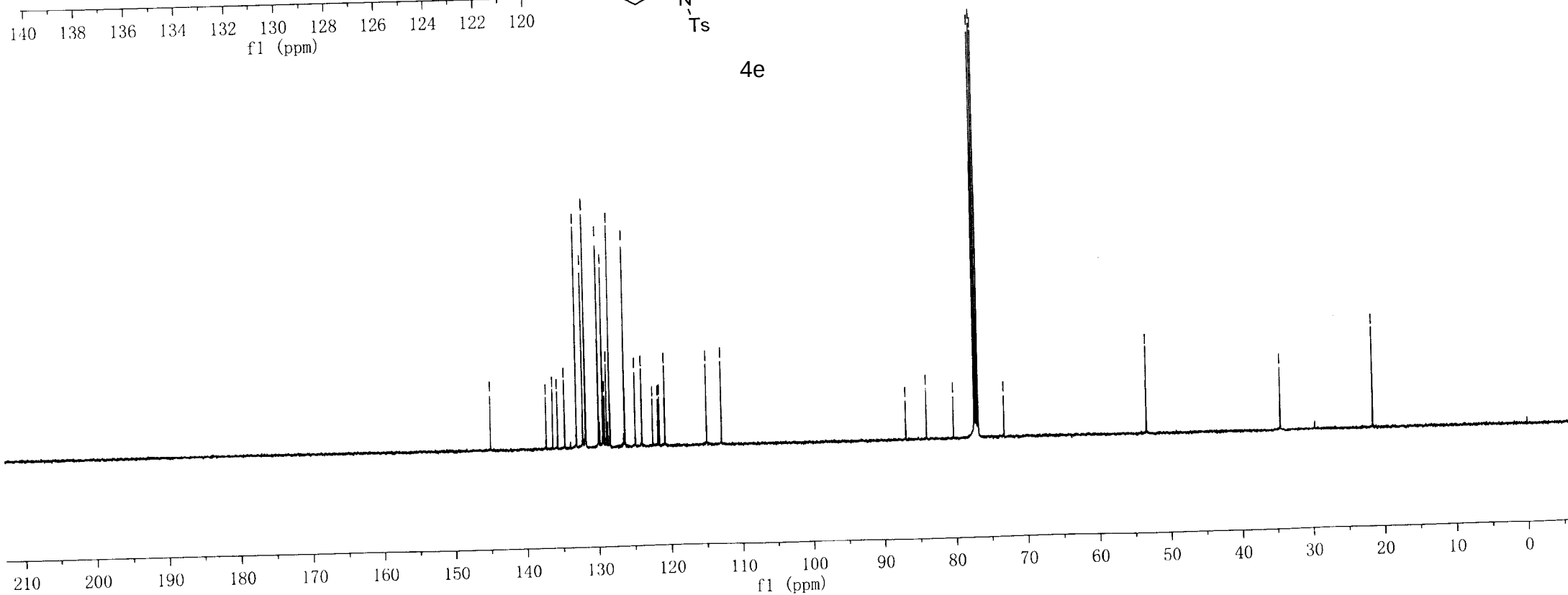
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128.27
126.23
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120.68
112.79

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80.21
77.25
77.00
76.75
73.15

53.31

34.49

21.50



8.134
8.118

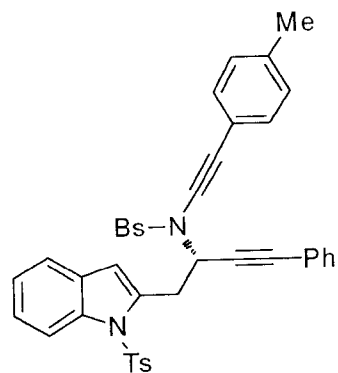
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7.251
7.159
7.154
7.136

5.573
5.559
5.513

3.667
3.664
3.651

2.368
2.279



4f

0.97

1.97

2.09

5.30

3.98

1.09

4.02

1.94

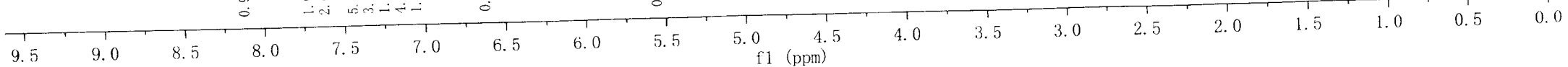
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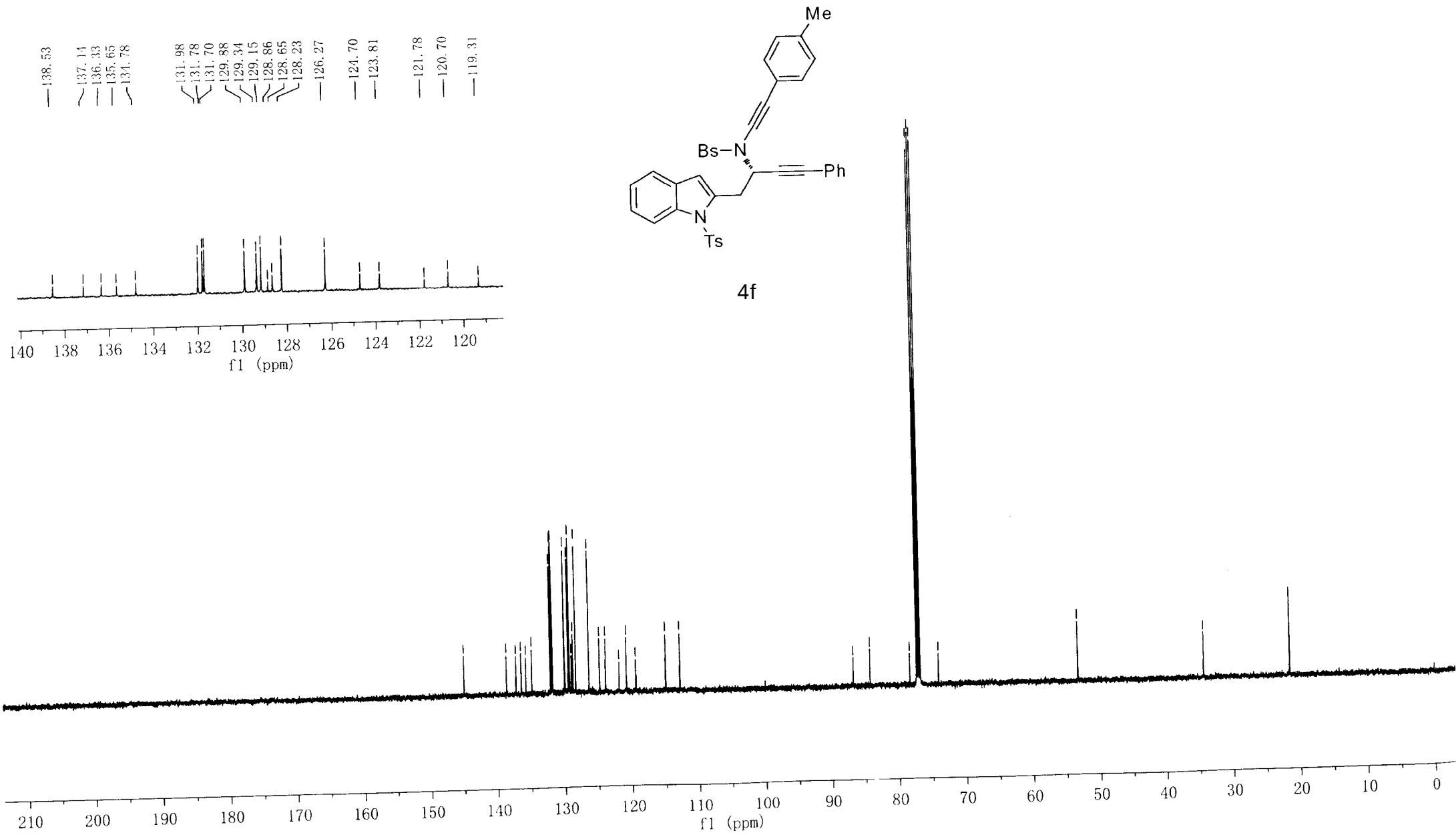
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1.93

3.00

3.07



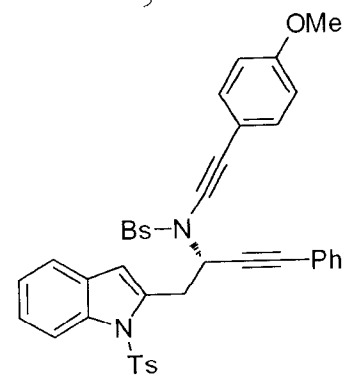


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8.120
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7.420
7.411
7.403
7.393
7.269
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6.875
6.857
6.634

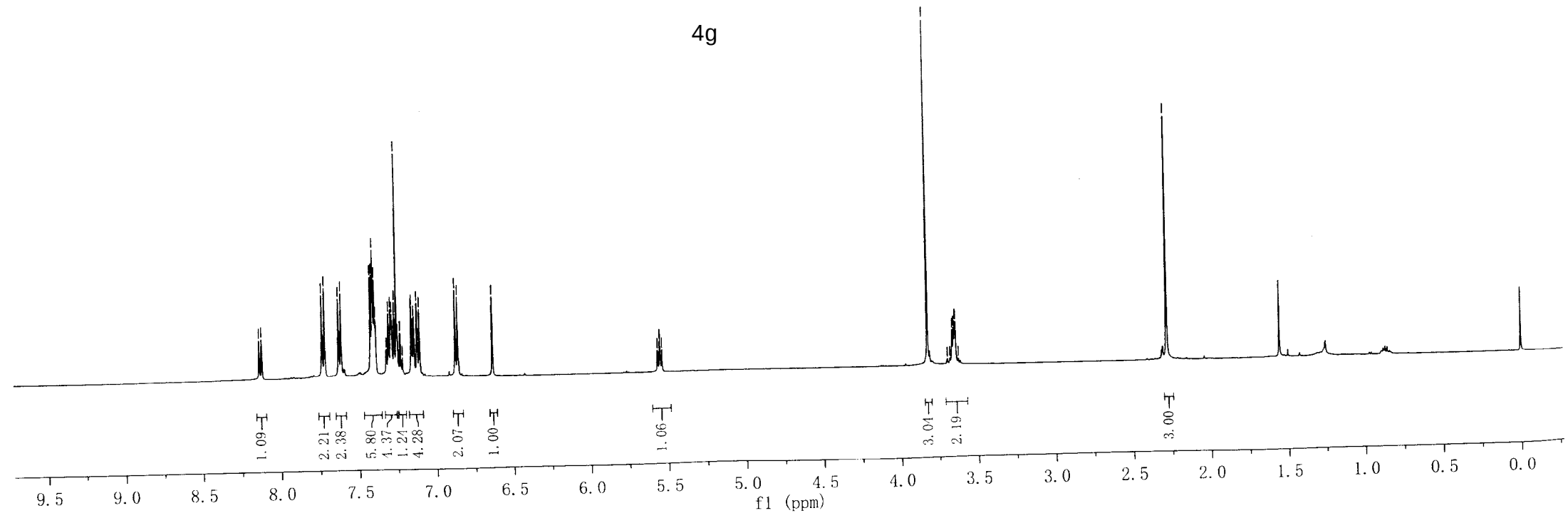
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5.551
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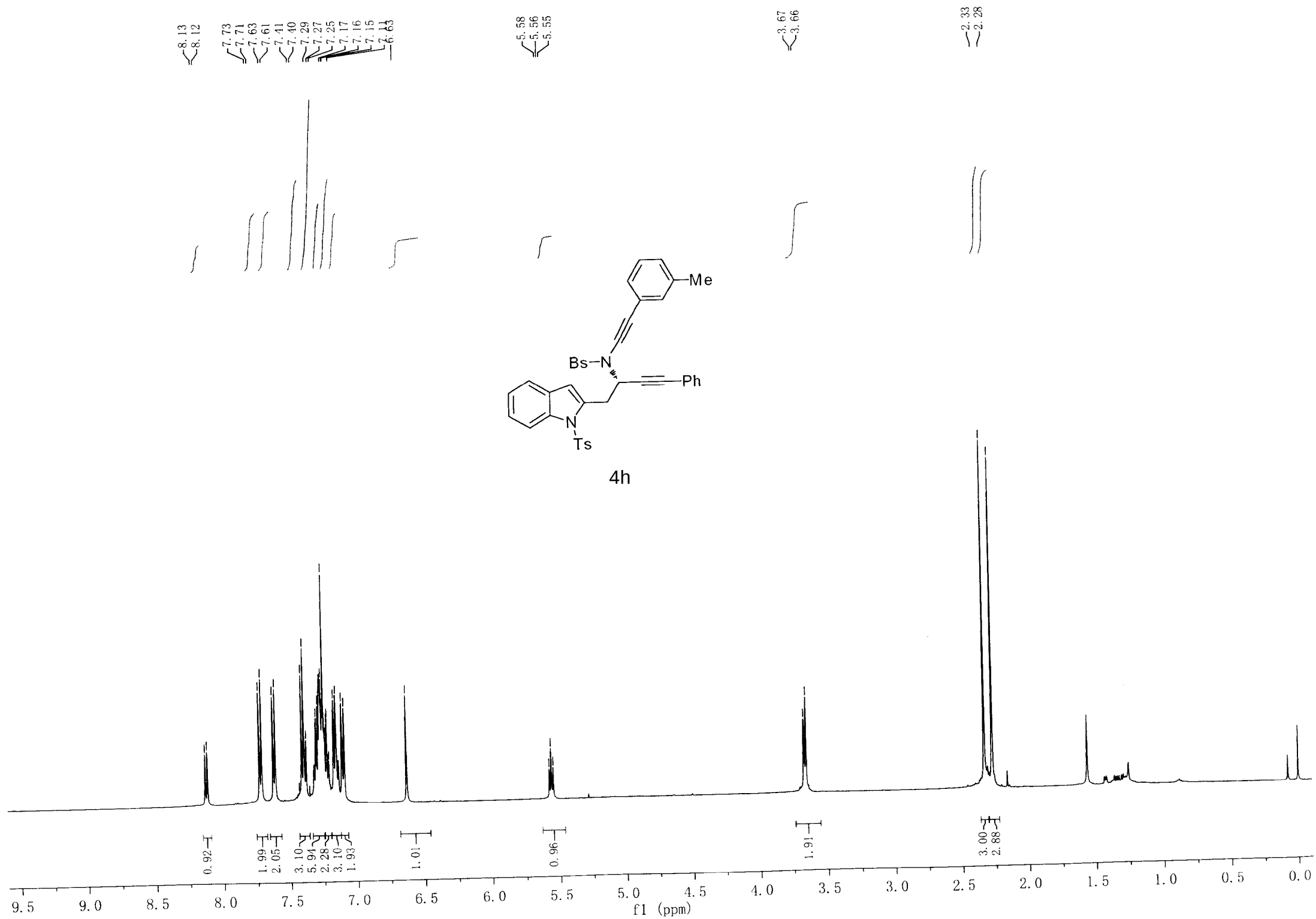
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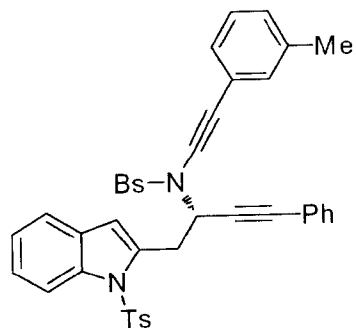
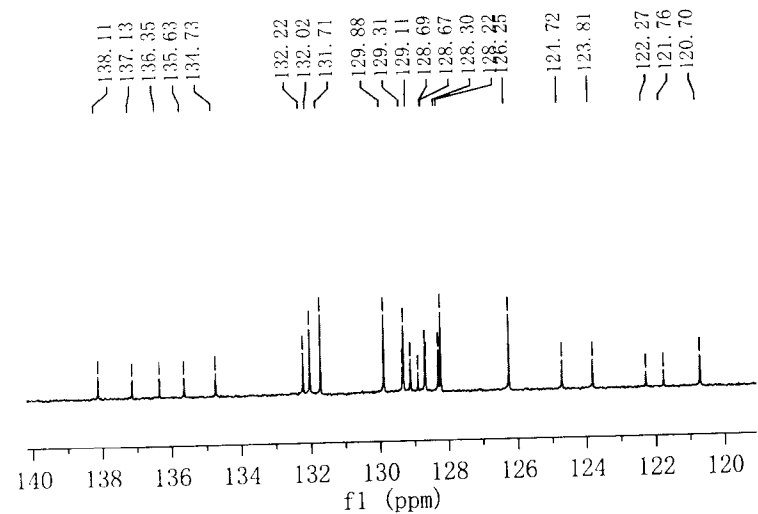
2.285



4g







4h

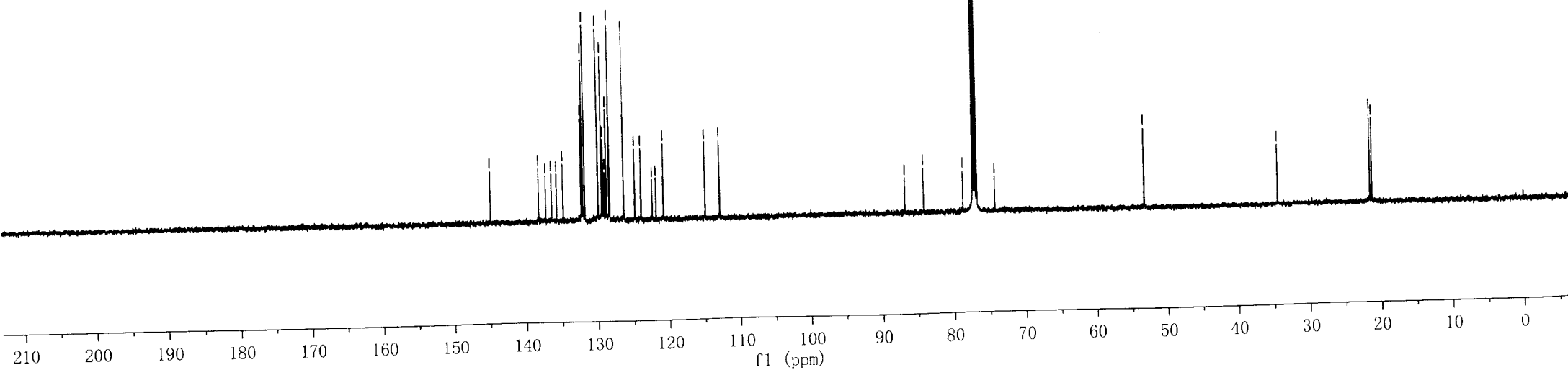
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120.70
114.89
112.77

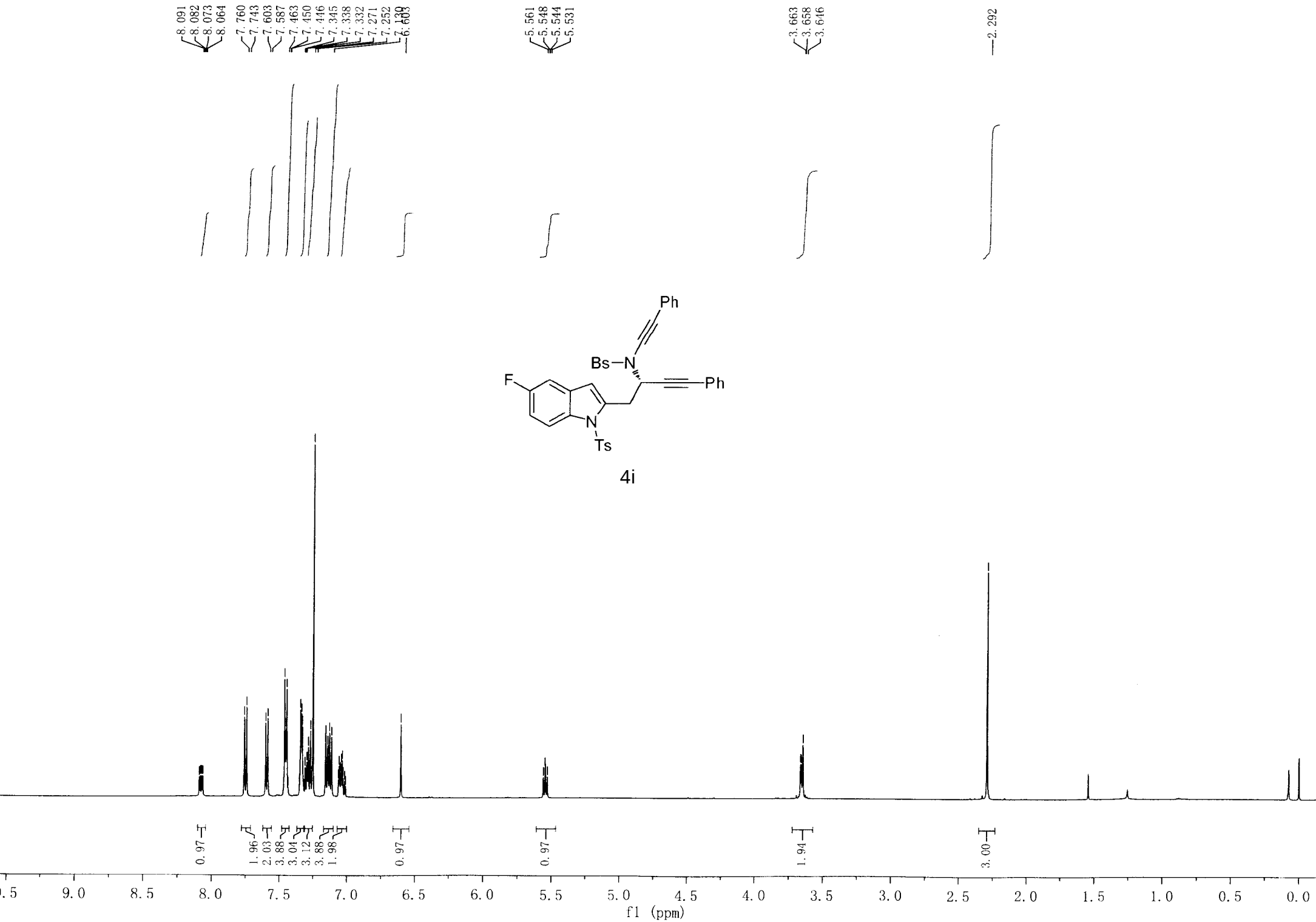
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76.75
74.20

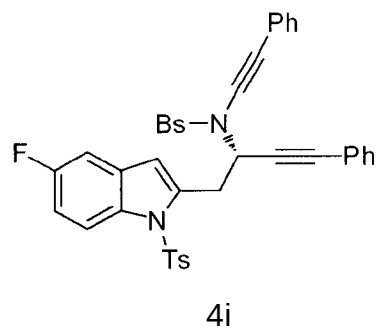
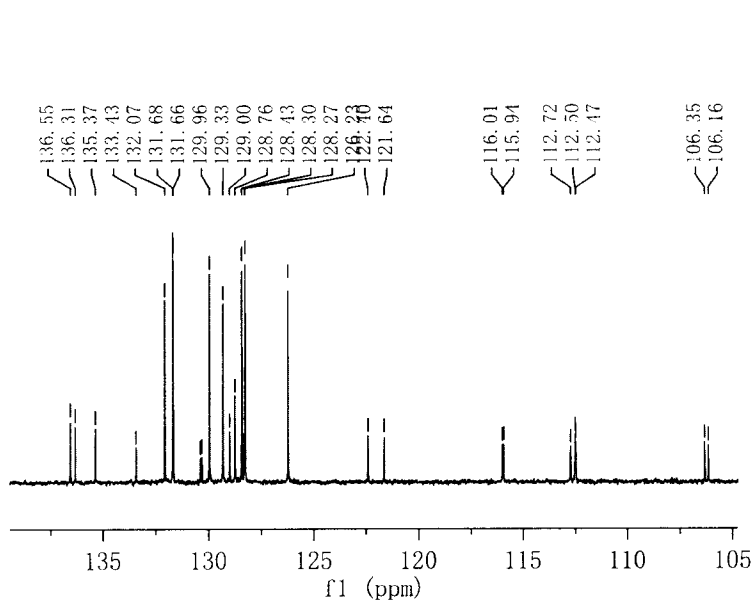
53.24

34.44

21.48
21.19







160.75
158.84

145.15

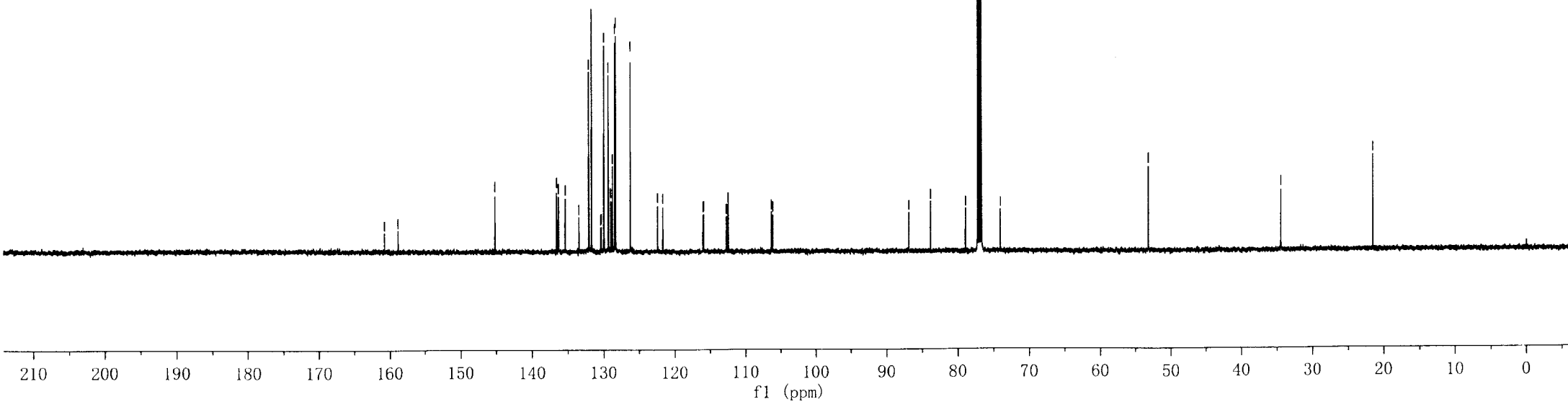
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106.16

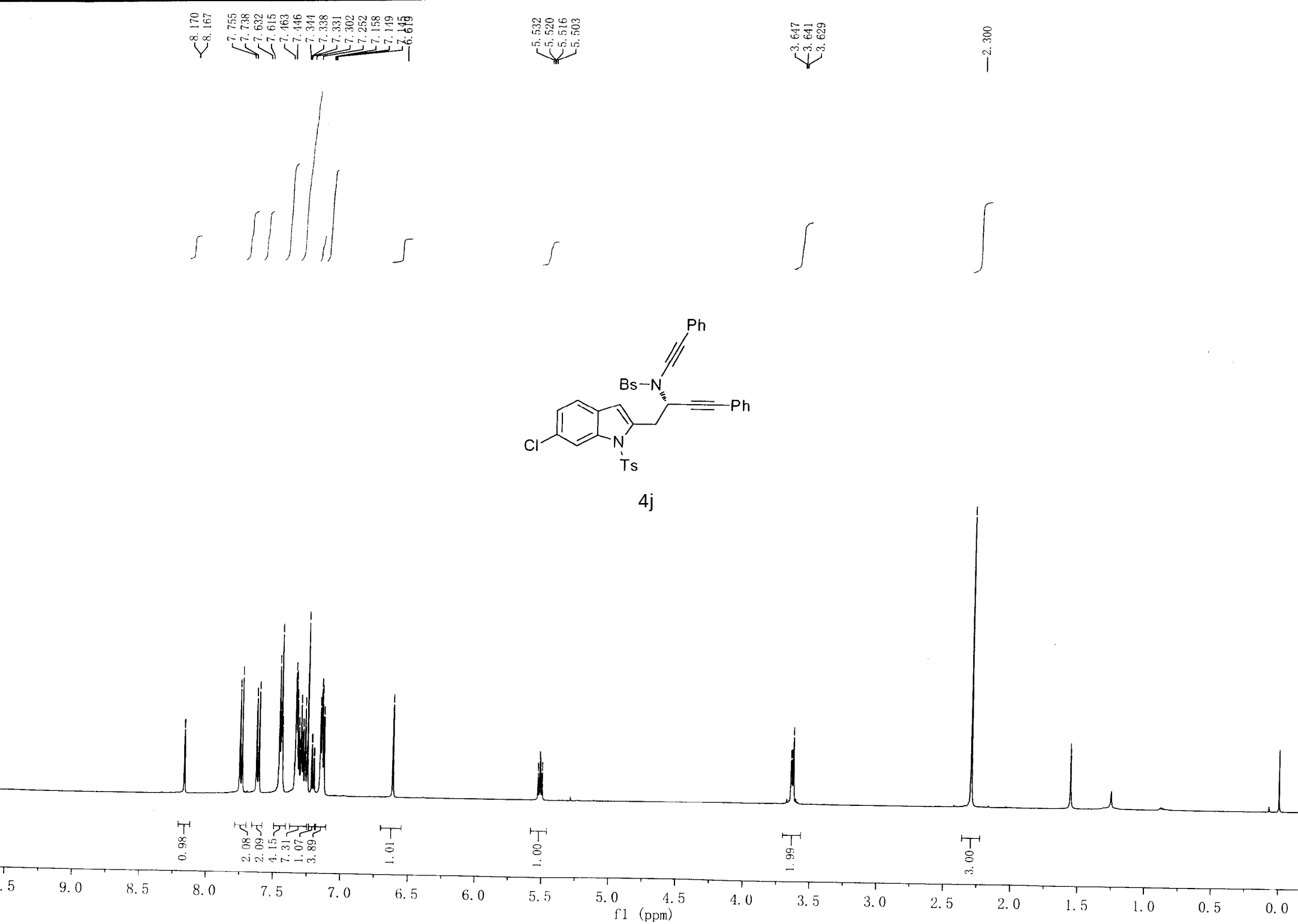
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74.08

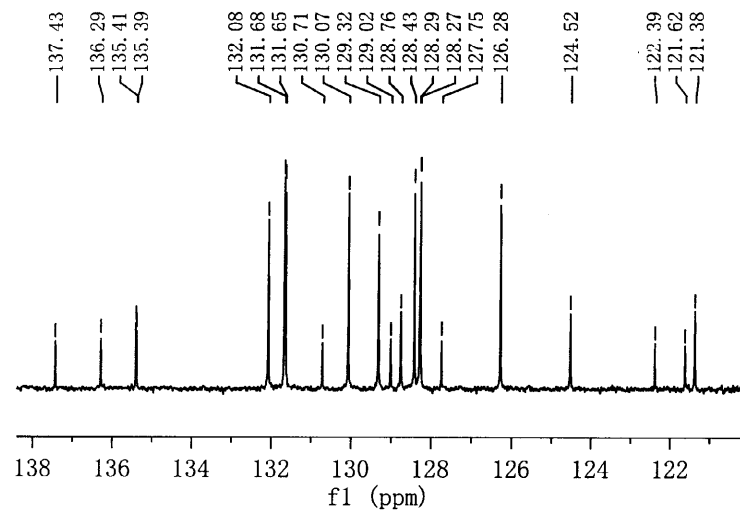
53.21

34.47

21.52







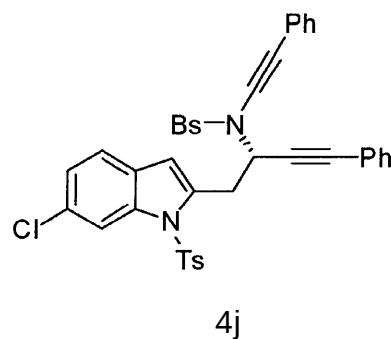
145.30
132.08
131.68
131.65
130.07
129.32
128.76
128.43
128.29
128.27
126.28
124.52
112.14

86.90
83.85
78.94
77.25
77.00
76.75
74.09

53.13

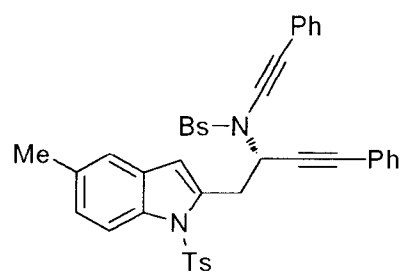
34.31

21.54

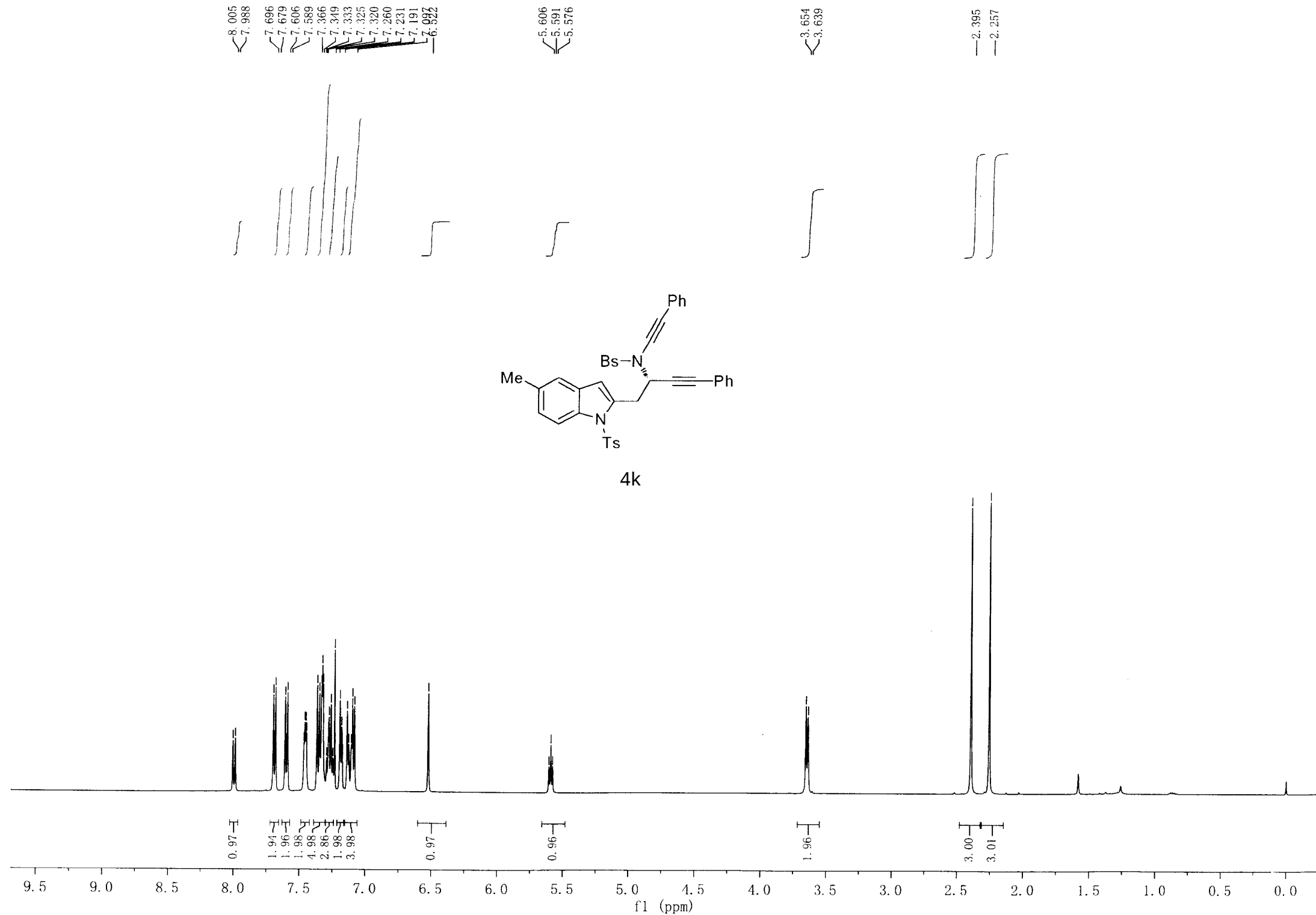


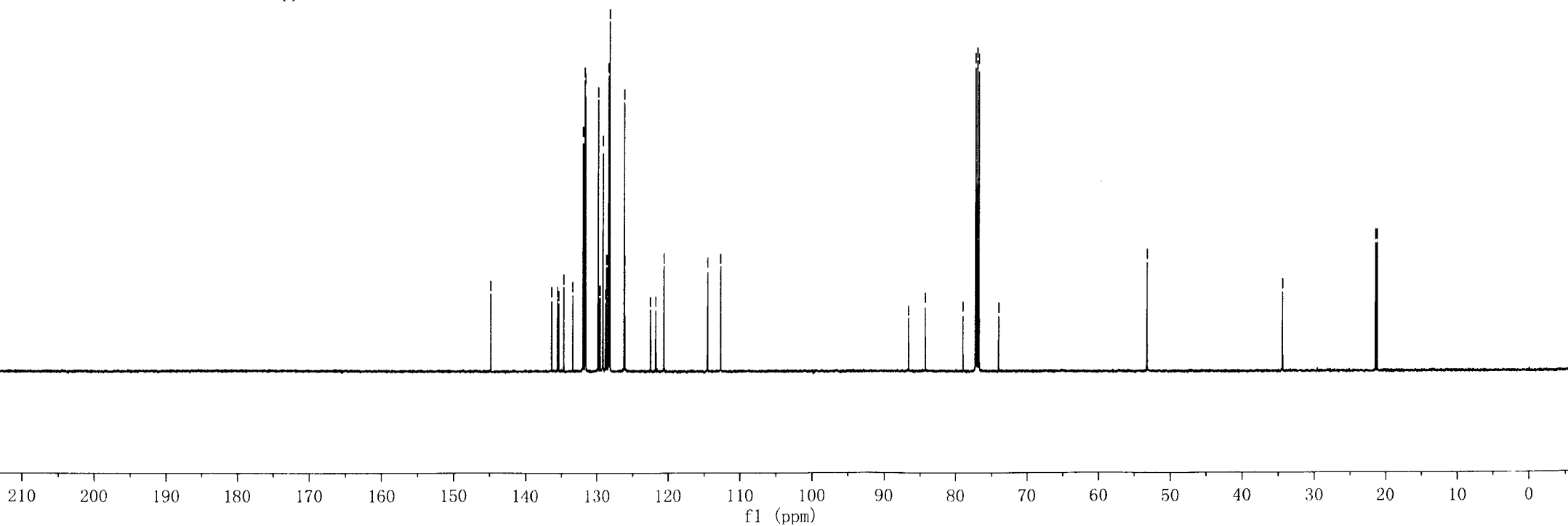
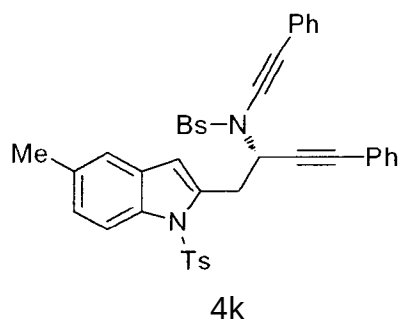
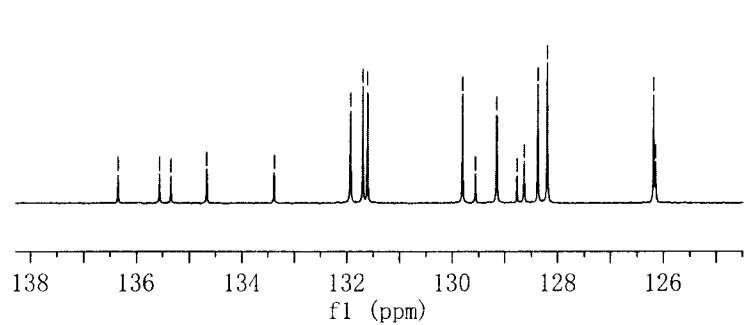
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

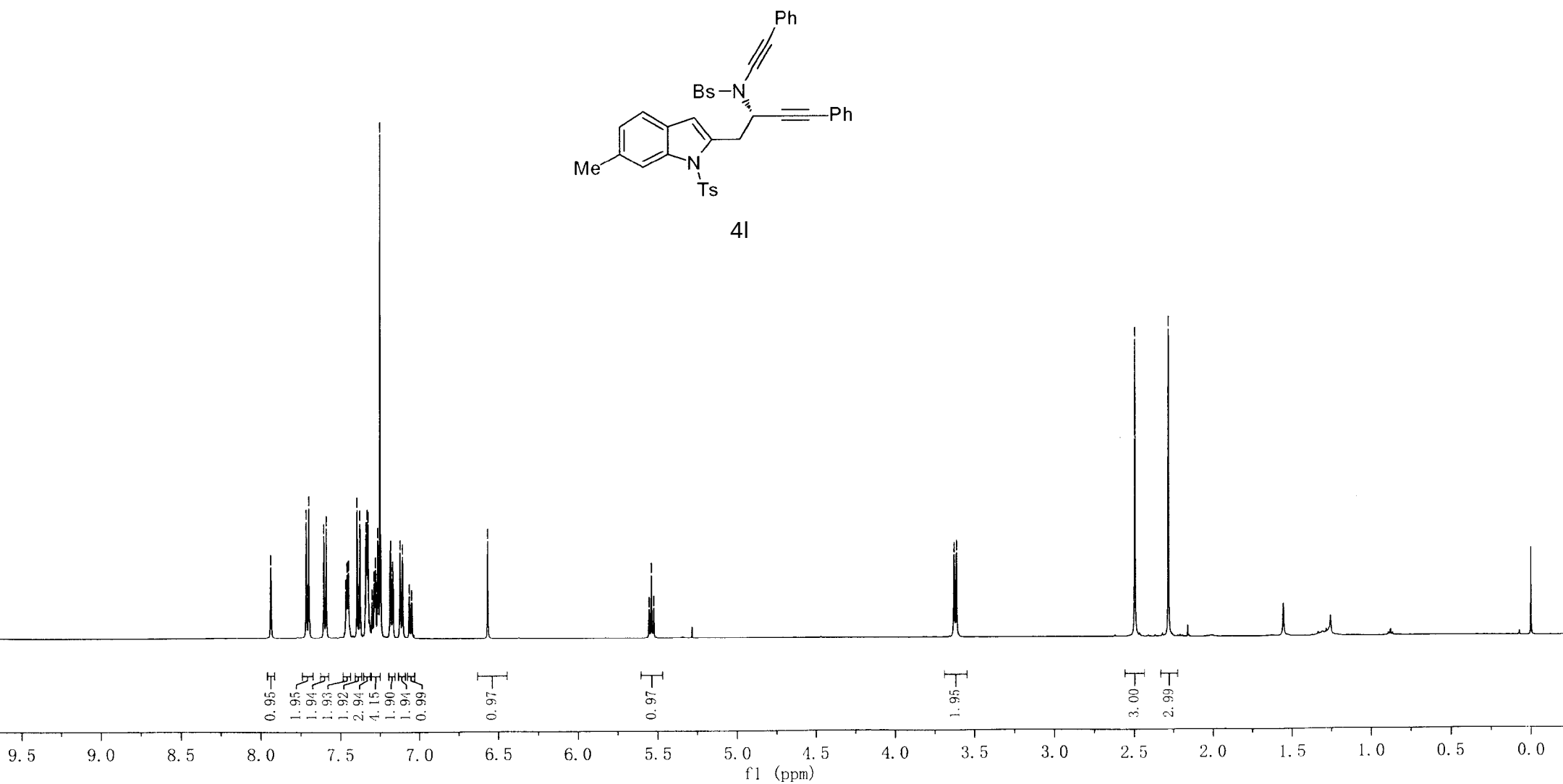
f1 (ppm)

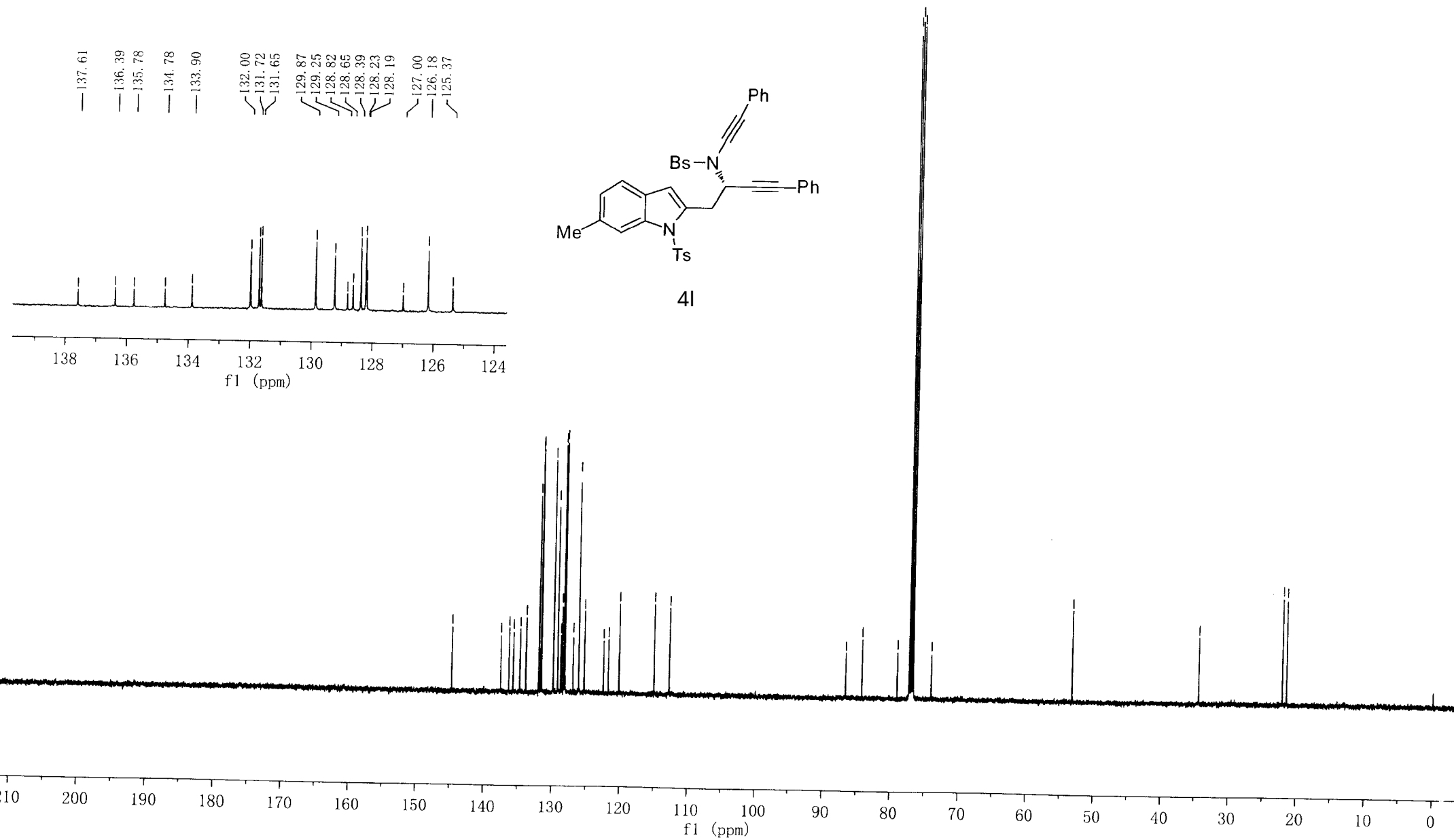


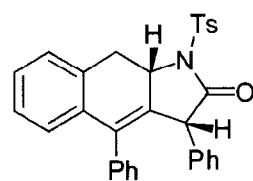
4k



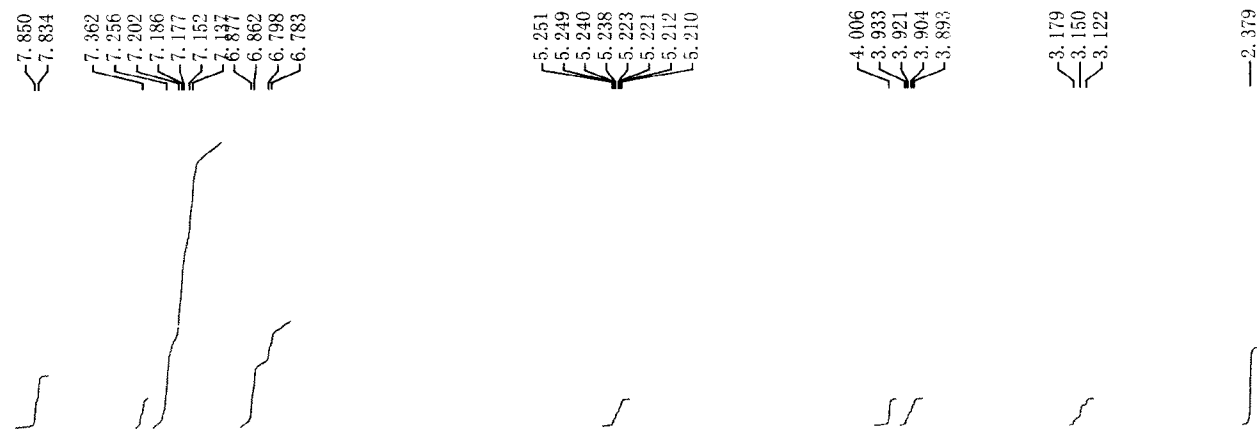








2a



7.850
7.834

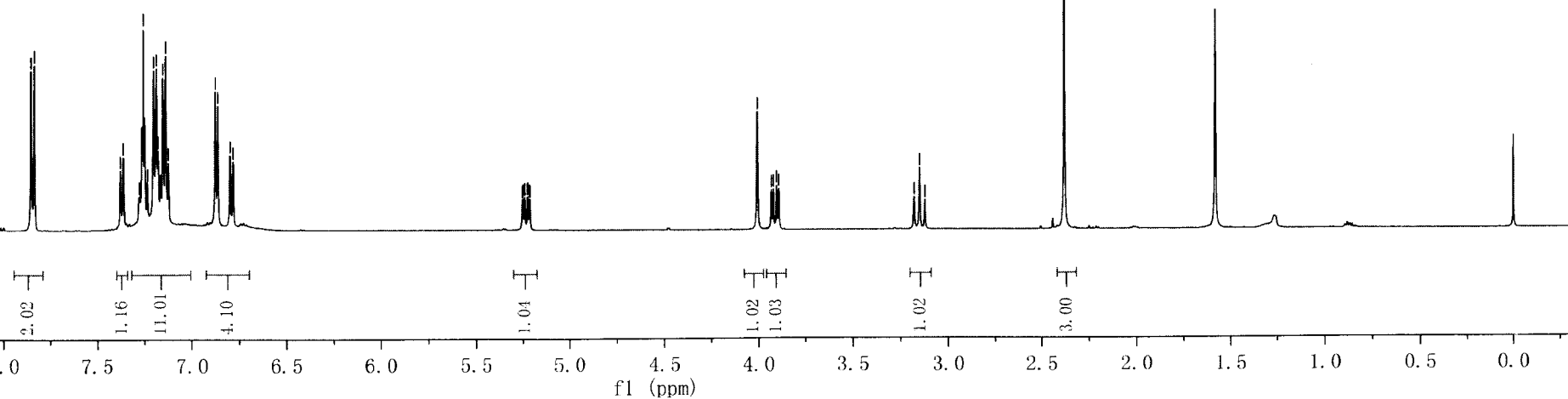
7.362
7.256
7.202
7.186
7.177
7.152
6.877
6.862
6.798
6.783

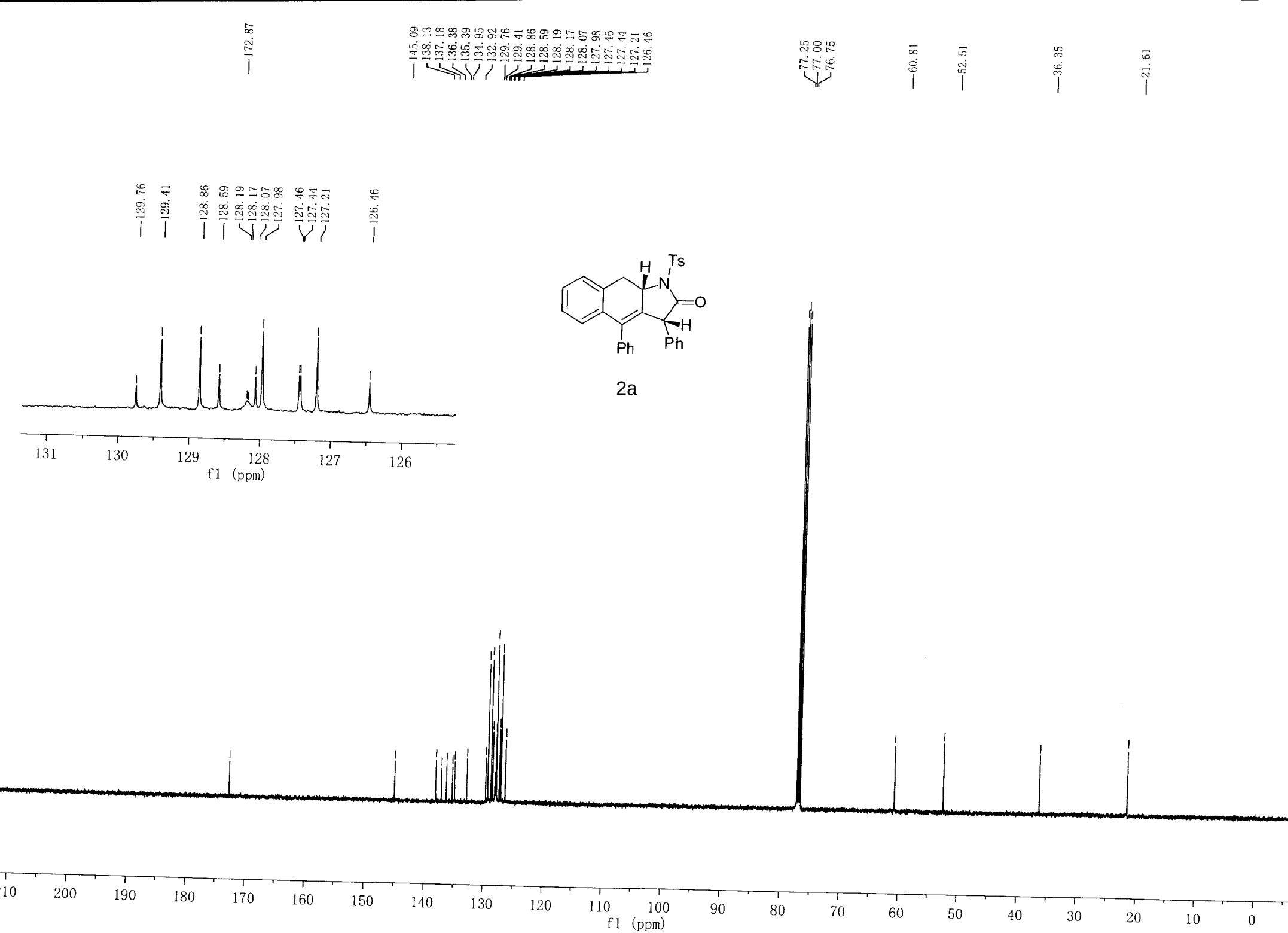
5.251
5.249
5.240
5.238
5.223
5.221
5.212
5.210

4.006
3.933
3.921
3.904
3.893

3.179
3.150
3.122

2.379





129.39
128.84
128.57
128.18
128.06
127.98
127.95
127.43
127.21
126.44

60.80

52.50

36.37

21.57

129.39

128.84

128.57

128.18

128.06

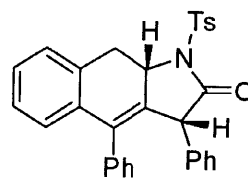
127.98

127.95

127.43

127.21

126.44



2a

130

129

f1 (ppm)

127

126

210

200

190

180

170

160

150

140

130

120

110

f1 (ppm)

100

90

80

70

60

50

40

30

20

10

0

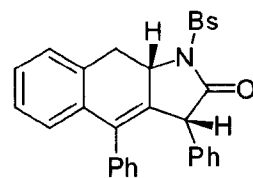
-10

7.783
7.762
7.506
7.484
7.267
7.248
7.181
7.162
6.896
6.878
6.814
6.796

5.220
5.207
5.185
5.172

4.025
3.898
3.883
3.862
3.848

3.198
3.162
3.127



2b

1.99
2.10
9.18
4.96

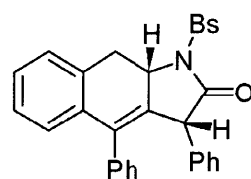
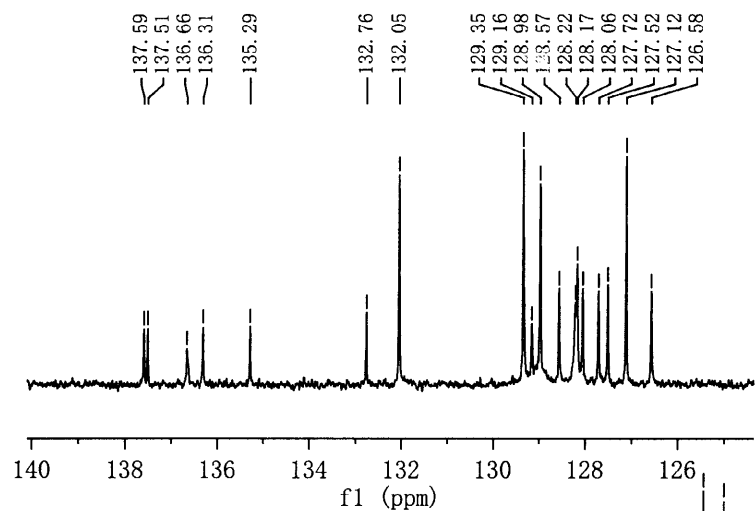
1.00

0.99
1.01

1.00

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

f1 (ppm)



2b

172.83
137.59
137.51
136.66
136.31
135.29
132.76
132.05
129.35
129.16
128.98
128.57
128.22
128.17
128.06
127.72
127.52
127.12
126.58

77.32
77.00
76.68

60.94

52.39

36.43

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

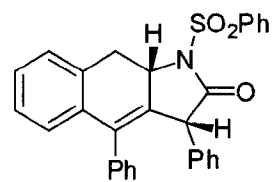
f1 (ppm)

7.981
7.963
7.557
7.435
7.415
7.269
7.187
7.170
7.156
6.838
6.856
6.802
6.784

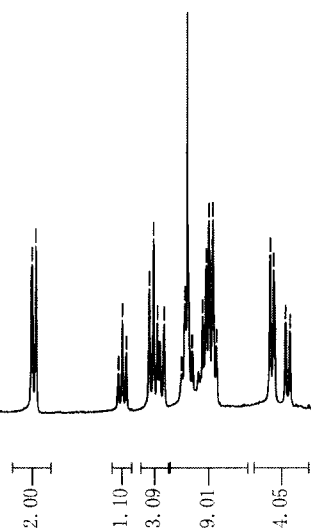
5.273
5.262
5.241
5.238
5.227

4.018
3.947
3.932
3.911
3.896

3.198
3.163
3.127



2c

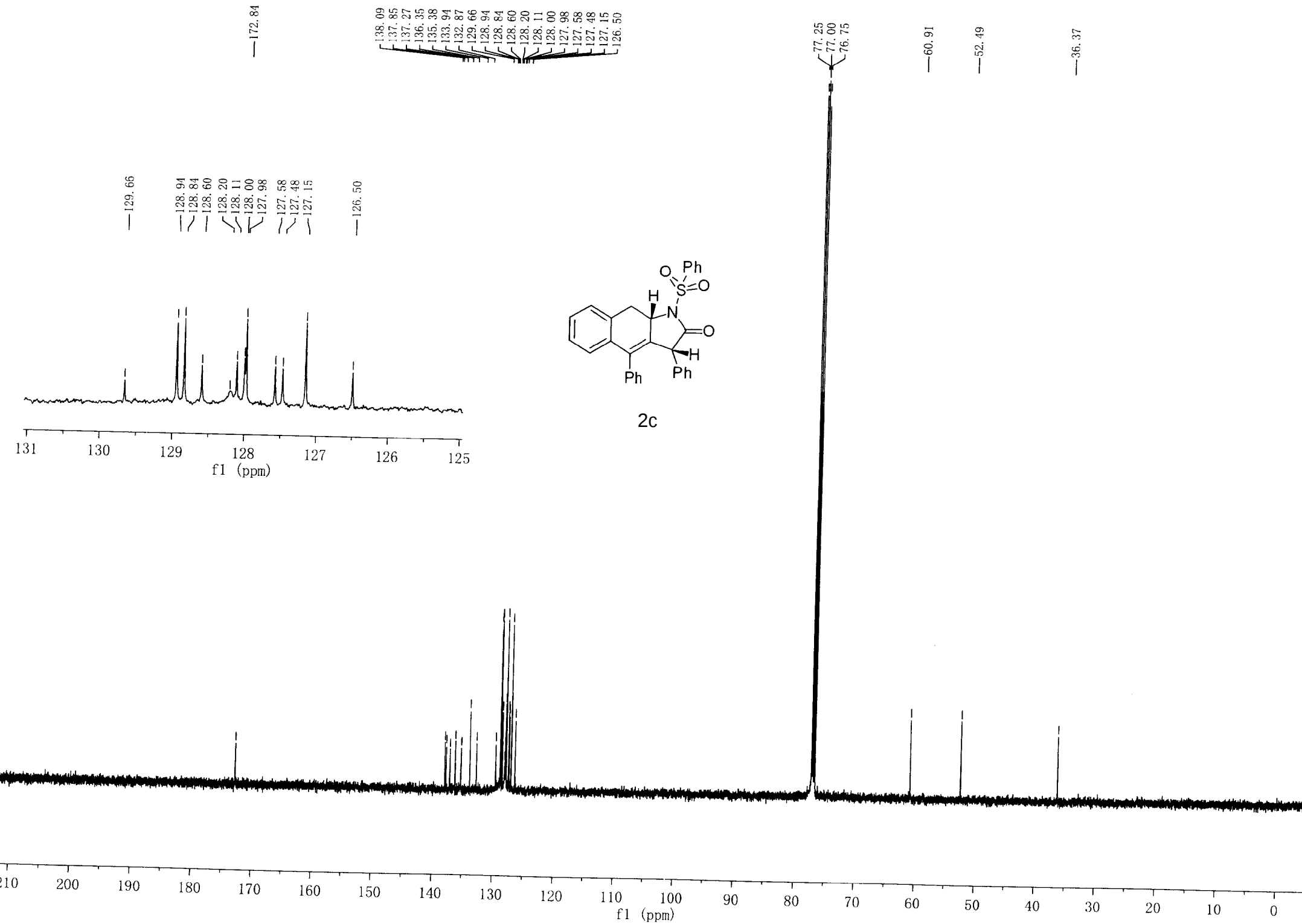


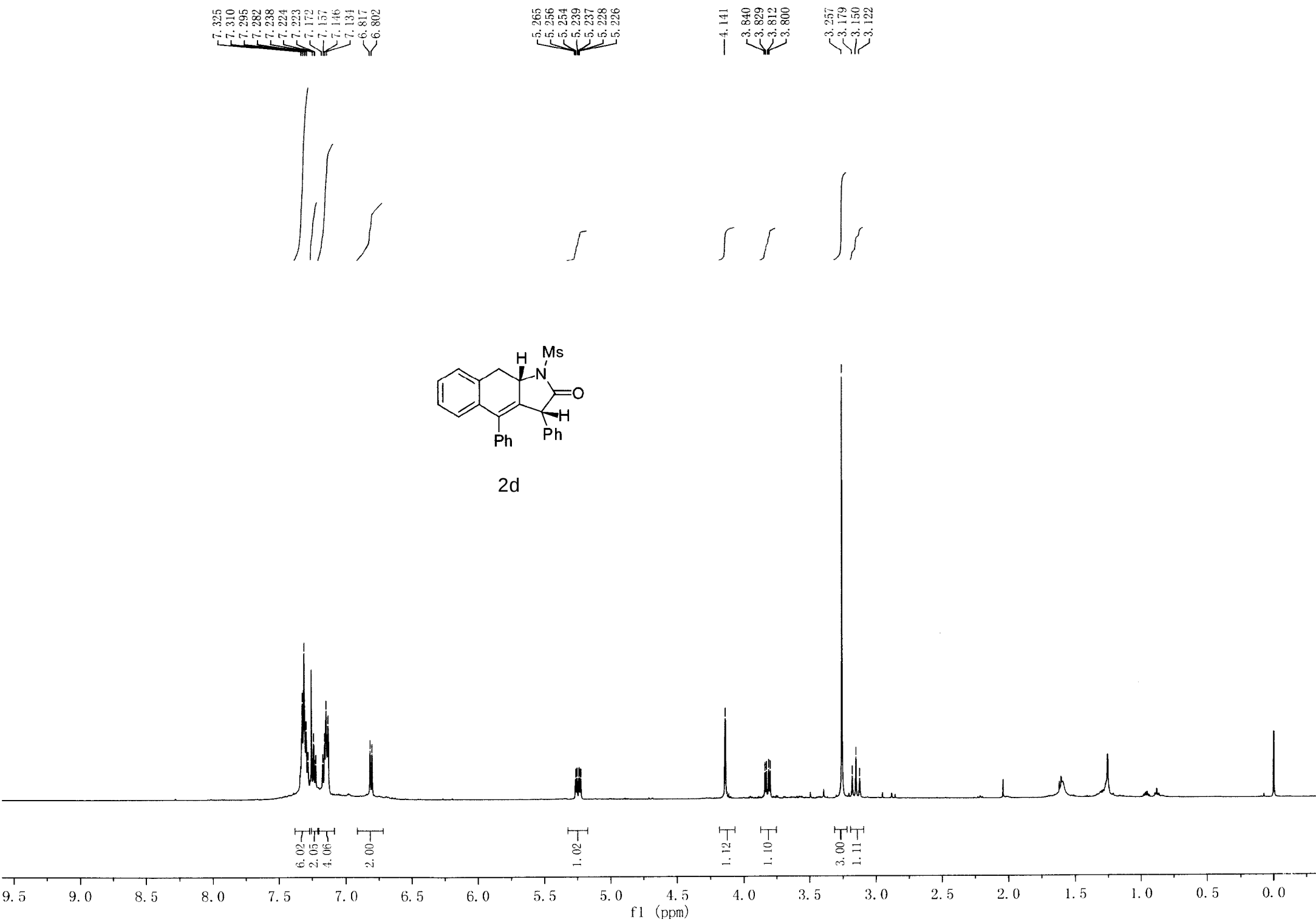
1.00

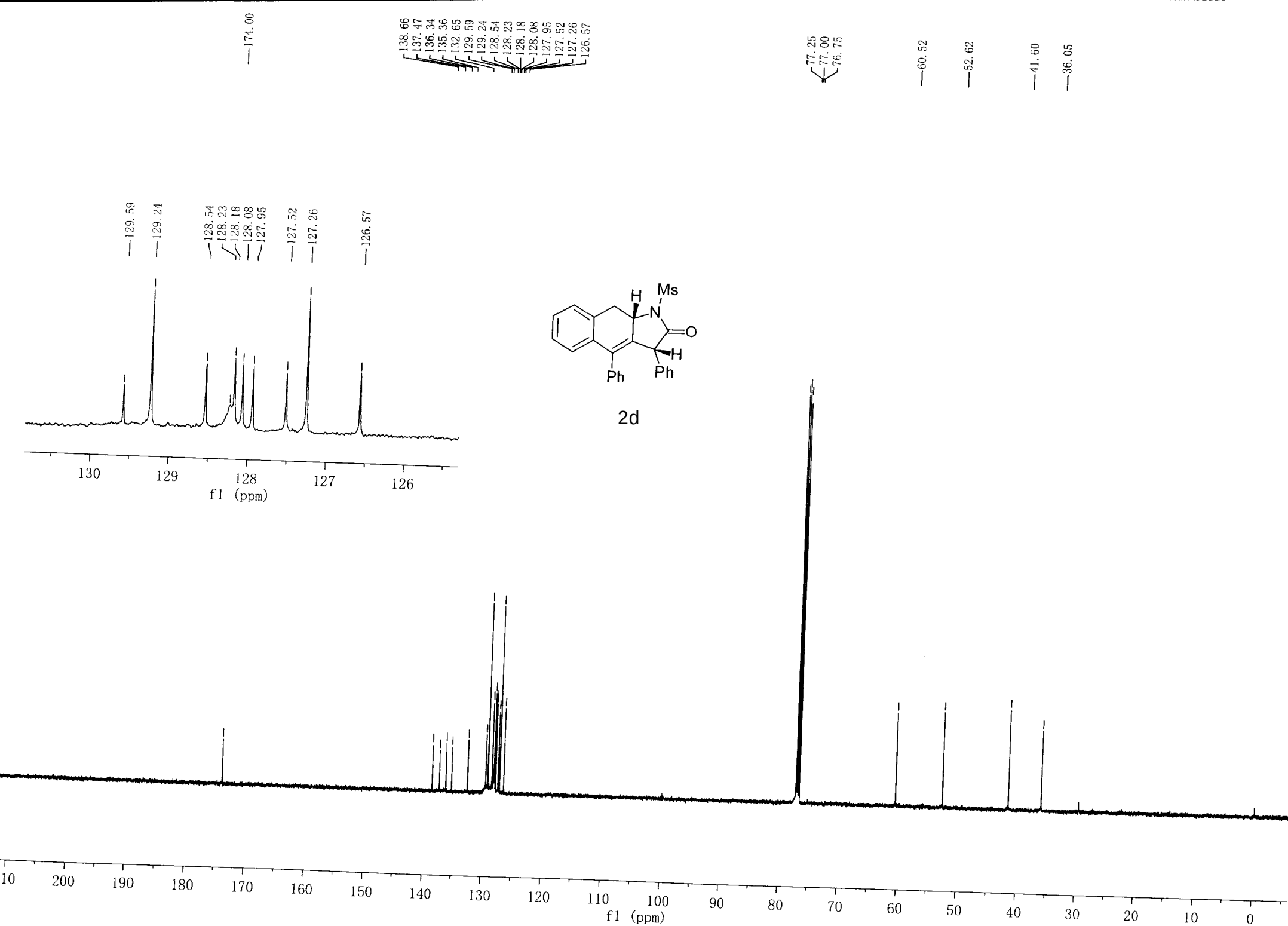
1.00
1.12

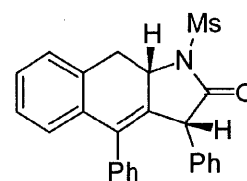
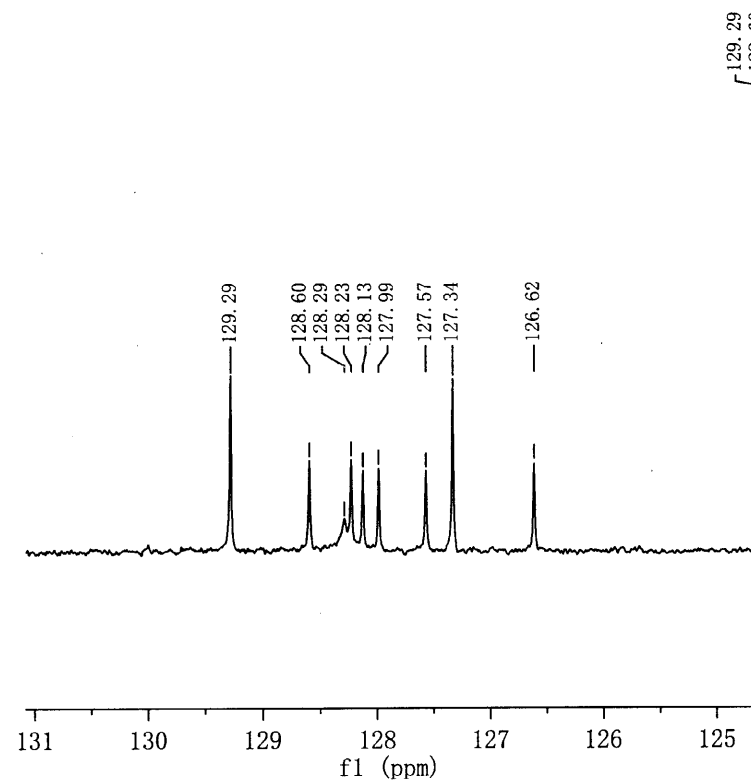
1.06

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
f1 (ppm)









2d

129.29
128.60
128.29
128.23
128.13
127.99
127.57
127.34
126.62

—60.57

—52.70

—41.64

—36.11

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

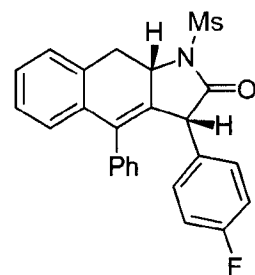
f1 (ppm)

7.330
7.311
7.293
7.242
7.223
7.180
7.161
7.143
7.129
7.116
7.107
7.091
7.037
7.020
7.015
6.994
6.819
6.802

5.256
5.252
5.241
5.238
5.221
5.217
5.206
5.203

4.126
3.845
3.831
3.809
3.795

3.278
3.172
3.137
3.101



2e

3.00
2.01
3.82
2.12
2.06

1.01

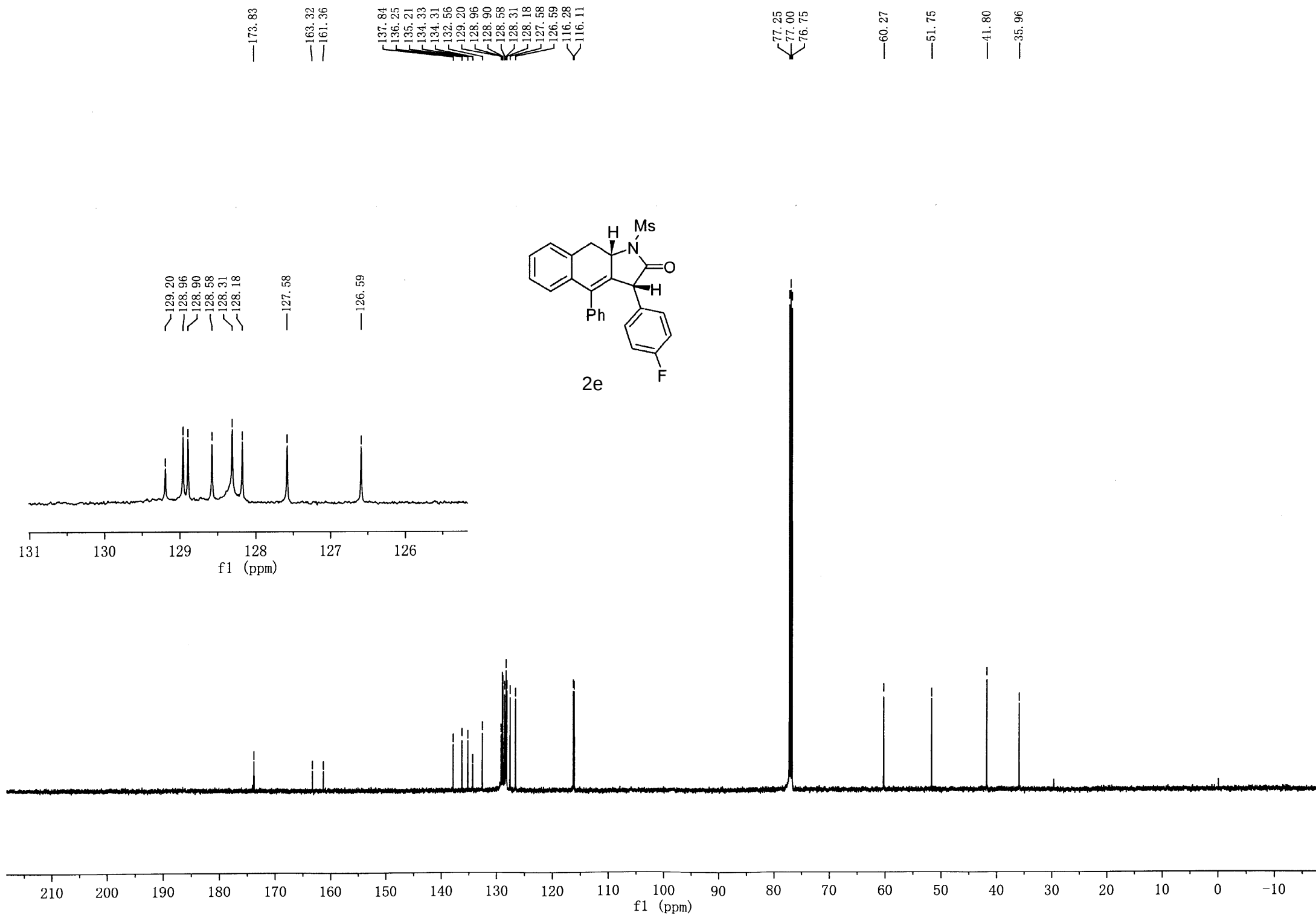
1.02

1.03

3.00
1.14

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

f1 (ppm)

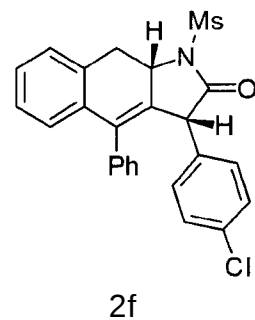


7.330
7.313
7.292
7.246
7.183
7.165
7.146
7.093
7.072
6.821
6.802

5.244
5.230
5.209
5.195

4.117
3.845
3.830
3.809
3.795

3.276
3.172
3.136
3.101



5.08
4.26
2.14
2.09

1.07

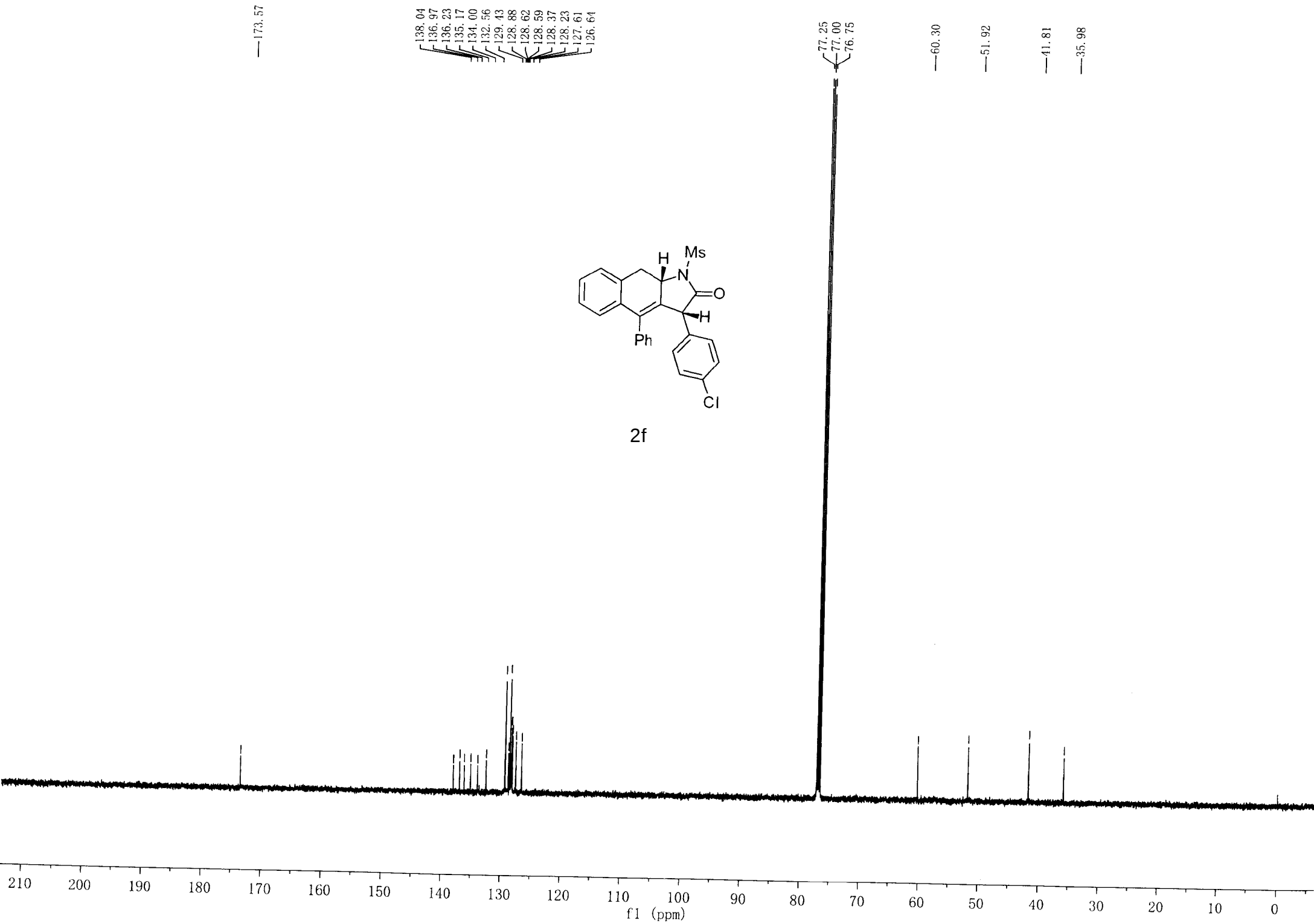
1.06

1.10

3.00
1.14

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

f1 (ppm)

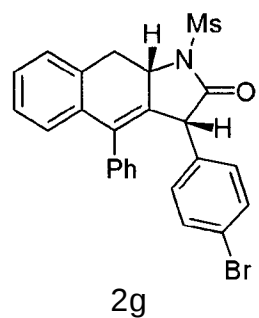


7.465
7.448
7.329
7.314
7.302
7.248
7.235
7.233
7.182
7.167
7.036
7.019
6.821
6.806

5.240
5.237
5.228
5.226
5.212
5.209
5.200
5.198

4.100
3.839
3.827
3.810
3.799

3.165
3.137
3.109



2.00
3.07
2.07
2.03
2.09
1.99

1.02

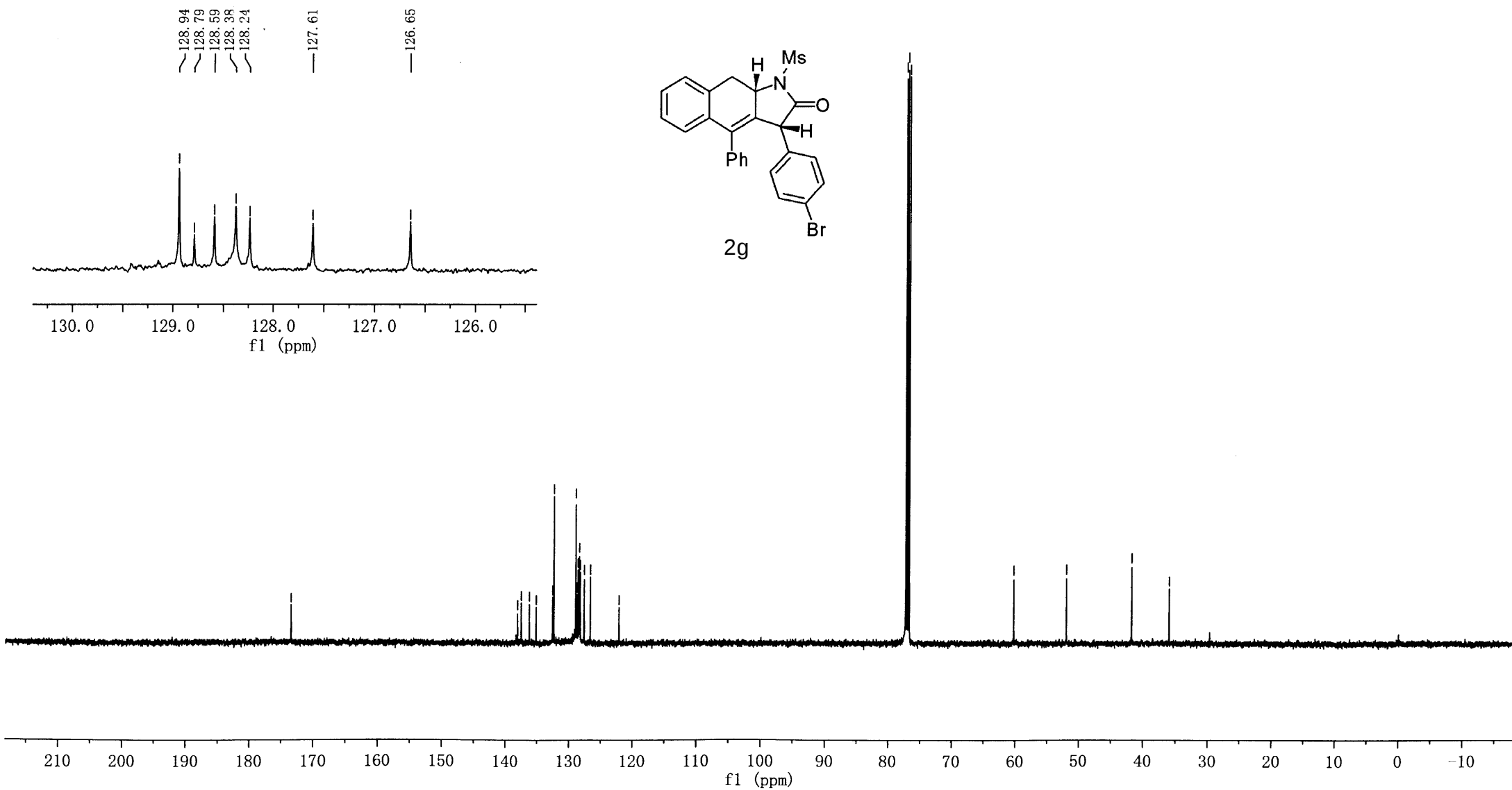
1.06

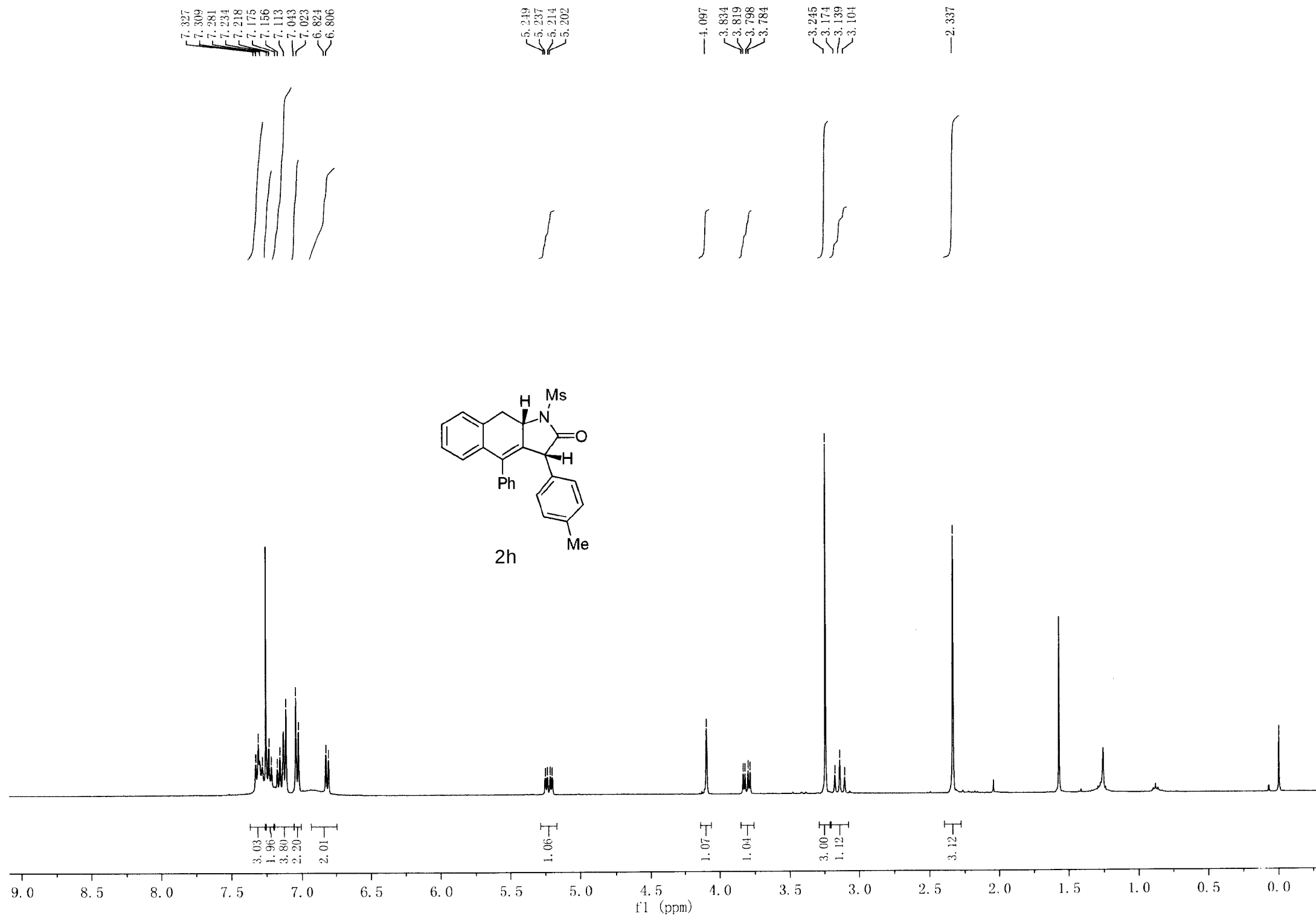
1.05

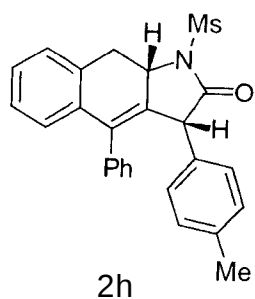
3.00
1.15

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

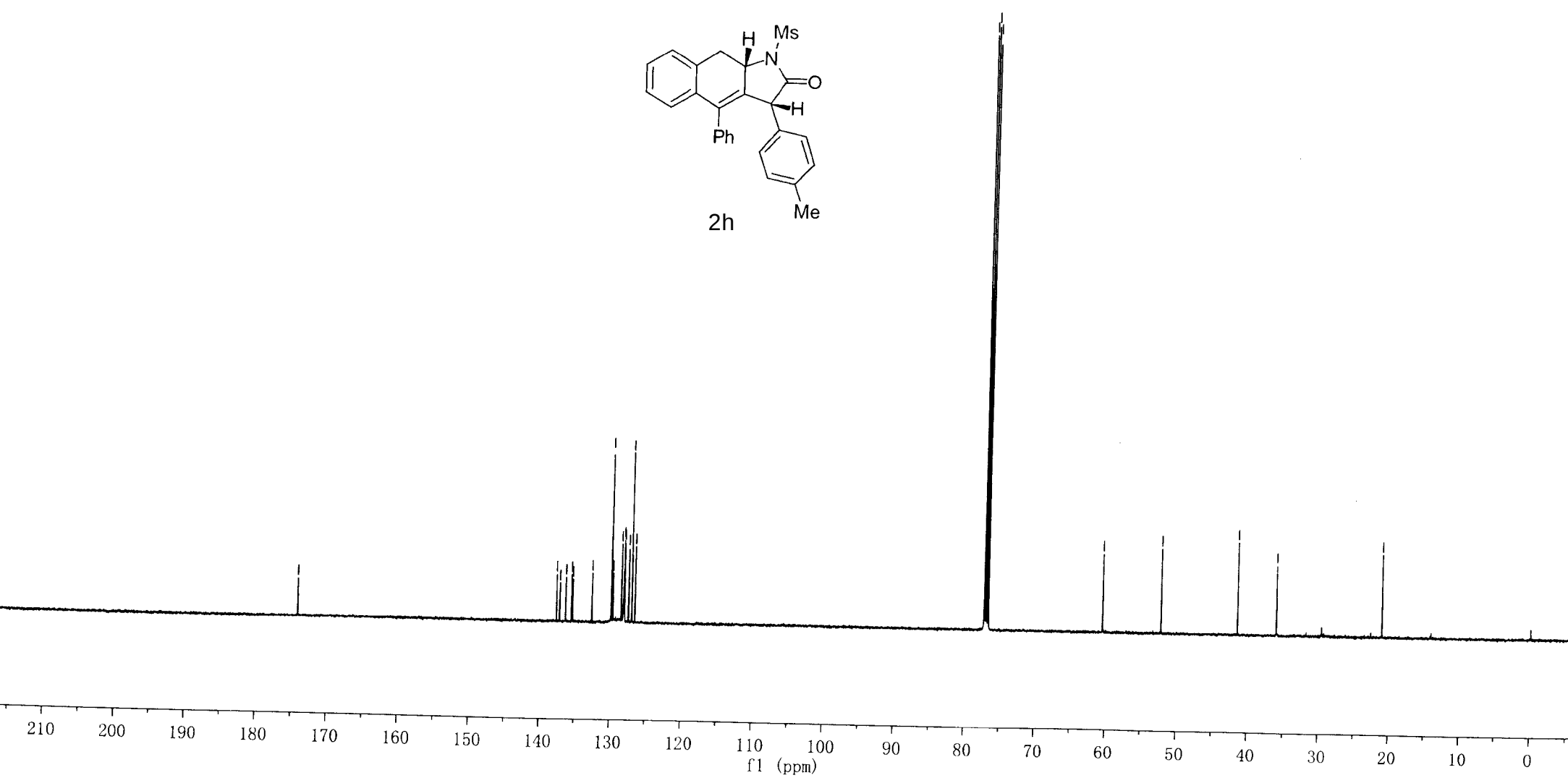
f1 (ppm)

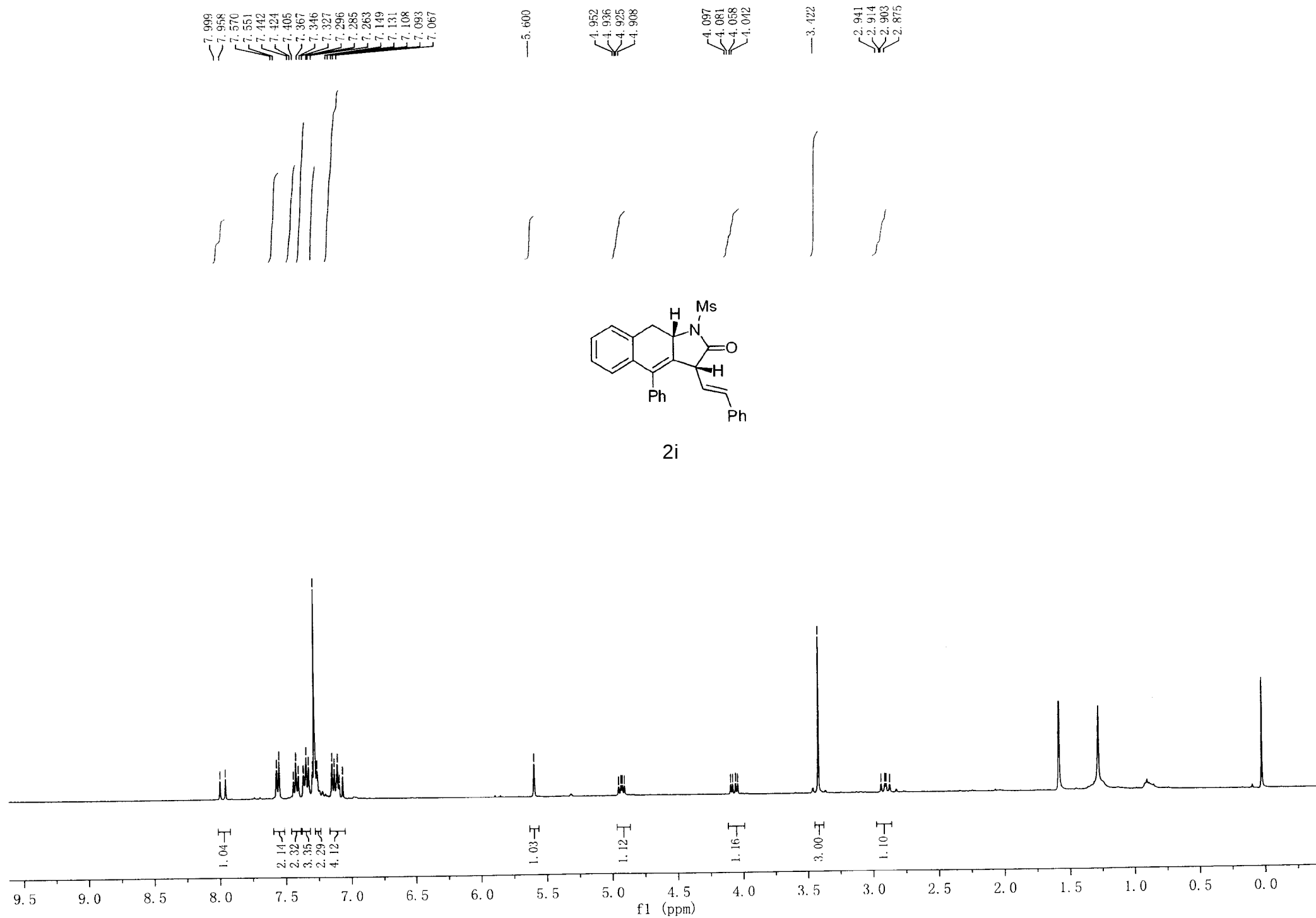


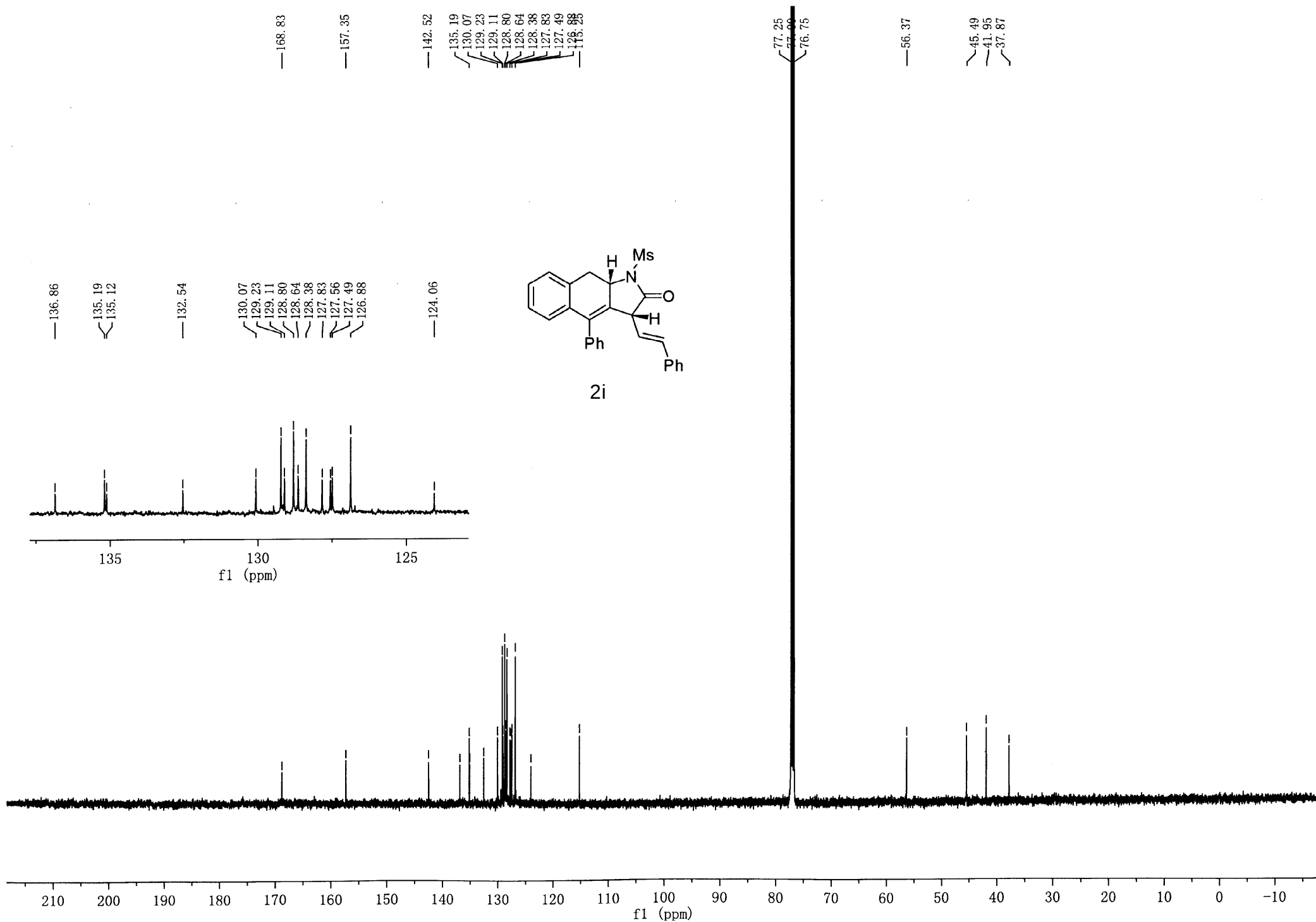


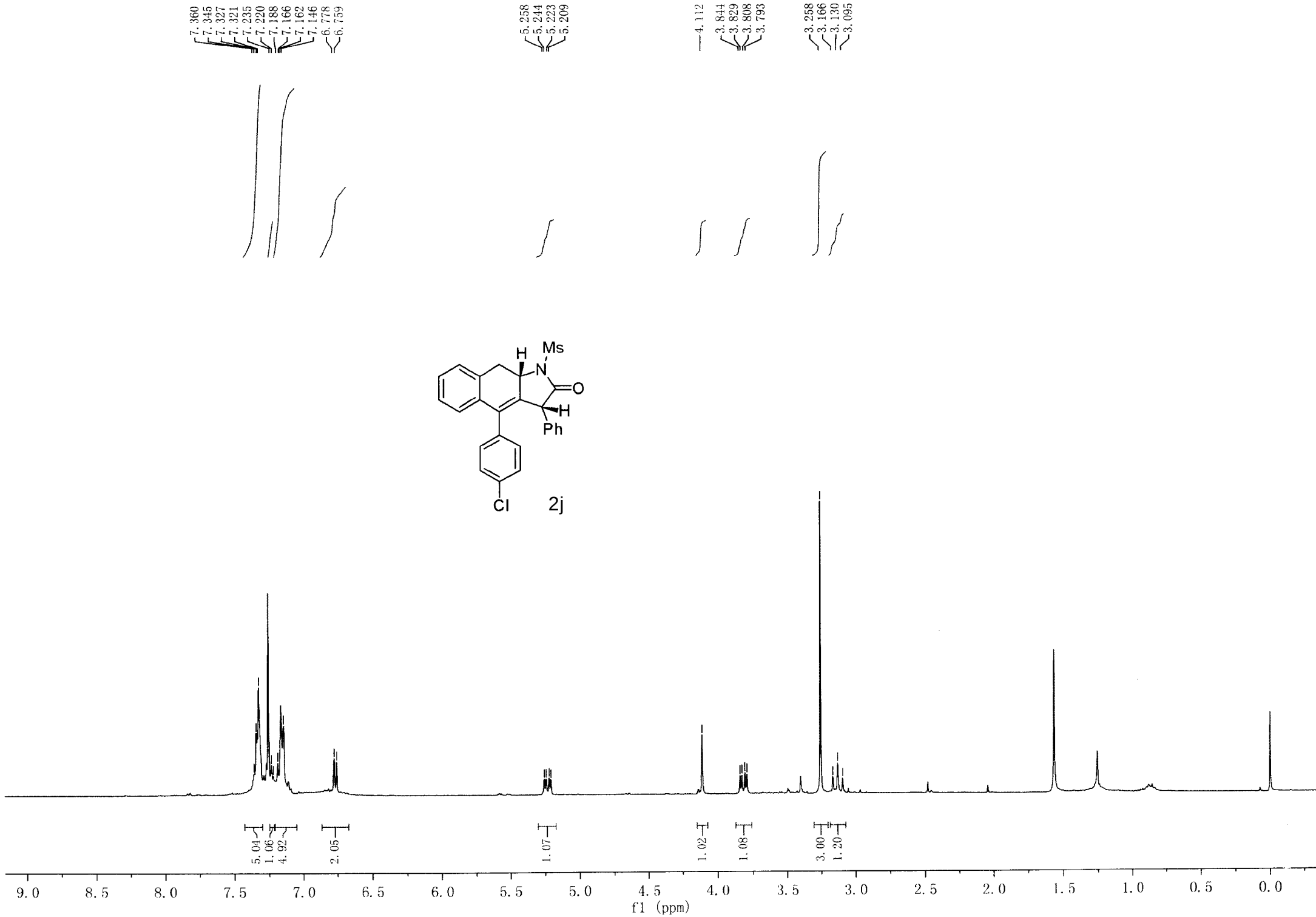


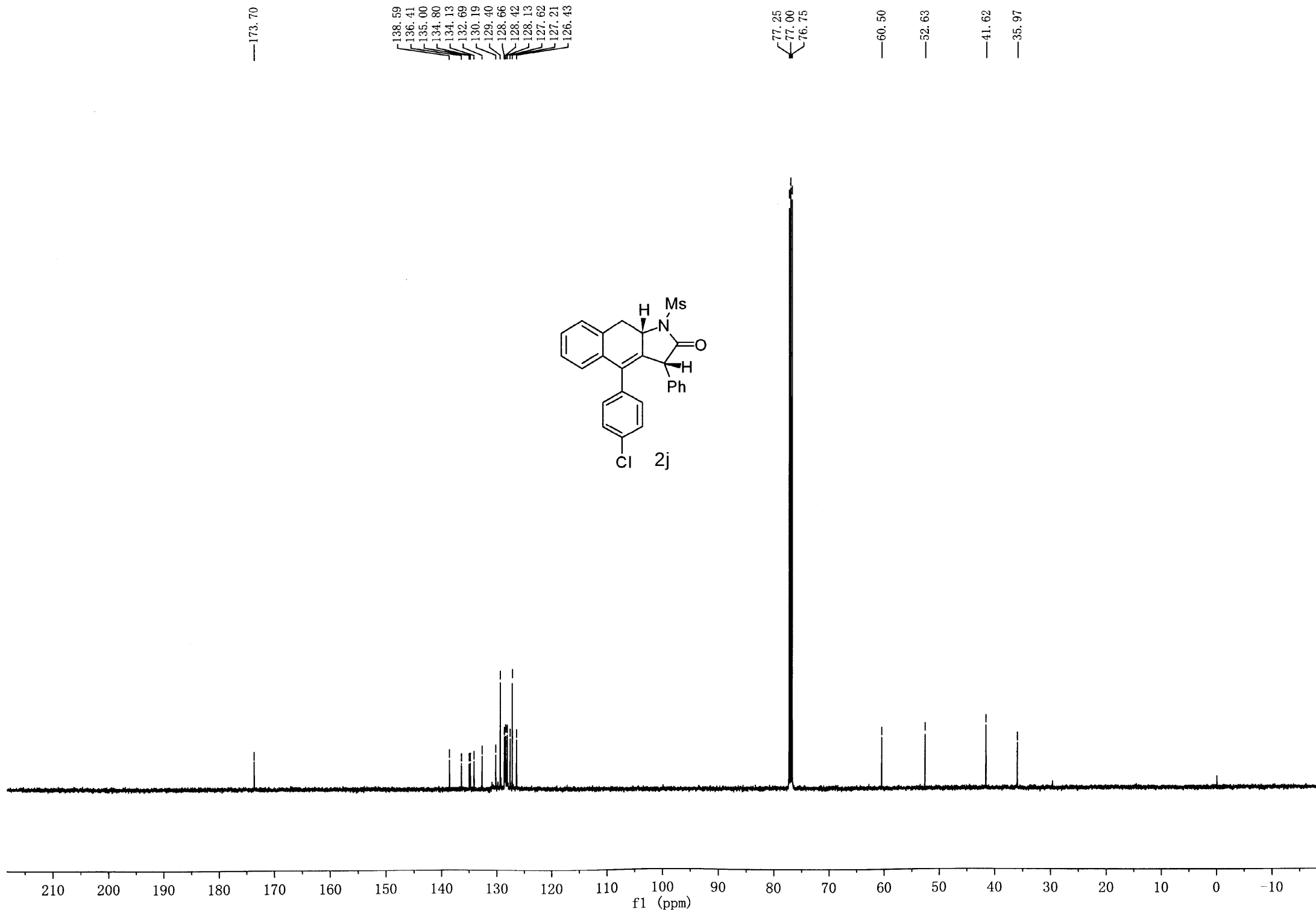
2h

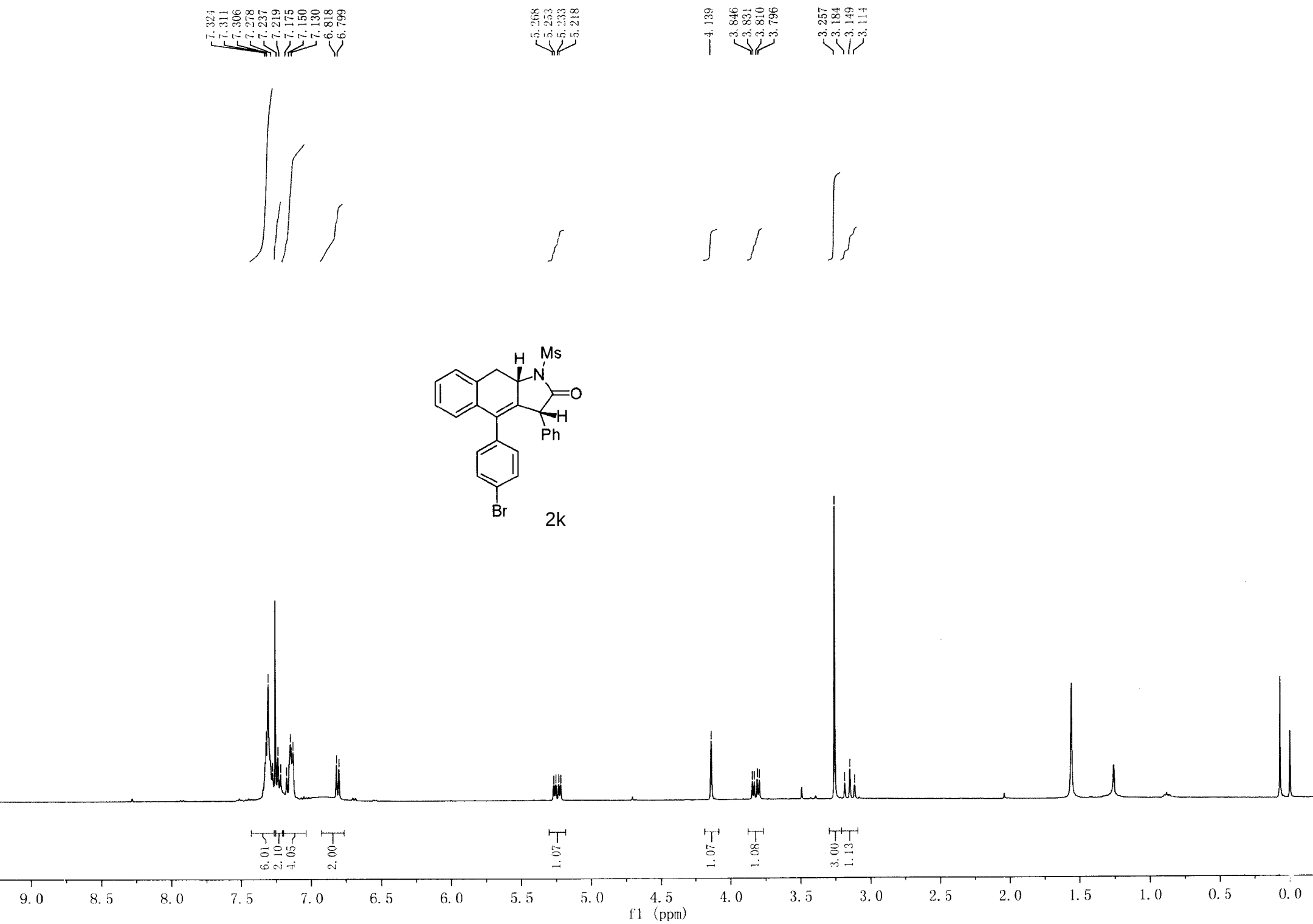


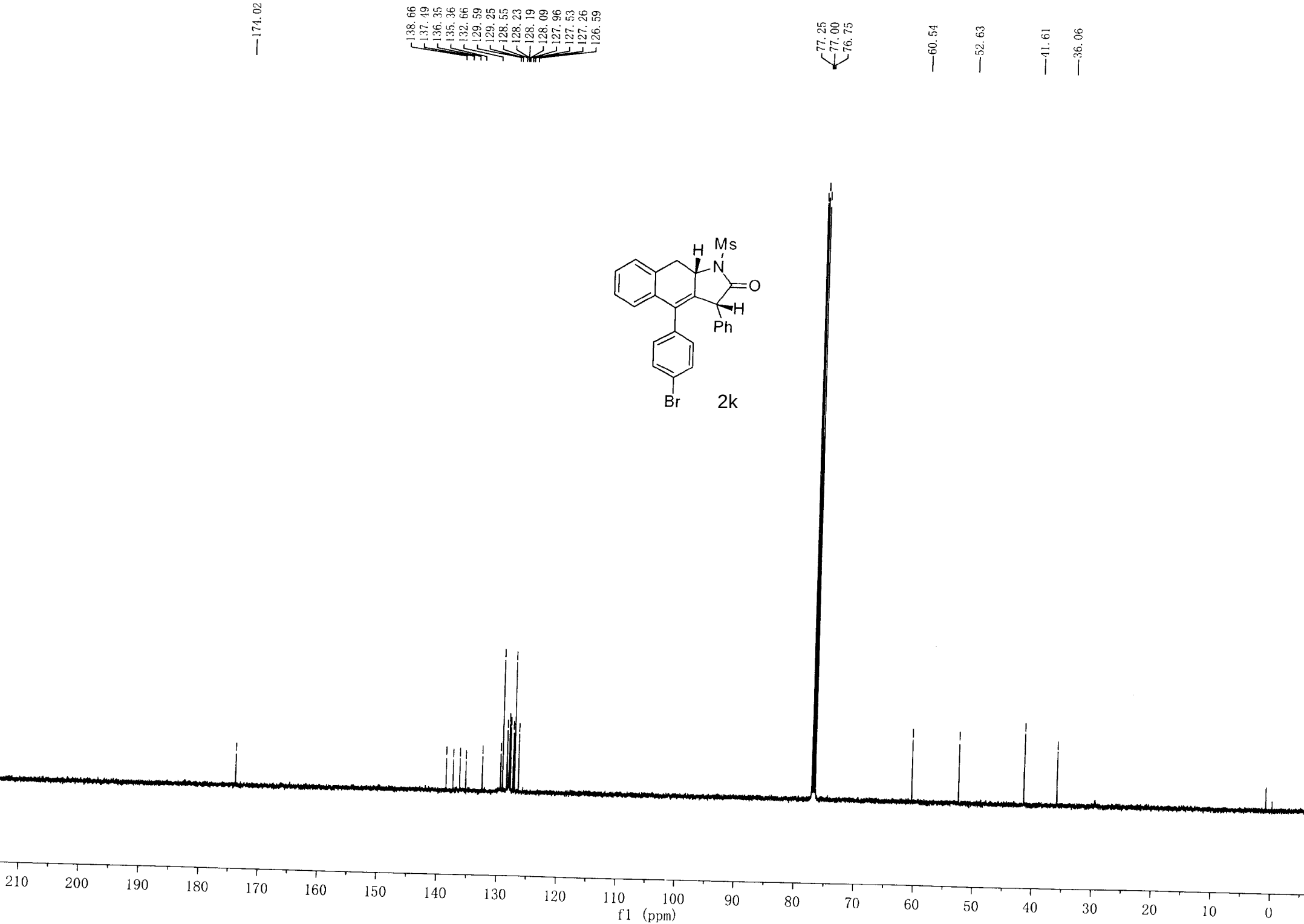












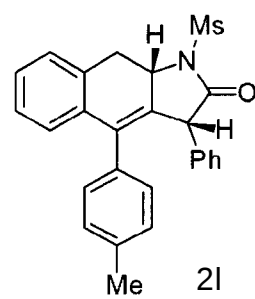
7.347
7.331
7.313
7.294
7.255
7.230
7.212
7.178
7.162
7.151
7.132
7.037
6.836
6.817

5.250
5.236
5.215
5.201

4.149
3.830
3.815
3.794
3.780

3.243
3.169
3.134
3.099

2.332



4.18
2.22
3.18
2.02
2.02

1.09

1.09

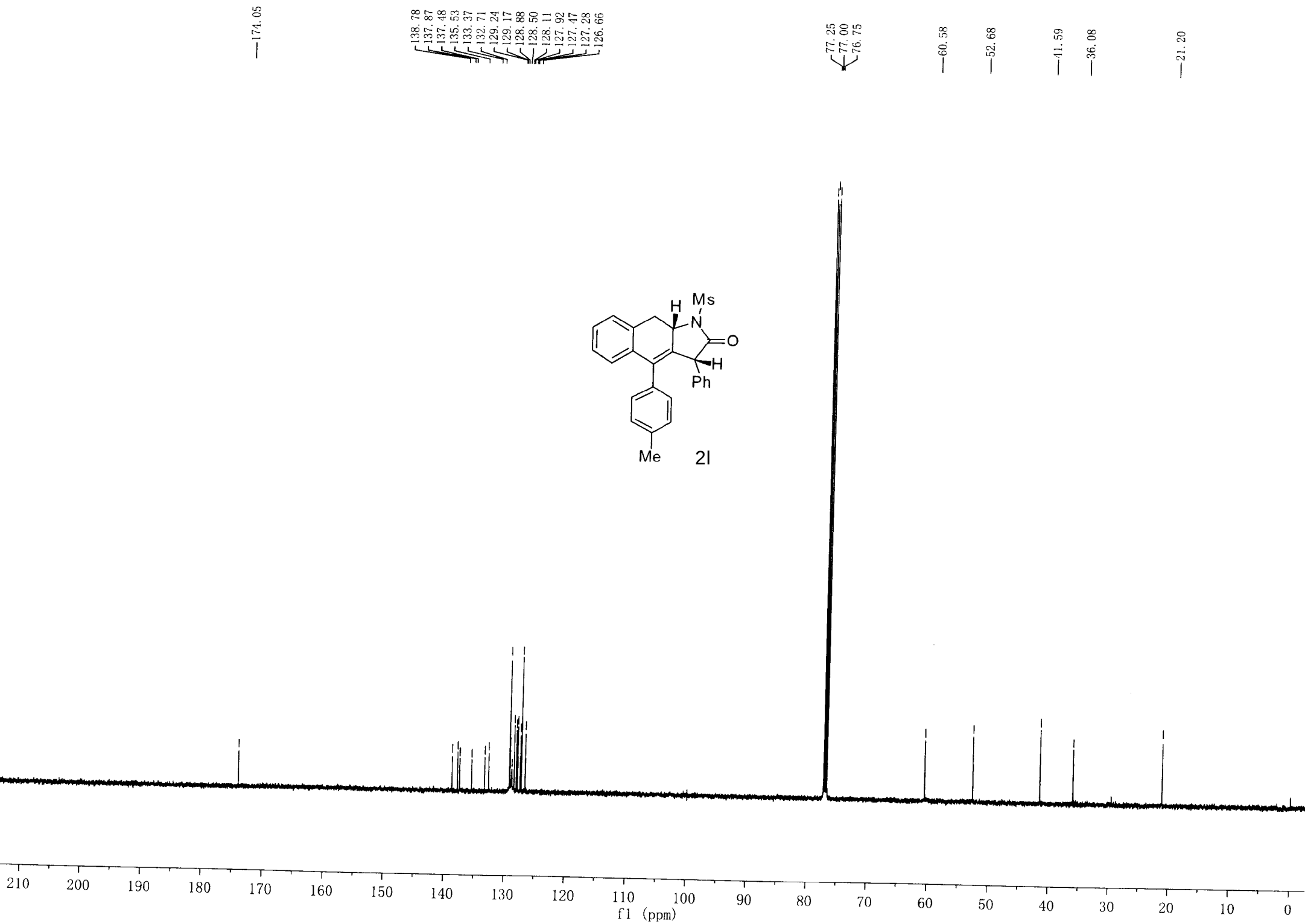
1.08

3.00
1.13

3.07

f1 (ppm)

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

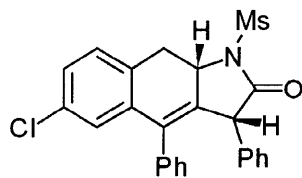


7.363
7.357
7.344
7.331
7.315
7.281
7.258
7.247
7.221
7.217
7.201
7.196
7.125
7.106
6.930
6.783

5.233
5.219
5.198
5.185

4.130
3.836
3.821
3.800
3.785

3.257
3.121
3.086
3.051



2m

7.01
1.97
2.17
2.15

1.08

1.06

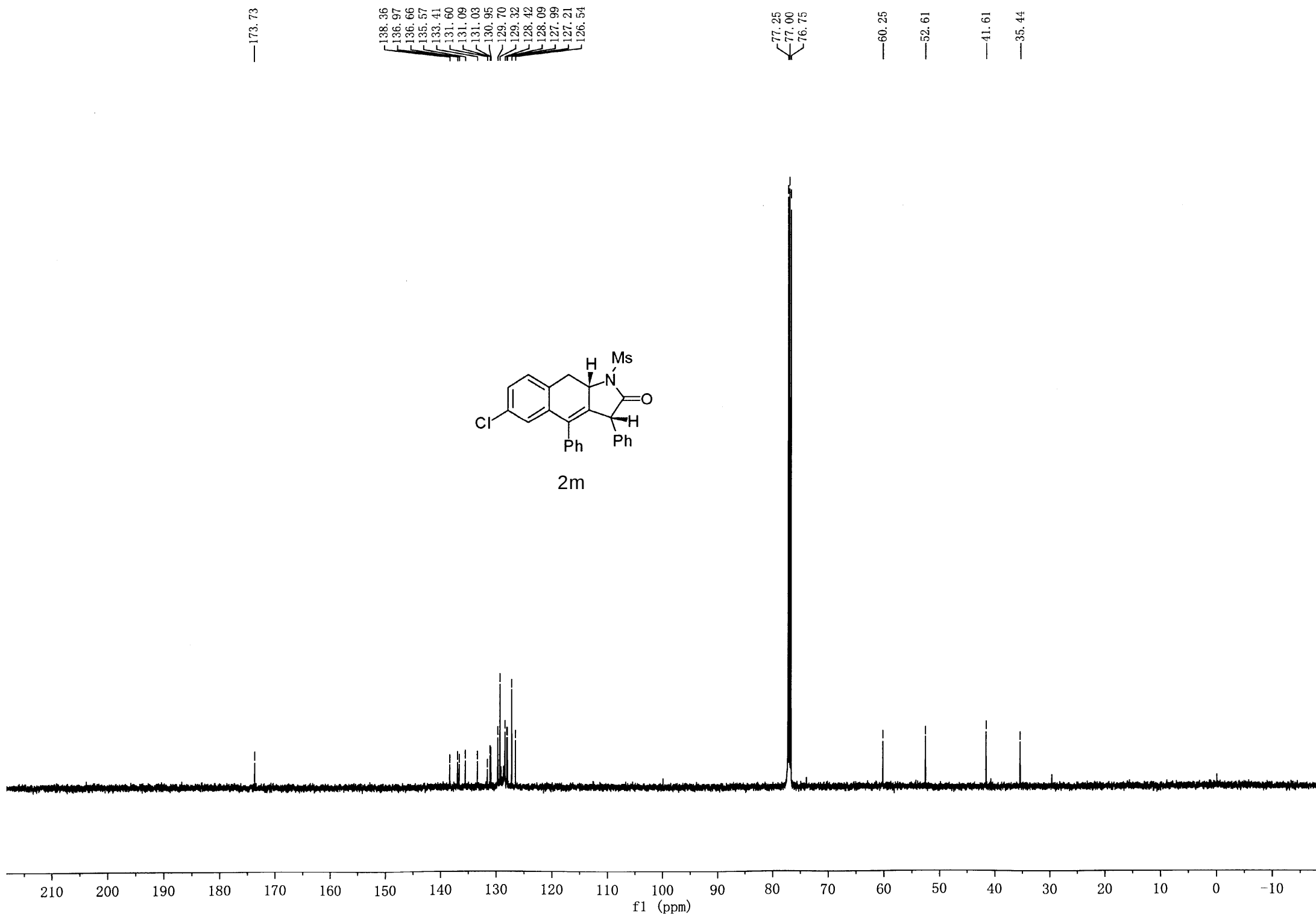
1.05

3.00

1.06

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

f1 (ppm)

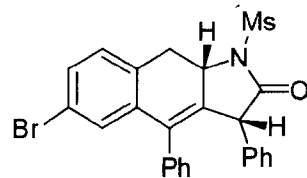


7.376
7.372
7.360
7.356
7.331
7.320
7.316
7.205
7.203
7.188
7.187
7.123
7.119
7.107
7.104
6.927
6.923

5.231
5.228
5.219
5.217
5.203
5.200
5.191
5.189

4.128
3.817
3.806
3.789
3.777

3.256
3.092
3.064
3.036



2n

6.06
2.10
3.04
2.05

1.01

1.06

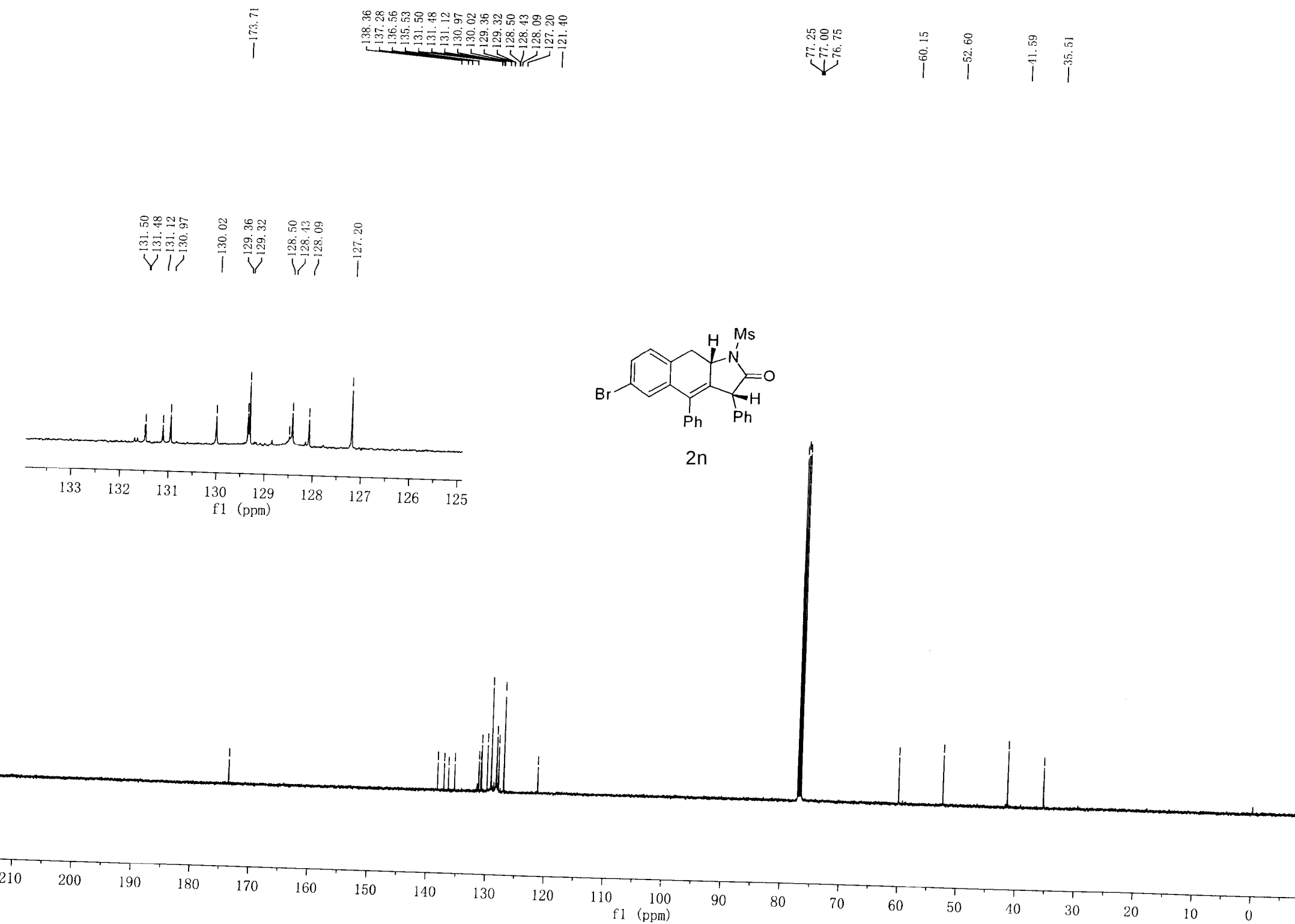
1.11

3.00

1.31

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

f1 (ppm)



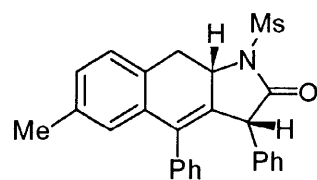
7.317
7.310
7.301
7.297
7.289
7.255
7.218
7.203
7.138
7.134
7.123
7.120
7.060
7.059
7.045
7.043
6.988
6.788
6.726
6.613

5.231
5.229
5.220
5.217
5.203
5.201
5.192
5.189

4.118
3.799
3.788
3.771
3.760

3.251
3.122
3.094
3.066

2.202



20

5.06
1.12
2.91
2.07
2.11

1.00

1.06

1.03

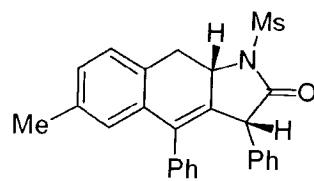
3.04

1.09

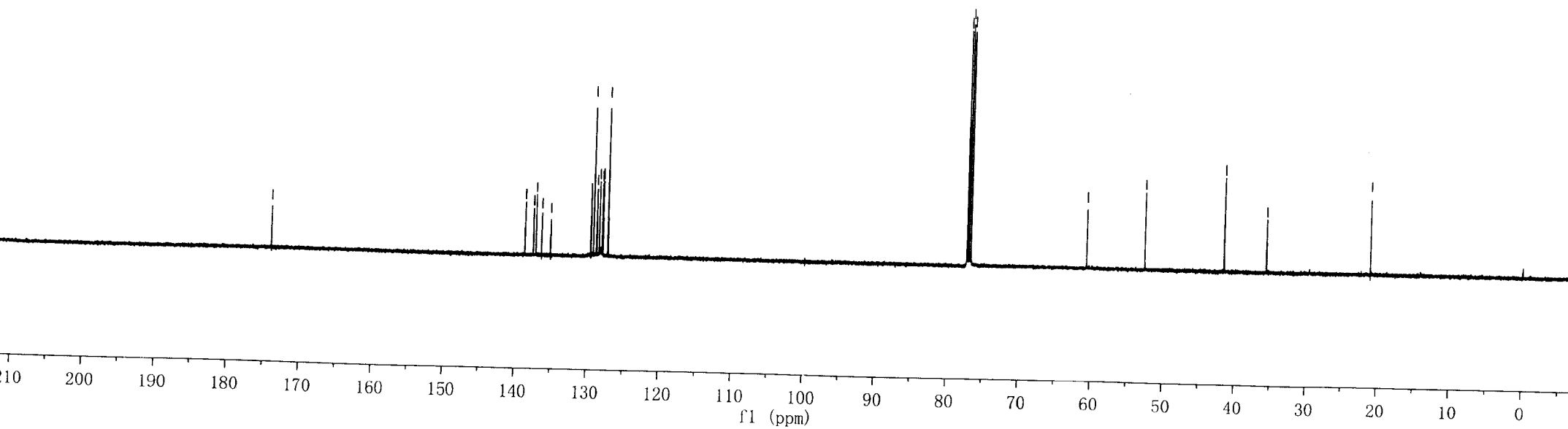
3.03

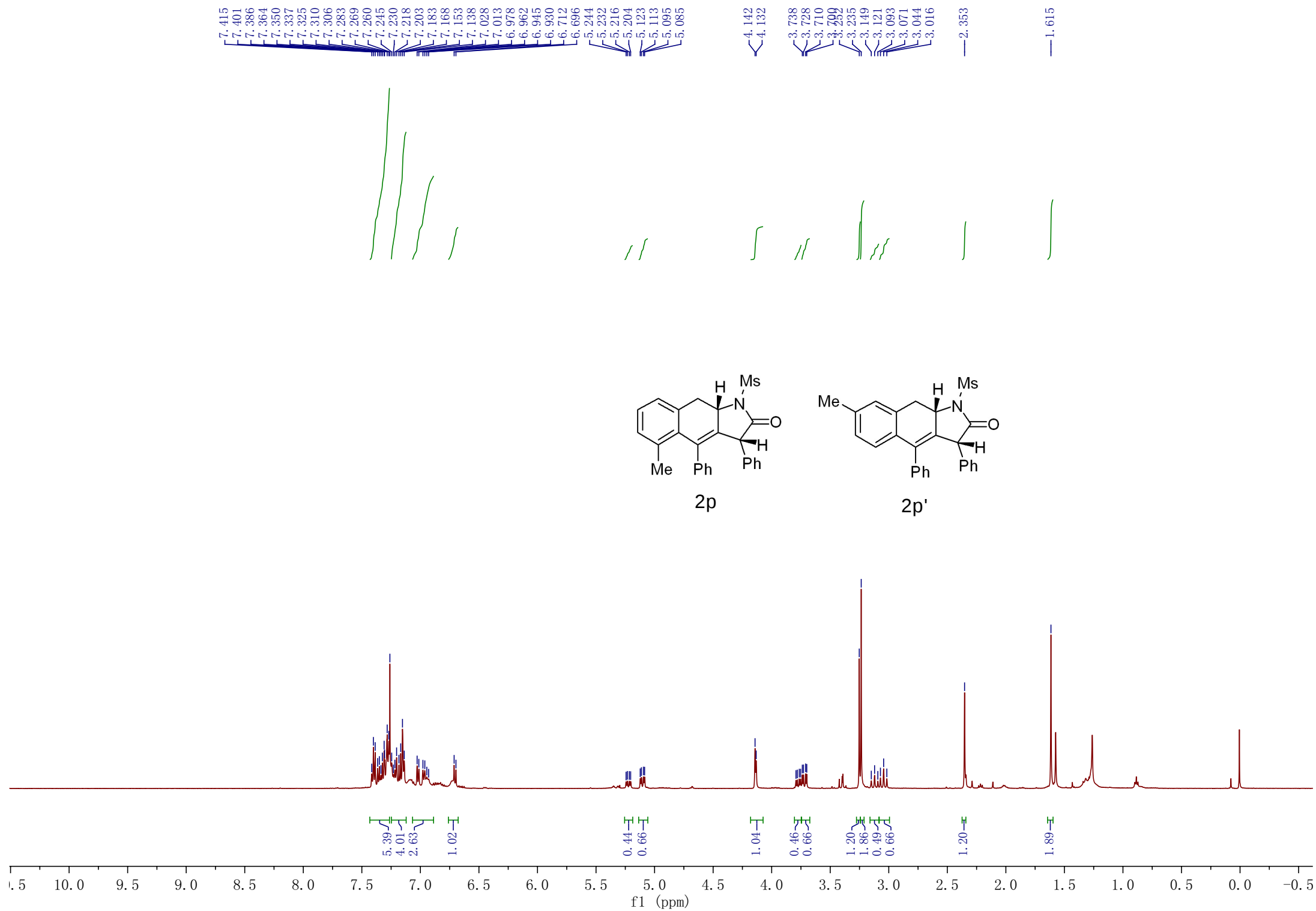
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

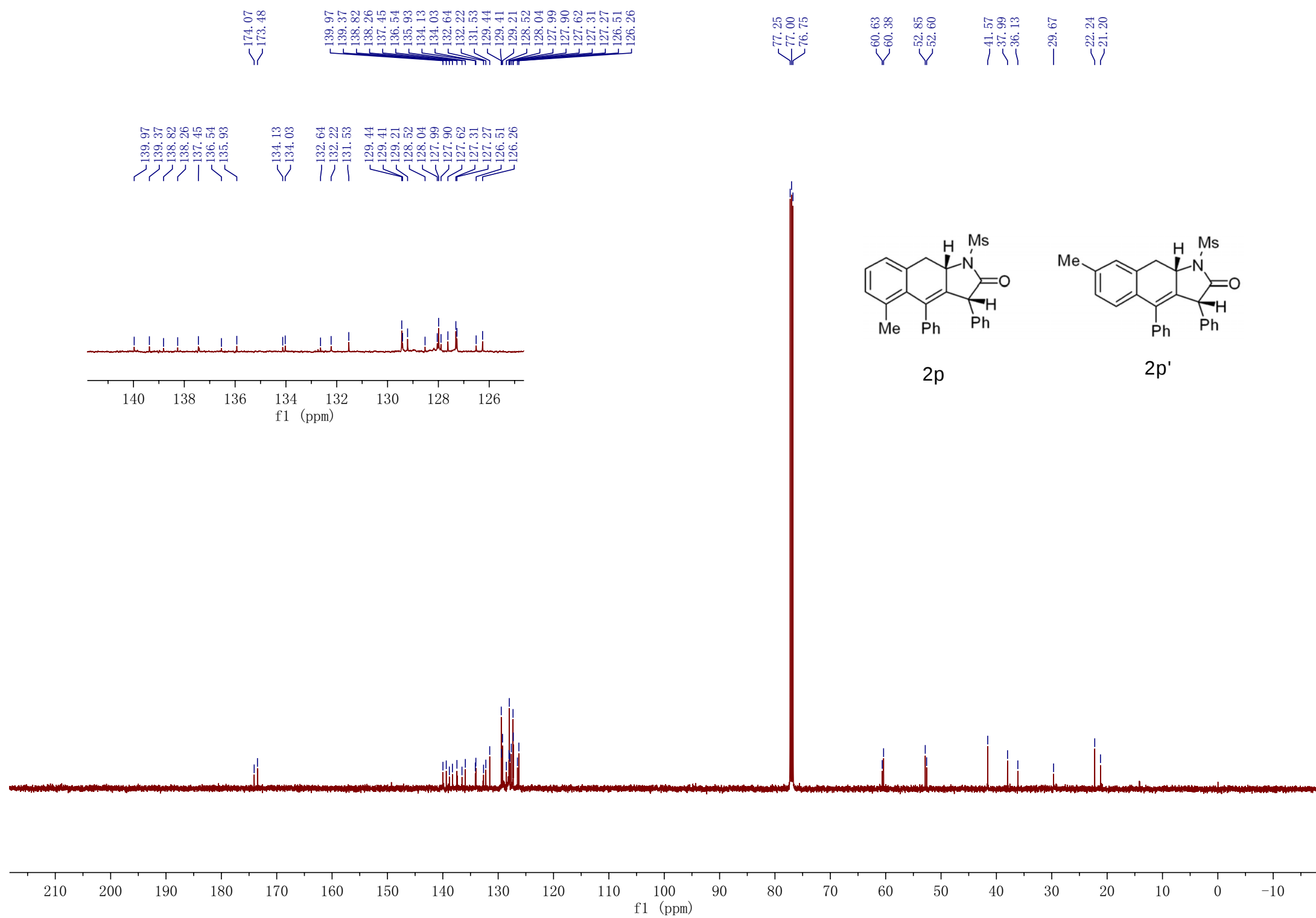
f1 (ppm)



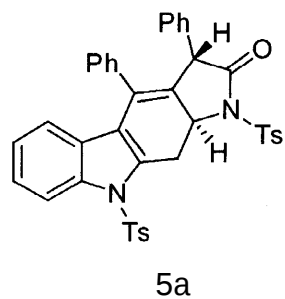
20







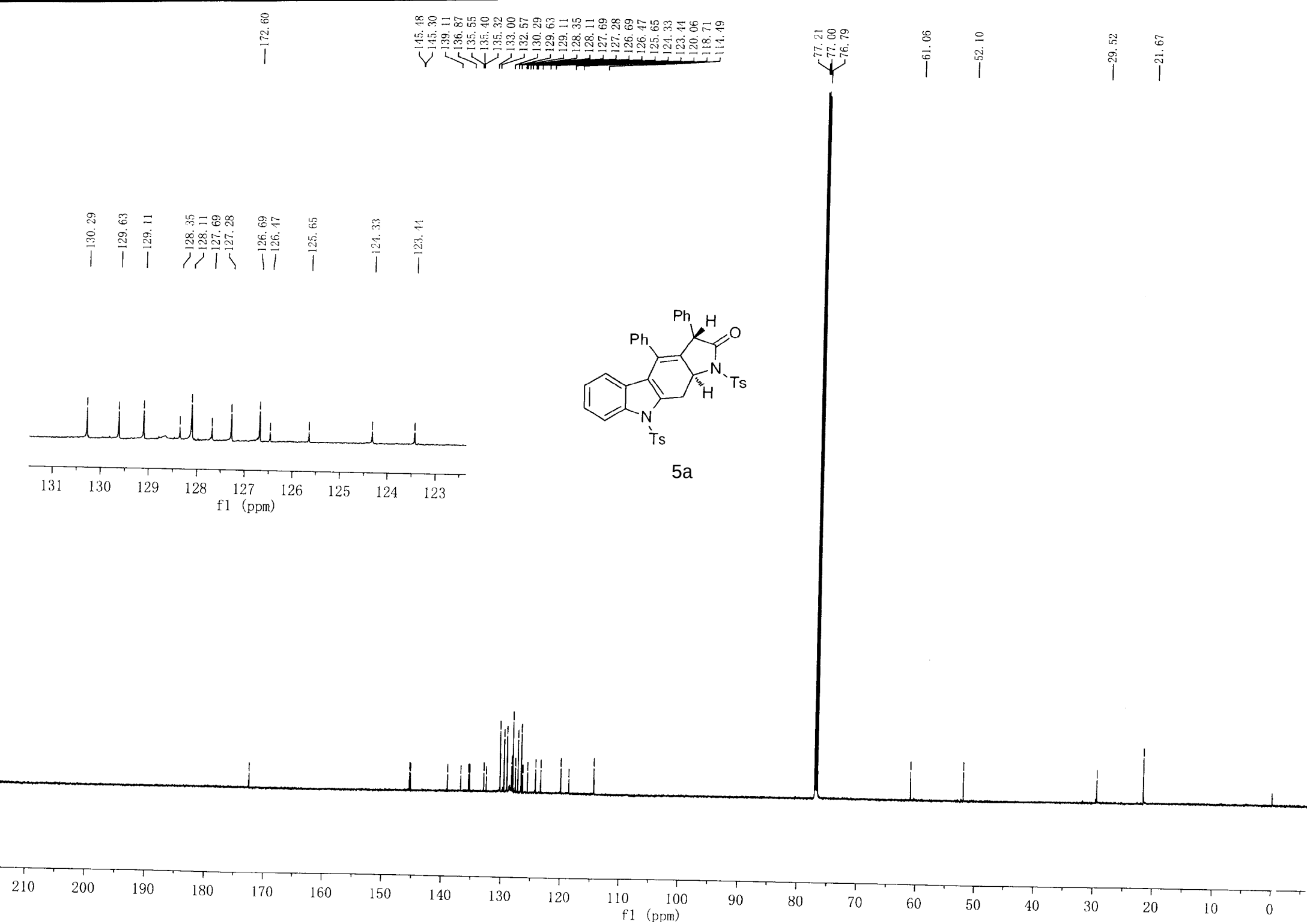
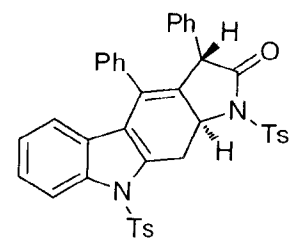
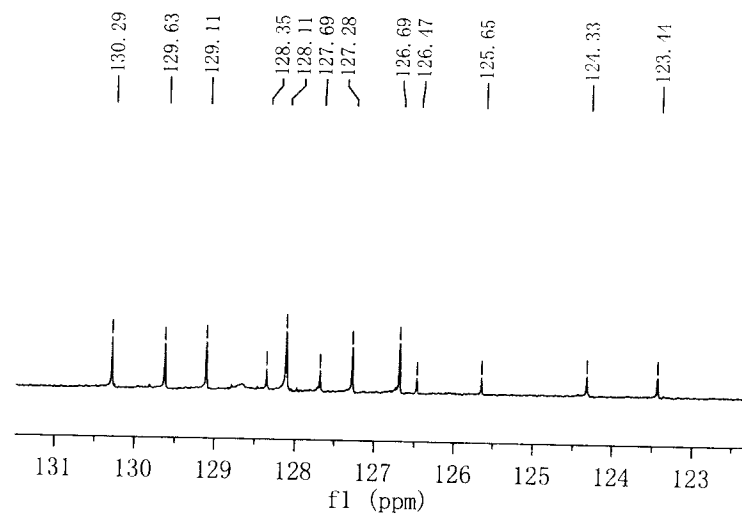
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 8.274
 7.957
 7.943
 7.928
 7.914
 7.354
 7.341
 7.289
 7.275
 7.259
 7.248
 7.238
 7.225
 7.024
 7.022
 7.012
 7.009
 6.938
 6.916
 6.303
 5.199
 5.197
 5.188
 5.185
 5.174
 5.171
 5.162
 5.160
 4.814
 4.802
 4.787
 4.775
 4.068
 3.098
 3.072
 3.045
 2.427
 2.420



1.09
 4.08
 2.13
 2.94
 8.45
 2.07
 1.17
 0.99
 1.00
 1.07
 0.98
 0.98
 2.98
 3.08

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

f1 (ppm)



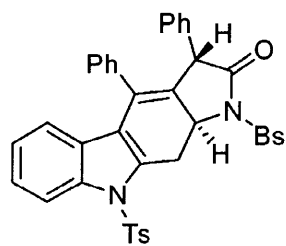
8.285
8.268
7.906
7.889
7.885
7.871
7.601
7.583
7.351
7.335
7.282
7.268
7.256
7.241
7.227
7.024
7.010
6.945
6.930
6.314

5.196
5.193
5.182
5.179
5.165
5.162
5.151
5.148
4.789
4.774
4.756
4.742

4.090

3.120
3.088
3.057

2.426



5b

1.08

4.06

2.05

2.15

9.80

2.10

1.19

0.98

1.01

1.08

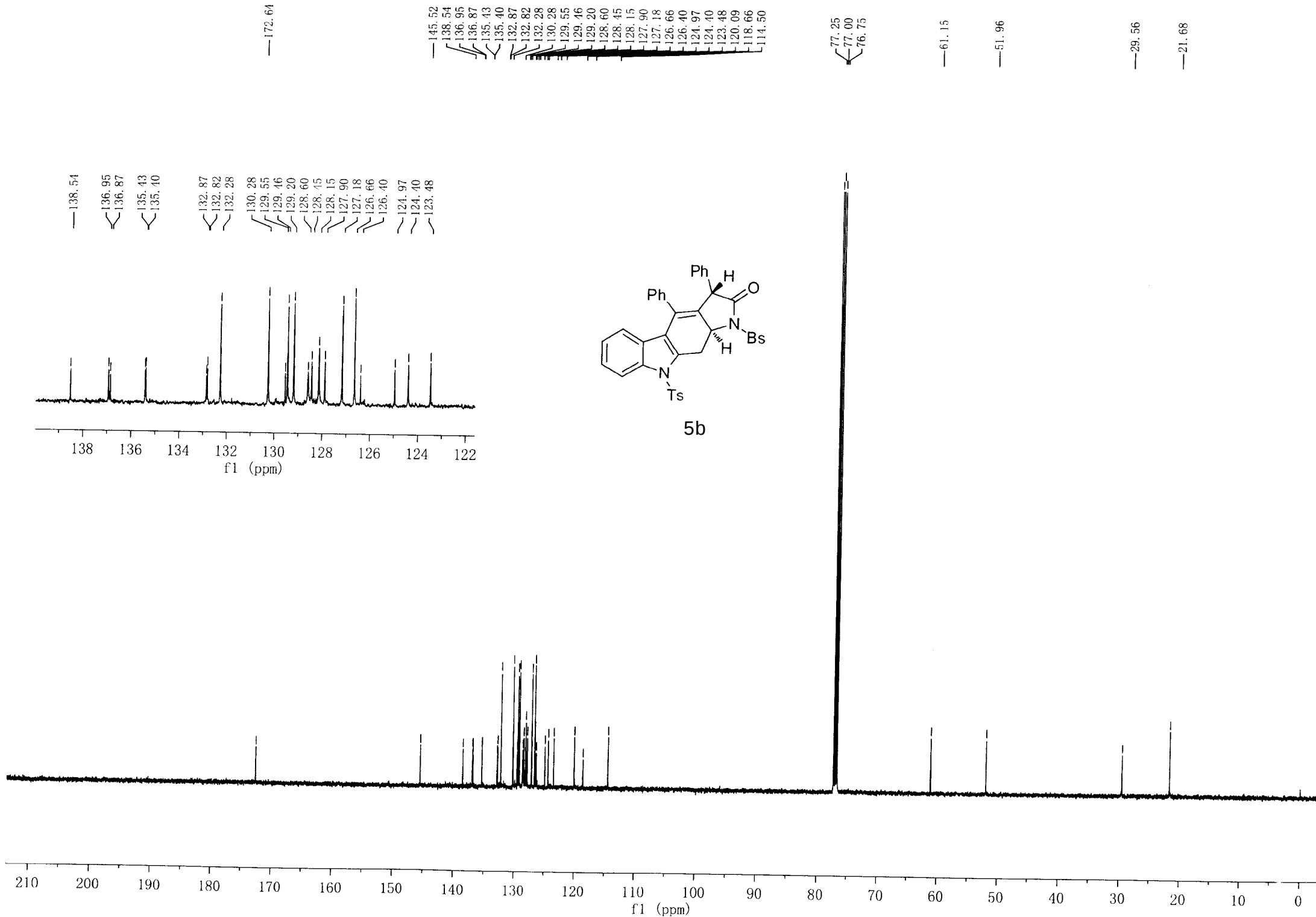
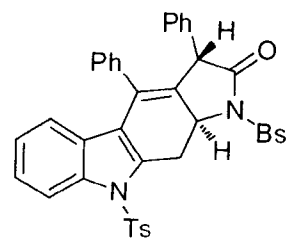
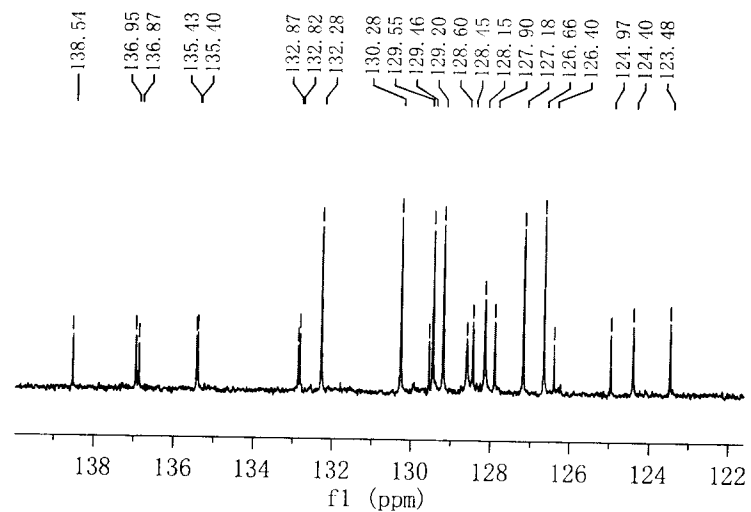
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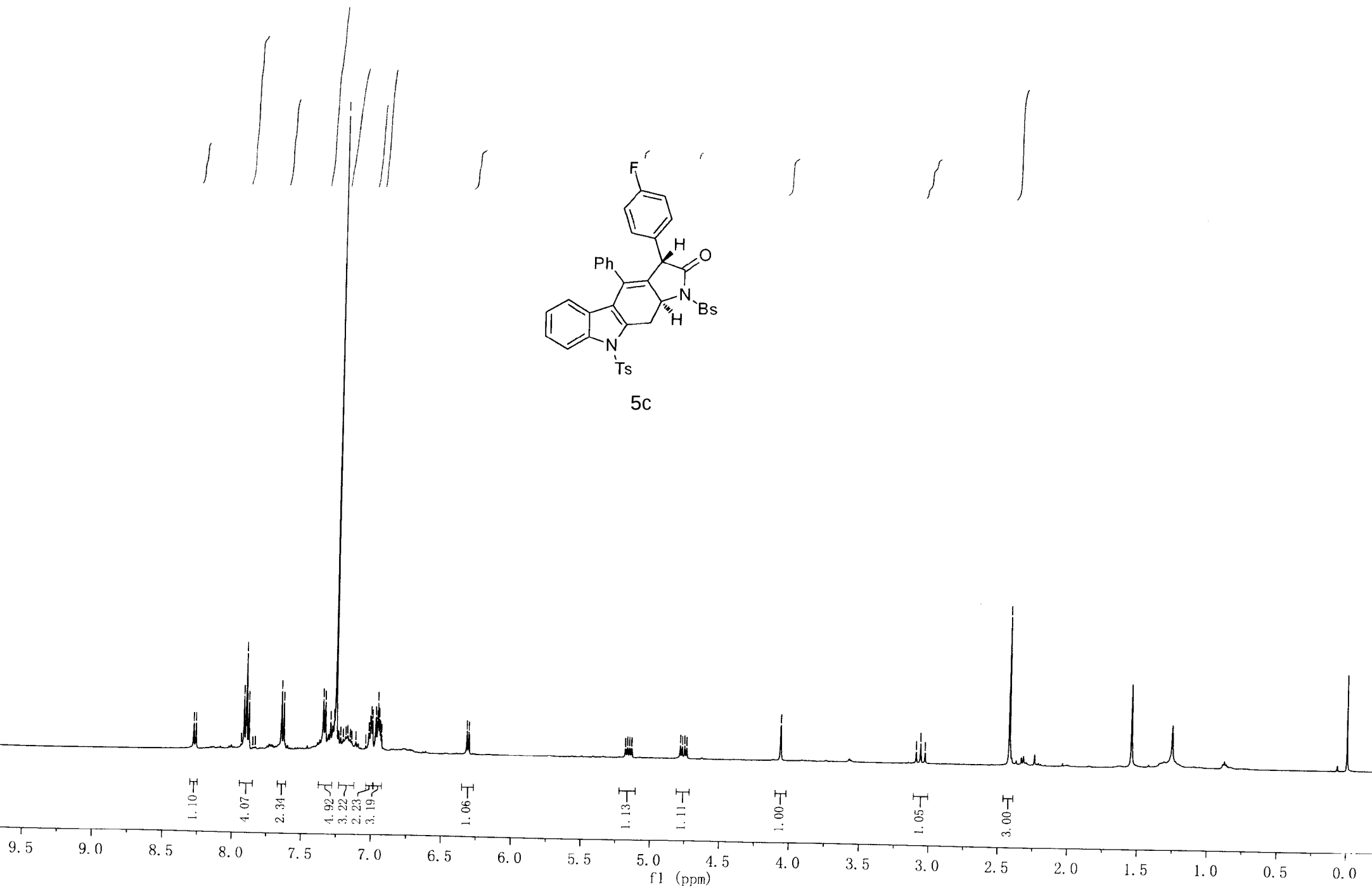
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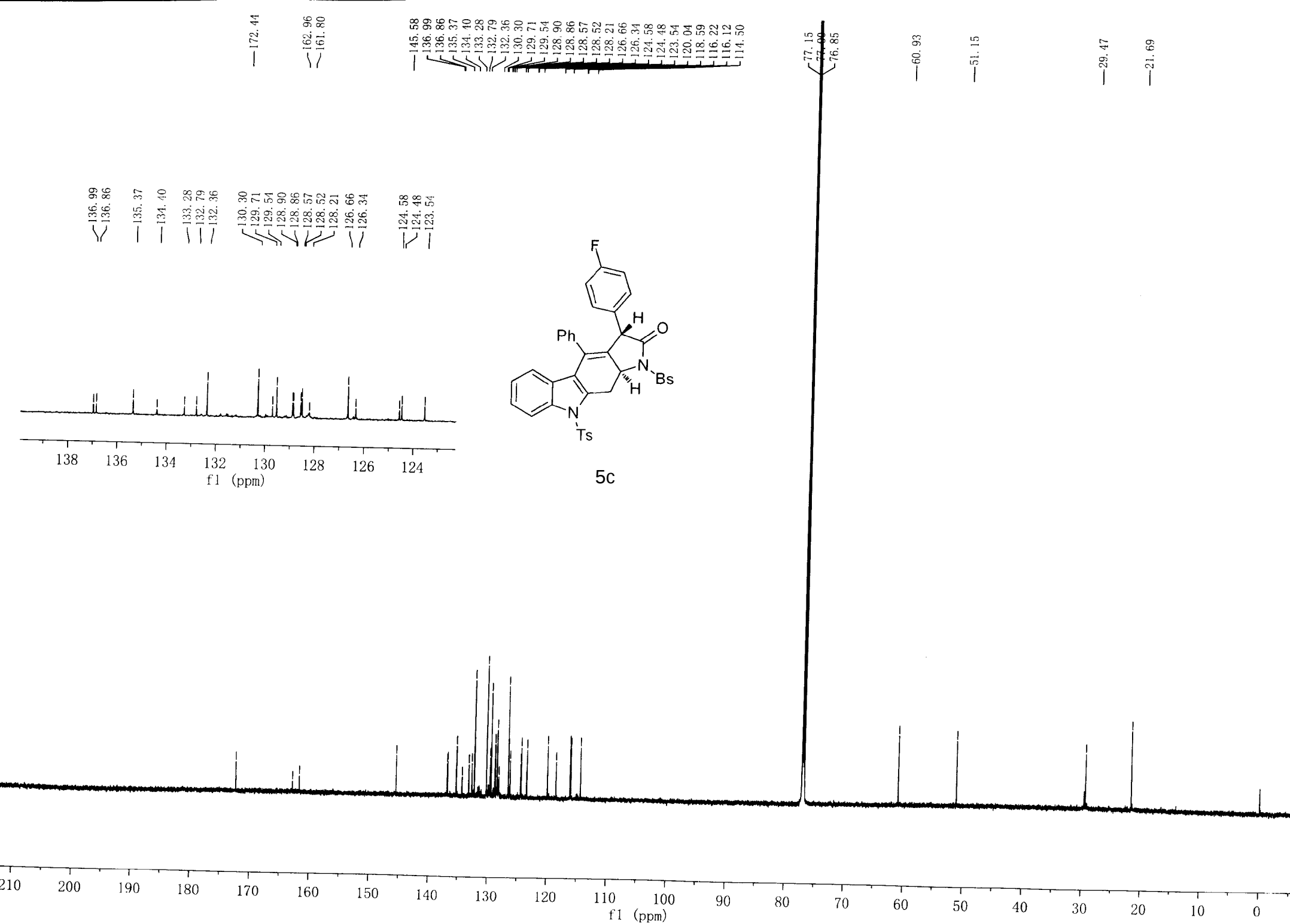
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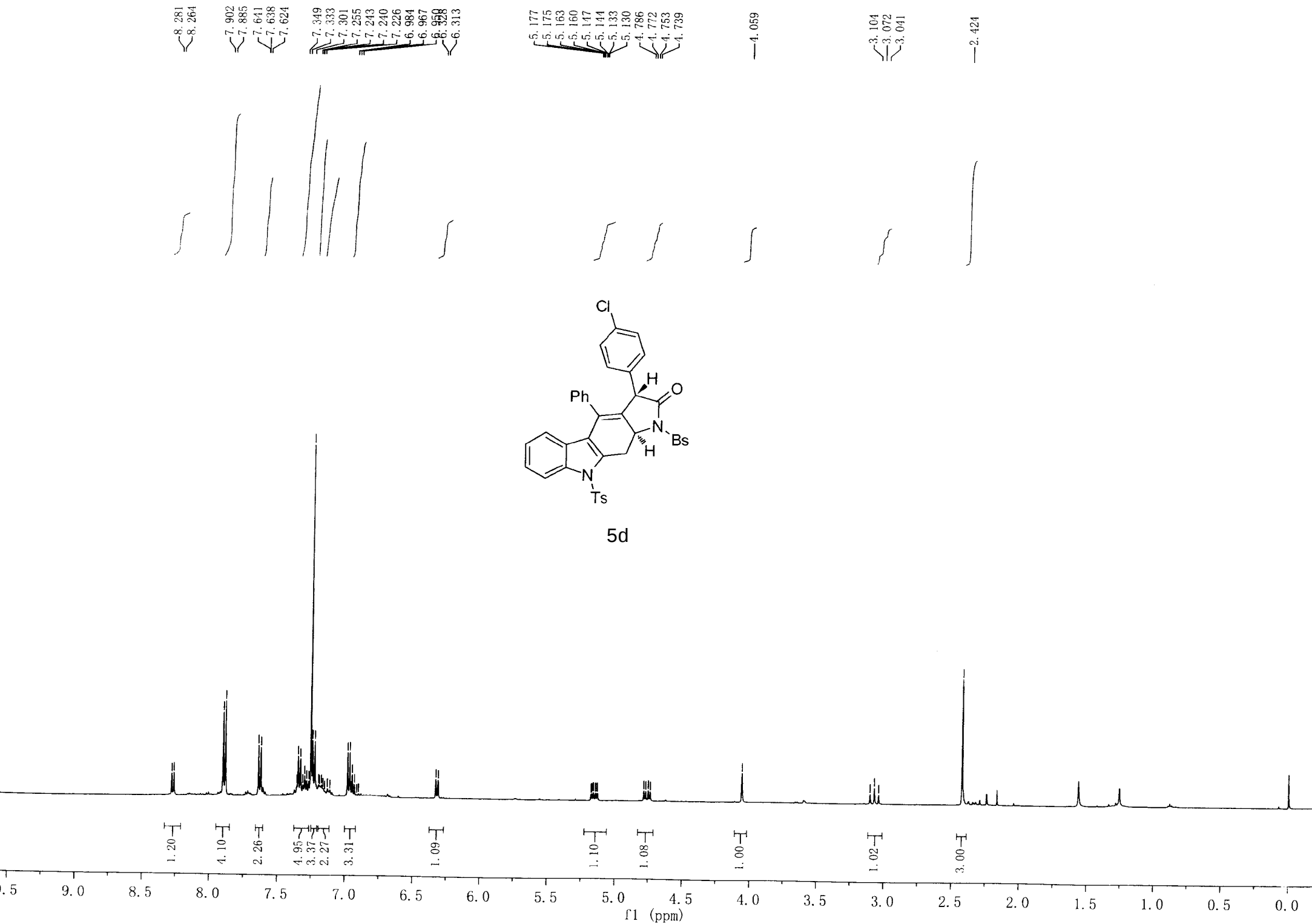
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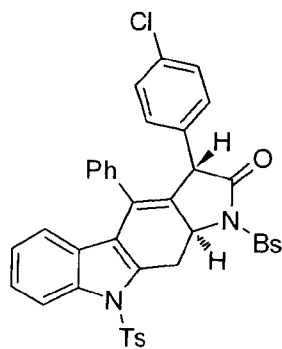
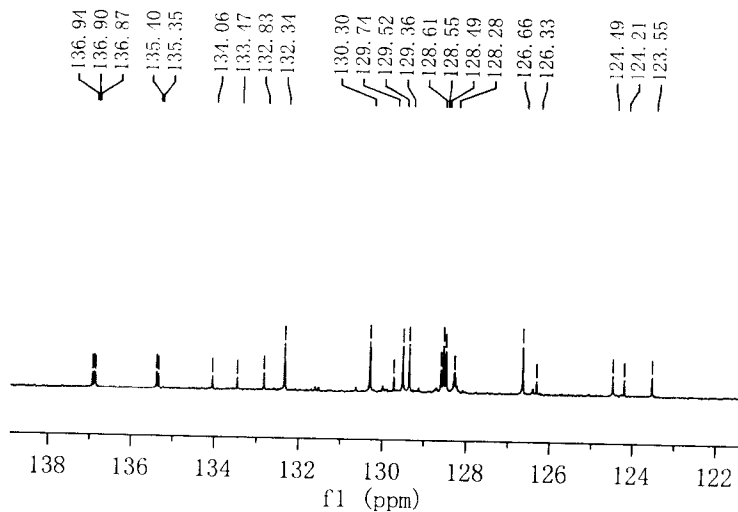
f1 (ppm)



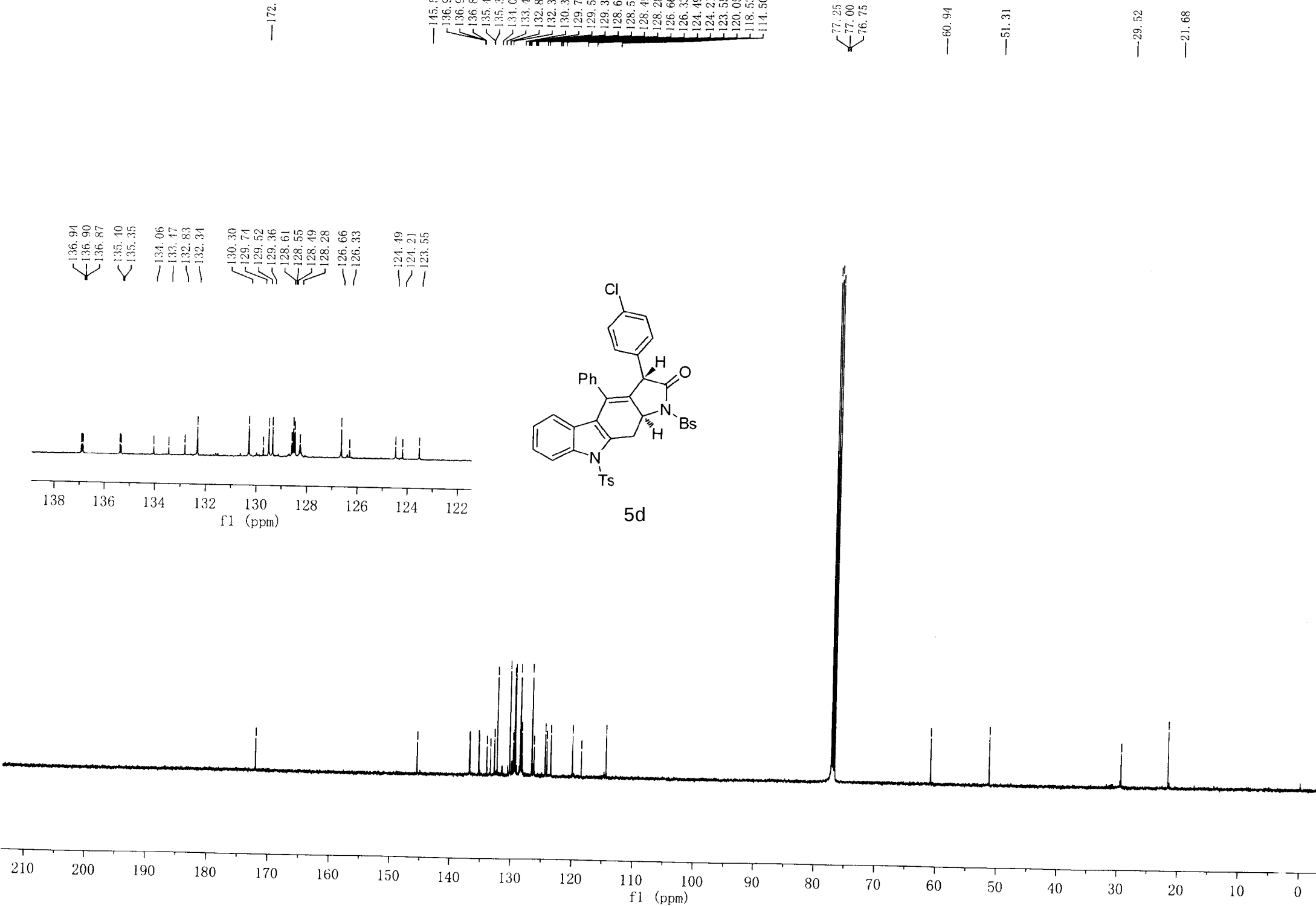


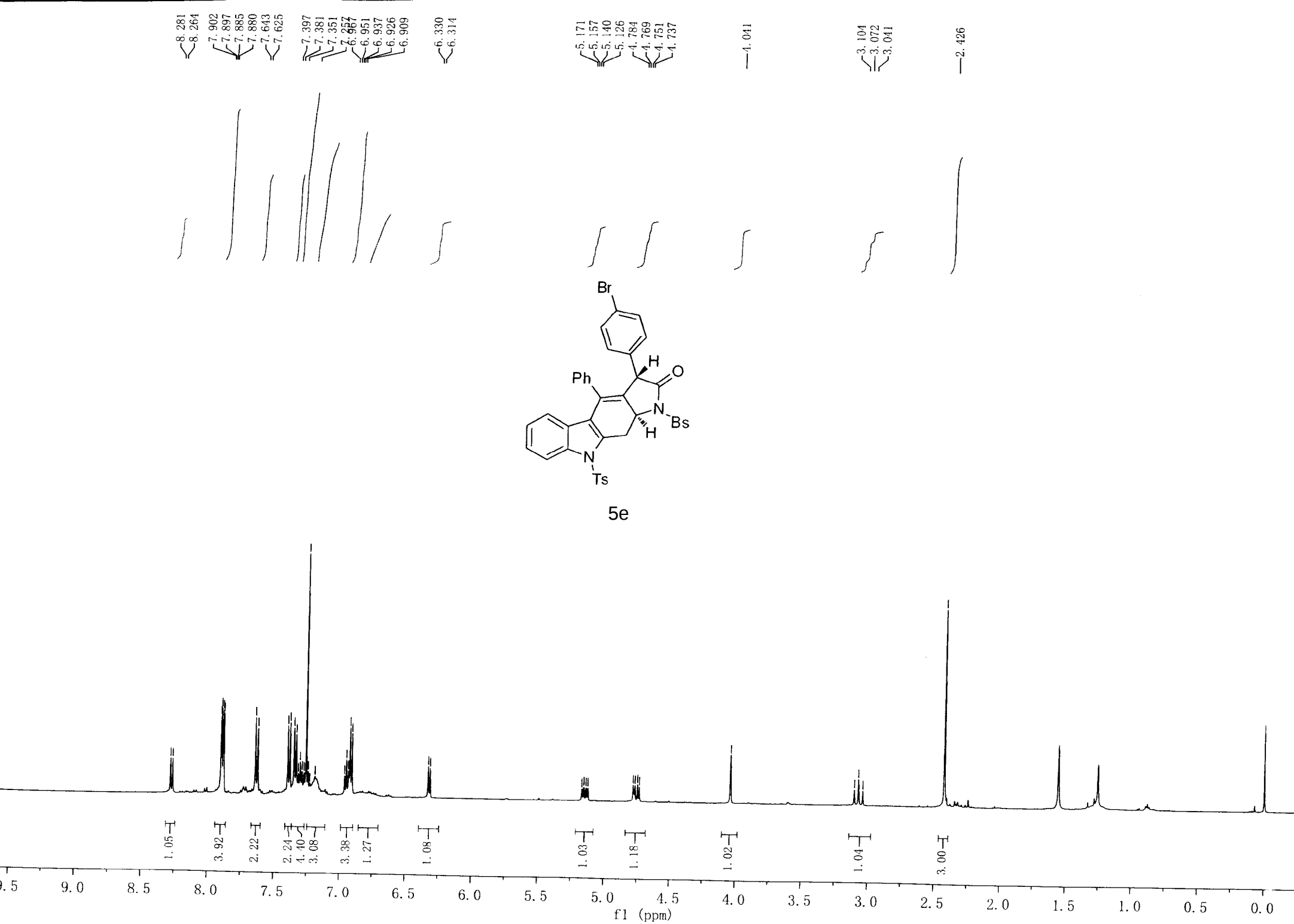


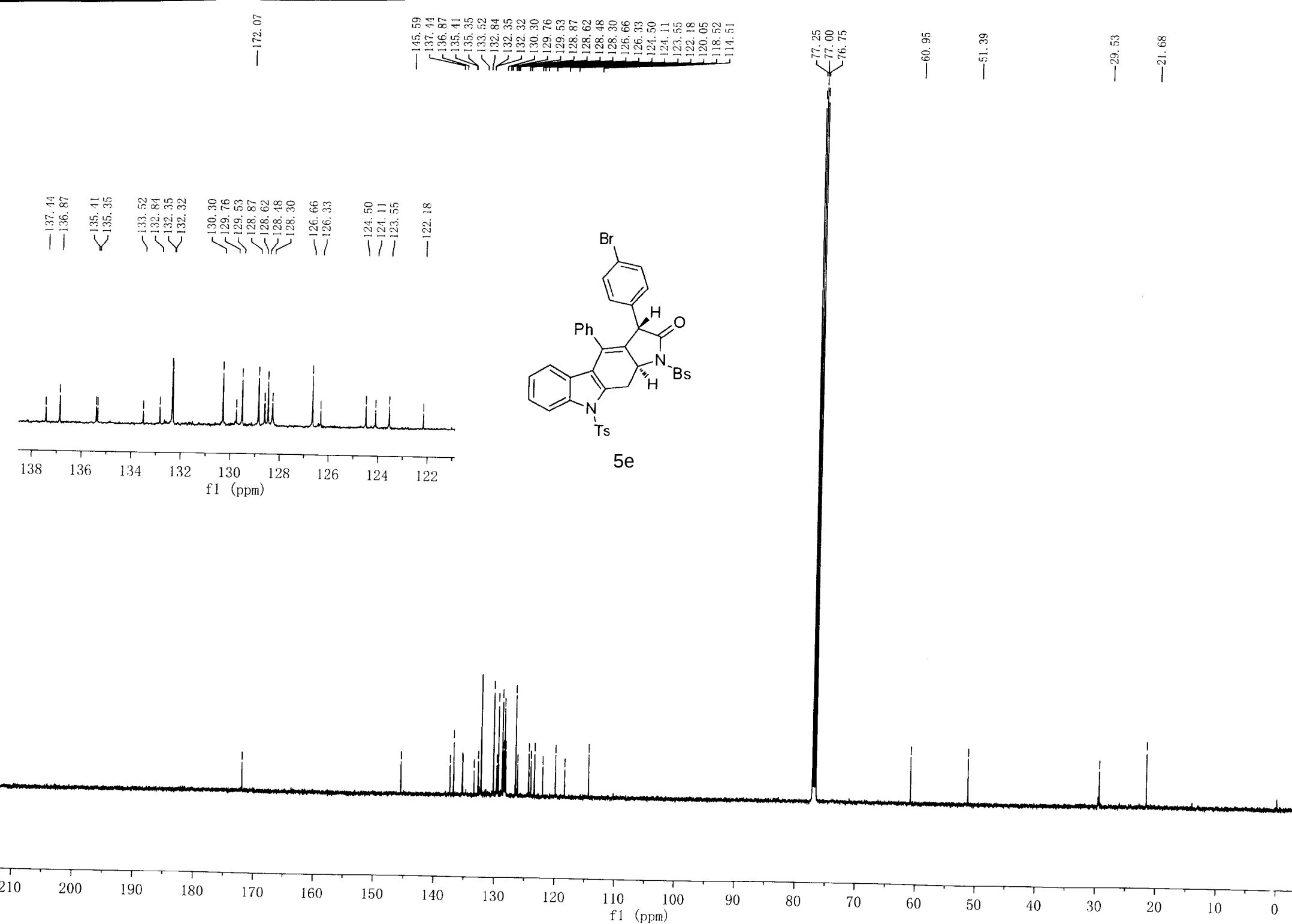


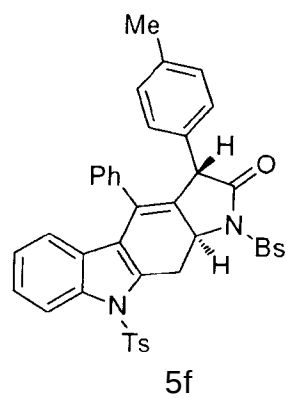
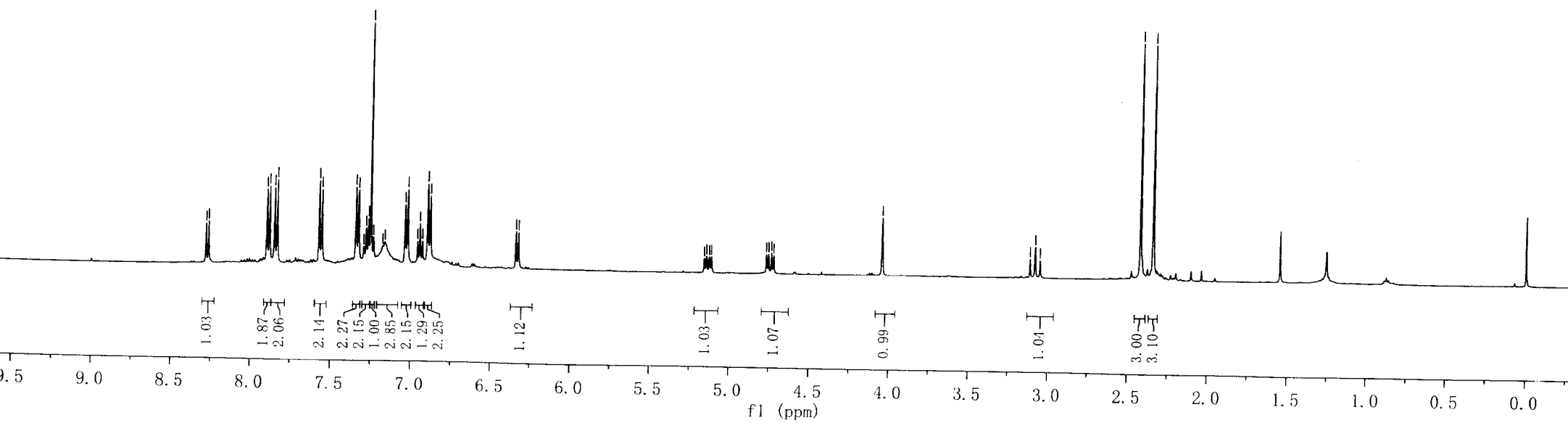


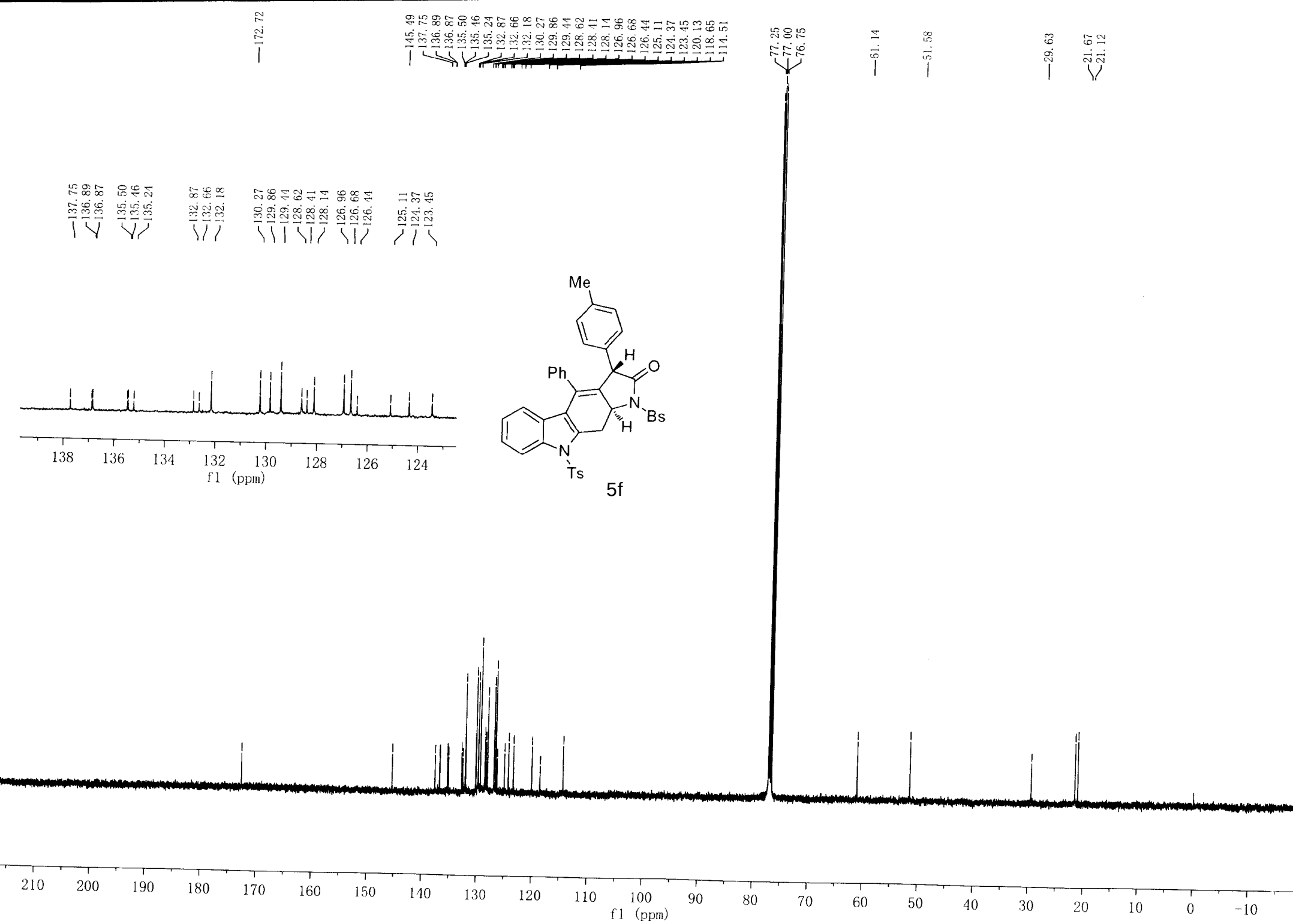
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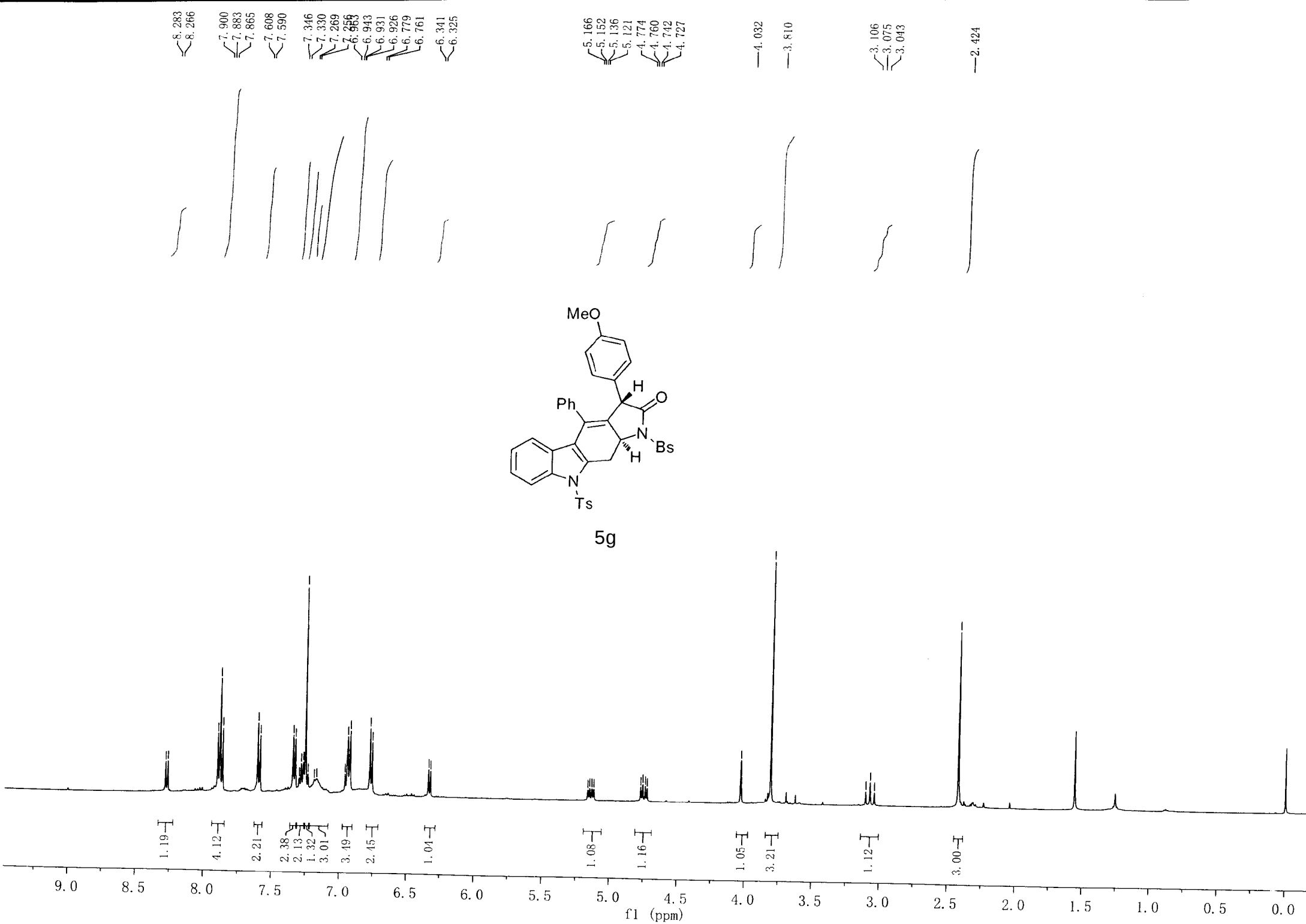


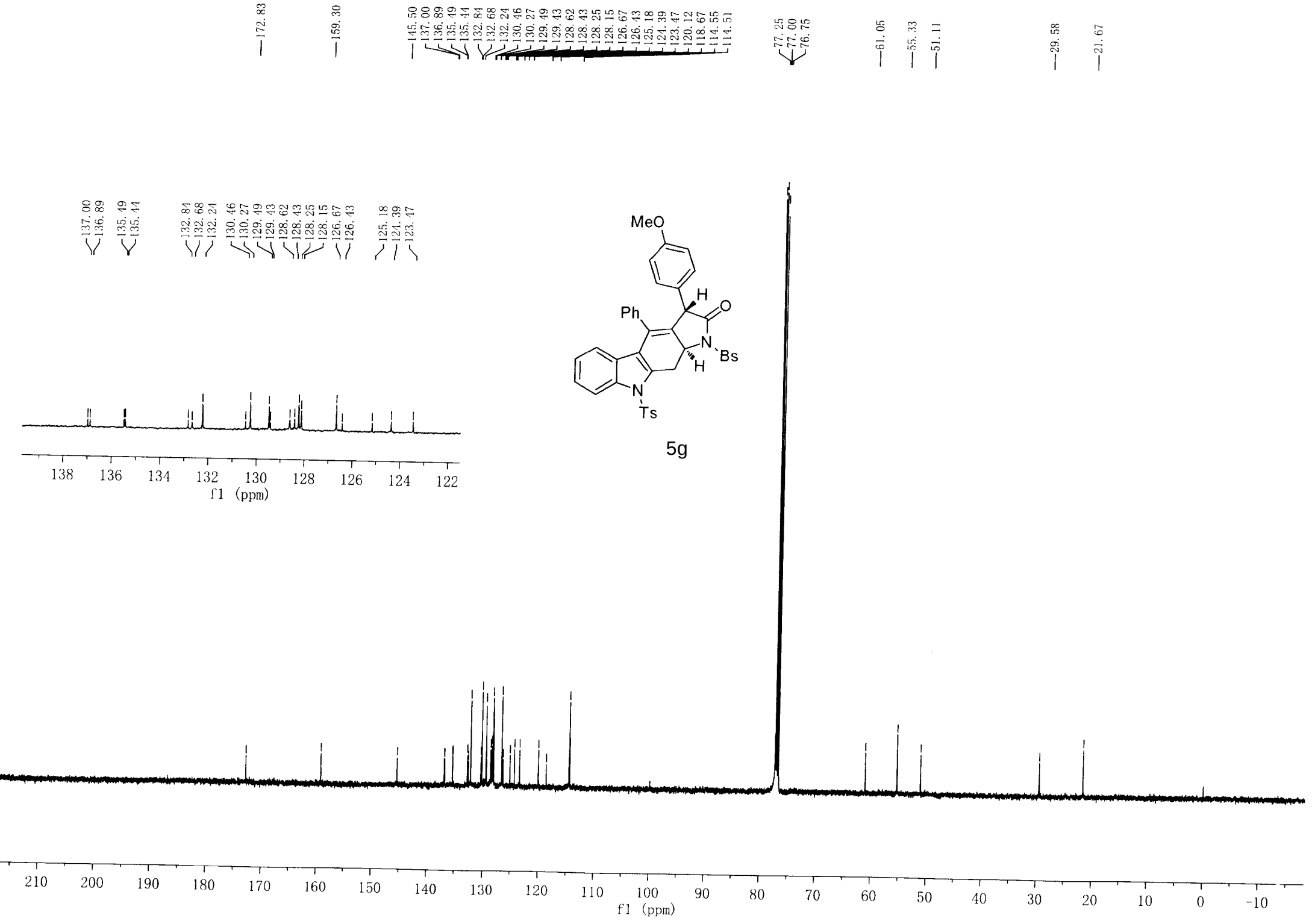
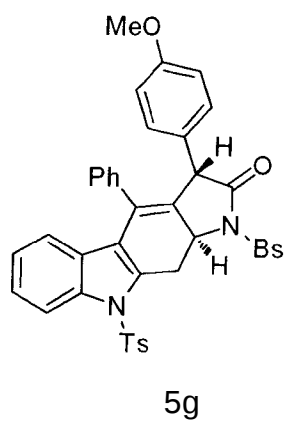
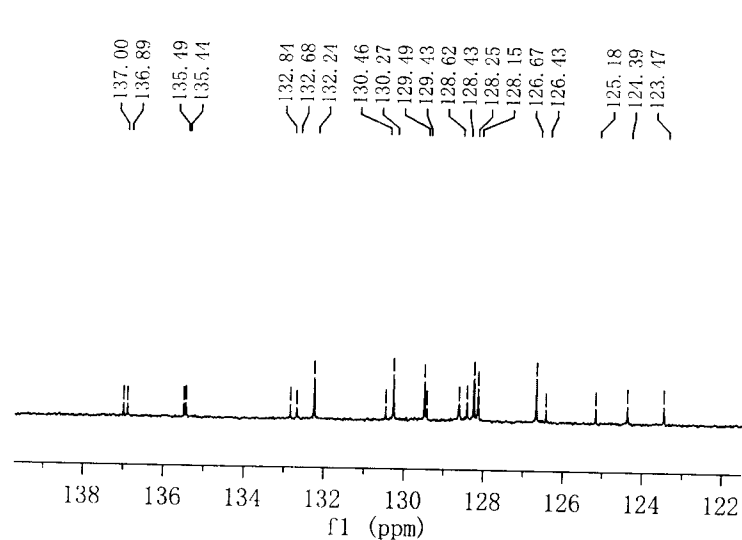


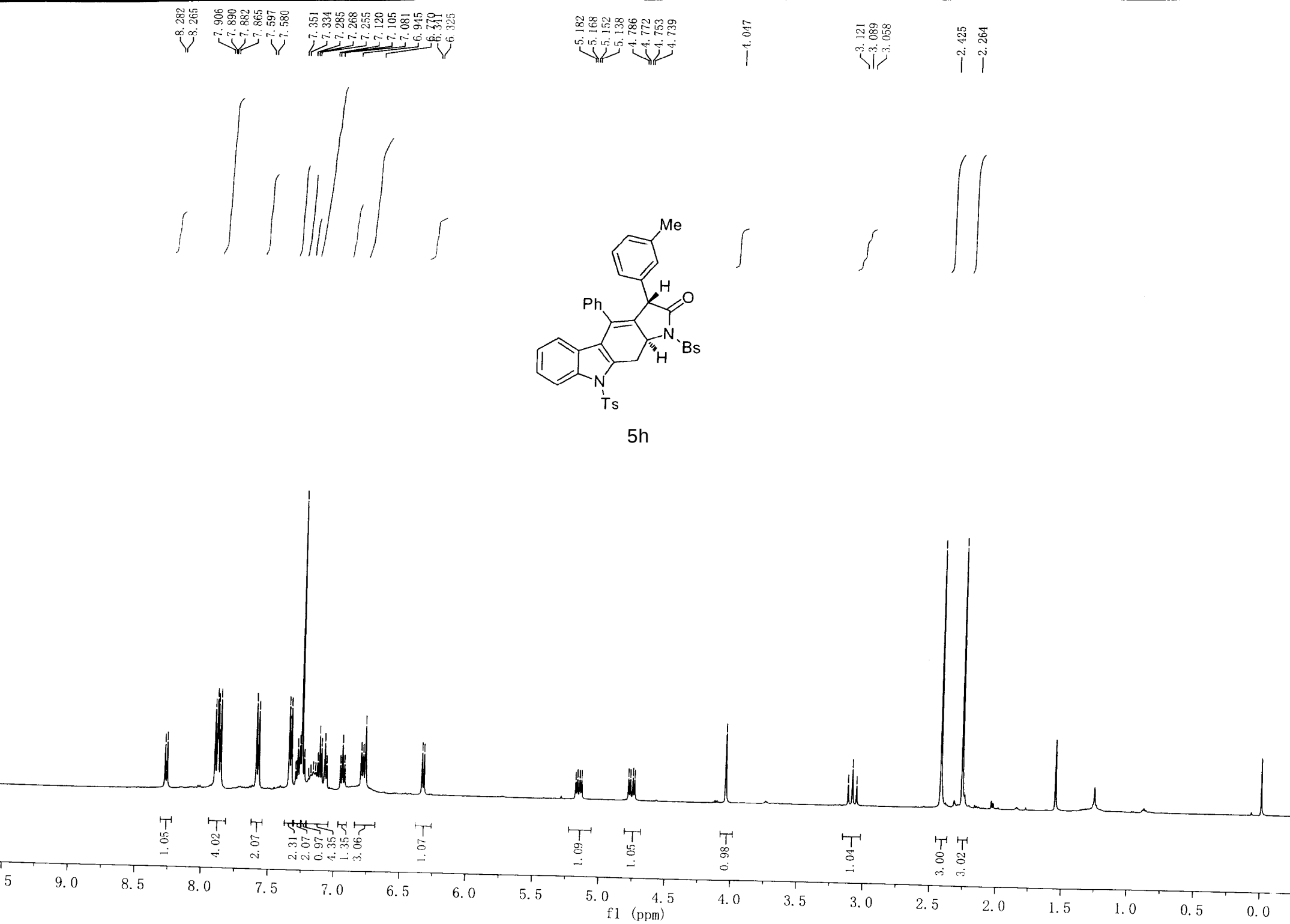


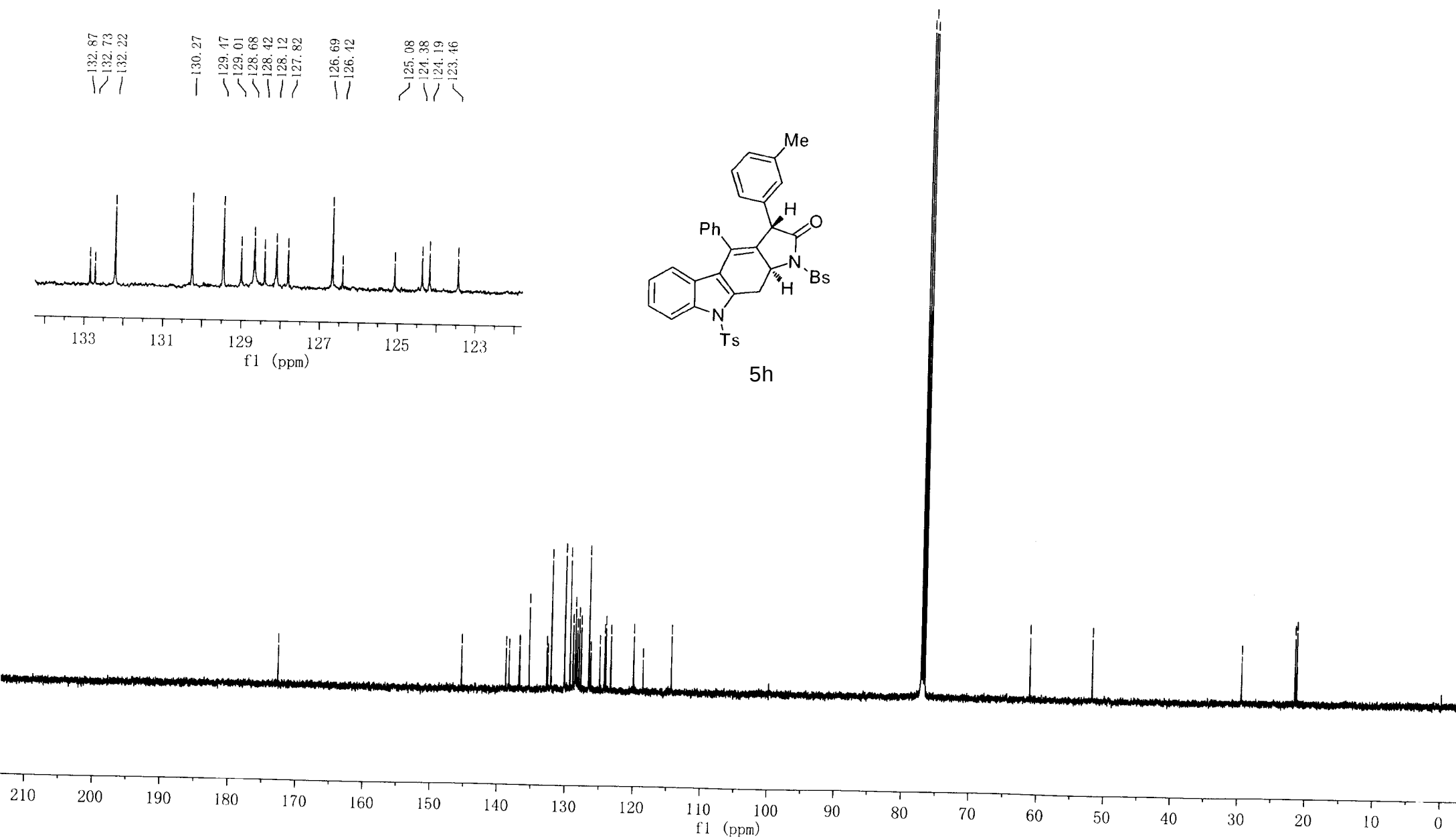


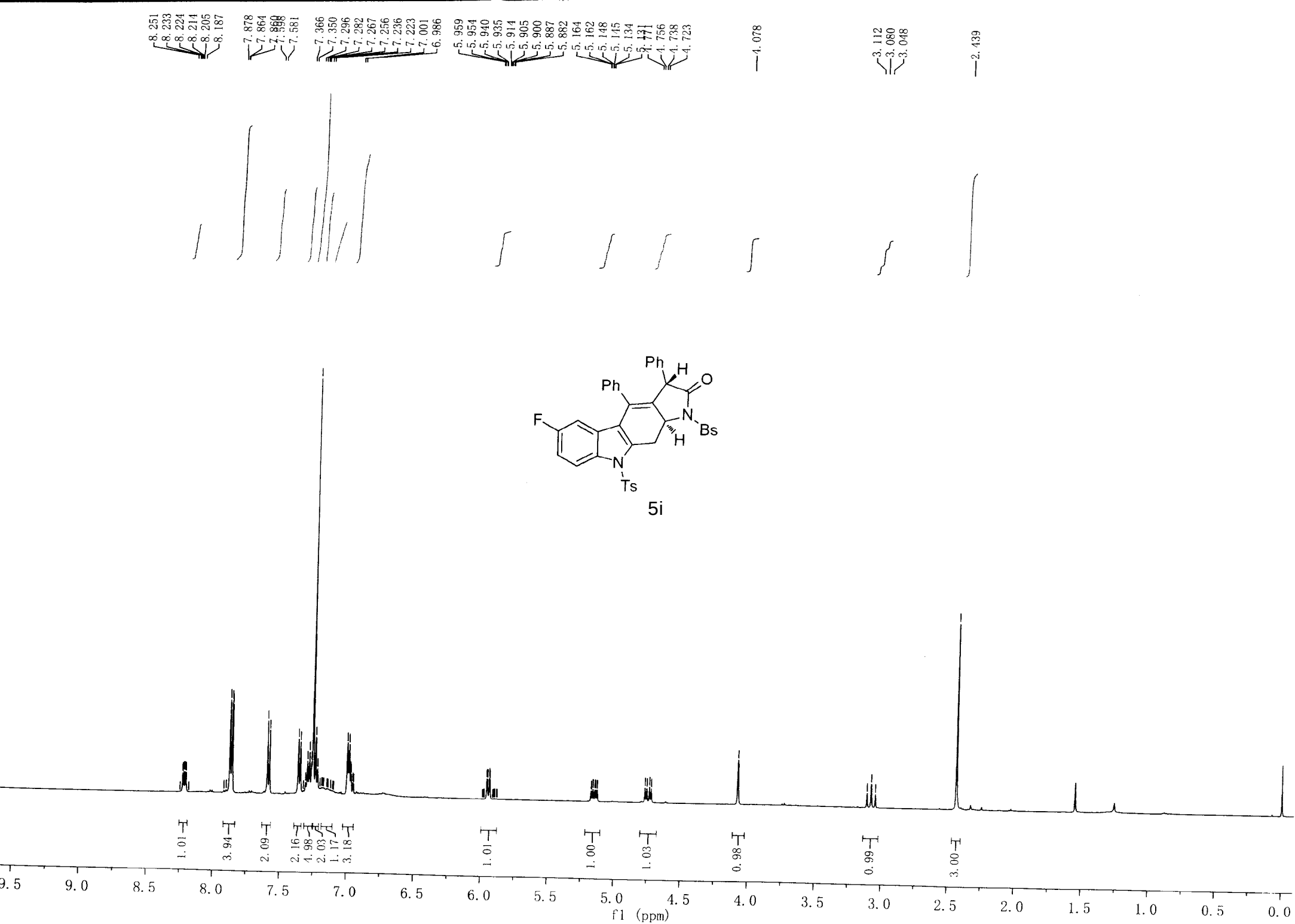


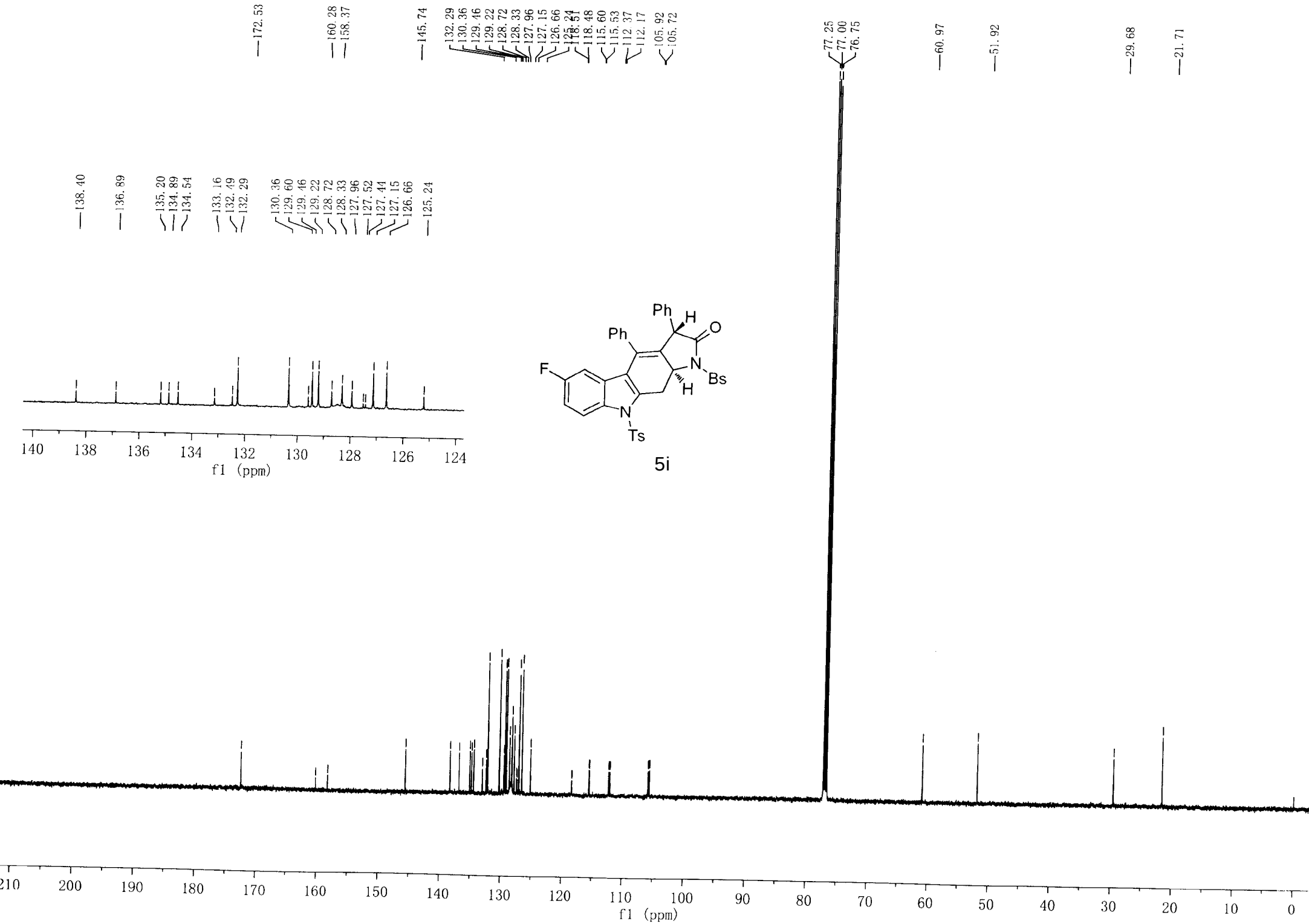
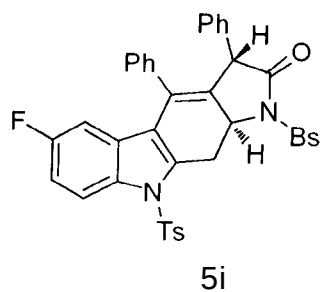
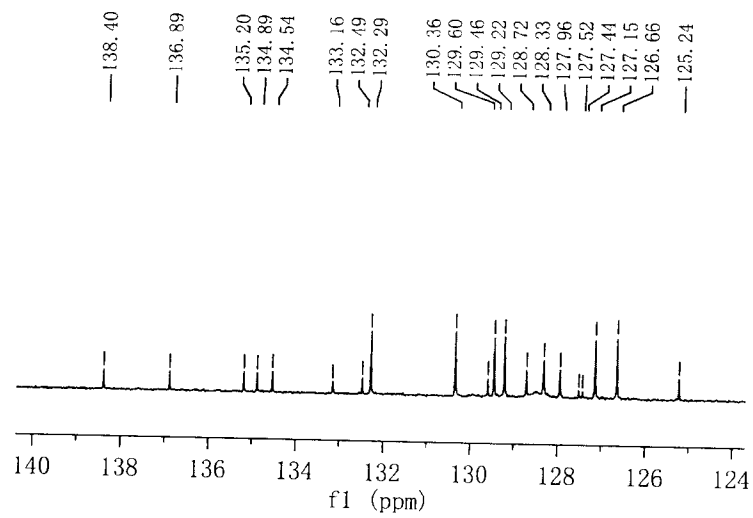












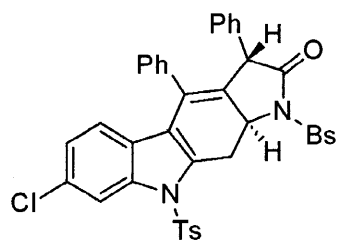
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7.579
7.391
7.374
7.288
7.281
7.267
7.258
7.251
7.236
7.002
6.988
6.930
6.219
6.202

5.178
5.175
5.163
5.161
5.147
5.144
5.133
5.130
4.747
4.733
4.714
4.700

4.075

3.101
3.070
3.038

2.451



5j

0.89
1.96
1.85
1.94
2.30
6.35
2.05
2.11
1.17

1.04

0.99

1.04

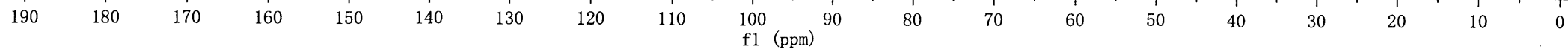
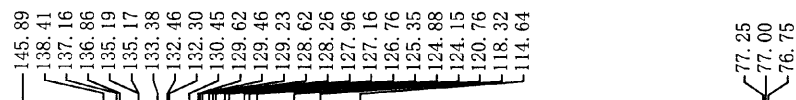
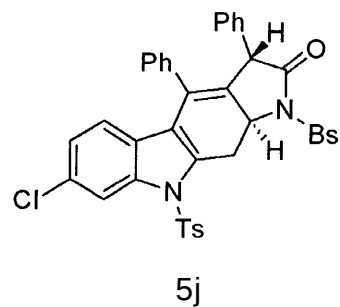
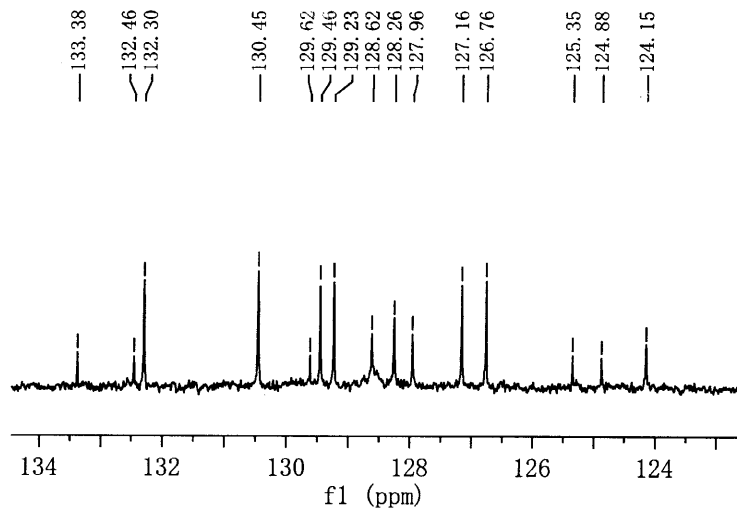
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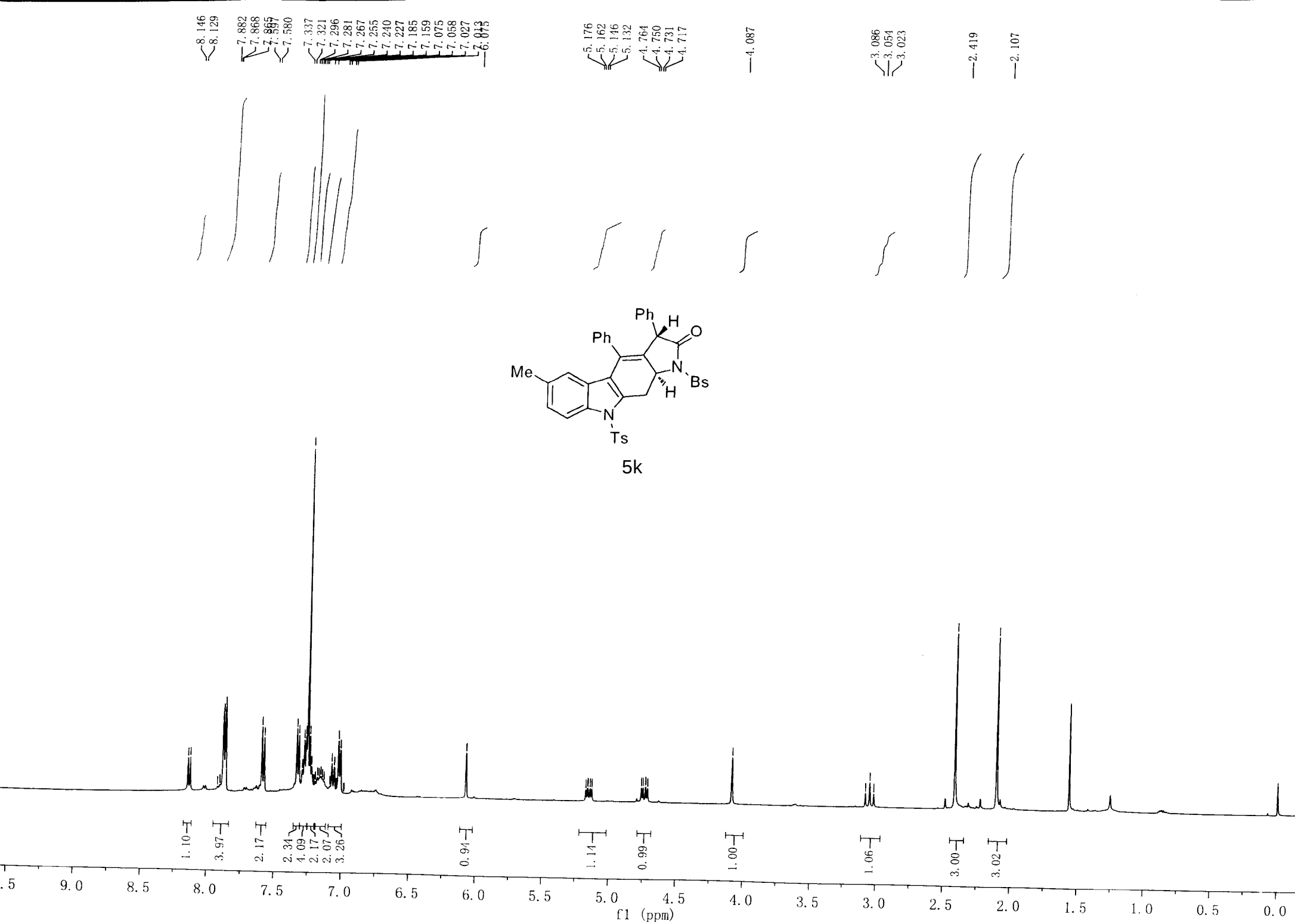
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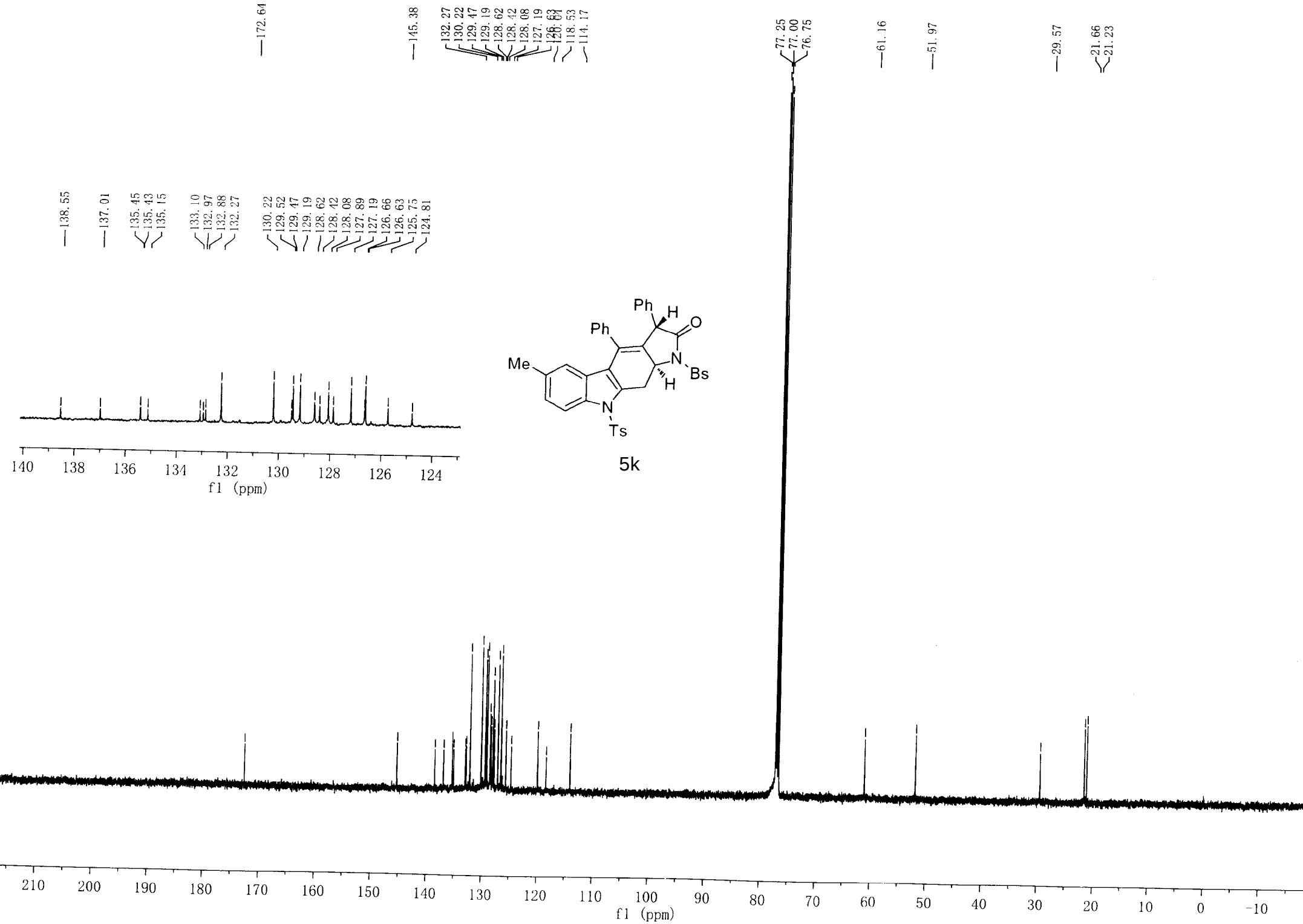
3.00

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

f1 (ppm)







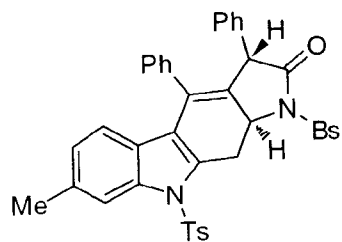
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7.854
7.574
7.351
7.335
7.275
7.272
7.262
7.258
7.252
7.237
7.022
7.008
6.781
6.262
6.186

5.186
5.184
5.172
5.169
5.156
5.153
5.142
5.139
4.748
4.734
4.715
4.701

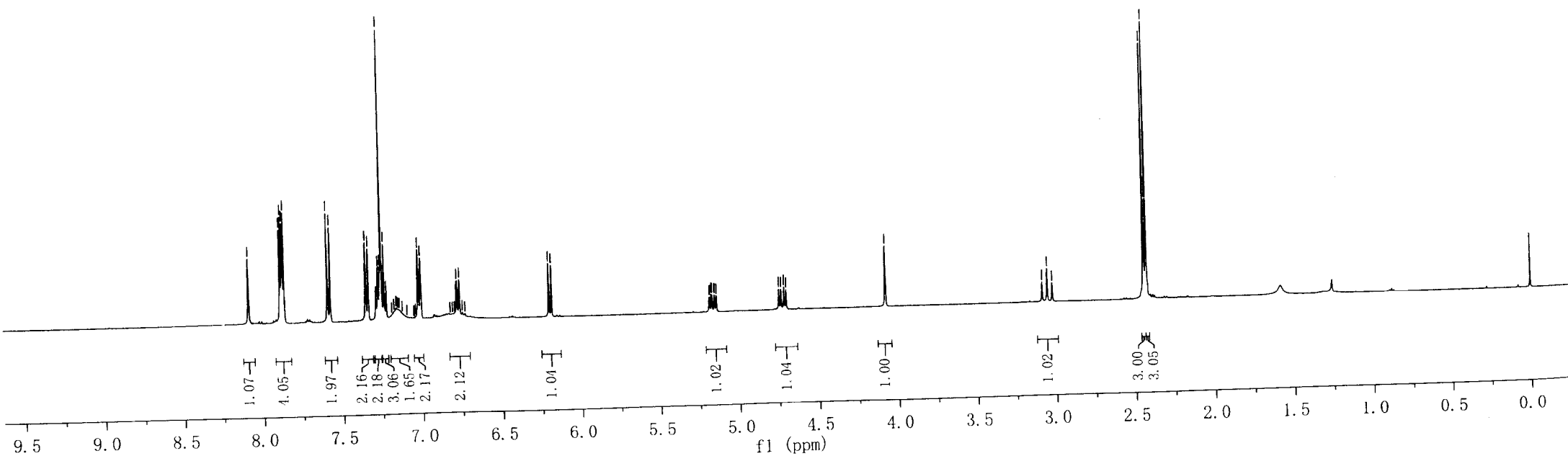
4.079

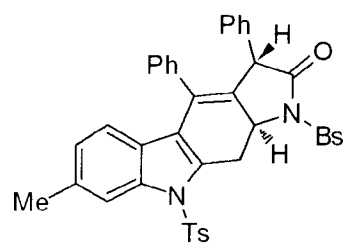
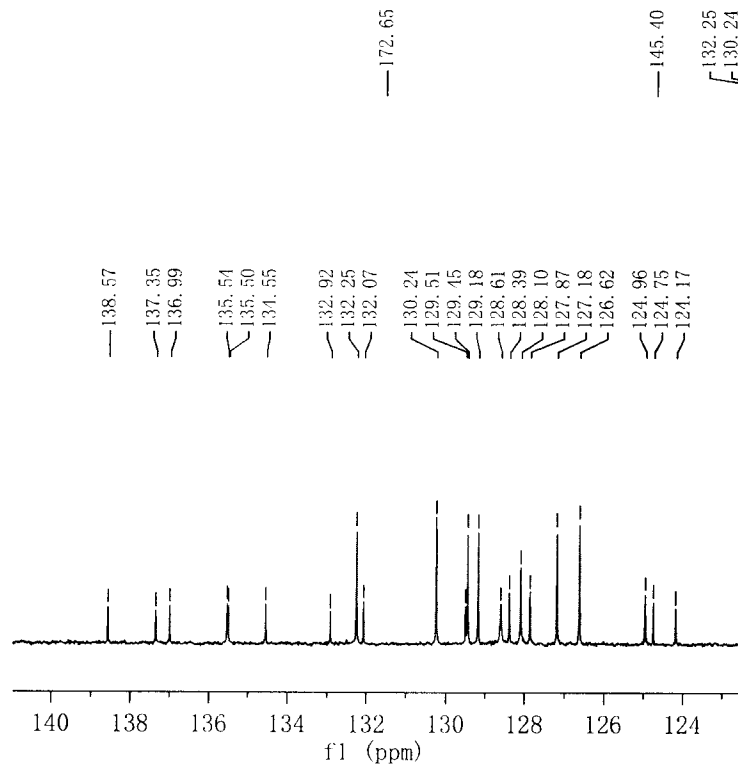
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3.054
3.022

2.443
2.428

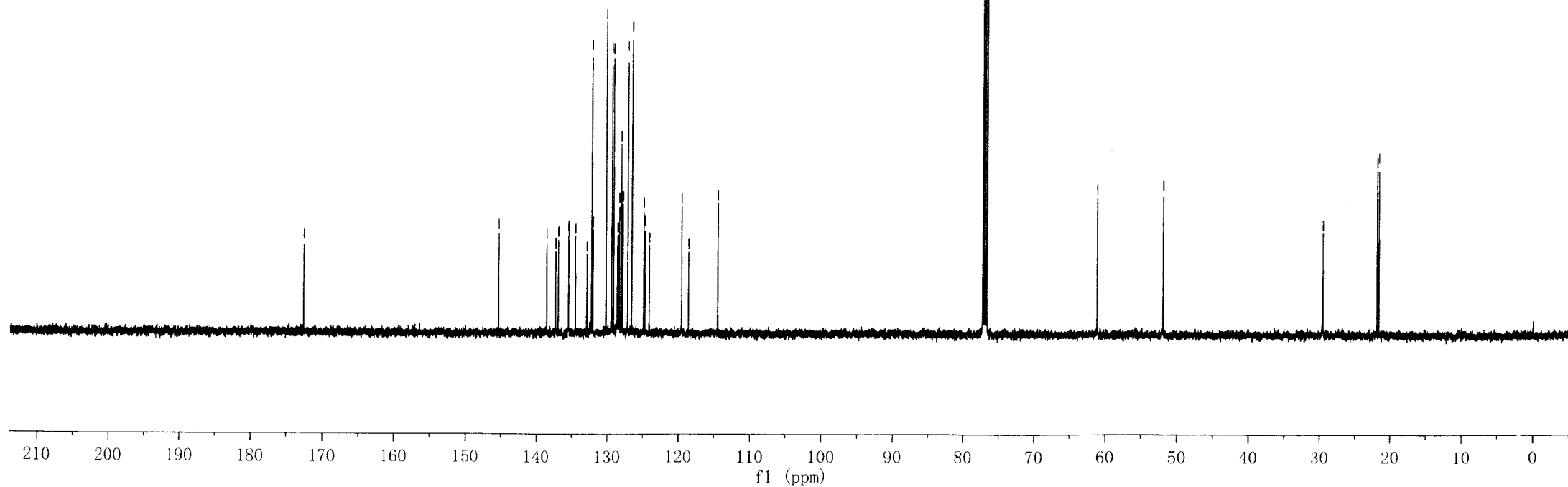
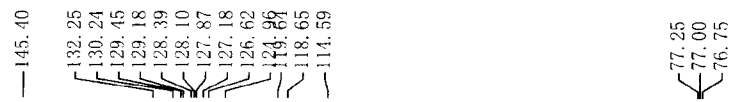


5l





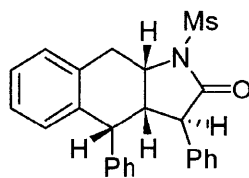
5l



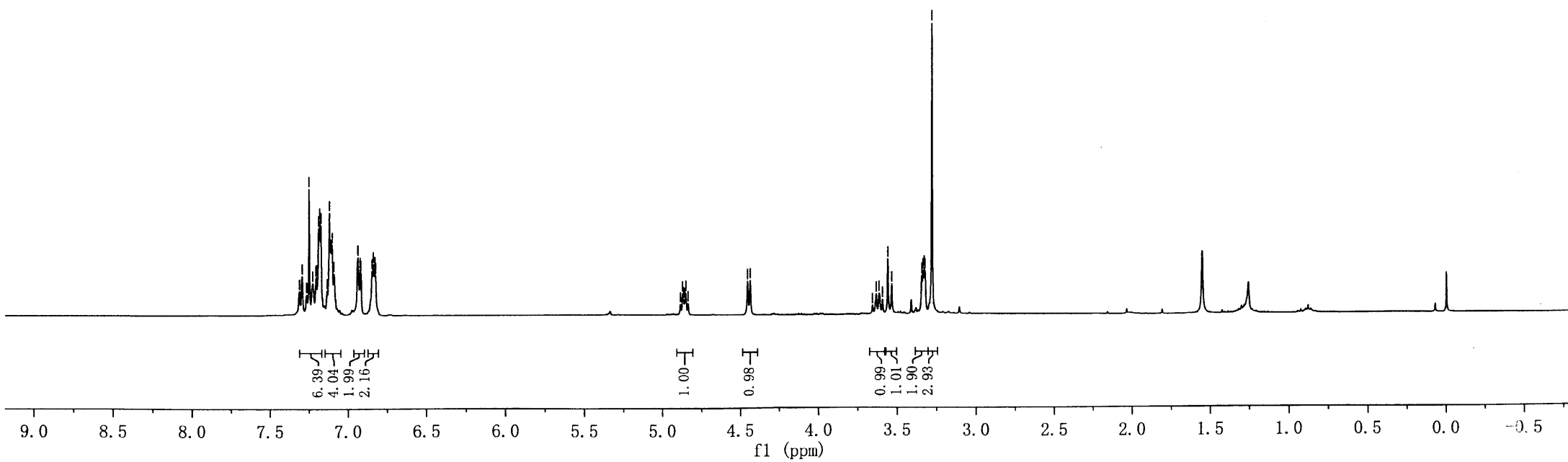
7.313
7.295
7.267
7.251
7.227
7.207
7.204
7.189
7.181
7.174
7.134
7.120
7.111
7.107
7.102
7.092
6.938
6.923
6.919
6.849
6.840
6.831
6.826

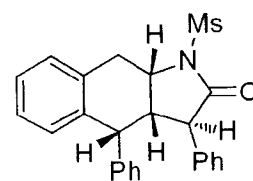
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4.871
4.864
4.856
4.850
4.835
4.455
4.438

3.656
3.633
3.615
3.593
3.560
3.536
3.346
3.338
3.330
3.325
3.281



2da





2da

—174.24

139.14
138.29
137.30
134.01
129.85
129.05
128.61
128.33
128.12
127.60
127.45
127.19
127.04

77.32
77.00
76.68

—57.94

51.32
46.90
42.97
41.90

—34.14

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (ppm)

