Supporting Information

Gold(I) Carbenes by Retro-Buchner Reaction: Generation and Fate

Yahui Wang, Paul R. McGonigal, Bart Herlé, Maria Besora, and Antonio M. Echavarren*

Institute of Chemical Research of Catalonia (ICIQ), Av. Països Catalans 16, 43007 Tarragona (Spain)

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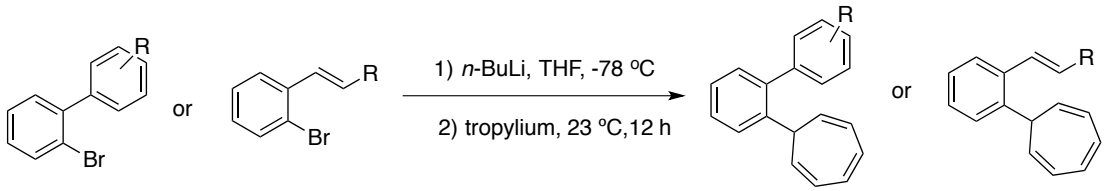
1. General Methods.

All reactions were carried out under Argon in solvents dried using a Solvent Purification System (SPS). Thin layer chromatography was carried out using TLC aluminum sheets with 0.2 mm of silica gel (Merck Gf234). Chromatographic purifications were carried out using flash grade silica gel (SDS Chromatogel 60 ACC, 40-60 μm). NMR spectra were recorded at 23 ºC on a Bruker Avance 400 Ultrashield and Bruker Avance 500 Ultrashield apparatus. Mass spectra were recorded on a Waster LCT Premier Spectrometer (ESI and APCI) or on an Autoflex Broker Daltonics (MALDI and LDI). Melting points were determined using a Büchi melting point apparatus.

2. General Procedure for the Synthesis of Arylcycloheptatrienes.



Procedure A:

n-BuLi (1.6 M in hexanes, 0.33 mL, 0.53 mmol) was added dropwise to the solution of corresponding aryl bromide[1] (0.5 mmol) in dry THF (2 mL, 0.2 M) at -78 ºC under argon. The mixture was stirred for 30 min at -78 ºC, and then tropylium tetrafluoroborate or tropylium bromide[2] (0.33 mmol) was added in one portion. The cooling bath was removed and the reaction was stirred at room temperature (23 ºC) for 12 h. The reaction was quenched by addition of water. The aqueous phase was extracted with ether, the combined organic extracts were dried over $MgSO_4$, and the solvent was evaporated. The crude reaction mixture was purified by column chromatography on silica gel with cyclohexane as eluent unless otherwise stated.

Procedure A-2:

n-BuLi (1.6 M in hexanes, 0.63 mL, 1 mmol) was added dropwise to the solution of corresponding aryl bromide (0.5 mmol) in dry THF (5 mL, 0.1 M) at -78 ºC under argon. The mixture was stirred for 30 min at -78 ºC, and then tropylium tetrafluoroborate or tropylium bromide (1 mmol) was added in one portion. The cooling bath was removed and the reaction was stirred at room temperature (23 ºC) for 12 h. The reaction was quenched by addition of water. The aqueous phase was extracted with ether, the combined organic extracts were dried over $MgSO_4$, and the solvent was evaporated. The crude reaction mixture was purified by column chromatography on silica gel with cyclohexane as eluent unless otherwise stated.

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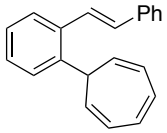
(1) The aryl bromides were prepared according to the literature procedures: (a) Li, C.-W.; Wang, C.-I.; Liao, H.-Y.; Chaudhuri, R.; Liu, R.-S. *J. Org. Chem.* **2007**, *72*, 9203–9207. (b) Rossi, R.; Carpita, A.; Ribecai, A.; Mannina, L. *Tetrahedron*. **2001**, *57*, 2847–2856. (c) Qi, W.-Y.; Zhu, T.-S.; Xu, M.-H. *Org. Lett.* **2011**, *13*, 3410–3413. (d) de Meijere, A.; Song, Z.-Z.; Lanskya, A.; Hyudaa, S.; Raucha, K.; Noltemeyera, M.; Konig, B.; Knieriem, B. *Eur. J. Org. Chem.* **1998**, 2289–2299.

(2) Tropylium bromide was prepared according to the reported procedure: Doering, W. E.; Knox, L. H. *J. Am. Chem. Soc*. **1957**, *79*, 352–356. Tropylium tetrafluoroborate was purchased from Alfa Aesar.

Experimental Details for the Synthesis of *o*-Alkenyl Cycloheptatrienes

(*E*)-7-(2-Styrylphenyl)cyclohepta-1,3,5-triene (7a)

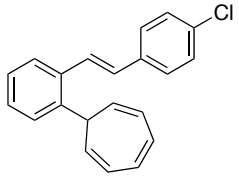


This compound was prepared as a yellow oil in 74% yield according to the general procedure A.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (dd, *J* = 6.9, 2.2 Hz, 1H), 7.52 - 7.42 (m, 3H), 7.39 - 7.26 (m, 6H), 6.96 (d, *J* = 16.1 Hz, 1H), 6.78 (t, *J* = 3.2 Hz, 2H), 6.35 - 6.29 (m, 2H), 5.48 (dd, *J* = 9.0, 5.4 Hz, 2H), 3.12 (tt, *J* = 5.6, 1.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.0, 137.5, 136.4, 130.9, 130.6, 128.6, 127.9, 127.6, 127.6, 126.9, 126.6, 126.6, 126.5, 124.5, 42.5.

HRMS-APCI calculated for $C_{21}H_{19}$ $[M+H]^+$: 271.1487; found: 271.1497

(*E*)-7-(2-(4-Chlorostyryl)phenyl)cyclohepta-1,3,5-triene (7b)



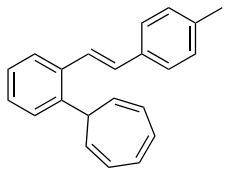
This compound was prepared as a colorless solid in 63% yield according to the general procedure A.

m.p. 65-67 ºC

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.66 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.52 (dd, *J* = 7.5, 1.6 Hz, 1H), 7.40 - 7.30 (m, 6H), 7.26 (d, *J* = 16.0 Hz, 1H), 6.91 (d, *J* = 16.0 Hz, 1H), 6.79 (t, *J* = 3.2 Hz, 2H), 6.35 - 6.30 (m, 2H), 5.47 (dd, *J* = 9.1, 5.4 Hz, 2H), 3.09 (t, *J* = 5.4 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.0, 136.0, 136.0, 133.1, 130.9, 129.2, 128.8, 128.1, 127.7, 127.6, 127.2, 126.9, 126.5, 126.4, 124.5, 42.5.

HRMS-APCI calculated for $C_{21}H_{18}Cl$ $[M+H]^+$: 305.1097; found: 305.1092

(*E*)-7-(2-(4-Methylstyryl)phenyl)cyclohepta-1,3,5-triene (7c)



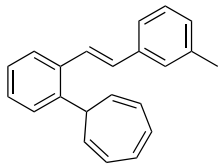
This compound was prepared as a colorless solid in 76% yield according to the general procedure A.

m.p. 70-72 ºC

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.68 (dd, *J* = 7.0, 2.3 Hz, 1H), 7.51 (dd, *J* = 7.2, 2.0 Hz, 1H), 7.39 - 7.33 (m, 4H), 7.25 (d, *J* = 15.9 Hz, 1H), 7.17 (d, *J* = 7.9 Hz, 2H), 6.94 (d, *J* = 16.1 Hz, 1H), 6.78 (t, *J* = 3.2 Hz, 2H), 6.33 - 6.29 (m, 2H), 5.49 (dd, *J* = 9.1, 5.4 Hz, 2H), 3.12 (t, *J* = 5.4 Hz, 1H), 2.38 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.9, 137.5, 136.6, 134.8, 130.9, 130.5, 129.3, 127.7, 127.6, 126.8, 126.6, 126.5, 126.4, 125.6, 124.5, 42.5, 21.2.

HRMS-APCI calculated for $C_{22}H_{21}$ $[M+H]^+$: 285.1643; found: 285.1641

(*E*)-7-(2-(3-Methylstyryl)phenyl)cyclohepta-1,3,5-triene (7d)

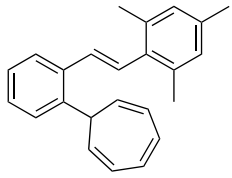


This compound was prepared as a yellow oil in 83% yield according to the general procedure A.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (dd, *J* = 7.0, 2.2 Hz, 1H), 7.51 (dd, *J* = 7.3, 1.9 Hz, 1H), 7.39 - 7.32 (m, 2H), 7.31 - 7.24 (m, 4H), 7.09 (d, *J* = 6.9 Hz, 1H), 6.93 (d, *J* = 16.1 Hz, 1H), 6.79 (t, *J* = 3.2 Hz, 2H), 6.36 - 6.29 (m, 2H), 5.49 (dd, *J* = 9.0, 5.4 Hz, 2H), 3.12(t, *J* = 5.3 Hz, 1H), 2.38 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.0, 138.2, 137.5, 136.5, 130.9, 130.8, 128.5, 128.4, 127.8, 127.6, 127.4, 126.9, 126.6, 126.5, 126.4, 124.5, 123.5, 42.5, 21.4.

HRMS-APCI calculated for $C_{22}H_{21}$ $[M+H]^+$: 285.1643; found: 285.1634

(*E*)-7-(2-(2,4,6-Trimethylstyryl)phenyl)cyclohepta-1,3,5-triene (7e)



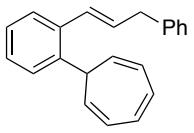
This compound was prepared as a white solid in 60% yield according to the general procedure A.

m.p. 89-91 ºC

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (dd, *J* = 7.1, 2.2 Hz, 1H), 7.53 (dd, *J* = 7.2, 2.0 Hz, 1H), 7.40 – 7.36 (m, 2H), 6.98 - 6.88 (m, 3H), 6.80 - 6.70 (m, 3H), 6.27 – 6.25 (m, 2H), 5.46 (dd, *J* = 9.0, 5.4 Hz, 2H), 3.07 (dd, *J* = 6.2, 4.6 Hz, 1H), 2.30 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.9, 137.1, 136.3, 136.1, 134.2, 131.6, 130.9, 129.1, 128.6, 127.8, 127.3, 126.8, 126.6, 126.5, 124.5, 42.2, 21.1, 20.9.

HRMS-APCI calculated for $C_{24}H_{25}$ $[M+H]^+$: 313.1956; found: 313.1960

(*E*)-7-(2-(3-Phenylprop-1-en-1-yl)phenyl)cyclohepta-1,3,5-triene (7f)

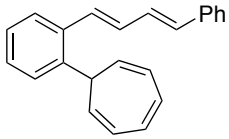


This compound was prepared as a yellow oil in 49% yield according to the general procedure A.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.47 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.33 - 7.30 (m, 3H), 7.28 - 7.19 (m, 4H), 6.76 (t, *J* = 3.2 Hz, 2H), 6.59 (d, *J* = 15.5 Hz, 1H), 6.29 - 6.27 (m, 2H), 6.19 (dt, *J* = 15.5, 6.9 Hz, 1H), 5.43 (dd, *J* = 9.1, 5.4 Hz, 2H), 3.52 (dd, *J* = 7.0, 1.5 Hz, 2H), 3.04 (t, *J* = 5.3 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.4, 140.1, 136.8, 131.4, 130.8, 129.0, 128.6, 128.4, 127.4, 127.3, 126.8, 126.7, 126.6, 126.0, 124.4, 42.2, 39.5.

HRMS-APCI calculated for $C_{22}H_{21}$ $[M+H]^+$: 285.1643; found: 285.1649

7-(2-((1*E*,3*E*)-4-Phenylbuta-1,3-dien-1-yl)phenyl)cyclohepta-1,3,5-triene (7g)



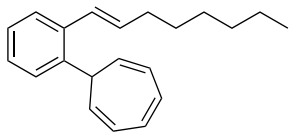
This compound was prepared as a colorless solid in 82% yield according to the general procedure A from 1-bromo-2-((1*E*,3*E*)-4-phenylbuta-1,3-dien-1-yl)benzene (see **7u** synthesis).

m.p. 124-125 ºC

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.68 - 7.64 (m, 1H), 7.49 - 7.44 (m, 3H), 7.37 - 7.30 (m, 4H), 7.25 (t, *J* = 7.3 Hz, 1H), 6.94 (ddd, *J* = 15.5, 5.9, 4.1 Hz, 1H), 6.90 - 6.84 (m, 2H), 6.79 (dd, *J* = 3.7, 2.7 Hz, 2H), 6.68 (d, *J* = 15.3 Hz, 1H), 6.36 - 6.29 (m, 2H), 5.45 (dd, *J* = 9.0, 5.3 Hz, 2H), 3.10 (t, *J* = 5.6 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.8, 137.3, 136.1, 132.8, 131.0, 130.9, 130.3, 129.5, 128.6, 127.9, 127.5, 126.8, 126.8, 126.4, 126.2, 124.5, 42.4.

HRMS-APCI calculated for $C_{23}H_{21}$ $[M+H]^+$: 297.1643; found: 297.1650

(*E*)-7-(2-(Oct-1-en-1-yl)phenyl)cyclohepta-1,3,5-triene (7h)

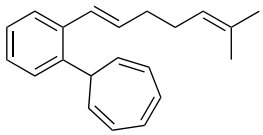


This compound was prepared as a yellow oil in 69% yield according to the general procedure A.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (dd, *J* = 7.2, 1.9 Hz, 1H), 7.45 (dd, *J* = 7.3, 1.8 Hz, 1H), 7.32 - 7.24 (m, 2H), 6.76 (t, *J* = 3.2 Hz, 2H), 6.50 (d, *J* = 15.5 Hz, 1H), 6.32 - 6.26 (m, 2H), 6.03 (dt, *J* = 15.5, 6.9 Hz, 1H), 5.43 (dd, *J* = 9.1, 5.5 Hz, 2H), 3.05 (t, *J* = 5.2 Hz, 1H), 2.17 (qd, *J* = 7.1, 1.5 Hz, 2H), 1.45 - 1.25 (m, 8H), 0.90 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.2, 137.2, 133.5, 130.8, 127.5, 127.4, 127.1, 126.9, 126.7, 126.6, 124.3, 42.3, 33.2, 31.7, 29.2, 28.8, 22.6, 14.1.

HRMS-APCI calculated for $C_{21}H_{27}$ $[M+H]^+$: 279.2113; found: 279.2108

(*E*)-7-(2-(6-Methylhepta-1,5-dien-1-yl)phenyl)cyclohepta-1,3,5-triene (7i)

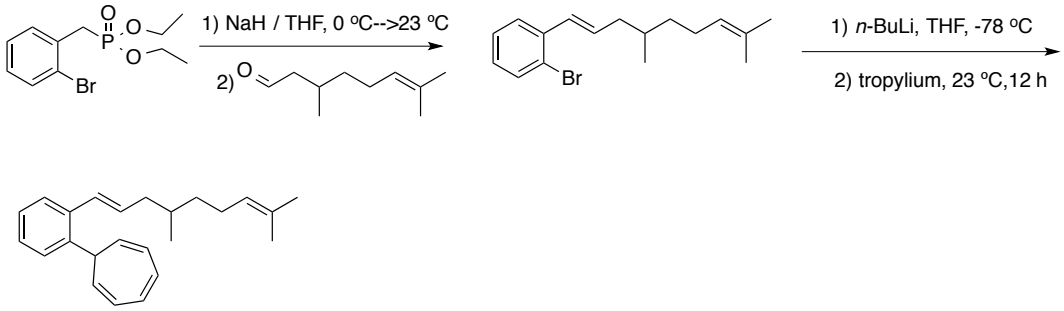


This compound was prepared as a colorless oil in 78% yield according to the general procedure A.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 - 7.44 (m, 2H), 7.34 - 7.22 (m, 2H), 6.76 (t, *J* = 3.2 Hz, 2H), 6.52 (d, *J* = 15.6 Hz, 1H), 6.30 - 6.26 (m, 2H), 6.05 (dt, *J* = 15.6, 6.7 Hz, 1H), 5.43 (dd, *J* = 9.1, 5.5 Hz, 2H), 5.17 - 5.13 (m, 1H), 3.04 (t, *J* = 5.6 Hz, 1H), 2.24 - 2.17 (m, 2H), 2.13 (q, *J* = 6.9 Hz, 2H), 1.71 (s, 3H), 1.62 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.2, 137.1, 132.9, 131.9, 130.8, 127.8, 127.4, 127.2, 126.9, 126.7, 126.6, 124.3, 123.7, 42.3, 33.4, 27.8, 25.7, 17.7.

HRMS-APCI calculated for $C_{21}H_{25}$ $[M+H]^+$: 277.1956; found: 277.1969

(*E*)-7-(2-(4,8-Dimethylnona-1,7-dien-1-yl)phenyl)cyclohepta-1,3,5-triene (7j)



To a suspension of NaH (60% in oil, 290 mg, 7.3 mmol) in THF (20 mL) at 0 ºC was slowly added diethyl 2-bromobenzylphosphonate[3] (2 g, 6.6 mmol). The resulting suspension was stirred for 1 h at room temperature (23 ºC). The reaction mixture was cooled to 0 ºC, and then (±)-citronellal (1.02 g, 6.6 mmol) was added dropwise and slowly warmed to room temperature. After stirring overnight (12 h), the reaction was quenched with ice water and the aqueous phase was extracted with Et_2O. The combined organic layers were washed with brine and dried over $MgSO_4$. After concentration in vacuo, the residue was purified by silica gel flash column chromatography to give 1.65g (*E*)-1-bromo-2-(4,8-dimethylnona-1,7-dien-1-yl)benzene as colorless oil in 81% yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.51 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.30 - 7.22 (m, 1H), 7.08 (ddd, *J* = 8.0, 7.3, 1.7 Hz, 1H), 6.72 (d, *J* = 15.7 Hz, 1H), 6.17 (dt, *J* = 15.7, 7.3 Hz, 1H), 5.19 - 5.05 (m, 1H), 2.35 – 2.27 (m, 1H), 2.19 - 1.98 (m, 3H), 1.77 - 1.61 (m, 7H), 1.50 - 1.42 (m, 1H), 1.28 - 1.20 (m, 1H), 0.98 (d, *J* = 6.7 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 137.76, 132.84, 132.80, 131.26, 129.84, 128.10, 127.35, 126.88, 124.74, 123.12, 40.48, 36.72, 32.80, 25.74, 25.61, 19.54, 17.69.

HRMS-APCI calculated for $C_{17}H_{24}Br$ $[M+H]^+$: 307.1056; found: 307.1050

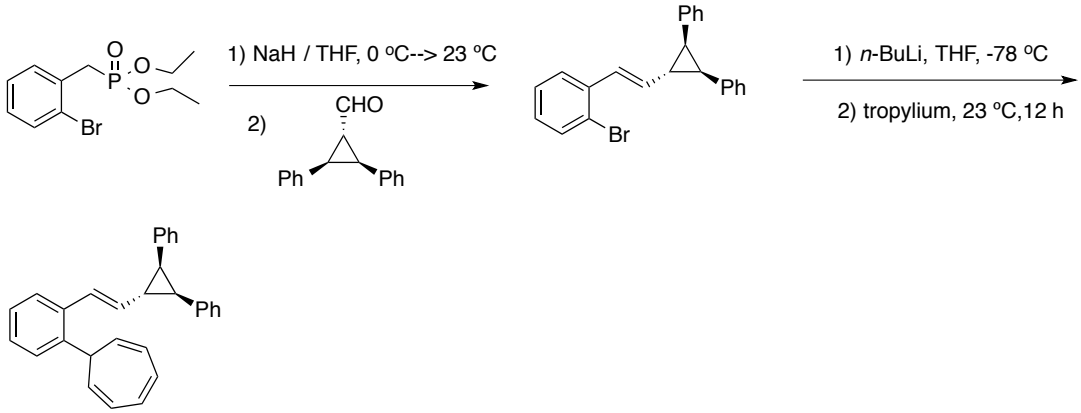
The title compound was prepared according to general procedure A from (*E*)-1-bromo-2-(4,8-dimethylnona-1,7-dien-1-yl)benzene as colorless oil in 71% yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 – 7.45 (m, 2H), 7.31 - 7.25 (m, 2H), 6.75 (dd, *J* = 3.7, 2.7 Hz, 2H), 6.50 (d, *J* = 15.6 Hz, 1H), 6.30 - 6.24 (m, 2H), 6.01(dt, *J* = 15.5, 7.3 Hz, 1H), 5.45 - 5.39 (m, 2H), 5.12 (ddt, *J* = 8.6, 5.7, 1.4 Hz, 1H), 3.13 - 3.00 (m, 1H), 2.24 - 2.16 (m, 1H), 2.07 - 1.95 (m, 3H), 1.71 (s, 3H), 1.64 - 1.56 (m, 4H), 1.43 - 1.34 (m, 1H), 1.20 – 1.15 (m, 1H), 0.91 (d, *J* = 6.7 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 140.25, 137.30, 132.05, 131.12, 130.83, 128.92, 127.44, 127.21, 126.95, 126.92, 126.68, 124.83, 124.35, 42.36, 40.65, 36.65, 32.83, 25.73, 25.62, 19.52, 17.67.

HRMS-APCI calculated for $C_{24}H_{31}$ $[M+H]^+$: 319.2420; found: 319.2429

7-(2-((*E*)-2-((1*R,2*S**,3*R**)-2,3-diphenylcyclopropyl)vinyl)phenyl)cyclohepta-1,3,5-triene (7k)**

(3) Alexander, J. B.; Mervyn, H.; John, T. S. *J. Chem. Soc., Perkin Trans. 1* **1994**, 3149–3161.



To a suspension of NaH (60% in oil, 99 mg, 2.47 mmol) in THF (4 mL) at 0 ºC was slowly added diethyl 2-bromobenzylphosphonate (759 mg, 2.47 mmol). The resulting suspension was stirred for 1 h at room temperature (23 ºC). The reaction mixture was cooled to 0 ºC, and then trans-2,trans-3-diphenylcyclopropanecarboxaldehyde[4] (500 mg, 2.25 mmol) in 1 mL THF was added dropwise and slowly warmed to room temperature. After stirring overnight (12 h), the reaction was quenched with ice water and the aqueous phase was extracted with Et_2O. The combined organic layers were washed with brine and dried over $MgSO_4$. After concentration in vacuo, the residue was purified by silica gel flash column chromatography to give 710 mg (((*E*)-2-bromostyryl)cyclopropane-1,2-diyl)dibenzene as a colorless solid in 84% yield.

m.p. 114-116 ºC

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 (dd, *J* = 8.1, 1.3 Hz, 1H), 7.56 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.29 (dd, *J* = 7.7 Hz, 1H), 7.20 - 7.08 (m, 7H), 7.05 - 6.99 (m, 5H), 6.15 (dd, *J* = 15.6, 8.3 Hz, 1H), 2.72 (d, *J* = 5.6 Hz, 2H), 2.61 - 2.56 (m, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 137.19, 137.13, 135.37, 132.98, 128.94, 128.24, 127.87, 127.58, 127.44, 126.51, 126.01, 123.11, 33.49, 30.01.

HRMS-APCI calculated for $C_{23}H_{20}Br$ $[M+H]^+$: 375.0743; found: 375.0740

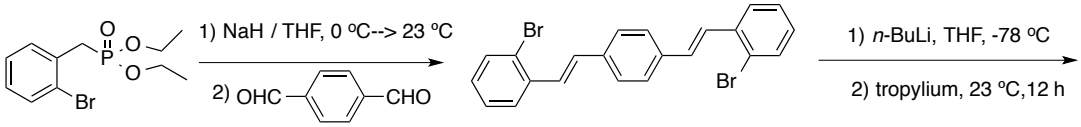
The title compound was prepared according to general procedure A from (((*E*)-2-bromostyryl)cyclopropane-1,2-diyl)dibenzene as colorless oil in 84% yield.

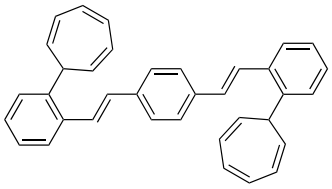
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (dd, *J* = 7.4, 1.8 Hz, 1H), 7.49 (dd, *J* = 7.4, 1.7 Hz, 1H), 7.35 - 7.29 (m, 2H), 7.18 - 7.09 (m, 6H), 6.99 - 6.95 (m, 4H), 6.82 - 6.76 (m, 3H), 6.34 - 6.30 (m, 2H), 5.99 (dd, *J* = 15.5, 8.3 Hz, 1H), 5.47 (dd, *J* = 9.1, 5.4 Hz, 2H), 3.13 - 3.09 (m, 1H), 2.63 (d, *J* = 5.5 Hz, 2H), 2.46 (dt, *J* = 8.3, 5.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.30, 137.39, 136.53, 134.51, 130.94, 128.95, 127.80, 127.65, 127.39, 126.88, 126.77, 126.49, 126.46, 125.90, 124.49, 42.31, 33.29, 30.11.

HRMS-APCI calculated for $C_{30}H_{27}$ $[M+H]^+$: 387.2107; found: 387.2105

1,4-Bis((*E*)-2-(cyclohepta-2,4,6-trien-1-yl)styryl)benzene (7l)

(4) Castellino, A. J.; Bruice, T. C. *J. Am. Chem. Soc.* **1988**, *110*, 7512–7519.





To a suspension of NaH (60% in oil, 217 mg, 5.42 mmol) in THF (4 mL) at 0 ºC was slowly added diethyl 2-bromobenzylphosphonate (1.51 g, 4.92 mmol). The resulting suspension was stirred for 1 h at room temperature (23 ºC). The reaction mixture was cooled to 0 ºC, and then a solution of terephthalaldehyde (300 mg, 2.24 mmol) in THF (2 mL) was added dropwise and slowly warmed to room temperature. After stirring for 2 d at room temperature, (during which time a precipitate formed) the reaction was quenched with ice water and the precipitate was collected by filtering, and washed with Et_2O and water, dried with vacuum. 1,4-bis((*E*)-2-bromostyryl)benzene was obtained as a light yellow solid. (620 mg, 63%).

m.p. 170-172 ºC

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (dd, *J* = 7.9, 1.6 Hz, 2H), 7.62 (dd, *J* = 8.1, 1.2 Hz, 2H), 7.59 (s, 4H), 7.53 (d, *J* = 16.2 Hz, 2H), 7.35 (td, *J* = 7.6, 1.2 Hz, 2H), 7.15 (td, *J* = 7.7, 1.7 Hz, 2H), 7.08 (d, *J* = 16.1 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.0, 136.8, 133.1, 130.9, 128.8, 127.5, 127.2, 126.6, 124.2.

HRMS-LDI+ calculated for $C_{22}H_{16}Br_2$ $[M]^+$: 437.9619; found: 437.9621

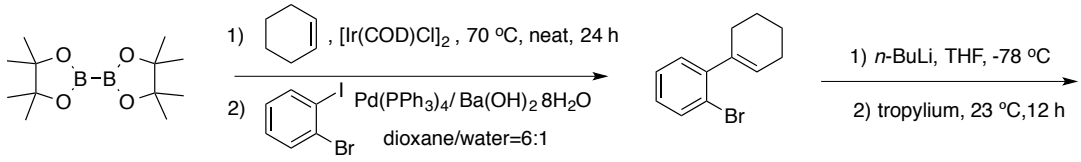
The title compound was prepared according to general procedure **A-2** from the 1,4-bis((*E*)-2-bromostyryl)benzene as yellow solid in 41% yield.

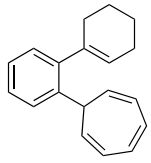
m.p. 161–163 ºC

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.73 - 7.66 (m, 2H), 7.54 - 7.26 (m, 12H), 6.97 (d, *J* = 16.0 Hz, 2H), 6.80 (t, *J* = 3.1 Hz, 4H), 6.32 - 6.30 (m, 4H), 5.50 (dd, *J* = 9.0, 5.3 Hz, 4H), 3.15 - 3.08 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.0, 136.9, 136.3, 130.9, 130.1, 127.9, 127.7, 126.9, 126.8, 126.6, 126.5, 126.5, 124.5, 42.6.

HRMS-LDI+ calculated for $C_{36}H_{29}$ $[M-H]^+$: 461.2269; found: 461.2264

2'-(Cyclohepta-2,4,6-trien-1-yl)-2,3,4,5-tetrahydro-1,1'-biphenyl (7m)





2'-bromo-2,3,4,5-tetrahydro-1,1'-biphenyl was prepared according to a reported procedure.[5]

$[Ir(COD)Cl]_2$ (2 mol %, 20 mg) and bis(pinacolato)diboron (1.5 mmol, 381 mg) were dissolved in 1 mL neat cyclohexene. The reaction mixture was stirred at 70 °C for 24 h under argon. After cooling to room temperature the reaction mixture was diluted with a dioxane/water (6:1) mixture (4 ml), then 2-bromoiodobenzene (1.5 mmol), $Pd(PPh_3)_4$ (5 mol %, 80 mg) and $Ba(OH)_2 \cdot 8H_2O$ (3.0 mmol, 946 mg) were added. Then stirring was continued for 24 h at 70 ºC. The crude reaction mixture was evaporated and the residue was purified by silica gel column chromatography to give 240 mg aryl bromide as colorless oil in 67% yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (dd, J = 8.0, 1.2 Hz, 1H), 7.25 (td, J = 7.4, 1.2 Hz, 1H), 7.17 (dd, J = 7.6, 1.9 Hz, 1H), 7.10 (td, J = 7.9, 1.8 Hz, 1H), 5.65 (tt, J = 3.8, 1.8 Hz, 1H), 2.32 – 2.28 (m, 2H), 2.22 - 2.16 (m, 2H), 1.83 - 1.76 (m, 2H), 1.75 - 1.66 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.4, 139.1, 132.6, 130.0, 127.9, 127.1, 127.0, 122.5, 29.3, 25.3, 22.8, 21.9.

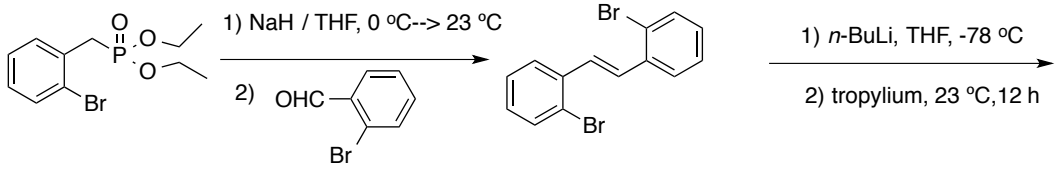
HRMS-EI calculated for $C_{12}H_{13}Br$ $[M]^+$: 236.0201; found: 236.0204

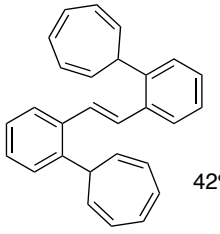
This title compound was prepared as a colorless oil in 55% yield according to the general procedure A from 2'-bromo-2,3,4,5-tetrahydro-1,1'-biphenyl.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (dd, J = 7.8, 1.4 Hz, 1H), 7.35 (td, J = 7.5, 1.5 Hz, 1H), 7.25 (td, J = 7.4, 1.4 Hz, 1H), 7.14 (dd, J = 7.7, 1.5 Hz, 1H), 6.73 (t, J = 3.2 Hz, 2H), 6.26 - 6.22 (m, 2H), 5.49 - 5.47 (m, 1H), 5.37 (dd, J = 9.0, 5.4 Hz, 2H), 2.95 (t, J = 5.6 Hz, 1H), 2.10 - 2.03 (m, 4H), 1.64 - 1.51 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 144.7, 141.5, 138.0, 130.6, 128.4, 127.8, 127.1, 126.1, 126.1, 124.0, 42.0, 30.9, 25.2, 22.9, 22.0.

HRMS-EI calculated for $C_{19}H_{20}$ $[M]^+$: 248.1565; found: 248.1562

(*E*)-1,2-Bis(2-(cyclohepta-2,4,6-trien-1-yl)phenyl)ethane (7n)





42%

To a suspension of NaH (60% in oil, 145 mg, 3.63 mmol) in THF (4 mL) at 0 ºC was slowly added diethyl 2-bromobenzylphosphonate (1 g, 3.3 mmol). The resulting suspension was stirred for 1 h at room temperature (23 ºC). The reaction mixture was cooled to 0 ºC, and then a solution of 2-bromobenzaldehyde (611 mg, 3.3 mmol) in THF (2 mL) was added dropwise and slowly warmed to room temperature. After stirring overnight, the reaction was quenched with ice water and the aqueous phase

(5) Olsson, V. J.; Szabó, K. J. *Angew. Chem. Int. Ed.* **2007**, *46*, 6891–6893.

was extracted with Et_2O. The combined organic layers were washed with brine and dried over Na_2SO_4. After concentration in vacuo, the residue was purified by silica gel flash column chromatography to give 730 mg (*E*)-1,2-bis(2-bromophenyl)ethene as a colorless solid in 65% yield. The spectroscopic data match with those reported in the literature.[6]

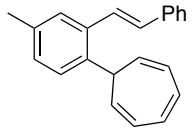
The title compound was prepared according to general procedure **A-2** from (*E*)-1,2-bis(2-bromophenyl)ethene as white solid in 42% yield.

m.p. 135-137ºC

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.56-7.48 (m, 4H), 7.38-7.27 (m, 4H), 7.10 (s, 2H), 6.76 (t, *J* = 3.1 Hz, 4H), 6.29 (d, *J* = 9.0 Hz, 4H), 5.45 (dd, *J* = 9.1, 5.5 Hz, 4H), 3.10 (t, *J* = 5.4 Hz, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 141.0, 136.6, 130.9, 128.5, 127.9, 127.6, 126.9, 126.7, 126.5, 124.5, 42.4.

HRMS-MALDI: calculated for $C_{28}H_{24}$ $[M]^+$: 360.1878; found: 360.1935

(*E*)-7-(4-Methyl-2-styrylphenyl)cyclohepta-1,3,5-triene (7p)



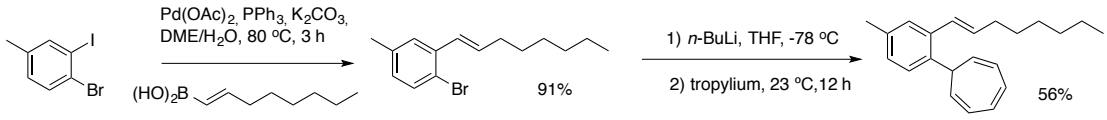
This compound was prepared as a white solid in 59% yield according to the general procedure A from (*E*)-1-bromo-4-methyl-2-styrylbenzene.[7]

m.p. 75-76 ºC

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (s, 1H), 7.44 (d, *J* = 7.8 Hz, 2H), 7.40 (d, *J* = 7.8 Hz, 1H), 7.36 (t, *J* = 7.7 Hz, 2H), 7.31 - 7.24 (m, 2H), 7.18 (dd, *J* = 7.9, 1.9 Hz, 1H), 6.96 (d, *J* = 16.0 Hz, 1H), 6.78 (t, *J* = 3.2 Hz, 2H), 6.34 - 6.28 (m, 2H), 5.47 (dd, *J* = 9.1, 5.5 Hz, 2H), 3.09 (t, *J* = 5.6 Hz, 1H), 2.43 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 138.2, 137.6, 136.3, 136.1, 130.9, 130.3, 128.7, 128.6, 127.6, 127.5, 127.1, 126.9, 126.6, 126.5, 124.4, 42.2, 21.1.

HRMS-APCI calculated for $C_{22}H_{21}$ $[M+H]^+$: 285.1643; found: 285.1613

(*E*)-7-(4-Methyl-2-(oct-1-en-1-yl)phenyl)cyclohepta-1,3,5-triene (7q)



(*E*)-1-Bromo-4-methyl-2-(oct-1-en-1-yl)benzene

To a DME/H_2O (5 ml / 2 ml) solution of 15 mg $Pd(OAc)_2$, 50 mg PPh_3, 424 mg K_2CO_3 and 243 mg (1.56 mmol) (*E*)-oct-1-en-1-ylboronic acid was added 1-bromo-2-iodo-4-methylbenzene (420 mg, 1.41 mmol) at room temperature. The mixture was then heated at 80 °C for 3 h. After cooling to room temperature, the mixture was

(6) Wyatt, P.; Hudson, A.; Charmant, J.; Orpen, A. G.; Phetmung, H. *Org. Biomol. Chem*. **2006**, *4*, 2218–2232.

(7) (*E*)-1-Bromo-4-methyl-2-styrylbenzene is a known compound: Watanabe, S.; Yamamoto, K.; Itagaki, Y.; Iwamura, T.; Iwama, T.; Kataoka, T. *Tetrahedron* **2000**, *56*, 855–863. It can be also prepared by the Heck reaction of 1-bromo-2-iodo-4-methylbenzene with styrene.

quenched by adding saturated $NH_4Cl_{(aq)}$. The mixture was extracted with ethyl acetate, and the combined organic extracts were dried over $MgSO_4$. The solvent was removed in vacuo, and the crude residue was purified by silica gel flash column chromatography (SiO_2, c-hexane) to give (*E*)-1-bromo-4-methyl-2-(oct-1-en-1-yl)benzene (360 mg) colorless oil in 91% yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, *J* = 8.2 Hz, 1H), 7.32 (s, 1H), 6.89 (d, *J* = 8.2 Hz, 1H), 6.69 (d, *J* = 15.7 Hz, 1H), 6.18 (dt, *J* = 15.7, 7.0 Hz, 1H), 2.32 (s, 3H), 2.30 - 2.22 (m, 2H), 1.54 - 1.46 (m, 2H), 1.41 - 1.30 (m, 6H), 0.92 (t, *J* = 6.9 Hz, 3H).

HRMS-APCI calculated for $C_{15}H_{22}Br$ $[M+H]^+$: 281.0899; found: 281.0901

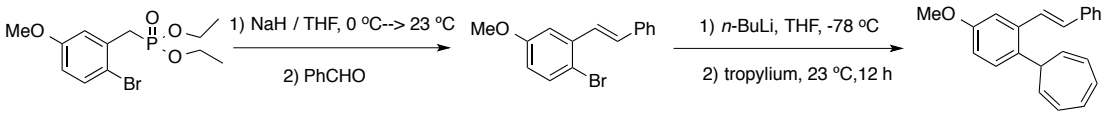
(*E*)-7-(4-Methyl-2-(oct-1-en-1-yl)phenyl)cyclohepta-1,3,5-triene

The title compound was prepared as a colorless oil in 56% yield according to general procedure A from (*E*)-1-bromo-4-methyl-2-(oct-1-en-1-yl)benzene.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (d, *J* = 7.8 Hz, 1H), 7.30 (s, 1H), 7.11 (d, *J* = 7.8 Hz, 1H), 6.75 (dd, *J* = 3.6, 2.6 Hz, 2H), 6.48 (d, *J* = 15.6 Hz, 1H), 6.31 - 6.24 (m, 2H), 6.03 (dt, *J* = 15.5, 7.0 Hz, 1H), 5.50 - 5.36 (m, 2H), 3.03 - 2.97 (m, 1H), 2.38 (s, 3H), 2.16 (qd, *J* = 7.1, 1.5 Hz, 2H), 1.47 - 1.40 (m, 2H), 1.35 – 1.27 (m, 6H), 0.92 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.38, 136.99, 136.08, 133.24, 130.79, 127.94, 127.63, 127.41, 127.37, 127.22, 124.23, 42.00, 33.20, 31.74, 29.28, 28.80, 22.65, 21.06, 14.12.

HRMS-APCI calculated for $C_{22}H_{29}$ $[M+H]^+$: 293.2264; found: 293.2263

(*E*)-7-(4-Methoxy-2-styrylphenyl)cyclohepta-1,3,5-triene (7r)



To a suspension of NaH (60% in oil, 131 mg, 3.28 mmol) in THF (4 mL) at 0 ºC was slowly added diethyl 2-bromo-5-methoxylbenzylphosphonate (1 g, 3 mmol). The resulting suspension was stirred for an additional 1 h at room temperature (23 ºC). The reaction mixture was cooled to 0 ºC, and then a solution of benzaldehyde (290 mg, 2.73 mmol) in THF (1 mL) was added dropwise and slowly warmed to room temperature. After stirring overnight (12 h), the reaction was quenched with ice water and extracted with Et_2O, dried with $MgSO_4$. (*E*)-1-bromo-4-methoxy-2-styrylbenzene was obtained as a colorless solid by silica gel column chromatography. (612 mg, 78%).

m.p. 65-67 ºC

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 (d, *J* = 7.5 Hz, 2H), 7.50 (d, *J* = 8.8 Hz, 1H), 7.45 (d, *J* = 16.2 Hz, 1H), 7.41 (t, *J* = 7.6 Hz, 2H), 7.33 (t, *J* = 7.4 Hz, 1H), 7.22 (d, *J* = 3.0 Hz, 1H), 7.05 (d, *J* = 16.2 Hz, 1H), 6.75 (dd, *J* = 8.8, 3.0 Hz, 1H), 3.88 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.04, 137.85, 136.92, 133.58, 131.51, 128.75, 128.14, 127.55, 126.88, 115.08, 114.95, 111.81, 55.56.

HRMS-APCI calculated for $C_{15}H_{14}BrO$ $[M+H]^+$: 289.0223; found: 289.0218

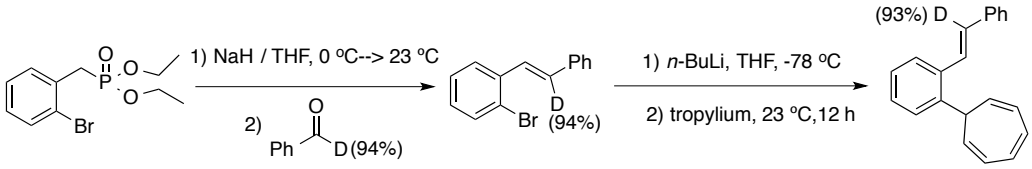
(*E*)-7-(4-Methoxy-2-styrylphenyl)cyclohepta-1,3,5-triene

The title compound was prepared according to general procedure A as colorless oil in 86% yield from (*E*)-1-bromo-4-methoxy-2-styrylbenzene.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.44 - 6.92 (m, 10H), 6.77 (t, *J* = 3.2 Hz, 2H), 6.31 - 6.26 (m, 2H), 5.51 - 5.38 (m, 2H), 3.90 (s, 3H), 3.04 (t, *J* = 5.5 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 158.37, 137.50, 137.42, 133.61, 130.93, 130.69, 128.81, 128.67, 127.69, 127.03, 126.59, 126.55, 124.39, 113.56, 111.62, 55.39, 41.95.

HRMS-APCI calculated for $C_{22}H_{21}O$ $[M+H]^+$: 301.1587; found: 301.1587

(*E*)-7-(2-styrylphenyl)cyclohepta-1,3,5-triene-d$_1$ (7a-*d*$_1$)



The isotopically labeled (*E*)-1-bromo-2-styrylbenzene-d$_1$[8] was synthesized as follows:

To a suspension of NaH (60% in oil, 145 mg, 3.63 mmol) in THF (4 mL) at 0 ºC was slowly added diethyl 2-bromobenzylphosphonate (1 g, 3.3mmol). The resulting suspension was stirred for an additional 1 h at room temperature (23 ºC). The reaction mixture was cooled to 0 ºC, and then a solution of benzaldehyde-α-d$_1$[9] (353 mg, 3.3 mmol) in THF (2 mL) was added dropwise and slowly warmed to room temperature. After stirring overnight (12h), the reaction was quenched with ice water and the aqueous phase was extracted with Et_2O. The combined organic layers were washed with brine and dried over Na_2SO_4. After concentration in vacuo, the residue was purified by silica gel flash column chromatography to give 650 mg isotopically labeled (*E*)-1-bromo-2-styrylbenzene-d$_1$ as colorless oil in 76% yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.63 - 7.57 (m, 3H), 7.50 (s, 1H), 7.42 (t, *J* = 7.5 Hz, 2H), 7.38 - 7.30 (m, 2H), 7.15 (td, *J* = 7.8, 1.7 Hz, 1H), 7.08 (d, *J* = 16.1 Hz, 6% residual signal). ^{13}C NMR (101 MHz, $CDCl_3$) δ 137.1, 136.9, 133.0, 131.1 (t, J_{CD} = 23.5 Hz), 128.7, 128.7, 128.0, 127.5, 127.3, 126.8, 126.7, 124.1.

HRMS-APCI calculated for $C_{14}H_{11}DBr$ $[M+H]^+$: 260.0185; found: 260.0189

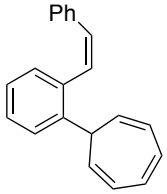
The title compound was prepared according to general procedure A from isotopically labeled (*E*)-1-bromo-2-styrylbenzene-d$_1$ as yellow oil in 82% yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (dd, *J* = 6.9, 2.2 Hz, 1H), 7.52 - 7.42 (m, 3H), 7.39 - 7.26 (m, 6H), 6.96 (residual signal, 7%), 6.78 (t, *J* = 3.2 Hz, 2H), 6.35 - 6.30 (m, 2H), 5.47 (dd, *J* = 9.0, 5.4 Hz, 2H), 3.12 (tt, *J* = 5.6, 1.6 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.0, 137.4, 136.4, 130.9, 130.2 (t, *J* = 23.1 Hz), 128.6, 127.9, 127.6, 127.6, 126.9, 126.6, 126.5, 126.4, 124.5, 42.5.

HRMS-APCI calculated for $C_{21}H_{18}D$ $[M+H]^+$: 272.1550; found: 272.1538

(*Z*)-7-(2-Styrylphenyl)cyclohepta-1,3,5-triene (*cis*-7a)

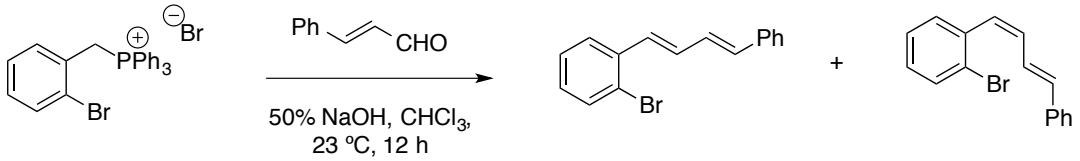
(8) Xue, F.; Li, X.; Wan, B. *J. Org. Chem*. **2011**, *76*, 7256–7262.
(9) Gajewski, J. J.; Bocian, W.; Harris, N. J.; Olson, L.P.; Gajewski, J. P. *J. Am. Chem. Soc.* **1999**, *121*, 326–334.



This compound was prepared as a colorless oil from (*Z*)-1-bromo-2-styrylbenzene[10] in 78% yield according to the general procedure A.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.35 (td, *J* = 7.5, 1.8 Hz, 1H), 7.22 - 7.13 (m, 5H), 7.12 - 7.03 (m, 2H), 6.71 (t, *J* = 3.2 Hz, 2H), 6.61 (d, *J* = 12.1 Hz, 1H), 6.55 (d, *J* = 12.0 Hz, 1H), 6.25 - 6.19 (m, 2H), 5.38 (dd, *J* = 9.1, 5.5 Hz, 2H), 3.09 - 3.05 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.7, 136.9, 136.6, 131.0, 130.7, 129.7, 129.1, 129.0, 128.0, 127.8, 127.3, 127.0, 126.5, 126.3, 124.5, 42.4.

HRMS-EI calculated for $C_{21}H_{18}$ $[M]^+$: 270.1409; found: 270.1400



To a solution of 2-bromobenzyltriphenylphosphonium bromide (2 g, 3.9 mmol) and (*E*)-cinnamaldehyde (516 mg, 3.9 mmol) in 30 mL chloroform was slowly added 50% $NaOH_{(aq)}$ (780 mg NaOH, 19.5 mmol). The resulting mixture was stirred overnight (12 h) at room temperature (23 ºC). The layers were separated, and the aqueous phase extracted twice with DCM. The combined organic extracts were washed with water then dried over $MgSO_4$. After concentration in vacuo, 5 mL *c*-hexane was added and the resulting triphenylphosphine oxide precipitate was removed by filtration. The *c*-hexane solution was passed through a short pad of silica gel then concentrated in vacuo to give 860 mg colorless oil (77%, *Z*:*E* = 1:1). The pure samples of *Z* (320mg, colorless oil) and *E* (280mg, light yellow solid) products were obtained by very careful silica gel chromatography using *c*-hexane as eluent.

Note: The (1*E,*3*E*) sample can be also prepared from diethyl 2-bromobenzylphosphonate and (*E*)-cinnamaldehyde using the same procedure described for deuterated (*E*)-1-bromo-2-styrylbenzene synthesis shown in this SI as well. By using this HWE olefination, only the desired (1*E,*3*E*) isomer was obtained, and the purification is easier.

1-Bromo-2-((1*E*,3*E*)-4-phenylbuta-1,3-dien-1-yl)benzene

m.p. 104-105 ºC

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.59 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.49 (d, *J* = 7.8 Hz, 2H), 7.37 (t, *J* = 7.7 Hz, 2H), 7.33 - 7.26 (m, 2H), 7.12 (ddd, *J* = 8.0, 7.3, 1.6 Hz, 1H), 7.08 - 7.03 (m, 2H), 6.97 - 6.90 (m, 1H), 6.75 (d, *J* = 16.1 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 137.1, 136.9, 134.0, 133.1, 131.8, 131.0, 129.0, 128.7, 128.6, 127.8, 127.4, 126.5, 126.3, 123.9.

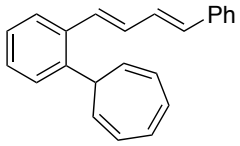
1-Bromo-2-((1*Z*,3*E*)-4-phenylbuta-1,3-dien-1-yl)benzene

(10) de Meijere, A.; Zhong Song, Z.; Lansky, A.; Hyuda, S.; Rauch, K.; Noltemeyer, M.; König, B.; Knieriem, B. *Eur. J. Org. Chem.,* **1998**, 2289–2299.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.47 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.41 - 7.22 (m, 6H), 7.18 (td, *J* = 7.7, 1.7 Hz, 1H), 7.12 (dd, *J* = 15.6, 10.4 Hz, 1H), 6.77 (d, *J* = 15.6 Hz, 1H), 6.63 - 6.50 (m, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 137.4, 137.1, 135.4, 132.7, 131.2, 131.2, 129.7, 128.6, 128.6, 127.8, 127.0, 126.6, 124.7, 124.0.

HRMS-MALDI: calculated for $C_{16}H_{13}Br$ $[M]^+$: 284.0195; found: 284.0166

7-(2-((1*E*,3*E*)-4-Phenylbuta-1,3-dien-1-yl)phenyl)cyclohepta-1,3,5-triene (7g)



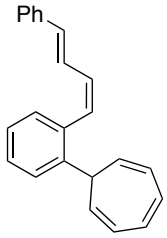
This compound was prepared as a white solid in 82% yield according to the general procedure A from 1-bromo-2-((1*E*,3*E*)-4-phenylbuta-1,3-dien-1-yl)benzene.

m.p. 124-125 ºC

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.68 - 7.64 (m, 1H), 7.49 - 7.44 (m, 3H), 7.37 - 7.30 (m, 4H), 7.25 (t, *J* = 7.3 Hz, 1H), 6.94 (ddd, *J* = 15.5, 5.9, 4.1 Hz, 1H), 6.90 - 6.84 (m, 2H), 6.79 (dd, *J* = 3.7, 2.7 Hz, 2H), 6.68 (d, *J* = 15.3 Hz, 1H), 6.36 - 6.29 (m, 2H), 5.45 (dd, *J* = 9.0, 5.3 Hz, 2H), 3.10 (t, *J* = 5.6 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 140.8, 137.3, 136.1, 132.8, 131.0, 130.9, 130.3, 129.5, 128.6, 127.9, 127.5, 126.8, 126.8, 126.4, 126.2, 124.5, 42.4.

HRMS-APCI calculated for $C_{23}H_{21}$ $[M+H]^+$: 297.1643; found: 297.1650

7-(2-((1*Z*,3*E*)-4-Phenylbuta-1,3-dien-1-yl)phenyl)cyclohepta-1,3,5-triene (7u)



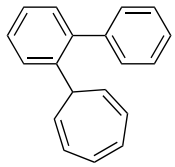
This compound was prepared as a colorless oil in 49% yield according to the general procedure A from1-bromo-2-((1*Z*,3*E*)-4-phenylbuta-1,3-dien-1-yl)benzene.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 7.8 Hz, 1H), 7.43 - 7.21 (m, 8H), 7.07 (ddd, *J* = 15.6, 10.9, 0.9 Hz, 1H), 6.73 (dd, *J* = 3.6, 2.8 Hz, 2H), 6.67 (d, *J* = 15.6 Hz, 1H), 6.51 (d, *J* = 11.3 Hz, 1H), 6.42 (td, *J* = 11.1, 0.8 Hz, 1H), 6.31 - 6.24 (m, 2H), 5.42 (dd, *J* = 8.8, 5.4 Hz, 2H), 3.02 (ddd, *J* = 5.4, 3.9, 1.5 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.0, 137.3, 136.3, 134.3, 131.0, 130.8, 130.5, 129.3, 128.5, 127.9, 127.6, 127.3, 126.5, 126.4, 126.3, 125.4, 124.6, 42.46.

HRMS-MALDI: calculated for $C_{23}H_{19}$ $[M-H]^+$: 295.1481; found: 295.1496

Experimental Details for the Synthesis of *o*-Aryl Cycloheptatrienes

2-(Cyclohepta-2,4,6-trien-1-yl)-1,1'-biphenyl (17a)



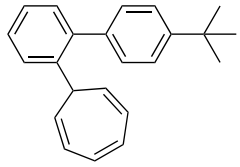
2-Biphenylmagnesium bromide solution (0.5 M, 5.6 mL, 2.8 mmol) was added dropwise to a solution of tropylium tetrafluoroborate (500 mg, 2.8 mmol) in 10 mL dry THF at 0 ºC under argon. The reaction was then stirred at room temperature (23 ºC) overnight (12 h). The reaction was quenched by addition of water. The aqueous phase was extracted with ether, the combined organic extracts were dried over $MgSO_4$, and the solvent was evaporated. The crude reaction mixture was purified by chromatography to give the title compound (460 mg) as a colorless solid in 67% yield.

m.p. 48-50 ºC

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.45 (td, *J* = 7.5, 1.7 Hz, 1H), 7.37 - 7.18 (m, 7H), 6.57 (t, *J* = 3.2 Hz, 2H), 6.22 - 6.13 (m, 2H), 5.37 (dd, *J* = 9.0, 5.3 Hz, 2H), 2.88 (t, *J* = 5.2 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.9, 141.0, 130.5, 130.1, 129.2, 128.0, 127.8, 127.7, 127.6, 126.8, 126.3, 124.1, 41.9.

HRMS-APCI calculated for $C_{19}H_{17}$ $[M+H]^+$: 245.1330; found: 245.1334

4'-(*tert*-Butyl)-2-(cyclohepta-2,4,6-trien-1-yl)-1,1'-biphenyl (17b)



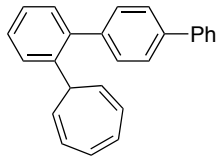
This compound was prepared as a colorless solid in 76% yield according to the general procedure A.

m.p. 87-89 ºC

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.66 (dd, *J* = 7.8, 1.1 Hz, 1H), 7.46 (t, *J* = 7.8 Hz, 1H), 7.38 - 7.31 (m, 4H), 7.19 (d, *J* = 8.4 Hz, 2H), 6.61 (t, *J* = 3.2 Hz, 2H), 6.25 - 6.16 (m, 2H), 5.40 (dd, *J* = 9.1, 5.2 Hz, 2H), 3.00 (t, *J* = 5.2 Hz, 1H), 1.35 (s, 9H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 149.6, 142.0, 141.7, 137.9, 130.5, 130.3, 128.9, 127.8, 127.8, 127.7, 126.2, 124.7, 124.1, 41.9, 34.4, 31.3.

HRMS-APCI calculated for $C_{23}H_{25}$ $[M+H]^+$: 301.1956; found: 301.1957

2-(Cyclohepta-2,4,6-trien-1-yl)-1,1':4',1''-terphenyl (17c)



This compound was prepared as a white solid in 59% yield according to the general procedure A.

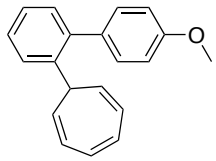
m.p. 86-89 ºC

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.6 Hz, 1H), 7.63 (d, *J* = 8.0 Hz, 2H), 7.57 (d, *J* = 8.2 Hz, 2H), 7.52 - 7.44 (m, 3H), 7.39 - 7.32 (m, 5H), 6.60 (t, *J* = 3.2 Hz, 2H),

6.24 – 6.21 (m, 2H), 5.43 (dd, *J* = 9.0, 5.3 Hz, 2H), 3.00 (t, *J* = 5.3 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.0, 141.4, 140.7, 140.0, 139.5, 130.6, 130.1, 129.7, 128.7, 128.0, 127.9, 127.6, 127.2, 127.0, 126.5, 126.3, 124.2, 41.9.

HRMS-APCI calculated for $C_{25}H_{21}$ $[M+H]^+$: 321.1643; found: 321.1647

2-(Cyclohepta-2,4,6-trien-1-yl)-4'-methoxy-1,1'-biphenyl (17d)



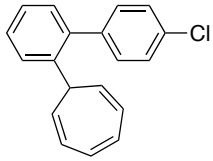
This compound was prepared as a white solid in 76% yield according to the general procedure A.

m.p. 74-75 ºC

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.46 (td, *J* = 7.5, 1.8 Hz, 1H), 7.38 - 7.29 (m, 2H), 7.18 (d, *J* = 8.7 Hz, 2H), 6.87 (d, *J* = 8.7 Hz, 2H), 6.62 (dd, *J* = 3.6, 2.6 Hz, 2H), 6.20-6.22 (m, 2H), 5.40 (dd, *J* = 9.0, 5.3 Hz, 2H), 3.83 (s, 3H), 2.91 (t, *J* = 5.3 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.5, 142.0, 141.5, 133.4, 130.6, 130.3, 130.2, 127.8, 127.7, 127.7, 126.2, 124.1, 113.3, 55.2, 41.9.

HRMS-APCI calculated for $C_{20}H_{19}O$ $[M+H]^+$: 275.1436; found: 275.1442

4'-Chloro-2-(cyclohepta-2,4,6-trien-1-yl)-1,1'-biphenyl (17e)



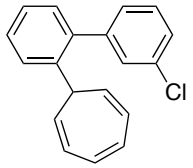
This compound was prepared as a white solid in 74% yield according to the general procedure A.

m.p. 114-115 ºC

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.49 (td, *J* = 7.6, 1.5 Hz, 1H), 7.36 (td, *J* = 7.5, 1.3 Hz, 1H), 7.31 - 7.25 (m, 3H), 7.18 (d, *J* = 8.4 Hz, 2H), 6.63 (t, *J* = 3.2 Hz, 2H), 6.24 - 6.18 (m, 2H), 5.38 (dd, *J* = 9.0, 5.3 Hz, 2H), 2.83 (tt, *J* = 5.3, 1.5 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 141.8, 140.6, 139.4, 132.9, 130.6, 130.5, 130.0, 128.3, 128.0, 127.8, 127.2, 126.4, 124.2, 41.9.

HRMS-APCI calculated for $C_{19}H_{16}Cl$ $[M+H]^+$: 279.0941; found: 279.0942

3'-Chloro-2-(cyclohepta-2,4,6-trien-1-yl)-1,1'-biphenyl (17f)



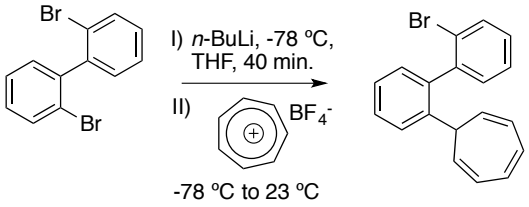
This compound was prepared as a white solid in 71% yield according to the general procedure A.

m.p. 89-90 ºC

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.50 (td, *J* = 7.5, 1.6 Hz, 1H), 7.36 (td, *J* = 7.5, 1.3 Hz, 1H), 7.31 - 7.24 (m, 4H), 7.12 (dt, *J* = 6.8, 1.7 Hz, 1H), 6.63 (t, *J* = 3.2 Hz, 2H), 6.24 - 6.20 (m, 2H), 5.39 (dd, *J* = 9.1, 5.3 Hz, 2H), 2.81 (tt, *J* = 5.4, 1.5 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.7, 141.8, 140.5, 133.7, 130.6, 129.9, 129.3, 129.0, 128.4, 127.8, 127.4, 127.1, 126.9, 126.4, 124.2, 41.9.

HRMS-APCI calculated for $C_{19}H_{16}Cl$ $[M+H]^+$: 279.0941; found: 279.0941

2-Bromo-2'-(cyclohepta-2,4,6-trien-1-yl)-1,1'-biphenyl (17g)

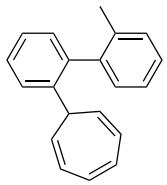


A solution of 2,2'-dibromobiphenyl (1.258 g, 4 mmol) in THF (16 mL) in a dried 50 mL round-bottom flask was cooled to -78 ºC and a *n*-BuLi solution (2.5 M in hexanes, 1.68 mL, 4.2 mmol) was added. After stirring for 40 minutes, tropylium tetrafluoroborate (1.424 g, 8 mmol) was added and the cooling bath was removed. When the reaction reached ambient temperature (23 ºC), cyclohexane (30 mL) was added and the mixture was loaded directly onto a column of SiO_2 and purified by flash chromatography (cyclohexane as eluent), yielding the desired cycloheptatriene (958 mg, 2.9 mmol, 74%) as a colorless oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.65 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.61 - 7.54 (m, 1H), 7.50 (td, *J* = 7.6, 1.5 Hz, 1H), 7.34 (td, *J* = 7.5, 1.3 Hz, 1H), 7.30 - 7.10 (m, 4H), 6.61 - 6.45 (m, 2H), 6.22 - 6.05 (m, 2H), 5.45 (dd, *J* = 9.4, 5.4 Hz, 1H), 5.23 (dd, *J* = 9.3, 5.4 Hz, 1H), 2.56 (tt, *J* = 5.5, 1.5 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 183.31, 132.48, 131.27, 130.86, 130.32, 129.98, 128.89, 128.79, 127.43, 127.15, 126.94, 126.42, 126.25, 124.54, 124.30, 42.24.

HRMS-APCI calcd for $C_{19}H_{16}Br$ $(M+H)^+$: 323.0430; found: 323.0427.

2-(Cyclohepta-2,4,6-trien-1-yl)-2'-methyl-1,1'-biphenyl (17h)



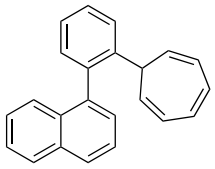
This compound was prepared as a colorless solid in 79% yield according to the general procedure A.

m.p. 58-60 ºC

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.48 (td, *J* = 7.6, 1.5 Hz, 1H), 7.34 (td, *J* = 7.5, 1.4 Hz, 1H), 7.24 - 7.11 (m, 4H), 7.05 (dd, *J* = 7.3, 1.4 Hz, 1H), 6.55 - 6.52 (m, 2H), 6.19 - 6.09 (m, 2H), 5.39 (dd, *J* = 9.4, 5.4 Hz, 1H), 5.26 (dd, *J* = 9.3, 5.3 Hz, 1H), 2.58 (tt, *J* = 5.4, 1.6 Hz, 1H), 2.03 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.4, 141.2, 140.5, 135.9, 130.5, 130.3, 129.6, 129.5, 129.5, 127.9, 127.3, 127.1, 127.0, 126.9, 126.1, 125.2, 124.5, 124.1, 41.9, 20.2.

HRMS-APCI calculated for $C_{20}H_{19}$ $[M+H]^+$: 259.1487; found: 259.1488

1-(2-(Cyclohepta-2,4,6-trien-1-yl)phenyl)naphthalene (17i)



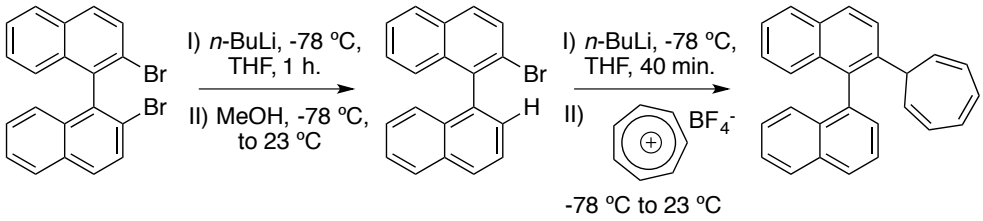
n-BuLi (1.6 M in hexanes, 0.23 mL, 0.37 mmol) was added dropwise to the solution of 1-(2-bromophenyl)naphthalene (100 mg, 0.23 mmol) in dry THF (1.4 mL, 0.25 M) at -78 ºC under argon. The mixture was stirred for 30 min at -78 ºC, and then tropylium tetrafluoroborate (75 mg, 0.42 mmol) was added in one portion. The cooling bath was removed and the reaction was stirred at room temperature (23 ºC) overnight (12 h). The reaction was quenched by addition of water. The aqueous phase was extracted with ether, the combined organic extracts were dried over $MgSO_4$, and the solvent was evaporated. The crude reaction mixture was purified by preparative TLC (eluent: pentane) to yield the title compound as a colorless oil that solidified upon standing (67 mg, 64%).

m.p. 80-81 ºC

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.1 Hz, 1H), 7.79 (d, *J* = 8.2 Hz, 1H), 7.72 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.54 (td, *J* = 7.6, 1.5 Hz, 1H), 7.49 (d, *J* = 8.4 Hz, 1H), 7.45 – 7.32 (m, 4H), 7.27 (ddd, *J* = 9.6, 7.3, 1.1 Hz, 2H), 6.39 (dd, *J* = 11.0, 5.6 Hz, 1H), 6.31 (dd, *J* = 11.0, 5.7 Hz, 1H), 6.08 (dd, *J* = 9.3, 5.7 Hz, 1H), 5.97 (dd, *J* = 9.3, 5.7 Hz, 1H), 5.37 (dd, *J* = 9.3, 5.4 Hz, 1H), 5.28 (dd, *J* = 9.3, 5.4 Hz, 1H), 2.54 (t, *J* = 5.4 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 143.4, 140.0, 138.7, 133.5, 132.4, 131.0, 130.6, 130.3, 128.4, 128.1, 127.7, 127.6, 127.2, 127.2, 127.0, 126.5, 126.2, 125.8, 125.7, 125.1, 124.5, 124.1, 42.3.

HRMS-MALDI: calculated for $C_{23}H_{17}$ $[M-H]^+$: 293.1330; found: 293.1361

2-(Cyclohepta-2,4,6-trien-1-yl)-1,1'-binaphthalene (17j).



Following a literature procedure, a solution of 2,2'-dibromo-1,1'-binaphtyl (412 mg, 1 mmol) in THF (10 mL) in a dried 25 mL round-bottom flask was cooled to -78 ºC and a *n*-BuLi solution (2.5 M in hexanes, 0.4 mL, 1 mmol) was added. After stirring for 1 hour, methanol (5 mL) was added and 10 minutes later the reaction was allowed to warm to room temperature (23 ºC). The solution was concentrated on a rotary evaporator and then purified by flash chromatography (cyclohexane) to yield 2-bromo-1,1'-binaphtyl (312 mg, 0.94 mmol, 94%) as a colorless solid. The spectroscopic data matched with those reported in the literature.[11]

A 10 mL round-bottom flask with a solution of 2-bromo-1,1'-binaphtyl (288 mg, 0.87 mmol) in THF (3.5 mL) was cooled to -78 ºC and *n*-BuLi solution (2.5 M in hexanes, 0.381 mL, 1.1 equiv.) was added. After stirring for 40 minutes, tropylium tetrafluoroborate (308 mg, 1.73 mmol, 2 equiv.) was added and the solution was

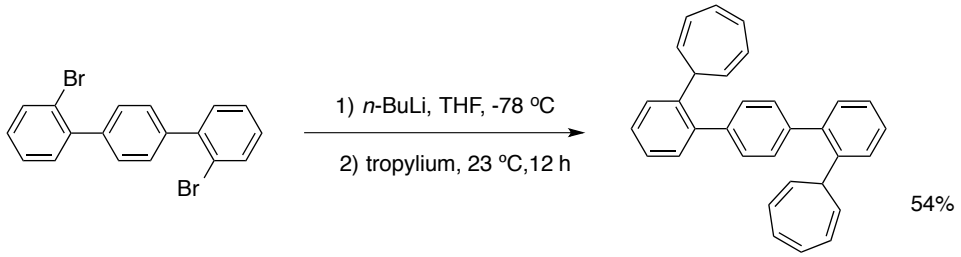
(11) Nagaki, A.; Takabayashi, N.; Tomida, Y. and Yoshida, J. *Org. Lett.* **2008**, *10*, 3937–3940.

allowed to warm to room temperature. The reaction was quenched with water, extracted with diethyl ether and washed with two portions of water and brine. After drying and concentrating, the mixture was purified by flash chromatography (cyclohexane) to yield the target compound (186 mg, 0.54 mmol, 62%) as a viscous pale-yellow oil.

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.6 Hz, 1H), 7.93 (d, *J* = 8.2 Hz, 1H), 7.86 (t, *J* = 7.9 Hz, 3H), 7.53 - 7.38 (m, 3H), 7.31 (d, *J* = 6.9 Hz, 1H), 7.26 - 7.19 (m, 3H), 7.08 (d, *J* = 8.5 Hz, 1H), 6.40 (d, *J* = 16.3 Hz, 1H), 6.30 (d, *J* = 16.3 Hz, 1H), 6.10 (dd, *J* = 9.3, 5.5 Hz, 1H), 5.96 (dd, *J* = 9.2, 5.5 Hz, 1H), 5.38 (d, *J* = 28.5 Hz, 2H), 2.58 (t, *J* = 5.1 Hz, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 140.51, 136.29, 133.46, 133.35, 133.04, 132.34, 130.67, 130.33, 128.89, 128.15, 128.09, 127.93, 127.88, 127.16, 127.00, 126.46, 126.29, 126.00, 125.87, 125.55, 125.52, 125.36, 124.58, 124.27, 42.94.

HRMS-APCI calcd for $C_{27}H_{21}Br$ $(M+H)^+$: 345.1638; found: 345.1646.

2,2''-Di(cyclohepta-2,4,6-trien-1-yl)-1,1':4',1''-terphenyl (17k)



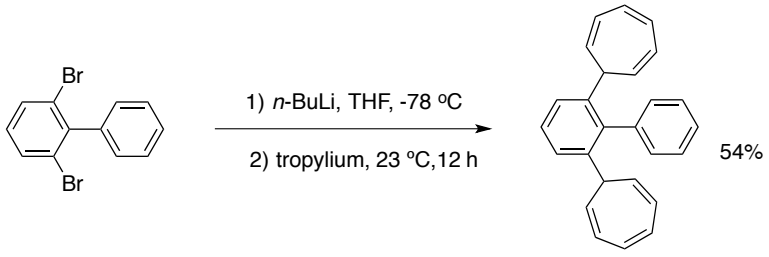
The title compound was prepared according to general procedure **A-2** from the known compound 2,2''-dibromo-1,1':4',1''-terphenyl[12] as a colorless solid in 54% yield.

m.p. 182-184 ºC

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.0 Hz, 2H), 7.47 (ddd, *J* = 7.8, 7.0, 1.8 Hz, 2H), 7.39 - 7.31 (m, 4H), 7.19 (s, 4H), 6.61 (dd, *J* = 3.8, 2.7 Hz, 4H), 6.23 - 6.18 (m, 4H), 5.39 (ddd, *J* = 9.5, 5.3, 0.8 Hz, 4H), 2.94 (ddd, *J* = 5.4, 3.8, 1.5 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 141.8, 141.5, 139.4, 130.6, 130.2, 128.8, 127.9, 127.8, 127.5, 126.3, 124.1, 41.8.

HRMS-APCI calculated for $C_{32}H_{27}$ $[M+H]^+$: 411.2113; found: 411.2113

2,6-Di(cyclohepta-2,4,6-trien-1-yl)-1,1'-biphenyl (17l)



n-BuLi (1.6 M in hexanes, 2.2 mL, 3.53 mmol) was added dropwise to the solution of 550 mg (1.76 mmol) 2,6-dibromo-1,1'-biphenyl[13] in 20 mL THF at -78 ºC under

(12) Velian, A.; Lin, S.; Miller, A. J. M.; Day, M. W.; Agapie, T. *J. Am. Chem. Soc.* **2010**, *132*, 6296–6297.
(13) Machuy, M. M.; Würtele, C.; Schreiner, P. R. *Synthesis* **2012**, *44*, 1405–1409.

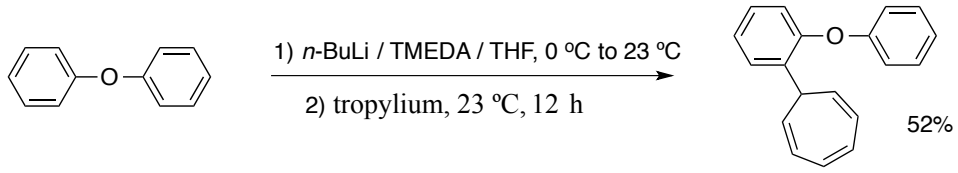
argon. After addition, the mixture was warmed to room temperature (23 ºC) slowly and allowed to stir for 1 h. After cooling down to -78 ºC again, tropylium tetrafluoroborate (628mg, 3.53mmol) was added in one portion. The cooling bath was removed and the reaction was stirred at room temperature overnight (12 h). The reaction was quenched by addition of water. The aqueous phase was extracted with ether, the combined organic extracts were dried over $MgSO_4$, and the solvent was evaporated. The crude reaction mixture was purified by chromatography to yield 320 mg of the title compound as a colorless crystalline solid (54%).

m.p. 137-138 ºC

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.62 - 7.55 (m, 3H), 7.18 – 7.16 (m, 3H), 7.02 - 6.97 (m, 2H), 6.49 (dd, J = 3.8, 2.7 Hz, 4H), 6.14 - 6.11 (m, 4H), 5.35 (dd, J = 8.7, 5.4 Hz, 4H), 2.52 (tt, J = 5.4, 1.5 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.7, 141.5, 138.4, 130.3, 129.4, 128.4, 127.5, 127.3, 126.6, 125.3, 123.9, 42.6.

HRMS-MALDI: calculated for $C_{26}H_{22}$ $[M]^+$: 334.1722; found: 334.1711

7-(2-Phenoxyphenyl)cyclohepta-1,3,5-triene (22a)

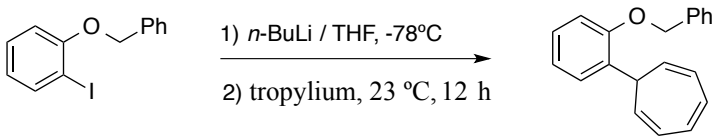


n-BuLi (1.6 M in hexanes, 15 mL, 24 mmol) was added dropwise to the solution of diphenyl ether (3.4 g, 20 mmol) and tetramethylethylenediamine (2.79 g, 3.58 mL, 24 mmol) in 50 mL THF at 0 ºC. After stirring at room temperature (23 ºC) for 5 h, tropylium tetrafluoroborate (3.56 g, 20 mmol) was added, and stirred at room temperature overnight. The reaction was quenched by addition of water. The aqueous phase was extracted with ether, the combined organic extracts were dried over $MgSO_4$, and the solvent was evaporated. The crude reaction mixture was purified by column chromatography on silica gel with cyclohexane as eluent to give 2.7 g colorless oil in 52% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50 (dd, J = 7.6, 1.7 Hz, 1H), 7.34 - 7.24 (m, 3H), 7.19 (td, J = 7.5, 1.3 Hz, 1H), 7.10 - 7.05 (m, 1H), 6.97 - 6.93 (m, 3H), 6.68 (dd, J = 3.6, 2.7 Hz, 2H), 6.22 - 6.25 (m, 2H), 5.46 (dd, J = 8.8, 5.6 Hz, 2H), 3.18 (tt, J = 5.6, 1.4 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.69, 154.74, 134.84, 130.78, 129.61, 129.34, 127.88, 126.28, 124.45, 123.94, 122.78, 119.52, 118.30, 40.18.

HRMS-MALDI: calculated for $C_{19}H_{15}O$ $[M-H]^+$: 259.1117; found: 259.1111

7-(2-(Benzyloxy)phenyl)cyclohepta-1,3,5-triene (22b)



n-BuLi (2.0 M in hexanes, 5.5 mL, 11 mmol) was added dropwise to the solution of 1-(benzyloxy)-2-iodobenzene[14] (3.1 g, 10 mmol) in 40 mL THF at -78 ºC. After stirring for 0.5 h, tropylium tetrafluoroborate (2.0 g, 11 mmol) was added, and stirred

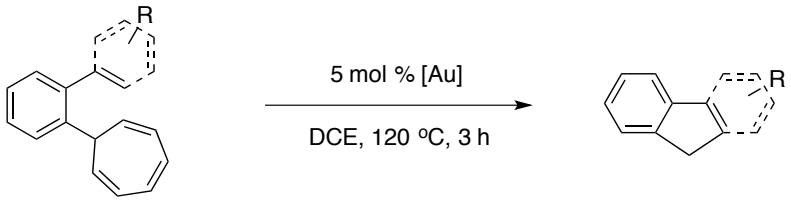
(14) 1-(Benzyloxy)-2-iodobenzene was prepared according to the reported procedure: Cakir, S. P.; Stokes, S.; Sygula, A.; Mead, K. T. *J. Org. Chem.* **2009**, *74*, 7529–7532.

at room temperature overnight (12 h). The reaction was quenched by addition of water. The aqueous phase was extracted with ether, the combined organic extracts were dried over $MgSO_4$, and the solvent was evaporated. The crude reaction mixture was purified by column chromatography on silica gel to give 1.7 g colorless oil in 62% yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 - 7.25 (m, 7H), 7.06 - 6.99 (m, 2H), 6.75 (dd, *J* = 3.7, 2.6 Hz, 2H), 6.27 (dddd, *J* = 8.9, 3.9, 2.6, 1.4 Hz, 2H), 5.52 (dd, *J* = 8.7, 5.6 Hz, 2H), 5.14 (s, 2H), 3.31 - 3.21 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 156.44, 137.32, 132.17, 130.79, 128.87, 128.44, 127.76, 127.57, 127.02, 126.75, 124.21, 121.13, 112.62, 70.04, 40.62.

HRMS-APCI calculated for $C_{20}H_{19}O$ $[M+H]^+$: 275.1430; found: 275.1428

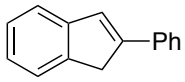
3. General Procedure B for the Gold-Catalyzed Formation of Indenes and Fluorenes.



A solution of the *o*-arylcycloheptatriene substrate (0.1 mmol) and gold complex (5 mol %) in 1,2-dichloroethane (DCE, 1 mL) was heated at 120 ºC in a sealed tube until the starting material had been fully consumed (2-3 h). The reaction was performed under an air atmosphere with no special precautions taken to exclude water. After the reaction mixture had been allowed to cool to room temperature, the solvent was removed in vacuo, and the crude residue was purified by preparative TLC.

Experimental Details on the Synthesis of Indenes.

2-Phenyl-1*H*-indene (8a)

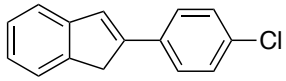


This compound was prepared as a colorless solid in 74% yield from **7a** according to the general procedure B.

The spectroscopic data match with those reported in the literature.[15]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 7.1 Hz, 2H), 7.52 (d, *J* = 7.4 Hz, 1H), 7.46 - 7.40 (m, 3H), 7.34 - 7.26 (m, 3H), 7.23 (td, *J* = 7.4, 1.2 Hz, 1H), 3.83 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.4, 145.3, 143.1, 136.0, 128.7, 127.5, 126.6, 126.5, 125.6, 124.7, 123.6, 121.0, 39.0.

2-(4-Chlorophenyl)-1*H*-indene (8b)



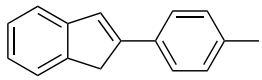
This compound was prepared as a colorless solid in 65% yield from **7b** according to the general procedure B.

(15) Deng, R.; Sun, L.; Li, Z. *Org. Lett.* **2007**, *9*, 5207–5210.

The spectroscopic data match with those reported in the literature.[16]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.6 Hz, 2H), 7.50 (d, *J* = 7.2 Hz, 1H), 7.43 (d, *J* = 7.6 Hz, 1H), 7.37 (d, *J* = 8.5 Hz, 2H), 7.31 (td, *J* = 7.5, 1.1 Hz, 1H), 7.26 - 7.18 (m, 2H), 3.79 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.1, 145.0, 143.0, 134.5, 133.1, 128.8, 127.1, 126.8, 126.7, 125.0, 123.7, 121.1, 38.9.

2-(*p*-Tolyl)-1*H*-indene (8c)

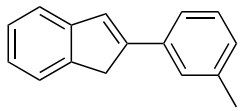


This compound was prepared as a colorless solid in 74% yield from **7c** according to the general procedure B.

The spectroscopic data match with those reported in the literature.[17]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 8.1 Hz, 2H), 7.50 (d, *J* = 7.3 Hz, 1H), 7.42 (d, *J* = 7.6 Hz, 1H), 7.32 (dd, *J* = 7.6, 1.1 Hz, 1H), 7.25 - 7.18 (m, 4H), 3.81 (s, 2H), 2.41 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.5, 145.5, 143.0, 137.4, 133.2, 129.3, 126.5, 125.6, 125.5, 124.5, 123.6, 120.8, 39.0, 21.2.

2-(*m*-Tolyl)-1*H*-indene (8d)

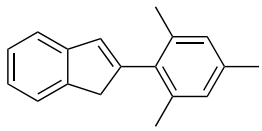


This compound was prepared as a colorless solid in 78% yield from **7d** according to the general procedure B.

The spectroscopic data match with those reported in the literature.[16]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 - 7.47 (m, 3H), 7.44 (d, *J* = 7.1 Hz, 1H), 7.32 (t, *J* = 7.5 Hz, 2H), 7.26 (s, 1H), 7.22 (td, *J* = 7.4, 1.2 Hz, 1H), 7.14 (d, *J* = 7.2 Hz, 1H), 3.83 (s, 2H), 2.44 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.6, 145.4, 143.1, 138.2, 135.9, 128.6, 128.3, 126.6, 126.4, 124.6, 123.6, 122.8, 120.9, 39.0, 21.5.

2-Mesityl-1*H*-indene (8e)



This compound was prepared as a colorless solid in 83% yield from **7e** according to the general procedure B.

The spectroscopic data match with those reported in the literature.[18]

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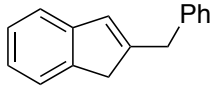
(16) Greifenstein, L. G.; Lambert, J. B.; Nienhuis, R. J.; Fried, H. E.; Pagani, G. A. *J. Org. Chem.* **1981**, *46*, 5125–5132.
(17) Jayamani, M.; Pant, N.; Ananthan, S.; Narayanan, K.; Pillai, C. N. *Tetrahedron* **1986**, *42*, 4325–4332.
(18) Lebedev, A. Y.; Izmer, V. V.; Asachenko, A. F.; Tzarev, A. A.; Uborsky, D. V.; Homutova, Y. A.; Shperber, E. R.; Canich, J. A. M.; Voskoboynikov, A. Z. *Organometallics* **2009**, *28*, 1800–1816.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.3 Hz, 1H), 7.46 (d, *J* = 7.3 Hz, 1H), 7.35 (td, *J* = 7.4, 1.0 Hz, 1H), 7.25 (td, *J* = 7.5, 1.2 Hz, 1H), 6.98 (s, 2H), 6.69 (s, 1H), 3.60 (s, 2H), 2.37 (s, 3H), 2.22 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.6, 145.4, 143.5, 136.7, 136.2, 134.7, 130.2, 128.0, 126.4, 124.2, 123.5, 120.7, 42.1, 21.0, 20.5.

2-Benzyl-1*H*-indene (8f)

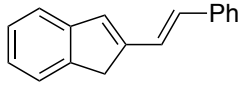


This compound was prepared as a colorless solid in 78% yield from **7f** according to the general procedure B.

The spectroscopic data match with those reported in the literature.[19]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 - 7.22 (m, 8H), 7.13 (td, *J* = 7.4, 1.3 Hz, 1H), 6.55 (s, 1H), 3.85 (s, 2H), 3.32 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.2, 145.3, 143.4, 140.0, 128.8, 128.4, 127.8, 126.2, 126.2, 123.8, 123.4, 120.2, 40.8, 37.9.

(*E*)-2-Styryl-1*H*-indene (8g)

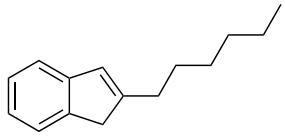


This compound was prepared as a colorless solid in 42% yield from **7g** according to the general procedure B.

The spectroscopic data match with those reported in the literature.[20]

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 (d, *J* = 7.2 Hz, 2H), 7.46 (d, *J* = 7.4 Hz, 1H), 7.40 - 7.35 (m, 3H), 7.31 - 7.19 (m, 4H), 6.88 (s, 1H), 6.81 (d, *J* = 16.2 Hz, 1H), 3.70 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 146.3, 145.1, 142.8, 137.3, 131.3, 129.4, 128.7, 127.5, 126.6, 126.3, 125.0, 124.9, 123.6, 120.9, 37.4.

2-Hexyl-1*H*-indene (8h)



This compound was prepared as a colorless solid in 89% yield from **7h** according to the general procedure B.

The spectroscopic data match with those reported in the literature.[21]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, *J* = 7.3 Hz, 1H), 7.31 - 7.22 (m, 2H), 7.13 (td, *J* = 7.3, 1.3 Hz, 1H), 6.53 (s, 1H), 3.34 (s, 2H), 2.51 (t, *J* = 7.6 Hz, 2H), 1.71 - 1.59 (m, 2H), 1.43 - 1.29 (m, 6H), 0.92 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.0, 145.7, 143.1, 126.2, 126.0, 123.4, 123.3, 119.8, 41.0, 31.7, 31.2, 29.1, 29.0, 22.6, 14.1.

2-(4-Methylpent-3-en-1-yl)-1*H*-indene (8i)

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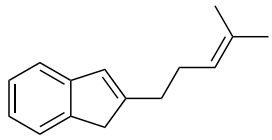
(19) Martinez, A.; Fernandez, M.; Estevez, J. C.; Estevez, R. J.; Castedo, L. *Tetrahedron* **2005**, *61*, 485–492.
(20) Deng, R.; Sun, L.; Li, Z. *Org. Lett.* **2007**, *9*, 5207–5210.
(21) Lee, D.-H.; Kwon, K.-H.; Yi, C. S. *Science* **2011**, *333*, 1613–1616.

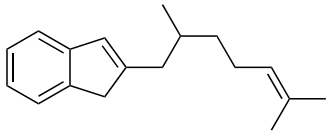


This compound was prepared as a colorless oil in 69% yield from **7i** according to the general procedure B.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 (d, *J* = 7.3 Hz, 1H), 7.30 (d, *J* = 7.4 Hz, 1H), 7.25 (t, *J* = 7.4 Hz, 1H), 7.13 (td, *J* = 7.3, 1.3 Hz, 1H), 6.55 (s, 1H), 5.21 (t, *J* = 7.0 Hz, 1H), 3.34 (d, *J* = 1.3 Hz, 2H), 2.58 - 2.51 (m, 2H), 2.33 (q, *J* = 7.4 Hz, 2H), 1.73 (d, *J* = 1.3 Hz, 3H), 1.66 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 150.6, 145.7, 143.1, 132.0, 126.2, 126.2, 123.9, 123.5, 123.3, 119.8, 41.1, 31.4, 27.6, 25.7, 17.7.

HRMS-EI calculated for $C_{15}H_{18}$ $[M]^+$: 198.1409; found: 198.1405

2-(2,6-Dimethylhept-5-en-1-yl)-1*H*-indene (8j)

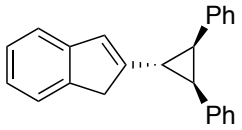


A 1 mL DCE solution of substrate **7j** (32 mg, 0.1 mmol) and gold catalyst **E** (4 mg, 5 mol %) was heated at 120 °C overnight. After cooling to room temperature, the solvent was removed in vacuo. The residue was purified with preparative TLC to give **8j** as a colorless oil (19.2mg, 80%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, *J* = 7.6 Hz, 1H), 7.30 (d, *J* = 7.3 Hz, 1H), 7.25 (t, *J* = 7.1 Hz, 1H), 7.13 (td, *J* = 7.3, 1.3 Hz, 1H), 6.54 (d, *J* = 1.1 Hz, 1H), 5.19 - 5.09 (m, 1H), 3.34 (d, *J* = 22.9 Hz, 1H), 3.32 (d, *J* = 22.7 Hz, 1H), 2.52 (ddd, *J* = 14.2, 6.1, 1.4 Hz, 1H), 2.33 (ddd, *J* = 14.0, 8.0, 1.2 Hz, 1H), 2.15 - 1.98 (m, 2H), 1.82 – 1.76 (m, 1H), 1.73 (s, 3H), 1.65 (s, 3H), 1.48 – 1.43 (m, 1H), 1.28 – 1.19 (m, 1H), 0.96 (d, *J* = 6.6 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 149.75, 145.72, 143.28, 131.27, 127.51, 126.21, 124.72, 123.50, 123.36, 119.83, 41.25, 39.06, 37.04, 32.67, 25.74, 25.64, 19.79, 17.69.

HRMS-APCI calculated for $C_{18}H_{25}$ $[M+H]^+$: 241.1951; found: 241.1953

2-((1*R,2*S**,3*R**)-2,3-diphenylcyclopropyl)-1*H*-indene (8k)**



This compound was prepared according to the general procedure B. The 1 mL DCE solution of substrate **7k** (39 mg, 0.1 mmol) and gold catalyst A (3.7 mg, 5 mol %) was heated at 120 °C for 2 h. After cooling to room temperature, the solvent was removed in vacuo. The residue was purified with preparative TLC to give **8k** as a colorless solid (19.2 mg, 62%).

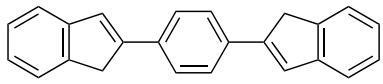
m.p. 129-131 ºC

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (d, *J* = 7.4 Hz, 1H), 7.34 (d, *J* = 7.1 Hz, 1H), 7.28 (t, *J* = 7.2 Hz, 1H), 7.21 - 7.11 (m, 7H), 7.05 - 7.01 (m, 4H), 6.75 (s, 1H), 3.48 (s, 2H), 2.85 - 2.75 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 150.25, 145.39, 142.44,

137.48, 128.92, 127.89, 126.50, 126.01, 125.56, 123.82, 123.52, 119.99, 39.79, 34.27, 27.76.

HRMS-APCI calculated for $C_{24}H_{21}$ $[M+H]^+$: 309.1638; found: 309.1637

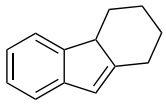
1,4-Di(1*H*-inden-2-yl)benzene (8l)



This compound was prepared from **7l** according to the general procedure B. A highly insoluble yellow solid was collected by filtration after cooling down to r.t. (in 41% yield). No further purification was necessary.

^{1}H NMR (500 MHz, 1,1,2,2-tetrachloroethane-d_2; 398 K) δ 7.60 (s, 4H), 7.44 (d, J = 7.3 Hz, 2H), 7.37 (d, J = 7.5 Hz, 2H), 7.24 (t, J = 7.4 Hz, 2H), 7.19 (s, 2H), 7.15 (t, J = 7.3 Hz, 2H), 3.78 (s, 4H). ^{13}C NMR (126 MHz, 1,1,2,2-tetrachloroethane-d_2; 398 K) δ ^{13}C NMR (126 MHz, 1,1,2,2-tetrachloroethane-d_2) δ 145.7, 144.8, 142.6, 134.9, 126.2, 126.1, 125.4, 124.3, 123.0, 120.4, 38.6. HRMS-MALDI calculated for $C_{24}H_{18}$ $[M]^+$: 306.1403; found 306.1402

2,3,4,4a-Tetrahydro-1*H*-fluorene (8m)

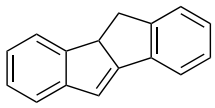


This compound was prepared as a colorless oil in 73% yield from **7m** according to the general procedure B.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 (d, J = 7.3 Hz, 1H), 7.31 (d, J = 7.4 Hz, 1H), 7.24 (td, J = 7.5, 1.1 Hz, 1H), 7.13 (td, J = 7.5, 1.3 Hz, 1H), 6.40 (s, 1H), 3.08 (dd, J = 12.5, 6.1 Hz, 1H), 2.82 - 2.76 (m, 1H), 2.59 - 2.54 (m, 1H), 2.42 - 2.34 (m, 1H), 2.07 - 2.00 (m, 1H), 1.92 - 1.88 (m, 1H), 1.65 - 1.58 (m, 1H), 1.29 - 1.21 (m, 1H), 0.94 (qd, J = 12.8, 3.5 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 153.6, 147.7, 144.8, 126.3, 123.4, 122.3, 121.7, 120.0, 50.0, 32.4, 29.2, 28.0, 25.4.

HRMS-APCI calculated for $C_{13}H_{15}$ $[M+H]^+$: 171.1174; found: 171.1169

4b,5-Dihydroindeno[2,1-*a*]indene (8n)



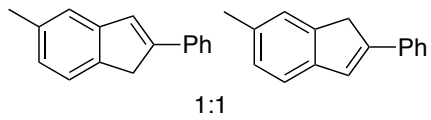
This compound was prepared from **7n** according to the general procedure B as a colorless solid in 31% yield.

m.p. 103-105 ºC

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (dd, J = 7.5, 0.6 Hz, 1H), 7.48 (d, J = 7.4 Hz, 1H), 7.39 (d, J = 7.5 Hz, 1H), 7.34 (d, J = 7.3 Hz, 1H), 7.31 - 7.26 (m, 2H), 7.23 – 7.16 (m, 2H), 6.75 (d, J = 2.5 Hz, 1H), 4.45 (td, J = 8.5, 2.6 Hz, 1H), 3.45 (dd, J = 14.8, 8.6 Hz, 1H), 2.70 (dd, J = 14.7, 8.5 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.8, 151.1, 149.2, 145.2, 136.9, 127.3, 127.0, 126.9, 125.7, 124.1, 123.5, 121.8, 121.7, 119.1, 58.5, 33.1.

HRMS-MALDI: calculated for $C_{16}H_{12}$ $[M]^+$: 204.0939; found: 204.0957

5-Methyl-2-phenyl-1*H*-indene (8p′) and 6-methyl-2-phenyl-1*H*-indene (8p)



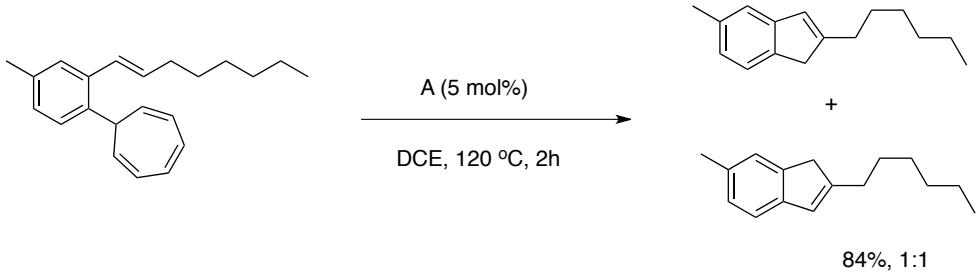
This mixture of compounds was prepared as a colorless solid in 81% yield (1:1 mixture) from **7p** according to the general procedure B.

m.p. 180-181 ºC

Some proton signals arising of the two isomers could be differentiated (labeled as *isomer a* and *isomer b*); however, these could not be assigned definitively to **8p** or **8p**. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.69 - 7.66 (m, 2H), 7.45 - 7.23 (m, 6H), 7.16 - 7.13 (d, *J* = 7.9 Hz, 1H, *isomer a*), 7.06 (dd, *J* = 7.7, 1.5 Hz, 1H, *isomer b*), 3.80 (s, 2H), 2.46 (s, 3H, *isomer a*), 2.45 (s, 3H, *isomer b*). ^{13}C NMR (126 MHz, $CDCl_3$, mixture of signals) δ 146.6, 145.6, 145.3, 143.5, 142.7, 140.2, 136.2, 136.1, 134.5, 128.6, 127.4, 127.3, 127.3, 126.5, 126.4, 125.6, 125.5, 124.6, 123.3, 121.7, 120.6, 38.8, 38.6, 21.5, 21.5.

HRMS-APCI calculated for $C_{16}H_{15}$ $[M+H]^+$: 207.1174; found: 207.1173

2-Hexyl-5-methyl-1*H*-indene (8q′) and 2-hexyl-6-methyl-1*H*-indene (8q)

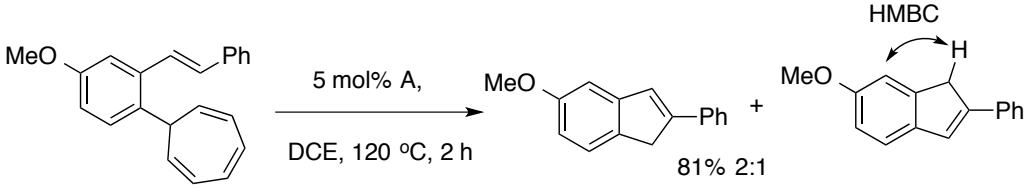


This mixture of compounds was prepared as a colorless oil in 84% yield (1:1 mixture) from **7q** according to the general procedure B.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (d, *J* = 7.7 Hz, 1H), 7.23 (s, 1H), 7.18 (d, *J* = 7.6 Hz, 1H), 7.12 (s, 1H), 7.05 (d, *J* = 7.7 Hz, 1H), 6.95 (d, *J* = 7.7 Hz, 1H), 6.48 (m, 2H), 3.29 (s, 4H), 2.53 - 2.47 (m, 4H), 2.40 (s, 6H), 1.68 - 1.58 (m, 4H), 1.39 - 1.29 (m, 12H), 0.94 (t, *J* = 6.8 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.33, 149.93, 146.02, 143.47, 143.09, 140.16, 135.73, 133.00, 126.83, 125.96, 125.79, 124.38, 124.23, 123.04, 120.61, 119.43, 40.84, 40.64, 31.77, 31.31, 31.25, 29.15, 29.05, 22.65, 21.46, 21.39, 14.12.

HRMS-APCI calculated for $C_{16}H_{23}$ $[M+H]^+$: 215.1794; found: 215.1801

5-Methoxyl-2-phenyl-1*H*-indene (8r′) and 6-methoxyl-2-phenyl-1*H*-indene (8r)



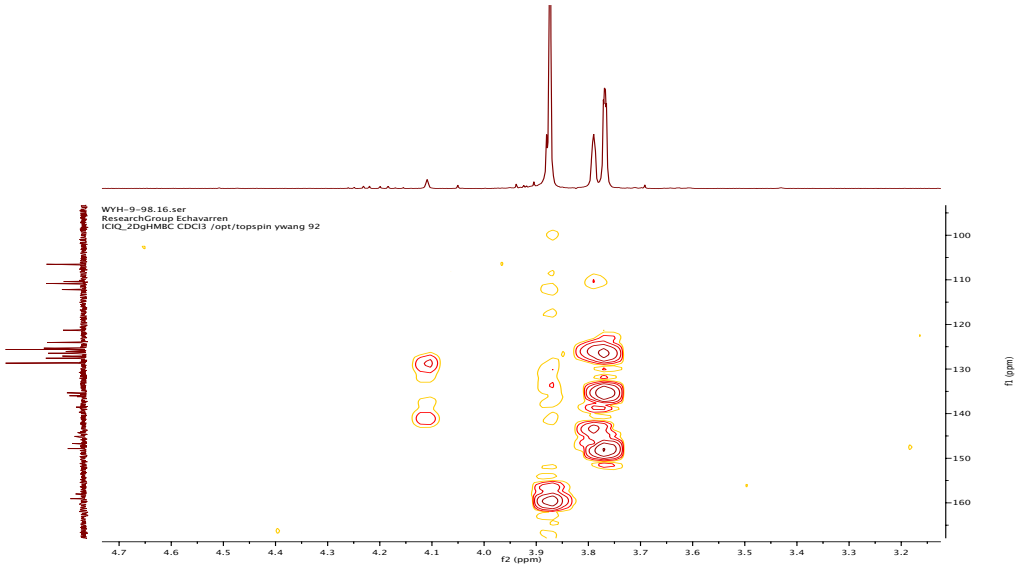
This mixture of compounds was prepared as a colorless solid in 81% yield (2:1 mixture, **8r′** as the major product) from **7r** according to the general procedure B. The

ratio of products was determined by integration of peaks in the ^{1}H NMR spectrum. HMBC was used to elucidate which were the major and minor products.

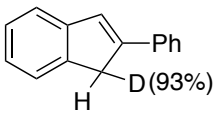
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 - 7.61 (m, major2H+minor2H), 7.44 - 7.31 (m, major4H+minor4H), 7.20 (s, major1H+minor1H), 7.10 (d, J = 0.7 Hz, minor1H), 6.99 (d, J = 2.4 Hz, major1H), 6.87 (dd, J = 8.2, 2.4 Hz, minor1H), 6.78 (dd, J = 8.1, 2.4 Hz, major1H), 3.87 (s, major3H+minor3H), 3.79 (s, minor2H), 3.77 (s, major2H). ^{13}C NMR (101 MHz, $CDCl_3$, mixed signals) δ 159.08, 158.01, 147.85, 146.70, 145.09, 144.25, 138.54, 136.21, 136.00, 135.34, 128.68, 128.65, 127.57, 127.09, 126.46, 126.06, 125.63, 125.32, 124.06, 121.29, 112.19, 110.82, 110.38, 106.50, 55.58, 55.51, 39.07, 38.26.

HRMS-APCI calculated for $C_{16}H_{15}O$ $[M+H]^+$: 223.1117; found: 223.1116

HMBC cross peak of **8r** (δ(H) 3.79, δ(C) 110.25)



2-Phenyl-1*H*-indene-d_1 (8a-d_1)

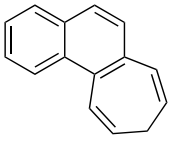


This compound was prepared as a colorless solid in 73% yield from **7a-d_1** according to the general procedure B.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.67 (d, J = 7.2 Hz, 2H), 7.51 (d, J = 7.2 Hz, 1H), 7.46 - 7.40 (m, 3H), 7.33 - 7.29 (m, 2H), 7.27 (d, J = 1.4 Hz, 1H), 7.22 (td, J = 7.4, 1.1 Hz, 1H), 3.81 (s, 1H and 7% residual signal). ^{13}C NMR (126 MHz, $CDCl_3$) δ 146.4, 145.4, 143.1, 136.0, 128.6, 127.5, 126.6, 126.5, 125.6, 124.7, 123.6, 120.9, 38.7 (t, J_{CD} = 19.7 Hz).

HRMS-APCI calculated for $C_{15}H_{12}D$ $[M+H]^+$: 194.1080; found: 194.1081

9*H*-Cyclohepta[*a*]naphthalene (12)

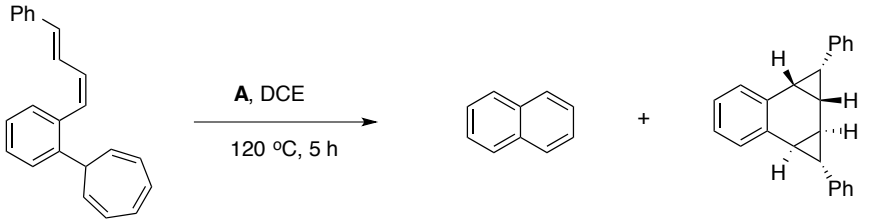


This compound was prepared as a colorless oil in 28% yield from ***cis*-7a** according to the general procedure B.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.24 (d, *J* = 8.6 Hz, 1H), 7.88 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.76 (d, *J* = 8.6 Hz, 1H), 7.61 - 7.51 (m, 2H), 7.48 (d, *J* = 8.6 Hz, 1H), 7.24 (d, *J* = 10.0 Hz, 1H), 6.82 (d, *J* = 10.0 Hz, 1H), 6.05 (ddt, *J* = 9.9, 8.6, 6.9 Hz, 2H), 2.41 (t, *J* = 6.9 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 134.8, 133.6, 132.2, 131.7, 130.3, 128.8, 128.3, 128.2, 126.9, 126.5, 126.2, 125.7, 125.2, 124.8, 26.5.

HRMS-EI calculated for $C_{15}H_{12}$ $[M]^+$: 192.0939; found: 192.0939

(1*R,1a*S**,1b*S**,2*S**,2a*S**,6b*S**)-1,2-diphenyl-1,1a,1b,2,2a,6b-hexahydrodicyclopropa[*a*,*c*]naphthalene (15)**

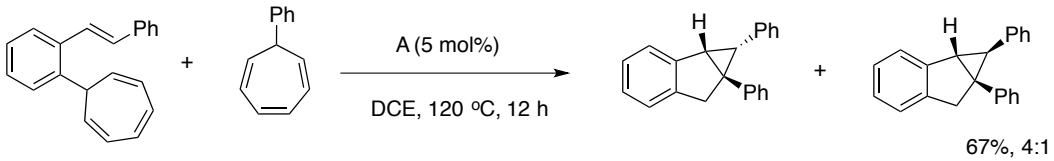


The 1 mL DCE solution of **7u** (45 mg, 0.15 mmol) and gold catalyst **A** (5.5 mg, 5 mol %) was heated at 120 °C for 5 h. After cooling to room temperature, the solvent was removed in vacuo. The residue was passed through a short column of silica, and naphthalene (colorless solid, 4.6 mg, 24%) was separated from the crude residue. The remaining mixture was purified carefully with preparative TLC to give **15** as a colorless solid (5.9 mg, 12%).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39 - 7.10 (m, 12H), 7.00 (td, *J* = 7.5, 1.4 Hz, 1H), 6.90 (dd, *J* = 7.6, 1.4 Hz, 1H), 2.59 (dd, *J* = 9.4, 8.2 Hz, 1H), 2.38 - 2.32 (m, 2H), 2.11 (t, *J* = 4.6 Hz, 1H), 2.06 (dd, *J* = 8.5, 4.7 Hz, 1H), 1.66 (dd, *J* = 8.6, 4.3 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 142.2, 136.6, 135.8, 131.3, 130.9, 130.1, 128.5, 128.3, 127.6, 125.7, 125.6, 125.5, 125.4, 125.3, 35.7, 29.7, 29.0, 25.4, 20.8, 20.2.

HRMS-APCI calculated for $C_{24}H_{21}$ $[M+H]^+$: 309.1643; found: 309.1649

(1*R,1a*S**,6a*R**)-1,6a-diphenyl-1,1a,6,6a-tetrahydrocyclopropa[*a*]indene (5a) and (5a′)**



The DCE solution of (*E*)-7-(2-styrylphenyl)cyclohepta-1,3,5-triene **7a** (27 mg, 0.1 mmol) and gold complex (3.7mg, 5 mol %) was heated at 120 °C for 2 h. After cooling to room temperature, 7-phenylcyclohepta-1,3,5-triene **1a**[22] (34 mg, 0.2 mmol) was added, and the mixture was heated to 120 °C overnight (12 h). The reaction mixture was cooled to room temperature, the solvent was removed in vacuo, and the resulting residue was purified by preparative TLC to give 19 mg of the title mixture (67%, 4:1) as a colorless solid.

m.p. 84.5-87.8 °C

(22) This compound was reported in: Solorio-Alvarado, C. R.; Wang, Y.; Echavarren, A. M. *J. Am. Chem. Soc*. **2011**, *133*, 11952-11955.

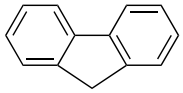
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 - 6.83 (m, aromatic 14H major + 14H minor), 3.68 (d, *J* = 16.9 Hz, 1H minor), 3.49 (d, *J* = 17.0 Hz, 1H minor), 3.42 (d, *J* = 17.3 Hz, 1H major), 3.34 (dd, *J* = 8.4, 1.6 Hz, 1H major), 3.26 (dd, *J* = 3.6, 1.5 Hz, 1H minor), 3.16 (d, *J* = 17.3 Hz, 1H major), 2.88 (d, *J* = 8.3 Hz, 1H major), 2.11 (d, *J* = 3.5 Hz, 1H minor). ^{13}C NMR (101 MHz, $CDCl_3$, major + minor) δ 146.3, 145.1, 142.6, 141.8, 139.8, 138.7, 135.4, 130.7, 129.8, 128.6, 128.1, 127.6, 127.2, 126.3, 126.1, 126.1, 125.8, 125.6, 125.3, 125.2, 124.2, 124.1, 123.3, 45.3, 41.7, 41.5, 38.5, 38.4, 37.7, 37.2, 35.9.

The relative configuration was confirmed by NOE.

HRMS-APCI: calculated for $C_{22}H_{19}$ $[M+H]^+$: 283.1481; found: 283.1498

Experimental Details on the Synthesis of Fluorenes

9*H*-Fluorene (18a)

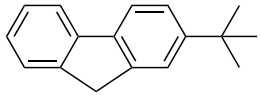


This compound was prepared as a colorless solid in 64% yield from **17a** according to the general procedure B.

The spectroscopic data match with those reported in the literature.[23]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 7.4 Hz, 2H), 7.58 (d, *J* = 7.4 Hz, 2H), 7.41 (td, *J* = 7.5, 1.1 Hz, 2H), 7.33 (td, *J* = 7.4, 1.2 Hz, 2H), 3.94 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.2, 141.7, 126.7, 126.6, 125.0, 119.8, 36.9.

2-(*tert*-Butyl)-9*H*-fluorene (18b)

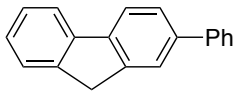


This compound was prepared as a colorless solid in 87% yield from **17b** according to the general procedure B.

The spectroscopic data match with those reported in the literature.[24]

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.5 Hz, 1H), 7.66 (d, *J* = 8.0 Hz, 1H), 7.53 (s, 1H), 7.47 (d, *J* = 7.3 Hz, 1H), 7.37 (d, *J* = 7.9 Hz, 1H), 7.29 (t, *J* = 7.3 Hz, 1H), 7.20 (t, *J* = 7.3 Hz, 1H), 3.83 (s, 2H), 1.33 (s, 9H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 149.9, 143.2, 143.0, 141.6, 139.0, 126.5, 126.1, 124.8, 123.8, 121.8, 119.5, 119.2, 36.9, 34.7, 31.5.

2-Phenyl-9*H*-fluorene (18c)



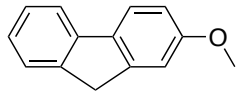
This compound was prepared as a colorless solid in 56% yield from **17c** according to the general procedure B using catalyst E.

(23) Clive, D. L. J.; Sunasee, R. *Org. Lett*. **2007**, *9*, 2677–2680.
(24) Fuchibe, K. *J. Am. Chem. Soc.* **2006**, *128*, 1434-1435.

The spectroscopic data match with those reported in the literature.[25]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 - 7.80 (m, 3H), 7.73 - 7.64 (m, 3H), 7.60 (d, *J* = 7.2 Hz, 1H), 7.48 (t, *J* = 7.9 Hz, 2H), 7.45 - 7.32 (m, 3H), 4.00 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.8, 143.4, 141.5, 141.4, 140.9, 139.8, 128.7, 127.1, 127.1, 126.8, 126.7, 126.0, 125.0, 123.8, 120.1, 119.9, 37.0.

2-Methoxy-9*H*-fluorene (18d)

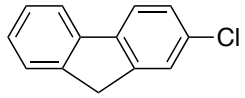


This compound was prepared as a colorless solid in 52% yield from **17d** according to the general procedure B using catalyst E.

The spectroscopic data match with those reported in the literature.[26]

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.73 – 7.69 (m, 2H), 7.53 (d, *J* = 7.5 Hz, 1H), 7.37 (t, *J* = 7.5 Hz, 1H), 7.26 (td, *J* = 7.4, 1.1 Hz, 1H), 7.13 (d, *J* = 2.4 Hz, 1H), 6.96 (dd, *J* = 8.4, 2.5 Hz, 1H), 3.90 (s, 5H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.2, 145.0, 142.6, 141.6, 134.7, 126.7, 125.5, 124.8, 120.5, 119.0, 112.9, 110.5, 55.5, 37.0.

2-Chloro-9*H*-fluorene (18e)

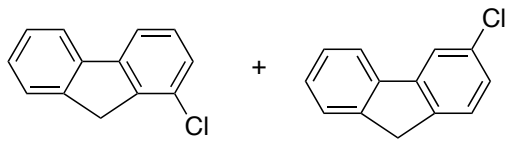


This compound was prepared as a colorless solid in 42% yield from **17e** according to the general procedure B.

The spectroscopic data match with those reported in the literature.[26]

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.78 (d, *J* = 7.6 Hz, 1H), 7.72 (d, *J* = 8.2 Hz, 1H), 7.59 - 7.53 (m, 2H), 7.41 (td, *J* = 7.5, 1.0 Hz, 1H), 7.38 (dd, *J* = 8.1, 2.0 Hz, 1H), 7.34 (td, *J* = 7.4, 1.2 Hz, 1H), 3.92 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 144.8, 142.9, 140.6, 140.2, 132.3, 127.0, 126.9, 126.9, 125.3, 125.0, 120.7, 119.9, 36.8.

1-Chloro-9*H*-fluorene (18f) and 3-Chloro-9*H*-fluorene (18f')



1.2 : 1

These compounds were prepared as a colorless solid in 56% yield from **17f** according to the general procedure B.

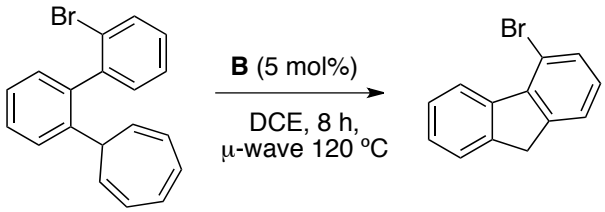
Their spectroscopic data match with those reported in the literature.[26]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 - 7.76 (m, major 1H, minor 2H), 7.70 (dd, *J* = 7.3, 1.1 Hz, major1H), 7.63 – 7.54 (m, major 1H, minor 1H), 7.48 – 7.27 (m, major 4H, minor 4H), 3.95 (s, major 2H), 3.88 (s, minor 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ major + minor : ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.7, 143.5, 143.5, 142.6, 141.3,

(25) Mu, B.; Li, T.; Li, J.; Wu, Y. *J. Organomet. Chem*. **2008**, *693*, 1243–1251.
(26) Hwang, S.-J.; Kim, H.-J.; Chang, S. *Org. Lett.*, **2009**, *11*, 4588-4591.

141.1, 140.6, 128.4, 127.3, 126.9, 126.6, 126.6, 125.9, 125.1, 120.3, 120.1, 118.2, 36.6, 36.5.

4-Bromo-9*H*-fluorene (18g)

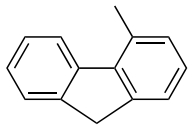


Gold catalyst **B** (13.5 mg, 0.015 mmol) and 2-bromo-2'-(cyclohepta-2,4,6-trien-1-yl)-1,1'-biphenyl **17g** (97 mg, 0.3 mmol) were mixed in a Biotage 2 – 5 mL microwave vial. The solids were dissolved in 1,2-dichloroethane (1.2 mL) before the vial was sealed and heated to 120 ºC in a Biotage initiator microwave for 8 h. Afterwards, the solution was filtered through Celite, concentrated and purified by flash chromatography (cyclohexane) to yield the desired fluorene (18.1 mg, 0.074 mmol, 25%) as a colorless solid.

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.64 (d, *J* = 9.0 Hz, 1H), 7.60 - 7.32 (m, 5H), 7.14 (t, *J* = 7.7 Hz, 1H), 3.95 (s, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 146.17, 143.68, 141.16, 140.01, 131.90, 127.64, 127.45, 126.61, 124.85, 123.93, 123.67, 117.05, 37.40.

HRMS-APCI calculated for $C_{13}H_9Br$ $[M]^+$: 243.9882; found: 243.9880.

4-Methyl-9*H*-fluorene (18h)

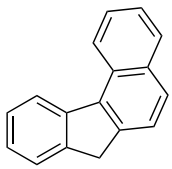


This compound was prepared as a colorless solid in 74% yield from **17h** according to the general procedure B.

The spectroscopic data match with those reported in the literature.[26]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 7.7 Hz, 1H), 7.61 (d, *J* = 7.4 Hz, 1H), 7.44 (td, *J* = 7.6, 1.1 Hz, 2H), 7.35 (td, *J* = 7.4, 1.2 Hz, 1H), 7.26 (t, *J* = 7.4 Hz, 1H), 7.20 (d, *J* = 7.5 Hz, 1H), 3.96 (s, 2H), 2.79 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.6, 143.6, 142.7, 139.8, 133.0, 128.9, 126.6, 126.4, 126.0, 124.8, 123.1, 122.4, 37.1, 21.1.

7*H*-benzo[*c*]fluorene (18i)

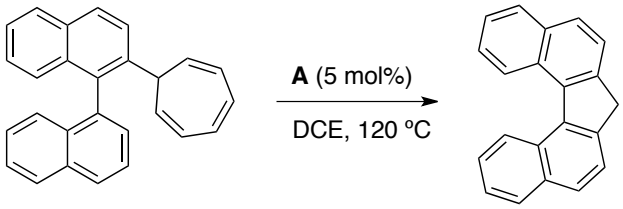


A solution of 1-(2-(cyclohepta-2,4,6-trien-1-yl)phenyl)naphthalene **17i** (20.2 mg, 69 μmol) and gold complex **A**(2.6 mg, 3.4 μmol) in DCE (0.68 mL) was heated at 120 ºC in a sealed tube until the starting material had been fully consumed (3 h). The reaction mixture was cooled to room temperature, the solvent was removed in vacuo, and the crude residue was purified by chromatography (Combiflash 4 g column, cyclohexane eluent) to give the title compound in 59% yield as a colorless solid (8.7 mg).

The spectroscopic data match with those reported in the literature.[27]

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.79 (d, *J* = 8.4 Hz, 1H), 8.41 (d, *J* = 7.8 Hz, 1H), 7.98 (d, *J* = 8.1 Hz, 1H), 7.83 (d, *J* = 8.2 Hz, 1H), 7.71 (d, *J* = 8.3 Hz, 1H), 7.68 – 7.63 (m, 2H), 7.56 – 7.48 (m, 2H), 7.36 (td, *J* = 7.4, 1.0 Hz, 1H), 4.03 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 144.3, 142.9, 142.4, 136.2, 133.5, 129.7, 129.3, 127.8, 127.0, 126.6, 125.8, 125.1, 125.0, 123.8, 123.4, 123.0, 37.9.

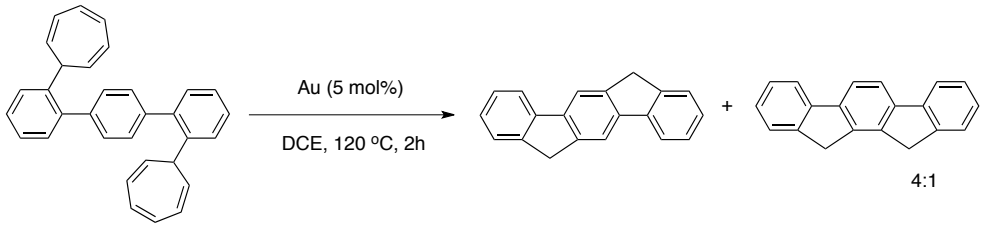
7*H*-Dibenzo[*c*,*g*]fluorene (18j)



This compound was synthesized in 67% yield as a colorless solid following the general procedure B, starting from 2-(cyclohepta-2,4,6-trien-1-yl)-1,1'-binaphthalene **17j** and gold catalyst **A**. After cooling to room temperature, the solution was filtered through Celite, concentrated and purified by flash chromatography (cyclohexane) to yield the title compound. The spectroscopic data matched with those reported in the literature.[28]

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.76 (dq, *J* = 7.9, 0.9 Hz, 2H), 8.00 (dd, *J* = 7.9, 1.7 Hz, 2H), 7.89 (d, *J* = 8.2 Hz, 2H), 7.76 (d, *J* = 8.2 Hz, 2H), 7.63 - 7.50 (m, 4H), 4.14 (s, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 143.02, 138.49, 134.02, 128.98, 128.89, 127.70, 126.82, 125.00, 124.88, 123.00, 39.02.

6,12-Dihydroindeno[1,2-*b*]fluorene (18k/18k′)



The 1 mL DCE solution of substrate **17k** (41 mg, 0.1 mmol) and gold catalyst **A** (3.7 mg, 5 mol %) was heated at 120 °C for 2 h. After cooling to room temperature, the solvent was removed in vacuo. 1 mL acetone was added to dissolve some of the residue. The liquid was decanted, leaving behind a colorless solid which was dried in vacuo to give a 4:1 mixture of **18k**/**18k′** (13.5 mg, 53%).

The spectroscopic data match with those reported in the literature.[29]

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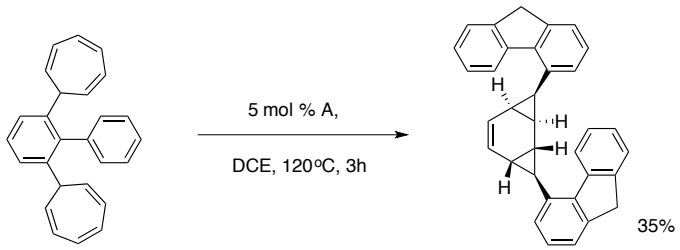
(27) Laali, K. K; Okazaki, T.; Sultana, F.; Bunge, S. D.; Banik, B. K.; Swartz, C. *Eur. J. Org. Chem.* **2008**, 1740–1752.

(28) (a) Laali, K. K.; Okazaki, T.; Sultana, F.; Bunge, S. D.; Banik, B. K.; Swartz, C. *Eur. J. Org. Chem.* **2008**, 1740–1752. (b) Harvey, R. D.; Pataki, J.; Cortez, C.; Raddo, P. D.; Yang, C.-X. *J. Org. Chem.* **1991**, *56*, 1210-1217.

(29) Major isomer: (a) Poriel, C.; Liang, J.-J.; Rault-Berthelot, J.; Barrière, F.; Cocherel, N.; Slawin, A. M. Z.; Horhant, D.; Virboul, M.; Alcaraz, G.; Audebrand, N.; Vignau, L.; Huby, N.; Wantz, G.; Hirsch, L. *Chem. Eur. J.* **2007**, *13*, 10055–

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (s, 2H, major), 7.85 - 7.81 (m, 2H major + 4H minor), 7.60 - 7.56 (m, 2H major + 2H minor), 7.42 (td, *J* = 7.5, 1.2 Hz, 2H major + 2H minor), 7.32 (td, *J* = 7.4, 1.3 Hz, 2H major + 2H minor), 4.00 (s, 4H major), 3.98 (s, 4H minor). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.6, 142.3, 141.8, 140.8, 126.8 (minor), 126.7, 126.5 (minor), 126.4, 125.1 (minor), 125.0, 119.9 (minor), 119.5, 118.7 (minor), 116.4, 36.7, 35.5 (minor).

(1*R,2*R**,3*R**,4*R**,7*R**,8*S**)-3,8-di(9*H*-fluoren-4-yl)tricyclo[5.1.0.0^{2,4}]oct-5-ene (19)**

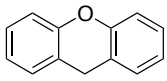


This compound (**19**) was prepared as a yellow oil in 35% yield from **17l** according to the general procedure B.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (d, *J* = 7.8 Hz, 1H), 8.20 (d, *J* = 8.0 Hz, 1H), 7.61 - 7.56 (m, 2H), 7.50 - 7.31 (m, 7H), 7.21 (t, *J* = 7.6 Hz, 1H), 7.16 (t, *J* = 7.5 Hz, 1H), 6.99 (d, *J* = 7.5 Hz, 1H), 5.76 (dd, *J* = 9.8, 4.5 Hz, 1H), 5.68 (dd, *J* = 9.8, 4.6 Hz, 1H), 3.95 (s, 2H), 3.90 (s, 2H), 2.83 (t, *J* = 8.5 Hz, 1H), 2.67 (t, *J* = 4.7 Hz, 1H), 2.54 (t, *J* = 8.5 Hz, 1H), 2.09 - 1.94 (m, 2H), 0.97 (dt, *J* = 8.6, 4.5 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 143.6, 143.6, 143.5, 142.6, 142.2, 141.9, 140.6, 136.1, 132.0, 130.6, 127.1, 126.6, 126.5, 126.3, 126.0, 125.9, 125.5, 124.9, 124.7, 124.7, 123.5, 123.2, 122.8, 122.6, 121.4, 37.1, 36.9, 35.3, 30.7, 21.9, 21.5, 20.5, 17.4.

HRMS-MALDI: calculated for $C_{34}H_{26}$ $[M]^+$: 434.2035; found: 434.2098

9*H*-xanthene (23a)



A solution of 7-(2-phenoxyphenyl)cyclohepta-1,3,5-triene **22a** (26 mg, 0.1 mmol) and gold complex **E** (4 mg, 5 mol %) in toluene (1 mL) was heated at 120 ºC in a sealed tube for 2 h. After cooling to room temperature, the solvent was removed in vacuo and the residue was purified by preparative TLC (eluent: cyclohexane) to give 5.5 mg the title compound in 30% yield as a colorless solid.

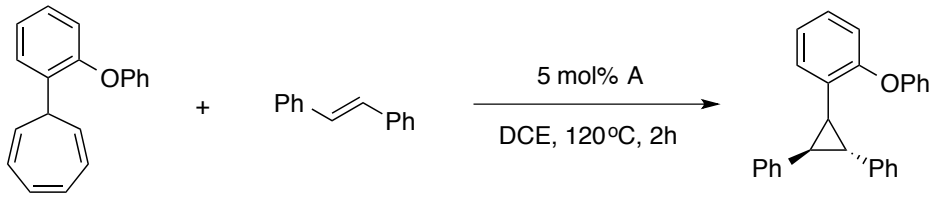
The spectroscopic data match with those reported in the literature.[30]

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.25 - 7.18 (m, 4H), 7.09 - 7.03 (m, 4H), 4.08 (s, 2H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 151.96, 128.90, 127.63, 122.94, 120.58, 116.45, 27.89.

((1*R**,2*R**)-3-(2-Phenoxyphenyl)cyclopropane-1,2-diyl)dibenzene (**24a**)

10069. Minor isomer: (b) Thirion, D., Poriel, C., Rault-Berthelot, J.; Barrière, F.; Jeannin, O. *Chem. Eur. J.* **2010**, *16*, 13646–13658.

(30) Okuma, K.; Nojima, A.; Matsunaga, N.; Shioji, K. *Org. Lett.* **2009**, *11*, 169–171.

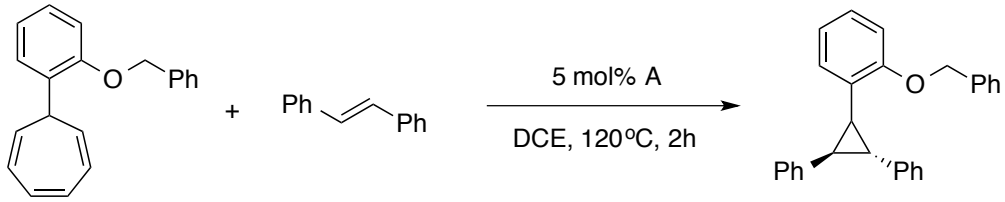


A solution of 7-(2-phenoxyphenyl)cyclohepta-1,3,5-triene **22a** (26 mg, 0.1 mmol), (*E*)-1,2-diphenylethene (36 mg, 0.2 mmol) and gold complex **A** (3.7 mg, 5%) in DCE (0.5 mL) was heated at 120 ºC in a sealed tube for 2 h. After cooling to room temperature, the solvent was removed in vacuo and the residue was purified by preparative TLC (eluent: cyclohexane) to give 29.2 mg the title compound in 81% yield as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 - 6.96 (m, 13H), 7.05 - 6.96 (m, 3H), 6.76 - 6.66 (m, 3H), 3.02 - 2.95 (m, 2H), 2.81 (dd, *J* = 8.6, 6.8 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.27, 156.45, 141.84, 138.23, 130.27, 129.55, 128.46, 128.39, 128.15, 127.73, 127.53, 126.59, 126.06, 125.73, 122.83, 122.81, 118.52, 118.16, 34.30, 30.27, 29.64.

HRMS-APCI: calculated for $C_{27}H_{23}O$ $[M+H]^+$: 363.1743; found: 363.1740

((1*R,2*R**)-3-(2-(benzyloxy)phenyl)cyclopropane-1,2-diyl)dibenzene (24b)**

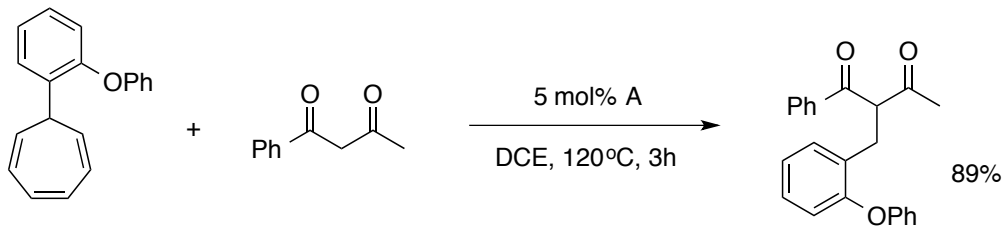


A solution of 7-(2-(benzyloxy)phenyl)cyclohepta-1,3,5-triene **22b** (27 mg, 0.1 mmol), (*E*)-1,2-diphenylethene (36 mg, 0.2 mmol) and gold complex **A** (3.7 mg, 5 mol %) in DCE (0.5 mL) was heated at 120 ºC in a sealed tube for 2 h. After cooling to room temperature, the solvent was removed in vacuo and the residue was purified by preparative TLC (eluent: cyclohexane) to give 28.4 mg the title compound in 75% yield as a colorless oil.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42 - 7.26 (m, 10H), 7.20 - 7.10 (m, 5H), 7.00 (dd, *J* = 7.7, 1.8 Hz, 2H), 6.88 (td, *J* = 7.5, 1.1 Hz, 1H), 6.81 - 6.77 (m, 1H), 5.06 (d, *J* = 12.2 Hz, 1H), 4.88 (d, *J* = 12.2 Hz, 1H), 3.06 (dd, *J* = 9.6, 6.4 Hz, 1H), 2.95 (t, *J* = 6.0 Hz, 1H), 2.83 (dd, *J* = 9.6, 5.7 Hz, 1H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.01, 142.23, 138.73, 137.49, 129.95, 128.47, 128.45, 127.97, 127.58, 127.57, 127.50, 126.96, 126.71, 126.14, 126.00, 125.56, 120.26, 111.58, 69.80, 34.18, 30.56, 29.74.

HRMS-APCI: calculated for $C_{28}H_{25}O$ $[M+H]^+$: 377.1900; found: 377.1890

2-(2-Phenoxybenzyl)-1-phenylbutane-1,3-dione (25a)

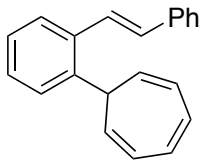


The solution of 7-(2-phenoxyphenyl)cyclohepta-1,3,5-triene **22a** (0.3mmol, 78mg), 1-phenylbutane-1, 3-dione (0.15mmol, 24mg) and gold complex A (5.5mg, 5mol %) in DCE (0.5mL) was heated at 120 ºC in a sealed tube for 3h. The reaction mixture was cooled down to room temperature, after removing the solvent in vacuum, purified by chromatography directly to give 46mg yellow oil in 89% yield.

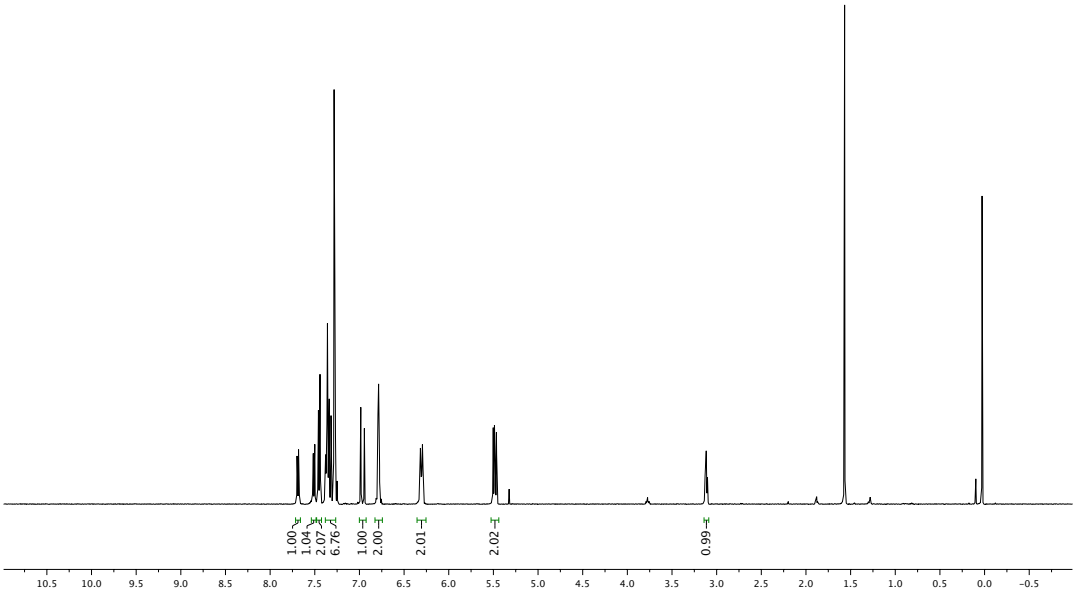
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.94 (d, *J* = 7.0 Hz, 2H), 7.55 (t, *J* = 7.4 Hz, 1H), 7.46 - 7.30 (m, 5H), 7.21 - 7.09 (m, 2H), 7.07 - 6.96 (m, 3H), 6.86 (dd, *J* = 8.1, 1.2 Hz, 1H), 4.99 (t, *J* = 7.1 Hz, 1H), 3.45 - 3.27 (m, 2H), 2.14 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 203.25, 196.10, 157.18, 154.84, 136.34, 133.62, 132.02, 129.91, 129.55, 128.76, 128.74, 128.29, 123.82, 123.22, 118.89, 118.11, 62.48, 30.15, 28.94.

HRMS-ESI: calculated for $C_{23}H_{20}NaO_3$ $[M+Na]^+$: 367.1305; found: 367.1314

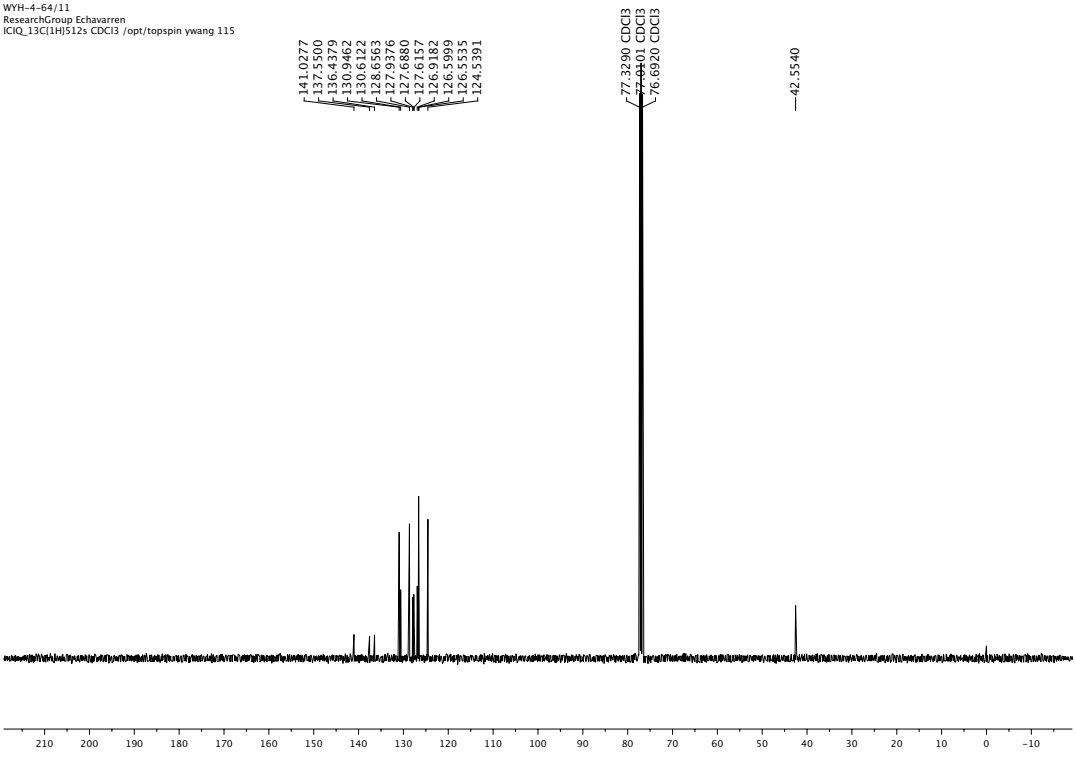
4. NMR Spectra

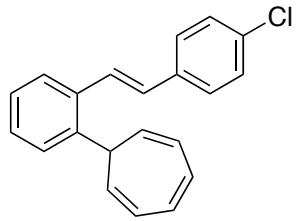


WYH-4-64/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 115

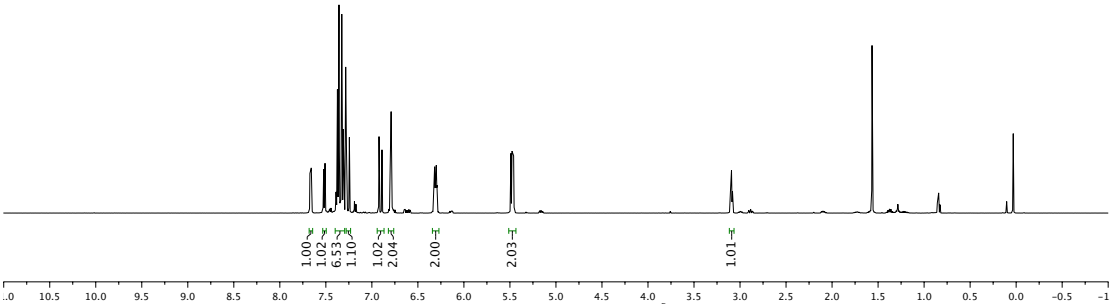


WYH-4-64/11
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 115





WYH-4-82N/1
1H Experiment



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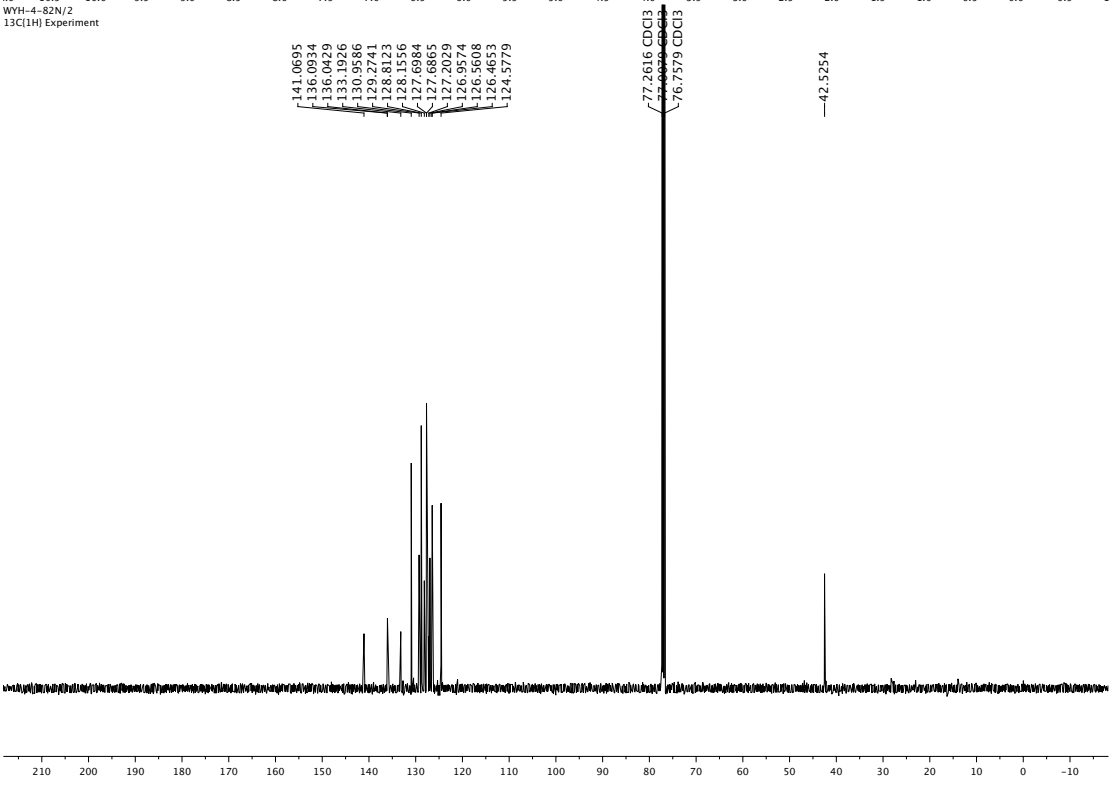
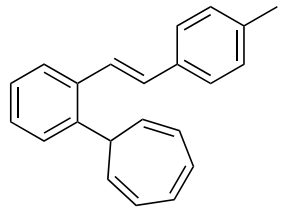
13C{1H} Experiment





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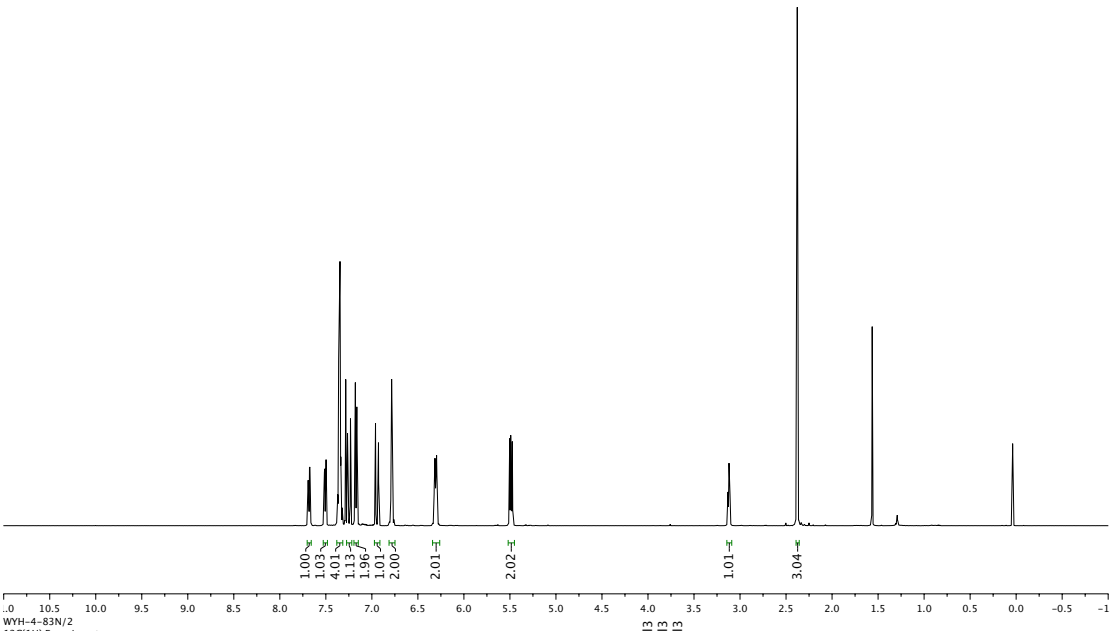
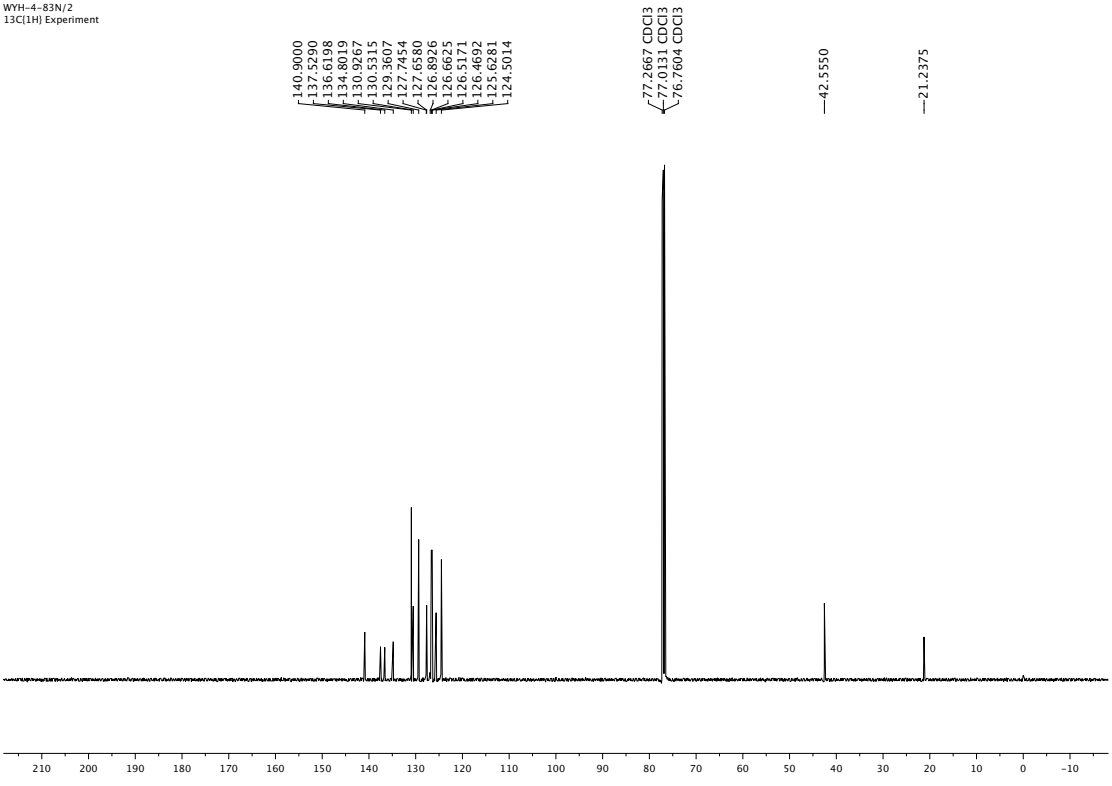
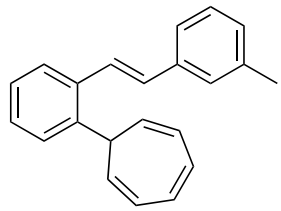
1H Experiment

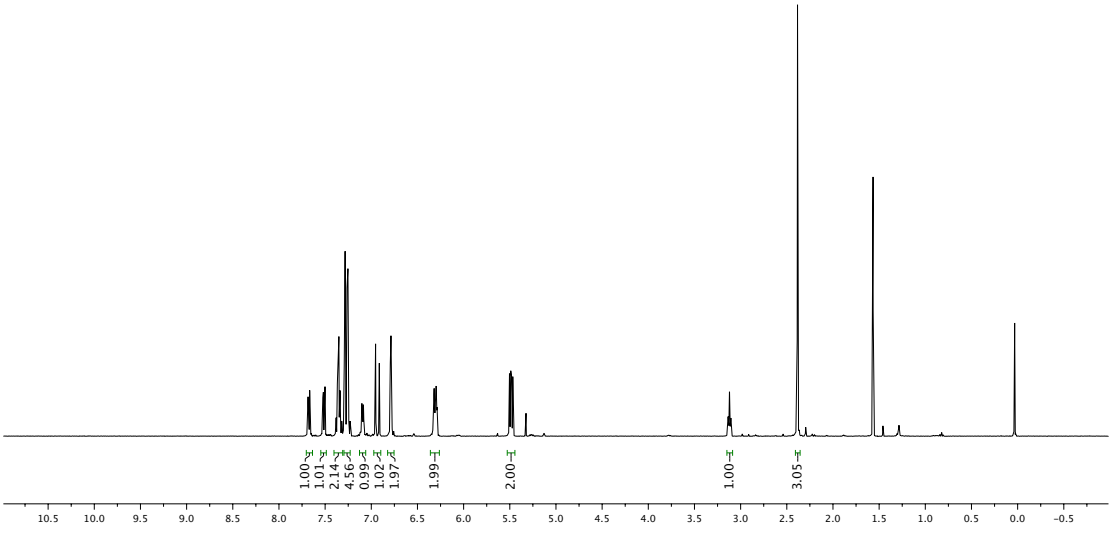


WYH-4-83N/2
13C{1H} Experiment

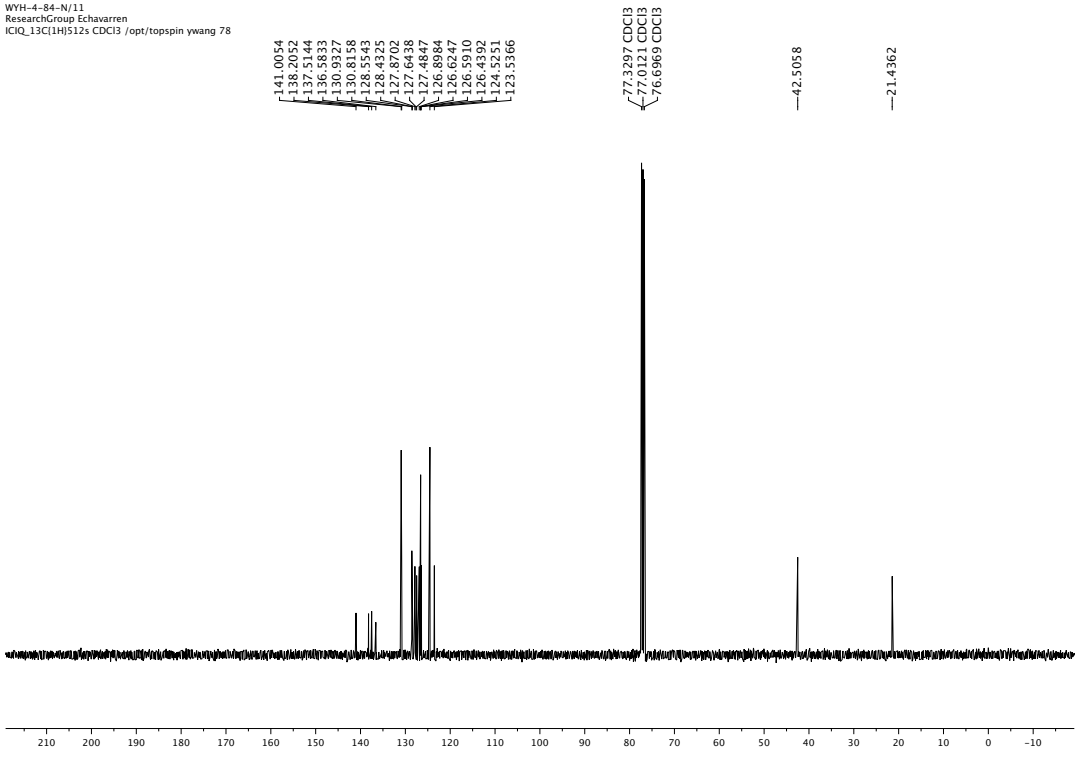


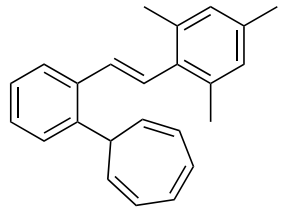


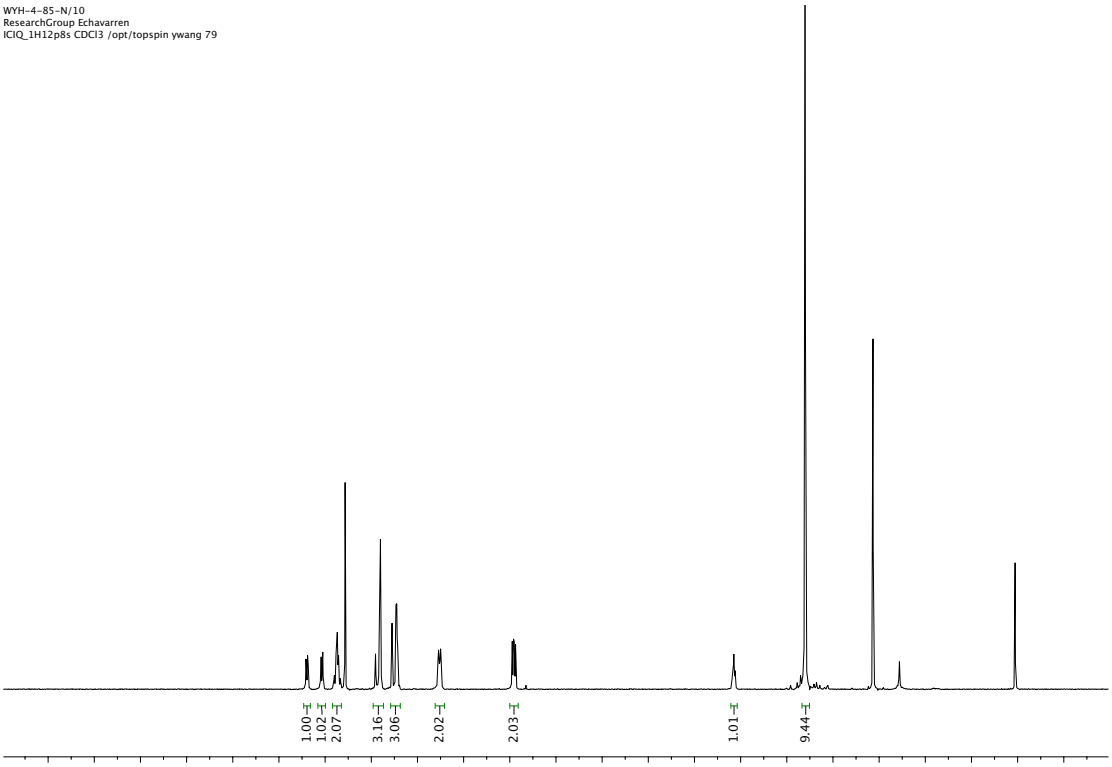
WYH-4-84-N/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 78

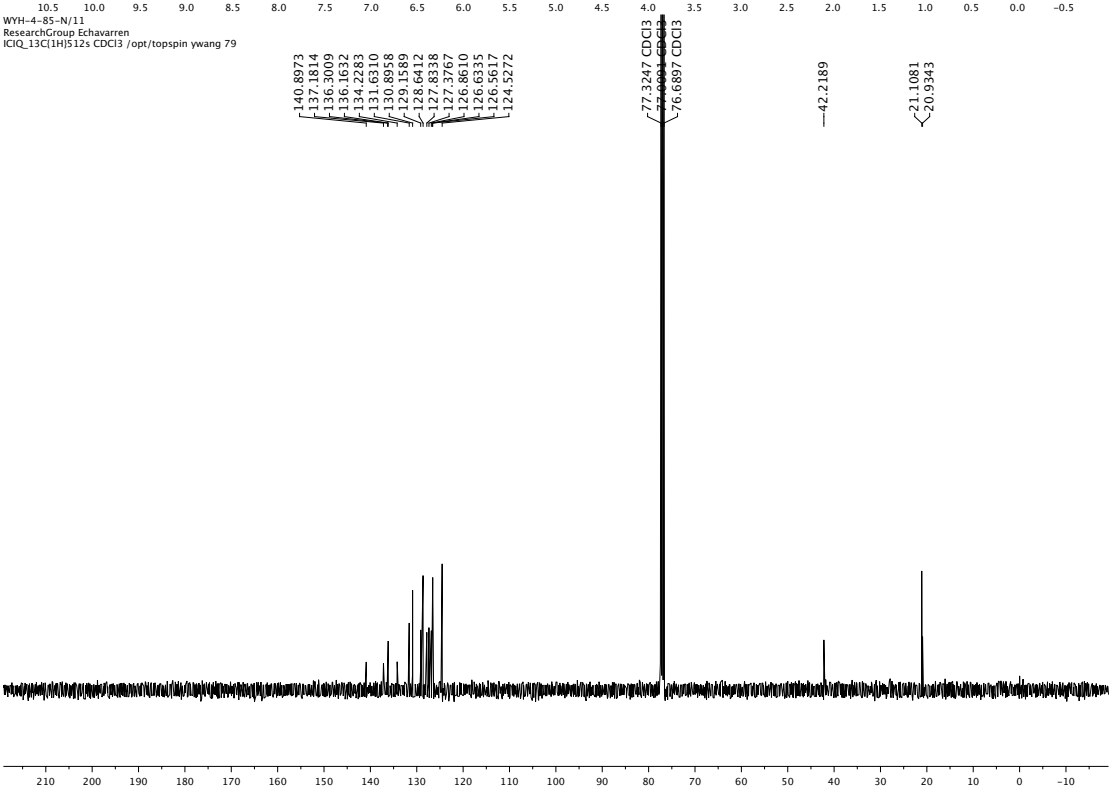


WYH-4-84-N/11
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 78






WYH-4-85-N/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 79
1.00
1.02
2.07
3.16
3.06
2.02
2.03
1.01
9.44
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5


WYH-4-85-N/11
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 79
140.8973
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136.3009
136.1632
134.2283
131.6310
130.8958
129.1589
128.6412
127.8338
127.3767
126.8610
126.6335
126.5617
124.5272
77.3247 CDCl3
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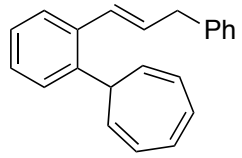
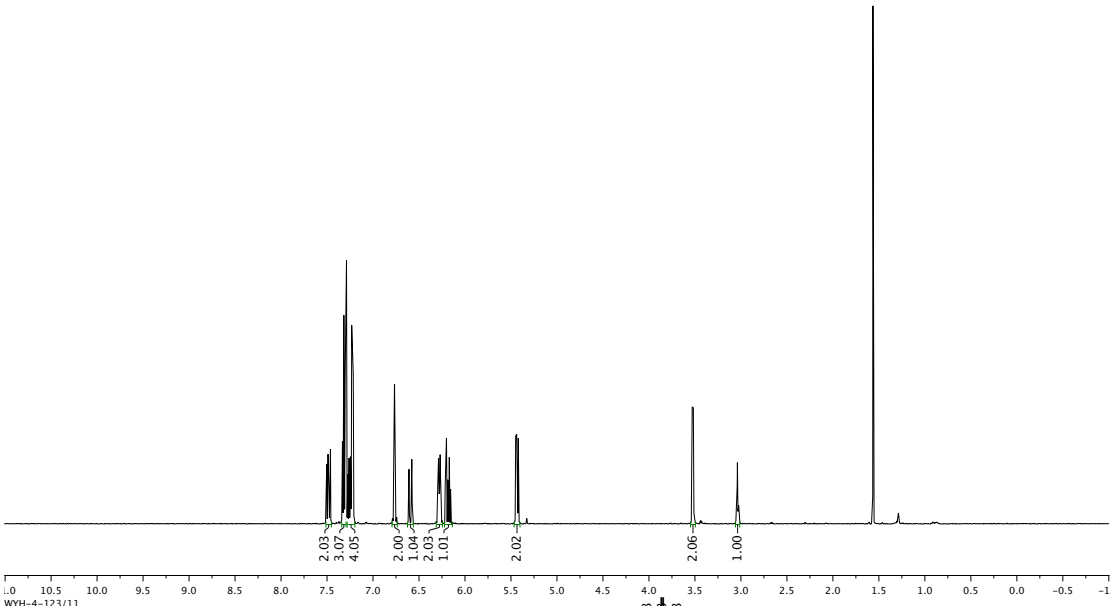
42.2189
21.1081
20.9343
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10



WYH-4-123/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 24



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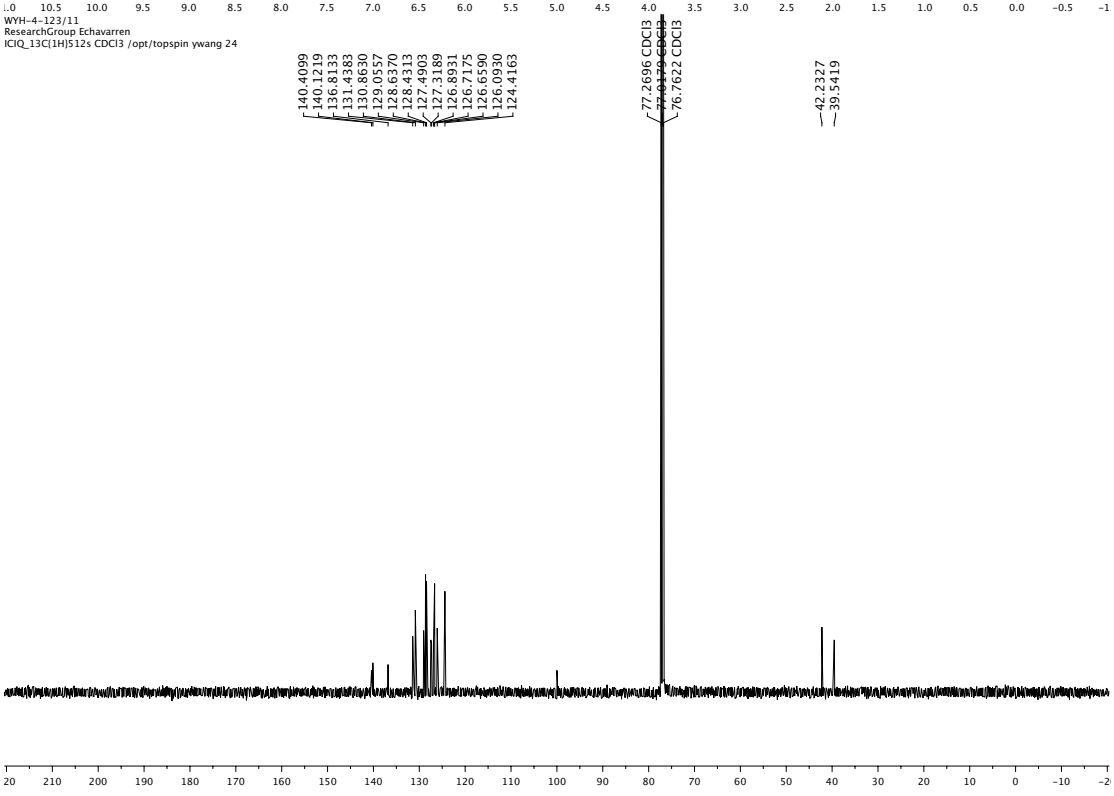
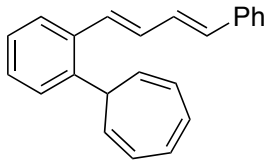
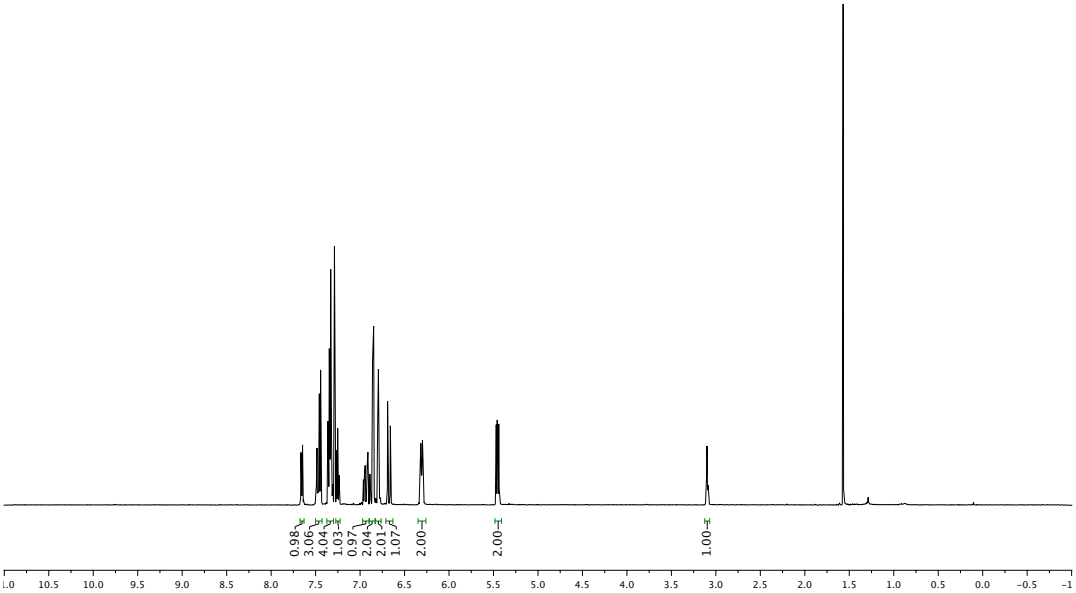
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 24

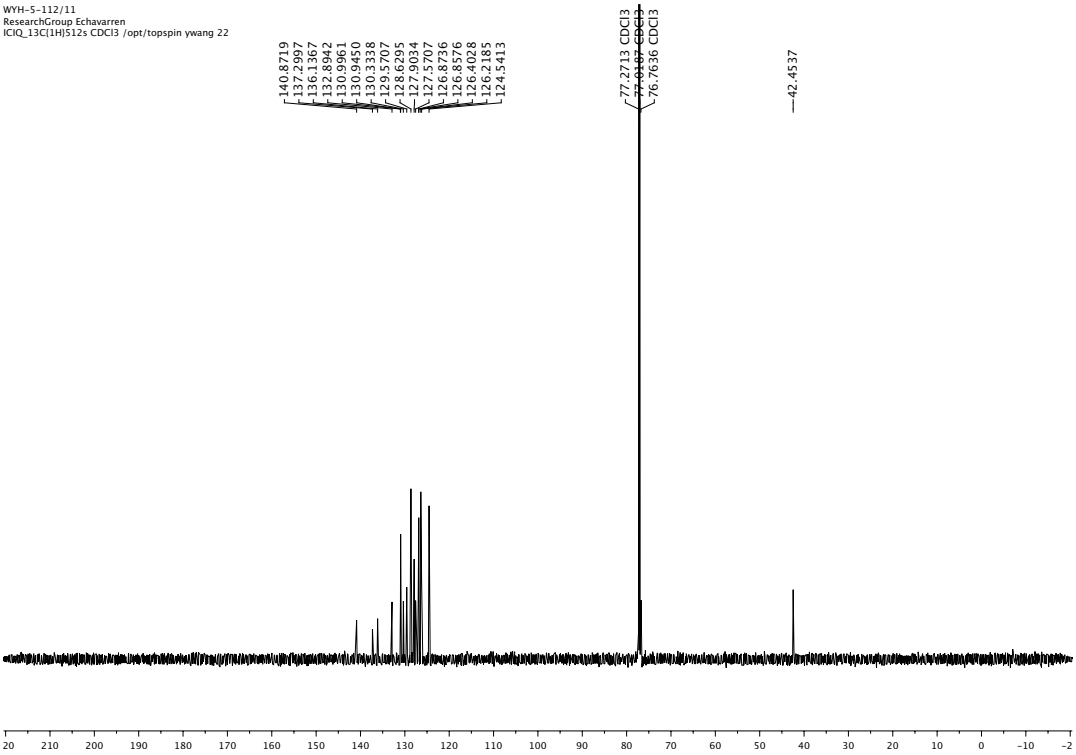


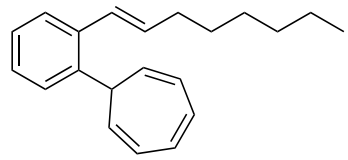


WYH-5-112/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 22

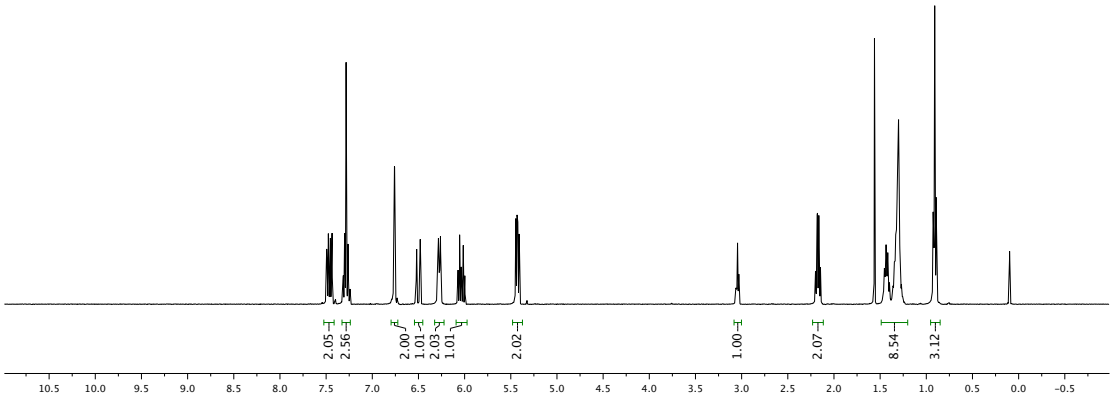


WYH-5-112/11
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 22

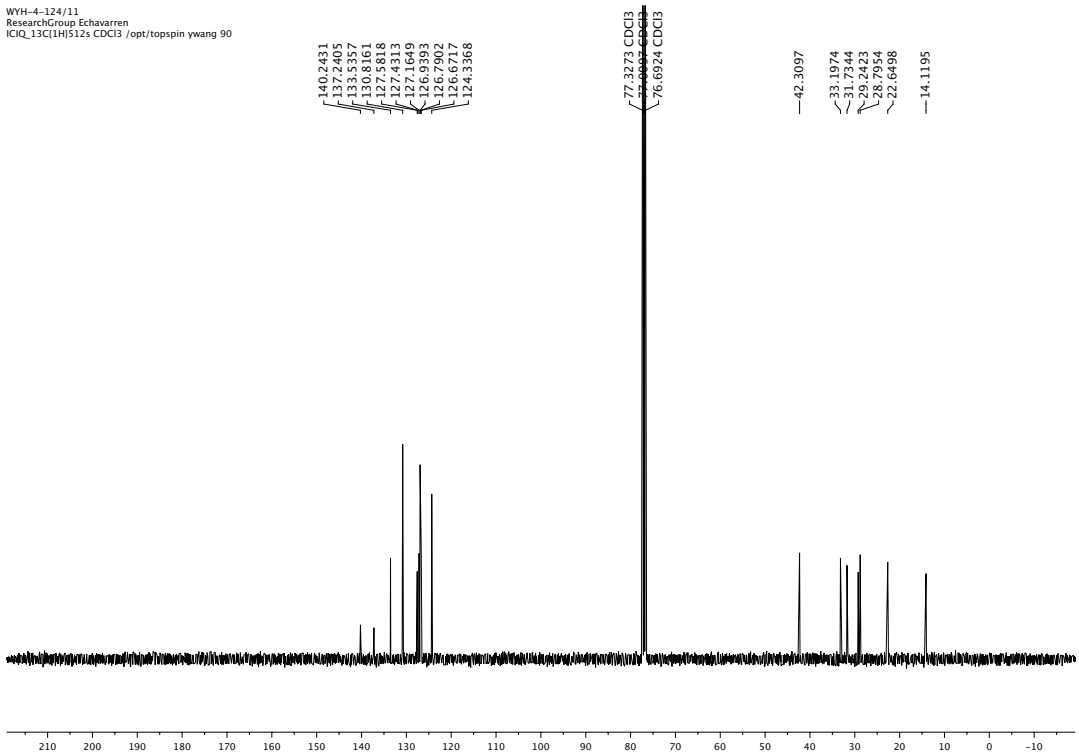


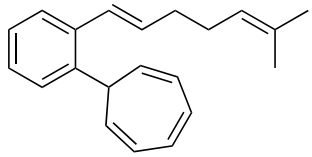


WYH-4-124/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 90

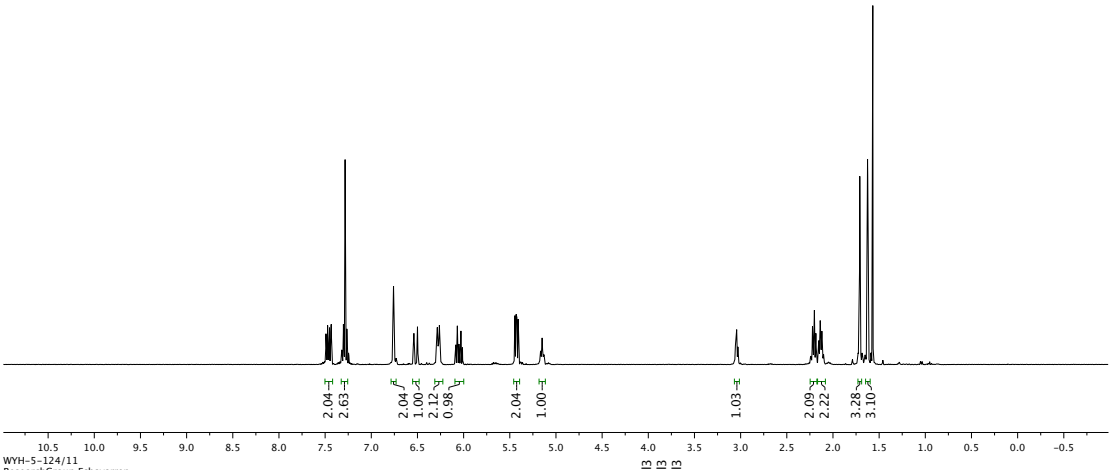


WYH-4-124/11
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 90

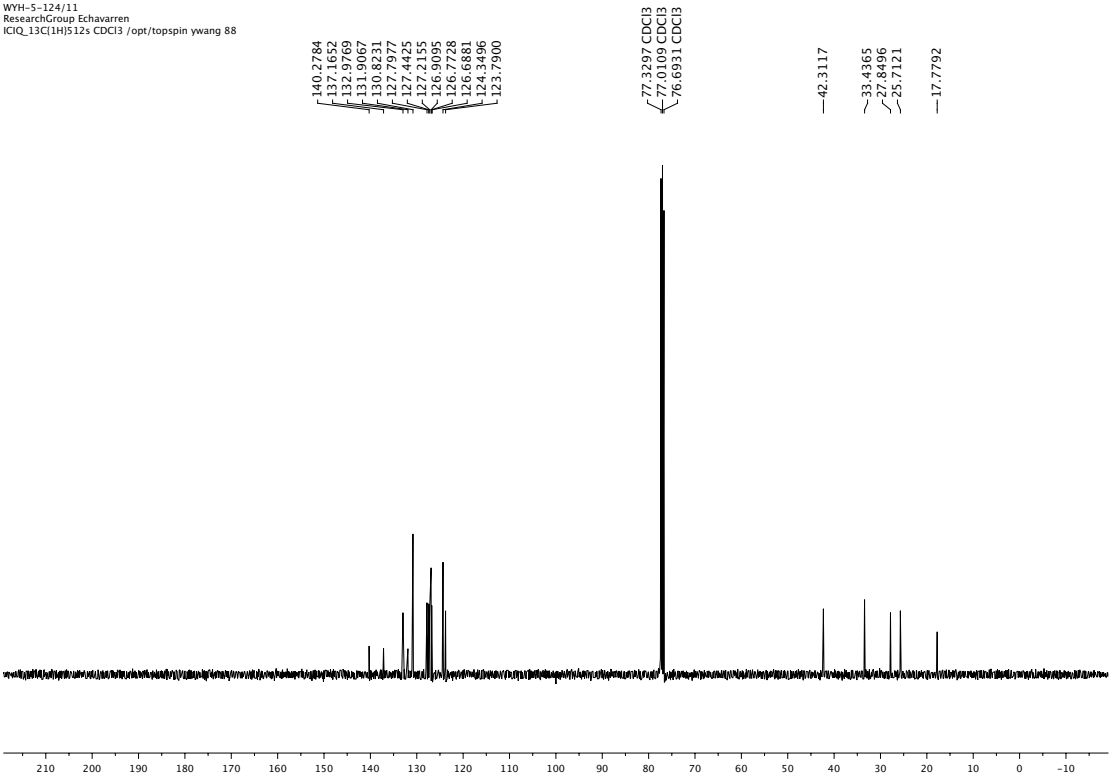


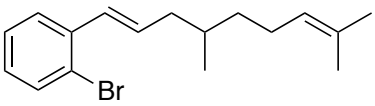


WYH-5-124/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 88

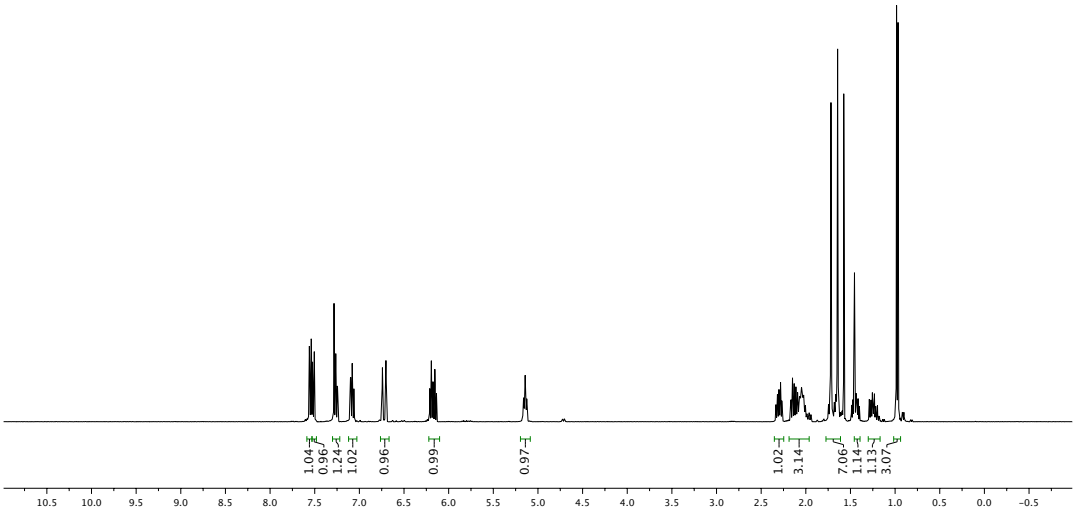


WYH-5-124/11
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 88



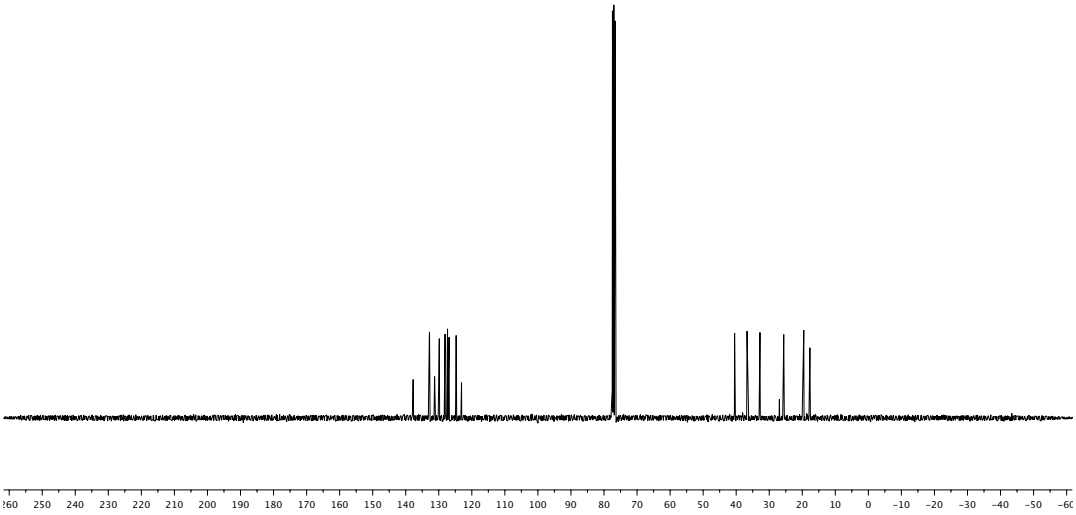


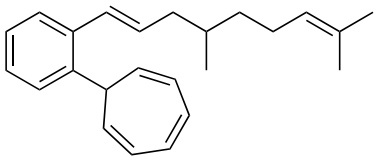
WYH-9-2.10.fid
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 73



WYH-9-2.10.fid
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 {C:\Bruker\TopSpin3.1} ywang 13

137.7588
132.8440
132.8021
131.2624
129.8423
128.0951
127.3483
126.6807
124.7404
123.1175
77.4402 CDCl3
77.0166 CDCl3
76.5950 CDCl3
40.4761
36.7163
32.7973
25.7435
25.6083
19.5389
17.6877





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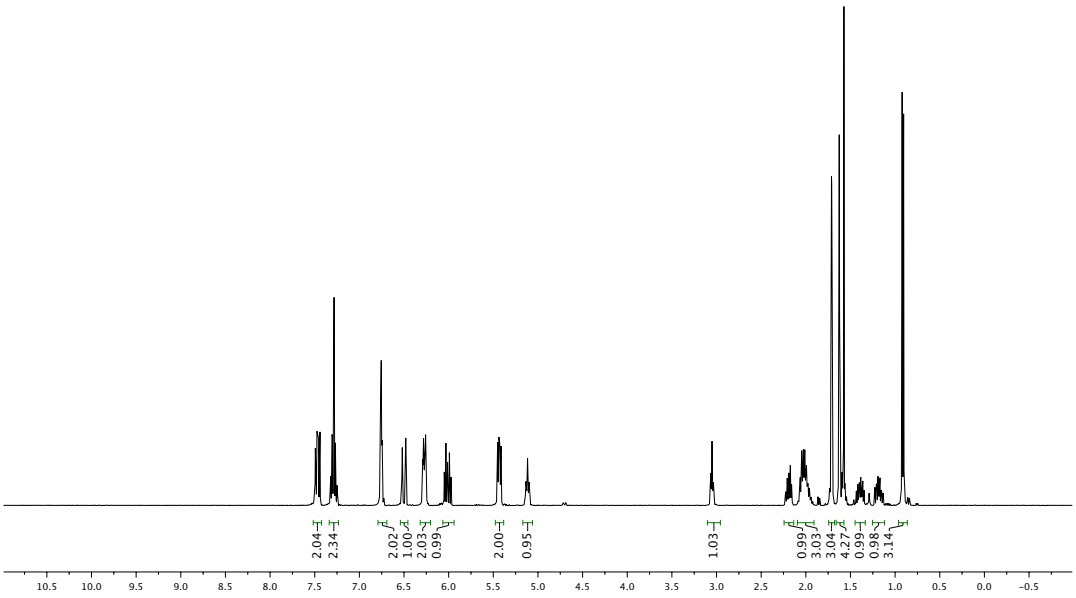
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 87



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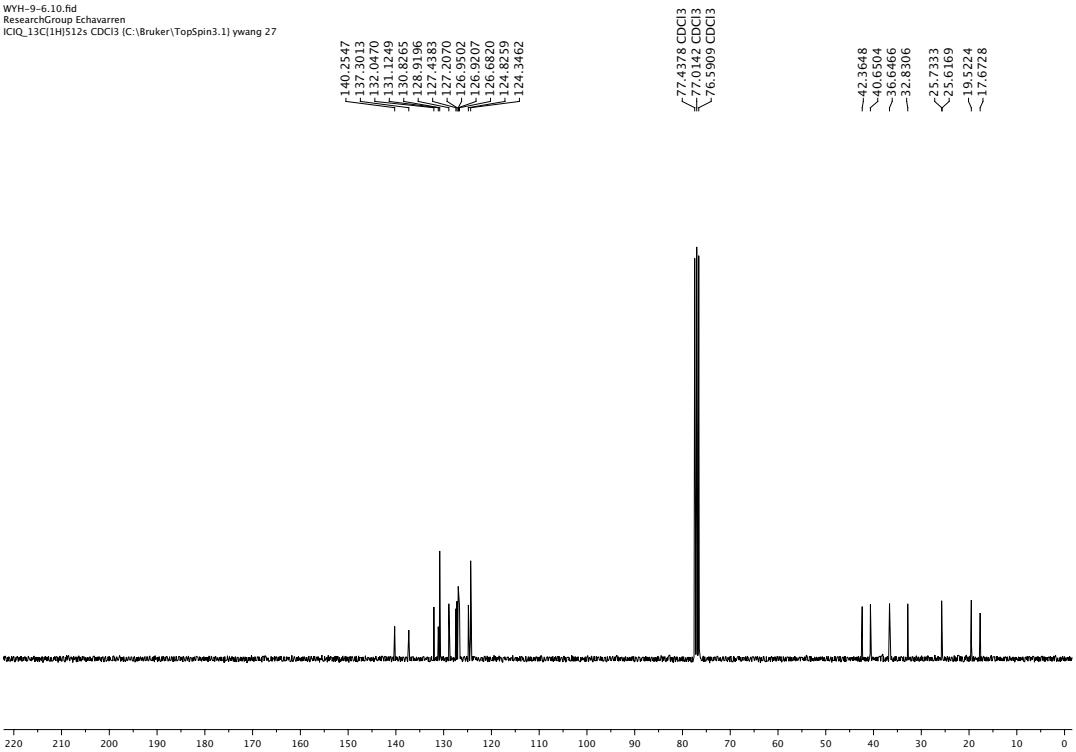
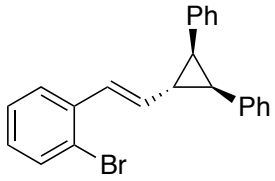
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 (C:\Bruker\TopSpin3.1) ywang 27





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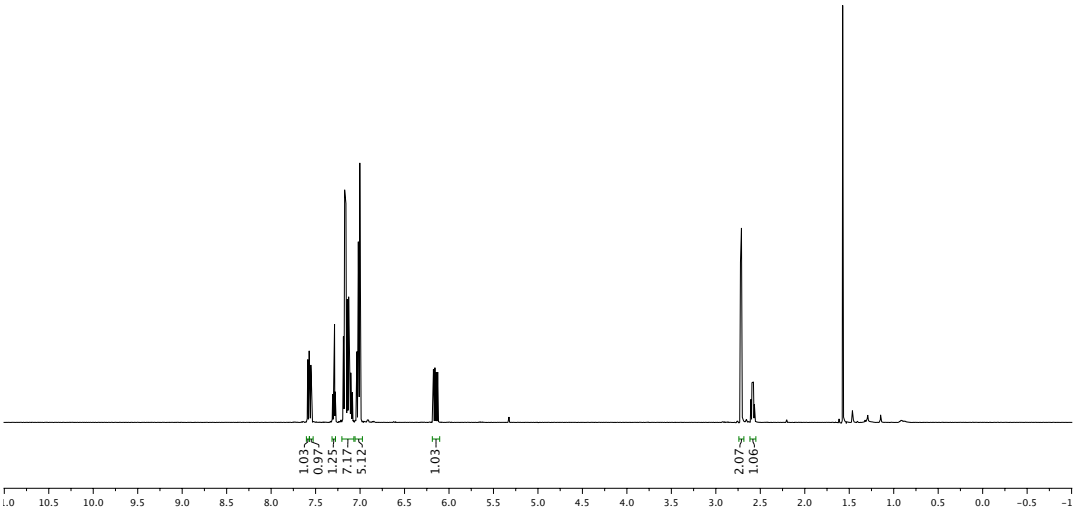
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 10



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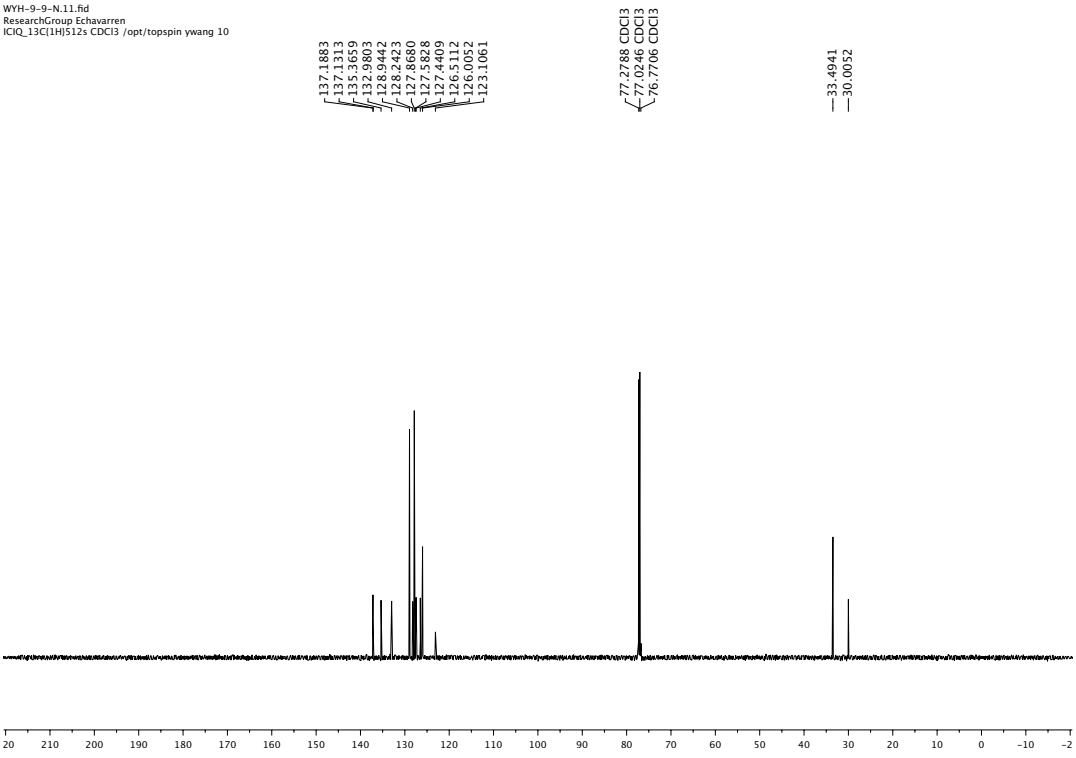
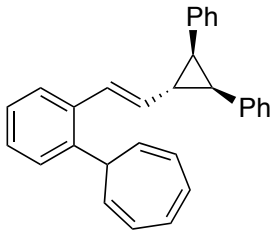
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 10





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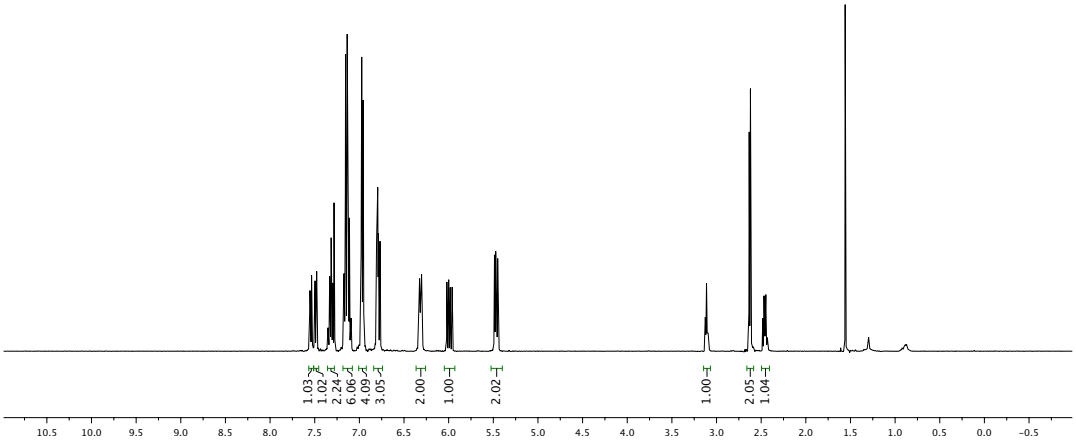
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 62



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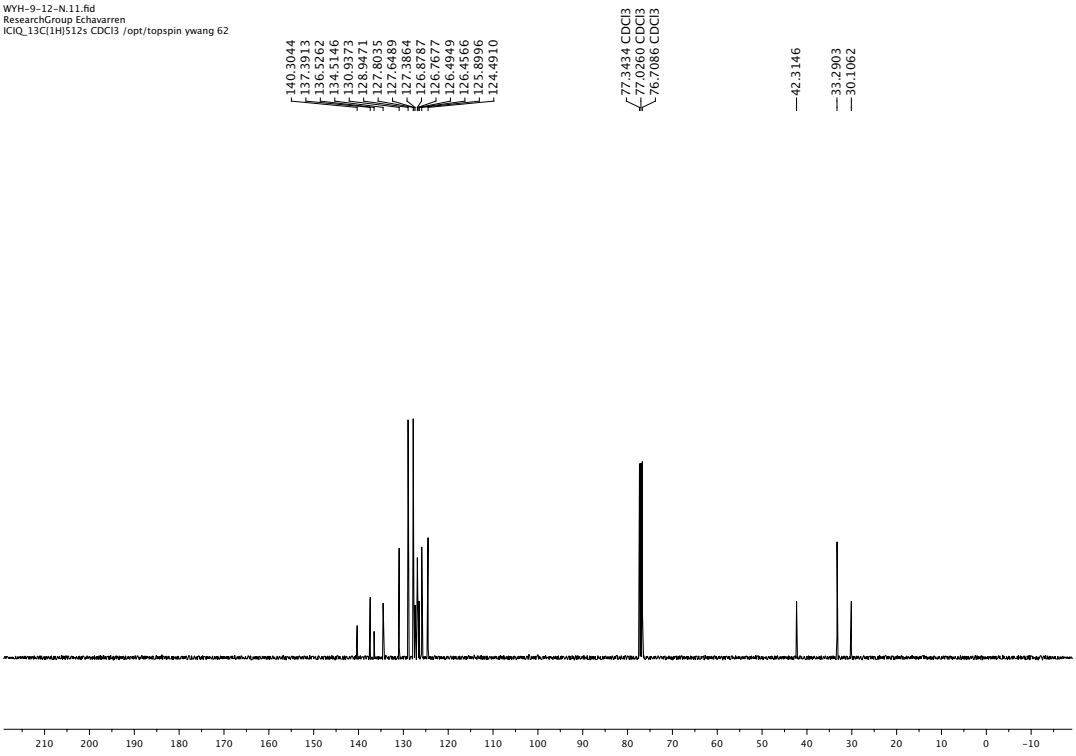
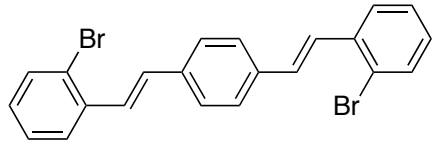
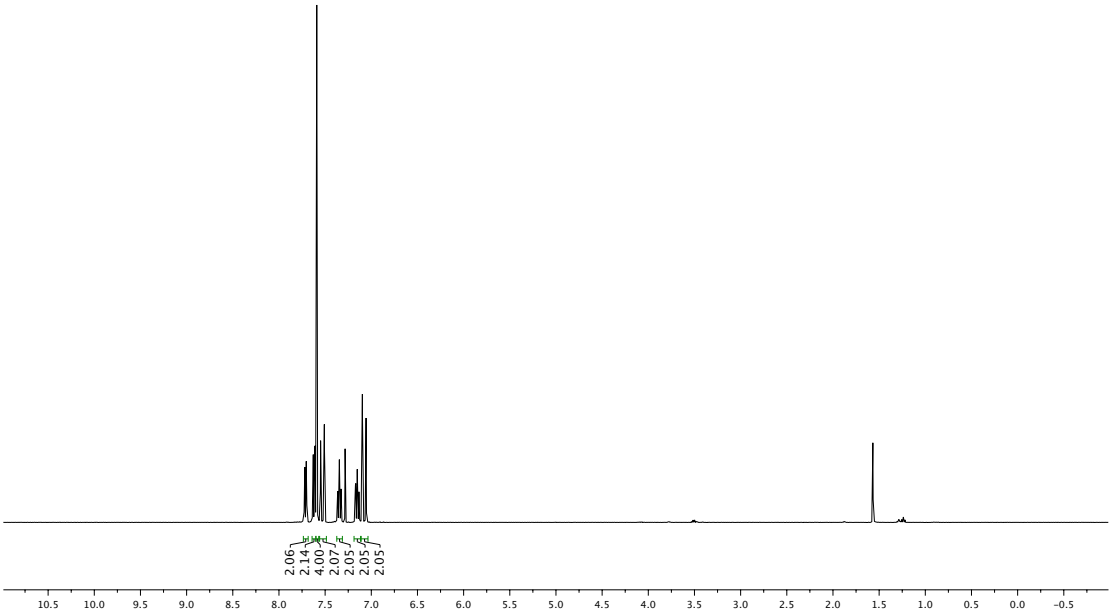
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 62



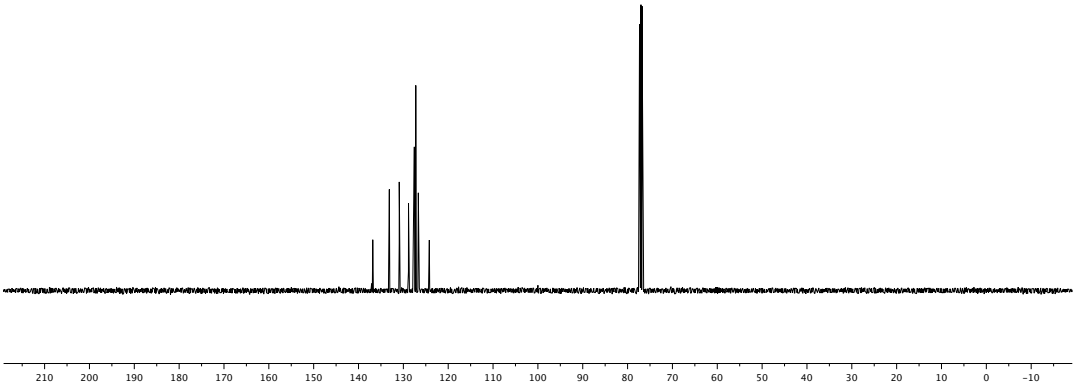


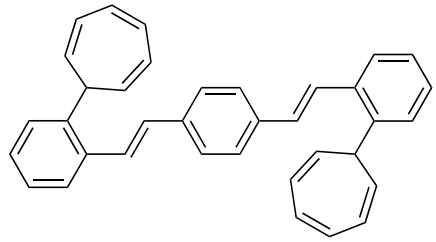
WYH-5-91-Solution/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 94



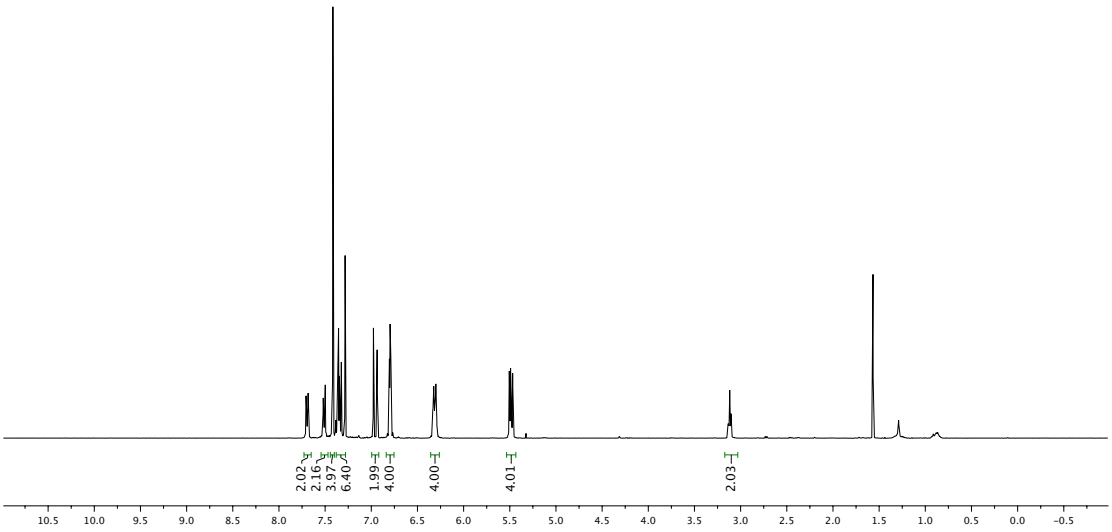
WYH-5-91-Solution/11
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 94

137.0582
136.8249
133.1279
130.9174
128.8504
127.5636
127.2291
126.6640
124.2114
77.3315 CDCl3
77.0164 CDCl3
76.6969 CDCl3

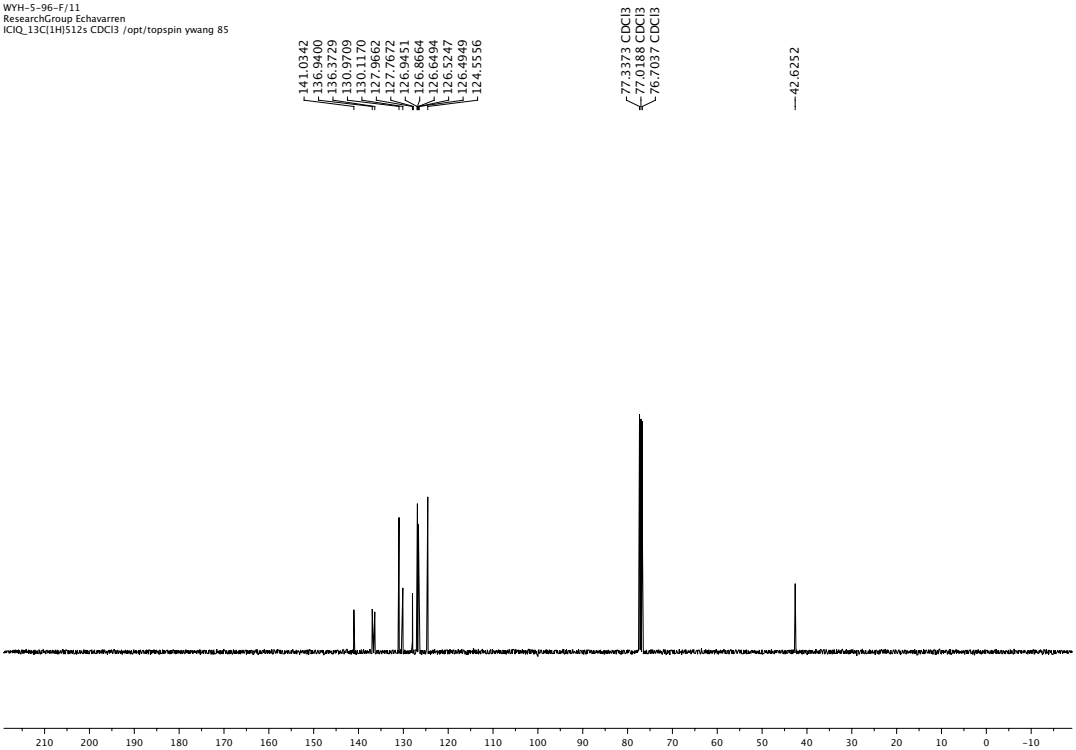


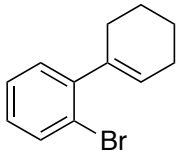


WYH-5-96-F/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 85

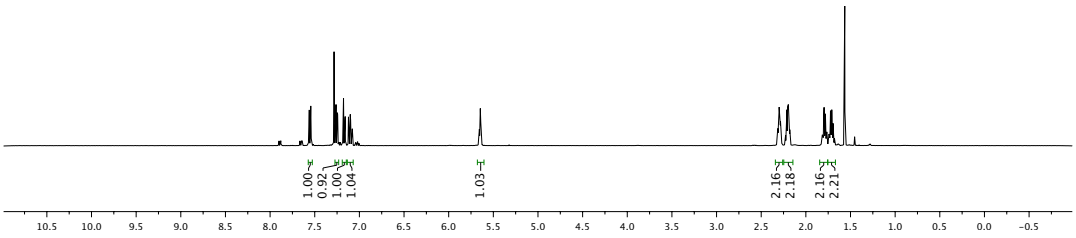


WYH-5-96-F/11
ResearchGroup Echavarren
ICIQ_13C(1H)512s CDCl3 /opt/topspin ywang 85

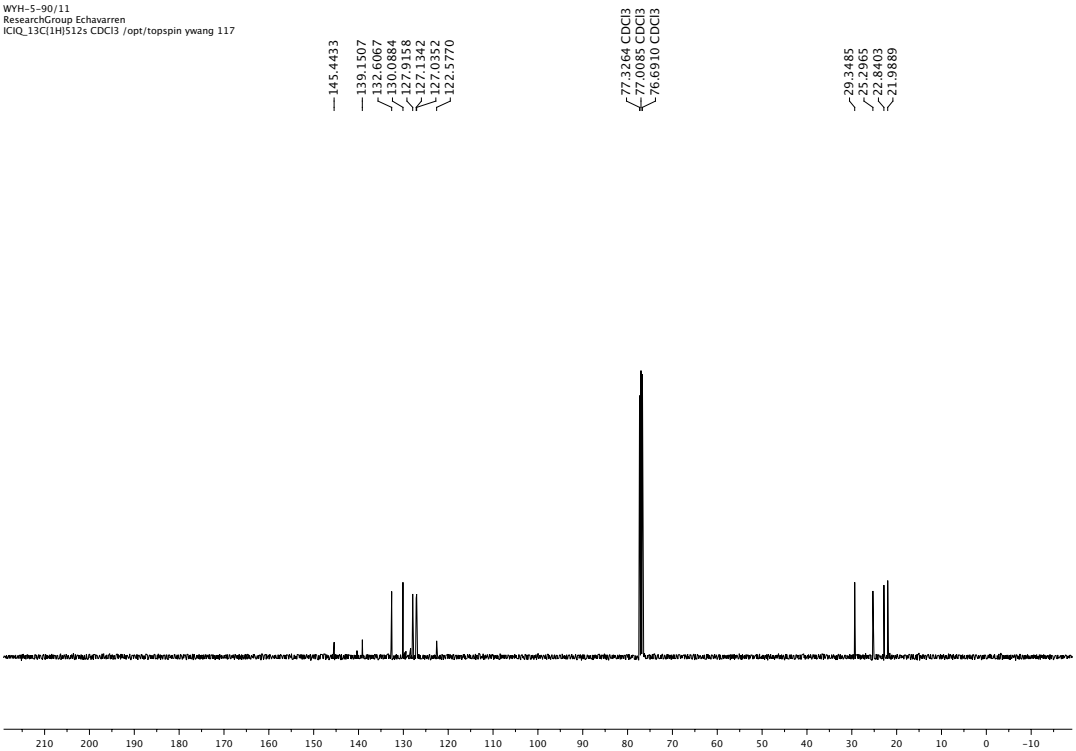


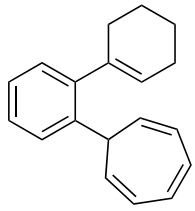


WYH-5-90/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 117

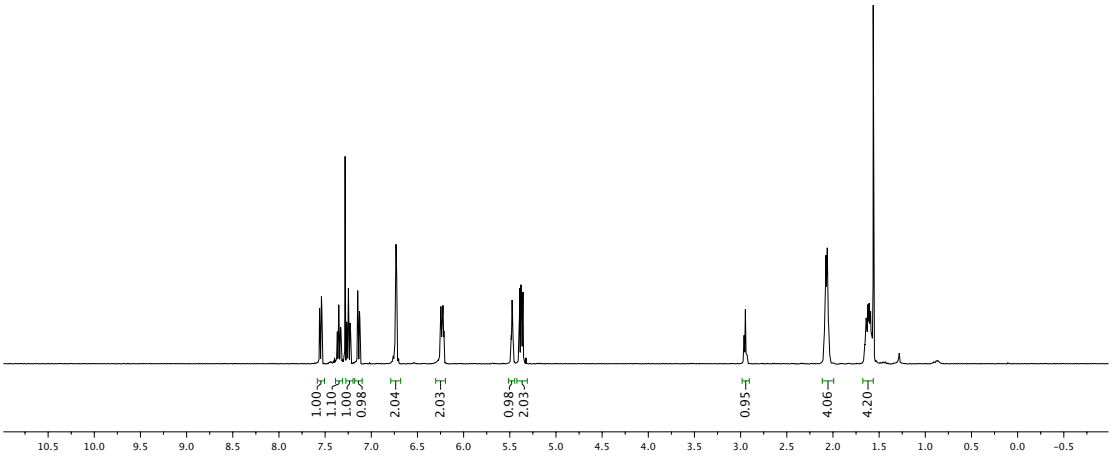


WYH-5-90/11
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 117

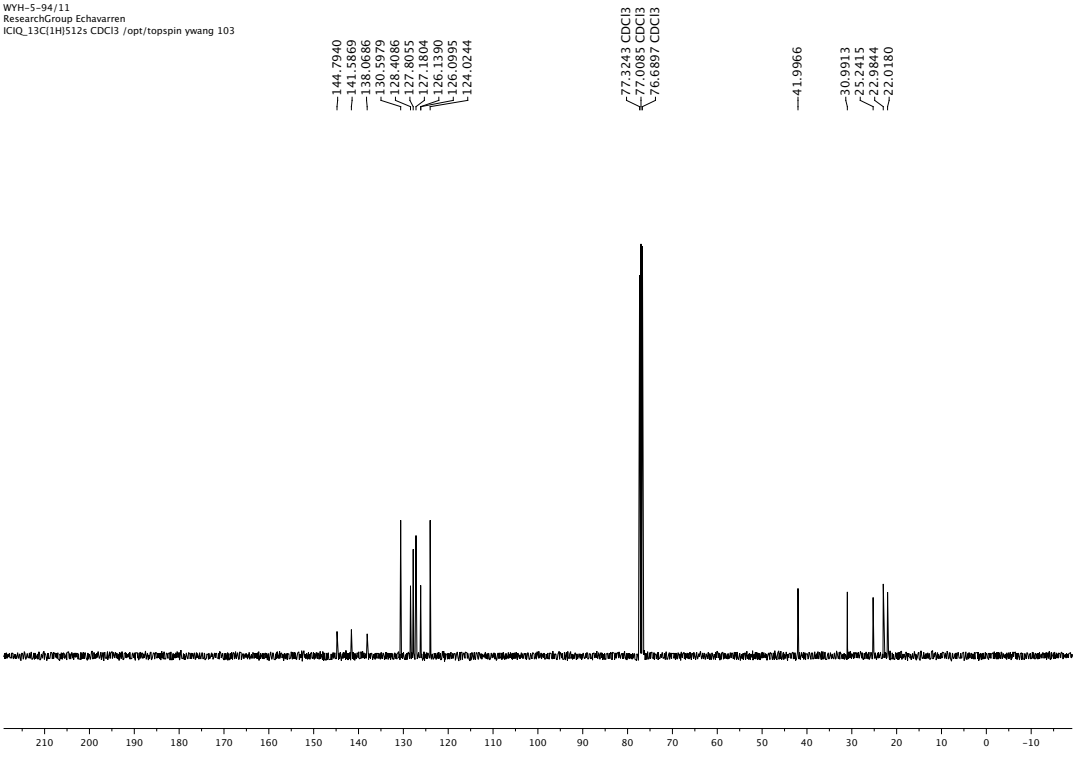


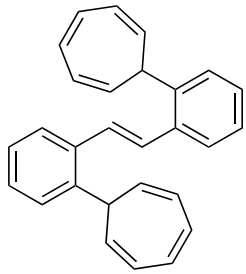


WYH-5-94/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 103



WYH-5-94/11
ResearchGroup Echavarren
ICIQ_13C(1H)512s CDCl3 /opt/topspin ywang 103





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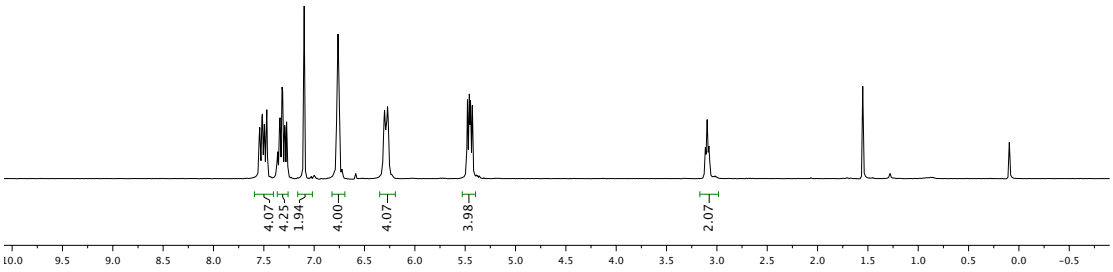
ResearchGroup Echavarren
ICIQ_1H20p8s CDCl3 {C:\Bruker\TopSpin3.1} ywang 48



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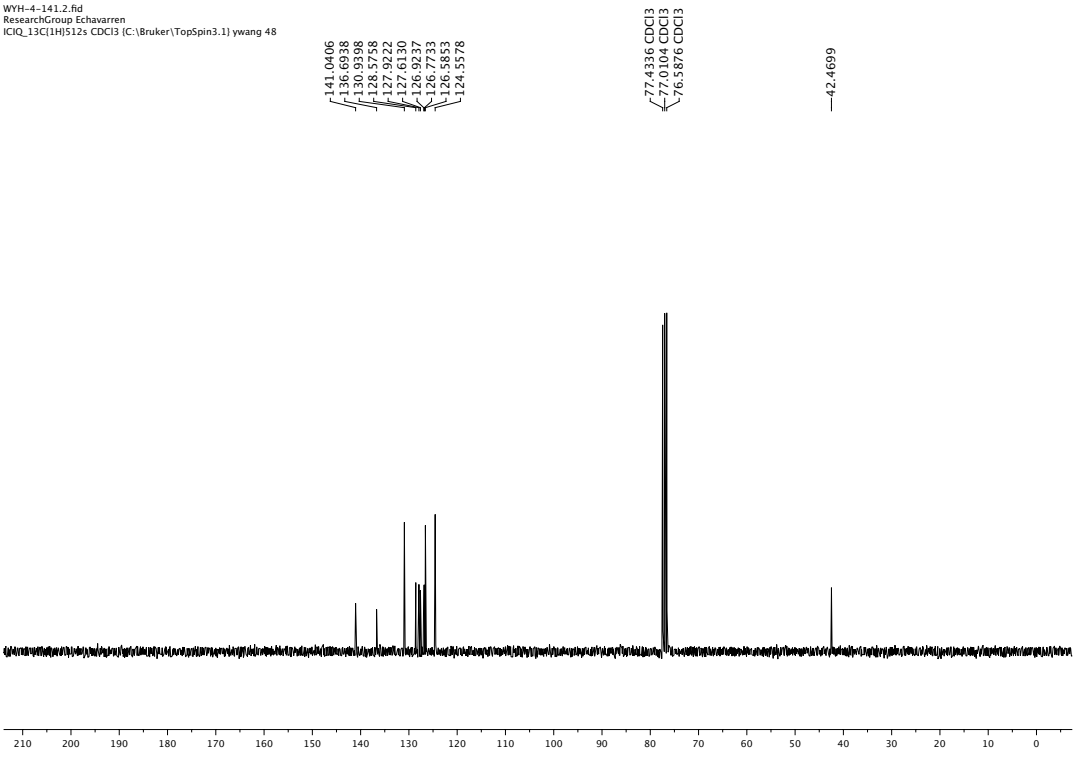
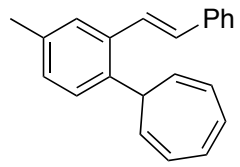
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 {C:\Bruker\TopSpin3.1} ywang 48





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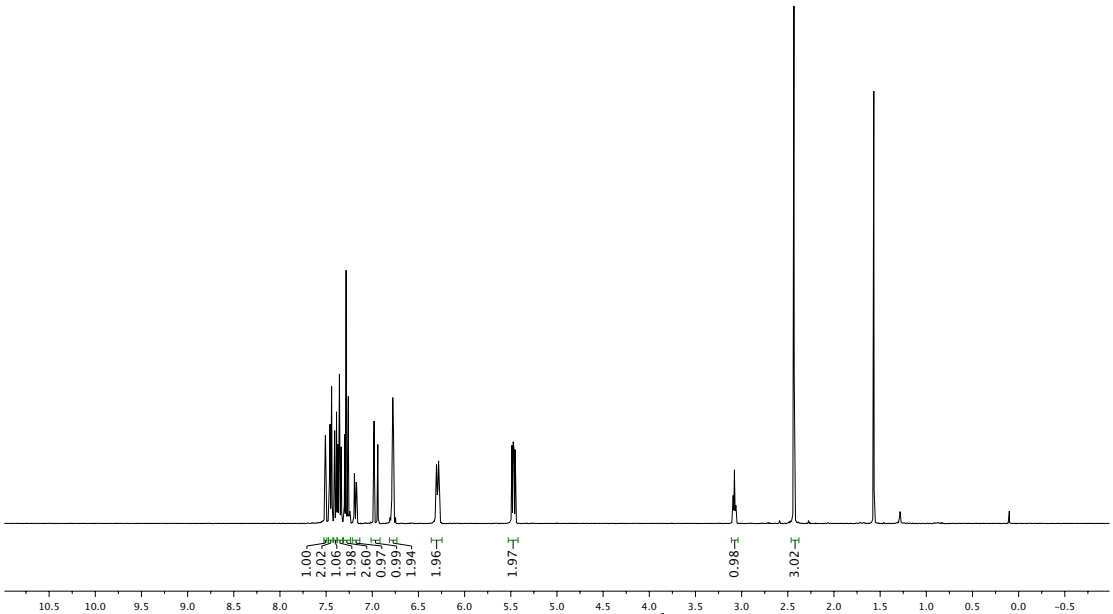
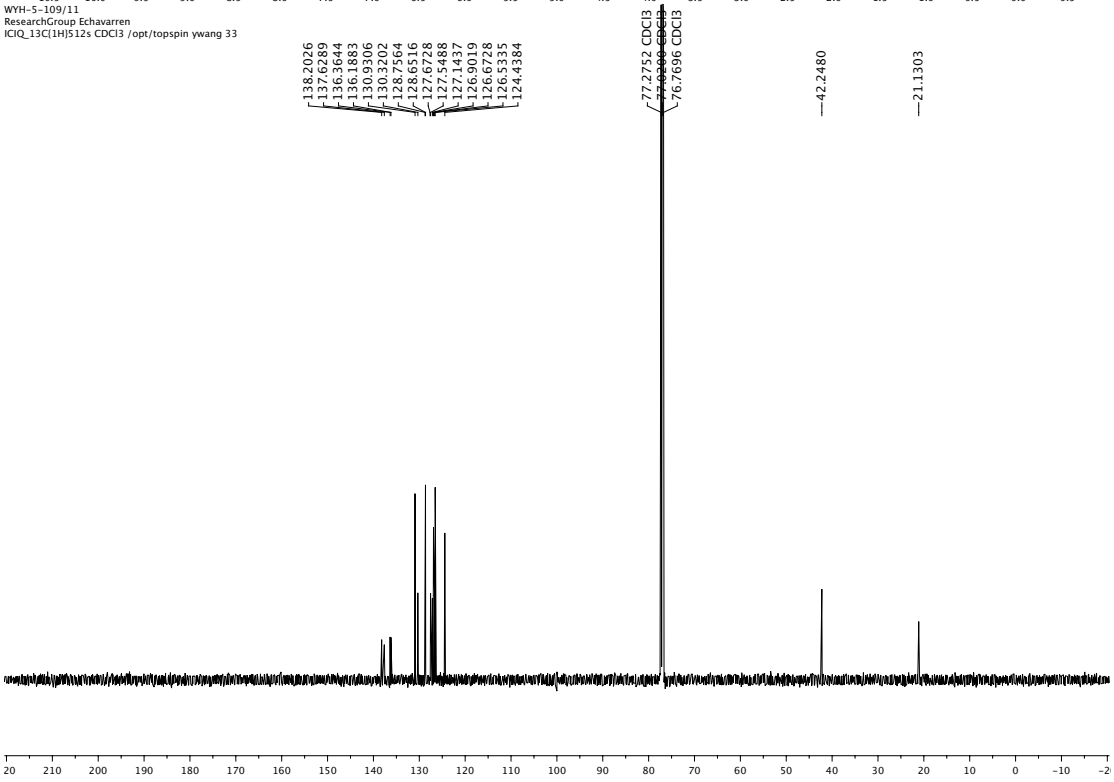
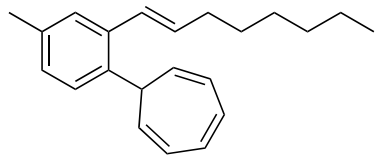
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 104

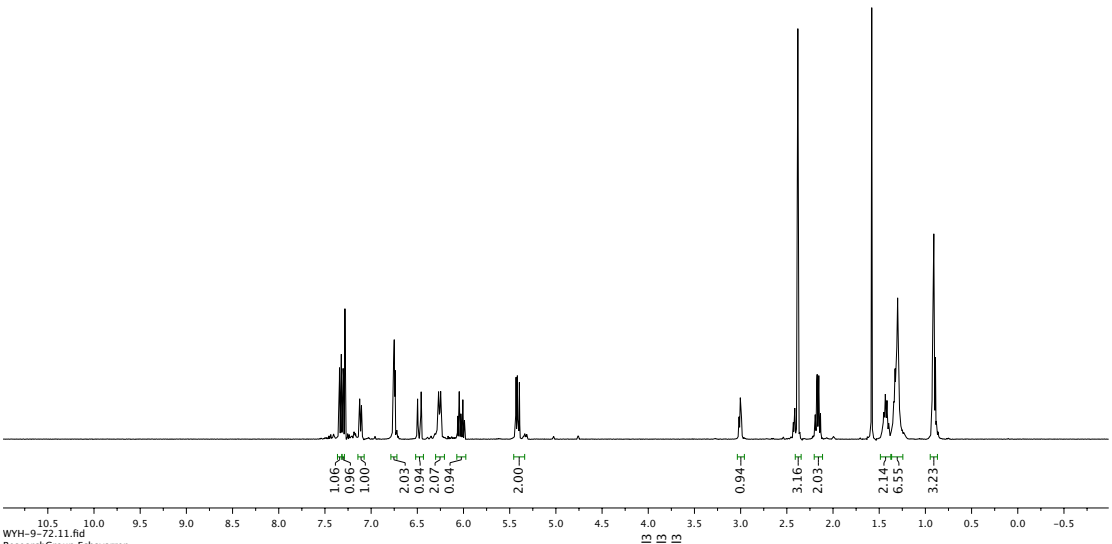


WYH-5-109/11
ResearchGroup Echavarren
ICIQ_13C(1H)512s CDCl3 /opt/topspin ywang 33





WYH-9-72.10.fid
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 97



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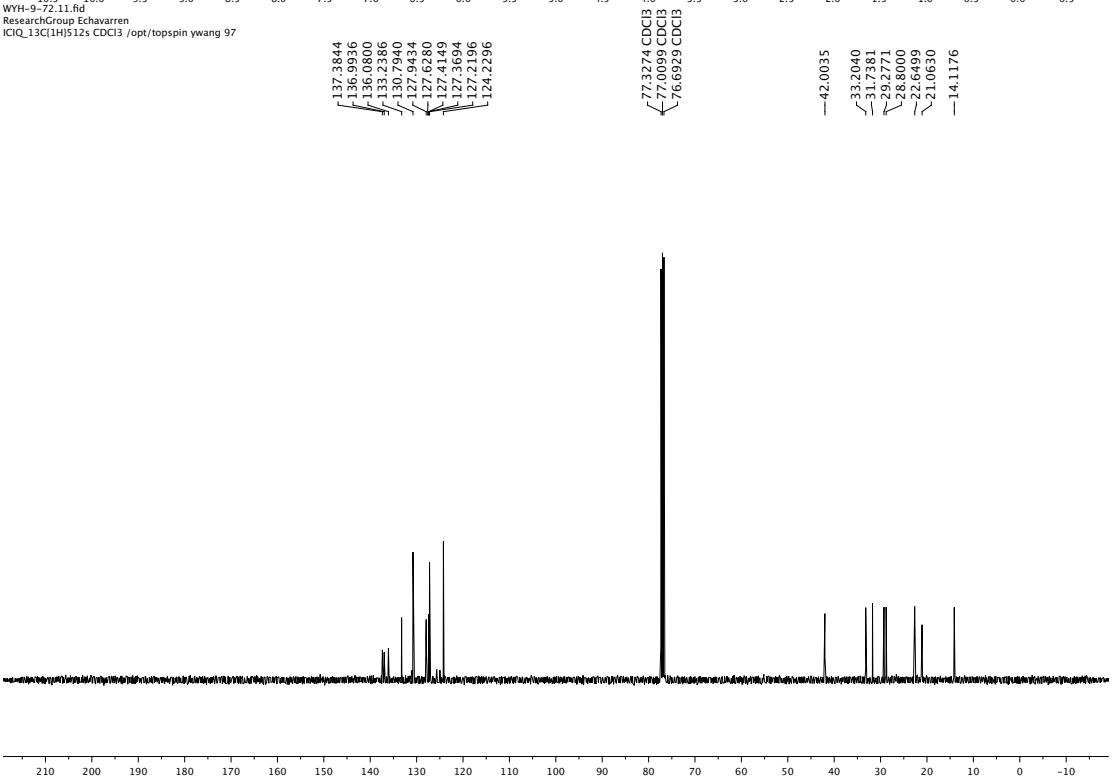
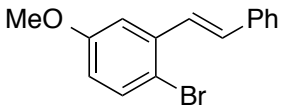
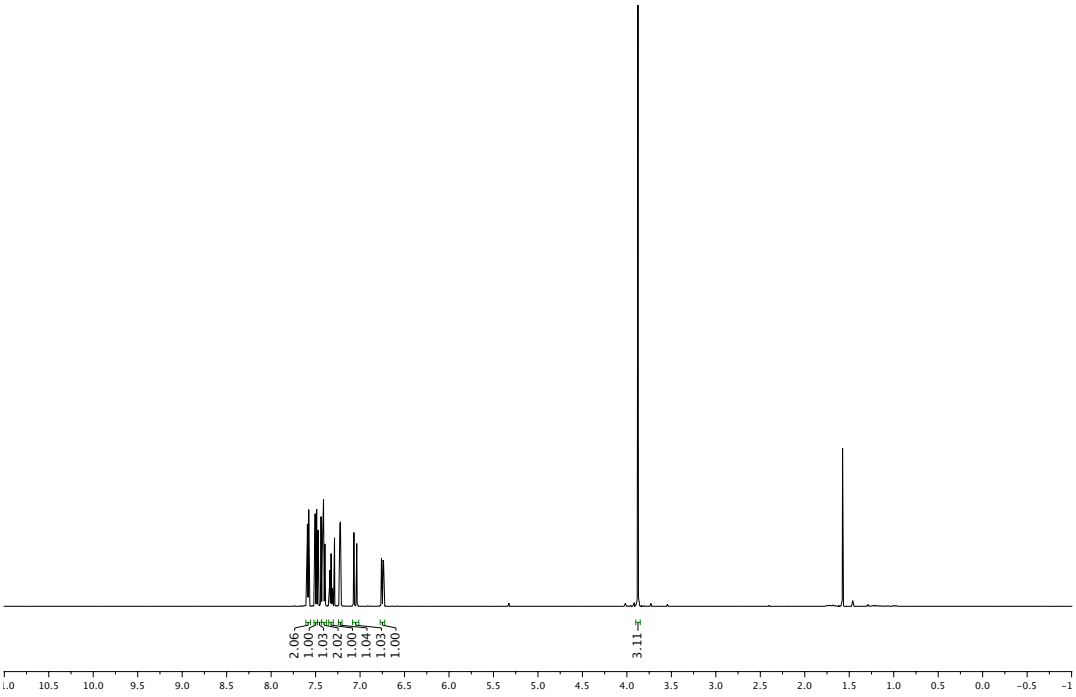
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 97





WYH-5-111.10.fid
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 35



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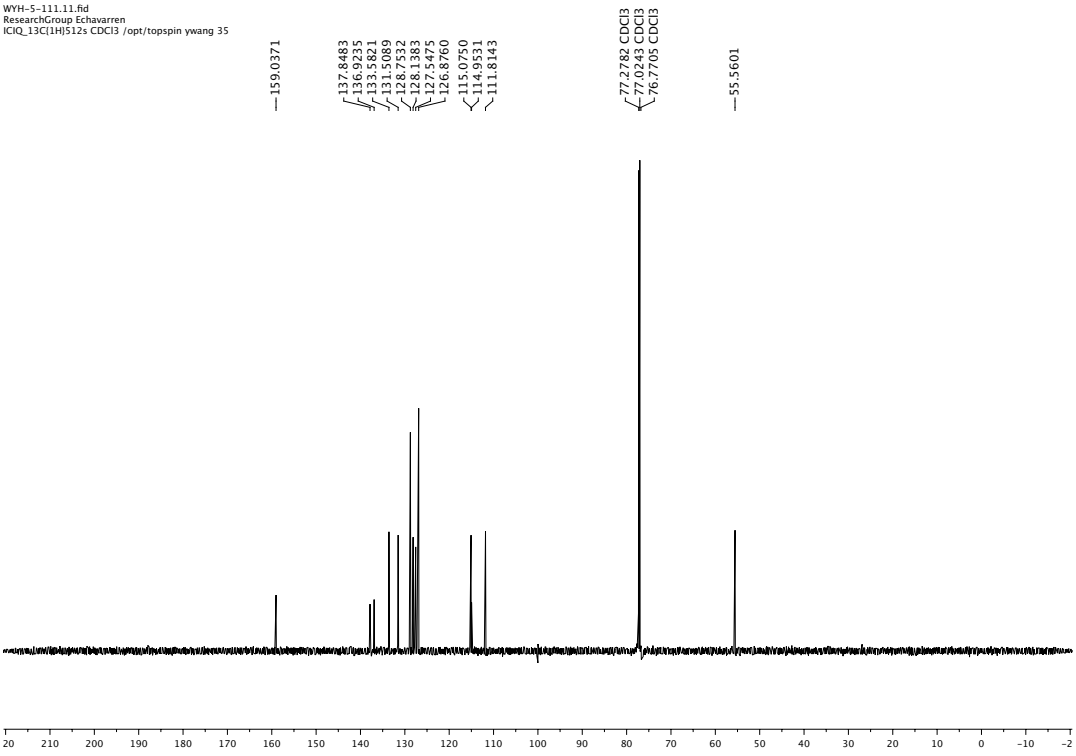
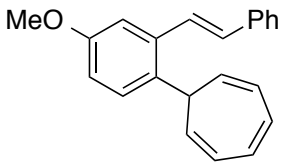
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 35





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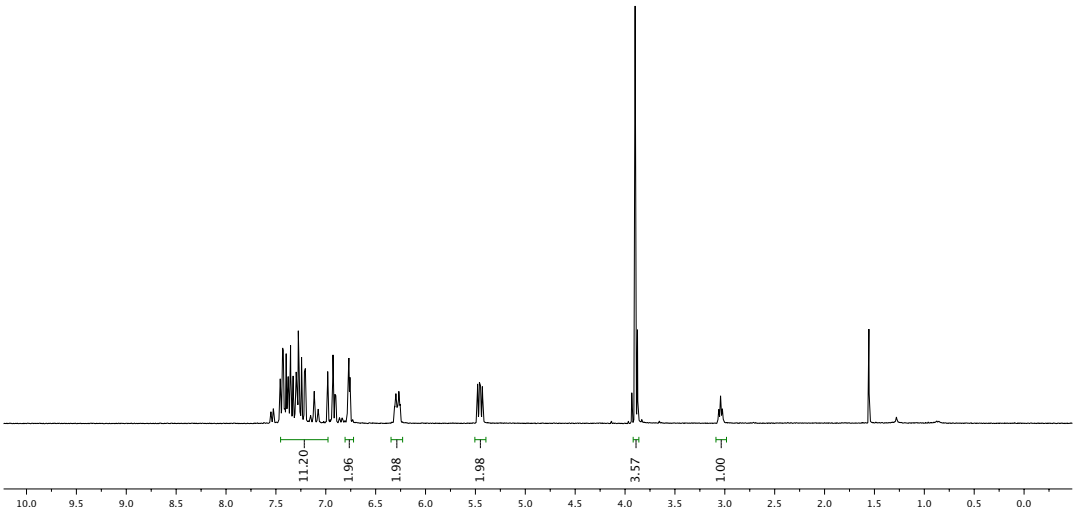
ResearchGroup Echavarren
ICIQ_1H20p8s CDCl3 (C:\Bruker\TopSpin3.1) ywang 33



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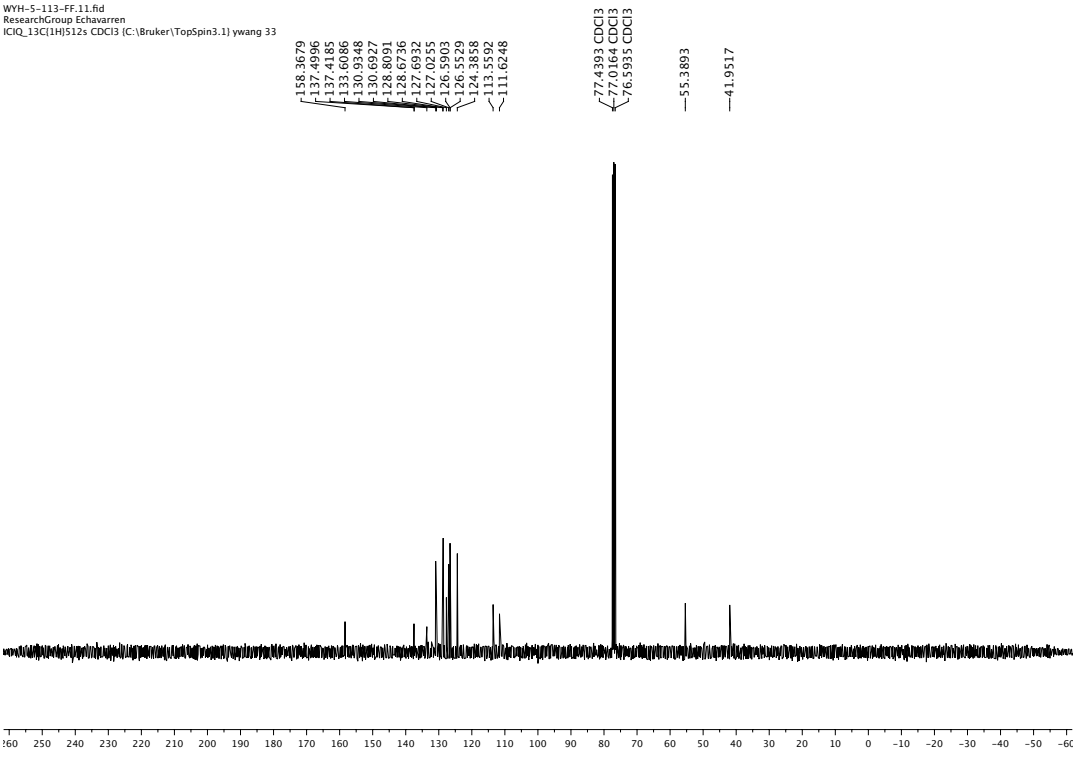
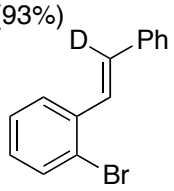
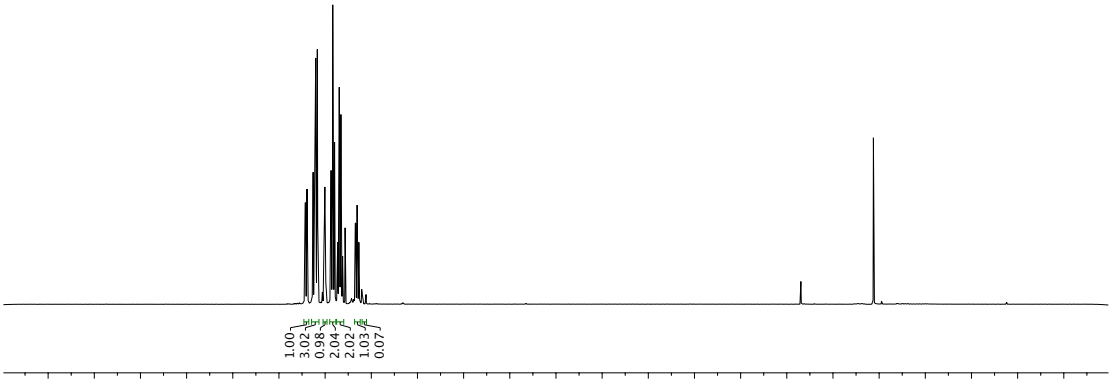
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 (C:\Bruker\TopSpin3.1) ywang 33



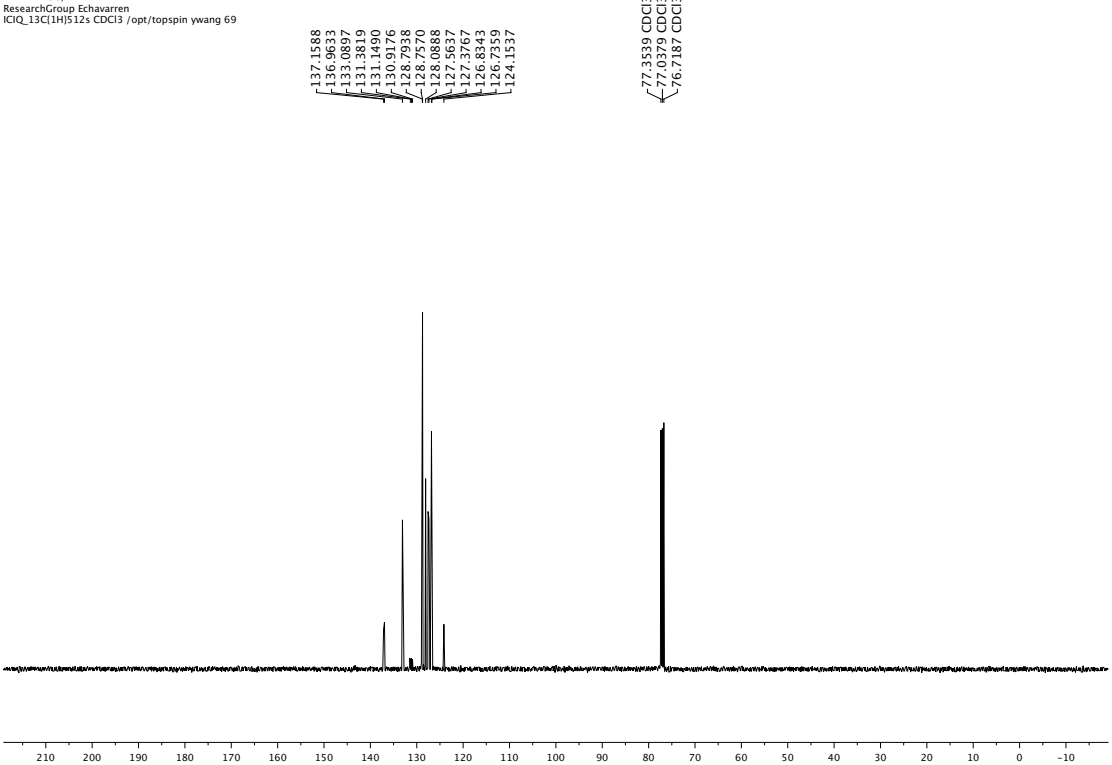
(93%)



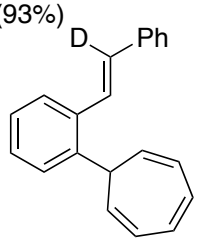
WYH-4-138/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 69



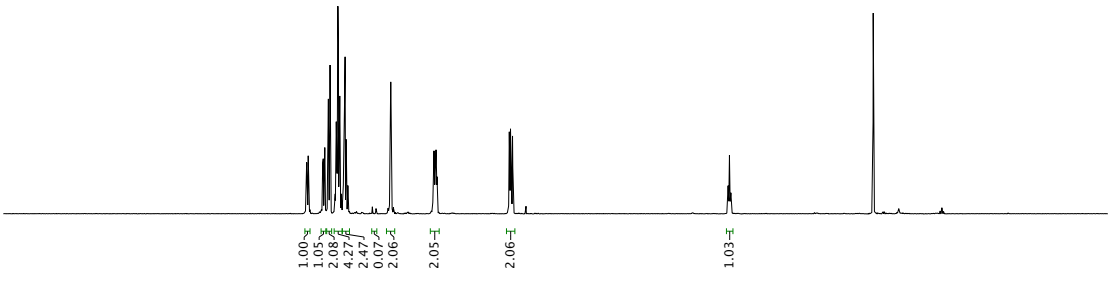
WYH-4-138/11
ResearchGroup Echavarren
ICIQ_13C(1H)512s CDCl3 /opt/topspin ywang 69



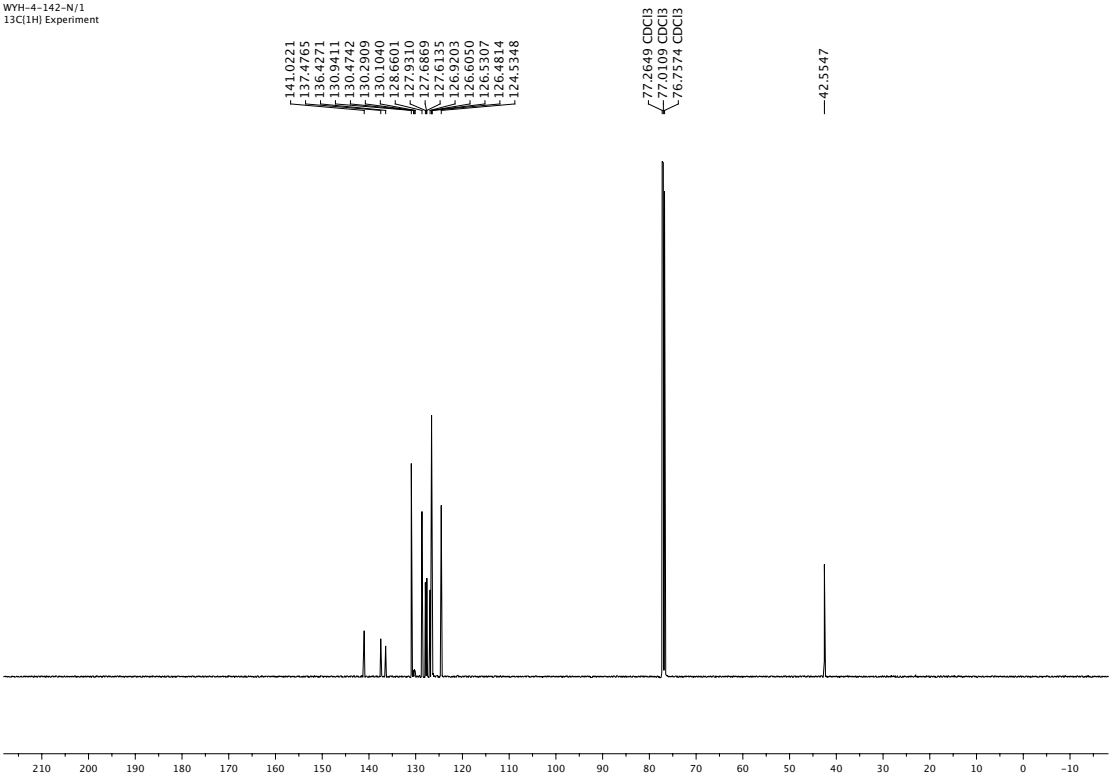
(93%)

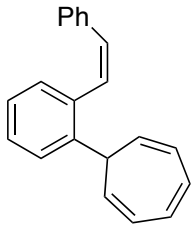


WYH-4-142/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 87



WYH-4-142-N/1
13C{1H} Experiment

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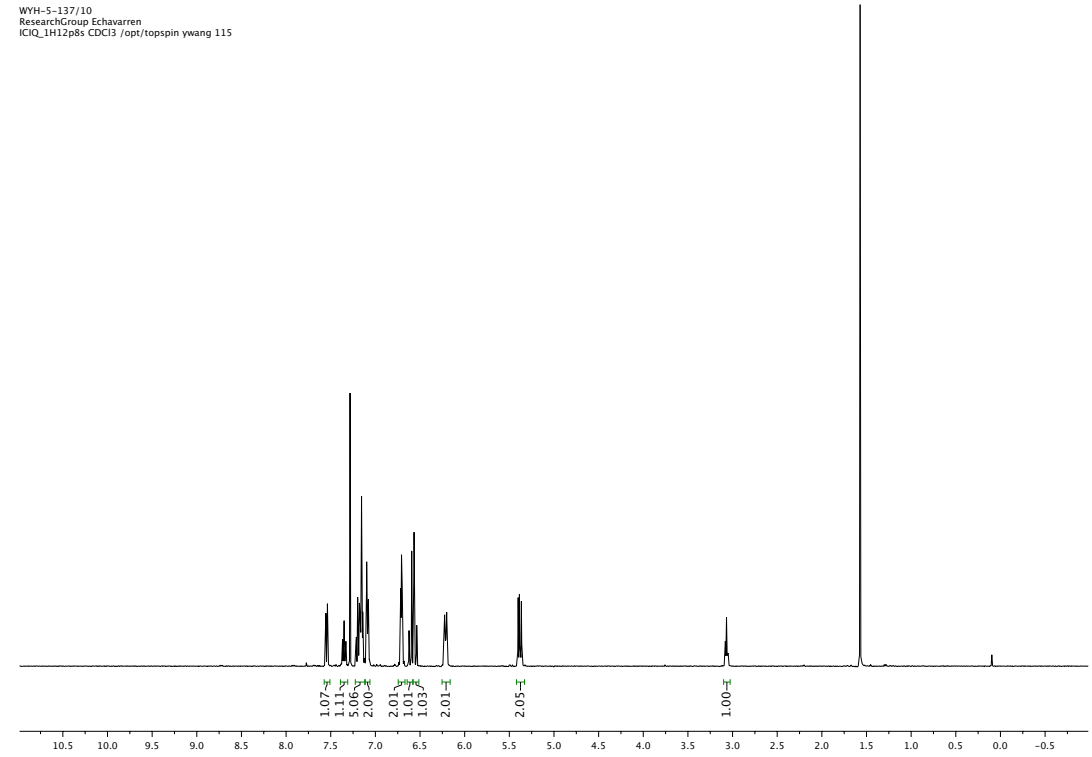
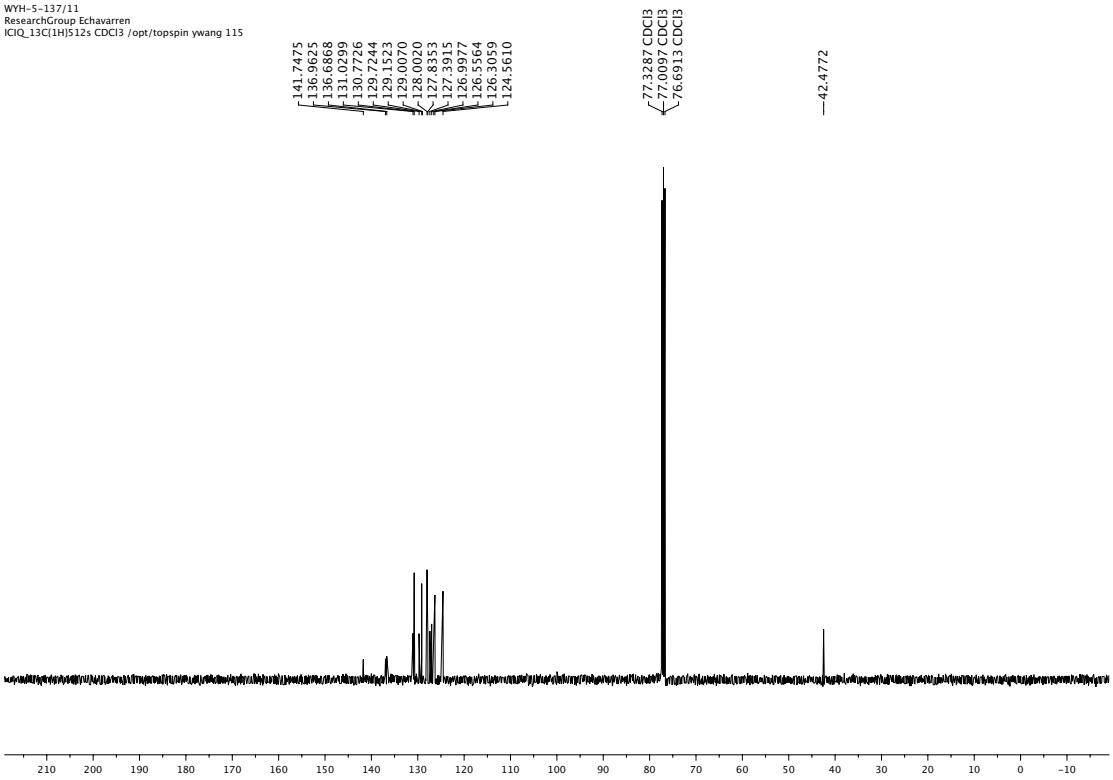
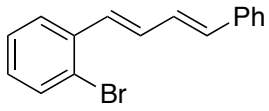
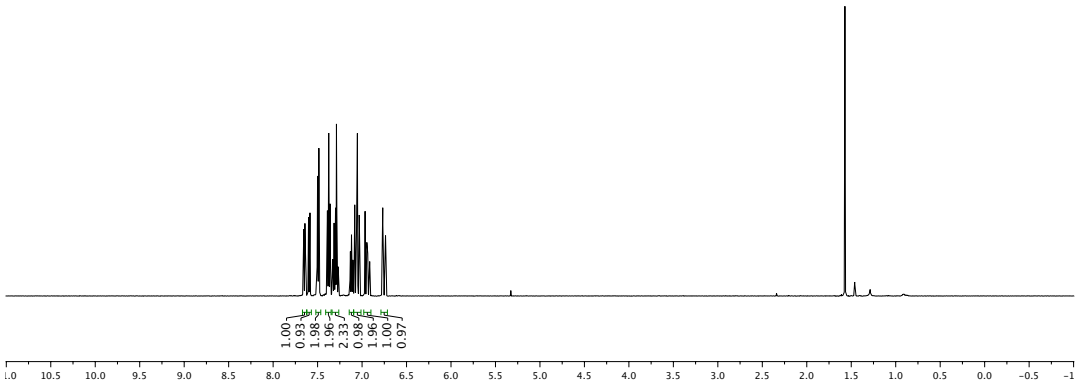

WYH-5-137/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 115
1.07
1.11
5.06
2.00
2.01
1.01
1.03
2.01
2.05
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

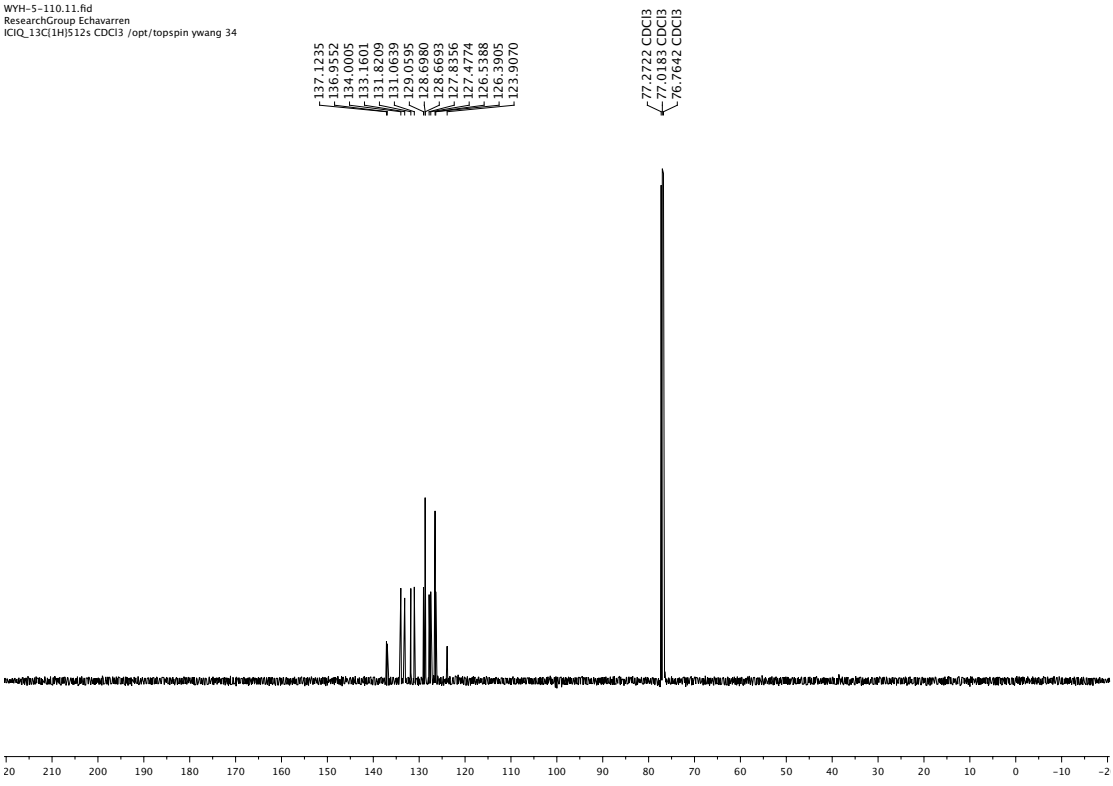

WYH-5-137/11
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 115
141.7475
136.9625
136.6868
131.0299
130.7726
129.7244
129.1523
129.0070
128.0020
127.8353
127.3915
126.9977
126.5564
126.3059
124.5610
77.3287 CDCl3
77.0097 CDCl3
76.6913 CDCl3
42.4772
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

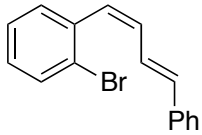


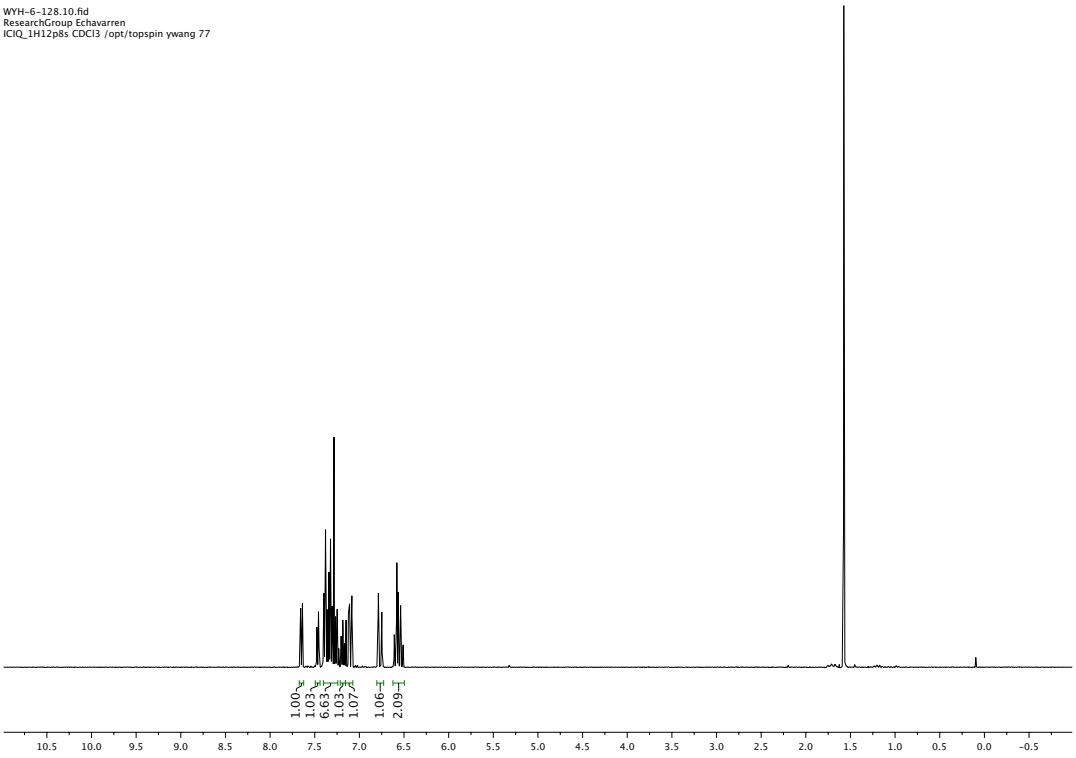
WYH-5-110.10.fid
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 34

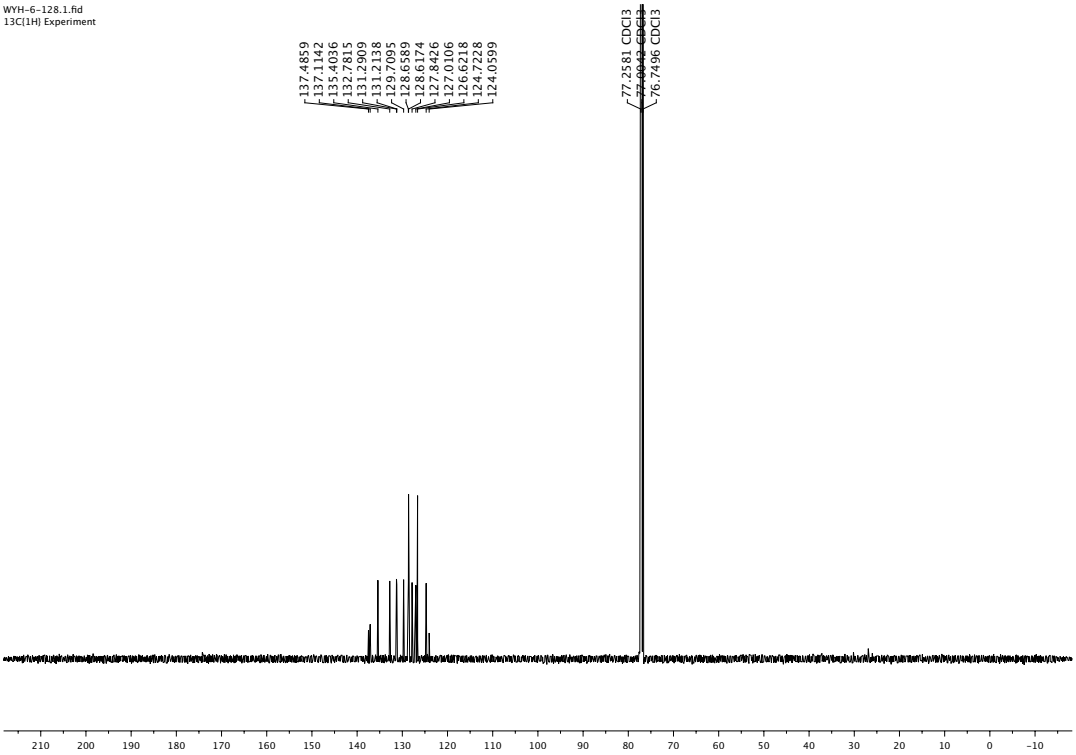


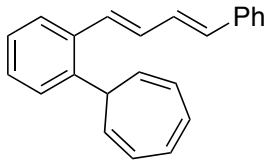
WYH-5-110.11.fid
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 34



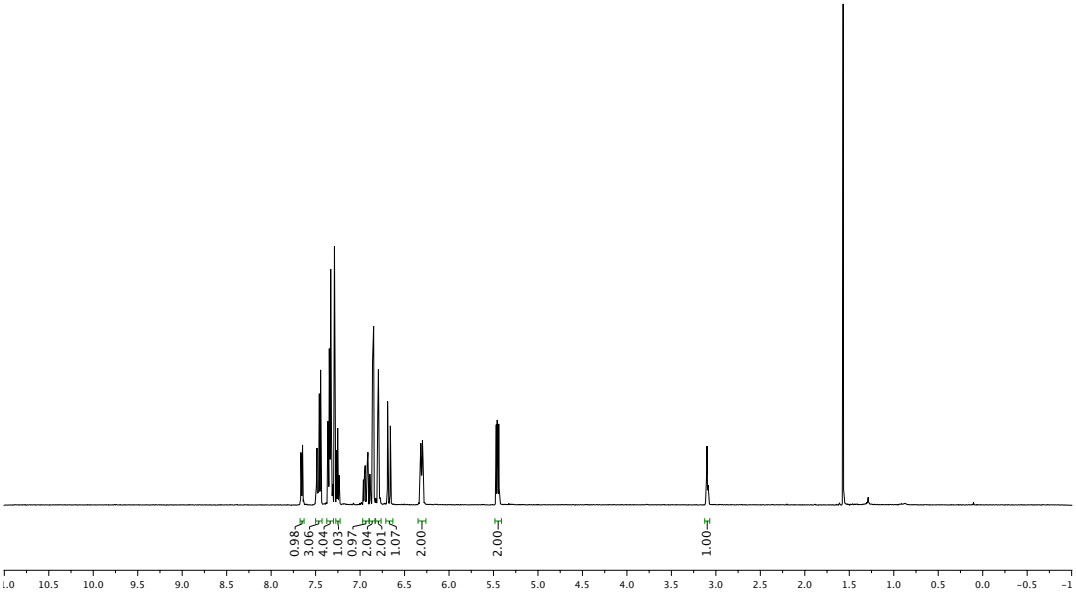

Br
Ph


WYH-6-128.10.fid
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 77
1.00
1.03
6.63
1.03
1.07
1.06
2.09
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

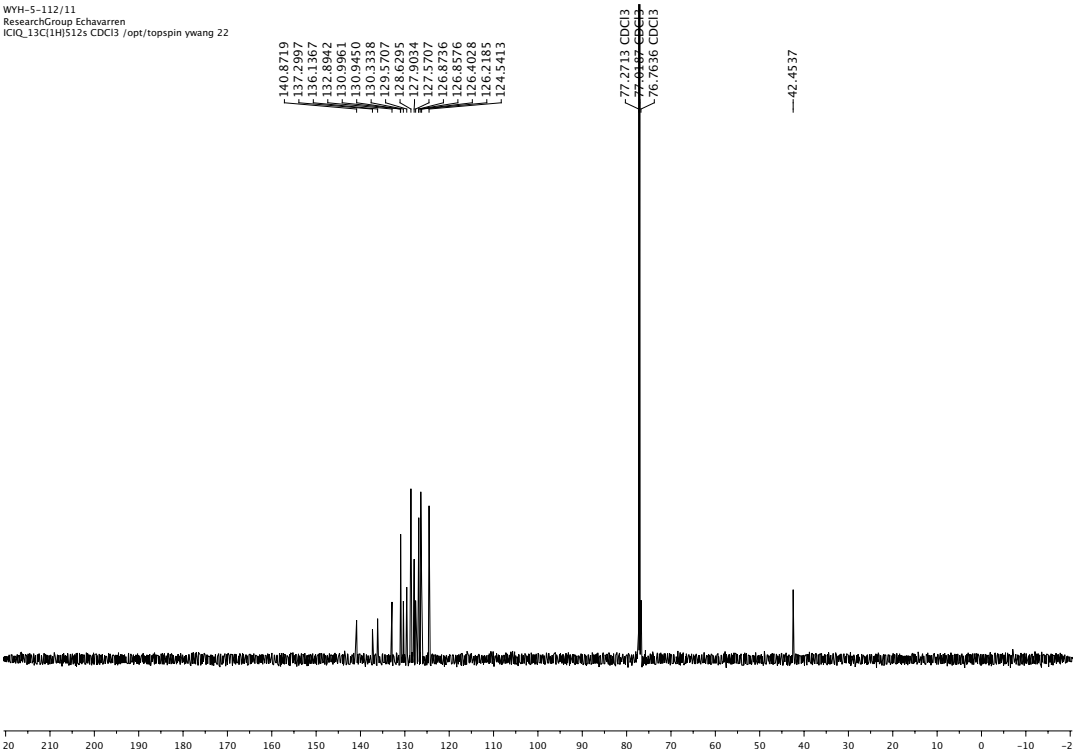

WYH-6-128.1.fid
13C{1H} Experiment
137.4859
137.1142
135.4036
132.7815
131.2909
131.2138
129.7095
128.6589
128.6174
127.8426
127.0106
126.6218
124.7228
124.0599
77.2581 CDCl3
77.0041 CDCl3
76.7496 CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

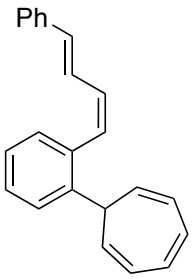


WYH-5-112/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 22



WYH-5-112/11
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 22





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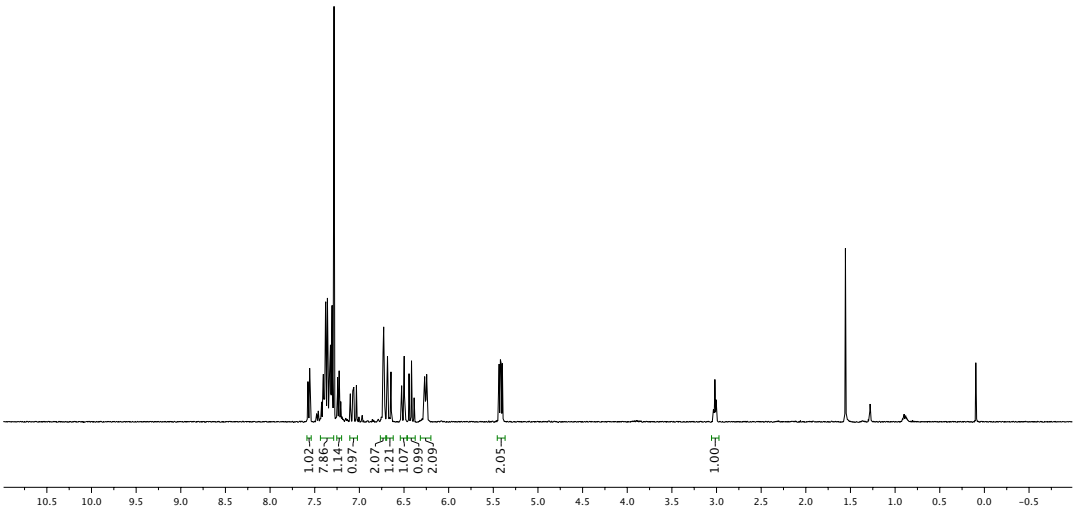
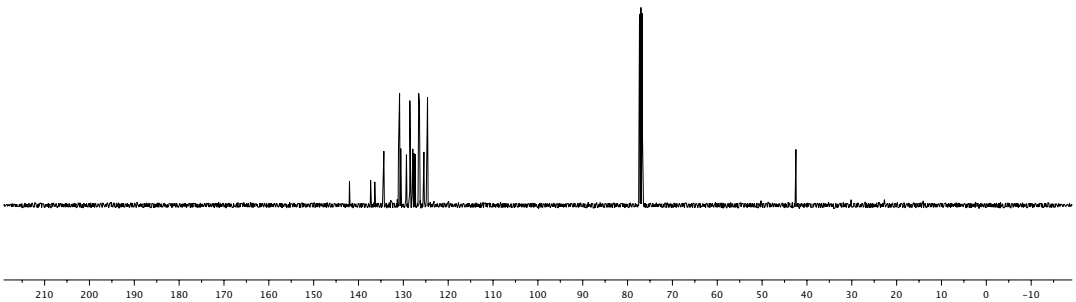
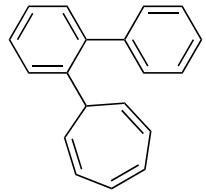
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 10



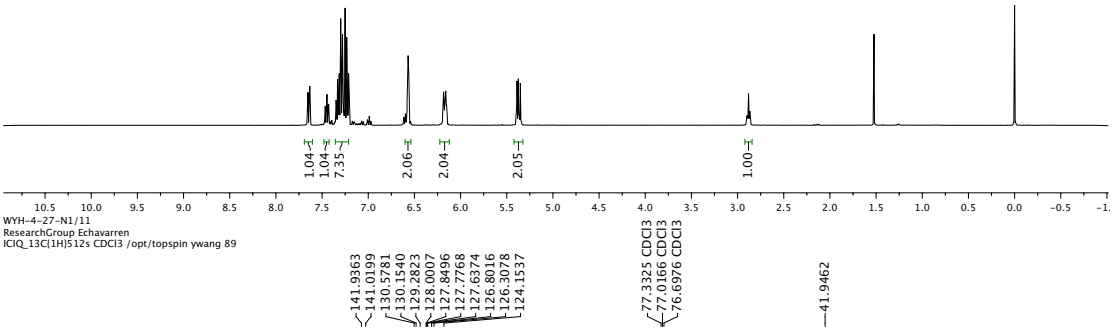
WYH-6-129-N.11.fid
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 75

142.0123
137.3008
136.3722
134.3489
131.0895
130.8421
130.5777
129.3129
128.5528
127.8957
127.6154
127.3588
126.5785
126.4154
126.3029
125.4172
124.6106
77.3376 CDCl3
77.0206 CDCl3
76.7031 CDCl3
42.4582

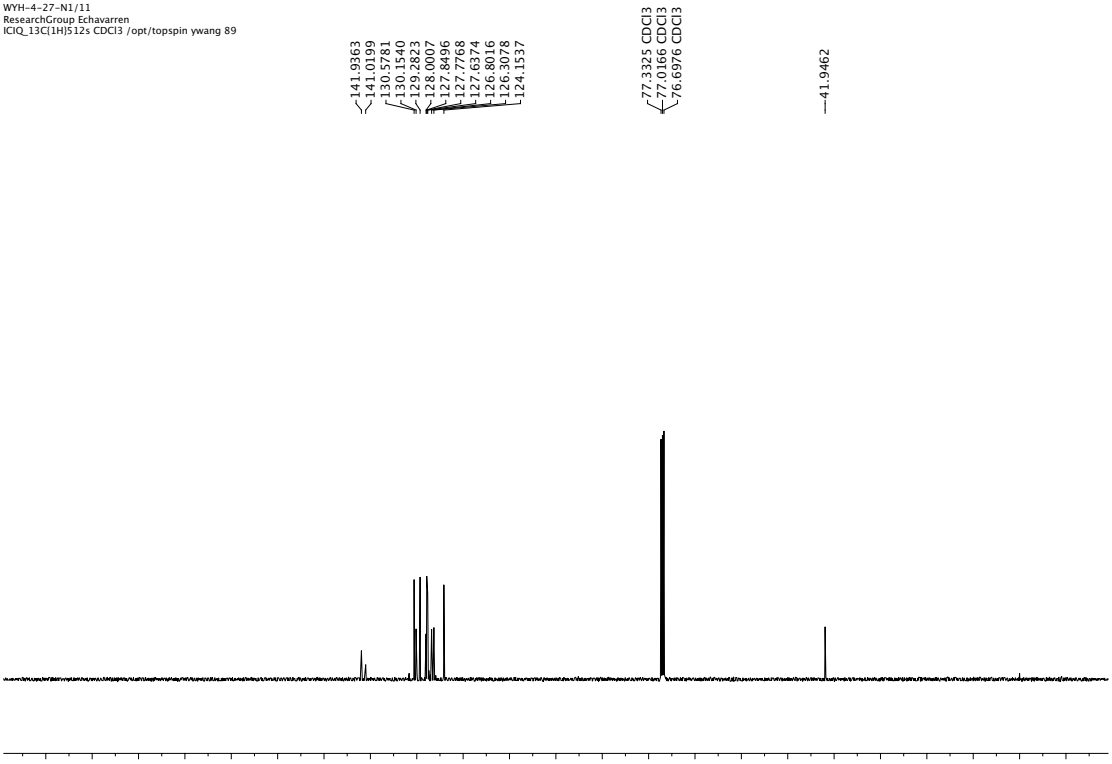


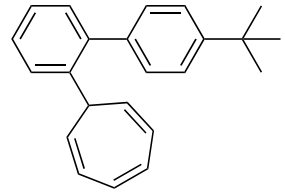


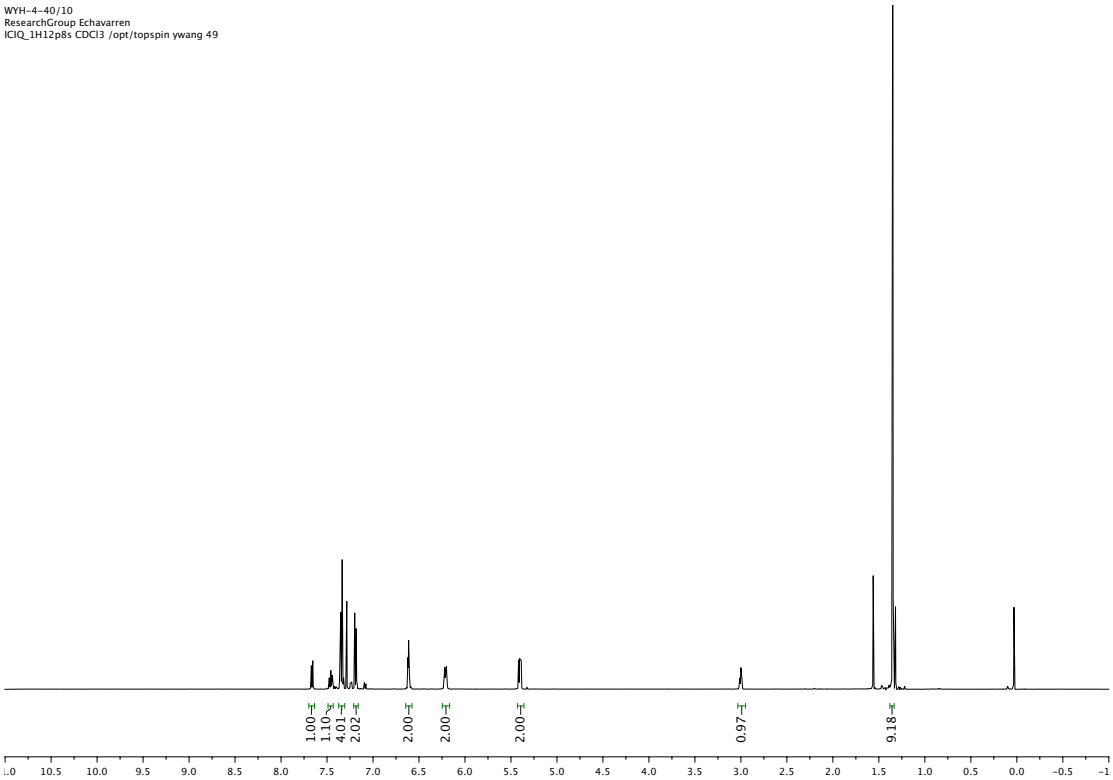
WYH-4-27-N1/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 89

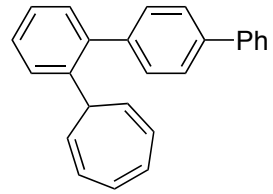


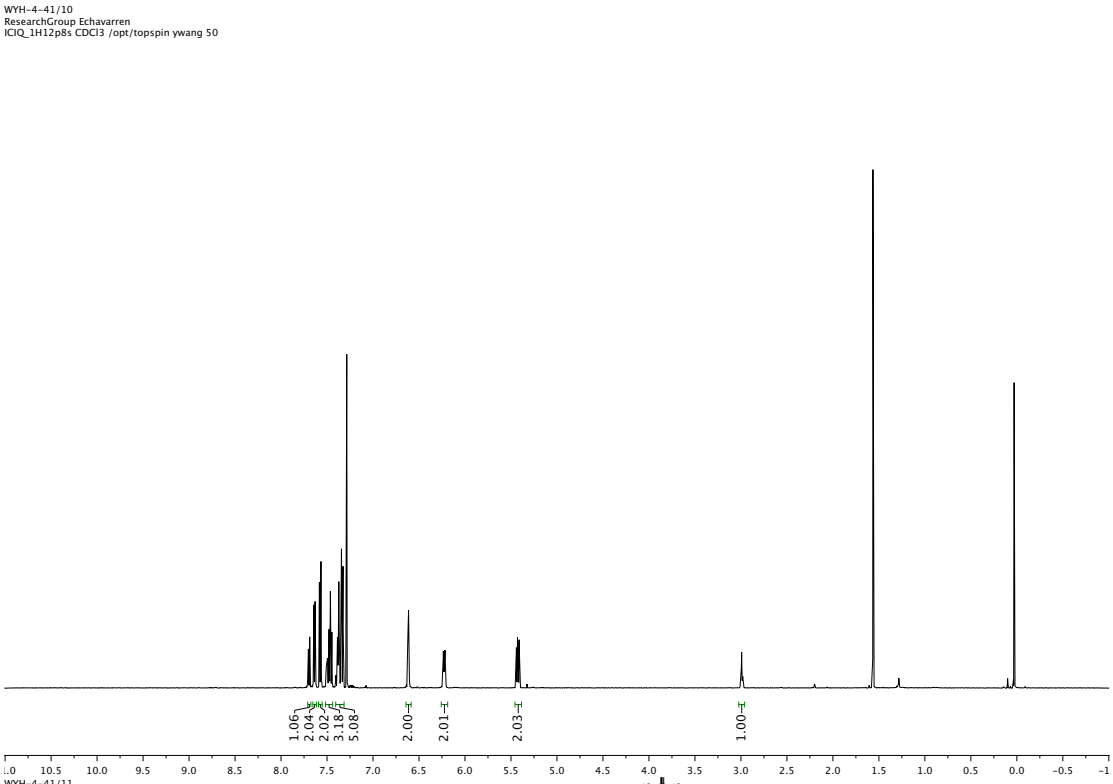
WYH-4-27-N1/11
ResearchGroup Echavarren
ICIQ_13C(1H)512s CDCl3 /opt/topspin ywang 89






WYH-4-40/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 49
1.00
1.10
4.01
2.02
2.00
2.00
2.00
0.97
9.18
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5


Ph


WYH-4-41/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 50
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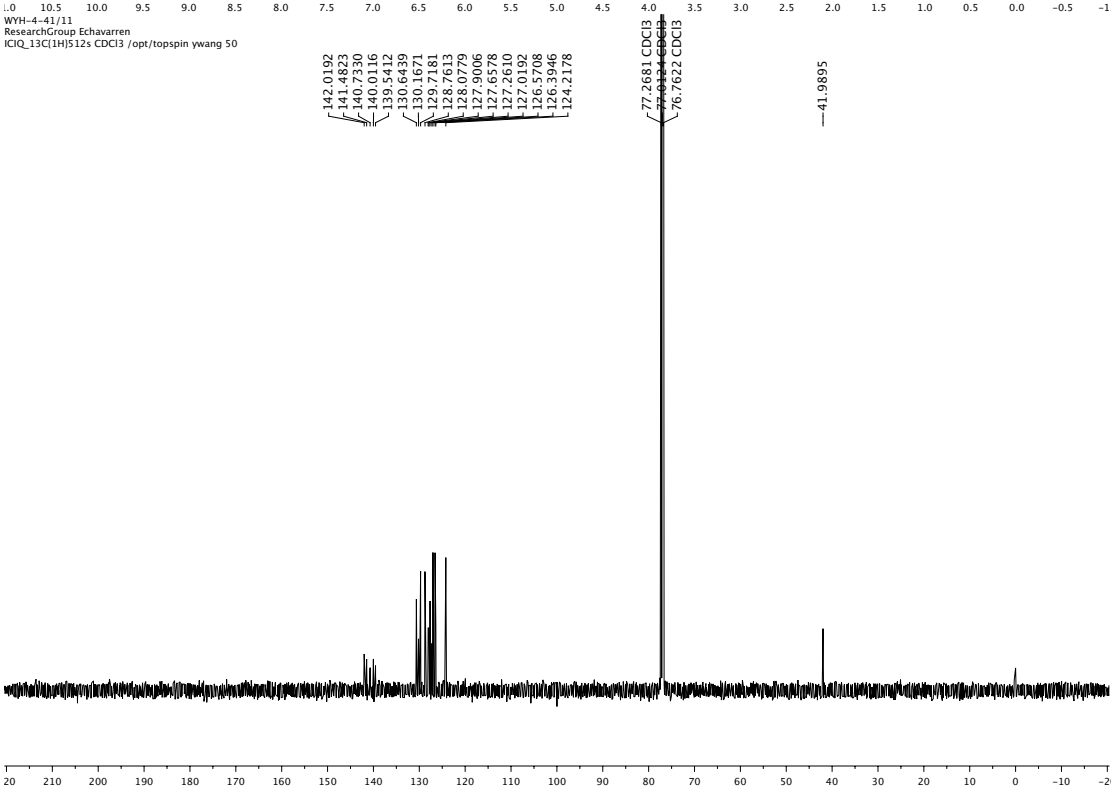
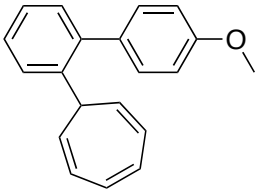
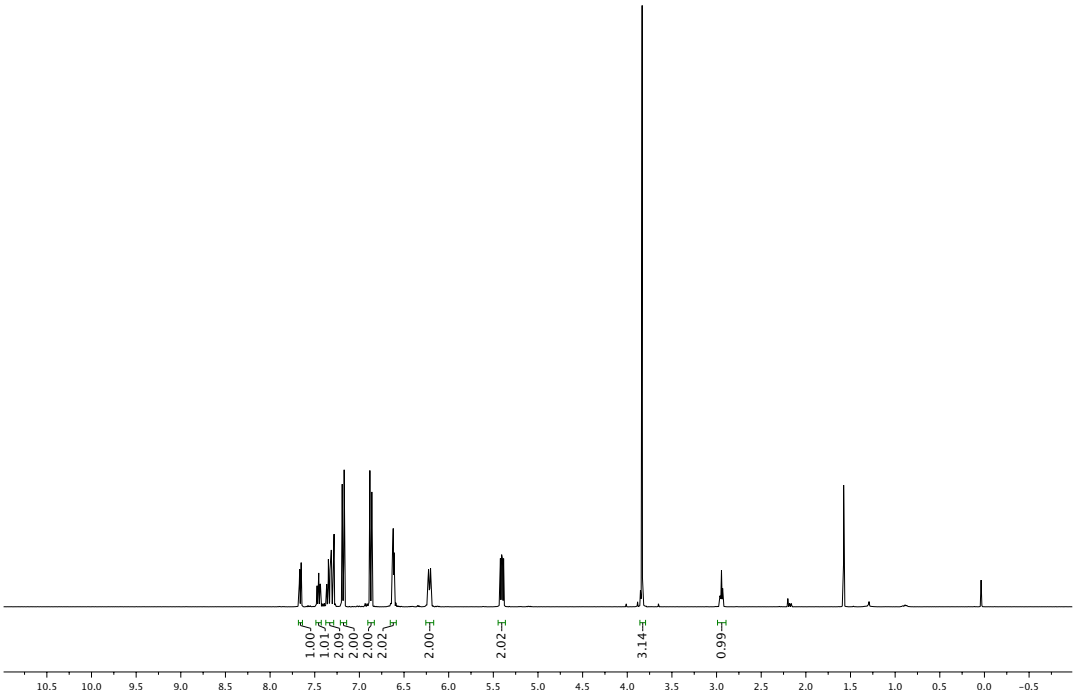
2.04
2.02
3.18
5.08
2.00
2.01
2.03
1.00

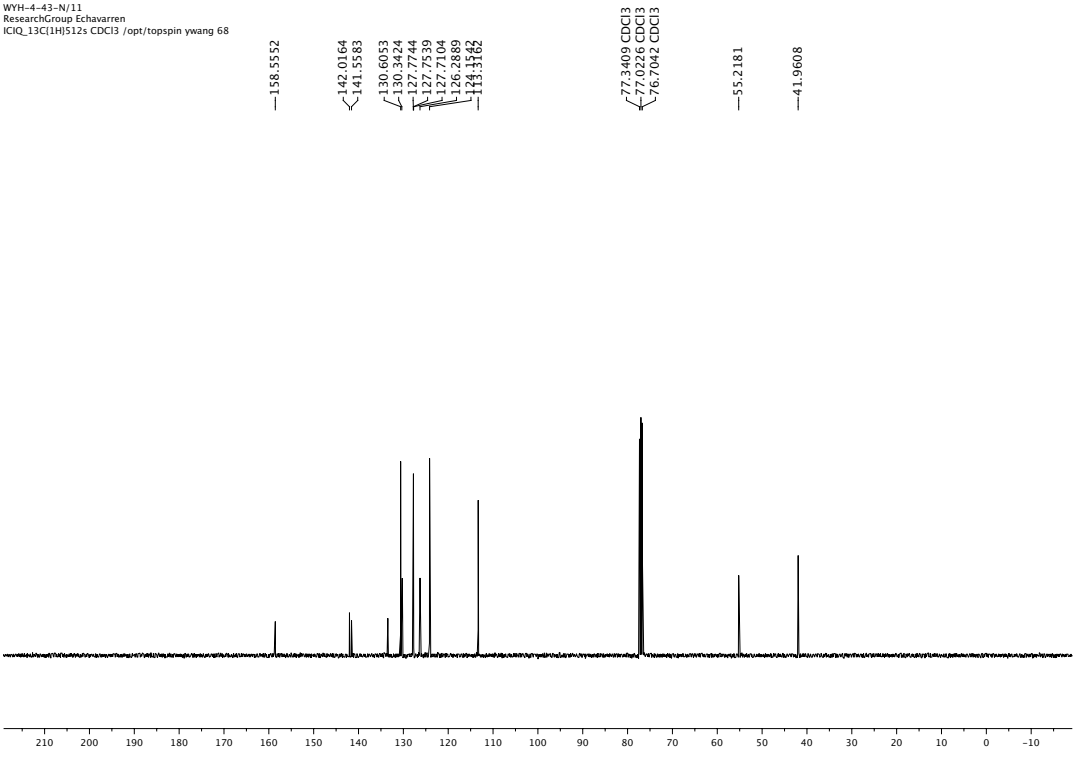

WYH-4-41/11
ResearchGroup Echavarren
ICIQ_13C(1H)512s CDCl3 /opt/topspin ywang 50
142.0192
141.4823
140.7330
140.0116
139.5412
130.6439
130.1671
129.7181
128.7613
128.0779
127.9006
127.6578
127.2610
127.0192
126.5708
126.3946
124.2178
77.2681 CDCl3
77.0164 CDCl3
76.7622 CDCl3
41.9895

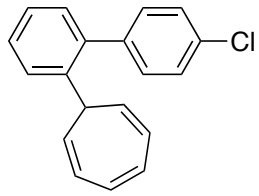


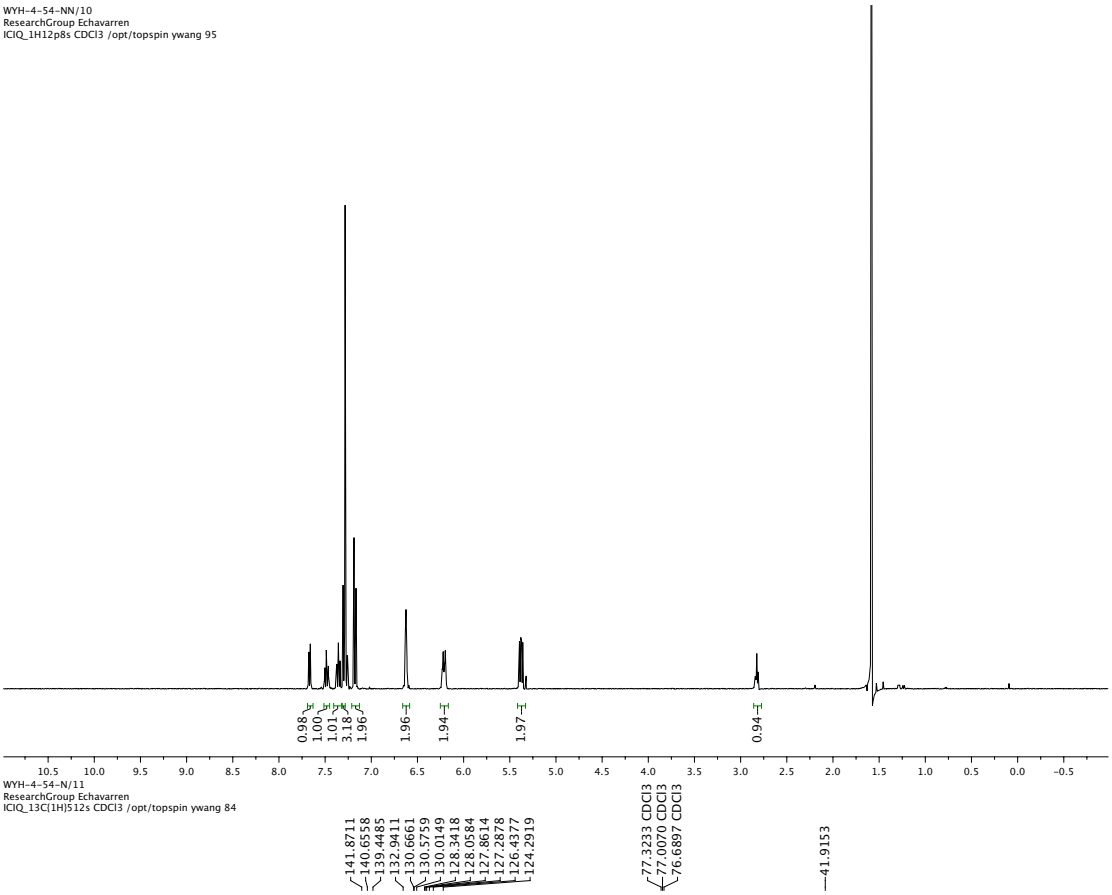
WYH-4-43-N/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 68

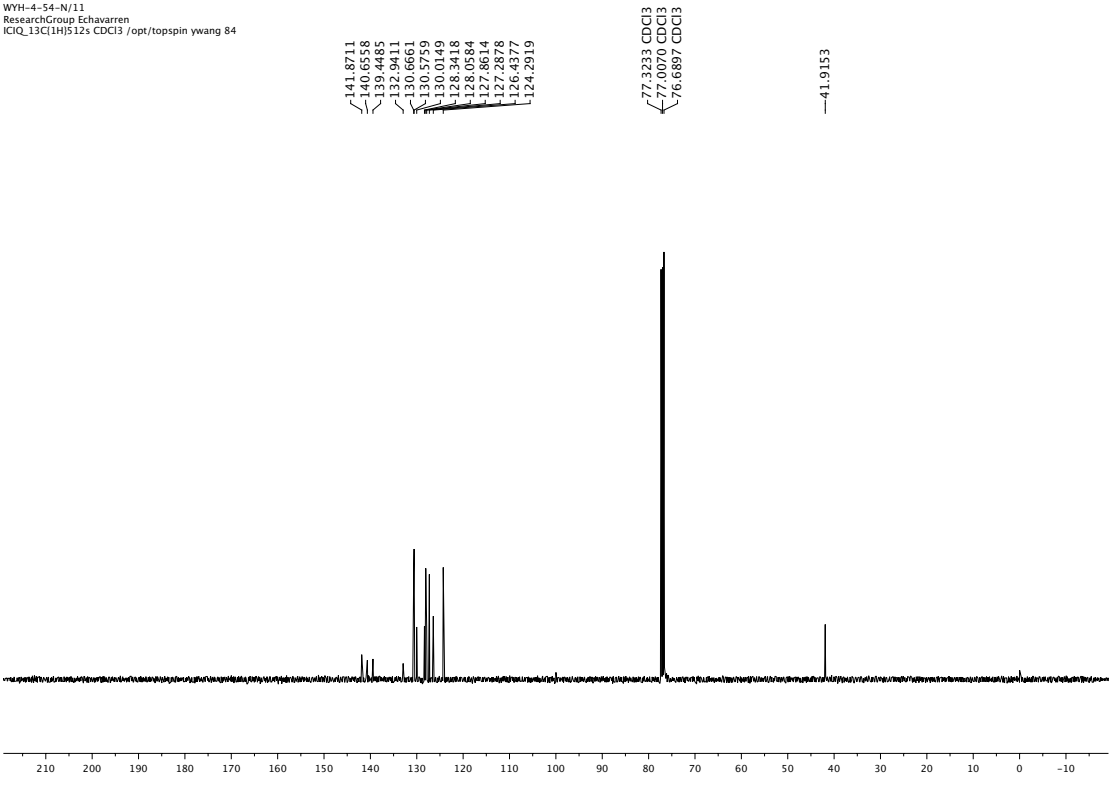


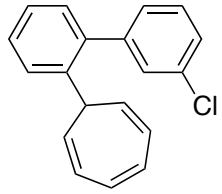
WYH-4-43-N/11
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 68



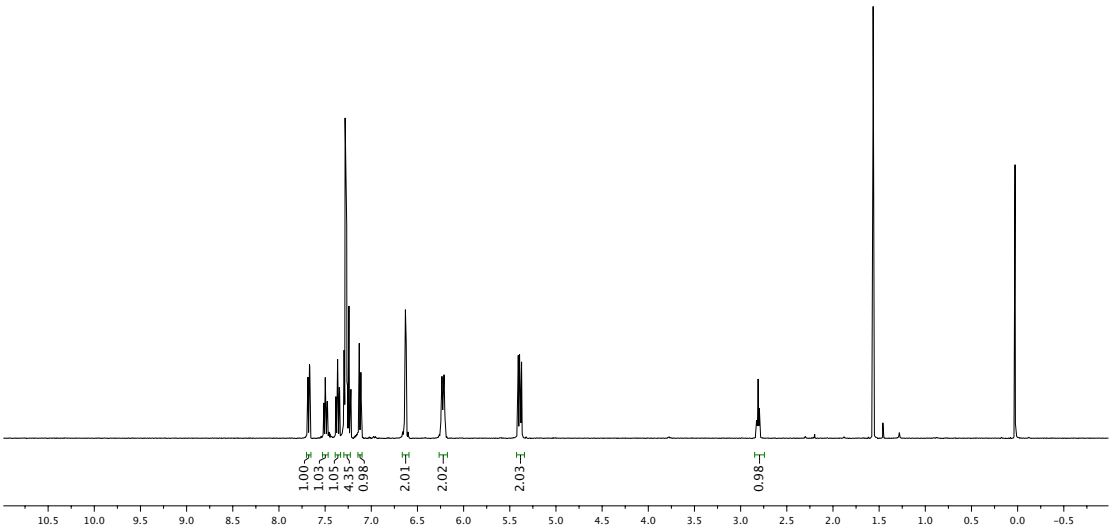

Cl


WYH-4-54-NN/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 95
0.98
1.00
1.01
3.18
1.96
1.96
1.94
1.97
0.94
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5

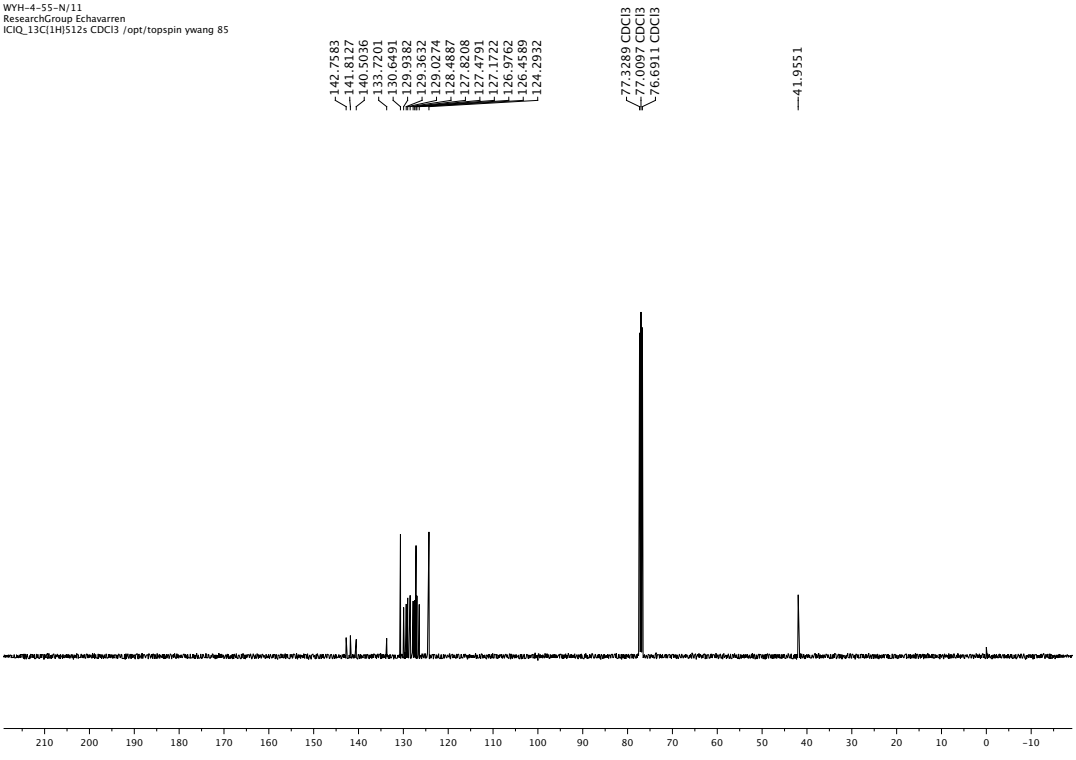

WYH-4-54-N/11
ResearchGroup Echavarren
ICIQ_13C(1H)512s CDCl3 /opt/topspin ywang 84
141.8711
140.6558
139.4485
132.9411
130.6661
130.5759
130.0149
128.3418
128.0584
127.8614
127.2878
126.4377
124.2919
77.3233 CDCl3
77.0070 CDCl3
76.6897 CDCl3
41.9153
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

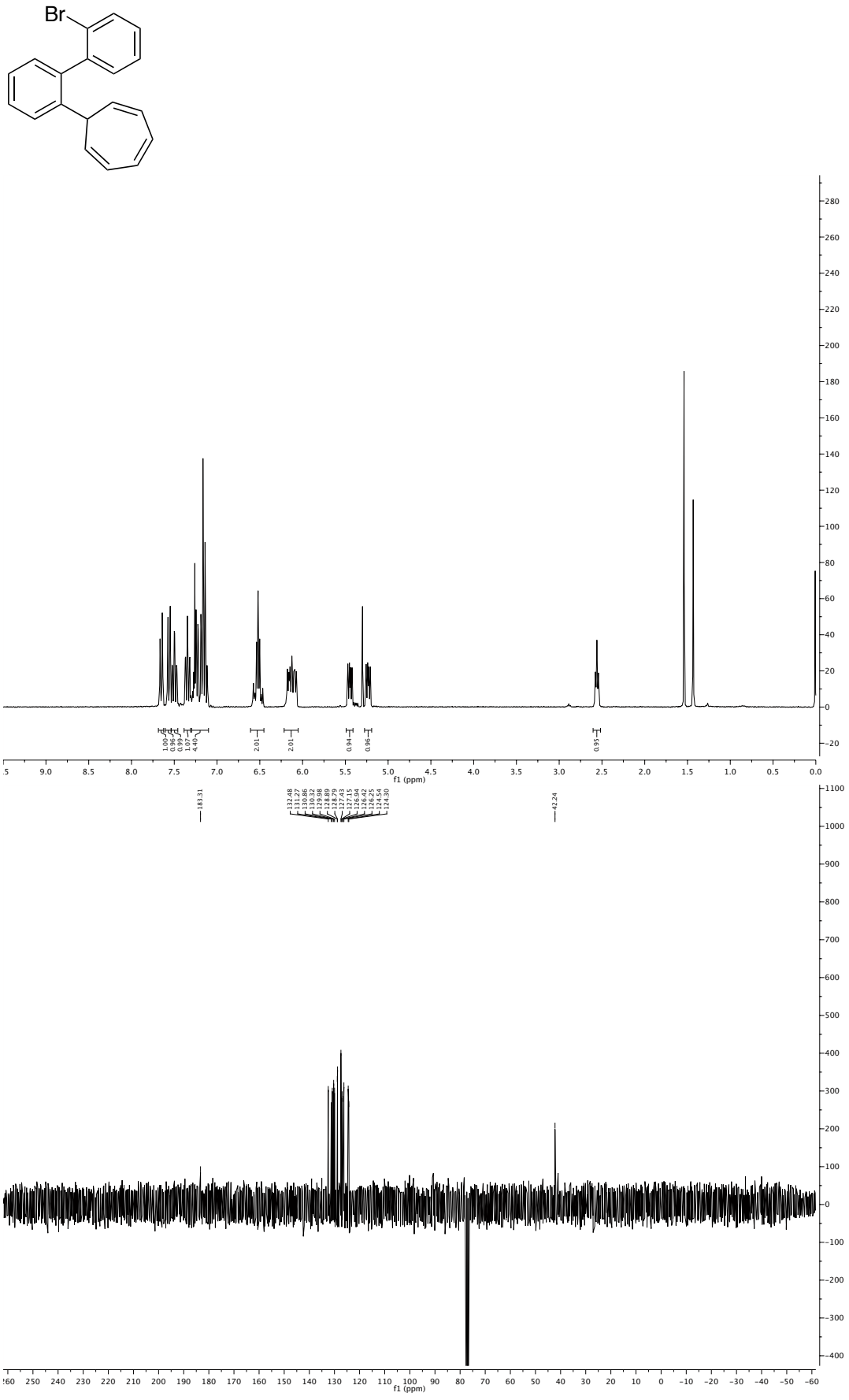


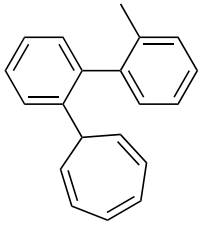
WYH-4-55-N/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 85



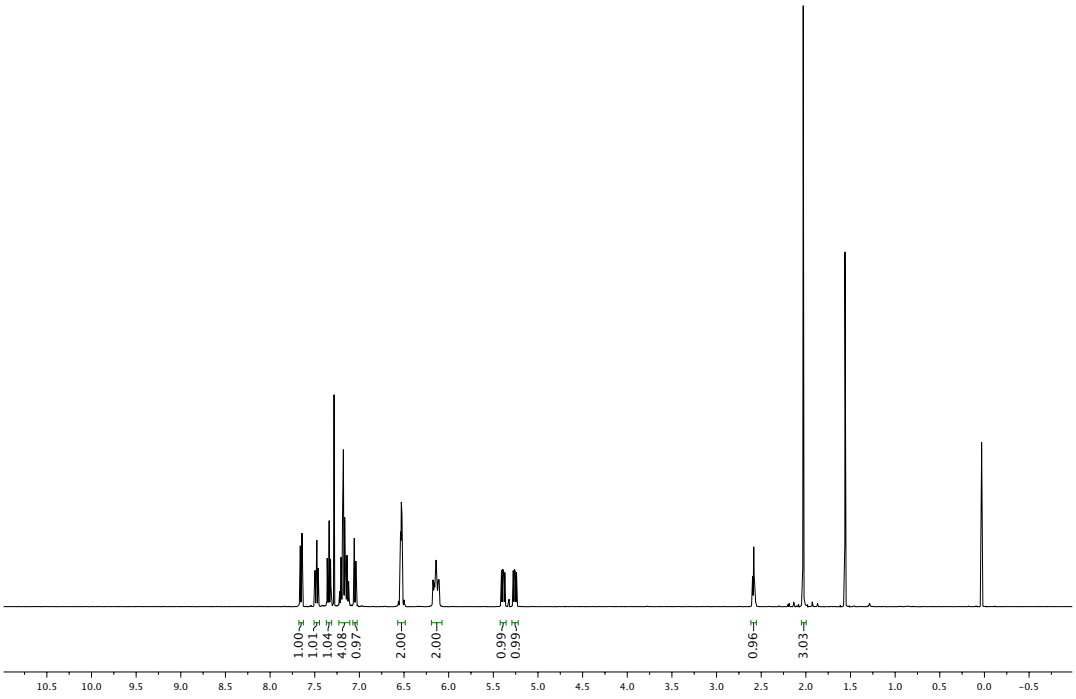
WYH-4-55-N/11
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 85



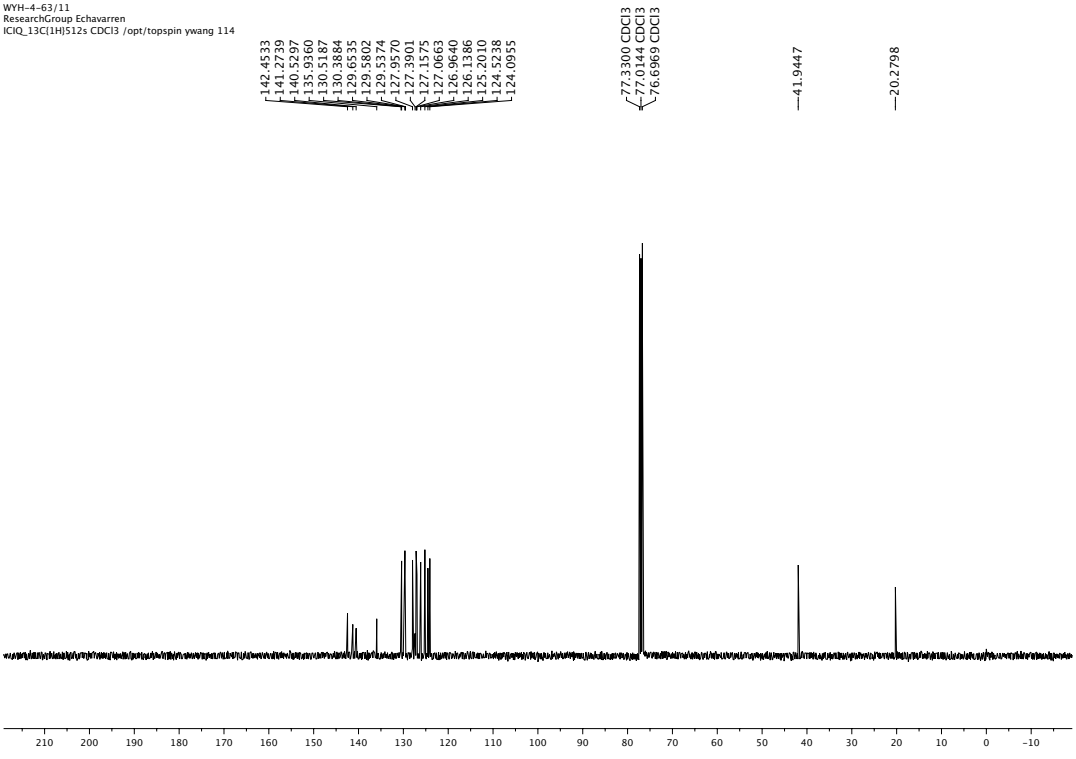

Br
1.00
0.96
0.99
1.00
4.40
2.01
2.01
0.94
0.96
0.95
f1 (ppm)
183.31
132.48
131.27
130.86
130.32
129.98
128.89
128.79
127.43
127.15
126.94
126.62
126.25
124.54
124.30
42.24
f1 (ppm)

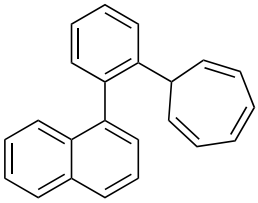


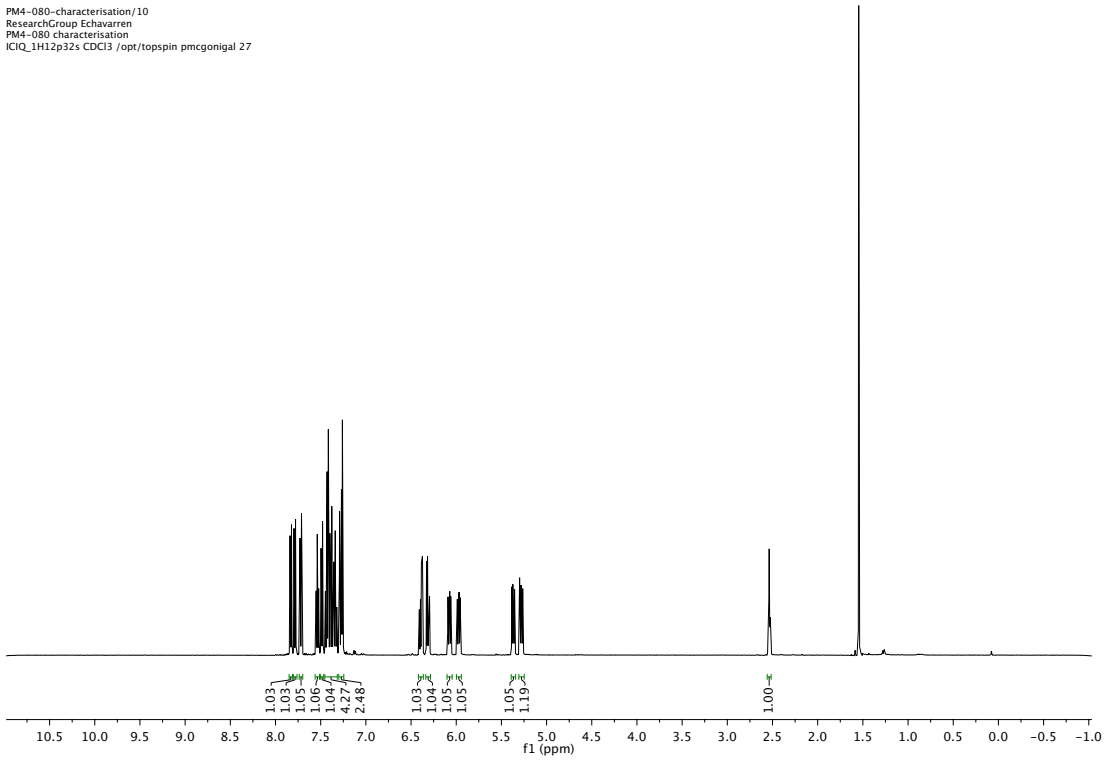
WYH-4-63/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 114

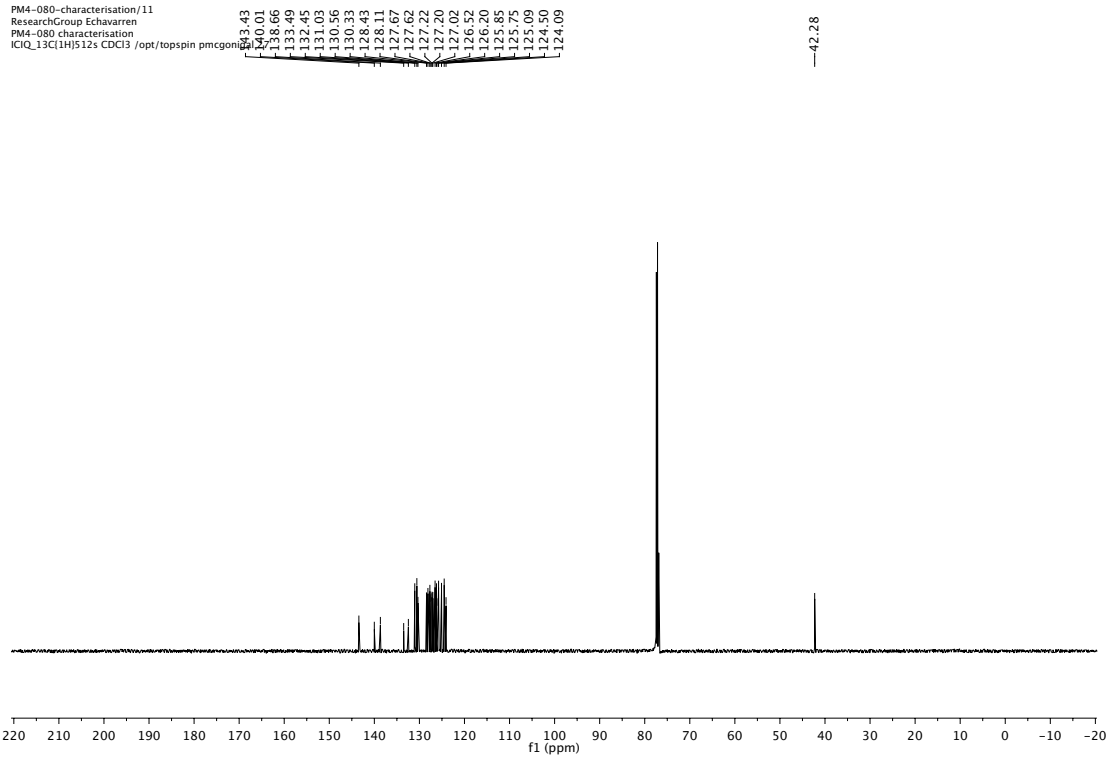


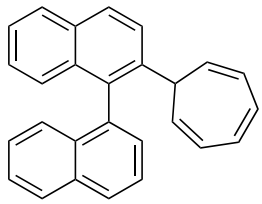
WYH-4-63/11
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 114

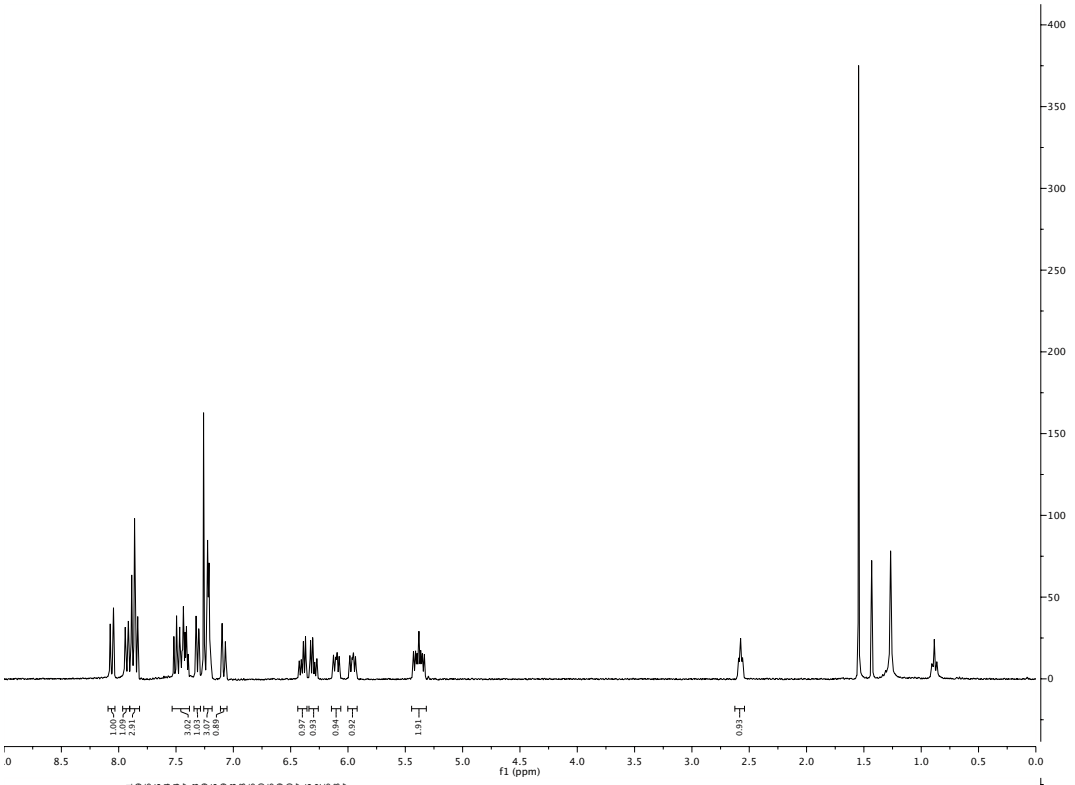


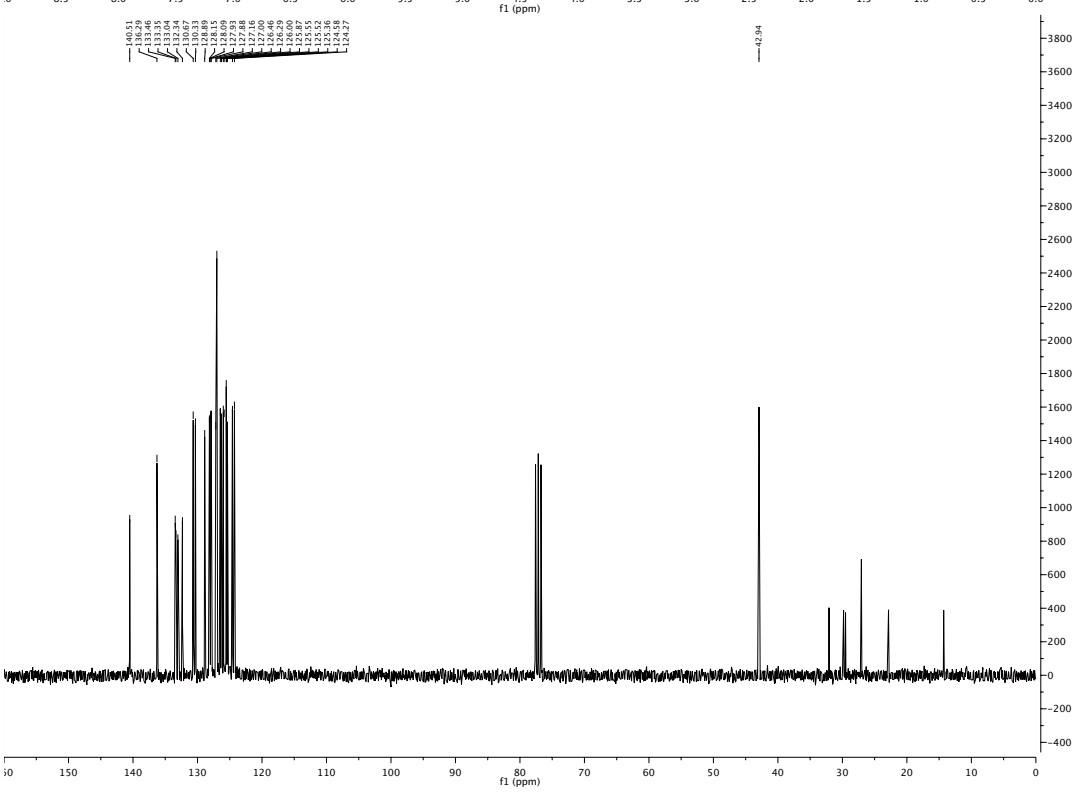


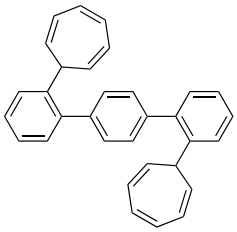

PM4-080-characterisation/10
ResearchGroup Echavarren
PM4-080 characterisation
ICIQ_1H12p32s CDCl3 /opt/topspin pmcgonigal 27
1.03
1.03
1.05
1.06
1.04
4.27
2.48
1.03
1.04
1.05
1.05
1.05
1.19
1.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


PM4-080-characterisation/11
ResearchGroup Echavarren
PM4-080 characterisation
ICIQ_13C{1H}512s CDCl3 /opt/topspin pmcgonigal
143.43
140.01
138.66
133.49
132.45
131.03
130.56
130.33
128.43
128.11
127.67
127.62
127.22
127.20
127.02
126.52
126.20
125.85
125.75
125.09
124.50
124.09
42.28
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

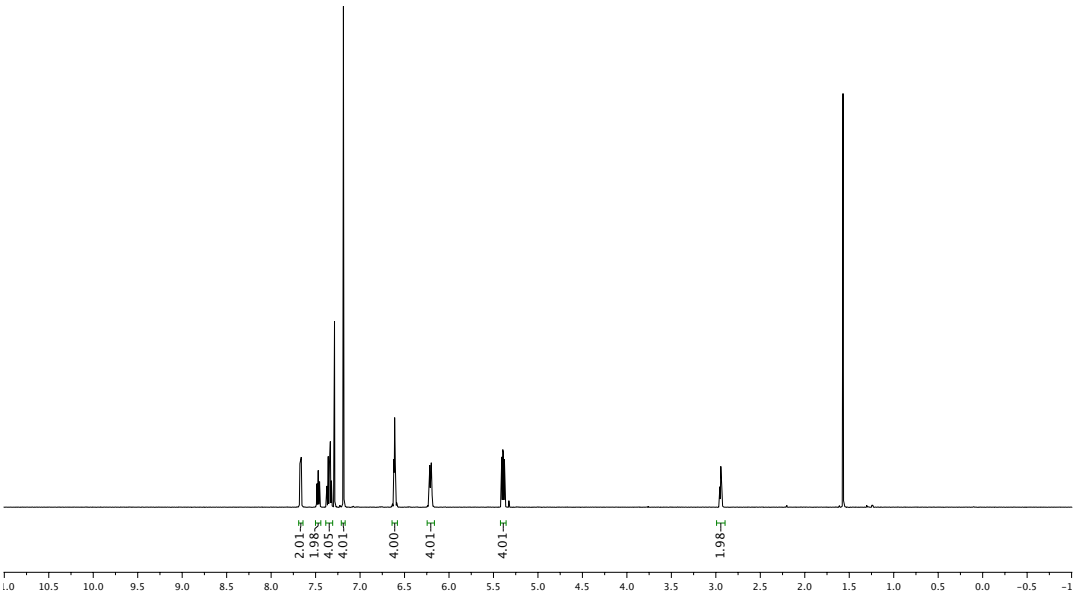



1.00
1.09
2.91
3.02
1.02
3.07
0.89
0.97
0.93
0.94
0.92
1.91
0.93
f1 (ppm)

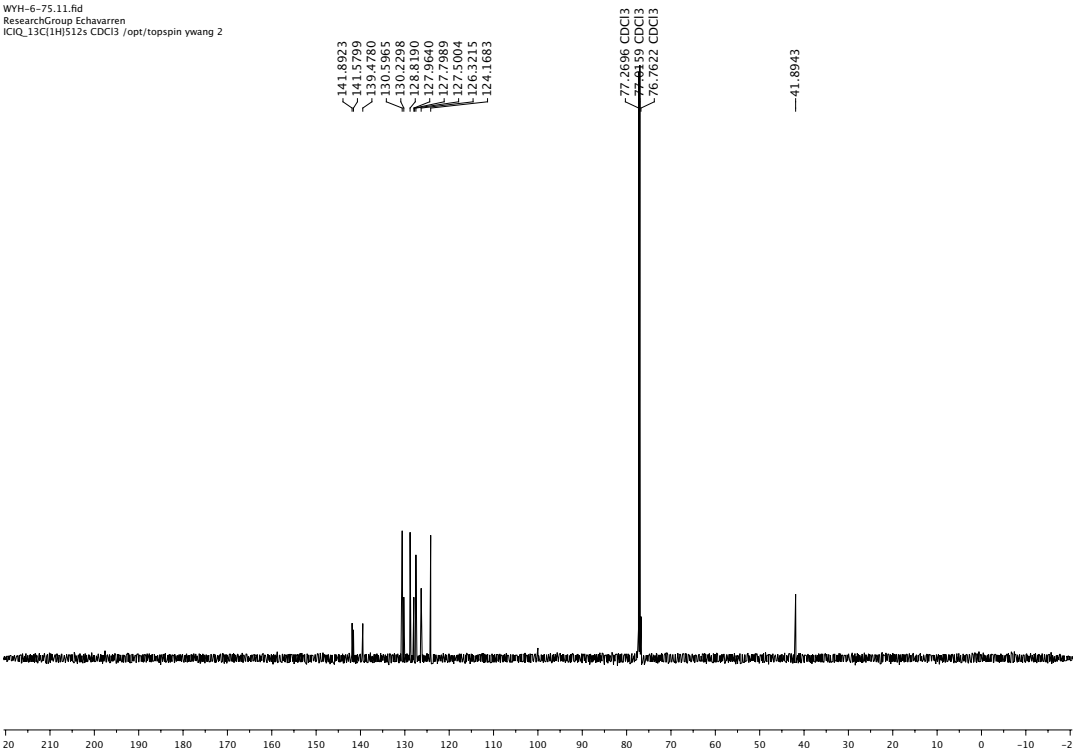

140.51
136.29
133.46
133.35
133.34
132.34
130.87
130.33
128.89
128.15
128.00
127.93
127.88
127.16
127.00
126.46
126.39
126.00
125.87
125.55
125.52
125.36
124.98
124.27
42.94
f1 (ppm)

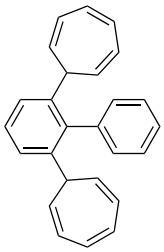


WYH-6-75.10.fid
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 2

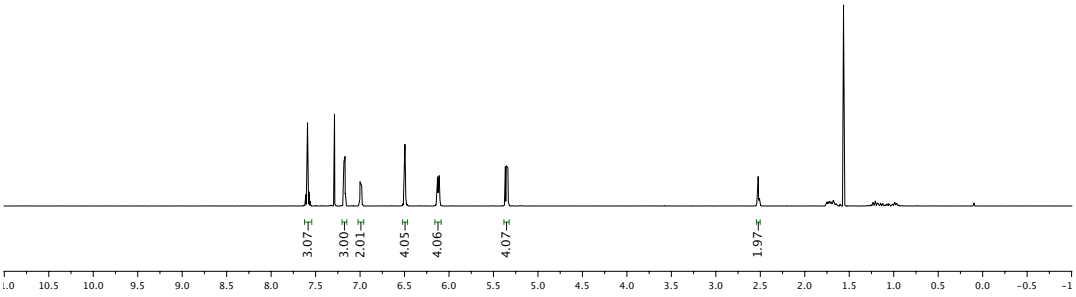


WYH-6-75.11.fid
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 2

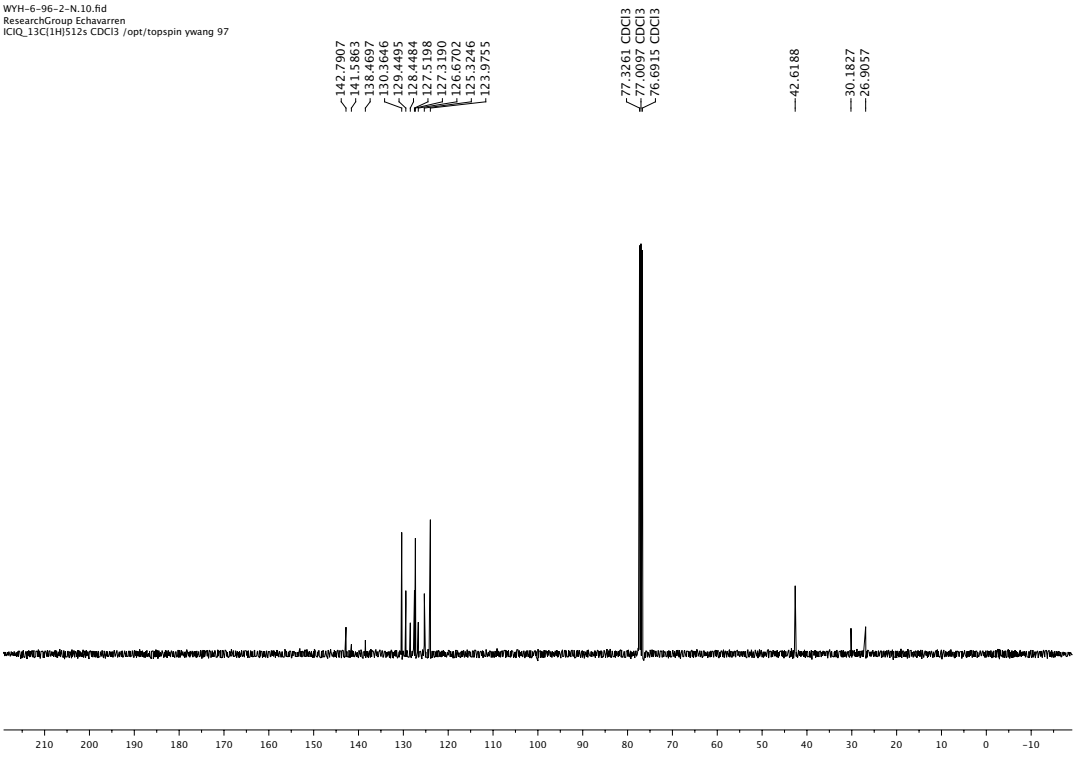


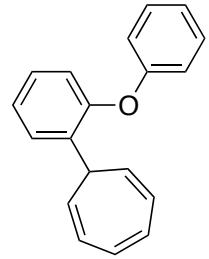


WYH-6-96-2.10.fid
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 32

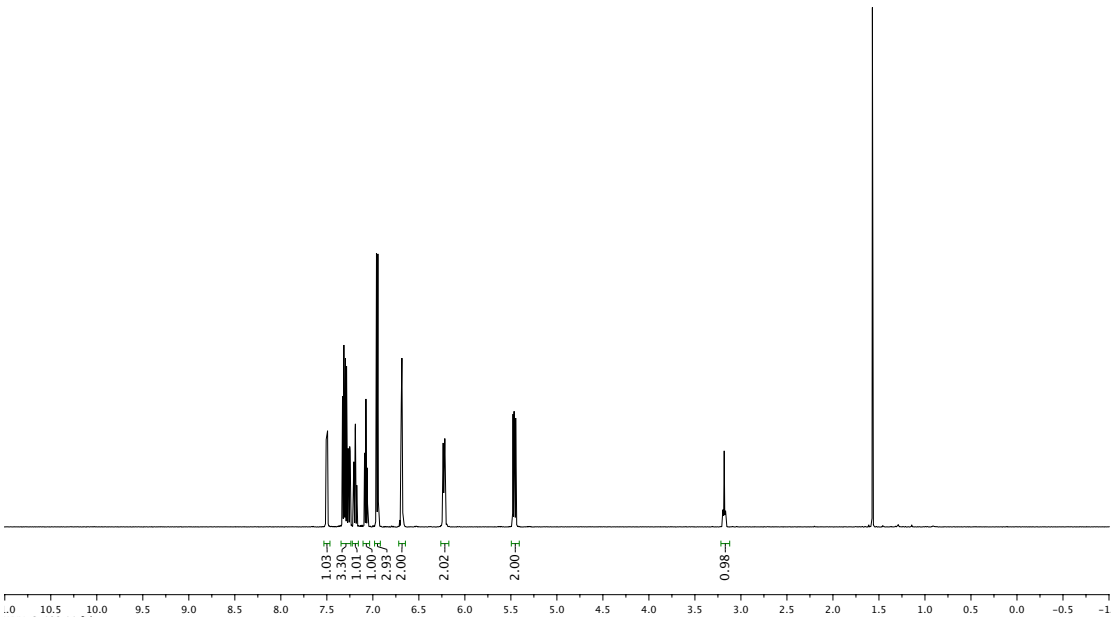


WYH-6-96-2-N.10.fid
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 97





WYH-6-103.10.fid
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 40



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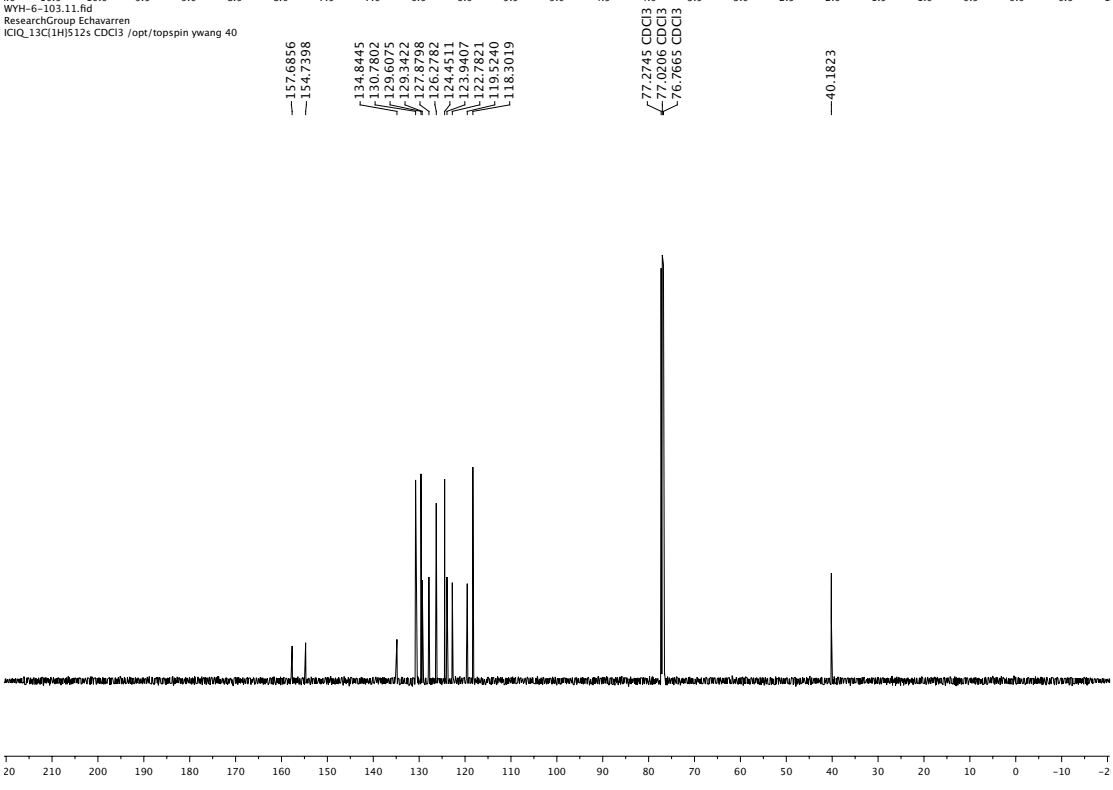
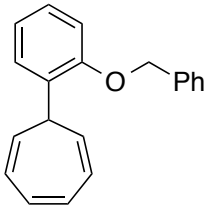
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 40





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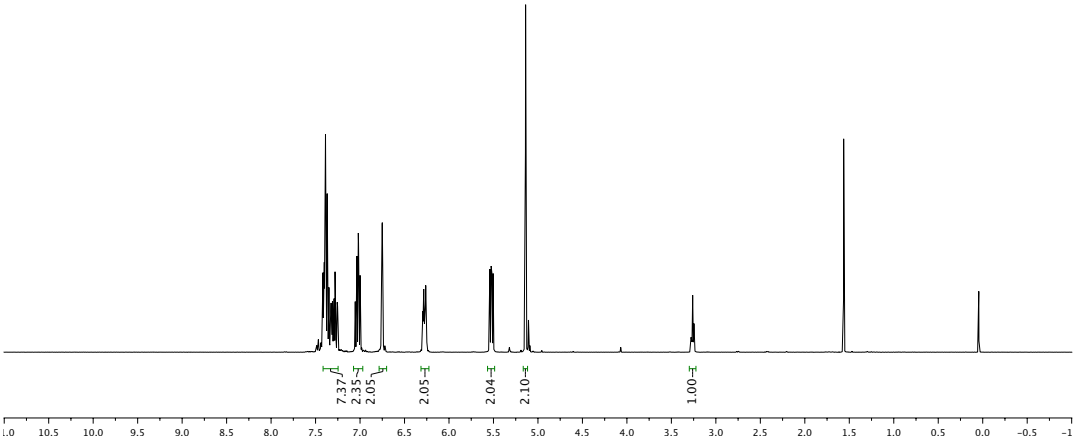
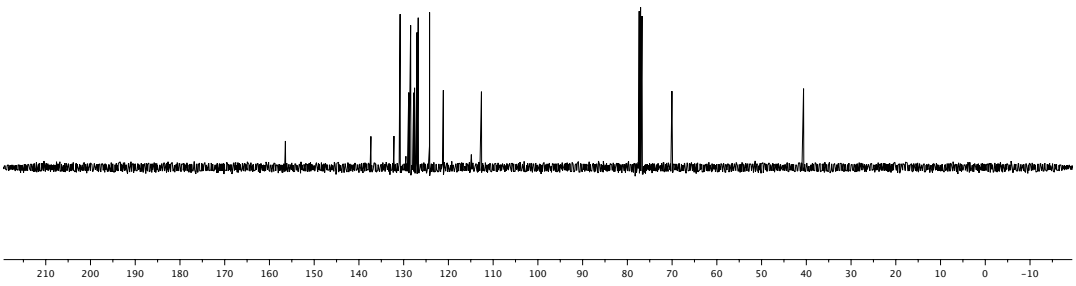
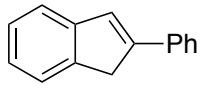
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 20



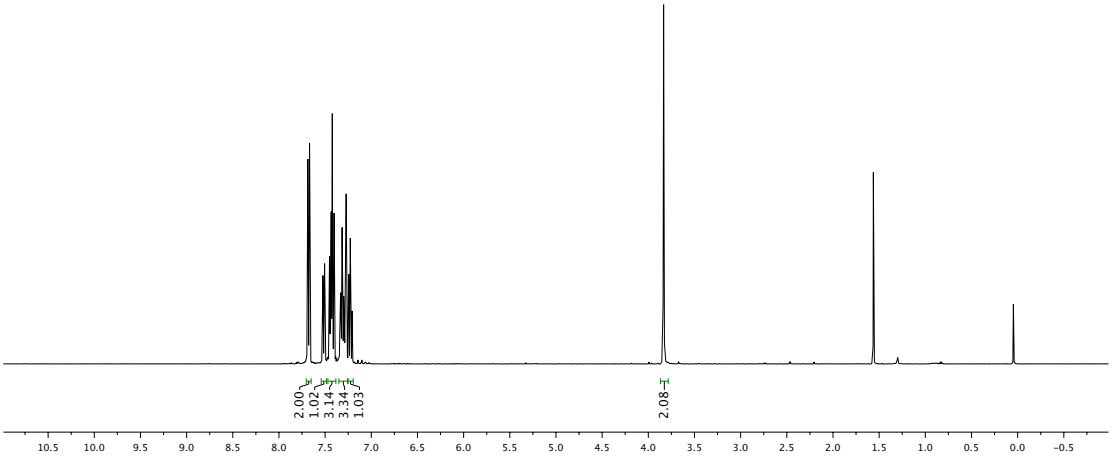
WYH-2-42-N.11.fid
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 20

156.4385
137.3212
132.1733
130.7947
128.8735
128.4385
127.7565
127.5652
127.0206
126.7483
124.2075
121.1346
112.6159
77.3625 CDCl3
77.0440 CDCl3
76.7280 CDCl3
70.0388
40.6180

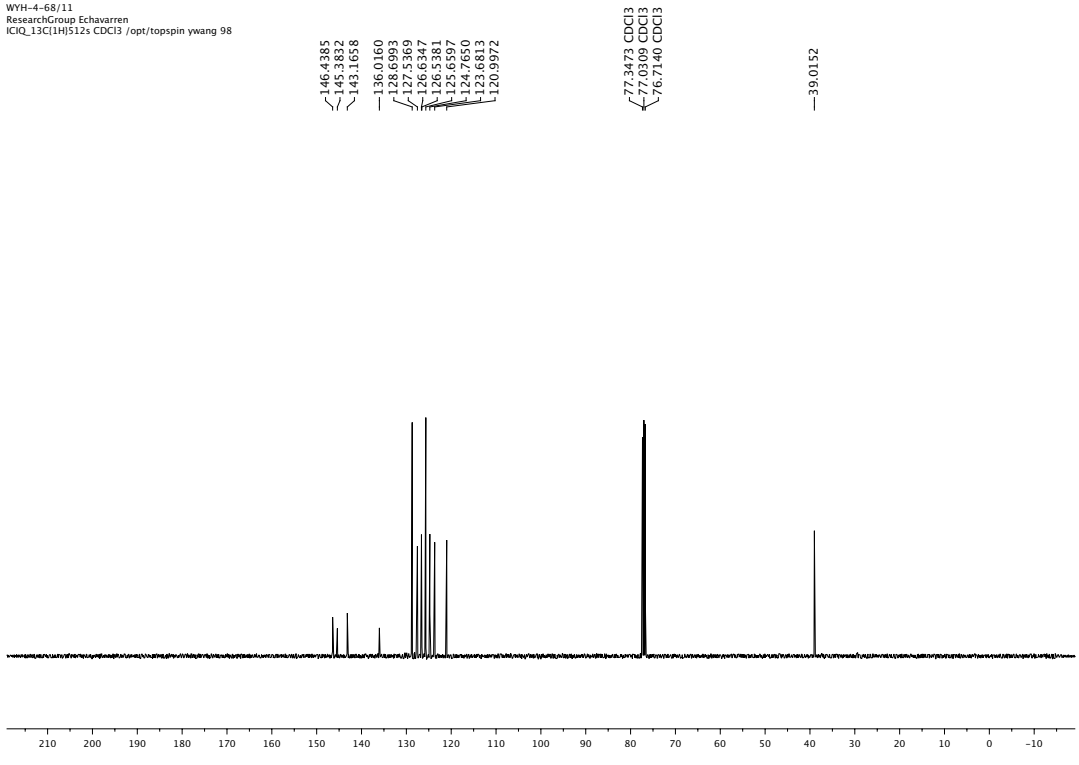


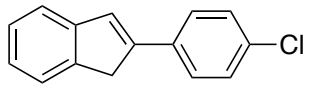


WYH-4-68/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 98

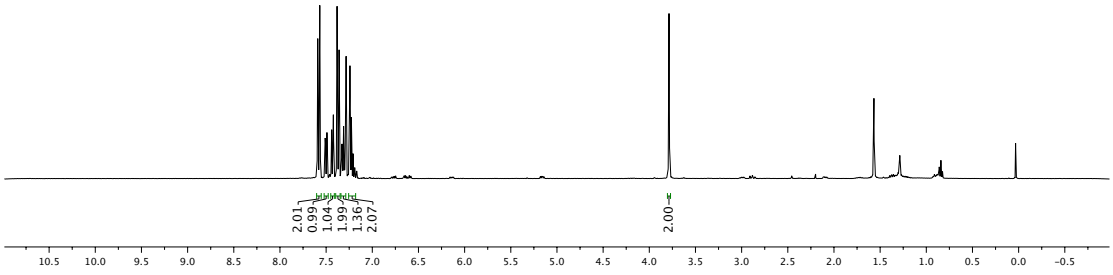


WYH-4-68/11
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 98



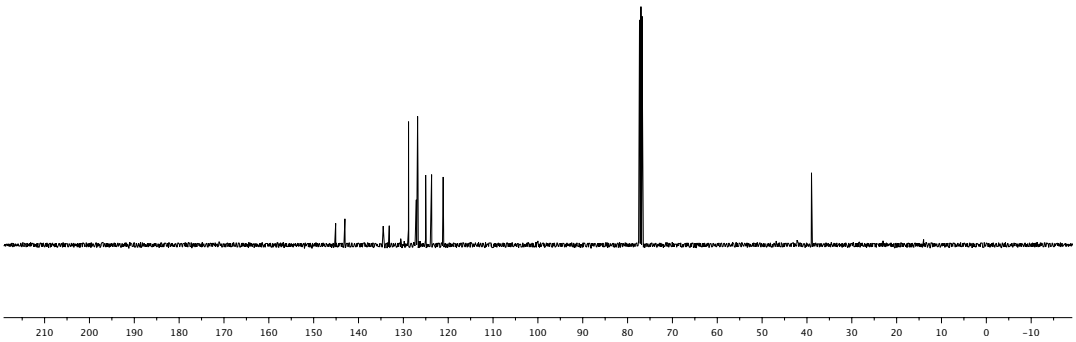


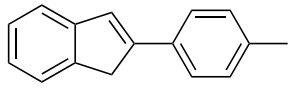
WYH-4-88/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 93



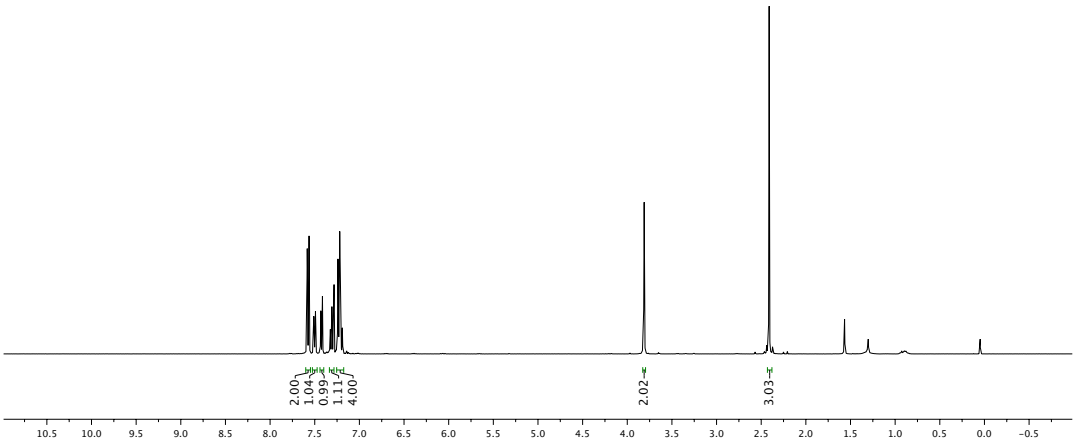
WYH-4-88/11
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 93

145.1162
145.0926
143.0356
134.4957
133.1446
128.8446
127.1083
126.8228
126.7356
125.0270
123.7033
121.1212
77.3360 CDCl3
77.0174 CDCl3
76.6990 CDCl3
38.9861

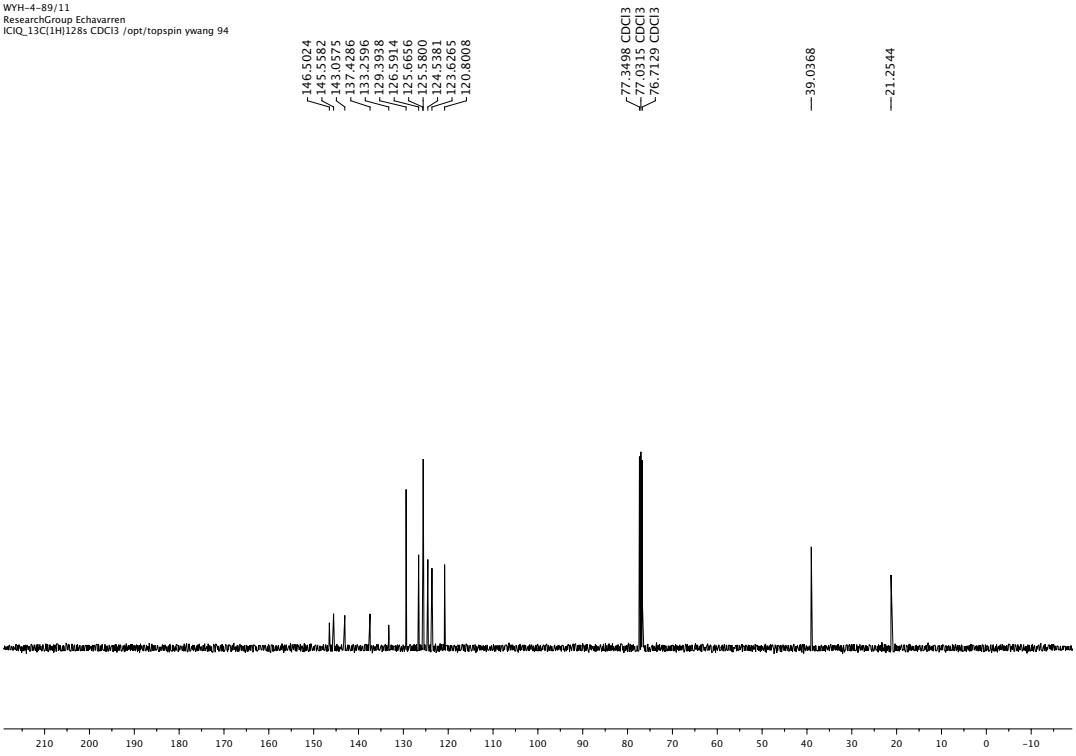


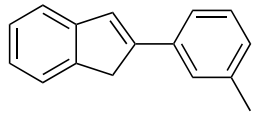


WYH-4-89/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 94

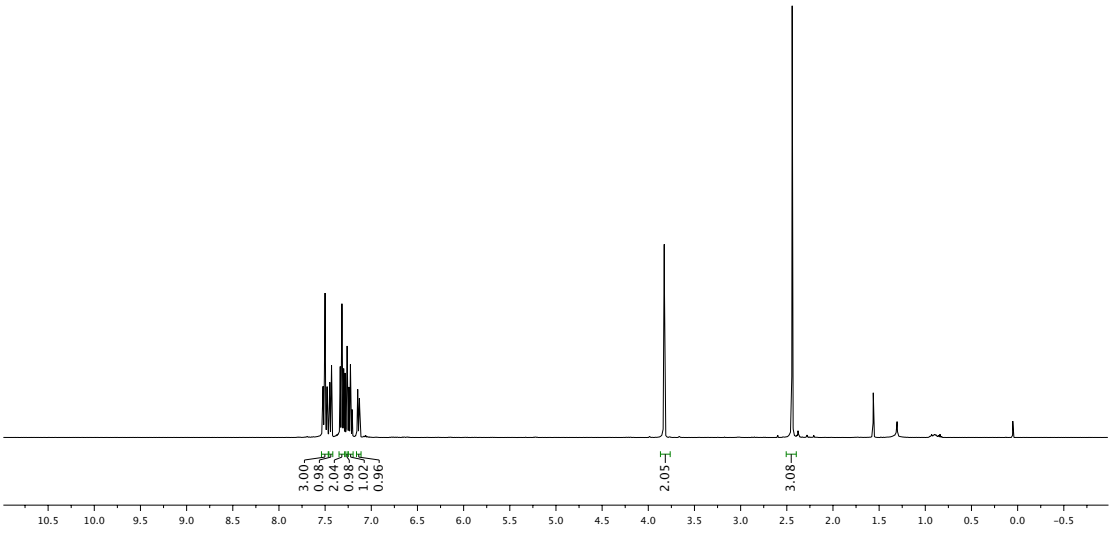


WYH-4-89/11
ResearchGroup Echavarren
ICIQ_13C{1H}128s CDCl3 /opt/topspin ywang 94

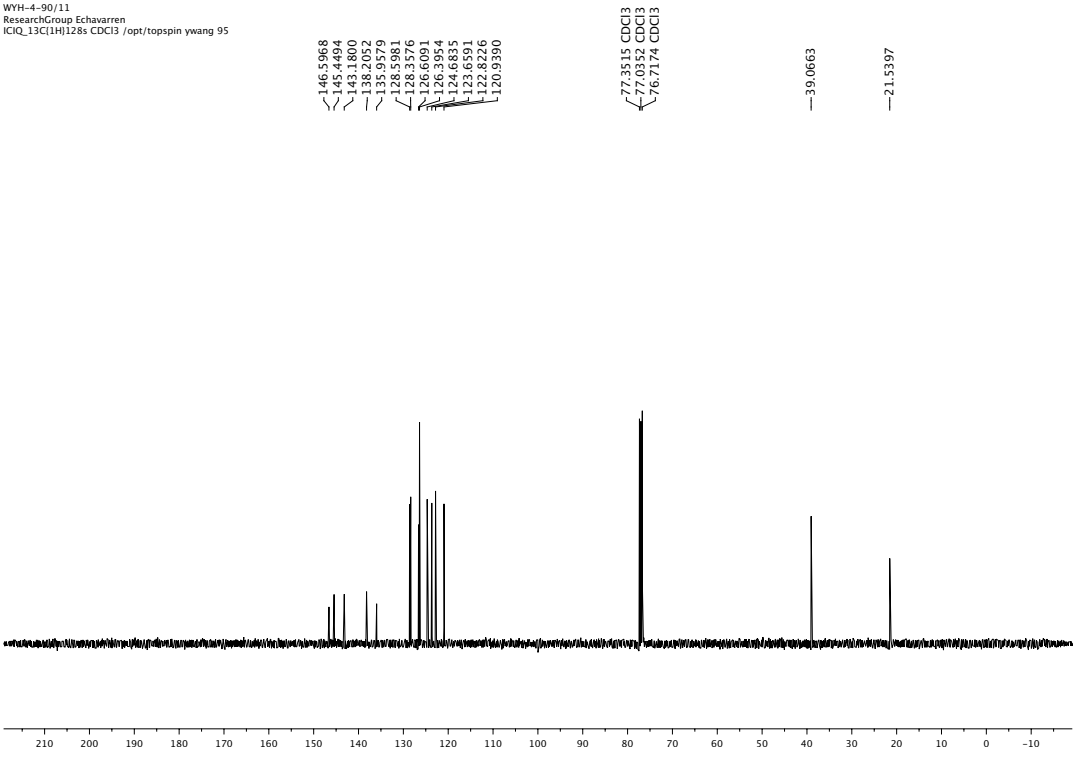


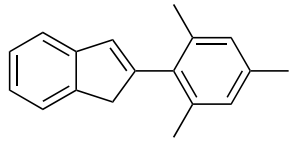


WYH-4-90/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 95

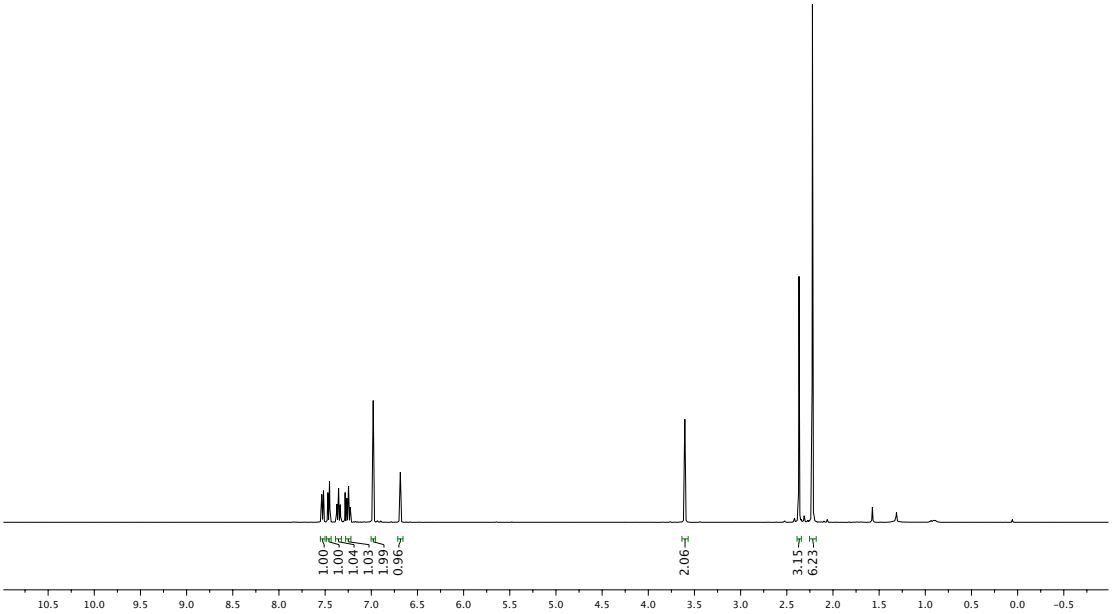


WYH-4-90/11
ResearchGroup Echavarren
ICIQ_13C{1H}128s CDCl3 /opt/topspin ywang 95



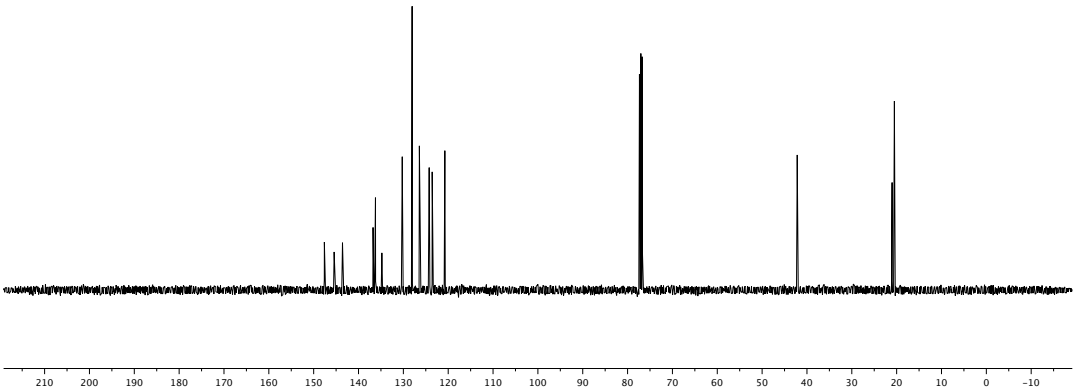


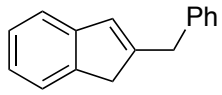
WYH-4-91/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 96



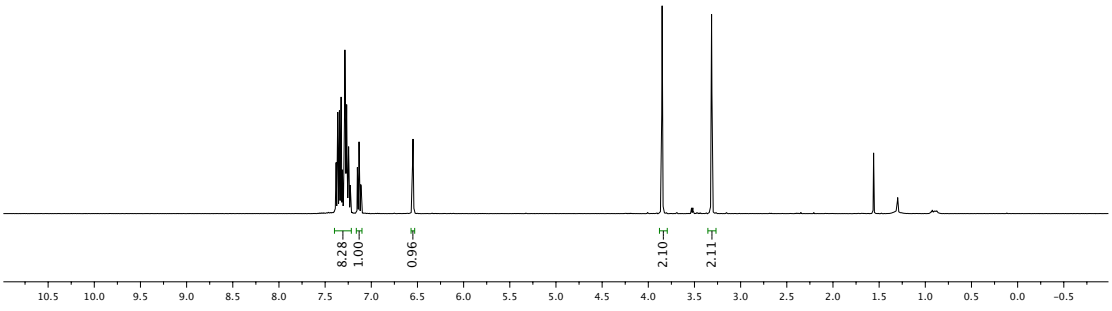
WYH-4-91/11
ResearchGroup Echavarren
ICIQ_13C{1H}128s CDCl3 /opt/topspin ywang 96

147.6178
145.4339
143.5728
136.7576
136.2211
134.7942
130.2477
128.0448
126.4297
124.2437
123.5701
120.7499
77.3540 CDCl3
77.0373 CDCl3
76.7190 CDCl3
42.1719
21.0149
20.5052

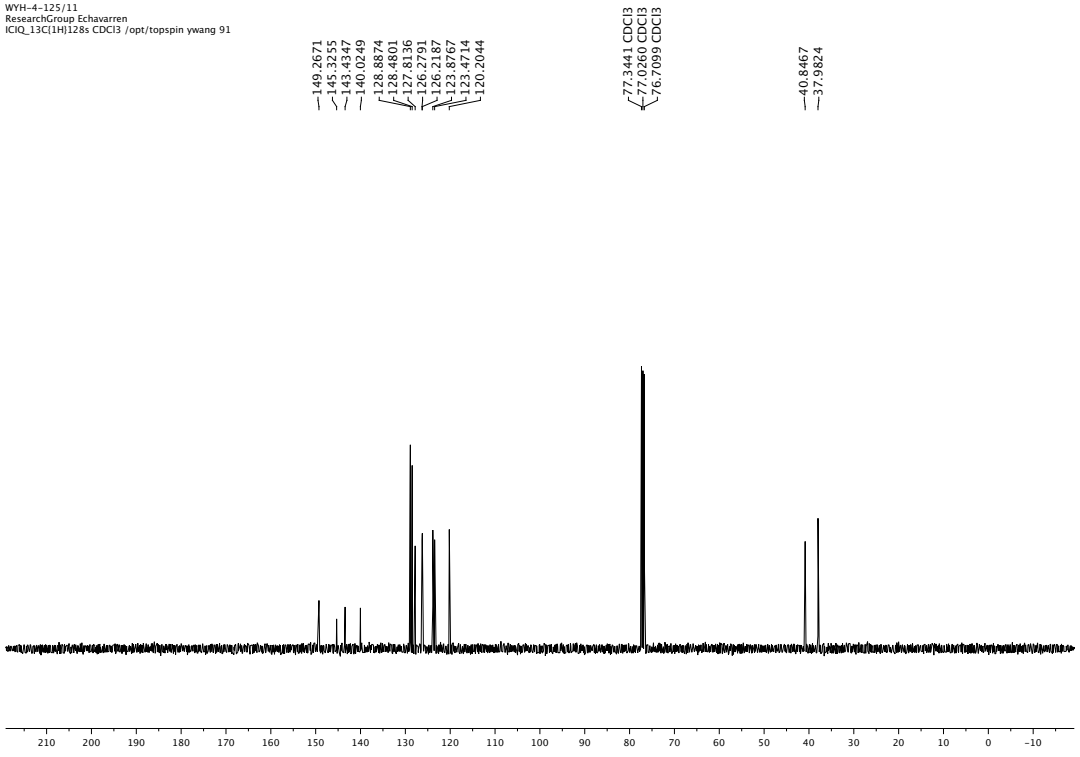


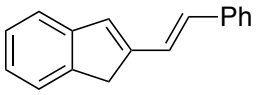


WYH-4-125/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 91

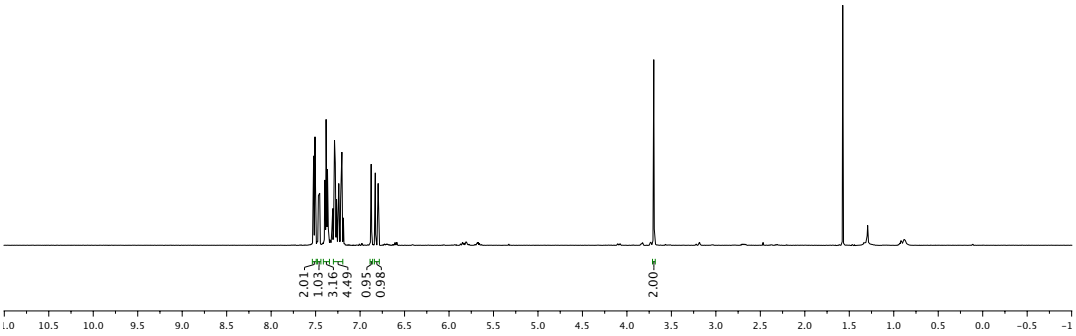


WYH-4-125/11
ResearchGroup Echavarren
ICIQ_13C{1H}128s CDCl3 /opt/topspin ywang 91

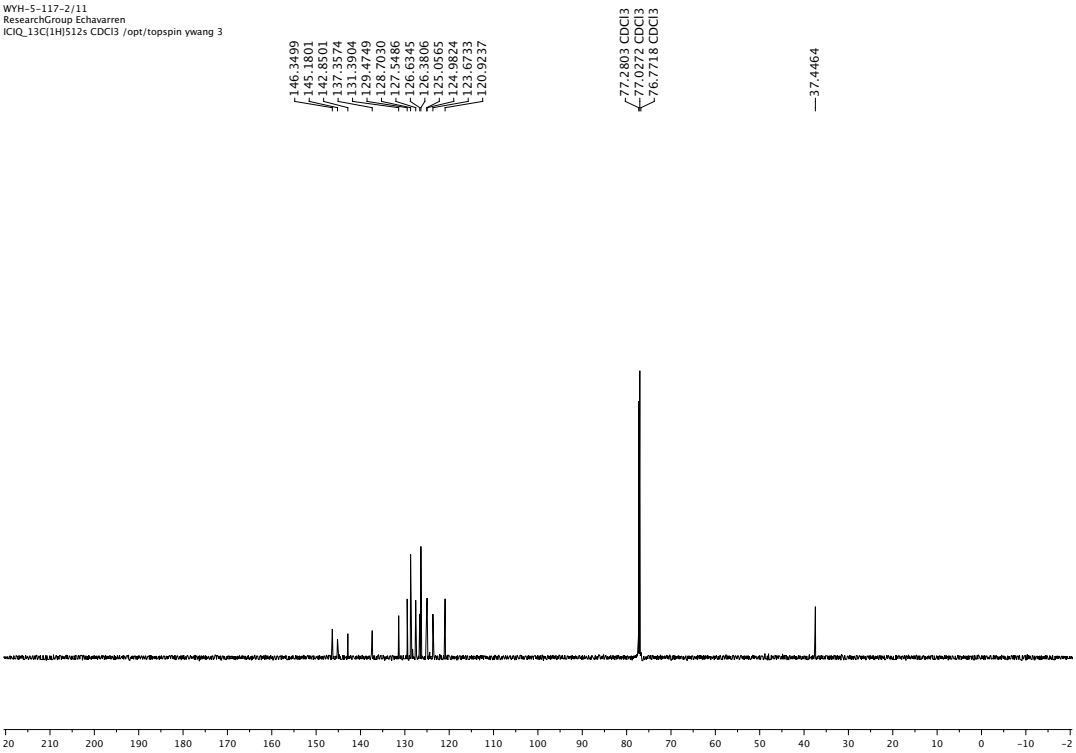


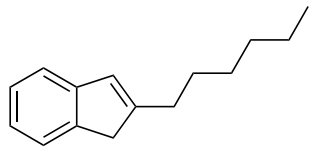


WYH-5-117-2/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 3

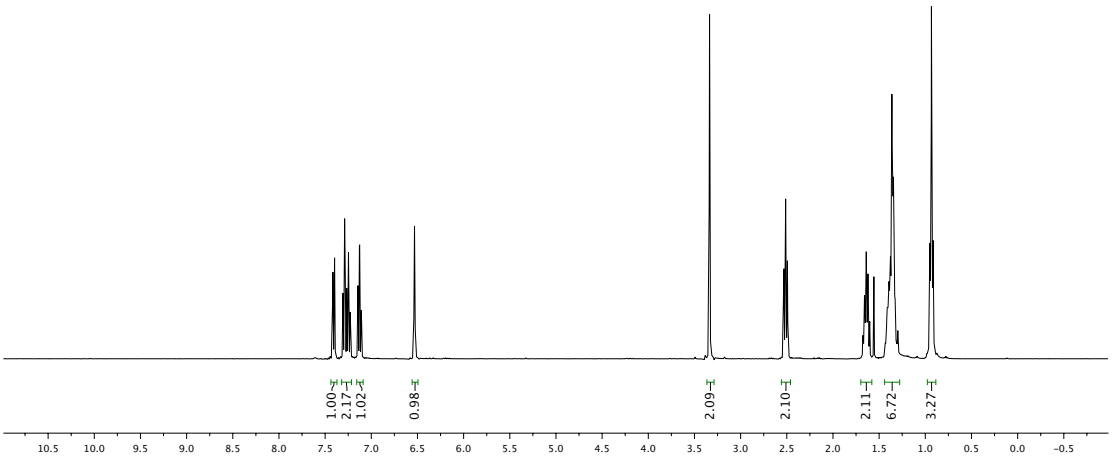


WYH-5-117-2/11
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 3

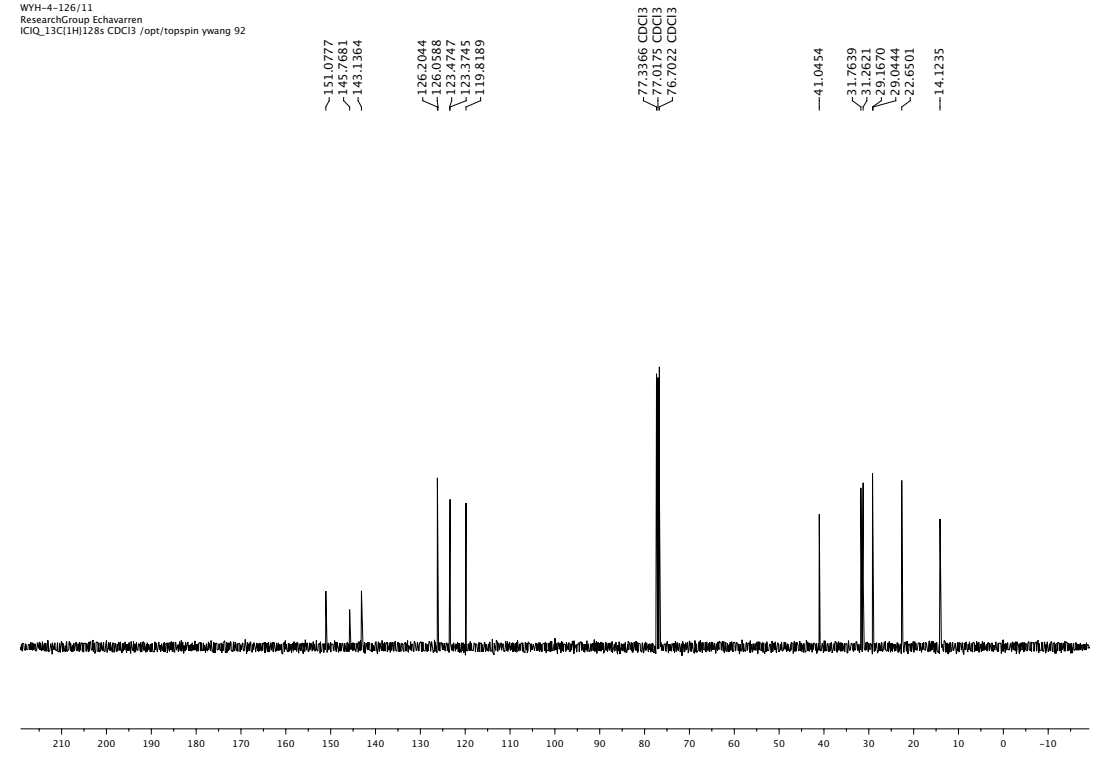


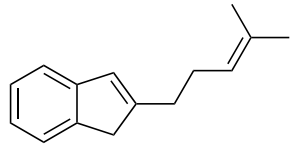


WYH-4-126/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 92

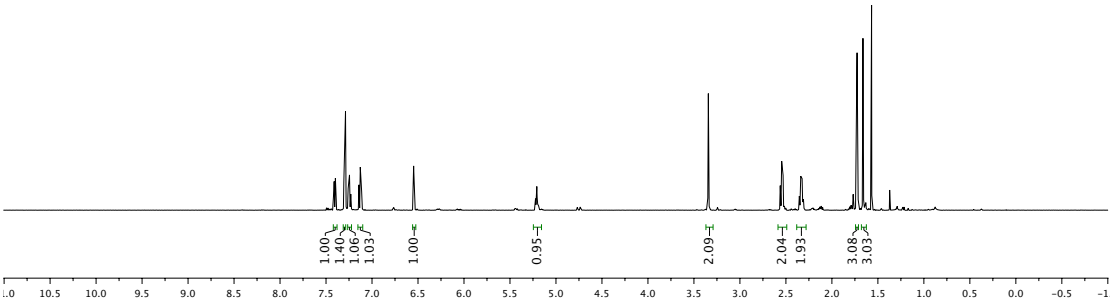


WYH-4-126/11
ResearchGroup Echavarren
ICIQ_13C{1H}128s CDCl3 /opt/topspin ywang 92





WYH-5-126-2/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 20



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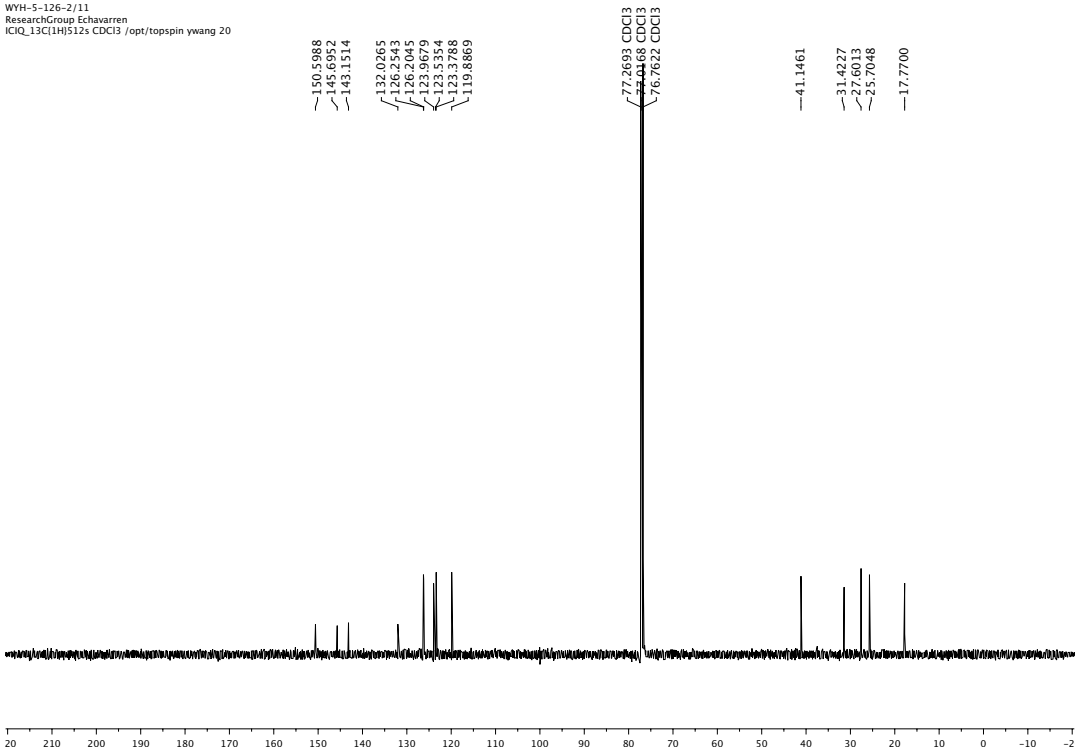
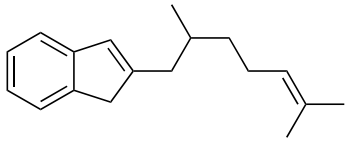
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 20





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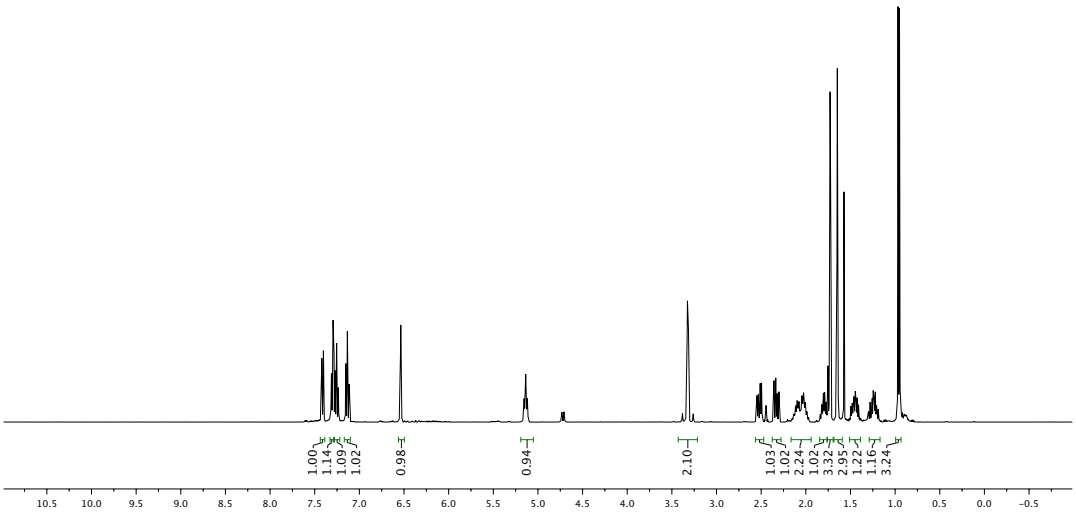
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 65



WYH-9-8-8.11.fid
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 65

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143.2769
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123.5014
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77.3424 CDCl3
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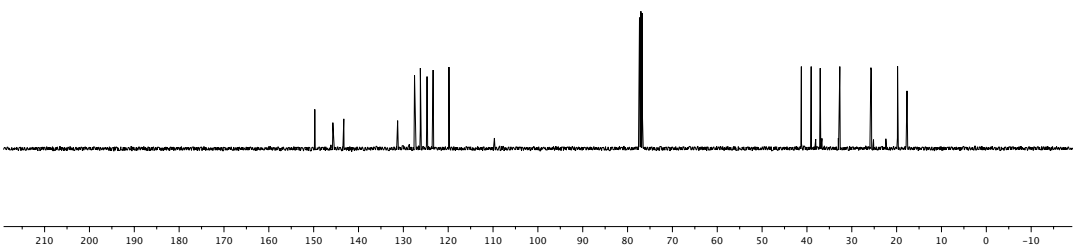
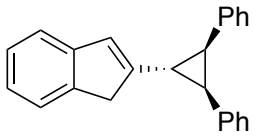
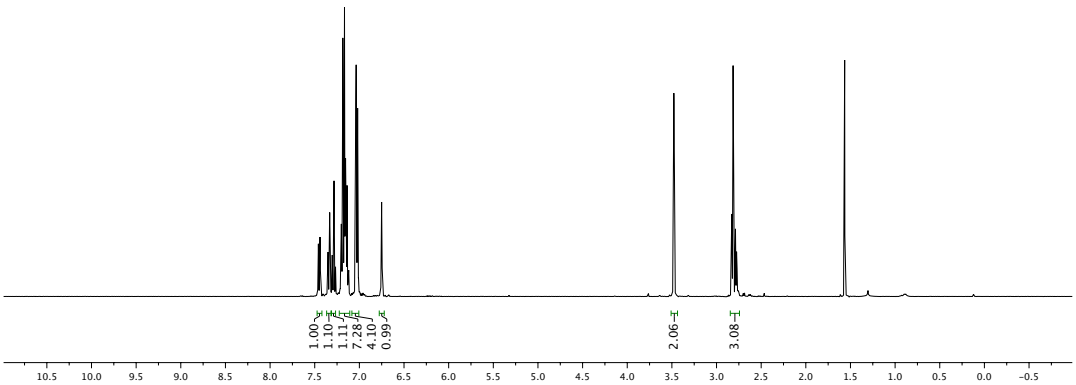




WYH-9-14.10.fid
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 77



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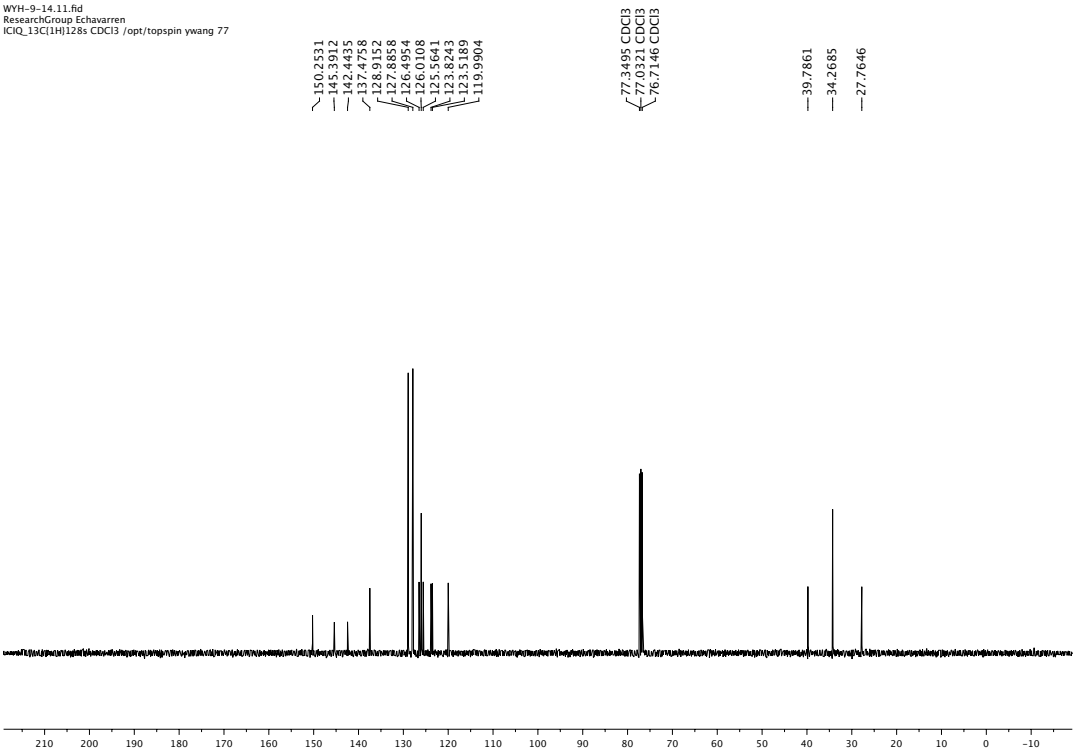
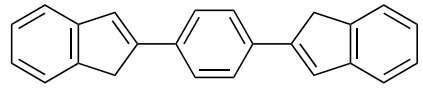
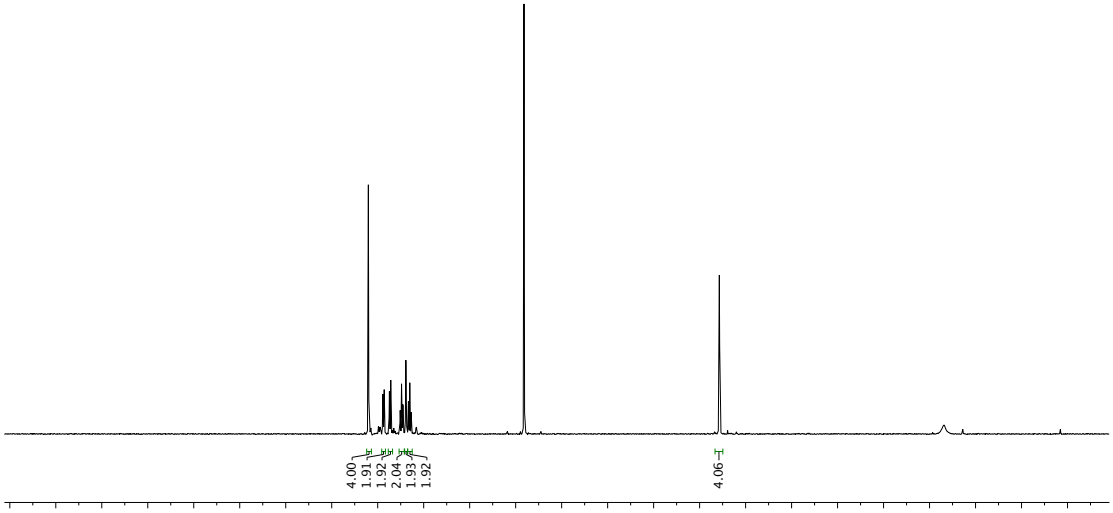
ResearchGroup Echavarren
ICIQ_13C{1H}128s CDCl3 /opt/topspin ywang 77

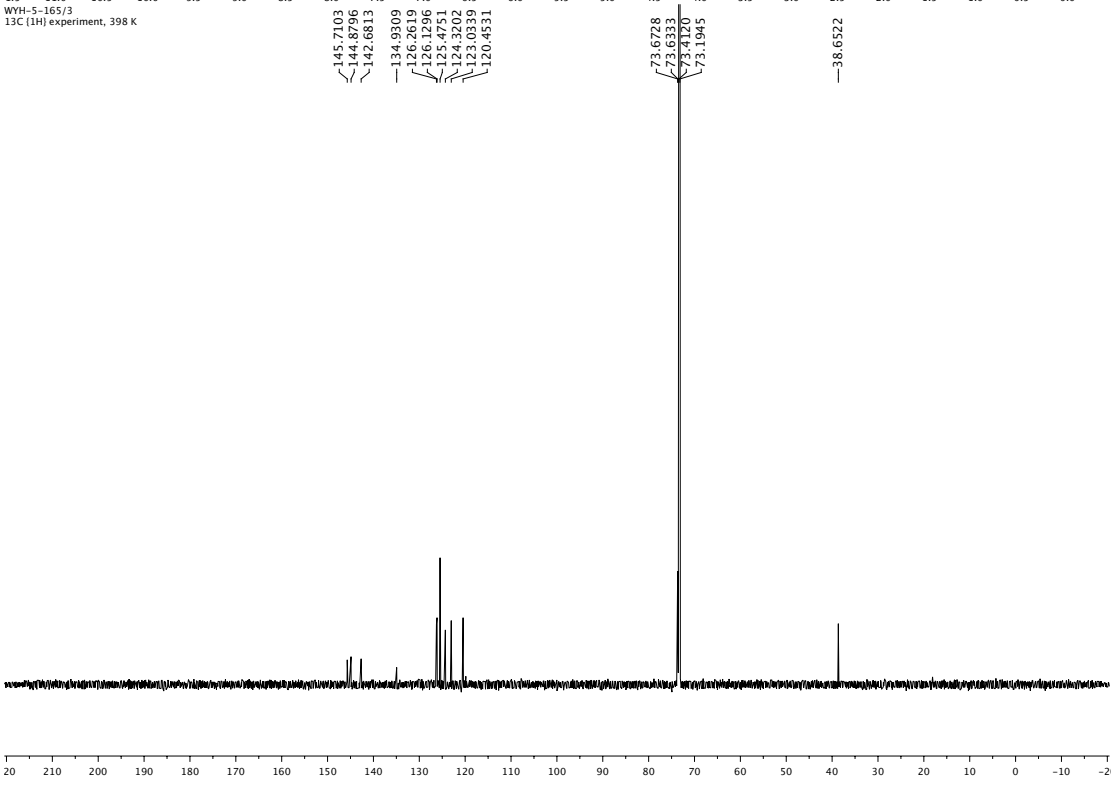


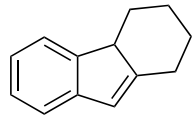


WYH-5-165/2
proton 398 K

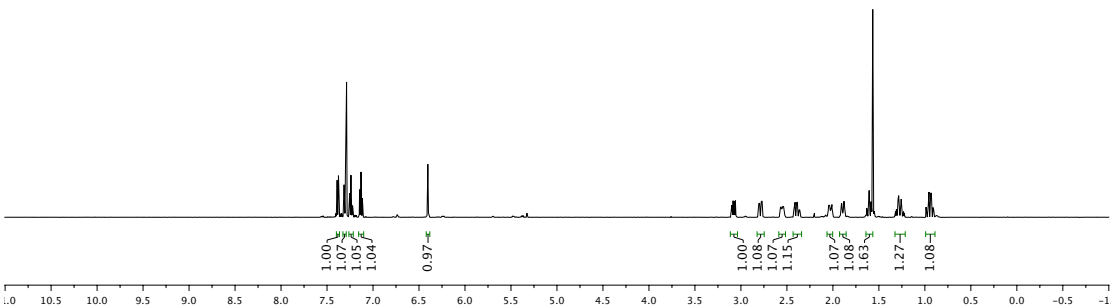


WYH-5-165/3
13C {1H} experiment, 398 K

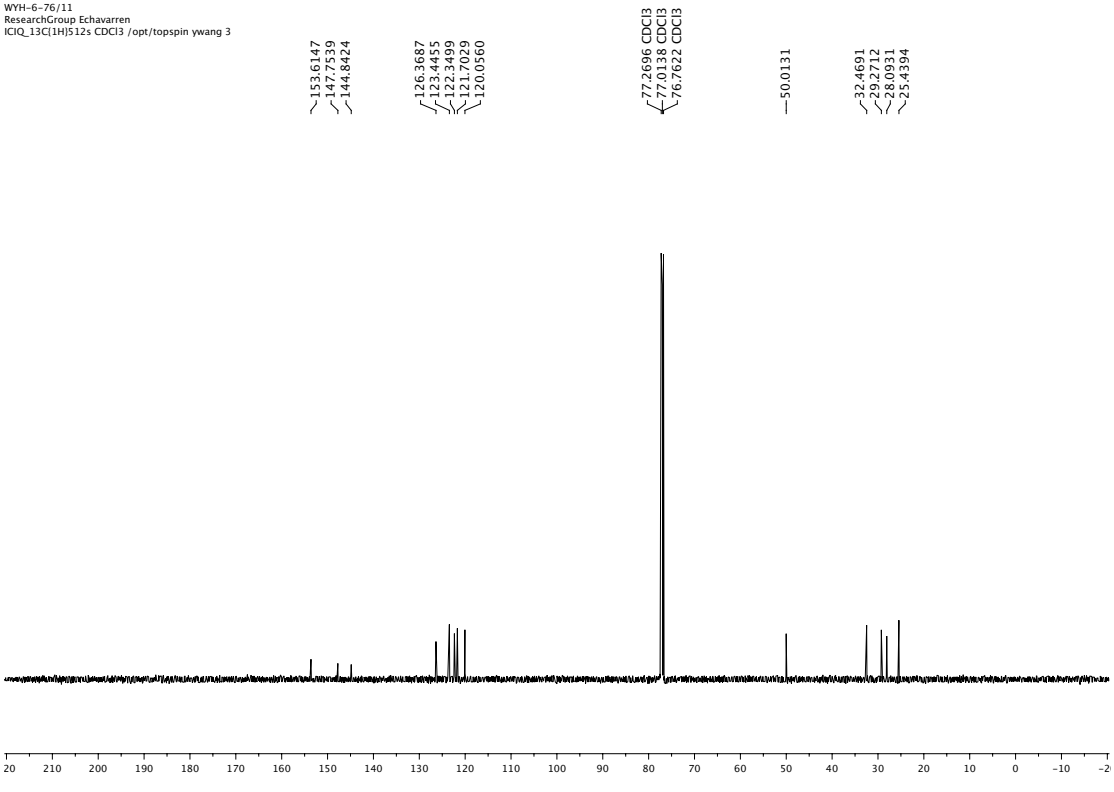


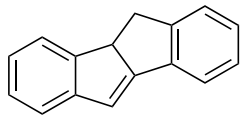


WYH-6-76/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 3



WYH-6-76/11
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 3





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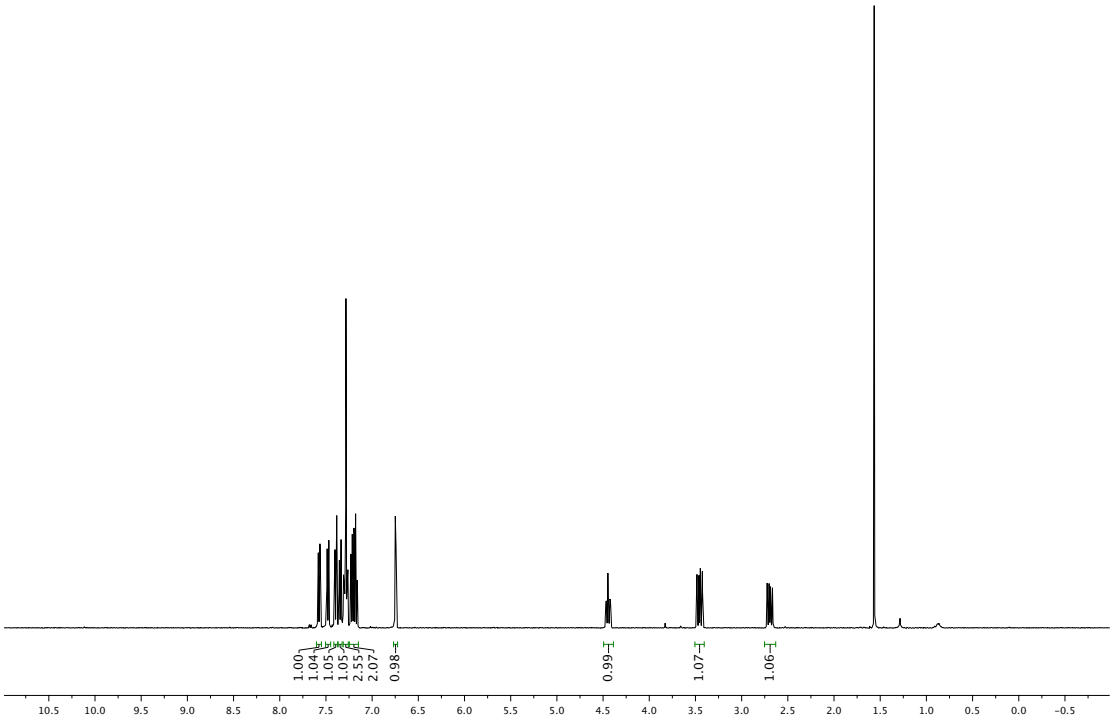
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 81



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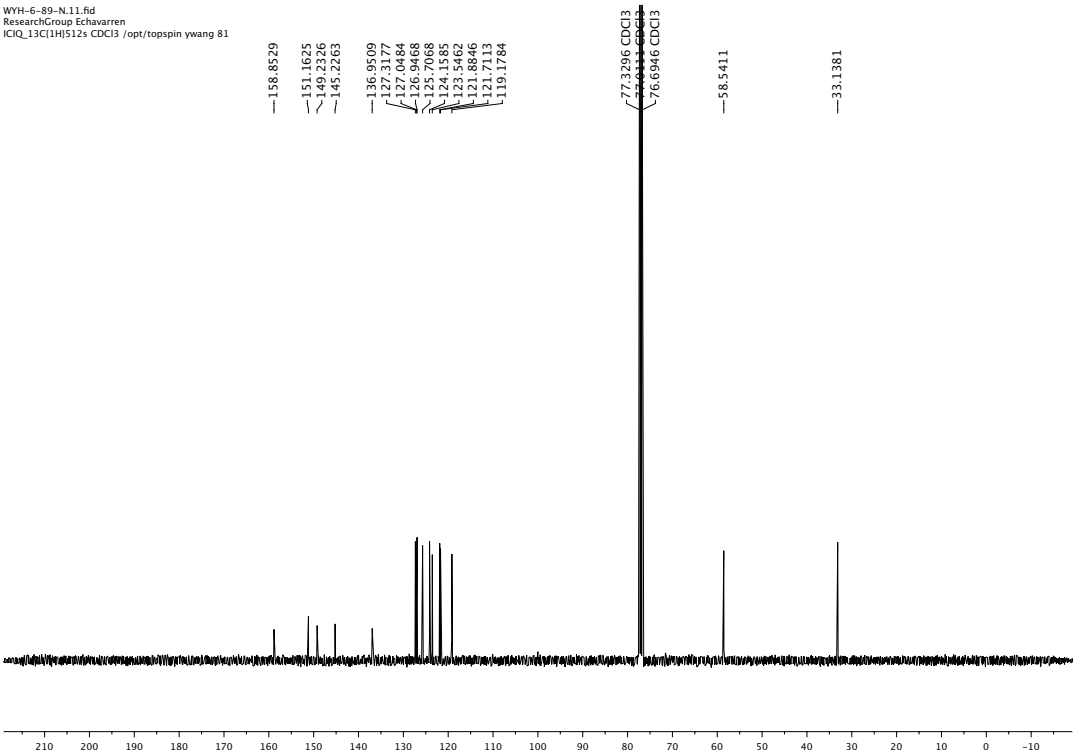
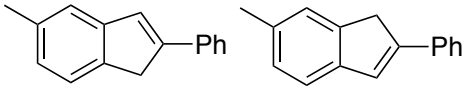
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 81

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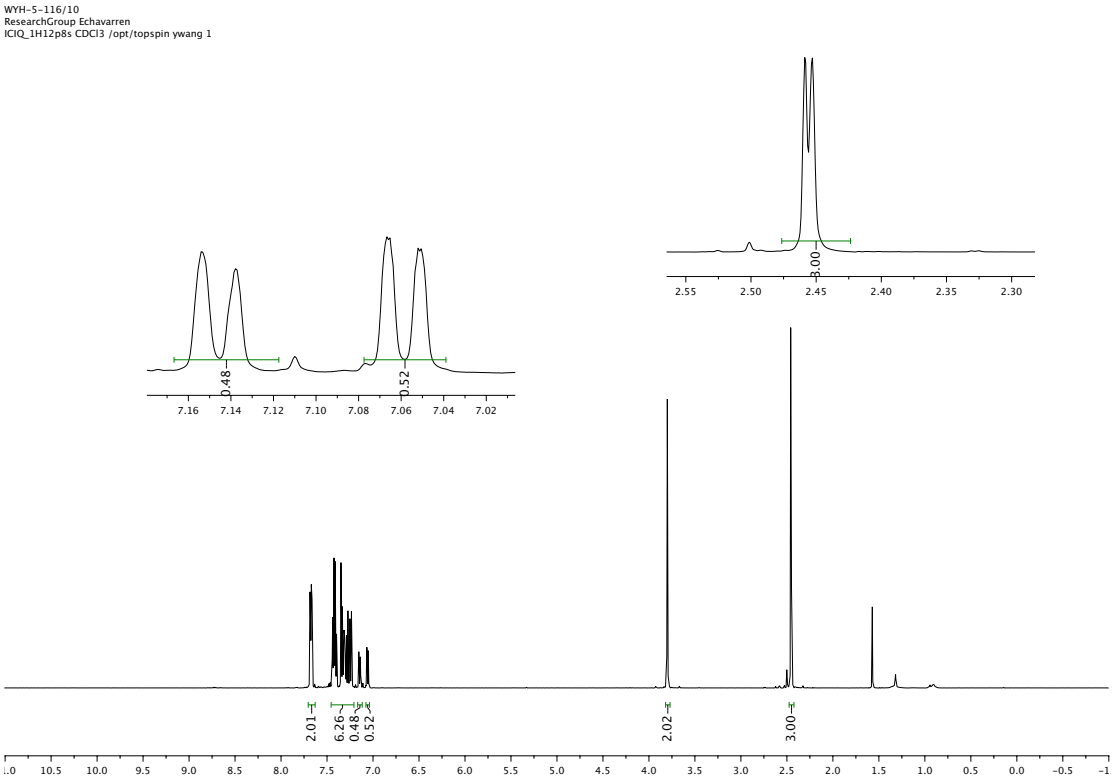
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ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 1
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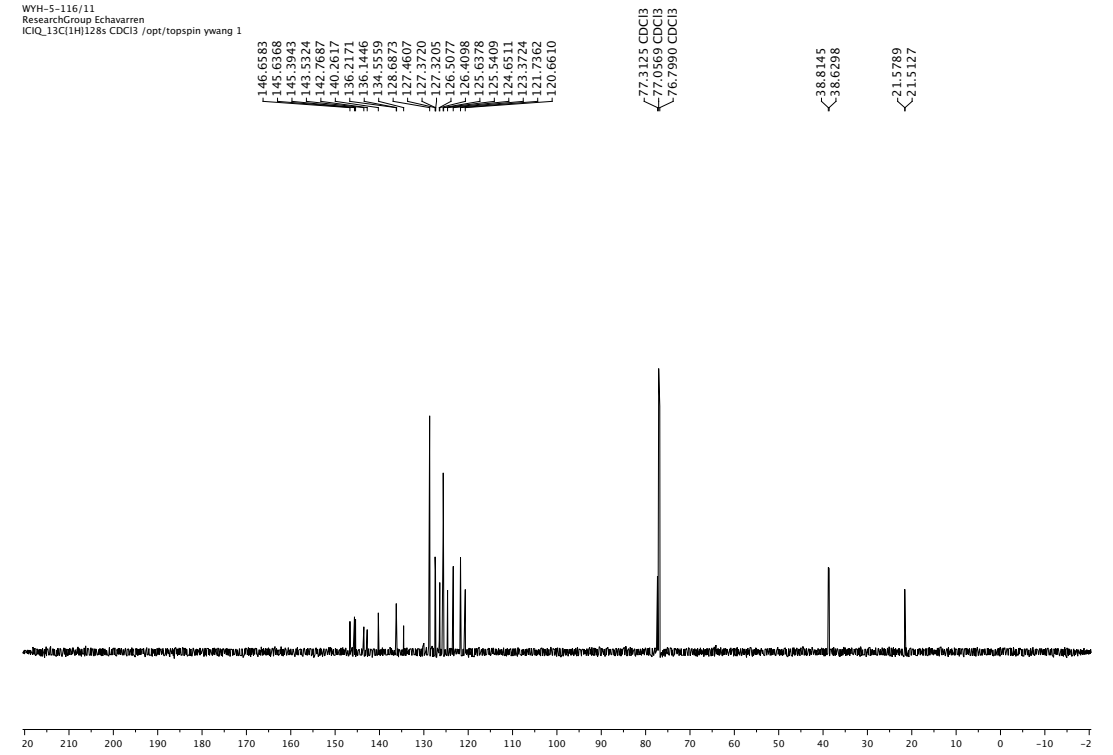
6.26
0.48
0.52
2.02
3.00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ResearchGroup Echavarren
ICIQ_13C{1H}128s CDCl3 /opt/topspin ywang 1
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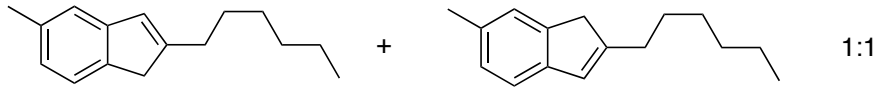

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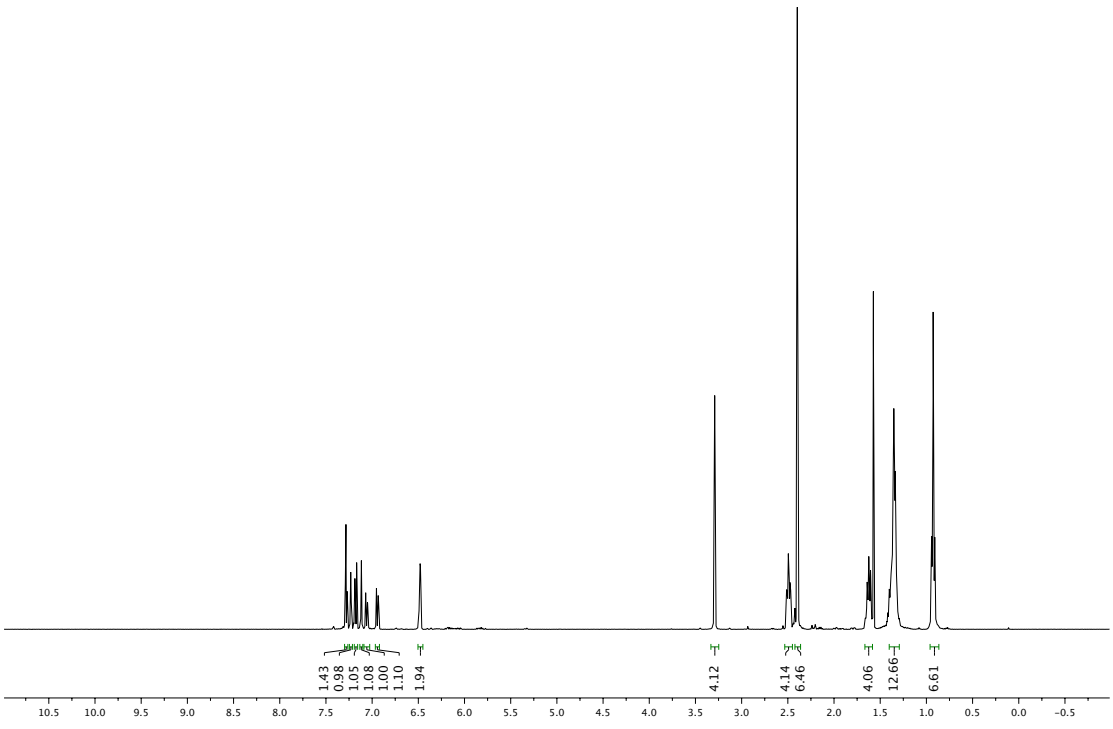
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 108



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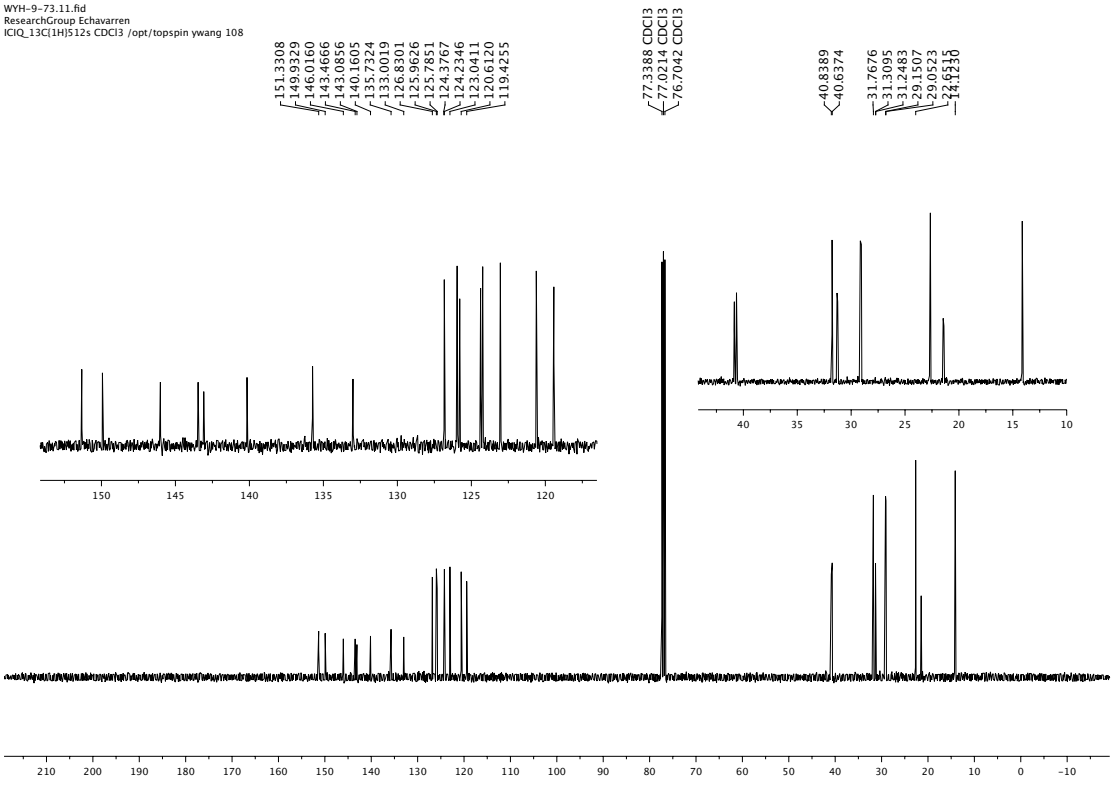
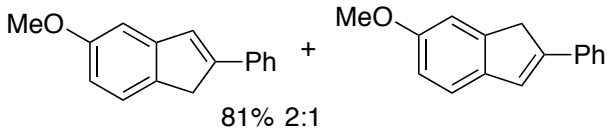
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 108





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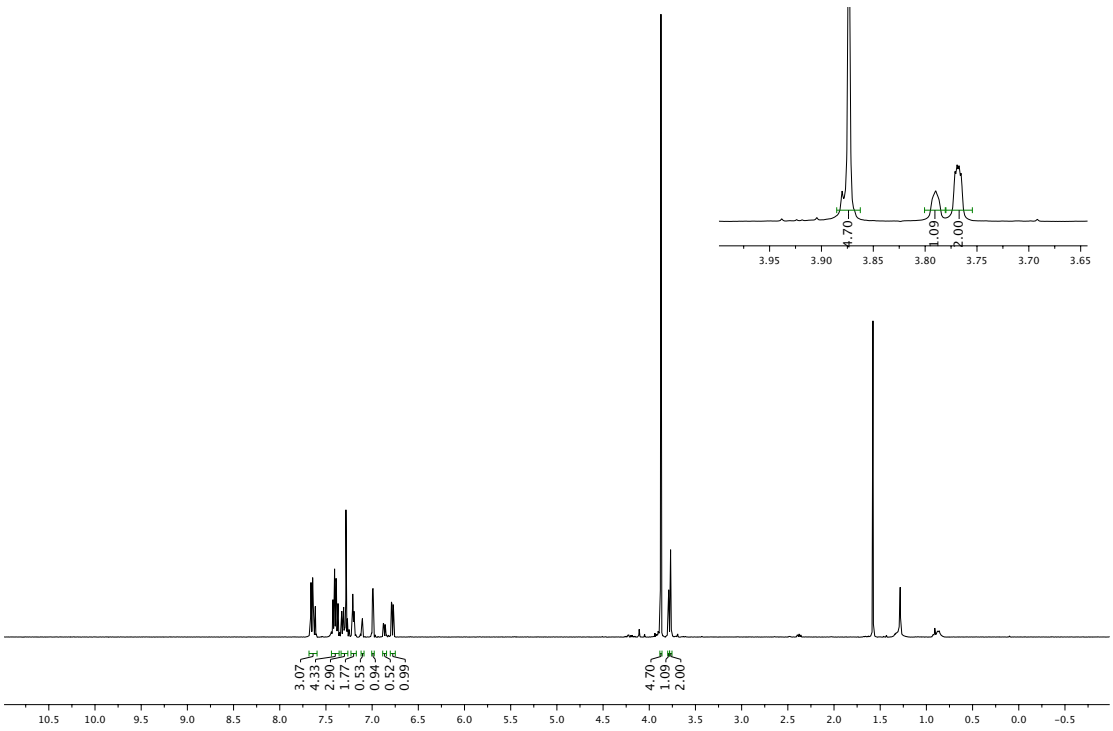
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 92



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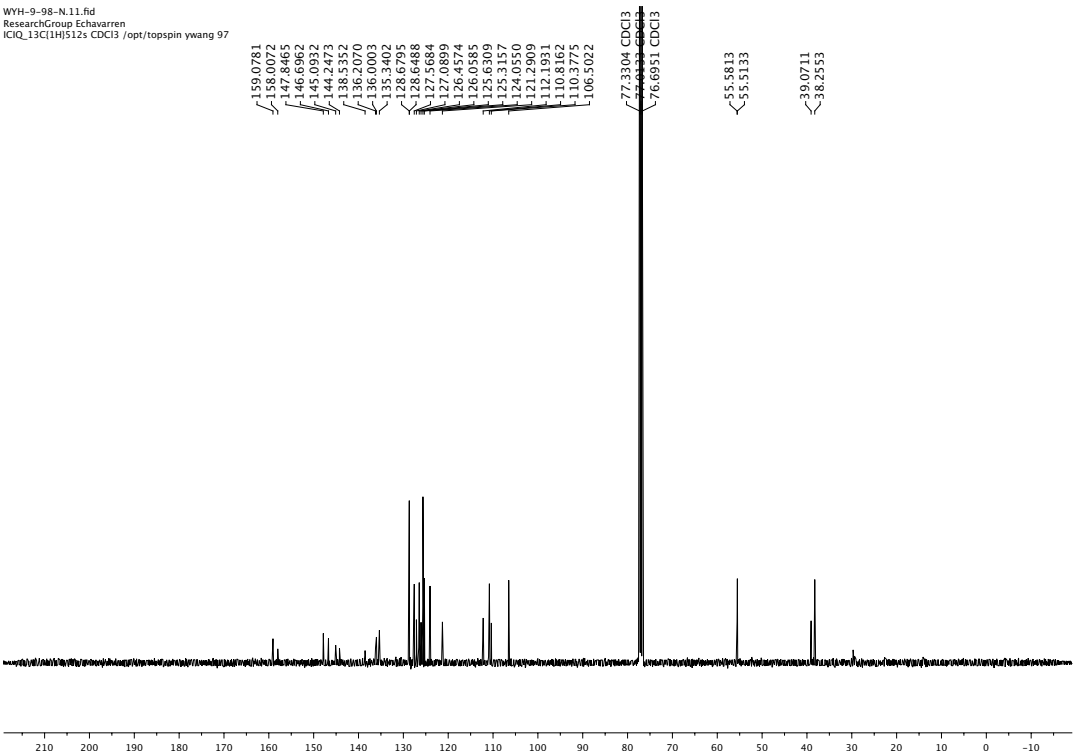
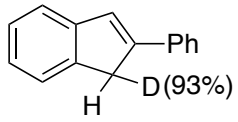
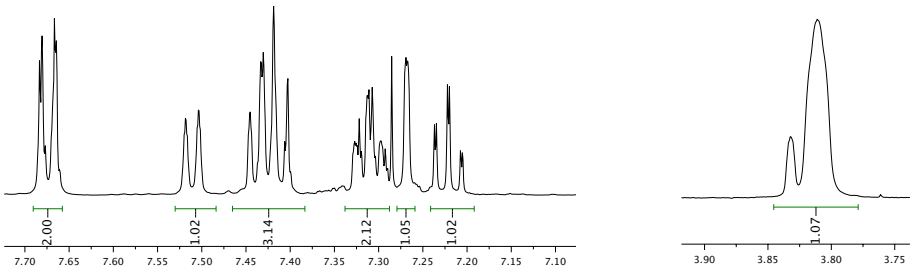
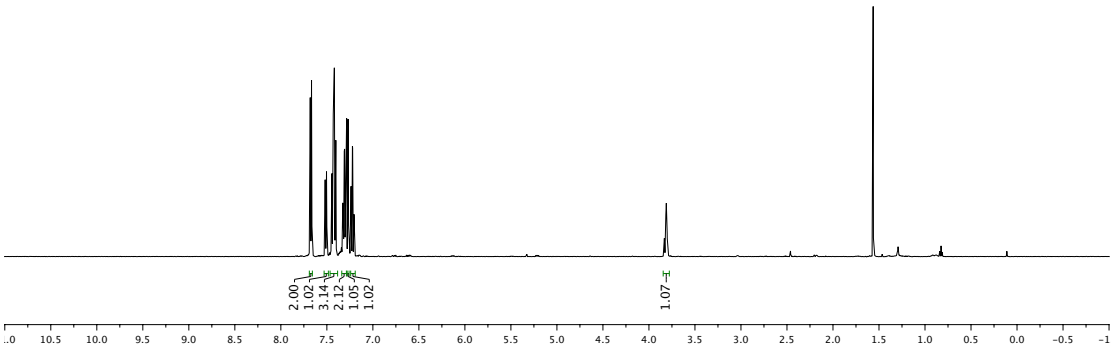
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 97





WYH-4-143/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 13





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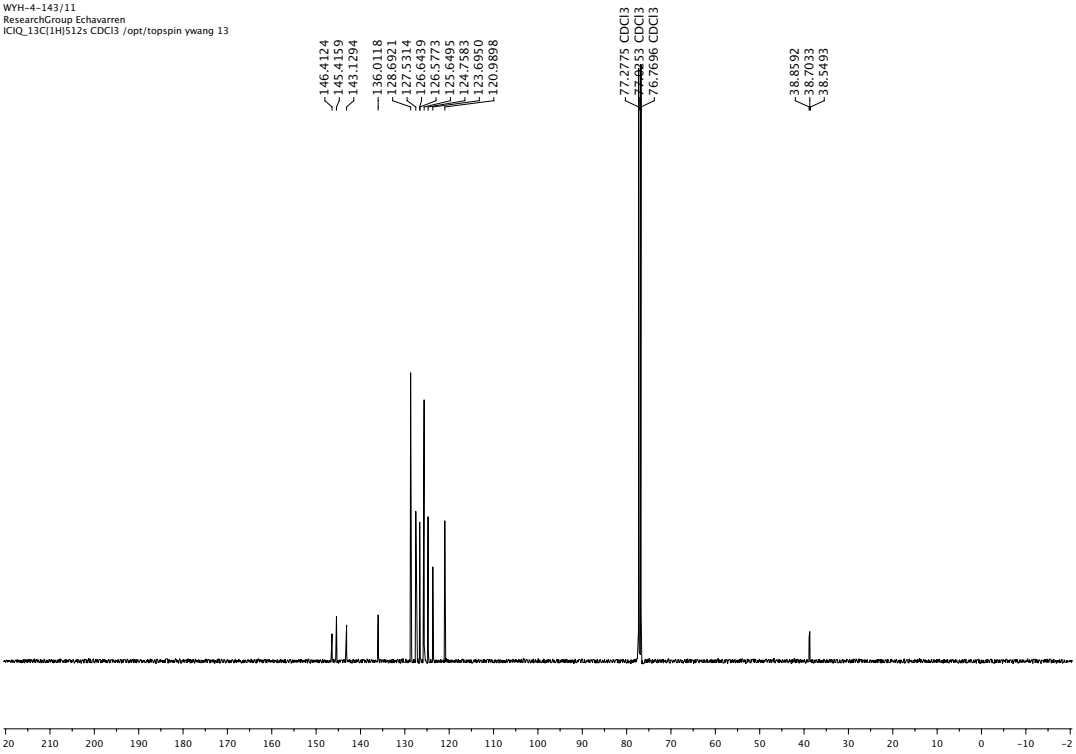
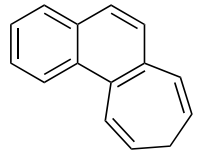
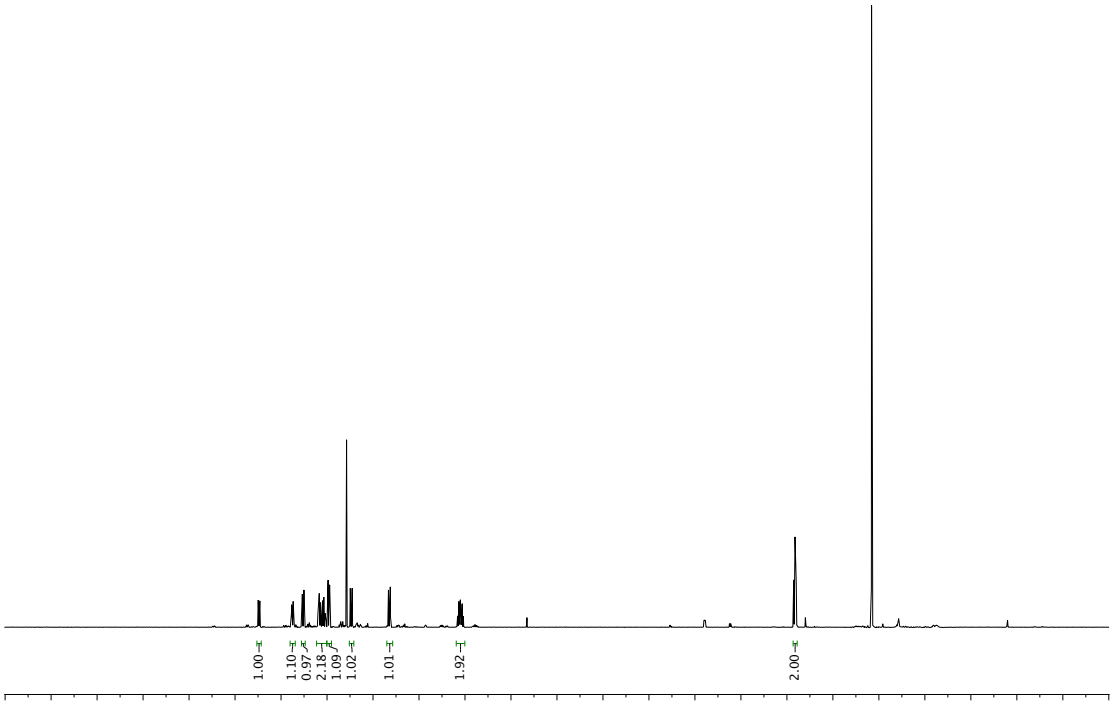
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 13





WYH-5-139-1-N/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 41



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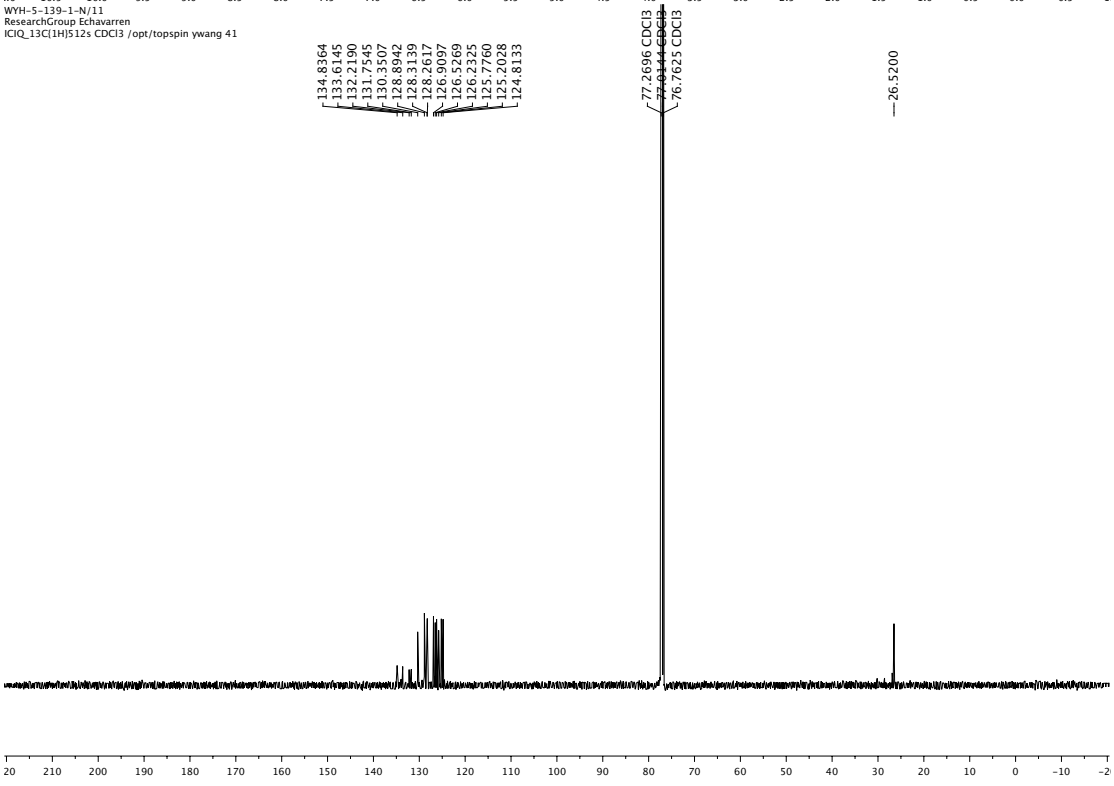
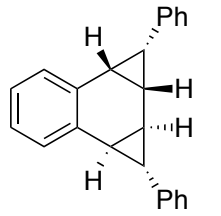
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 41





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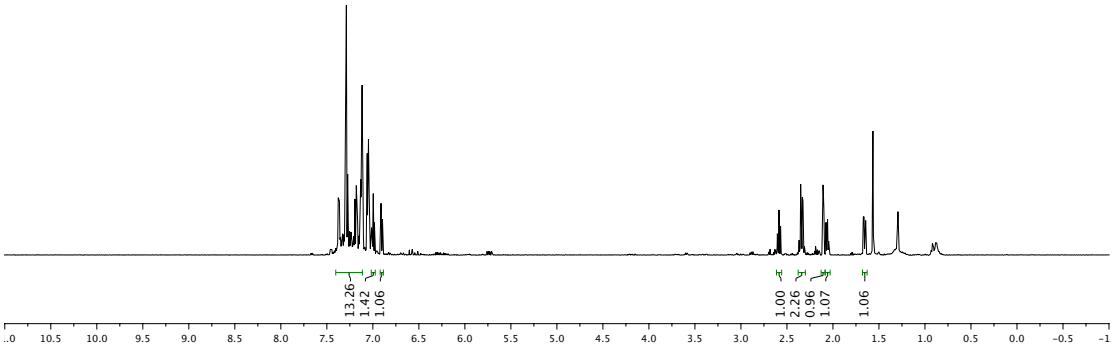
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 15



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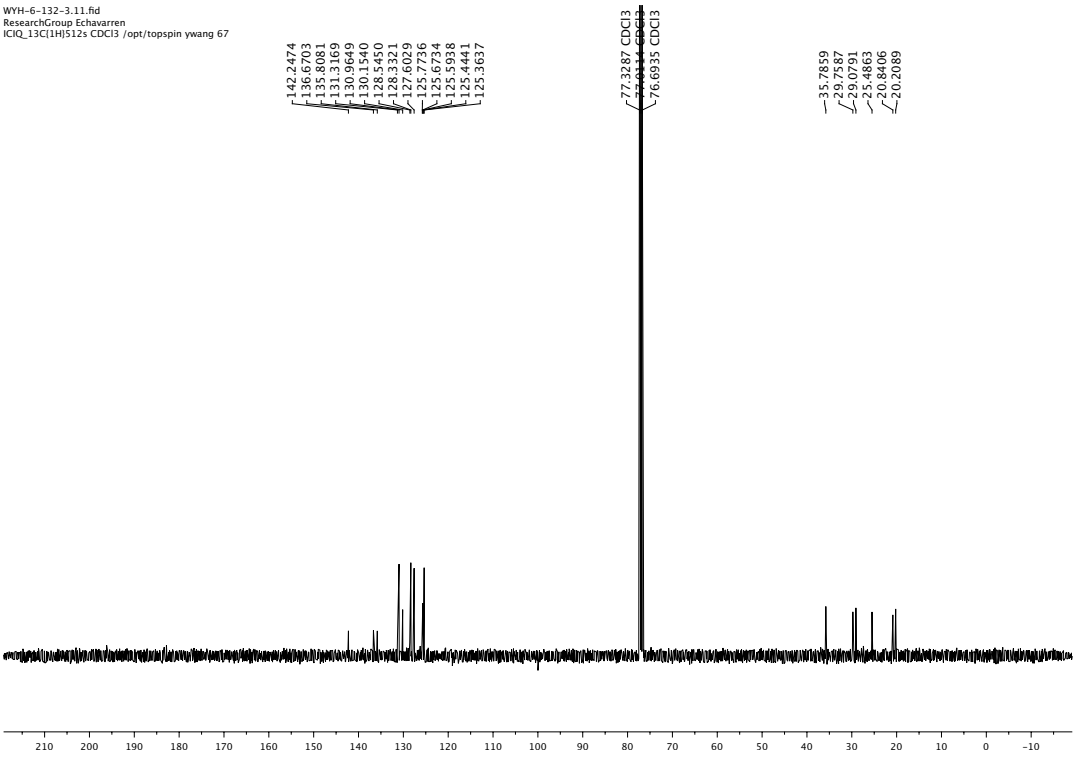
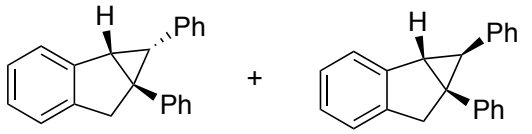
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 67





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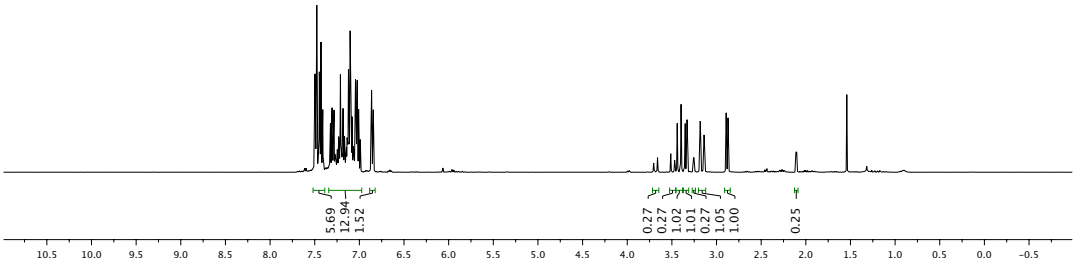
WYH-6-83-N.10.fid
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 86



WYH-6-83-N.11.fid
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 86

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138.7378
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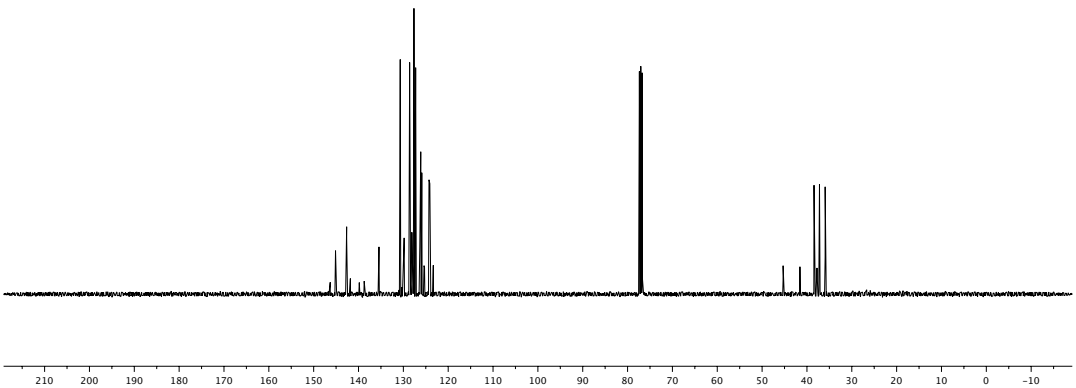
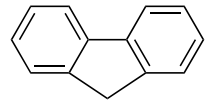
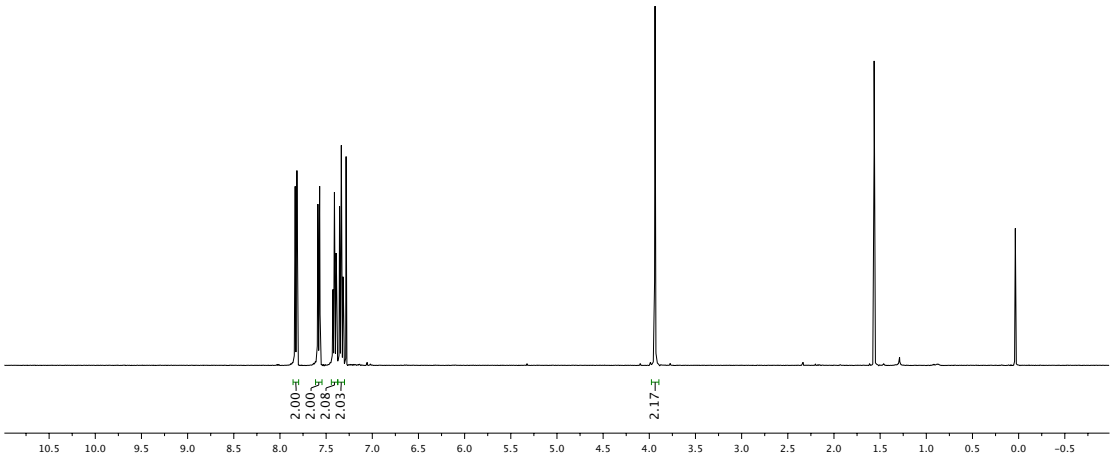
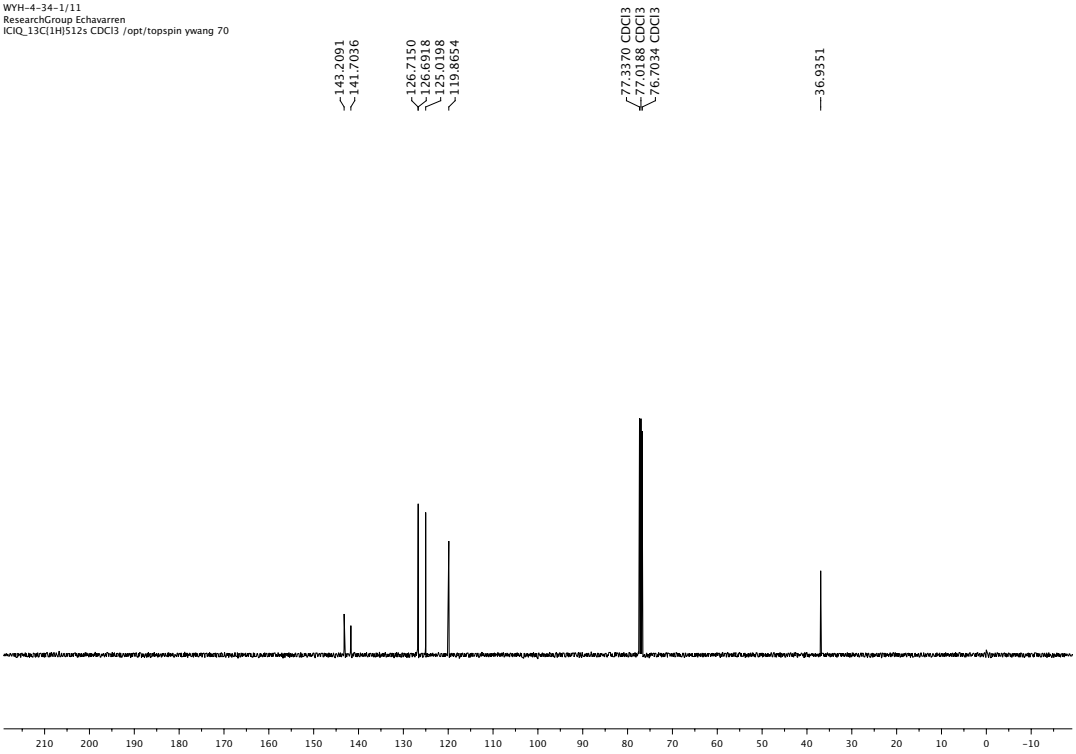


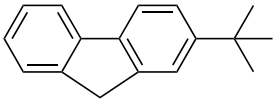


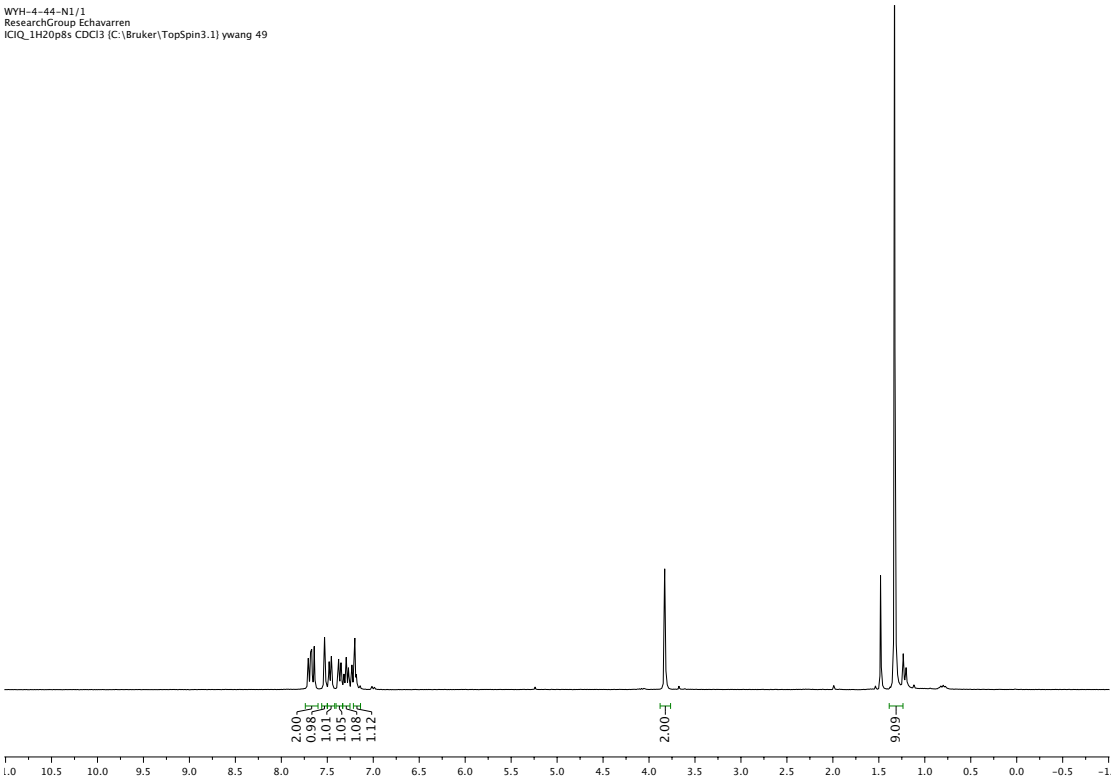
WYH-4-34-1/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 70



WYH-4-34-1/11
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 70



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ResearchGroup Echavarren
ICIQ_1H20p8s CDCl3 {C:\Bruker\TopSpin3.1} ywang 49
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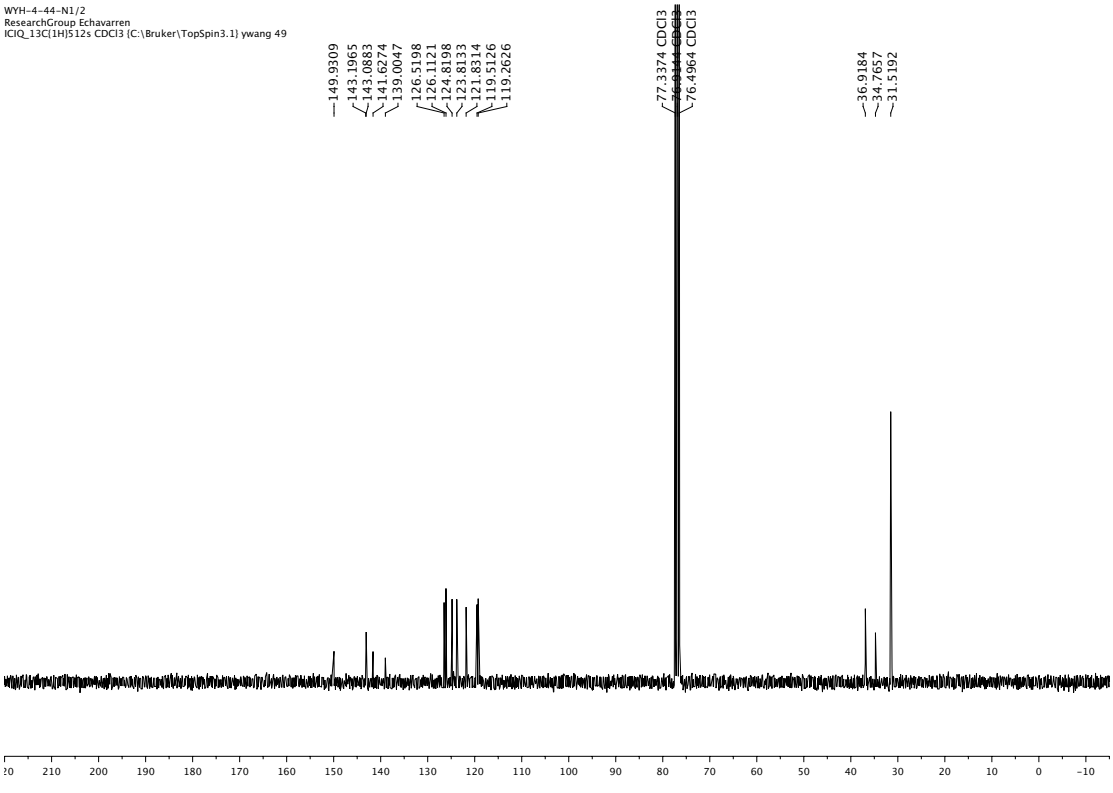
1.01
1.05
1.08
1.12
2.00
9.09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ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 {C:\Bruker\TopSpin3.1} ywang 49
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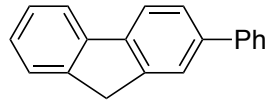
143.1965
143.0883
141.6274
139.0047
126.5198
126.1121
124.8198
123.8133
121.8314
119.5126
119.2626
77.3374 CDCl3
76.4964 CDCl3
36.9184
34.7657
31.5192



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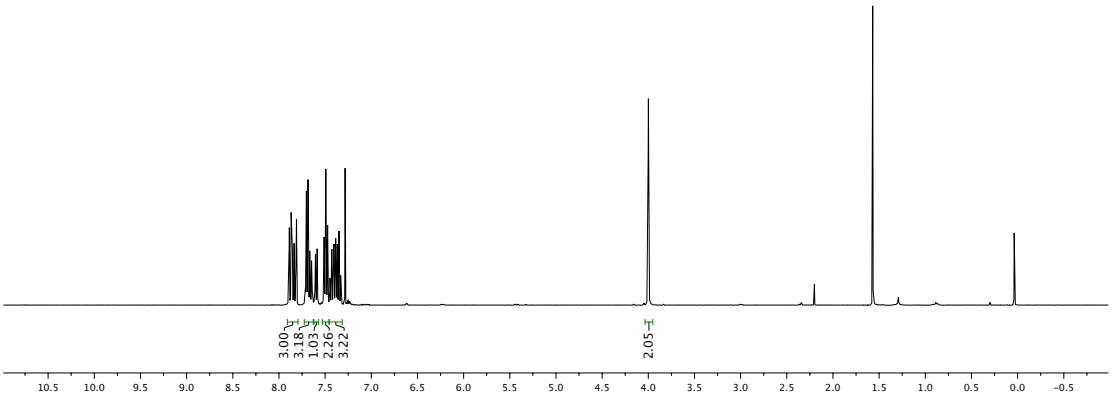
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 70



WYH-4-45/11
ResearchGroup Echavarren
ICIQ_13C(1H)512s CDCl3 /opt/topspin ywang 70

143.8928
143.4642
141.5006
141.3984
140.9335
139.8799
128.7725
127.1876
127.1137
126.8296
126.7356
126.0019
125.0555
123.8059
120.1105
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77.0209 CDCl3
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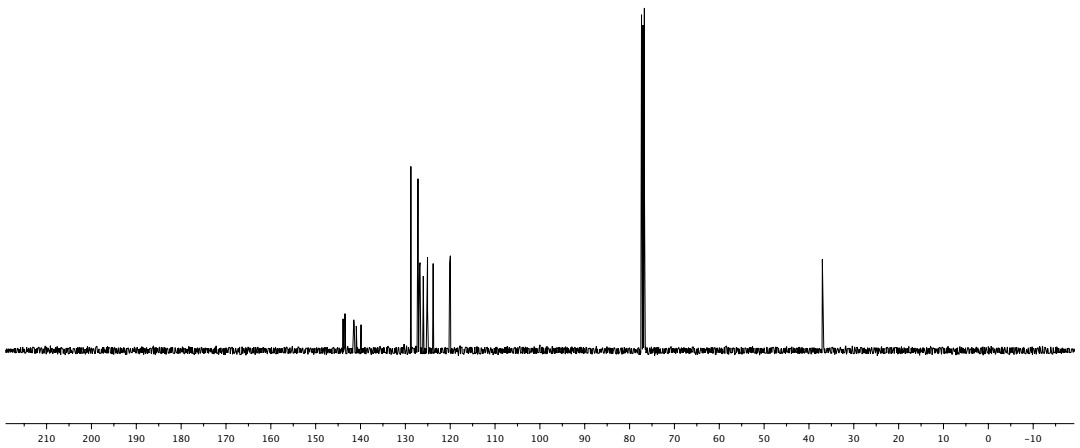
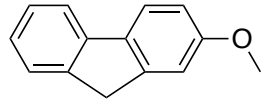
37.0149





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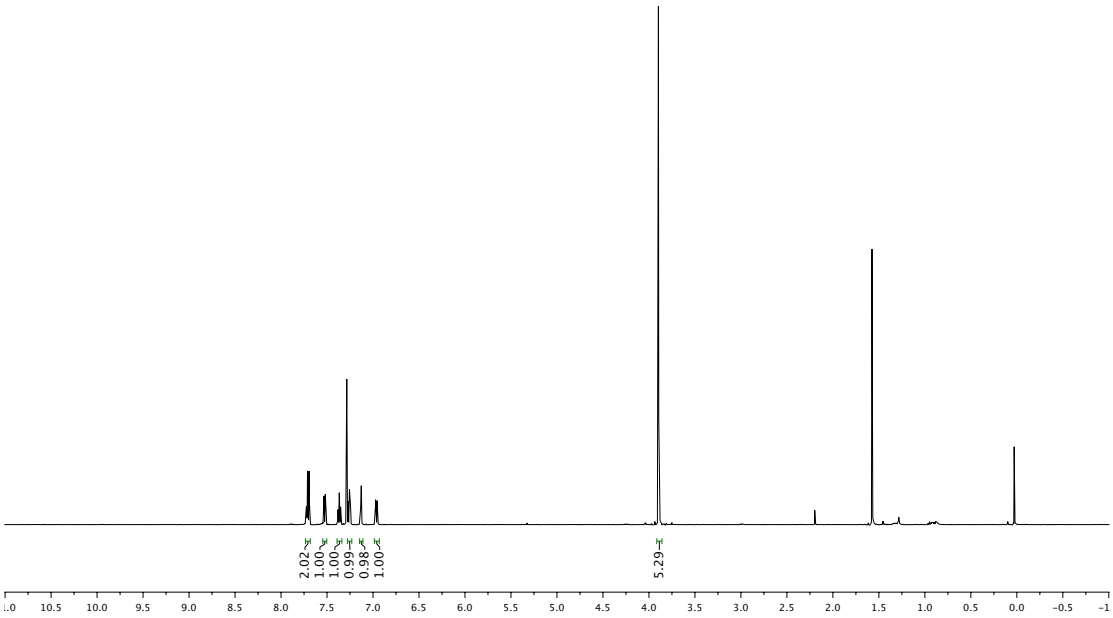
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 31



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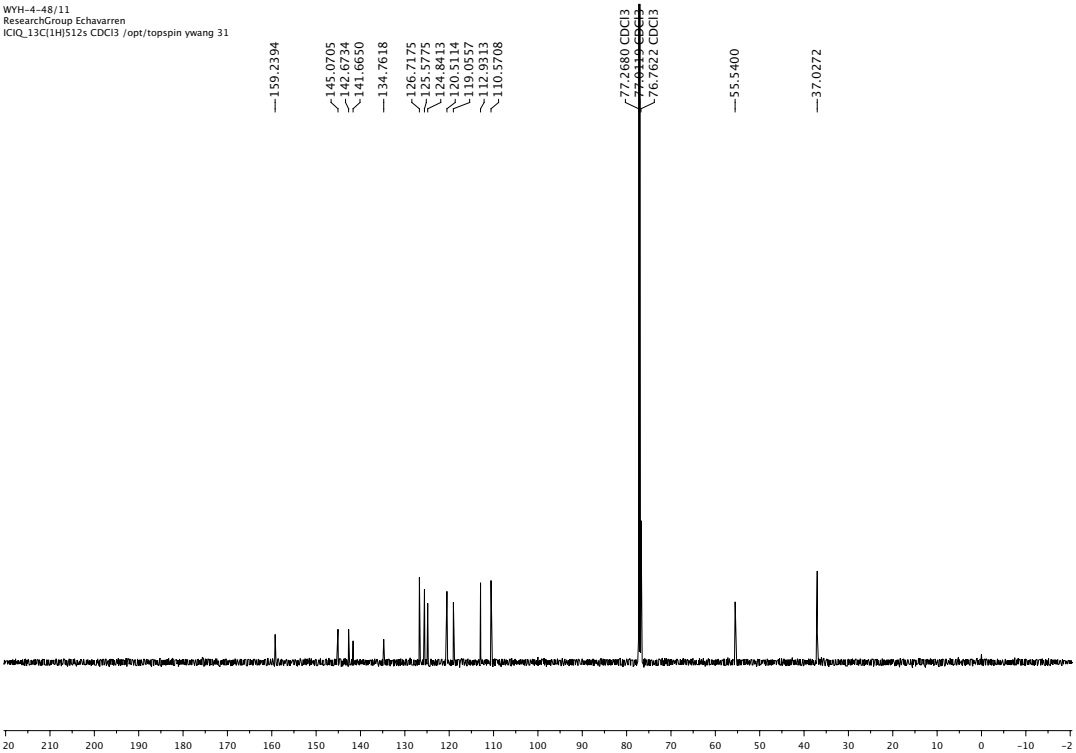
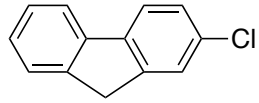
ResearchGroup Echavarren
ICIQ_13C(1H)512s CDCl3 /opt/topspin ywang 31





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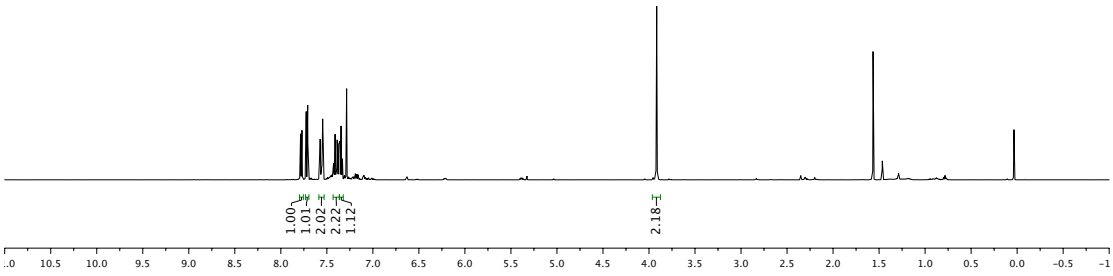
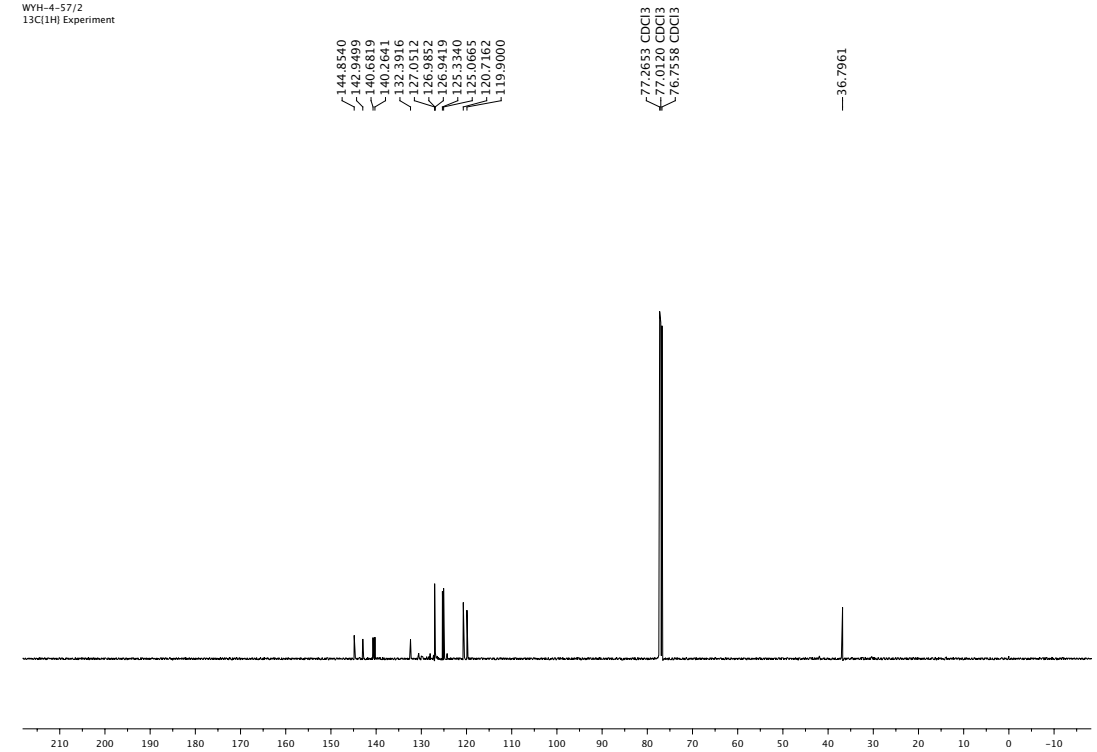
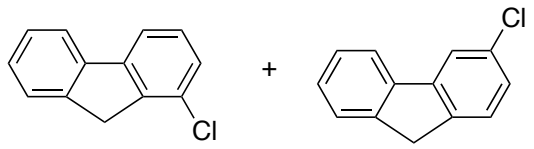
1H Experiment



WYH-4-57/2
13C{1H} Experiment





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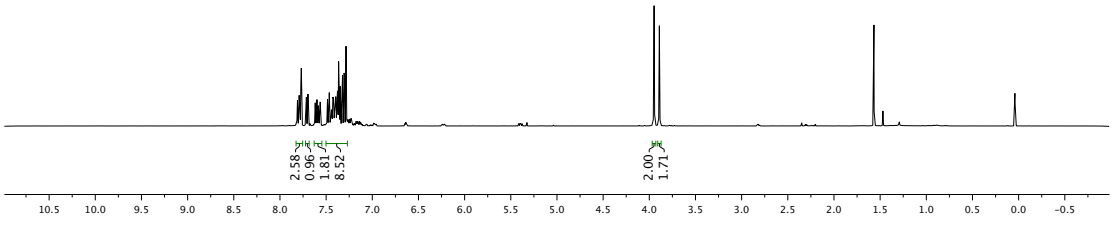
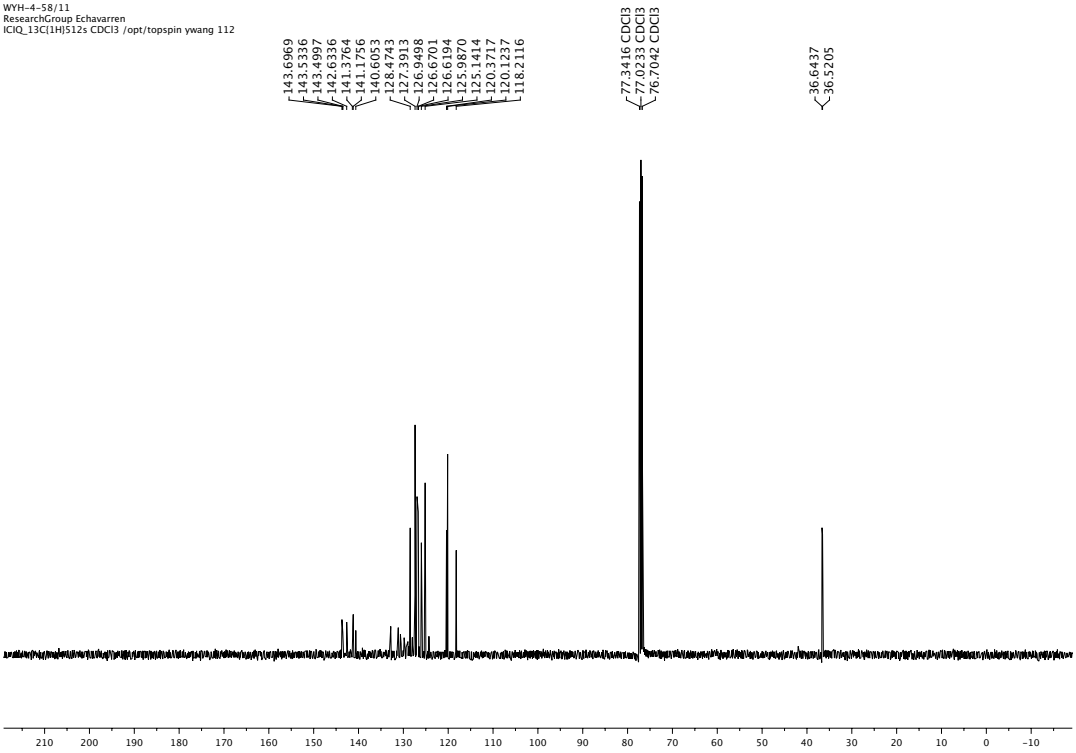
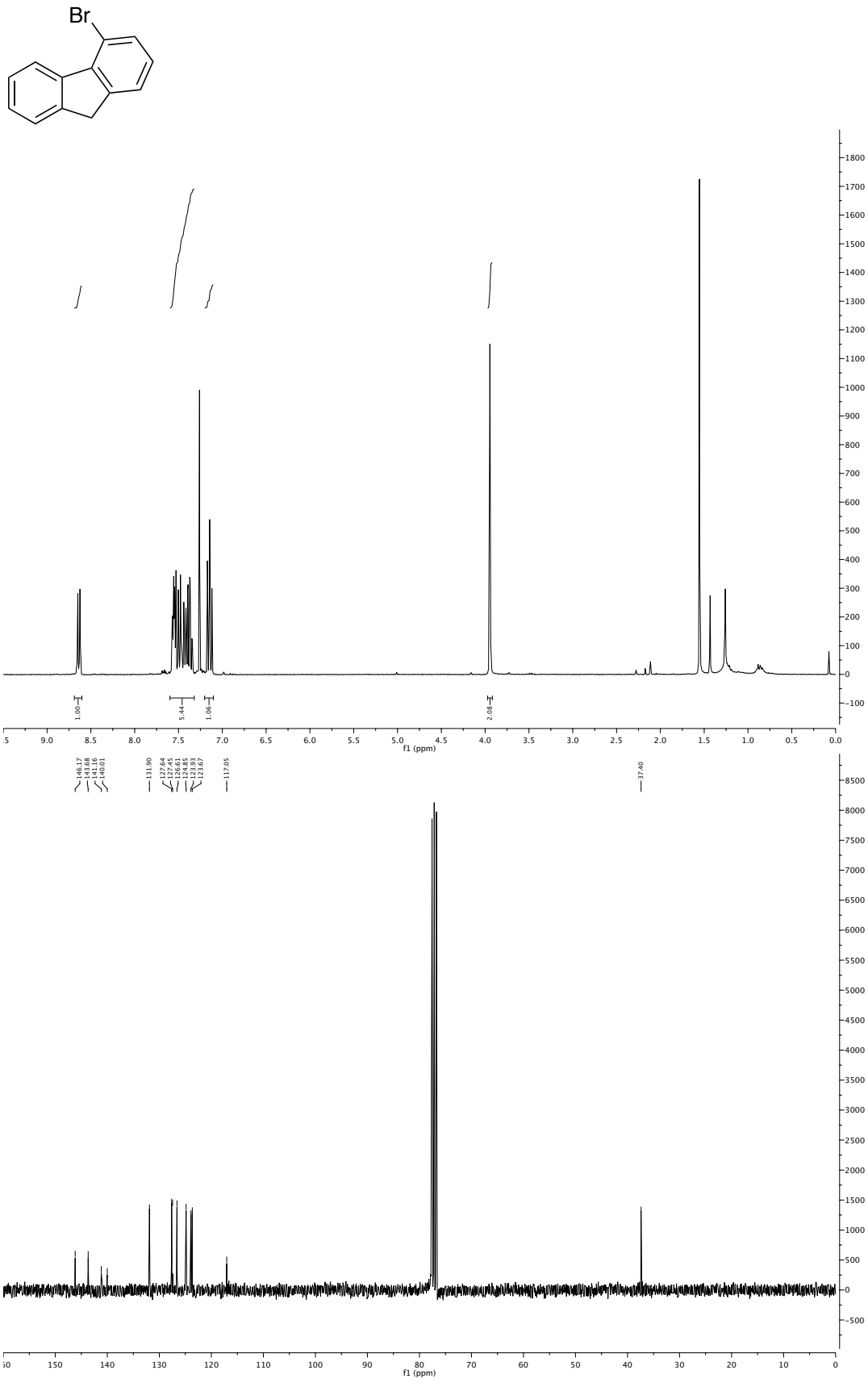
WYH-4-58/10
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 112



WYH-4-58/11
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 112

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5.44
1.06
2.08
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143.68
141.16
140.01
131.90
127.64
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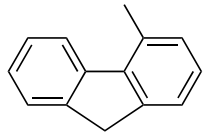
123.89
123.67
117.05
37.40
f1 (ppm)



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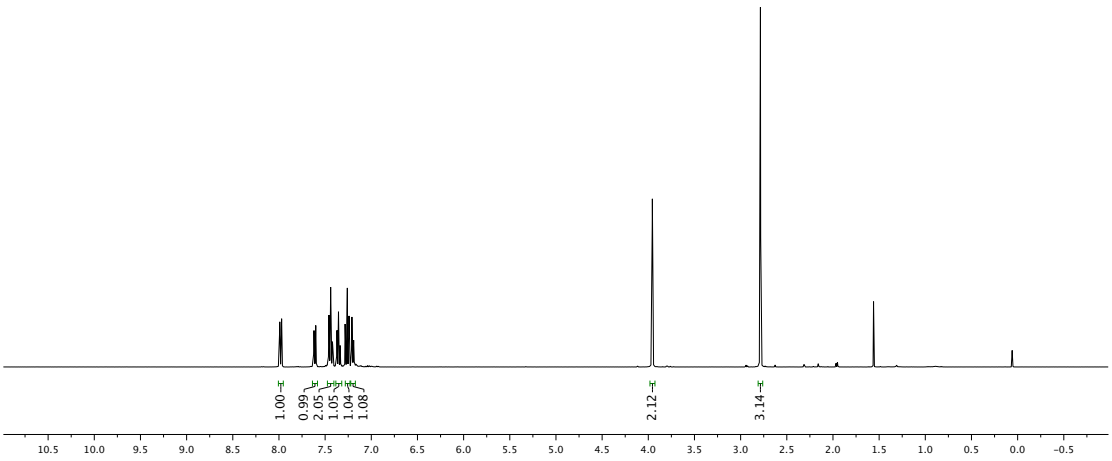
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 97



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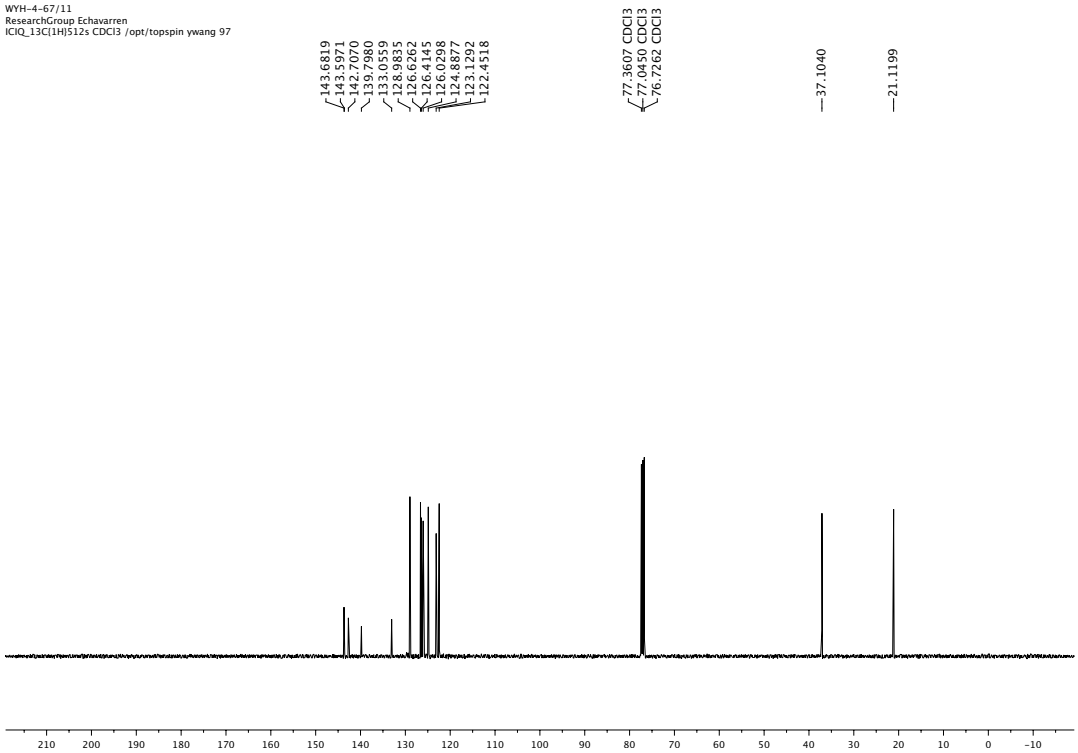
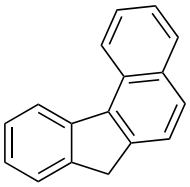
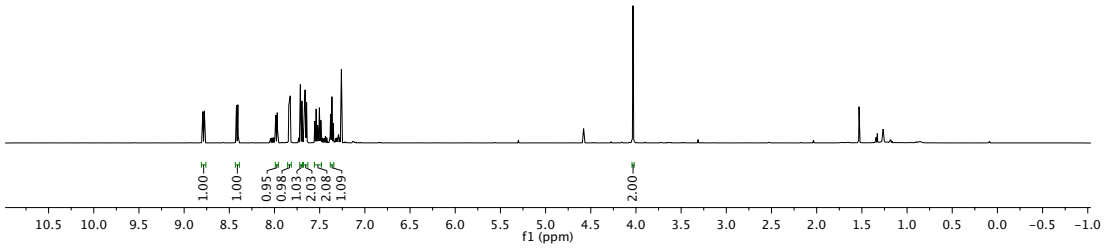
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 97

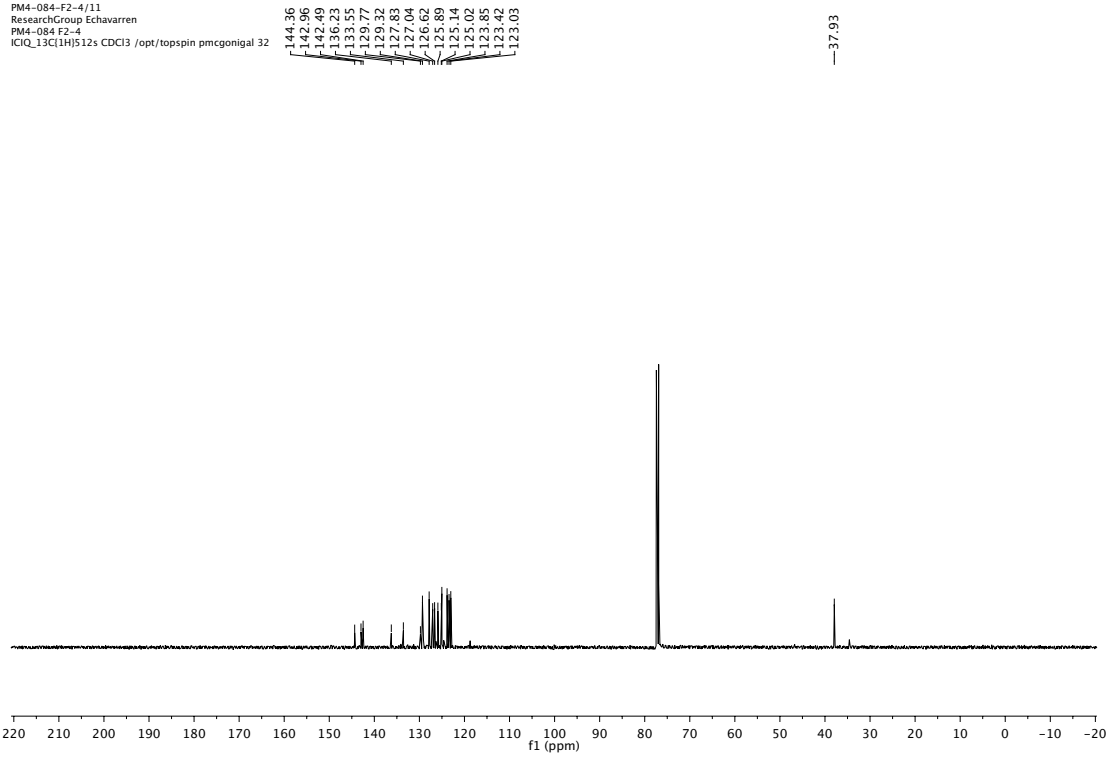


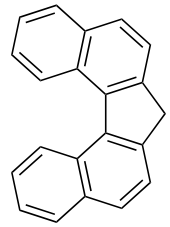


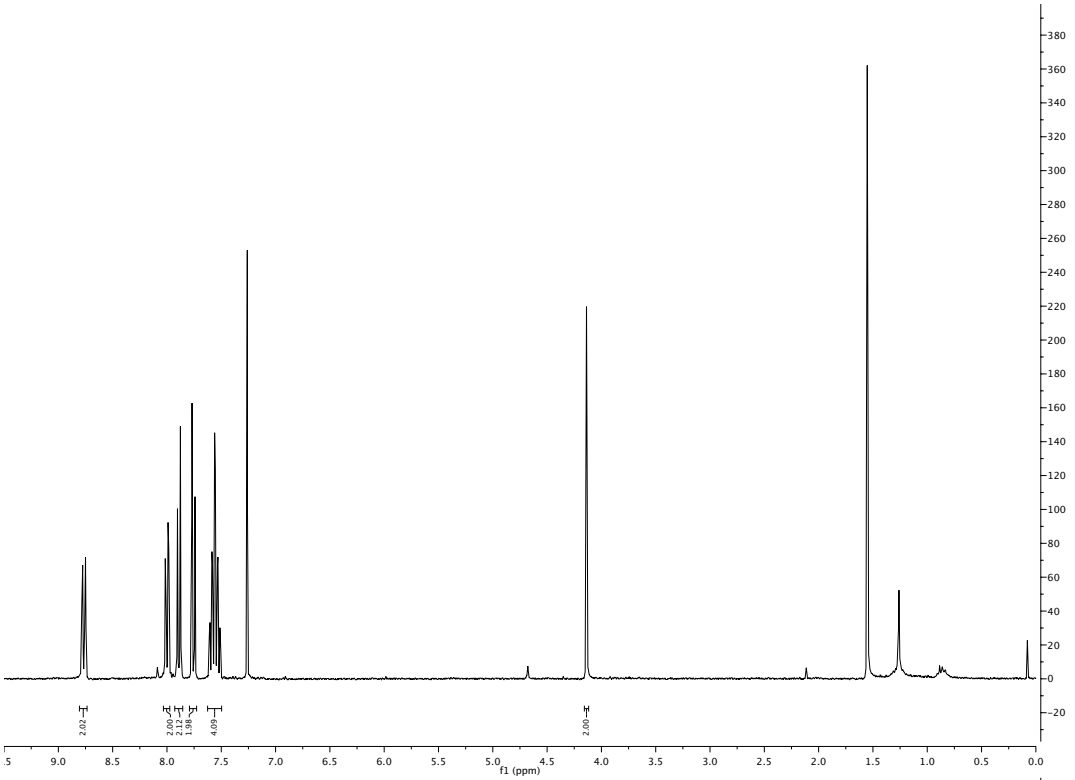
PM4-084-F2-4/10
ResearchGroup Echavarren
PM4-084 F2-4
ICIQ_1H12p32s CDCl3 /opt/topspin pmcgonigal 32



PM4-084-F2-4/11
ResearchGroup Echavarren
PM4-084 F2-4
ICIQ_13C(1H)512s CDCl3 /opt/topspin pmcgonigal 32



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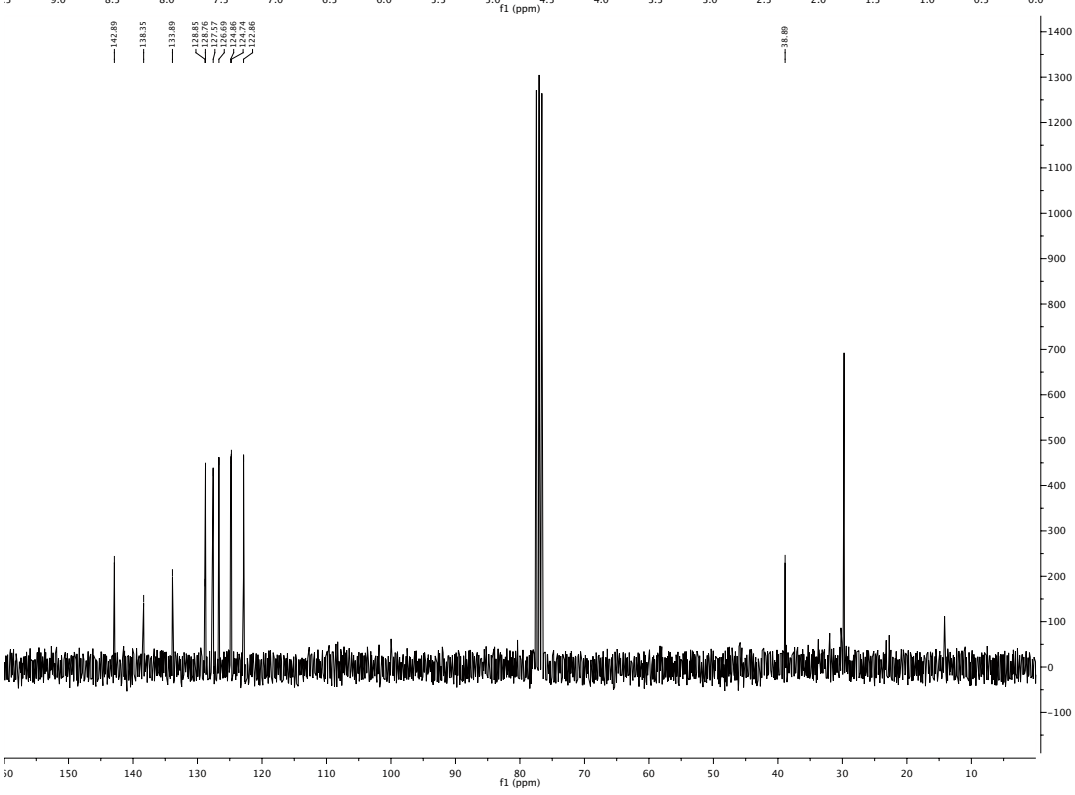
2.00
2.13
1.98
4.09
2.00
f1 (ppm)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126.68
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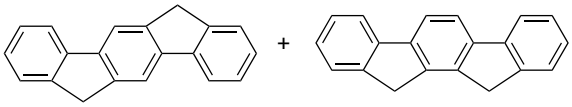
124.74
122.68
38.89
f1 (ppm)



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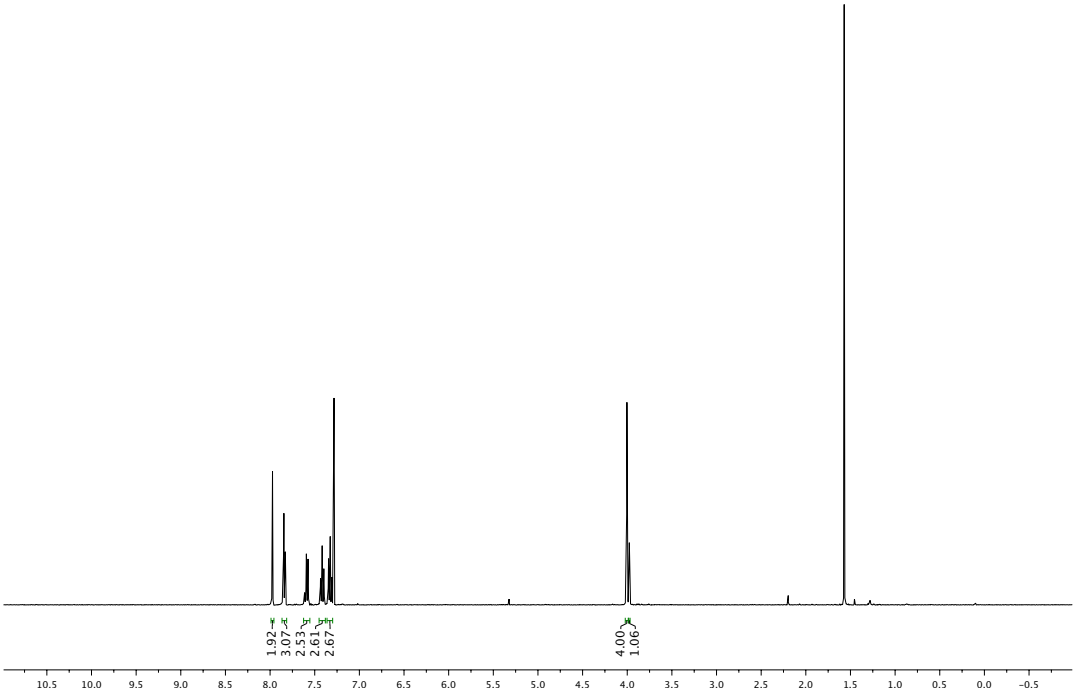
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 77



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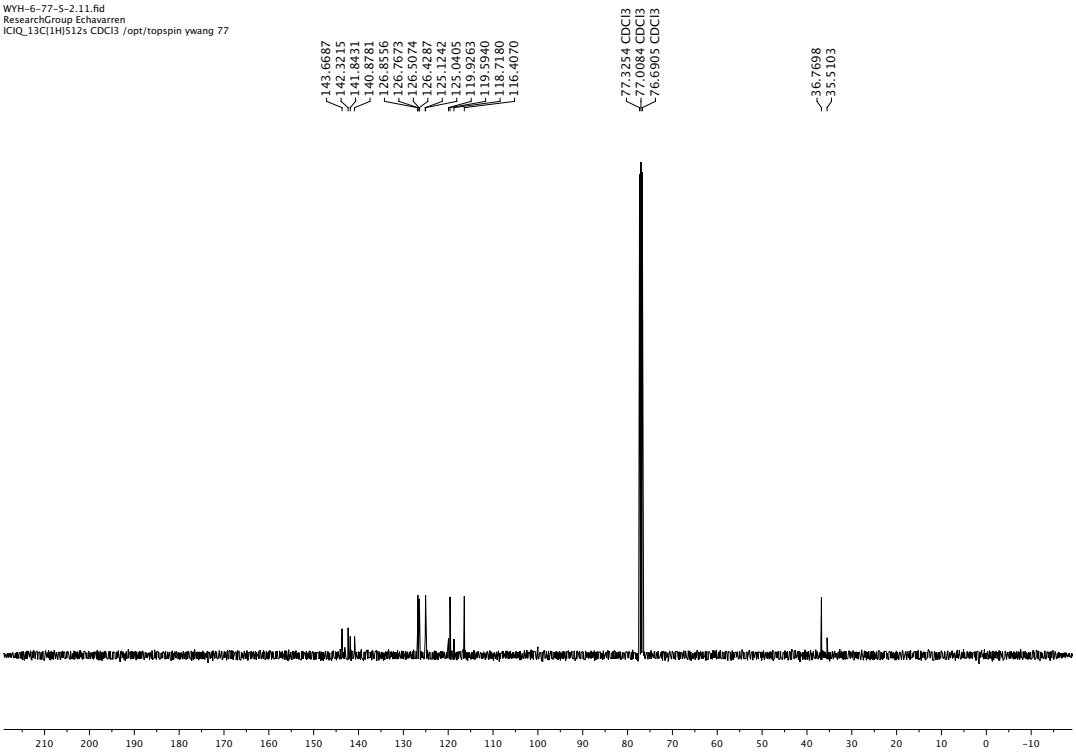
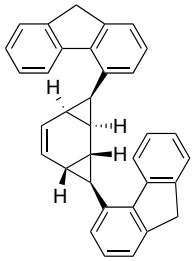
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 77





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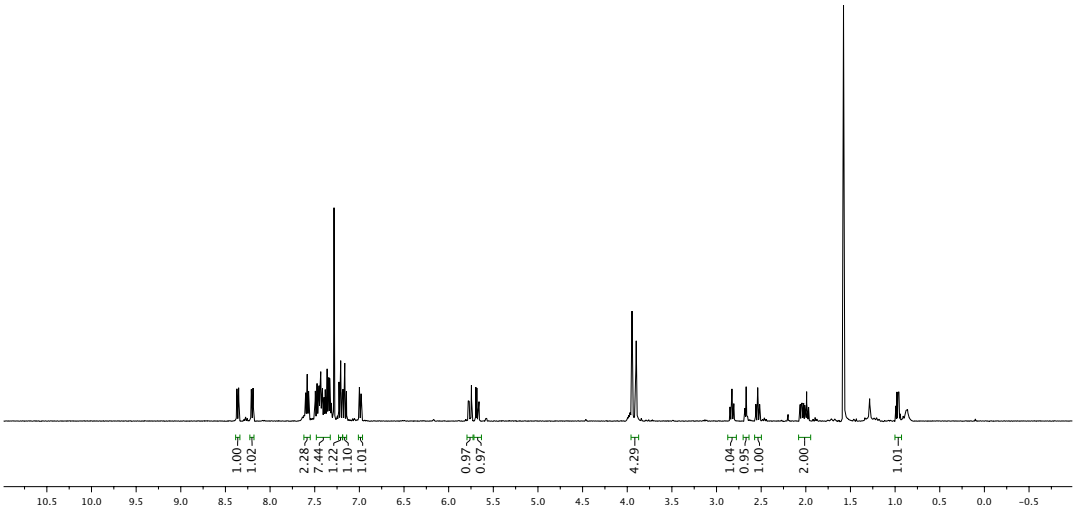
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 74



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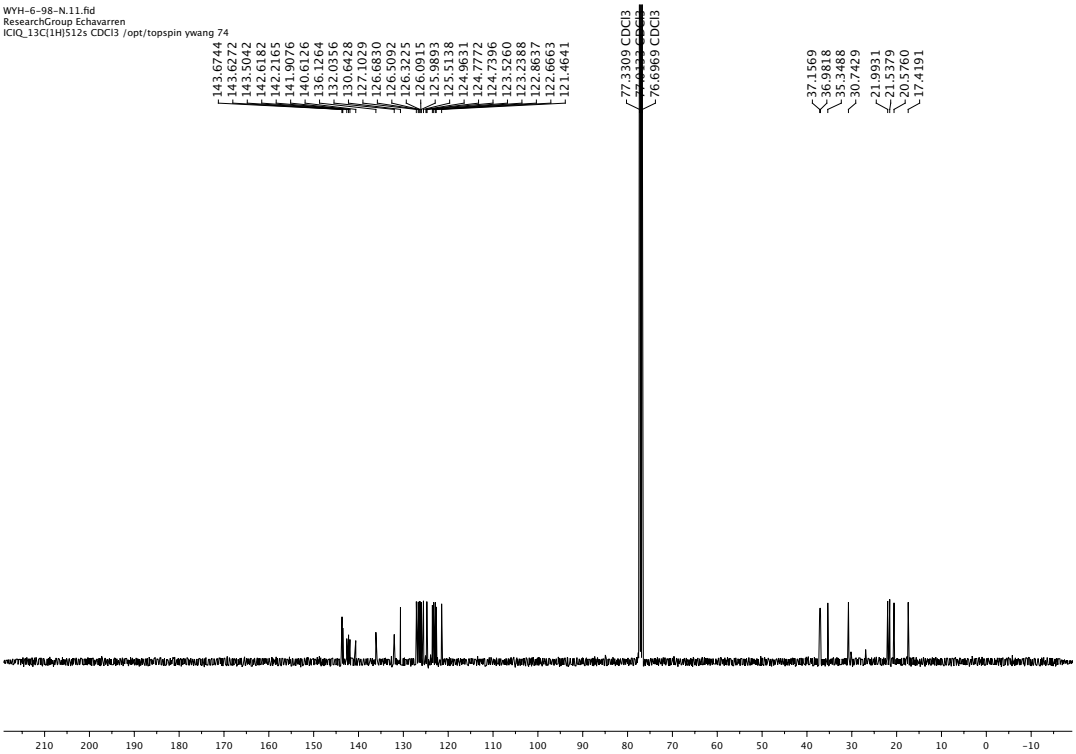
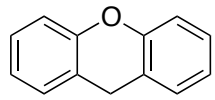
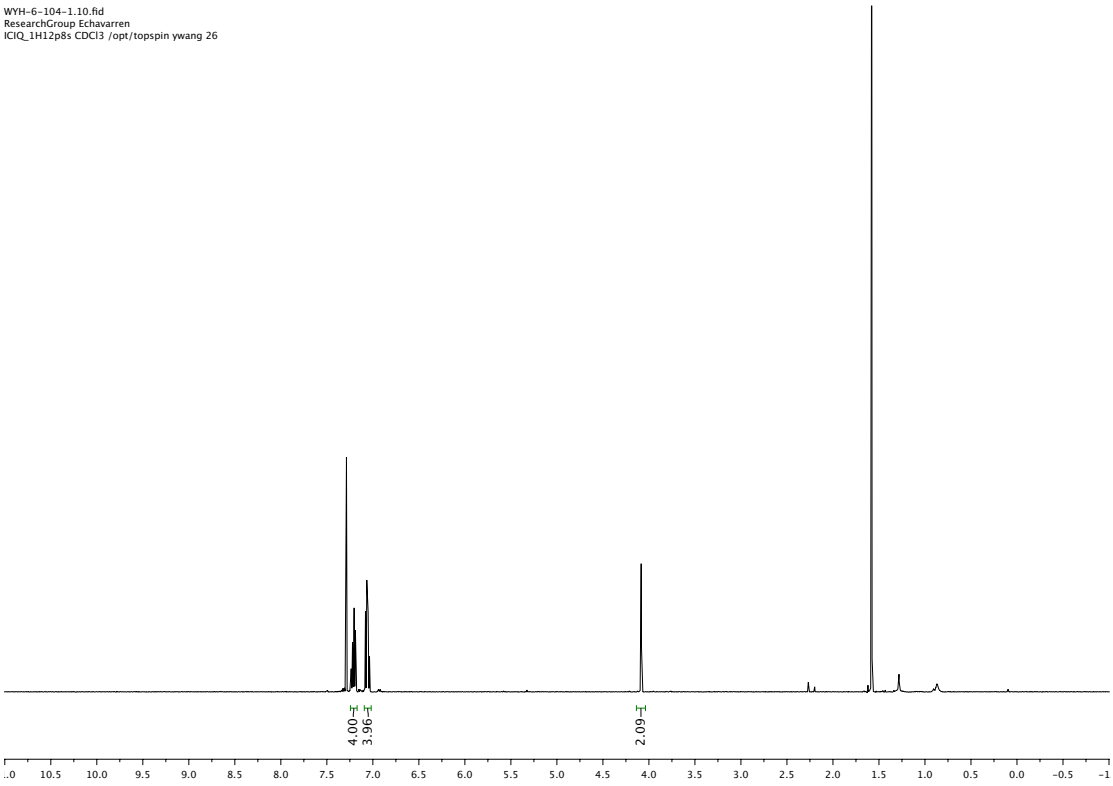
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 74



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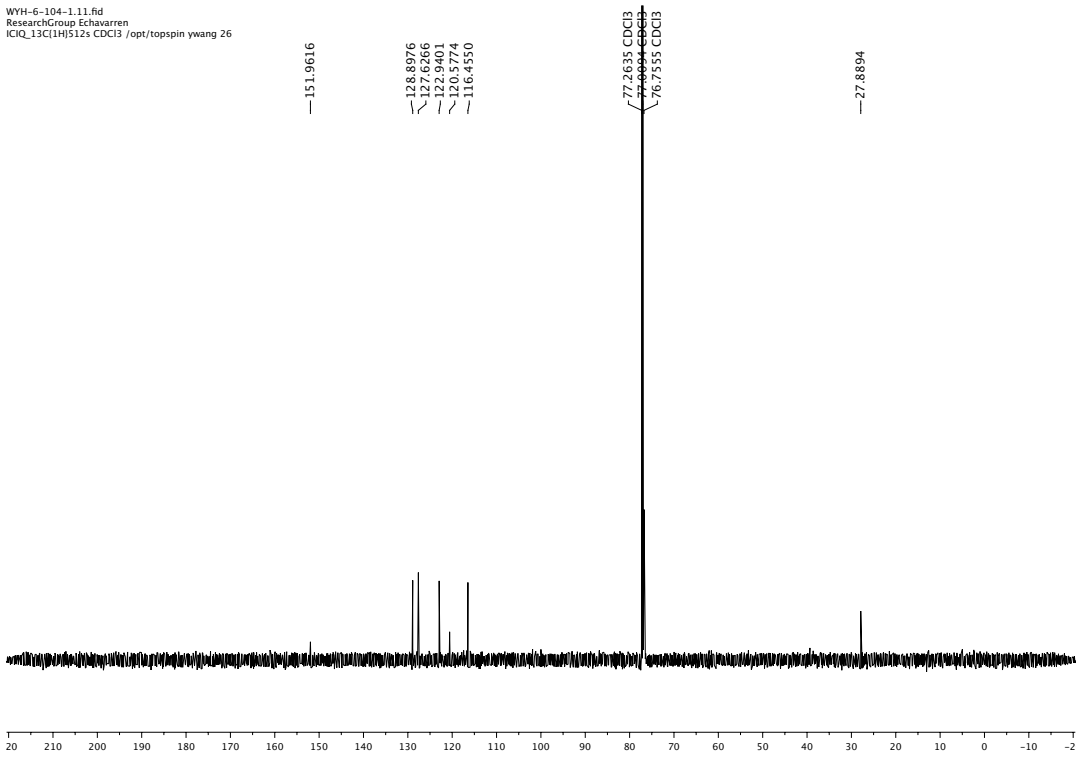
ResearchGroup Echavarren
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 26
4.00
3.96
2.09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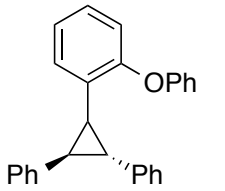
ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 26
151.9616
128.8976
127.6266
122.9401
120.5774
116.4550
77.2635 CDCl3
77.0004 CDCl3
76.7555 CDCl3
27.8894



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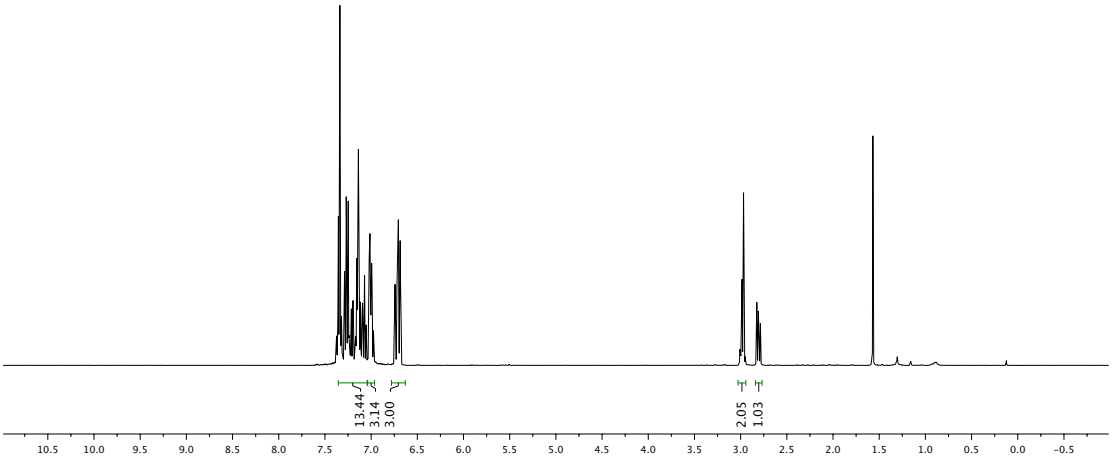
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 113



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ResearchGroup Echavarren
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 113

157.2652
156.4531
141.8402
138.2333
130.2667
129.5512
128.4603
128.3892
128.1460
127.7322
127.5287
126.5943
126.0613
125.7271
122.8309
122.8070
118.5243
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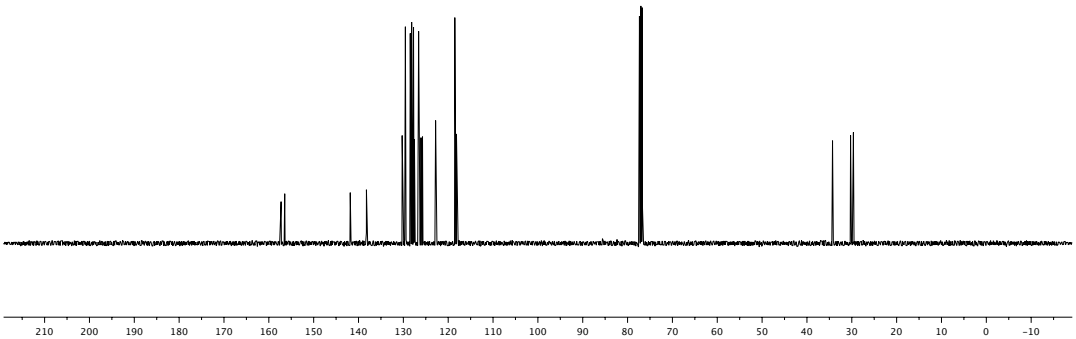
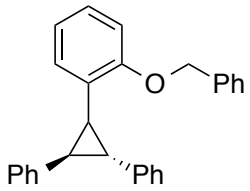
30.2733
29.6393





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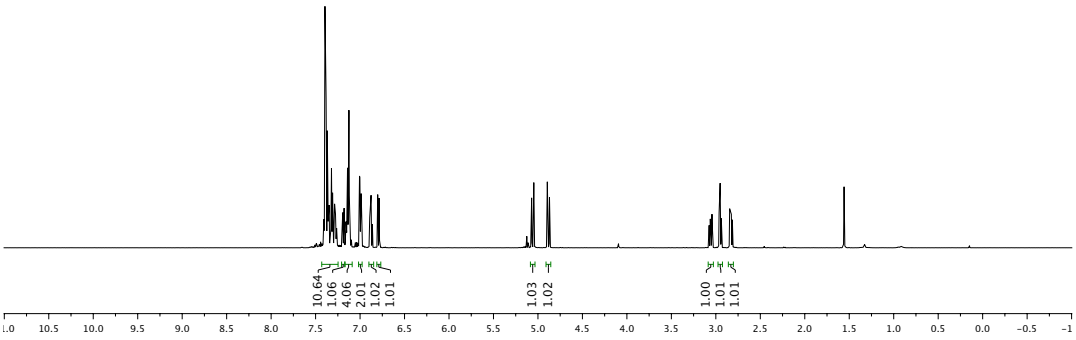
ICIQ_1H12p8s CDCl3 /opt/topspin ywang 34



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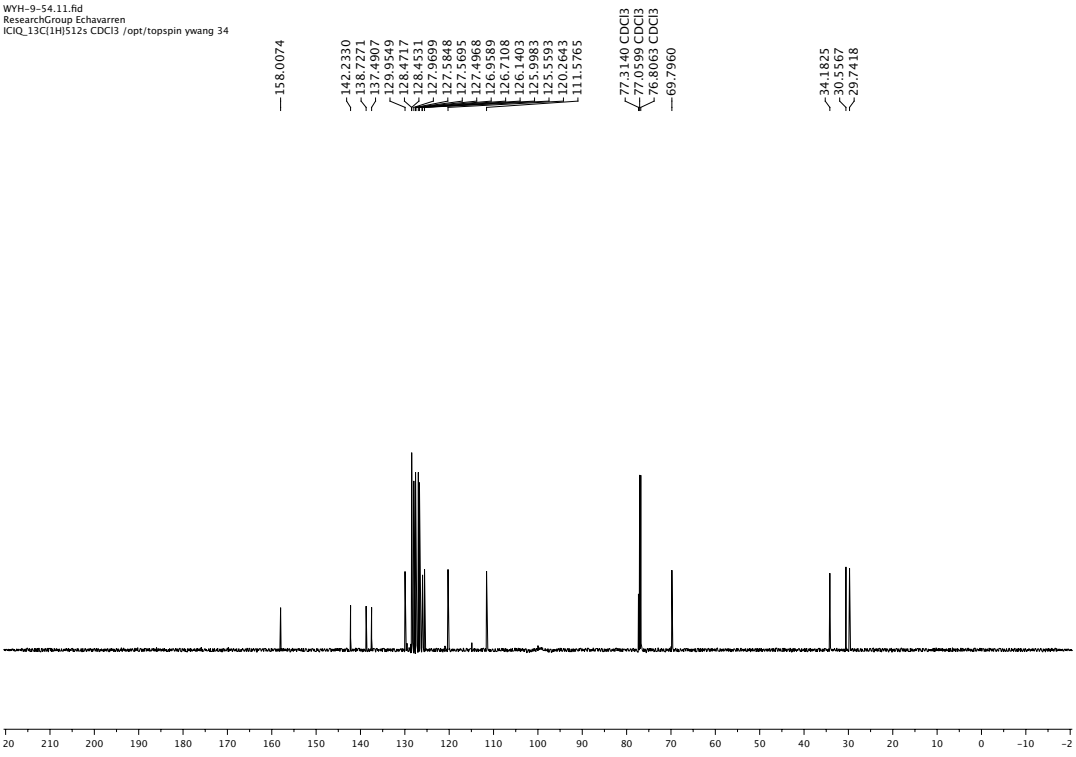
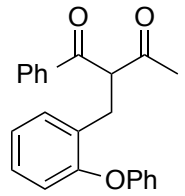
ICIQ_13C{1H}512s CDCl3 /opt/topspin ywang 34





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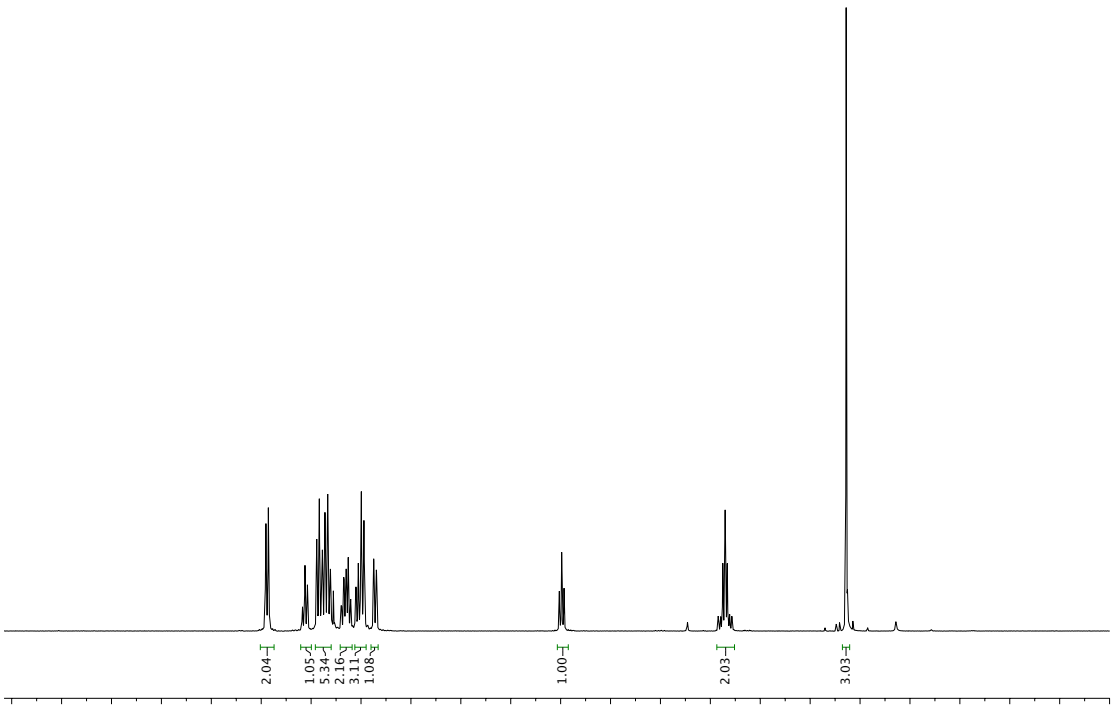
ResearchGroup Echavarren
ICIQ_1H20p8s CDCl3 {C:\Bruker\TopSpin3.1} ywang 35



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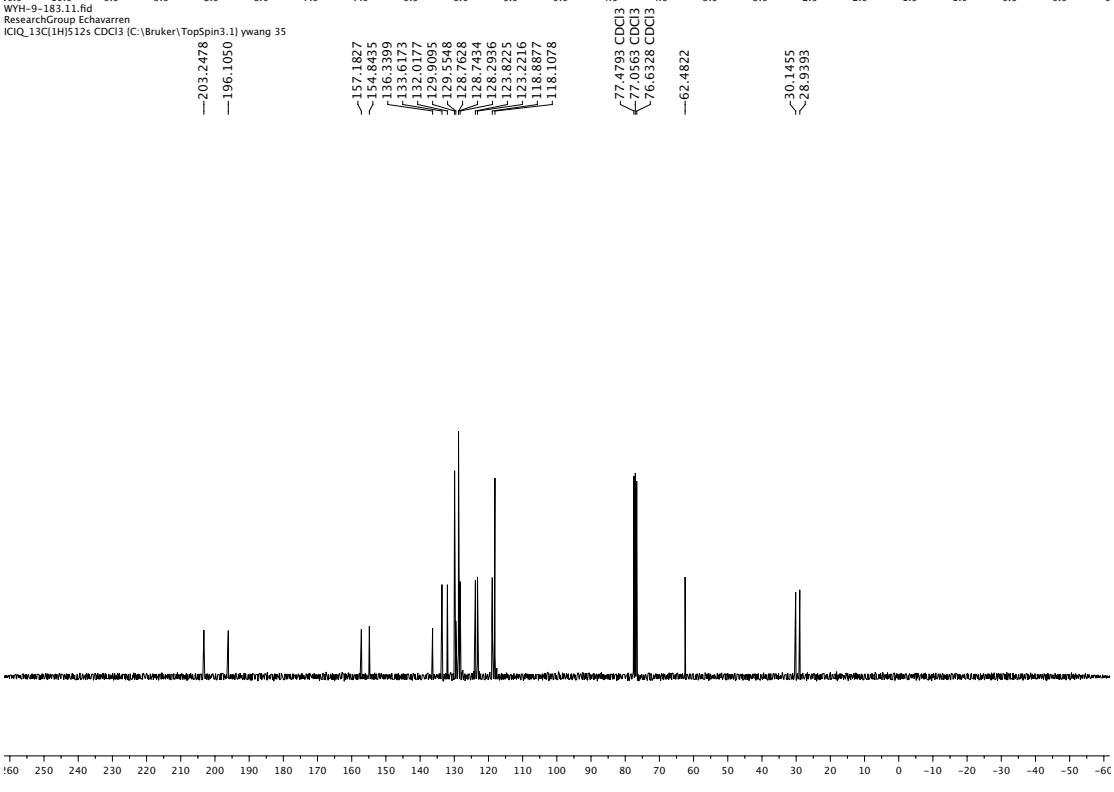
ICIQ_13C{1H}512s CDCl3 {C:\Bruker\TopSpin3.1} ywang 35



Computational Supporting Information

Table of Contents

1.- Computational methods.

Calculations were performed using the M06[1] functional together with the standard 6-31G(d) basis set to describe the H, C and P atoms.[2] The large core scalar relativistic pseudopotentials by Dolg et al. were used for Gold coupled to a double-zeta quality basis set.[3] Full geometry optimizations were performed in solution, with the Polarizable Continuum Model (IEFPCM) method,[4] and using Gaussian 09[5] defaults for dichloroethane (DCE). Some test calculations presented in the text as notes, were performed instead with the B3LYP[6] functional. Unless otherwise stated, all the energies presented correspond to free energies in solution. The nature of the stationary points was characterized by a vibrational analysis performed within the harmonic approximation at 298 K and 1 atm. Transition states were identified by the presence of one imaginary frequency and minima by a full set of real frequencies.

---

[1] Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc*. **2008**, *120*, 215-241.
[2] Hehre, W. J.; Ditchfield, R.; Pople, J.A. *J. Chem. Phys*. **1972**, *56*, 2257.
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[4] Cossi, M.; Barone, V.; Mennucci B.; Tomasi, J. *Chem. Phys. Lett.* **1998**, *286*, 253. Miertus, S.; Tomasi, J. *Chem. Phys.* **1982**, *65*, 239. Mennucci, B.; Tomasi, J. *J. Chem. Phys.* **1997**, *106*, 5151.
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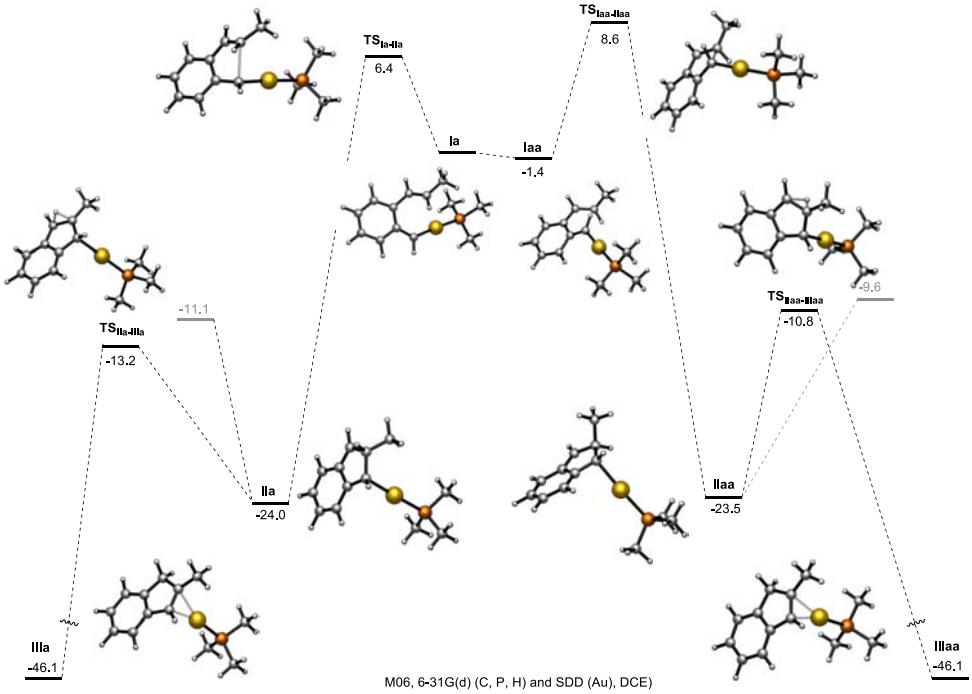
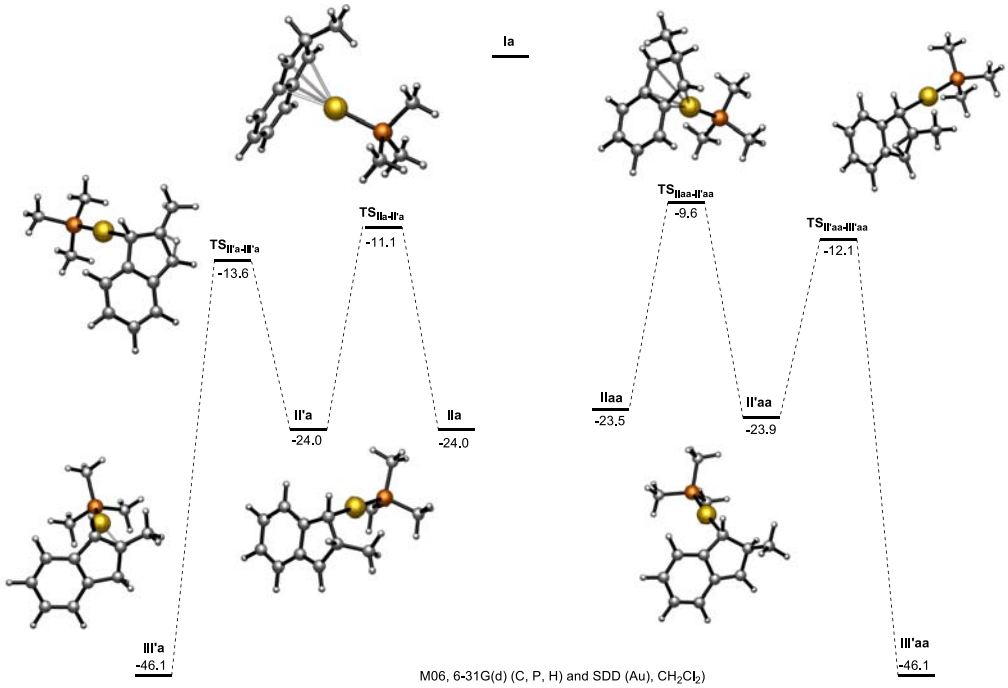
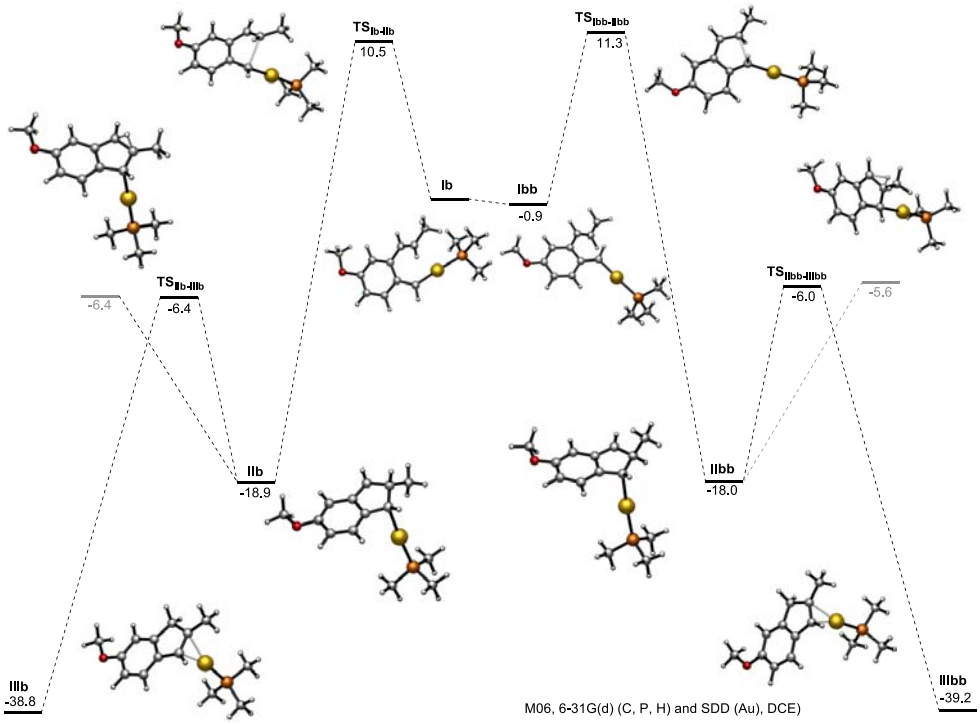
2.- Free energy reaction profiles for the formation of IIIa-c, III'a-c and the anti-rotamers IIIaa-cc and III'aa-cc.



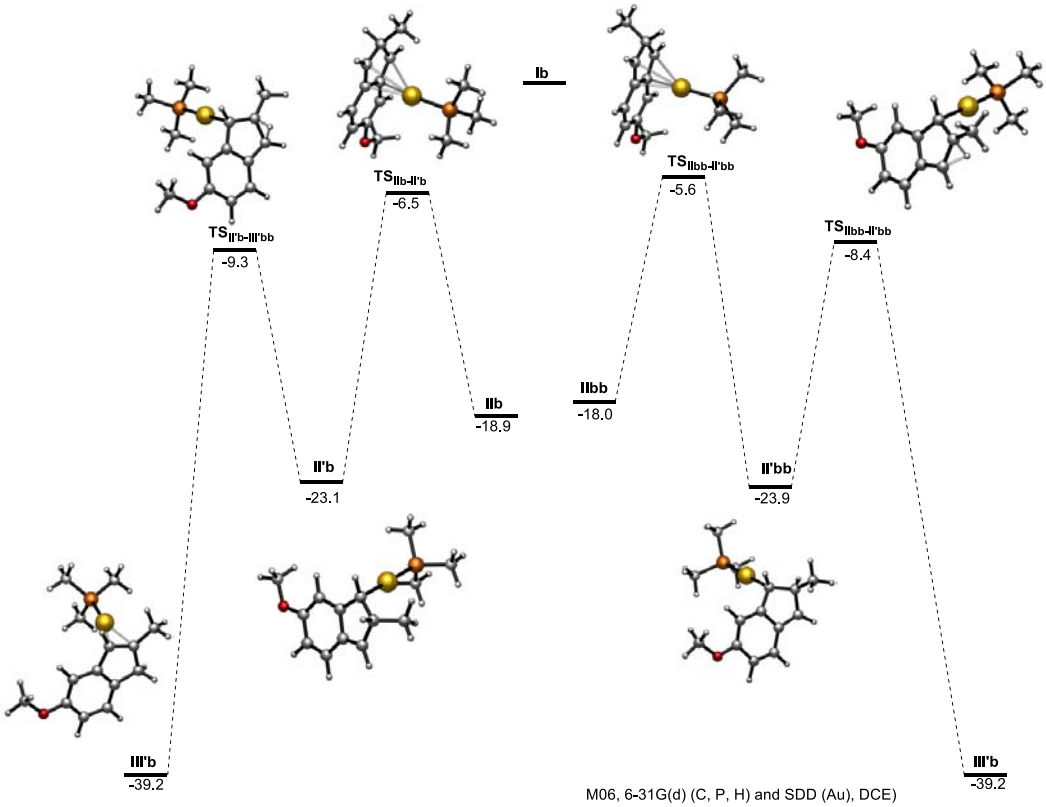
Free energy reaction profile for the formation of IIIa and the *anti*-rotamer IIIaa, energies correspond to free energies in solution, in kcal/mol. Energies in grey correspond to the transition states for the metal-migration competitive process.



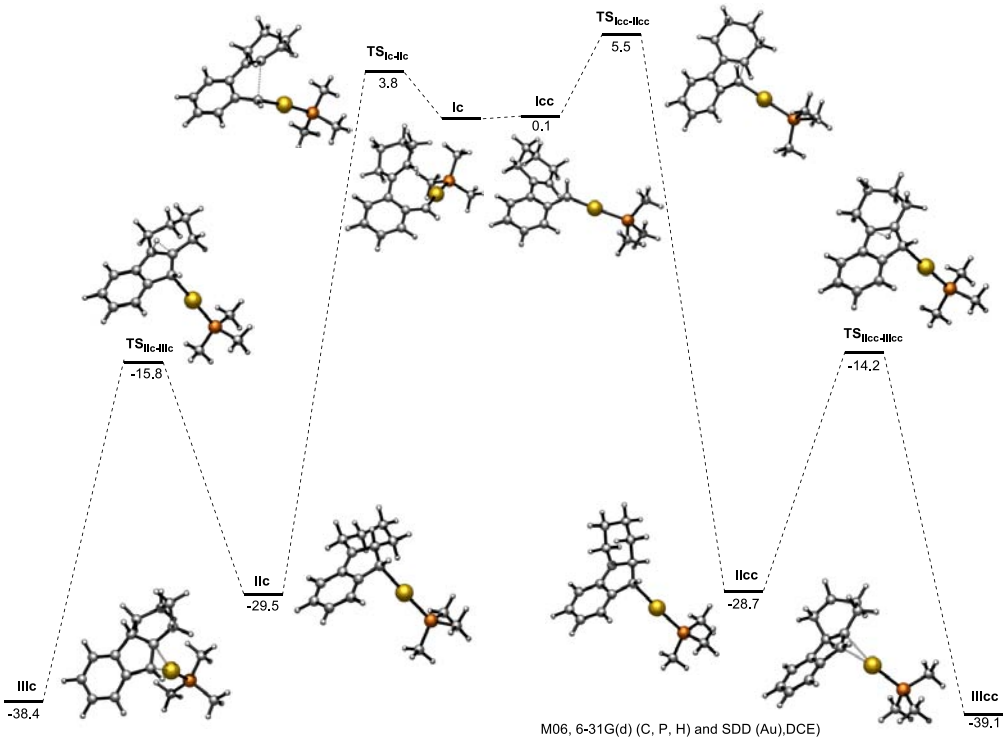
Free energy reaction profile for the formation of III'a and the *anti*-rotamer III'aa, through the metal-migration mechanism, energies correspond to free energies in solution, in kcal/mol.



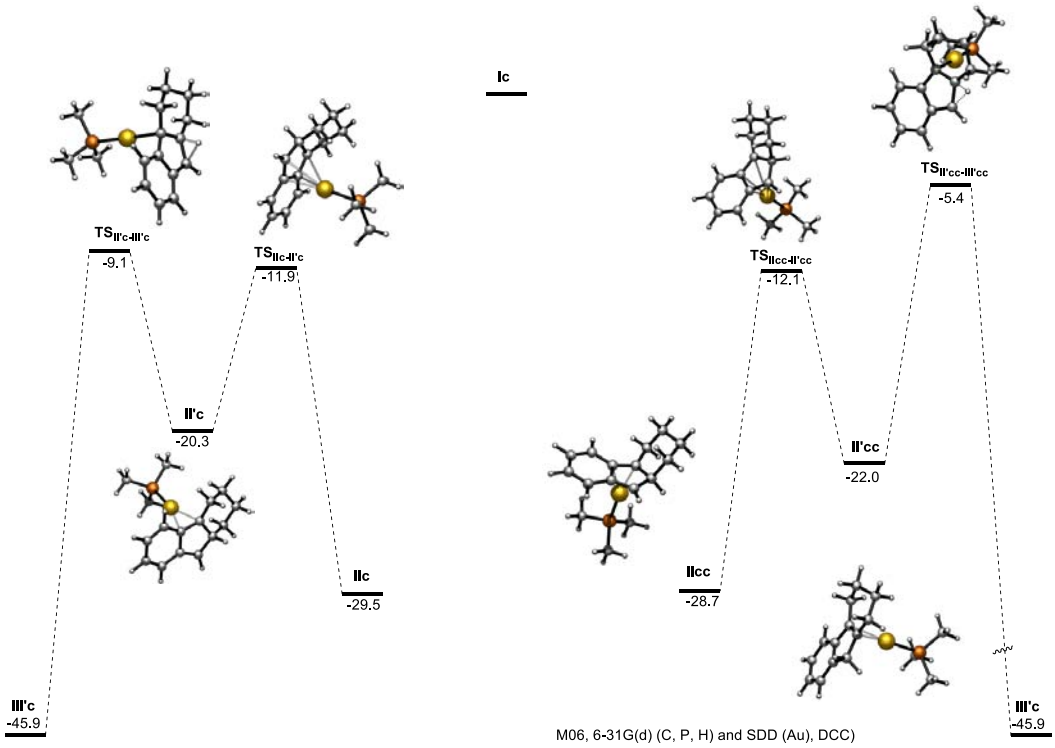
Free energy reaction profile for the formation of IIIb and the *anti*-rotamer IIIbb, energies correspond to free energies in solution, in kcal/mol. Energies in grey correspond to the transition states for the metal-migration competitive process.



Free energy reaction profile for the formation of III'b and the *anti*-rotamer III'bb, through the metal-migration mechanism, energies correspond to free energies in solution, in kcal/mol.

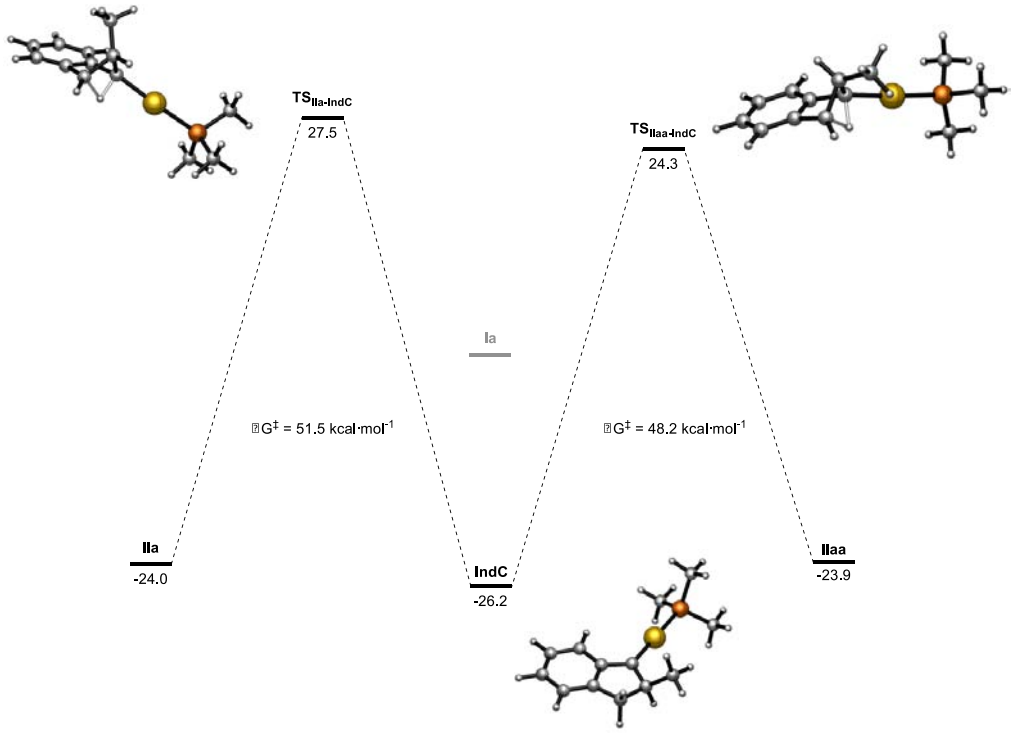


Free energy reaction profile for the formation of IIIc and the *anti*-rotamer IIIcc, energies correspond to free energies in solution, in kcal/mol.



Free energy reaction profile for the formation of III'c and the *anti*-rotamer III'cc, through the metal-migration mechanism, energies correspond to free energies in solution, in kcal/mol.

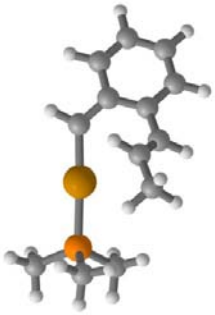
3. Free energy reaction profiles for the isomerization via 1,4-H-shift.



Free energy reaction profile for the isomerization via 1,4-H-shift, energies correspond to free energies in solution, in kcal/mol.

4.- Energies (hartree) and coordinates (angstrom) of the structures presented.

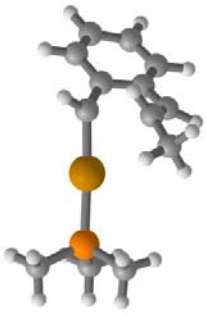
Ia



ΔE(DCE) -983.050536 h.
ΔG(DCE)-983.097758 h.

79	-0.578043	-0.487161	-0.266964
15	-2.807697	-0.071098	0.426246
6	-3.671985	1.269945	-0.459703
1	-3.661848	1.079482	-1.538777
1	-4.712589	1.332948	-0.114565
1	-3.175594	2.227876	-0.265828
6	-3.918955	-1.506034	0.246863
1	-3.536008	-2.351058	0.829897
1	-4.926019	-1.248953	0.601414
1	-3.972802	-1.805242	-0.805951
6	-2.957908	0.399613	2.182017
1	-2.397095	1.323183	2.368195
1	-4.012815	0.561175	2.439473
1	-2.548283	-0.392258	2.819206
6	1.341091	-1.015125	-0.794699
1	1.450636	-1.908355	-1.424009
6	2.575846	-0.512975	-0.377030
6	3.699794	-1.396246	-0.473746
6	2.731522	0.721415	0.358672
6	4.844186	-1.174601	0.253457
1	3.600842	-2.290549	-1.087556
6	3.892085	0.892432	1.122505
6	4.923938	-0.033196	1.071707
1	5.676536	-1.872506	0.205693
1	4.002614	1.796463	1.719538
1	5.826631	0.146411	1.653178
6	1.770033	1.793986	0.294373
6	1.022687	2.088034	-0.793863
6	0.057632	3.213376	-0.868677
1	1.184892	1.520562	-1.713574
1	-0.898036	2.874538	-1.291442
1	0.428580	3.995280	-1.547099
1	1.718665	2.456307	1.163173
1	-0.127252	3.663139	0.114239

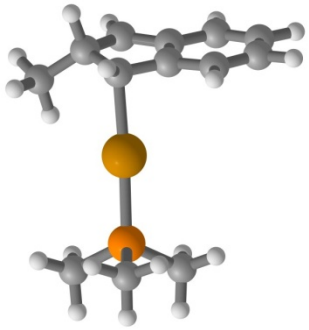
TSIa-IIa



ΔE(DCE) -983.039943 h.
ΔG(DCE) -983.087485 h.

79	-0.600288	-0.153969	-0.381283
15	-2.789375	-0.381395	0.447243
6	-3.547897	1.220670	0.876939
1	-3.561086	1.873220	-0.003810
1	-4.576535	1.071029	1.230484
1	-2.962705	1.709508	1.664570
6	-3.958393	-1.136121	-0.729556
1	-3.628582	-2.149292	-0.985122
1	-4.961599	-1.183848	-0.285857
1	-3.997640	-0.538992	-1.647576
6	-2.952246	-1.382813	1.960719
1	-2.345165	-0.948082	2.762585
1	-4.002549	-1.412728	2.279276
1	-2.603527	-2.404256	1.771870
6	1.322793	-0.014768	-1.181564
1	1.378243	-0.099539	-2.277156
6	2.545904	-0.269309	-0.512283
6	3.459727	-1.270197	-0.927804
6	2.835908	0.491152	0.660991
6	4.489416	-1.625161	-0.085001
1	3.291650	-1.801445	-1.863475
6	3.885529	0.098759	1.516540
6	4.693152	-0.952902	1.143936
1	5.157163	-2.438252	-0.363487
1	4.077872	0.658834	2.430433
1	5.525133	-1.249634	1.779601
6	2.040836	1.654296	0.778062
6	1.369307	2.122821	-0.334227
6	0.272393	3.133130	-0.280433
1	1.858508	2.015477	-1.310085
1	-0.457387	2.970840	-1.082421
1	0.688911	4.139845	-0.431924
1	1.899420	2.139940	1.746516
1	-0.255353	3.114508	0.680352

IIa=II'a

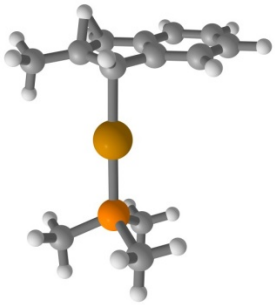


ΔE(DCE) -983.087670 h.
ΔG(DCE) -983.135936 h.

79	0.526829	0.201924	-0.326001
15	2.663970	-0.488230	0.345648
6	3.579049	0.788193	1.268875
1	3.012838	1.080635	2.160272
1	4.559246	0.399148	1.574773
1	3.722457	1.672980	0.638609
6	2.664939	-1.939030	1.448866
1	2.191509	-2.790126	0.946925
1	3.696626	-2.204327	1.715933
1	2.102408	-1.711423	2.361267
6	3.775134	-0.948550	-1.022083
1	3.910948	-0.095173	-1.695669
1	4.751198	-1.252280	-0.621078
1	3.344195	-1.780170	-1.590404
6	-2.789574	1.450244	0.894343
1	-3.218661	1.983879	1.741289
6	-2.928162	0.114272	0.637250
6	-3.681181	-0.902331	1.309867
6	-2.182745	-0.193986	-0.574360
6	-3.740280	-2.141177	0.749077
1	-4.201669	-0.668976	2.237087
6	-2.307105	-1.490048	-1.144910
6	-3.066159	-2.420758	-0.489199
1	-4.310803	-2.936238	1.224101

1	-1.792230	-1.731624	-2.073816
1	-3.167825	-3.418193	-0.914735
6	-1.447861	0.947322	-0.990419
6	-1.954164	2.104524	-0.140799
1	-1.251566	1.107075	-2.055680
1	-2.668277	2.656767	-0.787342
6	-0.950606	3.119134	0.402087
1	-0.355737	3.544284	-0.414397
1	-1.469247	3.939608	0.913374
1	-0.262191	2.648762	1.117289

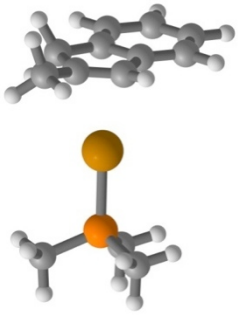
TSIIa-IIIa = TSII'a-III'a



ΔE(DCE) -983.071726 h.
ΔG(DCE) -983.119500 h.

79	0.588890	0.208686	-0.279760
15	2.725597	-0.527971	0.328100
6	3.873312	0.807864	0.793216
1	3.476558	1.358952	1.653111
1	4.850990	0.382668	1.056072
1	3.995780	1.503516	-0.044300
6	2.745617	-1.664357	1.752802
1	2.164516	-2.563234	1.518621
1	3.779225	-1.951997	1.986947
1	2.300244	-1.175851	2.626610
6	3.593789	-1.436245	-0.991410
1	3.705971	-0.795820	-1.873344
1	4.586933	-1.746438	-0.640348
1	3.017403	-2.324367	-1.273585
6	-2.702604	1.465185	0.944931
1	-3.074645	2.045244	1.787530
6	-3.015105	0.114935	0.624831
6	-3.916181	-0.785521	1.223714
6	-2.265365	-0.239799	-0.531747
6	-4.065702	-2.032139	0.653750
1	-4.475656	-0.499665	2.113235
6	-2.462373	-1.503156	-1.115132
6	-3.349212	-2.378004	-0.515549
1	-4.748601	-2.755865	1.094168
1	-1.913170	-1.788379	-2.012066
1	-3.502667	-3.363667	-0.952995
6	-1.407691	0.870228	-0.916451
6	-1.772514	1.979288	-0.027327
1	-1.215130	1.075746	-1.974737
1	-2.978222	2.218986	-0.225518
6	-1.054167	3.290794	0.095585
1	-0.704641	3.635376	-0.884008
1	-1.701584	4.062684	0.527439
1	-0.180413	3.181088	0.749435

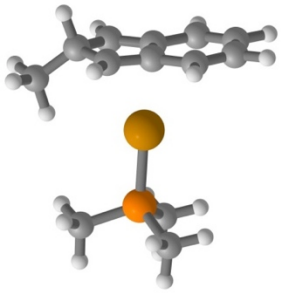
IIIa = III'a = IIIaa = III'aa



ΔE(DCE) -983.123010 h.
ΔG(DCE) -983.171280 h.

79	0.573360	0.317458	-0.206964
15	2.614702	-0.729412	0.222046
6	3.606536	0.105701	1.498690
1	3.055613	0.124502	2.445392
1	4.553596	-0.431068	1.642140
1	3.818022	1.136255	1.192906
6	2.435733	-2.445101	0.801290
1	1.919379	-3.042388	0.041806
1	3.426438	-2.878665	0.990978
1	1.848362	-2.467075	1.725769
6	3.698811	-0.826004	-1.235939
1	3.939498	0.182848	-1.588683
1	4.628038	-1.348086	-0.972583
1	3.195266	-1.370709	-2.042032
6	-2.125194	1.347766	1.214437
1	-1.508256	1.213294	2.115976
6	-2.763592	0.082518	0.719357
6	-3.600661	-0.816369	1.363812
6	-2.396843	-0.126211	-0.622817
6	-4.077531	-1.918581	0.649031
1	-3.890126	-0.664550	2.403302
6	-2.868099	-1.224199	-1.336547
6	-3.718379	-2.118409	-0.686589
1	-4.742642	-2.628929	1.137495
1	-2.581592	-1.380632	-2.375927
1	-4.105695	-2.982382	-1.224127
6	-1.497120	0.962451	-1.028440
6	-1.327175	1.838732	0.031272
1	-1.219992	1.183325	-2.060583
1	-2.873131	2.114052	1.477063
6	-0.732952	3.203121	-0.009240
1	-0.144809	3.365786	-0.919543
1	-1.539497	3.950956	0.016256
1	-0.095617	3.392979	0.863988

TSIIa-II'a

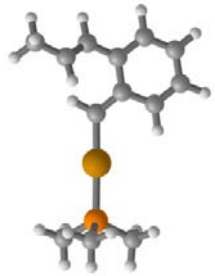


ΔE(DCE) -983.068742 h.
ΔG(DCE)-983.115452 h.

79	0.241519	-0.052303	-0.001364
15	2.537885	-0.250075	-0.000760
6	3.352674	1.371537	-0.113203
1	3.057358	1.992869	0.739958
1	4.442967	1.241991	-0.107808
1	3.051523	1.876758	-1.037793
6	3.208581	-1.027749	1.499564
1	2.810993	-2.043170	1.602914
1	4.303549	-1.071790	1.431625
1	2.922812	-0.444376	2.381633
6	3.194068	-1.230487	-1.383629
1	2.907290	-0.772204	-2.336177
1	4.288969	-1.275739	-1.315711
1	2.788204	-2.247247	-1.344407
6	-1.984282	1.339622	1.181311
1	-1.957599	1.676868	2.214275
6	-2.169580	0.049950	0.746097
6	-2.409727	-1.191036	1.447683
6	-2.172078	0.050217	-0.743208
6	-2.641817	-2.316809	0.727168
1	-2.414230	-1.200109	2.536388
6	-2.414477	-1.190526	-1.444409
6	-2.644305	-2.316532	-0.723540

1	-2.835768	-3.256977	1.240580
1	-2.422661	-1.199222	-2.533097
1	-2.840062	-3.256468	-1.236691
6	-1.988473	1.340027	-1.178669
6	-1.939311	2.254245	0.001384
1	-1.965159	1.677477	-2.211650
1	-2.921085	2.777048	0.003447
6	-0.839996	3.312940	-0.000656
1	-0.915473	3.951072	-0.888853
1	-0.909640	3.948558	0.889835
1	0.152053	2.835302	-0.004645

Iaa

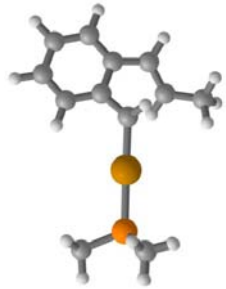


ΔE(DCE) -983.050303 h.

ΔG(DCE) -983.100068 h.

79	-0.862905	0.143417	-0.146163
15	-3.220099	-0.008773	0.114311
6	-3.835117	0.648448	1.701012
1	-3.578849	1.710020	1.789571
1	-4.925701	0.534056	1.757046
1	-3.373331	0.106175	2.533774
6	-4.181636	0.890518	-1.147685
1	-3.949563	0.495396	-2.143091
1	-5.256327	0.773089	-0.955855
1	-3.925483	1.955709	-1.125639
6	-3.881583	-1.707365	0.051399
1	-3.426649	-2.314614	0.841940
1	-4.970555	-1.690047	0.190824
1	-3.650295	-2.163349	-0.917798
6	1.168130	0.322565	-0.376258
1	1.541437	1.214437	-0.892893
6	2.173482	-0.578091	-0.019018
6	1.800367	-1.922486	0.297237
6	3.578015	-0.263347	-0.151086
6	2.732816	-2.929736	0.334241
1	0.741177	-2.132413	0.444673
6	4.496002	-1.320052	-0.157596
6	4.082543	-2.622578	0.081742
1	2.436489	-3.954921	0.542206
1	5.553603	-1.103856	-0.301509
1	4.824192	-3.419381	0.101330
6	4.067693	1.094709	-0.222182
6	3.497623	2.152935	0.392187
6	4.024436	3.538246	0.333120
1	2.620479	1.990431	1.024977
1	4.264742	3.907313	1.339827
1	3.265681	4.223680	-0.070426
1	4.921731	3.607773	-0.292340
1	5.021541	1.239589	-0.737103

TSIaa-IIaa

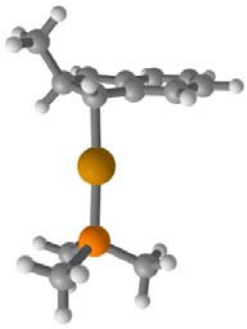


ΔE(DCE) -983.037932 h.

ΔG(DCE) -983.086327 h.

79	-0.733147	0.063184	-0.197407
15	-3.042587	-0.303964	0.198251
6	-3.719517	0.583020	1.641658
1	-3.583701	1.662738	1.512335
1	-4.790282	0.364769	1.749335
1	-3.195354	0.270594	2.551793
6	-4.123394	0.203022	-1.181156
1	-3.854236	-0.349897	-2.088204
1	-5.173048	-0.001976	-0.932335
1	-4.001634	1.274462	-1.375941
6	-3.490301	-2.047009	0.495244
1	-2.967260	-2.420703	1.382801
1	-4.573540	-2.136424	0.650463
1	-3.199184	-2.658791	-0.366070
6	1.271519	0.398199	-0.588880
1	1.487521	1.044762	-1.445725
6	2.369809	-0.441418	-0.200093
6	2.306582	-1.844484	-0.091459
6	3.604250	0.218999	0.073283
6	3.476537	-2.552334	0.105094
1	1.356259	-2.356543	-0.236409
6	4.791617	-0.518271	0.249653
6	4.716870	-1.894460	0.263109
1	3.447745	-3.640094	0.127578
1	5.735782	-0.002504	0.416661
1	5.615747	-2.485730	0.425169
6	3.432586	1.619342	0.187946
6	2.146414	2.082430	0.410170
1	1.532753	1.526542	1.128163
1	4.257601	2.312950	0.009252
6	1.686367	3.470434	0.125521
1	1.631748	4.061291	1.049885
1	2.343167	3.985885	-0.583590
1	0.671290	3.451782	-0.294300

IIaa=II'aa



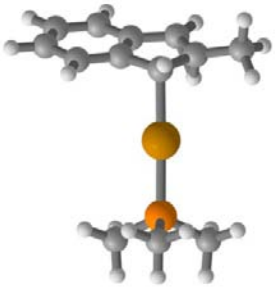
ΔE(DCE) -983.087330 h.

ΔG(DCE) -983.135908 h.

79	-0.601191	-0.255352	-0.223005
15	-2.812661	0.358426	0.265299
6	-4.042109	-0.485026	-0.782454
1	-3.961542	-1.569889	-0.651545
1	-5.054579	-0.161635	-0.507065
1	-3.861166	-0.245639	-1.836257
6	-3.326257	-0.022963	1.970820
1	-2.692140	0.518896	2.681111
1	-4.373086	0.271067	2.123302
1	-3.223065	-1.097858	2.157372
6	-3.175120	2.132269	0.057326
1	-2.969387	2.435379	-0.975341
1	-4.230924	2.327537	0.287795
1	-2.543875	2.724685	0.728846
6	2.779829	-1.115734	1.218664
1	3.236842	-1.500509	2.129080
6	2.895396	0.162997	0.747200
6	3.649116	1.280492	1.233508
6	2.133924	0.263363	-0.488346
6	3.687775	2.411488	0.476819
1	4.184883	1.205317	2.178099
6	2.222177	1.455900	-1.255624
6	2.985501	2.485078	-0.774655

1	4.260831	3.276125	0.804593
1	1.684489	1.541354	-2.198916
1	3.065748	3.403287	-1.354715
6	1.426030	-0.946169	-0.715697
6	1.923391	-1.933772	0.329307
1	1.104035	-2.366815	0.934284
1	1.270930	-1.293547	-1.742928
6	2.695462	-3.103433	-0.303878
1	2.028173	-3.684563	-0.950757
1	3.526211	-2.723229	-0.912500
1	3.100941	-3.770466	0.465521

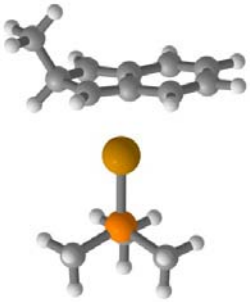
TSIIaa-IIIaa = TSII'aa-III'aa



ΔE(DCE) -983.069878 h.
ΔG(DCE) -983.117221 h.

79	-0.609529	0.217243	-0.261134
15	-2.765438	-0.500937	0.314475
6	-2.817540	-2.153406	1.080599
1	-2.216626	-2.160056	1.996667
1	-3.854698	-2.417601	1.326174
1	-2.409631	-2.897988	0.388091
6	-3.621930	0.581135	1.504720
1	-3.724005	1.588684	1.086438
1	-4.619743	0.178129	1.723424
1	-3.046368	0.642928	2.435120
6	-3.909252	-0.617158	-1.099483
1	-3.514517	-1.318005	-1.843543
1	-4.891060	-0.969657	-0.756454
1	-4.023177	0.366473	-1.568859
6	1.406615	0.861774	-0.839604
1	1.196436	1.144658	-1.876366
6	2.287613	-0.252746	-0.528048
6	2.422142	-1.520757	-1.119408
6	3.075604	0.070977	0.611027
6	3.324865	-2.413990	-0.573671
1	1.826684	-1.788400	-1.992027
6	3.960489	-0.862534	1.180995
6	4.086502	-2.094972	0.573845
1	3.451788	-3.393289	-1.033296
1	4.543570	-0.605876	2.064261
1	4.779065	-2.831854	0.976053
6	2.794071	1.422831	0.969123
6	1.784525	1.936343	0.083483
1	1.429571	1.549659	1.235533
1	3.252669	2.006333	1.765298
6	1.436722	3.377455	-0.098986
1	1.598029	3.957352	0.815997
1	2.079631	3.798577	-0.882386
1	0.394149	3.492065	-0.415227

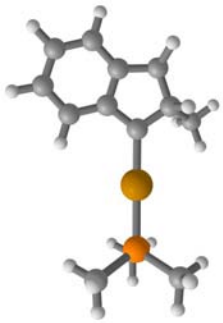
TSIIaa-II'aa



ΔE(DCE) -983.066050 h.
ΔG(DCE) -983.113129 h.

79	-0.356515	-0.047802	0.005223
15	-2.659829	-0.101328	0.000090
6	-3.338648	-1.618741	-0.736294
1	-3.000571	-2.493714	-0.170517
1	-4.435473	-1.574772	-0.713803
1	-3.000446	-1.714232	-1.773631
6	-3.399920	0.000865	1.657330
1	-3.100544	0.935668	2.143324
1	-4.494468	-0.030989	1.574827
1	-3.059704	-0.840953	2.270047
6	-3.395251	1.264710	-0.947716
1	-3.055171	1.221099	-1.988185
1	-4.489984	1.182981	-0.920919
1	-3.092229	2.224924	-0.516445
6	2.077705	-1.049768	1.177736
1	2.125928	-1.383815	2.210990
6	2.049914	0.251562	0.743540
6	2.104460	1.515243	1.444875
6	2.047135	0.251686	-0.747120
6	2.166992	2.662188	0.723928
1	2.112077	1.524826	2.533592
6	2.097853	1.515668	-1.448178
6	2.163393	2.662409	-0.727135
1	2.225994	3.620560	1.236864
1	2.100412	1.525766	-2.536913
1	2.219434	3.620963	-1.240044
6	2.073261	-1.049469	-1.181694
6	2.171916	-1.964208	-0.002298
1	1.363249	-2.714853	-0.000649
1	2.117294	-1.383200	-2.215238
6	3.513264	-2.723795	-0.005195
1	3.588870	-3.358605	-0.895429
1	4.352367	-2.016143	-0.006734
1	3.592616	-3.359329	0.884180

IndC

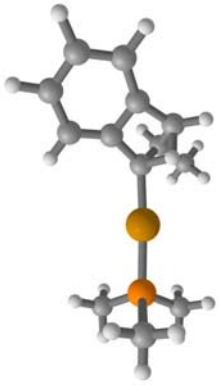


ΔE(DCE) -983.091201 h.
ΔG(DCE) -983.139522 h.

6	1.309736	0.529667	-0.111323
6	2.372342	-0.393517	-0.017131
6	2.302382	-1.799717	0.122129
6	3.626668	0.271929	-0.088083
6	3.479180	-2.515770	0.172306
1	1.331803	-2.291110	0.183435
6	4.804861	-0.461008	-0.042736
6	4.716172	-1.845148	0.087599
1	3.463908	-3.598223	0.275144
1	5.776052	0.026903	-0.103048
1	5.632462	-2.432423	0.126941
6	3.418735	1.741067	-0.196659
6	1.890804	1.887680	-0.324421
1	3.971635	2.181786	-1.037221
1	1.633137	2.126926	-1.375624
6	1.279773	2.974735	0.556725
1	1.744548	3.943515	0.337434
1	0.199510	3.062389	0.389058
1	1.446480	2.749923	1.618669
1	3.782996	2.250229	0.709503
79	-0.703769	0.114634	-0.039038
15	-3.032720	-0.359773	0.013251

6	-3.769195	-0.337154	1.681507
1	-3.637223	0.652248	2.133585
1	-4.841497	-0.565523	1.620812
1	-3.277741	-1.081303	2.318100
6	-3.478915	-1.997996	-0.652425
1	-4.564460	-2.148411	-0.585189
1	-3.170303	-2.070207	-1.701377
1	-2.970145	-2.784205	-0.083363
6	-4.058033	0.807387	-0.942108
1	-3.746758	0.806252	-1.992785
1	-5.115456	0.518235	-0.878761
1	-3.937488	1.820573	-0.542356

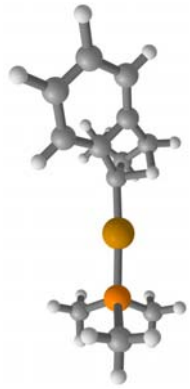
TSIIaa-IndC



ΔE(DCE) -983.011355 h.
ΔG(DCE) -983.058992 h.

6	-1.344707	0.536311	-0.171118
6	-2.495094	-0.442523	-0.225714
6	-2.782087	-1.678457	-0.763499
6	-3.424371	0.287290	0.518586
6	-4.077118	-2.163895	-0.519573
1	-2.055974	-2.254847	-1.334819
6	-4.691122	-0.186226	0.787959
6	-5.001103	-1.440802	0.237577
1	-4.366352	-3.134222	-0.919529
1	-5.414338	0.360536	1.389324
1	-5.988171	-1.865999	0.411442
6	-2.538884	1.472385	0.746597
6	-1.933979	1.860978	-0.597400
1	-1.461995	0.861955	1.145563
1	-2.524676	2.206086	1.557907
79	0.711252	0.095519	0.007787
15	2.997668	-0.446821	0.081956
6	3.605085	-1.319109	-1.397491
1	3.446254	-0.701223	-2.288121
1	4.677041	-1.531176	-1.290871
1	3.062668	-2.262779	-1.523452
6	3.468141	-1.527429	1.472278
1	4.546334	-1.732794	1.438131
1	3.224673	-1.039663	2.422708
1	2.919005	-2.473647	1.412548
6	4.090884	1.002701	0.240227
1	3.859048	1.546345	1.163092
1	5.140119	0.680367	0.265035
1	3.941105	1.676914	-0.610403
1	-2.647137	1.774965	-1.418712
6	-1.050414	3.077277	-0.622772
1	-0.403698	3.121962	0.264335
1	-0.405229	3.060441	-1.509214
1	-1.654018	3.992122	-0.653374

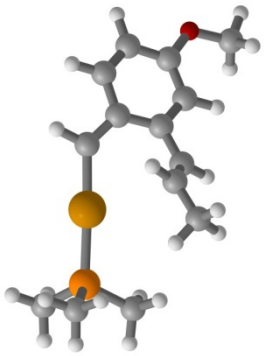
TSIIa-IndC



ΔE(DCE) -983.006724 h.
ΔG(DCE) -983.053887 h.

6	-1.275502	-0.553936	0.010256
6	-2.408841	0.437083	0.138458
6	-2.708158	1.583705	0.840238
6	-3.316211	-0.169345	-0.731857
6	-3.991030	2.114407	0.624921
1	-2.002124	2.059454	1.519281
6	-4.570987	0.348927	-0.968783
6	-4.892625	1.517406	-0.257411
1	-4.287760	3.018849	1.153279
1	-5.279136	-0.102067	-1.660898
1	-5.871315	1.972377	-0.400762
6	-2.450408	-1.342720	-1.075218
6	-1.899832	-1.918098	0.225544
1	-1.348301	-0.714956	-1.340414
1	-1.190905	-2.727331	0.022269
6	-2.798105	-2.206395	1.397680
1	-3.342428	-3.142601	1.229762
1	-2.195221	-2.326405	2.305416
1	-3.529927	-1.410515	1.576547
1	-2.424130	-1.949741	-1.984330
79	0.790559	-0.149036	-0.049577
15	3.092749	0.331686	-0.002764
6	3.822870	0.319591	1.666458
1	3.691505	-0.667714	2.123120
1	4.894758	0.550132	1.607130
1	3.327923	1.066435	2.296995
6	3.526802	1.965928	-0.681569
1	4.611723	2.121498	-0.617117
1	3.215800	2.027511	-1.730414
1	3.015054	2.753611	-0.117501
6	4.113019	-0.842701	-0.952619
1	3.801126	-0.846042	-2.003020
1	5.170568	-0.553731	-0.891046
1	3.991487	-1.853311	-0.546857

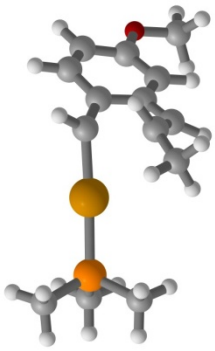
Ib



ΔE(DCE) -1097.493812 h.
ΔG(DCE) -1097.544848 h.

79	-1.138502	-0.584420	-0.158148
15	-3.244360	0.204495	0.589906
6	-4.468529	0.457604	-0.739951
1	-4.663815	-0.491873	-1.251209
1	-5.407889	0.843528	-0.322045
1	-4.080919	1.174780	-1.473081
6	-4.091866	-0.889606	1.777578
1	-3.466388	-1.029107	2.666676
1	-5.052843	-0.451279	2.077567
1	-4.268795	-1.869209	1.319536
6	-3.173553	1.816907	1.441583
1	-2.772485	2.580325	0.764387
1	-4.178063	2.118523	1.767141
1	-2.516422	1.747511	2.316089
6	0.683136	-1.355226	-0.739137
1	0.678626	-2.385287	-1.118758
6	1.971514	-0.854507	-0.621786
6	3.059316	-1.793583	-0.710385
6	2.288244	0.493530	-0.186637
6	4.305399	-1.504481	-0.243369
1	2.846919	-2.784936	-1.108675
6	3.552869	0.758144	0.327917
6	4.553407	-0.222918	0.312297
1	5.118517	-2.226130	-0.267918
1	3.772848	1.763393	0.680374
6	1.362720	1.602276	-0.304748
6	0.483130	1.766291	-1.314059
6	-0.409572	2.944006	-1.462076
1	0.456071	1.028323	-2.119086
1	-1.451442	2.623829	-1.608474
1	-0.141809	3.525137	-2.356034
1	1.473567	2.404149	0.430720
1	-0.363313	3.606595	-0.589375
8	5.785179	-0.034802	0.763425
6	6.146478	1.219879	1.340801
1	7.187606	1.113935	1.647220
1	6.057879	2.022313	0.599273
1	5.521630	1.435789	2.215170

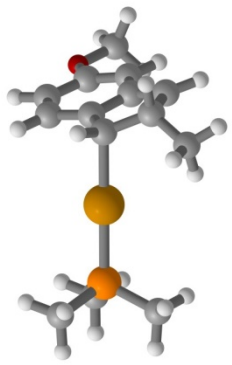
TSIb-IIb



ΔE(DCE) -1097.476911 h.
ΔG(DCE) -1097.528054 h.

79	-1.137533	0.076999	-0.434102
15	-3.112500	-0.826857	0.462508
6	-4.484142	-0.993227	-0.725967
1	-4.192826	-1.670737	-1.536306
1	-5.371818	-1.396077	-0.220663
1	-4.726388	-0.015511	-1.157294
6	-2.927583	-2.493499	1.176532
1	-2.193478	-2.470912	1.989778
1	-3.891044	-2.844936	1.568854
1	-2.575878	-3.190439	0.407533
6	-3.802549	0.178253	1.819266
1	-4.041684	1.183225	1.451787
1	-4.714976	-0.287955	2.213841
1	-3.064969	0.267844	2.625034
6	0.626843	0.799282	-1.297979
1	0.512405	1.163980	-2.329945
6	1.944590	0.427802	-0.957362
6	2.846768	-0.184930	-1.870352
6	2.377526	0.638290	0.388543
6	3.995538	-0.753909	-1.393532
1	2.578681	-0.274377	-2.921932
6	3.560263	0.044220	0.872662
6	4.351116	-0.661342	-0.015991
1	4.672517	-1.294946	-2.052169
1	3.855560	0.207735	1.906376
6	1.539203	1.537031	1.083820
6	0.672340	2.335074	0.354908
6	-0.478442	3.071323	0.958744
1	1.029625	2.743395	-0.597392
1	-1.287573	3.206087	0.231546
1	-0.153819	4.078607	1.259074
1	1.506787	1.551226	2.175443
1	-0.881511	2.558806	1.840428
8	5.511635	-1.262763	0.296422
6	5.964250	-1.197631	1.639955
1	6.891924	-1.771492	1.674304
1	6.163844	-0.158470	1.933730
1	5.229834	-1.643447	2.323559

IIb

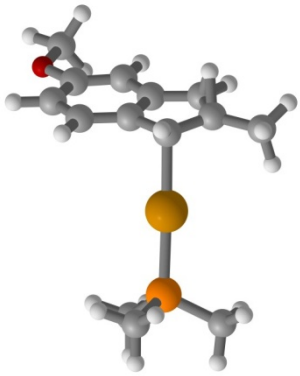


ΔE(DCE) -1097.523592 h.
ΔG(DCE) -1097.574930 h.

6	3.494482	0.058683	0.698812
6	2.435291	0.950746	0.327831
6	1.609825	0.693298	-0.842164
6	1.946759	-0.401239	-1.692545
6	2.979613	-1.209051	-1.330014
6	3.747207	-1.001766	-0.123728
1	4.070738	0.258201	1.598391
1	1.374801	-0.590582	-2.599621
6	0.576595	1.656019	-0.933884
79	-1.024296	0.266567	-0.273701
15	-2.818508	-1.098725	0.365620
6	-2.344079	-2.778243	0.889259
1	-1.670152	-2.723063	1.751371
1	-3.239904	-3.349545	1.166972
1	-1.827646	-3.292684	0.071301
6	-4.043361	-1.356309	-0.957921
1	-4.866051	-1.983406	-0.589724
1	-4.444817	-0.392010	-1.288720
1	-3.567429	-1.850339	-1.812423

6	-3.778895	-0.436189	1.764440
1	-4.610493	-1.113226	2.000320
1	-3.133947	-0.337627	2.644753
1	-4.178218	0.551612	1.509080
6	2.018676	2.130694	0.879689
6	0.901063	2.721590	0.099970
6	-0.234559	3.284224	0.951042
1	1.338448	3.565456	-0.472719
1	-1.031999	3.685208	0.314567
1	-0.668580	2.505281	1.592993
1	0.179069	1.945309	-1.912172
1	2.423889	2.590567	1.779897
1	0.131531	4.093872	1.594465
1	3.264355	-2.060394	-1.947035
8	4.698997	-1.938994	0.061453
6	5.507416	-1.831623	1.220494
1	4.891520	-1.867230	2.129764
1	6.185066	-2.687000	1.201473
1	6.088615	-0.899327	1.205859

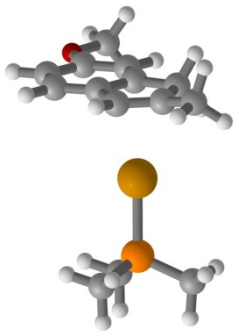
TSIIb-IIIb



ΔE(DCE) -1097.503991 h.
ΔG(DCE) -1097.555021 h.

6	3.653792	0.094143	0.676603
6	2.511779	0.842245	0.320052
6	1.714204	0.518552	-0.807524
6	2.101581	-0.561746	-1.623973
6	3.213152	-1.292601	-1.274557
6	3.986988	-0.981591	-0.124209
1	4.233872	0.370703	1.553662
1	1.521494	-0.825368	-2.507784
1	3.532484	-2.142396	-1.876327
6	0.601519	1.449059	-0.912139
79	-1.114972	0.250760	-0.246566
15	-2.957312	-1.052770	0.371985
6	-2.521239	-2.619392	1.194023
1	-1.955054	-2.412127	2.109024
1	-3.431840	-3.176732	1.451438
1	-1.899976	-3.229260	0.528812
6	-4.004785	-1.541977	-1.036067
1	-4.851833	-2.145742	-0.684840
1	-4.385337	-0.648284	-1.543212
1	-3.417285	-2.127605	-1.751905
6	-4.099508	-0.232043	1.530428
1	-4.935888	-0.902253	1.769157
1	-3.570449	0.026241	2.454558
1	-4.490815	0.687661	1.081509
6	1.964310	2.017787	0.906323
6	0.826635	2.451842	0.130828
6	-0.133239	3.522870	0.556238
1	1.926071	2.988598	-0.117656
1	-0.670697	3.926989	-0.308927
1	-0.872521	3.111233	1.254054
1	0.239353	1.770866	-1.894478
1	2.305776	2.525630	1.806748
1	0.382292	4.346317	1.063565
8	5.039808	-1.807993	0.086515
6	5.876854	-1.540560	1.195454
1	5.318669	-1.611696	2.139638
1	6.659054	-2.302280	1.178332
1	6.334409	-0.544564	1.112601

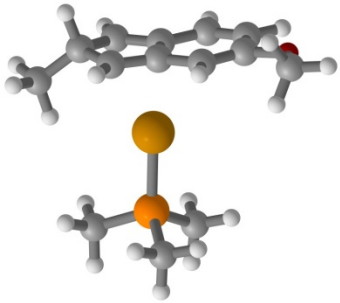
IIIb



ΔE(DCE) -1097.556006 h.
ΔG(DCE) -1097.606620 h.

6	-3.386483	-0.039157	-0.763626
6	-2.301611	0.745029	-0.395133
6	-1.811425	0.741094	0.920214
6	-2.419557	-0.047681	1.898063
6	-3.512810	-0.822943	1.543586
6	-3.994776	-0.825513	0.223557
1	-3.751146	-0.027883	-1.788590
1	-2.047632	-0.058602	2.921843
1	-4.021014	-1.448036	2.275724
6	-0.647738	1.629369	0.981793
79	1.108619	0.352370	0.126441
15	2.785961	-1.240509	-0.186760
6	2.144151	-2.921787	-0.455397
1	1.507734	-2.939054	-1.346999
1	2.979280	-3.621095	-0.592861
1	1.548046	-3.235239	0.408613
6	3.923474	-1.384143	1.226384
1	4.678346	-2.152841	1.015126
1	4.423047	-0.425198	1.402134
1	3.366922	-1.663006	2.127791
6	3.853446	-0.903694	-1.621746
1	4.621880	-1.683702	-1.701533
1	3.253627	-0.892706	-2.538507
1	4.338992	0.071506	-1.505818
6	-1.471647	1.679094	-1.227413
6	-0.421323	2.187487	-0.267022
6	0.448279	3.352016	-0.596595
1	-2.060605	2.536135	-1.593683
1	-0.172999	4.253936	-0.703086
1	1.191322	3.541640	0.186650
1	-0.183042	1.978183	1.905360
1	-1.039087	1.208753	-2.123677
1	0.970491	3.209436	-1.551464
8	-5.064734	-1.624349	-0.000660
6	-5.601057	-1.681879	-1.309263
1	-4.859165	-2.060815	-2.025994
1	-6.444165	-2.374304	-1.261703
1	-5.958768	-0.695695	-1.635920

TSIIb-II'b

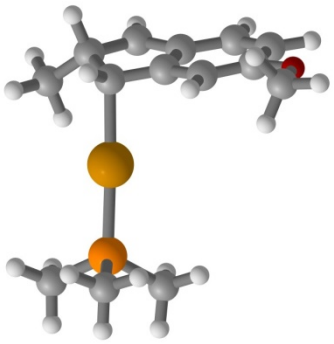


ΔE(DCE) -1097.506008 h.
ΔG(DCE) -1097.555155 h.

79	0.549090	0.045021	0.067395
15	2.550360	-1.091318	-0.041951

6	3.974134	0.039698	-0.095096
1	3.978972	0.674524	0.797859
1	4.904850	-0.542201	-0.132091
1	3.911541	0.678196	-0.983341
6	2.854914	-2.178002	1.383772
1	2.072560	-2.941566	1.450180
1	3.830881	-2.667644	1.267547
1	2.852924	-1.588598	2.307176
6	2.726809	-2.154159	-1.505832
1	2.653284	-1.550303	-2.416992
1	3.704901	-2.652339	-1.478722
1	1.934914	-2.910779	-1.517606
6	-0.731749	2.442402	0.957862
1	-0.395010	2.949840	1.858315
6	-1.470210	1.286518	0.900434
6	-2.044490	0.449916	1.931444
6	-1.745102	0.961632	-0.526399
6	-2.819584	-0.595129	1.568104
1	-1.855158	0.676740	2.979260
6	-2.574573	-0.172190	-0.853345
6	-3.090988	-0.908166	0.171825
1	-3.278768	-1.245084	2.310836
1	-2.780131	-0.395591	-1.897179
6	-1.146387	1.922646	-1.305458
6	-0.551302	2.975907	-0.425204
1	-1.184842	1.989831	-2.389640
1	-1.251129	3.838518	-0.486117
6	0.842134	3.477186	-0.788342
1	0.858341	3.868585	-1.812434
1	1.159632	4.277004	-0.108584
1	1.575843	2.659901	-0.722626
8	-3.894764	-1.979820	0.035856
6	-4.246052	-2.379461	-1.278184
1	-3.352052	-2.657475	-1.852834
1	-4.898666	-3.247546	-1.169824
1	-4.783631	-1.575164	-1.798431

II'b

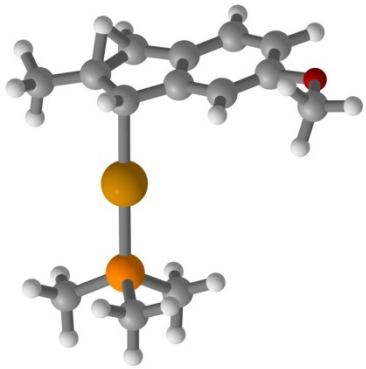


ΔE(DCE) -1097.530057 h.

ΔG(DCE)-1097.581629 h.

79	0.873934	0.198482	-0.310169
15	2.792071	-0.949718	0.407534
6	4.270697	0.107294	0.544050
1	4.096643	0.898336	1.282270
1	5.135789	-0.493211	0.855421
1	4.484960	0.573332	-0.424314
6	2.641690	-1.734754	2.045472
1	1.812655	-2.451122	2.040963
1	3.572474	-2.260089	2.297099
1	2.441827	-0.971850	2.806194
6	3.304136	-2.302394	-0.701775
1	3.508399	-1.904777	-1.702188
1	4.210781	-2.784395	-0.312461
1	2.503774	-3.046904	-0.776820
6	-1.862826	2.624045	0.634070
1	-2.044545	3.445345	1.326168
6	-2.423262	1.383632	0.709914
6	-3.409568	0.845633	1.602157
6	-1.910877	0.578239	-0.388309
6	-3.902073	-0.391458	1.353204
1	-3.759513	1.434046	2.448235
6	-2.468673	-0.687158	-0.647338
6	-3.447479	-1.152078	0.212343
1	-4.661229	-0.849532	1.983379
1	-2.113134	-1.277195	-1.489209
6	-0.872599	1.295069	-1.060856
6	-0.949708	2.727216	-0.532057
1	-0.767759	1.150868	-2.142125
1	-1.507842	3.309578	-1.294153
6	0.348225	3.476298	-0.244016
1	0.987691	3.495019	-1.134425
1	0.140081	4.512621	0.051169
1	0.908741	2.991942	0.567619
8	-4.064048	-2.326819	0.087942
6	-3.720633	-3.170959	-1.005779
1	-2.667977	-3.472684	-0.943666
1	-4.362630	-4.048670	-0.920067
1	-3.910977	-2.662120	-1.958739

TSII'b-III'b

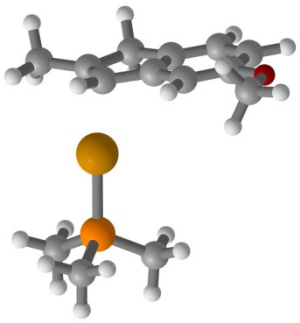


ΔE(DCE) -1097.508858 h.

ΔG(DCE) -1097.559719 h.

79	0.927027	0.198600	-0.287699
15	2.830676	-0.977443	0.398973
6	4.321019	0.054712	0.581002
1	4.151686	0.822262	1.344465
1	5.174887	-0.568333	0.878600
1	4.550011	0.549706	-0.369330
6	2.655794	-1.814276	2.008080
1	1.820573	-2.522450	1.971849
1	3.579402	-2.356125	2.251000
1	2.455299	-1.074816	2.791362
6	3.327254	-2.298843	-0.753522
1	3.543513	-1.872052	-1.739279
1	4.223413	-2.808298	-0.375292
1	2.515332	-3.027281	-0.856921
6	-1.718297	2.575638	0.749452
1	-1.799580	3.390928	1.466415
6	-2.427230	1.341918	0.764346
6	-3.480448	0.881594	1.580550
6	-1.953816	0.555868	-0.320541
6	-4.041822	-0.339537	1.302264
1	-3.839031	1.480107	2.416398
6	-2.557620	-0.673275	-0.622610
6	-3.592690	-1.109609	0.194904
1	-4.851310	-0.744321	1.906312
1	-2.205304	-1.260735	-1.467864
6	-0.865916	1.257964	-0.988196
6	-0.795586	2.577563	-0.356663
1	-0.743694	1.176902	-2.073186
1	-1.926866	3.132523	-0.502265
6	0.260323	3.615334	-0.588363
1	0.569068	3.625742	-1.639726
1	-0.092441	4.617047	-0.317349
1	1.143896	3.394164	0.023011
8	-4.253044	-2.271249	0.021748
6	-3.885260	-3.098763	-1.068830
1	-2.841094	-3.426847	-0.978847
1	-4.544825	-3.967658	-1.026804
1	-4.028061	-2.575950	-2.024110

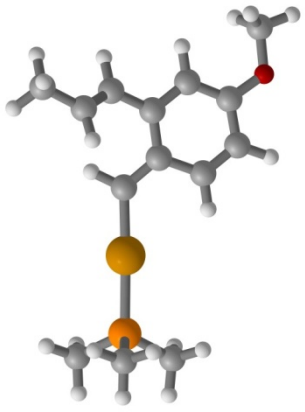
III'b



ΔE(DCE) -1097.556038 h.
ΔG(DCE) -1097.607252 h.

79	0.981714	0.254864	-0.260727
15	2.728492	-1.177952	0.325534
6	4.281657	-0.304814	0.696857
1	4.132614	0.383518	1.535770
1	5.059970	-1.033336	0.959478
1	4.604506	0.269987	-0.178099
6	2.384877	-2.187250	1.799110
1	1.510997	-2.822969	1.619640
1	3.253270	-2.819690	2.025372
1	2.177449	-1.538270	2.656970
6	3.159079	-2.368525	-0.981805
1	3.445213	-1.832765	-1.893692
1	3.999995	-2.991826	-0.650111
1	2.299340	-3.009734	-1.205024
6	-1.097897	2.363262	0.977510
1	-0.410366	2.278802	1.833398
6	-2.114417	1.262793	0.897985
6	-3.056563	0.823149	1.821064
6	-2.021270	0.629288	-0.349148
6	-3.898568	-0.228734	1.479527
1	-3.148441	1.295105	2.798876
6	-2.856013	-0.428542	-0.709549
6	-3.806254	-0.850978	0.223789
1	-4.652201	-0.592191	2.176225
1	-2.755894	-0.897839	-1.685668
6	-0.930272	1.262259	-1.104397
6	-0.378879	2.283393	-0.346673
1	-0.754261	1.123794	-2.172485
1	-1.562439	3.359277	1.066427
6	0.551686	3.350557	-0.806099
1	1.012539	3.106550	-1.769930
1	-0.003978	4.293015	-0.921040
1	1.344538	3.537520	-0.070544
8	-4.686384	-1.860279	0.009348
6	-4.647965	-2.530023	-1.236171
1	-3.673404	-3.011979	-1.398632
1	-5.426634	-3.294629	-1.194267
1	-4.859733	-1.840115	-2.064993

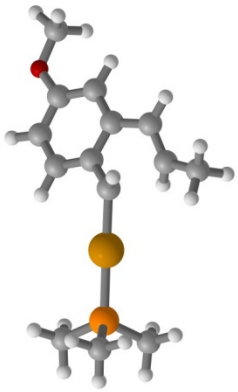
Ibb



ΔE(DCE) -1097.493511 h.
ΔG(DCE) -1097.546308 h.

79	-1.372567	0.145711	-0.126878
15	-3.660100	-0.458185	0.082916
6	-4.405925	-0.006685	1.685677
1	-4.330461	1.075700	1.838822
1	-5.463567	-0.301349	1.705690
1	-3.875857	-0.512487	2.500657
6	-4.753790	0.323551	-1.150524
1	-4.444816	0.033014	-2.160951
1	-5.793532	0.010379	-0.987097
1	-4.688929	1.414185	-1.065593
6	-4.008163	-2.241920	-0.078511
1	-3.476320	-2.796922	0.702528
1	-5.086364	-2.424390	0.021318
1	-3.670614	-2.603336	-1.056284
6	0.586305	0.739057	-0.313456
1	0.768117	1.715538	-0.775707
6	1.742988	0.053716	0.021243
6	1.654673	-1.343155	0.350642
6	3.069079	0.624563	-0.130733
6	2.751357	-2.149455	0.376480
1	0.661617	-1.757763	0.522964
6	4.173840	-0.218914	-0.144022
6	4.026670	-1.591782	0.097546
1	2.686536	-3.214558	0.585877
1	5.162073	0.212547	-0.286821
6	3.303695	2.053262	-0.236198
6	2.585998	3.008154	0.386214
6	2.876647	4.461228	0.297630
1	1.758439	2.716439	1.038323
1	3.067720	4.884155	1.293544
1	2.008577	5.003597	-0.103338
1	3.740536	4.668256	-0.344682
1	4.196345	2.351674	-0.792834
8	5.033095	-2.452546	0.115810
6	6.358022	-2.003995	-0.171928
1	6.984041	-2.896294	-0.139219
1	6.403705	-1.554829	-1.170696
1	6.693934	-1.287318	0.586297

TSIbb-IIbb

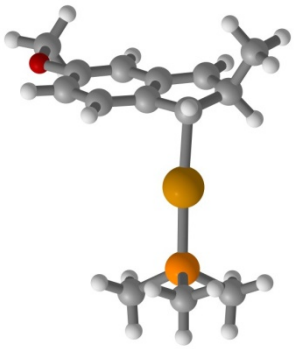


ΔE(DCE) -1097.474331 h.
ΔG(DCE)-1097.526850 h.

79	-1.267440	0.087089	-0.224920
15	-3.467289	-0.657597	0.258470
6	-4.154660	0.011433	1.810642
1	-4.194571	1.105397	1.759678
1	-5.168276	-0.378483	1.972935
1	-3.519152	-0.276328	2.655746
6	-4.721012	-0.232909	-0.996710
1	-4.451577	-0.678911	-1.960762
1	-5.704563	-0.610414	-0.686391
1	-4.775379	0.854867	-1.117500
6	-3.623725	-2.465401	0.445129
1	-2.971659	-2.815204	1.253536
1	-4.662841	-2.732135	0.678977
1	-3.325817	-2.963582	-0.484508
6	0.651613	0.751938	-0.638267

1	0.741192	1.473519	-1.456301
6	1.858774	0.051411	-0.320387
6	1.996437	-1.355296	-0.294524
6	3.000027	0.847912	-0.008167
6	3.246096	-1.903821	-0.151891
1	1.126590	-1.988051	-0.462922
6	4.284182	0.284113	0.124440
6	4.398169	-1.092276	0.045527
1	3.393421	-2.981615	-0.194301
1	5.135207	0.924787	0.342900
6	2.634423	2.199211	0.188724
6	1.290021	2.457242	0.422734
1	0.773429	1.807533	1.138323
1	3.352231	3.012178	0.058368
6	0.639598	3.780026	0.196172
1	0.505011	4.317128	1.144717
1	1.216038	4.412358	-0.488127
1	-0.363748	3.637490	-0.228363
8	5.546448	-1.778216	0.180524
6	6.745878	-1.046778	0.380481
1	6.696943	-0.460154	1.307547
1	7.542061	-1.788952	0.461163
1	6.946058	-0.382587	-0.470693

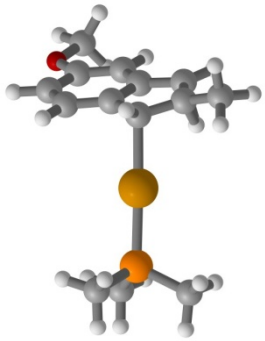
IIbb



ΔE(DCE) -1097.522724 h.
ΔG(DCE) -1097.573536 h.

79	-1.092135	0.300519	-0.194426
15	-2.980463	-1.000484	0.294510
6	-3.767575	-0.577101	1.882256
1	-4.084455	0.471774	1.873888
1	-4.643209	-1.218651	2.047614
1	-3.053932	-0.721796	2.700965
6	-4.314860	-0.846749	-0.935986
1	-3.955981	-1.173792	-1.918242
1	-5.171307	-1.466538	-0.639468
1	-4.634980	0.198527	-1.009149
6	-2.657191	-2.790339	0.406355
1	-1.913842	-2.986146	1.187099
1	-3.586194	-3.322569	0.650167
1	-2.268625	-3.160217	-0.548986
6	0.605624	1.631066	-0.656233
1	0.253148	2.083704	-1.588850
6	1.606252	0.631097	-0.685728
6	1.924663	-0.348189	-1.672420
6	2.424117	0.705399	0.514990
6	2.949024	-1.209572	-1.425765
1	1.351754	-0.403190	-2.596722
6	3.467046	-0.245489	0.763352
6	3.716175	-1.178456	-0.202340
1	3.227128	-1.968242	-2.155996
1	4.038034	-0.190039	1.686910
6	2.031507	1.808685	1.221769
6	0.922143	2.516102	0.537705
1	0.069044	2.602666	1.237489
1	2.453461	2.138382	2.169730
6	1.311715	3.939315	0.108016
1	1.599318	4.544779	0.975345
1	2.157610	3.904909	-0.591085
1	0.466958	4.427651	-0.391655
8	4.666035	-2.134265	-0.149079
6	5.487250	-2.174014	1.005024
1	4.888052	-2.373262	1.904090
1	6.196163	-2.989151	0.848825
1	6.033813	-1.228937	1.126708

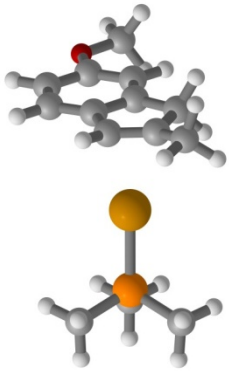
TSIIbb-IIIbb



ΔE(DCE) -1097.503443 h.
ΔG(DCE) -1097.554456 h.

79	-1.135691	0.256607	-0.232244
15	-2.996006	-1.039930	0.361678
6	-2.576937	-2.573745	1.252164
1	-2.041855	-2.331620	2.177205
1	-3.491714	-3.128843	1.499305
1	-1.931192	-3.200990	0.627617
6	-4.183869	-0.190003	1.450959
1	-4.568465	0.709138	0.957007
1	-5.021518	-0.859985	1.685798
1	-3.687548	0.106429	2.381745
6	-3.987211	-1.590160	-1.064384
1	-3.374083	-2.216181	-1.722471
1	-4.854401	-2.169213	-0.720570
1	-4.335915	-0.721045	-1.633218
6	0.611421	1.435275	-0.843577
1	0.224858	1.816090	-1.794699
6	1.741380	0.521844	-0.793694
6	2.077747	-0.587423	-1.594248
6	2.562343	0.835572	0.319009
6	3.194474	-1.323788	-1.274585
1	1.465447	-0.856719	-2.454345
6	3.683051	0.055823	0.671538
6	3.997125	-1.015449	-0.144266
1	3.493072	-2.177012	-1.882099
1	4.276073	0.318510	1.544137
6	2.032367	2.010602	0.931243
6	0.842416	2.408644	0.223494
1	0.719981	1.768742	1.313405
1	2.437291	2.555549	1.782102
6	0.171945	3.738814	0.329247
1	0.294901	4.182523	1.323190
1	0.622484	4.422602	-0.401683
1	-0.897574	3.657922	0.105700
8	5.053018	-1.844703	0.039512
6	5.912178	-1.589066	1.134283
1	5.373384	-1.671140	2.088792
1	6.694315	-2.349923	1.092430
1	6.367392	-0.591859	1.053540

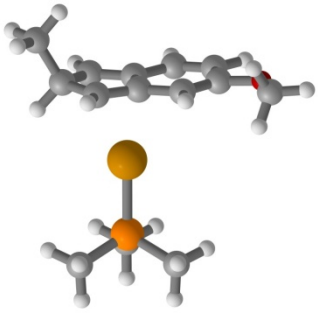
IIIbb



ΔE(DCE) -1097.556262 h.
ΔG(DCE) -1097.607248 h.

79	1.106977	0.345768	0.119064
15	2.804638	-1.226835	-0.189952
6	2.216748	-2.827449	-0.824355
1	1.733694	-2.688138	-1.797838
1	3.064692	-3.515951	-0.936351
1	1.489384	-3.260181	-0.128724
6	4.093279	-0.693127	-1.358814
1	4.555055	0.235572	-1.005598
1	4.862817	-1.471843	-1.442033
1	3.652104	-0.514950	-2.345452
6	3.696735	-1.621298	1.346945
1	3.000183	-2.024461	2.090014
1	4.476672	-2.365837	1.140097
1	4.160465	-0.715424	1.752652
6	-0.651161	1.608893	0.992997
1	-0.183146	1.947135	1.918823
6	-1.816080	0.722824	0.925640
6	-2.423056	-0.074566	1.897204
6	-2.311185	0.742590	-0.387688
6	-3.520755	-0.841784	1.538798
1	-2.046985	-0.098032	2.919266
6	-3.400583	-0.033289	-0.760248
6	-4.008336	-0.827565	0.220905
1	-4.028376	-1.472886	2.266168
1	-3.769703	-0.009215	-1.783395
6	-1.482360	1.683862	-1.212708
6	-0.428174	2.180485	-0.250425
1	-1.053499	1.222535	-2.115376
1	-2.071129	2.545611	-1.568062
6	0.440223	3.348800	-0.570259
1	0.958206	3.217060	-1.528966
1	-0.181488	4.251906	-0.663604
1	1.186703	3.529490	0.211826
8	-5.083370	-1.618358	-0.007693
6	-5.625320	-1.657597	-1.314665
1	-4.889011	-2.034210	-2.038349
1	-6.473560	-2.344014	-1.271377
1	-5.976705	-0.665142	-1.628933

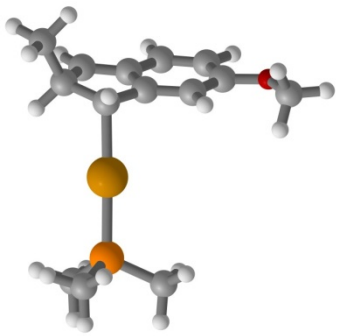
TSIIbb-II'bb



ΔE(DCE) -1097.503492 h.
ΔG(DCE) -1097.553766 h.

79	0.650896	0.168444	0.035710
15	2.793318	-0.667761	-0.078405
6	3.849107	0.219909	-1.262902
1	3.929810	1.274293	-0.976920
1	4.850073	-0.231326	-1.270336
1	3.416194	0.157397	-2.267089
6	3.688141	-0.609061	1.503810
1	3.148506	-1.190740	2.259176
1	4.693890	-1.029983	1.372183
1	3.771348	0.427179	1.848821
6	2.848594	-2.410547	-0.592593
1	2.404202	-2.522851	-1.587527
1	3.892267	-2.750379	-0.619202
1	2.285993	-3.026618	0.117183
6	-1.063967	2.254677	0.947880
1	-0.827805	2.828801	1.840278
6	-1.568750	0.980429	0.911612
6	-1.963656	0.063951	1.959364
6	-1.805115	0.596883	-0.508914
6	-2.548367	-1.104616	1.618027
1	-1.801306	0.332540	3.001737
6	-2.418737	-0.673196	-0.811702
6	-2.780316	-1.476727	0.228656
1	-2.876422	-1.816413	2.373536
1	-2.598603	-0.944413	-1.848982
6	-1.416219	1.646842	-1.303622
6	-1.006449	2.803275	-0.442935
1	0.003662	3.170705	-0.691627
1	-1.504350	1.700837	-2.385663
6	-1.985741	3.982338	-0.601006
1	-1.979910	4.344538	-1.635496
1	-3.006196	3.666012	-0.347972
1	-1.701998	4.810671	0.058722
8	-3.379968	-2.677068	0.114995
6	-3.678132	-3.146467	-1.189202
1	-2.760273	-3.263231	-1.781095
1	-4.158226	-4.118436	-1.061522
1	-4.364051	-2.458847	-1.701989

II'bb

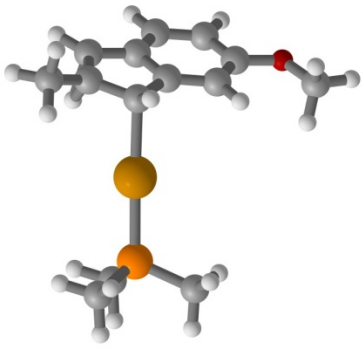


ΔE(DCE) -1097.529760 h.
ΔG(DCE) -1097.582896 h.

79	0.938201	0.281712	-0.259970
15	2.960289	-0.760589	0.325603
6	4.305337	-0.512464	-0.879404
1	4.522807	0.556519	-0.981896
1	5.210263	-1.034740	-0.541776
1	4.006781	-0.904520	-1.858049
6	3.663229	-0.197502	1.910310
1	2.953856	-0.391882	2.722511
1	4.601265	-0.730262	2.115418
1	3.862211	0.879327	1.869220
6	2.842023	-2.571070	0.502016
1	2.501738	-3.015440	-0.440024
1	3.823753	-2.987868	0.764023
1	2.120960	-2.821829	1.288068
6	-1.942127	2.355294	1.022453
1	-2.173672	3.082885	1.799120
6	-2.438462	1.087908	0.949497
6	-3.392445	0.401491	1.772979
6	-1.892818	0.442252	-0.235228
6	-3.816941	-0.824686	1.385324
1	-3.771404	0.870474	2.679030
6	-2.373571	-0.819964	-0.629613
6	-3.321112	-1.431278	0.171691

1	-4.548222	-1.391423	1.957611
1	-1.986199	-1.290250	-1.530461
6	-0.910422	1.294342	-0.829274
6	-1.032091	2.639019	-0.113438
1	-0.069939	3.013140	0.280838
1	-0.834881	1.304516	-1.922753
6	-1.607267	3.727915	-1.034436
1	-0.915894	3.917292	-1.863791
1	-2.569202	3.401234	-1.451765
1	-1.762204	4.667681	-0.491343
8	-3.867959	-2.620730	-0.075953
6	-3.478428	-3.330918	-1.247096
1	-4.059817	-4.253878	-1.243578
1	-3.712701	-2.747484	-2.146058
1	-2.407432	-3.566068	-1.217833

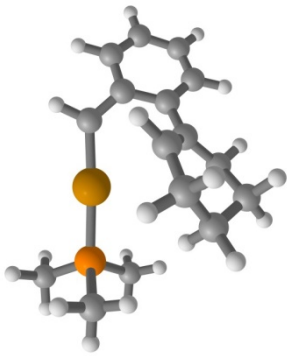
TSII'bb-III'bb



ΔE(DCE) -1097.506978 h.
ΔG(DCE) -1097.558189 h.

79	0.944157	0.227374	-0.259697
15	2.880096	-0.928634	0.380470
6	4.430718	-0.160175	-0.189535
1	4.525938	0.846870	0.231945
1	5.287521	-0.768342	0.129765
1	4.430060	-0.084879	-1.282617
6	3.096291	-1.109444	2.180471
1	2.236659	-1.636054	2.609663
1	4.011486	-1.678516	2.391609
1	3.171716	-0.121077	2.647454
6	2.954443	-2.631666	-0.263851
1	2.922058	-2.615797	-1.359041
1	3.884532	-3.114514	0.063816
1	2.098691	-3.208285	0.104411
6	-1.891608	2.565590	0.760737
1	-2.123079	3.423079	1.390013
6	-2.554843	1.302798	0.734263
6	-3.596852	0.787844	1.529801
6	-1.995372	0.531785	-0.318852
6	-4.098407	-0.454623	1.229505
1	-4.011496	1.370342	2.350810
6	-2.501292	-0.745114	-0.608120
6	-3.559745	-1.215593	0.158023
1	-4.919647	-0.888696	1.796408
1	-2.066883	-1.336001	-1.412117
6	-0.878237	1.262232	-0.904770
6	-0.877105	2.575626	-0.256029
1	-0.557182	2.378127	0.977012
1	-0.698937	1.246724	-1.985047
6	-0.172670	3.784598	-0.774201
1	0.831042	3.532281	-1.134001
1	-0.744681	4.189990	-1.619011
1	-0.092308	4.570767	-0.015539
8	-4.158455	-2.409950	-0.030883
6	-3.685024	-3.238469	-1.077954
1	-4.303349	-4.138012	-1.058023
1	-3.792516	-2.741271	-2.051564
1	-2.633594	-3.512500	-0.916738

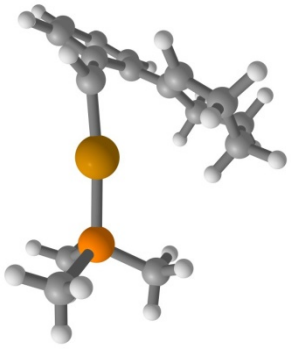
Ic



ΔE(DCE) -1099.637072 h.
ΔG(DCE) -1099.686760 h.

79	-0.654748	-0.843141	-0.203598
15	-2.861800	-0.244870	0.423938
6	-3.723969	0.902954	-0.702768
1	-3.784915	0.464773	-1.705343
1	-4.739466	1.095035	-0.331645
1	-3.184083	1.855049	-0.769366
6	-3.995311	-1.668833	0.542075
1	-3.607868	-2.394136	1.266544
1	-4.990997	-1.334187	0.861964
1	-4.076986	-2.159807	-0.434419
6	-2.979653	0.551915	2.061592
1	-2.381755	1.470920	2.082557
1	-4.025413	0.798554	2.287977
1	-2.596264	-0.129282	2.829817
6	1.229290	-1.524372	-0.674405
1	1.293256	-2.506549	-1.162356
6	2.491227	-1.011144	-0.359547
6	3.577564	-1.941650	-0.328624
6	2.694903	0.319819	0.165551
6	4.739755	-1.650600	0.344864
1	3.436759	-2.917227	-0.792531
6	3.875533	0.567246	0.873694
6	4.873333	-0.395245	0.960633
1	5.545620	-2.378230	0.404045
1	4.053224	1.548494	1.307885
1	5.794298	-0.153855	1.488876
6	1.724487	1.372074	-0.087396
6	1.108359	1.436835	-1.296984
6	1.417834	2.376199	0.996295
6	0.082576	2.458245	-1.658852
1	1.430039	0.759858	-2.090158
6	0.682812	3.604111	0.473583
1	0.804820	1.868683	1.764434
1	2.337429	2.680602	1.514407
6	-0.460857	3.192645	-0.441913
1	-0.724200	1.968376	-2.226546
1	0.534879	3.173781	-2.368048
1	0.317031	4.203082	1.317687
1	1.384666	4.241578	-0.088434
1	-1.055613	4.061372	-0.753623
1	-1.139680	2.523129	0.114700

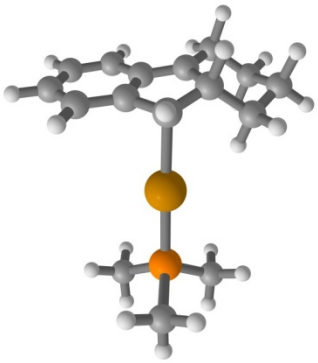
TSIc-IIc



ΔE(DCE) -1099.630768 h.
ΔG(DCE) -1099.680767 h.

79	-0.754831	-0.541457	-0.393218
15	-2.902196	-0.338145	0.558958
6	-3.399729	1.358686	1.005075
1	-3.371947	2.003278	0.118898
1	-4.417834	1.353602	1.416460
1	-2.711613	1.762945	1.756667
6	-4.245628	-0.929325	-0.522599
1	-4.081892	-1.982283	-0.777911
1	-5.212232	-0.827250	-0.011733
1	-4.263882	-0.343143	-1.448251
6	-3.115254	-1.281990	2.104134
1	-2.399869	-0.930163	2.856096
1	-4.135733	-1.149543	2.486702
1	-2.933699	-2.346730	1.919866
6	1.117878	-0.910799	-1.217362
1	1.129622	-1.382183	-2.211806
6	2.339048	-1.035202	-0.505397
6	3.121773	-2.213401	-0.566930
6	2.737673	0.029471	0.354481
6	4.127676	-2.398269	0.357838
1	2.869128	-2.993533	-1.283843
6	3.755007	-0.188502	1.299742
6	4.431018	-1.394144	1.301164
1	4.696909	-3.325862	0.361816
1	4.049651	0.603322	1.986206
1	5.239623	-1.556340	2.011368
6	2.071225	1.268453	0.086631
6	1.522650	1.433204	-1.171081
6	1.876269	2.301362	1.158885
6	0.599991	2.554845	-1.523636
1	1.981079	0.912775	-2.017000
6	1.265551	3.597907	0.638907
1	1.226034	1.861731	1.936656
1	2.836826	2.496837	1.658268
6	0.099258	3.302330	-0.295033
1	-0.231520	2.168486	-2.131383
1	1.148050	3.244395	-2.188980
1	0.947943	4.219054	1.485989
1	2.029758	4.173606	0.092042
1	-0.406442	4.227355	-0.600385
1	-0.649850	2.689210	0.235186

IIc

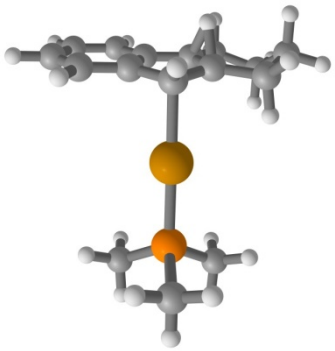


ΔE(DCE) -1099.681796 h.
ΔG(DCE) -1099.733809 h.

6	-3.310329	1.812726	1.109643
6	-2.664272	0.866411	0.256883
6	-1.622557	1.279605	-0.655322
6	-1.317248	2.658725	-0.763881
6	-1.982161	3.544733	0.045306
6	-2.966992	3.128648	0.997441
1	-4.069944	1.485807	1.818204
1	-0.558570	2.998638	-1.467966
1	-1.754106	4.607141	-0.029332
1	-3.445629	3.879643	1.621992
6	-1.071243	0.146300	-1.334134
79	0.907863	0.035862	-0.402496
15	3.058823	-0.123405	0.530129

6	3.446598	1.145862	1.778869
1	2.729224	1.085829	2.604994
1	4.461179	0.990643	2.168995
1	3.380788	2.143095	1.329840
6	4.408291	0.011268	-0.688126
1	5.379979	-0.093474	-0.187419
1	4.306184	-0.773882	-1.445649
1	4.363083	0.986038	-1.186899
6	3.373250	-1.704825	1.381426
1	4.393676	-1.717269	1.786860
1	2.658162	-1.835836	2.201350
1	3.254846	-2.535912	0.677006
6	-2.898735	-0.480805	0.070625
6	-3.861106	-1.367687	0.760756
6	-1.993445	-1.013166	-0.984398
6	-3.204827	-2.707822	1.128763
1	-4.691095	-1.568711	0.060073
1	-4.303423	-0.877983	1.637918
6	-1.386861	-2.362611	-0.563717
1	-2.635167	-1.207389	-1.868221
6	-2.469818	-3.309891	-0.062251
1	-3.976734	-3.391113	1.504633
1	-2.491984	-2.548392	1.953303
1	-0.829369	-2.789917	-1.407786
1	-0.654187	-2.185785	0.243081
1	-2.019585	-4.270775	0.220978
1	-3.186533	-3.522579	-0.873294
1	-0.785585	0.275349	-2.384743

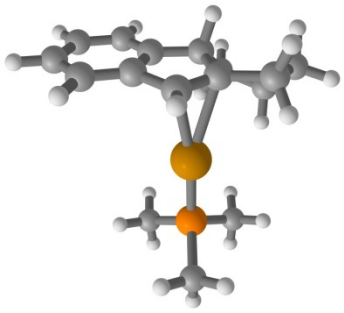
TSIIc-IIIc



ΔE(DCE) -1099.661586 h.
ΔG(DCE) -1099.711975 h.

6	-3.336591	1.819375	1.109565
6	-2.635479	0.893623	0.322813
6	-1.692269	1.307210	-0.651563
6	-1.491305	2.678081	-0.871412
6	-2.193016	3.585591	-0.095235
6	-3.101224	3.165783	0.899233
1	-4.047881	1.484096	1.864267
1	-0.783185	3.018867	-1.626616
1	-2.038150	4.652505	-0.250545
1	-3.624666	3.910838	1.495192
6	-1.085996	0.136076	-1.284585
79	0.910858	0.026559	-0.397621
15	3.061971	-0.065147	0.525889
6	3.459554	1.311814	1.651947
1	2.750146	1.327206	2.486871
1	4.477585	1.190862	2.045600
1	3.390118	2.265049	1.116087
6	4.406901	-0.050192	-0.703767
1	5.378603	-0.108412	-0.195551
1	4.302455	-0.905885	-1.379993
1	4.364245	0.870995	-1.295385
6	3.375591	-1.563593	1.515715
1	4.394322	-1.534114	1.924496
1	2.657131	-1.623973	2.340777
1	3.265101	-2.455102	0.888232
6	-2.713037	-0.542704	0.287255
6	-3.474757	-1.460513	1.189315
6	-1.820398	-1.009663	-0.744831
6	-2.936524	-2.890473	1.117364
1	-4.544078	-1.428350	0.928486
1	-3.409684	-1.062044	2.211663
6	-1.564876	-2.476841	-0.950130
1	-3.046415	-0.817809	-1.023124
6	-2.671516	-3.322968	-0.321889
1	-3.644890	-3.572279	1.603333
1	-1.995758	-2.951560	1.687248
1	-1.441640	-2.694326	-2.019741
1	-0.603102	-2.715736	-0.470910
1	-2.381921	-4.380338	-0.356151
1	-3.597789	-3.234804	-0.913903
1	-0.858247	0.159749	-2.355360

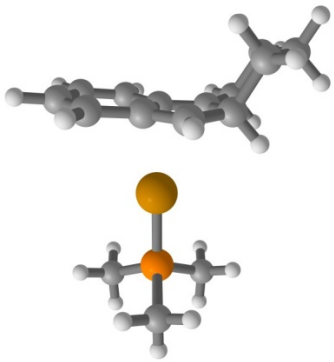
IIIc



ΔE(DCE) -1099.698196 h.
ΔG(DCE) -1099.747897 h.

6	3.352272	-0.989448	1.402504
6	2.638084	-0.273532	0.453939
6	2.193880	-0.898584	-0.726711
6	2.481427	-2.236204	-0.981621
6	3.213448	-2.947861	-0.030350
6	3.637342	-2.335193	1.151392
1	3.692755	-0.514593	2.323170
1	2.139930	-2.717677	-1.897452
1	3.452191	-3.995233	-0.208527
1	4.200660	-2.911731	1.883426
6	1.405135	0.078132	-1.502304
79	-0.643583	-0.077148	-0.460328
15	-2.725672	-0.632651	0.432094
6	-2.675906	-2.053119	1.568198
1	-1.978708	-1.849903	2.388385
1	-3.677717	-2.230884	1.980806
1	-2.340277	-2.948372	1.033512
6	-3.980290	-1.062683	-0.812539
1	-4.927582	-1.300912	-0.311158
1	-4.134816	-0.220591	-1.495806
1	-3.650603	-1.931713	-1.392060
6	-3.462872	0.718765	1.404042
1	-4.443989	0.405330	1.784739
1	-2.811804	0.968252	2.249899
1	-3.585318	1.609033	0.777146
6	2.218387	1.166962	0.436118
6	1.493486	1.756982	1.659523
6	1.413446	1.287557	-0.828748
6	0.537017	2.893151	1.252910
1	2.242153	2.118637	2.377297
1	0.934554	0.956183	2.167308
6	0.963426	2.656991	-1.229971
1	3.115598	1.787851	0.242622
6	0.986359	3.605424	-0.021384
1	0.437918	3.611800	2.076384
1	-0.472754	2.480389	1.083009
1	1.635349	3.029436	-2.019711
1	-0.037391	2.618440	-1.682520
1	0.344567	4.471414	-0.225473
1	2.002917	4.004876	0.121269
1	1.102681	-0.059604	-2.541784

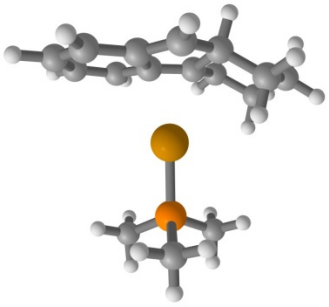
TSIIc-II'c



ΔE(DCE) -1099.656383 h.
ΔG(DCE) -1099.706059 h.

79	-0.761290	0.076063	0.097794
15	-2.905476	-0.737632	-0.109707
6	-2.969638	-2.362187	-0.924888
1	-2.404981	-3.096170	-0.339714
1	-4.013287	-2.692730	-1.011214
1	-2.527891	-2.292647	-1.924951
6	-3.763340	-0.958488	1.478360
1	-3.851073	0.005931	1.990783
1	-4.766623	-1.368186	1.302095
1	-3.198240	-1.647040	2.115719
6	-3.990674	0.337013	-1.095817
1	-3.577317	0.462664	-2.102427
1	-4.987678	-0.117830	-1.166696
1	-4.075238	1.321208	-0.622790
6	1.568328	0.223066	1.773719
1	1.481607	0.234928	2.856791
6	1.290357	1.264050	0.920955
6	0.868295	2.627592	1.154582
6	1.575780	0.832003	-0.476658
6	0.782484	3.479738	0.102250
1	0.646324	2.952767	2.169990
6	1.460058	1.794794	-1.548537
6	1.084815	3.065034	-1.254399
1	0.481406	4.512785	0.268468
1	1.684482	1.496152	-2.571875
1	1.002162	3.804241	-2.049146
6	2.021115	-0.472076	-0.450372
6	2.125660	-0.909458	0.979132
6	2.605099	-1.313420	-1.523250
6	3.634057	-1.147223	1.264728
1	1.603030	-1.864224	1.162052
6	4.079864	-1.593733	-1.178128
1	2.069568	-2.275780	-1.579992
1	2.516439	-0.835617	-2.507940
6	4.224062	-2.116711	0.245609
1	3.751417	-1.519298	2.290932
1	4.154759	-0.177122	1.206482
1	4.494959	-2.309257	-1.900395
1	4.654088	-0.659178	-1.283123
1	5.284901	-2.284577	0.477703
1	3.723295	-3.095456	0.335386

II'c



ΔE(DCE) -1099.669195 h.
ΔG(DCE) -1099.719148 h.

6	-1.725306	-1.634569	-1.493001
6	-1.854904	-0.629051	-0.461545
6	-2.294057	-1.039441	0.894951
6	-2.424790	-2.442143	1.188621
6	-2.234146	-3.347993	0.195106
6	-1.909506	-2.937542	-1.154650
1	-1.482734	-1.338783	-2.513193
1	-2.694386	-2.755330	2.196390
1	-2.343162	-4.411759	0.398302
1	-1.816693	-3.707914	-1.918609
6	-2.515995	0.071847	1.648329
79	0.443758	-0.112336	-0.118608
15	2.748010	-0.201077	0.202724
6	3.568444	-1.567005	-0.675298
1	3.384345	-1.482273	-1.751811
1	4.649607	-1.528985	-0.488068
1	3.173346	-2.526078	-0.322876
6	3.244391	-0.386081	1.942997
1	4.339764	-0.399484	2.014859
1	2.853967	0.449667	2.534074
1	2.844320	-1.322414	2.347117
6	3.582387	1.308960	-0.375333
1	4.663811	1.226614	-0.203426
1	3.396054	1.449355	-1.446089
1	3.194104	2.179367	0.165963
6	-1.779781	0.766274	-0.499941
6	-1.597144	1.745932	-1.613953
6	-2.307691	1.283221	0.807003
6	-0.832410	2.973646	-1.095053
1	-2.592034	2.065716	-1.971292
1	-1.086093	1.292654	-2.474846
6	-1.522252	2.490725	1.318019
1	-3.327879	1.649934	0.555801
6	-1.429996	3.529880	0.197949
1	-0.820843	3.753573	-1.868254
1	0.221085	2.692987	-0.916678
1	-2.010094	2.917523	2.204746
1	-0.514371	2.166698	1.627494
1	-0.835926	4.389448	0.536970
1	-2.442751	3.915047	-0.010385
1	-2.833973	0.095169	2.687757

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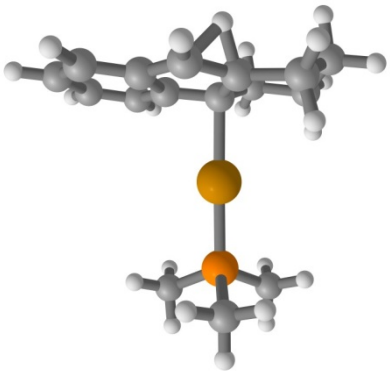
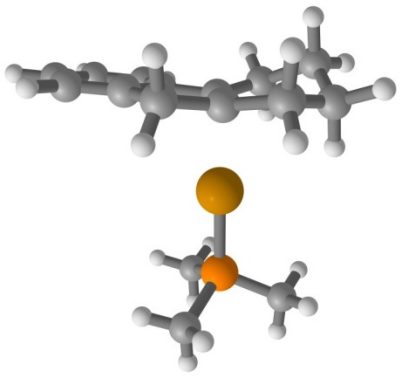


ΔE(DCE) -1099.652190 h.
ΔG(DCE) -1099.701280 h.

6	-2.116409	-1.632213	-1.447622
6	-2.028552	-0.677825	-0.416220
6	-2.562481	-0.991643	0.871675
6	-3.112967	-2.259262	1.145951
6	-3.147379	-3.190789	0.130846
6	-2.665171	-2.867086	-1.160463
1	-1.745872	-1.403290	-2.446897
1	-3.502465	-2.488356	2.136859
1	-3.563149	-4.180191	0.310919
1	-2.733675	-3.616726	-1.947685
6	-2.465500	0.170251	1.682400
79	0.629786	0.078319	-0.086906
15	2.876302	-0.513550	0.161383
6	3.295675	-2.163013	-0.489244
1	3.074475	-2.208916	-1.561280
1	4.363982	-2.363064	-0.331191

1	2.705313	-2.929323	0.025129
6	3.443556	-0.549388	1.892209
1	4.504372	-0.830344	1.929934
1	3.315020	0.438541	2.348289
1	2.856850	-1.279075	2.461243
6	4.033388	0.615289	-0.678610
1	5.064513	0.267080	-0.533119
1	3.811986	0.647205	-1.751193
1	3.932898	1.626439	-0.268598
6	-1.503668	0.676207	-0.411356
6	-1.537397	1.635950	-1.587426
6	-1.889572	1.230160	0.890607
6	-0.976176	2.998068	-1.174117
1	-2.583476	1.757619	-1.923787
1	-0.980569	1.237699	-2.447444
6	-1.473057	2.618121	1.295242
1	-3.123387	1.206594	0.926278
6	-1.642058	3.546168	0.089004
1	-1.105460	3.714374	-1.996746
1	0.110368	2.906364	-1.002823
1	-2.063933	2.967205	2.152414
1	-0.422547	2.595317	1.620787
1	-1.239258	4.538977	0.328389
1	-2.719697	3.682539	-0.104453
1	-2.767351	0.275410	2.722570

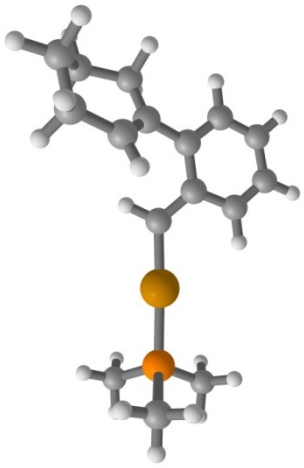
III'c



ΔE(DCE) -1099.708955 h.
ΔG(DCE) -1099.759893 h.

79	0.638511	0.116987	0.083808
15	2.771836	-0.806062	-0.092866
6	4.052900	0.418744	-0.501912
1	4.103060	1.184387	0.280076
1	5.027860	-0.079359	-0.583705
1	3.814283	0.903287	-1.455061
6	3.355035	-1.616434	1.427764
1	2.678077	-2.434030	1.698451
1	4.363725	-2.019519	1.266989
1	3.382474	-0.893476	2.250203
6	2.898146	-2.076619	-1.389979
1	2.634790	-1.644855	-2.361799
1	3.925451	-2.461837	-1.432073
1	2.211447	-2.901741	-1.172045
6	-1.946063	0.182869	1.823159
1	-2.746266	0.677515	2.398547
6	-2.498636	-0.865351	0.899386
6	-3.137982	-2.063600	1.179777
6	-2.286184	-0.472336	-0.435224
6	-3.574093	-2.856856	0.114210
1	-3.307667	-2.379704	2.208811
6	-2.717867	-1.260467	-1.498555
6	-3.369024	-2.459414	-1.209576
1	-4.085523	-3.796292	0.318546
1	-2.550606	-0.951532	-2.530436
1	-3.719610	-3.093300	-2.022365
6	-1.585559	0.820931	-0.436470
6	-1.334119	1.192587	0.879267
6	-1.469135	1.761927	-1.604924
6	-0.935309	2.582107	1.268343
1	-1.241206	-0.213698	2.568811
6	-1.388176	3.213523	-1.125508
1	-0.599961	1.506744	-2.231460
1	-2.348367	1.621224	-2.251194
6	-0.444577	3.380775	0.062296
1	-0.184522	2.566094	2.072092
1	-1.826042	3.071015	1.701874
1	-1.082571	3.860605	-1.957384
1	-2.395206	3.543740	-0.823147
1	-0.359888	4.440804	0.334243
1	0.570222	3.048610	-0.218103

Icc



ΔE(DCE) -1099.634469 h.
ΔG(DCE)-1099.686582 h.

79	1.404926	-0.106003	-0.117392
15	3.758637	-0.398988	0.033157
6	4.315174	-1.170524	1.589383
1	3.851590	-2.157404	1.700417
1	5.407258	-1.284512	1.581922
1	4.023433	-0.548526	2.443067
6	4.462257	-1.469678	-1.264780
1	4.261911	-1.042504	-2.253707
1	5.547195	-1.564639	-1.125712
1	4.004591	-2.463981	-1.213039
6	4.730222	1.140702	-0.078968
1	4.446684	1.821568	0.731433
1	5.802155	0.915812	-0.002146
1	4.534814	1.635231	-1.037175
6	-0.633066	0.078310	-0.270489
1	-1.174845	-0.748584	-0.743320
6	-1.452918	1.153960	0.081106
6	-0.841027	2.425459	0.308610
6	-2.895030	1.074558	0.024738
6	-1.586591	3.578974	0.320527
1	0.244055	2.456730	0.404542
6	-3.619361	2.271741	-0.006820
6	-2.979048	3.494413	0.141498
1	-1.111543	4.547618	0.456460
1	-4.703939	2.245780	-0.090284
1	-3.574892	4.405718	0.149050
6	-3.585112	-0.205585	0.046505
6	-3.096350	-1.228748	0.790768
6	-4.886281	-0.345668	-0.709636
6	-3.736212	-2.571721	0.897474
1	-2.205847	-1.061986	1.400757
6	-5.245085	-1.807418	-0.947026
1	-5.697902	0.141134	-0.142411
1	-4.818842	0.195589	-1.664616
6	-5.160961	-2.592835	0.353450
1	-3.704249	-2.910062	1.943156
1	-3.108548	-3.292522	0.343405
1	-6.250725	-1.874897	-1.382502
1	-4.549895	-2.241252	-1.684507
1	-5.492565	-3.629595	0.211288
1	-5.842236	-2.141298	1.092531

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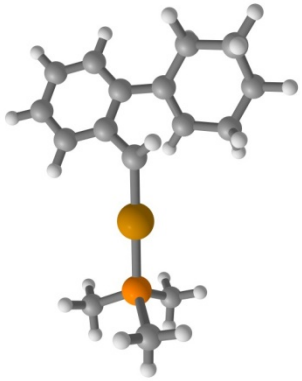
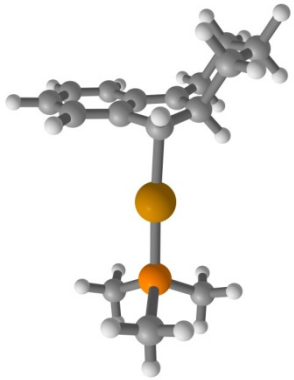


ΔE(DCE) -1099.626766
ΔG(DCE) -1099.678063

79	1.189266	0.012627	-0.209453
15	3.517940	-0.216542	0.182813
6	3.955713	-1.359918	1.535487
1	3.575434	-2.363775	1.315842
1	5.046836	-1.404238	1.650030
1	3.509962	-1.014240	2.475007
6	4.457815	-0.837344	-1.251554
1	4.339374	-0.150806	-2.097379
1	5.523417	-0.918244	-0.999681
1	4.080966	-1.823243	-1.546717
6	4.363182	1.336581	0.632458
1	3.935317	1.737989	1.558118
1	5.434970	1.150320	0.782571
1	4.234342	2.079356	-0.162840
6	-0.830582	0.210803	-0.587761
1	-1.240718	-0.386593	-1.406951
6	-1.672622	1.301041	-0.180310
6	-1.232273	2.635727	-0.088326
6	-3.029753	0.992825	0.112743
6	-2.162799	3.636710	0.118447
1	-0.180867	2.868667	-0.252836
6	-3.967011	2.022738	0.301498
6	-3.526713	3.333021	0.301390
1	-1.842099	4.676681	0.133516
1	-5.013205	1.790491	0.496574
1	-4.235202	4.140568	0.475184
6	-3.259681	-0.416284	0.226057
6	-2.147337	-1.186828	0.526616
6	-4.591425	-1.043972	-0.055871
6	-2.105095	-2.673293	0.336144
1	-1.393309	-0.759645	1.193186
6	-4.446168	-2.482771	-0.547906
1	-5.176483	-1.031386	0.880387
1	-5.155466	-0.435612	-0.775522
6	-3.509292	-3.277089	0.350234
1	-1.466636	-3.134514	1.100065
1	-1.623831	-2.891511	-0.633335
1	-5.436783	-2.952684	-0.593720
1	-4.050867	-2.477217	-1.576340
1	-3.462853	-4.326790	0.032786
1	-3.899144	-3.274614	1.380562

IIcc



ΔE(DCE) -1099.681479 h.
ΔG(DCE) -1099.732543 h.

79	1.049271	-0.123879	-0.309115
15	3.277323	-0.223960	0.434130
6	3.623312	-1.658349	1.505438
1	3.398214	-2.586629	0.968247
1	4.680684	-1.660186	1.802223
1	2.997045	-1.613074	2.403502
6	4.497729	-0.365907	-0.913344
1	4.443066	0.516632	-1.560375
1	5.510203	-0.444415	-0.495475
1	4.286091	-1.256152	-1.516264
6	3.845080	1.209590	1.406057
1	3.216446	1.331702	2.295173
1	4.886827	1.058043	1.718703
1	3.779442	2.120983	0.801416
6	-1.003828	-0.136616	-1.040315
1	-0.848396	-0.292076	-2.115037
6	-1.500093	1.138243	-0.618192
6	-1.241204	2.439638	-1.112752
6	-2.432637	0.981561	0.475363
6	-1.850837	3.508000	-0.504211
1	-0.560938	2.581027	-1.951634
6	-3.027185	2.118657	1.102093
6	-2.731849	3.358267	0.613404
1	-1.659440	4.512820	-0.878527
1	-3.704359	1.990646	1.945247
1	-3.169150	4.247874	1.061427
6	-2.643553	-0.367959	0.678740
6	-1.846786	-1.156510	-0.292083
6	-3.614935	-1.055876	1.551885
6	-2.844247	-1.931989	-1.189390
1	-1.251121	-1.914587	0.249417
6	-4.573933	-1.861783	0.645521
1	-3.081246	-1.760011	2.210456
1	-4.167187	-0.355558	2.190353
6	-3.808443	-2.743658	-0.332649
1	-2.277796	-2.572167	-1.878535
1	-3.397709	-1.201304	-1.802595
1	-5.239971	-2.461678	1.278627
1	-5.209739	-1.156617	0.087331
1	-4.515555	-3.278140	-0.981710
1	-3.247251	-3.513147	0.222760

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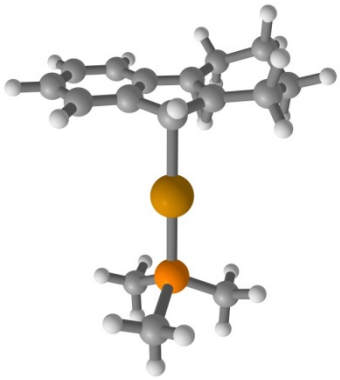
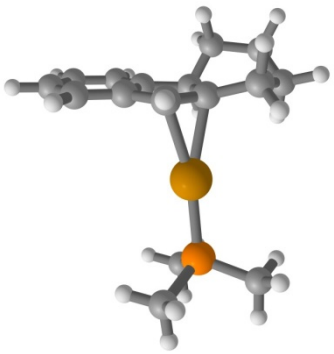


ΔE(DCE) -1099.658625 h.

ΔG(DCE)-1099.709429 h.

79	0.972086	-0.013215	-0.354132
15	3.158747	-0.123360	0.491014
6	3.623116	-1.773869	1.110256
1	3.511741	-2.517837	0.313315
1	4.665800	-1.766000	1.454274
1	2.971184	-2.054330	1.945221
6	4.450284	0.282407	-0.728727
1	4.305496	1.301286	-1.104552
1	5.440936	0.207090	-0.261191
1	4.396952	-0.413056	-1.573630
6	3.490428	0.994077	1.892410
1	2.826014	0.749571	2.728707
1	4.534173	0.886551	2.216610
1	3.310080	2.032930	1.594249
6	-1.055751	0.085957	-1.160482
1	-0.832408	-0.008290	-2.228574
6	-1.665459	1.306339	-0.633506
6	-1.402074	2.657734	-0.904411
6	-2.644080	0.971703	0.337115
6	-2.116259	3.626099	-0.218730
1	-0.650422	2.935633	-1.643154
6	-3.338439	1.959514	1.050682
6	-3.074490	3.285357	0.757950
1	-1.932363	4.677992	-0.433518
1	-4.077616	1.688513	1.804034
1	-3.609074	4.075747	1.281503
6	-2.763853	-0.464581	0.382635
6	-1.814443	-1.007362	-0.552816
6	-3.762139	-1.308915	1.116279
6	-1.838613	-2.449403	-0.949005
1	-1.541743	-0.936597	0.712401
6	-3.921803	-2.676722	0.449423
1	-3.467484	-1.417701	2.171288
1	-4.716153	-0.764459	1.129061
6	-2.574861	-3.297228	0.087652
1	-0.819108	-2.815234	-1.128941
1	-2.365633	-2.500596	-1.915768
1	-4.488029	-3.342633	1.112004
1	-4.518925	-2.562659	-0.469199
1	-2.715254	-4.310854	-0.306941
1	-1.953581	-3.397321	0.993689

IIIcc



ΔE(DCE) -1099.697981 h.

ΔG(DCE) -1099.749134 h.

79	-0.820562	0.039920	-0.317320
15	-3.010205	-0.280175	0.437248
6	-4.017781	1.235380	0.409110
1	-4.064457	1.634748	-0.609895
1	-5.034582	1.007846	0.755609
1	-3.573926	1.992171	1.065236
6	-3.939776	-1.483953	-0.562553
1	-3.433208	-2.454885	-0.544467
1	-4.953140	-1.597044	-0.155389
1	-4.003363	-1.138064	-1.600051
6	-3.126596	-0.893407	2.146516
1	-2.654023	-0.182870	2.833467
1	-4.182795	-1.013168	2.421461
1	-2.618733	-1.860218	2.233501
6	1.238646	-0.144262	-1.385900
1	0.920272	-0.178053	-2.428886
6	1.953022	-1.233579	-0.705800
6	2.135881	-2.564322	-1.072885
6	2.505564	-0.724827	0.484059
6	2.890397	-3.382976	-0.233277
1	1.706842	-2.954626	-1.995190
6	3.242931	-1.548134	1.322472
6	3.437231	-2.881412	0.951286
1	3.057622	-4.424548	-0.502844
1	3.672444	-1.164325	2.248361
1	4.027370	-3.536955	1.589834
6	2.150886	0.725527	0.625429
6	1.348959	1.011646	-0.630465
6	3.320576	1.718999	0.643414
6	1.186034	2.443665	-1.053246
1	1.545695	0.894374	1.535151
6	2.809325	3.164738	0.755643
1	4.000900	1.476364	1.470190
1	3.896798	1.578324	-0.285044
6	1.412867	3.362684	0.142576
1	0.213221	2.623834	-1.528860
1	1.944274	2.647396	-1.829586
1	2.781056	3.466742	1.811832
1	3.528920	3.834429	0.264645
1	1.274557	4.409686	-0.154007
1	0.636778	3.153230	0.896196

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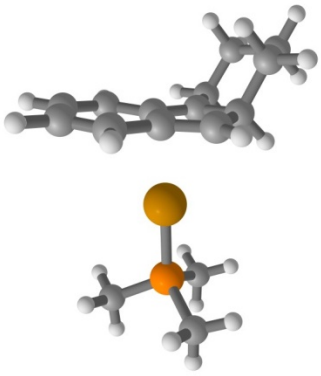


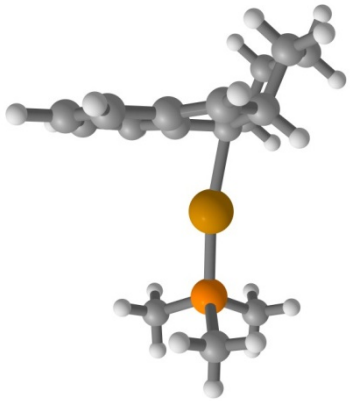
ΔE(DCE) -1099.656383 h.

ΔG(DCE) -1099.706059 h.

79	-0.761290	0.076063	0.097794
15	-2.905476	-0.737632	-0.109707
6	-2.969638	-2.362187	-0.924888
1	-2.404981	-3.096170	-0.339714
1	-4.013287	-2.692730	-1.011214
1	-2.527891	-2.292647	-1.924951
6	-3.763340	-0.958488	1.478360
1	-3.851073	0.005931	1.990783
1	-4.766623	-1.368186	1.302095
1	-3.198240	-1.647040	2.115719
6	-3.990674	0.337013	-1.095817
1	-3.577317	0.462664	-2.102427
1	-4.987678	-0.117830	-1.166696
1	-4.075238	1.321208	-0.622790

6	1.568328	0.223066	1.773719
1	1.481607	0.234928	2.856791
6	1.290357	1.264050	0.920955
6	0.868295	2.627592	1.154582
6	1.575780	0.832003	-0.476658
6	0.782484	3.479738	0.102250
1	0.646324	2.952767	2.169990
6	1.460058	1.794794	-1.548537
6	1.084815	3.065034	-1.254399
1	0.481406	4.512785	0.268468
1	1.684482	1.496152	-2.571875
1	1.002162	3.804241	-2.049146
6	2.021115	-0.472076	-0.450372
6	2.125660	-0.909458	0.979132
6	2.605099	-1.313420	-1.523250
6	3.634057	-1.147223	1.264728
1	1.603030	-1.864224	1.162052
6	4.079864	-1.593733	-1.178128
1	2.069568	-2.275780	-1.579992
1	2.516439	-0.835617	-2.507940
6	4.224062	-2.116711	0.245609
1	3.751417	-1.519298	2.290932
1	4.154759	-0.177122	1.206482
1	4.494959	-2.309257	-1.900395
1	4.654088	-0.659178	-1.283123
1	5.284901	-2.284577	0.477703
1	3.723295	-3.095456	0.335386

II'cc



ΔE(DCE) -1099.671281 h.
ΔG(DCE) -1099.721874 h.

79	-0.690379	-0.206677	-0.065823
15	-3.017030	-0.237511	0.129651
6	-3.752584	-1.880327	-0.143054
1	-3.355487	-2.592489	0.588940
1	-4.843700	-1.820686	-0.033769
1	-3.509857	-2.238191	-1.149570
6	-3.615485	0.271964	1.771670
1	-3.285419	1.293340	1.990833
1	-4.712493	0.232891	1.793936
1	-3.214762	-0.400236	2.538356
6	-3.869727	0.861507	-1.044925
1	-3.621133	0.576593	-2.073267
1	-4.955459	0.785286	-0.900627
1	-3.555661	1.898096	-0.880359
6	2.165134	0.533374	1.832193
1	2.427939	0.698966	2.874784
6	1.878982	1.496400	0.912684
6	1.868592	2.930252	1.005020
6	1.567181	0.847485	-0.369762
6	1.659706	3.659217	-0.122215
1	2.043506	3.408607	1.967621
6	1.404250	1.665186	-1.539562
6	1.455183	3.018780	-1.399876
1	1.659646	4.746544	-0.080874
1	1.238069	1.204316	-2.512750
1	1.338360	3.650905	-2.278853
6	1.569124	-0.551425	-0.199051
6	2.103933	-0.808067	1.198458
6	1.750402	-1.594885	-1.269055
6	3.542261	-1.395273	1.089973
1	1.488259	-1.521825	1.773220
6	3.198676	-2.097468	-1.287170
1	1.094220	-2.457141	-1.067440
1	1.455044	-1.198858	-2.251092
6	3.615534	-2.551780	0.103293
1	3.879960	-1.690064	2.092218
1	4.213574	-0.591416	0.746864
1	3.290673	-2.915968	-2.013832
1	3.865661	-1.286960	-1.625533
1	4.642249	-2.943075	0.088072
1	2.965204	-3.378141	0.436619

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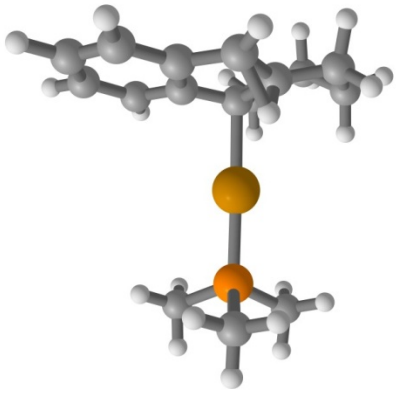
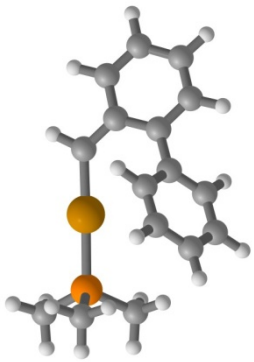


ΔE(DCE) -1099.645262 h.
ΔG(DCE) -1099.695360 h.

79	0.661271	0.113649	-0.082650
15	2.918695	-0.438706	0.134329
6	4.058847	0.955447	-0.137021
1	3.872474	1.740140	0.604699
1	5.096421	0.608069	-0.042564
1	3.908712	1.374393	-1.138110
6	3.367061	-1.083869	1.777178
1	2.778677	-1.980058	2.002884
1	4.435111	-1.338120	1.794791
1	3.164724	-0.326999	2.543148
6	3.470577	-1.721603	-1.034427
1	3.328035	-1.374583	-2.063839
1	4.534005	-1.939838	-0.869701
1	2.887591	-2.637537	-0.888038
6	-2.485766	0.099144	1.704229
1	-2.829781	0.209493	2.730133
6	-2.557408	-1.056999	0.882452
6	-3.056297	-2.347891	1.149673
6	-2.022327	-0.725640	-0.397718
6	-3.078233	-3.267137	0.123374
1	-3.437625	-2.597989	2.138720
6	-2.051096	-1.687136	-1.429630
6	-2.587107	-2.929894	-1.161949
1	-3.481932	-4.263639	0.293068
1	-1.656414	-1.448732	-2.417730
1	-2.630993	-3.676436	-1.953776
6	-1.506493	0.628400	-0.381141
6	-1.841034	1.152414	0.950333
6	-1.518087	1.565136	-1.592513
6	-1.853241	2.625063	1.262702
1	-1.146284	0.516482	1.781787
6	-1.950308	2.981375	-1.207960
1	-0.535173	1.619511	-2.084360
1	-2.204774	1.152464	-2.346864
6	-1.296762	3.432366	0.093425
1	-1.316793	2.840324	2.195919
1	-2.901120	2.916047	1.436038
1	-1.706924	3.670329	-2.027085
1	-3.045403	3.015336	-1.082831
1	-1.484756	4.498120	0.275957
1	-0.202579	3.310503	0.026119

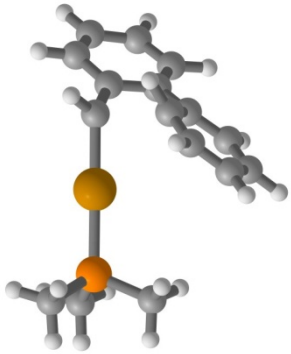
IV



ΔE(DCE)-1097.286187 h.
ΔG(DCE)-1097.336036 h.

79	-0.613679	-0.871876	-0.113651
15	-2.843513	-0.175635	0.307666
6	-3.596719	0.770800	-1.059086
1	-3.595188	0.171102	-1.976328
1	-4.630800	1.038358	-0.804008
1	-3.022524	1.688374	-1.238664
6	-4.023298	-1.530722	0.620746
1	-3.703841	-2.107721	1.495959
1	-5.026713	-1.123717	0.803360
1	-4.057981	-2.200661	-0.245751
6	-3.018760	0.923333	1.752112
1	-2.423237	1.831291	1.597798
1	-4.072229	1.201308	1.888022
1	-2.658094	0.418062	2.655118
6	1.297957	-1.551147	-0.429281
1	1.406068	-2.604022	-0.721946
6	2.542351	-0.932905	-0.248885
6	3.693985	-1.777572	-0.200748
6	2.692981	0.460987	0.087538
6	4.904533	-1.316446	0.265796
1	3.581024	-2.818444	-0.500936
6	3.924024	0.894351	0.570303
6	5.007321	0.021771	0.666504
1	5.767329	-1.975326	0.322112
1	5.959723	0.400503	1.033959
6	1.613229	1.436121	-0.107504
6	1.279373	2.338682	0.912584
6	0.931333	1.510729	-1.333584
6	0.268094	3.273505	0.720862
6	-0.063376	2.464949	-1.529963
1	1.214480	0.845416	-2.148605
6	-0.403483	3.340190	-0.500881
1	0.003157	3.954640	1.527783
1	-0.570509	2.524366	-2.491848
1	-1.185674	4.082920	-0.652359
1	4.055284	1.943564	0.829934
1	1.795804	2.282990	1.870776

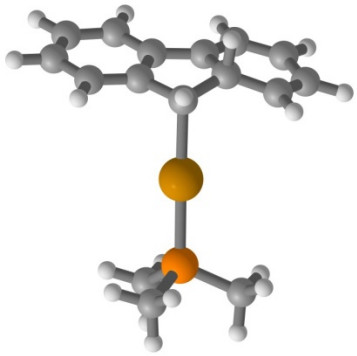
TSIV-V



ΔE(DCE)-1097.267084 h.
ΔG(DCE) -1097.315563 h.

79	-0.707493	-0.527733	-0.385815
15	-2.857115	-0.375772	0.553555
6	-4.207724	-0.966093	-0.518387
1	-4.059747	-2.025649	-0.755102
1	-5.173338	-0.841069	-0.010682
1	-4.216285	-0.395794	-1.454065
6	-3.077234	-1.288309	2.115330
1	-2.359497	-0.927251	2.860539
1	-4.096945	-1.142313	2.494794
1	-2.902781	-2.357361	1.950518
6	-3.310407	1.343390	0.957554
1	-3.284587	1.954444	0.047519
1	-4.318258	1.381221	1.391734
1	-2.592406	1.757384	1.675643
6	1.203786	-0.679139	-1.213072
1	1.255833	-1.046004	-2.248716
6	2.429352	-0.830441	-0.472910
6	3.216558	-1.996315	-0.522917
6	2.810257	0.240711	0.371624
6	4.264596	-2.133589	0.370693
1	2.961040	-2.800252	-1.211901
6	3.878715	0.089775	1.262888
6	4.589956	-1.099411	1.266147
1	4.851301	-3.050359	0.375484
1	5.433574	-1.221732	1.942551
6	2.032217	1.429315	0.112938
6	1.685048	2.391505	1.073386
6	1.433073	1.491031	-1.177855
6	0.723140	3.341778	0.776217
6	0.440592	2.460700	-1.456062
1	1.973434	1.079874	-2.038295
6	0.089449	3.371398	-0.482641
1	0.432826	4.065092	1.536154
1	-0.002867	2.506213	-2.448679
1	-0.660499	4.132547	-0.688378
1	2.122139	2.346641	2.069989
1	4.177473	0.914049	1.909357

V

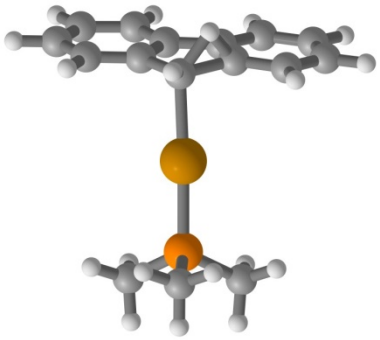


ΔE(DCE)-1097.292523 h.
ΔG(DCE) -1097.342815 h.

79	-0.845315	-0.086707	-0.414642
15	-2.994702	-0.080248	0.540172
6	-3.745062	1.576273	0.677670
1	-3.840571	2.026072	-0.317092
1	-4.740292	1.497557	1.135205
1	-3.113417	2.223239	1.296949
6	-4.232949	-1.051977	-0.380900
1	-3.924142	-2.102176	-0.429978
1	-5.208617	-0.984865	0.118954
1	-4.324498	-0.665032	-1.401982
6	-3.070670	-0.746376	2.236254
1	-2.420084	-0.160583	2.895291
1	-4.101723	-0.698258	2.610929
1	-2.731704	-1.788356	2.244751
6	1.132102	-0.062807	-1.293506
1	0.972785	-0.214189	-2.367978
6	1.889086	-1.112684	-0.626812
6	1.837261	-2.507088	-0.805634
6	2.793389	-0.573853	0.337328
6	2.617635	-3.310465	0.002237
1	1.171207	-2.940818	-1.551026
6	3.570019	-1.412480	1.167920

6	3.475010	-2.773631	0.995627
1	2.572141	-4.391845	-0.119743
1	4.066162	-3.447803	1.611758
6	2.731414	0.834447	0.263122
6	3.247444	1.820806	1.120946
6	1.902248	1.210868	-0.905224
6	2.809443	3.116067	0.969112
6	1.374656	2.587795	-0.910538
1	2.671344	1.279512	-1.719446
6	1.857630	3.500225	-0.031367
1	3.172109	3.879215	1.656088
1	0.668617	2.869396	-1.690880
1	1.524521	4.534857	-0.068281
1	4.241479	-0.988213	1.913297
1	3.913175	1.555095	1.939919

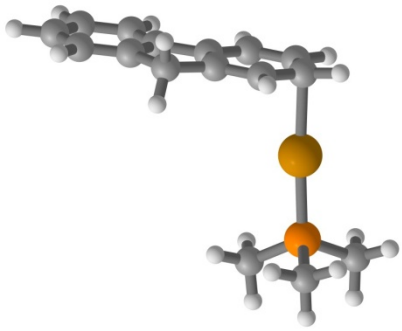
TSV-VI



ΔE(DCE) -1097.272389 h.
ΔG(DCE) -1097.322036 h.

79	-0.869189	-0.044632	-0.419427
15	-2.974219	-0.081559	0.556181
6	-3.308588	1.334099	1.650361
1	-3.255194	2.268373	1.080504
1	-4.311140	1.232731	2.086810
1	-2.566322	1.369377	2.455214
6	-4.342227	-0.081181	-0.644444
1	-4.265970	-0.957244	-1.297610
1	-5.300904	-0.111617	-0.109707
1	-4.301170	0.823349	-1.260864
6	-3.260368	-1.553603	1.586979
1	-2.510460	-1.606157	2.383662
1	-4.261901	-1.499181	2.033596
1	-3.186827	-2.458668	0.973869
6	1.165738	-0.100738	-1.325741
1	0.793334	-0.211703	-2.352578
6	1.902053	-1.161971	-0.640202
6	1.860459	-2.545005	-0.856620
6	2.738342	-0.616295	0.361811
6	2.628643	-3.364242	-0.045642
1	1.222213	-2.964321	-1.633876
6	3.511930	-1.460293	1.173535
6	3.446501	-2.826945	0.967060
1	2.599918	-4.442837	-0.191465
1	4.038582	-3.496750	1.588154
6	2.649244	0.819737	0.328535
6	3.222112	1.798720	1.151522
6	1.770895	1.229036	-0.714545
6	2.921012	3.131674	0.930213
6	1.456743	2.589669	-0.929901
1	2.112421	0.682058	-1.788316
6	2.045808	3.524227	-0.104377
1	3.364832	3.894577	1.566942
1	0.783029	2.881625	-1.733667
1	1.829406	4.580404	-0.251404
1	4.156344	-1.047083	1.948711
1	3.889232	1.511071	1.962766

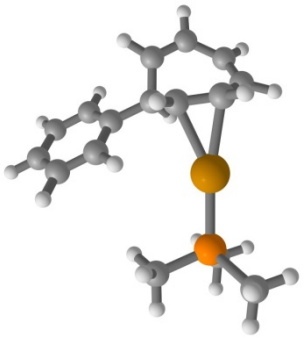
VI



ΔE(DCE) -1097.352248 h.
ΔG(DCE) -1097.403101 h.

79	-1.421874	-0.498731	0.017232
15	-3.012180	1.193882	-0.030134
6	-4.390913	0.854540	-1.168112
1	-4.913464	-0.058539	-0.862641
1	-5.096423	1.695879	-1.157102
1	-4.007618	0.717883	-2.185264
6	-3.790695	1.511494	1.583658
1	-3.029903	1.818756	2.309592
1	-4.537934	2.309718	1.483643
1	-4.279875	0.602290	1.949910
6	-2.348377	2.803407	-0.559743
1	-1.921470	2.717494	-1.564995
1	-3.154849	3.548478	-0.570204
1	-1.562604	3.130401	0.130072
6	2.843060	-0.220138	1.834134
1	2.326989	0.525949	2.456818
6	3.823249	0.412730	0.885369
6	4.939089	1.193119	1.159329
6	3.479003	0.112592	-0.444877
6	5.704884	1.668154	0.093716
1	5.214227	1.431491	2.186523
6	4.244764	0.586238	-1.510192
6	5.361704	1.367560	-1.229080
1	6.582483	2.280798	0.294421
1	5.975140	1.747751	-2.044184
6	2.279899	-0.717634	-0.434959
6	1.551283	-1.265143	-1.490987
6	1.893553	-0.926640	0.906980
6	0.435945	-2.047486	-1.201599
6	0.786496	-1.702763	1.203737
1	3.330303	-0.916385	2.532914
6	0.035229	-2.270886	0.140952
1	-0.121316	-2.523886	-2.006163
1	0.498983	-1.904320	2.235106
1	-0.711775	-3.036791	0.358228
1	3.980130	0.350882	-2.540857
1	1.850699	-1.101166	-2.525054

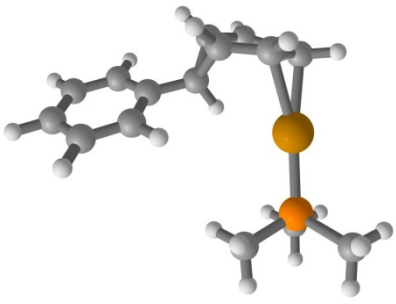
VIIa



ΔE(DCE) -1098.649400 h.
ΔG(DCE) -1098.700023 h.

6	-0.882143	-3.130294	0.344309
6	-2.120429	-3.311348	0.867067
6	-3.319897	-2.628883	0.453721
6	-0.607558	-2.241778	-0.765711
6	-3.374117	-1.357279	0.021594
6	-1.250638	-1.040988	-0.965573
6	-2.161616	-0.474046	0.085601
1	-0.092079	-3.816296	0.637731
1	-4.241034	-3.206339	0.490699
1	-2.246354	-4.140449	1.560213
1	-0.032208	-2.664915	-1.590583
1	-4.299694	-0.947397	-0.376116
1	-1.247793	-0.595998	-1.959903
1	-1.689136	-0.664959	1.064502
6	-2.441555	1.005703	-0.013567
6	-3.522062	1.539795	0.688792
6	-1.619332	1.875784	-0.725480
6	-3.781282	2.902034	0.670750
1	-4.165717	0.879188	1.265021
6	-1.875621	3.241930	-0.744397
1	-0.758306	1.496515	-1.271448
6	-2.958787	3.759599	-0.049706
1	-4.628098	3.296285	1.224061
1	-1.222518	3.902084	-1.307549
1	-3.160894	4.825954	-0.066073
79	0.967413	-0.583590	-0.241798
15	2.752232	0.805028	0.359700
6	3.067188	0.893710	2.143804
1	3.870103	1.613172	2.334891
1	2.161631	1.213798	2.663788
1	3.363484	-0.088688	2.517780
6	2.430334	2.517489	-0.148969
1	1.514799	2.872784	0.331234
1	3.269625	3.155555	0.145866
1	2.300981	2.562815	-1.233075
6	4.347488	0.366196	-0.383181
1	4.266428	0.379299	-1.472074
1	5.108801	1.086038	-0.065238
1	4.639059	-0.636002	-0.061490

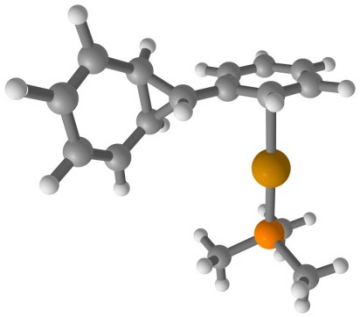
VIIb



ΔE(DCE) -1098.649650 h.
ΔG(DCE) -1098.701019 h.

6	-1.645722	-1.466932	-0.963225
6	-1.988857	-0.650866	0.245244
6	-2.324624	-2.102434	0.295304
6	-0.284765	-1.910776	-1.254941
6	-1.482944	-2.993242	1.089036
6	0.449103	-2.636740	-0.341970
6	-0.164883	-3.146050	0.870734
1	-2.288526	-1.297198	-1.822243
1	-1.131895	-0.363796	0.859652
1	-3.376149	-2.361226	0.201331
1	0.055697	-1.860955	-2.286129
1	-1.966185	-3.564754	1.876769
1	1.388589	-3.083831	-0.661332
1	0.427365	-3.789096	1.512422
6	-3.036378	0.397285	0.113828
6	-4.263769	0.300691	0.760698
6	-2.760505	1.528198	-0.654829
6	-5.204049	1.317389	0.638759
1	-4.484588	-0.573699	1.367096
6	-3.694884	2.545650	-0.773759
1	-1.801893	1.597530	-1.167594
6	-4.921307	2.440091	-0.126449
1	-6.160500	1.231566	1.145425
1	-3.471043	3.420515	-1.376521
1	-5.656886	3.232763	-0.222243
79	1.305945	-0.450195	-0.219239
15	2.459767	1.513863	0.325481
6	1.509999	3.010680	-0.062743
1	0.574218	3.009307	0.501045
1	2.094709	3.896737	0.205241
1	1.279357	3.035733	-1.130263
6	2.864544	1.656376	2.088158
1	3.507542	0.826084	2.387853
1	3.383260	2.603592	2.269224
1	1.947215	1.626027	2.680424
6	4.038474	1.712749	-0.545940
1	4.505459	2.656602	-0.246446
1	4.704934	0.883473	-0.298993
1	3.866569	1.719634	-1.624459

VIIc

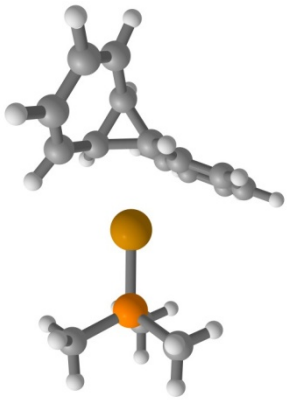


ΔE(DCE) -1098.646245 h.
ΔG(DCE) -1098.697565 h.

6	2.614644	-0.828042	0.912821
6	2.409382	0.158269	-0.217727
6	3.766454	0.065973	0.437622
6	2.711703	-2.252573	0.603466
6	4.852021	-0.601157	-0.280100
6	3.674601	-2.731232	-0.203921
6	4.763454	-1.889959	-0.652617
1	2.111635	-0.553132	1.837802
1	4.032460	0.920007	1.055906
1	1.993532	-2.922680	1.067590
1	5.750564	-0.026750	-0.485904
1	3.705857	-3.790107	-0.442314
1	5.574849	-2.347641	-1.210545
79	-0.988874	0.288746	-0.335353
15	-2.597454	-1.283251	0.257982
6	-1.885669	-2.861870	0.798390
1	-1.257693	-2.703635	1.677931
1	-2.691119	-3.560360	1.047425
1	-1.275120	-3.282534	-0.003574
6	-3.679888	-0.758127	1.615658
1	-4.215458	0.150222	1.331119
1	-4.401239	-1.552132	1.835726

1	-3.082806	-0.553124	2.506933
6	-3.712827	-1.708211	-1.108187
1	-3.134978	-2.105544	-1.945605
1	-4.434233	-2.461225	-0.774584
1	-4.246504	-0.814691	-1.439509
1	2.340150	-0.288888	-1.207598
6	1.544829	1.323106	-0.001321
6	1.543631	2.067733	1.182870
6	0.662921	1.723481	-1.039722
6	0.725794	3.177365	1.324125
1	2.202785	1.791707	2.000856
6	-0.164105	2.855503	-0.875401
1	0.783701	1.286249	-2.030897
6	-0.137491	3.575440	0.307182
1	0.760371	3.744671	2.248994
1	-0.798904	3.167615	-1.698440
1	-0.771685	4.445584	0.433051

VIId

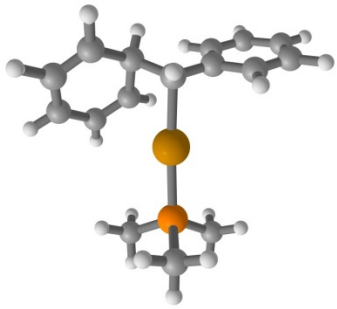


ΔE(DCE) -1098.628265

ΔG(DCE) -1098.680711

6	-1.938635	-0.904351	-0.859673
6	-1.946268	0.138232	0.333863
6	-3.227050	-0.294196	-0.335822
6	-1.740733	-2.337649	-0.603281
6	-4.143961	-1.187265	0.378232
6	-2.574728	-3.031451	0.187452
6	-3.797998	-2.444039	0.694043
1	-1.573947	-0.512386	-1.807786
1	-3.671637	0.493343	-0.940015
1	-0.913960	-2.829129	-1.108496
1	-5.125514	-0.797036	0.628664
1	-2.391062	-4.085845	0.368764
1	-4.485650	-3.074208	1.249002
79	0.520685	-0.334623	-0.052870
15	2.811811	-0.512540	0.045429
6	3.450866	-0.399811	1.737159
1	3.039547	-1.209089	2.343915
1	4.542888	-0.477537	1.717161
1	3.162009	0.557523	2.176224
6	3.462186	-2.066009	-0.620956
1	3.177369	-2.166405	-1.670238
1	4.554029	-2.064891	-0.537576
1	3.055522	-2.908998	-0.058467
6	3.643931	0.805089	-0.878739
1	3.346925	1.777894	-0.480017
1	4.728288	0.686390	-0.784006
1	3.362585	0.751767	-1.932515
1	-1.818270	-0.289310	1.328487
6	-1.497043	1.548275	0.171923
6	-1.575206	2.228653	-1.046131
6	-0.996944	2.224352	1.289595
6	-1.155853	3.547529	-1.140942
1	-1.962116	1.731281	-1.932332
6	-0.581216	3.543168	1.190186
1	-0.937782	1.704200	2.242574
6	-0.656205	4.209329	-0.026399
1	-1.221545	4.061815	-2.094645
1	-0.199039	4.053260	2.068925
1	-0.330776	5.241558	-0.105384

TSVIId-VIII

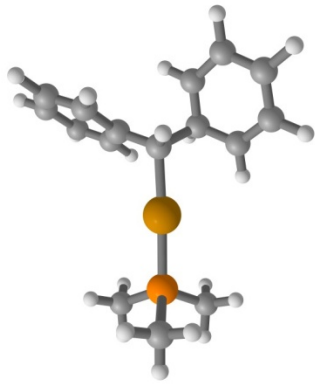


ΔE(DCE) -1098.614032 h.

ΔG(DCE) -1098.663856 h.

6	-0.562379	1.779958	1.044426
6	-1.474361	0.729359	-0.662582
6	-1.527610	2.124006	-0.021852
6	0.625098	2.522765	1.253690
6	-1.042786	3.188341	-0.935458
6	0.927332	3.552655	0.415306
6	0.103891	3.856028	-0.721356
1	-0.904839	1.097700	1.817989
1	-2.535071	2.370618	0.349452
1	1.272010	2.262741	2.084561
1	-1.671410	3.427290	-1.788999
1	1.818486	4.146729	0.591642
1	0.416092	4.642872	-1.399464
79	0.463466	-0.159393	-0.179785
15	2.573372	-1.228353	0.119932
6	3.487236	-1.516888	-1.425085
1	3.639059	-0.567143	-1.943675
1	4.459756	-1.969902	-1.206170
1	2.915081	-2.183994	-2.073789
6	3.708308	-0.236678	1.137967
1	3.273406	-0.088424	2.129634
1	4.674513	-0.742386	1.235660
1	3.855024	0.740966	0.671297
6	2.525081	-2.852380	0.934327
1	1.930784	-3.547112	0.336483
1	3.540587	-3.246787	1.043928
1	2.065100	-2.756227	1.920555
1	-1.321789	0.781511	-1.742949
6	-2.480935	-0.261982	-0.242652
6	-3.292700	-0.108076	0.886106
6	-2.659370	-1.412060	-1.029813
6	-4.246765	-1.064588	1.211682
1	-3.191750	0.763416	1.526304
6	-3.616088	-2.356520	-0.708876
1	-2.035058	-1.547456	-1.910100
6	-4.414860	-2.190468	0.419705
1	-4.865570	-0.922331	2.092411
1	-3.741523	-3.230824	-1.340332
1	-5.161803	-2.934737	0.676346

VIII

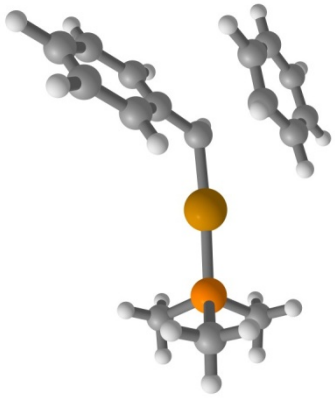


ΔE(DCE) -1098.617404 h.

ΔG(DCE) -1098.670156 h.

6	1.257630	-2.522042	-0.667477
6	1.313471	-0.178467	0.282273
6	1.949569	-1.256385	-0.822828
6	1.845964	-3.585179	-0.053422
6	3.347070	-1.253316	-0.455233
6	3.176826	-3.473715	0.389538
6	3.929474	-2.320537	0.184716
1	0.227442	-2.578627	-1.009052
1	1.733353	-0.766605	-1.777182
1	1.305367	-4.512265	0.096253
1	3.912043	-0.340990	-0.625410
1	3.630440	-4.315713	0.904715
1	4.956564	-2.270866	0.525704
79	-0.816238	-0.088194	0.110964
15	-3.170522	0.099951	0.002262
6	-4.019373	-0.172732	1.588122
1	-3.800298	-1.177249	1.957573
1	-5.100895	-0.061493	1.458110
1	-3.666827	0.555023	2.322827
6	-3.970940	-1.071147	-1.137159
1	-3.590071	-0.919045	-2.149877
1	-5.055058	-0.917209	-1.131387
1	-3.749227	-2.095805	-0.829075
6	-3.769986	1.728631	-0.543258
1	-3.423659	2.498217	0.150579
1	-4.864634	1.733068	-0.574258
1	-3.377789	1.952815	-1.537987
1	1.579071	-0.588302	1.264553
6	1.909325	1.177055	0.115975
6	1.789448	1.895614	-1.078373
6	2.577039	1.783998	1.182960
6	2.315658	3.171486	-1.200113
1	1.261645	1.451730	-1.920719
6	3.085399	3.071085	1.070509
1	2.693932	1.235933	2.115492
6	2.962888	3.768926	-0.123431
1	2.211963	3.709099	-2.137905
1	3.591061	3.525747	1.917278
1	3.369456	4.770969	-0.217148

TSVIII-IX

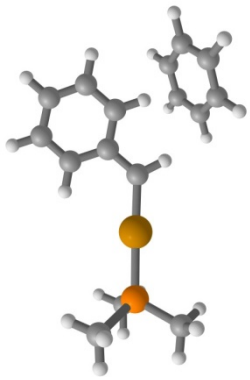


ΔE(DCE) -1098.615621 h.

ΔG(DCE) -1098.667797 h.

6	-1.030388	2.551103	0.725317
6	-1.245400	0.120634	-0.353510
6	-1.540372	3.573487	-0.035589
6	-1.829144	1.418442	1.043407
6	-2.879722	3.533610	-0.437644
6	-3.202651	1.454538	0.699579
6	-3.713592	2.485208	-0.062168
1	0.005354	2.570130	1.051965
1	-0.917254	4.415833	-0.314164
1	-1.511126	0.781149	1.864708
1	-3.276175	4.339335	-1.047905
1	-3.838120	0.624628	0.993417
1	-4.754606	2.480180	-0.364397
79	0.845572	0.008889	-0.127688
15	3.197988	-0.207041	-0.007812
6	4.119997	1.357419	-0.115969
1	3.890755	1.855656	-1.060905
1	5.195794	1.160777	-0.061399
1	3.830812	2.014933	0.707387
6	3.902916	-1.237099	-1.330039
1	3.469645	-2.239041	-1.283650
1	4.989110	-1.305723	-1.211330
1	3.670660	-0.799895	-2.303889
6	3.805688	-0.978892	1.522903
1	3.506616	-0.379211	2.385664
1	4.897673	-1.053879	1.494044
1	3.376997	-1.978754	1.624472
1	-1.597293	0.701456	-1.211857
6	-2.035183	-1.097980	-0.157039
6	-1.711950	-2.021065	0.846596
6	-3.095355	-1.396764	-1.023620
6	-2.421460	-3.201961	0.977618
1	-0.886552	-1.799692	1.519952
6	-3.785248	-2.592779	-0.913690
1	-3.367387	-0.678368	-1.793815
6	-3.454606	-3.493518	0.092508
1	-2.162944	-3.906398	1.761649
1	-4.590283	-2.820464	-1.605019
1	-4.002908	-4.425524	0.187630

IX



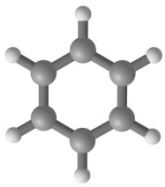
ΔE(DCE) -1098.628727 h.

ΔG(DCE) -1098.685404 h.

6	-3.823964	-2.488359	-0.662833
6	-0.615892	0.080403	-0.254063
6	-4.890560	-1.802540	-1.233502
6	-3.586650	-2.392177	0.703788
6	-5.719792	-1.021396	-0.436764
6	-4.414652	-1.609501	1.499660
6	-5.481746	-0.925191	0.929364
1	-3.178775	-3.102374	-1.284484
1	-5.076824	-1.879350	-2.300478
1	-2.755616	-2.930785	1.149958
1	-6.554574	-0.487935	-0.881769
1	-4.230694	-1.535516	2.567250
1	-6.130035	-0.315326	1.551554
79	1.413909	-0.116273	-0.080157
15	3.776279	-0.388995	0.076988
6	4.433289	-0.294453	1.770180
1	3.981022	-1.074544	2.386721
1	5.519674	-0.429649	1.752389
1	4.196495	0.679227	2.205116
6	4.390604	-1.979980	-0.552657
1	4.127556	-2.085889	-1.607574
1	5.478823	-2.028671	-0.442763
1	3.934172	-2.799681	0.007026
6	4.728787	0.858679	-0.841318
1	4.489478	1.855376	-0.463282
1	5.800895	0.673143	-0.719316
1	4.472015	0.814347	-1.902188
1	-1.213929	-0.812514	-0.474197
6	-1.398283	1.234248	-0.149324
6	-0.809282	2.495635	0.135701
6	-2.805921	1.162382	-0.331633

6	-1.590131	3.621801	0.230165
1	0.267371	2.542696	0.273937
6	-3.581608	2.294042	-0.233139
1	-3.257124	0.199047	-0.556747
6	-2.971997	3.517123	0.046242
1	-1.145245	4.586614	0.445228
1	-4.656063	2.237746	-0.370007
1	-3.584842	4.410235	0.122024
1	3.916351	-2.110788	-0.016271
6	5.041690	1.080482	-0.002341
1	3.825806	2.857866	0.012337
1	6.042073	-0.825758	-0.017771
1	5.971894	1.640517	-0.002558

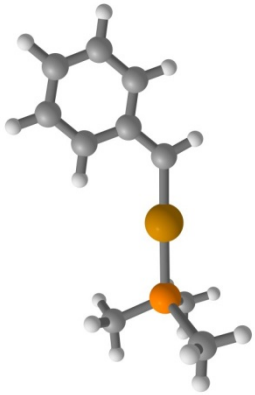
benzene



ΔE(DCE) -232.015548 h.
ΔG(DCE) -232.043028 h.

6	-0.157356	1.380635	0.000001
6	-1.274652	0.554000	-0.000027
6	-1.117048	-0.826638	0.000020
6	0.157379	-1.380632	-0.000004
6	1.274642	-0.554021	-0.000016
6	1.117035	0.826656	0.000021
1	-0.280103	2.459598	0.000001
1	-2.270453	0.987251	-0.000014
1	-1.990159	-1.472538	0.000016
1	0.280058	-2.459603	0.000007
1	2.270470	-0.987210	-0.000012
1	1.990186	1.472501	0.000031

IX (no benzene)



ΔE(DCE) -866.608514 h.
ΔG(DCE) -866.653884 h.

79	-0.461167	-0.390117	0.004322
15	-2.717346	0.380402	-0.003593
6	-3.734674	-0.304607	-1.346110
1	-3.777578	-1.392562	-1.257823
1	-4.748509	0.104906	-1.287895
1	-3.294604	-0.047398	-2.312403
6	-3.648696	-0.013377	1.508060
1	-3.166201	0.449778	2.371898
1	-4.673836	0.361480	1.420238
1	-3.671013	-1.095513	1.655824
6	-2.888680	2.181148	-0.184330
1	-2.441412	2.500520	-1.128617
1	-3.947324	2.459777	-0.172826
1	-2.372947	2.685265	0.636319
6	1.465138	-1.079421	0.000949
1	1.633843	-2.162727	-0.002890
6	2.658711	-0.350604	-0.001019
6	2.649084	1.069713	0.006327
6	3.909604	-1.025139	-0.009798
6	3.829091	1.774099	0.006095
1	1.689377	1.579194	0.012568
6	5.086477	-0.314188	-0.010779