Supporting Information

Gold(I)-Catalyzed High-Yielding Synthesis of Indenes by Direct C_{sp}^3-H Bond Activation

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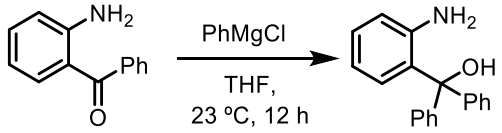
1. General Information

All moisture and oxygen sensitive reactions were carried out in flame–dried round bottom flasks or using Schlenk techniques under an inert atmosphere of nitrogen. Unless otherwise specified, all commercial materials were used as received without further purification. Anhydrous solvents were purchased from Sigma Aldrich in SureSeal® bottles. Column chromatography was performed using silica gel of size 100–200 and 230–400 mesh (Sigma Aldrich). Thin layer chromatography was performed with TLC Silica gel 60 F256 plates, and visualization was done with short wavelength UV light (254 nm).

Compounds were characterized using ^{1}H–NMR, ^{13}C–NMR, Melting Point, IR and Mass spectroscopy. (Copies of ^{1}H–NMR and ^{13}C–NMR spectra are provided starting from page S41, Section 9, for all new compounds). Data of known compounds were compared with existing literature characterization data and the references are given. ^{1}H and ^{13}C NMR spectra were recorded with 500 MHz and Bruker advance 400 MHz instruments using deuterated solvents purchased from Sigma Aldrich like $CDCl_3$.^{1}H spectra were referenced to tetramethylsilane (TMS, 0.0 ppm) and chloroform ($CDCl_3$, 7.26 ppm) and are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constant (Hz), and integration. Chemical shifts of the ^{13}C NMR spectra were measured relative to $CDCl_3$ (δ = 77.16 ppm) Melting points were measured using a Fisher–Johns apparatus. IR spectra were measured using a Perkin–Elmer System 2000 FT–IR. Compounds were applied in a thin film on a KBr pellet or ATR diamond. High resolution mass (HRMS) analysis was obtained using GC-MS Thermo Scientific™ DFS™

2. Synthesis of starting materials 1–5.

Spectroscopic data for **1**–**3**, **5**–**7**, **10**, **13**, **18**–**19**, **22** and **25** matches with those in literature.[1, 2] Spectroscopic data for unknown compounds **4**, **8**–**9**, **11**–**12**, **14**–**17**, **20**–**21**, **23**–**24**, and **26**–**29** are described here.



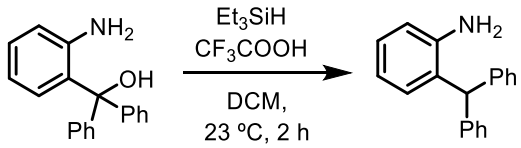
1

Synthesis of (2−aminophenyl)diphenylmethanol **(1).**[1] Phenylmagnesium Chloride (2 *M* in 2−methyltetrahydrofuran; 15 mL, 30 mmol) was added to a flame dried 250 mL round bottom flask containing a solution of (2−aminophenyl)(phenyl)methanone (7.0 g, 15.0 mmol) in THF (40 mL) at room temp. The mixture was stirred at room temp. for 12 h. Then the reaction was quenched with saturated aqueous NH_4Cl (50 mL), and the mixture was extracted with CH_2Cl_2 (2 × 30 mL). The combined organic layers were dried with anhydrous Na_2SO_4. The solvent was evaporated under reduced pressure, and the residue was purified by column chromatography (petroleum ether/EtOAc, 5:1) to give (2−aminophenyl)diphenylmethanol **1** (6.8 g, 70 %) as a pale−yellow solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 –7.31 (m, 10H), 7.14 (t, *J* = 7.6 Hz, 1H), 6.73 (d, *J* = 7.8 Hz, 1H), 6.70 (t, *J* = 7.6 Hz, 1H), 6.49 (d, *J* = 7.8 Hz, 1H), 5.21 (s, 1H), 3.67 (s, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 145.8, 144.1, 133.4, 129.9, 128.8, 128.2, 127.9, 127.5, 119.3, 119.2, 82.4.

Spectral data match with those reported on the literature[1].



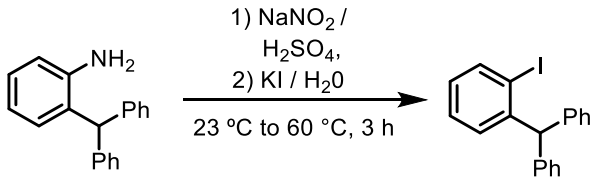
1 2

Synthesis of 2−benzohydrylaniline **(2).**[1] Et_3SiH (2.78 mL, 36 mmol) and CF_3COOH (5.5 mL, 72 mmol) were added to a flame dried 250 mL round bottom flask containing a solution of (2−aminophenyl)diphenylmethanol **1** (5 g, 18 mmol) in CH_2Cl_2 (20 mL). The reaction mixture was stirred at room temp. for 2 h. Solid Na_2CO_3 (7.6 g, 72 mmol) and water (60 mL) were then successively added. The mixture was extracted with CH_2Cl_2 (2 × 30 mL). The combined organic layers were dried with anhydrous Na_2SO_4. The solvent was evaporated under reduced pressure, and the residue was purified

by column chromatography (petroleum ether/EtOAc, 10:1) to give 2–benzohydrylaniline **2** (4 g, 85 %) as a pale–yellow solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35–7.26 (m, 6H), 7.17 (d, *J* = 7.3 Hz, 4H), 7.11 (t, *J* = 7.4 Hz, 1H), 6.75 – 6.68 (m, 3H), 5.51 (s, 1H), 3.49 (s, 2H).

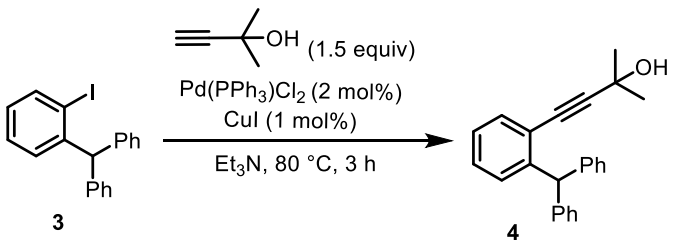
^{13}C NMR (126 MHz, $CDCl_3$) δ 144.3, 142.5, 130.0, 129.6, 129.2, 128.6, 127.5, 126.7, 118.7, 116.3, 52.3. Spectral data match with those reported on the literature[1].



2 **3**

[(2–iodophenyl)methylene]dibenzene **(3).**[1] A flame dried 250 mL round bottom flask containing a solution of 2–benzohydrylaniline **2** (4 g, 15 mmol), CH_3COOH (12 mL), concentrated H_2SO4 (12 mL), and water (12 mL) was stirred at 0 °C for 15 min. After this time, a solution of $NaNO_2$ (2.2 g, 32 mmol) in water (7 mL) was slowly added to the mixture. After the mixture became a brown liquid, a solution of KI (10.7 g, 65 mmol) in water (4 mL) was added in one portion. The mixture was warmed to room temp. and stirred for 1 h at 60 °C. Sodium sulfite (7.5 g, 56 mmol) was then added, and the mixture was extracted with CH_2Cl_2 (2 × 30 mL). The combined organic layers were dried with anhydrous Na_2SO_4. The solvent was evaporated under reduced pressure, and the residue was purified by column chromatography (hexanes) to give [(2–iodophenyl)methylene]dibenzene **3** (4.1 g, 71 %) as a white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89–7.80 (m, 2H), 7.30 –7.28 (m, 5H), 7.07 (d, *J* = 7.4 Hz, 5H), 6.93 (d, *J* = 6.2 Hz, 2H), 5.84 (s, 1H). Spectral data match with those reported on the literature[1].



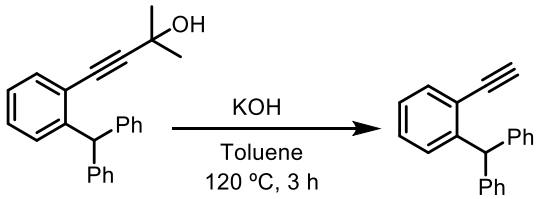
3 **4**

4–(2–benzohydrylphenyl)–2–methylbut–3–yn–2–ol **(4).** A flame dried 100 mL round bottom flask charged with nitrogen containing $Pd(PPh_3)_2Cl_2$ (67 mg, 2 mol%) and CuI (10 mg, 1 mol%) were dissolved in Et_3N (10 mL), and [(2–iodophenyl)methylene]dibenzene **3** (1.8 g, 4.8 mmol) and

2–methylbut–3–yn–2–ol (613 mg, 7.29 mmol) were added to the solution. The resulting mixture was stirred under a nitrogen atmosphere at room temp. for 2 h. The reaction was then quenched with saturated aqueous NH_4Cl (15 mL), and the mixture was extracted with CH_2Cl_2 (2 × 15 mL). The combined organic layers were dried with anhydrous Na_2SO_4. The solvent was removed under reduced pressure, and the residue was purified by column chromatography (9:1 Hexanes/EtOAc) to give compound **4** (862 mg, 55 %) as a yellow solid. M.p= 113–115 ˚C; IR (ATR Diamond) cm^{-1} 3141, 3021, 1595, 1492, 1476, 1447, 1373, 1361, 1286, 1265, 1162, 1076, 1028, 968, 917, 818, 757, 747, 726, 700.

^1H NMR (500 MHz, $CDCl_3$) δ 7.46 (d, *J* = 7.2 Hz, 1H), 7.32 (d, *J* = 7.3 Hz, 2H), 7.29 (d, *J* = 8.2 Hz, 2H), 7.25 (d, *J* = 7.3 Hz, 2H), 7.23 (d, *J* = 6.2 Hz, 1H), 7.20 (d, *J* = 7.4 Hz, 1H), 7.11 (d, *J* = 7.4 Hz, 4H), 6.92 (d, *J* = 7.5 Hz, 1H), 5.99 (s, 1H), 1.49 (s, 6 H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 145.9, 143.4, 132.5, 129.7, 129.5, 128.4, 128.3, 126.43, 126.41, 123.1, 99.0, 81.1, 65.6, 54.8, 31.3. HRMS (EI) *m/z* calcd for $C_{29}H_{24}$ $[M+H]^+$: 327.1749; found: 327.1744.



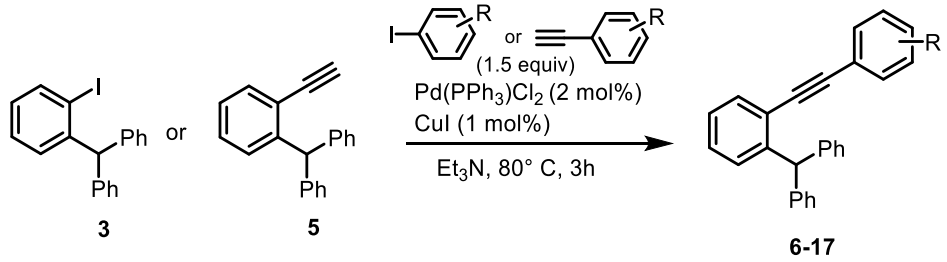
4 5

4 ((2–ethynylphenyl)methylene)dibenzene **(5).**[2] A flame dried 100 mL round bottom flask containing 4–(2–benzohydrylphenyl)–2–methylbut–3–yn–2–ol **4** (862 mg, 2.64 mmol) was dissolved in toluene (20 ml), and freshly powdered KOH (593 mg, 10.57 mmol) was added. After heating to reflux for 3 hours, the solvent was removed on a rotary evaporator. The mixture was extracted with CH_2Cl_2 (2 × 15 mL). The combined organic layers were dried with anhydrous Na_2SO_4. The solvent was removed under reduced pressure, and the residue was purified by column chromatography (petroleum ether) to give compound **5** (637 mg, 89 %) as a clear liquid.

^1H NMR (500 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.6 Hz, 1H), 7.26 (s, 6H), 7.31–7.18(m, 8H), 7.11 (d, *J* = 7.4 Hz, 4H), 7.01 (d, *J* = 7.8 Hz, 1H), 6.12 (s, 1H), 3.21 (s, 1H).

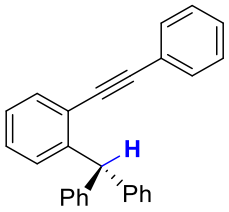
^{13}C NMR (126 MHz, $CDCl_3$) δ 146.5 143.3, 133.2, 129.7, 129.6, 128.8, 128.3, 126.4, 126.3, 122.5, 82.3, 81.9, 54.3. Spectral data match with those reported on the literature[1].

3. **General procedure A** for the synthesis starting alkynes **6–17.**



In a flame dried pressure tube charged with nitrogen containing $Pd(PPh_3)_2Cl_2$ (2 mol%) and CuI (1 mol%), these were dissolved in Et_3N (5 mL), and [(2−iodophenyl)methylene]dibenzene (1 equiv) or aryiodides (1.5equiv) and phenyl acetylene (1.5 equiv) or ((2−ethynylphenyl)methylene)dibenzene (1 equiv) were added to the solution. The resulting mixture was stirred under a nitrogen atmosphere at 80 ˚C for 3 h. The reaction was then quenched with saturated aqueous NH_4Cl (15 mL), and the mixture was extracted with CH_2Cl_2 (2 × 15 mL). The combined organic layers were dried with anhydrous Na_2SO_4. The solvent was removed under reduced pressure, and the residue was purified by column chromatography (hexanes) to give compound corresponding alkynes **6–17.**

{[2(Phenylethynyl)phenyl]methylene}dibenzene **(6).**

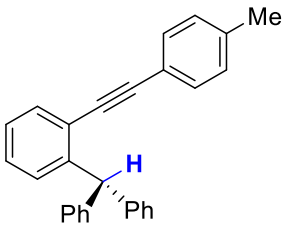


This compound was synthesized according to the general procedure **A** by using ((2−iodophenyl)methylene)dibenzene **3** and phenyl acetylene in 78% yield as white solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 (d, *J* = 7.2 Hz, 1H), 7.37 (d, *J* = 3.6 Hz, 2H), 7.31–7.21 (m, 11H), 7.15 (d, *J* = 7.5 Hz, 4H), 7.00 (d, *J* = 7.4 Hz, 1H), 6.15 (s, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 146.1, 143.4, 132.5, 131.6, 129.7, 129.5, 128.4, 128.39, 128.35, 126.4, 123.7, 123.4, 94.3, 88.3, 54.8. Spectral data match with those reported on the literature[1]

((2–(*p*–tolylethynyl)phenyl)methylene)dibenzene **(7).**

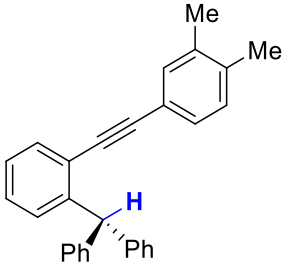


This compound was synthesized according to the general procedure **A** by ((2–ethynylphenyl)methylene)dibenzene **5** and 1–iodo–4–methylbenzene in 93% yield as white solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 (dd, *J* = 7.2, 1.7 Hz, 1H), 7.33–7.22 (m, 11H), 7.15 (t, *J* = 8.3 Hz, 6H), 7.00 (d, *J* = 8.7 Hz, 1H), 6.17 (s, 1H), 2.38 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 146.0, 143.4, 138.4, 132.4, 131.5, 129.7, 129.5, 129.1, 128.4, 128.2, 126.4, 123.8, 120.3, 94.4, 87.6, 54.8, 21.6. Spectral data match with those reported on the literature[1]

((2–((3,5–dimethylphenyl)ethynyl)phenyl)methylene)dibenzene **(8).**



This compound was synthesized according to the general procedure **A** by using ((2–ethynylphenyl)methylene)dibenzene **5** and 1–iodo–3,4–dimethylbenzene in 76% yield as white solid.

m.p=124–126 ˚C.

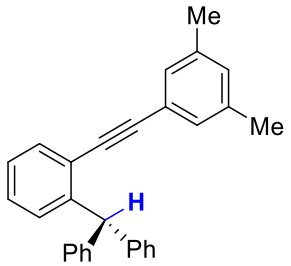
IR (ATR Diamond) cm^{-1} 2920, 1597, 1492, 1479, 1443, 1076, 1030, 847, 818, 760, 741, 723, 696.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.52 (s, 1H), 7.30 –7.06 (m, 15H), 6.98 (d, *J* = 6.8 Hz, 1H), 6.14 (s, 1H), 2.26 (s, 3H), 2.24 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 146.0, 143.5, 137.3, 136.7, 132.7, 132.4, 129.7, 129.7, 129.5, 129.0, 128.3, 128.1, 126.3, 123.8, 120.6, 94.6, 87.4, 54.8, 19.9, 19.7.

HRMS (EI) *m*/*z* calcd for $C_{29}H_{24}$ $[M]^+$: 372.1878; found: 372.1873.

((2–((3,5–dimethylphenyl)ethynyl)phenyl)methylene)dibenzene **(9).**



This compound was synthesized according to the general procedure **A** by using ((2–ethynylphenyl)methylene)dibenzene and 1–iodo–3,5–dimethylbenzene in 62% yield as white solid. m.p= 122–124 ˚C.

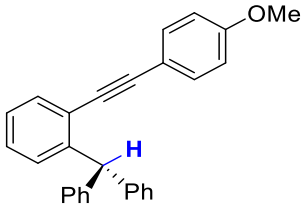
IR (ATR Diamond) cm^{-1} 2918, 2850, 1595, 1494, 1473, 1448, 1078, 1022, 890, 812, 756, 727, 700.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 (d, *J* = 6.8 Hz, 1H), 7.32 –7.22 (m, 8H), 7.15 (d, *J* = 7.3 Hz, 4H), 6.99–6.95 (s,4 H), 6.15 (s, 1H), 2.30 (s, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 146.0, 143.5, 137.9, 132.4, 130.2, 129.8, 129.5, 129.3, 128.4, 128.2, 126.4, 123.8, 123.0, 94.7, 87.6, 123.0, 54.8, 21.2.

HRMS (EI) *m*/*z* calcd for $C_{29}H_{24}$ $[M]^+$: 372.1878; found: 372.1876.

((2–((4–methoxyphenyl)ethynyl)phenyl)methylene)dibenzene **(10).**

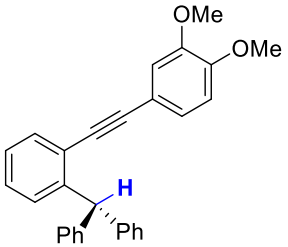


This compound was synthesized according to the general procedure **A** by using ((2–ethynylphenyl)methylene)dibenzene **5** and 1–iodo–4–methoxybenzene in 90% yield as white solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 (d, *J* = 7.4 Hz, 1H), 7.30 (t, *J* = 7.3 Hz, 6H), 7.23 (t, *J* = 6.8 Hz, 4H), 7.15 (d, *J* = 7.6 Hz, 4H), 6.98 (d, *J* = 6.9 Hz, 1H), 6.85 (d, *J* = 8.6 Hz, 2H), 6.15 (s, 1H), 3.82 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 159.7, 145.9, 143.5, 133.0, 132.3, 129.7, 129.5, 128.3, 128.0, 126.3, 124.0, 115.5, 114.0, 94.3, 87.0, 55.4, 54.8. Spectral data match with those reported on the literature[1]

((2–((3,4–dimethoxyphenyl)ethynyl)phenyl)methylene)dibenzene **(11).**



This compound was synthesized according to the general procedure **A** by using ((2–ethynylphenyl)methylene)dibenzene **5** and 1–iodo–3,4–dimethoxybenzene in 88% yield as white solid.

m.p. 125–127 °C.

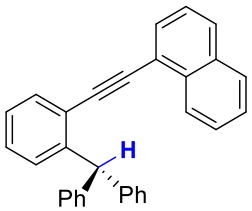
IR (ATR Diamond) cm^{-1} 2920, 1597, 1514, 1443, 1327, 1251, 1228, 1130, 1024, 845, 800, 761, 726, 700.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.7 Hz, 1H), 7.29 (t, *J* = 7.4 Hz, 4H), 7.23 –7.20 (m, 4H), 7.15 (t, *J* = 8.8 Hz, 4H), 6.97 (t, *J* = 8.0 Hz, 2H), 6.80 (d, *J* = 7.6 Hz, 2H), 6.13 (s, 1H), 3.89 (s, 3H), 3.87 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 149.5, 148.6, 145.9, 143.5, 132.3, 129.7, 129.5, 128.3, 128.1, 126.43, 126.40, 124.8, 123.9, 115.6, 114.3, 111.0, 94.4, 86.8, 56.8, 56.0, 54.8.

HRMS (EI) *m*/*z* calcd for $C_{29}H_{24}O_2$ $[M]^+$: 404.1776; found: 404.1771.

1–((2–benzohydrylphenyl)ethynyl)naphthalene **(12).**



This compound was synthesized according to the general procedure **A** by using ((2–ethynylphenyl)methylene)dibenzene **5** and 1–iodonapthalene in 85% yield as white solid.

m.p. 93–95°C.

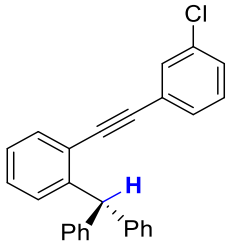
IR (ATR Diamond) cm^{-1} 2920, 2851, 1594, 1492, 1477, 1396, 1157, 1078, 1030, 910, 859, 793, 768, 756, 726, 699.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.09 (d, *J* = 7.8 Hz, 1H), 7.86 (t, *J* = 7.8 Hz, 2H), 7.73 (d, *J* = 7.4 Hz, 1H), 7.65 (d, *J* = 6.2 Hz, 1H), 7.45–7.54 (m, 3 H), 7.36 –7.27 (m, 8H), 7.20 (d, *J* = 7.4 Hz, 4H), 7.07 (d, *J* = 6.6 Hz, 1H), 6.33 (s, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 145.7, 143.6, 133.2, 132.8, 130.5, 129.8, 128.8, 128.5, 128.4, 128.3, 126.8, 126.5, 126.5, 126.4, 125.3, 123.8, 121.1, 93.0, 92.2, 54.8.

HRMS (EI) *m/z* calcd for $C_{31}H_{22}$ $[M]^+$: 394.1722 found: 394.1704.

((2–((3–chlorophenyl)ethynyl)phenyl)methylene)dibenzene **(13).**

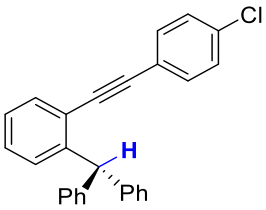


This compound was synthesized according to the general procedure **A** by using ((2–ethynylphenyl)methylene)dibenzene **5** and 3–chloro –4–iodobenzene in 93% yield as white solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.6 Hz, 1H), 7.36–7.26 (m, 12H), 7.17 (d, *J* = 7.2 Hz, 4H), 7.02 (d, *J* = 7.6 Hz, 1H), 6.14 (s, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 146.2, 143.2, 134.2, 132.6, 131.5, 129.7, 129.65, 129.61, 128.7, 128.5, 128.4, 126.52, 126.51, 125.1, 123.1, 92.8, 89.5, 54.9. Spectral data match with those reported on the literature[1].

((2–((4–chlorophenyl)ethynyl)phenyl)methylene)dibenzene **(14).**



This compound was synthesized according to the general procedure **A** by using ((2–ethynylphenyl)methylene)dibenzene **5** and 1–chloro–4–iodobenzene in 91% yield as white solid. m.p. 107–109°C.

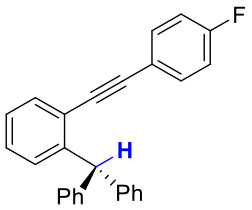
IR (ATR Diamond) cm^{-1} 2922, 1597, 1489, 1446, 1089, 1032, 1012, 823, 809, 756, 745, 736, 719, 697.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44 (d, *J* = 6.8 Hz, 1H), 7.20–7.13 (m, 12H), 7.03 (d, *J* = 6.9 Hz, 4H), 6.89 (d, *J* = 7.1 Hz, 1H), 6.01 (s, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 146.1, 143.3, 134.3, 132.8, 132.5, 129.7, 129.6, 128.7, 128.6, 128.4, 126.4, 123.3, 121.9, 93.1, 89.3, 54.8.

HRMS (EI) *m/z* calcd for $C_{27}H_{19}Cl$ $[M]^+$: 378.1175; found: 378.1167.

((2–((4–fluorophenyl)ethynyl)phenyl)methylene)dibenzene **(15).**



This compound was synthesized according to the general procedure **A** by using ((2–ethynylphenyl)methylene)dibenzene **5** and 1–fluoro–4–iodobenzene in 96% yield as white solid. m.p=112–114 ˚C.

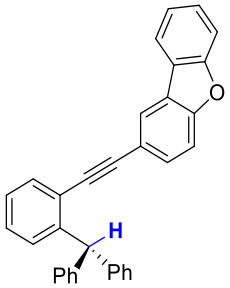
IR (ATR Diamond) cm^{-1} 2922, 1599, 1449, 1224, 1155, 1079, 841, 799, 756, 726, 702.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 (d, *J* = 6.6 Hz, 1H), 7.34–7.15 (m, 14H), 7.02 (d, *J* = 7.7 Hz, 3H), 6.14 (s, 1H).

^{13}C NMR (126 MHz) δ 162.62 (d, *J* = 249.5 Hz), 146.1, 143.3, 133.48 (d, *J* = 8.5 Hz), 132.5, 129.7, 129.6, 128.4, 126.4, 123.5, 119.52 (d, *J* = 3.3 Hz), 115.71 (d, *J* = 22.0 Hz), 93.2, 88.0, 54.8.

HRMS (EI) *m*/*z* calcd for $C_{27}H_{19}F$ $[M]^+$: 362.1471; found: 362.1465.

2–((2–benzohydrylphenyl)ethynyl)dibenzo[*b*,*d*]furan **(16).**



This compound was synthesized according to the general procedure **A** by using ((2–ethynylphenyl)methylene)dibenzene **5** and 2–iododibenzo[*b*,*d*]furan in 85% yield as white solid.

m.p. 92–94°C.

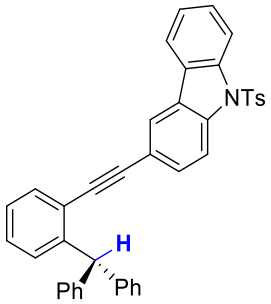
IR (ATR Diamond) cm^{-1} 3024, 1597, 1485, 1448, 1242, 1192, 1118, 1021, 838, 808, 744, 725, 699.

^{1}H NMR (500 MHz,) δ 8.17–7.71 (m, 7H), 7.64 –7.44 (m, 14H), 6.45 (s, 1H).

^{13}C NMR (126 MHz,) δ 156.7, 155.9, 146.0, 143.5, 132.4, 130.7, 129.8, 129.6, 128.4, 128.3, 127.7, 126.4, 126.4, 124.5, 124.2, 123.8, 123.7, 123.1, 120.9, 117.9, 111.9, 111.8, 94.5, 87.5, 54.9.

HRMS (EI) *m*/*z* calcd for $C_{33}H_{22}O$ $[M]^+$: 434.1671; found: 434.1652.

3–((2–benzohydrylphenyl)ethynyl)–9–tosyl–9*H*–carbazole **(17).**



This compound was synthesized according to the general procedure **A** by using ((2–ethynylphenyl)methylene)dibenzene **5** and 3–iodo–9–tosyl–9*H*–carbazole in 91% yield as white solid.

m.p=190–192 ˚C.

IR (ATR Diamond) cm^{-1} 2924, 1595, 1445, 1368, 1172, 1089, 980, 809, 823, 755, 715, 670, 570, 699, 650, 610, 590, 539, 485.

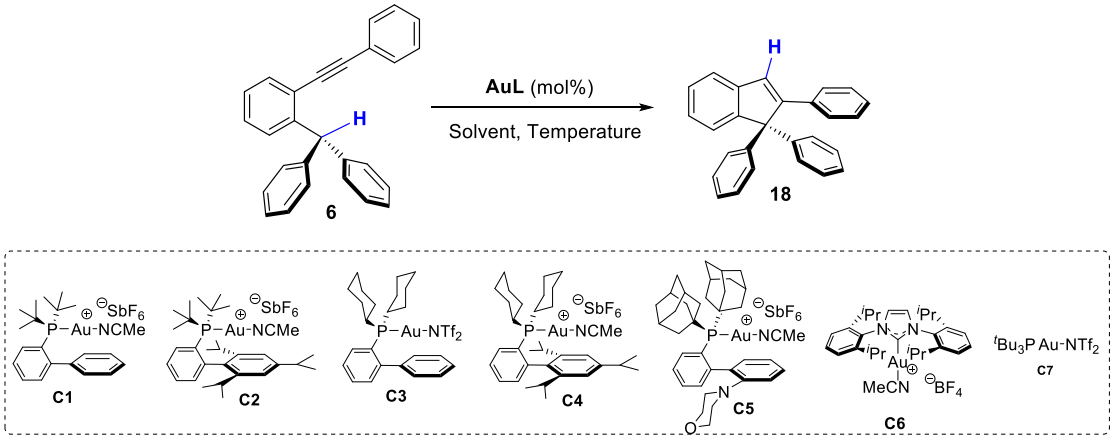
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (d, *J* = 8.4 Hz, 1H), 8.26 (d, *J* = 8.7 Hz, 1H), 7.88 (d, *J* = 7.7 Hz, 1H), 7.81 (s, 1H), 7.68 (d, *J* = 8.1 Hz, 2H), 7.57 (d, *J* = 8.1 Hz, 1H), 7.51 (t, *J* = 7.8 Hz, 1H), 7.46 (d, *J* = 8.7 Hz, 1H), 7.39 (t, *J* = 7.5 Hz, 1H), 7.32 (t, *J* = 7.4 Hz, 4H), 7.25–7.23 (m, 4H), 7.16 (d, *J* = 7.6 Hz, 4H), 7.11 (d, *J* = 8.1 Hz, 2H), 6.98 (d, *J* = 8.3 Hz, 1H), 6.16 (s, 1H), 2.27 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 146.0, 145.2, 143.4, 138.8. 138.0, 134.9, 132.5, 130.7, 129.89, 129.81, 129.6, 128.4, 128.4, 127.9, 126.6, 126.5, 126.4, 125.9, 124.2, 123.6, 123.4, 120.2, 119.0, 115.3, 115.2, 94.2, 88.2, 54.9, 21.6.

HRMS (EI) *m*/*z* calcd for $C_{40}H_{29}NO_2S$ $[M]^+$: 587.1919; found: 587.1916.

4. Optimization of reaction conditions and chromatograms

Table 1. Optimization of the new gold(I)–catalyzed C_{sp}^3–H bond activation mode in the synthesis of 1,1,2–triarylindenes– The yields were obtained by gas chromatography with flame ionization detection (GC–FID).



Entry	Au(I)L (mol%)	Solvent	Temp (°C)	Yield (%)[a]
1	C1 (5)	MeCN	23	n.r.
2	C1 (5)	DCE	23	n.r.
3	C1 (10)	DCE	23	n.r.
4	C1 (5)	DCE	60	n.r.
5	C1 (5)	DCE	80	n.r.
6	C1 (10)	DCE	90	48
7	C1 (15 + 5)	DCE	105	78
8	*C1 (20)*	*DCE*	*105*	***>99***
9	C2 (20)	DCE	105	9
10	C3 (20)	DCE	105	81
11	C4 (20)	DCE	105	25
12	C5 (20)	DCE	105	30
13	C6 (20)	DCE	105	45
14	C7 (20)	DCE	105	11
15	–	DCE	105	n.r.

[a]The chemical yields were determined by GC. n.r. = no reaction observed.

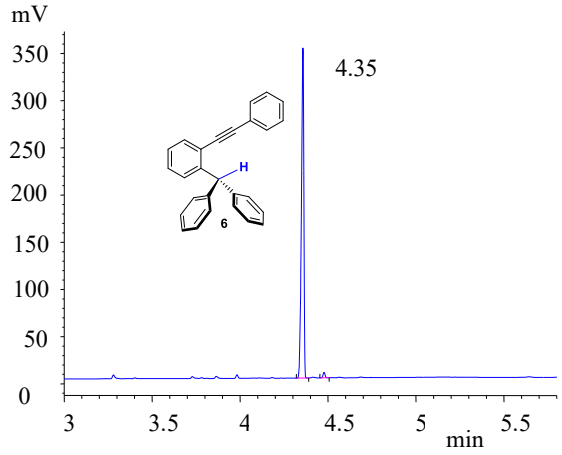
Gas chromatography with flame ionization detection (GC–FID): A Clarus 500 gas chromatograph with flame ionization detector (Perkin–Elmer, USA) was used with a ZB–5 INFERNO capillary column (30 m x 0.25 mm, film 0.1 µm, Phenomenex, USA). The reaction mixture in hexane (1 µl) was injected in a split mode (50:1) with inlet temperature of 250 °C. Separation was carried out with He as a carrier gas at the flow rate 1 ml/min, applying temperature gradient from 200 °C to 340 °C within 6 min. FID was operated

at 350 °C with 45 ml/min hydrogen and 450 ml/min air. The reaction yield (Yield %) was evaluated based on the peak areas of the product (A_p) and the substrate (A_s), as follows: Yield % = $A_p/(A_s+A_p)*100$.

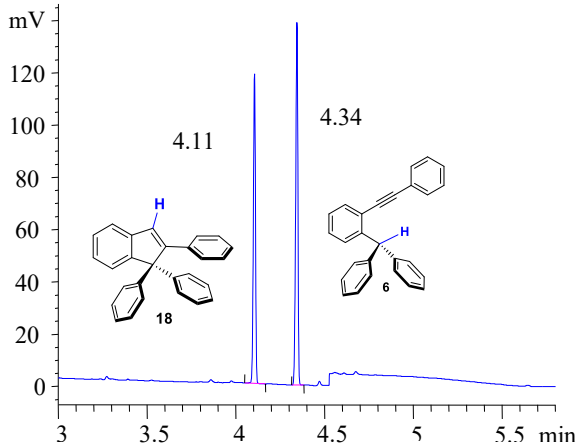
Chromatograms:

Following are the chromatograms obtained for selected reactions with substrate **6.** Entries **6**, **7**, **8** and **9** in table **1**.

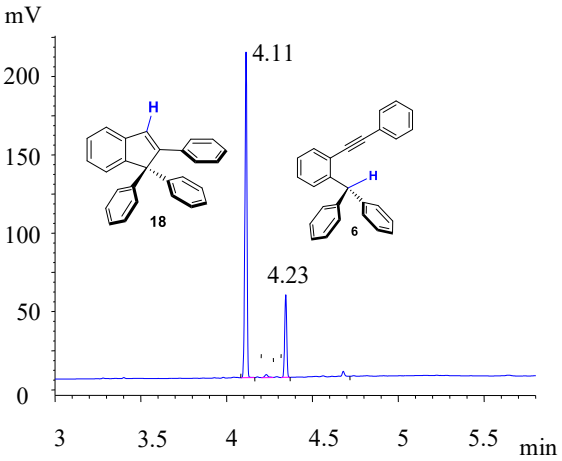
Reaction substrate **6**



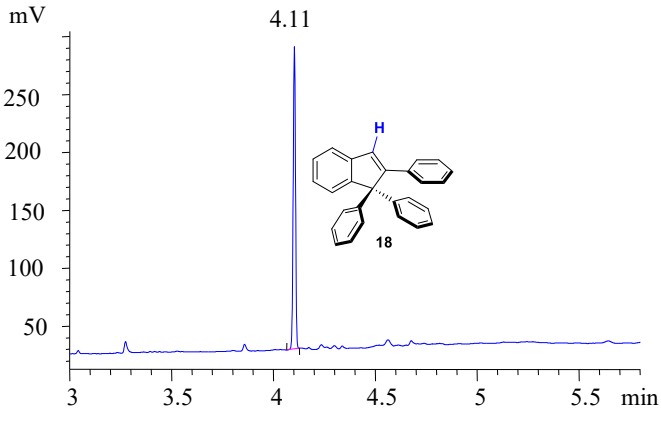
Entry **6**, C**1**(10 mol%) 48% yield



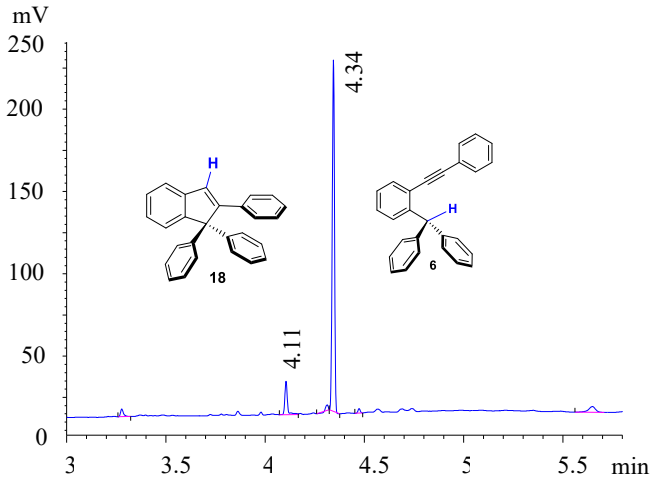
Entry **7**, C**1**(15+5 mol%) 78% yield



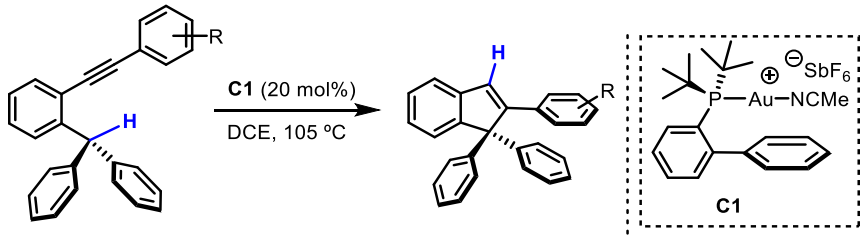
Entry **8**, **C1**(20 mol%) 99.8% yield



Entry **9**, **C2**(20 mol%) 9% yield

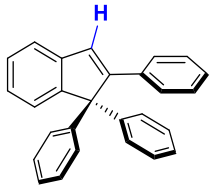


5. General procedure B *for the synthesis of the 1,1,2-triarylindenes* 18–29.



In a flame dried pressure tube charged with nitrogen the starting alkynes **6–17** (0.2 mmol, 1 equiv) and catalyst **C1** (20 mol%) were dissolved in DCE (3 mL). The resulting mixture was stirred at 105 ˚C for 2–18 h. The reaction was monitored by TLC until fully consumption of the starting alkyne. Then the solvent was removed under reduced pressure, and the residue was purified by column chromatography (hexanes) to give compound corresponding indenes **18–29.**

1,1,2–triphenyl–1*H*–indene **(18).**

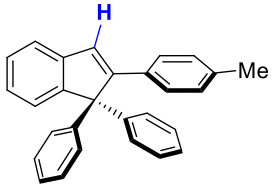


This compound was synthesized according to the general procedure **B** using compound **6** in 98% of yield as white solid. The reaction time for this example is 2 h.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42 (d, *J* = 7.5 Hz, 1H), 7.37 (dd, *J* = 7.5, 2.1 Hz, 2H), 7.32 (dd, *J* = 7.5, 2.1 Hz, 4H), 7.24 (s, 1H), 7.24 –7.16 (m, 11H), 7.11 (t, *J* = 7.4 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 155.4, 155.0, 142.1, 135.5, 129.0, 128.8, 128.2, 128.0, 127.9, 127.5, 127.1, 126.8, 126.2, 124.6, 121.6, 68.9. Spectral data match with those reported on the literature[1].

1,1–diphenyl–2–(*p*–tolyl)–1*H*–indene **(19).**[1]

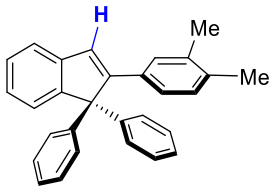


This compound was synthesized according to the general procedure **B** using compound **7** in 97% yield as white solid. The reaction time for this example is 2.5 h.

^{1}H NMR (400 MHz) δ 7.50 (d, *J* = 7.5 Hz, 1H), 7.43 –7.28 (m, 14H), 7.20 (t, *J* = 7.4 Hz, 1H), 7.09 (d, *J* = 8.0 Hz, 2H), 2.36 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.4, 154.9, 142.3, 142.2, 137.3, 132.5, 128.85, 128.81, 128.2, 127.8, 127.0, 126.7, 126.0, 124.6, 121.4, 68.7, 21.2. Spectral data match with those reported on the literature[1].

2–(3,4–dimethylphenyl)–1,1–diphenyl–1*H*–indene **(20).**



This compound was synthesized according to the general procedure **B** using compound **8** in 91% yield as white solid. The reaction time for this example is 3 h.

m.p=103–105 ˚C.

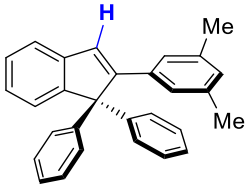
IR (ATR Diamond) cm[1] 2919, 1596, 1489, 1449, 1187, 1080, 1020, 989, 920, 876, 819, 750, 739, 698, 668.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 (d, *J* = 7.4 Hz, 1H), 7.34 –7.33 (m, 4H), 7.24–7.17 (m, 10H), 7.10 (d, *J* = 7.4 Hz, 1H), 7.07 (d, *J* = 7.8 Hz, 1H), 6.92 (d, *J* = 7.9 Hz, 1H), 2.18 (s, 3H), 2.15 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 155.5, 155.0, 142.4, 142.3, 136.16, 136.13, 132.9, 129.2, 129.1, 128.8, 128.17, 128.10, 127.0, 126.7, 125.9, 125.4, 124.6, 121.3, 68.7, 29.8, 19.9, 19.6.

HRMS (EI) *m*/*z* calcd for $C_{29}H_{24}$ $[M]^+$: 372.1878; found: 327.1862.

2–(3,5–dimethylphenyl)–1,1–diphenyl–1*H*–indene **(21).**



This compound was synthesized according to the general procedure **B** using compound **9** in 91% yield as white solid. The reaction time for this example is 2.5 h.

m.p=128–130 ˚C.

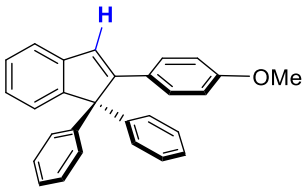
IR (ATR Diamond) cm[1] 2916, 1488, 1183, 1080, 1032, 918, 841, 745, 731, 667, 696.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 (d, *J* = 7.4 Hz, 1H), 7.33 (dd, *J* = 7.5, 1.9 Hz, 4H), 7.25 –7.18 (m, 9H), 7.11 (t, *J* = 7.4 Hz, 1H), 6.98 (s, 2H), 6.82 (s, 1H), 2.18 (s, 6H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 155.5, 155.2, 142.34, 142.3,1 137.2, 135.4 129.3, 128.8, 128.1, 127.0, 126.7, 126.0, 125.9, 124.6, 121.4, 68.8, 21.4.

HRMS (EI) *m*/*z* calcd for $C_{29}H_{24}$ $[M]^+$: 372.1878; found: 372.1865.

2–(4–methoxyphenyl)–1,1–diphenyl–1*H*–indene **(22).**[1]

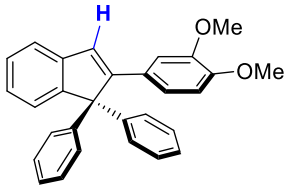


This compound was synthesized according to the general procedure **B** using compound **10** in 96% yield as white solid. The reaction time for this example is 2 h.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 (d, *J* = 7.4 Hz, 1H), 7.38 (d, *J* = 7.4 Hz, 1H), 7.32 –7.30 (m, 6H), 7.24 –7.14 (m, 9H), 7.08 (t, *J* = 8.0 Hz, 1H), 6.71 (d, *J* = 8.9 Hz, 2H), 3.74 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 159.1, 155.3, 154.73, 142.5, 142.3, 129.2, 128.8, 128.2, 128.1, 127.3, 127.0, 126.7, 125.8, 124.6, 121.2 113.5, 68.7, 55.2. Spectral data match with those reported on the literature[1].

2–(3,4–dimethoxyphenyl)–1,1–diphenyl–1*H*–indene **(23).**



This compound was synthesized according to the general procedure **B** using compound **11** in 89%yield as white solid. The reaction time for this example is 3.5 h.

m.p=95–97 ˚C.

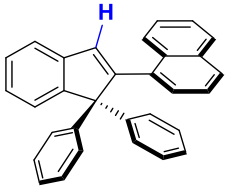
IR (ATR Diamond) cm^{-1} 2922, 1594, 1506, 1446, 1369, 1242, 1167, 1140, 1023, 980, 743, 699, 670, 614, 572.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39 (d, *J* = 7.4 Hz, 1H), 7.33 (d, *J* = 9.2 Hz, 4H), 7.25–7.17 (m, 8H) 7.15 (s, 1H), 7.10 (t, *J* = 7.5 Hz, 1H), 6.98 (dd, *J* = 8.4, 1.9 Hz, 1H), 6.85 (s, 1H), 6.70 (d, *J* = 8.5 Hz, 1H), 3.81 (3, 1H), 3.64 (s, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 155.2, 154.8, 148.6, 148.2, 142.4, 142.2, 128.9, 128.6, 128.2, 127.7, 127.1, 126.8, 125.9, 124.6, 121.3, 120.7, 111.2, 110.7, 68.6, 55.8, 55.7.

HRMS (EI) *m/z* calcd for $C_{29}H_{24}O_2$ [M]+: 404.1776; found: 404.1773.

1–(1,1–diphenyl–1*H*–inden–2–yl)naphthalene **(24).**



This compound was synthesized according to the general procedure **B** using compound **12** in 93% yield as white solid. The reaction time for this example is 18 h.

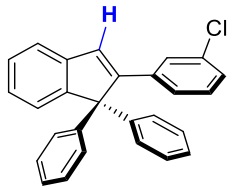
m.p=176–178 ˚C.

IR (ATR Diamond) cm^{-1} 2917, 2849, 1595, 1487, 1391, 1242, 1212, 1460, 1019, 772, 739, 698, 671, 654, 575.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.2 Hz, 1H), 7.48 (d, *J* = 7.5 Hz, 1H), 7.41 (d, *J* = 7.2 Hz, 1H), 7.37 (d, *J* = 8.7 Hz, 1H), 7.33 (dd, *J* = 7.5, 0.9 Hz, 1H), 7.28 (d, *J* = 7.3 Hz, 1H), 7.21 (dd, *J* = 7.5, 0.9 Hz, 1H), 7.18 (dd, *J* = 8.2, 1.4 Hz, 4H), 7.13 –7.03 (m, 6H), 6.94 (s, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 153.3, 151.6, 142.5, 141.1, 135.0, 133.5, 133.4, 133.3, 128.6, 128.0, 127.8, 127.7, 127.1, 126.7, 126.0, 125.7, 125.6, 125.5, 125.4, 125.3, 124.6, 121.9, 71.8. HRMS (EI) *m*/*z* calcd for $C_{31}H_{22}$ $[M]^+$: 394.17221; found: 394.1717.

2–(3–chlorophenyl)–1,1–diphenyl–1*H*–indene **(25).**

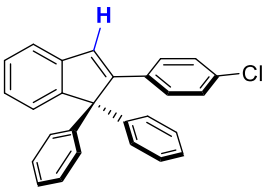


This compound was synthesized according to the general procedure **B** using compound **13** in 88% yield as white solid. The reaction time for this example is 3.5 h.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42 (d, *J* = 7.5 Hz, 1H), 7.37 (t, *J* = 1.8 Hz, 1H), 7.29 (dd, *J* = 7.4, 2.4 Hz, 4H), 7.2 (s, 1H), 7.23 –7.18 (m, 8H), 7.17 (s, 1H), 7.14 (t, *J* = 7.0 Hz, 2H), 7.08 (t, *J* = 7.8 Hz, 1H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 155.5, 153.5, 141.8, 141.7, 137.3, 133.9, 130.1, 129.2, 128.7, 128.3, 127.8, 127.5, 127.2, 127.0, 126.6, 126.0, 124.7, 121.9, 68.8. Spectral data match with those reported on the literature[1]

2–(4–chlorophenyl)–1,1–diphenyl–1*H*–indene **(26).**



This compound was synthesized according to the general procedure **B** using compound **14** in 91% yield as white solid. The reaction time for this example is 2.5 h.

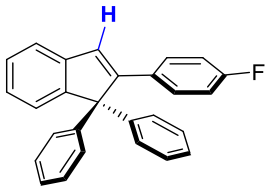
m.p= 205–207 ˚C.

IR (ATR Diamond) cm^{-1} 2920, 1594, 1487, 1444, 1179, 1089, 1034, 1014, 924, 824, 745, 697, 665, 459, 531.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.45 (d, *J* = 7.5 Hz, 1H), 7.34–7.28 (m, 7H), 7.26 (s, 1H), 7.25–7.22 (m, 6H), 7.20 –7.14 (m, 4H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 155.5, 153.7, 141.9, 141.8, 133.9, 133.3, 129.4, 129.1, 128.7, 128.3, 128.2, 127.2, 126.9, 126.4, 124.6, 121.7, 68.8. HRMS (EI) *m/z* calcd for $C_{27}H_{19}Cl$ $[M]^+$: 378.1175; found: 387.1151.

2–(4–fluorophenyl)–1,1–diphenyl–1*H*–indene **(27).**



This compound was synthesized according to the general procedure **B** using compound **15** in 93% yield as white solid. The reaction time for this example is 3.5 h.

m.p= 161–163 ˚C.

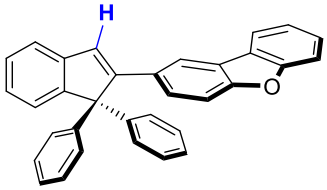
IR (ATR Diamond) cm^{-1} 2923, 2853, 1596, 1504, 1465, 1448, 1224, 1161, 1098, 1080, 923, 875, 751, 829, 796, 743, 695, 666.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 (d, *J* = 7.4 Hz, 1H), 7.34–7.28 (m, 6H), 7.24 –7.15 (m, 9H), 7.12 (dd, *J* = 7.0 Hz, 1H), 6.86 (t, *J* = 8.7 Hz, 2H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 162.28 (d, *J* = 247.7 Hz), 155.3, 154.0, 142.1, 141.9, 131.73 (d, *J* = 3.4 Hz), 129.62 (d, *J* = 7.9 Hz), 128.8, 128.7, 128.3, 127.1, 126.9, 126.2, 124.7, 121.6, 115.02 (d, *J* = 21.3 Hz), 68.9.

HRMS (EI) *m/z* calcd for $C_{27}H_{19}F$ $[M]^+$: 362.1471; found: 362.1468.

2–(1,1–diphenyl–1*H*–inden–2–yl)dibenzo[*b*,*d*]furan **(28).**



This compound was synthesized according to the general procedure **B** using compound **16** in 91% yield as white solid. The reaction time for this example is 18 h.

m.p=183–185 ˚C.

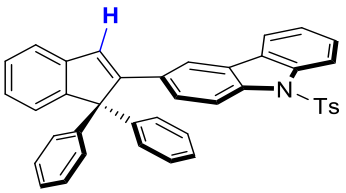
IR (ATR Diamond) cm^{-1} 2924, 1728, 1595, 1448, 1246, 1194, 1141, 1021, 917, 815, 744, 68, 672, 643, 619, 545, 575, 509

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (s, 1H), 7.77 (d, *J* = 7.6 Hz, 1H), 7.55–7.36 (m, 10H), 7.29 (dd, *J* = 10.7, 5.2 Hz, 3H), 7.22 (dd, *J* = 10.7, 5.2 Hz, 8H), 7.14 (t, *J* = 7.4 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 156.5, 155.2, 142.3, 142.1, 130.8, 128.9, 128.8, 128.31, 127.4, 127.3, 127.1, 126.9, 126.1, 124.7, 124.2, 124.0, 122.8, 121.5, 120.6, 120.0, 111.7, 111.1, 69.1.

HRMS (EI) *m*/*z* calcd for $C_{33}H_{22}O$ $[M]^+$: 434.1671; found: 434.1655.

3–(1,1–diphenyl–1*H*–inden–2–yl)–9–tosyl–9*H*–carbazole **(29).**



This compound was synthesized according to the general procedure A using compound **17** in 95% yield as white solid. The reaction time for this example is 3 h.

m.p= 246–248 ˚C.

IR (ATR Diamond) cm^{-1} 3030, 1594, 1509, 1446, 1369, 1242, 1167, 1140, 1023, 980, 808, 743, 699, 670, 614, 572.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.27 (d, *J* = 8.4 Hz, 1H), 8.14 (d, *J* = 8.8 Hz, 1H), 7.81 (d, *J* = 1.6 Hz, 1H), 7.69 (dd, *J* = 8.4 Hz, 3H), 7.55 (dd, *J* = 8.8, 1.8 Hz, 1H), 7.46 (dd, *J* = 7.1, 5.3 Hz, 2H), 7.37 –7.35 (m, 3H), 7.33 –7.27(m, 5H), 7.22 –7.21 (m, 6H), 7.16 (dd, *J*= 8.3Hz, 1H), 7.12 (d, *J* = 8.3 Hz, 2H), 2.30 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 155.3, 154.7, 145.0, 142.2, 142.0, 138.6, 137.6, 135.0, 131.8, 129.8, 129.2, 128.8, 128.3, 127.5, 127.2, 126.9, 126.6, 126.4, 126.2, 126.1, 124.7, 123.9, 121.6, 120.0, 119.2, 115.1, 114.6, 69.0, 21.6; HRMS (EI) *m*/*z* calcd for $C_{40}H_{29}NO_2S$ $[M]^+$: 587.1919; found: 587.1902.

6. Computational Methodology.

We have performed gas-phase geometry optimizations using the Gaussian16 rev. A.03 program.[3] The potential energy surface (PES) of the reactions reported in this work was explored using a combined semi-empirical-DFT approach (two-layered ONIOM scheme)[4] (see Figure S1). We treated the diphenyl phosphine part of Au(I) complex, the isonitrile core and the [2(phenylethynyl)phenyl]methylene (Figure S1) with the global-hybrid, meta-GGA density-functional M08-HX developed by Zhao and Truhlar,[5] in combination with the split-valence double-ζ quality basis set with one function 6-31G(d) for C and H and two polarization functions, 6-31G(2d) for N and P and the modified LANL2DZ pseudopotential for Au.[6] For the outer part, we defined the t-Butyl groups of the Au(I) complex, phenyl groups of the substrate and the methyl group of isonitrile as the steric hindrance contributors, described at the semi-empirical PM6 level[7] as this can give good weak interactions such as hydrogen bonds, and has been shown to be significantly better for reproducing ab initio TS structures and barrier heights.[8] We also utilized electronic embedding in our calculations to incorporate the partial charges of the PM6 region into the DFT Hamiltonian.[9] This computational level of theory is called ONIOM(M08-HX/*mixed–basis*:PM6) where *mixed–basis* stands for the combination described above (6-31G(d)–6-31G(2d)–mod-LANL2DZ). Finally, we have computed the S-value test which is low (0.63 kcal·mol^{-1}) and therefore, our ONIOM2 partition scheme is very suitable for this study.

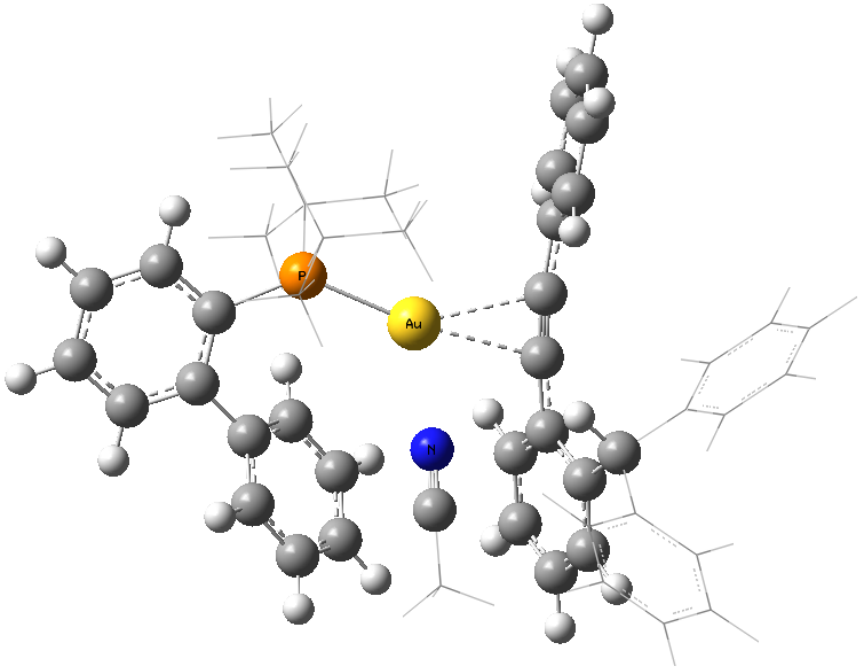


Figure S1. Partition scheme used for ONIOM calculations. The high layer is represented in ball and stick mode whereas the low layer is shown as wireframe draw.

Also, the solvent effect was considered by performing single-point calculations over each optimized geometry using the polarizable continuum model (PCM) and setting up Truhlar and coworkers' SMD solvation radii[10] using dichloroethane as the solvent of reaction.

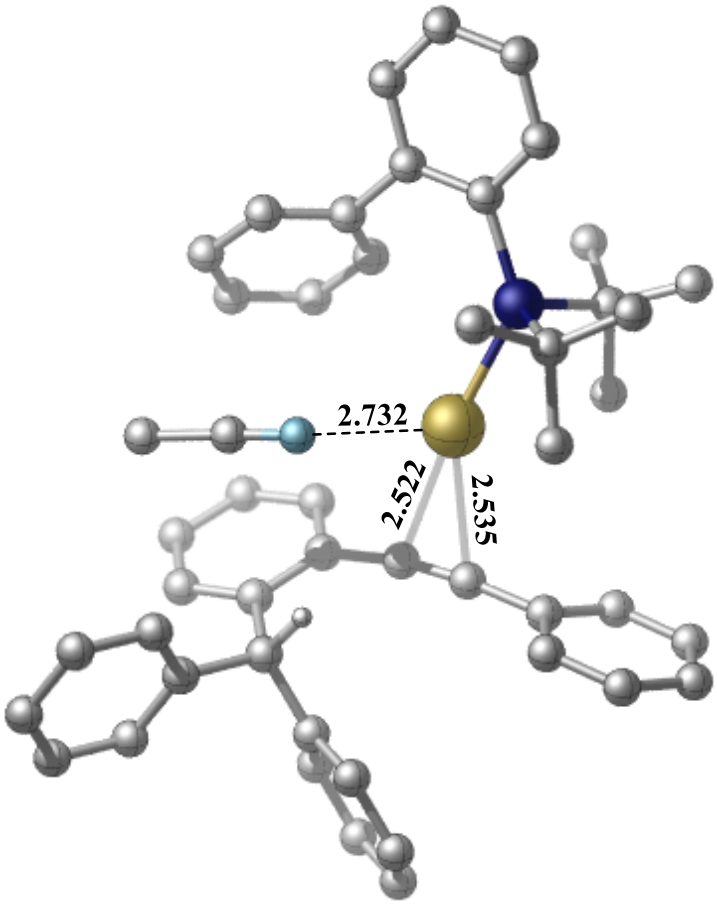


Figure S2. Optimized geometry of the reaction adduct **I**. Bond distances are given in Angstroms. Hydrogens were omitted for clarity.

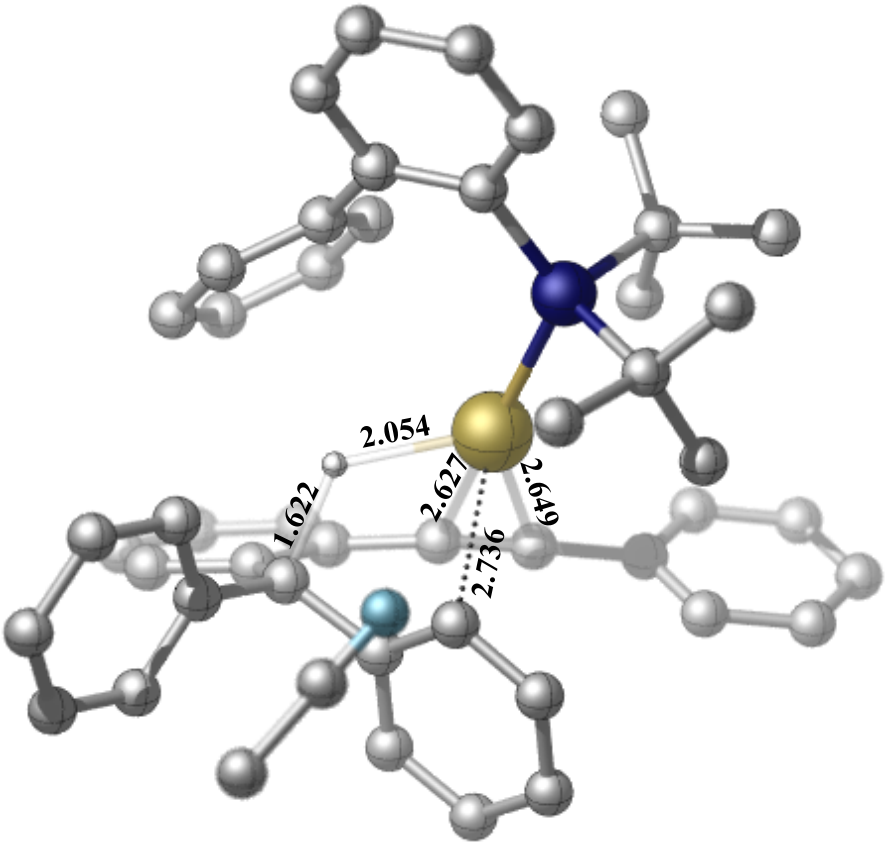


Figure S3. Optimized geometry of the transition state **I→II**. Bond distances are given in Angstroms. Hydrogens were omitted for clarity.

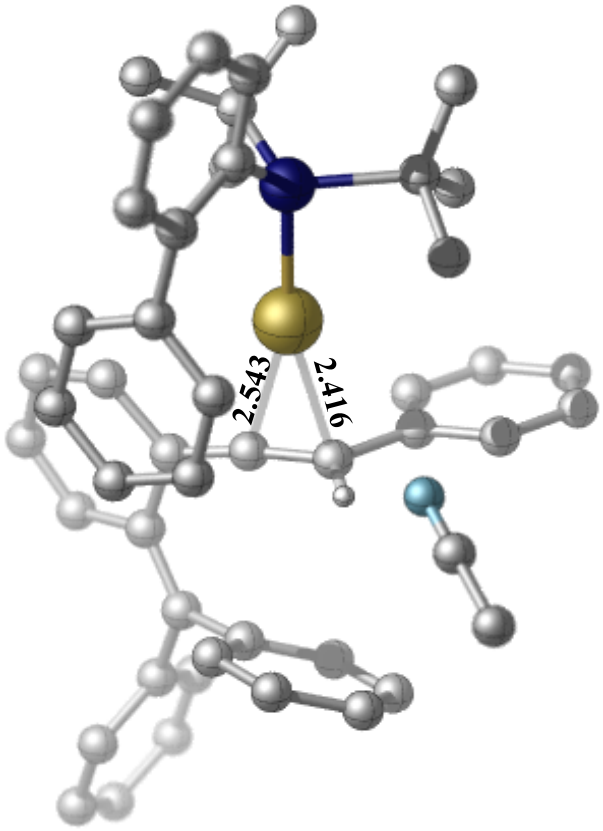


Figure S4. Optimized geometry of the intermediate **II**. Bond distances are given in Angstroms. Hydrogens were omitted for clarity.

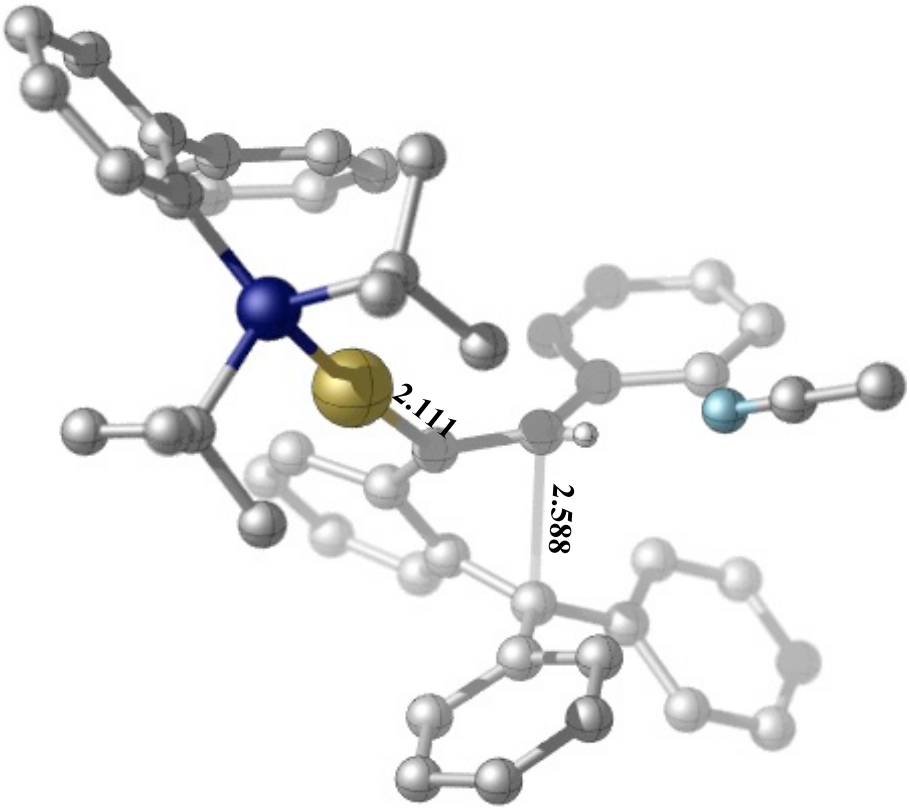


Figure S5. Optimized geometry of the transition state **II→III**. Bond distances are given in Angstroms. Hydrogens were omitted for clarity.

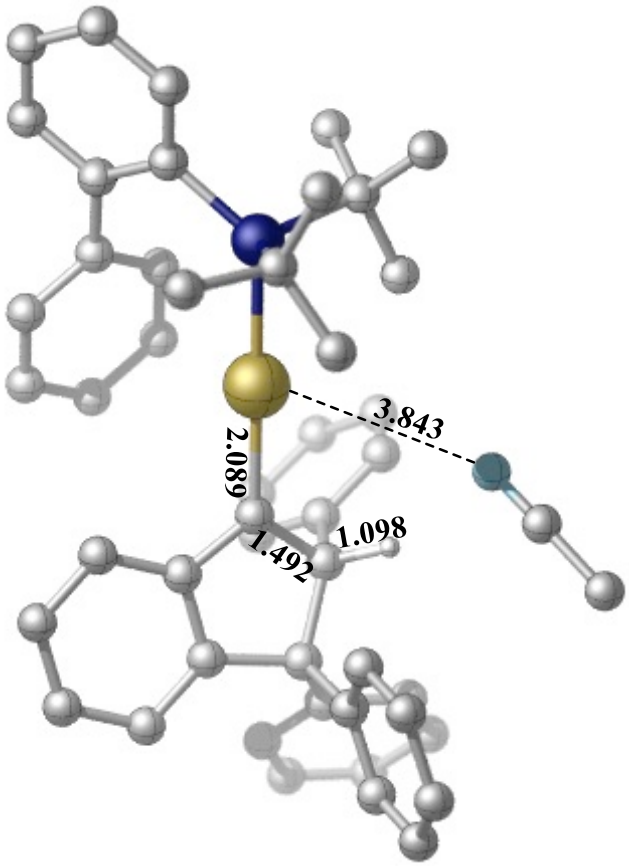


Figure S6. Optimized geometry of the intermediate **III**. Bond distances are given in Angstroms. Hydrogens were omitted for clarity.

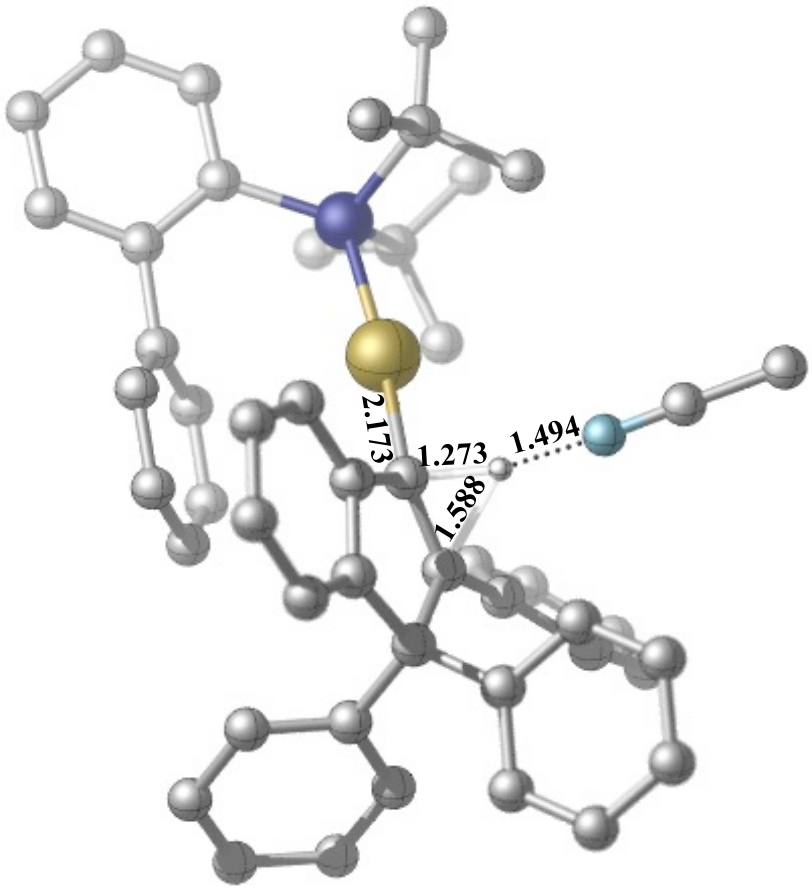


Figure S7. Optimized geometry of the transition state **III→IV**. Bond distances are given in Angstroms. Hydrogens were omitted for clarity.

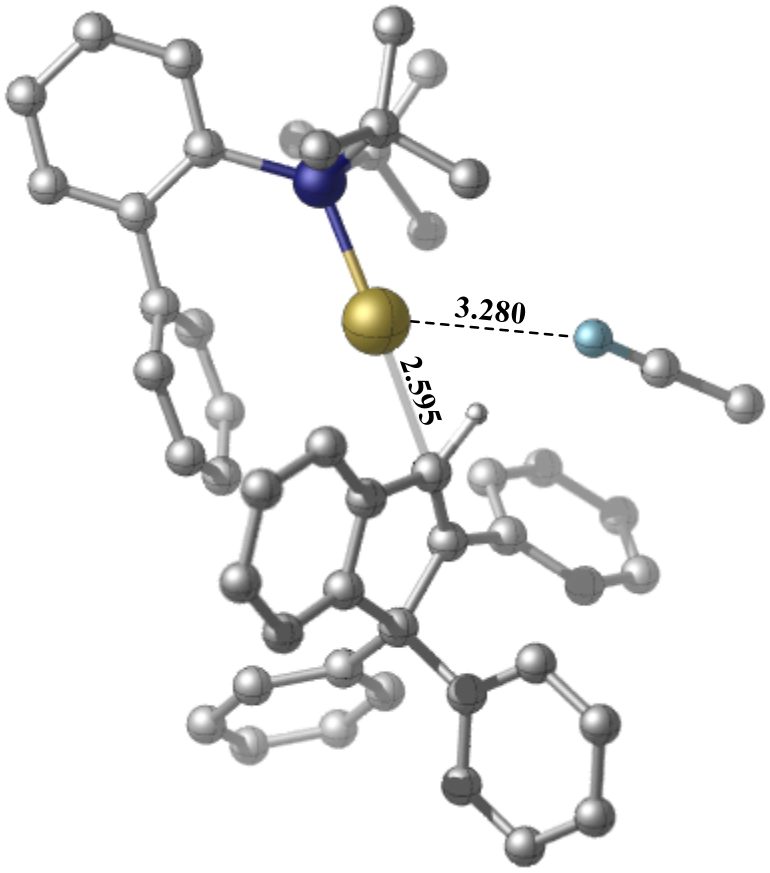


Figure S8. Optimized geometry of the intermediate **IV**. Bond distances are given in Angstroms. Hydrogens were omitted for clarity.

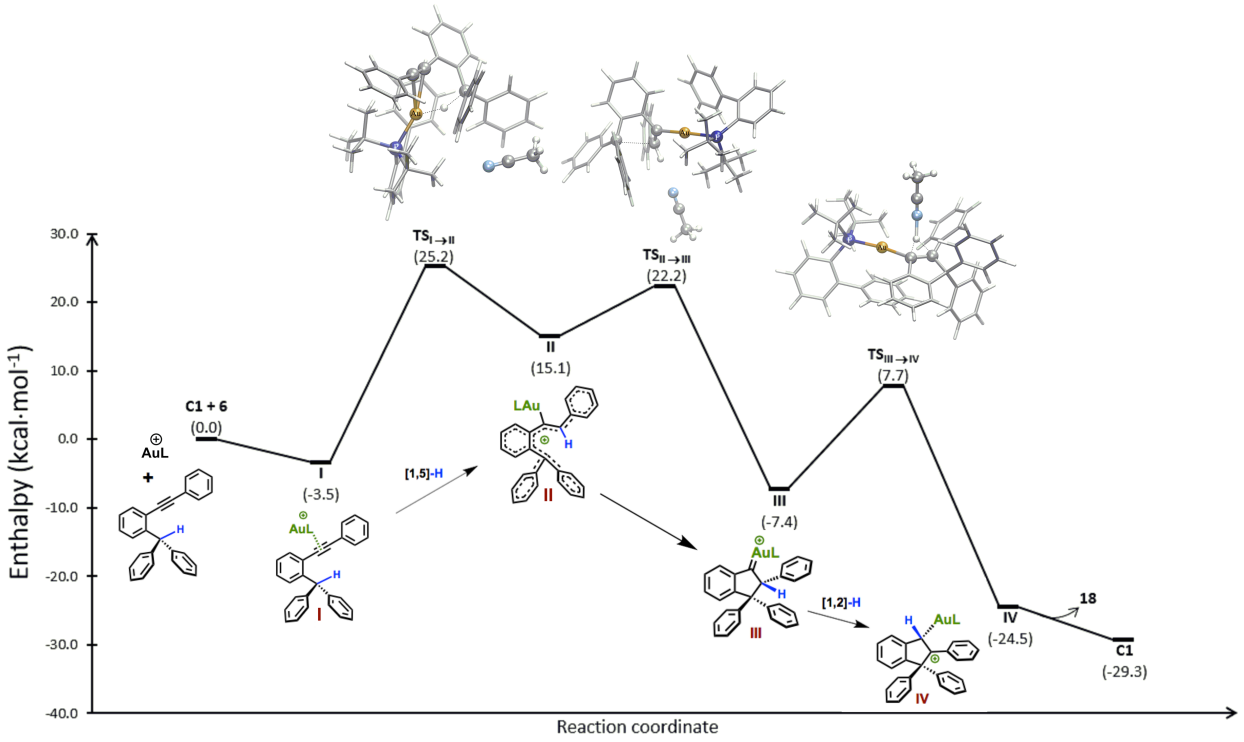


Figure S9. Free energy profile for the calculated reaction mechanism between **C1** and **6** to get product **18**. Calculations were done at the (SMD:dichloroethane)ONIOM(M08-HX/*mixed–basis*:PM6) level.

Table 2. Cartesian coordinates (xyz) of the optimized geometries for all the compounds involved in the reaction mechanism.

C1

E(scf) = –578.519481534200 a.u.

C	2.495086	1.983280	0.484145
C	1.273426	1.391684	0.160731
C	0.103017	2.172992	0.286062
C	0.183134	3.505677	0.717595
C	1.413220	4.072652	1.029945
C	2.572153	3.307945	0.913649
H	3.413773	1.396682	0.390548
H	–0.735800	4.085456	0.804273
H	1.466825	5.109504	1.362826
H	3.542914	3.742417	1.154260
C	–1.177207	1.602605	–0.018537
C	–2.251291	1.098315	–0.265998
C	–3.511570	0.476092	–0.547216
C	–4.622063	1.245104	–0.929794
C	–3.644136	–0.917985	–0.439667
C	–5.839087	0.628099	–1.200603
H	–4.516346	2.326648	–1.011915
C	–4.864345	–1.527172	–0.712200
H	–2.778740	–1.508956	–0.133323
C	–5.963787	–0.757300	–1.093673
H	–6.696638	1.232253	–1.497595
H	–4.959244	–2.609755	–0.624689
H	–6.919194	–1.237455	–1.306720
C	1.157882	–0.057915	–0.338123
H	0.447203	–0.035136	–1.203568
C	2.495928	–0.579850	–0.834779
C	3.363009	–1.298700	0.000257
C	2.869174	–0.327187	–2.164796
C	4.586162	–1.763335	–0.491452
H	3.083100	–1.502103	1.034115
C	4.093429	–0.792055	–2.651024
H	2.207265	0.236538	–2.820126
C	4.954566	–1.511905	–1.816365
H	5.252724	–2.324517	0.161519
H	4.376907	–0.593093	–3.683236
H	5.906478	–1.875185	–2.197187

I

E(scf) = –1612.310359278357 a.u.

C	3.634379	–2.362721	–1.416669
C	3.130700	–1.165275	–0.903816
C	2.021590	–0.594648	–1.570160
C	1.459259	–1.202266	–2.699032
C	1.984539	–2.393843	–3.188094
C	3.070195	–2.975872	–2.538548
H	4.494302	–2.831871	–0.932487
H	0.614169	–0.718780	–3.191448
H	1.552604	–2.859874	–4.074295
H	3.497694	–3.905282	–2.914129
C	1.467442	0.650216	–1.099202
C	1.188712	1.784323	–0.725820
C	1.009002	3.157600	–0.333689
C	0.454439	4.082506	–1.232340
C	1.420643	3.571786	0.942635
C	0.309845	5.411117	–0.848794
H	0.157676	3.752843	–2.228256
C	1.272854	4.903959	1.314050
H	1.867046	2.845850	1.623254
C	0.715624	5.821526	0.422403
H	–0.112590	6.132591	–1.547006
H	1.599807	5.229602	2.300693
H	0.604380	6.864741	0.716523
C	3.718949	–0.458913	0.332037
H	2.836785	–0.140553	0.947541
C	4.573773	–1.391969	1.171866
C	5.901580	–1.674696	0.817456
C	4.032177	–1.959741	2.334836
C	6.670805	–2.532343	1.607634
H	6.341109	–1.210061	–0.066733
C	4.806301	–2.817313	3.122542
H	3.018115	–1.717349	2.645487
C	6.123865	–3.109559	2.758584
H	7.704054	–2.744926	1.330468
H	4.385122	–3.249742	4.029759
H	6.727559	–3.774896	3.375306

C	0.559031	−0.985479	0.707851
C	−0.104304	−2.145893	0.276265
C	0.658574	−0.715822	2.079584
C	−0.665781	−3.020489	1.209247
H	−0.174567	−2.370180	−0.786776
C	0.092156	−1.593227	3.009008
H	1.170715	0.181913	2.425430
C	−0.570854	−2.745766	2.577623
H	−1.176410	−3.920023	0.869922
H	0.167394	−1.374977	4.073117
H	−1.011498	−3.426227	3.302709

6

E(scf) = −1033.777359752151 a.u.

Au	1.134564	−0.464531	−0.135759
P	−1.123295	−0.678022	0.097077
C	−1.262106	−1.341781	1.893082
C	−1.355873	−2.052010	−1.210969
C	−0.270545	−3.097805	−0.914778
H	−0.399663	−3.596281	0.062115
H	−0.334418	−3.917643	−1.654874
H	0.769704	−2.737046	−1.003693
C	−1.039388	−1.347983	−2.537403
H	−1.058106	−2.072773	−3.369938
H	−1.782960	−0.584649	−2.815112
H	−0.039365	−0.885532	−2.576995
C	−2.733966	−2.695943	−1.247619
H	−2.811830	−3.389281	−2.102275
H	−2.963397	−3.298606	−0.358937
H	−3.555436	−1.973636	−1.381378
C	−1.953638	−2.698157	1.973772
H	−1.432630	−3.493475	1.416549
H	−1.993735	−3.046340	3.019872
H	−2.999392	−2.672449	1.637274
C	0.205120	−1.456293	2.348094
H	0.736038	−0.489385	2.417022
H	0.236169	−1.840356	3.387371
H	0.802578	−2.191708	1.781979
C	−2.012732	−0.318387	2.742577
H	−1.554874	0.686519	2.747709
H	−3.064557	−0.195512	2.445046
H	−2.041476	−0.636771	3.797387
C	4.503936	0.790190	−0.033559
C	4.678385	1.778773	0.948737
C	5.067959	0.966757	−1.303524
C	5.402758	2.936193	0.655167
H	4.268862	1.637118	1.946826
C	5.789757	2.129523	−1.592350
H	4.950202	0.204726	−2.072615
C	5.957289	3.115971	−0.616778
H	5.542155	3.698840	1.420696
H	6.225834	2.263594	−2.582232
H	6.522244	4.019166	−0.843520
Au	−0.908445	0.431203	−0.279871
P	−3.148756	0.478991	0.287952
C	−3.775708	1.657547	−1.095535
C	−2.876115	1.390853	1.959435
C	−1.563611	2.174101	1.775205
H	−1.519352	2.809190	0.873081
H	−1.446029	2.895885	2.607491
H	−0.650055	1.551199	1.871286
C	−2.669429	0.278984	2.992757
H	−2.381499	0.707022	3.966518
H	−3.579442	−0.306194	3.190991
H	−1.865685	−0.428768	2.735656
C	−4.003527	2.318777	2.391903
H	−3.837022	2.674206	3.421834
H	−4.080926	3.224517	1.768996
H	−4.991765	1.831790	2.403610
C	−4.744461	2.732506	−0.619533
H	−4.312455	3.418961	0.126108
H	−5.061425	3.366745	−1.463812
H	−5.673302	2.320710	−0.201618
C	−2.490192	2.289518	−1.659800
H	−1.865974	1.596829	−2.254151
H	−2.760885	3.074193	−2.393955
H	−1.886719	2.833457	−0.908580
C	−4.452987	0.790192	−2.158834
H	−3.838412	−0.051164	−2.522365
H	−5.412159	0.368728	−1.819190
H	−4.697568	1.390526	−3.049660
C	−4.413196	−0.792140	0.560920
C	−5.603566	−0.362719	1.166025
C	−4.230053	−2.155618	0.254908
C	−6.613913	−1.263460	1.481331

C	−2.278121	0.681687	−0.203108
C	−3.620588	0.397618	−0.484187
C	−1.815272	2.014155	−0.230154
C	−4.505348	1.420029	−0.811202
H	−3.972563	−0.638260	−0.469872
C	−2.716299	3.026085	−0.579288
C	−4.047055	2.735076	−0.866547
H	−5.545769	1.188013	−1.029223
H	−2.360791	4.055901	−0.603811
H	−4.731673	3.540396	−1.128194
C	−0.409658	2.377979	0.109253
C	0.451762	2.870779	−0.878442
C	0.070808	2.204507	1.413522
C	1.781869	3.159291	−0.569222
H	0.078048	3.011221	−1.893724
C	1.398725	2.498850	1.724471
H	−0.610084	1.828102	2.188628
C	2.257258	2.970952	0.729940
H	2.445338	3.540852	−1.344866
H	1.759305	2.369159	2.744224
H	3.292355	3.210062	0.972601
N	3.284928	−0.385107	−0.374731
C	4.421011	−0.329636	−0.512090
C	5.858178	−0.263797	−0.686592
H	6.379662	0.016269	0.251884
H	6.282213	−1.237213	−1.010317
H	6.150808	0.483197	−1.453194
H	−5.727514	0.696732	1.415450
C	−5.259994	−3.048323	0.590130
C	−6.434844	−2.614950	1.193547
H	−7.530383	−0.912096	1.950952
H	−5.134462	−4.101664	0.339810
H	−7.217174	−3.334057	1.431693
C	−3.029110	−2.719425	−0.419457
C	−2.418160	−3.864311	0.108560
C	−2.555042	−2.200131	−1.631389
C	−1.358639	−4.474727	−0.558511
H	−2.783320	−4.276962	1.050196
C	−1.483392	−2.799952	−2.289339
H	−3.063792	−1.339350	−2.088684
C	−0.881017	−3.938283	−1.754561
H	−0.911264	−5.378791	−0.144747
H	−1.143644	−2.400195	−3.244595
H	−0.055657	−4.415691	−2.282629
N	0.335836	−1.567147	1.108490
C	0.874763	−2.566217	0.908999
C	1.593319	−3.812940	0.710968
H	1.611363	−4.108930	−0.355356
H	2.652659	−3.721883	1.036387
H	1.147061	−4.643947	1.286731

$TS_{I \rightarrow II}$

E(scf) = −1612.251094142660 a.u.
ν_{min} = −637.2 cm^{-1}

C	3.815804	1.033067	−2.392836
C	2.711144	1.267842	−1.567626
C	1.706575	2.140488	−2.042955
C	1.824651	2.750780	−3.299302
C	2.942692	2.513359	−4.093099
C	3.939001	1.651764	−3.636364
H	4.598148	0.346875	−2.059801
H	1.033717	3.417772	−3.640587
H	3.032227	2.997174	−5.064627
H	4.816248	1.454170	−4.251416
C	0.534460	2.438931	−1.262661

II

E(scf) = −1612.272396054096 a.u.

C	4.009186	−2.920719	−0.843183
C	3.500054	−1.635665	−0.356550
C	2.013837	−1.464493	−0.420585
C	1.195924	−2.676234	−0.579767
C	1.762869	−3.851495	−0.910451
C	3.200228	−3.967563	−1.094583
H	5.091900	−3.028952	−0.938060
H	0.113179	−2.582967	−0.464394
H	1.138464	−4.732080	−1.058670
H	3.617996	−4.921214	−1.411921
C	1.467211	−0.255085	−0.406120
C	1.112307	1.033248	−0.436391

C	−0.433155	2.911209	−0.678206
C	−1.548611	3.596973	−0.082743
C	−2.498703	4.211144	−0.916432
C	−1.683655	3.676214	1.311765
C	−3.569517	4.895811	−0.353821
H	−2.382403	4.149683	−1.998158
C	−2.761498	4.360264	1.863910
H	−0.929181	3.211462	1.950268
C	−3.703694	4.968622	1.033918
H	−4.302042	5.377724	−0.999981
H	−2.862587	4.426441	2.946128
H	−4.544059	5.507513	1.470057
C	2.543362	0.568488	−0.251374
H	1.242134	−0.363430	−0.513173
C	3.615664	−0.401900	0.151934
C	4.903541	0.069091	0.460689
C	3.336030	−1.770169	0.257298
C	5.904978	−0.828269	0.836491
H	5.121343	1.136033	0.405918
C	4.341717	−2.665251	0.636455
H	2.331524	−2.139253	0.050402
C	5.627929	−2.197773	0.919485
H	6.907355	−0.460890	1.060051
H	4.120448	−3.730294	0.710474
H	6.415146	−2.898023	1.199480
C	2.084552	1.398356	0.917241
C	1.164611	0.858041	1.833881
C	2.620962	2.675645	1.135744
C	0.820541	1.586544	2.979021
H	0.846569	−0.199322	1.766905
C	2.248059	3.406810	2.268230
H	3.330049	3.100544	0.423229
C	1.350671	2.863204	3.192888
H	0.155876	1.141500	3.722545
H	2.667545	4.401428	2.434133
H	1.080716	3.426236	4.086832
Au	−0.649913	0.347308	−0.149238
P	−2.237309	−1.303801	0.262002
C	−3.791428	−0.535319	−0.597034
C	−2.398087	−1.204063	2.170577
C	−2.450164	0.298761	2.484517
H	−3.390367	0.775616	2.152760
H	−2.425395	0.449663	3.578069
C	0.993485	1.860692	−1.667549
C	1.322672	1.347030	−2.929237
C	0.524454	3.173952	−1.550571
C	1.190741	2.146357	−4.058466
H	1.691027	0.322234	−3.012193
C	0.393667	3.971091	−2.686426
H	0.261837	3.560240	−0.563172
C	0.725370	3.459057	−3.939287
H	1.455556	1.748479	−5.037481
H	0.033885	4.995047	−2.591639
H	0.626128	4.082815	−4.826897
C	4.362732	−0.711241	0.153794
H	0.971261	1.561561	0.520715
C	5.835558	−0.935074	0.092028
C	6.523407	−0.723350	−1.112499
C	6.531564	−1.328920	1.243657
C	7.906492	−0.915353	−1.161824
H	5.983004	−0.409162	−2.003740
C	7.914491	−1.523284	1.183755
H	5.998365	−1.480288	2.180823
C	8.602295	−1.317126	−0.016441
H	8.444899	−0.749944	−2.095162
H	8.458205	−1.832596	2.076676
H	9.681292	−1.466496	−0.058857
C	3.957480	0.542271	0.846048
C	3.405566	0.479674	2.134389
C	4.201535	1.786054	0.243813
C	3.095632	1.660628	2.814476
H	3.228086	−0.487114	2.605939
C	3.879766	2.961671	0.926964
H	4.644885	1.833247	−0.750850
C	3.329868	2.900915	2.212064
H	2.689034	1.613029	3.823431
H	4.071307	3.927945	0.460154
H	3.102125	3.819551	2.748595
Au	−1.064428	−0.015100	−0.430443
P	−3.311588	−0.408956	−0.553852
C	−3.407508	−1.775765	−1.894776
C	−3.753864	1.319428	−1.244588
C	−2.871945	1.536933	−2.480489
H	−3.111976	0.852486	−3.312543
H	−3.045503	2.548955	−2.889367
H	−1.783432	1.508939	−2.293263

H	−1.604704	0.890414	2.098886
C	−1.098878	−1.818589	2.692842
H	−1.027809	−1.727261	3.790458
H	−1.007963	−2.897695	2.500689
H	−0.175331	−1.337487	2.322261
C	−3.599990	−1.910354	2.788503
H	−3.583158	−1.797258	3.884910
H	−4.571189	−1.516444	2.459397
H	−3.604997	−2.998146	2.606927
C	−4.938983	−0.248273	0.367305
H	−4.682880	0.490976	1.144767
H	−5.800100	0.173305	−0.175688
H	−5.318261	−1.149440	0.872411
C	−3.261678	0.787756	−1.177441
H	−2.472923	0.677150	−1.940621
H	−4.077372	1.300549	−1.723892
H	−2.969338	1.523291	−0.406791
C	−4.276882	−1.466581	−1.705782
H	−3.514552	−1.680246	−2.475672
H	−4.639069	−2.434486	−1.330332
H	−5.127183	−1.020167	−2.244854
C	−2.061716	−3.040967	−0.251390
C	−2.826114	−4.010411	0.412809
C	−1.149039	−3.441383	−1.253123
C	−2.683388	−5.363219	0.124951
H	−3.536091	−3.705013	1.188278
C	−1.011775	−4.811158	−1.518285
C	−1.763650	−5.764151	−0.840679
H	−3.285507	−6.096973	0.656852
H	−0.314511	−5.118689	−2.297720
H	−1.639736	−6.820078	−1.075955
C	−0.333291	−2.498650	−2.063976
C	1.052385	−2.681048	−2.167533
C	−0.930049	−1.449092	−2.772411
C	1.823317	−1.811284	−2.935824
H	1.524279	−3.503445	−1.627185
C	−0.158277	−0.570378	−3.533303
H	−2.024514	−1.341987	−2.748986
C	1.221346	−0.750767	−3.614583
H	2.903272	−1.953775	−2.997394
H	−0.637282	0.243107	−4.078242
H	1.827631	−0.066781	−4.209309
N	1.988938	−1.762635	3.699862
C	−3.311930	2.276665	−0.128566
H	−3.498595	3.321967	−0.428297
H	−3.872121	2.148021	0.809197
H	−2.232090	2.243268	0.108122
C	−5.226190	1.519087	−1.575775
H	−5.392539	2.529504	−1.985841
H	−5.609230	0.827095	−2.335563
H	−5.879249	1.455785	−0.693813
C	−4.353742	−1.429026	−3.038675
H	−4.063641	−0.516775	−3.585985
H	−4.361975	−2.236623	−3.789360
H	−5.398156	−1.317748	−2.718817
C	−1.955197	−1.885039	−2.396400
H	−1.247179	−2.288009	−1.645747
H	−1.906110	−2.625137	−3.218995
H	−1.554543	−0.964250	−2.852085
C	−3.836174	−3.083947	−1.230086
H	−3.199000	−3.393611	−0.392060
H	−4.872672	−3.062638	−0.862302
H	−3.800314	−3.913114	−1.955270
C	−4.386064	−0.818296	0.841935
C	−5.772077	−0.869781	0.639505
C	−3.841912	−1.105824	2.110451
C	−6.627168	−1.181622	1.691199
H	−6.184883	−0.669646	−0.350781
C	−4.719411	−1.417709	3.154705
C	−6.096565	−1.450220	2.951845
H	−7.702036	−1.217791	1.525229
H	−4.302821	−1.642648	4.135976
H	−6.758932	−1.695073	3.780967
C	−2.367947	−1.142093	2.361638
C	−1.656496	0.016989	2.693622
C	−1.681358	−2.354651	2.224734
C	−0.271635	−0.037528	2.867459
H	−2.181601	0.969584	2.787625
C	−0.298132	−2.406564	2.399116
H	−2.238994	−3.258863	1.975665
C	0.409273	−1.245939	2.713460
H	0.276238	0.874762	3.108097
H	0.230611	−3.352123	2.278940
H	1.493858	−1.281980	2.832179
N	−0.534907	3.101288	1.844723
C	−0.356502	3.906457	2.648988

C	3.098051	−1.650187	3.988539
C	4.500986	−1.507022	4.346979
H	5.129363	−1.356177	3.448217
H	4.663027	−0.642128	5.015098
H	4.879278	−2.403083	4.871600
C	−0.137116	4.925120	3.663090
H	0.601664	5.679303	3.332205
H	−1.070389	5.469056	3.903742
H	0.238742	4.489958	4.607844

$TS_{II \rightarrow III}$

E(scf) = −1612.261221791709 a.u.
ν_{min} = −91.5 cm^{-1}

C	−3.689220	−2.310348	−2.119461
C	−2.977524	−1.236653	−1.549201
C	−1.577507	−1.382496	−1.314510
C	−0.874515	−2.473692	−1.868664
C	−1.592653	−3.491936	−2.465241
C	−2.996624	−3.418081	−2.575622
H	−4.764975	−2.231082	−2.275265
H	0.206034	−2.537179	−1.736803
H	−1.073543	−4.372319	−2.841693
H	−3.538605	−4.227301	−3.060855
C	−1.018004	−0.422166	−0.412382
C	−1.787646	−0.013259	0.664637
C	−2.598738	−0.874422	1.553943
C	−2.572035	−2.278010	1.491404
C	−3.349312	−0.252599	2.564344
C	−3.304476	−3.033785	2.402136
H	−1.957689	−2.775861	0.739229
C	−4.085405	−1.017792	3.467540
H	−3.337314	0.836077	2.636899
C	−4.066722	−2.410271	3.387753
H	−3.268433	−4.121684	2.347557
H	−4.666706	−0.522625	4.243914
H	−4.629769	−3.006229	4.104058
C	−3.591508	0.029966	−1.191373
H	−1.582888	0.969785	1.100438
C	−4.962912	0.050579	−0.669221
C	−5.832694	1.131243	−0.951792
C	−5.451969	−1.025609	0.103114
C	−7.136560	1.135428	−0.465197
H	−5.492062	1.962099	−1.575295
C	−6.757643	−1.010557	0.595659
H	−4.802461	−1.877136	0.331165
C	−7.601528	0.067729	0.315421

III

E(scf) = −1612.310387577454 a.u.

C	−3.618268	−1.241919	−2.864584
C	−2.949084	−0.773835	−1.738520
C	−1.532799	−0.784536	−1.717889
C	−0.781395	−1.271347	−2.805537
C	−1.459584	−1.762603	−3.909285
C	−2.864046	−1.738962	−3.931206
H	−4.706027	−1.204749	−2.931114
H	0.309054	−1.251705	−2.759503
H	−0.914204	−2.148197	-4.769049
H	−3.383014	−2.107615	−4.816608
C	−1.020933	−0.168189	−0.529973
C	−2.177680	0.056103	0.385964
C	−1.915034	−1.044424	1.431447
C	−2.182330	−2.391830	1.169181
C	−1.342990	−0.681509	2.656569
C	−1.952399	−3.356545	2.150009
H	−2.596698	−2.691181	0.202175
C	−1.094398	−1.648867	3.627448
H	−1.121399	0.371420	2.849325
C	−1.409562	−2.987036	3.380681
H	−2.195671	−4.400097	1.950154
H	−0.671546	−1.355651	4.587661
H	−1.230748	−3.740824	4.146656
C	−3.494857	−0.083796	−0.471929
H	−2.100322	1.017516	0.910746
C	−4.581969	−0.821731	0.285809
C	−5.152612	−2.017107	−0.167049
C	−5.028793	−0.266197	1.500105
C	−6.160755	−2.643144	0.576244
H	−4.824331	−2.486038	−1.092067
C	−6.030915	−0.894782	2.239296
H	−4.588800	0.660253	1.866715
C	−6.602977	−2.085931	1.777290
H	−6.600669	−3.572198	0.212779

H	−7.802154	1.969600	−0.694109
H	−7.118464	−1.843584	1.201598
H	−8.623985	0.078468	0.699960
C	−3.015877	1.298811	−1.691794
C	−3.031796	2.465992	−0.903003
C	−2.526063	1.356215	−3.009664
C	−2.597042	3.677200	−1.440734
H	−3.372854	2.417140	0.134074
C	−2.102425	2.575991	−3.542891
H	−2.491102	0.453274	−3.622427
C	−2.143631	3.736782	−2.764440
H	−2.615377	4.580540	−0.830601
H	−1.744576	2.621961	−4.572468
H	−1.824711	4.689972	−3.188948
Au	1.027714	0.096969	−0.347333
P	3.277986	0.703834	−0.103422
C	3.113709	1.960624	1.347469
C	3.540109	1.578513	−1.790951
C	2.142594	2.121097	−2.141986
H	1.671416	2.717675	−1.342466
H	2.213217	2.808169	−3.003487
H	1.433881	1.341712	−2.481594
C	3.933269	0.473226	−2.778145
H	3.966161	0.870586	−3.805006
H	4.937283	0.065023	−2.589101
H	3.232127	−0.371331	−2.809522
C	4.585766	2.686054	−1.805905
H	4.776886	3.023561	−2.836704
H	4.270804	3.582575	−1.248471
H	5.561250	2.366087	−1.408048
C	3.982757	3.205700	1.211471
H	3.749091	3.808528	0.319928
H	3.837120	3.872253	2.075729
H	5.056863	2.977932	1.192870
C	1.620224	2.329903	1.356893
H	0.953279	1.519784	1.710422
H	1.439778	3.140244	2.089585
H	1.245407	2.733854	0.404600
C	3.484259	1.219526	2.635554
H	2.930739	0.276381	2.789037
H	4.556596	0.981883	2.698991
H	3.263787	1.842039	3.515715
C	4.708602	−0.360038	0.215800
H	−6.368972	−0.458626	3.179505
H	−7.387542	−2.575456	2.354011
C	−3.985364	1.287013	−0.935633
C	−5.359478	1.531257	−1.088924
C	−3.076488	2.304026	−1.270805
C	−5.814434	2.773011	−1.541183
H	−6.090942	0.753538	−0.856111
C	−3.533346	3.543951	−1.726102
H	−2.003106	2.138105	−1.194299
C	−4.903799	3.784643	−1.858641
H	−6.885607	2.948715	−1.652183
H	−2.817392	4.320096	−1.994344
H	−5.260462	4.748997	−2.219969
Au	0.986650	0.231572	−0.110832
P	3.250326	0.799405	0.230420
C	3.279831	1.169370	2.121183
C	3.275468	2.394308	−0.834871
C	1.861093	2.977448	−0.667260
H	1.526311	3.084395	0.377641
H	1.831381	4.004812	−1.072787
H	1.084191	2.443625	−1.244724
C	3.468923	1.917035	−2.280053
H	3.356134	2.760940	−2.979753
H	4.475951	1.515599	−2.469677
H	2.741476	1.161706	−2.605253
C	4.346993	3.414334	−0.472569
H	4.439777	4.175985	−1.263346
H	4.117266	3.970339	0.448252
H	5.350698	2.974446	−0.360792
C	3.870270	2.526453	2.485729
H	3.365839	3.375673	2.003640
H	3.780539	2.702244	3.570274
H	4.943875	2.597087	2.264930
C	1.794682	1.094954	2.512304
H	1.355254	0.085133	2.426446
H	1.677679	1.342962	3.583439
H	1.151484	1.838957	2.005444
C	4.074960	0.064822	2.820259
H	3.699417	−0.954202	2.621232
H	5.144293	0.074017	2.564630
H	4.028636	0.191132	3.913228
C	4.691861	−0.205327	−0.214528
C	5.947463	0.410767	−0.298544

C	5.989239	0.194428	0.084022
C	4.557693	−1.728834	0.521594
C	7.125666	−0.589462	0.247794
H	6.089763	1.253550	−0.173431
C	5.716878	−2.503844	0.669840
C	6.984111	−1.945500	0.539171
H	8.113982	−0.146316	0.142398
H	5.607193	−3.561543	0.910583
H	7.865956	−2.571381	0.668779
C	3.238575	−2.407749	0.674595
C	2.939747	−3.511117	-0.136210
C	2.298809	−1.995318	1.628236
C	1.725988	−4.181942	0.000393
H	3.667743	−3.837676	-0.880454
C	1.075396	−2.656525	1.756756
H	2.533440	−1.145671	2.284884
C	0.791320	−3.753887	0.944145
H	1.509520	−5.042971	-0.632497
H	0.345300	−2.318653	2.494673
H	−0.154991	−4.284909	1.054333
N	−1.508409	2.827206	2.642394
C	−1.481245	3.721030	3.368292
C	−1.442802	4.854998	4.276541
H	−0.750434	5.662126	3.893196
H	−2.471445	5.308160	4.399462
H	−1.082231	4.545048	5.302275

$TS_{III \rightarrow IV}$

E(scf) = −1612.280089910452 a.u.
ν_{min} = −687.9 cm^{-1}

C	−3.255454	−2.090986	−2.641372
C	−2.704004	−1.263672	−1.664289
C	−1.373779	−0.845015	−1.753791
C	−0.556158	−1.270394	−2.799933
C	−1.103253	−2.110175	−3.769893
C	−2.441359	−2.512577	−3.696467
H	−4.303485	−2.400242	−2.588559
H	0.481053	−0.947351	−2.859924
H	−0.486782	−2.455781	−4.602174
H	−2.850010	−3.160686	−4.466226
C	−1.022868	0.021468	−0.603396
C	−2.162738	0.177601	0.156588
C	4.547801	−1.566929	−0.557183
C	7.061331	−0.302771	−0.728028
H	6.042761	1.471712	−0.044044
C	5.678202	−2.263647	−1.002952
C	6.920934	−1.643055	−1.086059
H	8.031608	0.186585	−0.789270
H	5.572008	−3.316563	−1.265572
H	7.786225	−2.210314	−1.426540
C	3.244586	−2.282691	−0.470483
C	2.694318	−2.884990	−1.608472
C	2.540432	−2.349763	0.738991
C	1.451979	−3.516937	−1.540215
H	3.241571	−2.843838	−2.551998
C	1.290264	−2.964551	0.805560
H	2.983809	−1.907057	1.642940
C	0.742540	−3.544599	−0.339469
H	1.031904	−3.982670	−2.432643
H	0.742663	−2.987842	1.749241
H	−0.233555	−4.028461	−0.289034
N	−1.028449	3.020086	1.602620
C	−1.842911	3.835151	1.593681
C	−2.882174	4.851353	1.572332
H	−3.436291	4.889752	2.529210
H	−2.467605	5.860921	1.396459
H	−3.623358	4.652070	0.772209

IV

E(scf) = −1612.337416783371 a.u.

C	−2.846808	−2.943652	−1.925378
C	−2.542736	−1.717327	−1.346352
C	−1.400848	−1.011602	−1.763366
C	−0.533424	−1.536133	−2.717854
C	−0.820490	−2.790195	−3.260648
C	−1.968525	−3.483614	−2.872537
H	−3.756561	−3.481903	−1.651329
H	0.349727	−0.978822	−3.038230
H	−0.154355	−3.223887	−4.006118
H	−2.191680	−4.451003	−3.321332
C	−1.343097	0.251931	−1.015608
C	−2.368455	0.335967	−0.128666
C	−2.568526	1.480079	0.784111

C	−2.248556	0.998985	1.387761
C	−1.233560	0.909658	2.350950
C	−3.299919	1.908444	1.583810
C	−1.263924	1.713202	3.486257
H	−0.450638	0.156389	2.215198
C	−3.324274	2.726537	2.709930
H	−4.098659	1.993631	0.833031
C	−2.306440	2.626807	3.662042
H	−0.487598	1.623925	4.237511
H	−4.138914	3.433023	2.847961
H	−2.328944	3.258863	4.543798
C	−3.362332	−0.650929	−0.419420
H	−1.311648	1.260513	−0.634509
C	−3.722338	−1.673244	0.647874
C	−3.467807	−3.042107	0.458049
C	−4.319903	−1.259288	1.854015
C	−3.790184	−3.969024	1.456001
H	−3.011001	−3.403712	−0.466046
C	−4.636756	−2.184910	2.843053
H	−4.550323	−0.210733	2.021825
C	−4.373199	−3.548565	2.651379
H	−3.586560	−5.030637	1.286487
H	−5.097687	−1.848548	3.774499
H	−4.625909	−4.269529	3.421906
C	−4.535593	0.201070	−0.869930
C	−5.864153	−0.133933	−0.547550
C	−4.293011	1.325680	−1.686109
C	−6.925308	0.663931	−0.997654
H	−6.091699	−1.022679	0.045862
C	−5.353071	2.111081	−2.141752
H	−3.281751	1.557377	−2.006580
C	−6.673884	1.784877	−1.793851
H	−7.950780	0.391982	−0.741907
H	−5.160660	2.971871	−2.785336
H	−7.502289	2.403047	−2.145814
Au	1.074005	0.394477	−0.170502
P	3.367789	0.583782	0.040522
C	3.642694	1.425310	1.748204
C	3.704261	1.787797	−1.410523
C	2.678060	2.930036	−1.241010
H	2.866334	3.531637	−0.331167
H	2.768178	3.630398	−2.084589
H	1.631190	2.597545	−1.241097
C	−1.596098	1.768448	1.751547
C	−3.694867	2.310986	0.681707
C	−1.725203	2.882970	2.578765
H	−0.754660	1.080322	1.878742
C	−3.819018	3.426681	1.504559
H	−4.466155	2.087501	-0.060278
C	−2.832340	3.718611	2.451027
H	−0.965238	3.091159	3.331153
H	−4.696648	4.066407	1.416150
H	−2.941978	4.583832	3.103698
C	−3.322482	−0.888157	−0.303585
H	−0.765662	1.146626	−1.303417
C	−3.589501	−1.585611	1.021778
C	−3.359039	−2.957080	1.200755
C	−4.126494	−0.850021	2.094245
C	−3.642061	−3.574912	2.424526
H	−2.956386	−3.570994	0.396708
C	−4.401522	−1.465523	3.316394
H	−4.355705	0.209066	1.975558
C	−4.159042	−2.832468	3.487580
H	−3.461060	−4.643724	2.543372
H	−4.815988	−0.879535	4.137194
H	−4.379980	−3.314373	4.439660
C	−4.619324	−0.427340	−0.965738
C	−5.867324	−0.891032	−0.528714
C	−4.562542	0.437382	−2.073850
C	−7.039888	−0.472961	−1.167809
H	−5.945043	−1.587810	0.308019
C	−5.734029	0.851808	−2.709185
H	−3.599935	0.774893	−2.457351
C	−6.978481	0.401821	−2.254501
H	−8.005117	−0.839206	−0.816199
H	−5.678983	1.519008	−3.568980
H	−7.892778	0.724326	−2.751893
Au	1.116420	0.485942	−0.222517
P	3.407510	0.461131	−0.114872
C	3.705835	1.754154	1.276471
C	3.707763	1.149595	−1.876313
C	2.523554	2.097062	−2.125990
H	2.333306	2.834894	−1.330108
H	2.723402	2.718679	−3.019919
H	1.575980	1.587932	−2.388692
C	3.596482	−0.066890	−2.804193

C	3.351034	0.970062	−2.659864	H	3.609698	0.255280	−3.858918
H	3.410698	1.598613	−3.566655	H	4.442251	−0.764958	−2.707235
H	4.045022	0.137959	−2.841334	H	2.670496	−0.645744	−2.682932
H	2.325810	0.565712	−2.653723	C	5.042468	1.852636	−2.084822
C	5.112868	2.348348	−1.510498	H	5.236294	2.000274	−3.160460
H	5.224746	2.969752	−2.410467	H	5.077460	2.857517	−1.642030
H	5.393452	2.992082	−0.662875	H	5.905330	1.283022	−1.703481
H	5.888688	1.563790	−1.593485	C	4.572509	2.931534	0.845372
C	4.362737	2.768198	1.659236	H	4.182003	3.481729	−0.021239
H	3.817257	3.513892	1.063109	H	4.645610	3.671282	1.660007
H	4.482564	3.203782	2.663164	H	5.609330	2.640288	0.626070
H	5.379721	2.684918	1.248646	C	2.285837	2.229768	1.635545
C	2.203623	1.620966	2.255740	H	1.648750	1.446840	2.085190
H	1.664207	0.671154	2.436200	H	2.347998	2.998109	2.430501
H	2.225212	2.115167	3.246851	H	1.758150	2.754880	0.816366
H	1.590215	2.285159	1.633581	C	4.353474	1.048315	2.467906
C	4.417725	0.475392	2.658149	H	3.776893	0.190749	2.855389
H	3.935224	−0.511769	2.794910	H	5.369828	0.685446	2.254620
H	5.444973	0.294682	2.317571	H	4.460590	1.742757	3.316324
H	4.514070	0.903613	3.669263	C	4.479363	−0.980004	0.117613
C	4.433643	−0.875312	−0.142692	C	5.825309	−0.896840	−0.260912
C	5.774444	−0.726293	−0.520599	C	3.948757	−2.190609	0.604019
C	3.888159	−2.168513	0.007173	C	6.647788	−2.015206	−0.168616
C	6.572398	−1.843751	−0.774552	H	6.224539	0.046641	−0.648369
H	6.199542	0.277071	−0.637758	C	4.785295	−3.308451	0.673012
C	4.701332	−3.280061	−0.270746	C	6.122274	−3.221848	0.292494
C	6.028455	−3.120156	−0.658510	H	7.693037	−1.946310	−0.463199
H	7.611772	−1.710903	−1.068989	H	4.376680	−4.247771	1.044249
H	4.273310	−4.277801	−0.152504	H	6.760381	−4.101710	0.360013
H	6.637239	−3.996097	−0.857509	C	2.524237	−2.267549	1.034414
C	2.491938	−2.410603	0.480136	C	1.568926	−2.887127	0.220739
C	1.539907	−2.971952	−0.379750	C	2.118120	−1.615057	2.203843
C	2.120768	−2.070888	1.784423	C	0.215631	−2.820246	0.553158
C	0.230628	−3.171078	0.063437	H	1.884517	−3.389837	−0.694509
H	1.823761	−3.233120	−1.402629	C	0.766382	−1.550844	2.540652
C	0.815160	−2.279708	2.230544	H	2.871826	−1.129163	2.835866
H	2.873723	−1.640718	2.462774	C	−0.184867	−2.140758	1.706664
C	−0.134286	−2.825109	1.359744	H	−0.524952	−3.285397	−0.099424
H	−0.514749	−3.584727	−0.624314	H	0.453777	−1.042691	3.452975
H	0.546244	−2.029669	3.257287	H	−1.243375	−2.079347	1.972068
H	−1.158881	−2.980726	1.709583	N	−0.267824	3.409808	−0.766223
N	−1.270635	2.753603	−0.643734	C	−1.026264	4.265422	−0.628842
C	−1.313361	3.866478	-0.960265	C	−1.974283	5.355631	-0.469534

C	−1.389591	5.261718	−1.343449
H	−2.434917	5.634559	−1.328360
H	−0.809939	5.913650	−0.658575
H	−1.001796	5.431640	−2.369767
H	−2.026873	5.699924	0.580714
H	−1.701290	6.229199	−1.091495
H	−2.997035	5.050084	−0.763242

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E(scf) = −578.566420934768 a.u.

C	−3.123165	−0.304684	0.126729
C	−1.872550	−0.476882	−0.447229
C	−1.739636	−1.126384	−1.686164
C	−2.858418	−1.614095	−2.358476
C	−4.114972	−1.445086	−1.774116
C	−4.248298	−0.797547	−0.544642
H	−3.231718	0.208382	1.085328
H	−2.756711	−2.115901	−3.321817
H	−5.002951	−1.819823	−2.284847
H	−5.237940	−0.671321	−0.104485
C	−0.321336	−1.151150	−2.044936
C	0.429932	−0.539604	−1.103408
C	1.899908	−0.426306	−1.135277
C	2.580664	0.605456	−0.472215
C	2.662032	−1.366459	−1.849851
C	3.968045	0.707537	−0.537912
H	2.015331	1.348251	0.098063
C	4.046697	−1.263112	−1.919307
H	2.158555	−2.204695	−2.333294
C	4.707677	−0.222713	−1.265118
H	4.473272	1.521763	−0.017422
H	4.616007	−2.008048	−2.476234
H	5.793925	−0.144605	−1.314144
C	−0.484474	−0.022244	0.042814
H	0.063724	−1.593019	−2.964316
C	−0.538444	1.494578	0.155468
C	−1.006940	2.097561	1.334277
C	−0.196914	2.305700	−0.937712
C	−1.103155	3.488124	1.425699
H	−1.297919	1.481202	2.185308
C	−0.294658	3.696560	−0.842535
H	0.142658	1.854279	−1.870789
C	−0.744003	4.292182	0.339534
H	−1.462739	3.945730	2.345857
H	−0.023068	4.316382	−1.695644
H	−0.818961	5.374926	0.412305

C	−0.066460	−0.706460	1.336194
C	0.904073	−0.133507	2.173201
C	−0.618100	−1.949047	1.685903
C	1.301211	−0.782110	3.344932
H	1.358496	0.822765	1.909894
C	−0.219932	−2.595412	2.859271
H	−1.359438	−2.421817	1.040467
C	0.738555	−2.013605	3.693752
H	2.054643	−0.327085	3.985531
H	−0.657367	−3.557541	3.120460
H	1.048153	−2.517563	4.606527

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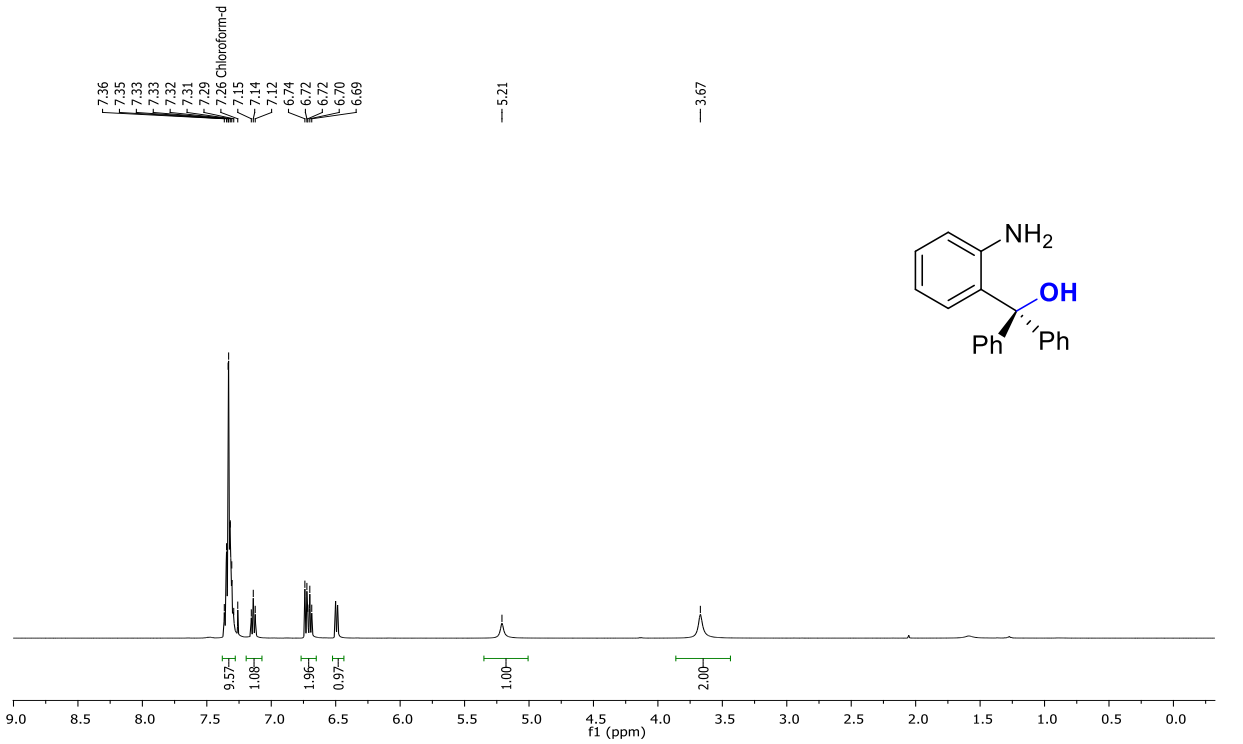
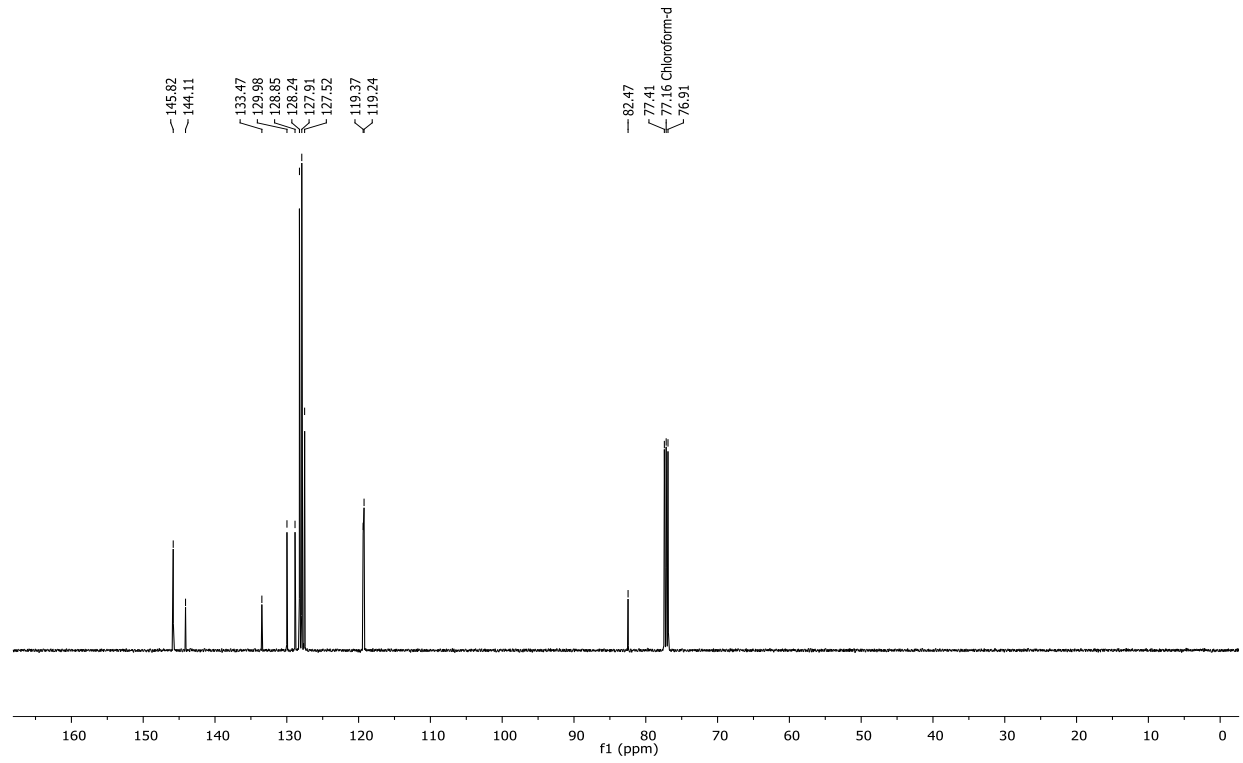
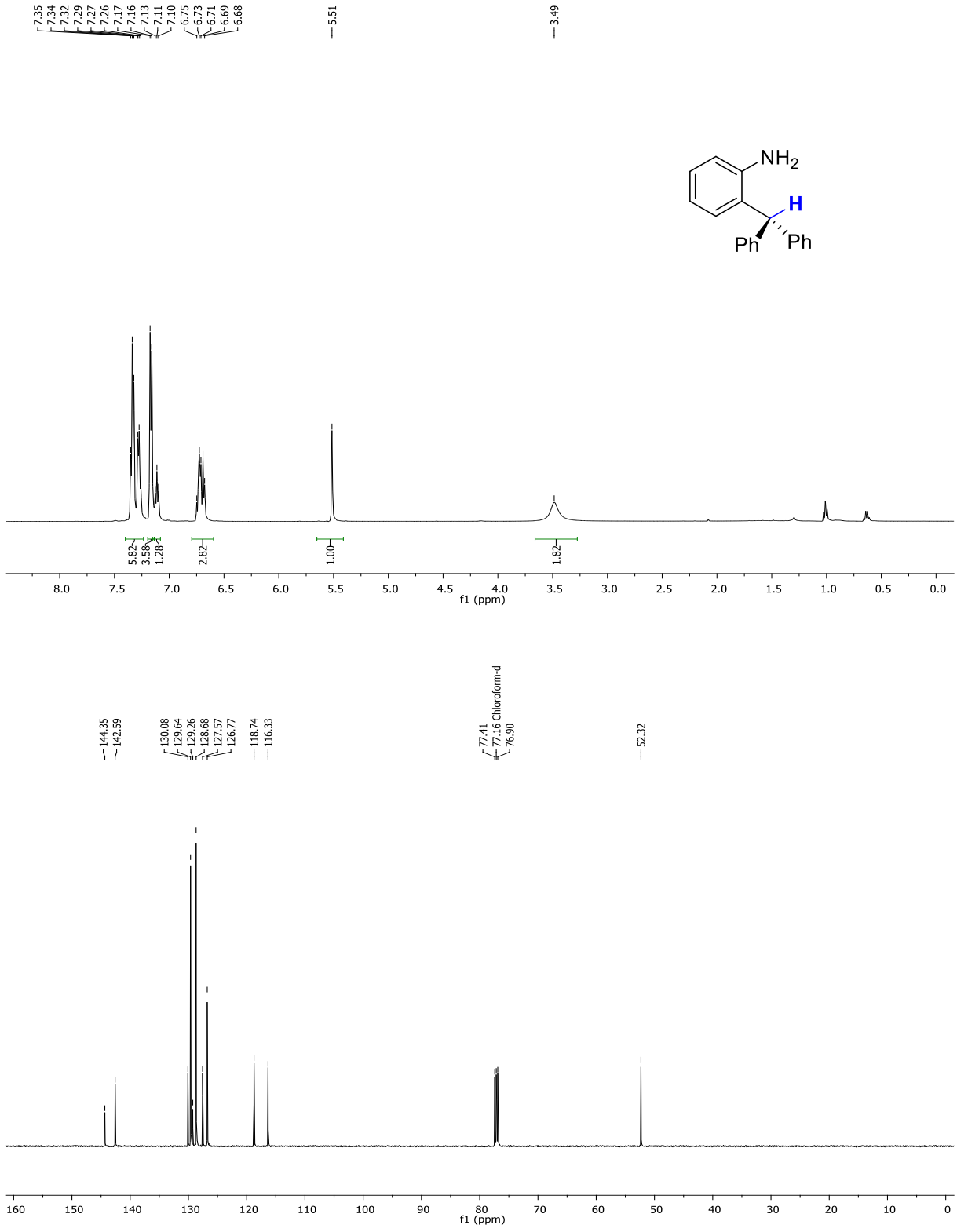
^{1}H and ^{13}C NMR SPECTRA

(2-aminophenyl)diphenylmethanol **(1)**

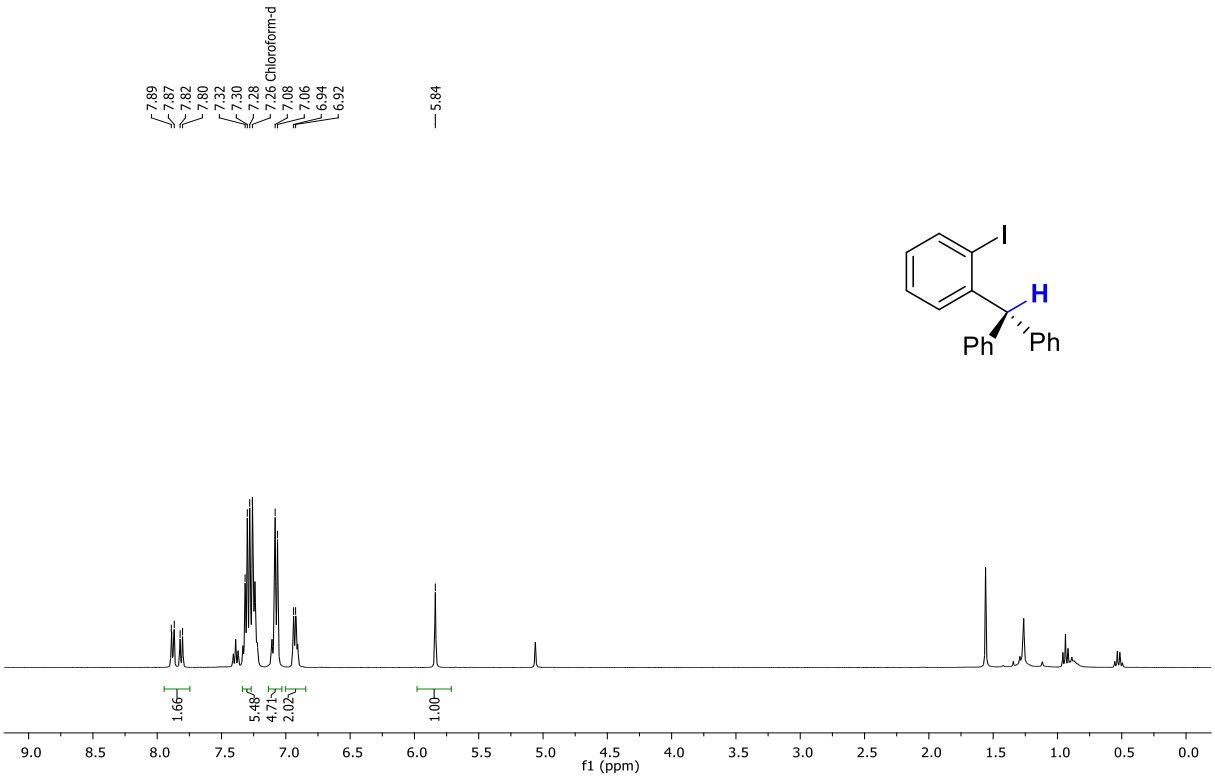




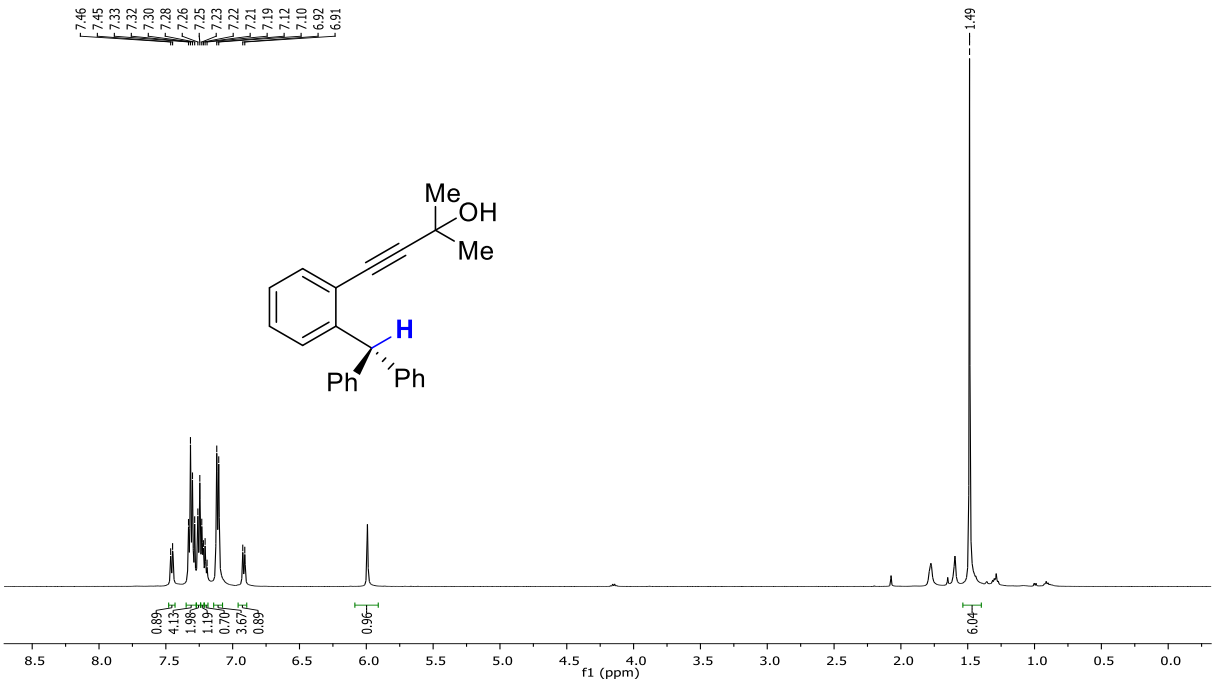
2-benzohydrylaniline **(2)**

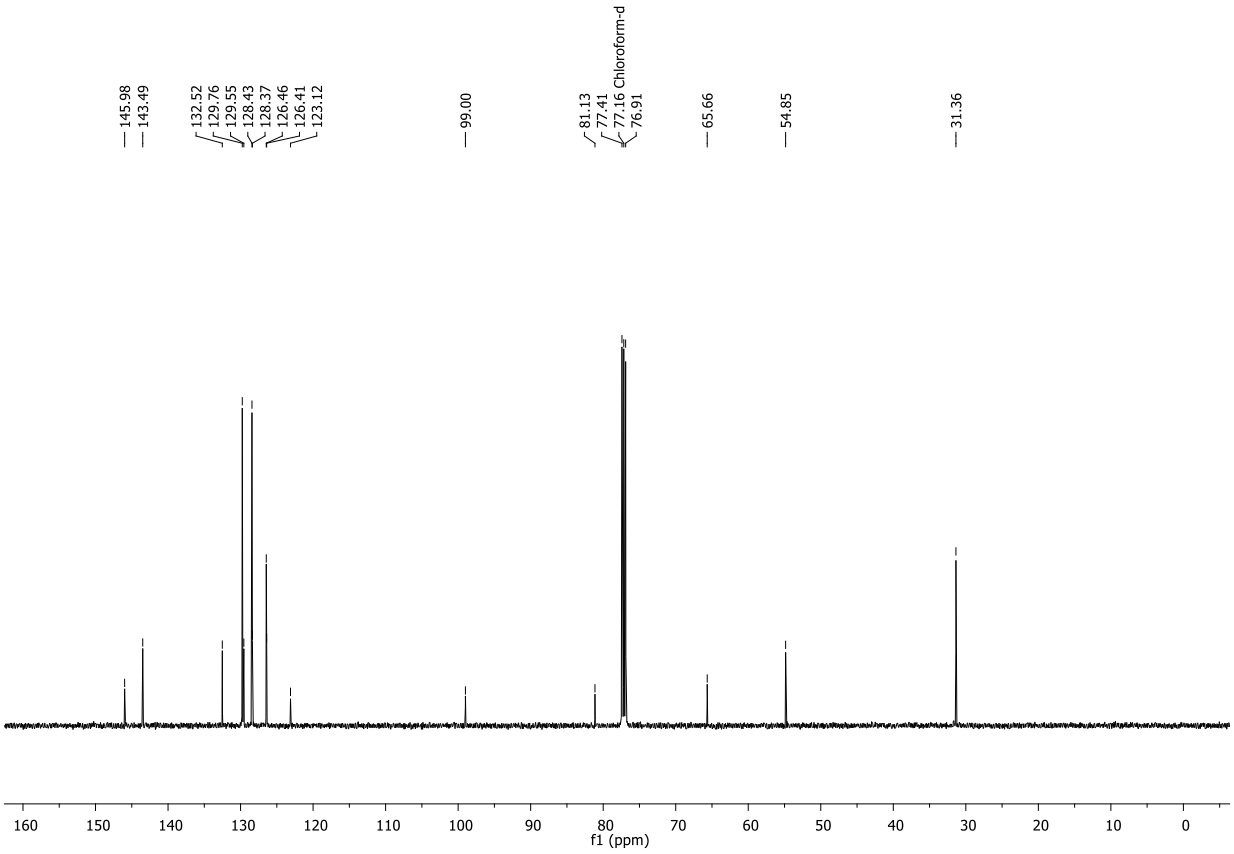


((2-iodophenyl)methylene)dibenzene **(3)**

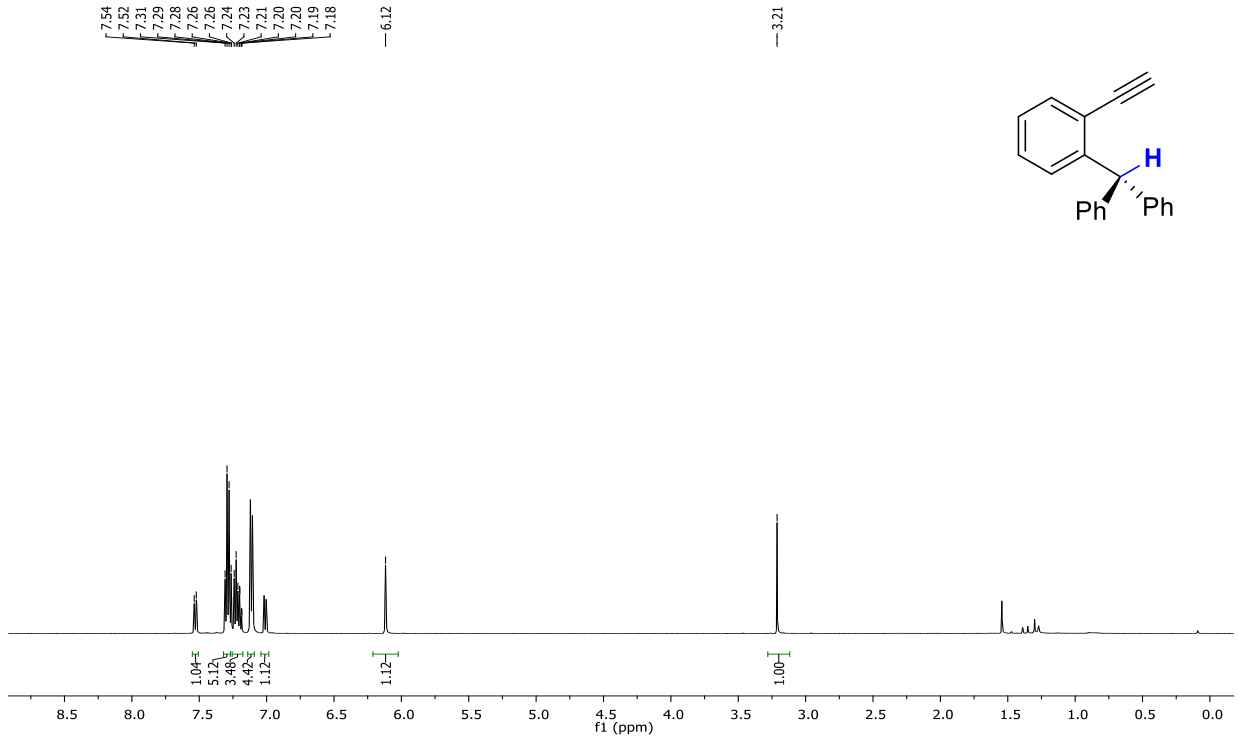


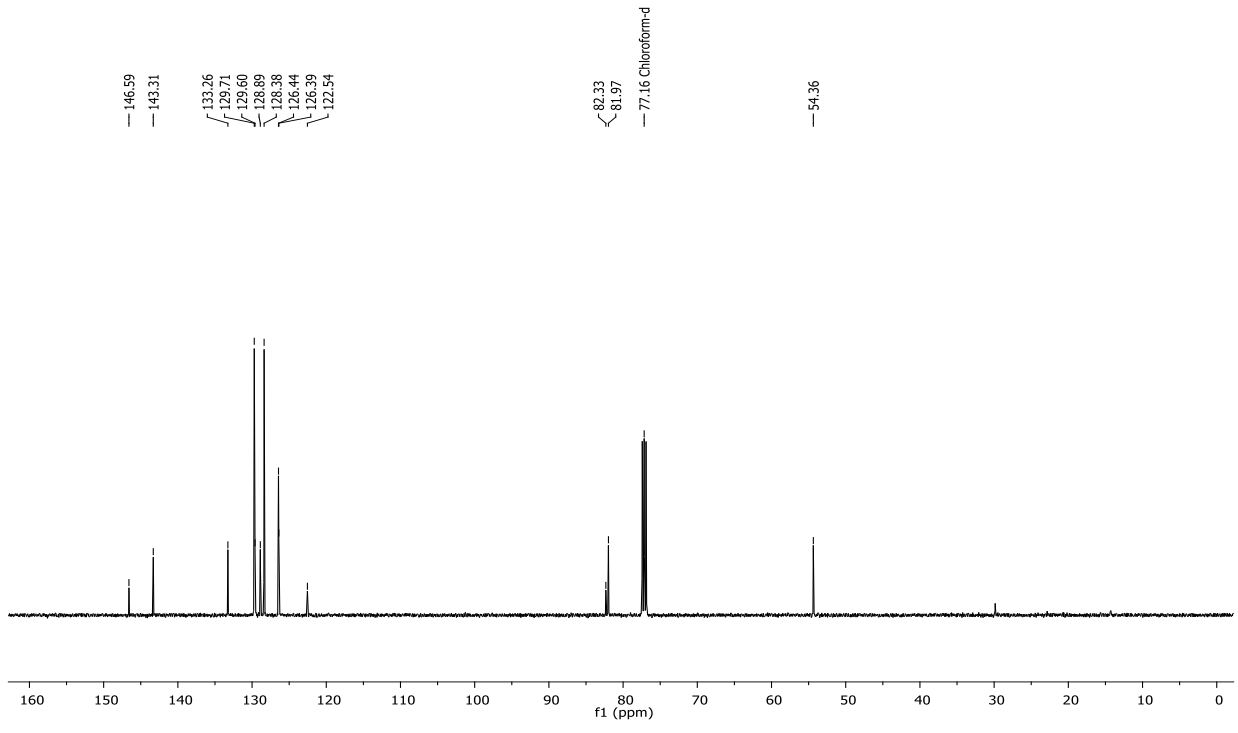
4-(2-benzohydrylphenyl)-2-methylbut-3-yn-2-ol **(4)**



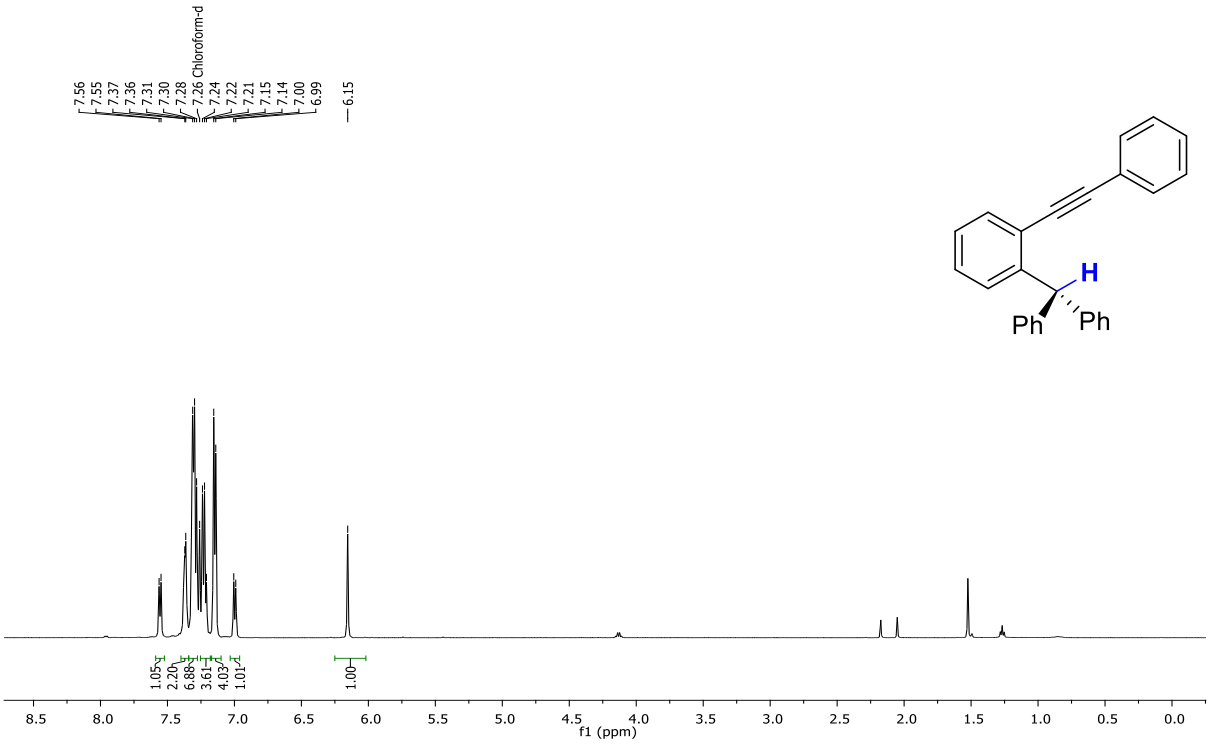


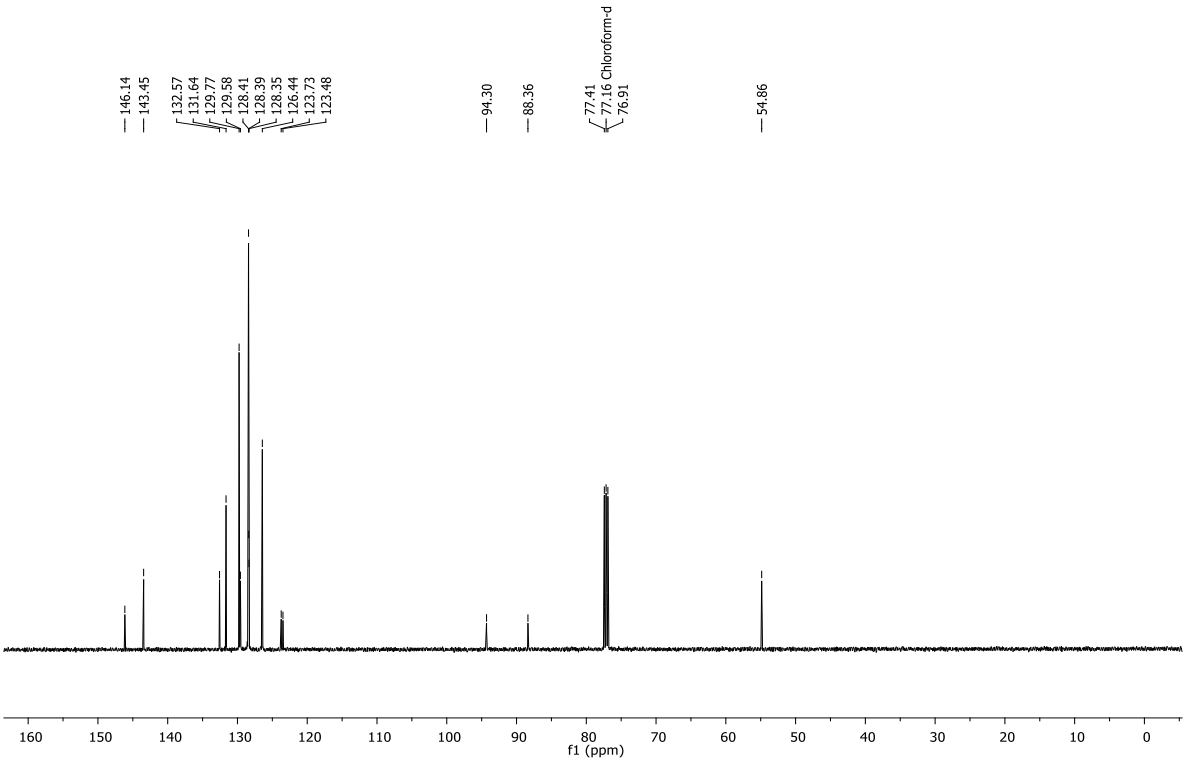
((2-ethynylphenyl)methylene)dibenzene **(5)**



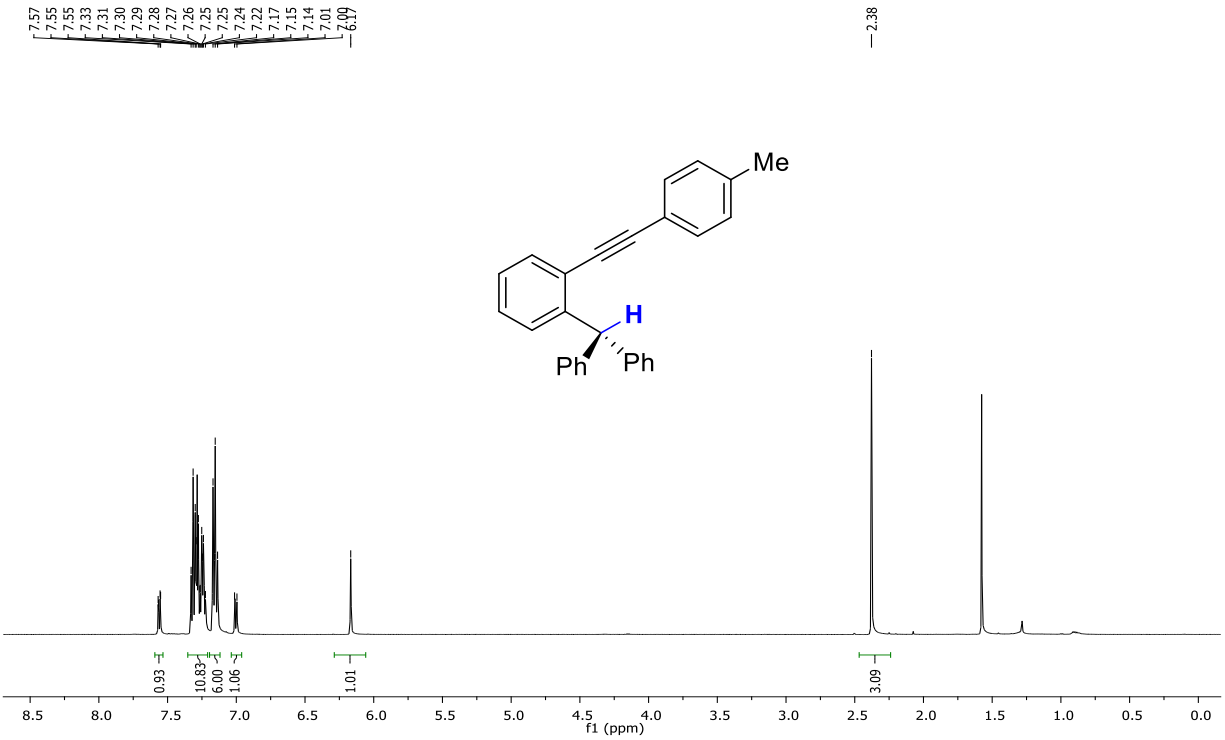


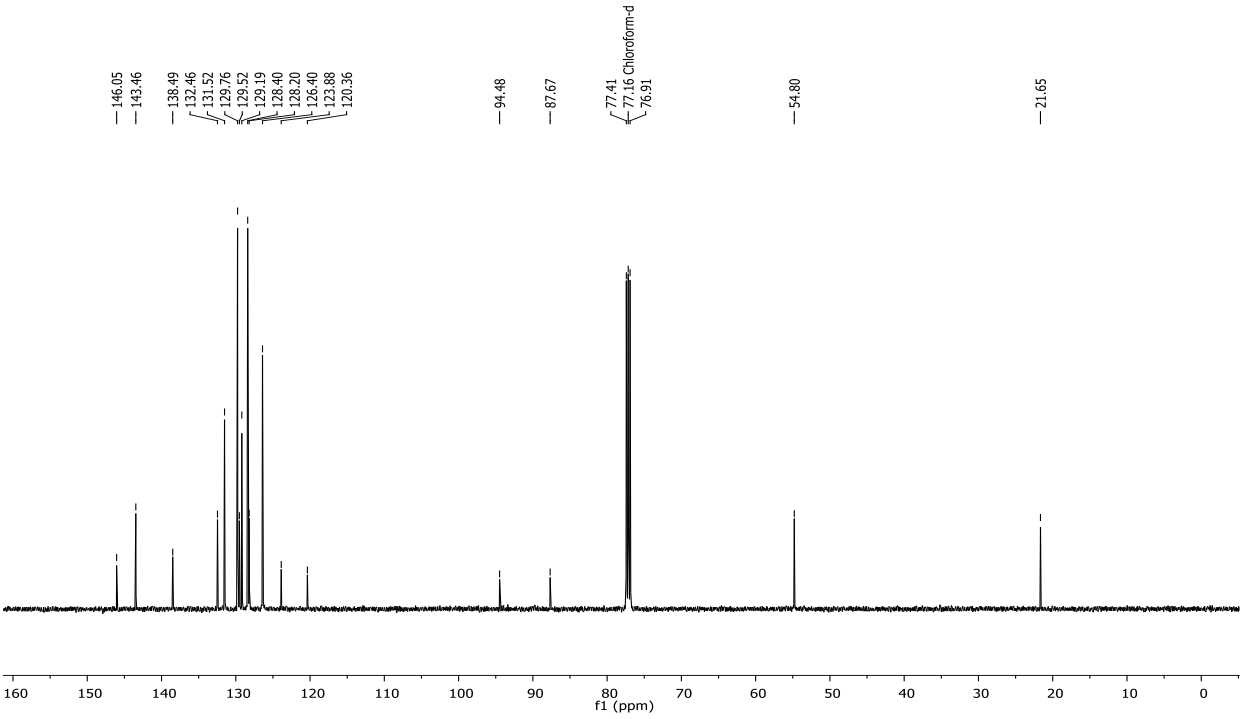
{[2(Phenylethynyl)phenyl]methylene}dibenzene **(6)**



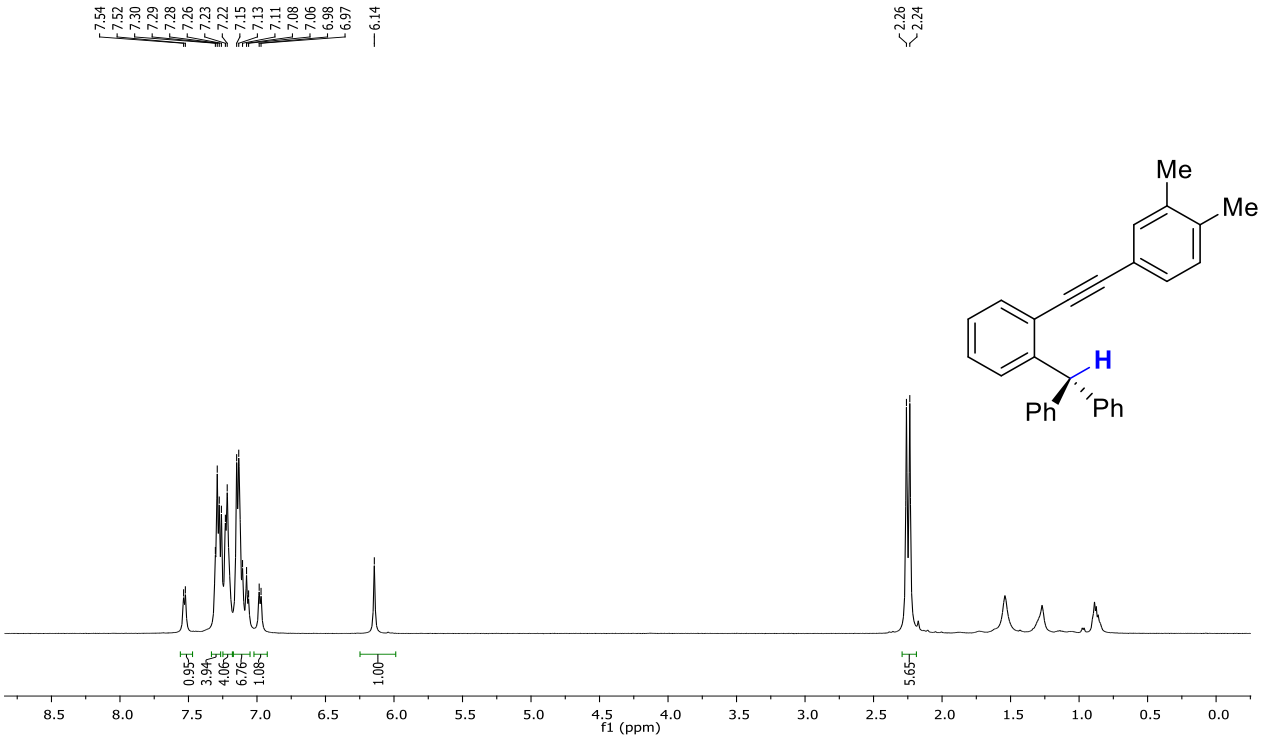


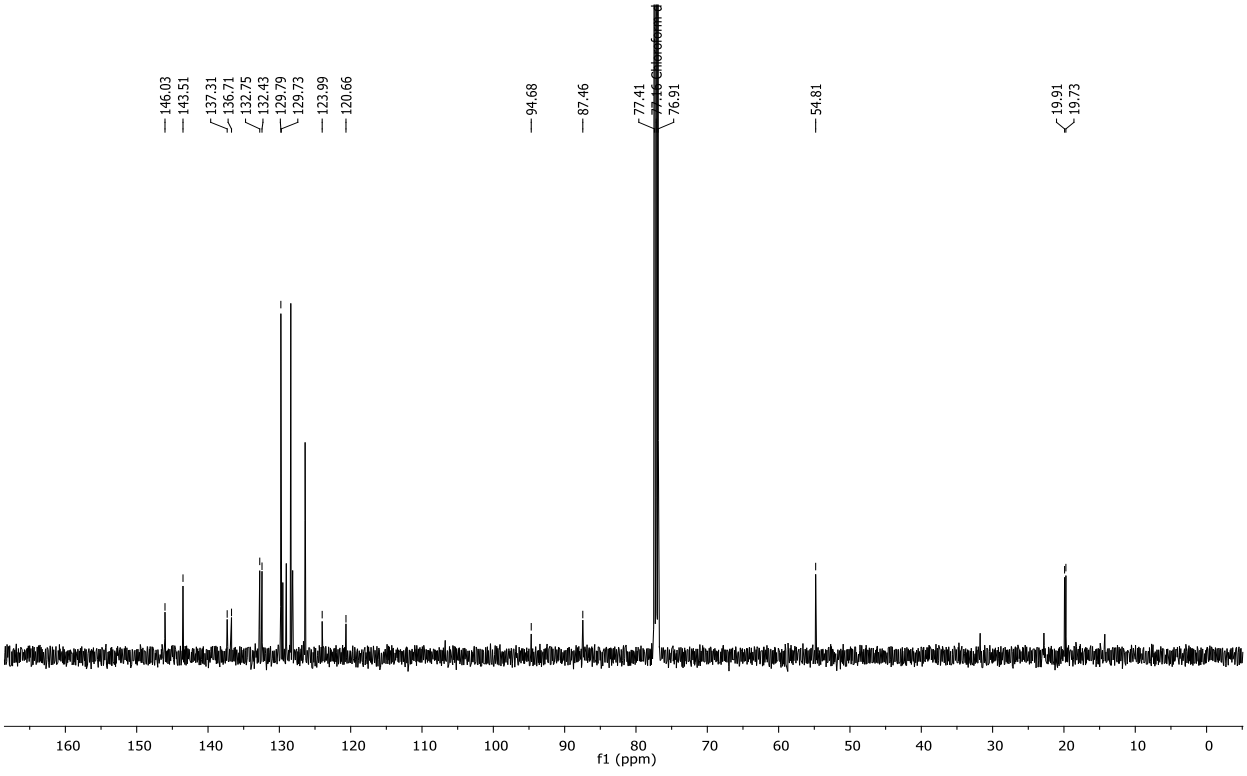
((2-(*p*-tolylethynyl)phenyl)methylene)dibenzene **(7)**



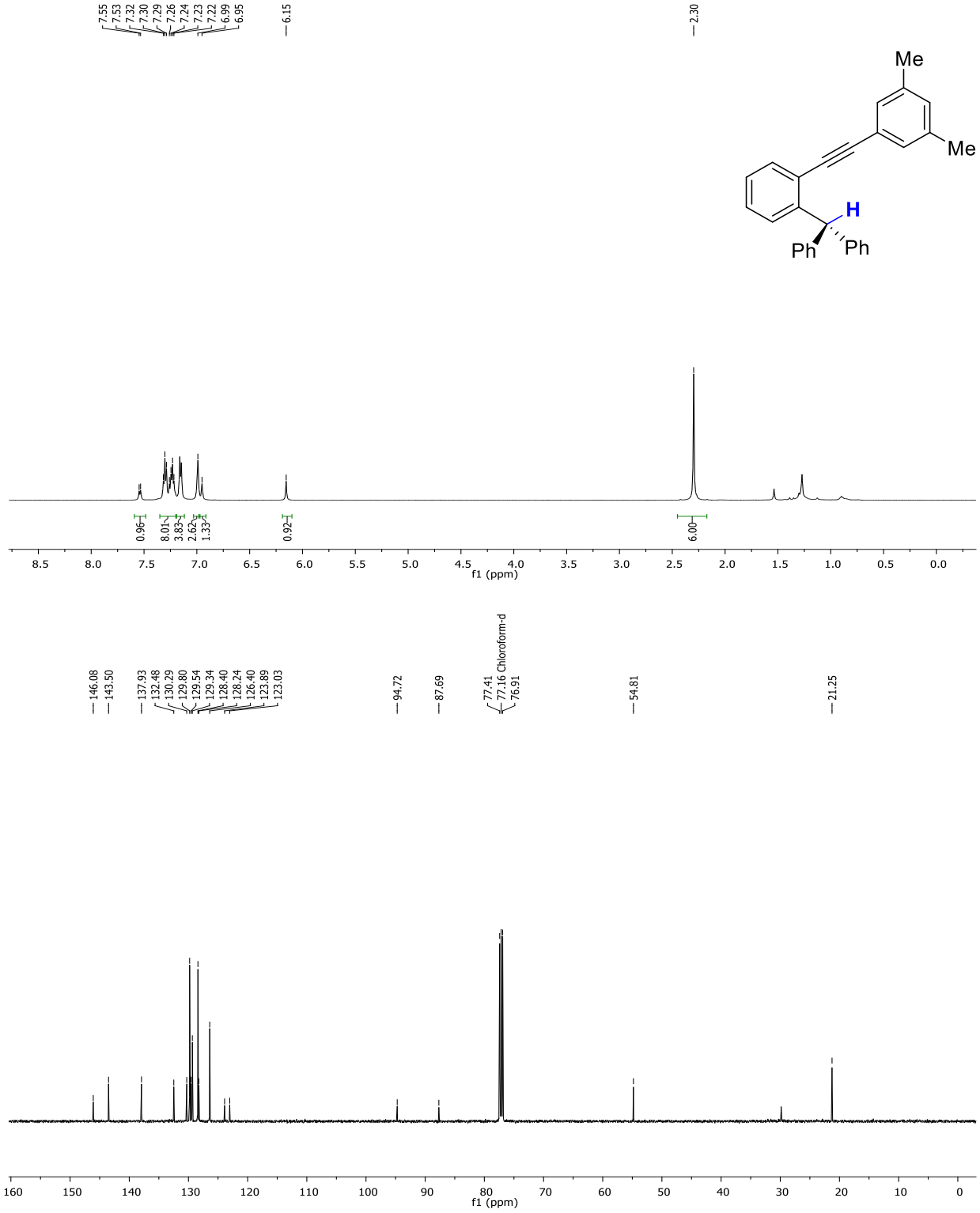


((2-((3,4-dimethylphenyl)ethynyl)phenyl)methylene)dibenzene **(8)**

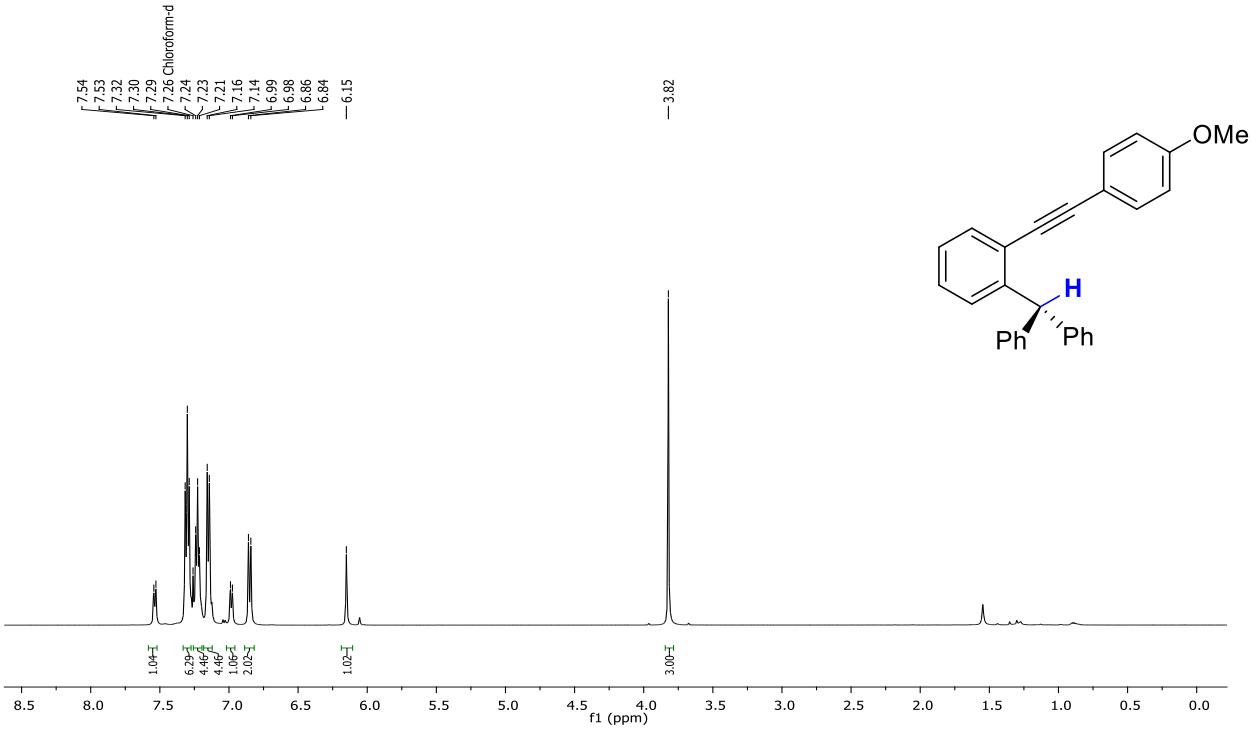


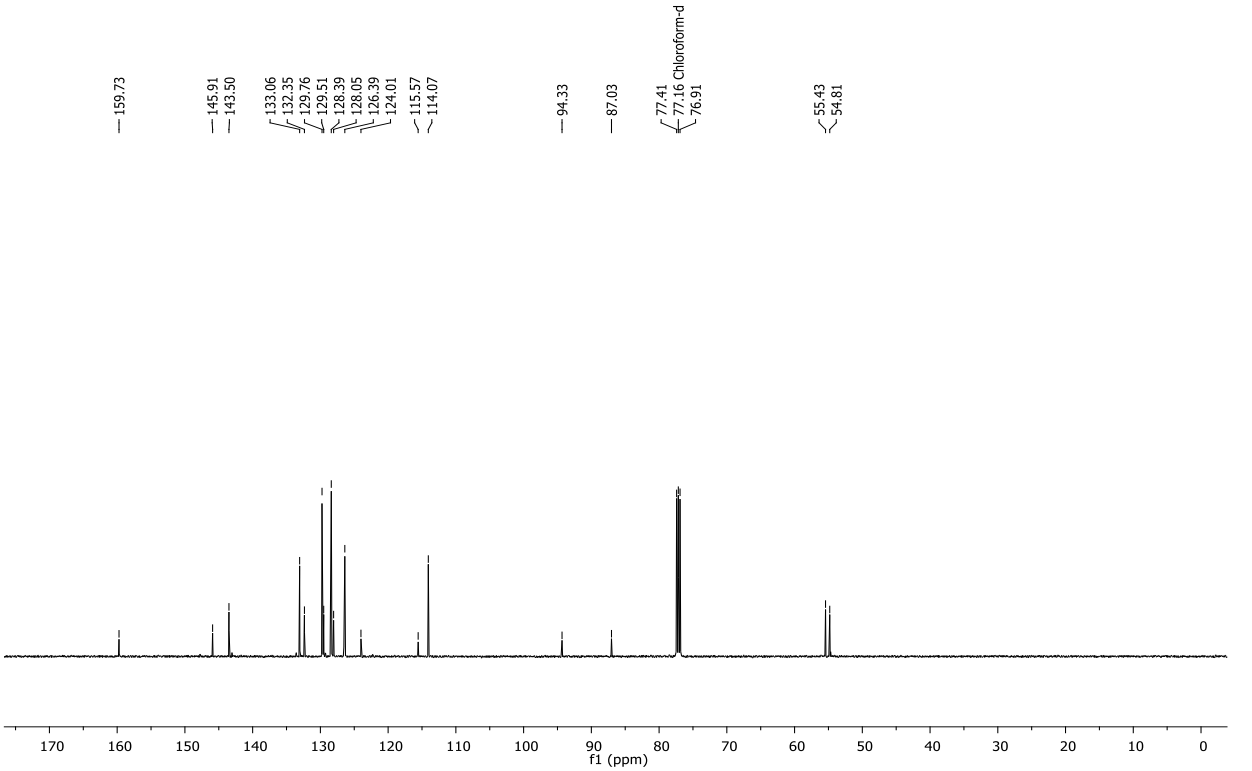


((2-((3,5-dimethylphenyl)ethynyl)phenyl)methylene)dibenzene **(9)**

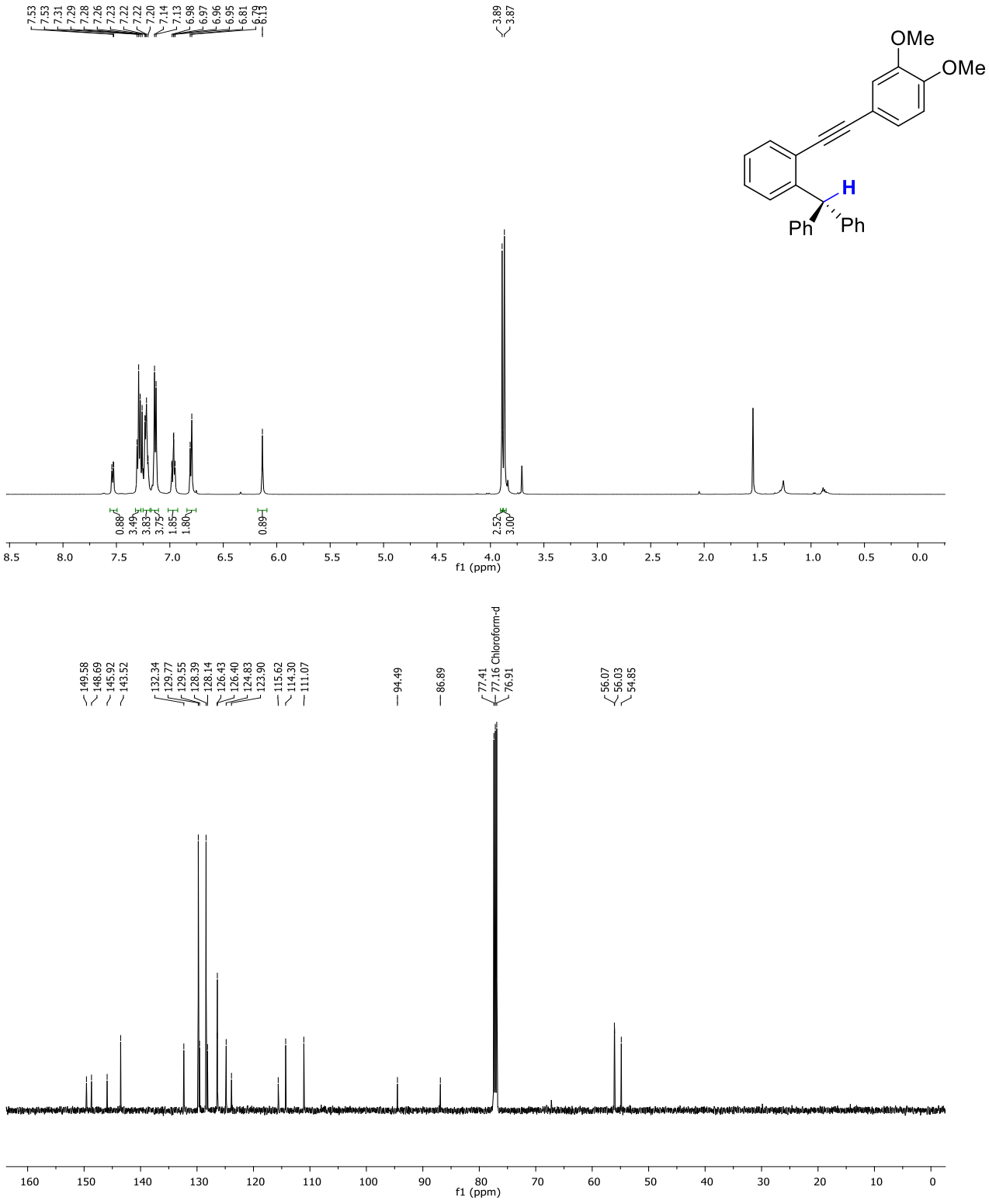


((2-((4-methoxyphenyl)ethynyl)phenyl)methylene)dibenzene **(10)**

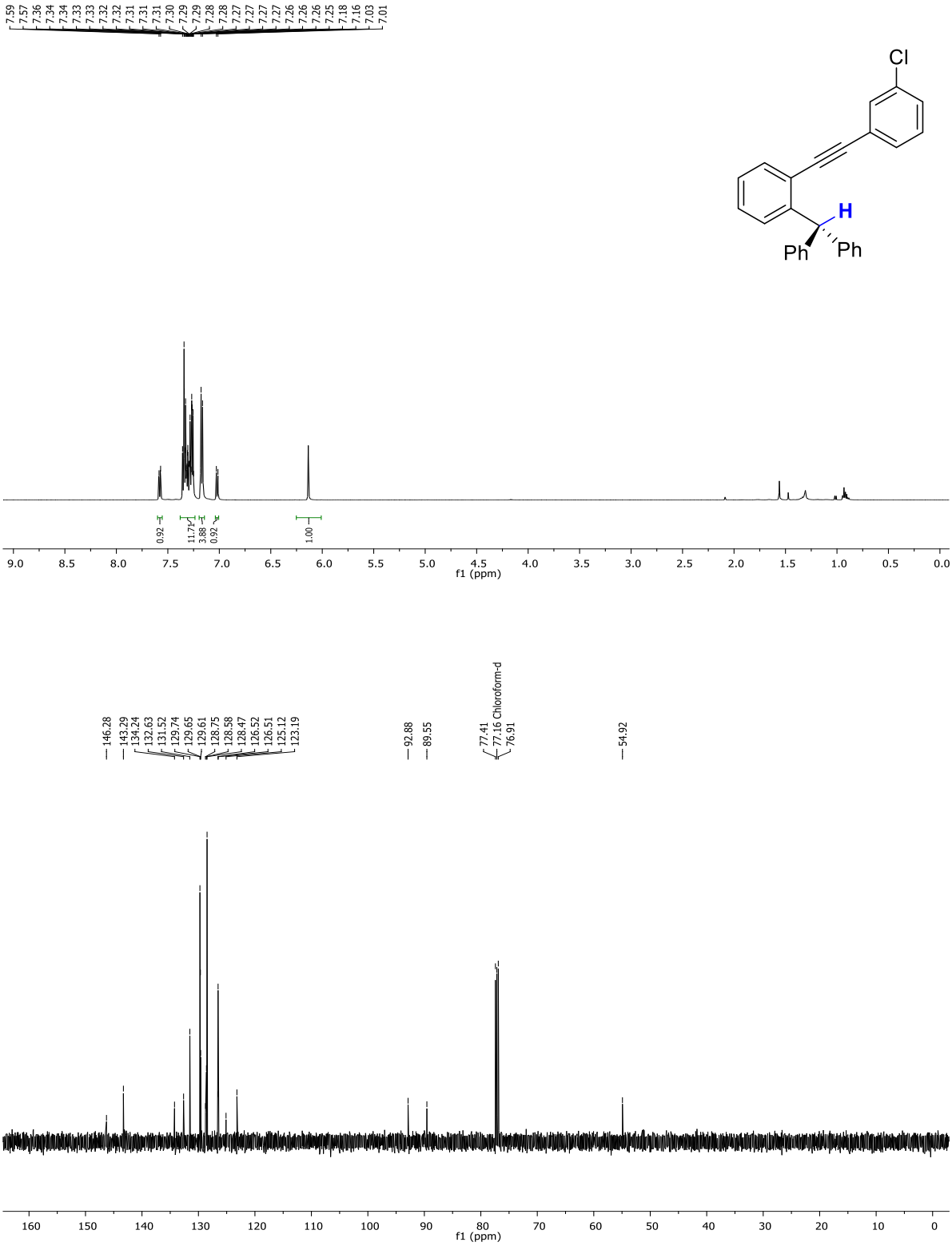




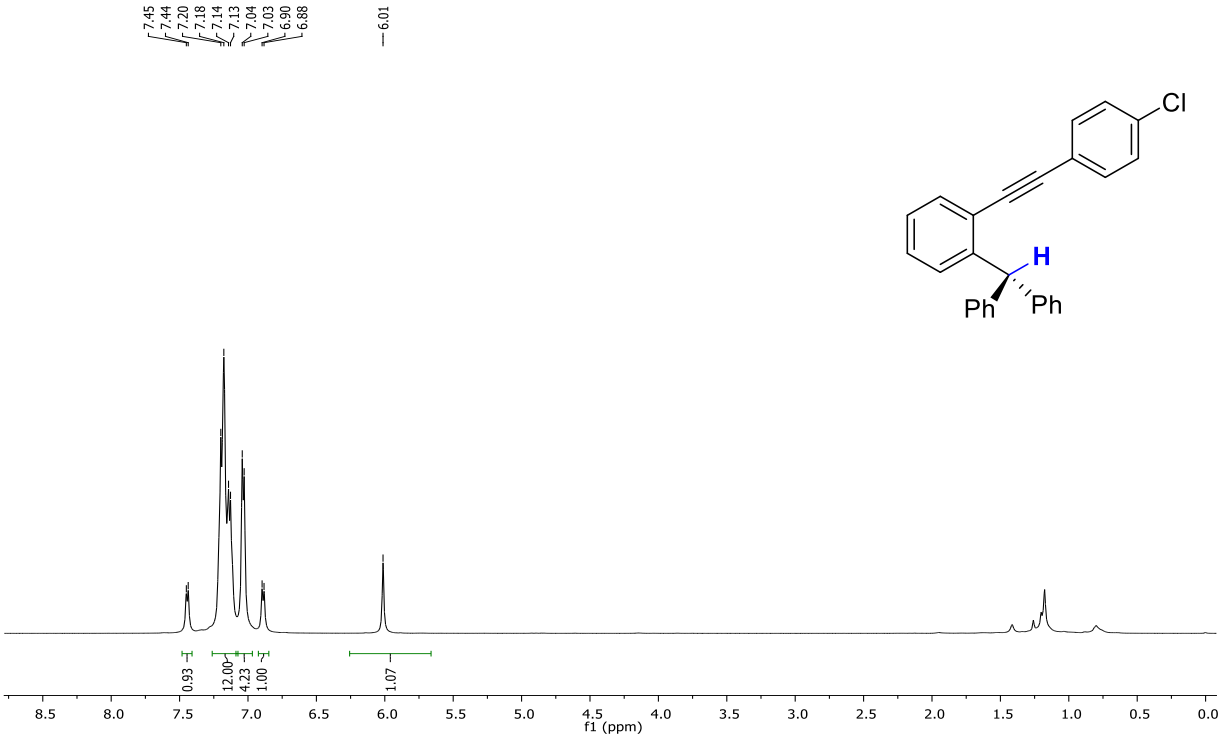
((2-((3,4-dimethoxyphenyl)ethynyl)phenyl)methylene)dibenzene **(11)**

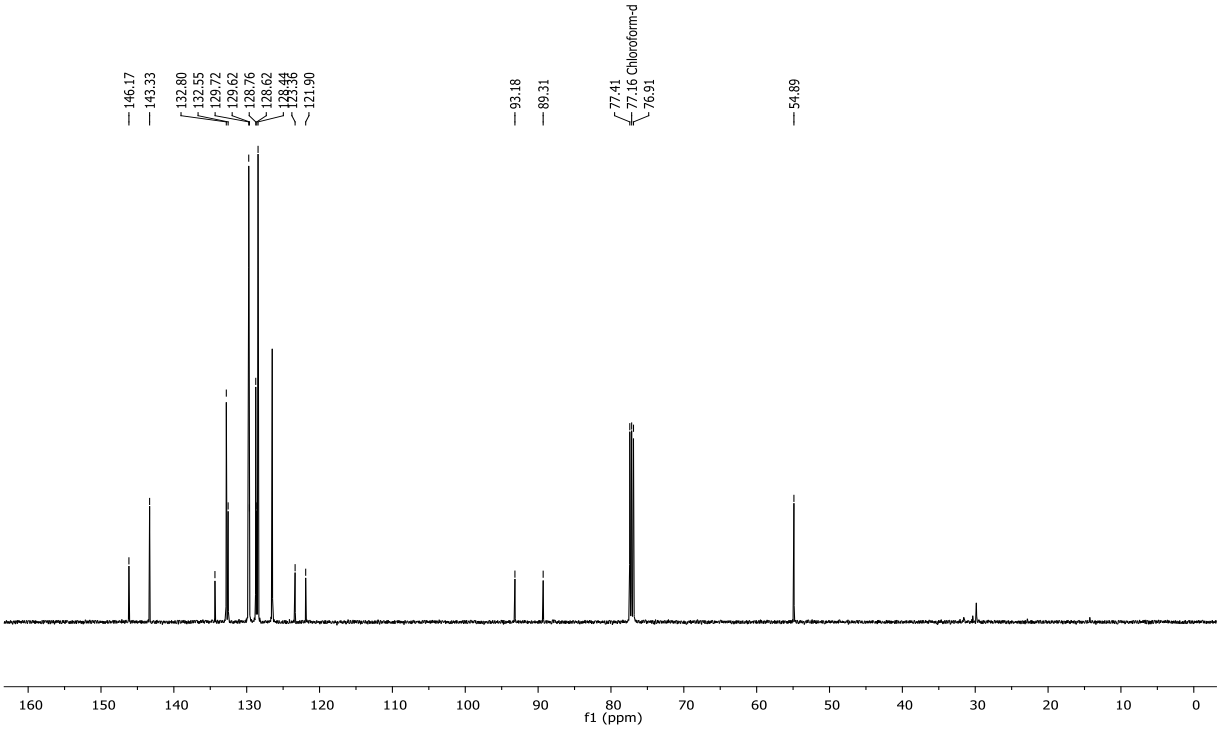


((2-((3-chlorophenyl)ethynyl)phenyl)methylene)dibenzene **(12)**

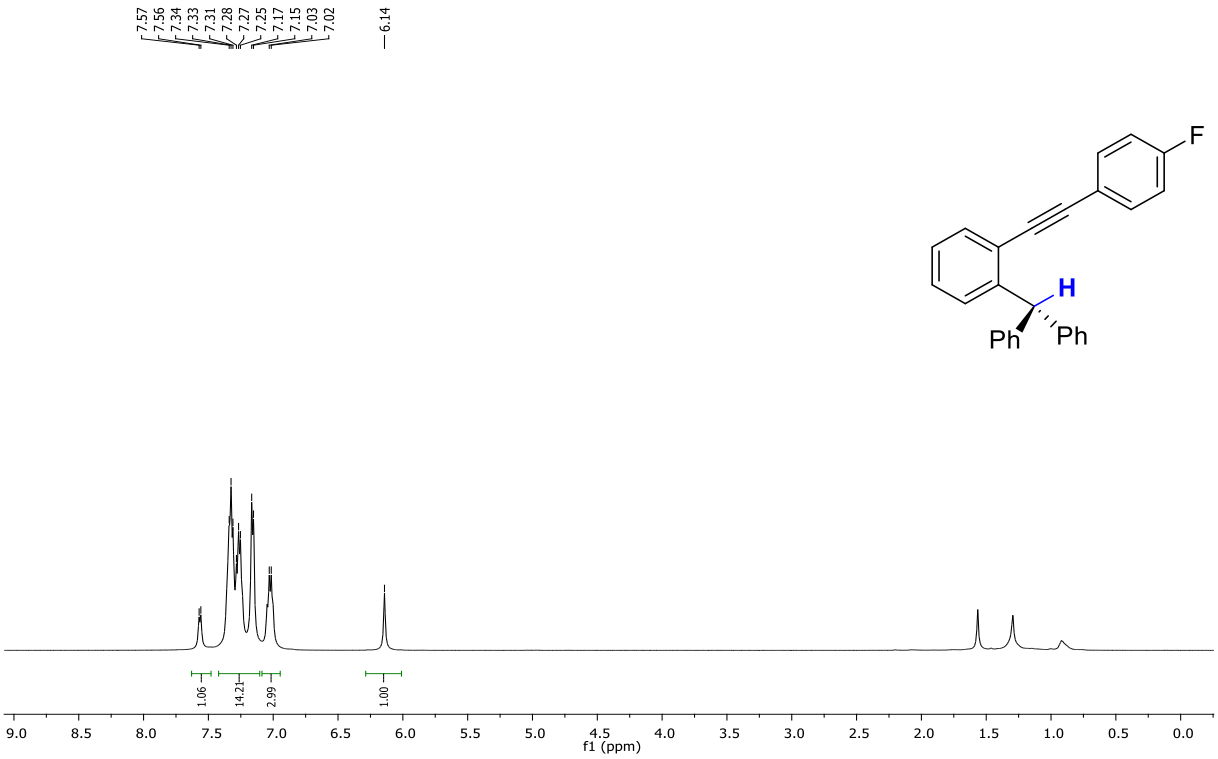


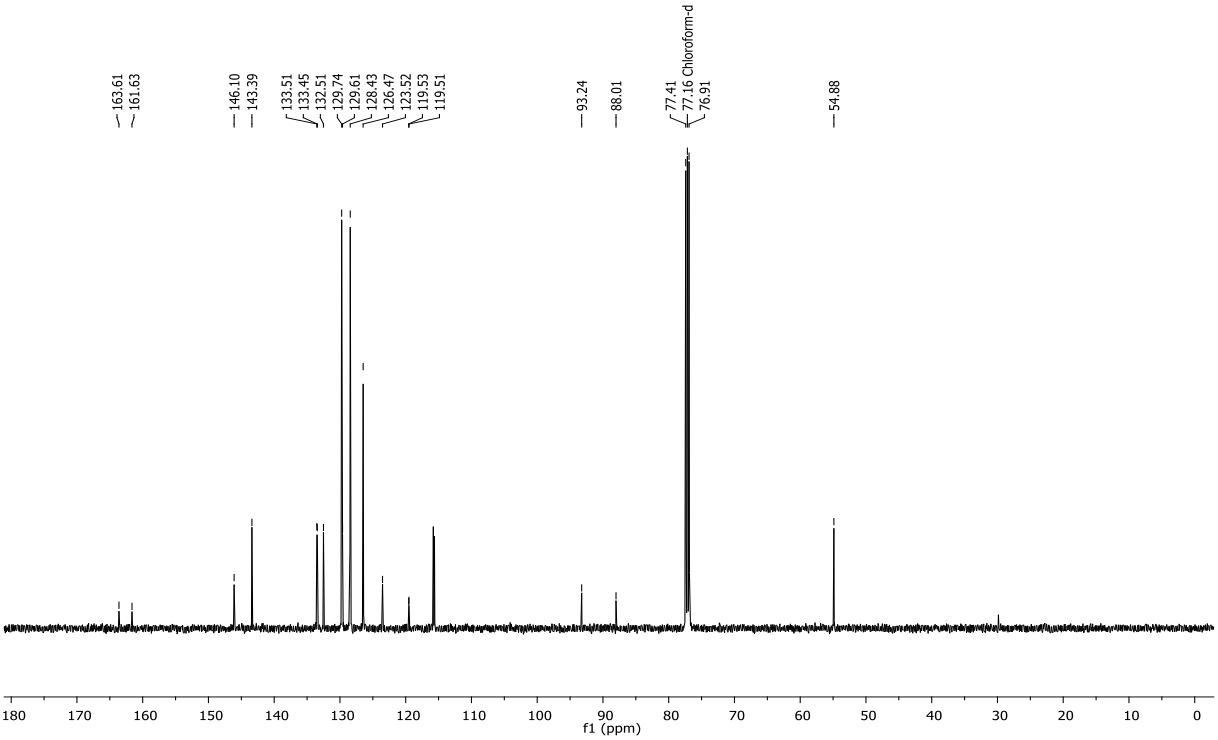
((2-((4-chlorophenyl)ethynyl)phenyl)methylene)dibenzene **(13)**



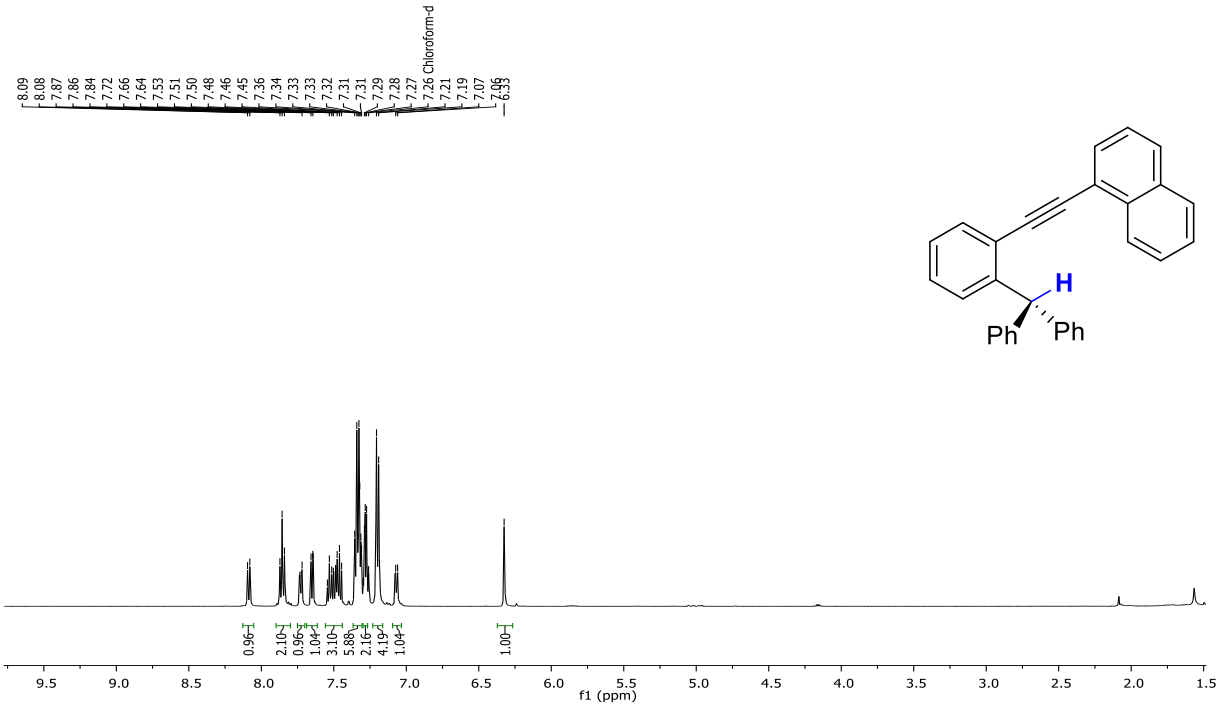


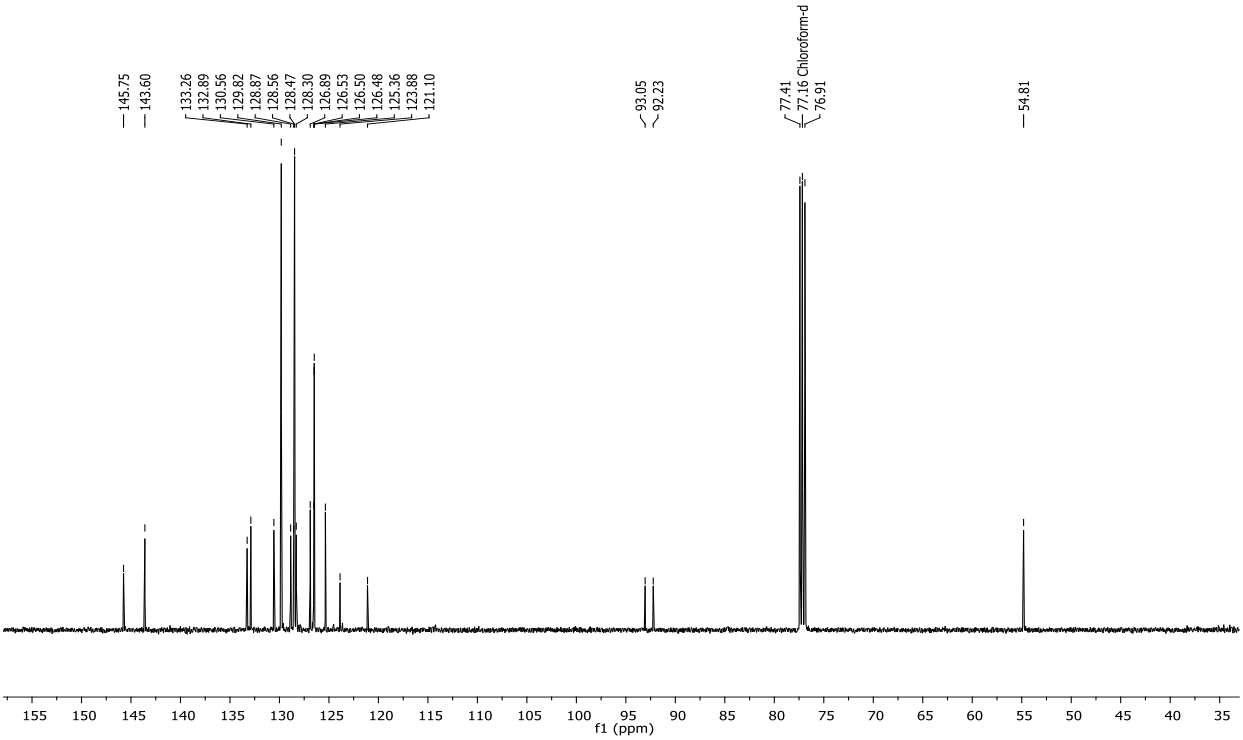
((2-((4-fluorophenyl)ethynyl)phenyl)methylene)dibenzene **(14)**



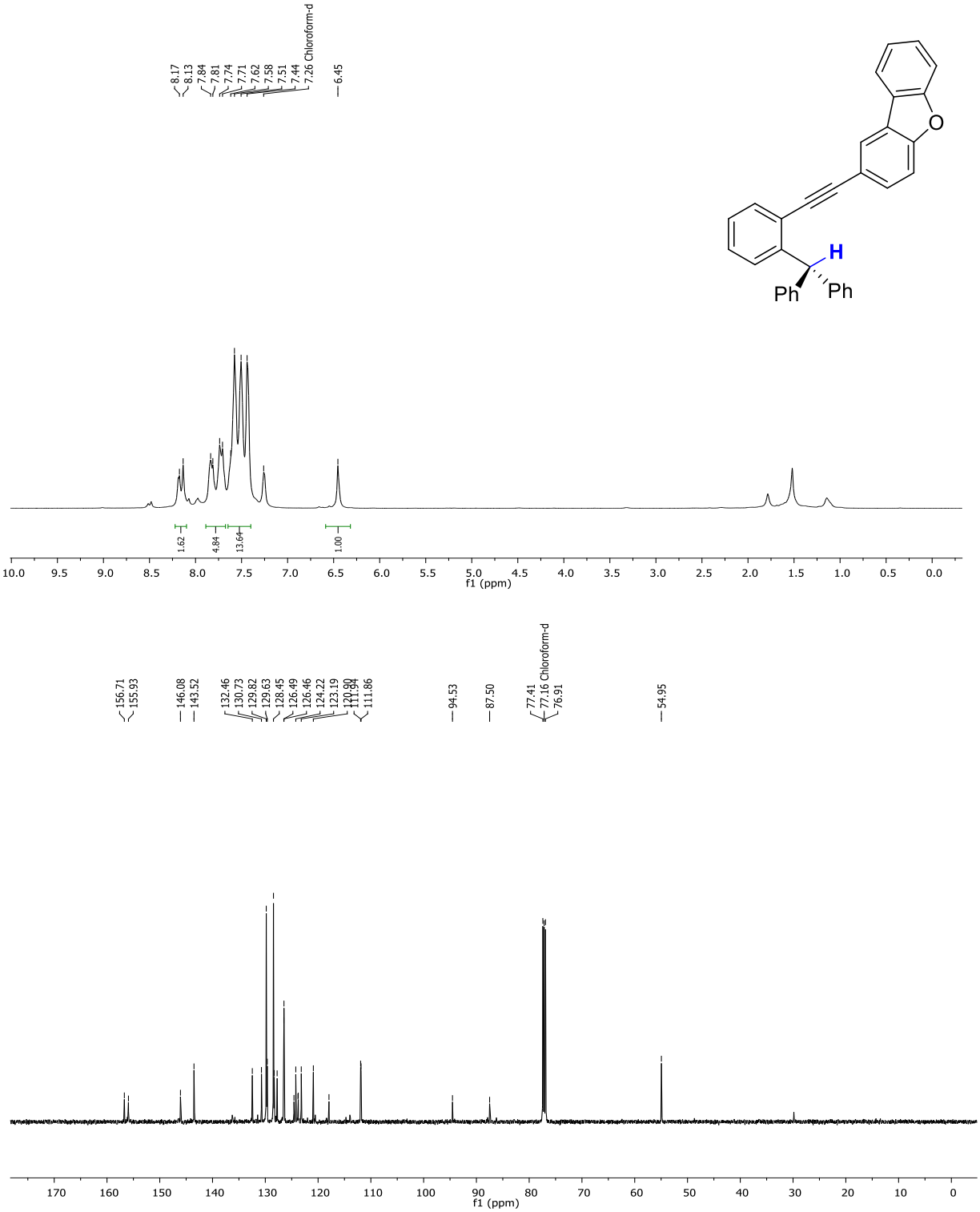


1-((2-benzohydrylphenyl)ethynyl)naphthalene **(15)**

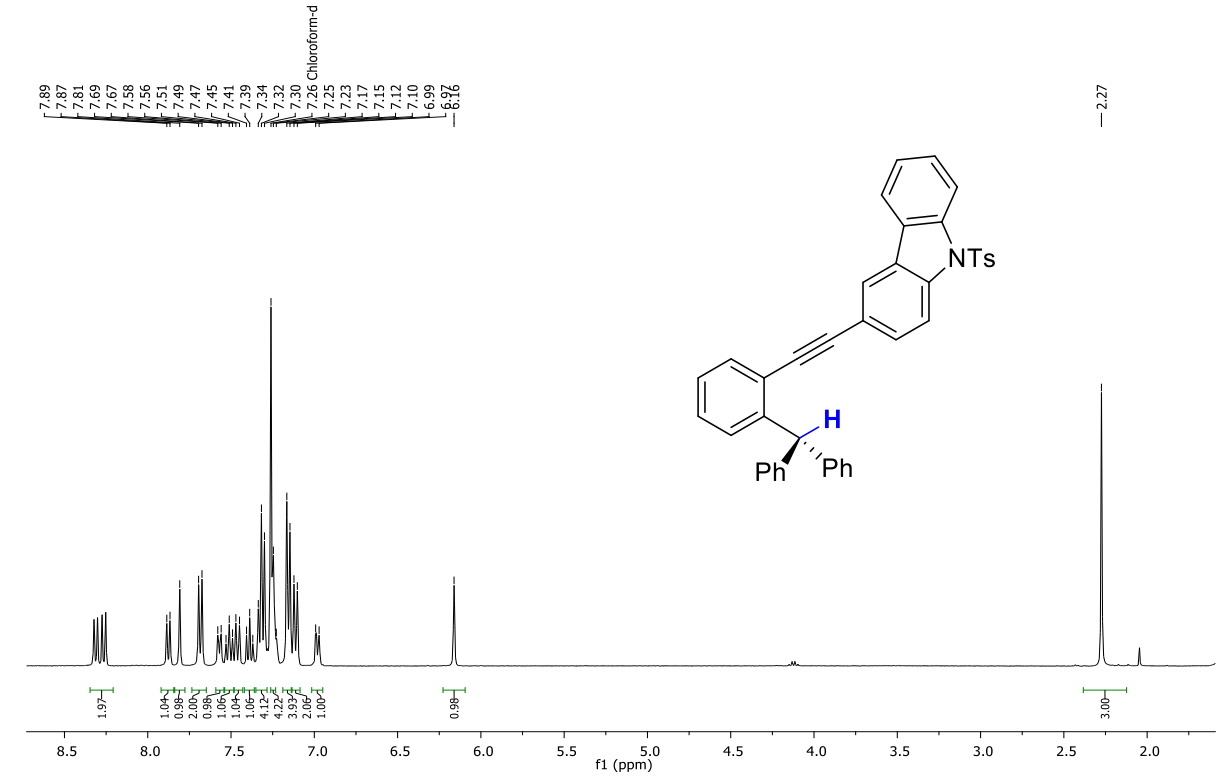


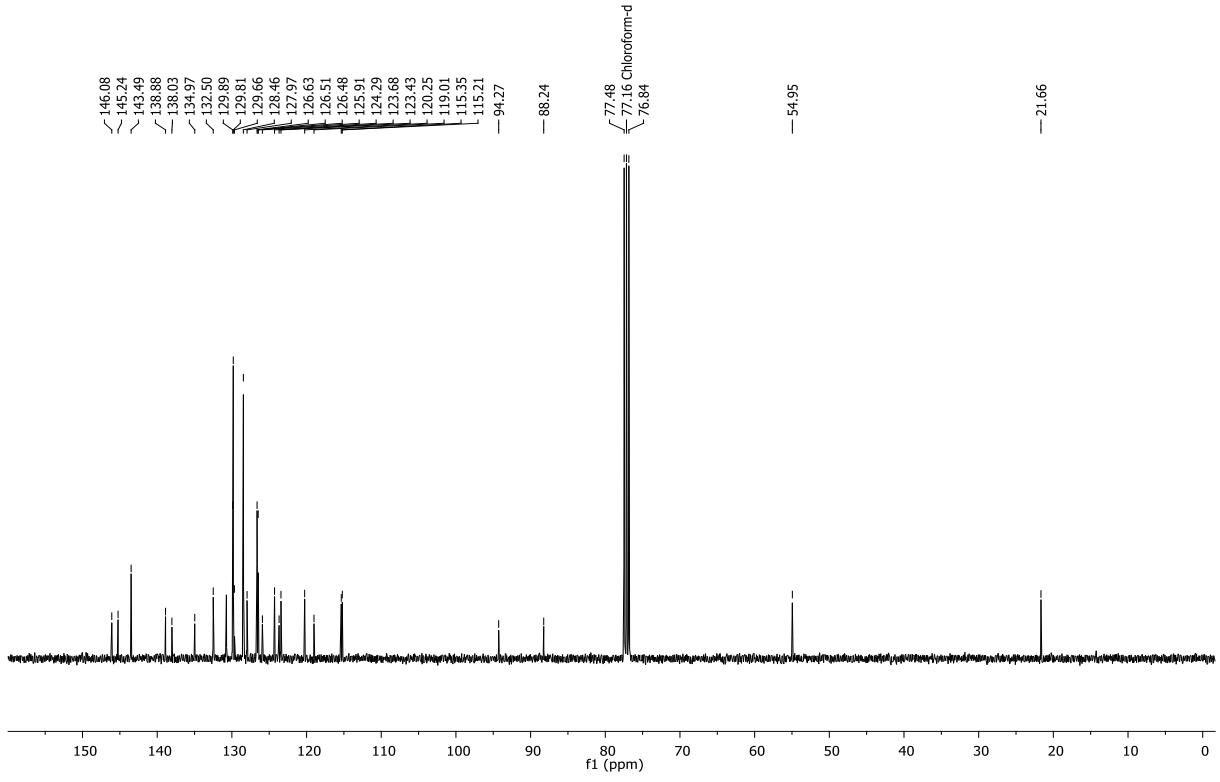


2-((2-benzohydrylphenyl)ethynyl)dibenzo[*b*,*d*]furan **(16)**

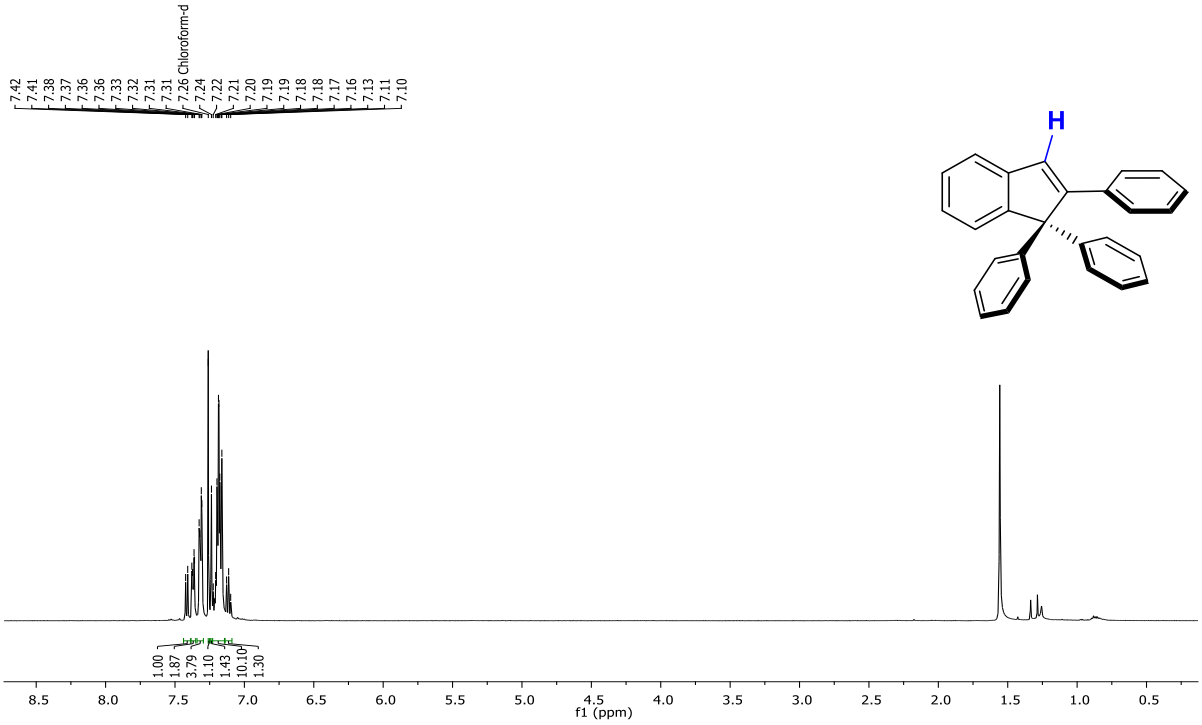


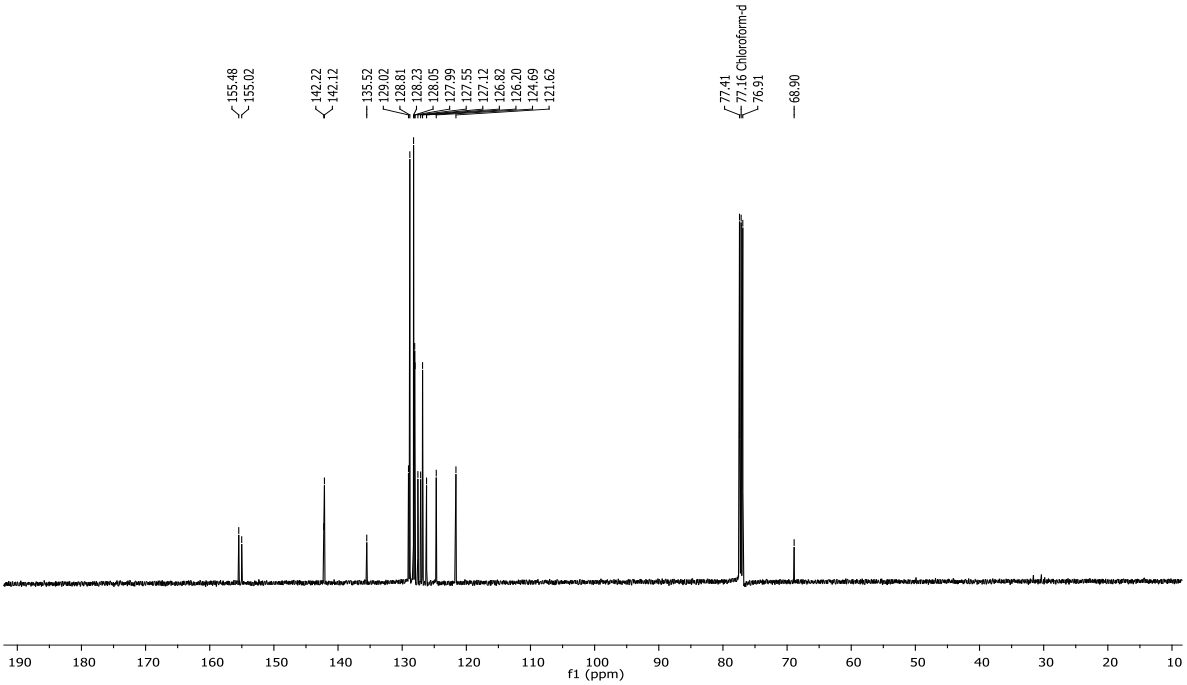
3-(1,1-diphenyl-1H-inden-2-yl)-9-tosyl-9H-carbazole **(17)**



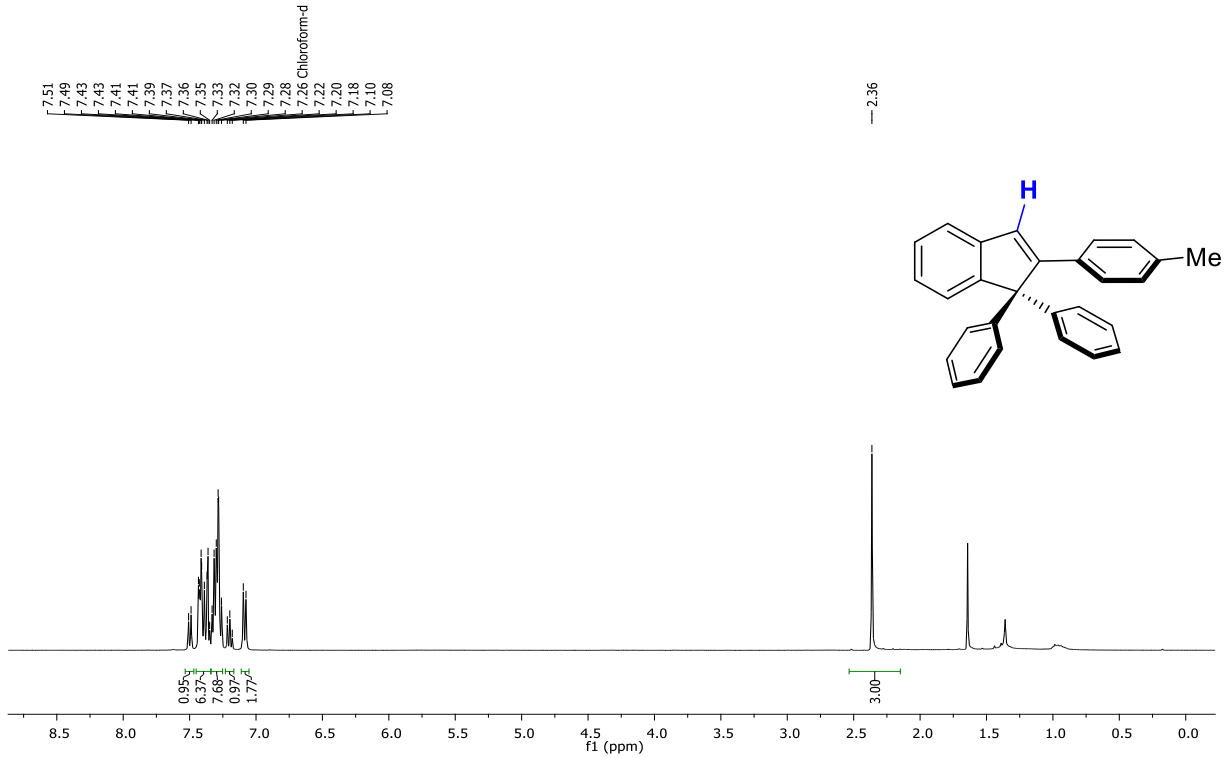


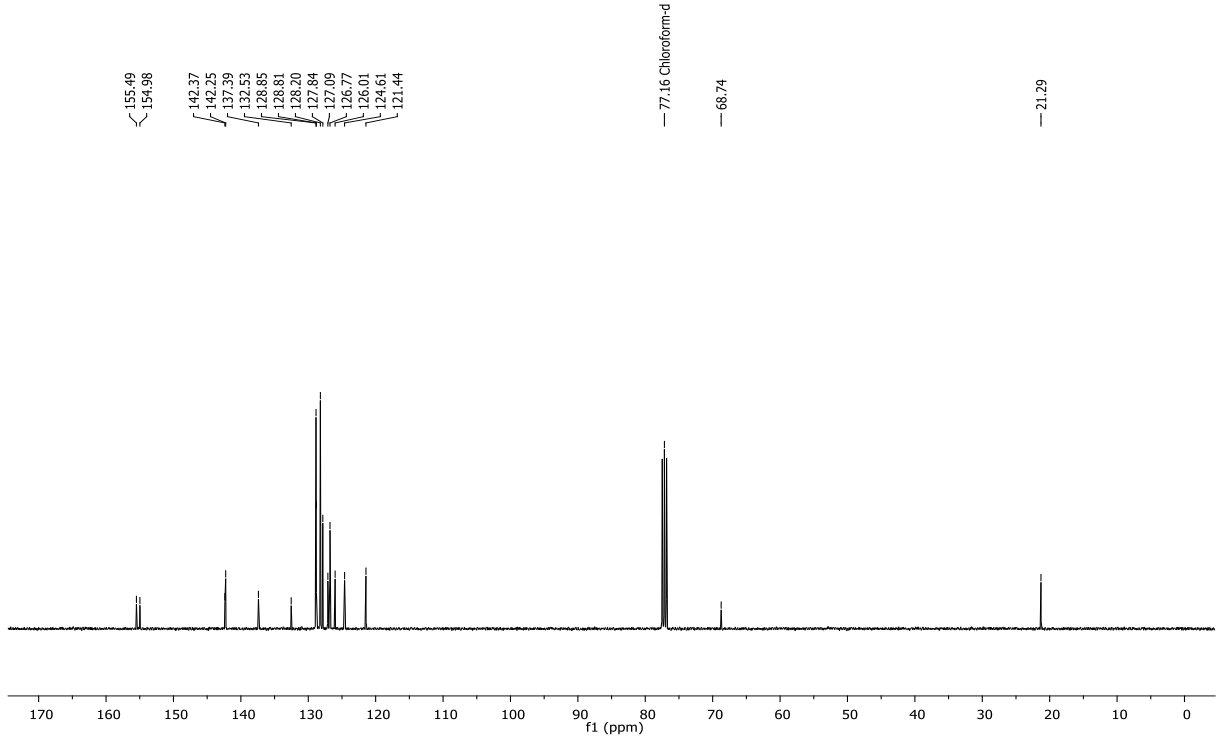
1,1,2-triphenyl-1*H*-indene **(18)**



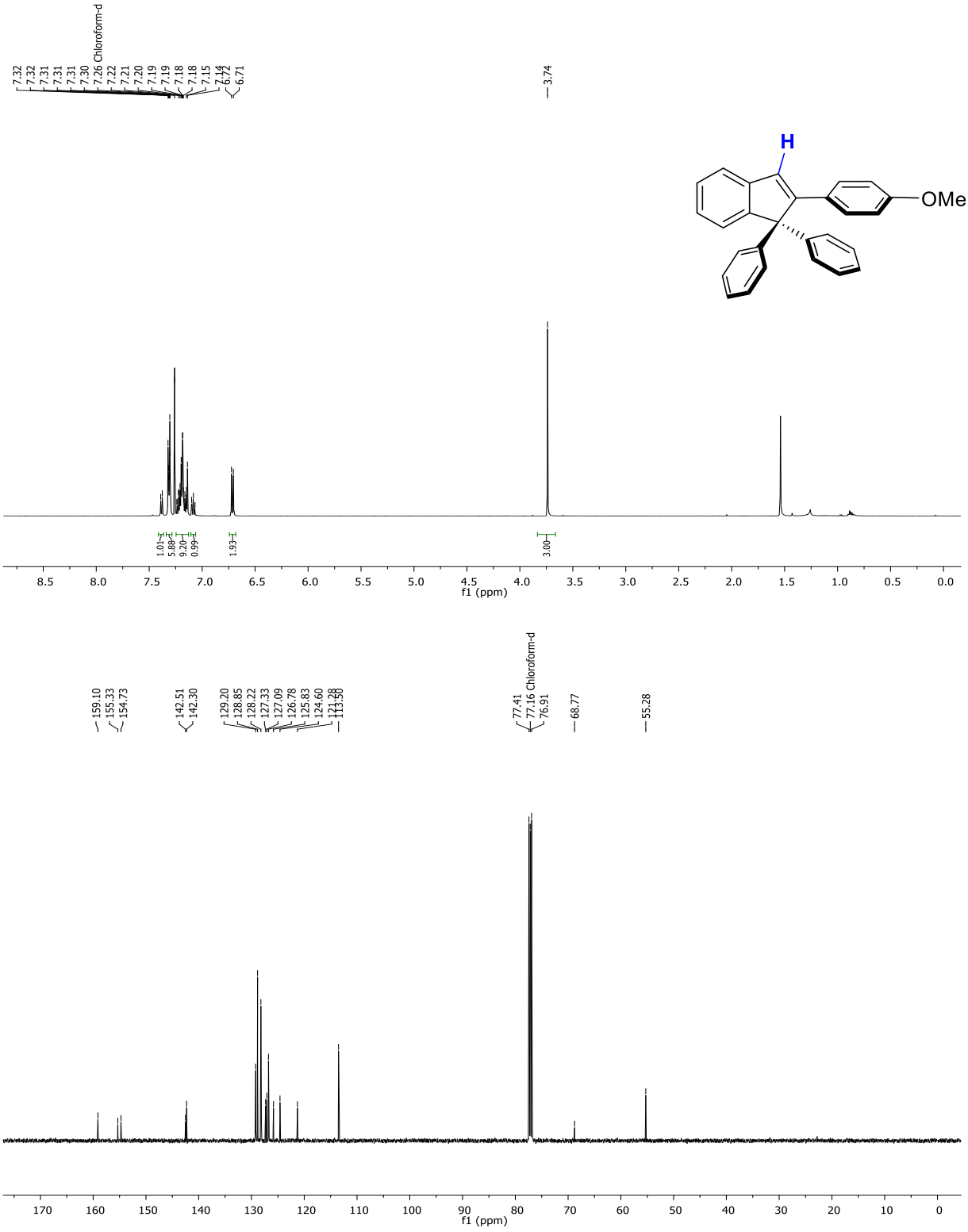


1,1-diphenyl-2-(*p*-tolyl)-1*H*-indene **(19)**

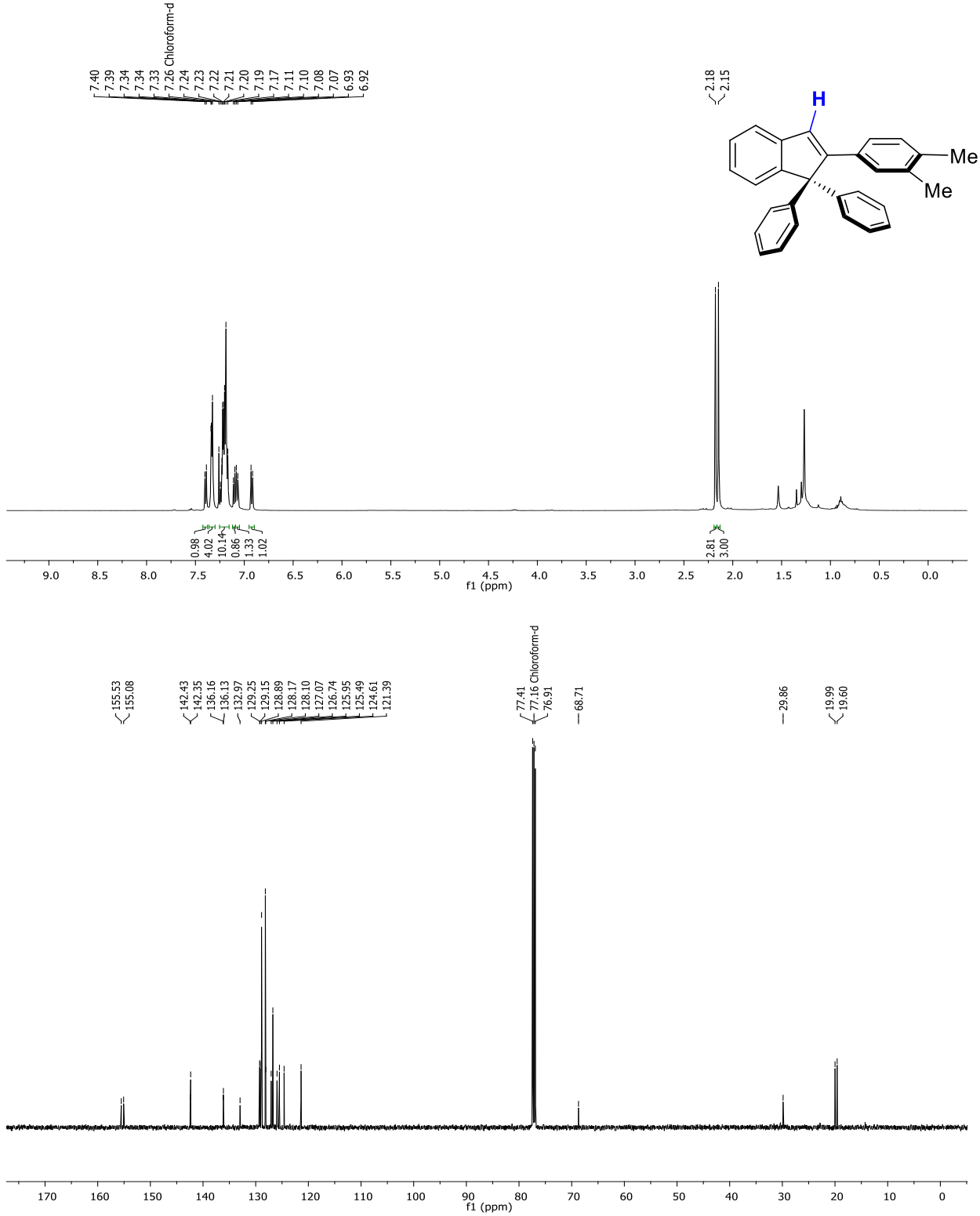




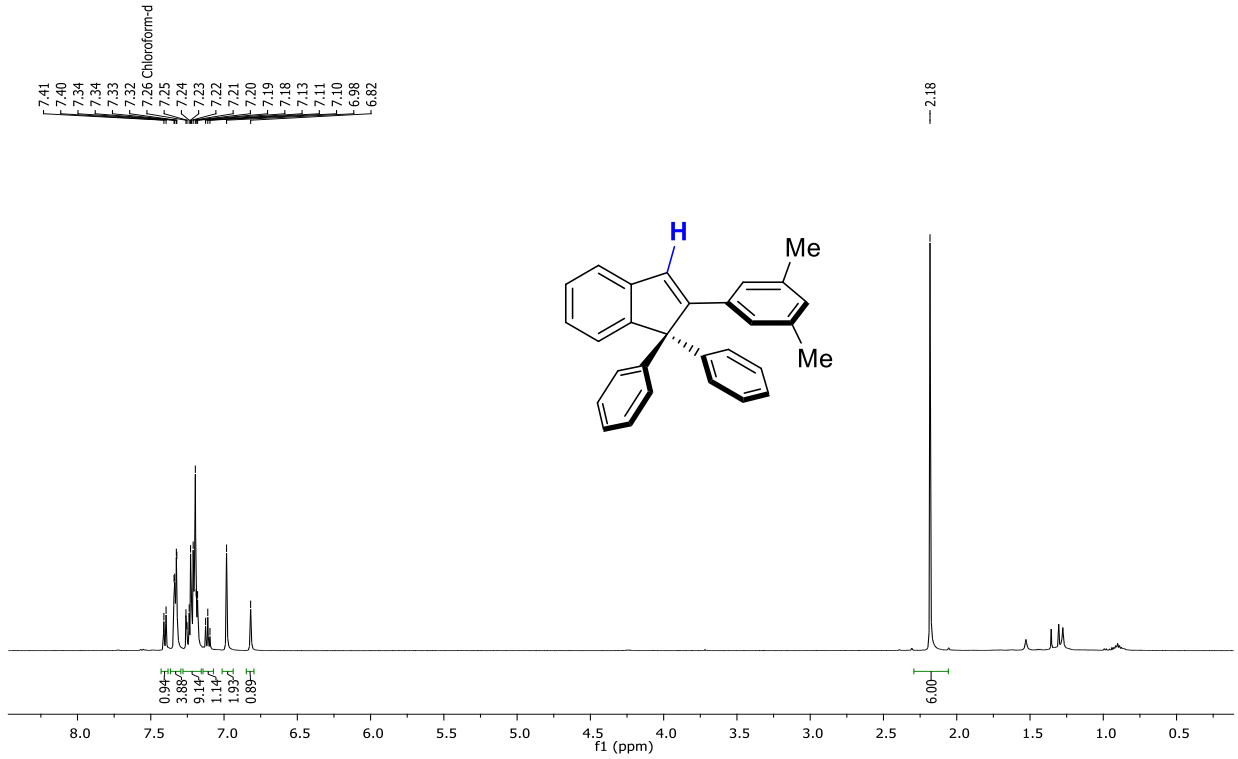
2-(4-methoxyphenyl)-1,1-diphenyl-1*H*-indene **(20)**

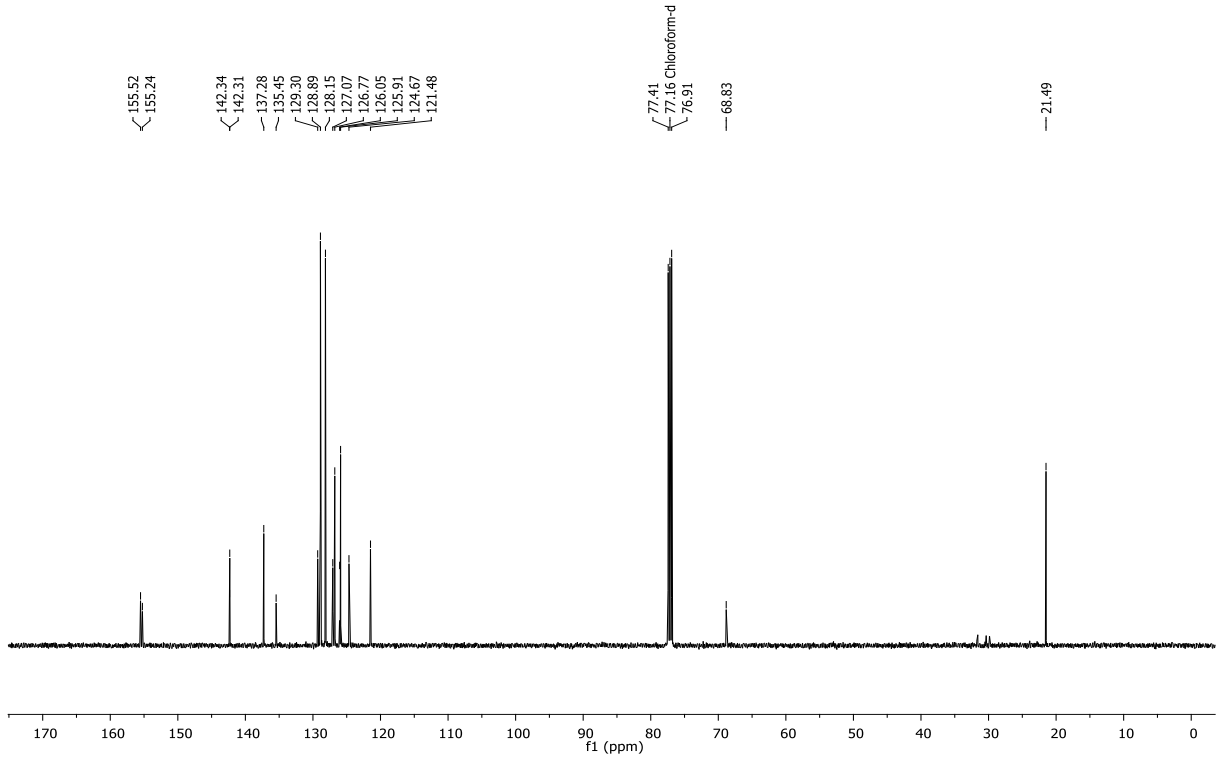


2-(3,4-dimethylphenyl)-1,1-diphenyl-1*H*-indene **(21)**

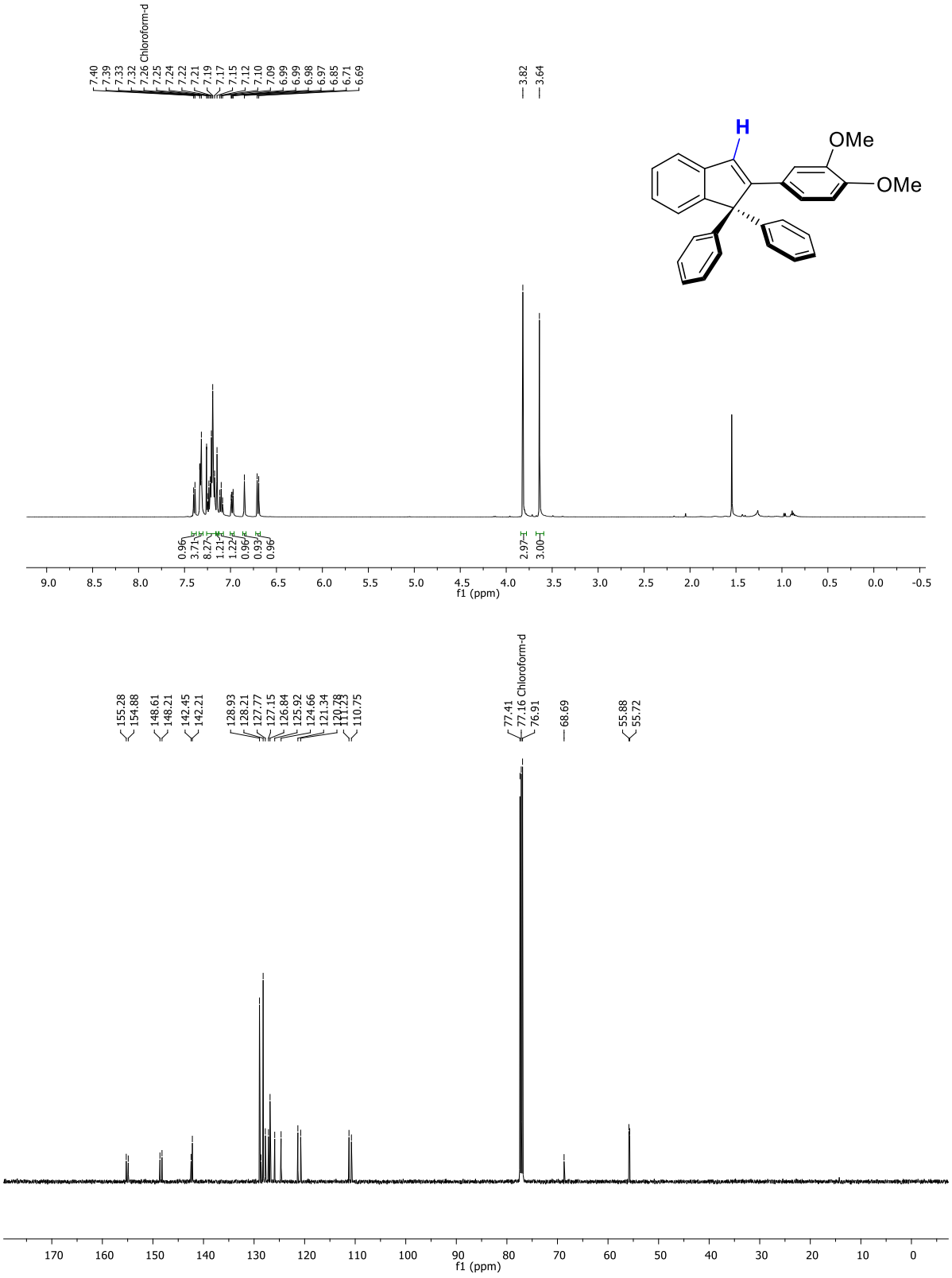


2-(3,5-dimethylphenyl)-1,1-diphenyl-1*H*-indene **(22)**

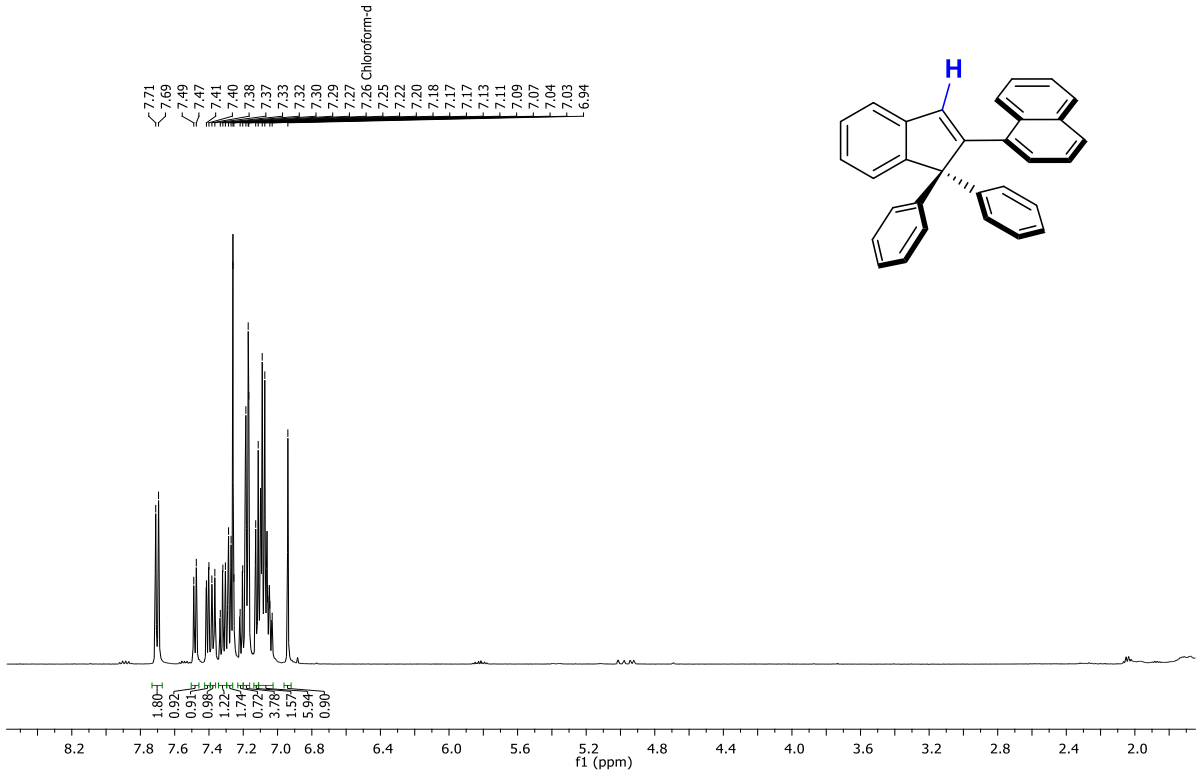


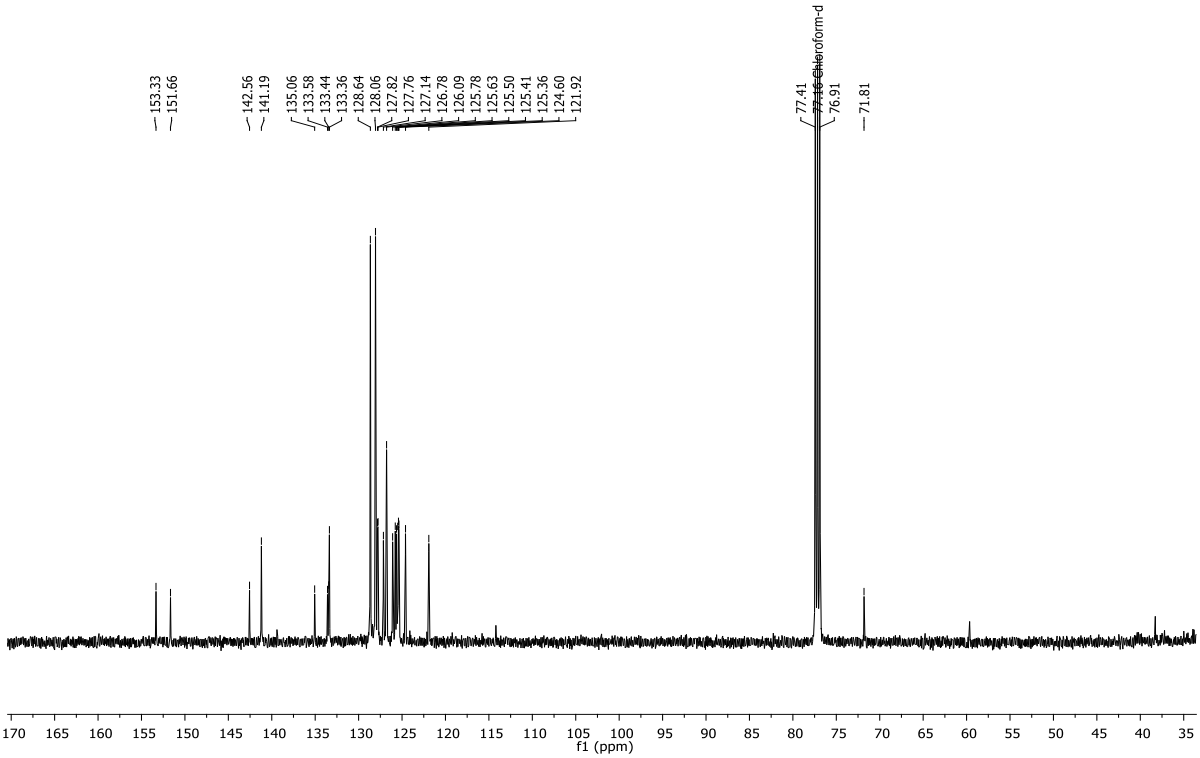


2-(3,4-dimethoxyphenyl)-1,1-diphenyl-1*H*-indene **(23)**

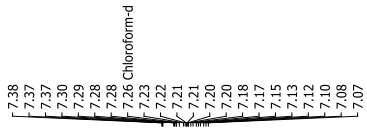


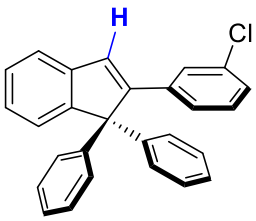
1-(1,1-diphenyl-1*H*-inden-2-yl)naphthalene **(24)**

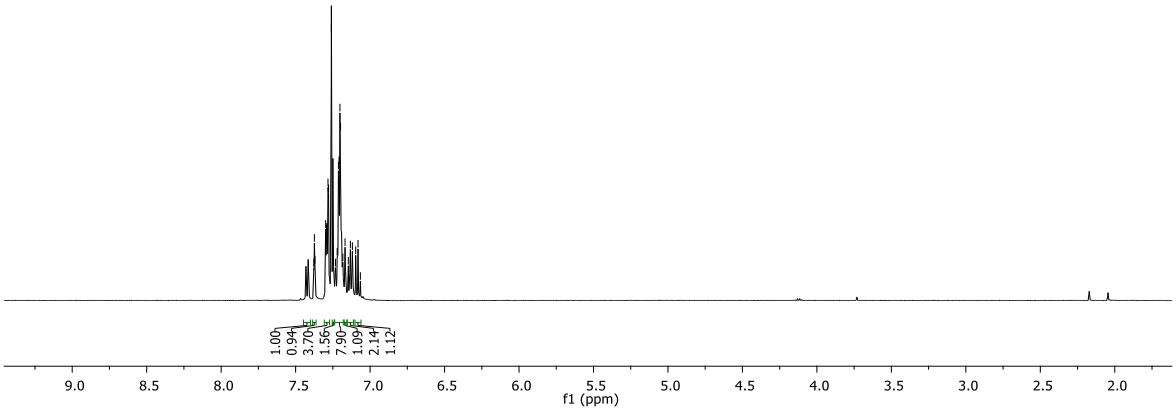


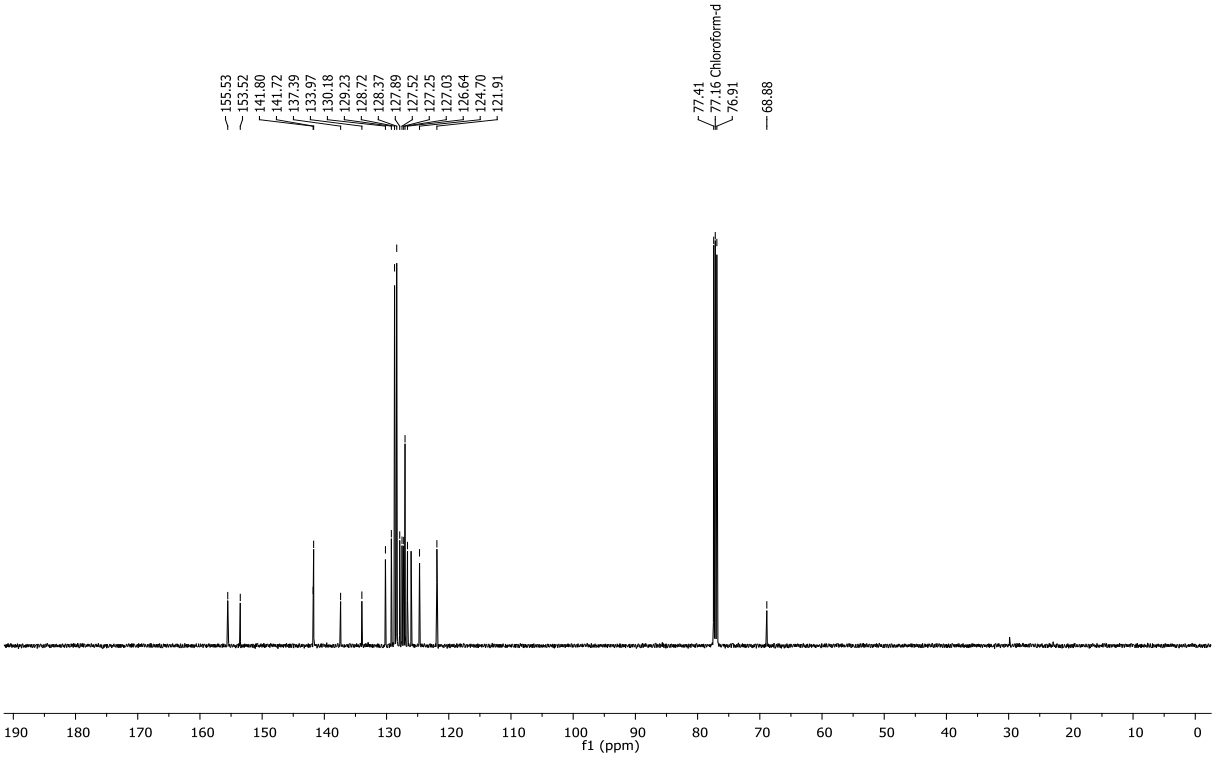


2-(3-chlorophenyl)-1,1-diphenyl-1*H*-indene **(25)**

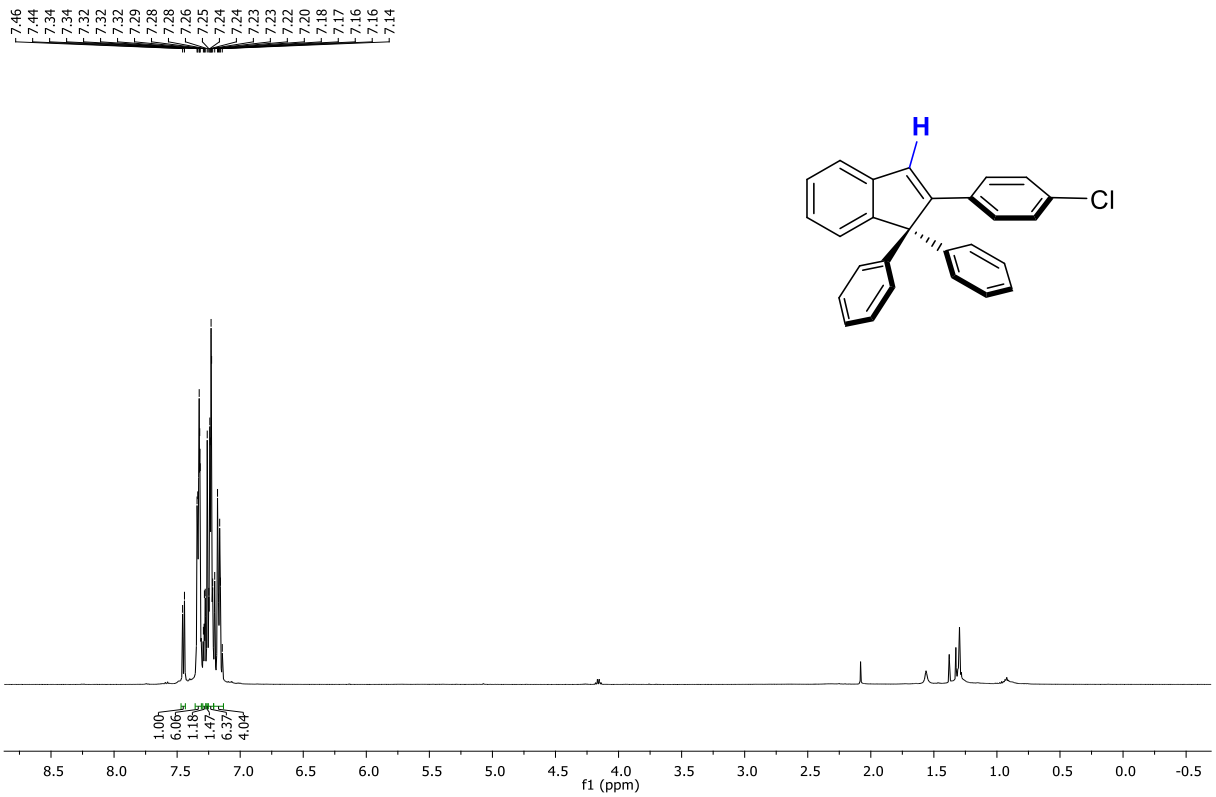


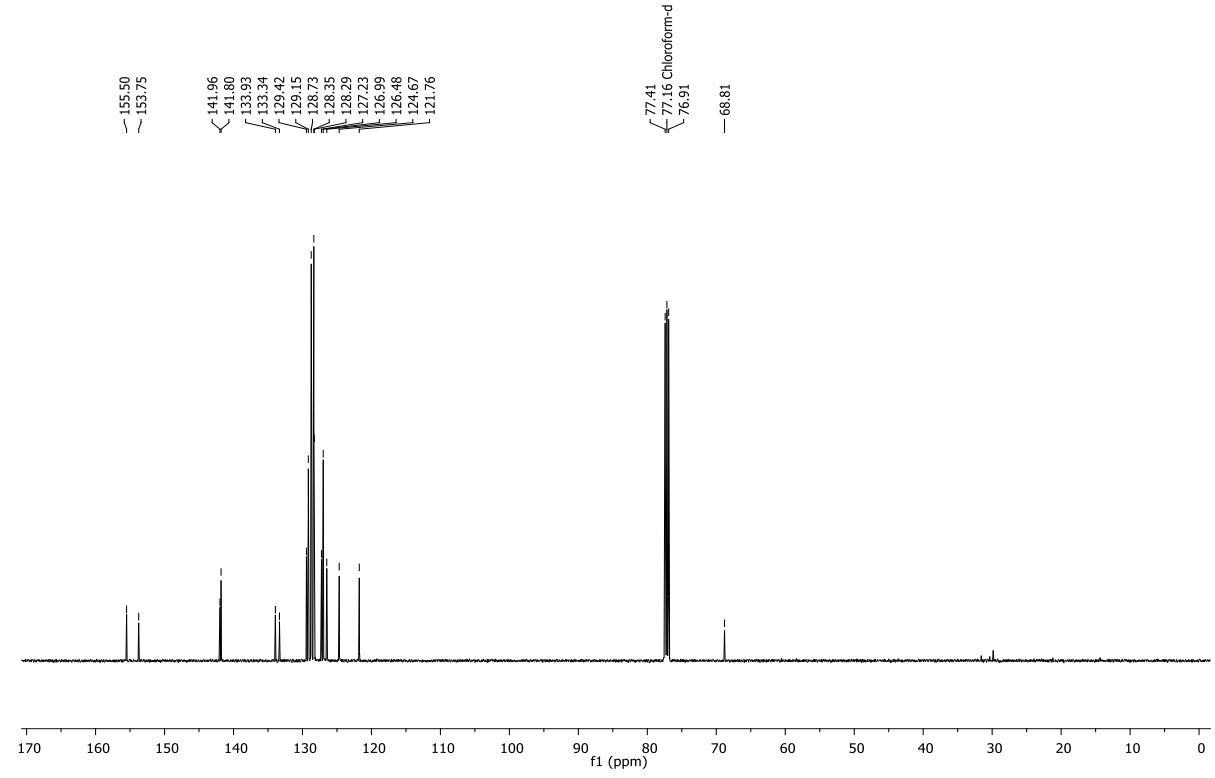




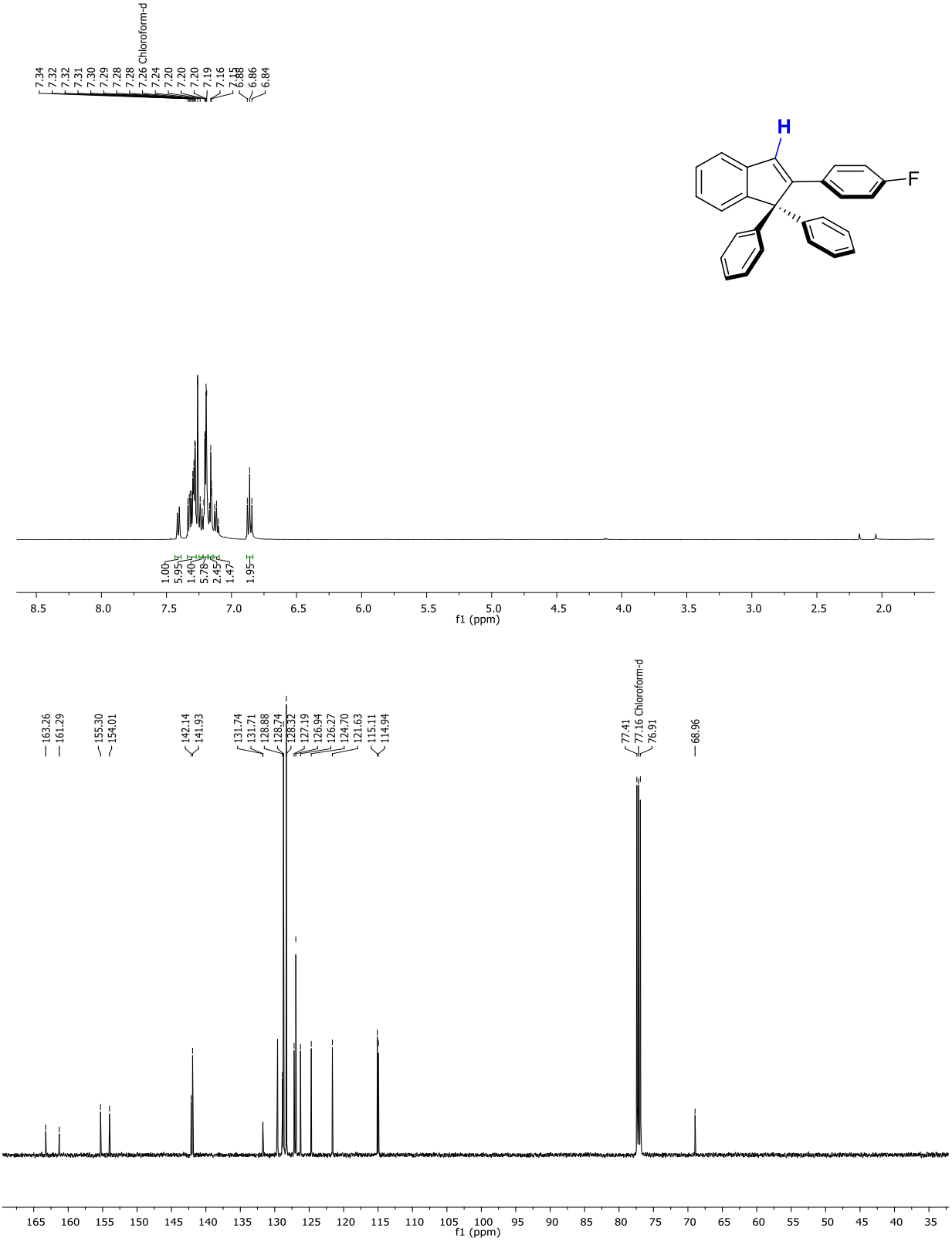


((2-((4-chlorophenyl)ethynyl)phenyl)methylene)dibenzene **(26)**

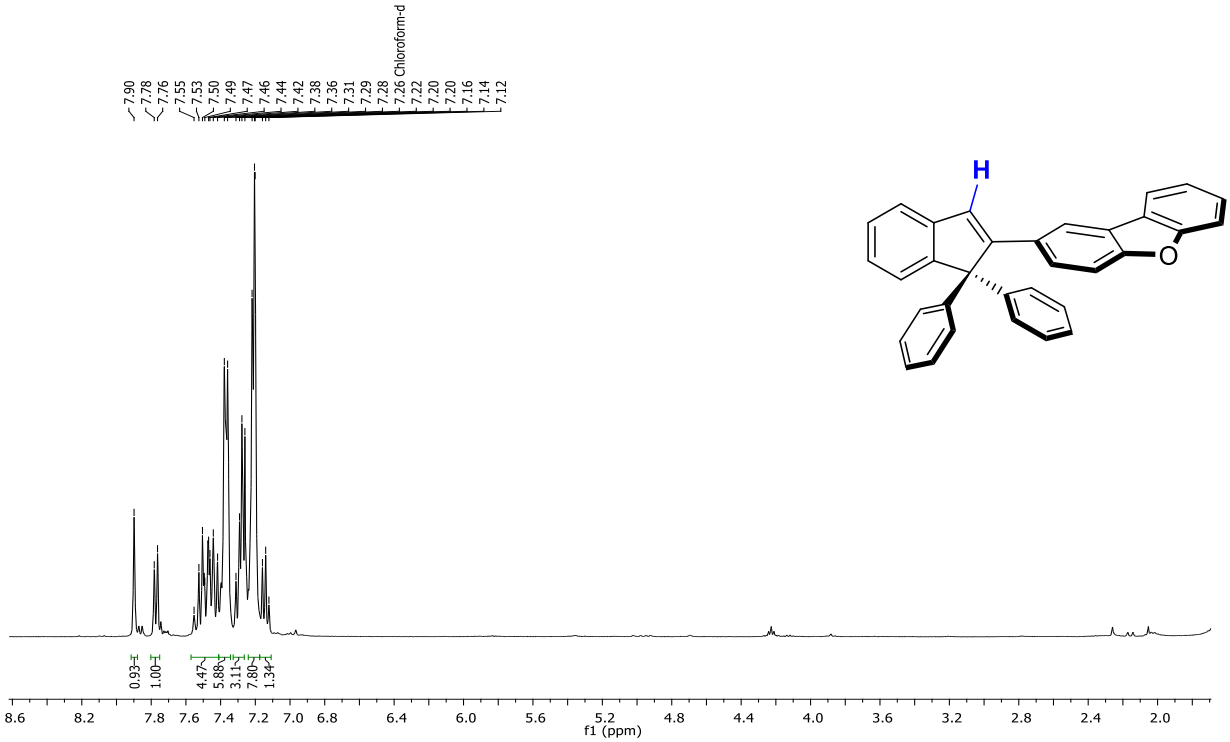


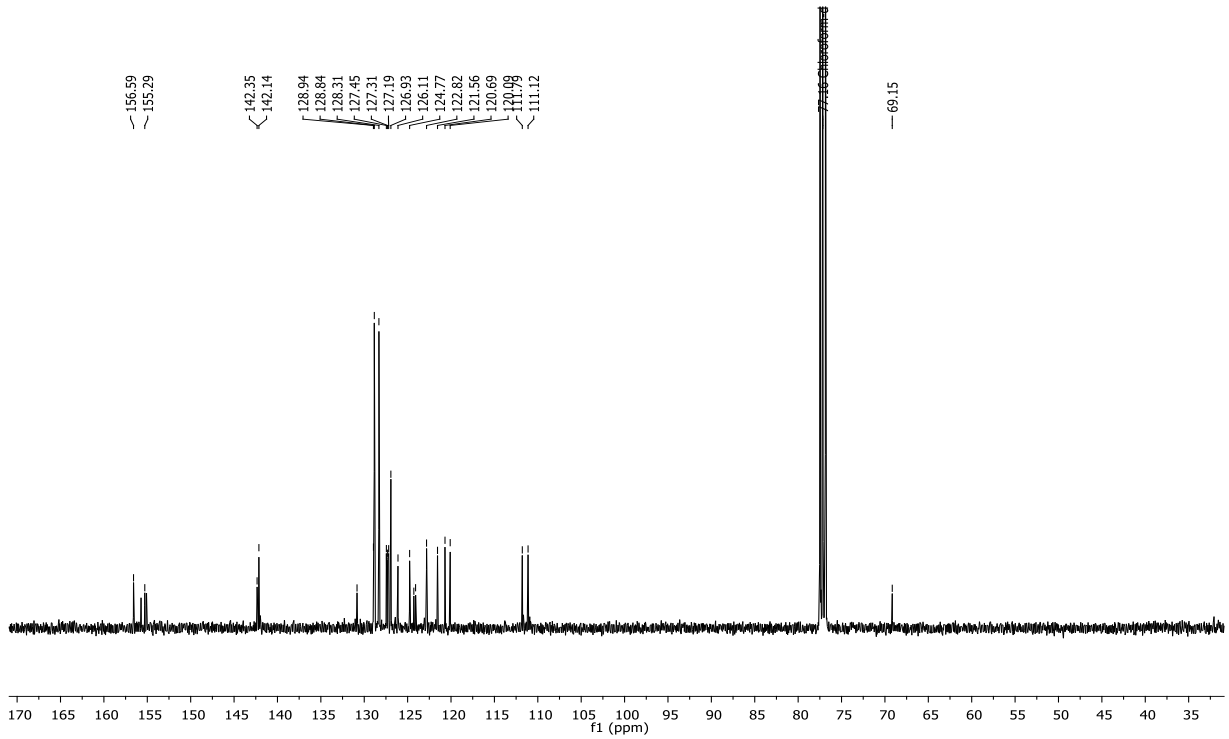


2-(4-fluorophenyl)-1,1-diphenyl-1*H*-indene **(27)**



2-(1,1-diphenyl-1*H*-inden-2-yl)dibenzo[*b*,*d*]furan **(28)**





(1,1-diphenyl-1*H*-inden-2-yl)-9-tosyl-9*H*-carbazole **(29)**