ESI for

Gold-Catalysed Rearrangement of Unconventional Cyclopropane-Tethered 1,5-Enynes

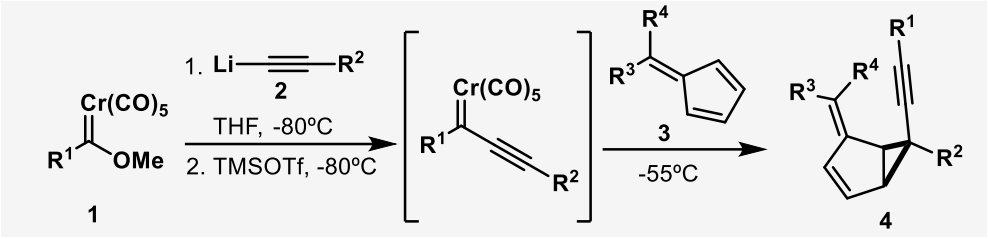
Rubén Vicente, Eva Tudela, Miguel A. Rodríguez, Ángel L. Suárez-Sobrino and Alfredo Ballesteros**

General remarks. All operations were carried out under argon atmosphere using conventional Schlenk techniques. Commercially available reagents were distilled and stored under Ar atmosphere at 0-4 ºC. Fischer carbene complexes[1] and fulvenes[2] were prepared as described in literature. Tetrahydrofuran (THF) and 1,2-dichloroethane (DCE) were distilled from sodium-benzophenone and CaH_2, respectively, under a nitrogen atmosphere, prior to use. TLC was performed on aluminium-backed plates coated with silica gel 60, with F254 indicator. Flash chromatographic columns were carried out on SiO_2 60, 230-400 mesh or deactivated SiO_2 (washed with saturated solution of $NaHCO_3$, filtered and dried at 120 ºC for 48 h). High-resolution mass spectra were determined on a Finnigan MAT95 spectrometer. NMR spectra were run on Bruker AV-300, AV-400 and NAV-400 spectrometer.

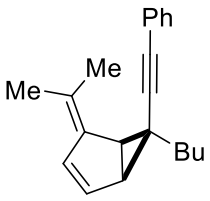
[1] (a) E. O. Fischer and A. Maasböl, *Angew. Chem. Int. Ed. Eng.,* 1964, **3**, 580–581; (b) R. Aumann and E. O. Fischer, *Chem. Ber.*, 1968, **101**, 954–962.

[2] (a) H. Alper and D. E. Laycock, *Synthesis,* 1980, **1980**, 799; (b) K. J. Stone and R. D. Little, *J. Org. Chem.*, 2002, **49**, 1849–1853; (c) N. Coskun and I. Erden, *Tetrahedron*, 2011, **67**, 8607-8614.

Synthesis of compounds 4.



To a solution of the alkyne (1.55 equiv.) in THF (50 mL) at -78 ºC, *n*-BuLi was added dropwise (1.6 M, 1.50 equiv.). After 5 min, the corresponding chromium(0) Fischer carbene complex (1.00 mmol) was added and the resulting mixture was stirred at -78 ºC until disappearance of the carbene complex (the solution turned from deep red to light yellow). Then, TMSOTf (1.66 equiv.) was added in one portion and the mixture was stirred at -78 ºC for 5 min. The resulting solution was transferred via cannula to a Schlenk flask containing the corresponding fulvene (5.00 mmol) in THF (5.0 mL) at -55 ºC. The resulting mixture was stirred at -55 ºC for 5-10 min and $NaHCO_3$ sat. (2 mL) was added subsequently. The solvent was removed under vacuum. The remaining residue was filtered through a short path of SiO_2 (10 g) using *n*-hexane. The solution was stored overnight on the fridge (0-4 ºC). The residue was purified by column chromatography on deactivated SiO_2 using a mixture of *n*-hexane/EtOAc as eluent to yield compounds **4a**. *[Note: Compounds **4** quickly decompose when neat. They were stored in stock 1,2-dichlorethane solution at –20 ºC. Under these conditions, compounds **4** can be stored for days, but appreciable decomposition was observed after 4-5 days].*



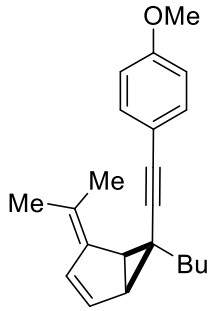
4a

(*1S*,5S*,6S)-6-Butyl-6-(phenylethynyl)-4-(propan-2-ylidene)bicyclo[3.1.0]hex-2-ene (4a).**
The representative procedure was followed using 1-hexyne (127 mg, 1.55 mmol) pentacarbonyl[(methoxy)benzylidene] chromium(0) (312 mg, 1.00 mmol) and 6,6-dimethylfulvene (530 mg, 5.00 mmol). Purification by column chromatography on silica gel (*n*-hexane) yielded **4a** as a yellow oil (222 mg, 75 %).

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 7.44-7.26 (m, 5H), 6.30 (d, *J* = 5.4 Hz, 1H), 5.96 (d, *J* = 5.4 Hz, 1H), 2.48-2.39 (m, 2H), 1.96 (bs, 6H), 1.79-1.65 (m, 3H), 1.58-1.42 (m, 3H), 1.05 (t, *J* = 7.3 Hz, 3H).

^{13}C-NMR (100 MHz, $CDCl_3$): δ = 137.8 (C), 131.5 (CH), 131.4 (CH), 130.7 (CH), 127.9 (CH), 127.1 (C), 126.9 (CH), 124.4 (C), 90.1 (C), 80.7 (C), 38.8 (CH), 37.4 (CH_2), 34.7 (CH), 30.6 (C), 30.0 (CH_2), 22.5 (CH_2), 21.7 (CH_3), 20.9 (CH_3), 14.1 (CH_3).

HR-MS (EI) calc. for $C_{21}H_{24}$ $[M]^+$ 276.1878, found 276.1877.



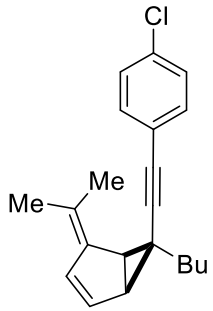
4b

(*1S*,5S*,6S)-6-Butyl-6-((4-methoxyphenyl)ethynyl)-4-(propan-2-ylidene)bicyclo[3.1.0]hex-2-ene (4b):** The representative procedure was followed using 1-hexyne (127 mg, 1.55 mmol), pentacarbonyl[(methoxy)(4-methoxybenzylidene)chromium(0)] (342 mg, 1.00 mmol) and 6,6-dimethylfulvene (530 mg, 5.00 mmol). After purification by column chromatography (hexanes/EtOAc, 5:1) yielded **4b** (214 mg, 70%) as a pale brown oil.

^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.25 (d, *J* = 8.9 Hz, 2H), 6.80 (d, *J* = 8.9 Hz, 3H), 6.33 (d, *J* = 5.5 Hz, 1H), 5.98 (d, J = 5.5 Hz, 1H), 3.81 (s, 3H), 2.47–2.26 (m, 2H), 1.91 (s, 3H), 1.90 (s, 3H), 1.81–1.56 (m, 3H), 1.51–1.34 (m, 3H), 0.98 (t, *J* = 7.3 Hz, 3H).

^{13}C-NMR (75 MHz, $CDCl_3$): δ = 158.7 (C), 138.0 (C), 133.0 (CH), 131.6 (CH), 130.8 (CH), 127.2 (C), 116.7 (C), 113.7 (CH), 88.4 (C), 80.4 (C), 55.3 (CH_3), 38.8 (CH), 37.6 (CH_2), 34.8 (CH), 30.8 (C), 30.1 (CH_2), 22.6 (CH_2), 21.8 (CH_3), 21.0 (CH_3), 14.3 (CH_3).

HR-MS (EI) calc. for $C_{22}H_{26}O$ $[M]^+$ 306.1984, found 306.1986.



4c

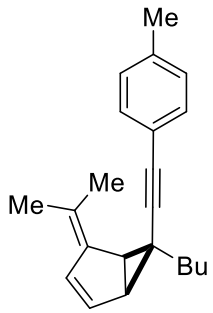
(*1S*,5S*,6S)-6-Butyl-6-((4-chlorophenyl)ethynyl)-4-(propan-2-ylidene)bicyclo[3.1.0]hex-2-ene (4c):** The representative procedure was followed using 1-hexyne (127 mg, 1.55 mmol), pentacarbonyl[(methoxy)(4-chlorobenzylidene)chromium(0)] (347 mg, 1.00 mmol) and 6,6-

dimethylfulvene (530 mg, 5.00 mmol). After purification by column chromatography (hexanes) yielded **4c** (171 mg, 55%) as a yellow oil.

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 7.22 (s, 4H), 6.31 (d, *J* = 5.5 Hz, 1H), 5.97 (dd, *J* = 5.5, 1.6 Hz, 1H), 2.40 (d, *J* = 5.7 Hz, 1H), 2.36 (dd, *J* = 5.6, 2.6 Hz, 1H), 1.90 (s, 3H), 1.88 (s, 3H), 1.70–1.58 (m, 3H), 1.53–1.36 (m, 3H), 0.97 (t, *J* = 7.4 Hz, 3H).

^{13}C-NMR (101 MHz, $CDCl_3$): δ = 137.8 (C), 132.9 (C), 132.8 (CH), 131.4 (CH), 130.8 (CH), 128.3 (CH), 127.5 (C), 123.0 (C), 91.5 (C), 79.7 (C), 39.0 (CH), 37.4 (CH_2), 34.9 (CH), 30.7 (C), 30.1 (CH_2), 22.6 (CH_2), 21.8 (CH_3), 21.0 (CH_3), 14.2 (CH_3).

HR-MS (EI) calc. for $C_{21}H_{23}Cl$ $[M]^+$ 310.1488, found 310.1493.



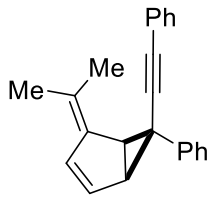
4d

(*1S*,5S*,6S)-6-Butyl-4-(propan-2-ylidene)-6-(p-tolylethynyl)bicyclo[3.1.0]hex-2-ene (4d):** The representative procedure was followed using 1-hexyne (127 mg, 1.55 mmol), pentacarbonyl[(methoxy)(4-methylbezylidene)chromium(0)] (326 mg, 1.00 mmol) and 6,6-dimethylfulvene (530 mg, 5.00 mmol). After purification by column chromatography (hexanes) yielded **4d** (166 mg, 57%) as a yellow oil.

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 7.19 (d, *J* = 8.0 Hz, 2H), 7.05 (d, *J* = 8.0 Hz, 2H), 6.31 (d, *J* = 5.6 Hz, 1H), 5.97 (d, *J* = 5.6 Hz, 1H), 2.40-2.30 (m, 2H, overlapped signal), 2.32 (s, 3H, overlapped signal), 1.89 (s, 3H), 1.88 (s, 3H), 1.68–1.58 (m, 3H), 1.46–1.38 (m, 3H), 0.98 (t, *J* = 7.2 Hz, 3H).

^{13}C-NMR (101 MHz, $CDCl_3$): δ = 137.9 (C), 137.0 (C), 131.5 (CH), 130.8 (CH), 128.8 (CH), 127.2 (C), 121.4 (C), 89.3 (C), 80.7 (C), 38.9 (CH), 37.5 (CH_2), 34.7 (CH), 30.8 (C), 30.1 (CH_2), 22.6 (CH_2), 21.8 (CH_3), 21.4 (CH_3), 21.0 (CH_3), 14.2 (CH_3) (one signal corresponding to aromatic CH is overlapping).

HR-MS (EI) calc. for $C_{22}H_{26}$ $[M]^+$ 290.2035, found 290.2033.



4e

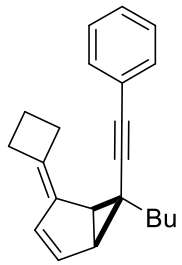
(*1S*,5S*,6S)-6-Phenyl-6-(phenylethynyl)-4-(propan-2-ylidene)bicyclo[3.1.0]hex-2-ene (4e)**

The representative procedure was followed using phenylacetylene (158 mg, 1.55 mmol) pentacarbonyl[(methoxy)benzylidene] chromium(0) (312 mg, 1.00 mmol) and 6,6-dimethylfulvene (530 mg, 5.00 mmol). Purification by column chromatography on silica gel (*n*-hexane) yielded **4e** as a pale yellow oil (215 mg, 78 %).

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 7.53 (d_{app}, *J* = 8.4 Hz, 2H), 7.42-7.36 (m, 4H), 7.34-7.23 (m, 4H), 6.52 (d, *J* = 5.5 Hz, 1H), 6.15 (d, *J* = 5.5 Hz, 1H), 3.00 (d, *J* = 5.7 Hz, 1H), 2.94 (dd, *J* = 5.7, 2.7 Hz, 1H), 1.99 (s, 3H), 1.93 (s, 3H).

^{13}C-NMR (100 MHz, $CDCl_3$): δ = 142.1 (C), 138.1 (C), 132.0 (CH), 131.5 (CH), 131.0 (CH), 129.6 (C), 128.2 (CH), 128.0 (CH), 127.3 (CH), 125.9 (CH), 125.3 (CH), 124.1 (C), 88.0 (C), 83.0 (C), 43.7 (CH), 39.4 (CH), 33.0 (C), 22.1 (CH_3), 21.1 (CH_3).

HR-MS (EI) calc. for $C_{23}H_{20}$ $[M]^+$ 296.1565, found 296.1579.



4f

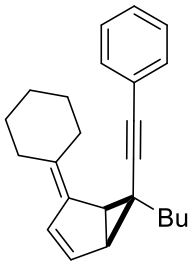
(*1S*,5S*,6S)-6-butyl-4-cyclobutylidene-6-(phenylethynyl)bicyclo[3.1.0]hex-2-ene (4f):**

The representative procedure was followed using 1-hexyne (127 mg, 1.55 mmol), pentacarbonyl[(methoxy)benzylidene] chromium(0) (312 mg, 1.00 mmol) and 5-cyclobutylidenecyclopenta-1,3-diene (590 mg, 5.00 mmol). After purification by column chromatography (hexanes) yielded **4f** (165 mg, 57%) as a pale yellow oil.

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 7.37–7.32 (m, 2H), 7.31–7.20 (m, 3H), 6.08 (d, *J* = 5.5 Hz, 1H), 5.94 (d, *J* = 5.5 Hz, 1H), 2.94-2.72 (m, 4H), 2.37 (dd, *J* = 5.6, 2.6 Hz, 1H), 2.24 (d, *J* = 5.6 Hz, 1H), 2.16–1.96 (m, 2H), 1.76–1.53 (m, 3H), 1.52–1.30 (m, 3H), 0.96 (t, *J* = 7.3 Hz, 3H).

^{13}C-NMR (101 MHz, $CDCl_3$): 136.3 (C), 134.7 (C), 131.7 (CH), 131.2 (CH), 130.0 (CH), 128.0 (CH), 127.1 (CH), 124.5 (C), 90.3(C), 80.8 (C), 39.0 (CH), 37.4 (CH_2), 33.9 (CH), 30.7 (C), 30.4 (CH_2), 30.3 (CH_2), 30.0 (CH_2), 22.5 (CH_2), 17.3 (CH_2), 14.2 (CH_3).

HR-MS (EI) calc. for $C_{22}H_{24}$ $[M]^+$ 288.1878, found 288.1871.



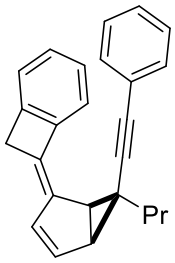
4g

(*1S*,5S*,6S)-6-butyl-4-cyclohexylidene-6-(phenylethynyl)bicyclo[3.1.0]hex-2-ene (4g):**

The representative procedure was followed using 1-hexyne (127 mg, 1.55 mmol), pentacarbonyl[(methoxy)benzylidene] chromium(0) (312 mg, 1.00 mmol) and cyclopenta-2,4-dien-1-ylidenecyclohexane (750 mg, 5.00 mmol). After purification by column chromatography (hexanes) yielded **4g** (155 mg, 49% determined by ^{1}H NMR, purity *ca.* 90%) as a pale yellow oil. *(Note: compound **4g** could not be purified by column chromatography, attempts to perform longer columns led to lower yields without an increase of the purity).*

^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.36–7.23 (m, 5H), 6.36 (dd, *J* = 5.5, 1.1 Hz, 1H), 5.99 (ddd, *J* = 5.5, 2.4, 0.8 Hz, 1H), 2.49–2.19 (m, 5H), 1.83–1.36 (m, 13H), 0.98 (t, *J* = 7.3 Hz, 3H).

^{13}C-NMR (75 MHz, $CDCl_3$): 136.3 (C), 134.8 (C), 131.6 (CH), 130.4 (CH), 128.0 (CH), 127.1 (CH), 124.6 (C), 90.3 (C), 80.9 (C), 38.7 (CH), 37.5 (CH_2), 34.6 (CH), 32.8 (CH_2), 31.9 (CH_2), 30.5 (C), 29.9 (CH_2), 28.6 (CH_2), 28.4 (CH_2), 26.9 (CH_2), 22.6 (CH_2), 14.2 (CH_3) (a signal corresponding to an aromatic CH is overlapping).



4h

(*Z*)-7-(*1S*,5S*,6S)-6-(phenylethynyl)-6-propylbicyclo[3.1.0]hex-3-en-2-ylidene)bicyclo[4.2.0]octa-1(6),2,4-triene (4h):**

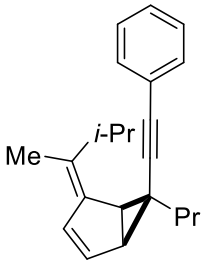
The representative procedure was followed using 1-pentyne (0.153 mL, 1.55 mmol) pentacarbonyl[(methoxy)benzylidene] chromium(0) (312 mg, 1.00 mmol) and 7-(cyclopenta-2,4-dien-1-ylidene)bicyclo[4.2.0]octa-1(6),2,4-triene (831 mg, 5.00 mmol). After purification by column chromatography (hexanes) yielded **4h** (170 mg, 53%) as a pale yellow oil. *(Note: A small amount of the E-isomer is observed; Z:E = 19:1).*

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 7.54–7.49 (m, 2H), 7.43–7.36 (m, 4H), 7.33–7.24 (m, 4H), 6.50 (dd, *J* = 5.5, 1.3 Hz, 1H), 6.20 (dd, *J* = 5.5, 2.5 Hz, 1H), 2.42 (dd, *J* = 5.3, 2.5 Hz, 1H), 2.30 (s,

3H), 2.25 (dd, *J* = 5.3, 1.0 Hz, 1H), 1.79–1.66 (m, 2H), 1.57–1.50 (m, 2H), 1.49–1.31 (m, 2H), 0.99 (t, *J* = 7.3 Hz, 3H).

^{13}C-NMR (101 MHz, $CDCl_3$): 145.3 (C), 144.8 (C), 135.0 (C), 134.7 (CH), 131.7 (CH), 131.2 (C), 130.9 (CH), 128.0 (CH), 127.8 (CH), 127.5 (CH), 127.2 (CH), 124.2 (C), 122.6 (CH), 118.8 (CH), 89.5 (C), 81.2 (C), 40.0 (CH_2), 39.8 (CH), 37.3 (CH_2), 35.6 (CH), 33.3 (C), 21.2 (CH_2), 14.2 (CH_3).

HR-MS (EI) calc. for $C_{25}H_{22}$ $[M]^+$ 322.1722, found 322.1715.



4i

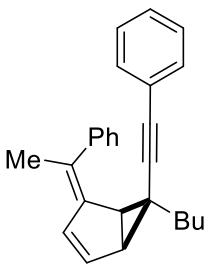
(*1S*,5S*,6S*,Z*)-4-(3-methylbutan-2-ylidene)-6-(phenylethynyl)-6-propylbicyclo[3.1.0]hex-2-ene (4i):

The representative procedure was followed using 1-pentyne (0.120 mg, 1.50 mmol) pentacarbonyl[(methoxy)benzylidene] chromium(0) (312 mg, 1.00 mmol) and 6-isopropyl-6-methylfulvene (670 mg, 5.00 mmol). After purification by column chromatography (hexanes) yielded **4i** (125 mg, 57%, *Z:E* = 8:1) as a pale yellow oil.

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 7.31–7.27 (m, 2H), 7.25–7.21 (m, 3H), 6.31 (dd, *J* = 5.5, 1.1 Hz, 1H), 6.00 (dd, *J* = 5.6, 2.4 Hz, 1H), 2.91 (p, *J* = 6.8 Hz, 1H), 2.45 (d, *J* = 5.6 Hz, 1H), 2.35 (dd, *J* = 5.7, 2.4 Hz, 1H), 1.78 (s, 3H), 1.74–1.59 (m, 3H), 1.44–1.34 (m, 1H), 1.08 (d, *J* = 6.6 Hz, 3H), 1.07 (d, *J* = 1.6 Hz, 3H), 1.00 (t, *J* = 7.0 Hz, 3H).

^{13}C-NMR (101 MHz, $CDCl_3$): 136.9 (C), 136.8 (C), 131.7 (CH), 131.6 (CH), 131.3 (CH), 128.0 (CH), 127.1 (CH), 124.5 (C), 90.1 (C), 81.0 (C), 40.0 (CH_2), 38.8 (CH), 34.5 (CH), 32.8 (CH), 30.8 (C), 21.0 (CH_3), 20.9 (CH_2), 20.3 (CH_3), 14.1 (CH_3), 13.1 (CH_3).

HR-MS (EI) calc. for $C_{22}H_{26}$ $[M]^+$ 290.2035, found 290.2030.



4j

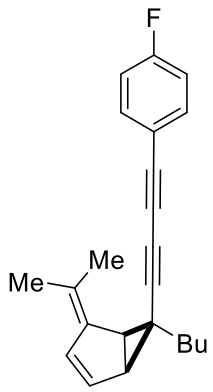
(*1S*,5S*,6S*,Z*)-6-butyl-4-(1-phenylethylidene)-6-(phenylethynyl)bicyclo[3.1.0]hex-2-ene (4j):

The representative procedure was followed using 1-hexyne (127 mg, 1.55 mmol), pentacarbonyl[(methoxy)benzylidene] chromium(0) (312 mg, 1.00 mmol) and 6-methyl-6-phenylfulvene (750 mg, 5.00 mmol). After purification by column chromatography (hexanes) yielded **4j** (175 mg, 52%) as a pale yellow oil.

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 7.54–7.49 (m, 2H), 7.43–7.36 (m, 4H), 7.33–7.24 (m, 4H), 6.50 (dd, *J* = 5.5, 1.3 Hz, 1H), 6.20 (dd, *J* = 5.5, 2.5 Hz, 1H), 2.42 (dd, *J* = 5.3, 2.5 Hz, 1H), 2.30 (s, 3H), 2.25 (dd, *J* = 5.3, 1.0 Hz, 1H), 1.79–1.66 (m, 2H), 1.57–1.50 (m, 2H), 1.49–1.31 (m, 2H), 0.99 (t, *J* = 7.3 Hz, 3H).

^{13}C-NMR (101 MHz, $CDCl_3$): 143.4 (C), 140.7 (C), 133.8 (CH), 131.8 (CH), 131.5 (CH), 130.3 (C), 128.5 (CH), 128.1 (CH), 127.7 (CH), 127.3 (CH), 126.6 (CH), 124.3 (C), 89.8 (C), 81.3 (C), 39.8 (CH), 37.7 (CH_2), 36.0 (CH), 31.6 (C), 29.4 (CH_2), 22.8 (CH_2), 20.1 (CH_3), 14.2 (CH_3).

HR-MS (EI) calc. for $C_{26}H_{26}$ $[M]^+$ 338.2035, found 338.2025.



4k

(*1S*,5S*,6S)-6-butyl-6-((4-fluorophenyl)buta-1,3-diyn-1-yl)-4-(propan-2-ylidene)bicyclo[3.1.0]hex-2-ene (4k):**

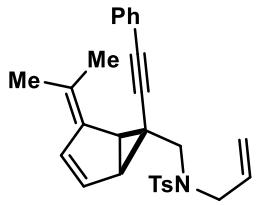
The representative procedure was followed using 1-hexyne (84 mg, 1.00 mmol), pentacarbonyl[3-(4-fluorophenyl)-1-methoxyprop-2-yn-1-ylidene)chromium(0)] (354 mg, 0.66 mmol) and 6-methyl-6-phenylfulvene (500 mg, 3.3 mmol). After purification by column chromatography (hexanes) yielded **4k** (136 mg, 64%) as a yellow oil.

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 7.53–7.39 (m, 2H), 6.98 (t, *J* = 8.7 Hz, 2H), 6.33 (d, *J* = 5.5 Hz, 1H), 5.96 (d, *J* = 5.3 Hz, 1H), 2.53–2.28 (m, 2H), 1.89 (s, 6H), 1.66–1.55 (m, 3H), 1.45–1.31 (m, 3H), 0.95 (t, *J* = 7.3 Hz, 3H).

^{13}C-NMR (75 MHz, $CDCl_3$): δ = 162.7 (d, *J* = 249.9 Hz, C), 137.2 (C), 134.4 (d, *J* = 8.3 Hz, CH), 131.1 (CH), 131.0 (CH), 128.6 (C), 118.5 (d, *J* = 3.8 Hz, C), 115.6 (d, *J* = 21.8 Hz, CH), 85.2 (C), 74.9 (C), 72.8 (C), 64.5 (C), 39.5 (CH), 37.3 (CH_2), 35.3 (CH), 30.9 (C), 30.0 (CH_2), 22.6 (CH_2), 21.8 (CH_3), 21.1 (CH_3), 14.1 (CH_3).

^{19}F-NMR (282 MHz, $CDCl_3$): δ = –109.7 (s).

HR-MS (EI) calc. for $C_{23}H_{23}F$ $[M]^+$ 318.1784, found 318.1782.



4l

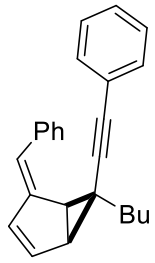
***N*-allyl-4-methyl-*N*-(((*1S*,5S*,6S**)-6-(phenylethynyl)-4-(propan-2-ylidene)bicyclo[3.1.0]hex-2-en-6-yl)methyl)benzenesulfonamide (4l):**

The representative procedure was followed using *N*-allyl-4-methyl-*N*-(prop-2-yn-1-yl)benzenesulfonamide[3] (386 mg, 1.55 mmol), pentacarbonyl[(methoxy)benzylidene] chromium(0) (312 mg, 1.00 mmol) and 6-methyl-6-phenylfulvene (750 mg, 5.00 mmol).. After purification by column chromatography (hexanes:EtOAc = 5:1) yielded **4l** (366 mg, 82%) as a colorless oil.

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 7.78 (d, *J* = 8.3 Hz, 2H), 7.38–7.16 (m, 7H), 6.34 (dd, *J* = 5.5, 1.0 Hz, 1H), 5.90 (dd, *J* = 5.7, 2.3 Hz, 1H), 5.78–5.62 (m, 1H), 5.27 (dd, *J* = 17.1, 1.5 Hz, 1H), 5.19 (dd, *J* = 10.2, 1.5 Hz, 1H), 4.26–4.10 (m, 2H), 3.47 (d, *J* = 1.5 Hz, 2H), 2.70 (d, *J* = 5.9 Hz, 1H), 2.63 (dd, *J* = 5.9, 2.4 Hz, 1H), 2.39 (s, 3H), 1.90 (s, 3H), 1.89 (s, 3H).

^{13}C-NMR (100 MHz, $CDCl_3$): δ =143.1 (C), 137.9 (C), 137.1 (C), 132.8 (CH), 131.5 (CH), 130.3 (CH), 129.6 (CH), 129.3 (C), 128.1 (CH), 127.5 (CH), 127.3 (CH), 123.9 (C), 119.1 (CH_2), 88.7 (C), 82.0 (C), 52.1 (CH_2), 50.3 (CH_2), 38.5 (CH), 33.7 (CH), 29.2 (C), 22.1 (CH_3), 21.5 (CH_3), 21.1 (CH_3) (a C(sp^2)–H is overlapping).

HR-MS (EI) calc. for $C_{28}H_{29}NO_2S$ $[M]^+$ 443.1919, found 443.1915.



4m

(*1S*,5S*,6S)-4-((Z)-benzylidene)-6-butyl-6-(phenylethynyl)bicyclo[3.1.0]hex-2-ene (4m):**

The representative procedure was followed using 1-hexyne (127 mg, 1.55 mmol), pentacarbonyl[(methoxy)benzylidene] chromium(0) (312 mg, 1.00 mmol) and 6-phenylfulvene (770 mg, 5.00 mmol). After purification by column chromatography (hexanes) yielded **4m** (198 mg, 61%, *Z:E* = 4:1) as a pale yellow oil.

[3] M. C. Patel, T. Livinghouse and B. L. Pagenkop, *Org. Synth.* 2003, **80**, 93

^{1}H-NMR (400 MHz, $CDCl_3$, data for *Z*-isomer, * indicates signal overlapping with *E*-isomer): δ = 7.56 (d, *J* = 7.7 Hz, 2H*), 7.42 (t, *J* = 7.7 Hz, 2H*), 7.39–7.32 (m, 3H*), 7.32–7.21 (m, 5H*), 6.71 (s, 1H), 6.31 (d, *J* = 5.4 Hz, 1H*), 6.27–6.19 (m, 1H), 2.67 (d, *J* = 5.2 Hz, 1H), 2.55 (dd, *J* = 5.2, 2.4 Hz, 1H*), 1.89–1.74 (m, 2H*), 1.73–1.59 (m, 2H*), 1.58–1.42 (m, 2H*), 1.05 (t, *J* = 7.3 Hz, 3H*).

^{13}C-NMR (101 MHz, $CDCl_3$, data for *Z*-isomer): 145.6 (C), 138.0 (C), 135.6 (CH), 134.2 (CH), 131.7 (CH), 128.5 (CH), 128.1 (CH), 127.9 (CH), 127.2 (CH), 126.4 (CH), 124.0 (C), 123.8 (CH), 88.9 (C), 81.3 (C), 40.3 (CH), 37.8 (CH_2), 34.7 (CH), 33.5 (C), 29.7 (CH_2), 22.7 (CH_2), 14.1 (CH_3).

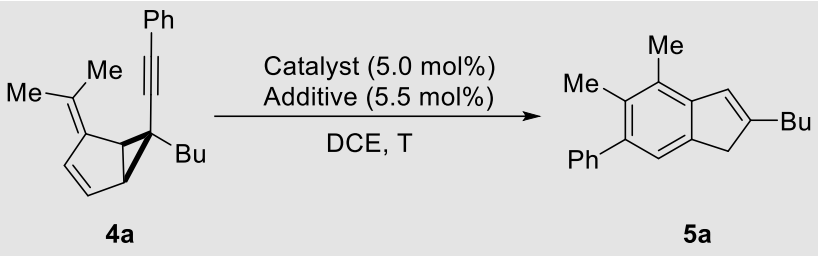
HR-MS (EI) calc. for $C_{25}H_{24}$ $[M]^+$ 324.1878, found 324.1879.

Catalyst screening for the reaction with model substrate 4a.

Representative procedure:

Under Ar atmosphere, the corresponding catalyst (5.0 mol%) and additive (5.5 mol%, when applicable) were dissolved in DCE and stirred for 10 min. Then, a stock solution of **4a** in DCE was added (final concentration ≈ 0.1 M) and the resulting mixture was stirred at the indicated temperature until consumption of the starting material (TLC). Solvent was removed and the residue was purified by flash column chromatography in SiO_2 (hexanes). The results are summarized in Table S1.

Table S1. Screening summary.

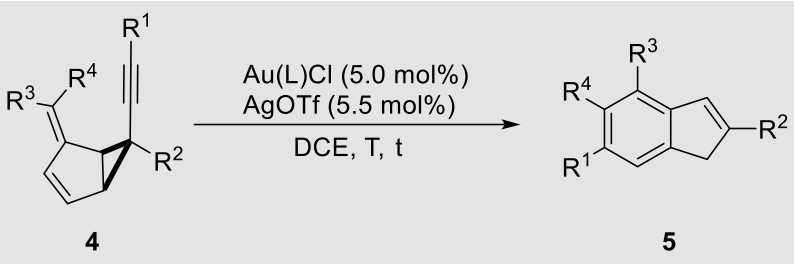


4a **5a**

Catalyst / Additive	5a (%)	T (°C)	Observations
no catalyst	n.d.	70	Degradation of **4a**
TfOH / —	n.d.	RT/70	Degradation of **4a**
$(Ph_3P)AuCl$ / AgOTf	37	RT	
$(Ph_3P)AuCl$ / AgOTf	62	50	
$(Ph_3P)AuCl$ / AgOTf	60	50	*After filtration of the in situ generated cationic gold catalyst*
$(Ph_3P)AuCl$ / AgOTf	55	70	
(JohnPhos)AuCl / AgOTf	37	50	
$(ArO)_3PAuCl$ / AgOTf	40	50	
(IPr)PAuCl / AgOTf	38	RT	
(IPr)PAuCl / AgOTf	77	50	*rr* = 10:1 *(isomerization of the indene double bond)*
(IPr)PAuCl / $AgNTf_2$	35	50	
(IPr)PAuCl / AgOTf	63	50	*rr* = 8:1. THF as solvent.
(IPr)PAuCl / AgOTf	31	50	*rr* = 10:1. Toluene as solvent.
(IPr)PAuCl / —	n.d.	50	Degradation of **4a**
AgOTf / —	n.d.	RT/50	Degradation of **4a**

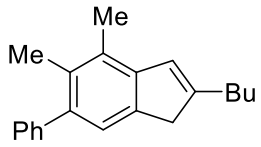
$AuCl_3$ / —	23	RT	
$AuCl_3$ / —	n.d.	50	Complex mixture
AuCl(pic) / —	n.d.	50	Complex mixture
$PtCl_2$ / —	n.d.	RT/50	Degradation of **4a**.
$PdCl_2(MeCN)$ / —	n.d.	RT/50	Degradation of **4a**.
$[Cu(MeCN)_2][BF_4]$/ —	n.d.	RT/50	Degradation of **4a**.
$FeCl_3$ / —	n.d.	RT/50	Degradation of **4a**.
n.d. = not detected. Ar = 2,6-di-*tert*-butylphenyl. IPr = 1,3-Bis(2,6-diisopropylphenyl)-1,3-dihydro-2*H*-imidazol-2-ylidene). pic = 2-picolinate.			

Gold-catalysed rearrangement of compounds 4 to indenes 5.



4 **5**

Under Ar atmosphere, the corresponding gold catalyst (5.0 mol%) and AgOTf (5.5 mol%) were dissolved in DCE and stirred for 10 min. Then, a stock solution of **4** in DCE was added (final concentration ≈ 0.1 M) and the resulting mixture was stirred at the indicated temperature until consumption of the starting material (TLC). Solvent was removed and the residue was purified by flash column chromatography in SiO_2 (hexanes/EtOAc).



5a

2-Butyl-4,5-dimethyl-6-phenyl-1*H*-indene (5a).

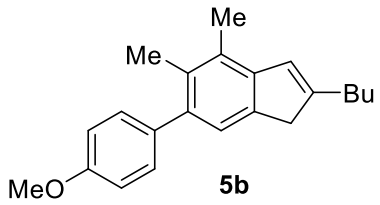
The representative procedure was followed using (IPr)AuCl (4.4 mg, 5.0 mol%), AgOTf (2.0 mg, 5.5 mol%) and **4a** (39 mg, 0.141 mmol). After 16 h at 50 ºC, purification by flash column chromatography (hexanes) yielded **5a** (34 mg, 77%, rr = 10:1) as an off-white solid (mixture of isomeric indenes). The reaction with Ph_3PAuCl led exclusively to the formation of **5a** (21 mg, 62%) as a white solid. Crystals of **5a** suitable for X-Ray analysis were obtained by slow diffusion of pentane into a solution of **5a** in CH_2Cl_2.

m. p. = 75–76 ºC (dec.).

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 7.48-7.41 (m, 2H), 7.36 (d_{app}, *J* = 7.3 Hz, 2H), 7.18 (bs, 1H), 6.69 (bs, 1H), 3.38 (s, 2H), 2.55 (t, *J* = 7.5 Hz, 2H), 2.43 (s, 3H), 2.23 (s, 3H), 1.65 (quint, *J* = 7.8 HzJJ, 2H), 1.44 (sextet, *J* = 7.8 Hz, 2H), 0.99 (t, *J* = 7.8 Hz, 3H).

^{13}C-NMR (100 MHz, $CDCl_3$): δ = 150.5 (C), 144.0 (C), 143.5 (C), 139.9 (C), 137.9 (C), 131.6 (C), 129.6 (CH), 128.0 (C), 127.8 (CH), 126.2 (CH), 124.6 (CH), 122.6 (CH), 41.1 (CH_2), 31.3 (CH_2), 31.1 (CH_2), 22.5 (CH_2), 17.0 (CH_3), 16.0 (CH_3), 13.9 (CH_3).

HR-MS (EI) calc. for $C_{21}H_{24}$ $[M]^+$ 276.1878, found 276.1883.



5b

2-Butyl-6-(4-methoxyphenyl)-4,5-dimethyl-1*H*-indene (5b)

The representative procedure was followed using Ph_3PAuCl (7.3 mg, 5.0 mol%), AgOTf (4.2 mg, 5.5 mol%) and **4b** (92 mg, 0.30 mmol). After 17 h at 70 ºC, purification by flash column chromatography (hexanes/EtOAc = 5:1) yielded **5b** (45 mg, 49%) as a white solid.

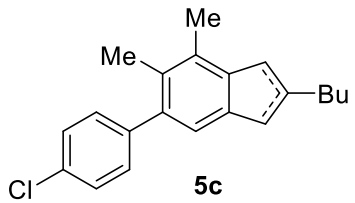
m. p. = 145–148 ºC (dec.).

^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.27 (d, *J* = 8.8 Hz, 2H), 7.15 (s, 1H), 6.97 (d, *J* = 8.9 Hz, 2H), 6.67 (s, 1H), 3.89 (s, 3H), 3.36 (s, 2H), 2.53 (t, *J* = 7.6 Hz, 2H), 2.41 (s, 3H), 2.22 (s, 3H), 1.73–1.56 (m, 2H), 1.42 (dq, *J* = 13.9, 7.2 Hz, 2H), 0.98 (t, *J* = 7.3 Hz, 3H).

7.72 (d, *J* = 7.8 Hz, 2H), 7.52-7.26 (m, 10H), 3.87 (s, 2H), 2.54 (s, 3H), 2.28 (s, 3H).

^{13}C-NMR (75 MHz, $CDCl_3$): δ = 158.5 (C), 150.9 (C), 144.3 (C), 140.4 (C), 137.9 (C), 136.4 (C), 132.3 (C), 131.1 (CH), 128.5 (C), 125.1 (CH), 123.2 (CH), 113.7 (CH), 55.7 (CH_3), 41.6 (CH_2), 31.8 (CH_2), 31.6 (CH_2), 23.0 (CH_2), 17.5 (CH_3), 16.6 (CH_3), 14.4 (CH_3).

HR-MS (EI) calc. for $C_{24}H_{22}O$ $[M]^+$ 326.1671, found 326.1675.



5c

2-Butyl-6-(4-chlorophenyl)-4,5-dimethyl-1*H*-indene (5c)

The representative procedure was followed using IPrAuCl (12.6 mg, 5.0 mol%), AgOTf (5.8 mg, 5.5 mol%) and **4c** (126 mg, 0.405 mmol). After 17 h at 50 ºC, purification by flash column chromatography (hexanes) yielded inseparable indene isomers **5c/5c'** (71 mg, 56% overall yield, *rr* = 4:1) as a white solid.

m. p. *(of the mixture)* = 135–138 ºC (dec.).

Major isomer 5c. *(* indicates that signals overlap with minor isomer **5c')***

^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.39 (d_{app}, *J* = 8.8 Hz, 2H*), 7.28 (d_{app}, *J* = 8.8 Hz, 2H*), 7.13 (s, 1H), 6.68 (s, 1H), 3.71 (s, 2H), 2.55 (t, *J* = 7.2 Hz, 2H), 2.42 (s, 3H), 2.21 (s, 3H), 1.70–1.60 (m, 2H*), 1.49-1.39 (m, 2H*), 0.99 (t, *J* = 7.2 Hz, 3H*).

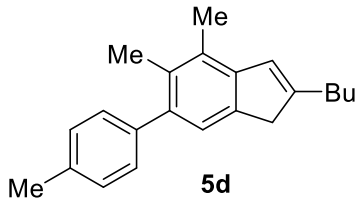
^{13}C-NMR (75 MHz, $CDCl_3$): δ = 150.9 (C), 144.4 (C), 142.0 (C), 140.1 (C), 136.7 (C), 132.3 (C), 131.6 (C), 131.0 (CH), 128.2 (C), 128.1 (CH), 124.6 (CH), 122.5 (CH), 41.2 (CH_2), 31.3 (CH_2), 31.2 (CH_2), 22.6 (CH_2), 17.0 (CH_3), 16.1 (CH_3), 14.0 (CH_3).

Minor isomer 5c'.

^{1}H-NMR (300 MHz, $CDCl_3$, *only non-overlapping signals are indicated*): δ = 7.03 (s, 1H), 6.51 (s, 1H), 3.32 (s, 2H), 2.36 (s, 3H), 2.20 (s, 3H).

^{13}C-NMR (75 MHz, $CDCl_3$, *only clearly assignable signals are indicated*): δ = 150.5 (C), 142.7 (C), 141.6 (C), 139.6 (C), 132.4 (C), 130.9 (CH), 129.1 (C), 126.1 (CH), 118.9 (CH), 40.5 (CH_2), 31.0 (CH_2), 16.8 (CH_3), 16.5 (CH_3).

HR-MS *(of the mixture)* (EI) calc. for $C_{21}H_{23}Cl$ $[M]^+$ 310.1488, found 310.1483.



5d

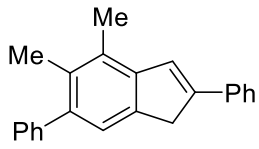
2-Butyl-4,5-dimethyl-6-(*p*-tolyl)-1*H*-indene (5d)

The representative procedure was followed using IPrAuCl (6.8 mg, 5.0 mol%), AgOTf (3.0 mg, 5.5 mol%) and **4d** (64 mg, 0.22 mmol). After 17 h at 50 ºC, purification by flash column chromatography (hexanes) yielded **5d** (26 mg, 40%) as a yellow oil.

^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.25 (bs, 4H), 7.17 (s, 1H), 6.68 (bs, 1H), 3.37 (s, 2H), 2.52 (t, *J* = 7.8 Hz, 2H), 2.45 (s, 3H), 2.43 (s, 3H), 2.30 (s, 3H), 1.69–1.55 (m, 2H), 1.49-1.36 (m, 2H), 0.99 (t, *J* = 7.2 Hz, 3H).

^{13}C-NMR (101 MHz, $CDCl_3$): δ = 150.5 (C), 143.9 (C), 140.6 (C), 140.0 (C), 137.9 (C), 135.8 (C), 131.8 (C), 129.6 (CH), 128.6 (CH), 128.0 (C),124.7 (CH), 122.8 (CH), 41.2 (CH_2), 31.4 (CH_2), 31.2 (CH_2), 22.6 (CH_2), 21.2 (CH_3), 17.1 (CH_3), 16.1 (CH_3), 14.0 (CH_3).

HR-MS (EI) calc. for $C_{22}H_{26}$ $[M]^+$ 290.2035, found 290.2042.



5e

4,5-Dimethyl-2,6-diphenyl-1*H*-indene (5e)

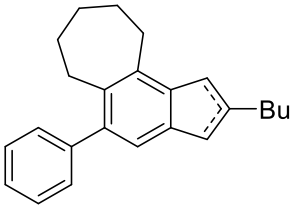
The representative procedure was followed using Ph_3PAuCl (7.4 mg, 5.0 mol%), AgOTf (4.2 mg, 5.5 mol%) and **4e** (87.3 mg, 0.290 mmol). After 16 h at 70 ºC, purification by flash column chromatography (hexanes/EtOAc = 50:1) yielded **5e** (65.4 mg, 75%) as a white solid.

m. p. = 131–135 ºC (dec.).

^{1}H-NMR (400 MHz, $CDCl_3$): δ = 7.72 (d, *J* = 7.8 Hz, 2H), 7.52-7.26 (m, 10H), 3.87 (s, 2H), 2.54 (s, 3H), 2.28 (s, 3H).

^{13}C-NMR (100 MHz, $CDCl_3$): δ = 145.8 (C), 143.7 (C), 143.3 (C), 140.0 (C), 139.2 (C), 136.2 (C), 132.0 (C), 129.5 (CH), 129.2 (C), 128.6 (CH), 127.9 (CH), 127.3 (CH), 126.3 (CH), 125.5 (CH), 125.1 (CH), 122.8 (CH), 39.1 (CH_2), 17.0 (CH_3), 16.1 (CH_3).

HR-MS (EI) calc. for $C_{23}H_{20}$ $[M]^+$ 296.1565, found 296.1566.



5f/5f'

2-Butyl-5-phenyl-3,6,7,8,9,10-hexahydrocyclohepta[*e*]indene (5f)

The representative procedure was followed using IPrAuCl (11.3 mg, 5.0 mol%), AgOTf (5.1 mg, 5.5 mol%) and **4f** (115 mg, 0.363 mmol). After 17 h at 50 ºC, purification by flash column chromatography (hexanes) yielded inseparable indene isomers **5f/5f'** (45 mg, 39% overall estimated yield, *rr* = 5:1) as a colorless oil. *(Note: The real yield should be slightly higher as **4f** was not pure, ca. 90% purity).*

Major isomer 5f. *(* indicates that signals overlap with minor isomer **5f')***

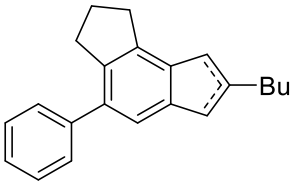
^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.49–7.41 (m, 2H*), 7.40–7.32 (m, 3H*), 7.18 (s, 1H), 6.76–6.70 (m, 1H), 3.40 (s, 2H), 3.12–3.01 (m, 2H), 2.88–2.77 (m, 2H*), 2.55 (t, *J* = 7.3 Hz, 2H*), 1.99–1.85 (m, 2H*), 1.83–1.73 (m, 2H*), 1.73–1.62 (m, 4H*), 1.54–1.36(m, 2H*), 1.01 (t, *J* = 7.3 Hz, 3H*).

^{13}C-NMR (75 MHz, $CDCl_3$): 150.5 (C), 143.8 (C), 143.3 (C), 140.2 (C), 139.1 (C), 137.3 (C), 135.3 (C), 129.7 (CH), 127.9 (CH), 126.2 (CH), 124.7 (CH), 123.0 (CH), 41.3 (CH_2), 32.6 (CH_2), 31.4 (CH_2), 31.2 (CH_2), 31.1 (CH_2), 31.0 (CH_2), 28.5 (CH_2), 27.9 (CH_2), 22.6 (CH_2), 14.0 (CH_3).

Minor isomer 5f'.

^{1}H-NMR (300 MHz, $CDCl_3$,*only non-overlapping signals are indicated*): δ = 7.06 (s, 1H), 6.55 (t, *J* = 1.5 Hz, 1H), 3.37 (s, 2H), 3.00–2.92 (m, 2H).

HR-MS *(of the mixture)* (EI) calc. for $C_{24}H_{28}$ $[M]^+$ 316.2191, found 316.2194.



5g/5g'

7-Butyl-4-phenyl-1,2,3,6-tetrahydro-*as*-indacene (5g)

The representative procedure was followed using IPrAuCl (7.0 mg, 5.0 mol%), AgOTf (3.2 mg, 5.5 mol%) and **4g** (67 mg, 0.232 mmol). After 17 h at 50 ºC, purification by flash column

chromatography (hexanes) yielded inseparable indene isomers **5g/5g'** (39 mg, 58% overall yield, *rr* = 4:1) as a colorless oil.

Major isomer 5g. *(* indicates that signals overlap with minor isomer **5g')***

^{1}H-NMR (400 MHz, $CDCl_3$): 7.55–7.49 (m, 2H*), 7.51–7.41 (m, 2H*), 7.41–7.33 (m, 1H*), 7.31 (s, 1H), 6.59 (bs, 1H*), 3.42 (s, 2H), 3.15–3.02 (m, 4H*), 2.57 (t, *J* = 7.4 Hz, 2H*), 2.15 (td, *J* = 7.4, 2.3 Hz, 2H*), 1.67 (p, *J* = 7.8 Hz, 2H*), 1.46 (h, *J* = 7.6 Hz, 2H*), 1.02 (t, *J* = 7.3 Hz, 3H*).

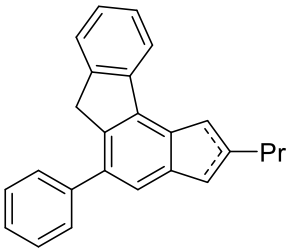
^{13}C-NMR (101 MHz, $CDCl_3$): 151.7 (C), 142.4 (C), 141.8 (C), 140.8 (C), 140.3 (C), 135.7 (C), 133.7 (C), 128.7 (CH), 128.2 (CH), 126.4 (CH), 124.3 (CH), 121.9 (CH), 41.1 (CH_2), 33.0 (CH_2), 31.4 (CH_2), 31.2 (CH_2), 31.2 (CH_2), 26.1 (CH_2), 22.6 (CH_2), 14.0 (CH_3).

Minor isomer 5g'.

^{1}H-NMR (300 MHz, $CDCl_3$, *only non-overlapping signals are indicated*): δ = 7.21 (s, 1H), 3.31 (s, 2H).

^{13}C-NMR (101 MHz, $CDCl_3$, *only non-overlapping signals are indicated*): δ = 150.3 (C), 144.7 (C), 139.4 (C), 137.9 (C), 137.6 (C), 136.6 (C), 126.5 (CH), 126.2 (CH), 118.5 (CH), 39.6 (CH_2), 32.8 (CH_2), 31.1 (CH_2), 26.0 (CH_3).

HR-MS *(of the mixture)* (EI) calc. for $C_{22}H_{24}$ $[M]^+$ 288.1878, found 288.1877.

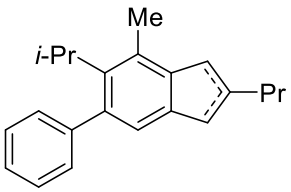


5h/5h'

5-Phenyl-2-propyl-3,6-dihydrocyclopenta[*c*]fluorene (5h)

The representative procedure was followed using Ph_3PAuCl (8.7 mg, 5.0 mol%), AgOTf (5.0 mg, 5.5 mol%) and **4h** (113 mg, 0.350 mmol). After 17 h at 50 ºC, purification by flash column chromatography (hexanes) yielded inseparable indene isomers **5h/5h'** (65 mg, 57% overall *estimated* yield) as a colorless oil.

*The yield given is an estimation since the mixture of indenes **5h/5h'** contains impurities which could not be removed by column chromatography (^{1}H-NMR and ^{13}C-NMR are included, see page 52).*



5i/5i'

5-Isopropyl-4-methyl-6-phenyl-2-propyl-1*H*-indene (5i)

The representative procedure was followed using IPrAuCl (5.3 mg, 5.0 mol%), AgOTf (2.4 mg, 5.5 mol%) and **4i** (50 mg, 0.172 mmol). After 17 h at 50 ºC, purification by flash column chromatography (hexanes) yielded inseparable indene isomers **5i/5i'** (21 mg, 42% overall yield, *rr* = 4:1) as a colorless oil. When the reaction was accomplished with Ph_3PAuCl, a mixture of indenes **5i/5i'** (19 mg, 38% overall yield, *rr* = 2:1) was obtained.

Major isomer 5i. *(* indicates that signals overlap with minor isomer **5i'**)*

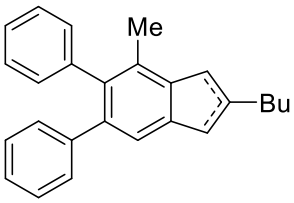
^{1}H-NMR (400 MHz, $CDCl_3$): 7.44–7.29 (m, 5H*), 7.08 (bs, 1H), 6.70 (bs, 1H), 3.45–3.23 (m, 3H*, CH_2 of indene + C$H(CH_3)_2$), 2.59 (s, 3H), 2.58–2.46 (m, 2H*), 1.83–1.61 (m, 2H*), 1.29 (d, *J* = 7.3 Hz, 6H*), 1.02 (t, *J* = 7.4 Hz, 3H*).

^{13}C-NMR (101 MHz, $CDCl_3$): 150.5 (C), 145.8 (C), 144.7 (C), 141.3 (C), 139.6 (C), 138.5 (C), 129.5 (CH), 127.7 (CH), 126.2 (CH), 124.9 (CH), 123.4 (CH), 41.1 (CH_2), 33.6 (CH_2), 30.5 (CH), 22.4 (CH_2), 21.9 (2 x CH_3), 17.1 (CH_3), 14.0 (CH_3) (one aromatic C signal could not be allocated, likely due to overlapping).

Minor isomer 5i'.

^{1}H-NMR (300 MHz, $CDCl_3$, *only non-overlapping signals are indicated*): δ = 6.98 (s, 1H), 6.58–6.46 (m, 1H).

HR-MS *(of the mixture)* (EI) calc. for $C_{22}H_{24}$ $[M]^+$ 288.1878, found 288.1877.



5j/5j'

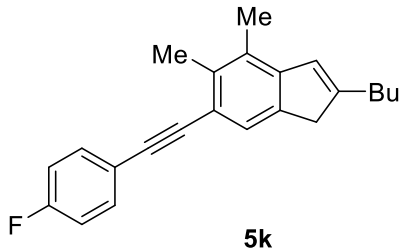
2-Butyl-4-methyl-5,6-diphenyl-1*H*-indene (5j)

The representative procedure was followed using Ph_3PAuCl (5.4 mg, 5.0 mol%), AgOTf (3.0 mg, 5.5 mol%) and **4j** (75 mg, 0.221 mmol). After 17 h at 50 ºC, purification by flash column chromatography (hexanes:EtOAc = 40:1) yielded inseparable indene isomers **5j/5j'** (59 mg, 78% overall yield, *rr* = 1:1) as a colorless oil. When the reaction was accomplished with IPrAuCl, inseparable indene isomers **5j/5j'** (30 mg, 40% overall yield, *rr* = 1:1) was obtained.

^{1}H-NMR *(of the **5j/5j'** mixture)* (400 MHz, $CDCl_3$): 7.38 (s, 1H), 7.31–7.09 (m, 10H+9H), 6.74 (bs, 1H), 6.63 (bs, 1H), 3.49 (bs, 2H), 3.39 (bs, 2H), 2.61 (t, *J* = 7.5 Hz, 2H+2H), 2.28 (s, 3H), 2.22 (s, 3H), 1.77–1.63 (m, 2H+2H), 1.56–1.43 (m, 2H+2H), 1.03 (d, *J* = 7.3 Hz, 3H+3H).

^{13}C-NMR *(of the **5j/5j'** mixture)* (101 MHz, $CDCl_3$): 152.0 (C), 151.7 (C), 144.7 (C), 143.4 (C), 142.3 (C), 141.8 (C), 141.3 (C), 141.2 (C), 139.2 (C), 137.9 (C), 136.7 (C), 131.4 (CH), 131.3 (CH), 130.5 (CH), 128.0 (CH), 127.9 (CH),127.8 (CH), 126.7 (CH), 126.5 (CH), 126.4 (CH), 126.2 (CH), 126.1 (CH), 125.2 (CH), 123.3 (CH), 119.8 (CH), 41.9 (CH_2), 41.1 (CH_2), 31.8 (CH_2), 31.7 (CH_2), 31.6 (CH_2), 31.5 (CH_2), 23.0 (CH_2), 17.8 (CH_3), 17.5 (CH_3), 14.4 (CH_3).

HR-MS *(of the mixture)* (EI) calc. for $C_{26}H_{26}$ $[M]^+$ 338.2035, found 338.2043.



5k

2-Butyl-6-((4-fluorophenyl)ethynyl)-4,5-dimethyl-1*H*-indene (5k)

The representative procedure was followed using Ph_3PAuCl (7.4 mg, 5.0 mol%), AgOTf (4.2 mg, 5.5 mol%) and **4k** (100 mg, 0.32 mmol). After 17 h at 70 ºC, purification by flash column chromatography (hexanes: EtOAc = 10:1) yielded **5k** (35 mg, 35%) as a yellow oil.

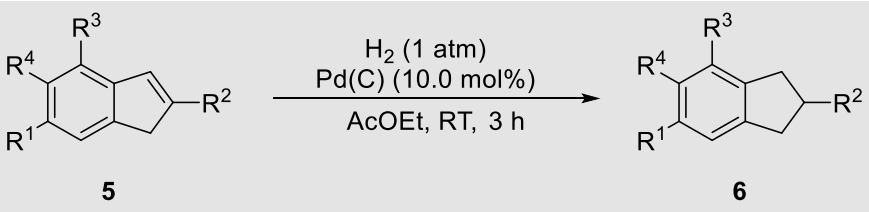
^{1}H-NMR (300 MHz, $CDCl_3$): 7.60–7.48 (m, 2H), 7.41 (s, 1H), 7.06 (t, *J* = 8.7 Hz, 2H), 6.62 (s, 1H), 3.33 (s, 2H), 2.57-2.46 (m, 2H, overlapped signal), 2.51 (s, 3H, overlapped signal), 1.73–1.53 (m, 2H), 1.50–1.31 (m, 2H), 0.97 (t, *J* = 7.3 Hz, 2H).

^{13}C-NMR (75 MHz, $CDCl_3$): δ = 162.6 (d, *J* = 248.7 Hz, C), 152.7 (C), 146.0 (C), 140.3 (C), 137.0 (C), 133.5 (d, *J* = 8.2 Hz), 128.2 (C), 125.2 (CH), 124.8 (CH), 120.64 (d, *J* = 3.5 Hz, C), 118.3 (C), 115.96 (d, *J* = 22.1 Hz, CH), 91.2 (C), 90.6 (C), 41.5 (CH_2), 31.6 (CH_2, two methylene groups), 23.0 (CH_2), 18.0 (CH_3), 16.3 (CH_3), 14.4 (CH_3).

^{19}F-NMR (282 MHz, $CDCl_3$): δ = –112.41 (s).

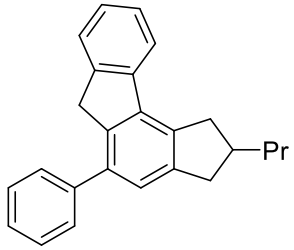
HR-MS (EI) calc. for $C_{23}H_{23}F$ $[M]^+$ 318.1784, found 318.1784.

Palladium-catalysed hydrogenation of 5h-j to indanes 6h-j.



5 **6**

Pd(C) (10 mol%) was added to a solution of the corresponding indene mixture **5/5'** in EtOAc under H_2 atmosphere. The resulting mixture was stirred at ambient temperature for 3 h (TLC analysis). The crude was filtered through a short pad of Celite® and washed with Et_2O (10 mL). Solvents were removed under reduced pressure and the residue was purified by flash column chromatography (hexanes:EtOAc) to yield indanes **6**.



6h

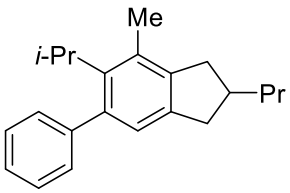
5-Phenyl-2-propyl-1,2,3,6-tetrahydrocyclopenta[c]fluorene (6h)

The representative procedure was followed using Pd(C) (10 mol%, 17 mg), indene mixture **5h/5h'** (50 mg, 0.155 mmol) in EtOAc (5.0 mL). Purification by flash column chromatography (hexanes) yielded indane **6h** (45 mg, 78% overall yield, *rr* = 7:1, mixture of regioisomers from benzyl/phenyl migration). *Only the signals from major isomer are indicated below.*

^{1}H-NMR (400 MHz, $CDCl_3$): 7.88 (d, *J* = 7.7 Hz, 1H), 7.63–7.57 (m, 2H), 7.57–7.50 (m, 3H), 7.46–7.39 (m, 2H), 7.33 (td, *J* = 7.4, 1.2 Hz, 1H), 7.22 (s, 1H), 3.98 (s, 2H), 3.58 (dd, *J* = 15.8, 8.0 Hz, 1H), 3.26–3.14 (m, 1H), 2.98 (dd, *J* = 15.0, 7.9 Hz, 1H), 2.79–2.65 (m, 2H), 1.75–1.59 (m, 2H), 1.60–1.48 (m, 2H), 1.05 (t, *J* = 7.1 Hz, 3H).

^{13}C-NMR (101 MHz, $CDCl_3$): 144.0 (C), 143.9 (C), 142.2 (C), 141.8 (C), 139.1 (C), 137.8 (C), 137.0 (C), 136.5 (C), 128.7 (CH), 128.4 (CH), 126.9 (CH), 126.6 (CH), 126.2 (CH), 124.8 (CH), 123.2 (CH), 122.1 (CH), 40.2 (CH), 38.8 (CH_2), 38.5 (CH_2), 38.2 (CH_2), 36.9 (CH_2), 21.6 (CH_2), 14.4 (CH_3).

HR-MS (EI) calc. for $C_{25}H_{24}$ $[M]^+$ 324.1878, found 324.1875.



6i

5-Isopropyl-4-methyl-6-phenyl-2-propyl-2,3-dihydro-1*H*-indene (6i)

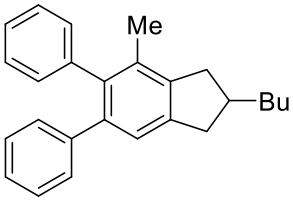
The representative procedure was followed using Pd(C) (10 mol%, 6.6 mg), indene mixture **5i/5i'** (18 mg, 0.062 mmol) in EtOAc (2.0 mL). Purification by flash column chromatography (hexanes) yielded indane **6i** (14 mg, 77%) as a white solid.

m.p. = 149-153 ºC (dec.)

^{1}H-NMR (400 MHz, $CDCl_3$): 7.45–7.34 (m, 3H), 7.32–7.27 (m, 2H), 6.88 (s, 1H), 3.26 (h, *J* = 7.3 Hz, 1H), 3.18–2.96 (m, 2H), 2.79–2.47 (m, 3H), 2.41 (s, 3H), 1.64–1.53 (m, 2H), 1.52–1.42 (m, 2H), 1.27 (d, *J* = 7.3 Hz, 3H), 1.26 (d, *J* = 7.3 Hz, 3H), 0.99 (t, *J* = 7.1 Hz, 3H).

^{13}C-NMR (101 MHz, $CDCl_3$): 144.5 (C), 143.8 (C), 141.1 (C), 140.9 (C), 140.1 (C), 132.5 (C), 129.3 (CH), 127.7 (CH), 126.3 (CH), 124.0 (CH), 39.4 (CH), 39.2 (CH_2), 38.9 (CH_2), 38.5 (CH_2), 30.3 (CH), 21.9 (CH_3), 21.8 (CH_3), 21.6 (CH_2), 17.7 (CH_3), 14.3 (CH_3).

HR-MS (EI) calc. for $C_{22}H_{28}$ $[M]^+$ 292.2191, found 292.2187.



6j

2-Butyl-4-methyl-5,6-diphenyl-2,3-dihydro-1*H*-indene (6j)

The representative procedure was followed using Pd(C) (10 mol%, 16 mg), indene mixture **5j/5j'** (50 mg, 0.148 mmol) in EtOAc (5.0 mL). Purification by flash column chromatography (hexanes:EtOAc = 40:1) to yield indane **6j** (40 mg, 79%) as a white solid.

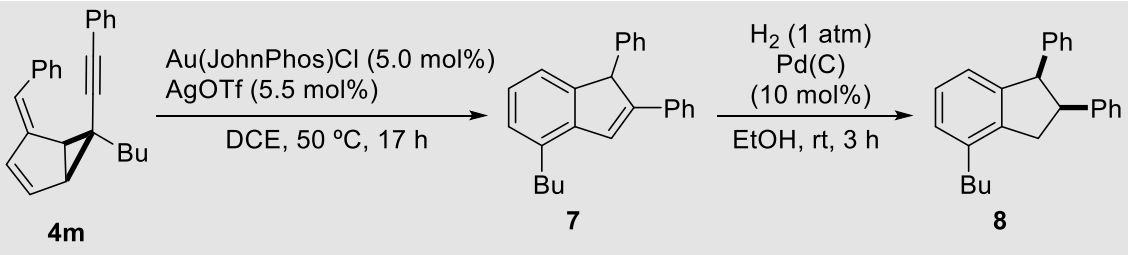
m.p. = 163-166 ºC (dec.)

^{1}H-NMR (400 MHz, $CDCl_3$): 7.32–7.06 (m, 11H), 3.33–3.09 (m, 2H), 2.76 (dd, *J* = 15.7, 8.4 Hz, 1H), 2.70–2.53 (m, 2H), 2.13 (s, 3H), 1.73–1.62 (m, 2H), 1.54–1.37 (m, 4H), 1.01 (t, *J* = 6.9 Hz, 3H).

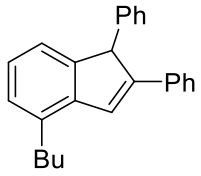
^{13}C-NMR (101 MHz, $CDCl_3$): 142.7 (C), 142.5 (C), 142.3 (C), 140.8 (C), 140.1 (C), 138.5 (C), 132.1 (C), 130.9 (CH), 130.8 (CH), 130.0 (CH), 127.6 (CH), 127.5 (CH), 126.1 (CH), 125.8 (CH), 123.5 (CH), 39.8 (CH), 39.7 (CH_2), 38.8 (CH_2), 36.0 (CH_2), 30.8 (CH_2), 23.0 (CH_2), 17.7 (CH_3), 14.3 (CH_3).

HR-MS (EI) calc. for $C_{26}H_{28}$ $[M]^+$ 340.2191, found 340.2188.

Gold-catalysed rearrangement of 4m to indene 7 and hydrogenation to indane 8.



Under Ar atmosphere, the (JonhPhos)AuCl (8.0 mg, 5.0 mol%) and AgOTf (4.0 mg, 5.5 mol%) were dissolved in DCE (1 mL) and stirred for 10 min. Then, a stock solution of **4m** (100 mg, 0.308 mmol, 2 mL) was added and the resulting mixtures was stirred at 50 ºC for 17 h. Solvent was removed and the residue was purified by flash column chromatography in SiO_2 (hexanes) to yield **7** (52 mg, 52%) as colorless oil.



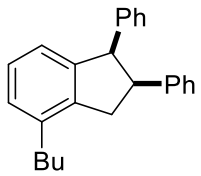
8

4-Butyl-1,2-diphenyl-1*H*-indene (8).

^{1}H-NMR (300 MHz, $CDCl_3$): δ = 7.59–7.52 (m, 2H), 7.49 (d, *J* = 1.6 Hz, 1H), 7.33–7.15 (m, 8H), 7.11–7.02 (m, 3H), 4.99 (d, *J* = 1.5 Hz, 1H), 2.99–2.74 (m, 2H), 1.82–1.65 (m, 2H), 1.55–1.41 (m, 2H), 1.01 (t, *J* = 7.3 Hz, 3H).

^{13}C-NMR (75 MHz, $CDCl_3$): δ = 149.74 (C), 149.69 (C), 142.1 (C), 140.7 (C), 136.0 (C), 135.7 (C), 129.3 (CH), 128.9 (CH), 128.3 (CH), 127.7 (CH), 127.6 (CH), 127.1 (CH), 126.7 (CH), 126.1 (CH), 121.9 (CH), 56.9 (CH), 34.1 (CH_2), 33.4 (CH_2), 23.1 (CH_2), 14.6 (CH_3) (a signal corresponding to a C(sp^2)–H is overlapping).

HR-MS (EI) calc. for $C_{25}H_{24}$ $[M]^+$ 324.1878, found 324.1875.



9

(*1R*,2S)-4-butyl-1,2-diphenyl-2,3-dihydro-1*H*-indene (9)**:

Pd(C) (10 mol%, 12 mg) was added to a solution of indene **8'** (38 mg, 0.111 mmol) in EtOAc (4.0 mL) under H_2 atmosphere. The resulting mixture was stirred at ambient temperature for 3 h (TLC analysis). The crude was filtered through a short pad of Celite® and washed with Et_2O (10

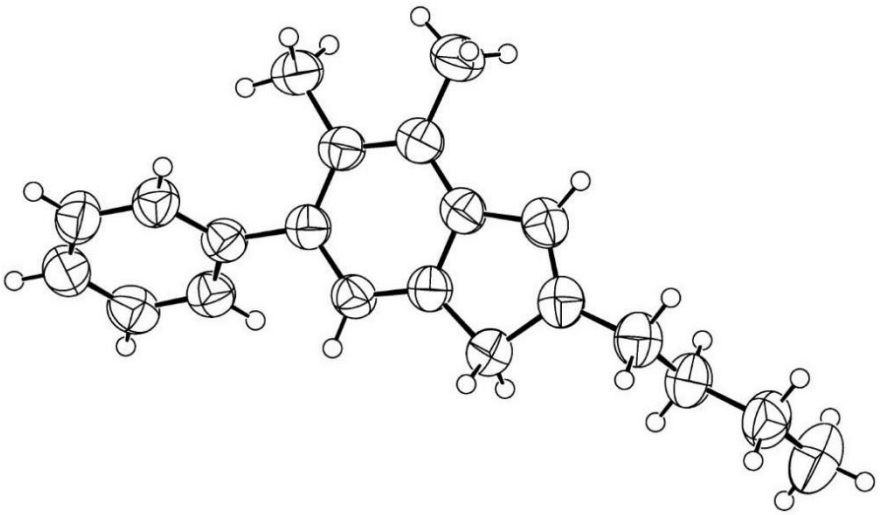
mL). Solvents were removed under reduced pressure and the residue was purified by flash column chromatography (hexanes) to yield indane **8** (25 mg, 69%) as a colorless oil.

^{1}H-NMR (600 MHz, $CDCl_3$): δ = 7.21 (t, *J* = 7.4 Hz, 1H), 7.15 (d, *J* = 7.5 Hz, 1H), 7.10–7.03 (m, 6H), 7.01 (d, *J* = 7.3 Hz, 1H), 6.91–6.80 (m, 2H), 6.67–6.60 (m, 2H), 4.71 (d, *J* = 8.2 Hz, 1H), 4.06 (q, *J* = 8.1 Hz, 1H), 3.35 (dd, *J* = 15.6, 8.4 Hz, 1H), 3.29 (dd, *J* = 15.7, 7.6 Hz, 1H), 2.76 (dd, *J* = 7.9, 7.8 Hz, 2H), 1.89–1.65 (m, 2H), 1.49 (h, *J* = 7.4 Hz, 2H), 1.02 (t, *J* = 7.4 Hz, 3H).

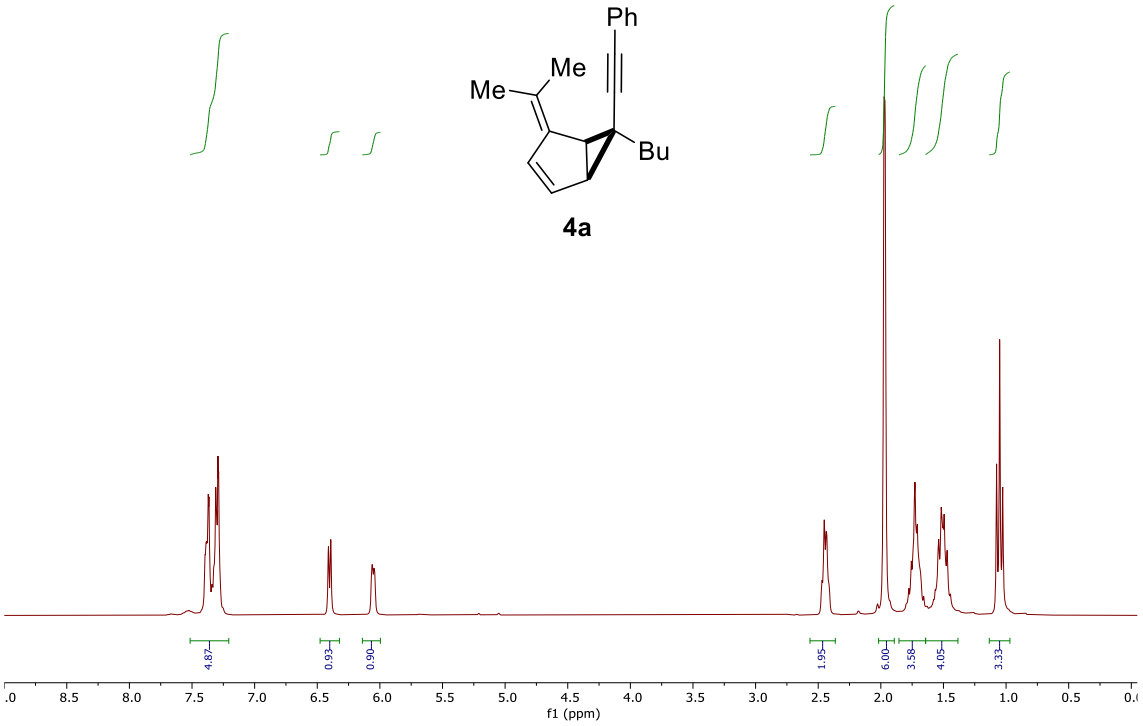
^{13}C-NMR (150 MHz, $CDCl_3$): δ = 145.4 (C), 142.3 (C), 141.5 (C), 141.0 (C), 138.6 (C), 129.1 (CH), 128.5 (CH), 127.6 (CH), 127.1 (CH), 127.0 (CH), 126.02 (CH), 125.98 (CH), 122.9 (CH), 57.1 (CH), 51.7 (CH), 35.4 (CH_2), 33.4 (CH_2), 32.7 (CH_2), 22.7 (CH_2), 14.1 (CH_3) (a signal corresponding to a C(sp^2)–H is overlapping)

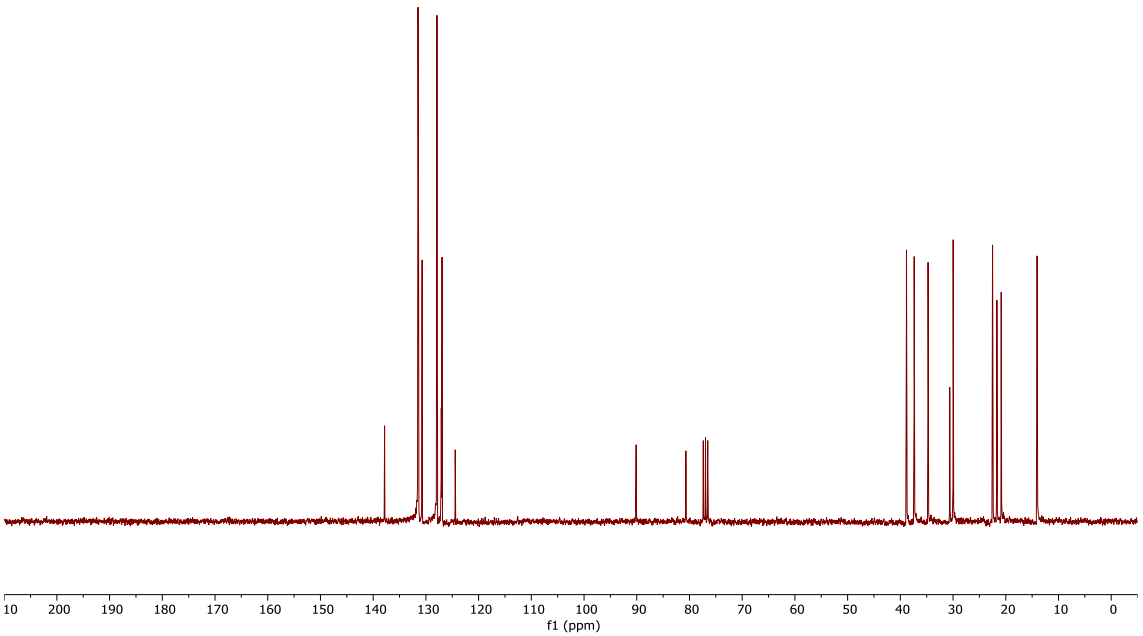
HR-MS (EI) calc. for $C_{25}H_{26}$ $[M]^+$ 326.2035, found 326.2034.

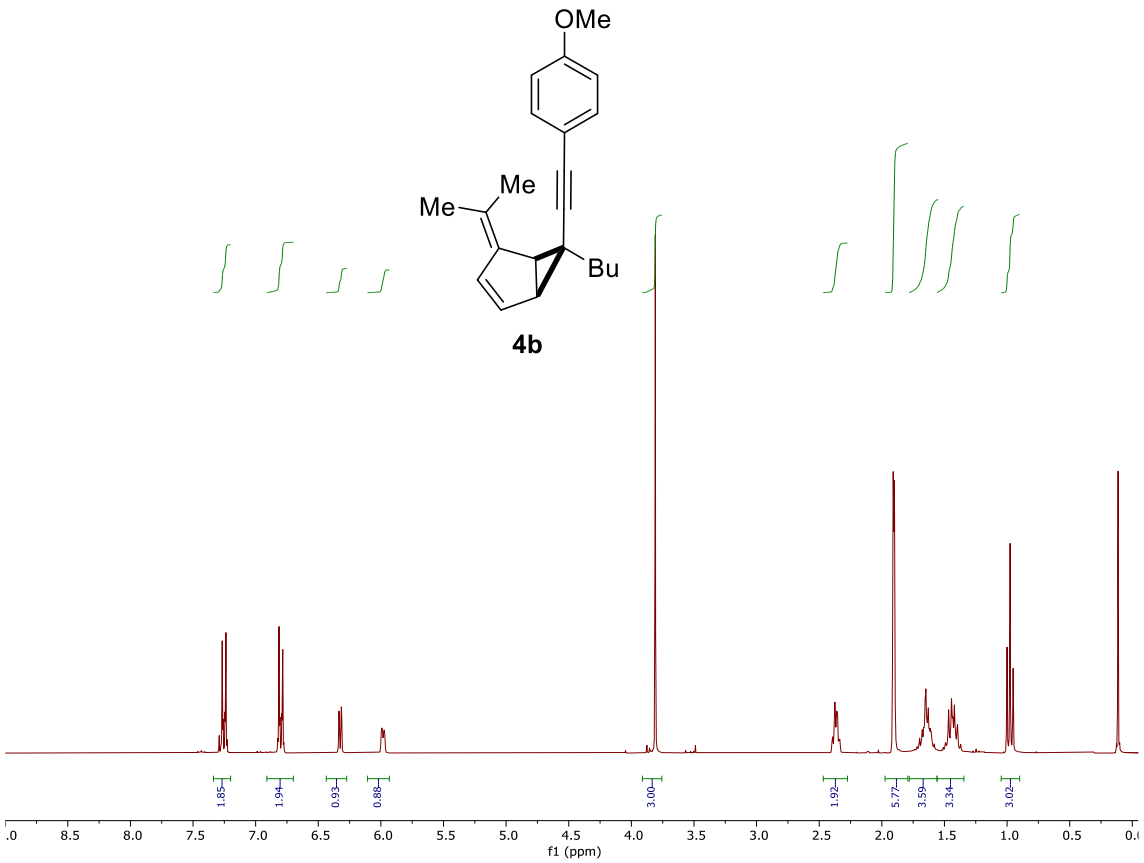
Crystallographic data for compound 5a.



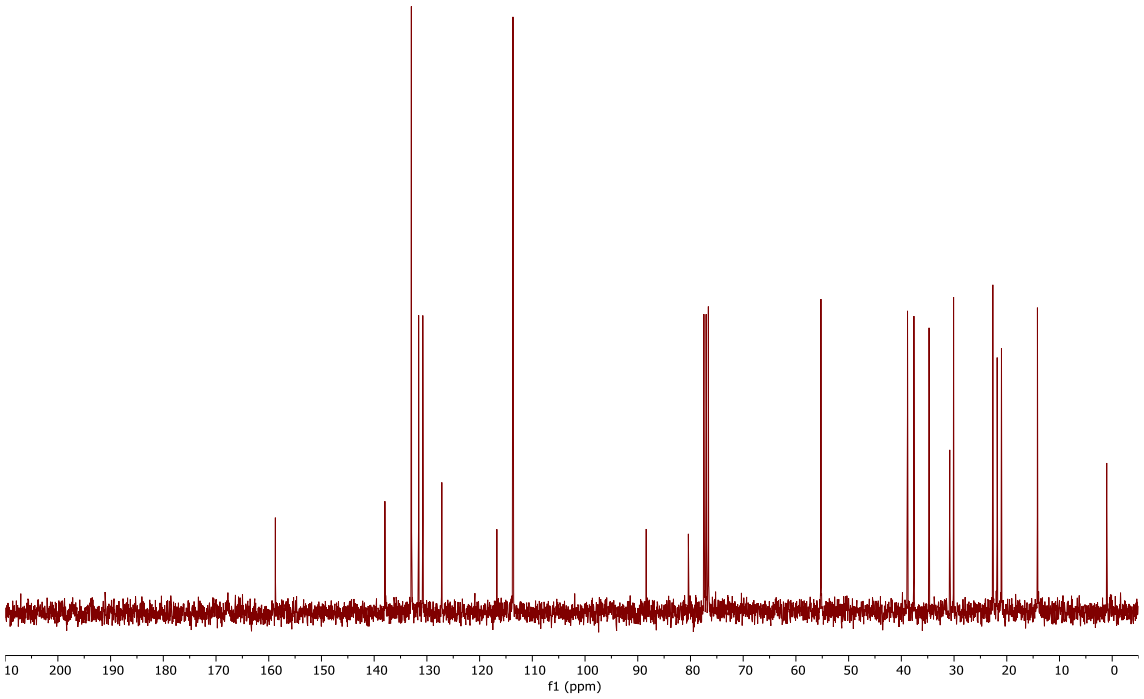
5a: empirical formula C21H24, M_r = 276.40, T = 294.0 (2) K, λ = 1.54184 Å, crystal system, space group: triclinic, *P-1*, unit cell dimensions: a = 9.9636 (14), b = 12.0181 (13), c = 14.0409 (16) Å, α = 85.976 (9)º , β = 84.279 (10)º , γ = 83.003 (10)º, V = 1657.6 (4) Å^3, Z = 4, ρ_{calcd} = 1.108 Mgm^{-3}, μ = 0.459 mm^{-1}, F(000) = 600, crystal size: 0.440 x 0.129 x 0.109 mm, θ range data collection: 3.169-74.019º, index ranges: -12≤*h*≤9, -14≤*k*≤12, -16≤*l*≤17, reflections collected/unique = 12141/6437, R_{int} = 0.0254, completeness to 2θ = 70.000 (98.40%), absorption correction: semiempirical from equivalents, max. and min. transmission = 1.0000 and 0.8631, refinement method: full matrix least-squares on F^2, data/restraints/parameters = 6437/0/379, goodness-of-fit on F^2 = 1.066, final R indices [I>2σ(I)]: R_1 = 0.0560, wR_2 = 0.1768, R indices (all data): R_1 = 0.0767, wR_2 = 0.1983, largest difference peak and hole = 0.279 and – 205 eÅ^{-3}. Deposit number: CCDC2173325.

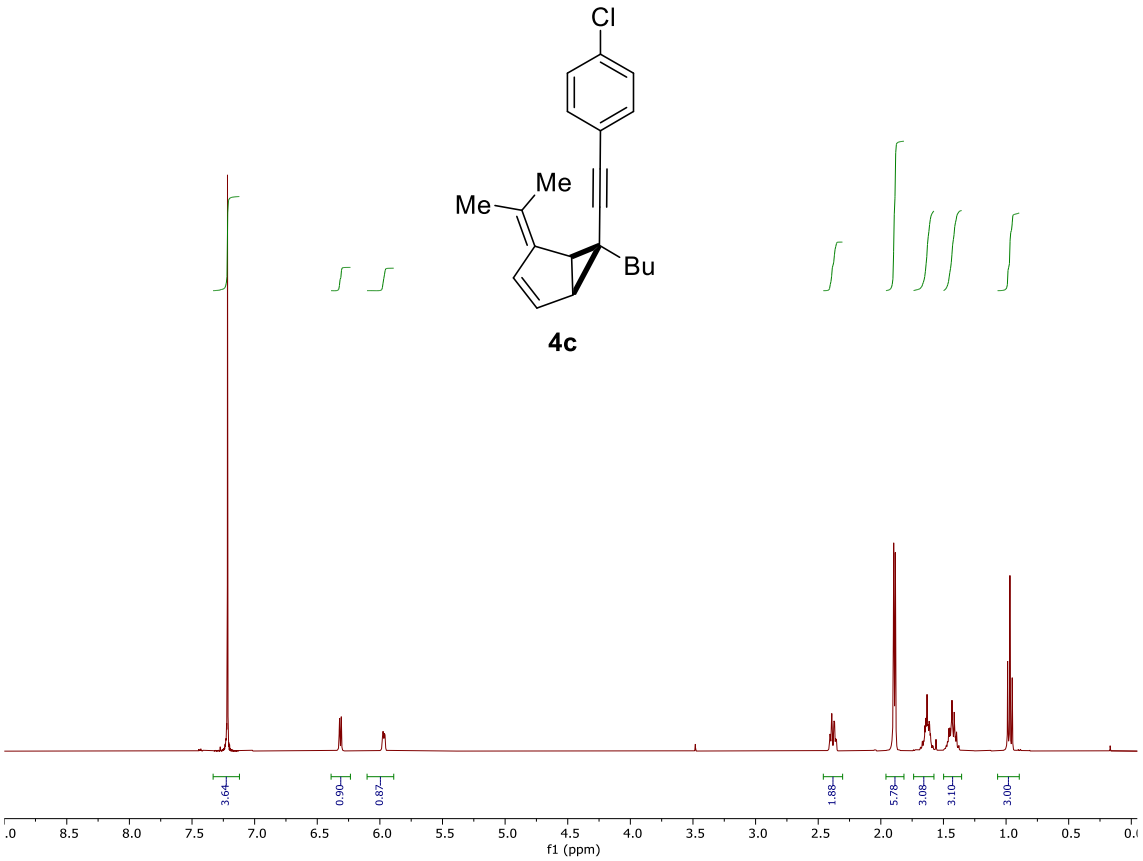




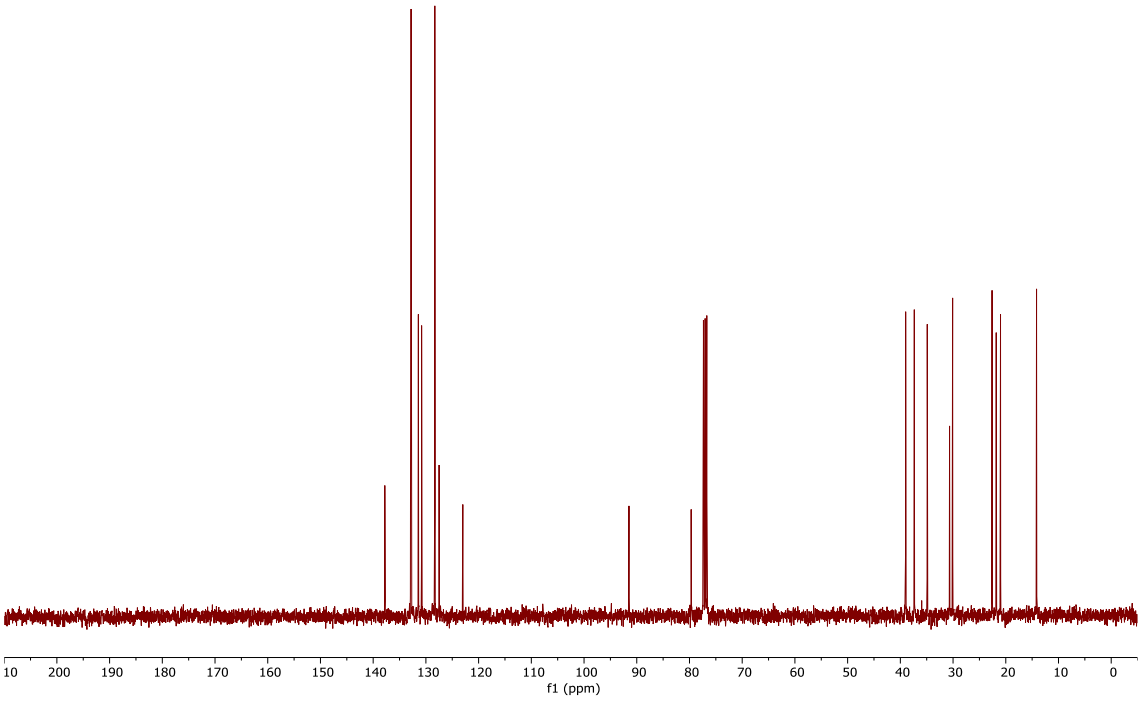


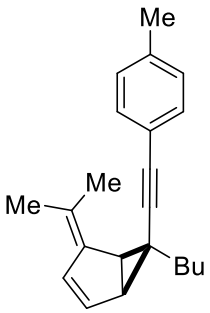
4b



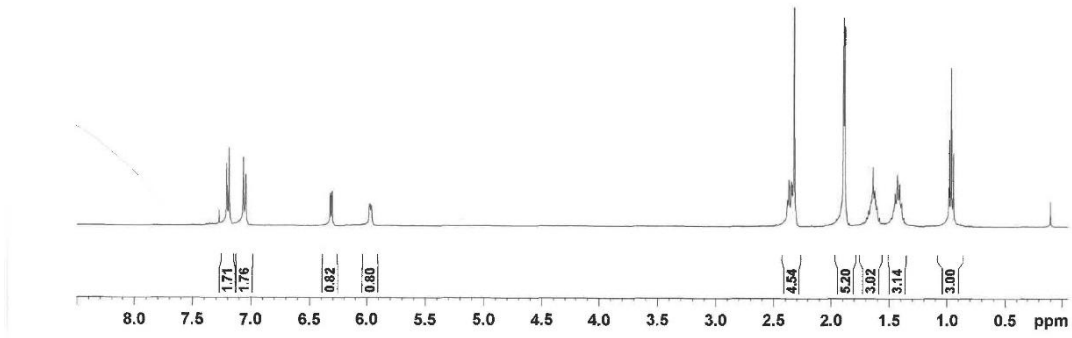


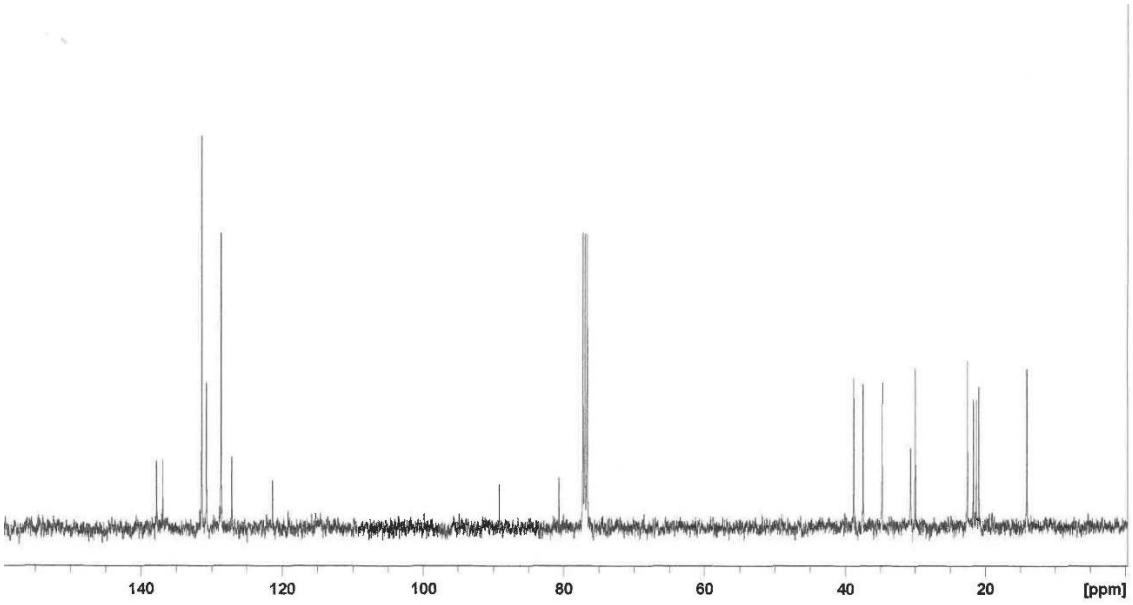
4c

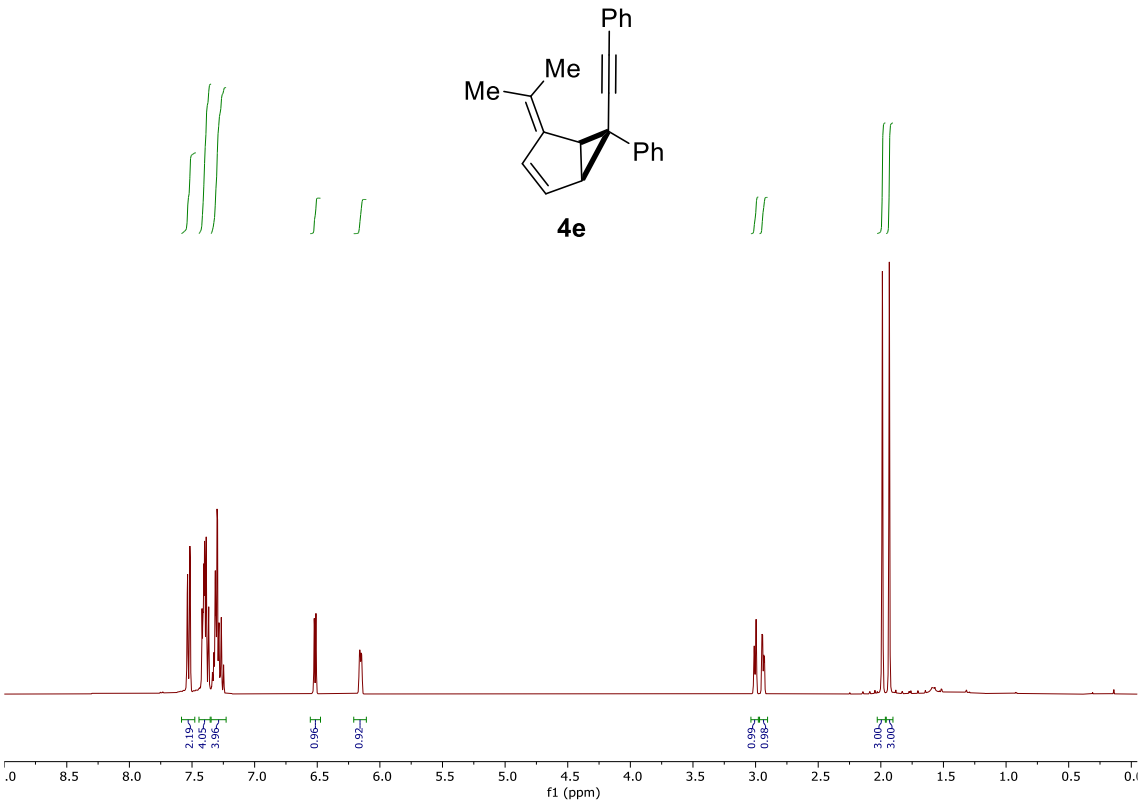


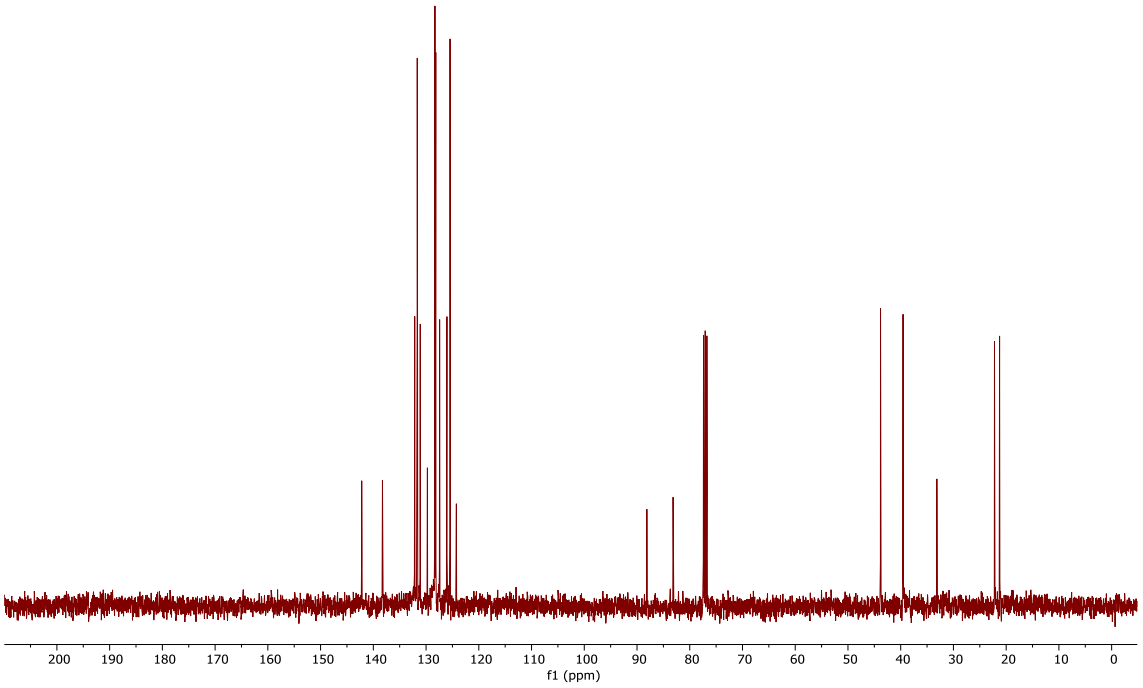


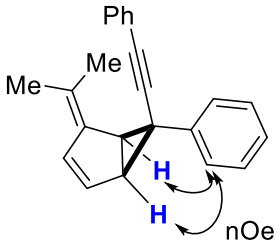
4d



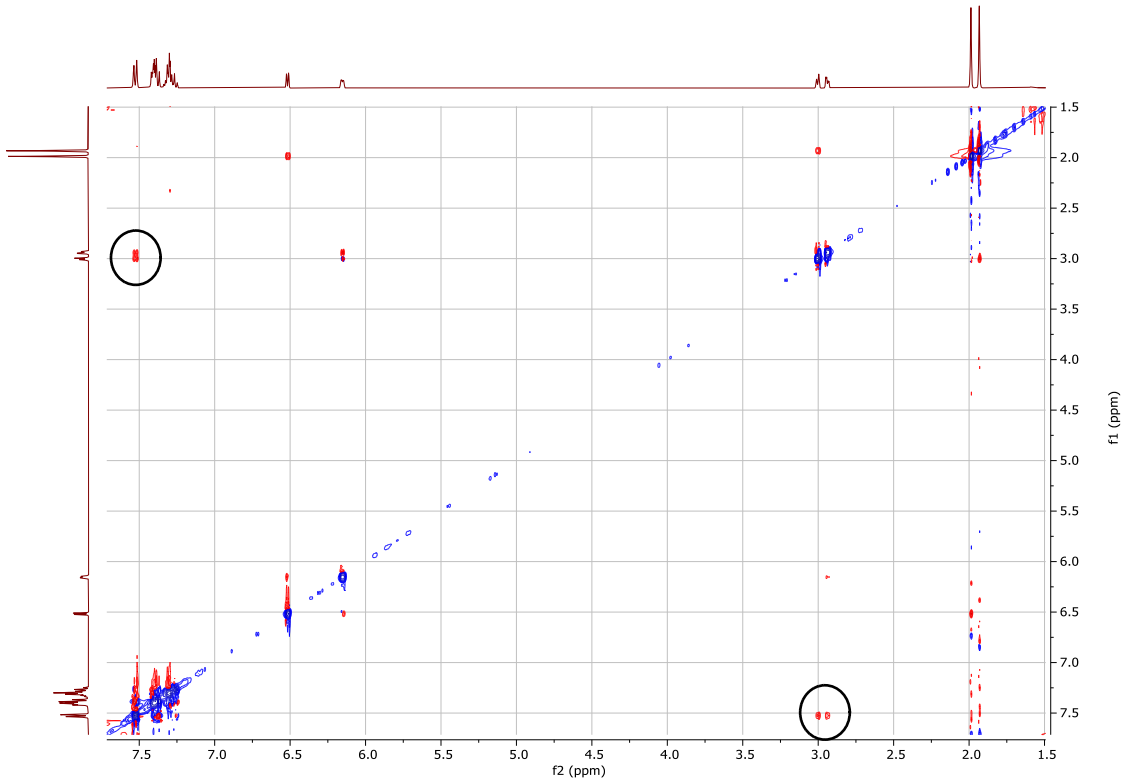


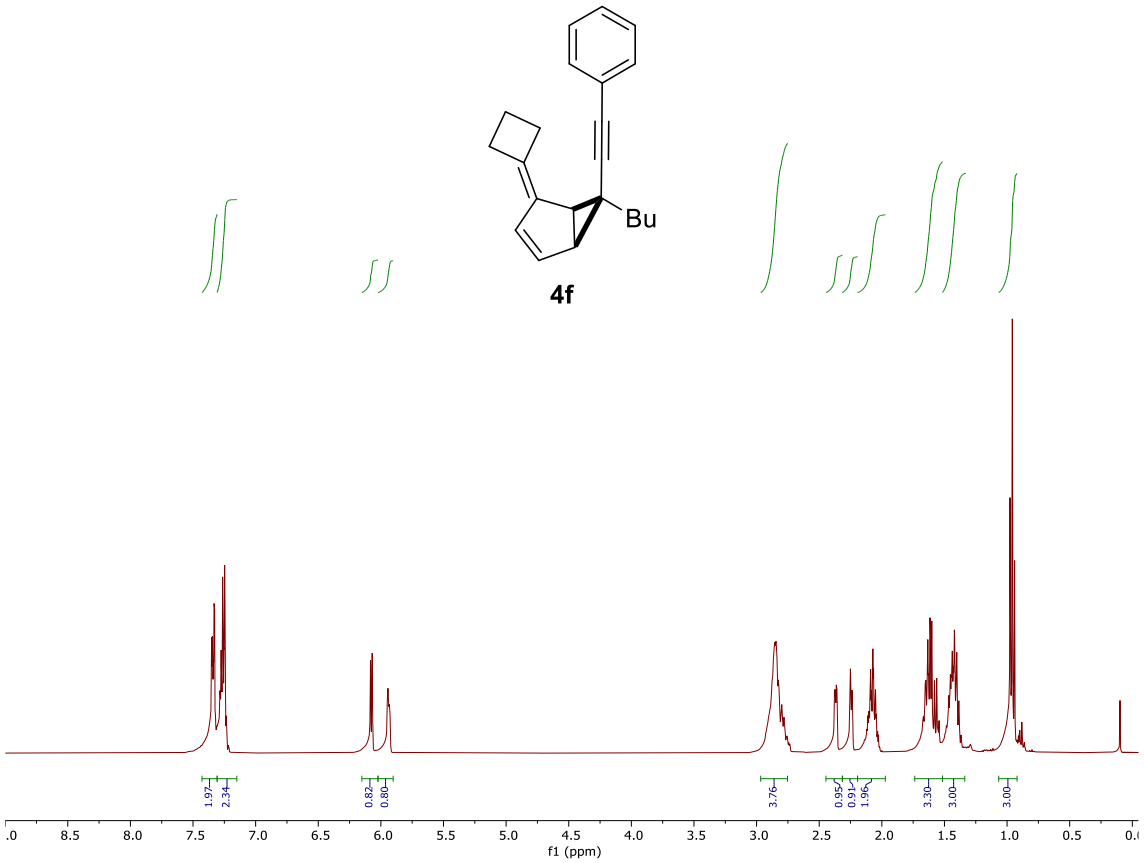


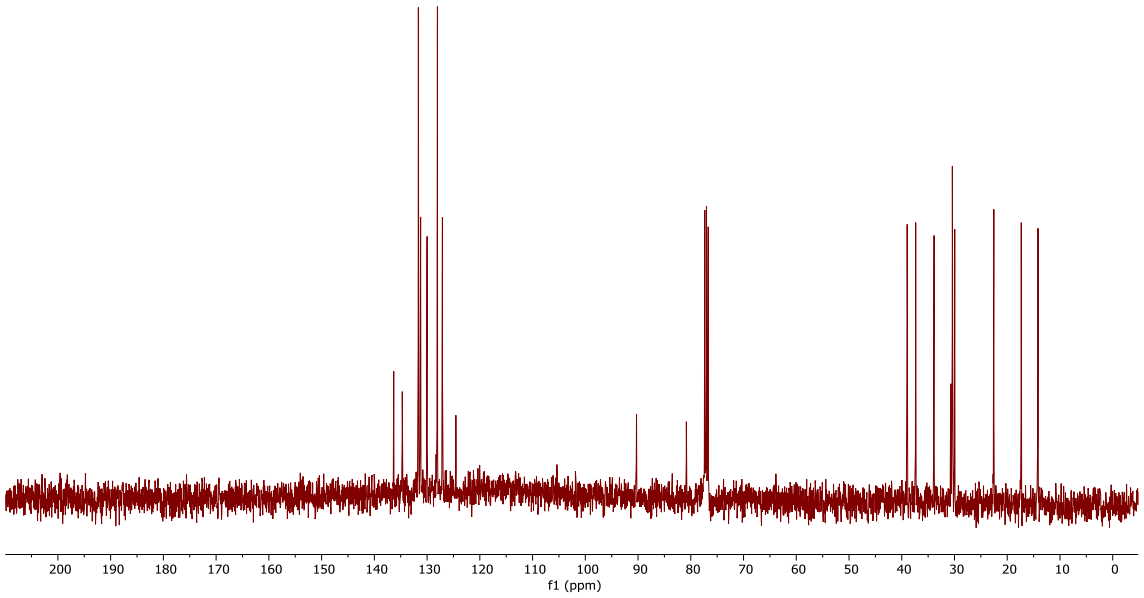


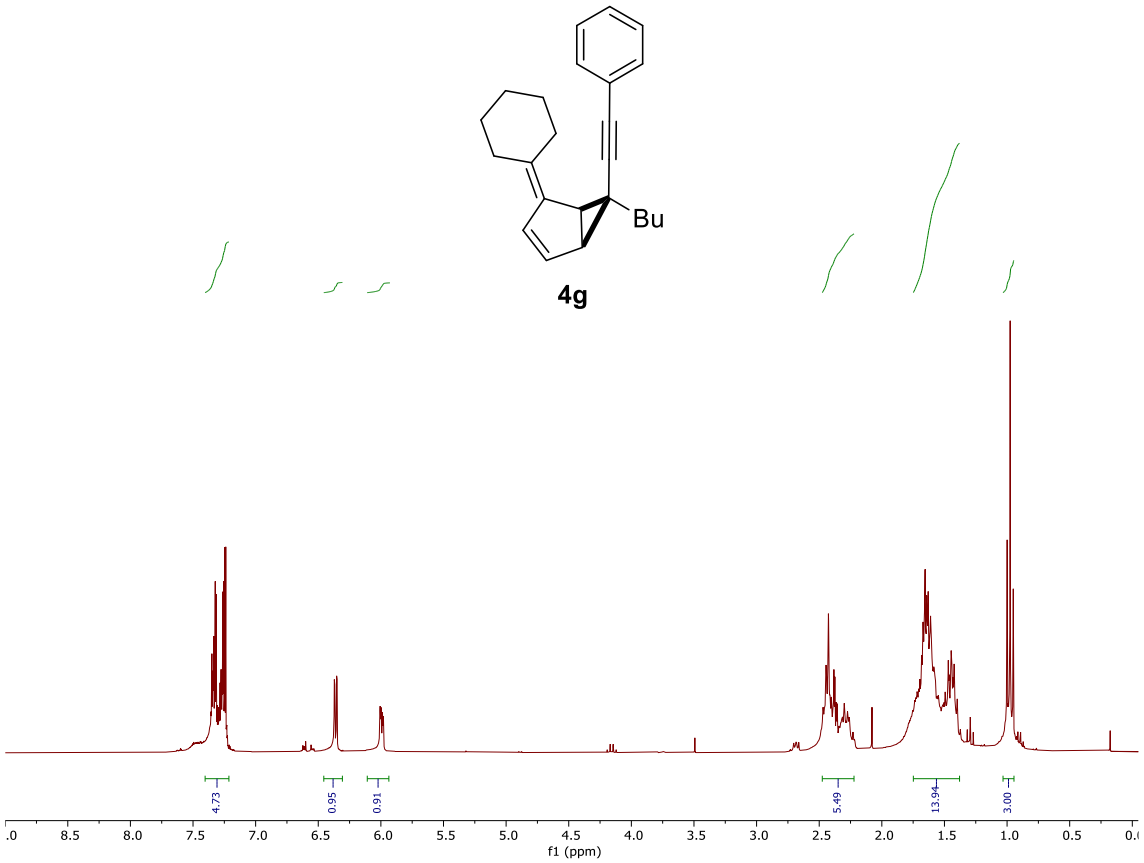


4e

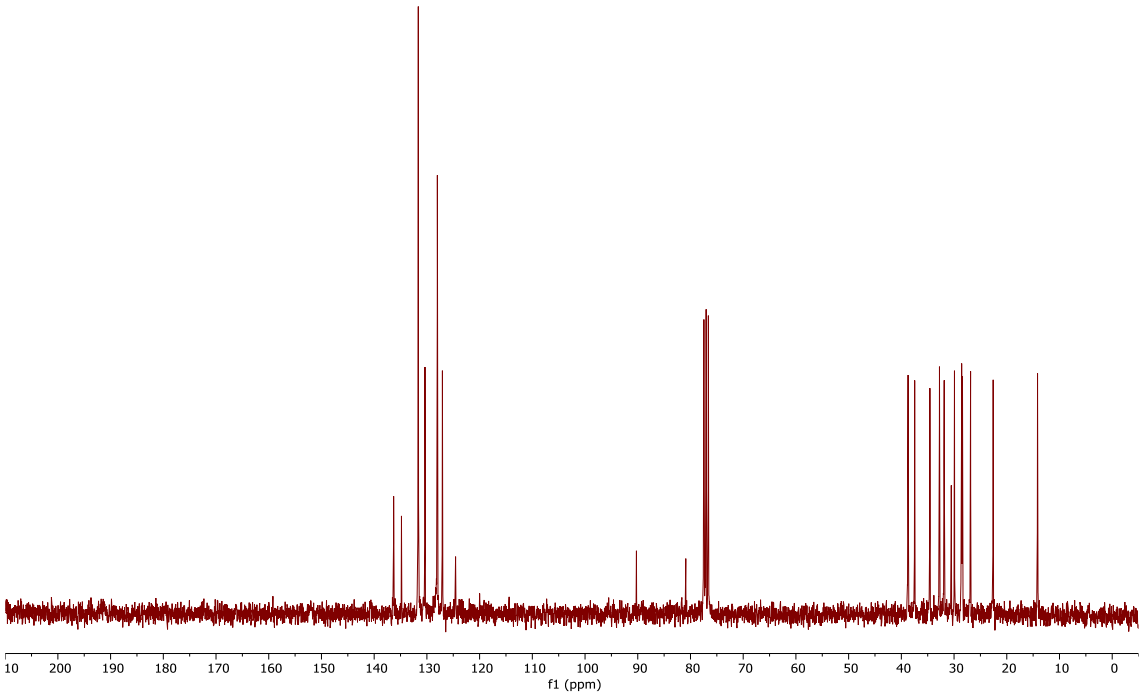


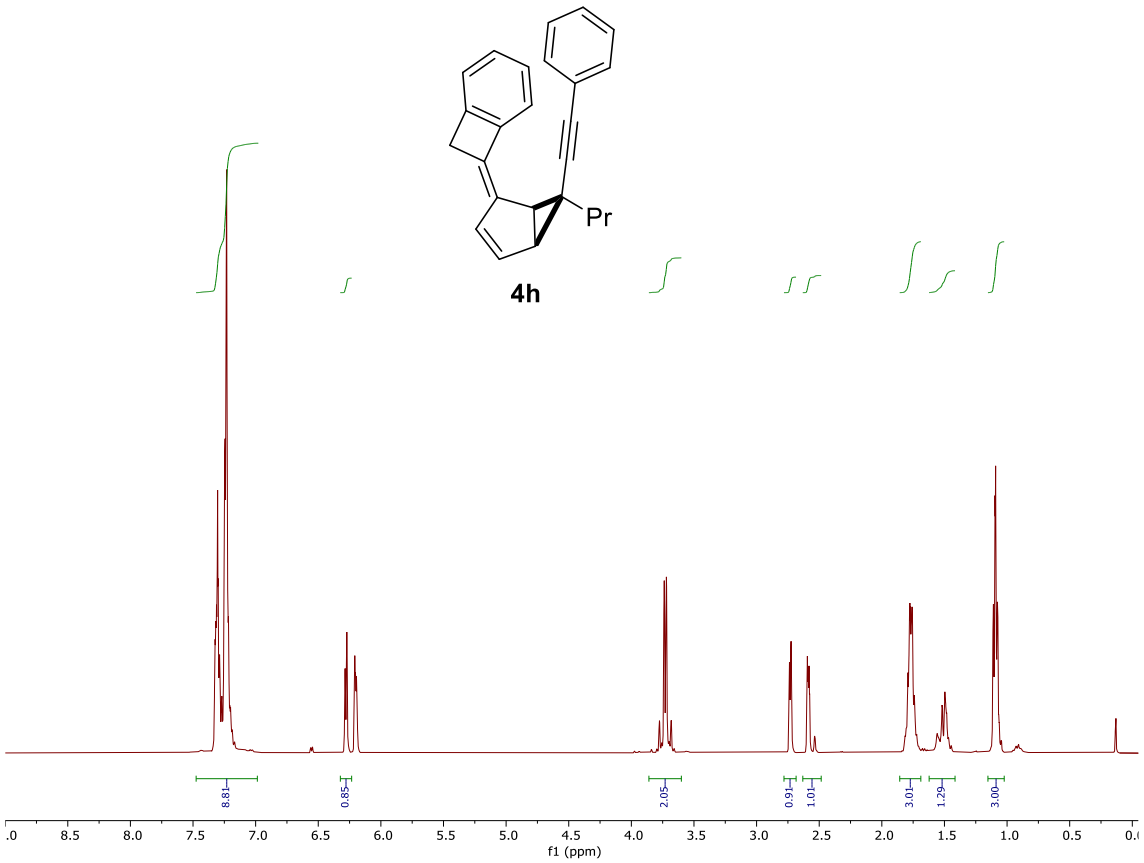


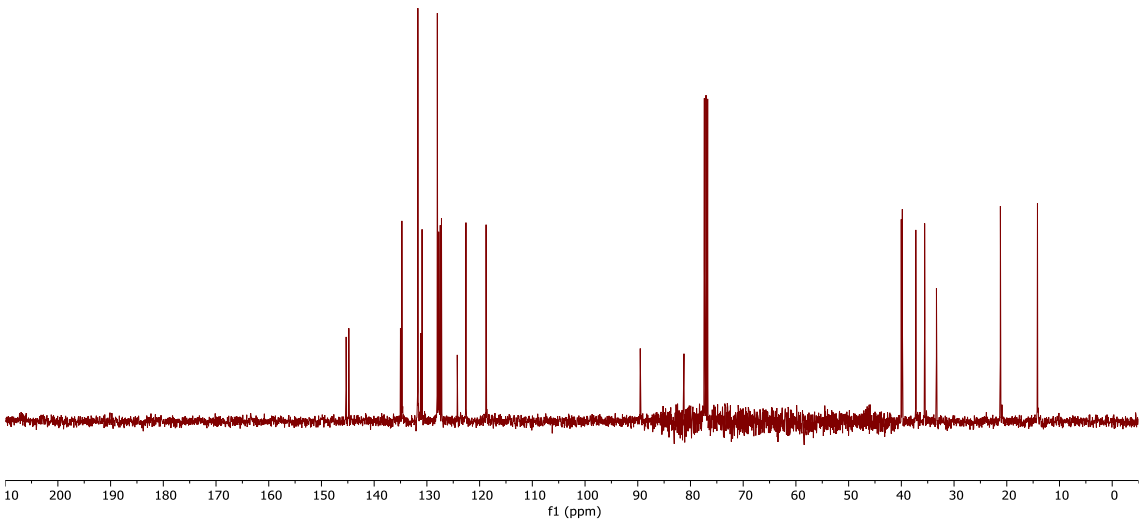


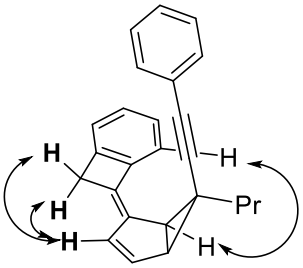


4g

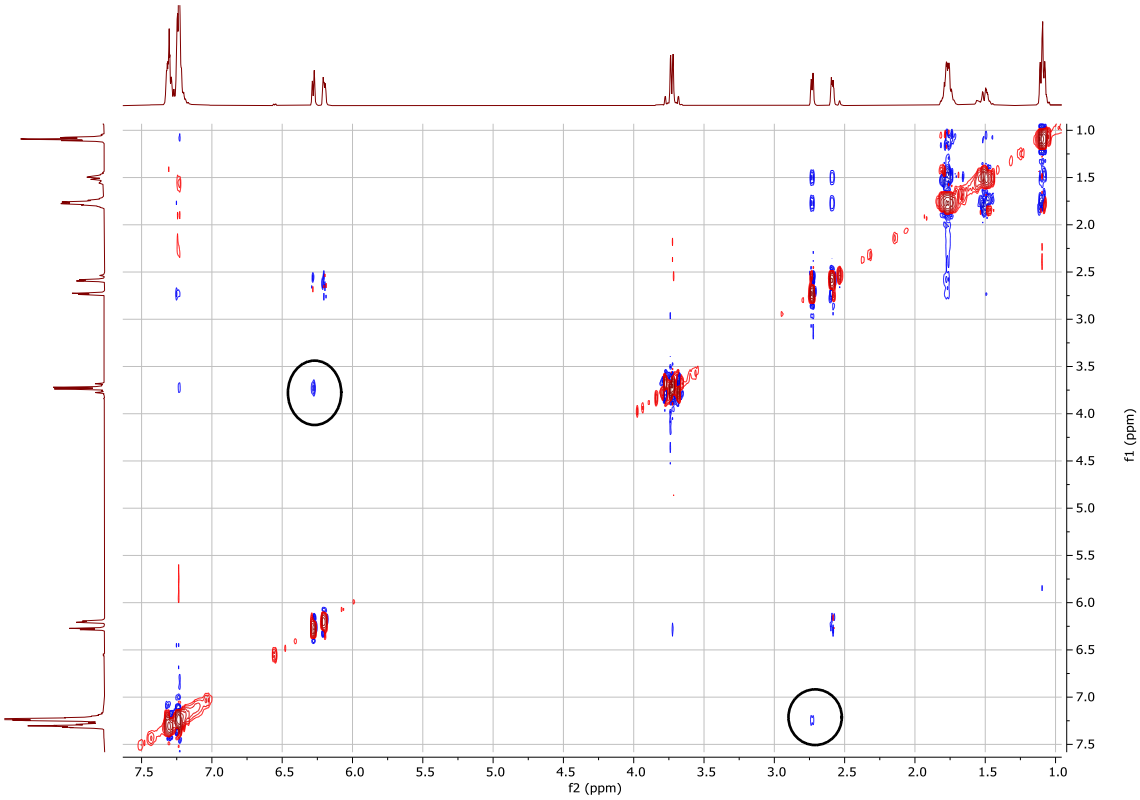


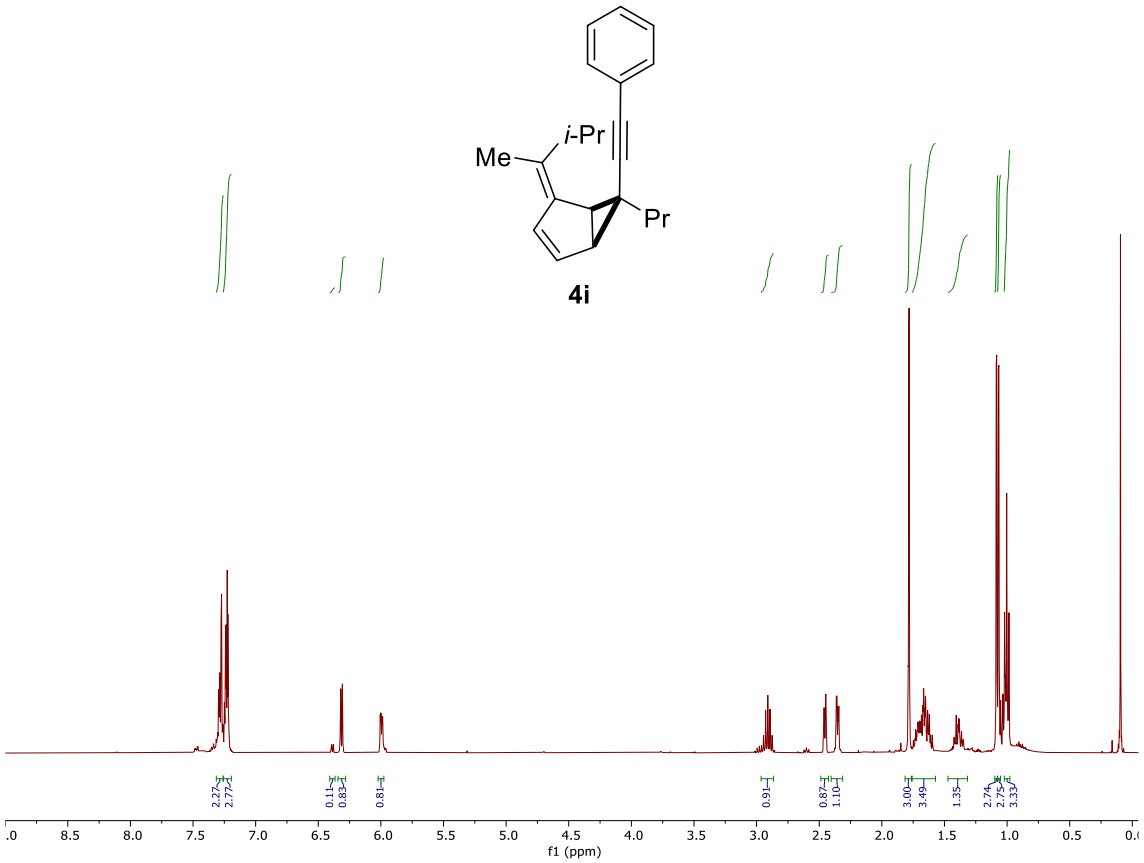


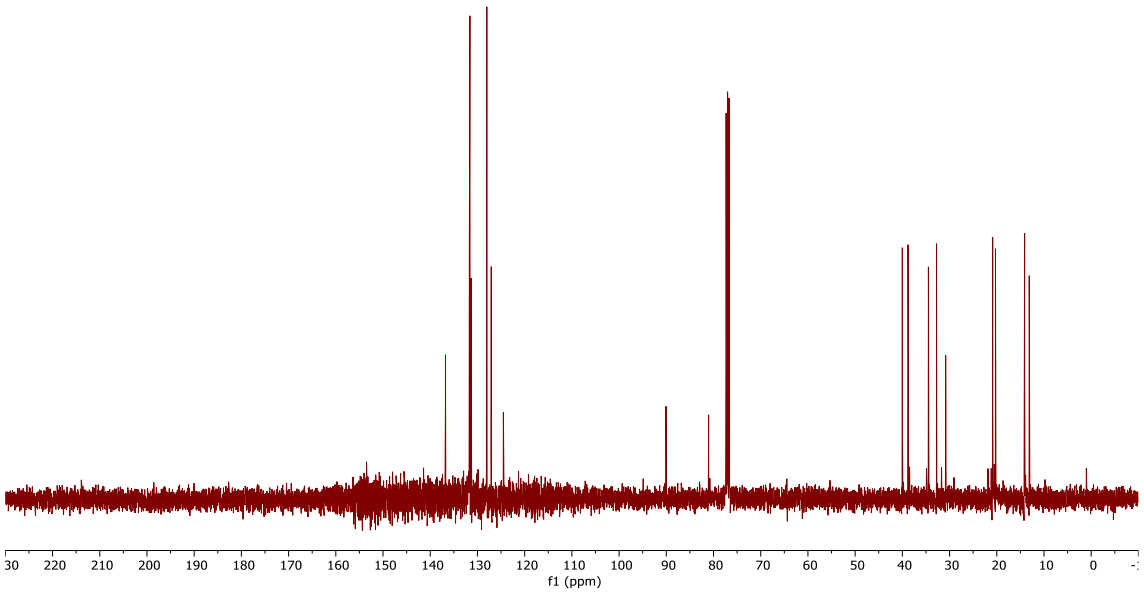


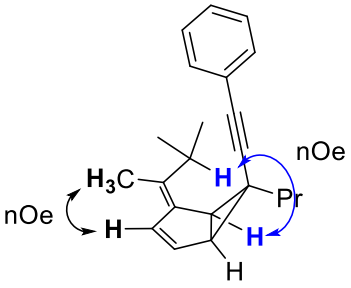


4h

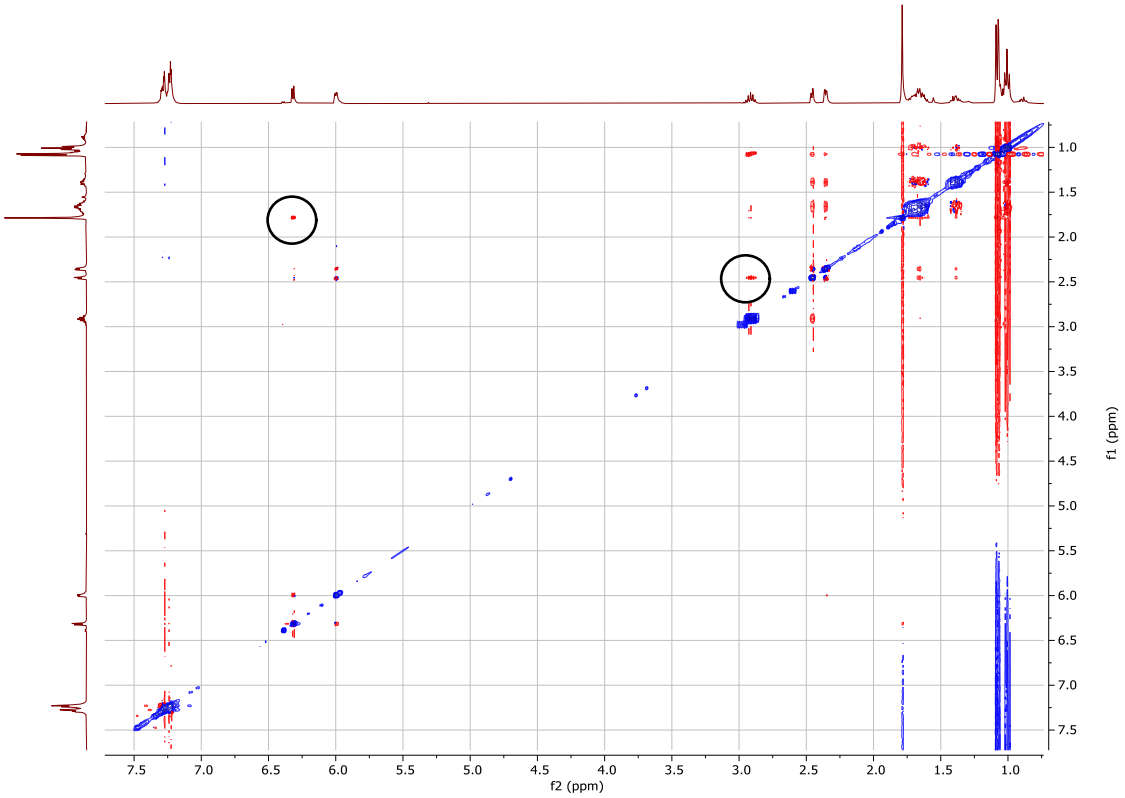


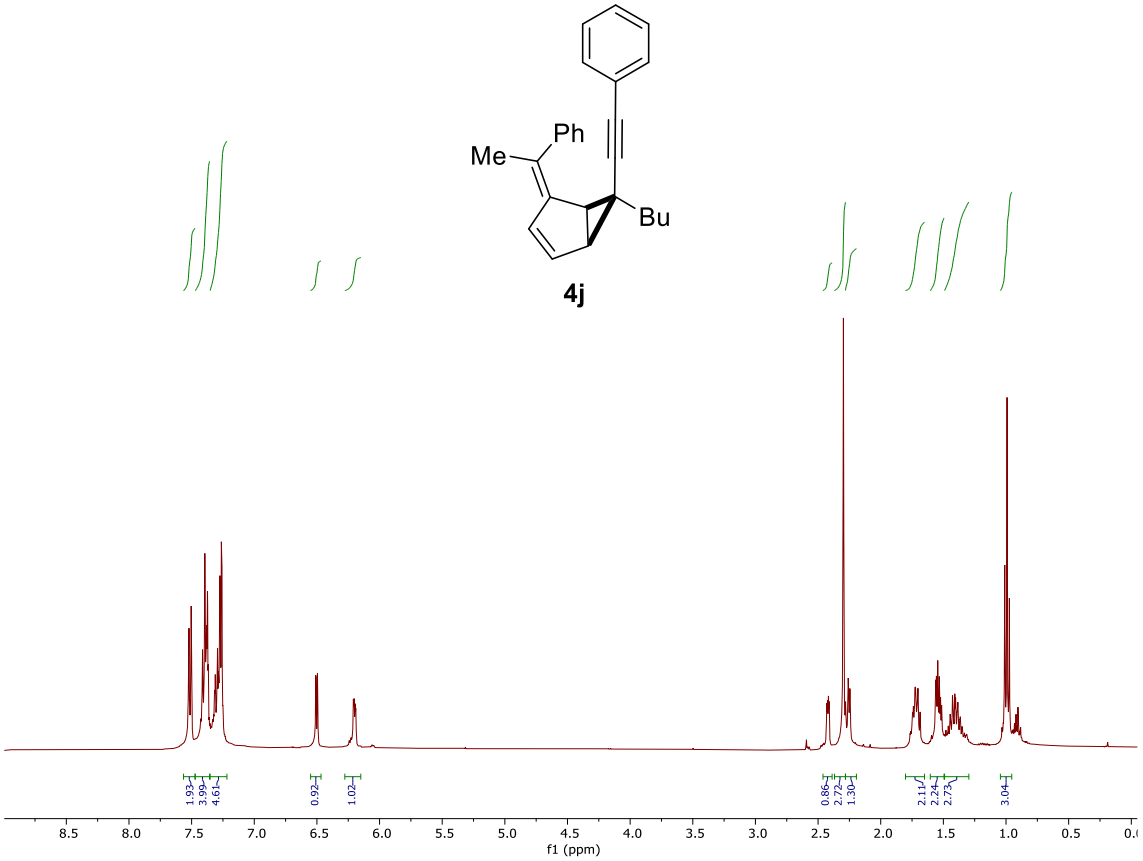




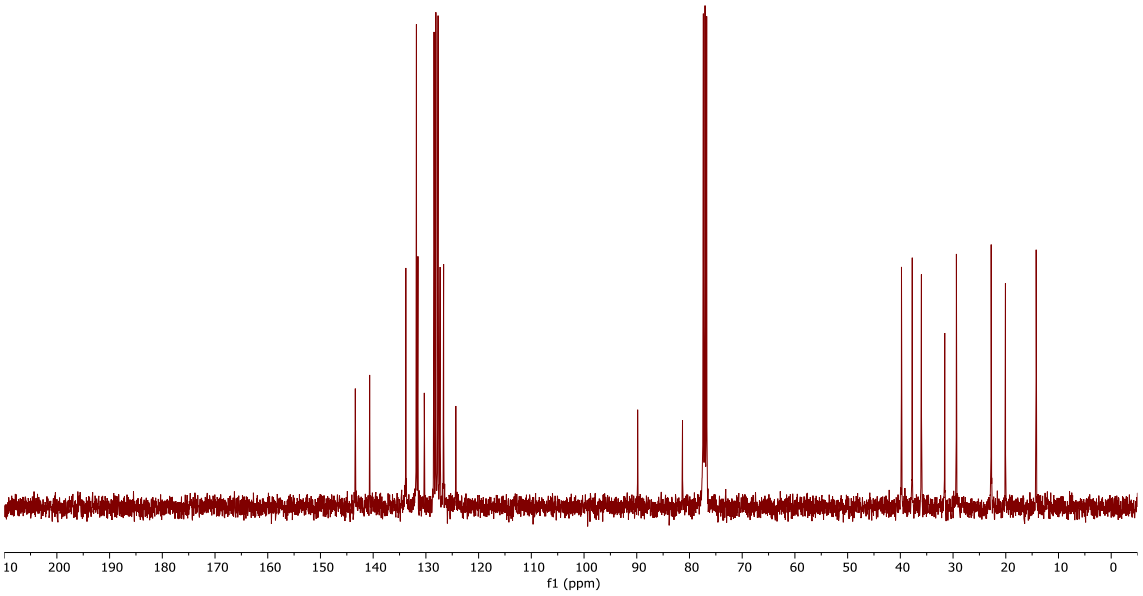


4i

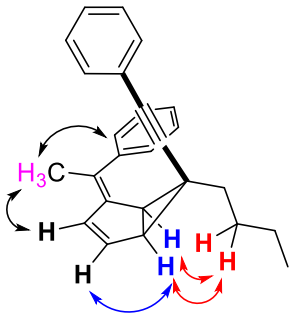




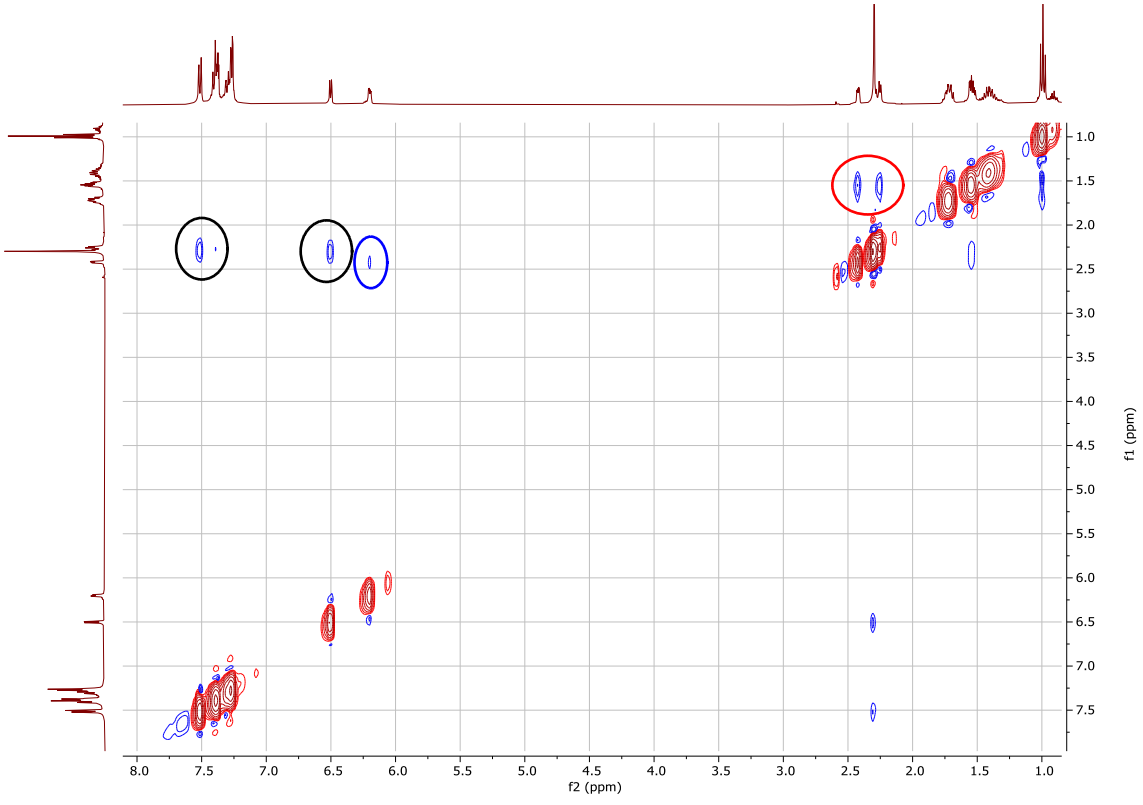
4j

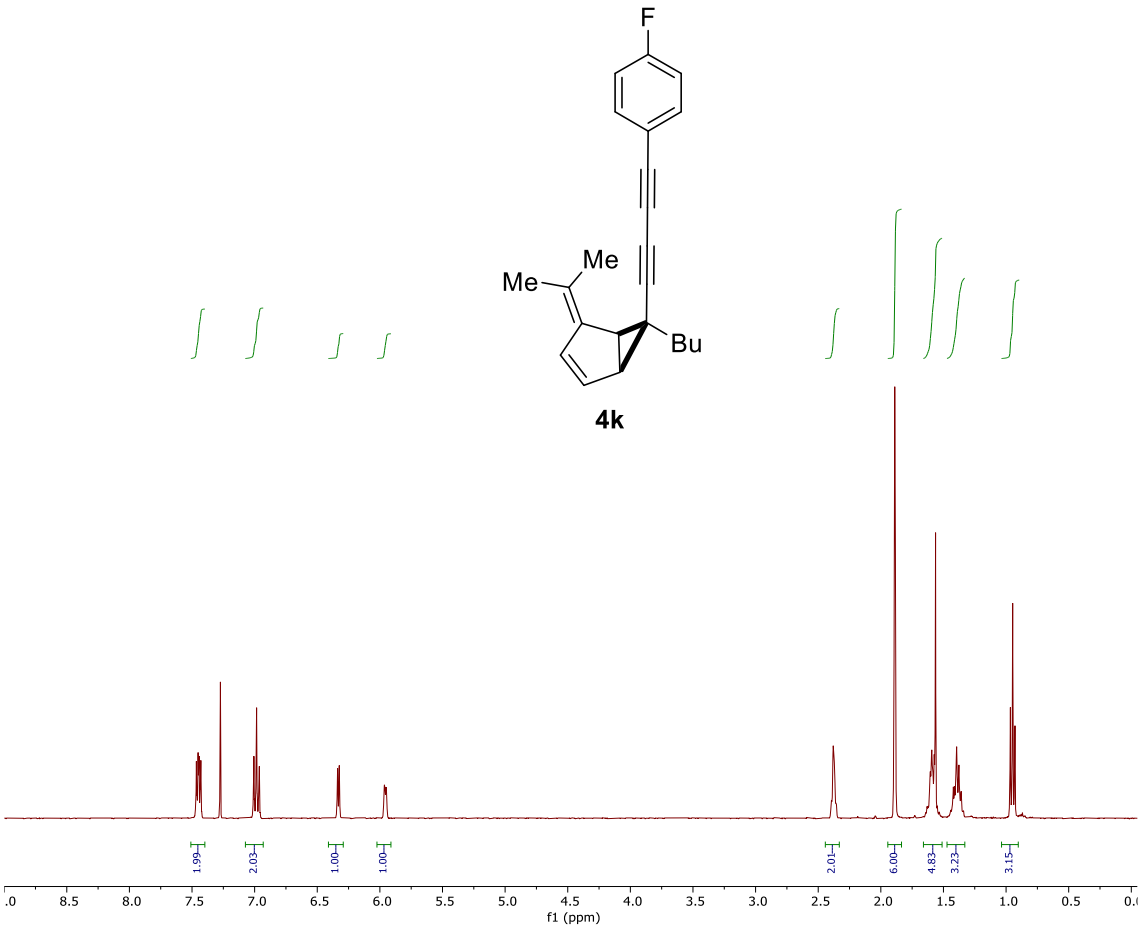


Observed nOe

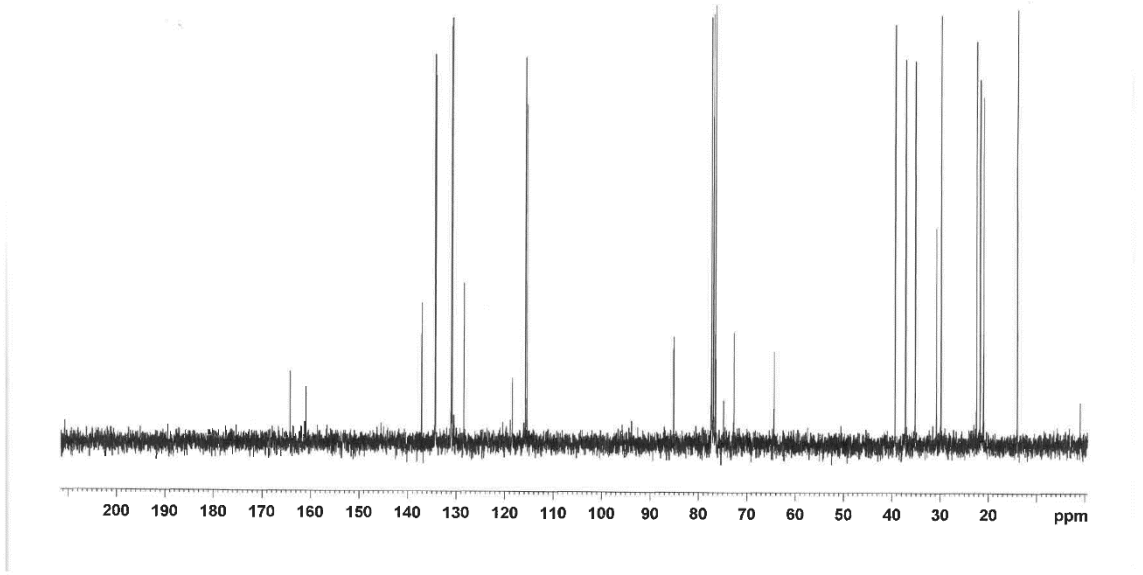


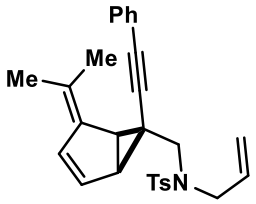
4j



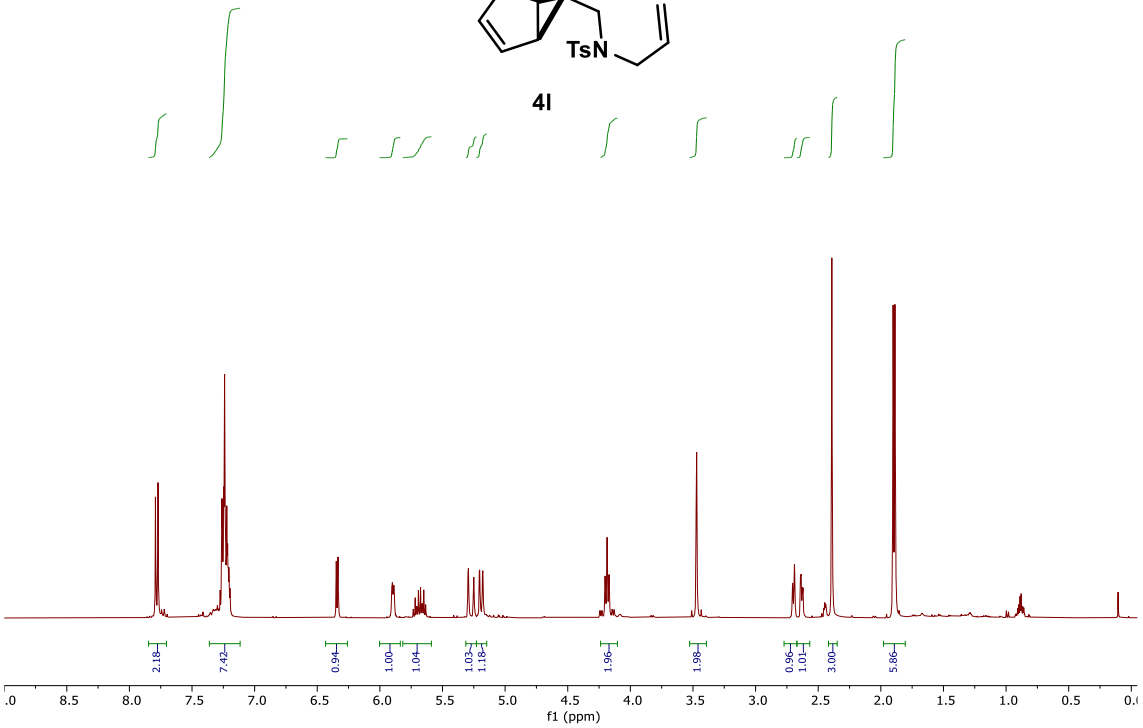


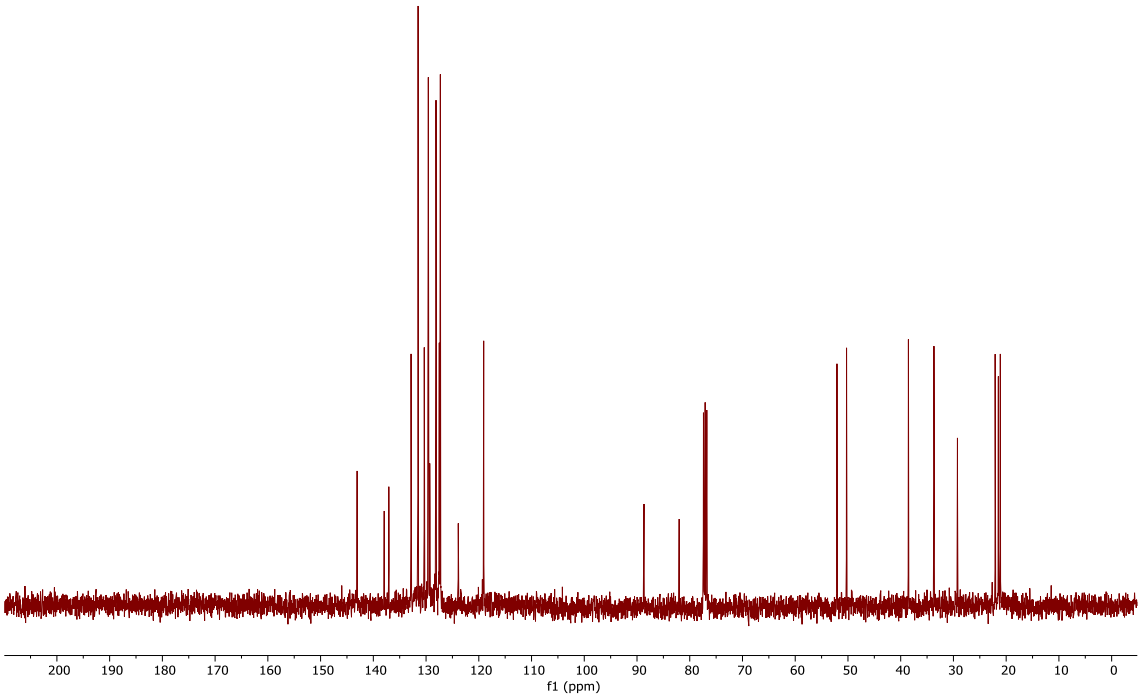
4k

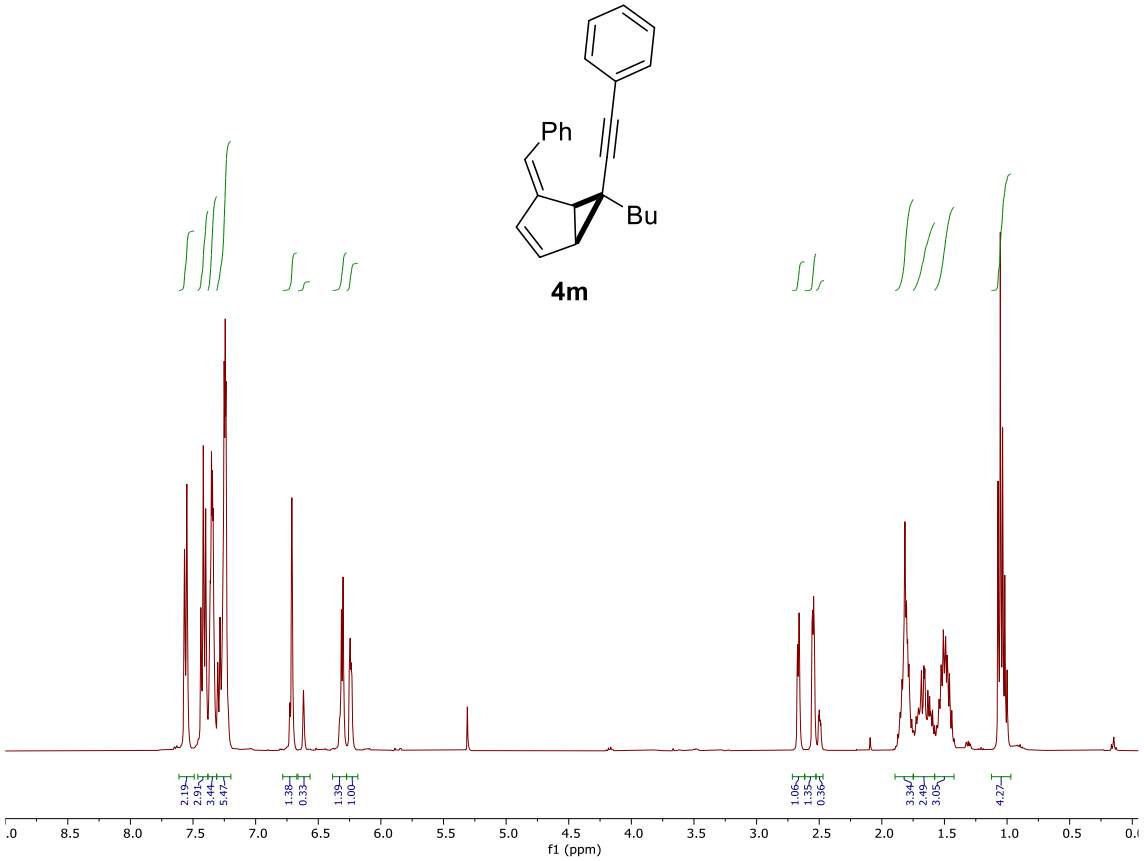


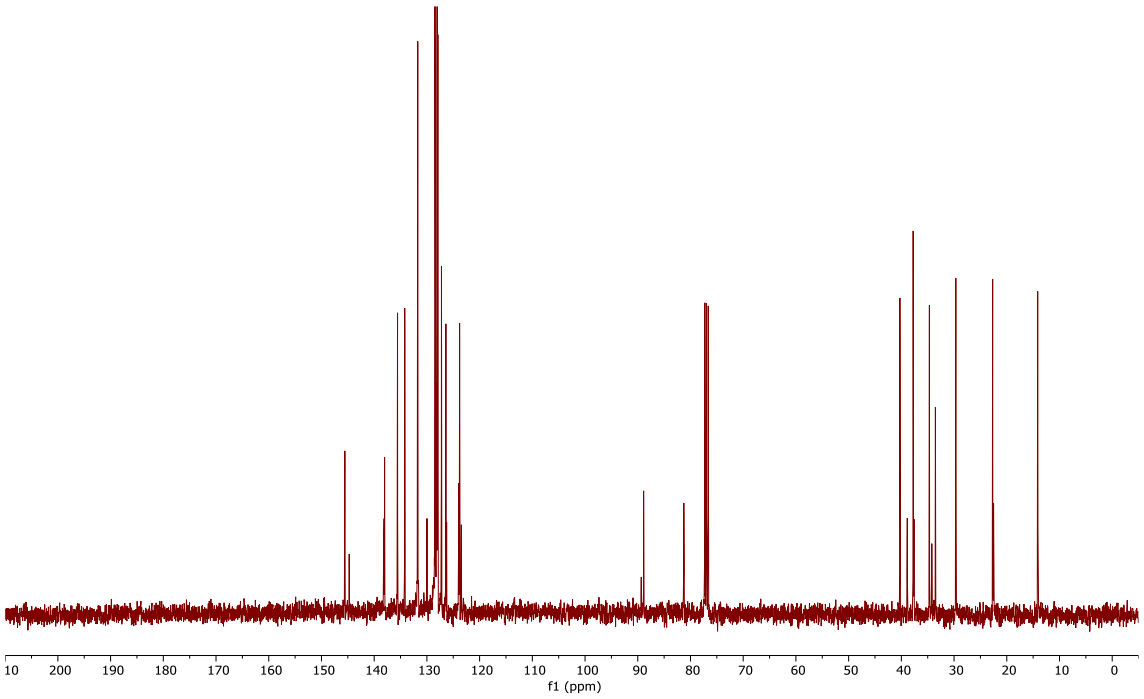


4l

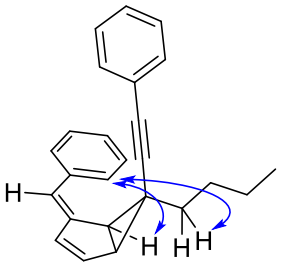




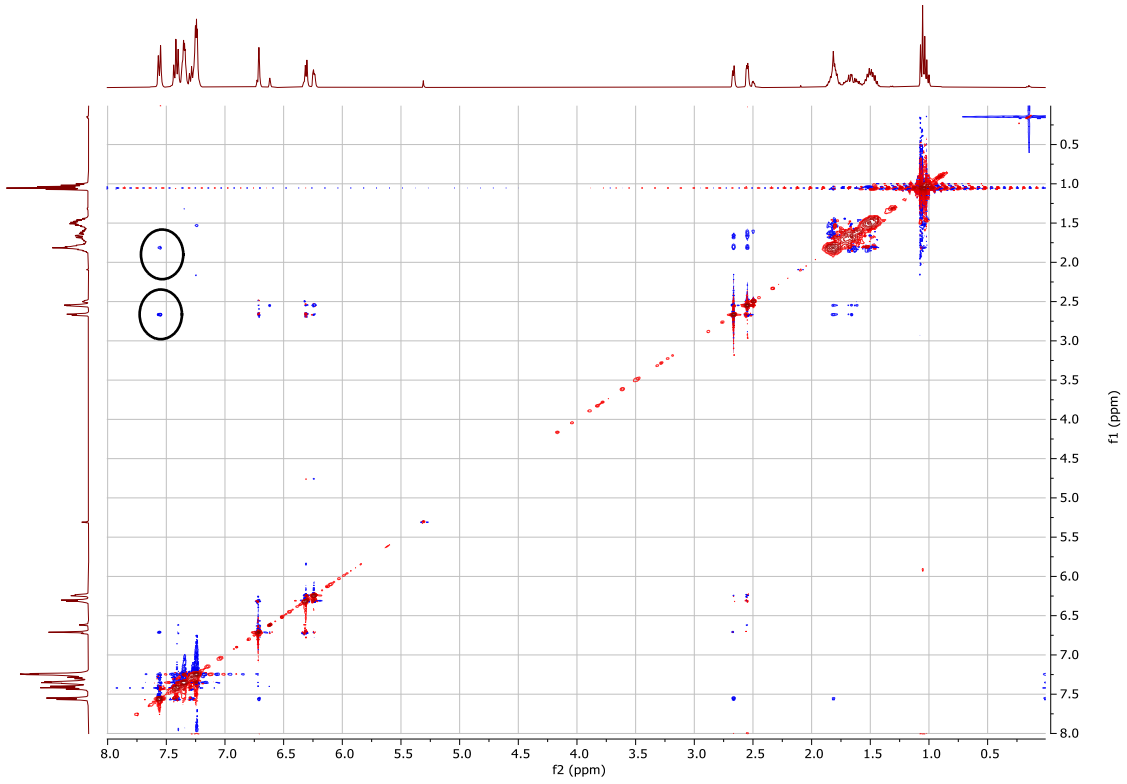


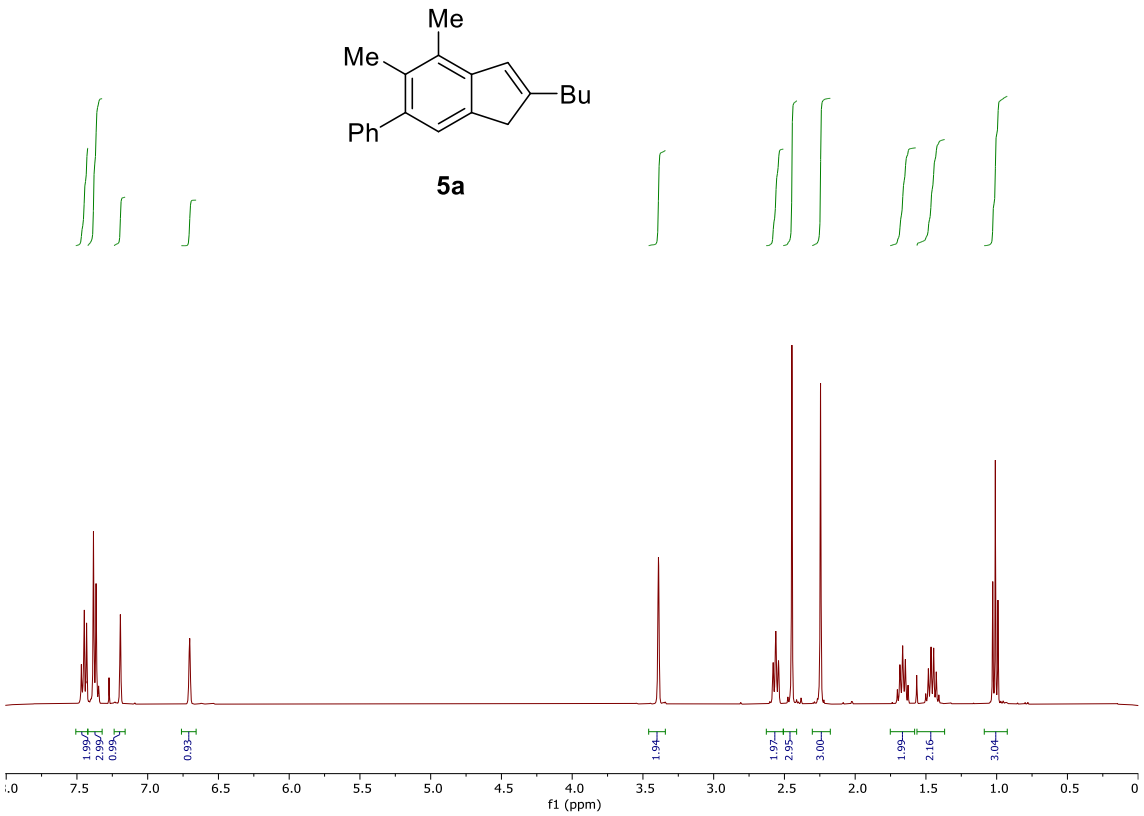


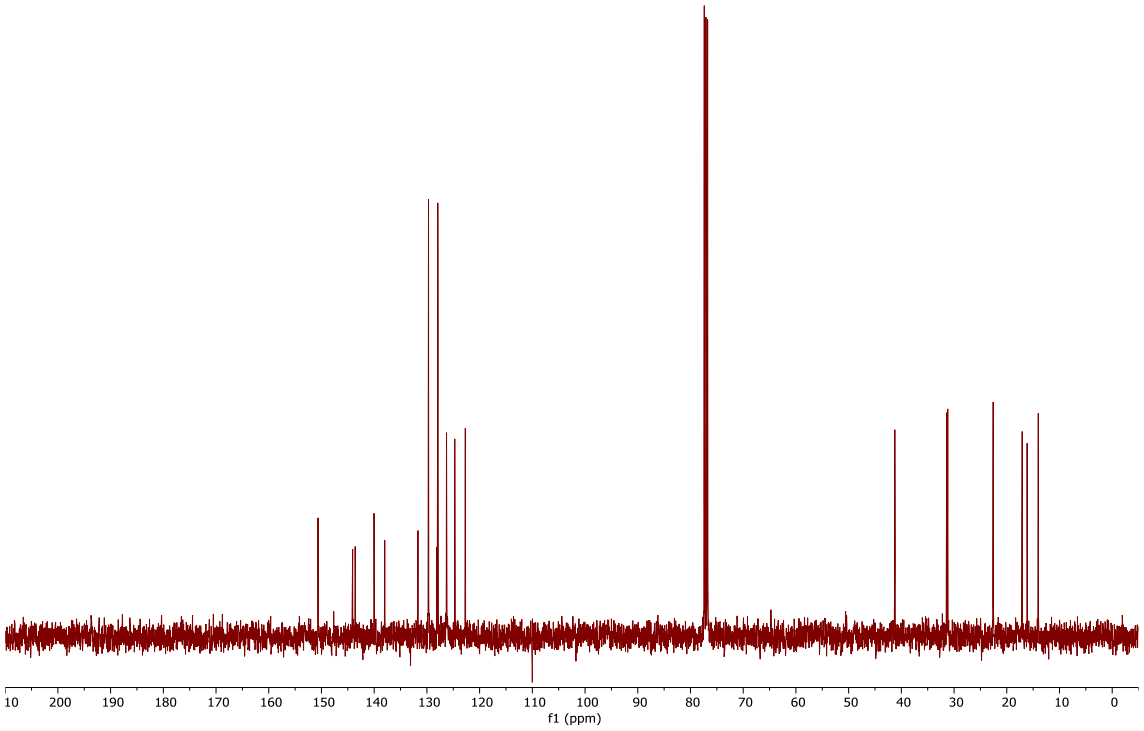
Observe nOe

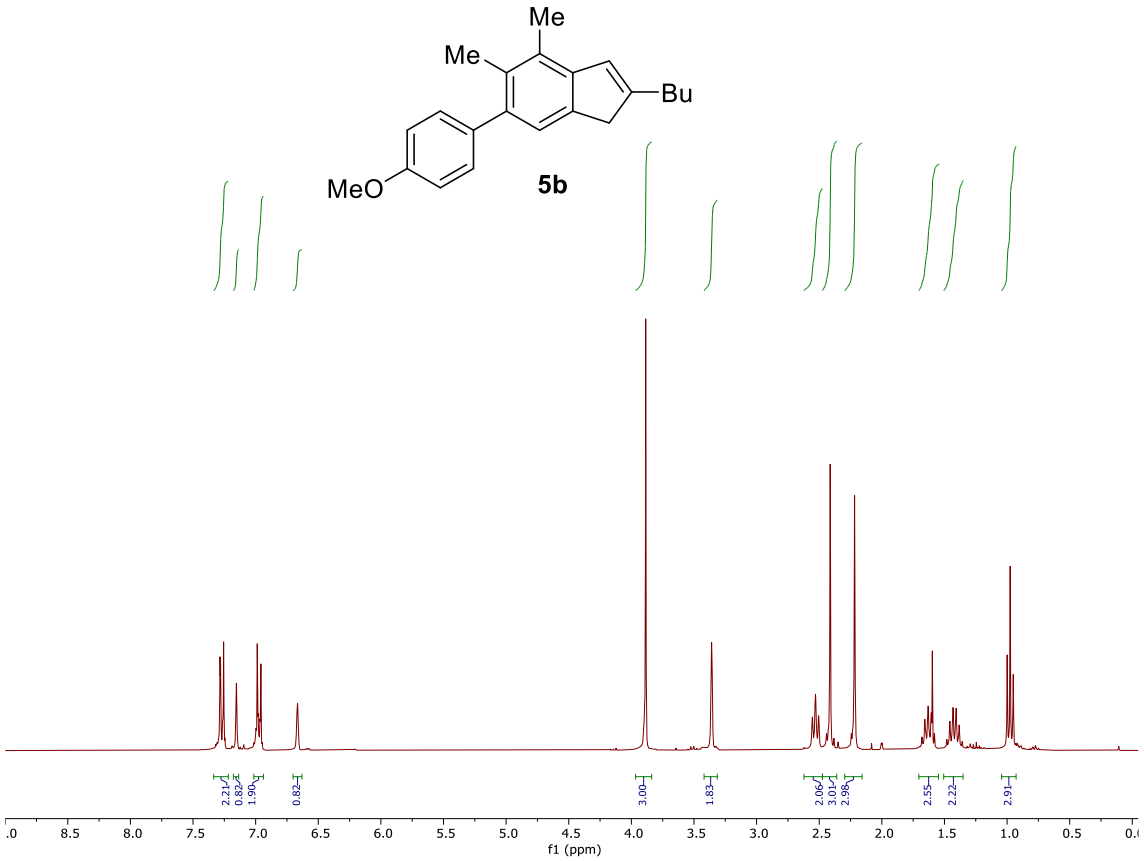


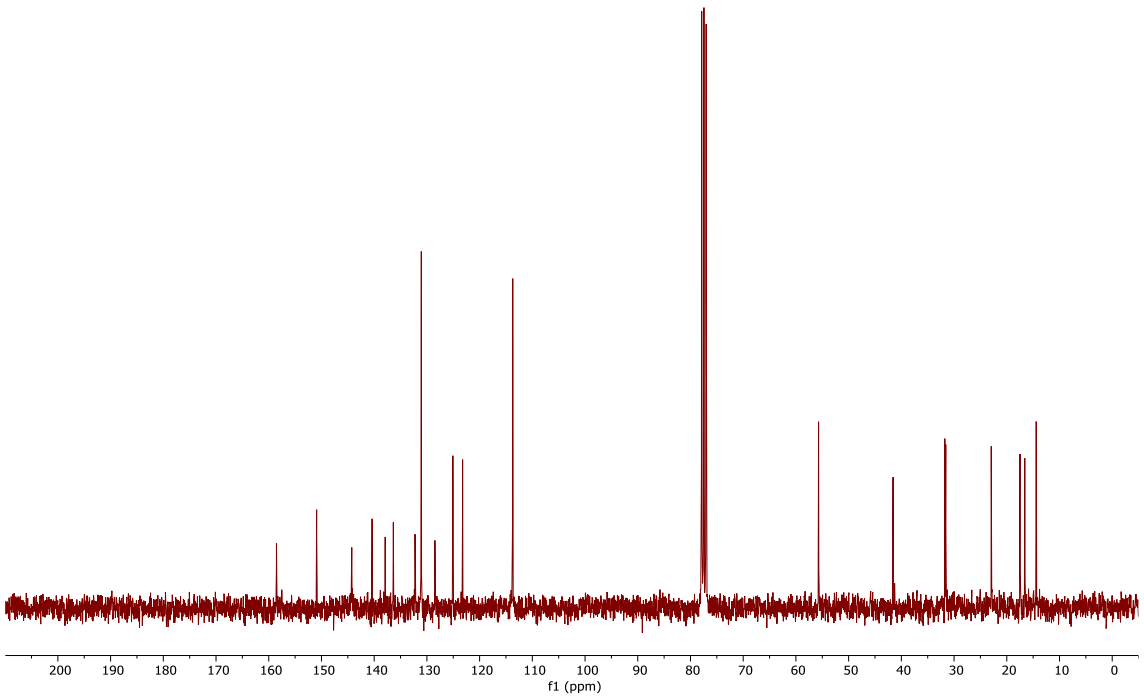
4m

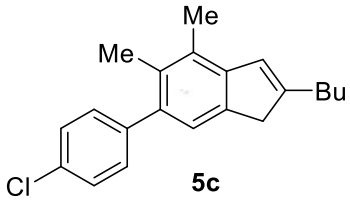




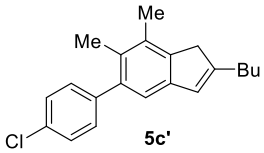




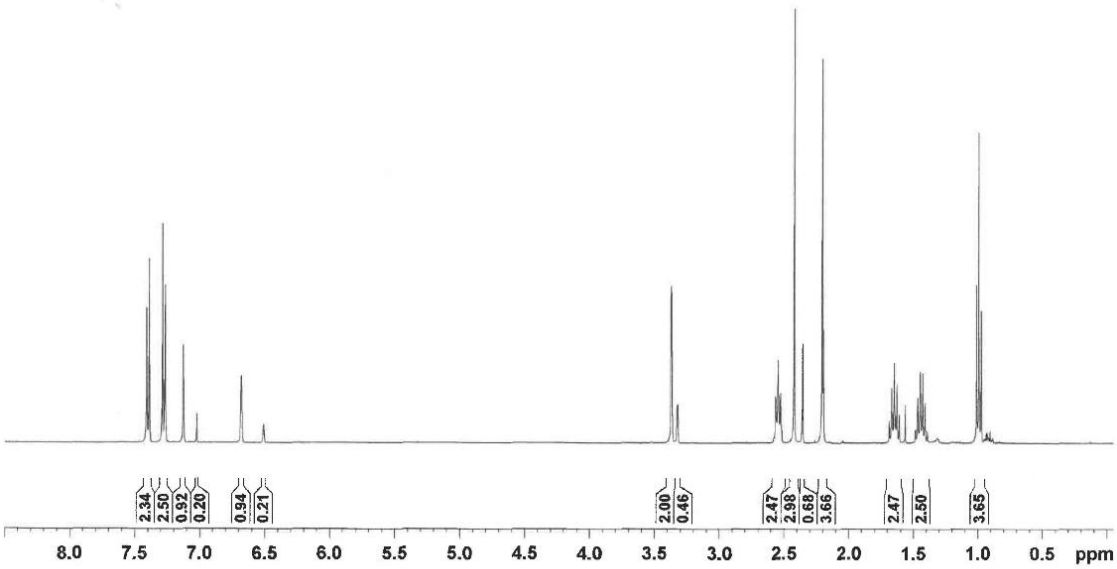


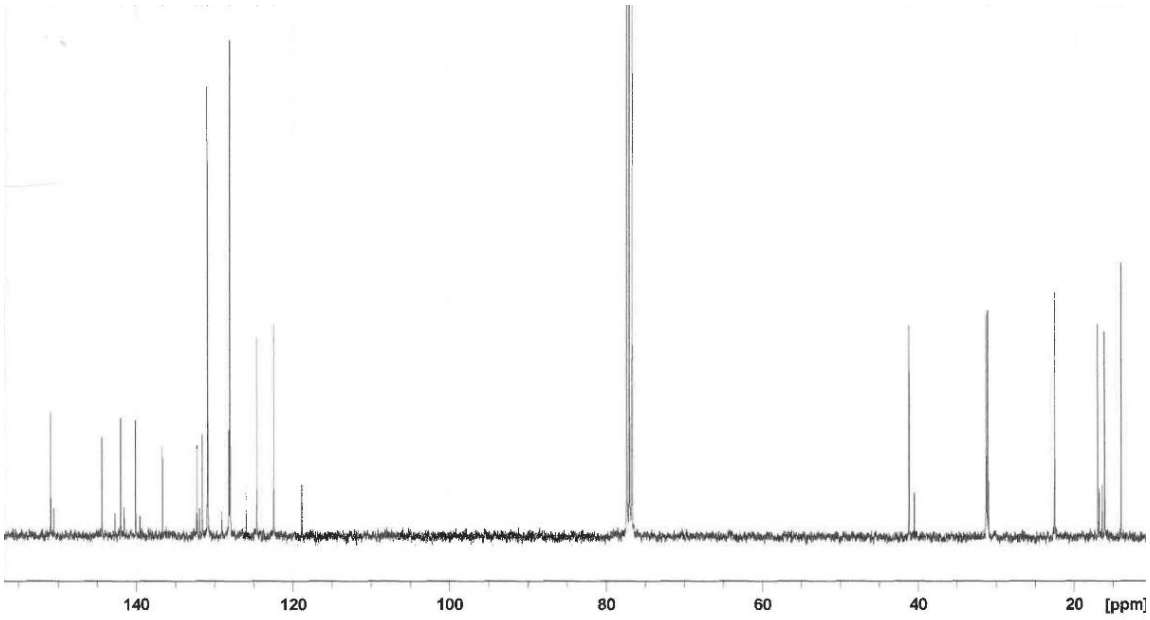


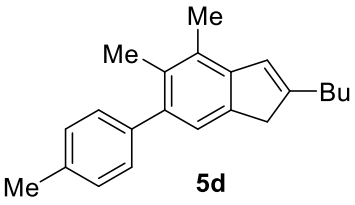
5c



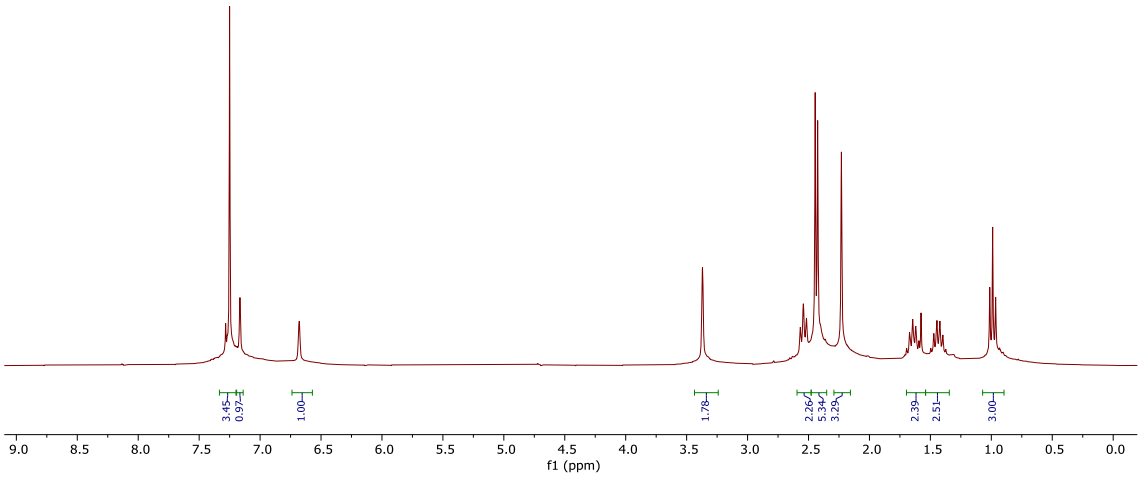
5c'

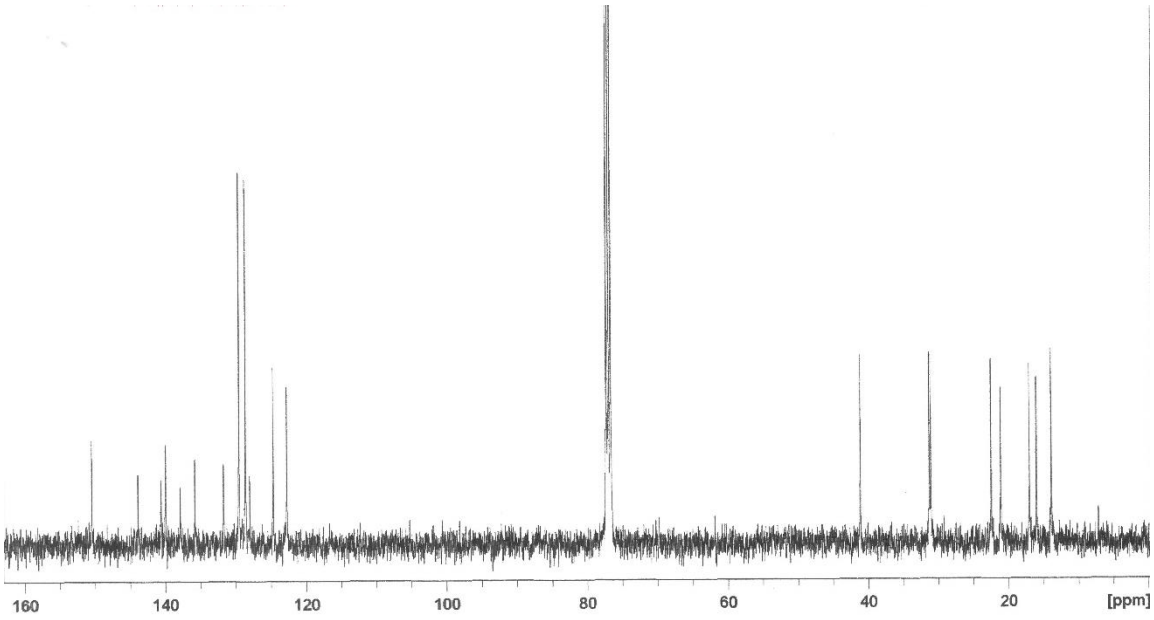


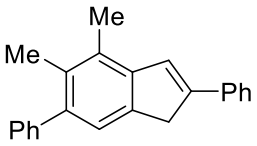




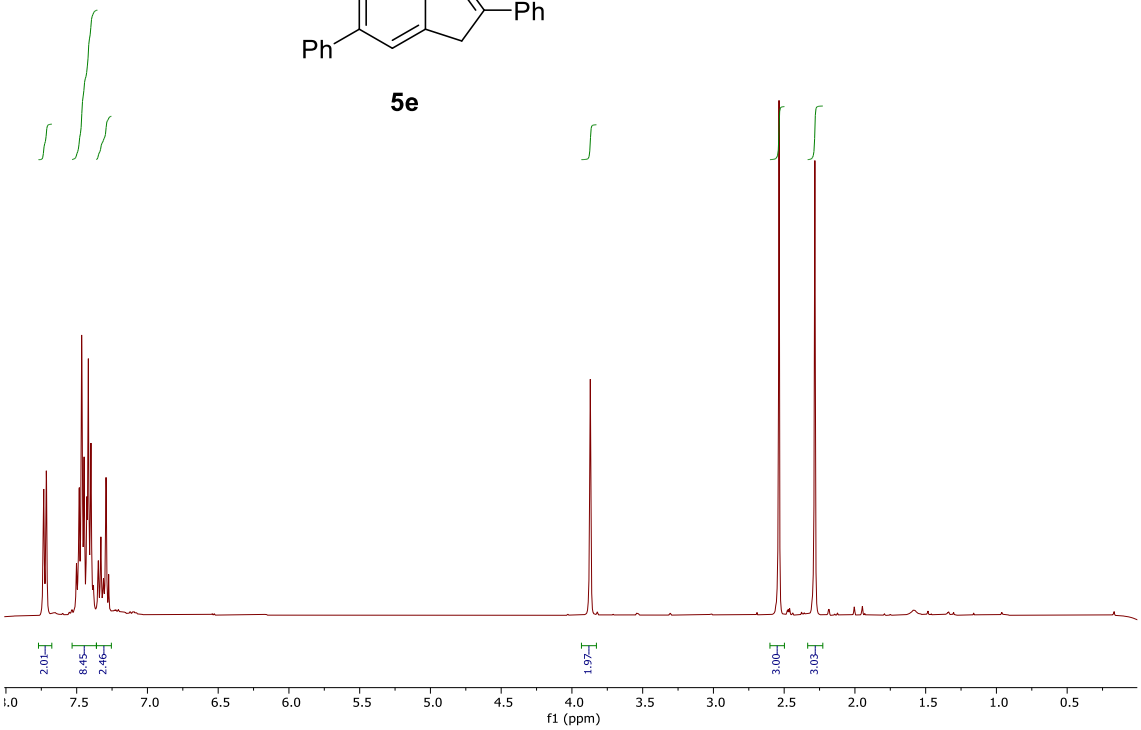
5d

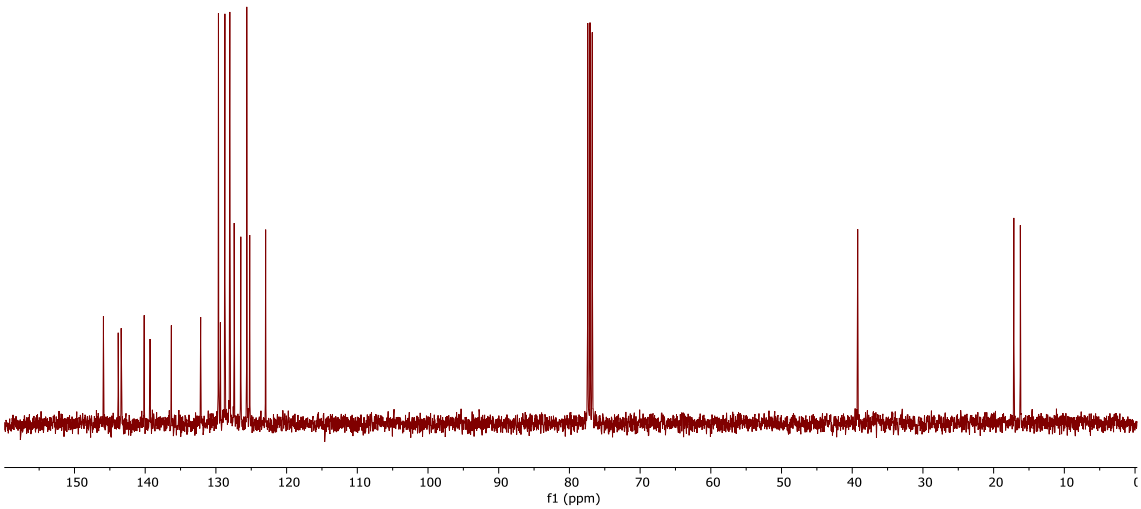


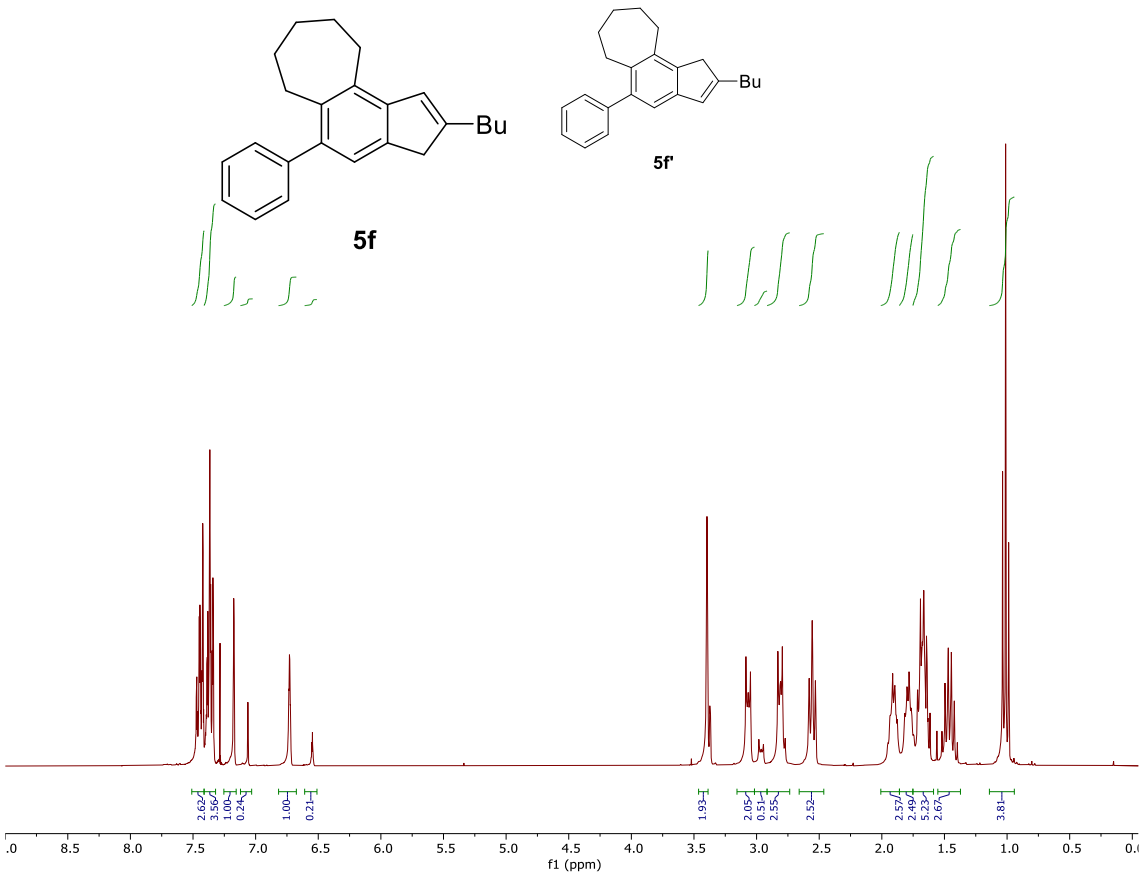


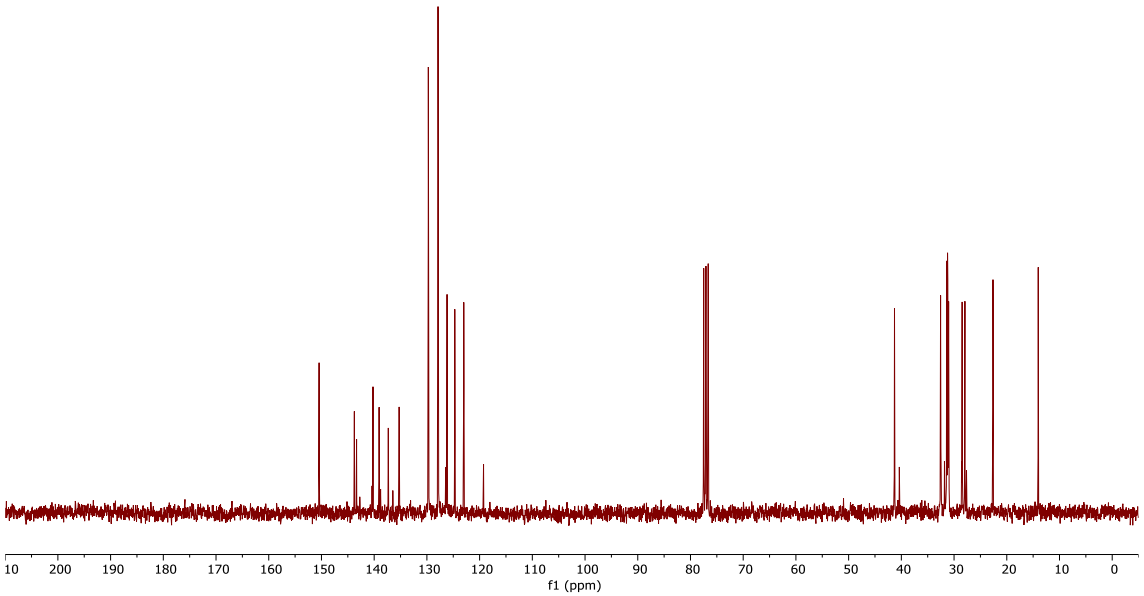


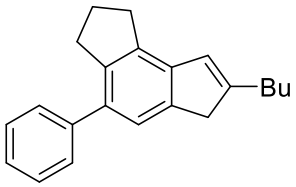
5e



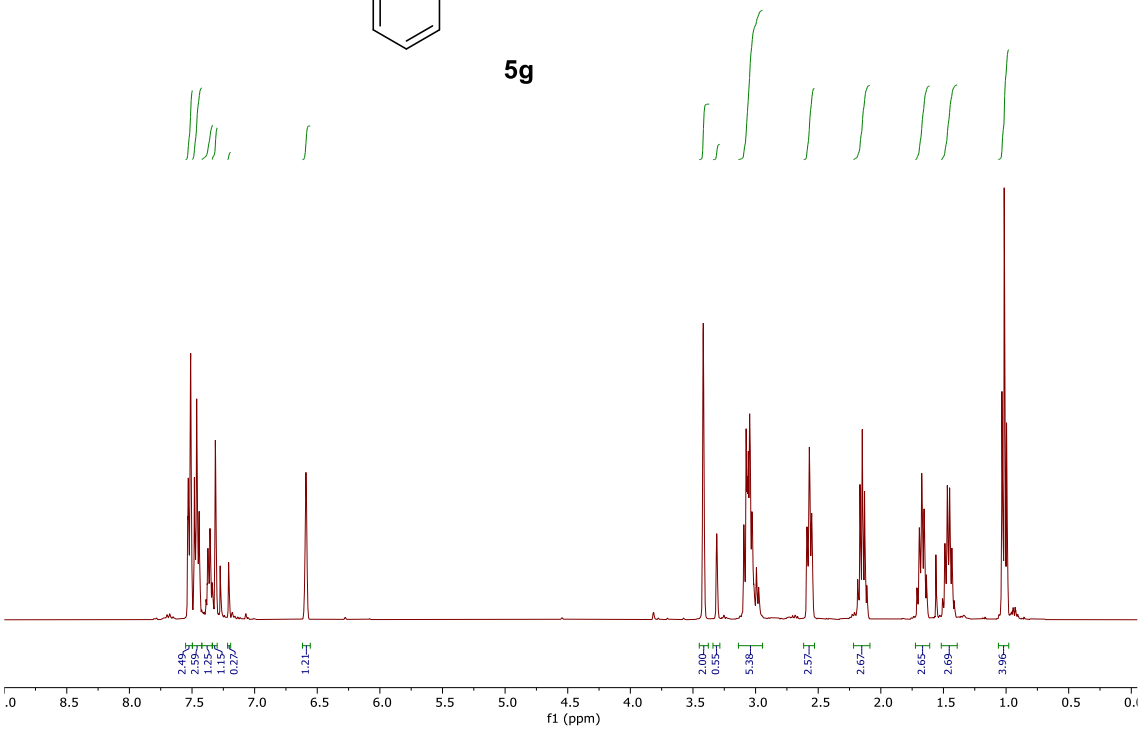


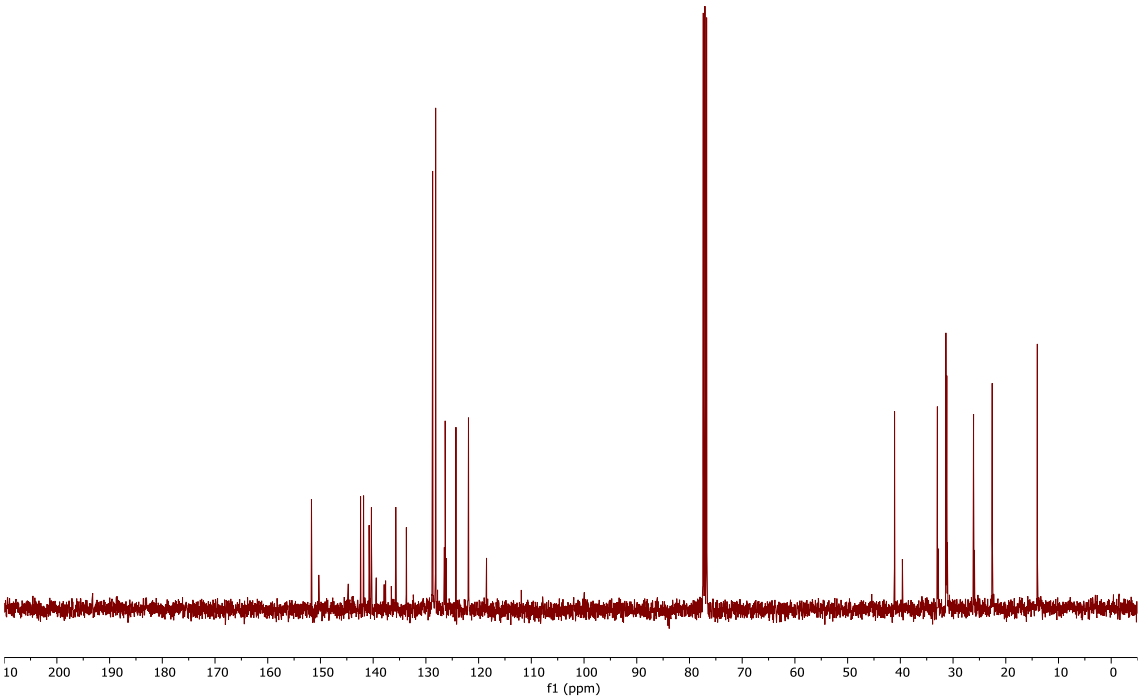


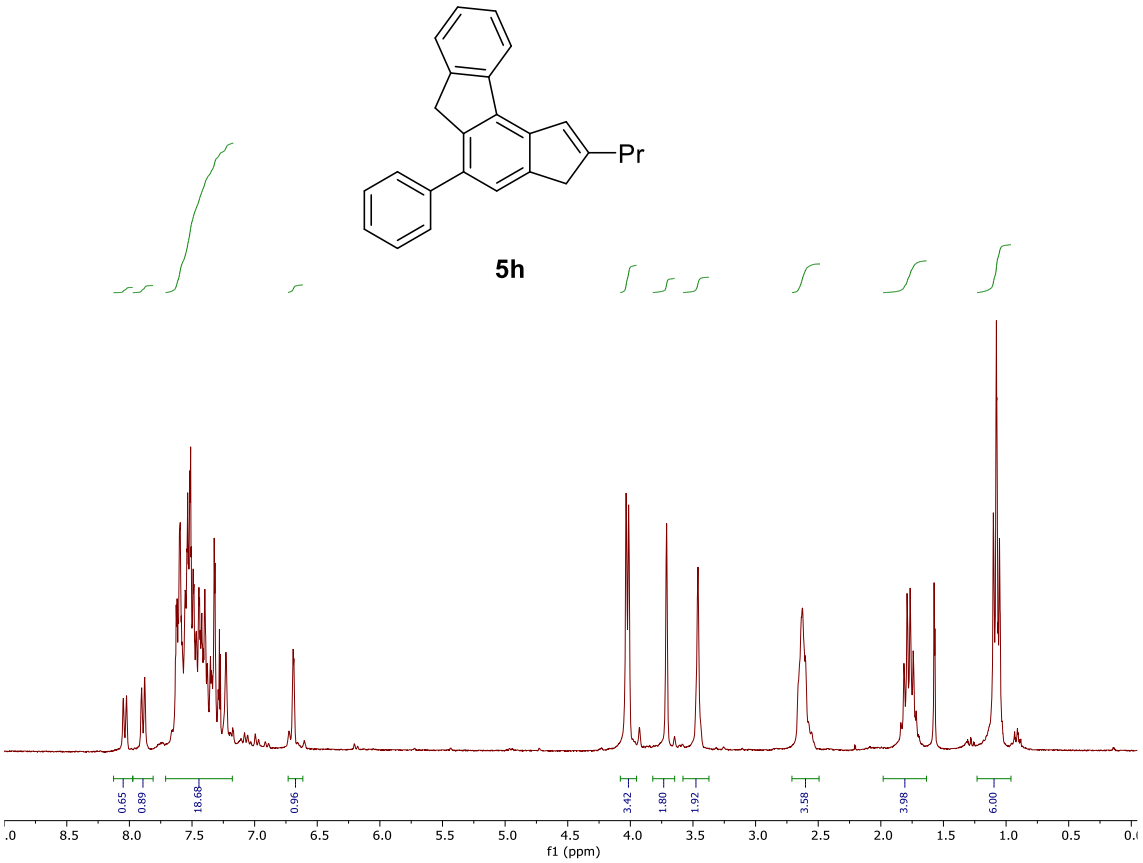


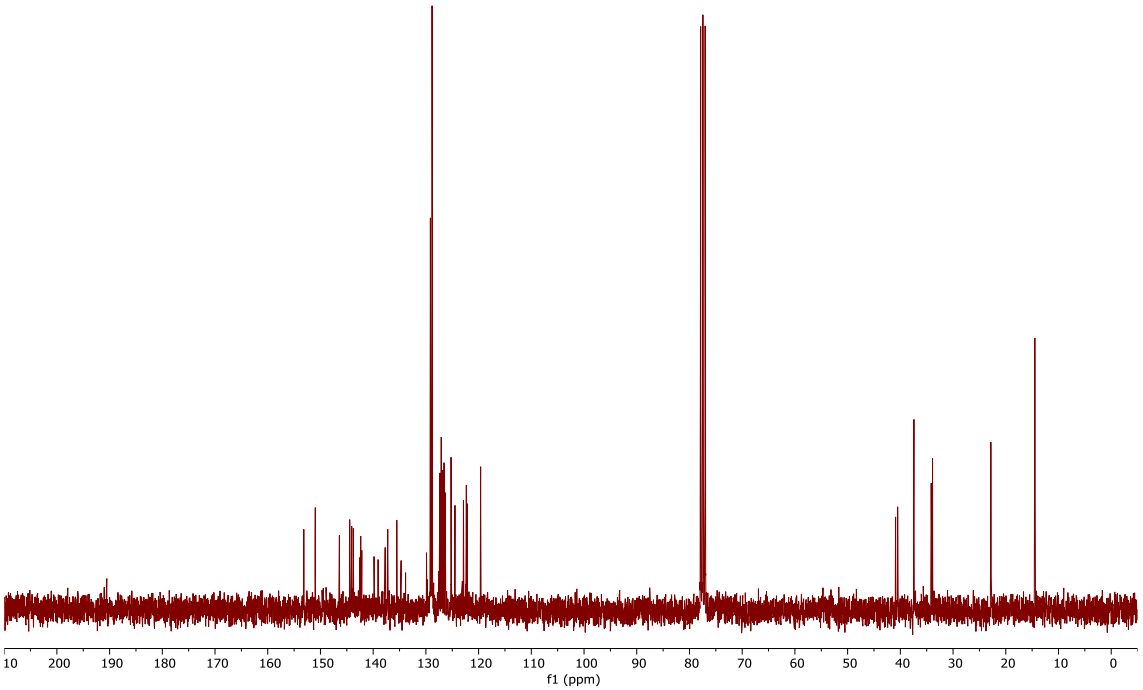


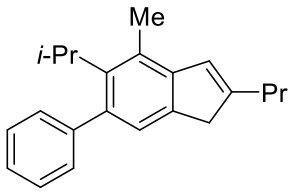
5g



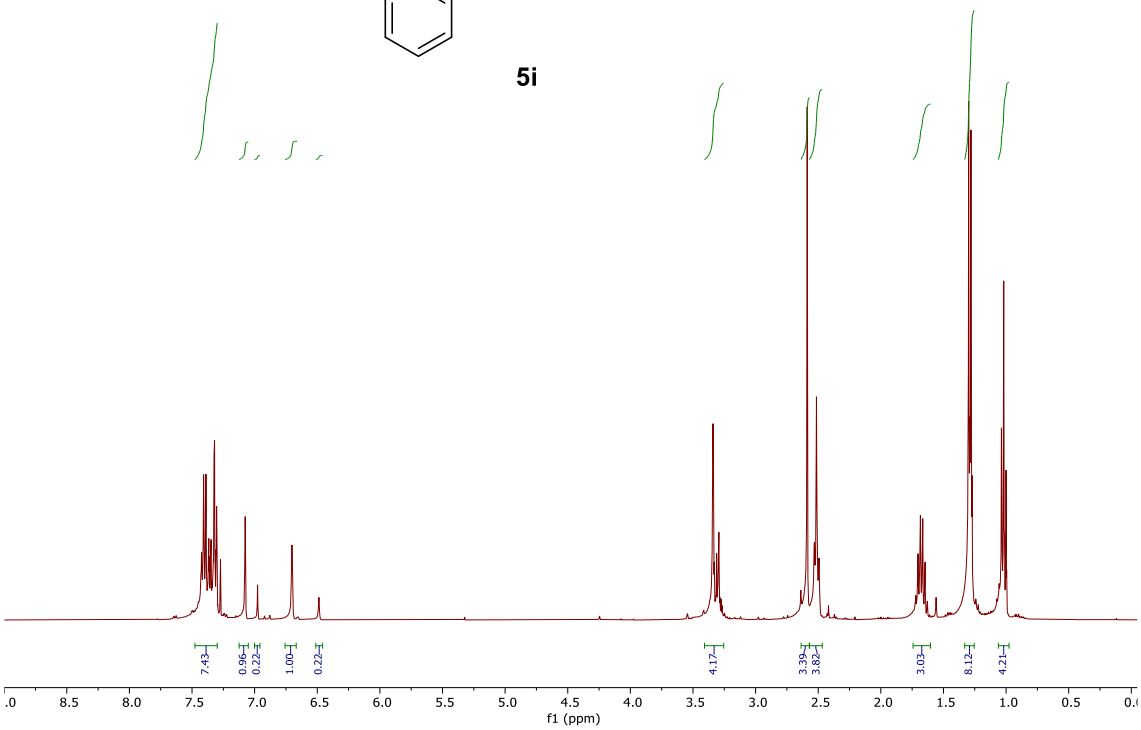


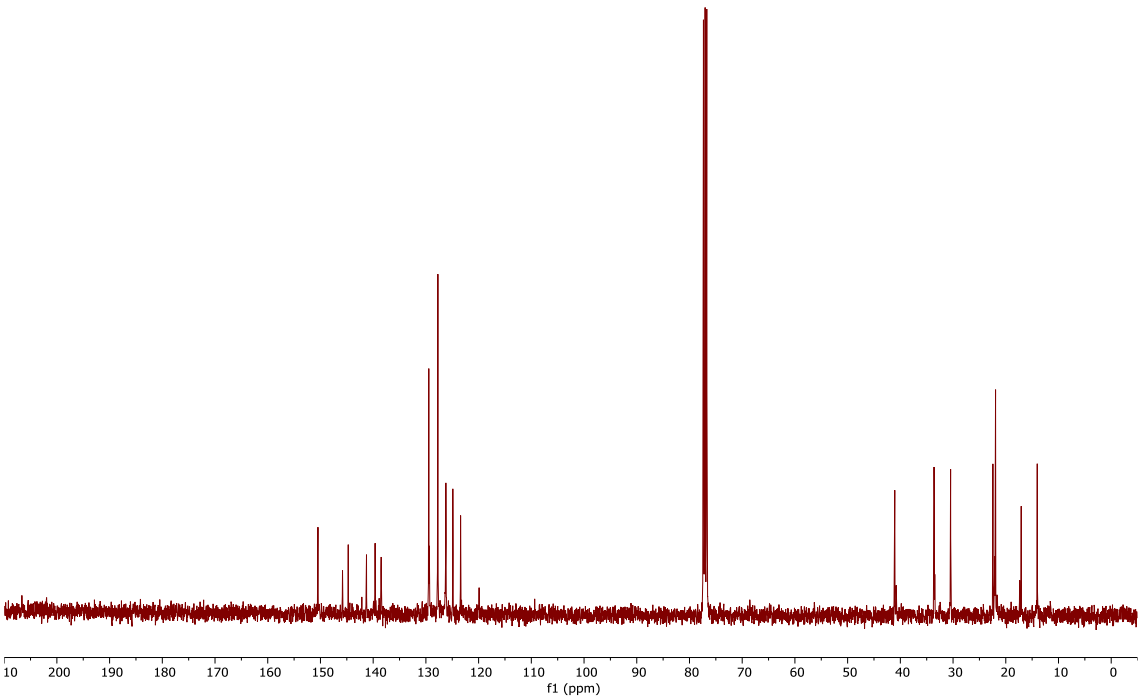


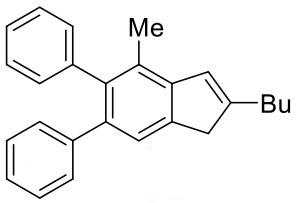




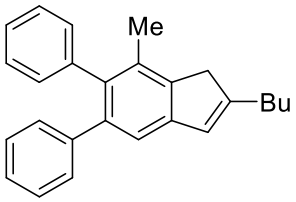
5i



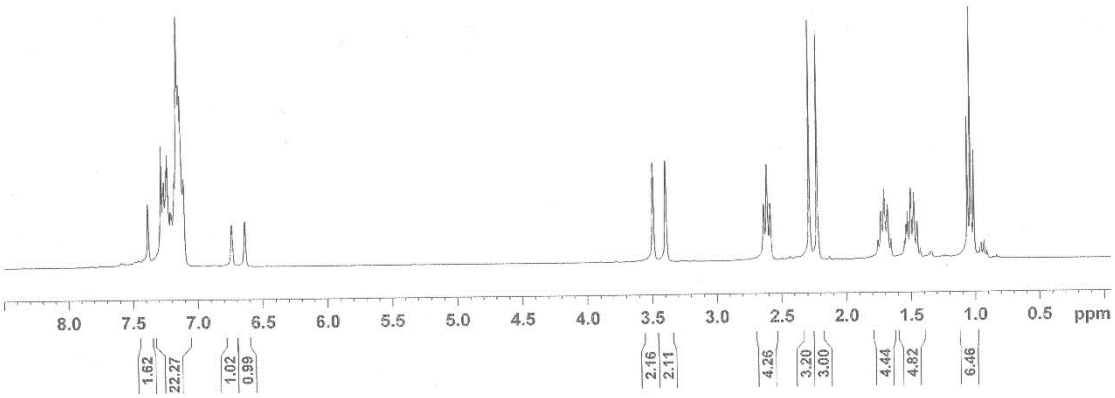


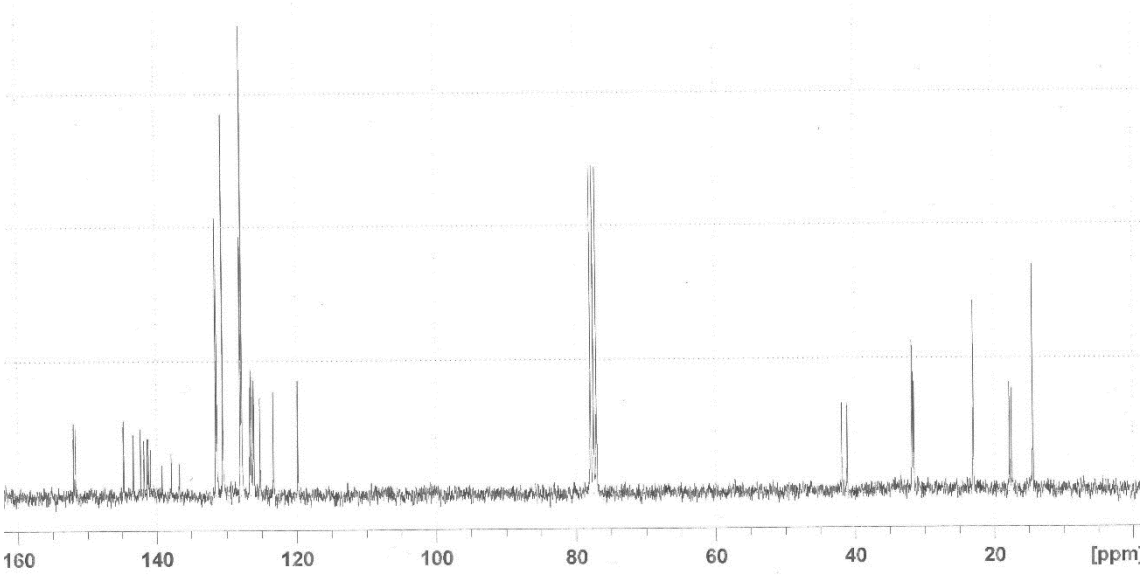


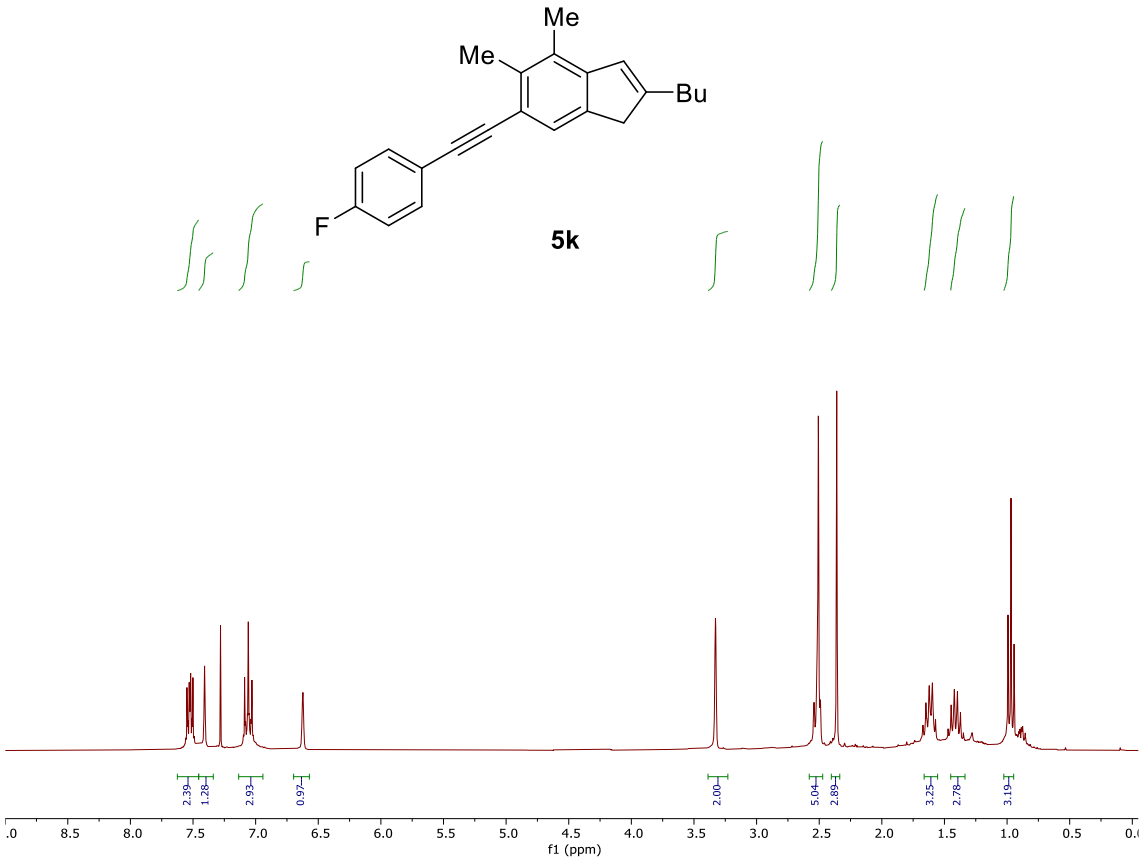
5j

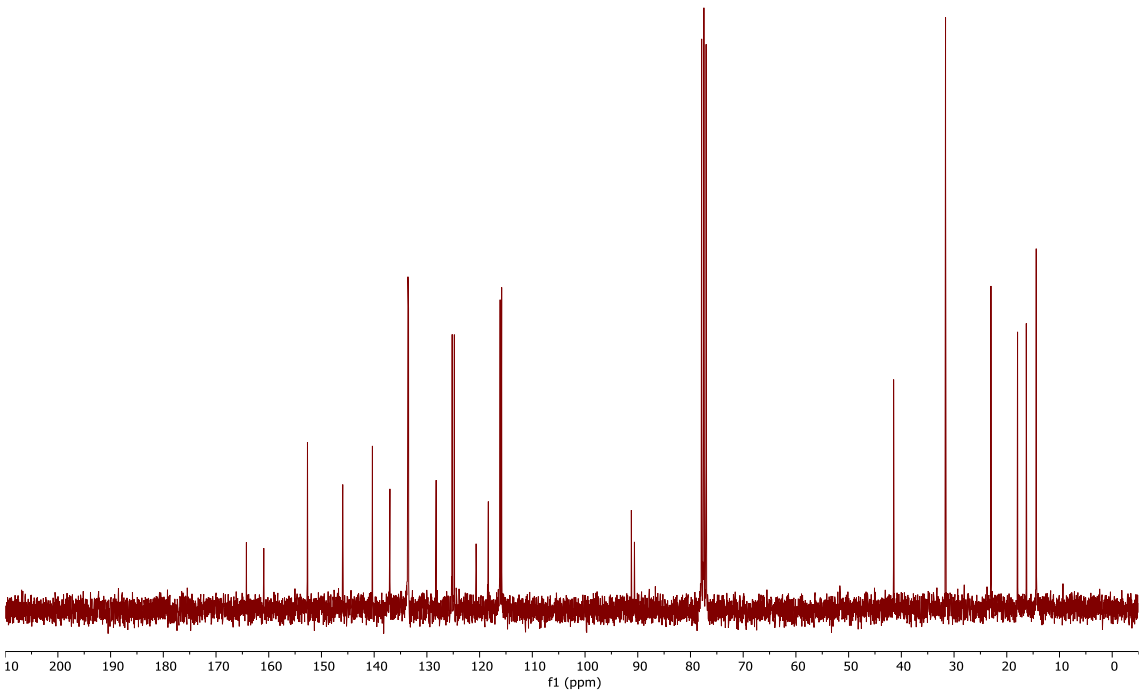


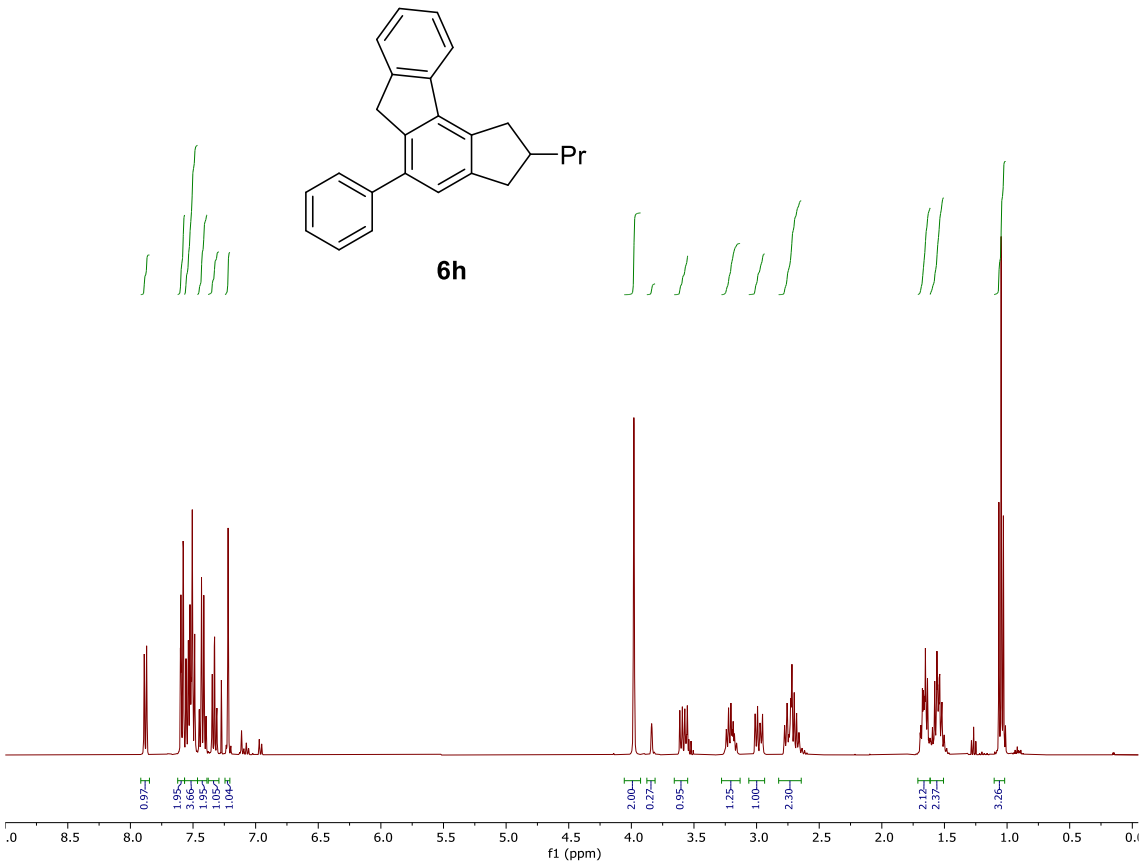
5j'

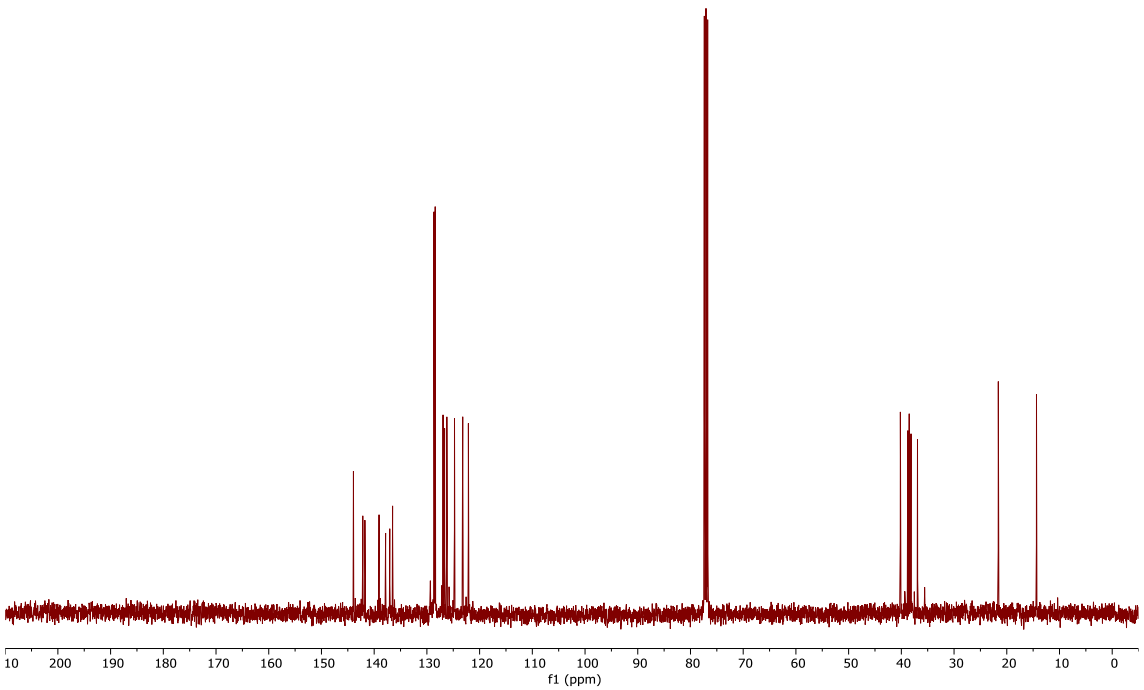




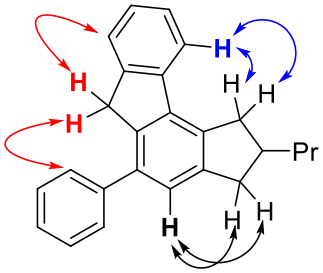




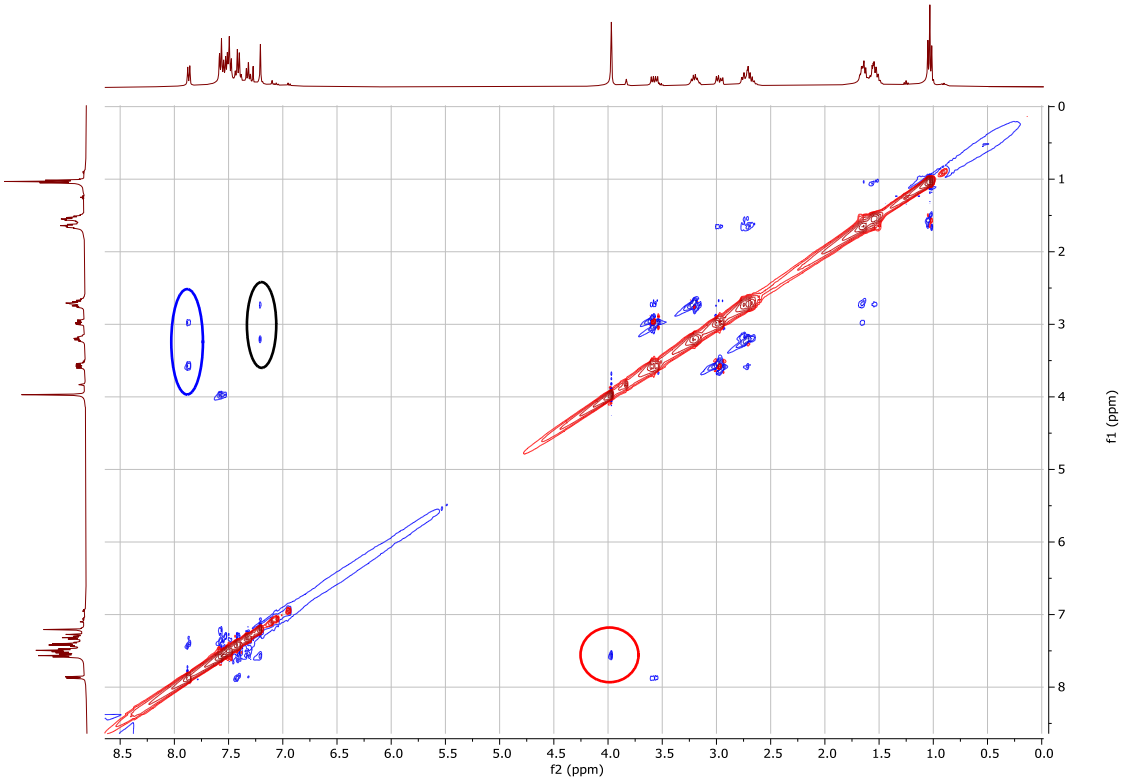


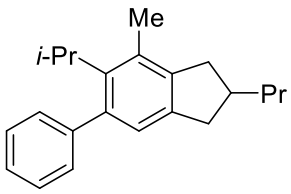


Observed nOe

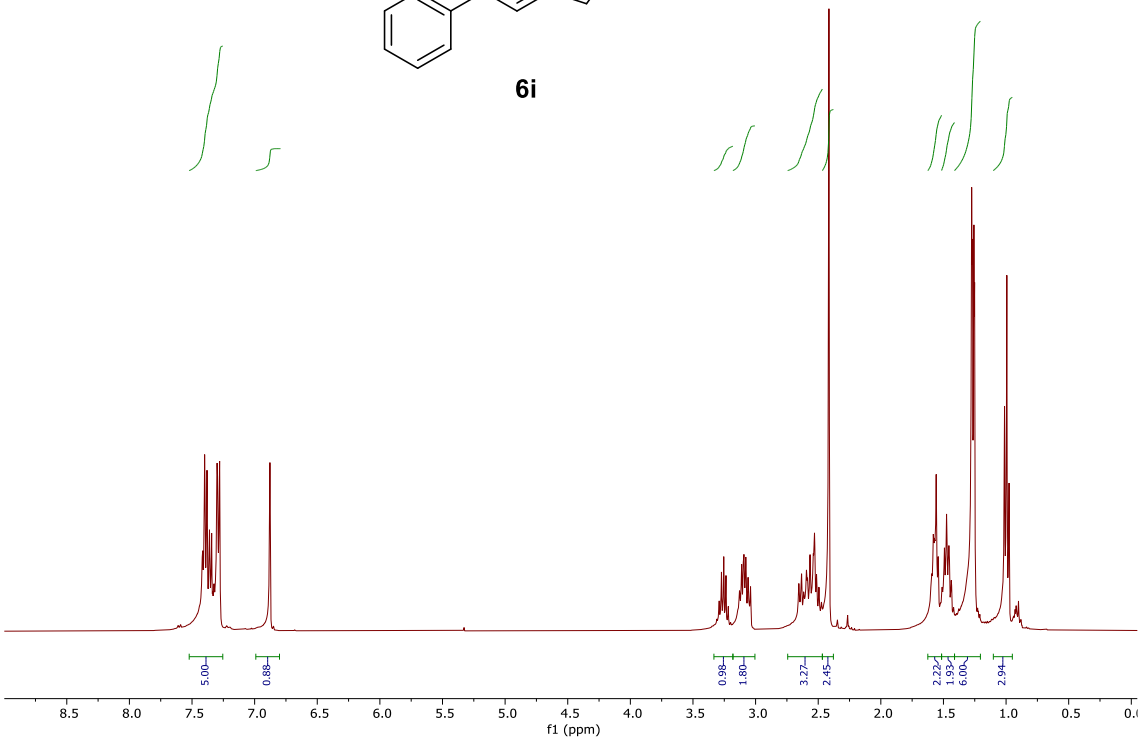


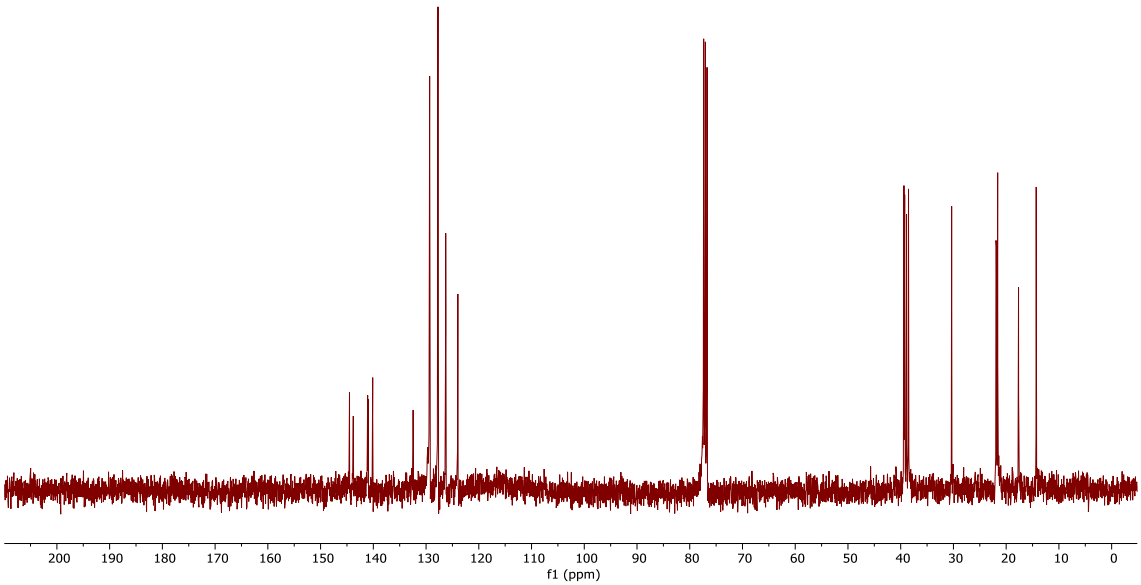
6h

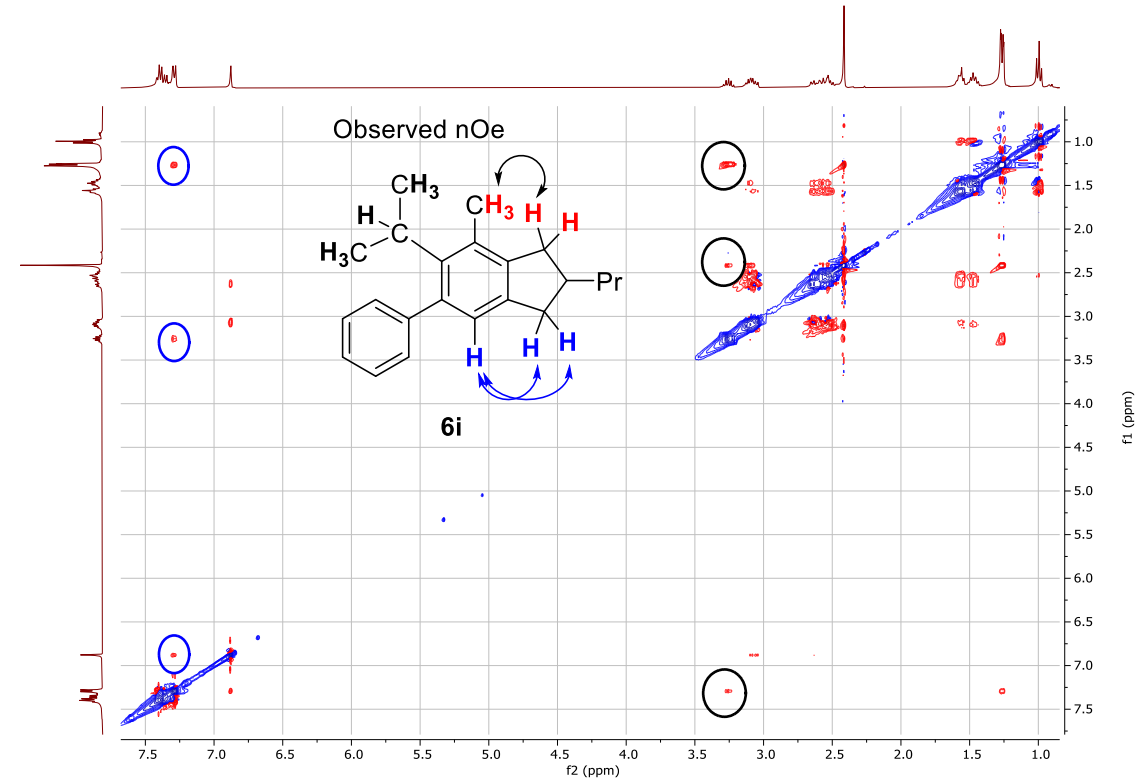


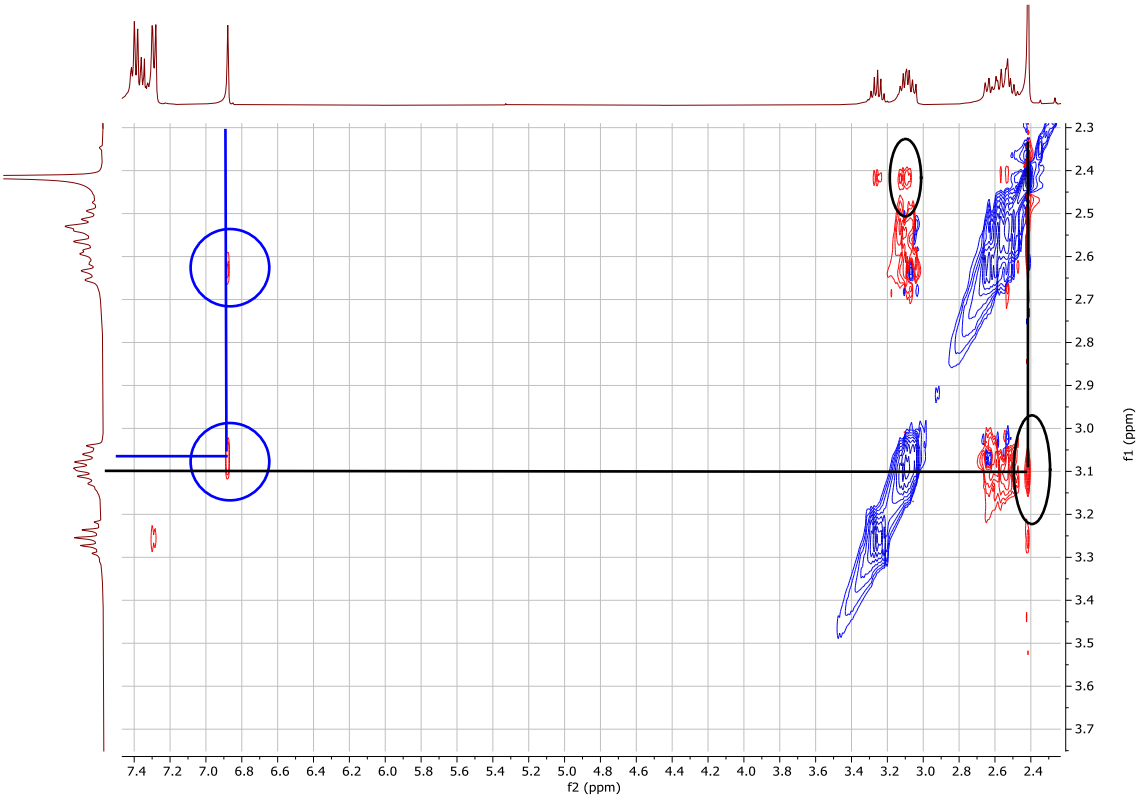


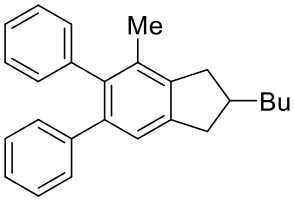
6i



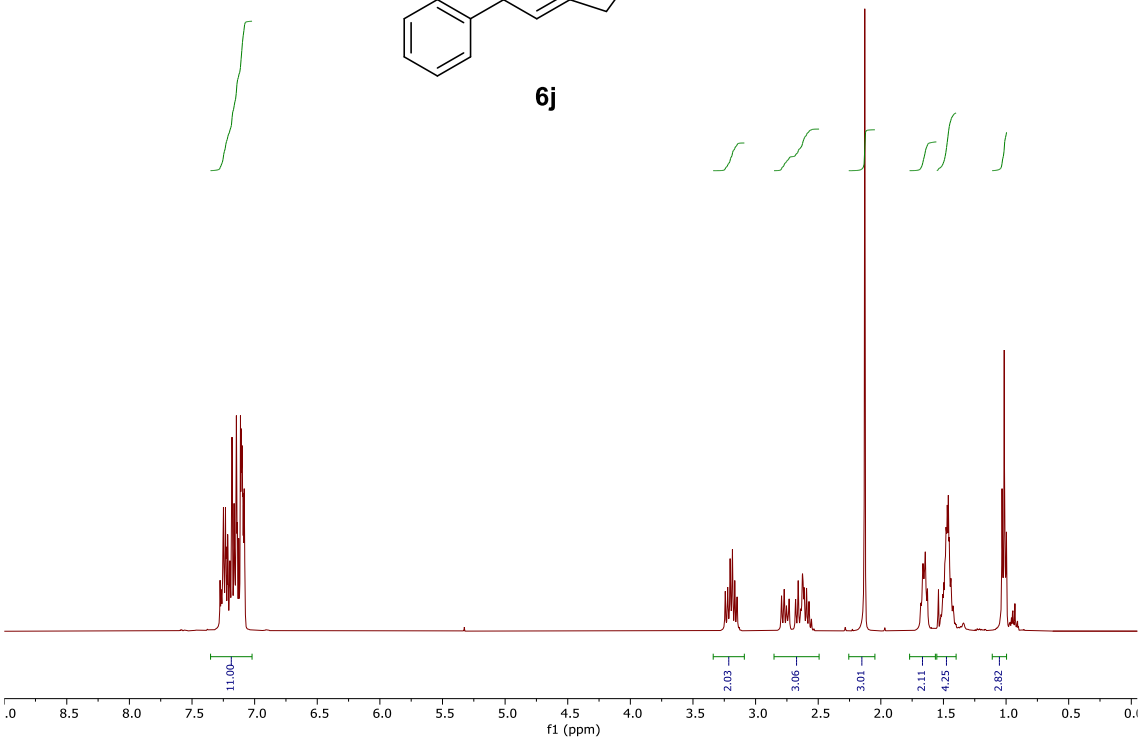


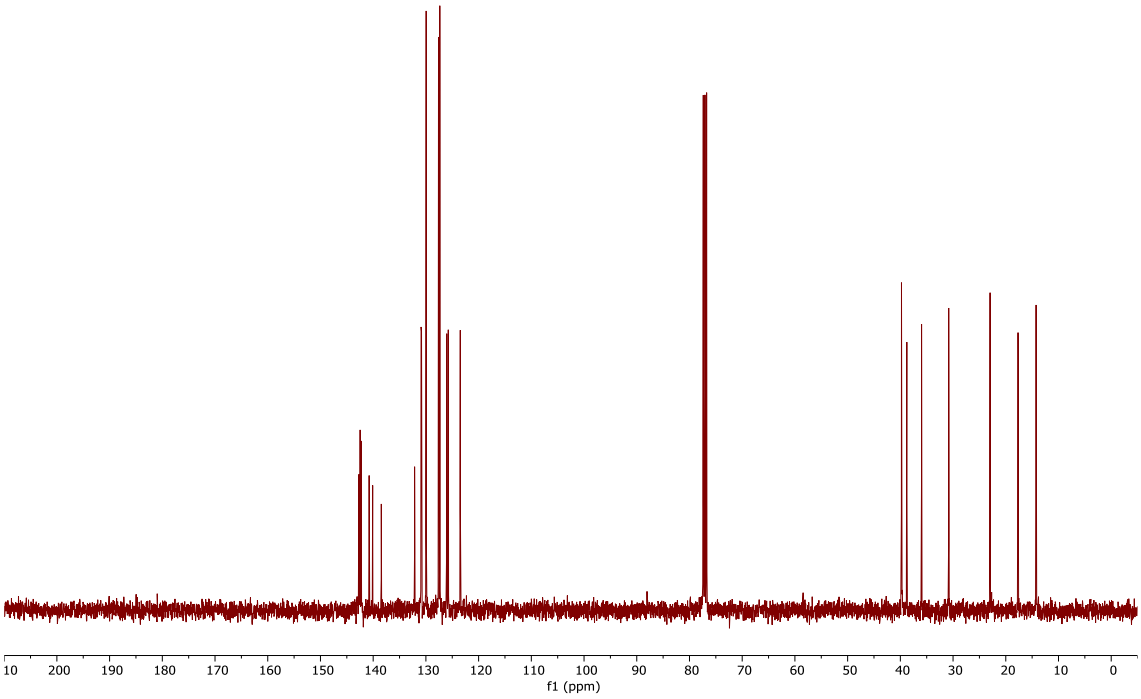


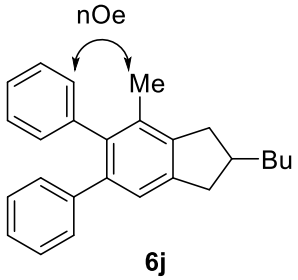




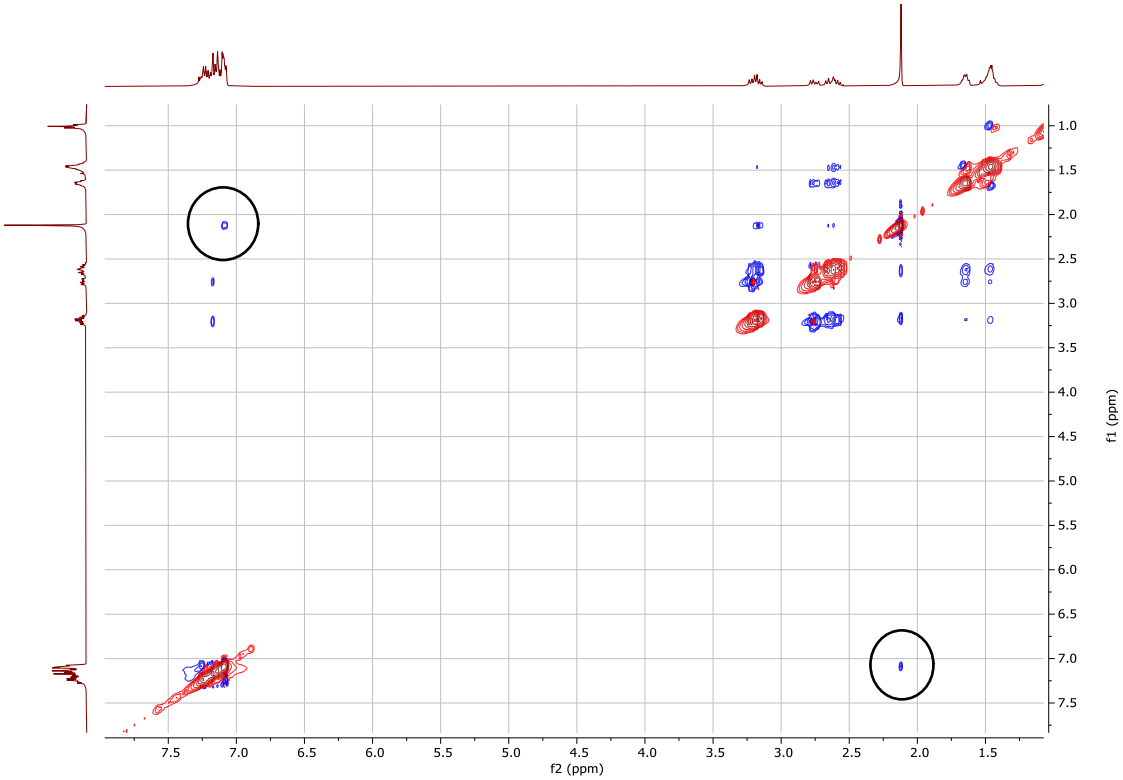
6j



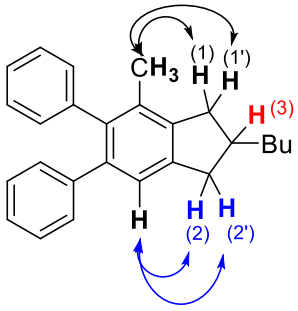




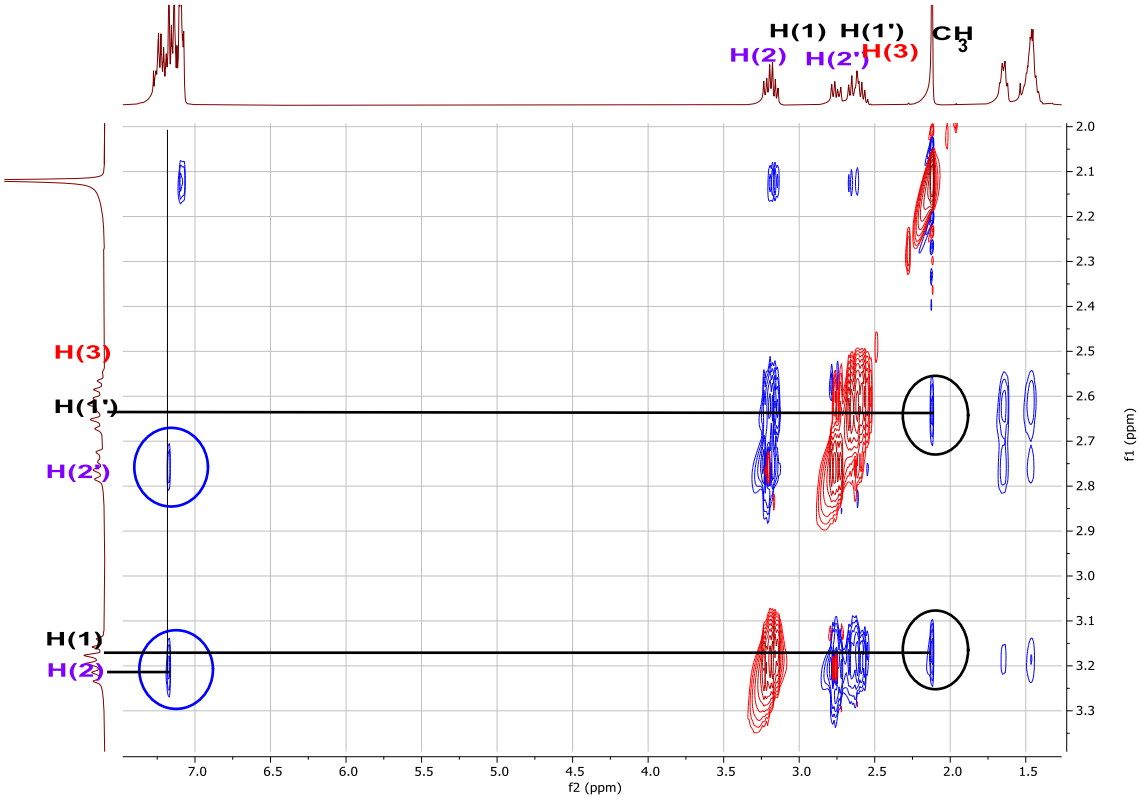
6j

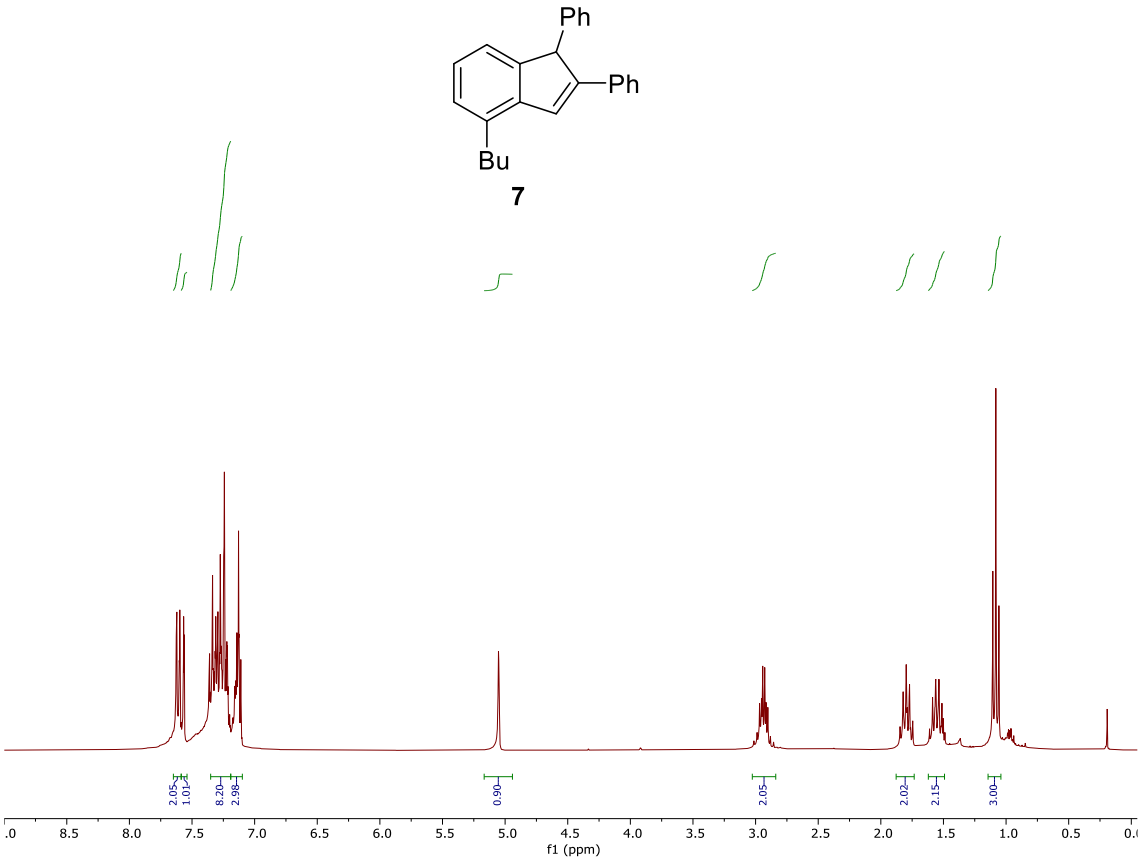


Observed nOe

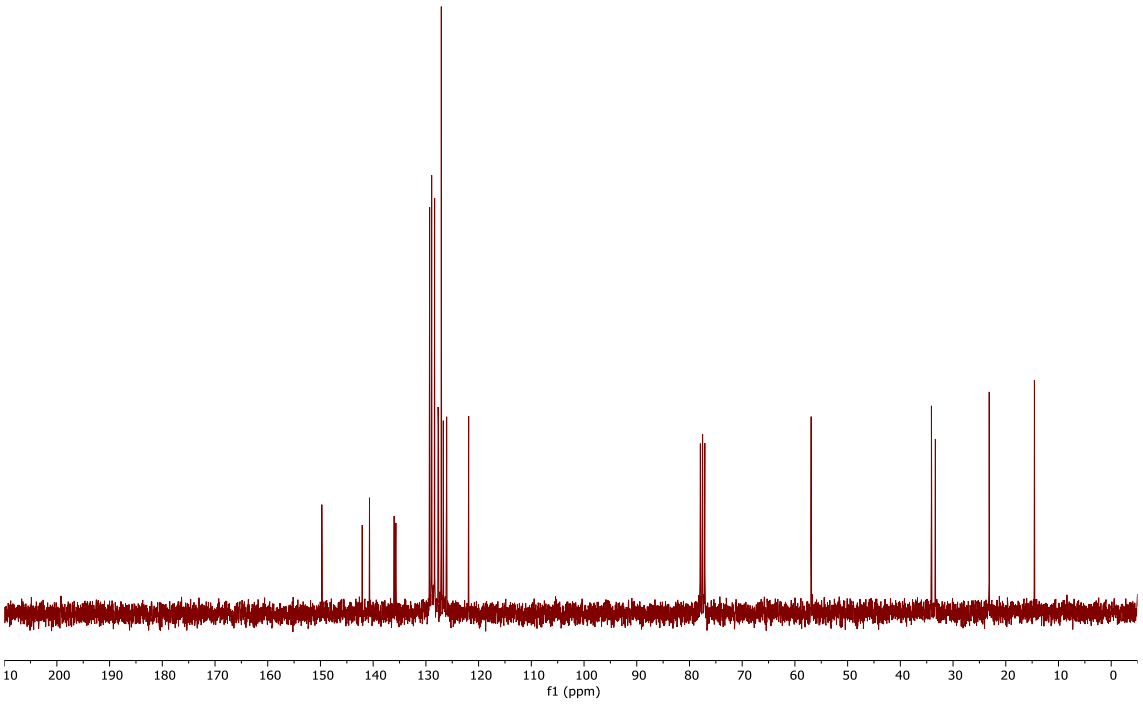


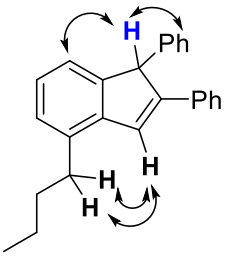
6j



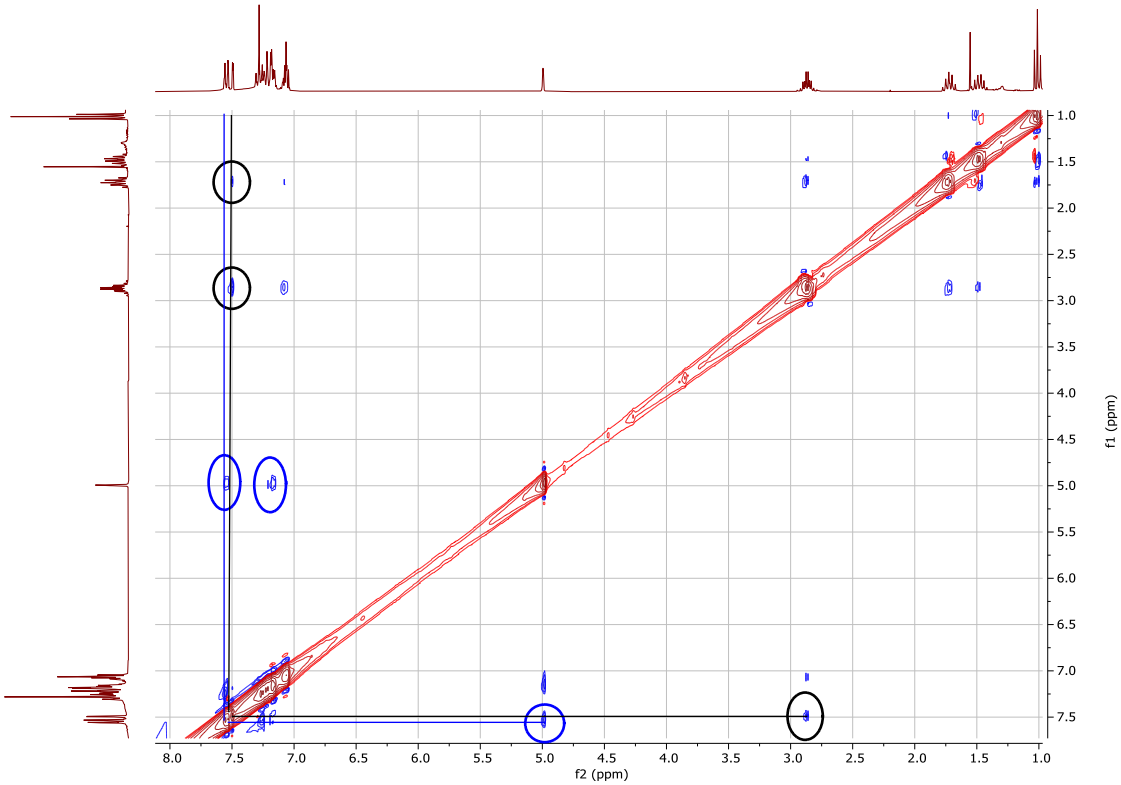


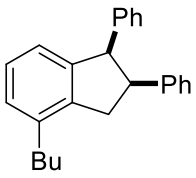
7



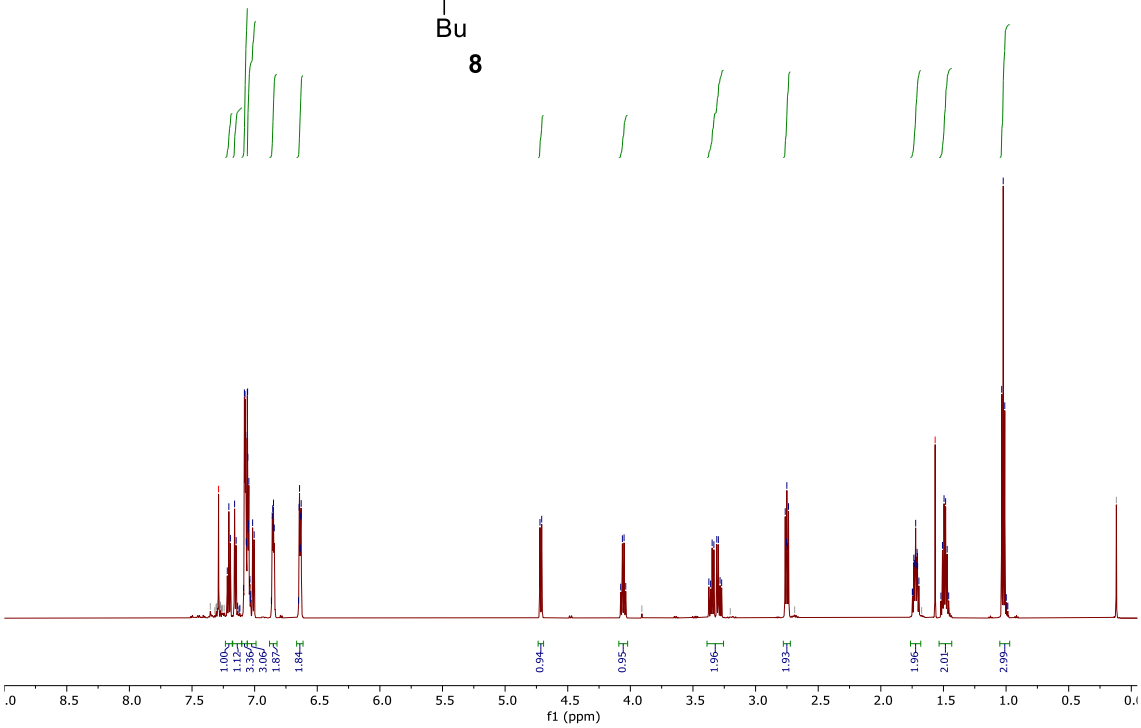


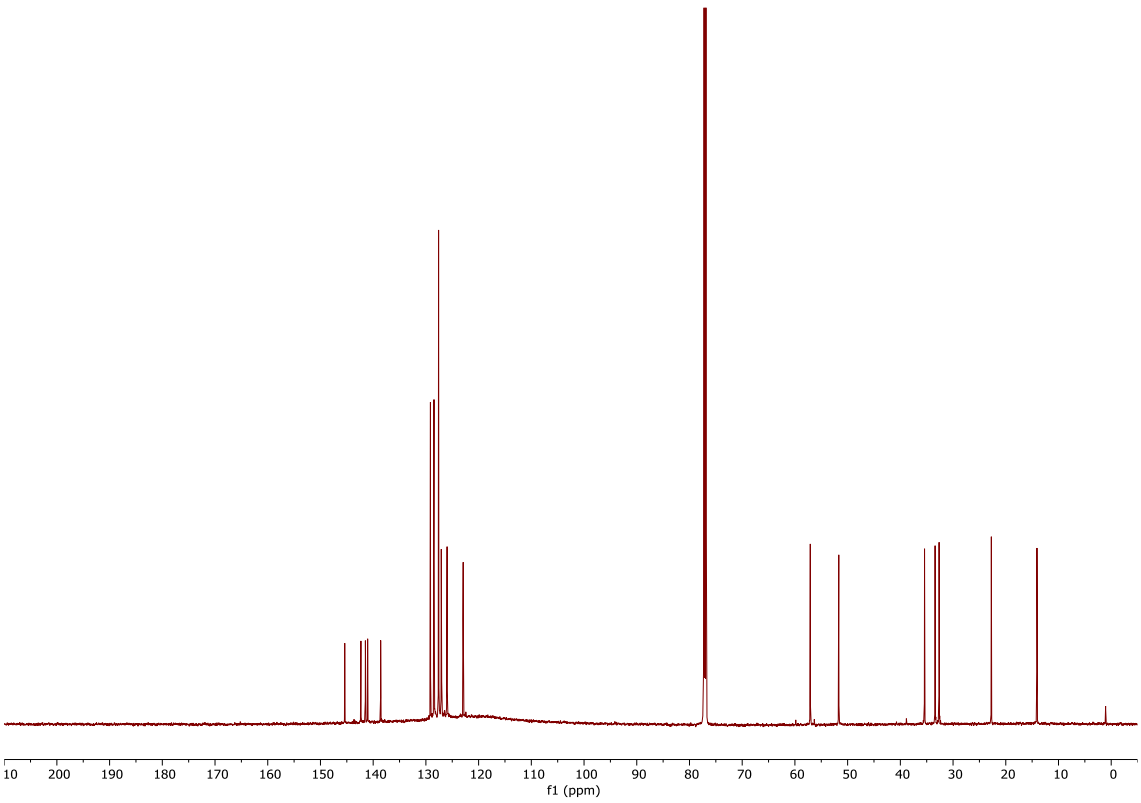
7



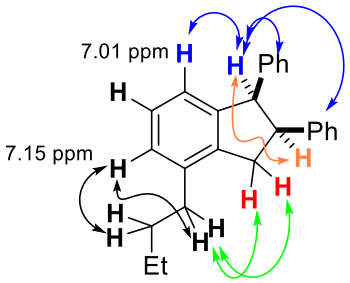


8

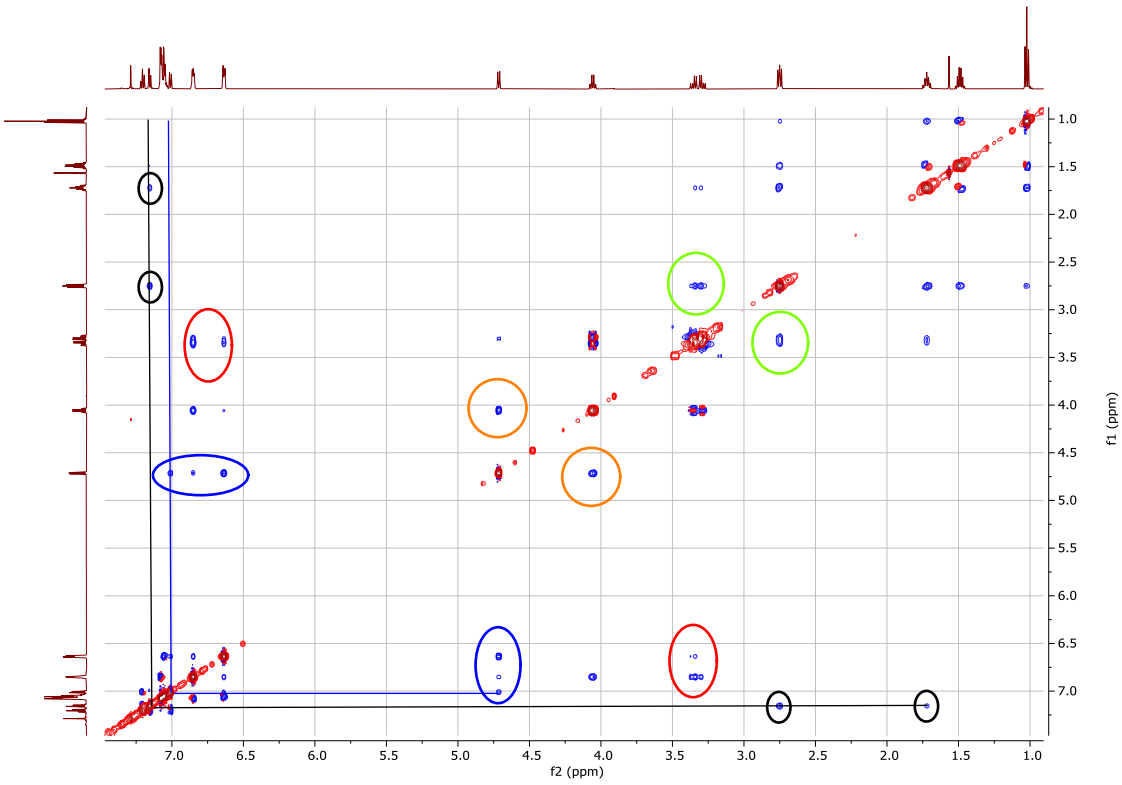




Observe nOe



8



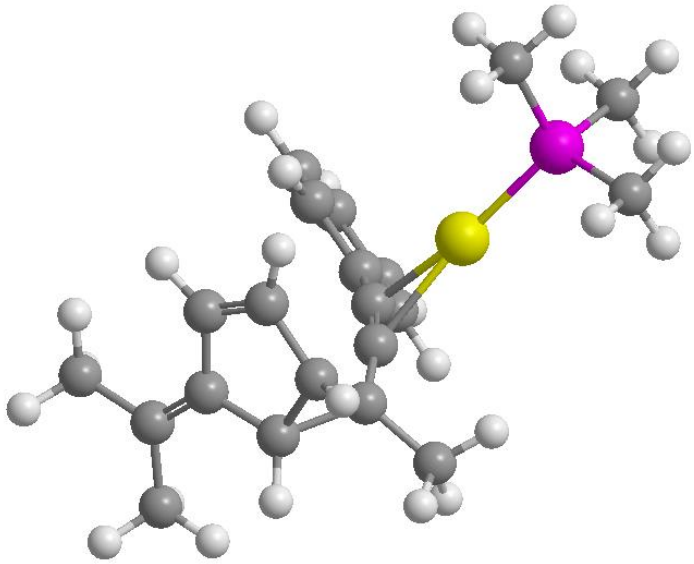
Computational details.

All calculations were carried out using the Gaussian 16 program package.[4] The molecular geometries were fully optimized without any molecular symmetry constraints for all model compounds using the Becke's three-parameter hybrid exchange potential (B3)[5] with the Perdew–Wang (PW91)[6] gradient-corrected correlation functional, B3PW91. This method has been shown to describe bond cleavage more accurately than pure DFT methods.[7] Regarding the atomic basis set, the cc-pVDZ-PP small-core relativistic basis set for gold[8] and cc-pVDZ for the remaining elements[9] appeared to be a good choice.[10] The optimized structures were characterized as minima or saddle points by frequency calculations. In order to fully prove the relevance of the transition structures we also computed the IRC (intrinsic reaction coordinate) connecting the critical points to confirm that the TS really relate the minima. Finally, to account for the dispersion effect and solvation effects on the reaction profile, punctual calculations on the optimized structures were performed by means of the Grimme's dispersion with the original D3 damping function[11] including the Polarizable Continuum Model (PCM), using the integral equation formalism variant and the dielectric constant of 1,2-dichloroethane (ε=10.1250).

[4] Gaussian 16, Revision C.01, Gaussian, Inc., Wallingford CT, 2019.
[5] A. D. Becke, *J. Chem. Phys.* 1993, **98**, 5648.
[6] J. P. Perdew, K. Burke and Y. Wang, *Phys. Rev. B* 1996, **54**, 16533.
[7] F. Jensen, *Introduction to Computational Chemistry*; Wiley, New York, 1999, p.283.
[8] (a) K. A. Peterson and C. Puzzarini, *Theor. Chem. Acc.* 2005, **114**, 283;(b) D. Figgen, G. Rauhut, M. Dolg and H. Stoll, *J. Chem. Phys.* 2005, **311**, 227.
[9] D. E. Woon, T. H. Dunning, *J. Chem. Phys.* 1993, **98**, 1358.
[10] This level of theory proved useful in the elucidation of reaction mechanisms of cationic gold-catalyzed reactions, see: (a) A. Fedorov, L. Batiste, A. Bach, D. M. Birney and P. Chen, *J. Am. Chem. Soc.* 2011, **133**, 12162; (b) A. S. K. Hashmi, A. M. Schuster, S. Litters, F. Rominger and M. Pernpointner, *Chem. Eur. J.* 2011, **17**, 5661; (c) J. Barluenga, R. Sigüeiro, R. Vicente, A. Ballesteros, M. Tomás and M. A. Rodríguez, *Angew. Chem. Int. Ed.* 2012, *51*, 10377; (d) E. Tudela, E.; J. González, R. Vicente, J. Santamaría, M. A. Rodríguez, A. Ballesteros, *Angew. Chem. Int. Ed.* 2014, **53**, 12097; e) J. González, D. Allegue, S. Fernández, M. A. Rodríguez, J. Santamaría, A. Ballesteros, *Adv. Synth. Catal.* 2020, **362**, 3912.
[11] (a) S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.* 2010, **132**, 154104; (b) J. Tomasi, B. Mennucci and R. Cammi, *Chem. Rev.* 2005, **105**, 2999.

Coordinates and Absolute Free-Energies (atomic units).

Model compound 4-Me-[Au]

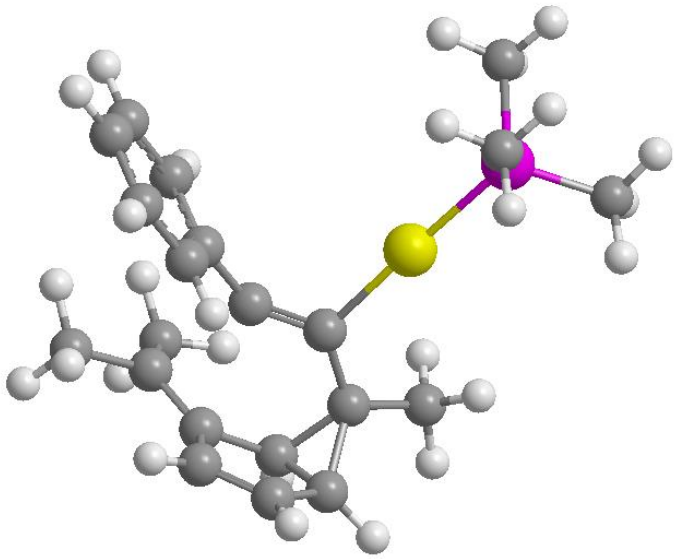


Au	1.28880000	-0.13730100	-0.12712800
P	3.53907000	-0.40176000	0.33974500
C	-1.31726300	-1.83212300	-1.02564400
C	-0.87375900	-0.49959800	-0.70072200
C	-0.75532500	0.71761900	-0.45424500
C	-2.55539800	-1.61569500	1.74255300
C	-1.49148500	-2.41157800	1.50064500
C	-1.49443400	-2.88068000	0.09116800
C	-2.72081500	-2.25992600	-0.52936900
H	-0.72288800	-2.68499000	2.22425500
H	-1.15404600	-3.88688100	-0.16529600
H	-3.30890800	-2.79179900	-1.27861800
C	-0.89383900	2.14157800	-0.28848700
C	-0.94585400	2.70716500	0.99886400
C	-0.99972500	2.96861100	-1.42199400
C	-1.11307300	4.08107200	1.14439800
H	-0.86761300	2.06095500	1.87484700
C	-1.16446300	4.34144600	-1.26244000
H	-0.95895200	2.52654700	-2.41881800
C	-1.22099700	4.89921100	0.01706900
H	-1.16191600	4.51707600	2.14399000

H	-1.25199100	4.98050700	-2.14308800
H	-1.35153800	5.97661300	0.13625900
H	-2.75248500	-1.12352200	2.69449300
C	-3.39896000	-1.47512900	0.55155600
C	-4.57458600	-0.80690900	0.43688200
C	-5.34242400	-0.73662300	-0.84935000
H	-6.37069500	-1.11079000	-0.70727500
H	-5.44260900	0.31235700	-1.17892500
H	-4.87995200	-1.30064000	-1.66885200
C	-5.21192800	-0.08070400	1.58438900
H	-5.33404100	0.98960800	1.34418700
H	-6.22778100	-0.47202000	1.76466600
H	-4.65075800	-0.15825300	2.52314200
C	-0.89655900	-2.33865600	-2.39297300
H	0.19950200	-2.40678500	-2.47313800
H	-1.30930400	-3.34231300	-2.57012900
H	-1.26064700	-1.67607100	-3.19271200
C	4.51152300	1.10765000	-0.01565200
H	4.13410900	1.94126100	0.59348300
H	5.57362800	0.93612700	0.21677900
H	4.40712200	1.37075000	-1.07784500
C	4.32613000	-1.73431700	-0.63766900
H	5.39460000	-1.80797900	-0.38366700
H	3.83326600	-2.69251700	-0.42008100
H	4.21984800	-1.51622900	-1.70982500
C	3.88307700	-0.80834900	2.09055000
H	3.38130400	-1.74988900	2.35531500
H	4.96697600	-0.91440600	2.24990900
H	3.49540900	-0.00795100	2.73667800

G: -1292,915894 u.a.

Model compound TS1

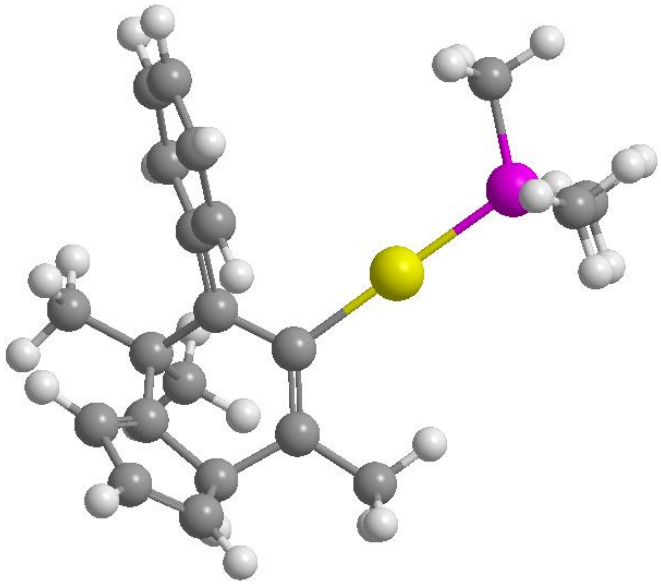


Au	1.31425100	-0.32457200	-0.07399600
P	3.56808100	0.23553300	0.00007900
C	-1.11043000	-2.28828100	-0.11483500
C	-0.69660100	-0.88423200	-0.13315200
C	-1.50327800	0.15448500	-0.21317600
C	-3.26973100	-1.08240000	1.67359600
C	-2.43937200	-2.02838300	2.17331700
C	-1.92798500	-2.90011100	1.10294700
C	-2.63025800	-2.47356300	-0.14578700
H	-2.13874300	-2.11680100	3.21808100
H	-1.68278600	-3.94357900	1.30474600
H	-3.05374900	-3.16911500	-0.87212000
C	-1.54075600	1.58444900	-0.00407900
C	-1.51233000	2.12334500	1.29806400
C	-1.59013100	2.46009200	-1.10725200
C	-1.54016000	3.50217300	1.48682600
H	-1.45931300	1.44763900	2.15323800
C	-1.59677800	3.83835600	-0.91100000
H	-1.59895300	2.04697700	-2.11771300
C	-1.58089600	4.36092600	0.38479800
H	-1.52006600	3.91194800	2.49873000
H	-1.61866900	4.50963100	-1.77178800

H	-1.59630300	5.44223000	0.53670500
H	-3.73761400	-0.28299700	2.24604100
C	-3.31810800	-1.21103600	0.21632800
C	-3.70213300	-0.26422600	-0.72733200
C	-3.69773800	-0.58617500	-2.19506200
H	-4.70340300	-0.93097800	-2.49626500
H	-3.48441100	0.31208300	-2.79280400
H	-2.97286200	-1.36306400	-2.46479800
C	-4.49869500	0.94424500	-0.33769800
H	-4.23795200	1.81696600	-0.95332000
H	-5.56489800	0.72649900	-0.52716700
H	-4.39468700	1.22027800	0.71809500
C	-0.25291800	-3.29595600	-0.84667100
H	0.73117500	-3.39704300	-0.36476100
H	-0.72660700	-4.28866100	-0.85649400
H	-0.08996800	-2.98485900	-1.88991700
C	4.68664500	-1.21658800	0.00142200
H	4.51863800	-1.80996600	-0.90876100
H	5.73822400	-0.89348900	0.03694600
H	4.46937400	-1.84623300	0.87611900
C	4.12459400	1.25594800	-1.41761400
H	5.19713400	1.48718500	-1.32963600
H	3.94454900	0.70988100	-2.35468500
H	3.54972600	2.19274300	-1.44203600
C	4.04435000	1.19637300	1.48686700
H	3.81425400	0.61213900	2.38933000
H	5.11970300	1.43041400	1.46745200
H	3.46743300	2.13170800	1.51823000

G: -1292,897868 u.a. (207i)

Model compound I

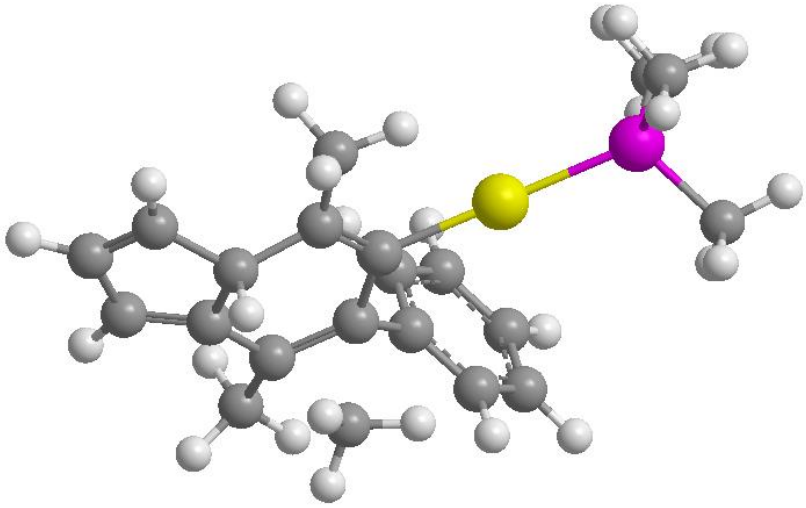


Au	-1.22625400	-0.46011000	0.06425600
P	-3.53297000	-0.12883200	0.02318400
C	1.41323000	-2.00581700	-0.08378800
C	0.82319200	-0.77843500	0.13645000
C	1.65927100	0.32855200	0.48063600
C	4.18293900	-0.21446000	-0.95683300
C	4.12461400	-1.18491400	-2.02807500
C	3.35943600	-2.23879100	-1.64013700
C	2.91804100	-2.03223600	-0.21449800
H	4.61866000	-1.07188500	-2.99323300
H	3.13054300	-3.12673500	-2.22888200
H	3.34578500	-2.81708800	0.43944100
C	1.29553700	1.67704600	0.01053800
C	0.95954400	1.86503200	-1.34502700
C	1.22136400	2.77573000	0.88605700
C	0.60014900	3.12347800	-1.81607800
H	1.01326100	1.01598700	-2.02935900
C	0.81801800	4.02457300	0.41832400
H	1.43784200	2.64563300	1.94637500
C	0.52219400	4.20524500	-0.93375600
H	0.37613100	3.26316900	-2.87556400
H	0.74346000	4.86359700	1.11280700

H	0.22970300	5.19097600	-1.30174300
H	4.67632500	0.75477400	-1.03153200
C	3.47887000	-0.68346500	0.12573600
C	2.94072100	0.07871000	1.30506800
C	2.73657600	-0.76791700	2.56633100
H	3.71362400	-1.07383000	2.96928900
H	2.22275000	-0.17575800	3.33823200
H	2.13674800	-1.66837300	2.38287000
C	3.79869400	1.29980900	1.63602400
H	3.40494900	1.84431500	2.50460500
H	4.81018500	0.95513200	1.89815300
H	3.88322000	2.00791100	0.80148700
C	0.67964000	-3.29808800	-0.20530400
H	-0.40322900	-3.15729100	-0.09283400
H	0.87019700	-3.79201800	-1.17215300
H	1.03103000	-3.99976700	0.57209000
C	-4.03633300	1.61890700	0.25880200
H	-3.59117800	2.23728200	-0.53372300
H	-5.13230400	1.71517200	0.22644800
H	-3.66693500	1.97761500	1.23021000
C	-4.43937400	-1.05212100	1.32295900
H	-5.52018700	-0.85460100	1.25722000
H	-4.25825300	-2.12970800	1.20118300
H	-4.07194100	-0.74610100	2.31297700
C	-4.33364600	-0.63402500	-1.54773100
H	-4.14832000	-1.70292900	-1.72647700
H	-5.41876600	-0.45442300	-1.50598900
H	-3.90078200	-0.06078900	-2.38009300

G: -1292,934840 u.a.

Model compound TS2

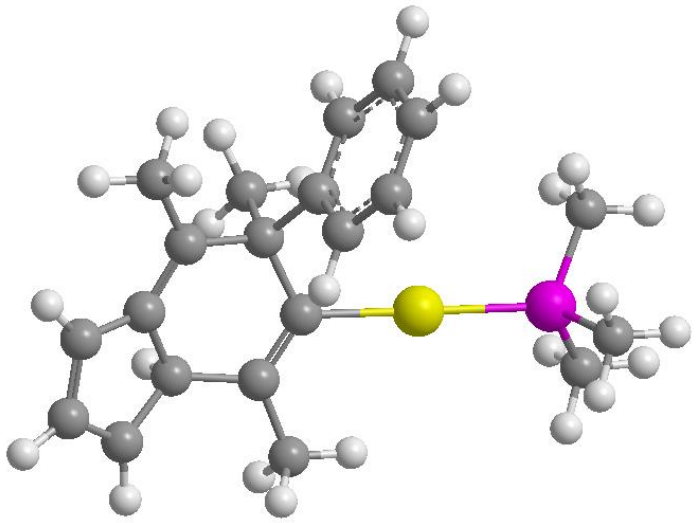


Au	1.12756400	-0.60636600	-0.06185300
P	3.45759200	-0.65590500	0.04671400
C	-1.70720800	-1.69921800	-0.01287100
C	-0.94169300	-0.57517700	-0.15634700
C	-1.60851300	0.73526600	-0.35126800
C	-5.02737500	-0.42671600	0.51517100
C	-5.25156700	-1.81989200	0.85816400
C	-4.17922000	-2.55829400	0.47705700
C	-3.20195600	-1.66675500	-0.23719900
H	-6.15290500	-2.19791800	1.34007500
H	-4.08055100	-3.64063800	0.55195700
H	-3.33110200	-2.00265700	-1.29629300
C	-0.78428000	1.96450400	-0.06515500
C	-0.66431700	2.29785900	1.29420500
C	-0.12711000	2.75358200	-1.01472900
C	0.09382900	3.39748200	1.69010900
H	-1.16072500	1.68172700	2.04777600
C	0.62953800	3.85765000	-0.61460600
H	-0.19198400	2.52662800	-2.08037000
C	0.74170400	4.18417100	0.73566600
H	0.17384400	3.64273600	2.75115700
H	1.12899000	4.46745100	-1.37022500
H	1.32827200	5.05174300	1.04424300
H	-5.71746900	0.38383100	0.75061400

C	-3.81545600	-0.30954000	-0.10176400
C	-3.03978000	0.88666700	-0.35088000
C	-2.33280500	0.81653700	-2.07228200
H	-2.93046700	1.65435900	-2.45003700
H	-1.29616100	0.96175700	-2.40563500
H	-2.67854900	-0.16169600	-2.40908000
C	-3.70076000	2.22244500	-0.13317900
H	-3.07616600	3.05812600	-0.46890100
H	-4.67415400	2.26440000	-0.64165600
H	-3.87636300	2.35460300	0.94556800
C	-1.13953200	-3.05030000	0.27915900
H	-0.04182100	-3.03120700	0.29736000
H	-1.50333700	-3.41142400	1.25716200
H	-1.47089700	-3.79145600	-0.46902600
C	4.18254000	-2.33961400	-0.03825400
H	3.88672600	-2.81812100	-0.98300500
H	5.28081200	-2.29563800	0.01987800
H	3.79865500	-2.94567200	0.79504500
C	4.14658600	0.05958800	1.58984900
H	5.24635000	0.01431900	1.58597000
H	3.82353000	1.10654300	1.68112500
H	3.76158500	-0.49988600	2.45459300
C	4.29865500	0.26852000	-1.29738900
H	3.98336500	1.32136000	-1.26778300
H	5.39223900	0.21164700	-1.18608900
H	4.00919400	-0.15603800	-2.26949100

G: -1292,897047 u.a. (477i)

Model compound II

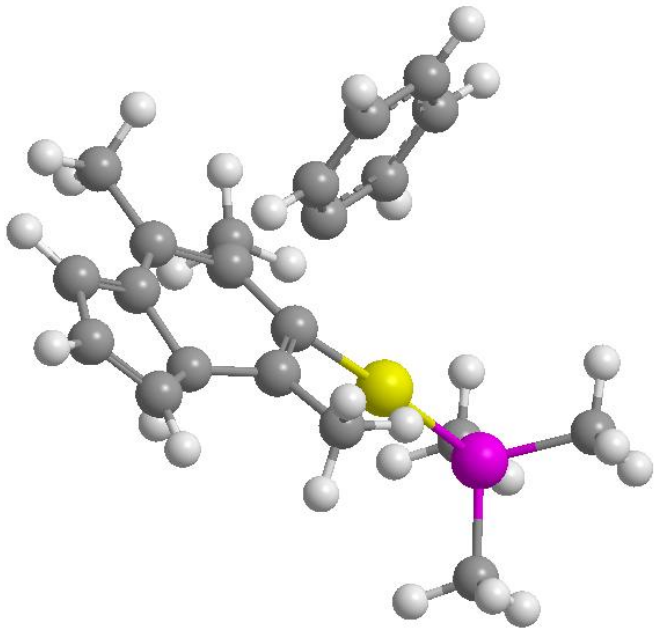


Au	1.14462000	-0.58631200	-0.08143300
P	3.47520100	-0.53694700	0.05458500
C	-1.64705800	-1.72237900	0.08276800
C	-0.92020000	-0.62133300	-0.21255800
C	-1.59027500	0.66459100	-0.73766400
C	-5.05211900	-0.48541000	0.42533400
C	-5.25335000	-1.81969900	0.85864500
C	-4.12842000	-2.55481300	0.55150900
C	-3.14342800	-1.71417200	-0.17333700
H	-6.15334900	-2.19437700	1.34459000
H	-4.00720700	-3.62475300	0.72862300
H	-3.25701500	-2.11519600	-1.21567800
C	-0.89387600	1.89561200	-0.13290000
C	-0.83417100	1.99512500	1.26762800
C	-0.33948200	2.92649000	-0.89863400
C	-0.24309000	3.09524400	1.88342800
H	-1.24495900	1.18744100	1.87974400
C	0.26236800	4.02754900	-0.28125300
H	-0.36217400	2.88616900	-1.98835500
C	0.30928900	4.11879500	1.10827500
H	-0.20837700	3.15313100	2.97364200
H	0.69150900	4.82094100	-0.89712600
H	0.77371400	4.98296100	1.58775700
H	-5.77539300	0.32150100	0.55391900

C	-3.77747200	-0.36376600	-0.15247000
C	-3.07446000	0.78859800	-0.45786900
C	-1.48419500	0.62962900	-2.29331600
H	-1.97011500	-0.27250600	-2.68970100
H	-1.93866800	1.51031400	-2.77034000
H	-0.41937400	0.58712400	-2.56435100
C	-3.72849800	2.12300500	-0.49073000
H	-3.29785600	2.74438900	-1.29013600
H	-4.81640300	2.06442800	-0.61819300
H	-3.50610100	2.66616600	0.44342900
C	-1.08315900	-3.03292100	0.54573000
H	0.01332700	-2.98703800	0.59462800
H	-1.46045400	-3.30505100	1.54752700
H	-1.35941900	-3.85752700	-0.13608000
C	4.26364100	0.71031500	-1.03732000
H	3.88007100	1.70903900	-0.78375500
H	5.35812800	0.69785100	-0.92082000
H	4.00652000	0.49345100	-2.08418900
C	4.30135600	-2.11462200	-0.39030200
H	5.39507500	-2.02170300	-0.30816700
H	3.95279000	-2.91194100	0.28192300
H	4.03498900	-2.38807000	-1.42147700
C	4.12138000	-0.14354200	1.72725300
H	3.76610700	-0.89879100	2.44310200
H	5.22202100	-0.12801400	1.72937600
H	3.74097700	0.83911000	2.04126900

G: -1292,928386 u.a.

Model compound TS3

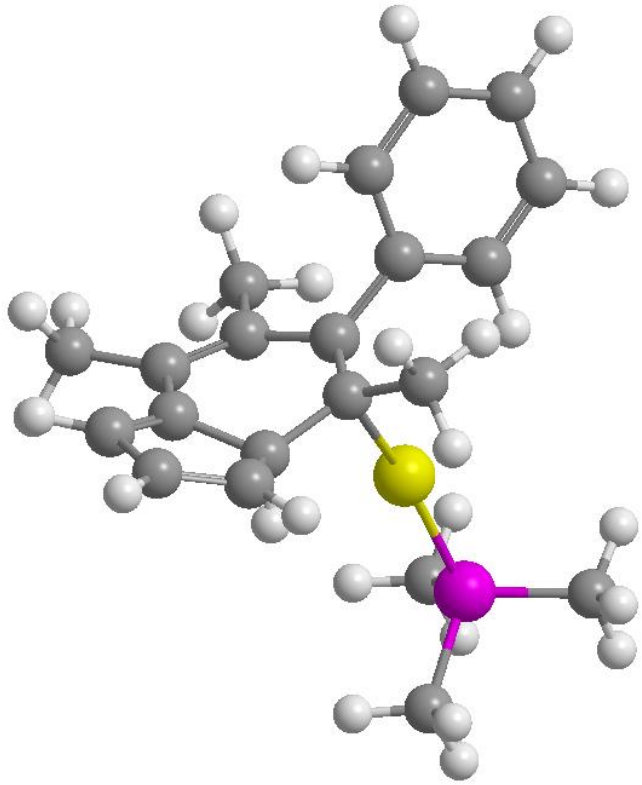


Au	-1.37335600	-0.23640300	0.04585400
P	-3.69970100	-0.31740600	0.03027300
C	1.33063700	-1.20442500	-0.79065300
C	0.72951400	-0.27158300	0.08516200
C	1.50647600	0.22837000	1.25024300
C	4.75885200	-1.52423300	0.42608000
C	4.80082000	-2.46023900	-0.64412900
C	3.54340200	-2.63851900	-1.17633800
C	2.58132000	-1.85666800	-0.35858100
H	5.70339000	-2.96743500	-0.98555500
H	3.27141700	-3.32081700	-1.98047000
H	2.17966900	-2.72510600	0.24558500
C	1.41038900	1.40470600	-0.15659500
C	2.52631000	1.55787100	-1.00302700
C	0.54070800	2.49497200	0.01897100
C	2.75980700	2.76769900	-1.64286100
H	3.22345600	0.73391800	-1.15862000
C	0.79396000	3.70629800	-0.62529100
H	-0.34303200	2.40511700	0.64754100
C	1.89826000	3.85482200	-1.46067300
H	3.63268800	2.86114100	-2.29251700
H	0.10342500	4.53834000	-0.47132200

H	2.08677200	4.80172300	-1.96885300
H	5.61821600	-1.24453800	1.03419700
C	3.44406400	-1.08591100	0.60825200
C	2.87923900	-0.14402900	1.46981800
C	0.77281900	0.81693500	2.43476300
H	0.80578200	0.09093100	3.26302700
H	1.21730100	1.75830900	2.78734400
H	-0.28699200	0.98778700	2.20543900
C	3.69568600	0.57413700	2.49612600
H	3.29032300	0.42750900	3.51003000
H	4.73888000	0.23672700	2.50410200
H	3.68907600	1.66178400	2.30613700
C	0.76349900	-1.59807900	-2.10179700
H	-0.16206600	-1.05514700	-2.33439900
H	1.51127600	-1.40419500	-2.89688900
H	0.55654300	-2.68305200	-2.15059400
C	-4.47170700	0.11794500	1.63577300
H	-4.18486300	1.14143600	1.91688800
H	-5.56838900	0.05409000	1.56733100
H	-4.11486400	-0.57249900	2.41347500
C	-4.37849500	-1.97200500	-0.37540200
H	-5.47892800	-1.95195000	-0.36444400
H	-4.03044100	-2.27730500	-1.37262800
H	-4.01999200	-2.70568800	0.36080200
C	-4.47856600	0.81527800	-1.18355100
H	-4.12715800	0.56657700	-2.19521300
H	-5.57513400	0.72789100	-1.14648500
H	-4.18765600	1.85128800	-0.95821200

G: -1292,871187 u.a. (493i)

Model compound III

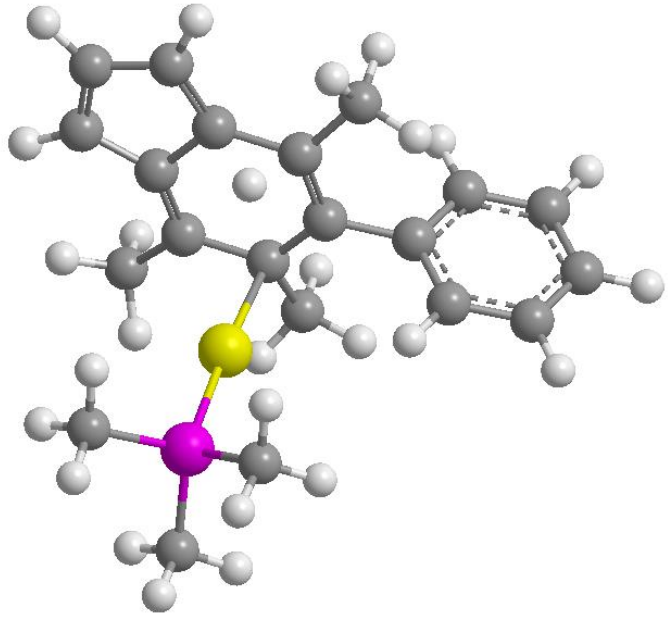


Au	-1.00463200	-0.06606200	-0.15945300
P	-3.28635500	-0.15786800	0.24794700
C	1.09706400	-0.44161400	-1.05798800
C	1.26952500	0.36534700	0.08497000
C	1.61151800	-0.21626000	1.40748600
C	2.90403500	-3.38396400	-0.06040900
C	2.65542100	-3.71114600	-1.45316200
C	1.75541100	-2.84407200	-1.98320000
C	1.27589200	-1.93936900	-0.88110900
H	3.12337900	-4.54123700	-1.98300300
H	1.34127300	-2.87270500	-2.99000500
H	0.27937400	-2.38666700	-0.64669600
C	1.54813300	1.83716500	-0.07974700
C	0.57211100	2.82366100	-0.26284800
C	2.89836200	2.22277700	-0.05486400
C	0.93216300	4.16314000	-0.42274700
H	-0.48533100	2.54331100	-0.27839100
C	3.25767900	3.55976300	-0.21615100
H	3.67315100	1.46543300	0.08732700

C	2.27564500	4.53472100	-0.39990400
H	0.15671200	4.91876300	-0.56390300
H	4.31278600	3.84043100	-0.19988100
H	2.55771400	5.58197100	-0.52425700
H	3.58982200	-3.92988300	0.58731000
C	2.15164100	-2.29648300	0.28705600
C	2.12506500	-1.49223100	1.48139900
C	1.51075700	0.68454500	2.61389100
H	1.13298700	0.13914200	3.49044200
H	2.48538500	1.11916200	2.89175600
H	0.83459800	1.52915300	2.42600800
C	2.73762900	-2.05938200	2.72892900
H	2.71096700	-1.36572700	3.57614400
H	2.23132000	-2.99216200	3.02517400
H	3.79334600	-2.31833800	2.54610500
C	1.15631400	0.08538600	-2.46284900
H	1.02123900	1.17180100	-2.51799700
H	2.14952200	-0.16812800	-2.87837200
H	0.41556200	-0.40437000	-3.11223900
C	-4.24298800	1.04046100	-0.75080300
H	-4.08017500	0.84281700	-1.81984900
H	-5.31593400	0.95192300	-0.52182500
H	-3.90595500	2.06213300	-0.52476500
C	-3.71935600	0.19516600	1.99108000
H	-4.81006100	0.13864800	2.12815700
H	-3.22984900	-0.53820000	2.64751400
H	-3.36935200	1.20146200	2.26180200
C	-4.01642200	-1.79617000	-0.11752100
H	-3.53448400	-2.56226400	0.50642100
H	-5.09704600	-1.78259000	0.09123000
H	-3.85326800	-2.04560500	-1.17564900

G: -1292,972670 u.a.

Model compound TS4

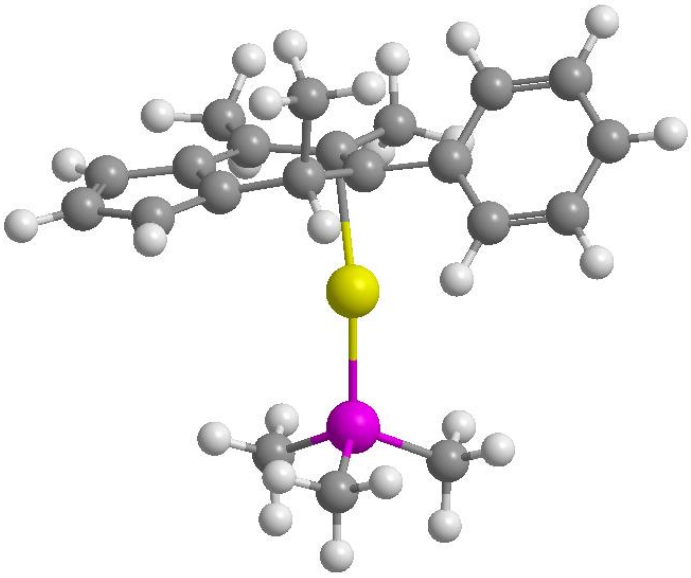


Au	0.98067600	-0.31672400	0.27658300
P	2.86728500	-1.34335600	-0.55431400
C	-1.75919400	1.28751200	-1.05488600
C	-1.71885200	0.34187400	0.01578700
C	-0.89623000	0.54854900	1.18960900
C	0.42126400	4.01528300	0.19483000
C	-0.00841300	4.56731400	-1.02362500
C	-0.84692700	3.67234700	-1.71786800
C	-0.98102000	2.53619200	-0.90263900
H	0.24784800	5.56680800	-1.37606400
H	-1.34032000	3.85768000	-2.66869700
H	-0.59924000	1.34080600	-1.49694500
C	-2.64517800	-0.82773300	-0.04268200
C	-2.22342400	-2.08518200	-0.49699100
C	-3.97933200	-0.66663700	0.36169000
C	-3.11368500	-3.15870300	-0.54388100
H	-1.18815400	-2.21795500	-0.82248500
C	-4.86712200	-1.74172300	0.31722800
H	-4.32407900	0.30705400	0.71815900
C	-4.43714000	-2.98957300	-0.13561100
H	-2.77204600	-4.13171600	-0.90319600
H	-5.90138500	-1.60149400	0.63807000

H	-5.13353800	-3.82956500	-0.17187500
H	1.06461000	4.50878000	0.91942200
C	-0.14832500	2.73417400	0.31182000
C	-0.12995800	1.77672200	1.33412500
C	-1.20931200	-0.27261600	2.43259900
H	-0.35713300	-0.34200700	3.11951800
H	-2.03833200	0.19973900	2.98677600
H	-1.52576200	-1.29059700	2.17784000
C	0.55955200	2.10457300	2.63021200
H	1.01833800	1.22910300	3.10723300
H	1.33859400	2.86259200	2.48374600
H	-0.17456300	2.51518100	3.34463300
C	-2.73771200	1.18885900	-2.19748100
H	-3.00493900	0.14893700	-2.41910000
H	-3.65929800	1.73508600	-1.94150500
H	-2.32881800	1.64878700	-3.10793200
C	3.70811100	-2.37485200	0.70162700
H	3.02190600	-3.15700100	1.05629400
H	4.60387600	-2.84378200	0.26658800
H	4.00274100	-1.74857700	1.55564100
C	4.13056400	-0.15859300	-1.14600500
H	5.01291900	-0.70129500	-1.51824200
H	3.71039200	0.45540700	-1.95518600
H	4.42892700	0.50294600	-0.32042800
C	2.54600100	-2.46110800	-1.96817300
H	2.09820000	-1.89224900	-2.79535900
H	3.48738200	-2.91888500	-2.30877500
H	1.84719100	-3.25231400	-1.66160500

G: -1292,937317 u.a. (1071i)

Model compound IV

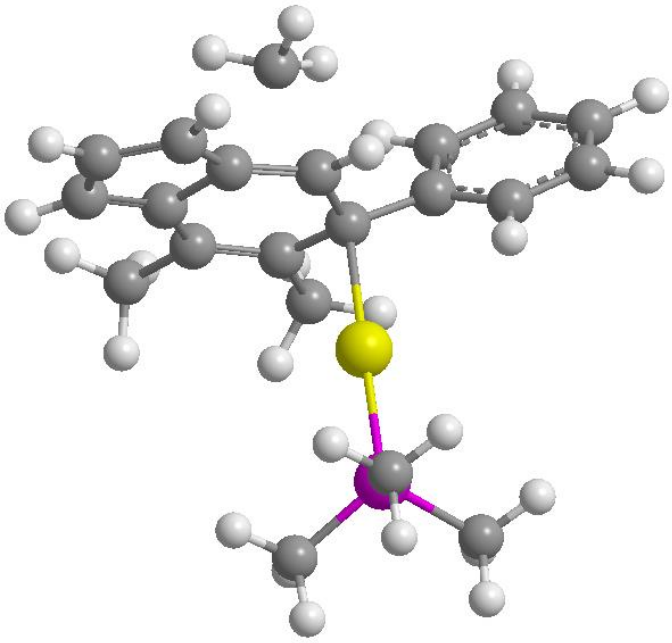


Au	-0.68294900	0.48384600	0.20016800
P	-2.60331700	1.69436200	-0.24670800
C	1.35394100	-1.36992600	-1.24732000
C	1.42940800	-0.48776400	-0.00184900
C	0.86359900	-0.91339400	1.21822400
C	-1.08466400	-4.00176400	-0.09072600
C	-1.15498700	-4.16996100	-1.44052700
C	-0.30217300	-3.17905100	-2.10822100
C	0.27616300	-2.39696500	-1.15661100
H	-1.75251600	-4.91827800	-1.96134600
H	-0.14661000	-3.11909500	-3.18581200
H	1.19882200	-0.72141500	-2.12605300
C	2.44049800	0.61355500	-0.08654300
C	2.30637900	1.62463800	-1.05326500
C	3.59524000	0.60365600	0.71281400
C	3.27485400	2.61743500	-1.18958700
H	1.42809900	1.63813500	-1.70406300
C	4.57097500	1.58887400	0.56619600
H	3.75046600	-0.19751400	1.43745700
C	4.41021800	2.60349900	-0.37801700
H	3.14630400	3.40124800	-1.93875800
H	5.46604200	1.55816300	1.19070400
H	5.17352600	3.37614500	-0.48859500

H	-1.62350100	-4.57220100	0.66213000
C	-0.20784600	-2.86239100	0.15178100
C	0.07853500	-2.18434800	1.30114100
C	1.19909700	-0.23767300	2.53026800
H	0.32324200	-0.17322200	3.18931500
H	1.95744400	-0.82938800	3.07028700
H	1.60406500	0.77035200	2.38608700
C	-0.40182500	-2.64940900	2.64238700
H	-1.08995200	-1.92410500	3.10641800
H	-0.92533900	-3.60860000	2.56358800
H	0.43702200	-2.78150300	3.34391500
C	2.73156000	-2.05885800	-1.43663300
H	3.53700700	-1.32079900	-1.55682700
H	2.96436600	-2.70531600	-0.57681600
H	2.69248700	-2.69055000	-2.33495600
C	-2.57732300	3.38384400	0.45393500
H	-1.72229900	3.93948700	0.04342600
H	-3.51096800	3.91109100	0.20537400
H	-2.46964200	3.32757700	1.54647900
C	-4.11425300	0.90191400	0.41513700
H	-4.99864500	1.50667900	0.16273000
H	-4.22106200	-0.10267900	-0.01822700
H	-4.03521200	0.81046500	1.50770300
C	-2.90339700	1.90117700	-2.03993000
H	-2.98604300	0.91300500	-2.51443800
H	-3.83447000	2.46517600	-2.20290700
H	-2.06392000	2.44532000	-2.49539300

G: -1292,976748 u.a.

Model compound TS5

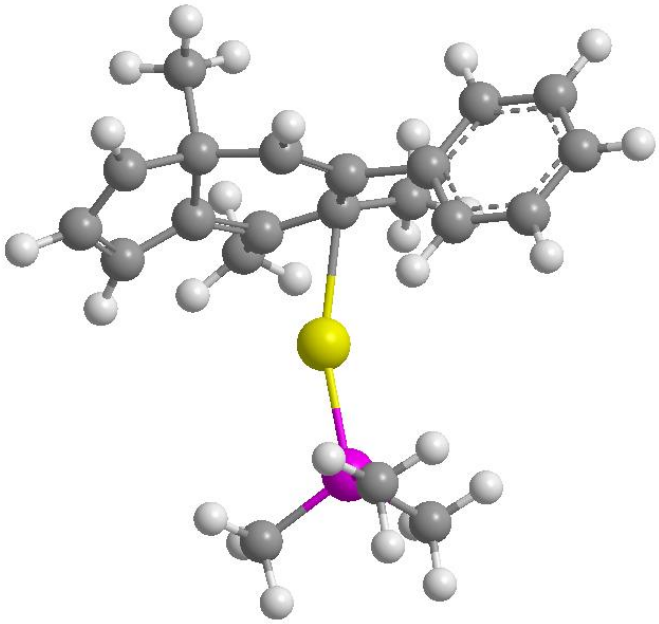


Au	-0.98524800	0.18146000	-0.01339400
P	-3.29485700	0.07941700	-0.05473800
C	1.52197800	-0.45384400	-1.17586800
C	1.21676700	0.30643400	0.03945200
C	1.34661900	-0.40848700	1.32009700
C	1.78373800	-3.90159500	-0.05968800
C	1.74260900	-4.08596800	-1.48763100
C	1.65802000	-2.88009500	-2.15308600
C	1.66880100	-1.86539800	-1.13991200
H	1.75587400	-5.06215800	-1.97518500
H	1.61877200	-2.71438300	-3.22690500
H	1.37210900	0.04764000	-2.13474800
C	1.66136100	1.75002300	-0.05509100
C	1.03373700	2.65746000	-0.92505400
C	2.80113900	2.18738600	0.64121700
C	1.51610800	3.95536800	-1.08310900
H	0.14739600	2.34174500	-1.48334700
C	3.28145200	3.48952600	0.48870400
H	3.32377700	1.50518500	1.31565800
C	2.64045300	4.37893600	-0.37215500
H	1.00656100	4.64259100	-1.76177000
H	4.16553500	3.80633700	1.04603000

H	3.01486900	5.39755500	-0.49029700
H	1.81574400	-4.70845500	0.66863600
C	1.70931700	-2.54737000	0.20122700
C	1.58271600	-1.78624700	1.39041300
C	1.16049500	0.36441400	2.60204800
H	0.42091400	-0.12717900	3.25251900
H	2.09733400	0.41604500	3.18183400
H	0.82925000	1.39365300	2.41834800
C	1.64441500	-2.49526700	2.71557400
H	0.63836200	-2.62729800	3.14948700
H	2.09200400	-3.49187200	2.61424900
H	2.24093500	-1.93816900	3.45225400
C	3.31293400	-0.86807300	-1.31432300
H	3.60783100	0.03984900	-0.76672900
H	3.80506700	-1.73539800	-0.85707200
H	3.51739300	-0.81220000	-2.38603400
C	-4.09483300	1.66695600	0.38552400
H	-3.77499000	2.44787200	-0.31899300
H	-5.19024100	1.56632100	0.34711200
H	-3.79076300	1.96310300	1.39963000
C	-4.00287700	-1.15312600	1.10094000
H	-5.10146100	-1.15506200	1.03174700
H	-3.61936900	-2.15273700	0.85147500
H	-3.70312600	-0.90672800	2.12951700
C	-3.97170200	-0.36209500	-1.69838200
H	-3.58974700	-1.34782000	-2.00013600
H	-5.07145900	-0.39154000	-1.66317300
H	-3.65061600	0.38287600	-2.44030700

G: -1292,914100 u.a. (579i)

Model compound V

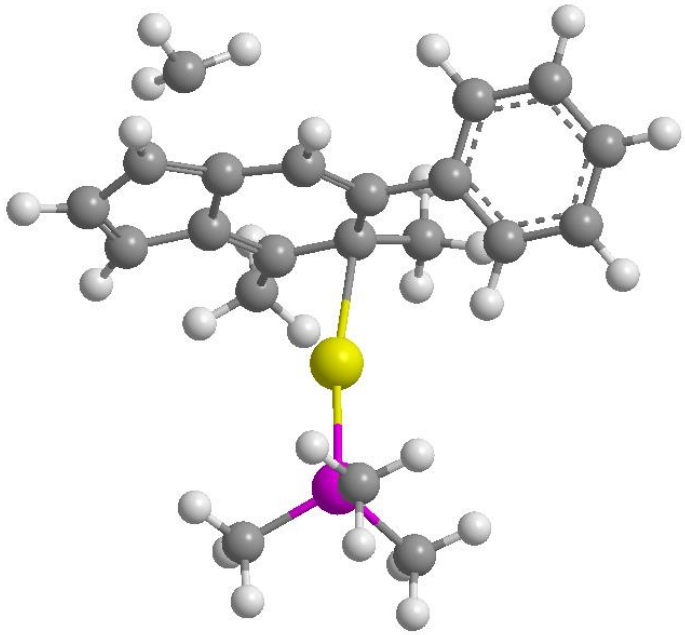


Au	-1.01493200	0.01144800	0.35258200
P	-2.90154100	1.09541200	-0.43254500
C	2.21746900	-0.95642400	-0.99405300
C	1.92993200	-0.04280600	-0.04047500
C	1.11386700	-0.41863300	1.16177600
C	-0.27528100	-3.40277600	-0.59259300
C	0.30539100	-3.85558800	-1.85035000
C	1.49457200	-3.23867500	-2.04497700
C	1.82566400	-2.39878100	-0.83951000
H	-0.15573700	-4.58643200	-2.51484400
H	2.18740400	-3.40780100	-2.87005900
H	2.84003000	-0.66717300	-1.84523200
C	2.43041200	1.35885600	-0.19025800
C	1.81760000	2.22857300	-1.10343500
C	3.54400400	1.81598400	0.52988900
C	2.29717500	3.52710100	-1.28536100
H	0.96650000	1.87179000	-1.68915400
C	4.02289900	3.11338000	0.34915200
H	4.05443800	1.14468700	1.22421300
C	3.39860700	3.97384100	-0.55562500
H	1.81469800	4.18934700	-2.00769300
H	4.89611800	3.45061300	0.91151300

H	3.77755300	4.98775900	-0.69866100
H	-1.24717400	-3.72081800	-0.21176100
C	0.57140900	-2.50554900	-0.01093400
C	0.40441800	-1.64237300	1.15834300
C	1.31480400	0.38302300	2.42407500
H	0.53961800	0.19398700	3.17569700
H	2.28445900	0.10910900	2.87561500
H	1.35216400	1.46025800	2.21843400
C	-0.25181200	-2.23884400	2.38085700
H	-0.60417200	-1.49238100	3.10304800
H	-1.10101500	-2.87638000	2.09900700
H	0.47801400	-2.88846800	2.89441500
C	3.01024600	-3.12118700	-0.11101600
H	3.91843400	-3.08059800	-0.73060200
H	3.22578800	-2.62164100	0.84496500
H	2.75588000	-4.17448100	0.07763900
C	-2.61349100	2.05486100	-1.96417400
H	-2.26117200	1.38294600	-2.75967600
H	-3.54629600	2.54341700	-2.28472300
H	-1.84651300	2.82005900	-1.77871000
C	-3.58133400	2.29076000	0.77464600
H	-4.47692100	2.77903800	0.36113000
H	-3.84737000	1.76563900	1.70300600
H	-2.82256900	3.05228900	1.00442700
C	-4.27858600	-0.04610800	-0.82323600
H	-4.55667700	-0.61048000	0.07816000
H	-5.15048500	0.52255200	-1.18102800
H	-3.96005000	-0.75418500	-1.60140900

G: -1292,967584 u.a.

Model compound TS6

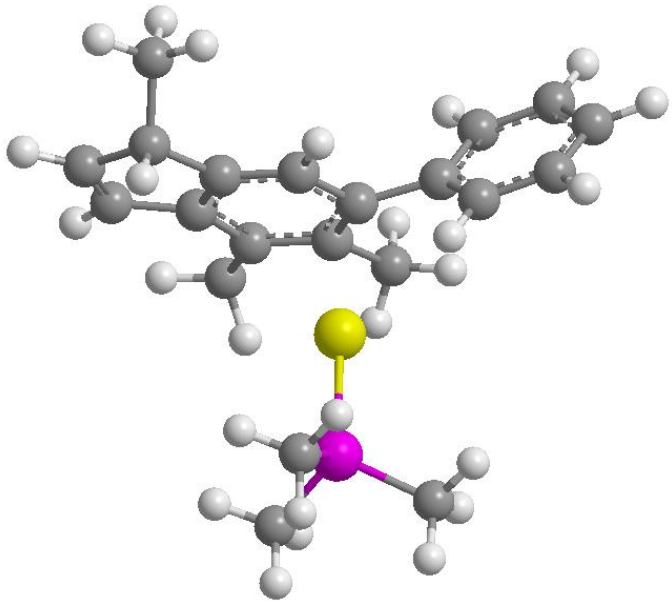


Au	1.02320000	-0.14916700	0.30927100
P	2.98867900	-0.93513300	-0.61015100
C	-2.08212700	0.87685100	-0.97457800
C	-1.83728100	-0.04984100	0.00456900
C	-1.01934900	0.28798000	1.19316100
C	0.00274300	3.73317600	-0.12341400
C	-0.52210100	4.22122800	-1.32305000
C	-1.50149900	3.32079700	-1.79200100
C	-1.59997300	2.22621900	-0.83692100
H	-0.25078100	5.15742800	-1.80748000
H	-1.99385300	3.34654900	-2.76250400
H	-2.67428000	0.59525700	-1.84820500
C	-2.43884800	-1.40660800	-0.13666400
C	-1.65947000	-2.57458700	-0.11986100
C	-3.82384800	-1.53403500	-0.32377900
C	-2.24467000	-3.82802900	-0.28694400
H	-0.57581500	-2.49464800	0.01032700
C	-4.41139600	-2.78873200	-0.48884300
H	-4.45076500	-0.63942600	-0.32258000
C	-3.62435500	-3.93951300	-0.47118300
H	-1.62048300	-4.72415400	-0.27856100
H	-5.49186400	-2.86554200	-0.62667900

H	-4.08326400	-4.92175000	-0.59979900
H	0.75767200	4.24338200	0.47460600
C	-0.61645000	2.50369500	0.19750400
C	-0.41110200	1.58416100	1.26749900
C	-1.24378500	-0.51691500	2.46029800
H	-0.43212300	-0.39914800	3.18816900
H	-2.17403600	-0.17448900	2.94651100
H	-1.36448300	-1.58625800	2.25455500
C	0.27435900	2.07654800	2.51731000
H	0.75668800	1.27855200	3.09441800
H	1.03310600	2.83447200	2.28207700
H	-0.47168600	2.55547800	3.17475400
C	-3.07788800	3.37961700	-0.52106100
H	-3.66656000	3.83899000	-1.32417000
H	-3.67044200	2.59379800	-0.04017700
H	-2.70482300	4.11914600	0.19338800
C	3.79977300	-2.21553300	0.41636100
H	3.12101000	-3.07073500	0.54388400
H	4.72946900	-2.55556400	-0.06482500
H	4.03229600	-1.79970000	1.40705000
C	4.25387400	0.36676400	-0.85079800
H	5.16463300	-0.06580800	-1.29250800
H	3.85730600	1.14476200	-1.51850800
H	4.49973500	0.82391400	0.11818900
C	2.76280200	-1.70014500	-2.25814000
H	2.34385600	-0.95785500	-2.95239000
H	3.72790000	-2.06045500	-2.64584300
H	2.06214600	-2.54358700	-2.18060200

G: -1292,935258 u.a. (620i)

Model compound VI

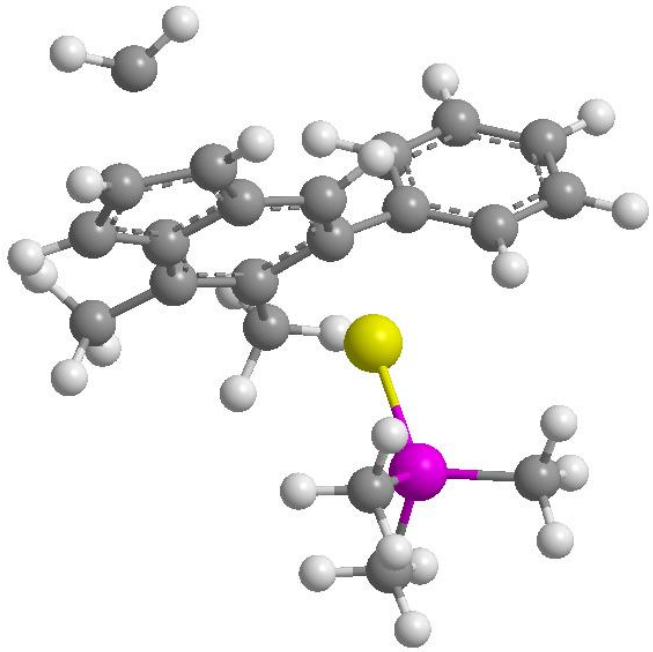


Au	-0.92466400	-0.05934800	0.08530900
P	-3.11742000	-0.55400700	-0.37896100
C	1.74443900	-0.09460000	-0.94934600
C	1.26724900	0.71780700	0.13107600
C	1.08475000	0.11674600	1.43109000
C	2.36953700	-3.38487900	0.46784300
C	2.77417800	-3.64535200	-0.79295200
C	2.62703700	-2.44317400	-1.68812000
C	2.06665700	-1.41625500	-0.73249400
H	3.17553800	-4.59682800	-1.14500500
H	1.86972800	-2.66549200	-2.46575300
H	1.90631600	0.37956200	-1.91972500
C	1.28387600	2.20433000	-0.07563500
C	0.51342000	2.81586600	-1.07614900
C	2.16820500	2.99909400	0.66950500
C	0.60436800	4.18803800	-1.30838800
H	-0.16688100	2.21024200	-1.68121900
C	2.26172500	4.37041600	0.43446900
H	2.80652200	2.53858400	1.42637500
C	1.47657200	4.97026500	-0.55074200
H	-0.00753100	4.64758400	-2.08732300
H	2.95971100	4.97173300	1.02052200
H	1.55001100	6.04417000	-0.73294300

H	2.38618500	-4.09383400	1.29464700
C	1.91601100	-1.99662700	0.55454700
C	1.41511600	-1.26309400	1.63534200
C	0.71497900	0.95705300	2.63140000
H	-0.02880300	0.45203300	3.26335500
H	1.60189900	1.12834100	3.26449600
H	0.31930700	1.93794000	2.34344000
C	1.27999100	-1.87404700	3.00180500
H	0.25231200	-1.79132800	3.38896100
H	1.54803500	-2.93686900	3.00014100
H	1.93377600	-1.36812800	3.73076200
C	3.92614400	-2.02623500	-2.39146700
H	3.76647600	-1.14245100	-3.02691400
H	4.71049800	-1.78801700	-1.65763100
H	4.29214900	-2.83898600	-3.03614800
C	-4.22824900	0.87808600	-0.12815600
H	-3.91613900	1.70538200	-0.78111300
H	-5.26615000	0.59701600	-0.36337500
H	-4.16750200	1.21214800	0.91730000
C	-3.80077800	-1.89419000	0.66389200
H	-4.85155600	-2.08318900	0.39580700
H	-3.21466400	-2.81205500	0.51449100
H	-3.74085200	-1.60364500	1.72229100
C	-3.39381500	-1.09468000	-2.10574400
H	-2.80449500	-2.00068900	-2.30624100
H	-4.46108200	-1.30946500	-2.26849100
H	-3.07155200	-0.30260800	-2.79640200

G: -1293,015402 u.a.

Model compound TS7

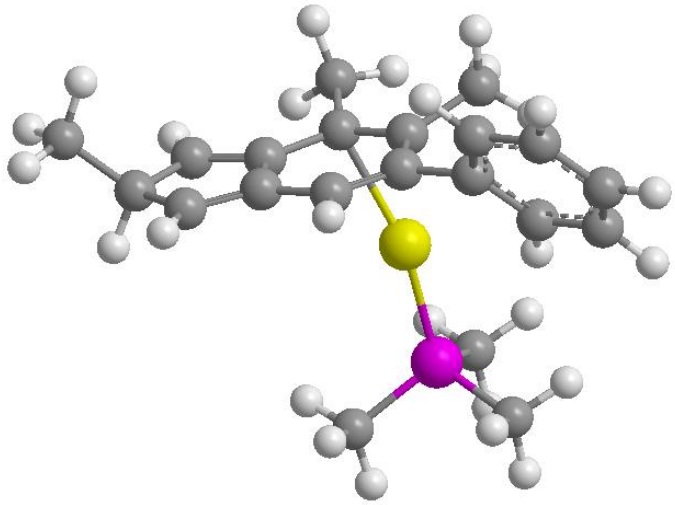


Au	-0.94497200	0.07138100	-0.17073800
P	-3.22370100	-0.09354700	0.12497000
C	1.20846200	-0.26144000	-1.01667600
C	1.32091200	0.60132600	0.10653300
C	1.56193100	0.03247000	1.43601600
C	1.82177400	-3.59178900	0.34937900
C	1.66250100	-3.93842600	-1.02095600
C	1.36809200	-2.72887300	-1.77492700
C	1.37088300	-1.65966900	-0.84385500
H	1.46846200	-4.94350700	-1.39378700
H	0.99957500	-2.69876600	-2.79792200
H	1.19171300	0.17749200	-2.01818400
C	1.58686000	2.05568500	-0.15330200
C	0.66594800	2.91284200	-0.77032800
C	2.86001100	2.55983200	0.16137200
C	1.00056500	4.23643800	-1.05958600
H	-0.33234000	2.54149700	-1.02170600
C	3.19428200	3.88180900	-0.12588200
H	3.60168800	1.90397800	0.62305900
C	2.26509300	4.72622500	-0.73583200
H	0.26572700	4.88807400	-1.53676100
H	4.19076300	4.25232000	0.12340300

H	2.52708300	5.76227300	-0.95898900
H	2.05617100	-4.29313500	1.14589300
C	1.66510900	-2.20193700	0.45688200
C	1.76299400	-1.33211000	1.59613600
C	1.58162400	0.96504100	2.62359800
H	0.96950000	0.57078900	3.44781000
H	2.60065300	1.10765500	3.01847400
H	1.19513000	1.95729600	2.36111300
C	2.07167600	-1.96270000	2.92255300
H	1.27609700	-2.66915800	3.21370700
H	3.00065300	-2.55162900	2.85371500
H	2.19566300	-1.23643000	3.73261100
C	3.18417300	-3.42491300	-1.97783000
H	3.18952400	-3.14334200	-3.03877300
H	3.73731700	-2.72204700	-1.34926300
H	3.59880200	-4.43874600	-1.89621500
C	-3.91868500	-1.69777900	-0.41929000
H	-3.44415000	-2.51346600	0.14449900
H	-5.00592700	-1.71829700	-0.24857400
H	-3.71410200	-1.84240800	-1.48959300
C	-4.15981500	1.18089100	-0.79669900
H	-5.23967300	1.05866100	-0.62202400
H	-3.84720700	2.18025700	-0.46205000
H	-3.95077800	1.08625600	-1.87175800
C	-3.74096100	0.09080000	1.87157400
H	-3.41773600	1.07134800	2.24891500
H	-4.83560900	0.00934000	1.95379400
H	-3.26926700	-0.69456800	2.47906400

G: -1292,938828 u.a. (693i)

Model compound VII

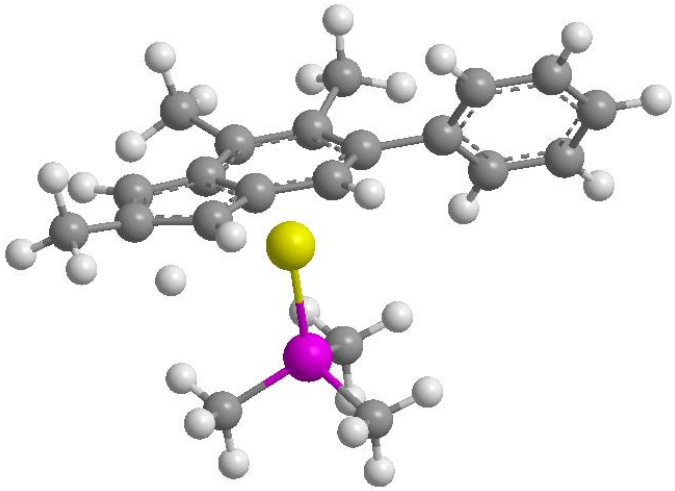


Au	-0.86962300	0.61256500	0.32656200
P	-2.18792000	2.25506300	-0.63883900
C	1.56107100	-1.67423800	-0.95869500
C	1.82079700	-0.71651500	-0.02014400
C	0.94621600	-0.56660300	1.17793300
C	-1.49092500	-3.29708300	0.20533700
C	-1.28706500	-4.11152400	-1.03694900
C	-0.03830300	-3.54335700	-1.63711000
C	0.41279700	-2.52600900	-0.85014400
H	-2.12990000	-3.87876800	-1.72568400
H	0.41913700	-3.90836200	-2.55669500
H	2.23400900	-1.78404800	-1.81216700
C	3.02610200	0.14416800	-0.17828900
C	2.92400200	1.53958000	-0.29970800
C	4.29755800	-0.44327700	-0.25871000
C	4.05914500	2.32400900	-0.49502700
H	1.93884000	2.01349300	-0.25990500
C	5.43457100	0.34235000	-0.45201600
H	4.39570300	-1.52641600	-0.15545300
C	5.31940300	1.72703300	-0.56966400
H	3.96080800	3.40699800	-0.59626600
H	6.41630500	-0.13255500	-0.50680400
H	6.20908700	2.34165700	-0.72016200
H	-2.31369800	-3.46126800	0.90034900

C	-0.49998000	-2.36516800	0.29410500
C	-0.21381100	-1.36872100	1.32748800
C	1.52839000	0.17531000	2.35766600
H	0.78898400	0.39615900	3.13495100
H	2.31063300	-0.45965500	2.80981900
H	2.01926600	1.10909100	2.06129100
C	-0.95762700	-1.51358100	2.63269100
H	-0.89655300	-0.62915900	3.27672700
H	-2.01958600	-1.73211700	2.45568200
H	-0.53840300	-2.36792300	3.19148700
C	-1.27269900	-5.63435700	-0.82351600
H	-0.45645800	-5.92395000	-0.14555200
H	-2.22397000	-5.97459500	-0.38864200
H	-1.13031600	-6.15693800	-1.78060100
C	-1.21980200	3.56051900	-1.48107800
H	-0.60046200	3.11012700	-2.26972000
H	-1.89822000	4.30330100	-1.92792800
H	-0.56280100	4.05911500	-0.75436400
C	-3.24437200	3.13064500	0.57176400
H	-3.84916500	3.89617700	0.06217300
H	-3.91013400	2.41071000	1.06858900
H	-2.61279800	3.61113700	1.33250300
C	-3.33044200	1.59698700	-1.90829200
H	-3.99829700	0.85244000	-1.45232500
H	-3.93126400	2.41416400	-2.33582400
H	-2.75190600	1.11158500	-2.70711300

G: -1292,987300 u.a.

Model compound TS8

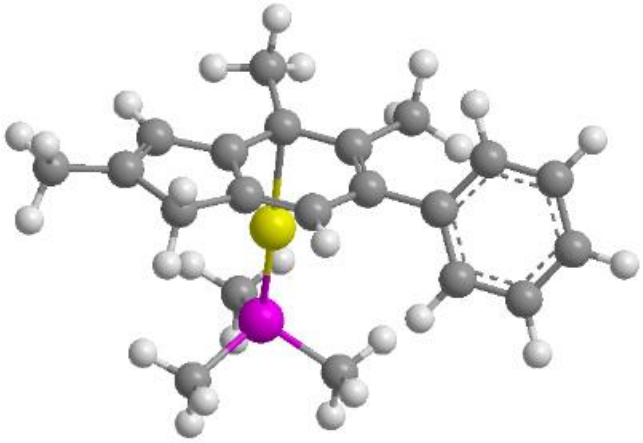


Au	0.71678600	-0.74996400	0.32001000
P	1.69124100	-2.60984000	-0.63931200
C	-1.19009900	1.94680000	-0.91180200
C	-1.66207900	1.04065900	0.01496200
C	-0.86923900	0.72415100	1.20620400
C	2.07318300	3.00179600	0.33330200
C	2.03074900	3.81692200	-0.84093000
C	0.73198900	3.54398900	-1.50685500
C	0.06643400	2.57208500	-0.73818400
H	2.02316400	3.00452800	-1.77770700
H	0.39194400	4.04473500	-2.41212400
H	-1.80455600	2.18662300	-1.78253200
C	-3.01029700	0.44065700	-0.19339300
C	-3.18526500	-0.94289100	-0.35802400
C	-4.13820000	1.27104500	-0.27339300
C	-4.44999300	-1.48034900	-0.59084700
H	-2.31378100	-1.60284600	-0.31826200
C	-5.40465600	0.73335600	-0.50711000
H	-4.02192400	2.34883300	-0.13738300
C	-5.56488900	-0.64284000	-0.66494800
H	-4.56663800	-2.55823900	-0.72295300
H	-6.27118300	1.39566600	-0.56119800
H	-6.55578500	-1.06357400	-0.84687800
H	2.90066500	2.99598300	1.03920800

C	0.89533100	2.25082100	0.39416500
C	0.42657400	1.30126400	1.38398200
C	-1.57134000	0.06374300	2.37231600
H	-0.88283800	-0.43372900	3.06518000
H	-2.10717800	0.84225800	2.94294800
H	-2.32105100	-0.66386900	2.04370800
C	1.16082200	1.26632200	2.70382000
H	0.93367700	0.38215800	3.31006900
H	2.24814900	1.30146000	2.55101400
H	0.88554800	2.15628700	3.29553300
C	2.91739000	4.98984000	-1.14847200
H	2.57952700	5.86901200	-0.57797700
H	3.96091100	4.78604200	-0.87077700
H	2.88898300	5.25478700	-2.21478000
C	1.08306300	-2.96588800	-2.32890900
H	1.29013700	-2.10688600	-2.98285000
H	1.58249500	-3.86067500	-2.73082200
H	-0.00286700	-3.13424100	-2.30278700
C	1.40184700	-4.14119100	0.32051500
H	1.89139500	-4.99514000	-0.17211100
H	1.80901000	-4.02214200	1.33464300
H	0.32185300	-4.33224100	0.39398900
C	3.51007800	-2.47096800	-0.79613400
H	3.95513200	-2.32747000	0.19870000
H	3.92148200	-3.38424800	-1.25252800
H	3.76060900	-1.60423700	-1.42405000

G: -1292,969259 u.a. (1050i)

Model compound 5-Me-[Au]



Au	1.02780700	-0.47800300	0.33066600
P	2.23951200	-2.23100800	-0.52455200
C	-1.53843300	1.56375700	-0.97707900
C	-2.02055800	0.68160100	0.01416500
C	-1.28722000	0.49119800	1.21085100
C	1.52519900	3.01699000	0.34233700
C	1.50095900	3.71469300	-0.82170600
C	0.32153700	3.28215200	-1.65508300
C	-0.34866800	2.24443300	-0.80208900
H	0.63897000	2.88800000	-2.63697300
H	-0.35231100	4.12918700	-1.87352000
H	-2.14035300	1.71884400	-1.87566700
C	-3.32135400	0.00114000	-0.24414500
C	-3.46196800	-0.84419000	-1.35551700
C	-4.44148100	0.23505600	0.56835900
C	-4.68441000	-1.45384400	-1.63744200
H	-2.60022500	-1.03070300	-2.00172400
C	-5.66515400	-0.36925300	0.28219500
H	-4.36125400	0.91503000	1.41940700
C	-5.78920400	-1.21854400	-0.81834200
H	-4.77493600	-2.11395800	-2.50275500
H	-6.52906000	-0.16881600	0.91933000
H	-6.74779800	-1.69158900	-1.04066600
H	2.26805600	3.14281300	1.12952900
C	0.40044600	2.08811400	0.38894200

C	-0.04218600	1.20230400	1.42272900
C	-1.82682100	-0.37834700	2.31717400
H	-1.03100400	-0.93523500	2.82971700
H	-2.32798200	0.23643700	3.08394000
H	-2.56292200	-1.09732200	1.93916700
C	0.55618100	1.32241600	2.81057000
H	0.51951400	0.38453200	3.37855600
H	1.60277000	1.65068200	2.77461000
H	-0.00704100	2.07513800	3.38830800
C	2.45396000	4.76843200	-1.26477400
H	3.24940700	4.93691300	-0.52653800
H	2.92352400	4.49912600	-2.22589000
H	1.93170100	5.72530300	-1.43274700
C	1.20761700	-3.66018200	-1.01751600
H	0.49432500	-3.34902800	-1.79377900
H	1.84324200	-4.46962900	-1.40798300
H	0.64429700	-4.02481200	-0.14688100
C	3.45366400	-2.89489200	0.67298600
H	4.01076600	-3.73034100	0.22217700
H	4.15680600	-2.10151700	0.96355500
H	2.92889100	-3.24916700	1.57155900
C	3.21052800	-1.79440100	-2.01364400
H	3.91224600	-0.98405700	-1.77027200
H	3.77283500	-2.67114500	-2.36974600
H	2.53232100	-1.44915100	-2.80685200

G: -1293,022823 u.a.