Supporting Information

Control Over Organometallic Intermediate Enables Cp*Co(III) Catalyzed Switchable Cyclization to Quinolines and Indoles

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General information

Unless otherwise noted, all reactions were carried out under an atmosphere of argon in oven-dried glassware cooled down under vacuum. Reaction temperatures are reported as the temperature of the heat transfer medium surrounding the vessel unless otherwise stated. Anhydrous 1,2-dichloroethane (DCE) was purchased from ROTH and stored over molecular sieves under argon. Commercially available chemicals were obtained from Acros Organics, Aldrich Chemical Co., Alfa Aesar, ABCR and TCI Europe and used as received unless otherwise stated. Acetanilide derivatives,[1] *N*-arylureas[2] and diphenylacetylene compounds[3] were prepared following literature procedures. Analytical thin layer chromatography was performed on Polygram SIL G/UV254 plates. TLC plates were visualized by exposure to short wave ultraviolet light (254 nm, 366 nm). Flash chromatography was performed on Merck silica gel (40-63 mesh) by standard techniques using appropriate mixtures of *n*-pentane, ethyl acetate. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker AV 300 or AV 400, Varian 500 MHz INOVA or Varian Unity plus 600 in solvents as indicated. Chemical shifts (δ) for ^{1}H and ^{13}C NMR spectra are given in ppm relative to TMS. The residual solvent signals were used as references for ^{1}H and ^{13}C NMR spectra and the chemical shifts converted to the TMS scale (TMS: δH = 0.00 ppm, and $CDCl_3$: δH = 7.26 ppm, δC = 77.16 ppm; CD_2Cl_2: δC = 54.00 ppm;).

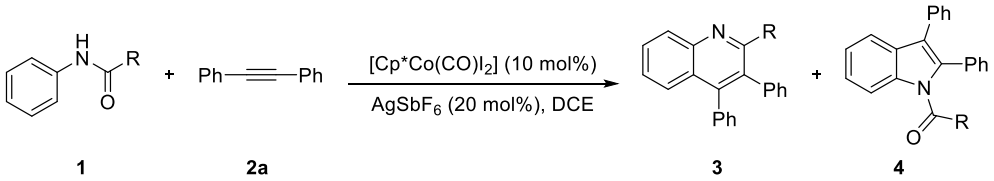
GC were recorded on an Agilent Technologies 7890A GC-system with an Agilent 5975C VL MSD or an Agilent 5975 inert Mass Selective Detector (EI) and a HP-5MS column (0.25 mm × 30 m, film: 0.25 µm). The methods used start with the injection temperature T0. After holding this temperature for 3 min, the column is heated to temperature T1 (ramp) and this temperature is held for an additional time t (method 50_40: T0 = 50 °C, T1 = 290 °C, ramp = 40 °C/min, t = 10 min).

Exact ESI mass spectra were recorded on a Bruker Daltonics MicroTof. Mass Calibration was carried out directly before the measurement of the sample using clusters of sodium formate. Infrared spectra were recorded neat on a Shimadzu FTIR-8400S. The wave numbers (υ) of recorded IR-signals are quoted in cm^{-1}.

Experimental section

1) Optimization of the reaction conditions.

Table S1. Optimization of the reaction conditions.[a]



1 **2a** **3** **4**

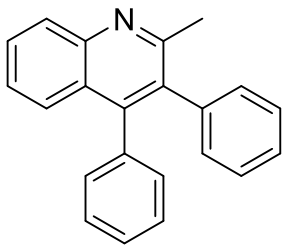
Entry	Amide: R (**1**)	Temp. / ºC	Additive	Yield of **3** (%)	Yield of **4** (%)
1	Me- (**1a**)	130	KOAc (10%)	18 (**3a**)	8 (**4a**)
2	Me- (**1a**)	130	NaOAc (10%)	13 (**3a**)	8 (**4a**)
3	Me- (**1a**)	130	$Fe(OAc)_2$ (10%)	25 (**3a**)	10 (**4a**)
4	Me- (**1a**)	130	$Fe(OAc)_2$ (10%), BF_3•OEt_2 (80%)	72 (**3a**)	9 (**4a**)
5	**Me- (1a)**	**135**	**$Fe(OAc)_2$ (10%), BF_3•OEt_2 (80%)**	**76 (74)** (**3a**)	**10** (**4a**)
6	Me- (**1a**)	120	$Fe(OAc)_2$ (10%), BF_3•OEt_2 (80%)	68 (**3a**)	7 (**4a**)
7[b]	Me- (**1a**)	120	$Fe(OAc)_2$ (10%), Ag_2O (1.0 equiv.)	(38) (**3a**)	(41) (**4a**)
8[b]	MeO- (**1b**)	120	$Fe(OAc)_2$ (10%), Ag_2O (1.0 equiv.)	complex mixture	
9[b]	**Me_2N- (1c)**	**120**	**$Fe(OAc)_2$ (10%), Ag_2O (1.0 equiv.)**	**0**	**(85)** (**4c**)
10[b,c]	Me_2N- (**1c**)	120	$Fe(OAc)_2$ (10%), Ag_2O (1.0 equiv.)	0	0
11[c]	Me- (**1a**)	130	$Fe(OAc)_2$ (10%), BF_3•OEt_2 (80%)	0 (**3a**)	0 (**4a**)

[a] Unless otherwise specified, all reactions were carried out using **1a** (0.2 mmol), **2a** (0.8 mmol), [Cp*Co(CO)I_2] (10 mol%), $AgSbF_6$ (20 mol%) in DCE (1.0 mL) for 12 h. Yields were determined by GC-FID using mesitylene as internal standard, isolated yield in parenthesis. [b] **2a** (0.4 mmol) was employed. [c] No [Cp*Co(CO)I_2].

2) Procedure and analytical data of compounds 3a-3o.

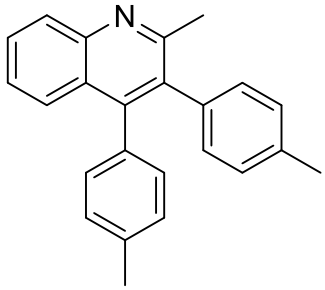
General procedure: In a 10 mL dry Schlenk tube with a stirring bar, acetanilide (**1**) (0.20 mmol), internal alkyne (**2**) (0.80 mmol) and [Cp*Co(CO)I_2] (10 mol%, 9.5 mg) were added under air. Then the tube was transferred into the glove box. $AgSbF_6$ (20 mol%, 13.7 mg), $Fe(OAc)_2$ (10 mol%, 3.5 mg) were added. After moving out, 1,2-dichloroethane (DCE) (1 mL) was added followed by BF_3·OEt_2 (0.16 mmol, 20.2 µL) under argon atmosphere. The tube was sealed and the mixture was stirred at 135 °C for 12 h. The crude reaction was diluted with dichloromethane, the volatiles were removed and the analytically pure product was obtained by flash chromatography (silica; gradient of pentane/EtOAc).

2-Methyl-3,4-diphenylquinoline (3a)[4]



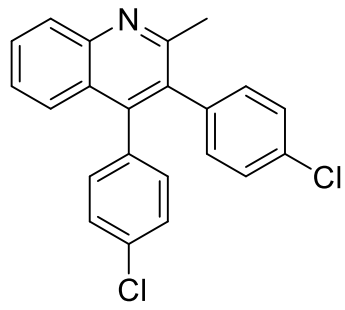
Following the general procedure, product **3a** was isolated in 74% yield. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.4 Hz, 1H), 7.61 (ddd, *J* = 8.4, 6.8, 1.4 Hz, 1H), 7.48 – 7.38 (m, 1H), 7.36 – 7.25 (m, 1H), 7.22 – 7.05 (m, 6H), 7.04 – 6.91 (m, 4H), 2.47 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 157.96, 147.05, 146.83, 138.71, 136.86, 134.20, 130.21, 130.15, 129.30, 128.65, 128.04, 127.82, 127.35, 126.96, 126.74, 126.42, 126.02, 25.52.

2-Methyl-3,4-di-*p*-tolylquinoline (3b)



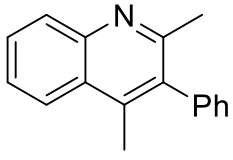
Following the general procedure, product **3b** was isolated in 67% yield. **^{1}H NMR (300 MHz, $CDCl_3$)** δ = 8.15 (d, *J* = 8.4, 1H), 7.68 (ddd, *J* = 8.4, 6.8, 1.5, 1H), 7.51 (dd, *J* = 8.4, 1.5, 1H), 7.38 (ddd, *J* = 8.2, 6.8, 1.1, 1H), 7.05 (t, *J* = 7.9, 4H), 7.00 – 6.90 (m, 4H), 2.55 (s, 3H), 2.32 (s, 3H), 2.30 (s, 3H); **^{13}C NMR (75 MHz, $CDCl_3$)** δ 158.17, 147.30, 146.53, 136.93, 136.46, 135.57, 134.30, 133.79, 130.06, 129.96, 129.30, 128.79, 128.55, 128.26, 126.83, 126.72, 125.97, 25.35, 21.38, 21.34; **HRMS**: m/z (ESI) calcd for $C_{22}H_{21}NH$ $[M+H]^+$ 324.1752, found 324.1750. **FT-IR** u_{max} (neat/cm^{-1}) 3047, 3024, 2920, 1558, 1516, 1377, 764.

3,4-Bis(4-chlorophenyl)-2-methylquinoline (3c)



Following the general procedure, product **3c** was isolated in 56% yield. **^{1}H NMR (400 MHz, $CDCl_3$)** δ = 8.15 (d, *J* = 8.4, 1H), 7.72 (ddd, *J* = 8.4, 5.9, 2.4, 1H), 7.49 – 7.39 (m, 2H), 7.31 – 7.21 (m, 4H), 7.05 – 6.96 (m, 4H), 2.54 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 157.59, 147.43, 136.85, 135.02, 133.81, 133.38, 133.04, 131.45, 131.42, 129.79, 128.74, 128.64, 128.44, 126.49, 126.39, 126.10, 25.38; **HRMS**: m/z (ESI) calcd for $C_{22}H_{15}NCl_2H$ $[M+H]^+$ 364.0654, found 364.0658. **FT-IR** u_{max} (neat/cm^{-1}) 3063, 3032, 1948, 1635, 1593, 1489, 1381, 1087, 1014, 806, 763, 740.

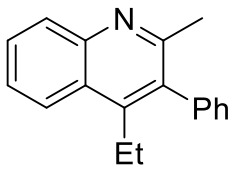
2,4-Dimethyl-3-phenylquinoline (3d)[4]



Following the general procedure, product **3d** was isolated in 66% yield. **^{1}H**

NMR (300 MHz, $CDCl_3$) δ 8.00 (dd, *J* = 8.4, 0.6 Hz, 1H), 7.92 (dd, *J* = 8.4, 0.9 Hz, 1H), 7.62 (ddd, *J* = 8.4, 6.8, 1.4 Hz, 1H), 7.52 – 7.29 (m, 4H), 7.17 – 7.08 (m, 2H), 2.36 (s, 3H), 2.32 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 157.71, 146.57, 141.55, 139.57, 135.07, 129.44, 129.16, 129.08, 128.84, 127.54, 126.87, 125.95, 124.24, 25.48, 16.08. **HRMS**: m/z (ESI) calcd for $C_{17}H_{15}NNa$ $[M+Na]^+$ 256.1102, found 256.1097. **FT-IR** u_{max} (neat/cm^{-1}) 3059, 2997, 1975, 1601, 1581, 1497, 1373, 980, 868, 752, 706.

4-Ethyl-2-methyl-3-phenylquinoline (3e)



Following the general procedure, product **3e** was isolated in 72% yield. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.00 (dd, *J* = 8.4, 0.9 Hz, 1H), 7.95 (dd, *J* = 8.4, 0.9 Hz, 1H), 7.61 (ddd, *J* = 8.4, 6.9, 1.5 Hz, 1H), 7.48 – 7.34 (m, 4H), 7.17 – 7.12 (m, 2H), 2.81 – 2.69 (q, *J* = 7.5 Hz, 2H), 2.32 (s, 3H), 1.07 (t, *J* = 7.7 Hz, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 157.94, 147.25, 139.40, 134.40, 129.45, 129.29, 128.95, 128.81, 127.54, 125.92, 125.69, 124.21, 25.52, 22.71, 15.23. **HRMS**: m/z (ESI) calcd for $C_{18}H_{17}NNa$ $[M+ Na]^+$ 270.1259, found 270.1253. **FT-IR** u_{max} (neat/cm^{-1}) 2974, 2931, 1578, 1559, 1508, 1497, 1366, 1065, 1026, 772, 756, 706.

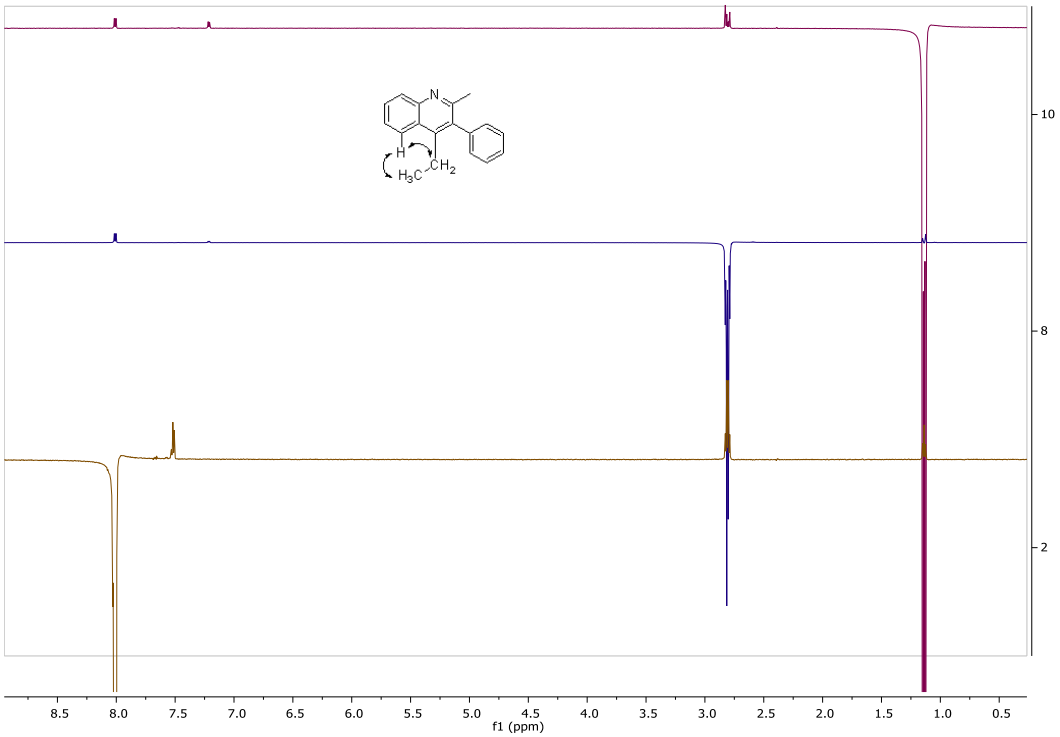
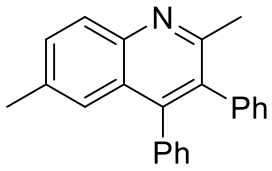


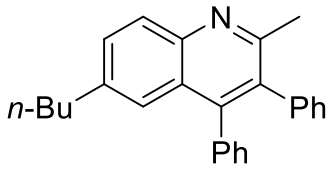
Figure S1. Determination of structure **3e** was achieved with TOCSY and NOE-Experiments.

2,6-Dimethyl-3,4-diphenylquinoline (3f)



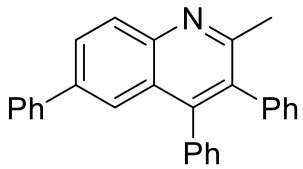
Following the general procedure, product **3f** was isolated in 73% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.4 Hz, 1H), 7.45 (dd, *J* = 8.8, 1.6 Hz, 1H), 7.25 – 7.06 (m, 7H), 7.04 – 6.86 (m, 4H), 2.45 (s, 1H), 2.32 (s, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 156.87, 146.30, 145.60, 138.88, 137.05, 135.87, 134.23, 131.56, 130.24, 130.19, 128.36, 128.00, 127.81, 127.28, 126.89, 126.35, 125.50, 25.33, 21.87. **HRMS**: m/z (ESI) calcd for $C_{23}H_{19}NNa$ $[M+Na]^+$ 332.1415, found 332.1410. **FT-IR** u_{max} (neat/cm^{-1}) 3055, 3028, 1716, 1559, 1489, 1442, 1072, 1018, 826, 698.

6-Butyl-2-methyl-3,4-diphenylquinoline (3g)



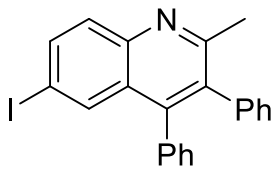
Following the general procedure, product **3g** was isolated in 78% yield. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.4 Hz, 1H), 7.47 (dd, *J* = 8.6, 2.0 Hz, 1H), 7.22 – 7.06 (m, 7H), 7.04 – 6.91 (m, 4H), 2.64 – 2.51 (t, *J* = 7.8 Hz, 2H), 2.44 (s, 3H), 1.56 – 1.41 (m, 2H), 1.31 – 1.15 (m, 2H), 0.80 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 156.90, 146.24, 145.93, 140.76, 138.98, 137.08, 134.14, 130.71, 130.26, 130.19, 128.52, 127.97, 127.77, 127.22, 126.84, 126.28, 124.98, 35.90, 33.69, 25.42, 22.45, 14.03. **HRMS**: m/z (ESI) calcd for $C_{26}H_{25}NNa$ $[M+Na]^+$ 374.1885, found 374.1879. **FT-IR** u_{max} (neat/cm^{-1}) 3055, 3028, 2920, 1948, 1559, 1489, 1010, 833, 760, 698.

2-Methyl-3,4,6-triphenylquinoline (3h)



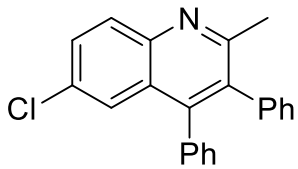
Following the general procedure, product **3h** was isolated in 73% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.4 Hz, 1H), 7.88 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.61 (d, *J* = 1.6 Hz, 1H), 7.51 – 7.42 (m, 2H), 7.32 (t, *J* = 7.4 Hz, 2H), 7.23 (tt, *J* = 7.2, 1.2 Hz, 1H), 7.20 – 7.08 (m, 6H), 7.07 – 7.02 (m, 2H), 7.01 – 6.93 (m, 2H), 2.49 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 157.96, 147.15, 146.40, 140.83, 138.82, 138.70, 136.74, 134.66, 130.25, 130.16, 129.08, 128.95, 128.08, 127.92, 127.58, 127.53, 127.48, 127.02, 126.62, 124.56, 25.47. **HRMS**: m/z (ESI) calcd for $C_{28}H_{21}NNa$ $[M+Na]^+$ 394.1572, found 394.1566. **FT-IR** u_{max} (neat/cm^{-1}) 3055, 3028, 1867, 1482, 1438, 1369, 1072, 1010, 841, 756.

6-Iodo-2-methyl-3,4-diphenylquinoline (3i)



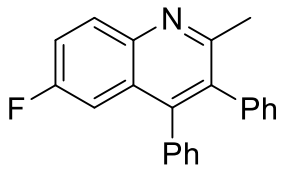
Following the general procedure, product **3i** was isolated in 71% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.85 (dd, *J* = 8.7, 2.1 Hz, 1H), 7.80 – 7.70 (m, 2H), 7.23 – 7.06 (m, 6H), 7.03 – 6.91 (m, 4H), 2.44 (s, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.78, 146.15, 145.64, 138.33, 138.00, 136.10, 135.41, 134.90, 130.58, 130.15, 130.01, 128.28, 128.11, 128.03, 127.67, 127.13, 91.65, 25.65. **HRMS**: m/z (ESI) calcd for $C_{22}H_{16}INNa$ $[M+Na]^+$ 444.0225, found 444.0220. **FT-IR** u_{max} (neat/cm^{-1}) 3059, 3012, 1566, 1474, 1366, 1072, 1007, 830.

6-Chloro-2-methyl-3,4-diphenylquinoline (3j)[5]



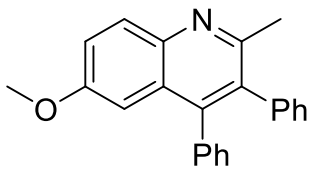
Following the general procedure, product **3j** was isolated in 76% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.97 (d, *J* = 9.0 Hz, 1H), 7.55 (dd, *J* = 8.9, 1.2 Hz, 1H), 7.39 (d, *J* = 1.1 Hz, 1H), 7.23 – 7.06 (m, 6H), 7.03 – 6.92 (m, 4H), 2.45 (s, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.43, 146.03, 145.55, 138.35, 136.19, 135.05, 131.80, 130.41, 130.14, 130.12, 130.00, 128.13, 128.05, 127.67, 127.25, 127.15, 125.52, 25.55. **HRMS**: m/z (ESI) calcd for $C_{22}H_{16}ClNNa$ $[M+Na]^+$ 352.0869, found 352.0863. **FT-IR** u_{max} (neat/cm^{-1}) 3063, 3028, 1604, 1559, 1477, 1439, 1366, 1157, 1072, 1011, 833, 764.

6-Fluoro-2-methyl-3,4-diphenylquinoline (3k)



Following the general procedure, product **3k** was isolated in 79% yield. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.05 (dd, *J* = 9.0, 5.4 Hz, 1H), 7.38 (td, *J* = 9.0, 2.7 Hz, 1H), 7.25 – 7.08 (m, 6H), 7.06 – 6.87 (m, 5H), 2.46 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 160.36 (d, ^{1}JCF = 244.7 Hz), 157.35 (d, ^{4}JCF = 2.6 Hz), 144.13, 138.43, 136.42, 134.88, 131.04 (d, ^{3}JCF = 8.9 Hz), 130.06, 130.02, 128.12, 128.04, 127.64, 127.30 (d, ^{3}JCF = 9.3 Hz), 127.14, 119.37 (d, ^{2}JCF = 25.5 Hz), 110.13 (d, ^{2}JCF = 22.9 Hz), 25.34. **^{19}F NMR** (282 MHz, $CDCl_3$) δ -113.67. **HRMS**: m/z (ESI) calcd for $C_{22}H_{16}FNNa$ $[M+Na]^+$ 336.1164, found 336.1159. **FT-IR** u_{max} (neat/cm^{-1}) 3066, 3028, 1620, 1559, 1489, 1215, 1195, 872, 733, 698.

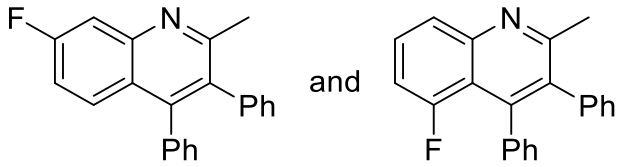
6-Methoxy-2-methyl-3,4-diphenylquinoline (3l)



Following the general procedure, $B(C_6F_5)_3$ (0.16 mmol) was used to

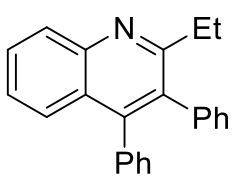
replace BF_3•OEt_2 and reaction time was prolonged to 24 h. Product **3l** was isolated in 73% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 9.2 Hz, 1H), 7.29 (dd, *J* = 9.2, 2.8 Hz, 1H), 7.23 – 7.06 (m, 6H), 7.06 – 6.91 (m, 4H), 6.69 (d, *J* = 2.4 Hz, 1H), 3.62 (s, 3H), 2.44 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 157.51, 155.23, 145.99, 142.97, 138.86, 137.07, 134.49, 130.15, 130.11, 129.98, 128.02, 127.95, 127.39, 127.34, 126.94, 121.50, 105.02, 55.48, 25.01. **HRMS**: m/z (ESI) calcd for $C_{23}H_{19}NNaO$ $[M+Na]^+$ 348.1364, found 348.1359. **FT-IR** u_{max} (neat/cm^{-1}) 3059, 3020, 1616, 1489, 1227, 1119, 1026, 833.

7-Fluoro-2-methyl-3,4-diphenylquinoline (3m) and 5-fluoro-2-methyl-3,4-diphenylquinoline (3m′)[4]



Following the general procedure, $B(C_6F_5)_3$ (0.16 mmol) was used to replace BF_3•OEt_2 and reaction time was prolonged to 24 h. Product **3m+3m′** was isolated in 43% (5:1) total yield. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.4 Hz, 1.0 H), 7.70 (d, *J* = 10.8 Hz, 0.2 H), 7.55 (td, *J* = 8.1, 5.3 Hz, 1.0 H), 7.42 (dd, *J* = 9.2, 6.2 Hz, 0.2 H), 7.21 – 7.04 (m, 8.5 H), 7.04 – 6.89 (m, 6.1 H), 2.47 (s, 0.6 H), 2.43 (d, 3.0 H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 160.46, 158.92, 158.90, 157.05, 148.53, 139.12, 139.08, 138.03, 135.92, 130.16, 130.12, 130.05, 129.10, 128.98, 128.94, 128.12, 128.00, 127.93, 127.57, 127.17, 127.08, 127.02, 126.91, 125.19, 125.13, 116.85, 116.40, 111.70, 111.40, 25.57, 25.53. **HRMS**: m/z (ESI) calcd for $C_{22}H_{16}FNNa$ $[M+Na]^+$ 336.1164, found 336.1159. **^{19}F NMR** (282 MHz, $CDCl_3$) δ -107.47, -110.83. **FT-IR** u_{max} (neat/cm^{-1}) 3059, 3028, 1624, 1559, 1230, 1072, 826, 745, 698.

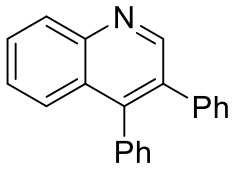
2-Ethyl-3,4-diphenylquinoline (3n)



Following the general procedure, product **3n** was isolated in 63% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 8.4 Hz, 1H), 7.61 (t, *J* = 7.0 Hz, 1H), 7.41 (d, *J* = 8.0 Hz, 1H), 7.31 (t, *J* = 7.2 Hz, 1H), 7.25 – 7.05 (m, 6H), 7.04 – 6.80 (m, 4H), 2.77 (q, *J* = 7.4 Hz, 2H), 1.16 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) ^{13}C NMR (101 MHz, $CDCl_3$) δ 162.42, 147.23, 147.18, 138.49, 137.06, 133.88, 130.42, 130.21, 129.23, 128.85, 127.86, 127.79, 127.29, 126.93, 126.74, 126.34, 126.01, 30.65, 13.92. **HRMS**: m/z (ESI) calcd for $C_{23}H_{19}NNa$ $[M+Na]^+$ 332.1415, found 332.1410. **FT-IR**

u_{max} (neat/cm^{-1}) 3055, 2974, 2931, 1559, 1481, 1439, 1397, 1053, 1026, 768, 698.

3,4-Diphenylquinoline (3o)[6]

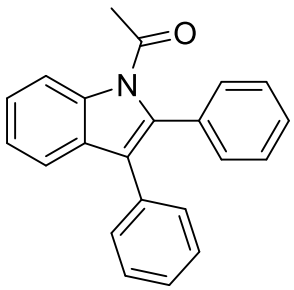


Following the general procedure, product **3o** was isolated in 45% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.93 (s, 1H), 8.13 (d, *J* = 8.4 Hz, 1H), 7.74 – 7.54 (m, 2H), 7.49 – 7.36 (m, 1H), 7.34 – 7.23 (m, 3H), 7.22 – 6.92 (m, 7H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 151.83, 147.53, 145.79, 138.20, 136.38, 133.29, 130.65, 130.29, 129.53, 129.32, 128.30, 128.21, 127.89, 127.39, 127.21, 127.06, 126.74.

1.2) Procedure and analytical data of compounds 4a-4o.

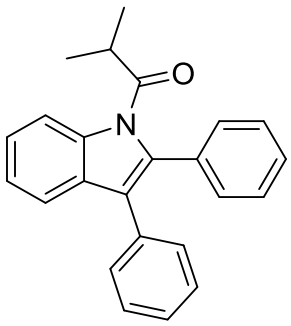
General procedure: In a 10 mL dry Schlenk tube with a stirring bar, acetanilide or *N*-arylurea (**1c**) (0.20 mmol), internal alkyne (**2**) (0.40 mmol), silver oxide (0.20 mmol, 46.3 mg) and [Cp*Co(CO)I_2] (10 mol%, 9.5 mg) were added under air. Then the tube was transferred into the glove box. $AgSbF_6$ (20 mol%, 13.7 mg), $Fe(OAc)_2$ (10 mol%, 3.5 mg) were added. After moving out, 1,2-dichloroethane (DCE) (1 mL) was added under argon atmosphere. The tube was sealed and the mixture was stirred at 120 °C for 12 h. The crude reaction was diluted with dichloromethane, the volatiles were removed and the analytically pure product was obtained by flash chromatography (silica; gradient of pentane/EtOAc).

1-(2,3-Diphenyl-1H-indol-1-yl)ethan-1-one (4a)[7]



Following the general procedure, product **4a** was isolated in 41% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.39 (d, *J* = 8.0 Hz, 1H), 7.48 (d, *J* = 7.6 Hz, 1H), 7.37 – 7.31 (m, 1H), 7.30 – 7.10 (m, 11H), 1.93 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 171.72, 136.92, 135.14, 133.20, 133.09, 130.92, 130.18, 129.40, 128.76, 128.75, 128.37, 127.06, 125.65, 123.92, 123.50, 119.70, 116.34, 28.09.

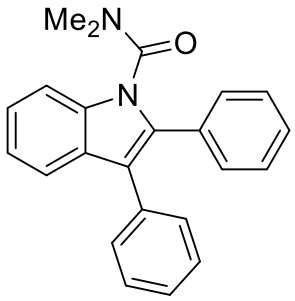
1-(2,3-Diphenyl-1H-indol-1-yl)ethan-1-one (4b)



Following the general procedure, product **4b** was isolated in 53% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.11 (d, *J* = 8.4 Hz, 1H), 7.52 – 7.43 (m, 1H), 7.27 (ddd, *J* = 8.2, 7.2, 1.4 Hz, 1H), 7.25 – 7.09 (m,

11H), 2.42 (hept, *J* = 6.8 Hz, 1H), 0.87 (d, *J* = 6.8 Hz, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 180.17, 137.04, 134.62, 133.42, 132.90, 130.23, 130.20, 129.15, 128.74, 128.46, 128.37, 126.97, 125.25, 123.38, 122.41, 119.65, 114.84, 37.26, 19.09. **HRMS**: m/z (ESI) calcd for $C_{24}H_{21}NNaO$ $[M+Na]^+$ 362.1521, found 362.1526. **FT-IR** u_{max} (neat/cm^{-1}) 3051, 3032, 2978, 2874, 1709, 1451, 1296, 1141, 1088, 750.

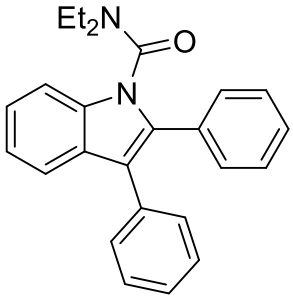
***N*,*N*-dimethyl-2,3-diphenyl-1*H*-indole-1-carboxamide (4c)[2a]**



Following the general procedure, product **4c** was isolated in 85% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 8.0 Hz, 1H), 7.44 (d, *J* = 8.0 Hz, 1H), 7.36 – 7.16 (m, 11H), 7.16 – 7.09 (m, 1H), 2.90 (s, 1H), 2.46 (s, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 154.10, 135.84, 135.01, 134.19, 131.45, 130.29, 129.76, 128.54, 128.43, 128.38, 128.16, 126.63, 123.86, 121.81, 119.99, 117.90, 111.57, 38.03, 36.62.

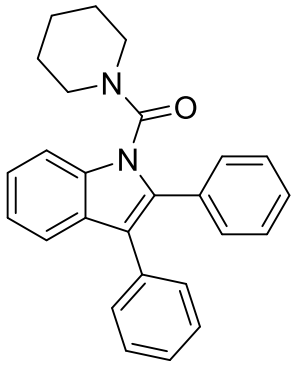
***N*,*N*-diethyl-2,3-diphenyl-1*H*-indole-1-carboxamide (4d)**

Following the general procedure, product **4d** was isolated in 84% yield. **^{1}H NMR** (300 MHz,



$CDCl_3$) δ 7.62 (d, *J* = 7.8 Hz, 1H), 7.39 (d, *J* = 8.4 Hz, 1H), 7.35 – 7.08 (m, 12H), 3.94 – 2.36 (m, 4H), 1.13 – 0.37 (br, 6H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 153.34, 135.99, 134.81, 134.30, 131.28, 130.25, 130.19, 128.49, 128.41, 128.19, 127.99, 126.48, 123.70, 122.62, 121.57, 119.97, 117.37, 111.88, 111.08, 42.75, 40.82, 13.85, 12.31. **HRMS**: m/z (ESI) calcd for $C_{25}H_{24}N_2NaO$ $[M+Na]^+$ 391.1786, found 391.1781. **FT-IR** u_{max} (neat/cm^{-1}) 3059, 2985, 2974, 1678, 1446, 1423, 1315, 1265, 1238, 1150, 760.

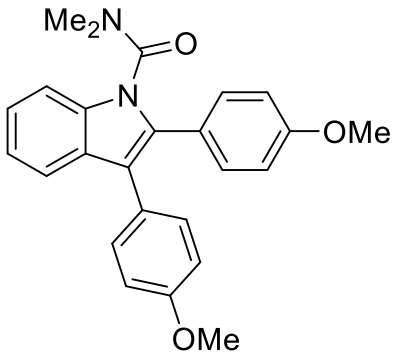
(2,3-Diphenyl-1*H*-indol-1-yl)(piperidin-1-yl)methanone (4e)



Following the general procedure, product **4e** was isolated in 66% yield. **^{1}H NMR** (600 MHz, cdcl$_3$) δ 7.59 (d, *J* = 7.8 Hz, 1H), 7.45 (d, *J* = 7.8 Hz, 1H), 7.33 – 7.14 (m, 11H), 7.12 (t, *J* = 7.5 Hz, 1H), 3.65 – 2.68 (br, 4H), 1.58 – 0.80 (m, 6H). **^{13}C NMR** (151 MHz, cdcl$_3$) δ 152.75, 136.07, 134.95, 134.27, 131.34, 130.31, 130.06, 128.51,

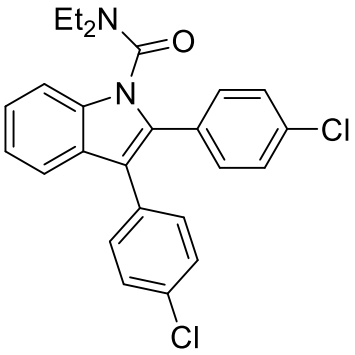
128.37, 128.25, 128.12, 126.56, 123.76, 121.71, 119.92, 117.65, 111.47, 47.47, 45.44, 25.69, 24.09. **HRMS**: m/z (ESI) calcd for $C_{26}H_{24}N_2NaO$ $[M+Na]^+$ 403.1786, found 403.1781. **FT-IR** u_{max} (neat/cm^{-1}) 3066, 2940, 2855, 1670, 1427, 1215, 1026, 752, 698.

2,3-Bis(4-methoxyphenyl)-*N*,*N*-dimethyl-1*H*-indole-1-carboxamide (4f)



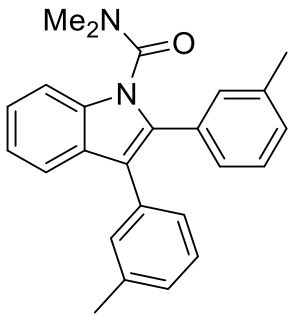
Following the general procedure, product **4f** was isolated in 67% yield. **^{1}H NMR (400 MHz, $CDCl_3$)** δ = 7.56 (dt, *J*=7.9, 1.1, 1H), 7.41 (dt, *J*=8.2, 0.9, 1H), 7.25 – 7.15 (m, 5H), 7.12 (ddd, *J*=8.1, 7.1, 1.1, 1H), 6.85 – 6.79 (m, 2H), 6.79 – 6.74 (m, 2H), 3.75 (s, 3H), 3.74 (s, 3H), 2.92 (bs, 3H), 2.46 (bs, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ δ 159.38, 158.32, 154.30, 135.66, 134.61, 131.30, 130.99, 128.64, 126.64, 123.93, 123.50, 121.63, 119.79, 116.83, 114.06, 113.95, 111.44, 55.35, 55.33, 38.05, 36.61; **HRMS**: m/z (ESI) calcd for $C_{25}H_{24}N_2O_3Na$ $[M+Na]^+$ 423.1693, found 423.1679. **FT-IR** u_{max} (neat/cm^{-1}) 3032, 2955, 2835, 1682, 1246, 1153, 1022, 837.

2,3-Bis(4-chlorophenyl)-*N*,*N*-diethyl-1*H*-indole-1-carboxamide (4g)



Following the general procedure, product **4g** was isolated in 77% yield. **^{1}H NMR (400 MHz, CD_2Cl_2)** δ = 7.64 (dt, *J*=8.0, 1.0, 1H), 7.42 (dt, *J*=8.2, 1.0, 1H), 7.36 – 7.26 (m, 9H), 7.23 (ddd, *J*=8.1, 7.0, 1.1, 1H), 3.46 (bs, 2H), 2.96 (bs, 2H), 0.99 (bs, 6H); **^{13}C NMR (101 MHz, CD_2Cl_2)** δ 153.14, 136.47, 134.84, 134.41, 133.15, 132.88, 132.00, 131.97, 130.16, 129.27, 129.25, 128.07, 124.46, 122.28, 120.11, 117.08, 111.55 (CH_3 and CH_2 peaks from diethylamide group are not visible); **HRMS**: m/z (ESI) calcd for $C_{25}H_{22}Cl_2N_2ONa$ $[M+Na]^+$ 459.1007, found 459.0994. **FT-IR** umax (neat/cm-1) 3048, 2982, 1686, 1455, 1427, 1277, 1088, 1011, 748.

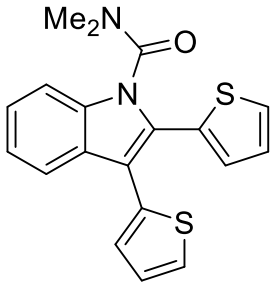
***N*, *N*-Diethyl-2,3-di-*m*-tolyl-1*H*-indole-1-carboxamide (4h)**



Following the general procedure, product **4h** was isolated in 56% yield. **^{1}H NMR (400 MHz, CDCl3)** δ = 7.59 (dt, J=7.9, 1.0, 1H), 7.44 (dt, J=8.3, 0.9, 0.9, 1H), 7.22 (ddd, J=8.3, 7.0, 1.2, 1H), 7.17 – 6.97

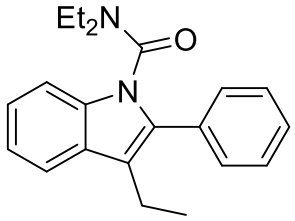
(m, 9H), 3.00 – 2.80 (m, 3H), 2.51 – 2.40 (m, 3H), 2.24 (s, 3H), 2.20 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 154.20, 137.91, 137.88, 135.80, 135.09, 134.11, 131.37, 130.84, 130.17, 128.87, 128.47, 128.33, 128.19, 127.39, 127.34, 126.91, 123.70, 121.68, 120.02, 117.84, 111.52, 38.11, 36.53, 21.61, 21.53; **HRMS: m/z (ESI)** calcd for $C_{25}H_{24}N_2ONa$ $[M+Na]^+$ 391.1782, found 391.1781. FT-IR u_{max} (neat/cm^{-1}) 3048, 3023, 2924, 1686, 1604, 1454, 1393, 1323, 1150, 795, 746, 691.

***N*, *N*-Dimethyl-2,3-di(thiophen-2-yl)-1*H*-indole-1-carboxamide (4i)**



Following the general procedure, product **4i** was isolated in 80% yield. **^{1}H NMR (400 MHz, $CDCl_3$)** δ = 7.67 (dt, *J*=7.9, 1.0, 1H), 7.33 – 7.28 (m, 2H), 7.27 – 7.21 (m, 2H), 7.18 – 7.09 (m, 2H), 7.05 – 6.94 (m, 3H), 3.03 (s, 3H), 2.65 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 153.46, 135.47, 134.77, 131.48, 129.19, 129.11, 128.29, 127.78, 127.41, 127.33, 127.23, 125.59, 124.42, 122.10, 120.36, 112.55, 111.11, 38.24, 36.75; **HRMS**: m/z (ESI) calcd for $C_{19}H_{16}N_2OS_2Na$ $[M+Na]^+$ 375.0596, found 375.0593. **FT-IR** u_{max} (neat/cm^{-1}) 3002, 1682, 1389, 1308, 1150, 729.

***N*, *N*, 3-triethyl-2-phenyl-1*H*-indole-1-carboxamide (4j)**



Following the general procedure, product **4j** was isolated in 75% yield. **^{1}H NMR (400 MHz, $CDCl_3$)** δ = 7.65 (dt, *J*=7.7, 1.1, 1H), 7.51 – 7.46 (m, 2H), 7.46 – 7.41 (m, 3H), 7.40 – 7.34 (m, 1H), 7.30 – 7.24 (m, 1H), 7.20 (ddd, *J*=8.1, 7.1, 1.1, 1H), 3.64 – 2.87 (bs, 4H), 2.81 (q, *J*=7.5, 2H), 1.29 (t, *J*=7.5, 3H), 0.91 (bs, 6H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 153.77, 136.17, 134.59, 131.94, 129.62, 128.50, 128.46, 128.04, 123.33, 120.82, 119.43, 118.34, 111.26, 41.88, 17.84, 15.68, 13.19 (one CH_3 and one CH_2 peak from diethylamide group are not visible); **HRMS**: m/z (ESI) calcd for $C_{21}H_{24}N_2ONa$ $[M+Na]^+$ 343.1781, found 343.1800. **FT-IR** u_{max} (neat/cm^{-1}) 3055, 2970, 2932, 1678, 1454, 1420, 1316, 741, 698.

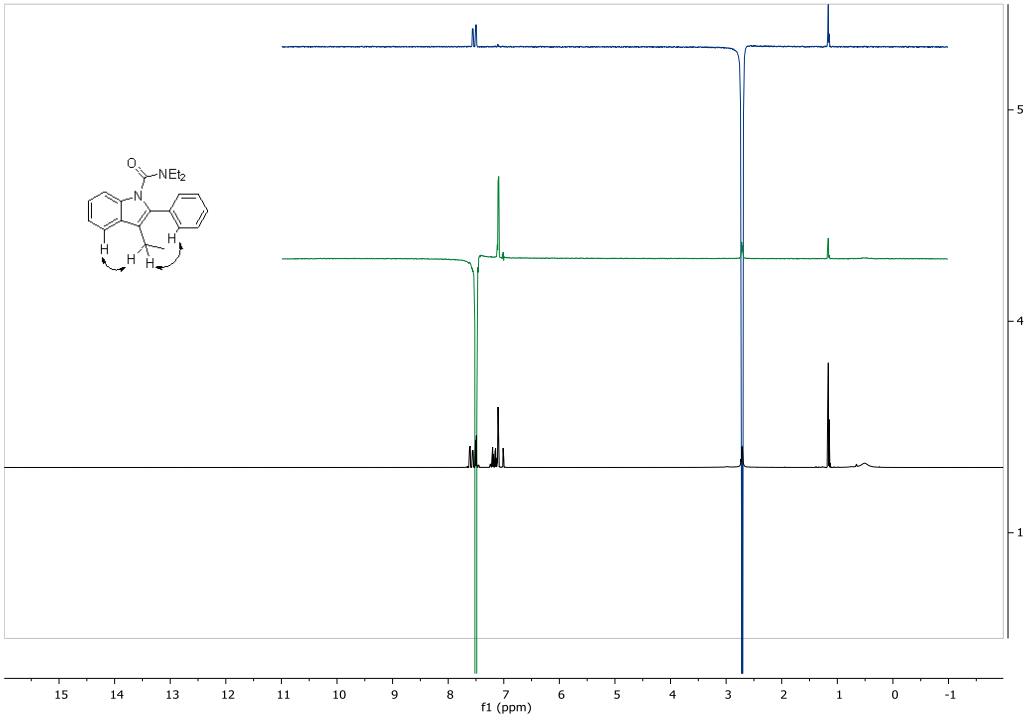
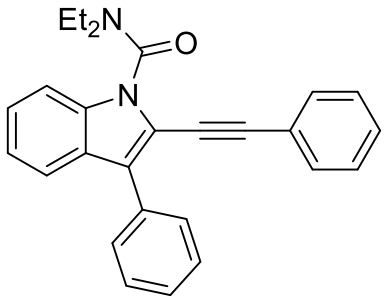


Figure S2. Determination of structure **4j** was achieved with TOCSY and NOE-Experiments.

***N*,*N*-diethyl-3-phenyl-2-(phenylethynyl)-1*H*-indole-1-carboxamide (4k)**



Following the general procedure, product **4k** was isolated in 55% yield. **^{1}H NMR (300 MHz, $CDCl_3$)** δ = 7.83 – 7.71 (m, 3H), 7.49 – 7.40 (m, 2H), 7.39 – 7.32 (m, 3H), 7.27 (dddd, *J*=8.8, 5.6, 3.3, 2.0, 5H), 7.20 – 7.09 (m, 1H), 3.43 (dq, *J*=13.9, 8.0, 7.1, 4H), 1.19 (t, *J*=7.8, 6H); **^{13}C NMR (75 MHz, $CDCl_3$)** δ 152.70, 136.29, 133.61, 131.45, 129.25, 128.78, 128.64, 128.56, 127.26, 126.48, 125.14, 124.77, 122.72, 122.04, 120.49, 116.86, 111.44, 96.61, 80.95, 42.87, 13.95 (one CH_3 and one CH_2 peak from diethylamide group are not visible); **HRMS**: m/z (ESI) calcd for C27H24N2ONa $[M+Na]^+$ 415.1781, found 415.1783. **FT-IR** umax (neat/cm-1) 3055, 2974, 1686, 1427, 1331, 1273, 737, 698.

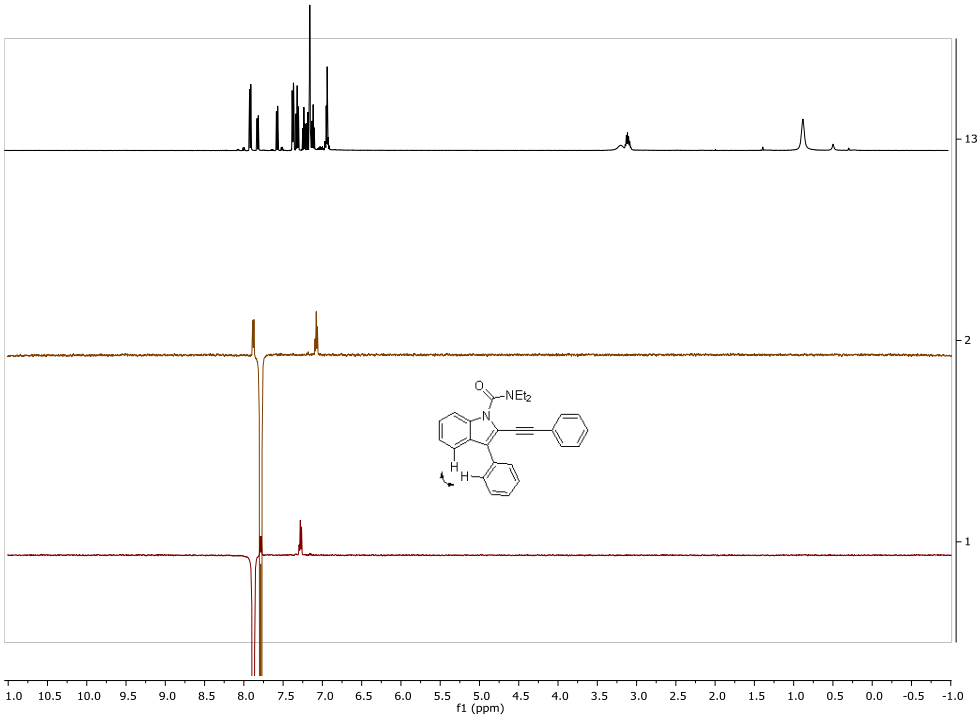
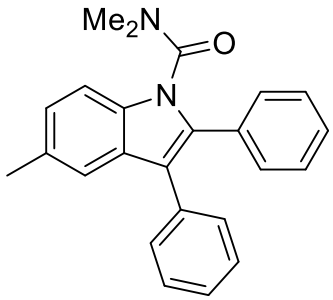


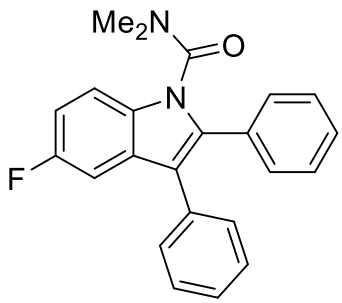
Figure S3. Determination of structure **4k** was achieved with TOCSY and NOE-Experiments.

***N*,*N*,5-trimethyl-2,3-diphenyl-1*H*-indole-1-carboxamide (4l)**[2a]



Following the general procedure, product **4l** was isolated in 84% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.36 (s, 1H), 7.32 (d, *J* = 8.4 Hz, 1H), 7.30 – 7.12 (m, 10H), 7.09 – 7.02 (m, 1H), 2.86 (s, 3H), 2.45 (s, 3H), 2.40 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 154.24, 135.11, 134.34, 134.21, 131.55, 131.24, 130.31, 129.70, 128.60, 128.51, 128.36, 128.03, 126.56, 125.37, 119.58, 117.61, 111.28, 37.98, 36.68, 21.58.

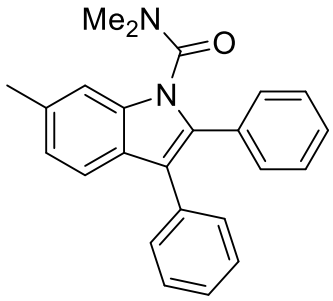
5-Fluoro-*N*,*N*-dimethyl-2,3-diphenyl-1*H*-indole-1-carboxamide (4m)[2a]



Following the general procedure, product **4m** was isolated in 85% yield. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.37 (dd, *J* = 9.0, 4.8 Hz, 1H), 7.31 – 7.14 (m, 11H), 6.97 (td, *J* = 9.0, 2.4 Hz, 1H), 2.88 (s, 3H), 2.43 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 159.16 (d, ^{1}*J*CF = 235.6 Hz), 13, 153.87, 136.52, 133.70, 132.26, 131.09, 130.07, 129.67, 128.97 (d, ^{3}*J*CF = 9.8 Hz), 128.67, 128.49, 128.42, 126.84, 117.78 (d, ^{4}*J*CF = 4.5 Hz), 112.48 (d, ^{3}*J*CF = 9.4 Hz), 112.07 (d, ^{2}*J*CF = 26.0 Hz), 105.08 (d, ^{2}*J*CF = 24.2 Hz),

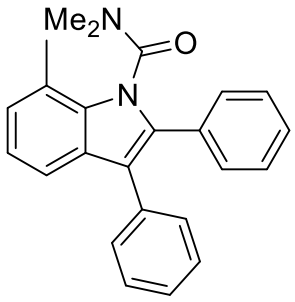
38.02, 36.66. **^{19}F NMR** (282 MHz, $CDCl_3$) δ -121.94.

***N*,*N*,6-trimethyl-2,3-diphenyl-1*H*-indole-1-carboxamide (4n)[2a]**



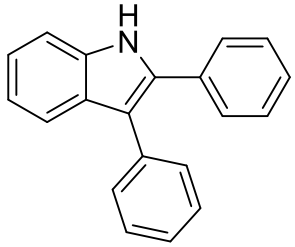
Following the general procedure, product **4n** was isolated in 83% yield. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.47 (d, *J* = 8.1 Hz, 1H), 7.32 – 7.11 (m, 11H), 6.96 (dd, *J* = 8.1, 0.9 Hz, 1H), 2.88 (s, 3H), 2.41 (br, 6H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 154.26, 136.18, 134.33, 134.25, 133.95, 131.54, 130.21, 129.65, 128.49, 128.38, 127.99, 126.53, 126.18, 123.48, 119.62, 117.66, 111.49, 38.07, 36.54, 21.92.

***N*,*N*,7-trimethyl-2,3-diphenyl-1*H*-indole-1-carboxamide (4o)[2a]**



Following the general procedure, product **4o** was isolated in 61% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.50 (dd, *J* = 5.9, 0.5 Hz, 1H), 7.36 – 7.30 (m, 2H), 7.29 – 7.12 (m, 8H), 7.08 – 6.96 (m, 2H), 2.84 (s, 3H), 2.44 (s, 3H), 2.36 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 154.95, 134.80, 134.44, 134.22, 131.24, 130.39, 130.37, 128.42, 128.39, 128.35, 128.29, 126.38, 125.74, 121.64, 121.57, 117.90, 117.51, 37.87, 36.43, 18.08.

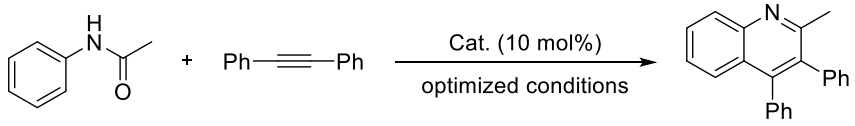
2,3-Diphenyl-1*H*-indole (5)[8]



Following the general procedure of removal of the carbamoyl moiety, product **5** was isolated in 76% yield. **^{1}H NMR (400 MHz, $CDCl_3$)** δ = 8.20 (s, 1H), 7.76 (d, *J*=7.9, 1H), 7.55 – 7.49 (m, 2H), 7.49 – 7.41 (m, 5H), 7.40 – 7.28 (m, 5H), 7.23 (ddd, *J*=8.0, 7.0, 1.1, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 136.00, 135.18, 134.20, 132.79, 130.28, 128.87, 128.78, 128.64, 128.30, 127.80, 126.35, 122.81, 120.55, 119.82, 115.15, 111.03.

3) Comparison of different catalyst precursors

Table S2. Comparison of Cp*Co(III) with second and third row transition metal catalyst pecursors in the dehydrative cyclization reaction.



Entry	Catalyst precursors	Yield[a]
1	**[Cp*Co(CO)I_2]**	**76%**
2[b]	[(*p*-cymene)$RuCl_2$]$_2$	trace
3[b]	[Cp*$RhCl_2$]$_2$	trace
4	$Pd(OAc)_2$	trace
5[b]	[Cp*$IrCl_2$]$_2$	trace

44	45
Ru	**Rh**
Ruthenium	Rhodium
101.07	102.906
46	77
Pd	**Ir**
Palladium	Iridium
106.42	192.2

[a] Yield was determined by GC-FID using mesitylene as internal standard. [b] Catalyst precursors (5 mol%) were used.

4) X-Ray Data.

X-Ray diffraction: Data sets for the compound **4c** were collected with a Kappa-CCD APEXII diffractometer. Programs used: data collection: APEX2 V2014.5-0 (Bruker AXS Inc., 2014); cell refinement: SAINT V8.34A (Bruker AXS Inc., 2013); data reduction: SAINT V8.34A (Bruker AXS Inc., 2013); absorption correction, SADABS V2014/2 (Bruker AXS Inc., 2014); structure solution SHELXT-2014 (Sheldrick, 2008); structure refinement SHELXL-2014 (Sheldrick, 2008). *R*-values are given for observed reflections, and wR^2 values are given for all reflections. Thermals ellipsoids are shown with 50% probability. *R*-values are given for observed reflections, and wR^2 values are given for all reflections.

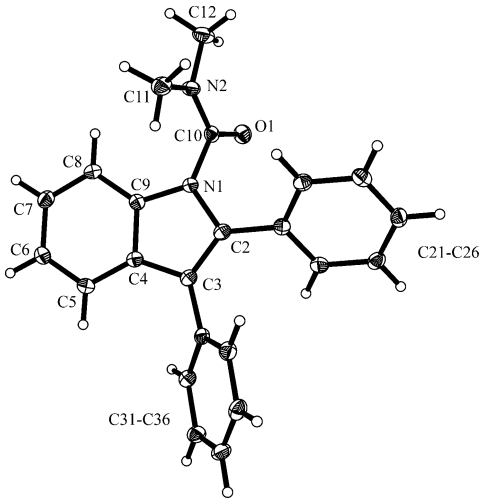


Figure S4. Crystal structure of compound **4c**. (Thermals ellipsoids are shown with 50% probability.)

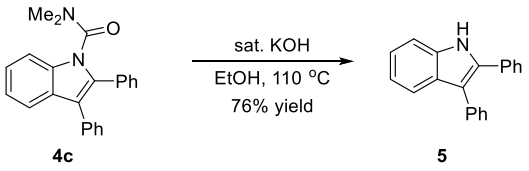
X-ray crystal structure analysis of *N*,*N*-dimethyl-2,3-diphenyl-1*H*-indole-1-carboxamide (4b, CCDC 1441958): A colorless prism-like specimen of $C_{23}H_{20}N_2O$, approximate dimensions 0.050 mm x 0.100 mm x 0.230 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. A total of 1785 frames were collected. The total exposure time was 21.64 hours. The frames were integrated with the Bruker SAINT software package using a wide-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 32407 reflections to a maximum θ angle of 67.87° (0.83 Å resolution), of which 3157 were independent (average redundancy 10.265, completeness = 99.5%, R_{int} = 5.01%, R_{sig} = 2.31%) and 2803 (88.79%) were greater than $2\sigma(F^2)$. The final cell constants of a = 10.4762(3) Å, b = 10.8341(3) Å, c = 15.5988(4) Å, β = 99.3150(10)°, volume = 1747.12(8) $Å^3$, are based upon the refinement of the XYZ-centroids of 9889 reflections above 20 σ(I) with 9.502° < 2θ < 135.0°. Data were corrected for absorption effects using the multi-scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.879. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.8700 and 0.9690. The final anisotropic full-matrix least-squares refinement on F^2 with 237 variables converged at R1 = 3.45%, for the observed data and wR2 = 8.69% for all data. The goodness-of-fit was 1.044. The largest peak in the final difference electron density synthesis was 0.196 $e^-/Å^3$ and the largest hole was -0.267 $e^-/Å^3$ with an RMS deviation of 0.063 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.294 g/cm^3 and F(000), 720 e^-.

References for X-Ray Part:

Bruker (2013). *APEX2*, *SAINT* and *SADABS* Bruker AXS Inc., Madison, Wisconsin, USA.

SHELXT und SHELXL Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

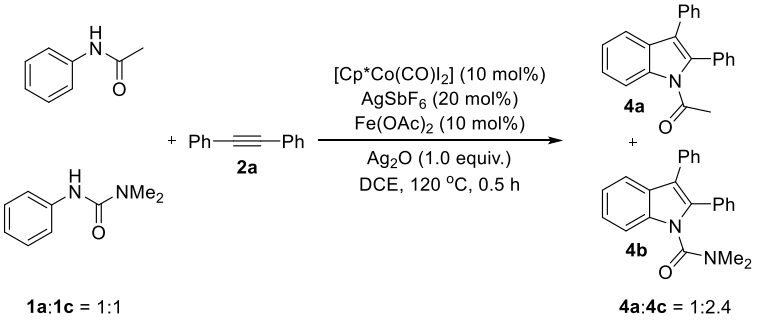
5) Removal of the carbamoyl moiety.



Scheme S1. Removal of the carbamoyl moiety.

General procedure: In a 50 mL dry Schlenk tube with a stirring bar, 3:1 EtOH/sat. aq. KOH (3.0 mL) and *N*,*N*-dimethyl-2,3-diphenyl-1*H*-indole-1-carboxamide (**4c**, 0.20 mmol, 68.1 mg) were added under air. Then the tube was closed tightly with a screwcap and stirred at 110ºC for 48 h. After reaction, the crude reaction was diluted with sat. aq. NH_4Cl and extracted with CH_2Cl_2 (three times). The combined organics were dried (Na_2SO_4) and concentrated in vacuum. The analytically pure product **5** was obtained in 76% yield by flash chromatography (silica; gradient of pentane/EtOAc).

6) Competition experiment.

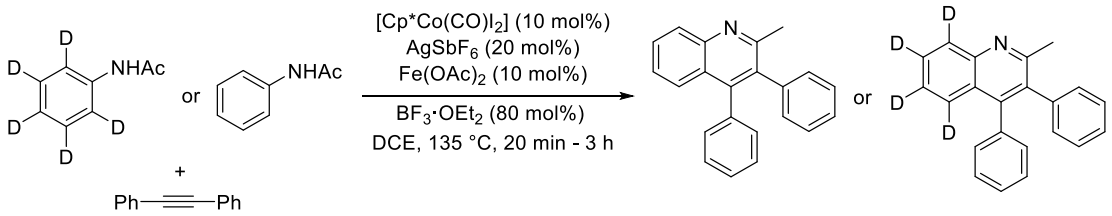


Scheme S2. Competition experiment between **1a** and **1c**.

General procedure: In a 10 mL dry Schlenk tube with a stirring bar, acetanilide **1a** (0.10 mmol, 13.5 mg), *N*-arylurea (**1c**) (0.10 mmol, 16.4 mg), diphenylacetylenes (**2a**) (0.40 mmol, 71.3 mg), silver oxide (0.20 mmol, 46.3 mg) and [Cp*Co(CO)I_2] (10 mol%, 9.5 mg) were added under air. Then the tube was transferred into the glove box. $AgSbF_6$ (20 mol%, 13.7 mg), $Fe(OAc)_2$ (10 mol%, 3.5 mg) were added. After moving out, 1,2-dichloroethane (DCE) (1 mL) was added under argon atmosphere. The tube was sealed and the mixture was stirred at 120 °C for 0.5 h. Afterwards, the crude reaction mixture was analyzed by GC-FID, The yields of **3a** and **4a** are 10% and 24% respectively (based on **1a** and **1c**).

7) KIE experiments.

a) Parallel experiments for the synthesis of quinoline.



Scheme S3. Parallel KIE experiment for the synthesis of quinoline.

As per general procedure A, [Cp*Co(CO)I_2] (10 mol %, 9.5 mg), $AgSbF_6$ (20 mol %, 13.7 mg), $Fe(OAc)_2$ (10 mol %, 3.5 mg) and $BF_3{\cdot}OEt_2$ (20.2 µL; 80 mol %), Diphenylacetylene (0.80 mmol, 142.6 mg), Acetanilide (0.20 mmol; 27.0 mg) or d_5-Acetanilide (0.20 mmol, 28 mg) and DCE (1 mL) and mesitylene (0.20 mmol, 28 µL) as internal standard were added under argon atmosphere in two different reaction tubes. The reactions were stirred at 135 °C and samples of 20 µL were taken at intervals to evaluate conversion of starting material by GC-FID. KIE value was measured averaging the slopes obtained for each run.

Table S3. Results for the parallel KIE experiment.

Acetanilide (H5)				**D_5-Acetanilide (D5)**			
Run 1		Run 2		Run 1		Run 2	
Time (min)	Conversion (%)	Time (min)	Conversion (%)	Time (min)	Conversion (%)	Time (min)	Conversion (%)
40	19	20	8.5	40	9	20	1
80	25	60	17	80	14	60	3.5
100	26	120	25	100	15	120	10
120	33	180	30	120	17	180	14

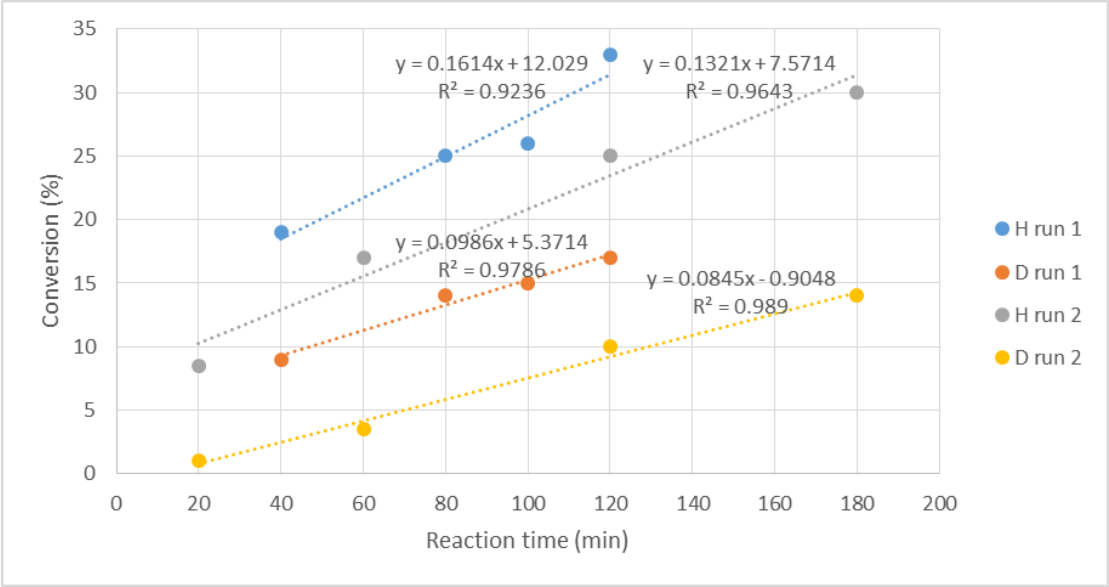
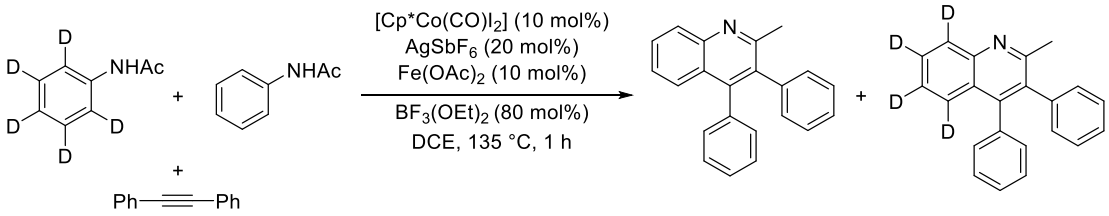


Figure S5. Parallel KIE experiment result: K_H/K_D = 1.6.

b) Competition experiment for the synthesis of quinoline.



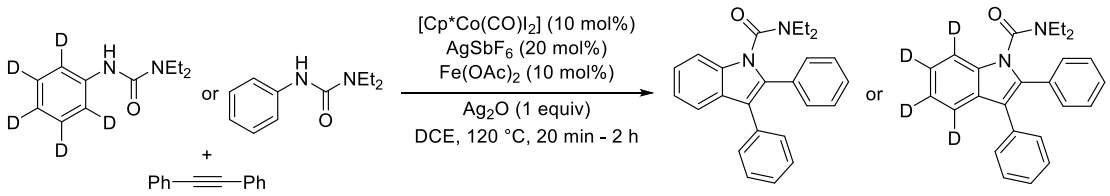
Scheme S4. Competition KIE experiment for the synthesis of quinoline.

As per general procedure A, [Cp*Co(CO)I_2] (10 mol %, 9.5 mg), $AgSbF_6$ (20 mol %, 13.7 mg), $Fe(OAc)_2$ (10 mol %, 3.5 mg) and $BF_3{\cdot}OEt_2$ (20.2 µL; 80 mol %), Diphenylacetylene (0.80 mmol, 142.6 mg), Acetanilide (0.20 mmol; 27.0 mg) and d_5-Acetanilide (0.20 mmol, 28 mg) and DCE (1 mL) were added under argon. The reaction was stirred at 135 °C for 1 h. Volatiles from the crude reaction mixture were removed and the ratio of H/D was found to be 3.2/1 by HRMS.

Table S4. Results for the competition KIE experiment. KIE = 3.2.

Product	m/z	Res.	S/N	I	FWHM
H	296.1442	6646	9543.8	1711996	0.0446
D	300.1693	6937	3055.3	532972	0.0433

a) Parallel experiments for the synthesis of indole.



Scheme S5. Parallel KIE experiment for the synthesis of indole.

As per general procedure B but in a 0.10 mmol scale, [Cp*Co(CO)I_2] (10 mol %, 4.8 mg), $AgSbF_6$ (20 mol %, 6.9 mg), $Fe(OAc)_2$ (10 mol %, 1.8 mg) and Ag_2O (0.10 mmol; 23.2 mg), Diphenylacetylene (0.20 mmol, 35.6 mg), 1,1-diethyl-3-phenylurea (0.10 mmol; 19.2 mg) or d_5-1,1-diethyl-3-phenylurea (0.10 mmol, 19.7 mg) and DCE (0.50 mL) and mesitylene (0.10 mmol, 14 μL) as internal standard were added under argon atmosphere in two different reaction tubes. The reactions were stirred at 120 °C and samples of 20 μL were taken at intervals to evaluate conversion of starting material by GC-FID. KIE value was measured averaging the results of two separate runs.

Table S5. Parallel KIE experiment for the synthesis of indole.

1,1-diethyl-3-phenylurea		**d_5-1,1-diethyl-3-phenylurea**	
Average		Average	
Time (min)	Conversion (%)	Time (min)	Conversion (%)
20	5.5	20	3
60	24	60	5
120	25	120	9.5

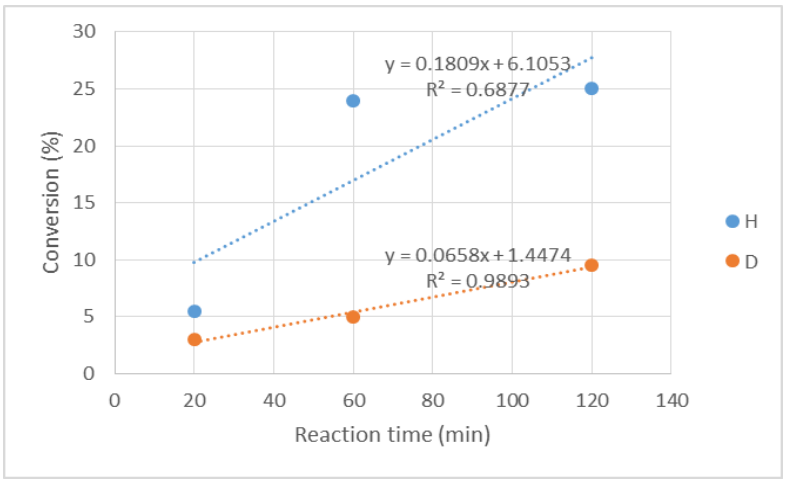
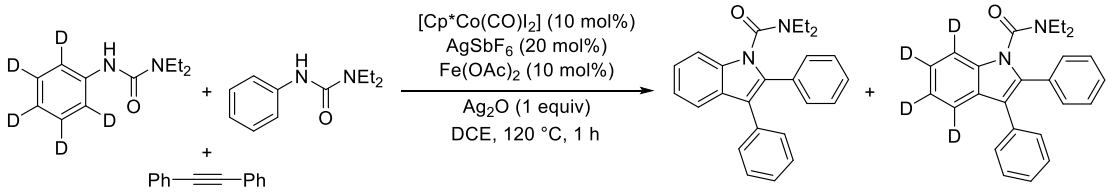


Figure S6. Parallel KIE experiment result: K_H/K_D = 2.75.

b) Competition experiment for the synthesis of indole.



Scheme S6. Competition KIE experiment for the synthesis of indole.

As per general procedure B but in a 0.10 mmol scale, [Cp*Co(CO)I_2] (10 mol %, 4.8 mg), $AgSbF_6$ (20 mol %, 6.9 mg), $Fe(OAc)_2$ (10 mol %, 1.8 mg) and Ag_2O (0.10 mmol; 23.2 mg), Diphenylacetylene (0.20 mmol, 35.6 mg), 1,1-diethyl-3-phenylurea (0.10 mmol; 19.2 mg) and d_5-1,1-diethyl-3-phenylurea (0.10 mmol, 19.7 mg) and DCE (0.50 mL) were added under argon. The reaction was stirred at 120 °C for 1 h. Volatiles from the crude reaction mixture were removed and the ratio of H/D was found to be 2.9/1 by HRMS.

Table S6. Competition KIE experiment for the synthesis of indole. KIE = 2.9.

Product	m/z	Res.	S/N	I	FWHM
H	391.1779	7847	1817.8	174994	0.0498
D	395.2031	8042	617.1	60703	0.0491

8) ^{13}C NMR of *N*-(*p*-tolyl)acetamide and 1,1-dimethyl-3-(*p*-tolyl)urea.

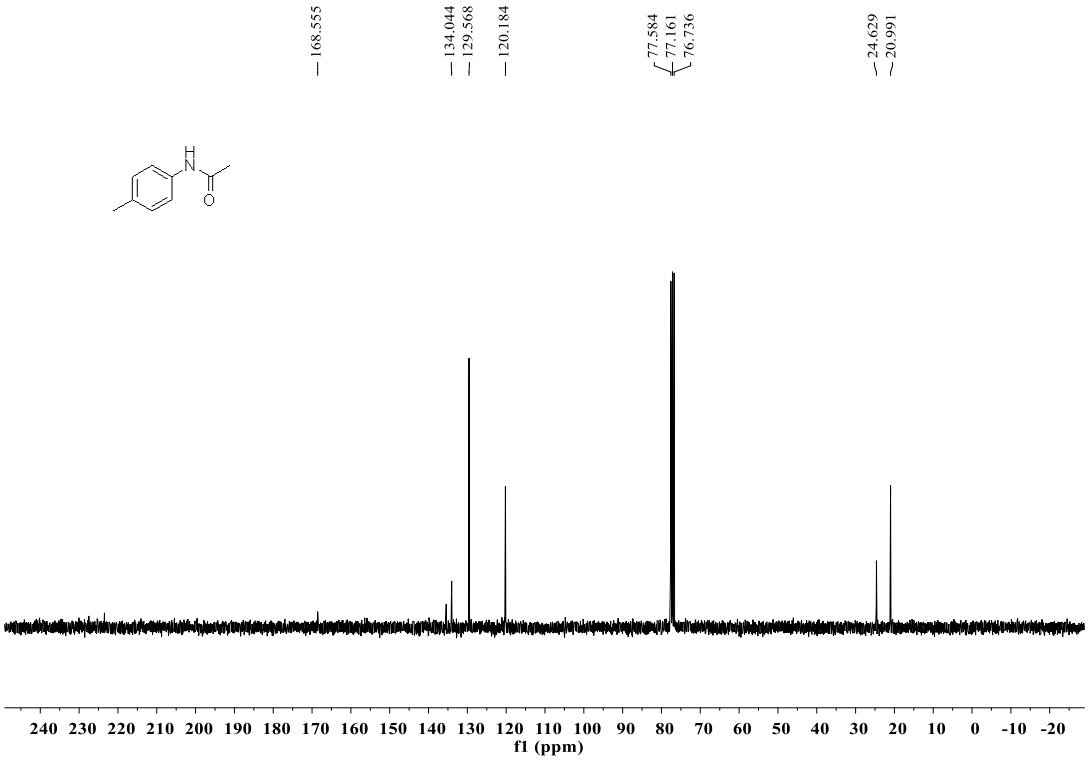


Figure S7. ^{13}C NMR of *N*-(*p*-tolyl)acetamide.

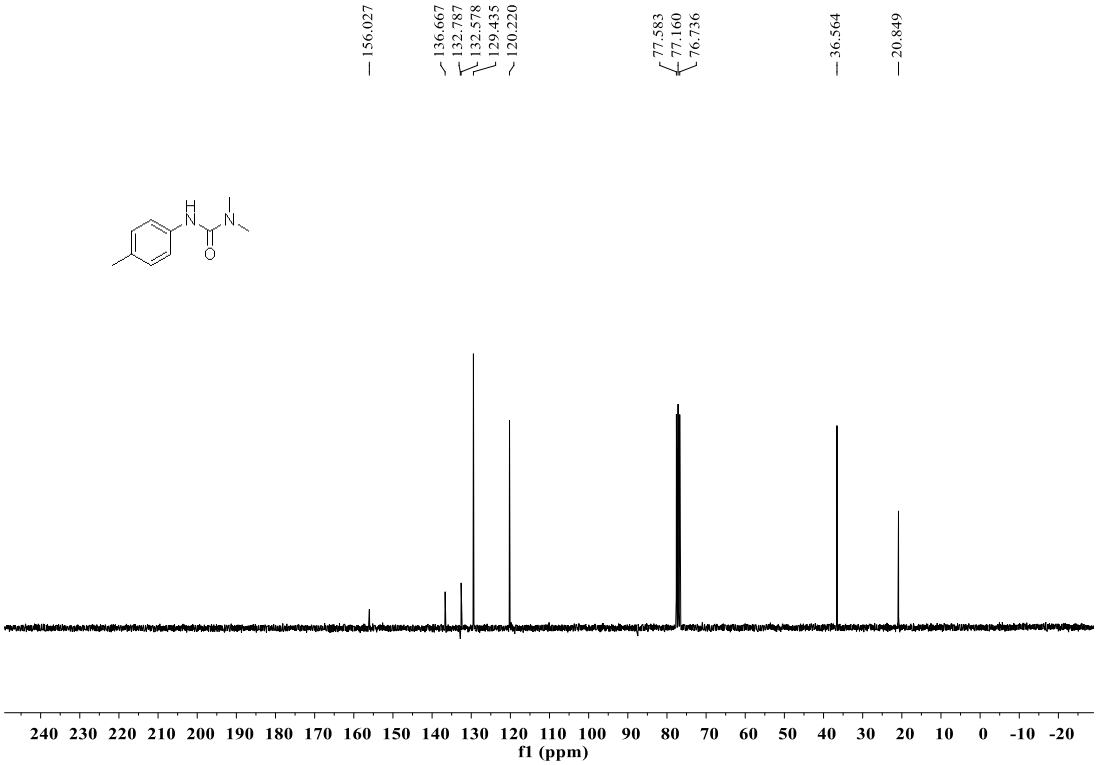


Figure S8. ^{13}C NMR of 1,1-dimethyl-3-(*p*-tolyl)urea.

9) Theoretical studies.

To better understand the origin of the observed selectivity, the mechanism of the alkyne insertion was studied computationally (Scheme 5). Alkyne insertion in **I** occurs readily to form the eight-membered cobaltacycle **II**. Nucleophilic attack in this intermediate is favored to the acetamide (R = Me) relative to the urea derivative (R = NMe_2) by 1.7 kcal mol^{-1}. Isomerization to a 6-membered, N,O-chelating cobaltacycle **IV** has a lower barrier by ca. 10 kcal mol^{-1} for either substrate. Subsequent reductive elimination to the indole (**V**) is favored for the more electron-rich urea derivative by 2.7 kcal mol^{-1} over the acetamide. Interestingly, from **IV** the acetamide derivative has a slightly lower barrier for the isomerization back to the 8-membered intermediate **II** (31.5 kcal mol^{-1}) than the reductive elimination (+32.2 kcal mol^{-1}), which means that the overall lowest barrier for product formation is the nucleophilic attack to the 6-membered ring **III** (+29.3 kcal mol^{-1}). Based on these results, a slight preference for the formation of quinolines over indoles should be expected from acetanilide substrates, as opposed to a selective formation of indole from arylurea. Importantly, the role of BF_3 can be rationalized to decrease the high barrier for nucleophilic addition by coordination to **II**.

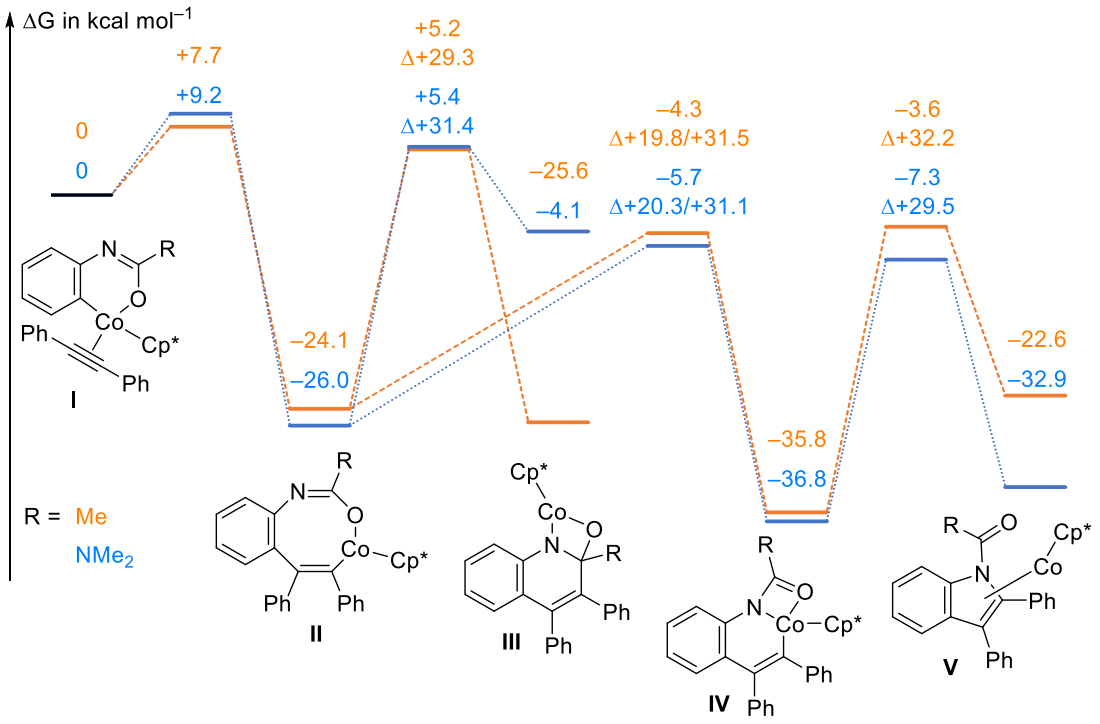
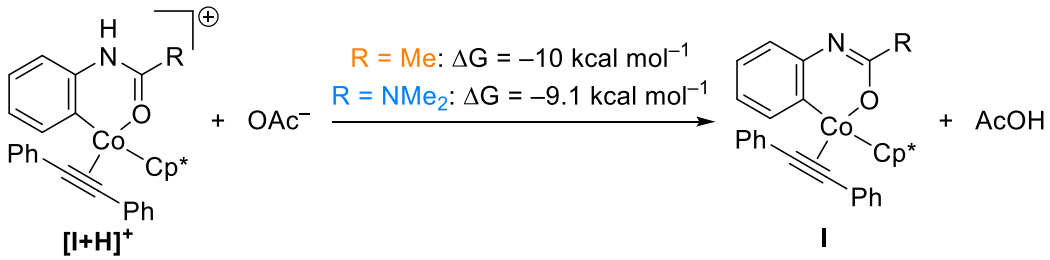


Figure S9. Free-energy profiles for two competitive reaction pathways at the IEFPCM(1,2-DCE) /M06/6-311G**//M06-L/6-31G**+LANL2DZ(Co) level.

Computational Details

All calculations were carried out with the Gaussian 09 suite. At the IEFPCM(1,2-DCE)/M06/6-311G**//M06-L/6-31G**+LANL2DZ(Co) level of theory. The optimization was carried out without symmetrical or internal constraints and frequencies were calculated at the same level as the optimization to confirm the absence of imaginary frequencies for minima and the presence of a single imaginary frequency for the transition states. Intrinsic reaction coordinate calculations were performed for all transition states to confirm the corresponding connected ground states. Free energies are reported at 298.15 K in kcal mol^{-1}. Only relevant structures are included; conformers of higher energy are not shown but have been accounted for in all cases.

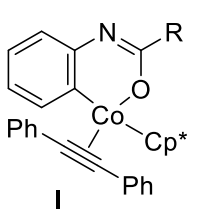
For the reaction pathway, only the deprotonated amide directing groups have been considered based on the following result on the deprotonation of intermediate **I**: The free energy of deprotonation by an acetate base at the IEFPCM(1,2-DCE)/M06/6-311+G(d,p)//M06-L/6-31G(d,p)+LANL2DZ(Co) level is –10.0 and –9.1 kcal mol^{-1} for both directing groups. Subsequent H-bond formation of the acetic acid with acetate, other HOAc molecules or other species present will likely lead to further stabilization under the actual reaction conditions. While we cannot definitely state if the deprotonation occurs at an earlier stage of the mechanism (C–H activation stage), all states relevant to the alkyne insertion process should be present in the deprotonated form.



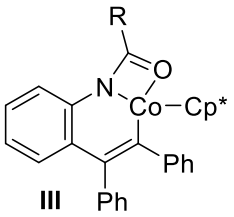
Scheme S7. Free energies of deprotonation for metallacycle **I**.

Co^{III} compounds can occur as singlet, triplet and quintuplet states. Only singlet states were considered in the discussion of the mechanism, based on the energy differences between singlet and triplet states in representative structures. The alkyne p-coordination compound I did not converge to a stable minimum in the triplet state. Vertical excitation to the triplet state has an

energy difference of +18.0 and +15.9 kcal mol^{-1}, though. Similarly, the vertical excitation energies for a later intermediate are around 20 kcal mol^{-1} and the adiabatic excitation free energy around 9 kcal mol^{-1}. While the triplet states are clearly accessible under the reaction conditions, they should not have a relevance to the mechanism.



I



III

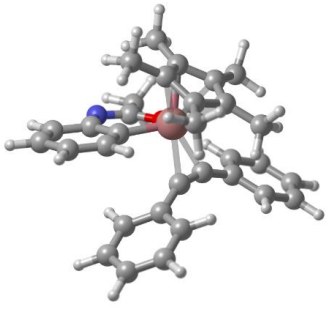
	$\Delta E(S-T)_{vertical}$	$\Delta G(S-T)_{adiabatic}$	$\Delta E(S-T)_{vertical}$	$\Delta G(S-T)_{adiabatic}$
R = Me	+18.0	n.c.	+19.9	+8.7
R = NMe_2	+15.9	n.c.	+21.0	+9.1

Scheme S8. Free energy differences between singlet and triplet states of representative intermediates. Vertical = G(T) at the singlet geometry; adiabatic = fully optimized at the triplet state; n.c. = no convergence of optimization in the triplet state.

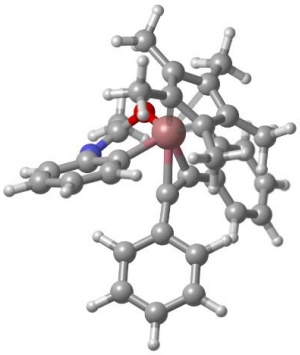
Full authorship for Gaussian 09, Revision D.01

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian 09, Revision D.01; Gaussian, Inc.: Wallingford, CT, 2013.

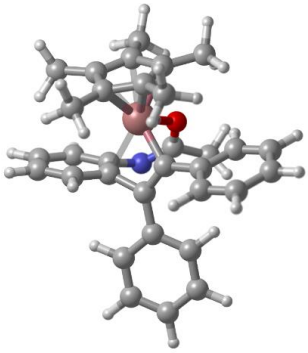
Minimum energy structures of the relevant intermediates and transition states.



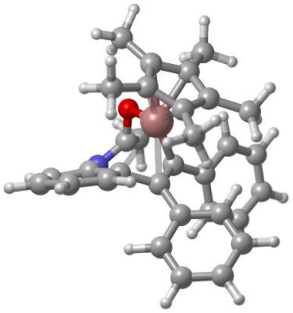
Me-I



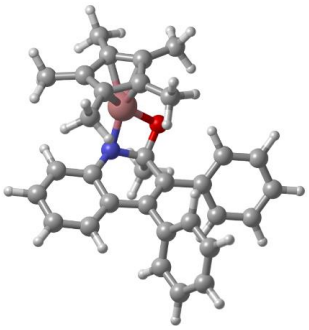
Me-I_II



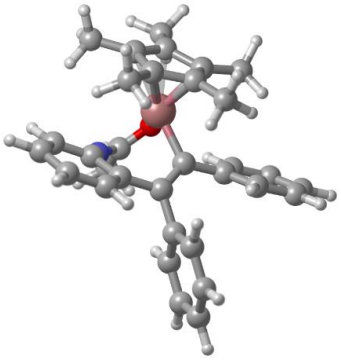
Me-II



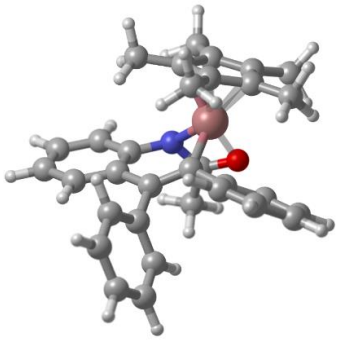
Me-II_III



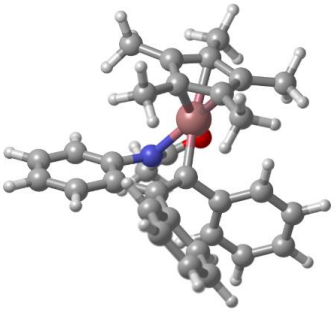
Me-III



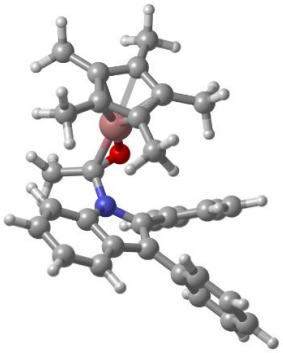
Me-II_IV



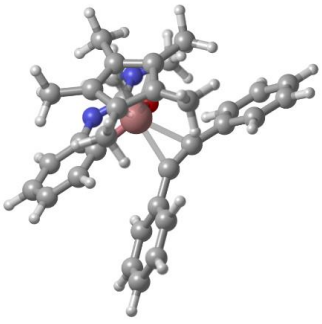
Me-IV



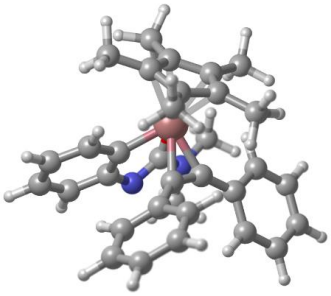
Me-IV_V



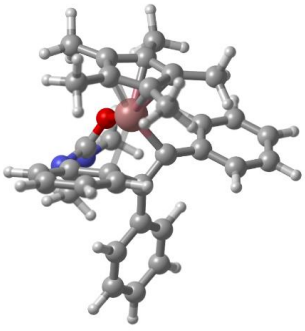
Me-V



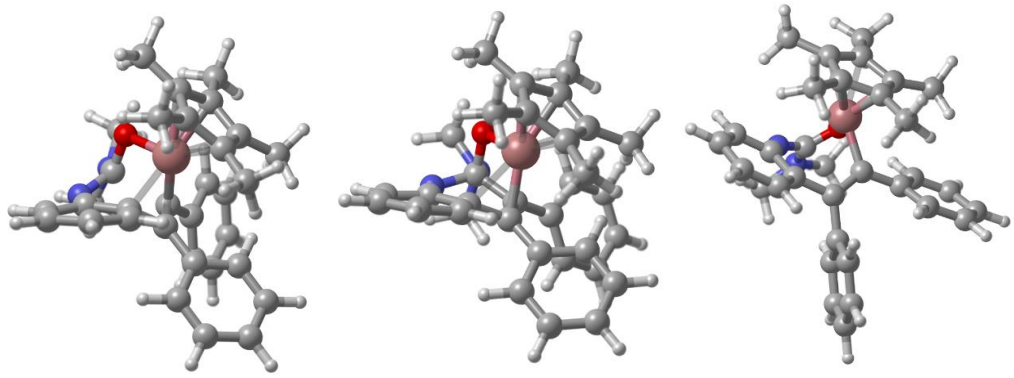
NMe2-I



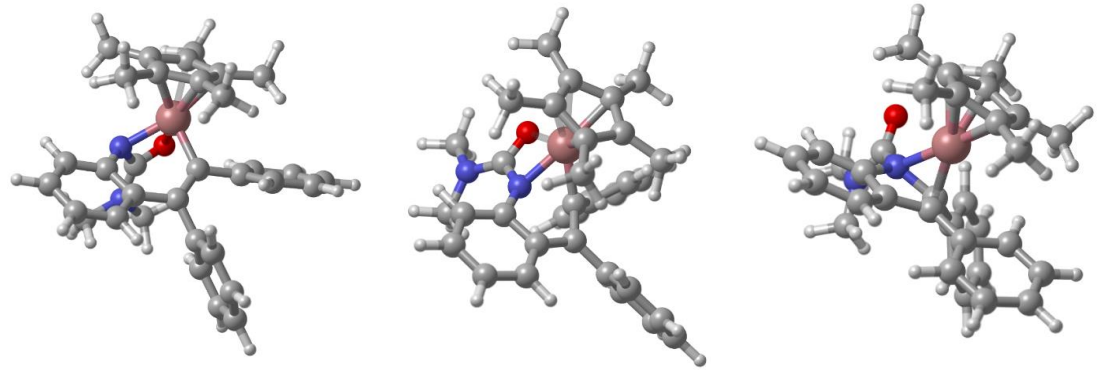
NMe2-I_II



NMe2-II



NMe2-II_III **NMe2-III** **NMe2-II_IV**



NMe2-IV **NMe2-IV_V** **NMe2-V**

Figure S10. Minimum energy structures of the relevant intermediates and transition states.

Cartesian coordinates of minimum energy structures

Me-S-I
Number of imaginary frequencies = 0

C	4.101047	-0.392115	-0.097313
C	4.361944	-1.279079	-1.138487
C	3.306724	-1.912801	-1.774257
C	1.958805	-1.698830	-1.404920
C	1.703313	-0.801568	-0.344226
C	2.779044	-0.165293	0.279570
H	4.908710	0.126531	0.413813
H	5.383607	-1.475669	-1.454581
H	3.477576	-2.606463	-2.593989
H	2.587985	0.548403	1.079837
N	1.039086	-2.424093	-2.157798
C	-0.233276	-2.220224	-2.009947
O	-0.862913	-1.423176	-1.191539
Co	-0.111670	-0.571944	0.370239
C	0.626322	-1.630970	2.079889
C	0.194078	-0.320984	2.443988
C	-1.224866	-0.237871	2.184284
C	-1.643323	-1.444648	1.580596
C	-0.480396	-2.291823	1.467904
C	1.949589	-2.256121	2.330493
C	0.978720	0.727333	3.152527
C	-2.055594	0.937832	2.544982
C	-2.991310	-1.796941	1.069897
C	-0.454749	-3.656066	0.882156
H	2.284840	-2.847118	1.473590
H	2.725556	-1.516805	2.535264
H	1.878111	-2.926853	3.195769
H	0.950462	1.685963	2.620350
H	0.582772	0.904830	4.159852
H	2.028767	0.445234	3.258466
H	-3.043292	0.910436	2.079738
H	-2.193856	0.983788	3.631889
H	-1.570074	1.873195	2.243503
H	-2.923677	-2.097495	0.017407

H -3.424906 -2.633420 1.630002
H -3.685436 -0.954748 1.128613
H -1.303140 -3.813641 0.211811
H 0.459371 -3.827427 0.305719
H -0.501605 -4.422089 1.665968
C 0.101919 1.460228 -0.301585
C -1.095077 1.115846 -0.421302
C -2.490453 1.290310 -0.702521
C -3.118231 2.455551 -0.218245
C -3.246787 0.380039 -1.459008
H -2.530885 3.169735 0.354015
C -4.462519 2.691241 -0.470451
C -4.592742 0.624835 -1.702132
H -2.756027 -0.511603 -1.832074
H -4.929267 3.596080 -0.090871
C -5.207684 1.773192 -1.208147
H -5.166623 -0.088345 -2.287790
H -6.260470 1.957054 -1.403426
C 1.205992 2.367304 -0.411143
C 2.176447 2.227236 -1.416699
C 1.301216 3.447529 0.482526
C 3.208496 3.148800 -1.522089
H 2.116116 1.380035 -2.093218
H 0.540411 3.567712 1.251105
C 2.343158 4.361385 0.374782
H 3.954178 3.027166 -2.302363
C 3.300557 4.212845 -0.625854
H 2.404273 5.192935 1.071387
H 4.115710 4.926271 -0.708807
C -1.169034 -2.990296 -2.902248
H -1.889912 -3.561788 -2.306063
H -1.752576 -2.303430 -3.524992
H -0.609900 -3.667201 -3.547600

Me-S-I_II

Number of imaginary frequencies = 1

C 0.625872 -0.986644 2.576115
C -0.513855 1.004996 0.049024
C 0.763531 0.932845 0.157850
C -1.619413 -0.860449 1.999996
C -2.900443 -1.099427 2.548813
C -4.034622 -1.217168 1.762604
H -2.955454 -1.186119 3.630703
C -2.693367 -0.807166 -0.183367
C -3.935985 -1.064506 0.377975
H -4.999395 -1.402137 2.228058
H -2.629603 -0.614818 -1.252025
H -4.818822 -1.114914 -0.253899
C -1.522066 -0.742114 0.587622
N -0.599773 -0.712427 2.919974
O 1.065380 -1.424230 1.430270
Co 0.254924 -0.900426 -0.261955
C 1.827909 -1.892078 -1.238217
C 0.743018 -2.825678 -1.010457
C -0.386946 -2.385822 -1.727991
C -0.052087 -1.121175 -2.330436
C 1.342930 -0.864613 -2.083278
C 3.196524 -2.083553 -0.696708
C 0.838038 -4.020900 -0.137448
C -1.669846 -3.133031 -1.824792
C -0.910548 -0.291614 -3.222329
C 2.095628 0.295862 -2.627192
H 3.844354 -1.226394 -0.895908
H 3.151632 -2.237447 0.388003
H 3.667947 -2.971334 -1.135173
H 1.463588 -4.800289 -0.589139
H 1.287460 -3.745703 0.822648
H -0.145384 -4.453156 0.063369
H -2.419060 -2.597599 -2.411973
H -1.502454 -4.102049 -2.308192
H -2.108318 -3.321301 -0.840022
H -1.900434 -0.733301 -3.361625
H -1.059493 0.719722 -2.825213
H -0.458841 -0.185065 -4.215474
H 1.525230 1.226462 -2.528373
H 3.050419 0.442852 -2.115132
H 2.303363 0.155166 -3.694776
C -1.569193 1.977520 -0.188269
C -1.394186 2.912680 -1.223474
C -2.707252 2.081663 0.625858
C -2.333474 3.915423 -1.443002
H -0.508608 2.839633 -1.852986
C -3.634667 3.091407 0.409338
H -2.848495 1.374908 1.438415
C -3.457431 4.007037 -0.626875
H -2.184746 4.624545 -2.252773

H	-4.504546	3.163780	1.056089
H	-4.191410	4.789930	-0.796035
C	2.014715	1.605955	0.370135
C	3.147104	0.917713	0.833765
C	2.128191	2.979787	0.084701
C	4.358932	1.579019	0.992280
H	3.039983	-0.134338	1.078419
C	3.341723	3.633993	0.248650
H	1.252525	3.519604	-0.268451
C	4.463750	2.936323	0.694871
H	5.226510	1.031980	1.352543
H	3.414923	4.694031	0.020647
H	5.413587	3.450180	0.813776
C	1.691918	-0.833858	3.622538
H	2.327408	0.026123	3.381433
H	1.250107	-0.681250	4.606859
H	2.342046	-1.713949	3.637215

Me-S-II

Number of imaginary frequencies = 0

C	-0.118505	-0.811725	2.442544
C	-1.206592	-0.644015	-0.357967
C	-0.706766	0.602058	-0.321661
C	0.308675	-2.368999	0.775963
C	1.107855	-3.530633	0.611222
C	1.466645	-3.979804	-0.640435
H	1.391259	-4.077360	1.505878
C	0.316122	-2.142410	-1.672498
C	1.074965	-3.285048	-1.803037
H	2.063961	-4.884278	-0.732021
H	-0.035156	-1.606079	-2.552567
H	1.356076	-3.654755	-2.785456
C	-0.088206	-1.648795	-0.404373
N	-0.152408	-2.046995	2.013276
O	0.572207	0.156986	1.937129
Co	1.142556	0.183059	0.064387
C	2.386017	1.745349	0.423657
C	3.136016	0.527743	0.677482
C	3.174201	-0.214509	-0.514930
C	2.423340	0.511880	-1.522902
C	2.013229	1.757731	-0.957934
C	2.143221	2.803052	1.436636
C	3.658789	0.134844	2.010729
C	3.866697	-1.507629	-0.739924
C	2.293169	0.128523	-2.954157
C	1.356558	2.868445	-1.692078
H	1.422114	3.545289	1.085931
H	1.751419	2.363665	2.359951
H	3.074073	3.327250	1.686278
H	4.549771	0.713513	2.282304
H	2.899713	0.309061	2.779692
H	3.925242	-0.924746	2.044521
H	3.286959	-2.172330	-1.385288
H	4.832644	-1.339417	-1.232230
H	4.060998	-2.039203	0.194739
H	2.366134	-0.953895	-3.087888
H	1.334549	0.453761	-3.370878
H	3.084654	0.589065	-3.559307
H	0.674338	2.500926	-2.463699
H	0.778572	3.519474	-1.031507
H	2.114384	3.485968	-2.189778
C	-2.598188	-1.120982	-0.305052
C	-3.650514	-0.288169	0.114588
C	-2.908213	-2.447052	-0.648869
C	-4.956067	-0.757696	0.161317
H	-3.435601	0.731915	0.419181
C	-4.216777	-2.914045	-0.601048
H	-2.110141	-3.118529	-0.959049
C	-5.249932	-2.071552	-0.200647
H	-5.751265	-0.094494	0.492684
H	-4.429040	-3.944136	-0.875735
H	-6.272750	-2.436109	-0.161386
C	-1.335470	1.907872	-0.321637
C	-2.011605	2.391603	-1.455116
C	-1.232648	2.745702	0.803459
C	-2.558699	3.669117	-1.464541
H	-2.098574	1.746852	-2.327452
C	-1.786858	4.020471	0.790644
H	-0.712544	2.363508	1.679547
C	-2.446870	4.491397	-0.344347
H	-3.076483	4.026302	-2.351275
H	-1.705092	4.651829	1.672240
H	-2.873613	5.490536	-0.354431
C	-0.902196	-0.466257	3.671684
H	-1.238207	-1.361709	4.194285
H	-0.314019	0.165668	4.342016

H -1.782528 0.114148 3.371641

Me-S-II_III

Number of imaginary frequencies = 1

C -0.306545 -1.172072 2.247182
C -1.356895 0.845642 2.285637
C -2.374279 1.592915 2.944951
C -3.111199 2.540514 2.284316
H -2.578764 1.332975 3.979135
C -1.794948 2.231688 0.288668
C -2.828489 2.858150 0.931869
H -3.917847 3.054938 2.799953
H -1.532472 2.520090 -0.726555
H -3.414261 3.615037 0.417214
C -1.012372 1.208051 0.910445
N -0.698880 -0.094167 2.959700
O -1.152502 -1.693966 1.365437
Co -0.881615 -0.709578 -0.225491
C -2.334431 -1.900853 -1.105802
C -2.506706 -0.573727 -1.559343
C -1.286019 -0.171226 -2.226788
C -0.381969 -1.272763 -2.198976
C -0.996330 -2.329854 -1.453853
C -3.298777 -2.706497 -0.317372
C -3.742252 0.237993 -1.391152
C -1.072259 1.093969 -2.983228
C 0.934241 -1.326974 -2.891520
C -0.460520 -3.689438 -1.180132
H -4.274769 -2.219687 -0.254869
H -3.442923 -3.694551 -0.767752
H -2.923193 -2.854027 0.701930
H -3.558193 1.302553 -1.549252
H -4.514436 -0.074742 -2.104384
H -4.157883 0.134244 -0.383892
H -0.102077 1.554036 -2.766991
H -1.107663 0.907336 -4.063760
H -1.845972 1.833517 -2.763819
H 1.724195 -1.752737 -2.266365
H 0.861283 -1.947730 -3.793149
H 1.258227 -0.333446 -3.211738
H 0.555976 -3.811838 -1.563626
H -0.452725 -3.893652 -0.103807
H -1.083080 -4.458083 -1.654065
C 0.366413 0.949700 0.441125
C 1.119075 2.035993 -0.238661
C 2.056371 1.736165 -1.238401
C 0.961353 3.378066 0.136092
C 2.788068 2.740036 -1.860188
H 2.209766 0.696687 -1.514813
C 1.701411 4.383085 -0.478333
H 0.258037 3.630640 0.925541
C 2.610873 4.070517 -1.484918
H 3.500972 2.483057 -2.639285
H 1.567948 5.415376 -0.165648
H 3.181502 4.857217 -1.970534
C 0.873621 -0.305601 0.687227
C 2.231205 -0.788213 0.661048
C 2.551082 -2.074523 0.188062
C 3.277006 -0.022369 1.221138
C 3.854418 -2.554387 0.222427
H 1.745788 -2.694141 -0.198227
C 4.575714 -0.508202 1.260521
H 3.048041 0.963332 1.620095
C 4.878139 -1.772974 0.754009
H 4.070527 -3.549836 -0.158139
H 5.362147 0.105607 1.692895
H 5.896802 -2.148592 0.787159
C 0.604375 -2.138726 2.940169
H 1.397459 -1.616642 3.479578
H 0.019457 -2.718234 3.661796
H 1.047657 -2.833722 2.224929

Me-S-III

Number of imaginary frequencies = 0

C 0.111491 -0.505035 -1.458458
C 0.469371 1.880043 -0.968838
C 1.298837 3.006016 -1.087715
C 0.824671 4.274741 -0.785443
H 2.314560 2.852015 -1.443625
C -1.314708 3.326159 -0.204248
C -0.485392 4.435663 -0.334551
H 1.475300 5.138022 -0.900025
H -2.323305 3.458252 0.176647
H -0.861262 5.422423 -0.079937
C -0.874316 2.036901 -0.530460
N 0.982041 0.630325 -1.213844

O	0.924599	-1.541869	-0.972380
Co	2.134089	-0.378300	-0.212368
C	3.199408	-1.671773	0.965454
C	4.085928	-0.848365	0.221066
C	3.806549	0.536836	0.542244
C	2.737135	0.562546	1.481459
C	2.325067	-0.802914	1.710472
C	3.029621	-3.145304	0.852059
C	5.105380	-1.298863	-0.761598
C	4.542179	1.704979	-0.010610
C	2.068923	1.759961	2.052990
C	1.191407	-1.234448	2.568869
H	3.778748	-3.588021	0.192015
H	3.115966	-3.636090	1.827470
H	2.043677	-3.387185	0.437781
H	5.190557	-0.598776	-1.597378
H	6.097736	-1.368804	-0.298494
H	4.864297	-2.280211	-1.176668
H	4.007361	2.640439	0.172339
H	5.535664	1.798922	0.444566
H	4.690754	1.615026	-1.091697
H	0.986686	1.609881	2.133651
H	2.444758	1.981920	3.058959
H	2.220980	2.648211	1.434227
H	0.336400	-0.558374	2.468139
H	0.850456	-2.238685	2.304413
H	1.476945	-1.248954	3.628178
C	-1.685070	0.830981	-0.334276
C	-3.007948	0.972974	0.330312
C	-3.256519	0.365532	1.565807
C	-4.042934	1.696760	-0.275839
C	-4.502106	0.473030	2.175409
H	-2.464327	-0.211681	2.037425
C	-5.290856	1.801492	0.329670
H	-3.864175	2.166327	-1.241252
C	-5.524280	1.190190	1.559284
H	-4.676047	-0.008383	3.134099
H	-6.084269	2.357778	-0.162312
H	-6.498260	1.271555	2.033877
C	-1.219619	-0.391393	-0.713377
C	-2.024307	-1.627620	-0.607906
C	-1.518277	-2.786174	0.000865
C	-3.323606	-1.674003	-1.138318
C	-2.296733	-3.935182	0.097770
H	-0.505242	-2.770167	0.387730
C	-4.096266	-2.824988	-1.047814
H	-3.724418	-0.788930	-1.626655
C	-3.587162	-3.961413	-0.424119
H	-1.889069	-4.819121	0.582331
H	-5.098292	-2.834788	-1.468783
H	-4.190058	-4.862617	-0.351183
C	-0.158904	-0.705212	-2.948668
H	-0.743663	0.126623	-3.355683
H	0.793899	-0.768086	-3.479473
H	-0.715618	-1.634453	-3.099751

Me-S-II_IV

Number of imaginary frequencies = 1

C	-0.955477	0.093294	2.502557
C	1.167891	0.870007	-0.041493
C	0.631865	-0.371635	-0.003114
C	-0.798392	2.134095	0.906812
C	-1.634451	3.272779	0.864290
C	-1.394281	4.317290	-0.017702
H	-2.445789	3.330089	1.585038
C	0.537218	3.162566	-0.843745
C	-0.292961	4.277972	-0.871607
H	-2.055533	5.180289	-0.013072
H	1.401565	3.123092	-1.503616
H	-0.081419	5.102922	-1.545042
C	0.298432	2.065905	-0.009093
N	-0.973752	1.256957	1.943660
O	-1.205802	-1.027470	1.899013
Co	-1.302850	-0.397934	0.089485
C	-3.098729	-1.435021	-0.282720
C	-3.285629	-0.087646	-0.626304
C	-2.282246	0.266257	-1.618663
C	-1.504095	-0.883028	-1.906104
C	-1.940435	-1.929187	-1.012740
C	-3.808865	-2.214739	0.762053
C	-4.266043	0.872919	-0.055565
C	-2.182195	1.589904	-2.280847
C	-0.419429	-0.974898	-2.916083
C	-1.427500	-3.320519	-0.946227
H	-3.119283	-2.493439	1.566320
H	-4.627628	-1.645627	1.207779

H	-4.228427	-3.137838	0.347210
H	-3.789236	1.836917	0.154444
H	-5.088160	1.068327	-0.754842
H	-4.701293	0.506844	0.877360
H	-1.222776	1.721782	-2.785117
H	-2.974346	1.698208	-3.032764
H	-2.295352	2.411553	-1.567123
H	0.258022	-1.804611	-2.701348
H	-0.835969	-1.131894	-3.917898
H	0.180633	-0.059336	-2.942165
H	-0.427985	-3.410340	-1.379511
H	-1.366011	-3.673539	0.088176
H	-2.091924	-4.005914	-1.488308
C	1.405770	-1.616619	-0.030226
C	2.328450	-1.875785	-1.061236
C	1.234465	-2.605177	0.955192
C	3.043741	-3.067410	-1.107139
H	2.482432	-1.120160	-1.827570
C	1.961000	-3.789648	0.914162
H	0.513953	-2.428087	1.747985
C	2.865076	-4.031823	-0.118308
H	3.749249	-3.239501	-1.916275
H	1.817143	-4.533536	1.694182
H	3.426797	-4.961520	-0.150872
C	2.644123	1.095287	-0.002673
C	3.387377	1.411861	-1.145664
C	3.318174	0.987788	1.219219
C	4.761611	1.621681	-1.068721
H	2.881979	1.473140	-2.108802
C	4.691564	1.192623	1.298379
H	2.745726	0.734203	2.109898
C	5.417900	1.513903	0.154282
H	5.322098	1.862461	-1.968414
H	5.196800	1.099738	2.256321
H	6.490975	1.673807	0.214441
C	-0.682099	-0.014610	3.974336
H	-0.625032	0.968874	4.439999
H	-1.452124	-0.615674	4.465678
H	0.269546	-0.536257	4.122260

Me-S-IV

Number of imaginary frequencies = 0

C	-1.150008	4.556576	0.510890
C	-1.607991	3.242722	0.518244
C	-0.821908	2.180986	0.042763
C	0.452567	2.515117	-0.480489
C	0.909161	3.832213	-0.488728
C	0.109913	4.859271	0.004726
H	-1.787941	5.346863	0.897129
H	-2.605017	3.034805	0.894743
H	1.897465	4.033238	-0.896370
H	0.468763	5.884600	-0.009290
N	1.264374	1.471289	-0.932921
C	1.226953	0.925974	-2.139608
O	1.586929	-0.301301	-2.152891
Co	1.447764	-0.250070	-0.095276
C	1.540235	-1.023750	1.834550
C	2.218777	0.234043	1.714059
C	2.135602	-1.936521	0.915022
C	0.415718	-1.296392	2.765900
C	3.320691	0.065775	0.792541
C	1.874603	1.475062	2.456491
C	3.247977	-1.254333	0.290141
C	1.780501	-3.368016	0.720886
H	-0.084389	-2.238430	2.531645
H	0.780369	-1.355477	3.798139
H	-0.337756	-0.502043	2.727201
C	4.261085	1.136157	0.367566
H	0.797797	1.543239	2.640645
H	2.378459	1.511154	3.430611
H	2.165845	2.371870	1.902013
C	4.083270	-1.848222	-0.785719
H	1.908394	-3.676235	-0.321319
H	2.414391	-4.020884	1.334828
H	0.738081	-3.568305	0.985491
H	4.606872	0.981563	-0.658776
H	3.780655	2.118405	0.401230
H	5.147237	1.181191	1.011807
H	4.788144	-2.581933	-0.376967
H	3.460422	-2.366318	-1.521334
H	4.661790	-1.090960	-1.319815
C	-0.501106	-0.309973	-0.132285
C	-1.025560	-1.677314	-0.290578
C	-0.603744	-2.457637	-1.382336
C	-1.912812	-2.267859	0.627886
C	-1.063166	-3.758257	-1.555842

H 0.097410 -2.020311 -2.088878
C -2.351506 -3.577547 0.465204
H -2.260046 -1.684631 1.476489
C -1.934262 -4.330045 -0.630347
H -0.730154 -4.333769 -2.416365
H -3.033033 -4.008289 1.194662
H -2.284362 -5.350507 -0.760994
C -1.304663 0.786061 -0.001448
C -2.788381 0.600554 0.064851
C -3.515466 0.232666 -1.071484
C -3.476252 0.733468 1.277642
C -4.884132 -0.007382 -0.997661
H -2.988767 0.112010 -2.016195
C -4.845365 0.496772 1.355007
H -2.918076 1.005503 2.172906
C -5.554030 0.122542 0.215977
H -5.428959 -0.301665 -1.890896
H -5.357967 0.596190 2.308517
H -6.621978 -0.069037 0.274709
C 0.745961 1.614622 -3.371121
H 0.831715 2.699912 -3.290138
H 1.294942 1.256850 -4.243630
H -0.311973 1.370695 -3.521975

Me-S-IV_V
Number of imaginary frequencies = 1
C 1.430545 4.280620 1.201571
C 1.906278 3.136512 0.573407
C 1.166153 1.939170 0.628069
C -0.048287 1.968583 1.363645
C -0.538954 3.115298 1.974625
C 0.215273 4.285593 1.893084
H 2.018455 5.193295 1.151133
H 2.863489 3.164174 0.062913
H -1.492685 3.095419 2.497530
H -0.143642 5.194812 2.365360
N -0.677994 0.729645 1.288003
C -1.522211 0.058244 2.120412
O -2.094272 -0.889276 1.523306
Co -1.379576 -0.180000 -0.304738
C -1.105688 -0.536977 -2.347264
C -1.268214 0.858555 -2.019950
C -2.249473 -1.212500 -1.858663
C 0.106048 -1.113945 -2.991141
C -2.596972 1.059269 -1.475846
C -0.309153 1.942479 -2.359894
C -3.181737 -0.213166 -1.337536
C -2.532999 -2.674390 -1.884563
H 0.068144 -2.206376 -3.031803
H 0.218306 -0.754348 -4.021305
H 1.020268 -0.834166 -2.452854
C -3.140982 2.370175 -1.029839
H 0.717803 1.567837 -2.402580
H -0.543311 2.378291 -3.340192
H -0.334357 2.757843 -1.628498
C -4.500663 -0.544757 -0.735610
H -2.766210 -3.056819 -0.883446
H -3.391992 -2.906388 -2.526508
H -1.680858 -3.247880 -2.260702
H -3.460126 2.990959 -1.876360
H -4.006834 2.245576 -0.372577
H -2.387736 2.948048 -0.479819
H -4.434664 -1.430968 -0.097268
H -4.885189 0.274593 -0.121508
H -5.251400 -0.756881 -1.507448
C 0.442336 -0.323976 0.424114
C 0.636706 -1.681325 0.973719
C 1.060939 -1.837526 2.302694
C 0.362083 -2.826983 0.219832
C 1.189012 -3.105361 2.862433
H 1.299893 -0.948036 2.884794
C 0.531181 -4.093660 0.763870
H 0.016203 -2.698740 -0.802427
C 0.931742 -4.236940 2.092721
H 1.503308 -3.210734 3.897798
H 0.333819 -4.973235 0.156444
H 1.040534 -5.227214 2.526107
C 1.489383 0.601003 0.209193
C 2.784298 0.237089 -0.383479
C 3.511498 -0.923890 -0.055450
C 3.330842 1.072727 -1.379577
C 4.715001 -1.218712 -0.684551
H 3.139298 -1.593539 0.713020
C 4.536173 0.776676 -2.003088
H 2.777134 1.955981 -1.687081
C 5.241258 -0.373249 -1.659325

H 5.254535 -2.118463 -0.398943
H 4.919909 1.445113 -2.769979
H 6.184700 -0.609010 -2.143709
C -1.691501 0.367246 3.564473
H -2.660962 0.844247 3.741211
H -1.680271 -0.563378 4.137275
H -0.906355 1.035389 3.924353

Me-S-V

Number of imaginary frequencies = 0

C 1.152266 4.436615 0.554009
C 1.979742 3.374862 0.220056
C 1.563043 2.068870 0.512564
C 0.332343 1.868070 1.184554
C -0.508351 2.934065 1.506461
C -0.083845 4.216598 1.181188
H 1.462659 5.453029 0.328372
H 2.938294 3.547922 -0.262589
H -1.466026 2.777157 1.990984
H -0.720197 5.063076 1.424487
N 0.159293 0.505307 1.379677
C -1.155222 -0.070989 1.661500
O -1.307516 -1.350404 1.322079
Co -2.187240 -0.412634 0.070083
C -2.313308 -0.947550 -1.924223
C -1.922258 0.446848 -1.702988
C -3.563728 -1.146106 -1.322250
C -1.443877 -1.958811 -2.580445
C -2.990534 1.124874 -1.043404
C -0.632101 1.036692 -2.148751
C -3.947772 0.118842 -0.705334
C -4.344185 -2.408202 -1.226841
H -1.831695 -2.972258 -2.454457
H -1.349574 -1.767609 -3.656513
H -0.431419 -1.944246 -2.161780
C -3.078330 2.572555 -0.711726
H 0.211507 0.369630 -1.933112
H -0.631833 1.216908 -3.231490
H -0.425970 1.988590 -1.650300
C -5.183542 0.325636 0.094637
H -4.730652 -2.568103 -0.215153
H -5.210943 -2.398075 -1.899880
H -3.738014 -3.280267 -1.483290
H -3.544015 2.737245 0.265918
H -2.093036 3.044344 -0.680746
H -3.684648 3.111211 -1.451114
H -5.401575 -0.536631 0.732436
H -5.105445 1.207233 0.736958
H -6.056381 0.471006 -0.554942
C 1.253372 -0.156553 0.819388
C 1.428618 -1.609255 0.886913
C 1.268836 -2.304806 2.092899
C 1.832810 -2.321411 -0.249788
C 1.505484 -3.671010 2.158685
H 0.955649 -1.759766 2.980287
C 2.065608 -3.690801 -0.183954
H 1.974704 -1.784481 -1.185836
C 1.904068 -4.370420 1.020606
H 1.379430 -4.193789 3.103023
H 2.375685 -4.227856 -1.076351
H 2.088887 -5.439826 1.073801
C 2.137015 0.774395 0.288094
C 3.435041 0.525149 -0.343404
C 4.362015 -0.389192 0.181965
C 3.788026 1.226509 -1.507663
C 5.588425 -0.596051 -0.437006
H 4.108863 -0.937743 1.085912
C 5.019275 1.023752 -2.122202
H 3.072164 1.922425 -1.940569
C 5.925513 0.110489 -1.590343
H 6.290738 -1.307420 -0.010605
H 5.268359 1.576954 -3.024183
H 6.887693 -0.049269 -2.069041
C -1.771132 0.390364 2.966017
H -1.021547 0.802724 3.650112
H -2.545245 1.151681 2.824620
H -2.245725 -0.470766 3.443123

NNMe2-S-I

Number of imaginary frequencies = 0

C 3.767055 -1.851861 -0.274156
C 3.437643 -3.043111 -0.915596
C 2.108710 -3.343391 -1.163070
C 1.048402 -2.484215 -0.785900
C 1.395569 -1.268183 -0.146691
C 2.739198 -0.986979 0.100982

H 4.802206 -1.587653 -0.070814
H 4.215113 -3.739839 -1.220903
H 1.827137 -4.270309 -1.657533
H 3.012056 -0.052516 0.587257
N -0.214153 -2.968741 -1.062636
O -1.322898 -0.944230 -0.590389
Co -0.015581 -0.126635 0.593116
C 0.479457 -1.023239 2.440673
C 0.825404 0.364299 2.457299
C -0.394112 1.120501 2.325610
C -1.470442 0.223519 2.140626
C -0.923679 -1.108914 2.186349
C 1.371030 -2.177341 2.722418
C 2.148058 0.959245 2.791015
C -0.441062 2.601547 2.399022
C -2.896491 0.540063 1.871160
C -1.707819 -2.361265 2.052693
H 1.128181 -3.037651 2.092568
H 2.420423 -1.936421 2.542151
H 1.261169 -2.484533 3.770016
H 2.464518 1.703975 2.050593
H 2.113459 1.465446 3.764023
H 2.929939 0.198689 2.842842
H -1.454447 2.989754 2.281369
H -0.058160 2.944725 3.367120
H 0.190072 3.056036 1.625503
H -3.202773 0.092112 0.917653
H -3.554750 0.141889 2.651534
H -3.072508 1.615996 1.793407
H -2.608030 -2.204662 1.452661
H -1.126550 -3.149679 1.566046
H -2.017376 -2.729916 3.038458
C 0.779838 1.433485 -0.680206
C -0.454720 1.608694 -0.677165
C -1.780402 2.086997 -0.895495
C -2.171679 3.334605 -0.370074
C -2.704888 1.361127 -1.668248
H -1.447684 3.926211 0.181662
C -3.459899 3.811773 -0.569519
C -3.992833 1.845454 -1.855630
H -2.391514 0.418133 -2.096271
H -3.744270 4.776939 -0.159389
C -4.381379 3.062079 -1.299096
H -4.697603 1.267180 -2.447965
H -5.390532 3.435222 -1.449295
C 2.122566 1.765432 -1.061324
C 2.785710 1.064589 -2.080969
C 2.787020 2.819617 -0.414289
C 4.077567 1.420046 -2.442978
H 2.283330 0.228728 -2.558426
H 2.270269 3.371124 0.368550
C 4.084914 3.162196 -0.775649
H 4.581472 0.868090 -3.231067
C 4.733891 2.462684 -1.790023
H 4.587648 3.979539 -0.266437
H 5.748908 2.728584 -2.071304
C -1.258833 -2.192239 -0.956270
N -2.497637 -2.767323 -1.246512
C -2.545686 -4.025581 -1.955673
C -3.673979 -1.950552 -1.391305
H -1.656124 -4.602926 -1.715105
H -3.443281 -4.577347 -1.653941
H -2.586555 -3.885527 -3.047695
H -3.650402 -1.114618 -0.691497
H -3.790511 -1.536209 -2.408899
H -4.561191 -2.559607 -1.184986

NNMe2-S-I_II
Number of imaginary frequencies = 1
C -0.825345 0.919318 -0.196862
C 0.428167 0.946090 -0.457874
C -0.581026 -0.244111 2.424053
C -1.408370 -0.192704 3.574113
C -2.736624 -0.581841 3.554994
H -0.937704 0.145009 4.494003
C -2.549506 -1.012693 1.203522
C -3.321697 -1.003885 2.359196
H -3.322796 -0.544131 4.469948
H -3.032307 -1.251003 0.260303
H -4.370904 -1.283733 2.316437
C -1.191914 -0.670522 1.208956
N 0.714435 0.159245 2.599576
O 1.493718 -1.213282 0.865238
Co -0.029364 -0.967054 -0.348576
C 1.037047 -2.098359 -1.807552
C 0.287463 -2.987309 -0.941292

C	-1.086203	-2.719682	-1.103669
C	-1.203057	-1.583927	-1.976627
C	0.116828	-1.257014	-2.465724
C	2.508480	-2.182659	-1.978289
C	0.900182	-4.002483	-0.051174
C	-2.191708	-3.525071	-0.516613
C	-2.474307	-1.012462	-2.499370
C	0.417124	-0.172411	-3.435987
H	2.906554	-1.368980	-2.589035
H	3.005393	-2.157701	-1.001868
H	2.790637	-3.127634	-2.458287
H	1.390617	-4.796093	-0.627374
H	1.657491	-3.530677	0.584661
H	0.157306	-4.467558	0.601108
H	-3.172293	-3.156306	-0.827060
H	-2.112000	-4.565377	-0.851566
H	-2.171674	-3.523470	0.577271
H	-3.193235	-0.778295	-1.707060
H	-2.300083	-0.087145	-3.054013
H	-2.962858	-1.717494	-3.183323
H	-0.053073	0.769622	-3.129956
H	1.490672	0.016253	-3.515449
H	0.040865	-0.417321	-4.435975
C	-2.052564	1.683930	-0.300494
C	-2.362959	2.277142	-1.536359
C	-2.870361	1.963161	0.805517
C	-3.472370	3.102346	-1.671509
H	-1.710457	2.087999	-2.386953
C	-3.973132	2.796986	0.665645
H	-2.612531	1.546294	1.774701
C	-4.285041	3.360677	-0.569977
H	-3.698276	3.548598	-2.636224
H	-4.590026	3.013493	1.533375
H	-5.152212	4.007457	-0.671567
C	1.613278	1.727896	-0.640016
C	2.864502	1.146542	-0.887577
C	1.526568	3.131765	-0.551479
C	3.994197	1.938998	-1.051832
H	2.929524	0.064287	-0.910399
C	2.658338	3.916281	-0.716156
H	0.561499	3.588626	-0.348035
C	3.897669	3.326160	-0.968279
H	4.957480	1.469522	-1.237371
H	2.575307	4.997419	-0.644398
H	4.781551	3.945204	-1.094299
C	1.650870	-0.359288	1.835200
N	2.957119	-0.011571	2.114487
C	3.276355	0.938858	3.149336
C	4.082465	-0.676904	1.519503
H	3.904944	0.479208	3.925414
H	3.830781	1.788580	2.725545
H	2.351515	1.294986	3.597802
H	3.743892	-1.355778	0.738424
H	4.779220	0.050943	1.080625
H	4.639285	-1.258719	2.269848

NNMe2-S-II

Number of imaginary frequencies = 0

C	-0.997004	-0.380787	-0.834450
C	-0.354063	0.788965	-0.670719
C	-0.007454	-2.451159	0.325040
C	0.572675	-3.737232	0.106749
C	1.104564	-4.083298	-1.109611
H	0.549747	-4.441375	0.933581
C	0.570639	-1.924766	-2.019800
C	1.118984	-3.172749	-2.194809
H	1.526814	-5.077054	-1.243209
H	0.515666	-1.220782	-2.848551
H	1.535302	-3.468293	-3.153834
C	-0.001741	-1.512673	-0.781061
N	-0.607889	-2.198071	1.491119
O	0.241201	-0.052591	1.783096
Co	1.268479	0.056500	0.068959
C	2.619280	1.342859	0.902752
C	3.088117	-0.008308	1.150392
C	3.293110	-0.635020	-0.091212
C	2.910207	0.300494	-1.131959
C	2.576537	1.547422	-0.509084
C	2.314145	2.325767	1.973731
C	3.215892	-0.604494	2.505046
C	3.814884	-2.004176	-0.328907
C	3.063318	0.081853	-2.595600
C	2.270039	2.813050	-1.223455
H	1.849023	3.231416	1.576014
H	1.631113	1.889492	2.711153
H	3.226085	2.623239	2.506242

H 4.046121 -0.157071 3.064682
H 2.297306 -0.436743 3.077141
H 3.386093 -1.683115 2.460302
H 3.284651 -2.506100 -1.142810
H 4.874556 -1.963955 -0.610305
H 3.731036 -2.635720 0.558690
H 3.005751 -0.979686 -2.853196
H 2.286475 0.604225 -3.163363
H 4.032807 0.455109 -2.950370
H 1.705307 2.631568 -2.142508
H 1.679274 3.501009 -0.613162
H 3.199810 3.324212 -1.501577
C -2.433186 -0.686823 -0.916900
C -3.415721 0.267927 -0.595248
C -2.863626 -1.979682 -1.260320
C -4.765448 -0.058686 -0.628921
H -3.113217 1.269409 -0.301615
C -4.214661 -2.304322 -1.288192
H -2.123046 -2.739178 -1.503131
C -5.175179 -1.346093 -0.974768
H -5.504853 0.696654 -0.373695
H -4.518390 -3.313078 -1.556387
H -6.231460 -1.599606 -0.994326
C -0.792759 2.168093 -0.696276
C -1.211377 2.788487 -1.886329
C -0.753914 2.940929 0.478745
C -1.575808 4.130462 -1.897200
H -1.246033 2.199097 -2.800204
C -1.126441 4.279427 0.464398
H -0.429463 2.454655 1.395697
C -1.534168 4.883659 -0.725218
H -1.895614 4.592475 -2.827961
H -1.097480 4.857048 1.385459
H -1.818806 5.931837 -0.737994
C -0.672944 -0.942935 1.945709
N -1.721450 -0.631079 2.768088
C -2.903617 -1.465815 2.788628
C -1.877832 0.720262 3.248289
H -2.620633 -2.490508 2.552455
H -3.358525 -1.430916 3.784076
H -3.647243 -1.130305 2.050534
H -0.900088 1.166954 3.426570
H -2.422672 1.354505 2.531371
H -2.441258 0.706024 4.186501

NNMe2-S-II_III
Number of imaginary frequencies = 1
C 0.771992 -1.443333 1.593189
C -1.095189 -0.421017 2.441868
C -2.112448 -0.476404 3.449963
C -3.371659 0.001503 3.226167
H -1.851085 -0.988598 4.371150
C -2.722287 0.840229 1.059362
C -3.691431 0.656481 2.004045
H -4.138559 -0.115720 3.987437
H -2.942557 1.412337 0.161038
H -4.694861 1.040158 1.840358
C -1.390378 0.330179 1.215739
N 0.055354 -1.010491 2.695972
O 0.107493 -2.162337 0.689361
Co -0.618234 -0.840982 -0.484617
C -1.481673 -2.378828 -1.567208
C -2.373891 -1.282705 -1.574968
C -1.686243 -0.155801 -2.165424
C -0.384367 -0.592502 -2.565861
C -0.231539 -1.951061 -2.159046
C -1.724961 -3.726510 -0.997265
C -3.775372 -1.317266 -1.075264
C -2.293436 1.160572 -2.505355
C 0.623845 0.207362 -3.314365
C 0.921713 -2.848903 -2.422393
H -2.716337 -3.801017 -0.544387
H -1.649855 -4.499532 -1.770681
H -0.981936 -3.949336 -0.223661
H -4.212486 -0.319245 -1.005635
H -4.409635 -1.907348 -1.747262
H -3.840426 -1.766360 -0.079091
H -1.617155 1.998205 -2.310638
H -2.559083 1.195941 -3.569250
H -3.212798 1.343971 -1.943332
H 1.601253 0.209937 -2.818944
H 0.770944 -0.207481 -4.318666
H 0.304370 1.245185 -3.435640
H 1.808116 -2.295498 -2.742537
H 1.179405 -3.427540 -1.529762
H 0.680309 -3.567655 -3.215794

C	-0.254120	0.992256	0.549037
C	-0.346763	2.417472	0.141796
C	0.363806	2.892128	-0.970685
C	-1.075700	3.343525	0.900912
C	0.327629	4.234076	-1.327386
H	0.957420	2.189765	-1.548186
C	-1.106835	4.689770	0.549460
H	-1.609982	3.004840	1.784594
C	-0.412621	5.140284	-0.569613
H	0.881984	4.574240	-2.198160
H	-1.672757	5.389962	1.158180
H	-0.440545	6.190564	-0.845954
C	0.869350	0.200893	0.416827
C	2.232297	0.537219	0.080092
C	3.025953	-0.361870	-0.654181
C	2.865177	1.677592	0.616989
C	4.377613	-0.124218	-0.871553
H	2.553449	-1.266797	-1.029656
C	4.216249	1.911399	0.401108
H	2.279601	2.373509	1.213835
C	4.982551	1.016371	-0.346451
H	4.964735	-0.839118	-1.443750
H	4.679150	2.799431	0.824825
H	6.040288	1.202427	-0.509931
N	2.066441	-1.854084	1.871365
C	2.683730	-2.980549	1.232568
C	2.811553	-1.218367	2.923322
H	2.041751	-3.333883	0.426407
H	3.666222	-2.711668	0.818290
H	2.834651	-3.810374	1.941306
H	2.292012	-0.313606	3.241887
H	2.925498	-1.868278	3.803963
H	3.813423	-0.944029	2.563513

NNMe2-S-III

Number of imaginary frequencies = 0

C	1.597396	-0.658010	-2.206248
C	2.810155	-0.677671	-2.982847
C	3.765987	0.281283	-2.836982
H	2.938846	-1.520367	-3.655913
C	2.413375	1.469833	-1.215577
C	3.572496	1.366464	-1.928200
H	4.687203	0.225945	-3.411283
H	2.256486	2.320111	-0.555571
H	4.345917	2.122007	-1.819580
C	1.381320	0.483307	-1.308778
N	0.751858	-1.649215	-2.312064
O	0.575026	-2.096037	-0.112712
Co	0.706088	-0.413339	0.710600
C	1.917163	-1.239124	2.136059
C	2.309052	0.115453	1.965726
C	1.173310	0.951979	2.251699
C	0.093582	0.103293	2.663894
C	0.534412	-1.251933	2.555660
C	2.731328	-2.449782	1.868177
C	3.666553	0.579938	1.574640
C	1.218880	2.439704	2.317370
C	-1.238687	0.511460	3.188730
C	-0.247875	-2.474707	2.873693
H	3.703579	-2.193523	1.440500
H	2.905612	-3.021251	2.787183
H	2.211675	-3.101118	1.156997
H	3.678093	1.644604	1.329874
H	4.374885	0.421482	2.396444
H	4.048737	0.042581	0.700290
H	0.237771	2.874004	2.516871
H	1.897627	2.766234	3.114433
H	1.573677	2.890854	1.384561
H	-2.063665	0.112585	2.585032
H	-1.375806	0.127966	4.206333
H	-1.349123	1.597537	3.233482
H	-1.298909	-2.242316	3.065355
H	-0.202125	-3.185152	2.041691
H	0.149575	-2.973677	3.765992
C	0.029177	0.752267	-0.861693
C	-0.439881	2.150206	-0.679632
C	-1.295087	2.519326	0.364909
C	-0.087382	3.131200	-1.617006
C	-1.770661	3.818155	0.482785
H	-1.592631	1.764686	1.084590
C	-0.565102	4.433946	-1.504463
H	0.561222	2.861838	-2.446718
C	-1.405003	4.785146	-0.451579
H	-2.428950	4.076135	1.308834
H	-0.280204	5.174973	-2.246465
H	-1.775308	5.802621	-0.362016

C -0.813922 -0.381748 -0.749026
C -2.253229 -0.334078 -0.426207
C -2.778602 -1.266090 0.480779
C -3.133599 0.568194 -1.038488
C -4.131930 -1.269634 0.797531
H -2.095319 -1.988362 0.918682
C -4.489944 0.560320 -0.727035
H -2.747701 1.280100 -1.764297
C -4.992766 -0.352131 0.197354
H -4.517906 -1.995189 1.509026
H -5.156048 1.268957 -1.211945
H -6.051300 -0.353851 0.442716
C -0.189142 -1.735736 -1.214294
N -1.216226 -2.732665 -1.489265
C -1.895516 -2.465223 -2.744144
C -0.676152 -4.081518 -1.484051
H -1.236761 -2.579688 -3.620585
H -2.740322 -3.154575 -2.846699
H -2.295735 -1.446321 -2.750882
H -0.182043 -4.276643 -0.530784
H -1.503423 -4.789154 -1.601936
H 0.050148 -4.256949 -2.295955

NNMe2-S-II_IV
Number of imaginary frequencies = 1
C -0.706942 0.205920 2.257963
C 1.120176 0.869291 -0.375560
C 0.616035 -0.382433 -0.323720
C -0.813697 2.163101 0.639056
C -1.664257 3.296298 0.555628
C -1.497488 4.277140 -0.408742
H -2.426276 3.398279 1.324062
C 0.372578 3.071570 -1.289381
C -0.464111 4.179209 -1.342138
H -2.165631 5.135297 -0.416812
H 1.184532 2.983361 -2.008725
H -0.312073 4.950167 -2.091089
C 0.215600 2.043045 -0.351981
N -0.955052 1.387469 1.756012
O -1.015557 -0.929008 1.702745
Co -1.307912 -0.409117 -0.123628
C -3.101423 -1.496574 -0.303566
C -3.348818 -0.171507 -0.687822
C -2.427842 0.161055 -1.766629
C -1.643333 -0.980231 -2.066528
C -1.988025 -1.996624 -1.099556
C -3.692720 -2.242699 0.835076
C -4.301783 0.795233 -0.082976
C -2.398573 1.464488 -2.473328
C -0.627315 -1.088957 -3.144017
C -1.449617 -3.377747 -1.029250
H -2.919664 -2.479258 1.574915
H -4.469015 -1.665214 1.341461
H -4.136682 -3.187154 0.501535
H -3.815717 1.761687 0.091694
H -5.155991 0.980166 -0.745640
H -4.691020 0.440987 0.874229
H -1.465867 1.609416 -3.022600
H -3.226688 1.524764 -3.191243
H -2.503633 2.304292 -1.779656
H 0.116683 -1.857086 -2.917658
H -1.098254 -1.348975 -4.099427
H -0.092131 -0.143495 -3.279939
H -0.478239 -3.465188 -1.522720
H -1.320327 -3.703433 0.007548
H -2.137115 -4.084652 -1.511869
C 1.412010 -1.612017 -0.364042
C 2.306841 -1.856788 -1.422640
C 1.292177 -2.599922 0.629698
C 3.046683 -3.032996 -1.484538
H 2.418316 -1.100961 -2.196754
C 2.041782 -3.768852 0.571675
H 0.592321 -2.432947 1.442178
C 2.919597 -3.996135 -0.486233
H 3.730439 -3.194279 -2.314336
H 1.936858 -4.512689 1.358176
H 3.500525 -4.913312 -0.532132
C 2.591121 1.125513 -0.340926
C 3.326092 1.482762 -1.477170
C 3.271160 0.997514 0.876064
C 4.695675 1.719051 -1.396494
H 2.820542 1.552240 -2.439285
C 4.639780 1.230356 0.959231
H 2.704861 0.700554 1.757827
C 5.356507 1.596996 -0.177280
H 5.249667 1.991252 -2.291251

H	5.149154	1.122995	1.913551
H	6.425876	1.779411	-0.114856
N	-0.240214	0.127482	3.550509
C	0.257936	1.299682	4.226149
C	0.093673	-1.148564	4.134887
H	-0.180798	2.187019	3.770846
H	-0.019028	1.260447	5.285561
H	1.353175	1.380188	4.165366
H	-0.524556	-1.931800	3.699242
H	1.151470	-1.412099	3.978135
H	-0.087656	-1.113496	5.214576

NNMe2-S-IV

Number of imaginary frequencies = 0

C	-1.181282	4.153253	1.661262
C	-1.625952	2.861985	1.400838
C	-0.866159	1.955477	0.644506
C	0.347355	2.426834	0.088145
C	0.796610	3.719575	0.370330
C	0.041792	4.584963	1.154189
H	-1.791192	4.820534	2.263966
H	-2.584366	2.540545	1.798431
H	1.743573	4.035796	-0.063478
H	0.400853	5.590295	1.357052
N	1.146940	1.572929	-0.690095
O	1.191733	-0.173324	-2.034310
Co	1.482118	-0.252598	-0.033641
C	1.939131	-1.047772	1.809444
C	2.647407	0.175330	1.580112
C	2.315832	-1.973943	0.782669
C	0.991653	-1.303248	2.925735
C	3.516408	-0.007261	0.442034
C	2.535347	1.415680	2.390140
C	3.294072	-1.317778	-0.048017
C	1.915508	-3.402625	0.681028
H	0.312164	-2.125984	2.688860
H	1.531252	-1.570849	3.842375
H	0.381289	-0.421156	3.145210
C	4.372058	1.053875	-0.152089
H	1.527083	1.548408	2.795406
H	3.231680	1.396551	3.238061
H	2.764947	2.303707	1.794731
C	3.849686	-1.912034	-1.292371
H	1.873747	-3.738549	-0.359010
H	2.633327	-4.047450	1.205088
H	0.927742	-3.585476	1.113662
H	4.770082	0.751971	-1.124275
H	3.794792	1.972355	-0.307585
H	5.225472	1.298451	0.491368
H	4.591744	-2.686422	-1.065603
H	3.055562	-2.380411	-1.882410
H	4.327359	-1.161827	-1.926190
C	-0.450142	-0.464803	0.173883
C	-0.931555	-1.841316	-0.016222
C	-0.627554	-2.563857	-1.183961
C	-1.675318	-2.498925	0.981072
C	-1.064210	-3.873061	-1.350263
H	-0.034707	-2.076019	-1.953266
C	-2.092757	-3.816049	0.821496
H	-1.926712	-1.956778	1.889501
C	-1.792397	-4.511118	-0.347510
H	-0.824535	-4.405620	-2.267962
H	-2.660711	-4.299229	1.612777
H	-2.122401	-5.538527	-0.475815
C	-1.305470	0.567218	0.413773
C	-2.784874	0.342006	0.379345
C	-3.418087	0.197593	-0.859915
C	-3.567955	0.255128	1.536465
C	-4.787944	-0.029015	-0.943953
H	-2.811118	0.248868	-1.762650
C	-4.939994	0.032019	1.456885
H	-3.085802	0.346105	2.508969
C	-5.554872	-0.109714	0.215647
H	-5.258302	-0.145784	-1.916920
H	-5.529019	-0.038556	2.367831
H	-6.625028	-0.287321	0.152959
C	0.752827	1.018775	-1.856043
N	-0.033803	1.606639	-2.793353
C	-0.403386	3.005208	-2.743759
C	-0.529834	0.831502	-3.909835
H	0.377220	3.588985	-2.255125
H	-0.518321	3.374163	-3.767274
H	-1.345767	3.170670	-2.203805
H	-0.346374	-0.225718	-3.723959
H	-1.607496	0.993955	-4.026411
H	-0.036686	1.116670	-4.847949

NNMe2-S-IV_V

Number of imaginary frequencies = 1

C	1.162301	4.310361	1.132704
C	1.776738	3.176425	0.619064
C	1.090792	1.947475	0.589933
C	-0.227113	1.926491	1.130488
C	-0.847839	3.065084	1.635380
C	-0.144843	4.267744	1.632243
H	1.707269	5.250705	1.142304
H	2.795961	3.234460	0.248080
H	-1.863645	3.003782	2.021104
H	-0.613833	5.169092	2.015451
N	-0.783003	0.661346	0.995138
C	-1.726478	-0.095055	1.632819
O	-2.189187	-1.001922	0.884036
Co	-1.158568	-0.167197	-0.733617
C	-0.552710	-0.288301	-2.730789
C	-0.903675	1.050463	-2.326063
C	-1.680980	-1.108381	-2.489115
C	0.790692	-0.685086	-3.232575
C	-2.311799	1.080686	-1.988340
C	-0.015491	2.238439	-2.426238
C	-2.775804	-0.246194	-2.048384
C	-1.804937	-2.579451	-2.685820
H	0.864264	-1.763821	-3.398056
H	1.016257	-0.195192	-4.187753
H	1.585532	-0.398990	-2.531649
C	-3.048167	2.287822	-1.526986
H	1.034946	1.963958	-2.287648
H	-0.107777	2.714779	-3.411242
H	-0.256008	2.996104	-1.673054
C	-4.122146	-0.752185	-1.671317
H	-2.162881	-3.078065	-1.777068
H	-2.512521	-2.822382	-3.488734
H	-0.845168	-3.035573	-2.945647
H	-3.340293	2.937372	-2.361868
H	-3.961852	2.022877	-0.986168
H	-2.430489	2.895396	-0.854300
H	-4.045552	-1.672476	-1.084425
H	-4.676252	-0.025471	-1.070667
H	-4.727926	-0.979889	-2.557450
C	0.538293	-0.345574	0.233192
C	0.666750	-1.742851	0.674191
C	0.654474	-2.067103	2.040935
C	0.753456	-2.787627	-0.255287
C	0.701696	-3.393949	2.458244
H	0.613074	-1.259064	2.770960
C	0.843169	-4.107926	0.161963
H	0.754786	-2.540308	-1.313353
C	0.802752	-4.419344	1.521889
H	0.675944	-3.627257	3.519995
H	0.931711	-4.901085	-0.576196
H	0.849188	-5.454639	1.847581
C	1.550071	0.628981	0.244622
C	2.964276	0.311894	-0.015470
C	3.644089	-0.742601	0.620172
C	3.686275	1.070242	-0.956797
C	4.973961	-1.020250	0.326599
H	3.126128	-1.340250	1.364219
C	5.017947	0.793855	-1.245451
H	3.177322	1.873685	-1.486075
C	5.672109	-0.255799	-0.605601
H	5.473044	-1.837558	0.841331
H	5.542680	1.395591	-1.983628
H	6.711790	-0.475903	-0.830899
N	-2.097185	0.055034	2.929953
C	-1.266096	0.719898	3.914260
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H	-0.421631	1.217419	3.440640
H	-1.842306	1.469520	4.467609
H	-0.881507	-0.015522	4.633412
H	-3.737384	-1.204928	2.664992
H	-2.578936	-1.765536	3.887668
H	-3.647654	-0.386301	4.247501

NNMe2-S-V

Number of imaginary frequencies = 0

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C	-0.468774	-0.702860	1.967616
C	0.848165	-1.123075	1.684472
C	1.514640	-2.111796	2.372023
C	0.820988	-2.748144	3.417160
H	-1.022594	-2.900928	4.497551
H	-2.180857	-1.150339	3.217032

H	2.525944	-2.402198	2.098860
H	1.310834	-3.532020	3.986523
N	1.266928	-0.450365	0.494633
C	2.664583	-0.432772	0.108204
O	3.042957	-0.990744	-0.908099
Co	-0.308240	-0.797033	-0.723927
C	-2.049128	-1.373909	-1.592717
C	-1.378999	-2.540316	-1.078976
C	-1.214272	-0.755241	-2.594945
C	-3.428656	-0.965139	-1.210636
C	-0.097763	-2.574075	-1.696143
C	-1.890340	-3.444167	-0.013313
C	0.003826	-1.485853	-2.649960
C	-1.550257	0.437285	-3.422169
H	-3.673281	0.044582	-1.547414
H	-4.164217	-1.650296	-1.650055
H	-3.574722	-0.983186	-0.124276
C	0.987621	-3.548440	-1.399262
H	-2.561078	-2.910199	0.668784
H	-2.450382	-4.297805	-0.417473
H	-1.073546	-3.844202	0.596568
C	1.141799	-1.245283	-3.577744
H	-0.711911	1.141850	-3.469632
H	-1.796689	0.156963	-4.454212
H	-2.411631	0.979289	-3.021227
H	0.962592	-4.393756	-2.098492
H	1.971124	-3.077529	-1.476052
H	0.890172	-3.960268	-0.389488
H	1.076357	-1.884482	-4.468800
H	1.156112	-0.208570	-3.929662
H	2.101751	-1.445624	-3.095176
C	0.362151	0.678238	0.194689
C	0.913249	1.996689	-0.158760
C	0.579575	3.135797	0.588552
C	1.805252	2.134769	-1.233317
C	1.131522	4.373565	0.277532
H	-0.112478	3.036341	1.421383
C	2.378346	3.368160	-1.522569
H	2.047863	1.259745	-1.833733
C	2.041341	4.493027	-0.770707
H	0.860295	5.246376	0.865274
H	3.078644	3.455232	-2.349209
H	2.479686	5.458932	-1.006445
C	-0.828117	0.307475	0.963232
C	-2.023778	1.154735	0.957333
C	-2.889325	1.252645	2.057774
C	-2.332219	1.931090	-0.177162
C	-4.029439	2.050969	2.010588
H	-2.653856	0.725348	2.975596
C	-3.460645	2.736307	-0.218507
H	-1.670021	1.876444	-1.038761
C	-4.328856	2.791605	0.872136
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H	-3.670976	3.316953	-1.113774
H	-5.220635	3.410658	0.835805
N	3.485846	0.215241	0.977364
C	3.061475	1.076705	2.064796
C	4.889660	0.319623	0.630637
H	2.008212	0.941230	2.300716
H	3.645005	0.843375	2.961588
H	3.226629	2.129290	1.800247
H	5.127577	-0.424049	-0.126891
H	5.115833	1.318396	0.234750
H	5.502104	0.154415	1.522252.

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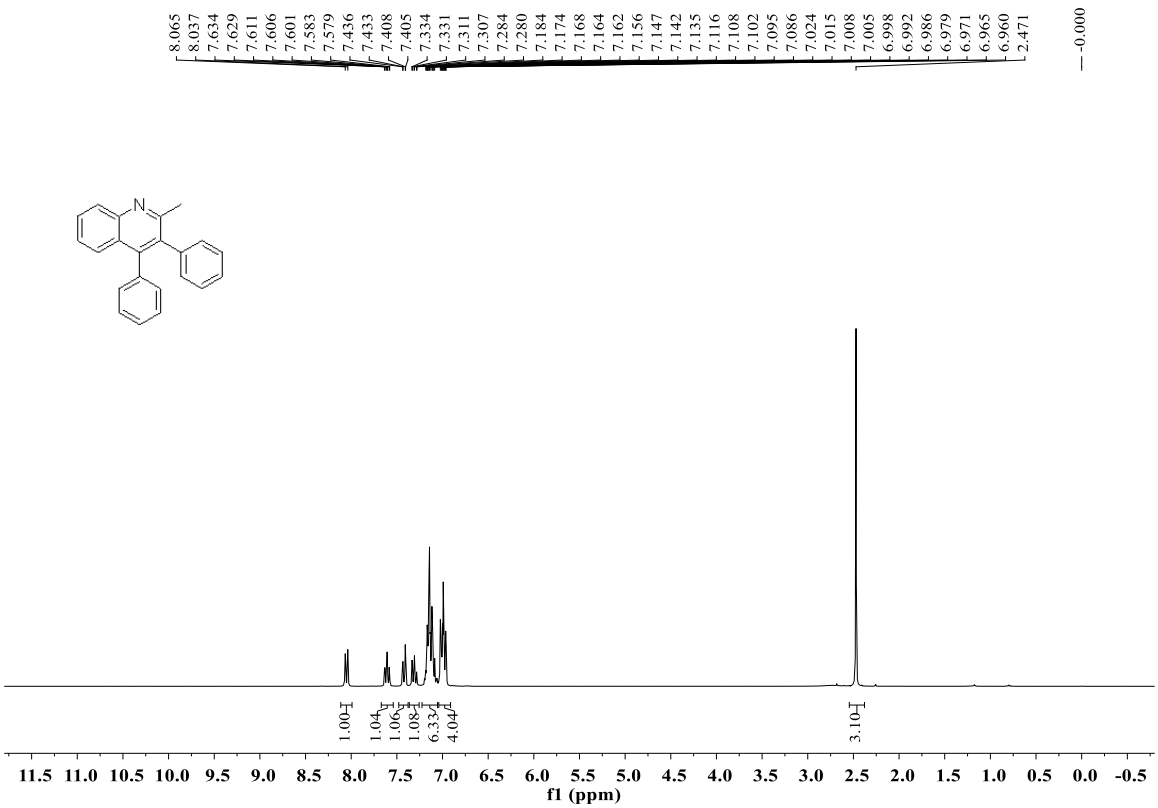
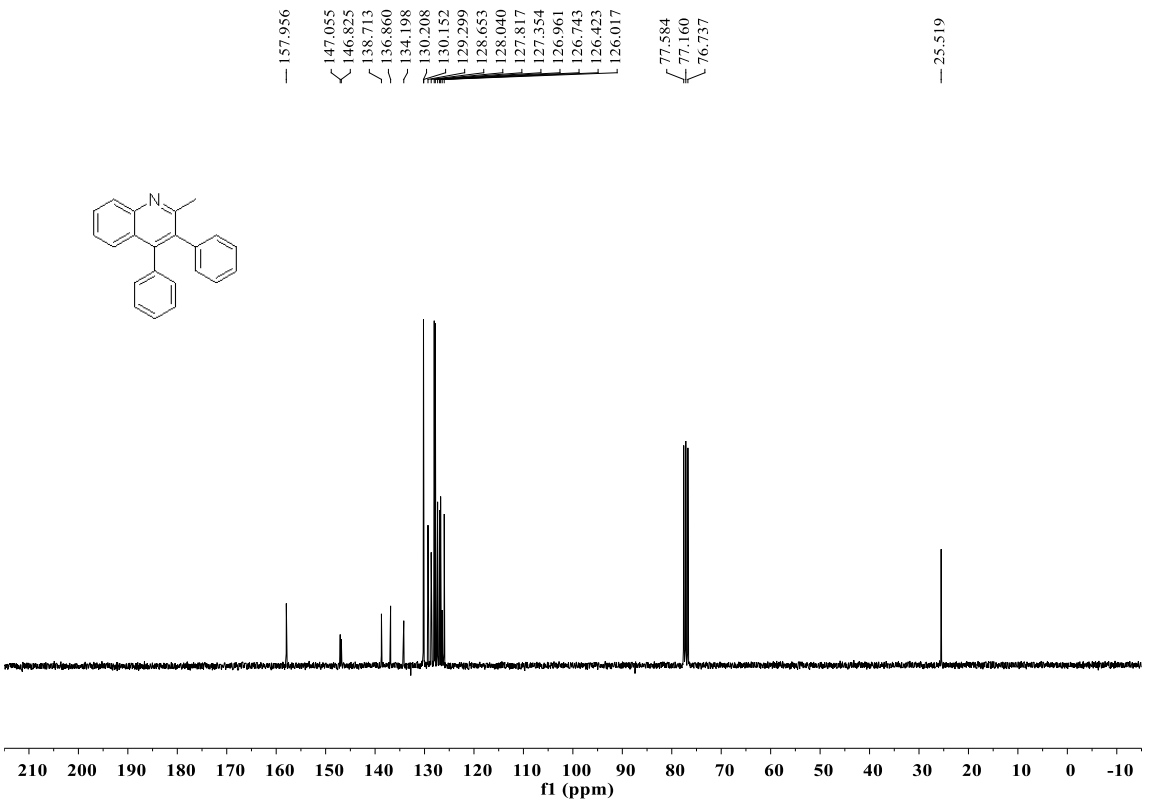
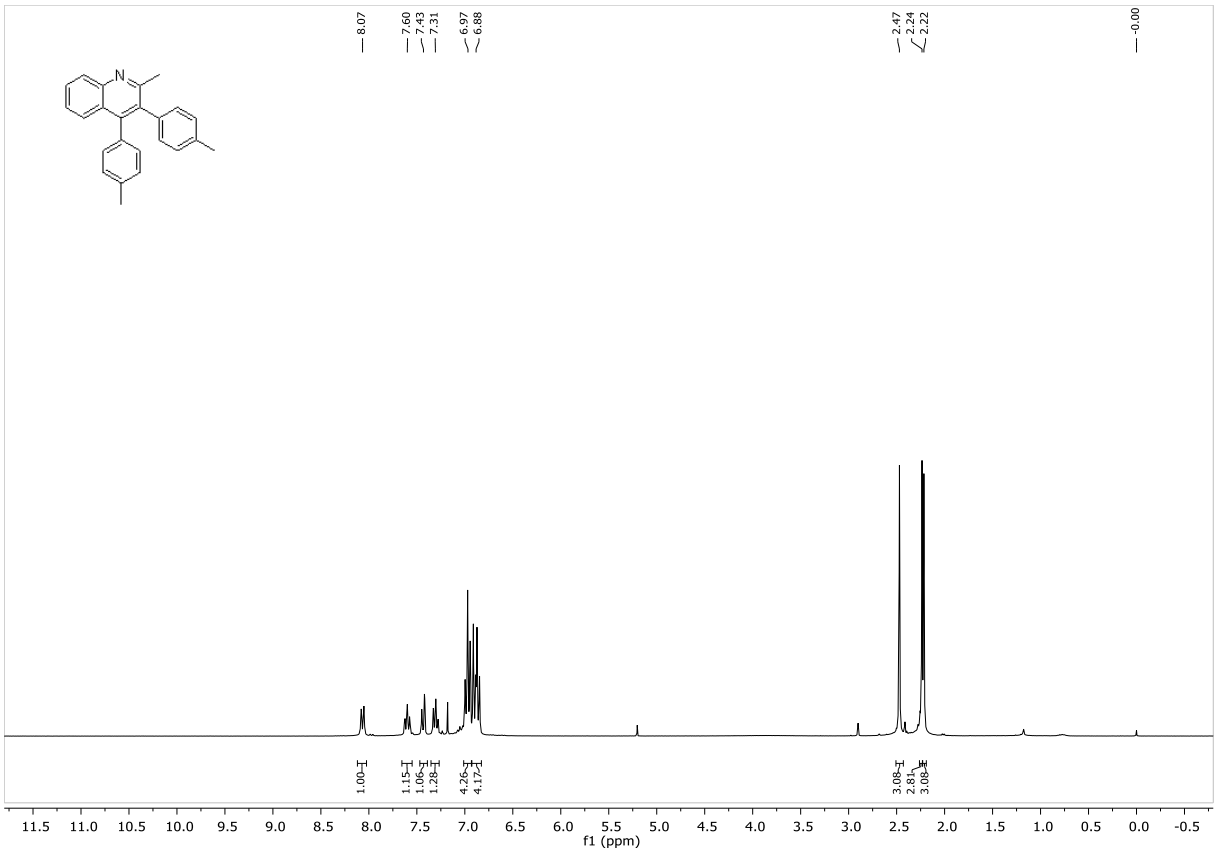
NMR Spectra of Products



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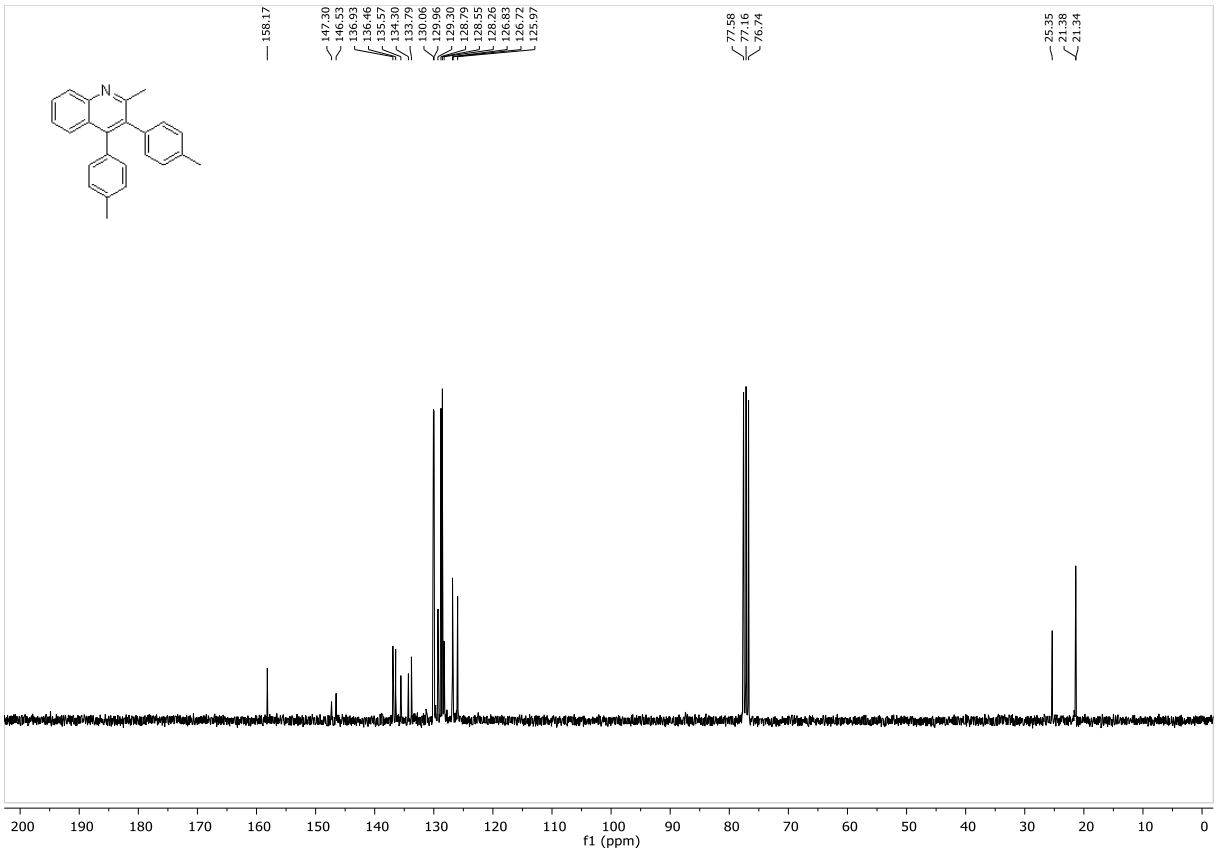
1.06
1.28
4.26
4.17
3.08
2.81
3.08
f1 (ppm)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77.58
77.16
76.74
25.35
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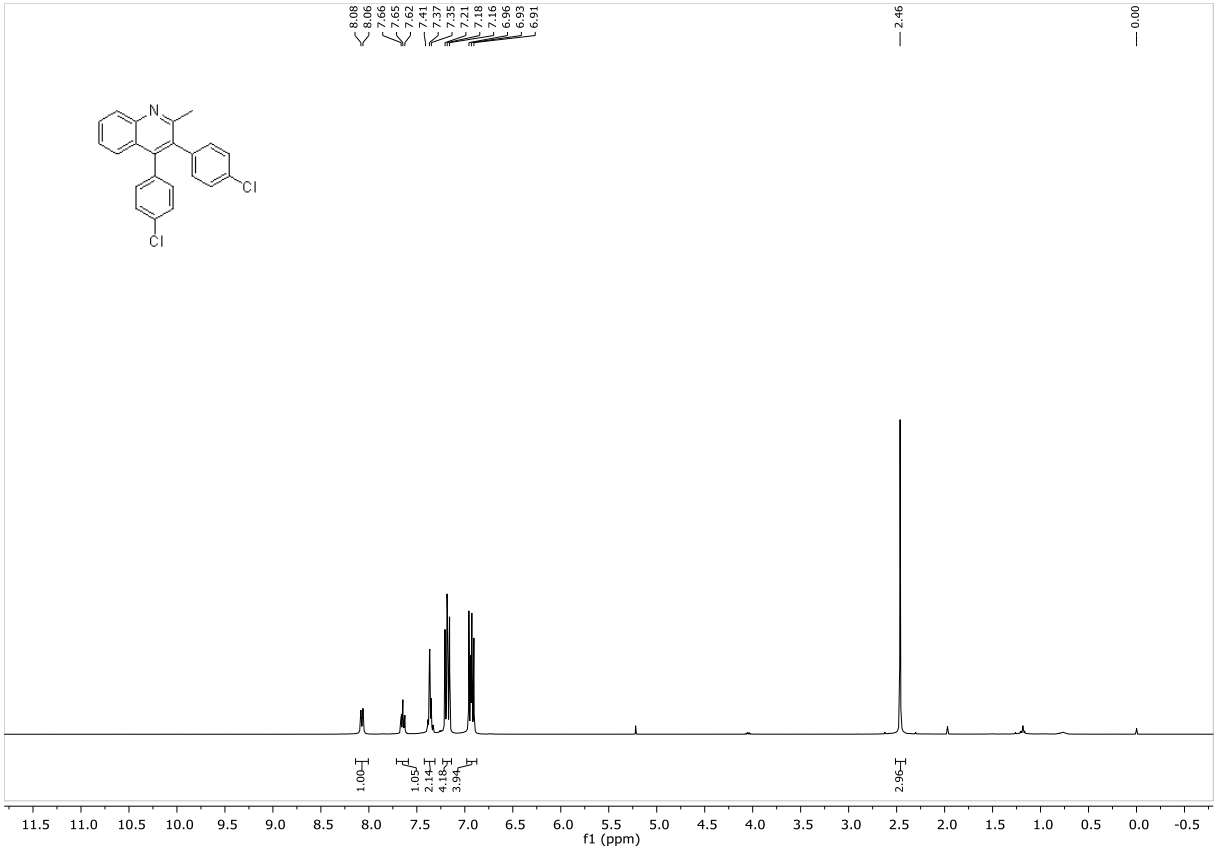
21.34
f1 (ppm)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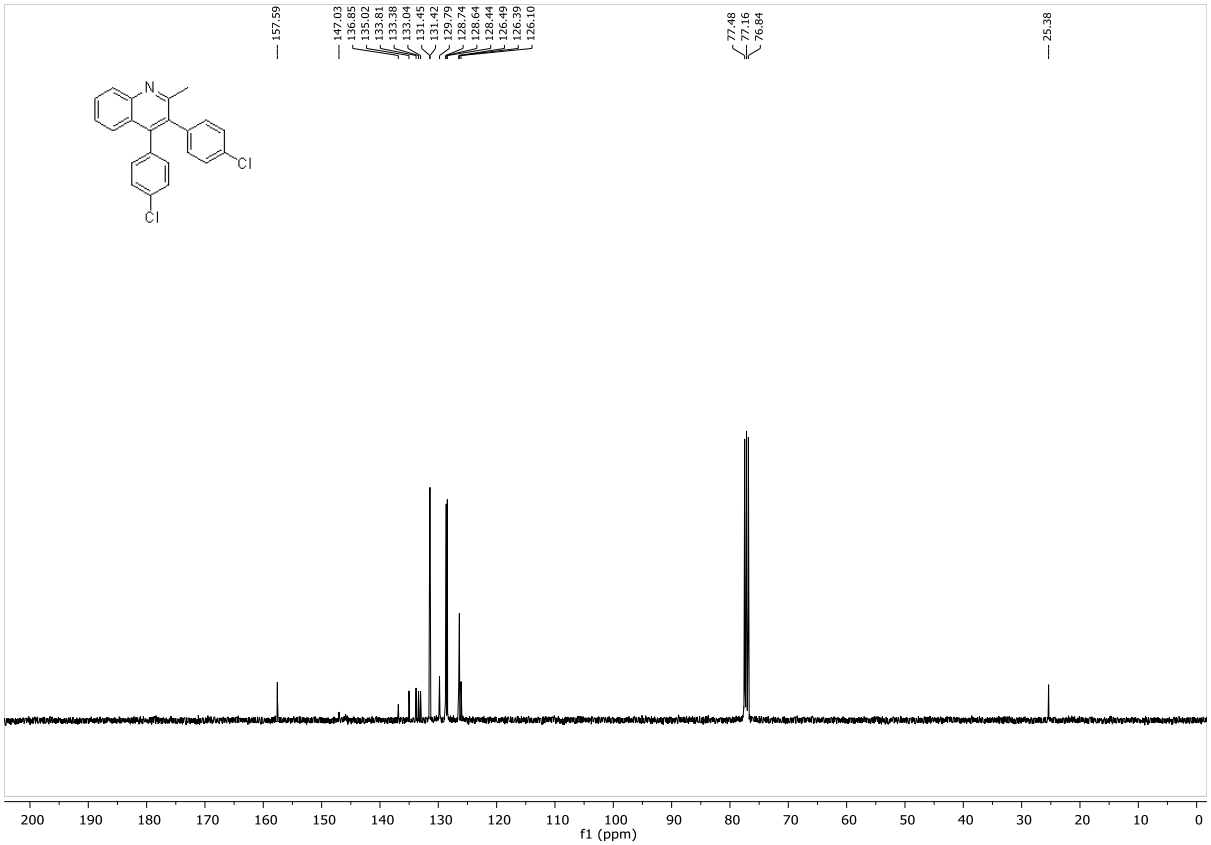
6.93
6.91
2.46
0.00
N
Cl
Cl
1.00
1.05
2.14
4.18
3.94
2.96
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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128.44
126.49
126.39
126.10
77.48
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76.84
25.38
N
Cl
Cl
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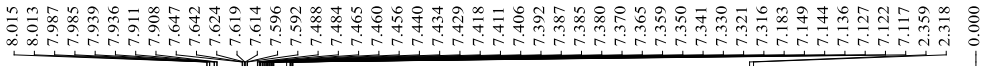
f1 (ppm)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7.596
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7.484
7.465
7.460
7.456
7.440
7.434
7.429
7.418
7.411
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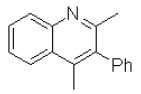
0.000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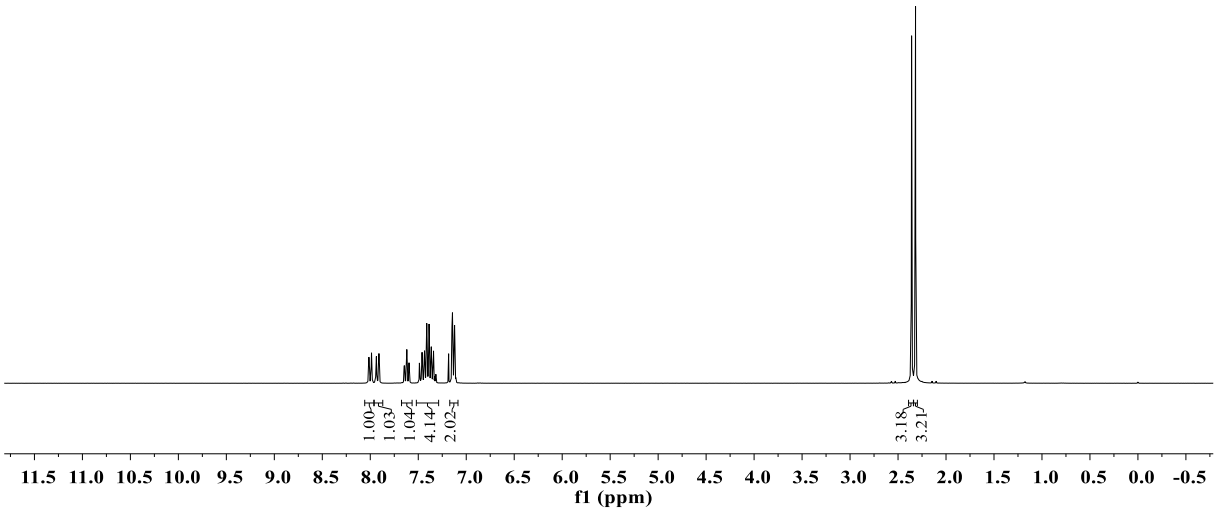
Ph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3.18
3.21
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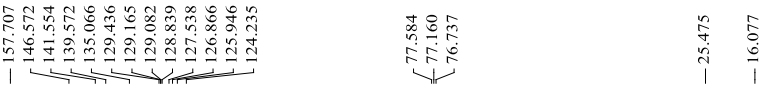
f1 (ppm)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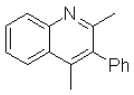
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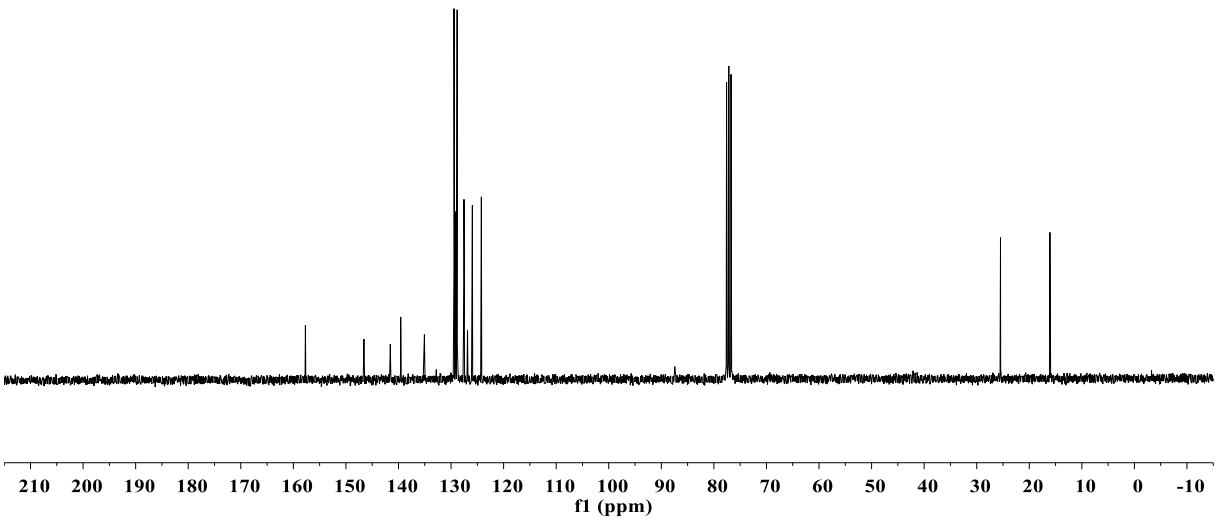
Ph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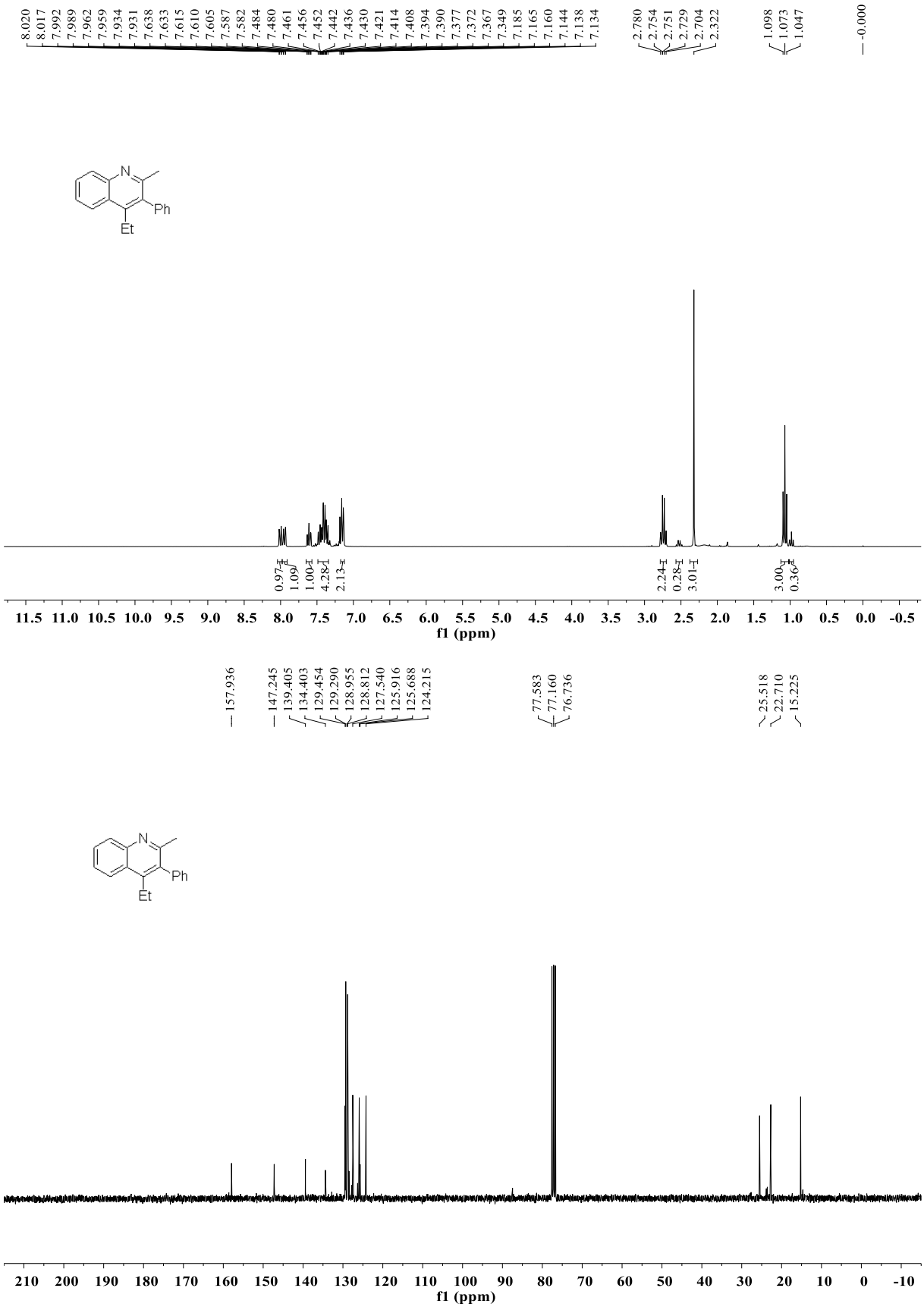
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1.047
-0.000
N
Ph
Et
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1.00
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2.24
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3.00
0.36
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124.215
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77.160
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N
Ph
Et
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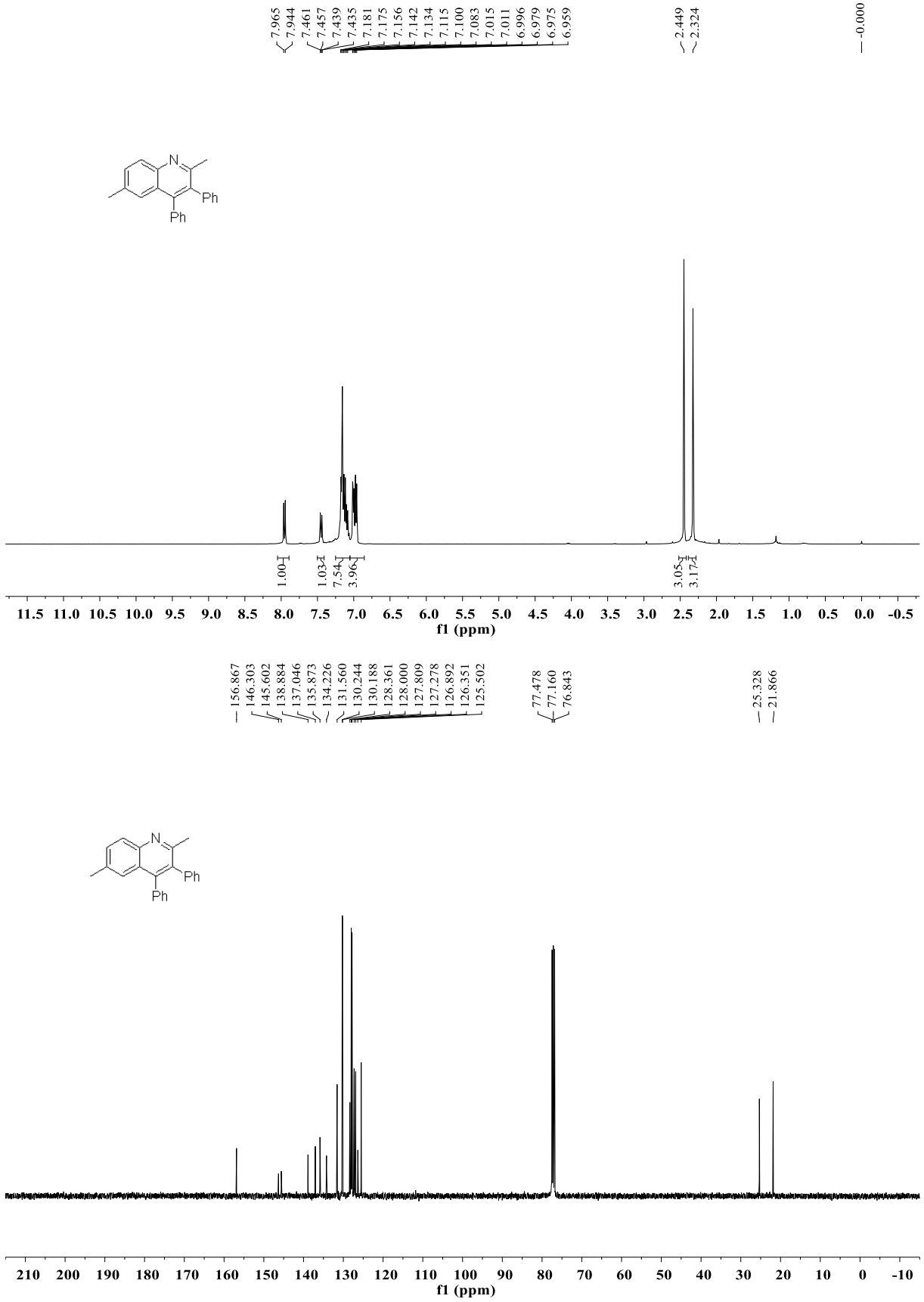
f1 (ppm)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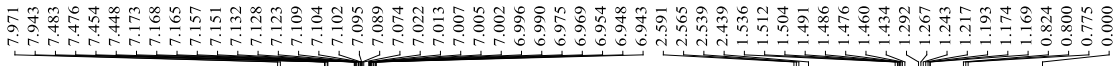
f1 (ppm)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7.022
7.013
7.007
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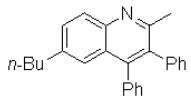
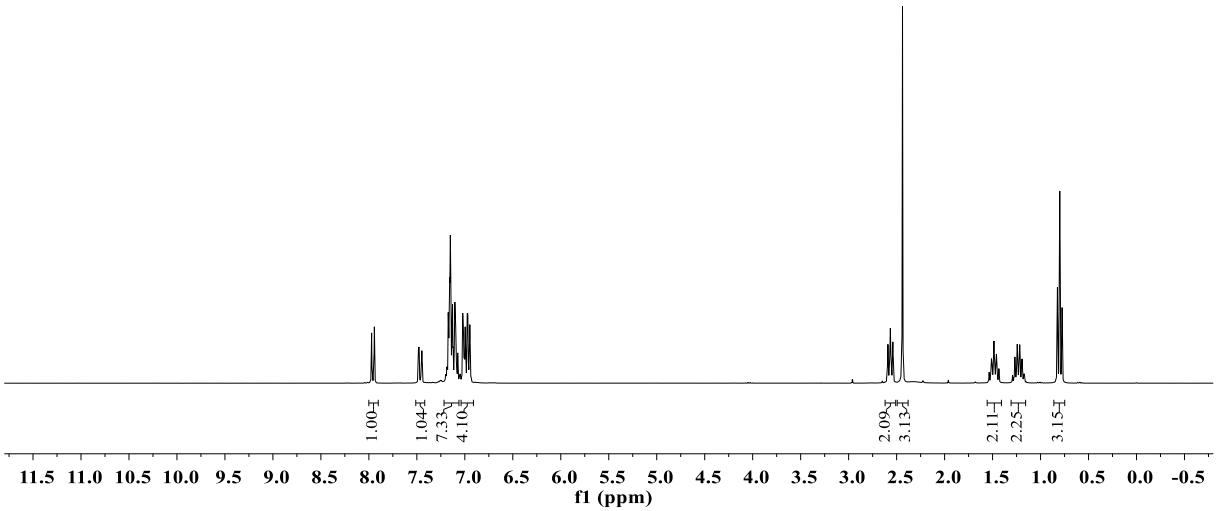
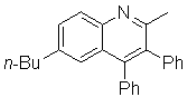
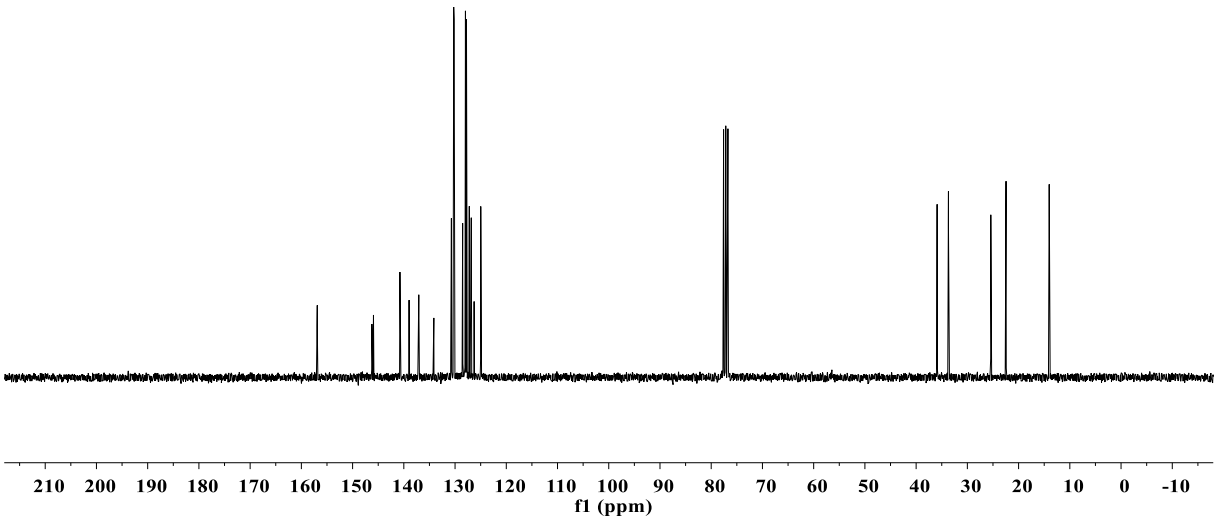
0.000


N
n-Bu
Ph
Ph


1.00
1.04
7.33
4.10
2.09
3.13
2.11
2.25
3.15
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


156.897
146.237
145.926
140.763
138.977
137.081
134.142
130.714
130.264
130.188
128.516
127.974
127.775
127.222
126.836
126.278
124.982
77.584
77.160
76.737
35.903
33.692
25.423
22.447
14.026


N
n-Bu
Ph
Ph


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)


8.141
8.120
7.897
7.892
7.875
7.870
7.616
7.612
7.473
7.469
7.452
7.338
7.320
7.301
7.257
7.239
7.224
7.221
7.176
7.173
7.169
7.157
7.152
7.141
7.139
7.136
7.133
7.121
7.117
7.114
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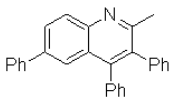
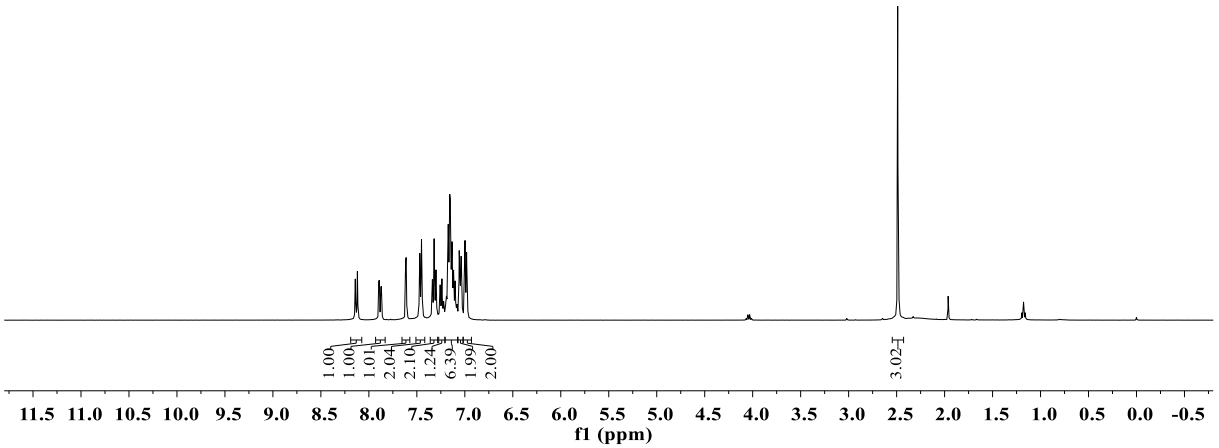
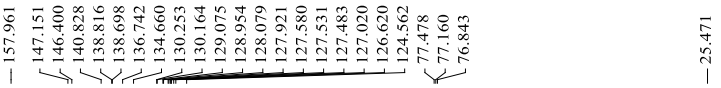
7.058
7.054
7.039
7.035
7.002
6.998
6.981
2.489
-0.000


N
Ph
Ph
Ph


1.00
1.00
1.01
2.04
2.10
1.24
6.39
1.99
2.00
3.02
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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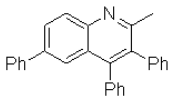
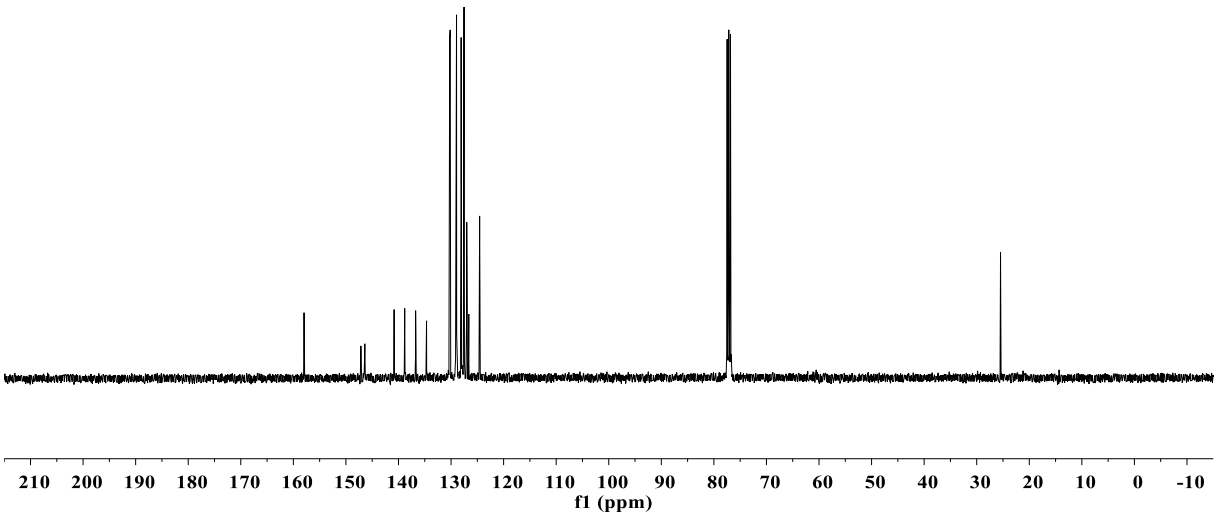
147.151
146.400
140.828
138.816
138.698
136.742
134.660
130.253
130.164
129.075
128.954
128.079
127.921
127.580
127.531
127.483
127.020
126.620
124.562
77.478
77.160
76.843
25.471


N
Ph
Ph
Ph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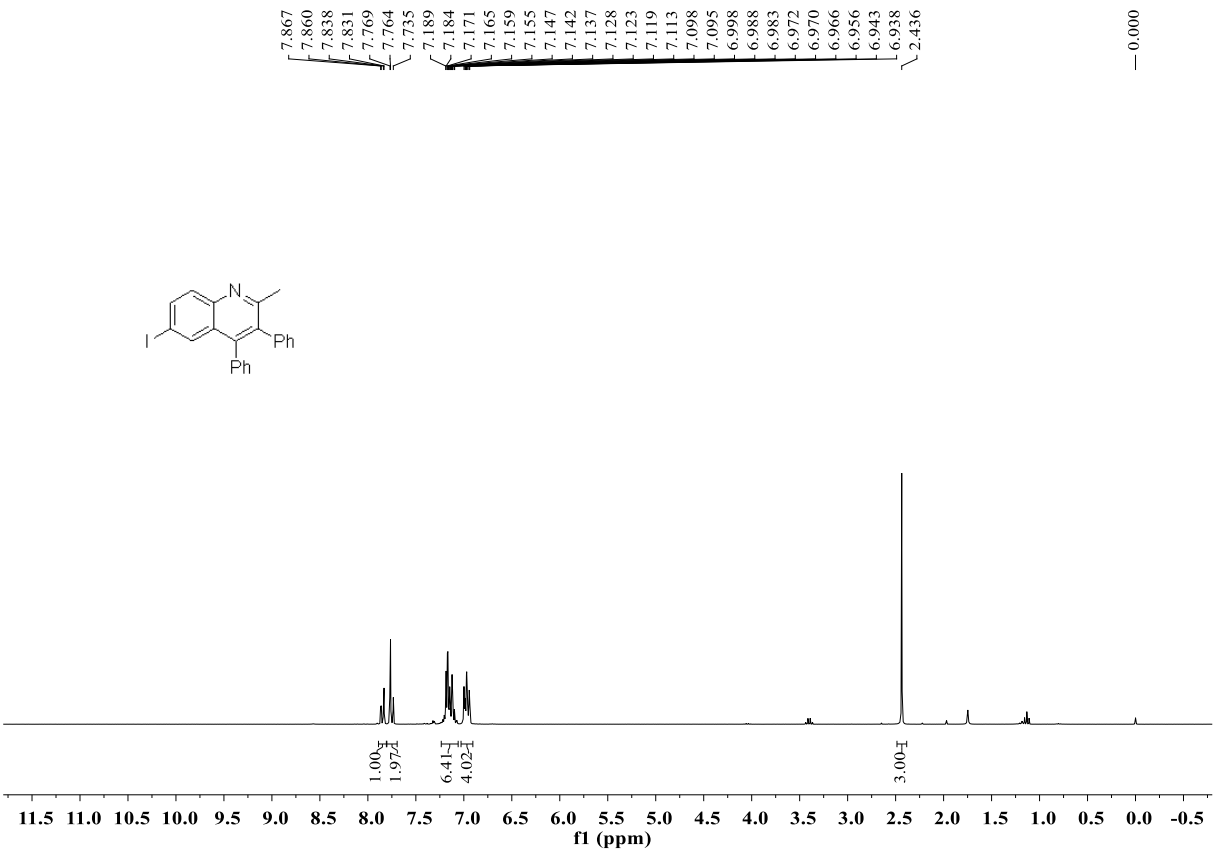
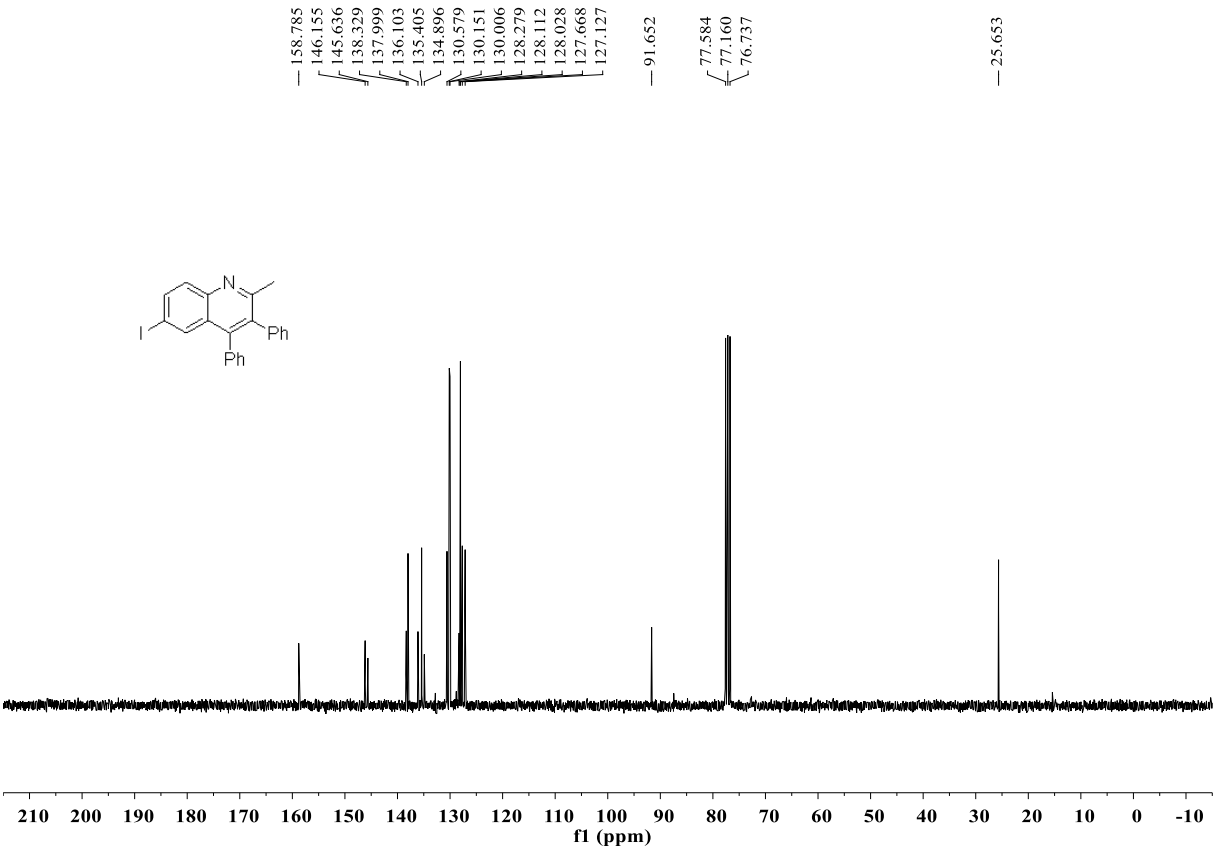
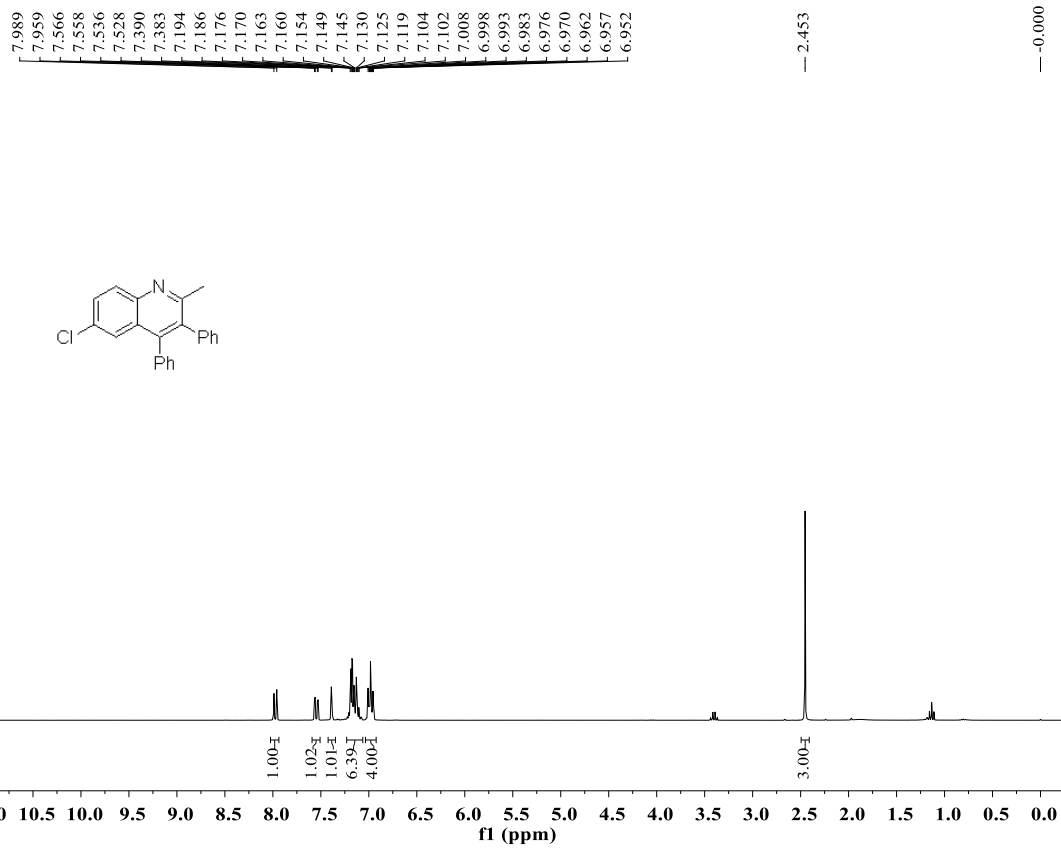
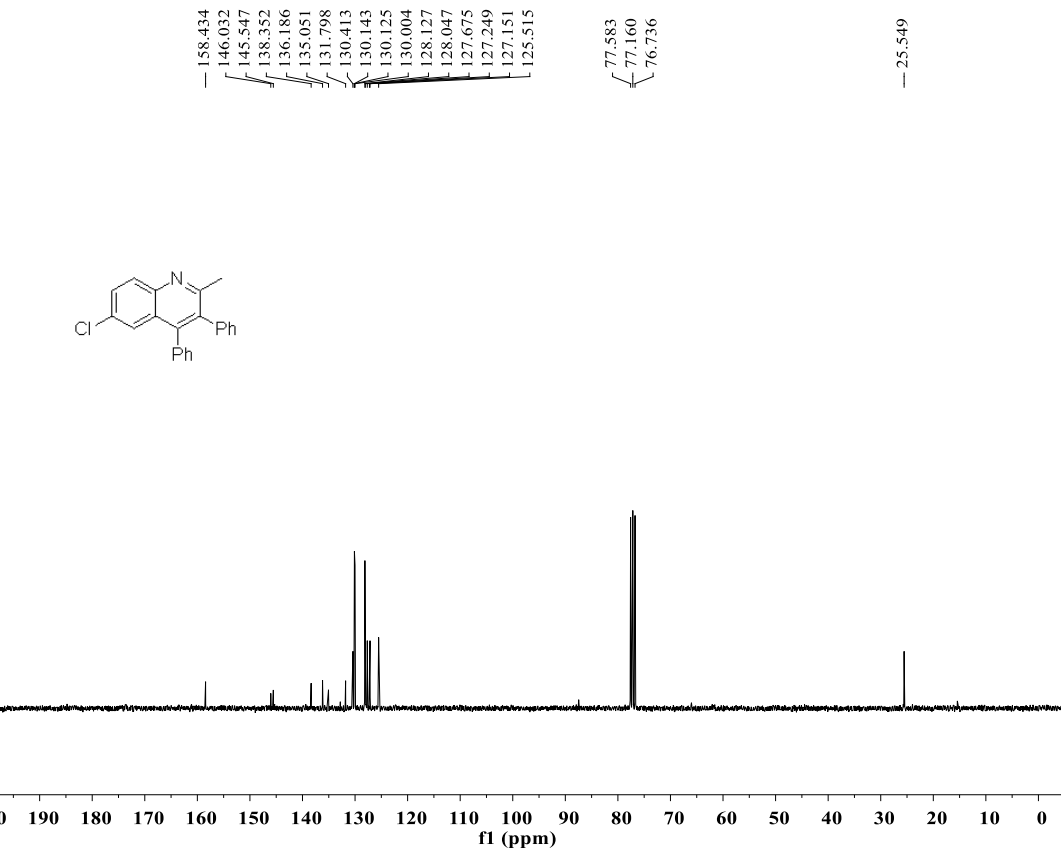
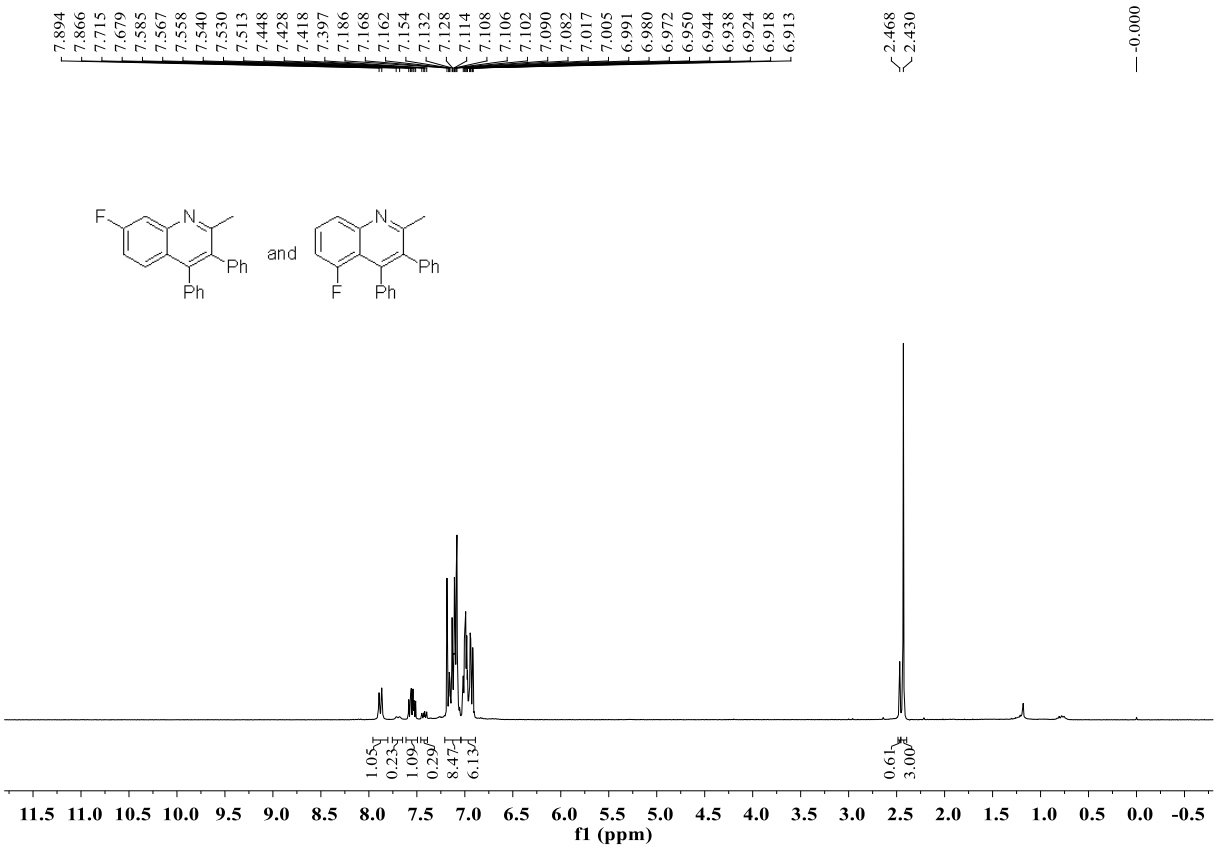
f1 (ppm)


7.867
7.860
7.838
7.831
7.769
7.764
7.735
7.189
7.184
7.171
7.165
7.159
7.155
7.147
7.142
7.137
7.128
7.123
7.119
7.113
7.098
7.095
6.998
6.988
6.983
6.972
6.970
6.966
6.956
6.943
6.938
2.436
0.000
N
I
Ph
Ph
1.00
1.97
6.41
4.02
3.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


158.785
146.155
145.636
138.329
137.999
136.103
135.405
134.896
130.579
130.151
130.006
128.279
128.112
128.028
127.668
127.127
91.652
77.584
77.160
76.737
25.653
N
I
Ph
Ph
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)


7.989
7.959
7.566
7.558
7.536
7.528
7.390
7.383
7.194
7.186
7.176
7.170
7.163
7.160
7.154
7.149
7.145
7.130
7.125
7.119
7.104
7.102
7.008
6.998
6.993
6.983
6.976
6.970
6.962
6.957
6.952
2.453
-0.000
N
Cl
Ph
Ph
1.00
1.02
1.01
6.39
4.00
3.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


158.434
146.032
145.547
138.352
136.186
135.051
131.798
130.413
130.143
130.125
130.004
128.127
128.047
127.675
127.249
127.151
125.515
77.583
77.160
76.736
25.549
N
Cl
Ph
Ph
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)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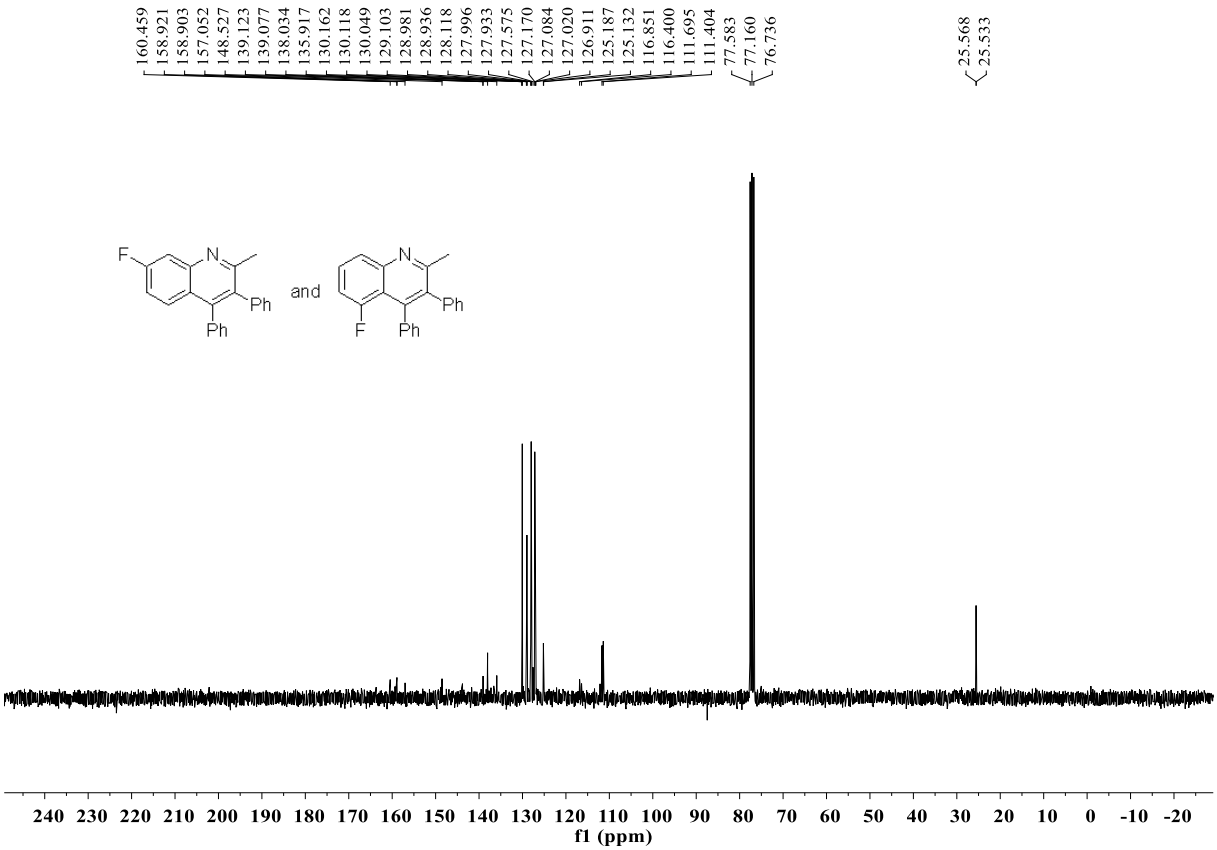
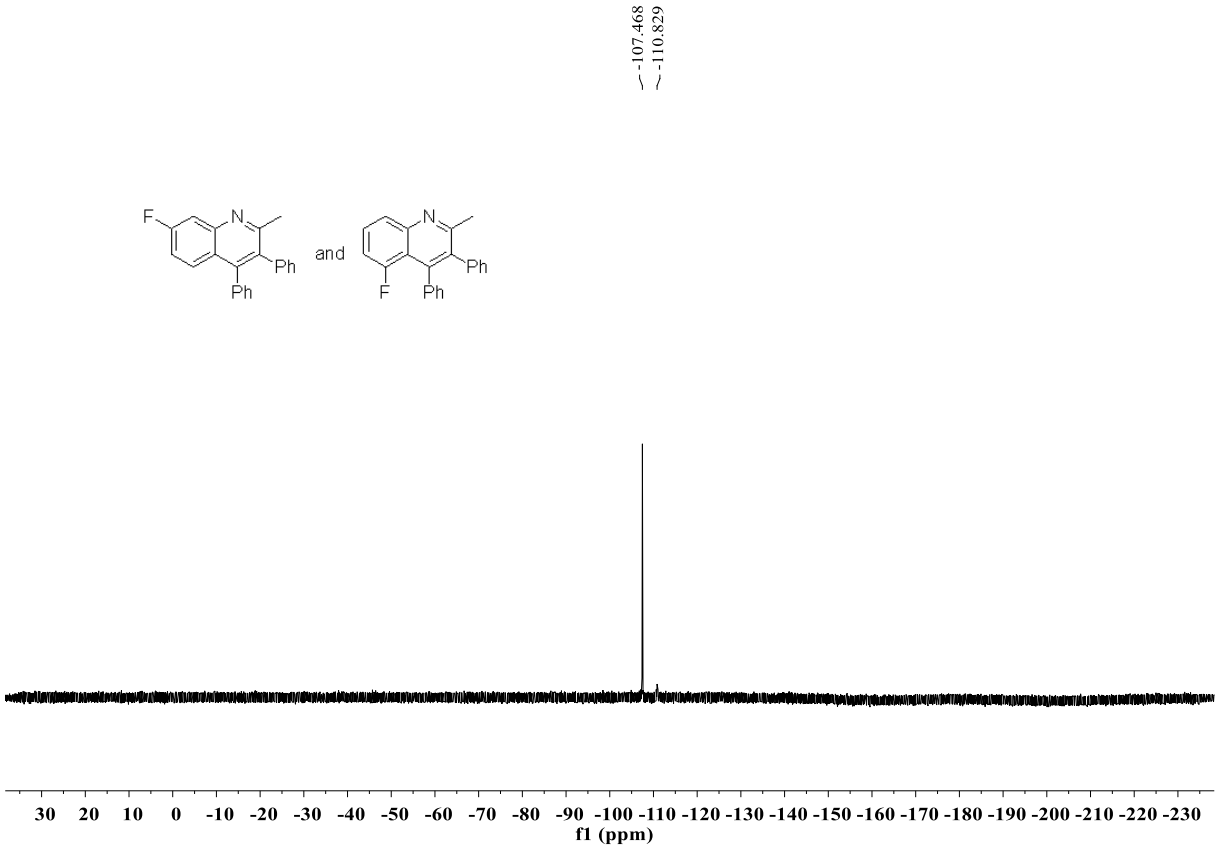
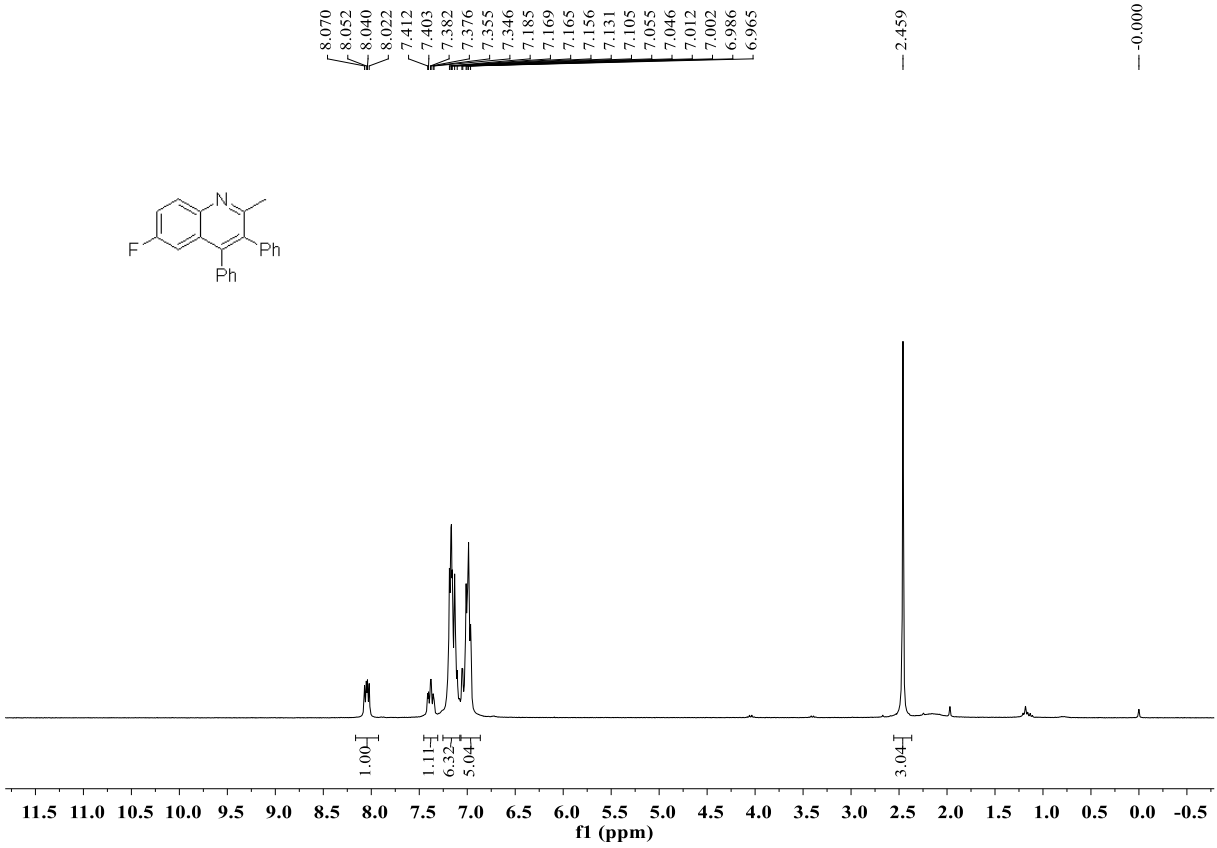
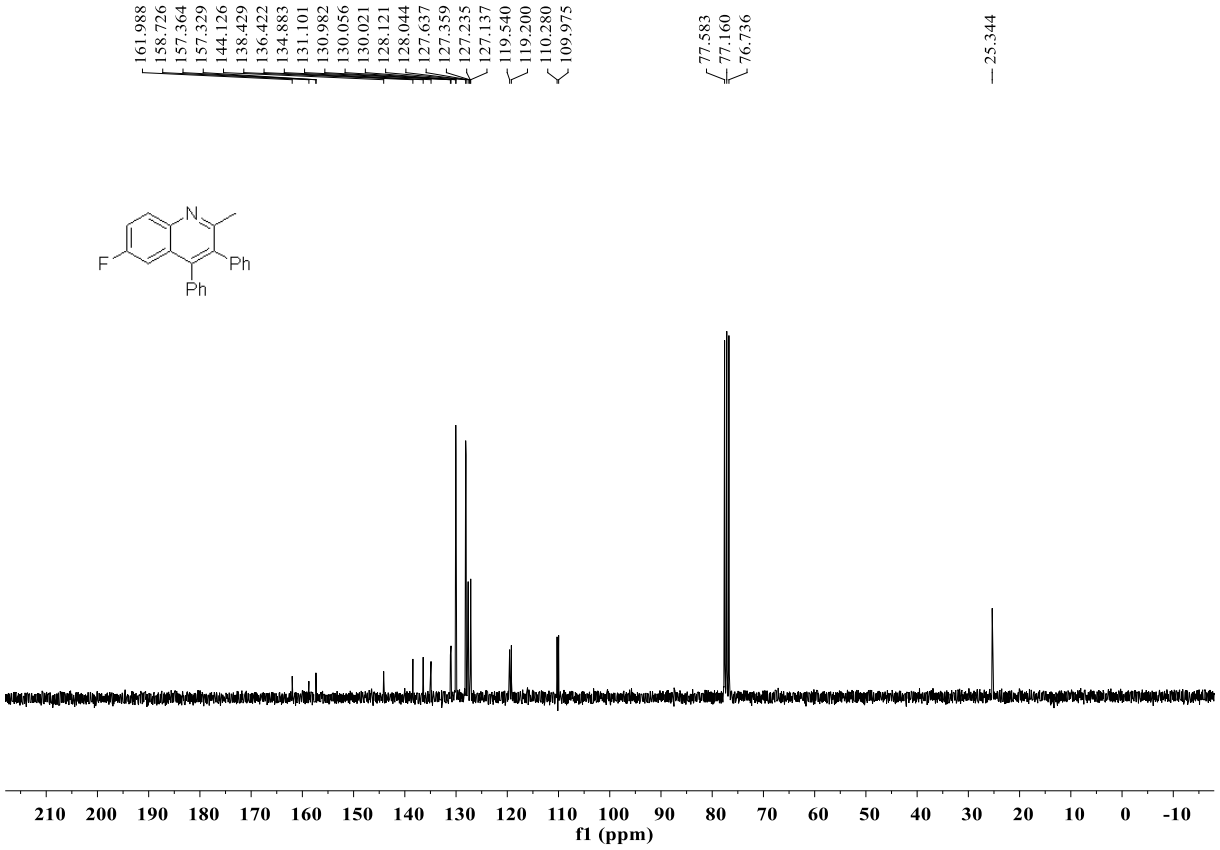
7.866
7.715
7.679
7.585
7.567
7.558
7.540
7.530
7.513
7.448
7.428
7.418
7.397
7.186
7.168
7.162
7.154
7.132
7.128
7.114
7.108
7.106
7.102
7.090
7.082
7.017
7.005
6.991
6.980
6.972
6.950
6.944
6.938
6.924
6.918
6.913
2.468
2.430
-0.000
F
N
Ph
Ph
and
F
N
Ph
Ph
1.05
0.23
1.09
0.29
8.47
6.13
0.61
3.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


160.459
158.921
158.903
157.052
148.527
139.123
139.077
138.034
135.917
130.162
130.118
130.049
129.103
128.981
128.936
128.118
127.996
127.933
127.575
127.170
127.084
127.020
126.911
125.187
125.132
116.851
116.400
111.695
111.404
77.583
77.160
76.736
25.568
25.533
F
N
Ph
Ph
and
F
N
Ph
Ph
240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


-107.468
-110.829
F
N
Ph
Ph
and
N
Ph
F
Ph
30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230
f1 (ppm)


8.070
8.052
8.040
8.022
7.412
7.403
7.382
7.376
7.355
7.346
7.185
7.169
7.165
7.156
7.131
7.105
7.055
7.046
7.012
7.002
6.986
6.965
2.459
0.000
N
F
Ph
Ph
1.00
1.11
6.32
5.04
3.04
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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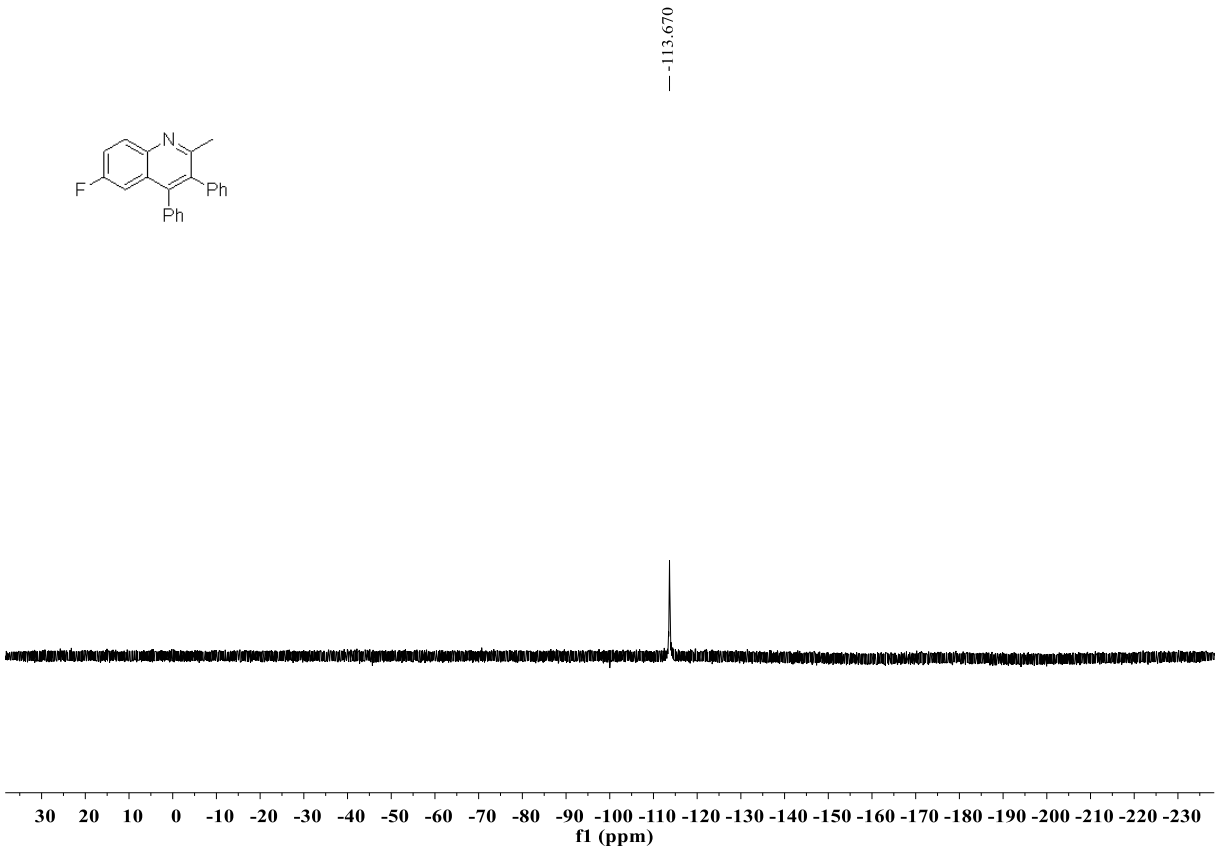
158.726
157.364
157.329
144.126
138.429
136.422
134.883
131.101
130.982
130.056
130.021
128.121
128.044
127.637
127.359
127.235
127.137
119.540
119.200
110.280
109.975
77.583
77.160
76.736
25.344
N
F
Ph
Ph
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-113.670
N
F
Ph
Ph
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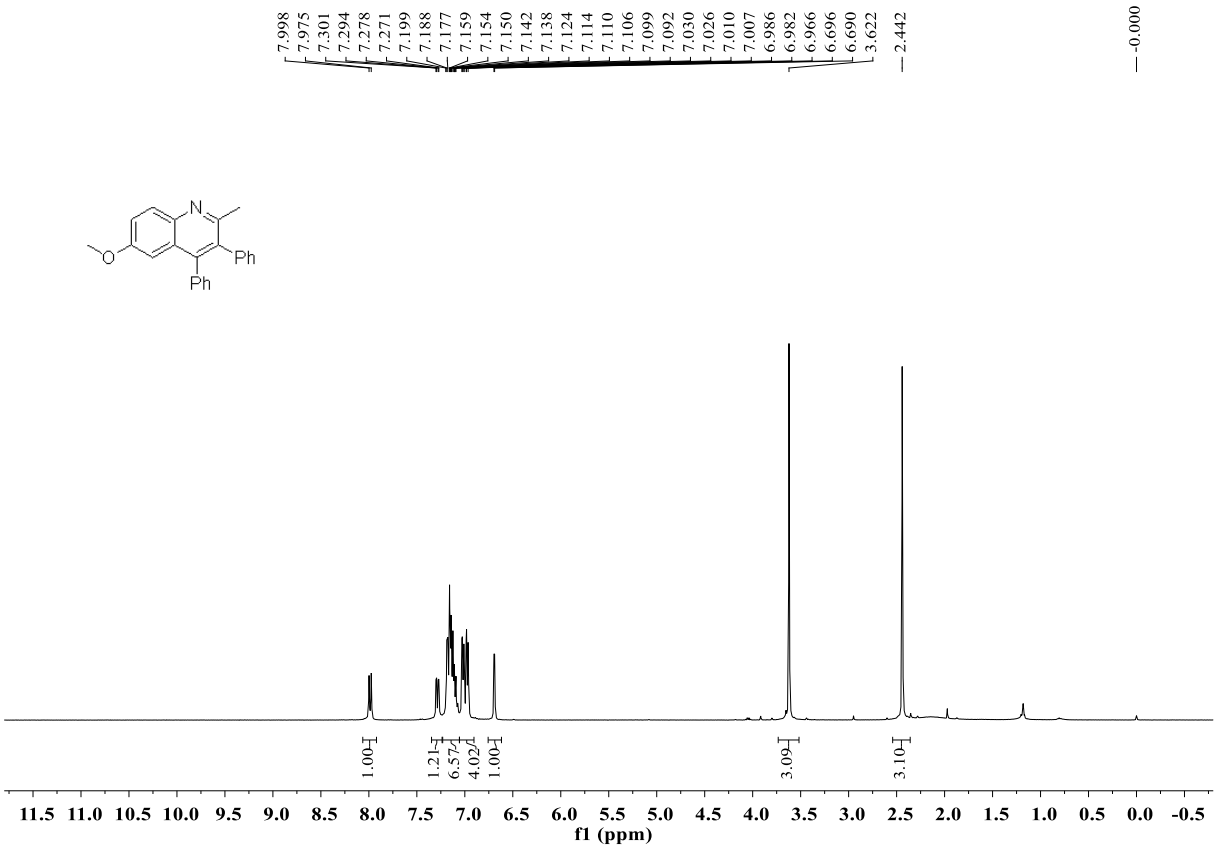
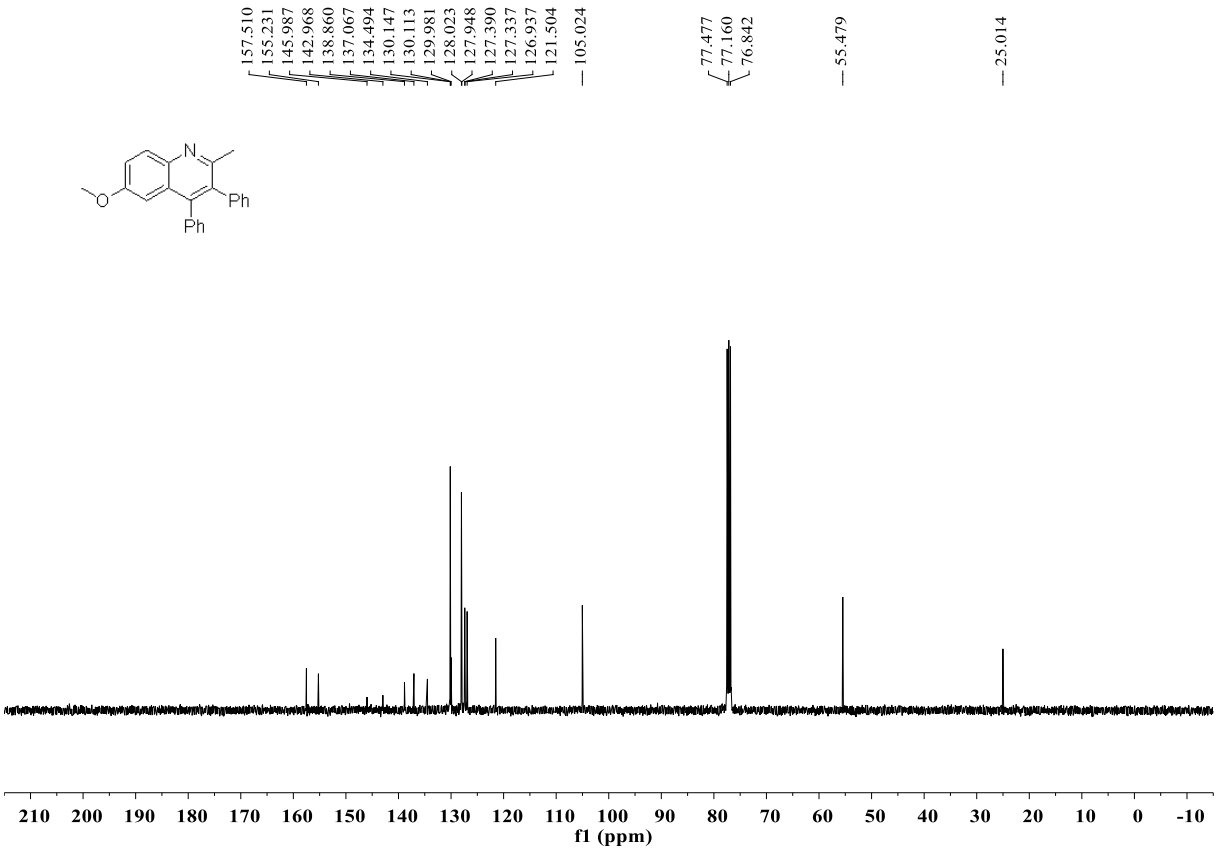
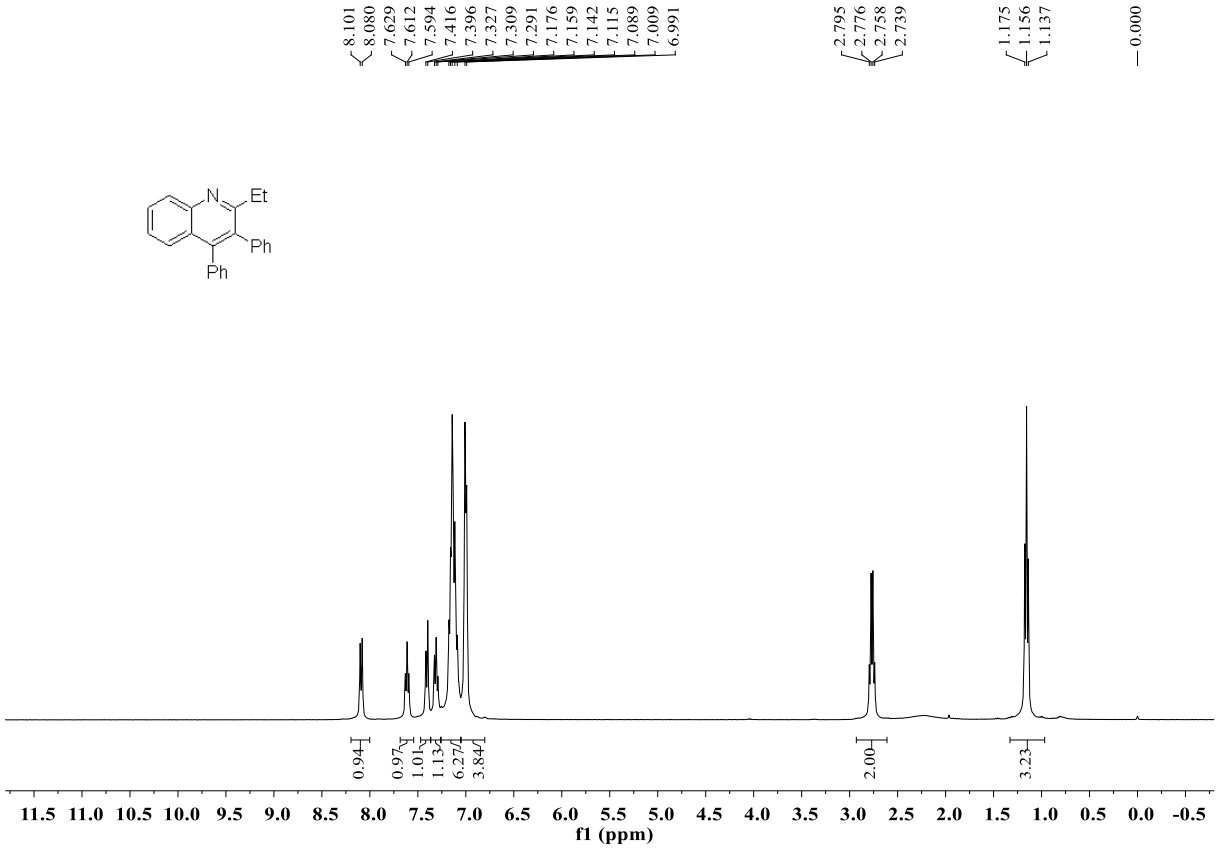
f1 (ppm)


7.998
7.975
7.301
7.294
7.278
7.271
7.199
7.188
7.177
7.159
7.154
7.150
7.142
7.138
7.124
7.114
7.110
7.106
7.099
7.092
7.030
7.026
7.010
7.007
6.986
6.982
6.966
6.696
6.690
3.622
2.442
-0.000
N
O
Ph
Ph
1.00
1.21
6.57
4.02
1.00
3.09
3.10
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


157.510
155.231
145.987
142.968
138.860
137.067
134.494
130.147
130.113
129.981
128.023
127.948
127.390
127.337
126.937
121.504
105.024
77.477
77.160
76.842
55.479
25.014
N
O
Ph
Ph
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)


8.101
8.080
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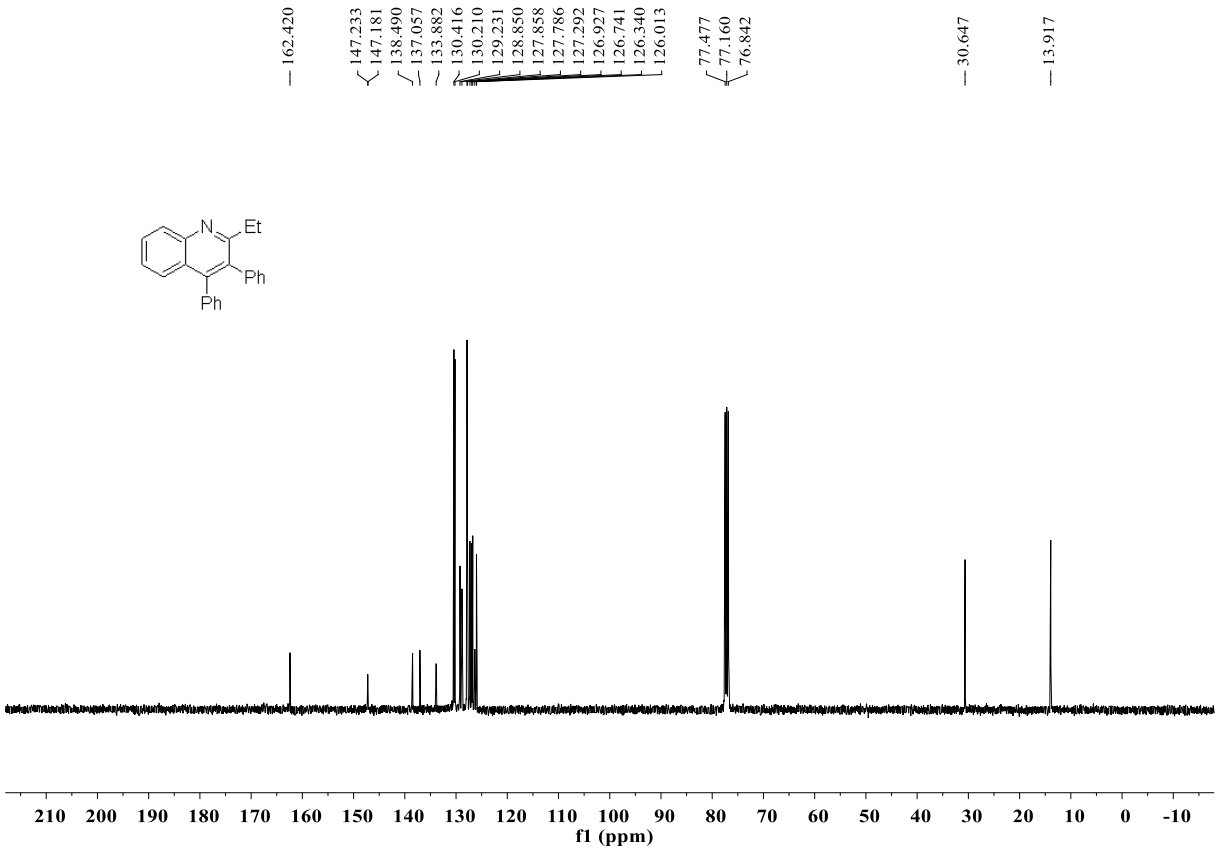
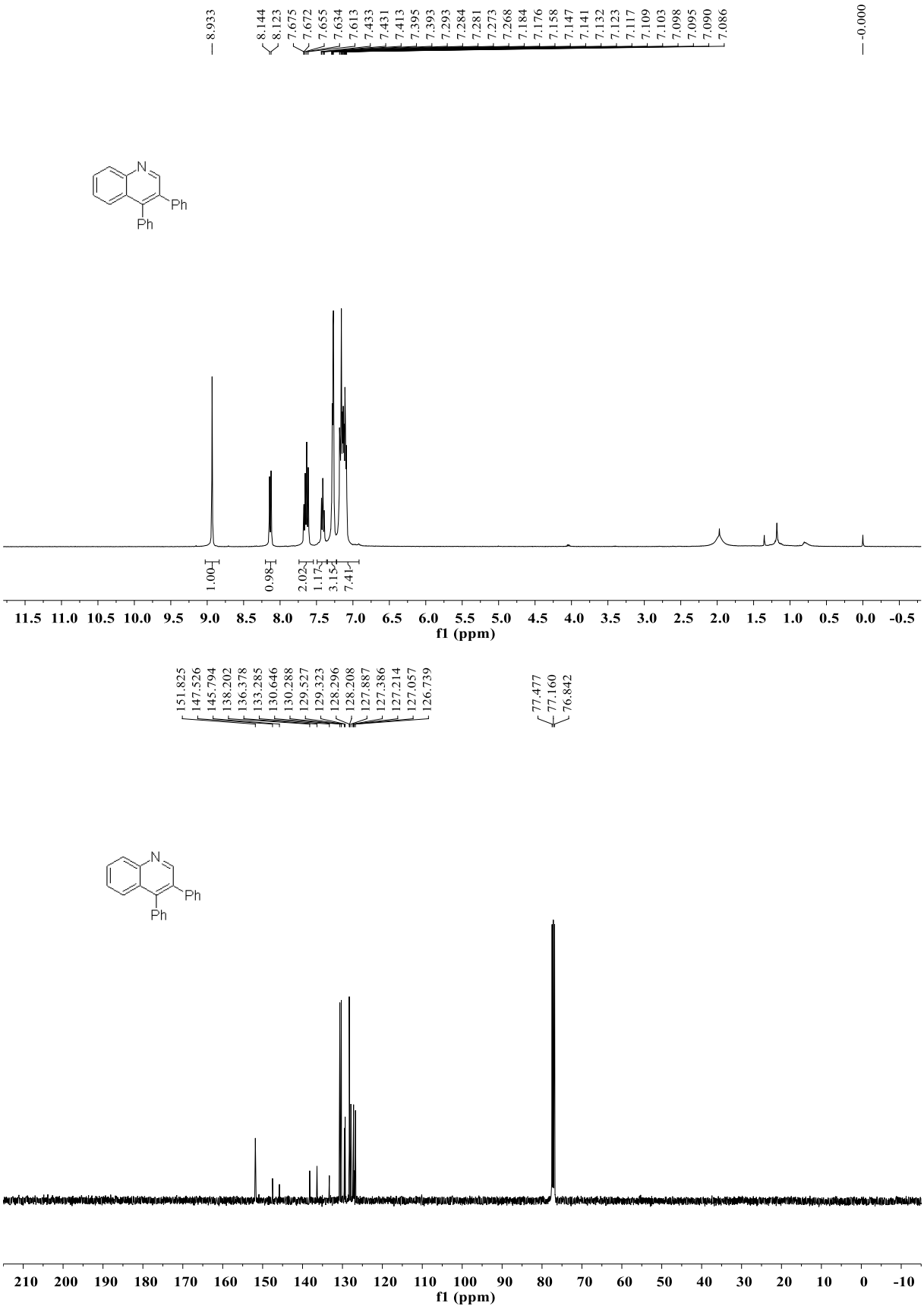
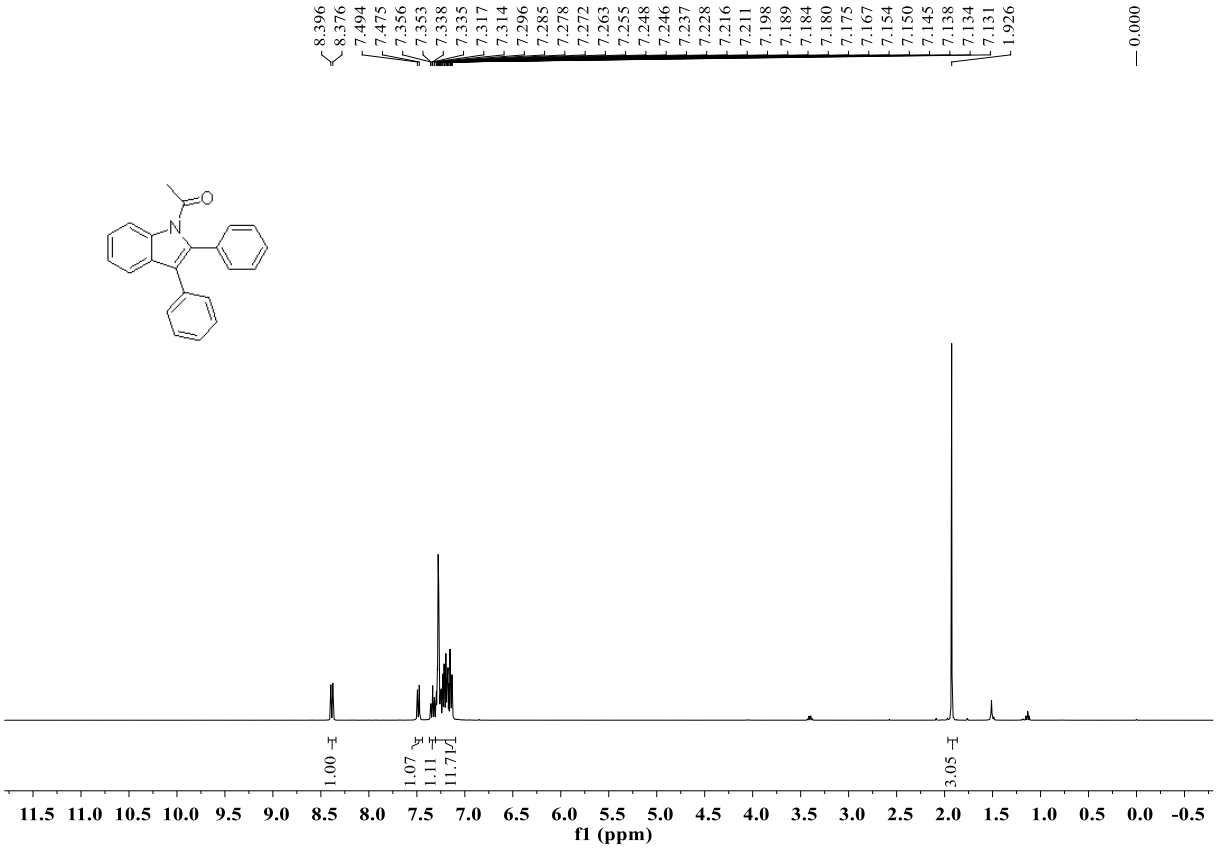
7.612
7.594
7.416
7.396
7.327
7.309
7.291
7.176
7.159
7.142
7.115
7.089
7.009
6.991
2.795
2.776
2.758
2.739
1.175
1.156
1.137
0.000
N
Et
Ph
Ph
0.94
0.97
1.01
1.13
6.27
3.84
2.00
3.23
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


162.420
147.233
147.181
138.490
137.057
133.882
130.416
130.210
129.231
128.850
127.858
127.786
127.292
126.927
126.741
126.340
126.013
77.477
77.160
76.842
30.647
13.917
N
Et
Ph
Ph
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)


8.933
8.144
8.123
7.675
7.672
7.655
7.634
7.613
7.433
7.431
7.413
7.395
7.393
7.293
7.284
7.281
7.273
7.268
7.184
7.176
7.158
7.147
7.141
7.132
7.123
7.117
7.109
7.103
7.098
7.095
7.090
7.086
-0.000
N
Ph
Ph
1.00
0.98
2.02
1.17
3.15
7.41
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
151.825
147.526
145.794
138.202
136.378
133.285
130.646
130.288
129.527
129.323
128.296
128.208
127.887
127.386
127.214
127.057
126.739
77.477
77.160
76.842
N
Ph
Ph
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)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8.376
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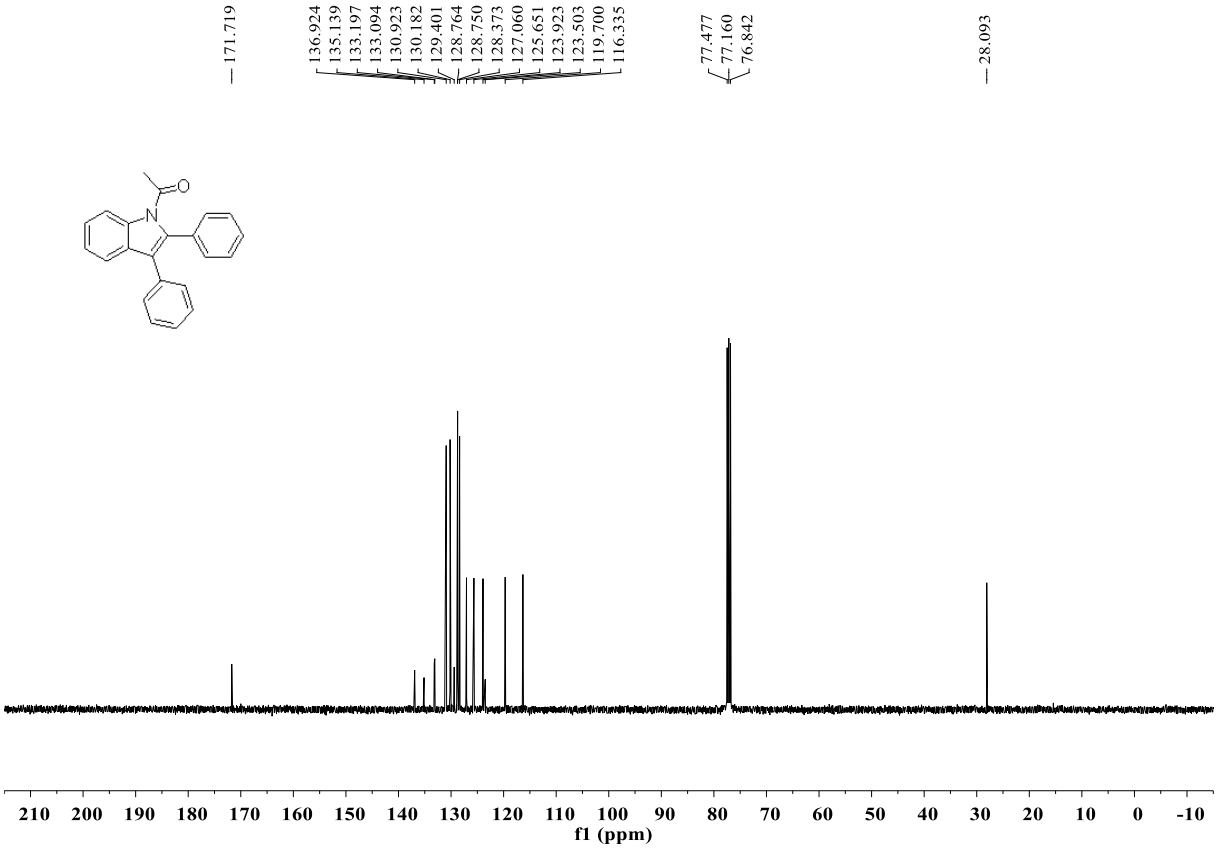
7.475
7.356
7.353
7.338
7.335
7.317
7.314
7.296
7.285
7.278
7.272
7.263
7.255
7.248
7.246
7.237
7.228
7.216
7.211
7.198
7.189
7.184
7.180
7.175
7.167
7.154
7.150
7.145
7.138
7.134
7.131
1.926
0.000
1.00
1.07
1.11
11.71
3.05
f1 (ppm)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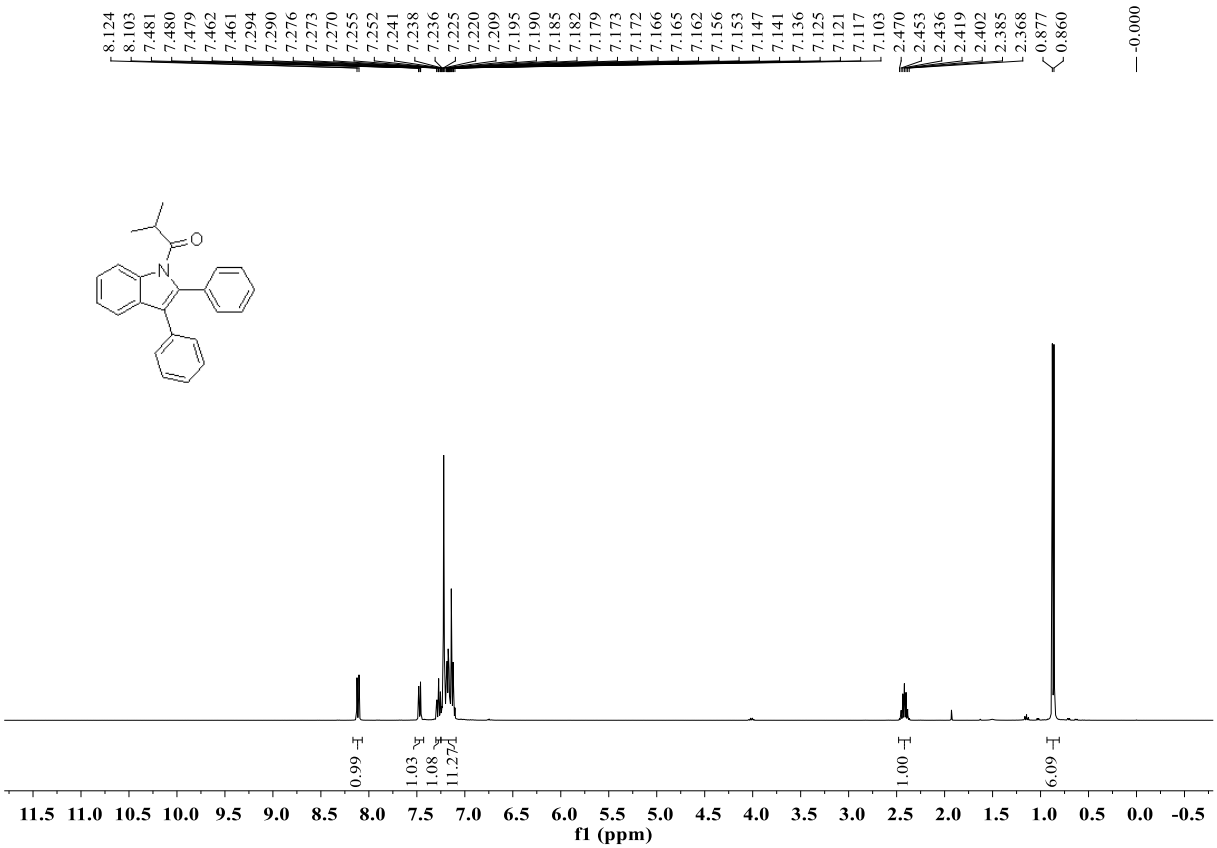
136.924
135.139
133.197
133.094
130.923
130.182
129.401
128.764
128.750
128.373
127.060
125.651
123.923
123.503
119.700
116.335
77.477
77.160
76.842
28.093
f1 (ppm)


8.124
8.103
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7.166
7.165
7.162
7.156
7.153
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7.117
7.103
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2.436
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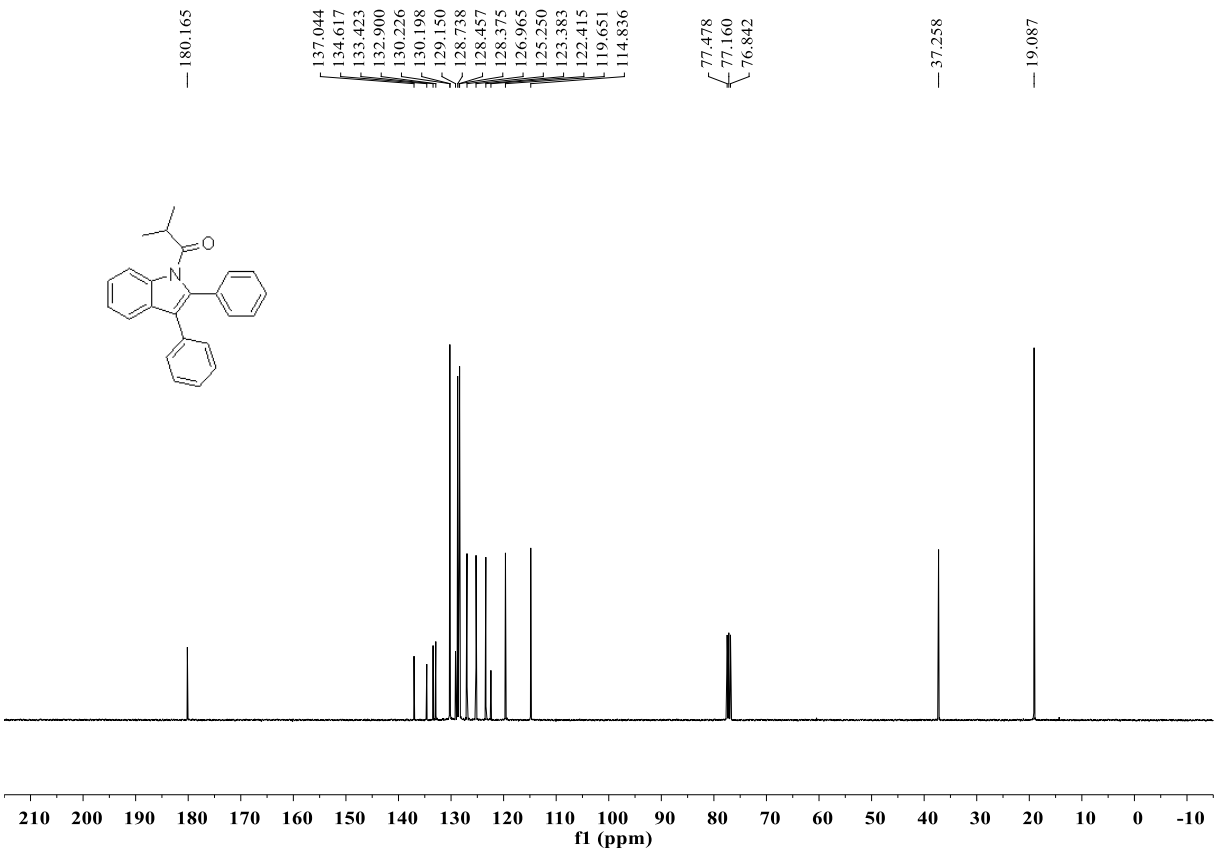
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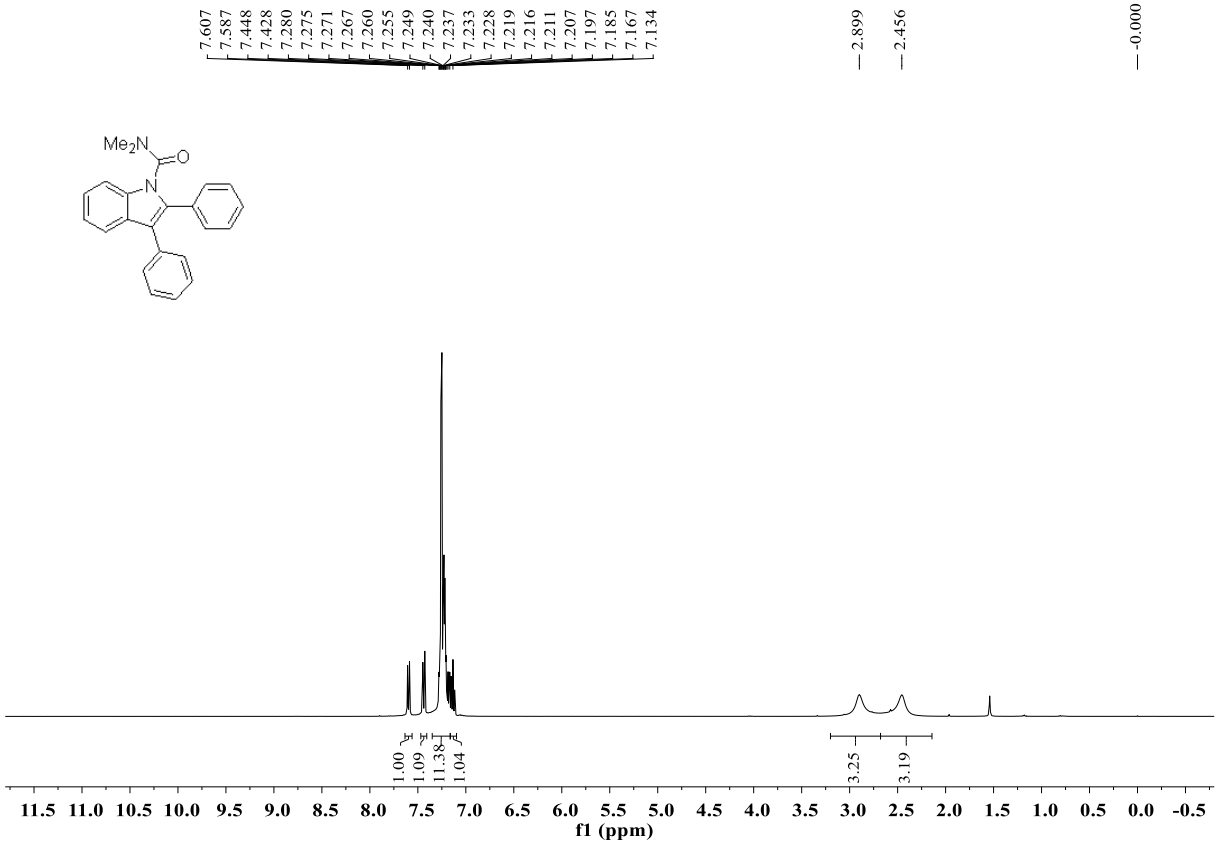
f1 (ppm)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7.167
7.134
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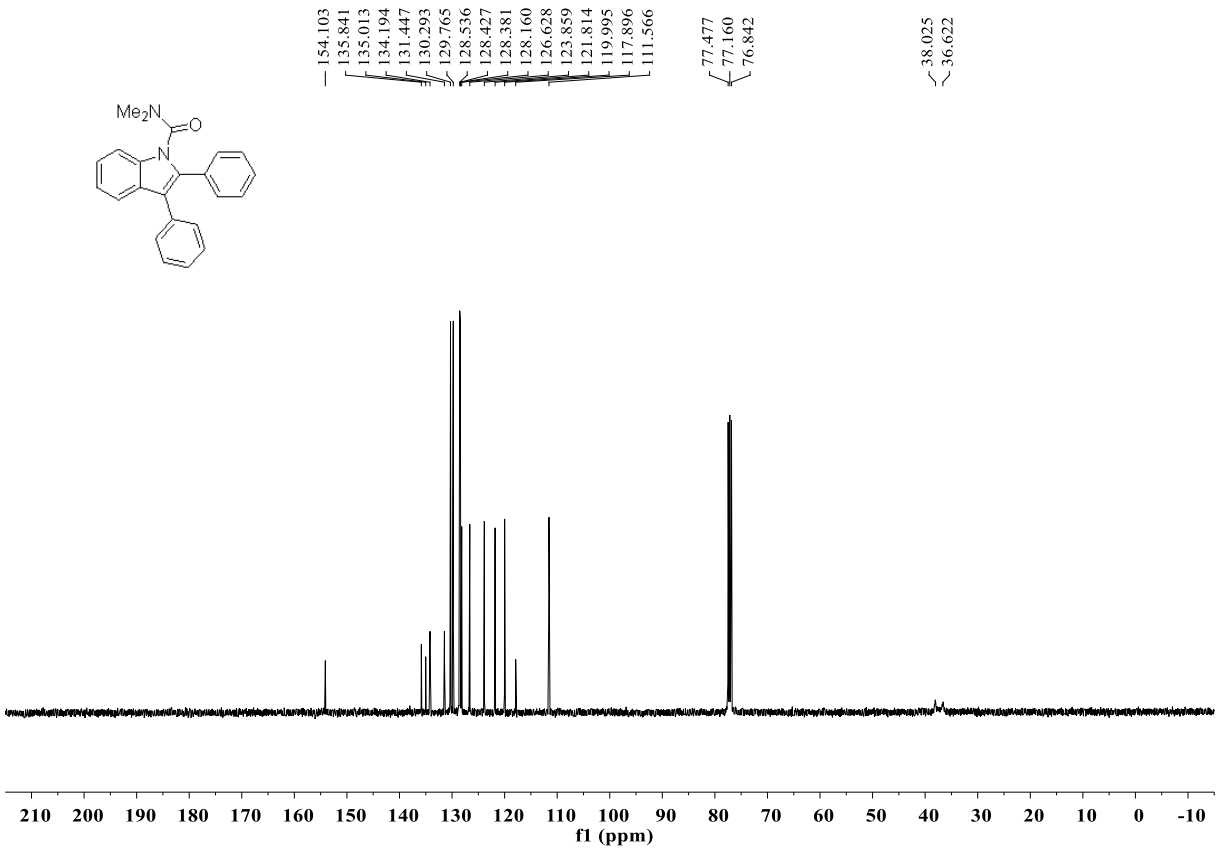
3.19
f1 (ppm)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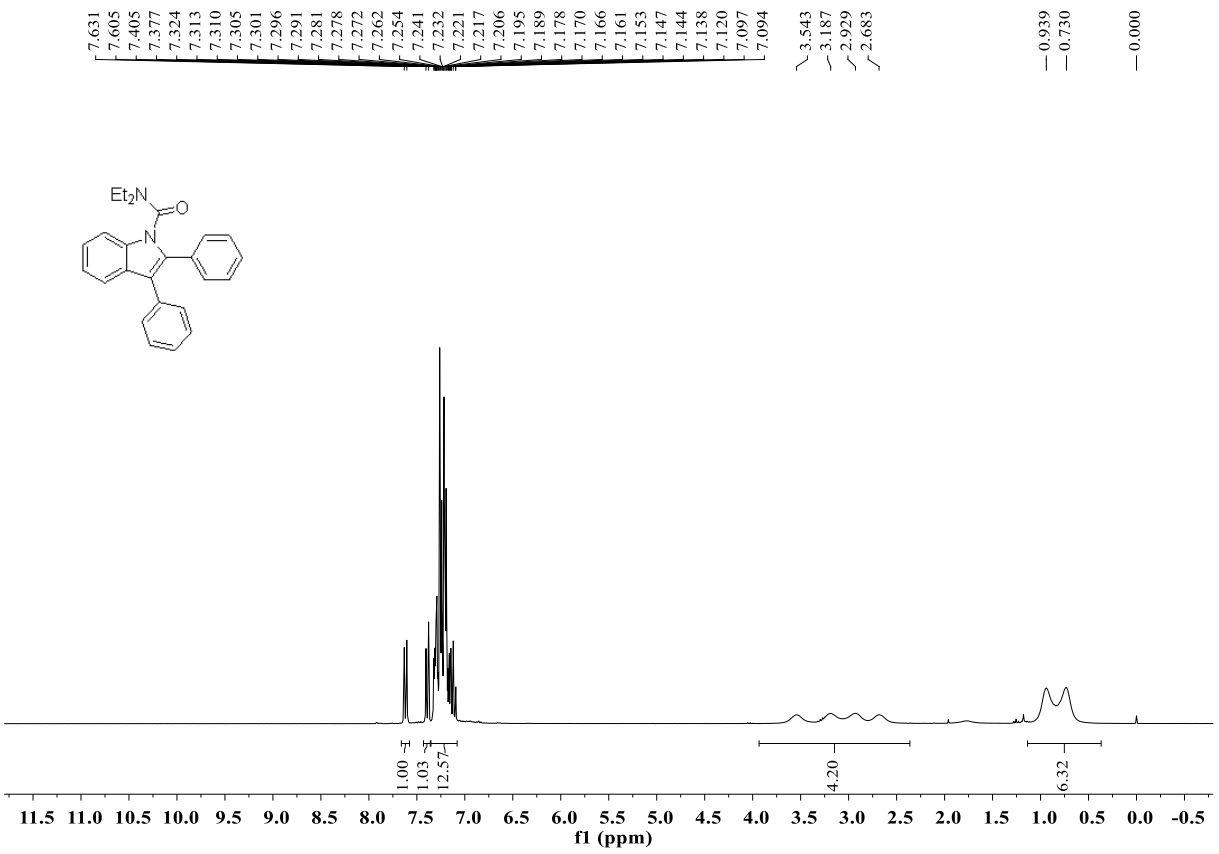
O
N
f1 (ppm)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7.170
7.166
7.161
7.153
7.147
7.144
7.138
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7.097
7.094
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3.187
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2.683
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O
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1.03
12.57
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6.32
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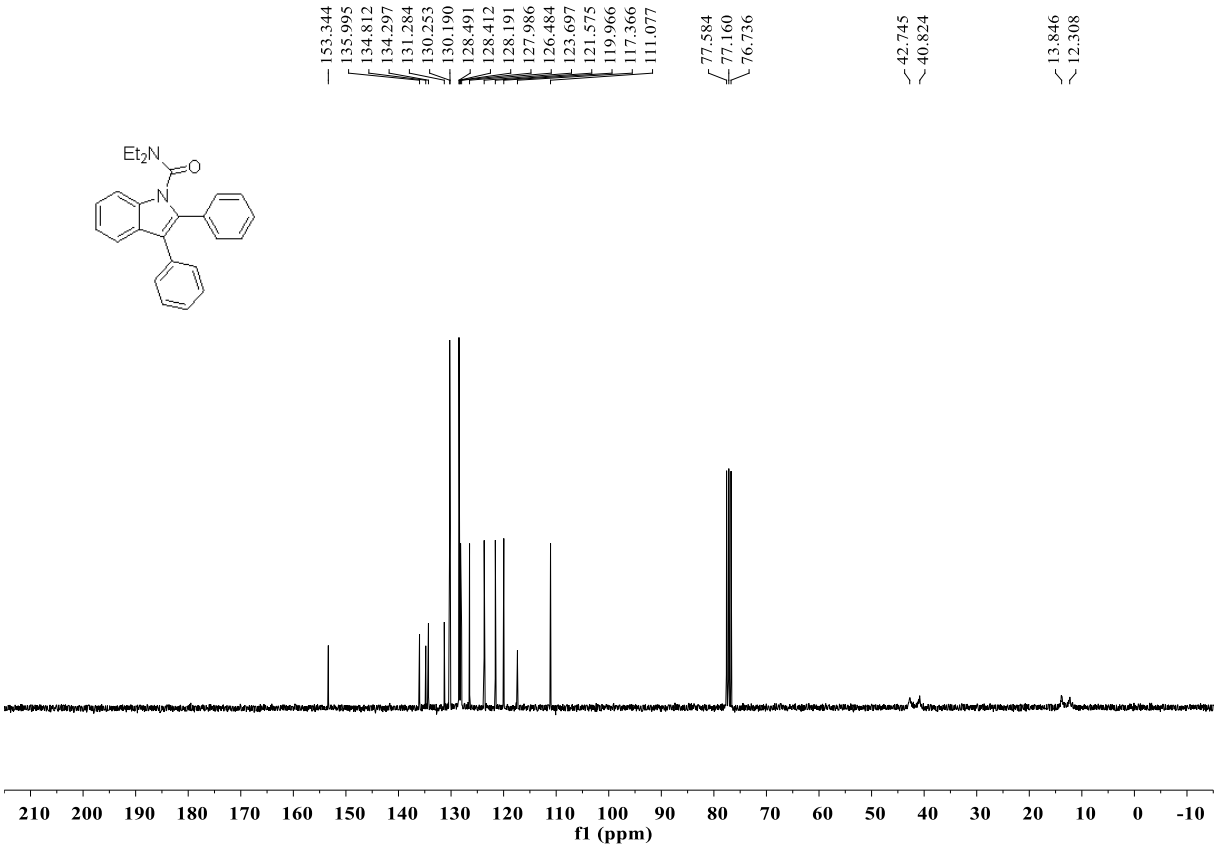
f1 (ppm)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42.745
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Et2N
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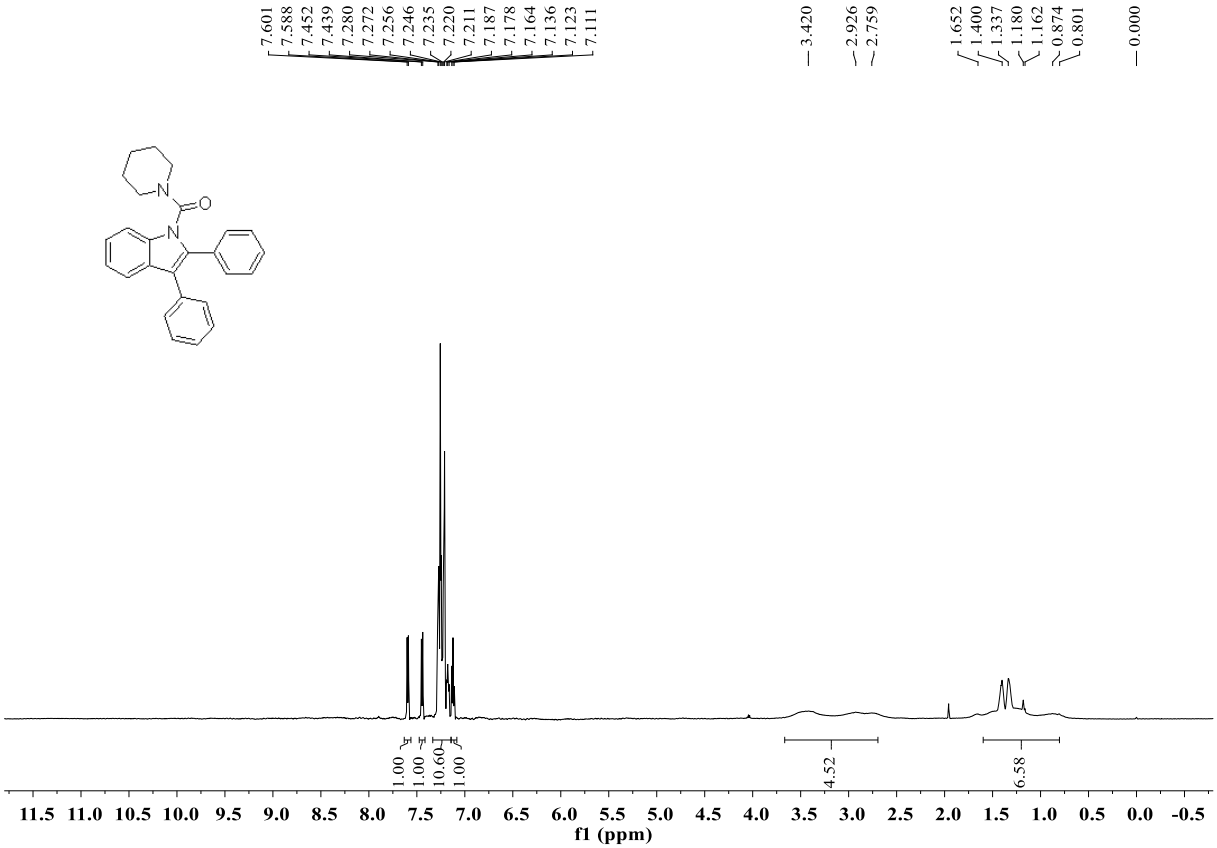
f1 (ppm)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7.164
7.136
7.123
7.111
3.420
2.926
2.759
1.652
1.400
1.337
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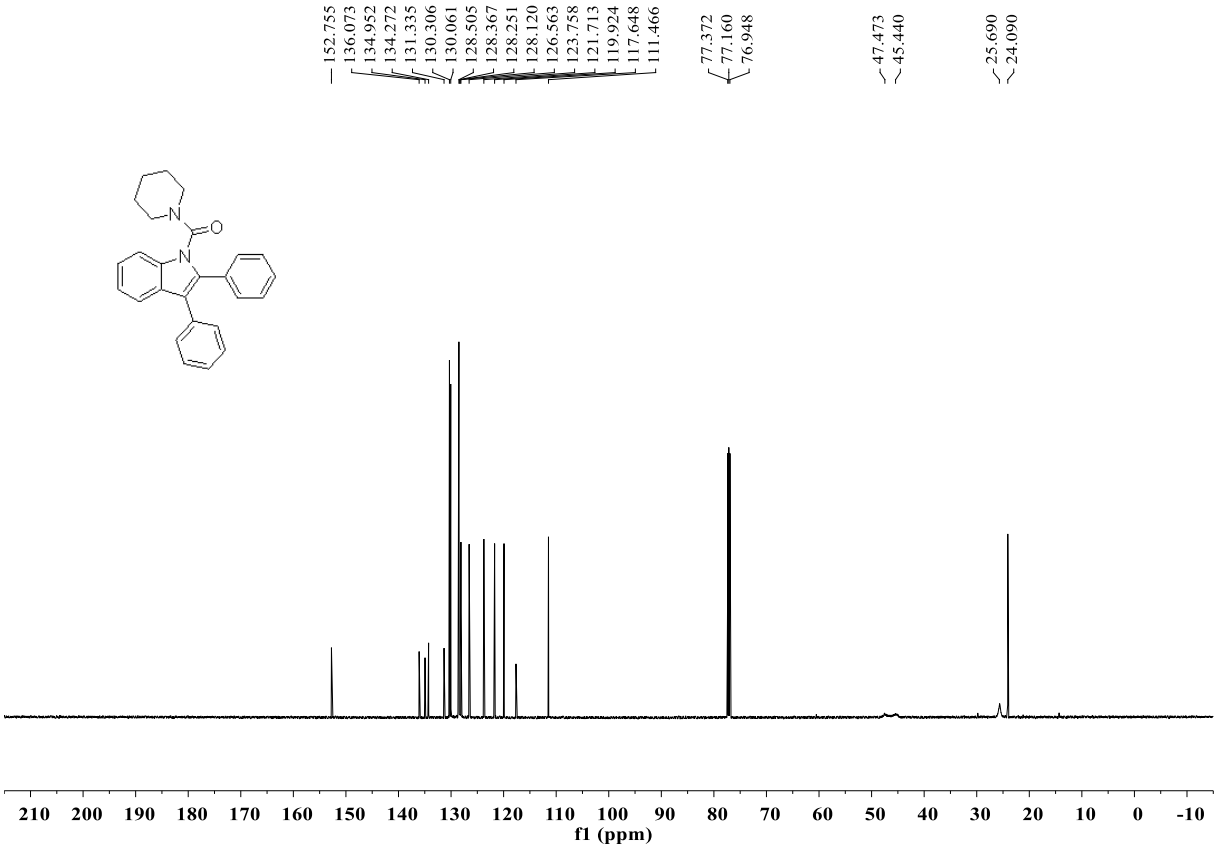
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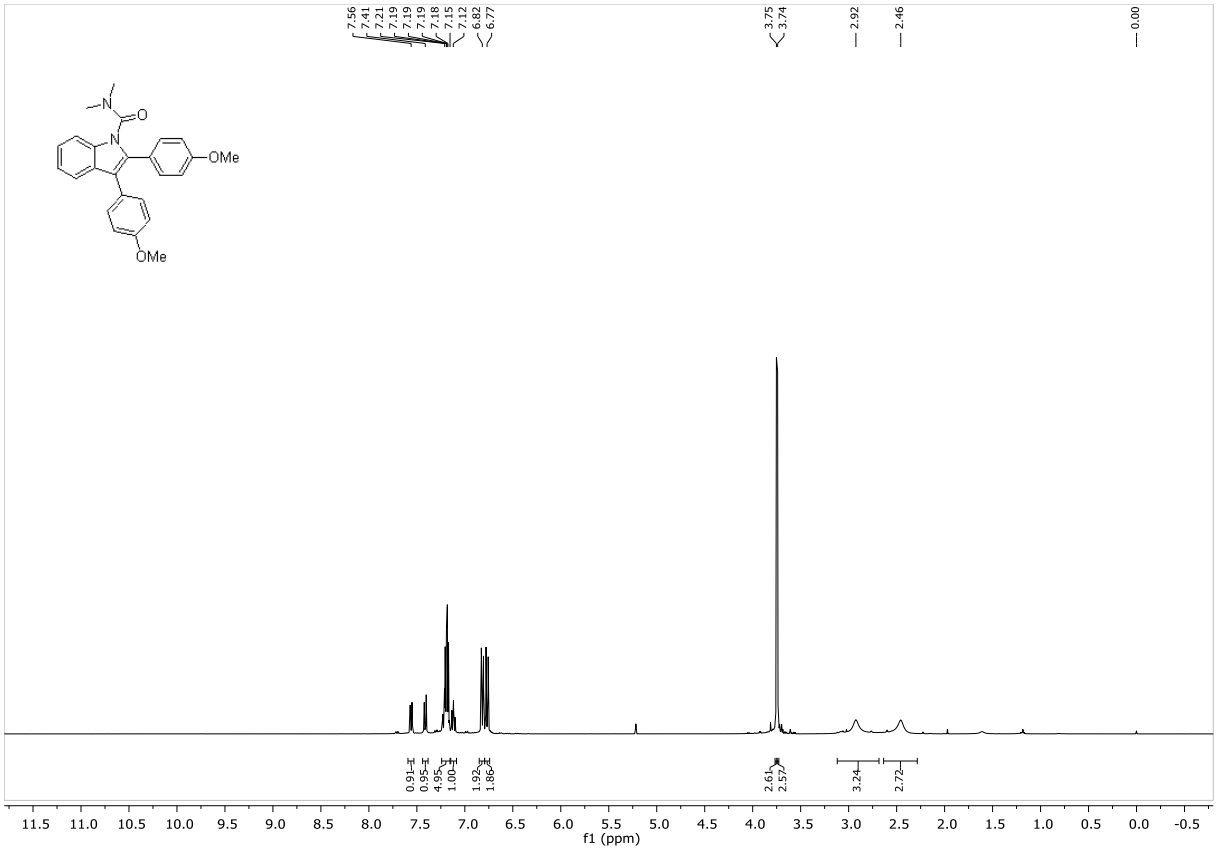
f1 (ppm)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7.19
7.18
7.15
7.12
6.82
6.77
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3.74
2.92
2.46
0.00
OMe
OMe
0.91
0.95
4.95
1.00
1.92
1.86
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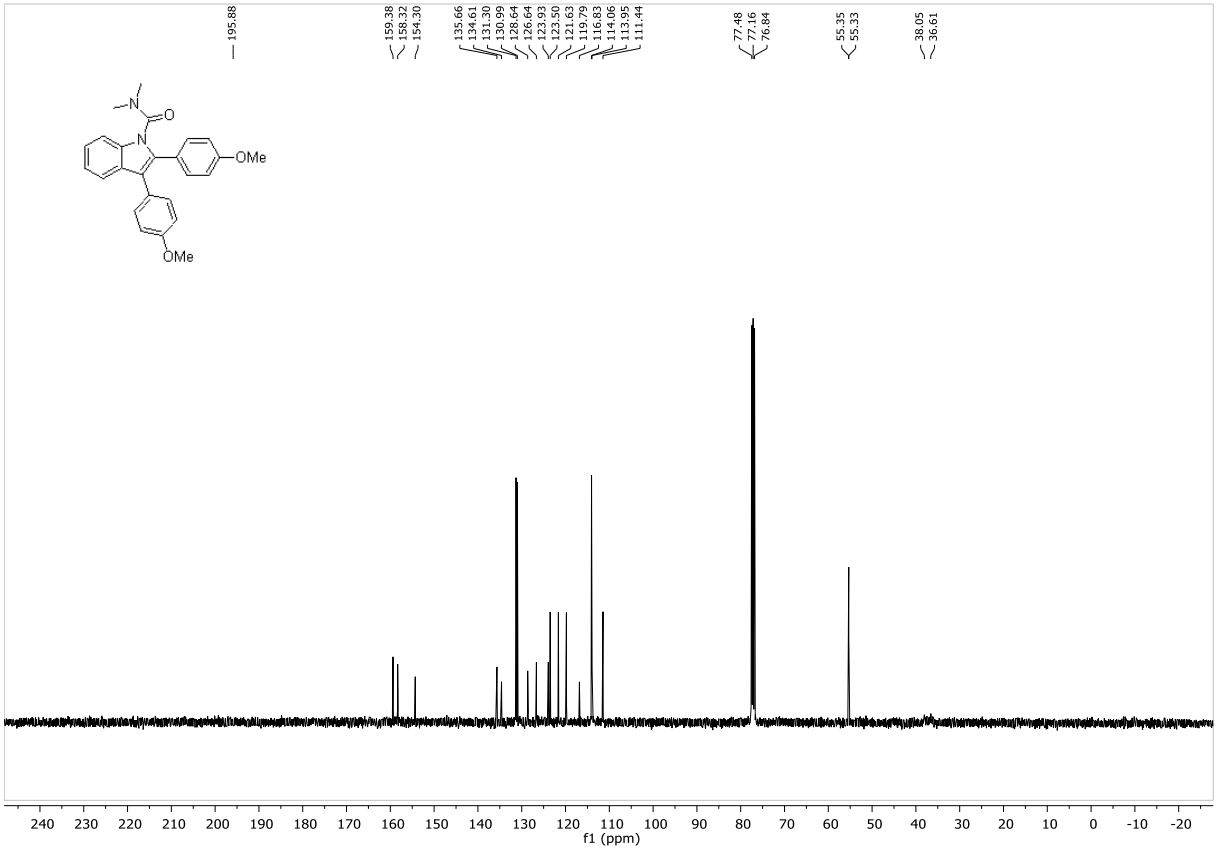
2.57
3.24
2.72
f1 (ppm)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116.83
114.06
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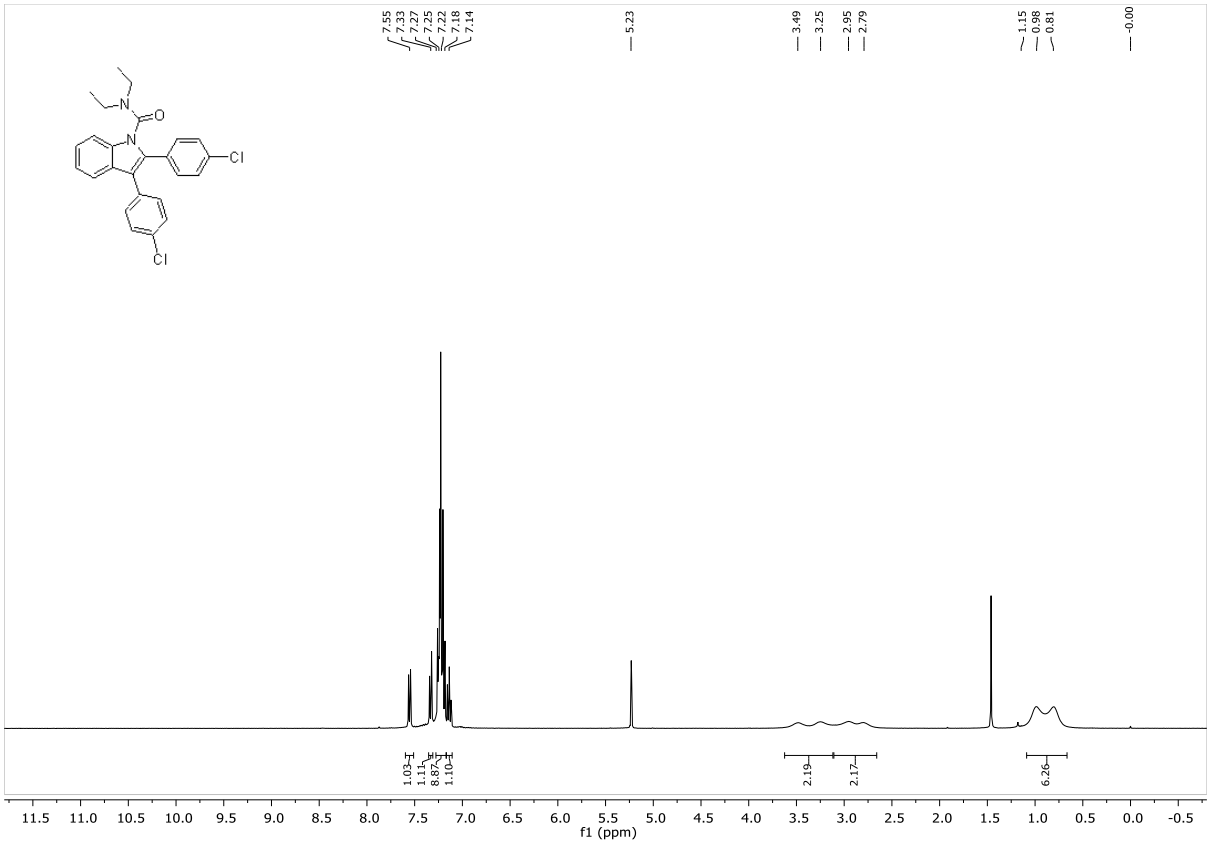
38.05
36.61
OMe
OMe
f1 (ppm)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1.15
0.98
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8.87
1.10
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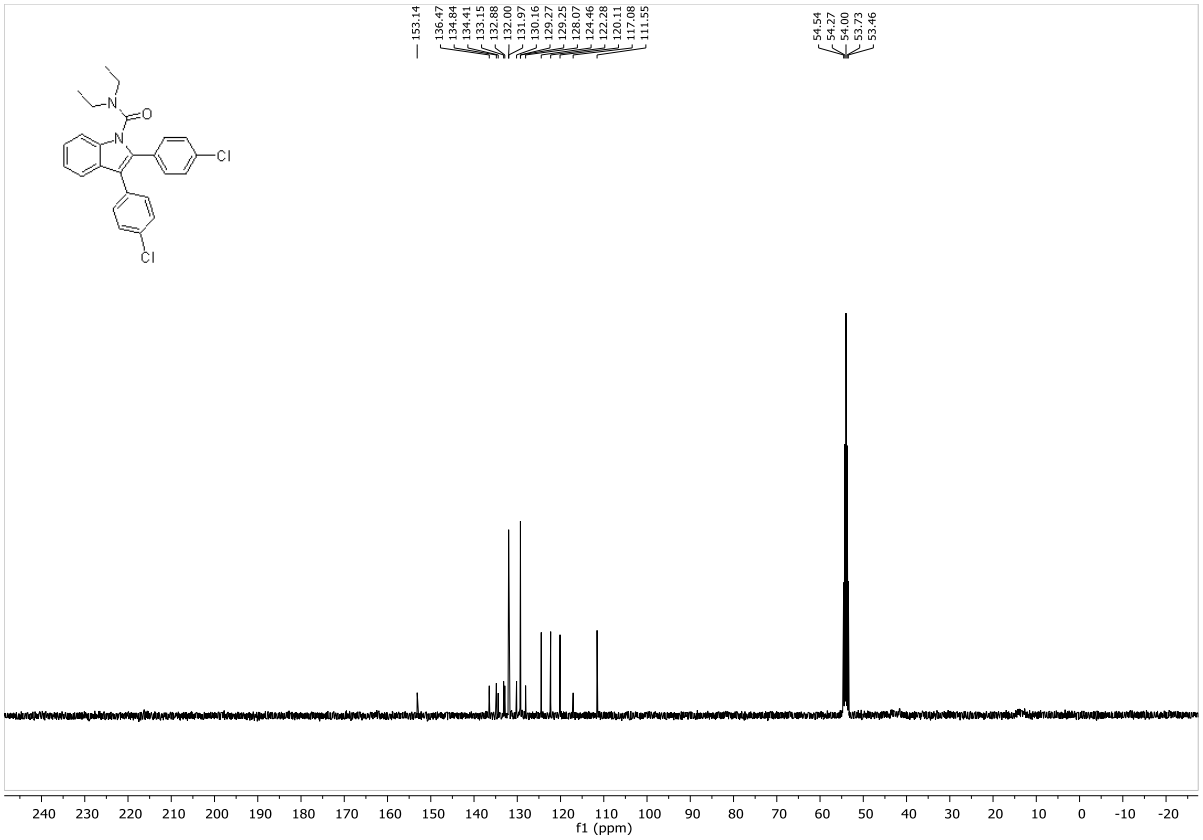
2.17
6.26
Cl
Cl
f1 (ppm)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53.73
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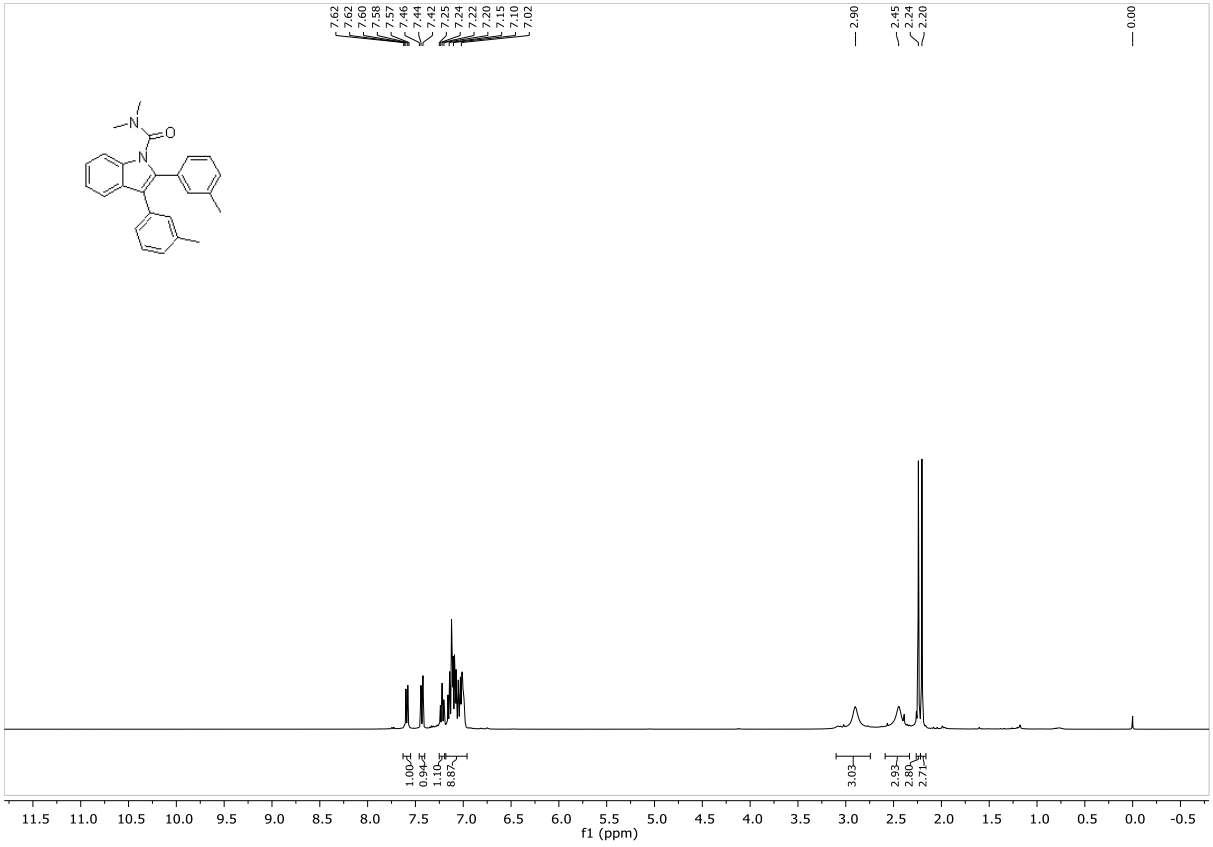
Cl
Cl
f1 (ppm)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7.22
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7.15
7.10
7.02
2.90
2.45
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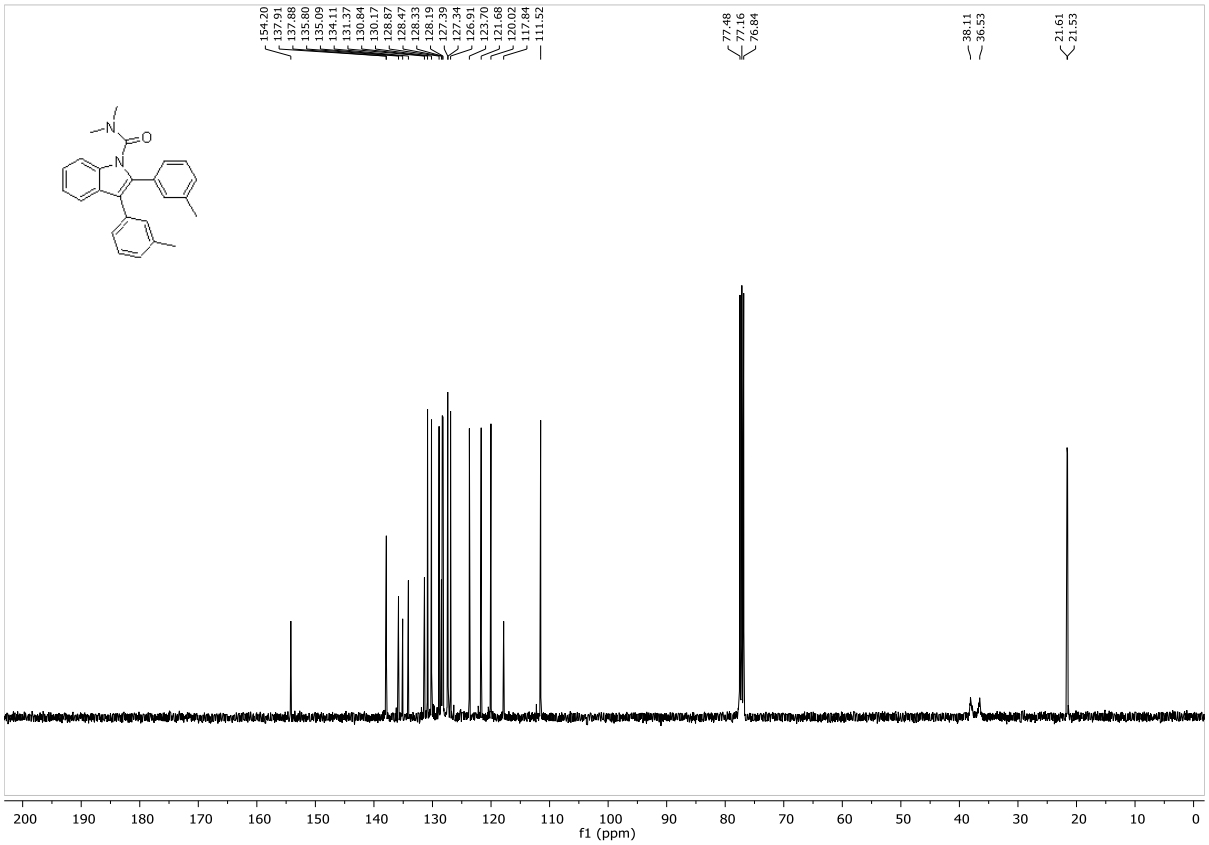
2.71
f1 (ppm)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127.39
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126.91
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77.16
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38.11
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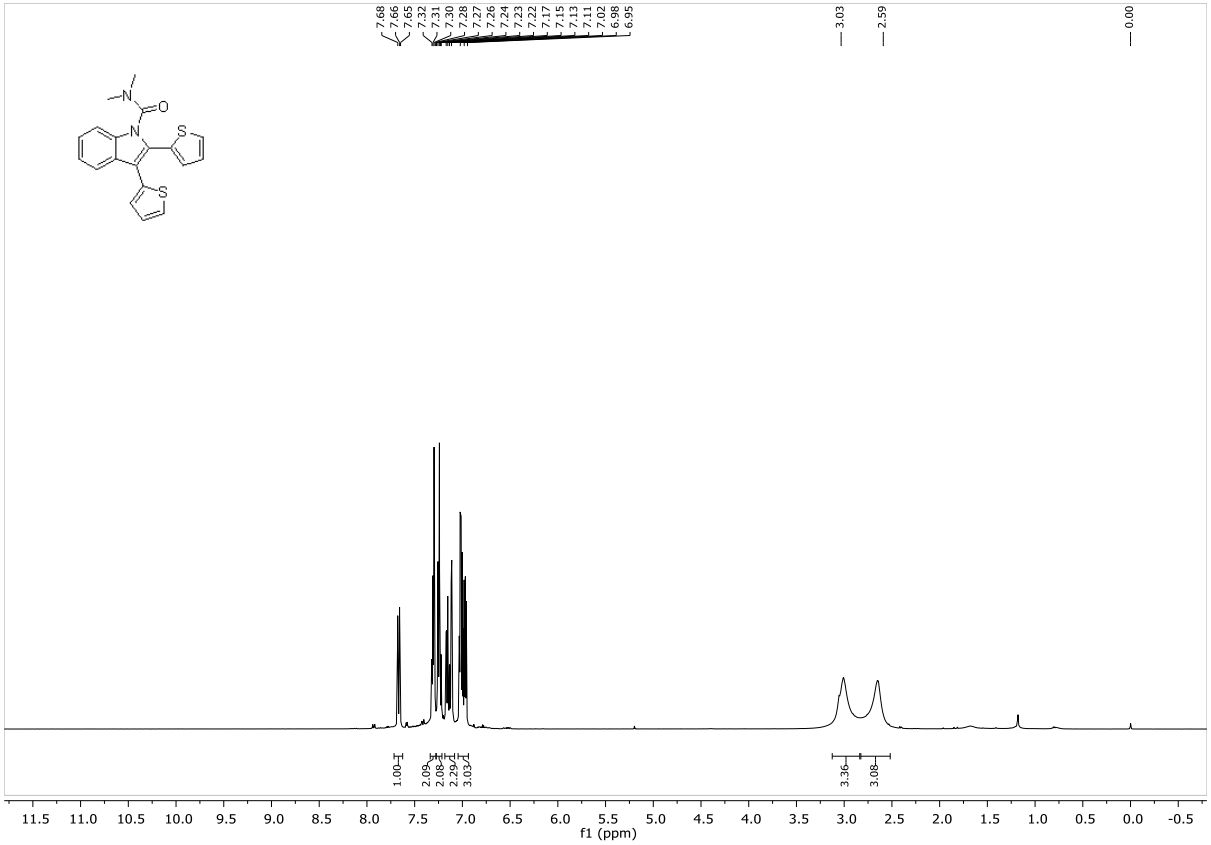
21.53
f1 (ppm)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7.22
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7.15
7.13
7.11
7.02
6.98
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1.00
2.09
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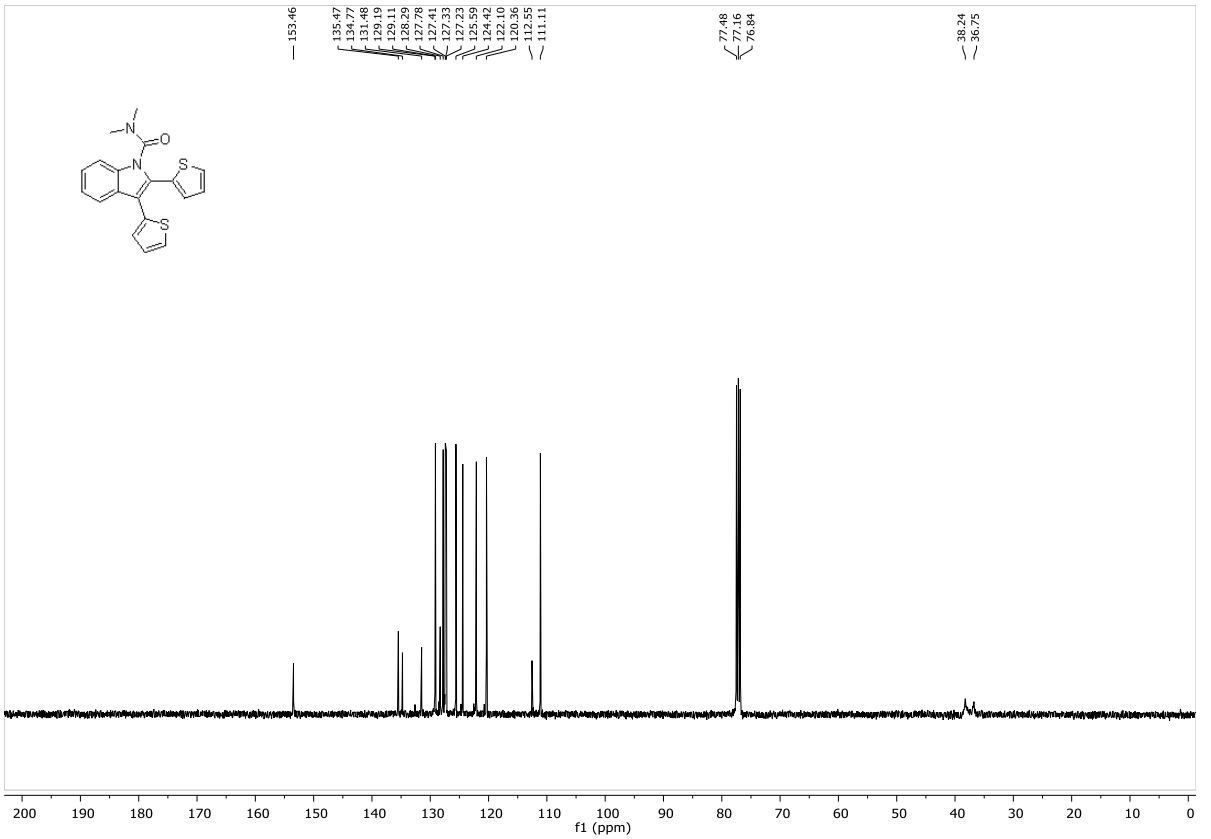
2.29
3.03
3.36
3.08
f1 (ppm)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127.23
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76.84
38.24
36.75
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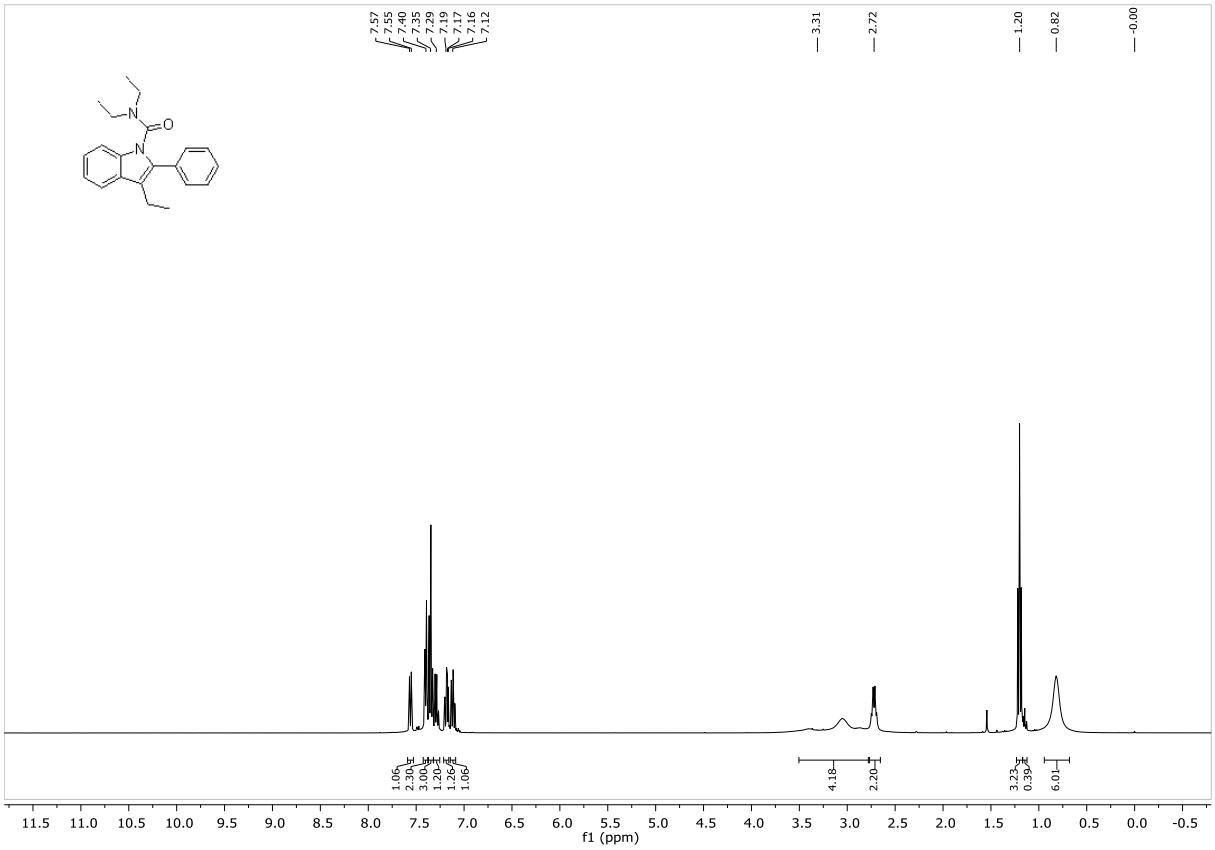
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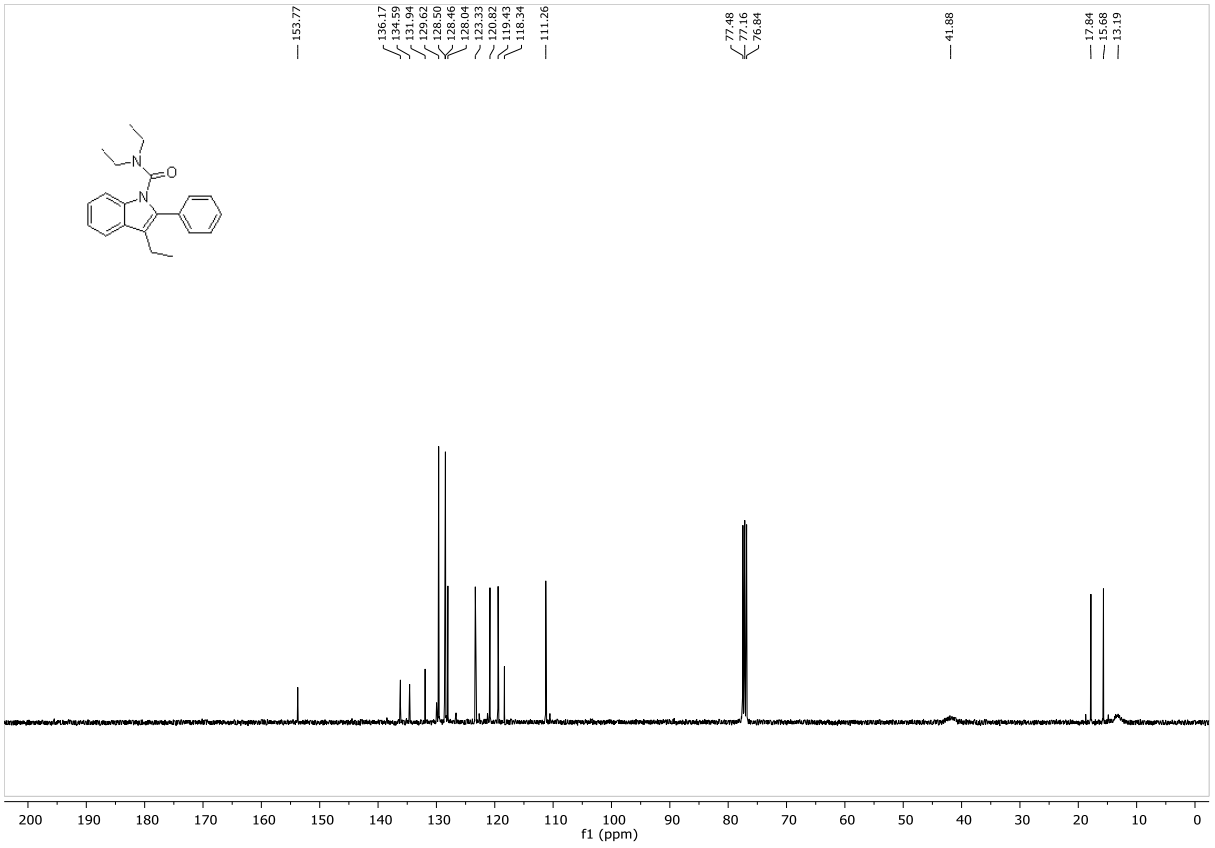
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77.16
76.84
41.88
17.84
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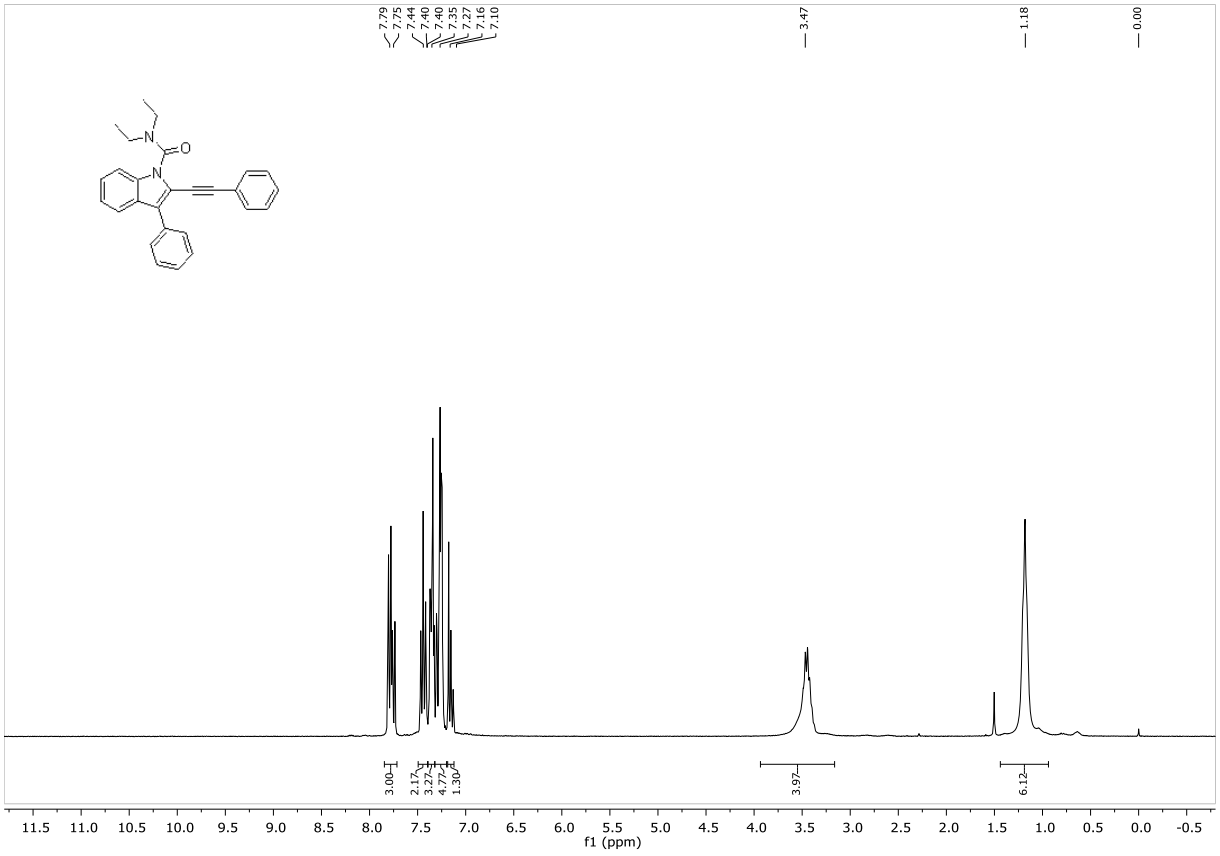
13.19
f1 (ppm)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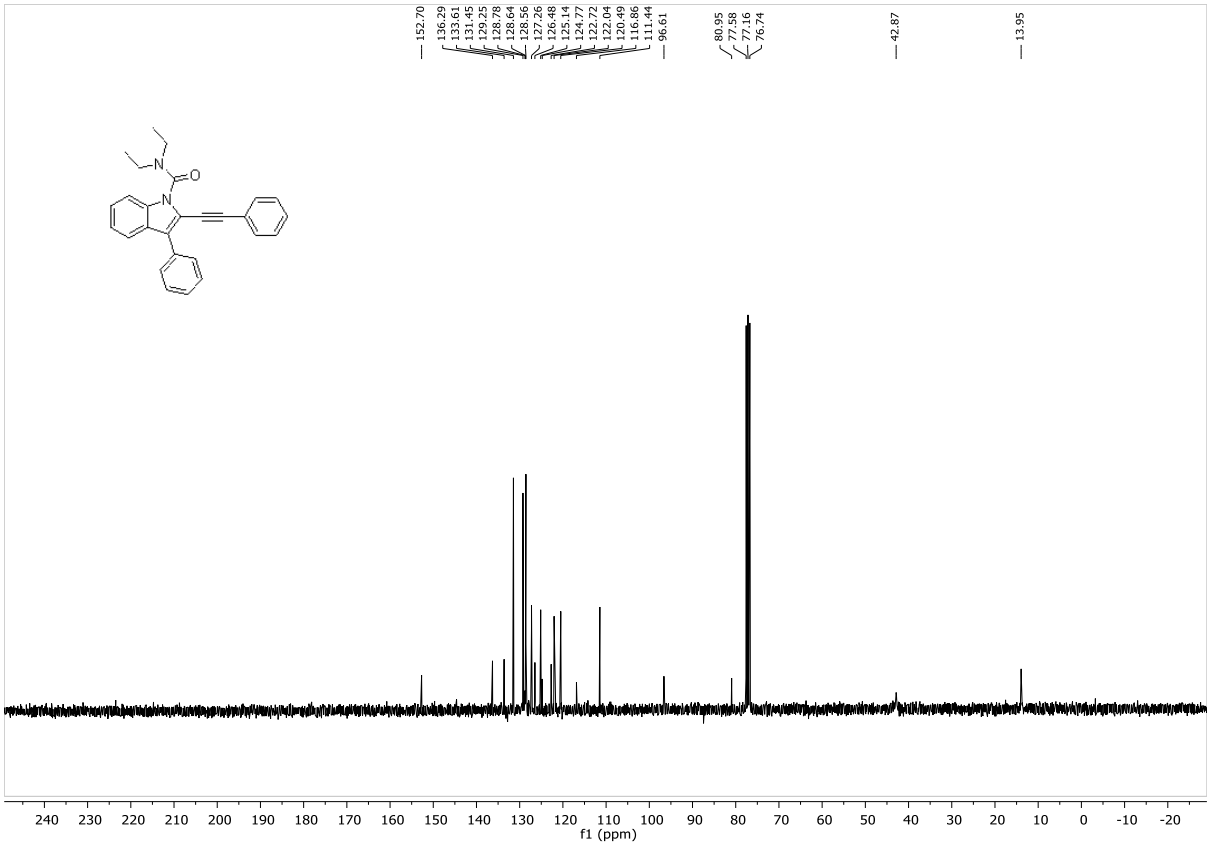
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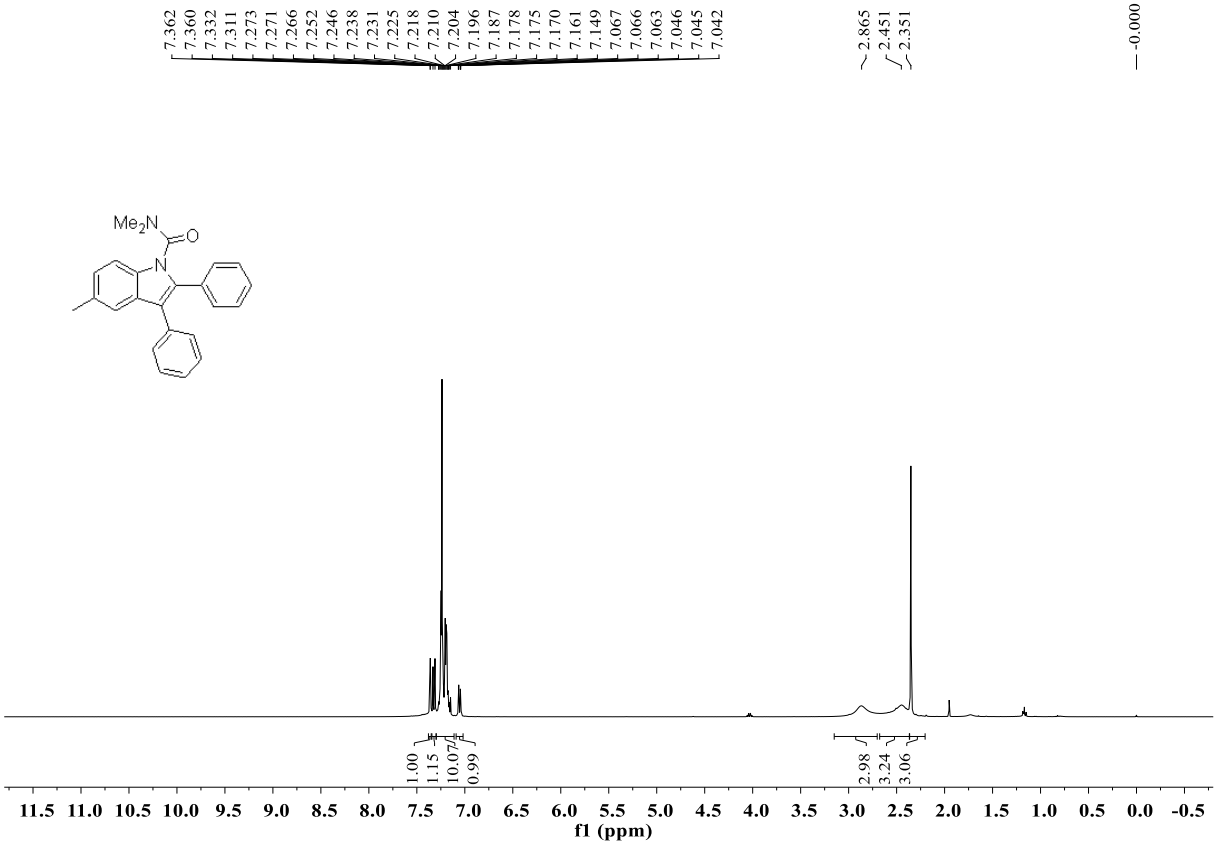
f1 (ppm)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7.170
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7.067
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7.063
7.046
7.045
7.042
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2.451
2.351
-0.000
Me2N
O
N
1.00
1.15
10.07
0.99
2.98
3.24
3.06
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
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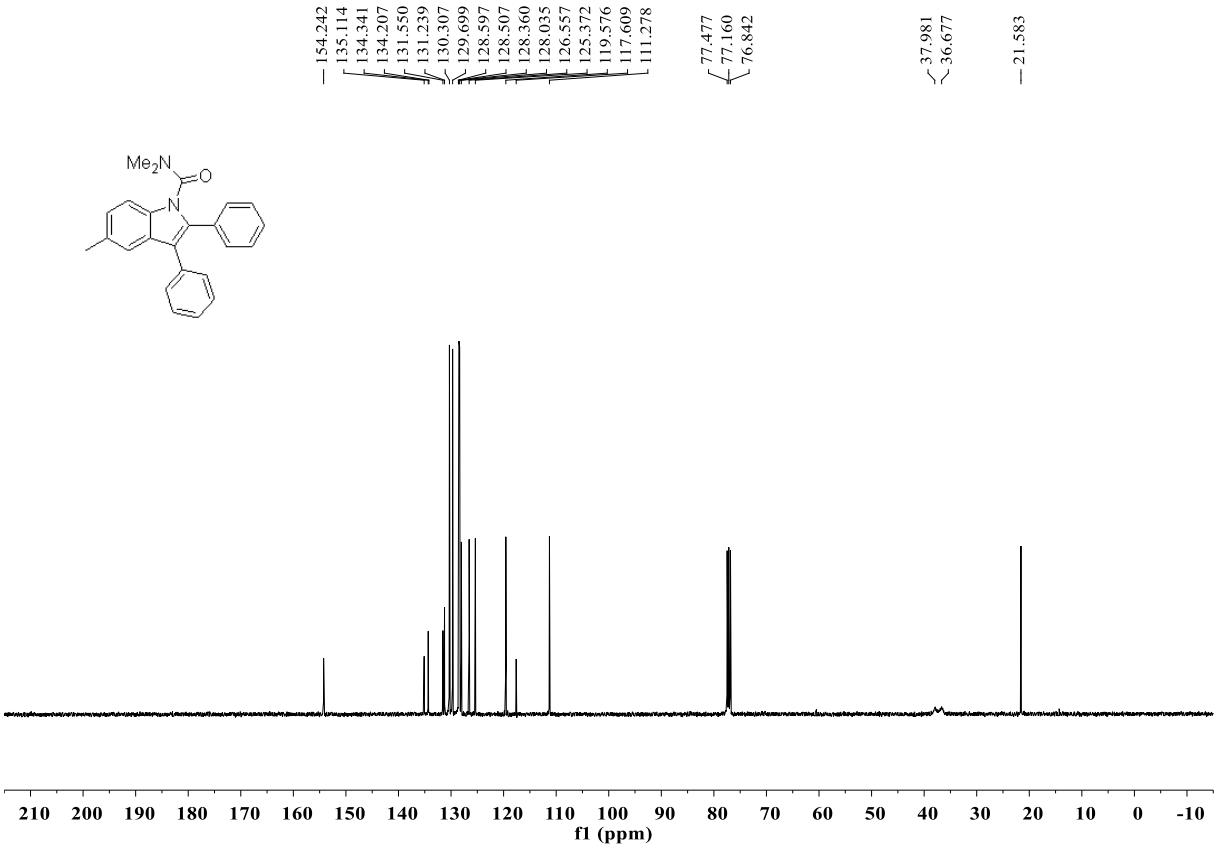
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117.609
111.278
77.477
77.160
76.842
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Me2N
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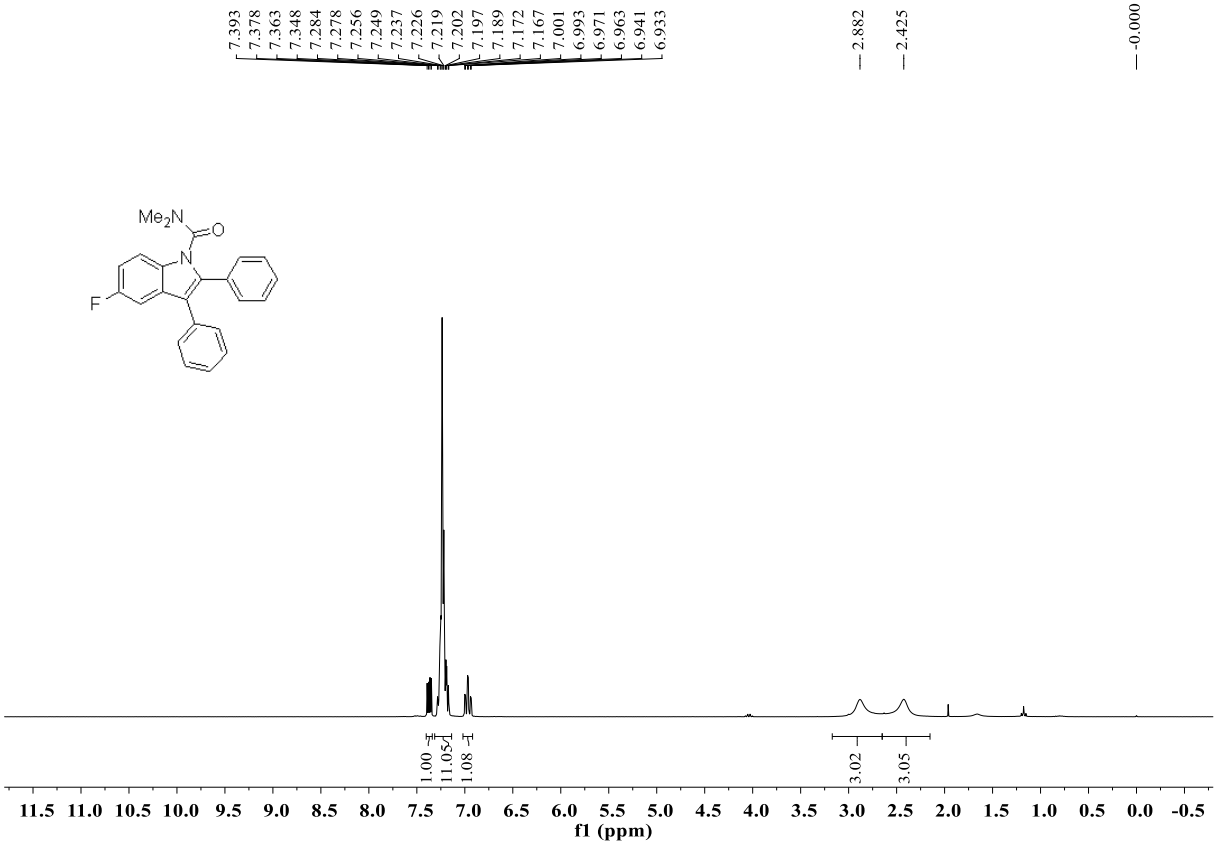
f1 (ppm)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F
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11.05
1.08
3.02
3.05
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
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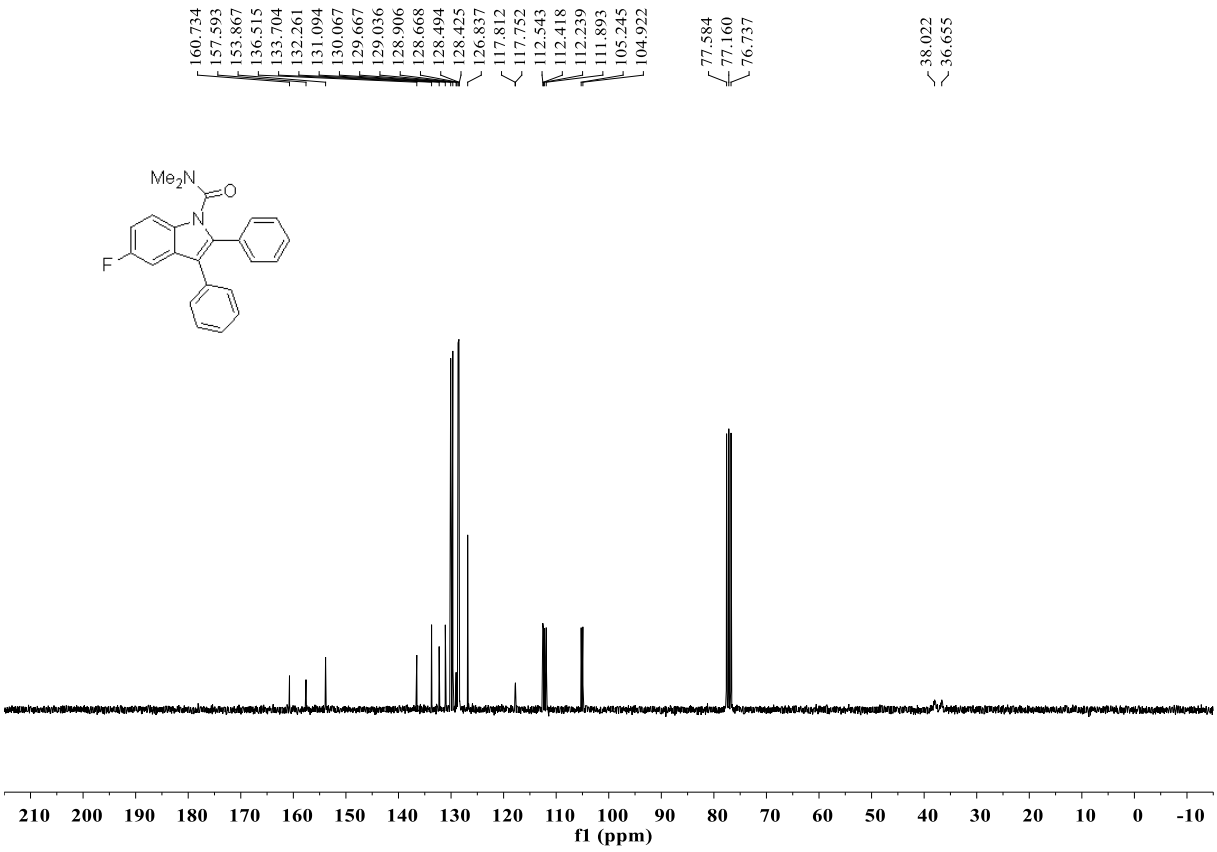
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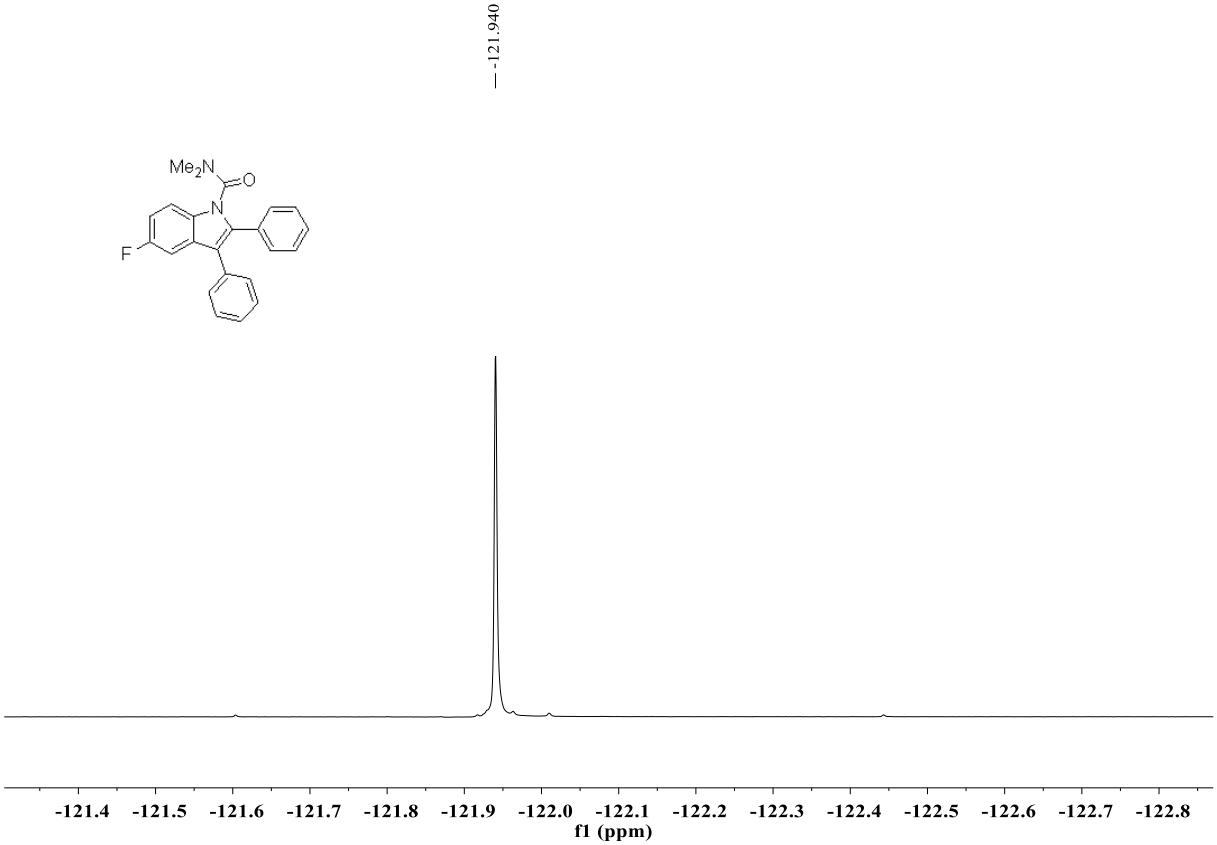
f1 (ppm)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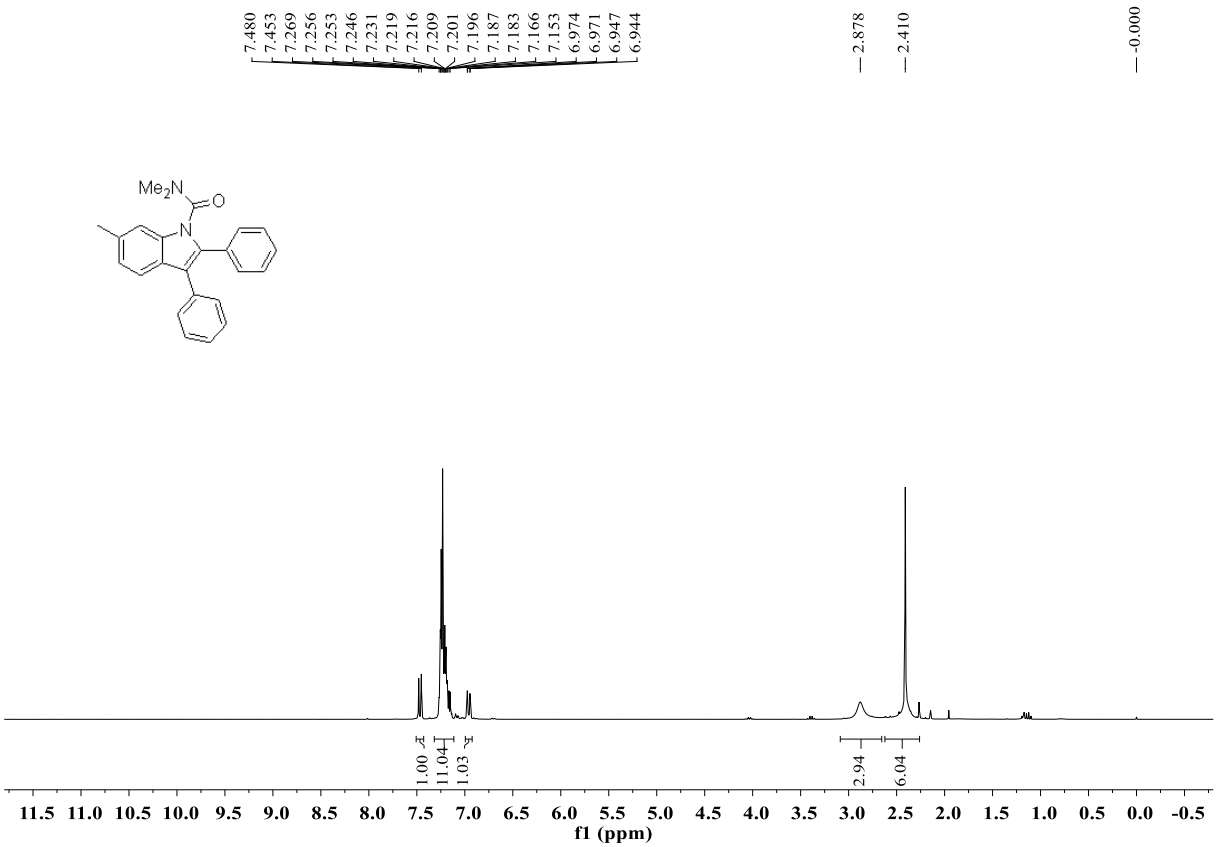
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7.166
7.153
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6.971
6.947
6.944
2.878
2.410
0.000
Me2N
O
N
1.00
11.04
1.03
2.94
6.04
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
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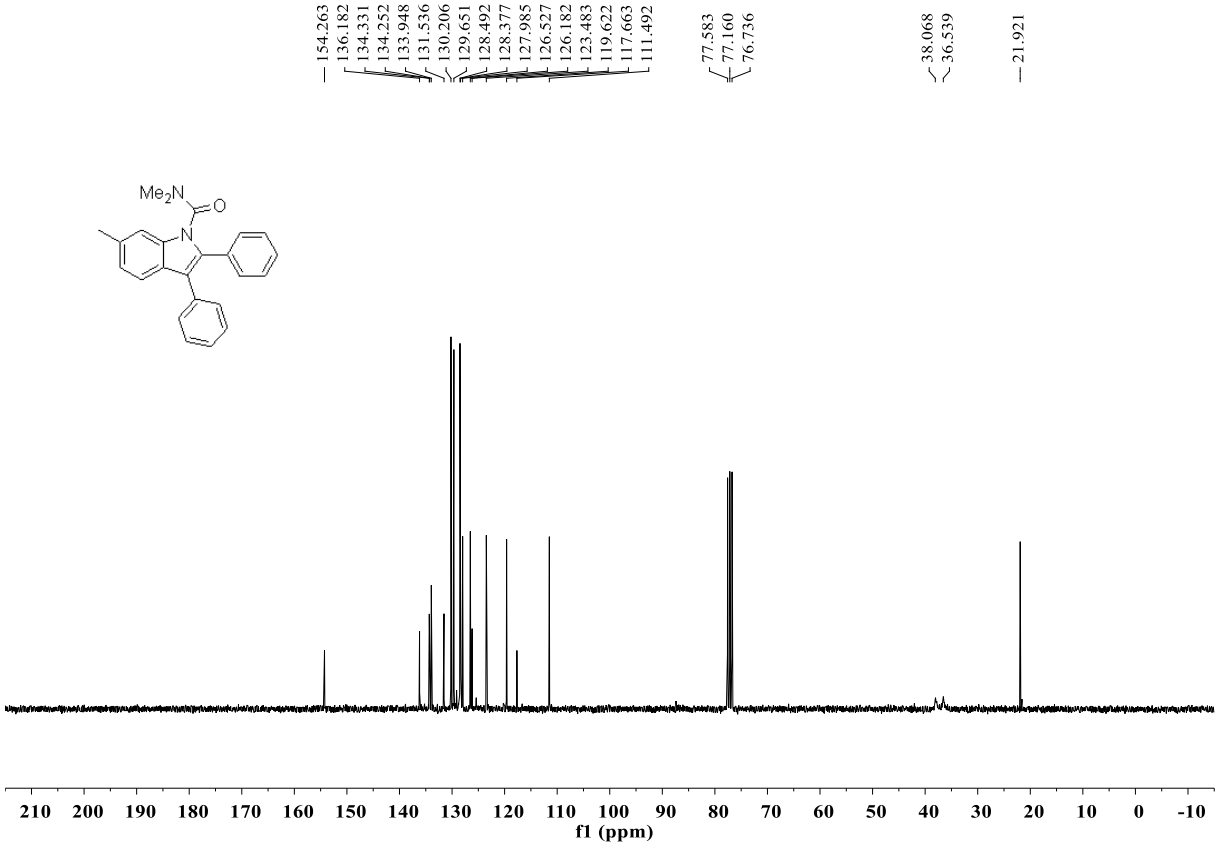
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76.736
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O
N
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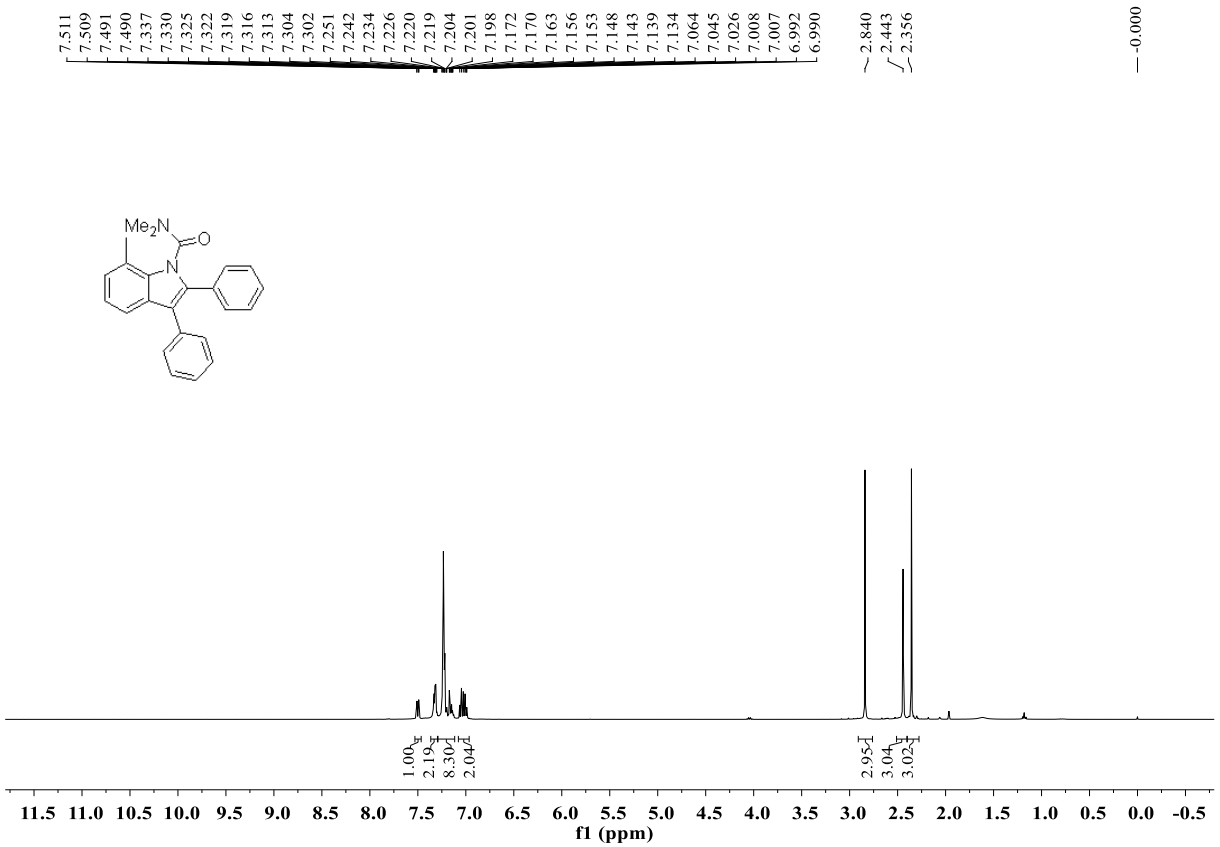
f1 (ppm)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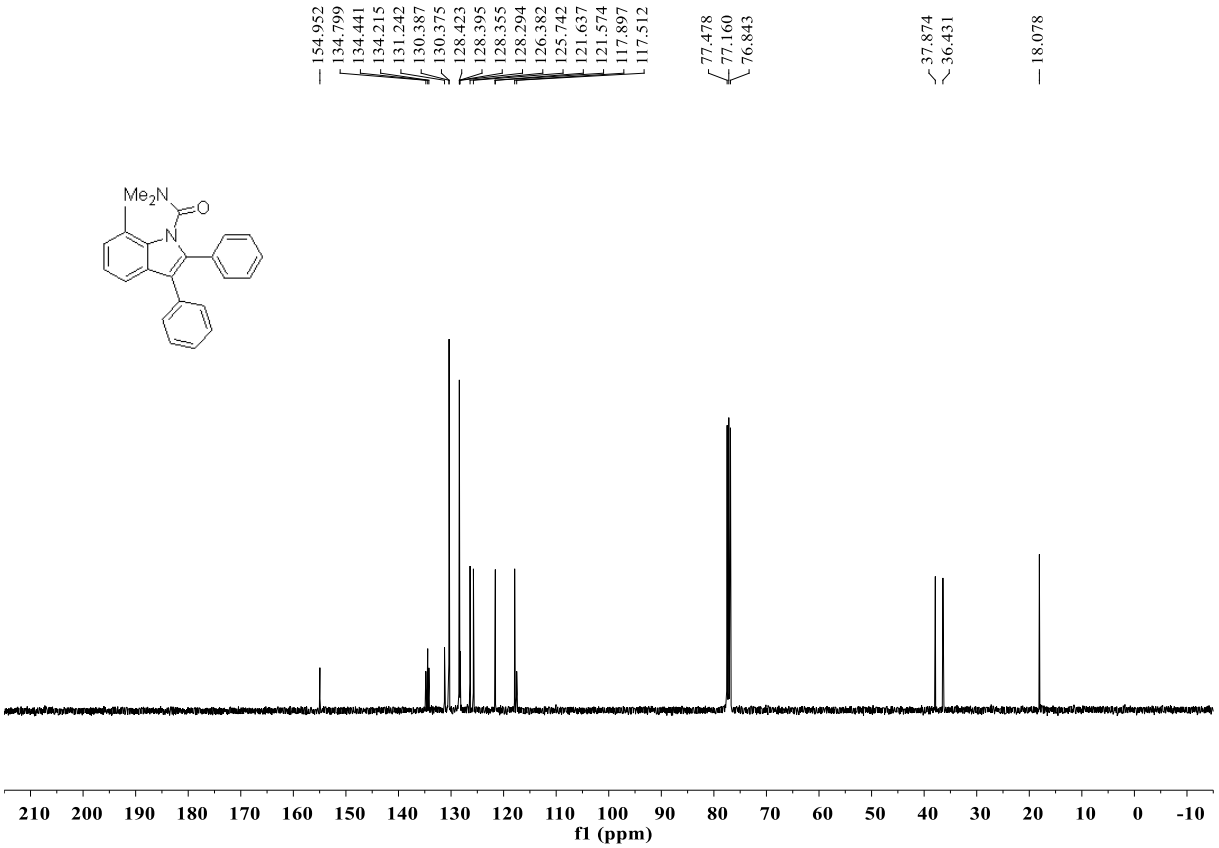
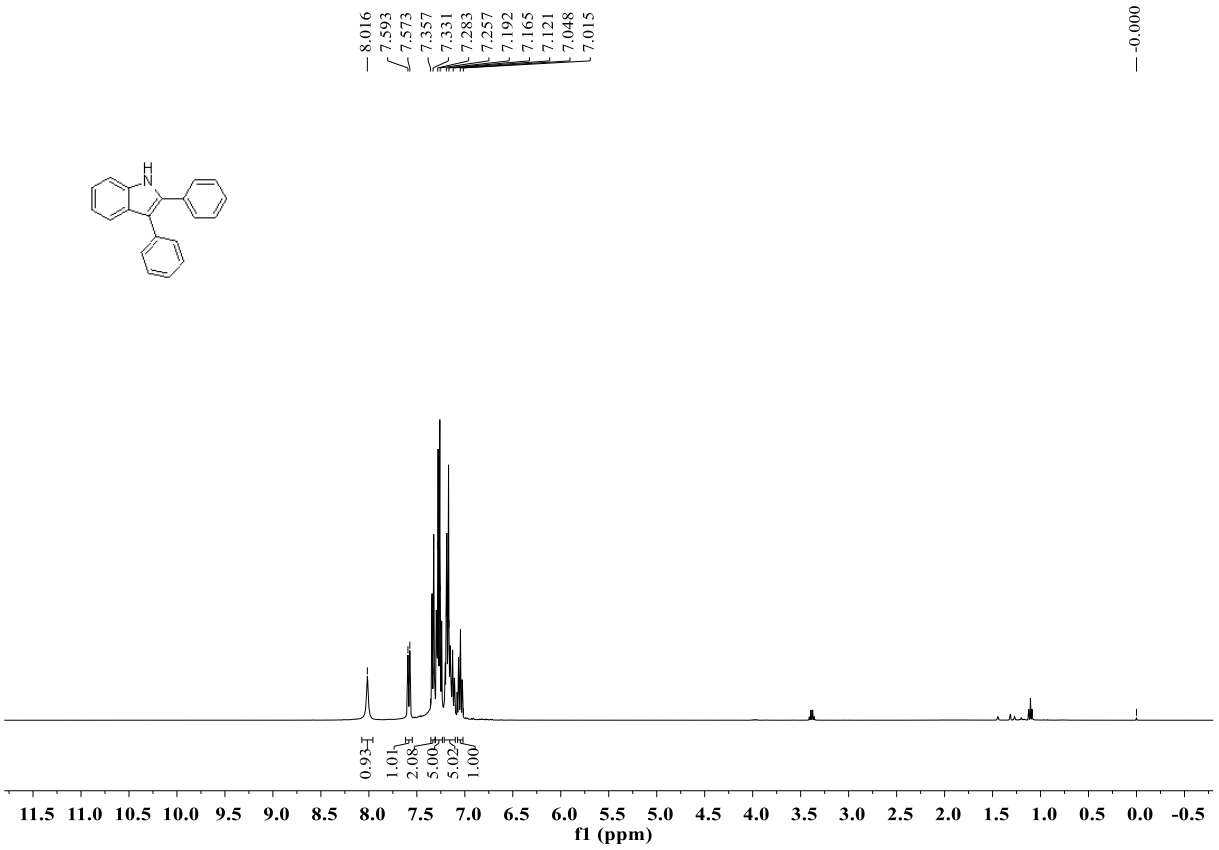
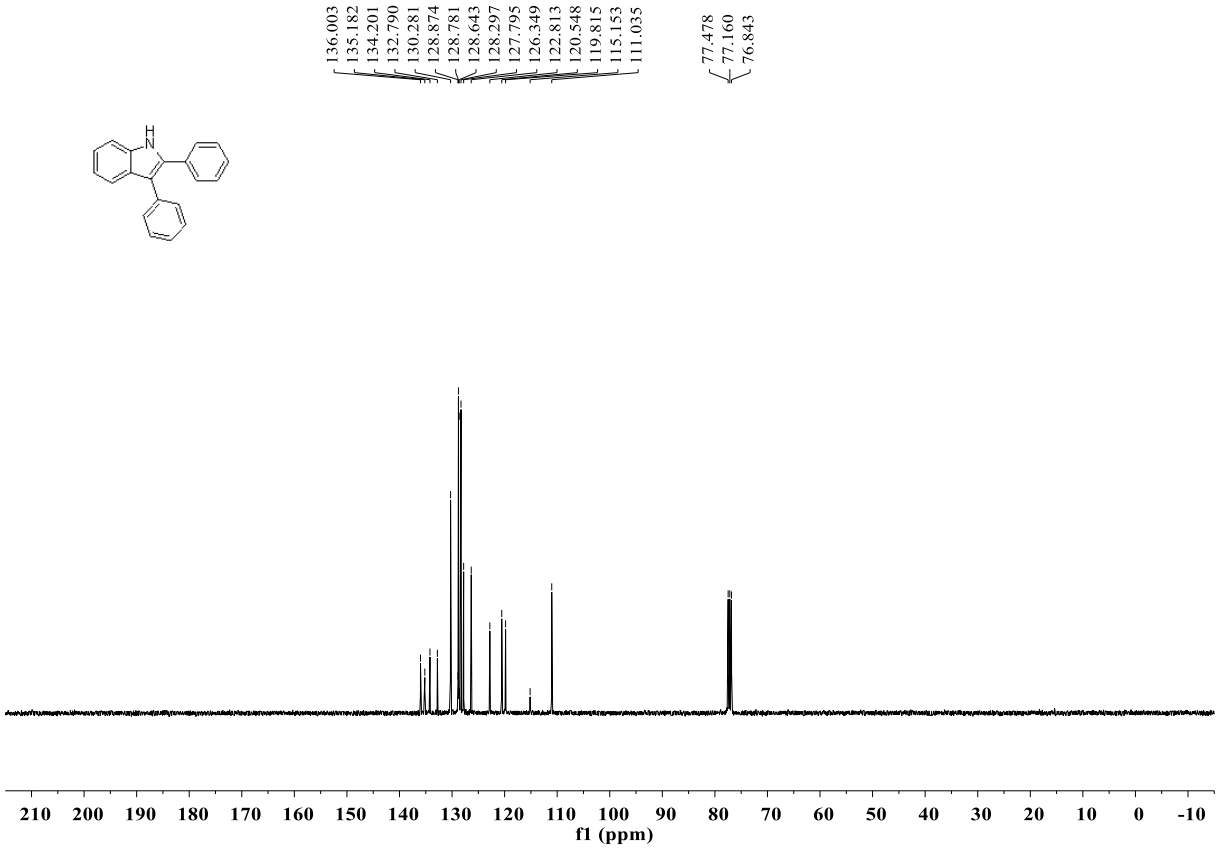
7.219
7.204
7.201
7.198
7.172
7.170
7.163
7.156
7.153
7.148
7.143
7.139
7.134
7.064
7.045
7.026
7.008
7.007
6.992
6.990
2.840
2.443
2.356
-0.000
Me2N
O
N
1.00
2.19
8.30
2.04
2.95
3.04
3.02
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


154.952
134.799
134.441
134.215
131.242
130.387
130.375
128.423
128.395
128.355
128.294
126.382
125.742
121.637
121.574
117.897
117.512
77.478
77.160
76.843
37.874
36.431
18.078
Me2N
O
N
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)


8.016
7.593
7.573
7.357
7.331
7.283
7.257
7.192
7.165
7.121
7.048
7.015
-0.000
H
N
0.93
1.01
2.08
5.00
5.02
1.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


136.003
135.182
134.201
132.790
130.281
128.874
128.781
128.643
128.297
127.795
126.349
122.813
120.548
119.815
115.153
111.035
77.478
77.160
76.843
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)