Supporting Information

An efficient class of bis-NHC salts: applications in Pd-catalyzed reactions under mild reaction conditions

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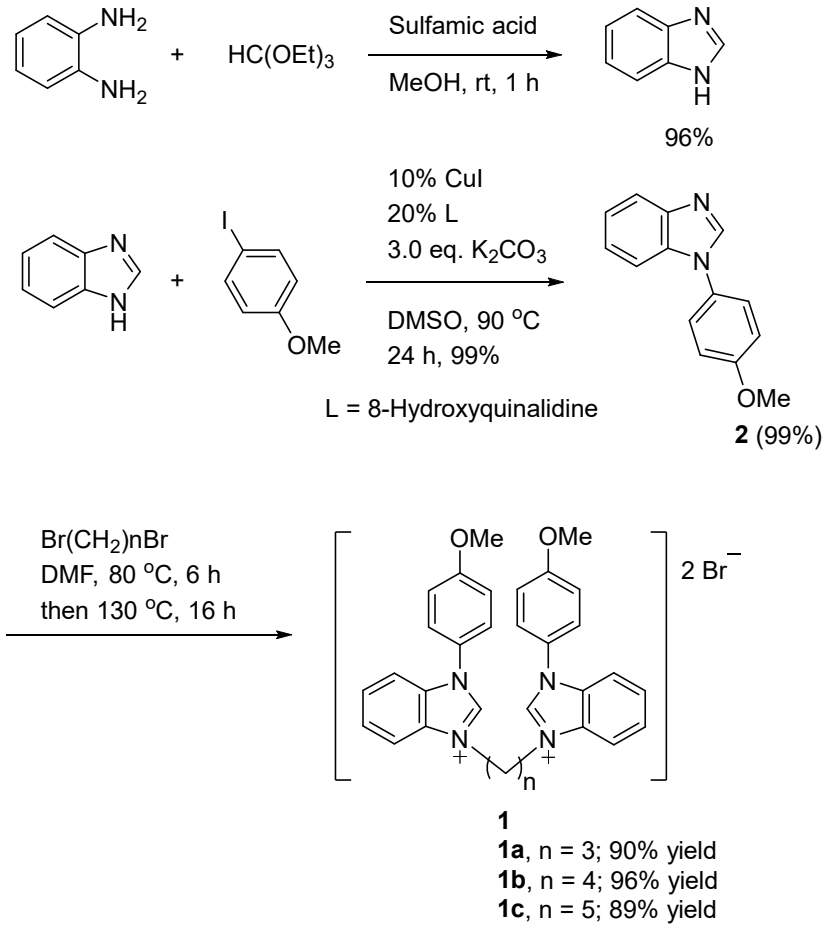
1. Experimental Section

1.1. General Aspects. Anhydrous solvents (PhMe, CH_3CN, and dioxane) were obtained by distillation over calcium hydride. *t*-BuOH was obtained by distillation over sodium. Pre-coated silica gel 60 F-254, layer thickness 0.2 mm, plates were used for analysis of reactions with detection by 0.5% phosphomolybdic acid solution in 95% EtOH. Merck silica gel 60 (0.040–0.063 μm) was used for chromatography. ^{1}H and ^{13}C NMR spectra were recorded on a Varian Mercury-400 spectrometer operating at 400 MHz (^{1}H) and 100 MHz (^{13}C). Chemical shifts (δ) given in ppm relative to TMS; *J*-values are in Hz. Melting points were determined with a Thermo 1001D digital melting point apparatus and are uncorrected. High-resolution mass spectra were recorded on a Finnigan/Thermo Quest MAT 95XL mass spectrometer. Mass spectra were obtained using either electron impact (EI) or electrospray ionization (ESI) method. Benzimidazole was synthesized according to similar literature procedures.[1]

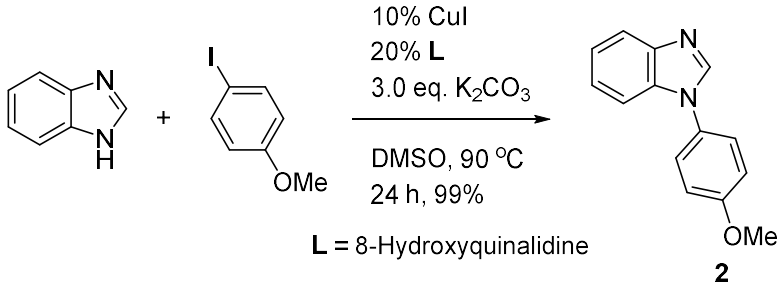
1.2. Experimental procedures and spectral data

1.2.1. Synthesis of *bis*-benzimidazolium salts 1



Scheme 1. Synthesis of bis-benzimidazolium salts **1**.

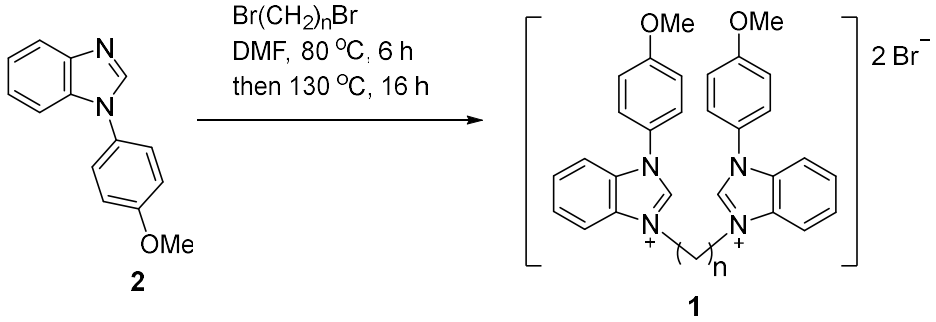
Procedure for the 1-(4-methoxyphenyl)-1*H*-benzo[d]imidazole (2)[2]



To a mixture of CuI (0.280 g, 1.50 mmol), K_2CO_3 (6.20 g, 44.9 mmol) and 8-hydroxyquinalidine (0.480 g, 3.00 mmol) in DMSO (15 mL) was added a solution of 4-iodoanisole (3.50 g, 15.0 mmol) and benzimidazole (2.21 g, 18.7 mmol) in DMSO (15 mL) at 30 °C. After stirring for 24 h at 90 °C, the reaction mixture was filtered through a small pad of Celite. The filtrate was treated with H_2O (30 mL) and EtOAc (30 mL). The aqueous layer was extracted with EtOAc (30 mL×2). The

combined organic layers were dried over $MgSO_4$ and then filtered. The solvent was removed under reduced pressure. The residue was purified by column chromatography to give the pure product **2** (3.33 g, 99%) as white solid. Mp = 92–94 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.05 (s, 1H), 7.89–7.86 (m, 1H), 7.47–7.44 (m, 1H), 7.42 (d, *J* = 8.8 Hz, 2H), 7.35–7.30 (m, 2H), 7.08 (d, *J* = 8.8 Hz, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 158.9, 143.5, 142.2, 133.8, 128.7, 125.3, 123.2, 122.2, 120.1, 114.7, 110.0, 55.3.

General procedures for the bis-benzimidazolium salts (1)[3]



To a solution of 1-(4-methoxyphenyl)-1*H*-benzo[d]imidazole **2** (4.46 mmol) in DMF (9.0 mL) was added dibromoalkane (2.23 mmol). After stirring for 6 h at 80 ºC, the resulting solution was heated at 130ºC for 16 h. The reaction mixture was cooled to room temperature. The *bis*-benzimidazolinum salt precipitate was filtered off and washed with EtOH.

3,3'-(propane-1,3-diyl)bis(1-(4-methoxyphenyl)-1*H*-benzo[d]imidazol-3-ium) bromide (1a)

Yield 90% (1.30 g); purple powder; Mp = 260–262 ºC (dec.); ^{1}H NMR (CD_3OD, 400 MHz): δ 8.20 (d, *J* = 8.8 Hz, 2H), 7.80–7.72 (m, 10H), 7.24 (d, *J* = 9.2 Hz, 4H), 3.91 (s, 6H), 4.93 (t, *J* = 7.6 Hz, 4H), 2.97 (quin, *J* = 7.6 Hz, 2H); ^{13}C NMR (CD_3OD, 100 MHz): δ 162.8, 133.5, 132.9, 129.0, 128.7, 127.9, 127.0, 116.6, 114.9, 114.8, 56.4, 45.9, 29.8; HRMS-ESI (*m*/*z*) $[M–Br]^+$ calcd for $C_{31}H_{30}BrN_4O_2$: 569.1547, found: 569.1552.

4,4'-(butane-1,4-diyl)bis(1-(4-methoxyphenyl)-1*H*-benzo[d]imidazol-3-ium) bromide (1b)

Yield 96% (1.42 g); pale-purple powder; Mp = 264–266 ºC (dec.); ^{1}H NMR (CD_3OD, 400 MHz): δ 8.14 (d, *J* = 8.8 Hz, 2H), 7.77–7.71 (m, 10H), 7.23 (d, *J* = 8.8 Hz, 4H), 4.75 (t, *J* = 7.6 Hz, 4H), 3.91 (s, 6H), 2.33 (quin, *J* = 7.6 Hz, 4H); ^{13}C NMR (CD_3OD, 100 MHz): δ 162.9, 133.5, 132.9, 128.9,

128.6, 127.9, 116.6, 114.9, 114.7, 56.4, 48.1, 27.3; HRMS-ESI (*m*/*z*) $[M–Br]^+$ calcd for $C_{32}H_{32}BrN_4O_2$: 583.1703, found: 583.1705.

5,5'-(pentane-1,5-diyl)bis(1-(4-methoxyphenyl)-1*H*-benzo[d]imidazol-3-ium) bromide (1c)

Yield 89% (1.35 g); white powder; Mp = 172–176 ºC; ^{1}H NMR (CD_3OD, 400 MHz): δ 8.09 (d, *J* = 8.0 Hz, 2H), 7.79–7.69 (m, 10H), 7.25 (d, *J* = 9.2 Hz, 4H), 4.67 (t, *J* = 7.6 Hz, 4H), 3.92 (s, 6H), 2.22 (quin, *J* = 7.6 Hz, 4H), 1.72–1.70 (quin, *J* = 7.6 Hz, 2H); ^{13}C NMR (CD_3OD, 100 MHz): δ 162.8, 133.5, 132.9, 128.9, 128.5, 127.9, 127.1, 116.6, 114.9, 114.7, 56.4, 48.5, 29.7, 24.7; HRMS-ESI (*m*/*z*) $[M–Br]^+$ calcd for $C_{33}H_{34}BrN_4O_2$: 597.1860, found: 597.1865.

1.2.2. Synthesis of 1c–Ag complex[4]

To a 50 mL of round-bottom flask, bis-NHC **1c** (0.420 g, 0.620 mmol) and silver(I) oxide (0.430 g, 1.85 mmol) in distilled water (21 mL) was allowed to stir for 18 h at room temperature with exclusion of light. The suspension was filtered through celite and the filtrate was collected in a conical flask. To the conical flask, KPF_6 (0.340 g, 1.85 mmol) was added with the instant formation of gray precipitate, the resulting suspension was stirred for 1 h and filtered through filter paper. The filtrate was dried under vacuum to afford **1c–**Ag complex in 80% yield as gray solid. Mp = 178–182 ºC (dec.); ^{1}H NMR (DMSO-d_6, 400 MHz): δ 8.05 (d, *J* = 8.0 Hz, 4H), 7.69 (t, *J* = 7.6 Hz, 4H), 7.60–7.51 (m, 8H), 7.02 (d, *J* = 8.0 Hz, 8H), 6.21 (d, *J* = 7.6 Hz, 8H), 4.23 (br, 8H), 3.65 (s, 12H), 1.64 (br. 8H), 0.56 (br, 4H); ^{13}C NMR (DMSO-d_6, 100 MHz): δ 159.8, 134.5, 133.3, 130.1, 126.9, 126.0, 125.6, 114.6, 113.2, 112.8, 56.0, 50.1, 28.7, 23.6.

1.2.3. Synthesis of 1c–Pd complex

To a 100 mL double-necked round-bottom flask (RBF), $Pd(MeCN)_2Cl_2$ (48.6 mg, 0.187 mmol) was charged in and dissolved with acetonitrile (30 mL), the solution of **1c-Ag** (120 mg, 0.0780 mmol) dissolved in acetonitrile (13 mL) was injected into the aforementioned double-necked RBF with syringe and auto-injector within 1 h at room temperature with exclusion of light. After stirring for 24 h at room temperature in dark, the resulting suspension was filtered through celite. The filtrate was dried under vacuum to afford Pd complex (89.1 mg) in 82% yield as yellow solid. Crystals suitable for X-ray diffraction were obtained by method of slow cooling in CH_2Cl_2. ^{1}H NMR (CD_2Cl_2,

400 MHz): δ 7.65 (d, J = 8.0 Hz, 4H), 7.55 (t, J = 8.0 Hz, 4H), 7.43 (t, J = 8.0 Hz, 4H), 7.33 (d, J = 8.0 Hz, 4H), 7.21 (br, 8H), 6.16 (br, 8H), 4.71–4.63 (m, 4H), 4.28–4.22 (m, 4H), 3.70 (s, 12H), 1.80–1.65 (m, 8H), 1.30–1.24 (m, 4H); ^{13}C NMR (CD_2Cl_2, 100 MHz): δ 175.8, 160.2, 135.8, 133.7, 129.8, 128.2, 125.0, 124.8, 114.3, 112.1, 111.8, 37.0, 27.9, 27.6.

1.2.4. Pd-catalyzed the Suzuki–Miyaura coupling reaction

General Procedures for Suzuki−Miyaura Coupling Reaction of Pd catalysts loading ranging from 0.5−1.0 mol%: A stock solution of $Pd(OAc)_2$ (11.3 mg, 0.0500 mmol), bis-NHC **1c** (33.9 mg, 0.0500 mmol) and $K_3PO_4 \cdot H_2O$ (57.5 mg, 0.250 mmol) in freshly distilled *t*-butanol (5.0 mL) was initially prepared with continuous stirring at 60 ºC for 1 h. Arylboronic acid **4** (1.50 mmol), aryl bromide **3** (1.00 mmol), $K_3PO_4 \cdot H_2O$ (3.00 mmol) were charged to the Schlenk tube with treatment of carefully evacuated and backfilled with nitrogen for 3 times. Stock solution of palladium complex (as indicated) was added to the Schlenk tube and then dry *t*-butanol was added up to final volume 3.0 mL. The mixture was stirred at room temperature for 24 h. After completion of the reaction, the reaction was quenched with water (3.0 mL). The aqueous layer was extracted with EtOAc (3.0 mL×3), the combined organic layers were dried over anhydrous $MgSO_4$ and then filtered. The solvent was evaporated under reduced pressure and the corresponding crude product of the Suzuki−Miyaura coupling reaction was purified by chromatography.

General Procedures for Suzuki−Miyaura Coupling Reaction of 0.005 mol% Pd catalysts loading: A stock solution of $Pd(OAc)_2$ (2.23 mg, 0.0100 mmol), bis-NHC **1c** (6.78 mg, 0.0100 mmol) and $K_3PO_4 \cdot H_2O$ (11.5 mg, 0.250 mmol) in freshly distilled *t*-butanol (5.0 mL) was initially prepared with continuous stirring at 60 ºC for 1 h. The stock solution was diluted to 100X working solution. Arylboronic acid **4** (1.50 mmol), aryl bromide **3** (1.00 mmol), $K_3PO_4 \cdot H_2O$ (3.00 mmol) were charged to the Schlenk tube with treatment of carefully evacuated and backfilled with nitrogen for 3 times. Working solution of palladium complex was added to the Schlenk tube and then dry *t*-butanol was added up to final volume 3.0 mL. The mixture was stirred at room temperature for 24 h. After completion of the reaction, the reaction was quenched with water (3.0 mL). The aqueous layer was extracted with EtOAc (3.0 mL×3), the combined organic layers were dried over anhydrous

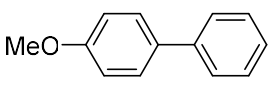
$MgSO_4$ and then filtered. The solvent was evaporated under reduced pressure and the corresponding crude product of the Suzuki−Miyaura coupling reaction was purified by chromatography.

General Procedures for Suzuki−Miyaura Coupling Reaction of 0.0005 mol% Pd catalysts loading: A stock solution of $Pd(OAc)_2$ (2.23 mg, 0.01 mmol), bis-NHC **1c** (6.78 mg, 0.01 mmol) and $K_3PO_4 \cdot H_2O$ (11.5 mg, 0.25 mmol) in freshly distilled *t*-butanol (5.0 mL) was initially prepared with continuous stirring at 60 ºC for 1 h. The stock solution was diluted to 1000X working solution by sequential dilution. Arylboronic acid **4** (1.50 mmol), aryl bromide **3** (1.00 mmol), $K_3PO_4 \cdot H_2O$ (3.00 mmol) were charged to the Schlenk tube with treatment of carefully evacuated and backfilled with nitrogen for 3 times. Working solution of palladium complex was added to the Schlenk tube and then dry *t*-butanol was added up to final volume 3.0 mL. The mixture was stirred at room temperature for 24 h. After completion of the reaction, the reaction was quenched with water (3.0 mL). The aqueous layer was extracted with EtOAc (3.0 mL×3), the combined organic layers were dried over anhydrous $MgSO_4$ and then filtered. The solvent was evaporated under reduced pressure and the corresponding crude product of the Suzuki−Miyaura coupling reaction was purified by chromatography.

General Procedures for Suzuki−Miyaura Coupling Reaction of 0.00005 mol% Pd catalysts loading: A stock solution of $Pd(OAc)_2$ (2.23 mg, 0.01 mmol), bis-NHC **1c** (6.78 mg, 0.01 mmol) and $K_3PO_4 \cdot H_2O$ (11.5 mg, 0.25 mmol) in freshly distilled *t*-butanol (5.0 mL) was initially prepared with continuous stirring at 60 °C for 1 h. The stock solution was diluted to 10000X working solution by sequential dilution. Arylboronic acid **4** (1.50 mmol), aryl bromide **3** (1.00 mmol), $K_3PO_4 \cdot H_2O$ (3.00 mmol) were charged to the Schlenk tube with treatment of carefully evacuated and backfilled with nitrogen for 3 times. Working solution of palladium complex was added to the Schlenk tube and then dry *t*-butanol was added up to final volume 3.0 mL. The mixture was stirred at room temperature for 24 h. After completion of the reaction, the reaction was quenched with water (3.0 mL). The aqueous layer was extracted with EtOAc (3.0 mL×3), the combined organic layers were dried over anhydrous $MgSO_4$ and then filtered. The solvent was evaporated under reduced pressure and the corresponding crude product of the Suzuki−Miyaura coupling reaction was purified by

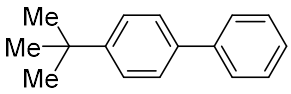
chromatography.

4-methoxybiphenyl (5aa)[5] (table 2, entry 1)



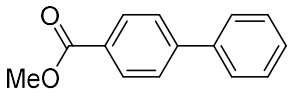
This compound was prepared from 4-bromoanisole **3a** and phenylboronic acid **4a** in 99% yield (0.183 g). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.57−7.52 (m, 4H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.30 (t, *J* = 7.2 Hz, 1H), 6.99 (d, *J* = 8.4 Hz, 2H), 3.86 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 159.1, 140.8, 133.7, 128.7, 128.1, 126.7, 126.6, 114.2, 55.3.

4-*tert*-butylbiphenyl (5ba)[5] (table 2, entry 4)



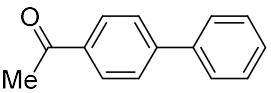
This compound was prepared from 1-bromo-4-*tert*-butylbenzene **3b** and phenylboronic acid **4a** in 99% yield (0.209 g). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.59 (d, *J* = 8.0 Hz, 2H), 7.54 (d, *J* = 8.0 Hz, 2H), 7.47 (d, *J* = 8.0 Hz, 2H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.32 (t, *J* = 7.4 Hz, 1H), 1.36 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 150.1, 141.0, 138.3, 128.7, 127.0, 126.9, 126.8, 125.7, 34.4, 31.3.

methyl biphenyl-4-carboxylate (5ca)[5] (table 2, entry 5)



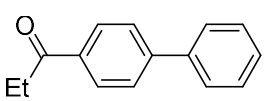
This compound was prepared from methyl 4-bromobenzoate **3c** and phenylboronic acid **4a** in 98% yield (0.208 g). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.11 (d, *J* = 8.4 Hz, 2H), 7.67 (d, *J* = 8.4 Hz, 2H), 7.63 (d, *J* = 8.8 Hz, 2H), 7.47 (t, *J* = 7.4 Hz, 2H), 7.41 (t, *J* = 7.2 Hz, 1H), 3.94 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 166.9, 145.6, 139.9, 130.0, 128.9, 128.8, 128.1, 127.2, 127.0, 52.1.

1-([1,1'-biphenyl]-4-yl)ethanone (5da)[5] (table 2, entry 6)



This compound was prepared from 4-bromoacetophenone **3d** and phenylboronic acid **4a** in 99% yield (0.194 g). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.04 (d, *J* = 8.4 Hz, 2H), 7.67 (d, *J* = 8.4 Hz, 2H), 7.63 (d, *J* = 7.6 Hz, 2H), 7.49 (t, *J* = 7.6 Hz, 2H), 7.41 (t, *J* = 7.6 Hz, 1H), 2.65 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 197.6, 145.6, 139.7, 135.7, 128.87, 128.82, 128.1, 127.2, 127.1, 26.6.

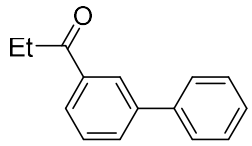
4'-phenylpropiophenone (5ea)[5] (table 2, entry 9)



This compound was prepared from 1-(4-bromophenyl)-1-propanone **3e** and phenylboronic acid **4a** in 99% yield (0.209 g). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.04 (d, *J* = 8.4 Hz, 2H), 7.68 (d, *J* = 8.4 Hz, 2H), 7.63 (d, J = 8.0 Hz, 2H), 7.47 (t, *J* = 8.0 Hz,

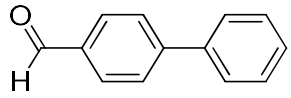
2H), 7.40 (t, J = 8.0 Hz, 1H), 3.04 (q, J = 7.2, 2H), 1.26 (t, J = 7.2, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 200.4, 145.5, 139.9, 135.6, 128.9, 128.5, 128.1, 127.2, 127.2, 31.8, 8.3.

3'-phenylpropiophenone (5fa)[5] (table 2, entry 12)



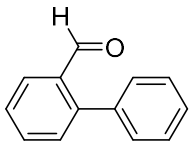
This compound was prepared from 3'-bromopropiophenone **3f** and phenylboronic acid **4a** in 99% yield (0.209 g). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.20 (t, J = 1.8 Hz, 1H), 7.95 (td, J = 7.6, 1.3 Hz, 1H), 7.78 (td, J = 7.6, 1.5 Hz, 1H), 7.64−7.62 (m, 2H), 7.54 (t, J = 7.6 Hz, 1H), 7.50−7.46 (m, 2H), 7.39 (td, J = 7.6, 1.2 Hz, 1H), 3.07 (q, J = 7.2 Hz, 2H), 1.26 (t, J = 7.2 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 200.1, 141.2, 139.8, 137.1, 131.0, 128.7, 128.6, 127.5, 126.8, 126.5, 126.2, 31.5, 7.9.

3'-phenylpropiophenone (5ga)[6] (table 2, entry 13)



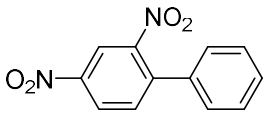
This compound was prepared from 3'-bromopropiophenone **3g** and phenylboronic acid **4a** in 99% yield (0.180 g). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 10.06 (s, 1H), 7.97−7.95 (m, 2H), 7.77−7.74 (m, 2H), 7.66−7.63 (m, 2H), 7.51−7.41 (m, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 192.0, 147.2, 139.7, 135.1, 130.3, 129.0, 128.5, 127.7, 127.4, 127.3.

2-phenylbenzaldehyde (5ha)[5] (table 2, entry 14)



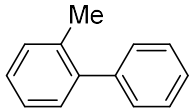
This compound was prepared from 2-bromobenzaldehyde **3h** and phenylboronic acid **4a** in 84% yield (0.153 g). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.99 (d, J = 0.8 Hz, 1H), 8.04 (dd, J = 7.8, 1.3 Hz, 1H), 7.64 (td, J = 7.5, 1.5 Hz, 1H), 7.55−7.43 (m, 5H), 7.41−7.36 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 192.4, 145.9, 137.7, 133.6, 133.5, 130.7, 130.0, 128.4, 128.1, 127.7, 127.5.

2,4-dinitro-1,1'-biphenyl (5ia)[5] (table 2, entry 15)



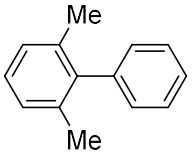
This compound was prepared from 1-bromo-2,4-dinitrobenzene **3i** and phenylboronic acid **4a** in 99% yield (0.242 g). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.72 (d, J = 2.4 Hz, 1H), 8.47 (dd, J = 2.4, 8.4 Hz, 1H), 7.68 (d, J = 8.4 Hz, 1H), 7.50−7.48 (m, 3H), 7.36−7.33 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 148.9, 146.7, 142.1, 135.1, 133.2, 129.4, 129.0, 127.6, 126.4, 119.6.

2-methyl-1,1'-biphenyl (5ja)[5] (table 2, entry 16)



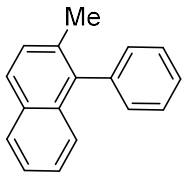
This compound was prepared from 1-bromo-2-methylbenzene **3j** and phenylboronic acid **4a** in 70% yield (0.118 g). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.60 (d, *J* = 7.2 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 1H), 7.41 (d, *J* = 7.2 Hz, 1H), 7.37–7.32 (m, 3H), 7.28–7.23 (m, 3H), 2.28 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 130.3, 129.8, 129.2, 128.7, 128.0, 127.21, 127.15, 126.7, 125.7, 20.4.

2,6-dimethyl-1,1'-biphenyl (5ka)[5] (table 2, entry 17)



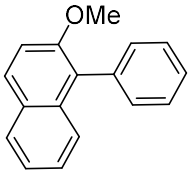
This compound was prepared from 1-bromo-2,6-dimethylbenzene **3k** and phenylboronic acid **4a** in 85% yield (0.155 g). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.47 (d, *J* = 7.2 Hz, 1H), 7.32–7.27 (m, 2H), 7.22–7.18 (m, 1H), 7.06–6.98 (m, 4H), 1.92 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 141.8, 141.2, 141.0, 136.0, 129.0, 128.7, 128.4, 127.24, 127.19, 127.1, 127.0, 126.6, 20.8.

2-methyl-1-phenylnaphthalene (5la)[5] (table 2, entry 18)



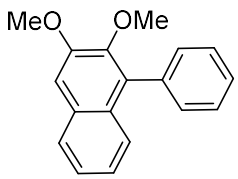
This compound was prepared from 1-bromo-2-methylnaphthalene **3l** and phenylboronic acid **4a** in 99% yield (0.216 g). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.84 (d, *J* = 8.4 Hz, 1H), 7.79 (d, *J* = 8.4 Hz, 1H), 7.60 (d, *J* = 8.0 Hz, 1H), 7.38–7.32 (m, 8H), 2.24 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 139.8, 138.1, 133.1, 132.9, 131.9, 130.1, 128.7, 128.6, 128.4, 127.7, 127.18, 127.14, 127.0, 126.1, 125.8, 124.7, 20.8.

2-methoxy-1-phenylnaphthalene (5ma)[5] (table 2, entry 19)



This compound was prepared from 1-bromo-2-methoxynaphthalene **3m** and phenylboronic acid **4a** in 99% yield (0.232 g). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.88 (d, *J* = 8.8 Hz, 1H), 7.83–7.81 (m, 1H), 7.52–7.48 (m, 3H), 7.44 (d, *J* = 7.6 Hz, 1H), 7.38–7.32 (m, 5H), 3.83 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 153.7, 136.4, 133.6, 130.9, 129.04, 128.98, 128.1, 127.8, 127.0, 126.27, 126.26, 125.2, 123.5, 113.8, 56.7.

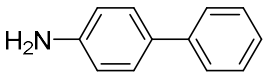
2,3-dimethoxy-1-phenylnaphthalene (5na) (table 2, entry 20)



This compound was prepared from 1-bromo-2,3-dimethoxynaphthalene **3n** and phenylboronic acid **4a** in 99% yield (0.262 g). White solid; Mp = 108–110 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.89 (d, *J* = 8.0 Hz, 1H), 7.66–7.63 (m, 3H), 7.59–7.58 (m, 3H), 7.53 (t, *J* = 8.0 Hz, 1H), 7.40–7.37 (m, 2H), 4.11 (s, 3H), 3.81 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 151.9, 146.2, 135.8, 131.9, 131.1, 130.3, 128.4,

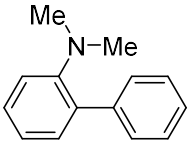
127.9, 127.1, 126.4, 125.5, 125.0, 123.7, 106.6, 60.7, 55.4; HRMS-EI (*m*/*z*) [M^+] calcd for $C_{18}H_{16}O_2$: 264.1150, found: 264.1155.

[1,1'-biphenyl]-4-amine (5oa)[7] (table 2, entry 21)



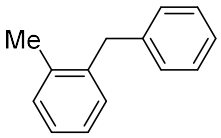
This compound was prepared from 4-bromoaniline **3o** and phenylboronic acid **4a** in 99% yield (0.168 g). Brown solid; ^{1}H NMR ($CDCl_3$, 400 MHz): 7.55–7.52 (m, 2H), 7.43–7.37 (m, 4H), 7.29–7.25 (m, 1H), 6.76 (d, *J* = 8.4 Hz, 2H), 3.74 (s, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 145.7, 140.9, 131.1, 128.5, 127.7, 126.12, 126.05, 115.2.

***N*,*N*-dimethyl-[1,1'-biphenyl]-2-amine (5pa)**[8] (table 2, entry 22)



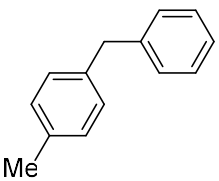
This compound was prepared from 2-bromo-*N*,*N*-dimethylaniline **3p** and phenylboronic acid **4a** in 70% yield (0.138 g). White solid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.58–7.56 (m, 2H), 7.40–7.31 (m, 3H), 7.30–7.21 (m, 2H), 7.04–7.00 (m, 2H), 2.54 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 151.1, 141.9, 134.1, 131.6, 128.6, 128.2, 128.0, 126.4, 121.4, 117.5, 43.3.

1-benzyl-2-methylbenzene (5qa)[9] (table 2, entry 23)



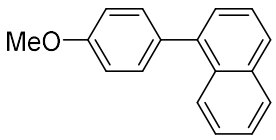
This compound was prepared from 1-(bromomethyl)-2-methylbenzene **3q** and phenylboronic acid **4a** in 89% yield (0.162 g). Coloreless oil; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.27–7.25 (m, 2H), 7.19–7.10 (m, 7H), 3.99 (s, 2H), 2.25 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 140.3, 138.8, 136.5, 130.2, 129.9, 128.7, 128.3, 126.4, 125.9, 125.8, 39.4, 19.6.

1-benzyl-4-methylbenzene (5ra)[9] (table 2, entry 24)



This compound was prepared from 1-(bromomethyl)-4-methylbenzene **3r** and phenylboronic acid **4a** in 77% yield (0.140 g). Colorless oil; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.29–7.09 (m, 9H), 3.94 (s, 2H), 2.31 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 141.4, 138.1, 135.5, 129.1, 128.9, 128.8, 128.4, 126.0, 41.5, 21.0.

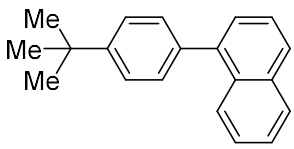
1-(4-methoxyphenyl)naphthalene (5ab)[10] (table 2, entry 25)



This compound was prepared from 4-bromoanisole **3a** and 1-naphthylboronic acid **4b** in 99% yield (0.232 g). White solid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.91 (t, *J* = 8.8 Hz, 2H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.53–7.47 (m, 2H), 7.45–7.40 (m, 4H), 7.04 (d, *J* = 8.8 Hz, 2H), 3.90 (s, 3H); ^{13}C NMR ($CDCl_3$,

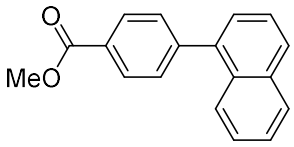
100 MHz): δ 158.8 139.8, 133.8, 133.0, 131.7, 131.0, 128.2, 127.3, 126.8, 126.0, 125.9, 125.6, 125.3, 113.6, 55.2.

1-(4-(*tert*-butyl)phenyl)naphthalene (5bb)[11] (table 2, entry 26)



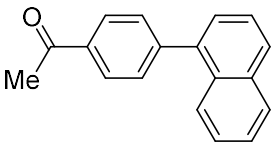
This compound was prepared from 1-bromo-4-*tert*-butylbenzene **3b** and 1-naphthylboronic acid **4b** in 96% yield (0.250 g). White solid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.96 (d, *J* = 8.4 Hz, 1H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.85 (d, *J* = 8.4 Hz, 1H), 7.54–7.41 (m, 8H), 1.41 (s, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 149.9, 140.2, 137.8, 133.8, 131.7, 129.7, 128.2, 127.4, 126.9, 126.2, 125.9, 125.7, 125.4, 125.1, 34.5, 31.5.

methyl 4-(naphthalen-1-yl)benzoate (5cb)[10] (table 2, entry 27)



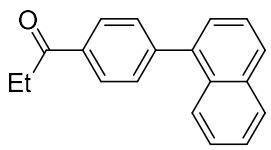
This compound was prepared from methyl 4-bromobenzoate **3c** and 1-naphthylboronic acid **4b** in 97% yield (0.254 g). White solid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.17 (d, *J* = 8.4, Hz, 2H), 7.92 (d, *J* = 8.8 Hz, 1H), 7.90 (d, *J* = 8.8 Hz, 1H), 7.84 (d, *J* = 8.4 Hz, 1H), 7.58 (d, *J* = 8.8 Hz, 2H), 7.56–7.49 (m, 2H), 7.47–7.42 (m, 2H), 3.98 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 166.7, 145.3, 138.8, 133.6, 130.9, 129.9, 129.4, 128.8, 128.2, 128.1, 126.7, 126.1, 125.7, 125.3, 125.1, 51.9.

1-(4-(naphthalen-1-yl)phenyl)ethan-1-one (5db)[12] (table 2, entry 28)



This compound was prepared from 4-bromoacetophenone **3d** and 1-naphthylboronic acid **4b** in 95% yield (0.234 g). Orange solid; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.10 (d, *J* = 8.0 Hz, 2H), 7.93 (d, *J* = 8.8 Hz, 1H), 7.90 (d, *J* = 8.8 Hz, 1H), 7.84 (d, *J* = 8.4 Hz, 1H), 7.61 (d, *J* = 8.0 Hz, 2H), 7.57–7.42 (m, 4H), 2.69 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 197.5, 145.4, 138.6, 135.6, 133.5, 130.1, 130.0, 128.2, 128.1, 126.7, 126.1, 125.7, 125.2, 125.1, 26.4.

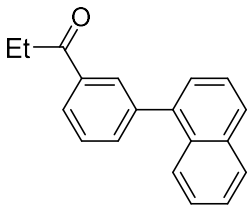
1-(4-(naphthalen-1-yl)phenyl)propan-1-one (5eb) (table 2, entry 29)



This compound was prepared from 1-(4-bromophenyl)-1-propanone **3e** and 1-naphthylboronic acid **4b** in 99% yield (0.258 g). White solid; Mp = 110–112 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.10 (d, *J* = 8.0 Hz, 2H), 7.93 (d, *J* = 8.8 Hz, 1H), 7.90 (d, *J* = 8.8 Hz, 1H), 7.85 (d, *J* = 8.4 Hz, 1H), 7.60 (d, *J* = 8.0 Hz, 2H), 7.56–7.50 (m, 2H), 7.47–7.42 (m, 2H), 3.09 (q, *J* = 7.2 Hz, 2H), 1.29 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 199.9, 145.1, 138.7, 135.3, 133.5, 130.8, 129.9, 128.1, 128.0, 127.7, 126.6, 126.1,

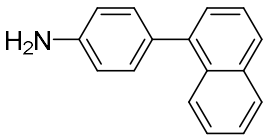
125.7, 125.2, 125.1, 31.5, 8.0; HRMS-EI (*m*/*z*) [M^+] calcd for $C_{19}H_{16}O$: 260.1201, found: 260.1196.

1-(3-(naphthalen-1-yl)phenyl)propan-1-one (5fb) (table 2, entry 30)



This compound was prepared from 1-(3-bromophenyl)-1-propanone **3f** and 1-naphthylboronic acid **4b** in 96% yield (0.250 g). Yellow oil; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.09 (s, 1H), 8.04 (d, *J* = 7.6 Hz, 1H), 7.93 (d, *J* = 8.8 Hz, 1H), 7.90 (d, *J* = 8.8 Hz, 1H), 7.81 (d, *J* = 8.4 Hz, 1H), 7.69 (d, *J* = 7.6 Hz, 1H), 7.42–7.61 (m, 5H), 3.05 (q, *J* = 7.2 Hz, 2H), 1.25 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 200.3, 140.8, 138.9, 136.7, 134.1, 133.5, 131.1, 129.3, 128.3, 128.2, 127.9, 126.8, 126.6, 126.1, 125.7, 125.3, 125.1, 31.6, 8.0; HRMS-EI (m/z) [M^+] calcd for $C_{19}H_{16}O$: 260.1201, found: 260.1205.

4-(naphthalen-1-yl)aniline (5ob)[12] (table 2, entry 31)

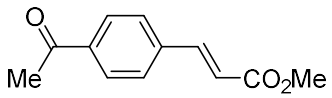


This compound was prepared from 4-bromoaniline **3o** and 1-naphthylboronic acid **4b** in 99% yield (0.217 g). Dark-red oil; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.97 (d, *J* = 8.4 Hz, 1H), 7.88 (d, *J* = 7.6 Hz, 1H), 7.81 (d, *J* = 8.4 Hz, 1H), 7.52–7.39 (m, 4H), 7.30 (d, *J* = 8.4 Hz, 2H), 6.82 (d, *J* = 8.8, 2H), 3.74 (br, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 145.6, 140.3, 133.8, 131.8, 130.9, 130.8, 128.2, 126.9, 126.7, 126.1, 125.7, 125.6, 125.4, 114.8.

1.2.5. Pd-catalyzed the Mizoroki–Heck coupling reaction

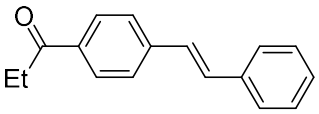
Olefin **6** (1.50 mmol), aryl halide **3** (1.00 mmol), CsF (2.00 mmol), bis-NHC **1c** (1.0 mol%) and $Pd(dba)_2$ (1.0 mol%) were charged to the Schlenk tube. Further dry DMF (5.0 mL) was added. The mixture was stirred at 60 °C for 24 h. After completion of the reaction, monitored by TLC, the reaction was quenched by water (5.0 mL). The aqueous layer was extracted with EtOAc (5.0 mL×3). The combined organic layers were dried over anhydrous $MgSO_4$ and then filtered. The solvent was evaporated under reduced pressure and the corresponding crude product of the Heck−Mizoroki coupling reaction was purified by chromatography.

methyl (*E*)-3-(4-acetylphenyl)acrylate (7da)[13] (table 4, entry 1)



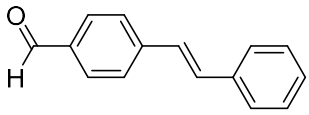
This compound was prepared from 4-bromoacetophenone **3d** and methyl acrylate **6a** in 44% yield (0.0892 g). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.94 (d, *J* = 8.4 Hz, 2H), 7.68 (d, *J* = 16.0 Hz, 1H), 7.58 (d, *J* = 8.4 Hz, 2H), 6.50 (d, *J* = 16.0 Hz, 1H), 3.80 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 197.3, 166.9, 143.2, 138.6, 137.9, 128.8, 128.1, 120.2, 51.8, 26.6.

(*E*)-1-(4-styrrlphenyl)propan-1-one (7eb) (table 4, entry 2)



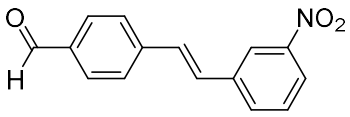
This compound was prepared from 1-(4-bromophenyl)propan-1-one **3e** and styrene **6b** in 93% yield (0.220 g). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.97 (d, *J* = 8.4 Hz, 2H), 7.59 (d, *J* = 8.4 Hz, 2H), 7.54 (d, *J* = 7.2 Hz, 2H), 7.40−7.28 (m, 3H), 7.23 (d, *J* = 16.4 Hz, 1H), 7.13 (d, *J* = 16.4 Hz, 1H), 3.01 (q, *J* = 7.2 Hz, 2H), 1.24 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 199.9, 141.5, 136.5, 135.5, 131.0, 128.6, 128.3, 128.1, 127.3, 126.6, 126.3, 31.5, 8.1.

(*E*)-4-styrylbenzaldehyde (7gb)[14] (table 4, entry 3)



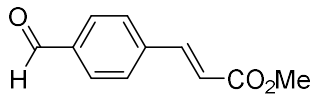
This compound was prepared from methyl 4-bromobenzaldehyde **3g** and styrene **6b** in 98% yield (0.154 g). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 10.00 (s, 1H), 7.88 (d, *J* = 7.6 Hz, 2H), 7.66 (d, *J* = 7.6 Hz, 2H), 7.55 (d, *J* = 8.0 Hz, 2H), 7.38 (d, *J* = 7.6 Hz, 2H), 7.32 (d, *J* = 7.6 Hz, 1H), 7.27 (d, *J* = 16.4 Hz, 1H), 7.15 (d, *J* = 16.4 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 191.5, 143.2, 136.4, 135.1, 132.0, 130.1, 128.7, 128.4, 127.1, 126.8, 126.7.

(*E*)-4-(3-nitrostyryl)benzaldehyde (7gc) (table 4, entry 4)



This compound was prepared from 4-bromobenzaldehyde **3g** and 3-nitrostyrene **6c** in 96% yield (0.243 g). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 10.03 (s, 1H), 8.42 (t, *J* = 2.0 Hz, 1H), 8.17−8.15 (m, 1H), 7.92 (d, *J* = 8.0 Hz, 2H), 7.90−7.83 (m, 1H), 7.70 (d, *J* = 8.0 Hz, 2H), 7.57 (t, *J* = 8.0 Hz, 1H), 7.29 (s, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 191.5, 148.7, 142.1, 138.3, 135.9, 132.6, 130.3, 130.2, 129.7, 129.3, 127.2, 122.7, 121.2.

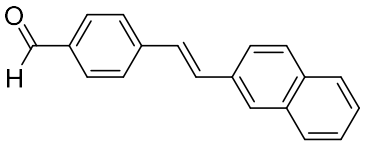
methyl (*E*)-3-(4-formylphenyl)acrylate (7ga)[15] (table 4, entry 5)



This compound was prepared from 4-bromobenzaldehyde **3g** and methyl acrylate **6a** in 98% yield (0.186 g). ^{1}H NMR ($CDCl_3$, 400 MHz):

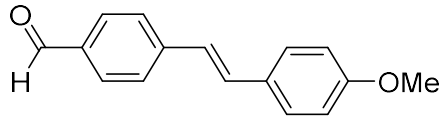
δ 9.95 (s, 1H), 7.82 (d, *J* = 8.0 Hz, 2H), 7.65−7.58 (m, 3H), 6.47 (d, *J* = 16.0 Hz, 1H), 3.75 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 191.3, 166.5, 142.9, 139.7, 136.9, 129.9, 128.3, 120.7, 51.7.

(*E*)-4-(2-(naphthalen-2-yl)vinyl)benzaldehyde (7gd)[16] (table 4, entry 6)



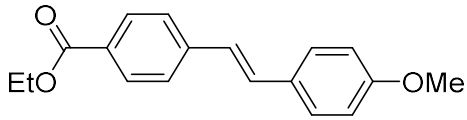
This compound was prepared from 4-bromobenzaldehyde **3g** and 2-vinylnaphthalene **6d** in 61% yield (0.156 g). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 10.01 (s, 1H), 7.91−7.82 (m, 6H), 7.77−7.70 (m, 3H), 7.55 (d, *J* = 8.0 Hz, 2H), 7.44 (d, *J* = 16.4 Hz, 1H), 7.27 (d, *J* = 16.4 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 191.6, 143.4, 135.3, 134.0, 133.6, 133.4, 132.2, 130.2, 129.0, 128.1, 127.7, 127.6, 127.5, 126.9, 126.5, 126.4, 123.3.

(*E*)-4-(4-methoxystyryl)benzaldehyde (7ge)[17] (table 4, entry 7)



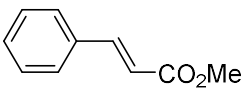
This compound was prepared from 4-bromobenzaldehyde **3g** and 1-methoxy-4-vinylbenzene **6e** in 67% yield (0.161 g). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.98 (s, 1H), 7.86 (d, *J* = 8.4 Hz, 2H), 7.63 (d, *J* = 8.4 Hz, 2H), 7.50 (d, *J* = 8.8 Hz, 2H), 7.23 (d, *J* = 16.4 Hz, 1H), 7.01 (d, *J* = 16.4 Hz, 1H), 6.93 (d, *J* = 8.8 Hz, 2H), 3.85 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 191.6, 159.9, 143.8, 134.9, 131.7, 130.2, 129.3, 128.2, 126.5, 125.1, 114.2, 55.3.

ethyl (*E*)-4-(4-methoxystyryl)benzoate (7se)[18] (table 4, entry 8)



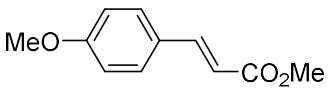
This compound was prepared from ethyl 4-bromobenzoate **3s** and 1-methoxy-4-vinylbenzene **6e** in 66% yield (0.185 g). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.01 (d, *J* = 8.0 Hz, 2H), 7.54 (d, *J* = 7.2 Hz, 2H), 7.48 (d, *J* = 7.6 Hz, 2H), 7.17 (d, *J* = 16.0 Hz, 1H), 6.99 (d, *J* = 16.0 Hz, 1H), 6.91 (d, *J* = 7.6 Hz, 2H), 4.38 (q, *J* = 8.4 Hz, 2H), 3.84 (s, 3H), 1.40 (t, *J* = 8.4 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 166.4, 159.7, 142.0, 130.6, 129.9, 129.5, 128.7, 128.0, 125.9, 125.4, 114.2, 60.8, 55.3, 14.3.

methyl cinnamate (7ta)[13] (table 4, entry 9)



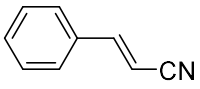
This compound was prepared from iodobenzene **3t′** and methyl acrylate **6a** in 96% yield (0.155 g). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.71 (d, *J* = 16.0 Hz, 1H), 7.50−7.48 (m, 2H), 7.36−7.33 (m, 3H), 6.46 (d, *J* = 16.0 Hz, 1H), 3.79 s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 166.9, 144.4, 134.0, 129.9, 128.5, 127.7, 117.4, 51.2.

methyl (*E*)-3-(4-methoxyohenyl)acrylate (7aa)[19] (table 4, entry 10)



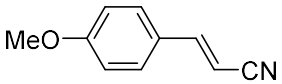
This compound was prepared from 4-iodoanisole **3a′** and methyl acrylate **6a** in 98% yield (0.189 g). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.61 (d, *J* = 16.0 Hz, 1H), 7.41 (s, br, 2H), 6.84 (s, br, 2H), 6.27 (d, *J* = 16.0 Hz, 1H), 3.75 (s, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 167.2, 161.0, 144.0, 129.3, 126.6, 114.8, 113.9, 54.8, 51.0.

cinnamonitrile (7tf)[20] (table 4, entry 11)



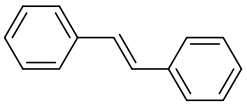
This compound was prepared from iodobenzene **3t′** and acrylonitrile **6f** in 78% yield (0.101 g). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.44–7.40 (m, 5H), 7.37 (d, *J* = 16.4 Hz, 1H), 5.86 (d, *J* = 16.4 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 150.4, 133.3, 131.0, 128.9, 127.2, 118.0, 96.1.

(*E*)-3-(4-methoxyphenyl)acrylonitrile (7af)[19] (table 4, entry 12)



This compound was prepared from 4-iodoanisole **3a′** and acrylonitrile **6f** in 71% yield (0.112 g). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.36 (d, *J* = 7.6 Hz, 2H), 7.28 (d, *J* = 164 Hz, 1H), 6.90 (d, *J* = 7.6 Hz, 2H), 5.68 (d, *J* = 164 Hz, 1H), 3.83 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 161.7, 149.7, 128.8, 126.0, 118.5, 114.2, 92.9, 55.2.

(*E*)-stilbene (7tb)[13] (table 4, entry 13)

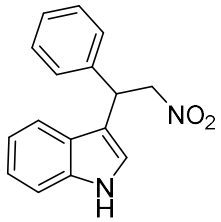


This compound was prepared from iodobenzene **3t′** and styrene **6b** in 72% yield (0.130 g). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.46–7.44 (m, 4H), 7.31–7.29 (m, 4H), 7.22–7.19 (m, 2H), 7.05–7.04 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 137.2, 128.6, 127.5, 126.4.

1.2.6. Pd-catalyzed the Friedel–Crafts alkylation reaction

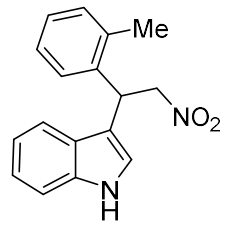
Indole **9** (1.50 mmol), nitroalkene **8** (0.500 mmol), **1c**–Ag (0.50 mol%), and $Pd(OAc)_2$ (1.0 mol%) were charged to the Schlenk tube. Isopropanol (HPLC grade, 3.0 mL) was added. The mixture was stirred at 30 °C for 24 h. After completion of the reaction, monitored by TLC, the reaction was quenched by water (3.0 mL). The aqueous layer was extracted with EtOAc (3.0 mL×3). The combined organic layers were dried over anhydrous $MgSO_4$ and then filtered. The solvent was evaporated under reduced pressure and the corresponding crude product of the Friedel−Crafts alkylation reaction was purified by chromatography.

3-(2-nitro-1-phenylethyl)-1*H*-indole (10aa)[21] (table 6, entry 1)



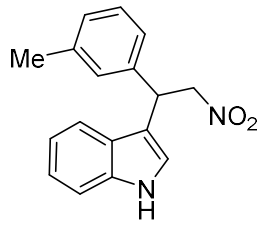
This compound was prepared from nitrostyrene **8a** and indole **9a** in 96% yield (0.128 g). Brown solid; Mp = 108–110 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.05 (s, 1H), 7.43 (d, *J* = 8.0 Hz, 1H), 7.34–7.23 (m, 6H), 7.19 (t, *J* = 8.0 Hz, 1H), 7.07 (t, *J* = 8.0 Hz, 1H), 6.99 (s, 1H), 5.17 (t, *J* = 8.0 Hz, 1H), 5.05 (dd, *J* = 12.4, 8.0 Hz, 1H), 4.92 (dd, *J* = 12.4, 8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 139.1, 136.4, 128.9, 127.7, 127.5, 126.0, 122.6, 121.6, 119.8, 118.8, 114.2, 111.4, 79.4, 41.5.

3-(1-(2-methylyphenyl)-2-nitroethyl)-1*H*-indole (10ba)[22] (table 6, entry 2)



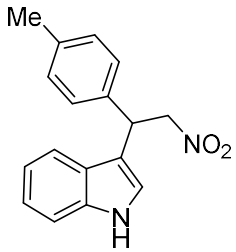
This compound was prepared from (*E*)-1-methyl-2-(2-nitrovinyl)benzene **8b** and indole **9a** in 86% yield (0.121 g). Green oil; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.01 (s, 1H), 7.46 (d, *J* = 8.0 Hz, 1H), 7.30 (d, *J* = 8.0 Hz, 1H), 7.24–7.14 (m, 5H), 7.08 (t, *J* = 8.0 Hz, 1H), 6.83 (s, 1H), 5.41 (t, *J* = 8.0 Hz, 1H), 4.99 (dd, *J* = 12.8, 8.0 Hz, 1H), 4.87 (dd, *J* = 12.8, 8.0 Hz, 1H), 2.41 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 137.1, 136.3, 136.1, 131.0, 127.2, 126.3, 126.1, 125.9, 122.5, 122.4, 119.7, 118.4, 113.7, 111.4, 78.4, 37.1, 19.3.

3-(1-(3-methylyphenyl)-2-nitroethyl)-1*H*-indole (10ca)[23] (table 6, entry 3)



This compound was prepared from (*E*)-1-methyl-3-(2-nitrovinyl)benzene **8c** and indole **9a** in 70% yield (0.0988 g). Brown oil; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.10 (s, 1H), 7.47 (d, *J* = 8.0 Hz, 1H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.23–7.03 (m, 7H), 5.15 (t, *J* = 8.0 Hz, 1H), 5.05 (dd, *J* = 12.4, 8.0 Hz, 1H), 4.93 (dd, *J* = 12.4, 8.0 Hz, 1H), 2.31 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 139.0, 138.4, 136.2, 128.6, 128.4, 128.2, 125.9, 124.5, 122.3, 121.5, 119.6, 118.7, 113.9, 111.3, 79.4, 41.3, 21.2.

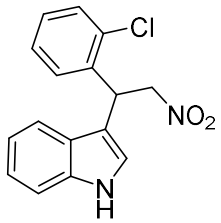
3-(1-(4-methylyphenyl)-2-nitroethyl)-1*H*-indole (10da)[24] (table 6, entry 4)



This compound was prepared from (*E*)-1-methyl-4-(2-nitrovinyl)benzene **8d** and indole **9a** in 81% yield (0.113 g). Brown oil; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.04 (s, 1H), 7.43 (d, *J* = 8.0 Hz, 1H), 7.31 (d, *J* = 8.0 Hz, 1H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.16 (t, *J* = 8.0 Hz, 1H), 7.10 (d, *J* = 8.0 Hz, 2H), 7.06 (t, *J* = 8.0 Hz, 1H), 6.96 (s, 1H), 5.13 (t, *J* = 8.0 Hz, 1H), 5.02 (dd, *J* = 12.4, 8.0 Hz, 1H),

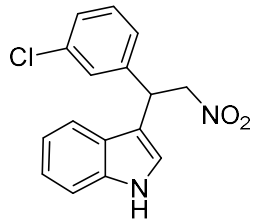
4.89 (dd, *J* = 12.4, 8.0 Hz, 1H), 2.29 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 137.1, 136.3, 136.0, 129.5, 127.5, 125.9, 122.4, 121.5, 119.7, 118.8, 114.2, 111.3, 79.5, 41.1, 20.9.

3-(1-(2-chlorophenyl)-2-nitroethyl)-1*H*-indole (10ea)[24] (table 6, entry 5)



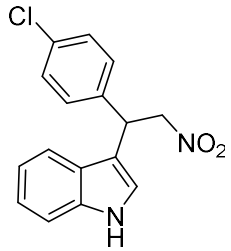
This compound was prepared from (*E*)-1-chloro-2-(2-nitrovinyl)benzene **8e** and indole **9a** in 80% yield (0.120 g). White solid; Mp = 108–110 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.12 (s, 1H), 7.44 (d, *J* = 8.0 Hz, 2H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.22–7.11 (m, 5H), 7.08 (t, *J* = 8.0 Hz, 1H), 5.74 (t, *J* = 8.0 Hz, 1H), 5.01 (dd, *J* = 12.4, 8.0 Hz, 1H), 4.97 (dd, *J* = 12.4, 8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 136.4, 133.8, 130.1, 128.9, 128.8, 127.3, 126.1, 122.7, 121.9, 120.0, 118.9, 113.1, 111.4, 77.6, 37.9.

3-(1-(3-chloroyphenyl)-2-nitroethyl)-1*H*-indole (10fa)[24] (table 6, entry 6)



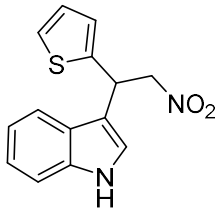
This compound was prepared from (*E*)-1-chloro-3-(2-nitrovinyl)benzene **8f** and indole **9a** in 71% yield (0.107 g). Yellow oil; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.14 (s, 1H), 7.42 (d, *J* = 8.0 Hz, 1H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.30 (s, 1H), 7.25–7.19 (m, 4H), 7.09 (t, *J* = 7.6 Hz, 1H), 7.02 (s, 1H), 5.16 (t, *J* = 8.0 Hz, 1H), 5.04 (dd, *J* = 12.4, 8.0 Hz, 1H), 4.93 (dd, *J* = 12.4, 8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 141.3, 136.4, 134.6, 130.1, 127.9, 127.8, 126.0, 125.8, 122.7, 121.6, 119.9, 118.6, 113.3, 111.5, 79.1, 41.1.

3-(1-(4-chlorophenyl)-2-nitroethyl)-1*H*-indole (10ga)[21] (table 6, entry 7)



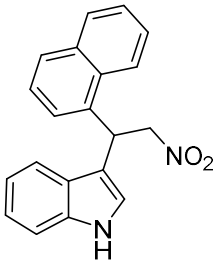
This compound was prepared from (*E*)-1-chloro-4-(2-nitrovinyl)benzene **8g** and indole **9a** in 70% yield (0.105 g). Yellow oil; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.12 (s, 1H), 7.40 (d, *J* = 8.0 Hz, 1H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.30–7.25 (m, 4H), 7.21 (t, *J* = 8.0 Hz, 1H), 7.08 (t, *J* = 8.0 Hz, 1H), 7.01 (s, 1H), 5.16 (t, *J* = 8.0 Hz, 1H), 5.05 (dd, *J* = 12.4, 8.0 Hz, 1H), 4.90 (dd, *J* = 12.4, 8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 137.6, 136.4, 133.3, 129.1, 129.0, 125.8, 122.7, 121.5, 119.9, 118.7, 113.6, 111.4, 79.2, 40.8.

3-(2-nitro-1-(thiophen-2-yl)ethyl)-1*H*-indole (10ha)[25] (table 6, entry 8)



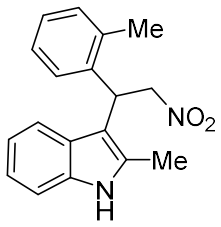
This compound was prepared from (*E*)-2-(2-nitroethyl)thiophene **8h** and indole **9a** in 87% yield (0.118 g). Brown solid; Mp = 108–110 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.09 (s, 1H), 7.51 (d, *J* = 8.0 Hz, 1H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.24–7.18 (m, 2H), 7.11 (t, *J* = 8.0 Hz, 1H), 7.09 (s, 1H), 6.98–6.92 (m, 2H), 5.45 (t, *J* = 8.0 Hz, 1H), 5.02 (dd, *J* = 12.4, 8.0 Hz, 1H), 4.98 (dd, *J* = 12.4, 8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 142.9, 136.3, 126.9, 125.6, 125.1, 124.8, 122.6, 122.0, 119.9, 118.7, 113.7, 111.5, 79.9, 36.8.

3-(1-(naphthalen-1-yl)-2-nitroethyl)-1*H*-indole (10ia)[24] (table 6, entry 9)



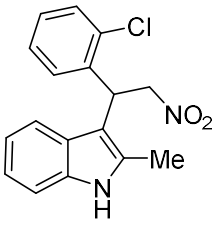
This compound was prepared from (*E*)-1-(2-nitrovinyl)naphthalene **8i** and indole **9a** in 90% yield (0.142 g). White solid; Mp = 108–110 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.28 (d, *J* = 8.0 Hz, 1H), 8.08 (s, 1H), 7.89 (d, *J* = 7.6 Hz, 1H), 7.79 (t, *J* = 4.8 Hz, 1H), 7.56–7.52 (m, 2H), 7.44 (d, *J* = 8.0 Hz, 1H), 7.39–7.35 (m, 3H), 7.38 (t, *J* = 7.2 Hz, 1H), 7.06 (t, *J* = 8.0 Hz, 1H), 7.02 (d, *J* = 2.0 Hz, 1H), 6.08 (t, *J* = 8.0 Hz, 1H), 5.12–5.09 (m, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 136.4, 134.5, 134.0, 131.0, 129.1, 128.2, 126.8, 125.9, 125.8, 125.3, 124.3, 122.6, 122.5, 119.8, 118.6, 113.9, 111.4, 78.4, 36.8.

3-[1-(2-methylphenyl)-2-nitroethyl]-2-methyl-1*H*-indole (10bb) (table 6, entry 10)



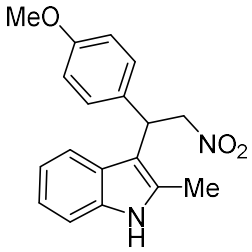
This compound was prepared from (*E*)-1-methyl-2-(2-nitrovinyl)benzene **8b** and 2-methylindole **9b** in 95% yield (0.140 g). Yellow solid; Mp = 110–112 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.83 (s, 1H), 7.45 (d, *J* = 7.6 Hz, 1H), 7.43 (d, *J* = 8.0 Hz, 1H), 7.26–7.13 (m, 4H), 7.09 (t, *J* = 8.0 Hz, 1H), 7.01 (t, *J* = 8.0 Hz, 1H), 5.25 (t, *J* = 8.0 Hz, 1H), 5.16–5.07 (m, 2H), 2.30 (s, 3H), 2.25 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 137.1, 136.7, 135.1, 132.8, 131.1, 127.1, 126.9, 125.9, 125.6, 121.0, 119.5, 118.1, 110.5, 107.2, 77.9, 37.7, 19.4, 11.8; HRMS-EI (m/z) $[M]^+$ calcd for $C_{18}H_{18}N_2O_2$: 294.1368, found: 294.1366; Anal. Calcd for $C_{18}H_{18}N_2O_2$: C, 73.45; H, 6.16; N, 9.52, found: C, 72.17; H, 6.18; N, 9.22.

3-[1-(2-chlorophenyl)-2-nitroethyl]-2-methyl-1*H*-indole (10eb)[26] (table 6, entry 11)



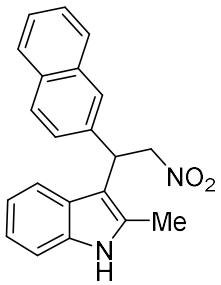
This compound was prepared from (*E*)-1-chloro-2-(2-nitrovinyl)benzene **8c** and 2-methylindole **9b** in 94% yield (0.148 g). Yellow solid; Mp = 110–112 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.89 (s, 1H), 7.53 (d, *J* = 7.6 Hz, 1H), 7.49 (d, *J* = 8.0 Hz, 1H), 7.38 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.27–7.19 (m, 3H), 7.11 (t, *J* = 8.0 Hz, 1H), 7.05 (t, *J* = 7.6 Hz, 1H), 5.50 (t, *J* = 8.0 Hz, 1H), 5.15–5.13 (m, 2H), 2.42 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 136.4, 135.2, 133.8, 133.6, 130.2, 128.5, 128.4, 127.0, 126.9, 121.1, 119.6, 118.3, 110.8, 106.6, 77.1, 38.3, 12.0.

3-(1-(4-methoxyphenyl)-2-nitroethyl)-2-methyl-1*H*-indole (10jb)[27] (table 6, entry 12)



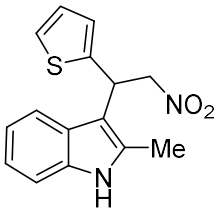
This compound was prepared from (*E*)-1-methoxy-4-(2-nitrovinyl)benzene **8j** and 2-methylindole **9b** in 89% yield (0.138 g). Yellow solid; Mp = 110–112 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.85 (s, 1H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.24–7.21 (m, 3H), 7.10 (t, *J* = 8.0 Hz, 1H), 7.02 (t, *J* = 8.0 Hz, 1H), 6.81 (d, *J* = 8.8 Hz, 2H), 5.20–5.04 (m, 3H), 3.75 (s, 3H), 2.38 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 158.4, 135.3, 132.7 131.4, 128.3, 126.7, 121.1, 119.6, 118.5, 114.0, 110.7, 108.8, 78.8, 55.1, 39.7, 11.8.

3-(2-naphthalen-1-yl-2-nitroethyl)-2-methyl-1*H*-indole (10kb) (table 6, entry 13)



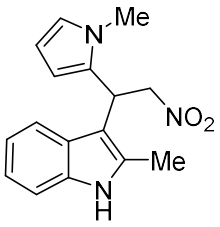
This compound was prepared from (*E*)-2-(2-nitrovinyl)naphthalene **8k** and 2-methylindole **9b** in 98% yield (0.161 g). White solid; Mp = 143–146 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.89 (s, 1H), 7.79–7.73 (m, 4H), 7.48–7.44 (m, 2H), 7.38 (d, *J* = 8.0 Hz, 2H), 7.27 (d, *J* = 8.0 Hz, 1H), 7.10 (t, *J* = 7.6 Hz, 1H), 7.00 (t, *J* = 7.6 Hz, 1H), 5.40–5.22 (m, 2H), 5.20–5.17 (m, 1H), 2.42 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 136.9, 135.3, 133.2, 133.0, 132.3, 128.6, 127.8, 127.5, 126.8, 126.3, 126.1, 126.0, 124.9, 121.3, 119.7, 118.4, 110.7, 108.6, 78.4, 40.4, 11.9; HRMS-EI (m/z) $[M]^+$ calcd for $C_{21}H_{18}N_2O_2$: 330.1368, found: 330.1369; Anal. Calcd for $C_{21}H_{18}N_2O_2$: C, 76.34; H, 5.49; N, 8.48, found: C, 75.86; H, 5.55; N, 8.51.

2-methyl-3-(2-nitro-1-(thiophen-2-yl)ethyl)-1*H*-indole (10hb)[27] (table 6, entry 14)



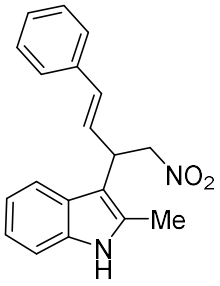
This compound was prepared from (*E*)-2-(2-nitroethyl)thiophene **8h** and 2-methylindole **9b** in 92% yield (0.132 g). Yellow oil; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.88 (s, 1H), 7.35 (d, *J* = 8.0 Hz, 1H), 7.26 (d, *J* = 8.0 Hz, 1H), 7.17 (d, *J* = 4.8 Hz, 1H), 7.11 (t, *J* = 7.6 Hz, 1H), 7.03 (t, *J* = 7.6 Hz, 1H), 6.93–6.90 (m, 2H), 5.35 (dd, *J* = 8.8, 6.8 Hz, 1H), 5.19 (dd, *J* = 12.4, 6.8 Hz, 1H), 5.08 (dd, *J* = 12.4, 8.8 Hz, 1H), 2.38 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 143.2, 135.2, 133.1, 126.7, 126.2, 124.7, 124.3, 121.2, 119.5, 118.5, 110.7, 108.2, 78.8, 36.4, 11.6.

2-methyl-3-(1-(1-methyl-1H-pyrrol-2-yl)-2-nitroethyl)-1*H*-indole (10lb) (table 6, entry 15)



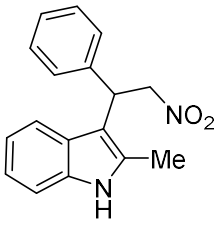
This compound was prepared from (*E*)-1-methyl-2-(2-nitroethyl)tpyrrole **8n** and 2-methylindole **9b** in 91% yield (0.129 g). Yellow solid; Mp = 113–116 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.82 (s, 1H), 7.37 (d, *J* = 8.0 Hz, 1H), 7.24 (d, *J* = 7.2 Hz, 1H), 7.10 (t, *J* = 7.2 Hz, 1H), 7.01 (t, *J* = 7.2 Hz, 1H), 6.54 (s, 1H), 6.18 (s, 1H), 6.10 (t, *J* = 3.2 Hz, 1H), 5.14–5.08 (m, 2H), 4.93 (dd, *J* = 14.4, 10.8 Hz, 1H), 3.28 (s, 3H), 2.29 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 135.1, 132.6, 129.4, 126.7, 122.6, 121.3, 119.6, 117.9, 110.4, 106.7, 106.4, 105.6, 77.6, 33.6, 33.4, 11.3; HRMS-EI (m/z) $[M]^+$ calcd for $C_{16}H_{17}N_3O_2$: 283.1321, found: 283.1328; Anal. Calcd for $C_{16}H_{17}N_3O_2$: C, 67.83; H, 6.05; N, 14.83, found: C, 67.08; H, 6.03; N, 14.33.

3-(1-nitro-4-phenylbut-3-en-2-yl)-2-methyl-1*H*-indole (10mb) (table 6, entry 16)



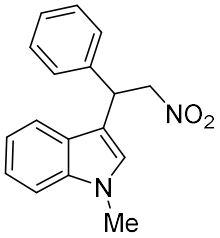
This compound was prepared from (2*E*,4*E*)-1-nitro-4-phenylbutadiene **8m** and 2-methylindole **9b** in 93% yield (0.142 g). Yellow solid; Mp = 115–117 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.87 (s, 1H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.32–7.18 (m, 5H), 7.15–7.06 (m, 2H), 6.51 (d, *J* = 2.8 Hz, 1H), 4.94 (dd, *J* = 12.0, 8.0 Hz, 1H), 4.81 (dd, *J* = 12.0, 8.0 Hz, 1H), 4.65 (t, *J* = 8.0 Hz, 1H), 2.44 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 136.4, 135.3, 132.6, 131.9, 128.5, 127.6, 126.5, 126.4, 126.3, 121.2, 119.6, 118.3, 110.8, 107.3, 78.6, 38.9, 11.7; HRMS-EI (m/z) $[M]^+$ calcd for $C_{19}H_{18}N_2O_2$: 306.1368, found: 306.1367; Anal. Calcd for $C_{19}H_{18}N_2O_2$: C, 74.49; H, 5.92; N, 9.14, found: C, 74.34; H, 5.92; N, 9.06.

2-methyl-3-(2-nitro-1-phenylethyl)-1*H*-indole (10ab)[27] (table 6, entry 17)



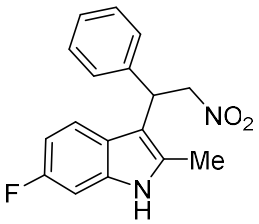
This compound was prepared from nitrostyrene **8a** and 2-methylindole **9b** in 84% yield (0.118 g). Yellow oil; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.86 (s, 1H), 7.36 (d, *J* = 8.0 Hz, 1H), 7.32–7.22 (m, 6H), 7.10 (t, *J* = 8.0 Hz, 1H), 7.02 (t, *J* = 8.0 Hz, 1H), 5.23–5.10 (m, 3H), 2.38 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 139.4, 135.3, 132.9, 128.7, 127.2, 127.0, 126.7, 121.1, 119.5, 118.4, 110.7, 108.5, 78.5, 40.3, 11.7.

***N*-methyl-3-(2-nitro-1-phenylethyl)-1*H*-indole (10ac)**[21] (table 6, entry 18)



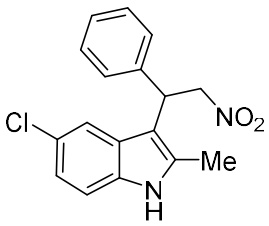
This compound was prepared from nitrostyrene **8a** and 1-methylindole **9c** at 80 °C for 24 h in 56% yield (0.0790 g). Brown oil; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.45 (d, *J* = 8.0 Hz, 1H), 7.36–7.26 (m, 6H), 7.23 (t, *J* = 8.0 Hz, 1H), 7.07 (t, *J* = 8.0 Hz, 1H), 6.87 (s, 1H), 5.17 (t, *J* = 8.0 Hz, 1H), 5.06 (dd, *J* = 12.4, 8.0 Hz, 1H), 4.94 (dd, *J* = 12.4, 8.0 Hz, 1H), 3.75 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 139.3, 137.1, 128.8, 127.6, 127.4, 126.4, 126.3, 122.1, 119.3, 118.9, 112.6, 109.4, 79.4, 41.4, 32.7.

6-fluoro-3-(2-nitro-1-phenylethyl)-1*H*-indole (10ad)[22] (table 6, entry 19)



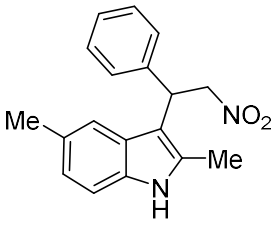
This compound was prepared from nitrostyrene **8a** and 6-fluoro-2-methylindole **9d** in 61% yield (0.0860 g). Brown oil; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.02 (s, 1H), 7.35–7.25 (m, 6H), 7.05–7.02 (m, 2H), 6.83 (t, *J* = 9.2 Hz, 1H), 5.15 (t, *J* = 8.0 Hz, 1H), 5.04 (dd, *J* = 12.4, 8.0 Hz, 1H), 4.92 (dd, *J* = 12.4, 8.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 138.9, 128.9, 127.6, 122.6, 121.7,121.6, 119.7, 119.6, 114.3, 108.8, 108.5, 97.8, 97.5, 79.5, 41.1.

5-chloro-2-methyl-3-(2-nitro-1-phenylethyl)-1*H*-indole (10ae)[28] (table 6, entry 20)



This compound was prepared from nitrostyrene **8a** and 5-chloro-2-methylindole **9e** in 90% yield (0.141 g). White solid; Mp = 115–117 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.91 (s, 1H), 7.34–7.25 (m, 6H), 7.17 (d, *J* = 7.2 Hz, 1H), 7.05 (d, *J* = 7.2 Hz, 1H), 5.22–5.08 (m, 3H), 2.39 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 138.8, 134.6, 133.6, 128.8, 127.7, 127.2, 127.1, 125.2, 121.4, 117.8, 111.6, 108.3, 78.3, 40.1, 11.8.

2,5-dimethyl-3-(2-nitro-1-phenylethyl)-1*H*-indole (10af) (table 6, entry 21)



This compound was prepared from nitrostyrene **8a** and 2,5-dimethylindole **9f** in 92% yield (0.135 g). Yellow solid; Mp = 112–114 ºC; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.26 (s, 1H), 7.33–7.27 (m, 4H), 7.25–7.22 (m, 1H), 7.16–7.14 (m, 2H), 6.93 (d, *J* = 7.6 Hz, 1H), 5.25–5.07 (m, 3H), 2.38 (s, 3H), 2.36 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 139.5, 133.5, 132.9, 128.7, 128.6, 127.2, 126.9, 126.8, 122.6, 118.1, 110.3, 107.9, 78.5, 40.3, 21.5, 11.7; HRMS-EI (m/z) $[M]^+$ calcd for $C_{18}H_{18}N_2O_2$: 294.1368, found: 294.1358.; Anal. Calcd for $C_{18}H_{18}N_2O_2$: C, 73.45; H, 6.16; N, 9.52, found: C, 73.25; H, 6.21; N, 9.34.

2. References and notes:

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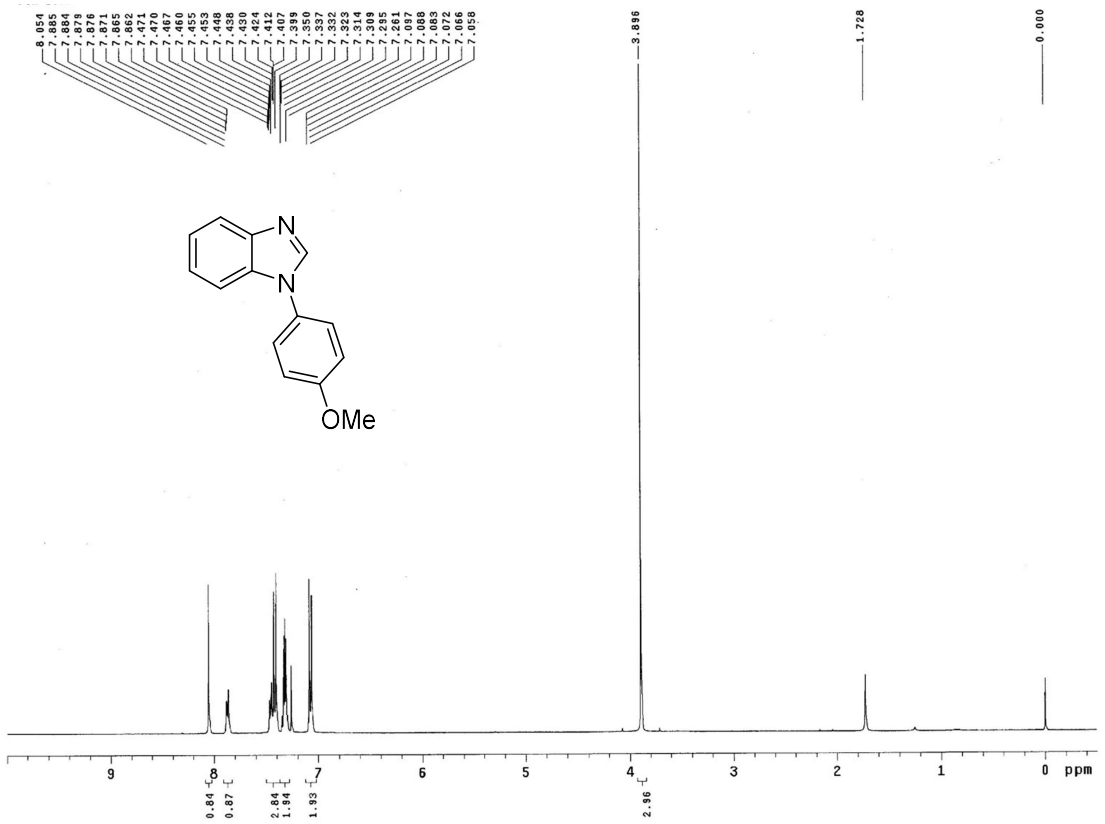
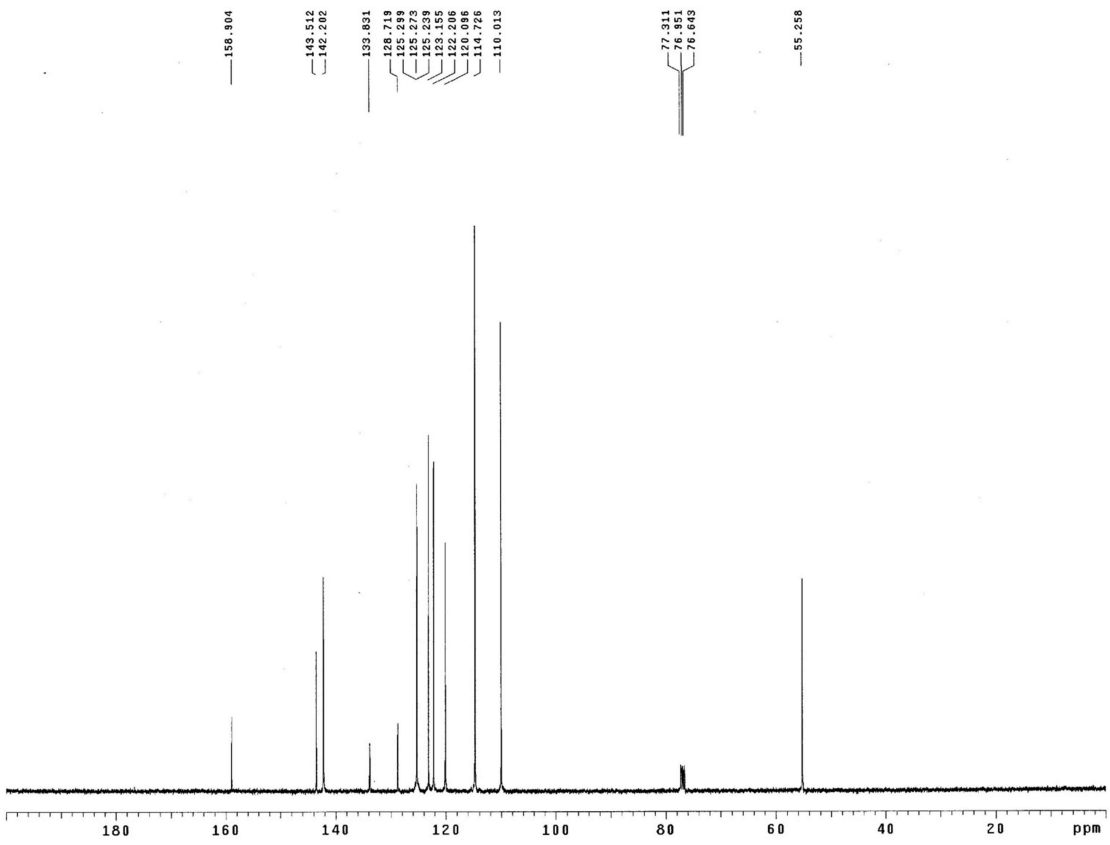
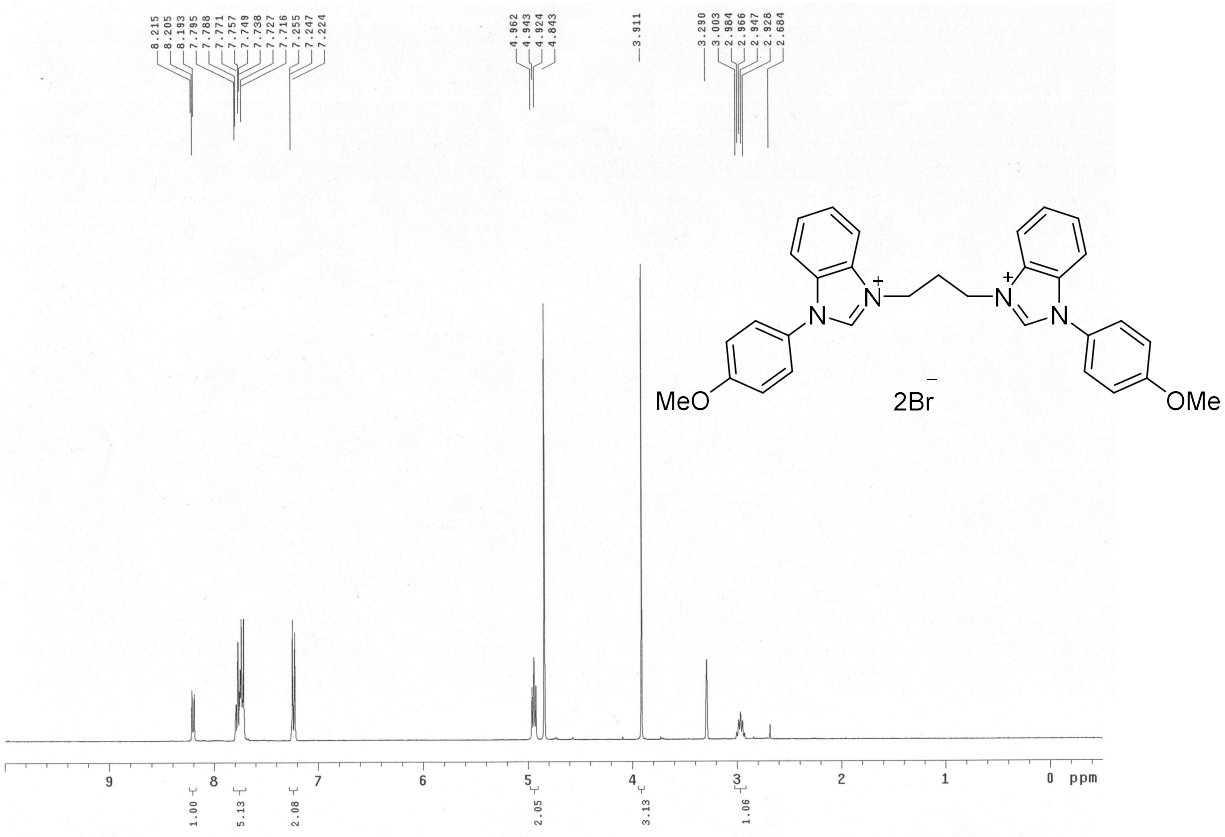
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **2**



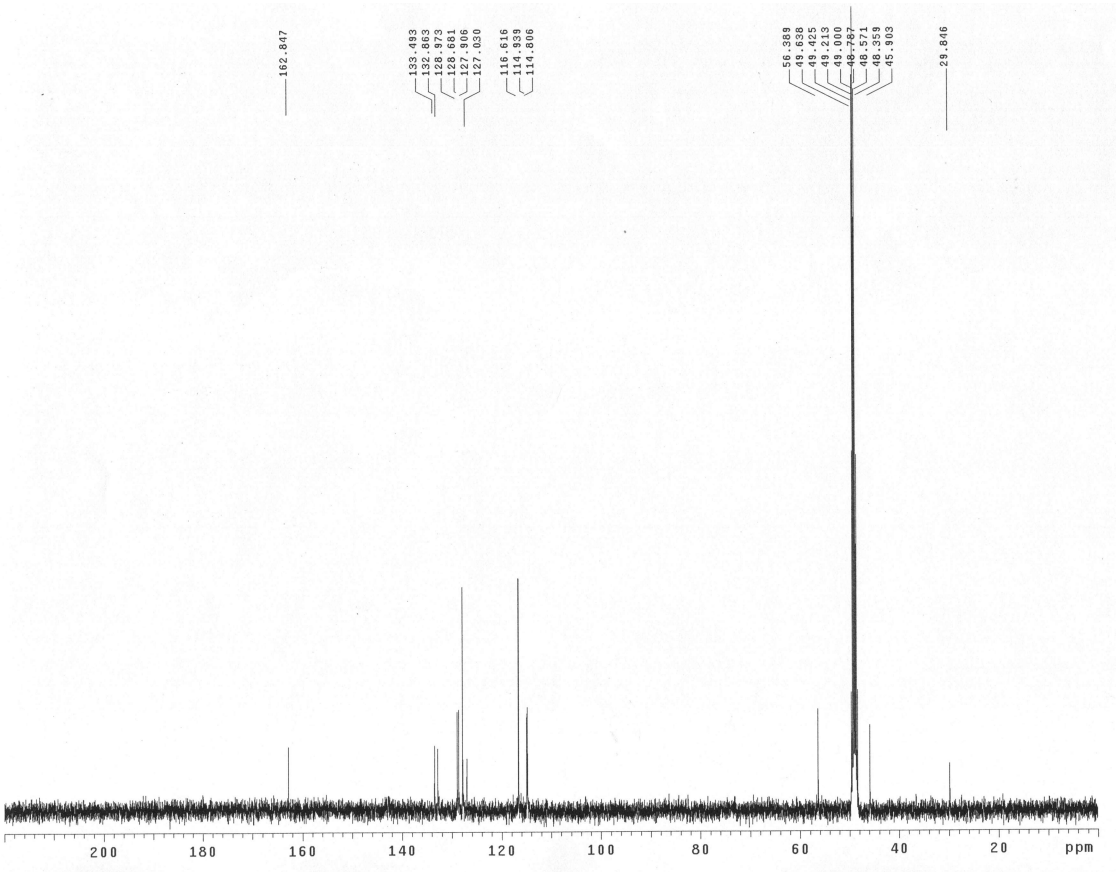
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **2**



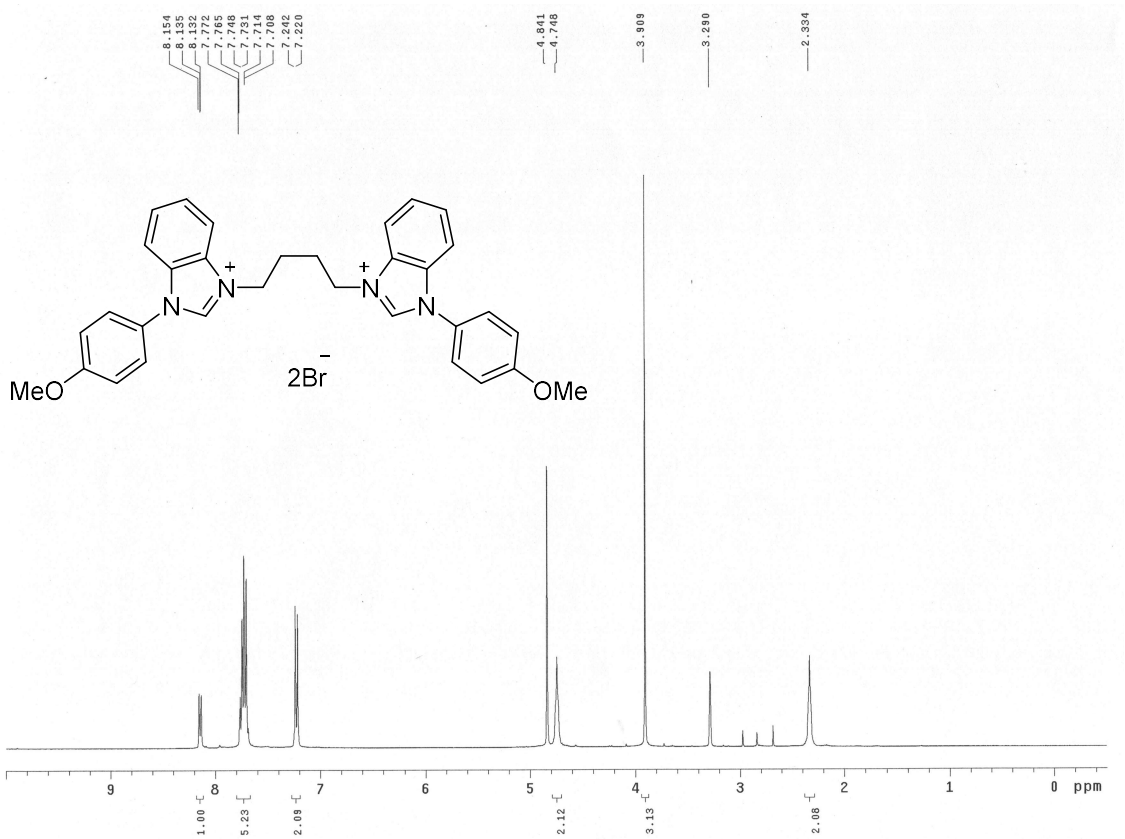
^{1}H NMR (CD_3OD, 400 MHz) spectrum of compound **1a**



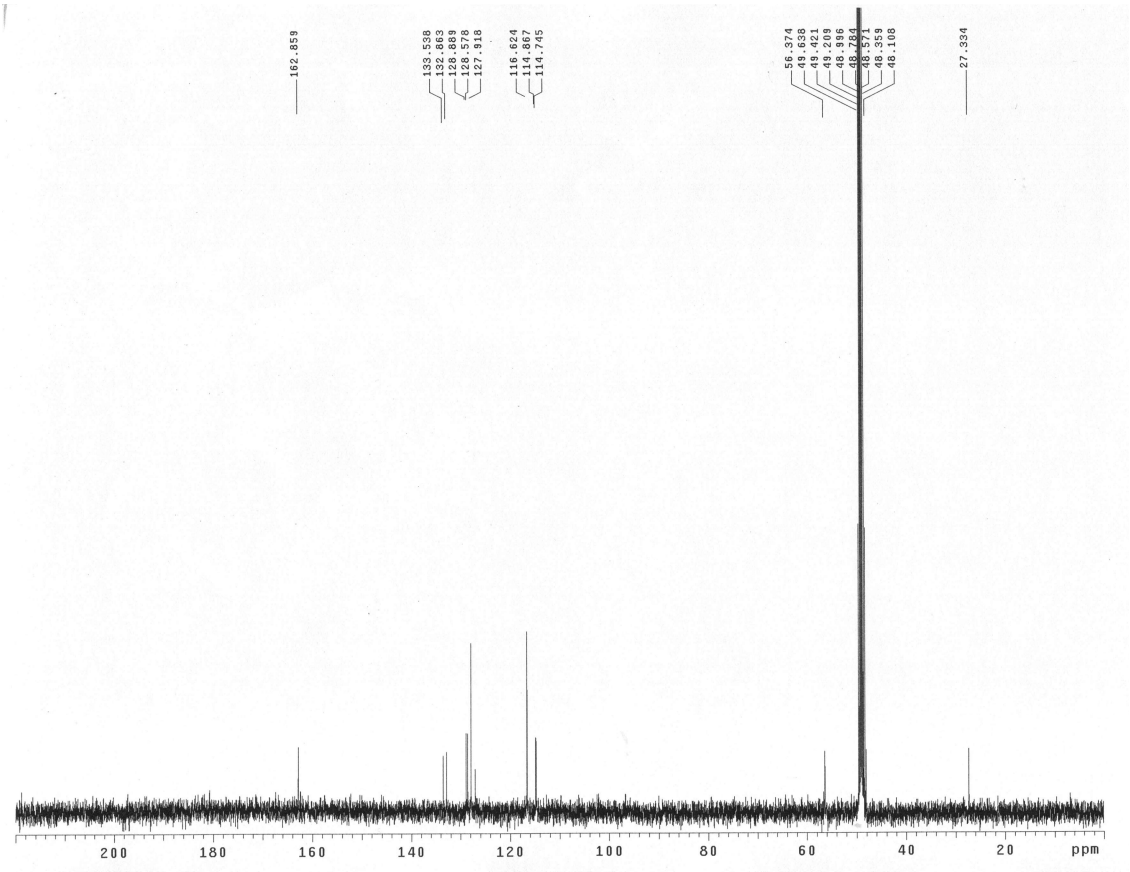
^{13}C NMR (CD_3OD, 100 MHz) spectrum of compound **1a**



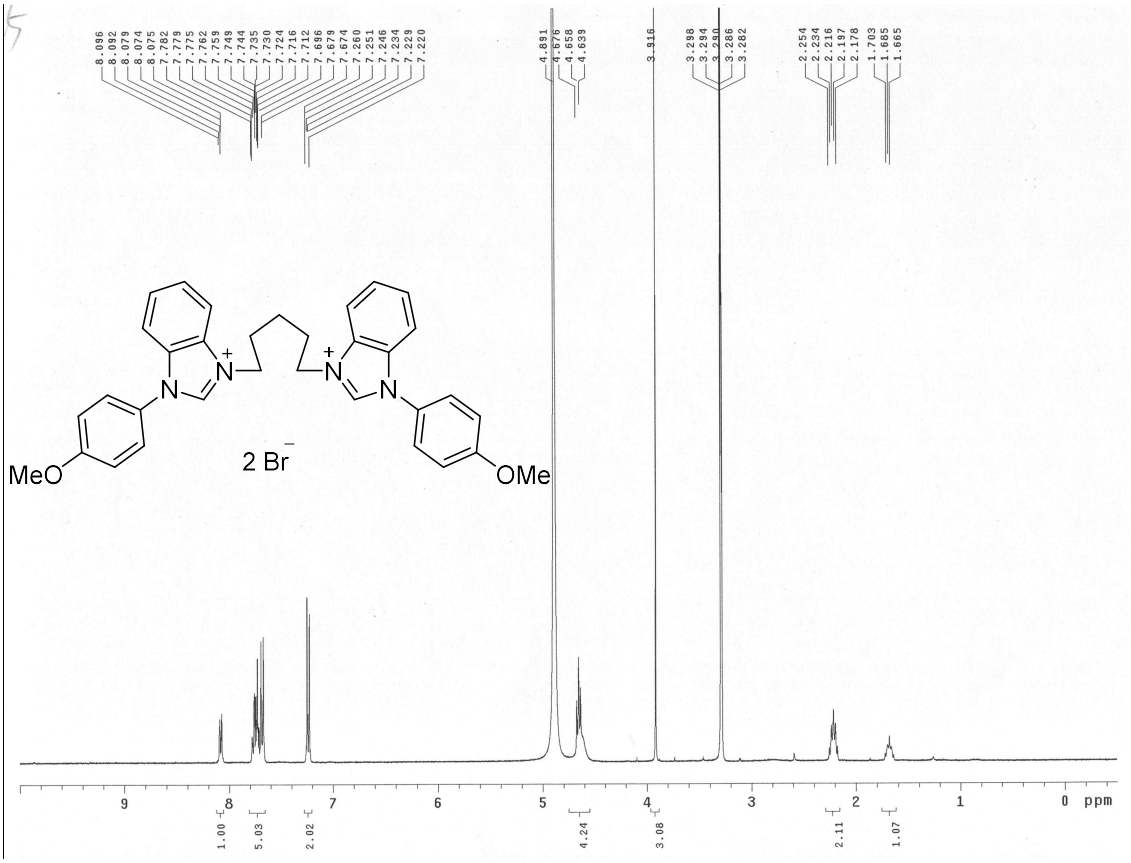
^{1}H NMR (CD_3OD, 400 MHz) spectrum of compound **1b**



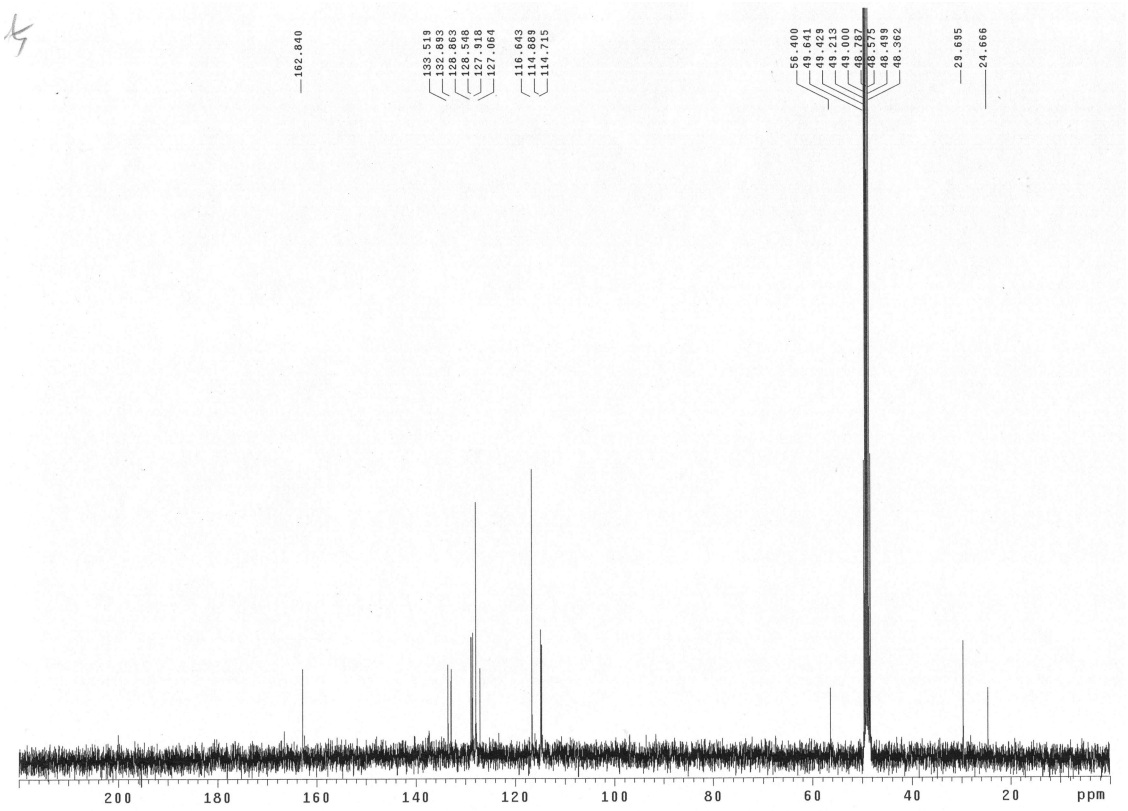
^{13}C NMR (CD_3OD, 100 MHz) spectrum of compound **1b**



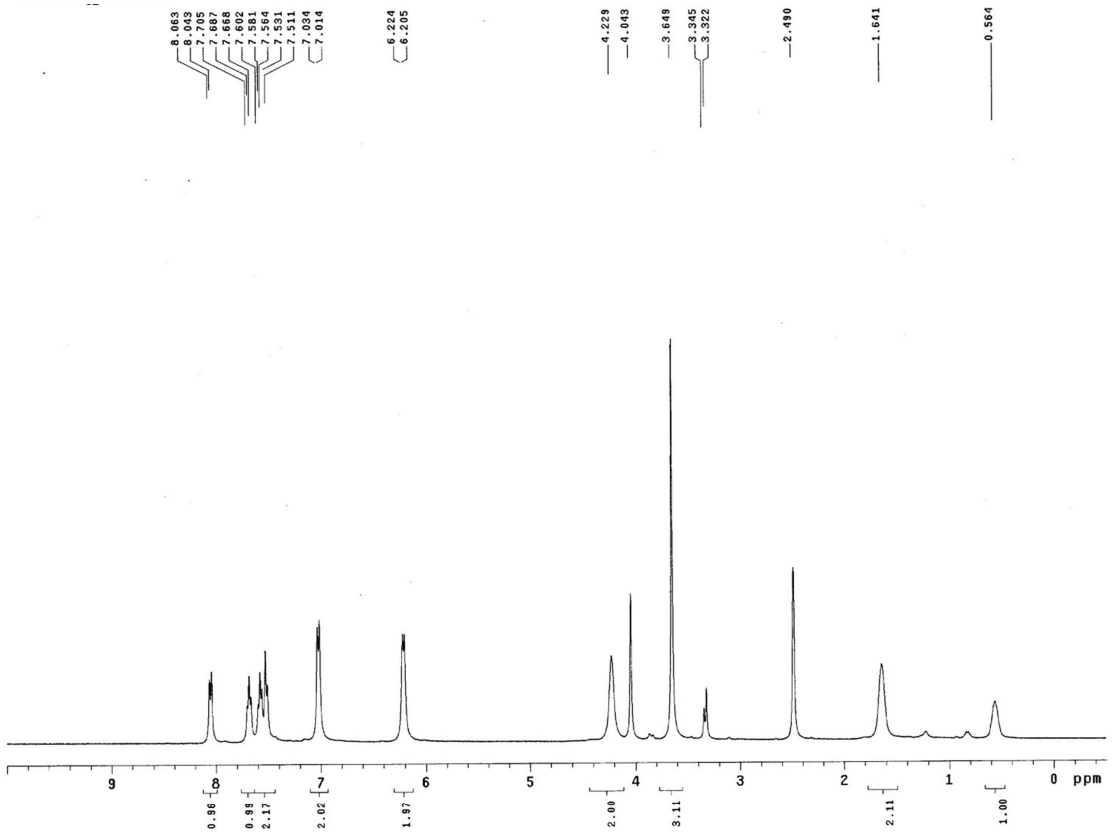
^{1}H NMR (CD_3OD, 400 MHz) spectrum of compound **1c**



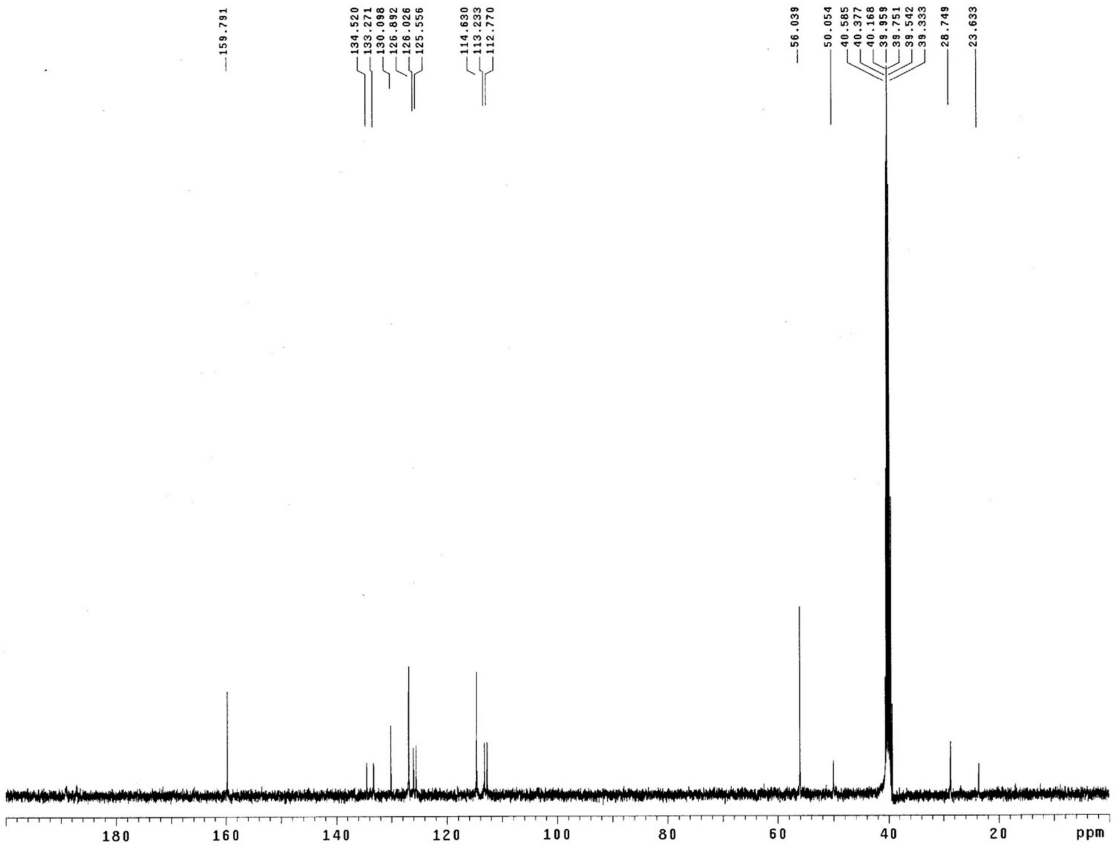
^{13}C NMR (CD_3OD, 100 MHz) spectrum of compound **1c**



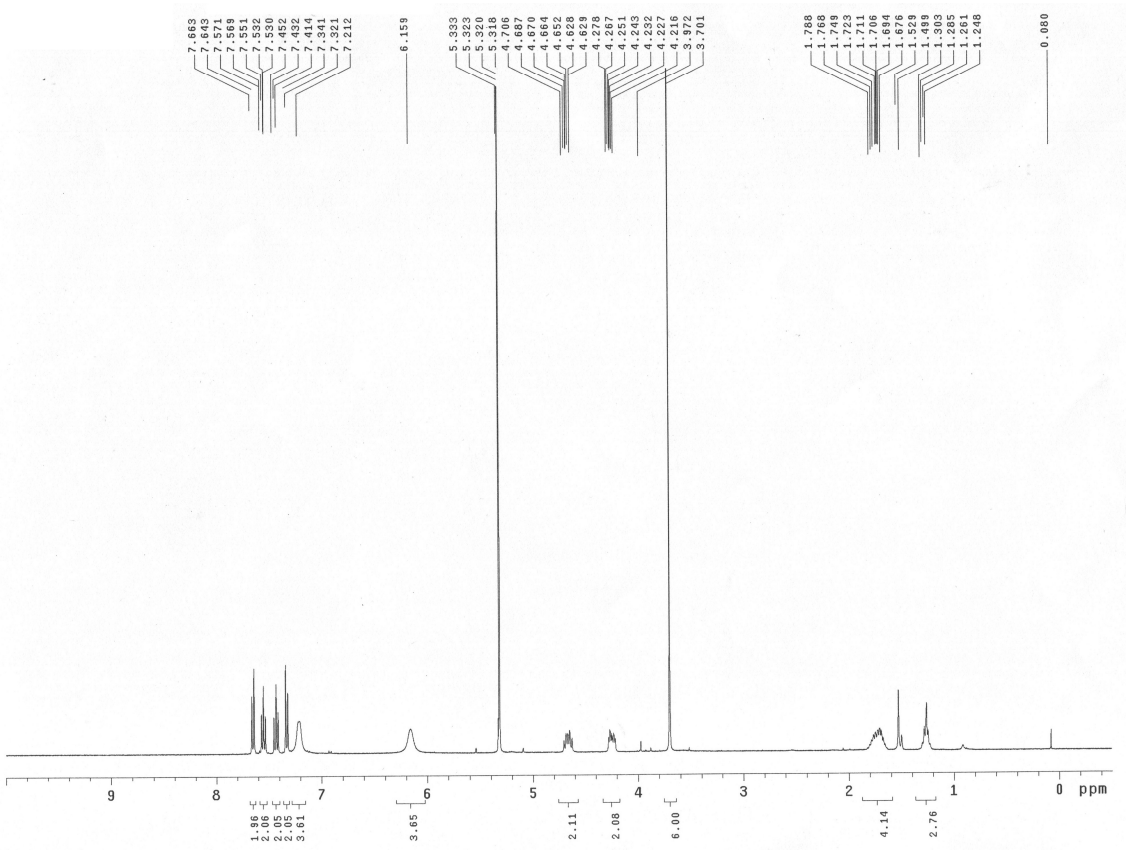
^{1}H NMR (DMSO-d_6, 400 MHz) spectrum of complex **1c**–**Ag**



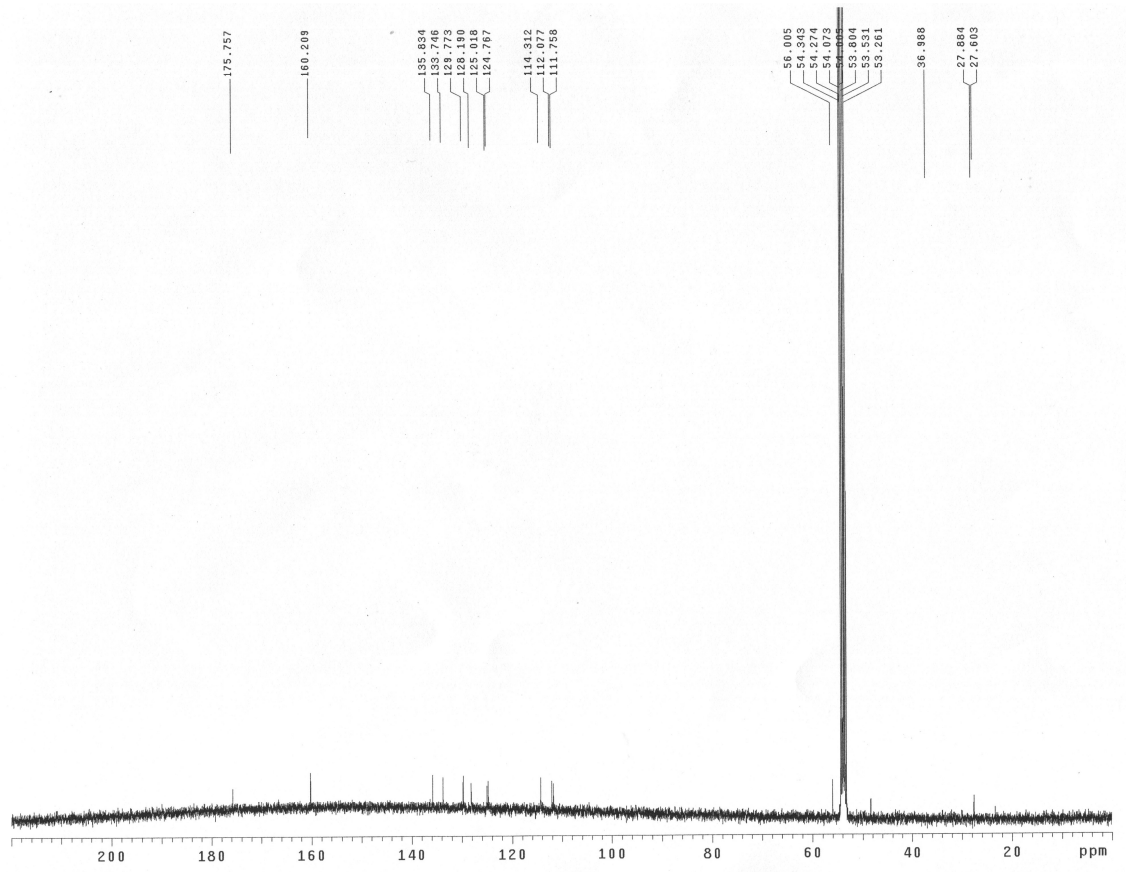
^{13}C NMR (DMSO-d_6, 100 MHz) spectrum of complex **1c**–**Ag**



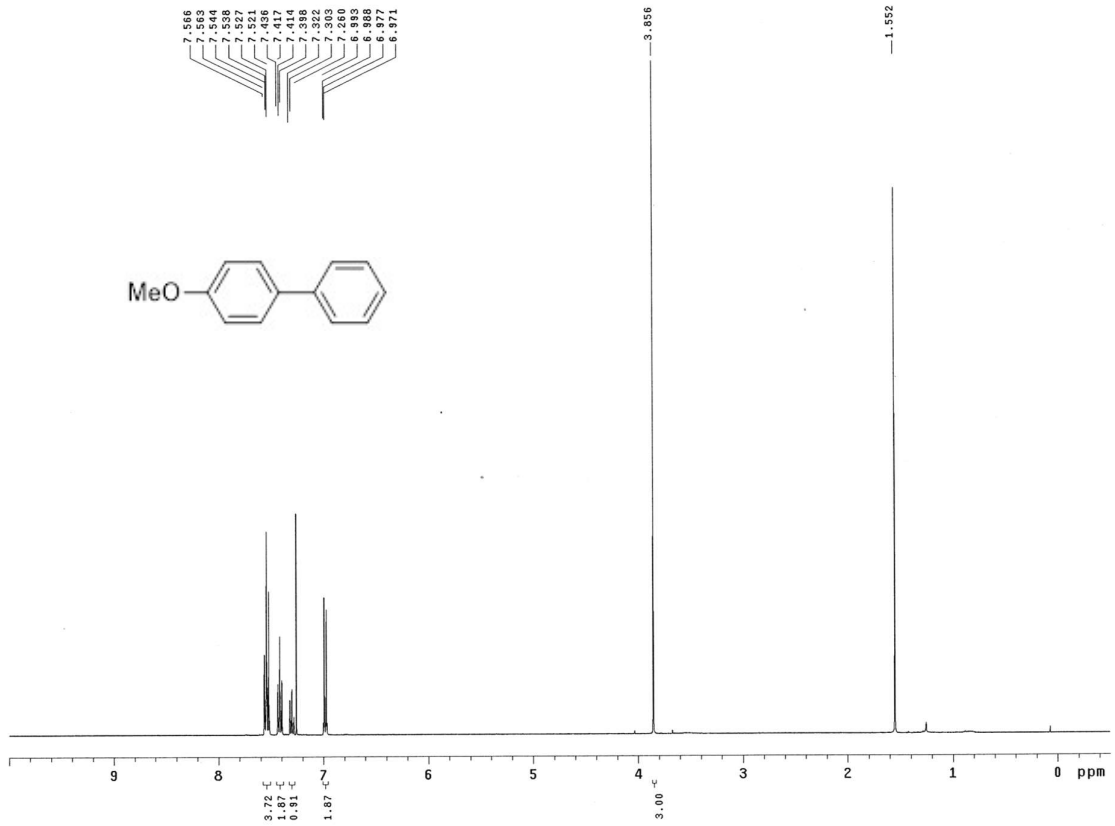
^{1}H NMR (CD_2Cl_2, 400 MHz) spectrum of complex **1c**–**Pd**



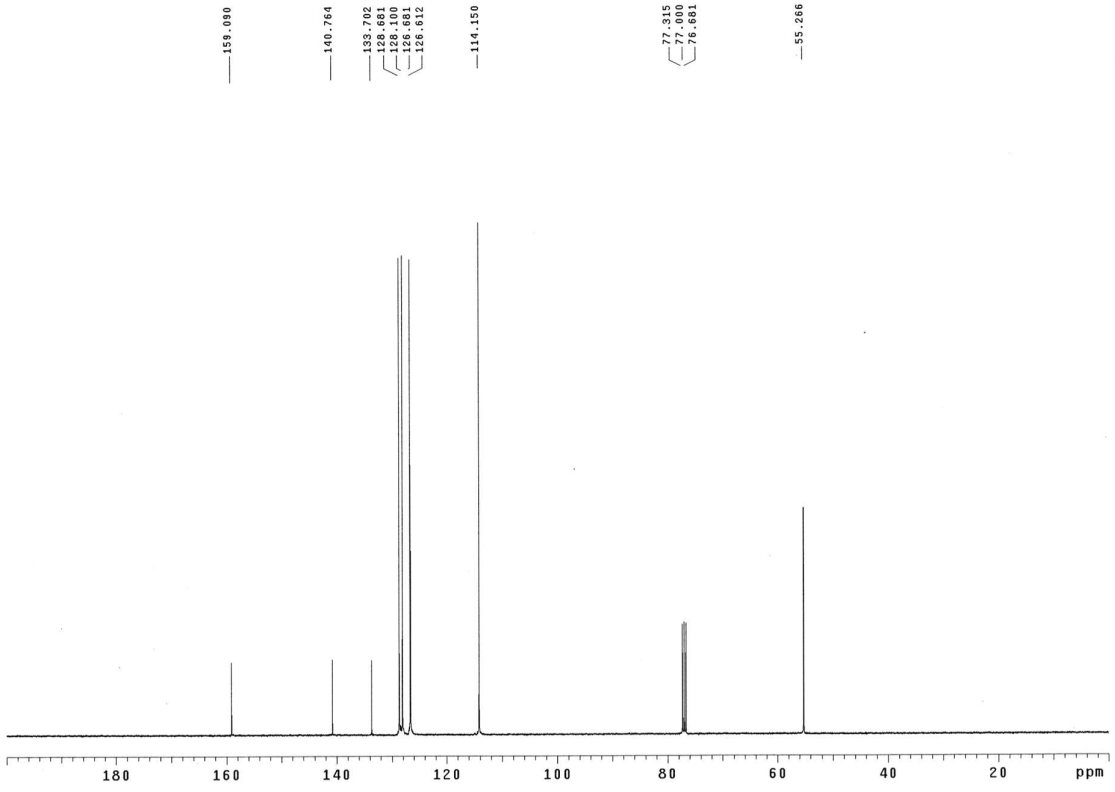
^{13}C NMR (CD_2Cl_2, 100 MHz) spectrum of complex **1c**–**Pd**



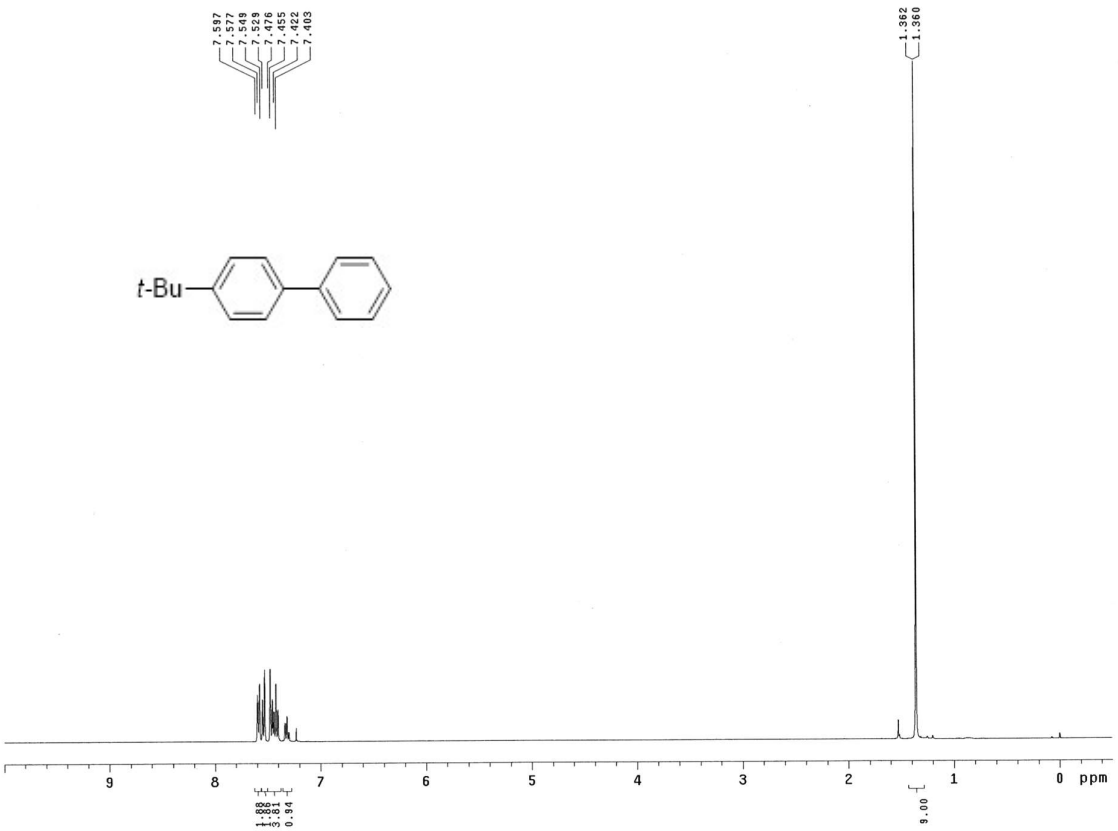
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **5aa** (table 2, entry 1)



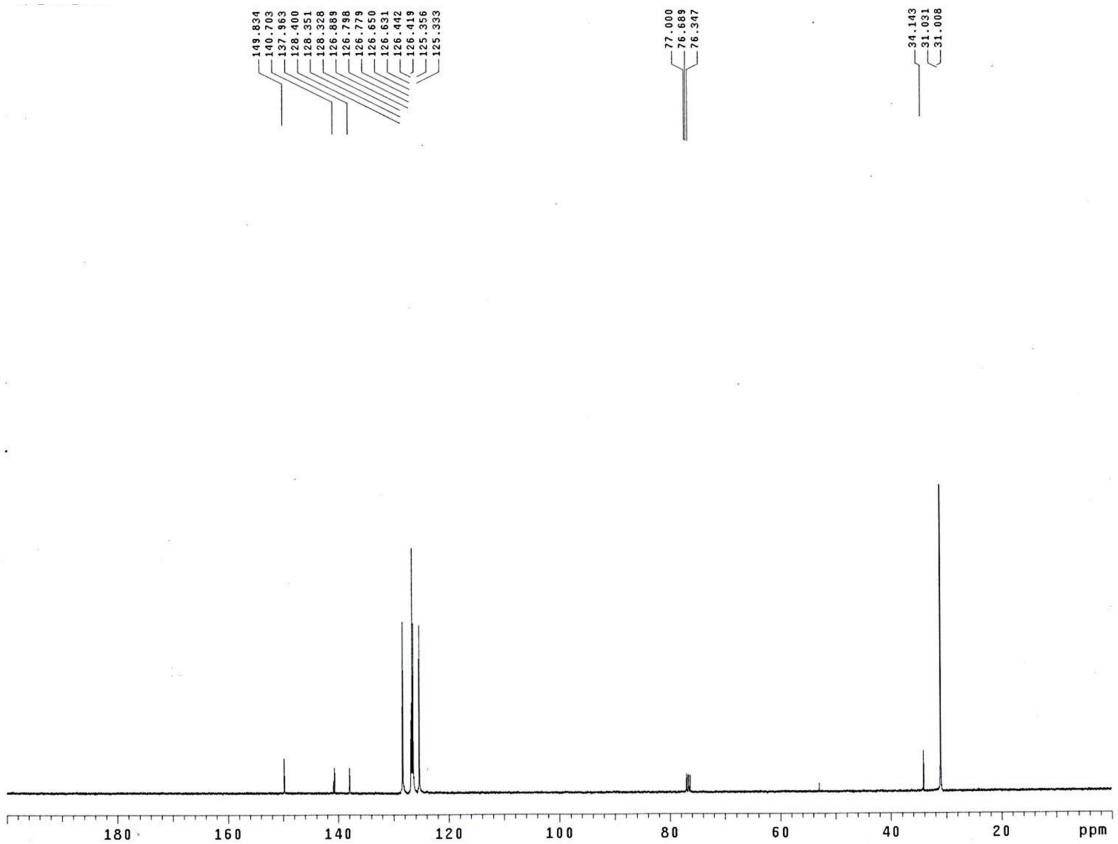
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **5aa**



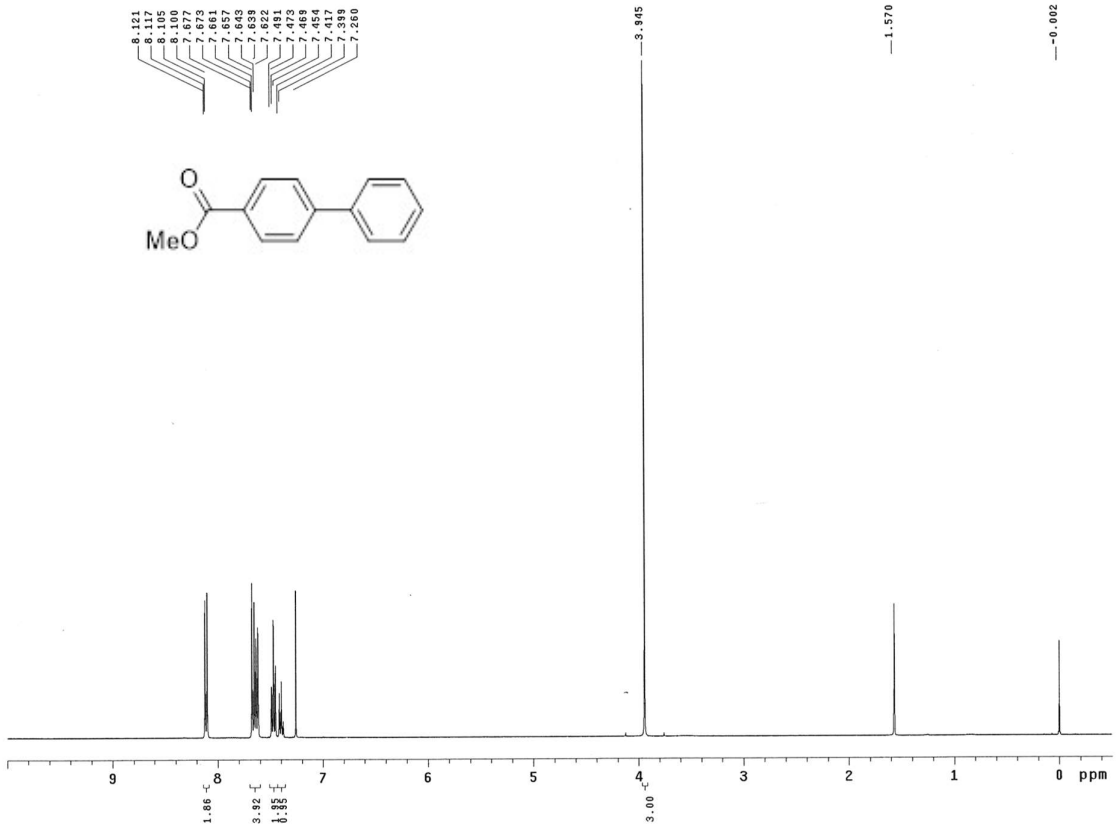
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **5ba** (table 2, entry 4)



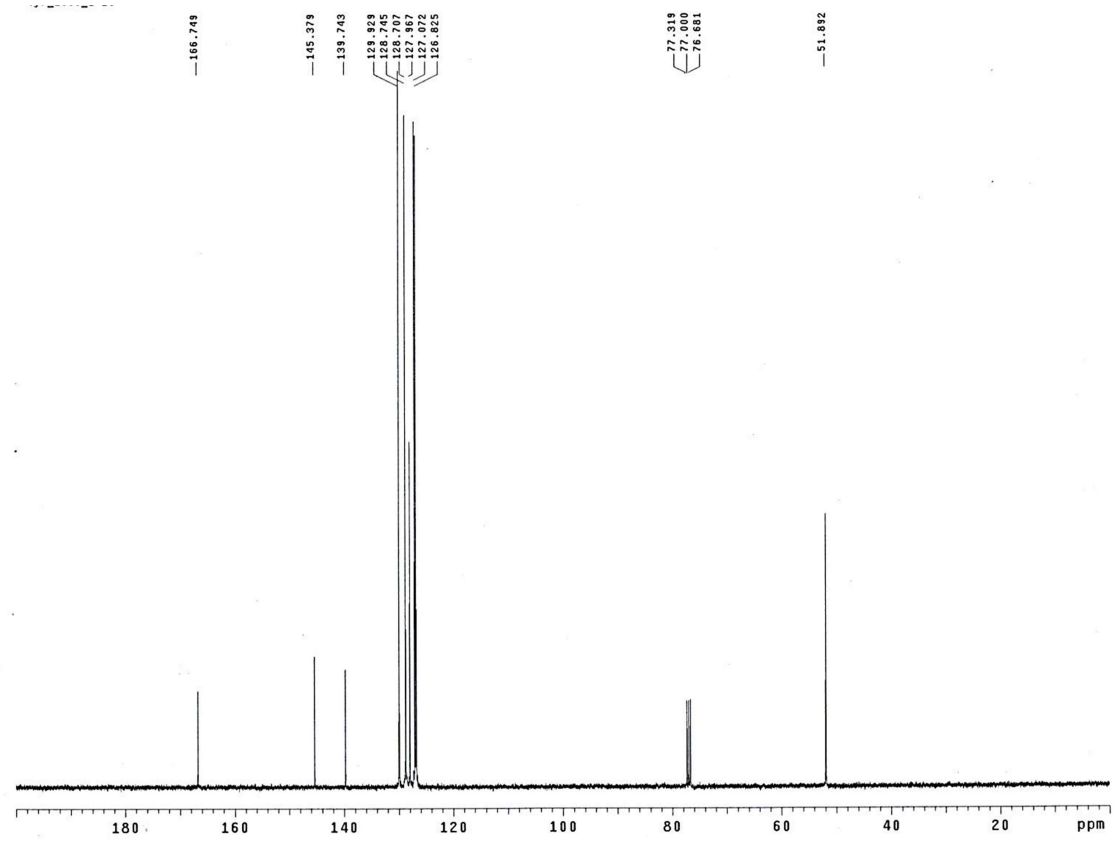
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **5ba**



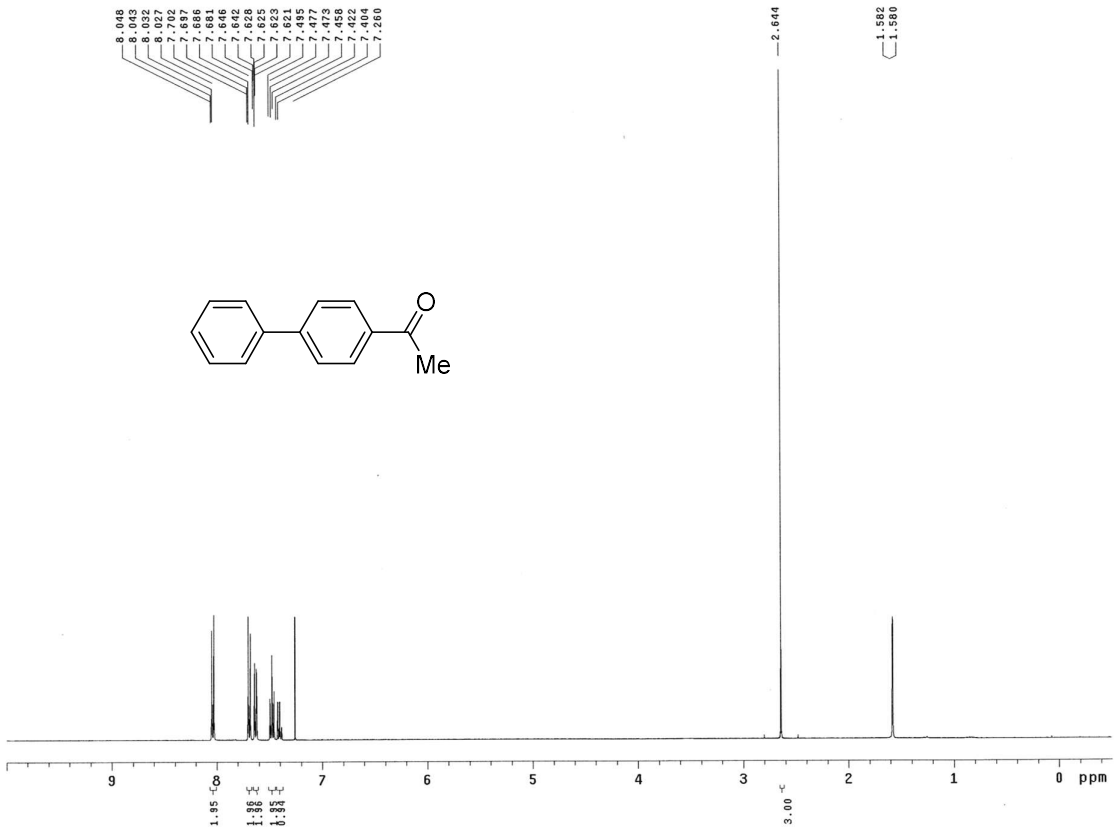
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **5ca** (table 2, entry 5)



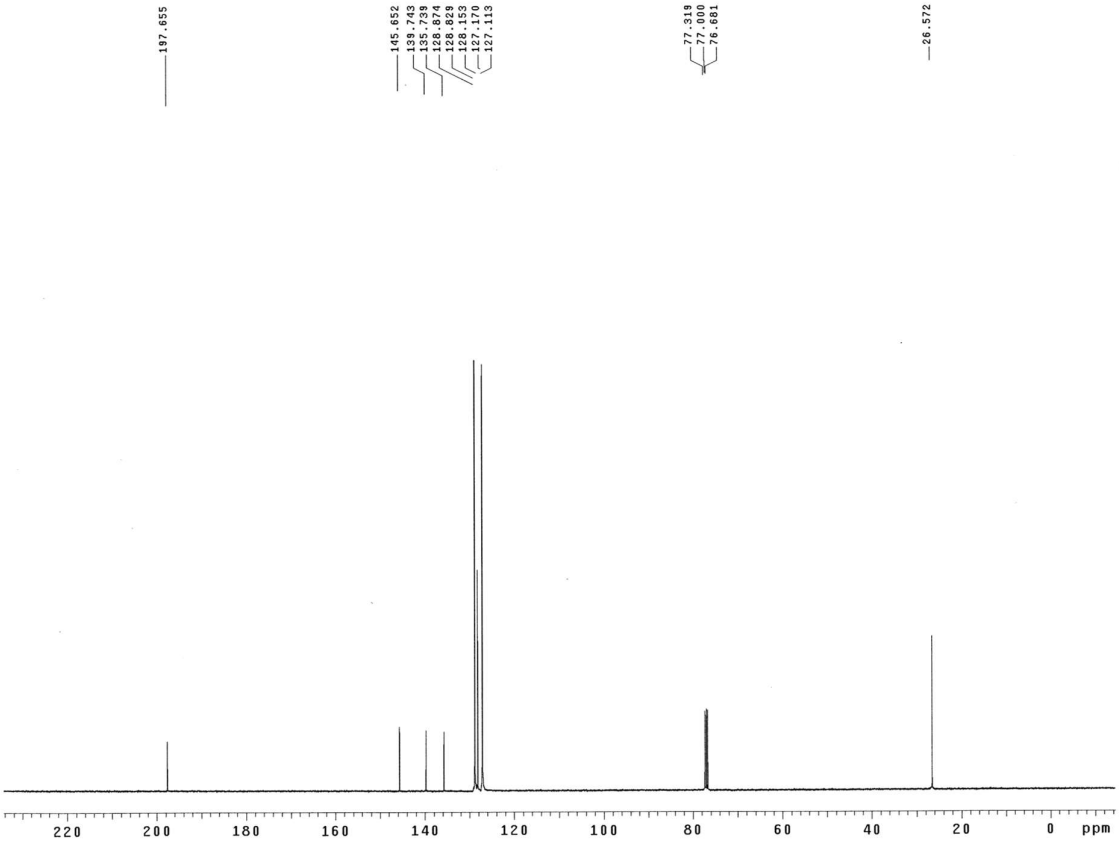
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **5ca**



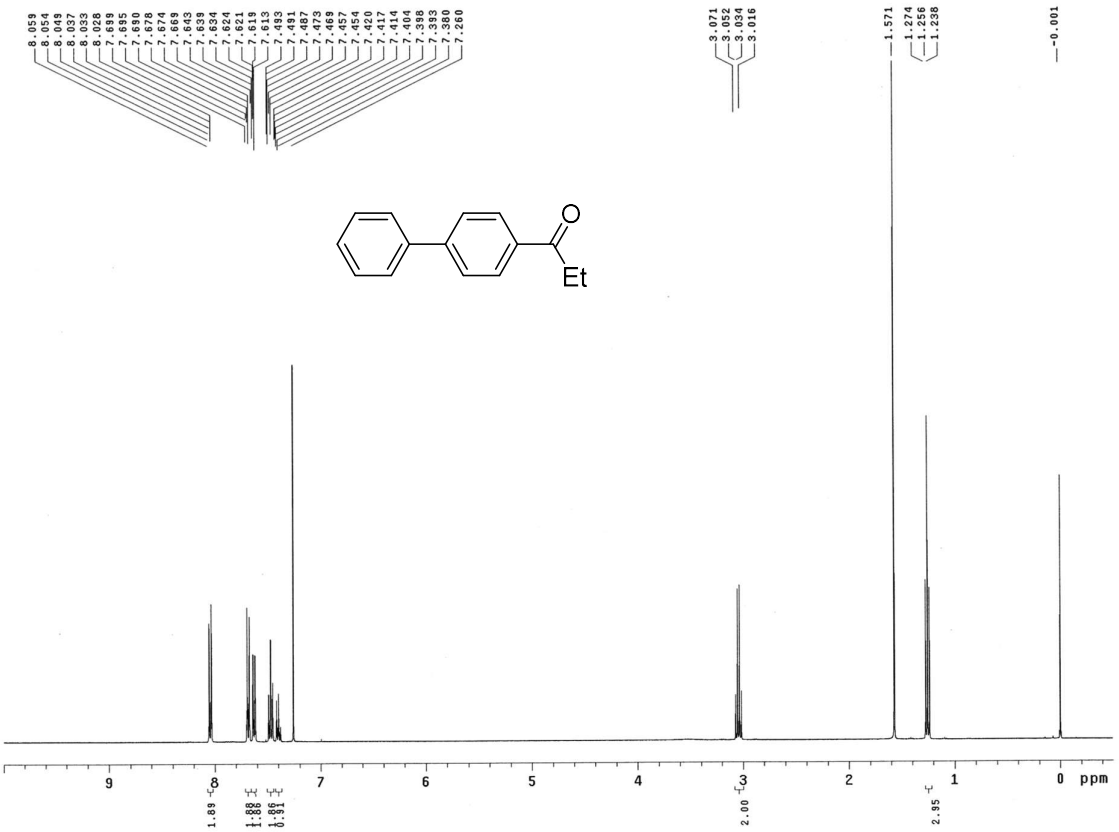
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **5da** (table 2, entry 6)



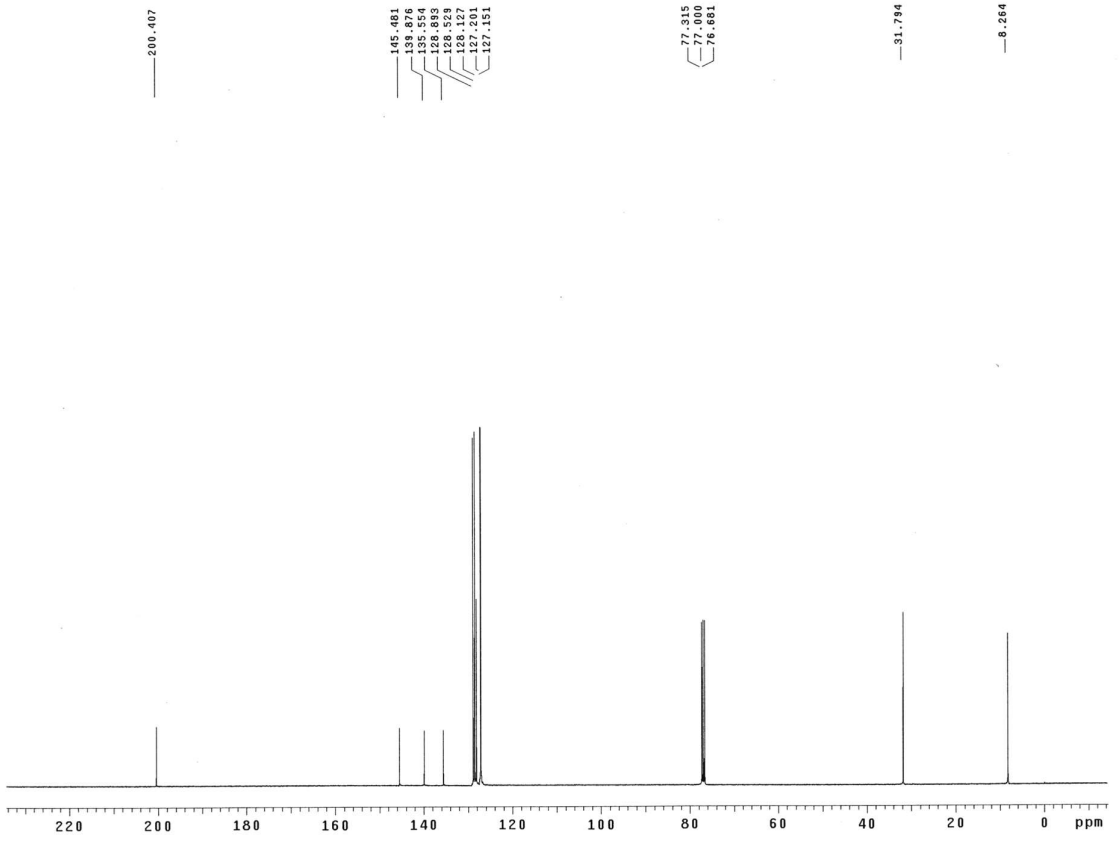
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **5da**



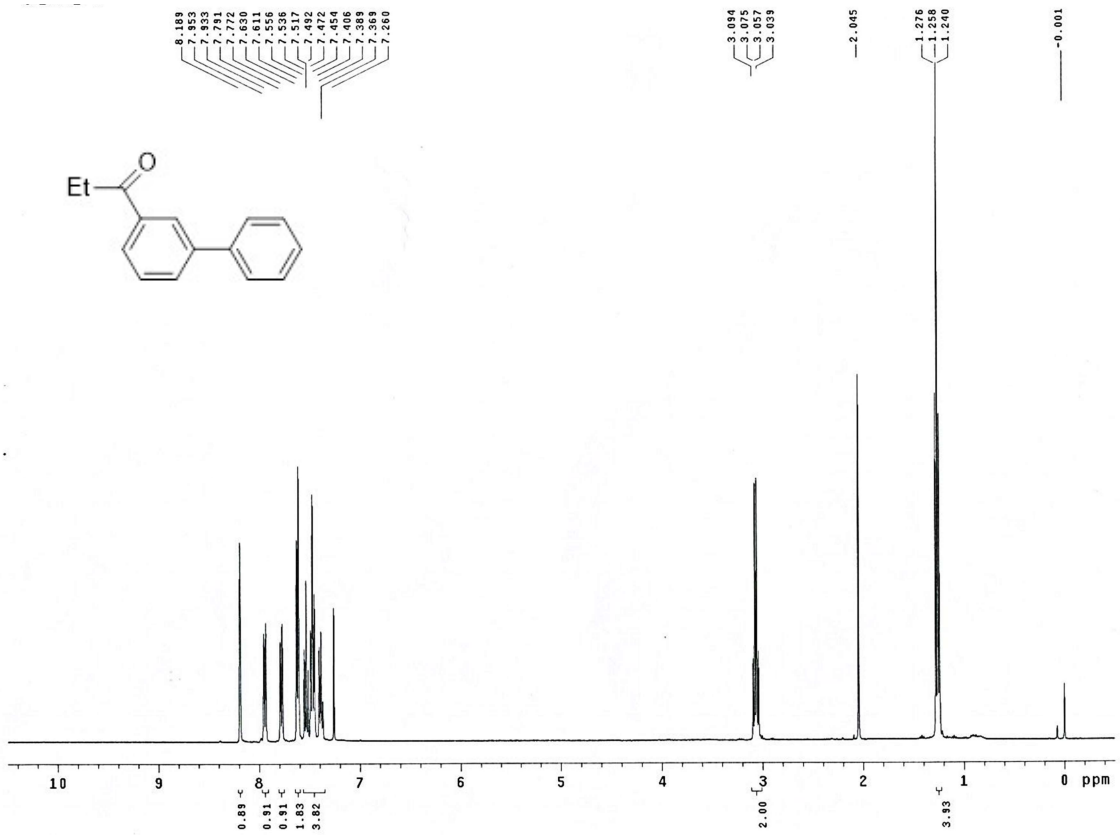
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **5ea** (table 2, entry 9)



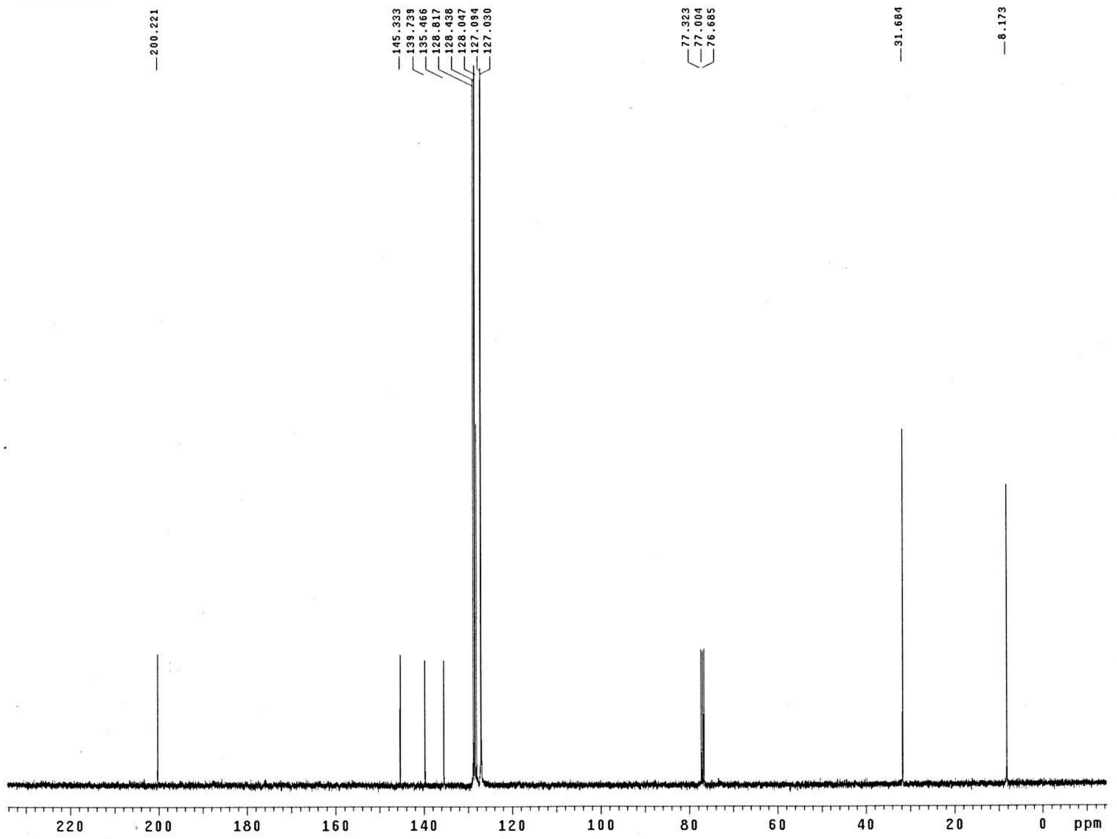
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **5ea**



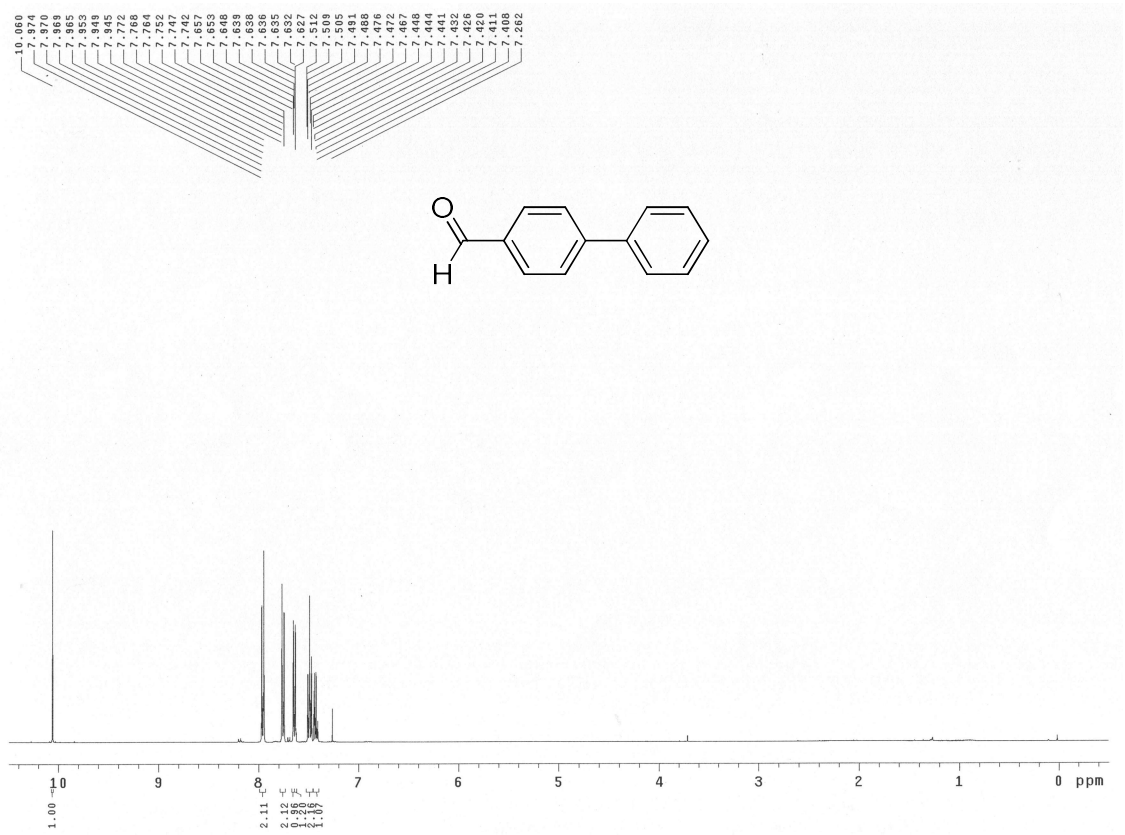
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **5fa** (table 2, entry 12)



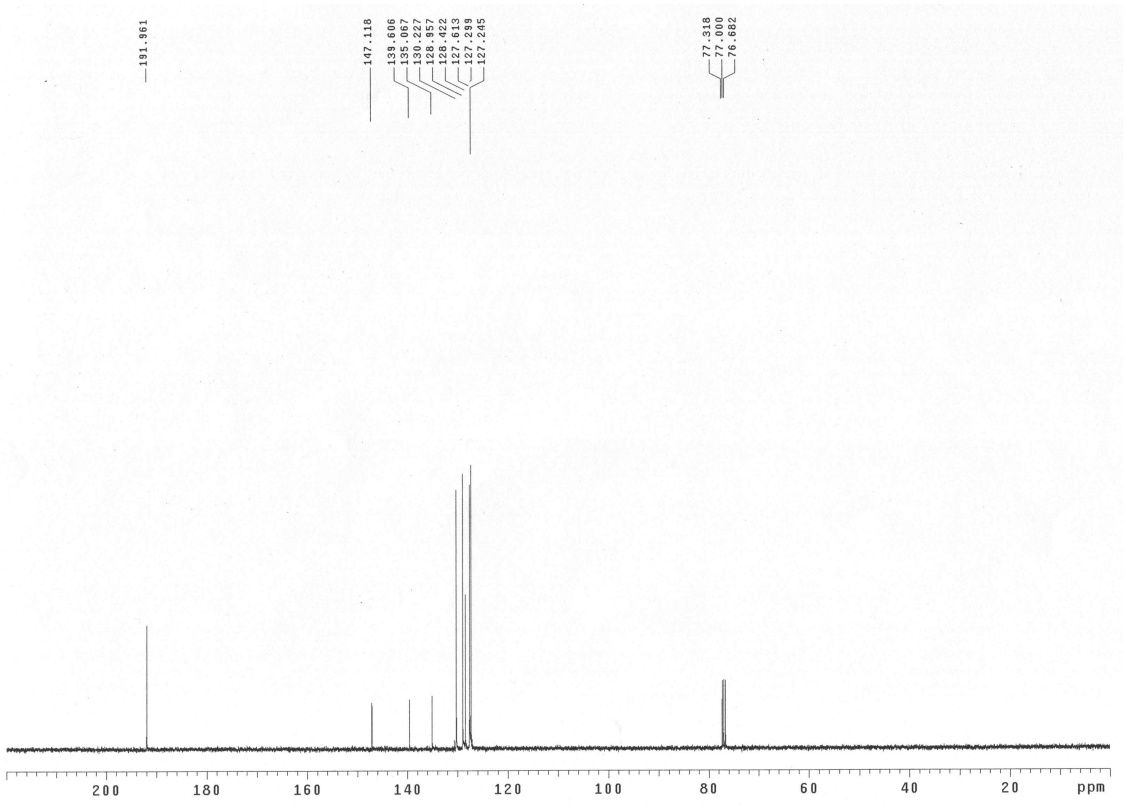
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **5fa**



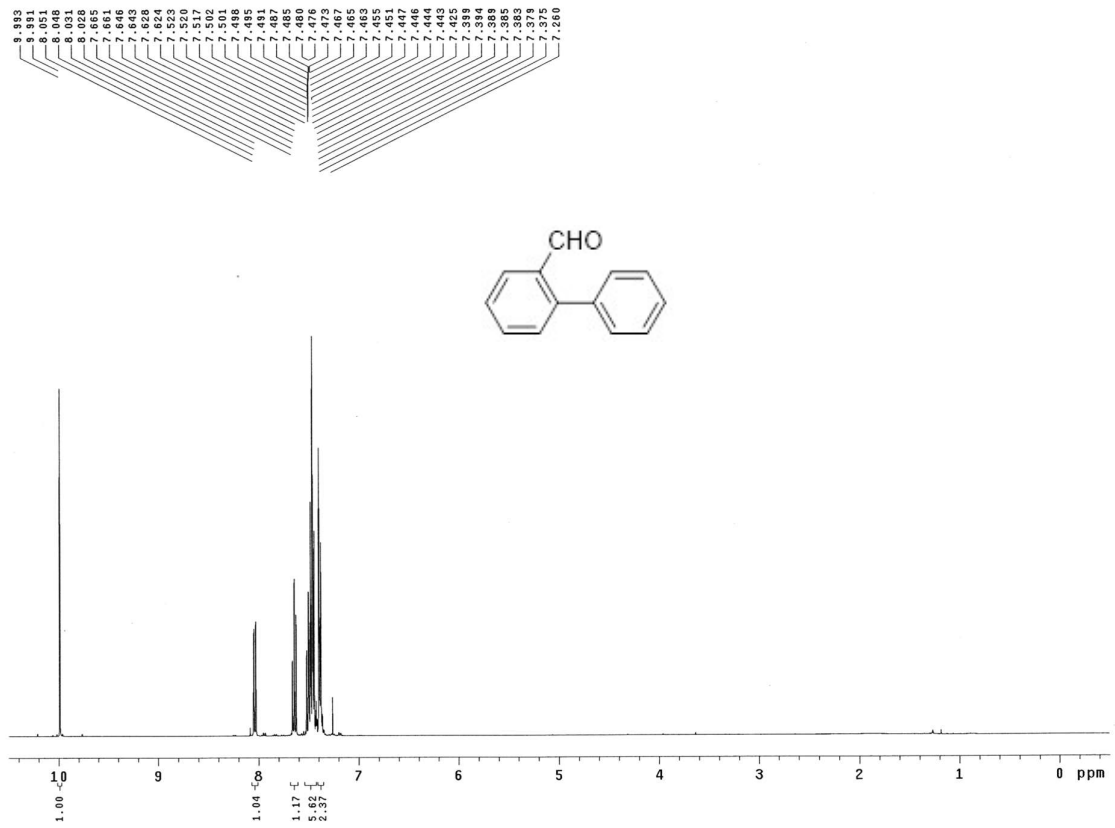
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **5ga** (table 2, entry 13)



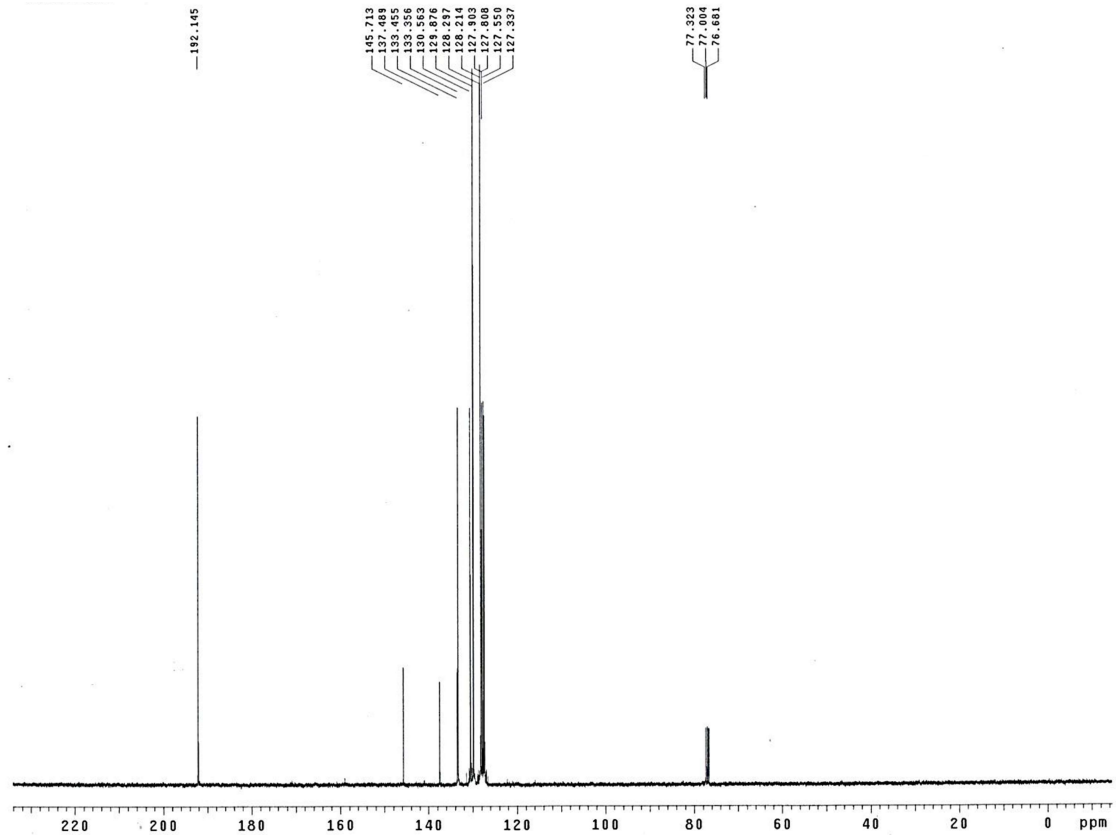
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **5ga**



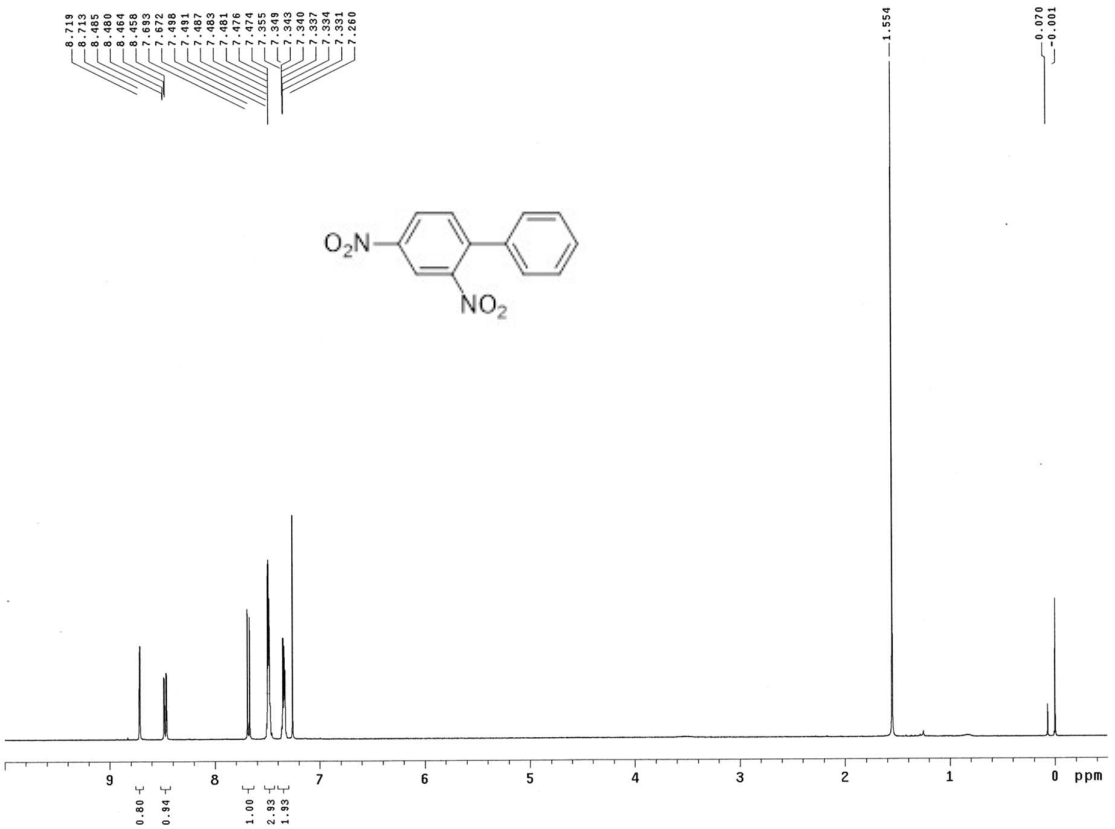
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **5ha** (table 2, entry 14)



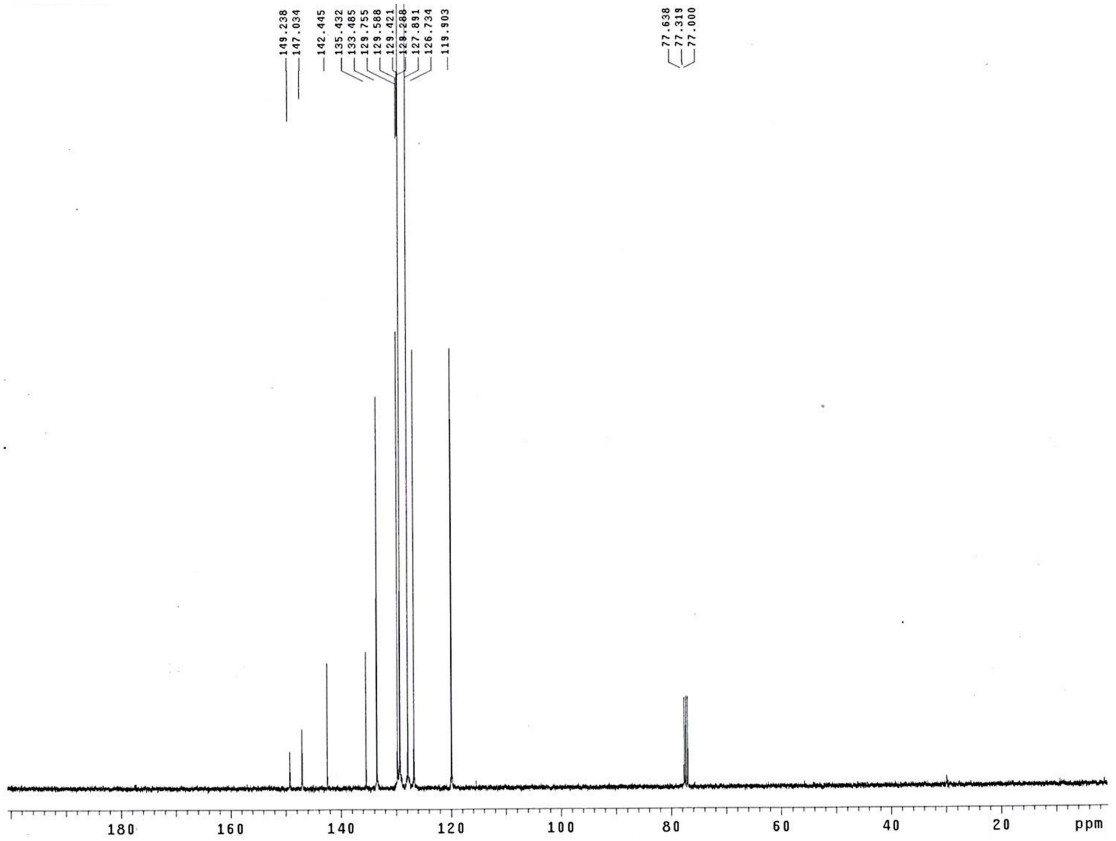
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **5ha**



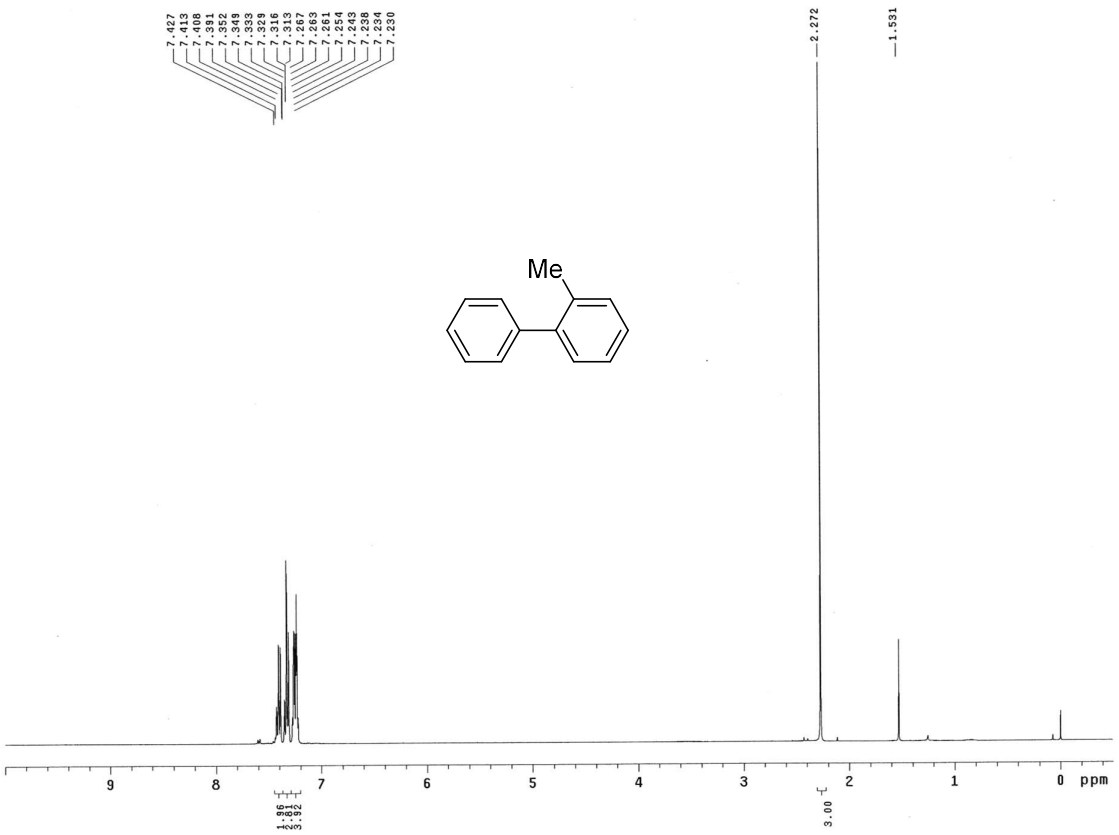
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **5ia** (table 2, entry 15)



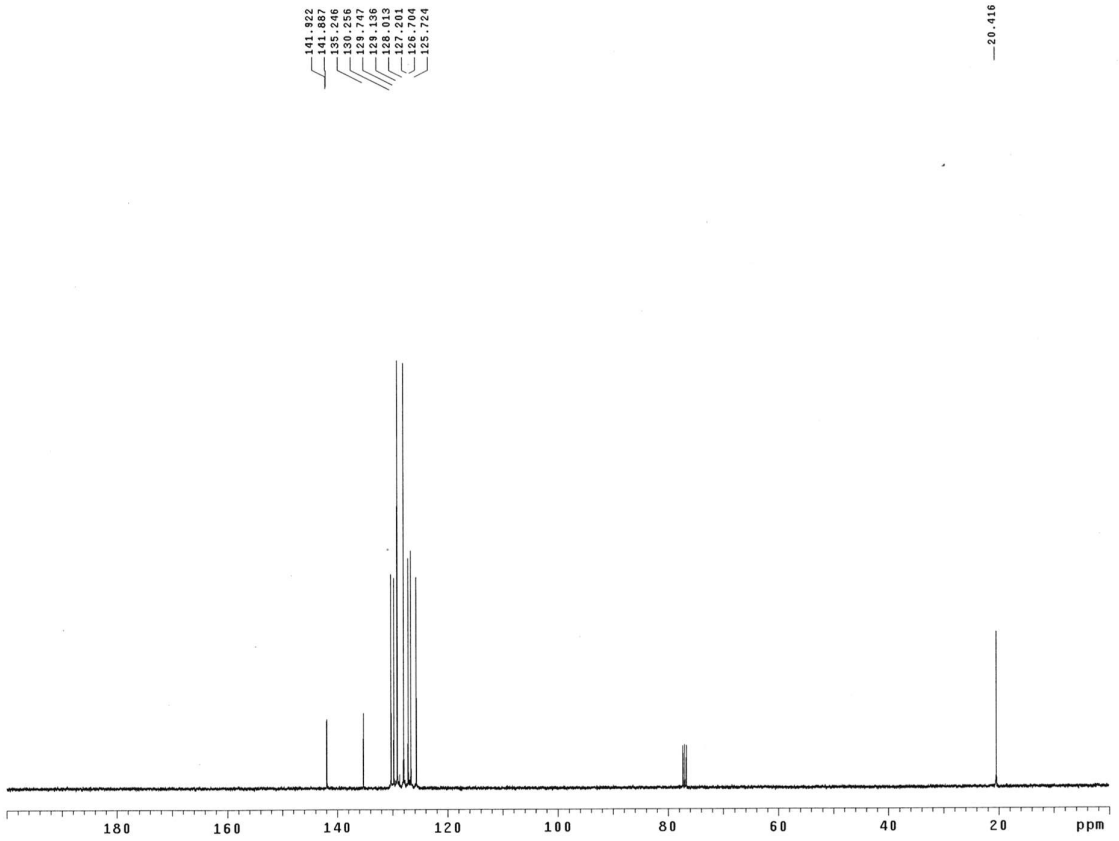
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **5ia**



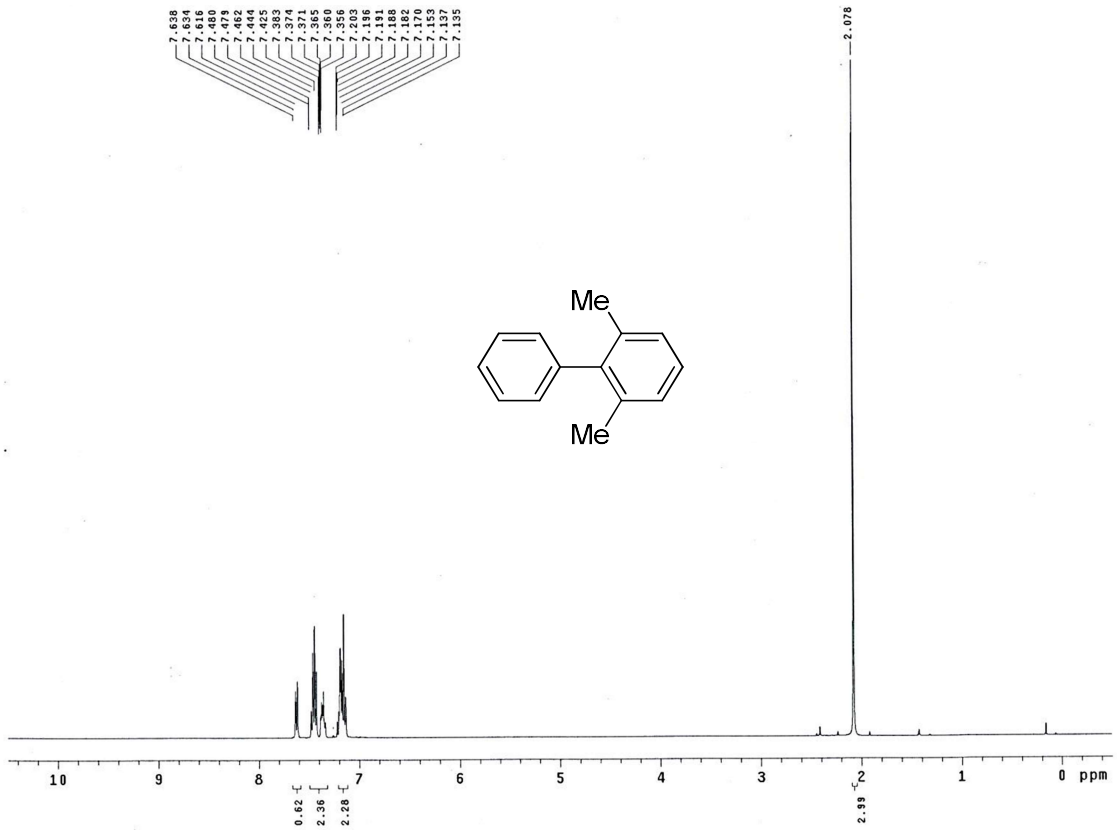
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **5ja** (table 2, entry 16)



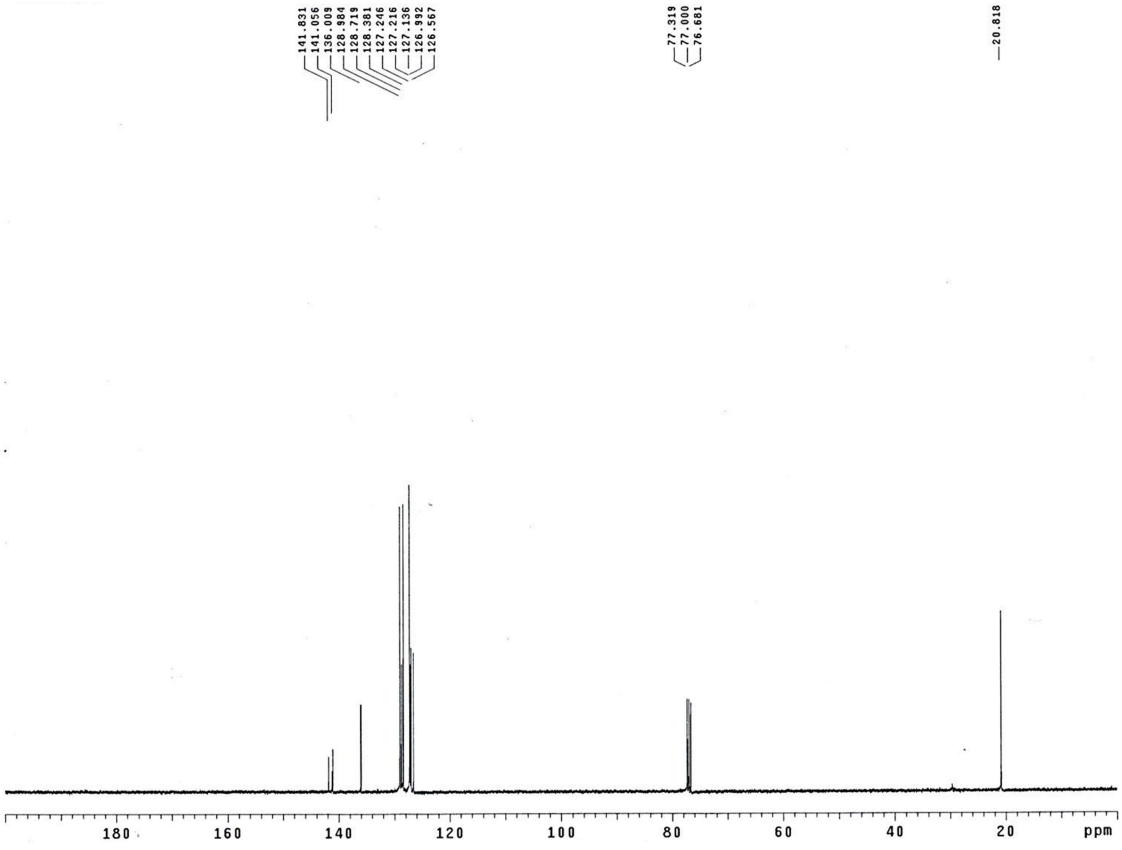
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **5ja**



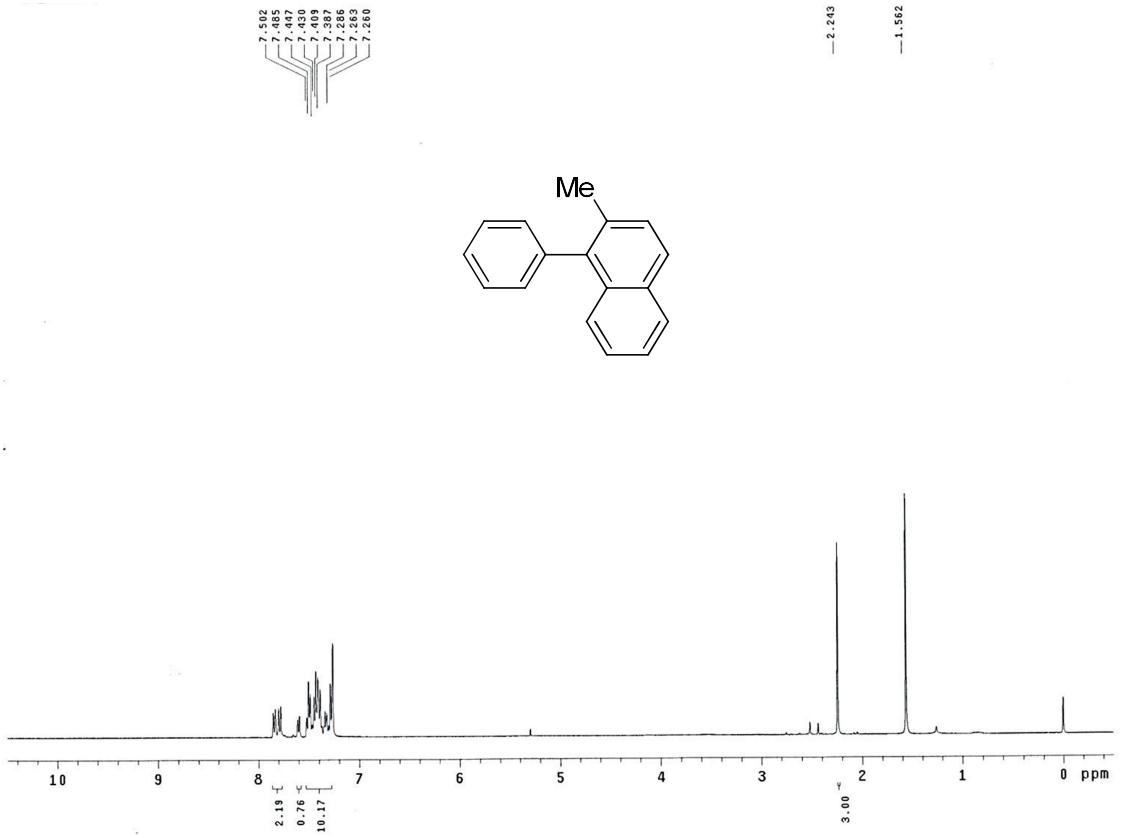
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **5ka** (table 2, entry 17)



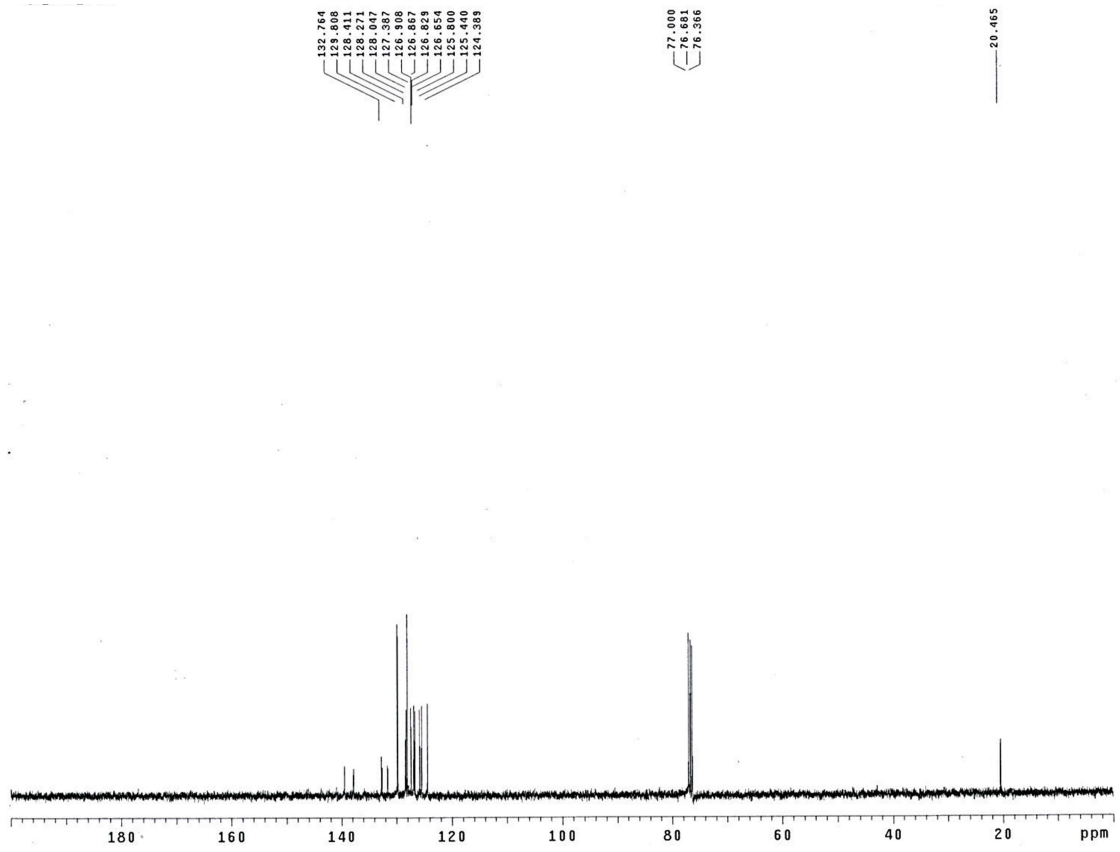
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **5ka**



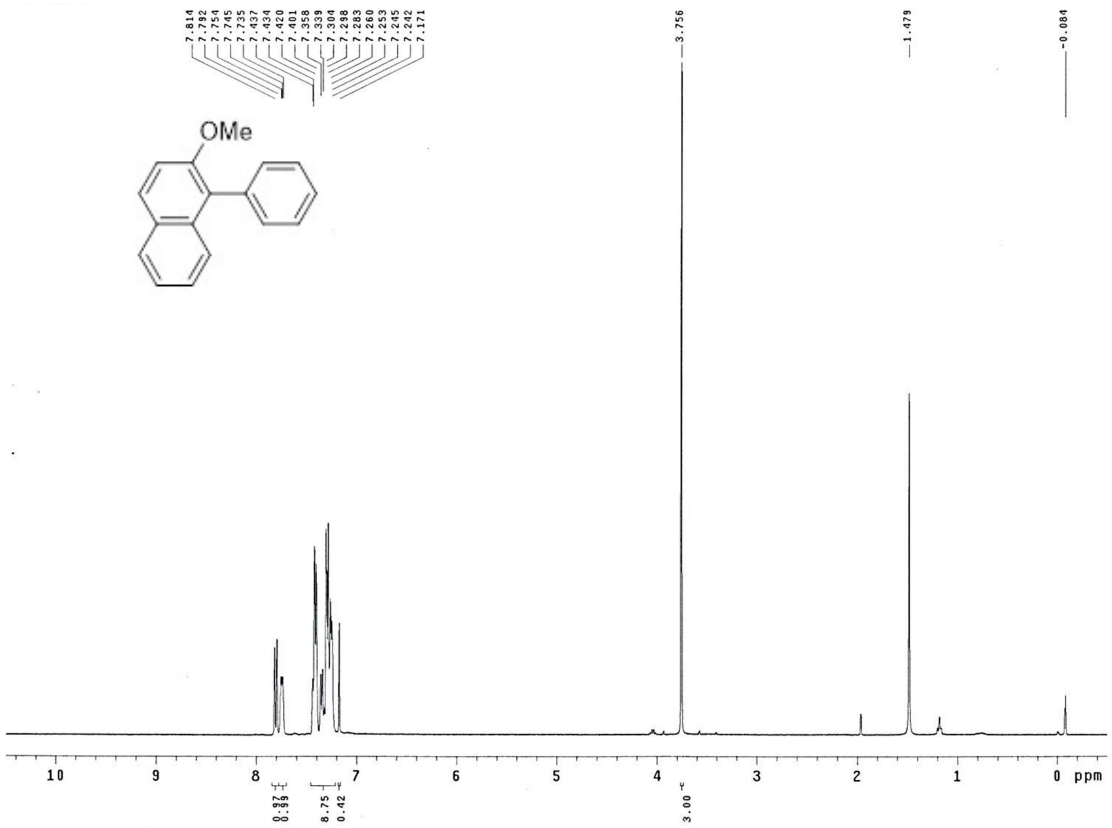
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **5la** (table 2, entry 18)



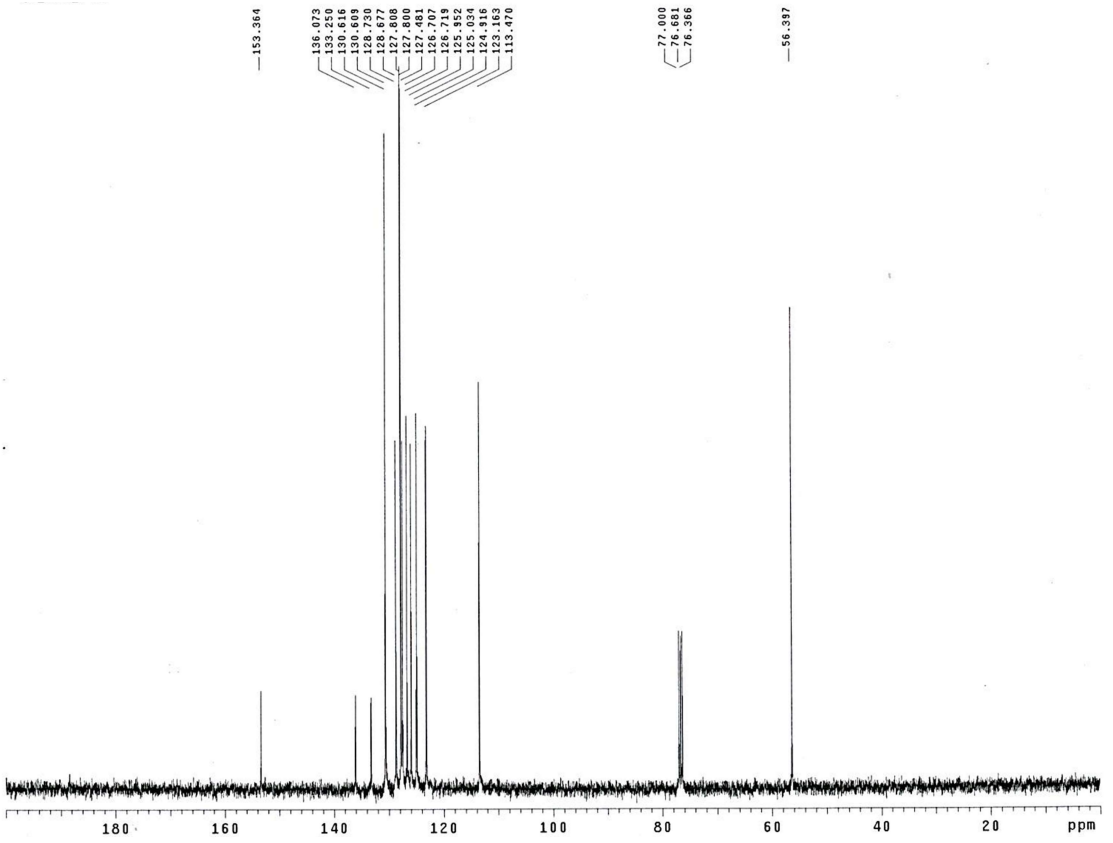
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **5la**



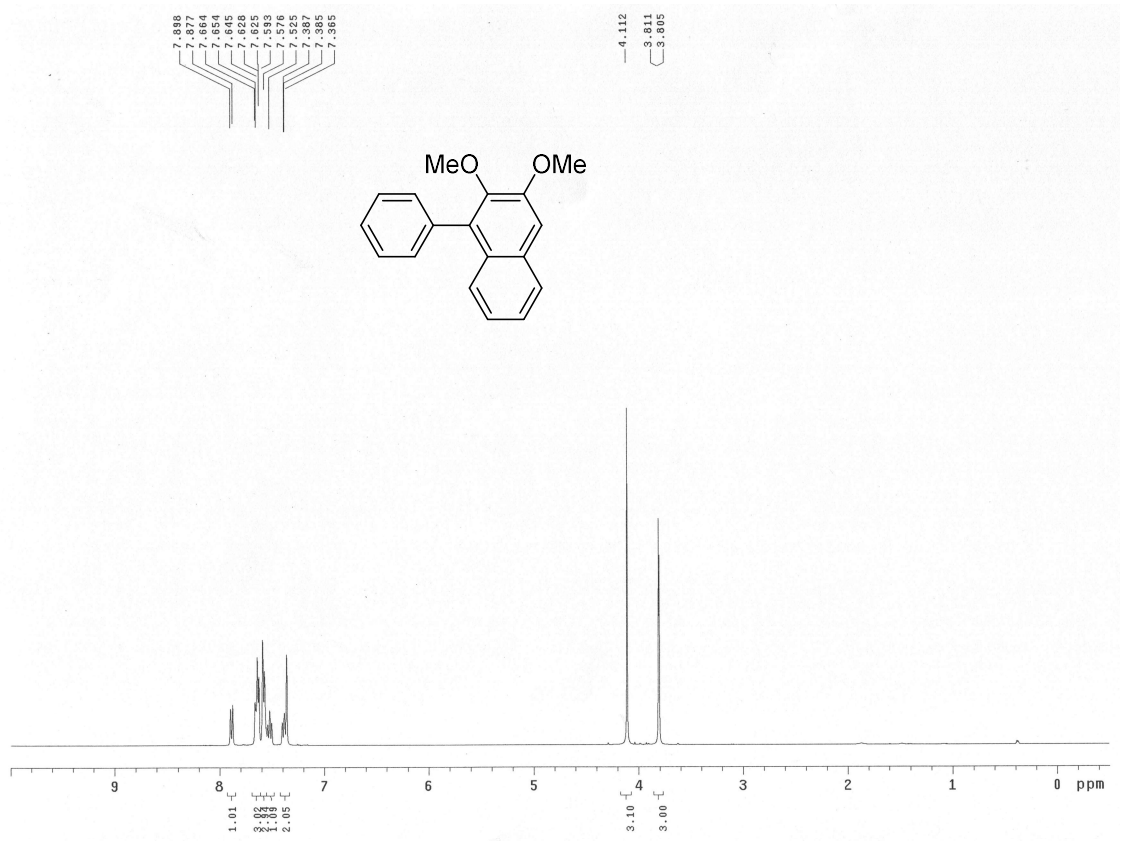
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **5ma** (table 2, entry 19)



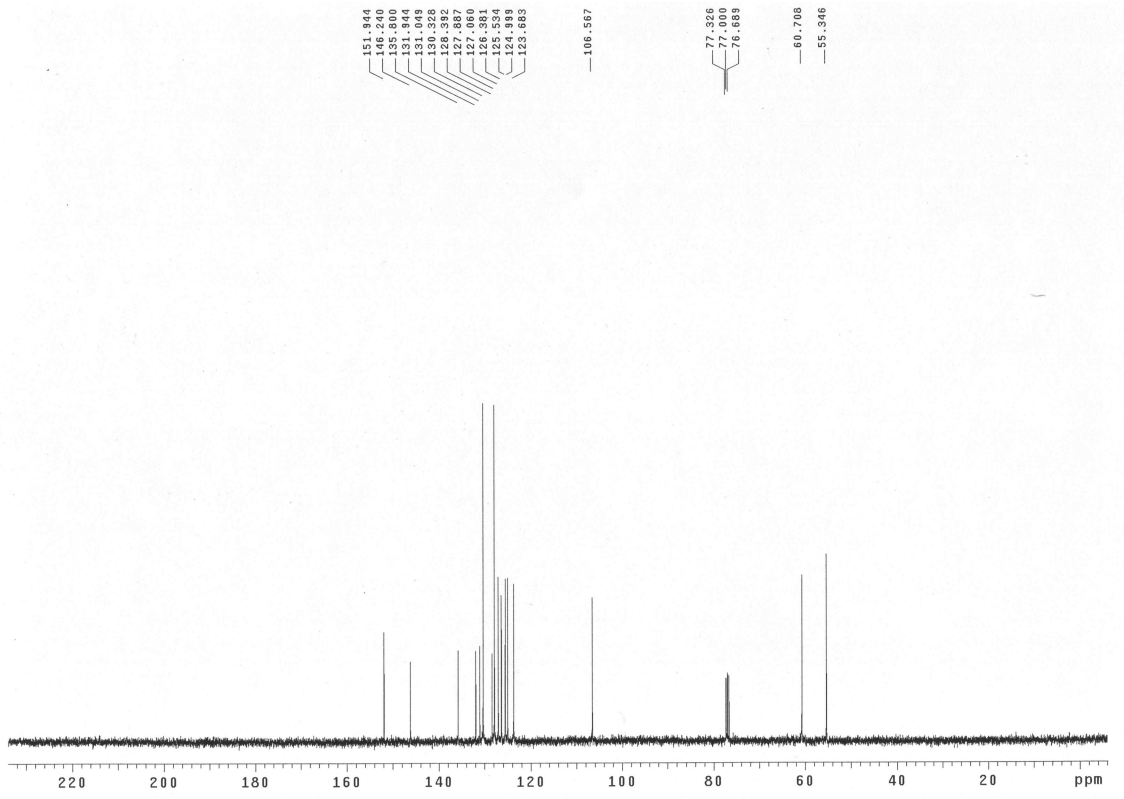
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **5ma**



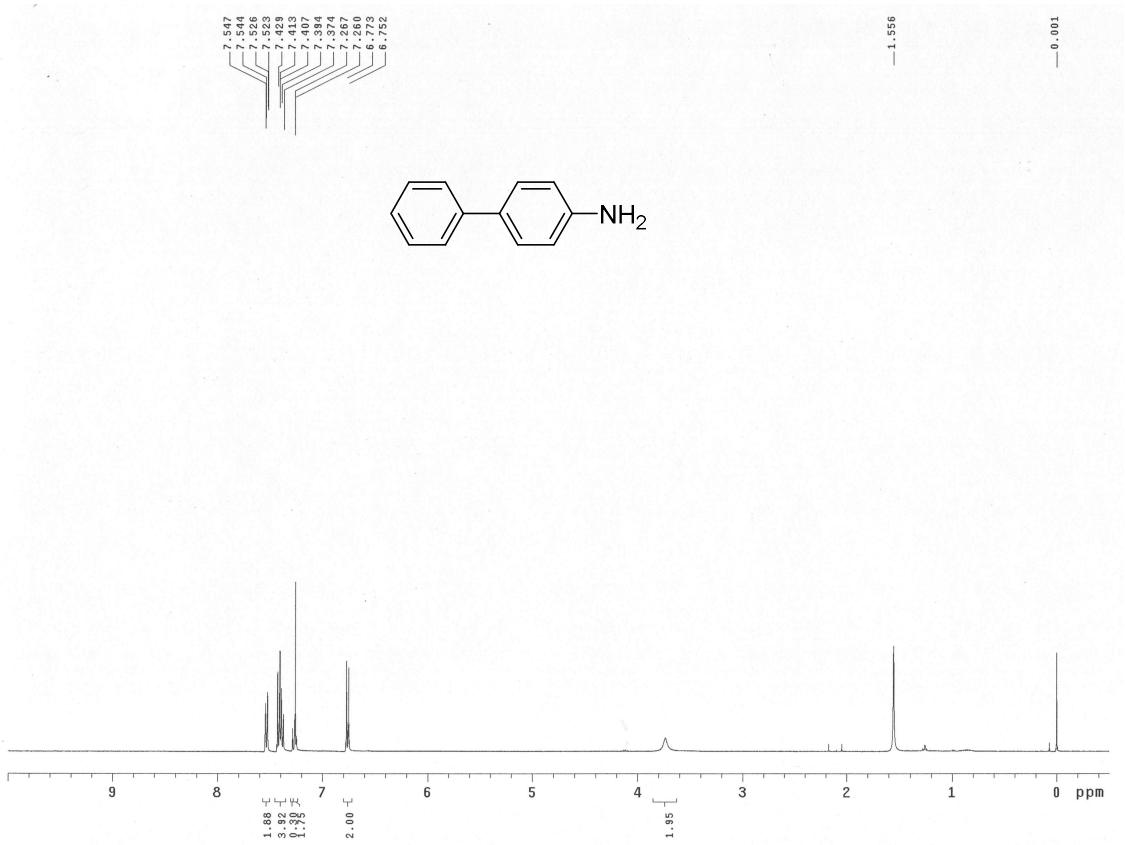
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **5na** (table 2, entry 20)



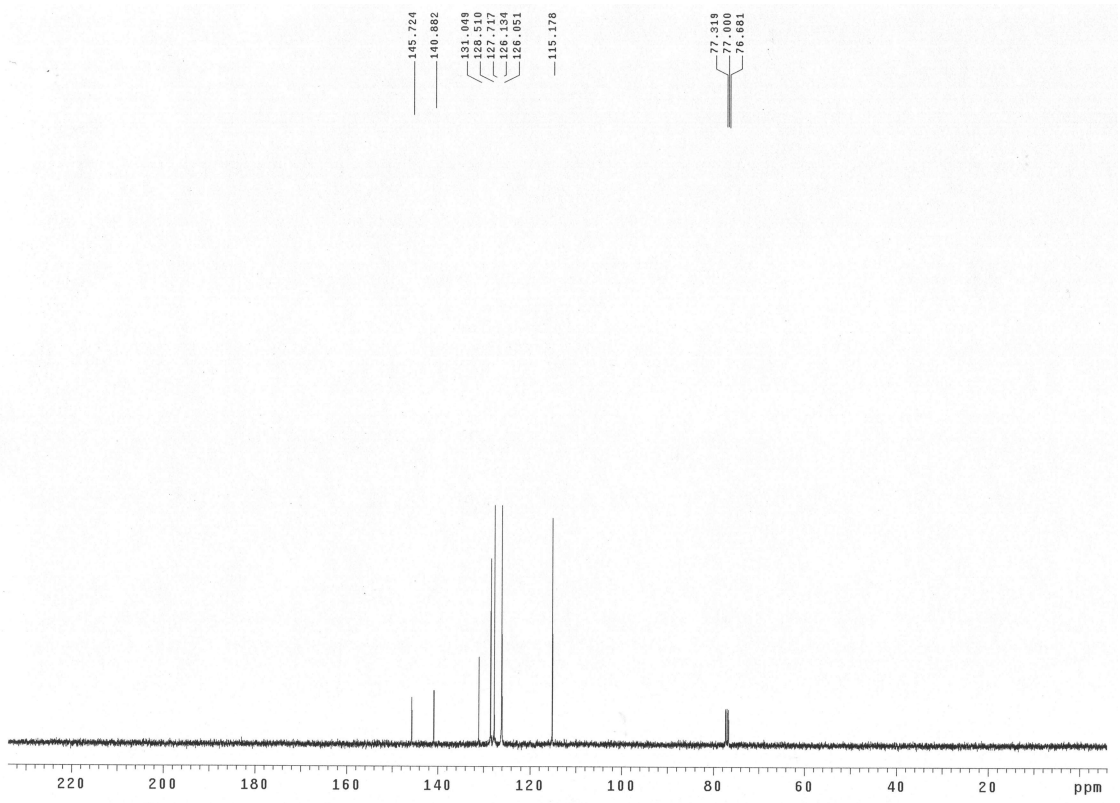
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **5na**



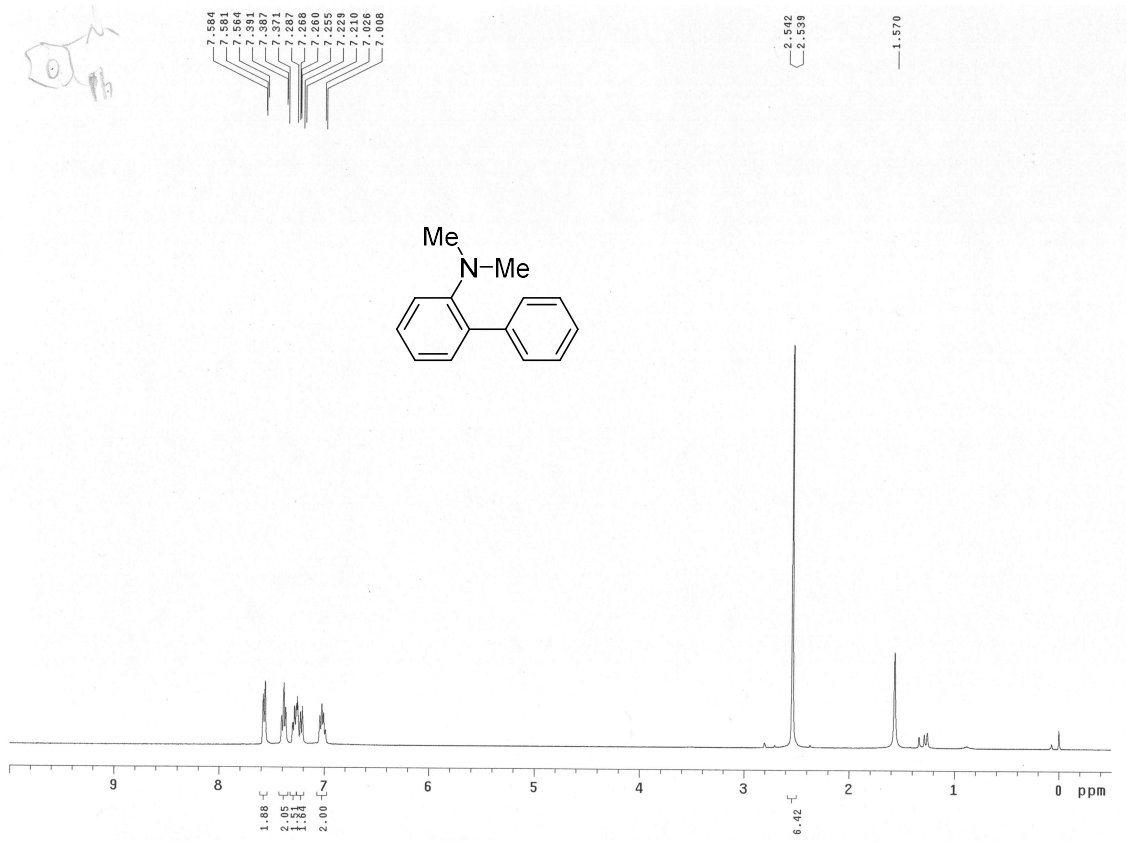
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **5oa** (table 2, entry 21)



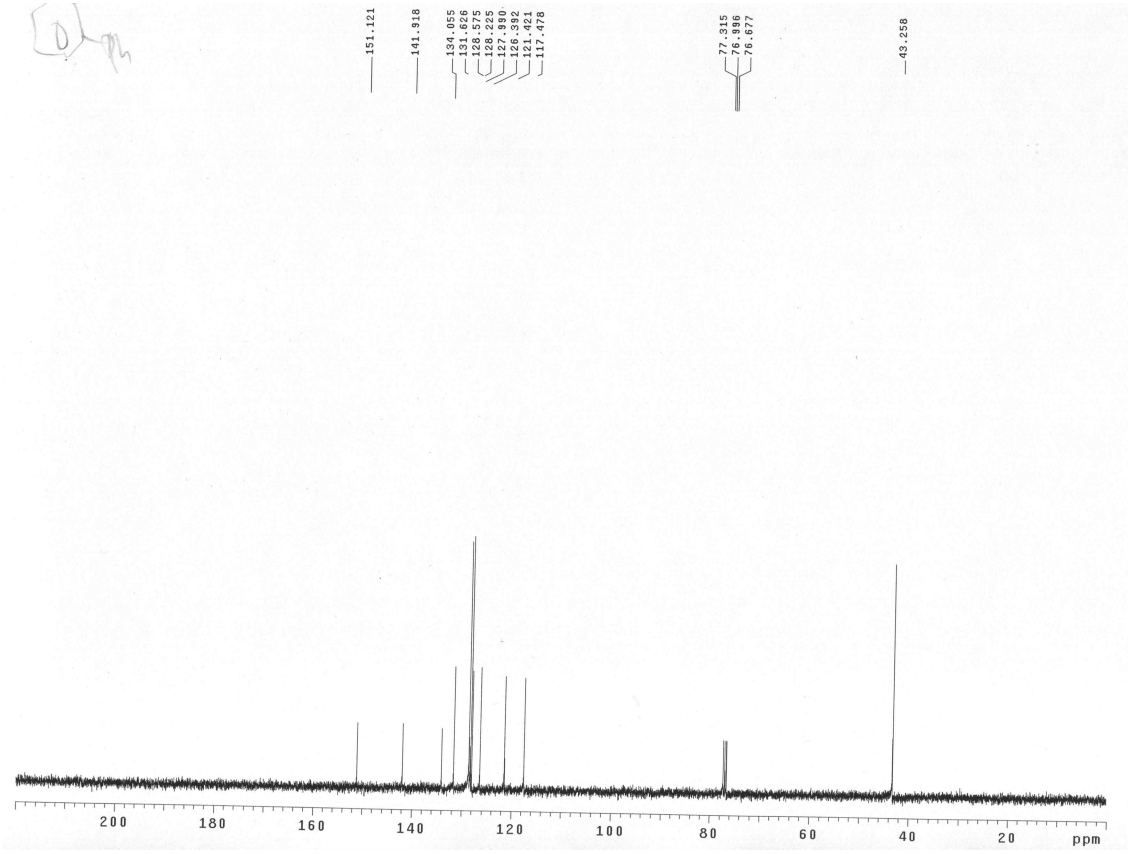
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **5oa**



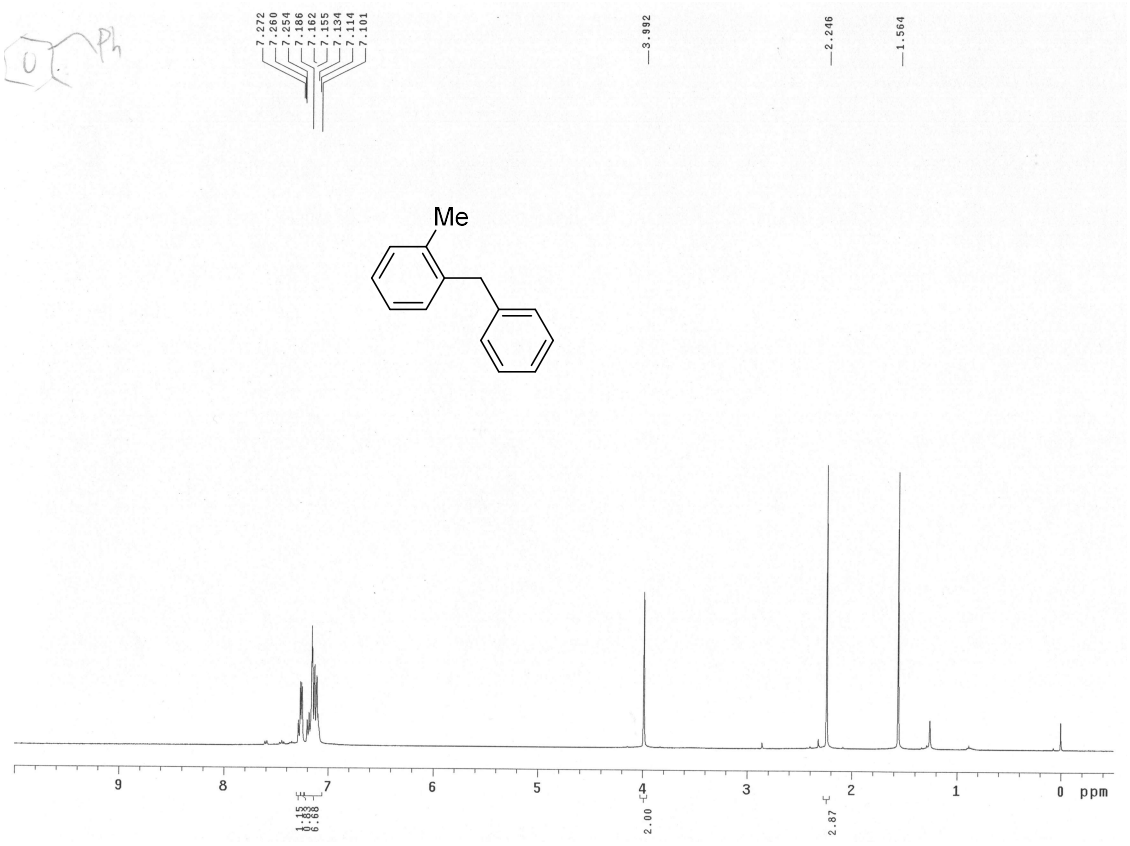
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **5pa** (table 2, entry 22)



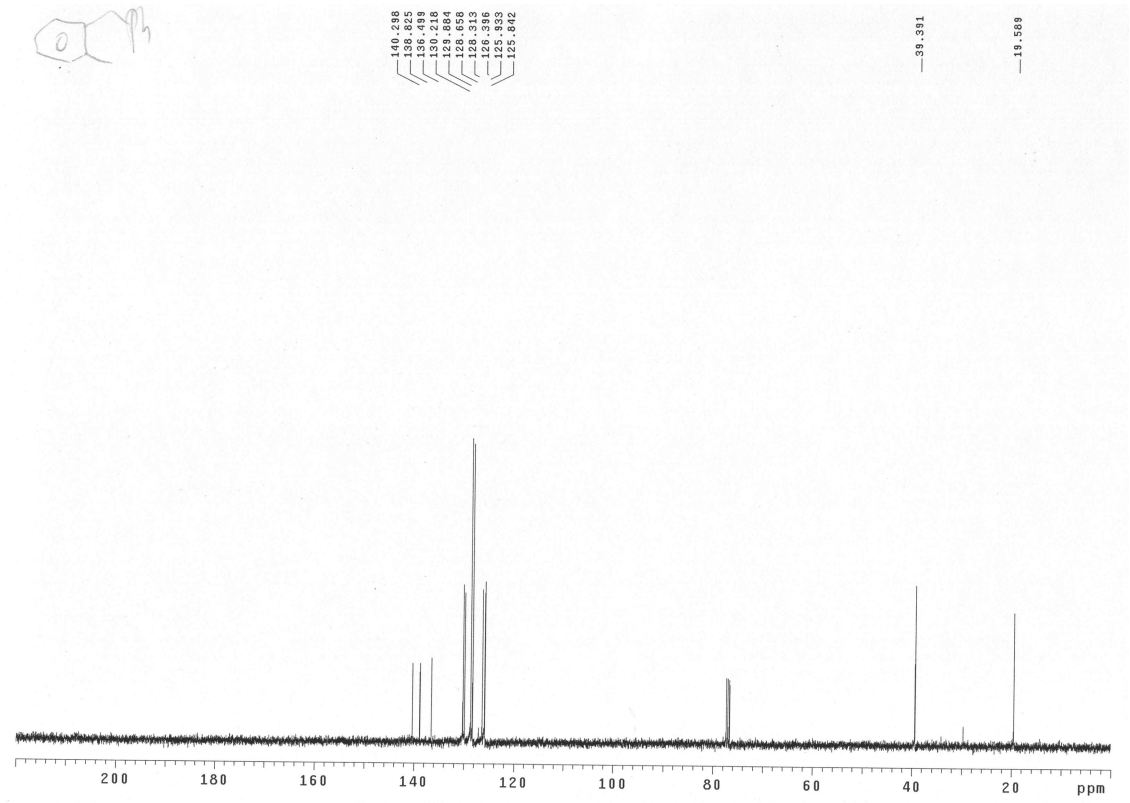
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **5pa**



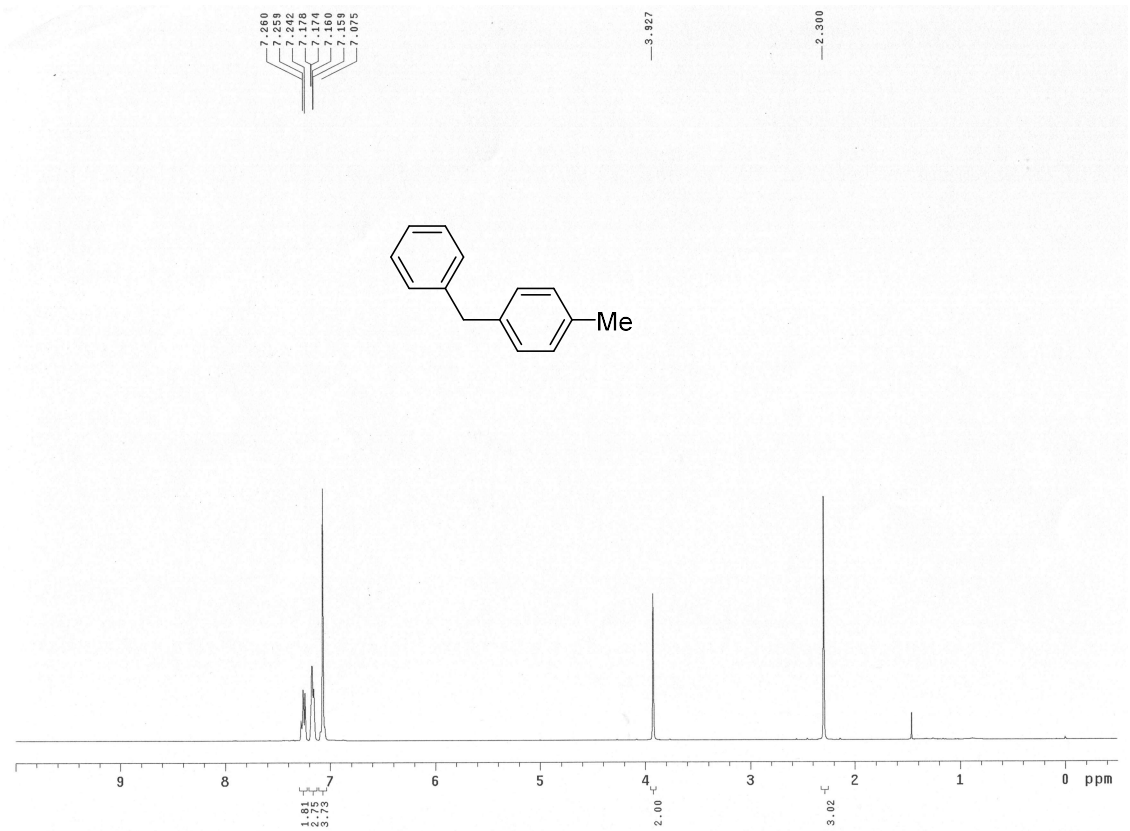
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **5qa** (table 2, entry 23)



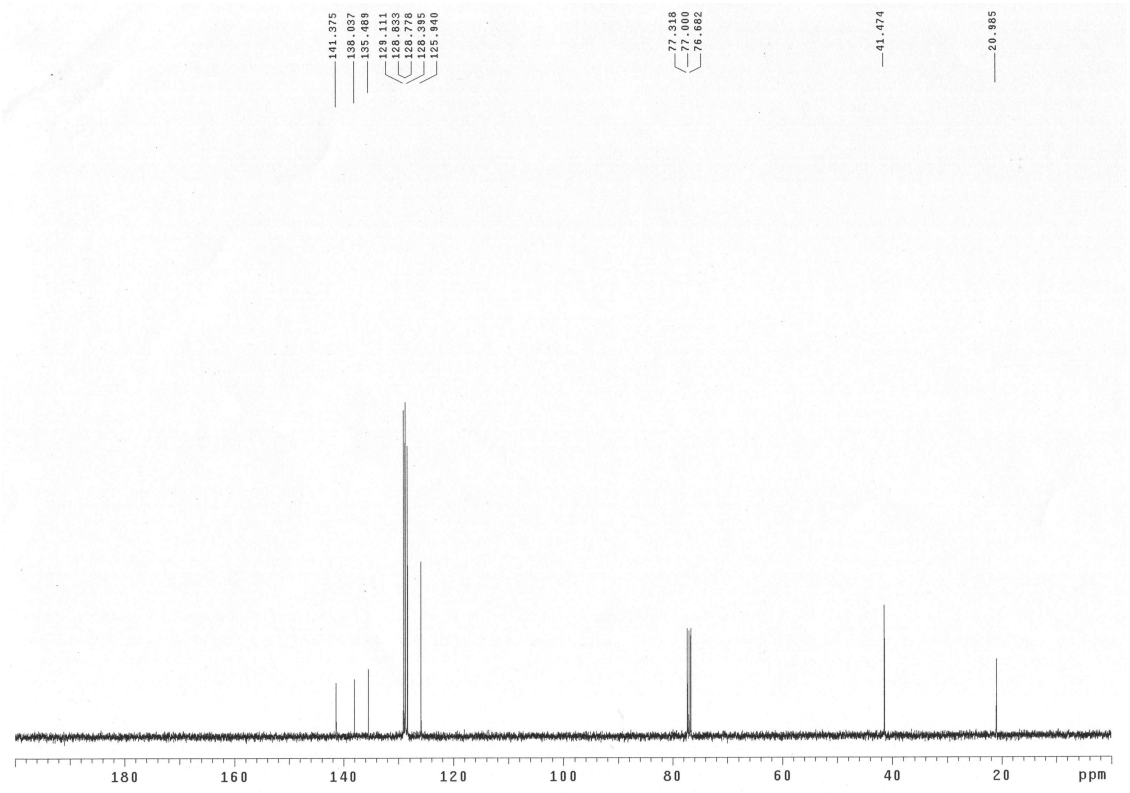
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **5qa**



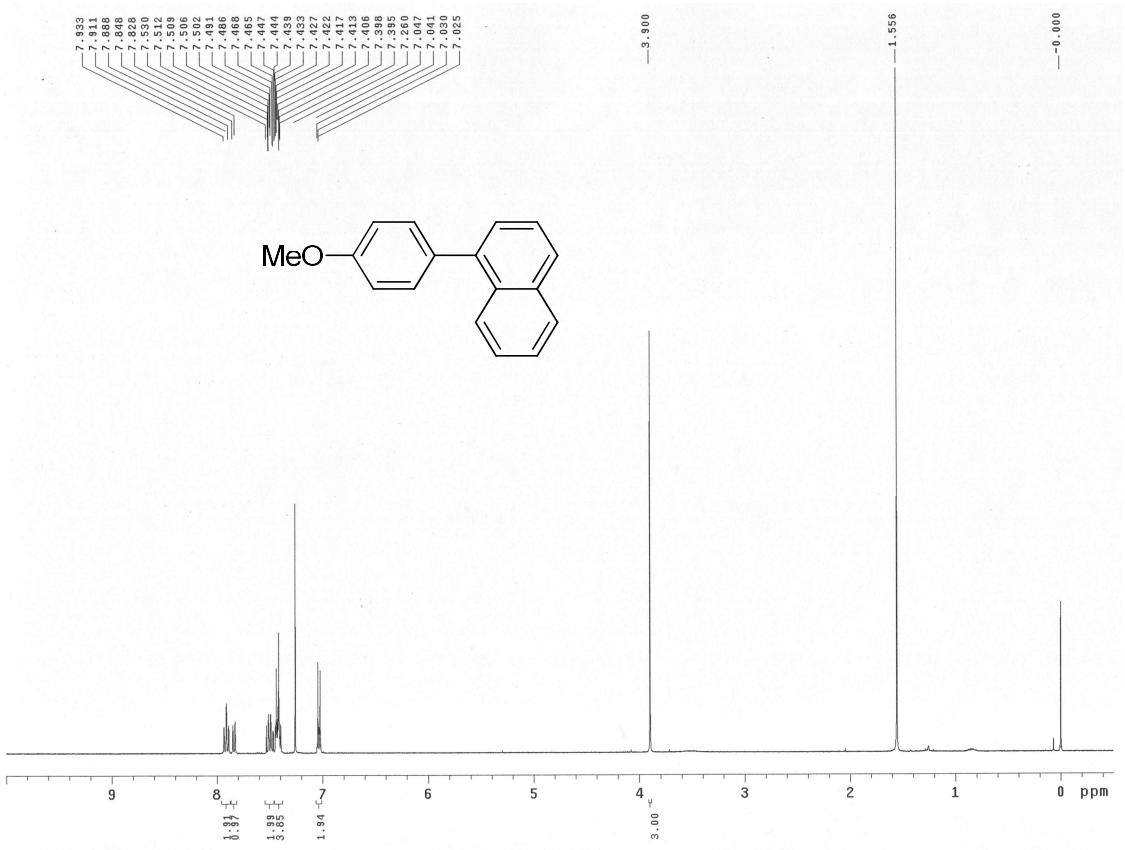
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **5ra** (table 2, entry 24)



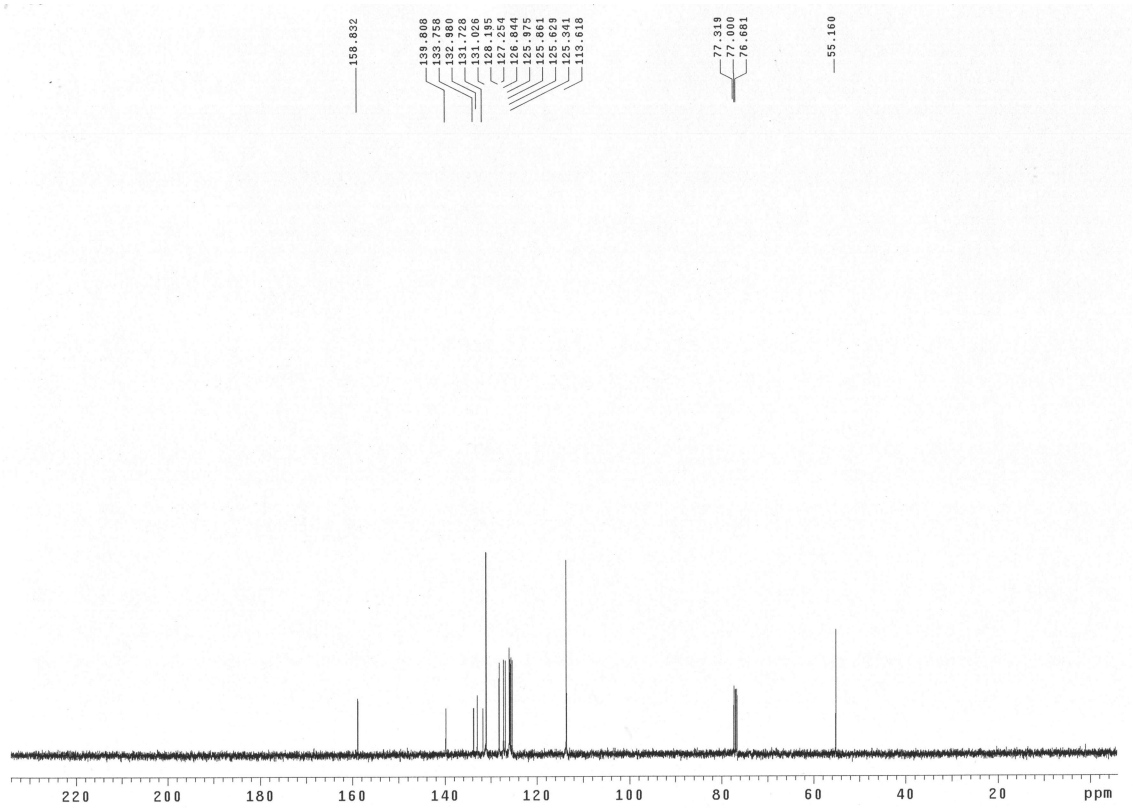
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **5ra**



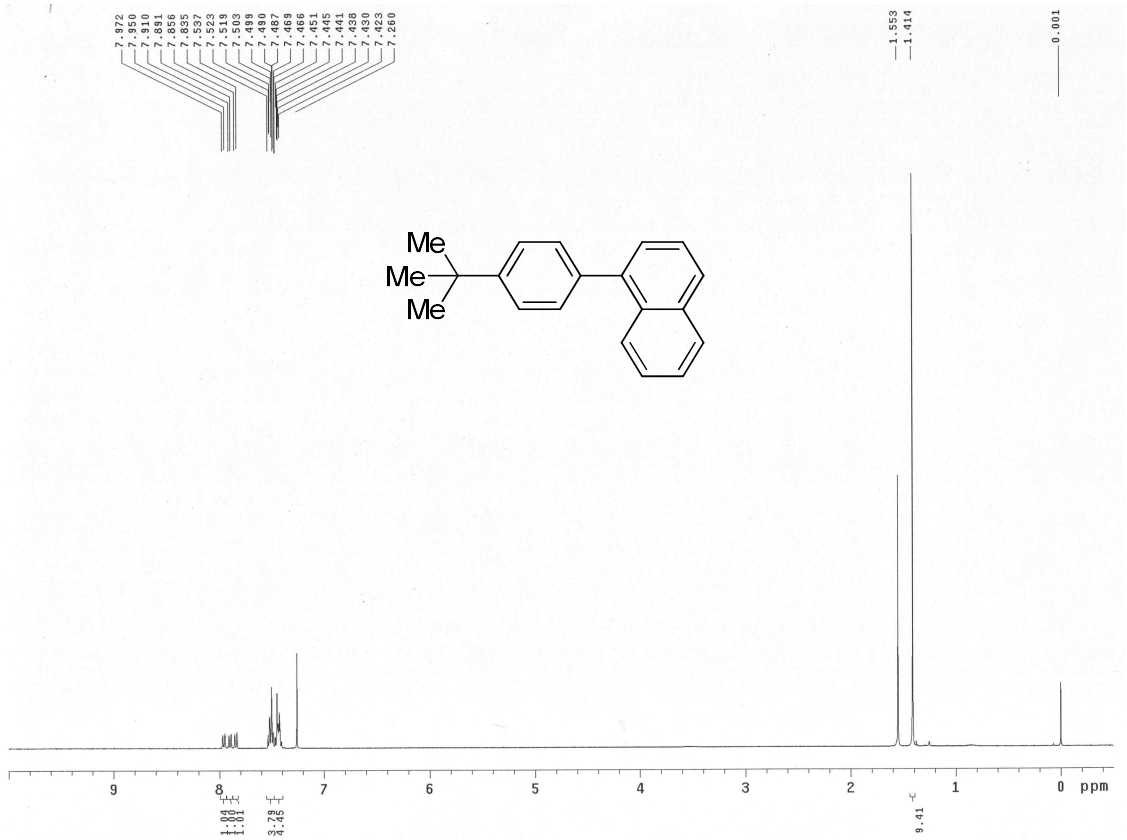
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **5ab** (table 2, entry 25)



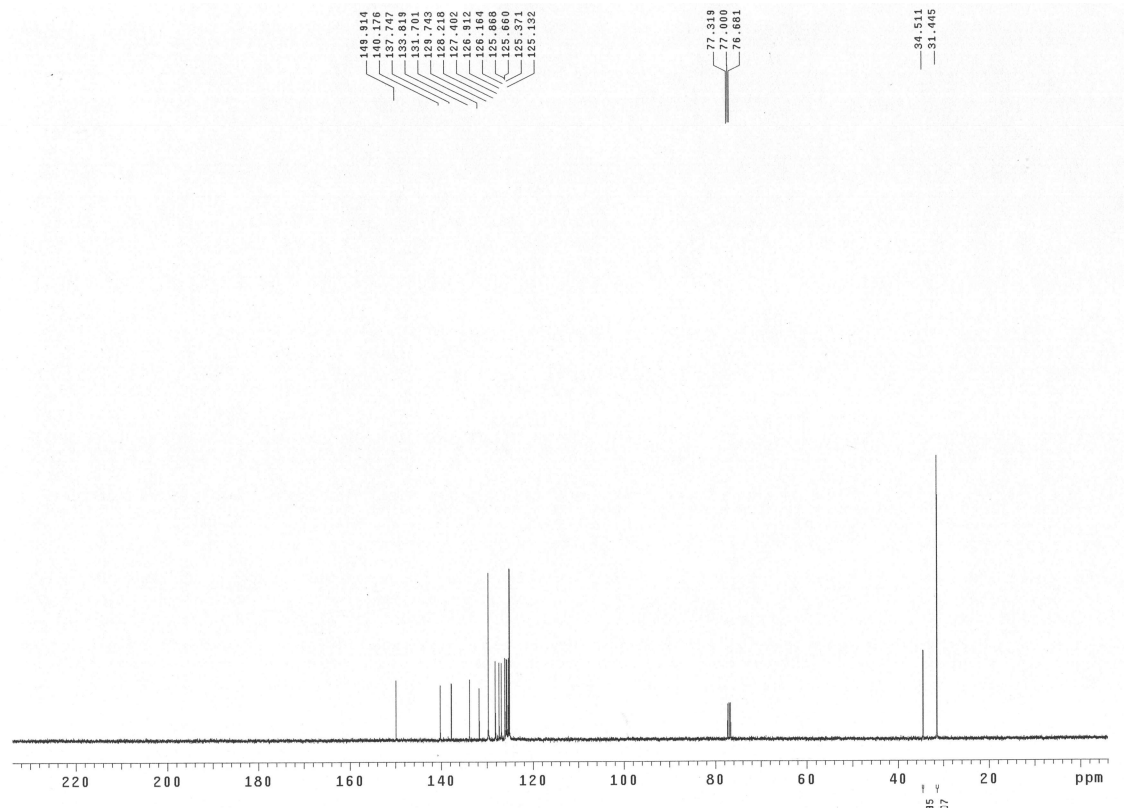
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **5ab**



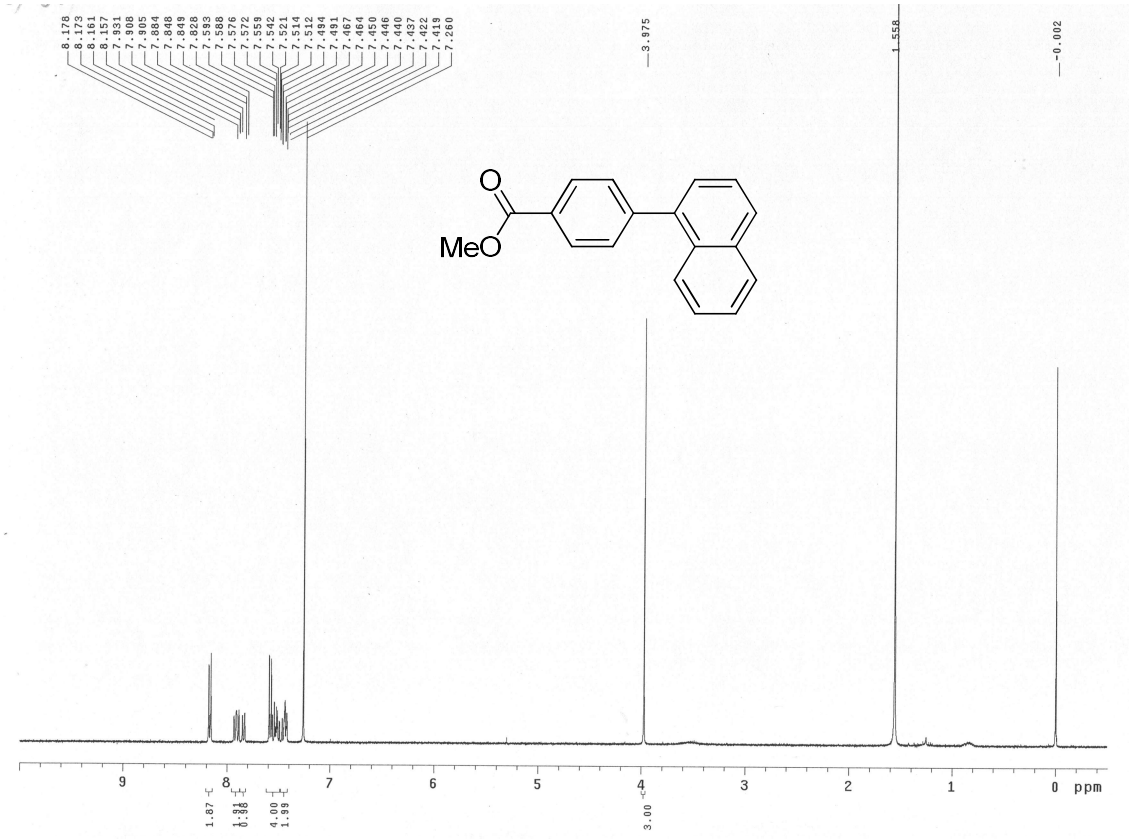
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **5bb** (table 2, entry 26)



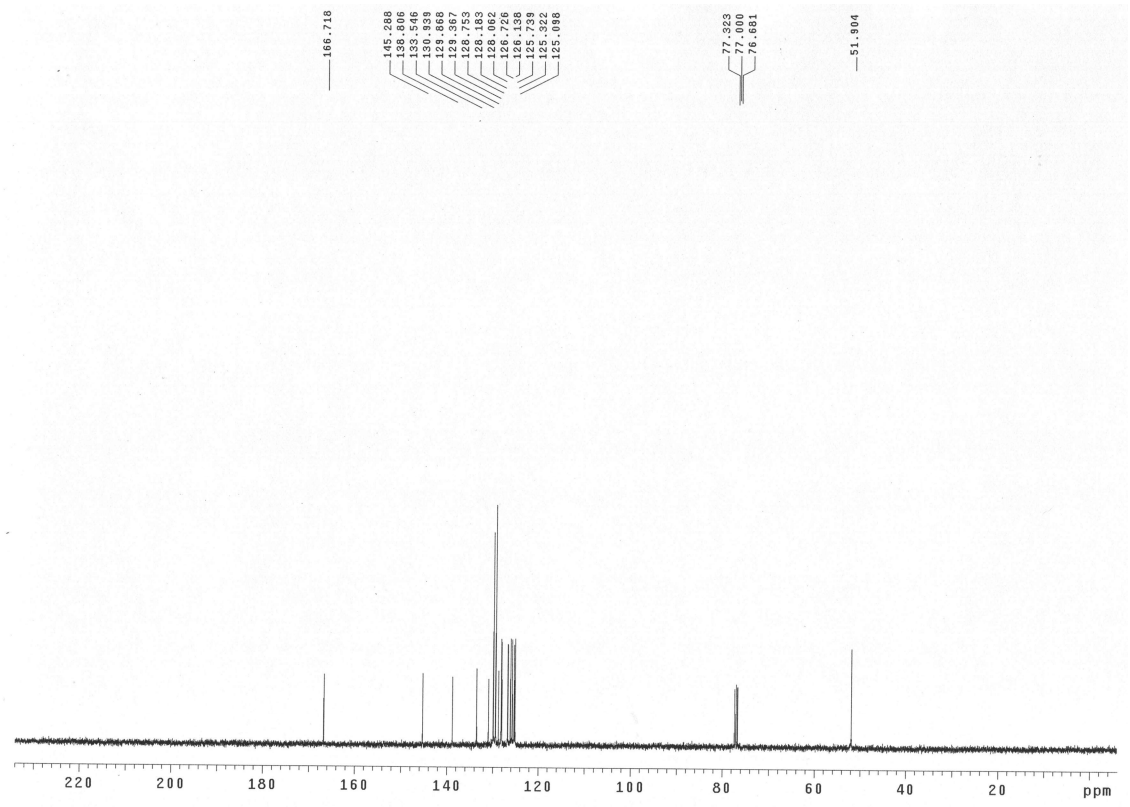
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **5bb**



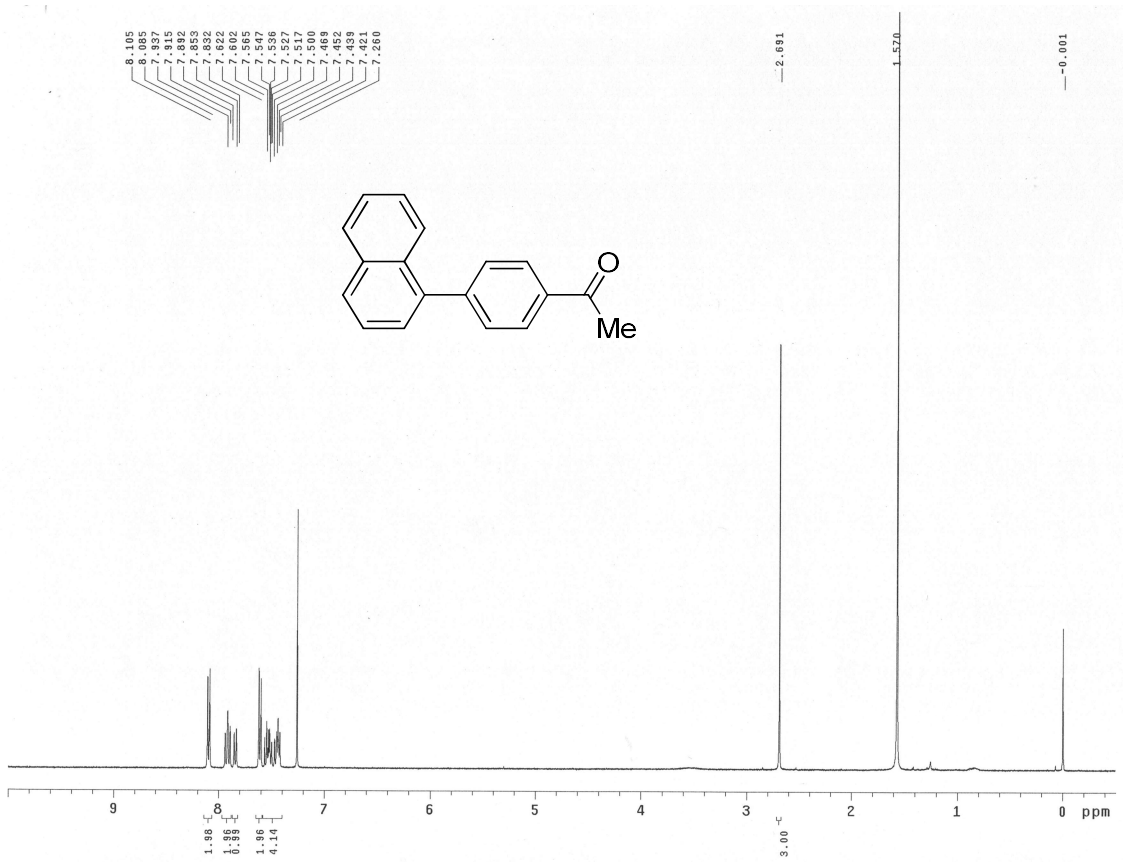
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **5cb** (table 2, entry 27)



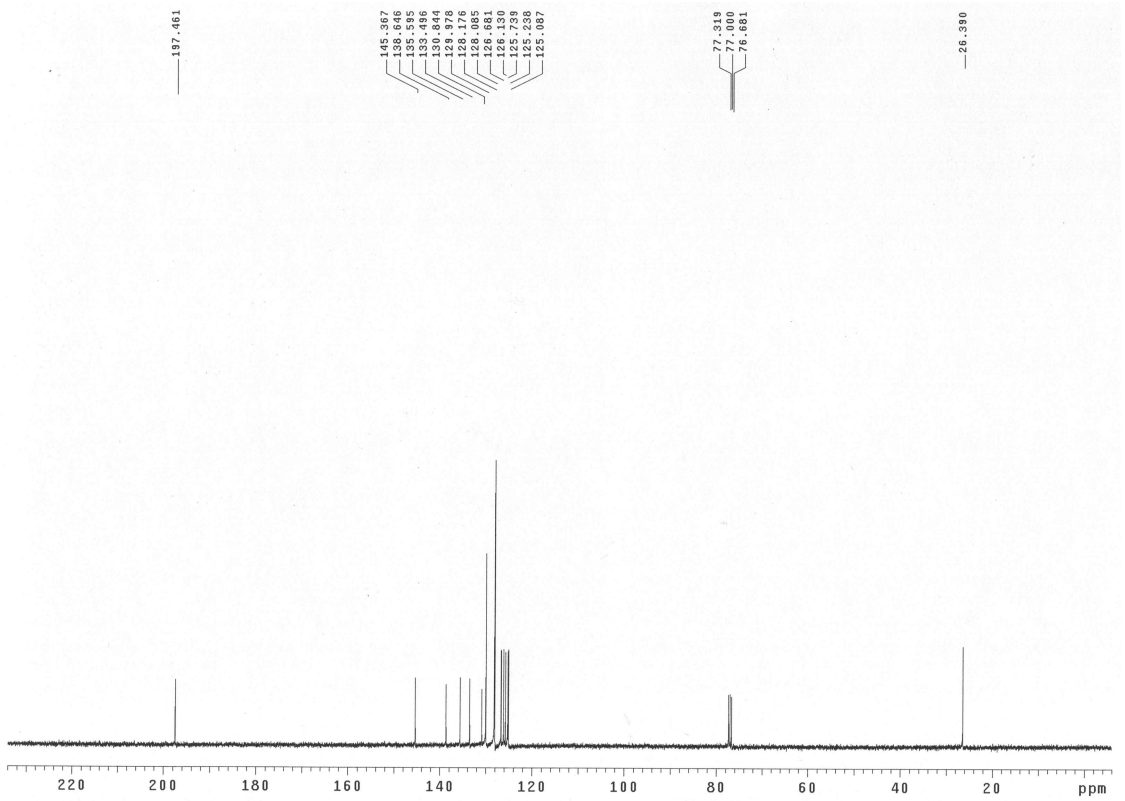
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **5cb**



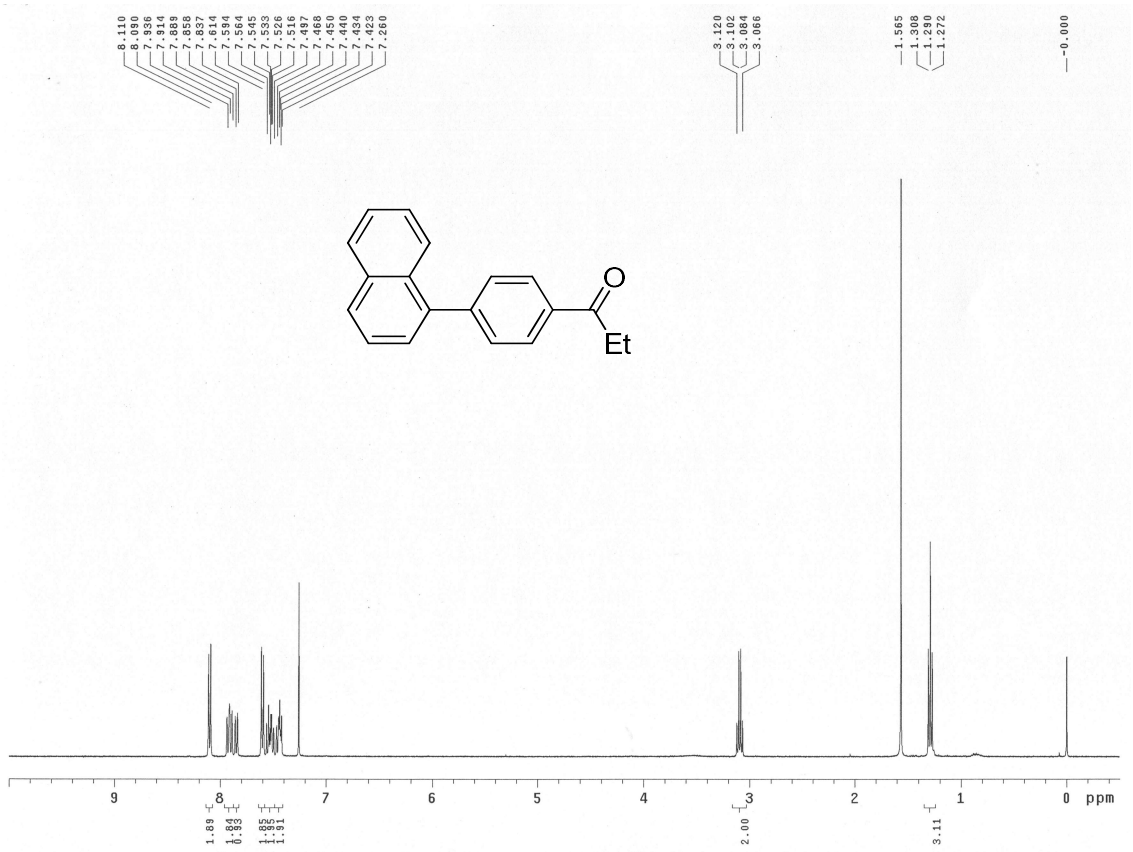
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **5db** (table 2, entry 28)



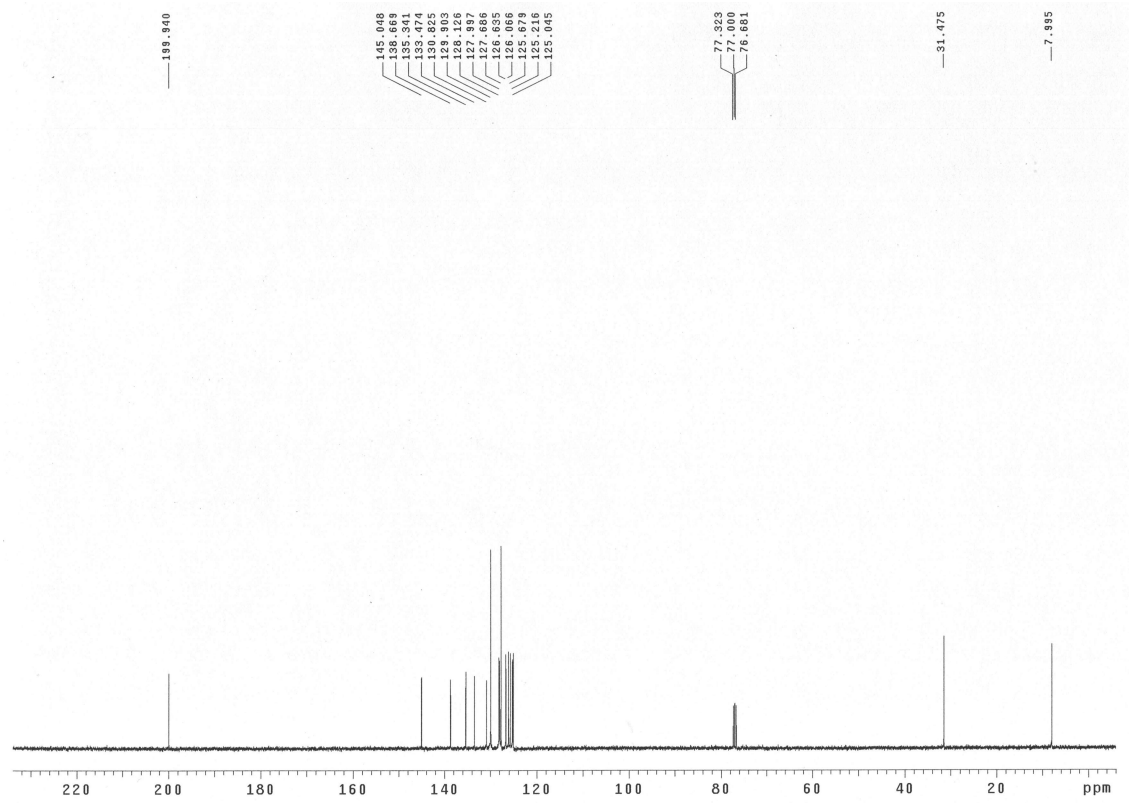
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **5db**



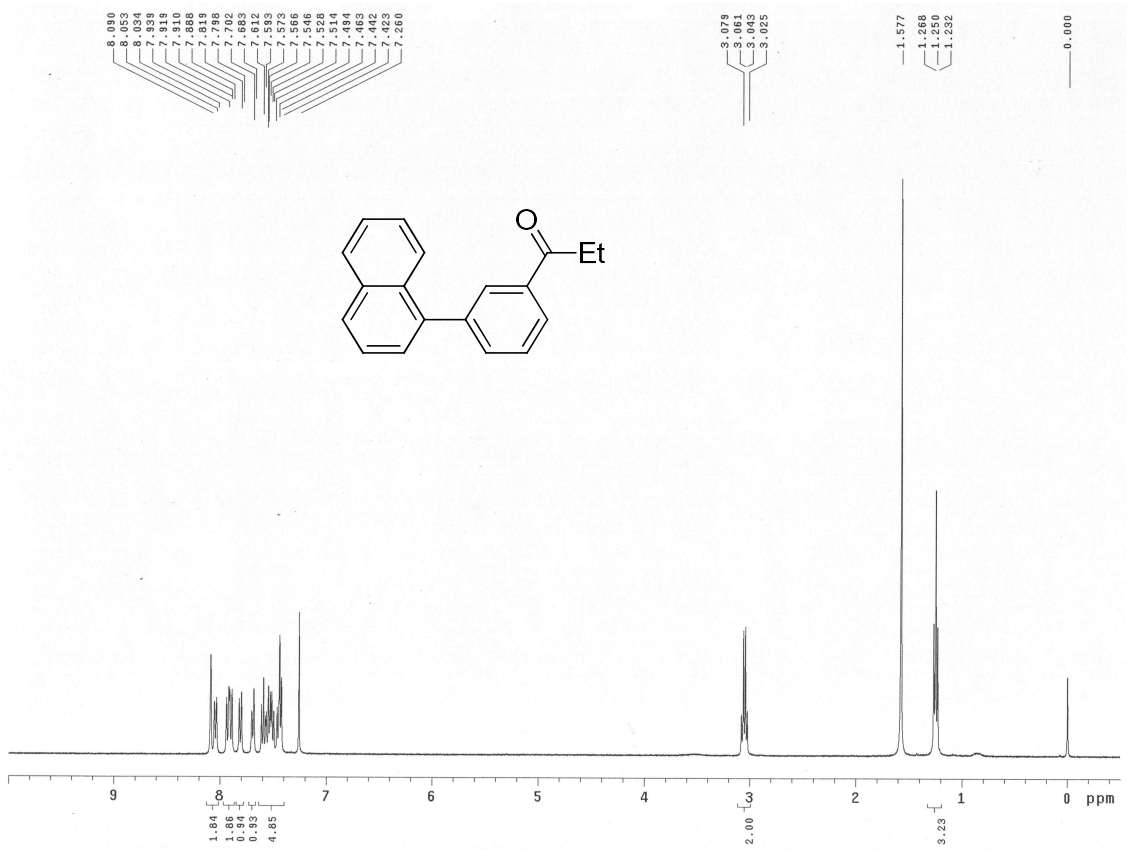
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **5eb** (table 2, entry 29)



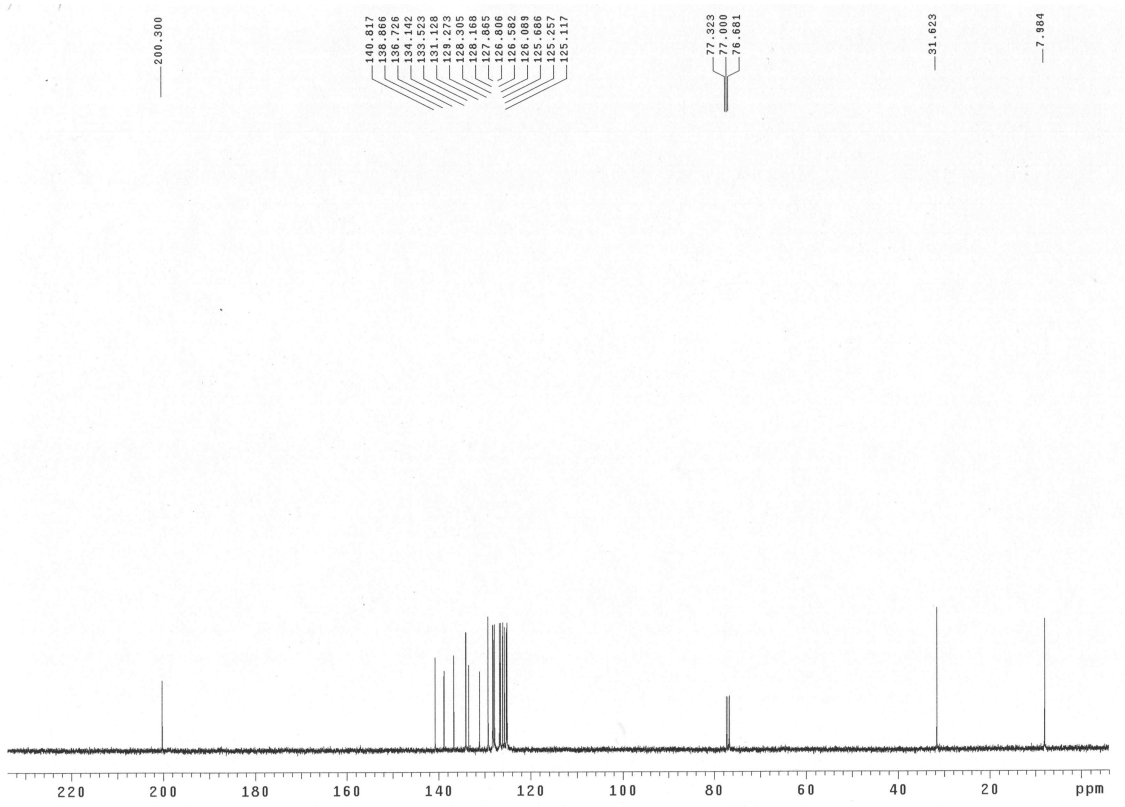
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **5eb**



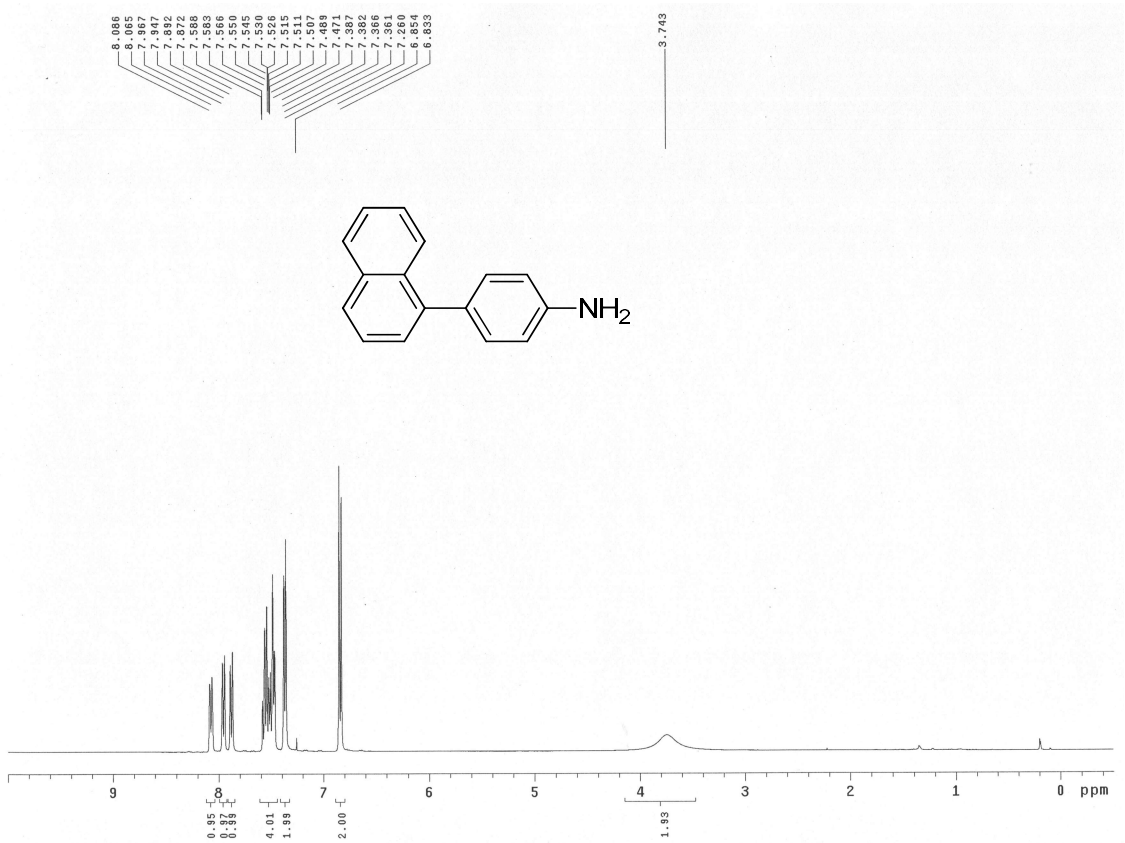
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **5fb** (table 2, entry 30)



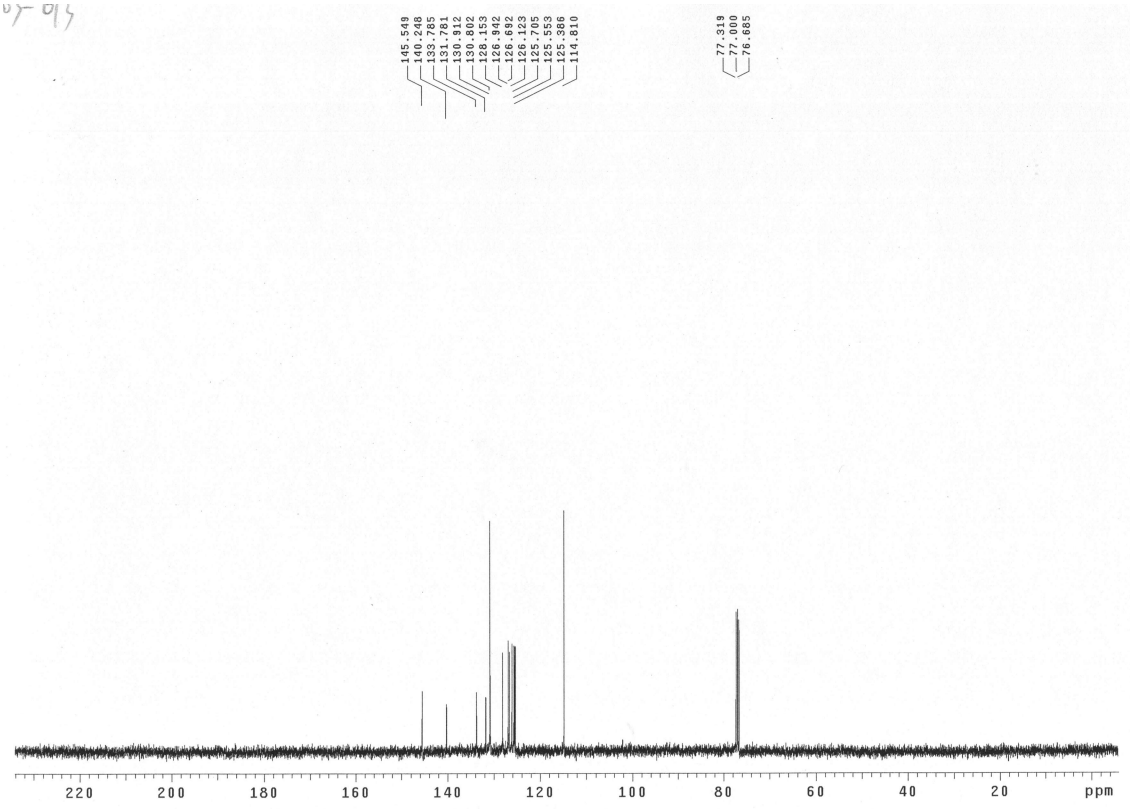
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **5fb**



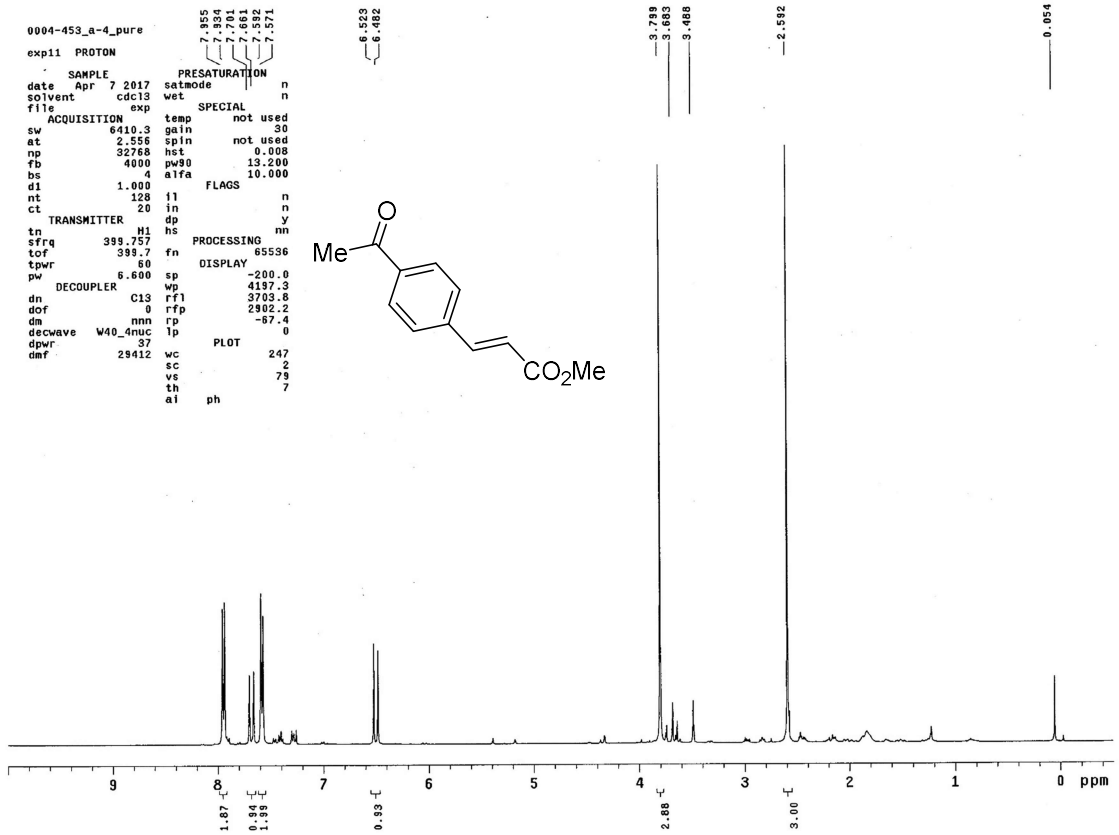
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **5ob** (table 2, entry 31)



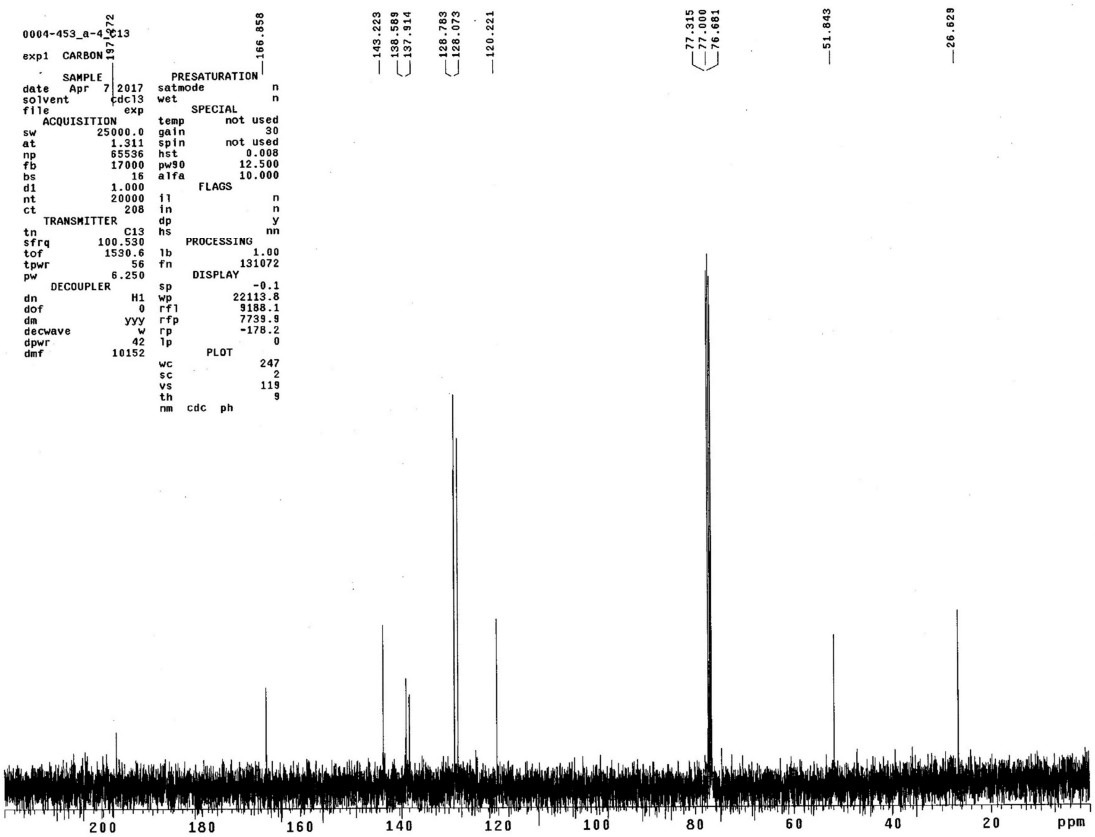
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **5ob**



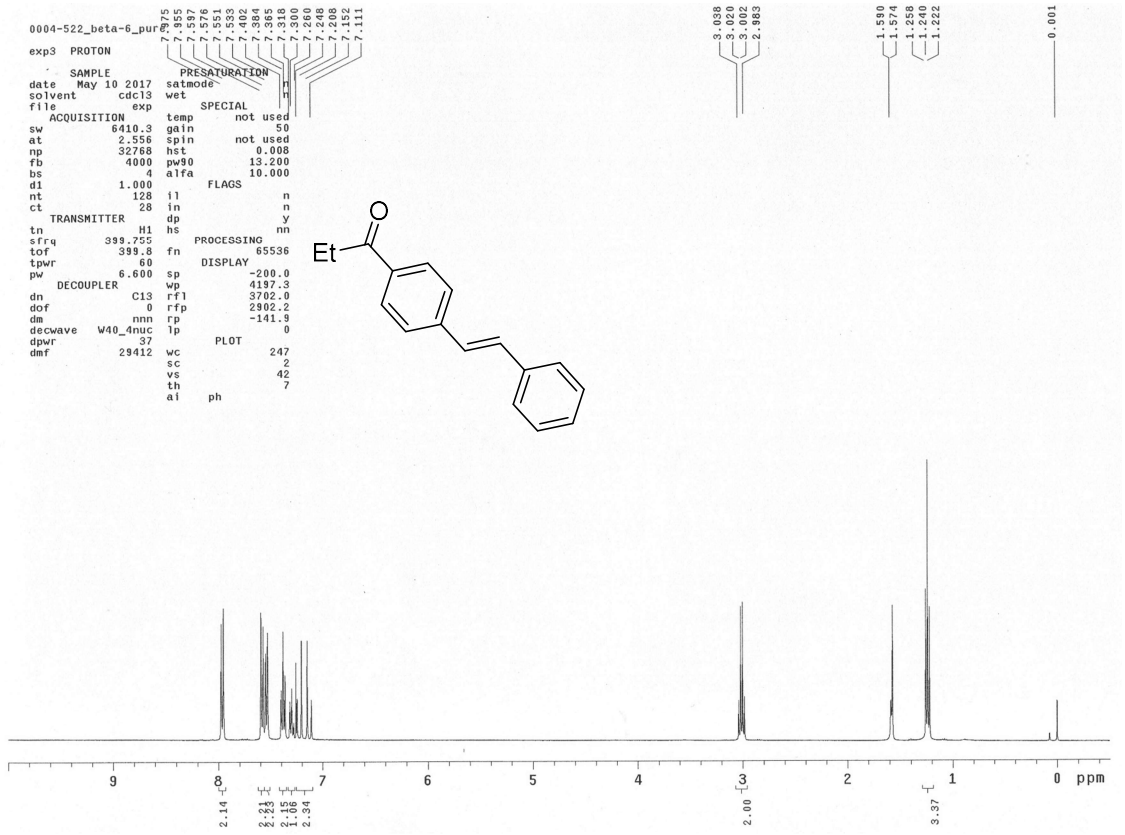
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **7da** (table 4, entry 1)



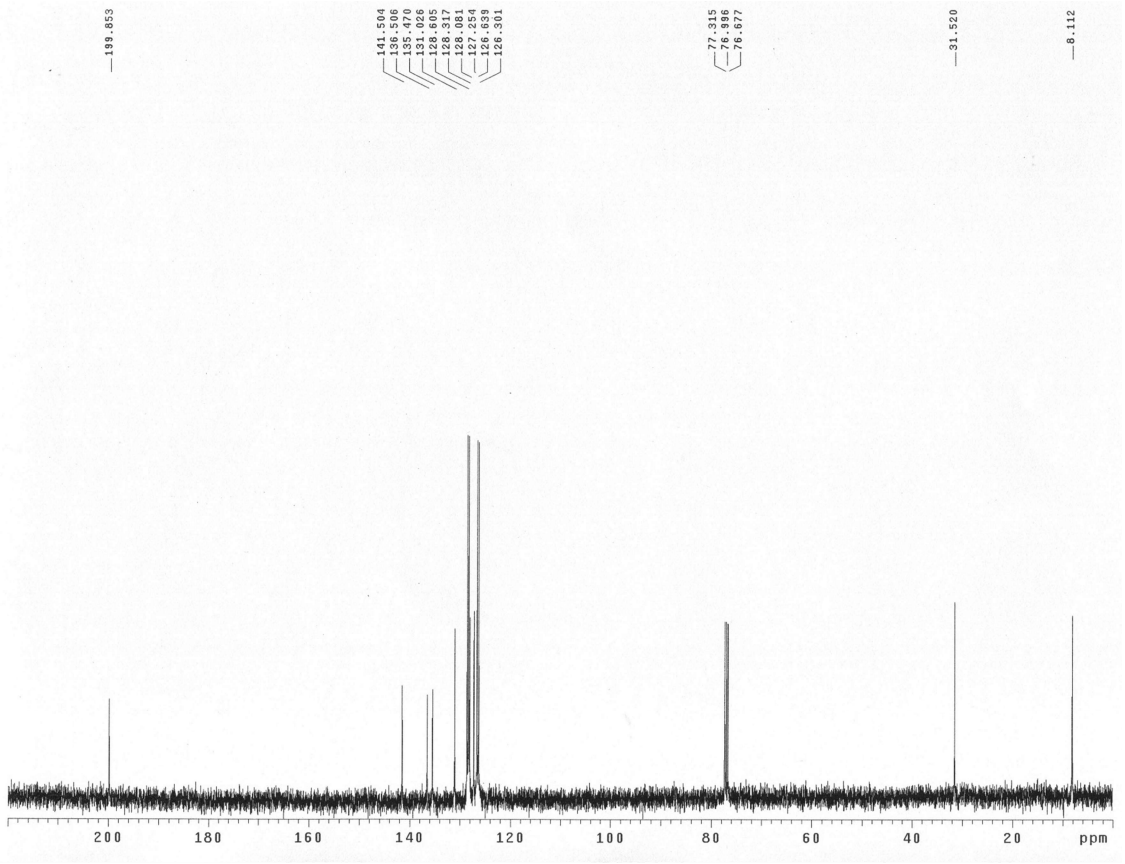
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **7da**



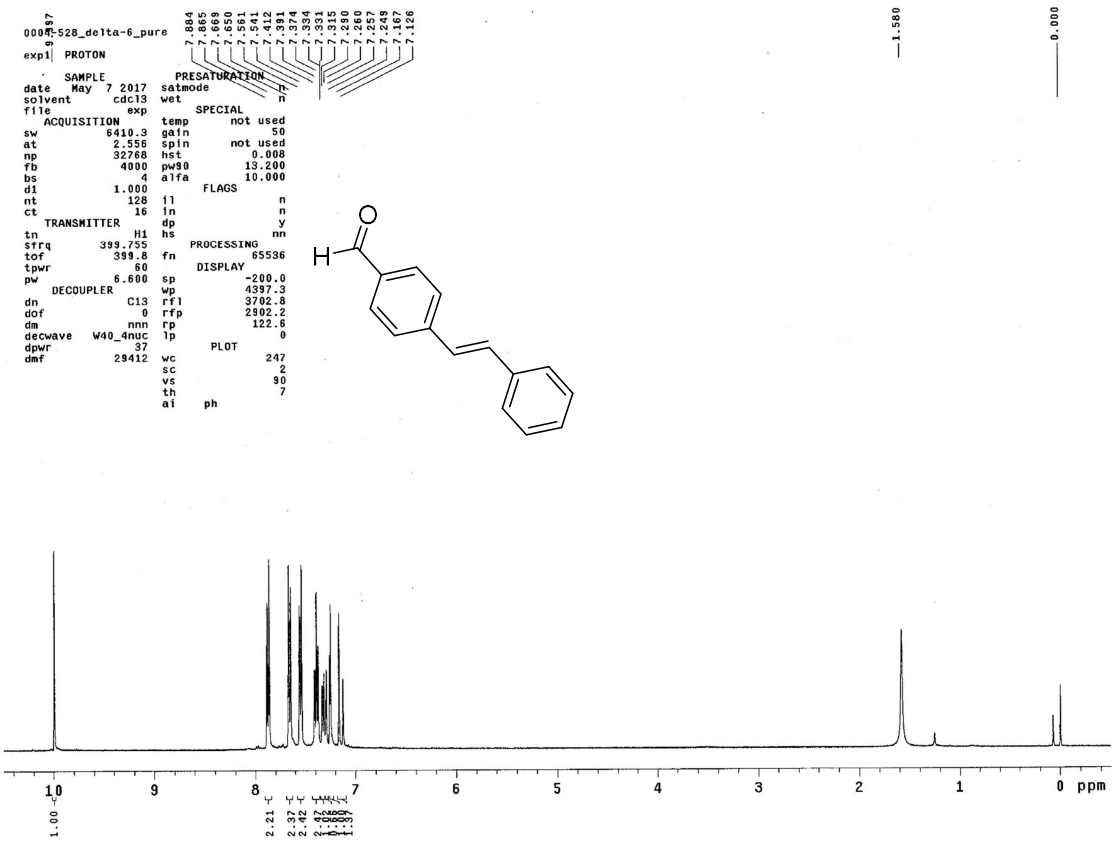
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **7eb** (table 4, entry 2)



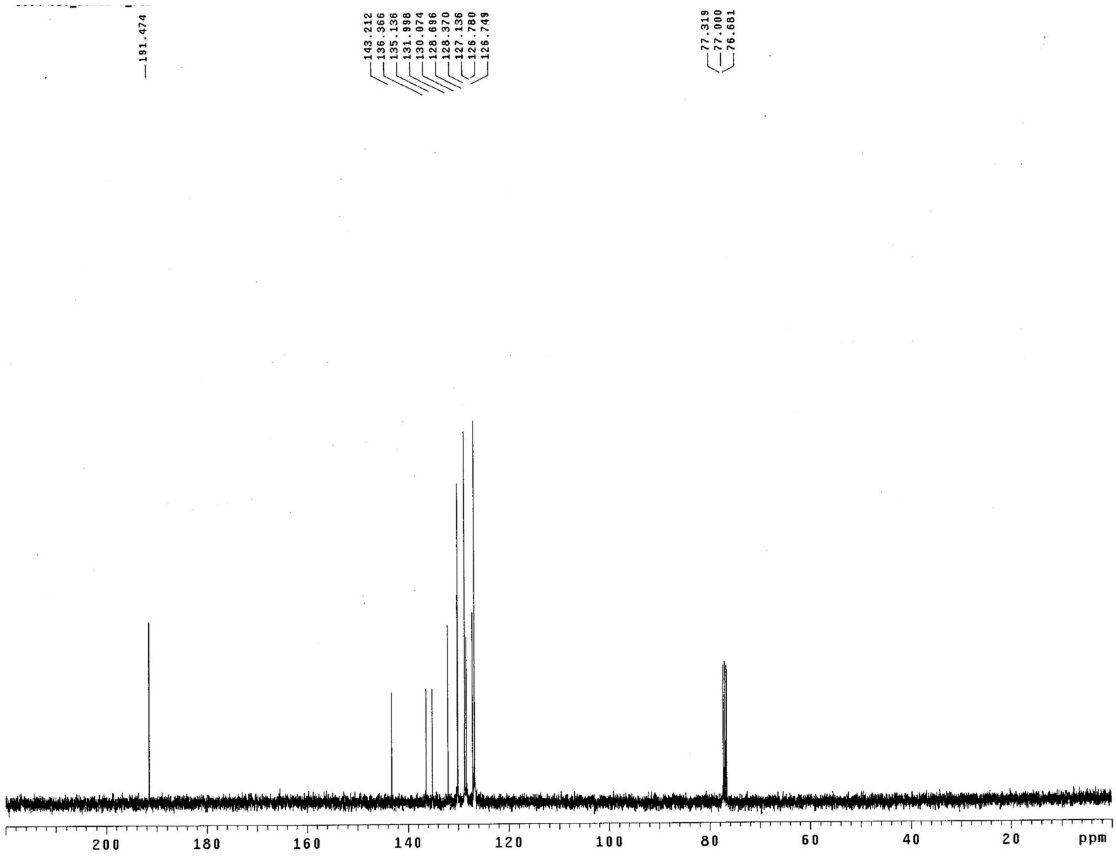
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **7eb**



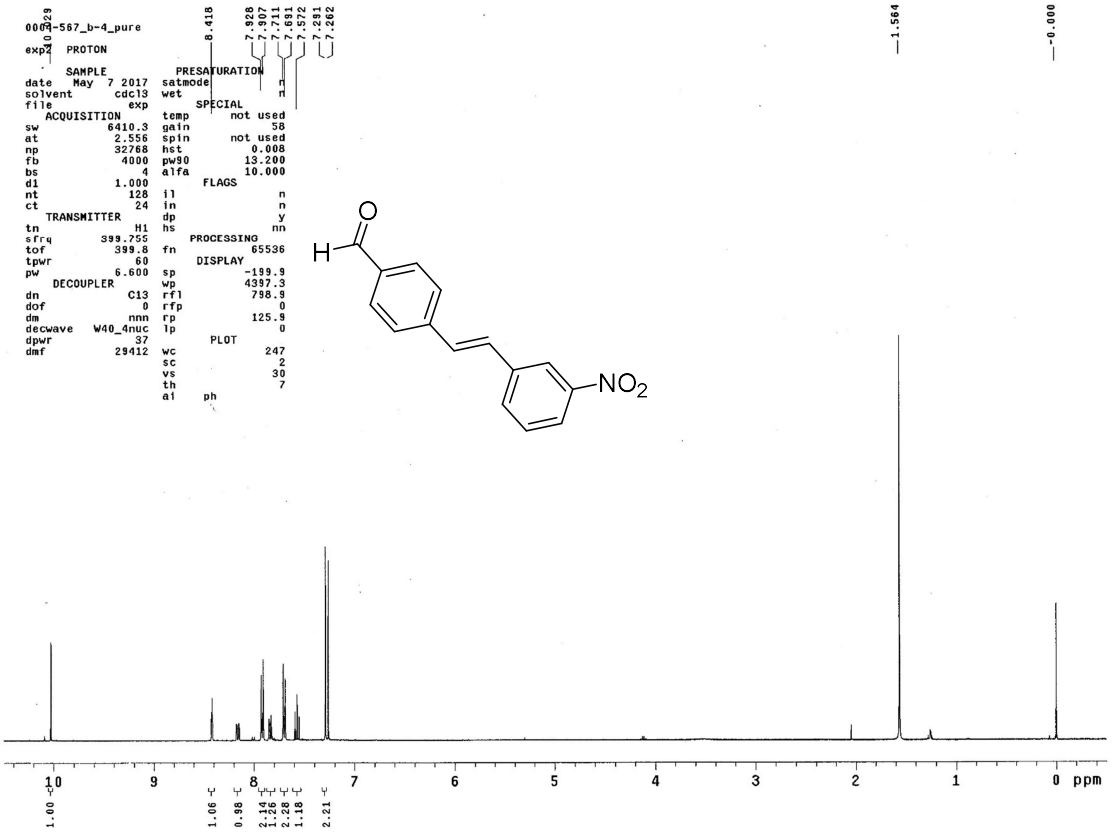
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **7gb** (table 4, entry 3)



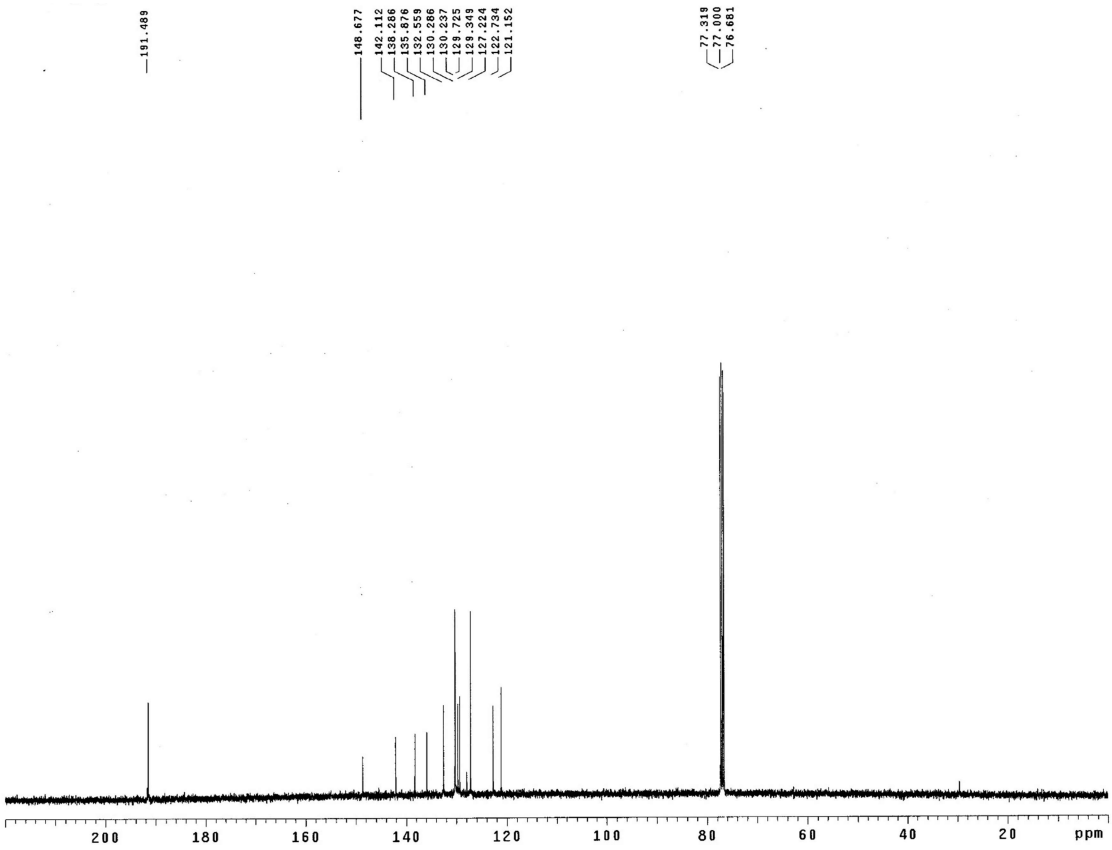
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **7gb**



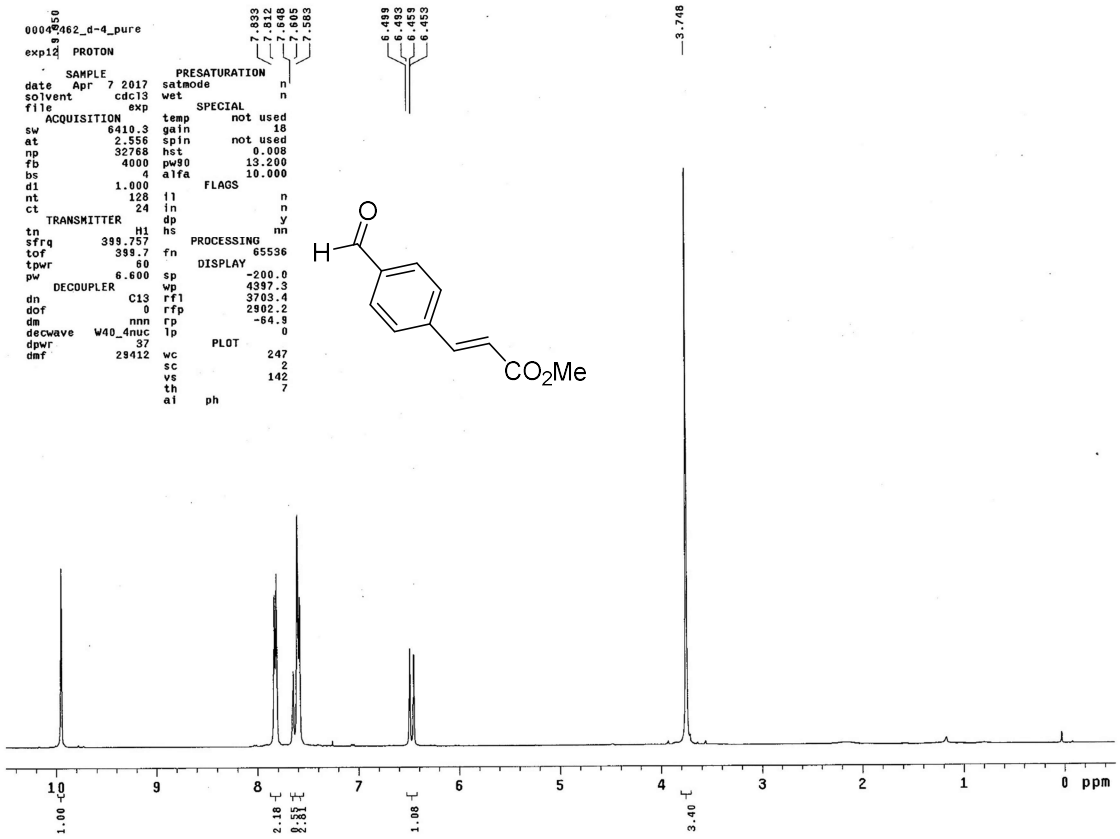
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **7ge** (table 4, entry 4)



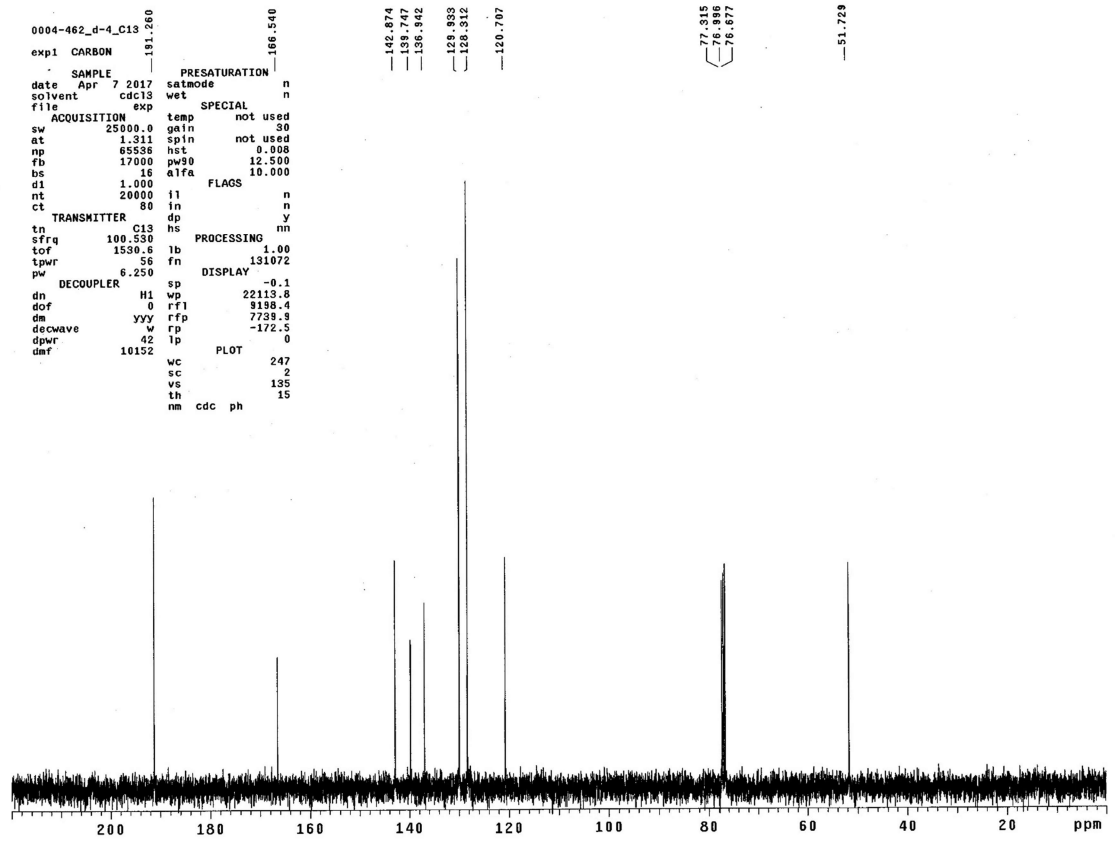
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **7ge**



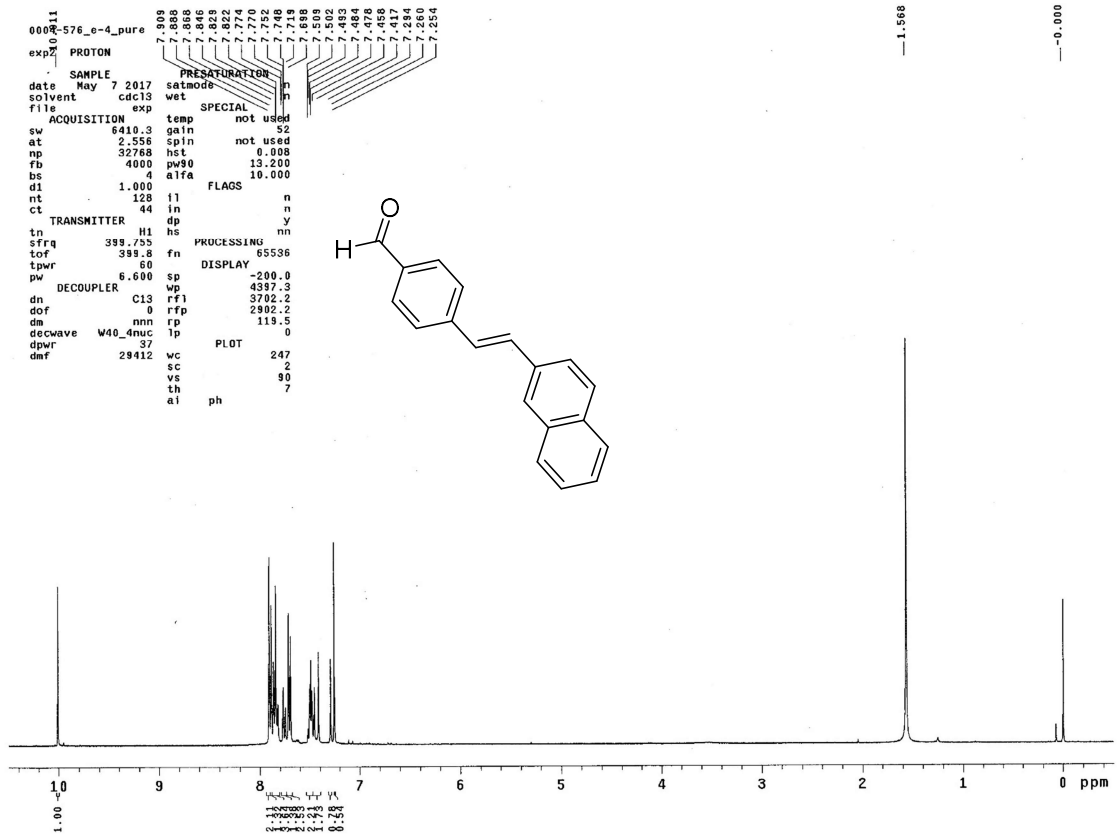
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **7ga** (table 4, entry 5)



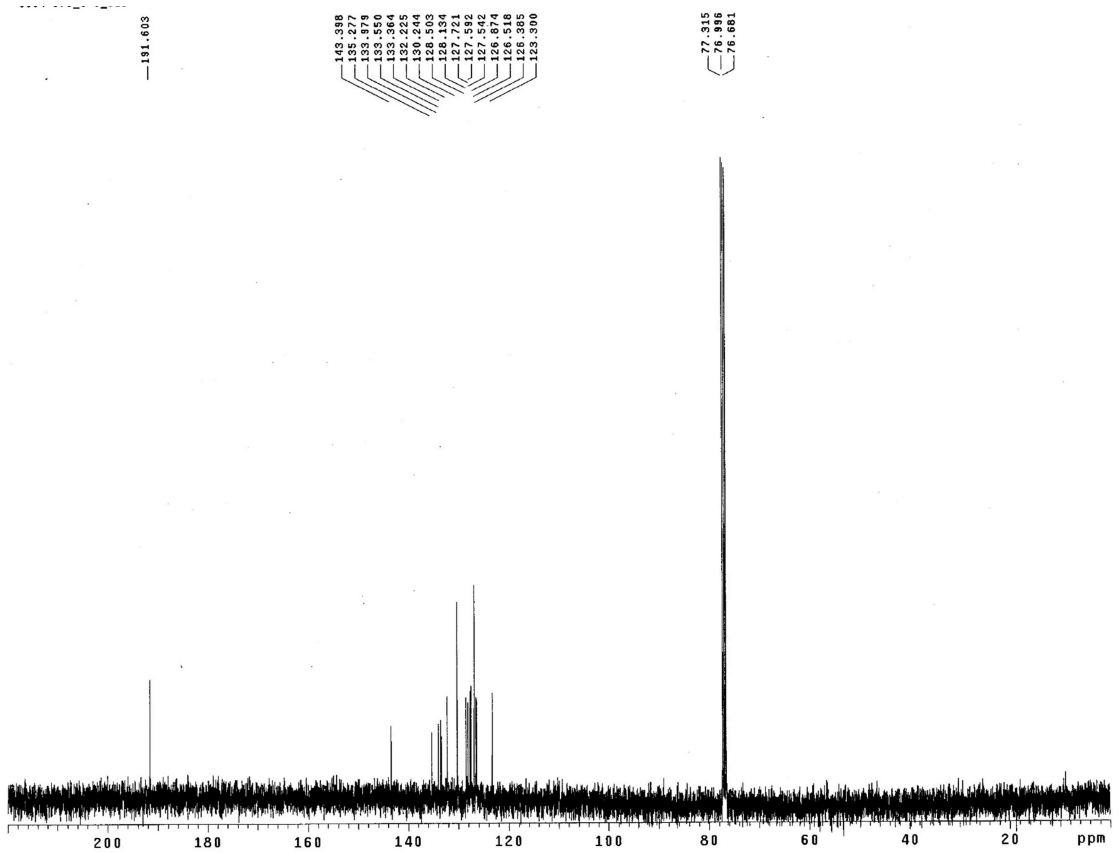
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **7ga**



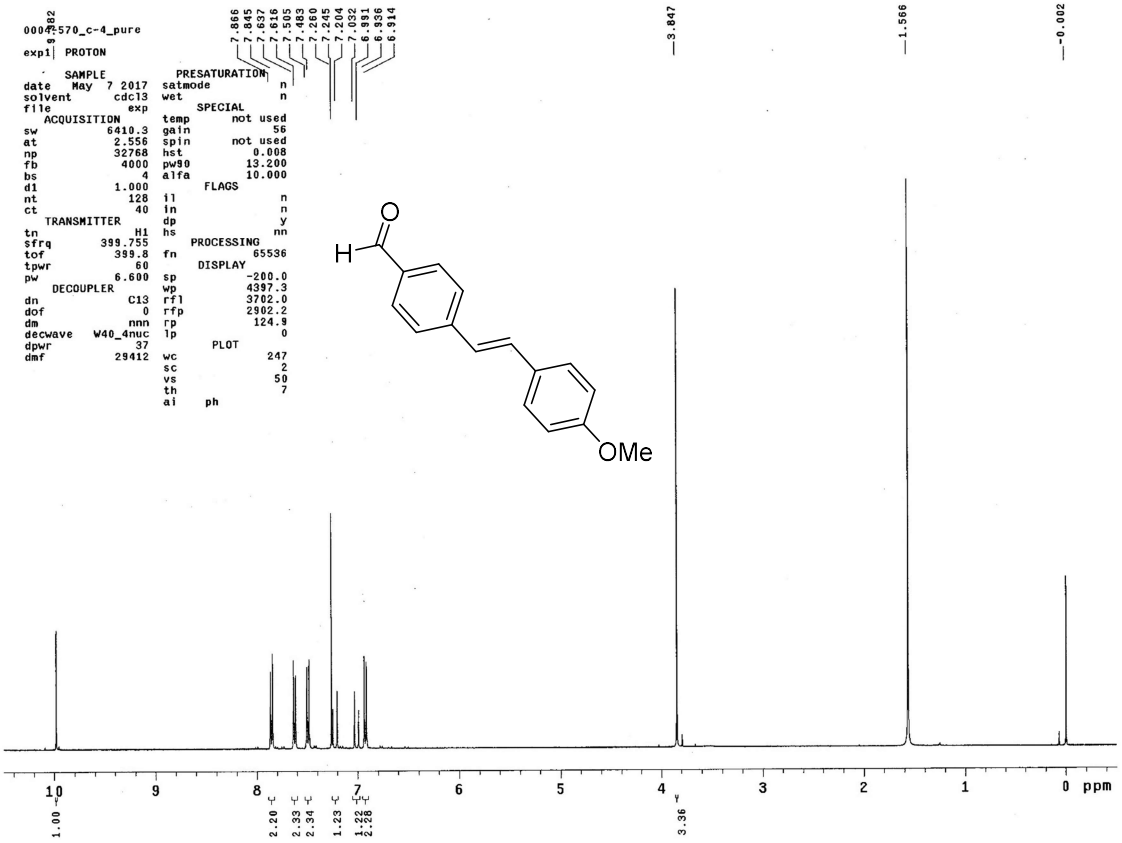
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **7gd** (table 4, entry 6)



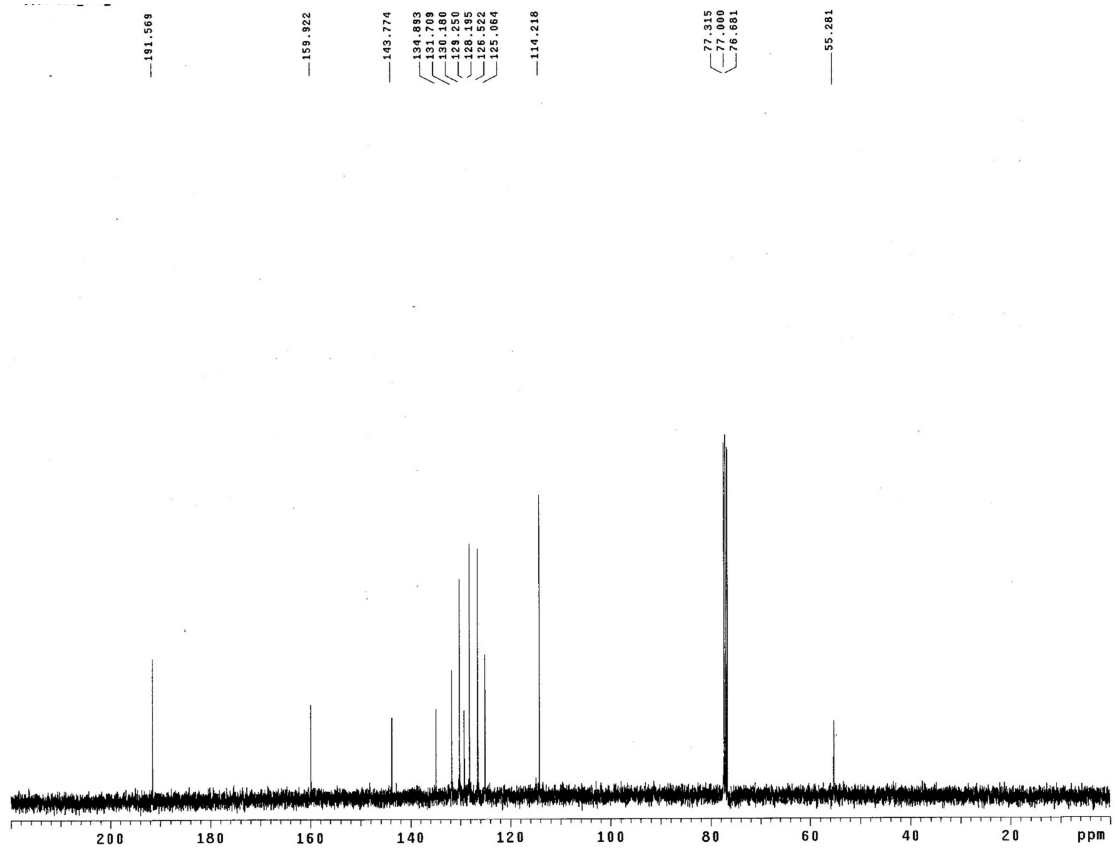
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **7gd**



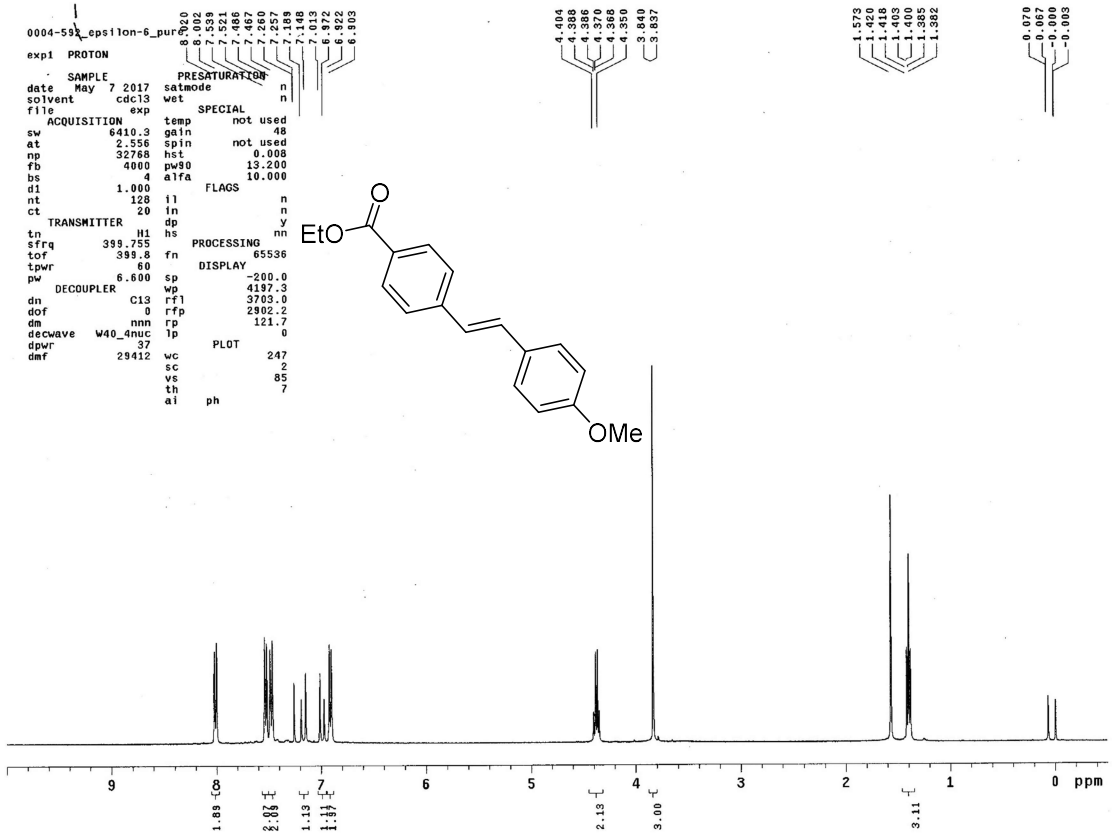
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **7ge** (table 4, entry 7)



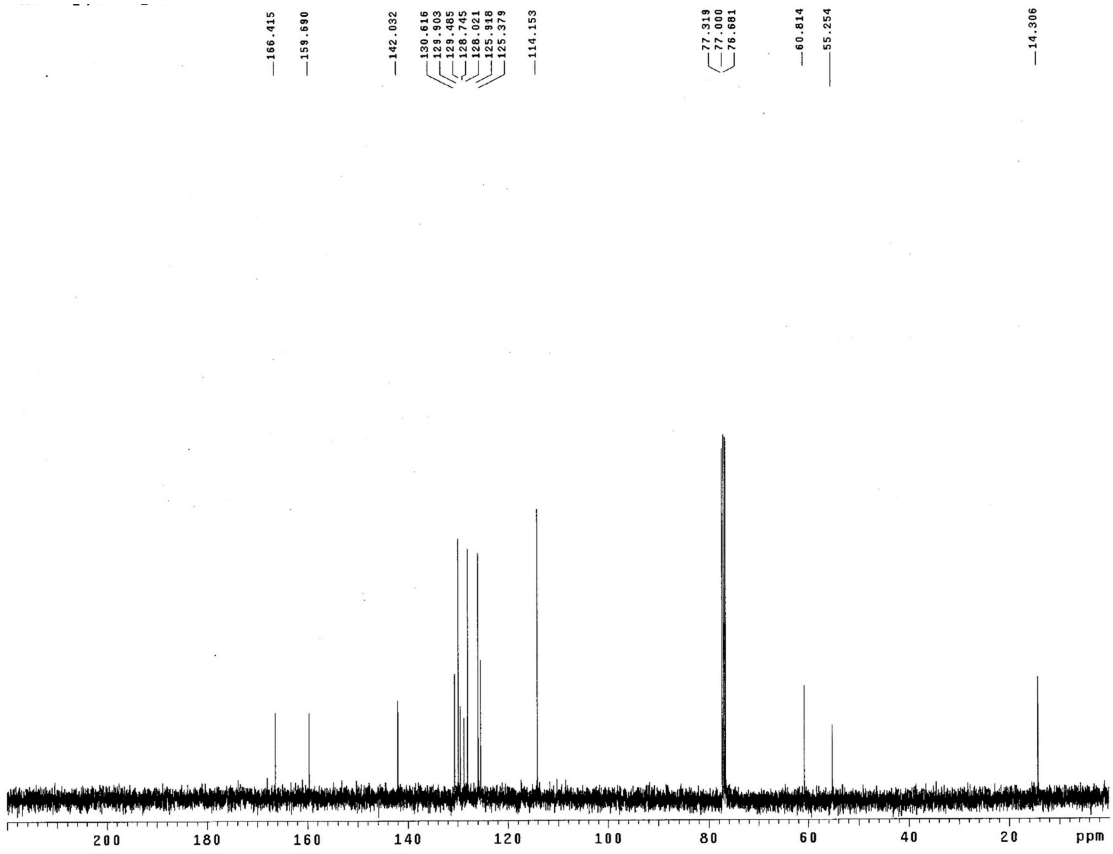
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **7ge**



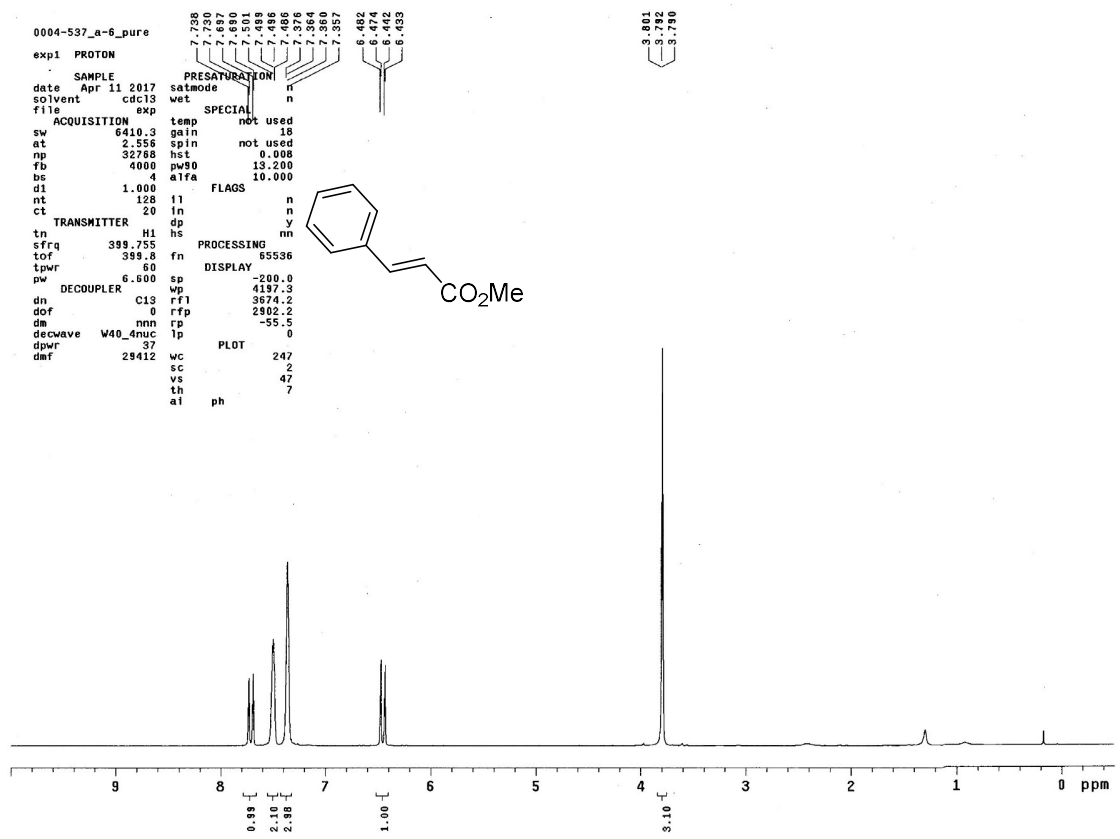
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **7se** (table 4, entry 8)



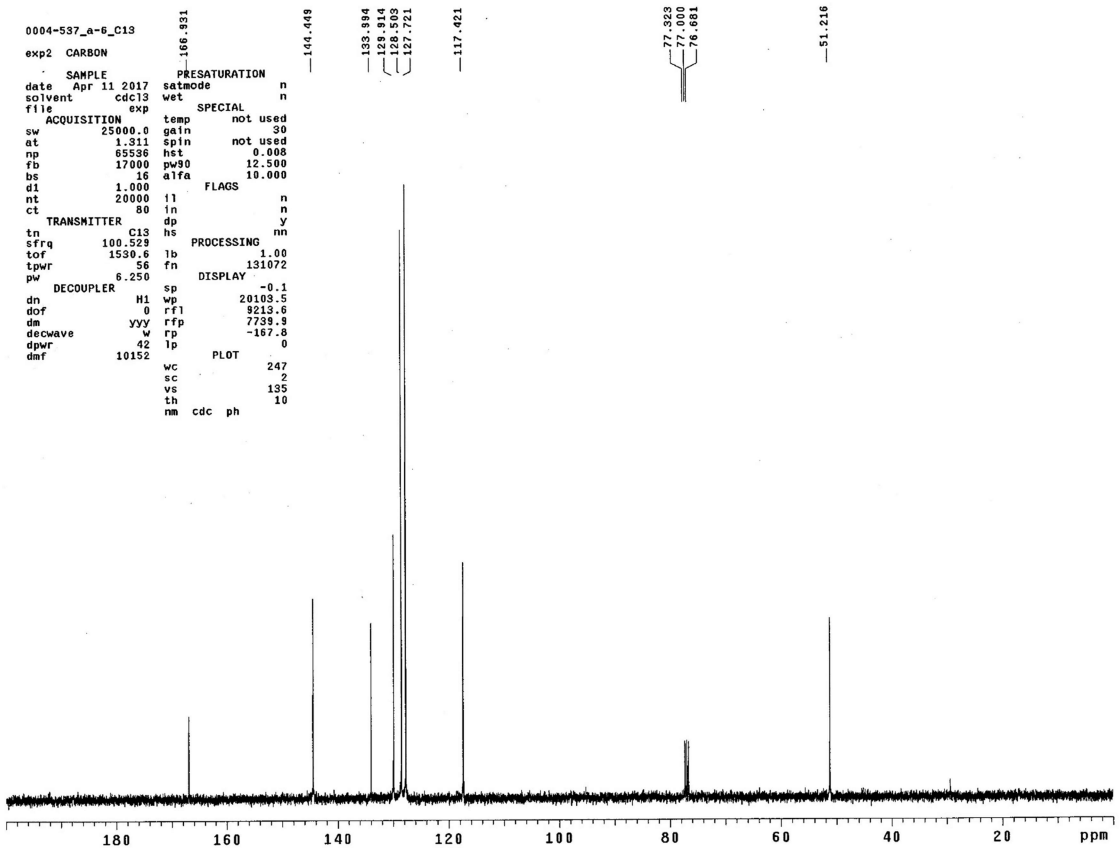
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **7se**



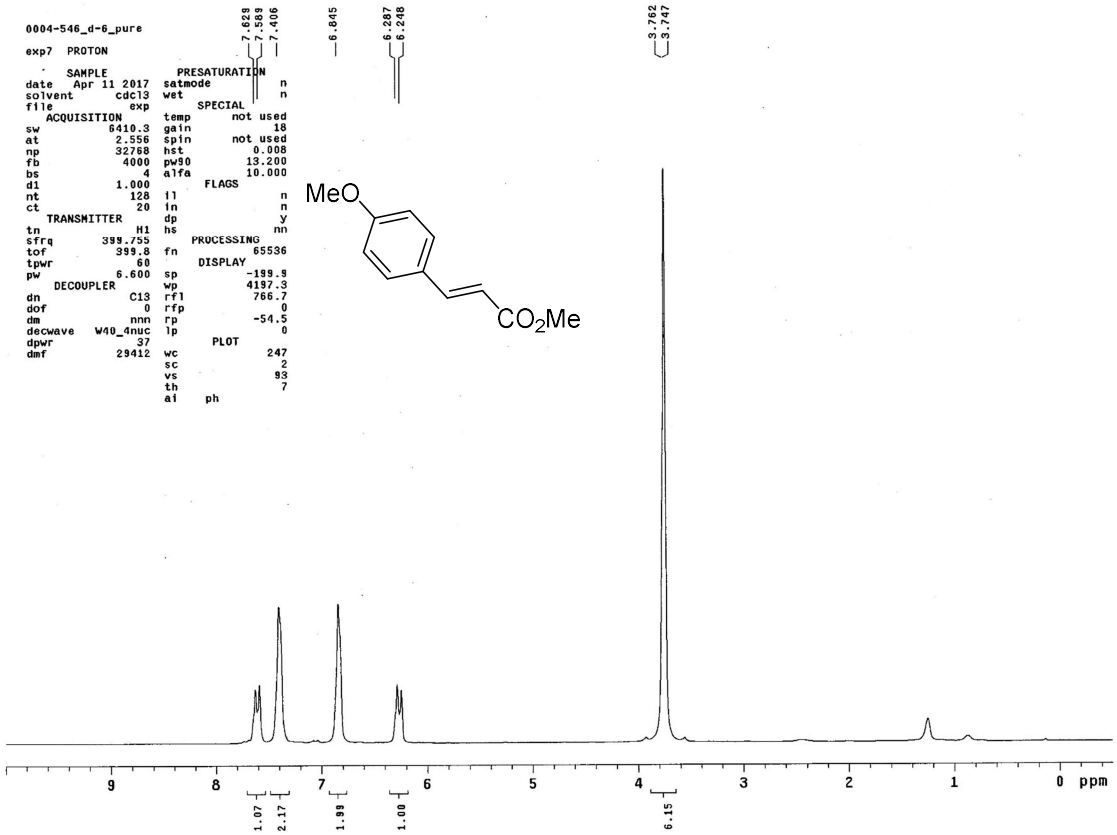
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **7ta** (table 4, entry 9)



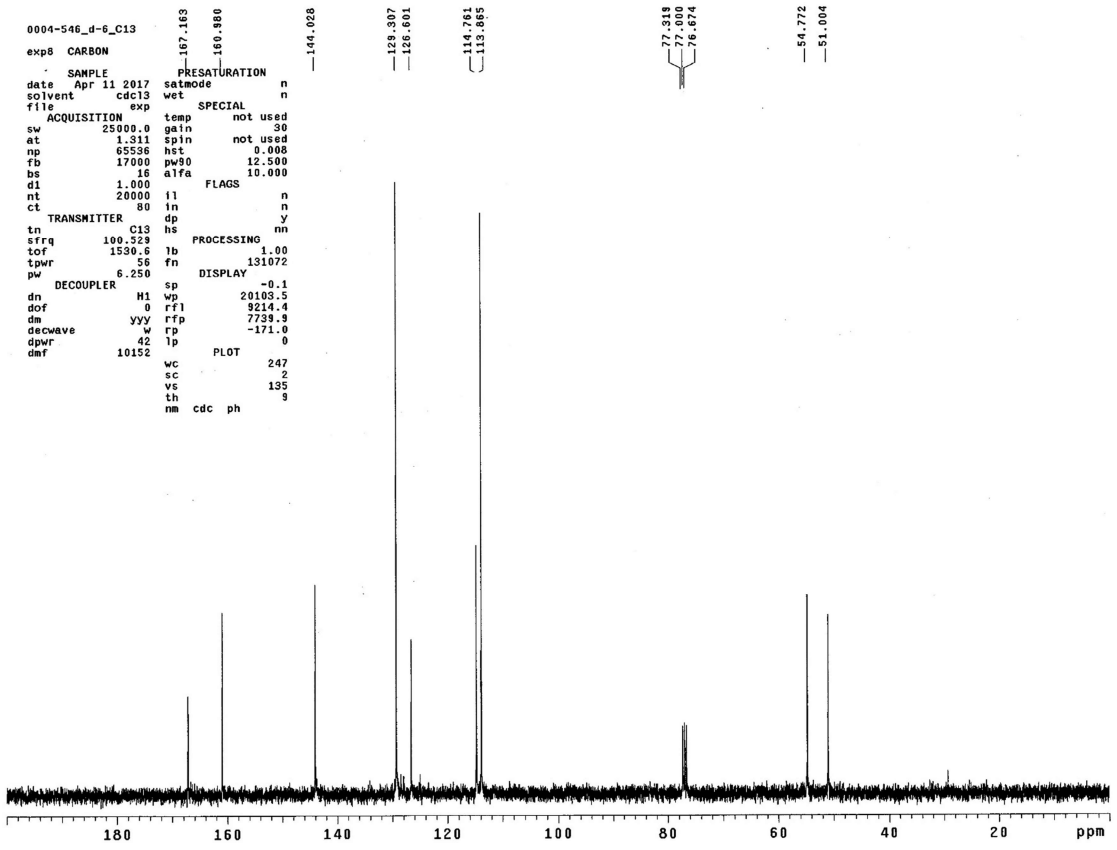
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **7ta**



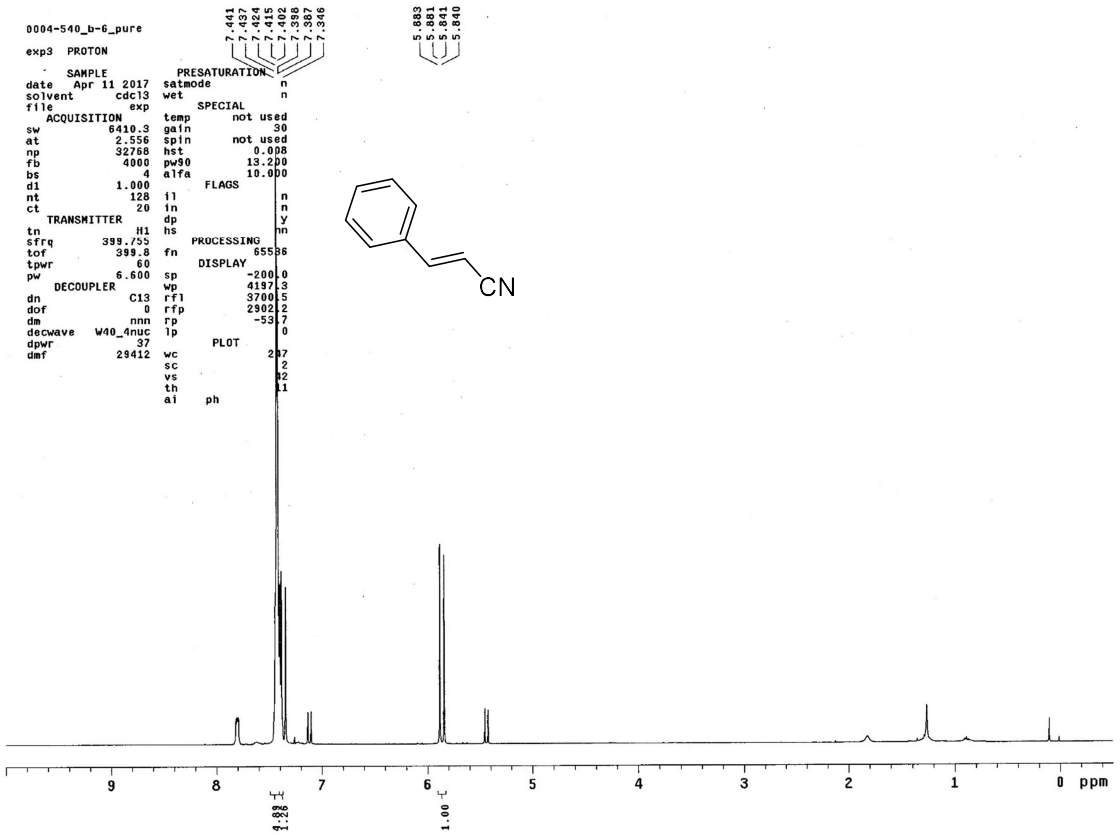
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **7aa** (table 4, entry 10)



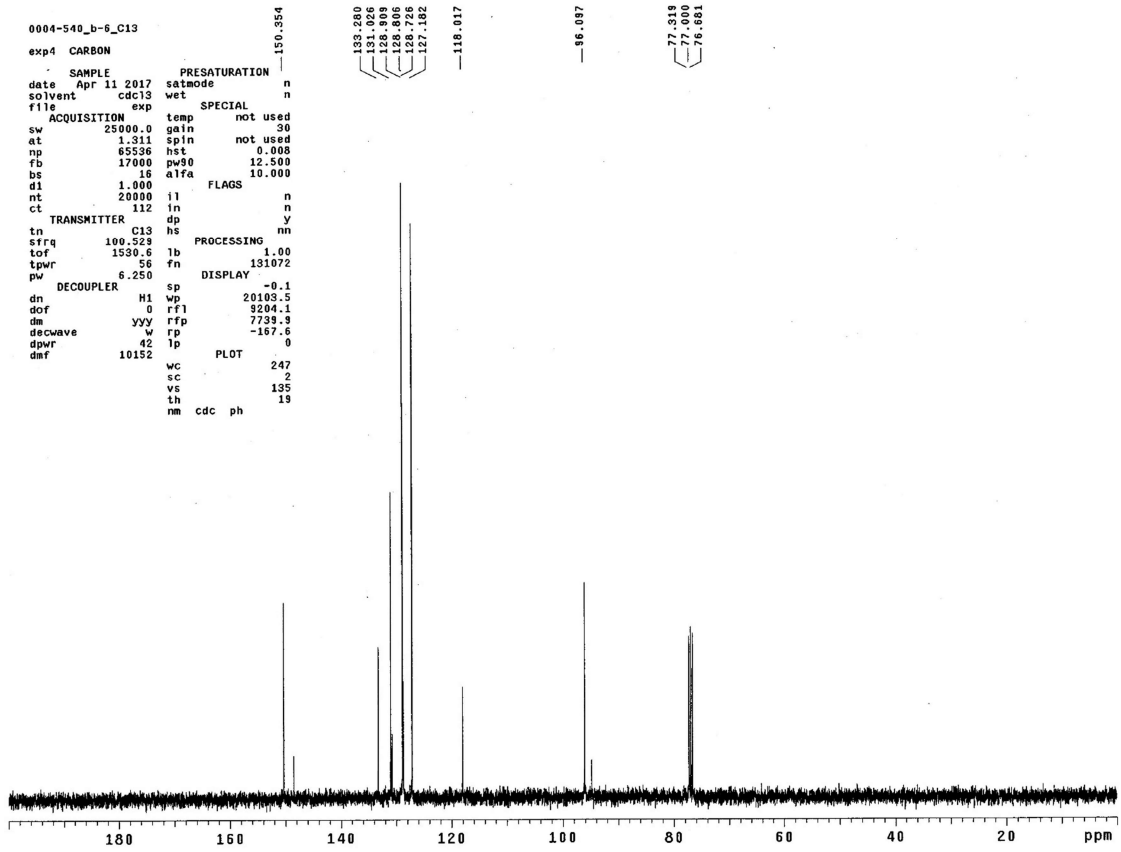
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **7aa**



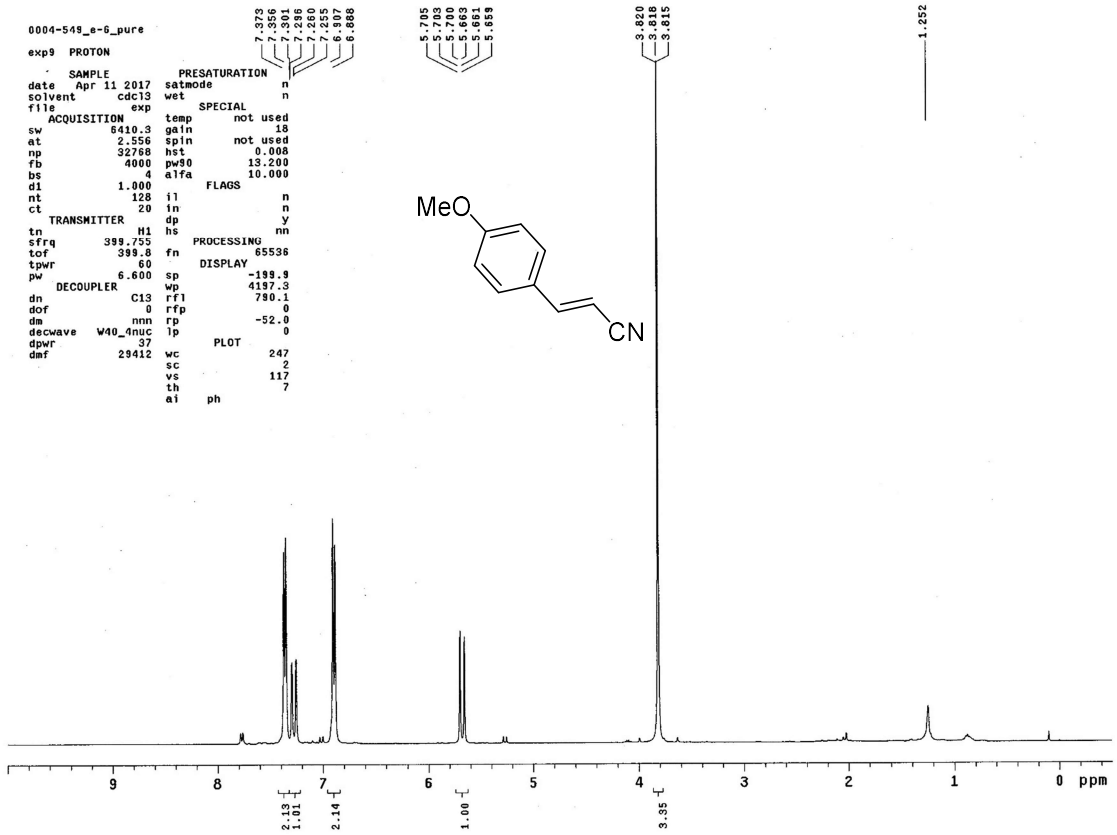
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **7tf** (table 4, entry 11)



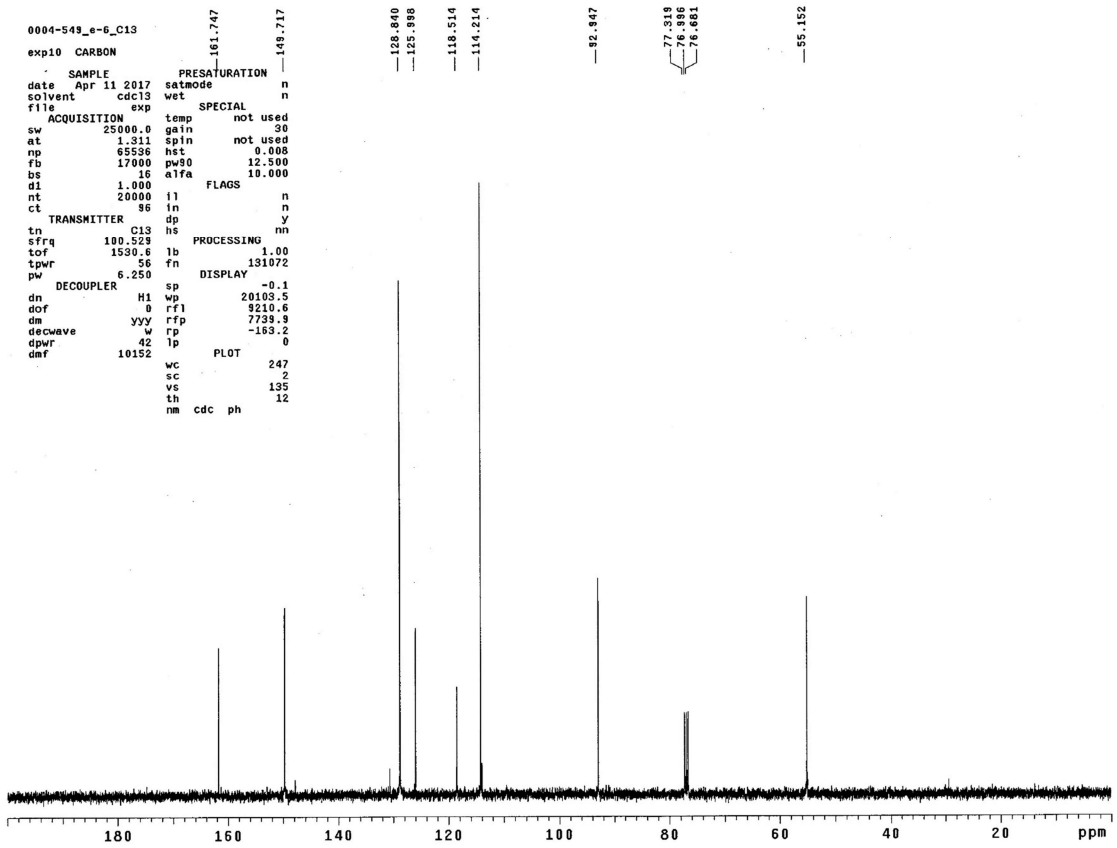
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **7tf**



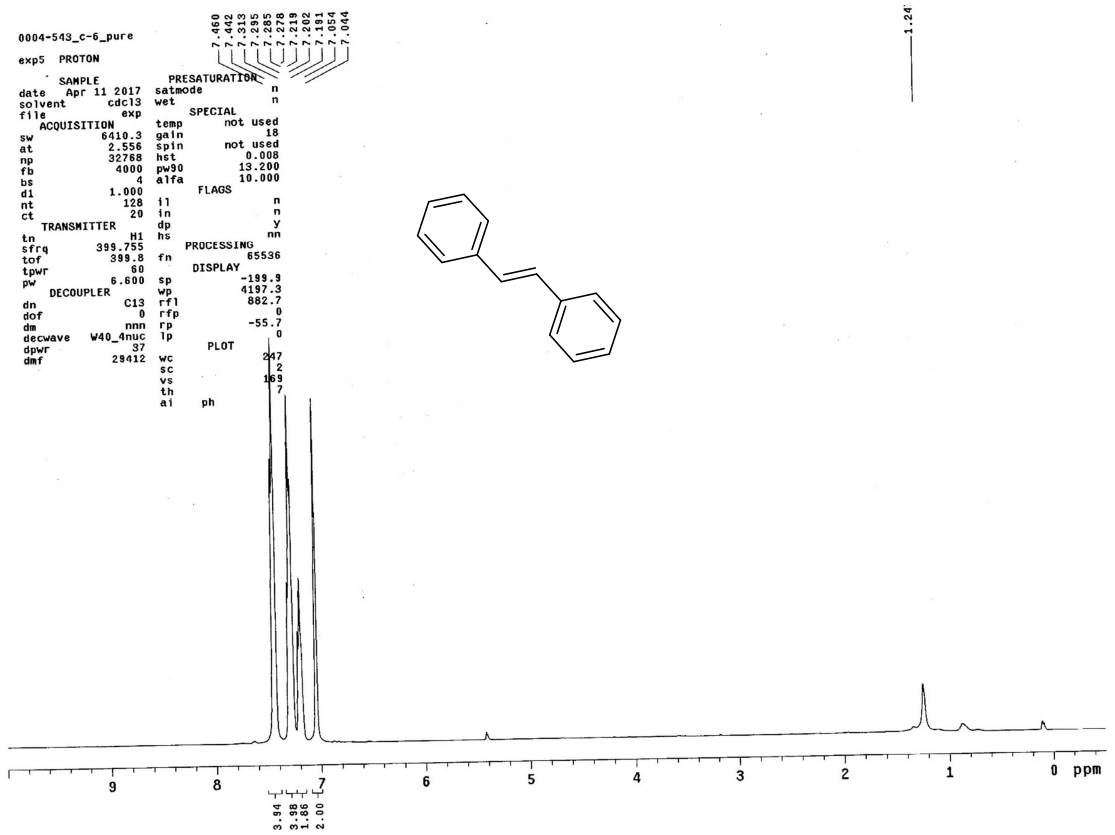
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **7af** (table 4, entry 12)



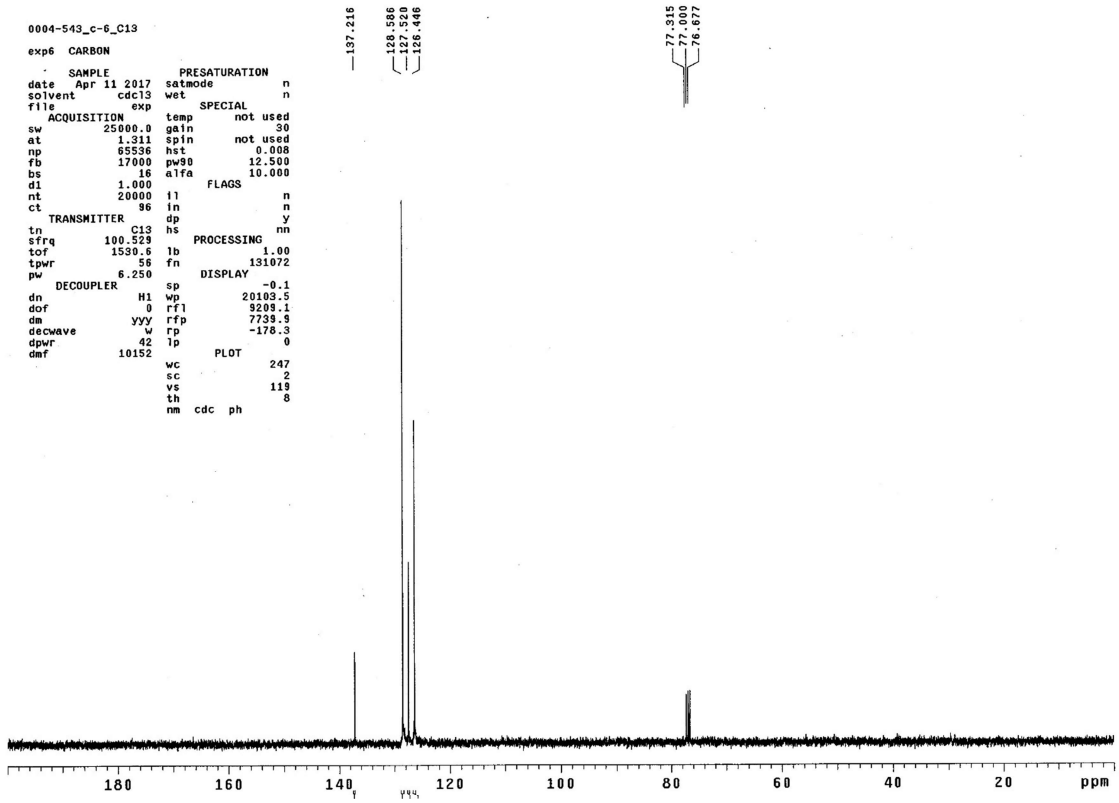
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **7af**



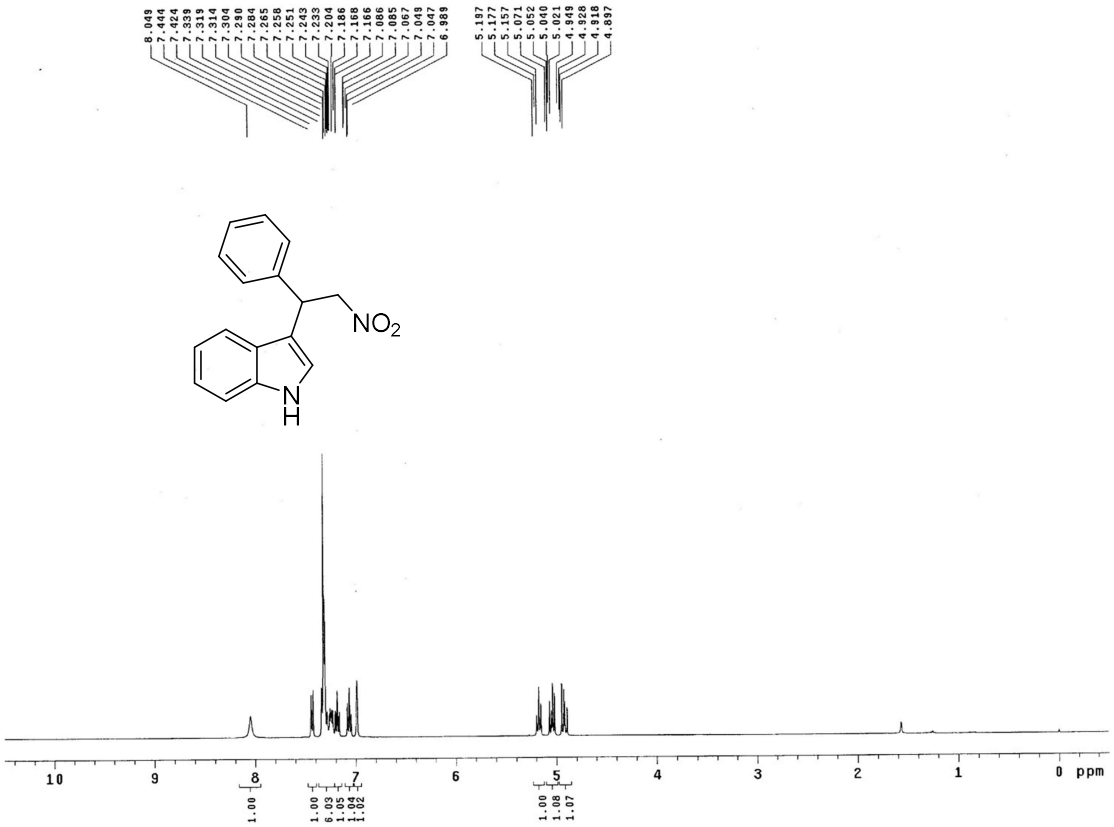
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **7tb** (table 4, entry 13)



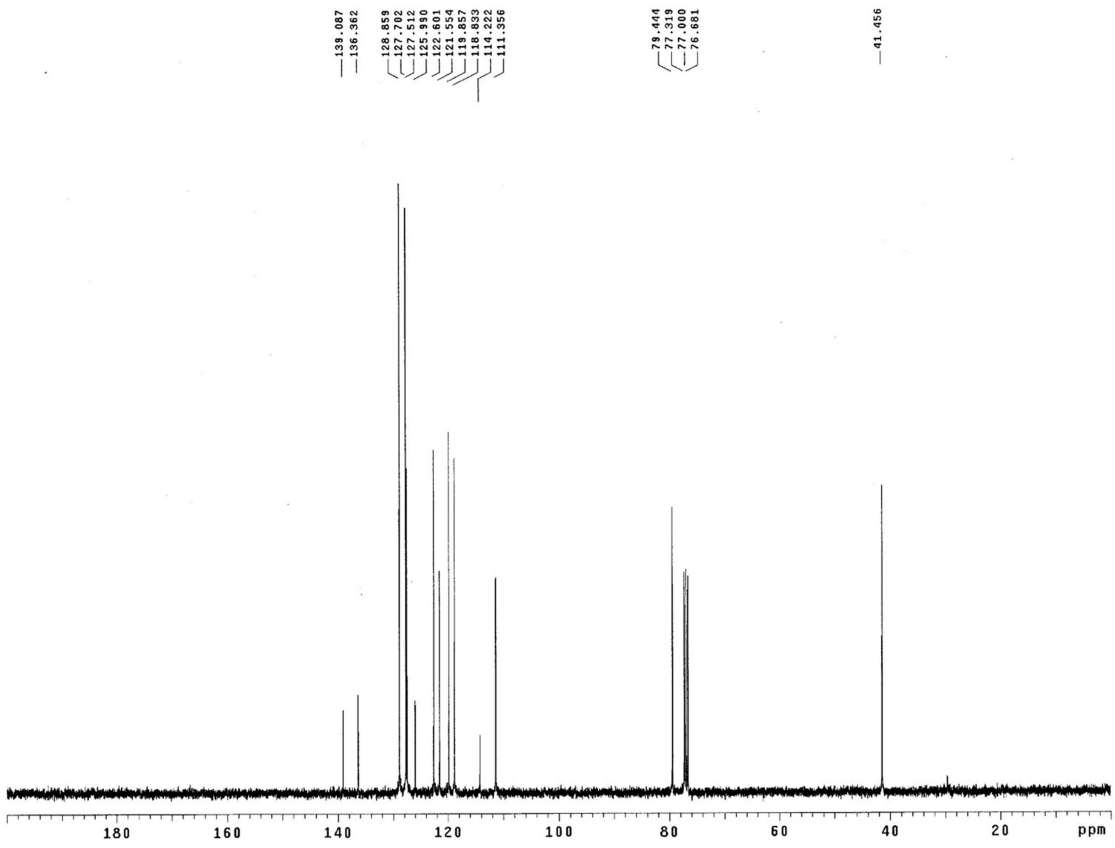
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **7tb**



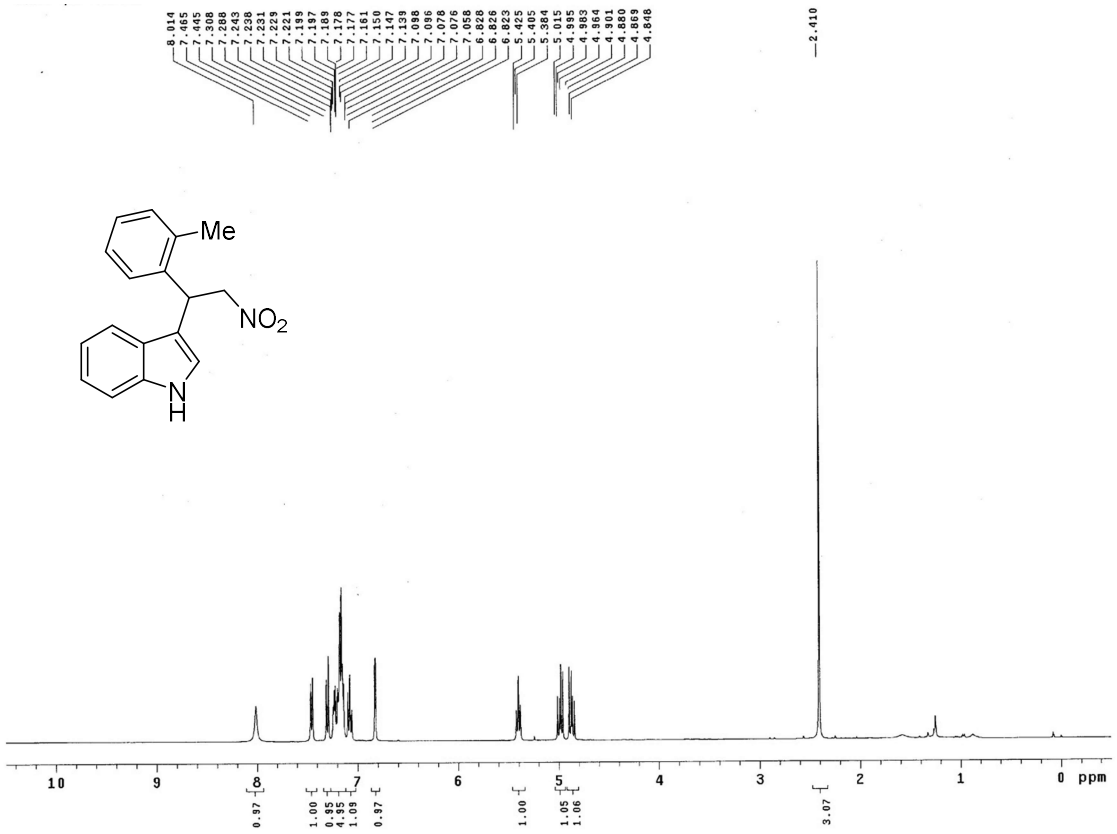
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **10aa** (table 6, entry 1)



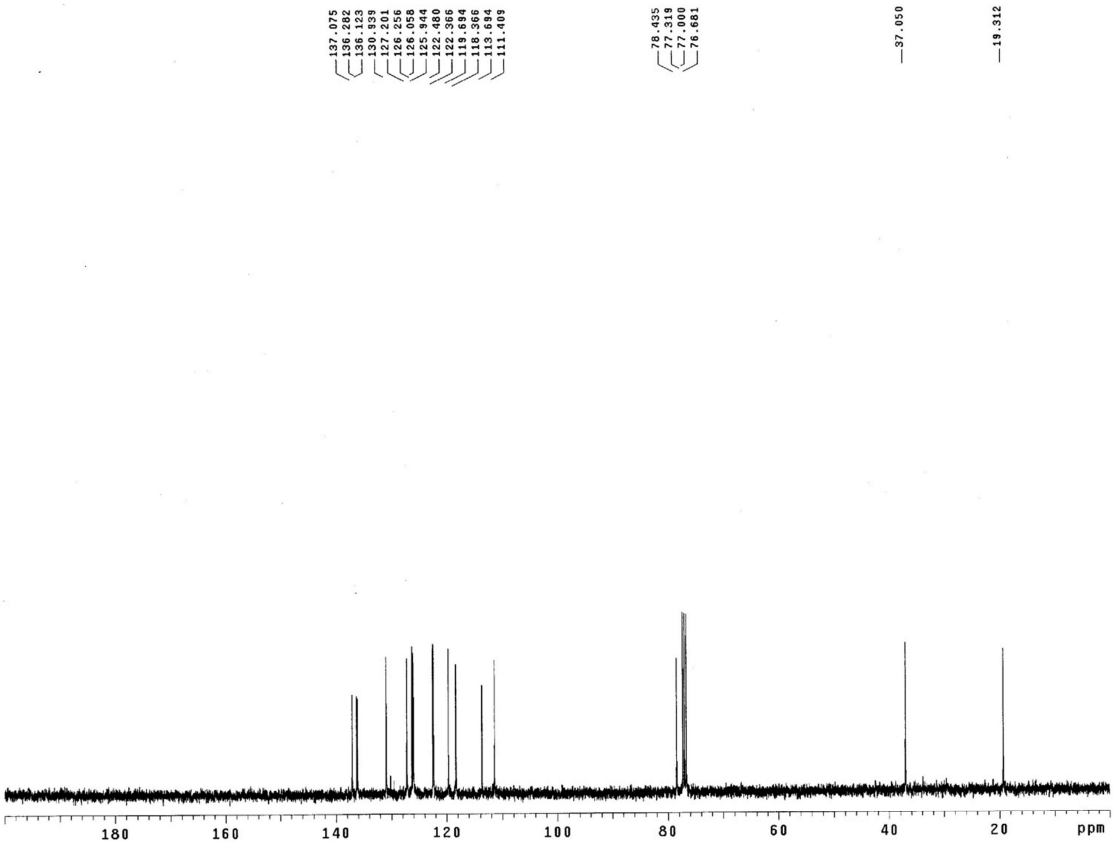
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **10aa**



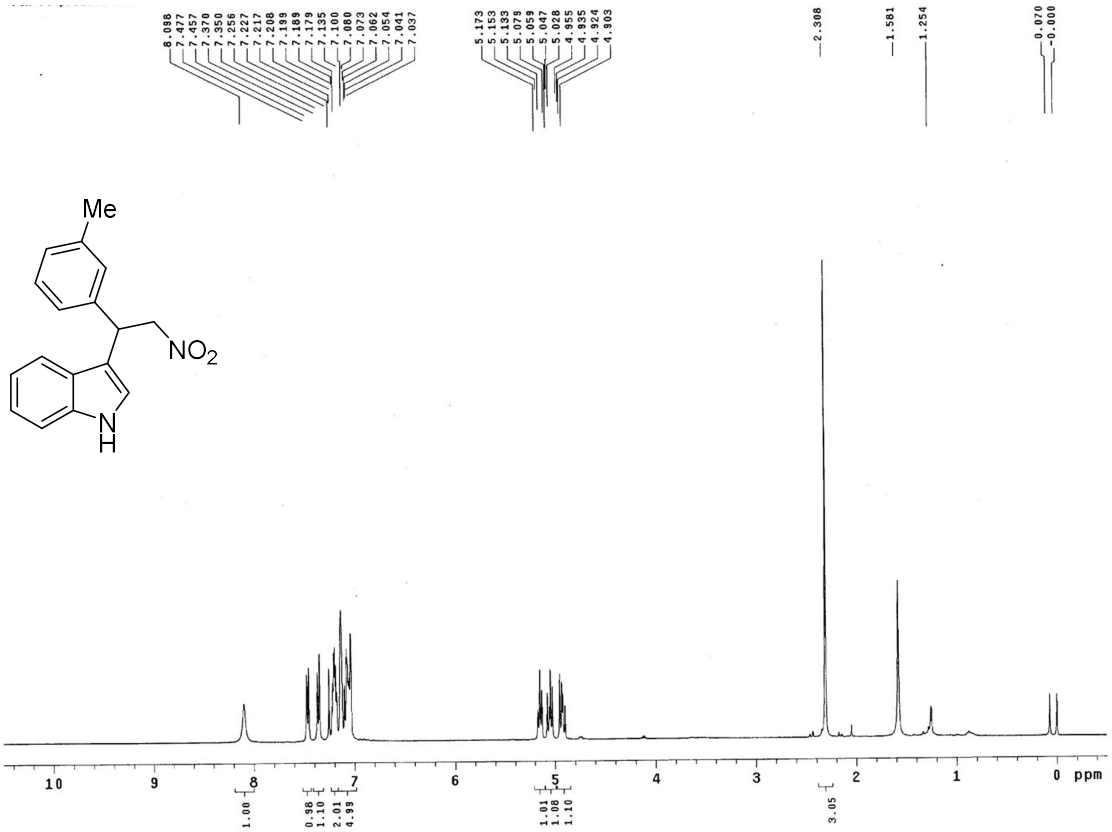
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **10ba** (table 6, entry 2)



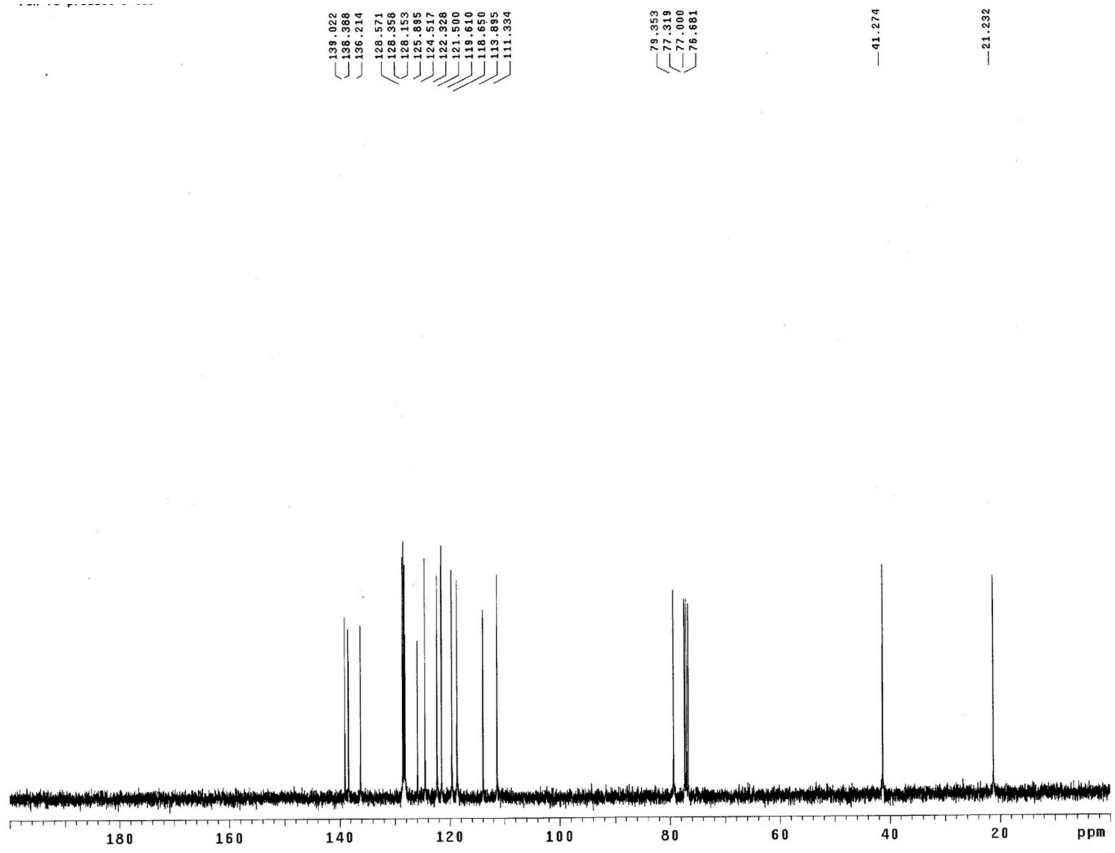
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **10ba**



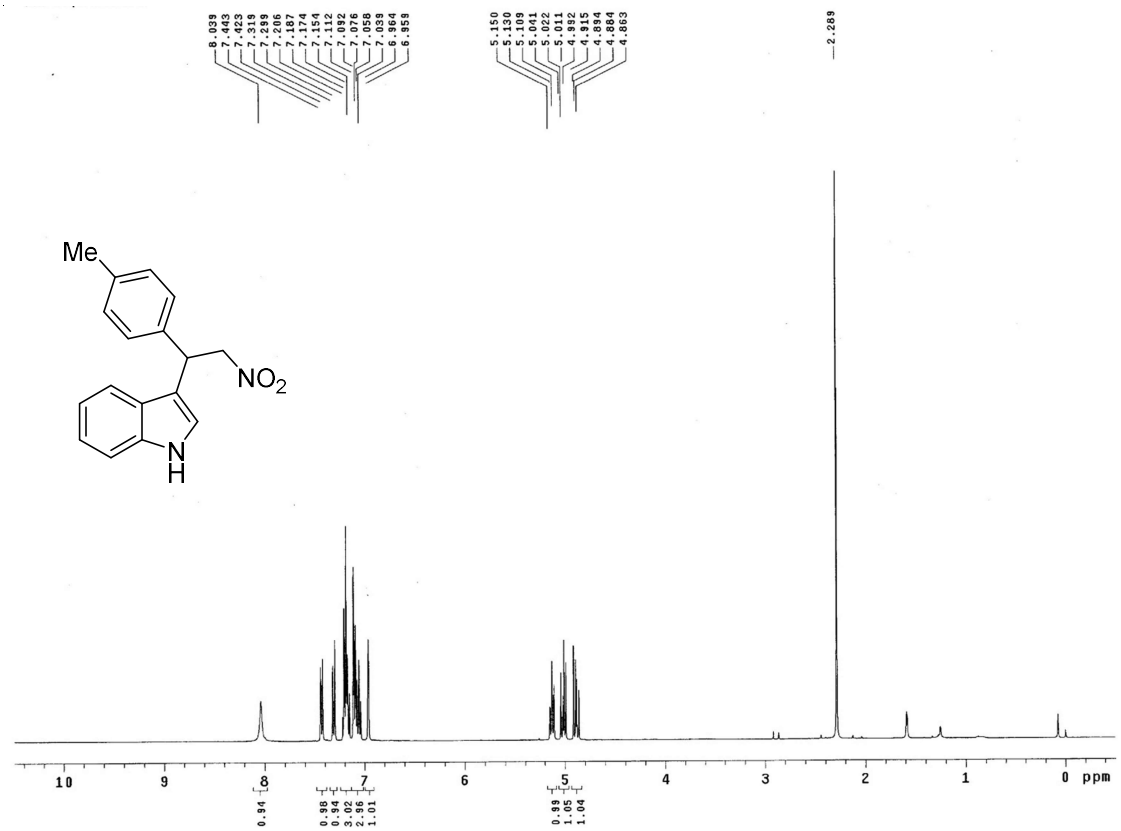
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **10ca** (table 6, entry 3)



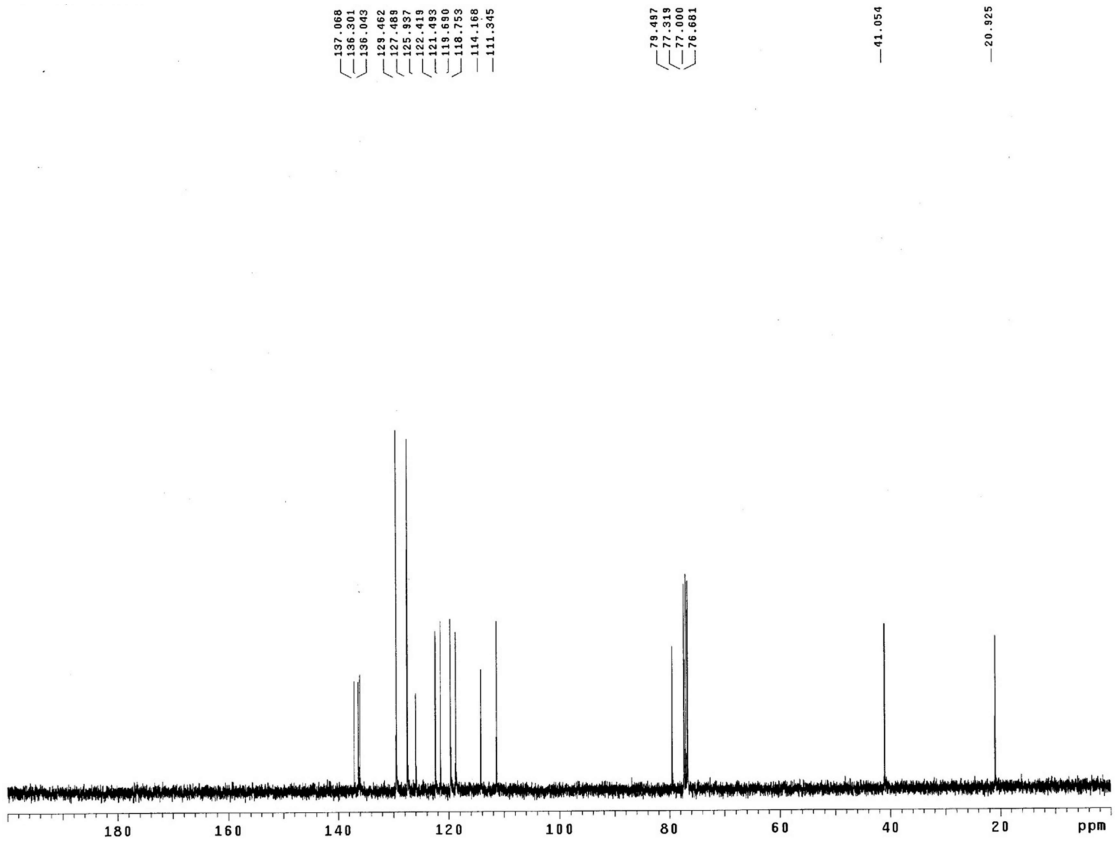
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **10ca**



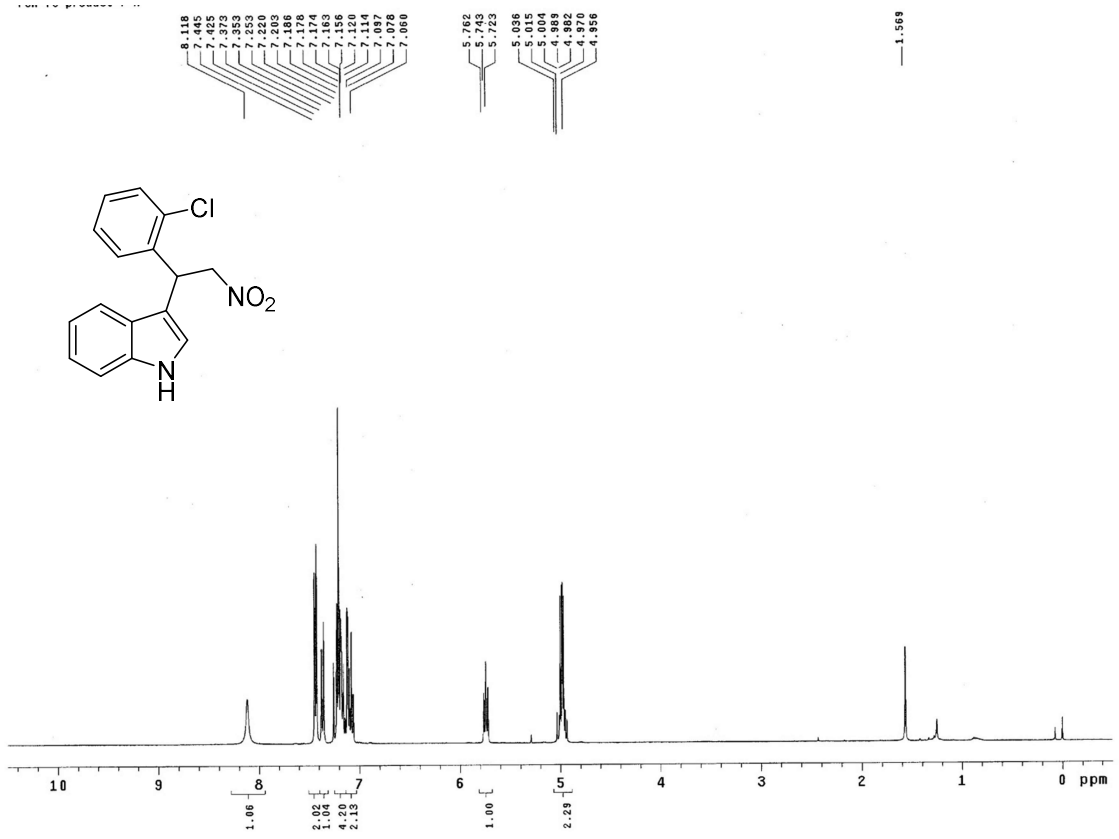
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **10da** (table 6, entry 4)



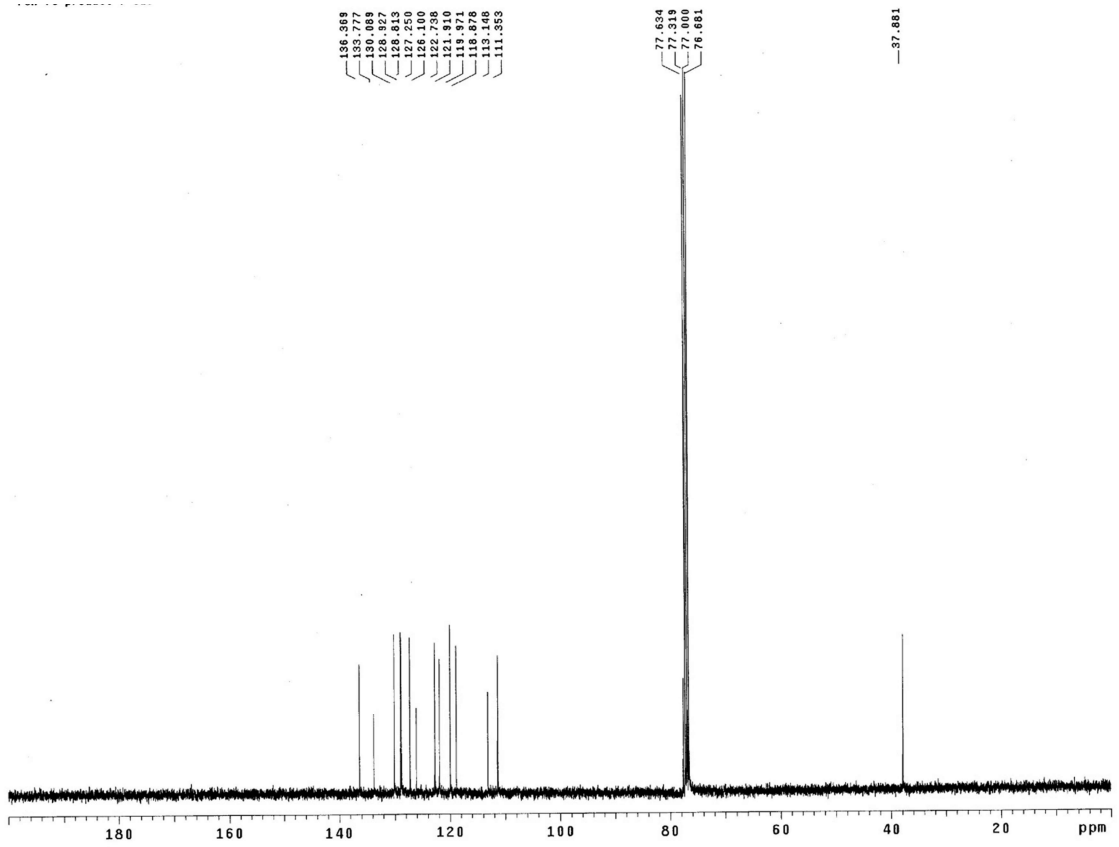
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **10da**



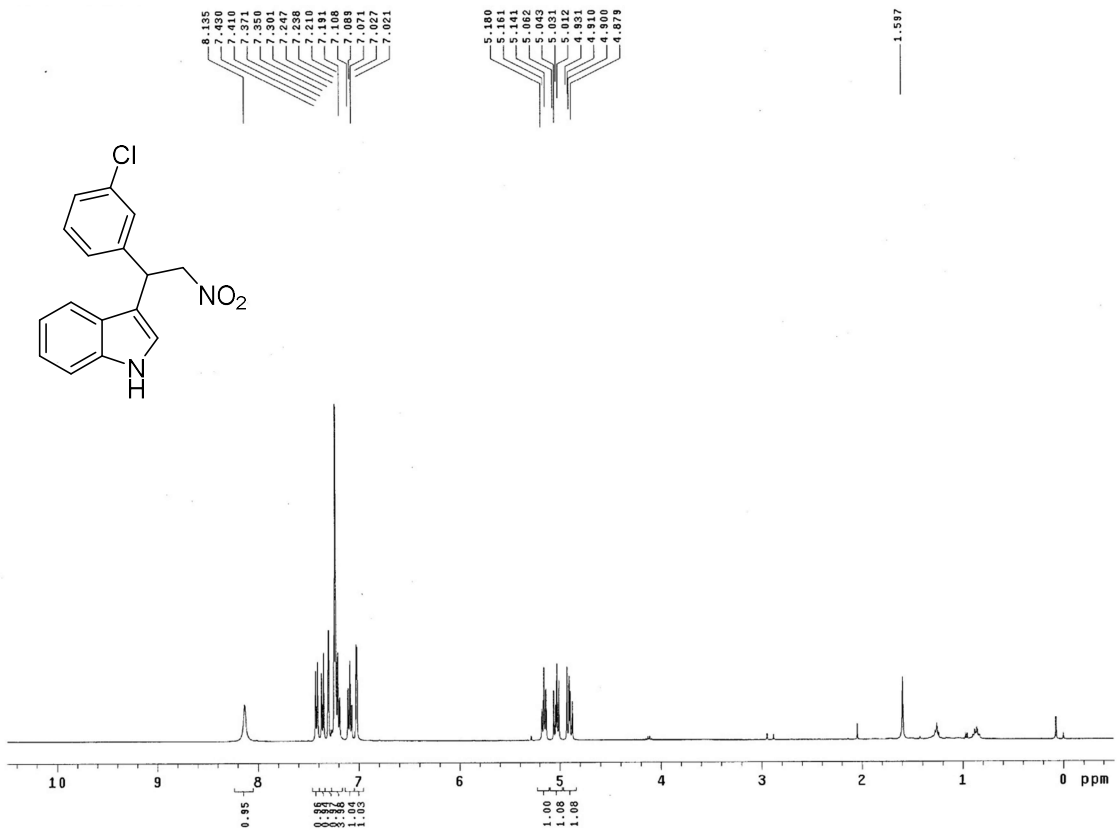
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **10ea** (table 6, entry 5)



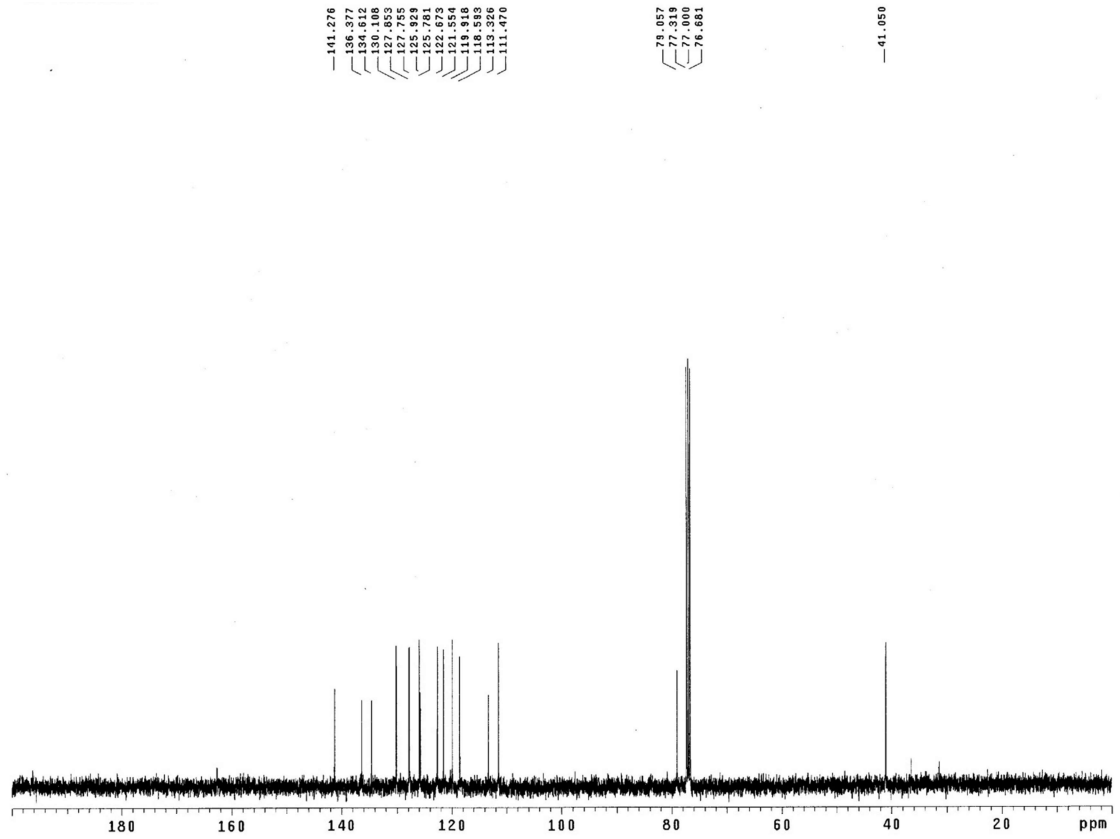
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **10ea**



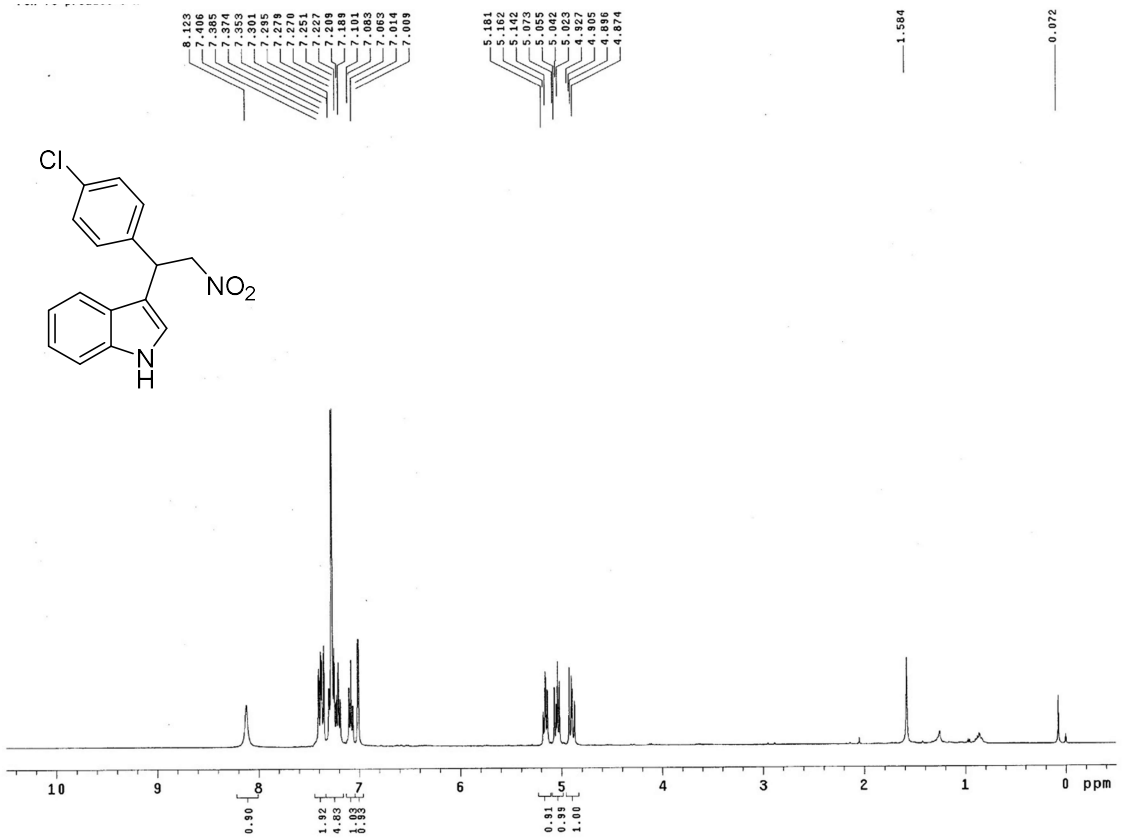
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **10fa** (table 6, entry 6)



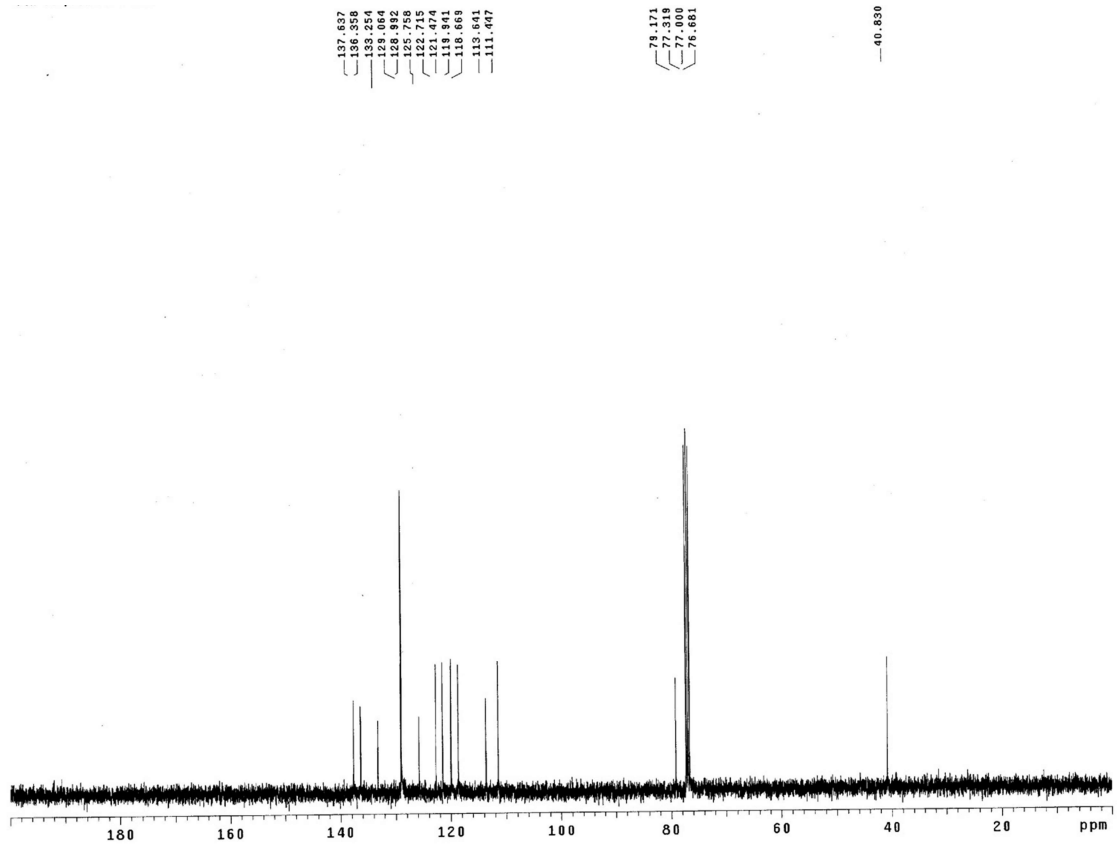
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **10fa**



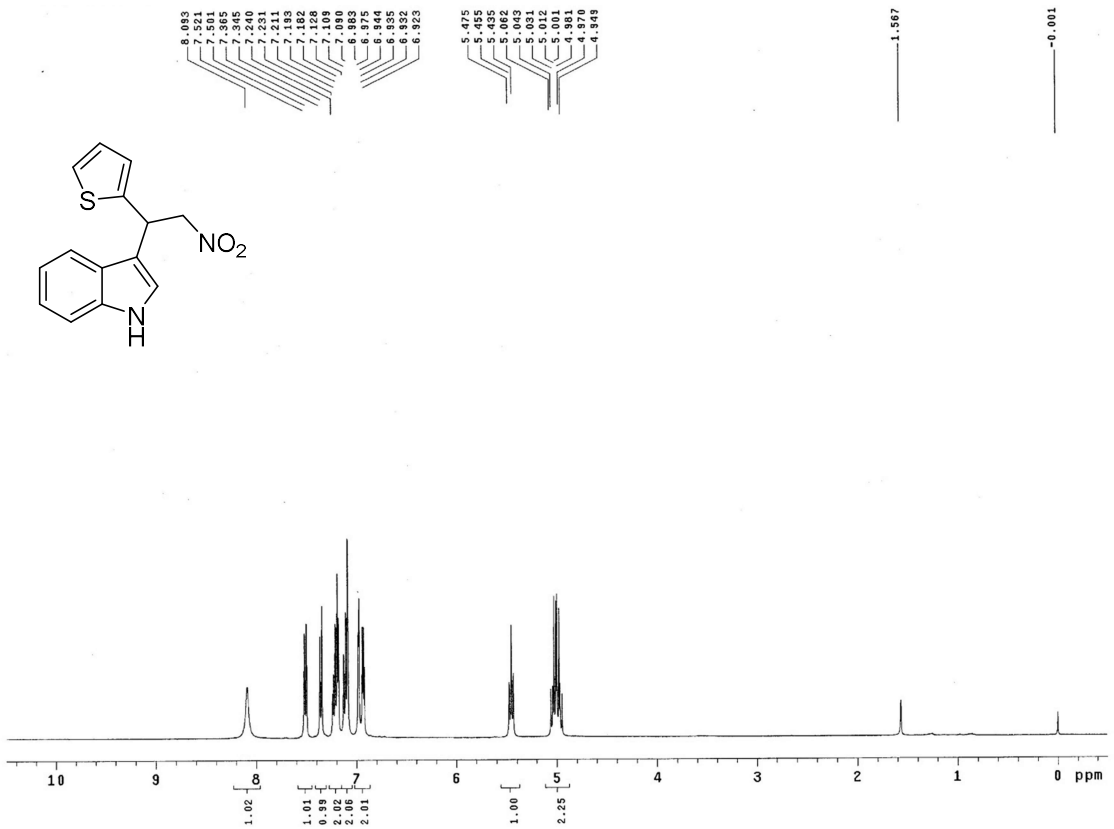
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **10ga** (table 6, entry 7)



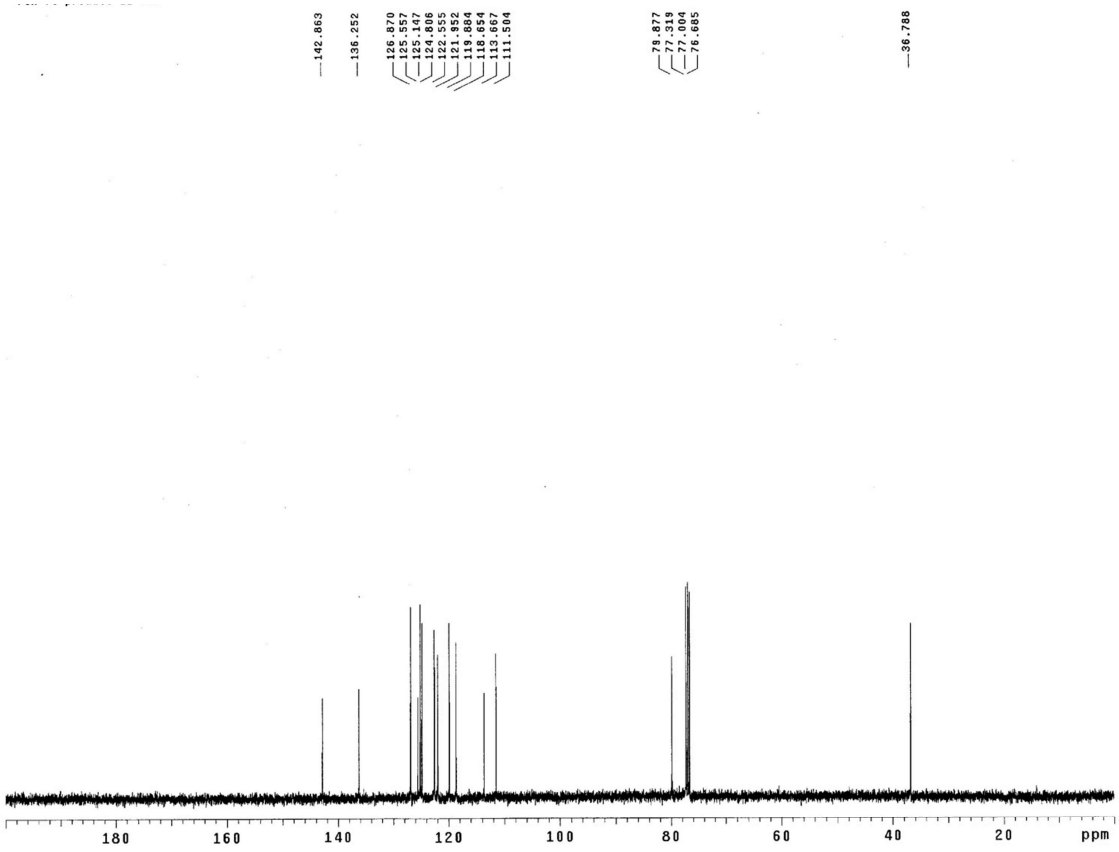
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **10ga**



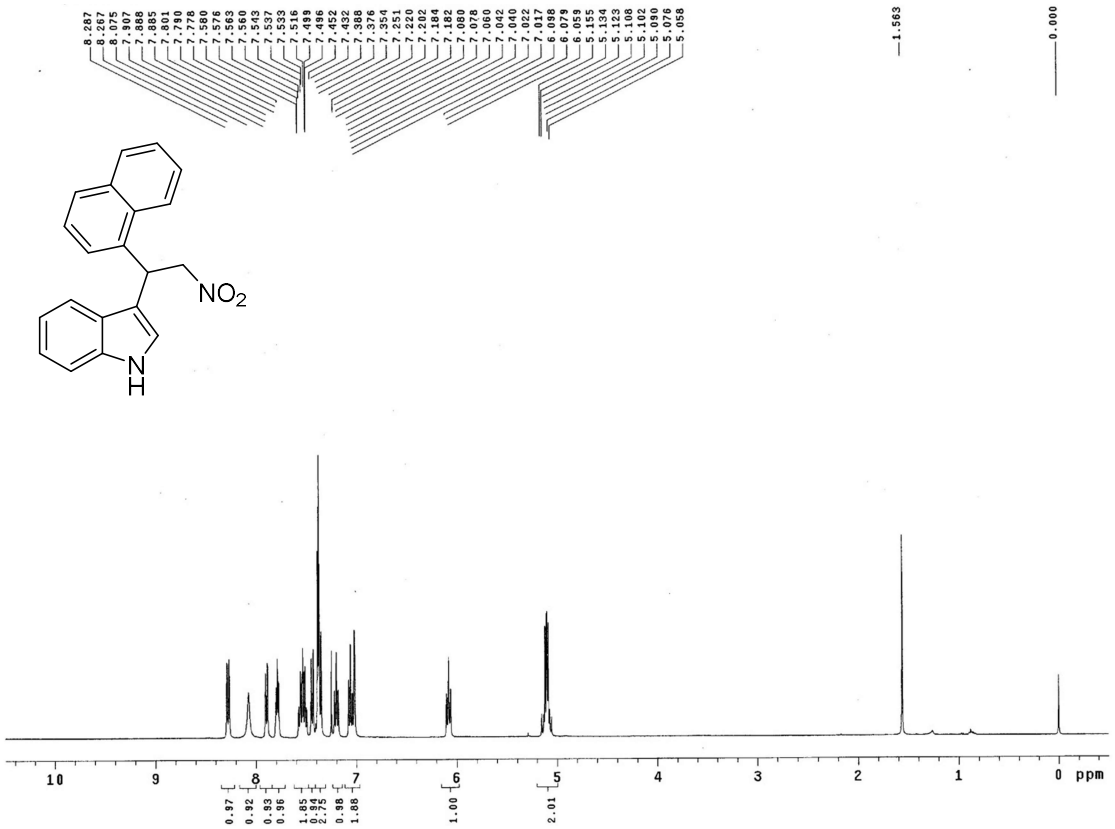
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **10ha** (table 6, entry 8)



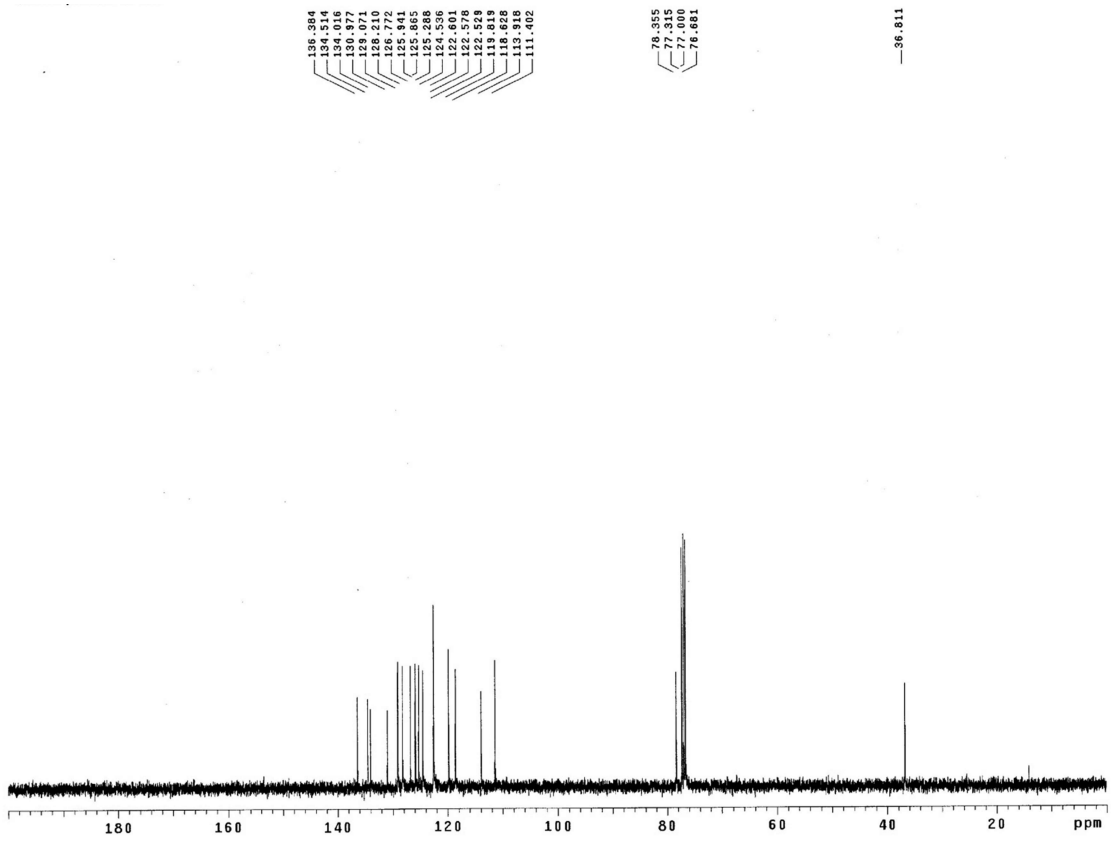
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **10ha**



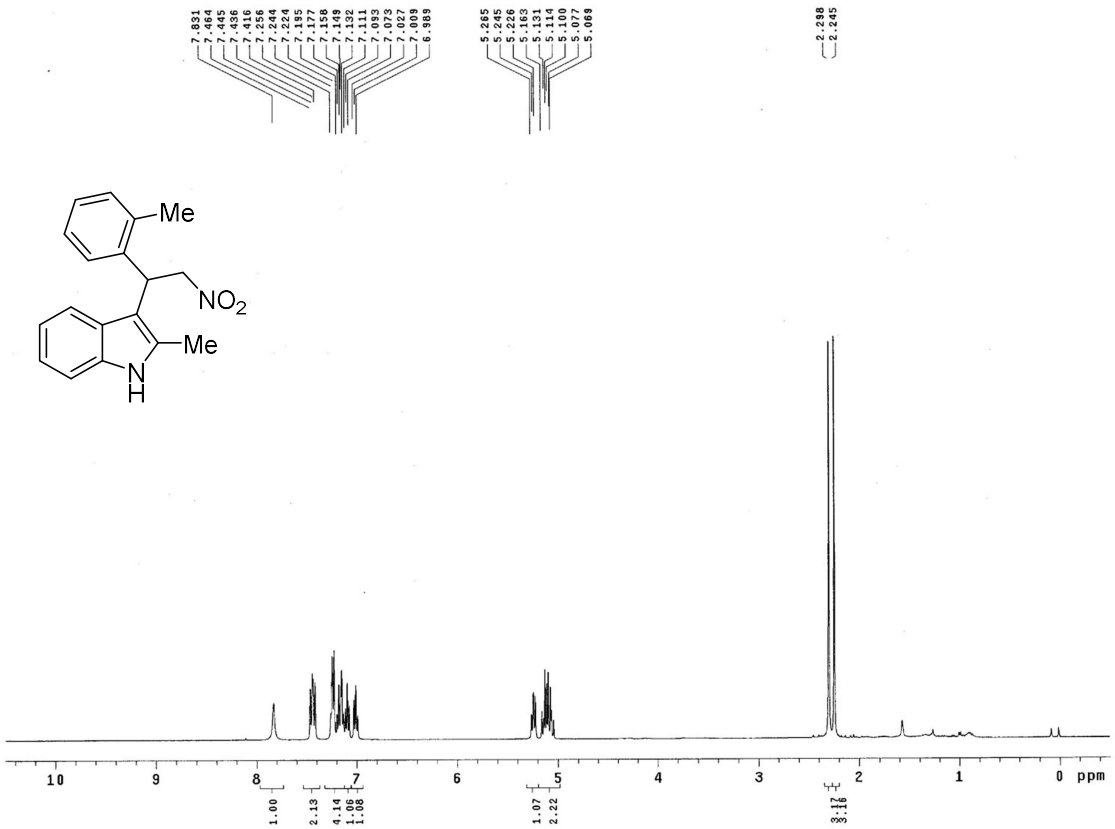
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **10ia** (table 6, entry 9)



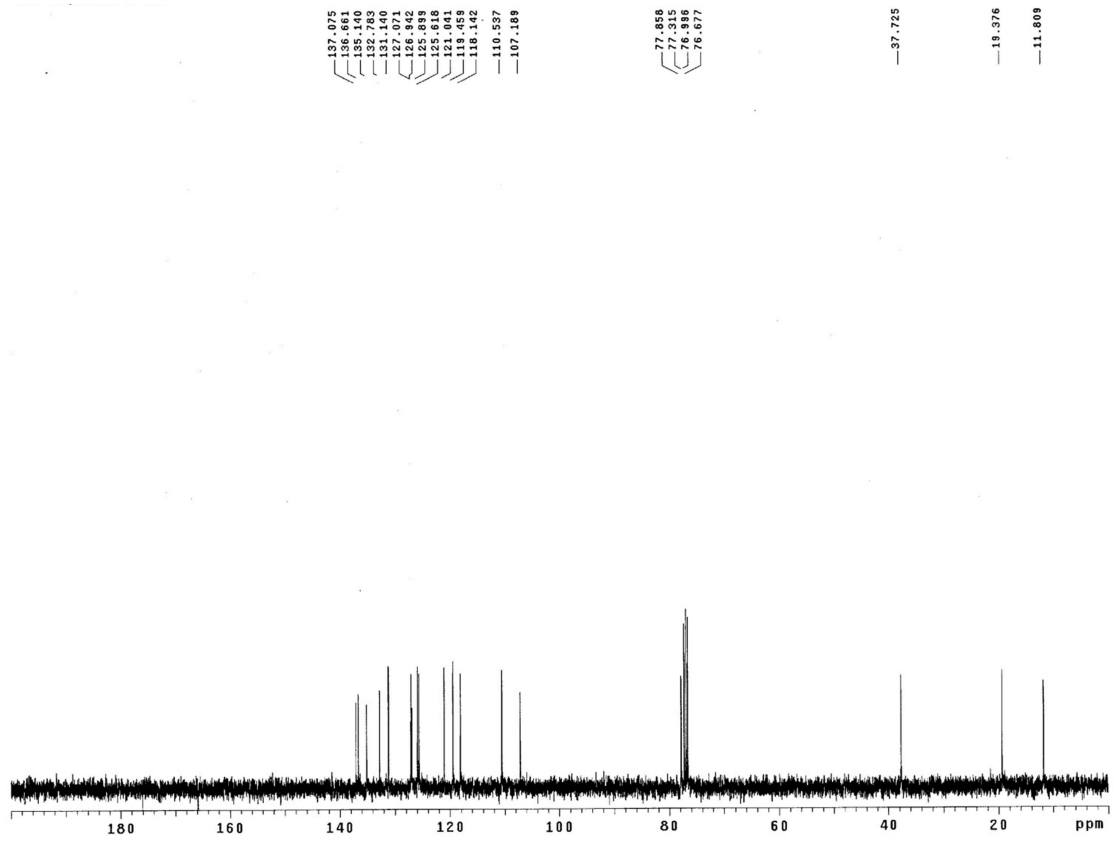
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **10ia**



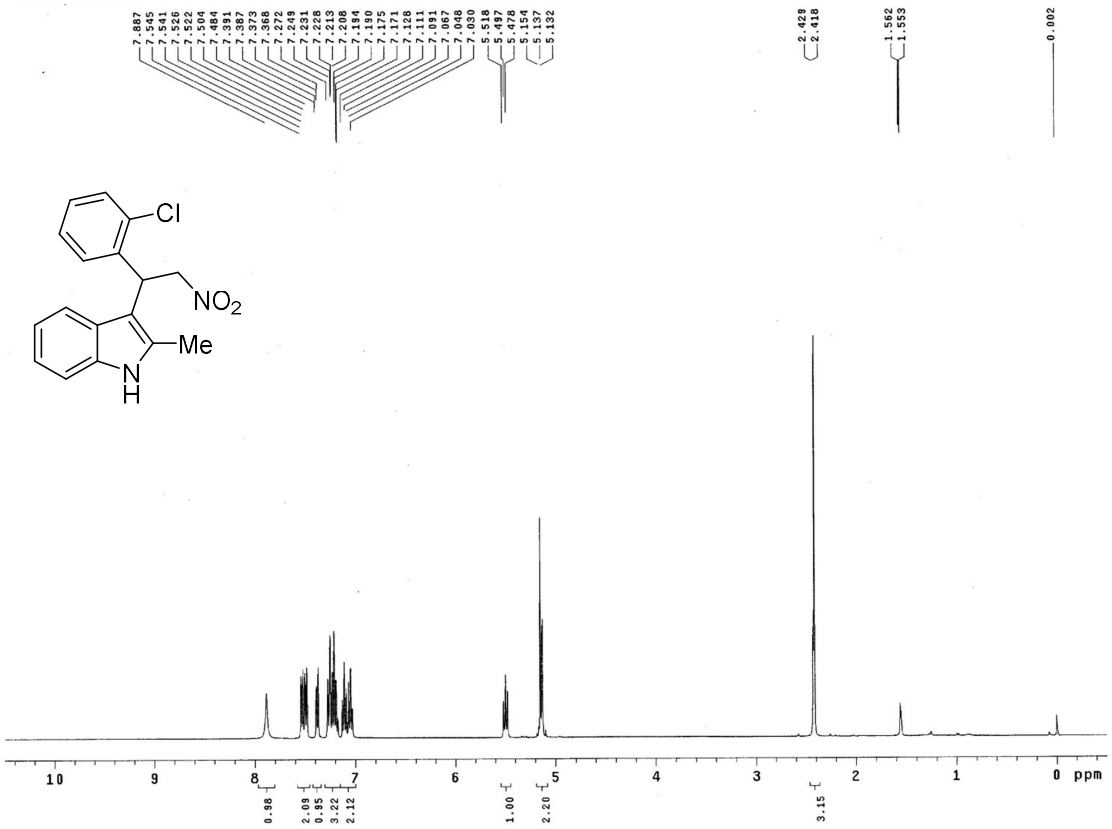
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **10bb** (table 6, entry 10)



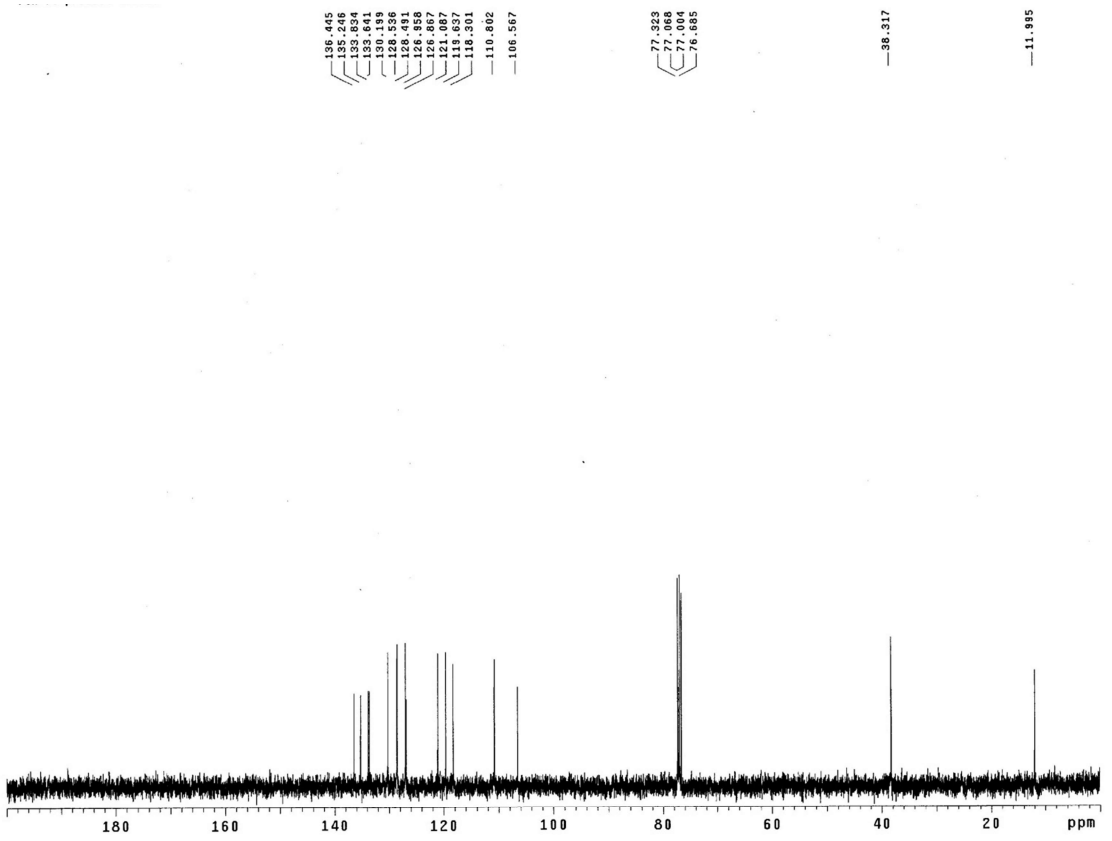
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **10bb**



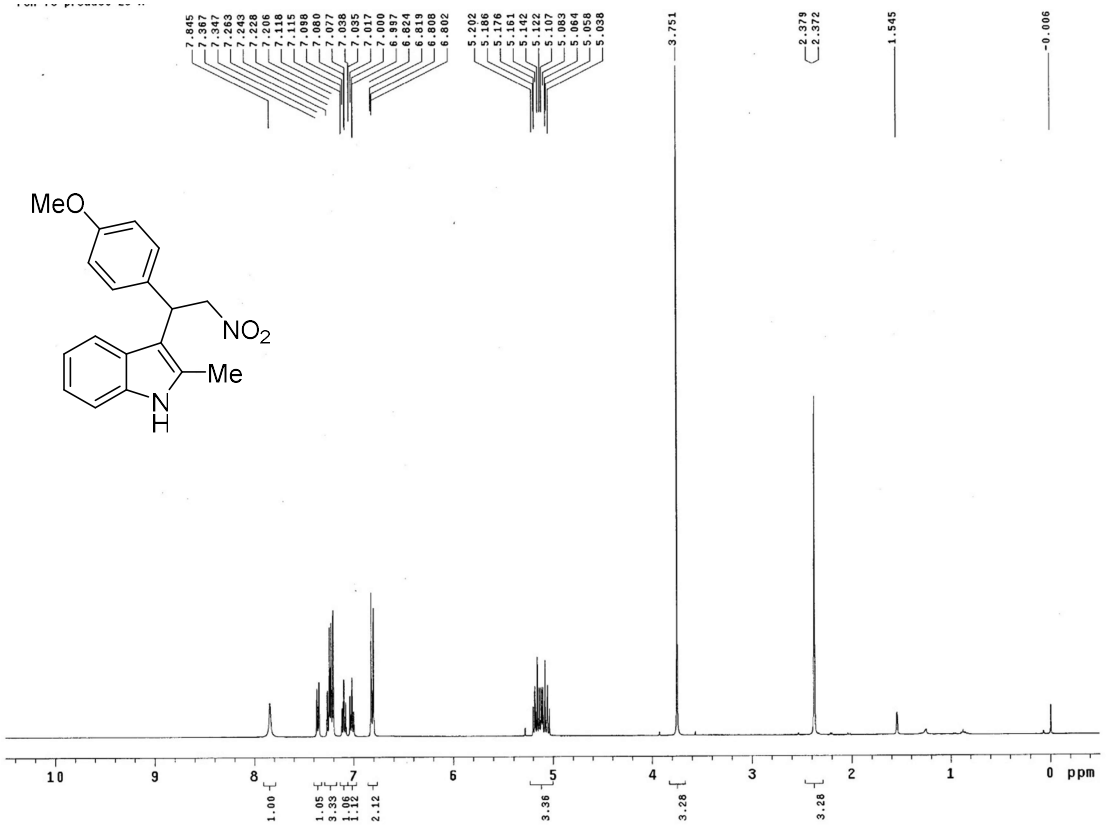
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **10eb** (table 6, entry 11)



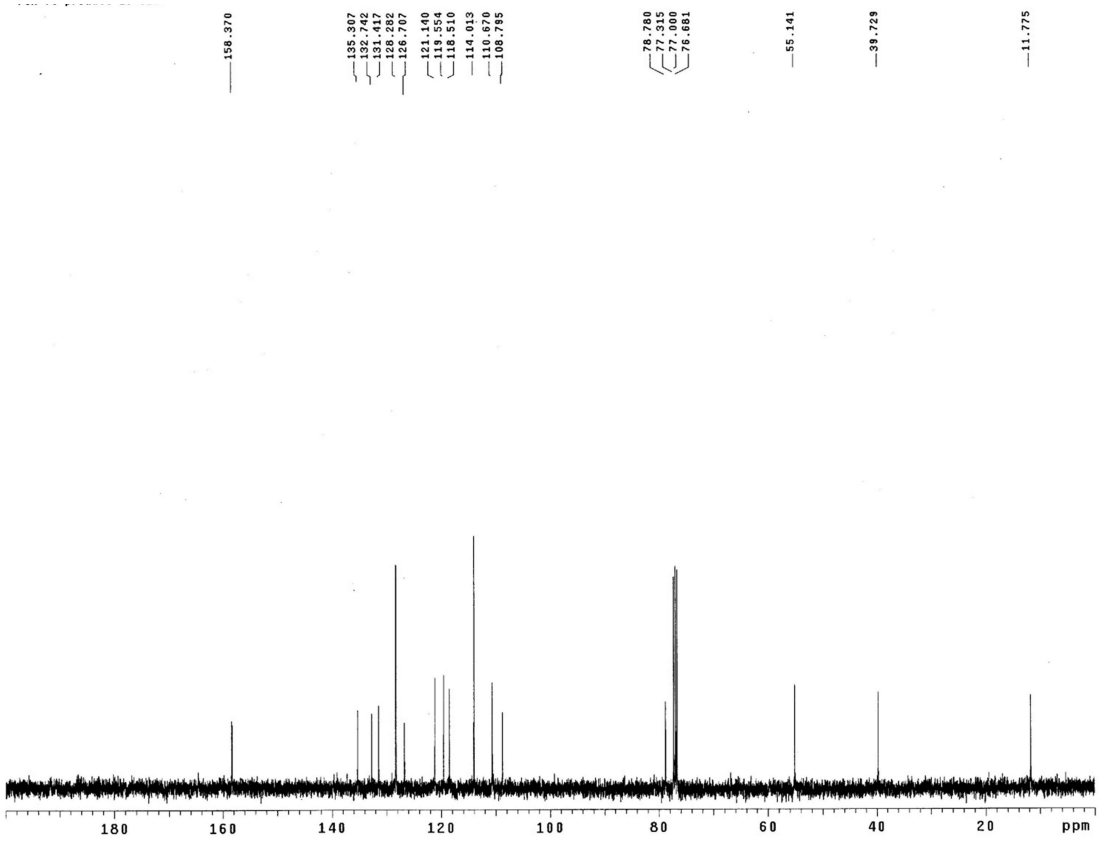
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **10eb**



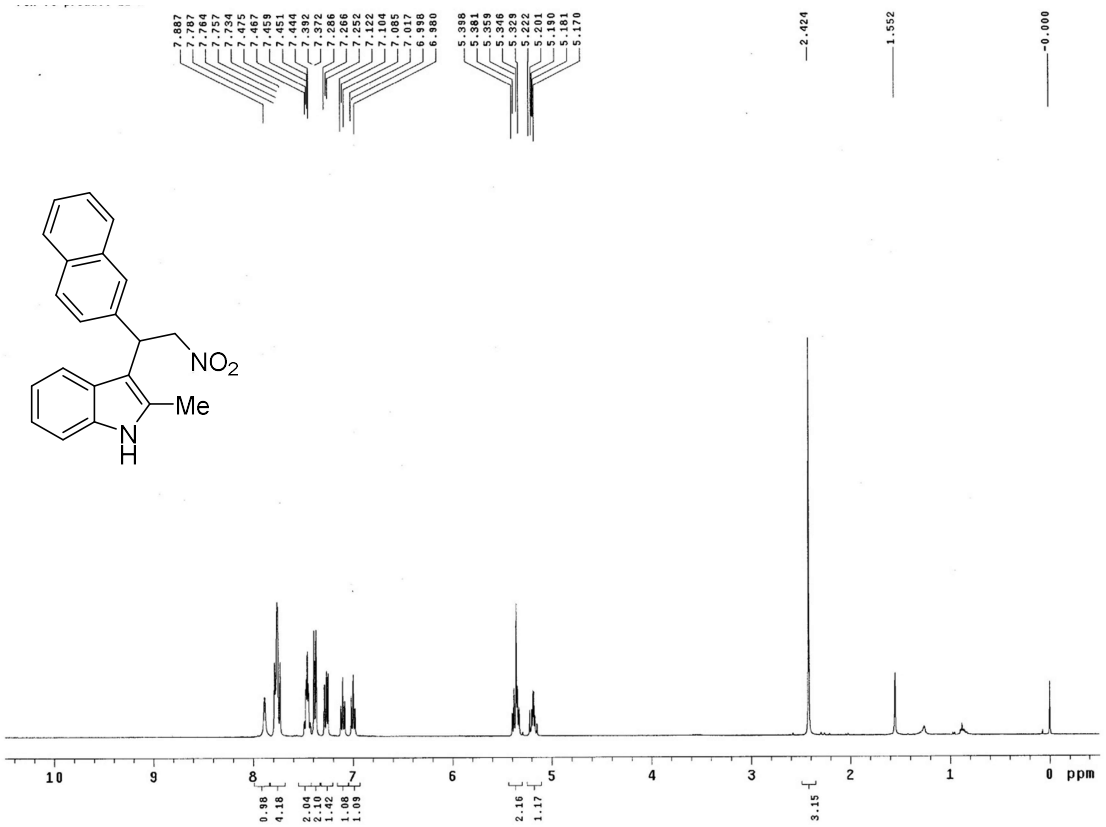
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **10jb** (table 6, entry 12)



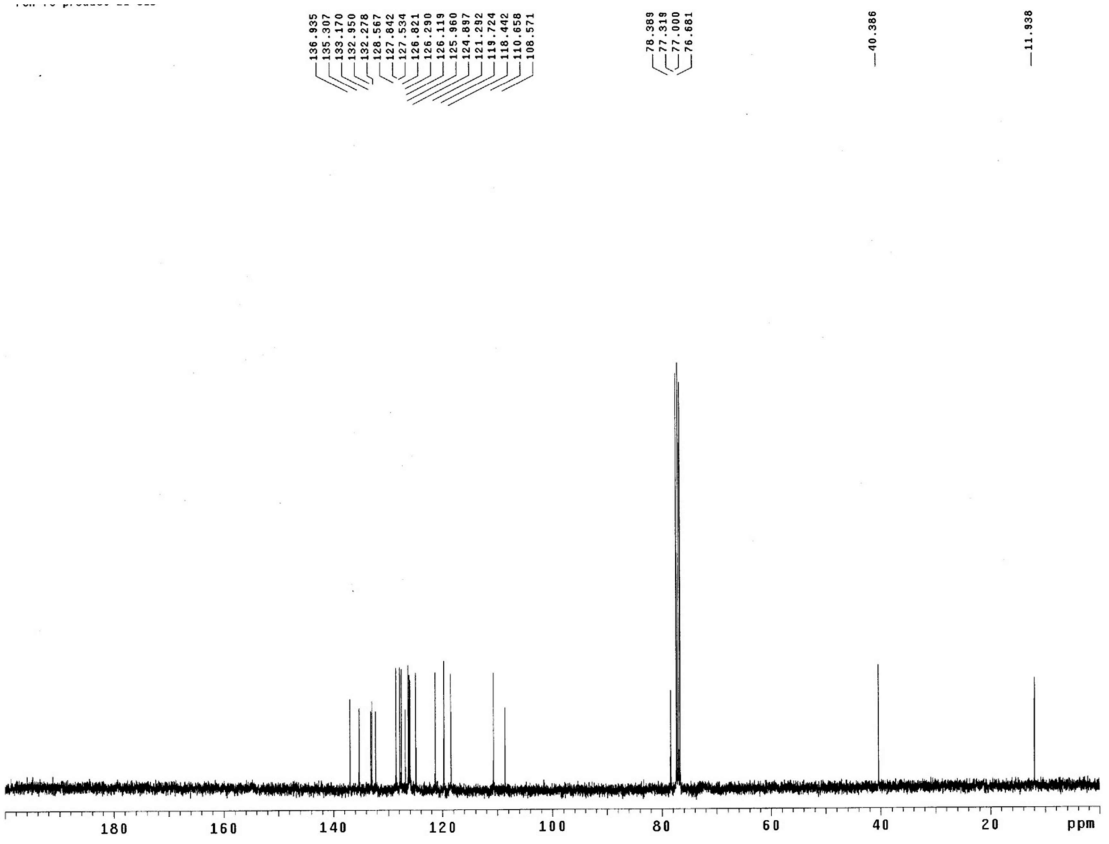
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **10jb**



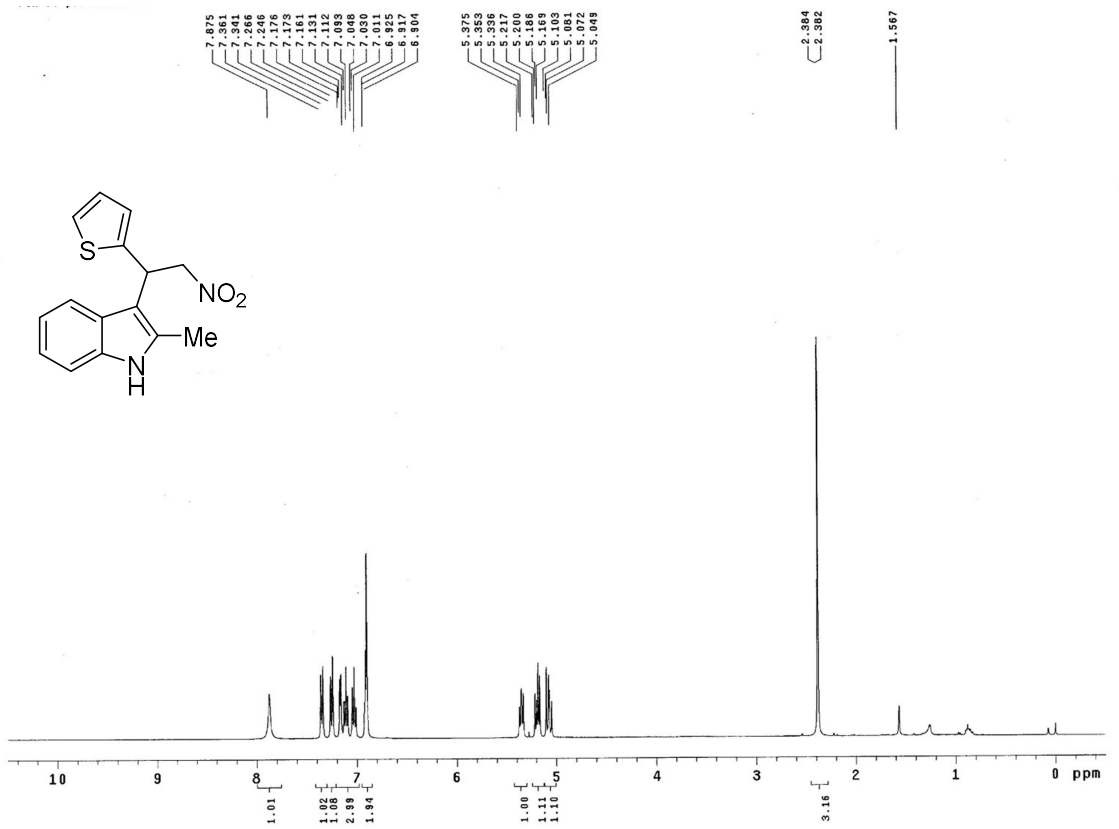
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **10kb** (table 6, entry 13)



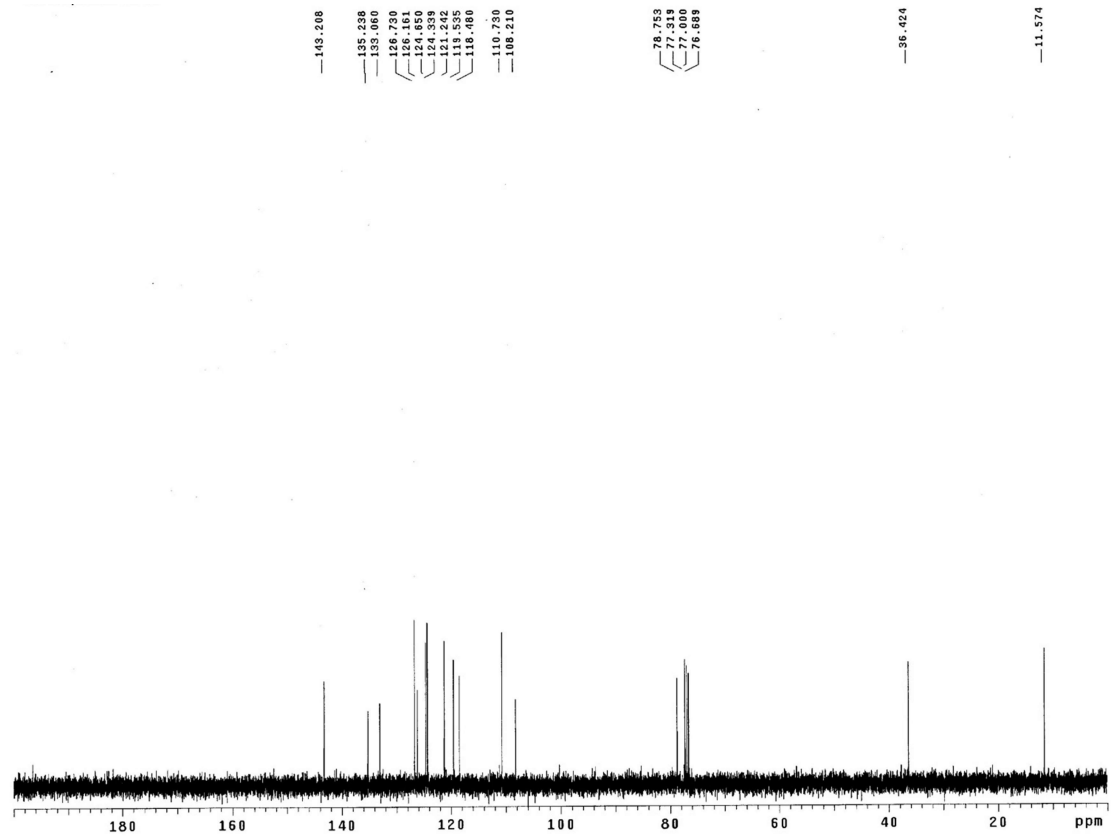
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **10kb**



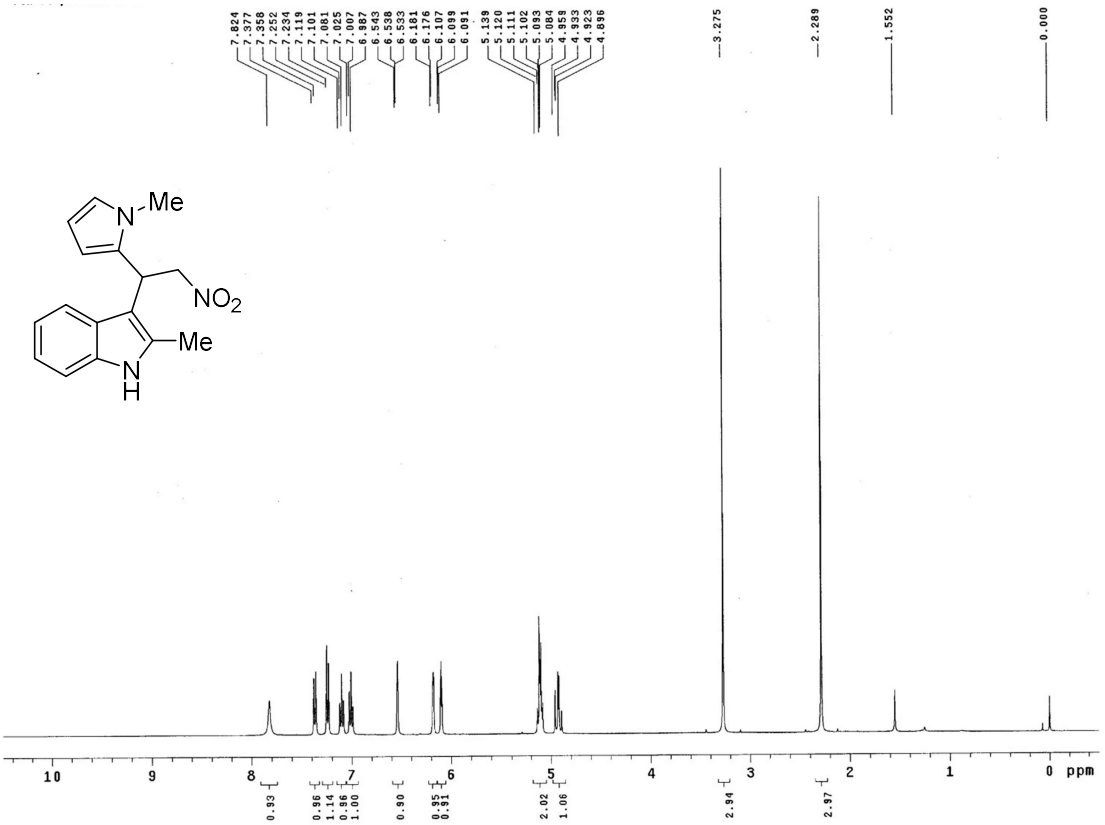
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **10hb** (table 6, entry 14)



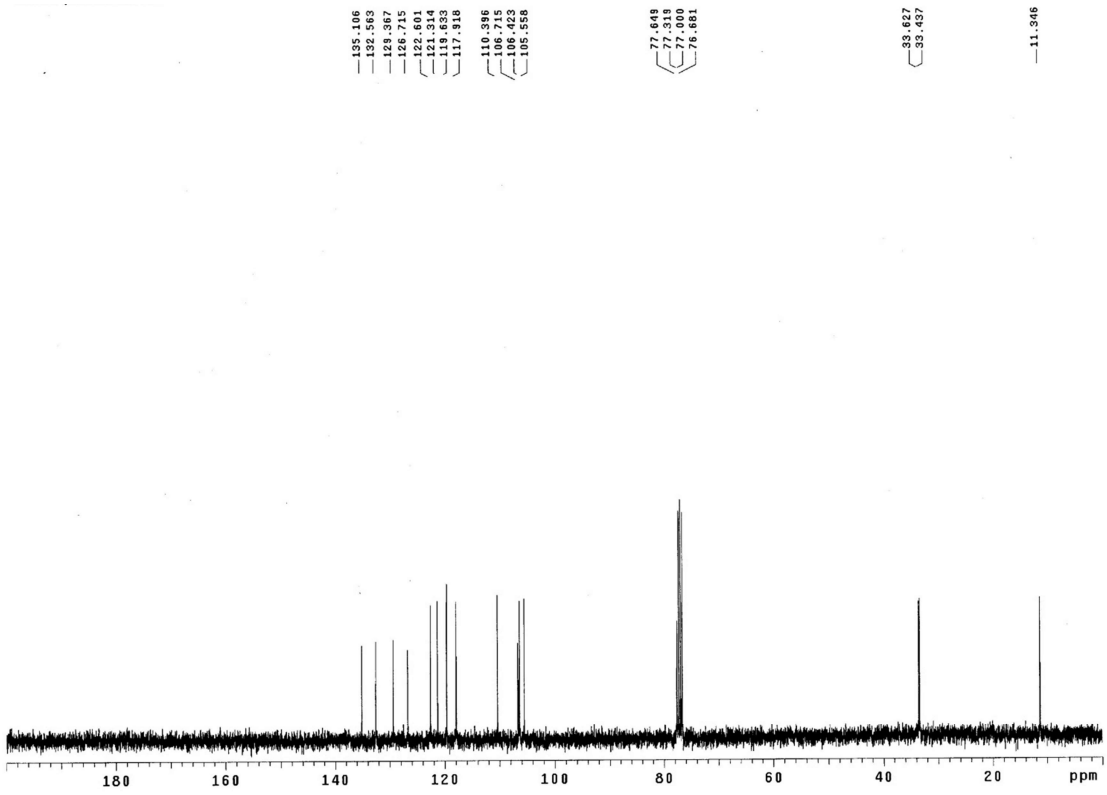
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **10hb**



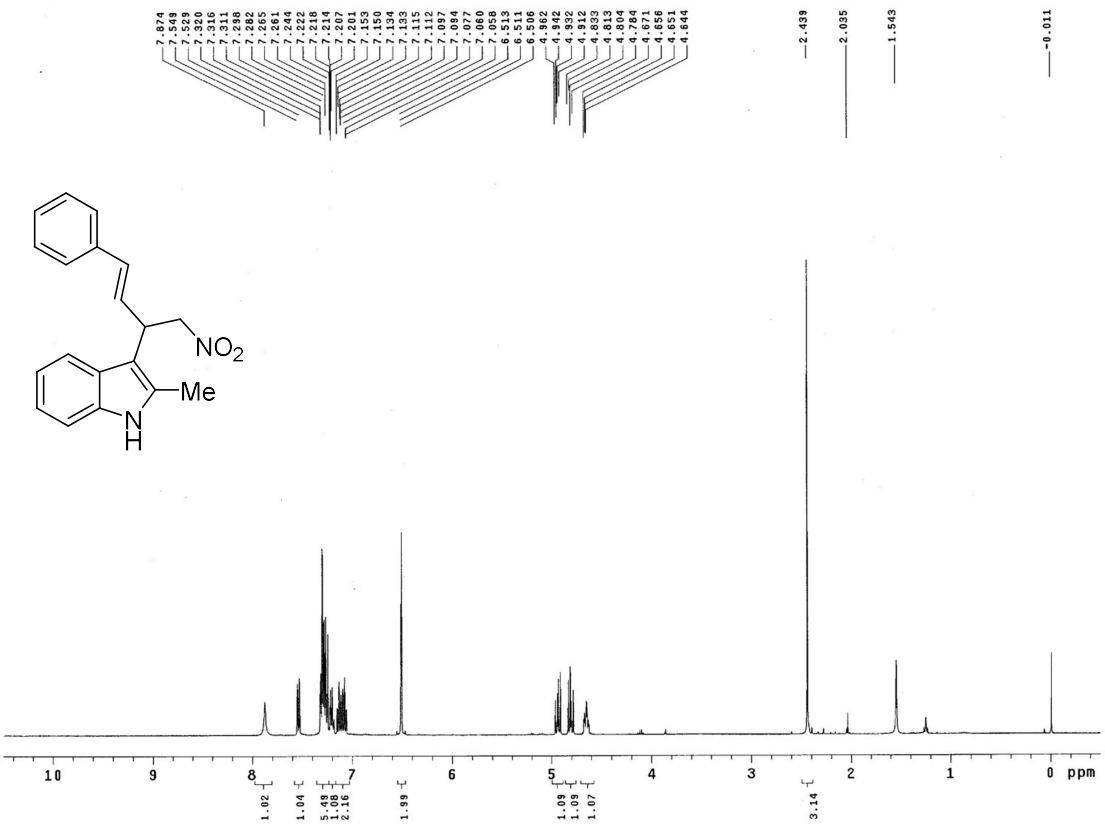
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **10lb** (table 6, entry 15)



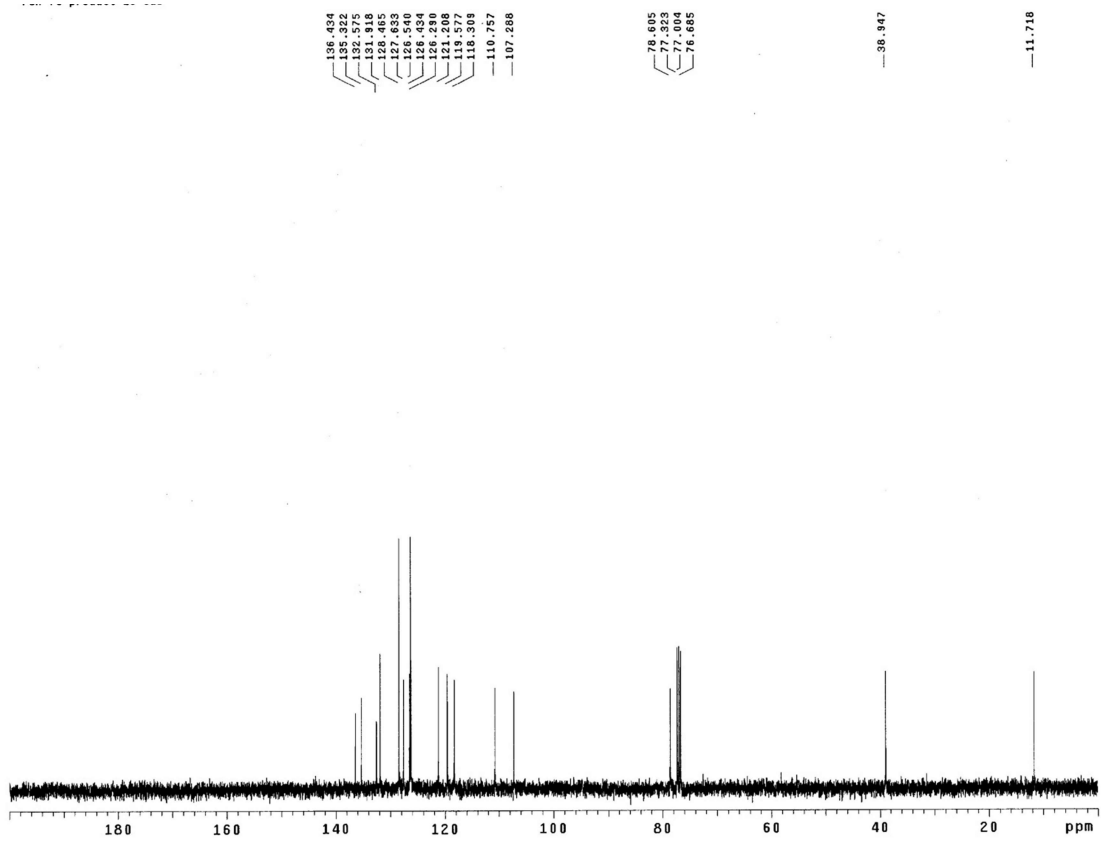
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **10lb**



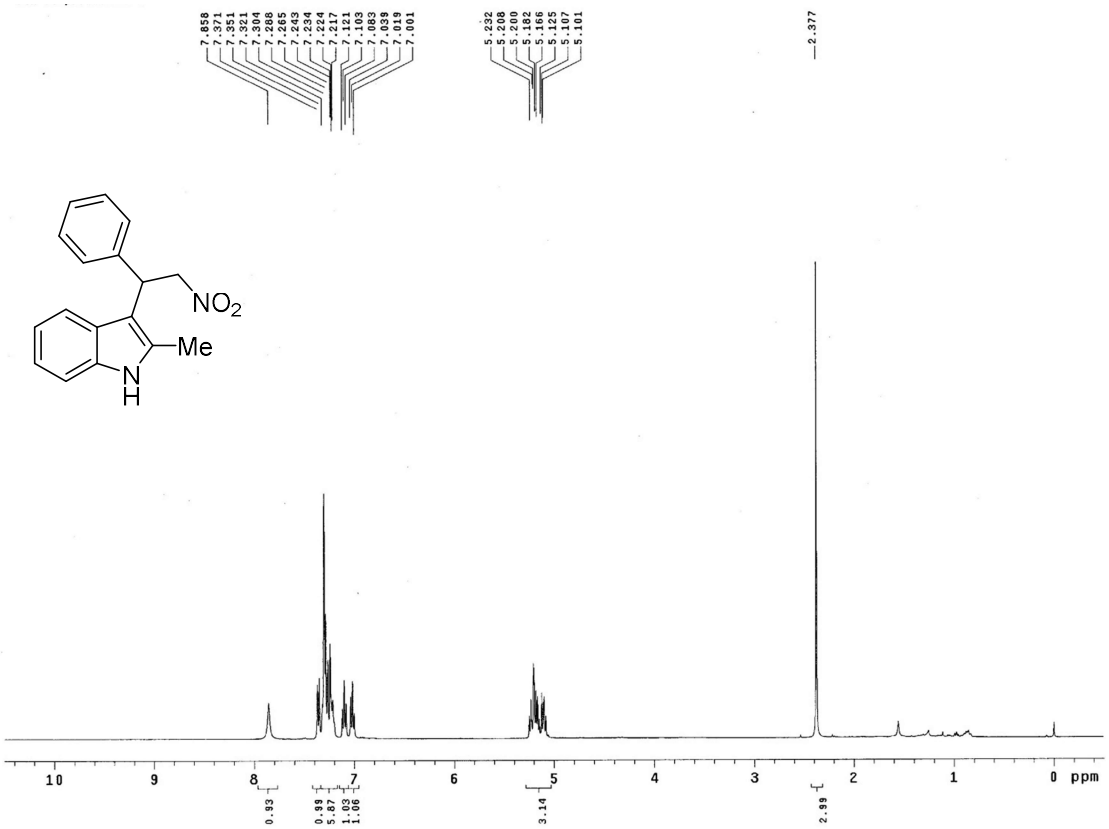
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **10mb** (table 6, entry 16)



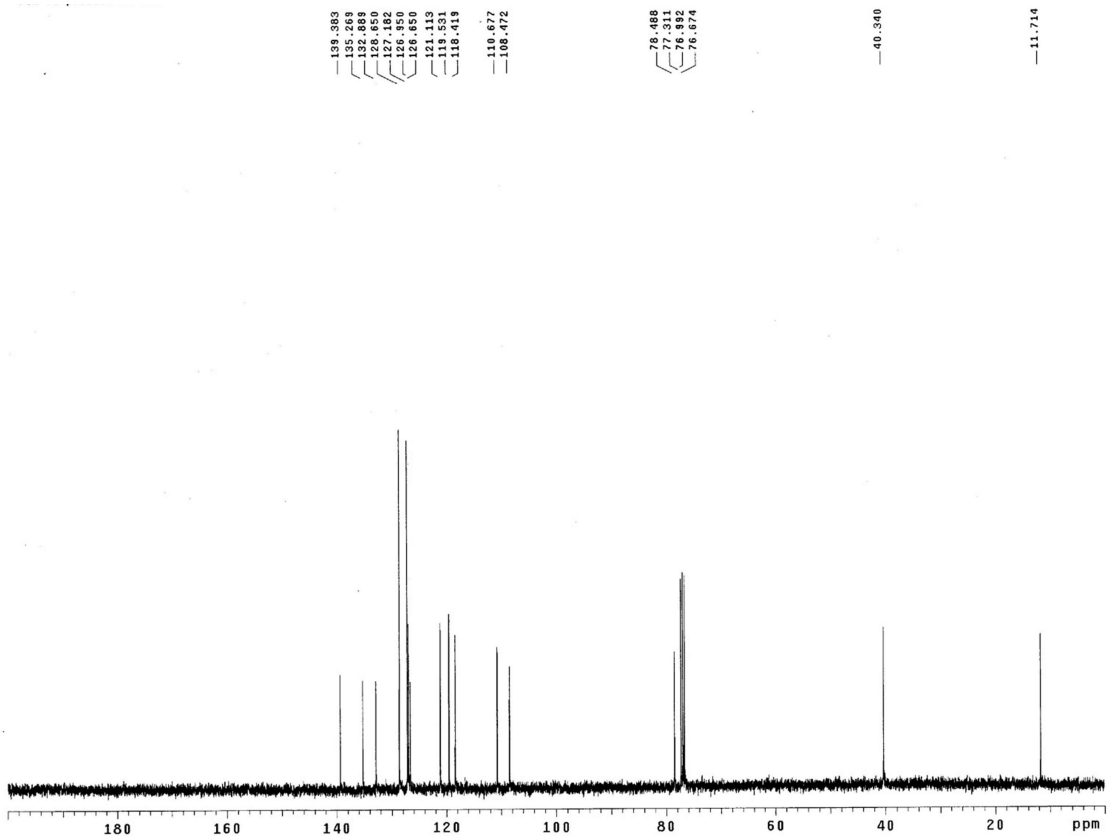
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **10mb**



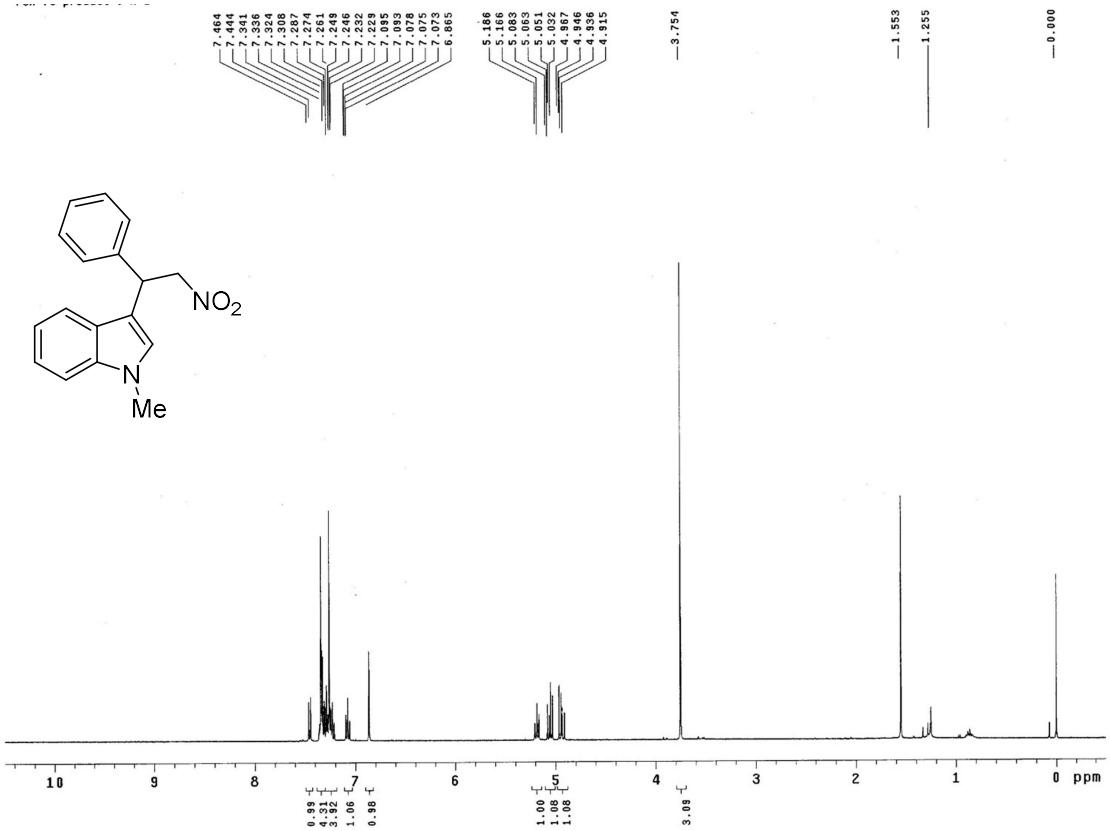
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **10ab** (table 6, entry 17)



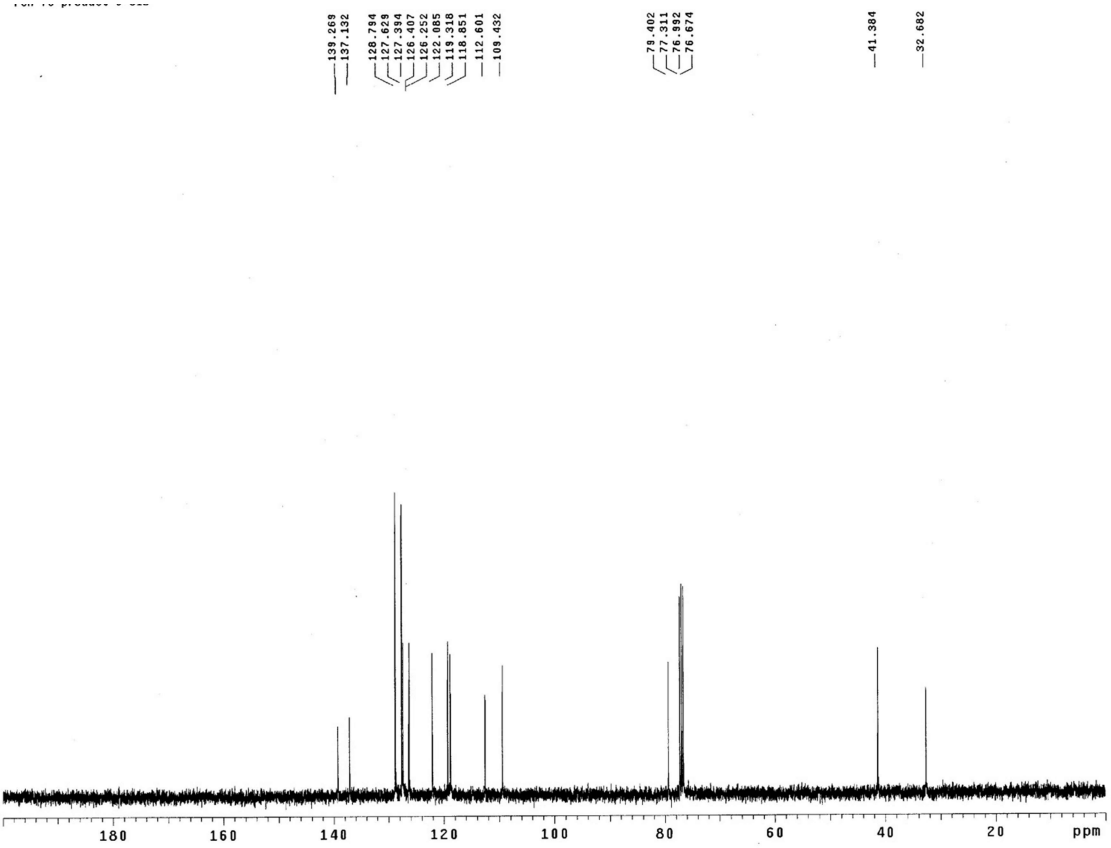
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **10ab**



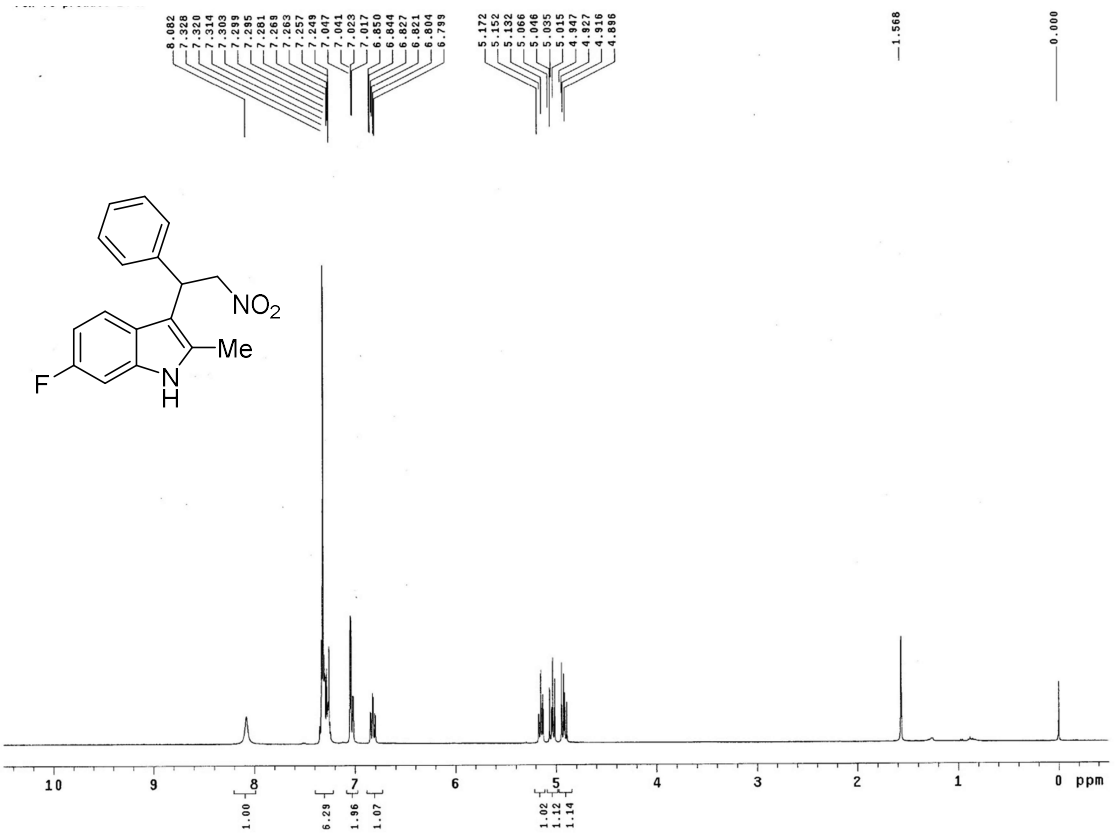
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **10ac** (table 6, entry 18)



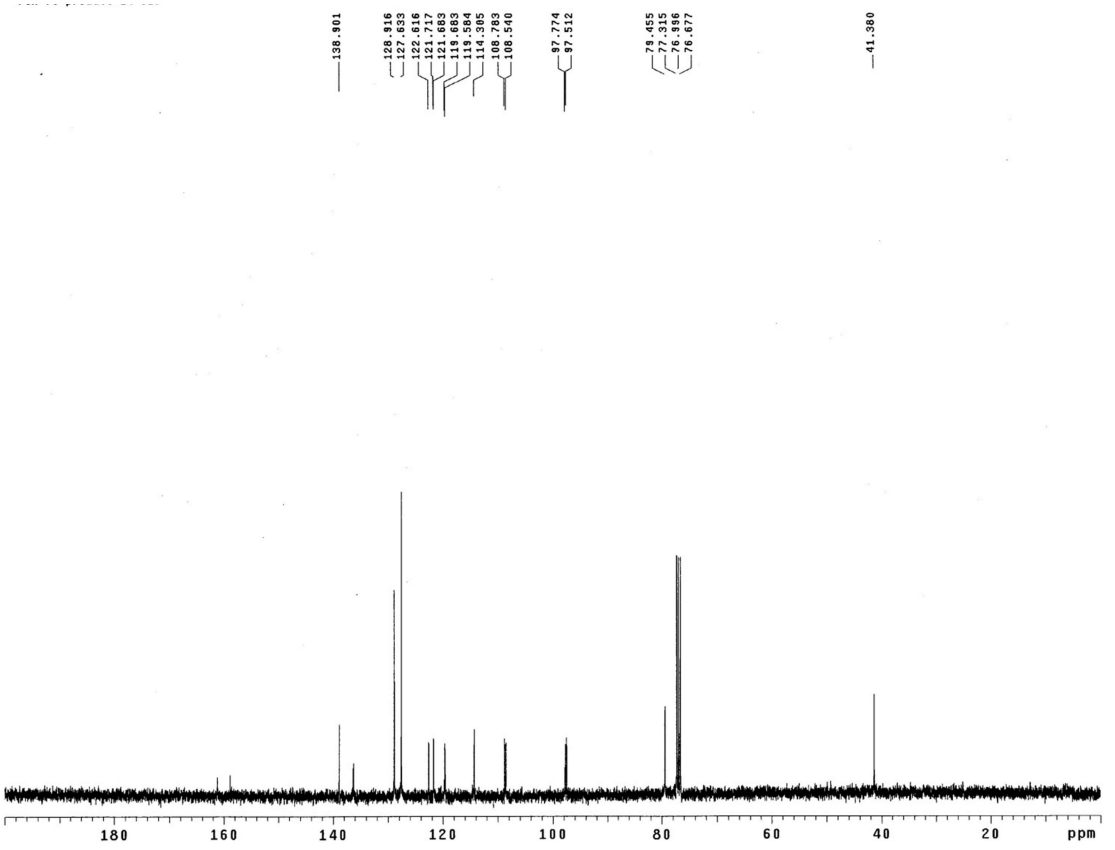
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **10ac**



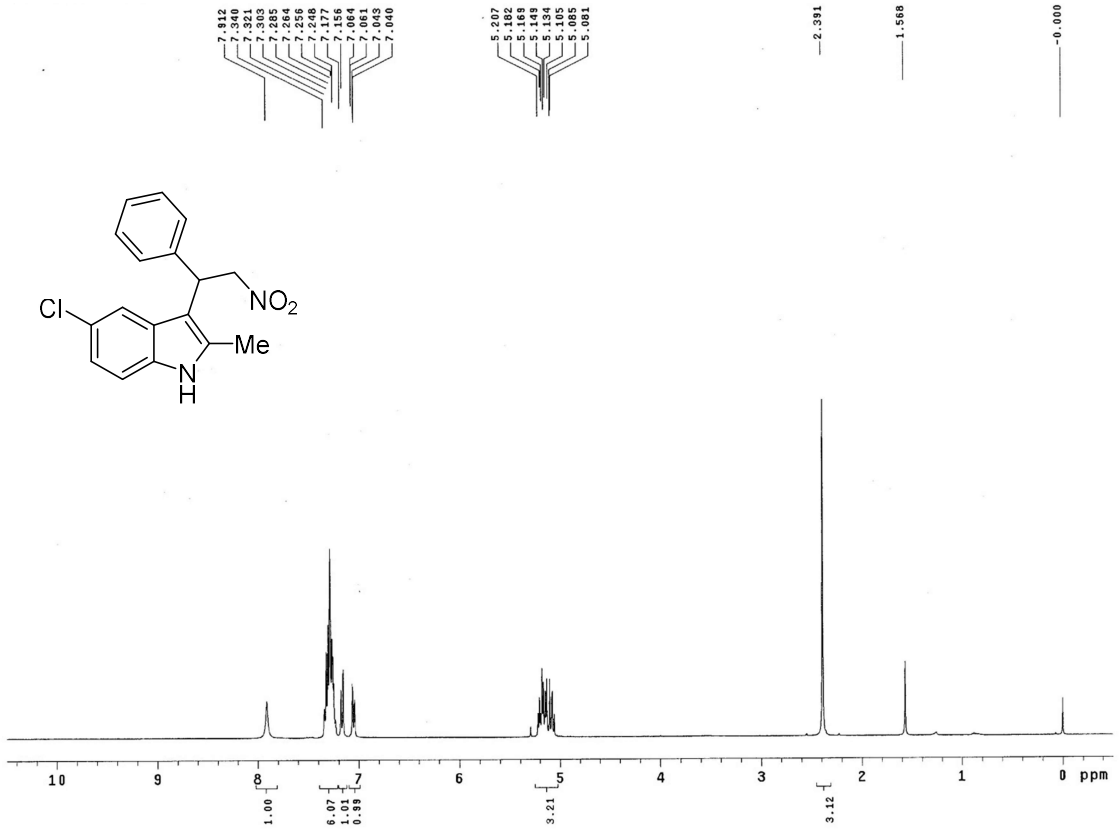
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **10ad** (table 6, entry 19)



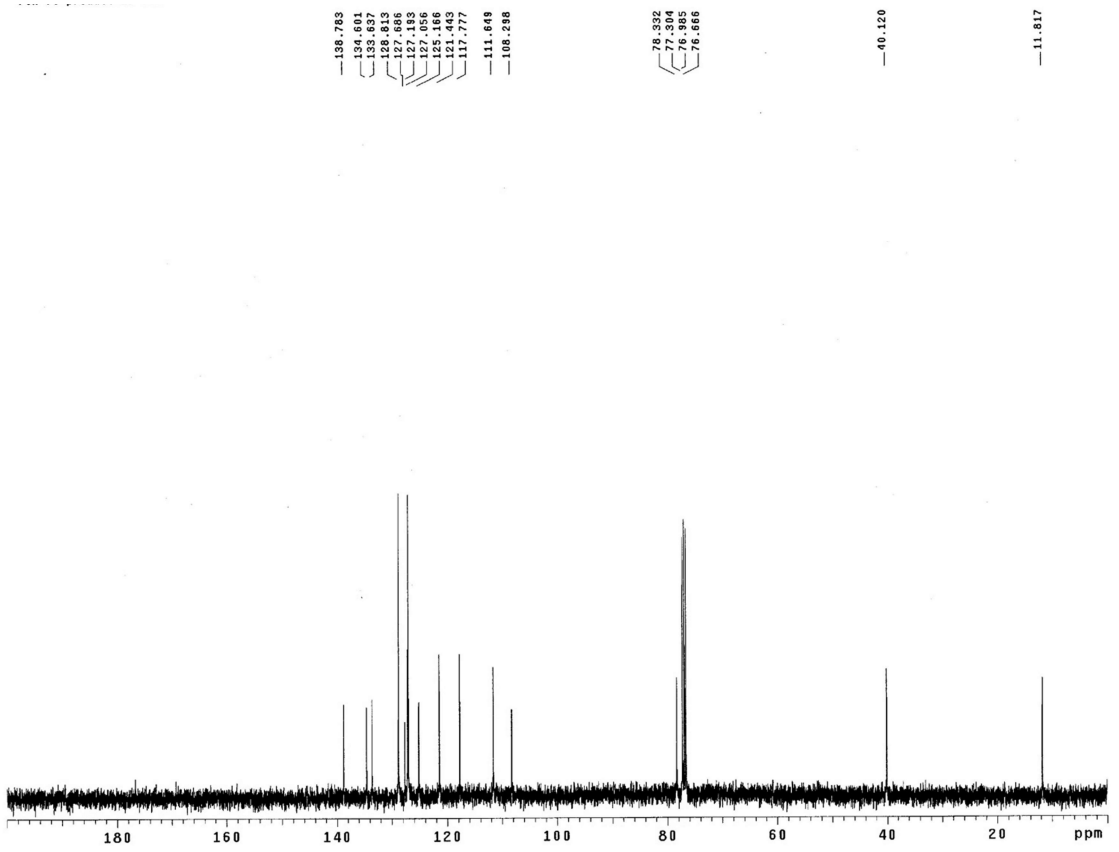
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **10ad**



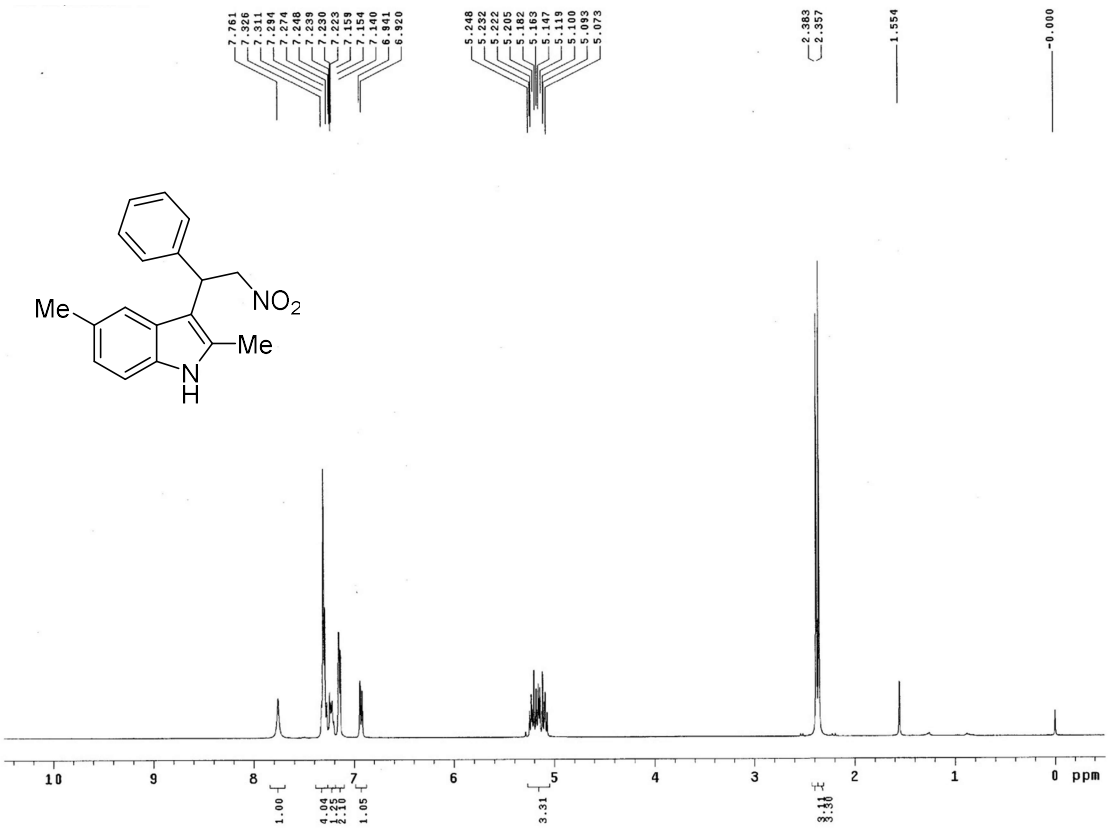
^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **10ae** (table 6, entry 20)



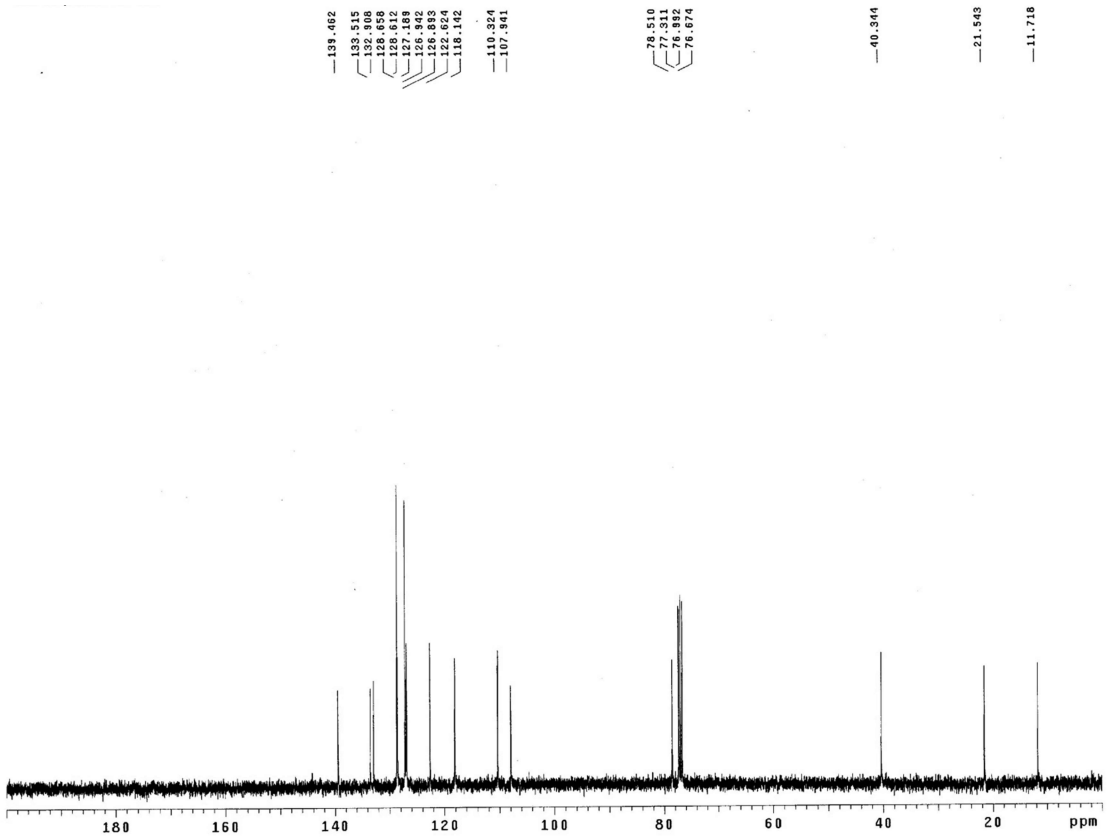
^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **10ae**



^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of compound **10af** (table 6, entry 21)



^{13}C NMR ($CDCl_3$, 100 MHz) spectrum of compound **10af**



4. X ray crystal structure of complexes 1c–Ag and 1c–Pd:

4.1 X ray crystal structure of 1c–Ag complex:

Table 1. Crystal data and structure refinement for l1ag_sq.

Identification code	l1ag_sq	
Empirical formula	C66 H64 Ag2 F12 N8 O4 P2	
Formula weight	1538.93	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 17.7431(6) Å	α= 90°.
	b = 15.6583(6) Å	β= 95.567(3)°.
	c = 26.3446(8) Å	γ = 90°.
Volume	7284.7(4) $Å^3$	
Z	4	
Density (calculated)	1.403 Mg/m^3	
Absorption coefficient	0.661 mm^{-1}	
F(000)	3120	
Crystal size	0.43 x 0.35 x 0.12 mm^3	
Theta range for data collection	2.816 to 29.183°.	
Index ranges	-23<=h<=22, -20<=k<=21, -34<=l<=23	
Reflections collected	38390	
Independent reflections	16974 [R(int) = 0.0433]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.88916	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	16974 / 2 / 893	
Goodness-of-fit on F^2	1.014	
Final R indices [I>2sigma(I)]	R1 = 0.0733, wR2 = 0.1780	
R indices (all data)	R1 = 0.1100, wR2 = 0.2013	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.229 and -1.440 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for l1ag_sq. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ag(1)	7559(1)	-2112(1)	2433(1)	32(1)
Ag(2)	7384(1)	796(1)	2447(1)	36(1)
O(1)	4852(4)	520(3)	615(2)	70(2)
O(2)	9272(3)	-1843(3)	436(2)	65(1)
O(3)	6143(3)	-2256(3)	4473(2)	55(1)
N(1)	5726(3)	679(3)	2708(2)	31(1)
N(2)	6493(2)	737(3)	3402(2)	29(1)
N(3)	8875(2)	-2024(3)	3288(2)	28(1)
N(4)	9316(2)	-1957(3)	2556(2)	30(1)
N(5)	5808(2)	-2170(3)	2344(2)	28(1)
N(6)	6205(2)	-2208(3)	1595(2)	29(1)
N(7)	8256(2)	832(3)	1488(2)	32(1)
N(8)	9044(3)	856(3)	2171(2)	37(1)
C(1)	5148(5)	1105(5)	271(3)	68(2)
C(2)	5070(4)	621(4)	1129(2)	45(2)
C(3)	4785(4)	13(4)	1448(3)	51(2)
C(4)	4981(4)	43(4)	1967(2)	43(1)
C(5)	5474(3)	674(3)	2172(2)	30(1)
C(6)	5727(3)	1297(3)	1854(2)	32(1)
C(7)	5533(3)	1273(4)	1330(2)	37(1)
C(8)	6471(3)	746(3)	2889(2)	28(1)
C(9)	5268(3)	621(3)	3110(2)	32(1)
C(10)	4491(3)	545(3)	3123(2)	39(1)
C(11)	4228(4)	491(4)	3601(3)	48(2)
C(12)	4728(4)	532(4)	4046(3)	46(2)
C(13)	5508(4)	619(3)	4038(2)	38(1)
C(14)	5765(3)	659(3)	3556(2)	32(1)
C(15)	7183(3)	857(3)	3751(2)	33(1)
C(16)	7493(4)	53(4)	4013(2)	39(1)
C(17)	7756(3)	-638(4)	3663(2)	35(1)
C(18)	8175(3)	-1351(4)	3978(2)	35(1)

C(19)	8342(3)	-2145(3)	3678(2)	29(1)
C(20)	8664(3)	-2017(3)	2782(2)	29(1)
C(21)	9664(3)	-1961(3)	3387(2)	31(1)
C(22)	10131(3)	-1978(4)	3840(2)	39(1)
C(23)	10910(3)	-1936(4)	3796(3)	47(2)
C(24)	11199(3)	-1868(4)	3327(3)	45(2)
C(25)	10726(3)	-1861(4)	2874(2)	38(1)
C(26)	9949(3)	-1914(3)	2919(2)	30(1)
C(27)	9327(3)	-1970(3)	2010(2)	32(1)
C(28)	8931(3)	-2586(4)	1725(2)	35(1)
C(29)	8895(3)	-2569(4)	1192(2)	42(1)
C(30)	9273(4)	-1935(4)	950(2)	44(2)
C(31)	9701(4)	-1336(4)	1240(2)	50(2)
C(32)	9724(4)	-1346(4)	1766(2)	42(1)
C(33)	8865(5)	-2481(5)	127(3)	73(2)
C(34)	5834(5)	-1588(5)	4764(2)	65(2)
C(35)	6001(4)	-2209(4)	3953(2)	39(1)
C(36)	6356(3)	-2840(4)	3683(2)	36(1)
C(37)	6270(3)	-2837(4)	3155(2)	33(1)
C(38)	5837(3)	-2203(3)	2889(2)	29(1)
C(39)	5464(3)	-1603(4)	3162(2)	35(1)
C(40)	5540(3)	-1599(4)	3693(2)	37(1)
C(41)	6446(3)	-2185(3)	2096(2)	28(1)
C(42)	5159(3)	-2176(3)	2002(2)	25(1)
C(43)	4392(3)	-2156(3)	2071(2)	31(1)
C(44)	3888(3)	-2168(3)	1629(2)	38(1)
C(45)	4146(3)	-2213(3)	1146(2)	37(1)
C(46)	4912(3)	-2232(3)	1076(2)	32(1)
C(47)	5412(3)	-2208(3)	1520(2)	28(1)
C(48)	6715(3)	-2281(4)	1191(2)	35(1)
C(49)	6792(4)	-1444(4)	900(2)	46(2)
C(50)	7146(3)	-697(4)	1220(2)	40(1)
C(51)	7339(4)	42(4)	881(2)	47(2)
C(52)	7555(3)	862(4)	1145(2)	43(1)
C(53)	8294(3)	831(3)	1998(2)	35(1)
C(54)	8982(3)	849(3)	1321(2)	35(1)

C(55)	9227(4)	846(4)	837(3)	42(1)
C(56)	10008(4)	854(4)	808(3)	51(2)
C(57)	10514(4)	870(4)	1247(3)	53(2)
C(58)	10267(3)	887(4)	1734(3)	46(2)
C(59)	9485(3)	861(3)	1760(2)	37(1)
C(60)	9320(4)	876(4)	2706(3)	51(2)
O(4)	10033(5)	760(5)	4261(3)	65(2)
C(61)	9047(7)	1380(7)	3036(5)	45(3)
C(62)	9285(8)	1339(11)	3553(5)	52(4)
C(63)	9831(6)	759(6)	3737(4)	47(2)
C(64)	10167(6)	239(6)	3408(3)	48(2)
C(66)	10705(9)	171(7)	4505(5)	145(9)
C(65)	9928(6)	274(6)	2882(4)	43(2)
O(4')	9536(14)	1247(16)	4294(8)	72(7)
C(61')	8815(18)	1680(30)	2982(15)	37(8)
C(62')	8936(16)	1784(19)	3505(11)	41(6)
C(63')	9398(19)	1260(30)	3778(12)	38(9)
C(64')	9780(20)	560(20)	3501(14)	48(2)
C(65')	9618(19)	460(20)	3001(13)	43(2)
C(66')	9160(30)	1850(20)	4590(17)	145(9)
P	7712(1)	-191(2)	7579(1)	104(1)
F(1)	7199(3)	-911(4)	7277(3)	133(3)
F(2)	7857(3)	-800(4)	8042(3)	110(2)
F(3)	8272(4)	440(4)	7821(4)	160(4)
F(4)	7559(4)	367(5)	7067(3)	142(3)
F(5)	8430(4)	-600(6)	7326(3)	156(3)
F(6)	6980(3)	168(5)	7805(3)	143(3)
P(2)	6768(2)	1553(2)	5404(1)	77(1)
F(7)	6417(5)	669(4)	5267(3)	145(3)
F(8)	6181(8)	1953(5)	4994(3)	218(6)
F(9)	7166(7)	2352(7)	5580(4)	230(6)
F(10)	7300(5)	1110(7)	5841(3)	180(4)
F(11)	6169(4)	1705(7)	5798(3)	172(4)
F(12)	7242(7)	1452(8)	4974(4)	251(7)

Table 3. Bond lengths [Å] and angles [°] for l1ag_sq.

Ag(1)-C(20)	2.089(5)
Ag(1)-C(41)	2.087(5)
Ag(2)-C(8)	2.087(5)
Ag(2)-C(53)	2.093(6)
O(1)-C(2)	1.380(7)
O(1)-C(1)	1.424(9)
O(2)-C(30)	1.360(7)
O(2)-C(33)	1.438(9)
O(3)-C(35)	1.372(6)
O(3)-C(34)	1.437(8)
N(1)-C(8)	1.365(7)
N(1)-C(9)	1.400(7)
N(1)-C(5)	1.440(7)
N(2)-C(8)	1.347(6)
N(2)-C(14)	1.396(7)
N(2)-C(15)	1.471(7)
N(3)-C(20)	1.348(6)
N(3)-C(21)	1.403(6)
N(3)-C(19)	1.476(6)
N(4)-C(20)	1.356(6)
N(4)-C(26)	1.403(6)
N(4)-C(27)	1.441(6)
N(5)-C(41)	1.362(6)
N(5)-C(42)	1.392(6)
N(5)-C(38)	1.433(6)
N(6)-C(41)	1.349(6)
N(6)-C(47)	1.403(6)
N(6)-C(48)	1.467(6)
N(7)-C(53)	1.339(7)
N(7)-C(54)	1.401(6)
N(7)-C(52)	1.466(7)
N(8)-C(53)	1.363(7)
N(8)-C(59)	1.397(7)
N(8)-C(60)	1.447(8)

C(2)-C(3)	1.396(9)
C(2)-C(7)	1.384(9)
C(3)-C(4)	1.380(8)
C(4)-C(5)	1.394(8)
C(5)-C(6)	1.389(7)
C(6)-C(7)	1.390(8)
C(9)-C(10)	1.387(8)
C(9)-C(14)	1.401(8)
C(10)-C(11)	1.388(9)
C(11)-C(12)	1.400(10)
C(12)-C(13)	1.394(9)
C(13)-C(14)	1.390(8)
C(15)-C(16)	1.514(8)
C(16)-C(17)	1.525(7)
C(17)-C(18)	1.538(7)
C(18)-C(19)	1.517(8)
C(21)-C(26)	1.380(7)
C(21)-C(22)	1.385(7)
C(22)-C(23)	1.398(8)
C(23)-C(24)	1.388(9)
C(24)-C(25)	1.390(8)
C(25)-C(26)	1.398(7)
C(27)-C(28)	1.372(8)
C(27)-C(32)	1.397(8)
C(28)-C(29)	1.401(8)
C(29)-C(30)	1.387(9)
C(30)-C(31)	1.389(9)
C(31)-C(32)	1.383(8)
C(35)-C(40)	1.393(8)
C(35)-C(36)	1.402(8)
C(36)-C(37)	1.385(7)
C(37)-C(38)	1.400(7)
C(38)-C(39)	1.388(7)
C(39)-C(40)	1.391(7)
C(42)-C(43)	1.392(7)
C(42)-C(47)	1.387(7)

C(43)-C(44)	1.398(8)
C(44)-C(45)	1.395(8)
C(45)-C(46)	1.388(8)
C(46)-C(47)	1.398(7)
C(48)-C(49)	1.531(8)
C(49)-C(50)	1.540(9)
C(50)-C(51)	1.521(8)
C(51)-C(52)	1.492(9)
C(54)-C(59)	1.390(8)
C(54)-C(55)	1.389(8)
C(55)-C(56)	1.394(9)
C(56)-C(57)	1.395(10)
C(57)-C(58)	1.395(10)
C(58)-C(59)	1.396(8)
C(60)-C(65')	1.11(4)
C(60)-C(61)	1.302(14)
C(60)-C(65)	1.473(13)
C(60)-C(61')	1.74(3)
O(4)-C(63)	1.392(12)
O(4)-C(66)	1.593(15)
C(61)-C(62)	1.389(19)
C(62)-C(63)	1.381(19)
C(63)-C(64)	1.368(14)
C(64)-C(65)	1.411(13)
O(4')-C(63')	1.36(4)
O(4')-C(66')	1.430(19)
C(61')-C(62')	1.38(5)
C(62')-C(63')	1.32(5)
C(63')-C(64')	1.51(6)
C(64')-C(65')	1.33(5)
P-F(3)	1.499(7)
P-F(2)	1.549(6)
P-F(5)	1.625(8)
P-F(4)	1.609(7)
P-F(6)	1.583(8)
P-F(1)	1.612(8)

P(2)-F(8)	1.557(10)
P(2)-F(12)	1.482(7)
P(2)-F(9)	1.489(7)
P(2)-F(10)	1.578(8)
P(2)-F(11)	1.576(7)
P(2)-F(7)	1.546(6)

C(20)-Ag(1)-C(41)	178.6(2)
C(8)-Ag(2)-C(53)	179.2(2)
C(2)-O(1)-C(1)	117.7(6)
C(30)-O(2)-C(33)	116.2(6)
C(35)-O(3)-C(34)	116.9(5)
C(8)-N(1)-C(9)	110.8(5)
C(8)-N(1)-C(5)	122.9(4)
C(9)-N(1)-C(5)	126.4(5)
C(8)-N(2)-C(14)	110.8(4)
C(8)-N(2)-C(15)	124.4(4)
C(14)-N(2)-C(15)	124.6(4)
C(20)-N(3)-C(21)	111.2(4)
C(20)-N(3)-C(19)	123.7(4)
C(21)-N(3)-C(19)	125.0(4)
C(20)-N(4)-C(26)	111.3(4)
C(20)-N(4)-C(27)	122.2(4)
C(26)-N(4)-C(27)	126.4(4)
C(41)-N(5)-C(42)	111.2(4)
C(41)-N(5)-C(38)	122.0(4)
C(42)-N(5)-C(38)	126.6(4)
C(41)-N(6)-C(47)	110.8(4)
C(41)-N(6)-C(48)	123.6(4)
C(47)-N(6)-C(48)	125.4(4)
C(53)-N(7)-C(54)	110.9(5)
C(53)-N(7)-C(52)	125.2(5)
C(54)-N(7)-C(52)	123.8(5)
C(53)-N(8)-C(59)	110.1(5)
C(53)-N(8)-C(60)	123.6(5)
C(59)-N(8)-C(60)	126.3(5)

O(1)-C(2)-C(3)	115.4(6)
O(1)-C(2)-C(7)	124.0(6)
C(3)-C(2)-C(7)	120.6(6)
C(2)-C(3)-C(4)	120.2(6)
C(5)-C(4)-C(3)	119.7(6)
C(4)-C(5)-C(6)	119.5(5)
C(4)-C(5)-N(1)	120.5(5)
C(6)-C(5)-N(1)	120.0(5)
C(5)-C(6)-C(7)	121.2(5)
C(2)-C(7)-C(6)	118.7(6)
N(2)-C(8)-N(1)	106.4(4)
N(2)-C(8)-Ag(2)	127.8(4)
N(1)-C(8)-Ag(2)	125.8(4)
N(1)-C(9)-C(10)	132.6(5)
N(1)-C(9)-C(14)	105.5(5)
C(10)-C(9)-C(14)	121.9(5)
C(11)-C(10)-C(9)	116.8(6)
C(10)-C(11)-C(12)	121.0(6)
C(11)-C(12)-C(13)	122.7(6)
C(14)-C(13)-C(12)	115.7(6)
N(2)-C(14)-C(13)	131.6(6)
N(2)-C(14)-C(9)	106.5(5)
C(13)-C(14)-C(9)	121.9(5)
N(2)-C(15)-C(16)	115.0(4)
C(17)-C(16)-C(15)	115.6(5)
C(16)-C(17)-C(18)	110.5(4)
C(17)-C(18)-C(19)	115.0(4)
N(3)-C(19)-C(18)	115.3(4)
N(4)-C(20)-N(3)	105.5(4)
N(4)-C(20)-Ag(1)	128.0(4)
N(3)-C(20)-Ag(1)	126.4(4)
C(26)-C(21)-N(3)	106.3(4)
C(26)-C(21)-C(22)	122.1(5)
N(3)-C(21)-C(22)	131.5(5)
C(21)-C(22)-C(23)	116.2(5)
C(22)-C(23)-C(24)	122.1(5)

C(25)-C(24)-C(23)	121.3(5)
C(24)-C(25)-C(26)	116.5(5)
C(21)-C(26)-N(4)	105.6(4)
C(21)-C(26)-C(25)	121.8(5)
N(4)-C(26)-C(25)	132.5(5)
C(28)-C(27)-C(32)	119.6(5)
C(28)-C(27)-N(4)	120.0(5)
C(32)-C(27)-N(4)	120.4(5)
C(27)-C(28)-C(29)	120.5(6)
C(30)-C(29)-C(28)	119.8(6)
O(2)-C(30)-C(31)	115.1(6)
O(2)-C(30)-C(29)	125.3(6)
C(31)-C(30)-C(29)	119.6(5)
C(32)-C(31)-C(30)	120.4(6)
C(31)-C(32)-C(27)	120.1(6)
C(40)-C(35)-C(36)	120.3(5)
C(40)-C(35)-O(3)	124.8(5)
C(36)-C(35)-O(3)	114.9(5)
C(35)-C(36)-C(37)	119.7(5)
C(38)-C(37)-C(36)	120.3(5)
C(37)-C(38)-C(39)	119.2(5)
C(37)-C(38)-N(5)	119.4(5)
C(39)-C(38)-N(5)	121.4(5)
C(38)-C(39)-C(40)	121.2(5)
C(35)-C(40)-C(39)	119.1(5)
N(6)-C(41)-N(5)	105.8(4)
N(6)-C(41)-Ag(1)	127.9(4)
N(5)-C(41)-Ag(1)	126.2(4)
C(43)-C(42)-C(47)	121.9(5)
C(43)-C(42)-N(5)	132.3(5)
C(47)-C(42)-N(5)	105.9(4)
C(42)-C(43)-C(44)	116.4(5)
C(43)-C(44)-C(45)	121.5(5)
C(46)-C(45)-C(44)	122.2(5)
C(47)-C(46)-C(45)	116.0(5)
C(46)-C(47)-C(42)	122.1(5)

C(46)-C(47)-N(6)	131.6(5)
C(42)-C(47)-N(6)	106.3(4)
N(6)-C(48)-C(49)	112.8(5)
C(48)-C(49)-C(50)	115.3(5)
C(51)-C(50)-C(49)	111.1(5)
C(52)-C(51)-C(50)	116.4(5)
C(51)-C(52)-N(7)	115.0(5)
N(7)-C(53)-N(8)	106.8(5)
N(7)-C(53)-Ag(2)	126.9(4)
N(8)-C(53)-Ag(2)	126.4(4)
C(59)-C(54)-N(7)	106.0(5)
C(59)-C(54)-C(55)	122.1(5)
N(7)-C(54)-C(55)	131.9(6)
C(56)-C(55)-C(54)	116.8(6)
C(55)-C(56)-C(57)	121.3(6)
C(58)-C(57)-C(56)	121.8(6)
C(57)-C(58)-C(59)	116.6(6)
C(54)-C(59)-N(8)	106.3(5)
C(54)-C(59)-C(58)	121.4(6)
N(8)-C(59)-C(58)	132.3(6)
C(65')-C(60)-N(8)	139.5(18)
C(61)-C(60)-N(8)	123.4(8)
C(61)-C(60)-C(65)	119.1(9)
N(8)-C(60)-C(65)	117.5(7)
C(65')-C(60)-C(61')	111(2)
N(8)-C(60)-C(61')	106.4(14)
C(63)-O(4)-C(66)	120.6(9)
C(60)-C(61)-C(62)	122.0(12)
C(63)-C(62)-C(61)	120.7(13)
C(64)-C(63)-C(62)	120.2(11)
C(64)-C(63)-O(4)	122.9(10)
C(62)-C(63)-O(4)	116.8(11)
C(63)-C(64)-C(65)	119.4(10)
C(64)-C(65)-C(60)	118.4(8)
C(63')-O(4')-C(66')	119(3)
C(62')-C(61')-C(60)	118(3)

C(63')-C(62')-C(61')	120(3)
O(4')-C(63')-C(62')	126(3)
O(4')-C(63')-C(64')	115(4)
C(62')-C(63')-C(64')	118(3)
C(65')-C(64')-C(63')	120(3)
C(60)-C(65')-C(64')	131(3)
F(3)-P-F(2)	91.1(4)
F(3)-P-F(5)	85.4(5)
F(2)-P-F(5)	90.1(4)
F(3)-P-F(4)	92.8(4)
F(2)-P-F(4)	174.8(5)
F(5)-P-F(4)	86.8(5)
F(3)-P-F(6)	98.1(5)
F(2)-P-F(6)	90.1(4)
F(5)-P-F(6)	176.4(5)
F(4)-P-F(6)	92.6(4)
F(3)-P-F(1)	172.4(6)
F(2)-P-F(1)	90.0(4)
F(5)-P-F(1)	87.1(5)
F(4)-P-F(1)	85.6(4)
F(6)-P-F(1)	89.4(4)
F(8)-P(2)-F(12)	84.6(7)
F(8)-P(2)-F(9)	98.2(7)
F(12)-P(2)-F(9)	92.4(5)
F(8)-P(2)-F(10)	174.7(7)
F(12)-P(2)-F(10)	99.7(8)
F(9)-P(2)-F(10)	84.8(6)
F(8)-P(2)-F(11)	87.0(6)
F(12)-P(2)-F(11)	171.5(7)
F(9)-P(2)-F(11)	89.8(5)
F(10)-P(2)-F(11)	88.7(5)
F(8)-P(2)-F(7)	88.4(4)
F(12)-P(2)-F(7)	88.5(5)
F(9)-P(2)-F(7)	173.4(7)
F(10)-P(2)-F(7)	88.6(5)
F(11)-P(2)-F(7)	90.3(5)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for l1ag_sq. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ag(1)	26(1)	45(1)	25(1)	-3(1)	0(1)	0(1)
Ag(2)	39(1)	35(1)	36(1)	-1(1)	13(1)	-5(1)
O(1)	112(5)	51(3)	42(3)	-9(2)	-20(3)	5(3)
O(2)	113(4)	56(3)	27(2)	2(2)	11(2)	6(3)
O(3)	90(4)	52(3)	23(2)	3(2)	9(2)	0(3)
N(1)	37(2)	23(2)	33(2)	-2(2)	6(2)	2(2)
N(2)	36(2)	22(2)	29(2)	-3(2)	5(2)	2(2)
N(3)	27(2)	34(2)	23(2)	2(2)	3(2)	0(2)
N(4)	31(2)	34(2)	25(2)	-1(2)	6(2)	0(2)
N(5)	33(2)	26(2)	26(2)	-3(2)	6(2)	-4(2)
N(6)	28(2)	34(2)	26(2)	-3(2)	2(2)	-4(2)
N(7)	30(2)	28(2)	39(3)	5(2)	11(2)	-1(2)
N(8)	37(3)	31(3)	44(3)	4(2)	6(2)	-12(2)
C(1)	111(7)	54(4)	35(4)	2(3)	-10(4)	25(4)
C(2)	63(4)	36(3)	34(3)	-4(3)	-6(3)	12(3)
C(3)	74(5)	27(3)	48(4)	-6(3)	-14(3)	-3(3)
C(4)	57(4)	21(3)	47(4)	2(3)	-8(3)	1(3)
C(5)	33(3)	21(2)	34(3)	-2(2)	2(2)	8(2)
C(6)	34(3)	27(3)	36(3)	-5(2)	7(2)	5(2)
C(7)	45(3)	28(3)	37(3)	0(2)	5(2)	12(2)
C(8)	32(3)	22(2)	31(3)	1(2)	3(2)	5(2)
C(9)	40(3)	22(3)	35(3)	-2(2)	12(2)	0(2)
C(10)	38(3)	26(3)	53(4)	-3(3)	9(3)	2(2)
C(11)	45(4)	32(3)	72(5)	-8(3)	27(3)	-2(3)
C(12)	63(4)	30(3)	52(4)	-6(3)	33(3)	-4(3)
C(13)	53(4)	23(3)	41(3)	-7(2)	15(3)	1(2)
C(14)	39(3)	19(2)	39(3)	-3(2)	14(2)	4(2)
C(15)	37(3)	33(3)	28(3)	-5(2)	-1(2)	-1(2)
C(16)	54(4)	37(3)	27(3)	-6(2)	3(2)	7(3)
C(17)	41(3)	38(3)	26(3)	-1(2)	3(2)	6(2)
C(18)	39(3)	41(3)	25(3)	2(2)	0(2)	5(2)

C(19)	25(2)	39(3)	25(2)	7(2)	6(2)	2(2)
C(20)	29(3)	33(3)	27(3)	-2(2)	5(2)	4(2)
C(21)	30(3)	29(3)	33(3)	9(2)	0(2)	-2(2)
C(22)	34(3)	47(4)	35(3)	9(3)	0(2)	-3(3)
C(23)	36(3)	53(4)	48(4)	15(3)	-10(3)	-5(3)
C(24)	23(3)	56(4)	56(4)	13(3)	0(2)	-7(3)
C(25)	30(3)	42(3)	45(3)	10(3)	7(2)	0(2)
C(26)	30(3)	31(3)	29(3)	7(2)	-1(2)	1(2)
C(27)	36(3)	34(3)	24(2)	-2(2)	0(2)	11(2)
C(28)	35(3)	40(3)	32(3)	1(2)	8(2)	7(2)
C(29)	47(3)	46(4)	33(3)	-8(3)	2(2)	6(3)
C(30)	70(4)	38(3)	26(3)	5(3)	7(3)	16(3)
C(31)	77(5)	36(3)	38(3)	9(3)	16(3)	0(3)
C(32)	60(4)	32(3)	35(3)	-2(3)	10(3)	-2(3)
C(33)	111(7)	80(6)	25(3)	-11(4)	1(4)	13(5)
C(34)	115(7)	54(4)	29(3)	-6(3)	17(4)	6(4)
C(35)	54(4)	40(3)	23(3)	1(2)	5(2)	-13(3)
C(36)	41(3)	36(3)	33(3)	7(2)	7(2)	-3(3)
C(37)	38(3)	31(3)	31(3)	4(2)	7(2)	1(2)
C(38)	31(3)	28(3)	27(3)	-2(2)	-2(2)	-7(2)
C(39)	41(3)	32(3)	31(3)	1(2)	6(2)	0(2)
C(40)	52(4)	29(3)	32(3)	-8(2)	8(2)	-3(3)
C(41)	25(2)	33(3)	26(2)	1(2)	3(2)	-5(2)
C(42)	27(2)	16(2)	31(3)	-1(2)	-1(2)	-4(2)
C(43)	31(3)	23(3)	39(3)	2(2)	10(2)	-3(2)
C(44)	25(3)	29(3)	58(4)	4(3)	-1(2)	-5(2)
C(45)	36(3)	28(3)	44(3)	0(2)	-11(2)	-1(2)
C(46)	39(3)	25(3)	31(3)	-1(2)	-2(2)	-3(2)
C(47)	30(3)	21(2)	32(3)	-2(2)	1(2)	0(2)
C(48)	35(3)	44(3)	28(3)	-7(2)	7(2)	-4(2)
C(49)	42(3)	66(4)	32(3)	4(3)	10(2)	-9(3)
C(50)	40(3)	48(4)	32(3)	5(3)	7(2)	1(3)
C(51)	42(3)	62(4)	38(3)	12(3)	10(3)	-4(3)
C(52)	34(3)	52(4)	45(3)	9(3)	9(2)	4(3)
C(53)	42(3)	26(3)	39(3)	1(2)	9(2)	-7(2)
C(54)	32(3)	27(3)	48(3)	4(2)	15(2)	0(2)

C(55)	44(3)	35(3)	50(4)	9(3)	18(3)	-2(3)
C(56)	52(4)	36(3)	70(5)	10(3)	33(3)	1(3)
C(57)	34(3)	40(4)	87(5)	10(3)	18(3)	-2(3)
C(58)	32(3)	35(3)	71(5)	14(3)	3(3)	-7(3)
C(59)	35(3)	27(3)	50(4)	4(2)	7(2)	-5(2)
C(60)	70(5)	45(4)	40(4)	-1(3)	10(3)	-35(4)
O(4)	90(6)	57(5)	44(4)	-6(3)	-3(4)	-13(4)
C(61)	33(6)	33(6)	69(7)	-3(5)	11(6)	-11(4)
C(62)	56(8)	53(8)	46(8)	-25(8)	9(7)	-18(6)
C(63)	53(6)	46(5)	43(5)	-9(4)	5(4)	-18(5)
C(64)	57(6)	41(5)	45(5)	-2(4)	-3(4)	-6(4)
C(66)	300(20)	50(7)	106(10)	-37(7)	135(14)	-65(11)
C(65)	55(6)	29(4)	45(5)	-6(4)	5(4)	-9(4)
O(4')	78(17)	78(17)	57(14)	-6(12)	-20(12)	-18(14)
C(61')	16(15)	50(20)	47(17)	-6(16)	15(12)	-3(12)
C(62')	34(14)	37(15)	52(17)	3(13)	13(12)	-4(11)
C(63')	16(13)	60(20)	34(18)	-20(20)	5(13)	-5(13)
C(64')	57(6)	41(5)	45(5)	-2(4)	-3(4)	-6(4)
C(65')	55(6)	29(4)	45(5)	-6(4)	5(4)	-9(4)
C(66')	300(20)	50(7)	106(10)	-37(7)	135(14)	-65(11)
P	41(1)	114(2)	155(3)	70(2)	0(1)	-11(1)
F(1)	78(4)	122(5)	187(7)	45(5)	-46(4)	-25(4)
F(2)	77(4)	115(5)	135(5)	58(4)	-12(3)	-21(3)
F(3)	120(6)	88(4)	260(10)	45(6)	-50(6)	-46(4)
F(4)	124(6)	131(6)	165(7)	61(5)	-10(5)	-5(5)
F(5)	67(4)	236(10)	161(7)	-11(6)	-4(4)	27(5)
F(6)	66(4)	137(6)	221(8)	29(6)	-6(4)	17(4)
P(2)	96(2)	100(2)	36(1)	-14(1)	10(1)	-53(1)
F(7)	170(7)	118(5)	137(6)	37(4)	-43(5)	-76(5)
F(8)	446(18)	103(6)	90(5)	17(4)	-50(8)	11(8)
F(9)	321(13)	202(9)	179(9)	-116(8)	81(9)	-180(10)
F(10)	155(7)	216(9)	150(7)	-31(7)	-83(6)	26(7)
F(11)	82(4)	338(13)	96(5)	2(6)	18(4)	-14(6)
F(12)	322(14)	289(13)	176(8)	-142(9)	190(10)	-153(11)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for l1ag_sq.

	x	y	z	U(eq)
H(1A)	4950	964	-79	102
H(1B)	4995	1687	352	102
H(1C)	5701	1067	304	102
H(3A)	4456	-422	1306	61
H(4A)	4781	-366	2184	51
H(6A)	6038	1747	1996	39
H(7A)	5715	1697	1114	44
H(10A)	4156	530	2820	46
H(11A)	3701	426	3627	58
H(12A)	4526	498	4367	56
H(13A)	5843	650	4341	46
H(15A)	7076	1278	4015	39
H(15B)	7580	1104	3555	39
H(16A)	7925	213	4261	47
H(16B)	7095	-192	4209	47
H(17A)	8098	-384	3429	42
H(17B)	7313	-882	3455	42
H(18A)	7867	-1518	4255	42
H(18B)	8660	-1119	4138	42
H(19A)	8551	-2587	3921	35
H(19B)	7859	-2366	3509	35
H(22A)	9935	-2017	4162	46
H(23A)	11251	-1954	4097	56
H(24A)	11731	-1825	3314	54
H(25A)	10920	-1822	2551	46
H(28A)	8681	-3026	1891	42
H(29A)	8611	-2990	996	50
H(31A)	9979	-917	1076	59
H(32A)	10010	-927	1962	50
H(33A)	8900	-2354	-234	109

H(33B)	9086	-3044	208	109
H(33C)	8332	-2479	196	109
H(34A)	5972	-1689	5129	98
H(34B)	6039	-1036	4668	98
H(34C)	5282	-1582	4695	98
H(36A)	6654	-3268	3862	44
H(37A)	6507	-3267	2971	40
H(39A)	5152	-1188	2983	42
H(40A)	5281	-1187	3875	45
H(43A)	4219	-2136	2401	37
H(44A)	3359	-2145	1658	45
H(45A)	3786	-2231	854	44
H(46A)	5085	-2259	747	38
H(48A)	6522	-2730	947	42
H(48B)	7222	-2461	1344	42
H(49A)	6282	-1268	750	56
H(49B)	7104	-1552	615	56
H(50A)	6787	-500	1460	48
H(50B)	7612	-896	1423	48
H(51A)	7763	-138	687	57
H(51B)	6896	151	631	57
H(52A)	7136	1041	1344	52
H(52B)	7610	1306	883	52
H(55A)	8880	840	539	50
H(56A)	10198	847	483	61
H(57A)	11043	870	1214	64
H(58A)	10613	913	2033	55
H(61A)	8674	1789	2919	53
H(62A)	9070	1715	3783	62
H(64A)	10558	-143	3533	58
H(66A)	10767	253	4875	218
H(66B)	10585	-429	4428	218
H(66C)	11175	325	4361	218
H(65A)	10154	-81	2647	52
H(61B)	8469	2031	2781	45
H(62B)	8689	2232	3667	49

H(64B)	10134	195	3684	58
H(65B)	9789	-70	2873	52
H(66D)	9318	1760	4953	218
H(66E)	9296	2431	4494	218
H(66F)	8612	1774	4527	218

4.2 X ray crystal structure of 1c–Pd complex:

Table 1. Crystal data and structure refinement for l1pd.

Identification code	l1pd	
Empirical formula	C68 H68 Cl7 F6 N8 O4 P Pd2	
Formula weight	1667.22	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 12.6608(10) Å	α= 87.943(3)°.
	b = 17.1920(14) Å	β= 84.738(3)°.
	c = 18.8963(15) Å	γ = 76.841(3)°.
Volume	3987.7(6) $Å^3$	
Z	2	
Density (calculated)	1.389 Mg/m^3	
Absorption coefficient	0.767 mm^{-1}	
F(000)	1688	
Crystal size	0.250 x 0.240 x 0.030 mm^3	
Theta range for data collection	2.838 to 26.500°.	
Index ranges	-15<=h<=15, -21<=k<=21, -23<=l<=23	
Reflections collected	84054	
Independent reflections	16416 [R(int) = 0.0687]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9281 and 0.7631	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	16416 / 2 / 870	
Goodness-of-fit on F^2	1.067	
Final R indices [I>2sigma(I)]	R1 = 0.1096, wR2 = 0.2830	
R indices (all data)	R1 = 0.1375, wR2 = 0.3036	
Extinction coefficient	0.0066(6)	
Largest diff. peak and hole	2.413 and -2.193 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for l1pd. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pd(1)	7912(1)	8298(1)	8636(1)	30(1)
Pd(2)	8274(1)	8328(1)	6277(1)	46(1)
Cl(1)	7887(2)	8704(2)	7455(1)	45(1)
Cl(2)	7767(3)	8072(2)	9837(1)	60(1)
Cl(3)	8639(3)	8115(2)	5088(1)	74(1)
O(1)	12143(6)	5570(4)	9069(4)	43(2)
O(2)	6156(9)	5270(6)	5864(6)	76(3)
O(3)	3462(8)	10846(5)	7925(5)	62(3)
O(4)	10491(9)	11386(6)	6637(5)	84(4)
N(1)	9987(7)	8757(4)	8968(4)	31(2)
N(2)	8761(7)	9830(4)	8733(4)	34(2)
N(3)	6292(7)	9702(6)	6156(4)	43(2)
N(4)	5948(7)	8540(6)	5930(4)	45(2)
N(5)	5822(7)	7763(5)	8419(4)	40(2)
N(6)	7161(7)	6753(4)	8643(4)	31(2)
N(7)	10264(8)	6974(8)	6338(5)	63(4)
N(8)	10665(7)	8115(8)	6547(5)	57(3)
C(1)	8943(8)	8999(6)	8762(5)	35(2)
C(2)	10420(8)	9413(6)	9051(5)	34(2)
C(3)	11454(9)	9469(7)	9236(5)	42(2)
C(4)	11608(10)	10230(7)	9282(5)	43(2)
C(5)	10818(10)	10905(6)	9143(5)	41(2)
C(6)	9830(9)	10850(6)	8926(5)	41(2)
C(7)	9655(9)	10105(6)	8910(5)	36(2)
C(8)	7791(9)	10342(6)	8480(5)	41(2)
C(9)	8017(9)	10696(6)	7732(6)	44(3)
C(10)	6962(10)	11146(7)	7432(6)	52(3)
C(11)	6317(9)	10611(8)	7118(6)	53(3)
C(12)	6815(9)	10295(7)	6391(5)	47(3)
C(13)	5196(8)	9851(8)	5990(5)	47(3)
C(14)	4402(9)	10556(8)	5950(5)	53(3)

C(15)	3371(8)	10466(9)	5764(6)	54(4)
C(16)	3173(9)	9742(9)	5623(6)	57(4)
C(17)	3966(9)	9035(8)	5657(5)	52(3)
C(18)	4984(9)	9126(8)	5834(5)	50(3)
C(19)	6717(8)	8907(7)	6119(5)	46(3)
C(20)	10520(8)	7927(5)	9000(5)	31(2)
C(21)	10629(9)	7458(6)	8418(5)	38(2)
C(22)	11168(8)	6662(6)	8454(5)	34(2)
C(23)	11612(8)	6352(5)	9073(5)	35(2)
C(24)	11533(9)	6842(6)	9664(5)	40(2)
C(25)	11001(8)	7625(6)	9615(5)	34(2)
C(26)	12649(9)	5246(6)	9684(7)	49(3)
C(27)	6048(8)	7715(8)	5901(6)	50(3)
C(28)	5776(11)	7374(8)	5299(6)	58(4)
C(29)	5845(14)	6557(9)	5286(9)	79(5)
C(30)	6128(12)	6070(9)	5862(8)	73(5)
C(31)	6426(10)	6394(10)	6448(9)	79(6)
C(32)	6370(9)	7220(9)	6482(6)	60(4)
C(33)	6592(17)	4872(13)	6465(16)	77(7)
C(33')	5757(18)	4929(16)	5346(11)	77(7)
C(34)	6886(9)	7560(5)	8556(5)	35(2)
C(35)	5415(9)	7053(6)	8420(5)	37(2)
C(36)	4388(9)	6943(7)	8309(6)	45(3)
C(37)	4288(10)	6145(7)	8329(6)	51(3)
C(38)	5154(11)	5516(7)	8468(5)	47(3)
C(39)	6153(10)	5636(6)	8606(6)	49(3)
C(40)	6274(9)	6431(6)	8548(5)	36(2)
C(41)	8253(9)	6282(6)	8771(5)	40(2)
C(42)	8803(10)	5802(6)	8140(6)	47(3)
C(43)	8920(9)	6315(6)	7477(5)	45(3)
C(44)	9537(11)	5834(9)	6839(6)	67(4)
C(45)	9677(11)	6383(10)	6202(6)	67(4)
C(46)	11394(9)	6837(11)	6449(6)	67(5)
C(47)	12190(11)	6107(10)	6408(6)	76(5)
C(48)	13241(12)	6196(13)	6512(7)	88(7)
C(49)	13484(10)	6917(12)	6626(7)	74(5)

C(50)	12686(9)	7617(10)	6667(6)	67(4)
C(51)	11635(9)	7569(9)	6582(6)	57(4)
C(52)	9841(10)	7752(8)	6400(5)	57(4)
C(53)	5229(8)	8554(6)	8315(5)	42(3)
C(54)	5253(9)	9144(6)	8787(5)	44(3)
C(55)	4676(10)	9927(7)	8673(6)	53(3)
C(56)	4050(10)	10092(6)	8087(6)	47(3)
C(57)	4002(9)	9513(7)	7639(6)	45(3)
C(58)	4590(9)	8716(6)	7739(5)	37(2)
C(59)	3533(12)	11476(7)	8334(7)	61(4)
C(60)	10565(9)	8958(8)	6598(6)	56(4)
C(61)	11006(9)	9265(9)	7168(6)	61(4)
C(62)	10993(9)	10063(8)	7175(6)	59(4)
C(63)	10532(10)	10598(9)	6658(6)	66(4)
C(64)	10079(10)	10273(9)	6095(6)	66(4)
C(65)	10138(9)	9495(10)	6069(6)	66(4)
C(66)	10981(13)	11691(10)	7175(8)	79(5)
Cl(4)	7985(4)	1954(3)	5236(3)	88(1)
Cl(6)	3955(5)	8111(3)	10105(3)	106(2)
Cl(5)	8320(5)	3541(3)	5476(3)	104(2)
Cl(7)	5647(6)	6896(4)	10593(5)	162(3)
C(67)	8608(11)	2557(9)	5739(7)	61(4)
C(68)	4409(15)	7067(12)	10295(9)	94(6)
P	8014(4)	3289(2)	8060(2)	69(1)
F(1)	8275(13)	2723(6)	7416(5)	126(5)
F(2)	8880(13)	2727(7)	8450(9)	162(7)
F(3)	7869(17)	3864(7)	8701(6)	194(9)
F(4)	7250(30)	3810(20)	7627(16)	390(30)
F(5)	8680(30)	3812(12)	7719(9)	317(18)
F(6)	7244(18)	2820(20)	8394(10)	293(16)

Table 3. Bond lengths [Å] and angles [°] for l1pd.

Pd(1)-C(1)	2.000(11)
Pd(1)-C(34)	2.031(11)
Pd(1)-Cl(2)	2.286(3)
Pd(1)-Cl(1)	2.315(2)
Pd(2)-C(19)	2.039(10)
Pd(2)-C(52)	2.036(10)
Pd(2)-Cl(3)	2.277(3)
Pd(2)-Cl(1)	2.318(3)
O(1)-C(23)	1.359(11)
O(1)-C(26)	1.414(13)
O(2)-C(30)	1.368(19)
O(2)-C(33)	1.40(3)
O(2)-C(33')	1.351(2)
O(3)-C(56)	1.379(12)
O(3)-C(59)	1.377(15)
O(4)-C(63)	1.344(19)
O(4)-C(66)	1.41(2)
N(1)-C(2)	1.382(12)
N(1)-C(1)	1.380(13)
N(1)-C(20)	1.434(11)
N(2)-C(1)	1.395(12)
N(2)-C(7)	1.393(14)
N(2)-C(8)	1.448(13)
N(3)-C(13)	1.416(14)
N(3)-C(12)	1.438(16)
N(3)-C(19)	1.352(15)
N(4)-C(19)	1.354(16)
N(4)-C(27)	1.398(16)
N(4)-C(18)	1.415(12)
N(5)-C(34)	1.358(14)
N(5)-C(35)	1.429(14)
N(5)-C(53)	1.412(13)
N(6)-C(34)	1.359(12)
N(6)-C(40)	1.390(13)

N(6)-C(41)	1.470(13)
N(7)-C(52)	1.328(17)
N(7)-C(46)	1.429(16)
N(7)-C(45)	1.43(2)
N(8)-C(52)	1.384(19)
N(8)-C(51)	1.371(13)
N(8)-C(60)	1.432(19)
C(2)-C(7)	1.386(14)
C(2)-C(3)	1.410(15)
C(3)-C(4)	1.373(15)
C(4)-C(5)	1.384(16)
C(5)-C(6)	1.375(16)
C(6)-C(7)	1.352(14)
C(8)-C(9)	1.547(13)
C(9)-C(10)	1.530(16)
C(10)-C(11)	1.529(19)
C(11)-C(12)	1.524(14)
C(13)-C(14)	1.392(14)
C(13)-C(18)	1.380(19)
C(14)-C(15)	1.425(18)
C(15)-C(16)	1.36(2)
C(16)-C(17)	1.392(16)
C(17)-C(18)	1.405(18)
C(20)-C(21)	1.366(13)
C(20)-C(25)	1.390(13)
C(21)-C(22)	1.386(13)
C(22)-C(23)	1.380(14)
C(23)-C(24)	1.406(14)
C(24)-C(25)	1.365(14)
C(27)-C(32)	1.397(14)
C(27)-C(28)	1.402(19)
C(28)-C(29)	1.39(2)
C(29)-C(30)	1.373(19)
C(30)-C(31)	1.38(2)
C(31)-C(32)	1.41(2)
C(33')-C(33')#1	2.38(4)

C(35)-C(40)	1.373(14)
C(35)-C(36)	1.391(16)
C(36)-C(37)	1.405(17)
C(37)-C(38)	1.390(17)
C(38)-C(39)	1.376(17)
C(39)-C(40)	1.408(15)
C(41)-C(42)	1.498(14)
C(42)-C(43)	1.520(15)
C(43)-C(44)	1.534(15)
C(44)-C(45)	1.53(2)
C(46)-C(47)	1.419(18)
C(46)-C(51)	1.40(2)
C(47)-C(48)	1.41(2)
C(48)-C(49)	1.37(3)
C(49)-C(50)	1.383(19)
C(50)-C(51)	1.377(19)
C(53)-C(58)	1.398(15)
C(53)-C(54)	1.382(16)
C(54)-C(55)	1.397(15)
C(55)-C(56)	1.405(18)
C(56)-C(57)	1.344(17)
C(57)-C(58)	1.418(14)
C(60)-C(65)	1.397(14)
C(60)-C(61)	1.43(2)
C(61)-C(62)	1.37(2)
C(62)-C(63)	1.391(16)
C(63)-C(64)	1.44(2)
C(64)-C(65)	1.33(2)
Cl(4)-C(67)	1.782(15)
Cl(6)-C(68)	1.79(2)
Cl(5)-C(67)	1.713(15)
Cl(7)-C(68)	1.67(2)
P-F(6)	1.483(19)
P-F(4)	1.450(17)
P-F(2)	1.515(11)
P-F(3)	1.562(11)

P-F(1)	1.550(9)
P-F(5)	1.463(17)
F(2)-F(5)	2.26(2)

C(1)-Pd(1)-C(34)	177.1(4)
C(1)-Pd(1)-Cl(2)	89.7(3)
C(34)-Pd(1)-Cl(2)	87.7(3)
C(1)-Pd(1)-Cl(1)	88.7(3)
C(34)-Pd(1)-Cl(1)	94.1(3)
Cl(2)-Pd(1)-Cl(1)	171.67(12)
C(19)-Pd(2)-C(52)	178.2(4)
C(19)-Pd(2)-Cl(3)	90.3(3)
C(52)-Pd(2)-Cl(3)	88.0(3)
C(19)-Pd(2)-Cl(1)	87.2(3)
C(52)-Pd(2)-Cl(1)	94.5(3)
Cl(3)-Pd(2)-Cl(1)	173.16(13)
Pd(1)-Cl(1)-Pd(2)	146.70(13)
C(23)-O(1)-C(26)	118.1(8)
C(30)-O(2)-C(33)	112.6(16)
C(30)-O(2)-C(33')	122.1(16)
C(56)-O(3)-C(59)	118.7(11)
C(63)-O(4)-C(66)	117.2(11)
C(2)-N(1)-C(1)	110.1(8)
C(2)-N(1)-C(20)	128.3(8)
C(1)-N(1)-C(20)	121.2(8)
C(1)-N(2)-C(7)	112.5(8)
C(1)-N(2)-C(8)	123.4(9)
C(7)-N(2)-C(8)	123.9(8)
C(13)-N(3)-C(12)	124.9(9)
C(13)-N(3)-C(19)	108.4(11)
C(12)-N(3)-C(19)	126.5(9)
C(19)-N(4)-C(27)	125.8(9)
C(19)-N(4)-C(18)	108.8(11)
C(27)-N(4)-C(18)	125.1(11)
C(34)-N(5)-C(35)	108.8(8)
C(34)-N(5)-C(53)	124.5(9)

C(35)-N(5)-C(53)	126.7(9)
C(34)-N(6)-C(40)	109.9(9)
C(34)-N(6)-C(41)	125.3(9)
C(40)-N(6)-C(41)	124.7(8)
C(52)-N(7)-C(46)	107.8(14)
C(52)-N(7)-C(45)	125.6(11)
C(46)-N(7)-C(45)	126.7(12)
C(52)-N(8)-C(51)	111.5(13)
C(52)-N(8)-C(60)	125.4(9)
C(51)-N(8)-C(60)	123.0(12)
N(1)-C(1)-N(2)	103.9(9)
N(1)-C(1)-Pd(1)	126.6(7)
N(2)-C(1)-Pd(1)	129.3(7)
N(1)-C(2)-C(7)	109.5(9)
N(1)-C(2)-C(3)	131.0(9)
C(7)-C(2)-C(3)	119.5(9)
C(4)-C(3)-C(2)	115.6(10)
C(5)-C(4)-C(3)	122.9(11)
C(4)-C(5)-C(6)	121.5(10)
C(7)-C(6)-C(5)	115.8(10)
C(6)-C(7)-C(2)	124.4(11)
C(6)-C(7)-N(2)	131.5(10)
C(2)-C(7)-N(2)	104.0(8)
N(2)-C(8)-C(9)	112.0(8)
C(8)-C(9)-C(10)	111.3(9)
C(9)-C(10)-C(11)	114.5(9)
C(12)-C(11)-C(10)	112.6(10)
N(3)-C(12)-C(11)	111.3(10)
N(3)-C(13)-C(14)	131.7(14)
N(3)-C(13)-C(18)	107.3(9)
C(14)-C(13)-C(18)	121.0(12)
C(13)-C(14)-C(15)	115.4(13)
C(16)-C(15)-C(14)	122.7(10)
C(15)-C(16)-C(17)	122.2(13)
C(18)-C(17)-C(16)	115.1(14)
C(17)-C(18)-N(4)	129.8(13)

C(17)-C(18)-C(13)	123.6(10)
N(4)-C(18)-C(13)	106.5(11)
N(4)-C(19)-N(3)	109.0(9)
N(4)-C(19)-Pd(2)	124.0(8)
N(3)-C(19)-Pd(2)	126.9(10)
C(21)-C(20)-N(1)	120.6(8)
C(21)-C(20)-C(25)	120.6(8)
N(1)-C(20)-C(25)	118.7(8)
C(20)-C(21)-C(22)	119.7(9)
C(23)-C(22)-C(21)	119.9(8)
O(1)-C(23)-C(22)	116.8(9)
O(1)-C(23)-C(24)	122.8(9)
C(22)-C(23)-C(24)	120.4(8)
C(25)-C(24)-C(23)	118.7(9)
C(24)-C(25)-C(20)	120.7(9)
C(32)-C(27)-N(4)	120.7(12)
C(32)-C(27)-C(28)	118.8(13)
N(4)-C(27)-C(28)	120.4(9)
C(29)-C(28)-C(27)	119.9(12)
C(28)-C(29)-C(30)	121.7(17)
C(31)-C(30)-O(2)	119.0(12)
C(31)-C(30)-C(29)	118.8(16)
O(2)-C(30)-C(29)	122.2(17)
C(30)-C(31)-C(32)	121.1(12)
C(27)-C(32)-C(31)	119.6(14)
O(2)-C(33')-C(33')#1	143(2)
N(6)-C(34)-N(5)	107.6(9)
N(6)-C(34)-Pd(1)	124.6(8)
N(5)-C(34)-Pd(1)	127.8(7)
C(40)-C(35)-N(5)	106.2(9)
C(40)-C(35)-C(36)	122.8(10)
N(5)-C(35)-C(36)	131.0(10)
C(35)-C(36)-C(37)	115.3(10)
C(36)-C(37)-C(38)	121.8(11)
C(39)-C(38)-C(37)	122.3(10)
C(38)-C(39)-C(40)	116.0(11)

C(35)-C(40)-N(6)	107.6(9)
C(35)-C(40)-C(39)	121.6(11)
N(6)-C(40)-C(39)	130.7(10)
N(6)-C(41)-C(42)	112.6(8)
C(41)-C(42)-C(43)	112.8(8)
C(42)-C(43)-C(44)	113.2(9)
C(43)-C(44)-C(45)	110.9(11)
N(7)-C(45)-C(44)	113.5(11)
N(7)-C(46)-C(47)	128.4(18)
N(7)-C(46)-C(51)	108.4(11)
C(47)-C(46)-C(51)	123.1(14)
C(48)-C(47)-C(46)	113.3(17)
C(47)-C(48)-C(49)	123.7(13)
C(50)-C(49)-C(48)	121.6(15)
C(49)-C(50)-C(51)	117.7(17)
N(8)-C(51)-C(50)	134.6(16)
N(8)-C(51)-C(46)	104.5(12)
C(50)-C(51)-C(46)	120.7(12)
N(8)-C(52)-N(7)	107.8(10)
N(8)-C(52)-Pd(2)	125.4(9)
N(7)-C(52)-Pd(2)	126.7(12)
C(58)-C(53)-N(5)	118.3(10)
C(58)-C(53)-C(54)	121.1(9)
N(5)-C(53)-C(54)	120.5(10)
C(55)-C(54)-C(53)	120.1(11)
C(54)-C(55)-C(56)	118.7(12)
O(3)-C(56)-C(57)	115.7(11)
O(3)-C(56)-C(55)	123.1(11)
C(57)-C(56)-C(55)	121.2(10)
C(56)-C(57)-C(58)	121.1(11)
C(53)-C(58)-C(57)	117.7(10)
C(65)-C(60)-N(8)	122.1(13)
C(65)-C(60)-C(61)	117.8(14)
N(8)-C(60)-C(61)	119.9(9)
C(62)-C(61)-C(60)	119.2(11)
C(61)-C(62)-C(63)	122.5(14)

O(4)-C(63)-C(62)	125.3(15)
O(4)-C(63)-C(64)	117.7(11)
C(62)-C(63)-C(64)	117.0(14)
C(65)-C(64)-C(63)	120.5(11)
C(64)-C(65)-C(60)	122.8(15)
Cl(4)-C(67)-Cl(5)	112.8(7)
Cl(7)-C(68)-Cl(6)	109.4(12)
F(6)-P-F(4)	97(2)
F(6)-P-F(2)	86.4(14)
F(4)-P-F(2)	174.7(18)
F(6)-P-F(3)	94.1(12)
F(4)-P-F(3)	96.8(12)
F(2)-P-F(3)	87.1(7)
F(6)-P-F(1)	90.3(11)
F(4)-P-F(1)	86.0(12)
F(2)-P-F(1)	89.8(8)
F(3)-P-F(1)	174.5(11)
F(6)-P-F(5)	174.4(19)
F(4)-P-F(5)	78(2)
F(2)-P-F(5)	98.9(17)
F(3)-P-F(5)	84.3(10)
F(1)-P-F(5)	91.6(8)
P-F(2)-F(5)	39.7(10)
P-F(5)-F(2)	41.4(8)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for l1pd. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pd(1)	39(1)	25(1)	23(1)	1(1)	5(1)	-1(1)
Pd(2)	25(1)	70(1)	23(1)	14(1)	5(1)	23(1)
Cl(1)	68(2)	39(1)	25(1)	8(1)	-9(1)	-3(1)
Cl(2)	109(3)	55(2)	23(1)	-3(1)	8(1)	-42(2)
Cl(3)	52(2)	113(3)	21(1)	11(1)	8(1)	50(2)
O(1)	51(4)	27(3)	43(4)	0(3)	-3(3)	4(3)
O(2)	83(7)	56(6)	71(7)	10(5)	-8(5)	18(5)
O(3)	80(6)	37(4)	52(5)	6(4)	18(4)	12(4)
O(4)	92(8)	73(7)	53(6)	34(5)	22(5)	40(6)
N(1)	39(4)	24(4)	25(4)	-5(3)	4(3)	2(3)
N(2)	49(5)	22(4)	28(4)	0(3)	2(3)	-4(3)
N(3)	28(4)	63(6)	22(4)	9(4)	8(3)	16(4)
N(4)	33(5)	69(6)	15(4)	7(4)	1(3)	24(4)
N(5)	41(5)	41(5)	30(4)	7(4)	12(3)	-2(4)
N(6)	46(5)	24(4)	23(4)	-3(3)	6(3)	-10(3)
N(7)	38(5)	96(9)	25(4)	6(5)	4(4)	41(6)
N(8)	19(4)	107(9)	27(4)	27(5)	5(3)	16(5)
C(1)	42(5)	32(5)	20(4)	3(4)	8(4)	7(4)
C(2)	46(6)	27(5)	28(5)	2(4)	10(4)	-13(4)
C(3)	41(6)	47(6)	35(5)	5(4)	6(4)	-7(5)
C(4)	54(7)	44(6)	33(5)	-7(4)	7(5)	-17(5)
C(5)	63(7)	28(5)	31(5)	-5(4)	13(5)	-14(5)
C(6)	55(6)	28(5)	35(5)	-1(4)	15(5)	-5(4)
C(7)	51(6)	30(5)	26(5)	2(4)	7(4)	-12(4)
C(8)	43(6)	32(5)	37(5)	8(4)	11(4)	8(4)
C(9)	57(7)	29(5)	38(6)	7(4)	14(5)	2(5)
C(10)	65(8)	34(6)	44(6)	15(5)	1(5)	11(5)
C(11)	32(5)	68(8)	39(6)	14(5)	15(4)	21(5)
C(12)	42(6)	61(7)	24(5)	16(5)	5(4)	17(5)
C(13)	29(5)	69(8)	21(5)	14(5)	9(4)	25(5)
C(14)	37(6)	70(8)	30(5)	19(5)	11(4)	25(5)

C(15)	25(5)	79(9)	36(6)	23(6)	4(4)	28(5)
C(16)	33(6)	79(9)	40(6)	14(6)	3(5)	20(6)
C(17)	36(6)	78(8)	25(5)	15(5)	6(4)	19(5)
C(18)	36(6)	73(8)	20(5)	15(5)	11(4)	20(5)
C(19)	32(5)	68(7)	20(4)	12(5)	7(4)	18(5)
C(20)	41(5)	26(4)	21(4)	1(3)	1(4)	0(4)
C(21)	51(6)	36(5)	20(4)	-3(4)	-3(4)	8(4)
C(22)	42(5)	32(5)	25(4)	-13(4)	-2(4)	-1(4)
C(23)	41(5)	25(4)	31(5)	1(4)	8(4)	5(4)
C(24)	52(6)	39(5)	25(5)	7(4)	-3(4)	0(5)
C(25)	49(6)	28(5)	24(4)	-3(4)	0(4)	-4(4)
C(26)	44(6)	33(5)	62(7)	18(5)	1(5)	-1(5)
C(27)	33(5)	67(8)	34(5)	26(5)	9(4)	13(5)
C(28)	73(8)	55(7)	26(5)	8(5)	10(5)	18(6)
C(29)	88(11)	64(9)	67(9)	24(7)	28(8)	3(8)
C(30)	64(9)	72(10)	57(8)	28(7)	24(7)	20(7)
C(31)	39(7)	80(10)	93(12)	60(9)	21(7)	22(7)
C(32)	38(6)	85(9)	35(6)	20(6)	12(5)	25(6)
C(33)	38(9)	44(9)	133(19)	12(11)	55(11)	-5(8)
C(33')	38(9)	44(9)	133(19)	12(11)	55(11)	-5(8)
C(34)	53(6)	24(4)	22(4)	1(3)	6(4)	-3(4)
C(35)	45(6)	33(5)	30(5)	-3(4)	10(4)	-7(4)
C(36)	39(6)	45(6)	44(6)	5(5)	8(5)	-3(5)
C(37)	46(6)	53(7)	51(7)	3(5)	10(5)	-11(5)
C(38)	77(8)	44(6)	29(5)	0(4)	3(5)	-37(6)
C(39)	63(7)	29(5)	51(7)	3(5)	0(5)	-3(5)
C(40)	48(6)	36(5)	21(4)	-5(4)	2(4)	-4(4)
C(41)	64(7)	25(5)	28(5)	1(4)	-5(4)	-2(4)
C(42)	58(7)	29(5)	44(6)	1(4)	0(5)	9(5)
C(43)	50(6)	38(6)	34(5)	4(4)	-5(5)	15(5)
C(44)	61(8)	73(9)	42(6)	-9(6)	-7(6)	40(7)
C(45)	45(7)	95(11)	35(6)	0(6)	-1(5)	35(7)
C(46)	31(6)	114(12)	26(5)	17(6)	4(4)	38(7)
C(47)	55(8)	104(11)	37(6)	-3(7)	-5(5)	47(8)
C(48)	55(8)	128(15)	43(7)	-11(8)	-15(6)	66(10)
C(49)	35(6)	118(14)	42(7)	8(8)	6(5)	35(8)

C(50)	33(6)	106(11)	37(6)	22(7)	9(5)	26(6)
C(51)	40(6)	80(9)	26(5)	18(6)	9(4)	29(6)
C(52)	44(6)	74(8)	26(5)	18(5)	9(4)	37(6)
C(53)	38(5)	44(6)	30(5)	8(4)	17(4)	8(4)
C(54)	49(6)	42(6)	28(5)	4(4)	18(4)	7(5)
C(55)	61(7)	39(6)	47(7)	3(5)	22(6)	5(5)
C(56)	53(6)	28(5)	47(6)	6(4)	20(5)	9(5)
C(57)	51(6)	42(6)	33(5)	8(4)	15(5)	2(5)
C(58)	51(6)	24(4)	26(5)	-5(4)	14(4)	3(4)
C(59)	89(10)	31(6)	50(7)	-5(5)	1(7)	14(6)
C(60)	32(5)	82(9)	30(5)	28(6)	13(4)	24(6)
C(61)	33(6)	95(10)	31(6)	28(6)	13(4)	22(6)
C(62)	42(6)	74(9)	37(6)	14(6)	15(5)	26(6)
C(63)	50(7)	81(10)	37(6)	17(6)	20(5)	31(7)
C(64)	48(7)	79(9)	40(7)	33(6)	20(5)	37(6)
C(65)	29(5)	108(12)	34(6)	32(7)	10(4)	29(6)
C(66)	82(11)	73(10)	57(9)	19(7)	5(8)	23(8)
Cl(4)	80(3)	86(3)	99(3)	-7(2)	-31(2)	-14(2)
Cl(6)	133(4)	73(3)	85(3)	18(2)	34(3)	13(3)
Cl(5)	136(4)	58(2)	106(4)	12(2)	1(3)	-2(3)
Cl(7)	107(5)	121(5)	239(9)	-59(5)	-40(5)	31(4)
C(67)	49(7)	82(10)	40(6)	8(6)	0(5)	6(6)
C(68)	95(13)	124(16)	60(10)	17(10)	14(9)	-29(12)
P	105(3)	51(2)	33(2)	-7(1)	-7(2)	22(2)
F(1)	247(15)	82(7)	58(6)	-33(5)	14(7)	-61(8)
F(2)	194(14)	77(7)	202(14)	-37(7)	-121(12)	47(8)
F(3)	370(20)	86(8)	56(6)	-23(5)	-51(10)	101(11)
F(4)	500(50)	330(40)	240(30)	-50(20)	-250(30)	230(40)
F(5)	730(50)	169(14)	126(13)	-23(9)	100(20)	-310(30)
F(6)	220(20)	560(50)	143(15)	-50(20)	119(15)	-220(30)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for l1pd.

	x	y	z	U(eq)
H(3A)	12008	9009	9323	51
H(4A)	12288	10296	9415	52
H(5A)	10961	11417	9199	49
H(6A)	9304	11308	8795	49
H(8A)	7506	10783	8818	49
H(8B)	7225	10030	8464	49
H(9A)	8389	10259	7408	53
H(9B)	8508	11065	7760	53
H(10A)	7142	11524	7058	63
H(10B)	6494	11464	7817	63
H(11A)	6284	10154	7447	64
H(11B)	5562	10919	7075	64
H(12A)	6743	10743	6042	57
H(12B)	7601	10058	6415	57
H(14A)	4538	11062	6041	64
H(15A)	2799	10929	5737	65
H(16A)	2471	9719	5498	68
H(17A)	3828	8529	5567	63
H(21A)	10336	7676	7989	46
H(22A)	11232	6329	8054	41
H(24A)	11843	6633	10090	49
H(25A)	10959	7968	10005	41
H(26A)	12999	4682	9609	73
H(26B)	13199	5540	9779	73
H(26C)	12100	5293	10090	73
H(28A)	5545	7701	4902	69
H(29A)	5693	6329	4867	95
H(31A)	6674	6055	6835	95
H(32A)	6550	7440	6897	72
H(33A)	6594	4303	6441	115

H(33B)	7339	4935	6482	115
H(33C)	6149	5099	6892	115
H(33D)	5854	4354	5445	115
H(33E)	4980	5172	5329	115
H(33F)	6148	5012	4887	115
H(36A)	3796	7377	8225	54
H(37A)	3609	6033	8246	61
H(38A)	5053	4986	8466	56
H(39A)	6727	5208	8733	59
H(41A)	8193	5917	9182	48
H(41B)	8708	6648	8893	48
H(42A)	8377	5408	8041	56
H(42B)	9534	5504	8254	56
H(43A)	9310	6729	7585	53
H(43B)	8186	6591	7348	53
H(44A)	9130	5439	6710	81
H(44B)	10261	5539	6969	81
H(45A)	10066	6055	5798	80
H(45B)	8949	6655	6060	80
H(47A)	12029	5608	6319	91
H(48A)	13816	5731	6504	106
H(49A)	14217	6936	6677	89
H(50A)	12857	8114	6752	80
H(54A)	5662	9017	9189	53
H(55A)	4707	10340	8987	64
H(57A)	3568	9641	7249	54
H(58A)	4551	8306	7425	44
H(59A)	3075	11970	8157	92
H(59B)	3284	11379	8829	92
H(59C)	4291	11527	8308	92
H(61A)	11306	8919	7538	73
H(62A)	11311	10260	7548	70
H(64A)	9736	10619	5739	79
H(65A)	9878	9293	5673	79
H(66A)	10899	12268	7102	118
H(66B)	10628	11586	7640	118

H(66C)	11757	11431	7154	118
H(67A)	9407	2348	5689	73
H(67B)	8355	2516	6247	73
H(68A)	3892	6894	10659	113
H(68B)	4437	6758	9859	113