Supporting Information

Rh(I)-Catalyzed Formal [5+1]/[2+2+1] Cycloaddition of 1-Yne-vinylcyclopropanes and Two CO Units: One-Step Construction of Multifunctional Angular Tricyclic 5/5/6 Compounds

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1. General

Air and moisture sensitive reactions were carried out in oven-dried glassware sealed with rubber septa under a positive pressure of dry argon. Similarly sensitive liquids and solutions were transferred via syringe. Reactions were stirred using Teflon-coated magnetic stir bars. Elevated temperatures were maintained using Thermostat-controlled silicone oil baths. Organic solutions were concentrated using a Büchi rotary evaporator with a desktop vacuum pump. Tetrahydrofuran, diethyl ether, and toluene were distilled from sodium and benzophenone prior to use. 1,2-Dichloromethane was distilled from CaH_2 prior to use. Dichloroethane was distilled from P_2O_5 prior to use. Synthetic reagents were purchased from Acros, Aldrich, and Alfa Aesar and used without further purification, unless otherwise indicated. Analytical TLC was performed with 0.25 mm silica gel G plates with a 254 nm fluorescent indicator. The TLC plates were visualized by ultraviolet light and treatment with phosphomolybdic acid stain followed by gentle heating. Purification of products was accomplished by flash chromatography on silica gel and the purified compounds showed a single spot by analytical TLC.

NMR spectra were measured on Bruker ARX 400 (^{1}H at 400 MHz, ^{13}C at 100 MHz) and Bruker AVANCE 600 (^{1}H at 600 MHz, ^{13}C at 150 MHz) nuclear magnetic resonance spectrometers. Data for ^{1}H-NMR spectra are reported as follows: chemical shift (ppm, referenced to TMS; s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, dt = doublet of triplets, dm = doublet of multiplet, ddd = doublet of doublet of doublets, tdd = triplet of doublet of doublets, m = multiplet), coupling constant (Hz), and integration. Data for ^{13}C-NMR are reported in terms of chemical shift (ppm) relative to residual solvent peak ($CDCl_3$: 77.0 ppm, C_6D_6: 128.0 ppm). 2D NMR experiments were conducted on a Bruker AVANCE 600 nuclear magnetic resonance spectrometer. Infrared spectra were recorded on Mettler-Toledo ReactIR iC10 system with an SiComp probe and are reported in wavenumbers (cm^{-1}). High-resolution mass spectra (HRMS) were recorded on a Bruker Apex IV FTMS mass spectrometer (ESI).

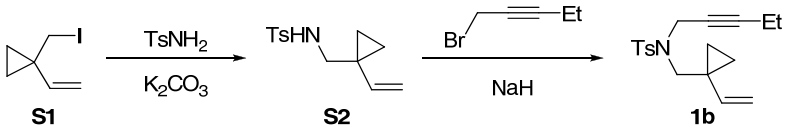
Abbreviations:

Cy = cyclohexyl
DCE = 1,2-dichloroethane
DCM = dichloromethane
DEAD = diethyl azodicarboxylate
DIBAL-H = diisobutylaluminum hydride
DMF = N,N-dimethylformamide
EA = ethyl acetate
LDA = lithium diisopropylamide
PCC = pyridinium chlorochromate
PE = petroleum ether
PPTS = pyridinium *p*-toluenesulfonate
TBAF = tetrabutylammonium fluoride
TBS = *tert*-butyldimethylsilyl
TFA = trifluoroacetic acid
THF = tetrahydrofuran
TLC = thin layer chromatography
TMS = trimethylsilyl

2. Experimental Procedures and Characterization Data

2.1 Synthesis of New Substrates

1-Yne-VCP (1b)



S1 **S2** **1b**

S1 to **S2**: To a stirred solution of 4-methylbenzenesulfonamide (1.71 g, 10.0 mmol), and potassium carbonate (1.38 g, 10.0 mmol) in acetone (20 mL) was added iodide **S1**[1] (1.04 g, 5.0 mmol). The mixture was then refluxed for 24 h. Saturated NH_4Cl solution was added to quench the reaction, and the mixture was extracted with ether. The combined extract was dried over $MgSO_4$. The mixture was concentrated and filtered through silica gel (eluted with PE/EA 30:1) to afford compound **S2** (988 mg, 79%).

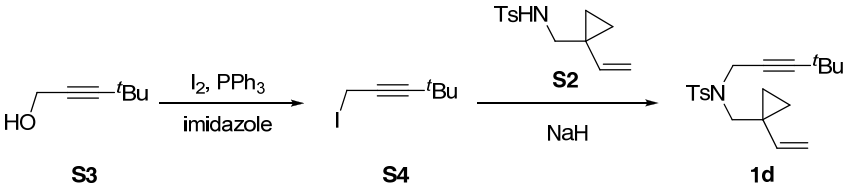
S2: Yellow oil: TLC R_f (20% EA/PE) = 0.34. ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.62 (s, 4H), 2.44 (s, 3H), 2.97 (d, J = 5.9 Hz, 2H), 4.57 (t, J = 5.9 Hz, 1H), 4.86 (d, J = 17.5 Hz, 1H), 4.94 (d, J = 10.8 Hz, 1H), 5.43 (dd, J = 10.8 and 17.5 Hz, 1H), 7.32 (d, J = 8.2 Hz, 2H), 7.75 (d, J = 8.2 Hz, 2H). ^{13}C NMR (100 MHz, CDCl3): δ 13.1, 21.5, 22.3, 48.7, 105.3, 112.6, 127.1, 129.7, 136.8, 140.5, 143.4. IR (neat): ν 3293, 2935, 1643, 1602, 1434, 1330, 1166 cm^{-1}. HRMS (ESI) calcd for $C_{13}H_{17}NNaO_2S$ (M+Na): 274.0872. Found: 274.0872.

S2 to **1b**: To a suspension of NaH (37 mg, 1.5 mmol) in DMF (1 mL) was added a solution of tosylamide **S2** (194 mg, 0.77 mmol) in DMF (1 mL) at 0 ºC. After stirred for 5 min, 1-bromopent-2-yne (171 mg, 1.16 mmol) in DMF (1 mL) was added and the reaction mixture was allowed to warm to room temperature and stirred for 1.5 h. Then saturated NH_4Cl solution (4 mL) was added to quench the reaction. The resulting mixture was washed with water (10 mL), extracted with ether and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/AE 30:1) to afford 1-yne-VCP **1b** (242 mg, 99%).

1b: Colorless oil: TLC R_f (20% EA/PE) = 0.64. ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.70-0.72 (m, 4H), 0.85 (t, J = 7.4 Hz, 3H), 1.85 (tq, J = 2.2 and 7.4 Hz, 2H), 2.40 (s, 3H), 3.21 (s, 2H), 4.19 (t, J = 2.2 Hz, 2H), 4.96 (dd, J = 1.2 and 11.0 Hz, 1H), 5.12 (dd, J = 1.2 and 17.4 Hz, 1H), 5.81 (dd, J = 11.0 and 17.4 Hz, 1H), 7.27 (d, J = 8.2 Hz, 2H), 7.72 (d, J = 8.2 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 12.0, 12.8, 13.5, 19.6, 21.4, 36.1, 51.4, 71.7, 87.9, 112.2, 113.8, 127.8, 129.2, 136.0, 140.2, 143.0. IR (neat): ν 2983, 1605, 1441, 1352, 1162 cm^{-1}. HRMS (ESI) calcd for $C_{18}H_{23}NNaO_2S$ (M+Na): 340.1342. Found: 340.1339.

[1] (a) Jiao, L.; Lin, M.; Zhuo, L.-G.; Yu, Z.-X. *Org. Lett.* **2010**, *12*, 2528. (b) Jiao, L.; Lin, M.; Yu, Z.-X. *Chem. Commun*. **2010**, *46*, 1059-1061.

1-Yne-VCP (1d)

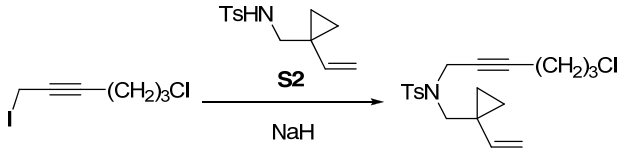


S3 **S4** **1d**

S3 to **1d**: To a stirred solution of alcohol **S3**[2] (2.24 g, 20.0 mmol), triphenylphosphine (6.29 g, 24.0 mmol), and imidazole (1.63 g, 24.0 mmol) at 0 ºC in DCM (20 mL) was added iodine (7.62 g, 30.0 mmol) in three potions. After 14 h, saturated aqueous $Na_2S_2O_3$ was added. The mixture was extracted with CH_2Cl_2, and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by a thin pad of silica gel eluted with pentane to afford the crude iodide **S4**. To a suspension of NaH (38 mg, 1.6 mmol) in DMF (1 mL) was added a solution of tosylamide **S2** (201 mg, 0.8 mmol) in DMF (1 mL) at 0 ºC. After stirred for 5 min, iodide **S4** in DMF (1 mL) was added and the reaction mixture was allowed to warm to room temperature and stirred for 6 h. Then saturated NH_4Cl solution (4 mL) was added to quench the reaction. The resulting mixture was washed with water (10 mL), extracted with ether and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/AE 30:1) to afford 1-yne-VCP **1d** (222 mg, two steps 56%).

1d: White solid: TLC R_f (20% EA/PE) = 0.68, m.p. 85-87 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.68-0.76 (m, 4H), 0.92 (s, 9H), 2.40 (s, 3H), 3.23 (s, 2H), 4.21 (s, 2H), 4.97 (dd, J = 1.0 and 11.8 Hz, 1H), 5.15 (dd, J = 1.0 and 17.4 Hz, 1H), 5.82 (dd, J = 11.8 and 17.4 Hz, 1H), 7.28 (d, J = 7.0 Hz, 2H), 7.71 (d, J = 7.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 12.7, 19.5, 21.4, 27.0, 30.5, 36.0, 51.1, 70.9, 95.1, 112.2, 127.7, 129.4, 136.1, 140.2, 143.0. IR (neat): ν 2980, 1602, 1352, 1162, 1099 cm^{-1}. HRMS (ESI) calcd for $C_{20}H_{27}NNaO_2S$ (M+Na): 368.1655. Found: 368.1652.

1-Yne-VCP (1e)



S5 **1e**

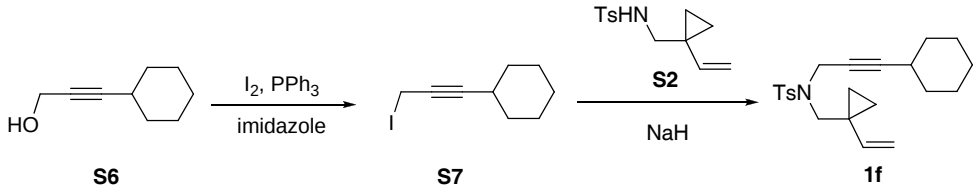
S5 to **1e**: To a suspension of NaH (70% in mineral oil, 25 mg, 1.5 mmol) in DMF (1 mL) was added a solution of tosylamide **S2** (176 mg, 1.0 mmol) in DMF (1 mL) at 0 ºC. After stirred for 5 min, iodide **S5**[3] (199 mg, 1.5 mmol) in DMF (1 mL) was added and the reaction mixture was allowed to warm to room temperature and stirred for 12 h. Then saturated NH_4Cl solution (4 mL) was added to quench the reaction. The resulting mixture was washed with water (10 mL), extracted with ether and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/AE 20:1

[2] Trost, B. M.; Rudd, M. T. *J. Am. Chem. Soc*. **2003**, *125*, 11516.
[3] Ohuchida, S.; Hamanaka, N.; Hayashi, M. *Tetrahedron* **1983**, *39*, 4237.

to 5:1) to afford 1-yne-VCP **1e** (139 mg, 46%).

1e: Light yellow solid: TLC R_f (20% EA/PE) = 0.51, m.p. 71-73 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.71 (s, 4H), 1.65 (quintet, J = 6.4 Hz, 2H), 2.07 (tt, J = 2.2 and 6.8 Hz, 2H), 2.42 (s, 3H), 3.22 (s, 2H), 3.36 (t, J = 6.4 Hz, 2H), 4.20 (t, J = 2.2 Hz, 2H), 4.96 (dd, J = 1.0 and 10.8 Hz, 1H), 5.12 (dd, J = 1.0 and 17.2 Hz, 1H), 5.81 (dd, J = 10.8 and 17.2 Hz, 1H), 7.29 (d, J = 8.4 Hz, 2H), 7.71 (d, J = 8.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 12.8, 15.8, 19.7, 21.5, 30.9, 36.0, 43.3, 51.5, 73.6, 84.4, 112.3, 127.8, 129.3, 136.1, 140.1, 143.2. IR (neat): ν 2924, 1646, 1352, 1166 cm^{-1}. HRMS (ESI) calcd for $C_{19}H_{24}ClNNaO_2S$ (M+Na): 388.1109. Found: 388.1106.

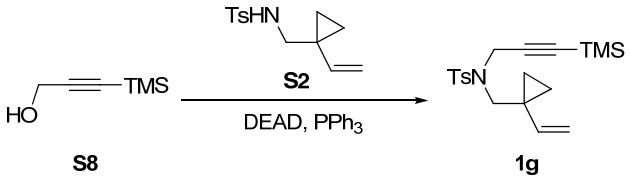
1-Yne-VCP (1f)



S6 to **1f**: To a stirred solution of alcohol **S6**[2] (552 mg, 4.0 mmol), triphenylphosphine (1.26 g, 4.8 mmol), and imidazole (408 mg, 6.0 mmol) at 0 ºC was added iodine (1.52 g, 6.0 mmol) in three potions. After 7 h, saturated aqueous $Na_2S_2O_3$ was added. The mixture was extracted with CH_2Cl_2, and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by a thin pad of silica gel eluted with pentane to afford the crude iodide **S7**. To a suspension of NaH (70% in mineral oil, 31 mg, 0.9 mmol) in DMF (1 mL) was added a solution of tosylamide **S2** (176 mg, 0.7 mmol) in DMF (1 mL) at 0 ºC. After stirred for 5 min, iodide **S7** in DMF (1 mL) was added and the reaction mixture was allowed to warm to room temperature and stirred for 6 h. Then saturated NH_4Cl solution (4 mL) was added to quench the reaction. The resulting mixture was washed with water (10 mL), extracted with ether and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/AE 30:1) to afford 1-yne-VCP **1f** (214 mg, two steps 26%).

1f: Light yellow oil: TLC R_f (20% EA/PE) = 0.51. ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.68-0.75 (m, 4H), 1.00-1.25 (m, 5H), 1.44-1.60 (m, 5H), 2.00-2.09 (m, 1H), 2.40 (s, 3H), 3.23 (s, 2H), 4.21 (d, J = 2.0 Hz, 2H), 4.96 (dd, J = 1.0 and 10.9 Hz, 1H), 5.12 (dd, J = 1.0 and 17.7 Hz, 1H), 5.82 (dd, J = 10.9 and 17.7 Hz, 1H), 7.27 (d, J = 8.2 Hz, 2H), 7.71 (d, J = 8.2 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 12.8, 19.6, 21.4, 24.6, 25.7, 28.7, 32.3, 36.1, 51.3, 72.2, 90.9, 112.2, 127.8, 129.3, 136.2, 140.2, 143.0. IR (neat): ν 2935, 2861, 1356, 1166, 1099 cm^{-1}. HRMS (ESI) calcd for $C_{22}H_{29}NNaO_2S$ (M+Na): 394.1811. Found: 394.1807.

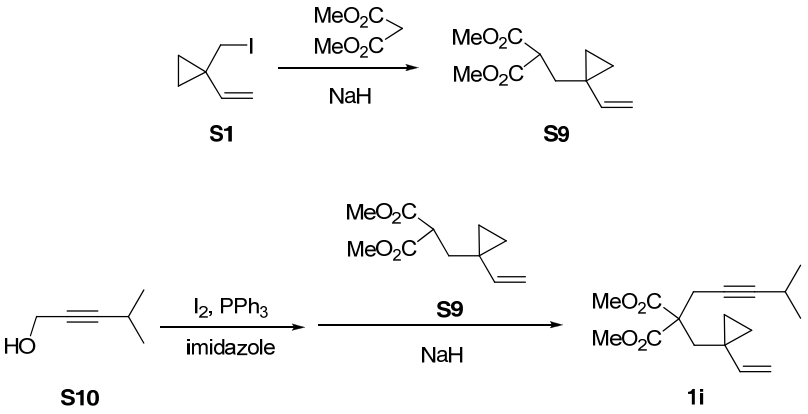
1-Yne-VCP (1g)



S8 to **1g**: To a stirred solution of alcohol **S8** (85 mg, 0.66 mmol), tosylamide **S2** (200 mg, 0.8 mmol), and PPh_3 (346 mg, 1.32 mmol) in anhydrous THF (5 mL) was added DEAD (230 mg, 1.32 mmol) at 0 ºC. The mixture was then stirred for 5 d at 25 ºC. The reaction mixture was concentrated and filtered through a pad of silica gel (eluted with PE/EA 10:1). The filtrate was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 20:1) to afford 1-yne-VCP **1g** (89 mg, 31%).

1g: White Solid: TLC R_f (20% EA/PE) = 0.60, m.p. 87-89 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ -0.04 (s, 9H), 0.72 (d, J = 6.1 Hz, 4H), 2.41 (s, 3H), 3.23 (s, 2H), 4.24 (s, 2H), 4.93 (d, J = 10.6 Hz, 1H), 5.14 (d, J = 17.5 Hz, 1H), 5.81 (dd, J = 10.6 and 17.5 Hz, 1H), 7.24 (d, J = 7.0 Hz, 2H), 7.71 (d, J = 8.2 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ -0.5, 12.7, 19.5, 21.5, 36.6, 51.3, 91.4, 98.0, 112.4, 127.8, 129.4, 135.8, 140.0, 143.2. IR (neat): ν 2961, 2369, 2183, 1356, 1166 cm^{-1}. HRMS (ESI) calcd for $C_{19}H_{27}NNaO_2SSi$ (M+Na): 384.1424. Found: 384.1428.

1-Yne-VCP (1i)



S1 to **S9**: To a suspension of NaH (70% in mineral oil, 140 mg, 6.0 mmol) in DMF (7 mL) was added a solution of dimethyl malonate (790 mg, 6.0 mmol) in DMF (3 mL) at 0 ºC. After stirred for 5 min, a solution of iodide **S1** (832 mg, 6.0 mmol) in DMF (3 mL) was added and the reaction mixture was allowed to warm to room temperature and stirred for 13 h. Then saturated NH_4Cl solution (4 mL) and water (50 mL) was added to quench the reaction. The resulting mixture was extracted with ether and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/AE 20:1 to 10:1) to afford **S9** (697 mg, 82%).

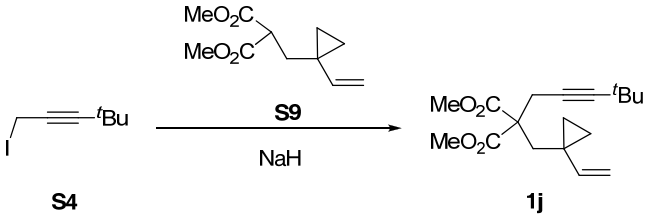
S9: Colorless oil: TLC R_f (20% EA/PE) = 0.57. ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.58-0.59 (m, 4H), 2.10 (d, J = 7.1 Hz, 2H), 3.63 (t, J = 7.1 Hz, 1H), 3.73 (s, 6H), 4.94 (dd, J = 0.7 and 17.1 Hz, 1H),

4.98 (dd, J = 1.2 and 10.7 Hz, 1H), 5.60 (dd, J = 10.7 and 17.1 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.3, 21.1, 35.2, 49.2, 52.4, 112.3, 141.7, 170.0. IR (neat): ν 2965, 2369, 1743, 1441, 1225, 1151 cm^{-1}. HRMS (ESI) calcd for $C_{11}H_{17}O_4$ (M+H): 213.1121. Found: 213.1122.

S10 to **1i**: To a stirred solution of alcohol **S10**[1] (588 mg, 6.0 mmol), triphenylphosphine (1.89 g, 7.2 mmol), and imidazole (612 mg, 9.0 mmol) at 0 ºC was added iodine (2.29 g, 9.0 mmol) in three potions. After 7 h, saturated aqueous $Na_2S_2O_3$ was added. The mixture was extracted with CH_2Cl_2, and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by a thin pad of silica gel eluted with pentane to afford the crude iodide. Then to a suspension of NaH (36 mg, 1.5 mmol) in DMF (3 mL) was added a solution of diester **S9** (211 mg, 1.0 mmol) in DMF (1 mL) at 0 ºC. After stirred for 5 min, the crude iodide in DMF (1 mL) was added and the reaction mixture was allowed to warm to room temperature and stirred for 6 h. Then saturated NH_4Cl solution (4 mL) was added to quench the reaction. The resulting mixture was washed with water (10 mL), extracted with ether and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/AE 30:1) to afford 1-yne-VCP **1i** (138 mg, two steps 16%).

1i: Colorless oil: TLC R_f (10% EA/PE) = 0.47. ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.63 (d, J = 5.4 Hz, 4H), 1.11 (d, J = 6.9 Hz, 6H), 2.25 (s, 2H), 2.48 (triplet of heptet, J = 2.0 and 6.9 Hz, 1H), 2.93 (d, J = 2.0 Hz, 2H), 3.89 (s, 6H), 4.81-4.84 (m, 2H), 5.93 (dd, J = 10.4 and 17.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.0, 19.6, 20.4, 22.9, 38.7, 52.3, 57.5, 74.3, 89.8, 111.9, 141.1, 170.8. IR (neat): ν 2980, 1743, 1441, 1285, 1203, 1054 cm^{-1}. HRMS (ESI) calcd for $C_{17}H_{24}NaO_4$ (M+Na): 315.1567. Found: 315.1564.

1-Yne-VCP (1j)



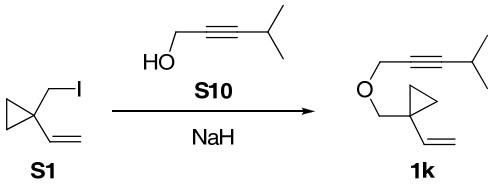
S4 **1j**

S4 to **1j**: To a suspension of NaH (29 mg, 1.2 mmol) in DMF (1 mL) was added a solution of diester **S9** (204 mg, 1.0 mmol) in DMF (1 mL) at 0 ºC. After stirred for 10 min, iodide **S4** (178 mg, 0.8 mmol) in DMF (1 mL) was added and the reaction mixture was allowed to warm to room temperature and stirred for 36 h. Then saturated NH_4Cl solution (4 mL) was added to quench the reaction. The resulting mixture was washed with water (10 mL), extracted with ether and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/AE 100:1) to afford 1-yne-VCP **1j** (91 mg, 37%).

1j: Colorless oil: TLC R_f (10% EA/PE) = 0.53. ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.63 (d, J = 6.8 Hz,

4H), 1.16 (s, 9H), 2.22 (s, 2H), 2.95 (s, 2H), 3.68 (s, 6H), 4.81-4.84 (m, 2H), 5.92 (dd, J = 10.6 and 16.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.0, 19.6, 22.9, 27.3, 31.0, 38.7, 52.3, 57.6, 73.7, 92.8, 111.9, 141.1, 170.8. IR (neat): ν 2972, 1747, 1441, 1211, 1050 cm^{-1}. HRMS (ESI) calcd for $C_{18}H_{26}NaO_4$ (M+Na): 329.1723. Found: 329.1725.

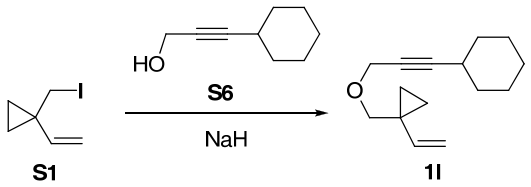
1-Yne-VCP (1k)



S1 to **1k**: To a suspension of NaH (29 mg, 1.2 mmol) in DMF (1 mL) was added a solution of diester **S10** (147 mg, 1.5 mmol) in dry DMF (4 mL) at 0 ºC. After 1 h, iodide **S1** (406 mg, 2.0 mmol) was added dropwise. The reaction mixture was stirred at 50 ºC for 48 h, then water was added to quench the reaction. The mixture was extracted with dichloromethane, and the combined organic layer was dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 200:1 to 100:1) to afford 1-yne-VCP **1k** (191 mg, 72%)

1k: Colorless oil: TLC R_f (2% EA/PE) = 0.53. ^{1}H NMR (400 MHz, C_6D_6): δ 0.52 (dd, J = 4.4 and 6.7 Hz, 2H), 0.66 (dd, J = 4.4 and 6.7 Hz, 2H), 1.02 (d, J = 6.9 Hz, 6H), 2.38 (triplet of heptet, J = 2.1 and 6.9 Hz, 1H), 3.44 (s, 2H), 4.02 (d, J = 2.1 Hz, 2H), 4.97 (dd, J = 1.3 and 10.7 Hz, 1H), 5.17 (dd, J = 1.3 and 17.8 Hz, 1H), 5.62 (dd, J = 10.7 and 17.8 Hz, 1H). ^{13}C NMR (100 MHz, C_6D_6): δ 12.6, 20.9, 22.5, 23.1, 58.2, 73.9, 76.3, 92.1, 111.4, 142.1. IR (neat): ν 2980, 2283, 1643, 1367, 1322, 1088 cm^{-1}. HRMS (ESI) calcd for $C_{12}H_{19}O$ (M+H): 179.1430. Found: 179.1426.

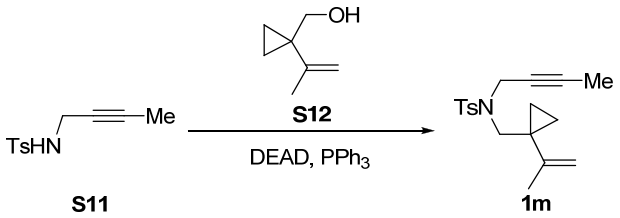
1-Yne-VCP (1l)



S1 to **1l**: To a stirred solution of alcohol **S6** (207 mg, 1.5 mmol) in dry DMF (4 mL) was added NaH (72mg, 3.0 mmol) at 25 ºC. After 1 h, iodide **S1** (343 mg, 1.65 mmol) was added dropwise. The reaction mixture was stirred at 25 ºC for 24 h, and then water was added to quench the reaction. The mixture was extracted with dichloromethane, and the combined organic layer was dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE) to afford 1-yne-VCP **1l** (149 mg, 46%).

1l: Colorless oil: TLC R_f (1% EA/PE) = 0.54. ^{1}H NMR (400 MHz, C_6D_6): δ 0.53 (dd, J = 4.4 and 6.4 Hz, 2H), 0.69 (dd, J = 4.4 and 6.4 Hz, 2H), 1.04-1.18 (m, 3H), 1.26-1.32 (m, 1H), 1.38-1.46 (m, 2H), 1.53-1.59 (m, 2H) 1.66-1.73 (m, 2H), 2.26-2.31 (m, 1H), 3.48 (s, 2H), 4.06 (d, J = 2.3 Hz, 2H), 4.98 (dd, J = 1.6 and 10.8 Hz, 1H), 5.19 (dd, J = 1.6 and 17.4 Hz, 1H), 5.64 (dd, J = 10.8 and 17.4 Hz, 1H). ^{13}C NMR (100 MHz, C_6D_6): δ 12.6, 22.5, 25.0, 26.1, 29.4, 33.0, 58.3, 73.8, 77.0, 90.8, 111.4, 142.1. IR (neat): ν 2935, 2861, 2361, 1639, 1456, 1363, 1095 cm^{-1}. HRMS (ESI) calcd for $C_{15}H_{23}O$ (M+H): 219.1743. Found: 219.1742.

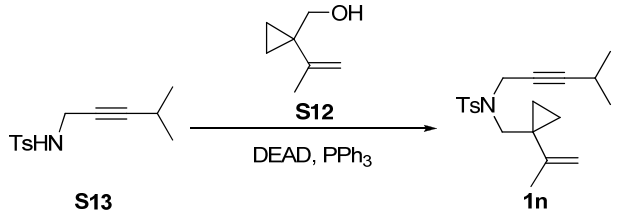
1-Yne-VCP (1m)



S11 to **1m**: To a stirred solution of alcohol **S12**[1] (120 mg, 1.0 mmol), tosylamide **S11**[1] (290 mg, 1.3 mmol), and PPh_3 (526 mg, 2.0 mmol) in anhydrous THF (10 mL) was added DEAD (348 mg, 2.0 mmol) at 0 ºC. The mixture was then stirred for 27 h at 25 ºC. The reaction mixture was concentrated and filtered through a pad of silica gel (eluted with PE/EA 20:1). The filtrate was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 20:1) to afford 1-yne-VCP **1m** (279 mg, 88%).

1m: Colorless oil: TLC R_f (20% EA/PE) = 0.64. ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.55-0.68 (m, 4H), 1.46 (t, J = 2.5 Hz, 3H), 1.87 (s, 3H), 2.41 (s, 3H), 3.14 (s, 2H), 4.17 (q, J = 2.5 Hz, 2H), 4.76 (s, 1H), 4.80 (s, 1H), 7.27 (d, J = 8.0 Hz, 2H), 7.71 (d, J = 8.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 3.1, 10.7, 20.4, 21.4, 24.3, 36.0, 50.9, 71.7, 81.2, 112.1, 128.0, 129.0, 136.0, 142.9, 145.5. IR (neat): ν 2924, 1602, 1445, 1348, 1162, 1099 cm^{-1}. HRMS (ESI) calcd for $C_{18}H_{24}NO_2S$ (M+H): 318.1522. Found: 318.1522.

1-Yne-VCP (1n)

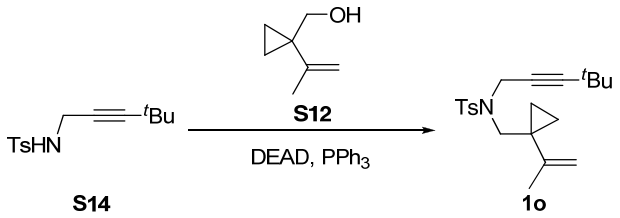


S13 to **1n**: To a stirred solution of alcohol **S12**[1] (33 mg, 0.3 mmol), tosylamide **S13**[2] (68 mg, 0.27 mmol), and PPh_3 (141 mg, 0.5 mmol) in anhydrous THF (2.5 mL) was added DEAD (89 mg,

0.5 mmol) at 0 ºC. The mixture was then stirred for 15 h at 25 ºC. The reaction mixture was concentrated and filtered through a pad of silica gel (eluted with PE/EA 20:1). The filtrate was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 20:1) to afford 1-yne-VCP **1n** (55 mg, 59%).

1n: Colorless oil: TLC R_f (33% EA/PE) = 0.79. ^{1}H NMR (600 MHz, C_6D_6): δ 0.51-0.56 (m, 4H), 0.72 (d, J = 6.6 Hz, 6H), 1.93 (s, 3H), 1.96 (s, 3H), 2.00 (triplet of heptet, J = 1.6 and 6.8 Hz, 1H), 3.29 (s, 2H), 4.33 (d, J = 1.6 Hz, 2H), 4.74 (s, 1H), 4.79 (s, 1H), 6.81 (d, J = 8.2 Hz, 2H), 7.76 (d, J = 8.2 Hz, 2H). ^{13}C NMR (150 MHz, C_6D_6): δ 10.9, 20.7, 21.1, 22.7, 24.6, 36.3, 51.1, 72.7, 84.2, 91.8, 112.4, 137.6, 142.6, 145.9. IR (neat): ν 2976, 1445, 1352, 1166, 1099 cm^{-1}. HRMS (ESI) calcd for $C_{20}H_{28}NO_2S$ (M+H): 346.1835. Found: 346.1842.

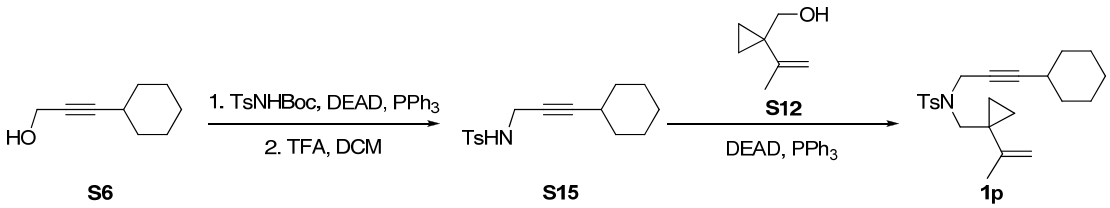
1-Yne-VCP (1o)



S14 to **1o**: To a stirred solution of alcohol **S12**[1] (63 mg, 0.56 mmol), tosylamide **S14**[2] (165 mg, 0.6 mmol), and PPh_3 (294 mg, 1.1 mmol) in anhydrous THF (7 mL) was added DEAD (195 mg, 1.1 mmol) at 0 ºC. The mixture was then stirred for 19 h at 25 ºC. The reaction mixture was concentrated and filtered through a pad of silica gel (eluted with PE/EA 20:1). The filtrate was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 20:1) to afford 1-yne-VCP **1o** (188 mg, 93%).

1o: White solid: TLC R_f (20% EA/PE) = 0.73, m.p. 75-77 ºC. ^{1}H NMR (600 MHz, C_6D_6): δ 0.55 (dd, J = 8.3 and 15.9 Hz, 4H), 0.84 (s, 9H), 1.93 (s, 3H), 1.97 (s, 3H), 3.30 (s, 2H), 4.32 (s, 2H), 4.74 (s, 1H), 4.79 (s, 1H), 6.82 (d, J = 8.0 Hz, 2H), 7.75 (d, J = 8.0 Hz, 2H). ^{13}C NMR (150 MHz, C_6D_6): δ 10.8, 20.7, 21.1, 24.6, 27.2, 30.0, 36.2, 51.0, 72.0, 94.5, 112.4, 127.9, 137.6, 142.6, 145.9. IR (neat): ν 2976, 1352, 1166, 1102 cm^{-1}. HRMS (ESI) calcd for $C_{21}H_{30}NO_2S$ (M+H): 360.1992. Found: 360.1997.

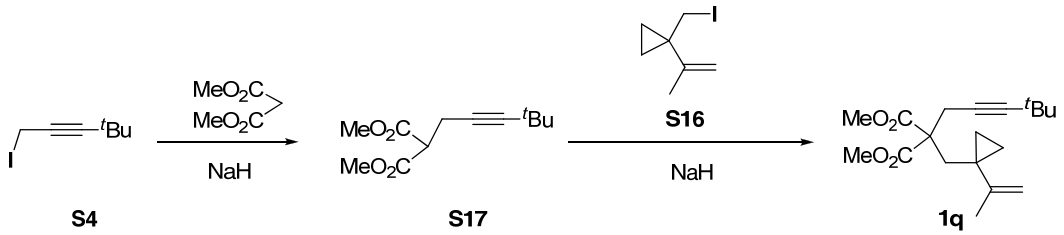
1-Yne-VCP (1p)



S6 to **1p**: To a stirred solution of alcohol **S6** (224 mg, 1.6 mmol), tosylamide[1] (482 mg, 1.8 mmol), and PPh_3 (807 mg, 3.0 mmol) in anhydrous THF (10 mL) was added DEAD (581 mg, 3.3 mmol) at 0 ºC. The mixture was then stirred for 22 h at 25 ºC. The reaction mixture was concentrated and filtered through a pad of silica gel (eluted with PE/EA 20:1). The crude oil was added to CH_2Cl_2 (10 ml) with TFA (749mg, 6.5 mmol) at room temperature for 20 h. The reaction mixture was concentrated and the crude product was purified by a thin pad of silica gel to afford the crude product **S15**. To a stirred solution of alcohol **S12**[1] (48 mg, 0.4 mmol), tosylamide **S15**, and PPh_3 (212 mg, 0.8 mmol) in anhydrous THF (10 mL) was added DEAD (150 mg, 0.86 mmol) at 0 ºC. The mixture was then stirred for 22 h at 25 ºC. The reaction mixture was concentrated and filtered through a pad of silica gel (eluted with PE/EA 20:1). The filtrate was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 20:1) to afford 1-yne-VCP **1p** (64 mg, two steps 30%).

1p: White solid: TLC R_f (20% EA/PE) = 0.54, m.p. 88-90 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.58-0.68 (m, 4H), 1.03-1.19 (m, 5H), 1.45-1.48 (m, 5H), 1.89 (s, 3H), 2.00-2.04 (m, 1H), 2.40 (s, 3H), 3.18 (s, 2H), 4.22 (d, J = 2.0 Hz, 2H), 4.78 (t, J = 0.9 Hz, 1H), 4.81 (t, J = 1.5 Hz, 1H), 7.26 (d, J = 8.0 Hz, 2H), 7.69 (d, J = 8.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 10.6, 20.4, 21.4, 24.2, 24.7, 25.7, 27.0, 28.7, 32.3, 36.0, 50.6, 72.2, 90.7, 112.1, 127.8, 129.1, 136.2, 143.0, 145.6. IR (neat): ν 2935, 2861, 1453, 1352, 1270, 1166, 1102 cm^{-1}. HRMS (ESI) calcd for $C_{23}H_{31}NNaO_2S$ (M+Na): 340.1342. Found: 340.1339.

1-Yne-VCP (1q)

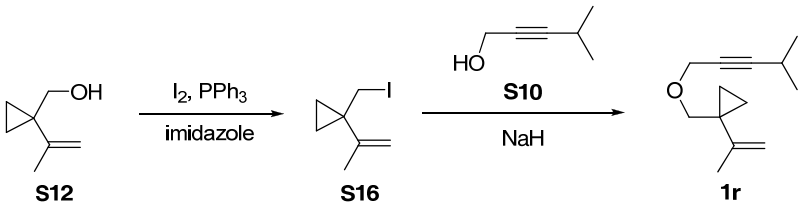


S4 to **1q**: To a suspension of NaH (74 mg, 3.0 mmol) in DMF (3 mL) was added a solution of dimethyl malonate (289 mg, 2.2 mmol) in DMF (3 mL) at 0 ºC. After stirred for 5 min, a solution of iodide **S4** (452 mg, 2.0 mmol) in DMF (3 mL) was added and the reaction mixture was allowed to warm to room temperature and stirred for 16 h. Then saturated NH_4Cl solution (4 mL) and water (50 mL) was added to quench the reaction. The resulting mixture was extracted with ether

and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by a thin pad of silica gel to afford the crude product **S17**. To a suspension of NaH (19 mg, 0.8 mmol) in DMF (7 mL) was added a solution of diester **S17** in DMF (1 mL) at 0 ºC. After stirred for 5 min, iodide **S16** (111 mg, 0.5 mmol) (see the preparation in the systhesis of substrate **1r**) in DMF (1 mL) was added and the reaction mixture was allowed to warm to room temperature and stirred for 27 h. Then saturated NH_4Cl solution (4 mL) was added to quench the reaction. The resulting mixture was washed with water (10 mL), extracted with ether and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/AE 100:1 to 50:1) to afford 1-yne-VCP **1q** (84 mg, two steps 30%).

1q: Colorless oil: TLC R_f (10% EA/PE) = 0.52. ^{1}H NMR (600 MHz, C_6D_6): δ 0.51 (dd, J = 4.4 and 5.5 Hz, 2H), 0.65 (dd, J = 4.4 and 5.5 Hz, 2H), 1.15 (s, 9H), 1.81 (s, 3H), 2.53 (s, 2H), 3.30 (s, 2H), 3.34 (s, 6H), 4.71 (s, 1H), 4.75 (s, 1H). ^{13}C NMR (150 MHz, C_6D_6): δ 12.7, 20.8, 23.2, 27.6, 31.2, 36.8, 51.1, 58.2, 75.2, 92.8, 113.2, 147.3, 170.7. IR (neat): ν 2976, 1743, 1438, 1218, 1062 cm^{-1}. HRMS (ESI) calcd for $C_{19}H_{28}NaO_4$ (M+Na): 343.1880. Found: 343.1881.

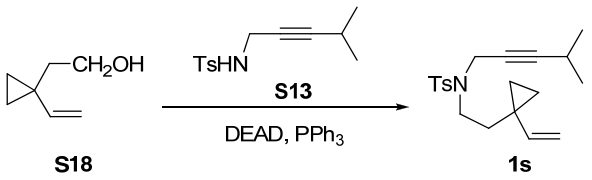
1-Yne-VCP (1r)



S12 to **1r**: To a stirred solution of alcohol **S12** (227 mg, 2.0 mmol), triphenylphosphine (629 mg, 2.4 mmol), and imidazole (171 mg, 2.5 mmol) in CH_2Cl_2 at 0 ºC was added iodine (772 mg, 3.0 mmol) in three potions. After 6 h, saturated aqueous $Na_2S_2O_3$ was added. The mixture was extracted with CH_2Cl_2, and the combined organic phase was dried over $MgSO_4$ and concentrated. The crude product was purified by a thin pad of silica gel to afford the crude iodide **S16**. To a suspension of NaH (25mg, 1.0 mmol) in DMF (5 mL) was added a solution of diester alcohol **S10** (74 mg, 0.75 mmol) at 0 ºC. After 1 h, iodide **S16** was added dropwise. The reaction mixture was stirred at 25 ºC for 24 h, then water was added to quench the reaction. The mixture was extracted with dichloromethane, and the combined organic layer was dried over $MgSO_4$ and concentrated. The crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 500:1) to afford 1-yne-VCP **1r** (41 mg, two steps 35%).

1r: Colorless oil: TLC R_f (2% EA/PE) = 0.52. ^{1}H NMR (600 MHz, C_6D_6): δ 0.56-0.63 (m, 4H), 1.03 (d, J = 7.0 Hz, 6H), 1.77 (s, 3H), 2.39 (triplet of heptet, J = 1.8 and 7.0 Hz, 1H), 3.43 (s, 2H), 4.05 (d, J = 1.8 Hz, 2H), 4.86 (s, 1H), 4.96 (s, 1H). ^{13}C NMR (150 MHz, C_6D_6): δ 10.9, 21.0, 23.1, 26.3, 58.2, 74.5, 76.4, 92.1, 111.6, 146.4. IR (neat): ν 2980, 1657, 1464, 1095 cm^{-1}. HRMS (ESI) calcd for $C_{13}H_{21}O$ (M+H): 193.1587. Found: 193.1586.

1-Yne-VCP (1s)



S18 to **1s**: To a stirred solution of alcohol **S18**[1] (176 mg, 1.6 mmol), tosylamide **S13** (358 mg, 1.4 mmol), and PPh_3 (749 mg, 2.9 mmol) in anhydrous THF (5 mL) was added DEAD (498 mg, 2.6 mmol) at 0 ºC. The mixture was then stirred for 40 h at 25 ºC. The reaction mixture was concentrated and the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 10:1) to afford 1-yne-VCP **1s** (331 mg, 67%).

1s: Colorless oil: TLC R_f (20% EA/PE) = 0.65. ^{1}H NMR (600 MHz, C_6D_6): δ 0.45 (d, J = 8.0 Hz, 4H), 0.81 (d, J = 6.6 Hz, 6H), 1.66-1.69 (m, 2H), 1.91 (s, 3H), 2.11 (heptet, J = 6.6 Hz, 1H), 3.43-3.45 (m, 2H), 4.06 (s, 2H), 4.93 (d, J = 10.5 Hz, 1H), 5.11 (d, J = 17.6 Hz, 1H), 5.34 (dd, J = 10.4 and 17.0 Hz, 1H), 6.78 (d, J = 7.7 Hz, 2H), 7.78 (d, J = 7.7 Hz, 2H). ^{13}C NMR (150 MHz, C_6D_6): δ 14.4, 20.8, 21.1, 22.7, 30.2, 34.5, 37.4, 44.9, 73.0, 91.3, 111.4, 129.4, 137.6, 142.7, 143.2. IR (neat): v 2931, 1461, 1356, 1162 cm^{-1}. HRMS (ESI) calcd for $C_{20}H_{28}NO_2S$ (M+H): 346.1835. Found: 346.1841.

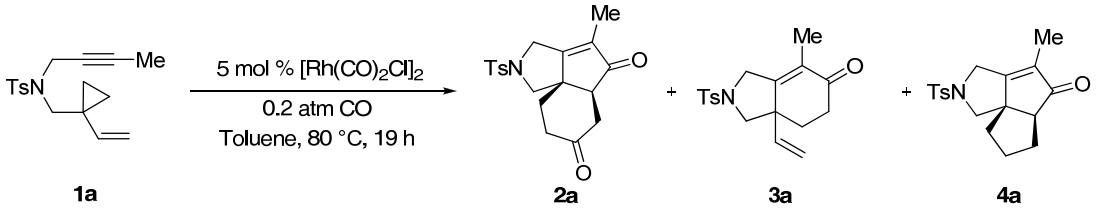
2.2 Experimental Details for the Rh(I)-Catalyzed Formal [5+1]/[2+2+1] Cycloaddition

General Procedures for the Rh(I)-Catalyzed Formal [5+1]/[2+2+1] Cycloaddition: A solution of 1-yne-VCP substrate and $[Rh(CO)_2Cl]_2$ (19.5 mg per mmol substrate, 5 mol %) in anhydrous DCE (20 mL per mmol) was degassed by bubbling CO or CO/N_2 (balloon pressured mixed gas of CO and N_2) for 5 min. Then the reaction mixture was immersed in an 80 ºC oil bath and stirred under the above atmosphere. When TLC indicated the disappearance of the starting material, the reaction mixture was cooled to room temperature and concentrated. The crude mixture was submitted to flash column chromatography on silica gel to afford the corresponding product (all reported yields were isolated yields).

All the reported results were obtained in their indicated CO pressures and the yields of the products were sensitive to the applied CO pressures.

We also must emphasize here that, very well stirring of the reaction is very important to make the CO gas enter the reaction system so that the [5+1]/[2+2+1] reaction can take place. Otherwise, the background reactions of [3+2] and [(3+2)+1] catalyzed by $[Rh(CO)_2Cl]_2$ without CO participation will happen to give the corresponding [3+2] and [(3+2)+1] cycloadducts only.[4,5]

Experimental Data for the Rh(I)-Catalyzed Formal [5+1]/[2+2+1] Cycloaddition Products (2a, 3a & 4a)



A solution of 1-yne-VCP **1a**[1] (31.0 mg, 0.10 mmol) substrate and $[Rh(CO)_2Cl]_2$ (2.0 mg, 0.005 mmol) in anhydrous toluene (2 mL) was degassed by bubbling 0.2 atm CO (balloon pressured mixed gas of CO and N_2, 1:4 V/V) for 5 min. Then the reaction mixture was immersed in an 80 ºC oil bath and stirred under the above atmosphere. When TLC indicated the disappearance of the starting material, the reaction mixture was cooled to room temperature and concentrated. The crude mixture was submitted to flash column chromatography on silica gel (eluted with PE/AE 2:1 to 1:2) to afford the corresponding products **2a** (11.7 mg, 32%), **3a**[1] (13.3 mg, 39%) and **4a** (1.4 mg, 4%). Substrate concentration: 0.05 M, reaction time: 19 h.

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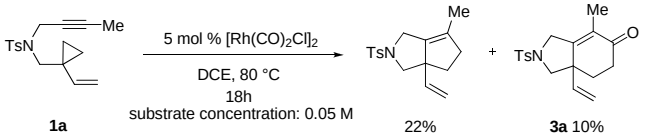
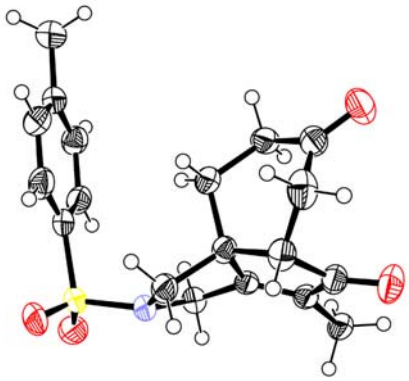
[4] Without CO, the reaction of **1a** catalyzed by $[Rh(CO)_2Cl]_2$ gave the [3+2] and [(3+2)+1] cycloadducts only. The [3+2] reaction in this case was not good in terms of reaction yield, compared to that obtained by the [3+2] reaction of **1a** catalyzed by $[Rh(dppp)]SbF_6$. For the [3+2] reaction of 1-yne-VCPs, see: Lei, J.; Li, M.; Yu, Z.-X. *Chem. Commum*. **2010**, *46*, 1059-1061.



[5] A solution of 1-yne-VCP **1a** (19.4 mg, 0.064 mmol) substrate and $[Rh(CO)_2Cl]_2$ (1.2 mg) in DCE (1.3 mL) was immersed in an 80 ºC oil bath and stirred under Ar atmosphere. When TLC indicated the disappearance of the starting material, the reaction mixture was cooled to room temperature and concentrated. The crude mixture was submitted to flash column chromatography on silica gel (eluted with PE/AE 20:1, 10:1 to 5:1) to afford the [3+2] product (4.3 mg, 22%) and **3a** (2.2 mg, 10%). Substrate concentration: 0.05 M, reaction time: 18 h.

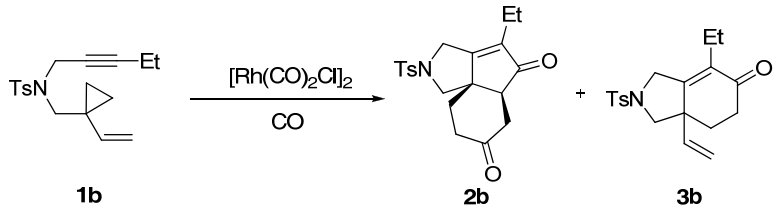
2a: Light yellow solid: TLC R_f (50% EA/PE) = 0.20, m.p. 166-168 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.74 (s, 3H), 1.78-1.87 (m, 3H), 2.22 (dt, J = 16.8 and 5.9 Hz, 1H), 2.43-2.47 (m, 4H), 2.56 (dd, J = 7.4 and 17.2 Hz, 1H), 2.88 (dd, J = 3.5 and 17.2 Hz, 1H), 2.93 (d, J = 9.8 Hz, 1H), 3.83 (d, J = 9.8 Hz, 1H), 4.08 (d, J = 16.2 Hz, 1H), 4.28 (d, J = 16.2 Hz, 1H), 7.37 (d, J = 8.3 Hz, 2H), 7.75 (d, J = 8.3 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 8.8, 21.5, 28.5, 35.2, 37.2, 45.4, 48.8, 49.8, 58.0, 127.3, 130.0, 133.5, 134.3, 144.2, 170.6, 207.3, 208.5. IR (neat): ν 2935, 1717, 1684, 1605, 1348, 1162 cm^{-1}. HRMS (ESI) calcd for $C_{19}H_{22}NO_4S$ (M+H): 360.1264. Found: 360.1255. Please see its relative 2D-NMR data in Section 5. For the Cambridge X-ray data, see CCDC number: 790092.



Empirical formula	$C_{19}H_{21}NO_4S$
Formula weight	359.43
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system, space group	orthorhombic, Pbca
Unit cell dimensions	a = 11.288(2) Å α = 90.00 deg.
	b = 14.489(3) Å β = 90.00 deg.
	c = 20.884(4) Å γ = 90.00 deg.
Volume	3415.7(12) Å^3
Z, Calculated density	8, 1.398 g/cm^3
Absorption coefficient	0.214 mm^{-1}
F(000)	1520
Crystal size	0.80 x 0.38 x 0.19 mm
Theta range for data collection	2.81 to 25.00 deg.
Limiting indices	$-12 \le h \le 10$, $-17 \le k \le 16$, $-13 \le l \le 24$
Reflections collected / unique	10821 / 2808
Completeness to theta = 25.00	98.8 %
Max. and min. transmission	0.9605 and 0.8475
Refinement method	Full-matrix least-squares on F^2
Goodness-of-fit on F^2	1.193
Final R indices [I>2sigma(I)]	R1 = 0.0517, wR^2 =0.1131
R indices (all data)	R1 = 0.0559, wR^2 = 0.1157
Largest diff. peak and hole	0.225 and -0.294 e Å^{-3}

4a: Colorless oil: TLC R_f (50% EA/PE) = 0.60. ^{1}H NMR (600 MHz, $CDCl_3$): δ 1.18 (m, 1H), 1.45 (dt, J = 6.6 and 12.2 Hz, 1H), 1.63-1.74 (m, 6H), 2.02 (dd, J = 4.7 and 11.1 Hz, 1H), 2.42-2.46 (m, 4H), 3.02 (d, J = 9.4 Hz, 1H), 3.67 (d, J = 9.4 Hz, 1H), 4.02 (d, J = 15.2 Hz, 1H), 4.20 (dd, J = 1.6 and 15.2 Hz, 1H), 7.34 (d, J = 7.5 Hz, 2H), 7.74 (d, J = 8.9 Hz, 2H). ^{13}C NMR (150 MHz, $CDCl_3$): δ 8.8, 21.6, 24.8, 29.3, 36.5, 46.0, 54.9, 57.8, 57.9, 127.4, 129.9, 133.8, 144.0, 172.5, 211.0. IR (neat): ν 2965, 2875, 1717, 1684, 1449, 1348, 1162. HRMS (ESI) calcd for $C_{18}H_{22}NO_3S$ (M+H): 332.1315. Found: 332.1312. See its relative 2D-NMR data in Section 5.

Products (2b & 3b)

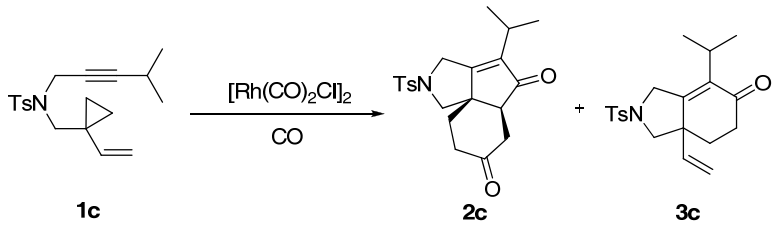


Following the general procedure, 1-yne-VCP **1b** (30.2 mg, 0.1 mmol) was converted to products **2b** (20.4 mg, 58%) and **3b** (1.2 mg, 4%). Substrate concentration: 0.05 M, CO pressure: 0.5 atm CO (balloon pressured mixed gas of CO and N_2, 1:1 V/V), temperature: 80 ºC, reaction time: 2.5 h.

2b: Colorless oil: TLC R_f (50% EA/PE) = 0.21. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.00 (t, J = 7.4 Hz, 3H), 1.74-1.91 (m, 3H), 2.09-2.30 (m, 3H), 2.42-2.45 (m, 4H), 2.55 (dd, J = 6.9 and 17.3 Hz, 1H), 2.87 (dd, J = 3.4 and 17.3 Hz, 1H), 2.92 (d, J = 9.9 Hz, 1H), 3.83 (d, J = 9.3 Hz, 1H), 4.13 (d, J = 15.7 Hz, 1H), 4.29 (d, J = 15.7 Hz, 1H), 7.37 (d, J = 8.0 Hz, 2H), 7.75 (d, J = 8.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 12.3, 17.5, 21.5, 28.7, 35.1, 37.1, 45.4, 49.0, 49.8, 57.9, 127.0, 130.0, 133.5, 140.0, 144.2, 169.8, 207.0, 208.4. IR (neat): ν 2939, 1724, 1684, 1602, 1352, 1162 cm^{-1}. HRMS (ESI) calcd for $C_{20}H_{23}NNaO_4$ (M+Na): 396.1240. Found: 396.1238.

3b: Colorless oil: TLC R_f (50% EA/PE) = 0.57. ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.94 (t, J = 7.3 Hz, 3H), 1.84 (dt, J = 4.9 and 13.3 Hz, 1H), 1.98 (ddd, J = 2.4, 4.9 and 12.8 Hz, 1H), 2.04 (dt, J = 21.2 and 7.5 Hz, 1H), 2.25 (dd, J = 7.8 and 13.4 Hz, 1H), 2.40 (dd, J = 4.9 and 13.9 Hz, 1H), 2.43-2.47 (m, 4H), 2.86 (d, J = 9.2 Hz, 1H), 3.72 (d, J = 8.7 Hz, 1H), 3.90 (d, J = 16.7 Hz, 1H), 4.19 (d, J = 16.1 Hz, 1H), 4.93 (d, J = 17.4 Hz, 1H), 5.15 (d, J = 10.8 Hz, 1H), 5.72 (dd, J = 10.8 and 17.4 Hz, 1H), 7.35 (d, J = 7.8 Hz, 2H), 7.72 (d, J = 7.8 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 13.2, 19.5, 21.5, 30.8, 33.1, 49.6, 57.8, 59.7, 117.3, 127.5, 129.8, 133.3, 136.1, 138.2, 143.9, 155.3, 196.8 cm^{-1}. HRMS (ESI) calcd for $C_{19}H_{23}NNaO_3$ (M+Na): 368.1291. Found: 368.1288.

Products (2c & 3c)



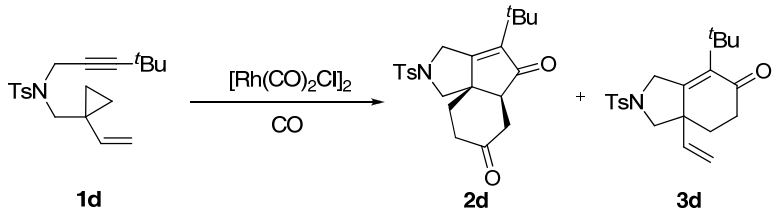
1c **2c** **3c**

Following the general procedure, 1-yne-VCP **1c**[1] (19.5 mg, 0.06 mmol) was converted to products **2c** (16.4 mg, 72%) and **3c** (2.0 mg, 9%). Substrate concentration: 0.05 M, CO pressure: 1 atm CO, temperature: 80 ºC, reaction time: 4 h.

2c: White solid: TLC R_f (50% EA/PE) = 0.23, m.p. 130-132 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.04 (d, J = 7.1 Hz, 3H), 1.09 (d, J = 7.0 Hz, 3H), 1.73-1.89 (m, 4H), 2.17-2.23 (m, 1H), 2.40 (q, J = 3.5 Hz, 1H), 2.45 (s, 3H), 2.52 (dd, J = 6.6 and 17.2 Hz, 1H), 2.70 (heptet, J = 7.1 Hz, 1H), 2.85-2.90 (m, 1H), 3.80 (d, J = 9.3 Hz, 1H), 4.22 (d, J = 16.3 Hz, 1H), 4.31 (d, J = 16.3 Hz, 1H), 7.37 (d, J = 8.4 Hz, 2H), 7.75 (d, J = 8.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 20.0, 21.6, 25.1, 29.1, 35.2, 37.1, 45.7, 49.1, 50.0, 57.8, 127.4, 130.0, 133.6, 143.5, 144.3, 168.5, 206.7, 208.4. IR (neat): ν 2935, 1717, 1669, 1348, 1158, 1099 cm^{-1}. HRMS (ESI) calcd for $C_{21}H_{26}NO_4S$ (M+H): 388.1577. Found: 388.1570.

3c: White solid: TLC R_f (50% EA/PE) = 0.58, m.p. 130-132 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.10 (d, J = 7.0 Hz, 3H), 1.13 (d, J = 7.0 Hz, 3H), 1.83 (dd, J = 5.1 and 13.7 Hz, 1H), 1.93 (ddd, J = 2.3, 5.1 and 12.5 Hz, 1H), 2.27 (ddd, J = 2.3 5.1 and 17.6 Hz, 1H), 2.37 (dd, J = 5.5 and 14.1 Hz, 1H), 2.44 (s, 3H), 2.69 (heptet, J = 7.0 Hz, 1H), 2.86 (d, J = 9.3 Hz, 1H), 3.68 (d, J = 9.3 Hz, 1H), 4.00 (d, J = 16.5 Hz, 1H), 4.20 (d, J = 16.5 Hz, 1H), 4.93 (d, J = 17.1 Hz, 1H), 5.15 (d, J = 10.1 Hz, 1H), 5.70 (dd, J = 10.1 and 17.1 Hz, 1H), 7.33 (d, J = 8.0 Hz, 2H), 7.71 (d, J = 8.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 20.3, 21.6, 28.3, 30.4, 33.8, 49.5, 49.8, 59.4, 117.3, 127.6, 129.8, 133.3, 138.5, 139.3, 143.9, 154.7, 196.9. IR (neat): ν 2942, 1676, 1356, 1166 cm^{-1}. HRMS (ESI) calcd for $C_{20}H_{25}NNaO_3S$ (M+Na): 382.1447. Found: 382.1449.

Products (2d & 3d)



1d **2d** **3d**

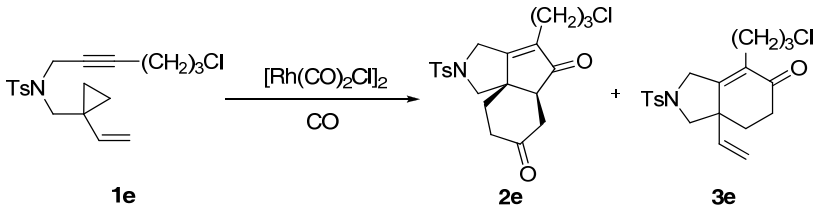
Following the general procedure, 1-yne-VCP **1d** (34.6 mg, 0.1 mmol) was converted to products **2d** (28.6 mg, 71%) and **3d** (9.7 mg, 26%). Substrate concentration: 0.05 M, CO pressure: 1 atm CO, temperature: 80 ºC, reaction time: 3.5 h.

2d: White solid: TLC R_f (50% EA/PE) = 0.25, m.p. 168-170 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.18 (s, 9H), 1.73-1.89 (m, 3H), 2.16-2.22 (m, 1H), 2.38 (dd, J = 3.0 and 6.9 Hz, 1H), 2.46 (s, 3H),

2.48 (dd, J = 6.9 and 17.7 Hz, 1H), 2.86-2.91 (m, 2H), 3.91 (d, J = 9.4 Hz, 1H), 4.31 (d, J = 16.8 Hz, 1H), 4.40 (d, J = 16.8 Hz, 1H), 7.38 (d, J = 8.4 Hz, 2H), 7.75 (d, J = 8.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.6, 28.5, 29.7, 33.1, 35.1, 36.9, 46.9, 49.6, 49.8, 57.4, 127.3, 130.0, 133.7, 144.2, 144.9, 167.8, 206.7, 208.4. IR (neat): ν 2924, 1721, 1356, 1266, 1166 cm^{-1}. HRMS (ESI) calcd for $C_{22}H_{27}NNaO_4S$ (M+Na):424.1553. Found: 424.1551.

3d: Colorless oil: TLC R_f (50% EA/PE) = 0.62. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.22 (s, 9H), 1.76 (dt, J = 6.3 and 13.3 Hz, 1H), 1.91 (ddd, J = 1.5, 6.3 and 12.9 Hz, 1H), 2.25 (ddd, J = 1.2 5.9 and 17.5 Hz, 1H),2.39 (dd, J = 6.3 and 13.2 Hz, 1H), 2.46 (s, 3H), 2.66 (d, J = 9.3 Hz, 1H), 3.59 (d, J = 8.9 Hz, 1H), 4.09 (d, J = 16.0 1H), 4.34 (d, J = 16.8, 1H), 4.92 (d, J = 17.1 Hz, 1H), 5.16 (d, J = 10.2 Hz, 1H), 5.70 (dd, J = 10.6 and 17.1 Hz, 1H), 7.36 (d, J = 7.8 H, 2H), 7.71 (d, J = 8.2 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.5, 29.2, 30.4, 35.0, 36.5, 50.8, 51.3, 58.2, 117.4, 127.7, 129.8, 132.5, 139.0, 142.6, 143.9, 152.0, 198.5. IR (neat): ν 2961, 1676, 1352, 1170 cm^{-1}. HRMS (ESI) calcd for $C_{21}H_{27}NNaO_3S$ (M+Na): 396.1604. Found: 396.1603.

Products (2e & 3e)



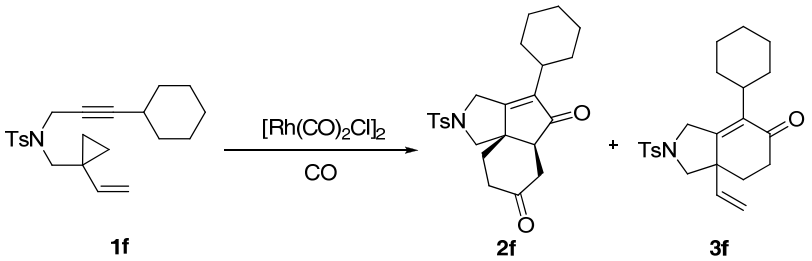
Following the general procedure, 1-yne-VCP **1e** (21.4 mg, 0.058 mmol) was converted to products **2e** (14.7 mg, 60%) and **3e** (6.7 mg, 29%). Substrate concentration: 0.05 M, CO pressure: 0.5 atm CO, temperature: 80 ºC, reaction time: 3.5 h.

2e: Colorless oil: TLC R_f (50% EA/PE) = 0.28. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.74-1.95 (m, 5H), 2.25 (ddd, J = 2.8, 5.5 and 17.6 Hz, 1H), 2.32 (t, J = 7.4 Hz, 1H), 2.38 (t, J = 7.4 Hz, 1H), 2.43-2.45 (m, 4H), 2.56 (dd, J = 7.1 and 17.2 Hz, 1H), 2.88 (dd, J = 3.5 and 17.6 Hz, 1H), 2.90 (d, J = 9.4 Hz, 1H), 3.39 (t, J = 5.9 Hz, 2H), 3.85 (d, J = 9.3 Hz, 1H), 4.13 (d, J = 16.3 Hz, 1H), 4.32 (d, J = 16.3 Hz, 1H), 7.37 (d, J = 8.3 Hz, 2H), 7.75 (d, J = 8.3 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.6, 28.8, 29.7, 35.2, 37.2, 44.0, 45.5, 49.1, 50.0, 58.0, 127.4, 130.1, 133.3, 136.7, 144.3, 172.0, 207.0, 208.1. IR (neat): ν 2928, 1721, 1345, 1166 cm^{-1}. HRMS (ESI) calcd for $C_{21}H_{25}ClNO_4S$ (M+H): 422.11873. Found: 422.1198.

3e: Colorless oil: TLC R_f (50% EA/PE) = 0.66. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.77-1.88 (m, 3H), 2.00 (ddd, J = 2.4, 5.1 and 12.9 Hz, 1H), 2.23 (dd, J = 7.4 and 13.3 Hz, 1H), 2.27-2.36 (m, 2H), 2.41 (dd, J = 5.1 and 13.8 Hz, 1H), 2.45 (s, 3H), 2.84 (d, J = 9.4 Hz, 1H), 3.46 (t, J = 6.3 Hz, 2H), 3.74 (d, J = 9.4 Hz, 1H), 3.95 (d, J = 17.0 Hz, 1H), 4.23 (d, J = 17.0 Hz, 1H), 4.92 (d, J = 17.1 Hz, 1H), 5.17 (d, J = 10.2 Hz, 1H), 5.73 (dd, J = 10.2 and 17.1 Hz, 1H), 7.35 (d, J = 8.2 Hz, 2H), 7.72 (d, J = 8.2 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.6, 23.8, 30.7, 31.1, 33.0, 44.5, 49.4, 49.8, 59.8, 117.4, 127.5, 129.8, 133.0, 138.1, 144.0, 157.2, 197.0. IR (neat): ν 2935, 1676, 1348, 1170

cm^{-1}. HRMS (ESI) calcd for $C_{20}H_{25}ClNO_3S$ (M+H): 394.1238. Found: 394.1243.

Products (2f & 3f)

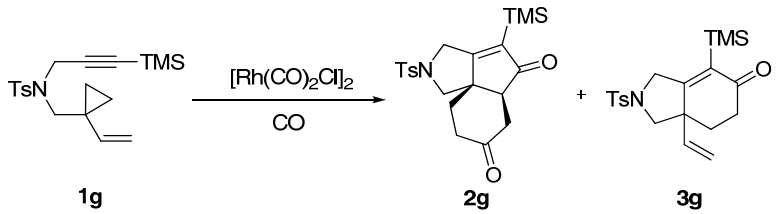


Following the general procedure, 1-yne-VCP **1f** (36.7 mg, 0.1 mmol) was converted to products **2f** (25.8 mg, 61%) and **3f** (5.6 mg, 14%). Substrate concentration: 0.05 M, CO pressure: 1 atm CO, temperature: 80 ºC, reaction time: 2 h.

2f: White solid: TLC R_f (50% EA/PE) = 0.20, m.p 164-166 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.16-1.35 (m, 5H), 1.55 (d, J = 11.8 Hz, 1H), 1.66-1.87 (m, 7H), 2.15-2.21 (m, 1H), 2.36 (dd, J = 2.5 and 8.8 Hz, 1H), 2.40 (q, J = 3.4 Hz, 1H), 2.45 (s, 3H), 2.52 (dd, J = 2.5 and 8.8 Hz, 1H), 2.87 (dd, J = 3.4 and 17.1 Hz, 1H), 2.91 (d, J = 9.3 Hz, 1H), 3.80 (d, J = 9.3 Hz, 1H), 4.24 (d, J = 16.3 Hz, 1H), 4.30 (d, J = 16.3 Hz, 1H), 7.37 (d, J = 8.0 Hz, 2H), 7.75 (d, J = 8.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.6, 26.1, 29.0, 30.0, 31.7, 34.9, 37.1, 45.8, 48.9, 50.0, 57.8, 127.4, 130.0, 133.6, 142.5, 144.2, 168.7, 206.8, 208.4. IR (neat): ν 2939, 2861, 1721, 1352, 1170 cm^{-1}. HRMS (ESI) calcd for $C_{24}H_{29}NNaO_4S$ (M+Na): 450.1710. Found: 450.1700.

3f: Colorless oil: TLC R_f (50% EA/PE) = 0.51. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.16-1.41 (m, 3H), 1.66-1.79 (m, 6H), 1.83 (dd, J = 5.1 and 13.7 Hz, 1H), 1.92 (ddd, J = 2.4, 5.5 and 12.9 Hz, 1H), 2.24-2.42 (m, 4H), 2.45 (s, 3H), 2.86 (d, J = 9.4 Hz, 1H), 3.67 (d, J = 9.4 Hz, 1H), 4.03 (d, J = 16.8 Hz, 1H), 4.21 (d, J = 16.8 Hz, 1H), 4.90 (d, J = 17.3 Hz, 1H), 5.11 (d, J = 10.1 Hz, 1H), 5.67 (dd, J = 10.1 and 17.3 Hz, 1H), 7.36 (d, J = 8.2 Hz, 2H), 7.73 (d, J = 8.2 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.5, 25.7, 26.8, 30.0, 33.8, 39.2, 49.5, 49.9, 59.2, 117.8, 127.6, 129.7, 133.4, 138.5, 138.6, 143.9, 154.9, 197.6. IR (neat): ν 2935, 2864, 2261, 1672, 1352, 1162 cm^{-1}. HRMS (ESI) calcd for $C_{23}H_{29}NNaO_3S$ (M+Na): 422.1760. Found: 422.1760.

Products (2g & 3g)

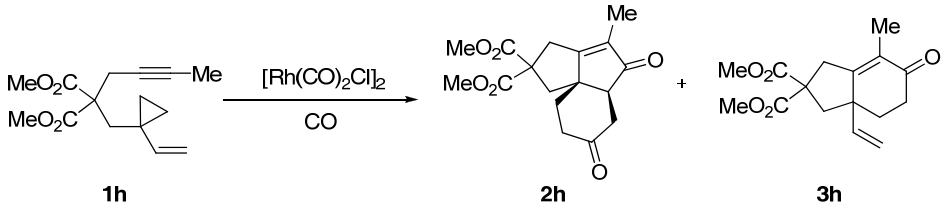


Following the general procedure, 1-yne-VCP **1g** (22.3 mg, 0.062 mmol) was converted to products **2g** (10.0 mg, 39%) and **3g** (1.4 mg, 6%). Substrate concentration: 0.05 M, CO pressure: 0.2 atm CO, temperature: 80 ºC, reaction time: 5 h.

2g: White solid: TLC R_f (50% EA/PE) = 0.23, m.p 158-159 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.17 (s, 9H), 1.72-1.89 (m, 3H), 2.16-2.23 (m, 1H), 2.41 (dd, J = 3.1 and 6.7 Hz, 1H), 2.45 (s, 3H), 2.51 (dd, J = 7.0 and 17.6 Hz, 1H), 2.87 (dd, J = 3.1 and 17.6 Hz, 1H), 2.93 (d, J = 9.5 Hz, 1H), 3.82 (d, J = 9.5 Hz, 1H), 4.12 (d, J = 16.4 Hz, 1H), 4.34 (d, J = 16.4 Hz, 1H), 7.37 (d, J = 8.1 Hz, 2H), 7.75 (d, J = 8.1 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ -1.53, 21.6, 29.3, 35.2, 36.9, 46.9, 50.3, 53.0, 57.6, 127.4, 130.0, 133.6, 138.0, 144.3, 184.6, 208.1, 210.8. IR (neat): ν 2931, 2369, 1728, 1624, 1352, 1255, 1166 cm^{-1}. HRMS (ESI) calcd for $C_{21}H_{27}NNaO_4SSi$ (M+Na): 440.1322. Found: 440.1320.

3g: Colorless oil: TLC R_f (50% EA/PE) = 0.45. ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.18 (s, 9H), 1.81 (dt, J = 5.2 and 13.3 Hz, 1H), 1.98 (ddd, J = 2.0, 5.5 and 12.9 Hz, 1H), 2.25 (ddd, J = 2.0, 5.2 and 17.6 Hz, 1H), 2.37 (ddd, J = 5.5, 13.7 and 17.9 Hz, 1H), 2.45 (s, 3H), 2.76 (d, J = 8.9 Hz, 1H), 3.70 (d, J = 9.3 Hz, 1H), 3.87 (d, J = 17.2 Hz, 1H), 4.21 (d, J = 17.2 Hz, 1H), 4.91 (d, J = 17.2 Hz, 1H), 5.18 (d, J = 10.1 Hz, 1H), 5.71 (dd, J = 10.1 and 17.2 Hz, 1H), 7.36 (d, J = 7.9 Hz, 2H), 7.70 (d, J = 7.9 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 0.49, 21.6, 30.2, 32.9, 50.3, 51.7, 58.8, 117.4, 127.7, 129.8, 133.0, 135.8, 138.2, 144.0, 168.8, 201.0. IR (neat): ν 2965, 1661, 1605, 1352, 1251, 1170, 1095, 1054 cm^{-1}. HRMS (ESI) calcd for $C_{20}H_{27}NNaO_3SSi$ (M+Na): 412.1373. Found: 412.1371.

Products (2h & 3h)

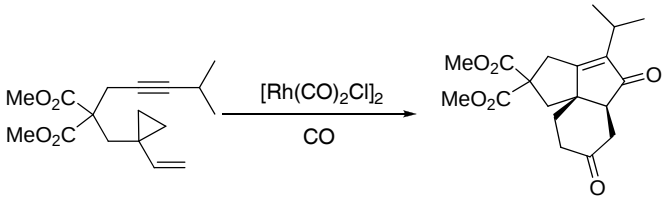


Following the general procedure, 1-yne-VCP **1h**[1] (16.1 mg, 0.07 mmol) was converted to products **2h** (9.1 mg, 47%) and **3h**[1] (3.4 mg, 19%). Substrate concentration: 0.05 M, CO pressure: 1 atm CO, temperature: 80 ºC, reaction time: 1 h.

2h: Colorless oil: TLC R_f (50% EA/PE) = 0.17. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.79 (s, 3H), 1.80-1.85 (m, 3H), 2.17-2.25 (m, 1H), 2.28 (d, J = 13.8 Hz, 1H), 2.49 (dd, J = 3.2 and 6.7 Hz, 1H), 2.58 (dd, J = 7.0 and 17.3 Hz, 1H), 2.75 (d, J = 13.8 Hz, 1H), 2.91 (dd, J = 3.6 and 17.3 Hz, 1H),

3.28 (d, J = 17.8 Hz, 1H), 3.40 (dd, J = 1.4 and 17.8 Hz, 1H), 3.76 (s, 3H), 3.82 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 8.8, 29.7, 33.0, 35.6, 37.5, 44.9, 50.8, 51.9, 53.4, 59.8, 133.5, 171.6, 172.1, 176.3, 208.8, 209.3. IR (neat): ν 2965, 2928, 1736, 1676, 1438, 1274 cm^{-1}. HRMS (ESI) calcd for $C_{17}H_{21}O_6$ (M+H): 321.1332. Found: 321.1331. See its relative 2D-NMR data in Section 5.

Product (2i)

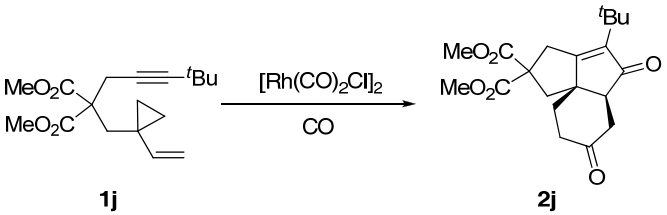


1i **2i**

Following the general procedure, 1-yne-VCP **1i** (36.6 mg, 0.125 mmol) was converted to product **2i** (39.7 mg, 91%). Substrate concentration: 0.05 M, CO pressure: 1 atm CO, temperature: 80 ºC, reaction time: 1 h.

2i: White solid: TLC R_f (33% EA/PE) = 0.20, m.p 98-100 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.15 (d, J = 6.8 Hz, 3H), 1.17 (d, J = 6.8 Hz, 3H), 1.75-1.84 (m, 3H), 2.17-2.23 (m, 1H), 2.27 (d, J = 13.8 Hz, 1H), 2.47 (q, J = 3.4 Hz, 1H), 2.56 (dd, J = 6.9 and 17.7 Hz, 1H), 2.73 (d, J = 13.3 Hz, 1H), 2.78 (heptet, J = 6.8 Hz, 1H), 2.90 (dd, J = 2.9 and 17.2 Hz, 1H), 3.38 (d, J = 17.7 Hz, 1H), 3.46 (d, J = 17.7 Hz, 1H), 3.76 (s, 3H), 3.82 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 20.4, 21.4, 25.1, 30.3, 33.5, 35.5, 37.3, 44.6, 50.8, 52.1, 53.3, 60.1, 74.1, 142.9, 171.1, 172.0, 174.3, 208.2, 209.3. IR (neat): ν 2965, 1728, 1724, 1661, 1439, 1263, 1065 cm^{-1}. HRMS (ESI) calcd for $C_{19}H_{24}NaO_6$ (M+Na): 371.1465. Found: 371.1466.

Product (2j)



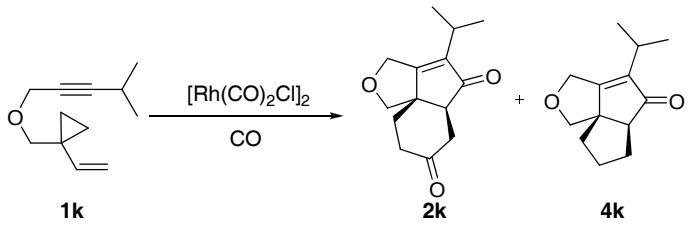
1j **2j**

Following the general procedure, 1-yne-VCP **1j** (30.5 mg, 0.1 mmol) was converted to product **2j** (26.8 mg, 74%). Substrate concentration: 0.05 M, CO pressure: 1 atm CO, temperature: 80 ºC, reaction time: 1.5 h.

2j: Colorless oil: TLC R_f (50% EA/PE) = 0.35. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.26 (s, 9H), 1.69-1.84 (m, 3H), 2.14-2.22 (m, 1H), 2.25 (d, J = 13.7 Hz, 1H), 2.43 (dd, J = 3.1 and 6.8 Hz, 1H), 2.52 (dd, J = 6.9 and 17.5 Hz, 1H), 2.73 (d, J = 13.7 Hz, 1H), 2.89 (dd, J = 3.2 and 17.5 Hz, 1H), 3.48 (d, J = 18.1, 1H), 3.64 (d, J = 18.1 Hz, 1H), 3.77 (s, 3H), 3.82 (s, 3H). ^{13}C NMR (100 MHz,

$CDCl_3$): δ 29.0, 30.8, 33.3, 34.9, 35.4, 37.1, 44.2, 50.1, 52.3, 53.3, 60.1, 144.2, 171.2, 173.2, 208.3, 209.4. IR (neat): ν 2961, 1728, 1646, 1438, 1263, 1222, 1065 cm^{-1}. HRMS (ESI) calcd for $C_{20}H_{26}NaO_6$ (M+Na): 385.1622. Found: 385.1626.

Products (2k & 4k)

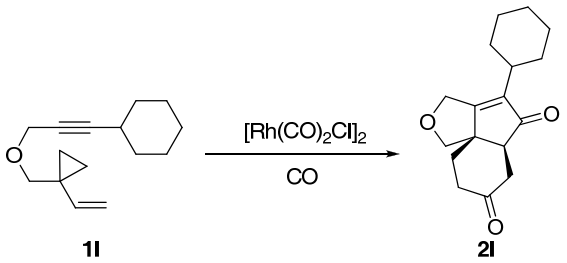


Following the general procedure, 1-yne-VCP **1k** (18.4 mg, 0.1 mmol) was converted to products **2k** (21.0 mg, 87%) and **4k** (2.4 mg, 11%). Substrate concentration: 0.05 M, CO pressure: 1 atm CO, temperature: 80 ºC, reaction time: 1.5 h.

2k: Colorless oil: TLC R_f (50% EA/PE) = 0.25. ^{1}H NMR (400 MHz, C_6D_6): δ 0.89 (d, J = 7.1 Hz, 3H), 0.91 (d, J = 7.1 Hz, 3H), 1.23-1.39 (m, 2H), 1.54 (ddd, J = 4.5, 12.1 and 17.5 Hz, 1H), 1.73 (dd, J = 3.3 and 7.1 Hz, 1H), 1.88 (dt, J = 17.5 and 4.5 Hz, 1H), 2.01 (dd, J = 7.1 and 17.6 Hz, 1H), 2.61 (heptet, J = 7.1 Hz, 1H), 2.89 (d, J = 8.2 Hz, 1H), 2.90 (dd, J = 3.3 and 17.6 Hz, 1H), 3.53 (d, J = 8.2 Hz, 1H) 4.14 (d, J = 15.7 Hz, 1H), 4.24 (d, J = 15.7 Hz, 1H). ^{13}C NMR (100 MHz, C_6D_6): δ 19.9, 21.5, 25.5, 30.4, 36.4, 37.3, 48.6, 51.0, 63.8, 76.5, 141.8, 173.2, 206.9, 207.4. IR (neat): ν 2369, 2287, 1728, 1337, 816 cm^{-1}. HRMS (ESI) calcd for $C_{14}H_{18}NaO_3$ (M+Na): 257.1148. Found: 257.1145. See its relative 2D-NMR data in Section 5.

4k: Colorless oil: TLC R_f (50% EA/PE) = 0.60. ^{1}H NMR (400 MHz, C_6D_6): δ 0.95 (d, J = 6.7 Hz, 3H), 0.96 (d, J = 6.7 Hz, 3H), 1.16 (dd, J = 7.3 and 16.6 Hz, 1H), 1.22 (q, J = 6.0 Hz, 1H), 1.25-1.31 (m, 2H), 1.55 (dd, J = 5.6 and 10.8 Hz, 1H), 2.09-2.15 (m, 2H), 2.68 (heptet, J = 6.7 Hz, 1H), 3.19 (d, J = 7.9 Hz, 1H), 3.59 (d, J = 7.9 Hz, 1H), 4.26 (d, J = 15.6 Hz, 1H), 4.33 (d, J = 15.6 Hz, 1H). ^{13}C NMR (100 MHz, C_6D_6): δ 20.0, 21.6, 24.9, 25.5, 29.4, 36.9, 54.4, 59.1, 64.1, 76.5, 141.7, 175.1, 210.1. IR (neat): ν 2957, 2875, 2369, 1710, 1669, 1032 cm^{-1}. HRMS (ESI) calcd for $C_{13}H_{19}O_2$ (M+H): 207.1380. Found: 207.1375. See its relative 2D-NMR data in Section 5.

Product (2l)

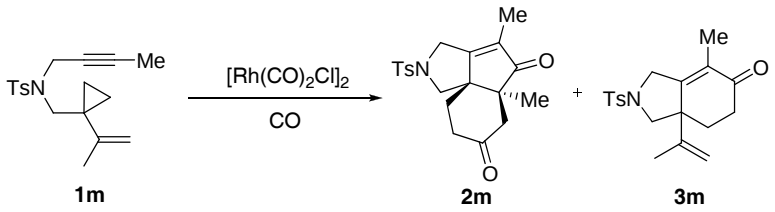


1l **2l**

Following the general procedure, 1-yne-VCP **1l** (33.2 mg, 0.15 mmol) was converted to product **2l** (32.2 mg, 77%). Substrate concentration: 0.05 M, CO pressure: 1 atm CO, temperature: 80 ºC, reaction time: 2 h.

2l: Light yellow oil: TLC R_f (50% EA/PE) = 0.20. ^{1}H NMR (400 MHz, C_6D_6): δ 0.90-1.21 (m, 5H), 1.31-1.43 (m, 2H), 1.52-1.64 (m, 6H), 1.76 (heptet, J = 3.1 Hz, 1H), 1.91 (dt, J = 17.8 and 3.8 Hz, 1H), 2.02 (ddd, J = 3.8, 6.6 and 17.8 Hz, 1H), 2.38 (tt, J = 2.5 and 12.0 Hz, 1H), 2.91 (dd, J = 3.5 and 11.1 Hz, 1H), 2.92-2.95 (m, 1H), 3.56 (q, J = 3.8 Hz, 1H), 4.18 (d, J = 15.5 Hz, 1H), 4.28 (d, J = 15.5 Hz, 1H). ^{13}C NMR (100 MHz, C_6D_6): δ 26.2, 26.6, 28.7, 30.2, 32.1, 35.3, 37.4, 48.3, 51.0, 64.0, 76.6, 104.9, 173.5, 207.1, 207.6. IR (neat): ν 2935, 2857, 2369, 1717, 1665, 1028 cm^{-1}. HRMS (ESI) calcd for $C_{17}H_{23}O_3$ (M+H): 275.1642. Found: 275.1639.

Products (2m & 3m)



1m **2m** **3m**

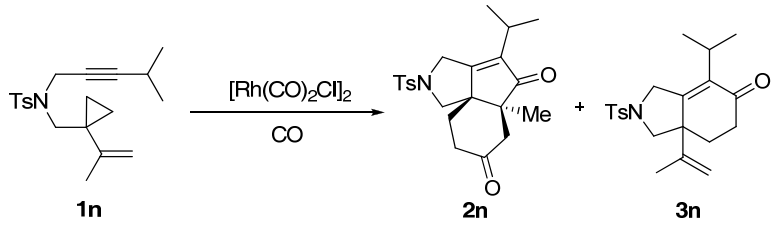
Following the general procedure, 1-yne-VCP **1m**[1] (33.4 mg, 0.1 mmol) was converted to products **2m** (14.3 mg, 36%) and **3m** (22.1 mg, 61%). Substrate concentration: 0.05 M, CO pressure: 0.2 atm CO, temperature: 80 ºC, reaction time: 4 h.

2m: Colorless oil: TLC R_f (50% EA/PE) = 0.23. ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.96 (s, 3H), 1.73 (s, 3H), 1.76-1.88 (m, 3H), 2.16-2.22 (m, 1H), 2.35 (d, J = 16.8 Hz, 1H), 2.45 (s, 3H), 2.74 (d, J = 16.8 Hz, 1H), 3.21 (d, J = 9.5 Hz, 1H), 3.57 (d, J = 9.5 Hz, 1H), 4.10 (d, J = 16.3 Hz, 1H), 4.23 (d, J = 16.3 Hz, 1H), 7.37 (d, J = 8.4 Hz, 2H), 7.76 (d, J = 8.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 9.0, 21.6, 29.8, 35.0, 45.7, 46.0, 49.7, 53.6, 127.3, 130.0, 131.8, 133.7, 144.2, 169.4, 208.5, 210.2. IR (neat): ν 2935, 1724, 1684, 1605, 1345, 1166 cm^{-1}. HRMS (ESI) calcd for $C_{20}H_{24}NO_4S$ (M+H): 374.1420. Found: 374.1420.

3m: Colorless oil: TLC R_f (50% EA/PE) = 0.58. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.69 (s, 3H), 1.74 (dd, J = 6.0 and 13.4 Hz, 1H), 1.80 (s, 3H), 2.12 (ddd, J = 2.9, 4.9 and 13.3 Hz, 1H), 2.27-2.40 (m, 2H), 2.45 (s, 3H), 2.72 (d, J = 9.8 Hz, 1H), 3.81 (d, J = 16.3 Hz, 1H), 3.93 (d, J = 9.8 Hz, 1H), 4.16 (d, J = 16.3 Hz, 1H), 4.60 (s, 1H), 4.96 (s, 1H), 7.35 (d, J = 8.4 Hz, 2H), 7.71 (d, J = 8.4 Hz,

2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 11.1, 18.9, 21.5, 29.4, 33.1, 49.8, 52.4, 57.7, 116.1, 127.6, 129.5, 129.7, 133.1, 141.8, 143.9, 157.4, 197.4. IR (neat): ν 2946, 1669, 1605, 1453, 1352, 1166 cm^{-1}. HRMS (ESI) calcd for $C_{19}H_{24}NO_3S$ (M+H): 346.1471. Found: 346.1471.

Products (2n & 3n)



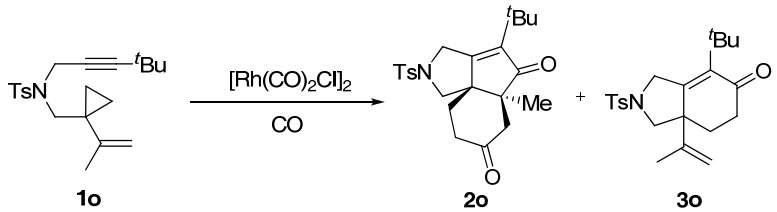
1n **2n** **3n**

Following the general procedure, 1-yne-VCP **1n** (39.6 mg, 0.1 mmol) was converted to products **2n** (14.2 mg, 31%) and **3n** (19.7 mg, 46%). Substrate concentration: 0.05 M, CO pressure: 1 atm CO, temperature: 80 ºC, reaction time: 1.5 h.

2n: Colorless oil: TLC R_f (33% EA/PE) = 0.31. ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.93 (s, 3H), 1.03 (d, J = 6.9 Hz, 3H), 1.09 (d, J = 6.9 Hz, 3H), 1.73-1.79 (m, 1H), 1.79-1.86 (m, 2H), 2.14-2.20 (m, 1H), 2.32 (d, J = 16.8 Hz, 1H), 2.45 (s, 3H), 2.65-2.69 (m, 1H), 2.72 (d, J = 16.8 Hz, 1H), 3.19 (d, J = 9.6 Hz, 1H), 3.53 (d, J = 9.6 Hz, 1H), 4.22 (d, J = 16.8 Hz, 1H), 4.29 (d, J = 16.8 Hz, 1H), 7.37 (d, J = 7.9 Hz, 2H), 7.76 (d, J = 7.9 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 19.8, 21.1, 21.7, 21.8, 24.9, 30.2, 34.8, 45.5, 49.7, 53.4, 53.5, 127.3, 129.0, 133.6, 141.0, 144.2, 166.9, 208.4, 209.7. IR (neat): ν 2969, 1724, 1676, 1464, 1348, 1166 cm^{-1}. HRMS (ESI) calcd for $C_{22}H_{28}NO_4S$ (M+H): 402.1734. Found: 402.1739.

3n: White solid: TLC R_f (33% EA/PE) = 0.55, m.p. 176-178 ºC. ^{1}H NMR (600 MHz, C_6D_6): δ 0.92 (dt, J = 5.0 and 13.8 Hz, 1H), 1.05 (d, J = 7.1 Hz, 3H), 1.11 (d, J = 7.1 Hz, 3H), 1.33-1.35 (m, 4H), 1.85 (s, 3H), 1.93 (ddd, J = 2.2, 5.0 and 17.5 Hz, 1H), 2.00 (ddd, J = 1.9, 14.3 and 17.7 Hz, 1H), 2.34 (d, J = 9.8 Hz, 1H), 2.39 (heptet, J = 7.1 Hz, 1H), 3.67 (d, J = 9.8 Hz, 1H), 3.87 (d, J = 16.5 Hz, 1H), 4.16 (d, J = 16.5 Hz, 1H), 4.48 (s, 1H), 4.64 (s, 1H), 6.78 (d, J = 8.2 Hz, 2H), 7.69 (d, J = 8.2 Hz, 2H). ^{13}C NMR (150 MHz, C_6D_6): δ 18.8, 20.4, 20.5, 28.9, 34.3, 49.9, 52.4, 57.7, 116.0, 130.0, 134.8, 138.7, 141.7, 142.8, 155.9, 195.8. IR (neat): ν 2965, 1676, 1464, 1352, 1166 cm^{-1}. HRMS (ESI) calcd for $C_{21}H_{28}NO_3S$ (M+H): 374.1784. Found: 374.1786.

Products (2o & 3o)



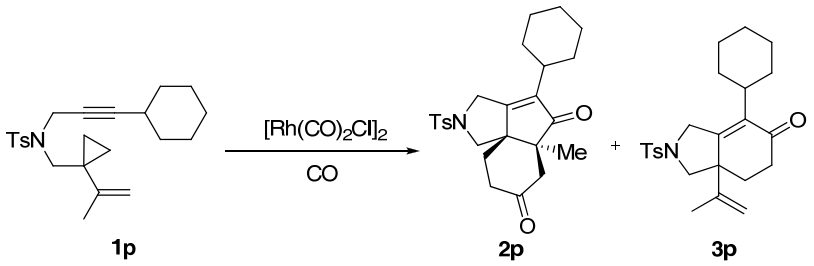
1o **2o** **3o**

Following the general procedure, 1-yne-VCP **1o** (40.5 mg, 0.1 mmol) was converted to products **2o** (15.0 mg, 32%) and **3o** (25.9 mg, 59%). Substrate concentration: 0.05 M, CO pressure: 1 atm CO, temperature: 80 ºC, reaction time: 1.5 h.

2o: Colorless oil: TLC R_f (33% EA/PE) = 0.20. ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.92 (s, 3H), 1.17 (s, 9H), 1.73-1.85 (m, 3H), 2.13-2.19 (m, 1H), 2.28 (d, J = 17.3 Hz, 1H), 2.46 (s, 3H), 2.72 (d, J = 17.3 Hz, 1H), 3.18 (d, J = 9.8 Hz, 1H), 3.51 (d, J = 9.8 Hz, 1H), 4.32 (d, J = 16.7 Hz, 1H), 4.38 (d, J = 16.7 Hz, 1H), 7.38 (d, J = 7.9 Hz, 2H), 7.75 (d, J = 7.9 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.5, 28.4, 30.8, 33.0, 34.7, 45.3, 46.9, 49.9, 53.0, 53.7, 127.3, 130.0, 133.7, 142.4, 144.2, 166.0, 208.5, 209.8. IR (neat): ν 2957, 1721, 1657, 1464, 1352, 1166, 1106 cm^{-1}. HRMS (ESI) calcd for $C_{23}H_{30}NO_4S$ (M+H): 416.1890. Found: 416.1900.

3o: White solid: TLC R_f (33% EA/PE) = 0.60, m.p. 142-144 ºC. ^{1}H NMR (600 MHz, C_6D_6): δ 0.92 (dt, J = 6.0 and 13.2 Hz, 1H), 1.19 (s, 9H), 1.38 (dd, J = 5.0 and 13.1 Hz, 1H), 1.40 (s, 3H), 1.89 (s, 3H), 1.91 (dd, J = 6.0 and 18.1 Hz, 1H), 2.08 (ddd, J = 5.5, 13.2 and 18.1 Hz, 1H), 2.28 (d, J = 9.3 Hz, 1H), 3.64 (d, J = 9.3 Hz, 1H), 4.16 (d, J = 16.5 Hz, 1H), 4.40 (d, J = 16.5 Hz, 1H), 4.61 (s, 1H), 4.76 (s, 1H), 6.83 (d, J = 8.3 Hz, 2H), 7.75 (d, J = 8.3 Hz, 2H). ^{13}C NMR (150 MHz, C_6D_6): δ 19.0, 21.2, 27.7, 30.4, 35.2, 36.8, 51.4, 53.8, 56.7, 116.6, 134.1, 141.9, 143.2, 143.6, 153.5, 197.4. IR (neat): ν 2957, 1676, 1356, 1170 cm^{-1}. HRMS (ESI) calcd for $C_{22}H_{30}NO_3S$ (M+H): 388.1941. Found: 388.1946.

Products (2p & 3p)



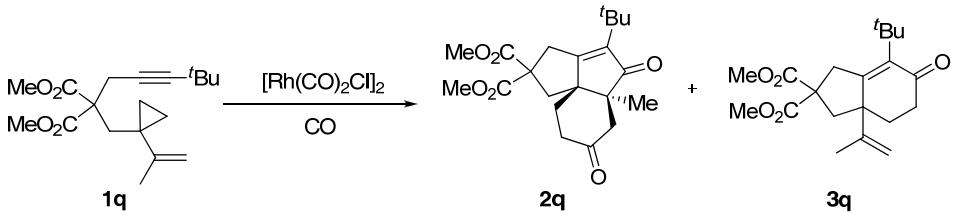
Following the general procedure, 1-yne-VCP **1p** (45.6 mg, 0.13 mmol) was converted to products **2p** (20.4 mg, 39%) and **3p** (27.9 mg, 57%). Substrate concentration: 0.05 M, CO pressure: 1 atm CO, temperature: 80 ºC, reaction time: 1.5 h.

2p: Colorless oil: TLC R_f (33% EA/PE) = 0.20. ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.93 (s, 3H), 1.16-1.30 (m, 6H), 1.64-1.80 (m, 8H), 2.12-2.18 (m, 1H), 2.31 (d, J = 17.2 Hz, 1H), 2.45 (s, 3H), 2.72 (d, J = 17.3 Hz, 1H), 3.20 (d, J = 9.9 Hz, 1H), 3.52 (d, J = 9.9 Hz, 1H), 4.26 (s, 2H), 7.37 (d, J = 8.0 Hz, 2H), 7.76 (d, J = 8.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.5, 21.8, 25.7, 26.1, 29.9, 31.5, 34.7, 45.5, 45.9, 49.5, 53.4, 53.8, 127.3, 129.9, 133.7, 140.0, 144.1, 167.1, 208.4, 209.8. IR (neat): ν 2935, 2857, 1724, 1672, 1460, 1352, 1166, 1095 cm^{-1}. HRMS (ESI) calcd for $C_{25}H_{32}NO_4S$ (M+H): 442.2047. Found: 442.2050.

3p: Colorless oil: TLC R_f (33% EA/PE) = 0.59. ^{1}H NMR (600 MHz, C_6D_6): δ 0.82-0.90 (m, 1H), 1.01 (dt, J = 5.0 and 13.1 Hz, 1H), 1.11-1.21 (m, 4H), 1.35-1.38 (m, 4H), 1.39 (s, 3H), 1.58 (d, J = 9.8 Hz, 1H), 1.64-1.68 (m, 2H), 1.88 (s, 3H), 1.95 (dq, J = 2.5 and 13.0 Hz, 1H), 2.01 (ddd, J = 1.6, 4.5 and 17.6 Hz, 1H), 2.07 (ddd, J = 4.9, 14.3 and 17.6 Hz, 1H), 3.74 (d, J = 9.9 Hz, 1H), 4.08 (d, J = 16.5 Hz, 1H), 4.33 (d, J = 16.4 Hz, 1H), 4.57 (s, 1H), 4.71 (s, 1H), 6.81 (d, J = 7.7 Hz, 2H), 7.74 (d, J = 7.7 Hz, 2H). ^{13}C NMR (150 MHz, C_6D_6): δ 18.8, 21.1, 26.2, 27.3, 28.9, 30.3, 34.3, 40.0, 50.0, 52.5, 57.7, 116.1, 130.0, 134.9, 138.2, 142.8, 143.5, 156.2, 195.9. IR (neat): ν 2931,

1672, 1453, 1348, 1166, 1095 cm^{-1}. HRMS (ESI) calcd for $C_{24}H_{32}NO_3S$ (M+H): 414.2097. Found: 414.2104.

Products (2q & 3q)

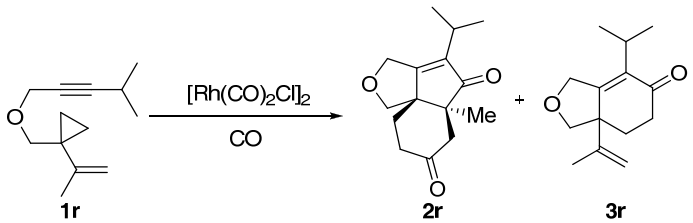


Following the general procedure, 1-yne-VCP **1q** (40.7 mg, 0.127 mmol) was converted to products **2q** (26.2 mg, 55%) and **3q** (7.9 mg, 18%). Substrate concentration: 0.05 M, CO pressure: 1 atm CO, temperature: 80 ºC, reaction time: 1.5 h.

2q: Colorless oil: TLC R_f (20% EA/PE) = 0.13. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.00 (s, 3H), 1.25 (s, 9H), 1.78 (s, 2H), 1.82 (q, J = 7.9 Hz, 1H), 2.12-2.17 (m, 1H), 2.28 (d, J = 17.2 Hz, 1H), 2.40 (d, J = 14.0 Hz, 1H), 2.56 (d, J = 14.0 Hz, 1H), 2.74 (d, J = 17.2 Hz, 1H), 3.50 (d, J = 18.7 Hz, 1H), 3.59 (d, J = 18.7 Hz, 1H), 3.77 (s, 3H), 3.82 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 22.7, 29.7, 32.3, 33.1, 34.8, 38.8, 45.4, 51.0, 53.3, 55.0, 59.6, 141.8, 172.0, 172.3, 209.6, 211.5. IR (neat): ν 2961, 1728, 1646, 1441, 1274 cm^{-1}. HRMS (ESI) calcd for $C_{21}H_{29}O_6$ (M+H): 377.1959. Found: 377.1963.

3q: Colorless oil: TLC R_f (20% EA/PE) = 0.40. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.22-1.27 (m, 1H), 1.30 (s, 9H), 1.71 (dd, J = 7.9 and 14.3 Hz, 1H), 1.73 (s, 3H), 2.02 (d, J = 13.3 Hz, 1H), 2.13-2.26 (m, 3H), 2.85 (dd, J = 2.0 and 13.3 Hz, 1H), 3.47 (d, J = 19.2 Hz, 1H), 3.66 (s, 3H), 3.74 (s, 3H), 4.48 (s, 1H), 4.83 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 19.1, 30.4, 30.7, 35.4, 36.3, 40.1, 42.8, 52.6, 53.2, 54.9, 59.0, 116.8, 141.9, 144.1, 158.3, 172.4, 199.7. IR (neat): ν 2957, 1743, 1680, 1438, 1259, 1211 cm^{-1}. HRMS (ESI) calcd for $C_{20}H_{29}O_5$ (M+H): 349.2010. Found: 349.2012.

Products (2r & 3r)



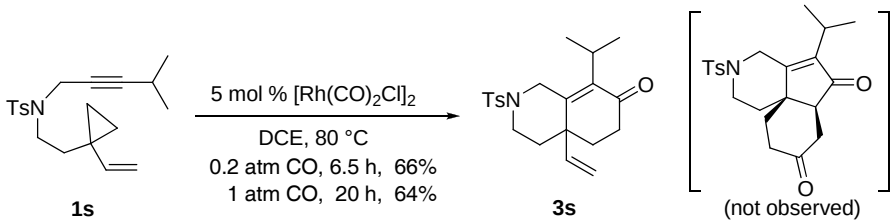
Following the general procedure, 1-yne-VCP **1r** (35.6 mg, 0.19 mmol) was converted to

products **2r** (26.0 mg, 57%) and **3r** (10.0 mg, 27%). Substrate concentration: 0.05 M, CO pressure: 1 atm CO, temperature: 80 ºC, reaction time: 1.5 h.

2r: Colorless oil: TLC R_f (20% EA/PE) = 0.08. ^{1}H NMR (400 MHz, C_6D_6): δ 0.57 (s, 3H), 0.87 (d, J = 7.0 Hz, 6H), 1.34 (dd, J = 3.5 and 13.7 Hz, 1H), 1.47-1.64 (m, 2H), 1.89 (d, J = 16.8 Hz, 1H), 1.92 (dt, J = 17.7 and 3.5 Hz, 1H), 2.59 (heptet, J = 7.0 Hz, 1H), 2.78 (d, J = 16.8 Hz, 1H), 3.29 (d, J = 8.4 Hz, 1H), 3.38 (d, J = 8.4 Hz, 1H), 4.14 (d, J = 15.8 Hz, 1H), 4.20 (d, J = 15.8 Hz, 1H). ^{13}C NMR (100 MHz, C_6D_6): δ 19.6, 20.8, 21.1, 25.1, 29.6, 34.9, 45.5, 49.4, 54.6, 63.9, 72.4, 139.1, 171.8, 206.7, 210.3. IR (neat): ν 2972, 1724, 1669, 1468, 1266, 1032 cm^{-1}. HRMS (ESI) calcd for $C_{15}H_{21}O_3$ (M+H): 249.1485. Found: 249.1485.

3r: Colorless oil: TLC R_f (20% EA/PE) = 0.50. ^{1}H NMR (400 MHz, C_6D_6): δ 1.23-1.31 (m, 1H), 1.26 (d, J = 7.1 Hz, 3H), 1.29 (d, J = 7.1 Hz, 3H), 1.51 (s, 3H), 1.56 (ddd, J = 2.2, 4.9 and 12.8 Hz, 1H), 2.18-2.34 (m, 2H), 2.65 (heptet, J = 7.1 Hz, 1H), 3.07 (d, J = 8.4 Hz, 1H), 3.98 (d, J = 8.4 Hz, 1H), 4.36 (d, J = 16.4 Hz, 1H), 4.50 (d, J = 16.4 Hz, 1H), 4.75 (s, 1H), 4.94 (s, 1H). ^{13}C NMR (100 MHz, C_6D_6): δ 18.8, 20.3, 27.7, 28.6, 34.1, 52.8, 68.4, 76.7, 115.2, 136.5, 143.6, 160.3, 196.1. IR (neat): ν 2931, 2287, 1676, 1062 cm^{-1}. HRMS (ESI) calcd for $C_{14}H_{21}O_2$ (M+H): 221.1536. Found: 221.1536.

2.3 Attempts to Forge Angular Tricyclic 6/5/6 Compounds



1s **3s**

By following the general procedure, we carried out the reaction of **1s** in DCE under the CO pressures of 0.2 atm, 1 atm, and 2 atm, respectively, to see whether the 6/5/6 compound can be generated. These results are:

0.2 atm CO pressure: 1-yne-VCP **1s** (32.4 mg, 0.094 mmol) was converted to products **3s** (23.1 mg, 66%). Substrate concentration: 0.05 M, 0.2 atm CO pressure, temperature: 80 ºC, reaction time: 6.5 h. In this case, no formal [5+1]/[2+2+1] product was found.

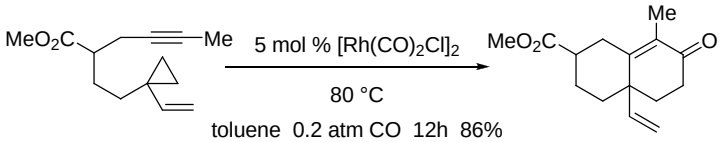
1 atm CO pressure: 1-yne-VCP **1s** (59.0 mg, 0.17 mmol) was converted to products **3s** (42.4 mg, 64%). Substrate concentration: 0.05 M, 1 atm CO pressure, temperature: 80 ºC, reaction time: 20 h. In this case, no formal [5+1]/[2+2+1] product was found.

2 atm CO pressure: in this case, no reaction was observed at 80 ºC within 4 hours.

3s: Colorless oil: TLC R_f (20% EA/PE) = 0.38. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.21 (d, J = 6.9 Hz, 6H), 1.69 (ddd, J = 3.1, 5.4 and 13.4 Hz, 1H), 1.75-1.85 (m, 3H), 2.27 (ddd, J = 2.5, 3.9 and 16.7 Hz, 1H), 2.39 (ddd, J = 5.4, 14.3 and 17.2 Hz, 1H), 2.44 (s, 3H), 2.64 (ddd, J = 4.9, 10.3 and 12.4 Hz, 1H), 3.07 (d, J = 14.3 Hz, 1H), 3.16 (heptet, J = 7.4 Hz, 1H), 3.68 (ddd, J = 3.4, 4.9 and 11.8 Hz, 1H), 4.76 (d, J = 17.2 Hz, 2H), 5.20 (d, J = 10.3 Hz, 1H), 5.44 (dd, J = 10.4 and 17.7 Hz, 1H), 7.34 (d, J = 8.4 Hz, 2H), 7.76 (d, J = 8.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.0, 21.2, 26.7, 34.2, 38.4, 42.3, 44.4, 118.2, 127.5, 129.8, 133.5, 140.0, 143.1, 143.7, 148.5, 198.4. IR (neat): ν 2942, 1680, 1352, 1166 cm^{-1}. HRMS (ESI) calcd for $C_{21}H_{28}NO_3S$ (M+H): 374.1784. Found: 374.1780.

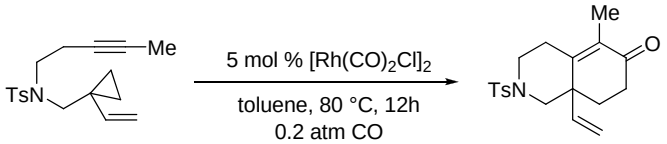
We have also tested the substrate in the reaction **a** (shown below) to see whether changing CO pressure could give the 6/5/6 product. In this case, only [(3+2)+1] product was obtained. [1a] In our previous report, the reactions **b** and **c** (shown below) also only gave [(3+2)+1] cycloadducts. [1a] All these results suggest that formation of the 6/5/6 compounds via the formal [5+1]/[2+2+1] reaction is disfavored with respect to the formation of the [(3+2)+1] cycloadducts.

a.

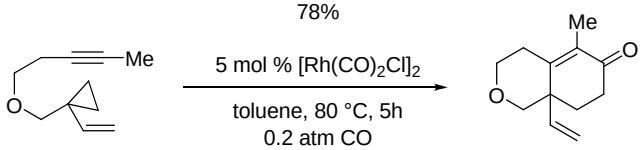


toluene	0.2 atm CO	12h	86%
DCE	0.2 atm CO	12h	53%
dioxane	0.2 atm CO	9h	76%
toluene	1 atm CO	6h	78%

b.

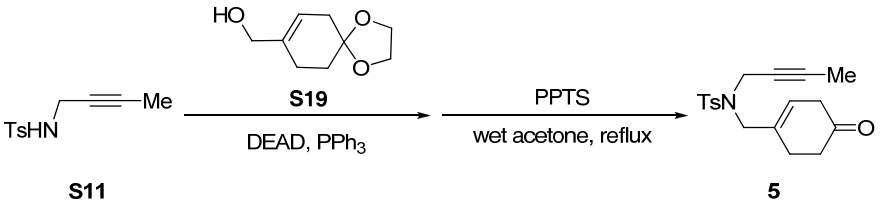


c.



2.4 Control Experiment to Study the Reaction Mechanism

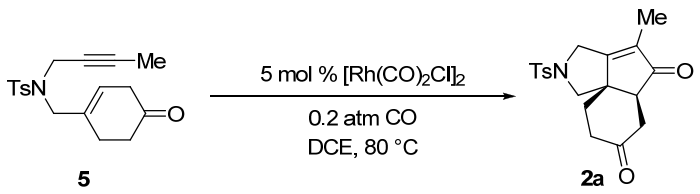
Synthesis of Substrate 5



S11 to **5**: To a stirred solution of alcohol **S19**[6] (102 mg, 0.6 mmol), tosylamide **S11** (174 mg, 0.8 mmol), and PPh_3 (314 mg, 1.2 mmol) in anhydrous THF (6 mL) was added DEAD (209 mg, 1.2 mmol) at 0 ºC. The mixture was then stirred for 24 h at 25 ºC. The reaction mixture was concentrated and the crude product was purified by a thin pad of silica gel to afford crude ketone. Then to the crude ketone with wet acetone (4 mL) was added PPTS (12 mg, 0.05 mmol). After the mixture was refluxed for 40 h, saturated aqueous NaCl was added to the reaction solution. The resulting mixture was extracted with CH_2Cl_2, and the combined organic phase was dried over $MgSO_4$ and concentrated. Then the crude product was purified by flash column chromatography on silica gel (eluted with PE/EA 10:1 to 5:1) to afford product **5** (92 mg, two steps 48%).

5: Colorless oil: TLC R_f (50% EA/PE) = 0.50. ^{1}H NMR (C_6D_6, 400 MHz): δ 1.15-1.16 (m, 3H), 1.90 (s, 3H), 2.01-2.07 (m, 4H), 2.40 (s, 2H), 3.61 (s, 2H), 3.88 (d, J = 2.0 Hz, 2H), 5.23 (s, 1H), 6.80 (d, J = 7.9 Hz, 2H), 7.78 (d, J = 7.9 Hz, 2H). ^{13}C NMR (C_6D_6, 100 MHz): δ 2.9, 21.1, 26.2, 36.4, 38.1, 39.3, 52.0, 72.4, 81.4, 123.9, 129.3, 133.3, 137.4, 142.9, 206.9. IR (neat): v 2928, 1724, 1352, 1166 cm^{-1}. HRMS (ESI) calcd for $C_{18}H_{21}NNaO_3S$ (M+Na): 354.1134. Found: 354.1139.

Experimental Data for the Control Experiment



A solution of substrate **5** (44.6 mg, 0.14 mmol) and $[Rh(CO)_2Cl]_2$ (2.7 mg, 0.007 mmol) in anhydrous DCE (2.7 mL) was degassed by bubbling 0.2 atm CO (balloon pressured mixed gas of CO and N_2, 1:4 V/V) for 5 min. Then the reaction mixture was immersed in an 80 ºC oil bath and stirred under the above atmosphere. One hour later, TLC indicated no appearance of compound **2a,** and that **5** was not consumed at all. We then stopped this reaction and the crude mixture was submitted to flash column chromatography on silica gel (eluted with PE/AE 2:1 to 1:2), getting the recovered starting material **5** (42.9 mg) in 96%. Substrate concentration: 0.05 M, reaction time: 1 h.

However, if we repeated this reaction and extended the reaction time to 24 h using the same

[6] Jung, M. E.; Rayle, H. L. *Synth. Commun.* **1994**, *24*, 197.

reaction conditions above, **5** (40.0mg, 0.12 mmol) was converted to **2a** (1.7mg, 3%) and 87% of the starting material **5** (34.8 mg) was recovered. These results clearly indicated that formation of **2a** from **1a** does not proceed via a cascade [5+1]/[2+2+1] mechanism, but via a formal [5+1]/[2+2+1] pathway.

3. DFT Study

3.1 Proposed Reaction Pathways

We proposed two pathways for this formal [5+1]/[2+2+1] cycloaddition (Figure S1). In pathway I, 1-yne-VCP and the Rh(I) catalyst undergo complexation, and cyclopropane cleavage, and alkyne complexation to generate intermediate **A**, which is then transformed to intermediate **B** via alkyne insertion into the C1-Rh bond. CO coordination and insertion into the C5-Rh bond give rhodacyclohexene intermediate **C**. If a direct elimination occurs on this intermediate, the [(3+2)+1] cycloadduct could be generated. Alternatively, if insertion of the Cα=Cβ double bond into the Rh–C(=O) bond takes place, a tricyclic rhodacyclohexane intermediate **D** is formed. Then another CO molecule participates in this reaction and the final angular tricyclic 5/5/6 product could be achieved through CO coordination, insertion into the C3-Rh bond, and reductive elimination (via intermediates **E** and **F**). There is another possible pathway (pathway II), starting from the same intermediates **A** and **B**. In the presence of CO, intermediate **B** undergoes CO complexation and insertion into the C3–Rh bond, producing rhodacycloheptanone intermediate **G**. At this stage, reductive elimination of this intermediate creates the C5–C(=O) bond between the carbonyl carbon and the C5 atom to furnish the [(3+2)+1] cycloadduct. Alternatively, insertion of the Cα=Cβ double bond into the Rh–C(=O) bond generates a tricyclic intermediate **H**. Coordination of another CO and insertion of this CO into the C5-Rh bond give intermediate **I**, which produces the final tricyclic product after reductive elimination. Both pathways above could explain how this formal [5+1]/[2+2+1] cycloaddition occurs. Our preliminary calculations indicate that pathway I is much more reasonable to explain the present formal [5+1]/[2+2+1] cycloaddition (see below). Even though several possible pathways could be proposed to explain how 5/5/5 compound forms (compound **4a** in Table 1), further investigation is required to reach a final conclusion about this.

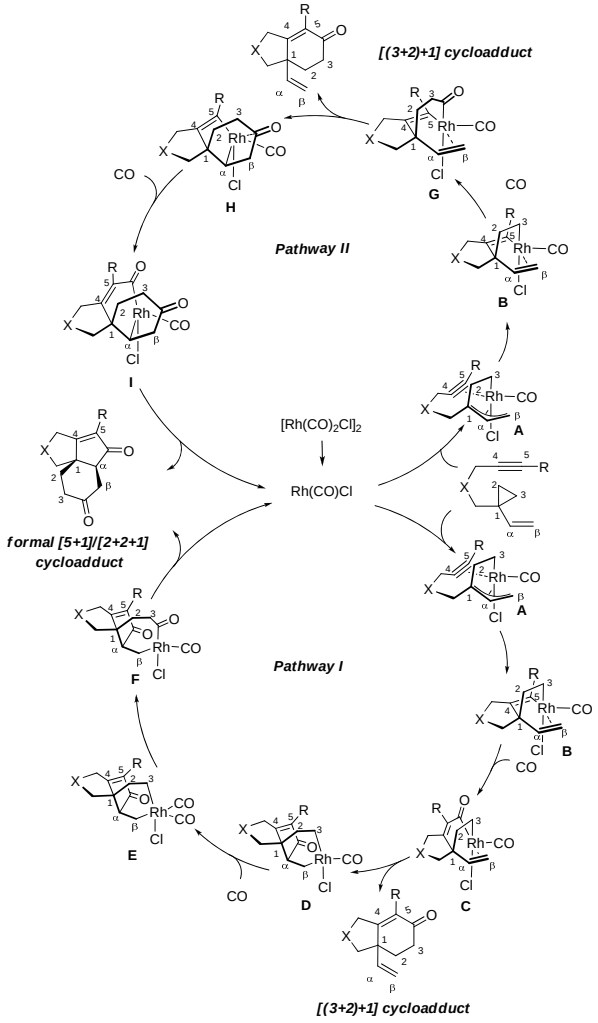


Figure S1. Proposed two possible pathways.

3.2 Computational Details and the DFT Computed Energy Surfaces

All calculations were performed with the Gaussian 03 program.[7] Density functional theory calculations using the B3LYP functional[8] were used to locate all the stationary points in the gas

[7] Full citation of Gaussian 03: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A. Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03*, Revision C.02; Gaussian Inc.: Wallingford CT, 2004.

[8] Other related computational references: (a) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648. (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785. (c) Hehre, W. J.; Radom, L.; Schleyer, P. v. R.; Pople, J. A. *Ab Initio Molecular Orbital Theory*; Wiley: New York, 1986.

phase. For the integration grid in the DFT calculations, the parameter Integral=FineGrid was applied. The default convergance criteria (RMS density matrix = 1.00×10^{-8}) for geometry optimization was used. The 6-31G(d) basis set was applied for all elements except Rh, which used the basis set of LANL2DZ.[9] The keyword "5D" in Gaussian 03 program was used to specify that five (instead of six) d-type STO orbitals were used as basis sets in all elements of the calculations. This method has been successfully applied to study structures and reaction mechanisms for reactions of carbonyl rhodium(I) complexes and other Rh-catalyzed cycloadditions.[10, 11] Frequency calculations at the same level had been performed to confirm each stationary point to be either a minimum or a transition structure.

Solvation energies in 1,2-dichloroethane were evaluated by a self-consistent reaction field (SCRF) using the CPCM approach, where simple united atom topological model (UA0) was used to define the atomic radii. Solvation calculations were carried out on the gas-phase obtained structures. The reported energies are zero-point energy-corrected enthalpies ($\Delta H_{\text{gas 298K}}$), Gibbs free energies ($\Delta G_{\text{gas 298K}}$), both in the gas phase, and Gibbs free energies in 1,2-dichloroethane solution ($\Delta G_{\text{sol 298K}}$). Unless specifically mentioned, all discussed relative energies in the paper are referred to the $\Delta H_{\text{gas 298K}}$.

We calculated the potential energy surfaces of this formal [5+1]/[2+2+1] cycloaddition employing 1-yne-VCP **1a** as the model substrate. The energy surfaces are shown in Figure S2. The Rh(I)-catalyzed formal [5+1]/[2+2+1] reaction of 1-yne-VCP and two units of CO starts with the ligand exchange between the product-Rh(I) complex **IN7**, which is generated in the previous catalytic cycle, and the substrate, 1-yne-VCP **1a**. The ligand exchange step is endothermic by 2.8 kcal/mol, giving a 14-e Rh(I) complex **IN1-1**. After coordination with a CO molecule, **IN1-1** is transformed to **IN1-2**, which then isomerizes to **IN1-3** through exchanging the positions of CO and the chlorine atom. The 16e complex **IN1-3** releases one molecule of CO to give a 14e complex **IN1-4**. The CP ring-opening reaction from **IN1-4** to **IN2-1** goes through the transition state **TS1**. Then **IN2-1** undergoes a geometric change by exchanging the positions of CO and Cl. This is followed by the coordination of the alkyne moiety to the Rh atom, generating a more stable 16e complex **IN2-3**. Insertion of alkyne into the C–Rh bond takes place, giving the rhodacyclohexane intermediate **IN3-1** via transition state **TS2**. After that, a CO molecule coordinates to the Rh center, converting the 16e complex **IN3-1** into an 18e complex **IN3-2**, which is much more stable than the former. It is found that the rate-determining step of the whole reaction is the CP ring-opening step, requiring an activation enthalpy of 30.4 kcal/mol (from **IN1-2** to **TS1**). The followed steps after the CP cleavage are much easier (see below).

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[9] (a) Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 299. (b) Dunning, T. H., Jr.; Hay, P. J. In *Modern Theoretical Chemistry*; Schaefer, H. F., III. Ed.; Plenum Press: New York, 1977; pp 1-28.

[10] (a) Yu, Z.-X.; Wender, P. A.; Houk, K. N. *J. Am. Chem. Soc.* **2004**, *126*, 9154. (b) Yu, Z.-X.; Cheong, P. H.-Y.; Liu, P.; Legault, C. Y.; Wender, P. A.; Houk, K. N. *J. Am. Chem. Soc.* **2008**, *130*, 2378. (c) Liu, P.; Cheong, P. H.-Y.; Yu, Z.-X.; Wender, P. A.; Houk, K. N. *Angew. Chem. Int. Ed.* **2008**, *47*, 3939. (d) Liu, P.; Sirois, L. E.; Cheong, P. H.-Y.; Yu, Z.-X.; Hartung, I. V.; Rieck, H.; Wender, P. A.; Houk, K. N. *J. Am. Chem. Soc.* **2010**, *132*, 10127.

[11] (a) Nakamura, E.; Yoshikai, N.; Yamanaka, M. *J. Am. Chem. Soc.* **2002**, *124*, 7181. (b) Baik, M.-H.; Baum, E. W.; Burland, M. C.; Evans, P. A. *J. Am. Chem. Soc.* **2005**, *127*, 1602. (c) Montero-Campillo, M. M.; Rodriguez-Otero, J.; Cabaleiro-Lago, E. M. *Tetrahedron* **2008**, *64*, 6215. (d) Wang, H.; Sawyer, J. R.; Evans, P. A.; Baik, M.-H. *Angew. Chem. Int. Ed.* **2008**, *47*, 342. (e) Montero-Campillo, M. M.; Cabaleiro-Lago, E. M.; Rodriguez-Otero, J. *J. Phys. Chem. A* **2008**, *112*, 9068. (f) Liang, Y.; Zhou, H.; Yu, Z.-X. *J. Am. Chem. Soc.* **2009**, *131*, 17783. (g) Hansen, J.; Autschbach, J.; Davies, H. M. L. *J. Org. Chem.* **2009**, *74*, 6555.

For the first CO insertion, calculations show that CO prefers to insert into the Rh–C(sp^2) bond (via **TS3**), rather than the Rh–C(sp^3) bond (via **TS3-a**). The pathway via **TS3** requires an activation enthalpy of only 12.1 kcal/mol, which is 10.3 kcal/mol lower than that of pathway via **TS3-a** (the red line). This suggests that pathway II is not favored compared to pathway I (see Figure S1).

The CO-insertion step in the favored pathway II transforms **IN3-2** into **IN4**, which could afford the [(3+2)+1] cycloadduct through a direct reductive elimination (the blue line, via **TS4-[(3+2)+1]**). Alternatively, **IN4** can give the formal [5+1]/[2+2+1] product-Rh complex **IN7**, through alkene insertion (via **TS4**), CO coordination and insertion (via **TS5**), and reductive elimination (via **TS6**). The potential energy profile indicates that the product distribution is determined by the relative energy of **TS4** and **TS4-[(3+2)+1]**. In Figure S2, **TS4** and **TS4-[(3+2)+1]** are close in energy, suggesting that both formal [5+1]/[2+2+1] and [(3+2)+1] products can be generated in equal amounts. This is very close to the experimental observations, showing that both 5/5/6 products and [(3+2)+1] cycloadducts are generated together with different ratios, depending on the substituents in the alkyne moieties.

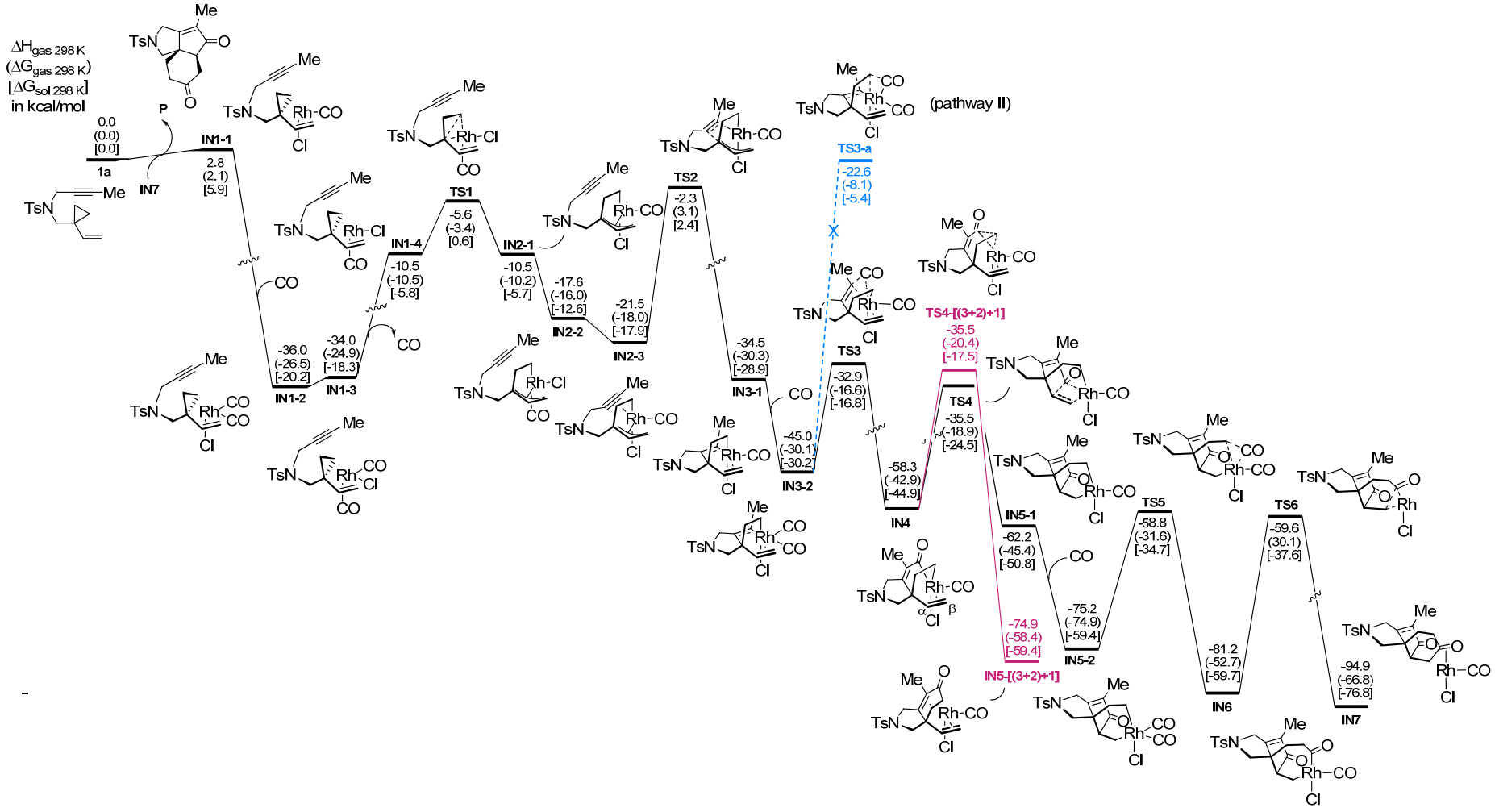


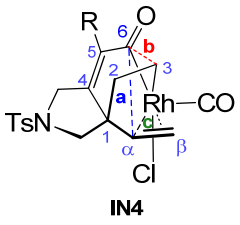
Figure S2. The DFT Computed Energy surfaces.

To explain how the steric bulkiness of the alkyne substitution R affects the product distribution of the 5/5/6 products and [(3+2)+1] cycloadducts, we computed the activation enthalpies of the reductive elimination step of the [(3+2)+1] pathway and alkene insertion step of the formal [5+1]/[2+2+1] pathway with different R groups (Table S1 and Figure 2). A cursory examination of the species involved in these two pathways suggests that steric effects are responsible for the above trend. No matter whether R is small or big, the activation enthalpies to the [(3+2)+1] pathway are almost the same (around 23.0 kcal/mol). However, when R becomes bigger, the activation enthalpies are reduced (from 24.6, to 22.8, to 21.8 kcal/mol), making the formal [5+1]/[2+2+1] pathway gradually favored with respect to the [(3+2)+1] pathway. The reason for the reduction of alkene insertion barrier with bigger R groups in **TS4** is due to the favored conformation changes in **IN4**. When R is bigger, the *a* bond between alkene and the C6 (carbonyl carbon bonded to the Rh atom) is shorter, the same as the *c* bond between Cα and Rh atom, suggesting that the alkene coordination to the Rh is stronger. Consequently, in this case, the alkene insertion into the Rh–C6(=O) bond is becoming easier. In contrast, when R is becoming bigger, the distance between C3 and C6 is longer (see the *b* bond in Table S1), indicating that the reductive elimination to form the C3-C6 bond is becoming much more difficult. The results mean that bigger R group in the 1-yne-VCPs favors the alkene coordination to the Rh atom and the alkene insertion into the Rh–C6(=O) bond, making the formal [5+1]/[2+2+1] reaction favored. These calculations results are in consistent with the experimental results.

Further studies of all the competitive pathways of the cycloadditions of 1-yne-VCPs and CO are ongoing and will be reported in due course.

Table S1. DFT Study on Reactivity

R	**IN4**	**TS4** (kcal/mol)	**TS4-[(3+2+)+1]**	bond length in **IN4**		
				a (Å)	**b** (Å)	**c** (Å)
H	0.0	24.6	23.2	2.96	2.87	2.38
Me	0.0	22.8	22.8	2.91	2.86	2.36
^{i}Pr	0.0	21.8	23.1	2.63	3.02	2.35



IN4

3.3 Computed Energies of All Stationary Points

Table S2. Sum of electronic and zero-point energies (*E*, in Hartree), sum of electronic and thermal enthalpies (*H*, in Hartree), sum of electronic and thermal free energies (*G*, in Hartree), thermal correction to Gibbs free energy (TCGFE, in Hartree), total free energy in solution (E_{sol}, in hartree), and thermo corrected Gibbs free energy in dichloroethane solution (G_{sol}, which equals to E_{sol} + TCGFE, in Hartree). Relative energies (ΔH, ΔG, and ΔG_{sol}) are reported in kcal/mol.

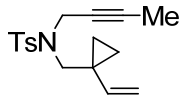
Structure	*E*	*H*	*G*	TCGFE	E_{sol}	G_{sol}	ΔH	ΔG	ΔG_{sol}
Potential energy surface									
S	-1263.286083	-1263.262377	-1263.342830	0.289202	-1263.626000	-1263.336798	0.0	0.0	0.0
CO	-113.301878	-113.298573	-113.321016	-0.014102	-113.304047	-113.318149			
IN1-1	-1946.376379	-1946.346849	-1946.441600	0.291064	-1946.731150	-1946.440086	2.8	2.1	5.9
IN1-2	-2059.739093	-2059.707278	-2059.808144	0.296930	-2060.096759	-2059.799829	-36.0	-26.5	-20.2
IN1-3	-2059.736075	-2059.704121	-2059.805696	0.296098	-2060.092894	-2059.796796	-34.0	-24.9	-18.3
IN1-4	-1946.397108	-1946.368101	-1946.461643	0.293062	-1946.751816	-1946.458754	-10.5	-10.5	-5.8
TS1	-1946.388676	-1946.360219	-1946.450376	0.294334	-1946.742870	-1946.448536	-5.6	-3.4	0.6
IN2-1	-1946.397113	-1946.368140	-1946.461171	0.293589	-1946.752185	-1946.458596	-10.5	-10.2	-5.7
IN2-2	-1946.408208	-1946.379424	-1946.470391	0.295521	-1946.765100	-1946.469579	-17.6	-16.0	-12.6
IN2-3	-1946.413749	-1946.385666	-1946.473544	0.298933	-1946.776946	-1946.478013	-21.5	-18.0	-17.9
TS2	-1946.382190	-1946.355046	-1946.439984	0.299867	-1946.745432	-1946.445565	-2.3	3.1	2.4
IN3-1	-1946.433539	-1946.406412	-1946.493276	0.300487	-1946.796010	-1946.495523	-34.5	-30.3	-28.9
IN3-2	-2059.751291	-2059.721608	-2059.813946	0.305816	-2060.121586	-2059.815770	-45.0	-30.1	-30.2
TS3	-2059.731308	-2059.702445	-2059.792405	0.307126	-2060.101448	-2059.794322	-32.9	-16.6	-16.8
TS3-a	-2059.715621	-2059.685959	-2059.778878	0.303735	-2060.079900	-2059.776165	-22.6	-8.1	-5.4
IN4	-2059.771815	-2059.742853	-2059.834381	0.307607	-2060.146836	-2059.839229	-58.3	-42.9	-44.9
TS4	-2059.734711	-2059.706511	-2059.796056	0.307855	-2060.114558	-2059.806703	-35.5	-18.9	-24.5
TS4-[(3+2)+1]	-2059.735670	-2059.706558	-2059.798404	0.305666	-2060.101226	-2059.795560	-35.5	-20.4	-17.5
IN5-1	-2059.777133	-2059.749090	-2059.838315	0.310555	-2060.159167	-2059.848612	-62.2	-45.4	-50.8
IN5-2	-2173.098998	-2173.068340	-2173.163085	0.315607	-2173.484020	-2173.168413	-75.2	-47.8	-51.9
IN5-[(3+2)+1]	-2059.797760	-2059.769246	-2059.858968	0.310912	-2060.173168	-2059.862256	-74.9	-58.4	-59.4
TS5	-2173.072854	-2173.042275	-2173.137393	0.313884	-2173.454939	-2173.141055	-58.8	-31.6	-34.7
IN6	-2173.107781	-2173.077929	-2173.170876	0.319255	-2173.500102	-2173.180847	-81.2	-52.7	-59.7
TS6	-2173.072977	-2173.043529	-2173.134982	0.318697	-2173.464364	-2173.145667	-59.6	-30.1	-37.6
IN7	-2173.129436	-2173.099684	-2173.193483	0.319673	-2173.527896	-2173.208223	-94.9	-66.8	-76.8
P	-1490.034874	-1490.010698	-1490.091383	0.315704	-1490.411266	-1490.095562			
Comparision of potential energy surface with different R groups									
IN4-H	-2020.482215	-2020.45501	-2020.542418	0.282108	-2020.83368	-2020.551572	0.0	0.0	0.0
TS4-H	-2020.442042	-2020.41574	-2020.500723	0.282758	-2020.798665	-2020.515907	24.6	26.2	22.4
TS4-H-[(3+2)+1]	-2020.445463	-2020.41811	-2020.506406	0.279528	-2020.788859	-2020.509331	23.2	22.6	26.5
IN4	-2059.771815	-2059.742853	-2059.834381	0.307607	-2060.146836	-2059.839229	0.0	0.0	0.0
TS4	-2059.734711	-2059.706511	-2059.796056	0.307855	-2060.114558	-2059.806703	22.8	24.0	20.4
TS4-[(3+2)+1]	-2059.735670	-2059.706558	-2059.798404	0.305666	-2060.101226	-2059.795560	22.8	22.6	27.4
IN4-^{i}Pr	-2138.336373	-2138.304948	-2138.400310	0.363952	-2138.764918	-2138.400966	0.0	0.0	0.0
TS4-^{i}Pr	-2138.300850	-2138.270166	-2138.364379	0.363290	-2138.734184	-2138.370894	21.8	22.5	18.9
TS4-^{i}Pr-[(3+2)+1]	-2138.299753	-2138.268088	-2138.364971	0.360731	-2138.719742	-2138.359011	23.1	22.2	26.3

3.4 Coordinates of All Stationary Points

CO

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	-0.650137
2	8	0	0.000000	0.000000	0.487603

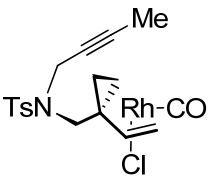
1a: 

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.885660	-3.912517	0.033361
2	6	0	2.577335	-3.224358	-0.459080
3	6	0	3.449369	-3.717591	-1.340692
4	1	0	3.494352	-4.781364	-1.558412
5	1	0	4.154416	-3.082467	-1.871106
6	6	0	3.596897	-0.845639	-0.162044
7	6	0	3.134349	-1.325684	1.192462
8	6	0	0.989969	-1.303739	-0.315477
9	1	0	3.408327	0.193613	-0.412151
10	1	0	4.533522	-1.236314	-0.549340
11	1	0	3.749003	-2.053107	1.715678
12	1	0	2.607025	-0.623810	1.831254
13	1	0	0.717053	-1.507064	-1.360322
14	1	0	0.316891	-1.898793	0.308573
15	6	0	0.868287	1.076734	-1.162058
16	1	0	-0.120734	1.481602	-1.419879
17	1	0	1.187871	0.487163	-2.028432
18	7	0	0.754366	0.122034	-0.033128
19	16	0	-0.352920	0.521884	1.179119
20	8	0	-0.128093	-0.430233	2.269310
21	8	0	-0.245931	1.968962	1.363831
22	6	0	-1.989545	0.195782	0.509639

23	6	0	-2.677127	1.216636	-0.153009
24	6	0	-2.560357	-1.073107	0.646876
25	6	0	-3.931040	0.950542	-0.701915
26	1	0	-2.247886	2.211706	-0.201696
27	6	0	-3.814484	-1.320086	0.092599
28	1	0	-2.042550	-1.841298	1.211160
29	6	0	-4.515115	-0.319556	-0.597769
30	1	0	-4.469974	1.747494	-1.208490
31	1	0	-4.263440	-2.303547	0.209109
32	6	0	-5.861066	-0.607761	-1.219167
33	1	0	-6.424007	-1.342372	-0.633810
34	1	0	-6.467728	0.299778	-1.301559
35	1	0	-5.746965	-1.017544	-2.231698
36	6	0	2.423780	-1.791056	-0.062146
37	6	0	1.814137	2.173022	-0.944172
38	6	0	2.594512	3.086391	-0.809753
39	6	0	3.526071	4.193083	-0.610089
40	1	0	4.442362	4.061119	-1.198239
41	1	0	3.074981	5.148827	-0.903278
42	1	0	3.814326	4.273002	0.444918

IN1-1:

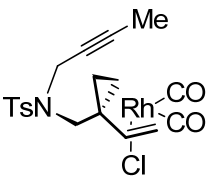


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.763561	-1.089209	-1.638116
2	6	0	-1.514281	-0.310702	-1.566569
3	6	0	-2.730259	-0.478641	-2.193645
4	1	0	-2.937884	-1.401439	-2.722953
5	1	0	-3.423956	0.340055	-2.370635
6	6	0	-2.379826	1.740211	-0.102222
7	6	0	-1.535006	2.266715	-1.226783
8	6	0	0.109821	0.772790	0.098111
9	1	0	-2.175979	2.115998	0.894150
10	1	0	-3.433048	1.562613	-0.324168

11	1	0	-2.003148	2.356034	-2.202989
12	1	0	-0.832007	3.058365	-0.985501
13	1	0	-0.103071	1.202233	1.078531
14	1	0	0.330189	-0.287840	0.265852
15	6	0	1.980147	2.403995	0.533386
16	1	0	2.808733	2.860621	-0.014851
17	1	0	2.409859	1.837339	1.376087
18	6	0	1.094013	3.448581	1.047462
19	6	0	0.380204	4.312214	1.504389
20	1	0	5.898390	-4.103907	1.251830
21	6	0	5.302306	-3.439080	1.890627
22	6	0	4.556994	-2.421580	1.060562
23	1	0	4.613577	-4.071071	2.461373
24	1	0	5.988406	-2.958129	2.594677
25	6	0	3.359979	-2.764609	0.414298
26	6	0	5.058867	-1.123390	0.888747
27	6	0	2.676369	-1.843609	-0.376602
28	1	0	2.959461	-3.769114	0.524990
29	6	0	4.389461	-0.187542	0.102094
30	1	0	5.992225	-0.842919	1.370286
31	6	0	3.192284	-0.551448	-0.521590
32	1	0	1.769554	-2.129524	-0.898208
33	1	0	4.802041	0.804228	-0.050175
34	16	0	2.296668	0.662852	-1.491832
35	8	0	1.390189	-0.064493	-2.384008
36	8	0	3.264529	1.642429	-1.987622
37	7	0	1.285929	1.500486	-0.416167
38	6	0	-1.138585	0.896124	-0.789934
39	45	0	-2.921953	-0.708230	0.076436
40	17	0	-3.617501	-2.939382	-0.136314
41	6	0	-3.097214	-0.857725	1.959622
42	8	0	-3.156379	-0.970839	3.102848
43	6	0	-0.465902	5.372275	2.048122
44	1	0	-0.642260	5.232080	3.121119
45	1	0	-0.001351	6.355712	1.909860
46	1	0	-1.441903	5.394406	1.548811

IN1-2:

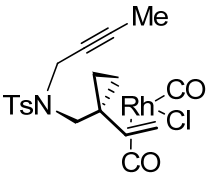


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.619722	-0.963813	1.979395
2	6	0	1.922339	0.051300	1.723092
3	6	0	3.249226	0.355625	1.905201
4	6	0	0.810610	0.970804	1.381921
5	1	0	3.902090	-0.363841	2.390070
6	1	0	3.621754	1.371986	1.815102
7	6	0	1.055102	2.449243	1.177526
8	6	0	0.442286	1.987857	2.465859
9	6	0	-0.323993	0.242556	0.642749
10	1	0	0.411181	2.964415	0.471727
11	1	0	2.079798	2.809895	1.192010
12	1	0	1.055254	1.995281	3.362641
13	1	0	-0.618790	2.148245	2.627884
14	1	0	0.095886	-0.273425	-0.230601
15	1	0	-0.715481	-0.534652	1.305968
16	6	0	-1.432452	1.564411	-1.211487
17	1	0	-2.303767	1.156193	-1.740089
18	1	0	-0.552880	1.117940	-1.689421
19	6	0	-1.393680	3.019477	-1.371948
20	6	0	-1.354814	4.214865	-1.549284
21	1	0	-5.937257	-4.244751	-1.938255
22	6	0	-5.076460	-4.391891	-1.278527
23	6	0	-4.579695	-3.081911	-0.715402
24	1	0	-5.370865	-5.084196	-0.482576
25	1	0	-4.292598	-4.888127	-1.865905
26	6	0	-3.815306	-3.052451	0.461120
27	6	0	-4.863502	-1.867438	-1.355375
28	6	0	-3.328359	-1.853611	0.976593
29	1	0	-3.607060	-3.980607	0.987554
30	6	0	-4.385631	-0.657016	-0.854639
31	1	0	-5.477962	-1.866336	-2.252195
32	6	0	-3.605625	-0.658357	0.305270
33	1	0	-2.769318	-1.836997	1.905967
34	1	0	-4.642601	0.282132	-1.332980
35	16	0	-2.943852	0.890745	0.926306
36	8	0	-2.680026	0.713729	2.356961
37	8	0	-3.786049	1.968166	0.408167
38	7	0	-1.429300	1.099022	0.197284
39	45	0	3.287865	-0.651682	-0.189995

40	6	0	3.680875	-1.587924	-1.807823
41	8	0	3.922851	-2.178250	-2.757467
42	17	0	3.323755	-2.798544	0.854981
43	6	0	3.302719	1.035033	-1.015109
44	8	0	3.334591	2.066951	-1.524318
45	6	0	-1.334022	5.662263	-1.742736
46	1	0	-0.325184	6.024119	-1.974860
47	1	0	-1.993827	5.959168	-2.566847
48	1	0	-1.677753	6.181481	-0.840148

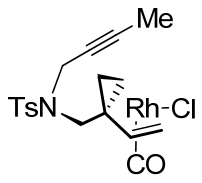
IN1-3:



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.004214	-0.212256	-2.412904
2	6	0	-2.158129	0.631398	-1.737419
3	6	0	-3.449608	1.009909	-1.472621
4	6	0	-0.913812	1.353856	-1.369725
5	1	0	-4.279086	0.569899	-2.019841
6	1	0	-3.664222	1.901372	-0.892578
7	6	0	-0.956071	2.809317	-0.984021
8	6	0	-0.501375	2.439343	-2.368063
9	6	0	0.181681	0.414277	-0.842013
10	1	0	-0.206342	3.167677	-0.287440
11	1	0	-1.926340	3.280181	-0.867025
12	1	0	-1.167296	2.638390	-3.203657
13	1	0	0.558673	2.488268	-2.600331
14	1	0	-0.233797	-0.200687	-0.033315
15	1	0	0.474505	-0.260405	-1.651005
16	6	0	1.380702	1.471351	1.091775
17	1	0	2.015205	0.769690	1.653294
18	1	0	0.355480	1.310410	1.444206
19	6	0	1.775120	2.851775	1.372741
20	6	0	2.073429	3.989407	1.651719
21	1	0	4.383213	-4.840601	2.176875

22	6	0	4.227070	-4.852750	1.093462
23	6	0	3.879911	-3.479629	0.569126
24	1	0	5.151743	-5.226056	0.633652
25	1	0	3.438025	-5.578616	0.870314
26	6	0	3.159831	-3.329236	-0.625625
27	6	0	4.300677	-2.324580	1.242919
28	6	0	2.859555	-2.067272	-1.133888
29	1	0	2.838011	-4.213409	-1.170671
30	6	0	4.011282	-1.053220	0.748831
31	1	0	4.870872	-2.420448	2.163650
32	6	0	3.279675	-0.930888	-0.436295
33	1	0	2.331627	-1.959509	-2.075340
34	1	0	4.369912	-0.164310	1.256865
35	16	0	2.859576	0.704552	-1.051184
36	8	0	2.605458	0.582574	-2.490381
37	8	0	3.842965	1.638116	-0.506197
38	7	0	1.373406	1.117069	-0.353587
39	45	0	-3.160721	-0.596171	0.201797
40	6	0	-3.253230	-1.698376	1.754090
41	8	0	-3.308221	-2.331207	2.705467
42	6	0	-3.570942	-2.004851	-0.969858
43	8	0	-3.821810	-2.865608	-1.692114
44	17	0	-2.667761	1.160949	1.740912
45	6	0	2.455750	5.362139	1.970432
46	1	0	1.963966	5.709613	2.887294
47	1	0	3.539204	5.450079	2.115583
48	1	0	2.171985	6.047144	1.162444

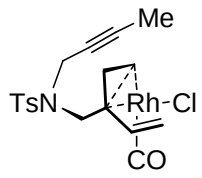


IN1-4:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.863182	-0.787882	-1.846965
2	6	0	-1.636901	-0.096689	-1.533812
3	6	0	-2.925950	-0.191806	-2.076387
4	1	0	-3.134001	-0.977584	-2.795635

5	1	0	-3.610127	0.653046	-2.122076
6	6	0	-2.348510	1.766411	0.167458
7	6	0	-1.622280	2.447948	-0.951326
8	6	0	0.119635	0.831074	0.097141
9	1	0	-2.100919	2.013141	1.193857
10	1	0	-3.407435	1.550045	0.009572
11	1	0	-2.165338	2.627205	-1.874640
12	1	0	-0.905336	3.218546	-0.685227
13	1	0	0.019547	1.264220	1.094262
14	1	0	0.288784	-0.241503	0.244688
15	6	0	2.080469	2.398220	0.348125
16	1	0	2.872199	2.818984	-0.277423
17	1	0	2.563926	1.840361	1.167489
18	6	0	1.270694	3.476557	0.913387
19	6	0	0.632790	4.367059	1.427362
20	1	0	5.105743	-4.429819	1.699758
21	6	0	5.210896	-3.394862	2.042132
22	6	0	4.493843	-2.434632	1.123794
23	1	0	4.797916	-3.346303	3.058304
24	1	0	6.278589	-3.164294	2.110016
25	6	0	3.261685	-2.780055	0.548533
26	6	0	5.036027	-1.175012	0.831195
27	6	0	2.577502	-1.893431	-0.279965
28	1	0	2.835217	-3.760587	0.744377
29	6	0	4.366609	-0.273883	0.004811
30	1	0	6.001644	-0.899041	1.247142
31	6	0	3.131069	-0.635350	-0.540287
32	1	0	1.642460	-2.182646	-0.746972
33	1	0	4.809634	0.684784	-0.243132
34	16	0	2.240319	0.536595	-1.566072
35	8	0	1.288811	-0.226364	-2.379259
36	8	0	3.220585	1.444373	-2.163726
37	7	0	1.293690	1.484297	-0.521277
38	6	0	-1.195980	1.035541	-0.670260
39	45	0	-2.909738	-0.787976	0.030855
40	17	0	-3.338298	-0.956190	2.346512
41	6	0	-3.260400	-2.545366	-0.291566
42	8	0	-3.466781	-3.659070	-0.507816
43	6	0	-0.124906	5.454233	2.043151
44	1	0	-0.887341	5.070533	2.731344
45	1	0	0.538100	6.113273	2.616211
46	1	0	-0.630411	6.066821	1.287465



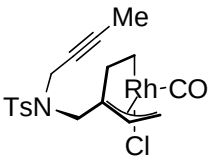
TS1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.572604	-2.145943	0.836692
2	6	0	1.217456	-1.409624	1.307425
3	6	0	2.393230	-1.812799	1.978651
4	1	0	2.605963	-2.874441	2.054222
5	1	0	2.848826	-1.203546	2.754418
6	6	0	2.608443	1.080191	1.167008
7	6	0	1.385383	1.046208	2.050331
8	6	0	-0.127149	0.350241	0.056349
9	1	0	2.605366	1.836921	0.389954
10	1	0	3.573008	0.934467	1.661838
11	1	0	1.555351	0.708379	3.073125
12	1	0	0.768250	1.943790	2.044638
13	1	0	0.409914	0.815917	-0.772701
14	1	0	-0.590362	-0.562901	-0.342556
15	6	0	-1.482899	2.429512	-0.444045
16	1	0	-2.073871	3.149196	0.129240
17	1	0	-2.120151	2.047904	-1.258721
18	6	0	-0.293427	3.060521	-1.008339
19	6	0	0.710979	3.515658	-1.507135
20	1	0	-6.151620	-3.332389	-2.062405
21	6	0	-6.106564	-2.263594	-2.293544
22	6	0	-5.203671	-1.527083	-1.333435
23	1	0	-5.743296	-2.165871	-3.325144
24	1	0	-7.126387	-1.865407	-2.269976
25	6	0	-4.184006	-2.198520	-0.644252
26	6	0	-5.360190	-0.149396	-1.116210
27	6	0	-3.328978	-1.519543	0.222819
28	1	0	-4.063210	-3.270353	-0.779396
29	6	0	-4.516844	0.546471	-0.253251
30	1	0	-6.161402	0.384115	-1.621510
31	6	0	-3.494450	-0.143940	0.406164
32	1	0	-2.565302	-2.050768	0.780494
33	1	0	-4.666153	1.604490	-0.065412
34	16	0	-2.369806	0.751147	1.479003

35	8	0	-1.726097	-0.228286	2.361743
36	8	0	-3.077379	1.925583	1.990251
37	7	0	-1.120441	1.335381	0.499217
38	6	0	0.871914	-0.023601	1.146178
39	45	0	2.869970	-0.831758	0.091037
40	17	0	3.815886	0.459526	-1.709761
41	6	0	3.279413	-2.451227	-0.881201
42	8	0	3.487964	-3.405569	-1.484284
43	6	0	1.932787	4.042203	-2.109850
44	1	0	2.697024	3.256361	-2.160474
45	1	0	1.745052	4.397642	-3.129922
46	1	0	2.337195	4.879701	-1.529331

IN2-1:

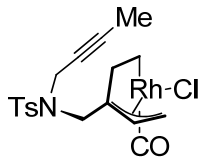


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.867841	-0.768107	-1.852803
2	6	0	-1.641301	-0.080849	-1.530411
3	6	0	-2.931918	-0.171741	-2.069892
4	1	0	-3.141442	-0.950388	-2.796432
5	1	0	-3.617187	0.672717	-2.104795
6	6	0	-2.346996	1.765096	0.192081
7	6	0	-1.627069	2.458018	-0.924084
8	6	0	0.121081	0.833013	0.101911
9	1	0	-2.094999	2.002076	1.219729
10	1	0	-3.406395	1.548751	0.037174
11	1	0	-2.175138	2.644584	-1.842982
12	1	0	-0.908947	3.226879	-0.655898
13	1	0	0.027295	1.262138	1.101384
14	1	0	0.288419	-0.240535	0.243764
15	6	0	2.081476	2.402059	0.345026
16	1	0	2.870543	2.823388	-0.283489
17	1	0	2.568385	1.846127	1.163686
18	6	0	1.270977	3.479290	0.911125
19	6	0	0.630404	4.368054	1.424734

20	1	0	5.112855	-4.427170	1.694779
21	6	0	5.216385	-3.392380	2.038189
22	6	0	4.497270	-2.432476	1.121124
23	1	0	4.803748	-3.345624	3.054578
24	1	0	6.283711	-3.160073	2.105800
25	6	0	3.263530	-2.777981	0.549258
26	6	0	5.039083	-1.173251	0.826226
27	6	0	2.577572	-1.891862	-0.278277
28	1	0	2.837250	-3.758222	0.746964
29	6	0	4.367869	-0.272569	0.000786
30	1	0	6.005811	-0.897244	1.239551
31	6	0	3.130923	-0.634158	-0.540979
32	1	0	1.641291	-2.181169	-0.742746
33	1	0	4.810570	0.685753	-0.249065
34	16	0	2.238285	0.536902	-1.566066
35	8	0	1.285637	-0.226982	-2.377045
36	8	0	3.217361	1.444345	-2.166182
37	7	0	1.293355	1.485663	-0.520629
38	6	0	-1.198168	1.043483	-0.657548
39	45	0	-2.908750	-0.790120	0.030848
40	17	0	-3.331519	-0.983609	2.345378
41	6	0	-3.257911	-2.544156	-0.309965
42	8	0	-3.463502	-3.655672	-0.537886
43	6	0	-0.135993	5.451420	2.036068
44	1	0	-0.196406	5.331933	3.124192
45	1	0	0.323285	6.425190	1.828972
46	1	0	-1.160555	5.478083	1.646222

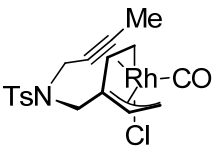
IN2-2:



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.764901	-0.421151	0.606385
2	6	0	-1.605769	2.448403	0.110963
3	6	0	-0.303686	0.307985	-0.178011

4	6	0	1.533532	0.372814	1.672439
5	6	0	3.028549	0.211754	1.417642
6	45	0	2.923771	-0.929007	-0.300630
7	1	0	1.237642	1.421878	1.599443
8	1	0	1.236426	0.011630	2.665354
9	1	0	3.588732	-0.308432	2.195782
10	1	0	3.535062	1.124853	1.105492
11	1	0	-2.196804	2.941457	0.887003
12	1	0	-2.258399	2.303419	-0.766128
13	1	0	-0.878782	-0.393898	-0.799561
14	1	0	0.203875	1.004094	-0.856245
15	6	0	0.955035	-1.786746	0.452347
16	6	0	2.116561	-2.458841	0.974637
17	1	0	2.431140	-2.261682	1.997701
18	1	0	2.264152	-3.493795	0.672389
19	1	0	0.337887	-2.302923	-0.282756
20	6	0	-0.454117	3.264683	-0.260921
21	6	0	0.521336	3.888417	-0.610720
22	1	0	-6.465798	-2.857796	-2.448016
23	6	0	-6.447398	-1.764143	-2.410243
24	6	0	-5.448635	-1.261992	-1.395146
25	1	0	-7.459829	-1.413345	-2.183654
26	1	0	-6.197238	-1.404877	-3.417269
27	6	0	-4.375156	-2.063661	-0.982850
28	6	0	-5.568506	0.024838	-0.847984
29	6	0	-3.434816	-1.596424	-0.065302
30	1	0	-4.278704	-3.072145	-1.377209
31	6	0	-4.639694	0.508859	0.070238
32	1	0	-6.407722	0.652826	-1.136837
33	6	0	-3.568124	-0.305171	0.451523
34	1	0	-2.625300	-2.232645	0.275992
35	1	0	-4.757380	1.492459	0.512569
36	16	0	-2.339952	0.325428	1.598750
37	8	0	-1.646014	-0.828887	2.177195
38	8	0	-2.986657	1.340910	2.432049
39	7	0	-1.177130	1.138300	0.672506
40	17	0	2.900664	0.923500	-1.878204
41	6	0	4.767507	-1.333403	-0.336858
42	8	0	5.890031	-1.578952	-0.321655
43	6	0	1.713655	4.608530	-1.046716
44	1	0	2.476589	3.894060	-1.379228
45	1	0	1.486398	5.276460	-1.886148
46	1	0	2.136248	5.216216	-0.237675



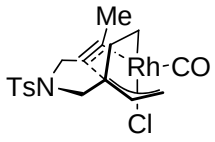
IN2-3:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.866724	-0.330275	-1.677818
2	6	0	-0.422937	-0.139793	1.138580
3	6	0	-0.607475	-0.264078	-1.348467
4	6	0	1.535092	-1.707598	-1.771237
5	6	0	2.818677	-1.642462	-0.932428
6	45	0	2.595013	0.309160	-0.186724
7	1	0	0.841521	-2.456055	-1.377983
8	1	0	1.719852	-1.959181	-2.825132
9	1	0	3.737903	-1.769217	-1.508356
10	1	0	2.812561	-2.339340	-0.092085
11	1	0	-1.028099	-0.448075	1.995171
12	1	0	-0.530695	0.945135	0.999938
13	1	0	-1.153638	-0.840166	-2.102672
14	1	0	-0.956963	0.778133	-1.380388
15	6	0	1.517268	0.833739	-2.080814
16	6	0	2.942596	0.901542	-2.223099
17	1	0	3.486599	0.102956	-2.720206
18	1	0	3.373522	1.891666	-2.341291
19	1	0	0.974992	1.772460	-1.998836
20	6	0	0.982323	-0.430873	1.469117
21	6	0	2.050389	-0.675362	2.019821
22	1	0	-6.682016	3.165108	0.934184
23	6	0	-6.802699	2.452082	0.112005
24	6	0	-5.699309	1.421335	0.108153
25	1	0	-7.783834	1.974892	0.236195
26	1	0	-6.829618	3.014716	-0.826563
27	6	0	-5.235499	0.868166	-1.094196
28	6	0	-5.136805	0.968840	1.310830
29	6	0	-4.237149	-0.104144	-1.104869
30	1	0	-5.666827	1.198078	-2.035974
31	6	0	-4.137411	-0.001736	1.320890
32	1	0	-5.489872	1.378112	2.254064
33	6	0	-3.686161	-0.528561	0.107380
34	1	0	-3.904617	-0.547005	-2.037662
35	1	0	-3.726618	-0.365570	2.256568

36	16	0	-2.358800	-1.735409	0.106155
37	8	0	-2.473368	-2.523285	-1.123250
38	8	0	-2.319225	-2.353377	1.432876
39	7	0	-0.904692	-0.873915	-0.044910
40	17	0	1.934407	2.639940	0.568227
41	6	0	4.373130	0.546141	0.418560
42	8	0	5.462224	0.714405	0.741528
43	6	0	3.142863	-1.085945	2.907548
44	1	0	3.738255	-0.223126	3.224853
45	1	0	2.731018	-1.568502	3.801460
46	1	0	3.810962	-1.800290	2.414332

TS2:

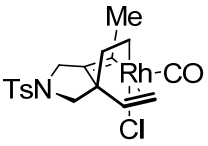


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.811715	-0.744658	-1.108732
2	6	0	-0.624183	-0.646909	1.243613
3	6	0	-0.709107	-0.843997	-1.124619
4	6	0	1.615694	-2.051223	-1.164460
5	6	0	3.018855	-1.758405	-0.603072
6	45	0	2.783980	0.291926	-0.158171
7	1	0	1.091400	-2.812356	-0.580002
8	1	0	1.641450	-2.407606	-2.204384
9	1	0	3.826885	-1.918988	-1.320754
10	1	0	3.233904	-2.324558	0.304523
11	1	0	-0.790141	-1.183749	2.181683
12	1	0	-1.096696	0.348322	1.313384
13	1	0	-1.005261	-1.501127	-1.948294
14	1	0	-1.147151	0.152778	-1.294893
15	6	0	1.311733	0.369535	-1.932356
16	6	0	2.486253	0.384225	-2.643017
17	1	0	3.054058	-0.509452	-2.870859
18	1	0	2.781300	1.297102	-3.150345
19	1	0	0.740330	1.293448	-1.880529
20	6	0	0.834157	-0.497232	1.004693

21	6	0	1.943721	-0.296616	1.615674
22	1	0	-5.078309	2.033380	2.061735
23	6	0	-4.819113	1.484548	1.159917
24	6	0	-5.226397	1.976947	-0.089144
25	6	0	-4.096249	0.298479	1.267933
26	6	0	-5.980562	3.280414	-0.195583
27	6	0	-4.903953	1.236115	-1.235565
28	6	0	-3.773604	-0.411677	0.107144
29	1	0	-3.809543	-0.091653	2.238792
30	1	0	-6.592697	3.317237	-1.102189
31	1	0	-5.286577	4.130496	-0.233236
32	1	0	-6.636838	3.435266	0.667085
33	6	0	-4.181036	0.047660	-1.148628
34	1	0	-5.230716	1.589988	-2.210083
35	16	0	-2.795952	-1.908897	0.228863
36	1	0	-3.960078	-0.535419	-2.036454
37	8	0	-3.036356	-2.706235	-0.974058
38	8	0	-2.957154	-2.446347	1.579933
39	7	0	-1.169661	-1.429470	0.131595
40	17	0	2.226273	2.713480	0.244572
41	6	0	4.547785	0.586682	0.317599
42	8	0	5.641946	0.776388	0.618490
43	6	0	2.540400	-0.281013	2.974306
44	1	0	3.414433	-0.939826	3.025688
45	1	0	2.870004	0.733989	3.221341
46	1	0	1.813222	-0.612150	3.725624

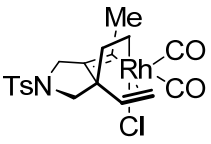
IN3-1:



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.466522	-0.673299	0.311651
2	6	0	-0.538388	0.984912	-1.261959
3	6	0	-1.032140	-0.976677	0.039915
4	6	0	0.798794	-0.238448	1.760315
5	6	0	2.232547	0.321448	1.845635

6	45	0	3.364338	-0.289704	0.147362
7	1	0	0.063462	0.505127	2.080901
8	1	0	0.678539	-1.099854	2.430292
9	1	0	2.801666	-0.096719	2.684225
10	1	0	2.233288	1.408238	1.938391
11	1	0	-0.699975	2.062769	-1.196945
12	1	0	-0.586347	0.700864	-2.322584
13	1	0	-1.568838	-1.271373	0.943566
14	1	0	-1.139390	-1.779819	-0.700125
15	6	0	1.401139	-1.777793	-0.140843
16	6	0	2.290758	-2.462266	0.623113
17	1	0	2.322061	-2.379740	1.705117
18	1	0	2.947817	-3.194710	0.166261
19	1	0	1.364186	-2.010325	-1.204983
20	6	0	0.751264	0.508296	-0.614901
21	6	0	2.002677	0.941290	-0.754639
22	1	0	-8.727679	-0.817133	-1.180198
23	6	0	-8.050506	-1.495364	-0.648455
24	6	0	-6.719526	-0.837466	-0.372309
25	1	0	-8.542790	-1.808666	0.277087
26	1	0	-7.927201	-2.386175	-1.277839
27	6	0	-6.135917	-0.890646	0.898633
28	6	0	-6.033081	-0.161743	-1.396343
29	6	0	-4.898646	-0.294777	1.152048
30	1	0	-6.656083	-1.399965	1.705829
31	6	0	-4.800041	0.436629	-1.163255
32	1	0	-6.476014	-0.101667	-2.387553
33	6	0	-4.236943	0.359018	0.114592
34	1	0	-4.452865	-0.324429	2.140248
35	1	0	-4.281022	0.963804	-1.957126
36	16	0	-2.670029	1.163822	0.437942
37	8	0	-2.375069	0.969126	1.866639
38	8	0	-2.691138	2.510918	-0.142270
39	7	0	-1.604084	0.261329	-0.530686
40	17	0	4.905079	-1.547143	-1.272218
41	6	0	4.596347	1.086639	0.367668
42	8	0	5.374225	1.912323	0.538939
43	6	0	2.490039	2.097480	-1.573181
44	1	0	2.936509	2.880356	-0.947253
45	1	0	3.247855	1.783592	-2.300113
46	1	0	1.656788	2.551169	-2.125642



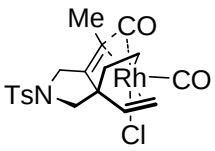
IN3-2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.265306	-0.642272	-0.063213
2	6	0	0.880610	1.457999	0.643454
3	6	0	1.224747	-0.906001	0.277845
4	6	0	-0.625088	-0.821671	-1.556791
5	6	0	-2.033996	-0.284650	-1.871592
6	1	0	0.128210	-0.309331	-2.164573
7	1	0	-0.553116	-1.885613	-1.819148
8	1	0	-2.583271	-0.931819	-2.559525
9	1	0	-1.990151	0.718774	-2.294493
10	1	0	1.059469	2.373250	0.075390
11	1	0	1.002888	1.697522	1.709144
12	1	0	1.707560	-1.579413	-0.432488
13	1	0	1.325919	-1.334315	1.283460
14	6	0	-1.236996	-1.416014	0.812052
15	6	0	-2.097698	-2.393180	0.421359
16	1	0	-2.091476	-2.812682	-0.579423
17	1	0	-2.734775	-2.873510	1.157501
18	1	0	-1.226100	-1.149244	1.866930
19	6	0	-0.461107	0.804040	0.359537
20	6	0	-1.707304	1.261546	0.500481
21	1	0	9.119637	-0.448107	0.961136
22	6	0	8.313373	-1.113162	1.297180
23	6	0	6.980135	-0.669151	0.743900
24	1	0	8.565141	-2.127056	0.971581
25	1	0	8.317618	-1.096362	2.392839
26	6	0	6.381869	-1.342208	-0.327758
27	6	0	6.321146	0.449036	1.283008
28	6	0	5.160815	-0.919136	-0.856744
29	1	0	6.877493	-2.207816	-0.760162
30	6	0	5.104217	0.884227	0.769924
31	1	0	6.771714	0.985815	2.114388
32	6	0	4.528072	0.189582	-0.298148
33	1	0	4.704682	-1.433349	-1.695657
34	1	0	4.606820	1.754311	1.186091
35	16	0	2.972929	0.760737	-0.980479

36	8	0	2.688288	-0.077766	-2.156408
37	8	0	3.020672	2.222208	-1.096396
38	7	0	1.874891	0.422015	0.264886
39	17	0	-4.192218	-0.123696	2.261521
40	6	0	-4.141851	1.285668	-0.706092
41	8	0	-4.751682	2.158829	-1.126262
42	45	0	-3.167340	-0.163190	-0.037256
43	6	0	-4.669693	-1.523984	-0.469691
44	8	0	-5.557724	-2.223073	-0.617597
45	6	0	-2.081152	2.607837	1.047016
46	1	0	-1.200752	3.136095	1.435596
47	1	0	-2.543850	3.254186	0.288963
48	1	0	-2.801958	2.496518	1.865497

TS3:

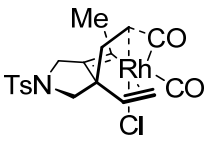


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.323091	-0.661470	0.058445
2	6	0	0.746474	1.460521	0.778822
3	6	0	1.176193	-0.857308	0.455059
4	6	0	-0.622604	-1.113140	-1.395265
5	6	0	-2.088256	-0.904377	-1.796711
6	1	0	0.056869	-0.579141	-2.065087
7	1	0	-0.361417	-2.176168	-1.472584
8	1	0	-2.557570	-1.819938	-2.159068
9	1	0	-2.198765	-0.143481	-2.570118
10	1	0	0.973614	2.430649	0.334391
11	1	0	0.723436	1.586678	1.871362
12	1	0	1.694862	-1.533825	-0.226220
13	1	0	1.257321	-1.266552	1.469508
14	6	0	-1.255950	-1.361743	1.051594
15	6	0	-2.010528	-2.468309	0.841093
16	1	0	-1.980666	-3.039234	-0.081166
17	1	0	-2.615474	-2.869012	1.648506
18	1	0	-1.286663	-0.916540	2.044651

19	6	0	-0.546491	0.835124	0.269907
20	6	0	-1.735970	1.464498	0.215851
21	1	0	9.002654	-0.528486	0.880664
22	6	0	8.214478	-1.268910	1.067664
23	6	0	6.872344	-0.761797	0.596702
24	1	0	8.497686	-2.192446	0.553867
25	1	0	8.209581	-1.467959	2.145656
26	6	0	6.232757	-1.328026	-0.511922
27	6	0	6.242870	0.306572	1.259434
28	6	0	4.998575	-0.850075	-0.957585
29	1	0	6.705419	-2.152391	-1.039546
30	6	0	5.014194	0.795591	0.831171
31	1	0	6.726033	0.760896	2.121074
32	6	0	4.396396	0.205544	-0.276288
33	1	0	4.508346	-1.281216	-1.823546
34	1	0	4.537902	1.624284	1.344801
35	16	0	2.832971	0.852932	-0.859378
36	8	0	2.463606	0.083807	-2.058780
37	8	0	2.900230	2.317187	-0.903732
38	7	0	1.799013	0.479857	0.446618
39	17	0	-4.202355	0.214772	2.179269
40	6	0	-3.279732	1.321406	-0.909114
41	8	0	-3.578802	2.194960	-1.616938
42	45	0	-3.178779	-0.301128	-0.025737
43	6	0	-4.713972	-1.369592	-0.481584
44	8	0	-5.674889	-1.932520	-0.746761
45	6	0	-1.988435	2.827633	0.809880
46	1	0	-2.196841	3.581520	0.042622
47	1	0	-2.856229	2.772065	1.478087
48	1	0	-1.132307	3.163669	1.403248

TS3-a:



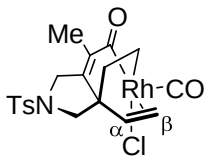
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.402101	0.876244	-0.321074

2	6	0	0.888396	-1.201635	-0.840245
3	6	0	1.108452	1.160302	-0.608018
4	6	0	-0.779719	1.217300	1.156922
5	6	0	-1.720178	0.253158	1.918480
6	1	0	0.139323	1.213831	1.755632
7	1	0	-1.176609	2.234680	1.213431
8	1	0	-2.093136	0.746311	2.819000
9	1	0	-1.157465	-0.642580	2.188665
10	1	0	1.095163	-2.115119	-0.281014
11	1	0	1.061475	-1.405757	-1.906712
12	1	0	1.525734	1.935651	0.035033
13	1	0	1.242908	1.468521	-1.652146
14	6	0	-1.259630	1.617744	-1.342339
15	6	0	-2.021271	2.709219	-1.181061
16	1	0	-2.138353	3.228402	-0.234058
17	1	0	-2.561954	3.128375	-2.024777
18	1	0	-1.197324	1.190575	-2.343015
19	6	0	-0.504403	-0.631977	-0.590335
20	6	0	-1.677548	-1.275301	-0.578059
21	1	0	9.070231	-0.413084	-0.945559
22	6	0	8.430072	0.447963	-1.168040
23	6	0	7.035728	0.253661	-0.621412
24	1	0	8.904502	1.340891	-0.749666
25	1	0	8.412319	0.563324	-2.259684
26	6	0	6.369576	1.289208	0.045788
27	6	0	6.372055	-0.974127	-0.779880
28	6	0	5.073680	1.119288	0.534871
29	1	0	6.872868	2.241329	0.193609
30	6	0	5.079921	-1.162505	-0.299630
31	1	0	6.879068	-1.795851	-1.279892
32	6	0	4.435336	-0.106321	0.350543
33	1	0	4.569311	1.916732	1.069579
34	1	0	4.581628	-2.120176	-0.408360
35	16	0	2.768151	-0.340172	0.962453
36	8	0	2.499941	0.756289	1.907781
37	8	0	2.626414	-1.742288	1.370566
38	7	0	1.805640	-0.122329	-0.414910
39	17	0	-4.474935	-0.779591	-1.910474
40	6	0	-3.209553	-0.768081	1.625243
41	8	0	-3.613998	-1.450699	2.484416
42	45	0	-3.213804	-0.002963	-0.047062
43	6	0	-4.784722	1.287088	0.295145
44	8	0	-5.714004	1.940282	0.395833
45	6	0	-1.894224	-2.730901	-0.857419

46	1	0	-2.590041	-2.856621	-1.693563
47	1	0	-0.955346	-3.243955	-1.104798
48	1	0	-2.345141	-3.240648	0.003605

IN4:

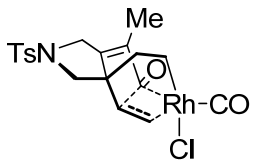


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.487801	-0.757790	-0.283163
2	6	0	-1.352672	0.888271	-0.443745
3	6	0	-0.823008	-1.416140	-0.798850
4	6	0	0.795845	-1.121501	1.192394
5	6	0	2.070506	-0.419446	1.676582
6	1	0	-0.060770	-0.859848	1.824915
7	1	0	0.900989	-2.211340	1.259614
8	1	0	2.585431	-1.013593	2.440251
9	1	0	1.841439	0.556484	2.112025
10	1	0	-1.732419	1.460554	0.408362
11	1	0	-1.656229	1.409390	-1.361293
12	1	0	-1.007760	-2.401302	-0.369601
13	1	0	-0.799564	-1.515137	-1.891920
14	6	0	1.665121	-1.110846	-1.166586
15	6	0	2.546651	-2.127036	-0.943641
16	1	0	2.477703	-2.779921	-0.077671
17	1	0	3.288380	-2.383903	-1.691259
18	1	0	1.703585	-0.610859	-2.133905
19	6	0	0.157657	0.720228	-0.385123
20	6	0	1.041064	1.733879	-0.445418
21	1	0	-9.151303	0.321607	-0.797951
22	6	0	-8.389333	1.088382	-0.987569
23	6	0	-7.025885	0.617692	-0.540866
24	1	0	-8.406056	1.299356	-2.063080
25	1	0	-8.693735	1.996618	-0.458889
26	6	0	-6.366328	-0.412821	-1.233635
27	6	0	-6.396260	1.179548	0.575802
28	6	0	-5.118854	-0.870834	-0.825699
29	1	0	-6.841175	-0.862891	-2.102074

30	6	0	-5.143619	0.732774	1.001310
31	1	0	-6.891868	1.975046	1.126152
32	6	0	-4.512471	-0.286558	0.291142
33	1	0	-4.620005	-1.671692	-1.361638
34	1	0	-4.661256	1.159808	1.873726
35	16	0	-2.929449	-0.900323	0.855276
36	8	0	-2.956890	-2.366219	0.878229
37	8	0	-2.572156	-0.139341	2.063772
38	7	0	-1.906770	-0.480115	-0.443006
39	17	0	5.324996	-0.646480	-1.472735
40	6	0	2.522375	1.545538	-0.361512
41	8	0	3.276782	2.466529	-0.546235
42	45	0	3.457431	-0.215381	0.086580
43	6	0	4.679799	0.760338	1.196992
44	8	0	5.422773	1.325759	1.854946
45	6	0	0.634764	3.186832	-0.577528
46	1	0	-0.447782	3.300010	-0.670968
47	1	0	0.966052	3.763525	0.293643
48	1	0	1.112622	3.639508	-1.452457

TS4:

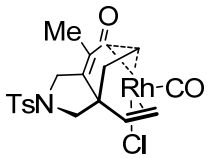


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.484475	-0.169101	0.406286
2	6	0	1.499738	0.958020	-0.527602
3	6	0	0.762854	-0.529380	1.249744
4	6	0	-0.835783	-1.275377	-0.635853
5	6	0	-2.100340	-0.934629	-1.428770
6	1	0	0.021873	-1.438876	-1.302085
7	1	0	-0.970469	-2.219485	-0.093296
8	1	0	-2.446198	-1.820328	-1.968496
9	1	0	-1.908354	-0.151807	-2.175584
10	1	0	1.750908	0.680277	-1.558772
11	1	0	2.002657	1.906001	-0.299125

12	1	0	0.839294	-1.589864	1.490820
13	1	0	0.778607	0.041070	2.187325
14	6	0	-1.725494	0.213979	1.191837
15	6	0	-2.690558	-0.823470	1.522003
16	1	0	-2.385011	-1.860507	1.403502
17	1	0	-3.352826	-0.642614	2.364494
18	1	0	-1.584371	0.977314	1.961436
19	6	0	0.013719	1.051889	-0.322874
20	6	0	-0.850160	2.039700	-0.591004
21	1	0	9.194856	0.481725	0.770160
22	6	0	8.464963	1.235385	0.447709
23	6	0	7.094465	0.623858	0.281167
24	1	0	8.460059	2.024474	1.208272
25	1	0	8.828212	1.668434	-0.489086
26	6	0	6.344971	0.239585	1.406756
27	6	0	6.547288	0.408443	-0.989223
28	6	0	5.089075	-0.341128	1.271688
29	1	0	6.755557	0.395752	2.401351
30	6	0	5.287712	-0.173571	-1.145504
31	1	0	7.113545	0.694755	-1.871733
32	6	0	4.565666	-0.538044	-0.010501
33	1	0	4.521859	-0.643667	2.145899
34	1	0	4.870625	-0.351563	-2.130703
35	16	0	2.959361	-1.304558	-0.194410
36	8	0	2.853700	-2.434955	0.732844
37	8	0	2.725016	-1.488593	-1.635723
38	7	0	1.918536	-0.104713	0.416547
39	17	0	-5.402215	0.814515	1.264061
40	6	0	-2.203425	1.819940	-0.046563
41	8	0	-3.093188	2.613895	-0.005703
42	45	0	-3.604663	-0.122736	-0.173241
43	6	0	-4.792026	-1.509916	-0.613413
44	8	0	-5.479937	-2.400441	-0.838128
45	6	0	-0.596367	3.336077	-1.310468
46	1	0	-0.993373	4.180230	-0.737075
47	1	0	0.473260	3.491002	-1.479177
48	1	0	-1.098443	3.347134	-2.285414

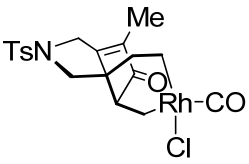
TS4-[(3+2)+1]:



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.279819	-0.292145	-1.100387
2	6	0	0.333390	0.874454	0.966062
3	6	0	1.144106	0.286239	-1.247348
4	6	0	-1.126186	-0.147990	-2.380076
5	6	0	-2.605734	-0.427464	-2.100243
6	1	0	-1.002963	0.868037	-2.772865
7	1	0	-0.759625	-0.838298	-3.150722
8	1	0	-2.768614	-1.501648	-1.965026
9	1	0	-3.280605	-0.097995	-2.887833
10	1	0	0.345307	1.890950	1.364727
11	1	0	0.276704	0.186103	1.817834
12	1	0	1.126700	1.199247	-1.856336
13	1	0	1.837238	-0.426137	-1.704488
14	6	0	-0.262217	-1.740602	-0.614544
15	6	0	0.790266	-2.441690	-0.190686
16	1	0	1.792118	-2.029407	-0.123371
17	1	0	0.667493	-3.472907	0.128667
18	1	0	-1.235588	-2.227504	-0.608432
19	6	0	-0.803620	0.641456	-0.001094
20	6	0	-1.932649	1.411574	-0.035095
21	1	0	7.902287	-2.405657	-1.146924
22	6	0	7.553511	-2.305035	-0.114598
23	6	0	6.385628	-1.353005	-0.014156
24	1	0	7.290252	-3.302015	0.255599
25	1	0	8.400646	-1.950436	0.486970
26	6	0	6.107962	-0.440102	-1.039149
27	6	0	5.566478	-1.347767	1.127856
28	6	0	5.045223	0.459432	-0.937981
29	1	0	6.733071	-0.427172	-1.928370
30	6	0	4.503013	-0.459163	1.247360
31	1	0	5.770423	-2.046478	1.935505
32	6	0	4.246956	0.437186	0.204740
33	1	0	4.839013	1.176668	-1.725113
34	1	0	3.883260	-0.449628	2.138067
35	16	0	2.887523	1.591156	0.358304
36	8	0	2.982860	2.540497	-0.759773
37	8	0	2.808251	2.063470	1.743777
38	7	0	1.541793	0.576666	0.147429
39	6	0	-3.031892	1.136049	-1.030368

40	8	0	-3.760450	1.919490	-1.579116
41	45	0	-3.274006	-0.493770	0.134126
42	6	0	-4.954435	-1.264560	-0.156099
43	8	0	-6.010095	-1.679621	-0.328855
44	17	0	-3.509273	-0.714091	2.455702
45	6	0	-2.206083	2.548071	0.929479
46	1	0	-2.376799	2.175298	1.943991
47	1	0	-1.360116	3.244388	0.950853
48	1	0	-3.093146	3.098311	0.609500

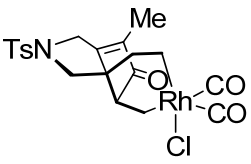


IN5-1:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.372949	-0.028030	-0.790730
2	6	0	-1.593422	1.130394	0.156832
3	6	0	-0.902733	-0.589355	-1.446875
4	6	0	0.915535	-0.983893	0.315969
5	6	0	2.186249	-0.548192	1.033910
6	1	0	0.135020	-1.125575	1.079213
7	1	0	1.067761	-1.968867	-0.141859
8	1	0	2.489517	-1.297179	1.766627
9	1	0	2.092978	0.415053	1.545643
10	1	0	-1.708453	0.982440	1.237955
11	1	0	-2.199720	1.995071	-0.137803
12	1	0	-0.944167	-1.676919	-1.512606
13	1	0	-1.034833	-0.175858	-2.454931
14	6	0	1.555916	0.454777	-1.676300
15	6	0	2.753375	-0.472544	-1.832539
16	1	0	2.451955	-1.506008	-2.022639
17	1	0	3.402163	-0.144196	-2.655131
18	1	0	1.135716	0.785085	-2.640441
19	6	0	-0.156295	1.283516	-0.238228
20	6	0	0.718085	2.309802	-0.311435
21	1	0	-9.304284	0.155413	0.073735

22	6	0	-8.582176	0.982270	0.089469
23	6	0	-7.166559	0.459693	0.142759
24	1	0	-8.755081	1.578920	-0.812854
25	1	0	-8.813848	1.604172	0.959569
26	6	0	-6.537255	-0.015867	-1.020446
27	6	0	-6.459403	0.412916	1.350528
28	6	0	-5.243576	-0.524477	-0.982573
29	1	0	-7.072000	0.010638	-1.966681
30	6	0	-5.160451	-0.094870	1.409131
31	1	0	-6.930463	0.773960	2.261196
32	6	0	-4.560616	-0.553922	0.237420
33	1	0	-4.767961	-0.897930	-1.883577
34	1	0	-4.618446	-0.143305	2.347290
35	16	0	-2.908969	-1.237794	0.300536
36	8	0	-2.863406	-2.472010	-0.489502
37	8	0	-2.487532	-1.236638	1.711552
38	7	0	-2.015786	-0.090263	-0.584054
39	17	0	5.401838	0.681847	1.608854
40	6	0	1.938648	1.695660	-0.872539
41	8	0	3.107244	1.971284	-0.563103
42	45	0	3.891798	-0.129754	-0.119600
43	6	0	4.437832	-1.862513	0.044910
44	8	0	4.771609	-2.958156	0.148755
45	6	0	0.640378	3.715835	0.195531
46	1	0	-0.293115	3.904408	0.732964
47	1	0	1.479673	3.914367	0.872272
48	1	0	0.717197	4.437372	-0.627020



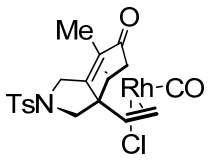
IN5-2:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.065506	-0.028976	-0.593150
2	6	0	-1.917263	1.180569	0.253402
3	6	0	-1.195551	-0.595432	-1.272748
4	6	0	0.570413	-0.958735	0.555147
5	6	0	1.848608	-0.518162	1.274922

6	1	0	-0.236783	-1.075141	1.293181
7	1	0	0.720123	-1.954345	0.118092
8	1	0	2.099385	-1.262699	2.035491
9	1	0	1.716105	0.440254	1.790297
10	1	0	-2.075190	1.074274	1.333817
11	1	0	-2.500760	2.040786	-0.096420
12	1	0	-1.245623	-1.683852	-1.307531
13	1	0	-1.294981	-0.208983	-2.295378
14	6	0	1.277409	0.421976	-1.455993
15	6	0	2.446351	-0.541829	-1.615163
16	1	0	2.106494	-1.571405	-1.752446
17	1	0	3.104611	-0.264473	-2.440694
18	1	0	0.886147	0.758940	-2.429677
19	6	0	-0.464802	1.302514	-0.094006
20	6	0	0.428685	2.312819	-0.160124
21	1	0	-9.569286	0.194752	-0.853420
22	6	0	-8.929393	0.950497	-0.383181
23	6	0	-7.528738	0.427350	-0.171618
24	1	0	-8.928083	1.826858	-1.043845
25	1	0	-9.394498	1.246744	0.561721
26	6	0	-6.820975	-0.159566	-1.235260
27	6	0	-6.903198	0.515405	1.077404
28	6	0	-5.527254	-0.637609	-1.062194
29	1	0	-7.295669	-0.247108	-2.209556
30	6	0	-5.604630	0.039626	1.271341
31	1	0	-7.438957	0.955147	1.914669
32	6	0	-4.924449	-0.527015	0.195220
33	1	0	-4.992057	-1.100897	-1.884622
34	1	0	-5.127031	0.092617	2.243648
35	16	0	-3.269578	-1.166395	0.430711
36	8	0	-3.149993	-2.449988	-0.267536
37	8	0	-2.958002	-1.057873	1.865295
38	7	0	-2.326492	-0.062097	-0.455529
39	17	0	5.646591	0.267337	-1.330878
40	6	0	1.658600	1.657088	-0.649170
41	8	0	2.815864	1.903544	-0.275362
42	6	0	4.031223	-1.978977	0.142571
43	8	0	4.286505	-3.097038	0.156850
44	45	0	3.610268	-0.187146	0.071875
45	6	0	4.822004	0.461464	1.645996
46	8	0	5.561365	0.833064	2.427735
47	6	0	0.354094	3.733215	0.305831
48	1	0	-0.599698	3.951440	0.794322
49	1	0	1.163862	3.938914	1.015833

50	1	0	0.480713	4.431025	-0.530846



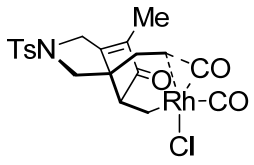
IN5-[(3+2)+1]:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.973285	-1.387148	-0.935538
2	6	0	-0.536514	0.458888	-0.225974
3	6	0	-0.292942	-1.257445	-1.836305
4	6	0	1.045142	-2.774621	-0.258806
5	6	0	1.997191	-2.853045	0.948349
6	1	0	0.034089	-3.016559	0.082760
7	1	0	1.318786	-3.528485	-1.006865
8	1	0	2.993892	-3.212034	0.671081
9	1	0	1.624466	-3.594025	1.665772
10	1	0	-1.107105	0.752630	0.656937
11	1	0	-0.353092	1.354853	-0.829253
12	1	0	-0.707164	-2.217225	-2.148048
13	1	0	-0.073417	-0.672090	-2.737029
14	6	0	2.236536	-0.949015	-1.670595
15	6	0	3.527680	-1.130441	-1.271076
16	1	0	3.820730	-1.747473	-0.431780
17	1	0	4.334035	-0.737457	-1.880564
18	1	0	2.079363	-0.404613	-2.600912
19	6	0	0.757291	-0.275368	0.113854
20	6	0	1.384946	-0.342458	1.367198
21	1	0	-7.390341	2.691389	1.198276
22	6	0	-7.182756	2.403234	0.163566
23	6	0	-5.998963	1.470224	0.074756
24	1	0	-8.087246	1.930599	-0.239669
25	1	0	-7.012559	3.318224	-0.415822
26	6	0	-5.482374	1.094909	-1.178037
27	6	0	-5.397787	0.951191	1.227316
28	6	0	-4.400617	0.228078	-1.280687
29	1	0	-5.937571	1.488334	-2.083636
30	6	0	-4.309720	0.080154	1.145498
31	1	0	-5.784609	1.228397	2.204415

32	6	0	-3.816482	-0.268706	-0.110533
33	1	0	-4.008176	-0.057647	-2.250893
34	1	0	-3.847754	-0.327926	2.037840
35	16	0	-2.463608	-1.432269	-0.221075
36	8	0	-2.813467	-2.527480	-1.131683
37	8	0	-2.021899	-1.731327	1.152716
38	7	0	-1.296594	-0.498389	-1.059098
39	6	0	2.170858	-1.566501	1.760089
40	8	0	2.866334	-1.567512	2.762139
41	45	0	2.660402	0.795148	-0.141693
42	6	0	2.338298	2.431021	0.738147
43	8	0	2.171677	3.457125	1.223461
44	17	0	4.312584	1.986725	-1.370059
45	6	0	0.914771	0.458344	2.565833
46	1	0	0.449033	1.406400	2.289153
47	1	0	0.175684	-0.133770	3.121880
48	1	0	1.752640	0.653290	3.239003

TS5:

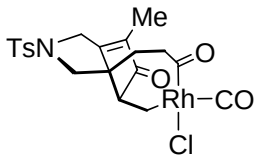


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.120570	0.045018	-0.594549
2	6	0	-1.873760	1.010875	0.504375
3	6	0	-1.138936	-0.353936	-1.394993
4	6	0	0.536817	-1.127756	0.343658
5	6	0	1.781500	-0.901159	1.198061
6	1	0	-0.301682	-1.352989	1.016154
7	1	0	0.666050	-2.027315	-0.270437
8	1	0	1.832760	-1.575930	2.054039
9	1	0	1.852141	0.113111	1.603370
10	1	0	-2.012191	0.632289	1.525011
11	1	0	-2.473732	1.921359	0.392049
12	1	0	-1.187875	-1.405348	-1.680332
13	1	0	-1.226277	0.255300	-2.303368

14	6	0	1.320654	0.670253	-1.355146
15	6	0	2.540701	-0.183669	-1.677303
16	1	0	2.268381	-1.184445	-2.023616
17	1	0	3.175641	0.285428	-2.428969
18	1	0	0.915810	1.097235	-2.289674
19	6	0	-0.429128	1.235520	0.173067
20	6	0	0.408444	2.286243	0.250663
21	1	0	-9.482130	0.652210	-0.705239
22	6	0	-8.823356	1.186960	-0.011204
23	6	0	-7.445400	0.570222	0.021512
24	1	0	-8.780664	2.230686	-0.347933
25	1	0	-9.292176	1.175123	0.977206
26	6	0	-6.746835	0.326924	-1.174185
27	6	0	-6.830984	0.233294	1.233157
28	6	0	-5.472871	-0.228977	-1.163016
29	1	0	-7.212662	0.573135	-2.125289
30	6	0	-5.551788	-0.326050	1.264959
31	1	0	-7.359705	0.404390	2.167267
32	6	0	-4.880302	-0.546131	0.063970
33	1	0	-4.944168	-0.422202	-2.090706
34	1	0	-5.081047	-0.598321	2.203288
35	16	0	-3.251511	-1.287172	0.084326
36	8	0	-3.182702	-2.340390	-0.933282
37	8	0	-2.922624	-1.583721	1.489404
38	7	0	-2.279951	-0.019122	-0.490844
39	17	0	5.629104	0.242225	-1.361493
40	6	0	1.650360	1.884622	-0.461633
41	8	0	2.763805	2.372009	-0.310900
42	6	0	3.215764	-1.878321	0.367245
43	8	0	3.184461	-3.043432	0.355672
44	45	0	3.734937	-0.156421	0.038634
45	6	0	5.067625	0.111217	1.602074
46	8	0	5.895679	0.248114	2.372754
47	6	0	0.258435	3.612057	0.928968
48	1	0	-0.703372	3.705493	1.441503
49	1	0	1.059223	3.753725	1.664427
50	1	0	0.350537	4.432892	0.207523

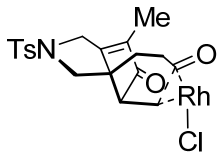
IN6:



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.036545	-0.090093	-0.538283
2	6	0	-1.990531	1.127091	0.194271
3	6	0	-1.193437	-0.672912	-1.264433
4	6	0	0.432904	-0.987648	0.675031
5	6	0	1.629123	-0.527439	1.552224
6	1	0	-0.439911	-1.081227	1.330374
7	1	0	0.634293	-1.999013	0.302945
8	1	0	1.518280	-0.974771	2.545493
9	1	0	1.656724	0.554937	1.684677
10	1	0	-2.200538	1.038944	1.267667
11	1	0	-2.558056	1.979998	-0.196457
12	1	0	-1.242036	-1.762039	-1.286757
13	1	0	-1.241405	-0.304055	-2.296840
14	6	0	1.271765	0.363797	-1.377428
15	6	0	2.478502	-0.557290	-1.607771
16	1	0	2.203252	-1.613749	-1.540691
17	1	0	2.888817	-0.392572	-2.610632
18	1	0	0.865950	0.716040	-2.339242
19	6	0	-0.523259	1.249327	-0.084392
20	6	0	0.370560	2.259822	-0.121534
21	1	0	-9.652363	0.224253	-0.569025
22	6	0	-8.950657	1.032593	-0.326822
23	6	0	-7.549445	0.497381	-0.153603
24	1	0	-9.001900	1.759178	-1.145847
25	1	0	-9.309472	1.521380	0.583817
26	6	0	-6.824237	0.029465	-1.263622
27	6	0	-6.948361	0.437911	1.109200
28	6	0	-5.540342	-0.483847	-1.120368
29	1	0	-7.276584	0.065652	-2.251648
30	6	0	-5.659582	-0.073534	1.273636
31	1	0	-7.494672	0.791746	1.979611
32	6	0	-4.963835	-0.525009	0.153544
33	1	0	-4.990462	-0.850494	-1.980980
34	1	0	-5.198410	-0.129563	2.253607
35	16	0	-3.331186	-1.226063	0.356162
36	8	0	-3.245994	-2.493485	-0.375255
37	8	0	-3.003804	-1.168694	1.791242
38	7	0	-2.364114	-0.127220	-0.514567
39	6	0	1.616024	1.610434	-0.579917

40	8	0	2.765529	1.891771	-0.212337
41	6	0	2.974503	-1.071540	1.037499
42	8	0	3.387830	-2.137494	1.395681
43	45	0	3.997076	0.055828	-0.280878
44	6	0	5.117582	-1.387394	-0.625537
45	8	0	5.825373	-2.255150	-0.868120
46	17	0	5.755117	1.180015	0.950030
47	6	0	0.275444	3.686893	0.319951
48	1	0	-0.695213	3.908201	0.772292
49	1	0	1.060414	3.906438	1.053095
50	1	0	0.428566	4.372113	-0.522645

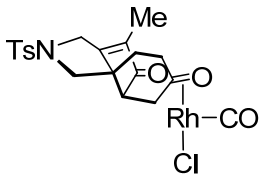


TS6:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.054355	-0.206052	-0.373685
2	6	0	-2.055795	1.137058	0.175713
3	6	0	-1.275813	-0.791930	-1.108942
4	6	0	0.299122	-1.022744	0.906672
5	6	0	1.639024	-0.631606	1.570294
6	1	0	-0.508734	-0.931681	1.640960
7	1	0	0.342329	-2.084344	0.634700
8	1	0	1.700828	-1.118793	2.548267
9	1	0	1.707009	0.445032	1.740654
10	1	0	-2.311503	1.149508	1.242404
11	1	0	-2.572684	1.973211	-0.310472
12	1	0	-1.363355	-1.877591	-1.061477
13	1	0	-1.277028	-0.489167	-2.164077
14	6	0	1.248598	0.122237	-1.157045
15	6	0	2.399673	-0.876542	-1.143575
16	1	0	2.082374	-1.918590	-1.174174
17	1	0	3.051893	-0.759829	-2.023489
18	1	0	0.958543	0.368319	-2.191570
19	6	0	-0.575160	1.181930	-0.048109
20	6	0	0.353418	2.158145	-0.138987
21	1	0	-9.722933	0.252365	-0.840466

22	6	0	-9.021530	1.070930	-0.635416
23	6	0	-7.637385	0.538865	-0.350877
24	1	0	-9.024080	1.724433	-1.515667
25	1	0	-9.414427	1.641536	0.211257
26	6	0	-6.894390	-0.088894	-1.366288
27	6	0	-7.069691	0.642377	0.924350
28	6	0	-5.624704	-0.597806	-1.119408
29	1	0	-7.321898	-0.182737	-2.361567
30	6	0	-5.795733	0.137416	1.192342
31	1	0	-7.631295	1.119431	1.723308
32	6	0	-5.080962	-0.473318	0.163592
33	1	0	-5.061753	-1.090007	-1.905750
34	1	0	-5.362089	0.205686	2.184049
35	16	0	-3.463934	-1.158394	0.501665
36	8	0	-3.365910	-2.494497	-0.092645
37	8	0	-3.191235	-0.951604	1.933860
38	7	0	-2.450338	-0.159128	-0.438280
39	17	0	5.783890	-1.432504	-0.877367
40	6	0	1.594201	1.452452	-0.496805
41	8	0	2.742997	1.795935	-0.176042
42	6	0	2.852129	-1.182144	0.784630
43	8	0	3.335371	-2.239333	1.081535
44	45	0	4.169581	0.180360	-0.256110
45	6	0	5.534444	1.092782	0.684178
46	8	0	6.336952	1.605550	1.325782
47	6	0	0.277051	3.621763	0.167497
48	1	0	-0.722072	3.912276	0.503773
49	1	0	0.995903	3.884325	0.952559
50	1	0	0.534782	4.223251	-0.712422



IN7:

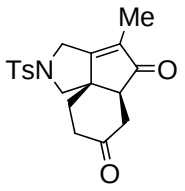
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.253011	-0.578605	0.403192

2	6	0	2.098115	0.619339	-0.711589
3	6	0	1.489777	-0.580559	1.330125
4	6	0	0.143106	-1.945329	-0.351561
5	6	0	-1.167360	-2.145513	-1.143513
6	1	0	1.001784	-2.084448	-1.015911
7	1	0	0.222110	-2.734026	0.406371
8	1	0	-1.297209	-3.211771	-1.373697
9	1	0	-1.160399	-1.627003	-2.108875
10	1	0	2.374899	0.138652	-1.658455
11	1	0	2.507101	1.636046	-0.709092
12	1	0	1.715378	-1.541515	1.793699
13	1	0	1.379392	0.170268	2.123276
14	6	0	-1.124572	-0.159169	0.983946
15	6	0	-2.142057	-1.315362	1.073662
16	1	0	-1.707948	-2.154426	1.629387
17	1	0	-3.076490	-1.001765	1.549355
18	1	0	-0.998628	0.305901	1.972117
19	6	0	0.618325	0.598639	-0.478285
20	6	0	-0.379323	1.483625	-0.682028
21	1	0	9.720461	1.515615	0.583769
22	6	0	8.903738	2.057525	0.090147
23	6	0	7.637528	1.235133	0.080971
24	1	0	8.764662	2.997227	0.636993
25	1	0	9.232137	2.300748	-0.924641
26	6	0	6.940236	0.989849	1.276976
27	6	0	7.138728	0.686686	-1.106561
28	6	0	5.781261	0.222459	1.290370
29	1	0	7.315576	1.404260	2.209416
30	6	0	5.976485	-0.087030	-1.114090
31	1	0	7.666934	0.861443	-2.040226
32	6	0	5.304151	-0.307303	0.086721
33	1	0	5.254871	0.029276	2.219355
34	1	0	5.597893	-0.522001	-2.032598
35	16	0	3.826952	-1.313840	0.098142
36	8	0	3.858276	-2.217034	1.252614
37	8	0	3.644836	-1.845304	-1.263135
38	7	0	2.615618	-0.167083	0.442733
39	17	0	-6.583437	-0.930922	-0.025126
40	6	0	-1.567112	0.965548	0.016566
41	8	0	-2.716479	1.371226	-0.182068
42	6	0	-2.382534	-1.652723	-0.376607
43	8	0	-3.420526	-1.331618	-0.948894
44	45	0	-4.629743	0.342375	-0.020542
45	6	0	-5.537251	1.768944	0.648461

46	8	0	-6.112114	2.677704	1.072833
47	6	0	-0.407287	2.750847	-1.478098
48	1	0	-0.768861	3.586254	-0.867997
49	1	0	0.580758	3.004025	-1.872732
50	1	0	-1.101853	2.655259	-2.321015

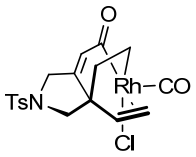
P:



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.899178	-0.184550	0.446920
2	6	0	0.080566	0.861977	-0.585466
3	6	0	-0.659714	-0.504945	1.310092
4	6	0	-2.213780	-1.367501	-0.513086
5	6	0	-3.543070	-1.182758	-1.256322
6	1	0	-1.392675	-1.515179	-1.222616
7	1	0	-2.263231	-2.287074	0.085641
8	1	0	-3.725739	-1.986332	-1.976318
9	1	0	-3.529267	-0.244243	-1.831291
10	1	0	0.254353	0.462927	-1.592680
11	1	0	0.645100	1.795978	-0.483734
12	1	0	-0.572535	-1.548365	1.615442
13	1	0	-0.637168	0.122914	2.210113
14	6	0	-3.182587	0.343052	1.137741
15	6	0	-4.412669	-0.573421	1.100426
16	1	0	-4.263946	-1.436418	1.765208
17	1	0	-5.294564	-0.038006	1.464357
18	1	0	-2.959571	0.590032	2.185541
19	6	0	-1.377407	1.037934	-0.286250
20	6	0	-2.224448	2.080810	-0.326222
21	1	0	7.663458	0.887362	0.827663
22	6	0	6.997637	1.380934	0.110163
23	6	0	5.649311	0.702839	0.057581
24	1	0	6.901782	2.427244	0.427531
25	1	0	7.488848	1.373528	-0.867375

26	6	0	4.932693	0.452014	1.240944
27	6	0	5.081092	0.314333	-1.160987
28	6	0	3.686069	-0.162359	1.210752
29	1	0	5.363146	0.738204	2.197588
30	6	0	3.829908	-0.304195	-1.211419
31	1	0	5.624447	0.491197	-2.085617
32	6	0	3.139456	-0.531869	-0.022821
33	1	0	3.143708	-0.362192	2.129121
34	1	0	3.395377	-0.616793	-2.154639
35	16	0	1.551304	-1.357271	-0.067387
36	8	0	1.511124	-2.385615	0.977739
37	8	0	1.284960	-1.711348	-1.472088
38	7	0	0.501804	-0.128377	0.446527
39	6	0	-3.444589	1.702260	0.439494
40	8	0	-4.457568	2.365792	0.556148
41	6	0	-4.723867	-1.123477	-0.292584
42	8	0	-5.834737	-1.508648	-0.594888
43	6	0	-2.064067	3.439861	-0.931691
44	1	0	-2.439107	4.209031	-0.248091
45	1	0	-1.020163	3.657942	-1.179455
46	1	0	-2.654113	3.526122	-1.852769

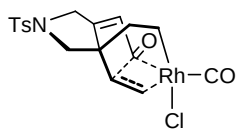


IN4-H:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.453304	0.416295	0.213170
2	6	0	1.139530	-1.012385	-1.042522
3	6	0	0.983820	1.015793	0.236700
4	6	0	-0.859487	-0.220045	1.569090
5	6	0	-2.253622	-0.858619	1.491114
6	1	0	-0.101195	-0.950632	1.876413
7	1	0	-0.835200	0.568923	2.330432
8	1	0	-2.755831	-0.823928	2.464695
9	1	0	-2.190277	-1.906730	1.187728
10	1	0	1.362017	-2.051837	-0.784973
11	1	0	1.431917	-0.852259	-2.089927
12	1	0	1.258837	1.400637	1.218915

13	1	0	1.075261	1.826669	-0.498326
14	6	0	-1.484365	1.439945	-0.214282
15	6	0	-2.260829	2.182009	0.623699
16	1	0	-2.203522	2.093392	1.705369
17	1	0	-2.894154	2.968742	0.229555
18	1	0	-1.492088	1.698170	-1.272617
19	6	0	-0.322765	-0.667688	-0.837888
20	6	0	-1.332379	-1.227954	-1.518649
21	1	0	-1.138089	-1.982780	-2.279223
22	1	0	9.189136	0.735317	-0.629788
23	6	0	8.374372	1.054539	-1.293082
24	6	0	7.034412	0.621187	-0.748020
25	1	0	8.437053	2.143811	-1.384130
26	1	0	8.566807	0.617749	-2.278388
27	6	0	6.319842	1.442139	0.137006
28	6	0	6.489296	-0.625107	-1.088976
29	6	0	5.096956	1.038659	0.668430
30	1	0	6.729414	2.408961	0.418892
31	6	0	5.267000	-1.046433	-0.568449
32	1	0	7.031850	-1.278598	-1.767588
33	6	0	4.575558	-0.204486	0.304302
34	1	0	4.559498	1.670001	1.367946
35	1	0	4.860242	-2.019911	-0.820627
36	16	0	2.989914	-0.717663	0.956921
37	8	0	2.784141	-0.014622	2.228013
38	8	0	2.922316	-2.180814	0.866017
39	7	0	1.866914	-0.094181	-0.151068
40	17	0	-5.071621	1.821784	-0.872998
41	6	0	-2.777496	-0.977093	-1.330951
42	8	0	-3.604626	-1.491232	-2.037270
43	45	0	-3.499206	0.224517	0.152880
44	6	0	-4.939798	-1.012486	0.388080
45	8	0	-5.813994	-1.731709	0.540880



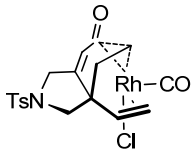
TS4-H:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.500784	0.074054	0.365818
2	6	0	1.488253	0.930943	-0.815201
3	6	0	0.744563	-0.056265	1.277369
4	6	0	-0.841719	-1.261882	-0.366502
5	6	0	-2.105228	-1.145775	-1.222417
6	1	0	0.019713	-1.581792	-0.967656
7	1	0	-0.970383	-2.037645	0.398285
8	1	0	-2.432984	-2.143120	-1.527487
9	1	0	-1.919146	-0.568890	-2.139034
10	1	0	1.740570	0.405854	-1.744703
11	1	0	1.985789	1.908039	-0.828961
12	1	0	0.819274	-1.018174	1.784925
13	1	0	0.758931	0.738136	2.034459
14	6	0	-1.751495	0.644855	1.013405
15	6	0	-2.712441	-0.280135	1.598423
16	1	0	-2.394417	-1.307494	1.762565
17	1	0	-3.380046	0.110298	2.362106
18	1	0	-1.614248	1.579127	1.564317
19	6	0	0.002099	1.068175	-0.647308
20	6	0	-0.873204	1.943756	-1.150296
21	1	0	-0.666974	2.721044	-1.879609
22	1	0	9.125791	0.827512	0.816060
23	6	0	8.478449	1.318762	0.079654
24	6	0	7.100954	0.700556	0.066512
25	1	0	8.433131	2.381065	0.349682
26	1	0	8.962879	1.241712	-0.898182
27	6	0	6.328027	0.662925	1.240733
28	6	0	6.563605	0.151493	-1.103274
29	6	0	5.057751	0.098995	1.248640
30	1	0	6.732557	1.077859	2.160726
31	6	0	5.289197	-0.419527	-1.115727
32	1	0	7.149170	0.163757	-2.018786
33	6	0	4.543995	-0.434436	0.061682
34	1	0	4.472385	0.065202	2.161728
35	1	0	4.878813	-0.856172	-2.019685
36	16	0	2.925177	-1.194953	0.069479
37	8	0	2.800580	-2.060535	1.245787
38	8	0	2.683048	-1.723141	-1.282773
39	7	0	1.904001	0.137221	0.365981
40	17	0	-5.437662	1.202125	0.908091
41	6	0	-2.228007	1.879448	-0.598252
42	8	0	-3.132858	2.632143	-0.783587
43	45	0	-3.628859	-0.067573	-0.219989
44	6	0	-4.787272	-1.539225	-0.271912

45	8	0	-5.459918	-2.468871	-0.248227

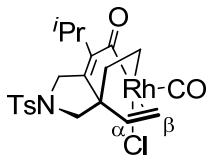


TS4-H-[(3+2)+1]:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.318054	-0.058588	-1.049233
2	6	0	0.304284	0.785299	1.172722
3	6	0	1.119092	0.508038	-1.100730
4	6	0	-1.163758	0.301481	-2.288973
5	6	0	-2.657409	0.030534	-2.065387
6	1	0	-1.008511	1.361149	-2.522656
7	1	0	-0.814460	-0.274334	-3.155477
8	1	0	-2.854333	-1.046093	-2.096692
9	1	0	-3.303718	0.496222	-2.807297
10	1	0	0.315758	1.741207	1.703218
11	1	0	0.231658	-0.012425	1.921109
12	1	0	1.120491	1.501791	-1.567269
13	1	0	1.803858	-0.139194	-1.656154
14	6	0	-0.341282	-1.562435	-0.783292
15	6	0	0.697687	-2.355182	-0.518443
16	1	0	1.717989	-1.993820	-0.436204
17	1	0	0.546092	-3.418300	-0.353493
18	1	0	-1.334640	-2.007909	-0.804663
19	6	0	-0.822399	0.704596	0.172808
20	6	0	-1.956819	1.447154	0.250029
21	1	0	-2.130460	2.108624	1.095533
22	1	0	7.927976	-2.037410	-1.565372
23	6	0	7.479715	-2.254217	-0.591273
24	6	0	6.330194	-1.322428	-0.290372
25	1	0	7.154589	-3.301165	-0.592423
26	1	0	8.268290	-2.163187	0.166438
27	6	0	6.065623	-0.213013	-1.102202
28	6	0	5.509642	-1.544625	0.829446
29	6	0	5.012709	0.658355	-0.815786
30	1	0	6.693440	-0.022204	-1.968763
31	6	0	4.456924	-0.687957	1.131902
32	1	0	5.705305	-2.397532	1.474784

33	6	0	4.212163	0.408475	0.297552
34	1	0	4.817691	1.526047	-1.436776
35	1	0	3.837087	-0.855745	2.006643
36	16	0	2.873492	1.526956	0.693981
37	8	0	2.960920	2.670282	-0.225312
38	8	0	2.818689	1.729404	2.144399
39	7	0	1.512249	0.578935	0.324903
40	6	0	-3.058617	1.412445	-0.767762
41	8	0	-3.730172	2.317613	-1.183753
42	45	0	-3.411523	-0.362151	0.115339
43	6	0	-5.099575	-1.023273	-0.341887
44	8	0	-6.159107	-1.371315	-0.611375
45	17	0	-3.734150	-0.907564	2.364756

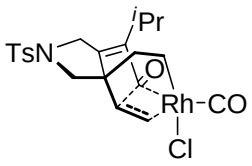


IN4-^{i}Pr:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.480548	-0.790242	-0.517608
2	6	0	-1.411842	0.730670	-0.091138
3	6	0	-0.825354	-1.381495	-1.103231
4	6	0	0.880539	-1.429879	0.836199
5	6	0	2.115335	-0.738276	1.406770
6	1	0	0.048458	-1.350481	1.548572
7	1	0	1.063328	-2.500905	0.691643
8	1	0	2.701956	-1.383510	2.063906
9	1	0	1.860378	0.192122	1.917094
10	1	0	-1.693376	0.917997	0.951652
11	1	0	-1.871262	1.514939	-0.706434
12	1	0	-0.948501	-2.446071	-0.900351
13	1	0	-0.854335	-1.236010	-2.191089
14	6	0	1.618884	-0.947830	-1.503135
15	6	0	2.578594	-1.930396	-1.491750
16	1	0	2.596720	-2.742609	-0.775755
17	1	0	3.264714	-2.029057	-2.327263
18	1	0	1.560927	-0.317089	-2.389827
19	6	0	0.089710	0.670032	-0.286485
20	6	0	0.985191	1.745856	-0.333295
21	1	0	-9.147766	0.325478	-0.605272

22	6	0	-8.380180	1.107922	-0.545956
23	6	0	-7.022118	0.512141	-0.261250
24	1	0	-8.389816	1.641032	-1.503454
25	1	0	-8.683227	1.809590	0.236985
26	6	0	-6.336457	-0.203704	-1.258262
27	6	0	-6.424204	0.641219	0.997700
28	6	0	-5.094296	-0.775461	-1.008265
29	1	0	-6.786104	-0.314248	-2.242060
30	6	0	-5.176827	0.074344	1.267668
31	1	0	-6.939711	1.190339	1.781420
32	6	0	-4.519088	-0.625281	0.257971
33	1	0	-4.573157	-1.329852	-1.781891
34	1	0	-4.716486	0.168115	2.245187
35	16	0	-2.942189	-1.397203	0.605313
36	8	0	-2.977793	-2.798179	0.173559
37	8	0	-2.585388	-1.057093	1.993592
38	7	0	-1.919507	-0.600738	-0.494532
39	17	0	5.259941	-1.929434	0.134924
40	6	0	2.387192	1.388183	-0.774242
41	8	0	3.044091	2.038119	-1.559168
42	45	0	3.425390	-0.259844	-0.160095
43	6	0	4.465418	0.757664	1.086176
44	8	0	5.110984	1.327909	1.837902
45	6	0	0.740528	3.102001	-0.021147
46	6	0	1.710601	4.202460	-0.386990
47	1	0	2.734478	3.997190	-0.055009
48	1	0	1.772670	4.342918	-1.472666
49	1	0	1.393620	5.149586	0.059809
50	6	0	-0.488332	3.581811	0.707708
51	1	0	-1.046632	2.794121	1.210713
52	1	0	-0.198191	4.315224	1.471183
53	1	0	-1.176857	4.108500	0.028494



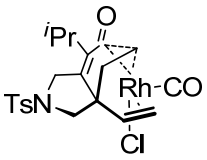
TS4-^{i}Pr:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.484345	-0.740415	0.681551
2	6	0	1.390862	0.699573	-0.026625
3	6	0	0.819806	-1.205165	1.371281
4	6	0	-0.842610	-1.637856	-0.530104
5	6	0	-2.101821	-1.180968	-1.252994
6	1	0	-0.010487	-1.640494	-1.248086
7	1	0	-0.948284	-2.671038	-0.179509
8	1	0	-2.541093	-1.977152	-1.855246
9	1	0	-1.955832	-0.291621	-1.867045
10	1	0	1.624549	0.684126	-1.099659
11	1	0	1.870814	1.584552	0.408627
12	1	0	0.965354	-2.286193	1.369130
13	1	0	0.850092	-0.857147	2.412047
14	6	0	-1.683340	-0.615143	1.601199
15	6	0	-2.732618	-1.627160	1.652853
16	1	0	-2.492453	-2.635984	1.326130
17	1	0	-3.366568	-1.611327	2.540522
18	1	0	-1.451382	-0.151952	2.564739
19	6	0	-0.087803	0.664572	0.251355
20	6	0	-1.010378	1.700592	0.418496
21	1	0	8.597053	1.801152	-0.885878
22	6	0	8.300627	1.359222	0.070068
23	6	0	6.959641	0.672010	-0.028982
24	1	0	9.084538	0.650525	0.366359
25	1	0	8.286216	2.155872	0.822865
26	6	0	6.305771	0.217863	1.129814
27	6	0	6.345065	0.458725	-1.268378
28	6	0	5.078961	-0.432014	1.056224
29	1	0	6.768283	0.375274	2.101224
30	6	0	5.112811	-0.191127	-1.362447
31	1	0	6.835331	0.802479	-2.175503
32	6	0	4.486857	-0.626967	-0.196074
33	1	0	4.581815	-0.781752	1.955037
34	1	0	4.639104	-0.361430	-2.323073
35	16	0	2.937209	-1.514507	-0.314079
36	8	0	3.038146	-2.786780	0.409188
37	8	0	2.536999	-1.502480	-1.732115
38	7	0	1.910786	-0.535705	0.619816
39	17	0	-4.103290	1.376998	-1.443642
40	6	0	-2.224215	1.194303	1.122817
41	8	0	-3.030736	1.762652	1.810348
42	45	0	-3.508563	-0.453499	0.111174
43	6	0	-4.838284	-1.592962	-0.583531
44	8	0	-5.627787	-2.297498	-1.028002

45	6	0	-0.934419	3.050334	0.032760
46	6	0	0.145845	3.558805	-0.880084
47	1	0	0.807140	4.266441	-0.357389
48	1	0	0.762076	2.771935	-1.317044
49	1	0	-0.310193	4.121057	-1.706394
50	6	0	-1.983649	4.054906	0.428212
51	1	0	-2.958127	3.777536	0.003690
52	1	0	-2.120117	4.112576	1.512927
53	1	0	-1.716976	5.049212	0.057352



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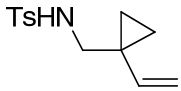
Standard orientation:

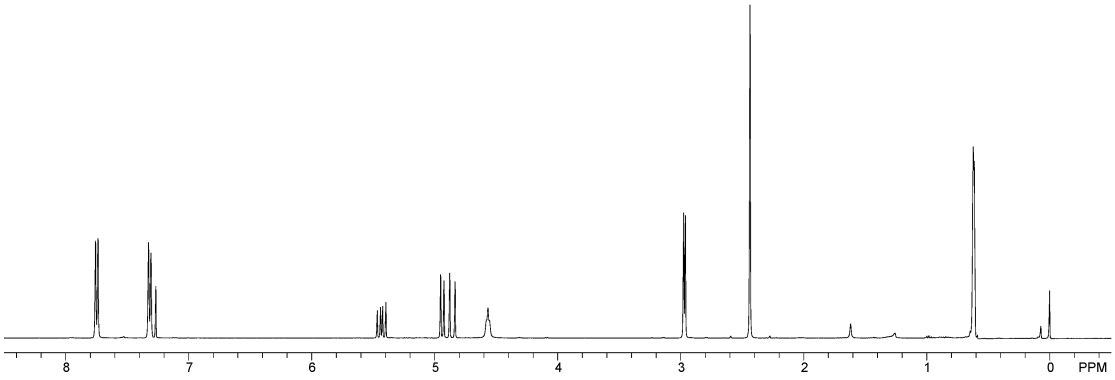
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.067231	-0.608051	-0.970168
2	6	0	0.489217	1.083397	0.719781
3	6	0	1.345434	-0.051057	-1.234554
4	6	0	-0.869819	-0.799677	-2.270902
5	6	0	-2.342341	-1.109110	-1.990810
6	1	0	-0.784930	0.112352	-2.873064
7	1	0	-0.431590	-1.617470	-2.857452
8	1	0	-2.437163	-2.139410	-1.631749
9	1	0	-2.990866	-1.005425	-2.858355
10	1	0	0.487899	2.173846	0.753677
11	1	0	0.433161	0.719557	1.751563
12	1	0	1.317046	0.699388	-2.036396
13	1	0	2.058981	-0.831525	-1.513992
14	6	0	-0.036402	-1.892803	-0.143854
15	6	0	1.027763	-2.502376	0.379452
16	1	0	2.039607	-2.120601	0.288703
17	1	0	0.906728	-3.420481	0.947806
18	1	0	-1.016470	-2.332755	0.039076
19	6	0	-0.644079	0.542748	-0.130533
20	6	0	-1.855847	1.146506	-0.298746
21	1	0	7.322478	-3.426272	0.598339
22	6	0	7.663213	-2.438238	0.267246
23	6	0	6.518676	-1.455215	0.204869

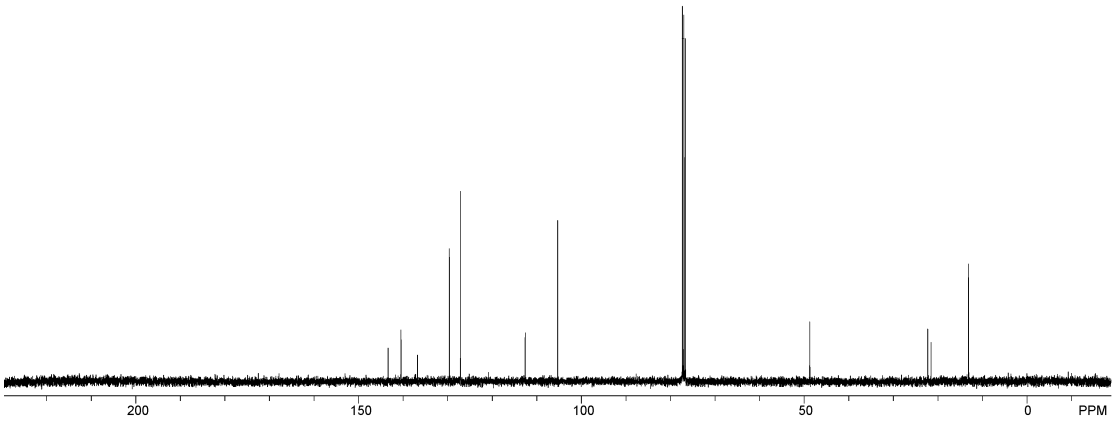
24	1	0	8.428374	-2.106365	0.980358
25	1	0	8.145578	-2.555520	-0.707693
26	6	0	6.284988	-0.687463	-0.942148
27	6	0	5.670425	-1.280640	1.312533
28	6	0	5.235504	0.232266	-0.995663
29	1	0	6.934042	-0.804724	-1.806111
30	6	0	4.620700	-0.369304	1.278922
31	1	0	5.841246	-1.863892	2.214147
32	6	0	4.406985	0.378267	0.115443
33	1	0	5.062700	0.836783	-1.879577
34	1	0	3.978010	-0.229144	2.141943
35	16	0	3.071155	1.567989	0.073973
36	8	0	3.170679	2.309232	-1.191928
37	8	0	3.007213	2.279209	1.354150
38	7	0	1.712242	0.550909	0.060760
39	6	0	-2.869231	0.587793	-1.279206
40	8	0	-3.570937	1.220000	-2.028002
41	45	0	-3.214854	-0.801562	0.144753
42	6	0	-4.828647	-1.658329	-0.197832
43	8	0	-5.849424	-2.134724	-0.419855
44	17	0	-3.713403	-0.718584	2.430606
45	6	0	-2.318184	2.478123	0.314404
46	1	0	-3.404213	2.494798	0.178132
47	6	0	-2.069189	2.649739	1.823049
48	1	0	-1.015521	2.807409	2.071126
49	1	0	-2.613394	3.536197	2.168261
50	1	0	-2.439728	1.787987	2.385458
51	6	0	-1.753926	3.650037	-0.517875
52	1	0	-2.037664	3.551210	-1.570272
53	1	0	-2.159375	4.597000	-0.144108
54	1	0	-0.661146	3.709664	-0.458269

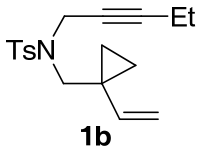
4. ^{1}H and ^{13}C-NMR Spectra for New Compounds



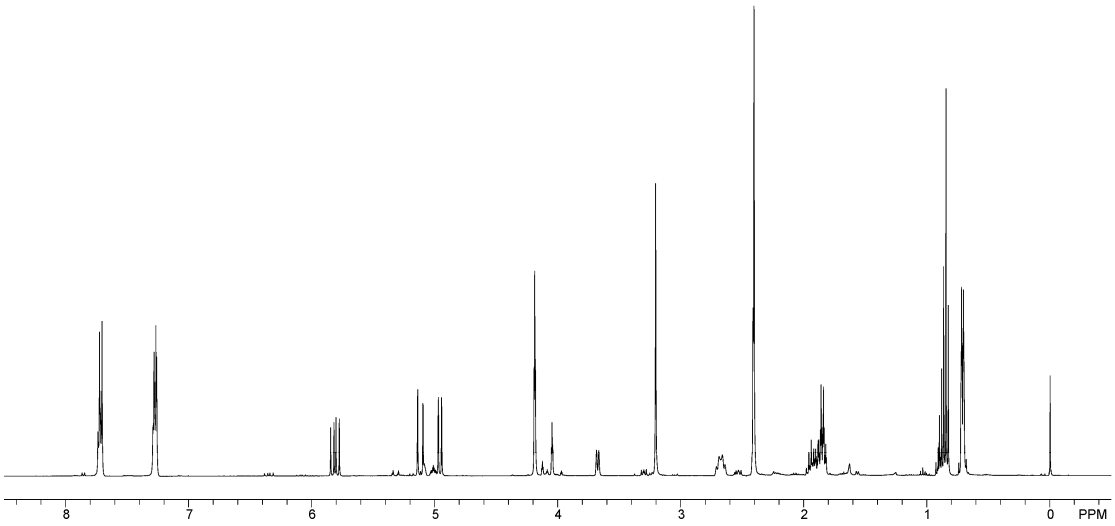
S2

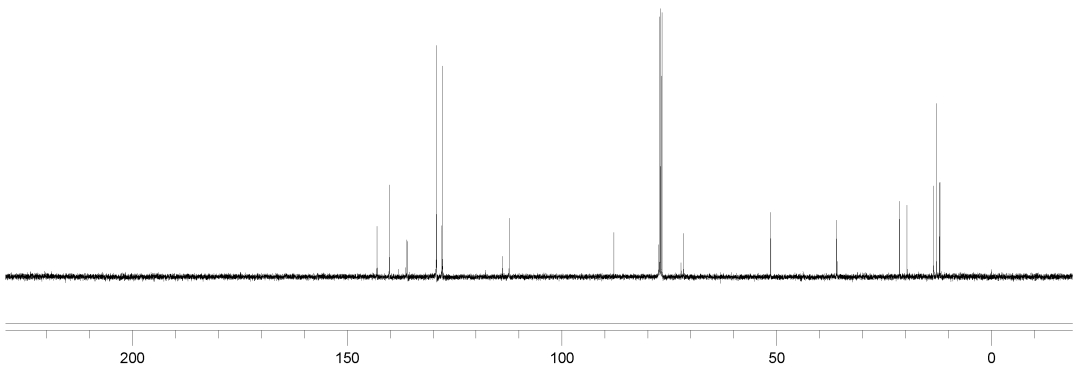


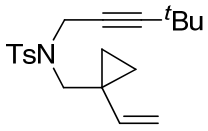




1b







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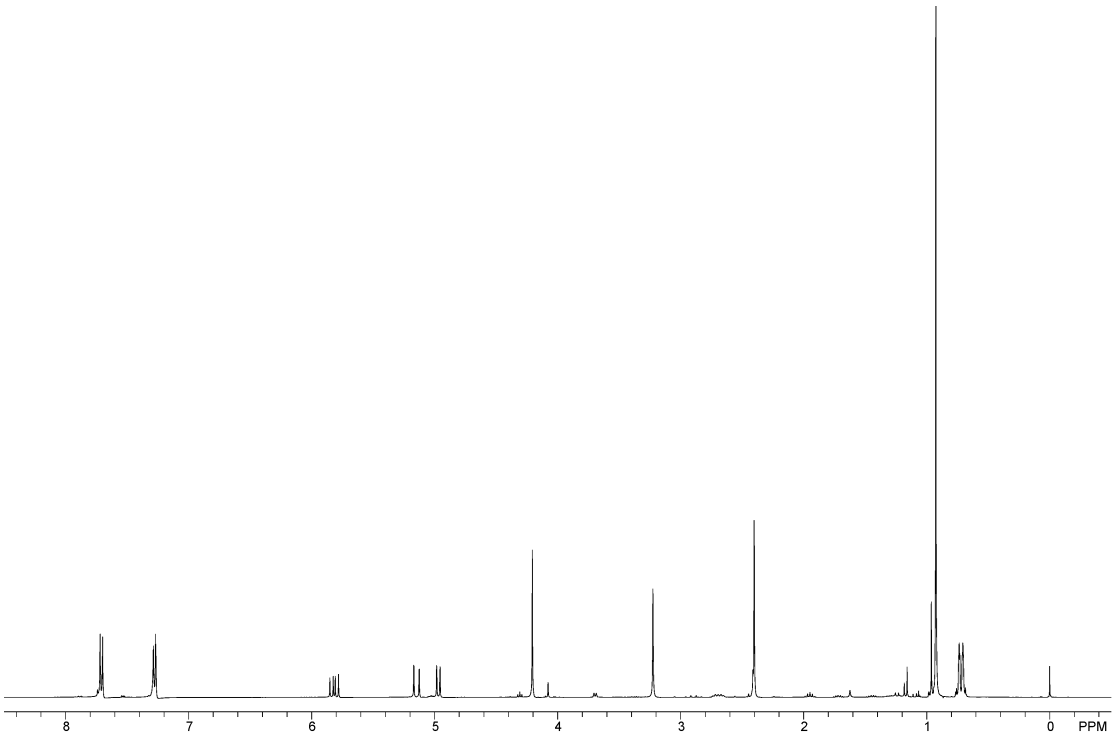

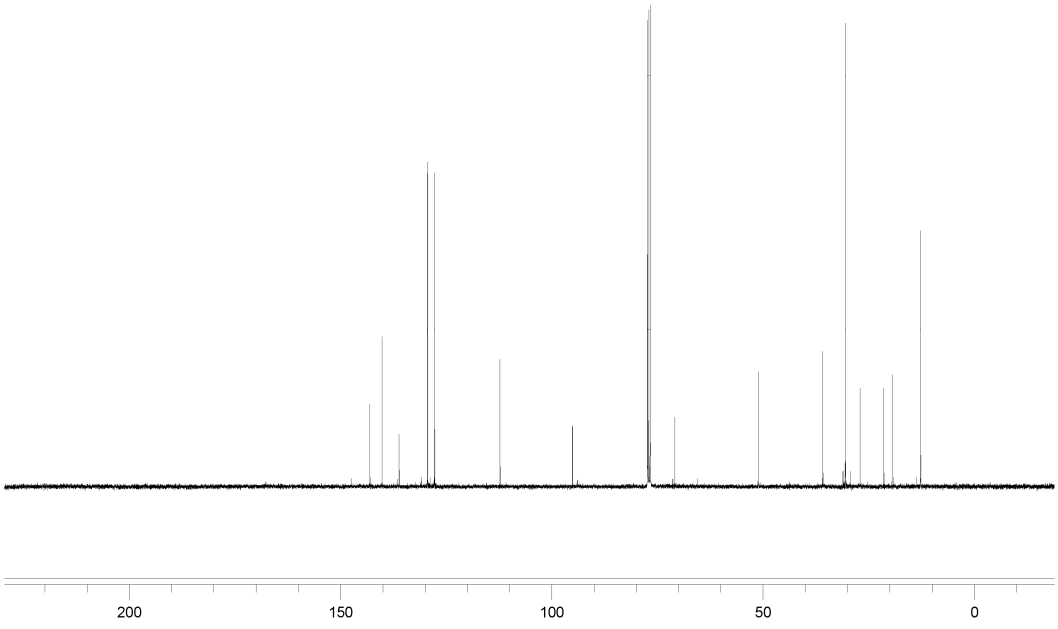

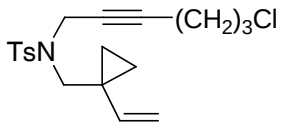

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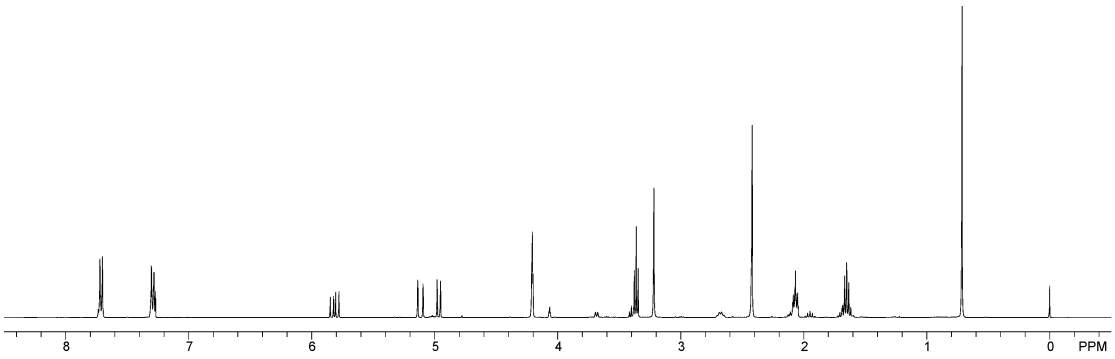

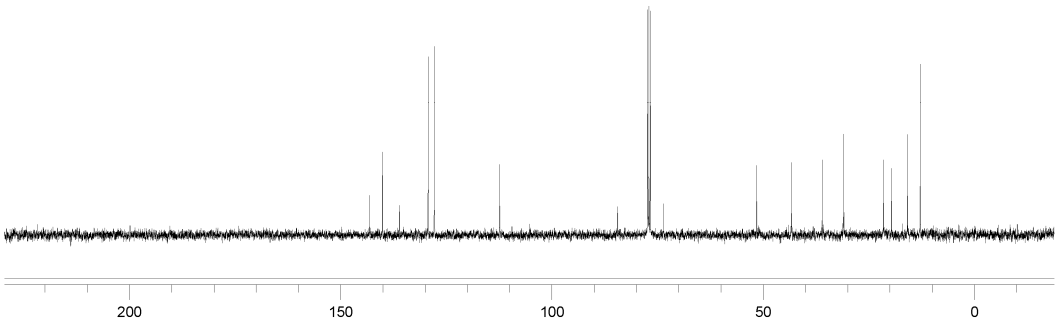

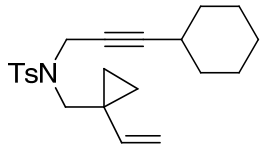

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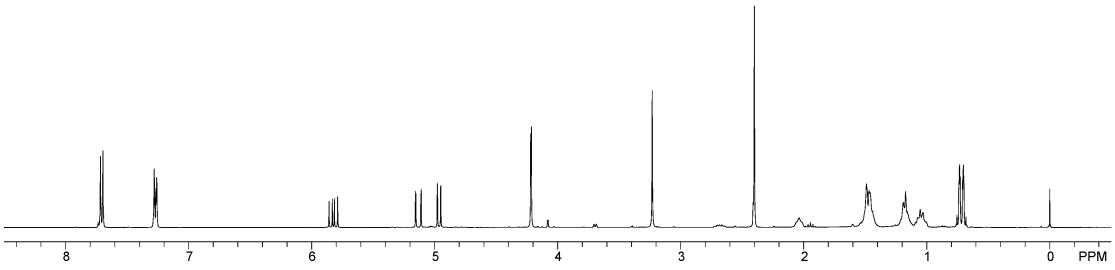

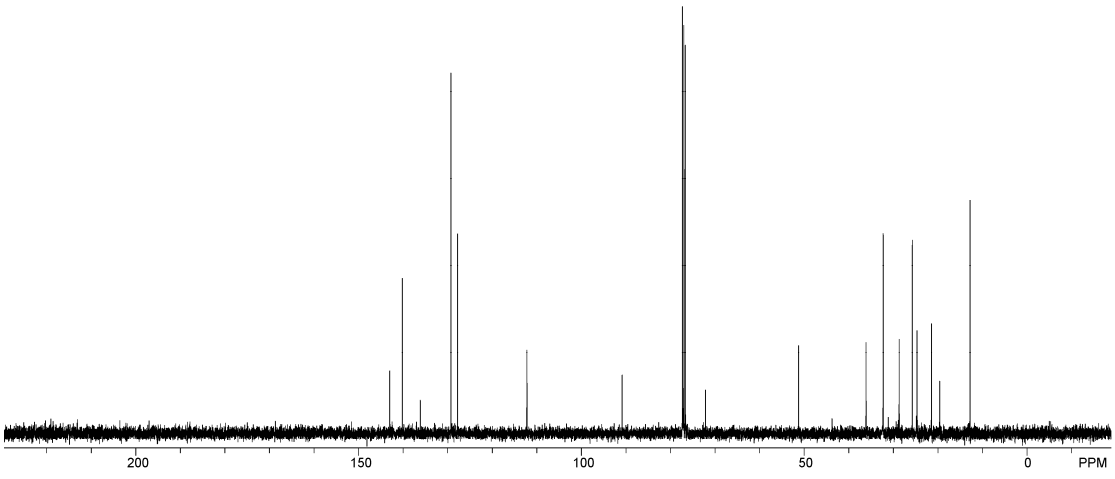

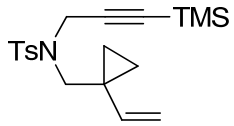

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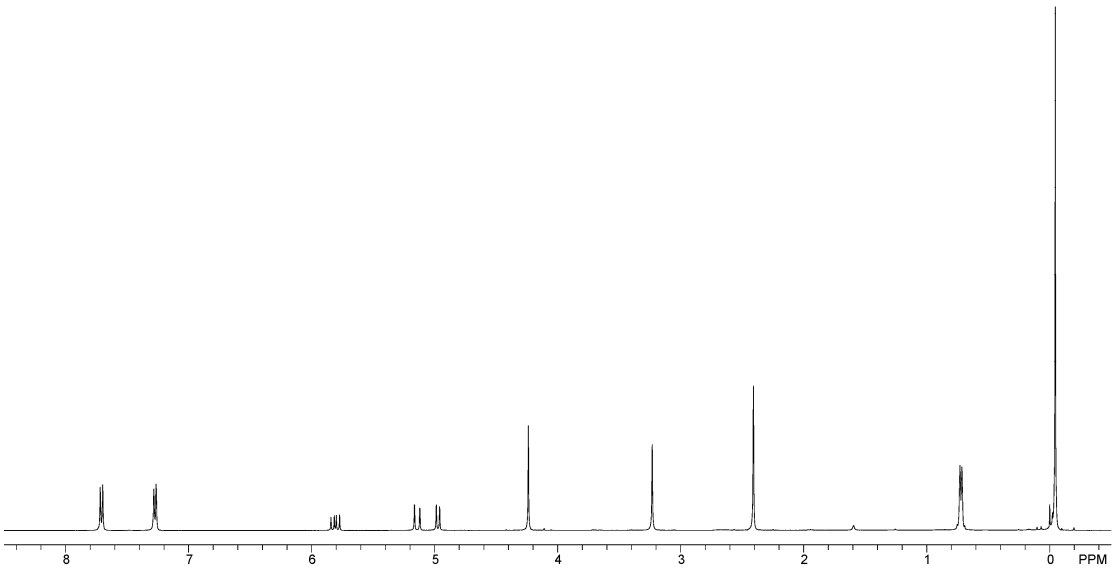
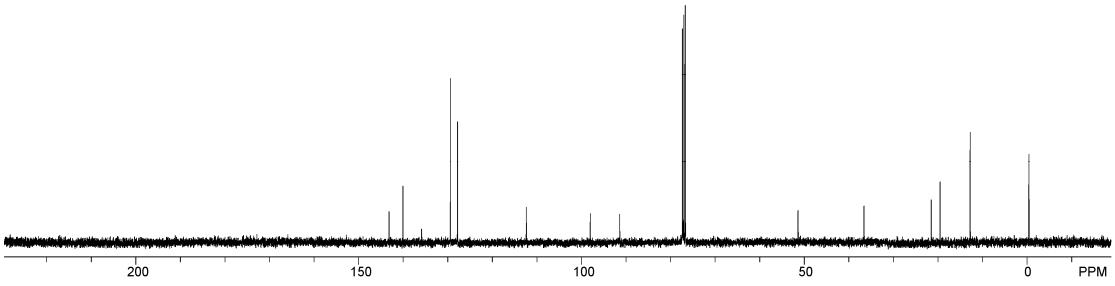
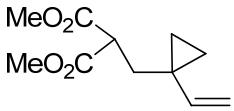
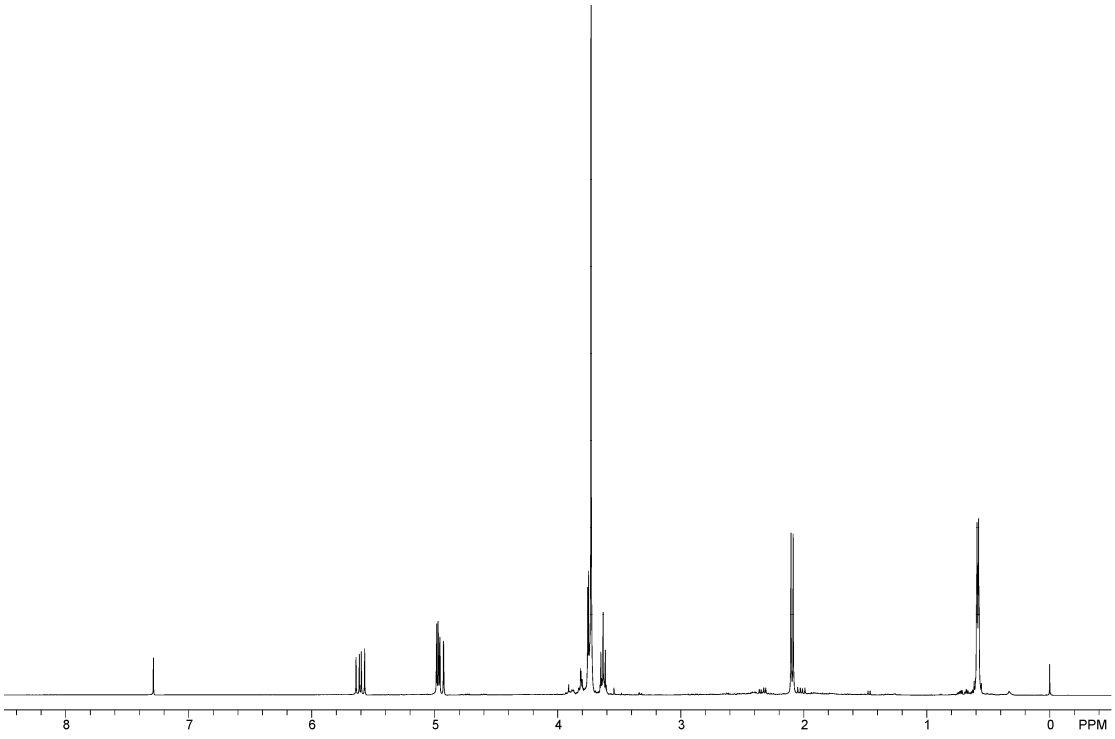
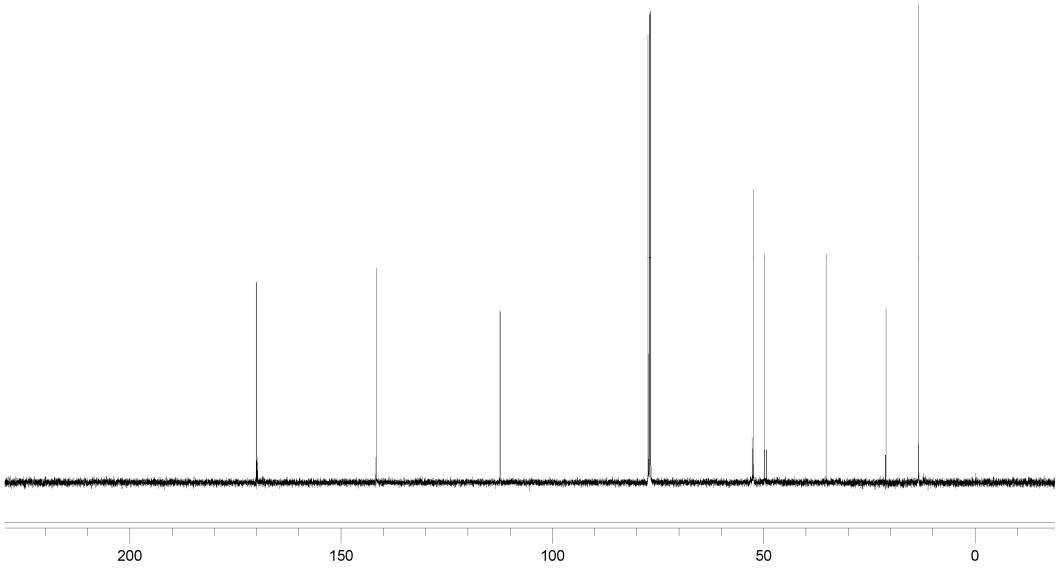


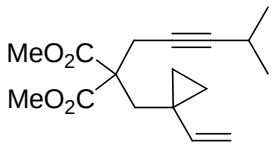




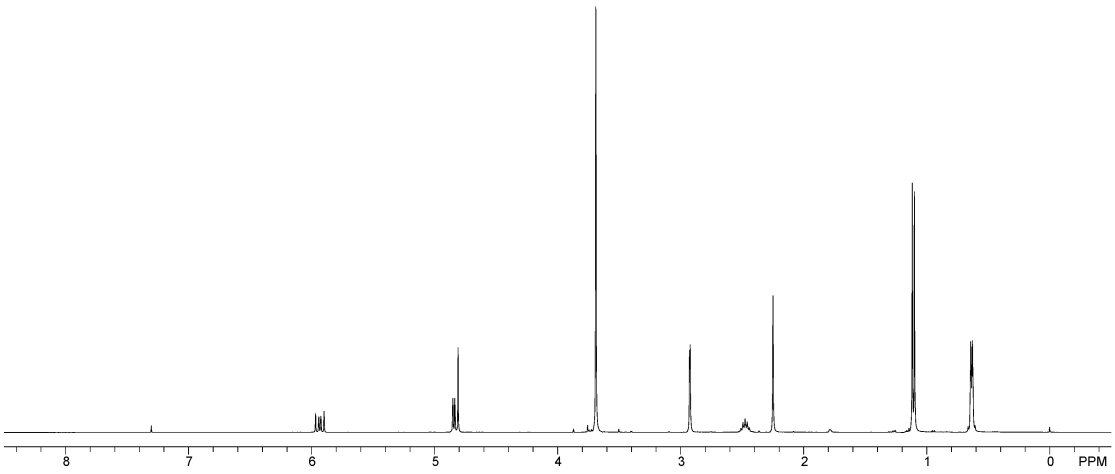
S9

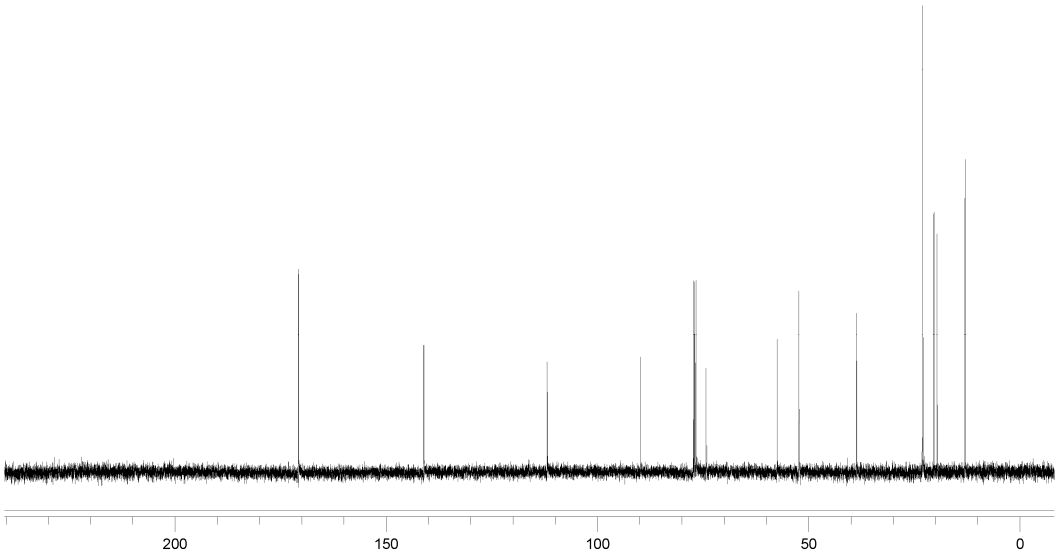


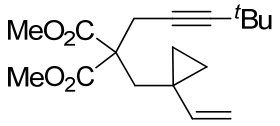




1i







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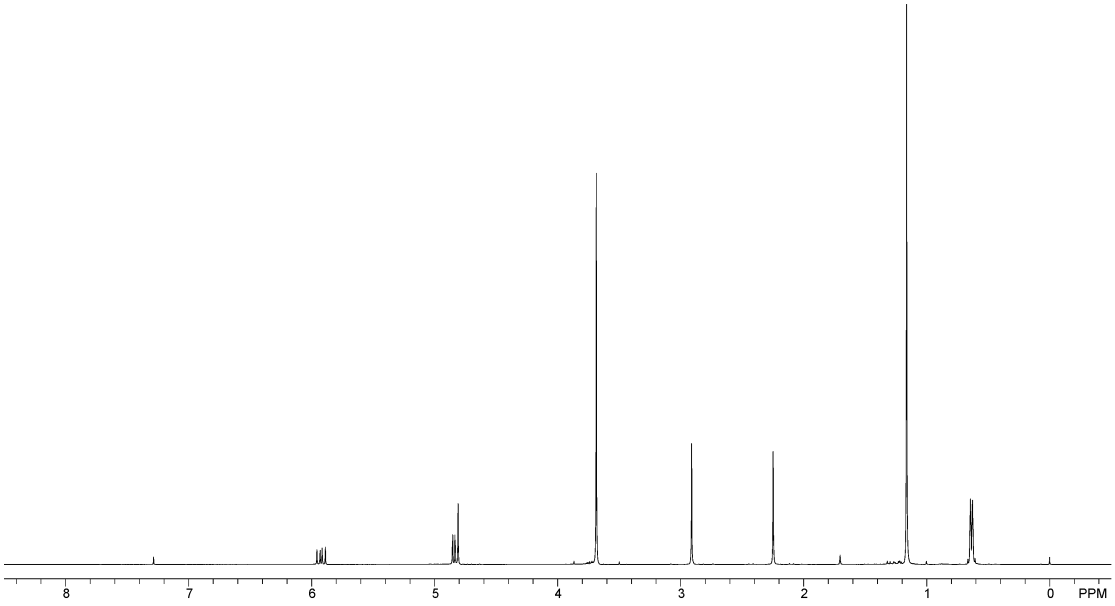

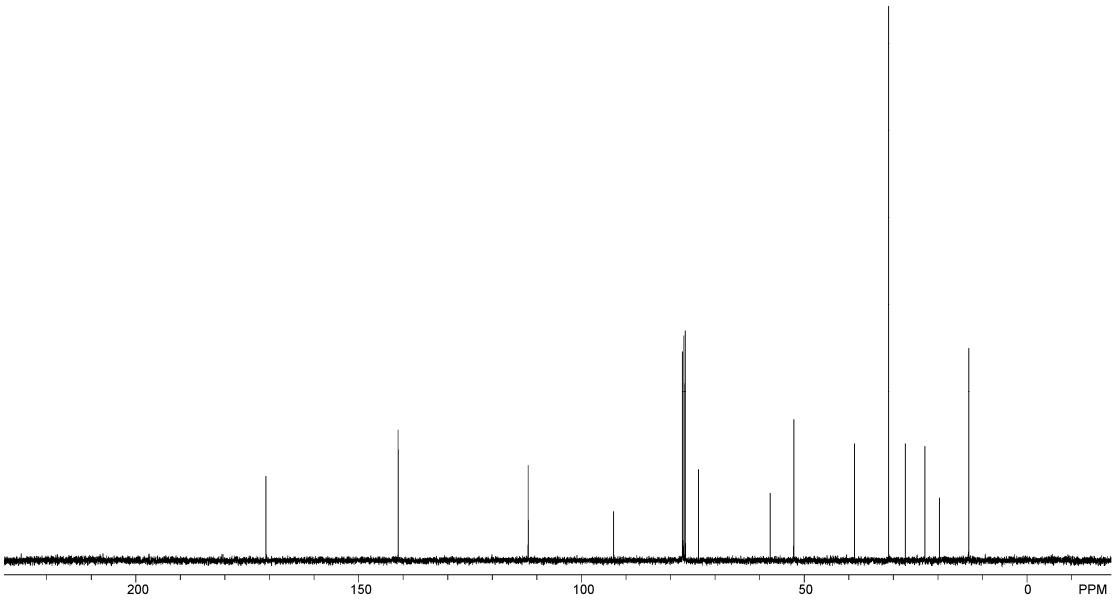

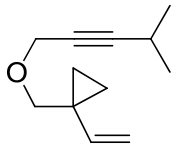

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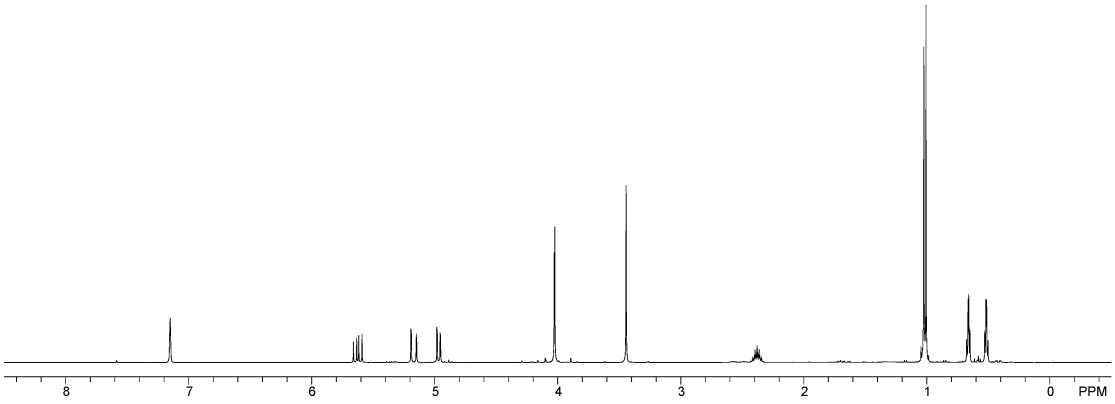

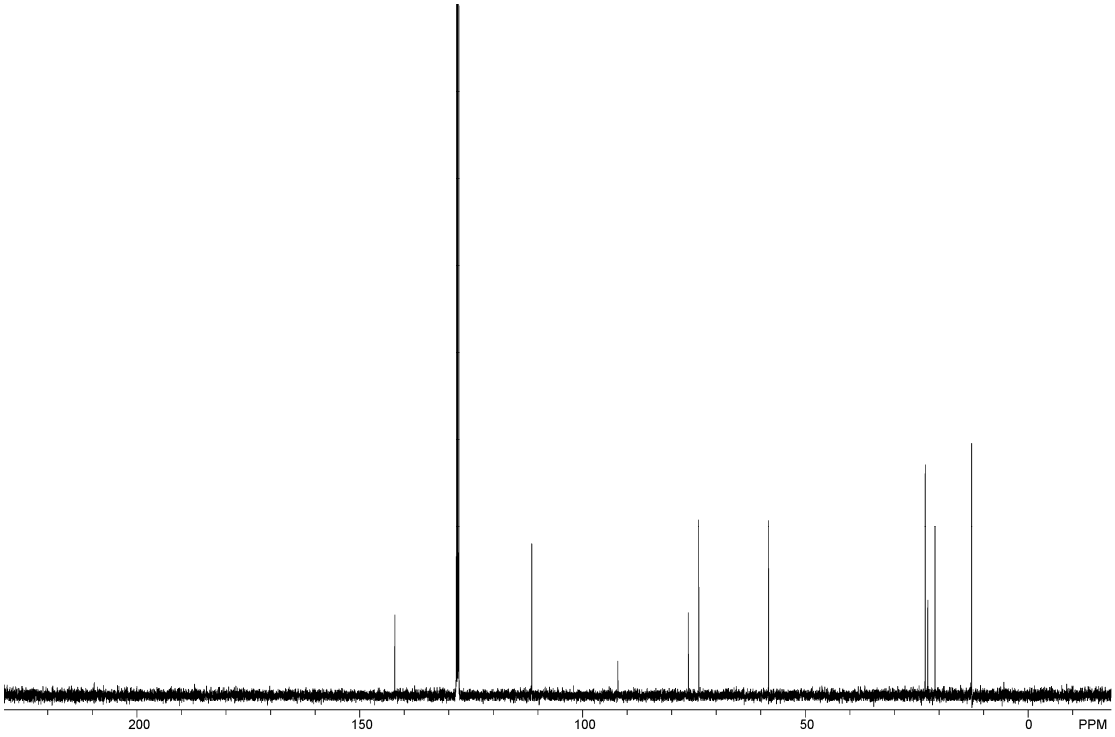

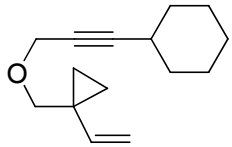

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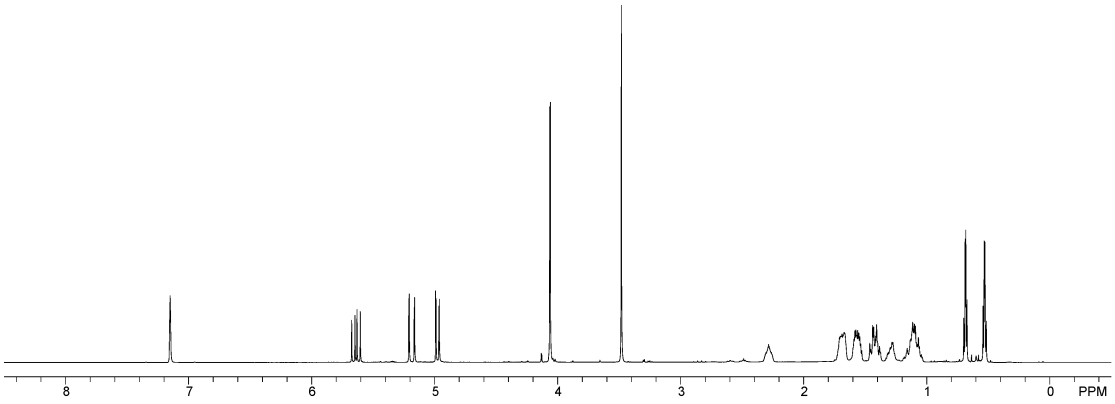

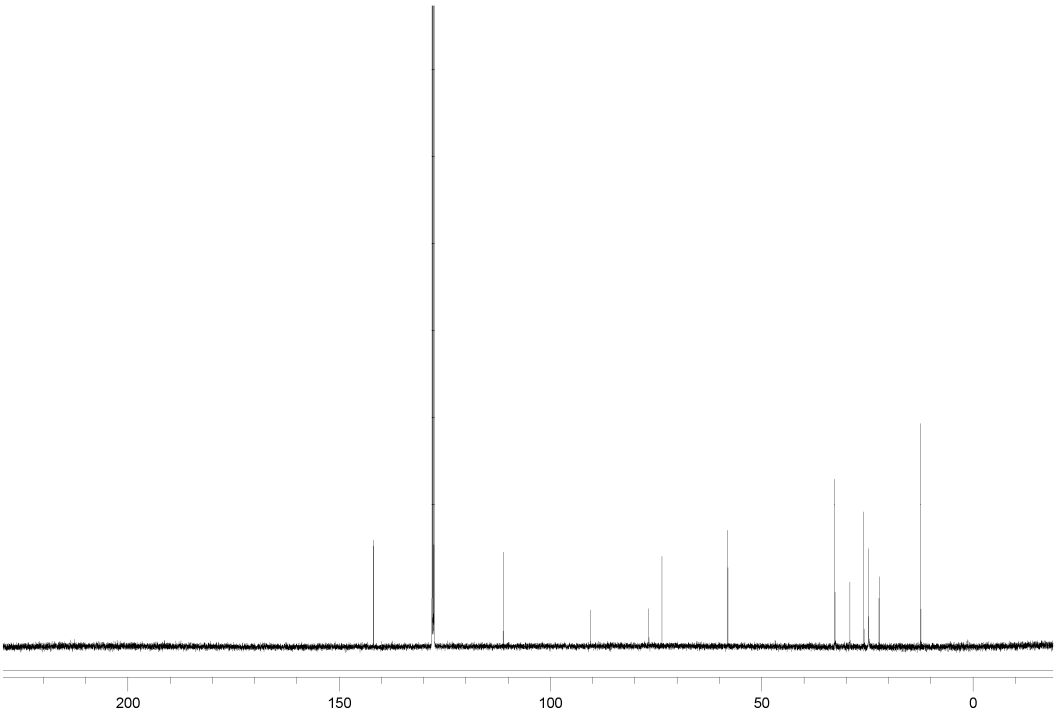

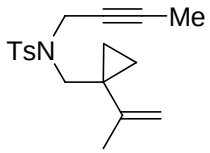

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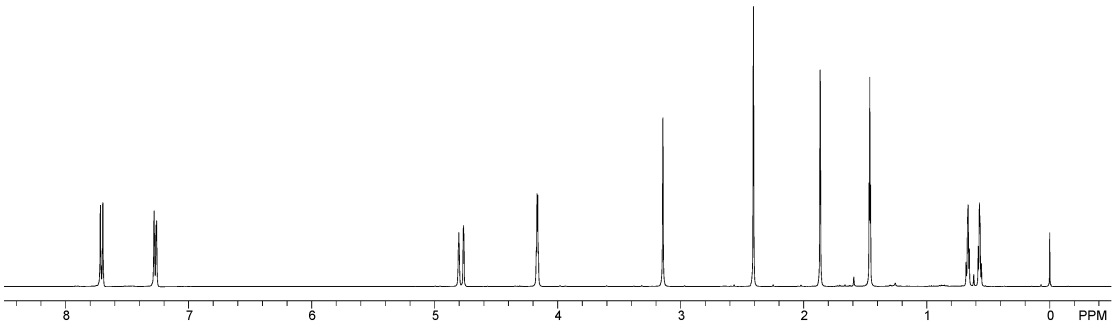

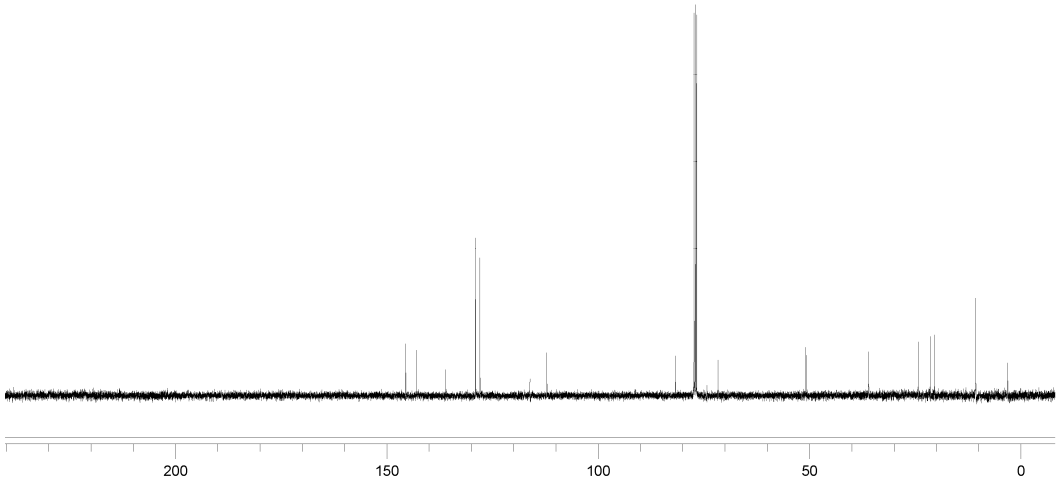

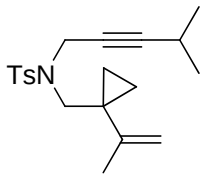

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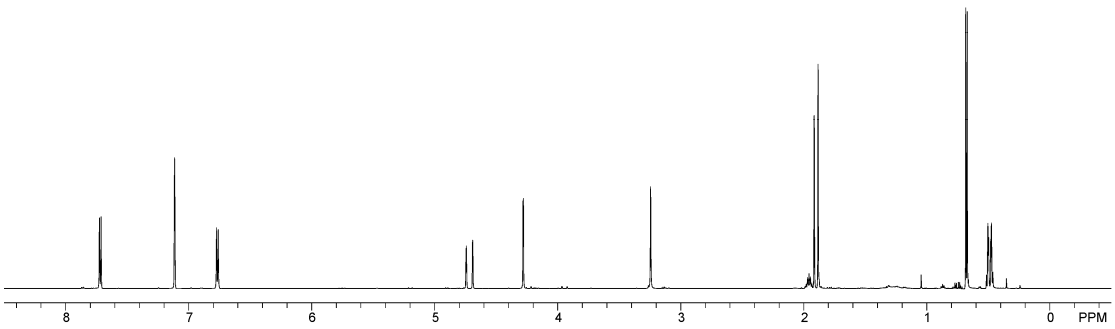

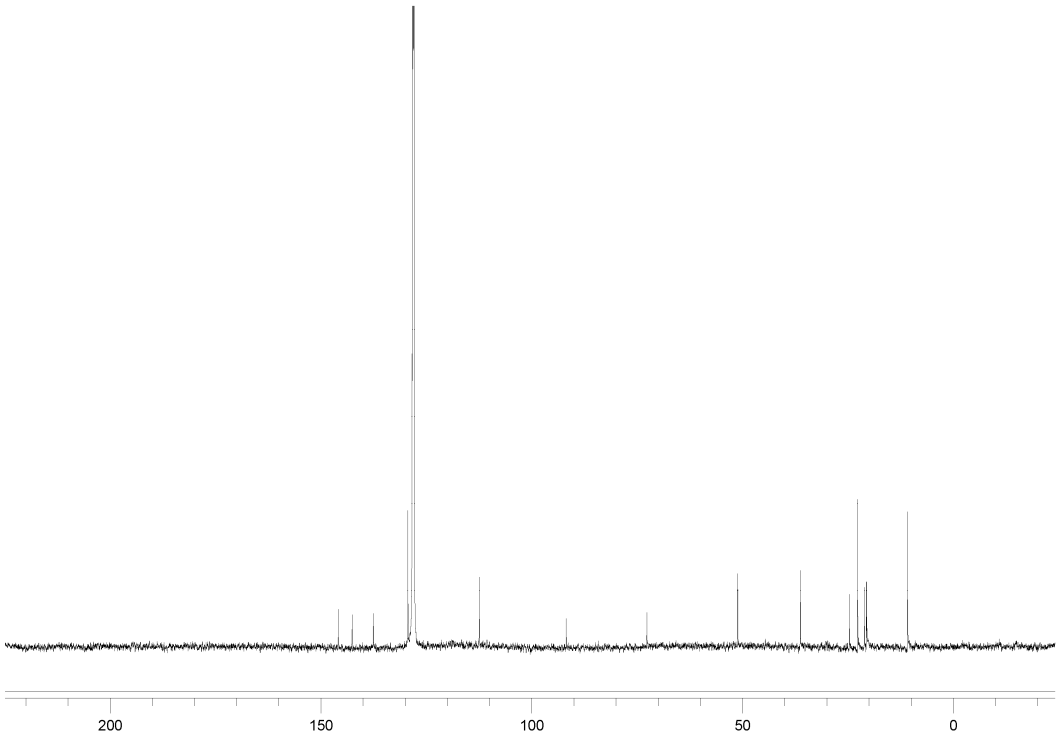

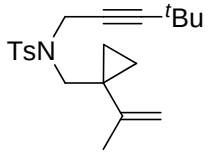

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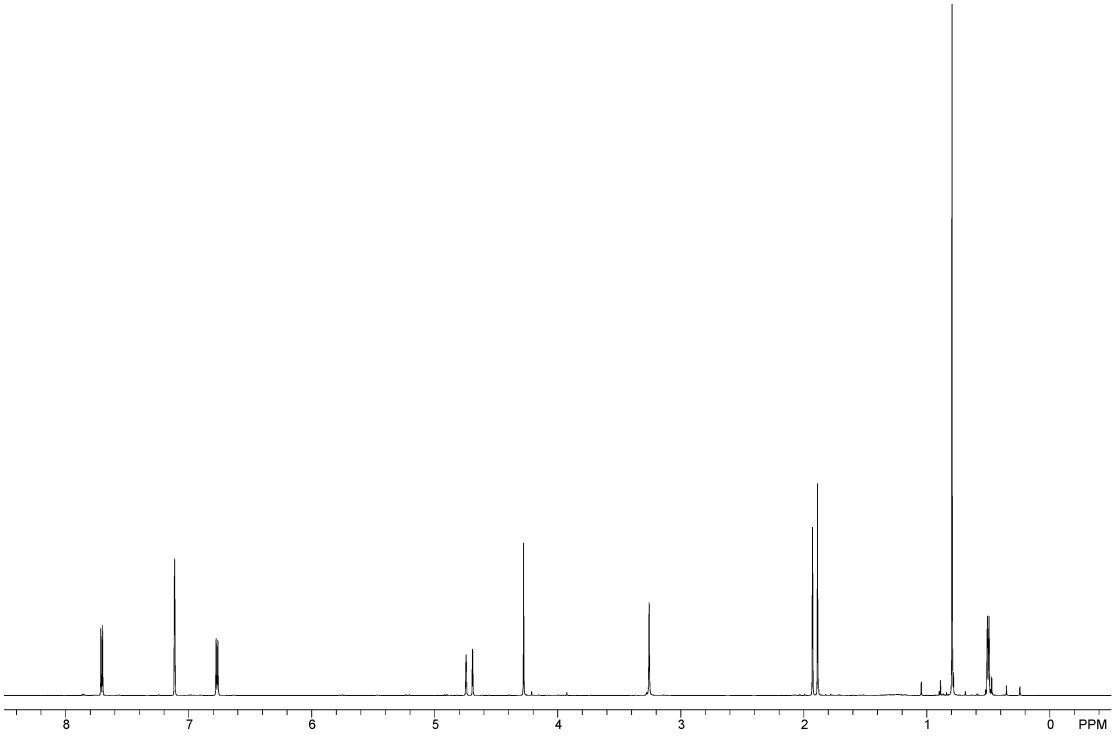

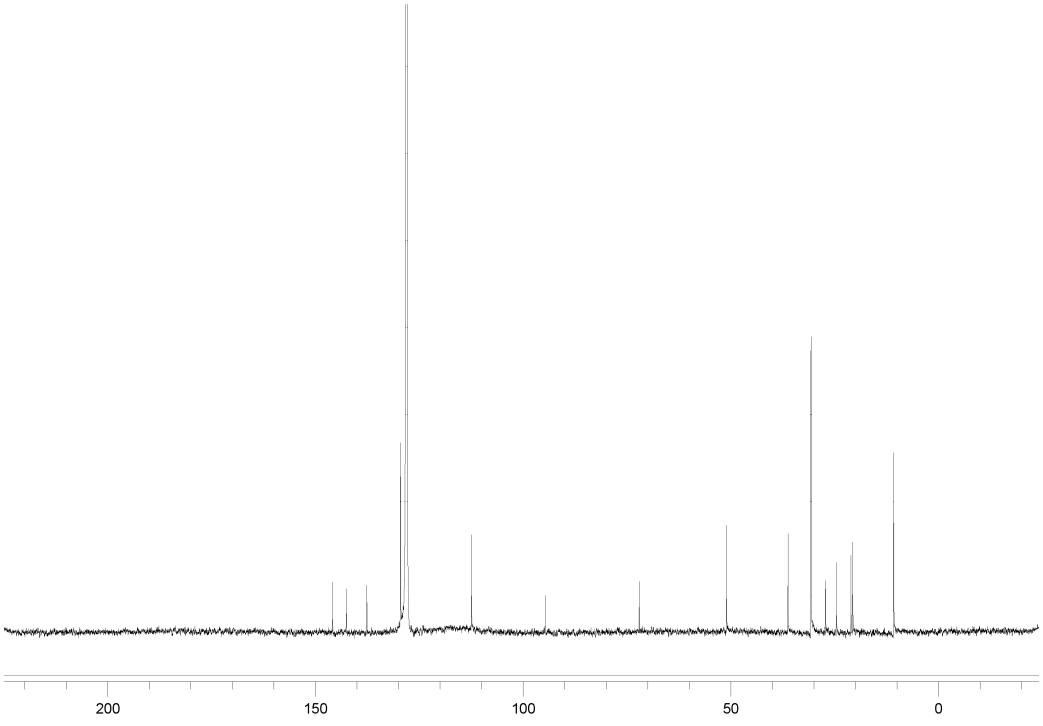

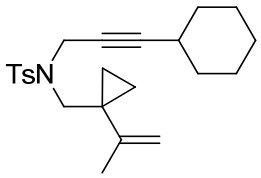

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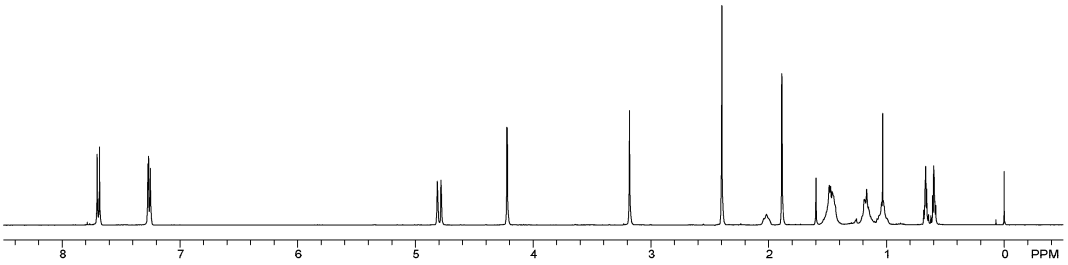

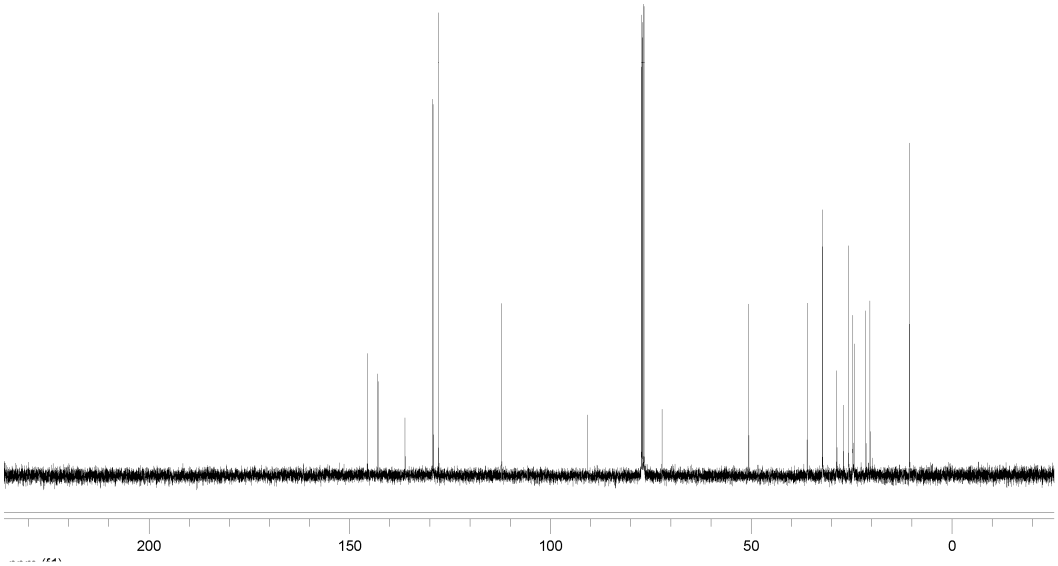

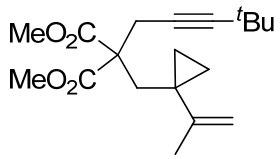

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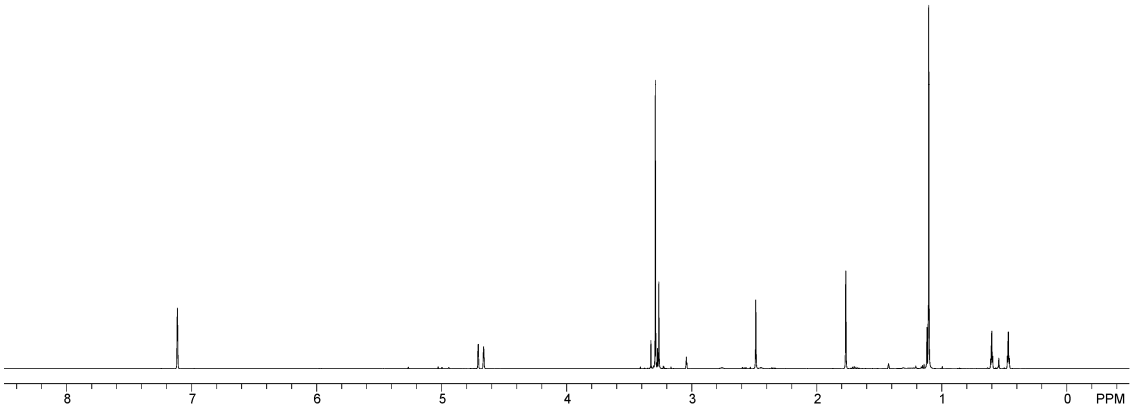

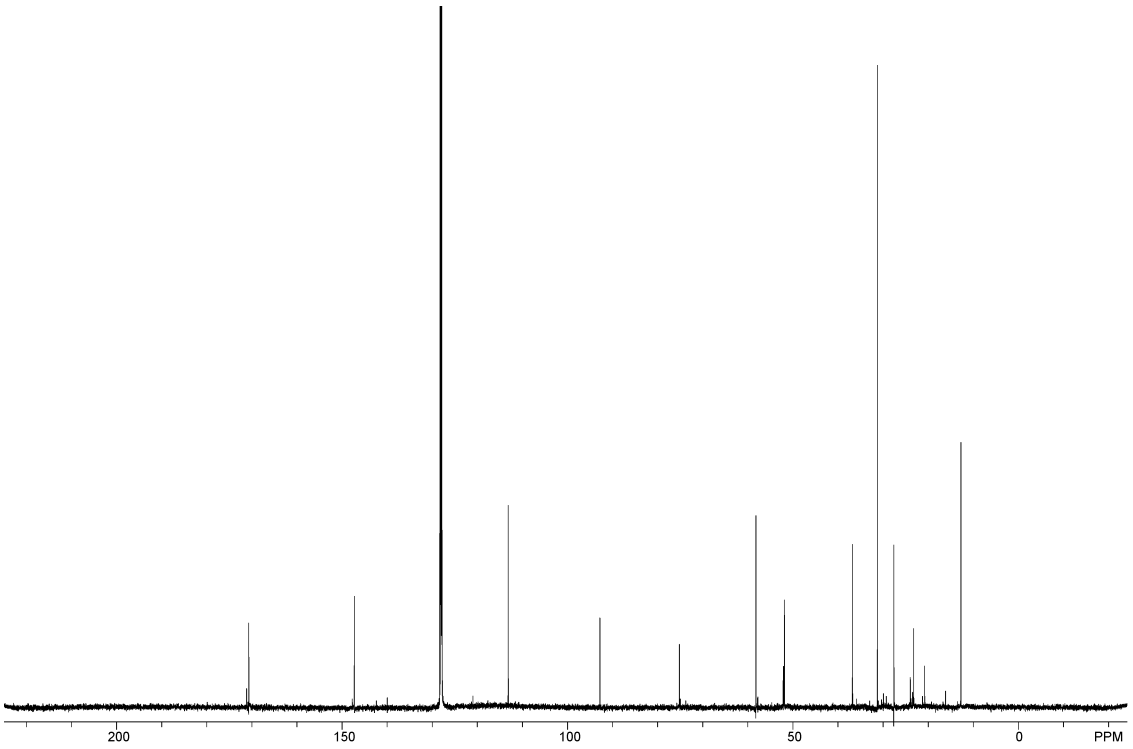

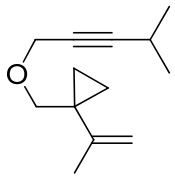

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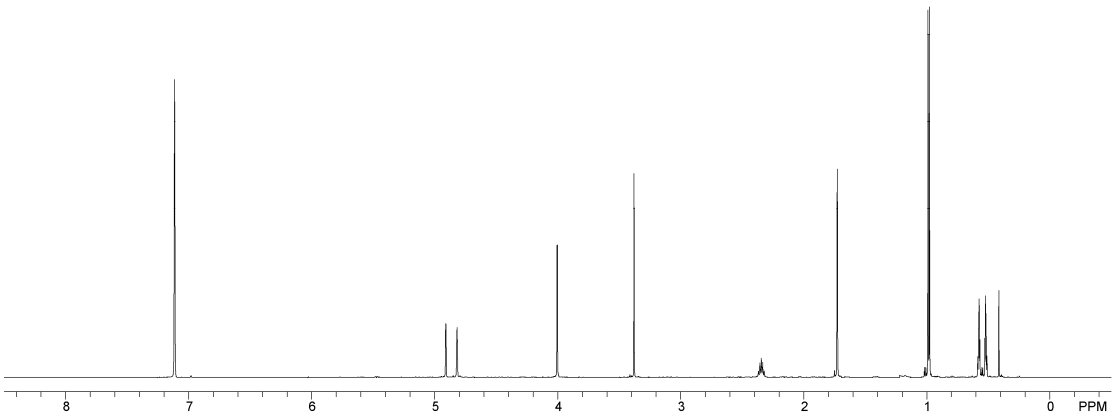

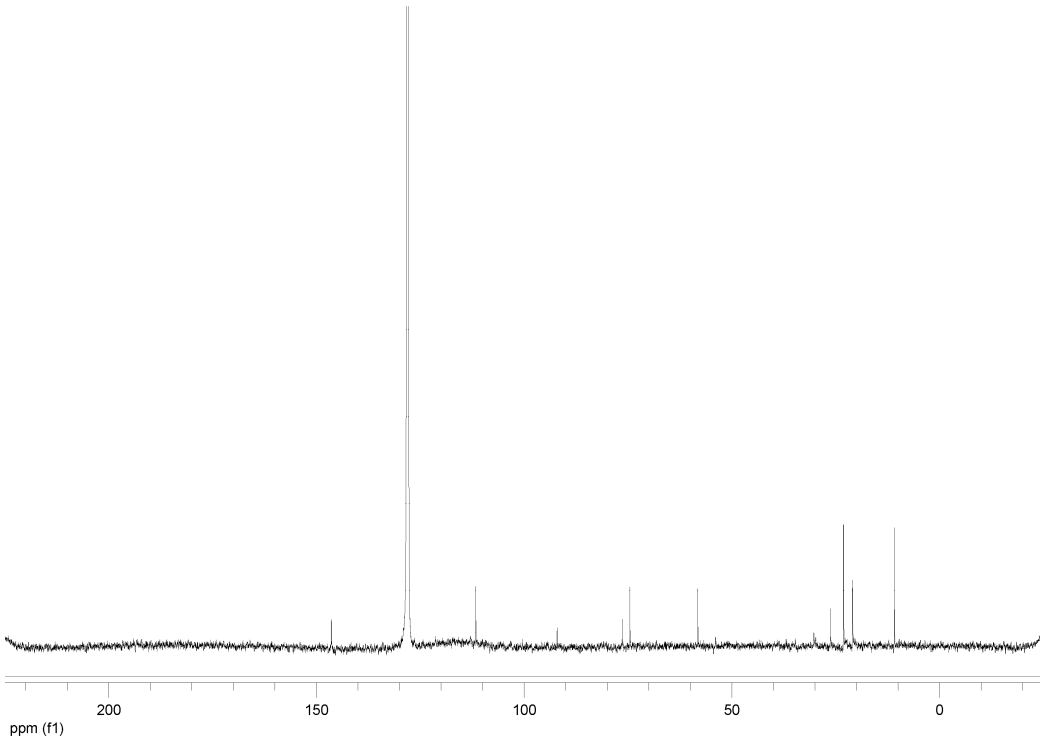

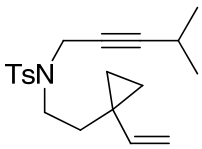

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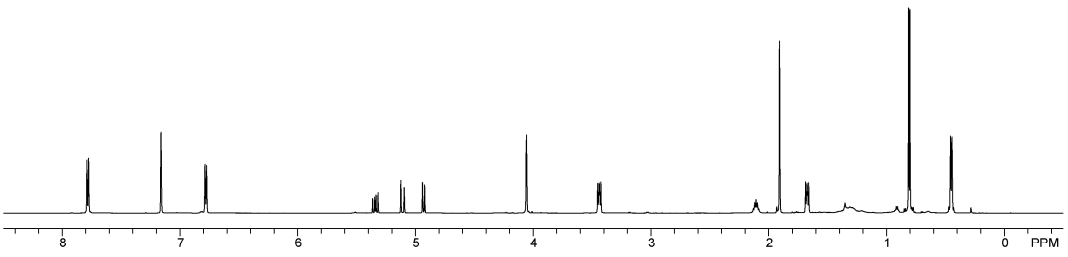

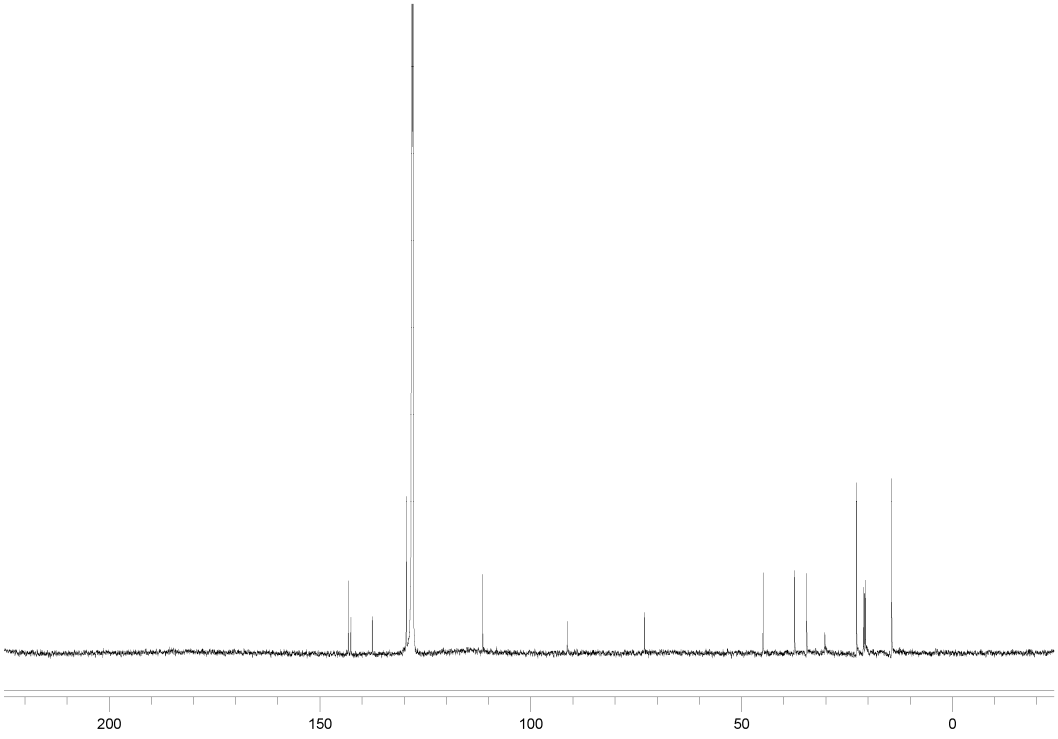

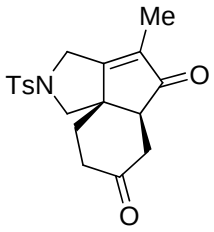
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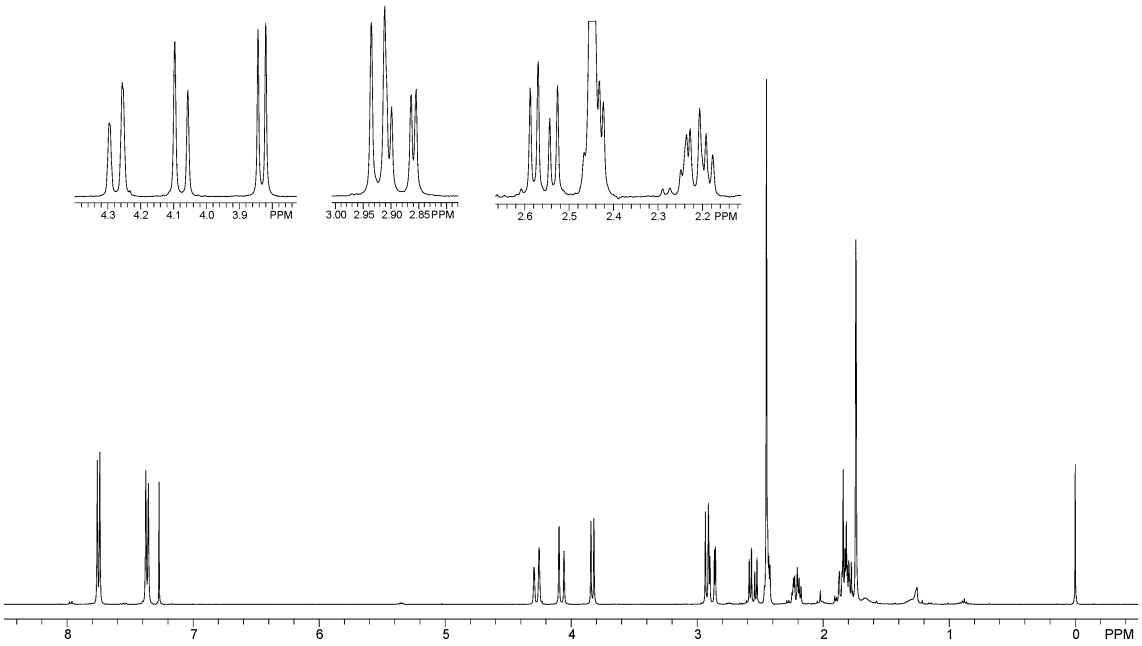
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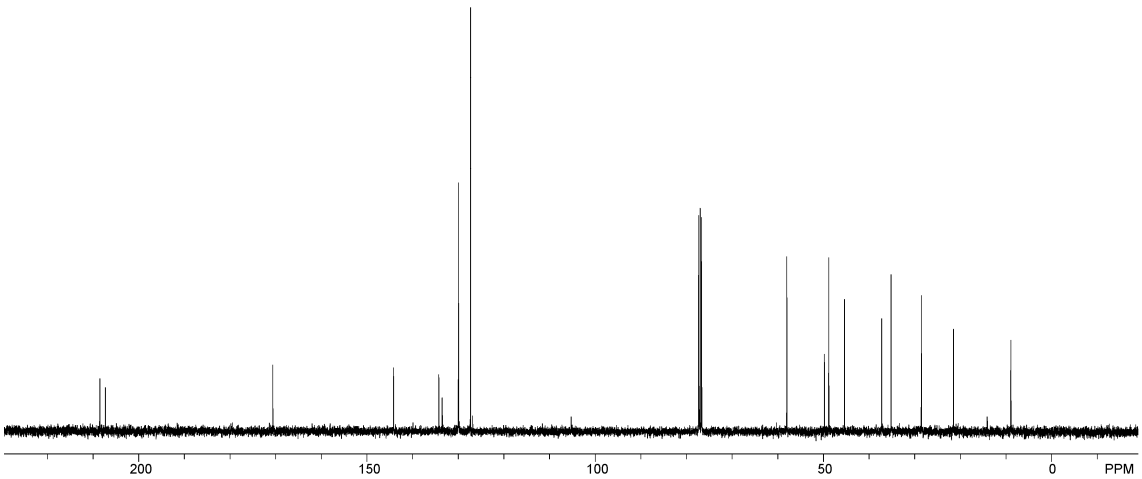
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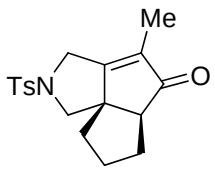

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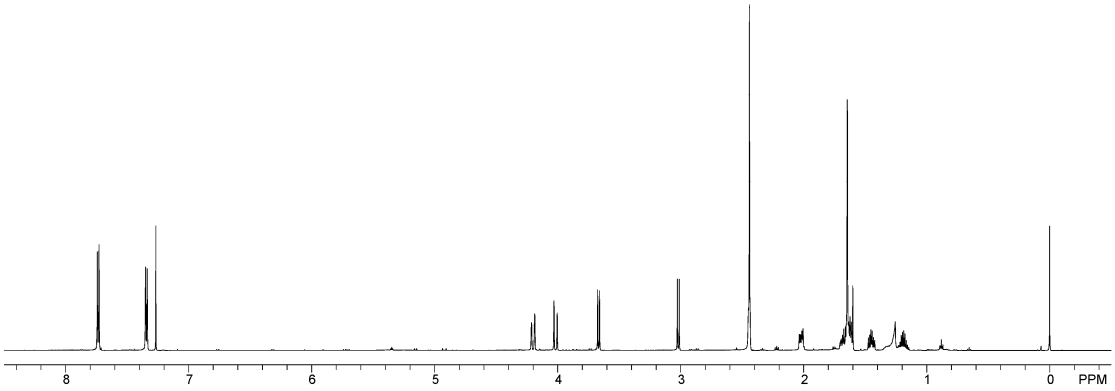

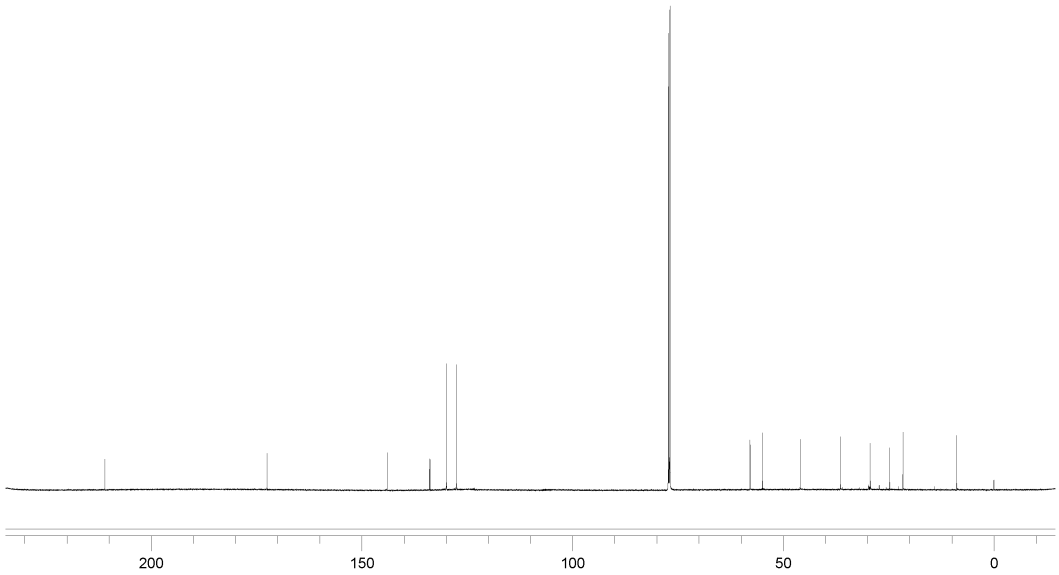

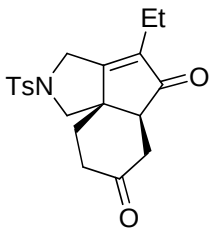

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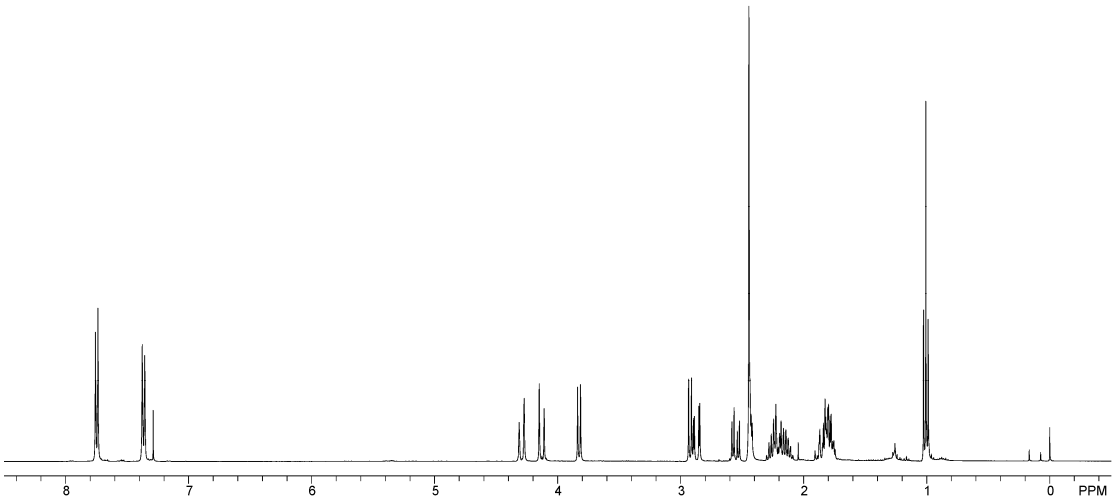

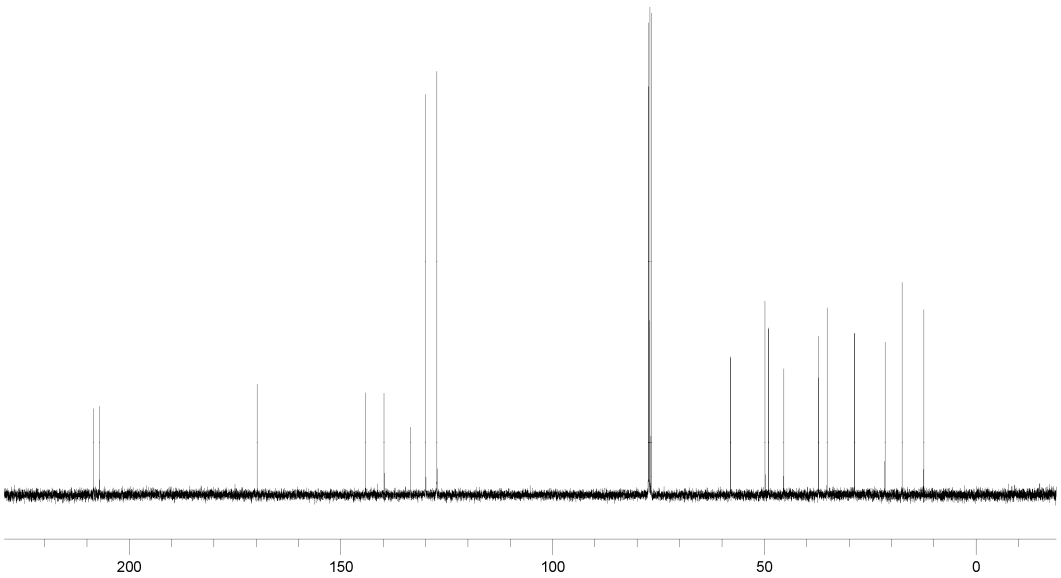

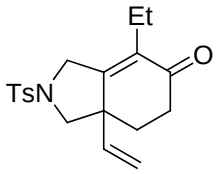

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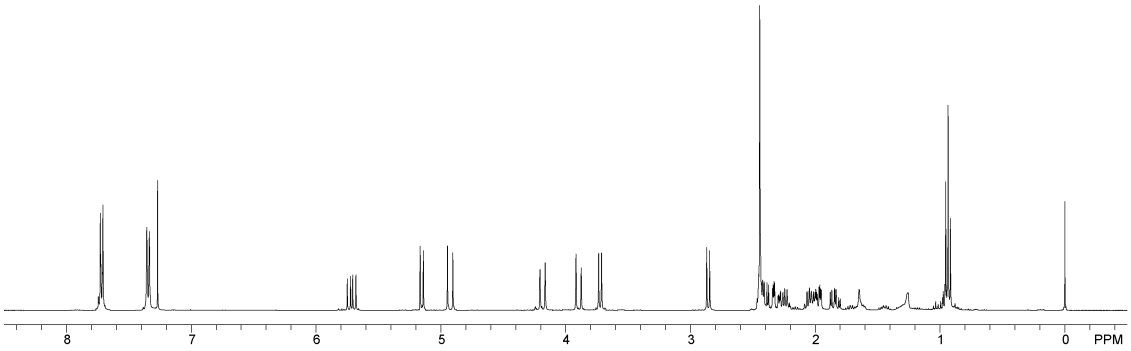

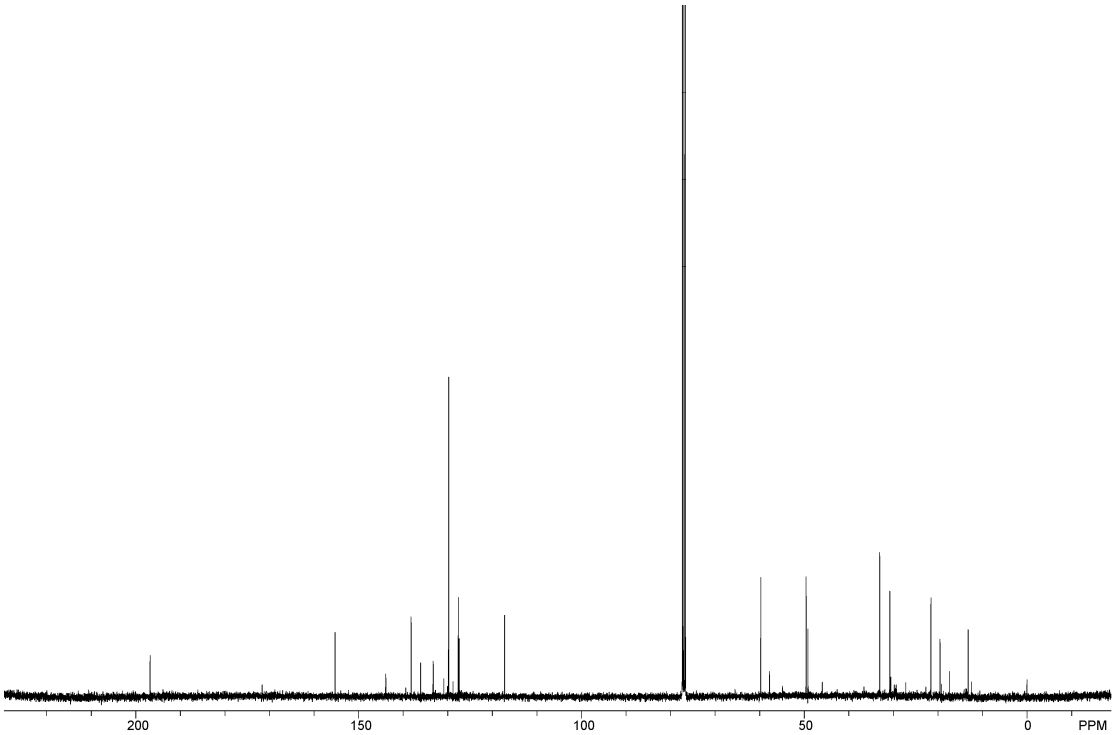

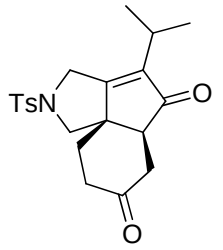

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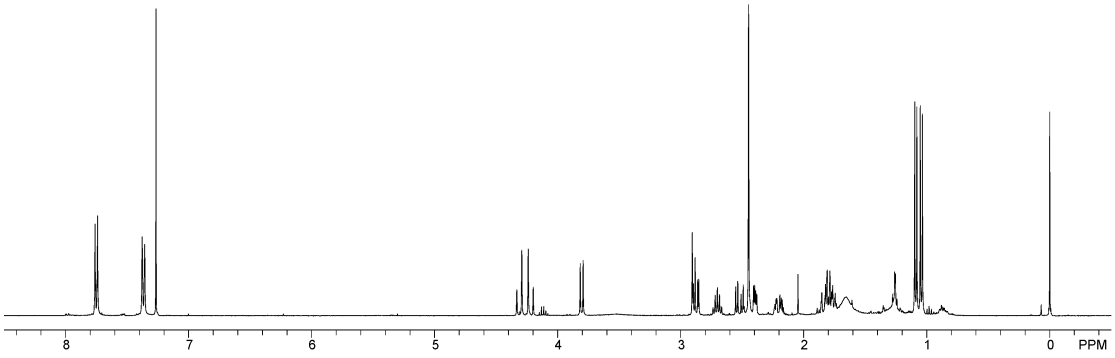

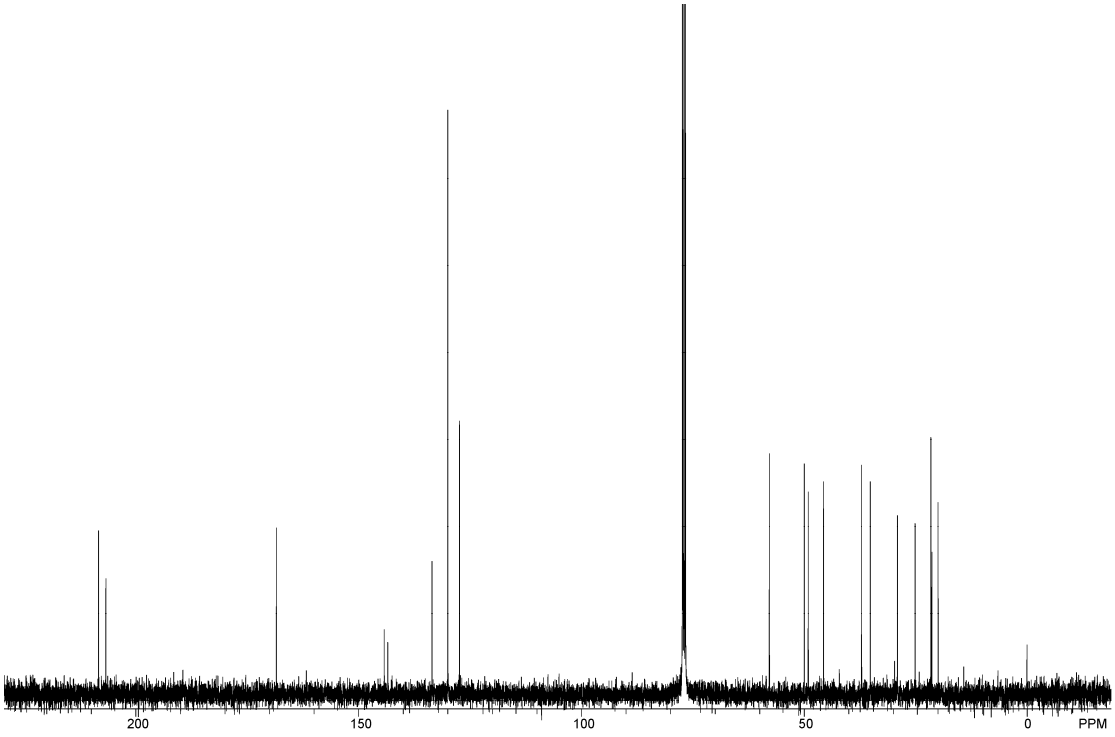

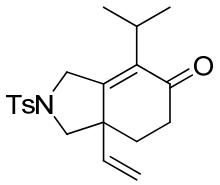

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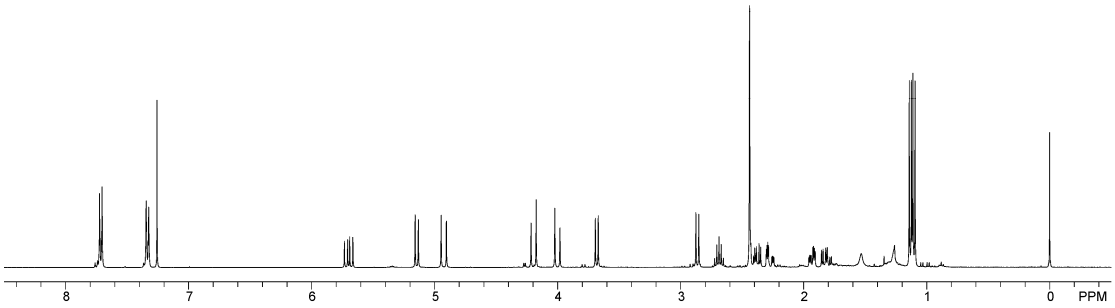

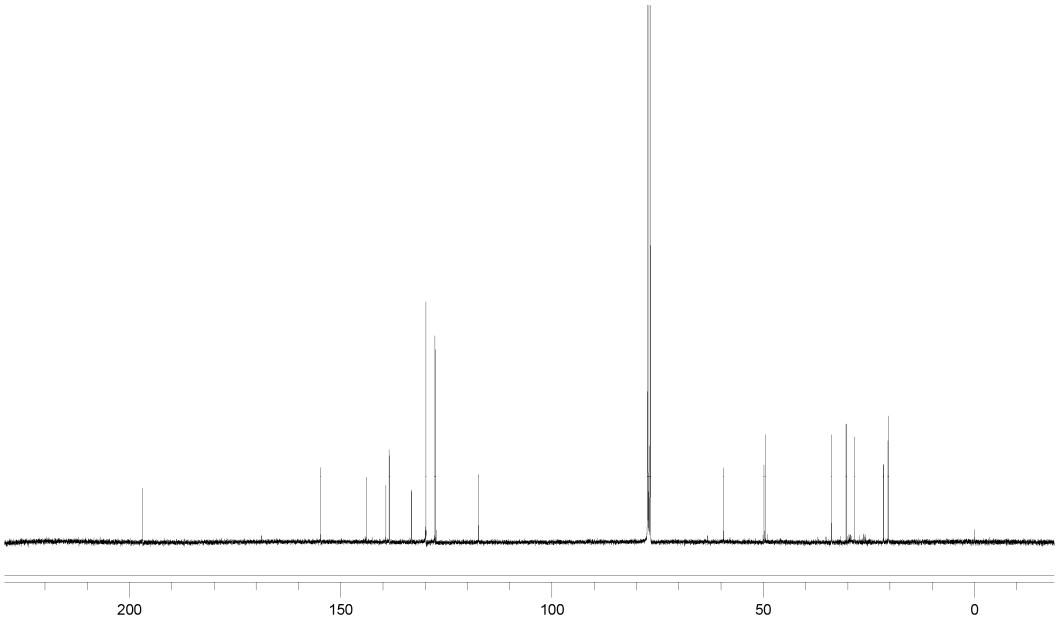

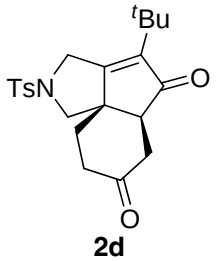

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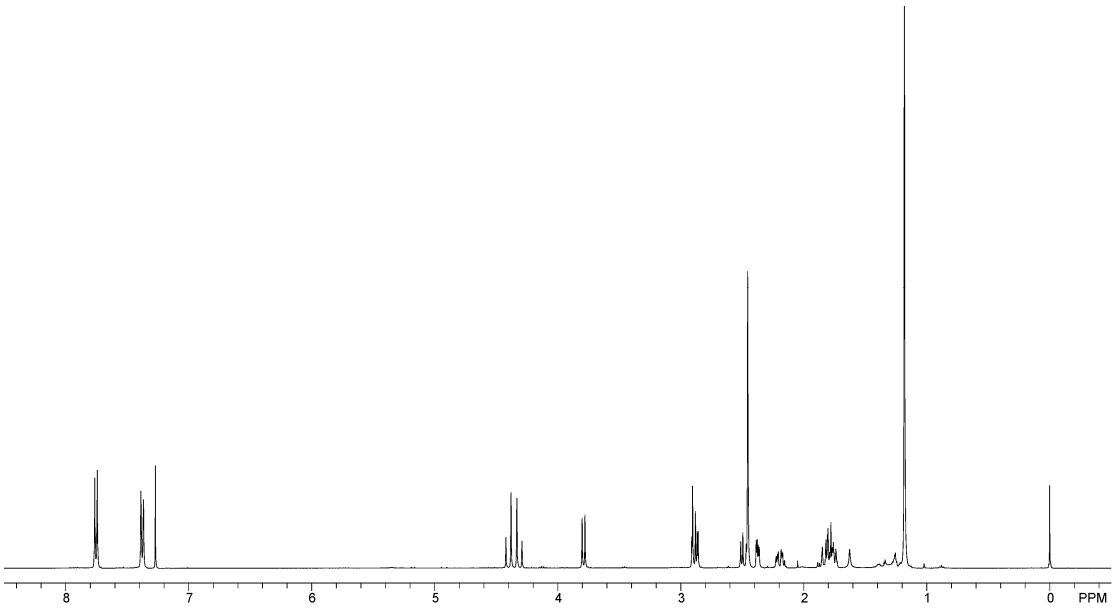

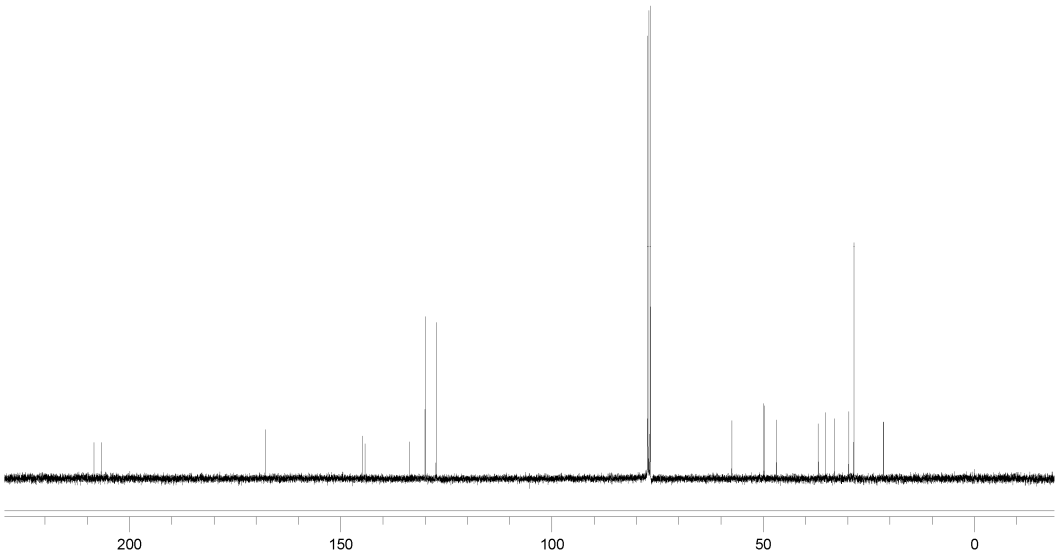

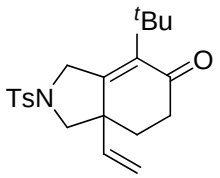

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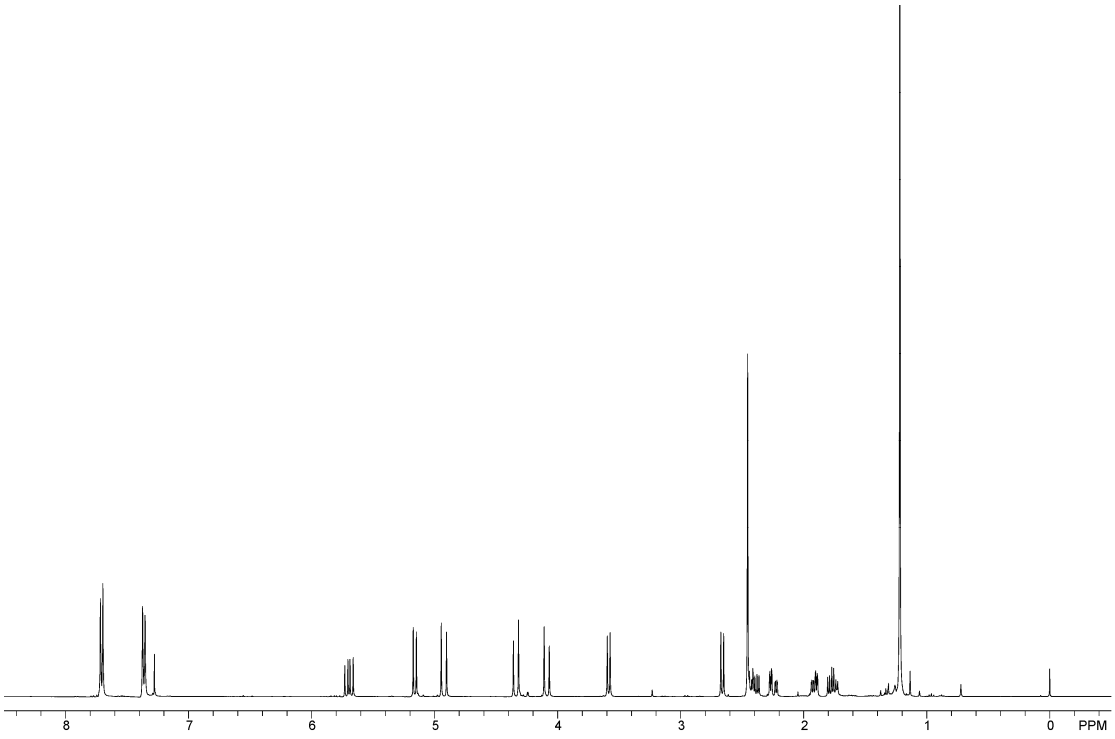

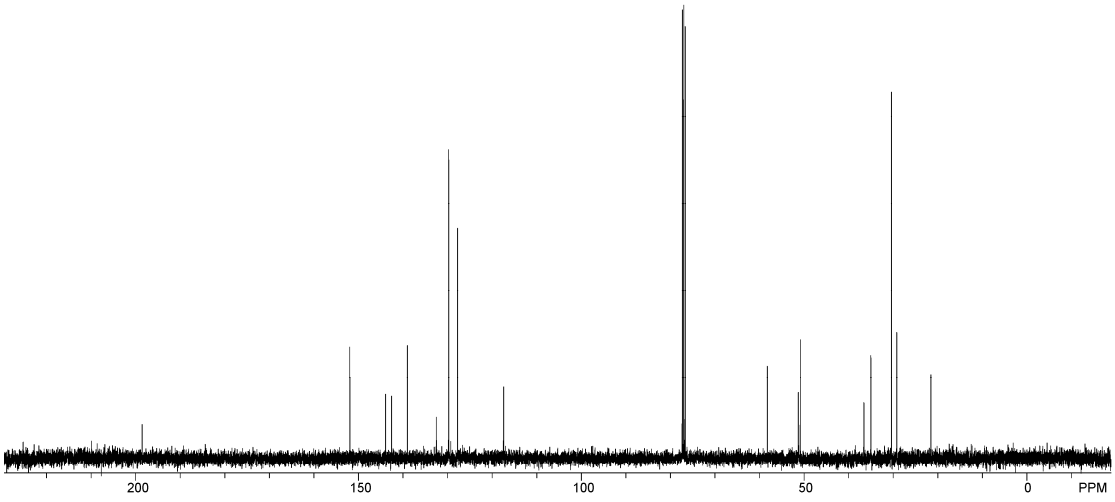

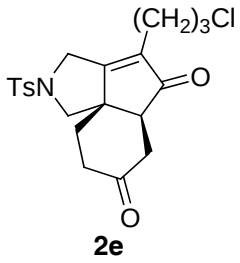

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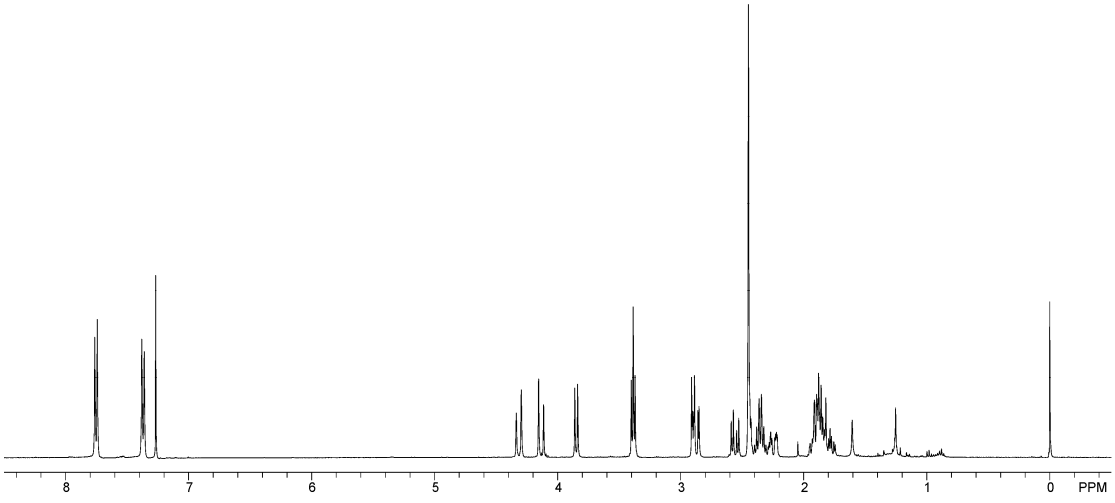

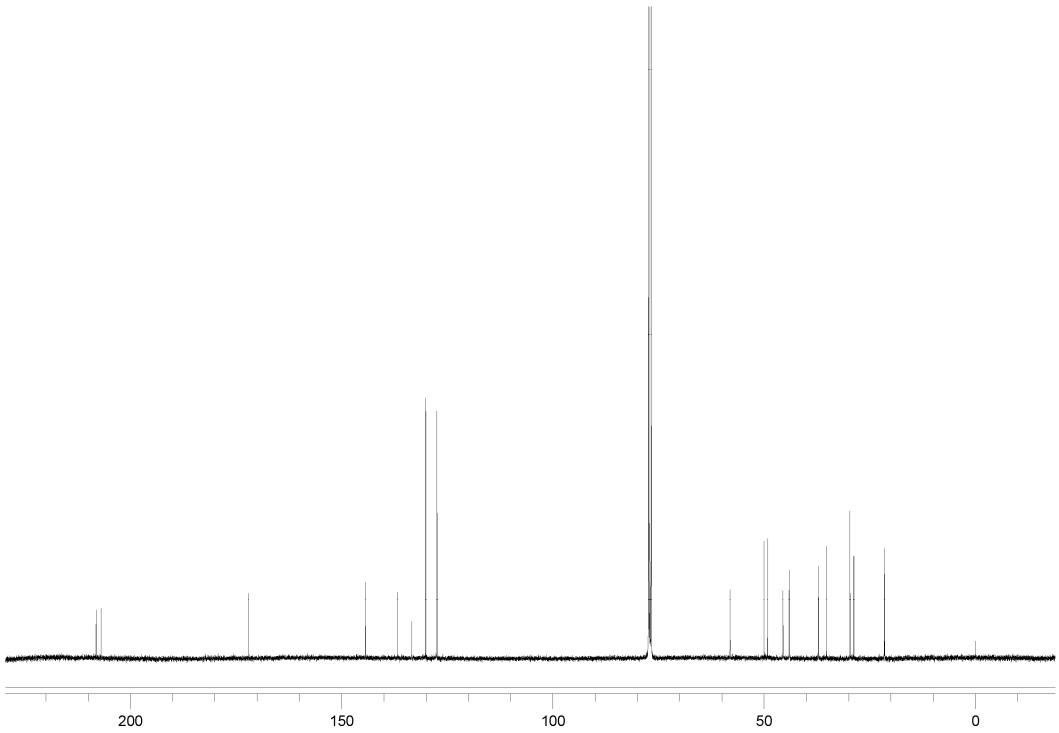

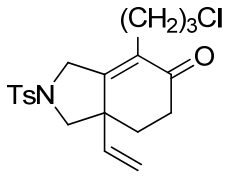

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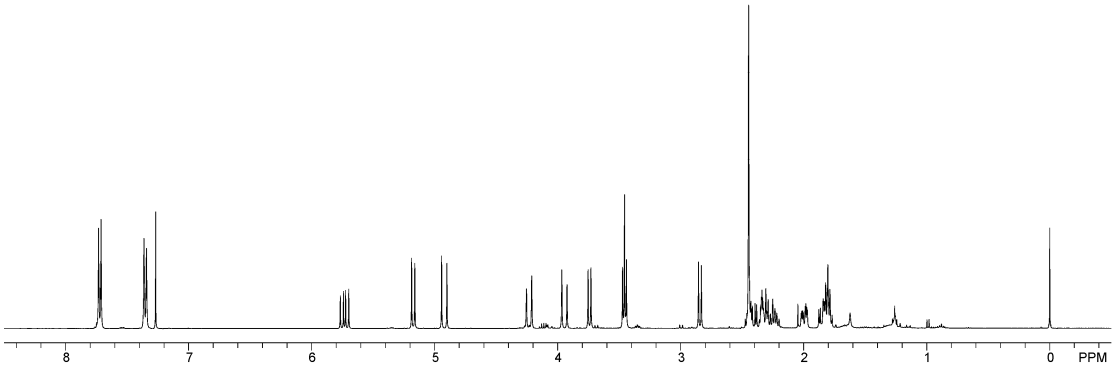

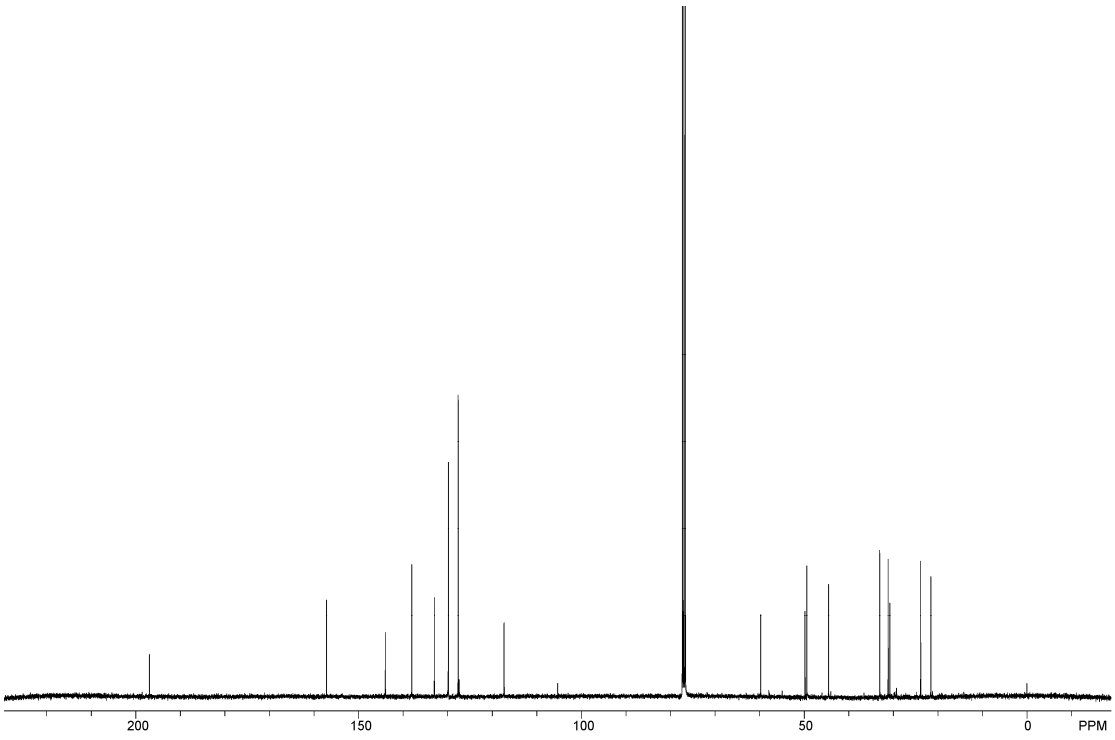

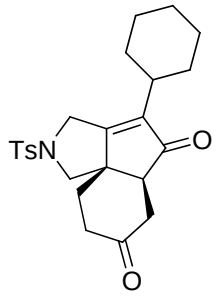

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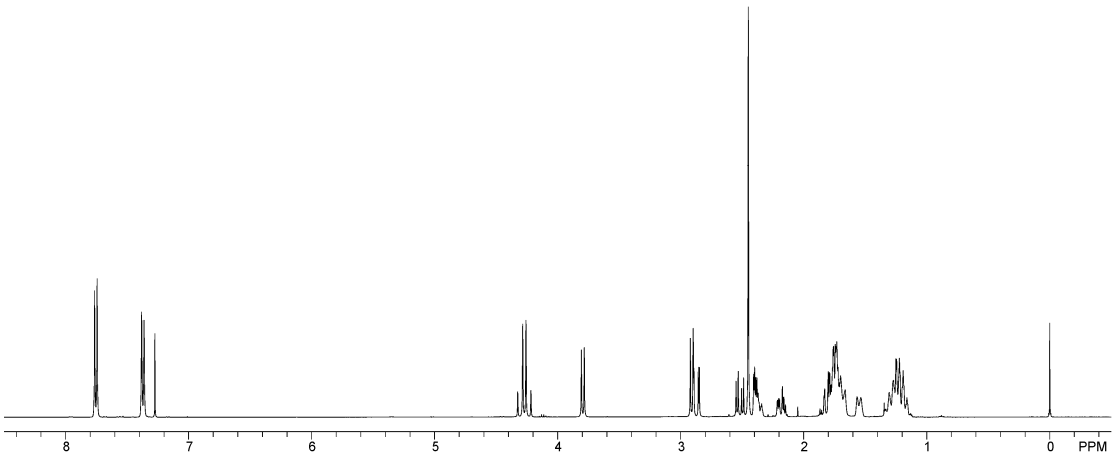

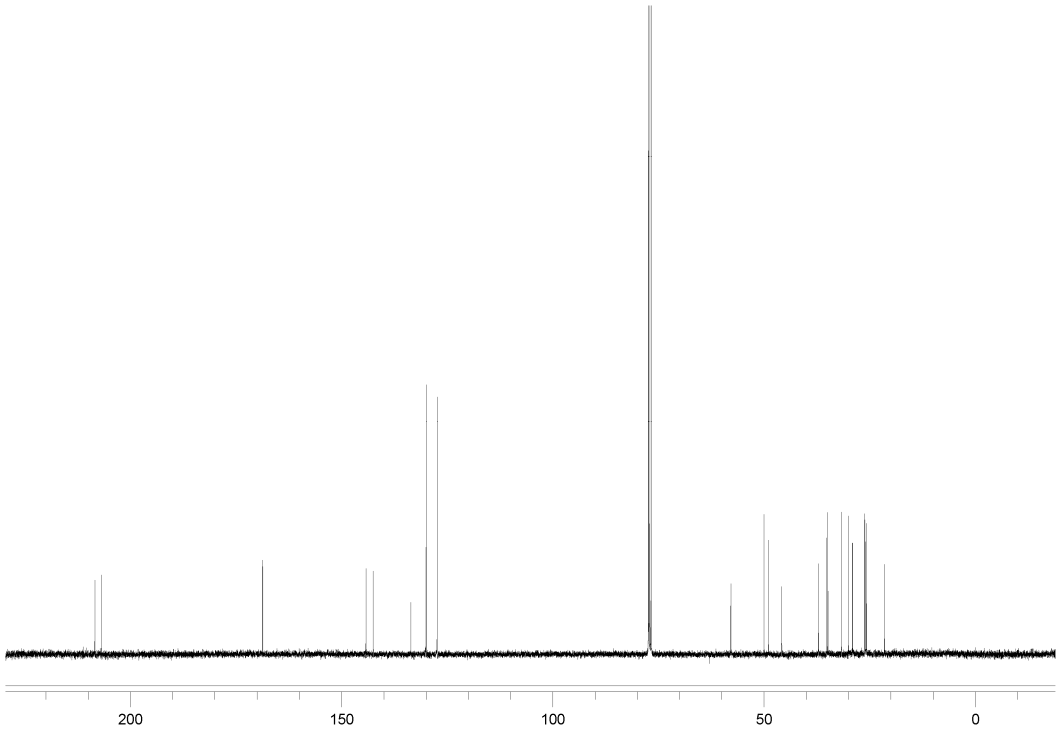

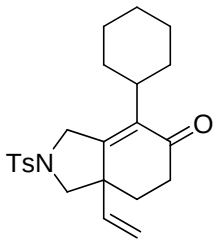

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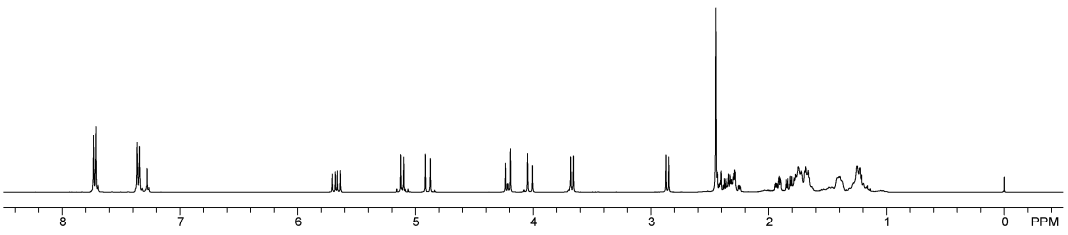

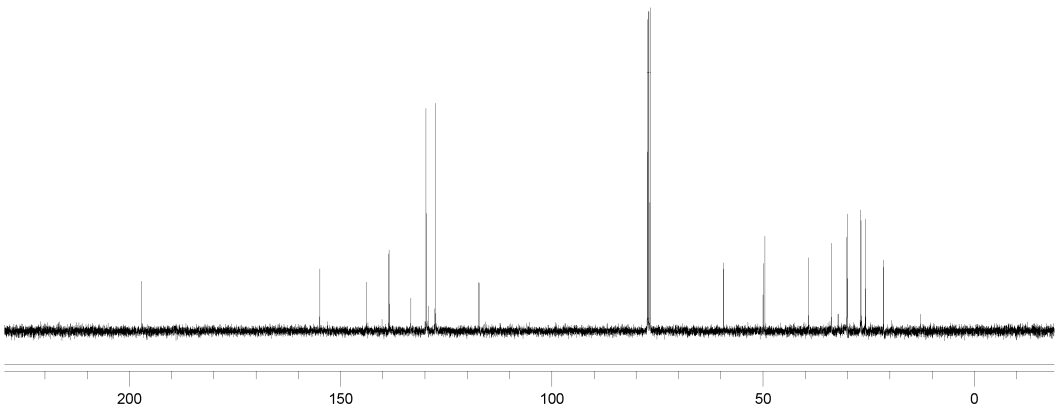

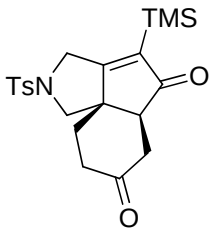

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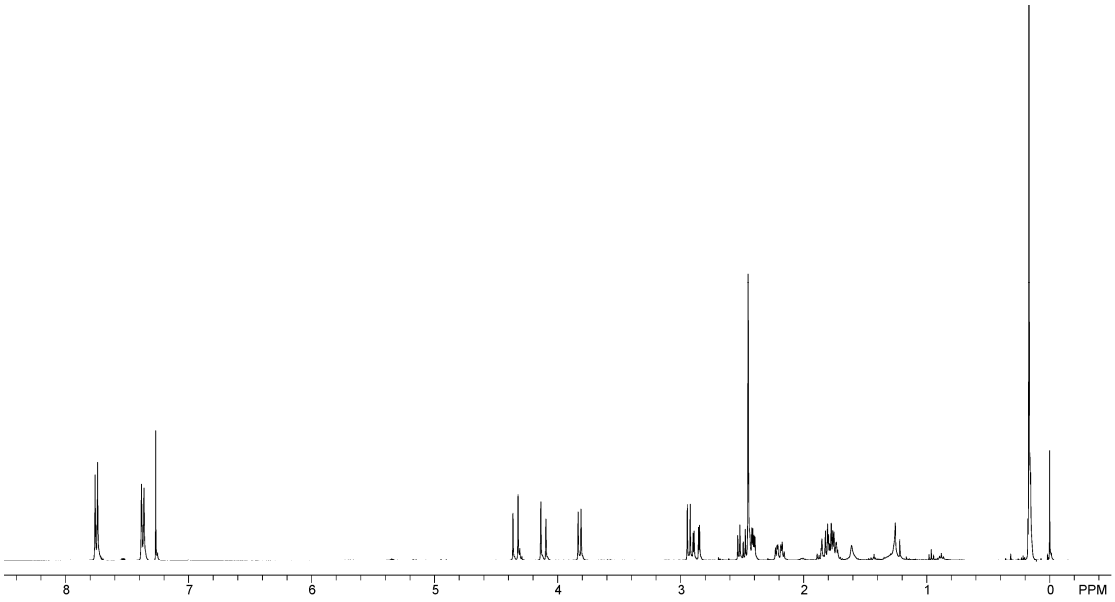

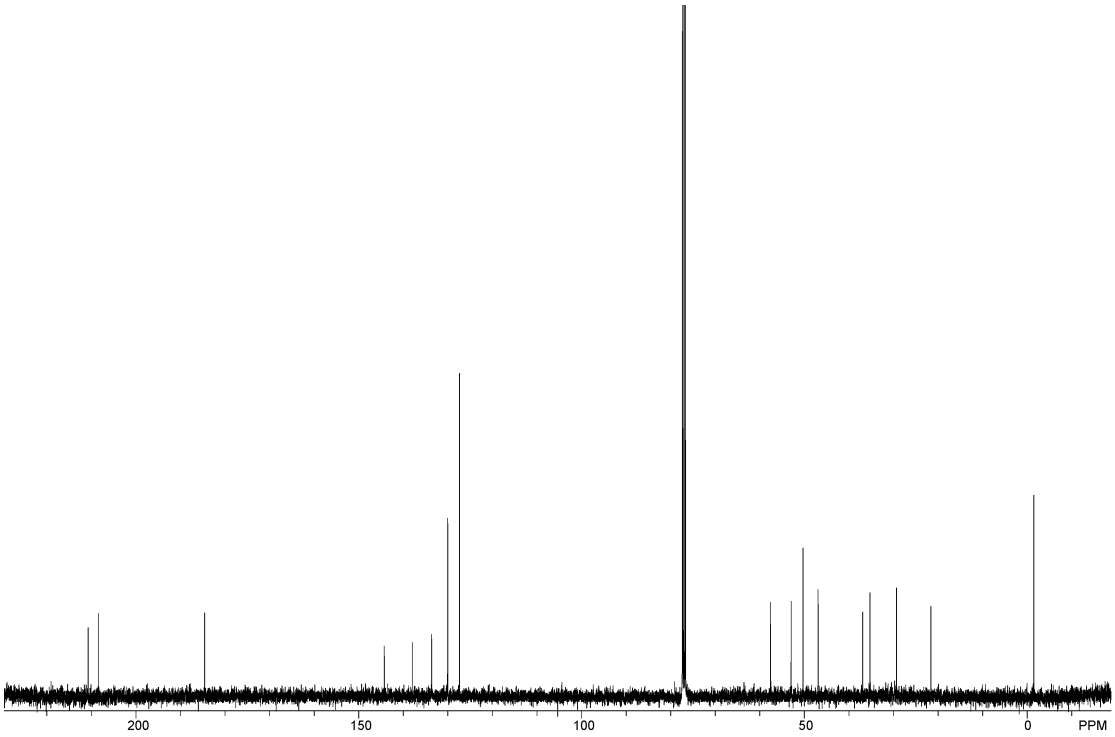

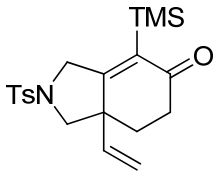

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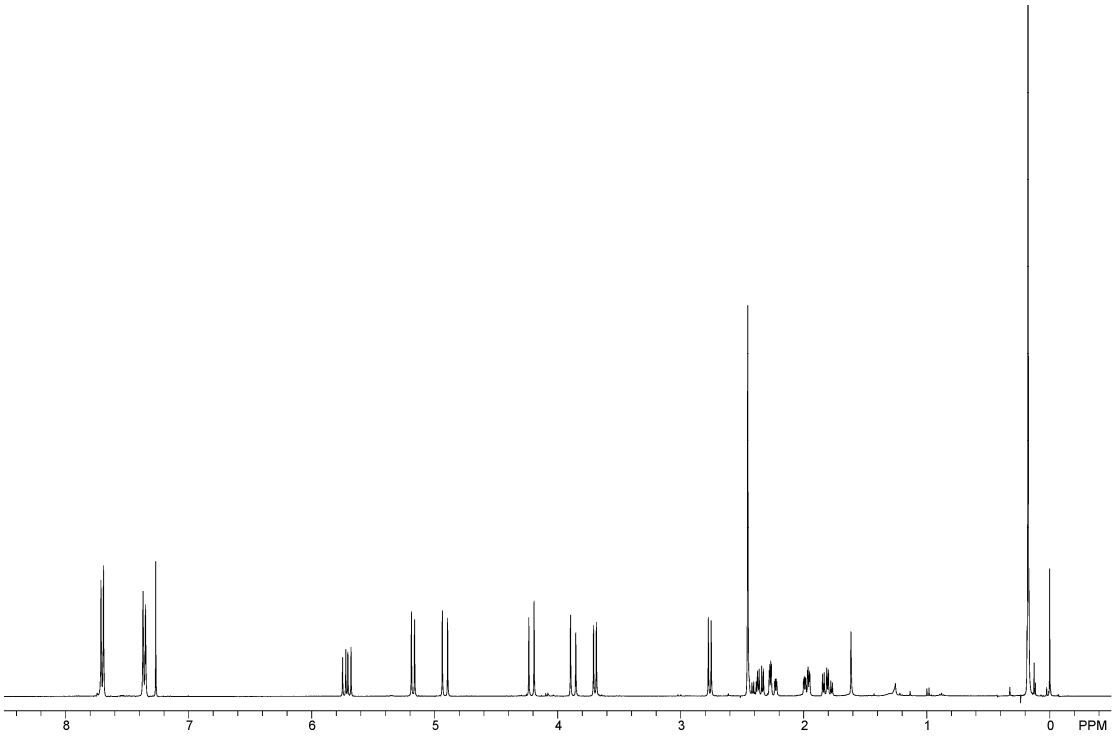

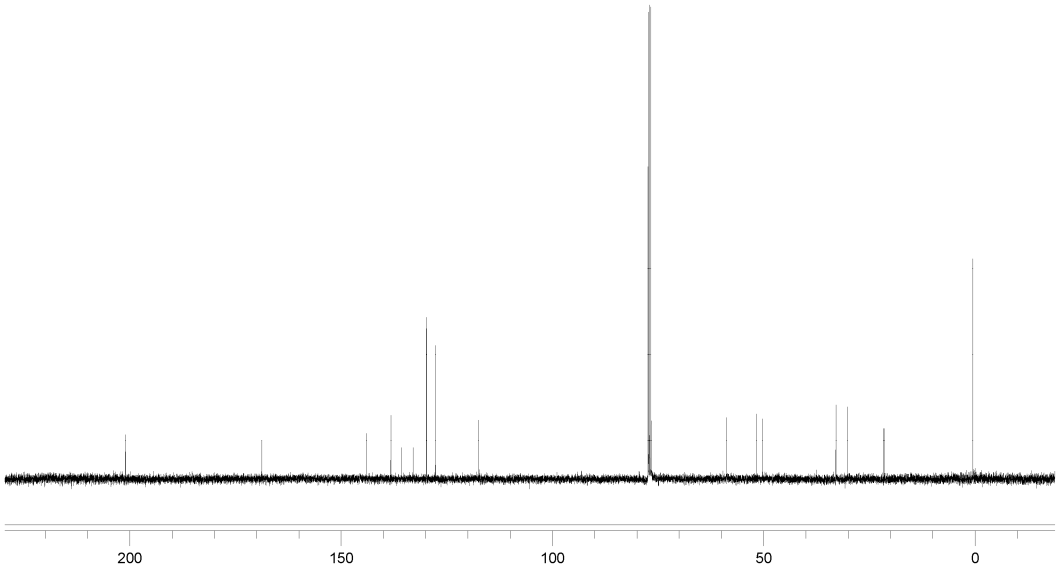

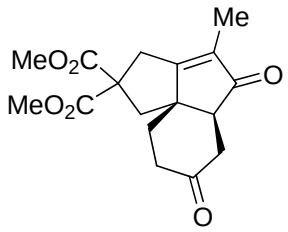

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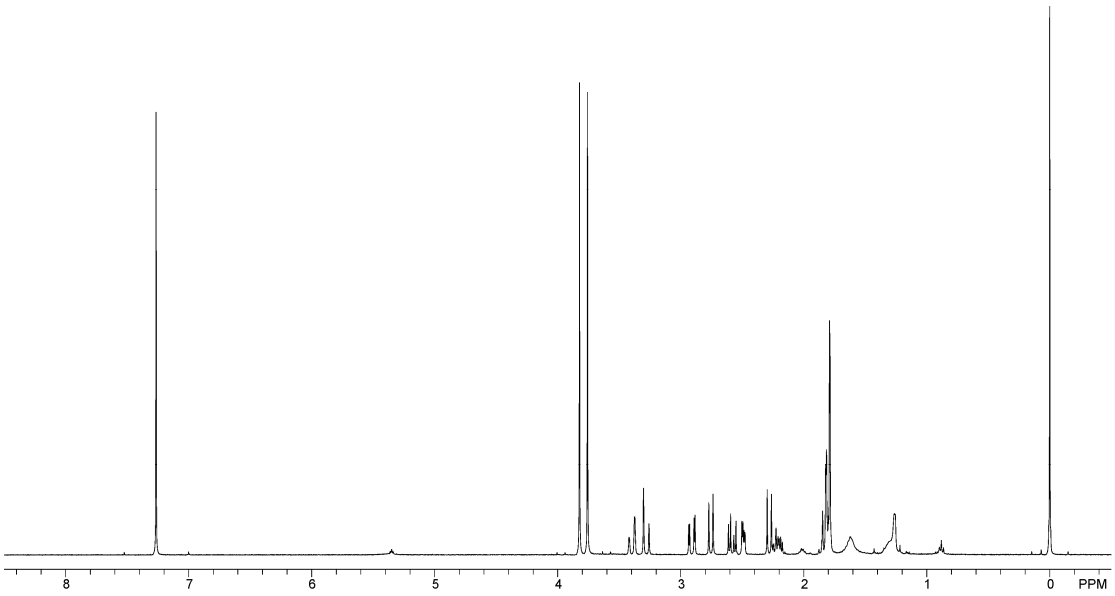

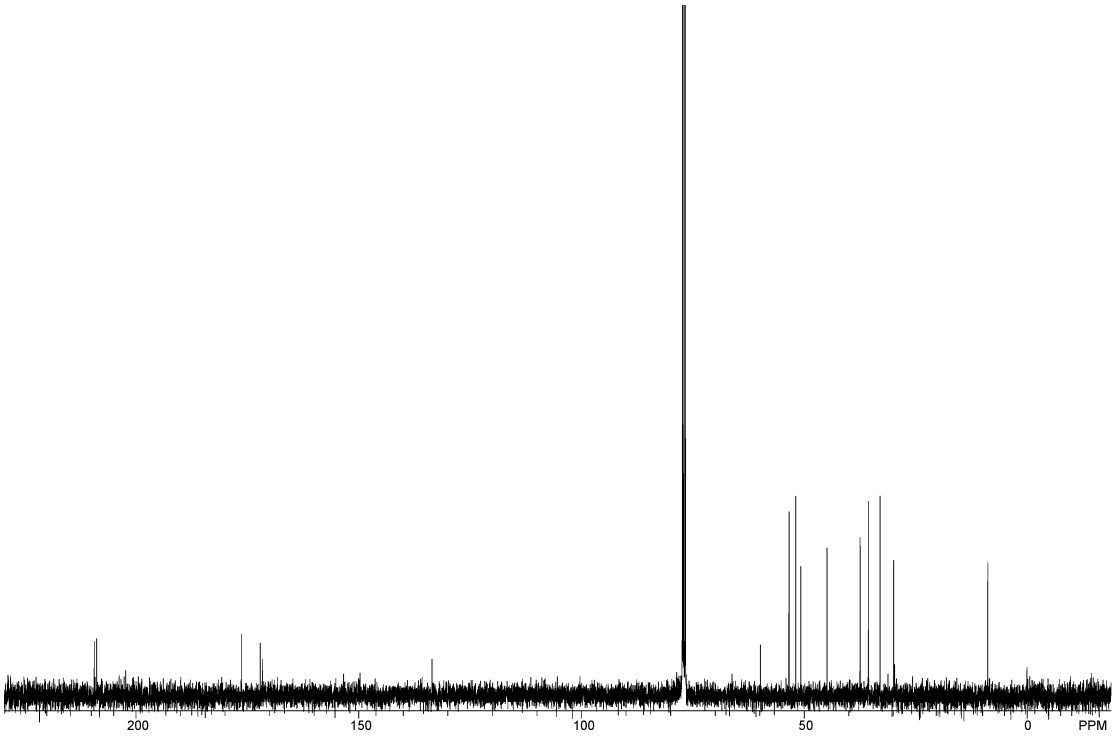

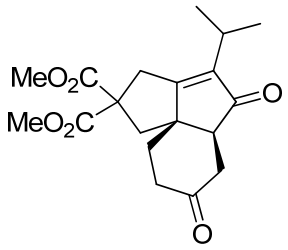

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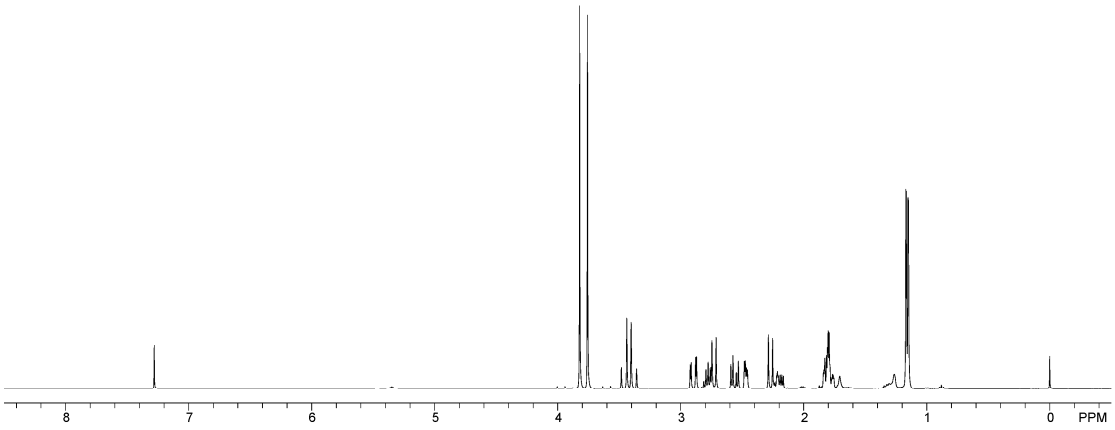

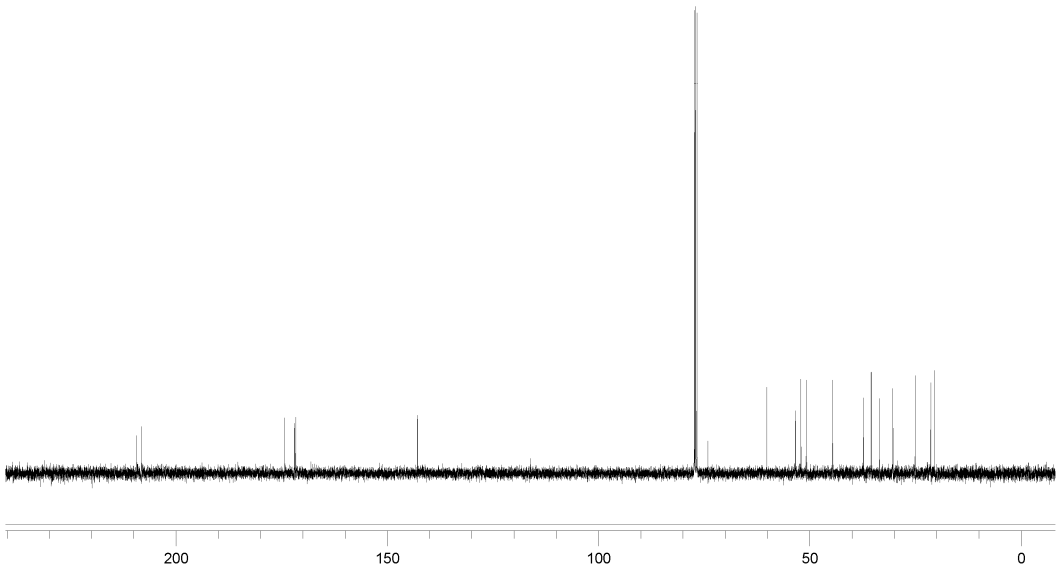

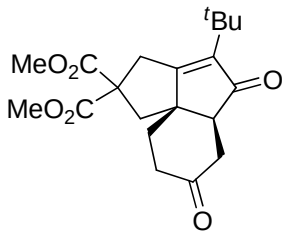

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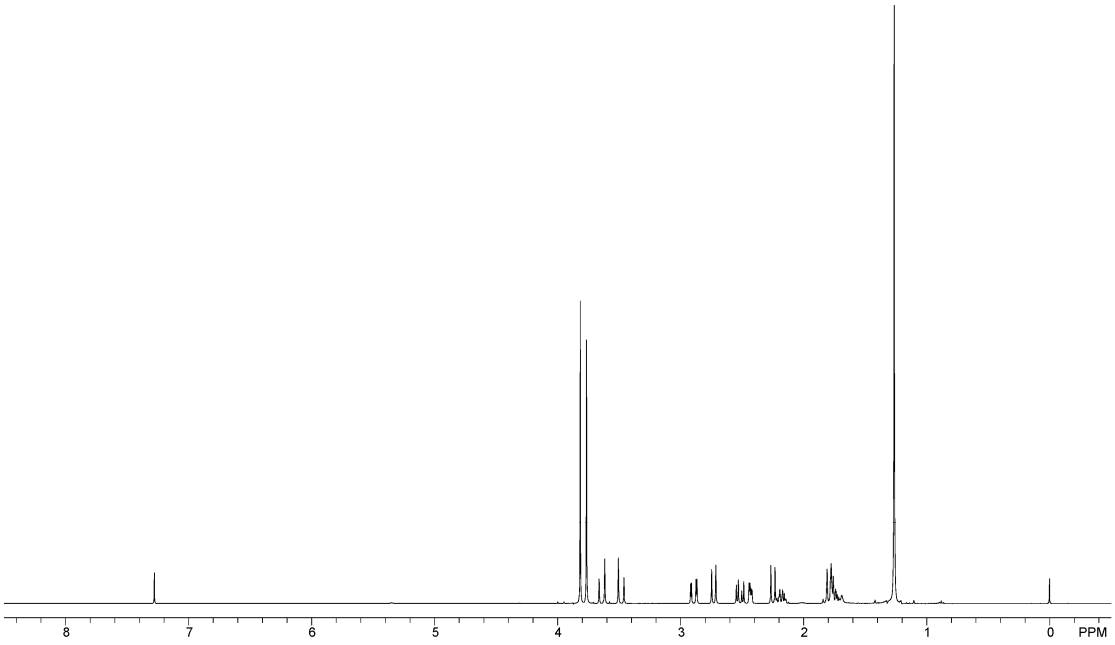

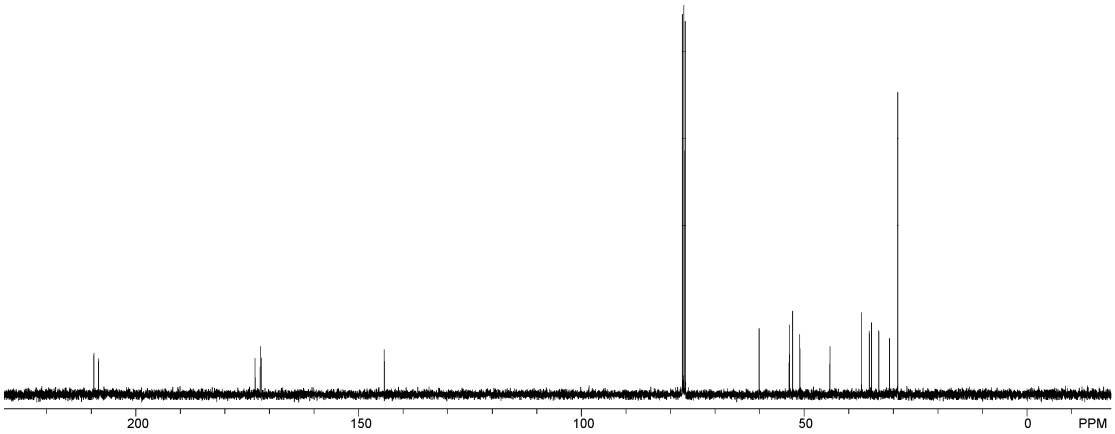

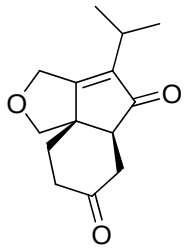

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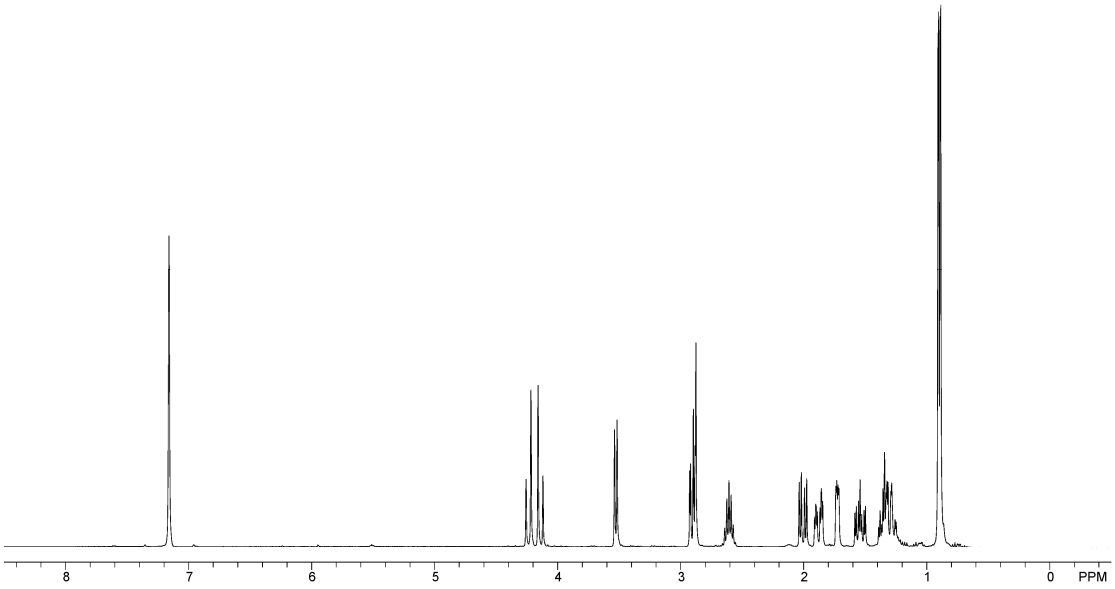

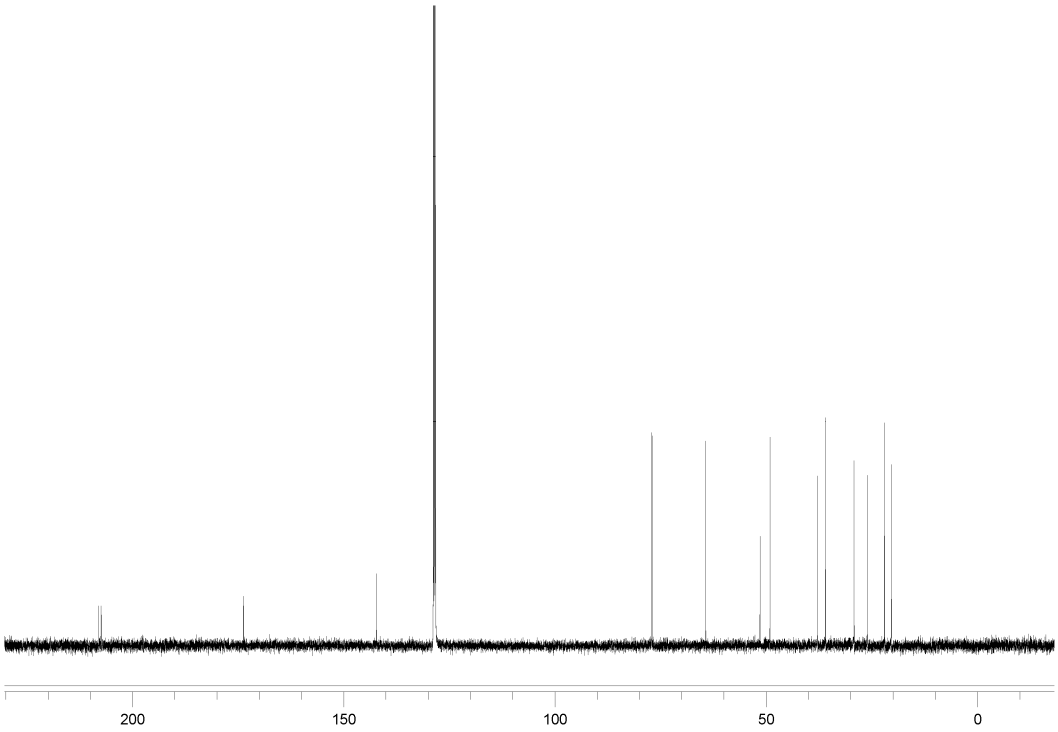

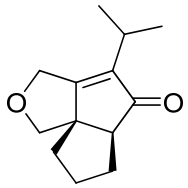

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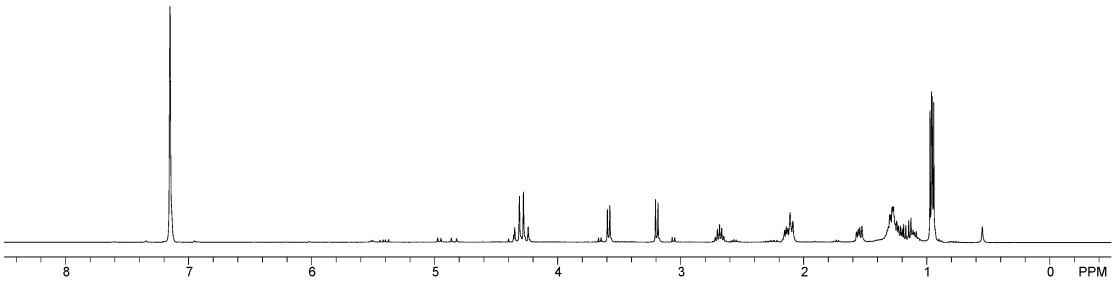

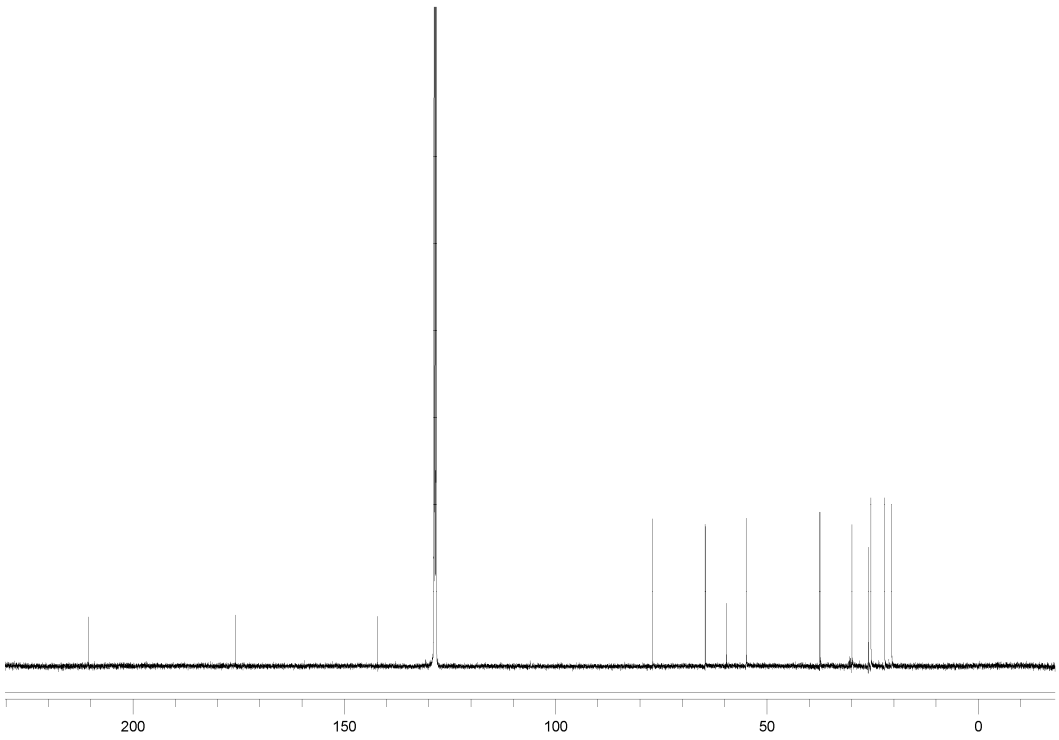

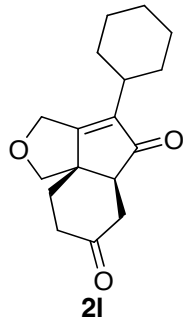

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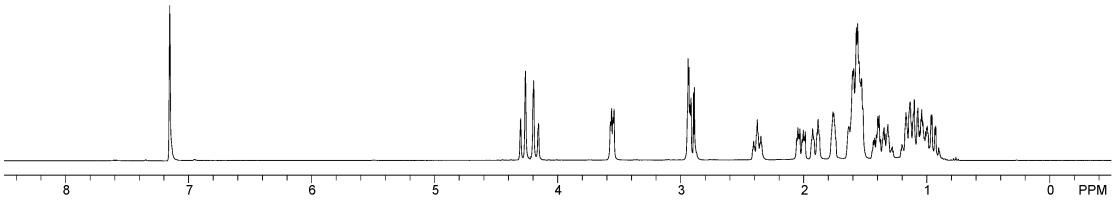

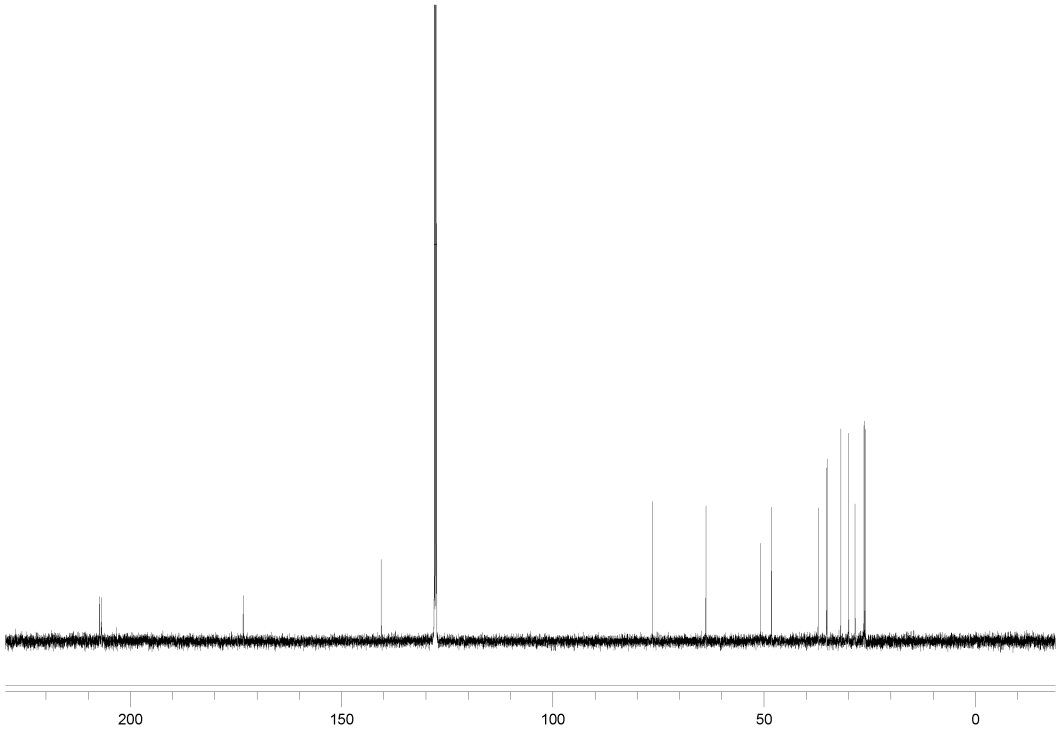

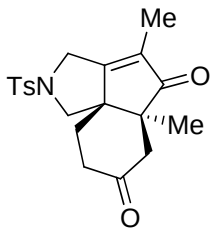

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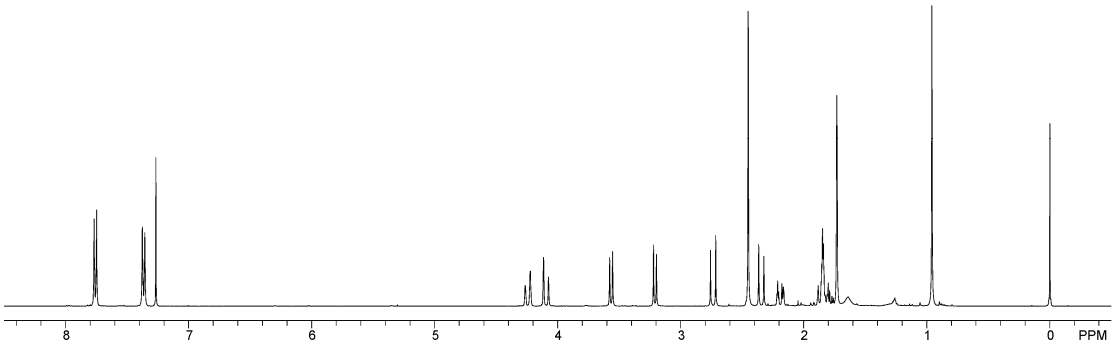

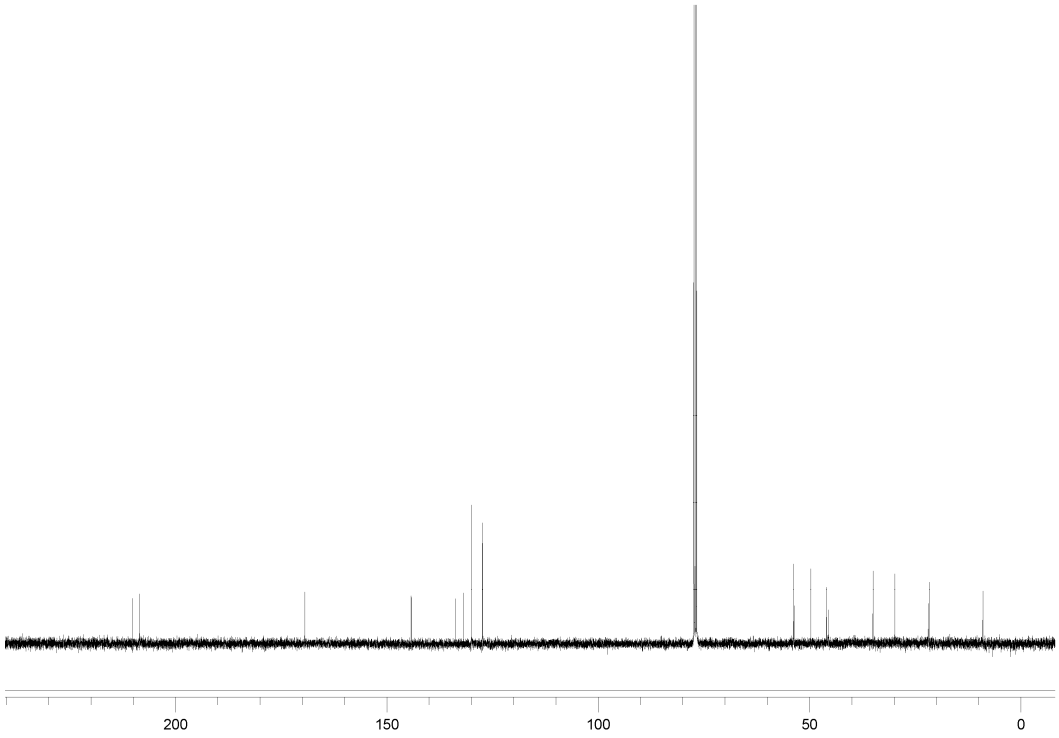

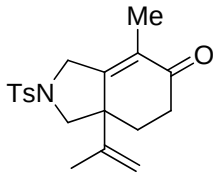

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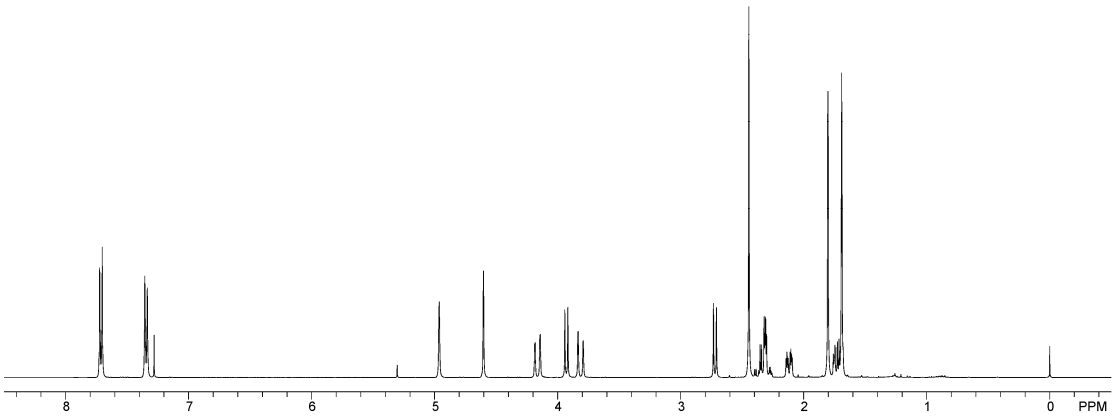

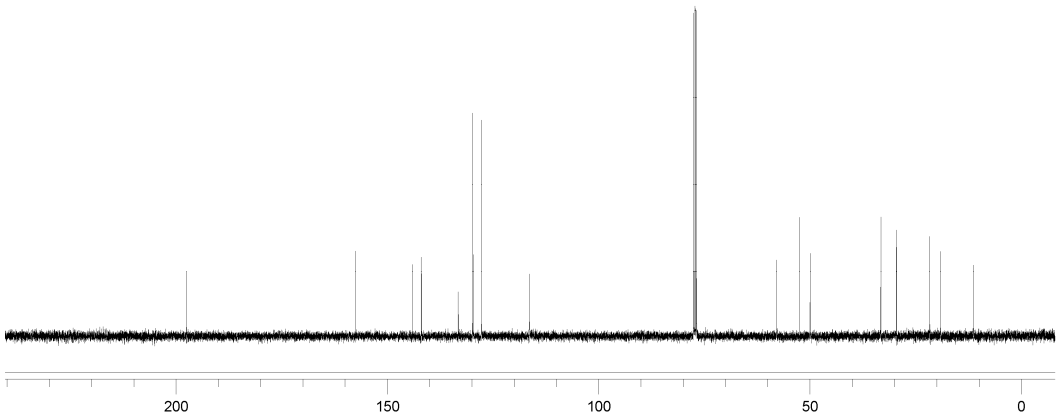

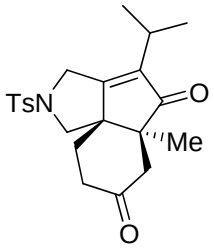

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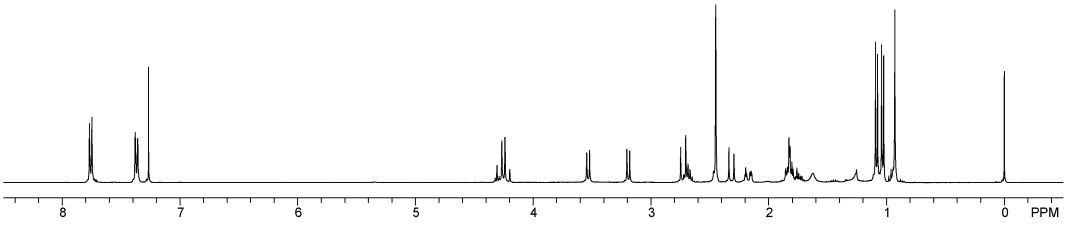

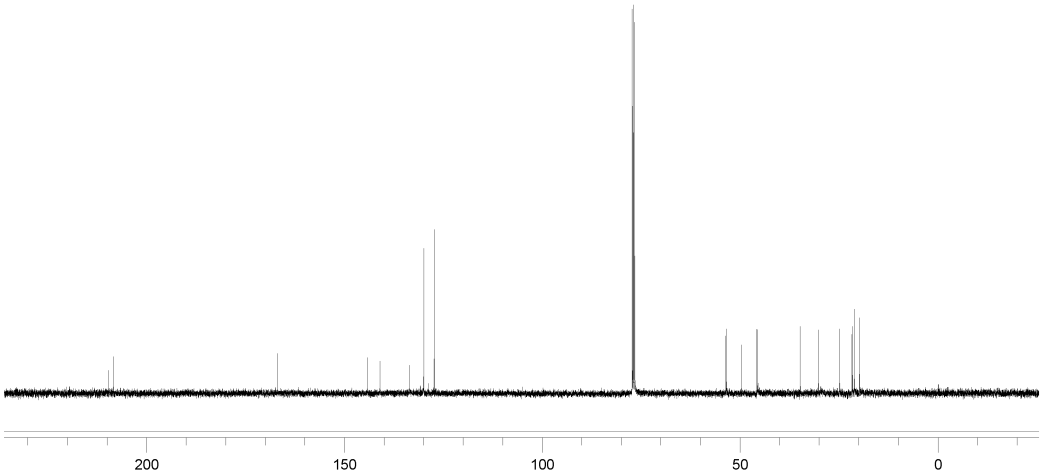

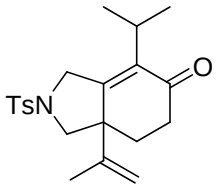

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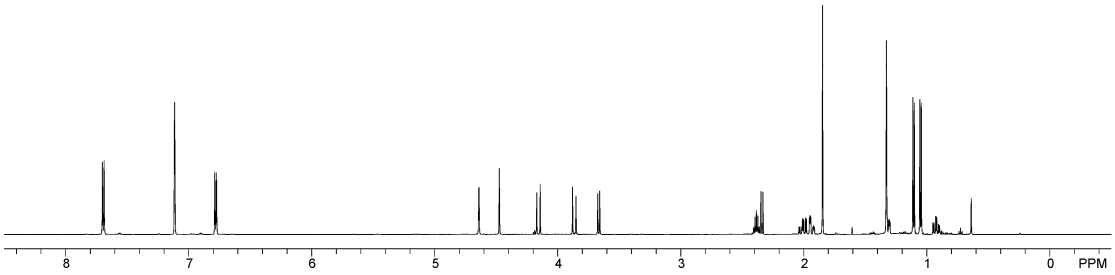

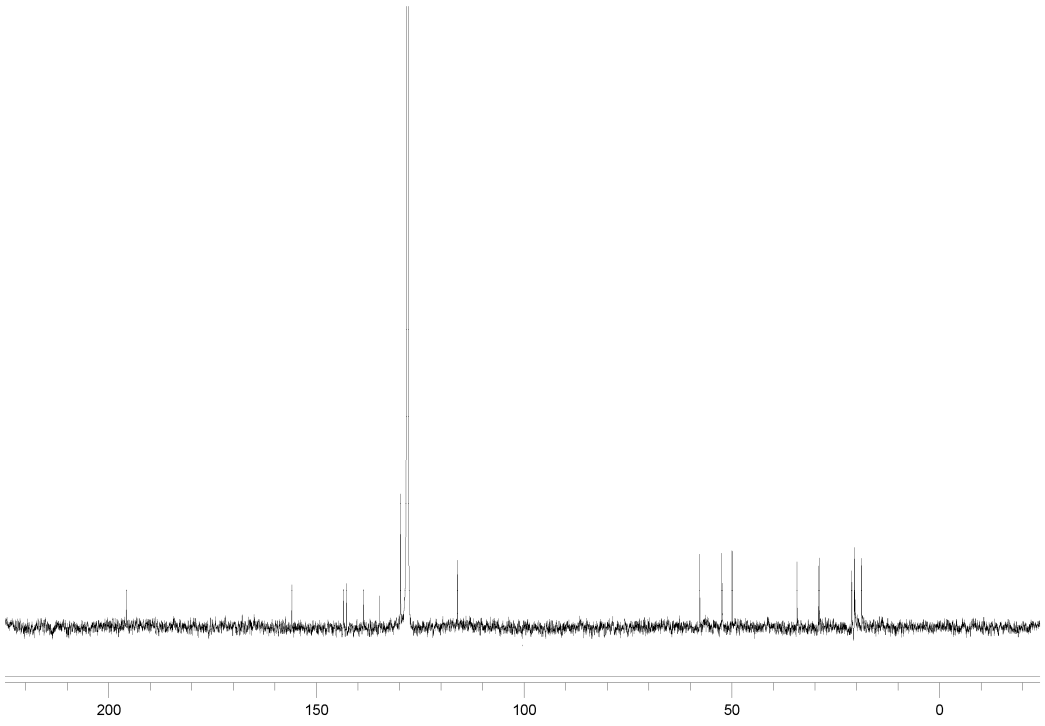

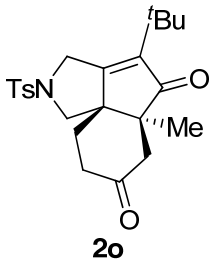

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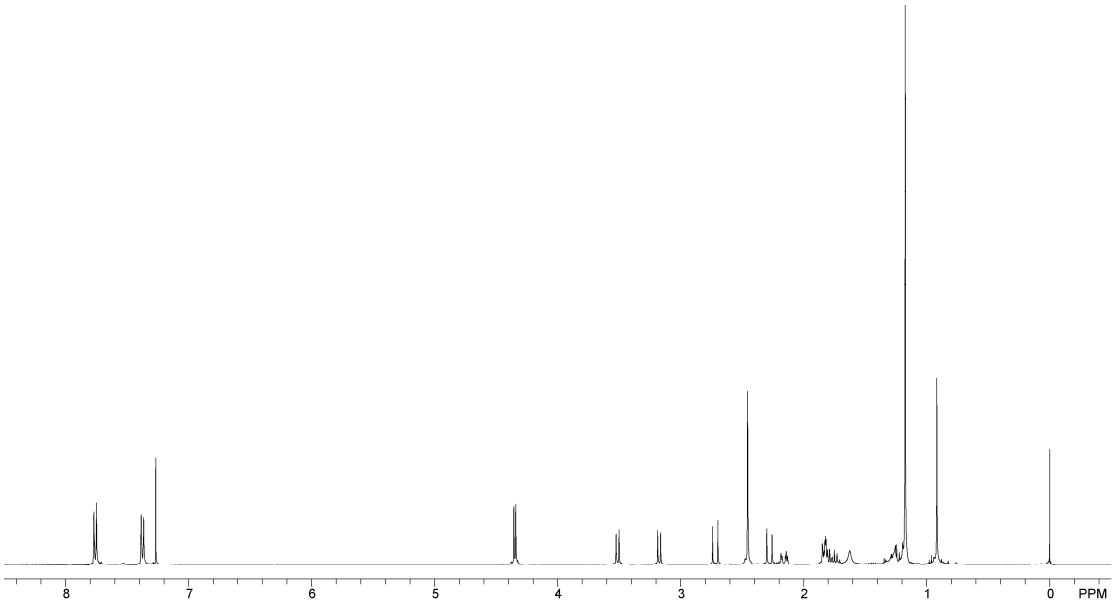

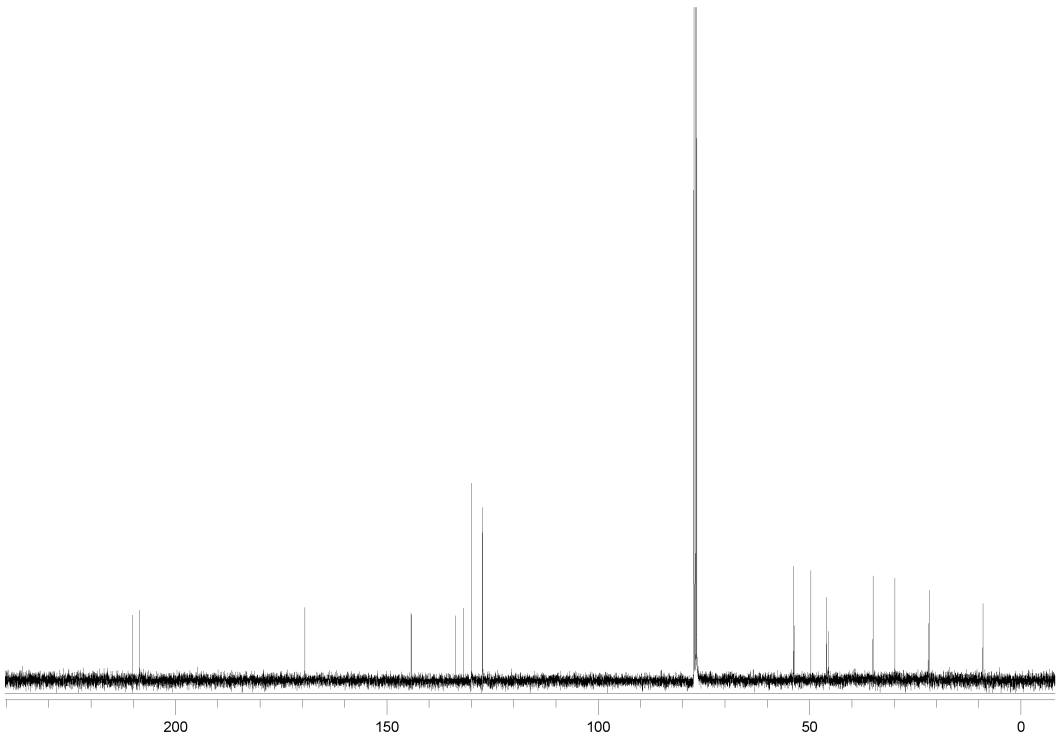

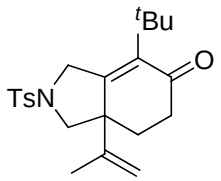

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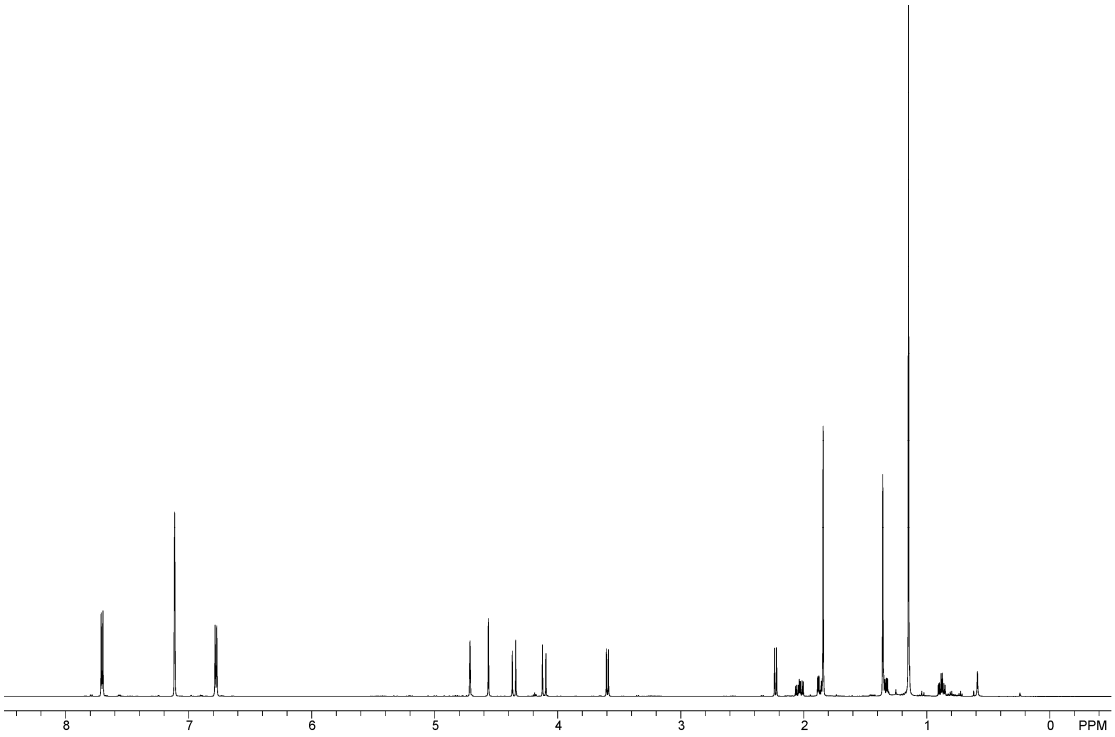

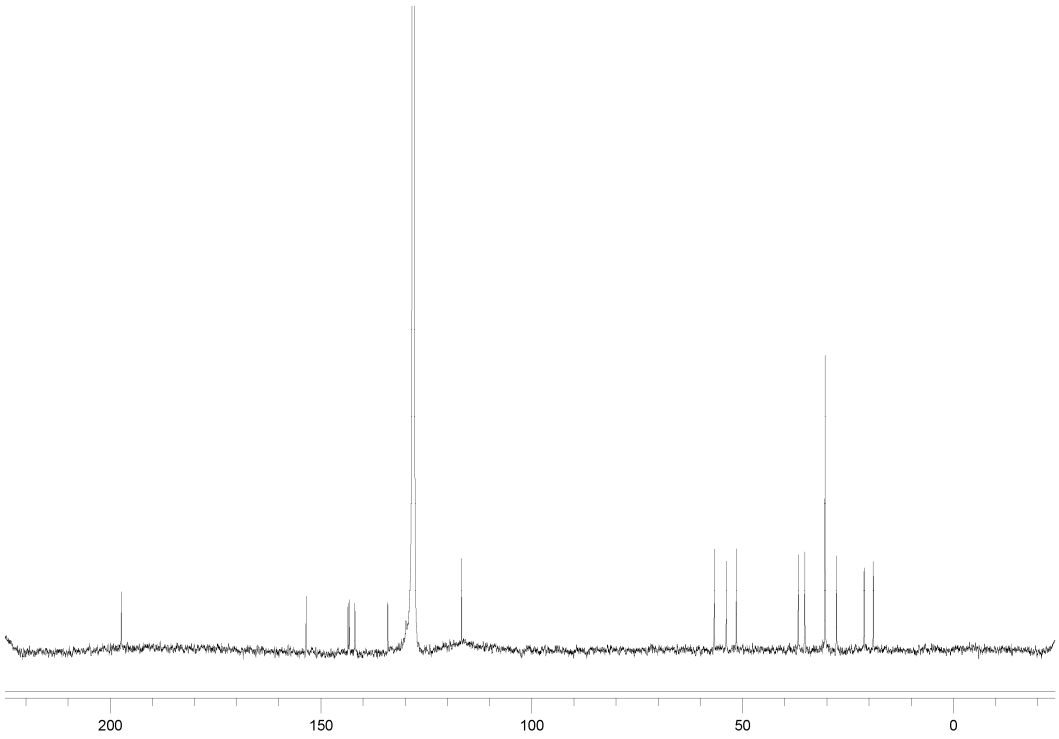

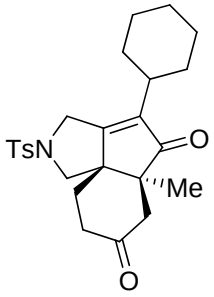

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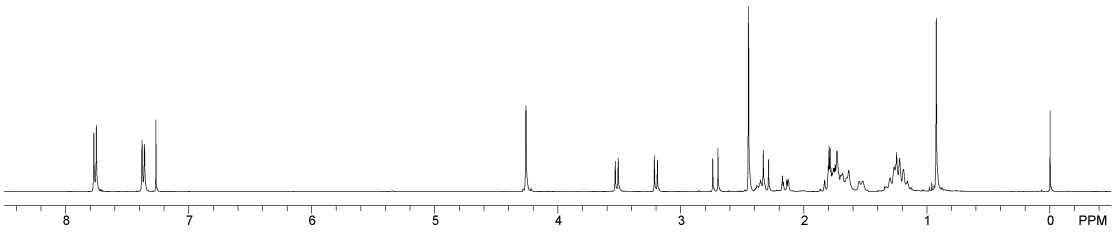

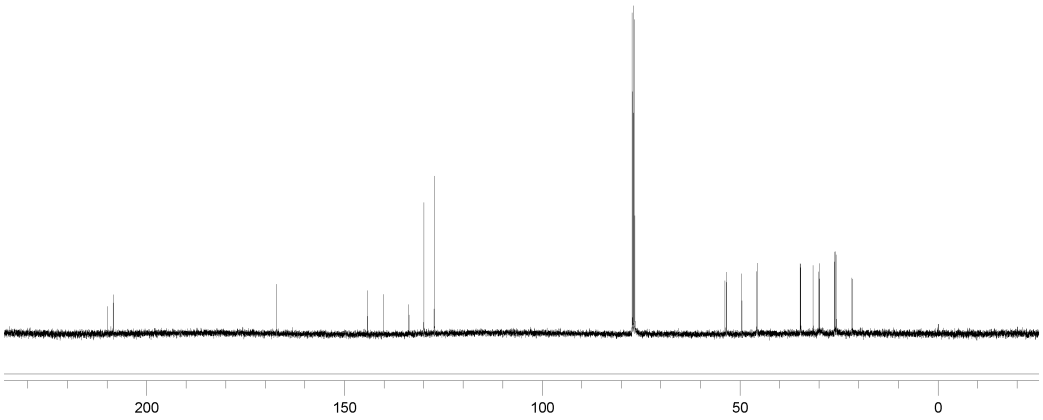

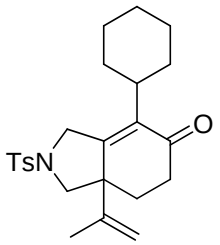

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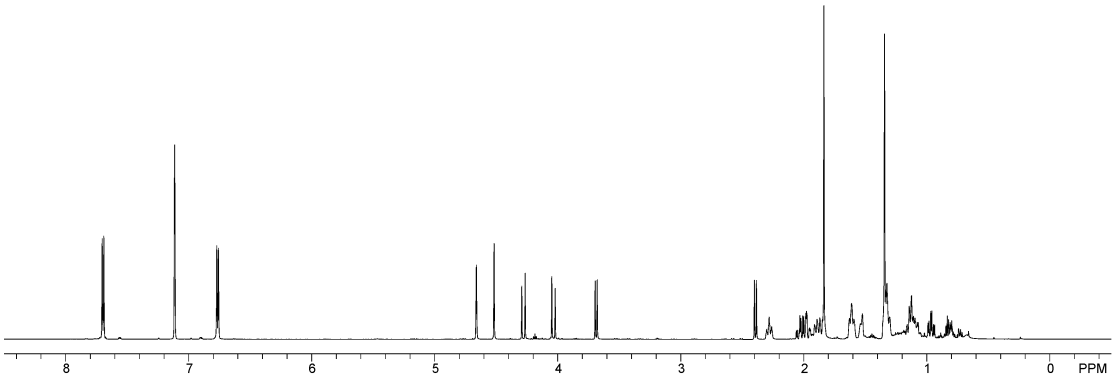

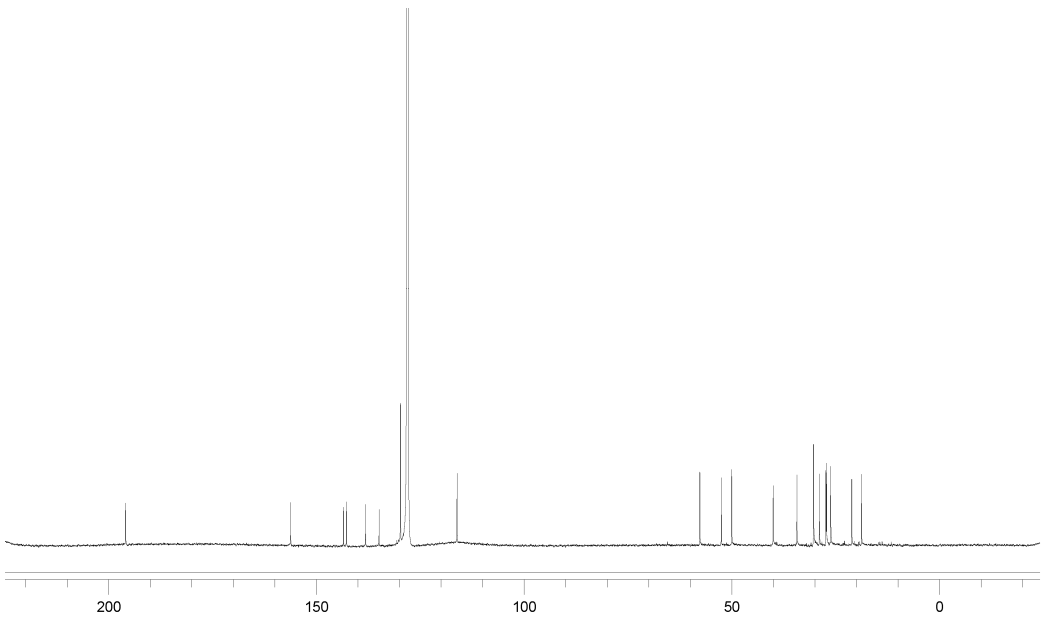

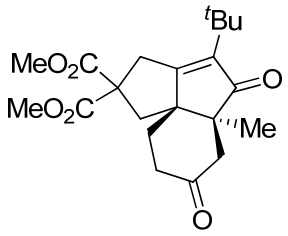

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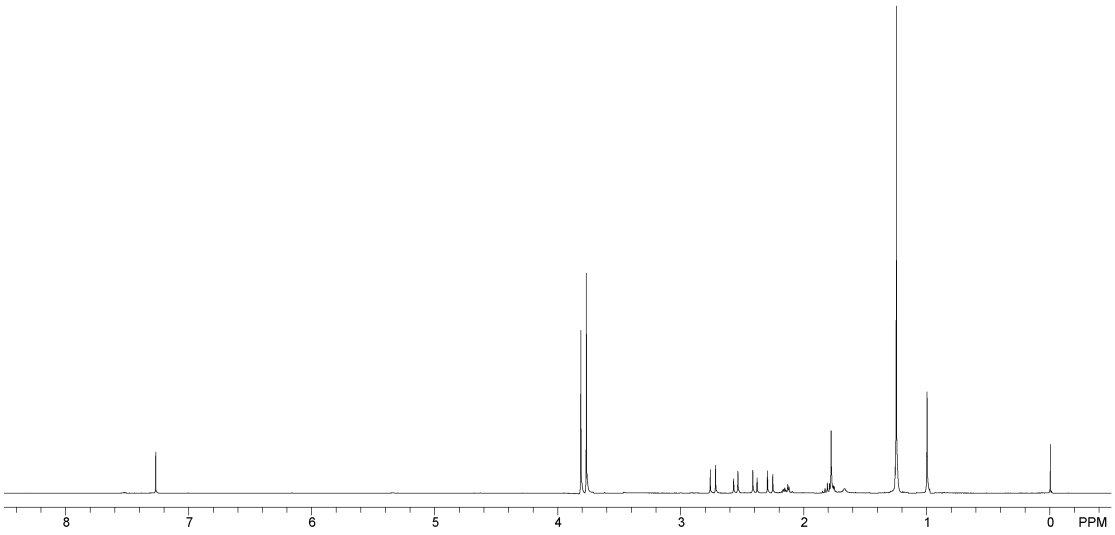

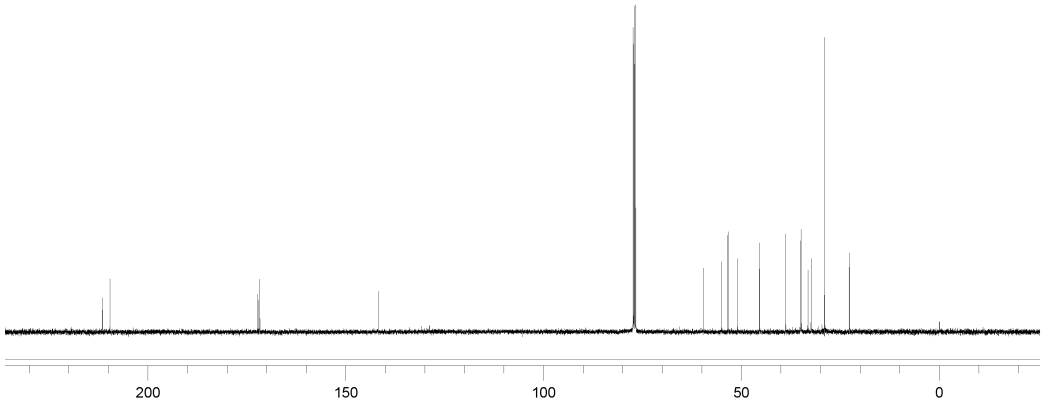

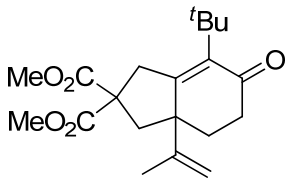

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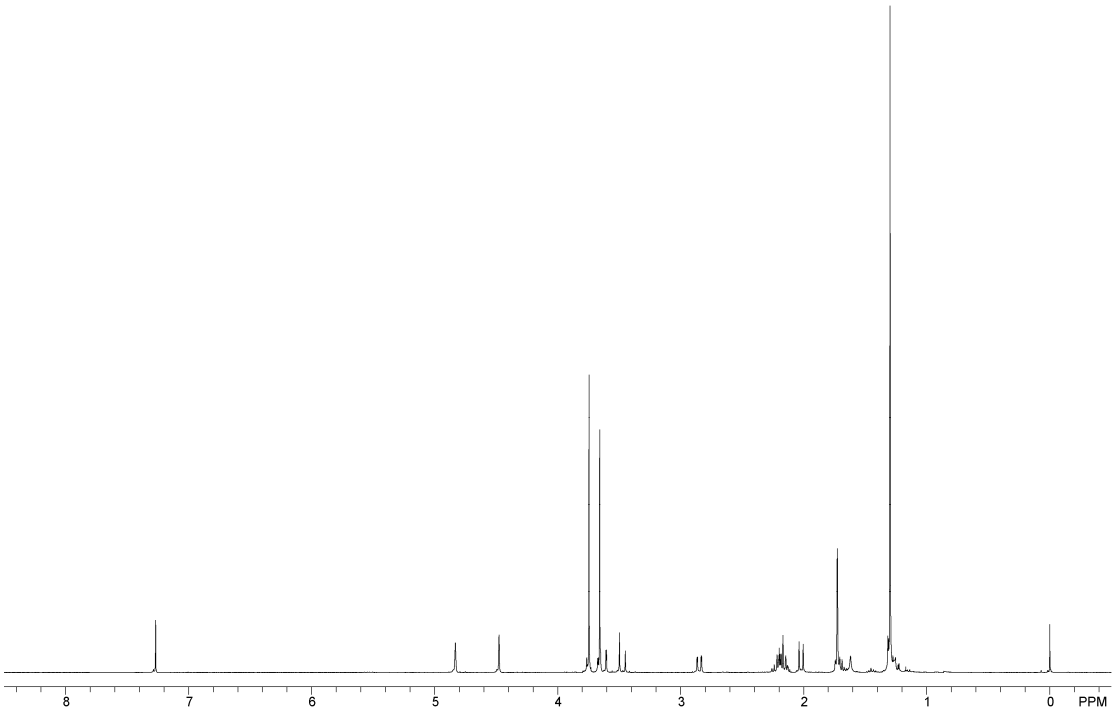

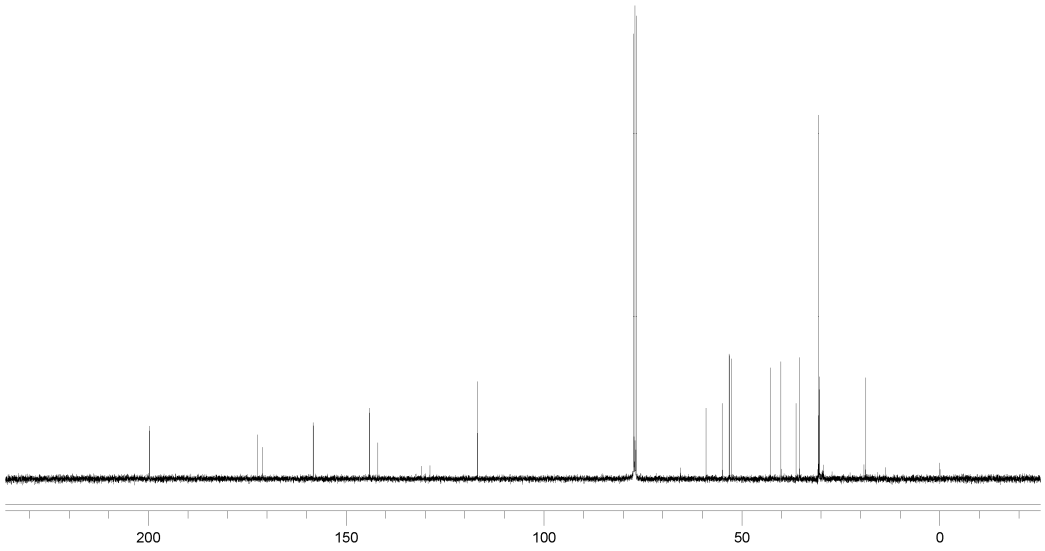

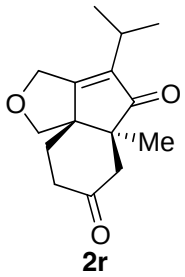

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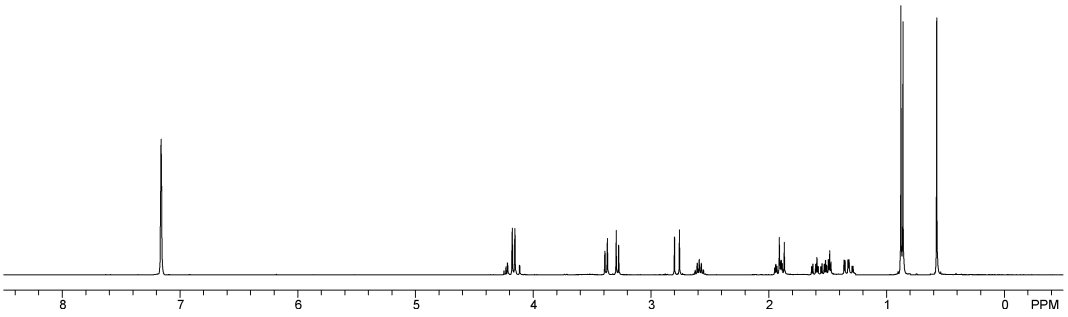
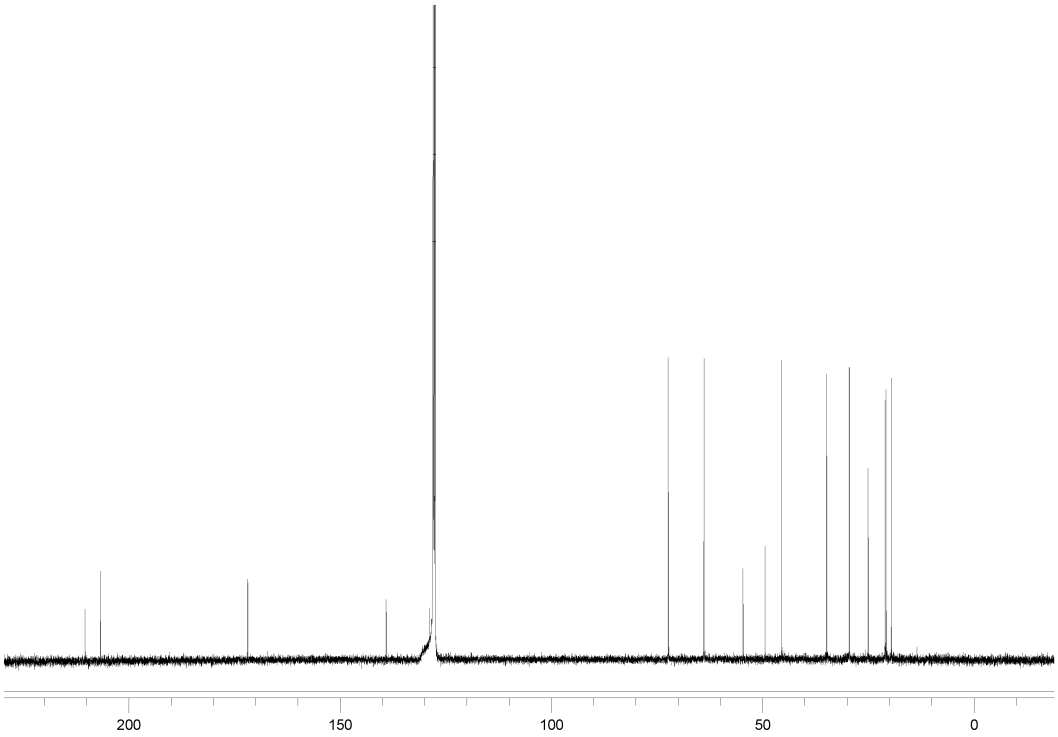
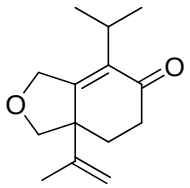
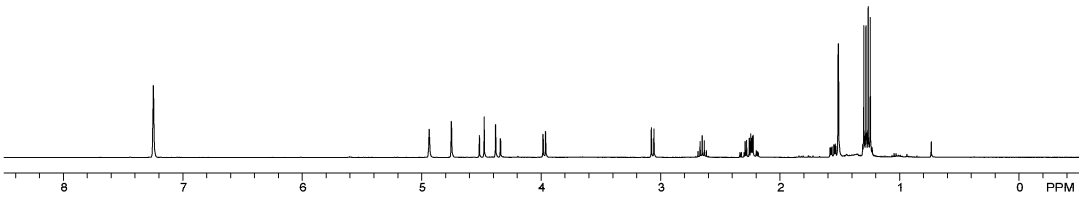
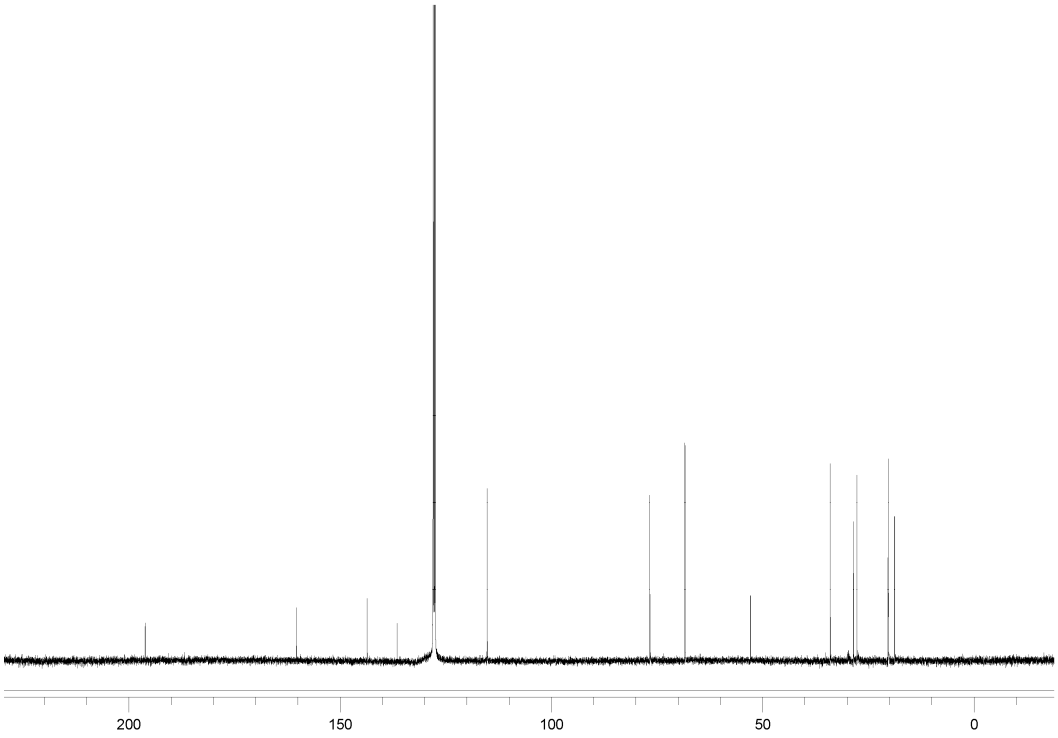


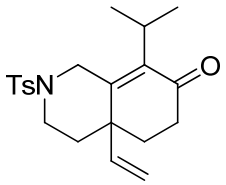




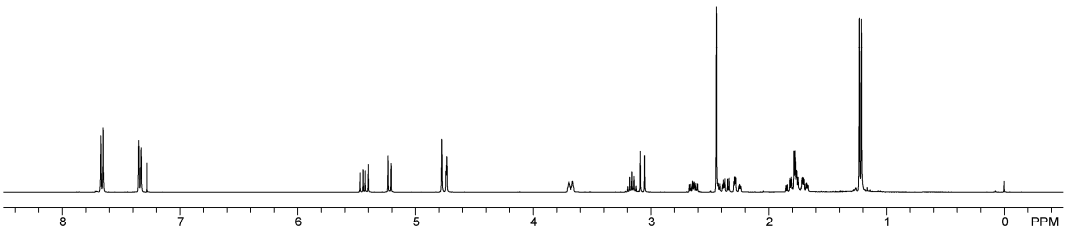
3r

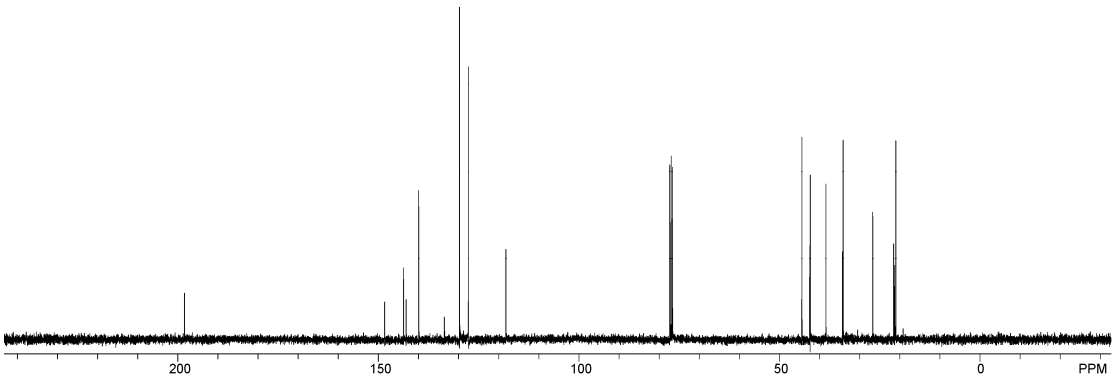


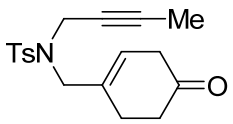




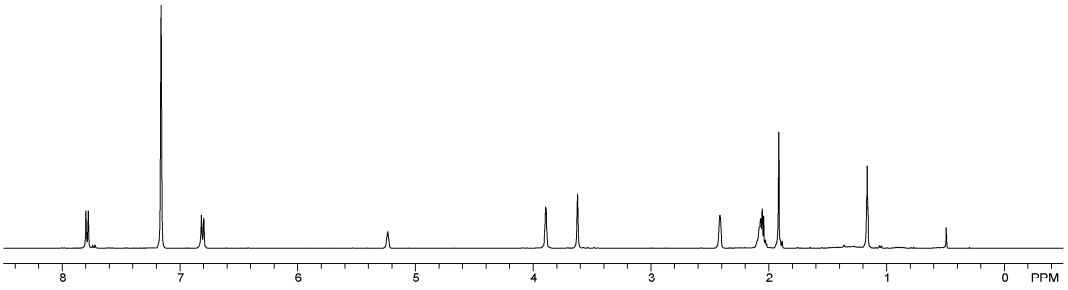
3s

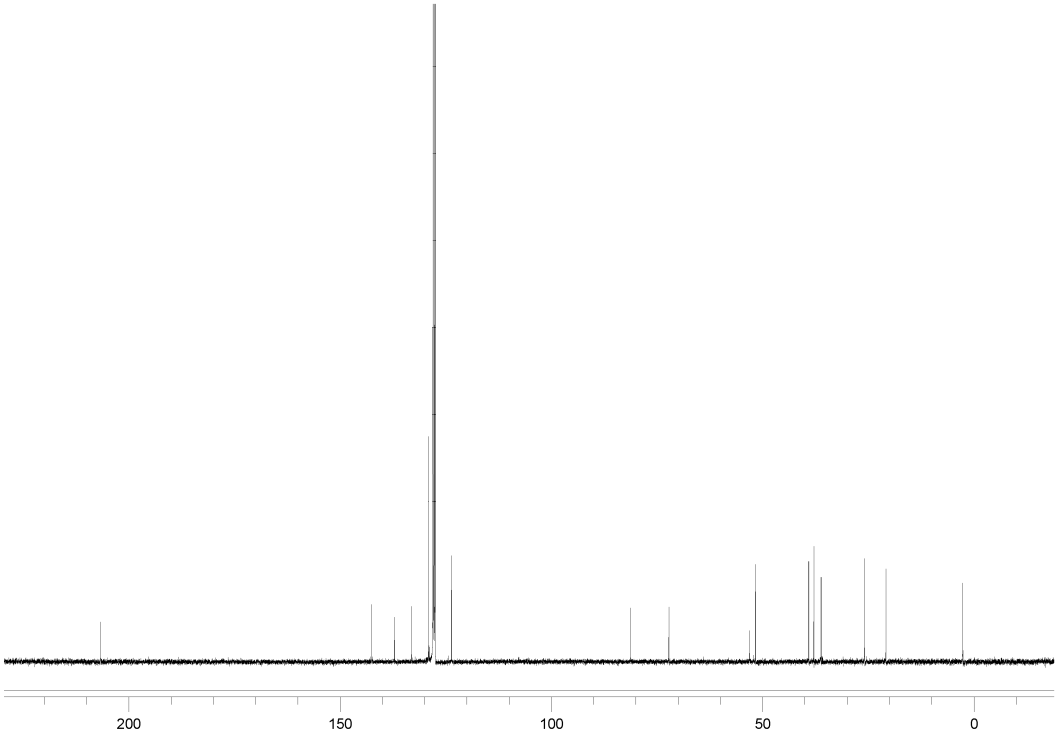






5

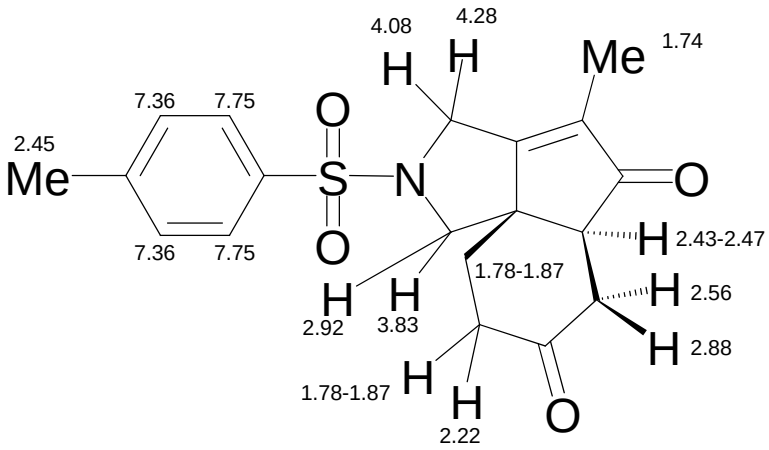




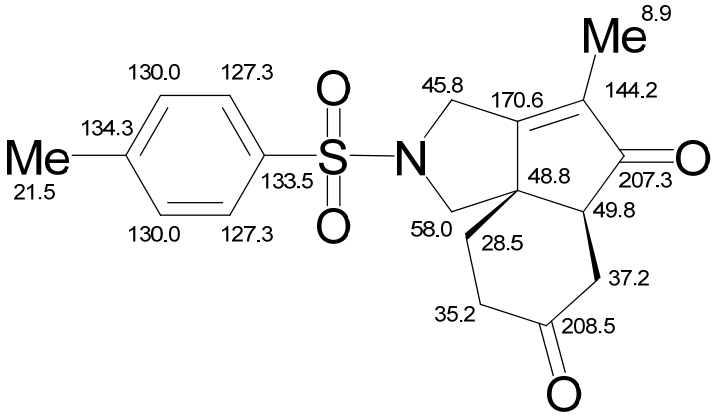
5. 2D-NMR Spectra of the Representive New Compounds

Compound **2a**:

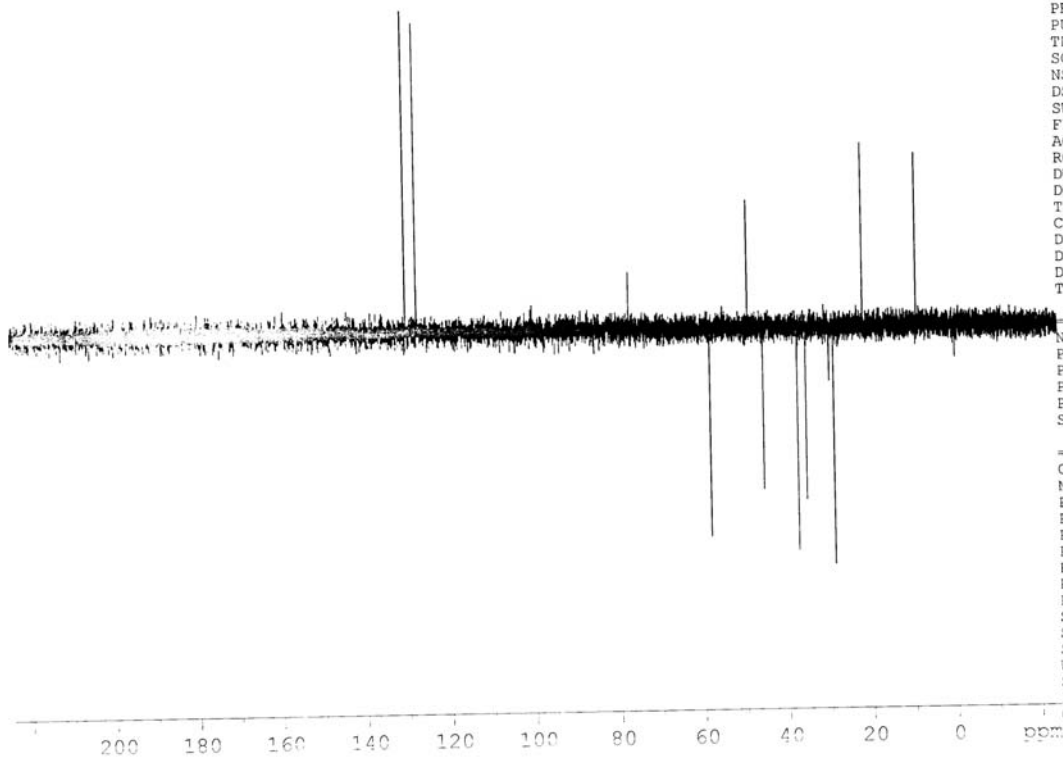
^{1}H NMR (ppm)



^{13}C NMR (ppm)

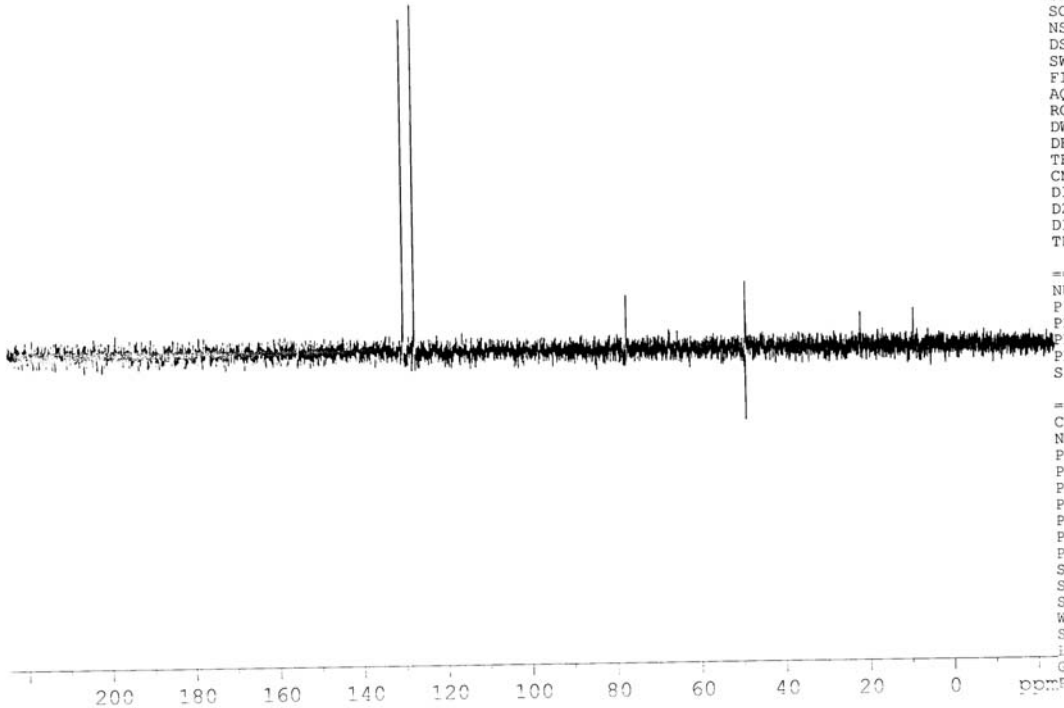


dept 135NMR
20101208

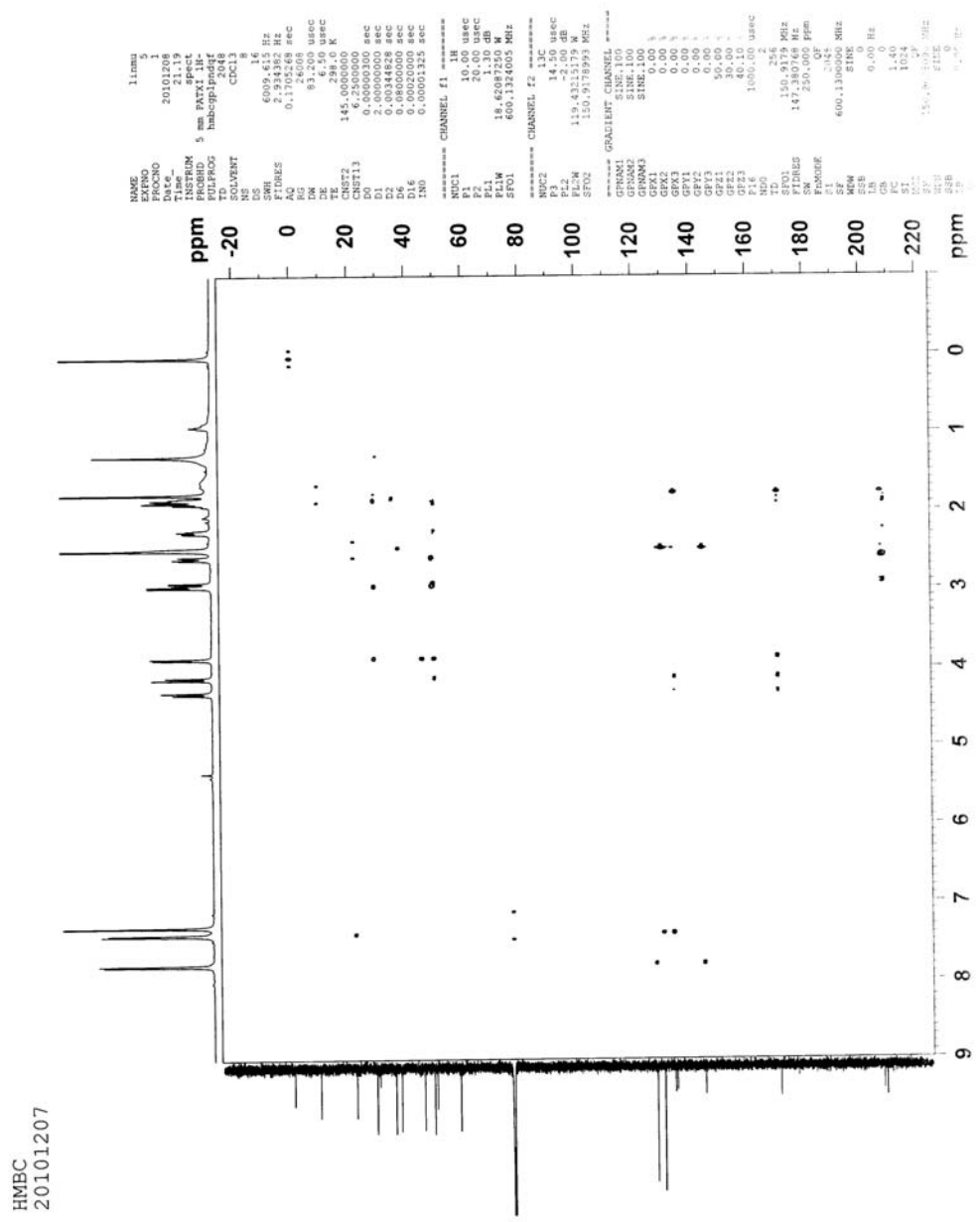


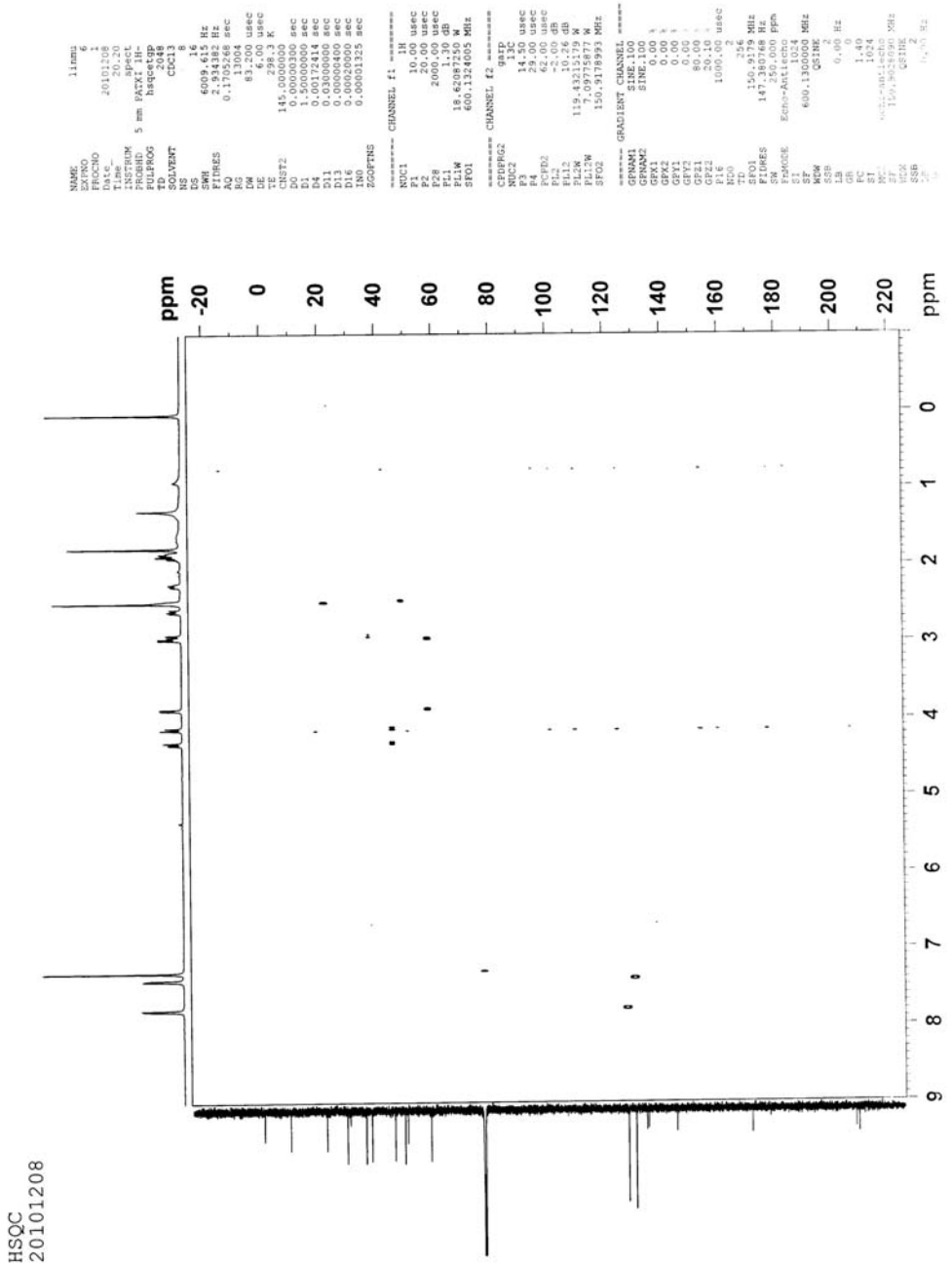
NAME	linmu
EXPNO	3
PROCNO	1
Date_	20101209
Time	3.07
INSTRUM	spect
PROBHD	5 mm PATXI 1H-
PULPROG	dept135
TD	32768
SOLVENT	CDCl3
NS	4096
DS	8
SWH	37593.984 Hz
FIDRES	1.147277 Hz
AQ	0.4358777 sec
RG	20642.5
DW	13.300 usec
DE	12.00 usec
TE	298.1 K
CNST2	145.0000000
D1	1.50000000 sec
D2	0.00344828 sec
D12	0.00002000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	14.50 usec
P2	29.00 usec
PL1	-2.00 dB
PL1W	119.43215179 W
SFO1	150.9178988 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz64
NUC2	1H
P3	10.00 usec
P4	20.00 usec
PCPD2	80.00 usec
PL2	1.30 dB
PL12	19.36 dB
PL2W	18.62087250 W
PL12W	0.29107168 W
SFO2	600.1327006 MHz
SI	32768
SF	150.9028090 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

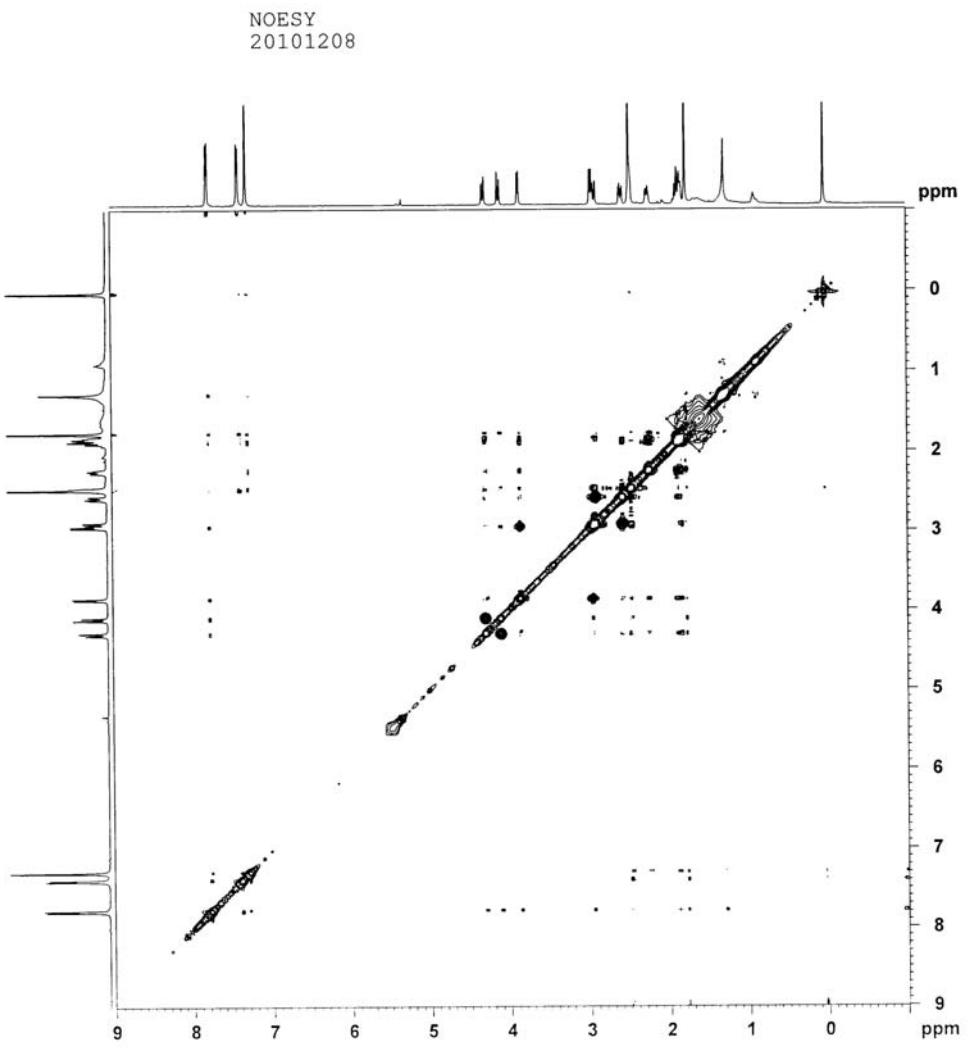
DPET90 CDCl3
ren weiwu
20100925



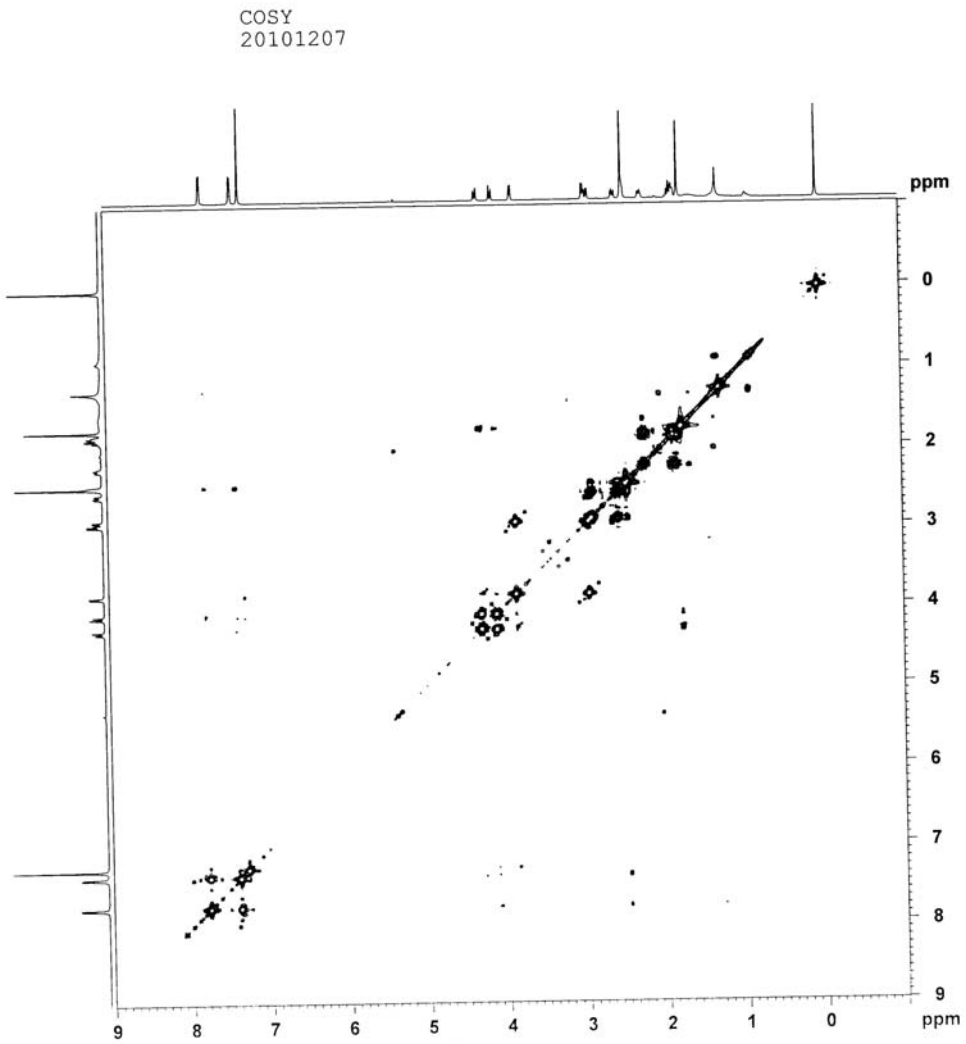
NAME	linmu
EXPNO	4
PROCNO	1
Date_	20101209
Time	0.52
INSTRUM	spect
PROBHD	5 mm PATXI 1H-
PULPROG	dept90
TD	32768
SOLVENT	CDCl3
NS	4096
DS	0
SWH	37593.984 Hz
FIDRES	1.147277 Hz
AQ	0.4358777 sec
RG	23170.5
DW	13.300 usec
DE	6.50 usec
TE	298.2 K
CNST2	145.0000000
D1	1.50000000 sec
D2	0.00344828 sec
D12	0.00002000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	14.50 usec
P2	29.00 usec
PL1	-2.00 dB
PL1W	119.43215179 W
SFO1	150.9178988 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
P3	10.00 usec
P4	20.00 usec
PCPD2	80.00 usec
PL2	1.30 dB
PL12	19.36 dB
PL2W	18.62087250 W
PL12W	0.29107168 W
SFO2	600.1324005 MHz
SI	32768
SF	150.9028090 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40


HMBC
20101207
ppm
ppm


HSQC
20101208
ppm
-20
0
20
40
60
80
100
120
140
160
180
200
220
ppm
0
1
2
3
4
5
6
7
8
9



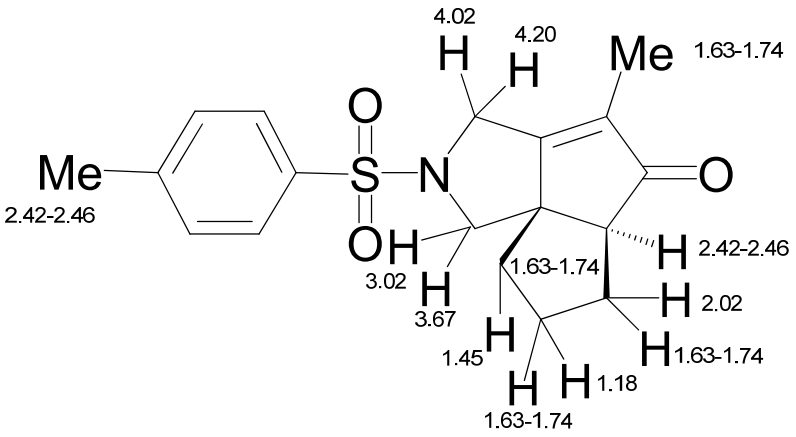
NAME	linmu
EXPNO	7
PROCNO	1
Date_	20101208
Time	18.07
INSTRUM	spect
PROBHD	5 mm PATXI 1H-
PULPROG	noesygpph
TD	2048
SOLVENT	CDC13
NS	8
DS	16
SWH	6009.615 Hz
FIDRES	2.934382 Hz
AQ	0.1705268 sec
RG	181
DW	83.200 usec
DE	6.50 usec
TE	298.0 K
D0	0.00007047 sec
D1	1.50000000 sec
D8	0.50000000 sec
D16	0.00020000 sec
IN0	0.00016640 sec
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
P2	20.00 usec
PL1	1.30 dB
PL1W	18.62087250 W
SFO1	600.1324005 MHz
====== GRADIENT CHANNEL =====	
GPNAM1	SINE.100
GPNAM2	SINE.100
GPX1	0.00 %
GPX2	0.00 %
GPY1	0.00 %
GPY2	0.00 %
GPZ1	40.00 %
GPZ2	-40.00 %
P16	1000.00 usec
ND0	1
TD	256
SFO1	600.1324 MHz
FIDRES	23.475023 Hz
SW	10.014 ppm
FnMODE	States-TPPI
SI	1024
SF	600.1300000 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	States-TPPI
SF	600.1300000 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0



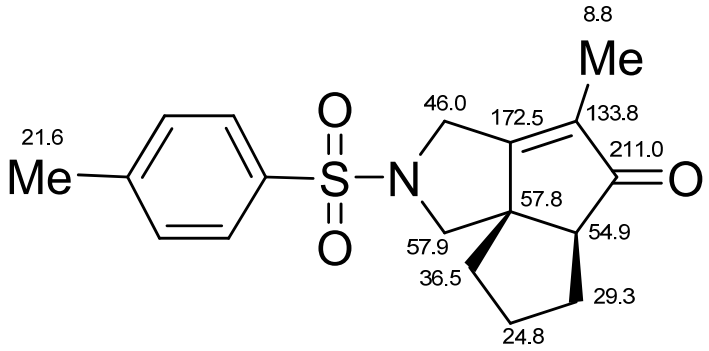
NAME	linmu
EXPNO	8
PROCNO	1
Date_	20101208
Time	19.22
INSTRUM	spect
PROBHD	5 mm PATXI 1H-
PULPROG	cosygpqf
TD	2048
SOLVENT	CDCl3
NS	8
DS	16
SWH	6009.615 Hz
FIDRES	2.934382 Hz
AQ	0.1705268 sec
RG	181
DW	83.200 usec
DE	6.50 usec
TE	298.1 K
D0	0.00000300 sec
D1	1.50000000 sec
D13	0.00000400 sec
D16	0.00020000 sec
IN0	0.00016640 sec
======== CHANNEL f1 ========	
NUC1	1H
P0	10.00 usec
P1	10.00 usec
PL1	1.30 dB
PL1W	18.62087250 W
SFO1	600.1324005 MHz
====== GRADIENT CHANNEL =====	
GPNAM1	SINE.100
GPX1	0.00 %
GPY1	0.00 %
GPZ1	10.00 %
P16	1000.00 usec
ND0	1
TD	256
SFO1	600.1324 MHz
FIDRES	23.475023 Hz
SW	10.014 ppm
FnMODE	QF
SI	1024
SF	600.1300000 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	4.00
SI	1024
MC2	QF
SF	600.1300000 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

Compound **4a**:

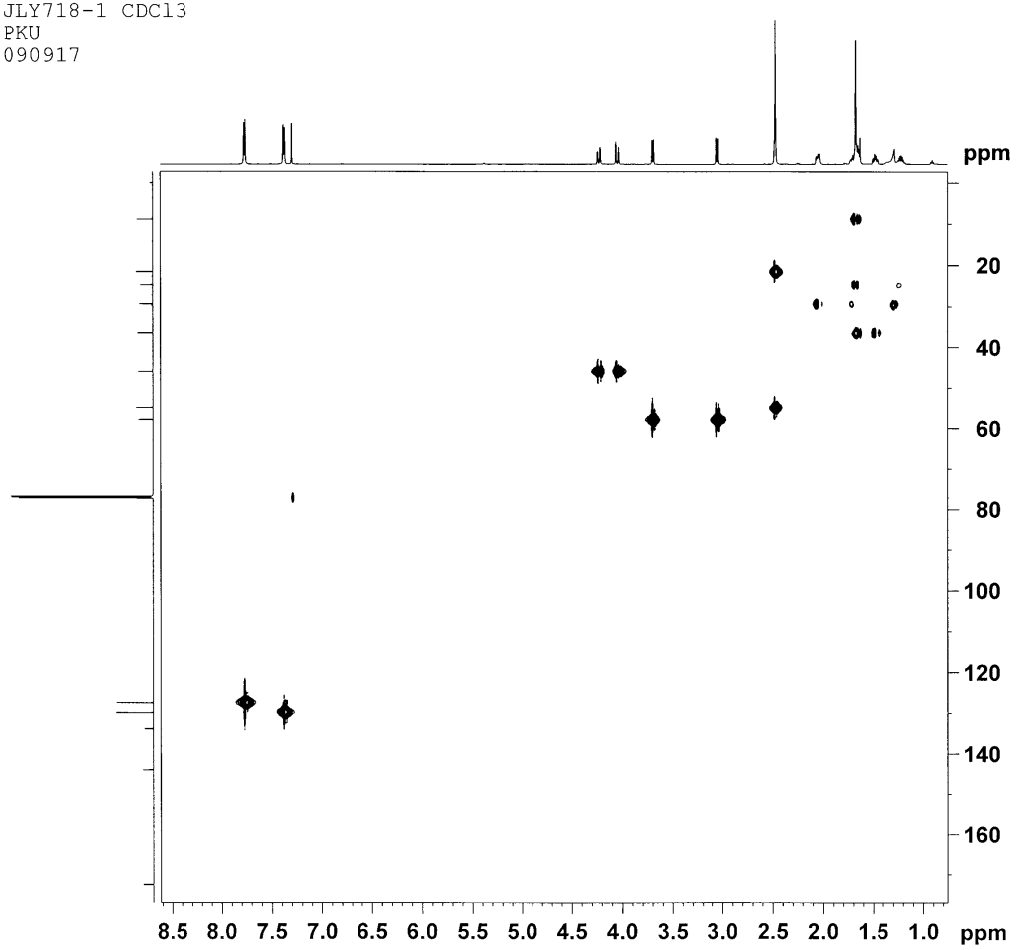
^{1}H NMR (ppm)



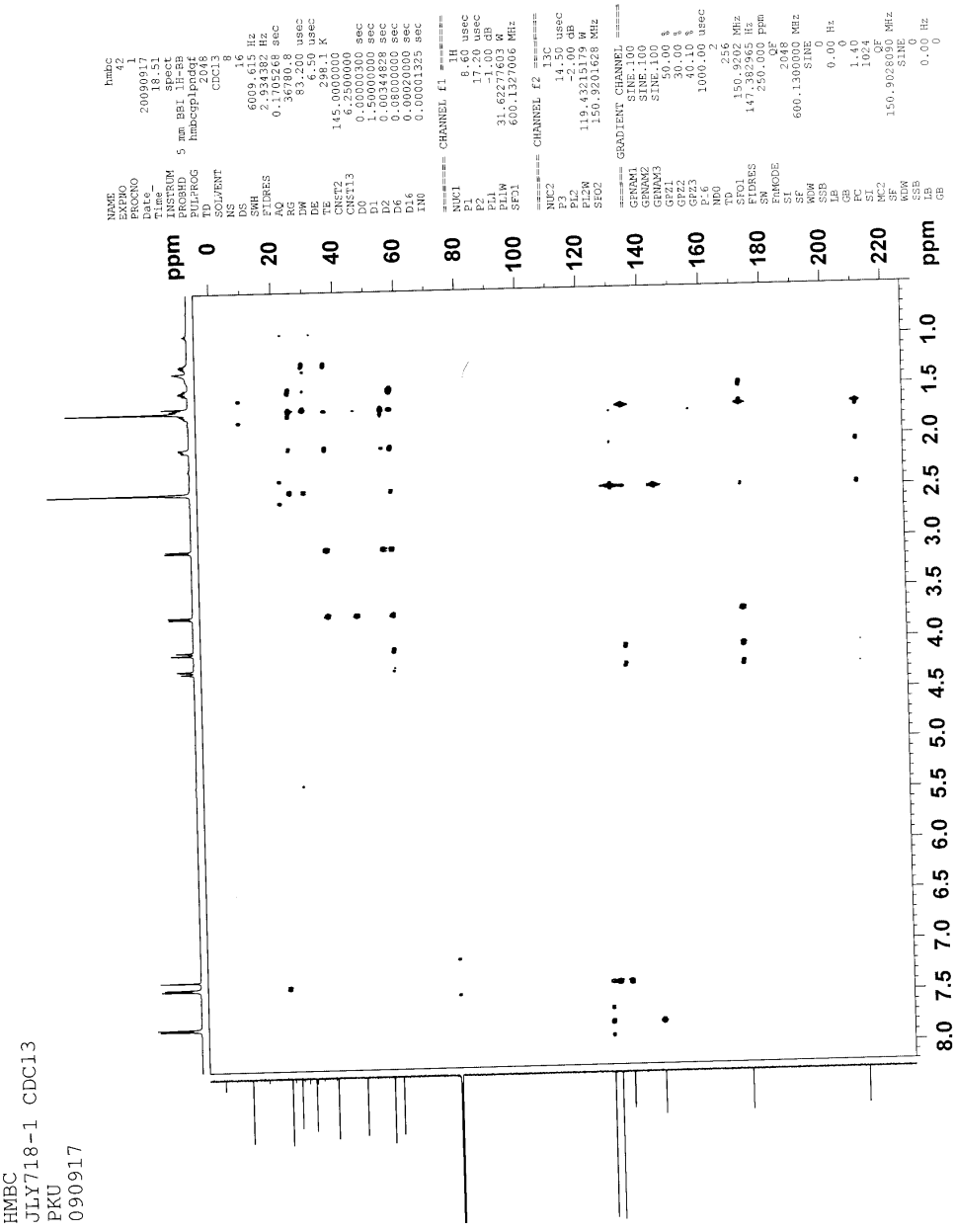
^{13}C NMR (ppm)

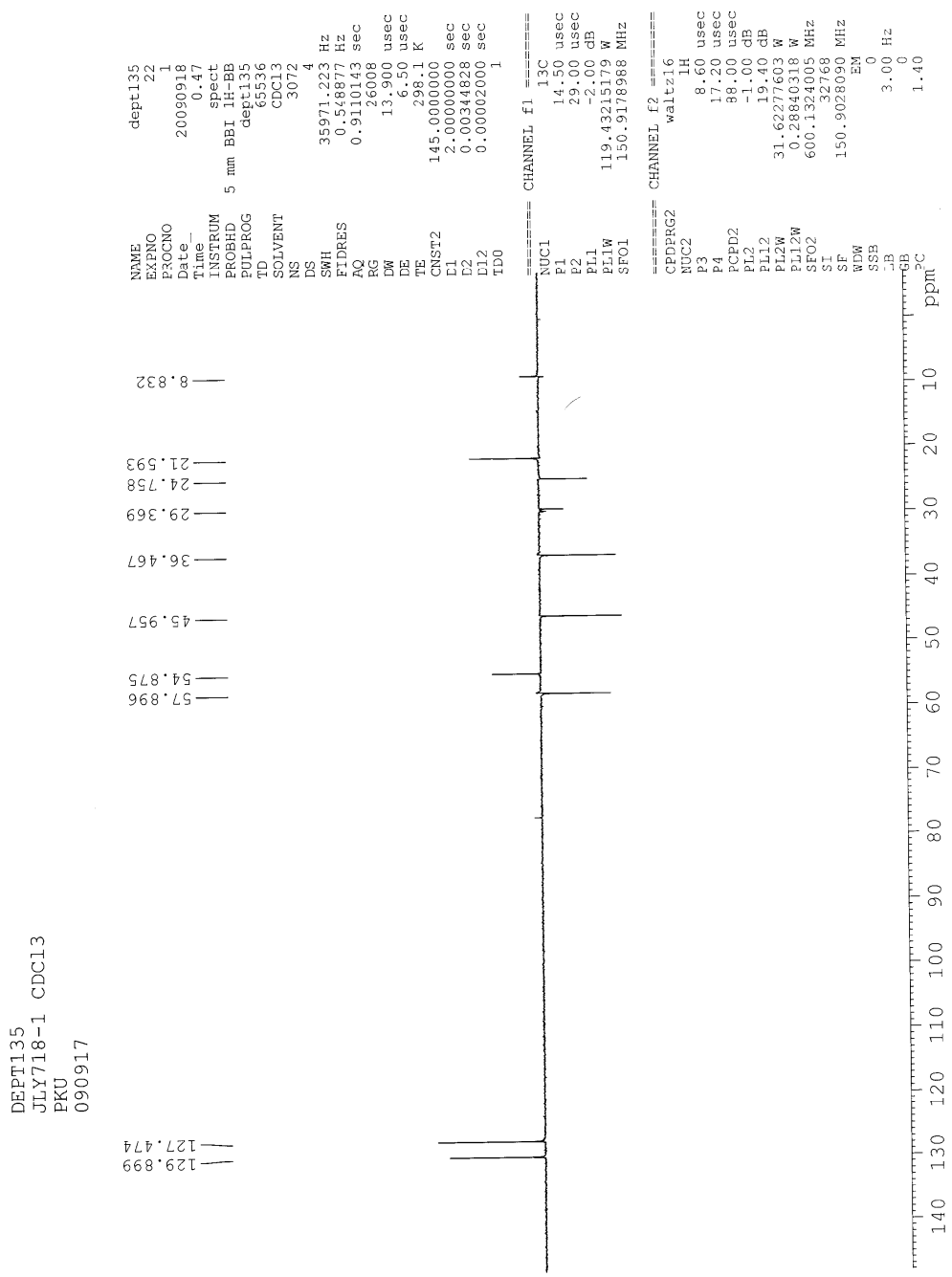


HSQC
JLY718-1 CDCl3
PKU
090917

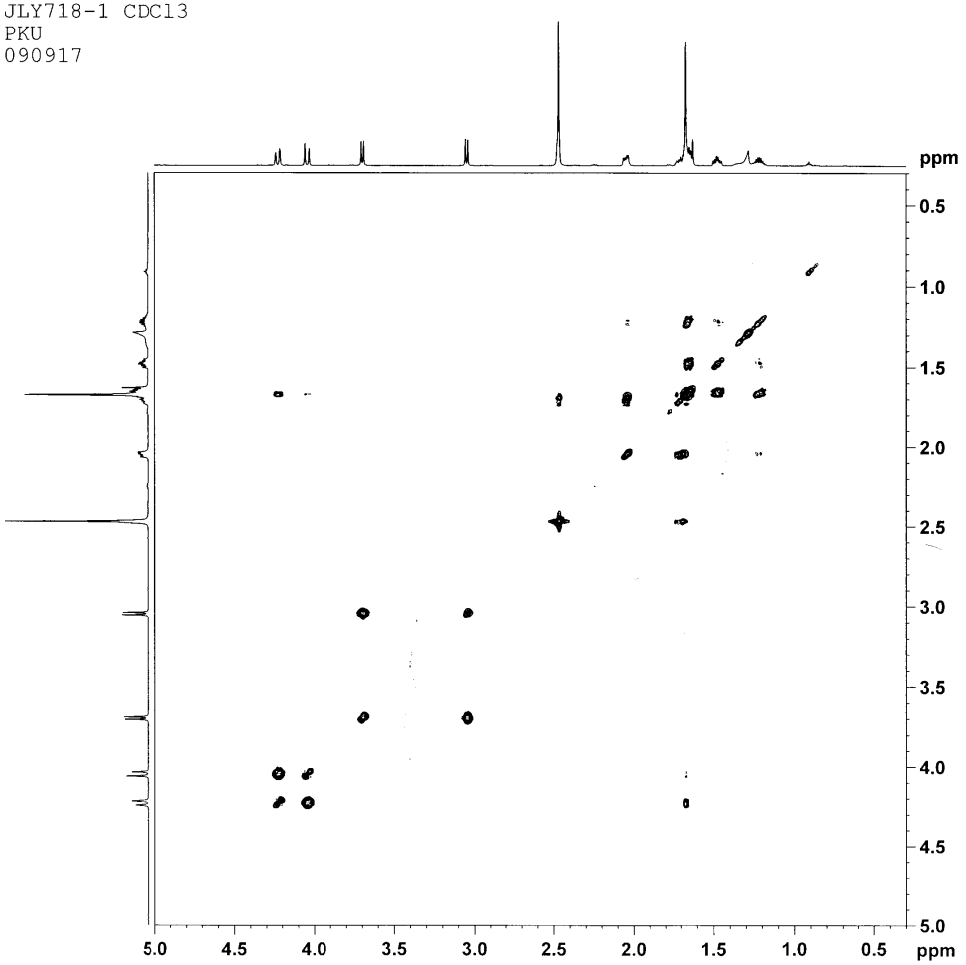


NAME	hsqc
EXPNO	51
PROCNO	1
Date_	20090917
Time	19.52
INSTRUM	spect
PROBHD	5 mm BBI 1H-BB
PULPROG	hsqcetgp
TD	2048
SOLVENT	CDCl3
NS	8
DS	16
SWH	6009.615 Hz
FIDRES	2.934382 Hz
AQ	0.1703268 sec
RG	32768
DW	83.200 usec
DE	5.50 usec
TE	298.1 K
CNST2	145.0000000
D0	0.00000300 sec
D1	1.50000000 sec
D4	0.00172414 sec
D11	0.03000000 sec
D13	0.00000400 sec
D16	0.00020000 sec
IN0	0.00001790 sec
ZGOPTNS	
======== CHANNEL f1 ========	
NUC1	1H
P1	8.60 usec
P2	17.20 usec
P28	0.10 usec
PL1	-1.00 dB
PL1W	31.62277603 W
SFO1	600.1327006 MHz
======== CHANNEL f2 ========	
CPDPRG2	garp
NUC2	13C
P3	11.50 usec
P4	29.00 usec
PCPD2	74.00 usec
PL2	-2.00 dB
PL12	12.00 dB
PL2W	119.43211179 W
PL12W	4.75467968 W
SFO2	150.9155357 MHz
======= GRADIENT CHANNEL =====	
GPNAM1	SINE.100
GPNAM2	SINE.100
GPZ1	80.00 %
GPZ2	20.10 %
P16	1000.00 usec
ND0	2
TD	256
SFO1	150.9156 MHz
FIDRES	109.060127 Hz
SW	185.000 ppm
FnMODE	Echo-Antiecho
SI	1024
SF	600.1300000 MHz
WDW	SINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	echo-antiecho
SF	150.9023090 MHz
WDW	SINE
SSB	2
LB	0.00 Hz
GB	0

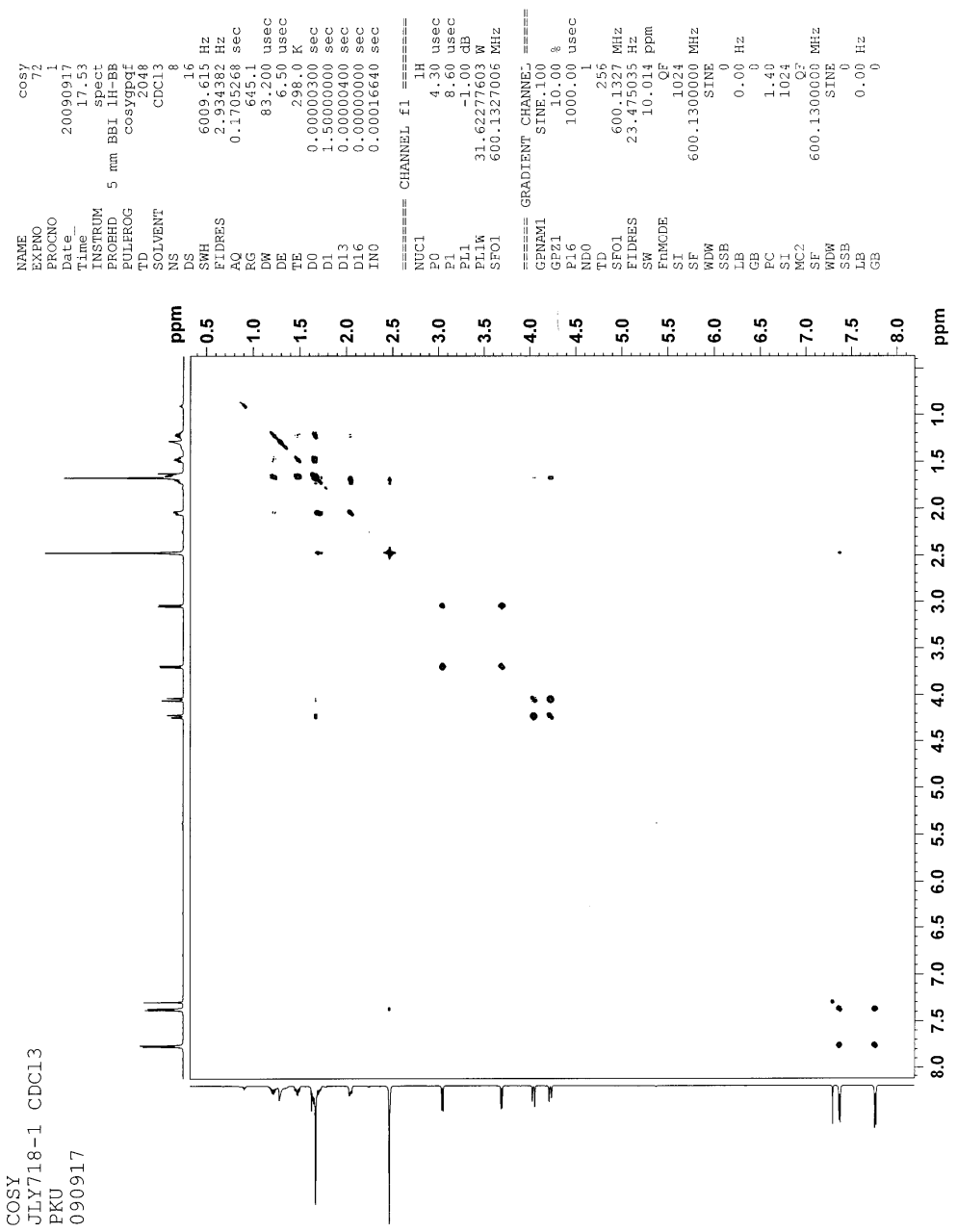

HMBC
JLY718-1 CDC13
PKU
090917
ppm
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
0 20 40 60 80 100 120 140 160 180 200 220 ppm

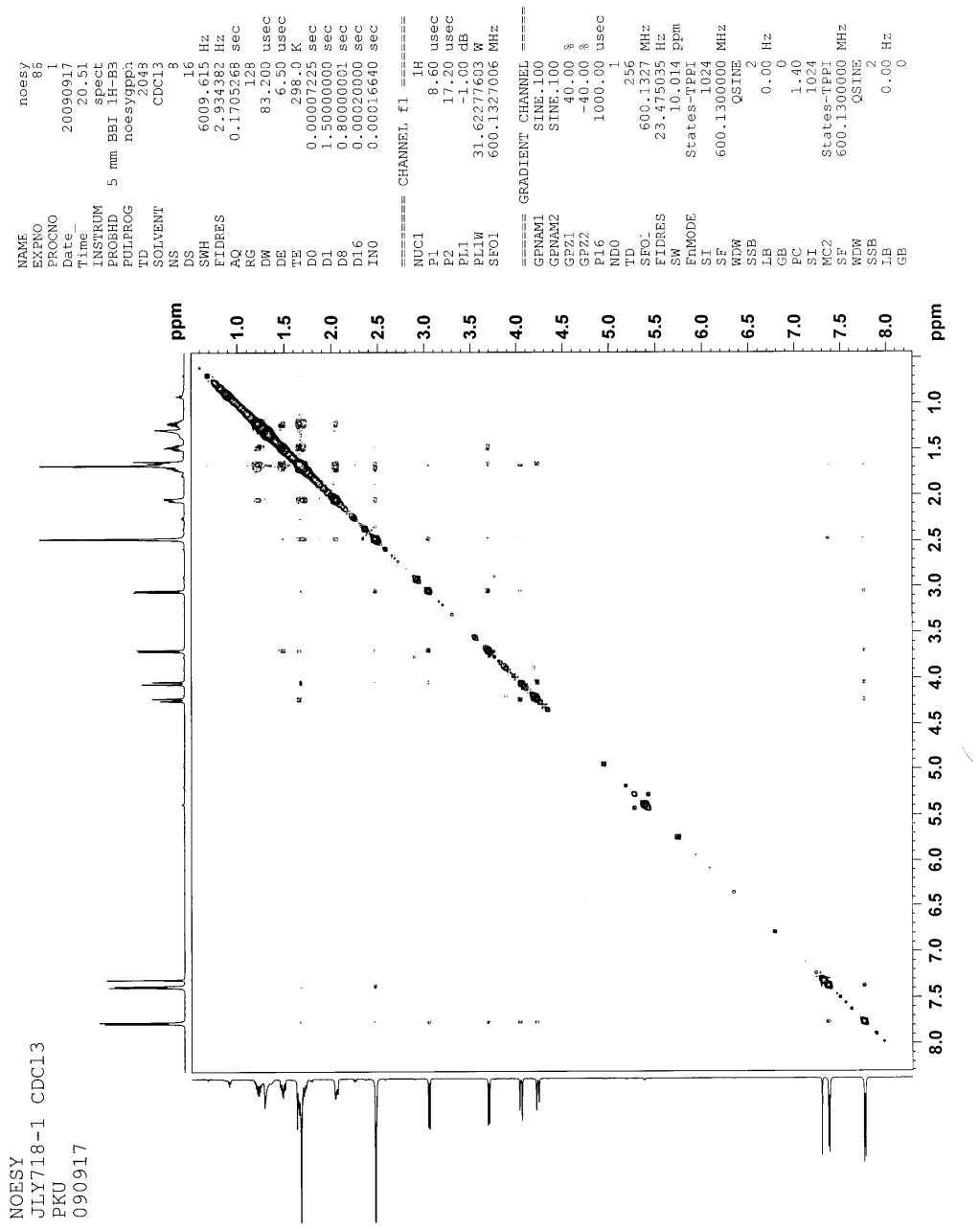

DEPT135
JLY718-1 CDC13
PKU
090917
8.832
21.593
24.758
29.369
36.467
45.957
54.875
57.896
127.474
129.899
dept135
22
1
20090918
0.47
spect
5 mm BBI 1H-BB
dept135
65536
CDCl3
3072
4
35971.223 Hz
0.548877 Hz
0.91110143 sec
26008
13.900 usec
6.50 usec
298.1 K
145.00000000
2.00000000 sec
0.00344828 sec
0.00002000 sec
1
CHANNEL f1
13C
14.50 usec
29.00 usec
-2.00 dB
119.43215179 W
150.9178988 MHz
CHANNEL f2
waltz16
1H
8.60 usec
17.20 usec
88.00 usec
-1.00 dB
19.40 dB
31.62277603 W
0.28840318 W
600.1324005 MHz
32768
150.9028090 MHz
EM
0
3.00 Hz
0
1.40
ppm

COSY
JLY718-1 CDCl3
PKU
090917



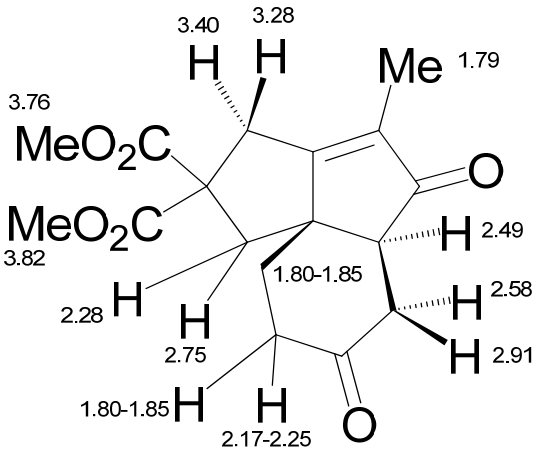
NAME	cosy
EXPNO	72
PROCNO	1
Date_	20090917
Time	17.53
INSTRUM	spect
PROBHD	5 mm BBI 1H-BB
PULPROG	cosygpqf
TD	2048
SOLVENT	CDCl3
NS	8
DS	16
SWH	6009.615 Hz
FIDRES	2.934382 Hz
AQ	0.1705268 sec
RG	645.1
DW	83.200 usec
DE	6.50 usec
TE	298.0 K
D0	0.00000300 sec
D1	1.50000000 sec
D13	0.00000400 sec
D16	0.00000000 sec
IN0	0.00016640 sec
======== CHANNEL f1 ========	
NUC1	1H
P0	4.30 usec
P1	8.60 usec
PL1	-1.00 dB
PL1W	31.62277603 W
SFO1	600.1327006 MHz
====== GRADIENT CHANNEL =====	
GPNAM1	SINE.100
GPZ1	10.00 %
P16	1000.00 usec
ND0	1
TD	256
SFO1	600.1327 MHz
FIDRES	23.475035 Hz
SW	10.014 ppm
FnMODE	QF
SI	1024
SF	600.1300000 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	QF
SF	600.1300000 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0


COSY
JLY718-1 CDC13
PKU
090917
NAME cosy
EXPNO 72
PROCNO 1
Date_ 20090917
Time 17.53
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG cosygpqf
TD 2048
SOLVENT CDC13
NS 8
DS 16
SWH 6009.615 Hz
FIDRES 2.934382 Hz
AQ 0.1705268 sec
RG 645.1
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D0 0.00000300 sec
D1 1.50000000 sec
D13 0.00000400 sec
D16 0.00000000 sec
IN0 0.00016640 sec
======== CHANNEL f1 ========
NUC1 1H
P0 4.30 usec
P1 8.60 usec
PL1 -1.00 dB
PL1W 31.62277603 W
SFO1 600.1327006 MHz
====== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPZ1 10.00 %
P16 1000.00 usec
ND0 1
TD 256
SFO1 600.1327 MHz
FIDRES 23.475035 Hz
SW 10.014 ppm
FnMODE QF
SI 1024
SF 600.1300000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 QF
SF 600.1300000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
ppm
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0
7.5
8.0

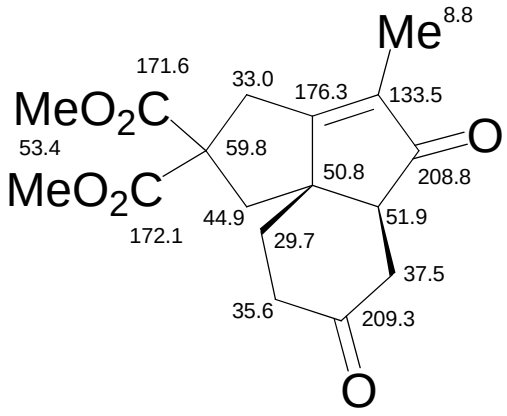

NOESY
JLY718-1 CDC13
PKU
090917
NAME noesy
EXPNO 86
PROCNO 1
Date_ 20090917
Time_ 20.51
INSTRUM spect
PROBHD 5 mm BBI 1H-B3
PULPROG noesygpph
TD 2048
SOLVENT CDC13
NS 8
DS 16
SWH 6009.615 Hz
FIDRES 2.934382 Hz
AQ 0.1705268 sec
RG 128
DW 83.200 usec
DE 6.50 usec
TE 298.0 K
D0 0.00007225 sec
D1 1.50000000 sec
D8 0.80000001 sec
D16 0.00020000 sec
IN0 0.00016640 sec
======== CHANNEL f1 ========
NUC1 1H
P1 8.60 usec
P2 17.20 usec
PL1 1.00 dB
PL1W 31.62277603 W
SFO1 600.1327006 MHz
======= GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPZ1 40.00 %
GPZ2 -40.00 %
P16 1000.00 usec
ND0 1
TD 256
SFO1 600.1327 MHz
FIDRES 23.475035 Hz
SW 10.014 ppm
FnMODE States-TPPI
SI 1024
SF 600.1300000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 States-TPPI
SF 600.1300000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
ppm
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0
7.5
8.0

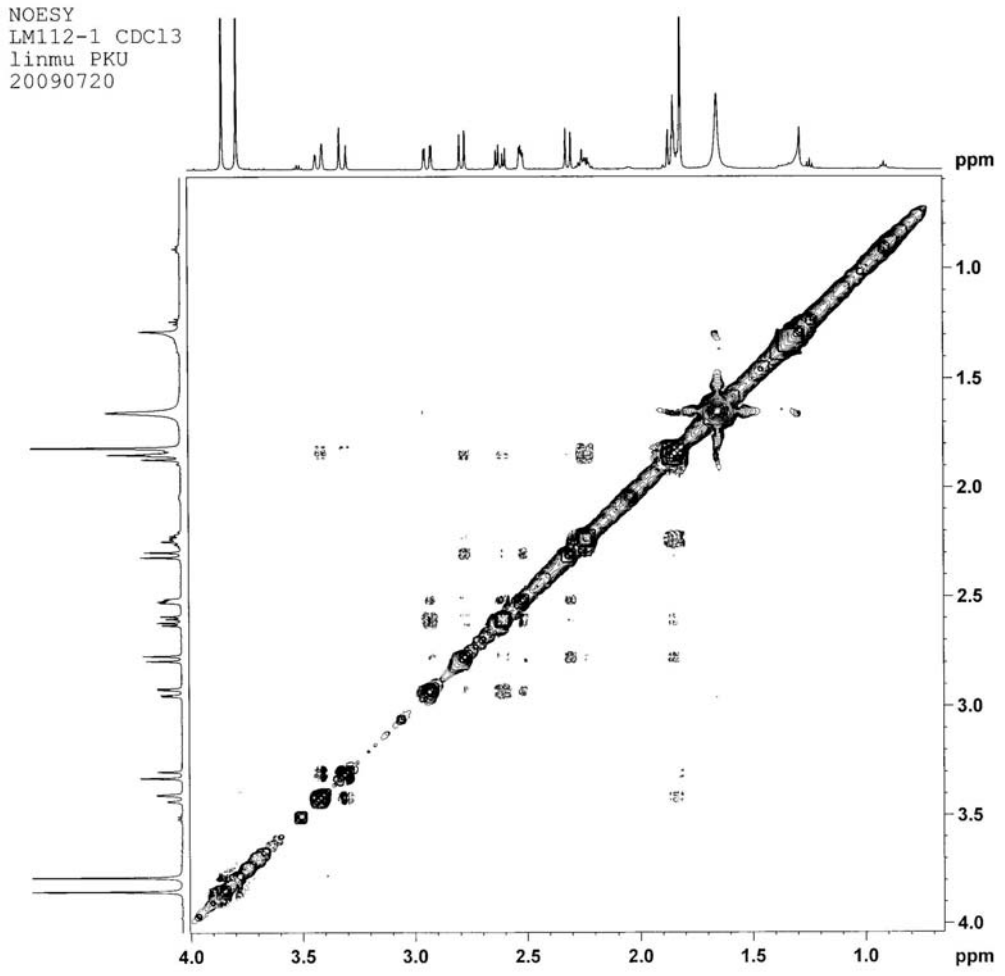
Compound **2h**:

^{1}H NMR (ppm)

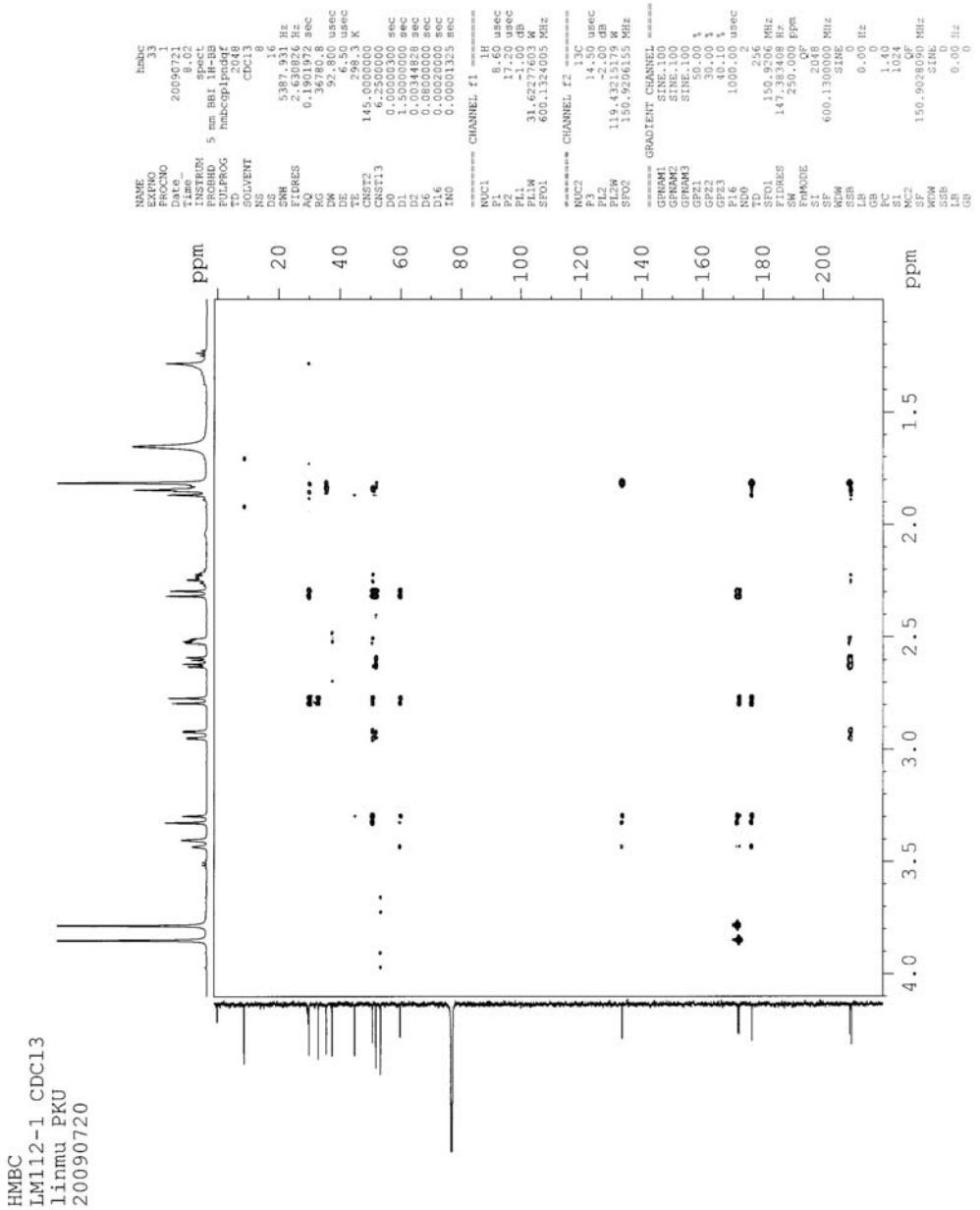


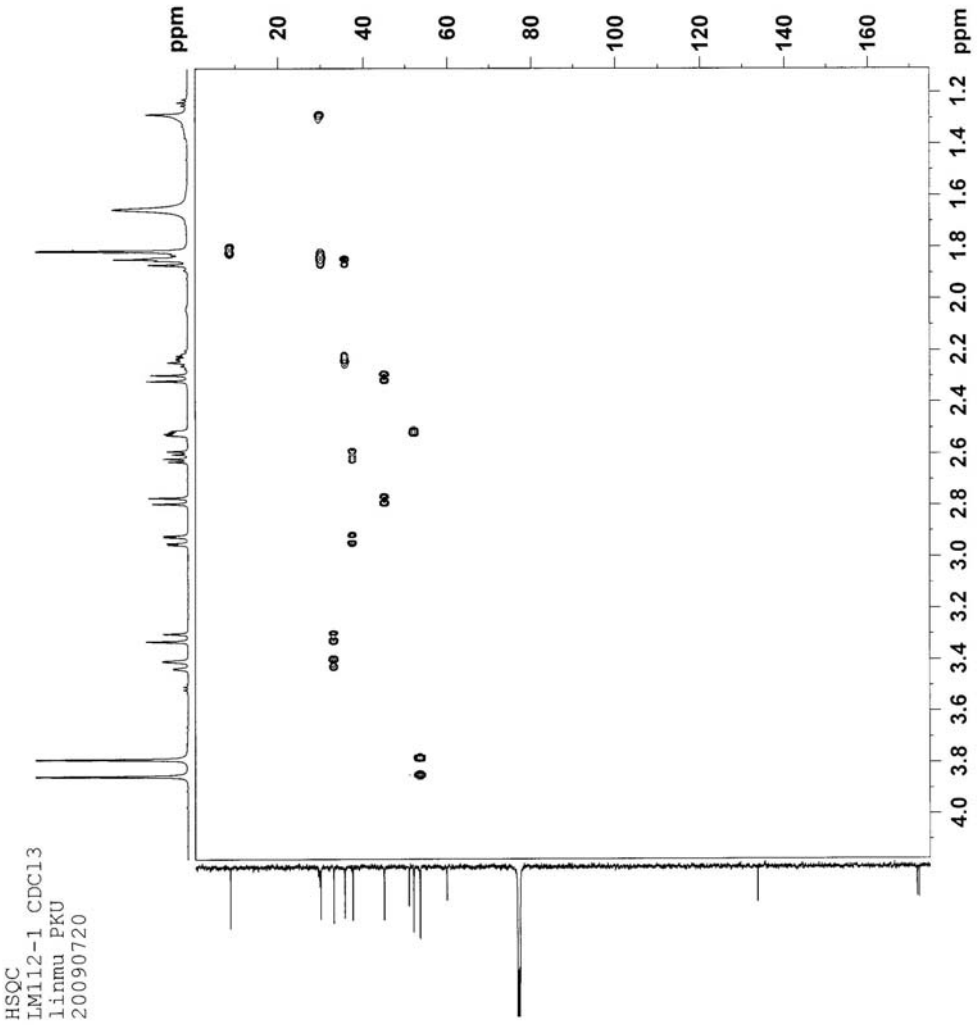
^{13}C NMR (ppm)



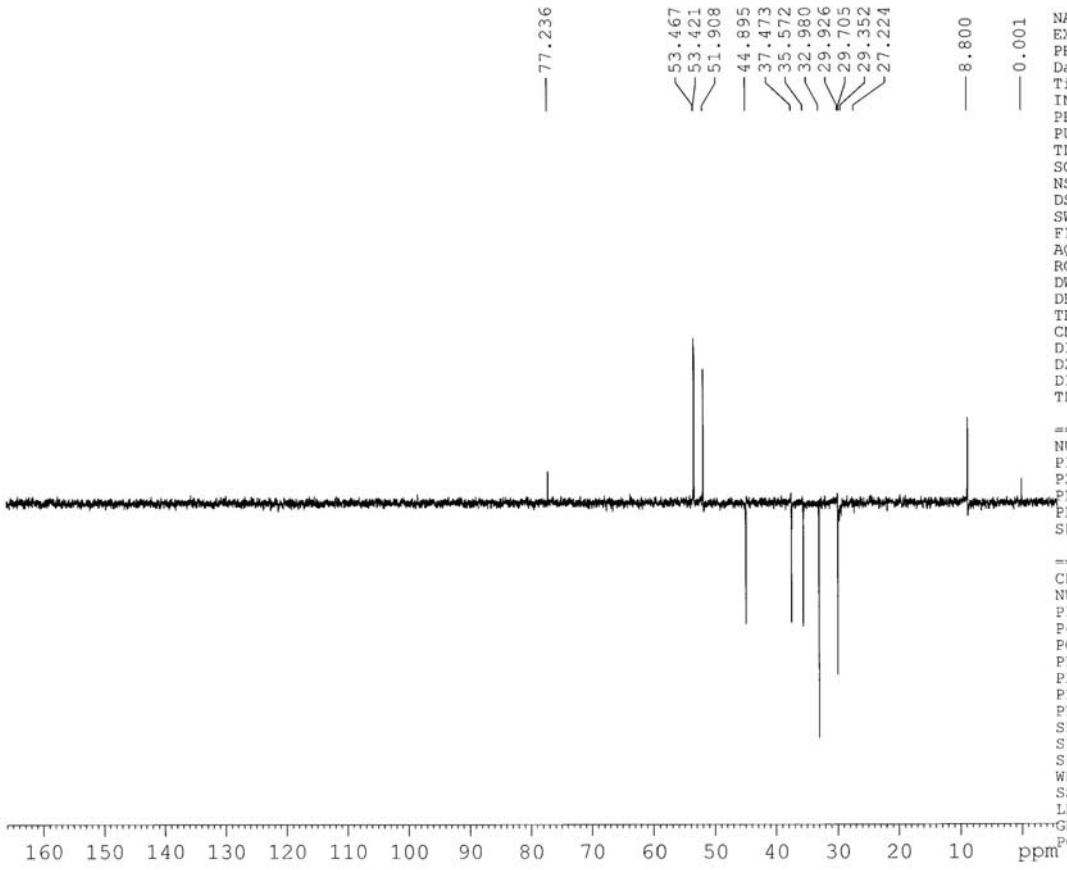


NAME	noesy	
EXPNO	65	
PROCNO	1	
Date_	20090720	
Time	17.58	
INSTRUM	spect	
PROBHD	5 mm BBI 1H-BB	
PULPROG	noesygpph	
TD	2048	
SOLVENT	CDCl3	
NS	8	
DS	16	
SWH	5387.931	Hz
FIDRES	2.630826	Hz
AQ	0.1901972	sec
RG	161.3	
DW	92.800	usec
DE	6.50	usec
TE	298.3	K
D0	0.00008185	sec
D1	1.50000000	sec
D8	0.80000001	sec
D16	0.00020000	sec
IN0	0.00018560	sec
======== CHANNEL f1 ========		
NUC1	1H	
P1	8.60	usec
P2	17.20	usec
PL1	-1.00	dB
PL1W	31.62277603	W
SFO1	600.1324005	MHz
====== GRADIENT CHANNEL =====		
GPNAM1	SINE.100	
GPNAM2	SINE.100	
GPZ1	40.00	%
GPZ2	-40.00	%
P16	1000.00	usec
ND0	1	
TD	256	
SFO1	600.1324	MHz
FIDRES	21.046597	Hz
SW	8.978	ppm
FnMODE	States-TPPI	
SI	1024	
SF	600.1300000	MHz
WDW	QSINE	
SSB	2	
LB	0.00	Hz
GB	0	
PC	1.40	
SI	1024	
MC2	States-TPPI	
SF	600.1300000	MHz
WDW	QSINE	
SSB	2	
LB	0.00	Hz
GB	0	


HMBC
LM112-1 CDCl3
linmu PKU
20090720
ppm
ppm

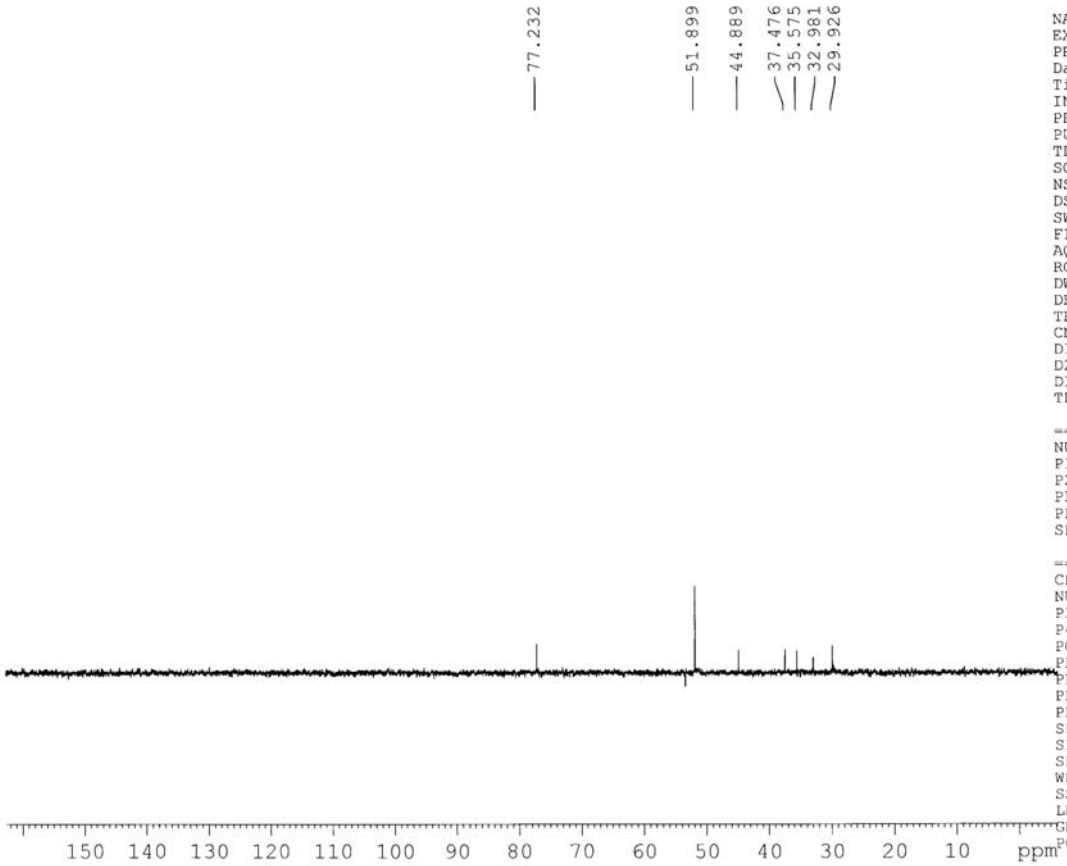

HSQC
LM112-1 CDCl3
linmu PKU
20090720
ppm
20
40
60
80
100
120
140
160
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
ppm

DEPT135
LM112-1 CDCl3
lin Mu PKU
20090722

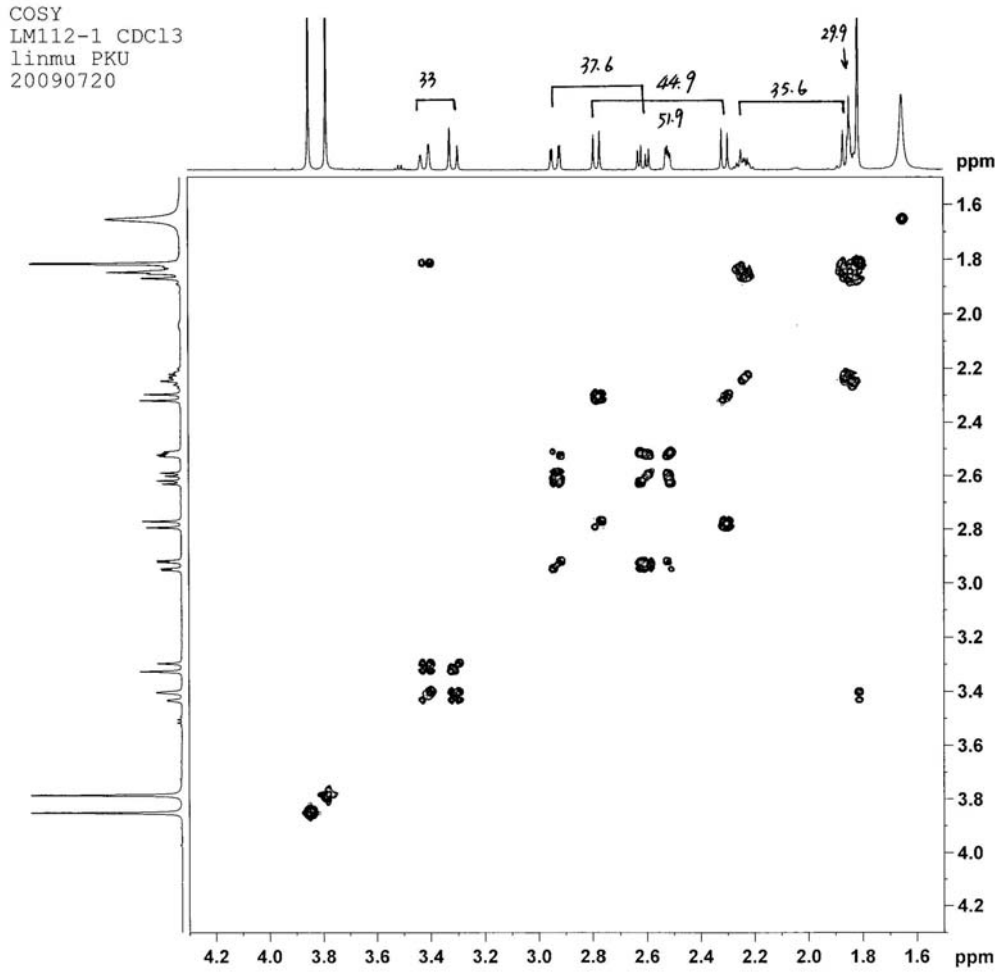


NAME	dept135
EXPNO	11
PROCNO	1
Date_	20090722
Time	11.59
INSTRUM	spect
PROBHD	5 mm BBI 1H-BB
PULPROG	dept135
TD	32768
SOLVENT	CDCl3
NS	3802
DS	8
SWH	35971.223 Hz
FIDRES	1.097755 Hz
AQ	0.4555391 sec
RG	26008
DW	13.900 usec
DE	6.50 usec
TE	298.2 K
CNST2	145.0000000
D1	1.50000000 sec
D2	0.00344828 sec
D12	0.00002000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	13.10 usec
P2	26.20 usec
PL1	-2.00 dB
PL1W	119.43215179 W
SFO1	150.9194083 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
P3	8.40 usec
P4	16.80 usec
PCPD2	88.00 usec
PL2	-1.00 dB
PL12	19.40 dB
PL2W	31.62277603 W
PL12W	0.28840318 W
SFO2	600.1324005 MHz
SI	32768
SF	150.9028090 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.20

DPET90
LM112-1 CDCl3
linmu PKU
20090720



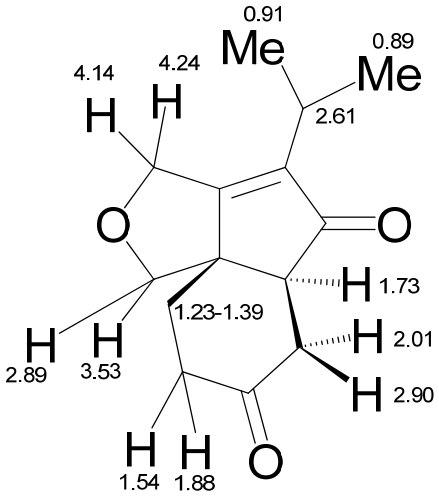
NAME	dept90	
EXPNO	5	
PROCNO	1	
Date_	20090721	
Time	2.15	
INSTRUM	spect	
PROBHD	5 mm BBI 1H-BB	
PULPROG	dept90	
TD	32768	
SOLVENT	CDCl3	
NS	2048	
DS	0	
SWH	37593.984	Hz
FIDRES	1.147277	Hz
AQ	0.4358777	sec
RG	23170.5	
DW	13.300	usec
DE	6.50	usec
TE	298.2	K
CNST2	145.0000000	
D1	2.00000000	sec
D2	0.00344828	sec
D12	0.00002000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	14.50	usec
P2	29.00	usec
PL1	-2.00	dB
PL1W	119.43215179	W
SFO1	150.9178988	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
P3	8.40	usec
P4	16.80	usec
PCPD2	88.00	usec
PL2	-1.00	dB
PL12	19.40	dB
PL2W	31.62277603	W
PL12W	0.28840318	W
SFO2	600.1324005	MHz
SI	32768	
SF	150.9028090	MHz
WDW	EM	
SSB	0	
LB	3.00	Hz
GB	0	
PC	1.40	



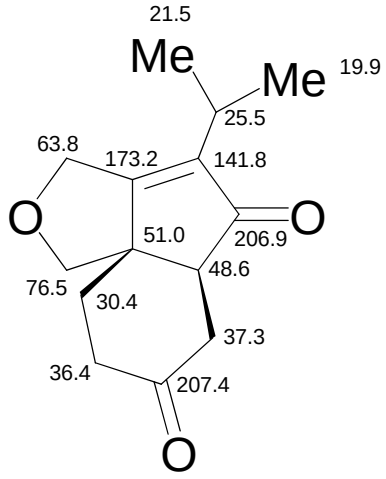
NAME	cosy	
EXPNO	60	
PROCNO	1	
Date_	20090720	
Time	19.24	
INSTRUM	spect	
PROBHD	5 mm BBI 1H-BB	
PULPROG	cosygpqf	
TD	2048	
SOLVENT	CDCl3	
NS	8	
DS	16	
SWH	5387.931	Hz
FIDRES	2.630826	Hz
AQ	0.1901972	sec
RG	812.7	
DW	92.800	usec
DE	6.50	usec
TE	298.4	K
D0	0.00000300	sec
D1	1.50000000	sec
D13	0.00000400	sec
D16	0.00000000	sec
IN0	0.00018560	sec
======== CHANNEL f1 ========		
NUC1	1H	
P0	4.30	usec
P1	8.60	usec
PL1	-1.00	dB
PL1W	31.62277603	W
SFO1	600.1324005	MHz
====== GRADIENT CHANNEL ======		
GPNAM1	SINE.100	
GPZ1	10.00	%
P16	1000.00	usec
ND0	1	
TD	256	
SFO1	600.1324	MHz
FIDRES	21.046597	Hz
SW	8.978	ppm
FnMODE	QF	
SI	1024	
SF	600.1300000	MHz
WDW	SINE	
SSB	0	
LB	0.00	Hz
GB	0	
PC	1.40	
SI	1024	
MC2	QF	
SF	600.1300000	MHz
WDW	SINE	
SSB	0	
LB	0.00	Hz
GB	0	

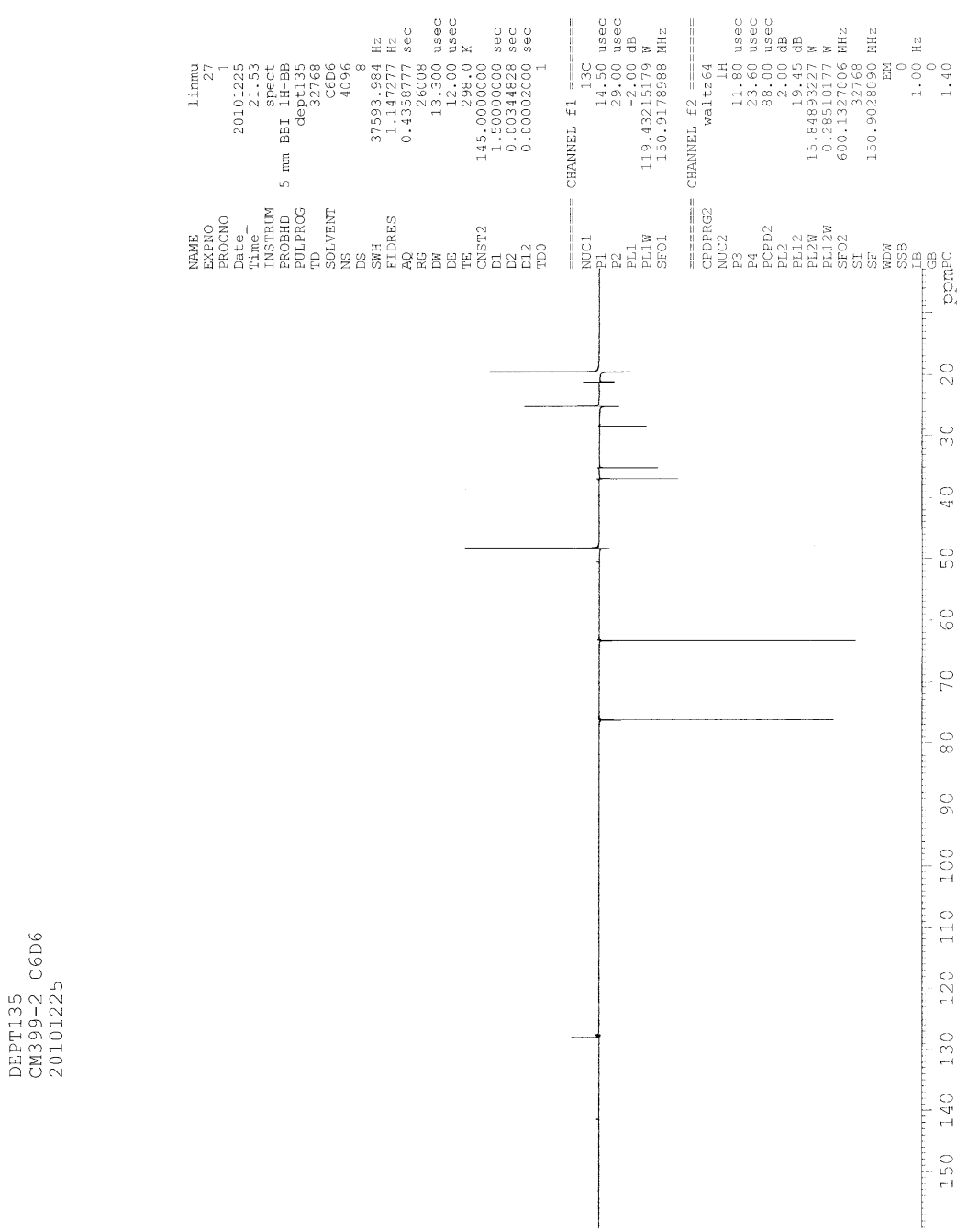
Compound **2k**:

^{1}H NMR (ppm):

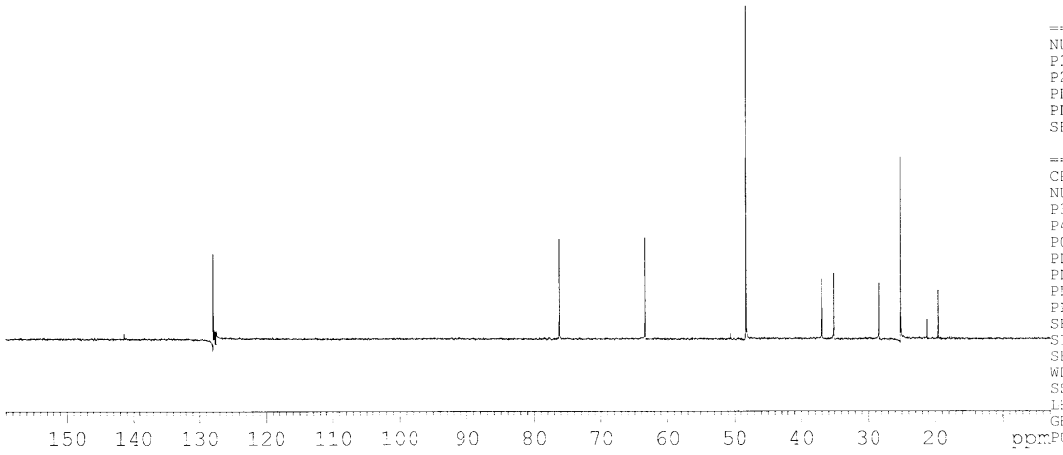


^{13}C NMR (ppm):

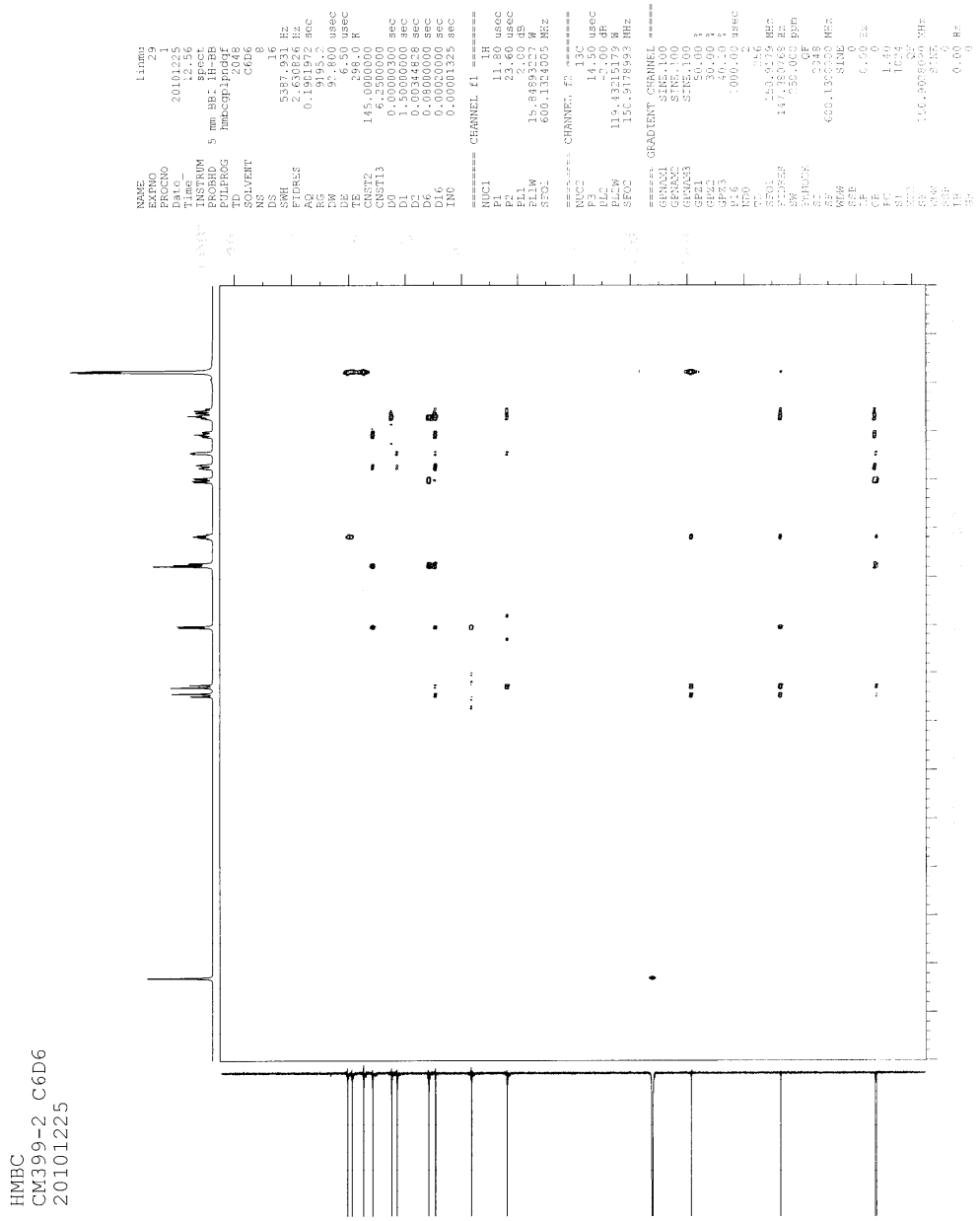


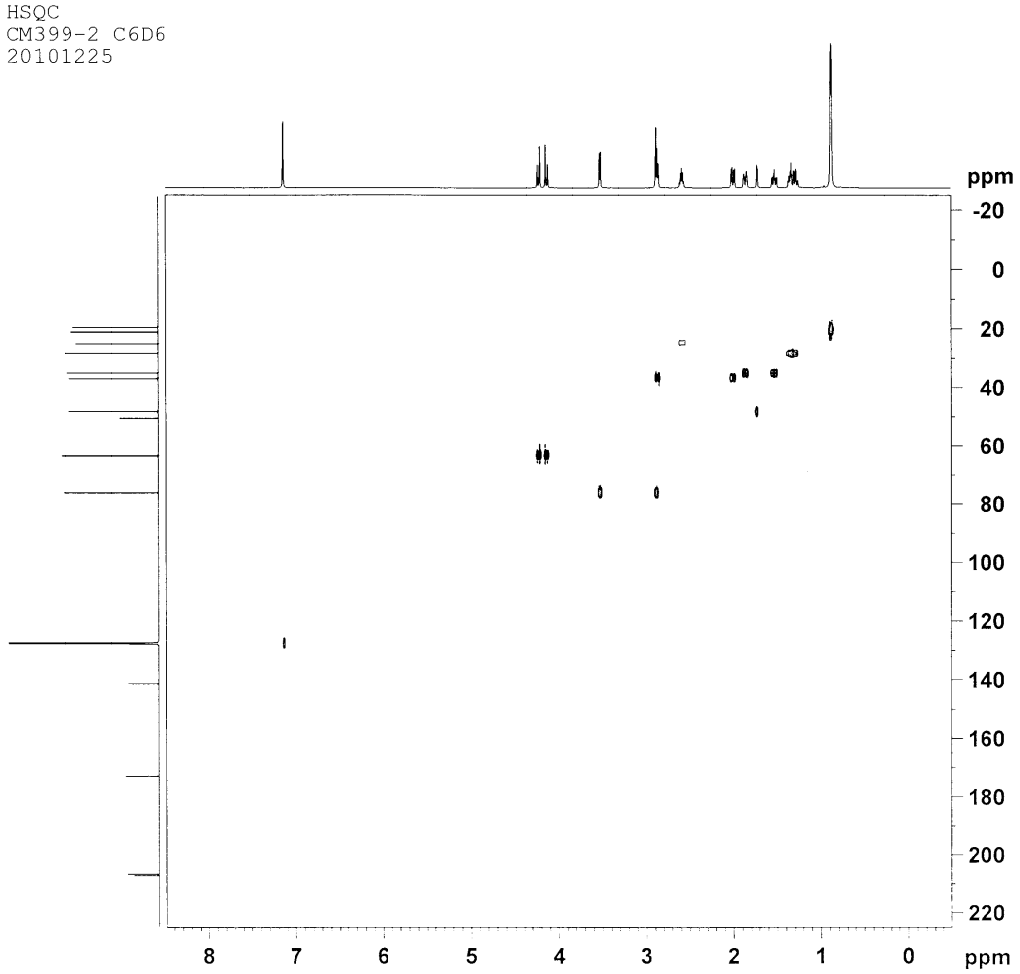

DEPT135
CM399-2 C6D6
20101225
linmu
27
1
20101225
21.53
spect
5 mm BBI 1H-BB
dept135
32768
C6D6
4096
8
37593.984 Hz
1.147277 Hz
0.4358777 sec
26008
13.300 usec
12.00 usec
298.0 K
145.0000000
1.50000000 sec
0.00344828 sec
0.00002000 sec
1
13C
14.50 usec
29.00 usec
-2.00 dB
119.4321179 W
150.9178988 MHz
waltz64
1H
11.80 usec
23.60 usec
88.00 usec
2.00 dB
19.45 dB
15.84993227 W
0.28510177 W
600.1327006 MHz
32768
150.9028090 MHz
EM
0
1.00 Hz
0
1.40
ppm

DPET90
CM399-2 C6D6
20101225



NAME	linmu
EXPNO	28
PROCNO	1
Date_	20101225
Time	19.37
INSTRUM	spect
PROBHD	5 mm BBI 1H-BB
PULPROG	dept90
TD	32768
SOLVENT	C6D6
NS	4096
DS	0
SWH	37593.984 Hz
FIDRES	1.147277 Hz
AQ	0.4358777 sec
RG	23170.5
DW	13.300 usec
DE	6.50 usec
TE	298.0 K
CNST2	145.0000000
D1	1.50000000 sec
D2	0.00344828 sec
D12	0.00002000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	14.50 usec
P2	29.00 usec
PL1	-2.00 cB
PL1W	119.43215179 W
SFO1	150.9178988 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
P3	11.80 usec
P4	23.60 usec
PCPD2	88.00 usec
PL2	2.00 dB
PL12	19.45 dB
PL2W	15.84893227 W
PL12W	0.28510177 W
SFO2	600.1324005 MHz
SI	32768
SF	150.9028090 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40


HMBC
CM399-2 C6D6
20101225

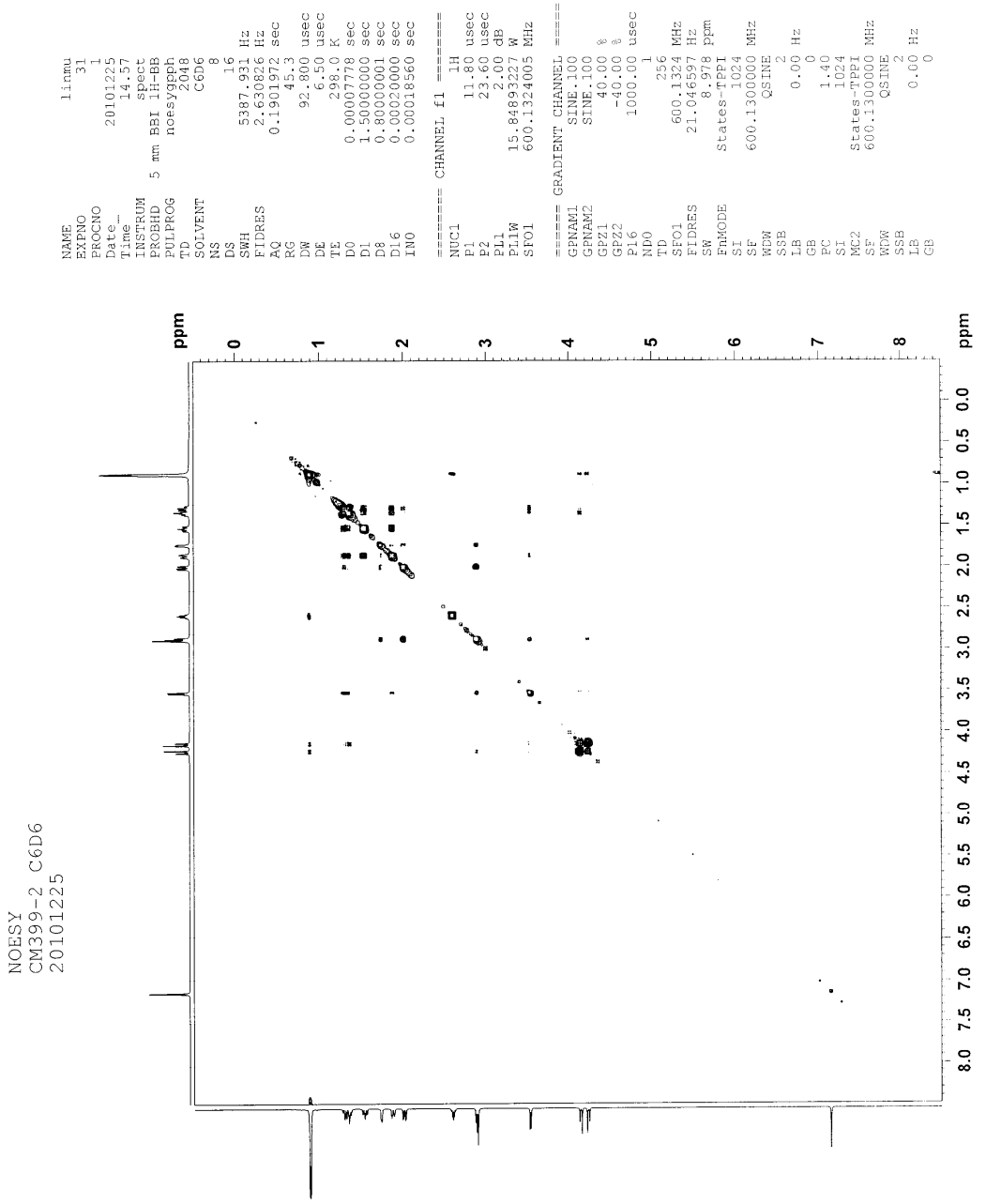


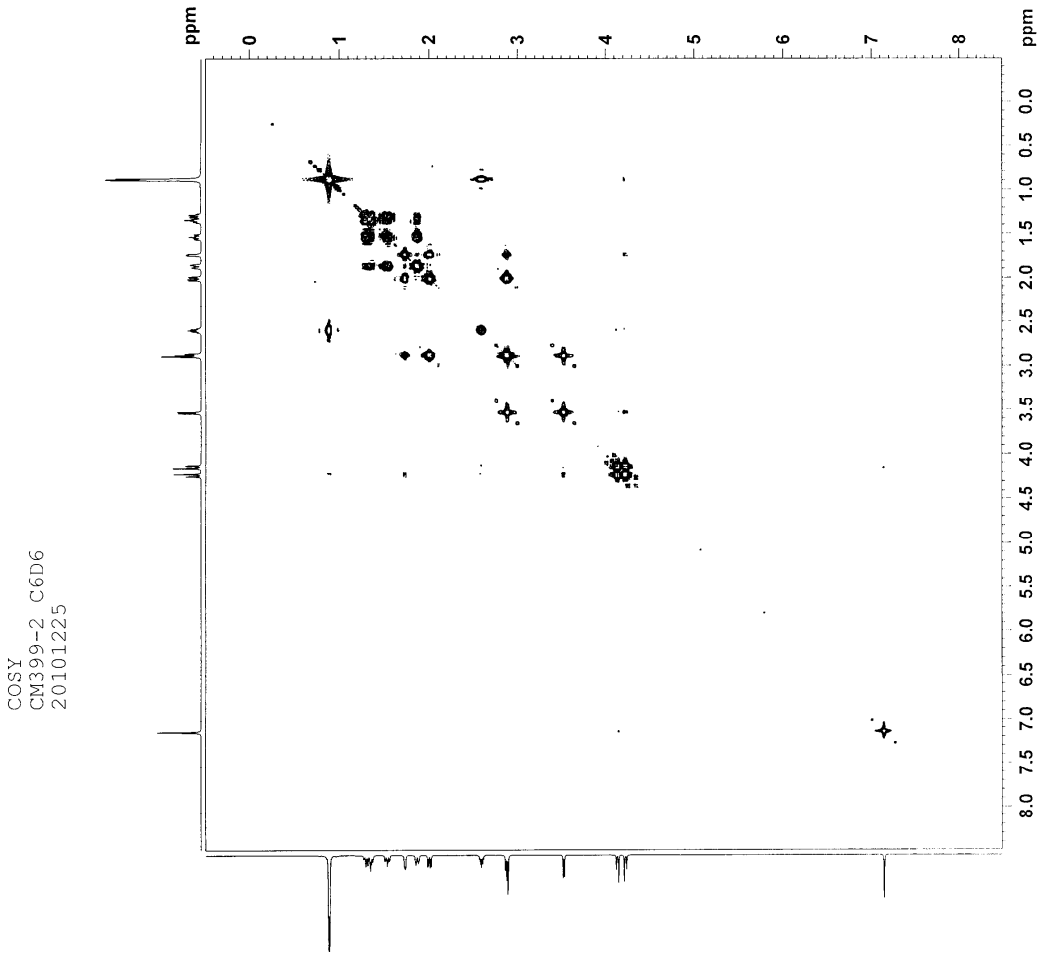
NAME 1inmu
EXPNO 30
PROCNO 1
Date_ 20101225
Time 13.58
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG hsqcetgp
TD 2048
SOLVENT C6D6
NS 8
DS 16
SWH 5387.931 Hz
FIDRES 2.630826 Hz
AQ 0.1901972 sec
RG 13004
DW 92.800 usec
DE 6.00 usec
TE 298.6 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
TN0 0.00001325 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1 1H
P1 11.80 usec
P2 23.60 usec
P28 0.10 usec
PL1 2.00 dB
PL1W 15.84893227 W
SFO1 600.1324005 MHz

======== CHANNEL f2 ========
GPPRG2 garp
NUC2 13C
P3 14.50 usec
P4 29.00 usec
PCPD2 60.00 usec
PL2 -2.00 dB
PL12 10.34 dB
PL2W 119.43215179 W
PL12W 6.96821022 W
SFO2 150.9174993 MHz

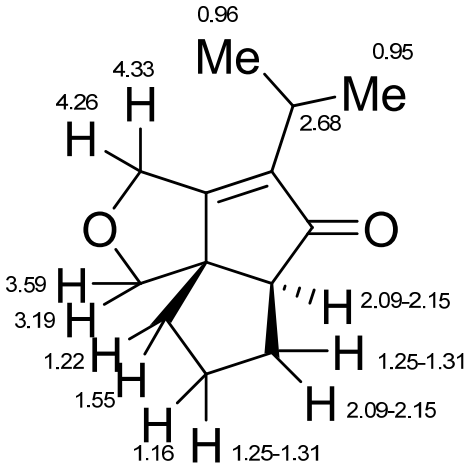
====== GRADIENT CHANNEL
GPNAM1 SINE.100
GPNAM2 SINE.100
GPZ1 80.09
GPZ2 20.19
P16 1000.00 usec
NDW 2
TD 256
SFO1 150.9179 MHz
FIDRES 147.380768 Hz
SW 250.000 ppm
FnMODE Echo-AntiEcho
SI 2024
SF 600.1300000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 echo-antiecho
SF 150.9026094 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0


NOESY
CM399-2 C6D6
20101225
ppm
ppm
NAME CM399-2 C6D6
EXPNO 31
PROCNO 1
Date_ 20101225
Time 14.57
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG noesygpph
TD 2048
SOLVENT C6D6
NS 8
DS 16
SWH 5387.931 Hz
FIDRES 2.630826 Hz
AQ 0.1901972 sec
RG 45.3
DW 92.800 usec
DE 6.50 usec
TE 298.0 K
D0 0.00007778 sec
D1 1.50000000 sec
D8 0.80000001 sec
D16 0.00020000 sec
IN0 0.00018560 sec
======== CHANNEL f1 ========
NUC1 1H
P1 11.80 usec
P2 23.60 usec
PL1 2.00 dB
PL1W 15.84893227 W
SFO1 600.1324005 MHz
====== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPZ1 40.00 %
GPZ2 -40.00 %
P16 1000.00 usec
NDO 1
TD 256
SFO1 600.1324 MHz
FIDRES 21.046597 Hz
SW 8.978 ppm
FnMODE States-TPPI
SI 1024
SF 600.1300000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40
SI 1024
MC2 States-TPPI
SF 600.1300000 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

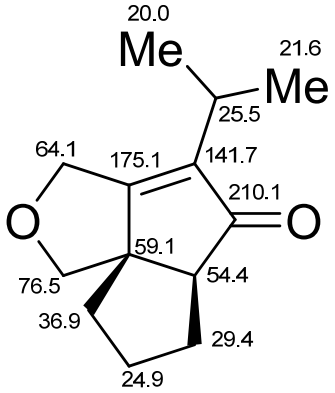

COSY
CM399-2 C6D6
20101225
ppm
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm
NAME lirmu
EXPNO 32
PROCNO 1
Date_ 20101225
Time 16.23
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG cosygpqf
TD 2048
SOLVENT C6D6
NS 8
DS 16
SWH 5387.931 Hz
FIDRES 2.630826 Hz
AQ 0.1901972 sec
RG 57
DW 92.800 usec
DE 6.50 usec
TE 298.1 K
D0 0.00000300 sec
D1 1.50000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00018560 sec
======== CHANNEL f1 ========
NUC1 1H
P0 11.80 usec
P1 11.80 usec
PL1 2.00 dB
PL1W 15.84893227 W
SFO1 600.1324005 MHz
====== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPZ1 10.00 %
P16 1000.00 usec
ND0 1
TD 256
SFO1 600.1324 MHz
FIDRES 21.046597 Hz
SW 8.978 ppm
FnMODE QF
SI 1024
SF 600.1300000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 4.00
SI 1024
MC2 QF
SF 600.1300000 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

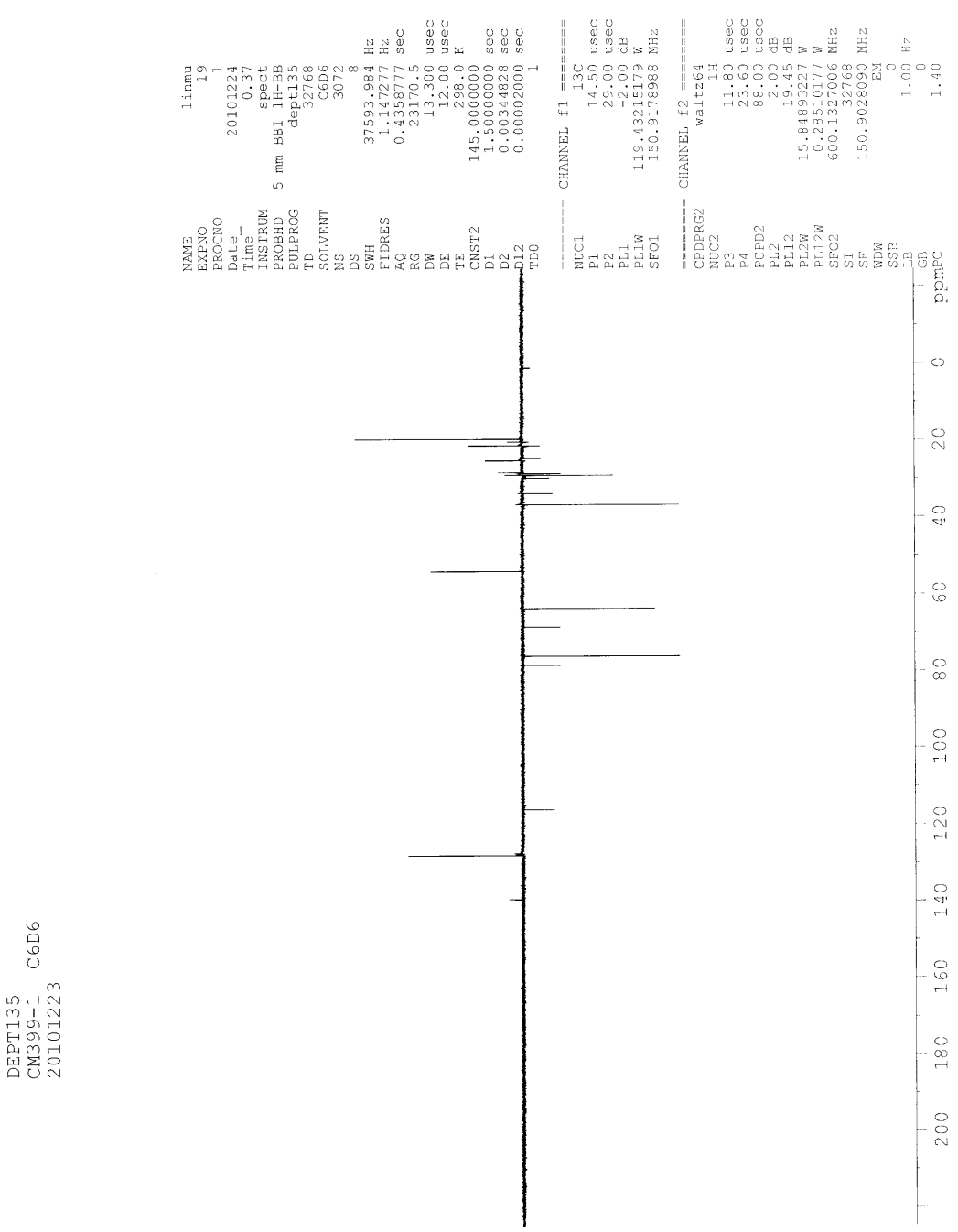
Compound **4k**:

^{1}H NMR (ppm)

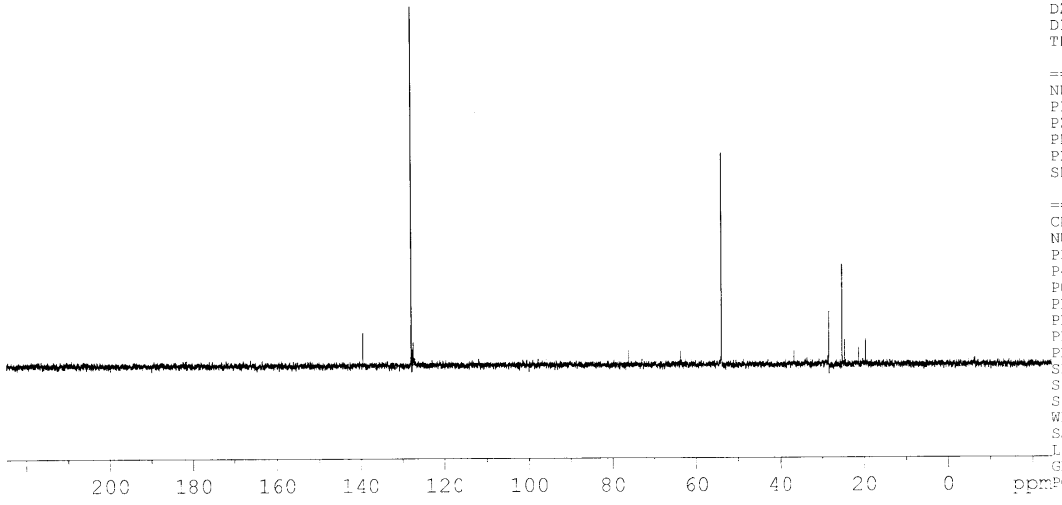


^{13}C NMR (ppm)

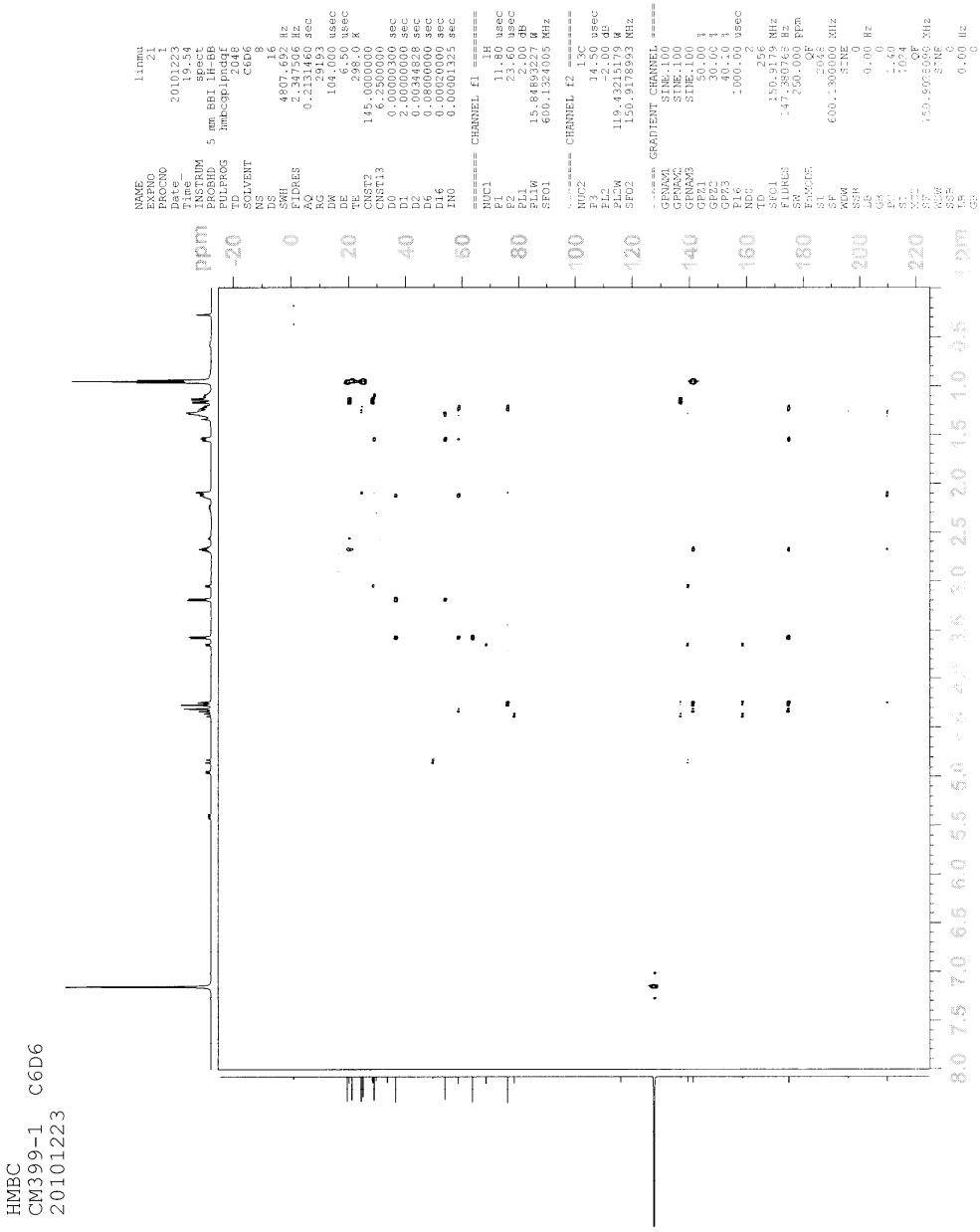


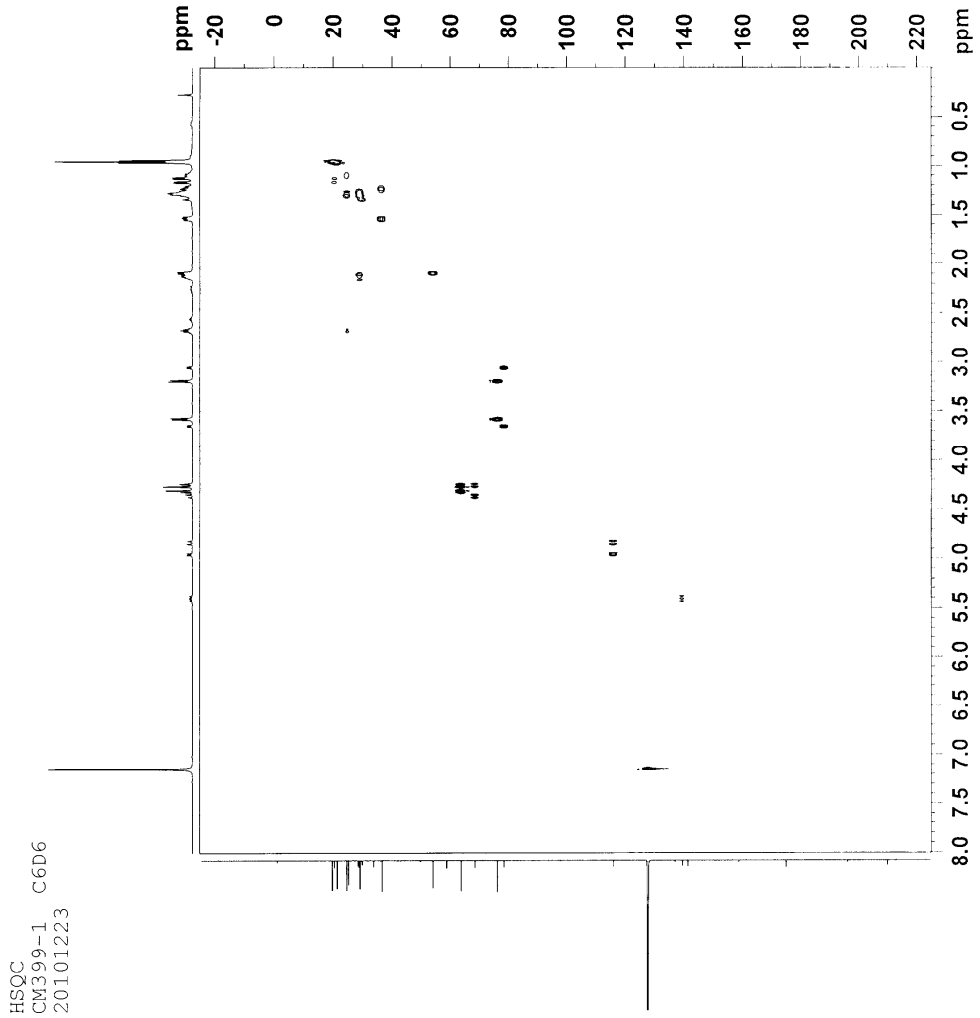

DEPT135
CM399-1 C6D6
20101223
NAME linmu
EXPNO 19
PROCNO 1
Date_ 20101224
Time_ 0.37
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG dept135
TD 32768
SOLVENT C6D6
NS 3072
DS 8
SWH 37593.984 Hz
FIDRES 1.147277 Hz
AQ 0.4358777 sec
RG 23170.5
DW 13.300 usec
DE 12.00 usec
TE 298.0 K
CNST2 145.0000000
D1 1.50000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 14.50 usec
P2 29.00 usec
PL1 -2.00 dB
PL1W 119.43215179 W
SFO1 150.9178988 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz64
NUC2 1H
P3 11.80 usec
P4 23.60 usec
PCPD2 88.00 usec
PL2 2.00 dB
PL12 19.45 dB
PL2W 15.84893227 W
PL12W 0.28510177 W
SFO2 600.1327006 MHz
SI 32768
SF 150.9028090 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm

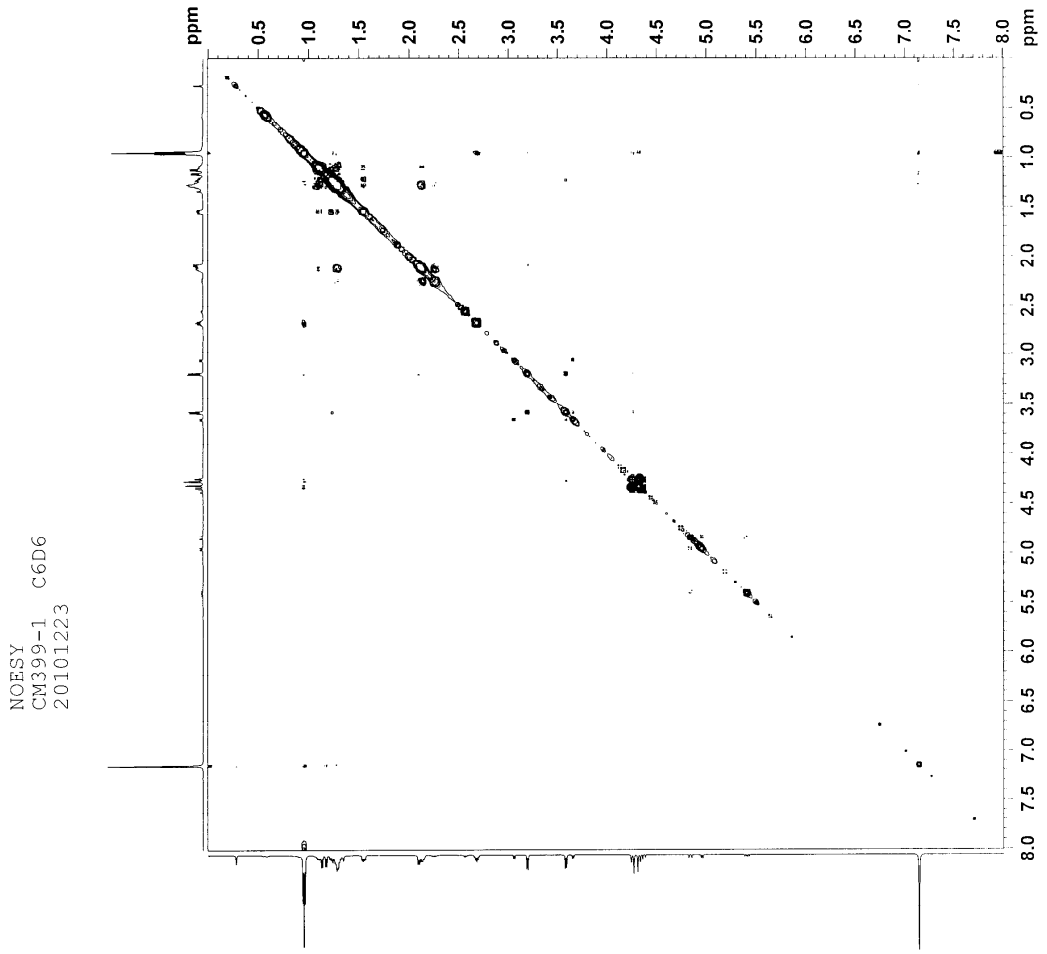
DPET90
CM399-1 C6D6
20101223



NAME	linmu	
EXPNO	20	
PROCNO	1	
Date_	20101223	
Time	22.54	
INSTRUM	spect	
PROBHD	5 mm BBI 1H-BB	
PULPROG	dept90	
TD	32768	
SOLVENT	C6D6	
NS	3072	
DS	0	
SWH	37593.984	Hz
FIDRES	1.147277	Hz
AQ	0.4358777	sec
RG	26008	
DW	13.300	usec
DE	6.50	usec
TE	298.1	K
CNST2	145.0000000	
D1	1.50000000	sec
D2	0.00344828	sec
D12	0.00002000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	14.50	usec
P2	29.00	usec
PL1	-2.00	dB
PL1W	119.43215179	W
SFO1	150.9178988	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
P3	11.80	usec
P4	23.60	usec
PCPD2	88.00	usec
PL2	2.00	dB
PL12	19.45	dB
PL2W	15.84893227	W
PL12W	0.28510177	W
SFO2	600.1324005	MHz
SI	32768	
SF	150.9028090	MHz
WDW	EM	
SSB	0	
LB	3.00	Hz
GB	0	
PC	1.40	


HMBC
CM399-1 C6D6
20101223

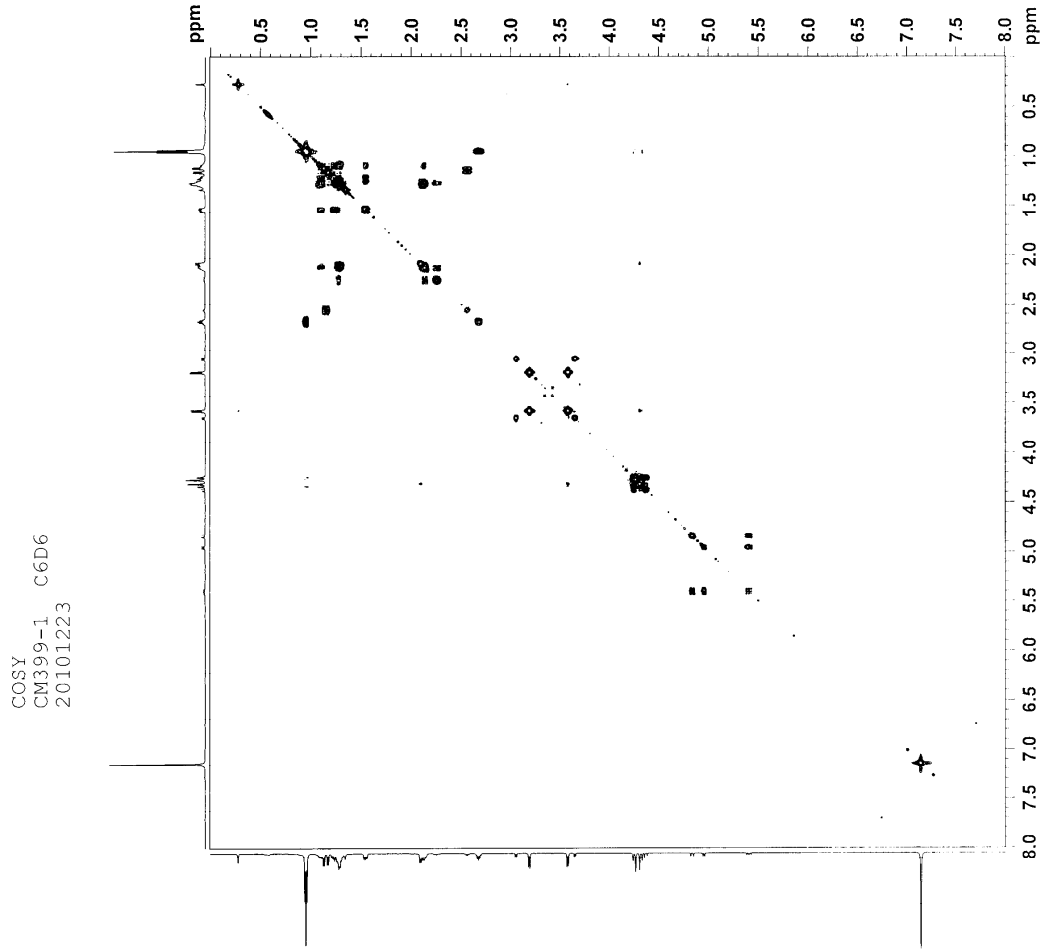

HSQC
CM399-1 C6D6
20101223
ppm
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
-20 0 20 40 60 80 100 120 140 160 180 200 220 ppm




```
NAME                 linmu
EXPNO                   23
PROCNO                   1
Date_             20101223
Time                 17.36
INSTRUM              spect
PROBHD     5 mm BBI 1H-BB
PULPROG          noesygpph
TD                    2048
SOLVENT               C6D6
NS                       8
DS                      16
SWH                4807.692 Hz
FIDRES             2.347506 Hz
AQ                 0.2131460 sec
RG                      57
DW                  104.000 usec
DE                    6.50 usec
TE                  298.0 K
D0                 0.00008898 sec
D1                 1.50000000 sec
D8                 0.50000000 sec
D16                0.00020000 sec
IN0                0.00020800 sec

======== CHANNEL f1 ========
NUC1                     1H
P1                    11.80 usec
P2                    23.60 usec
PL1                    2.00 dB
PLIW               15.84893227 W
SFO1              600.1324005 MHz

======= GRADIENT CHANNEL =====
GPNAM1             SINE.100
GPNAM2             SINE.100
GPZ1                  40.00 %
GPZ2                 -40.00 %
P16                1000.00 usec
NDO                      1
TD                     256
SFO1              600.1324 MHz
FIDRES             18.780159 Hz
SW                  8.011 ppm
FnMODE           States-TPPI
SI                     1024
SF                600.1300000 MHz
WDW                  QSINE
SSB                      2
LB                    0.00 Hz
GB                       0
PC                    1.40
SI                     1024
MC2              States-TPPI
SF                600.1300000 MHz
WDW                  QSINE
SSB                      2
LB                    0.00 Hz
GB                       0
```




```
NAME                 limmu
EXPNO                   24
PROCNO                   1
Date_             20101223
Time                 16.36
INSTRUM              spect
PROBHD     5 mm BBI 1H-BB
PULPROG          cosygpqf
TD                    2048
SOLVENT              C6D6
NS                      8
DS                     16
SWH              4807.692 Hz
FIDRES           2.347506 Hz
AQ               0.2131460 sec
RG                     57
DW                104.000 usec
DE                   6.50 usec
TE                 298.0 K
D0               0.00000300 sec
D1               1.50000000 sec
D13              0.00000400 sec
D16              0.00020000 sec
IN0              0.00020800 sec

======== CHANNEL f1 ========
NUC1                   1H
P0                 11.80 usec
P1                 11.80 usec
PL1                 2.00 dB
PL1W           15.84893227 W
SFO1           600.1324005 MHz

====== GRADIENT CHANNEL =====
GPNAM1          SINE.100
GPZ1               10.00 %
P16              1000.00 usec
ND0                    1
TD                   256
SFO1           600.1324 MHz
FIDRES          18.780159 Hz
SW                8.011 ppm
FnMODE                QF
SI                  1024
SF           600.1300000 MHz
WDW                 SINE
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  4.00
SI                  1024
MC2                   QF
SF           600.1300000 MHz
WDW                 SINE
SSB                    0
LB                  0.00 Hz
GB                     0
```