

Supplementary Information

Polycationic ligands in gold catalysis: Synthesis and applications of extremely π -acidic catalysts

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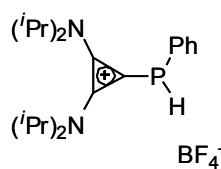
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Experimental procedures

General: All reactions were carried out in flame-dried glassware under Ar. All solvents were purified by distillation over the drying agents indicated and were transferred under Ar. IR: Nicolet FT-7199 spectrometer, wavenumbers in cm^{-1} . MS (EI): Finnigan MAT 8200 (70 eV), ESIMS: Finnigan MAT 95, accurate mass determinations: Bruker APEX III FT-MS (7 T magnet). NMR: Spectra were recorded on a Bruker AV 400 or DPX 300; ^1H and ^{13}C chemical shifts (δ) are given in ppm relative to TMS, coupling constants (J) in Hz. The solvent signals were used as references and the chemical shifts converted to the TMS scale. All flash chromatography was performed on Merck 60 silica gel (40-63 μm). Thin-layer chromatography (TLC) analysis was performed using Merck silica gel 60 F254 TLC plates, and visualized by UV and/or phosphomolybdic acid 10% in EtOH.

All commercially available compounds (Acros, ABCR, Alfa Aesar, Aldrich) were used as received. 2,3-bis(diisopropylamino)-1-chlorocyclopropenium tetrafluoroborate **2**,¹ 2-bromo-3-methylbenzaldehyde,² 1-*tert*-butyl-2-iodobenzene,³ 2-bromo-3-hydroxybenzaldehyde **41**,⁴ 3-bromo-2,6-dimethoxyphenol⁵ and Ohira-Bestmann reagent⁶ were prepared according to literature procedures.

Compound 4:



A solution of phenylphosphine in hexane (7.4 mL, 5.3 mmol, 10 %) was evaporated until 1/3 of the volume and chlorocyclopropenium salt **2** (630.0 mg, 1.8 mmol) in THF (6.0 mL) was added. The resulting mixture was heated at 60 $^{\circ}\text{C}$ overnight. After cooling to room temperature, the solvent was removed *in vacuo*, the residue dissolved in DCM (15 mL) and the solution was washed with a saturated solution of NaBF_4 (3×25 mL). Once dried over Na_2SO_4 , the organic phase was concentrated and the residue was purified by chromatography column ($\text{CH}_2\text{Cl}_2/\text{Acetone}$, 9/1) to afford compound **4** as a white solid (575 mg, 76%).

^1H NMR (400 MHz, CDCl_3) δ = 1.12 (d, J = 6.9 Hz, 6H), 1.31 - 1.46 (m, 18H), 3.64 - 3.80 (m, 2H), 4.14 (sept, J = 6.9 Hz, 2H), 5.63 (d, J = 233.6 Hz, 1H) 7.44 - 7.51 (m, 3H), 7.64 - 7.72 ppm (m, 2H) ppm.

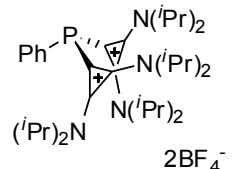
^{13}C NMR (101 MHz, CD_2Cl_2) δ = 21.6, 21.8, 22.9, 50.8, 56.7, 105.5 (d, J = 58.7 Hz), 126.0, 130.4 (d, J = 8.1 Hz), 132.3, 137.1 (d, J = 20.2 Hz), 138.7 ppm (d, J = 4.1 Hz) ppm.

^{31}P NMR (161 MHz, CDCl_3) δ = -70.9 ppm.

HRMS calcd. for $\text{C}_{21}\text{H}_{34}\text{N}_2\text{P}^+$: 345.245415; found 345.245568.

IR: $\tilde{\nu}$ = 729, 1032, 1349, 1558, 1872, 2984 cm^{-1} .

Compound 1:



Dry THF (6 mL) was added to a cooled (- 40 $^{\circ}\text{C}$) solid mixture of KHMDS (215.7 mg, 1.08 mmol) and phosphonium salt **4** (425.0 mg, 0.98 mmol) and the solution stirred at this temperature for 2 h. Then chlorocyclopropenium salt **2** (353.0 mg, 0.98 mmol) was added, the reaction mixture was allowed to warm

¹ Weiss, R.; Wagner, K. G.; Priesner, C.; Macheleid, J. *J. Am. Chem. Soc.* **1985**, 107, 4491-4499.

² Miyano, S.; Fukushima, H., Inagawa, H.; Hashimoto, H. *Bull. Chem. Soc. Jpn.*, **1986**, 59, 3285.

³ Gan, Z.; Kawamura, K.; Eda, K.; Hayashi, M. *J. Organomet. Chem.* **2010**, 695, 2022–2029.

⁴ Stavrakov, G.; Keller, M.; Breit, B. *Eur. J. Org. Chem.* **2007**, 5726-5733

⁵ Giles, R. G. F.; Hughes, A. B.; Sargent, M. V. *J. Chem. Soc., Perkin Trans. 1*, **1991**, 1581-1587.

⁶ (a) Müller, S.; Liepold, B.; Roth, G. J.; Bestmann, H. J. *Synlett* **1996**, 521-522; (b) Callant, P.; D'Haenens, L.; Vandewalle, M. *Synth. Commun.* **1984**, 14, 155-161.

to room temperature and stirred overnight. The solvent was removed *in vacuo*, the residue was dissolved in DCM (15 mL) and the solution washed with a saturated solution of NaBF₄ (3 × 15 mL) under Argon. Once dried over Na₂SO₄, the organic phase was concentrated and the residue washed with THF (4 × 5 mL), affording the desired compound as a white solid (516 mg, 69%).

¹H NMR (400 MHz, CD₂Cl₂) δ = 1.21 (d, *J* = 6.9 Hz, 12H), 1.25 (d, *J* = 6.9 Hz, 12H), 1.38 (d, *J* = 6.9 Hz, 12H), 1.44 (d, *J* = 6.9 Hz, 12H), 3.64 (sept, *J* = 6.9 Hz, 4H), 4.17 (sept, *J* = 6.9 Hz, 4H), 7.62 - 7.68 (m, 3H), 7.73 - 7.80 ppm (m, 2H) ppm.

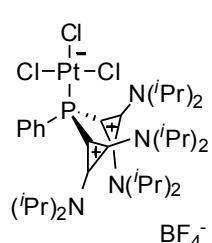
¹³C NMR (101 MHz, CD₂Cl₂) δ = 21.2, 21.5, 21.5, 21.6, 21.6, 21.7, 53.4, 54.8, 98.2 (d, *J* = 59.5 Hz), 125.0 (d, *J* = 4.6 Hz), 131.1 (d, *J* = 8.9 Hz), 133.0, 134.8 (d, *J* = 22.9 Hz), 140.0 ppm.

³¹P NMR (161 MHz, CD₂Cl₂) δ = -48.3 ppm.

HRMS calcd. for C₃₆H₆₁BF₄N₄P⁺: 667.467509; found 667.467401.

IR (neat) $\tilde{\nu}$ = 694, 1029, 1151, 1357, 1555, 1858, 2974 cm⁻¹.

Compound 5:



K₂PtCl₄ (48.4 mg, 0.117 mmol) was added to a solution of salt **1** (88.0 mg, 0.117 mmol) in dry DCM (3.0 mL). The reaction mixture was allowed to warm to room temperature and stirred overnight. The solvent was then removed *in vacuo* affording the desired product as a pale yellow solid (111 mg, 98%).

¹H NMR (400 MHz, CD₂Cl₂) δ = 1.10 (d, *J* = 6.4 Hz, 12H), 1.14 (d, *J* = 6.4 Hz, 12H), 1.33 (d, *J* = 7.0 Hz, 12H), 1.36 (d, *J* = 7.0 Hz, 12H), 4.05-4.18 (m, 4H), 4.29-4.43 (m, 4H), 7.58-7.67 (m, 3H), 8.37-8.46 ppm (m, 2H) ppm.

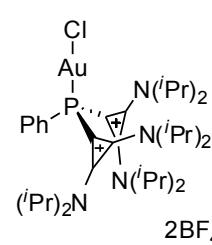
¹³C NMR (101 MHz, CD₂Cl₂) δ = 17.5, 18.1, 18.5, 53.4, 90.6 (d, *J* = 51.5 Hz), 118.9 (d, *J* = 70.8 Hz), 126.8 (d, *J* = 12.9 Hz), 130.9 (d, *J* = 2.3 Hz), 133.5 (d, *J* = 13.5 Hz), 134.7 ppm (d, *J* = 8.6 Hz) ppm.

³¹P NMR (161 MHz, CD₂Cl₂) δ = -21.2 ppm (*J* = 1994.8 Hz).

HRMS calcd. for C₃₆H₆₁Cl₃N₄PPt⁺: 880.333066; found 880.333903.

IR: $\tilde{\nu}$ = 679, 1050, 1148, 1376, 1557, 1850, 2977 cm⁻¹.

Compound 6:



[AuCl(Me₂S)] (39.0 mg, 0.13 mmol) was added to a cooled (-20 °C) suspension of salt **1** (100.0 mg, 0.13 mmol) in dry DCM (4 mL). The reaction mixture was allowed to warm to room temperature and stirred at this temperature for 30 min. The solvent was then removed *in vacuo* affording the desired product as a white solid (129 mg, 98%).

¹H NMR (400 MHz, CD₂Cl₂) δ = 1.25 (d, *J* = 7.0 Hz, 12H), 1.34 (d, *J* = 7.0 Hz, 12H), 1.45 (d, *J* = 7.0 Hz, 24H), 3.86 (sept, *J* = 7.0 Hz, 4H), 4.24 (sept, *J* = 7.0 Hz, 4H), 7.72 - 7.78 (m, 3H), 8.08 - 8.17 ppm (m, 2H) ppm.

¹³C NMR (101 MHz, CD₂Cl₂) δ = 21.6, 21.7, 21.9, 55.6, 56.3, 90.9 (d, *J* = 54.6 Hz), 121.7 (d, *J* = 70.0 Hz), 131.6 (d, *J* = 14.3 Hz), 135.5 (d, *J* = 17.8 Hz), 135.6 (d, *J* = 2.5 Hz), 138.9 ppm (d, *J* = 7.0 Hz) ppm.

³¹P NMR (161 MHz, CD₂Cl₂) δ = -10.0 ppm.

HRMS calcd. for C₃₆H₆₁AuBClF₄N₄P⁺: 899.401161; found 899.401924.

IR: $\tilde{\nu}$ = 694, 1030, 1151, 1358, 1556, 1858, 2973 cm⁻¹.



2-bromo-3-methylbenzaldehyde was prepared according to literature procedure.²

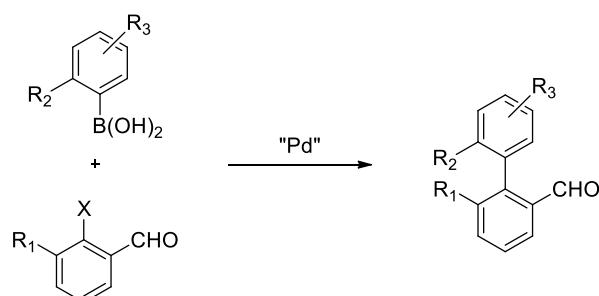
¹H NMR (400 MHz, CDCl₃) δ = 2.48 (s, 3H), 7.32 (t, J = 7.6 Hz, 1H), 7.48 (d, J = 7.4 Hz 1H), 7.74 (d, J = 7.7 Hz, 1H), 10.45 (s, 1H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ = 23.0, 127.5, 127.6, 129.7, 134.2, 136.4, 139.8, 192.8 ppm.

HRMS calcd. for C₈H₇BrO: 197.967926; found 197.968041.

IR: ν = 690, 778, 911, 1006, 1031, 1105, 1168, 1238, 1296, 1373, 1448, 1572, 1675, 1694, 2867, 2982 cm⁻¹.

General Procedures for the Suzuki coupling

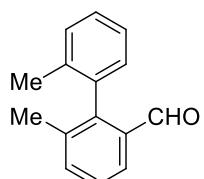


General procedure A: A suspension of the corresponding aldehyde, the boronic acid (1.1 eq.), Pd(OAc)₂ (0.02 eq.) and K₂CO₃ (2.5 eq.) in a degassed mixture of THF and water (9:1) was vigorously stirred overnight at room temperature. The mixture was diluted with water, the aqueous phase was extracted with EtOAc, the combined organic layers were dried over Na₂SO₄ and evaporated, and the crude product was purified by flash chromatography.

General procedure B: The corresponding aldehyde, the boronic acid (1.1 eq.), Pd(PPh₃)₄ (0.01 eq.), and Na₂CO₃ (2 eq.) were suspended in a degassed mixture of 1,4-dioxane:water 1.5:1 (0.9 M). The vial was sealed tightly with a Teflon crimp top. The mixture was irradiated for 25 min. at a preselected temperature of 120°C. Then, the mixture was cooled to room temperature and the crude material was extracted with ethyl acetate, the combined organic layers were dried over Na₂SO₄ and evaporated, and the crude product was purified by flash chromatography.

General procedure C: The corresponding aldehyde, the boronic acid (1.3 eq.), Pd(PPh₃)₄ (0.05 eq.), and Cs₂CO₃ (3 eq.) were suspended in a degassed mixture of 1,4-dioxane:ethanol 2:1 (0.125 M). The vial was sealed tightly with a Teflon crimp top. The mixture was irradiated for 15 min at a preselected temperature of 130°C. Then, the mixture was cooled to room temperature and the crude material was filtered through a pad of celite. The crude product was purified by flash chromatography.

General procedure D: A suspension of the corresponding aldehyde, the boronic acid (1.5 eq.), Pd₂(dba)₃ (0.032 eq.), PCy₃ (0.074 eq.) and Cs₂CO₃ (1.7 eq.) in a degassed mixture of 1,4-dioxane:toluene 2:3 was vigorously stirred 24 h at 85°C. Then, the mixture was cooled to room temperature and the crude material was filtered through a pad of celite. The crude product was purified by flash chromatography.



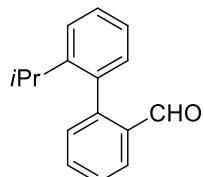
Using general procedure B, this compound was prepared from 2-bromo-3-methylbenzaldehyde (250 mg, 1.26 mmol) and o-tolylboronic acid (188 mg, 1.39 mmol) to obtain after flash chromatography (hexanes/ethyl acetate 100/1) a colorless oil (257 mg, 75%).

¹H NMR (300 MHz, CDCl₃) δ = 1.93 (s, 3H), 1.98 (s, 3H), 7.04 (d, J = 7.2 Hz, 1H), 7.17 - 7.30 (m, 3H), 7.35 (t, J = 7.6 Hz, 1H), 7.43 - 7.51 (m, 1H), 7.81 (dd, J = 7.7, 0.7 Hz, 1H), 9.56 (d, J = 0.8 Hz, 1H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ = 19.6, 20.0, 124.8, 126.1, 127.8, 128.3, 129.8, 130.2, 134.2, 135.7, 136.3, 136.5, 137.4, 145.2, 192.8 ppm.

HRMS calcd. for C₁₅H₁₄O: 210.104454; found 210.104462.

IR (neat) ν = 730, 759, 781, 918, 1006, 1120, 1214, 1235, 1381, 1458, 1491, 1591, 1684, 1739, 2856, 2921, 3017 cm⁻¹.



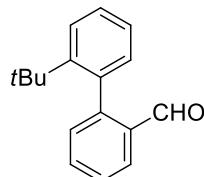
Using general procedure A, this compound was prepared from 2-bromobenzaldehyde (222 mg, 1.2 mmol) and (2-isopropylphenyl)boronic acid (216 mg, 1.32 mmol) to obtain after flash chromatography (hexanes) a colorless oil (254 mg, 94%).

¹H NMR (300 MHz, CDCl₃) δ = 1.02 (d, J = 6.9 Hz, 3H), 1.05 (d, J = 6.8 Hz, 3H), 2.67 (hept, J = 6.9 Hz, 1H), 7.07 (dt, J = 7.4, 0.9 Hz, 1H), 7.12 - 7.20 (m, 1H), 7.24 (dd, J = 7.6, 0.8 Hz, 1H), 7.31 - 7.38 (m, 2H), 7.43 (tt, J = 7.5, 1.1 Hz, 1H), 7.55 (td, J = 7.5, 1.5 Hz, 1H), 7.95 (dd, J = 7.8, 1.2 Hz, 1H), 9.69 (d, J = 0.7 Hz, 1H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ = 23.5, 24.5, 30.2, 125.4, 125.7, 127.1, 127.9, 128.8, 130.4, 131.1, 133.6, 134.3, 136.3, 145.8, 147.2, 192.4 ppm.

HRMS calcd. for C₁₇H₁₆ONa: 247.108915; found 247.109335.

IR: ν = 715, 755, 825, 1004, 1033, 1193, 1251, 1389, 1442, 1473, 1596, 1692, 2747, 2868, 2927, 2961, 3023, 3060 cm⁻¹.



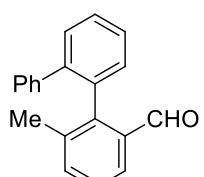
Using general procedure C, this compound was prepared from 1-(tert-butyl)-2-iodobenzene (260 mg, 1.0 mmol) and (2-formylphenyl)boronic acid (195 mg, 1.3 mmol) to obtain after flash chromatography (hexanes/AcOEt 500/1) a white solid (100 mg, 42%).

¹H NMR (400 MHz, CDCl₃) δ = 1.17 (s, 9H), 7.00 (dd, J = 7.5, 1.2 Hz, 1H), 7.20 (dd, J = 10.8, 3.9 Hz, 1H), 7.37 (dt, J = 8.1, 2.6 Hz, 2H), 7.48 (t, J = 7.5 Hz, 1H), 7.53 - 7.64 (m, 2H), 8.01 (d, J = 7.6 Hz, 1H), 9.77 (s, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ = 32.7, 36.8, 125.2, 126.8, 127.4, 127.8, 128.3, 131.8, 132.7, 132.7, 134.5, 136.6, 148.2, 148.6, 192.5 ppm.

HRMS calcd. for C₁₇H₁₈O: 238.135776; found 238.135831.

IR : ν = 685, 742, 766, 824, 880, 1002, 1053, 1103, 1193, 1242, 1263, 1364, 1390, 1432, 1442, 1471, 1596, 1650, 1687, 2750, 2842, 2960 cm⁻¹.



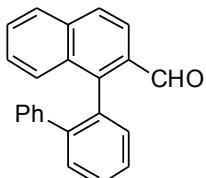
Using general procedure B, this compound was prepared from 2-bromo-3-methylbenzaldehyde (200 mg, 1.0 mmol) and 2-biphenylboronic acid (218.9 mg, 1.1 mmol) to obtain after flash chromatography (hexanes) a colorless oil (204 mg, 75%).

¹H NMR (400 MHz, CDCl₃) δ = 1.90 (s, 3H), 6.86 - 6.93 (m, 2H), 6.96 - 7.02 (m, 3H), 7.09 - 7.16 (m, 2H), 7.21 (dd, J = 7.5, 0.7 Hz, 1H), 7.26 - 7.33 (m, 1H), 7.34 - 7.38 (m, 2H), 7.59 (dd, J = 7.7, 0.8 Hz, 1H), 9.63 (d, J = 0.7 Hz, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ = 20.0, 124.8, 126.9, 127.3, 127.6, 128.0, 128.6, 129.0, 130.2, 131.0, 134.3, 135.0, 135.4, 137.4, 140.6, 141.8, 144.6, 192.4 ppm.

HRMS calcd. for C₂₀H₁₆O: 272.119921; found 272.120111.

IR (neat) $\tilde{\nu}$ = 699, 715, 747, 781, 921, 1008, 1074, 1116, 1162, 1239, 1448, 1459, 1480, 1591, 1686, 2744, 2852, 3058 cm⁻¹.



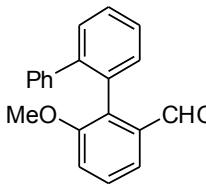
A modification of procedure C was employed, using only dioxane as solvent. Thus, this compound was prepared from 1-bromo-2-naphthaldehyde (235 mg, 1.0 mmol) and 2-biphenylboronic acid (257.4 mg, 1.3 mmol) to obtain after flash chromatography (hexanes/AcOEt 200/1) a white solid (194 mg, 63%).

¹H NMR (400 MHz, CDCl₃) δ = 6.90 - 7.06 (m, 5H), 7.42 (dd, *J* = 7.5, 0.8 Hz, 1H), 7.47 (ddd, *J* = 8.2, 6.9, 1.2 Hz, 1H), 7.52 (td, *J* = 7.3, 1.7 Hz, 1H), 7.56 - 7.65 (m, 3H), 7.75 (d, *J* = 8.5 Hz, 1H), 7.82 (d, *J* = 8.7 Hz, 1H), 7.84 - 7.91 (m, 2H), 9.85 (d, *J* = 0.6 Hz, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ = 122.1, 127.0, 127.1, 127.2, 127.8, 128.1, 128.4, 128.4, 128.8, 128.8, 129.1, 130.3, 131.0, 132.1, 133.0, 133.8, 136.1, 140.5, 143.3, 145.9, 192.4 ppm.

HRMS calcd. for C₂₃H₁₆O: 308.120113; found 308.120174.

IR: $\tilde{\nu}$ = 670, 703, 746, 823, 869, 910, 921, 974, 1009, 1025, 1070, 1121, 1233, 1260, 1326, 1379, 1427, 1445, 1456, 1478, 1594, 1615, 1677, 2850, 3056 cm⁻¹.



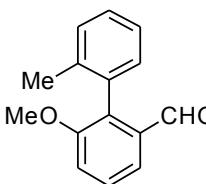
Using general procedure D, this compound was prepared from 2-chloro-3-methoxy-benzaldehyde (713 mg, 4.18 mmol) and 2-biphenylboronic acid (1.2 g, 6.27 mmol) to obtain after flash chromatography (hexanes/AcOEt 7/1) a white solid (1.18 g, 98%).

¹H NMR (300 MHz, CDCl₃) δ = 3.60 (s, 3H), 6.99 - 7.15 (m, 6H), 7.15 - 7.27 (m, 2H), 7.41 - 7.49 (m, 4H), 9.74 (m, 1H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ = 55.8, 115.9, 119.2, 126.9, 127.1, 127.9, 128.6, 128.9, 129.0, 129.9, 132.0, 132.1, 134.7, 135.2, 141.3, 143.0, 157.2, 192.2 ppm.

HRMS calcd. for C₂₀H₁₆O₂Na₁: 311.104249, found: 311.103990.

IR: $\tilde{\nu}$ = 699, 715, 748, 778, 798, 880, 912, 1000, 1009, 1066, 1114, 1156, 1185, 1239, 1260, 1301, 1387, 1437, 1463, 1483, 1574, 1592, 1684, 1947, 2750, 2837, 2857, 2938, 2960, 3011, 3055 cm⁻¹.



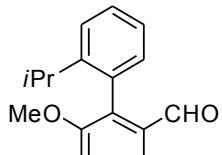
Using general procedure D, this compound was prepared from 2-chloro-3-methoxy-benzaldehyde (200 mg, 1.17 mmol) and 2-methylphenylboronic acid (239 mg, 1.98 mmol) to obtain after flash chromatography (hexanes/AcOEt 15/1) a white solid (182 mg, 69%).

¹H NMR (300 MHz, CDCl₃) δ = 2.06 (s, 3H), 3.78 (s, 3H), 7.11-7.14 (m, 1H), 7.20 (dd, *J* = 8.1 Hz, 0.8 Hz, 1H), 7.23 - 7.36 (m, 3H), 7.47 (td, *J* = 8.0 Hz, 8.0 Hz, 0.6 Hz, 1H), 7.63 (dd, *J* = 7.8 Hz, 1.1 Hz, 1H), 9.62 (d, *J* = 0.7, 1H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ = 20.2, 56.4, 116.3, 119.1, 125.7, 128.4, 128.9, 130.0, 131.0, 133.3, 134.9, 135.4, 137.5, 157.5, 192.6 ppm.

HRMS calcd. for C₁₅H₁₄O₂Na₁: 249.088595, found: 249.088542.

IR: $\tilde{\nu}$ = 729, 744, 762, 794, 911, 943, 983, 1003, 1067, 1119, 1185, 1240, 1262, 1298, 1389, 1467, 1494, 1575, 1592, 1682, 1697, 2341, 2742, 2837, 2948, 3011, 3067 cm⁻¹.



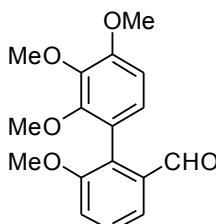
Using general procedure D, this compound was prepared from 2-chloro-3-methoxy-benzaldehyde (200 mg, 1.17 mmol) and 2-*i*-iso-propyl-phenylboronic acid (288 mg, 1.76 mmol) to obtain after flash chromatography (hexanes/AcOEt 10/1) a white solid (208 mg, 70%).

¹H NMR (300 MHz, CDCl₃) δ = 1.01 (d, *J* = 6.9 Hz, 3H), 1.17 (d, *J* = 6.9, 3H), 2.61 (hept., *J* = 6.9 Hz, 1H), 3.76 (s, 3H), 7.05 - 7.08 (m, 1H), 7.18 (dd, *J* = 8.1 Hz, 1.0 Hz, 1H), 7.19 - 7.26 (m, 1H), 7.40-7.42 (m, 2H), 7.46 (td, *J* = 8.0 Hz, 0.8 Hz, 1H), 7.62 (dd, *J* = 7.9 Hz, 1.2 Hz, 1H), 9.64 (d, *J* = 0.8 Hz, 1H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ = 23.6, 24.1, 30.8, 56.0, 115.9, 119.1, 125.5, 125.6, 129.1, 130.9, 132.0, 135.0, 135.8, 148.3, 157.5, 192.5 ppm.

HRMS calcd. for C₁₇H₁₈O₂Na₁: 254.130677, found: 254.130555.

IR: ν = 666, 716, 744, 755, 784, 794, 872, 912, 949, 1002, 1035, 1066, 1098, 1168, 1186, 1201, 1240, 1259, 1301, 1345, 1362, 1389, 1436, 1467, 1492, 1576, 1592, 1688, 1925, 1948, 1979, 2837, 2867, 2961, 3018, 3064 cm⁻¹.



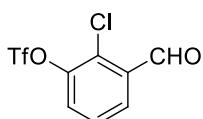
Using general procedure D, this compound was prepared from 2-chloro-3-methoxy-benzaldehyde (226 mg, 1.32 mmol) and 2,3,4-trimethoxyphenylboronic acid (421 mg, 1.98 mmol) to obtain after flash chromatography (hexanes/AcOEt 2/1) a white solid (386 mg, 97%).

¹H NMR (300 MHz, CDCl₃) δ = 3.64 (s, 3H), 3.80 (s, 3H), 3.91 (s, 3H), 3.92 (s, 3H), 6.81 (dd, *J* = 38.4 Hz, 8.51 Hz, 2H), 7.44 (td, *J* = 8.0 Hz, 8.0 Hz, 0.73 Hz, 1H), 7.61 (dd, *J* = 7.8 Hz, 1.1 Hz, 1H), 9.7 (d, *J* = 0.8 Hz, 1H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ = 56.2, 60.7, 61.1, 107.1, 116.0, 119.1, 119.9, 126.6, 128.8, 131.3, 135.7, 142.3, 152.2, 154.1, 157.7, 192.7 ppm.

HRMS calcd. for C₁₇H₁₈O₃Na₁: 325.104643, found: 325.104246.

IR: ν = 667, 689, 719, 744, 771, 788, 795, 815, 867, 916, 1001, 1012, 1071, 1091, 1111, 1167, 1181, 1203, 1242, 1257, 1289, 1395, 1409, 1428, 1462, 1501, 1578, 1592, 1681, 1693, 1874, 1977, 2163, 2761, 2838, 2868, 2939, 2977 cm⁻¹.



2-Chloro-3-hydroxybenzaldehyde (522 mg, 3.33 mmol) and 6.5 ml of a potassiumphosphate solution (c = 1.4 M) were united in a 50 ml Flask. The solution was stirred at rt until a clear solution remained and then 6.5 ml of Toluene were added. This two-phase mixture was cooled down to 0 °C under vigorous stirring. After this 0.67 ml (1.1 g, 4.00 mmol) of trifluoromethanesulfonic anhydride were added over 10 min, so that the temperature of the reaction solution remained below 6 °C. Then the reaction mixture was stirred for 40 min at rt. The organic layer was separated and the aqueous layer extracted with toluene (2 × 40 mL). The organic layers were combined, washed two times with briene and dried over Na₂SO₄. After removal of the solvents *in vacuo*, the product was obtained as colorless oil in 94% yield (904 mg).

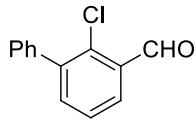
¹H NMR (300 MHz, CDCl₃) δ = 7.51 (td, *J* = 8.3 Hz, 0.7 Hz, 1H), 7.61 (dd, *J* = 8.2 Hz, 1.6 Hz, 1H), 7.97 (dd, *J* = 7.8 Hz, 1.6 Hz, 1H), 10.48 (s, 1H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ = 118.8 (q, *J* = 320.6 Hz, CF₃), 128.2, 128.4, 131.1, 129.1, 134.7, 146.4, 188.0 ppm.

¹⁹F NMR (282 MHz, CDCl₃) δ = -73.2 ppm.

HRMS calcd. for C₈H₄Cl₁F₃O₄S₁: 287.947094, found: 287.947140.

IR: $\tilde{\nu}$ = 708, 745, 774, 798, 826, 949, 1052, 1134, 1165, 1209, 1388, 1427, 1460, 1568, 1594, 1702, 1777, 2877, 3091 cm^{-1} .



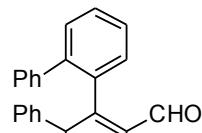
2-Chloro-3-formylphenyl trifluoromethanesulfonate (400 mg, 1.39 mmol), phenylboronic acid (169 mg, 1.39 mmol), K_3PO_4 (588 mg, 2.72 mmol), $\text{Pd}(\text{OAc})_2$ (15.6 mg, 0.069 mmol) and tricyclohexylphosphine (38.9 mg, 0.139 mmol) were added into a Schlenk-Flask under Argon. Subsequently 9 mL of dry and degassed THF and 6.2 μL of water were added. The reaction mixture was heated at 80 °C under argon with vigorous stirring for 20 h. After the reaction was finished, the mixture was filtered over a short pad of silica and rinsed with Ethylacetate. Final purification through a silica gel column chromatography (hexane/EtOAc 15/1) afforded the product as a white solid (75 mg, 25 %).

^1H NMR (300 MHz, CDCl_3) δ = 7.42 - 7.47 (m, 6H), 7.57 (dd, J = 7.5 Hz, 1.8 Hz, 1H), 7.94 (dd, J = 7.7 Hz, 1.8 Hz, 1H), 10.60 (s, 1H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ = 127.1, 128.3, 128.4, 128.6, 129.6, 133.4, 136.4, 136.8, 138.4, 142.5, 190.6 ppm.

HRMS calcd. for $\text{C}_{13}\text{H}_9\text{Cl}_1\text{O}_1$: 216.034192, found: 216.033995.

IR: $\tilde{\nu}$ = 698, 726, 757, 768, 800, 918, 972, 1028, 1042, 1072, 1109, 1159, 1173, 1239, 1268, 1301, 1336, 1380, 1421, 1447, 1457, 1479, 1569, 1603, 1682, 1710, 1728, 1813, 1979, 2884, 3015, 3056 cm^{-1} .



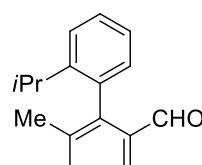
Using general procedure D, this compound was prepared from 2-chloro-biphenyl-carbaldehyde (170 mg, 0.79 mmol) and 2-biphenylboronic acid (233 mg, 1.18 mmol) to obtain after flash chromatography (hexanes/AcOEt 15/1) a white solid (159 mg, 61%).

^1H NMR (300 MHz, CDCl_3) δ = 6.60 - 6.65 (m, 4H), 7.01 - 7.16 (m, 6H), 7.24 - 7.27 (m, 1H), 7.31 - 7.50 (m, 5H), 7.98 (dd, J = 7.3 Hz, 1.8 Hz, 1H), 9.97 (s, 1H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ = 126.5, 126.7, 126.8, 127.7, 127.8, 128.0, 128.8, 129.4, 129.6, 130.4, 133.3, 134.3, 135.3, 135.7, 139.9, 140.3, 142.1, 142.6, 143.5, 192.9 ppm.

HRMS calcd. for $\text{C}_{25}\text{H}_{18}\text{O}_1$: 334.135767, found: 334.135729.

IR: $\tilde{\nu}$ = 696, 715, 745, 764, 807, 866, 910, 951, 982, 1008, 1026, 1075, 1117, 1158, 1181, 1231, 1263, 1294, 1329, 1386, 1425, 1434, 1448, 1456, 1480, 1497, 1570, 1584, 1687, 1731, 1805, 1903, 1954, 2746, 2803, 2852, 3029, 3057 cm^{-1} .



Using general procedure C, this compound was prepared from 2-bromo-3-methylbenzaldehyde (100 mg, 0.5 mmol) and (2-isopropylphenyl)boronic acid (90.2 mg, 0.55 mmol) to obtain after flash chromatography (hexanes) a colorless oil (98 mg, 66%).

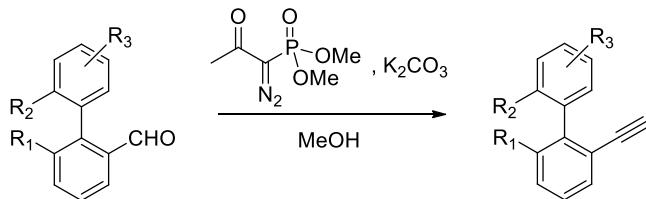
^1H NMR (400 MHz, CDCl_3) δ = 0.92 (d, J = 6.9 Hz, 3H), 1.06 (d, J = 6.9 Hz, 3H), 1.97 (s, 3H), 2.44 (hept, J = 6.9 Hz, 1H), 6.96 (dd, J = 7.7, 0.9 Hz, 1H), 7.16 (ddd, J = 7.6, 6.7, 2.0 Hz, 1H), 7.26 - 7.39 (m, 3H), 7.43 (dd, J = 7.5, 0.4 Hz, 1H), 7.78 (dd, J = 7.7, 0.4 Hz, 1H), 9.56 (d, J = 0.6 Hz, 1H) ppm.

^{13}C NMR (101 MHz, CDCl_3) δ = 20.0, 23.6, 24.1, 30.3, 124.7, 125.9, 127.7, 128.7, 129.8, 134.6, 135.0, 135.5, 137.7, 145.1, 147.1, 192.8, 192.8 ppm.

HRMS calcd. for $\text{C}_{17}\text{H}_{18}\text{O}$: 238.135875; found 238.135768.

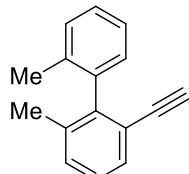
IR (neat) $\tilde{\nu}$ = 716, 756, 787, 920, 1004, 1034, 1127, 1216, 1234, 1362, 1382, 1443, 1460, 1591, 1687, 1740, 2867, 2960 cm⁻¹.

General Procedure for the Ohira-Bestmann reaction



The corresponding aldehyde, dimethyl (1-diazo-2-oxopropyl)phosphonate (Ohira-Bestmann reagent) (1.5 eq.) and K₂CO₃ (2 eq.) were suspended in dry MeOH (0.13 M) and stirred overnight. Afterwards, the solvent was evaporated and the crude partitioned between CH₂Cl₂ and brine. The combined organic layers were dried (Na₂SO₄), evaporated, and the residue was purified by flash chromatography.

Compound 7:



Prepared from the corresponding aldehyde (229 mg, 1.09 mmol) following the general procedure and purified by flash chromatography (hexanes). White solid (211 mg, 94%).

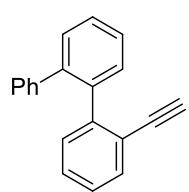
¹H NMR (300 MHz, CDCl₃) δ = 1.91 (s, 3H), 1.96 (s, 3H), 2.72 (s, 1H), 6.96 - 7.02 (m, 1H), 7.09 - 7.23 (m, 5H), 7.35 (dd, *J* = 7.3, 1.3 Hz, 1H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ = 19.6, 20.4, 79.5, 82.9, 122.1, 125.8, 127.1, 127.6, 129.1, 129.9, 130.5, 130.6, 136.0, 136.6, 139.8, 144.5 ppm.

HRMS calcd. for C₁₆H₁₄: 206.109326; found 206.109547.

IR (neat) $\tilde{\nu}$ = 727, 746, 756, 785, 915, 1006, 1120, 1268, 1379, 1454, 1489, 1574, 2921, 3016, 3061, 3286 cm⁻¹.

Compound 9:



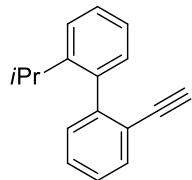
The starting aldehyde was prepared from 2-bromo-benzaldehyde (0.19 mL, 1.62 mmol) and 2-biphenylboronic acid (353 mg, 1.78 mmol) following general procedure A (using DMF/H₂O; 5:1 mixture as solvent) and purified by flash chromatography (hexanes/EtOAc, 95/5). Pale yellow solid (370 mg, 88%). Submission to the general Ohira-Bestmann conditions and purification by flash chromatography (hexanes/EtOAc, 95/5) afforded the desired alkyne as a white solid (350 mg, 96%).

¹H NMR (400 MHz, CDCl₃) δ = 2.95 (s, 1H), 6.98 - 7.04 (m, 1H), 7.12 - 7.21 (m, 7H), 7.38 - 7.52 (m, 5H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ = 80.4, 83.1, 122.0, 126.6, 126.8, 126.9, 127.8, 128.1, 128.3, 129.9, 130.2, 131.0, 131.1, 133.1, 139.2, 141.4, 141.4, 144.8 ppm.

HRMS calcd. for C₂₀H₁₄: 254.109546; found 254.109501.

IR: $\tilde{\nu}$ = 698, 742, 756, 770, 913, 948, 1008, 1073, 1159, 1240, 1265, 1429, 1449, 1467, 1488, 1597, 1735, 3020, 3057, 3283 cm⁻¹.

Compound 11:

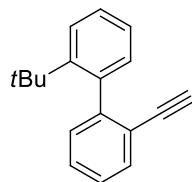
Prepared from the corresponding aldehyde (200 mg, 1.13 mmol) following the general procedure and purified by flash chromatography (hexanes). Pale yellow solid (167 mg, 85%).

¹H NMR (300 MHz, CDCl₃) δ = 1.00 (d, *J* = 6.9 Hz, 3H), 1.12 (d, *J* = 6.9 Hz, 3H), 2.73 (hept, *J* = 6.9 Hz, 1H), 2.82 (s, 1H), 7.03 - 7.10 (m, 1H), 7.10 - 7.20 (m, 2H), 7.20 - 7.38 (m, 4H), 7.51 (dd, *J* = 7.6, 1.4 Hz, 1H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ = 23.6, 24.6, 30.1, 80.3, 82.9, 122.2, 125.2, 125.3, 127.0, 128.2, 128.5, 129.8, 130.0, 132.9, 139.6, 145.2, 146.9 ppm.

HRMS calcd. for C₁₇H₁₆: 220.125307; found 220.125200.

IR: $\tilde{\nu}$ = 665, 747, 757, 1004, 1031, 1043, 1089, 1105, 1203, 1257, 1330, 1364, 1385, 1433, 1446, 1470, 2867, 2961, 3020, 3057, 3267 cm⁻¹.

Compound 12:

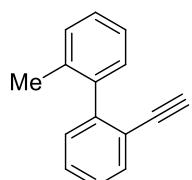
Prepared from the corresponding aldehyde (84 mg, 0.35 mmol) following the general procedure and purified by flash chromatography (hexanes). White solid (67 mg, 81%).

¹H NMR (300 MHz, CDCl₃) δ = 1.21 (s, 9H), 2.92 (s, 1H), 6.99 (dd, *J* = 7.5, 1.6 Hz, 1H), 7.19 (td, *J* = 7.4, 1.3 Hz, 1H), 7.21 - 7.32 (m, 4H), 7.54 - 7.58 (m, 2H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ = 32.5, 36.7, 81.0, 83.3, 122.8, 125.1, 126.9, 127.2, 127.6, 127.6, 130.7, 132.3, 132.6, 139.9, 147.8, 148.4 ppm.

HRMS calcd. for C₁₈H₁₈: 234.140848; found 234.140650.

IR: $\tilde{\nu}$ = 663, 753, 948, 1003, 1052, 1106, 1200, 1248, 1264, 1362, 1391, 1430, 1442, 1471, 1924, 2867, 2966, 3006, 3052, 3269 cm⁻¹.

Compound 13:

The starting aldehyde was prepared from 2-bromo-benzaldehyde (0.31 mL, 2.65 mmol) and o-tolylboronic acid (400 mg, 2.94 mmol) following the general procedure A and purified by flash chromatography (hexanes/EtOAc, 9/1) to afford a yellow oil (327 mg, 63%). Submission of this material to the general Ohira-Bestmann conditions afforded the desired alkyne that was further purified by flash chromatography (hexanes/EtOAc, 12/1). Yellow oil (223 mg, 94%).

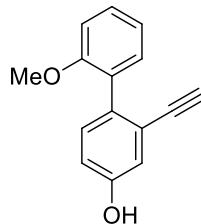
¹H NMR (400 MHz, CDCl₃) δ = 2.24 (s, 3H), 2.96 (s, 1H), 7.23 - 7.36 (m, 5H), 7.38 (dd, *J* = 7.5, 1.6 Hz, 1H), 7.45 (td, *J* = 7.5, 1.5 Hz, 1H), 7.66 (dd, *J* = 7.6, 1.3 Hz, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ = 20.1, 79.9, 82.8, 121.9, 125.5, 127.1, 127.8, 128.7, 129.7, 129.8, 129.9, 133.0, 136.3, 140.6, 145.1 ppm.

HRMS calcd. for C₁₅H₁₂: 192.093896; found 192.094011.

IR: $\tilde{\nu}$ = 725, 745, 755, 875, 950, 1005, 1042, 1101, 1122, 1159, 1264, 1378, 1438, 1456, 1472, 1495, 1595, 3019, 3060, 3283 cm⁻¹.

Compound 14:



The aldehyde employed as starting material was prepared following the general procedure A (DMF/H₂O 5:1 at 50°C) from 2-bromo-5-hydroxybenzaldehyde (387 mg, 1.92 mmol) and 2-methoxyphenylboronic acid (380 mg, 2.50 mmol) and purified by flash chromatography (hexanes/EtOAc, 7/3). Pale yellow solid (328 mg, 75%). Submission of this material to the general Ohira-Bestmann conditions and purification by flash chromatography (hexanes/EtOAc, 7/3) gives the desired alkyne as a white solid (227 mg, 96%).

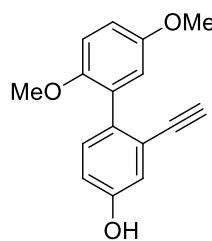
¹H NMR (400 MHz, CDCl₃) δ = 2.91 (s, 1H), 3.79 (s, 3H), 4.83 (s, 1H), 6.87 (dd, J = 8.4, 2.7 Hz, 1H), 6.97 (d, J = 8.3 Hz, 1H), 7.01 (dd, J = 7.4, 1.0 Hz, 1H), 7.05 (d, J = 2.7 Hz, 1H), 7.21 (d, J = 8.4 Hz, 1H), 7.26 - 7.29 (m, 1H), 7.34 (ddd, J = 8.2, 7.5, 1.8 Hz, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ = 55.7, 79.3, 82.9, 111.3, 116.3, 119.6, 120.4, 123.2, 129.0, 129.3, 131.6, 131.8, 134.5, 154.4, 157.0 ppm.

HRMS calcd. for C₁₅H₁₁O₂: 223.076455; found 223.076432.

IR: ν = 675, 700, 719, 760, 793, 829, 868, 936, 946, 1004, 1015, 1050, 1101, 1122, 1160, 1181, 1227, 1266, 1283, 1306, 1432, 1463, 1477, 1507, 1578, 1596, 2840, 3241, 3408 cm⁻¹.

Compound 15:



Following the general procedure A (DMF/H₂O 5:1 at 50°C), the aldehyde employed as starting material was prepared from 2-bromo-5-hydroxybenzaldehyde (200 mg, 0.99 mmol) and 2,5-dimethoxyphenylboronic acid (199 mg, 1.09 mmol) and purified by flash chromatography (hexanes/EtOAc, 3/2). Pale yellow solid (240 mg, 93%). Submission of this material to the general Ohira-Bestmann conditions and purification by flash chromatography (hexanes/EtOAc, 7/3) afforded the desired alkyne as a white solid (203 mg, 87%).

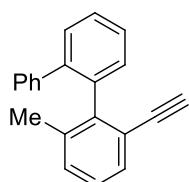
¹H NMR (400 MHz, CDCl₃) δ = 2.94 (s, 1H), 3.73 (s, 3H), 3.79 (s, 3H), 5.00 (s, 1H), 6.83 - 6.93 (m, 4H), 7.04 (d, J = 2.7 Hz, 1H), 7.21 (d, J = 8.4 Hz, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ = 55.9, 56.5, 79.5, 82.8, 112.6, 113.8, 116.3, 117.4, 119.6, 123.1, 130.2, 131.8, 134.3, 151.4, 153.3, 154.5 ppm.

HRMS calcd. for C₁₆H₁₄O₃Na₁: 277.083515; found 277.083378.

IR: ν = 675, 699, 727, 751, 793, 831, 864, 875, 944, 1014, 1044, 1100, 1149, 1157, 1179, 1205, 1220, 1260, 1287, 1432, 1481, 1508, 1589, 1599, 2832, 2945, 3241, 3391 cm⁻¹.

Compound 16:



Prepared from the corresponding aldehyde (204 mg, 0.75 mmol) following the general procedure and purified by flash chromatography (hexanes). White solid (158 mg, 78%).

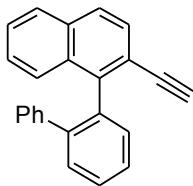
¹H NMR (400 MHz, CDCl₃) δ = 1.88 (s, 3H), 2.96 (s, 1H), 7.08 (d, J = 7.6 Hz, 1H), 7.15 (t, J = 7.6 Hz, 1H), 7.17 - 7.27 (m, 5H), 7.27 - 7.34 (m, 1H), 7.37 - 7.54 (m, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ = 20.5, 80.4, 83.6, 122.8, 126.7, 127.0, 127.2, 127.7, 127.9, 129.2, 130.0, 130.3, 130.4, 130.6, 136.6, 138.4, 141.4, 141.4, 144.4 ppm.

HRMS calcd. for C₂₁H₁₆: 268.125101; found 268.125200.

IR (neat) $\tilde{\nu}$ = 668, 698, 742, 749, 757, 772, 915, 952, 1008, 1074, 1105, 1159, 1262, 1428, 1449, 1468, 1488, 1598, 1967, 3059, 3270 cm^{-1} .

Compound 17:



Prepared from the corresponding aldehyde (150 mg, 0.48 mmol) following the general procedure and purified by flash chromatography (hexanes). White solid (112 mg, 80%).

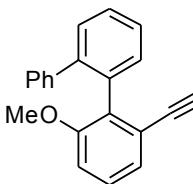
^1H NMR (400 MHz, CDCl_3) δ = 3.01 (s, 1H), 6.95 - 7.07 (m, 3H), 7.07 - 7.19 (m, 2H), 7.30 - 7.45 (m, 3H), 7.45 - 7.52 (m, 3H), 7.52 - 7.62 (m, 2H), 7.70 (d, J = 8.5 Hz, 1H), 7.76 (d, J = 8.0 Hz, 1H) ppm.

^{13}C NMR (101 MHz, CDCl_3) δ = 81.1, 83.8, 120.0, 126.5, 126.6, 126.9, 127.2, 127.5, 127.5, 128.0, 128.3, 128.7, 129.0, 130.1, 131.4, 132.4, 133.0, 137.2, 141.3, 142.6, 143.5 ppm.

HRMS calcd. for $\text{C}_{24}\text{H}_{16}$: 304.125197; found 304.155273.

IR: $\tilde{\nu}$ = 658, 698, 741, 761, 775, 816, 863, 876, 911, 975, 1008, 1025, 1073, 1101, 1152, 1198, 1281, 1332, 1380, 1435, 1447, 1478, 1503, 1593, 2923, 3054, 3272 cm^{-1} .

Compound 18:



Prepared from the corresponding aldehyde (179 mg, 0.62 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 15/1). Yellow solid (125 mg, 71%).

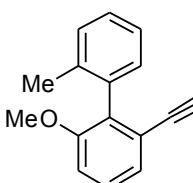
^1H NMR (300 MHz, CDCl_3) δ = 2.94 (s, 1H), 3.41 (s, 3H), 6.70 (dd, J = 7.2 Hz, 2.4 Hz, 1H), 7.11 - 7.18 (m, 7H), 7.35 - 7.45 (m, 4H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ = 55.5, 80.5, 83.0, 111.5, 123.7, 125.1, 126.5, 127.0, 127.4, 128.0, 128.3, 129.0, 129.5, 131.2, 134.0, 135.3, 142.0, 142.4, 156.7 ppm.

HRMS calcd. for $\text{C}_{21}\text{H}_{16}\text{O}_1$: 284.120115, found: 284.120047.

IR: $\tilde{\nu}$ = 672, 698, 742, 759, 779, 794, 845, 911, 948, 1008, 1065, 1117, 1159, 1187, 1265, 1292, 1427, 1435, 1449, 1460, 1484, 1503, 1565, 1597, 1634, 1927, 1950, 1970, 2837, 2934, 2967, 3014, 3051, 3262 cm^{-1} .

Compound 19:



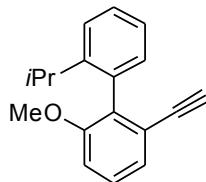
Prepared from the corresponding aldehyde (140 mg, 0.62 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 20/1). White solid (113 mg, 82%).

^1H NMR (300 MHz, CDCl_3) δ = 2.04 (s, 3H), 2.79 (s, 1H), 3.67 (s, 3H), 6.90 (dd, J = 8.1 Hz, 1.1 Hz, 1H), 7.07 - 7.23 (m, 6H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ = 19.8, 56.0, 79.9, 82.5, 111.7, 123.4, 125.3, 125.4, 127.7, 128.4, 129.7, 130.2, 133.9, 136.6, 136.9, 157.0 ppm.

HRMS calcd. for $\text{C}_{16}\text{H}_{14}\text{O}_1$: 222.104464, found: 222.104228.

IR: $\tilde{\nu}$ = 667, 729, 758, 795, 810, 909, 945, 967, 1004, 1068, 1120, 1159, 1171, 1186, 1260, 1292, 1378, 1436, 1462, 1566, 1589, 1602, 1672, 1701, 1842, 1931, 2836, 2934, 2956, 3018, 3063, 3277 cm^{-1} .

Compound 20:

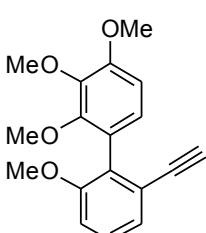
Prepared from the corresponding aldehyde (158 mg, 0.62 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 10/1). White solid (139 mg, 89%).

¹H NMR (300 MHz, CDCl₃) δ = 1.04 (d, *J* = 3.3 Hz, 3H), 1.06 (d, *J* = 3.3 Hz, 3H), 2.56 (hept., *J* = 6.9 Hz, 1H), 2.77 (s, 1H), 3.64 (s, 3H), 6.88 (d, *J* = 7.9 Hz, 1H), 7.02 (d, *J* = 7.1 Hz, 1H), 7.12 - 7.21 (m, 3H), 7.30 - 7.32 (m, 2H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ = 23.7, 24.2, 55.7, 80.3, 82.6, 111.4, 123.8, 125.0, 125.2, 125.4, 128.1, 128.2, 130.2, 134.1, 135.4, 147.6, 157.2 ppm.

HRMS calcd. for C₁₈H₁₈O₁: 250.135768, found: 250.135996.

IR: $\tilde{\nu}$ = 660, 731, 739, 758, 789, 909, 948, 1004, 1034, 1069, 1098, 1169, 1187, 1201, 1253, 1293, 1343, 1361, 1381, 1431, 1461, 1493, 1569, 1591, 2834, 2863, 2958, 3019, 3060, 3263, 3314 cm⁻¹.

Compound 21:

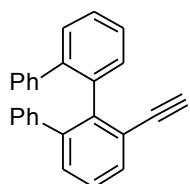
Prepared from the corresponding aldehyde (187 mg, 0.62 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 2/1). White solid (180 mg, 97%).

¹H NMR (300 MHz, CDCl₃) δ = 2.86 (s, 1H), 3.65 (s, 3H), 3.71 (s, 3H), 3.86 (s, 3H), 3.87 (s, 3H), 6.69 (d, *J* = 8.6 Hz, 1H), 6.86 (d, *J* = 9.1 Hz, 1H), 6.91 - 6.94 (m, 1H), 7.15 - 7.25 (m, 2H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ = 56.0, 61.0, 79.9, 80.0, 82.9, 106.9, 111.7, 123.7, 124.0, 125.3, 125.6, 128.4, 131.0, 142.2, 152.1, 153.4, 157.5 ppm.

HRMS calcd. for C₁₈H₁₈O₄: 321.109730, found: 321.109738.

IR: $\tilde{\nu}$ = 690, 746, 795, 872, 920, 1004, 1070, 1092, 1115, 1169, 1206, 1261, 1296, 1410, 1432, 1462, 1501, 1568, 1590, 2102, 2837, 2936, 3000, 3278 cm⁻¹.

Compound 22:

Prepared from the corresponding aldehyde (135 mg, 0.41 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 20/1). White solid (115 mg, 85%).

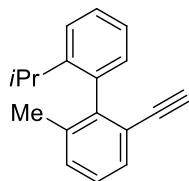
¹H NMR (300 MHz, CDCl₃) δ = 2.99 (s, 1H), 6.48 - 6.52 (m, 2H), 6.58 - 6.61 (m, 2H); 6.93 - 7.14 (m, 8H), 7.24 (d, *J* = 1.6 Hz, 1H), 7.28 - 7.38 (m, 2H), 7.49 - 7.52 (m, 1H), 7.58 (dd, *J* = 7.5 Hz, 1.4 Hz, 1H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ = 80.9, 83.6, 123.6, 126.3, 126.4, 126.4, 126.4, 127.3, 127.4, 128.0, 129.4, 129.6, 129.9, 130.7, 132.1, 132.7, 137.6, 140.5, 141.0, 141.5, 142.0, 143.1 ppm.

HRMS calcd. for C₂₆H₁₈: 330.140849, found: 330.140613.

IR: $\tilde{\nu}$ = 654, 671, 697, 730, 741, 749, 760, 810, 854, 910, 966, 979, 1008, 1027, 1073, 1092, 1115, 1157, 1182, 1253, 1284, 1419, 1434, 1455, 1481, 1496, 1578, 1597, 1748, 1804, 1819, 1881, 1900, 1947, 3029, 3056, 3278 cm⁻¹.

Compound 23:



Prepared from the corresponding aldehyde (97 mg, 0.4 mmol) following the general procedure and purified by flash chromatography (hexanes). Pale yellow oil (66 mg, 71%).

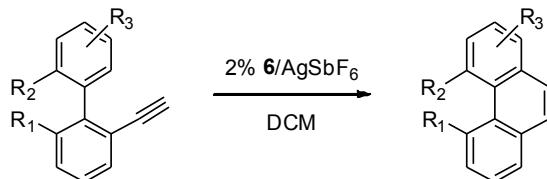
¹H NMR (400 MHz, CDCl₃) δ = 1.18 (d, *J* = 6.9 Hz, 3H), 1.23 (d, *J* = 6.8 Hz, 3H), 2.08 (s, 3H), 2.65 (hept, *J* = 6.9 Hz, 1H), 2.89 (s, 1H), 7.09 (dd, *J* = 7.6, 0.9 Hz, 1H), 7.27 - 7.35 (m, 3H), 7.40 - 7.48 (m, 2H), 7.50 (dd, *J* = 7.4, 0.9 Hz, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ = 20.7, 23.9, 24.4, 30.4, 80.1, 83.3, 122.5, 125.4, 125.7, 127.0, 128.0, 129.2, 130.4, 130.4, 136.9, 138.5, 144.5, 146.8 ppm.

HRMS calcd. for C₁₈H₁₈: 234.140849; found 234.140643.

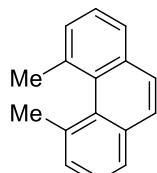
IR: ν = 756, 786, 1005, 1035, 1085, 1258, 1362, 1381, 1456, 1575, 2867, 2960, 3286 cm⁻¹.

General Procedure for the Au catalysed cycloisomerization:



A suspension of alkyne (1 eq.), AgSbF₆ (0.02 eq.) and compound **6** (0.02 eq.) in dry DCM (0.05 M) was stirred at r.t. under Ar. Reaction progress was followed by GC and once completed, the mixture was diluted with dichloromethane, and filtered through over a short pad of silica. The solvent was evaporated and the residue purified by flash chromatography.

Compound 8:



Prepared from compound **7** (20.6 mg, 0.1 mmol) following the general procedure and purified by flash chromatography (hexanes). White solid (20.1 mg, 98%).

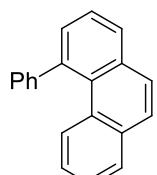
¹H NMR (400 MHz, CDCl₃) δ = 2.62 (s, 6H), 7.43 (dd, *J* = 7.2, 0.6 Hz, 2H), 7.50 (t, *J* = 7.4 Hz, 2H), 7.51 (s, 2H), 7.66 (dd, *J* = 7.6, 0.8 Hz, 2H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ = 22.9, 124.8, 126.0, 126.6, 128.6, 130.5, 134.0, 135.9 ppm.

HRMS calcd. for C₁₆H₁₄: 206.109638; found 206.109547.

IR: ν = 697, 718, 748, 756, 773, 814, 887, 1160, 1234, 1372, 1436, 1457, 2853, 2924, 2951, 3044 cm⁻¹.

Compound 10:



Prepared from compound **9** (33.3 mg, 0.13 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 95/5). Pale yellow solid (30.6 mg, 92%).

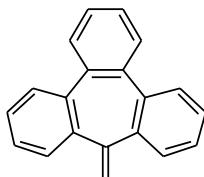
¹H NMR (400 MHz, CDCl₃) δ = 7.12 (ddd, *J* = 8.6, 7.0, 1.5 Hz, 1H), 7.38-7.54 (m, 7H), 7.60 (t, *J* = 7.5 Hz, 1H), 7.73 (d, *J* = 9.4 Hz, 1H), 7.77 (q, *J* = 8.6 Hz, 2H), 7.84 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.90 (dd, *J* = 7.9, 1.4 Hz, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ = 125.0, 125.8, 126.1, 127.2, 127.5, 127.7, 128.4, 128.5, 128.6, 128.7, 129.1, 129.2, 130.5, 130.9, 133.6, 133.8, 140.7, 145.5 ppm.

HRMS calcd. for C₂₀H₁₄: 254.109551; found 254.109307.

IR: $\tilde{\nu}$ = 673, 698, 721, 738, 765, 779, 799, 826, 872, 910, 948, 957, 1024, 1040, 1072, 1091, 1164, 1178, 1254, 1305, 1393, 1434, 1491, 1521, 1599, 2851, 2922, 3052 cm⁻¹.

Compound 11:



Prepared from compound **9** (20.6 mg, 0.1 mmol) with Ph₃PAuCl and AgSbF₆ as catalytic mixture. Purified by semi-preparative HPLC (YMC, 2 cm x 15 cm, CH₃CN, 10 mL/min; 35.9 mg in 1.5 mL of CH₃CN).

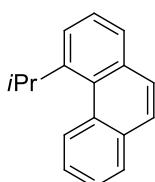
¹H NMR (400 MHz, CDCl₃) δ = 5.31 (s, *J* = 2.4 Hz, 2H), 7.31-7.41 (m, 6H), 7.42-7.47 (m, 2H), 7.56-7.62 (m, 4H), ppm.

¹³C NMR (101 MHz, CDCl₃) δ = 116.0, 127.1, 127.7, 128.0, 128.0, 129.1, 130.7, 137.1, 138.8, 145.0, 150.9 ppm.

HRMS calcd. for C₂₀H₁₄: 254.109551; found 254.109338.

IR (neat) $\tilde{\nu}$ = 664, 702, 739, 761, 788, 905, 946, 1040, 1101, 1161, 1276, 1326, 1430, 1475, 1488, 1629, 1819, 3013, 3055 cm⁻¹.

Compound 24:



Prepared from compound **11** (32.4 mg, 0.15 mmol) following the general procedure and purified by semi-preparative HPLC (YMC, 2 cm x 15 cm, CH₃CN/H₂O 75/25, 15 mL/min; 32.4 mg in 1.0 mL of CH₃CN) to obtain a colorless oil (22.7 mg, 70%).

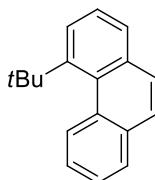
¹H NMR (400 MHz, CDCl₃) δ = 1.54 (d, *J* = 6.7 Hz, 6H), 4.34 (hept, *J* = 6.7 Hz, 1H), 7.56-7.63 (m, 3H), 7.68 (d, *J* = 1.3 Hz, 2H), 7.72 (d, *J* = 7.8 Hz, 2H), 7.88-7.95 (m, 1H), 8.60-8.67 (m, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ = 25.5, 31.2, 125.4, 125.7, 126.0, 126.2, 126.7, 126.8, 128.0, 128.1, 128.6, 129.4, 130.5, 133.5, 133.7, 147.0 ppm.

HRMS calcd. for C₁₇H₁₆: 220.125282; found 220.125198.

IR: $\tilde{\nu}$ = 666, 713, 723, 740, 771, 797, 827, 865, 965, 1040, 1162, 1176, 1261, 1324, 1363, 1384, 1436, 1452, 1495, 1594, 1714, 2866, 2961, 3048 cm⁻¹.

Compound 25:



Prepared from compound **12** (30.5 mg, 0.13 mmol) following the general procedure and purified by flash chromatography (hexanes). White solid (29.0 mg, 95%).

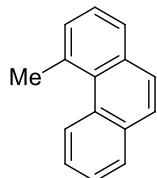
¹H NMR (400 MHz, CDCl₃) δ = 1.65 (s, 9H), 7.45 - 7.55 (m, 3H), 7.63 (s, 2H), 7.64 (dd, *J* = 7.6, 1.3 Hz, 1H), 7.83 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.92 (dd, *J* = 7.7, 1.3 Hz, 1H), 8.60 (dd, *J* = 8.1, 0.8 Hz, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ = 34.3, 38.0, 123.3, 125.3, 126.0, 126.2, 126.6, 127.3, 127.9, 128.4, 131.2, 131.2, 132.0, 133.2, 134.0, 148.5 ppm.

HRMS calcd. for C₁₈H₁₈: 234.140849; found 234.140826.

IR: $\tilde{\nu}$ = 722, 746, 769, 797, 828, 867, 901, 944, 963, 994, 1038, 1094, 1143, 1192, 1259, 1306, 1363, 1370, 1398, 1431, 1468, 1480, 1519, 1561, 1922, 2951, 3046 cm⁻¹.

Compound 26:



Prepared from compound **13** (28.0 mg, 0.15 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 20/1). White solid (24.7 mg, 88%).

¹H NMR (400 MHz, CDCl₃) δ = 3.18 (s, 3H), 7.49 - 7.55 (m, 2H), 7.58 - 7.63 (m, 1H), 7.63 - 7.68 (m, 1H), 7.74 (s, J = 9.5 Hz, 2H), 7.77 - 7.83 (m, 1H), 7.91 - 7.96 (m, 1H), 8.95 (dd, J = 9.3, 8.2 Hz, 1H) ppm.

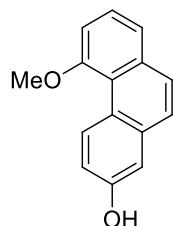
¹³C NMR (101 MHz, CDCl₃) δ = 27.5, 125.7, 125.9, 126.0, 127.2, 127.6, 127.7, 128.1, 128.9, 130.2, 131.4, 131.8, 133.6, 133.9, 135.7 ppm.

These NMR data was in agreement with those reported: Jana, R.; Biswas, A.; Samanta, S.; Ray, J. K. *Synthesis* **2010**, 2092-2100.

HRMS calcd. for C₁₅H₁₂: 192.093898; found 192.093722.

IR: $\tilde{\nu}$ = 666, 709, 735, 793, 820, 862, 895, 943, 957, 993, 1027, 1106, 1165, 1215, 1295, 1315, 1376, 1438, 1449, 1497, 1597, 2875, 2963, 3048 cm⁻¹.

Compound 27:



Prepared from compound **14** (32.6 mg, 0.15 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 7/3). White solid (30.2 mg, 93%).

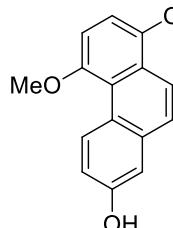
¹H NMR (400 MHz, CDCl₃) δ = 4.12 (s, 3H), 5.10 (s, 1H), 7.14 (dd, J = 6.9, 2.2 Hz, 1H), 7.20 (dd, J = 9.2, 2.9 Hz, 1H), 7.23 (d, J = 2.8 Hz, 1H), 7.45 - 7.54 (m, 2H), 7.60 (d, J = 8.8 Hz, 1H), 7.69 (d, J = 8.8 Hz, 1H), 9.59 (d, J = 9.2 Hz, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ = 55.8, 108.5, 111.8, 116.2, 121.1, 121.8, 124.9, 125.7, 127.2, 128.0, 130.8, 133.7, 134.7, 153.4, 158.3 ppm.

HRMS calcd. for C₁₅H₁₂O₂: 224.083727; found 224.083483.

IR: $\tilde{\nu}$ = 708, 752, 788, 805, 827, 859, 877, 943, 966, 994, 1073, 1098, 1139, 1154, 1220, 1256, 1266, 1312, 1336, 1352, 1429, 1449, 1529, 1573, 1614, 2833, 2934, 3192 cm⁻¹.

Compound 28:



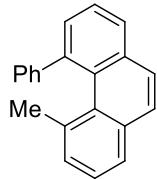
Prepared from compound **15** (33 mg, 0.13 mmol) following the general procedure and purified by flash chromatography (hexanes/EtOAc, 7/3). Pale brown solid (30 mg, 91%).

¹H NMR (400 MHz, CDCl₃) δ = 4.00 (s, 3H), 4.06 (s, 3H), 5.10 (s, 1H), 6.91 (d, J = 8.6 Hz, 1H), 7.05 (d, J = 8.6 Hz, 1H), 7.18 (dd, J = 9.3, 2.9 Hz, 1H), 7.23 (d, J = 2.8 Hz, 1H), 7.63 (d, J = 9.1 Hz, 1H), 8.23 (d, J = 9.1 Hz, 1H), 9.61 (d, J = 9.3 Hz, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ = 56.3, 56.3, 105.3, 108.7, 111.5, 116.2, 121.2, 122.1, 124.2, 124.7, 126.6, 130.9, 134.9, 150.2, 152.4, 153.6 ppm.

HRMS calcd. for C₁₆H₁₄O₃Na₁: 277.083513; found 277.083444.

IR: $\tilde{\nu}$ = 712, 726, 780, 798, 825, 860, 944, 970, 1016, 1064, 1106, 1149, 1217, 1242, 1264, 1307, 1353, 1426, 1453, 1500, 1530, 1613, 2832, 2935, 3328 cm⁻¹.

Compound 29:

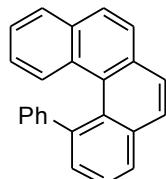
Prepared from compound **16** (30 mg, 0.11 mmol) following the general procedure and purified by flash chromatography (hexanes). Colorless oil (28.8 mg, 96%).

¹H NMR (400 MHz, CDCl₃) δ = 1.85 (s, 3H), 6.35 - 8.30 (m, 4H), 7.06 (d, J = 6.9 Hz, 1H), 7.25 (t, J = 7.3 Hz, 1H), 7.43 (t, J = 7.5 Hz, 1H), 7.58 - 7.70 (m, 5H), 7.79 (dd, J = 6.3, 2.8 Hz, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ = 23.4, 125.0, 126.4, 126.4, 126.5, 126.8, 126.8, 127.6, 128.4, 128.8, 129.5, 130.6, 133.9, 135.0, 136.8, 141.6, 144.9 ppm.

HRMS calcd. for C₂₁H₁₆: 268.125017; found 268.125200.

IR: ν = 696, 722, 749, 766, 813, 826, 882, 916, 965, 1030, 1074, 1115, 1164, 1176, 1244, 1263, 1302, 1376, 1412, 1437, 1493, 1568, 1596, 1927, 2851, 2922, 3044 cm⁻¹.

Compound 30:

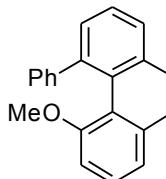
Prepared from compound **17** (40 mg, 0.13 mmol) following the general procedure and purified by flash chromatography (hexanes). Pale yellow solid (29.2 mg, 73%).

¹H NMR (400 MHz, CDCl₃) δ = 5.85 - 8.45 (m, 4H), 6.92 - 6.99 (m, 2H), 7.23 (t, J = 7.4 Hz, 1H), 7.70 - 7.78 (m, 3H), 7.81 - 7.90 (m, 3H), 7.95 (d, J = 8.4 Hz, 2H), 8.00 (dq, J = 7.1, 3.7 Hz, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ = 124.4, 125.2, 126.1, 126.3, 126.4, 126.6, 126.9, 127.2, 127.5, 127.5, 127.6, 128.0, 128.9, 129.4, 130.1, 130.7, 131.8, 132.0, 135.0, 141.3, 144.2 ppm.

HRMS calcd. for C₂₁H₁₆: 304.125200; found 304.125216.

IR: ν = 655, 680, 700, 734, 752, 835, 864, 921, 954, 963, 1029, 1072, 1176, 1237, 1261, 1361, 1425, 1441, 1485, 1597, 2851, 2922, 3047 cm⁻¹.

Compound 31:

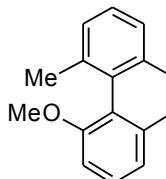
Prepared from compound **18** (42.6 mg, 0.15 mmol) following the general procedure and purified by filtration over a short pad of silica. White solid (40 mg, 93%).

¹H NMR (300 MHz, CDCl₃) δ = 3.04 (s, 3H), 6.63 (q, J = 4.4 Hz, 1H), 7.16 - 7.28 (m, 5H), 7.40 (d, J = 4.5 Hz, 2H), 7.55 (d, J = 5.2 Hz, 2H), 7.60 (d, J = 8.6 Hz, 1H), 7.65 (d, J = 8.6 Hz, 1H), 7.71 - 7.79 (m, 1H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ = 53.5, 107.1, 120.0, 120.9, 126.0, 126.1, 126.3, 126.7, 126.9, 127.3, 127.7, 128.4, 129.9, 134.3, 135.2, 135.6, 141.9, 146.9, 156.1 ppm.

HRMS calcd. for C₂₁H₁₆O₁: 284.120116; found 284.120169.

IR: ν = 667, 689, 719, 744, 771, 788, 815, 867, 916, 1001, 1062, 1091, 1111, 1167, 1181, 1203, 1242, 1257, 1289, 1395, 1409, 1428, 1462, 1501, 1578, 1592, 1681, 1693, 2761, 2869, 2939, 2977 cm⁻¹.

Compound 32:

Prepared from compound **19** (32.2 mg, 0.15 mmol) following the general procedure and purified by filtration over a short pad of silica. White solid (29 mg, 91%).

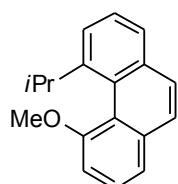
¹H NMR (300 MHz, CDCl₃) δ = 2.61 (s, 3H), 3.97 (s, 3H), 7.06 (d, *J* = 7.7 Hz, 1H), 7.46 - 7.67 (m, 7 H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ = 24.2, 55.0, 107.5, 120.0, 120.9, 124.9, 125.8, 125.9, 127.0, 127.9, 128.8, 129.3, 133.5, 135.2, 137.4, 157.0 ppm.

HRMS calcd. for C₁₆H₁₄O₁: 222.104467, found: 222.104643.

IR: $\tilde{\nu}$ = 698, 716, 750, 793, 817, 860, 888, 921, 977, 994, 1020, 1096, 1145, 1164, 1185, 1240, 1261, 1311, 1332, 1374, 1414, 1432, 1450, 1491, 1522, 1568, 1600, 1777, 1907, 2832, 2926, 2956, 2992, 3048 cm⁻¹.

Compound 33:



Prepared from compound **20** (32.2 mg, 0.15 mmol) following the general procedure and purified by filtration over a short pad of silica. White solid (29 mg, 91%).

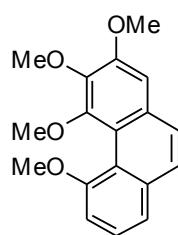
¹H NMR (300 MHz, CDCl₃) δ = 1.23 (bs, 6H), 3.59 (hept., *J* = 6.7 Hz, 1H), 3.91 (s, 3H), 7.01 (dd, *J* = 7.6 Hz, 1.5 Hz, 1H), 7.45 (dd, *J* = 7.9 Hz, 1.5 Hz, 1H), 7.48 - 7.63 (m, 6H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ = 33.2, 38.2, 55.4, 107.3, 120.1, 120.7, 124.0, 124.9, 125.9, 126.4, 126.5, 126.7, 127.8, 133.5, 135.3, 149.3, 156.8 ppm.

HRMS calcd. for C₁₈H₁₈O₁: 250.135764, found: 250.135535.

IR: $\tilde{\nu}$ = 699, 723, 757, 815, 824, 860, 891, 920, 988, 1043, 1085, 1151, 1171, 1221, 1235, 1259, 1302, 1328, 1359, 1379, 1416, 1431, 1451, 1491, 1521, 1567, 1601, 1613, 1726, 1777, 1912, 2867, 2932, 2951, 2984, 3047 cm⁻¹.

Compound 34:



Prepared from compound **21** (44.7 mg, 0.15 mmol) following the general procedure and purified by filtration over a short pad of silica. White solid (44 mg, 98%).

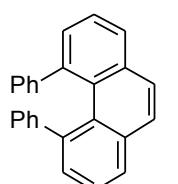
¹H NMR (300 MHz, CDCl₃) δ = 3.75 (s, 3H), 4.01 (ps, 6H), 4.02 (s, 3H), 7.00 (s, 1H), 7.06 (dd, *J* = 7.6 Hz, 1.2 Hz, 1H), 7.40 (dd, *J* = 7.8 Hz, 1.3 Hz, 1H), 7.45 (d, *J* = 7.6 Hz, 1H), 7.49 - 7.53 (m, 2H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ = 56.1, 60.9, 61.4, 103.6, 108.1, 117.1, 119.7, 119.9, 126.2, 126.3, 126.7, 130.5, 133.9, 142.5, 152.5, 152.8, 157.6 ppm.

HRMS calcd. for C₁₈H₁₈O₂Na₁: 321.109729, found: 321.109738.

IR: $\tilde{\nu}$ = 688, 728, 766, 782, 814, 835, 908, 925, 953, 1003, 1048, 1079, 1096, 1111, 1138, 1197, 1229, 1342, 1386, 1423, 1465, 1496, 1510, 1560, 1602, 2249, 2832, 2853, 2932, 2996, 3047 cm⁻¹.

Compound 35:



Prepared from compound **22** (47.9 mg, 0.15 mmol) following the general procedure and purified by filtration over a short pad of silica. Yellow solid (43 mg, 90%).

¹H NMR (400 MHz, CDCl₃) δ = 6.51 - 6.60 (m, 4H); 6.93 - 6.98 (m, 4H), 7.04 - 7.09 (m, 2H), 7.13 (dd, *J* = 7.32 Hz, 1.24 Hz, 2H), 7.50 (t, *J* = 7.44 Hz, 2H), 7.69 (s, 2H), 7.76 (dd, *J* = 7.8 Hz, 1.5 Hz, 2H) ppm.

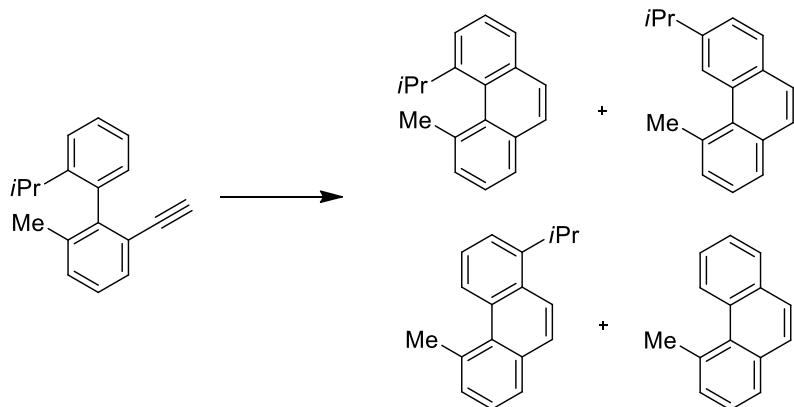
¹³C NMR (75 MHz, CDCl₃) δ = 125.6, 126.7, 126.9, 127.2, 128.0, 128.3, 129.6, 129.7, 134.8, 142.2, 143.7 ppm.

HRMS calcd. for C₂₆H₁₈: 330.140852, found: 330.140898.

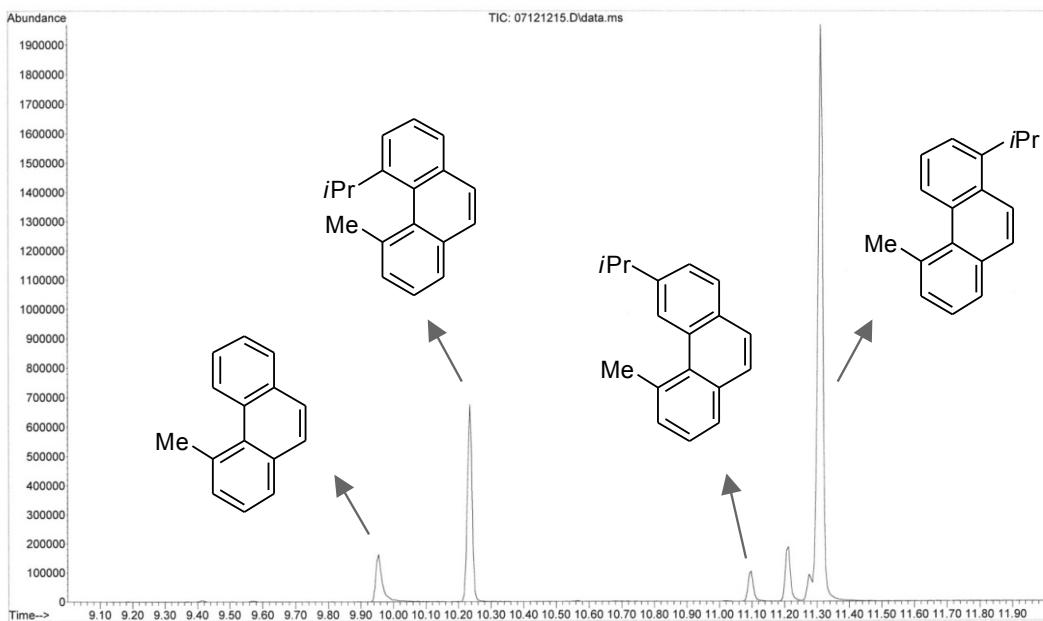
IR: $\tilde{\nu}$ = 693, 726, 744, 771, 828, 868, 909, 943, 961, 1025, 1075, 1130, 1155, 1176, 1260, 1278, 1307, 1410, 1437, 1491, 1596, 1666, 1799, 1871, 1934, 2849, 2923, 3027, 3047, 3075 cm⁻¹.

Compounds 36, 37 and 38:

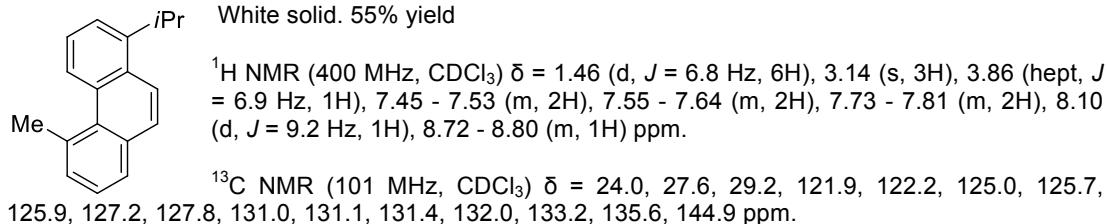
Starting from compound **23** (95.7 mg, 0.41 mmol) following the general procedure, a mixture of different products was obtained, which were separated by HPLC (YMC, 2 cm x 15 cm, CH₃CN/H₂O 75/25, 10 mL/min; 19.5 mg in 1.4 mL of CH₃CN and 0.1 mL of H₂O).



GC-MS of the crude reaction (Agilent 19091S-433 column (30 m × 0.25 mm); T = 70 → 280 °C. T_{detector} = 250 °C T_{inlet} = 250 °C).



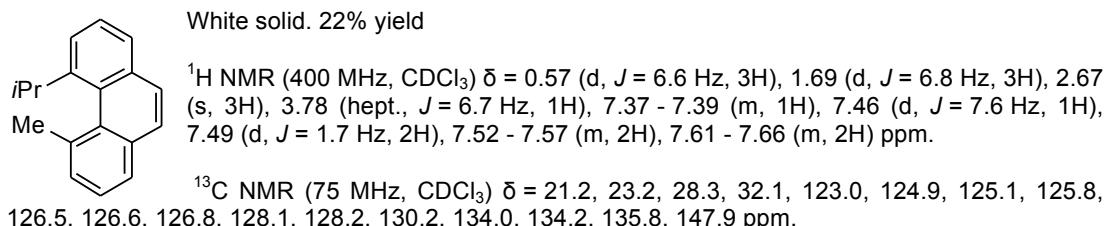
Compound 36:



HRMS calcd. for $\text{C}_{18}\text{H}_{18}$: 234.140849; found 234.140628.

IR $\tilde{\nu}$ = 721, 747, 774, 819, 829, 893, 960, 1054, 1102, 1164, 1190, 1216, 1275, 1310, 1359, 1377, 1410, 1434, 1448, 1594, 1784, 1922, 2867, 2923, 2959, 3047 cm^{-1} .

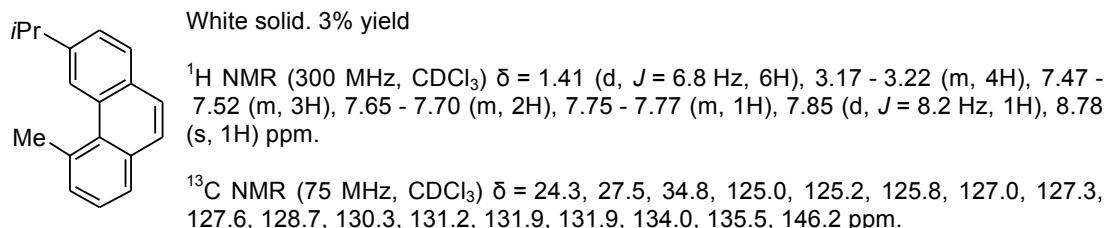
Compound 37:



HRMS calcd. for $\text{C}_{18}\text{H}_{18}$: 234.140848, found: 234.140779.

IR: $\tilde{\nu}$ = 699, 725, 751, 768, 792, 813, 824, 862, 891, 925, 961, 979, 995, 1037, 1044, 1044, 1090, 1114, 1172, 1216, 1230, 1265, 1300, 1361, 1383, 1418, 1438, 1459, 1565, 1594, 1716, 1772, 2865, 2924, 2952, 3044 cm^{-1} .

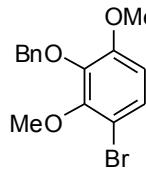
Compound 38:



HRMS calcd. for $\text{C}_{18}\text{H}_{18}$: 234.140848, found: 234.140779.

IR: $\tilde{\nu}$ = 716, 757, 791, 812, 838, 893, 957, 1018, 1032, 1052, 1078, 1104, 1133, 1149, 1193, 1216, 1234, 1292, 1312, 1359, 1378, 1407, 1431, 1450, 1459, 1500, 1522, 1569, 1595, 1615, 2869, 2928, 2957, 3047 cm^{-1} .

Synthesis of Bulbophyllantrin and Marylaurencinol A



To the stirred solution of 3-bromo-2,6-dimethoxyphenol (1.8 g, 7.72 mmol) in acetone (40 mL), potassium carbonate (1.6 g, 11.59 mmol) and benzyl bromide (0.97 mL, 8.11 mmol) were added. The reaction was stirred overnight at room temperature. The mixture was evaporated, and the remaining residue was purified by column chromatography, using hexane/EtOAc (9:1) as eluent, to give compound (2.2 g, 88%) as a colorless oil.

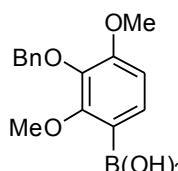
¹H NMR (400 MHz, CDCl₃) δ = 3.82 (s, 3H), 3.91 (s, 3H), 5.04 (s, 2H), 6.59 (d, J = 9.0 Hz, 1H), 7.22 (d, J = 8.9 Hz, 1H), 7.30 - 7.41 (m, 3H), 7.48 - 7.53 (m, 2H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ = 56.3, 61.3, 75.6, 108.6, 108.9, 127.1, 128.2, 128.5, 128.5, 137.5, 142.7, 151.5, 153.8 ppm.

HRMS calcd. for C₁₅H₁₅O₃Br₁Na₁: 345.009686; found 345.009358.

IR (neat) ν = 694, 734, 791, 876, 915, 980, 1008, 1088, 1179, 1214, 1226, 1271, 1293, 1371, 1413, 1438, 1460, 1473, 1574, 2837, 2937 cm⁻¹.

Compound 42:



2-(Benzylxy)-4-bromo-1,3-dimethoxybenzene (1.6 g, 4.95 mmol) in 40 mL of diethyl ether was cooled to -78°C. n-BuLi (1.98 mL, 4.95 mmol, 2.5 M) was added at that temperature. The solution was stirred for an additional 1 h at -78°C. Then, trimethylborate (1.69 mL, 14.85 mmol) was added and the solution was allowed to warm to room temperature overnight. The reaction was quenched with the addition of HCl (20 mL, 3 M) and stirred for 2 h. The two phases were separated, and the water phase was extracted with *tert*-butyl methyl ether and then dried over Na₂SO₄. The mixture was evaporated, and the remaining residue was purified by column chromatography, using hexane/EtOAc (6:4) as eluent, to give compound **42** (935 mg, 66%) as a white solid.

¹H NMR (300 MHz, CD₃CN) δ = 3.86 (s, 3H), 3.94 (s, 3H), 4.99 (s, 2H), 6.32 (s, 2H), 6.82 (d, J = 8.4 Hz, 1H), 7.32 - 7.43 (m, 1H), 7.46 (d, J = 8.4 Hz, 1H), 7.48 - 7.52 (m, 2H).

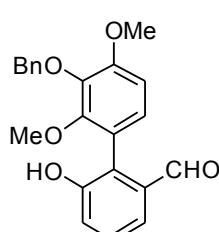
¹³C NMR (75 MHz, CD₃CN) δ = 56.7, 62.5, 75.6, 109.3, 129.0, 129.3, 129.3, 132.1, 138.9, 141.0, 157.7, 160.2.

¹¹B NMR (96 MHz, CD₃CN) δ = 28.7 ppm.

HRMS calcd. for C₁₅H₁₇B₁O₅Na₁: 311.107456; found 311.107270.

IR: ν = 693, 725, 751, 805, 896, 981, 1004, 1063, 1089, 1185, 1225, 1278, 1342, 1377, 1434, 1457, 1498, 1596, 2838, 2929, 3000, 3358 cm⁻¹.

Compound 43:



A suspension of aldehyde **41** (60.5 mg, 0.30 mmol), boronic acid **42** (130 mg, 0.45 mmol, 1.5 eq.), Pd₂(dba)₃ (0.05 eq.), PCy₃ (0.11 eq.) and Cs₂CO₃ (2.5 eq.) in a degassed mixture of 1,4-dioxane:toluene 2:3 was vigorously stirred for 24 h at 85°C. Then, the mixture was cooled to room temperature and the crude material was filtered through a pad of celite. The crude product was purified by flash chromatography (hexanes/EtOAc, 7/3) to afford **43** as a pale yellow solid (93 mg, 85%).

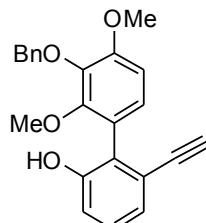
¹H NMR (400 MHz, CDCl₃) δ = 3.63 (s, 3H), 3.92 (s, 3H), 5.13 (s, 2H), 5.67 (s, 1H), 6.81 (d, J = 8.6 Hz, 1H), 6.88 (d, J = 8.5 Hz, 1H), 7.22 - 7.27 (m, 1H), 7.30 - 7.43 (m, 4H), 7.45 - 7.49 (m, 2H), 7.61 (dd, J = 7.7, 1.2 Hz, 1H), 9.67 (d, J = 0.6 Hz, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ = 56.3, 61.6, 75.4, 108.4, 118.0, 120.3, 121.8, 127.5, 127.9, 128.4, 128.5, 128.7, 129.2, 135.6, 137.2, 141.5, 152.2, 154.0, 155.2, 192.2 ppm.

HRMS calcd. for C₂₂H₂₀O₅Na₁: 387.120290; found 387.120626.

IR (neat) ν = 692, 723, 742, 785, 797, 887, 909, 978, 1012, 1089, 1113, 1167, 1176, 1218, 1267, 1283, 1370, 1416, 1440, 1454, 1482, 1497, 1578, 1593, 1667, 2839, 2938, 3223 cm⁻¹.

Compound 44:



Prepared from compound **43** (150 mg, 0.44 mmol) following the general procedure for the Ohira-bestmann reaction and purified by flash chromatography (hexanes/EtOAc, 7/3). White solid (135 mg, 91%).

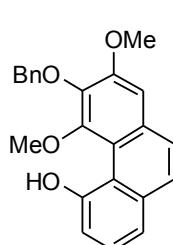
¹H NMR (400 MHz, CDCl₃) δ = 2.91 (s, 1H), 3.67 (s, 3H), 3.90 (s, 3H), 5.12 (s, 2H), 5.43 (s, 1H), 6.79 (d, J = 8.6 Hz, 1H), 7.02 (dd, J = 5.5, 3.9 Hz, 1H), 7.06 (d, J = 8.6 Hz, 1H), 7.20 - 7.23 (m, 2H), 7.29 - 7.39 (m, 3H), 7.48 (dd, J = 7.9, 1.6 Hz, 2H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ = 56.1, 61.9, 75.3, 79.9, 83.1, 108.2, 117.4, 121.0, 123.2, 126.0, 127.3, 128.0, 128.2, 128.4, 128.6, 128.8, 137.6, 141.1, 151.9, 153.6, 154.6 ppm.

HRMS calcd. for C₂₃H₂₀O₄Na₁: 383.125379; found 383.125089.

IR: ν = 668, 695, 743, 795, 804, 891, 973, 990, 1088, 1116, 1173, 1204, 1216, 1284, 1344, 1421, 1454, 1480, 1508, 1573, 1598, 2836, 2938, 3245, 3309 cm⁻¹.

Compound 45:



Prepared from compound **44** (100 mg, 0.27 mmol) following the general procedure for the Au-catalysed cycloisomerization and purified by flash chromatography (hexanes/EtOAc, 7/3). Pale yellow solid (90 mg, 90%).

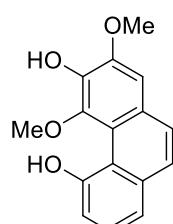
¹H NMR (400 MHz, CDCl₃) δ = 3.82 (s, 3H), 4.03 (s, 3H), 5.26 (s, 2H), 7.18 (s, 1H), 7.25 (dd, J = 7.7, 1.5 Hz, 1H), 7.34 - 7.44 (m, 4H), 7.48 - 7.53 (m, 2H), 7.54 - 7.59 (m, 2H), 7.62 (d, J = 8.8 Hz, 1H), 10.41 (s, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ = 56.2, 63.0, 76.4, 107.0, 116.4, 117.4, 118.2, 120.6, 126.2, 127.6, 128.4, 128.6, 128.6, 130.9, 134.5, 137.5, 141.5, 148.5, 152.7, 154.4 ppm.

HRMS calcd. for C₂₃H₂₀O₄Na₁: 383.125376; found 383.125101.

IR (neat) ν = 683, 696, 737, 752, 790, 819, 853, 882, 923, 959, 980, 993, 1066, 1097, 1142, 1200, 1244, 1265, 1277, 1342, 1366, 1438, 1451, 1467, 1499, 1516, 1559, 1605, 2878, 2943, 2986, 3143 cm⁻¹.

Compound 39, Bulbophyllanthrin:



A solution of compound **45** (31 mg, 0.084 mmol) in AcOEt (1 mL) was added over a suspension of 10% Pd/C (7 mg) in AcOEt (1 mL) and an atmosphere of H₂ was set up in the flask. After 24 h at r.t. the reaction mixture was filtered over celite and the compound was purified by flash chromatography (hexanes/EtOAc, 7/3) to obtain **39** as a white solid (19 mg, 81%). Compound **40** could also be isolated from the reaction mixture as a white solid (4 mg, 17%).

¹H NMR (400 MHz, CDCl₃) δ = 3.85 (s, 3H), 4.07 (s, 3H), 6.01 (s, 1H), 7.16 (s, 1H), 7.24 (dd, J = 7.6, 1.5 Hz, 1H), 7.42 (dd, J = 7.7, 1.5 Hz, 1H), 7.50 (dd, J = 8.6, 6.5 Hz, 2H), 7.57 (d, J = 8.8 Hz, 1H), 10.31 (s, 1H) ppm.

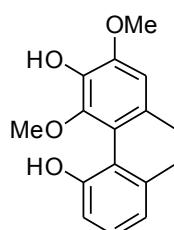
¹³C NMR (101 MHz, CDCl₃) δ = 56.4, 62.4, 106.2, 115.9, 117.3, 117.9, 120.5, 126.3, 127.0, 127.5, 127.6, 134.7, 139.1, 140.9, 147.1, 154.4 ppm.

NMR data was in agreement with those reported: Majumder, P. L.; Kar, A.; Shoolery, J. N. *Phytochemistry*, **1985**, 24, 2083-2087.

HRMS calcd. for C₁₆H₁₄O₄Na₁: 293.078431; found 293.078210.

IR: $\tilde{\nu}$ = 679, 728, 770, 789, 819, 850, 873, 926, 959, 998, 1064, 1077, 1097, 1144, 1200, 1253, 1275, 1293, 1357, 1421, 1438, 1462, 1475, 1506, 1525, 1569, 1617, 2934, 2968, 3171, 3277 cm⁻¹.

Compound 40, Marylaurencinol A:



A solution of compound **45** (22 mg, 0.06 mmol) in MeOH (1 mL) was added over a suspension of 10% Pd/C (11 mg) in MeOH (1 mL). H₂ was bubbled through the reaction mixture until an atmosphere of H₂ was set up in the flask and the mixture stirred at rt overnight. Filtration over celite and purification of the reaction crude by flash chromatography (hexanes/EtOAc, 7/3) afforded **40** as a white solid (16 mg, 97%).

¹H NMR (400 MHz, CDCl₃) δ = 2.62 - 2.69 (m, 2H), 2.69 - 2.78 (m, 2H), 3.77 (s, 3H), 3.95 (s, 3H), 5.52 (s, 1H), 6.71 (s, 1H), 6.85 (dd, *J* = 7.3, 1.2 Hz, 1H), 6.97 (dd, *J* = 8.2, 1.3 Hz, 1H), 7.16 (dd, *J* = 8.1, 7.3 Hz, 1H), 8.56 (s, 1H) ppm.

¹³C NMR (101 MHz, CDCl₃) δ = 30.7, 31.4, 56.5, 62.1, 108.0, 118.1, 119.2, 119.9, 120.1, 128.5, 132.4, 137.3, 140.7, 142.6, 146.3, 153.7 ppm.

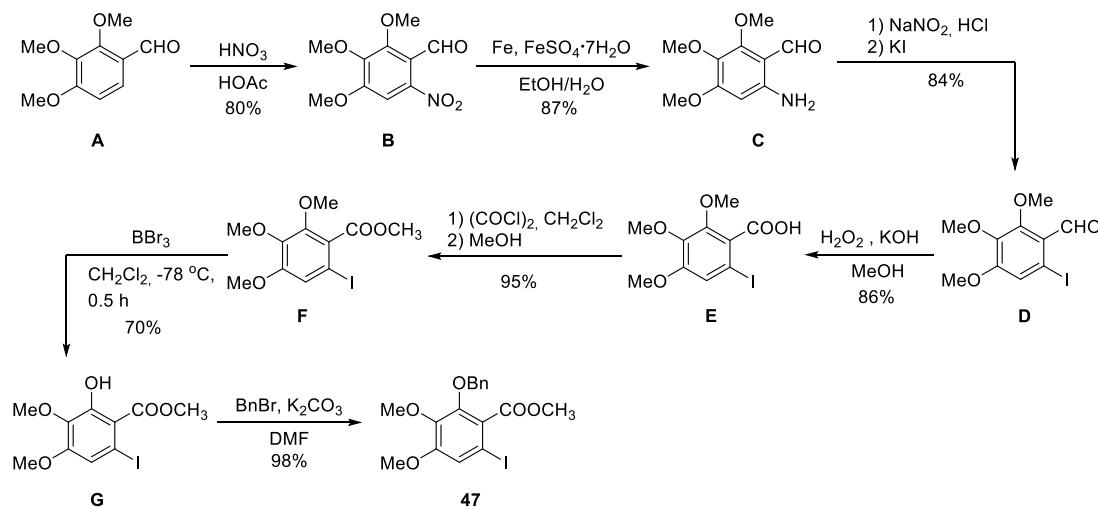
NMR data was in agreement with those reported: Yoshikawa, K.; Ito, T.; Iseki, K.; Baba, C.; Imagawa, H.; Yagi, Y.; Morita, H.; Asakawa, Y.; Kawano, S.; Hashimoto T. *J. Nat. Prod.*, **2012**, 75, 605-609.

HRMS calcd. for C₁₆H₁₆O₄Na₁: 295.094081; found 295.093913.

IR: $\tilde{\nu}$ = 676, 701, 740, 793, 838, 878, 923, 999, 1050, 1066, 1093, 1144, 1194, 1236, 1307, 1328, 1441, 1455, 1500, 1583, 1614, 2928, 3291 cm⁻¹.

Starting materials for the synthesis of Ochrolide and Coeliginin:

Preparation of methyl 2-(benzyloxy)-6-iodo-3,4-dimethoxybenzoate **47**:



Compound B: Prepared by a procedure reported by Cherkoui⁷. A solution of **A** (11.30 g, 41.4 mmol) in glacial acetic acid (100 mL) at 0 °C was treated dropwise with a 1:2 v/v mixture of glacial acetic acid: fuming nitric acid (100 mL). The resulting mixture was stirred at 0 °C for 90 min, then poured into ice water (400 mL) and extracted with CH₂Cl₂. The combined organic layers were washed with sat. NaHCO₃, brine, dried over Na₂SO₄, and concentrated *in vacuo*. Purification of the crude by flash chromatography (Hexane/EtOAc, 5/1) afforded **B** as a yellow solid (7.34 g, 80%).

¹H NMR (300 MHz, CDCl₃) δ = 10.22 (s, 1H), 7.28 (s, 1H), 3.97 (s, 9H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ = 186.8, 155.7, 153.2, 146.7, 143.3, 120.9, 103.6, 62.8, 61.2, 56.6.

HRMS (ESI): calculated for C₁₀H₁₁NO₅Na 264.047856, found 264.047856.

Compound C: Prepared by a procedure reported by Nimgirawath⁸. A mixture of **B** (8.00 g, 40.6 mmol), FeSO₄·7H₂O (2.00 g), iron powder (20.00 g), EtOH (70 mL) and water (25 mL) was refluxed for 4 h. The iron was filtered and the solvent was removed *in vacuo*. The residue was dissolved in EtOAc, washed with brine, dried over Na₂SO₄ and concentrated *in vacuo*. Purification of the crude by flash chromatography (Hexane/EtOAc, 5/1 to 2/1) afforded **C** as a yellow oil (6.08 g, 87%).

¹H NMR (300 MHz, CDCl₃) δ = 10.12 (s, 1H), 6.33 (br, 2H), 5.82 (s, 1H), 3.98 (s, 3H), 3.84 (s, 3H), 3.76 (s, 3H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ = 190.0, 160.6, 157.0, 149.0, 132.0, 106.6, 93.2, 62.0, 61.1, 55.8 ppm.

HRMS (EI): calculated for C₁₀H₁₃NO₄ 211.084241, found 211.084455.

Compound D: Prepared by a procedure reported by Nimgirawath⁸. A solution of sodium nitrite (1.90 g) in water (16 mL) was added to a mechanic stirred solution of **3** (5.32 g, 25.2 mmol) in 20% HCl (50 mL) at 0-5 °C and stirred for 15 min. Then, a solution of potassium iodide (20.00 g) in water (50 mL) was slowly added to the diazonium solution and stirred overnight. When this time has passed, CHCl₃ (200 mL) and excess Na₂S₂O₃ were added and the organic layer was separated, washed with brine, dried over Na₂SO₄ and concentrated *in vacuo*. Purification of the reaction crude by flash chromatography (Hexane/EtOAc, 5/1) afforded **D** as a pale yellow solid (6.79 g, 84%).

¹H NMR (300 MHz, CDCl₃) δ = 10.05 (s, 1H), 7.29 (s, 1H), 3.96 (s, 3H), 3.93 (s, 3H), 3.87 (s, 3H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ = 190.70, 157.9, 157.0, 142.9, 123.2, 120.7, 89.7, 62.5, 61.0, 56.4 ppm.

HRMS (ESI): calculated for C₁₀H₁₁O₄INa 344.959709, found 344.959427.

Compound E: Prepared by a procedure reported by Lv⁹. To a stirred solution of 50% aq. KOH (3.5 mL) and **D** (3.86 g, 12 mmol) in MeOH (20 mL) at 65 °C, hydrogen peroxide (30%, 9.6 mL) was added dropwise during 40 min. The mixture was then stirred at the same temperature for 30 min, cooled to room temperature and acidified with concentrated aq. HCl. The obtained mixture was then extracted

⁷ Cherkoui, M. Z.; Scherowsky, G. *New J. Chem.* **1997**, *21*, 1203.

⁸ Nimgirawath, S.; Udomputtimakul, P.; Taechowisan, T.; Wanbanjob, A.; Shen, Y. *Chem. Pharm. Bull.* **2009**, *57*, 368.

⁹ Lv, P.; Huang, K.; Xie, L.; Xu X. *Org. Biomol. Chem.* **2011**, *9*, 3133.

with CH_2Cl_2 , washed by brine, dried over Na_2SO_4 and concentrated *in vacuo*. Purification of the reaction crude by flash chromatography (Hexane/EtOAc, 5/1 to 1/1) afforded **E** as a white solid (3.48 g, 86%). Spectral data were consistent with those reported in the literature¹⁰.

¹H NMR (300 MHz, CDCl_3): δ = 8.91 (s, 1H), 7.11 (s, 1H), 3.90 (s, 3H), 3.85 (s, 6H) ppm.

¹³C NMR (75 MHz, CDCl_3): δ = 171.6, 155.2, 151.5, 142.5, 127.3, 118.6, 84.3, 62.2, 61.1, 56.4 ppm.

HRMS (ESI): calculated for $\text{C}_{10}\text{H}_{11}\text{O}_5\text{INa}$ 360.954480, found 360.954343.

Compound F: Prepared by a procedure reported by Lv⁹. To a stirred solution of **E** (3.00 g, 8.9 mmol) in CH_2Cl_2 (50 mL), oxalyl chloride (4.52 g, 17.8 mmol) was added. Then DMF was added dropwise in order to catalyze the formation of benzoyl chloride. The mixture was stirred for 3 h, after which the solvent and excess oxalyl chloride were removed *in vacuo*. Afterwards dry Methanol (30 mL) was added to the residue, and the resulting solution was stirred for 30 min. Then CH_2Cl_2 (70 mL) was added and the mixture was washed with water, brine, dried over Na_2SO_4 and concentrated *in vacuo*. Purification of the reaction crude by flash chromatography (Hexane/EtOAc, 5/1) afforded **F** as a white solid (2.97 g, 95%). Spectral data were consistent with those reported in the literature¹¹.

¹H NMR (300 MHz, CDCl_3) δ = 7.06 (s, 1H), 3.93 (s, 3H), 3.90 (s, 3H), 3.86 (s, 3H), 3.85 (s, 3H) ppm.

¹³C NMR (75 MHz, CDCl_3) δ = 167.4, 155.0, 151.4, 142.5, 128.7, 118.2, 83.9, 61.9, 60.9, 56.4, 52.7 ppm.

HRMS (ESI): calculated for $\text{C}_{11}\text{H}_{13}\text{O}_5\text{INa}$ 374.969715, found 374.969990.

Compound G: Prepared by a procedure reported by Fujita¹². To a stirred solution of **F** (2.00 g, 5.7 mmol) in CH_2Cl_2 (20 mL), BBr_3 (1.50 g, 6.0 mmol) was added dropwise at -78 °C. After stirring for 30 min, CH_2Cl_2 (40 mL) and water (2 mL) were added sequentially. The reaction mixture was allowed to reach room temperature, and then washed with brine, dried over Na_2SO_4 and concentrated *in vacuo*. Purification of the reaction crude by flash chromatography (Hexane/EtOAc, 5/1) afforded **G** as a white solid (1.55 g, 70%). Spectral data was consistent with those reported in the literature¹².

¹H NMR (300 MHz, CDCl_3) δ = 10.74 (s, 1H), 7.15 (s, 1H), 3.95 (s, 3H), 3.88 (s, 3H), 3.85 (s, 3H) ppm.

¹³C NMR (75 MHz, CDCl_3) δ = 168.9, 156.3, 156.2, 137.1, 118.2, 112.3, 87.4, 61.8, 56.4, 52.0 ppm.

HRMS (ESI): calculated for $\text{C}_{10}\text{H}_{11}\text{O}_5\text{INa}$ 360.954480, found 360.954343.

Compound 47: A mixture of **G** (1.50 g, 4.4 mmol), K_2CO_3 (1.80 g, 13.2 mmol) and BnBr (0.43 ml, 4.9 mmol) in DMF (20 mL) was stirred at room temperature for 18 h. The mixture was then poured to cold water (50 mL) and extracted with Et_2O , washed with brine, dried over Na_2SO_4 and concentrated *in vacuo*. Purification of the crude by flash chromatography (Hexane/EtOAc, 5/1) afforded **8** as a white solid (1.85 g, 98%).

¹⁰ Arthuis, M.; Pontikis, R.; Chabot, G. G.; Seguin, J.; Quentin, L.; Bourg, S.; Morin-Allory, L.; Florent, J.-F. *ChemMedChem* **2011**, *6*, 1693.

¹¹ Hewgill, F. R.; Slamet, R.; Stewart, J. M. *J. Chem. Soc. Perkin Trans. I* **1991**, 3033.

¹² Fujita, M.; Mori, K.; Shimogaki, M.; and Sugimura, T. *Org. Lett.* **2012**, *14*, 1294.

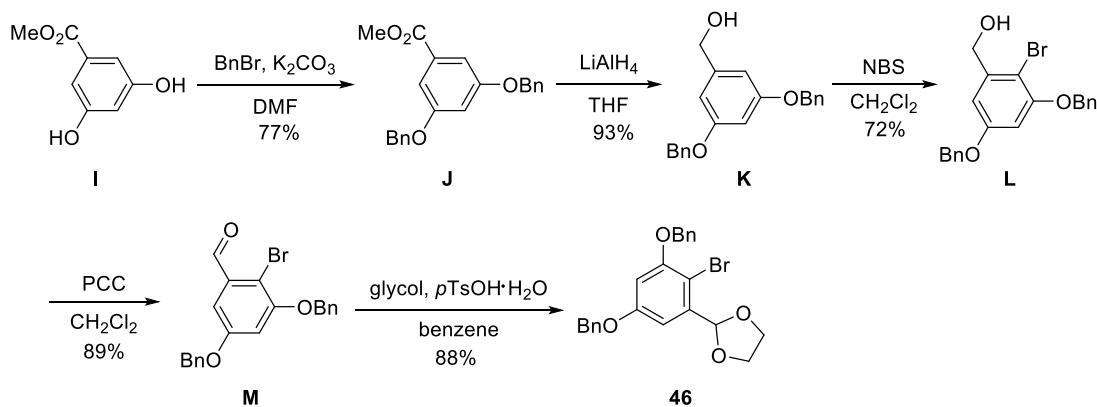
¹H NMR (300 MHz, CDCl₃) δ = 7.40 – 7.34 (m, 5H), 7.10 (s, 1H), 5.09 (s, 2H), 3.87 (s, 3H), 3.87 (s, 3H), 3.82 (s, 3H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ = 167.6, 155.2, 150.6, 142.9, 137.1, 129.2, 128.6, 128.4, 128.3, 118.5, 84.3, 76.6, 61.2, 56.6, 52.7 ppm.

HRMS (ESI): calculated for C₁₀H₁₁O₅Na 360.954480, found 360.954343.

IR: $\tilde{\nu}$ = 654, 700, 722, 757, 778, 798, 814, 908, 945, 962, 978, 1019, 1103, 1153, 1184, 1192, 1266, 1279, 1304, 1362, 1413, 1427, 1442, 1485, 1580, 1729, 2580, 2829, 2884, 2937, 2091 cm⁻¹.

Preparation of 2-(3,5-bis(benzyloxy)-2-bromophenyl)-1,3-dioxolane 46.



Compound J: Prepared by a modified procedure reported by Denmark¹³. A mixture of **I** (5.00 g, 29.8 mmol) and K₂CO₃ (12.31 g, 13.2 mmol) and BnBr (5.49 ml, 4.9 mmol) in DMF (50 mL) was stirred at room temperature for 18 h. The mixture was then poured to cold water (200 mL) and extracted with Et₂O, washed with brine, dried over Na₂SO₄ and concentrated *in vacuo*. Purification of the crude by flash chromatography (Hexane/EtOAc, 5/1) afforded **J** as a white solid (7.98 g, 77%). Spectral data were consistent with those reported in the literature¹³.

¹H NMR (500 MHz, CDCl₃) δ = 7.45 (d, J = 7.1 Hz, 2H), 7.41 (t, J = 7.1 Hz, 2H), 7.37 (d, J = 7.1, 2H), 7.34 (d, J = 2.2 Hz, 2H), 6.83 (t, J = 2.4 Hz, 1H), 5.09 (s, 4H), 3.92 (s, 3H) ppm.

¹³C NMR (125 MHz, CDCl₃) δ 166.2, 159.7, 136.4, 132.0, 128.6, 128.1, 127.5, 108.3, 107.2, 70.2, 52.2 ppm.

HRMS (ESI): calculated for C₂₂H₂₀O₄Na 371.125173, found 371.125379.

Compound K: Prepared by a modified procedure reported by Denmark¹³. A Schlenk charged with **J** (5.00 g, 14.4 mmol) and THF (10 mL) was cooled to 0 °C. LiAlH₄ (1.20 g, 31.6 mmol) was added portionwise over 30 min. After the addition was complete, the resulting solution was stirred at room temperature for 16 h, whereupon the solution was once again cooled to 0 °C and water (1.5 mL), 15% aq. NaOH (1.5 mL), H₂O (7.5 mL) were added sequentially. Upon warming to room temperature, the

¹³ Denmark, S. E.; Regens, C. S.; Kobayashi, T. *J. Am. Chem. Soc.* **2007**, *129*, 2774.

white suspension was eluted through Celite and washed with THF (20 mL). The filtrate was concentrated under reduced pressure by rotary evaporation. The resulting white suspension was dissolved in EtOAc (20 ml), washed with brine, dried over Na_2SO_4 and concentrated *in vacuo*. Purification of the crude by flash chromatography (Hexane/EtOAc, 5/1) afforded **K** as a white solid (4.29 g, 93%). Spectral data were consistent with these reported in the literature¹³.

¹H NMR (500 MHz, CDCl_3) δ = 7.34 (m, 10H), 6.63 (d, J = 2.2 Hz, 2 H), 6.56 (t, J = 2.3 Hz, 1H), 5.04 (s, 4H), 4.62 (d, J = 5.2 Hz, 2H), 1.90 (t, J = 5.2 Hz, 1H) ppm.

¹³C NMR (126 MHz, CDCl_3) δ = 160.1, 143.4, 136.7, 128.6, 127.9, 127.5, 105.6, 101.2, 69.9, 65.2 ppm.

HRMS (ESI): calculated for $\text{C}_{21}\text{H}_{20}\text{O}_3\text{Na}$ 343.130430, found 343.130461.

Compound L: Prepared by a modified procedure reported by Henry¹⁴. To a solution of **K** (4.00 g, 12.5 mmol) in CH_2Cl_2 (20 mL) was added NBS (2.45 g, 13.8 mmol) at 0 °C. The mixture was stirred for 18 h and then diluted with EtOAc (50 mL). The pink suspension was eluted through Celite, washed with EtOAc (50 mL). Water (20 mL) was added to the resulting solution and the aqueous layer was separated and extracted with EtOAc. The combined organic layers were washed with saturated aq. Na_2SO_3 thiosulfate and brine, dried over Na_2SO_4 and concentrated *in vacuo*. Purification of the crude by flash chromatography (Hexane/EtOAc, 4/1) afforded **L** as a white solid (3.58 g, 72%). Spectral data were consistent with these reported in the literature¹⁵.

¹H NMR (300 MHz, CDCl_3) δ = 7.47 - 7.32 (m, 10H) 6.81 (d, J = 2.7 Hz, 1H), 6.57 (d, J = 2.7 Hz, 1H), 5.11 (s, 2H), 5.04 (s, 2H), 4.75 (s, 2H) ppm.

¹³C NMR (75 MHz, CDCl_3) δ = 159.1, 155.7, 141.9, 136.5, 136.4, 128.7, 128.6, 128.2, 128.0, 127.5, 127.0, 106.5, 101.4, 71.0, 70.4, 65.4 ppm.

HRMS (ESI): calculated for $\text{C}_{21}\text{H}_{19}\text{O}_3\text{BrNa}$ 421.041078, found 421.040986.

Compound M: To a solution of **L** (3.50 g, 8.8 mmol) in CH_2Cl_2 (20 mL) was added PCC (1.99 g, 9.7 mmol) at room temperature. The mixture was stirred for 16 h, then MTBE (50 mL) was added to precipitate the chromium salts, eluted through Celite and washed the Celite pad with MTBE (100 ml). Then the combined organic layers were washed with brine, dried over Na_2SO_4 and concentrated *in vacuo*. Purification of the crude by flash chromatography (Hexane/EtOAc, 5/1) afforded **L** as a white solid (3.10 g, 89%).

¹H NMR (300 MHz, CDCl_3) δ = 10.43 (s, 1H), 7.48 - 7.34 (m, 10H), 7.16 (d, J = 2.7 Hz, 1H), 6.85 (d, J = 2.7 Hz, 1H), 5.15 (s, 2H), 5.07 (s, 2H) ppm.

¹³C NMR (75 MHz, CDCl_3) δ = 191.9, 158.9, 156.2, 136.0, 135.8, 134.9, 128.7, 128.3, 128.2, 127.7, 127.0, 109.9, 108.0, 105.2, 71.3, 70.6 ppm.

HRMS (ESI): calculated for $\text{C}_{21}\text{H}_{17}\text{O}_3\text{BrNa}$ 419.025470, found 419.025340.

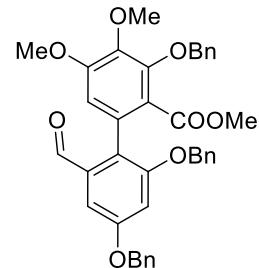
¹⁴ Henry, K. M.; Townsend C. A. *J. Am. Chem. Soc.* **2007**, *129*, 2774.

¹⁵ Sinhababu, A. K.; Borchardt, R. T. *J. Org. Chem.* **1983**, *48*, 2356.

Compound 46: Prepared by a modified procedure reported by Hsu¹⁶. *p*-TsOH·H₂O (117 mg, 0.63 mmol) and ethylene glycol (1.96 g, 31.5 mmol) were added to a solution of **M** (2.50 g, 6.3 mmol) in benzene (50 mL) at room temperature. The reaction mixture was heated under reflux for 8 h in a Dean–Stark apparatus. The contents were cooled to room temperature and quenched with saturated aqueous NaHCO₃. The aqueous layer was separated and extracted with EtOAc. The combined organic layers were washed with brine, dried over Na₂SO₄ and concentrated *in vacuo*. Purification of the crude by flash chromatography (Hexane/EtOAc, 5/1) afforded **46** as a white solid (2.44 g, 88%).
¹H NMR (400 MHz, CDCl₃) δ = 7.47 - 7.32 (m, 10H), 6.90 (d, *J* = 2.7 Hz, 1H), 6.62 (d, *J* = 2.7 Hz, 1H), 5.11 (s, 1H), 5.03 (s, 2H), 4.15 - 4.11 (m, 2H), 4.10 – 4.05 (m, 2H) ppm.
¹³C NMR (101 MHz, CDCl₃) δ = 159.0, 156.0, 138.7, 136.6, 136.5, 128.8, 128.7, 128.3, 128.1, 127.8, 127.2, 105.3, 104.8, 103.2, 102.7, 71.2, 70.6, 65.6.
HRMS (ESI): calculated for C₂₃H₂₁O₄BrNa 463.051955, found 419.051551.
IR (neat) $\tilde{\nu}$ = 665, 693, 741, 822, 832, 901, 933, 953, 1019, 1029, 1048, 1069, 1168, 1217, 1282, 1334, 1375, 1398, 1434, 1455, 1473, 2883, 2968, 3037 cm⁻¹.

Preparation of Orchrolide 53 and Coeloginin 54:

Compound 48: Prepared by a modified procedure reported by Buchwald¹⁷. A Schlenk was charged with **46** (660 mg, 1.5 mmol) and dry THF (2 mL). The resulting solution was cooled to –78 °C and then *n*-BuLi (0.66 ml, 2.5 M in hexane) was added dropwise *via* syringe through the septum and stirred at –78 °C for 1 h. After that freshly prepared ZnCl₂ (3.6 mL, 1 M in THF) was added dropwise *via* syringe through the septum. After 30 min at –78 °C, the Schlenk was removed from the cooling bath and the resulting solution stirred at room temperature for 1 h. Then, Pd₂(dba)₃ (23 mg, 2.5 mol%), S-Phos (28 mg, 6.0 mol%) and **47** (428 mg, 1.0 mmol) were added with the aid of THF (0.5 mL) which was used to rinse the walls of the tube. The septum was replaced with a glass cap and the Schlenk was sealed. The reaction mixture was placed in a preheated oil bath at 70 °C for 16 h. After that, the reaction mixture was cooled to room temperature, diluted with saturated NaHCO₃ (1 mL) and filtered through Celite. The result solution was concentrated *in vacuo* and the residue purified by flash chromatography (Hexane/EtOAc, 4/1) affording **48** as a yellow solid (400 mg, 65%).



¹H NMR (400 MHz, CDCl₃) δ = 9.69 (s, 1H), 7.44 - 7.18 (m, 16H), 6.82 (d, *J* = 2.3 Hz, 1H), 6.57 (s, 1H), 5.16 (s, 2H), 5.10 (s, 2H), 4.99 (s, 2H), 3.95 (s, 3H), 3.83 (s, 3H), 3.40 (s, 3H) ppm.
¹³C NMR (100 MHz, CDCl₃) δ = 191.6, 166.8, 159.5, 157.4, 154.4, 150.5, 142.3, 137.3, 136.6, 136.4, 136.0, 128.8, 128.5, 128.4, 128.3, 128.2, 127.9, 127.2, 126.8, 123.6, 111.4, 107.0, 102.2, 76.4, 70.7, 70.5, 61.3, 56.3, 51.8 ppm.

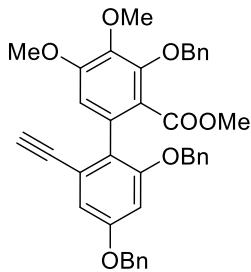
HRMS (ESI): calculated for C₃₈H₃₄O₈Na 641.215050, found 641.214592.

¹⁶ Hsu, D. –S.; Lin, S. –C. *J. Org. Chem.* **2012**, 77, 6139.

¹⁷ Milne, J. E.; Buchwald, S. L. *J. Am. Chem. Soc.* **2004**, 126, 13028.

IR (neat) $\tilde{\nu}$ = 697, 754, 791, 839, 911, 946, 976, 992, 1030, 1057, 1110, 1133, 1159, 1207, 1206, 1274, 1325, 1368, 1297, 1417, 1447, 1497, 1596, 1691, 2861, 2938 cm⁻¹.

Compound 49: Prepared by a modified procedure reported in our group¹⁸. Ohira-Bestmann reagent



(135 mg, 0.070 mmol) and K₂CO₃ (130 mg, 0.094 mmol) were added to a solution of **48** (290 mg, 0.047 mmol) in dry MeOH (20 mL) and the resulting mixture was stirred for 2 d. Afterwards, the solvent was evaporated and the crude partitioned between CH₂Cl₂ and brine. The combined organic layers were washed by brine, dried over Na₂SO₄ and concentrated *in vacuo*. Purification of the crude by flash chromatography (Hexane/EtOAc, 5/1) afforded **49** as a white solid (268 mg, 79%).

¹H NMR (300 MHz, CDCl₃) δ = 7.48 - 7.24 (m, 15H), 6.81 (s, 1H), 6.66 (s, 1H), 6.63 (s, 1H), 5.15 (s, 2H), 5.03 (s, 2H), 4.95 (s, 2H), 3.94 (s, 3H), 3.85 (s, 3H), 3.46 (s, 3H) 2.93 (s, 1H) ppm.

¹³C NMR (75 MHz, CDCl₃) δ = 166.9, 158.8, 156.9, 154.4, 151.0, 141.9, 137.8, 137.0, 136.7, 132.3, 128.8, 128.5, 128.4, 128.3, 128.0, 127.8, 127.0, 126.9, 123.3, 122.5, 111.3, 110.2, 102.9, 82.3, 80.5, 76.3, 70.7, 70.4, 61.2, 56.2, 51.7.

HRMS (ESI): calculated for C₃₉H₃₄O₇Na 637.220165, found 637.219677.

IR (neat) $\tilde{\nu}$ = 658, 698, 744, 835, 910, 946, 973, 1034, 1061, 1105, 1129, 1155, 1207, 1271, 1327, 1369, 1413, 1428, 1447, 1497, 1570, 1594, 1721, 2939, 3033, 3305 cm⁻¹.

Compound 50: A mixture of **49** (250 mg, 0.041 mmol) and AlCl₃ (163 mg, 0.123 mol) in dry benzene

(10 mL) was refluxed for 3 h. Then the reaction was cooled to room temperature and saturated NaHCO₃ (1 mL) was added. The result mixture was eluted through silica gel and washed with EtOAc. The combined organic layers were concentrated *in vacuo*. Purification of the crude by flash chromatography (Hexane/EtOAc, 5/1) afforded **50** as a pale yellow foam (157 mg, 73%).

¹H NMR (300 MHz, CDCl₃) δ = 11.37 (s, 1H), 7.45 - 7.24 (m, 8H), 7.15 - 7.12 (m, 2H), 6.81 (d, J = 2.3 Hz, 1H), 6.65 (d, J = 2.3 Hz, 1H), 6.39 (s, 1H), 5.07 (s, 2H), 4.95 (s, 2H), 3.96 (s, 3H), 3.85 (s, 3H), 3.45 (s, 3H), 2.91 (s, 1H) ppm.

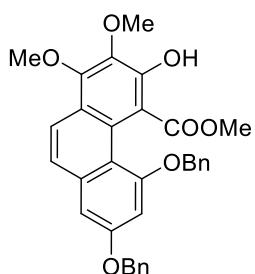
¹³C NMR (75 MHz, CDCl₃) δ = 171.4, 158.4, 156.4, 156.3, 156.2, 136.8, 136.7, 136.0, 134.8, 129.3, 128.8, 128.6, 128.3, 127.9, 127.7, 126.8, 122.3, 109.9, 109.0, 107.7, 102.7, 82.4, 80.3, 77.6, 77.2, 76.7, 70.5, 70.5, 60.8, 56.1, 51.9 ppm.

HRMS (ESI): calculated for C₃₂H₂₆O₇Na 547.172929, found 637.172273.

IR (neat) $\tilde{\nu}$ = 696, 736, 807, 832, 907, 959, 987, 1028, 1061, 1116, 1157, 1210, 1274, 1313, 1405, 1442, 1567, 1596, 1654, 2937, 3282 cm⁻¹.

¹⁸ Carreras, J.; Patil, M.; Thiel, W.; Alcarazo, M. *J. Am. Chem. Soc.* **2012**, *134*, 16753.

Compound 52: $\text{ClCH}_2\text{CH}_2\text{Cl}$ (2 ml) was added to a mixture of **50** (155 mg, 0.030 mmol), AgSbF_6 (10



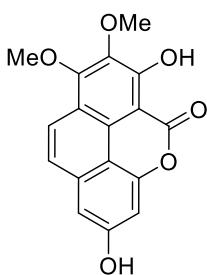
mg, 10 mol%), **6** (16 mg, 5 mol%) and AgSbF_6 (5 mol%) at room temperature. After 1 h, the reaction was completed by TLC. Then the solvents were evaporated *in vacuo* and the residue purified by flash chromatography (Hexane/EtOAc, 5/1) affording **52** as a pale yellow solid (116 mg, 75%).

^1H NMR (300 MHz, CDCl_3) δ = 11.36 (s, 1H), 8.62 (d, J = 8.9 Hz, 1H), 8.18 – 7.90 (m, 11H), 7.62 (d, J = 2.4 Hz, 1H), 7.40 (d, J = 2.4 Hz, 1H), 5.83 (s, 2H), 5.69 (br, 2H), 4.78 (s, 3H), 4.67 (s, 3H), 4.31 (s, 3H) ppm.

^{13}C NMR (75 MHz, CDCl_3) δ = 171.6, 158.01, 158.00, 157.9, 154.9, 151.8, 138.4, 136.8, 136.1, 135.8, 128.83, 128.81, 128.80, 128.79, 128.4, 128.3, 128.1, 127.73, 127.72, 125.0, 124.0, 121.3, 120.9, 117.3, 107.7, 102.2, 102.1, 77.48, 72.7, 70.4, 61.78, 61.77, 61.2, 51.7.

HRMS (ESI): calculated for $\text{C}_{32}\text{H}_{28}\text{O}_7\text{Na}$ 547.172947, found 637.172726.

IR (neat) $\tilde{\nu}$ = 655, 695, 735, 781, 836, 907, 967, 1007, 1059, 1091, 1140, 1161, 1217, 1252, 1275, 1311, 1330, 1395, 1443, 1485, 1578, 1613, 1662, 2940 cm^{-1} .



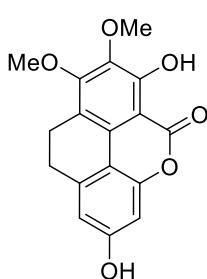
Compound 53: A Schlenk containing **52** (53 mg, 0.10 mmol), 10% Pd/C (10 mg) and EtOAc (3 mL) was bubbled with H_2 for 30 min. Then, a balloon full with H_2 was installed and the reaction stirred for 2 h. The suspension was then filtered through a pad of Celite, washed with EtOAc and concentrated *in vacuo*. Purification of the crude by flash chromatography (Hexane/EtOAc, 3/1) afforded **53** as a yellow solid (29 mg, 93%). Spectral data were consistent with those reported in the literature¹⁹.

^1H NMR (500 MHz, $(\text{CD}_3)_2\text{CO}$) δ = 7.97 (d, J = 9.1 Hz, 1H), 7.65 (d, J = 9.1 Hz, 1H), 7.25 (d, J = 2.1 Hz, 1H) 7.07 (d, J = 2.1 Hz, 1H), 4.28 (s, 3H), 4.03 (s, 3H) ppm.

^{13}C NMR (125 MHz, CD_3COCD_3) δ = 166.6, 159.3, 158.8, 156.4, 152.2, 139.2, 134.3, 125.8, 124.2, 122.6, 116.4, 109.1, 107.9, 103.1, 98.8, 62.3, 61.6 ppm.

HRMS (ESI): calculated for $\text{C}_{17}\text{H}_{12}\text{O}_6\text{Na}$ 335.052726, found 335.052612.

IR: $\tilde{\nu}$ = 680, 732, 767, 797, 842, 922, 938, 976, 1051, 1093, 1105, 1127, 1105, 1206, 1270, 1379, 1404, 1439, 1466, 1603, 1627, 1662, 2853, 2943, 3367 cm^{-1} .



Compound 54: An autoclave containing **52** (53 mg, 0.10 mmol), 10% Pd/C (20 mg) and EtOAc (5 mL) was pressurized to 20 bar H_2 and stirred during three days. The thus obtained suspension was then eluted through a pad of Celite and washed with EtOAc. Concentration of the residue afforded a residue that was then purified by flash chromatography (Hexane/EtOAc, 3/1) affording **54** as

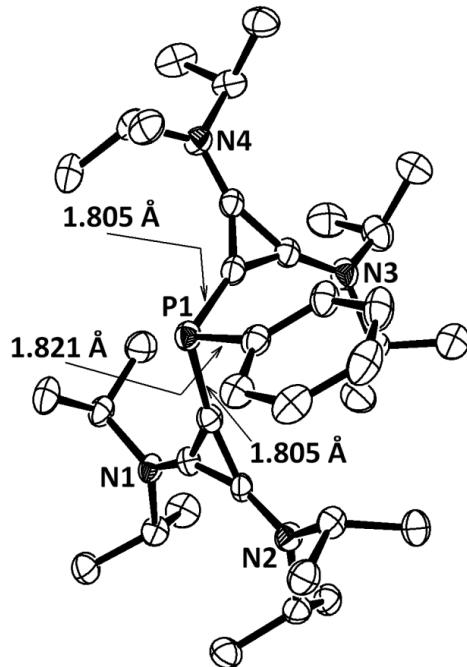
¹⁹ Bhaskar, M. U.; Mohan Rao, L. J.; Prakasa Rao, N. S.; Mohana, Rao P. R. *Phytochemistry*, **1989**, 28, 3545.

a yellow solid (29 mg, 93%). Spectral data were consistent with these reported in the literature²⁰

²⁰ Majumder, P. L.; Bandyopadhyay, D.; Joardar, S. J. *Chem. Soc. Perkin Trans I* **1982**, 1131.

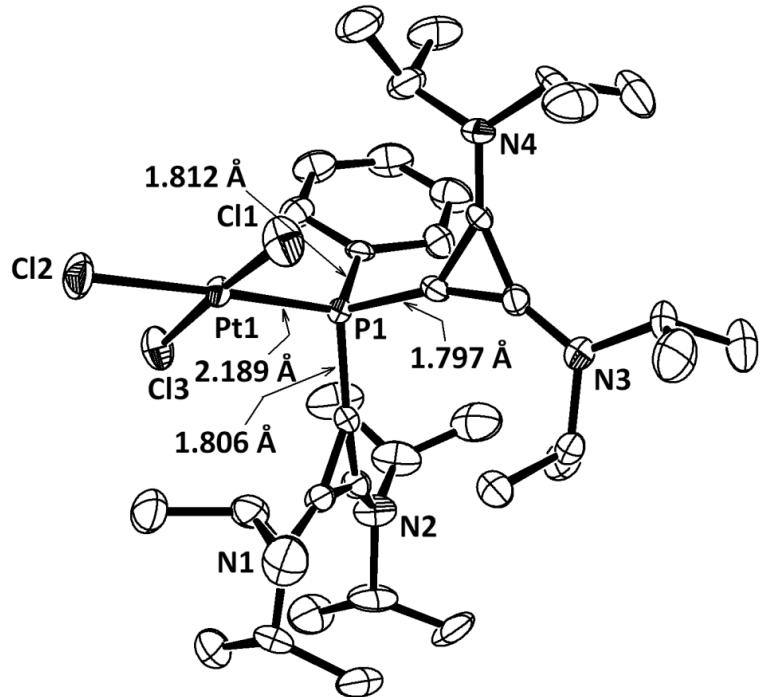
X-ray Structures

Compound 1



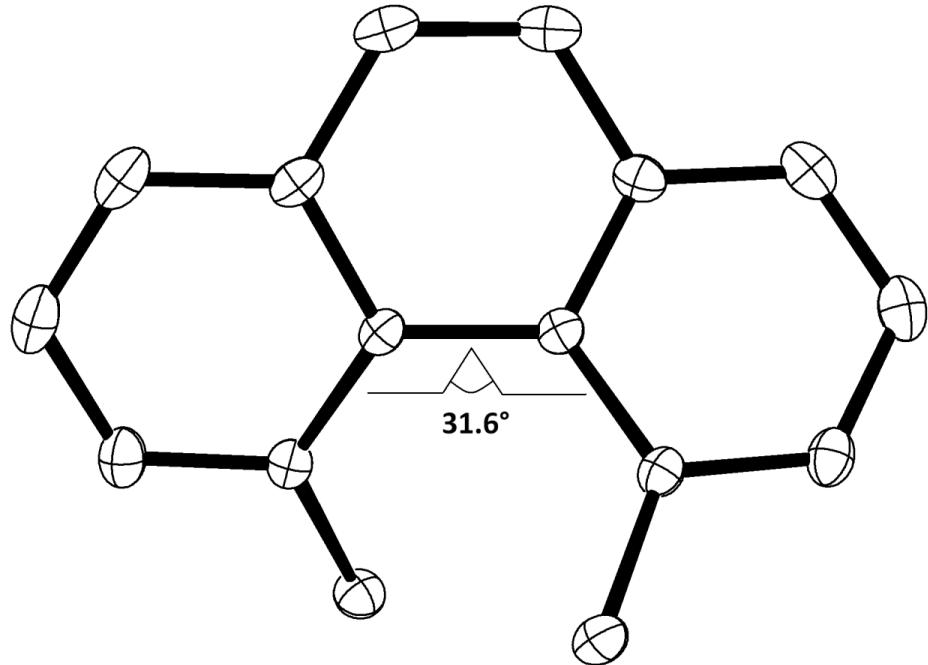
Empirical formula	$C_{36}H_{61}B_2F_8N_4P$
Color	colourless
Formula weight	754.48 g · mol ⁻¹
Temperature	100 K
Wavelength	1.54178 Å
Crystal system	Orthorhombic
Space group	Pbcn, (no. 60)
Unit cell dimensions	$a = 45.8483(14)$ Å $\alpha = 90^\circ$. $b = 11.6679(3)$ Å $\beta = 90^\circ$. $c = 15.3567(5)$ Å $\gamma = 90^\circ$.
Volume	8215.1(4) Å ³
Z	8
Density (calculated)	1.220 Mg · m ⁻³
Absorption coefficient	1.160 mm ⁻¹
F(000)	3216 e
Crystal size	0.59 x 0.51 x 0.04 mm ³
θ range for data collection	1.93 to 67.48°.
Index ranges	-54 ≤ h ≤ 54, -13 ≤ k ≤ 13, -18 ≤ l ≤ 18
Reflections collected	205006
Independent reflections	7325 [R _{int} = 0.1118]
Reflections with I > 2σ(I)	6324
Completeness to θ = 67.48°	99.0 %
Absorption correction	Gaussian
Max. and min. transmission	0.96 and 0.51
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	7325 / 0 / 495
Goodness-of-fit on F ²	2.065
Final R indices [I > 2σ(I)]	R ₁ = 0.0794 wR ² = 0.1689
R indices (all data)	R ₁ = 0.0895 wR ² = 0.1718
Extinction coefficient	0.00099(8)
Largest diff. peak and hole	0.608 and -0.429 e · Å ⁻³

Compound 5



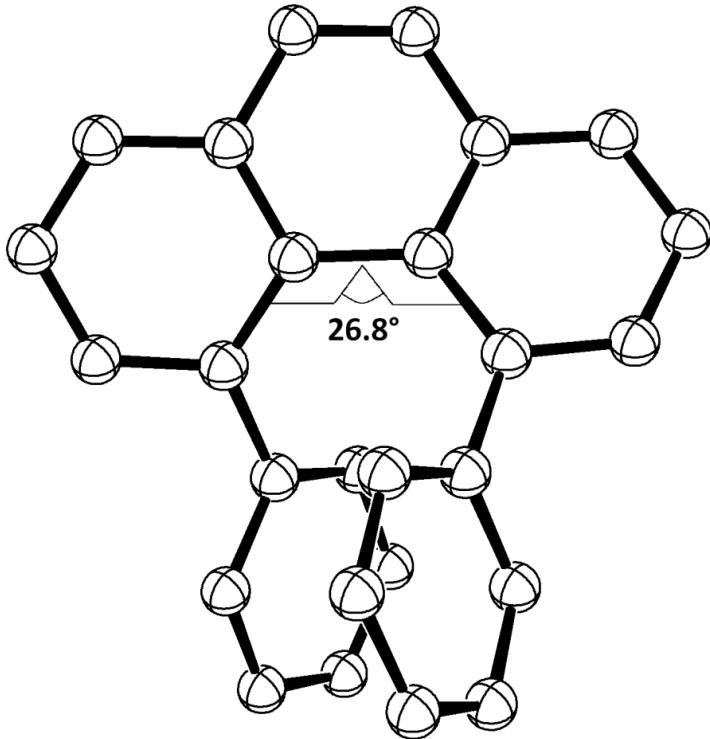
Empirical formula	$C_{37}H_{61.50}BCl_6F_4N_4PPt$
Color	?
Formula weight	1087.97 g · mol ⁻¹
Temperature	200 K
Wavelength	0.71073 Å
Crystal system	MONOCLINIC
Space group	P2 ₁ /c, (no. 14)
Unit cell dimensions	$a = 25.819(3)$ Å $\alpha = 90^\circ$. $b = 15.859(2)$ Å $\beta = 113.707(6)^\circ$. $c = 25.450(2)$ Å $\gamma = 90^\circ$.
Volume	9541.1(19) Å ³
Z	8
Density (calculated)	1.515 Mg · m ⁻³
Absorption coefficient	3.357 mm ⁻¹
F(000)	4380 e
Crystal size	0.153 x 0.152 x 0.050 mm ³
θ range for data collection	2.71 to 27.50°
Index ranges	-33 ≤ h ≤ 33, -20 ≤ k ≤ 20, -33 ≤ l ≤ 32
Reflections collected	129550
Independent reflections	21869 [R _{int} = 0.0612]
Reflections with I > 2σ(I)	18230
Completeness to θ = 27.50°	99.8 %
Absorption correction	Gaussian
Max. and min. transmission	0.85 and 0.35
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	21869 / 0 / 998
Goodness-of-fit on F ²	1.208
Final R indices [I > 2σ(I)]	R ₁ = 0.0822 wR ² = 0.2045
R indices (all data)	R ₁ = 0.0969 wR ² = 0.2135
Largest diff. peak and hole	4.066 and -2.870 e · Å ⁻³

Compound 8



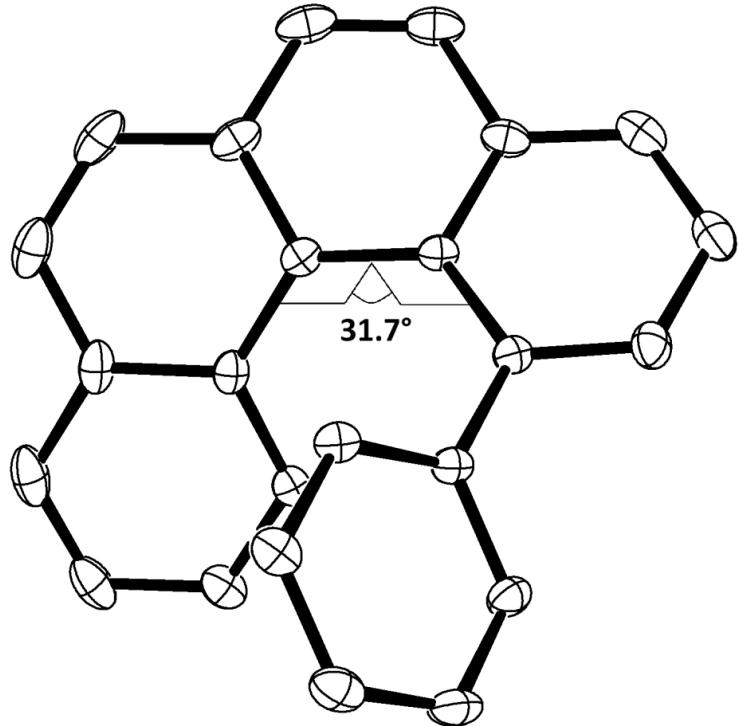
Empirical formula	$C_{16}H_{14}$
Color	colorless
Formula weight	$206.27 \text{ g} \cdot \text{mol}^{-1}$
Temperature	100 K
Wavelength	0.71073 Å
Crystal system	MONOCLINIC
Space group	P 2₁, (no. 4)
Unit cell dimensions	$a = 8.3090(8) \text{ \AA}$ $b = 8.0817(7) \text{ \AA}$ $c = 8.7050(8) \text{ \AA}$
Volume	$555.22(9) \text{ \AA}^3$
Z	2
Density (calculated)	$1.234 \text{ Mg} \cdot \text{m}^{-3}$
Absorption coefficient	0.069 mm^{-1}
F(000)	220 e
Crystal size	$0.39 \times 0.36 \times 0.16 \text{ mm}^3$
θ range for data collection	2.46 to 34.97°
Index ranges	$-13 \leq h \leq 13, -12 \leq k \leq 13, -14 \leq l \leq 14$
Reflections collected	19639
Independent reflections	4809 [$R_{\text{int}} = 0.0396$]
Reflections with $I > 2\sigma(I)$	4635
Completeness to $\theta = 34.97^\circ$	99.9 %
Absorption correction	Gaussian
Max. and min. transmission	0.99 and 0.97
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4809 / 1 / 147
Goodness-of-fit on F^2	1.085
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0360$
R indices (all data)	$R_1 = 0.0381$
Absolute structure parameter	0(8)
Largest diff. peak and hole	0.438 and $-0.194 \text{ e} \cdot \text{\AA}^{-3}$
	$wR^2 = 0.1003$
	$wR^2 = 0.1029$

Compound 30



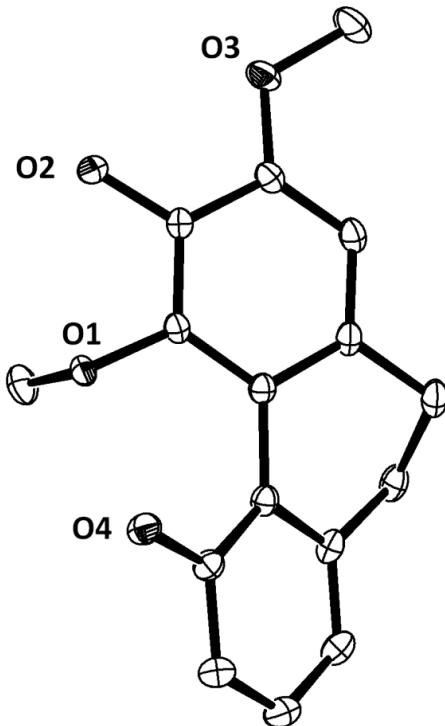
Empirical formula	$C_{26} H_{18}$
Color	colourless
Formula weight	330.40 g · mol ⁻¹
Temperature	100 K
Wavelength	0.71073 Å
Crystal system	MONOCLINIC
Space group	P2 ₁ /n, (no. 14)
Unit cell dimensions	$a = 8.9259(3)$ Å $\alpha = 90^\circ$. $b = 12.5274(11)$ Å $\beta = 105.646(5)^\circ$. $c = 16.0569(10)$ Å $\gamma = 90^\circ$.
Volume	1728.93(19) Å ³
Z	4
Density (calculated)	1.269 Mg · m ⁻³
Absorption coefficient	0.072 mm ⁻¹
F(000)	696 e
Crystal size	0.46 x 0.30 x 0.25 mm ³
θ range for data collection	2.63 to 33.10°.
Index ranges	-13 ≤ h ≤ 13, -19 ≤ k ≤ 19, -24 ≤ l ≤ 24
Reflections collected	35362
Independent reflections	6570 [R _{int} = 0.0302]
Reflections with I > 2σ(I)	5307
Completeness to θ = 33.10°	99.9 %
Absorption correction	Gaussian
Max. and min. transmission	0.98 and 0.96
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	6570 / 0 / 235
Goodness-of-fit on F ²	1.115
Final R indices [I > 2σ(I)]	R ₁ = 0.0460 wR ² = 0.1293
R indices (all data)	R ₁ = 0.0600 wR ² = 0.1381
Largest diff. peak and hole	0.577 and -0.594 e · Å ⁻³

Compound 35



Empirical formula	$C_{24}H_{16}$
Color	yellow
Formula weight	304.37 g · mol ⁻¹
Temperature	100 K
Wavelength	0.71073 Å
Crystal system	MONOCLINIC
Space group	Cc, (no. 9)
Unit cell dimensions	$a = 15.4509(5)$ Å $\alpha = 90^\circ$. $b = 10.9866(12)$ Å $\beta = 104.463(8)^\circ$. $c = 19.235(3)$ Å $\gamma = 90^\circ$.
Volume	3161.8(6) Å ³
Z	8
Density (calculated)	1.279 Mg · m ⁻³
Absorption coefficient	0.072 mm ⁻¹
F(000)	1280 e
Crystal size	0.31 x 0.18 x 0.13 mm ³
θ range for data collection	2.69 to 34.00°.
Index ranges	-24 ≤ h ≤ 24, -17 ≤ k ≤ 17, -30 ≤ l ≤ 30
Reflections collected	45761
Independent reflections	12696 [R _{int} = 0.0489]
Reflections with I > 2σ(I)	10427
Completeness to θ = 27.50°	99.8 %
Absorption correction	Gaussian
Max. and min. transmission	0.99 and 0.98
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	12696 / 2 / 433
Goodness-of-fit on F ²	1.121
Final R indices [I > 2σ(I)]	R ₁ = 0.0575 wR ² = 0.1487
R indices (all data)	R ₁ = 0.0763 wR ² = 0.1645
Largest diff. peak and hole	0.488 and -0.418 e · Å ⁻³

Compound 40



Empirical formula	$C_{16}H_{16}O_4$
Color	colorless
Formula weight	272.29 g · mol ⁻¹
Temperature	100 K
Wavelength	0.71073 Å
Crystal system	MONOCLINIC
Space group	P2 ₁ /n, (no. 14)
Unit cell dimensions	$a = 18.7373(19)$ Å $\alpha = 90^\circ$. $b = 7.5768(8)$ Å $\beta = 114.173(2)^\circ$. $c = 20.604(2)$ Å $\gamma = 90^\circ$.
Volume	2668.7(5) Å ³
Z	8
Density (calculated)	1.355 Mg · m ⁻³
Absorption coefficient	0.097 mm ⁻¹
F(000)	1152 e
Crystal size	0.38 x 0.22 x 0.06 mm ³
θ range for data collection	1.91 to 31.00°.
Index ranges	-27 ≤ h ≤ 27, -10 ≤ k ≤ 10, -29 ≤ l ≤ 29
Reflections collected	75168
Independent reflections	8476 [R _{int} = 0.0256]
Reflections with I > 2σ(I)	7693
Completeness to θ = 27.50°	100.0 %
Absorption correction	Gaussian
Max. and min. transmission	1.00 and 0.89
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	8476 / 0 / 369
Goodness-of-fit on F ²	1.165
Final R indices [I > 2σ(I)]	R ₁ = 0.0783 wR ² = 0.2149
R indices (all data)	R ₁ = 0.0825 wR ² = 0.2178
Largest diff. peak and hole	1.2 and -0.4 e · Å ⁻³

Computational Methods

Geometry optimizations were carried out using BP86^{21,22} functional in combination with def2-SVP basis sets.^{23,24,25} In the case of gold, the 60 inner-shell core electrons were replaced by an effective core potential (ECP) generated for the neutral atom using quasi-relativistic methods, and the explicitly treated electrons were described by the standard def2-ECP basis set.²⁶ The resolution-of-identity (RI) approximation^{27,28,29} was applied in conjunction with the appropriate auxiliary basis sets to speed up the calculations. This approach is computationally efficient and has been employed successfully in our previous computations on gold chemistry.^{30,31,32} All low-energy conformations of the substrate and the catalyst were considered during initial screening, and all relevant stationary points were characterized as minima or first-order transition states by evaluating the harmonic vibrational frequencies at the same level (RI-BP86/def2-SVP) that had been applied for geometry optimization.

The influence of the solvent environment (dichloromethane, dielectric constant $\epsilon = 8.93$) on the relative energies was investigated through single-point calculations with the conductor-like screening model (COSMO)³³ at the RI-BP86/def2-SVP level. In order to evaluate the best estimate of the total energies, all located stationary points were re-optimized at the RI-BP86 level employing the def2-TZVPP basis set.²⁴ Empirical Grimme-type dispersion corrections were also incorporated during this step using the latest parametrization (DFT-D3).³⁴ Relative free energies (ΔG) at standard pressure (1 bar) and 273.15K were determined at the RI-BP86/def2-SVP level. The required thermal and entropic contributions were evaluated within the rigid-rotor harmonic-oscillator approximation. All geometry optimizations were carried out using the TURBOMOLE (version 6.4) suite of programs.^{35,36}

To gain insight into the electronic structure of the complexes, a fragment molecular orbital (MO) analysis was performed for selected molecules using the *Amsterdam Density Functional* (ADF) package.^{37,38,39} The MOs were expanded in terms of Slater-type orbitals (STO) employing a triple- ζ basis set (TZP) with one polarization function. Relativistic effects were taken into account by the zero-order regular approximation (ZORA) approach,^{40,41} as implemented in ADF.

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³⁶ TURBOMOLE V6.4 **2012**, a development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, **1989-2007**, TURBOMOLE GmbH, since 2007; available from <http://www.turbomole.com>

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⁴⁰ van Lenthe, E.; Baerends, E. J.; Snijders, J. G. *J. Chem. Phys.* **1994**, *101*, 9783-9792.

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Computational Results Presented as Supporting Information

Cyclization of substrate **7** to the 6-endo product: Table S1 lists the computed relative free energies [total energy (RI-BP86/def2-TZVPP + dispersion corrections) + free energy corrections (RI-BP86/def2-SVP)] with and without solvent corrections, for catalyst-**6** and PPh₃Au⁺. Corresponding single-point relative energies are given in Table S2, for all methods currently applied and for both pathways considered. The computed free energy profiles are plotted as Figure S1. Optimized geometries of all relevant stationary points are shown in Figures S2-S24: catalyst-**6** see Figure S2; substrate see Figure S3; catalyst-substrate complex for catalyst-**6** see Figure S4; pathway for catalyst-**6** see Figures S5-S13; catalyst-substrate complex for PPh₃Au⁺ see Figure S14; pathway for PPh₃Au⁺ see Figures S15-S23; final product see Figure S24.

Cyclization of substrate **9** to the 6-endo product: Table S3 lists the computed relative free energies [total energy (RI-BP86/def2-TZVPP + dispersion corrections) + free energy corrections (RI-BP86/def2-SVP)] with and without solvent corrections, for catalyst-**6** and PMe₃Au⁺. Corresponding single-point relative energies are given in Table S4, for all methods currently applied and for both pathways considered. The computed free energy profiles are plotted as Figure S25. Optimized geometries of all relevant stationary points are shown in Figures S26-S43: substrate-**9** see Figure S26; pathway for catalyst-**6** see Figures S27-S34; 6-endo product see Figure S35; pathway for PMe₃Au⁺ see Figures S36-S43.

Cyclization of substrate **9** to the 7-exo product: The computed free energy profiles are plotted as Figure S44. The optimized geometries of all relevant stationary points are shown in Figures S45-S53: pathway for catalyst-**6** see Figures S45-S48; 7-exo product see Figure S49; pathway for PMe₃Au⁺ see Figures S50-53.

Figure S54 sketches the frontier orbital interactions in complexes **55** and **56**.

The Cartesian coordinates of all optimized geometries (RI-BP86/def2-TZVPP) are listed at the end of the computational section for documentation.

Note:

In the main paper, catalyst-**6** and PPh₃Au⁺ are labelled as **55** and **57**, respectively.

Table S1. Cyclization of substrate **7** to the 6-endo product: Relative free energies (with and without solvent corrections, in kcal/mol) with respect to the free reactants, of the species considered in the potential energy profile (see methodology section for details). The abbreviations used in the table are as follows: Cat = catalyst, Sub = substrate, Int-1_{a/b} = reactant complex, TS1_{a/b} = transition state for cyclisation, Int-2_{a/b} = cyclized intermediate, TS2_{a/b} = transition state for ring opening, Int-3_{a/b} = ring-opened intermediate, TS3_{a/b} = transition state for 1,2-hydride shift, Int-4_{a/b} = product resulting from hydride shift, TS-4_{a/b} = transition state for 1,2-hydride shift leading to the product complex, Prod-cplx_{a/b} = product complex, Prod = final product: the subscripts a and b designate pathways A (catalyst-**6**) and B (PPh_3Au^+), respectively.

Profile	Pathway	Cat + Sub	Int-1 _{a/b}	TS1 _{a/b}	Int-2 _{a/b}	TS2 _{a/b}	Int-3 _{a/b}	TS3 _{a/b}	Int-4 _{a/b}	TS4 _{a/b}	Prod-cplx _{a/b}	Prod + Cat
Relative free energy	Catalyst- 6	0	-56.2	-49.1	-56.2	-51.6	-58.1	-48.7	-72.9	-59.1 -58.9	-92.4	-36.0
	PPh_3Au^+	0	-39.2	-18.3	-21.7	-15.4	-19.3	-15.8	-40.6	-29.7 -27.4	-68.4	
Relative free energy with solvent corrections	Catalyst- 6	0	-29.1	-25.8	-27.4	-22.7	-28.6	-20.8	-45.5	-33.0 -32.6	-70.1	-35.2
	PPh_3Au^+	0	-30.7	-9.5	-13.0	-7.9	-12.9	-8.9	-32.1	-21.9 -19.6	-60.4	

Table S2. Cyclization of substrate **7** to the 6-endo product: Relative energies (in kcal/mol) with respect to the free reactants, of the species considered in the potential energy profile, at different levels of theory (BP86-D/def2-TZVPP gas-phase geometries, please refer to Table S1 for abbreviations).

Profile	Functional/ Basis set	Cat + Sub	Int-1 _{a/b}	TS1 _{a/b}	Int-2 _{a/b}	TS2 _{a/b}	Int-3 _{a/b}	TS3 _{a/b}	Int-4 _{a/b}	TS4 _{a/b}	Prod-cplx _{a/b}	Prod + Cat
Catalyst-6	B3LYP/def2-SVP	0	-61.7	-45.5	-58.6	-54.2	-63.8	-53.5	-79.6	-65.6 -65.4	-93.8	-42.3
	BP86/def2-SVP	0	-64.5	-49.6	-68.0	-62.4	-71.2	-63.2	-85.7	-73.1 -73.0	-98.8	-45.9
	B3LYP-D/def2-SVP	0	-67.8	-55.3	-67.4	-63.3	-72.9	-62.3	-88.6	-74.4 -74.4	-105.3	-42.2
	B3LYP/def2-TZVPP	0	-59.7	-43.8	-52.4	-49.1	-57.9	-47.0	-73.6	-59.3 -59.0	-88.2	-38.6
	BP86/def2-TZVPP	0	-62.5	-48.1	-62.0	-57.5	-65.6	-57.2	-80.1	-67.1 -67.0	-93.7	-42.5
	M06/6-31+G*	0	-52.3	-41.9	-57.4	-50.9	-58.7	-47.4	-74.7	-59.9 -60.1	-91.1	-41.2
PPh ₃ Au ⁺	B3LYP/def2-SVP	0	-34.9	-20.4	-25.4	-19.1	-24.0	-18.5	-49.3	-36.1 -35.6	-73.9	-42.3
	BP86/def2-SVP	0	-38.7	-27.3	-36.3	-29.1	-34.0	-29.9	-56.7	-44.8 -44.4	-80.1	-45.9
	B3LYP-D/def2-SVP	0	-39.2	-27.0	-30.6	-24.7	-29.3	-23.5	-54.5	-41.1 -40.6	-81.2	-42.2
	B3LYP/def2-TZVPP	0	-34.2	-19.1	-20.4	-15.7	-19.7	-13.5	-44.7	-31.0 -30.6	-69.5	-38.6
	BP86/def2-TZVPP	0	-38.0	-26.1	-31.5	-25.9	-30.0	-25.4	-52.6	-40.1 -39.8	-76.2	-42.5
	M06/6-31+G*	0	-24.7	-13.4	-21.0	-11.8	-14.7	-8.5	-40.7	-26.5 -26.1	-66.6	-41.2

Table S3. Cyclization of substrate **9** to the 6-endo product: Relative free energies (with and without solvent corrections, in kcal/mol) with respect to the free reactants, of the species considered in the potential energy profile (see methodology section for details). The abbreviations used in the table are as follows: Cat = catalyst, Sub = substrate, Int-1_{a/b} = reactant complex, TS1_{a/b} = transition state for cyclisation, Int-2_{a/b} = cyclized intermediate, TS2_{a/b} = transition state for 1,2-hydride shift, Int-3_{a/b} = product resulting from hydride shift, TS-3_{a/b} = transition state for 1,2-hydride shift leading to the product complex, Prod-cplx_{a/b} = product complex, Prod = final product: the subscripts a and b designate pathways A (catalyst-**6**) and B (PMe₃Au⁺), respectively.

Profile	Pathway	Cat + Sub	Int-1 _{a/b}	TS1 _{a/b}	Int-2 _{a/b}	TS2 _{a/b}	Int-3 _{a/b}	TS3 _{a/b}	Prod-cplx _{a/b}	Prod + Cat
Relative free energy	Catalyst- 6	0	-64.0	-44.8	-62.1	-56.8	-82.3	<u>-68.9</u> <u>-67.8</u>	-100.6	-45.9
	PMe ₃ Au ⁺	0	-46.8	-25.4	-30.7	-28.0	-54.7	<u>-44.6</u> <u>-44.3</u>	-80.1	
Relative free energy with solvent corrections	Catalyst- 6	0	-34.8	-21.0	-30.5	-27.1	-53.0	<u>-41.1</u> <u>-39.9</u>	-76.7	-44.9
	PMe ₃ Au ⁺	0	-30.8	-9.5	-14.4	-11.7	-37.5	<u>-28.4</u> <u>-28.1</u>	-65.5	

Table S4. Cyclization of substrate **9** to the 6-endo product: Relative energies (in kcal/mol) with respect to the free reactants, of the species considered in the potential energy, at different levels of theory (BP86-D/def2-TZVPP gas-phase geometries, please refer to Table S3 for abbreviations).

Profile	Functional/ Basis set	Cat + Sub	Int-1 _{a/b}	TS1 _{a/b}	Int-2 _{a/b}	TS2 _{a/b}	Int-3 _{a/b}	TS3 _{a/b}	Prod-cplx _{a/b}	Prod + Cat
Catalyst-6	B3LYP/def2-SVP	0	-64.5	-45.0	-69.7	-61.1	-87.1	-74.2 -73.9	-104.0	-52.2
	BP86/def2-SVP	0	-67.1	-48.9	-76.5	-70.0	-92.9	-80.8 -80.6	-107.9	-54.9
	B3LYP-D/def2-SVP	0	-71.3	-54.0	-78.0	-68.9	-95.4	-82.0 -81.6	-116.0	-51.7
	B3LYP/def2-TZVPP	0	-62.2	-43.4	-63.7	-54.7	-81.0	-67.8 -67.6	-98.1	-48.2
	BP86/def2-TZVPP	0	-64.8	-47.6	-70.8	-64.0	-87.1	-74.8 -74.6	-102.5	-51.1
	M06/6-31+G*	0	-52.8	-37.4	-60.4	-50.6	-78.1	-64.0 -63.6	-98.8	-50.6
PM ₃ Au ⁺	B3LYP/def2-SVP	0	-41.6	-24.7	-36.9	-32.6	-62.8	-50.9 -50.7	-88.2	-52.2
	BP86/def2-SVP	0	-46.0	-32.3	-46.5	-43.6	-70.2	-59.4 -59.1	-94.2	-54.9
	B3LYP-D/def2-SVP	0	-45.1	-30.0	-41.2	-36.6	-66.9	-54.7 -54.4	-93.7	-51.7
	B3LYP/def2-TZVPP	0	-40.6	-23.2	-32.1	-27.3	-57.8	-45.5 -45.3	-83.7	-48.2
	BP86/def2-TZVPP	0	-45.1	-31.0	-42.1	-38.7	-65.6	-54.4 -54.2	-90.2	-51.1
	M06/6-31+G*	0	-27.5	-12.9	-23.4	-18.3	-50.1	-37.1 -36.8	-76.2	-50.6

Figure Captions

Figure S1. Free energy profile (ΔG in kcal/mol) for the cyclization of substrate **7** to the 6-endo product using catalyst-**6** (in green) and PPh_3Au^+ (in red). Enlarged views of the reaction centers for all stationary points are also shown. Relative energies are given with respect to the sum of the energies of the isolated catalyst and substrate.

Figure S2. Optimized geometry of catalyst-**6** at the BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. Also shown is the color code of different elements used here and in the following figures.

Figure S3. Optimized geometry of the substrate at the BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S4. Optimized geometry of the catalyst-substrate complex (**Int-1_a**) for green pathway at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S5. Optimized geometry of the transition state for cyclization (**TS1_a**) for green pathway at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S6. Optimized geometry of the cyclized intermediate (**Int-2_a**) for green pathway at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S7. Optimized geometry of the transition state for ring opening (**TS2_a**) for green pathway at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S8. Optimized geometry of the ring-opened intermediate (**Int-3_a**) for green pathway at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S9. Optimized geometry of the transition state for 1,2-hydride shift (**TS3_a**) for green pathway at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S10. Optimized geometry of the product resulting from hydride shift (**Int-4_a**) for green pathway at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S11. Optimized geometry of the transition state for 1,2-hydride shift leading to the product complex (**TS4_{a1}**) for green pathway at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S12. Optimized geometry of the transition state for 1,2-hydride shift resulting in product complex (**TS-4_{a2}**) for green pathway at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S13. Optimized geometry of the product complex (**Prod-cplx_a**) for green pathway at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S14. Optimized geometry of the catalyst-substrate complex (**Int-1_b**) for red pathway at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S15. Optimized geometry of the transition state for cyclization (**TS1_b**) for red pathway at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S16. Optimized geometry of the cyclized intermediate (**Int-2_b**) for red pathway at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S17. Optimized geometry of the transition state for ring opening (**TS2_b**) for red pathway at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S18. Optimized geometry of the ring-opened intermediate (**Int-3_b**) for red pathway at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S19. Optimized geometry of the transition state for 1,2-hydride shift (**TS3_b**) for red pathway at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S20. Optimized geometry of the product resulting from hydride shift (**Int-4_b**) for red pathway at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S21. Optimized geometry of the transition state for 1,2-hydride shift leading to the product complex (**TS4_{b1}**) for red pathway at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S22. Optimized geometry of the transition state for 1,2-hydride shift resulting in product complex (**TS4_{b2}**) for red pathway at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S23. Optimized geometry of the product complex (**Prod-cplx_b**) for red pathway at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S24. Optimized geometry of the final product at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S25. Free energy profile (ΔG in kcal/mol) for the cyclization of substrate **9** to the 6-endo product: using catalyst-**6** (in green) and PMe_3Au^+ (in red). Enlarged views of the reaction centers for all stationary points are also shown. Relative energies are given with respect to the sum of the energies of the isolated catalyst and substrate.

Figure S26. Optimized geometry of substrate **9** at the BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S27. Optimized geometry of the catalyst-substrate complex (**Int-1_a**) for green pathway leading to 6-endo product at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S28. Optimized geometry of the transition state for cyclization (**TS1_a**) for green pathway leading to 6-endo product at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S29. Optimized geometry of the cyclized intermediate (**Int-2_a**) for green pathway leading to 6-endo product at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S30. Optimized geometry of the transition state for 1,2-hydride shift (**TS2_a**) for green pathway leading to 6-endo product at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S31. Optimized geometry of the product resulting from hydride shift (**Int-3_a**) for green pathway leading to 6-endo product at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S32. Optimized geometry of the transition state for 1,2-hydride shift leading to product complex (**TS3_{a1}**) for green pathway (6-endo product) at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S33. Optimized geometry of the transition state for 1,2-hydride shift leading to product complex (**TS3_{a2}**) for green pathway (6-endo product) at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S34. Optimized geometry of the product complex (**Prod-cplx_a**) for green pathway leading to 6-endo product at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S35. Optimized geometry of the 6-endo product at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S36. Optimized geometry of the catalyst-substrate complex (**Int-1_b**) for red pathway leading to 6-endo product at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S37. Optimized geometry of the transition state for cyclization (**TS1_b**) for red pathway leading to 6-endo product at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S38. Optimized geometry of the cyclized intermediate (**Int-2_b**) for red pathway leading to 6-endo product at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S39. Optimized geometry of the transition state for 1,2-hydride shift (**TS2_b**) for red pathway leading to 6-endo product at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S40. Optimized geometry of the product resulting from hydride shift (**Int-3_b**) for red pathway leading to 6-endo product at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S41. Optimized geometry of the transition state for 1,2-hydride shift leading to product complex (**TS3_{b1}**) for red pathway (6-endo product) at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S42. Optimized geometry of the transition state for 1,2-hydride shift leading to product complex (**TS3_{b2}**) for red pathway (6-endo product) at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S43. Optimized geometry of the product complex (**Prod-cplx_b**) for green pathway pathway leading to 6-endo product at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S44. Free energy profile (ΔG in kcal/mol) for the cyclization of substrate **9** to the 7-exo product using catalyst-**6** (in green, labeled **55** in the main paper) and PMe_3Au^+ (in red). Enlarged views of the reaction centers for all stationary points are also shown. Relative energies are given with respect to the sum of the energies of the isolated catalyst and substrate.

Figure S45. Optimized geometry of the transition state for cyclization (**TS1_a**) for green pathway leading to 7-exo product at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S46. Optimized geometry of the cyclized intermediate (**Int-2_a**) for green pathway leading to 7-exo product at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S47. Optimized geometry of the transition state for 1,2-hydride shift (**TS2_a**) for green pathway leading to 7-exo product at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S48. Optimized geometry of the product complex (**Prod-cplx_a**) for green pathway leading to 7-exo product at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S49. Optimized geometry of the 7-exo product at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S50. Optimized geometry of the transition state for cyclization (**TS1_b**) for red pathway leading to 7-exo product at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S51. Optimized geometry of the cyclized intermediate (**Int-2_b**) for red pathway leading to 7-exo product at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S52. Optimized geometry of the transition state for 1,2-hydride shift (**TS2_b**) for red pathway leading to 7-exo product at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S53. Optimized geometry of the product complex (**Prod-cplx_a**) for red pathway leading to 7-exo product at BP86/def2-TZVPP level. The hydrogen atoms are omitted for clarity. For the color code of different elements, please refer to Figure 2.

Figure S54. Frontier orbitals interactions in complexes **55** (left) and **56** (right). Shown are the LUMOs that are mainly responsible for the catalyst-substrate interaction and contain a very strong 6s(Au) contribution. The fragments **1** and (MeO)₃P (left and right) were calculated at their geometries in the complexes **55** and **56**.

Note:

Figures S1-S24 refer to the cyclization of substrate **7** to the 6-endo-product.

Figures S25-S43 refer to the cyclization of substrate **9** to the 6-endo-product.

Figures S44-S53 refer to the cyclization of substrate **9** to the 7-exo-product.

Figure S1

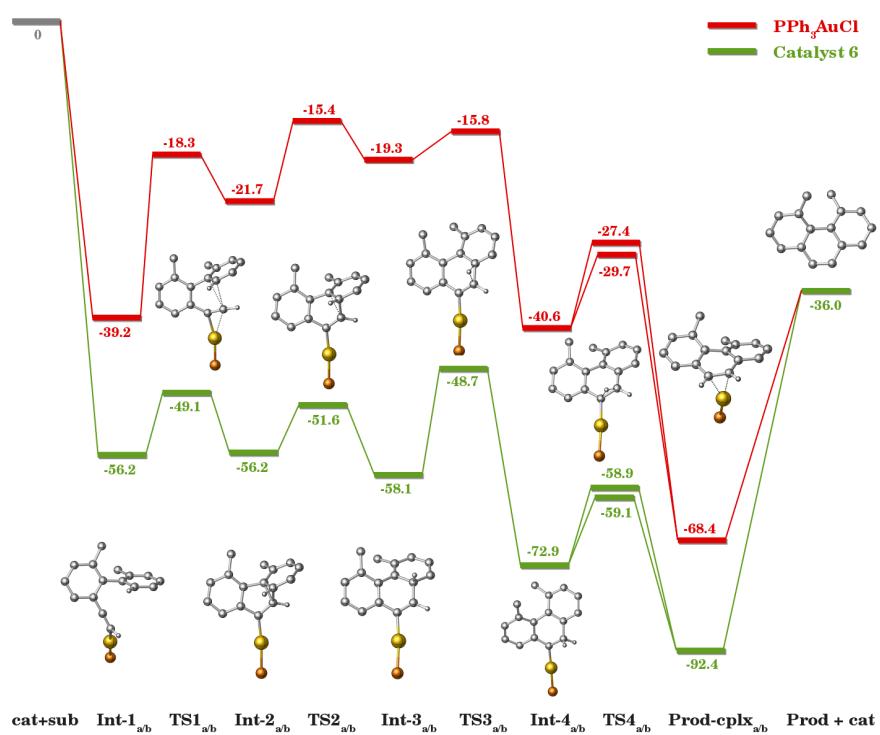
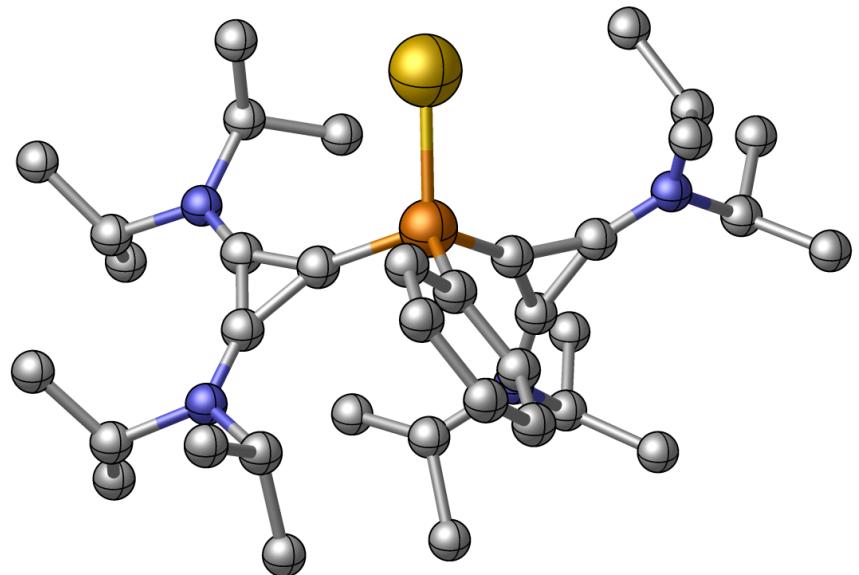


Figure S2



○ Au ○ P ● C ● N ● H

Figure S3

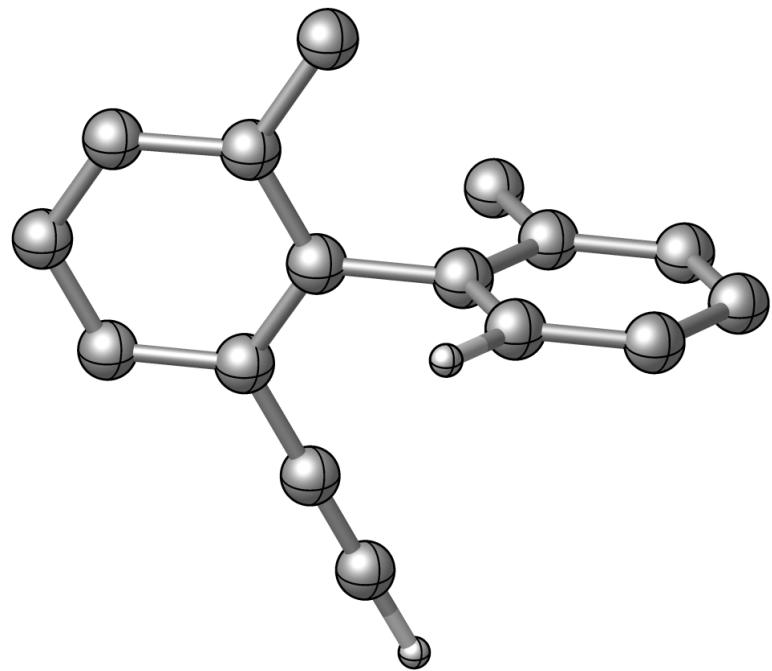


Figure S4

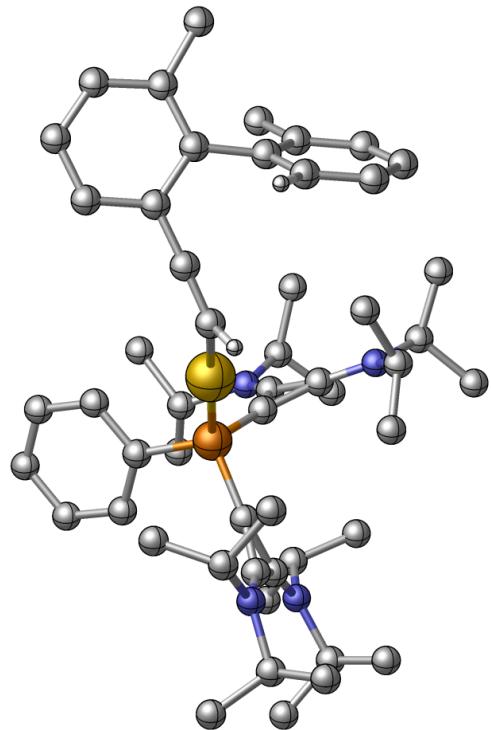


Figure S5

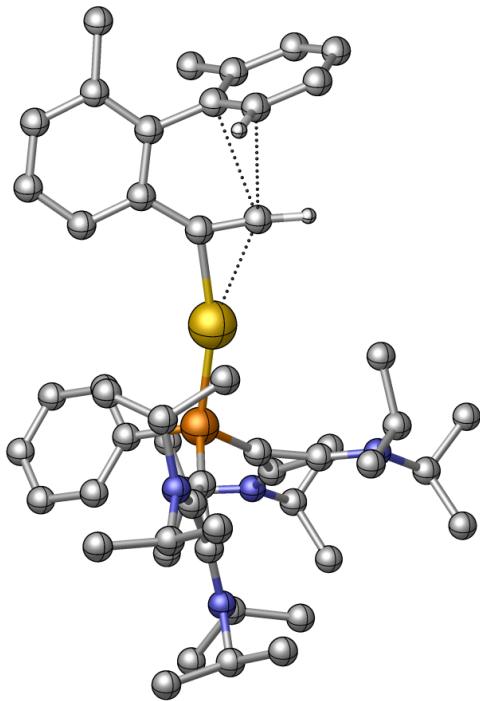


Figure S6

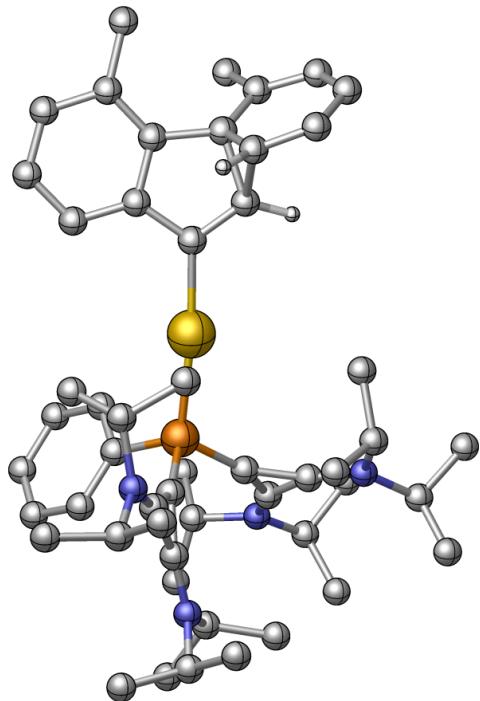


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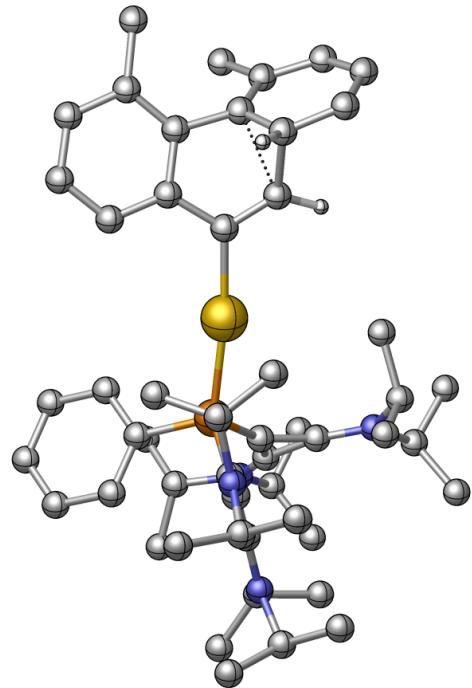


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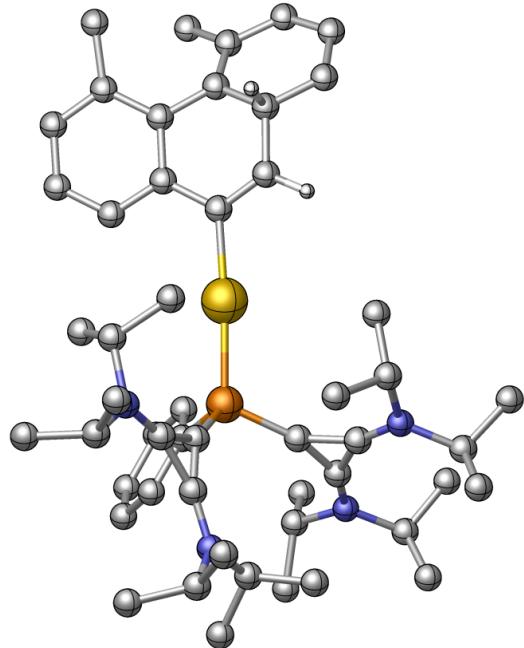


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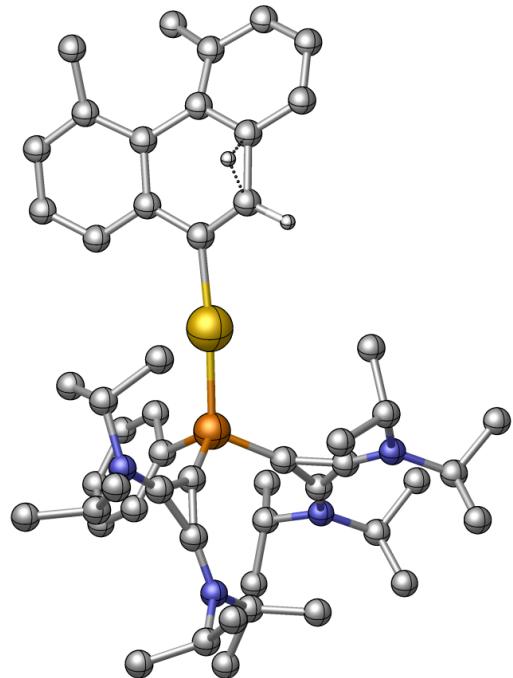


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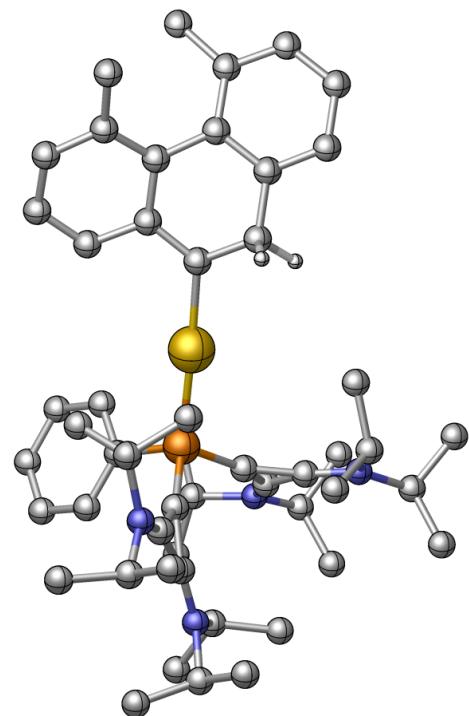


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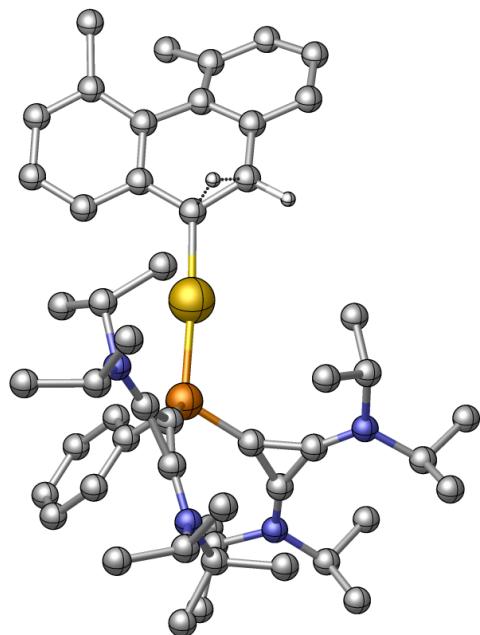


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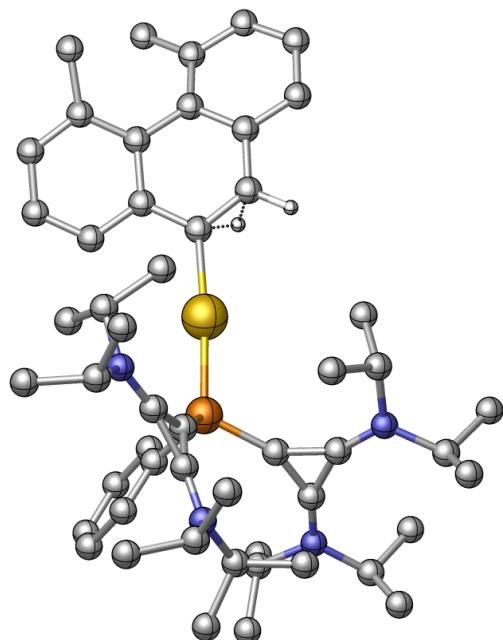


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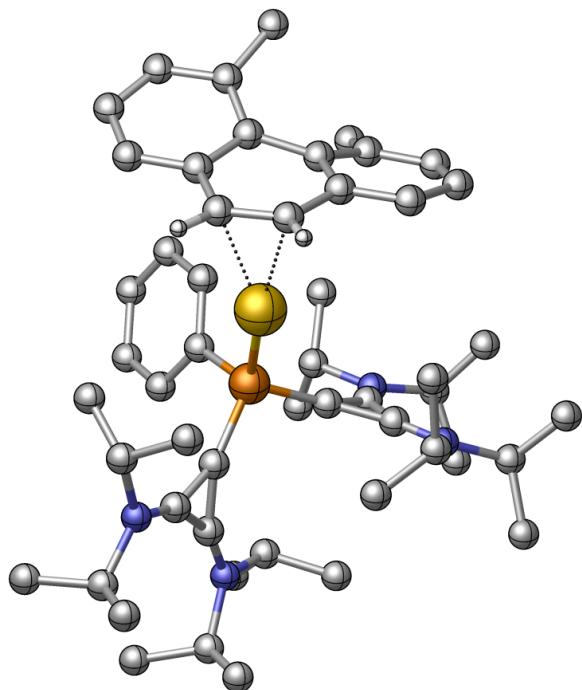


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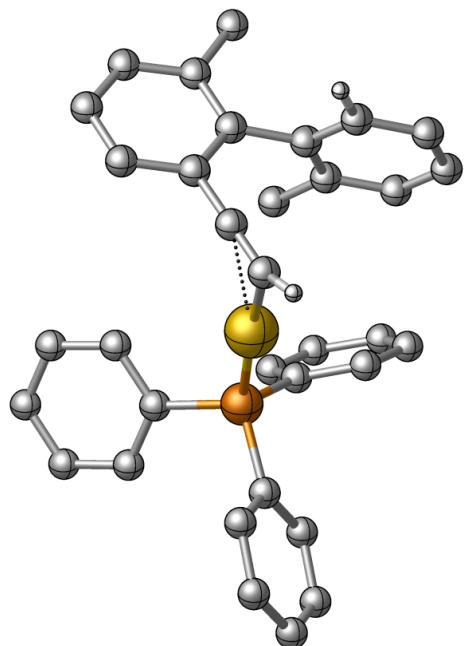


Figure S15

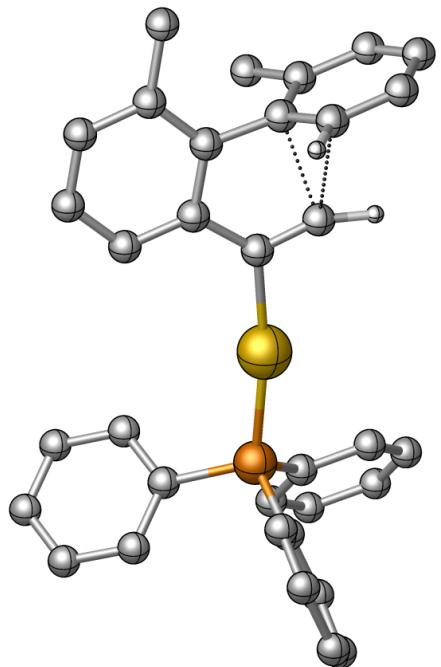


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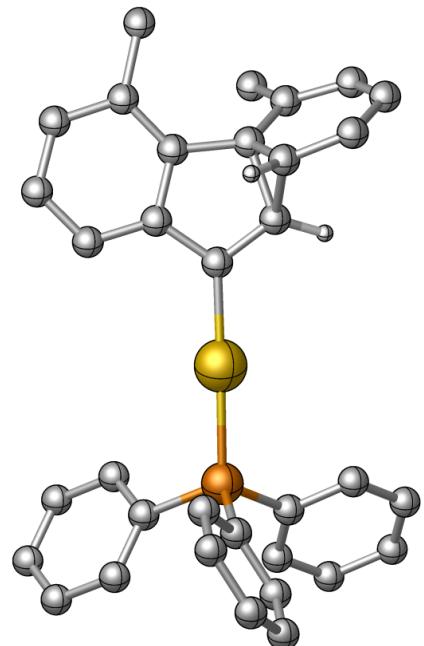


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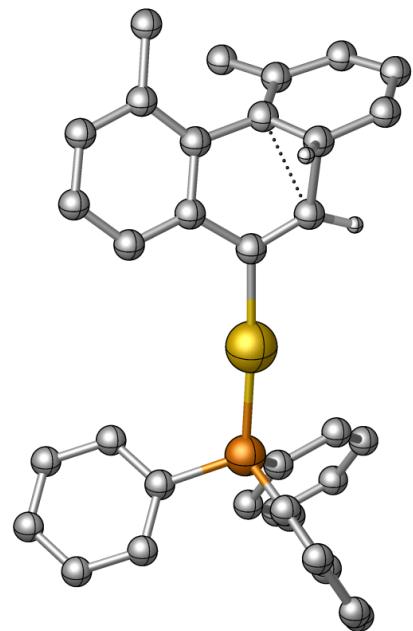


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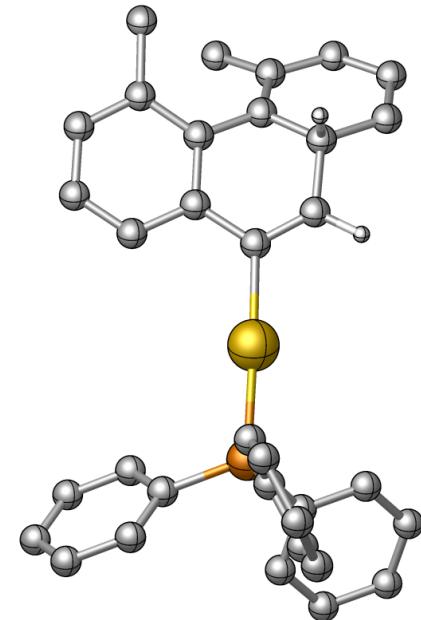


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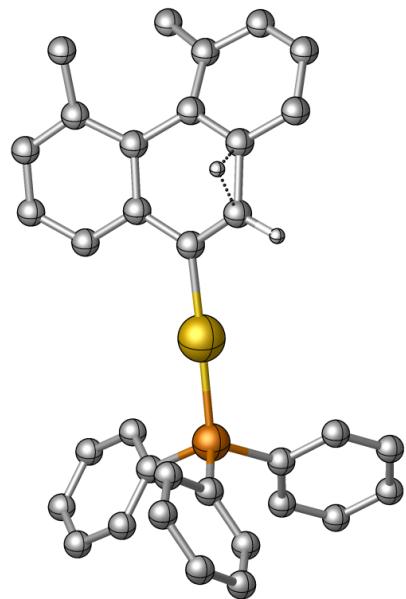


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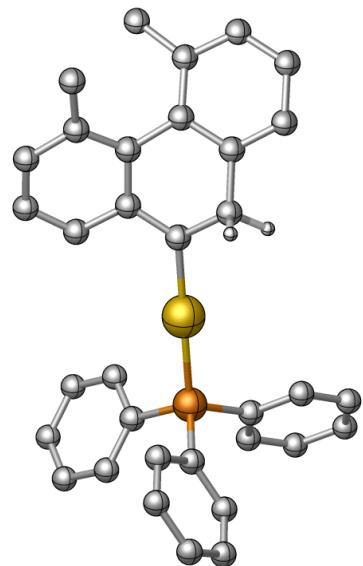


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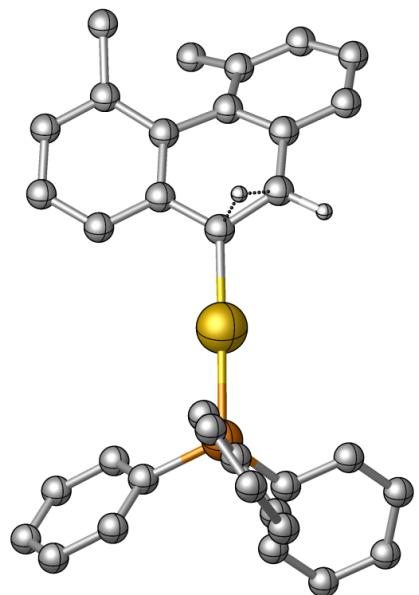


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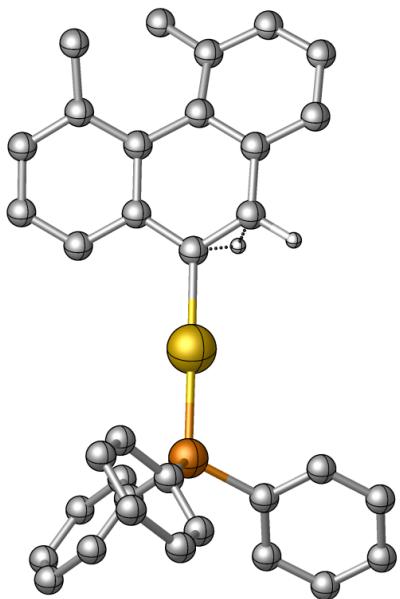


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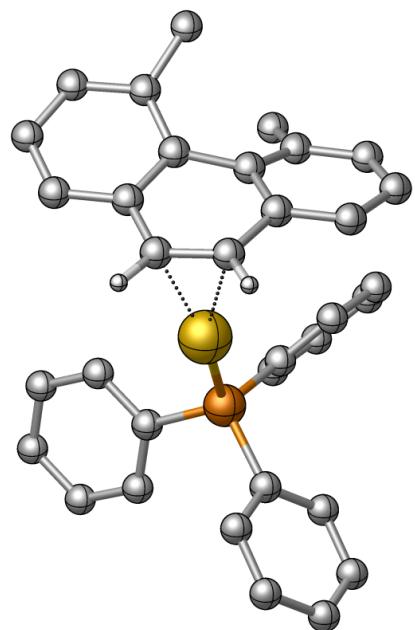


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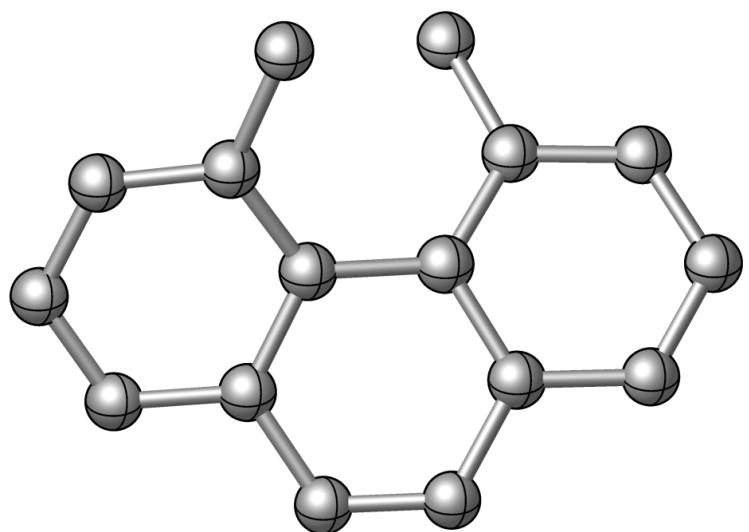


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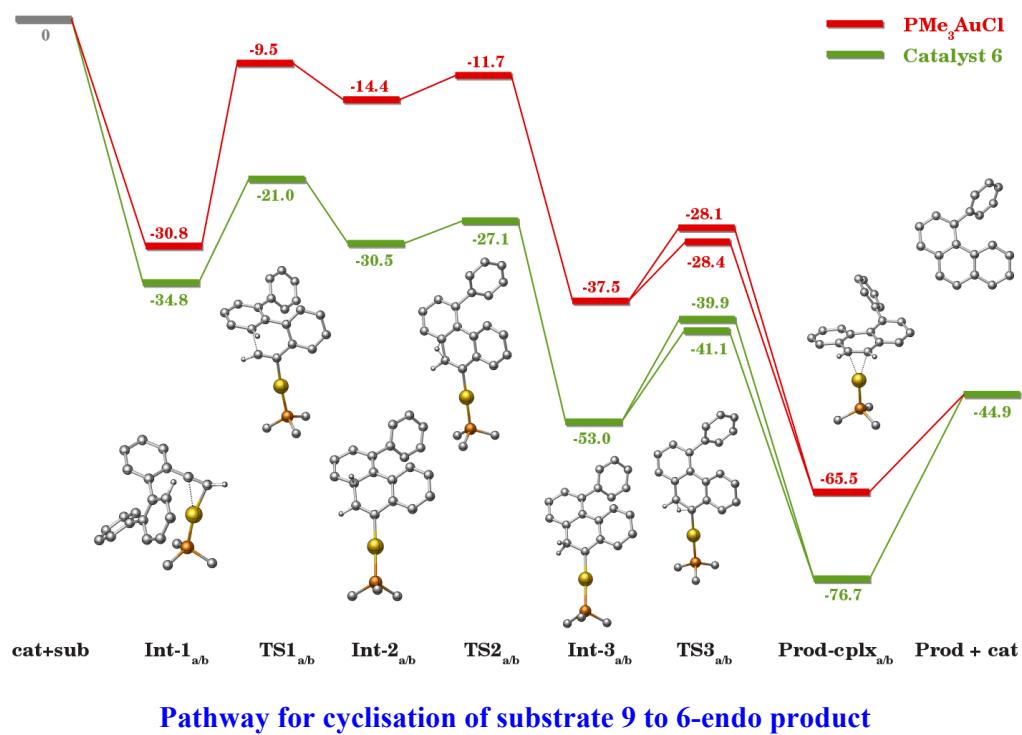


Figure S26

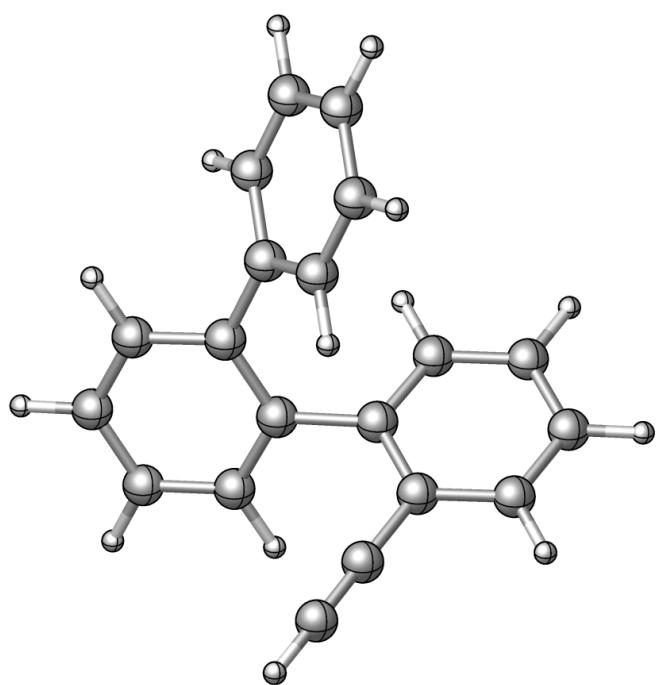


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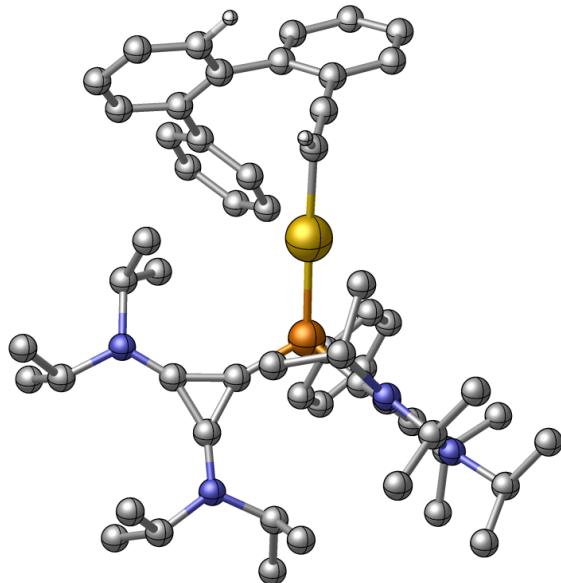


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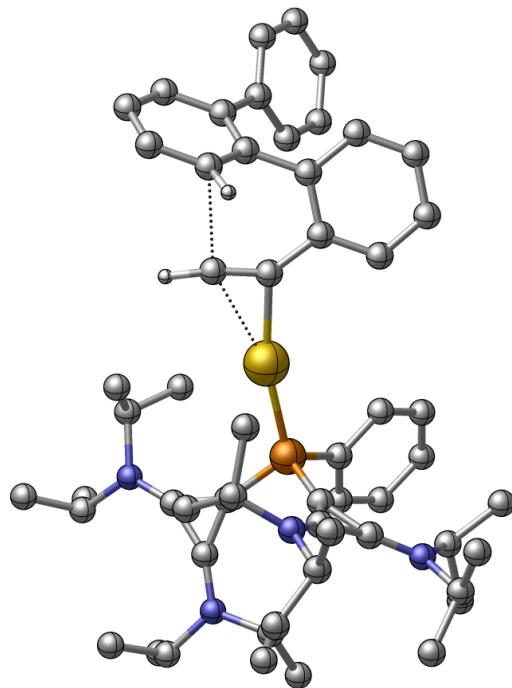


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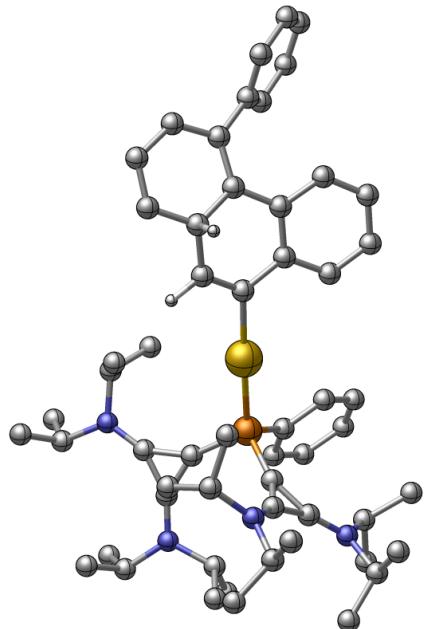


Figure S30

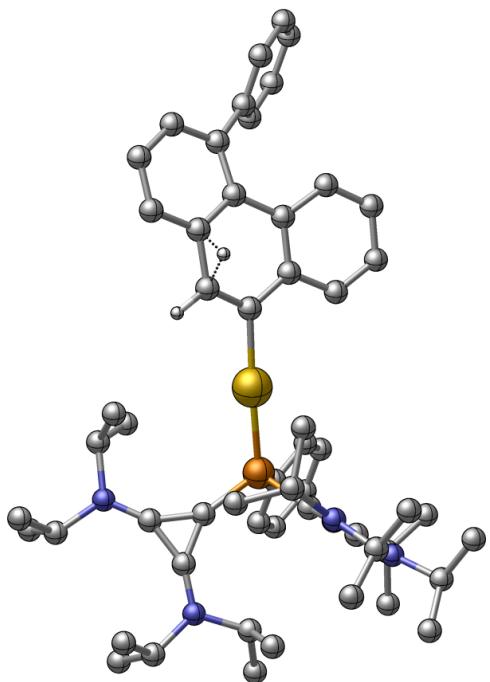


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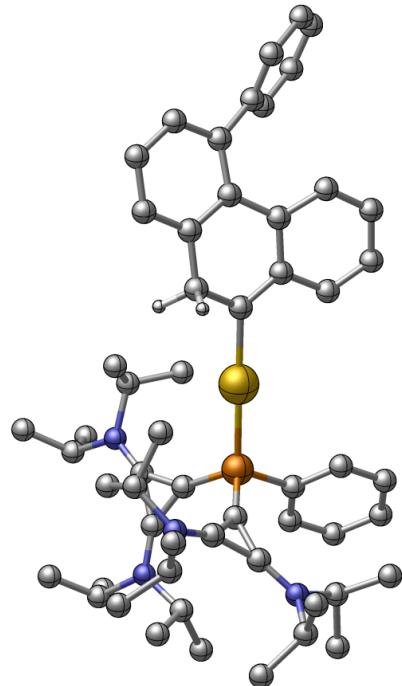


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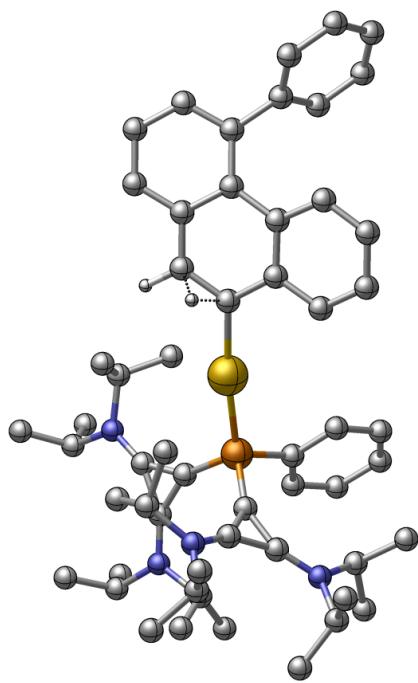


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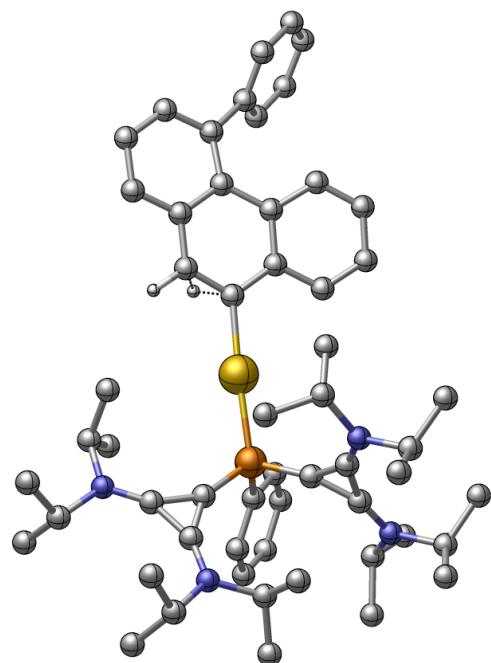


Figure S34

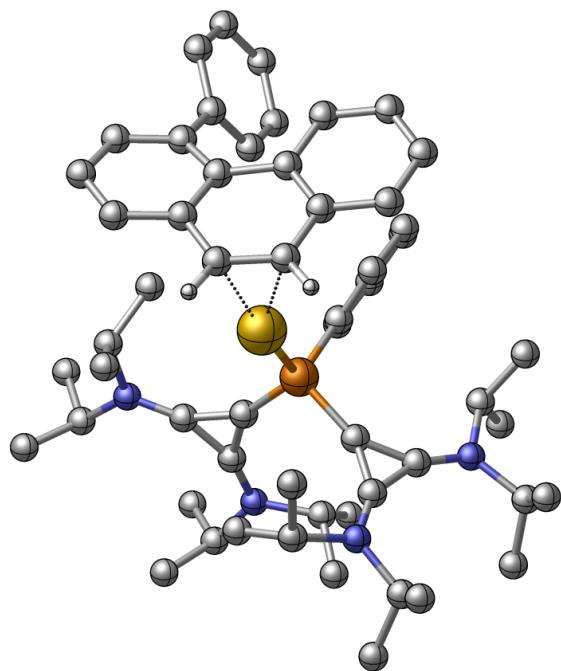


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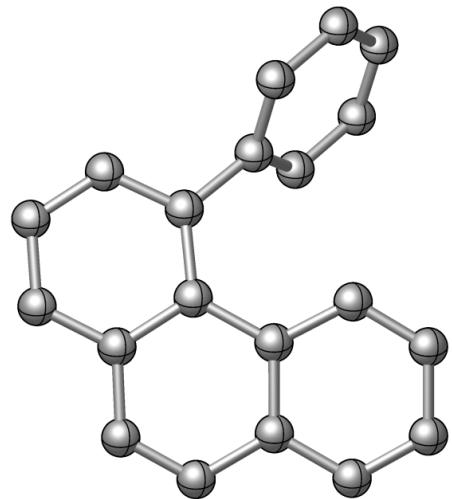


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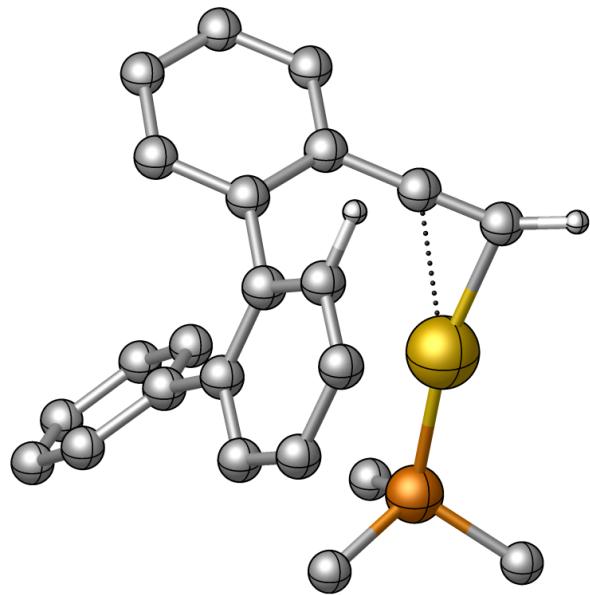


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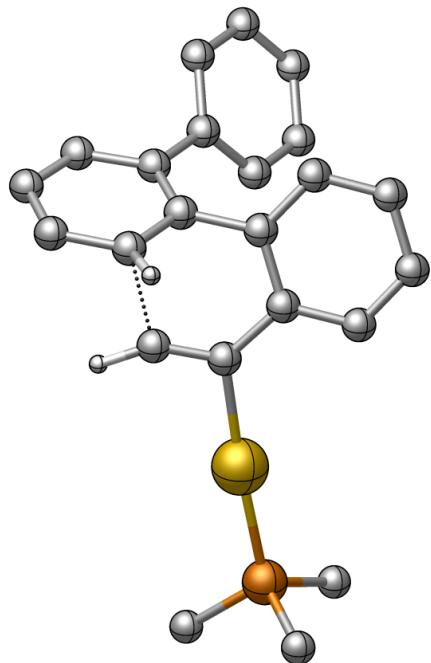


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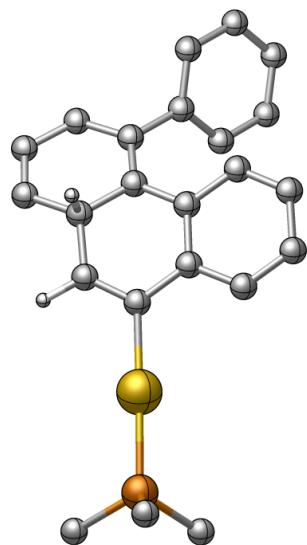


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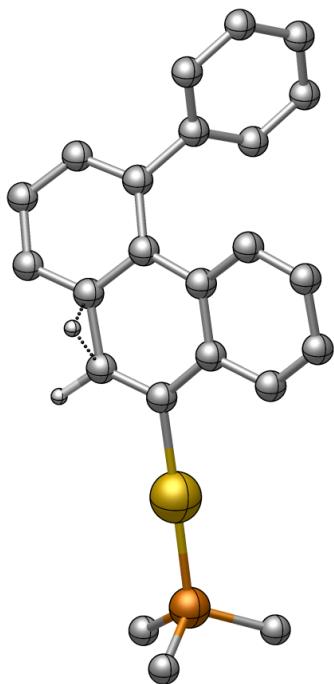


Figure S40

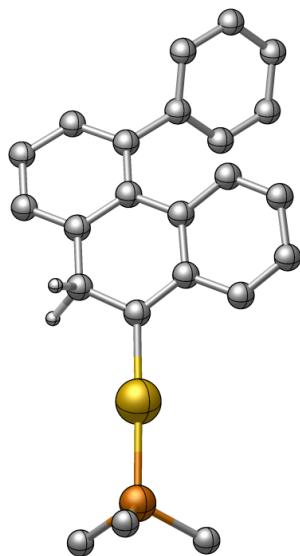


Figure S41

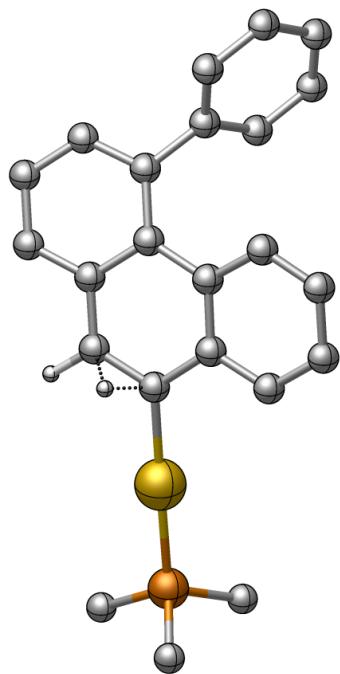


Figure S42

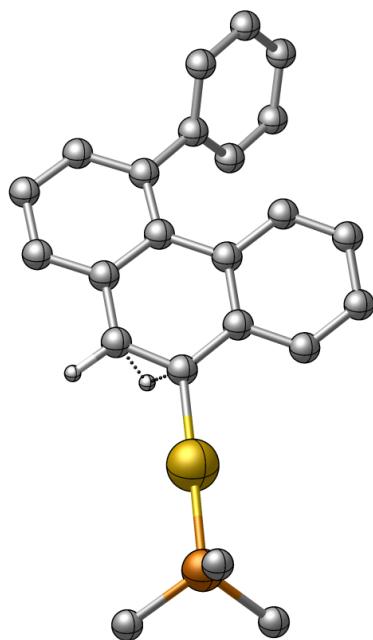


Figure S43

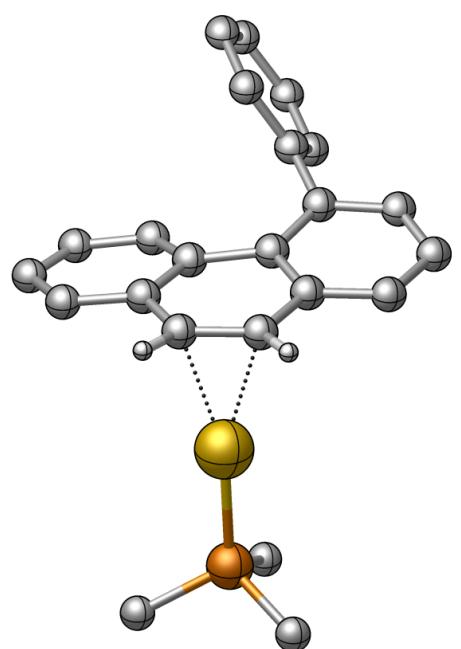


Figure S44

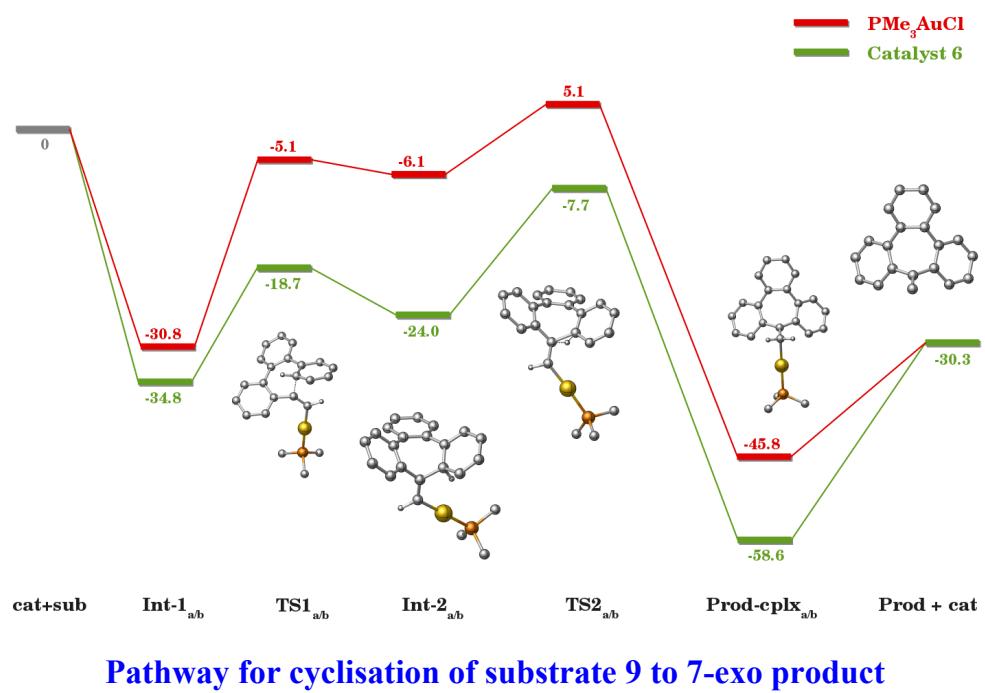


Figure S45

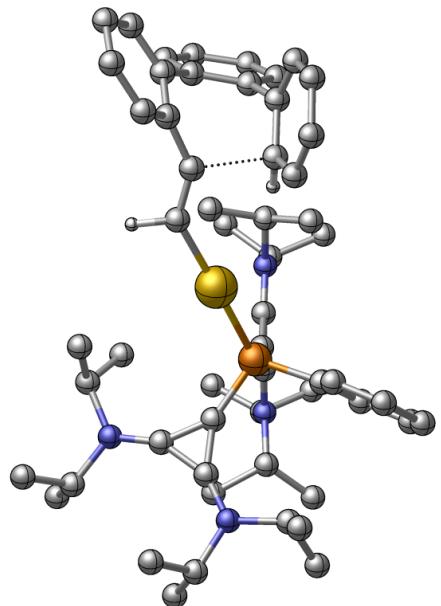


Figure S46

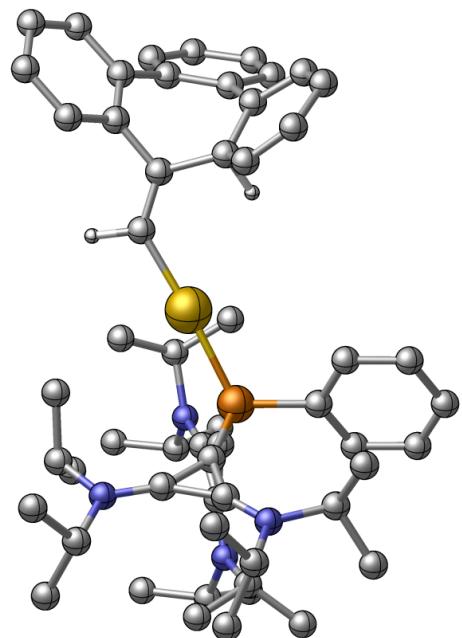


Figure S47

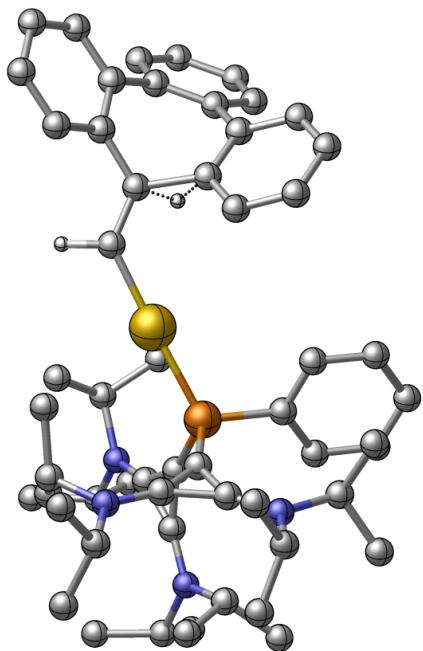


Figure S48

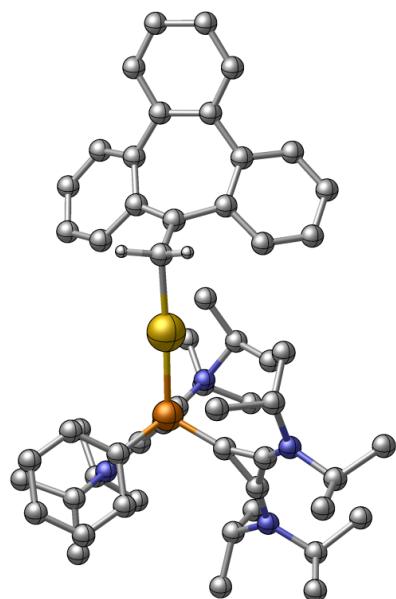


Figure S49

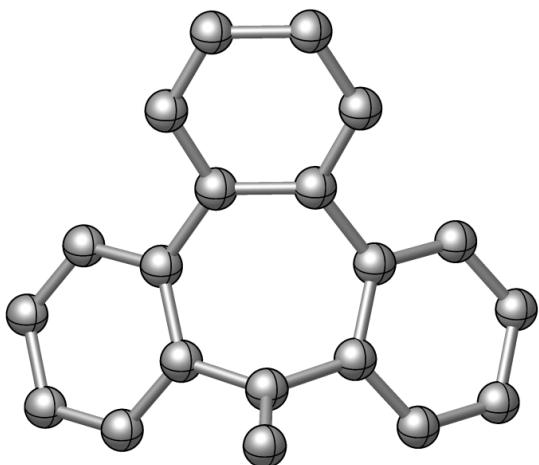


Figure S50

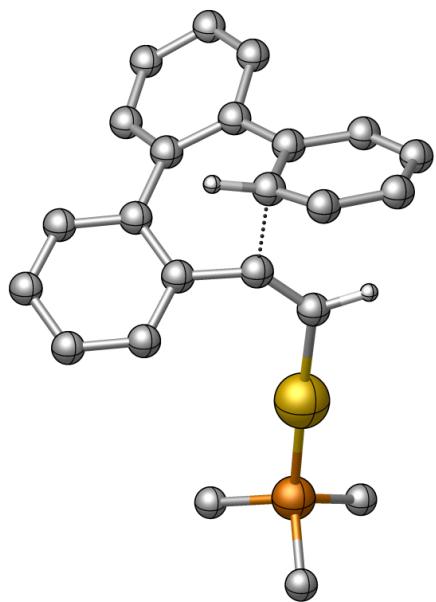


Figure S51

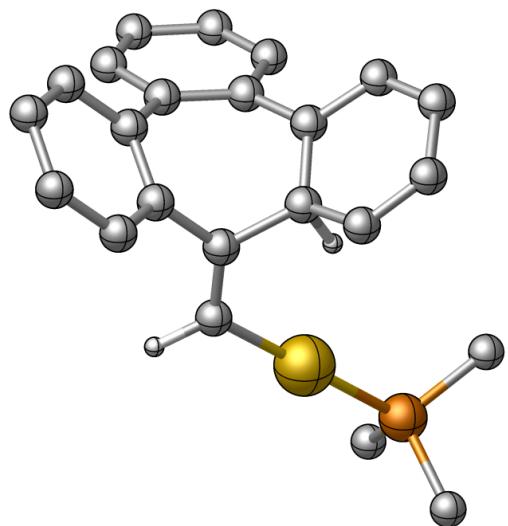


Figure S52

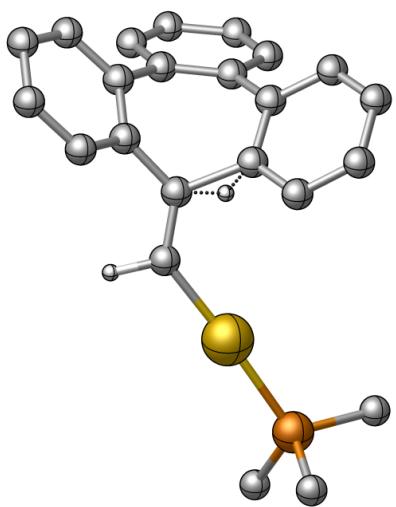


Figure S53

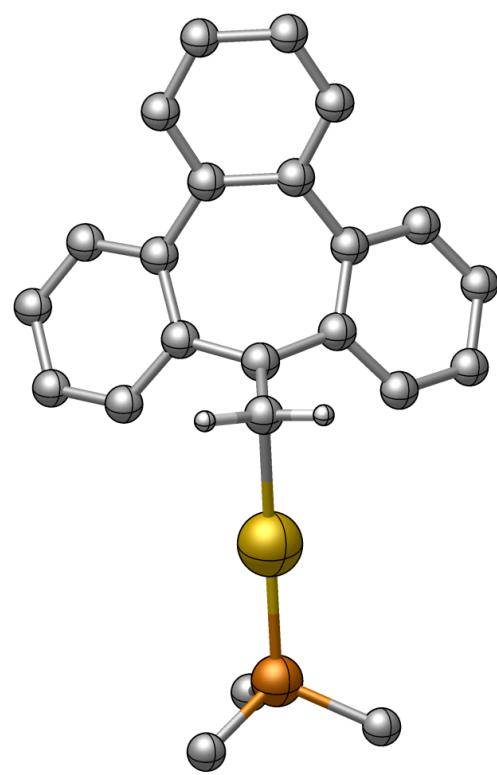
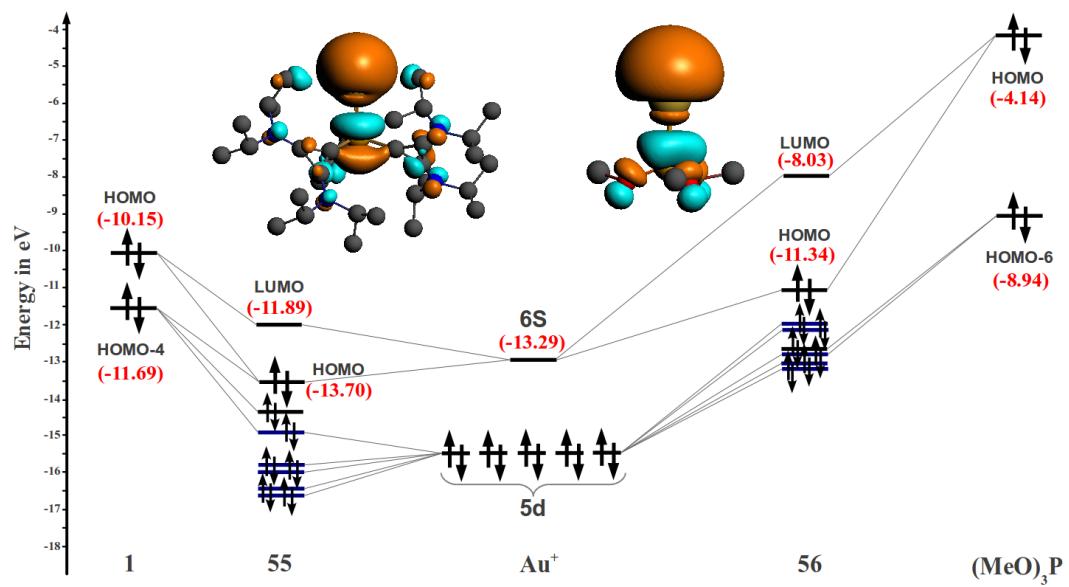


Figure S54



**CARTESIAN COORDINATES OF OPTIMIZED GEOMETRIES
(BP86/def2-TZVPP, Å)**

Catalyst-6

C	4.4391792750	2.5479010545	1.5535455004
C	3.4516597045	2.8424401410	0.6129706718
C	3.8340453174	3.1701908331	-0.7004561191
C	5.1899723743	3.1792034044	-1.0787729518
C	6.1635797940	2.8842007165	-0.1271784975
C	5.7890835540	2.5714896777	1.1859306776
P	2.6048351116	3.6726749031	-1.9062683077
C	0.9875533557	3.2366878343	-1.3222833687
C	-0.0843987050	2.3352554075	-1.2395647159
N	-0.5938286691	1.1709112704	-1.5125389429
C	0.1835441936	0.1726645203	-2.3264077479
C	0.2270193201	0.5997486509	-3.7927303449
C	2.6336325212	5.4428760250	-2.0497845560
C	2.3098988691	6.6073823124	-2.7570417268
N	1.7100423804	7.1786148397	-3.7629129700
C	1.0145919018	6.3538998900	-4.8079308979
C	2.0364675851	5.6363838665	-5.6902579859
C	3.1368373279	6.6654793375	-1.5830948201
N	3.8565866558	7.2876926626	-0.6962007806
C	4.0716289153	8.7783585227	-0.7148465679
C	2.7603644490	9.5147259915	-0.4444202038
C	4.5427116062	6.4830037513	0.3767950404
C	6.0601347240	6.5696707490	0.2213180990
C	4.0464292644	6.8992706456	1.7603125022
C	1.7068977620	8.6753165954	-3.9318235169
C	0.2880911447	9.2191569070	-3.7676278834
C	2.3706543120	9.0853388864	-5.2442187608
C	-0.0323419185	5.4227849174	-4.2028273264
C	4.8232434770	9.2016035012	-1.9758691727
C	-0.1518955424	3.6263372972	-0.6155936427
N	-0.7197430025	4.5507142603	0.1054200413
C	-2.1536895312	4.4648443316	0.5597428765
C	-2.3149387232	3.4109091848	1.6543181482
C	0.0814766281	5.7757809184	0.4427490068
C	0.0526117821	6.0536449918	1.9450768921
C	-0.3791970645	6.9629550804	-0.4016630119
C	-1.9485139799	0.7613194737	-0.9940767736
C	-2.8906420310	0.4163396718	-2.1453708622
C	-1.8020636687	-0.3584325078	0.0356779088
C	1.5533410624	-0.1059349030	-1.7139509158
C	-3.0865030245	4.3141413719	-0.6417357233
H	-0.4099858532	-0.7466435761	-2.2579046036
H	-0.7757032285	0.7472534722	-4.2106924916
H	0.7399259251	-0.1659603250	-4.3875301279
H	0.7817320143	1.5521653134	-3.8998278001
H	2.2330020962	0.7548219354	-1.7957465537
H	2.0249412582	-0.9407258195	-2.2459674247
H	1.4685657585	-0.3822048102	-0.6561871653
H	-2.3273707891	1.6559229220	-0.4887919768
H	-2.9766081452	1.2424963118	-2.8629409576
H	-3.8886171767	0.2178559385	-1.7358378828
H	-2.5794852925	-0.4887116406	-2.6828788131
H	-1.4415102955	-1.2924683318	-0.4137442952
H	-2.7860654185	-0.5708279074	0.4722206673

H	-1.1219994387	-0.0740422176	0.8487243549
H	-2.3476174328	5.4481924952	1.0047936996
H	-2.0280446367	2.4097370201	1.3082130800
H	-3.3627709456	3.3676661346	1.9744932092
H	-1.7025459409	3.6535543425	2.5308627596
H	-2.9756599752	5.1601385767	-1.3314351126
H	-4.1272794926	4.2912380959	-0.2973949591
H	-2.9029644954	3.3897892657	-1.2035091077
H	1.1138132653	5.5192624984	0.1608243827
H	-0.9516053684	6.3067798864	2.3062154819
H	0.6896414116	6.9208398085	2.1588278753
H	0.4287229550	5.2004659816	2.5224504677
H	-1.4096249210	7.2563023643	-0.1636845041
H	-0.3209772301	6.7311447957	-1.4726815597
H	0.2639305102	7.8281875183	-0.1971934988
H	0.4896122000	7.0926667254	-5.4251907784
H	2.7566546921	6.3309308675	-6.1371800045
H	1.5210734191	5.1057499659	-6.5000080300
H	2.6039629649	4.8950567705	-5.0967765190
H	0.4204724235	4.6193976612	-3.6041664559
H	-0.5979770206	4.9451728304	-5.0117554730
H	-0.7419521021	5.9747974131	-3.5746483056
H	2.3194068762	9.0422121905	-3.1022133050
H	-0.3793125377	8.8947298137	-4.5765663472
H	0.3206851168	10.3152520927	-3.7989703680
H	-0.1497330329	8.9190254089	-2.8067938200
H	3.3891764207	8.6856298001	-5.3268930680
H	2.4326382195	10.1799633937	-5.2800570604
H	1.7927509605	8.7691171166	-6.1219692848
H	4.7332169083	8.9566318711	0.1407249503
H	2.0006306014	9.3068151062	-1.2084013962
H	2.9382089183	10.5967839263	-0.4366196788
H	2.3504878697	9.2338227651	0.5339840347
H	5.8017146830	8.7098481860	-2.0310364399
H	4.9885643500	10.2855609057	-1.9590813155
H	4.2708266392	8.9621375159	-2.8927335694
H	4.2315320276	5.4484900751	0.1913925464
H	6.3797591641	6.2518443764	-0.7788287918
H	6.5293819351	5.9049702753	0.9569102317
H	6.4407799250	7.5819290026	0.4080248513
H	4.3363395390	7.9251157308	2.0198028915
H	4.4938647755	6.2374346383	2.5121639094
H	2.9550119110	6.8126409973	1.8359960385
H	5.4809575431	3.4087627162	-2.1050740857
H	7.2150406889	2.8820780168	-0.4118054124
H	6.5543713834	2.3276547588	1.9225400136
H	4.1547644900	2.2875802610	2.5725148565
H	2.4000345479	2.8179151492	0.8979617534
Au	2.9303777847	2.7451286638	-3.9252510286

Substrate

C	-2.0914442800	-1.2383422613	-0.7534517806
C	-1.2787632197	-0.0877186146	-0.7177522350
C	-1.7055099315	1.0949775032	-1.3692969891
C	-2.9327334780	1.1133152673	-2.0622477282
C	-3.7254556311	-0.0285284597	-2.0998793816
C	-3.3073942648	-1.1916570310	-1.4486243693
C	0.0215980650	-0.1111331384	0.0128034670
C	0.1031512315	0.3503455877	1.3433737514

C	1.3416573864	0.2926691319	1.9957720437
C	2.4790031890	-0.2051180008	1.3561429608
C	2.3921303152	-0.6578143522	0.0385889599
C	1.1646680015	-0.6105608345	-0.6242637431
C	-1.1156436209	0.9041169041	2.0347776792
C	-0.9007177781	2.2700585415	-1.3192761848
C	-0.2241895249	3.2769662485	-1.2710417546
C	-1.6573189177	-2.4952139029	-0.0425461701
H	1.4129556098	0.6470016773	3.0258120115
H	3.4308877637	-0.2380955809	1.8869583409
H	3.2739967851	-1.0448454578	-0.4721980976
H	1.0834862592	-0.9579250111	-1.6551104594
H	-3.2456267793	2.0295414861	-2.5611917408
H	-4.6747022798	-0.0141456398	-2.6355835148
H	-3.9366187587	-2.0828114036	-1.4760629458
H	-0.9121062245	1.1220424834	3.0903897826
H	-1.4482537600	1.8338581484	1.5498458255
H	-1.9607079789	0.2023504642	1.9820435785
H	-1.4324315498	-2.2943453909	1.0148313288
H	-2.4338405853	-3.2684323041	-0.0920619592
H	-0.7352534166	-2.9023100928	-0.4804725833
H	0.3816018919	4.1567540120	-1.2277775506

RC (catalyst-6)

C	5.2480801973	2.9616088586	1.9756616437
C	3.8811846258	3.1900609033	2.1677290780
C	3.0203217533	3.2491991873	1.0711119007
C	3.5354827548	3.0779748680	-0.2248760362
C	4.9048663312	2.8260022045	-0.4164186301
C	5.7578305429	2.7761719416	0.6866090886
P	2.5032615029	3.2524731077	-1.7034222693
Au	3.0207711888	1.8661523935	-3.4515355667
C	0.8142157829	3.0686752274	-1.1234903311
C	-0.2701793787	3.6397987141	-0.4635688467
N	-0.7539043331	4.6978871431	0.1318382731
C	0.1354845039	5.8959870521	0.2727389799
C	-0.2508092877	6.9629671093	-0.7507457014
C	2.5948015147	4.9960045218	-2.1402511746
C	3.1157621367	6.2706131994	-1.9044467732
N	3.8402166664	7.0440226960	-1.1409192862
C	4.4853744795	6.4555605870	0.0819720570
C	4.0725444614	7.2159695273	1.3398427681
C	-0.3268652375	2.2853624308	-0.9208104788
N	-0.9456825157	1.1446112486	-1.0392294077
C	-2.2942075342	0.9112484103	-0.4226813836
C	-2.1902598973	-0.1182650930	0.7026276708
C	-0.2949549311	0.0093078151	-1.7761760183
C	1.0442931233	-0.3678091460	-1.1478010307
C	-0.2262355120	0.3295037009	-3.2683666934
C	2.3271353897	6.0033130800	-3.0687562540
N	1.7587567873	6.3790805749	-4.1837943306
C	1.7593536229	7.8137267221	-4.6197534123
C	2.4550722856	7.9872812404	-5.9687062773
C	1.1065458356	5.3669752387	-5.0809735762
C	0.0612869903	4.5346863963	-4.3419850474
C	2.1688738213	4.5210425838	-5.7789791109
C	4.1419561309	8.4738865335	-1.4840932002
C	4.8976818541	8.5703425432	-2.8094818337
C	2.8826271261	9.3339989494	-1.3791414019

C	6.0000154825	6.3705760156	-0.1028149481
C	0.3387202545	8.3773304944	-4.5941415883
C	-2.1828673759	4.7928919474	0.5858892870
C	-3.1399215040	4.5309292446	-0.5769657767
C	-2.4136061629	3.9356669450	1.8301406033
C	0.1452178529	6.4097014194	1.7118904783
C	-3.3290314899	0.5506829884	-1.4870901302
H	-0.9819037981	-0.8332723585	-1.6355065915
H	-1.2233515922	0.5237600737	-3.6813633316
H	0.2110016581	-0.5190505871	-3.8088409679
H	0.4052232475	1.2116211082	-3.4559524917
H	1.7936457523	0.4286423472	-1.2555447004
H	1.4447329696	-1.2563907574	-1.6501595367
H	0.9310096259	-0.5986017305	-0.0818390497
H	-2.5669333454	1.8772158943	0.0151086499
H	-3.3817069403	1.3134373325	-2.2748859906
H	-4.3164808742	0.4791961519	-1.0152450912
H	-3.1238772784	-0.4216437048	-1.9537998563
H	-1.9275041626	-1.1159843573	0.3275363912
H	-3.1638046612	-0.2068716334	1.2006312836
H	-1.4470559282	0.1805703652	1.4528469890
H	-2.3014333503	5.8446066313	0.8738223861
H	-2.1979730750	2.8756840230	1.6444739084
H	-3.4591870127	4.0153925525	2.1509380565
H	-1.7771975153	4.2670739575	2.6593875703
H	-2.9638328848	5.2411205843	-1.3948150233
H	-4.1751317644	4.6537092362	-0.2367283072
H	-3.0429142778	3.5158139483	-0.9810499562
H	1.1443408641	5.5274197882	0.0353044278
H	-0.8358780833	6.7812763766	2.0316478470
H	0.8405825824	7.2544926318	1.7870017146
H	0.4712180886	5.6333391209	2.4146051733
H	-1.2576664357	7.3595153852	-0.5656253580
H	-0.2190981092	6.5554397535	-1.7699566166
H	0.4498773865	7.8049576201	-0.6896096037
H	0.5844614366	5.9716433466	-5.8320375545
H	2.8804506875	5.1378187589	-6.3377601986
H	1.7035596141	3.8261585927	-6.4887858199
H	2.7353727484	3.9204281301	-5.0504273346
H	0.5234273873	3.8245176039	-3.6438713552
H	-0.5083776103	3.9440255572	-5.0695900429
H	-0.6429861907	5.1688794082	-3.7890399900
H	2.3493470817	8.3318647730	-3.8570906580
H	-0.3088036574	7.9007508482	-5.3414942710
H	0.3699382451	9.4483922831	-4.8287436629
H	-0.1214302059	8.2580552584	-3.6044912571
H	3.4741882776	7.5813951799	-5.9503246192
H	2.5171267049	9.0569000091	-6.2040396311
H	1.9006376434	7.5082388092	-6.7858599264
H	4.8278317766	8.7966144635	-0.6920131345
H	2.0956684222	9.0013385624	-2.0681826584
H	3.1188081102	10.3776398049	-1.6197921694
H	2.4781559631	9.3061300698	-0.3593833722
H	5.8385857527	8.0090391430	-2.7606047961
H	5.1364933615	9.6186911291	-3.0255050014
H	4.3137451235	8.1805644216	-3.6521106121
H	4.0836032714	5.4386404732	0.1467187881
H	6.2587824575	5.7936803653	-0.9996513618
H	6.4382852957	5.8647304093	0.7658580519
H	6.4644919874	7.3626652587	-0.1744882770
H	4.4728734400	8.2372064753	1.3658219706

H	4.4659590049	6.6903798846	2.2189383569
H	2.9810886776	7.2653383912	1.4340824031
H	5.2997673562	2.6686611433	-1.4214411475
H	6.8195168039	2.5794695236	0.5419724763
H	5.9149615074	2.9106160283	2.8357888834
H	3.4850766677	3.3133935688	3.1750811839
H	1.9564567315	3.4244666868	1.2301667540
C	3.3486707262	0.5277513761	-5.0032511969
C	4.5086674406	0.4183153713	-5.5111301013
H	2.4682851670	-0.0248628634	-5.3394765227
C	5.7886451896	0.3141423335	-6.0083236081
C	6.6884797422	-0.6043169422	-5.3871290398
C	7.9733130370	-0.7202027124	-5.8772943007
C	8.3594631130	0.0516135052	-6.9831522860
C	7.5006587944	0.9643984199	-7.6285337712
C	6.1902393266	1.1105385205	-7.1420828002
H	6.3424878837	-1.2014891791	-4.5448726534
H	8.6773754936	-1.4186626944	-5.4275976660
H	9.3671428706	-0.0760378595	-7.3832288576
C	8.0054368752	1.7048662174	-8.8371396480
C	5.1895733470	1.9895389923	-7.7955485608
C	4.0915284924	1.3810019427	-8.4341473967
C	3.1480076401	2.1417315421	-9.1206672035
C	3.2896380672	3.5307633824	-9.1655440890
C	4.3616425937	4.1407120786	-8.5130526907
C	5.3267055778	3.3959014273	-7.8196185951
H	4.0122405387	0.2933657276	-8.4288053135
H	2.3253162315	1.6515990583	-9.6399024017
H	2.5734449573	4.1367345137	-9.7202374876
H	4.4678996009	5.2266053369	-8.5531999393
C	6.4657234461	4.1089701204	-7.1357218255
H	7.1904393512	2.1237783692	-9.4362072130
H	8.6666191069	2.5302555807	-8.5358832096
H	8.5987452804	1.0385153618	-9.4757765464
H	6.9365098856	3.4968278124	-6.3565357775
H	7.2486486486	4.3815426846	-7.8580031668
H	6.1217406925	5.0452438528	-6.6763390664

TS-1 (catalyst-6)

C	-0.5548742092	0.3370577583	-5.8807615892
C	-1.8721928499	-0.1761454932	-5.8517586613
C	-0.8905642772	-0.0861660584	-3.2646829822
C	-0.3456556932	1.7375256704	-5.9456546116
C	-2.9765109618	0.6780140370	-5.9019740506
C	-2.7702323320	2.0561835223	-5.9725539491
C	-1.4697452877	2.5717552881	-5.9898136660
C	0.5971767879	-0.6049891338	-5.8373161033
C	0.9771436551	-1.1742359935	-4.5847628297
C	2.0656513498	-2.0473640494	-4.4711989132
C	2.7899141458	-2.3767430356	-5.6142144304
C	2.4214846520	-1.8368277229	-6.8458605150
C	1.3356264050	-0.9512580154	-6.9838072508
C	0.1517878417	-0.7625817709	-3.4769047579
Au	0.4213863565	-1.1378775623	-1.4076706518
P	1.1982854643	-1.7915628879	0.6490344721
C	0.8233099905	-0.6432011519	1.9782104263
C	-0.1106743373	0.1556522632	2.6416625087
N	-1.3537988398	0.5179210392	2.8185003476
C	-2.4355628744	-0.0330302204	1.9376866055

C	-2.2911453192	0.4980305175	0.5128915030
C	1.0014407677	-0.3997183380	-8.3449126614
C	1.0455655869	2.3088464577	-5.9886766945
C	3.0003454684	-1.9858767519	0.6533497181
C	3.6367062978	-2.9495460421	1.4549285003
C	5.0301749593	-3.0042090691	1.4903715644
C	5.7882776170	-2.1065905868	0.7301181132
C	5.1549390669	-1.1586760493	-0.0798537995
C	3.7618462287	-1.0974870296	-0.1268814116
C	0.5508479901	-3.3486500775	1.2465476541
C	0.0148277946	-4.6183597240	1.0118423801
N	-0.4092389837	-5.5158165552	0.1684203810
C	-0.4690757477	-5.1896180544	-1.2980929226
C	-1.5468551853	-4.1379393378	-1.5553681011
C	0.3313043550	-4.1834582599	2.3386972333
N	0.4295861790	-4.3277415788	3.6329641048
C	-0.1310744348	-5.5155080297	4.3632805297
C	0.7097152039	-6.7632835296	4.0944154434
C	1.0696350799	-3.2202604406	4.4163041393
C	2.1795132314	-3.7548494995	5.3202622086
C	0.0097456581	-2.4141252360	5.1660075914
C	1.2836482815	0.2472021507	2.9527748282
N	2.3031400991	0.7485609546	3.5946132445
C	2.1670197458	1.8532062447	4.6025596745
C	1.4378938883	1.3574067585	5.8514445617
C	3.6829898206	0.2550554420	3.2612053226
C	4.4867372242	1.3476039987	2.5575428830
C	4.3758275172	-0.3065292701	4.5011704129
C	-1.7448942505	1.4966859561	3.8873130390
C	-2.6100946906	0.8119443719	4.9452665466
C	-2.3909661719	2.7432441819	3.2844806034
C	-2.5055943171	-1.5567480005	2.0097153043
C	-0.8129870667	-6.8912143855	0.6151045165
C	-2.2713094524	-7.1749624936	0.2594633484
C	0.1637301497	-7.9325776877	0.0694499686
C	0.9115401335	-4.8279023883	-1.8425815765
C	-1.6253134617	-5.6664218079	4.0798476886
C	1.5910885923	3.1130941703	3.9565692970
H	-0.7822306307	-6.1273851075	-1.7719918749
H	-2.5331065789	-4.4936020986	-1.2349687062
H	-1.5914847230	-3.9039186710	-2.6258839022
H	-1.3269949236	-3.2019795455	-1.0193484485
H	1.3077231112	-3.9072811625	-1.3911721395
H	0.8437232402	-4.6546993270	-2.9235425221
H	1.6325236050	-5.6349522072	-1.6656241788
H	-0.7187905204	-6.8634866098	1.7063433813
H	-2.9435539976	-6.4109550433	0.6703132577
H	-2.5591423342	-8.1455671838	0.6818139744
H	-2.4297004270	-7.2367458955	-0.8248576878
H	0.1135434607	-8.0130827844	-1.0243087484
H	-0.0946769816	-8.9176559895	0.4775677006
H	1.1981532105	-7.7034507254	0.3568348470
H	-0.0220079072	-5.2531065757	5.4229656004
H	0.7256591791	-7.0230585357	3.0281250505
H	0.2955110390	-7.6180557562	4.6424397191
H	1.7461077588	-6.6195551663	4.4223053792
H	-2.1718659893	-4.7593011112	4.3670747273
H	-2.0286744602	-6.5047189089	4.6605026909
H	-1.8304333047	-5.8682893903	3.0210174154
H	1.5318788737	-2.5712127156	3.6576899488
H	1.7972310859	-4.4119972255	6.1111915091

H	2.6716606445	-2.9114986835	5.8198215805
H	2.9373598978	-4.3029938072	4.7472892459
H	-0.4958374605	-3.0165351996	5.9316775219
H	-0.7467589306	-2.0244818730	4.4727561127
H	0.4850655615	-1.5659720315	5.6747389233
H	-3.3615270570	0.3688226248	2.3649571264
H	-2.2726961310	1.5937514681	0.4916599281
H	-3.1351346722	0.1529091014	-0.0974668680
H	-1.3633658997	0.1263331966	0.0479319964
H	-1.6241748917	-2.0271226925	1.5542231304
H	-3.3864894256	-1.9064843431	1.4576342222
H	-2.5963557789	-1.9029739118	3.0468358396
H	-0.7970868736	1.7886902672	4.3508001303
H	-3.5823560980	0.4956502029	4.5455895667
H	-2.8110518605	1.5189978069	5.7594916529
H	-2.1030274696	-0.0634488519	5.3710636473
H	-1.7418810684	3.2114252945	2.5332835406
H	-2.5697522054	3.4742666809	4.0824415905
H	-3.3633977845	2.5269405511	2.8230991326
H	3.2012365294	2.0763625981	4.8903083366
H	0.4243960900	1.0009261953	5.6260103583
H	1.3516165457	2.1701827609	6.5828206613
H	1.9909341912	0.5355163185	6.3228501160
H	2.2316008099	3.4555354783	3.1344786405
H	1.5320651319	3.9173974134	4.6996664929
H	0.5823543281	2.9544670598	3.5557332897
H	3.5210573159	-0.5671206329	2.5566046231
H	3.9719084018	1.7021403791	1.6555008177
H	5.4588398005	0.9389594724	2.2556329062
H	4.6805963135	2.2062334206	3.2130758748
H	4.6068531791	0.4681020808	5.2429697835
H	5.3272528492	-0.7618336731	4.1994931645
H	3.7652036530	-1.0810975425	4.9816870760
H	3.2709819618	-0.3603489770	-0.7643020701
H	5.7462866175	-0.4719986286	-0.6843922819
H	6.8763524670	-2.1573825252	0.7574971737
H	5.5274506886	-3.7537275531	2.1051103878
H	3.0556197986	-3.6564240540	2.0460723357
H	-1.7571283757	0.4733557563	-2.9631186628
H	2.3371473334	-2.4564871022	-3.4982094839
H	3.6410661918	-3.0533962175	-5.5497712275
H	2.9911248167	-2.1038066636	-7.7370223609
H	-2.0145289879	-1.2574642599	-5.8346060630
H	-3.9853355445	0.2670522752	-5.9139597467
H	-3.6209025130	2.7347365865	-6.0301251449
H	-1.3226814413	3.6506570316	-6.0541611443
H	1.7859945333	0.2938774762	-8.6811253161
H	0.9535848901	-1.2061785164	-9.0886507809
H	0.0466969587	0.1355065269	-8.3559236310
H	1.6967198324	1.8466849264	-5.2335945105
H	1.5146172656	2.1227004807	-6.9660426113
H	1.0384720680	3.3927545367	-5.8280213646

Int-1 (catalyst-6)

C	-1.0144851205	0.4815785915	-4.1348627730
C	-1.9720012250	-0.4011421377	-5.3048303124
C	1.0672080285	-1.3760416759	-6.6893681957
C	0.4655491746	-0.6955665250	-5.6313325282
C	0.7915493428	-0.9745568106	-4.2735589188

C	1.7987108091	-1.9022623788	-3.9625874553
C	2.4508015540	-2.5444289431	-5.0130503135
C	2.0884171650	-2.2868296337	-6.3417888887
C	-0.0537100196	-0.2069528861	-3.3870809238
C	-0.6899184239	0.2603354213	-5.6761877175
C	-0.7458965128	1.4977274795	-6.4644414596
C	-1.9795268410	2.0316720808	-6.7607757609
C	-3.1945568726	1.3747809231	-6.4074101805
C	-3.2055411779	0.1825240263	-5.7178088158
Au	0.2114913192	-0.0823397958	-1.3677324401
P	0.7245744425	-0.0300336248	0.8921527257
C	0.1372158968	1.4377944583	1.7589258156
C	-0.9079146940	2.3234904823	2.0234282715
N	-2.1766643157	2.6259232855	1.9216405000
C	-3.0960866168	1.7685769214	1.1047529686
C	-2.7849007232	1.9129032012	-0.3841834950
C	0.5396882976	2.1537960727	-6.8379880071
C	0.6923377904	-1.1617887644	-8.1303397585
C	2.5100992043	-0.0780011628	1.2217116561
C	3.3494935600	0.5998508048	0.3200300577
C	4.7202348834	0.6710105955	0.5716421817
C	5.2577306982	0.0572046353	1.7071324384
C	4.4263464045	-0.6381996381	2.5919262700
C	3.0533929988	-0.7088277423	2.3536813772
C	0.0429601998	-1.3584308226	1.8928996904
C	-0.4914455606	-2.6437038264	2.0117286101
N	-0.8575294806	-3.7638003810	1.4531585472
C	-0.7817443539	-3.9120301039	-0.0393413009
C	-1.8076537472	-2.9989937427	-0.7082548301
C	-0.3079368913	-1.8127950518	3.1606712500
N	-0.3640561200	-1.5437062988	4.4386649318
C	-1.0223233859	-2.4567973685	5.4323522538
C	-0.1776545145	-3.7096408077	5.6596534382
C	0.1755398349	-0.2253932886	4.9055136515
C	1.1697379868	-0.4121079984	6.0504367536
C	-0.9702257185	0.7274880727	5.2436579891
C	0.4189854662	2.6034447064	2.4755549408
N	1.3146811871	3.3460366930	3.0701349516
C	0.9972812817	4.6908481341	3.6550037614
C	0.1188121209	4.5492845586	4.8980840830
C	2.7422709787	2.8801295678	3.0935984472
C	3.6085368466	3.7621121856	2.1956141313
C	3.2606260064	2.7810838716	4.5269182200
C	-2.7555141001	3.8270192702	2.6074989935
C	-3.7283536315	3.3965859889	3.7058298550
C	-3.3677832488	4.7998182330	1.6014346151
C	-3.0937235230	0.3174269121	1.5805049454
C	-1.3305478171	-4.9329339429	2.2646954686
C	-2.7621840354	-5.3138708739	1.8915249573
C	-0.3414153401	-6.0930185698	2.1529822782
C	0.6476587720	-3.7273246430	-0.5431308465
C	-2.4788868415	-2.7140834666	5.0460283974
C	0.4711872195	5.6437747631	2.5820061054
H	-1.0727617090	-4.9528117580	-0.2233218299
H	-2.8235207106	-3.2241777446	-0.3615303546
H	-1.7721364495	-3.1355343433	-1.7958385809
H	-1.5924864689	-1.9397673809	-0.5034434200
H	1.0106924034	-2.7016783345	-0.3896535441
H	0.6804822342	-3.9225901186	-1.6220243955
H	1.3366987838	-4.4199353014	-0.0451207764
H	-1.3250253925	-4.5703834073	3.2981994626

H	-3.4452320174	-4.4599593174	1.9881951203
H	-3.1098453134	-6.1070338569	2.5649112230
H	-2.8331819861	-5.7055731377	0.8686014160
H	-0.3044952695	-6.5076465109	1.1372114632
H	-0.6584200281	-6.9030037577	2.8213671027
H	0.6715933036	-5.7861396658	2.4433459981
H	-1.0271499469	-1.8790551164	6.3645788782
H	-0.0363708221	-4.2809325142	4.7333362996
H	-0.6686614315	-4.3658764897	6.3884756715
H	0.8140697545	-3.4504719188	6.0496244934
H	-3.0368776789	-1.7717426028	4.9796794631
H	-2.9586110558	-3.3409868654	5.8071425265
H	-2.5693712302	-3.2332242449	4.0841055495
H	0.7214166558	0.1778083489	4.0400056035
H	0.6964356881	-0.8139199267	6.9546306841
H	1.5951428124	0.5619409425	6.3220264426
H	1.9937354026	-1.0760040950	5.7622434280
H	-1.5556069988	0.3752667817	6.1031285888
H	-1.6456410923	0.8454544534	4.3861690403
H	-0.5645111539	1.7129640591	5.5034083349
H	-4.0924883889	2.1848281103	1.2958240049
H	-2.8258144579	2.9617415269	-0.7001141527
H	-3.5162459686	1.3446987535	-0.9724565560
H	-1.7848917297	1.5153133169	-0.6192048415
H	-2.1493325809	-0.1877619599	1.3403967024
H	-3.8949477249	-0.2324864074	1.0722042908
H	-3.2648491289	0.2490948029	2.6622070026
H	-1.8961311249	4.3138972249	3.0787255684
H	-4.6175649902	2.8970313535	3.2996752204
H	-4.0759139018	4.2836178397	4.2495444386
H	-3.2456960115	2.7228328563	4.4259778340
H	-2.6414376530	5.0952749792	0.8335322417
H	-3.6921509320	5.7051262109	2.1295289475
H	-4.2533234186	4.3817950352	1.1054777564
H	1.9713308584	5.0729288907	3.9824650653
H	-0.8385430391	4.0600814012	4.6761989238
H	-0.0999931998	5.5386567827	5.3175291676
H	0.6304635184	3.9606738631	5.6697824907
H	1.2075261369	5.7676814298	1.7786386604
H	0.2783448904	6.6295598116	3.0221625352
H	-0.4645226701	5.2902313754	2.1321254278
H	2.7130514465	1.8710437698	2.6691476631
H	3.2239709057	3.7809271600	1.1681975680
H	4.6272849164	3.3569688808	2.1709996329
H	3.6732854408	4.7932495937	2.5666763292
H	3.3585132635	3.7616074302	5.0099094129
H	4.2574851796	2.3235047824	4.5134177655
H	2.6060467118	2.1518789505	5.1428496988
H	2.9329889769	1.0700823160	-0.5720152690
H	5.3711241596	1.1965967477	-0.1260485074
H	6.3299395152	0.1056344333	1.8949154543
H	4.8512853777	-1.1332032182	3.4644542095
H	2.4161050765	-1.2577088818	3.0465103747
H	-1.6028627853	1.3293448319	-3.7987670120
H	2.0620405661	-2.1032619626	-2.9240805466
H	3.2480103696	-3.2581734283	-4.8087665562
H	2.6173849248	-2.8046217453	-7.1432434702
H	-1.9329799168	-1.4493019535	-5.0128688953
H	-4.1367910204	-0.3532131410	-5.5409432874
H	-4.1371011757	1.8112068200	-6.7389198839
H	-2.0317247444	2.9606993641	-7.3285544257

H	-0.2430747733	-0.5996771509	-8.2384075602
H	1.4804632554	-0.6118811285	-8.6657028081
H	0.5738760092	-2.1227450923	-8.6474997513
H	1.1248732809	2.3822816245	-5.9324712793
H	1.1665351918	1.4814265324	-7.4412621244
H	0.3783652296	3.0815499747	-7.3965842574

TS-2 (catalyst-6)

C	-1.4157016152	-0.1124336429	-3.9399297023
C	-0.7648164895	0.0515945398	-5.8439794868
C	3.0598050922	-0.6151558140	2.3109208104
C	2.4770033817	-0.0674291808	1.1555273200
C	3.2809815678	0.5634380127	0.1899462237
C	4.6564476711	0.6715477554	0.3997414343
C	5.2333830168	0.1405254917	1.5574646164
C	4.4370851947	-0.5088059797	2.5072239358
P	0.6819536657	-0.0608924772	0.8803040323
C	0.0551111484	-1.3515098881	1.9620605206
C	-0.2636126353	-1.7579505284	3.2539600247
N	-0.3191487790	-1.4300496052	4.5184455128
C	0.1667328313	-0.0687057844	4.9143478041
C	-1.0161479449	0.8536407535	5.2049690666
Au	0.0946156001	-0.2167102137	-1.3480615249
C	-0.2262197155	-0.4335589769	-3.3662283145
C	0.5551876452	-0.5990214431	-5.6333731787
C	0.8175358000	-0.9090449429	-4.2712905891
C	-1.8988721104	-0.7615708230	-5.3967573347
C	-0.9830902648	1.3435921567	-6.3969219228
C	-2.3007018732	1.7257917619	-6.6410202769
C	-3.4127348719	0.8864729402	-6.3642793591
C	-3.2328263088	-0.3408414551	-5.7822460390
C	1.9911968824	-1.5813451531	-3.9202847661
C	2.8817761744	-1.9694802179	-4.9264114778
C	2.5971042870	-1.6877587995	-6.2600609741
C	1.4194653074	-1.0099327355	-6.6518227661
C	1.1494496885	-0.7716393066	-8.1132349251
C	0.1737347257	2.2371370598	-6.7366906651
C	0.0985107766	1.4378342920	1.6926691552
C	0.3801305359	2.6382607229	2.3489698354
N	1.2799857431	3.4169914231	2.8885410928
C	2.7141919269	2.9711634549	2.8934281533
C	3.2605153691	2.9064336244	4.3181446607
C	-0.9514318256	2.3235660575	1.9342646589
N	-2.2247098878	2.6081847293	1.8369501698
C	-2.8044861623	3.8352507188	2.4748356849
C	-3.4417201638	4.7552804497	1.4350455516
C	-3.1459128010	1.7090883159	1.0680480515
C	-3.0986100654	0.2694029922	1.5751280929
C	-2.8773288859	1.8208955015	-0.4323909337
C	-0.4160875234	-2.6532595333	2.1499114217
N	-0.7270460715	-3.8170523111	1.6506361550
C	-1.1265438413	-4.9696175437	2.5230139774
C	-0.0719415767	-6.0745108753	2.4585902556
C	-0.6576865444	-4.0331870515	0.1656379869
C	0.7527613758	-3.7877161324	-0.3653377727
C	-1.7454674675	-3.2179936339	-0.5316661739
C	-0.9341866592	-2.3190022599	5.5603512667
C	-2.3776996812	-2.6624548358	5.1926025781
C	-0.0326511868	-3.5183336740	5.8503501883

C	1.1673244663	-0.1532929146	6.0655085136
C	0.9566646337	4.7764826091	3.4339281531
C	0.4041309085	5.6881088025	2.3383470223
C	0.0977584489	4.6658730785	4.6938639377
C	3.5517484207	3.8456380733	1.9614004824
C	-3.7557766534	3.4490380745	3.6078865330
C	-2.5359418788	-5.4507733313	2.1827257689
H	-0.8866191942	-5.0975493827	0.0358460909
H	-2.7414031161	-3.4898012287	-0.1618591335
H	-1.7124879257	-3.4015574091	-1.6123274423
H	-1.5957412361	-2.1389318464	-0.3780640161
H	1.0570323220	-2.7374372951	-0.2605306376
H	0.7860982017	-4.0263627939	-1.4353371172
H	1.4864887065	-4.4172870469	0.1521687987
H	-1.1352214188	-4.5569968472	3.5376298888
H	-3.2673117438	-4.6343626095	2.2451320948
H	-2.8316319733	-6.2289404287	2.8969988169
H	-2.5911965754	-5.8953763134	1.1806532034
H	-0.0151731086	-6.5336423323	1.4630707563
H	-0.3380017644	-6.8689990034	3.1665583089
H	0.9228070732	-5.6959181202	2.7269020264
H	-0.9655100996	-1.6941816112	6.4613098583
H	0.1384543120	-4.1286241096	4.9540839094
H	-0.4942045299	-4.1596279951	6.6110975397
H	0.9445823439	-3.1933722277	6.2268327244
H	-2.9778967114	-1.7510109504	5.0778361231
H	-2.8281079347	-3.2685319275	5.9877617729
H	-2.4457583140	-3.2357761332	4.2600699571
H	0.6958853883	0.3098574837	4.0275146607
H	0.7126073940	-0.5336789421	6.9882393657
H	1.5441896455	0.8521042378	6.2902400675
H	2.0227729972	-0.7899760219	5.8088821730
H	-1.5877383552	0.5219965359	6.0817470036
H	-1.6943600458	0.9012373880	4.3431339585
H	-0.6505731116	1.8665213596	5.4142197945
H	-4.1459503363	2.1077610294	1.2768991599
H	-2.9557005414	2.8579550093	-0.7782105485
H	-3.6083735916	1.2157708184	-0.9835842667
H	-1.8725493174	1.4438960724	-0.6807460649
H	-2.1588600853	-0.2282947575	1.3024937938
H	-3.9129496042	-0.3031406504	1.1147810827
H	-3.2213959017	0.2210765913	2.6644193716
H	-1.9421725047	4.3507044932	2.9089678634
H	-4.6486217414	2.9271071051	3.2397007853
H	-4.0996708434	4.3575787936	4.1174678406
H	-3.2570830202	2.8105530366	4.3487709483
H	-2.7304544235	5.0208890597	0.6425646167
H	-3.7656446287	5.6813289345	1.9260983631
H	-4.3313866025	4.3071169861	0.9741662988
H	1.9310135078	5.1792010394	3.7352039102
H	-0.8593733869	4.1639534684	4.5013533115
H	-0.1222317262	5.6657615705	5.0868595410
H	0.6256309917	4.1038386222	5.4744226539
H	1.1310928362	5.8022468824	1.5251241087
H	0.1957110946	6.6824971920	2.7511506618
H	-0.5280000967	5.3030468232	1.9071506669
H	2.6906312260	1.9542883138	2.4884578154
H	3.1460688815	3.8415431938	0.9419369106
H	4.5737629908	3.4497964857	1.9232761578
H	3.6145345690	4.8841092092	2.3116813492
H	3.3423571403	3.8963426218	4.7848049172

H	4.2680200648	2.4733253703	4.2932412690
H	2.6328230951	2.2701123841	4.9543618565
H	2.8332014745	0.9694124279	-0.7184638117
H	5.2802676019	1.1616403931	-0.3468244318
H	6.3089920690	0.2182649999	1.7133753331
H	4.8924500136	-0.9385656228	3.3987560580
H	2.4488609003	-1.1242696647	3.0559349722
H	-2.1838826424	0.5334263499	-3.5250806932
H	2.2087226747	-1.7871383170	-2.8714864210
H	3.8036059228	-2.4902276480	-4.6704915749
H	3.3024464882	-1.9920588462	-7.0343578622
H	-1.7247051369	-1.8394737720	-5.3325847865
H	-4.0714977645	-1.0145984591	-5.6109968341
H	-4.4099036983	1.2178899471	-6.6522973228
H	-2.4839805625	2.7012787393	-7.0942997955
H	0.1177445765	-0.4549804206	-8.3061913098
H	1.8251122718	-0.0015939612	-8.5140006067
H	1.3341120230	-1.6847903406	-8.6939182904
H	0.9748877355	2.1510197071	-5.9916348468
H	0.6082282011	1.9610856936	-7.7086260287
H	-0.1406749746	3.2845567957	-6.8056123872

Int-2 (catalyst-6)

C	-1.3873922913	0.5541329804	-3.8518549764
C	-0.5374072478	0.1803558176	-6.2091632339
C	3.1336142283	-0.4281867869	2.2584462317
C	2.4989216999	0.1718890954	1.1578981689
C	3.2514026073	0.9069553654	0.2247733939
C	4.6245048833	1.0671813419	0.4155967341
C	5.2516837161	0.4854481091	1.5215279396
C	4.5082277051	-0.2680993633	2.4363972416
P	0.7005128927	0.1073138094	0.9036603341
C	0.1499675869	-1.2656097355	1.9279012085
C	-0.1104972201	-1.7424460273	3.2088567533
N	-0.1042238664	-1.4831966803	4.4904451029
C	0.4130222614	-0.1495898805	4.9376515821
C	-0.7417665651	0.7473354923	5.3815488255
Au	0.0952265967	0.0420647400	-1.3213756829
C	-0.2916152279	-0.0587360150	-3.3511371646
C	0.3211447175	-0.8569550696	-5.6803809803
C	0.5602134152	-0.8405436888	-4.2530658319
C	-1.6839339795	0.5806063834	-5.3437057112
C	-0.3011948571	0.9031374538	-7.4047150175
C	-1.2391865707	1.8704318338	-7.7901279081
C	-2.3902259267	2.2189756184	-7.0415539777
C	-2.5774915745	1.6532694172	-5.8175941648
C	1.6015933181	-1.6333626219	-3.7510808070
C	2.3170525118	-2.4959797747	-4.5776099586
C	1.9558410685	-2.6381072274	-5.9179436728
C	0.9553404518	-1.8460718908	-6.4897677821
C	0.5005988735	-2.1856197725	-7.8858777051
C	0.9573564806	0.7950214581	-8.2272181224
C	0.0611605885	1.5231479284	1.8220056126
C	0.2978398055	2.7062382627	2.5257268616
N	1.1714820585	3.5122359396	3.0696188887
C	2.6267344902	3.1473869123	3.0112374555
C	3.2328021888	3.0928004940	4.4123131681
C	-1.0286973556	2.3286180236	2.1540430893

N	-2.3208220744	2.5365817073	2.1315419283
C	-2.9430695123	3.6899739178	2.8581742399
C	-3.6758463005	4.6221523961	1.8945315394
C	-3.2236083880	1.6140741639	1.3700430099
C	-3.1074518963	0.1729213145	1.8611890487
C	-2.9959469166	1.7557236046	-0.1345059296
C	-0.3378502679	-2.5673804062	2.0637123250
N	-0.7102947909	-3.6903906579	1.5148649343
C	-1.1053180554	-4.8779821026	2.3395311618
C	-0.1005465367	-6.0146689422	2.1527502305
C	-0.7248407348	-3.8192967001	0.0183122638
C	0.6658803096	-3.5899951722	-0.5680860113
C	-1.8134968181	-2.9260626046	-0.5738752435
C	-0.6657518440	-2.4279194796	5.5126756421
C	-2.1357712020	-2.7271945455	5.2185334109
C	0.2310727337	-3.6555004299	5.6675535556
C	1.5016870749	-0.3102807976	5.9974372040
C	0.7935707028	4.8318162770	3.6742039902
C	0.1320521512	5.7399250723	2.6378502246
C	0.0081779320	4.6310978823	4.9704140449
C	3.3758918018	4.0824810581	2.0631362230
C	-3.8226529509	3.1884793118	4.0040827225
C	-2.5489719435	-5.2867880889	2.0517998196
H	-0.9997199301	-4.8653556793	-0.1608944238
H	-2.7992280571	-3.1820474228	-0.1666194457
H	-1.8431617363	-3.0486192006	-1.6633340327
H	-1.6125849451	-1.8638117106	-0.3716294355
H	1.0156756490	-2.5615925116	-0.4048797036
H	0.6352239753	-3.7499441190	-1.6527247795
H	1.3983778197	-4.2817838312	-0.1347339495
H	-1.0433721344	-4.5271857845	3.3753578836
H	-3.2428033688	-4.4497563975	2.2032421803
H	-2.8363612337	-6.0963615239	2.7339400643
H	-2.6757181144	-5.6660978787	1.0294631641
H	-0.1191517776	-6.4182526208	1.1319786162
H	-0.3564133459	-6.8379419910	2.8309947776
H	0.9219249747	-5.6875898310	2.3812722255
H	-0.6270156204	-1.8618080207	6.4512800199
H	0.3288593000	-4.2115081721	4.7265142730
H	-0.1896916973	-4.3355968537	6.4182613155
H	1.2374452579	-3.3681798470	5.9952092123
H	-2.7264176694	-1.8026794690	5.2060341911
H	-2.5441509637	-3.3826126978	5.9970251276
H	-2.2725942810	-3.2321163623	4.2544328014
H	0.8700626944	0.2911662594	4.0402322516
H	1.1165712309	-0.7415135619	6.9295268155
H	1.9113368105	0.6758813206	6.2485844494
H	2.3243881868	-0.9384634893	5.6348328390
H	-1.2414015365	0.3581008616	6.2782039402
H	-1.4878543004	0.8476516903	4.5818633136
H	-0.3592004186	1.7460247140	5.6250426502
H	-4.2331550275	1.9711142277	1.6052096712
H	-3.1121314582	2.7967026783	-0.4582679052
H	-3.7240949325	1.1395298035	-0.6772419192
H	-1.9881272866	1.4114735684	-0.4173333544
H	-2.1436789292	-0.2711894026	1.5834955888
H	-3.8927508311	-0.4347585599	1.3955407493
H	-3.2252941924	0.1094743555	2.9502966059
H	-2.0954551593	4.2335643370	3.2868906343
H	-4.6969046490	2.6310481607	3.6428627644
H	-4.1996077930	4.0466343346	4.5740379652

H	-3.2563827310	2.5457071440	4.6905181366
H	-3.0150784987	4.9698229047	1.0898199027
H	-4.0322626586	5.5009686517	2.4459980035
H	-4.5560214483	4.1451159797	1.4446085744
H	1.7557190441	5.2863953123	3.9395020276
H	-0.9209067900	4.0688291018	4.8098931749
H	-0.2589092158	5.6031209594	5.4021747846
H	0.6107551807	4.0871838619	5.7085390487
H	0.8050606979	5.9132349320	1.7894619127
H	-0.1037412886	6.7108417669	3.0901096538
H	-0.8022924690	5.3179649238	2.2483959783
H	2.6435607084	2.1360348665	2.5915005690
H	2.9329952123	4.0671194587	1.0593089085
H	4.4179366885	3.7506470575	1.9809793001
H	3.3879866424	5.1180256129	2.4274159605
H	3.2916215564	4.0806575673	4.8864523657
H	4.2557941869	2.7032499161	4.3418323391
H	2.6586117145	2.4251415875	5.0670012360
H	2.7648366219	1.3519364874	-0.6445773311
H	5.2073403559	1.6377565802	-0.3065549703
H	6.3255588338	0.6044748678	1.6625140461
H	5.0032242502	-0.7381711009	3.2854887988
H	2.5661595496	-1.0231040056	2.9733427783
H	-2.1408835673	1.0279258933	-3.2219513713
H	1.8310875949	-1.5843962353	-2.6865405841
H	3.1267583040	-3.0995073800	-4.1677486378
H	2.4440920531	-3.3955437658	-6.5319747159
H	-2.3712474071	-0.3098297034	-5.4354592569
H	-3.4011126747	1.9548861720	-5.1691008499
H	-3.0693944747	2.9812293617	-7.4210090631
H	-1.0479649394	2.4193560587	-8.7148249573
H	-0.3903584884	-1.6329076802	-8.1988360401
H	1.2957618440	-2.0173196590	-8.6243780645
H	0.2556657899	-3.2560983110	-7.9306961672
H	1.7686544079	0.3003295568	-7.6845757524
H	0.7862396675	0.2435829833	-9.1612023384
H	1.2958409639	1.8003196143	-8.5088070496

TS-3 (catalyst-6)

C	-1.5267126785	0.3859379142	-3.8417563665
H	-2.1543405810	-0.4228734354	-4.7492066215
C	1.0204944855	-1.6838872692	-6.5131108870
C	0.3276855175	-0.7459174969	-5.6916823444
C	0.5684520754	-0.7673940199	-4.2621328038
C	1.6780588885	-1.4937276104	-3.7693875054
C	2.4588947187	-2.2603916729	-4.6142509306
C	2.0863863489	-2.3972020263	-5.9575985175
C	-0.3556952166	-0.1529373624	-3.3426430378
C	-1.7253948350	0.5934417600	-5.3357878773
C	-0.6405212011	0.2094787654	-6.2114180548
C	-2.8372042544	1.3605143737	-5.8018992046
C	-2.8074297239	1.8469466574	-7.0871546768
C	-1.6566749010	1.6503338309	-7.8750711747
C	-0.5630762989	0.8786228562	-7.4654310938
Au	0.0019235455	-0.0743907478	-1.3118345556
P	0.6255808269	-0.0317994349	0.9117638983
C	0.1565703812	1.4620100781	1.8048730881
C	-0.8304417957	2.3953843907	2.1231639366

N	-2.0866370343	2.7588289271	2.0821496554
C	-3.0827094877	1.9511552542	1.3056913269
C	-2.8229086644	2.0754639981	-0.1952803220
C	0.6767584092	0.9151801786	-8.3216043510
C	0.5836174424	-2.0612519325	-7.9074338285
C	2.4238583417	-0.1609152140	1.1379170858
C	2.9987640676	-0.7830917088	2.2589157590
C	4.3843213460	-0.7707035562	2.4219852804
C	5.1973135516	-0.1407206759	1.4733106545
C	4.6273890097	0.4657376524	0.3496415634
C	3.2429976878	0.4514079069	0.1727765386
C	-0.0496648588	-1.3285116052	1.9565432421
C	-0.5534996468	-2.6234314202	2.1025529439
N	-0.9023790252	-3.7575177545	1.5619258812
C	-0.8530668458	-3.9142019825	0.0686524061
C	-1.9189211518	-3.0350545932	-0.5835471126
C	-0.3534257328	-1.7780144013	3.2378943593
N	-0.3659611478	-1.5046334464	4.5163462738
C	-0.9938114603	-2.4139796938	5.5329543458
C	-0.1305040223	-3.6549177314	5.7562339302
C	0.1852736049	-0.1824952095	4.9584425530
C	1.1985963121	-0.3558302610	6.0885432685
C	-0.9517063183	0.7774379011	5.3055937539
C	0.5298886677	2.6109975444	2.5061585036
N	1.4924250975	3.3082022845	3.0489529477
C	1.2673118226	4.6461774780	3.6882816637
C	0.4355658946	4.5047919115	4.9631113800
C	2.8981824425	2.7845659466	2.9679419246
C	3.7560712560	3.6811043198	2.0764148097
C	3.4837382955	2.5751997510	4.3624749612
C	-2.5705978830	3.9929907932	2.7833774010
C	-3.5233139015	3.6225386106	3.9202140754
C	-3.1649887633	4.9952791037	1.7956045994
C	-3.1416617944	0.5027498976	1.7860499790
C	-1.3270342482	-4.9314684889	2.3927315789
C	-2.7538214409	-5.3563154554	2.0497392990
C	-0.3074198527	-6.0639495559	2.2724741342
C	0.5610152967	-3.6942043479	-0.4647872023
C	-2.4543743256	-2.6933743346	5.1785893191
C	0.7427629774	5.6586358904	2.6702829894
H	-1.1181436363	-4.9639926806	-0.1033505009
H	-2.9235138881	-3.3142039260	-0.2437789013
H	-1.8757139439	-3.1454208857	-1.6738531736
H	-1.7537677965	-1.9717063596	-0.3544422484
H	0.9050506149	-2.6620491991	-0.3130919940
H	0.5771992951	-3.8811287901	-1.5454503320
H	1.2757096260	-4.3733354987	0.0155210167
H	-1.3128608659	-4.5591200254	3.4228113079
H	-3.4588544452	-4.5209583836	2.1502109411
H	-3.0667817980	-6.1515886162	2.7374402365
H	-2.8320146880	-5.7609911064	1.0323521005
H	-0.2762254602	-6.4849276517	1.2591123243
H	-0.5895732000	-6.8774008779	2.9521484540
H	0.7013536361	-5.7261728947	2.5427561654
H	-0.9880822549	-1.8255789764	6.4585405255
H	0.0113321592	-4.2245807955	4.8288839854
H	-0.6070934236	-4.3173606126	6.4890610370
H	0.8605393615	-3.3823353481	6.1384978591
H	-3.0228779994	-1.7580731883	5.1021674705
H	-2.9136311501	-3.3080555851	5.9619521015
H	-2.5574905940	-3.2347481559	4.2302580058

H	0.7169044820	0.2079345200	4.0782670316
H	0.7415112933	-0.7509651200	7.0039189044
H	1.6225622792	0.6231199939	6.3446079086
H	2.0210246400	-1.0187141338	5.7935714042
H	-1.5208986351	0.4372195500	6.1806832520
H	-1.6427068191	0.8860876951	4.4599369051
H	-0.5391280076	1.7652770432	5.5447561771
H	-4.0466364038	2.4218159445	1.5331366487
H	-2.8146537977	3.1239653162	-0.5145617351
H	-3.6125526210	1.5508614284	-0.7483465299
H	-1.8580067649	1.6194539038	-0.4687607220
H	-2.2254449948	-0.0475080083	1.5356621369
H	-3.9760118483	-0.0098939989	1.2919438132
H	-3.3017239517	0.4461693723	2.8698339727
H	-1.6674894563	4.4323198896	3.2182696010
H	-4.4521795052	3.1687382750	3.5508166903
H	-3.8032233905	4.5304569658	4.4686116048
H	-3.0514305202	2.9287033412	4.6281032921
H	-2.4549467477	5.2418194814	0.9959073239
H	-3.4114415027	5.9217427599	2.3291135471
H	-4.0944282915	4.6289332100	1.3406932521
H	2.2718005762	4.9689946342	3.9863601373
H	-0.5617499246	4.0909484332	4.7647270204
H	0.3018258889	5.4861021951	5.4340236634
H	0.9400593270	3.8490934234	5.6839846800
H	1.4606793705	5.7947692930	1.8526208908
H	0.5901057225	6.6304364798	3.1551670678
H	-0.2140721158	5.3496586497	2.2314161592
H	2.8028890335	1.8068503054	2.4854718465
H	3.3120492373	3.7914724828	1.0789651982
H	4.7464902443	3.2244789792	1.9601697104
H	3.9042125136	4.6794820039	2.5085969427
H	3.6237964201	3.5181926951	4.9064526542
H	4.4695594548	2.1032692287	4.2681131316
H	2.8475067761	1.9139647568	4.9640229928
H	2.8005191355	0.9185416868	-0.7084476735
H	5.2624482780	0.9422231678	-0.3963056920
H	6.2791397350	-0.1361418737	1.6033186405
H	4.8328576377	-1.2581728174	3.2869231986
H	2.3750204910	-1.2769458558	3.0037201557
H	-2.3313212295	0.7693267259	-3.2164995591
H	1.8793580036	-1.4745092623	-2.6971798750
H	3.3160612459	-2.8116675181	-4.2292182299
H	2.6245197739	-3.1048305905	-6.5898876908
H	-3.6613811665	1.5829941857	-5.1245939317
H	-3.6342941748	2.4416609689	-7.4724962537
H	-1.5991056212	2.1474082598	-8.8444599787
H	-0.3899620822	-1.6422674361	-8.1795157008
H	1.3158804639	-1.7576972004	-8.6666224612
H	0.5042159382	-3.1549509145	-7.9690933755
H	1.5591768973	0.5315178721	-7.8007133310
H	0.5517273059	0.3486810748	-9.2535020281
H	0.8783983204	1.9554180586	-8.6095684393

Int-3 (catalyst-6)

C	-1.4982523963	0.3905175637	-3.7886021094
H	-2.2037948364	-0.4409279225	-3.5625444089
C	0.8327635354	-1.6950429560	-6.5278672376
C	0.2913026061	-0.6729196169	-5.7014487025

C	0.6672680094	-0.6827690493	-4.2883430918
C	1.8193558440	-1.4297850382	-3.8746029129
C	2.4723612361	-2.2514028692	-4.7584888907
C	1.9256172436	-2.4265426324	-6.0469474649
C	-0.1843346374	-0.1243006466	-3.3291146969
C	-1.6233619347	0.7843399731	-5.2303494167
C	-0.6473494040	0.3406867032	-6.1661451082
C	-2.6728800394	1.6071482698	-5.6336385478
C	-2.7222338421	2.0685503393	-6.9481264482
C	-1.6784887360	1.7699205644	-7.8270520034
C	-0.6162933884	0.9361587801	-7.4638372814
Au	0.1966817381	-0.1253714713	-1.3123457676
P	0.7570764641	-0.0788633909	0.9419660958
C	0.2231766830	1.4203540021	1.7877551373
C	-0.7941462365	2.3376550040	2.0561133209
N	-2.0564898553	2.6717581227	1.9761013090
C	-3.0186197492	1.8235732964	1.2003263994
C	-2.7269098430	1.9106705146	-0.2969902135
C	0.5534190461	0.8386671760	-8.4096483901
C	0.2395601809	-2.1086587643	-7.8506780661
C	2.5447449652	-0.1757991088	1.2418582914
C	3.0846853393	-0.7784953234	2.3907067611
C	4.4621524141	-0.7394732238	2.6087495043
C	5.3012136295	-0.1027416089	1.6876046385
C	4.7665972100	0.4833389047	0.5360938627
C	3.3910095200	0.4427228107	0.3043292463
C	0.0466616786	-1.3708117442	1.9666079754
C	-0.5152765259	-2.6419886923	2.1070371714
N	-0.9082550288	-3.7601877519	1.5639703779
C	-0.8415639240	-3.9265436494	0.0727757589
C	-1.8561239759	-3.0045161324	-0.6016616210
C	-0.3097989171	-1.7974498477	3.2427329864
N	-0.3556618923	-1.5067331699	4.5159482714
C	-1.0347554522	-2.3870093925	5.5256270450
C	-0.2207156138	-3.6559813202	5.7731212511
C	0.2203865551	-0.1957241976	4.9605479134
C	1.2162513119	-0.3910949870	6.1027002954
C	-0.8978850809	0.7919933198	5.2907258590
C	0.5496996073	2.5937150986	2.4724063015
N	1.4783357010	3.3242836299	3.0292030147
C	1.2071956050	4.6791902703	3.6143733294
C	0.3443459280	4.5651335095	4.8711794350
C	2.8939079395	2.8218626334	3.0247794097
C	3.7727160895	3.6947903926	2.1302889718
C	3.4255390101	2.6824798764	4.4497509996
C	-2.5848560180	3.9104083196	2.6370177880
C	-3.5560353940	3.5435790626	3.7593942139
C	-3.1774198309	4.8756230032	1.6119135748
C	-3.0597264360	0.3886689675	1.7208318032
C	-1.4059245577	-4.9084292572	2.3911076696
C	-2.8463474293	-5.2618351312	2.0252781891
C	-0.4427623176	-6.0912625425	2.2915752380
C	0.5884670017	-3.7704024867	-0.4393451746
C	-2.4970994738	-2.6161261565	5.1436468697
C	0.6914367088	5.6425249094	2.5457427030
H	-1.1504612231	-4.9644209931	-0.0981561749
H	-2.8725465801	-3.2015213225	-0.2398657507
H	-1.8371489620	-3.1634492770	-1.6867126188
H	-1.6164712921	-1.9463260013	-0.4175086702
H	0.9692601126	-2.7490169635	-0.3008087270
H	0.6151273975	-3.9800247319	-1.5156087852

H	1.2686370406	-4.4670224682	0.0652295534
H	-1.3898790022	-4.5327872704	3.4199628139
H	-3.5105292477	-4.3925372821	2.1147977166
H	-3.2091689201	-6.0403078401	2.7077334387
H	-2.9286321698	-5.6627638974	1.0067777164
H	-0.4175824352	-6.5191680678	1.2809359847
H	-0.7761638698	-6.8857855879	2.9704368662
H	0.5774315064	-5.8033900727	2.5762044229
H	-1.0246429431	-1.7933512114	6.4477743908
H	-0.1015920993	-4.2497797096	4.8578995731
H	-0.7232336099	-4.2837279228	6.5189330439
H	0.7803182521	-3.4149791713	6.1508507473
H	-3.0326005438	-1.6621299933	5.0593416477
H	-2.9917652404	-3.2167907161	5.9162291307
H	-2.5997126096	-3.1511943330	4.1917133838
H	0.7709210899	0.1805062273	4.0856877876
H	0.7381621080	-0.7695554622	7.0145032420
H	1.6657144223	0.5762421950	6.3594232686
H	2.0226545343	-1.0784025515	5.8196530657
H	-1.4859920310	0.4693529441	6.1597274380
H	-1.5757223765	0.9141080796	4.4360211025
H	-0.4642547220	1.7704426407	5.5316226809
H	-3.9964475859	2.2812276159	1.3919924283
H	-2.7270005087	2.9500879745	-0.6453505817
H	-3.4924766018	1.3575157524	-0.8556244314
H	-1.7477496249	1.4636238389	-0.5328598913
H	-2.1248652827	-0.1464755209	1.5110227738
H	-3.8684341729	-0.1566335962	1.2192615859
H	-3.2471508437	0.3594962405	2.8013494433
H	-1.7027113314	4.3798354599	3.0829210875
H	-4.4683533242	3.0661390019	3.3788110069
H	-3.8642072519	4.4565197540	4.2837645405
H	-3.0873954388	2.8723649729	4.4910444603
H	-2.4533468793	5.1217580556	0.8248525989
H	-3.4597658096	5.8072408170	2.1179418248
H	-4.0858453100	4.4767730574	1.1422307963
H	2.1964399423	5.0343327516	3.9262489430
H	-0.6333739004	4.1109183389	4.6645398637
H	0.1675385886	5.5607222874	5.2956729015
H	0.8479149925	3.9571801717	5.6331927853
H	1.4193463512	5.7452052490	1.7317911364
H	0.5302395945	6.6341949072	2.9853409642
H	-0.2590363600	5.3115955183	2.1096471508
H	2.8327328478	1.8224245796	2.5823232828
H	3.3718693818	3.7486749504	1.1102628709
H	4.7766918294	3.2563140323	2.0797077589
H	3.8799101956	4.7152177915	2.5206747519
H	3.5373890824	3.6503517158	4.9548420517
H	4.4174239107	2.2152572239	4.4157536304
H	2.7701408192	2.0445256532	5.0560247601
H	2.9759912870	0.8965593102	-0.5970307147
H	5.4228451098	0.9647539300	-0.1879517746
H	6.3766292278	-0.0772401264	1.8609412032
H	4.8844351519	-1.2124247681	3.4946724151
H	2.4404926920	-1.2800981550	3.1124934783
H	-1.8580924985	1.2036249619	-3.1391359104
H	2.1199160261	-1.3764187045	-2.8271194715
H	3.3470985097	-2.8252236699	-4.4563797761
H	2.3636349924	-3.1828813297	-6.7016604584
H	-3.4330603716	1.9141840165	-4.9144242397
H	-3.5375669388	2.7144186604	-7.2721836169

H	-1.6693417852	2.2255805996	-8.8177729271
H	-0.7190907446	-1.6213881433	-8.0519817618
H	0.9161117386	-1.9017036127	-8.6894952581
H	0.0727819463	-3.1944915712	-7.8392819189
H	1.4415105545	0.3938366491	-7.9501398122
H	0.3051514194	0.2640968545	-9.3122876446
H	0.8246343717	1.8478128744	-8.7474084572

TS-4a (catalyst-6)

C	-0.3584572002	-0.2035087846	-3.3302709846
H	-1.5582137553	-0.7383964026	-3.4568500100
C	3.2809375439	0.4564042719	0.1925905666
C	2.4622919756	-0.1451083675	1.1648242243
C	3.0353984728	-0.7398791683	2.3018326334
C	4.4196619703	-0.7100461276	2.4729752272
C	5.2321643956	-0.0907288940	1.5167229906
C	4.6638219782	0.4875314238	0.3774915997
P	0.6663341924	-0.0414622513	0.9272770305
C	-0.0137856363	-1.3198472349	1.9889545384
C	-0.3317716605	-1.7320234349	3.2798160918
N	-0.3501120836	-1.4232188073	4.5495888438
C	0.2149884934	-0.0960619146	4.9592049256
C	-0.9116704247	0.8841330741	5.2831533134
Au	0.0308631920	-0.1299509178	-1.2873540304
C	-1.4689371206	0.5129678075	-3.8980790624
C	-1.5983539911	0.7542570613	-5.3057611183
C	-0.5864876446	0.2494871535	-6.1861965005
C	0.2718027088	-0.8279108601	-5.6823067866
C	0.5047695785	-0.9170592924	-4.2627379258
C	1.4950211371	-1.7858331034	-3.7627232052
C	2.1935499972	-2.6226453624	-4.6167699449
C	1.8131215420	-2.6844190758	-5.9611154507
C	0.8389072558	-1.8401985926	-6.5092587283
C	-0.4557478198	0.8743824487	-7.4566534838
C	-1.4724903507	1.7470240759	-7.8717105425
C	-2.5691239877	2.0821133131	-7.0676651864
C	-2.6061706303	1.6272965589	-5.7602097309
C	0.3557657653	-2.1586570873	-7.9025445782
C	0.7708040055	0.7740569800	-8.3280432003
C	0.1675201278	1.4719351225	1.7672755409
C	0.5209166504	2.6472632387	2.4351418663
N	1.4682977807	3.3705212298	2.9688358965
C	2.8777739616	2.8509656284	2.9406466060
C	3.4435702491	2.7341126743	4.3545096992
C	-0.8328803412	2.4050251084	2.0423706037
N	-2.0912811613	2.7557826411	1.9763465519
C	-2.5930041725	4.0065567496	2.6361209409
C	-3.1981747596	4.9684966753	1.6155235077
C	-3.0752209061	1.9138430819	1.2214159370
C	-3.1061462729	0.4745391005	1.7304602522
C	-2.8227642107	2.0110667879	-0.2829498855
C	-0.5432550922	-2.6011616305	2.1637704860
N	-0.9154849786	-3.7410881101	1.6521022287
C	-1.3620254370	-4.8858274410	2.5131560943
C	-0.3647379923	-6.0406135972	2.4193873429
C	-0.8721169724	-3.9402641820	0.1640250164
C	0.5427047726	-3.7561129437	-0.3792134751
C	-1.9259615453	-3.0641982053	-0.5111809320
C	-0.9921452930	-2.2971807297	5.5889717690

C	-2.4554337858	-2.5664322420	5.2386604775
C	-0.1456302556	-3.5422407610	5.8484343110
C	1.2276055765	-0.2534034347	6.0922799345
C	1.2255618034	4.7360637121	3.5418637238
C	0.7064242099	5.6939363714	2.4698928198
C	0.3808649824	4.6489377327	4.8132059055
C	3.7438329201	3.6960882521	2.0079355817
C	-3.5426638513	3.6603787277	3.7830985839
C	-2.7975353940	-5.2905538550	2.1834131390
H	-1.1547010512	-4.9900644671	0.0228220693
H	-2.9272373640	-3.2716544195	-0.1148632804
H	-1.9332253164	-3.2609566299	-1.5904205238
H	-1.7057403073	-1.9953461655	-0.3681172068
H	0.9029955725	-2.7256763460	-0.2539650838
H	0.5518599972	-3.9721204513	-1.4546186669
H	1.2490718173	-4.4332859374	0.1157298749
H	-1.3377328515	-4.4877760035	3.5333460154
H	-3.4869489134	-4.4407324614	2.2699013237
H	-3.1222403828	-6.0661581205	2.8878839780
H	-2.8874309925	-5.7141364041	1.1747270944
H	-0.3480605091	-6.4919305450	1.4188246419
H	-0.6584408246	-6.8282634714	3.1240706333
H	0.6519783005	-5.7149743796	2.6744155614
H	-0.9794744127	-1.6839889405	6.4982350622
H	-0.0376843153	-4.1584032307	4.9466379563
H	-0.6154634426	-4.1595023568	6.6238511252
H	0.8594645924	-3.2710231274	6.1932417773
H	-3.0145722791	-1.6266585083	5.1484640468
H	-2.9211597388	-3.1645067182	6.0310244276
H	-2.5640552926	-3.1207013486	4.2985347750
H	0.7502189148	0.2679058432	4.0697812033
H	0.7678305714	-0.6241773187	7.0164766535
H	1.6613018624	0.7266595047	6.3265691700
H	2.0436515559	-0.9301426664	5.8114471887
H	-1.4861055224	0.5702518414	6.1644646426
H	-1.6003399226	0.9819954416	4.4340484400
H	-0.4879188212	1.8722934461	5.5009746595
H	-4.0467693279	2.3715459919	1.4427547367
H	-2.8299878830	3.0524818773	-0.6246545390
H	-3.6059553810	1.4634412366	-0.8228996062
H	-1.8507174598	1.5633471833	-0.5457522171
H	-2.1866545656	-0.0682672553	1.4755390155
H	-3.9408127683	-0.0586468637	1.2591438721
H	-3.2481345662	0.4362451358	2.8176306143
H	-1.6964583783	4.4708706183	3.0580891981
H	-4.4683737189	3.1896043979	3.4272228788
H	-3.8293601996	4.5812114143	4.3059156434
H	-3.0651635952	2.9904630887	4.5101234414
H	-2.4880564385	5.2028549038	0.8122740715
H	-3.4621805439	5.9063256088	2.1199709322
H	-4.1194658644	4.5739787706	1.1678439189
H	2.2245504700	5.0806524719	3.8340095317
H	-0.6045591208	4.2021264540	4.6279262142
H	0.2206804864	5.6523608171	5.2256779142
H	0.8896894994	4.0467612376	5.5762762397
H	1.4208222864	5.7736386006	1.6415210959
H	0.5699646197	6.6937546511	2.8992460414
H	-0.2573317532	5.3735032478	2.0555378999
H	2.7940010411	1.8434498505	2.5205643910
H	3.3273457693	3.7218357841	0.9931049200
H	4.7463696408	3.2547467057	1.9543143117

H	3.8581128755	4.7268345123	2.3680710826
H	3.6006930566	3.7114487645	4.8285651798
H	4.4188664343	2.2343023112	4.3069113356
H	2.7858067362	2.1349715616	4.9965713397
H	2.8404539406	0.9008190567	-0.7013085533
H	5.2991068213	0.9543124171	-0.3742985725
H	6.3130974515	-0.0733014099	1.6528742305
H	4.8677652629	-1.1765994811	3.3495721857
H	2.4116268211	-1.2270649261	3.0509965295
H	-2.1602310660	1.0207634272	-3.2217643133
H	1.6795839396	-1.8115052333	-2.6872717827
H	2.9750355986	-3.2804891976	-4.2385392344
H	2.2651297402	-3.4391736163	-6.6066626396
H	-3.3771465467	1.9696938232	-5.0692508772
H	-3.3406086627	2.7505448968	-7.4468899030
H	-1.3829076611	2.2084463781	-8.8564954500
H	-0.5597913780	-1.6222939598	-8.1689398415
H	1.1160389805	-1.9464556947	-8.6650233924
H	0.1422427725	-3.2345514768	-7.9623739241
H	1.6096059469	0.2836791557	-7.8248784581
H	0.5713342957	0.2426000463	-9.2677758942
H	1.0909705450	1.7881643160	-8.6026935579

TS-4b (catalyst-6)

C	-0.0426316396	0.3564456588	-3.3376534394
H	-0.0160267932	1.6567490428	-3.6518144108
C	3.4253441991	0.6663134425	0.5185616194
C	2.5488943530	-0.0982713686	1.3090490875
C	3.0486150161	-0.8802842501	2.3640235323
C	4.4164845412	-0.8748161735	2.6387421245
C	5.2851151381	-0.0949075984	1.8674200761
C	4.7906523673	0.6704990901	0.8068720127
P	0.7742940833	0.0404535696	0.9569625508
C	0.0282474171	-1.3856041065	1.7510598122
C	-0.3726283166	-1.9905753691	2.9384629547
N	-0.4621801391	-1.8865859899	4.2381227409
C	0.1040853213	-0.6593148055	4.8874961751
C	-1.0210810407	0.2772380190	5.3258178827
Au	0.2944092432	0.2699285365	-1.2854961716
C	-1.1681713549	1.0766204980	-3.8710110941
C	-1.4904024444	1.1061390309	-5.2721250815
C	-0.6569305961	0.3772085269	-6.1841690300
C	0.2407208135	-0.6376233025	-5.6240867637
C	0.7005902082	-0.4765094164	-4.2683915209
C	1.7646340769	-1.2672156015	-3.7858711375
C	2.2952686960	-2.2807281752	-4.5645156181
C	1.6859015321	-2.5822639207	-5.7879589381
C	0.6462641711	-1.8119135890	-6.3226674121
C	-0.7125620283	0.7484079629	-7.5566696195
C	-1.7540203507	1.5913725456	-7.9720642805
C	-2.6896383499	2.1427379057	-7.0887893775
C	-2.5176551233	1.9531053339	-5.7274670109
C	-0.0680408986	-2.3573065394	-7.5347758868
C	0.3545891981	0.4174069680	-8.5698043334
C	0.1969608681	1.4051444475	1.9823538808
C	0.4858746182	2.4658458146	2.8450274838
N	1.3840691624	3.1071697072	3.5431440307
C	2.8007722876	2.6063826708	3.5327301953
C	3.2788077408	2.2953002963	4.9493568202

C	-0.8369218448	2.2731815374	2.3367062802
N	-2.0966960630	2.6155041429	2.2518241870
C	-2.6625873220	3.7399324103	3.0677916814
C	-3.2282321866	4.8426285163	2.1748397338
C	-3.0198051567	1.8878298663	1.3215801120
C	-3.0702806106	0.3917651290	1.6230818578
C	-2.6700532456	2.1956328865	-0.1343782297
C	-0.5321044368	-2.6643592110	1.6868126934
N	-0.8934460880	-3.6971655392	0.9782332682
C	-1.4289033929	-4.9440015204	1.6184594132
C	-0.4639907050	-6.1099825694	1.4049805053
C	-0.7513432228	-3.6635055886	-0.5176127058
C	0.7022321384	-3.4420619422	-0.9292753430
C	-1.7367878937	-2.6615096976	-1.1163094204
C	-1.1722498829	-2.9020815665	5.0865526060
C	-2.6215729064	-3.0673057323	4.6284207262
C	-0.3640492793	-4.1964627441	5.1748319568
C	1.0639698615	-1.0298189542	6.0174788791
C	1.0829692978	4.3716091883	4.2940055434
C	0.6038207232	5.4703151625	3.3453290067
C	0.1730301676	4.0899677941	5.4892705290
C	3.7090712377	3.5818875430	2.7863120747
C	-3.6697737213	3.2049157391	4.0858229895
C	-2.8512413955	-5.2336731243	1.1412550850
H	-1.8218887007	1.6072891582	-3.1748158918
H	-1.0441969368	-4.6693875651	-0.8399934326
H	-2.7707915220	-2.9173368183	-0.8553646948
H	-1.6435889023	-2.6566145539	-2.2089424579
H	-1.5295242105	-1.6401015336	-0.7631549459
H	1.0771776643	-2.4602392769	-0.6095334512
H	0.7832010766	-3.4730792332	-2.0229291860
H	1.3555671512	-4.2162690300	-0.5090215370
H	-1.4607402962	-4.7113780946	2.6882571356
H	-3.5172305733	-4.3783809339	1.3141491990
H	-3.2480744301	-6.0926052653	1.6962860029
H	-2.8850560774	-5.4950832104	0.0756680318
H	-0.3972630216	-6.4031072084	0.3493006533
H	-0.8266313194	-6.9837050602	1.9604101972
H	0.5441532397	-5.8688161798	1.7661201666
H	-1.1937888505	-2.4483980277	6.0848829981
H	-0.2065956786	-4.6487142753	4.1874723949
H	-0.8935616172	-4.9263060125	5.7989721488
H	0.6204836432	-4.0164927759	5.6234282569
H	-3.1563625146	-2.1105111150	4.6726932700
H	-3.1384289369	-3.7772639371	5.2850943546
H	-2.6937154596	-3.4507281313	3.6032164169
H	0.6833487772	-0.1625845597	4.0953780455
H	0.5568957831	-1.5322046268	6.8504241304
H	1.5119442282	-0.1151281802	6.4249214625
H	1.8737855512	-1.6775081125	5.6601523452
H	-1.6434653308	-0.1703469151	6.1117365768
H	-1.6666016493	0.5354596569	4.4759179717
H	-0.5934399408	1.2023844736	5.7317788453
H	-4.0084146848	2.3097705434	1.5382720369
H	-2.6667521178	3.2748820181	-0.3251419087
H	-3.4096066849	1.7274249467	-0.7964745668
H	-1.6783064793	1.7905993779	-0.3935208317
H	-2.1256599128	-0.1054324211	1.3685990275
H	-3.8579810245	-0.0746504077	1.0188747000
H	-3.2944779984	0.2037709181	2.6804508238
H	-1.8023097752	4.1434553764	3.6111096946

H	-4.5583865775	2.7756040801	3.6046864842
H	-4.0139638633	4.0297940968	4.7216418289
H	-3.2178374121	2.4418942928	4.7328577775
H	-2.4794328849	5.2052876902	1.4590604053
H	-3.5360153095	5.6880564802	2.8023940887
H	-4.1161422237	4.5144872449	1.6188118446
H	2.0576171371	4.6819902724	4.6883118705
H	-0.7912294235	3.6631594913	5.1846927069
H	-0.0291516339	5.0201911677	6.0337937127
H	0.6511965473	3.3887815930	6.1848890254
H	1.3630519876	5.6824680575	2.5831777904
H	0.4192037472	6.3931723951	3.9085417376
H	-0.3270166578	5.2024837253	2.8298535929
H	2.7599426237	1.6678916224	2.9706204765
H	3.3470066190	3.7606177612	1.7659483560
H	4.7166010593	3.1535083103	2.7201580978
H	3.7953294061	4.5463463722	3.3032483042
H	3.3753947154	3.1959403149	5.5690613282
H	4.2701354800	1.8286375568	4.8963220575
H	2.6002702255	1.5950888413	5.4530395435
H	3.0419891389	1.2579379369	-0.3143471441
H	5.4703670503	1.2634607688	0.1959800200
H	6.3529675019	-0.0973444906	2.0838726131
H	4.8086188063	-1.4862109405	3.4508014558
H	2.3818928099	-1.4960659104	2.9671541308
H	2.1382980431	-1.0890005726	-2.7760081140
H	3.1297252969	-2.8816212666	-4.2052156374
H	2.0132255156	-3.4641151899	-6.3413078871
H	-3.1439364693	2.4788609772	-5.0059483417
H	-3.4900331925	2.7772097849	-7.4663915162
H	-1.8099620603	1.8556141084	-9.0292807551
H	-1.0081154536	-1.8376302830	-7.7440836739
H	0.5552994377	-2.3207067554	-8.4371242872
H	-0.3022114532	-3.4158506515	-7.3579914980
H	1.2490550563	-0.0213065881	-8.1171989548
H	-0.0095568275	-0.2628558891	-9.3509445144
H	0.6569094882	1.3437306391	-9.0766275700

PRDT_{cplx} (catalyst-6)

C	-0.9315727469	-2.4977930870	-3.1492715900
H	-1.1316803464	-3.5122229244	-2.7985350692
C	2.4521111792	-0.2871030136	-1.2093547762
C	2.0512269550	-0.4286358855	0.1316069675
C	3.0102373309	-0.5852048815	1.1466597663
C	4.3667278011	-0.5785416132	0.8187568790
C	4.7665958533	-0.4186496299	-0.5128594576
C	3.8103386344	-0.2775448933	-1.5238608088
P	0.2801332830	-0.3361728063	0.5050681524
C	0.0494900145	-1.0971804731	2.1053898908
C	0.1215784072	-0.9625295055	3.4894228097
N	0.4377285765	-0.1883726453	4.4921730801
C	1.0255535514	1.1558417897	4.1829790202
C	-0.0161827090	2.2530271234	4.3990782991
Au	-0.9299994399	-1.1781996666	-1.2197285194
C	-1.9856693816	-1.5719220493	-3.2403706133
C	-1.7585251289	-0.2591486625	-3.8111474476
C	-0.4318081926	0.0910278680	-4.2477741466
C	0.5301197402	-0.9934750362	-4.4818620179

C	0.3369696868	-2.2347658966	-3.7802331911
C	1.3167104699	-3.2464645922	-3.8039340588
C	2.4512186415	-3.0856237954	-4.5807406257
C	2.5465616443	-1.9682713541	-5.4195150386
C	1.5940160147	-0.9403259965	-5.4286141102
C	-0.1344479185	1.4805634587	-4.3508189940
C	-1.1917044509	2.3991555923	-4.3199249263
C	-2.5226302116	2.0116205006	-4.1265001137
C	-2.7967678679	0.6912077143	-3.8092265351
C	1.6637318237	0.0546579838	-6.5610956865
C	1.2682867583	2.0390296544	-4.3635753449
C	-0.0709796605	1.3982288326	0.8062122108
C	0.3714294833	2.7230483273	0.8322798413
N	1.3772079567	3.5508849202	0.7479224689
C	2.7557977553	2.9917905051	0.5404061360
C	3.7011539759	3.4432359544	1.6514840249
C	-1.0194771372	2.4113170456	0.9603426855
N	-2.2676983769	2.7650758632	1.1116938323
C	-2.6549187035	4.1931636261	1.3628417312
C	-3.5787760718	4.7198261303	0.2661851931
C	-3.3601138027	1.7413325586	1.0210135361
C	-3.1462542510	0.5873575054	1.9978538189
C	-3.5330100986	1.2798368274	-0.4250650763
C	-0.3583473122	-2.1744444078	2.8980961231
N	-0.8158421867	-3.3904690078	2.9879958407
C	-0.9704303191	-4.0799377870	4.3139061460
C	0.0080334835	-5.2491338608	4.4207019362
C	-1.1721831802	-4.1503729086	1.7423661694
C	0.0289461145	-4.2788208163	0.8078738074
C	-2.4124673035	-3.5412293334	1.0909470227
C	0.1546958751	-0.5537379479	5.9222204643
C	-1.3372393223	-0.8193674589	6.1237267183
C	1.0859962944	-1.6707761763	6.3912662796
C	2.3200927085	1.3828390377	4.9622022287
C	1.2058855491	5.0420715293	0.7667316758
C	0.3309715756	5.5028465939	-0.3990036527
C	0.7678996372	5.5211652793	2.1510515289
C	3.2625695653	3.3239607040	-0.8618101982
C	-3.2317689576	4.3464660198	2.7701349143
C	-2.4256848001	-4.4756511753	4.5560113321
H	-1.4290409156	-5.1533005327	2.1024987105
H	-3.2609392360	-3.5241464105	1.7851309706
H	-2.7001926028	-4.1331837396	0.2132168328
H	-2.2180176799	-2.5109678015	0.7536126628
H	0.3360173743	-3.3108051856	0.3874568372
H	-0.2366129526	-4.9304323811	-0.0335278580
H	0.8886467360	-4.7230590298	1.3237436630
H	-0.6877045070	-3.3211082546	5.0512559240
H	-3.0982269652	-3.6120024341	4.4752539204
H	-2.5196164657	-4.8873233555	5.5683996917
H	-2.7662900736	-5.2528682493	3.8599352707
H	-0.2278175560	-6.0518709524	3.7101829416
H	-0.0558232812	-5.6805408444	5.4273870961
H	1.0432522756	-4.9247775645	4.2529306631
H	0.4054348012	0.3543951212	6.4840799904
H	0.9636356232	-2.5842573314	5.7955266978
H	0.8719048455	-1.9203424297	7.4375023964
H	2.1362450798	-1.3626379607	6.3237130535
H	-1.9320932018	0.0586494938	5.8419636821
H	-1.5343370426	-1.0386662315	7.1797628805
H	-1.6926845865	-1.6749151351	5.5357294979

H	1.2740320273	1.1136034387	3.1119762359
H	2.1525073362	1.4447567572	6.0444697867
H	2.7624016214	2.3387969626	4.6558705504
H	3.0518147604	0.5893378845	4.7670051867
H	-0.3033886336	2.3390377628	5.4547270527
H	-0.9195439947	2.0571531456	3.8064110015
H	0.3980934087	3.2204914244	4.0892481294
H	-4.2630843215	2.2818739914	1.3283613009
H	-3.7051562365	2.1231113002	-1.1026041640
H	-4.3865583120	0.5947943812	-0.5003637240
H	-2.6365293274	0.7439718588	-0.7759841728
H	-2.3012577850	-0.0477349957	1.7008849057
H	-4.0403533628	-0.0477986454	2.0066797894
H	-2.9752127106	0.9505479253	3.0190788101
H	-1.7107908594	4.7443574095	1.3147608269
H	-4.1861195892	3.8169411205	2.8870654525
H	-3.4250250086	5.4081219064	2.9681647766
H	-2.5307837021	3.9805807299	3.5316033982
H	-3.1326217779	4.5990441650	-0.7292778197
H	-3.7560556747	5.7895974662	0.4319781559
H	-4.5585074274	4.2255623087	0.2754135053
H	2.2176654552	5.4265775667	0.5898089633
H	-0.1930906344	5.0869515948	2.4561689490
H	0.6577828300	6.6122524939	2.1521807829
H	1.5164413136	5.2562725690	2.9082669084
H	0.7759598341	5.2061696889	-1.3565457405
H	0.2421563233	6.5956684703	-0.3875900394
H	-0.6816426703	5.0845614531	-0.3524421736
H	2.6299113345	1.9064805114	0.6149439097
H	2.5697966464	2.9539395586	-1.6279024536
H	4.2322982469	2.8354441058	-1.0176742510
H	3.4092067425	4.4022106823	-1.0056992288
H	3.8940483981	4.5233456338	1.6286385488
H	4.6668864844	2.9385520457	1.5249297350
H	3.3061487703	3.1793881859	2.6402852958
H	1.7127206445	-0.1951502545	-2.0075622929
H	4.1197128700	-0.1758717459	-2.5633588237
H	5.8269162694	-0.4217232408	-0.7637583018
H	5.1139823956	-0.7079953679	1.6009941337
H	2.7060522268	-0.7162296542	2.1852086019
H	-3.0082076709	-1.8836151559	-3.0167414677
H	1.1453100136	-4.1699039849	-3.2502195353
H	3.2167936675	-3.8596618343	-4.6133220084
H	3.3637520009	-1.9199367044	-6.1413183363
H	-3.8033749910	0.3780292122	-3.5308216108
H	-3.3216737637	2.7509232678	-4.1679068281
H	-0.9598921516	3.4583917743	-4.4444339543
H	0.7489451667	0.6470707251	-6.6623240546
H	2.5174334942	0.7393305407	-6.4708938859
H	1.8037853050	-0.4957992013	-7.5009608050
H	2.0230789588	1.2847900304	-4.1168291377
H	1.5380036865	2.4817385188	-5.3309014045
H	1.3356858073	2.8486797984	-3.6229008982

RC (PPh_3Au^+)

C	4.8740741816	3.3723598484	-6.6441861741
C	5.1451156313	2.0815257566	-7.1502217426
C	4.5309510068	1.6458869181	-8.3328090324
C	3.6515500832	2.4751065341	-9.0293203621

C	3.3802354612	3.7530537541	-8.5380839355
C	3.9882116537	4.1890688080	-7.3594613469
C	6.0495653815	1.1561500286	-6.4151843599
C	5.4845800341	0.1194647368	-5.6241545106
C	6.2971328797	-0.7585778699	-4.8732453670
C	7.6756954560	-0.6132739667	-4.9307410722
C	8.2376960861	0.3860275962	-5.7330509548
C	7.4504750039	1.2739884478	-6.4834101578
C	4.0776612353	-0.0425546716	-5.5963923957
C	2.8416094914	-0.2010928489	-5.5754658231
Au	2.8553194998	1.4241592144	-4.1524487412
P	2.5869138875	3.0548663427	-2.5644725233
C	2.8549320961	4.7196149928	-3.2423407186
C	8.0916435238	2.2962122659	-7.3841877010
C	5.5038922753	3.8639053736	-5.3663770970
C	3.7618881740	2.8434014437	-1.1922831946
C	3.4042996395	3.1991161600	0.1172133763
C	4.3389425514	3.0807200330	1.1476070558
C	5.6273639203	2.6123930828	0.8770859293
C	5.9844462072	2.2544880658	-0.4266942984
C	5.0543046729	2.3635639518	-1.4597335945
C	0.9245225020	3.0479288760	-1.8329088995
H	5.3312784689	2.0687285689	-2.4733942700
H	6.9862419654	1.8815318926	-0.6377118778
H	6.3526982311	2.5182729113	1.6848168708
H	4.0572270909	3.3514383601	2.1647485337
H	2.3982460701	3.5593488790	0.3324569665
H	1.9312176198	-0.6635221518	-5.9219027168
H	5.8328542901	-1.5375915007	-4.2707118496
H	8.3196358490	-1.2839125636	-4.3633770103
H	9.3236932854	0.4754036814	-5.7872069629
H	4.7508730762	0.6444053012	-8.7046387533
H	3.1848683656	2.1247529058	-9.9493833636
H	2.6974850432	4.4123286444	-9.0738763385
H	3.7741482278	5.1871211460	-6.9771695694
H	7.8627014775	2.0760422546	-8.4367705545
H	7.7126576429	3.3083411329	-7.1923573170
H	9.1808135702	2.3063148745	-7.2647584707
H	5.3187318449	3.1664566200	-4.5366836089
H	6.5958043155	3.9582627853	-5.4551822966
H	5.1024816858	4.8411453189	-5.0765303075
C	0.2502171903	4.2434488483	-1.15440556747
C	-0.9953504871	4.1997323384	-0.9134624006
C	-1.5657711113	2.9717046385	-0.5692634952
C	-0.8945926450	1.7789711779	-0.8594495103
C	0.3462851153	1.8134863033	-1.14937325658
H	0.6932108459	5.2024364552	-1.8113166832
H	-1.5197446094	5.1287222705	-0.6915130517
H	-2.5376650908	2.9424930107	-0.0774094340
H	-1.3412237015	0.8208635521	-0.5956145465
H	0.8694028746	0.8836876360	-1.7232454097
C	3.7231733968	5.6343656761	-2.6304920455
C	3.8963084678	6.9030408537	-3.1888931028
C	3.1969166465	7.2638485685	-4.3431793071
C	2.3261502570	6.3522566345	-4.9496129702
C	2.1634437569	5.0774494744	-4.4107503583
H	4.2670650352	5.3563533134	-1.7281441601
H	4.5776557673	7.6107399863	-2.7178106839
H	3.3315659611	8.2556712435	-4.7739210460
H	1.7807309020	6.6317311728	-5.8505901358
H	1.5063649464	4.3574159581	-4.9008126714

TS-1 (PPh_3Au^+)

C	-0.6525109755	0.3390570361	-5.9982463464
C	-1.1212474622	0.5646660825	-3.8311143315
C	-1.8285928411	-0.4325543826	-6.1968231310
C	1.5046022908	-0.7954809564	-6.7153858151
C	0.6403291332	-0.3406166557	-5.7086893926
C	0.9815780331	-0.5074481603	-4.3422258221
C	2.1811944629	-1.1226436725	-3.9735973748
C	3.0411996070	-1.5730644214	-4.9751945422
C	2.7049759775	-1.4111520622	-6.3211500757
C	-3.0270976542	0.1731514543	-6.5603945102
C	-3.0657143370	1.5593366752	-6.7468781912
C	-1.9141061333	2.3338744686	-6.5760541556
C	-0.6935696027	1.7537138293	-6.2150532025
C	-0.0290523478	0.0230161285	-3.4343304803
Au	0.0454807836	0.0645244238	-1.3443512833
P	0.4281432702	-0.0093424575	0.9256140856
C	-0.0355128538	1.5276202704	1.7809395488
C	0.5515509090	2.5739260874	-6.0475834059
C	1.1480970176	-0.6323435530	-8.1701977749
C	2.2003134381	-0.2660722160	1.2532257892
C	3.1273370379	0.5226127351	0.5503634018
C	4.4914241172	0.3830929680	0.8007532011
C	4.9381452382	-0.5506282247	1.7421184399
C	4.0189386788	-1.3420683394	2.4342745406
C	2.6493561699	-1.2021689475	2.1948243930
C	-0.4594136002	-1.3507544969	1.7721893847
H	2.7784292954	1.2464430291	-0.1884989227
H	5.2075577507	0.9994450278	0.2579340479
H	6.0051670196	-0.6626583471	1.9325730222
H	4.3660409290	-2.0720869675	3.1650048143
H	1.9348026576	-1.8204120567	2.7376709834
H	-2.0845766866	1.0408059186	-3.7499673783
H	2.4306417165	-1.2429520078	-2.9199429358
H	3.9808990329	-2.0550533938	-4.7075242607
H	3.3884668188	-1.7706453263	-7.0911773677
H	-1.7696774679	-1.5110961854	-6.0511226884
H	-3.9225949858	-0.4291587918	-6.7064420991
H	-3.9990896418	2.0416854985	-7.0371186448
H	-1.9604063373	3.4110702563	-6.7389422551
H	0.9246239149	0.4166056767	-8.4130693674
H	1.9611474474	-0.9682173611	-8.8237109782
H	0.2475343282	-1.2110822520	-8.4221657709
H	0.9790371347	2.4302701249	-5.0444892985
H	1.3267192036	2.2611049990	-6.7622541642
H	0.3533078167	3.6410975638	-6.1944615228
C	-0.8771788663	-1.2087100464	3.1045741421
C	-1.5001345907	-2.2766368063	3.7526250993
C	-1.7068043048	-3.4833300396	3.0786776598
C	-1.2933533378	-3.6255551208	1.7506273252
C	-0.6740519322	-2.5616542412	1.0949332229
H	-0.7209020101	-0.2670187572	3.6309228529
H	-1.8266985113	-2.1639319693	4.7860671249
H	-2.1967351215	-4.3131378010	3.5874505405
H	-1.4596912497	-4.5641083945	1.2226738457
H	-0.3584175044	-2.6685463412	0.0557043298
C	0.7997154587	2.1160457187	2.7414058473
C	0.3781337105	3.2650308826	3.4148144804

C	-0.8702650537	3.8252182263	3.1344844386
C	-1.7030621239	3.2402113065	2.1744522963
C	-1.2871511018	2.0967976778	1.4945635449
H	1.7737314400	1.6800825975	2.9628407887
H	1.0279674882	3.7214489560	4.1609840930
H	-1.1951497146	4.7218105350	3.6617909755
H	-2.6755126964	3.6791228090	1.9530668075
H	-1.9329031233	1.6411353087	0.7418260886

Int-1 (PPh_3Au^+)

C	2.8809580119	-1.0526491977	2.5073667566
C	2.4753303856	-0.2759608928	1.4125987436
C	3.4330409795	0.4174383231	0.6539113244
C	4.7825235932	0.3433849101	0.9976064340
C	5.1844745296	-0.4305613443	2.0911219324
C	4.2351507873	-1.1288983954	2.8414389942
P	0.7194357948	-0.0883489055	0.9642669022
C	-0.1662995517	-1.4219206787	1.8326583147
Au	0.3788072428	-0.1094655258	-1.3410656621
C	0.1097764924	-0.1507443454	-3.3539499308
C	-0.9679471073	0.4552155047	-4.0365708143
C	-0.6504318398	0.4198847040	-5.5878707397
C	0.6160325047	-0.3783551496	-5.6501568886
C	1.0118952155	-0.7241853435	-4.3268829059
C	-1.8144663978	-0.4317796773	-5.1662762146
C	-0.9211488068	1.6801874689	-6.2829277580
C	-2.2266685566	2.0651228225	-6.4640749150
C	-3.3273183003	1.2271093134	-6.0987545635
C	-3.1423933485	0.0068443709	-5.5031577035
C	2.1315795148	-1.5416152728	-4.1082571321
C	2.8293431378	-2.0130565909	-5.2184705550
C	2.4025758292	-1.6963589144	-6.5142940146
C	1.2690039692	-0.8949696907	-6.7680855047
C	0.8270272635	-0.6203048251	-8.1810807895
C	0.2435859666	2.5320623581	-6.6691781905
C	0.1677461551	1.4627136615	1.7453458520
H	3.1186369012	1.0163481688	-0.2027647872
H	5.5222602648	0.8860427587	0.4095632820
H	6.2398974077	-0.4921825074	2.3553795820
H	4.5476293080	-1.7356448193	3.6910106802
H	2.1427801262	-1.5982464347	3.0949745795
H	-1.6065257179	1.2256305675	-3.6145090641
H	2.4348184804	-1.7932355789	-3.0922795622
H	3.7101416268	-2.6400684696	-5.0847248733
H	2.9667749992	-2.0817242229	-7.3652524137
H	-1.6294851541	-1.4930104164	-5.0049442833
H	-3.9808924545	-0.6646892412	-5.3249495750
H	-4.3358259945	1.5540986650	-6.3522966162
H	-2.4337191198	3.0205036265	-6.9466457874
H	-0.1901011981	-0.2118868175	-8.2214065641
H	1.4976050366	0.0994823162	-8.6744976243
H	0.8503978950	-1.5389185696	-8.7813796403
H	0.8298888419	2.7956502481	-5.7742653208
H	0.9305782606	1.9924713689	-7.3356085146
H	-0.0756561908	3.4562191930	-7.1628420192
C	-0.7313637996	-1.2244886694	3.1011733678
C	-1.3568566807	-2.2875760294	3.7559586643
C	-1.4191969464	-3.5459675535	3.1518995199
C	-0.8587014367	-3.7446091796	1.8862224890

C	-0.2373957964	-2.6857536417	1.2245383689
H	-0.6859498479	-0.2433699599	3.5739278730
H	-1.7966634211	-2.1309276926	4.7406156990
H	-1.9096829972	-4.3724516505	3.6656042386
H	-0.9113175584	-4.7242635383	1.4117972699
H	0.1932674579	-2.8371583057	0.2331150022
C	0.9256711360	2.1073950836	2.7332930111
C	0.4373908325	3.2702664663	3.3347192605
C	-0.8036500330	3.7887321883	2.9572875274
C	-1.5604658598	3.1479793334	1.9704260117
C	-1.0754417587	1.9917150137	1.3606420561
H	1.8940214645	1.7051198792	3.0305473019
H	1.0293446981	3.7705100460	4.1007630879
H	-1.1813254934	4.6954854553	3.4291392176
H	-2.5275608779	3.5529422664	1.6733938451
H	-1.6610704376	1.4931041463	0.5864607884

TS-2 (PPh_3Au^+)

C	-0.5500978999	-0.0858054610	-4.6240105106
C	-1.2839002218	-0.6614204336	-2.6943920755
C	-2.5024494822	1.4230338418	2.3837923752
C	-1.2069029264	1.3594666682	2.9223227310
C	-0.8314087364	2.2427993706	3.9448776576
C	-1.7506837338	3.1767566195	4.4282731096
C	-3.0418374829	3.2312171036	3.8974612649
C	-3.4172458657	2.3537894768	2.8749247055
P	-0.0754846529	0.0743817657	2.3017834816
C	-0.4849606800	-1.4398076565	3.2284958215
C	-1.2444383503	-1.4039754342	4.4069796906
C	-1.4933572019	-2.5859398002	5.1087260899
C	-0.9854151374	-3.8006794856	4.6416323356
C	-0.2292831708	-3.8388216807	3.4655450037
C	0.0165635147	-2.6639605954	2.7560872108
Au	-0.1622752669	-0.2073748099	0.0045194056
C	-0.1296517435	-0.4280450725	-2.0466155987
C	1.0954869991	-0.3347298977	-2.8430682003
C	0.8792768422	-0.1196348764	-4.2341943534
C	-1.2883519846	-1.2954613981	-4.2764263128
C	2.3979892916	-0.4211172411	-2.3486308793
C	3.4782349092	-0.3330443789	-3.2337289897
C	3.2541354428	-0.1614705618	-4.5956205424
C	1.9509667077	-0.0640965799	-5.1304813588
C	-1.2218451353	1.0301809782	-5.1773192045
C	-2.5603917688	0.8679872549	-5.5370558572
C	-3.2591693950	-0.3520988889	-5.3608824787
C	-2.6417538700	-1.4278207079	-4.7753018080
C	1.7710189859	0.0748241423	-6.6206349872
C	-0.5062765805	2.3367062692	-5.3782252942
C	1.5913801204	0.5598568173	2.8563018541
C	2.1426983268	0.0717196380	4.0500884519
C	3.4077216133	0.5009532654	4.4584979441
C	4.1237967556	1.4157789764	3.6823191733
C	3.5768845601	1.9031645358	2.4907056762
C	2.3165494163	1.4745362664	2.0745959548
H	1.8914916966	1.8489364750	1.1416455591
H	4.1356636386	2.6140920606	1.8824658751
H	5.1113182257	1.7464442524	4.0032131088
H	3.8339249368	0.1176158678	5.3852152222
H	1.5875489689	-0.6439702798	4.6561546310

H	-2.2991863825	-0.4879847018	-2.3543038229
H	2.5600760907	-0.5454229746	-1.2780331634
H	4.4979526911	-0.3968774637	-2.8557196221
H	4.1030200784	-0.0949119883	-5.2776259375
H	-0.7031205719	-2.2172086627	-4.2059726313
H	-3.1579920446	-2.3799891055	-4.6567078717
H	-4.2867736293	-0.4319660577	-5.7139448962
H	-3.0862979958	1.7132068917	-5.9836892307
H	0.7264956539	-0.0467616143	-6.9301791218
H	2.1191083211	1.0588111152	-6.9678031780
H	2.3678081134	-0.6783179999	-7.1525664128
H	0.1440830431	2.5622262279	-4.5235690432
H	0.1342895300	2.3058600461	-6.2712581634
H	-1.2173904335	3.1602041876	-5.5095056520
H	-1.6427516395	-0.4579195378	4.7736054747
H	-2.0864328764	-2.5559055320	6.0225204785
H	-1.1829257069	-4.7206713713	5.1913420861
H	0.1633151671	-4.7864429619	3.0976760826
H	0.5978310992	-2.6932881999	1.8327989962
H	0.1753620751	2.2030194250	4.3609461346
H	-1.4559883033	3.8627619747	5.2220885014
H	-3.7561584291	3.9613424186	4.2771959877
H	-4.4225920829	2.3990444409	2.4569305305
H	-2.7903641869	0.7417297786	1.5811463083

Int-2 (PPh_3Au^+)

C	1.4234758804	-1.1416367510	-6.5872910023
C	0.5300403127	-0.4816341091	-5.6925494008
C	0.7878597612	-0.5212682657	-4.2660609115
C	2.0397941485	-0.9926399294	-3.8349648156
C	2.9621192617	-1.5118577515	-4.7347255402
C	2.6296637424	-1.6341395374	-6.0875487989
C	-0.2313235773	-0.1349989641	-3.2937572741
C	-1.4768017235	0.1429246511	-3.7364431026
C	-1.8015230081	0.2368515222	-5.2306021453
C	-0.6154233627	0.2857414427	-6.1231472640
C	-2.9908063167	1.0153995219	-5.6036538811
C	-3.0032593118	1.7554622048	-6.7466411174
C	-1.8175552473	1.8588005660	-7.5151758385
C	-0.6327133595	1.1736146967	-7.2299213533
Au	0.1385521408	-0.0493151048	-1.2554366577
P	0.6187950209	0.0174340447	1.0071471587
C	0.1603478922	1.5846621708	1.8165767610
C	0.5888462238	1.5301380776	-8.0394382622
C	1.0585854816	-1.4762834385	-8.0136470091
C	2.4061037168	-0.1836091628	1.3115402107
C	2.9036278750	-1.0226619483	2.3180618660
C	4.2820405016	-1.1130162927	2.5297054865
C	5.1642755658	-0.3663244986	1.7456005553
C	4.6702695239	0.4707845517	0.7393731652
C	3.2966741543	0.5582252327	0.5169753366
C	-0.2000895659	-1.2934053792	1.9723363343
H	2.9095812612	1.2061129561	-0.2718624596
H	5.3570413483	1.0532770280	0.1254853021
H	6.2383369137	-0.4380515759	1.9154446724
H	4.6654537772	-1.7684024388	3.3114683593
H	2.2183378590	-1.6050992731	2.9336525104
H	-2.3397948406	0.2426433299	-3.0782230606

H	2.2575444165	-0.9829140783	-2.7669429090
H	3.9241726340	-1.8780945604	-4.3769666660
H	3.3094894999	-2.1513296192	-6.7659239851
H	-2.1689192172	-0.8228051603	-5.3418742643
H	-3.8544605680	0.9754732784	-4.9387270067
H	-3.8874220712	2.3193442959	-7.0408546832
H	-1.8138406388	2.5479642734	-8.3621161419
H	0.0316846215	-1.1968206024	-8.2693429447
H	1.7390772954	-0.9982824543	-8.7314488293
H	1.1518510197	-2.5607377044	-8.1641664984
H	1.5164035362	1.2578590990	-7.5255567842
H	0.5869596746	1.0354965434	-9.0195730627
H	0.6035482558	2.6118663176	-8.2239907381
C	-0.6299406112	-1.0795198299	3.2904832427
C	-1.2054694127	-2.1270466333	4.0127465154
C	-1.3509057146	-3.3873911020	3.4273682807
C	-0.9253387144	-3.6027302624	2.1129830083
C	-0.3554864139	-2.5590093643	1.3840591483
H	-0.5194699638	-0.0969322038	3.7495316444
H	-1.5417086402	-1.9565029335	5.0352800088
H	-1.8017148929	-4.2018833578	3.9938998822
H	-1.0437334284	-4.5835439843	1.6529644465
H	-0.0318736431	-2.7223043870	0.3545160301
C	0.9783131273	2.1864469477	2.7840960607
C	0.5593078388	3.3591433469	3.4168203584
C	-0.6721558870	3.9321294818	3.0898246031
C	-1.4876460244	3.3360615617	2.1223637242
C	-1.0720920659	2.1688398859	1.4826682441
H	1.9401238823	1.7422656498	3.0407110512
H	1.1975249751	3.8248051704	4.1674851128
H	-0.9957688725	4.8472516921	3.5852979729
H	-2.4462104512	3.7849697862	1.8629753872
H	-1.7013426373	1.7066776586	0.7201401488

TS-3 (PPh_3Au^+)

H	-1.0791354274	-1.7977441309	-3.5427066880
C	-1.5124006961	-0.7696690274	-4.0372510697
C	-1.2910741575	-0.8292990371	-2.5259906043
C	1.9635333102	2.1309267450	2.1298047318
C	1.5234618705	1.0433626376	2.9025334220
C	2.2391642739	0.6670361029	4.0477808519
C	3.3829453695	1.3783674591	4.4176553738
C	3.8127634583	2.4650101370	3.6526228855
C	3.1015013928	2.8415315607	2.5088394146
P	-0.0063275603	0.1910988059	2.3956352052
C	-0.0370174518	-1.3749009301	3.3256638641
Au	-0.1010673165	-0.0996324856	0.0975404890
C	-0.1364304619	-0.3438562405	-1.9525712795
C	-0.4679022040	-0.1687296634	-4.8387551902
C	0.8660641951	-0.1271340369	-4.2602048941
C	0.9780679515	-0.0368757550	-2.8191848632
C	2.2365535166	0.2680667318	-2.2524325451
C	3.3677673717	0.3646823023	-3.0426687450
C	3.2799710616	0.0705840464	-4.4090071785
C	2.0606977034	-0.1983929409	-5.0348359278
C	-0.8628638530	0.4308706486	-6.0674703088
C	-2.1582694024	0.1989886565	-6.5392142846
C	-3.1119919526	-0.5614380532	-5.8350328002
C	-2.8169033229	-1.0155002682	-4.5726288185

C	2.1033774835	-0.6998771470	-6.4594379713
C	-0.0088972495	1.4185495949	-6.8230583896
C	-1.3754591229	1.1921548368	3.0612786714
H	1.4102618839	2.4211741606	1.2345145095
H	3.4365966802	3.6879710570	1.9096786418
H	4.7051369367	3.0179207411	3.9451757188
H	3.9383695012	1.0815720116	5.3070690106
H	1.9067365370	-0.1807096152	4.6470475313
H	-2.1273845363	-1.2397800395	-1.9623715790
H	2.3044242504	0.3719011786	-1.1690120982
H	4.3338763229	0.5962212819	-2.5954984917
H	4.1933620287	0.0164271112	-5.0036399675
H	-3.5625810518	-1.5142660988	-3.9539043409
H	-4.1004761853	-0.7239951131	-6.2624531162
H	-2.4518319810	0.6592574950	-7.4838332231
H	1.1452671054	-1.1101747330	-6.7935455868
H	2.4080959979	0.0831787898	-7.1661245615
H	2.8513266220	-1.5012609467	-6.5324327938
H	0.8404559218	1.7729401704	-6.2301226947
H	0.3787772349	0.9981046289	-7.7599049932
H	-0.6218592648	2.2889028015	-7.0919245724
C	-0.6967509617	-1.4892221081	4.5581707981
C	-0.6517665987	-2.6954354085	5.2612152126
C	0.0497289147	-3.7862528748	4.7411033822
C	0.7061404111	-3.6754941730	3.5110393112
C	0.6604604870	-2.4756234290	2.8014675469
H	-1.2463641747	-0.6406044459	4.9651005436
H	-1.1673731125	-2.7819024856	6.2173059294
H	0.0810280236	-4.7260147213	5.2919291841
H	1.2489694594	-4.5270824716	3.1015282419
H	1.1652411539	-2.3903215171	1.8375090916
C	-1.1762810713	2.1415247547	4.0742064981
C	-2.2659991504	2.8495452960	4.5868477136
C	-3.5521716893	2.6118557138	4.0957377459
C	-3.7529426769	1.6669140842	3.0841392598
C	-2.6683656224	0.9621349215	2.5631993993
H	-0.1738531951	2.3291647435	4.4588432317
H	-2.1079353363	3.5885140611	5.3718979716
H	-4.3995370451	3.1667579610	4.4977040686
H	-4.7551472418	1.4841637535	2.6972512223
H	-2.8208946704	0.2305204851	1.7678739627

Int-3 (PPh_3Au^+)

C	3.4131060997	0.4283543526	0.5931482114
C	2.4805190990	-0.2837054124	1.3661685653
C	2.9236324354	-1.1171578264	2.4028288538
C	4.2910551854	-1.2318181806	2.6650910307
C	5.2157563786	-0.5155207111	1.9013041715
C	4.7760062280	0.3157622215	0.8657803327
P	0.7099022622	-0.0497938611	1.0090946267
C	-0.1664254799	-1.3811578999	1.8889081933
Au	0.2778302402	-0.0362963943	-1.2837598716
C	-0.0840106218	0.0095702408	-3.2940483947
C	-1.4066552645	0.5014895916	-3.7528538568
C	-1.5345733098	0.9421554058	-5.1801634172
C	-0.5600957224	0.5304726735	-6.1253909255
C	0.3957110055	-0.4885048419	-5.6845075485
C	0.7760583834	-0.5178319328	-4.2826268288
C	1.9190587490	-1.2696387399	-3.8794008864

C	2.5741256254	-2.0831654442	-4.7783022904
C	2.0314998405	-2.2338992535	-6.0642767047
C	0.9393697142	-1.4869831235	-6.5305721117
C	-0.5209536931	1.1735002066	-7.3963809224
C	-1.5707872799	2.0357904375	-7.7316867056
C	-2.6120170350	2.3146193646	-6.8450193747
C	-2.5714417845	1.7979309891	-5.5520665949
C	0.3440811690	-1.8731686774	-7.8621038943
C	0.6501480783	1.0948591282	-8.3452055408
C	0.2295467109	1.4993670845	1.8362284929
H	-2.0725404275	-0.3706248740	-3.5579057288
H	3.0690325354	1.0741133031	-0.2170599076
H	5.4963810373	0.8740014021	0.2683278511
H	6.2813552193	-0.6065783923	2.1103039368
H	4.6329412972	-1.8823833759	3.4697009594
H	2.2045274750	-1.6764679940	3.0010875169
H	-1.8055051820	1.2682042511	-3.0716244867
H	2.2143242573	-1.2334478177	-2.8301243981
H	3.4437793509	-2.6654578922	-4.4778656977
H	2.4648135731	-2.9798028267	-6.7341216474
H	-3.3254506487	2.0855829362	-4.8185690617
H	-3.4174682780	2.9851108812	-7.1430019321
H	-1.5494646199	2.5297268909	-8.7040187374
H	-0.6139436277	-1.3781495540	-8.0492952120
H	1.0184208805	-1.6484638322	-8.6986106828
H	0.1720539326	-2.9583257832	-7.8726502106
H	1.5381212726	0.6482956048	-7.8861795167
H	0.4095371876	0.5235844947	-9.2522854201
H	0.9175920390	2.1086665102	-8.6715928656
C	-0.6735960384	-1.1943760475	3.1832686532
C	-1.2960237568	-2.2552069022	3.8444915324
C	-1.4128994351	-3.5002538204	3.2212462489
C	-0.9099470944	-3.6881326988	1.9300468687
C	-0.2915848849	-2.6316454962	1.2619718283
H	-0.5860182919	-0.2234759189	3.6709525748
H	-1.6914450397	-2.1069767780	4.8490492087
H	-1.9011486867	-4.3247597318	3.7401666265
H	-1.0057414809	-4.6571327426	1.4407849322
H	0.0949601062	-2.7752490441	0.2513241940
C	1.0411295745	2.1018108612	2.8081028264
C	0.6080466950	3.2645112734	3.4500421990
C	-0.6306974855	3.8245127763	3.1288780133
C	-1.4411819316	3.2254430723	2.1587574730
C	-1.0117137261	2.0692843322	1.5087934479
H	2.0077578268	1.6666558780	3.0616242922
H	1.2412134240	3.7321430691	4.2035941898
H	-0.9647968507	4.7318499962	3.6314558358
H	-2.4066032953	3.6630642876	1.9060132870
H	-1.6399401284	1.6029088891	0.7478386029

TS-4a (PPh_3Au^+)

H	-0.3555680566	-1.7094703835	-2.1521395420
C	-1.3085892115	-0.8830711738	-2.6153887989
C	-0.1195819156	-0.4394273025	-1.9539953506
C	-2.8071308358	-0.9746987988	-4.5556521369
C	-1.5271551312	-0.7233997209	-4.0294248545
C	-0.4973575083	-0.1224928040	-4.8177906043
C	-0.8817969269	0.4695206182	-6.0520889370
C	-2.1686216117	0.2085139429	-6.5427145862

C	-3.1099580628	-0.5518726257	-5.8404759718
C	0.8589940847	-0.1013410294	-4.2554362456
C	1.0051058811	-0.0906735255	-2.8255860942
C	2.2663719140	0.1392558946	-2.2466606239
C	3.3933817462	0.2688246447	-3.0435399792
C	3.2766049973	0.0540878097	-4.4189206426
C	2.0425217084	-0.1665516864	-5.0436583483
Au	-0.0794725898	-0.2015250115	0.1154618499
P	-0.0117045429	0.1942690253	2.3932309581
C	-1.4103151412	1.1957389936	2.9892273166
C	2.0696177440	-0.6098688406	-6.4874617504
C	-0.0478782025	1.4863944886	-6.7928326220
C	1.4968261949	1.0985579021	2.8681969981
C	1.9266565141	2.1556391835	2.0488953315
C	3.0489971916	2.9019479956	2.4050659559
C	3.7538533870	2.5916484438	3.5725542879
C	3.3334353724	1.5358197831	4.3846030896
C	2.2055888888	0.7886403635	4.0376756499
C	-0.0210567062	-1.3310031580	3.3872508459
H	1.3787683311	2.3945439942	1.1353654391
H	3.3770468297	3.7242151350	1.7695726243
H	4.6343695981	3.1722013212	3.8468617981
H	3.8841334354	1.2908962238	5.2924955313
H	1.8807868947	-0.0352758962	4.6733294501
H	-2.1490215177	-1.2146646265	-2.0007876327
H	2.3459618468	0.1692189312	-1.1589364834
H	4.3694433648	0.4545987732	-2.5972748529
H	4.1794233868	0.0192689779	-5.0312388673
H	-3.5598340121	-1.4567618720	-3.9313053088
H	-4.0923737208	-0.7412510654	-6.2706616266
H	-2.4546938091	0.6514122310	-7.4982693192
H	1.1094361961	-1.0143492758	-6.8223581032
H	2.3580758733	0.2011565015	-7.1689989587
H	2.8229091437	-1.4015293635	-6.5996697302
H	0.8158414480	1.8242337366	-6.2112598499
H	0.3126673400	1.1076058618	-7.7580428188
H	-0.6711725619	2.3649771914	-7.0077900731
C	-0.7240406699	-1.4163030377	4.5979625806
C	-0.6643905114	-2.5895085977	5.3539794768
C	0.0946185930	-3.6747735647	4.9086126428
C	0.7953211777	-3.5922549666	3.7006940830
C	0.7355304227	-2.4261470163	2.9381070522
H	-1.3178029213	-0.5717725873	4.9472128313
H	-1.2135260158	-2.6542919705	6.2929030222
H	0.1369721940	-4.5887133807	5.5004775383
H	1.3837980705	-4.4397332848	3.3501473152
H	1.2766585751	-2.3626561261	1.9924270553
C	-1.2419894720	2.1934885231	3.9602789236
C	-2.3514898786	2.9031474923	4.4257531215
C	-3.6262316147	2.6185732976	3.9298099251
C	-3.7961385542	1.6244077139	2.9606156097
C	-2.6918579135	0.9172553898	2.4865500478
H	-0.2485245937	2.4175517657	4.3485470391
H	-2.2178309006	3.6802431820	5.1777763125
H	-4.4889969613	3.1752012432	4.2948712443
H	-4.7895278487	1.4045700383	2.5704320893
H	-2.8211807264	0.1458422907	1.7253993534

TS-4b (PPh_3Au^+)

H	-1.0994065811	1.1161104061	-2.2484329593
C	-1.4944798632	-0.0879071829	-2.6279559300
C	-0.2384253625	0.1547245949	-1.9834876880
C	-2.9442718567	-0.2600758878	-4.6071185245
C	-1.6524686040	-0.1817640561	-4.0583346865
C	-0.4928946941	-0.0488643296	-4.8853135893
C	-0.7044587896	0.2809345021	-6.2538046073
C	-2.0054537848	0.1907262698	-6.7665604921
C	-3.1129895064	-0.1365411957	-5.9771017009
C	0.8210688906	-0.1731068201	-4.2440538491
C	0.9364646789	0.1629728886	-2.8509473452
C	2.2084263839	0.3089201273	-2.2643527550
C	3.3535068734	0.0243719151	-2.9907537114
C	3.2228843559	-0.5208596305	-4.2713901943
C	1.9826063912	-0.6638029435	-4.9047023121
Au	-0.1186861570	0.2020754390	0.0994868125
P	0.0325883252	0.1942707766	2.4073863065
C	-1.4643772785	0.8443586121	3.2149512485
C	1.9445063924	-1.4729460301	-6.1797878070
C	0.3549273450	0.8678474553	-7.1546232737
C	1.4187079714	1.2076858295	3.0138119604
C	1.6812188562	2.4323078942	2.3780105835
C	2.7004659316	3.2588415008	2.8494096095
C	3.4677330026	2.8643362064	3.9499038913
C	3.2136878210	1.6433598033	4.5795464050
C	2.1905244937	0.8134873954	4.1162616742
C	0.2866607774	-1.4725097951	3.0946602935
H	-2.3787827293	-0.2182153256	-1.9997189442
H	1.0846078594	2.7371371383	1.5161513413
H	2.8999121024	4.2092888840	2.3550800602
H	4.2679512043	3.5083184177	4.3139675422
H	3.8134902806	1.3336818604	5.4350611002
H	1.9953889574	-0.1389084888	4.6092954918
H	2.2713382951	0.6028910501	-1.2156678451
H	4.3388793475	0.1450926174	-2.5426995009
H	4.1128268699	-0.8821526733	-4.7897343804
H	-3.8018187608	-0.3838743775	-3.9450119789
H	-4.1026360583	-0.2128705454	-6.4252390057
H	-2.1597843460	0.4251203862	-7.8212587499
H	0.9264735978	-1.7380182919	-6.4810920602
H	2.4302832168	-0.9571635776	-7.0183646431
H	2.4981639563	-2.4082246115	-6.0186120256
H	1.2570516894	1.1596069617	-6.6070327441
H	0.6481756673	0.1796305517	-7.9583478169
H	-0.0495522324	1.7672244848	-7.6381207147
C	-0.3283906787	-1.8759765633	4.2891016023
C	-0.0664821871	-3.1449333242	4.8105155965
C	0.8078817754	-4.0098247511	4.1476824752
C	1.4212199786	-3.6099511141	2.9559927740
C	1.1591054554	-2.3470184402	2.4261891999
H	-1.0124364375	-1.2040077864	4.8075634386
H	-0.5483129748	-3.4576360223	5.7365313700
H	1.0083144789	-4.9997966237	4.5566793785
H	2.0996352793	-4.2857860849	2.4360037898
H	1.6306701083	-2.0371421198	1.4919180818
C	-1.3962326768	1.7230485420	4.3050779144
C	-2.5728026733	2.1555825433	4.9221772586
C	-3.8135432910	1.7117104847	4.4591245760
C	-3.8834876533	0.8355295500	3.3707390521
C	-2.7137690753	0.4064613712	2.7454696052
H	-0.4295296549	2.0699543146	4.6695808103

H	-2.5174250681	2.8409414440	5.7675371275
H	-4.7286647285	2.0511352245	4.9436939789
H	-4.8511259848	0.4902722601	3.0074990017
H	-2.7659511262	-0.2745898208	1.8939840883

PRDT_{cplx} (PPh₃Au⁺)

C	-3.0527707213	-0.3737930747	-3.1823342898
C	-1.8285661414	-0.9598873763	-3.5561349865
C	-0.8170195534	-0.1943072565	-4.2312124159
C	-0.9611957957	1.2215374017	-4.2168389269
C	-2.1948349214	1.7670298245	-3.8407183751
C	-3.2597120308	0.9818503328	-3.3866805853
C	0.3300574295	-0.9130192000	-4.8001589128
C	0.6875178727	-2.1772951505	-4.2245374233
C	-0.2446693472	-2.8437586253	-3.3400179058
C	-1.5117665203	-2.3003930485	-3.1108651780
C	1.8710235801	-2.8382890156	-4.6004352326
C	2.6671050421	-2.3093516673	-5.6031919847
C	2.2253314812	-1.1771066188	-6.2961141898
C	1.0582854700	-0.4873018654	-5.9480368593
Au	-0.1161515560	-1.6955995001	-1.3194702281
P	0.6746265542	-0.4774721928	0.4370487602
C	0.4541504276	1.2953469642	0.0898329301
C	0.5649024885	0.5657563517	-6.9119882810
C	0.1871518350	2.1805311585	-4.4177166134
C	2.4488291655	-0.7387554934	0.7260991113
C	3.3027069072	-0.8548197981	-0.3832386814
C	4.6764503433	-0.9891219958	-0.1898189924
C	5.2017773152	-1.0166074076	1.1066175344
C	4.3524727595	-0.9095155789	2.2106684785
C	2.9750608833	-0.7690017484	2.0258451172
C	-0.1829740006	-0.8381491596	1.9951757216
H	-0.0405890573	-3.8815334147	-3.0686056534
H	2.8910788165	-0.8430573668	-1.3943197462
H	5.3380898686	-1.0799727282	-1.0506395422
H	6.2754688296	-1.1283294275	1.2555659958
H	4.7608697114	-0.9370665487	3.2204596089
H	2.3132730437	-0.6875887734	2.8880209617
H	-2.3013075344	-2.9088960572	-2.6658245581
H	2.1259953783	-3.7856235640	-4.1241493531
H	3.5864805890	-2.8106467371	-5.9034119768
H	2.7835505050	-0.8393208612	-7.1709841855
H	-3.8101602916	-0.9895170319	-2.6968488821
H	-4.2106111322	1.4436534690	-3.1238931737
H	-2.3076757327	2.8520571737	-3.8695595822
H	-0.4780656326	0.8456612304	-6.7309067866
H	1.1742660485	1.4787144446	-6.8846733674
H	0.6312508103	0.1692414520	-7.9338939975
H	1.1530864472	1.6703833131	-4.4808620846
H	0.0652871662	2.8037136287	-5.3132431424
H	0.2251587697	2.8590682330	-3.5531518382
C	-0.6866291026	0.1844083153	2.8115596029
C	-1.3177861118	-0.1407743879	4.0148965574
C	-1.4419026545	-1.4762191741	4.4046006663
C	-0.9384385332	-2.4967490173	3.5899666086
C	-0.3153512816	-2.1821682063	2.3838200280
H	-0.5906844989	1.2270524023	2.5093808544
H	-1.7135345531	0.6531967028	4.6473680236
H	-1.9364890029	-1.7251406805	5.3430613293

H	-1.0381964481	-3.5386231015	3.8926834591
H	0.0701407877	-2.9766847593	1.7426602134
C	1.3776781146	2.2363845984	0.5721527991
C	1.1662615122	3.5969149174	0.3422541116
C	0.0367644015	4.0224706447	-0.3628739416
C	-0.8808335975	3.0853936518	-0.8471984795
C	-0.6737371322	1.7234993447	-0.6298555923
H	2.2603757419	1.9070712805	1.1204149222
H	1.8853607285	4.3251888595	0.7158150758
H	-0.1259539047	5.0855898739	-0.5386285051
H	-1.7594594682	3.4114901763	-1.4023044769
H	-1.3854237423	0.9986171501	-1.0302569042

Final Product

C	-0.5857325480	-2.3446059946	-3.1606963849
H	-0.4619135704	-3.1606356484	-2.4471988890
C	-1.7395360909	-1.6227876826	-3.1999026091
C	-1.8559987434	-0.4680570499	-4.0442162480
C	-0.7570526576	-0.0964028393	-4.8915123327
C	0.2977817675	-1.0867744743	-5.1084272939
C	0.4549045177	-2.1200499465	-4.1229239451
C	1.5673500496	-2.9866795680	-4.1725310516
C	2.4632272763	-2.9186026728	-5.2256566434
C	2.1923551693	-2.0534742320	-6.2934485530
C	1.1119708662	-1.1674772413	-6.2786324022
C	-0.7257100325	1.2478134160	-5.3727019725
C	-1.8695838031	2.0405302752	-5.2454041486
C	-3.0244717184	1.5859102183	-4.5956122600
C	-2.9950043075	0.3600416512	-3.9527800326
C	0.7693163411	-0.4801693987	-7.5821742379
C	0.5351892961	1.9328443059	-5.8520593386
H	-2.5701149831	-1.8621628655	-2.5339859381
H	1.6837375780	-3.7386504875	-3.3904660099
H	3.3250645844	-3.5848870874	-5.2654270111
H	2.8109257600	-2.1035057377	-7.1917916298
H	-3.8323390887	0.0357768025	-3.3330944445
H	-3.9044830497	2.2258672894	-4.5304381304
H	-1.8364642596	3.0648901350	-5.6216439428
H	-0.2374824906	-0.0495796622	-7.5716198536
H	1.4789263103	0.3174249898	-7.8411759804
H	0.8093155485	-1.2190207931	-8.3946803970
H	1.4322141644	1.3362522631	-5.6550677907
H	0.5088400870	2.1669112341	-6.9250497139
H	0.6447676955	2.8877597352	-5.3191927452

Substrate (9)

c	-2.2803965652	1.0392528657	1.8946788365
c	-1.2655897580	0.1160767813	2.2022361179
c	-1.4691020791	-0.7708557607	3.2726871702
c	-2.6567743497	-0.7458413270	4.0070893081
c	-3.6603460881	0.1720369656	3.6864833184
c	-3.4649304365	1.0673638832	2.6301383811
c	0.0035063245	0.0879947781	1.4308184153
c	0.0247305730	0.0592426365	0.0156218706
c	1.2597211574	0.0882707471	-0.6515748496

c	2.4621460885	0.1262003549	0.0515691674
c	2.4449009299	0.1364246764	1.4482821306
c	1.2261051370	0.1188086900	2.1238592906
c	-1.2220528423	-0.0722211359	-0.7851874465
c	-1.5843241932	0.8937653364	-1.7600180838
c	-2.7619296793	0.7108806704	-2.5159474784
c	-3.5728642923	-0.4011889464	-2.3126649854
c	-3.2221051274	-1.3500422008	-1.3463830885
c	-2.0606037110	-1.1801504579	-0.5949189250
c	-0.8081016193	2.0729471773	-1.9554202064
c	-0.1744006095	3.0948776434	-2.1236961012
h	1.2074617442	0.1594837929	3.2135099928
h	3.3779821523	0.1698280802	2.0110106364
h	3.4084224970	0.1426804295	-0.4896606567
h	1.2659683573	0.0635774817	-1.7411862890
h	-3.0295435759	1.4646529068	-3.2555911829
h	-4.4802555671	-0.5254710871	-2.9032891541
h	-3.8541981258	-2.2218653254	-1.1784079722
h	-1.7889772889	-1.9134549880	0.1639712287
h	-0.6944119302	-1.4998128781	3.5147880568
h	-2.8010792783	-1.4496601536	4.8272531622
h	-4.5896046327	0.1902066012	4.2562365145
h	-4.2387977358	1.7928230867	2.3781277444
h	-2.1311733152	1.7413477500	1.0747768558
h	0.3971085738	3.9868230586	-2.2666899597

Int-1_a (catalyst-6) [6-endo]

c	3.6859170340	-1.1284228119	-6.0826966064
c	4.2311209788	-0.2452177310	-7.0474003099
c	3.4955890463	0.0608749651	-8.2076281760
c	2.2542262592	-0.5255546370	-8.4439428179
c	1.7324311893	-1.4324825232	-7.5170823494
c	2.4401867268	-1.7203619154	-6.3494685478
c	5.6047317125	0.2798844358	-6.9168665271
c	5.8707221365	1.6939861330	-6.9562227485
c	7.2122032357	2.1873203373	-6.9324610149
c	8.2650675522	1.2994619856	-6.8515773199
c	8.0037692268	-0.0833262523	-6.7757160221
c	6.6999578415	-0.5803242652	-6.7955060626
c	4.8097148863	2.5711126060	-6.9222198362
c	3.8103430123	3.3342880024	-6.7536981792
au	3.2875484290	3.5103147319	-4.7431746450
p	2.6825166092	3.8509680521	-2.5611775600
c	2.6410807798	5.6118003909	-2.1809230830
c	2.2640984123	6.9029341288	-2.5587203767
n	1.6050790018	7.6948329353	-3.3635223243
c	0.9163082364	7.1479288079	-4.5792108200
c	1.9392734947	6.7844751836	-5.6547097096
c	4.3584228668	-1.3769345779	-4.7848219660
c	3.7949510829	3.1170664747	-1.3347752760
c	3.3278423893	2.6366746017	-0.1005111749
c	4.2400773723	2.1616804337	0.8428395728
c	5.6105184116	2.1730457206	0.5615964190
c	6.0735117149	2.6407610198	-0.6726721127
c	5.1690682411	3.1024019521	-1.6294247723
c	1.0300508647	3.3173731429	-2.1217867865
c	-0.0722106660	2.4830742857	-2.3290252976

n	-0.6017662215	1.4647578004	-2.9439717092
c	0.2230126123	0.6881882209	-3.9335879998
c	0.3983489640	1.4726830408	-5.2309811419
c	-0.1069468126	3.5215364470	-1.3455987846
n	-0.6668550630	4.2083966788	-0.3851019614
c	-2.1118515844	4.0469417749	-0.0085700920
c	-2.3476234780	2.7073868323	0.6880723111
c	0.1611144294	5.2352814020	0.3258890049
c	0.1368727973	5.0068474882	1.8370857039
c	-0.2690343367	6.6434301753	-0.0808260983
c	3.1093975016	6.6883933344	-1.4236118251
n	3.8350163786	7.0946867517	-0.4168038106
c	4.0417762434	8.5454082243	-0.0898573174
c	2.7467468620	9.1819107828	0.4152214467
c	4.5515349413	6.0700675677	0.4159585594
c	6.0640929102	6.1944749866	0.2385043614
c	4.1023328017	6.1447408703	1.8736813777
c	-1.9767599243	0.9675394142	-2.6107733447
c	-2.8630956443	0.9506753055	-3.8548156110
c	-1.8995025383	-0.3829455776	-1.8978999608
c	1.5350753628	0.2314777791	-3.3057730732
c	1.5348166399	9.1754617213	-3.1217285990
c	0.1038667791	9.5968843252	-2.7872828024
c	2.1376285109	9.9610210360	-4.2850470329
c	-0.0216896287	5.9911451883	-4.2405654203
c	4.7273995447	9.2733949611	-1.2461209132
c	-3.0119108601	4.3239730761	-1.2124980534
h	-0.3802078242	-0.2031283433	-4.1456341725
h	-0.5660922703	1.6944018066	-5.7031088683
h	1.0092630588	0.8902199793	-5.9333576559
h	0.9192526780	2.4258966694	-5.0454975879
h	2.2411575824	1.0584099944	-3.1491298195
h	2.0321348977	-0.4702923406	-3.9817705800
h	1.3705490458	-0.2743932878	-2.3466770272
h	-2.3766757289	1.7087613301	-1.9102403667
h	-2.9091170090	1.9388114171	-4.3294454536
h	-3.8811774159	0.6623136000	-3.5652524242
h	-2.5194868557	0.2188200792	-4.5971076477
h	-1.5237494110	-1.1764211857	-2.5565951739
h	-2.9055236389	-0.6784333201	-1.5754936466
h	-1.2552592344	-0.3338421484	-1.0103737265
h	-2.2883724574	4.8445498215	0.7234567066
h	-2.0853837583	1.8590611741	0.0441336660
h	-3.4056399837	2.6085736635	0.9595992917
h	-1.7529801490	2.6318687959	1.6061676605
h	-2.8423035487	5.3358680477	-1.6023509656
h	-4.0646310270	4.2464494558	-0.9154446815
h	-2.8436017062	3.6123592187	-2.0311261024
h	1.1880798728	5.0627342570	-0.0294025955
h	-0.8606896874	5.1605193353	2.2671194909
h	0.8044791797	5.7298725489	2.3218721153
h	0.4774968614	3.9973519845	2.0971451088
h	-1.2915771025	6.8696570025	0.2476825376
h	-0.2173509937	6.7675023295	-1.1699545290
h	0.3963291522	7.3804042269	0.3853101042
h	0.3051773594	7.9840637168	-4.9401670770
h	2.5720208112	7.6379853612	-5.9205811615
h	1.4214930684	6.4438244194	-6.5601252007
h	2.5901472555	5.9660306308	-5.3080088136
h	0.5333915437	5.0804552722	-3.9796201541
h	-0.6317229896	5.7550843406	-5.1208453090

h	-0.6987607660	6.2443828360	-3.4151567746
h	2.1580894902	9.3365104764	-2.2368792741
h	-0.5774812877	9.4644117219	-3.6375568606
h	0.0944460928	10.6632474931	-2.5298770555
h	-0.2909157181	9.0369765970	-1.9302396630
h	3.1676482098	9.6464718144	-4.4959269611
h	2.1543529827	11.0263742357	-4.0241773902
h	1.5444965801	9.8644539619	-5.2037192121
h	4.7468047911	8.5278253090	0.7499928276
h	1.9457959834	9.1485123948	-0.3347817633
h	2.9226110378	10.2340867559	0.6692621721
h	2.3893161429	8.6711848037	1.3179855926
h	5.7036494052	8.8232590284	-1.4643774998
h	4.8898777043	10.3246182352	-0.9787423597
h	4.1319180268	9.2507674678	-2.1668943732
h	4.2314384386	5.1061836263	0.0072725789
h	6.3471708842	6.1149544249	-0.8186554125
h	6.5559538312	5.3806220874	0.7850806838
h	6.4538508716	7.1397616914	0.6376978990
h	4.4019804691	7.0822549598	2.3592400187
h	4.5691885170	5.3247865696	2.4331529127
h	3.0135178713	6.0388670026	1.9590856162
h	5.5285742705	3.4523369843	-2.5982906659
h	7.1399543240	2.6343074526	-0.8951169259
h	6.3188411740	1.8026468435	1.3020345253
h	3.8822845889	1.7786591252	1.7978560755
h	2.2614288573	2.6289041309	0.1245865029
h	3.1905239892	3.8323103016	-7.4984709976
h	7.3804002922	3.2619858914	-6.9845950576
h	9.29197477821	1.6613207159	-6.8502508714
h	8.8381251978	-0.7825141541	-6.7176186179
h	3.9370500729	0.7159113730	-8.9593882859
h	1.7135503687	-0.3036807042	-9.3631708482
h	0.7763554524	-1.9196794409	-7.7071253608
h	2.0196208742	-2.4108803248	-5.6171269038
h	6.5252851779	-1.6543511360	-6.7510345595
c	4.4913623641	-2.6815803642	-4.2798586194
c	5.0860595230	-2.9073120117	-3.0371535021
c	5.5457901324	-1.8316723522	-2.2720912196
c	5.4096198256	-0.5274960408	-2.7581456087
c	4.8274471163	-0.3025097208	-4.0040951479
h	4.1495493802	-3.5259705254	-4.8791763574
h	5.1984784213	-3.9266974298	-2.6693874296
h	6.0114553574	-2.0116092542	-1.3036027364
h	5.7563870827	0.3160146742	-2.1617042735
h	4.7041229015	0.7196189679	-4.3704902790

TS1_a (catalyst-6) [6-endo]

c	-0.0929981829	2.9927880476	1.7800228963
c	1.0324440801	5.0936780309	2.8993557320
c	1.0569685886	5.5302473061	1.5526615290
c	0.2955422830	8.4556982669	-0.5132488062
c	0.1767731272	7.0799632046	-0.2523988824
c	0.0197542813	6.1969202299	-1.3349761694
c	-0.0131569063	6.6772174604	-2.6435600744
c	0.1193411766	8.0467220219	-2.8923445540
c	0.2730741524	8.9342232889	-1.8241123446

c	0.2057163785	6.5855217689	1.1454970099
c	0.1861862949	5.6924925695	3.8388145185
c	-0.6457642663	6.7377034787	3.4386759945
c	-0.6286125692	7.1749502640	2.1118314733
c	2.0119927070	4.8916296008	0.6150551106
c	1.9102708600	3.5067447689	0.2982409928
c	2.8114424947	2.9023171025	-0.5932013494
c	3.8261225812	3.6552213383	-1.1750487290
c	3.9381924105	5.0166436328	-0.8706935467
c	3.0409940630	5.6233458719	0.0096626044
c	0.8079482836	2.8129083554	0.9153499903
au	0.0066322183	0.9126552029	0.3834835513
p	-0.4305225774	-1.1370608104	-0.5500321445
c	-2.0020530007	-1.8887102112	-0.1415248845
c	-2.7532468068	-3.0540601392	-0.0150656312
n	-2.7620310853	-4.3583279869	-0.0869310184
c	-1.4999433578	-5.0484643662	-0.5114304694
c	-0.8211684844	-5.7079351850	0.6878973700
c	-0.3612052068	-1.1290272228	-2.3597160126
c	0.5064068863	-0.2190381315	-2.9886524944
c	0.6536404378	-0.2532948280	-4.3758222995
c	-0.0684665312	-1.1793145205	-5.1352481584
c	-0.9486975271	-2.0706058663	-4.5111112959
c	-1.0987717655	-2.0496971110	-3.1246759525
c	0.7704153338	-2.3615493479	-0.0119134938
c	1.7892262576	-3.2616927405	-0.3359143793
n	2.4773873505	-3.8539809623	-1.2733833490
c	2.1636381370	-3.5364762400	-2.7081579847
c	1.7570875419	-4.7955964404	-3.4696444264
c	1.4844204303	-2.9578794104	1.0303192226
n	1.6922585368	-3.1042833983	2.3119449726
c	2.6788190341	-4.1075801932	2.8373114267
c	3.7830214082	-3.4333755311	3.6497686053
c	0.9639865390	-2.2465100435	3.3051053801
c	-0.5502119982	-2.3055290805	3.1175403316
c	1.5112430469	-0.8202145452	3.2808386451
c	-3.3602936456	-1.7705397097	0.1637195716
n	-4.3923356095	-1.0073015670	0.3854150737
c	-5.7687670709	-1.5734601299	0.5826257261
c	-6.6717701540	-1.1917365438	-0.5901782108
c	-4.2212746339	0.4855224488	0.3992276863
c	-3.6556149401	0.9944168718	-0.9249825034
c	-3.4159648571	0.9103149273	1.6258110281
c	-3.9572924104	-5.1840798019	0.2960978928
c	-4.3794227868	-4.8856202518	1.7345130131
c	-5.0652691153	-5.0493203991	-0.7478191156
c	-1.7608793149	-6.0124840345	-1.6679590982
c	3.6195719310	-4.7844974064	-0.9832937898
c	4.7428775142	-4.0578269366	-0.2439305577
c	3.1156410357	-6.0683017892	-0.3234082198
c	3.3212930856	-2.7788247918	-3.3562137879
c	1.9544814185	-5.2163955741	3.6012464296
c	-6.3325550464	-1.1731519532	1.9443725213
h	-5.2412204228	0.8742325437	0.5032603012
h	-3.8972393142	0.5832810992	2.5549337155
h	-3.3293087731	2.0036937209	1.6452221873
h	-2.3991771914	0.4885140487	1.5944659201
h	-2.6171001043	0.6727054869	-1.0868877369
h	-3.6562026109	2.0911187784	-0.9233570316
h	-4.2607529435	0.6528236175	-1.7731870091
h	-5.6227882496	-2.6590553667	0.5718209263

h	-5.6623247658	-1.4683706151	2.7616771665
h	-7.2957182317	-1.6765428426	2.0943618589
h	-6.5200730017	-0.0940066939	2.0145863352
h	-6.8614871462	-0.1111824551	-0.6315671062
h	-7.6441310910	-1.6855219742	-0.4716262920
h	-6.2412817694	-1.5087685319	-1.5486343094
h	-3.5878112800	-6.2164426307	0.2693355621
h	-5.4078845398	-4.0116555904	-0.8475720809
h	-5.9278852763	-5.6615849044	-0.4586232575
h	-4.7232845598	-5.3887161395	-1.7328620351
h	-3.5552815180	-5.0791579184	2.4329113933
h	-5.2204789152	-5.5313172796	2.0144099947
h	-4.7023319649	-3.8452512220	1.8673067653
h	-0.8508951692	-4.2407809638	-0.8802271834
h	-2.4070419091	-6.8494069317	-1.3773097192
h	-0.8078218558	-6.4467448542	-1.9949052101
h	-2.2161862672	-5.5010319605	-2.5248740917
h	-1.4295628625	-6.5198155163	1.1071007544
h	-0.6263980552	-4.9728980750	1.4786121937
h	0.1365014241	-6.1425061191	0.3742850694
h	1.2015610770	-2.6995572214	4.2750495767
h	2.5914577452	-0.7959108480	3.4613659375
h	1.0192304262	-0.2193388443	4.0555752370
h	1.3126422994	-0.3416505582	2.3088371155
h	-0.8716757928	-1.7725031254	2.2125950101
h	-1.0370786175	-1.8172982550	3.9705536256
h	-0.9121096592	-3.3401234329	3.0676669203
h	3.1283644865	-4.5434366968	1.9394726708
h	1.4745228846	-4.8449983689	4.5159869974
h	2.6824876340	-5.9784694360	3.9053431590
h	1.1932416893	-5.7025508675	2.9777356196
h	4.2907260622	-2.6511547405	3.0712914875
h	4.5292678235	-4.1873178737	3.9288134132
h	3.4052642217	-2.9937044134	4.5817138496
h	3.9995721576	-5.0526446458	-1.9764548087
h	2.6181589749	-5.8745454679	0.6357522101
h	3.9560645005	-6.7466966371	-0.1331114440
h	2.4034723373	-6.5867395854	-0.9777018075
h	5.1181127959	-3.2154689443	-0.8378732810
h	5.5769297901	-4.7472639757	-0.0668225154
h	4.4191272687	-3.6678807098	0.7289050323
h	1.2972856825	-2.8694647872	-2.6614498316
h	3.5681300386	-1.8708674666	-2.7910788711
h	3.0277730626	-2.4797025195	-4.3699512687
h	4.2250430707	-3.3950964749	-3.4446488618
h	2.5828687594	-5.5111168114	-3.5752511036
h	1.4412072806	-4.5132384229	-4.4817365168
h	0.9154137534	-5.3004101751	-2.9791847626
h	1.0606113251	0.5151427322	-2.4012385634
h	1.3227387158	0.4528910252	-4.8659285080
h	0.0416463281	-1.1958633113	-6.2191728012
h	-1.5236340829	-2.7777772193	-5.1079752993
h	-1.7865695665	-2.7471372705	-2.6470416157
h	-0.8804984220	2.9833558290	2.5102789668
h	2.7138894951	1.8387908075	-0.8147155148
h	4.5302482325	3.1895214833	-1.8630344925
h	4.7298078526	5.6119214406	-1.3242273661
h	1.7613393212	4.3497367721	3.2244450749
h	0.2117402862	5.3708707297	4.8794450745
h	-1.3004874865	7.2257203918	4.1600363211
h	-1.2868243057	7.9877036983	1.8038438506

h	3.1303796371	6.6851810359	0.2348656095
h	0.4299032766	9.1511258361	0.3162110842
h	0.3789435674	10.0022479952	-2.0114470393
h	0.0989234028	8.4219220090	-3.9149013189
h	-0.1479407168	5.9846848865	-3.4745262922
h	-0.0931109175	5.1286722589	-1.1439304761

Int-2_a (catalyst-6) [6-endo]

c	-0.6953702599	3.2549267261	1.5768144878
c	-0.31118159542	5.6955290204	0.9650892681
c	-0.1575912315	-2.5879290007	-3.2462866079
c	0.4010498654	-1.5470990724	-2.4856281777
c	1.2914131651	-0.6382496794	-3.0830695295
c	1.6439747021	-0.7931866739	-4.4240441236
c	1.1019203159	-1.8406476631	-5.1748366950
c	0.1958341667	-2.7308682196	-4.5885955281
p	0.0841713586	-1.3533234454	-0.7066726450
c	1.3381260417	-2.3803267986	0.0882742767
c	1.9617239439	-2.7895781075	1.2681018729
n	1.9870686054	-2.8161519821	2.5760149324
c	0.9941256314	-2.0230042611	3.3718288282
c	1.2997295677	-0.5290464800	3.2780695613
au	0.0884206503	0.8385140015	0.0215937695
c	0.0941834877	2.8361278840	0.5583561412
c	0.7569586489	5.2418657038	0.1060771645
c	0.9245121512	3.8276820335	-0.1264383302
c	-0.7990939597	4.7066540013	1.9712280883
c	-0.9028498521	6.9890429835	0.9481385553
c	-1.8751866527	7.2963152944	1.9089528670
c	-2.3666248852	6.3789756095	2.8707164079
c	-1.9049797323	5.0978830363	2.8667307651
c	1.9367778599	3.4235507939	-1.0152928093
c	2.7969224903	4.3353544944	-1.6149290747
c	2.6777160307	5.7047087685	-1.3321582957
c	1.6668262250	6.1476630868	-0.4970843230
c	-0.6272154326	8.0217636652	-0.0850993499
c	-0.1972670859	9.3034825276	0.2936090654
c	0.0257324761	10.2835173086	-0.6758918237
c	-0.1985673479	9.9978025724	-2.0246174120
c	-0.6472178668	8.7281760612	-2.4049277755
c	-0.8559281699	7.7418555188	-1.4431515023
c	-1.4093226030	-2.3101443000	-0.4132312778
c	-2.7792829485	-2.3756053884	-0.1536342188
n	-3.9172531709	-1.7644435573	0.0282795526
c	-3.9665856814	-0.2637875323	0.0230155163
c	-3.2667855573	0.2914182985	1.2628579992
c	-1.9931007634	-3.5639779188	-0.2640899167
n	-1.8109022983	-4.8588684537	-0.2635375884
c	-2.8919948894	-5.8292182322	0.1122226770
c	-3.9652508672	-5.8948669571	-0.9743989638
c	-0.4420989514	-5.3787457458	-0.5817039155
c	-0.4960808251	-6.4126824110	-1.7053711738
c	0.2422817647	-5.8913850294	0.6849231256
c	2.5009101167	-3.1482645018	-0.0056503544
n	3.3907554808	-3.7166511105	-0.7766084733
c	4.6052836469	-4.4147394988	-0.2398377913
c	4.2189045222	-5.7100130194	0.4739929408

c	3.2394126160	-3.5979568546	-2.2653934161
c	4.3346951015	-2.7055823424	-2.8472695007
c	3.1710693904	-4.9770911889	-2.9186373359
c	3.0082663189	-3.6205531950	3.3231646775
c	2.3386337337	-4.7751761440	4.0688696004
c	3.8665029683	-2.7338722919	4.2243300303
c	-0.4459463439	-2.3595804742	2.9878639586
c	-5.1981871847	-2.5215707782	0.2098223279
c	-5.8314604168	-2.2047909147	1.5636954373
c	-6.1352784706	-2.2808011637	-0.9738334402
c	-3.4455417871	0.3050883811	-1.2949823642
c	-3.4078370419	-5.5401514490	1.5221845859
c	5.4779206696	-3.4530843953	0.5667903216
h	-5.0351945827	-0.0293073861	0.0948654282
h	-3.7201940879	-0.0954188913	2.1832159602
h	-3.3426858693	1.3858117724	1.2658794168
h	-2.1961221176	0.0373224576	1.2620381538
h	-2.3699462564	0.1265731514	-1.4282341986
h	-3.5924463558	1.3918176063	-1.3052858506
h	-3.9815251003	-0.1226743372	-2.1507365035
h	-4.8981077527	-3.5749464683	0.2051803507
h	-5.1351724445	-2.3997024271	2.3895199532
h	-6.7148631806	-2.8395962191	1.7043703207
h	-6.1694103569	-1.1625050506	1.6281384498
h	-6.4846116662	-1.2412984120	-1.0194524507
h	-7.0229293272	-2.9163707152	-0.8667399922
h	-5.6493487382	-2.5280202236	-1.9263174875
h	-2.3830764646	-6.8005070975	0.1420145396
h	-4.4423841478	-4.9201812192	-1.1389198081
h	-4.7470715933	-6.6078173685	-0.6863867673
h	-3.5381199597	-6.2254523760	-1.9286798876
h	-2.5917652605	-5.5949629396	2.2542506964
h	-4.1650047874	-6.2827768510	1.8002977999
h	-3.8701175339	-4.5483614061	1.6016826658
h	0.1132792216	-4.5034013674	-0.9487406717
h	-1.0373309049	-7.3205362521	-1.4119959840
h	0.5244315651	-6.7210733762	-1.9631782182
h	-0.9663000709	-6.0012530807	-2.6067472107
h	-0.2715904443	-6.7665624748	1.1025994718
h	0.2779841542	-5.1074361551	1.4534200571
h	1.2707694724	-6.1933823621	0.4513103211
h	1.1542025517	-2.3526604652	4.4053357053
h	2.3244628312	-0.3059924599	3.5955850925
h	0.6107192956	0.0316184285	3.9223670316
h	1.1665125102	-0.1631243695	2.2478598931
h	-0.7092485556	-1.9479085565	2.0058642689
h	-1.1282800738	-1.9123876988	3.7208121573
h	-0.6184148231	-3.4431775670	2.9764178458
h	3.6496456598	-4.0413935552	2.5425427563
h	1.6730799797	-4.4228870756	4.8679406038
h	3.1091807196	-5.3972615727	4.5412144298
h	1.7597990117	-5.4100439553	3.3854495767
h	4.3395294696	-1.9219845704	3.6578323167
h	4.6604687906	-3.3430094174	4.6736712556
h	3.2892690418	-2.2969173264	5.0494165698
h	5.1702316000	-4.6910577122	-1.1385897612
h	3.5474520785	-5.5304743427	1.3230911907
h	5.1167199033	-6.2106260863	0.8560070084
h	3.7167070183	-6.3984778490	-0.2173606623
h	5.7940080498	-2.6049616689	-0.0527800773
h	6.3774859657	-3.9726809949	0.9184362440

h	4.9586099452	-3.0532728216	1.4465504040
h	2.2731522516	-3.1025436350	-2.4086093122
h	4.3306830685	-1.7152951002	-2.3747527978
h	4.1555034379	-2.5716262202	-3.9210676685
h	5.3334153160	-3.1470077789	-2.7333747228
h	4.1196471795	-5.5241321342	-2.8496474586
h	2.9410295876	-4.8552291912	-3.9841589296
h	2.3804545737	-5.5900002215	-2.4678589844
h	1.7055274981	0.1857805077	-2.5005247545
h	2.3344733473	-0.0892692848	-4.8870284361
h	1.3726173950	-1.9542798133	-6.2241102688
h	-0.2414680465	-3.5333405214	-5.1817232200
h	-0.8686375125	-3.2834549452	-2.8017075348
h	-1.2514440202	2.5604236616	2.2079216406
h	2.0590182307	2.3562822200	-1.2061559911
h	3.5774965973	3.9864917421	-2.2908073856
h	3.3764622437	6.4191576119	-1.7646075554
h	0.0458016151	4.7700724523	2.7239682594
h	-2.2918572871	4.3482358609	3.5580168968
h	-3.1443784695	6.6937681291	3.5653569359
h	-2.3100097472	8.2965871901	1.8764506957
h	1.5899295903	7.2083121001	-0.2762635267
h	-0.0163903321	9.5273760478	1.3457862244
h	0.3703642440	11.2721360363	-0.3752026022
h	-0.0333931538	10.7661904719	-2.7789116045
h	-0.8427471502	8.5107587044	-3.4545056667
h	-1.2055165798	6.7527572872	-1.7404433123

TS2_a (catalyst-6) [6-endo]

c	-1.1940243048	3.2807066621	1.3604143626
h	-0.6843447431	4.0860459378	2.3687492568
c	-0.3697514110	7.9061592616	-1.4058111296
c	-0.3985296321	8.0975283348	-0.0132310931
c	0.0788747072	9.3028848405	0.5265821006
c	0.6011555157	10.2901097112	-0.3116710652
c	0.6323700637	10.0907411880	-1.6939871933
c	0.1383916611	8.9005251668	-2.2394211533
c	-0.9908668077	7.0600925045	0.8683813150
c	-0.5595034762	5.6982124177	0.8982222321
c	-1.4006015968	4.7594606687	1.6144362834
c	-2.5176504734	5.1937861917	2.4009760823
c	-2.8245961481	6.5306223893	2.4390483203
c	-2.0823065341	7.4384843898	1.6569559652
c	-0.1833321965	2.8103404359	0.5417117761
c	0.7915278513	3.7518942444	0.0571033706
c	0.6489438517	5.1735828849	0.2850107023
c	1.9525728267	3.2886433865	-0.6149735094
c	2.9670421238	4.1448966143	-0.9914890048
c	2.8673311909	5.5152345911	-0.6828034382
c	1.7342951354	6.0140598843	-0.0666459416
au	-0.1584219704	0.8079429469	0.0390175981
p	-0.0462233773	-1.3857559107	-0.6816919269
c	-1.4471819299	-2.4530022088	-0.3306357411
c	-1.9374363766	-3.7404262776	-0.1351668568
n	-1.6581559318	-5.0163328373	-0.0686070898
c	-0.2460466712	-5.4410664654	-0.3354061160
c	0.4568952859	-5.8085092676	0.9699701973

c	0.2172416420	-1.5663097135	-2.4695842482
c	-0.2595458022	-2.6746319227	-3.1901869914
c	0.0464226808	-2.8017567337	-4.5454353982
c	0.8241651311	-1.8294473632	-5.1837824857
c	1.2843887973	-0.7177233645	-4.4718405981
c	0.9776925404	-0.5777222112	-3.1177741419
c	1.3204797469	-2.2820815626	0.0807940486
c	2.5278146556	-2.9718319648	-0.0494461838
n	3.4154011733	-3.5008570614	-0.8495778249
c	3.1888650223	-3.4214106410	-2.3319229781
c	3.1866582154	-4.8126834443	-2.9618821885
c	2.0294861955	-2.6034988510	1.2394776762
n	2.1245715683	-2.5756963417	2.5436579215
c	3.2238045919	-3.2995155577	3.2635065962
c	4.0722638403	-2.3439702920	4.1012172132
c	1.1359554817	-1.7988379771	3.3617658807
c	-0.3084395797	-2.1709893534	3.0305198974
c	1.4023787232	-0.2989035409	3.2386593781
c	-2.8191830469	-2.6156782340	-0.1301032171
n	-4.0107493965	-2.0911522983	-0.0579645713
c	-5.2363669959	-2.9400965747	0.1029830570
c	-6.1001565958	-2.8759092181	-1.1566011279
c	-4.1792670952	-0.6051922647	-0.1898957620
c	-3.6121751653	-0.0937726279	-1.5127508913
c	-3.6150434023	0.1023574079	1.0414656318
c	-2.6695878074	-6.0490878070	0.3368209201
c	-3.2636737227	-5.7137551513	1.7050448842
c	-3.6916798058	-6.2781478563	-0.7773600941
c	-0.1941557665	-6.5496908545	-1.3853477662
c	4.6966416439	-4.1073108290	-0.3579937874
c	5.5449241429	-3.0729942468	0.3817246077
c	4.4257541239	-5.4037629669	0.4050390303
c	4.1918456447	-2.4656022978	-2.9765722434
c	2.6549307303	-4.4674449916	4.0702287412
c	-5.9910320673	-2.5733656370	1.3796267222
h	-5.2655157548	-0.4572377439	-0.2069426117
h	-4.0963789890	-0.2509481254	1.9610676754
h	-3.7868730396	1.1820103156	0.9497095008
h	-2.5289866928	-0.0577689935	1.1274687759
h	-2.5167292913	-0.1688306637	-1.5529140150
h	-3.8638160210	0.9670555767	-1.6309983672
h	-4.0333211590	-0.6421598732	-2.3640116530
h	-4.8509983852	-3.9601549367	0.2074109507
h	-5.3473104867	-2.6515764512	2.2653219367
h	-6.8339986616	-3.2631636153	1.5085131798
h	-6.4084901967	-1.5589905569	1.3365312603
h	-6.5492278688	-1.8846206990	-1.3004262849
h	-6.9247771403	-3.5939090213	-1.0658538019
h	-5.5209668333	-3.1303363364	-2.0536181546
h	-2.0821248094	-6.9686347112	0.4517178411
h	-4.2356803028	-5.3588656272	-1.0300409187
h	-4.4268588102	-7.0282243430	-0.4623830196
h	-3.2043750349	-6.6417273819	-1.6899306020
h	-2.4741362240	-5.6276958402	2.4625346220
h	-3.9492045267	-6.5109515230	2.0160785806
h	-3.8302810822	-4.7741564487	1.6963959136
h	0.2399800866	-4.5491555893	-0.7564440552
h	-0.6571814142	-7.4798956609	-1.0346181019
h	0.8538063733	-6.7829731607	-1.6107278406
h	-0.6842066291	-6.2439598719	-2.3178099779
h	0.0019858845	-6.6872032996	1.4449995647

h	0.4231832431	-4.9712520735	1.6794738369
h	1.5082867116	-6.0498847341	0.7687549292
h	1.3368516930	-2.1112658844	4.3936047139
h	2.4281019591	-0.0442530531	3.5270717263
h	0.7148934835	0.2545055125	3.8907548536
h	1.2350192653	0.0449238510	2.2059002684
h	-0.6188809543	-1.7698751024	2.0570521407
h	-0.9731472472	-1.7337498083	3.7853872601
h	-0.4587016129	-3.2580129862	3.0326373607
h	3.8520761492	-3.7063426416	2.4648747035
h	1.9723705277	-4.1314606051	4.8618193998
h	3.4769464635	-5.0045920777	4.5592100755
h	2.1196392827	-5.1759281453	3.4254442730
h	4.4798768704	-1.5262794731	3.4932701259
h	4.9145402343	-2.8999008273	4.5309013226
h	3.5097322177	-1.9128785970	4.9393503091
h	5.2330469816	-4.3729255991	-1.2772532741
h	3.8030678326	-5.2390145759	1.2939175904
h	5.3714522593	-5.8480177456	0.7378835774
h	3.9164680711	-6.1327657578	-0.2376758095
h	5.7800792537	-2.2256545637	-0.2736957488
h	6.4895569889	-3.5276128138	0.7037771086
h	5.0425019011	-2.6808925677	1.2746354977
h	2.1854901299	-2.9956701364	-2.4372397773
h	4.1401694213	-1.4693741063	-2.5190501663
h	3.9548027869	-2.3633417501	-4.0425756428
h	5.2230235705	-2.8348507235	-2.9027715785
h	4.1736333965	-5.2916649505	-2.9328195492
h	2.8982604817	-4.7241160448	-4.0164168156
h	2.4631345586	-5.4715666901	-2.4658696572
h	1.3247733637	0.2981264056	-2.5673329205
h	1.8731727958	0.0483843109	-4.9750104885
h	1.0576061748	-1.9310011482	-6.2432117165
h	-0.3273234028	-3.6567774447	-5.1077705343
h	-0.8672123889	-3.4366636313	-2.7027778254
h	-1.9120554953	2.6293009538	1.8572148144
h	2.0454105403	2.2160009290	-0.7942521655
h	3.8527589764	3.7634997426	-1.4984113643
h	3.6861916709	6.1905634782	-0.9276516398
h	-3.1078619732	4.4561351873	2.9446960715
h	-3.6682119080	6.8877904019	3.0280364362
h	-2.3902373750	8.4838601535	1.6284961911
h	1.6868405805	7.0731837665	0.1662995570
h	0.0609890022	9.4577306688	1.6060713099
h	0.9793520155	11.2176965134	0.1163384178
h	1.0314282529	10.8655608026	-2.3474973880
h	0.1408283935	8.7533719299	-3.3190565972
h	-0.7574863415	6.9799654710	-1.8312829391

Int-3_a (catalyst-6) [6-endo]

c	-0.0961344347	3.1485908857	1.6496977175
h	0.8141680890	2.8254511963	2.2012590794
c	-1.5686668228	7.7948020836	-0.8088934593
c	-0.8197185695	8.0120562860	0.3640027233
c	-0.2612877689	9.2825080288	0.5923537208
c	-0.4195515207	10.3008597979	-0.3477549546
c	-1.1549588089	10.0711656980	-1.5149002663
c	-1.7368504026	8.8180940644	-1.7381947117

c	-0.6731122203	6.9306769682	1.3641030400
c	-0.2420087306	5.6017053090	1.0355479673
c	-0.4048329885	4.5731021908	2.0045085669
c	-0.8276923350	4.8751437423	3.2983589422
c	-1.1254275605	6.1907598431	3.6460934215
c	-1.0682791951	7.1967434269	2.6785796211
c	0.1913861030	2.8121088314	0.2352251735
c	0.4936997233	3.8526964980	-0.6429895393
c	0.4180148226	5.2481413398	-0.2109034791
c	0.9890952567	3.5612685438	-1.9630771298
c	1.5129536589	4.5405716433	-2.7639282423
c	1.5945034368	5.8635039391	-2.2610887915
c	1.0555775585	6.2044348912	-1.0316700552
au	0.2269715151	0.8166995084	-0.2515791911
p	0.2532471057	-1.4279600990	-0.8408554520
c	-1.2725164488	-2.3336106933	-0.5673960425
c	-1.8805385642	-3.5687288240	-0.3645545345
n	-1.7147557629	-4.8619482901	-0.2759397503
c	-0.3405585481	-5.4138768612	-0.5069216983
c	0.2849982945	-5.8581413349	0.8147374725
c	0.6875644463	-1.7373454214	-2.5744730967
c	0.1452051681	-2.8015198007	-3.3134796841
c	0.5872962814	-3.0330370953	-4.6167132894
c	1.5649460553	-2.2083328756	-5.1836220003
c	2.0930122698	-1.1384342217	-4.4542199766
c	1.6529299173	-0.8944421476	-3.1530483879
c	1.4441915750	-2.3893594984	0.1112210063
c	2.6021846595	-3.1702209237	0.1493024656
n	3.5310213736	-3.8040113614	-0.5156833300
c	3.4714988061	-3.8109148017	-2.0162046165
c	3.4289733413	-5.2406132650	-2.5522448046
c	1.9906102499	-2.7065850467	1.3556236725
n	1.9370985478	-2.6295598452	2.6605071651
c	2.9023720444	-3.3797313737	3.5302530004
c	3.7014250773	-2.4306847728	4.4219669450
c	0.8981159266	-1.7826551142	3.3308626343
c	-0.5153954706	-2.1546177604	2.8866087141
c	1.2089564334	-0.2980254329	3.1432646952
c	-2.6518773466	-2.3643001988	-0.3488500238
n	-3.7849072335	-1.7302165396	-0.2301472398
c	-5.0827644163	-2.4614305572	-0.0529362959
c	-5.9803841233	-2.2601689612	-1.2739486676
c	-3.8141233922	-0.2302075158	-0.2994678516
c	-3.2471232153	0.2755830454	-1.6237343880
c	-3.1463628419	0.3665843267	0.9389407139
c	-2.8222141593	-5.7976932033	0.1128216147
c	-3.3866934122	-5.4221189294	1.4832181876
c	-3.8541111121	-5.9131196778	-1.0092408889
c	-0.3630422298	-6.5108928521	-1.5702045940
c	4.7037436082	-4.4612637333	0.1517771287
c	5.5337789428	-3.4383498389	0.9279876822
c	4.2602138213	-5.6916733262	0.9434360650
c	4.6106600897	-2.9780899066	-2.6018629979
c	2.1771928872	-4.4784434697	4.3074085787
c	-5.7498747133	-2.0747450191	1.2658628653
h	-4.8809370833	0.0205363735	-0.2702187871
h	-3.6324022711	0.0208229205	1.8588672808
h	-3.2111052820	1.4610732451	0.9006794204
h	-2.0799636625	0.0977868449	0.9827730877
h	-2.1733444717	0.0647535635	-1.7232470731
h	-3.3681290305	1.3641337021	-1.6793627934

h	-3.7713575744	-0.1724108996	-2.4763904709
h	-4.7982267973	-3.5179384598	-0.0028112368
h	-5.0809383823	-2.2408446458	2.1202217611
h	-6.6456606702	-2.6914332040	1.4087864876
h	-6.0753387052	-1.0266173428	1.2734780380
h	-6.3135265001	-1.2192976298	-1.3753422152
h	-6.8799647687	-2.8784589208	-1.1654235106
h	-5.4707583939	-2.5562961966	-2.1997416565
h	-2.3273081933	-6.7710474817	0.2168501057
h	-4.3119906393	-4.9443680919	-1.2478004615
h	-4.6555998992	-6.5996270074	-0.7113312912
h	-3.3955859994	-6.3028001046	-1.9258987438
h	-2.6002034552	-5.4467191366	2.2485580307
h	-4.1653500887	-6.1377174011	1.7728439055
h	-3.8361230103	-4.4212475136	1.4894377633
h	0.2406116361	-4.5672488664	-0.9007318778
h	-0.9223093792	-7.3964647936	-1.2448429178
h	0.6633051004	-6.8401802803	-1.7731231381
h	-0.7969606603	-6.1492263004	-2.5103306629
h	-0.2552307565	-6.7030875677	1.2603062168
h	0.2980659519	-5.0312112872	1.5379006800
h	1.3188611044	-6.1825010535	0.6419780582
h	0.9948731559	-2.0302460977	4.3944017427
h	2.2122203315	-0.0466738877	3.5053816699
h	0.4799240525	0.3053171161	3.6992207531
h	1.1403708208	-0.0157371166	2.0805189216
h	-0.7171370113	-1.8228674772	1.8607865554
h	-1.2425653230	-1.6560407086	3.5386035052
h	-0.6851638310	-3.2370514271	2.9487825607
h	3.5927782543	-3.8545466990	2.8260895481
h	1.4607789775	-4.0703136982	5.0327993090
h	2.9100935022	-5.0663890629	4.8738366457
h	1.6424021889	-5.1594258754	3.6322379420
h	4.2148819797	-1.6608727616	3.8326097168
h	4.4610727429	-3.0065171049	4.9645154433
h	3.0729363693	-1.9375134183	5.1748395933
h	5.3199687854	-4.8132059726	-0.6841189348
h	3.5296058702	-5.4428262060	1.7230415216
h	5.1262987135	-6.1571047507	1.4291317280
h	3.8060392314	-6.4369858600	0.2784431963
h	5.9021415422	-2.6513045417	0.2588667799
h	6.4004102796	-3.9322917246	1.3835679863
h	4.9633172536	-2.9573069597	1.7322529964
h	2.5204781114	-3.3243383910	-2.2599800615
h	4.5897937688	-1.9511707169	-2.2162976589
h	4.5000493619	-2.9352301004	-3.6920313475
h	5.5947874344	-3.4150101710	-2.3881694630
h	4.3679964453	-5.7830790112	-2.3840496851
h	3.2605046501	-5.2095792002	-3.6356937408
h	2.6104023705	-5.8108522698	-2.0954642089
h	2.0625285054	-0.0568731277	-2.5855554957
h	2.8431182757	-0.4883373005	-4.9029675433
h	1.9045340161	-2.3913586897	-6.2026135623
h	0.1634928610	-3.8532486308	-5.1951420692
h	-0.6216790181	-3.4447814423	-2.8830291850
h	-0.8722741916	2.4779450797	2.0569411476
h	0.9795237394	2.5197950526	-2.2888949940
h	1.9033532185	4.3083396446	-3.7535374466
h	2.0856461096	6.6339758825	-2.8556049491
h	-0.9296942825	4.0778860422	4.0361283957
h	-1.4531435630	6.4295671585	4.6573721217

h	-1.3931916687	8.2058736531	2.9303997137
h	1.1260461813	7.2351316077	-0.6962248569
h	0.3205062770	9.4607905310	1.4971842366
h	0.0300947712	11.2768253408	-0.1685924282
h	-1.2852547669	10.8709043138	-2.2431270971
h	-2.3340304281	8.6465611736	-2.6333776692
h	-2.0329165576	6.8220812549	-0.9754095996

TS-3_{a1} (catalyst-6) [6-endo]

c	-0.1019127113	2.8395965373	0.6544537571
h	-0.0789769684	2.9459857539	1.9743245388
c	1.0514322473	-0.4789670932	-2.9838881332
c	0.2360617312	-1.4612503583	-2.3947533676
c	-0.2744004985	-2.5145031089	-3.1726589419
c	0.0528105824	-2.5946737082	-4.5265656164
c	0.8842748255	-1.6302580014	-5.1063975233
c	1.3776710099	-0.5720542542	-4.3372323594
p	-0.0494825867	-1.3553448800	-0.6054145981
c	1.2815059506	-2.3162826789	0.1381627965
c	1.9617703302	-2.7114405673	1.2915613342
n	2.0311653489	-2.7527559734	2.5965248786
c	1.0313208231	-2.0125285272	3.4342471739
c	1.2972535681	-0.5087358111	3.3791442246
au	-0.1102483254	0.8143590986	0.1772759497
c	-1.1749811985	3.4217663403	1.4122165786
c	-1.3916596796	4.8369836419	1.5164052744
c	-0.5405831678	5.7307003321	0.7880199178
c	0.6988093547	5.1836518408	0.2257533231
c	0.8909998264	3.7612249497	0.1287969784
c	-2.4872047014	5.3018663206	2.2720852428
c	-2.7787342403	6.6532812254	2.2904080239
c	-2.0258725998	7.5244610383	1.4910091418
c	-0.9422719894	7.0990167903	0.7110909761
c	1.7801929271	6.0057498563	-0.1679002798
c	2.9456844355	5.4750100691	-0.6988314636
c	3.0942354239	4.0875794403	-0.8662800239
c	2.0818226991	3.2502918935	-0.4383802221
c	-0.3408315721	8.0980615900	-0.2084466336
c	-0.3298494624	7.8596343796	-1.5940938323
c	0.1896096207	8.8135525435	-2.4674561341
c	0.7107247814	10.0126992304	-1.9691749869
c	0.6950414691	10.2609518425	-0.5944385851
c	0.1629466877	9.3134352382	0.2828608237
c	-1.4864997219	-2.3869010344	-0.3072840355
c	-2.8569845513	-2.5280082104	-0.0796950515
n	-4.0316612077	-1.9821804705	0.0674587020
c	-4.1677901987	-0.4872024781	0.0544717610
c	-3.5415860252	0.1122931893	1.3127675553
c	-2.0050693495	-3.6720915272	-0.1802120552
n	-1.7562973616	-4.9551513388	-0.1960240399
c	-2.7873257829	-5.9871238111	0.1612810606
c	-3.8362495781	-6.1140597466	-0.9436797754
c	-0.3601127573	-5.3980119590	-0.5143874559
c	-0.3559144169	-6.4343746176	-1.6370177735
c	0.3525028820	-5.8709777202	0.7517890389
c	2.4773847108	-3.0242425345	-0.0057370597
n	3.3693644433	-3.5331305049	-0.8130081824
c	4.6321323930	-4.1825977121	-0.3263899345

c	4.3283542997	-5.5074401487	0.3725499212
c	3.1701519801	-3.3892178466	-2.2947116666
c	4.2018793590	-2.4279473545	-2.8832513680
c	3.1549929863	-4.7548234213	-2.9788727169
c	3.1088194082	-3.5243099300	3.3004893601
c	2.5110560019	-4.7219544104	4.0393125464
c	3.9509449821	-2.6187638963	4.1975277712
c	-0.4080673465	-2.3710008841	3.0674785904
c	-5.2740679287	-2.8113179981	0.2120265135
c	-5.9654571792	-2.5301104030	1.5451404878
c	-6.1856031788	-2.6239875330	-1.0007464663
c	-3.6389110812	0.1108610071	-1.2473845738
c	-3.3432584341	-5.7299298178	1.5619447322
c	5.4822076396	-3.1953421978	0.4729063604
h	-5.2499161091	-0.3150683241	0.0926129016
h	-3.9676953128	-0.3285082948	2.2217835689
h	-3.7322144151	1.1925494658	1.3315899068
h	-2.4507626916	-0.0390868546	1.3245908863
h	-2.5497684322	0.0002847944	-1.3430217180
h	-3.8564531999	1.1855651228	-1.2693820860
h	-4.1153954087	-0.3516451065	-2.1200335822
h	-4.9134808775	-3.8455141566	0.2187167943
h	-5.2870813540	-2.6892047115	2.3933171043
h	-6.8174535950	-3.2117426715	1.6572798228
h	-6.3617982429	-1.5079168105	1.5987491274
h	-6.5953235801	-1.6073569882	-1.0577842780
h	-7.0371587047	-3.3110195786	-0.9207091732
h	-5.6569098058	-2.8410251222	-1.9377982187
h	-2.2227361008	-6.9270793182	0.2003853910
h	-4.3702140102	-5.1701070993	-1.1135836861
h	-4.5770546720	-6.8747884457	-0.6703088574
h	-3.3746275053	-6.4144838665	-1.8919124284
h	-2.5381797210	-5.7349591756	2.3080847806
h	-4.0577051873	-6.5181028252	1.8271729310
h	-3.8680989761	-4.7691512070	1.6334638132
h	0.1445668734	-4.4930790345	-0.8830639181
h	-0.8457182637	-7.3708723678	-1.3434382103
h	0.6808338570	-6.6860849897	-1.8917479990
h	-0.8460308846	-6.0508722322	-2.5400451776
h	-0.1140195093	-6.7713523865	1.1713173762
h	0.3475017144	-5.0854570966	1.5195387890
h	1.3953707249	-6.1187161987	0.5173557763
h	1.2192452150	-2.3687148258	4.4541623846
h	2.3177866808	-0.2648775225	3.6942259560
h	0.5980557354	0.0160541083	4.0425359768
h	1.1470623802	-0.1252443787	2.3573652174
h	-0.7125154263	-1.9099577686	2.1189271626
h	-1.0821235122	-1.9886419463	3.8436229411
h	-0.5508253260	-3.4567499601	2.9972873565
h	3.7461551193	-3.8996612543	2.4939397122
h	1.8549006504	-4.4155646633	4.8644236347
h	3.3215947665	-5.3186758964	4.4760386018
h	1.9408816086	-5.3678388696	3.3592159031
h	4.3743483546	-1.7754971893	3.6373569870
h	4.7822152111	-3.2021989176	4.6121919665
h	3.3785718359	-2.2253424551	5.0475538164
h	5.1810628424	-4.4147119584	-1.2473309996
h	3.6832897554	-5.3748236029	1.2506948277
h	5.2607057394	-5.9752435371	0.7107633148
h	3.8307568615	-6.2035584862	-0.3144033762
h	5.7352629826	-2.3198630718	-0.1375609730

h	6.4177966065	-3.6762330288	0.7829764783
h	4.9737593242	-2.8411633231	1.3781317642
h	2.1761870283	-2.9413200975	-2.3997496614
h	4.1587556369	-1.4488695789	-2.3894209373
h	3.9879837336	-2.2814033406	-3.9490579257
h	5.2247853212	-2.8183317923	-2.8041838803
h	4.1324400205	-5.2525878157	-2.9499225796
h	2.8887136326	-4.6204254114	-4.0343991510
h	2.4105376822	-5.4190637456	-2.5223420262
h	1.4275786510	0.3553047862	-2.3894618633
h	2.0087289696	0.1889907421	-4.7946755024
h	1.1339615763	-1.6950364823	-6.1649965873
h	-0.3471778475	-3.4060590846	-5.1337289112
h	-0.9261970991	-3.2683771995	-2.7320091589
h	-1.9289702053	2.7558008248	1.8384298463
h	2.2010748146	2.1663673107	-0.4994302806
h	4.0091233493	3.6809332291	-1.2950842697
h	3.7557995044	6.1466561201	-0.9811292892
h	-3.1013966165	4.5896700834	2.8243181635
h	-3.6128681946	7.0357929733	2.8768454268
h	-2.3114920769	8.5750619045	1.4338620860
h	1.7090690794	7.0810253847	-0.0411750793
h	0.1574953758	9.5063031268	1.3562245783
h	1.0934111710	11.1962171608	-0.2027973760
h	1.1175757710	10.7566521030	-2.6530769099
h	0.1787293858	8.6285172051	-3.5412777651
h	-0.7404346142	6.9268464078	-1.9822870736

TS-3_{a2} (catalyst-6) [6-endo]

h	-1.6382836635	3.1661699769	-0.8537014100
c	-0.6784202338	2.7753804955	-0.0308968197
c	0.7790808437	-0.9426010295	-3.4040613873
c	0.1492248495	-1.9019199101	-2.5922820396
c	-0.2161968577	-3.1500990297	-3.1243858601
c	0.0679504613	-3.4405375956	-4.4591538206
c	0.7153703192	-2.4939667085	-5.2611136110
c	1.0670574788	-1.2468132553	-4.7352212877
p	-0.0842871329	-1.4980813035	-0.8396986552
c	1.4074566187	-2.0884794303	-0.0182122203
c	2.1992787706	-2.1219002516	1.1312863330
n	2.3592409832	-1.8291086579	2.3951949783
c	1.3556477737	-0.9700579865	3.1083480967
c	1.4926931345	0.4845874255	2.6608217670
au	-0.4595771043	0.7347692112	-0.3987179108
c	-1.9344055469	3.3048382321	0.4264486006
c	-2.1322463852	4.6750628586	0.8026538633
c	-1.0504790472	5.6061197305	0.6623117321
c	0.2805950282	5.0680807514	0.3644263050
c	0.4400143716	3.7013360624	-0.0565088625
c	-3.4016260918	5.0721833288	1.2690060235
c	-3.6243865502	6.3961246509	1.5992496890
c	-2.6132423941	7.3364475163	1.3592646923
c	-1.3521722065	6.9888631708	0.8565907058
c	1.4612943420	5.8291724245	0.5330558511
c	2.7114261892	5.3164237303	0.2244900537
c	2.8494059728	4.0119961959	-0.2806694879
c	1.7243335358	3.2196057027	-0.4038027218

c	-0.4535755925	8.1079825443	0.4733841751
c	-0.0279241693	8.2360141430	-0.8606698914
c	0.7674654155	9.3144979996	-1.2441507150
c	1.1542562939	10.2726282018	-0.3006035652
c	0.7287837016	10.1563830520	1.0251235270
c	-0.0802402963	9.0849570277	1.4103703860
c	-1.3411707859	-2.6466344316	-0.2703181937
c	-2.6888298467	-2.9354434139	-0.0406358238
n	-3.9387933348	-2.5662188397	-0.0801141077
c	-4.2973411511	-1.1742409279	-0.5097298633
c	-3.9001040323	-0.1680590025	0.5688216666
c	-1.6772885420	-3.9212103912	0.1776024683
n	-1.2547571281	-5.1171006750	0.4944273453
c	-2.1445818755	-6.1552246540	1.1163241019
c	-3.1064208743	-6.7383517796	0.0818721669
c	0.2026799324	-5.4174636765	0.3161165338
c	0.4088357122	-6.7190285441	-0.4571301960
c	0.9174781096	-5.3956157559	1.6663250983
c	2.6671533214	-2.6876113719	-0.0980350731
n	3.5619629627	-3.2771344019	-0.8450121117
c	4.9059602397	-3.7031938127	-0.3303357898
c	4.7654712223	-4.8489215782	0.6715686068
c	3.2683853376	-3.4683711638	-2.3064197654
c	4.2052178113	-2.6139760682	-3.1595245372
c	3.2869963094	-4.9484644122	-2.6799114143
c	3.5544560816	-2.3076126743	3.1662319522
c	3.1289427229	-3.3071043809	4.2430265417
c	4.3717695520	-1.1405357537	3.7171354834
c	-0.0663476892	-1.5083866242	2.9697600023
c	-5.0530022230	-3.5188899426	0.2421131855
c	-5.8958816451	-3.0033789952	1.4070979775
c	-5.8683123372	-3.8274901939	-1.0132911337
c	-3.7363124975	-0.8506484653	-1.8929374649
c	-2.8016607780	-5.6138715394	2.3861425202
c	5.7137249519	-2.5001000035	0.1558615564
h	-2.7722014480	2.6145264442	0.5410982321
h	-5.3909350705	-1.1895435277	-0.5826794286
h	-4.3366466661	-0.4258581381	1.5408585139
h	-4.2634163122	0.8274617386	0.2837212146
h	-2.8052955375	-0.1163484955	0.6772349766
h	-2.6414002741	-0.7580351686	-1.8866507825
h	-4.1386053317	0.1117072383	-2.2317988477
h	-4.0187391865	-1.6145016182	-2.6272895630
h	-4.5460003841	-4.4358325296	0.5609620903
h	-5.2796157951	-2.7989750264	2.2918890240
h	-6.6365716798	-3.7661267207	1.6758637883
h	-6.4519631883	-2.0930447845	1.1472516323
h	-6.4085198939	-2.9464606332	-1.3830419965
h	-6.6196267046	-4.5907358624	-0.7767346567
h	-5.2318160566	-4.2115693590	-1.8208210639
h	-1.4532365058	-6.9499931273	1.4210679090
h	-3.7476961200	-5.9662904781	-0.3613349939
h	-3.7559085153	-7.4855588714	0.5538552048
h	-2.5603111252	-7.2295654446	-0.7322341958
h	-2.0437544008	-5.2818672061	3.1067826254
h	-3.3969298123	-6.4042323773	2.8590175601
h	-3.4730198924	-4.7703875349	2.1838775179
h	0.5850840484	-4.5901681959	-0.2998214521
h	0.0441073490	-7.5950257050	0.0927134604
h	1.4830689086	-6.8734245562	-0.6182965639
h	-0.0850026233	-6.6887759582	-1.4355673734

h	0.5652101699	-6.1983806536	2.3270338215
h	0.7643501046	-4.4343211470	2.1731760943
h	1.9941248735	-5.5424641830	1.5156792672
h	1.6410597315	-1.0440334236	4.1645793223
h	2.5092668697	0.8626380575	2.8151933938
h	0.8006212774	1.1182838651	3.2290705225
h	1.2425316988	0.5915966105	1.5936151701
h	-0.4592936234	-1.3752569810	1.9527395083
h	-0.7276815784	-0.9512288625	3.6443832146
h	-0.1242949538	-2.5705901713	3.2383053995
h	4.1624025775	-2.8370375826	2.4255311035
h	2.5164210306	-2.8390079962	5.0248917006
h	4.0232350150	-3.7114274006	4.7327262602
h	2.5670264464	-4.1455877925	3.8126405687
h	4.6763594860	-0.4486753523	2.9216783715
h	5.2788367738	-1.5337072547	4.1924525510
h	3.8248582499	-0.5765058108	4.4835229165
h	5.4121943251	-4.1033960754	-1.2166575792
h	4.1947207837	-4.5539254198	1.5615057709
h	5.7570585773	-5.1778392561	1.0052838037
h	4.2609811745	-5.7073721271	0.2106012939
h	5.8570410071	-1.7748687345	-0.6544278269
h	6.7026171286	-2.8297497787	0.4965635773
h	5.2275273973	-1.9828754591	0.9919259621
h	2.2479195395	-3.0946070802	-2.4354035184
h	4.1457905026	-1.5555963669	-2.8765841952
h	3.9067147873	-2.7020394165	-4.2111744118
h	5.2504450887	-2.9406468774	-3.0865642410
h	4.2858202483	-5.3945191526	-2.5878010770
h	2.9783919640	-5.0551346452	-3.7273887979
h	2.5874451220	-5.5226375487	-2.0600041772
h	1.0419572370	0.0355076029	-2.9983984263
h	1.5547791555	-0.5048836580	-5.3663394178
h	0.9319659864	-2.7240410356	-6.3038637835
h	-0.2202068902	-4.4042825168	-4.8775501278
h	-0.7164097350	-3.8942676068	-2.5046125278
h	1.8123264512	2.1893702965	-0.7553575627
h	3.8321418899	3.6287936854	-0.5522339972
h	3.5933819294	5.9387398417	0.3729792419
h	-4.1968775787	4.3316867513	1.3618039255
h	-4.5898984300	6.7202981867	1.9846236835
h	-2.8211366108	8.3944436580	1.5208218888
h	1.3952675783	6.8406311249	0.9204602289
h	-0.4092216260	8.9940295873	2.4461736843
h	1.0212645188	10.9045604584	1.7610054199
h	1.7759661272	11.1148594700	-0.6019103793
h	1.0770945347	9.4166203694	-2.2838563181
h	-0.3357342947	7.4932659490	-1.5974827647

Prod-cplx_a (catalyst-6) [6-endo]

c	2.1497465513	2.3913299843	2.3360196874
h	2.8867652861	1.8020029747	2.8858951720
c	1.4477635475	0.9390012331	-1.8006975980
c	0.3569706639	0.0624961248	-1.6563898860
c	-0.4346901775	-0.2724769628	-2.7689061407
c	-0.1178251446	0.2508878215	-4.0228767601
c	0.9791237618	1.1072684713	-4.1693612496
c	1.7549424050	1.4540175584	-3.0594901700

p	0.0253747610	-0.6461676794	-0.0194631102
c	0.9900779971	-2.1525620340	0.1007096708
c	1.5014159016	-3.1781721117	0.8986525771
n	1.5455908937	-3.7844146499	2.0546676702
c	0.8304328922	-3.2070663328	3.2414053390
c	1.5636911778	-1.9680438439	3.7543880783
au	0.5688743424	0.8485300653	1.6070185846
c	0.9328963401	2.7321986883	2.9506923270
c	0.0424124903	3.6940331759	2.3412757891
c	0.3204892763	4.1782866066	1.0167245527
c	1.6479576997	3.9256526009	0.4452140508
c	2.5468602213	3.0207099156	1.1038361009
c	-1.0904185294	4.1328224876	3.0565521910
c	-1.9714074397	5.0277569709	2.4751890387
c	-1.7973867007	5.3790580366	1.1287821553
c	-0.7104057689	4.9293730094	0.3704929375
c	2.1499417350	4.6009093279	-0.6917263656
c	3.4233739532	4.3508952074	-1.1820242299
c	4.2688030616	3.4101746533	-0.5649159317
c	3.8328881725	2.7613252198	0.5758454448
c	-0.7618873212	5.1616821290	-1.0947902031
c	-0.6834472862	4.0646381117	-1.9723465064
c	-0.7936222706	4.2526857780	-3.3483574154
c	-0.9755858642	5.5376358364	-3.8714617735
c	-1.0575797588	6.6324126867	-3.0072507591
c	-0.9608462610	6.4457427945	-1.6264331620
c	-1.6609825897	-1.2333519239	-0.0745048188
c	-3.0217660178	-1.0217779331	0.1627813298
n	-3.9668752161	-0.2312939590	0.5825658331
c	-3.6007252732	1.1070456685	1.1598064861
c	-2.9039116119	0.9238263758	2.5060337959
c	-2.5575525544	-2.2364802855	-0.4331319979
n	-2.7201515246	-3.4149120981	-0.9717921808
c	-4.0422903325	-4.1303020623	-0.9676754432
c	-5.0097007065	-3.4873468740	-1.9607641014
c	-1.5132102939	-4.1035119571	-1.5343571511
c	-1.7721335504	-4.5960390488	-2.9576469646
c	-1.0406951216	-5.2070633832	-0.5888750606
c	1.9044747259	-3.0409856043	-0.4687527517
n	2.5944832321	-3.3792434176	-1.5233324181
c	3.5867403633	-4.5061091803	-1.5218175422
c	2.8739853667	-5.8528883114	-1.3995998047
c	2.4582647076	-2.5450088996	-2.7660791511
c	3.7349762645	-1.7424635946	-3.0123851975
c	2.0390344849	-3.4025609560	-3.9579050275
c	2.3164983508	-5.0594851977	2.2438222165
c	1.3615159051	-6.2208271150	2.5220747672
c	3.4033130734	-4.9021319596	3.3053119217
c	-0.6470798826	-2.9486938822	2.9549937824
c	-5.4174089749	-0.5985922776	0.4731314501
c	-6.0770200749	-0.6283687339	1.8507914023
c	-6.1226285936	0.3218358374	-0.5231191362
c	-2.8128165836	1.9478407195	0.1594125207
c	-4.5739089951	-4.2710884664	0.4587734794
c	4.6958165868	-4.2561086413	-0.5004745851
h	-4.5641832180	1.6016778165	1.3325726134
h	-3.5393939124	0.3864705030	3.2196048676
h	-2.6536550859	1.9063024455	2.9239408280
h	-1.9620025821	0.3631001030	2.3918295022
h	-1.8261985507	1.5198039142	-0.0645775895
h	-2.6336111515	2.9430724133	0.5821061657

h	-3.3570004049	2.0669410982	-0.7848036566
h	-5.4134433611	-1.6158002706	0.0659160998
h	-5.5487790664	-1.3028251725	2.5366942539
h	-7.1081153754	-0.9873782622	1.7455806421
h	-6.1277332787	0.3683822160	2.3074156702
h	-6.1647299930	1.3596298425	-0.1676713232
h	-7.1578454671	-0.0164696282	-0.6553091458
h	-5.6288632252	0.3073756049	-1.5031593877
h	-3.8018423529	-5.1375167130	-1.3295161571
h	-5.2048806137	-2.4347678050	-1.7173672836
h	-5.9685822730	-4.0191143030	-1.9454961221
h	-4.6134482324	-3.5294663662	-2.9821513203
h	-3.8540065579	-4.8021521736	1.0942888273
h	-5.5075516113	-4.8458797666	0.4491278961
h	-4.7878633513	-3.2999604367	0.9224037516
h	-0.7408667655	-3.3206479304	-1.5792868913
h	-2.5359747851	-5.3827677712	-2.9964861846
h	-0.8497177606	-5.0334683756	-3.3587334959
h	-2.0792089963	-3.7768962980	-3.6190057201
h	-1.7811319546	-6.0128222728	-0.5015456105
h	-0.8433635021	-4.8053346716	0.4133630217
h	-0.1142206808	-5.6505553211	-0.9743255825
h	0.8946469449	-3.9939176195	4.0026760344
h	2.6101062789	-2.1861735398	3.9946887467
h	1.0726354512	-1.5936325852	4.6609733190
h	1.5396775680	-1.1641977924	2.9995323626
h	-0.7906721827	-2.0917796612	2.2830016023
h	-1.1585779579	-2.7086921353	3.8950775909
h	-1.1338718686	-3.8299527005	2.5188639386
h	2.7991185177	-5.2320428033	1.2762547225
h	0.8404841718	-6.1082015064	3.4819215105
h	1.9349767559	-7.1545262021	2.5747369121
h	0.6134095001	-6.3251808998	1.7257662038
h	4.0758300133	-4.0662204318	3.0753108699
h	4.0024100735	-5.8203530760	3.3401601803
h	2.9857737157	-4.7529793942	4.3094464953
h	4.0405671233	-4.4597091756	-2.5187782938
h	2.3076949925	-5.9359534860	-0.4630890058
h	3.6074144684	-6.6682266849	-1.4202624679
h	2.1787661039	-6.0031832793	-2.2351123173
h	5.2194569825	-3.3168773733	-0.7165800319
h	5.4285488925	-5.0711410308	-0.5417816899
h	4.3133976197	-4.2034777370	0.5261591515
h	1.6457684492	-1.8451063747	-2.5432507250
h	3.9866926736	-1.1221875065	-2.1427445538
h	3.5799200665	-1.0773703696	-3.8705051119
h	4.5908881976	-2.3889800477	-3.2454595090
h	2.8193978637	-4.1105923165	-4.2626711504
h	1.8417820213	-2.7476494329	-4.8155201919
h	1.1220503668	-3.9650169579	-3.7411758304
h	2.0524840856	1.2326037250	-0.9414605997
h	2.5914866980	2.1433768665	-3.1629074792
h	1.2181842312	1.5192045721	-5.1493370201
h	-0.7325944560	-0.0021738085	-4.8859211448
h	-1.2936456978	-0.9350258197	-2.6619118318
h	0.7469617227	2.4286180652	3.9831111046
h	4.4892317345	2.0692945950	1.1050923315
h	5.2692289511	3.2296055405	-0.9561454953
h	3.7791143958	4.9124792085	-2.0456824463
h	-1.2446741808	3.7802902466	4.0770983696
h	-2.8202187909	5.4169051003	3.0361003479

h	-2.5548220231	5.9858722813	0.6316762464
h	1.5441849221	5.3543064849	-1.1843673920
h	-1.0129465570	7.3041580216	-0.9562010150
h	-1.1969745293	7.6357587417	-3.4079715994
h	-1.0583372410	5.6854737317	-4.9476560025
h	-0.7434861428	3.3937771111	-4.0172437413
h	-0.5273199670	3.0639530053	-1.5659085730

Final Product [6-endo]

c	2.2361172590	2.3765293258	1.6831998147
h	2.8591703946	1.4980470575	1.8581360926
c	1.1527648194	2.6279207141	2.4684719260
c	0.3011106156	3.7549757836	2.2242106480
c	0.5681164557	4.6359816713	1.1220307323
c	1.8252852945	4.4582208541	0.3952227247
c	2.6193316305	3.2914796391	0.6513744364
c	-0.8146410552	3.9730349338	3.0654519149
c	-1.6845152130	5.0191968635	2.8293172092
c	-1.4925567922	5.8237936772	1.6960640098
c	-0.4166007729	5.6339877768	0.8266245151
c	2.3586906313	5.4117642227	-0.5081355184
c	3.5478446545	5.1928582900	-1.1847566821
c	4.2747718936	4.0045278937	-0.9902044568
c	3.8174245969	3.0781981694	-0.0719279820
c	-0.4502153840	6.4350597639	-0.4286115697
c	-0.5538987430	5.7917180180	-1.6739548946
c	-0.6425065857	6.5326095171	-2.8512170237
c	-0.6301005658	7.9310453016	-2.8061977055
c	-0.5396438065	8.5808343232	-1.5732741053
c	-0.4566939736	7.8379697704	-0.3925127820
h	0.8986727763	1.9606306796	3.2935657604
h	4.3910741145	2.1718466888	0.1295938651
h	5.2021848148	3.8302379061	-1.5359657441
h	3.9223729939	5.9562963706	-1.8669433213
h	-0.9769662846	3.2933574260	3.9032095151
h	-2.5378768449	5.1931214803	3.4845701361
h	-2.2271372870	6.5900419724	1.4469948760
h	1.8405460012	6.3514540263	-0.6686754701
h	-0.3745018133	8.3445965759	0.5697604822
h	-0.5310537058	9.6702451356	-1.5283083889
h	-0.6946677012	8.5099402146	-3.7276029939
h	-0.7233699196	6.0174566073	-3.8088236752
h	-0.5517285728	4.7021484965	-1.7080856802

PMe₃Au⁺ (Catalyst)

c	4.2621952973	2.1704918789	1.4105467934
p	3.7565831695	1.5348884363	3.0292245285
au	2.0800725315	0.0753003116	2.8113256524
c	3.2562862672	2.9379261697	4.0592412682
c	5.1904489240	0.7447918500	3.8036875988
h	5.9952495490	1.4893382140	3.8881305891
h	4.9210508513	0.3807214325	4.8017032244
h	5.5310921618	-0.0963876017	3.1890090568
h	4.1064335054	3.6310498199	4.1405852223
h	2.4049565150	3.4533023289	3.6000346780

h	2.9731276144	2.5863891450	5.0580671305
h	5.0883471520	2.8806664834	1.5588526096
h	4.5974737263	1.3444500144	0.7728827106
h	3.4197375929	2.6814984878	0.9305125600

Int-1_b (PMe₃Au⁺) [6-endo]

c	5.0515698449	-0.5726926189	-4.4125910053
c	4.1241397261	-1.0819804906	-5.3417931721
c	3.5146074002	-2.3166991940	-5.0498695732
c	3.8062641778	-3.0048366719	-3.8711924586
c	4.7201885486	-2.4780519884	-2.9549041868
c	5.3455136632	-1.2601857083	-3.2349498517
c	3.7333396913	-0.3323172062	-6.5643916196
c	4.6561671004	0.3735915722	-7.3756521140
c	4.1931593274	1.1036347708	-8.4827349089
c	2.8401828085	1.1436526238	-8.8102710604
c	1.9247843745	0.4425201710	-8.0227363287
c	2.3716885821	-0.2814313193	-6.9197776443
c	6.1161237063	0.3595488727	-7.1080946940
c	6.7967418726	1.5622787503	-6.7662068642
c	8.1829690653	1.5522348475	-6.4876525311
c	8.8950618871	0.3629126314	-6.5728903620
c	8.2309484188	-0.8233786596	-6.9104034647
c	6.8583891098	-0.8231801416	-7.1647715787
c	6.0797206878	2.7765707002	-6.6518295712
c	5.4686931068	3.8545975209	-6.5255236445
au	4.2433732196	2.8897057998	-5.0201608767
p	2.7862653477	2.3244155056	-3.3480251143
c	1.6775651769	0.9330419718	-3.7206185667
c	1.6964394374	3.7218559209	-2.9196294198
c	3.6306730920	1.8597404191	-1.8035206721
h	5.2277074784	4.8551486375	-6.8489055706
h	8.6779841004	2.4825363999	-6.2133276361
h	9.9654236606	0.3556521961	-6.3729819621
h	8.7888148228	-1.7573004990	-6.9732716565
h	4.9185778092	1.6290771193	-9.1042796586
h	2.5051967418	1.7085856518	-9.6793763255
h	0.8629305364	0.4586723740	-8.2671994578
h	1.6477901801	-0.8110788480	-6.3008514089
h	6.3458162725	-1.7519891288	-7.4121944964
h	2.8172587790	-2.7518678609	-5.7660497484
h	3.3253211400	-3.9625994331	-3.6737734699
h	4.9522030149	-3.0178763975	-2.0373732715
h	6.0738014616	-0.8461469238	-2.5367745646
h	5.5471680684	0.3776375705	-4.6057225909
h	2.8884758171	1.6521182250	-1.0213137264
h	4.2291741309	0.9593900788	-1.9876466366
h	4.2895475983	2.6734095678	-1.4794502243
h	1.0270553390	3.4349591352	-2.0982051299
h	2.3024146867	4.5829271428	-2.6142120835
h	1.0998197792	4.0028177604	-3.7953830972
h	0.9672656323	0.7982631377	-2.8942628051
h	1.1355856894	1.1331391120	-4.6514609162
h	2.2774084813	0.0239102175	-3.8479144398

TS1_b (PMe₃Au⁺) [6-endo]

c	0.2864090766	8.5003325528	-0.4573350448
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c	0.2526694566	7.1054479073	-0.2956709746
c	0.1861277446	6.2889231555	-1.4376008286
c	0.1552600012	6.8568451984	-2.7102278912
c	0.2012364755	8.2460083383	-2.8617636811
c	0.2667998720	9.0663730977	-1.7326321106
c	0.2660517872	6.5154311131	1.0640375232
c	1.1598674041	5.4796349197	1.4243838170
c	1.0897015423	4.9102554140	2.7319671036
c	0.1886433387	5.4231965809	3.6938489764
c	-0.6726875801	6.4487729865	3.3367913509
c	-0.6279343271	6.9839658451	2.0406763334
c	2.1561081425	4.9022092460	0.4978755355
c	2.0569632513	3.5176293141	0.1892771836
c	2.9755374976	2.9361696098	-0.6927024926
c	3.9980307593	3.7049365105	-1.2510035011
c	4.1007878115	5.0625494875	-0.9403784013
c	3.1807271663	5.6595320546	-0.0734443144
c	0.9355871408	2.8087943642	0.7983725514
c	0.1917299654	3.2496935947	1.7601766962
au	0.2277669979	0.9123306745	0.2393316182
p	-0.4296490494	-1.1738607222	-0.4609164007
c	-2.0669150922	-1.6844514779	0.1624768599
c	-0.5442906904	-1.3258627529	-2.2750854248
c	0.7095671917	-2.5020256843	0.0553122711
h	-0.6880097741	3.1261251029	2.3700887721
h	2.8803137094	1.8794388270	-0.9411586256
h	4.7099244710	3.2456415033	-1.9356279700
h	4.8931083691	5.6658543020	-1.3818788040
h	1.9097707351	4.2709091818	3.0630418329
h	0.1899928902	5.0177841374	4.7050021348
h	-1.3797688090	6.8518375619	4.0611006127
h	-1.3221532887	7.7790080998	1.7670976465
h	3.2512950956	6.7221315156	0.1549606152
h	0.3530440692	9.1426075254	0.4217809322
h	0.3070106339	10.1495606518	-1.8443373013
h	0.1840239508	8.6880080818	-3.8576214937
h	0.0923647365	6.2138771395	-3.5877605211
h	0.1440326016	5.2059599908	-1.3231630906
h	0.3516930567	-3.4731723674	-0.3113986383
h	1.7096791476	-2.3052382543	-0.3489420292
h	0.7734390207	-2.5250910271	1.1495726823
h	-0.8541525024	-2.3421231332	-2.5525027662
h	-1.2752369878	-0.6036459419	-2.6573760370
h	0.4320302915	-1.1074657146	-2.7237926674
h	-2.3177552922	-2.6870269713	-0.2086929632
h	-2.0541449934	-1.6936364198	1.2586837868
h	-2.8266494460	-0.9693083317	-0.1741921844

Int-2_b (PMe_3Au^+) [6-endo]

c	-0.2186347338	3.3226422413	1.5577754681
c	0.4524138446	2.7563439902	0.5223240749
c	1.4724642973	3.5605794018	-0.1424366884
c	1.6571947030	4.9651761239	0.1467347434
c	0.7165898738	5.6320406045	1.0101163992
c	-0.0186650077	4.7623719286	1.9676330311
c	2.7619710938	5.6446368873	-0.4325275965
c	3.6204489942	5.0049360374	-1.3060492003
c	3.3869366546	3.6639094003	-1.6597901843

c	2.3384109770	2.9641841515	-1.0826489139
c	-1.0195695440	5.3784955658	2.8552710051
c	-1.1820203085	6.7298066108	2.8789460901
c	-0.4678927613	7.5335945531	1.9546845362
c	0.4370724825	7.0285439420	1.0186391059
au	0.0024688761	0.8004307122	-0.0016434762
p	-0.5202863788	-1.3799369651	-0.5494065039
c	-2.1305781975	-1.9554937838	0.0957092697
c	0.9762021943	7.9880248983	0.0164775979
c	0.7014790228	7.8118799174	-1.3497425329
c	1.1743352638	8.7316636166	-2.2841102250
c	1.9311427220	9.8320570473	-1.8676853721
c	2.2011913643	10.0172485459	-0.5099211904
c	1.7185850340	9.1041616026	0.4306114938
c	-0.6133132028	-1.7003561065	-2.3465194415
c	0.6799281341	-2.6123148190	0.0678319156
h	-0.8784600628	2.7493443943	2.2106546810
h	2.1809872930	1.9134461089	-1.3268867408
h	4.0438529717	3.1668781634	-2.3734602750
h	4.4750546139	5.5408694671	-1.7167462295
h	0.7955144220	4.5566418006	2.7279622714
h	-1.5873340593	4.7213209869	3.5150575241
h	-1.8915872541	7.1961045334	3.5611592101
h	-0.6655899160	8.6062658329	1.9340603177
h	2.9578462153	6.6775547597	-0.1596807702
h	1.9377804034	9.2435766131	1.4901468051
h	2.7877298913	10.8740762307	-0.1797656075
h	2.3033495558	10.5470428222	-2.6006549877
h	0.9491405319	8.5920304396	-3.3410674720
h	0.1185326729	6.9501832393	-1.6751612339
h	0.3671362849	-3.6283079161	-0.2074191416
h	1.6677616352	-2.4063802092	-0.3617098056
h	0.7533597639	-2.5356990340	1.1591306056
h	-0.8822885221	-2.7474188428	-2.5395137251
h	-1.3655000314	-1.0413044752	-2.7961308516
h	0.3584824248	-1.4840022861	-2.8063723544
h	-2.3147163516	-2.9970890409	-0.1988812849
h	-2.1329645195	-1.8802475894	1.1896629852
h	-2.9306035758	-1.3177003560	-0.2989429113

TS-2_b (PMe₃Au⁺) [6-endo]

c	0.3983482983	0.2347479111	1.6492129865
h	1.5268803394	1.1279552481	1.8515581450
c	0.3878308047	6.2647969040	0.1437738719
c	-0.3098996049	5.0485819199	0.2060647857
c	-1.4078405975	4.8426112924	-0.6466499014
c	-1.7894657154	5.8310099022	-1.5521679538
c	-1.0775911177	7.0334633829	-1.6227380316
c	0.0096246334	7.2489654999	-0.7725722536
c	0.0632024512	4.0136330660	1.2069342407
c	0.3775720064	2.6611839193	0.8727247446
c	0.4769209989	1.7164119681	1.9710722032
c	0.4055793871	2.1510350445	3.3400564033
c	0.2079894969	3.4790800562	3.6128991858
c	0.0144888231	4.3877050645	2.5514671656
c	0.3318479603	-0.2343026811	0.3537494791
c	0.5040048698	0.7227599845	-0.7130865955
c	0.6025242679	2.1436419427	-0.4638949005

c	0.9508263421	2.9882306668	-1.5477811816
c	1.1121775592	2.4906926516	-2.8275955352
c	0.9167446641	1.1215238761	-3.0901013885
c	0.6296498476	0.2619787718	-2.0484488630
au	-0.0108528995	-2.2563903222	0.0784874199
p	-0.3856476051	-4.5203117884	-0.1985831069
c	1.1423177530	-5.5165481683	-0.3019175734
c	-1.3472496732	-5.2962358899	1.1470200355
c	-1.3087569418	-4.9393916986	-1.7185487077
h	0.4221363109	-0.4166209562	2.5223537234
h	0.5263343454	-0.8084554616	-2.2290048110
h	1.0181583112	0.7391899277	-4.1052727897
h	1.3934528590	3.1664655280	-3.6345667102
h	0.4998141663	1.4111294472	4.1349203129
h	0.1489839277	3.8288066924	4.6425575296
h	-0.2271267373	5.4253087729	2.7816810208
h	1.1155882691	4.0465504490	-1.3711621878
h	1.2430768439	6.4286201805	0.8002959124
h	0.5656308378	8.1847848173	-0.8208510053
h	-1.3751854120	7.8029561041	-2.3343539288
h	-2.6478945008	5.6656065313	-2.2025759558
h	-1.9592142481	3.9037625532	-0.5952823620
h	0.8994486198	-6.5790082563	-0.4348369491
h	1.7468719800	-5.1718372221	-1.1493941783
h	1.7259394798	-5.3873877077	0.6170918841
h	-1.4362344983	-6.0266853498	-1.8040263439
h	-2.2932579814	-4.4574937986	-1.6918386871
h	-0.7619942120	-4.5675332907	-2.5932987713
h	-1.4792328928	-6.3695080608	0.9560738150
h	-0.8217529593	-5.1582913102	2.0996055793
h	-2.3300051046	-4.8148803681	1.2175906576

Int-3_b (PMe₃Au⁺) [6-endo]

c	1.8583498411	6.0036122892	-0.1670563675
c	0.7689148752	5.1746751474	0.1687328340
c	0.8895155379	3.7638519545	-0.1565835096
c	1.9950718931	3.3243304753	-0.9548379692
c	3.0000120922	4.1844440862	-1.3291002672
c	2.9429839436	5.5234850781	-0.8887894602
c	-0.4164601846	5.6798185150	0.8608251022
c	-1.2064325025	4.7379199552	1.5669786785
c	-0.9507946944	3.2703700329	1.4066620649
c	0.0088174851	2.8056295966	0.3811177480
c	-2.2345941285	5.1587936850	2.4147444982
c	-2.5187448882	6.5131724857	2.5467089201
c	-1.8181290468	7.4456110153	1.7761674320
c	-0.7930608878	7.0597939332	0.9079708838
c	-0.2326936964	8.0976618330	0.0063342743
c	-0.2749276416	7.9191679078	-1.3880091127
c	0.2186055315	8.9035428406	-2.2422480933
c	0.7647943328	10.0798008522	-1.7176542493
c	0.7999602418	10.2721355190	-0.3341529873
c	0.2969196256	9.2914537893	0.5233001186
au	0.0108870692	0.8031282557	-0.0614234942
p	-0.0628197639	-1.4673426045	-0.5579857620
c	1.0267937871	-2.4865451865	0.4950309118
c	-1.7195850315	-2.2120343833	-0.3723324400
c	0.4359088377	-1.8668359655	-2.2685695880

h	-0.5372452096	2.8589205016	2.3548649965
h	-1.9045160135	2.7233233891	1.3192007524
h	2.0397956585	2.2661740152	-1.2152184489
h	3.8452639157	3.8341404042	-1.9193058192
h	3.7642579496	6.2021424245	-1.1202619553
h	-2.8191197404	4.4173439574	2.9610772335
h	-3.3182303191	6.8451401375	3.2083832391
h	-2.1043255648	8.4967750174	1.8070337014
h	1.8577291862	7.0442949752	0.1427519588
h	0.3345671771	9.4375037195	1.6033678609
h	1.2196104755	11.1885534785	0.0800772578
h	1.1527432755	10.8477228840	-2.3862004588
h	0.1696303472	8.7581488677	-3.3212783931
h	-0.7046998544	7.0040418717	-1.7964819402
h	-1.6896847064	-3.2811039943	-0.6209019246
h	-2.0624039941	-2.0887376907	0.6619691042
h	-2.4269337731	-1.7031819883	-1.0381229653
h	0.3726223023	-2.9488492460	-2.4429937356
h	-0.2229376754	-1.3448652145	-2.9726407339
h	1.4656722988	-1.5306827485	-2.4387222078
h	0.9454943477	-3.5455527272	0.2169799216
h	2.0655530485	-2.1566937426	0.3745120886
h	0.7412070052	-2.3624403352	1.5463096282

TS3_{b1} (PMe₃Au⁺) [6-endo]

c	0.3755632854	9.2914994754	0.3993536660
c	-0.1762466337	8.1085954605	-0.1167665612
c	-0.2359877685	7.9327523510	-1.5097181639
c	0.2640480863	8.9124508652	-2.3658782816
c	0.8335337850	10.0786546458	-1.8436715910
c	0.8857857988	10.2669770562	-0.4606220163
c	-0.7517420116	7.0784160448	0.7883392622
c	-0.3530173067	5.7074841891	0.8036481328
c	-1.1796868466	4.7962060412	1.5308172985
c	-2.2513953258	5.2395048661	2.3307255416
c	-2.5442802446	6.5892090417	2.3985616871
c	-1.8119575732	7.4839111705	1.6076676484
c	0.8565412410	5.1714216079	0.1659001398
c	1.0260666305	3.7541865865	0.0145049883
c	0.0545900253	2.8102532878	0.5604240908
c	-0.9707456345	3.3801575498	1.3800683965
c	2.1758248757	3.2499890284	-0.6317020395
c	3.1765983480	4.0919520353	-1.0831048261
c	3.0556120945	5.4722995699	-0.8612350710
c	1.9246080293	5.9970841502	-0.2530124839
au	0.0114629744	0.7758082437	0.0896071371
p	-0.0958524535	-1.4488346489	-0.5076577392
c	-1.6770896217	-2.2579845921	-0.0866812049
c	0.1075287642	-1.7289620477	-2.3000667059
c	1.1840519753	-2.4874431618	0.2772627894
h	0.1564104337	2.8535334538	1.8647038700
h	-1.7035206623	2.7072683423	1.8325947653
h	2.2706124074	2.1691581090	-0.7448024764
h	4.0597316906	3.6867224679	-1.5751389230
h	3.8578296801	6.1451696749	-1.1631066162
h	-2.8492937266	4.5086291638	2.8762285379
h	-3.3633032894	6.9513788634	3.0183368131
h	-2.0960165658	8.5364286168	1.5888078810

h	1.8751455841	7.0678552558	-0.0861382401
h	0.4254757956	9.4340952345	1.4794929987
h	1.3238375901	11.1754931059	-0.0480058088
h	1.2281303076	10.8413970619	-2.5142432061
h	0.2050493010	8.7693164989	-3.4446126582
h	-0.6762097550	7.0217317484	-1.9157968999
h	1.0842763274	-3.5299839309	-0.0523637693
h	2.1778163405	-2.1126818908	0.0051436298
h	1.0785523778	-2.4380771420	1.3675090150
h	0.0591346356	-2.8022140963	-2.5259833606
h	-0.6869992749	-1.2049896192	-2.8444593948
h	1.0755100719	-1.3309214348	-2.6267083727
h	-1.6662135813	-3.3076861202	-0.4084416775
h	-1.8358907414	-2.2115214438	0.9973042563
h	-2.5010113044	-1.7329295920	-0.5844982538

TS3_{b2} (PMe₃Au⁺) [6-endo]

c	-0.3323431406	-0.2231644967	-0.1390344374
h	-1.0220425915	0.0155502533	-1.2261510516
c	-0.1011998338	6.1899880373	0.8684288607
c	-0.2169143576	5.1575072835	-0.0750661090
c	0.5512918250	5.2152985770	-1.2501259606
c	1.4303222970	6.2752328527	-1.4663109239
c	1.5563078326	7.2896238699	-0.5114327652
c	0.7876670316	7.2458777193	0.6540372311
c	-1.1920655663	4.0513434374	0.1226310059
c	-0.8535221958	2.6634250237	0.1386757803
c	-1.9356793823	1.7313118313	0.0609568400
c	-3.2814325552	2.1444662258	0.1135600251
c	-3.5831743980	3.4880628132	0.2372362656
c	-2.5393963469	4.4217104106	0.2099315880
c	-1.6530412066	0.3292278136	-0.0959837757
c	0.7588543382	0.7319419606	0.0157922888
c	0.5082963905	2.1262679368	0.2519625895
c	2.0832014568	0.2419281038	0.0505369264
c	3.1472340935	1.0620302617	0.3797608703
c	2.8945070335	2.4009053970	0.7157996862
c	1.6096047775	2.9185971662	0.6493378673
au	-0.0841496854	-2.2994719292	-0.1504878096
p	0.1555300227	-4.5910264416	-0.0643219373
c	1.5718998493	-5.2260585165	-1.0250680357
c	0.4126668121	-5.2301716374	1.6261479381
c	-1.2880173840	-5.5119234605	-0.6974397966
h	-2.4991957990	-0.3610947002	-0.1365689195
h	2.2468088851	-0.8155572821	-0.1622755136
h	4.1620182396	0.6673410334	0.4064474037
h	3.7125356756	3.0470841799	1.0331428162
h	-4.0723720721	1.3959370479	0.0556038836
h	-4.6168910301	3.8243309803	0.3023636265
h	-2.7742823882	5.4862731519	0.2112389241
h	1.4551636094	3.9568261709	0.9229909711
h	-0.6949873611	6.1514437398	1.7824135495
h	0.8776191156	8.0363559823	1.3987246843
h	2.2460181321	8.1160631228	-0.6803910202
h	2.0150620757	6.3141313547	-2.3851770505
h	0.4540789658	4.4226732121	-1.9926022717
h	-1.1179182517	-6.5933797500	-0.6125991100
h	-2.1789442216	-5.2373604632	-0.1204223038

h	-1.4569060624	-5.2513645185	-1.7490661070
h	1.6342654854	-6.3187614899	-0.9365634689
h	1.4510830418	-4.9521272701	-2.0799154271
h	2.4996412471	-4.7771356884	-0.6510620310
h	0.5177241743	-6.3229309665	1.6086990824
h	1.3184151945	-4.7830978089	2.0527091708
h	-0.4415841376	-4.9557028139	2.2565189374

Prod-cpx_b (PMe₃Au⁺) [6-endo]

c	2.1952351870	6.2260872244	2.0683258963
c	1.0466093773	6.2555911486	1.2629879276
c	0.8500806980	7.3428360938	0.3944642125
c	1.7926282829	8.3667087867	0.3201011330
c	2.9457677809	8.3192784854	1.1103253362
c	3.1431814449	7.2490873952	1.9856259182
c	0.0048156956	5.1983592306	1.3669056284
c	-0.4596943096	4.4198648066	0.2604446693
c	-1.6663459840	3.6682656218	0.4513656416
c	-2.2802602798	3.5738196525	1.7177425266
c	-1.7338235116	4.2306911237	2.8039976519
c	-0.6167599901	5.0554665712	2.6112032833
c	0.2174693879	4.3320200906	-1.0395873031
c	-0.4594732149	3.7367111626	-2.1539777577
c	-1.7430198462	3.1085722206	-1.9569744560
c	-2.3030058614	3.0313766475	-0.6789723288
c	0.1435438427	3.7011322613	-3.4312261539
c	1.4249996221	4.1852543194	-3.6202496358
c	2.1371292069	4.6812927123	-2.5146529753
c	1.5497808951	4.7532119731	-1.2600442385
au	-1.1721092665	1.0230504139	-1.0437108198
p	-0.2828019579	-1.0481093069	-0.7287909930
c	-1.4800496161	-2.2382084180	-0.0449215969
c	0.3378686442	-1.8020009047	-2.2666621840
c	1.1277324167	-1.0487281419	0.4231890667
h	-2.3278112897	2.8192130059	-2.8329157622
h	-3.3283583789	2.6760945375	-0.5535591830
h	-0.4131963911	3.2646586382	-4.2618046022
h	1.8860796876	4.1599795145	-4.6069613847
h	3.1656991090	5.0190393212	-2.6391595231
h	-3.1932825197	2.9861183355	1.8203430939
h	-2.1946087603	4.1568277892	3.7882181020
h	-0.2413169118	5.6534260812	3.4419163111
h	2.1373085759	5.1388910030	-0.4335953171
h	2.3526779799	5.3874522270	2.7476910126
h	4.0361815296	7.2101752330	2.6089469402
h	3.6824202363	9.1197777777	1.0501748543
h	1.6244900324	9.2081174250	-0.3519303458
h	-0.0482084605	7.3773530702	-0.2227422134
h	0.7501098476	-2.7973518445	-2.0533488313
h	-0.4819628105	-1.8935147057	-2.9888713622
h	1.1199696587	-1.1658527573	-2.6975640502
h	1.5140627024	-2.0699125633	0.5408978036
h	1.9200567042	-0.3992628110	0.0326834901
h	0.8042859037	-0.6643997759	1.3976320567
h	-1.0017934455	-3.2180674361	0.0852082175
h	-1.8430892042	-1.8763701369	0.9240396608
h	-2.3325505471	-2.3345924082	-0.7273619374

TS1_a (Catalyst-6) [7-exo]

c	1.0900156022	3.9814731437	0.2644146397
c	-0.0156370875	4.0394976879	-1.4654357420
c	-0.8084142174	5.2118254384	-1.2573096867
c	-0.4571643890	6.3825656297	-1.9120943182
c	0.6607086010	6.4058384458	-2.7660297454
c	1.4356753509	5.2585818393	-2.9911332695
c	1.0766144561	4.0671560831	-2.3777159573
c	-1.7852690024	5.1899720763	-0.1411049713
c	-1.2906331502	5.5056702668	1.1524336281
c	-2.1820376836	5.4638121809	2.2373551251
c	-3.5246625503	5.1306287592	2.0525289038
c	-4.0091451683	4.8590645960	0.7704406775
c	-3.1393859079	4.8940345029	-0.3236926865
c	0.1008721402	5.9951656507	1.3235372255
c	1.2261716444	5.3119589113	0.7710261890
c	2.5115831523	5.8925190979	0.8203613717
c	2.7070352427	7.1054081777	1.4743183000
c	1.6190935269	7.7514735784	2.0691313483
c	0.3337800805	7.2041683947	1.9871041468
c	1.4038249604	2.7459145934	0.5774895472
au	0.9573326951	0.8911363527	-0.1635066232
p	0.3135923582	-1.2127926947	-0.8296616973
c	-1.3572888417	-1.6492540546	-0.3312750542
c	-2.2432913879	-2.6653397874	0.0109434100
n	-2.4330578699	-3.9547370475	0.1142167967
c	-1.3294088989	-4.8676088232	-0.3267753563
c	-0.6573574740	-5.5156627302	0.8827389171
c	1.2973584556	-2.5043867911	-0.0443855684
c	2.1731500595	-3.5866226952	-0.1607359421
n	2.7730231681	-4.4456329013	-0.9412401529
c	2.4914389074	-4.4040688318	-2.4154611834
c	1.9856651967	-5.7579968381	-2.9102978495
c	0.3977820999	-1.5719953378	-2.6034245397
c	-0.5270874032	-2.4074284683	-3.2515475363
c	-0.3546772200	-2.7084356820	-4.6031800422
c	0.7340692863	-2.1816616171	-5.3065684079
c	1.6460907264	-1.3374753788	-4.6650435628
c	1.4779450333	-1.0231980356	-3.3161424989
c	1.9049572628	-2.9952186971	1.1132667243
n	2.0696267359	-2.9398342885	2.4094642124
c	2.8750921257	-3.9735068359	3.1410495249
c	4.0332021415	-3.3422025130	3.9115764364
c	1.4468701593	-1.8360276953	3.2112844588
c	-0.0470359397	-1.6897029778	2.9273670722
c	2.2151188329	-0.5308789152	3.0085986484
c	-2.6375480716	-1.2931587929	0.1007177548
n	-3.5266448499	-0.3735761799	0.3573480767
c	-4.9215670198	-0.7268315531	0.7771218999
c	-5.9185241162	-0.3765466058	-0.3276877231
c	-3.1898349135	1.0778777829	0.1617892774
c	-2.6971083370	1.3342955762	-1.2596881867
c	-2.2418268050	1.5643649021	1.2543527036
c	-3.6809002220	-4.5488179612	0.6989919111
c	-3.8835863626	-4.0649352846	2.1354455264
c	-4.8725461354	-4.3416089785	-0.2358789852
c	-1.8347037342	-5.8781140359	-1.3563448600

c	3.8043892564	-5.4148130882	-0.4416703732
c	4.9842793507	-4.6769899791	0.1921276296
c	3.1605336088	-6.4997919012	0.4226622262
c	3.7146354980	-3.9006270101	-3.1806662267
c	-5.2606060840	-0.0951175321	2.1262245584
c	1.9645545434	-4.8356528901	4.0165694895
h	-4.1474057124	1.5990473322	0.2813025283
h	-2.6866392774	1.4450841400	2.2492562210
h	-2.0143307025	2.6281440814	1.1048662059
h	-1.2906018986	1.0128894799	1.2257854021
h	-1.6984576566	0.9105757565	-1.4379215323
h	-2.6295278436	2.4163144644	-1.4196050900
h	-3.3893142610	0.9219482703	-2.0039670686
h	-4.9069122941	-1.8148668442	0.8988632818
h	-4.5360287577	-0.3820971106	2.8988319171
h	-6.2530007367	-0.4379318496	2.4428952963
h	-5.2982319514	1.0006465602	2.0713158358
h	-5.9922529961	0.7067239750	-0.4892658683
h	-6.9163670535	-0.7303696302	-0.0400142678
h	-5.6471130990	-0.8523955665	-1.2789180445
h	-3.4716188178	-5.6247631399	0.7418144583
h	-5.0800866986	-3.2780563113	-0.4078789935
h	-5.7718277631	-4.7940856921	0.1987217228
h	-4.6930127749	-4.8116640700	-1.2104825138
h	-3.0367361177	-4.3580493933	2.7688796515
h	-4.7926783630	-4.5126351993	2.5544789708
h	-3.9903629069	-2.9743445025	2.1969424574
h	-0.6006220773	-4.2097212063	-0.8224686039
h	-2.5593612029	-6.5831862340	-0.9299402278
h	-0.9896441383	-6.4724728837	-1.7232627203
h	-2.2985784034	-5.3783338155	-2.2154936482
h	-1.3384140484	-6.1897637260	1.4178795098
h	-0.2998806551	-4.7517017050	1.5856824163
h	0.2018798153	-6.1116585268	0.5511023244
h	1.5639996480	-2.1612725537	4.2521050636
h	3.2716712283	-0.6353095743	3.2775389725
h	1.7770864341	0.2598209553	3.6309010918
h	2.1528463817	-0.2072581189	1.9581325530
h	-0.2262797348	-1.1980817262	1.9631106491
h	-0.4992481964	-1.0553263439	3.6990795345
h	-0.5606268081	-2.6595293220	2.9361297560
h	3.2924621161	-4.6048137359	2.3503765472
h	1.5127950759	-4.2614592888	4.8358995989
h	2.5566805372	-5.6385714164	4.4727252760
h	1.1619939103	-5.2969754458	3.4272503256
h	4.6746663495	-2.7401866969	3.2558962874
h	4.6467123881	-4.1403937866	4.3475918211
h	3.6878605313	-2.7120728768	4.7414048694
h	4.1755692136	-5.8984645645	-1.3529329777
h	2.6372822426	-6.0827987562	1.2926598682
h	3.9289631330	-7.1896637285	0.7919747927
h	2.4372096815	-7.0823308220	-0.1614271321
h	5.4618375341	-4.0118356036	-0.5379103909
h	5.7336904895	-5.4003020754	0.5348833304
h	4.6860104604	-4.0694833357	1.0553293630
h	1.6824356405	-3.6731840675	-2.5254321893
h	4.0265525192	-2.9111680584	-2.8237164642
h	3.4637630954	-3.8160500026	-4.2450351681
h	4.5659710256	-4.5890162794	-3.0974407369
h	2.7631711742	-6.5323422344	-2.8860470695
h	1.6589221450	-5.6575045774	-3.9524508922

h	1.1312676887	-6.1050690636	-2.3154102023
h	2.1841825881	-0.3589377024	-2.8151561250
h	2.4848028954	-0.9169817397	-5.2186254116
h	0.8628940805	-2.4180193358	-6.3624076845
h	-1.0741662991	-3.3489171276	-5.1122592050
h	-1.3802991826	-2.8179136554	-2.7120092789
h	1.9063014919	2.7164458151	1.5586641387
h	3.3479595942	5.3612557438	0.3675164206
h	3.7023734302	7.5446763264	1.5231901866
h	1.7651819648	8.7012373407	2.5827533110
h	-1.8120101122	5.6978450332	3.2356772607
h	-4.1983673695	5.1103989075	2.9084175576
h	-5.0663496122	4.6432156171	0.6173509783
h	-3.5156548519	4.7144041412	-1.3312610834
h	-0.5100387865	7.7443674598	2.4160352736
h	-1.0194948086	7.2971924320	-1.7269770820
h	0.9380592814	7.3424415362	-3.2504913354
h	2.2995599574	5.3060437692	-3.6522025877
h	1.6460980910	3.1536094956	-2.5447423384
h	-0.4591441109	3.0853728464	-1.1925732435

Int-2_a (Catalyst-6) [7-exo]

c	0.8623216342	4.0461452685	0.4348286791
c	1.0516073415	4.2121625081	-1.0751415553
c	0.4117363589	5.3746106058	-1.7617249464
c	0.9591621089	5.7982372833	-2.9824556883
c	2.1836215780	5.3148508621	-3.4308458582
c	2.9225588106	4.3379828066	-2.7092401391
c	2.3966943692	3.8163710042	-1.5642291311
c	-0.7787370125	5.9987099515	-1.2276772403
c	-0.8725975435	6.4261670932	0.1387038001
c	-2.0689936122	7.0453241542	0.5420669428
c	-3.1289977420	7.2488147945	-0.3376463334
c	-3.0188942226	6.8633692562	-1.6823747700
c	-1.8493546474	6.2660651922	-2.1204885534
c	0.2667201837	6.4002656261	1.0813238539
c	1.1031859305	5.2694410158	1.2329458329
c	2.1496839975	5.2979543294	2.1648898278
c	2.3846959507	6.4313634348	2.9437937984
c	1.5671253556	7.5544206043	2.7948564887
c	0.5178866133	7.5338407968	1.8790686465
c	0.6106808879	2.8478130191	0.9986330052
au	0.2916094406	1.0015832698	0.1951148787
p	-0.1480510236	-1.1415327011	-0.5681717439
c	-1.6974627370	-1.8657383783	-0.0069462431
c	-2.4274586370	-3.0203656209	0.2583169527
n	-2.4434408015	-4.3282664454	0.2494770997
c	-1.2440260800	-5.0466177856	-0.2886065300
c	-0.4374983587	-5.6632967526	0.8536995822
c	1.0502702471	-2.3623908524	0.0152923205
c	2.0537695929	-3.2928894234	-0.2623855948
n	2.7102835073	-3.9698730264	-1.1689084306
c	2.3394567928	-3.7893896735	-2.6119749984
c	1.9258698652	-5.1187528458	-3.2398817824
c	-0.1727080597	-1.3595182460	-2.3720171239
c	-0.9741485753	-2.3176736336	-3.0151940716
c	-0.8694668789	-2.4934144635	-4.3955027066
c	0.0311247173	-1.7197314491	-5.1358919047

c	0.8161766760	-0.7532579918	-4.4996674877
c	0.7113530689	-0.5635610886	-3.1209863552
c	1.7876348373	-2.8841659723	1.0805284794
n	2.0237502173	-2.9441442182	2.3664423812
c	3.0222494327	-3.9070957915	2.9343860515
c	4.1565199196	-3.1748294766	3.6502282438
c	1.3172449540	-2.0238002582	3.3173163691
c	-0.2004549165	-2.1477124805	3.2060965382
c	1.8144498118	-0.5897301808	3.1493709675
c	-2.9929848502	-1.7298295641	0.4984317921
n	-3.9722696123	-0.9636153051	0.8922646675
c	-5.3013356242	-1.5290474791	1.2927504626
c	-6.3841856171	-1.0949492855	0.3047982024
c	-3.7867632807	0.5265895428	0.9359502803
c	-3.4272427244	1.0809107810	-0.4408571885
c	-2.8013824420	0.8985454893	2.0425703690
c	-3.5686359777	-5.1309431607	0.8338364306
c	-3.7763352194	-4.7755811755	2.3060322761
c	-4.8167884474	-5.0376462269	-0.0435050076
c	-1.6449732108	-6.0558174193	-1.3642143615
c	3.8692795055	-4.8640371705	-0.8412435594
c	5.0035219274	-4.0739590542	-0.1894086677
c	3.4047338639	-6.1027851781	-0.0751013084
c	3.4599328292	-3.0821805171	-3.3730036721
c	-5.6289994358	-1.1858969746	2.7449745685
c	2.3248261469	-4.9483940172	3.8103069967
h	-4.7760830604	0.9129155852	1.2083325772
h	-3.1413657059	0.5266539069	3.0163394845
h	-2.6987932634	1.9886932940	2.1010275960
h	-1.8010632186	0.4890150440	1.8384758391
h	-2.4347332287	0.7479381872	-0.7727981087
h	-3.3978759326	2.1761595562	-0.3927067269
h	-4.1689147452	0.7860292971	-1.1932779713
h	-5.1746612549	-2.6138126911	1.2118982082
h	-4.8356796117	-1.5178684267	3.4269622383
h	-6.5597198991	-1.6907328184	3.0320907023
h	-5.7873630472	-0.1095242870	2.8902616167
h	-6.5698291145	-0.0136227318	0.3444234372
h	-7.3270875076	-1.5945540533	0.5597996533
h	-6.1194768852	-1.3669804501	-0.7251213586
h	-3.2072762761	-6.1659561907	0.7950777875
h	-5.1806127342	-4.0061539743	-0.1307874381
h	-5.6230530180	-5.6437051405	0.3868860586
h	-4.6141377994	-5.4095442254	-1.0551980656
h	-2.8586066341	-4.9496403780	2.8816839345
h	-4.5696138473	-5.4020945762	2.7312346063
h	-4.0700707425	-3.7280382077	2.4441025467
h	-0.6348756691	-4.2632772706	-0.7625196262
h	-2.2565453801	-6.8735175115	-0.9631089178
h	-0.7414300771	-6.5127716885	-1.7859434048
h	-2.1982965475	-5.5748544571	-2.1802521331
h	-0.9967475097	-6.4548863999	1.3687578526
h	-0.1580926545	-4.8982534806	1.5895744856
h	0.4797548465	-6.1144361297	0.4555137442
h	1.6136509777	-2.3842260102	4.3092976591
h	2.9033716563	-0.5262108503	3.2579378301
h	1.3547830235	0.0551210064	3.9085790838
h	1.5392728128	-0.1891829380	2.1609328777
h	-0.5692875311	-1.7479526159	2.2537141264
h	-0.6711331948	-1.5641756370	4.0066042131
h	-0.5275915613	-3.1907784013	3.3043997187

h	3.4396672077	-4.4166837835	2.0601973782
h	1.8798610576	-4.5029918904	4.7095339576
h	3.0606417741	-5.6892162048	4.1469971583
h	1.5396854774	-5.4765465376	3.2544520522
h	4.6422656679	-2.4425123577	2.9924923548
h	4.9124373215	-3.9051344637	3.9637522353
h	3.8112694905	-2.6575437521	4.5546154620
h	4.2274697623	-5.2008578869	-1.8214837663
h	2.9355862259	-5.8471231729	0.8834733077
h	4.2597711065	-6.7571064132	0.1341952680
h	2.6791977861	-6.6746171148	-0.6672186443
h	5.3427265904	-3.2666201650	-0.8500955037
h	5.8550258257	-4.7372471506	0.0040990093
h	4.7055771971	-3.6259633909	0.7663152383
h	1.4640325010	-3.1328478843	-2.5944739668
h	3.7115731167	-2.1216043805	-2.9052616158
h	3.1260258855	-2.8843919465	-4.3989886656
h	4.3701076212	-3.6925357814	-3.4348873499
h	2.7601080796	-5.8285536152	-3.3137766491
h	1.5634369491	-4.9353405698	-4.2589907765
h	1.1154630442	-5.5898873910	-2.6697668636
h	1.3188140548	0.1931062501	-2.6215120230
h	1.5060377301	-0.1419973641	-5.0803819335
h	0.1091352308	-1.8608578969	-6.2135181335
h	-1.4943894537	-3.2314558794	-4.8972181082
h	-1.6811725895	-2.9229651852	-2.4489062530
h	0.5651277014	2.8641667625	2.0955017107
h	2.7825873180	4.4165828181	2.2715493806
h	3.2044727800	6.4397991493	3.6612249417
h	1.7513516164	8.4504087397	3.3860978802
h	-2.1646361057	7.3722939511	1.5766045337
h	-4.0430480985	7.7220779890	0.0203137502
h	-3.8423222484	7.0315667905	-2.3748161335
h	-1.7631430557	5.9484225415	-3.1596782217
h	-0.1000854724	8.4229122551	1.7553422613
h	0.4739245425	6.6053294226	-3.5302191022
h	2.6103116318	5.7321301885	-4.3439950494
h	3.9038264964	4.0298328511	-3.0678784014
h	2.9162091426	3.0547836083	-0.9826200479
h	0.4188604214	3.3868247915	-1.5064851896

TS2_a (Catalyst-6) [7-exo]

c	0.6183633212	4.0584536918	0.8007174767
h	0.0004057559	3.8114708940	-0.2694984899
c	0.8554828341	-0.0624873846	-2.7679922338
c	-0.0174085595	-1.0179727609	-2.2181354386
c	-0.6905477608	-1.9236090516	-3.0551666194
c	-0.4691317142	-1.8880332071	-4.4323720000
c	0.4200041280	-0.9546964344	-4.9764655511
c	1.0756623671	-0.0410986833	-4.1454840878
p	-0.1677647991	-1.0703192729	-0.4099856189
c	1.0967630389	-2.2356258703	0.1320428001
c	1.8006137415	-2.8188536468	1.1876271194
n	1.9478883581	-3.0073756358	2.4729941644
c	1.0870486900	-2.2672405921	3.4536965037
c	1.4940400689	-0.7961274952	3.5207403790
au	0.0524066671	1.0067569933	0.5844021834
c	0.2555169999	2.8694066813	1.3917864485

c	0.7489305390	5.3554849015	1.5038877173
c	0.1859898623	6.5576708203	1.0221140765
c	0.4099079114	7.7302800492	1.7670536817
c	1.1623341946	7.7183800637	2.9389677659
c	1.7141709493	6.5215869687	3.4051543038
c	1.5111220855	5.3481515168	2.6851359297
c	-0.6529036772	6.6205537650	-0.1945086299
c	-0.2948000203	5.9960753573	-1.4193013649
c	-1.1041938386	6.1988401535	-2.5569408371
c	-2.2497486316	6.9840950619	-2.5023816726
c	-2.6106041642	7.5908480456	-1.2957188303
c	-1.8186286125	7.4098045895	-0.1659097304
c	0.9029621433	5.1468231587	-1.5837532226
c	1.2442542689	4.1068608131	-0.6691882688
c	2.2761106884	3.1784608010	-0.9541745129
c	3.0150760460	3.3132960549	-2.1173525077
c	2.7266633581	4.3602018869	-3.0099484182
c	1.6918127818	5.2506925970	-2.7468632865
c	-1.6834817963	-1.9773989713	-0.0910511174
c	-3.0264963263	-2.0113257333	0.2929831938
n	-4.1048189225	-1.3776463127	0.6599106236
c	-4.0678146588	0.1123431783	0.8484817855
c	-3.2302820654	0.4667018616	2.0761681252
c	-2.3224360437	-3.2121286467	-0.0349738891
n	-2.2162404916	-4.5037886033	-0.2050611677
c	-3.3154578608	-5.4612409635	0.1535669787
c	-4.4829544257	-5.3365059400	-0.8253039333
c	-0.9149939644	-5.0441265459	-0.7162631950
c	-1.1323115491	-5.9232498798	-1.9469071925
c	-0.1518435258	-5.7459132845	0.4062472129
c	2.1940033538	-3.0457109145	-0.1684373003
n	2.9693746470	-3.5571635982	-1.0878254307
c	4.1868655111	-4.3728405380	-0.7655980130
c	3.7943973829	-5.7297091781	-0.1808640865
c	2.6867420657	-3.2364784310	-2.5271667463
c	3.7655580224	-2.3135235514	-3.0917898484
c	2.4931937218	-4.5114210817	-3.3449457260
c	2.9772337011	-3.9557746254	3.0134496175
c	2.3007369212	-5.1575082260	3.6736287188
c	3.9683748488	-3.2396857495	3.9289017974
c	-0.4010450948	-2.4576225816	3.1678509717
c	-5.4064010732	-2.0926959456	0.8742028087
c	-5.8954181674	-1.9156848500	2.3104427085
c	-6.4300588799	-1.6639956027	-0.1770156658
c	-3.6343677740	0.8224690738	-0.4322912355
c	-3.6837053121	-5.3280236052	1.6313974566
c	5.1843547203	-3.5628230758	0.0627046886
h	-5.1105615291	0.3845789537	1.0493686770
h	-3.6308372103	-0.0052475310	2.9811572736
h	-3.2286418620	1.5533695328	2.2243738073
h	-2.1848147272	0.1483942003	1.9491662647
h	-2.5804232437	0.6296153381	-0.6769274035
h	-3.7420531600	1.9059475601	-0.3003072730
h	-4.2531562747	0.5174116383	-1.2847829354
h	-5.1688824982	-3.1501569404	0.7155631223
h	-5.1397294532	-2.2410015012	3.0366806282
h	-6.7965013180	-2.5232587139	2.4592379453
h	-6.1685310901	-0.8755349057	2.5303774761
h	-6.7212433410	-0.6114055168	-0.0656867817
h	-7.3400934763	-2.2653172819	-0.0598391605
h	-6.0479261933	-1.8154165104	-1.1945517663

h	-2.8642685048	-6.4517806135	0.0165631268
h	-4.9029868481	-4.3226296959	-0.8348746535
h	-5.2839740909	-6.0303251531	-0.5434410579
h	-4.1670085051	-5.5794421923	-1.8470603245
h	-2.8105043460	-5.5157543261	2.2691232786
h	-4.4567875539	-6.0617715567	1.8888398213
h	-4.0752713541	-4.3327359381	1.8759970372
h	-0.3438435245	-4.1564722573	-1.0264179580
h	-1.6883843267	-6.8394285628	-1.7125842444
h	-0.1591662665	-6.2360158969	-2.3448846753
h	-1.6674818090	-5.3830544003	-2.7374602600
h	-0.6787227070	-6.6407292358	0.7623537896
h	-0.0004152072	-5.0686229264	1.2567123873
h	0.8305859039	-6.0671199714	0.0390408091
h	1.3102547854	-2.7407011599	4.4171670539
h	2.5547357838	-0.6813418993	3.7705255377
h	0.9018247129	-0.2807561153	4.2870514592
h	1.3062327161	-0.2945941817	2.5579766032
h	-0.7197998553	-1.8884473813	2.2851992962
h	-0.9825854747	-2.0842983823	4.0196317943
h	-0.6532422972	-3.5152426918	3.0186455079
h	3.5169449031	-4.3072730069	2.1284981810
h	1.7318887574	-4.8732142736	4.5686139462
h	3.0675861244	-5.8742626926	3.9921182926
h	1.6249681531	-5.6697188905	2.9766156070
h	4.4448641514	-2.3913566066	3.4215222905
h	4.7550309100	-3.9447552390	4.2245932811
h	3.4966970828	-2.8776543274	4.8514636619
h	4.6478783078	-4.5566961749	-1.7435457724
h	3.2131362130	-5.6297448878	0.7447582106
h	4.6938123103	-6.3132607248	0.0501316098
h	3.1955640913	-6.3033063798	-0.8994078052
h	5.4921964419	-2.6583527320	-0.4762702281
h	6.0803873525	-4.1643524515	0.2573652624
h	4.7720917384	-3.2551125091	1.0314578901
h	1.7363921226	-2.6931783931	-2.5094783744
h	3.8520700938	-1.3965750378	-2.4954192070
h	3.4946552064	-2.0294341625	-4.1160315398
h	4.7476854097	-2.8020118377	-3.1334834457
h	3.4220537444	-5.0842795988	-3.4584610981
h	2.1520910120	-4.2404599493	-4.3519414133
h	1.7344406910	-5.1625775055	-2.8928679810
h	1.3566410166	0.6645884670	-2.1263836757
h	1.7523113470	0.6987578316	-4.5716902421
h	0.5880970394	-0.9294552537	-6.0526925064
h	-0.9955707385	-2.5842733801	-5.0843821454
h	-1.3879725512	-2.6515989036	-2.6413074843
h	-0.0023494894	2.9805212970	2.4524484621
h	1.9628298581	4.4153830000	3.0254498244
h	2.3131984167	6.5068507772	4.3145797364
h	1.3321679338	8.6475459719	3.4813450495
h	-2.1075445607	7.8844113526	0.7713921846
h	-3.5080263870	8.2056397054	-1.2359092375
h	-2.8601482097	7.1201656777	-3.3941138478
h	-0.8347117359	5.7118116946	-3.4942169322
h	0.0042764645	8.6726149298	1.4008954312
h	1.4861739224	6.0604906606	-3.4450548914
h	3.3310963613	4.4904039042	-3.9072220658
h	3.8529453263	2.6440041747	-2.3092487470
h	2.5346162775	2.4293592536	-0.2087898053

Prod-cplx_a (Catalyst-6) [7-exo]

c	-0.1277530531	3.7762577104	-0.1326739194
h	-0.7703205001	3.4198460022	-2.1295492209
c	-0.2557117619	-1.1291998795	-4.0792826609
c	-0.7513229339	-1.9261185787	-3.0330061636
c	-1.2660521991	-3.2064901974	-3.3006572609
c	-1.2627050378	-3.6908378700	-4.6087992013
c	-0.7486862214	-2.9058071567	-5.6471474254
c	-0.2492485130	-1.6267014986	-5.3830763616
p	-0.6237544597	-1.2783887729	-1.3447983268
c	0.9505542581	-1.8810878099	-0.7147830464
c	1.9376683512	-1.8223131445	0.2708582942
n	2.3468424723	-1.3733611399	1.4288856308
c	1.5644693061	-0.3214164960	2.1598300848
c	1.7316837500	1.0327489481	1.4727442746
au	-0.8005323459	0.9994251523	-1.1527665727
c	-0.9975557934	3.1394802987	-1.0948290399
c	-0.5662062958	3.9309271180	1.2466168898
c	-0.2554507158	5.0480899777	2.0890597328
c	-0.6115262288	4.9675213874	3.4535056762
c	-1.2952986580	3.8831985881	3.9834125339
c	-1.6779600185	2.8286783686	3.1411529356
c	-1.3233717786	2.8659545834	1.8055947918
c	0.2477994395	6.3306527889	1.5839580851
c	1.2659482818	6.4442751167	0.5986248329
c	1.6804300325	7.7347557142	0.2025307926
c	1.1193239599	8.8822971224	0.7462651157
c	0.1174433107	8.7699036645	1.7172032933
c	-0.3044005799	7.5118986621	2.1254088587
c	1.9303798190	5.2939650523	-0.0265482603
c	1.2299230022	4.1360452085	-0.5034275128
c	1.9225372776	3.2495419602	-1.3743544341
c	3.2606099036	3.4097793862	-1.6802166433
c	3.9669400375	4.4915307432	-1.1337845944
c	3.3015652913	5.4134482627	-0.3391195220
c	-1.8231956504	-2.2274581059	-0.4052663409
c	-3.1276244260	-2.3826457714	0.0735694993
n	-4.3404583495	-1.9202657414	0.1931520801
c	-4.6669864087	-0.5440738305	-0.3133963089
c	-3.9777290765	0.5016274676	0.5603016892
c	-2.1504470535	-3.4111988443	0.2503364842
n	-1.7473431219	-4.5898739046	0.6482208164
c	-2.5791919588	-5.4769534056	1.5299673353
c	-3.7233150434	-6.1100959110	0.7382515501
c	-0.3537445123	-5.0111742935	0.2920514739
c	-0.3310440307	-6.4185700105	-0.3022941457
c	0.5722431780	-4.8483380777	1.4966908292
c	2.1393182188	-2.5848038065	-0.9239414906
n	2.8450597119	-3.3395951404	-1.7230775479
c	4.2325467733	-3.8057152175	-1.3948557562
c	4.2110227781	-4.7948878162	-0.2303690306
c	2.2780336854	-3.6898258260	-3.0702183975
c	3.0812064776	-3.0155718208	-4.1817367469
c	2.1577646909	-5.2022411449	-3.2392048182
c	3.6311623623	-1.8489923215	2.0407348623
c	3.3505533322	-2.6408093459	3.3179393202
c	4.6162834378	-0.6999675421	2.2485451025
c	0.1017430187	-0.7133599301	2.3555151632

c	-5.4414770685	-2.7382861124	0.8014465265
c	-6.0203371802	-2.0468869547	2.0347329359
c	-6.4912873168	-3.0841896036	-0.2548803424
c	-4.3648391649	-0.4096106802	-1.8044546803
c	-2.9967034491	-4.7386260268	2.8016886970
c	5.1853766283	-2.6218948335	-1.2319295646
h	-5.7510418835	-0.4544544670	-0.1773919512
h	-4.2802546204	0.4095031443	1.6099727172
h	-4.2306445660	1.5106442300	0.2131937975
h	-2.8844351615	0.3908535649	0.5011969644
h	-3.2875071569	-0.4456453848	-2.0168009582
h	-4.7306739210	0.5601852339	-2.1625875549
h	-4.8618343730	-1.1971677718	-2.3833385698
h	-4.9513521781	-3.6646353849	1.1202136638
h	-5.2412316424	-1.8245135463	2.7751439515
h	-6.7577363416	-2.7097825952	2.5039465469
h	-6.5416339202	-1.1146008074	1.7811112241
h	-7.0294837507	-2.1957326997	-0.6091402209
h	-7.2359641395	-3.7595273380	0.1848127623
h	-6.0399405471	-3.5873827579	-1.1194795448
h	-1.8908222591	-6.2770252167	1.8282211896
h	-4.3979984429	-5.3532207291	0.3187856030
h	-4.3144166136	-6.7632475604	1.3912652974
h	-3.3399031171	-6.7164799446	-0.0912133946
h	-2.1176107155	-4.3906771798	3.3586897691
h	-3.5652656416	-5.4150511142	3.4510786348
h	-3.6326717454	-3.8701164213	2.5910614272
h	-0.0409345479	-4.3060842124	-0.4919158245
h	-0.6433365875	-7.1841847841	0.4181843608
h	0.6968593101	-6.6649239890	-0.5968448497
h	-0.9699551436	-6.4921253782	-1.1905951806
h	0.2994600343	-5.5282957407	2.3138746227
h	0.5433084330	-3.8180260327	1.8746646395
h	1.6034389892	-5.0821693138	1.2032482605
h	2.0344345920	-0.2772263904	3.1494509669
h	2.7848571000	1.3144412685	1.3705276512
h	1.2170720310	1.8103600058	2.0498591301
h	1.2813896724	1.0150878011	0.4688216136
h	-0.4589022943	-0.6974675175	1.4113367504
h	-0.3747360967	0.0187409410	3.0190172136
h	0.0061732092	-1.7066587290	2.8118513256
h	4.0503717160	-2.5341379022	1.2968030969
h	2.9291285262	-2.0104177209	4.1119460741
h	4.2914005911	-3.0551636674	3.7011166444
h	2.6624357692	-3.4736599190	3.1285705669
h	4.8060773587	-0.1553780863	1.3147913578
h	5.5697749170	-1.1091492902	2.6039724587
h	4.2683481886	0.0132207009	3.0068984919
h	4.5438008796	-4.3583675146	-2.2895010080
h	3.82665552947	-4.3403171069	0.6918223105
h	5.2263265378	-5.1553415852	-0.0259702352
h	3.5847306313	-5.6635113455	-0.4702431957
h	5.2188306815	-2.0221553574	-2.1495548524
h	6.1990595528	-2.9862160970	-1.0257865218
h	4.8931673363	-1.9625332951	-0.4055736961
h	1.2704134093	-3.2627422639	-3.0660214755
h	3.1230157492	-1.9285512042	-4.0382516428
h	2.5920857142	-3.2123479487	-5.1437291701
h	4.1060650165	-3.4029280830	-4.2496504220
h	3.1340370731	-5.7022544320	-3.2710360781
h	1.6519929494	-5.4145922172	-4.1894048301

h	1.5622546697	-5.6457652660	-2.4317331114
h	0.1205722426	-0.1254088540	-3.8757997184
h	0.1331097069	-1.0100531448	-6.1955541811
h	-0.7533390161	-3.2864934157	-6.6681085439
h	-1.6676813299	-4.6796266662	-4.8218203889
h	-1.6657519993	-3.8257610724	-2.4979797151
h	-2.0597830842	3.2705376465	-0.8599726223
h	-1.5588324668	2.0123958707	1.1718727182
h	-2.2282287929	1.9757831015	3.5376797440
h	-1.5330868663	3.8573626910	5.0463142418
h	-1.1125759913	7.4359213280	2.8512937059
h	-0.3451475147	9.6615592540	2.1382787863
h	1.4462327346	9.8625213829	0.4019115058
h	2.4294494802	7.8345260731	-0.5815326173
h	-0.3290428367	5.7879209708	4.1109692810
h	3.8528141004	6.2614258067	0.0637801303
h	5.0303649808	4.6158241442	-1.3358344897
h	3.7653873429	2.6887510655	-2.3221149628
h	1.3951200224	2.3735774176	-1.7529493606

Final Product [7-exo]

c	-0.2237651996	4.2183881609	-0.1677390740
h	-0.9894223788	3.5556371722	-2.0322394763
c	-1.1812061106	3.7331403852	-0.9740717705
c	-0.4288436952	4.4212488396	1.2893115731
c	-0.1782799423	5.6723200236	1.9001162548
c	-0.3169544823	5.7721408415	3.2973095826
c	-0.7115005637	4.6833131153	4.0719047971
c	-0.9872616773	3.4590018938	3.4583378285
c	-0.8369170000	3.3342563215	2.0782644164
c	0.1275417332	6.8867398747	1.1069138133
c	1.0370400820	6.9099566189	0.0168967954
c	1.2541879431	8.1320309254	-0.6504854624
c	0.6108084397	9.3062244209	-0.2720646968
c	-0.2844490719	9.2831593624	0.7997276421
c	-0.5163874065	8.0864239954	1.4703591944
c	1.7870892473	5.7224183434	-0.4579335403
c	1.1666349906	4.4627542462	-0.6289589156
c	1.8900999223	3.4061250867	-1.2039450176
c	3.2174723228	3.5686375804	-1.5966999093
c	3.8462479942	4.8003827305	-1.4003797369
c	3.1341734243	5.8598793160	-0.8421537141
h	-2.1821911083	3.5240618193	-0.5969512974
h	-1.0187529236	2.3772273820	1.5884849944
h	-1.3004506108	2.6006886111	4.0528253317
h	-0.7974543540	4.7897269889	5.1533945925
h	-1.2379487708	8.0631408367	2.2870072303
h	-0.8135810458	10.1874863267	1.1004010662
h	0.7937300673	10.2290977797	-0.8225871058
h	1.9289537939	8.1454109005	-1.5065387282
h	-0.0957218663	6.7232856580	3.7822261523
h	3.6324063824	6.8169504007	-0.6848150643
h	4.8923211512	4.9353659285	-1.6758497447
h	3.7625166965	2.7334542496	-2.0367065388
h	1.3944671508	2.4421529119	-1.3220586141

TS1_b (PMe₃Au⁺) [7-exo]

c	0.9521678377	1.0773735594	-0.4132795170
c	0.1906124089	3.0639952112	-1.4769564527
c	1.5527903656	2.6644524969	-1.2057577247
c	-0.2824131701	2.8500590124	-2.7895576049
c	2.4351600325	2.3210932048	-2.2880782492
c	1.9423857877	2.1486147829	-3.5553780622
c	0.5640571189	2.3904039584	-3.7880319435
c	-0.6948809438	3.6047172734	-0.4324683304
c	-0.5837510087	3.3145905556	0.9628673319
c	-1.5898049562	3.8296434554	1.8037855048
c	-2.6051962836	4.6679365251	1.3480914673
c	-2.6581233727	5.0155237279	-0.0001388365
c	-1.7228818676	4.4686403898	-0.8702708793
c	0.4600208792	2.4756768134	1.6224548309
c	0.8155159921	2.7584754081	2.9548503811
c	1.6879263676	1.9454544925	3.6794128159
c	2.2412938071	0.8118447776	3.0844088403
c	1.9577019825	0.5394393764	1.7474912826
c	1.0897074661	1.3623301698	1.0096811654
c	0.6178996620	0.0500125556	-1.1553361309
au	0.0354491884	-1.7470908541	-0.3216069621
p	-0.6863602944	-3.7539323578	0.5378246121
c	0.5869392157	-5.0635351753	0.5583610506
c	-1.2709247918	-3.6510695963	2.2651513994
c	-2.0851229600	-4.4858441236	-0.3801125935
h	-1.3320981777	3.0167694071	-3.0210344959
h	0.6130378540	0.1230824805	-2.2483921061
h	2.4239513351	-0.3046821746	1.2407446906
h	2.9221122271	0.1679050269	3.6398866813
h	1.9391235671	2.2075054888	4.7065334753
h	-1.5897715732	3.5437127803	2.8539063288
h	-3.3486139640	5.0458552979	2.0491900200
h	-3.4247898433	5.6917238776	-0.3754326069
h	-1.7658356054	4.7475443618	-1.9218737511
h	0.4112533564	3.6471813036	3.4363968266
h	2.0336666119	3.1037801024	-0.3335226861
h	3.4871433052	2.1527298618	-2.0613827189
h	2.5884899577	1.8406611639	-4.3757492731
h	0.1588832854	2.2271250126	-4.7874089988
h	-1.6118883999	-4.6345818809	2.6145662026
h	-0.4543457930	-3.2979616815	2.9060601213
h	-2.0980731886	-2.9340102012	2.3275924607
h	-2.3897812282	-5.4362302907	0.0776944477
h	-2.9311696051	-3.7884114465	-0.3726520684
h	-1.7864583356	-4.6604997975	-1.4204693951
h	0.1686230919	-5.9991603410	0.9526827484
h	0.9567114724	-5.2294542668	-0.4604247154
h	1.4271690868	-4.7458202411	1.1869768799

Int-2_b (PMe₃Au⁺) [7-exo]

c	0.8490196194	7.6821522046	1.6586580802
c	0.6038592725	6.4226751081	1.0797612257
c	1.5028312628	5.3647141575	1.3553860838

c	2.5972014144	5.5797245331	2.2023625690
c	2.8190722372	6.8329550916	2.7732166958
c	1.9476654022	7.8887819586	2.4898878204
c	-0.6159652740	6.2163670588	0.2639472446
c	-0.6462495391	5.5294719238	-0.9933118236
c	-1.8443985575	5.5078849292	-1.7476697351
c	-3.0094285459	6.0889225939	-1.2734817420
c	-2.9901736427	6.7448053015	-0.0357037410
c	-1.8126234917	6.8135279498	0.7024572351
c	0.5308444227	4.9037687026	-1.5726945862
c	1.3806341844	4.0078483209	-0.7692775103
c	2.6852022406	3.6329517474	-1.3335981842
c	2.9928121057	3.8971234687	-2.6412811184
c	2.0636393479	4.6081149582	-3.4394984114
c	0.8650367580	5.0908090984	-2.9230370199
c	1.2493702252	4.0442188497	0.7450555697
c	0.8922781560	2.9194087090	1.3962921790
au	0.3695821674	1.1989238337	0.4109953289
p	-0.2889958172	-0.7517094151	-0.6850234202
c	-0.5105213142	-0.5716140072	-2.4916067805
c	-1.8855055855	-1.4223950907	-0.1004475488
c	0.8791989110	-2.1468758098	-0.5117273953
h	0.8250865256	2.9830589164	2.4887762395
h	3.2697179869	4.7480539240	2.4131292116
h	3.6718672622	6.9874609673	3.4336149912
h	2.1254177078	8.8755206848	2.9159470298
h	-1.8154225605	7.3248110005	1.6641537809
h	-3.8992988335	7.2007036084	0.3557081406
h	-3.9290910519	6.0272584434	-1.8534904721
h	-1.8560730725	4.9784622034	-2.7003827817
h	0.1795295320	8.5132464265	1.4364712421
h	0.2221164771	5.7064058280	-3.5514558524
h	2.3108251813	4.8171456126	-4.4810228325
h	3.9420765986	3.5754083959	-3.0674059083
h	3.3499502654	3.0584295839	-0.6883059777
h	0.8405358758	2.9799930789	-0.9418221059
h	-0.8263045772	-1.5227524626	-2.9401936813
h	-1.2705570739	0.1932903833	-2.6912276173
h	0.4357076249	-0.2533613991	-2.9455772619
h	0.5047960395	-3.0347065098	-1.0383922804
h	1.8542038490	-1.8613924804	-0.9245475225
h	1.0086587695	-2.3825820441	0.5514382251
h	-2.1472376734	-2.3368165927	-0.6491475531
h	-1.8144262021	-1.6487610540	0.9702830296
h	-2.6716233128	-0.6717234886	-0.2445408165

TS2_b (PMe₃Au⁺) [7-exo]

h	-0.0798666693	0.9316106609	-0.4008933804
c	0.3328392481	1.1910095441	0.8162458870
c	1.1160140597	1.3234743493	-0.5870287502
c	-0.1439889484	4.8115681610	1.9001331669
c	-0.2213680866	3.6667227716	1.0850793602
c	0.3435081362	2.4691033178	1.5697585889
c	0.9733728334	2.4416596118	2.8253327088
c	1.0319278771	3.5858614520	3.6168292304
c	0.4717693787	4.7771187532	3.1485979897
c	-0.9116432229	3.7539477956	-0.2205017770
c	-0.3702711132	3.2173212143	-1.4169140641

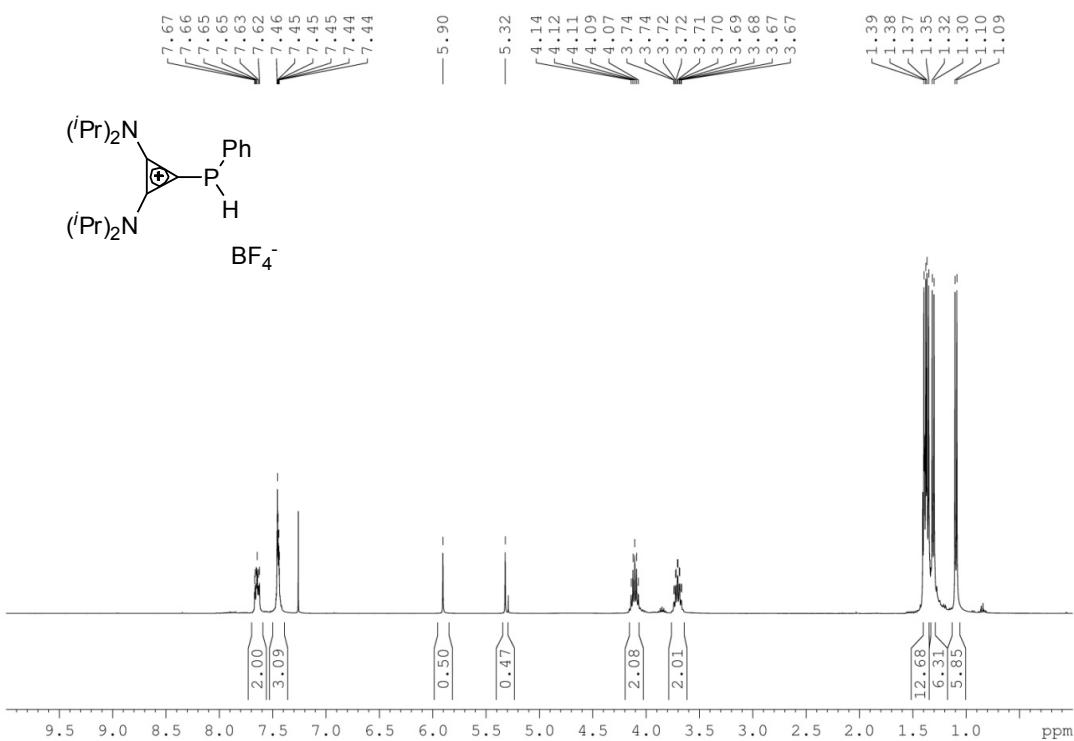
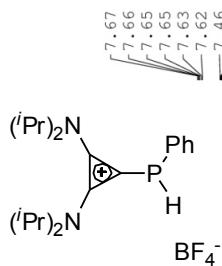
c	-1.0443953015	3.4377576673	-2.6354213218
c	-2.2358572287	4.1528320418	-2.6867000355
c	-2.7797712292	4.6685264215	-1.5071267479
c	-2.1197250468	4.4725617544	-0.2979480789
c	0.8761291789	2.4226459128	-1.4667413642
c	1.8101760734	2.6289421084	-2.4969806497
c	2.8970867464	1.7774561489	-2.6746057277
c	3.0855963463	0.6677913070	-1.8344522385
c	2.2005974807	0.4358218385	-0.7959038835
c	-0.0656826168	-0.0255853457	1.2973872099
au	-0.1828078839	-1.8673762606	0.4175114253
p	-0.4052756221	-3.9871467429	-0.4907485768
c	0.8589659195	-5.1745202393	0.0822132919
c	-1.9996114343	-4.7863155553	-0.0980453839
c	-0.2980898479	-4.0434129812	-2.3133601767
h	-0.4385626231	0.0420087900	2.3281823392
h	1.4234037833	1.5119235363	3.1743567852
h	1.5230231480	3.5494031835	4.5884175899
h	0.5265752775	5.6834689256	3.7503847905
h	-2.5509384997	4.8702039511	0.6203337761
h	-3.7204644548	5.2177483232	-1.5289195678
h	-2.7440820271	4.2958872818	-3.6394209441
h	-0.6344323273	3.0120250962	-3.5512636915
h	-0.5578278499	5.7491592026	1.5301153144
h	1.6715831230	3.4773024615	-3.1655372564
h	3.6097670712	1.9776149802	-3.4743038334
h	3.9417692272	0.0099159919	-1.9761722957
h	2.3511035846	-0.3838913294	-0.0970697990
h	-0.4280412798	-5.0724014931	-2.6739336220
h	-1.0782635780	-3.4054692934	-2.7455229411
h	0.6799744263	-3.6660466074	-2.6349199084
h	0.6917592032	-6.1610550445	-0.3699755030
h	1.8557621819	-4.8112591351	-0.1945435923
h	0.8101657651	-5.2611542090	1.1741625513
h	-2.0436375219	-5.7914791298	-0.5375879119
h	-2.1136854370	-4.8585314822	0.9902049422
h	-2.8215204750	-4.1781017486	-0.4943333268

Prod-cpx_b (PMe₃Au⁺) [7-exo]

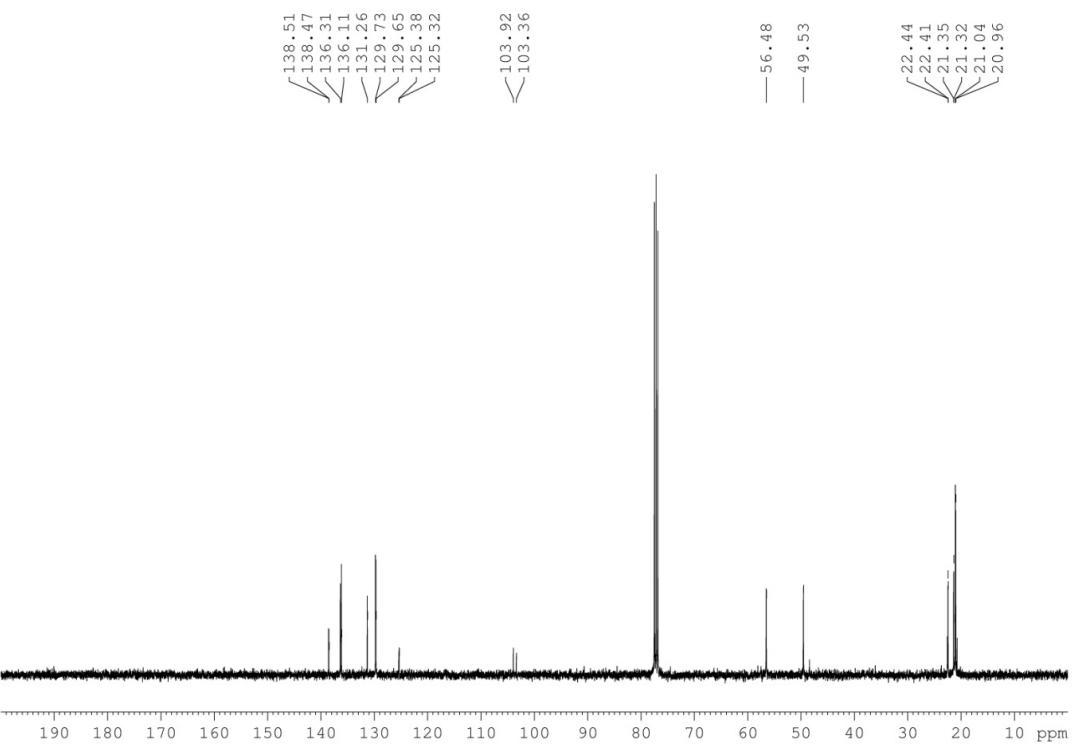
c	3.1409255030	5.8086972126	-0.9076566456
c	1.8122924251	5.6136506741	-0.4847332123
c	1.2191055886	4.3419122317	-0.7206166202
c	1.9506514457	3.3659113786	-1.4304579451
c	3.2551040229	3.5913653311	-1.8483139720
c	3.8616870871	4.8184950904	-1.5665581740
c	1.0527576209	6.7693797889	0.0343795449
c	0.1430125175	6.6887944661	1.1181825310
c	-0.5234778788	7.8610409723	1.5293959977
c	-0.3076961865	9.0847045289	0.9058351119
c	0.5903605130	9.1646356074	-0.1614309950
c	1.2543933542	8.0192737651	-0.5858291508
c	-0.1428553466	5.4406342902	1.8542773444
c	-0.3825452771	4.1974250567	1.2051854020
c	-0.8648991182	3.1101031351	1.9643667524
c	-1.0540846656	3.2040598504	3.3364469002
c	-0.7669418791	4.4074931558	3.9864391566
c	-0.3317965507	5.5027941071	3.2481325103

c	-0.1237291836	3.9954424565	-0.2292999961
c	-1.0855765610	3.4187249482	-1.0713985126
au	-0.7203357451	1.2476525117	-0.9270747487
p	-0.5328981910	-1.0261578593	-0.9323862499
c	-1.8365613452	-1.8553050735	0.0339014275
c	-0.6317465244	-1.7481495120	-2.6022448232
c	1.0426279738	-1.6212171486	-0.2351818666
h	-0.9402336343	3.5521168376	-2.1474484094
h	-2.1221192794	3.4450342959	-0.7219843628
h	-1.0386209832	2.1568583876	1.4594727071
h	-1.3995216405	2.3380157846	3.8996058935
h	-0.8788989596	4.4905936413	5.0669010051
h	-1.2501297915	7.7969367985	2.3384836303
h	-0.8511114026	9.9681032653	1.2391231167
h	0.7590109195	10.1115639968	-0.6729364339
h	1.9258442532	8.0806178834	-1.4415641426
h	-0.1169818631	6.4399634291	3.7599129836
h	3.6172597676	6.7659174646	-0.6990985541
h	4.8953979119	5.0019833337	-1.8575511141
h	3.8040256810	2.8072892600	-2.3682493269
h	1.4895077373	2.3905734490	-1.6022005883
h	-1.7010861039	-2.9441988559	-0.0091469937
h	-1.7884180419	-1.5224710150	1.0772644030
h	-2.8195629133	-1.5927075804	-0.3743492839
h	-0.5414855976	-2.8411503030	-2.5447838415
h	-1.5925225095	-1.4846936110	-3.0602062135
h	0.1763855943	-1.3468946269	-3.2251262361
h	1.0741853859	-2.7186529193	-0.2612390189
h	1.8783104134	-1.2174607493	-0.8187579337
h	1.1391285703	-1.2765772432	0.8011284628

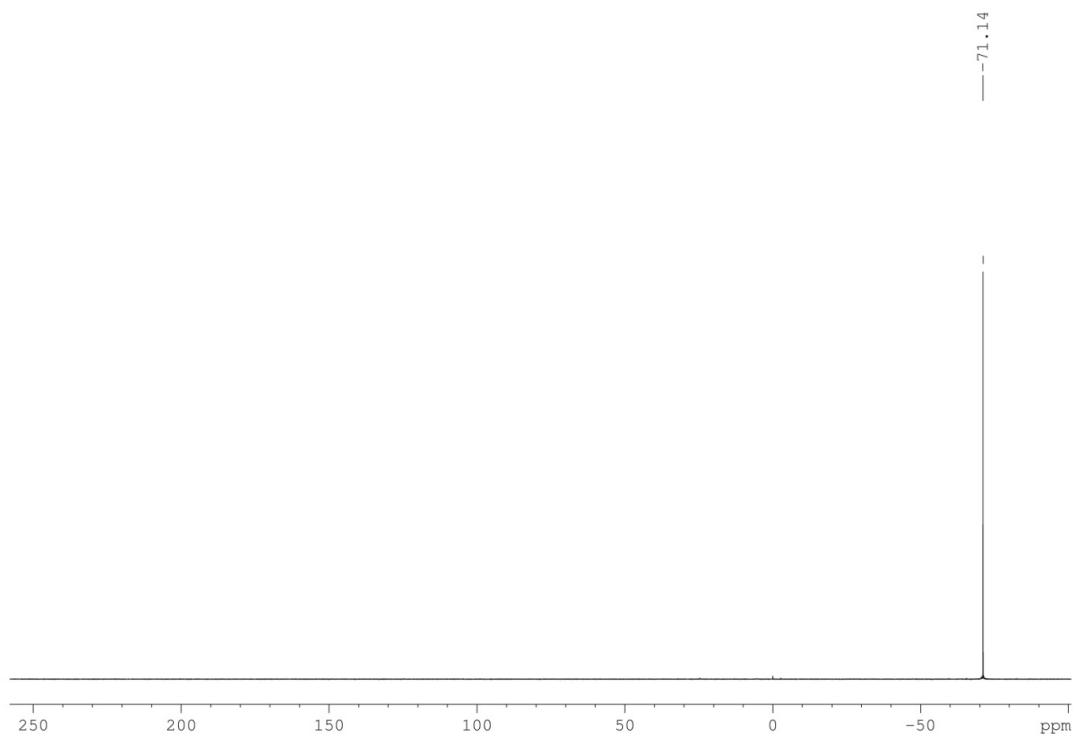
¹H NMR (400 MHz, CD₂Cl₂) 4



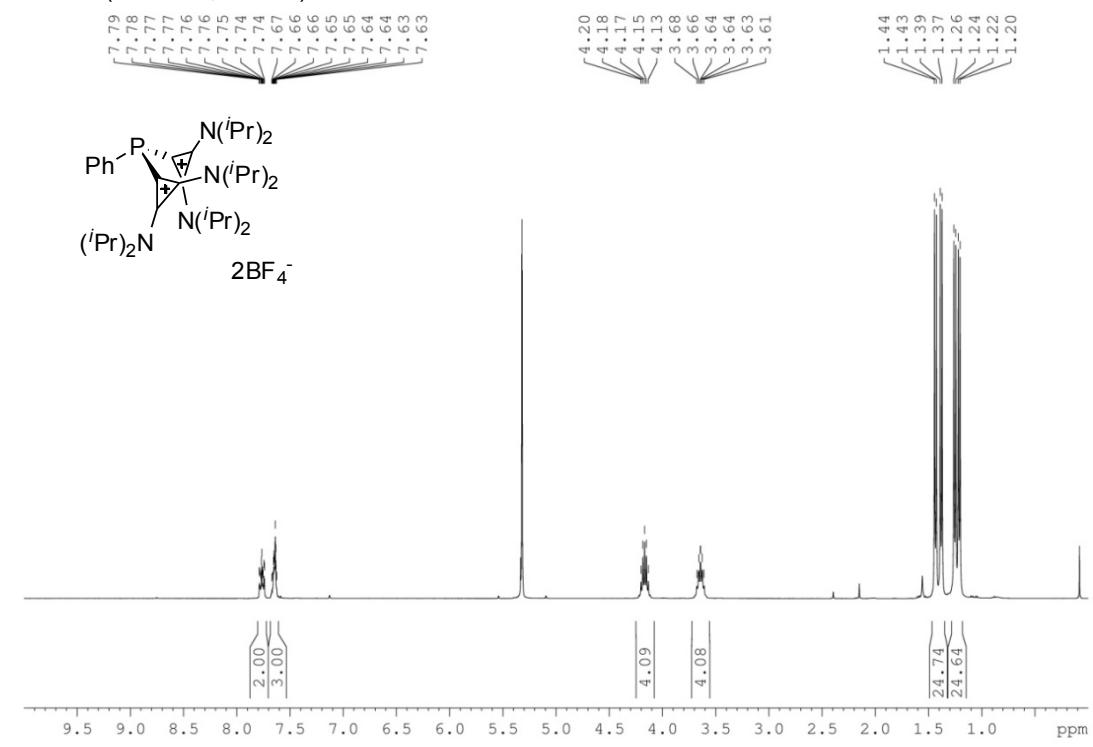
¹³C NMR (101 MHz, CD₂Cl₂) 4



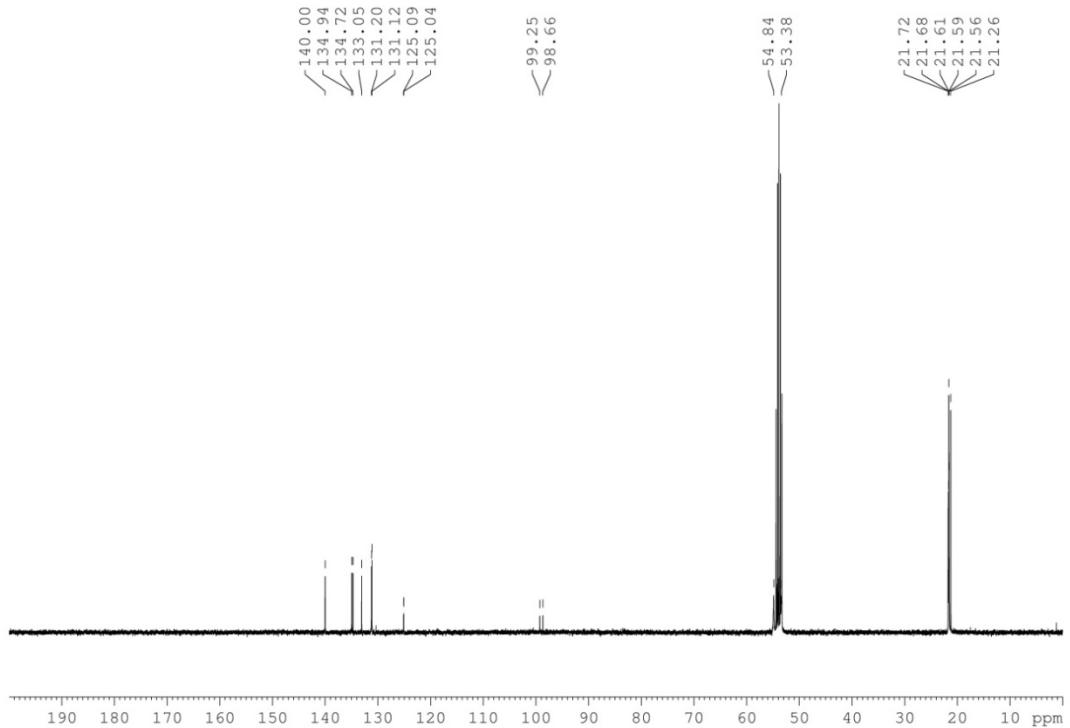
^{31}P NMR (161 MHz, CD_2Cl_2) **4**



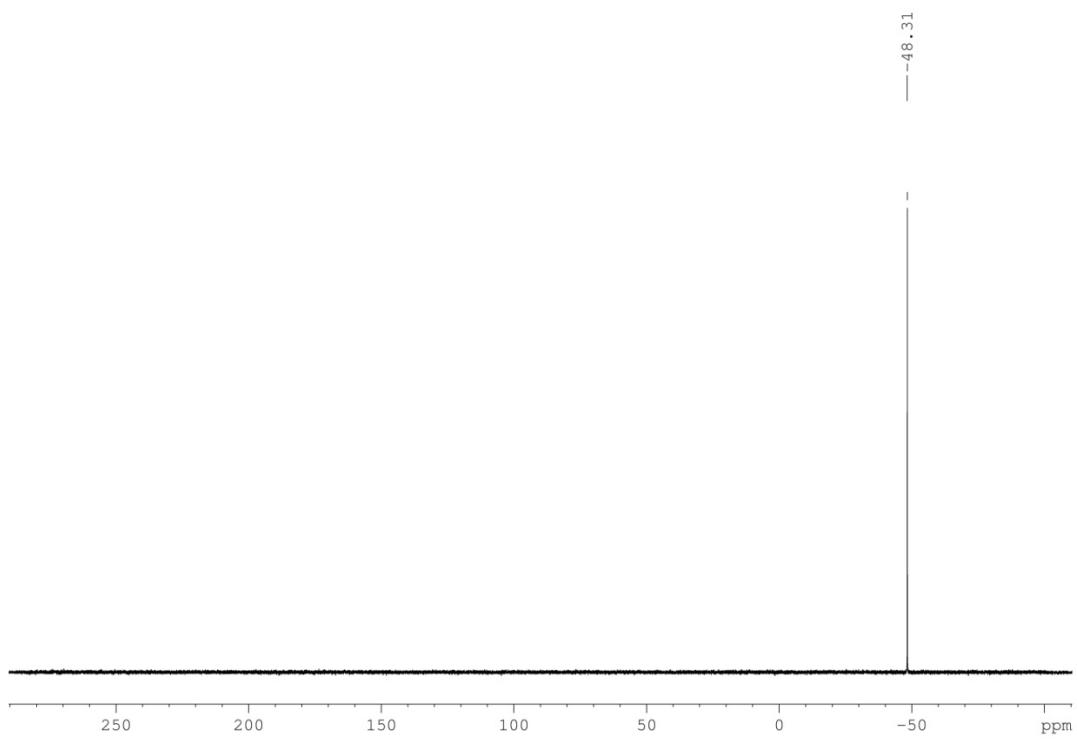
¹H NMR (400 MHz, CD₂Cl₂) **1**



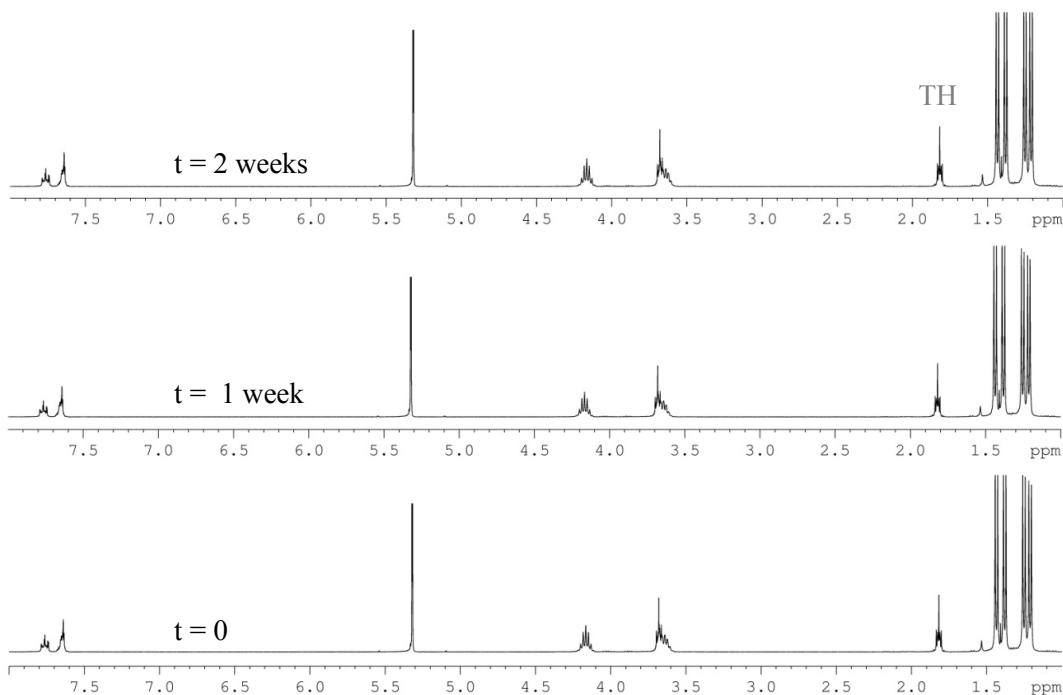
¹³C NMR (101 MHz, CD₂Cl₂) **1**



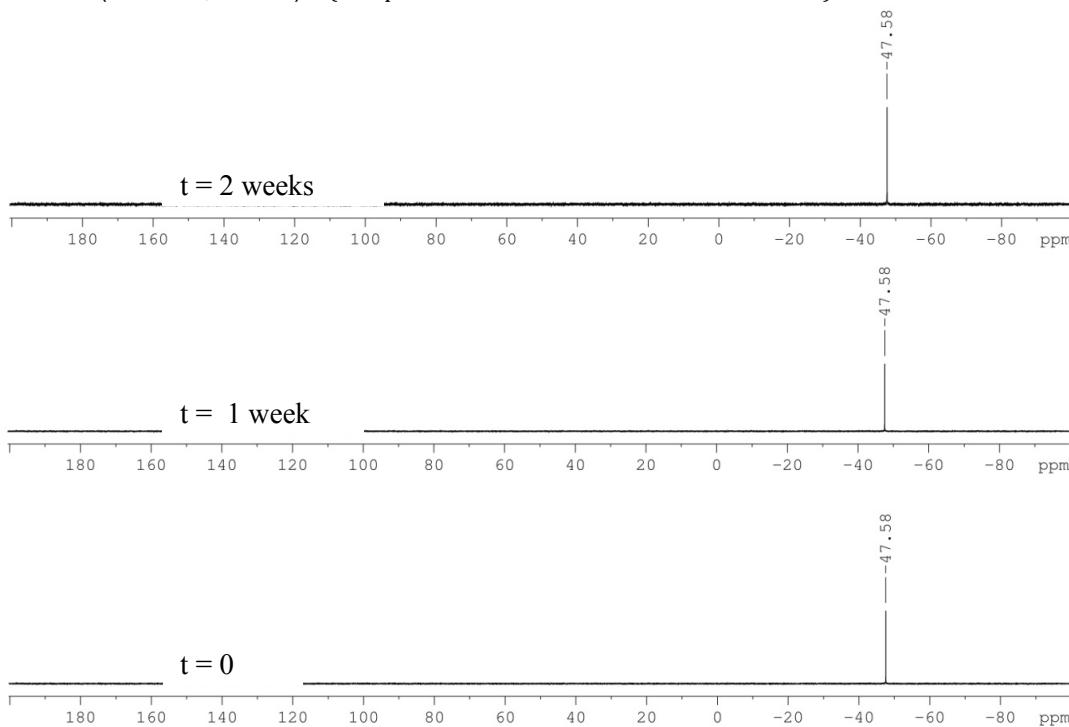
^{31}P NMR (161 MHz, CD_2Cl_2) **1**



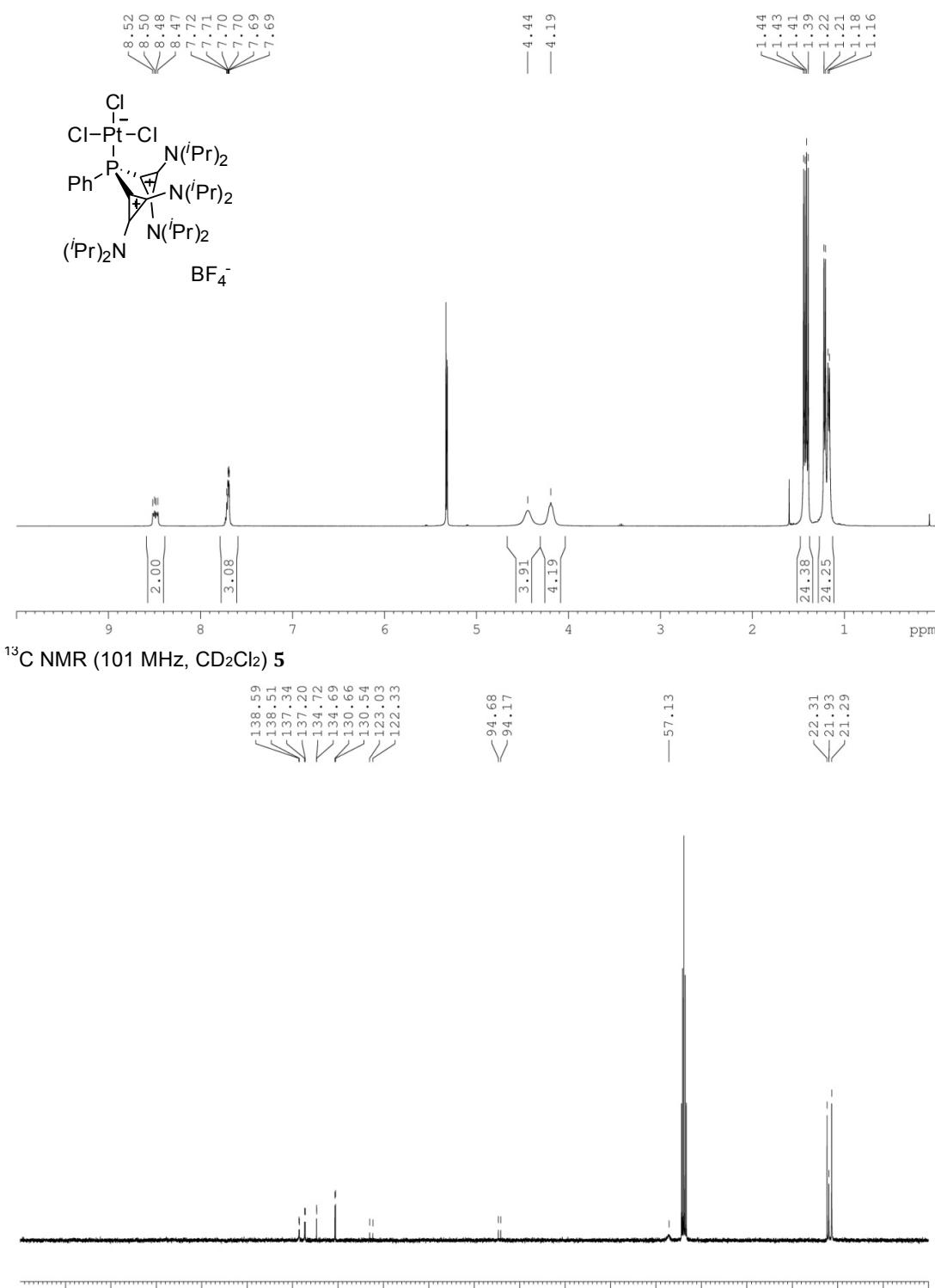
^1H NMR (400 MHz, CD_2Cl_2) **1** (Compound stored in an unsealed vial under air)

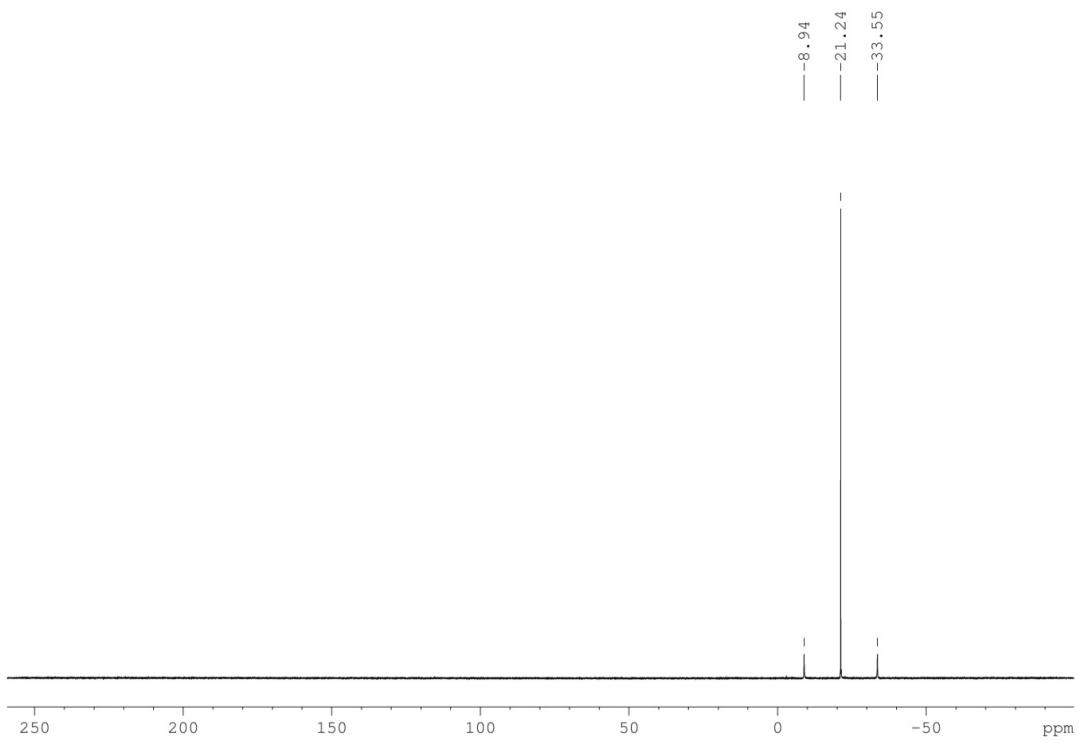


^{31}P NMR (161 MHz, CD_2Cl_2) **1** (Compound stored in an unsealed vial under air)

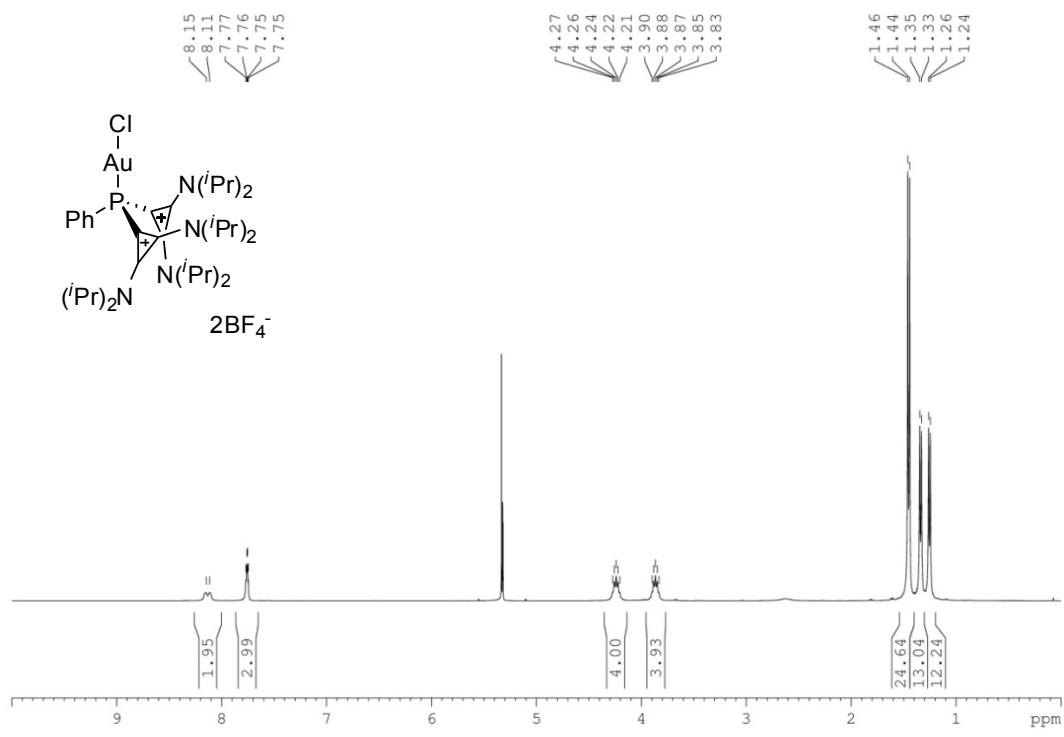


^1H NMR (400 MHz, CD_2Cl_2) **5**

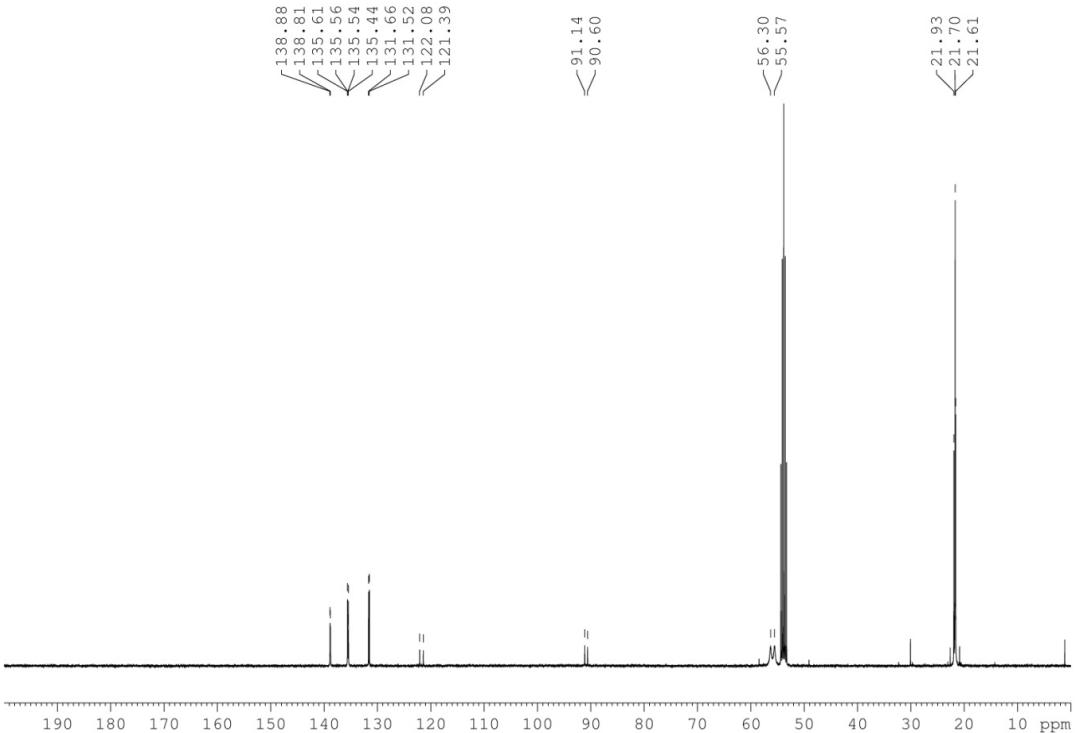




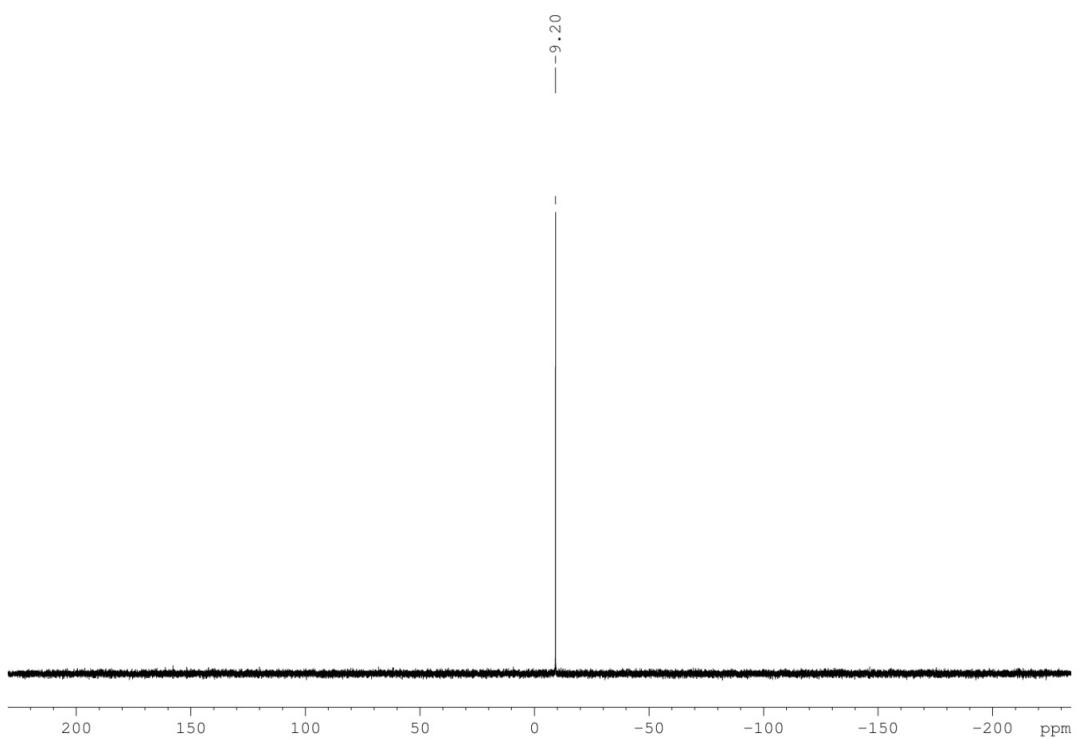
¹H NMR (400 MHz, CD₂Cl₂) **6**



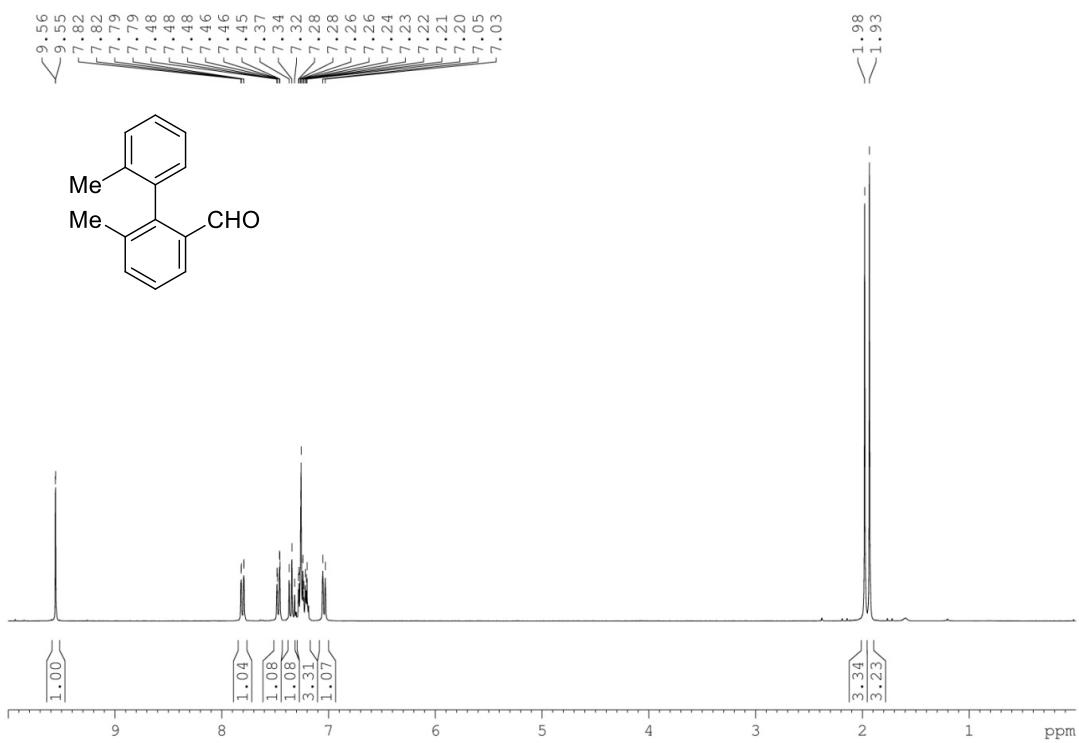
¹³C NMR (101 MHz, CD₂Cl₂) **6**



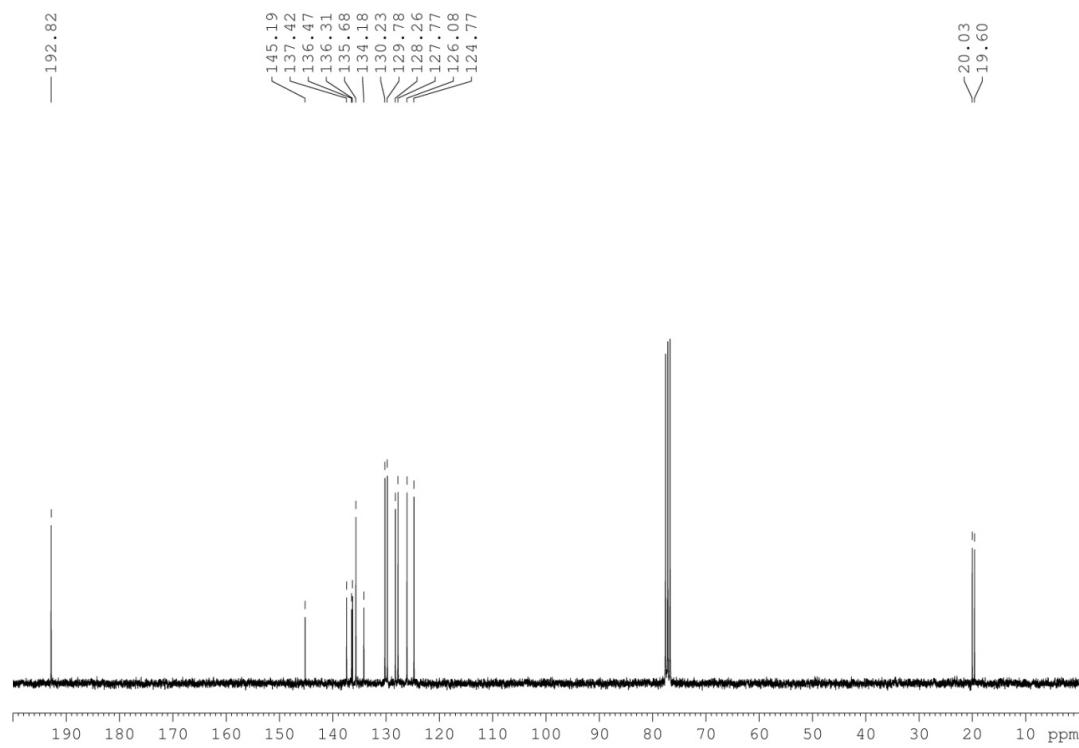
^{31}P NMR (161 MHz, CD_2Cl_2) 6



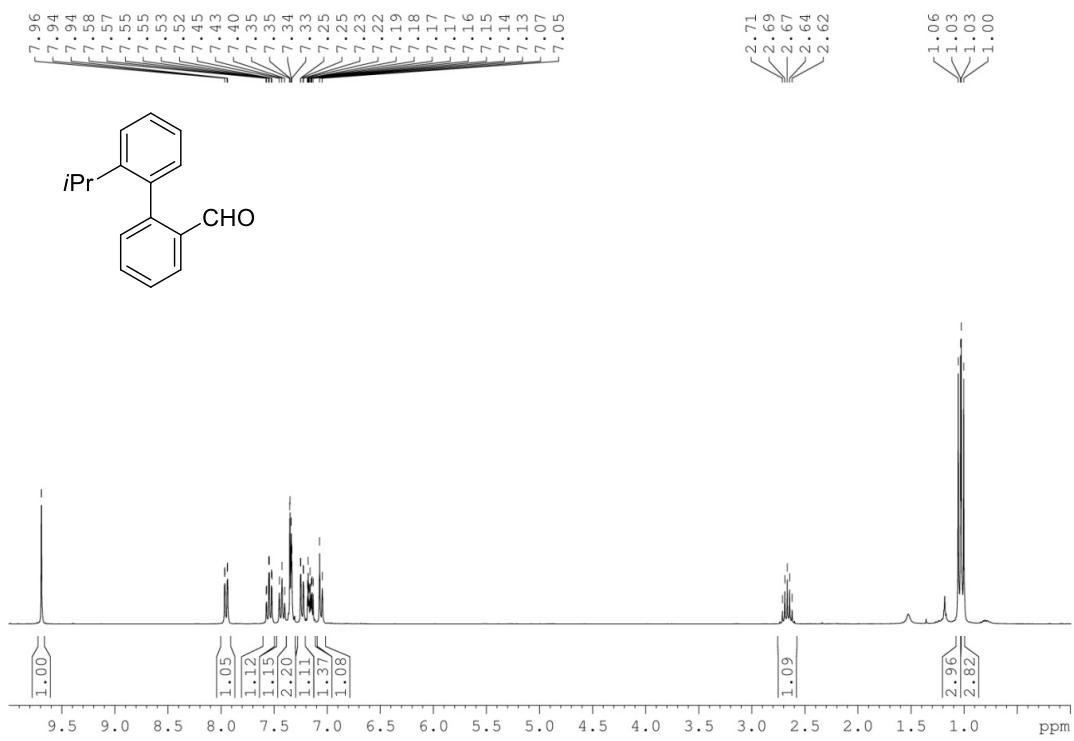
¹H NMR (400 MHz, CDCl₃)



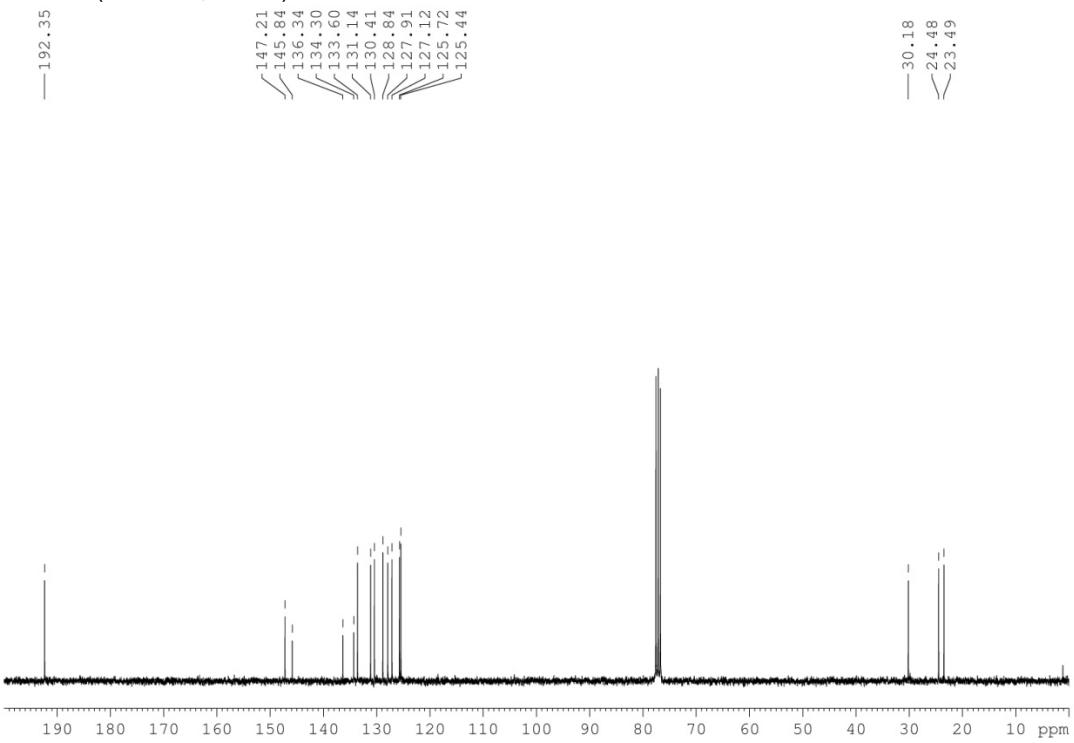
¹³C NMR (101 MHz, CDCl₃)



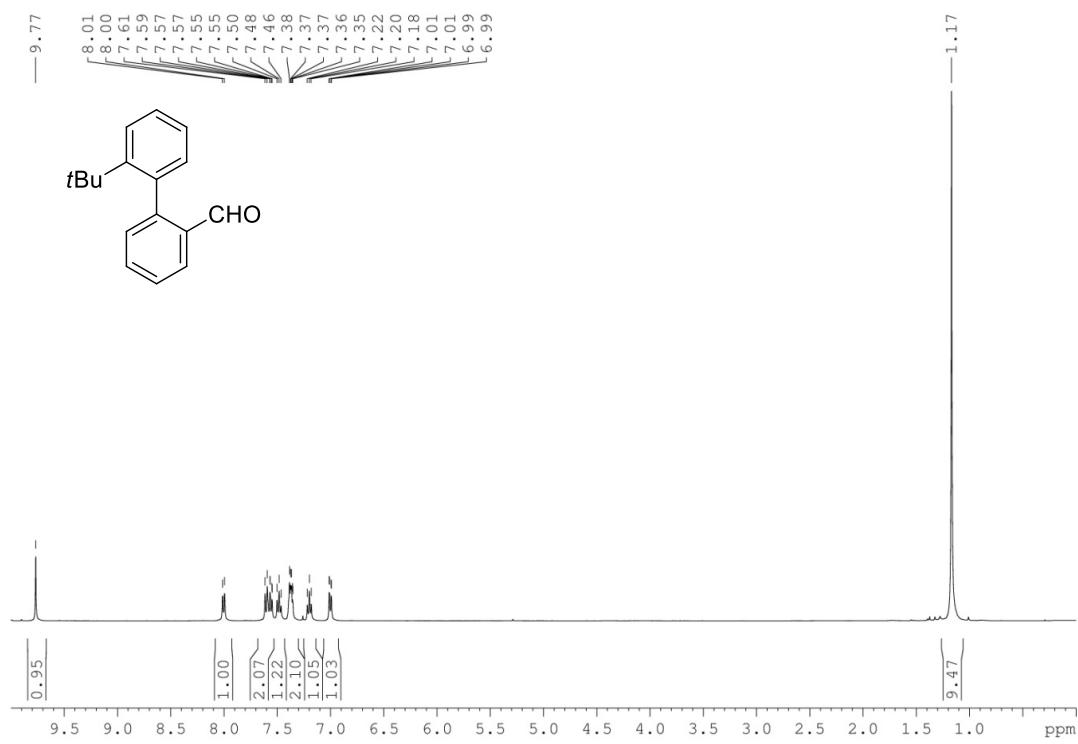
¹H NMR (400 MHz, CDCl₃)



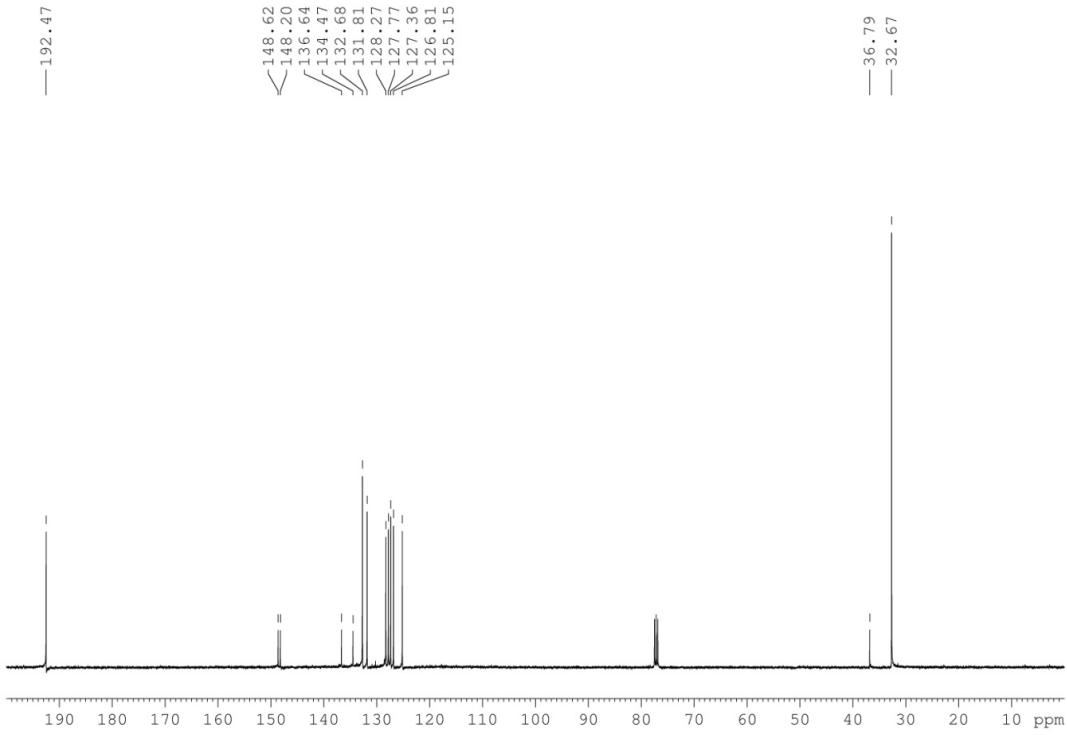
¹³C NMR (101 MHz, CDCl₃)



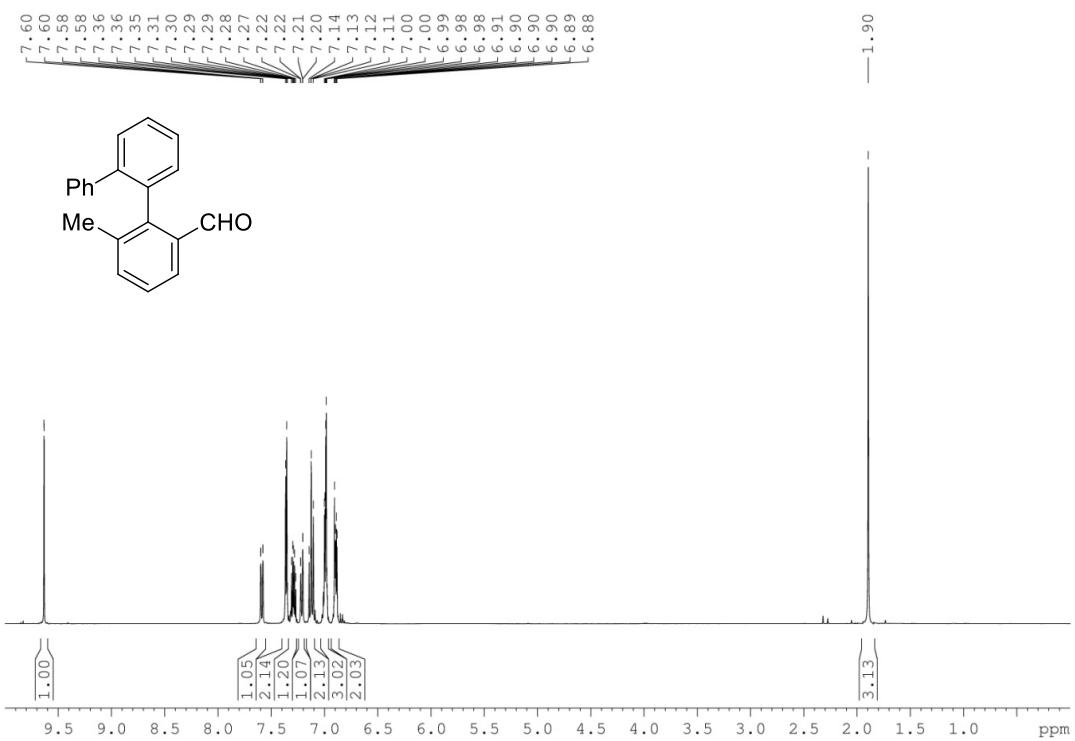
¹H NMR (400 MHz, CDCl₃)



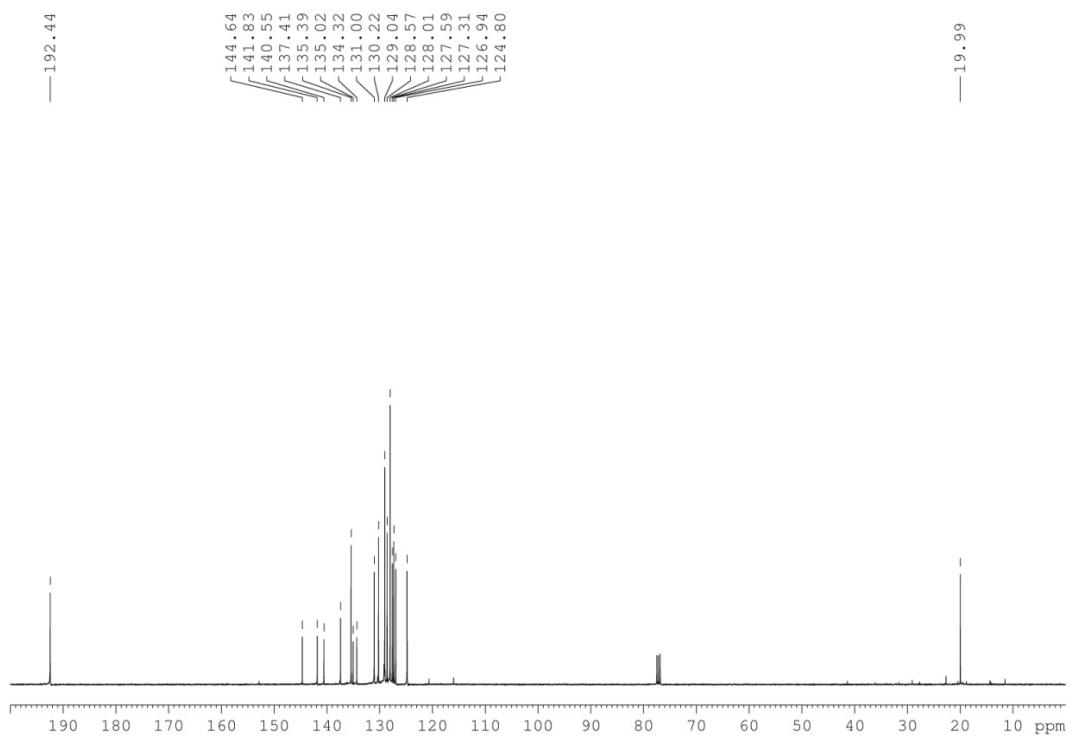
¹³C NMR (101 MHz, CDCl₃)



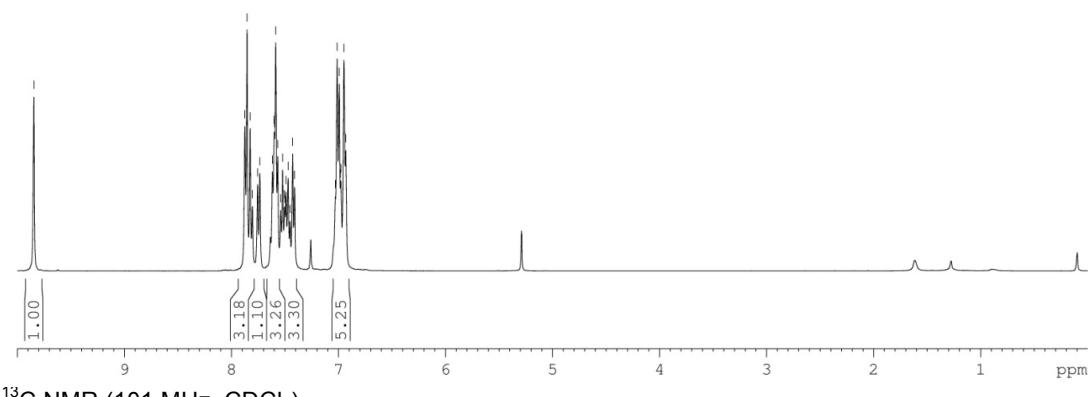
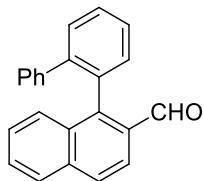
¹H NMR (400 MHz, CDCl₃)



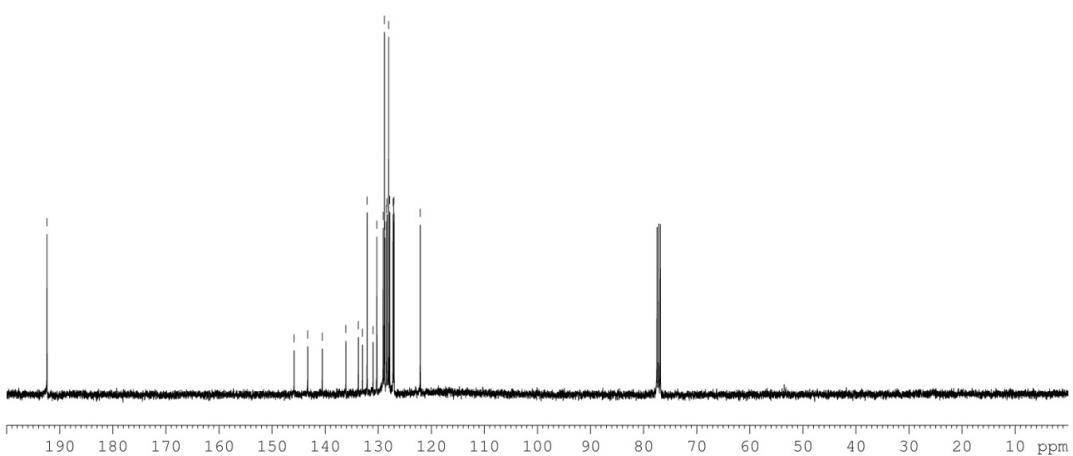
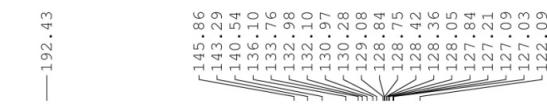
¹³C NMR (101 MHz, CDCl₃)



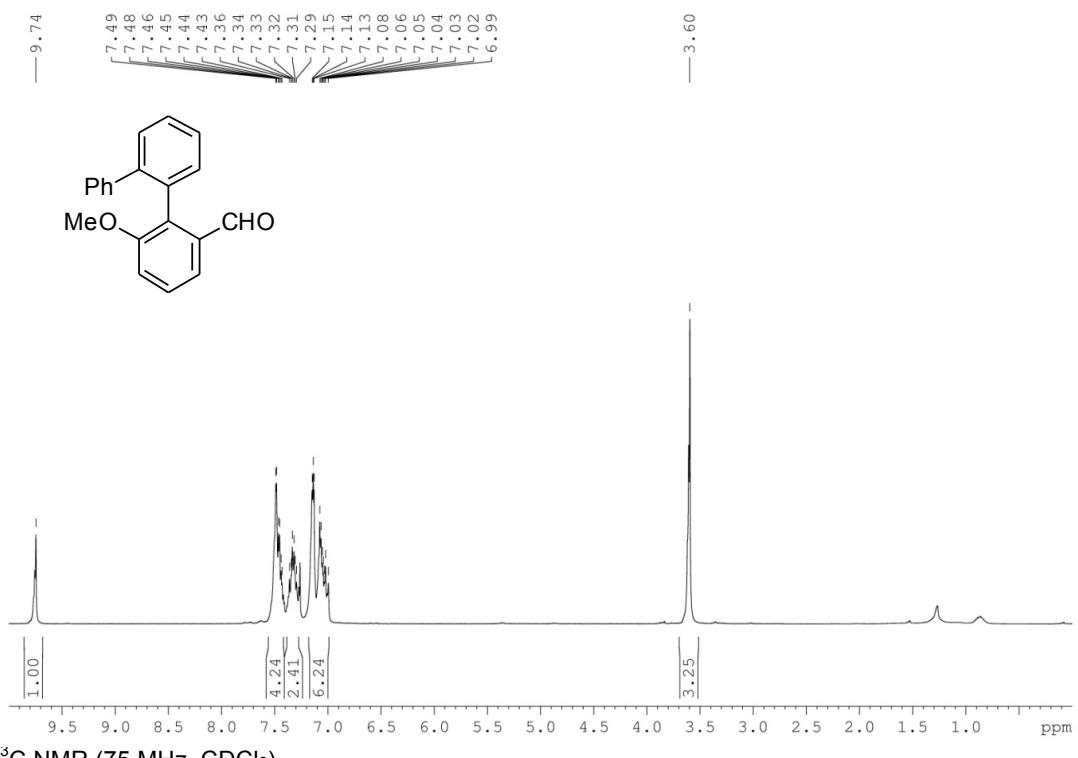
¹H NMR (400 MHz, CDCl₃)



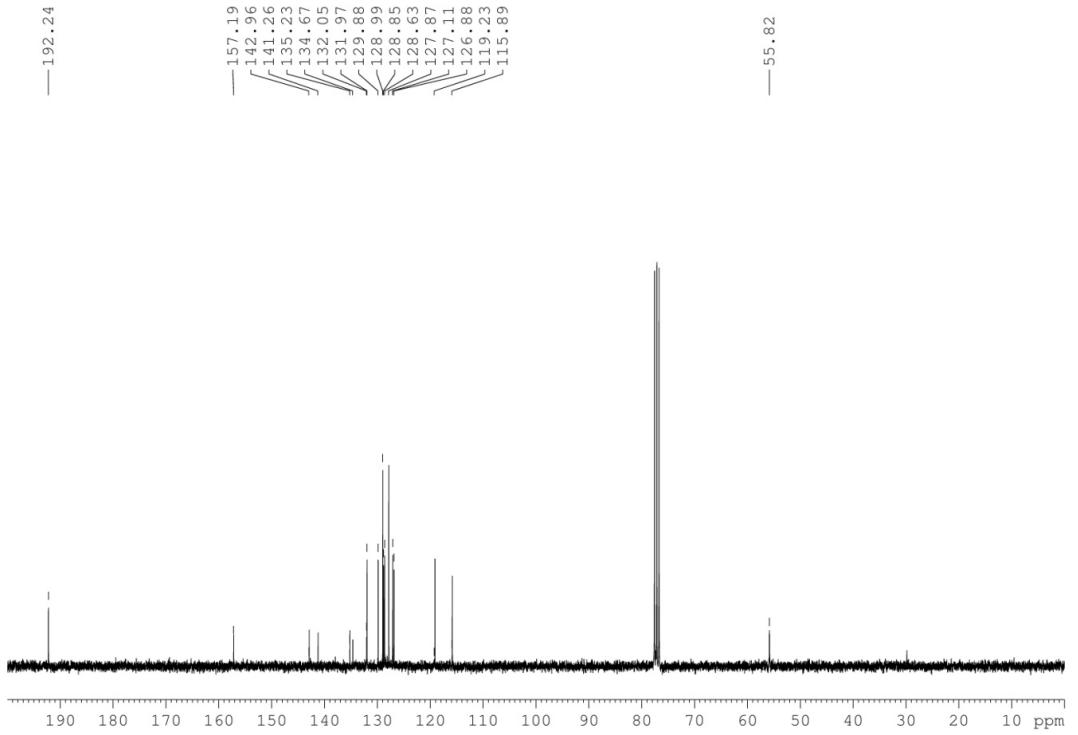
¹³C NMR (101 MHz, CDCl₃)



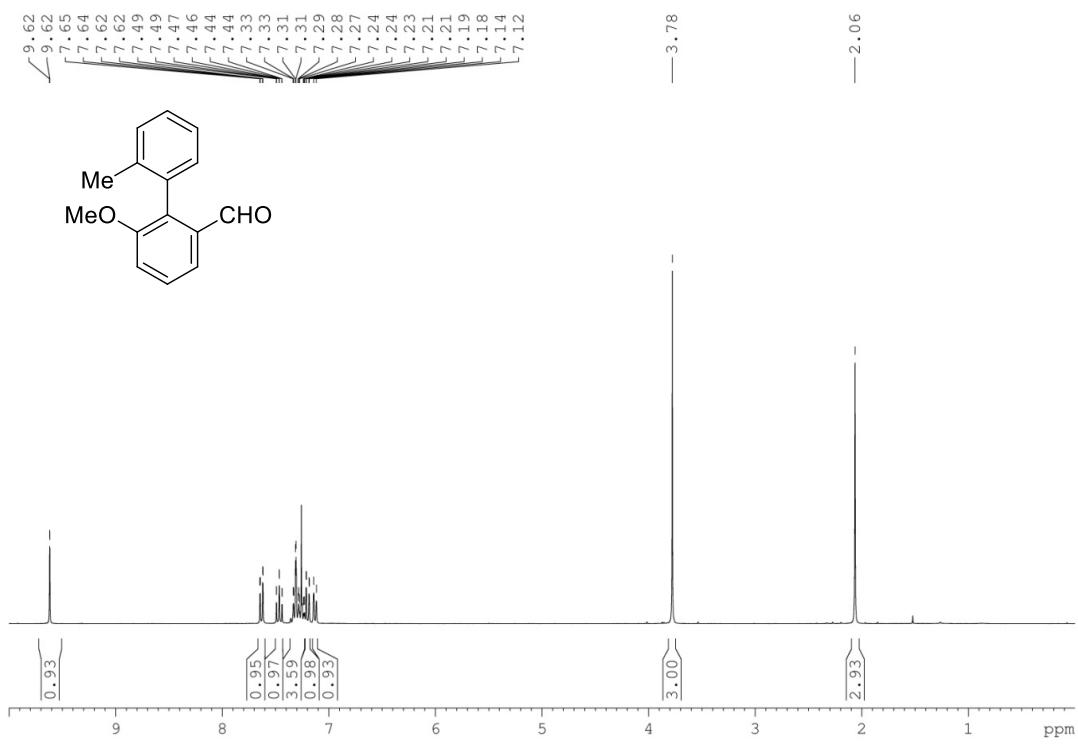
¹H NMR (300 MHz, CDCl₃)



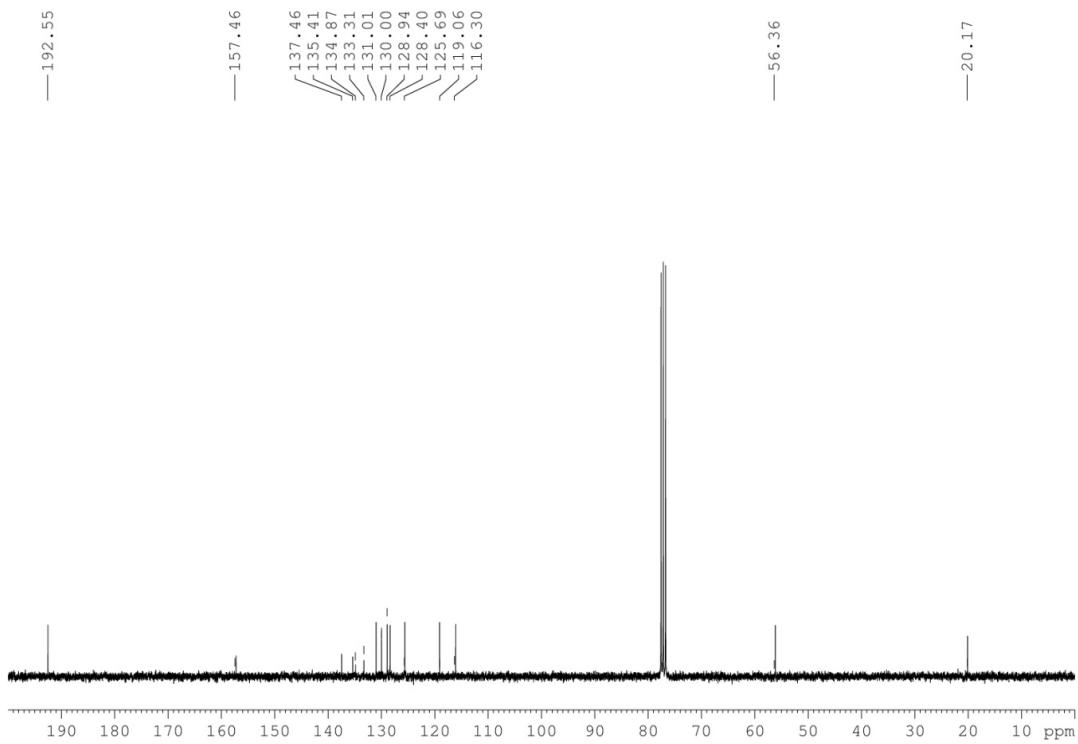
¹³C NMR (75 MHz, CDCl₃)



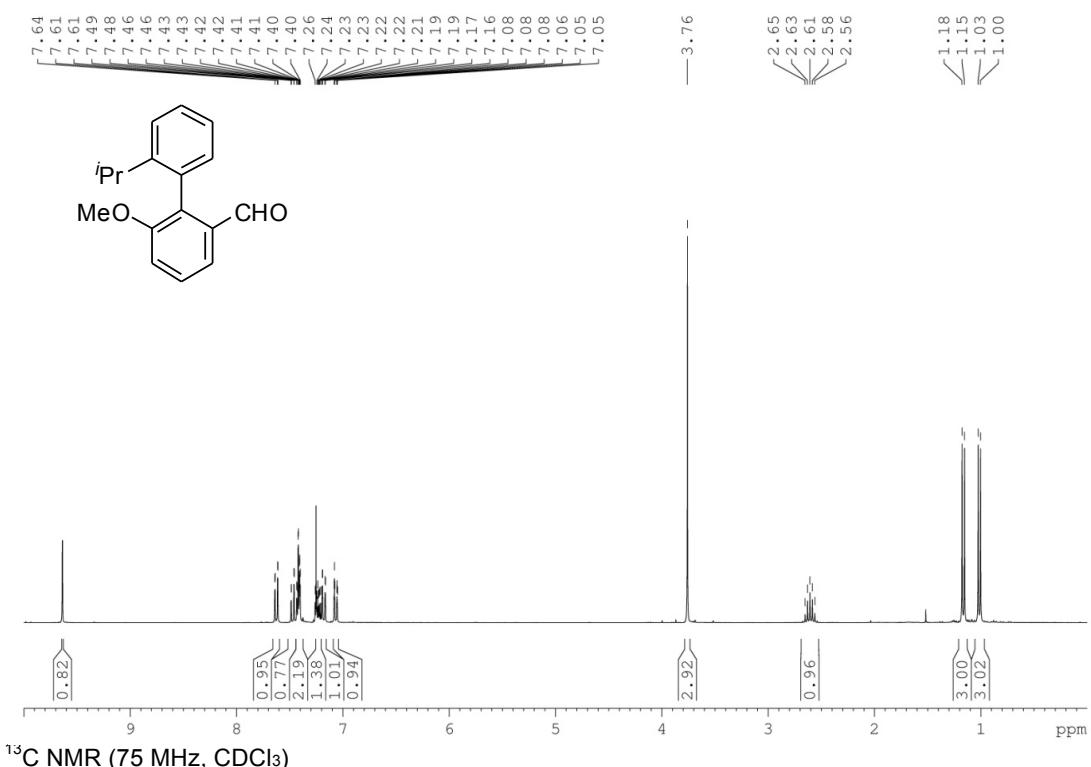
¹H NMR (300 MHz, CDCl₃)



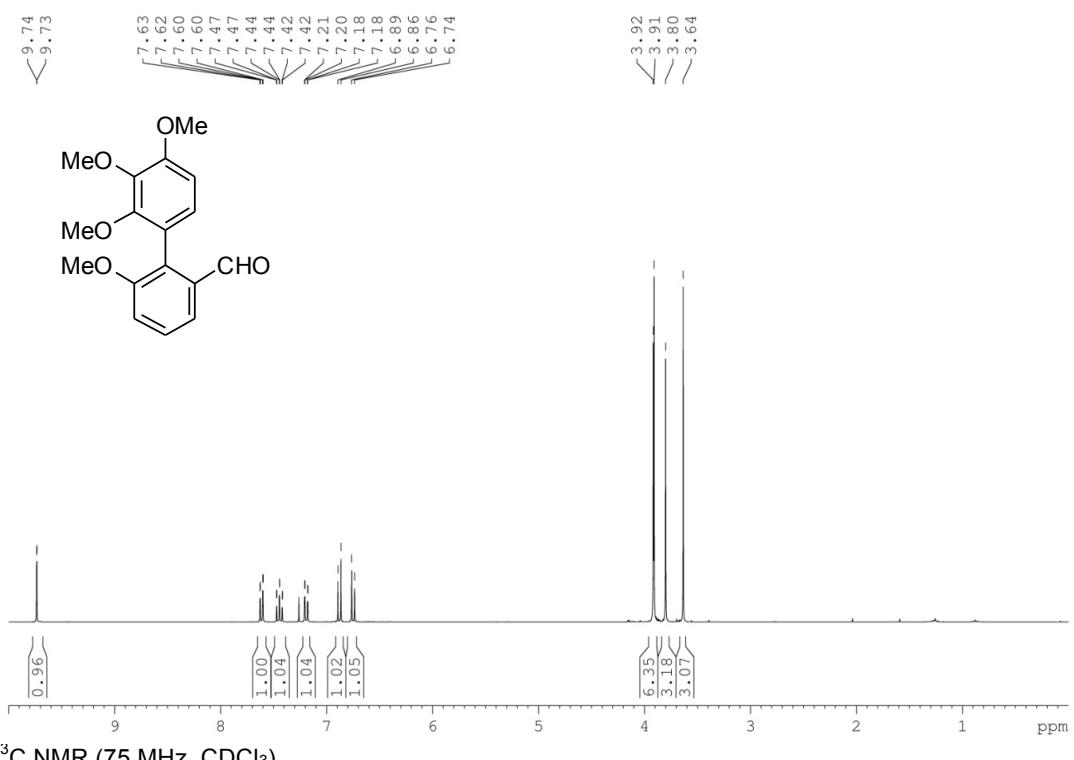
¹³C NMR (75 MHz, CDCl₃)



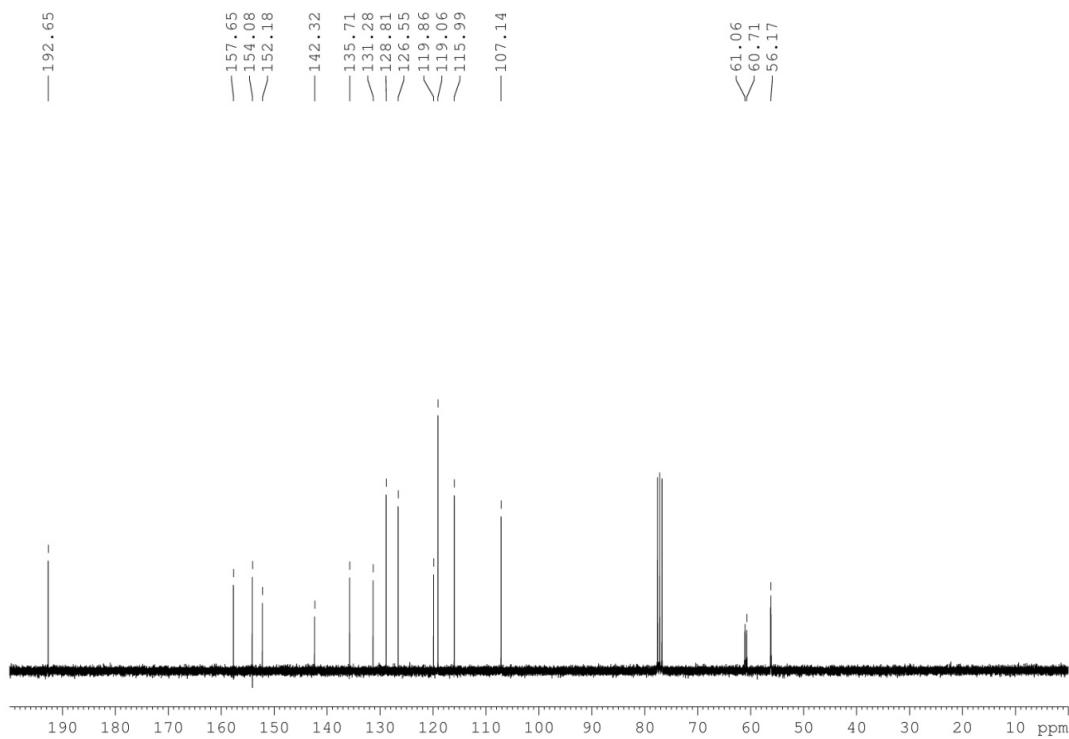
¹H NMR (300 MHz, CDCl₃)



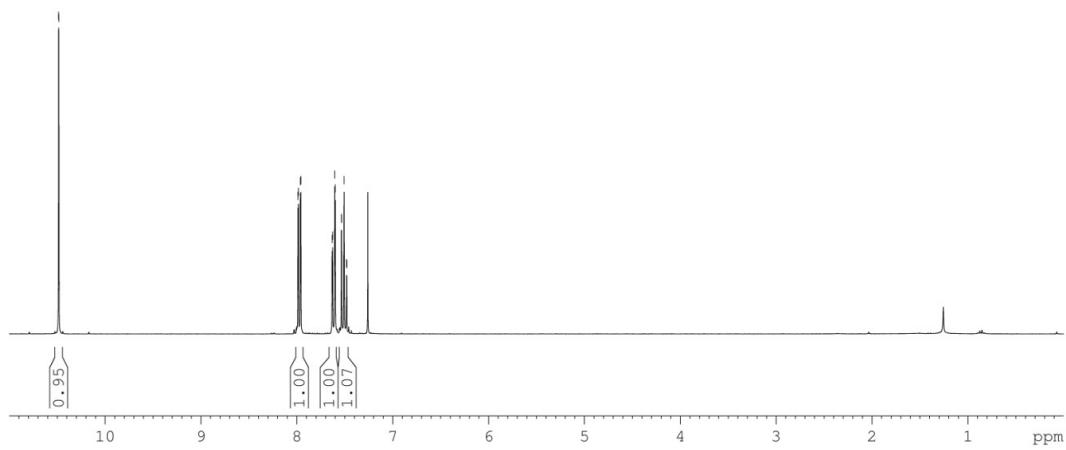
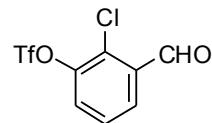
¹H NMR (300 MHz, CDCl₃)



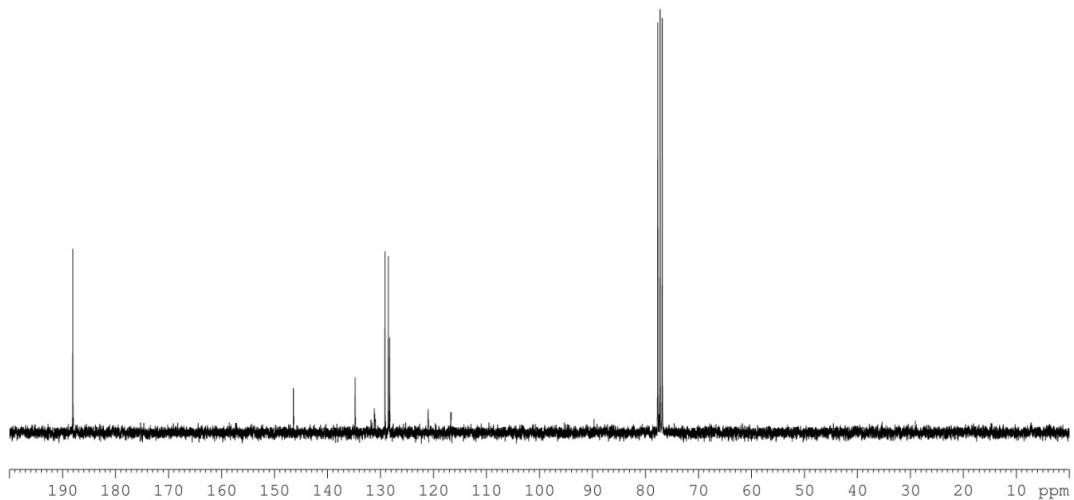
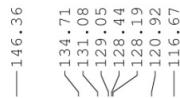
¹³C NMR (75 MHz, CDCl₃)



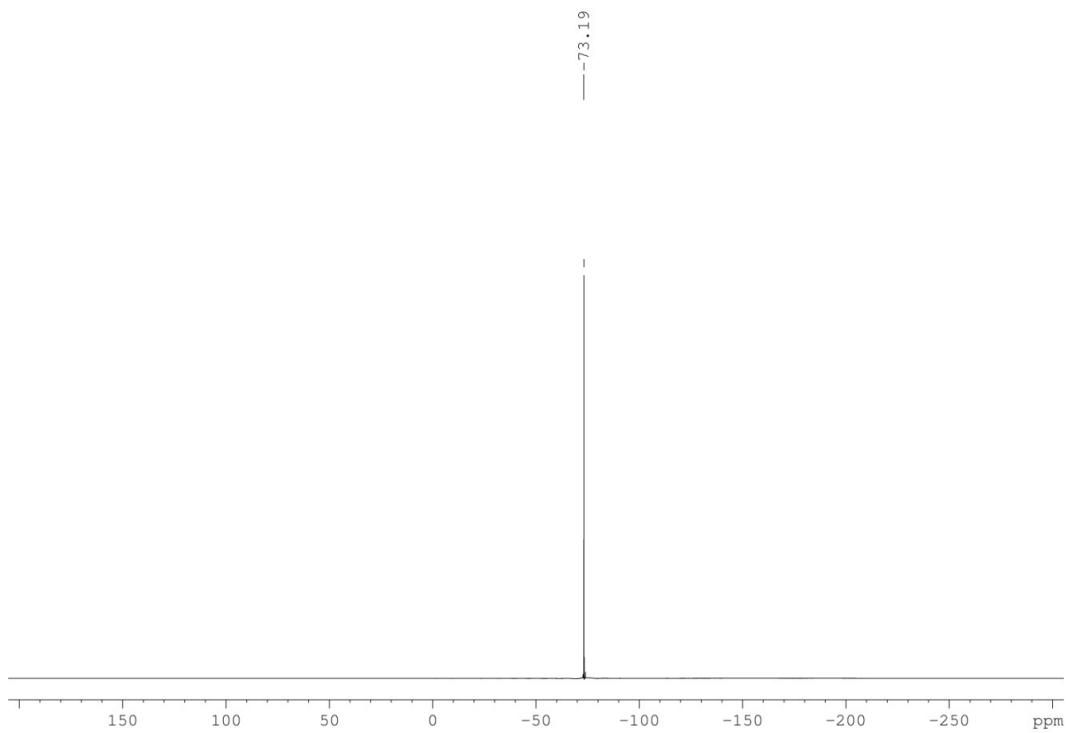
¹H NMR (300 MHz, CDCl₃)



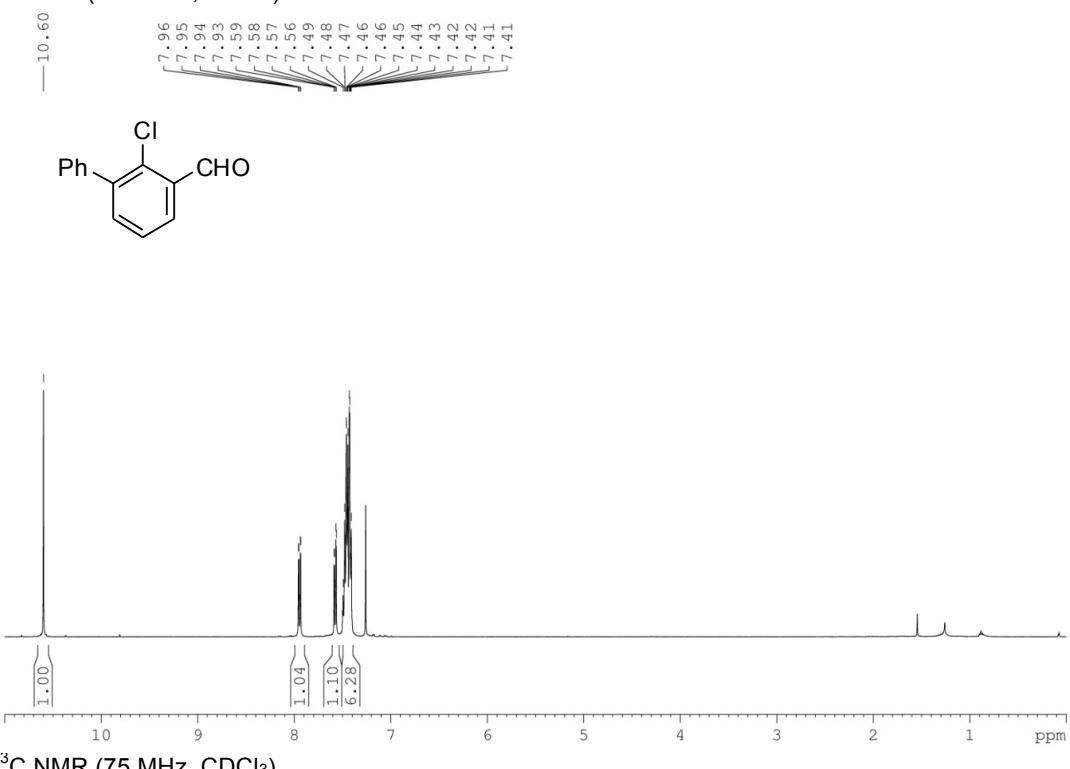
¹³C NMR (75 MHz, CDCl₃)



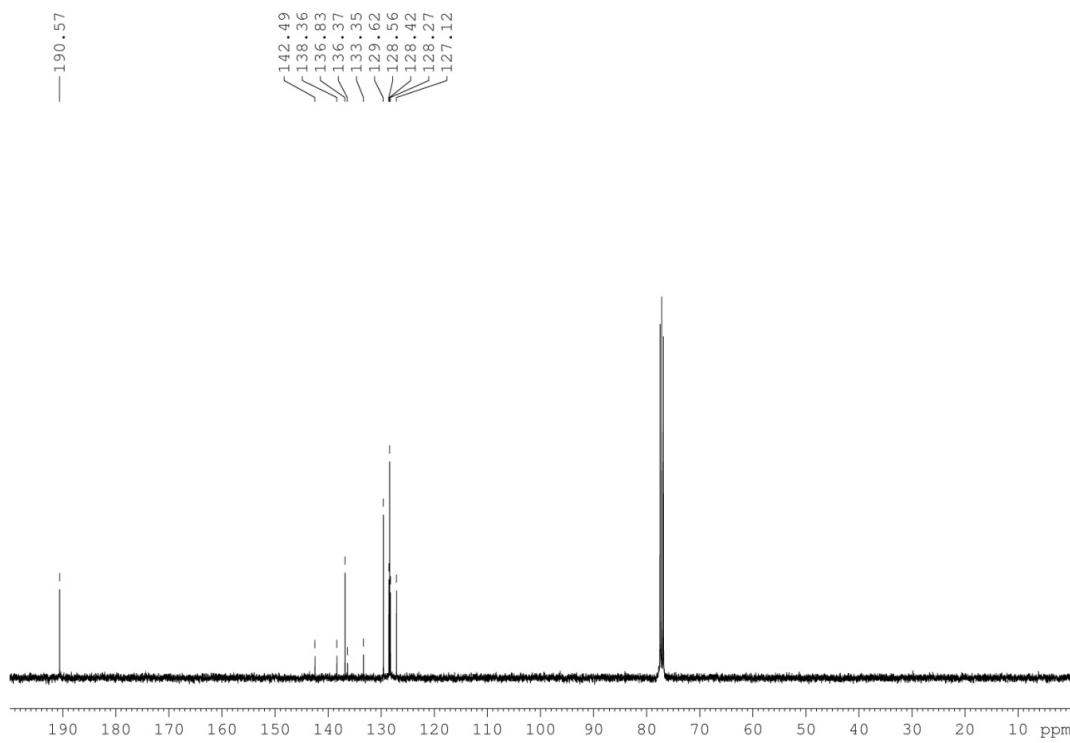
¹⁹F NMR (282 MHz, CDCl₃)



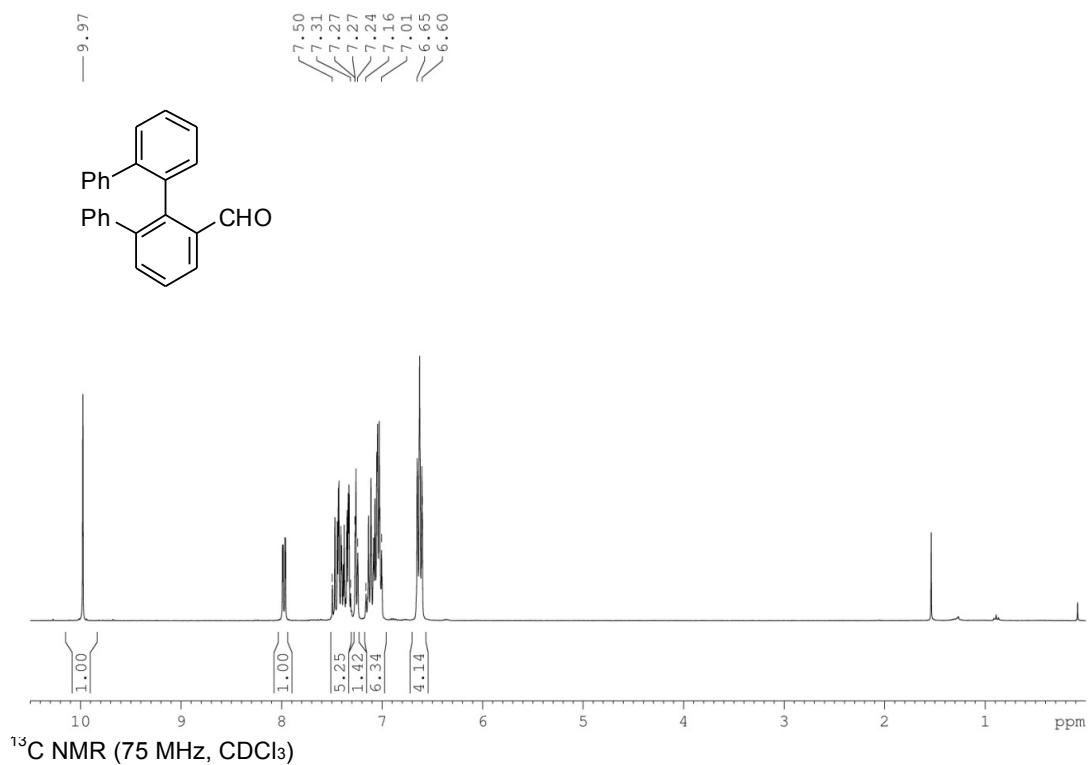
¹H NMR (300 MHz, CDCl₃)



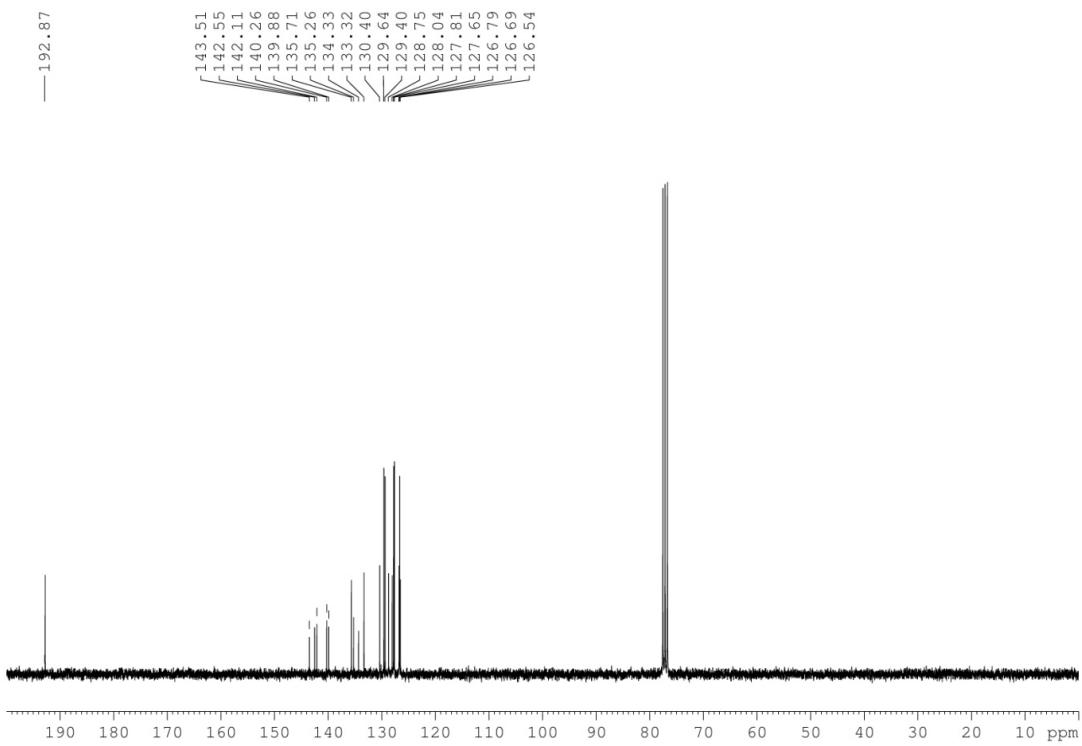
¹³C NMR (75 MHz, CDCl₃)



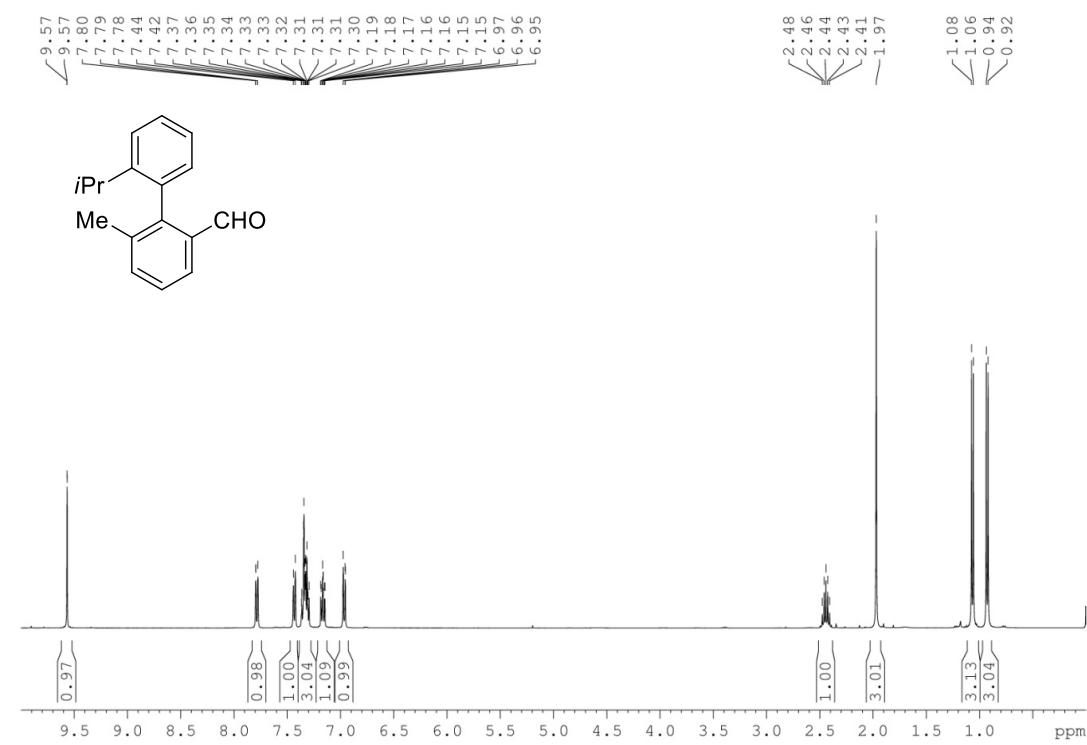
¹H NMR (300 MHz, CDCl₃)



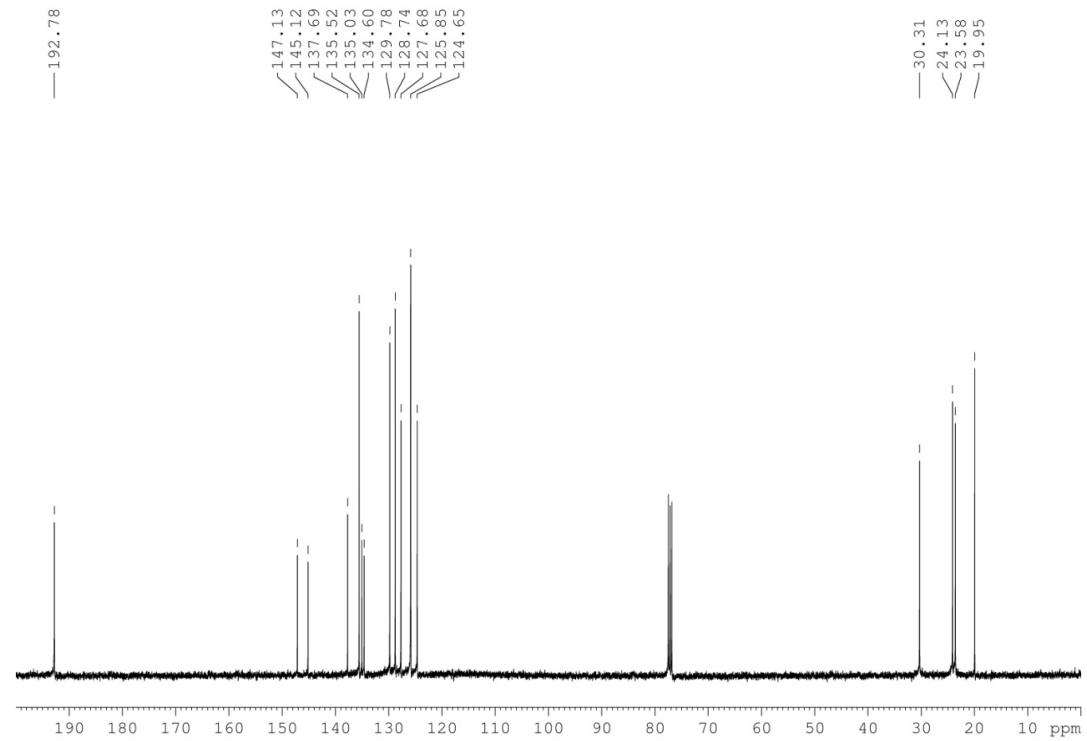
¹³C NMR (75 MHz, CDCl₃)



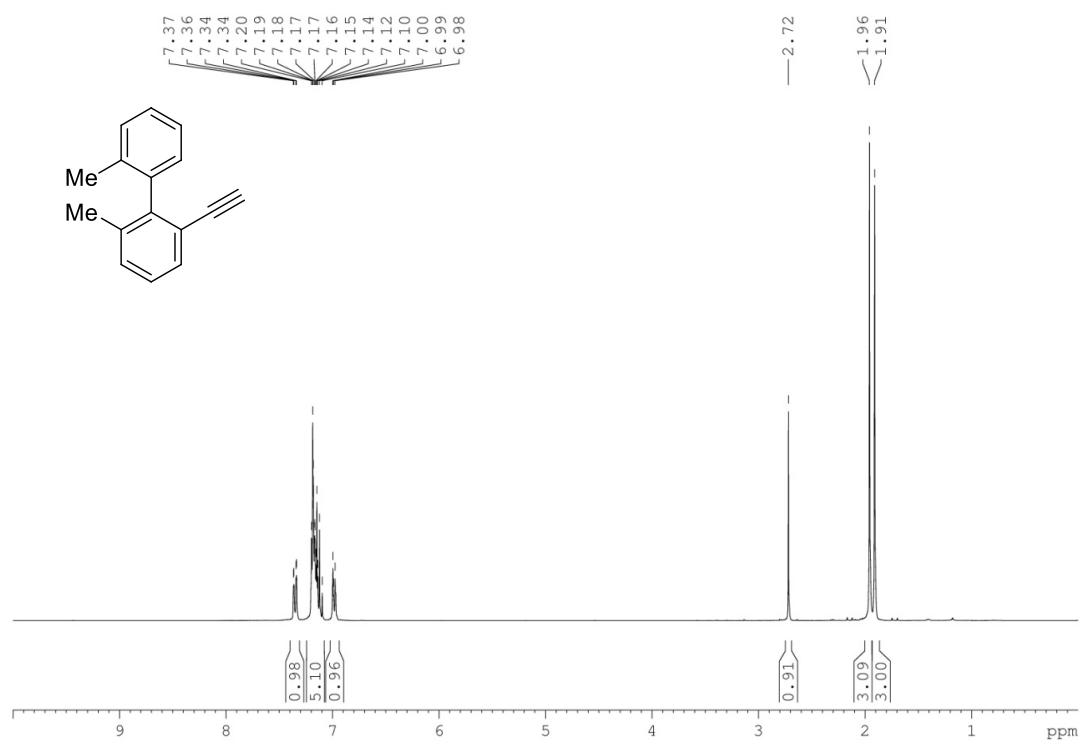
¹H NMR (400 MHz, CDCl₃)



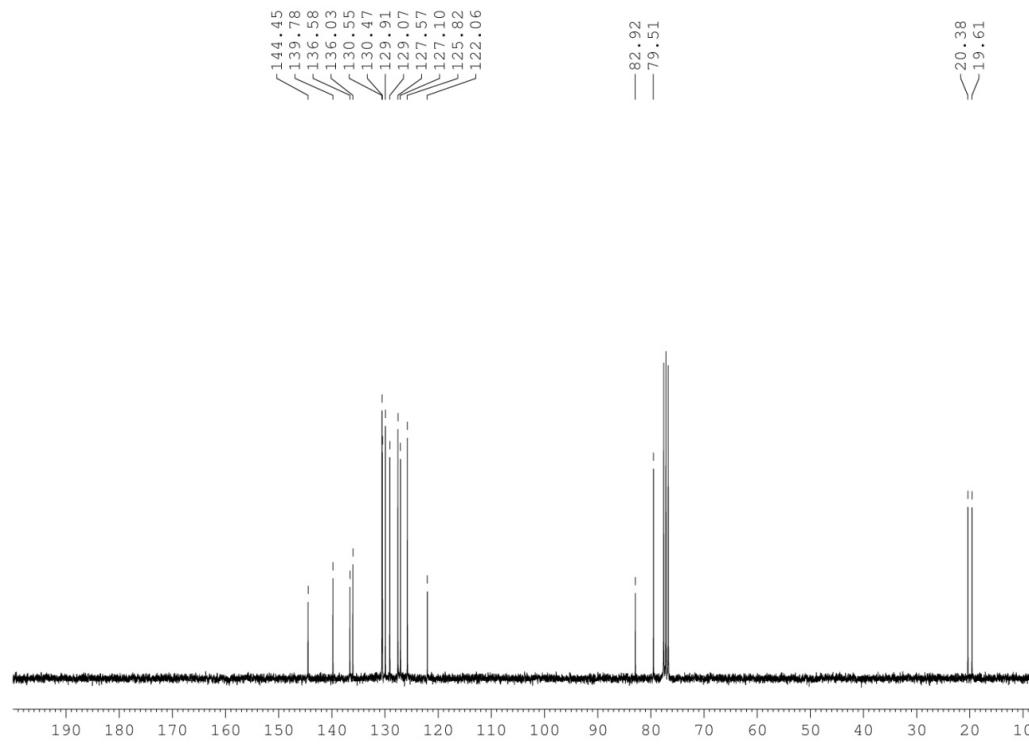
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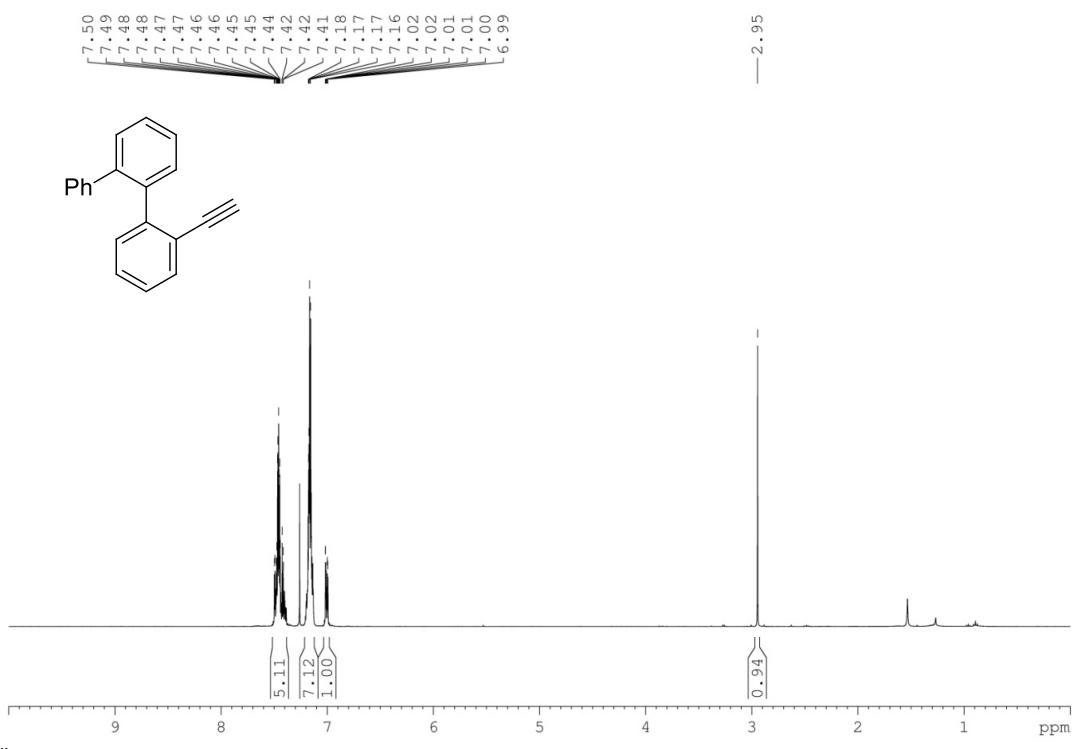
¹H NMR (400 MHz, CDCl₃) 7



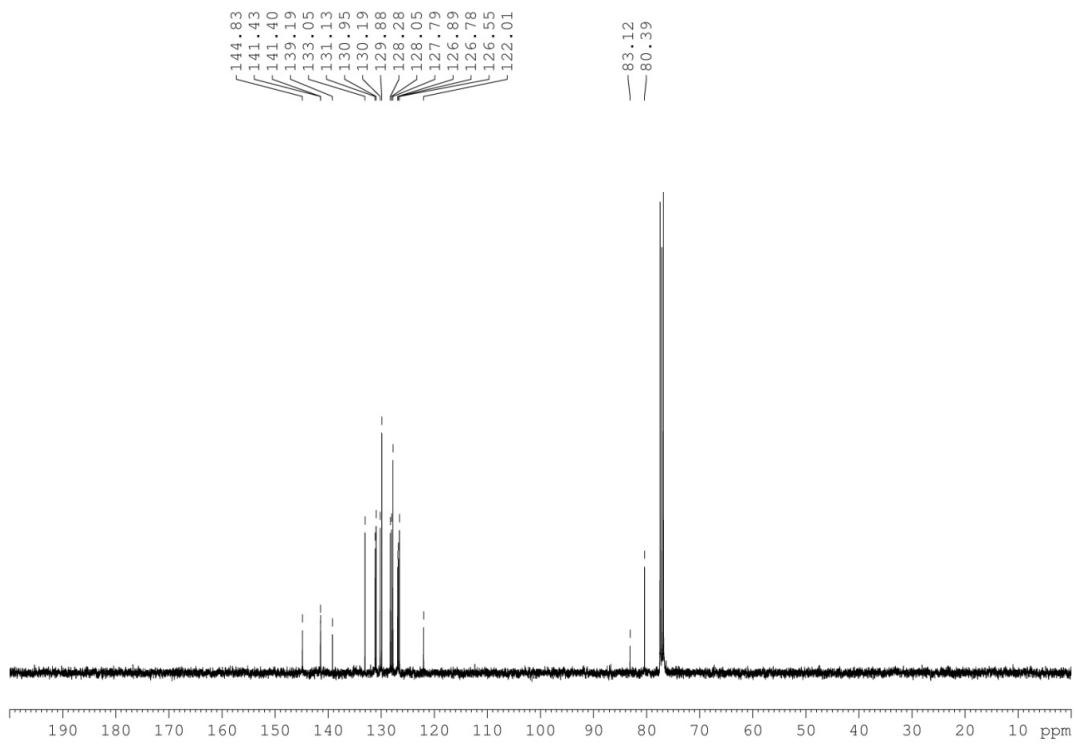
¹³C NMR (101 MHz, CDCl₃) 7



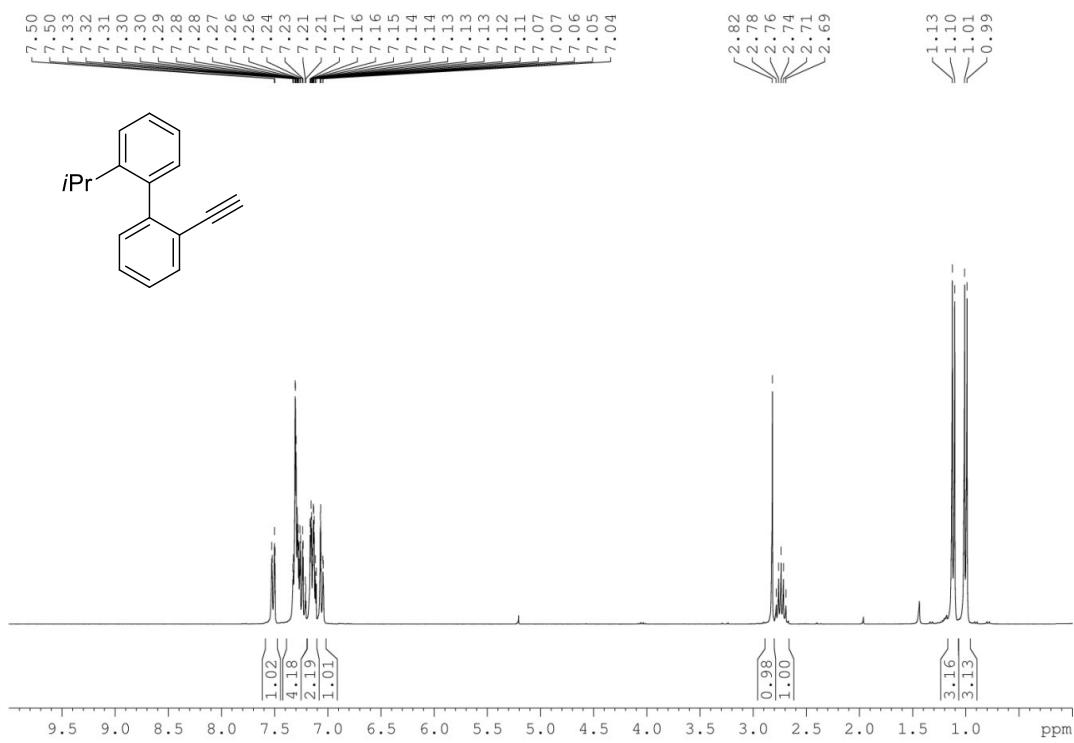
¹H NMR (400 MHz, CDCl₃) **9**



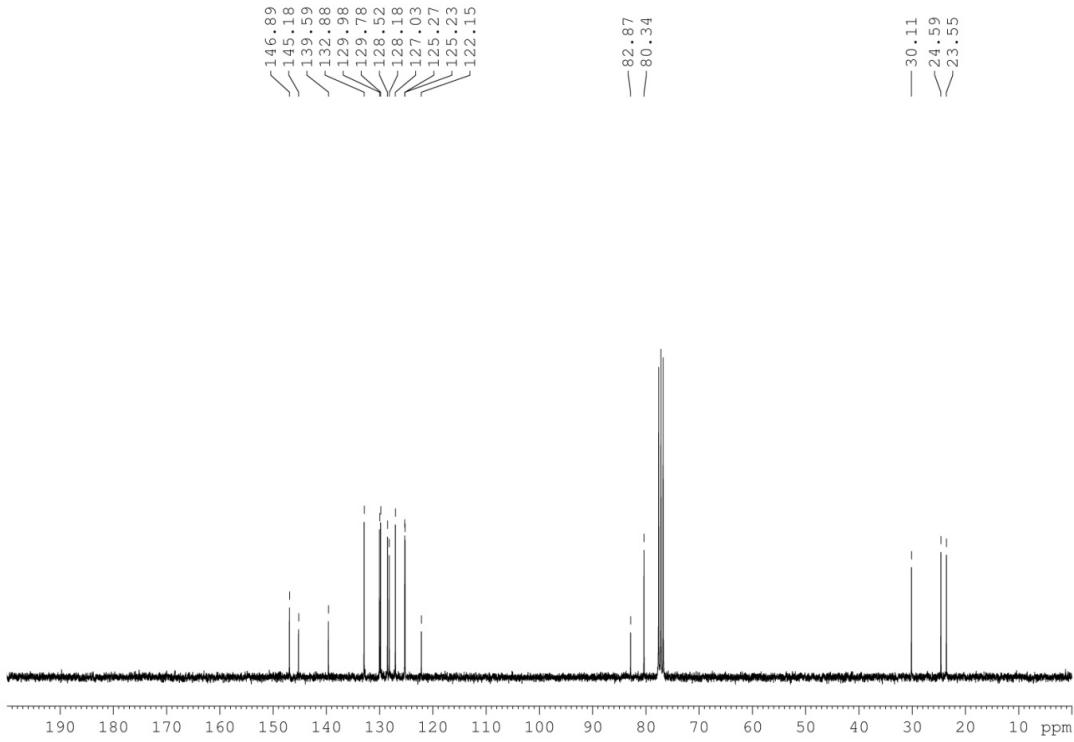
¹³C NMR (101 MHz, CDCl₃) **9**



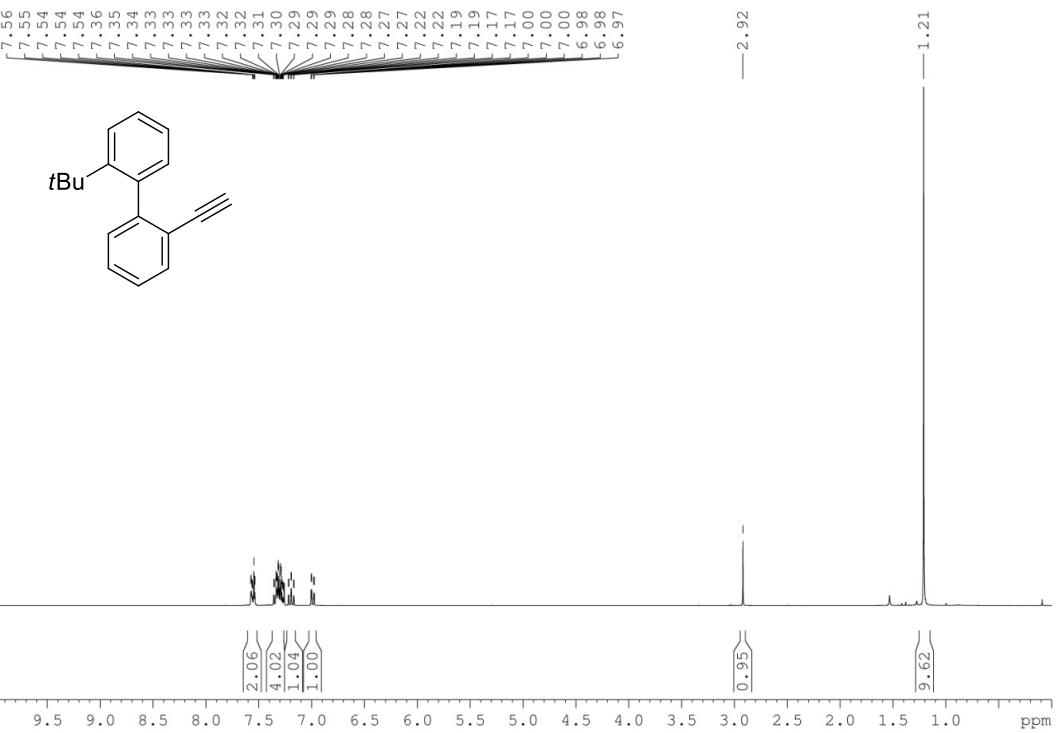
¹H NMR (400 MHz, CDCl₃) **11**



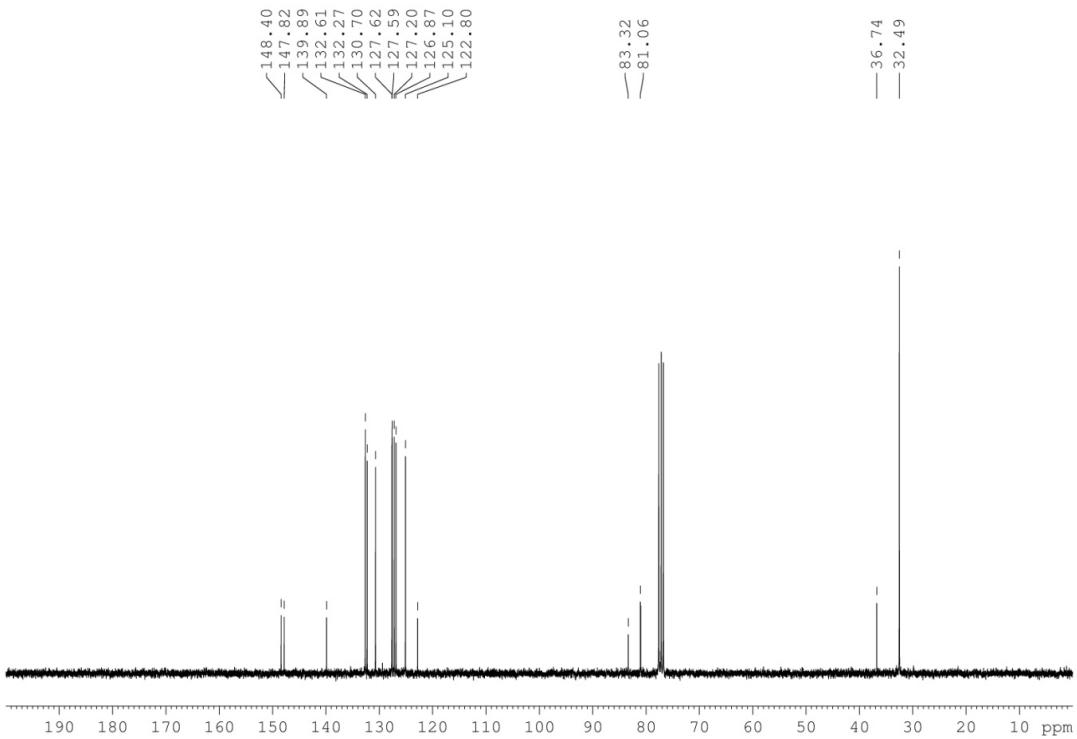
¹³C NMR (101 MHz, CDCl₃) **11**



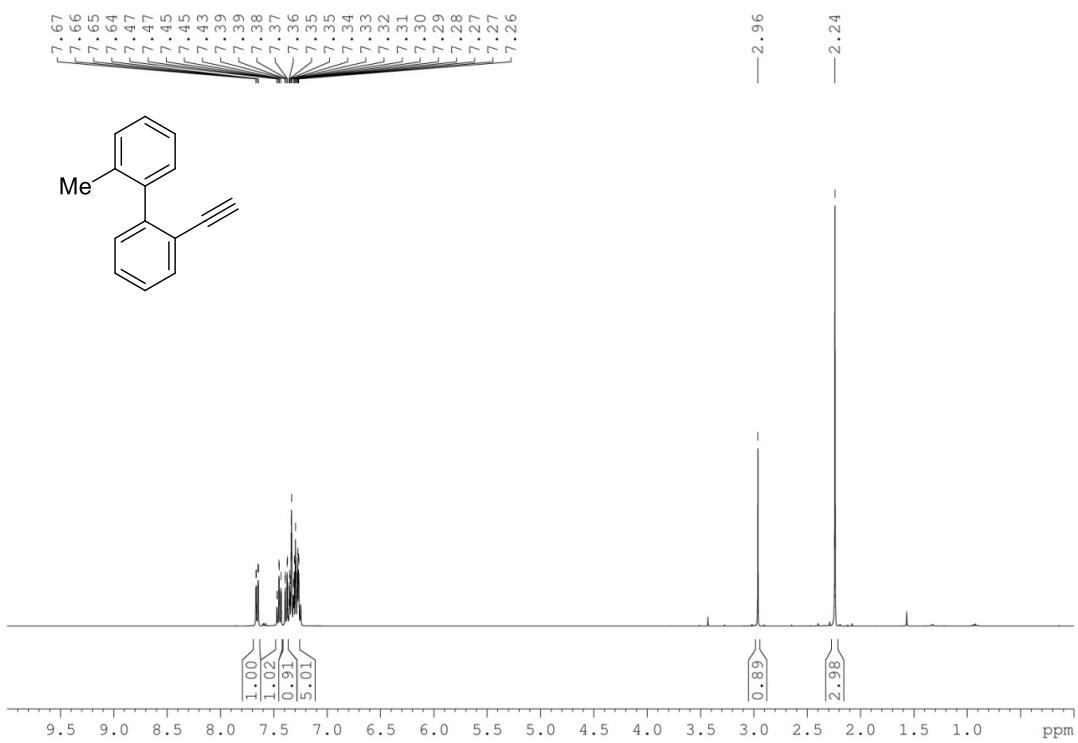
¹H NMR (400 MHz, CDCl₃) 12



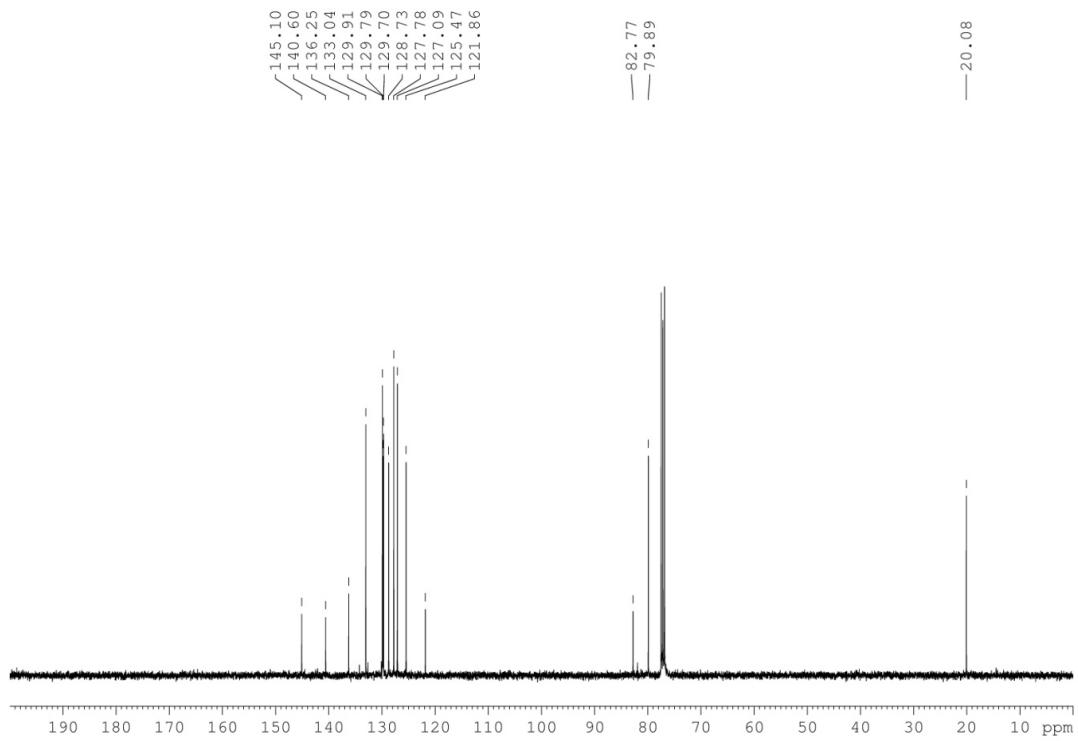
¹³C NMR (101 MHz, CDCl₃) 12



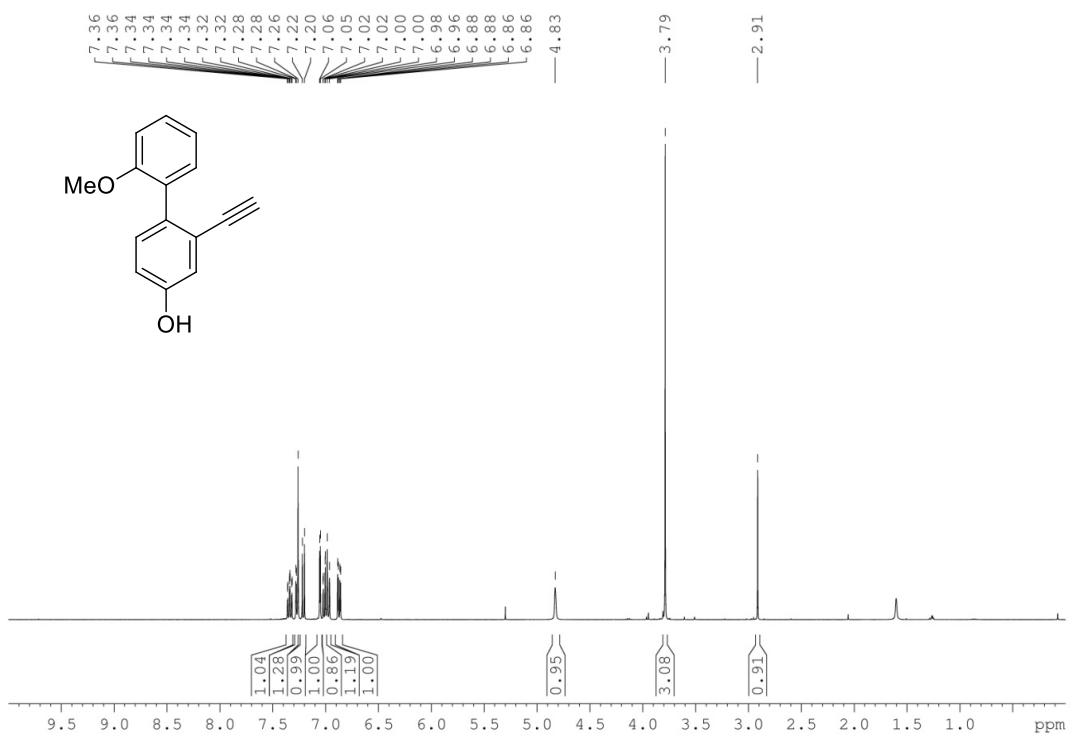
¹H NMR (400 MHz, CDCl₃) **13**



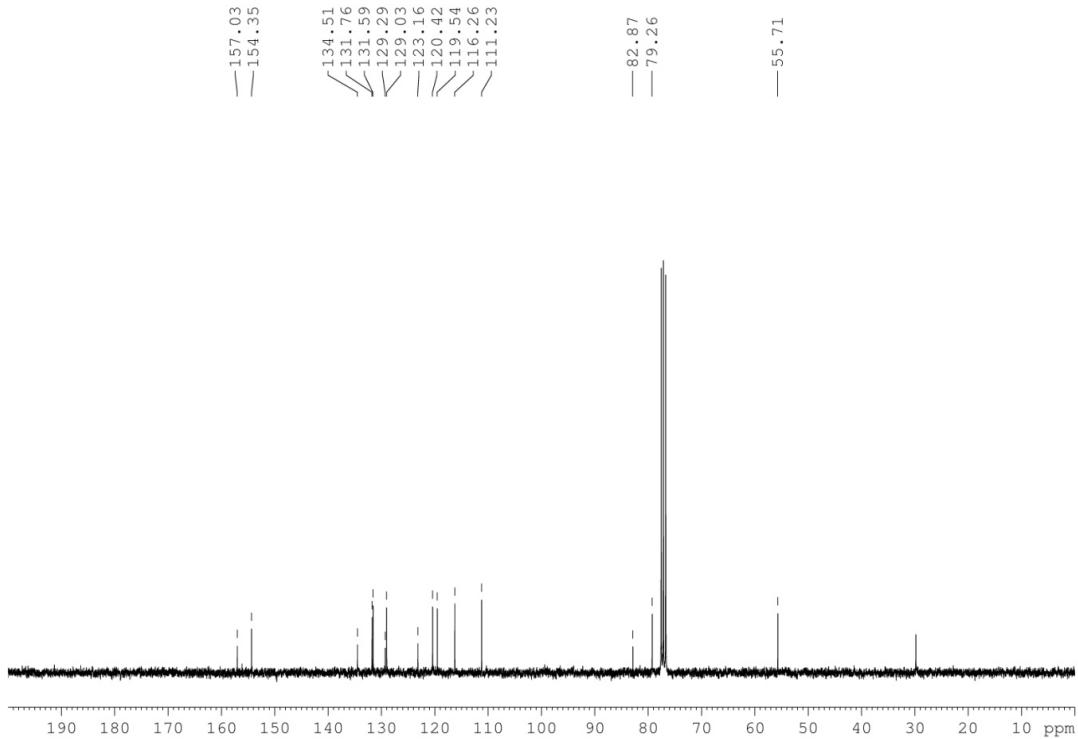
¹³C NMR (101 MHz, CDCl₃) **13**



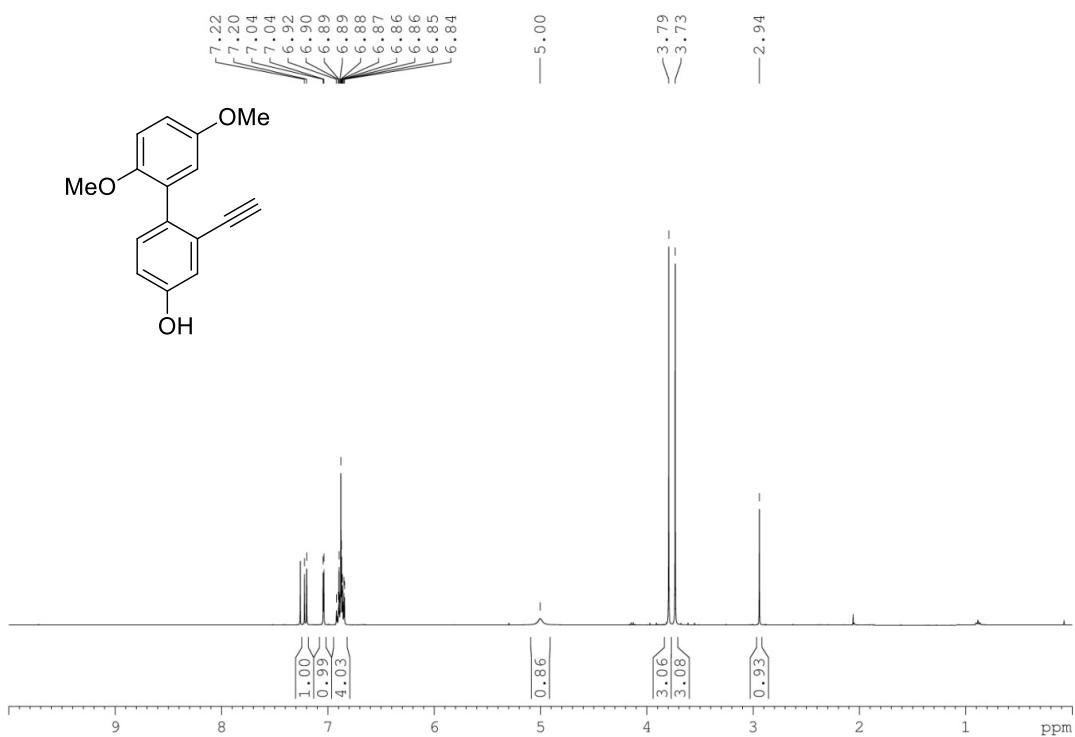
¹H NMR (400 MHz, CDCl₃) **14**



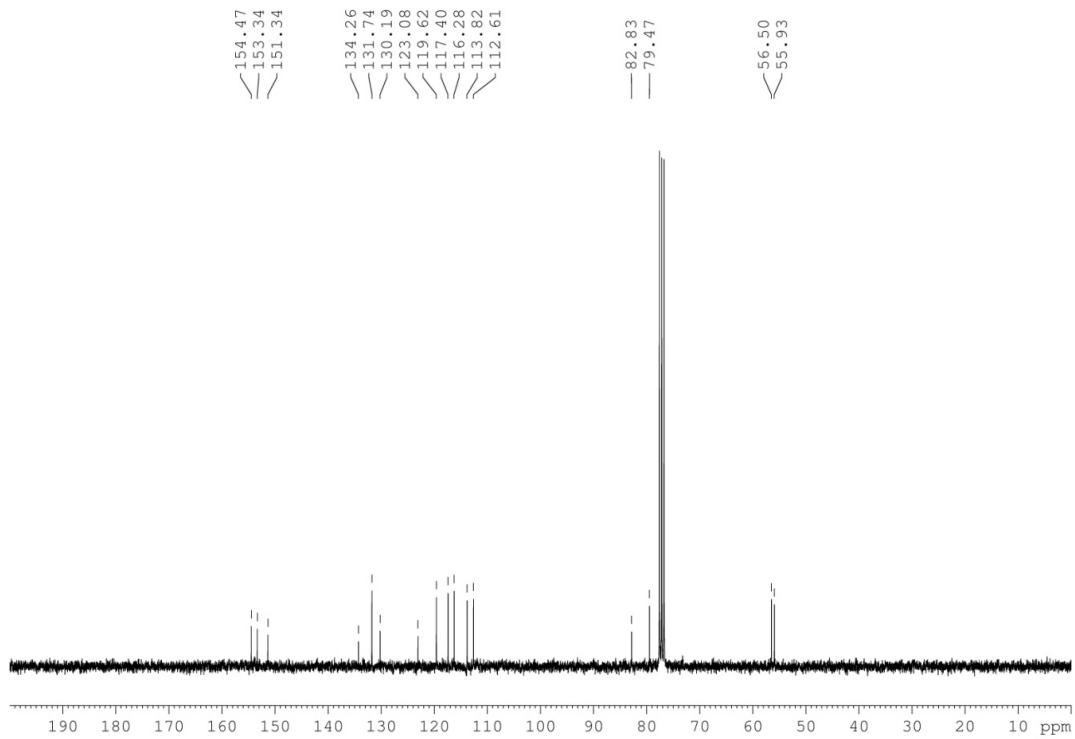
¹³C NMR (101 MHz, CDCl₃) 14



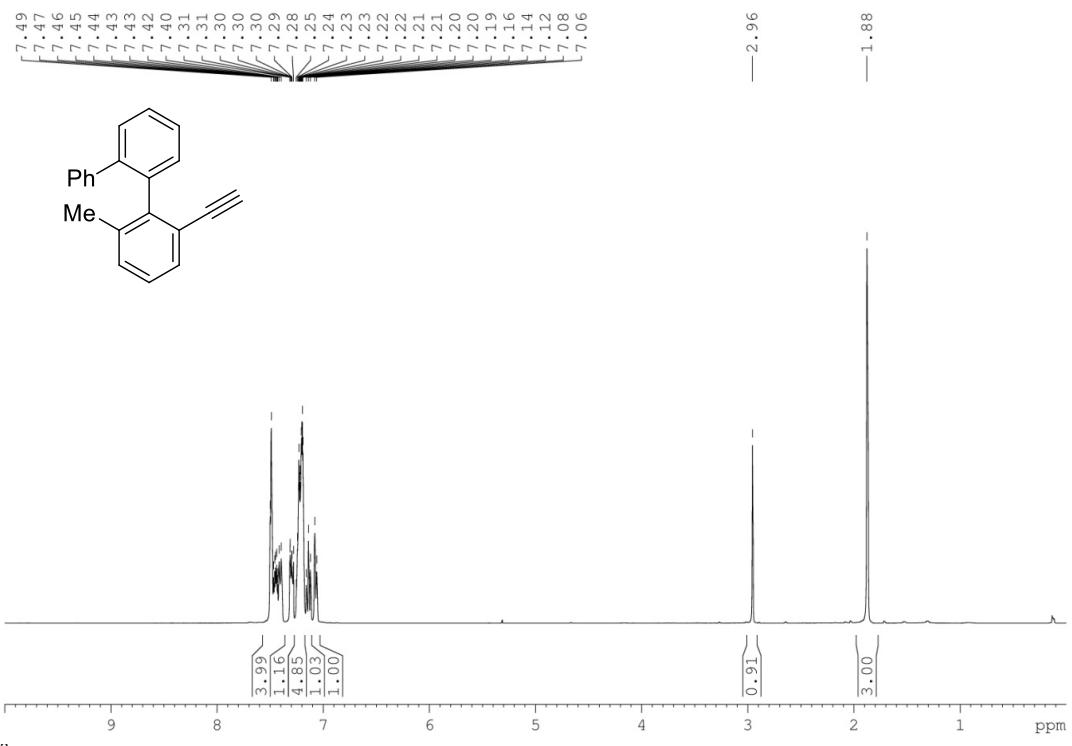
¹H NMR (400 MHz, CDCl₃) **15**



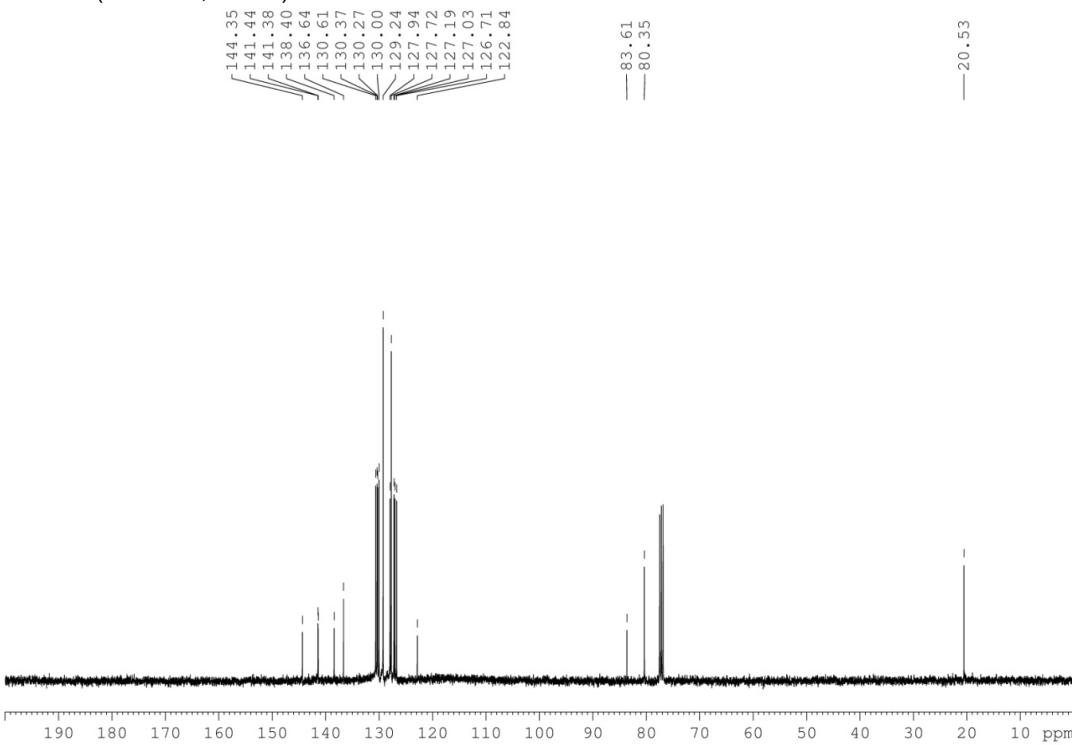
¹³C NMR (101 MHz, CDCl₃) **15**



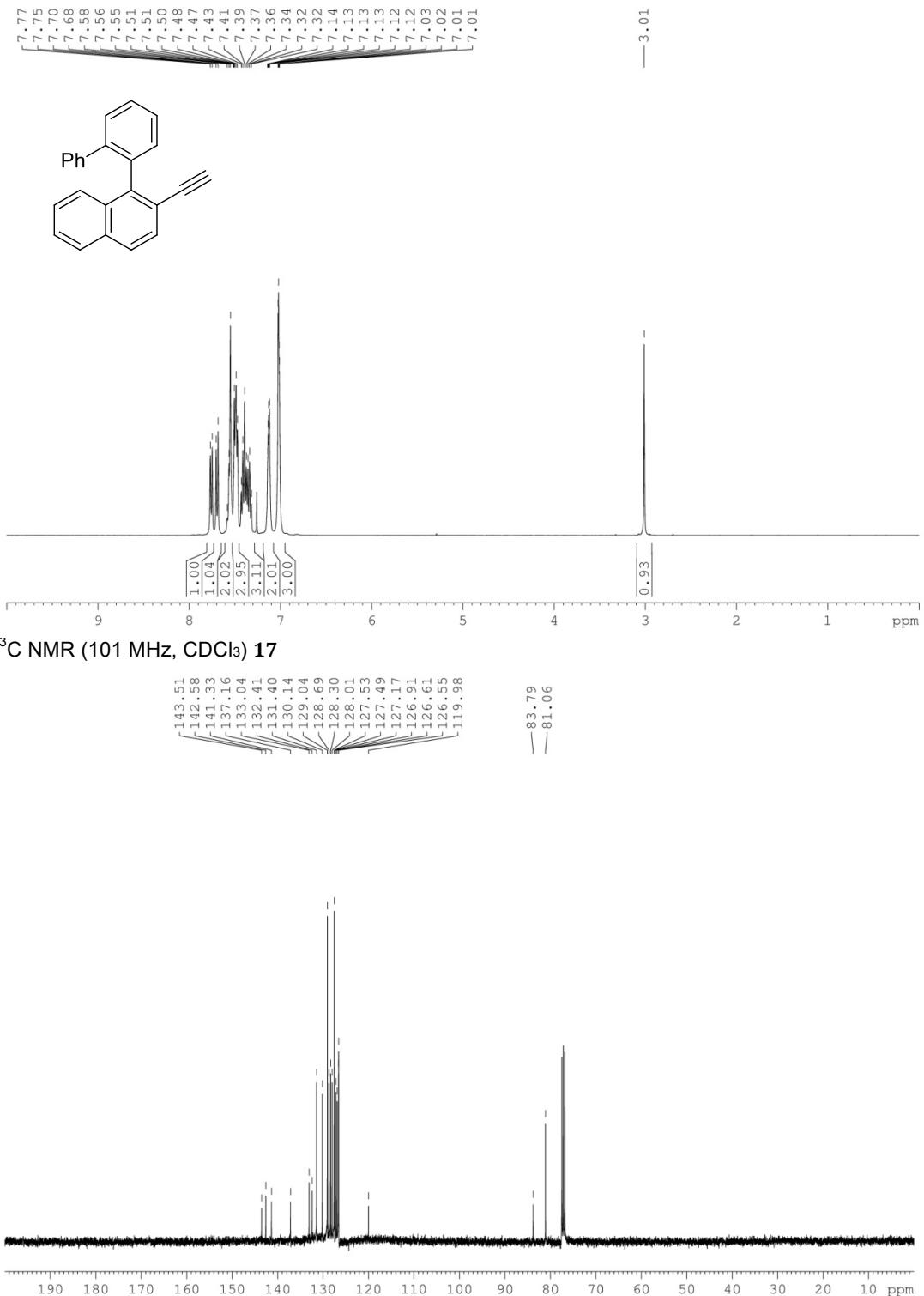
¹H NMR (400 MHz, CDCl₃) **16**



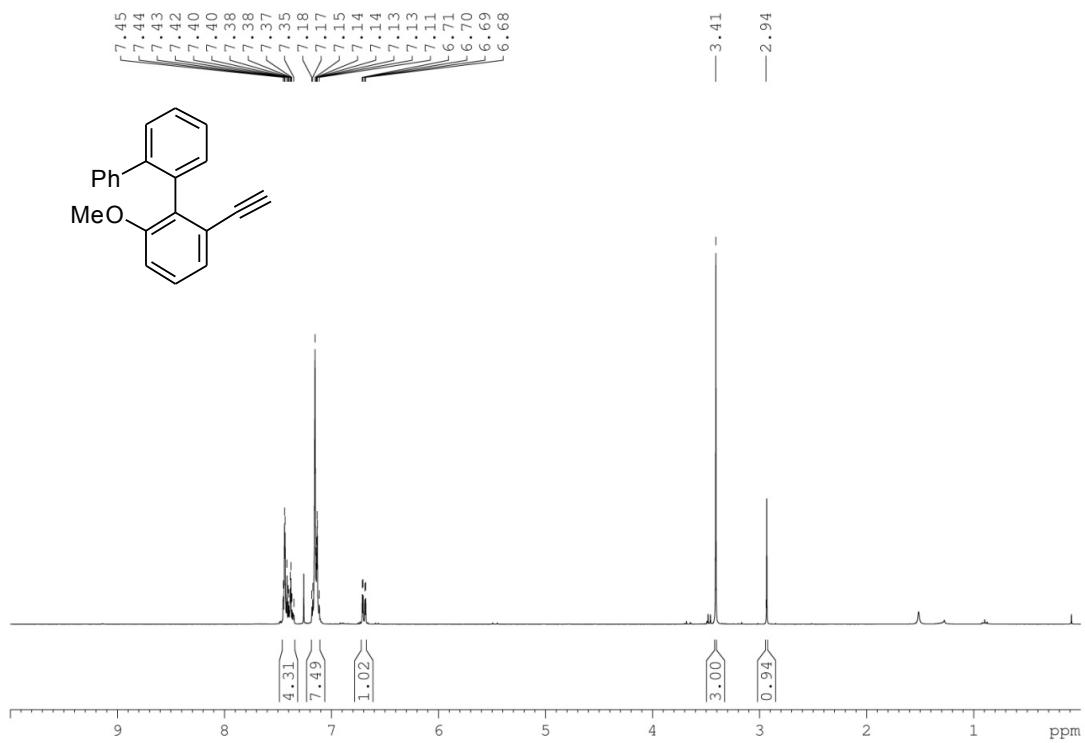
¹³C NMR (101 MHz, CDCl₃) **16**



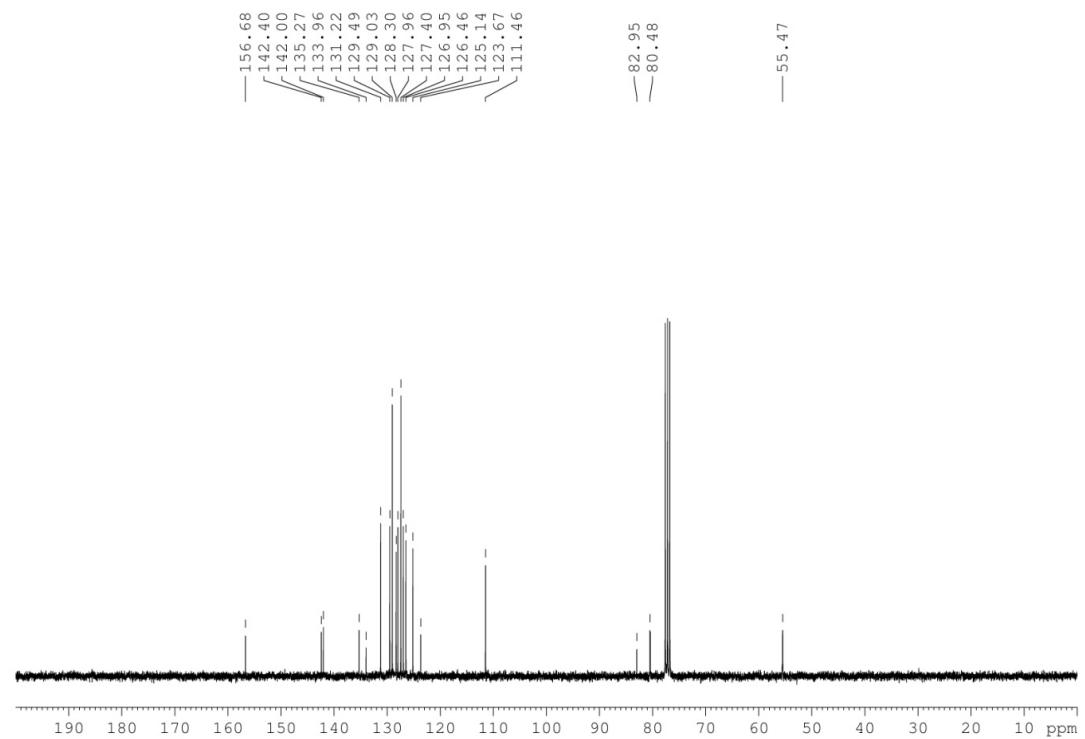
¹H NMR (400 MHz, CDCl₃) **17**



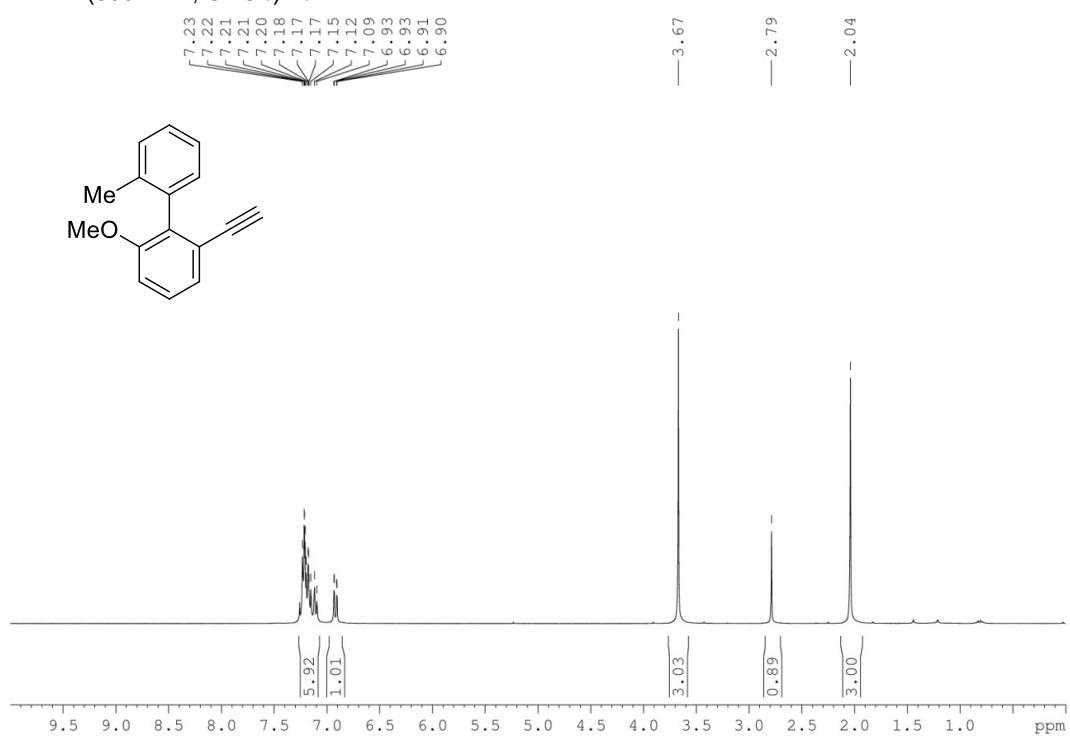
¹H NMR (400 MHz, CDCl₃) **18**



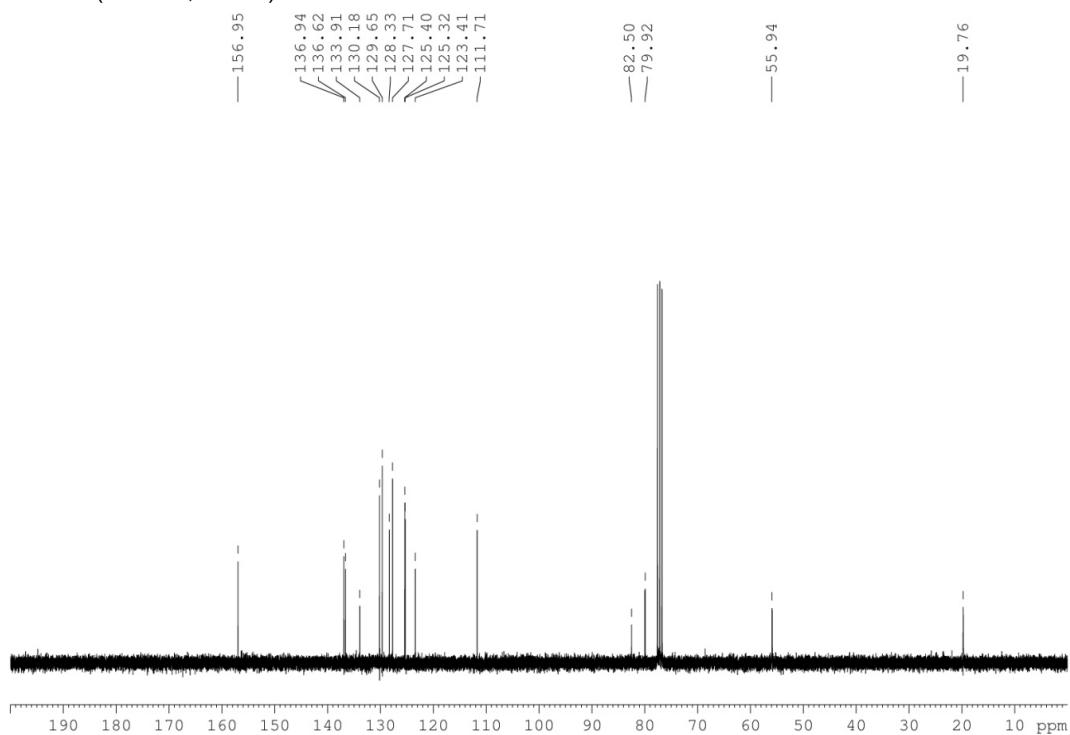
¹³C NMR (101 MHz, CDCl₃) **18**



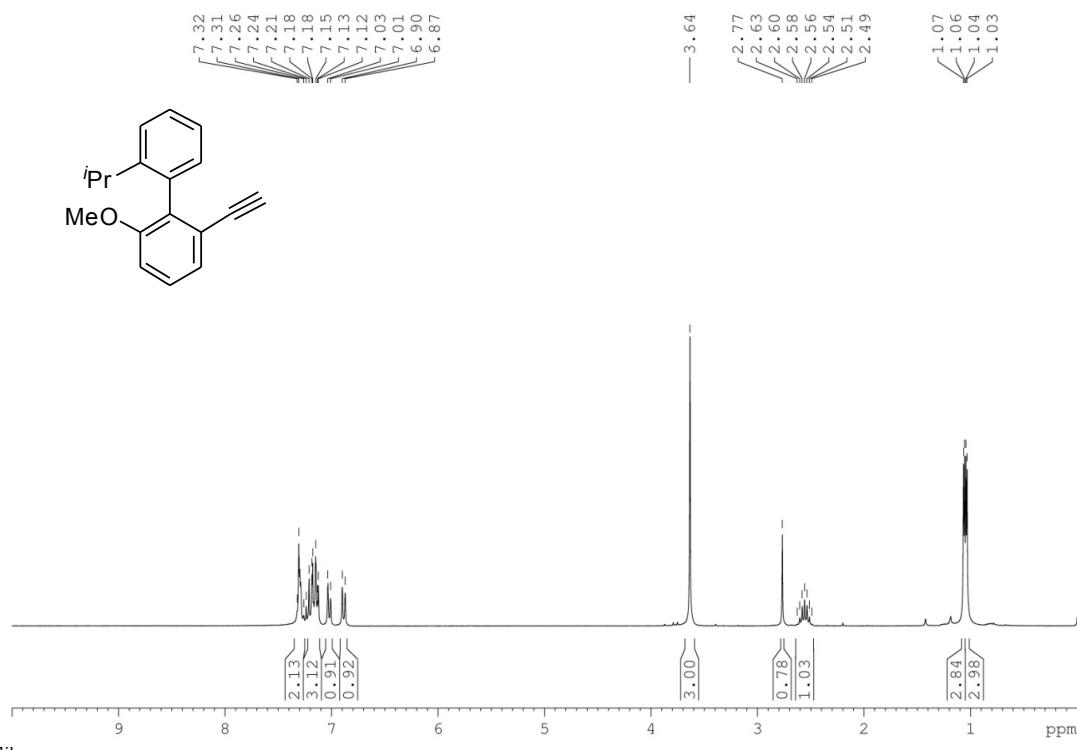
¹H NMR (300 MHz, CDCl₃) **19**



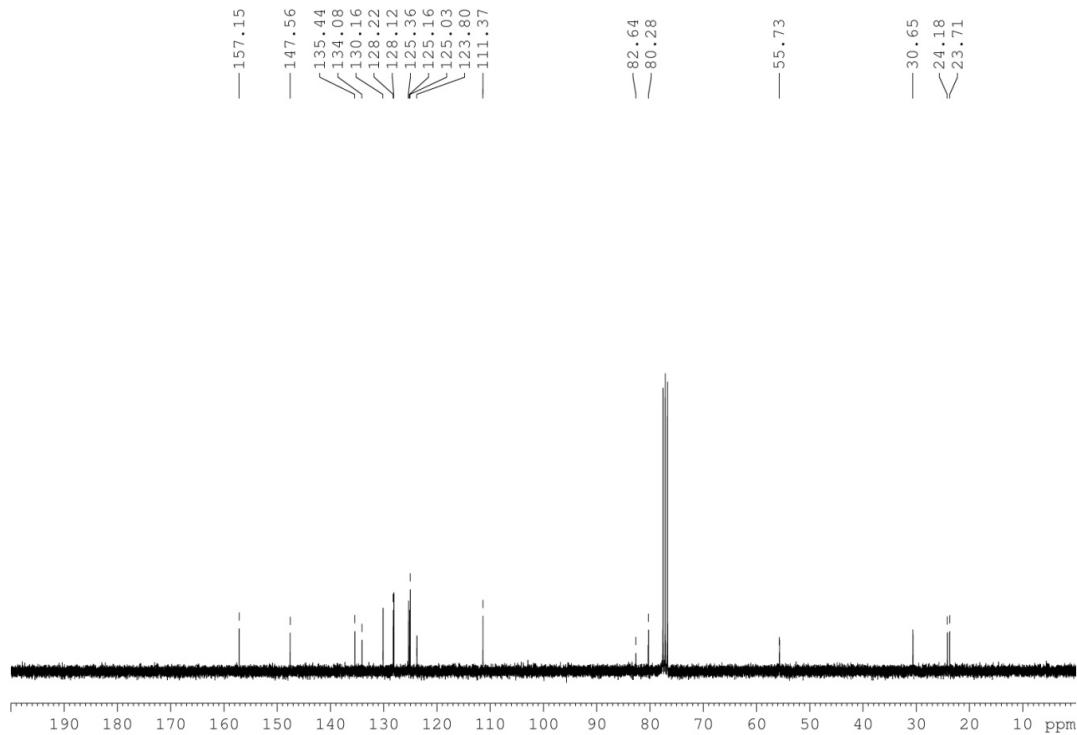
¹³C NMR (75 MHz, CDCl₃) **19**



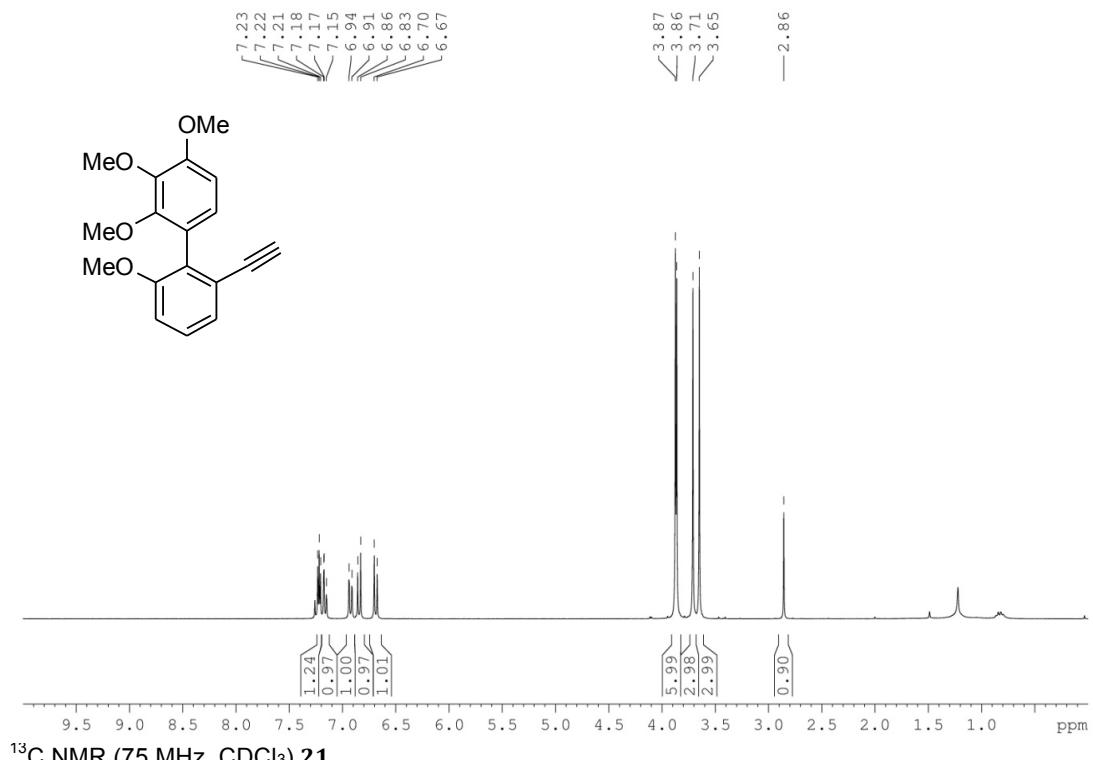
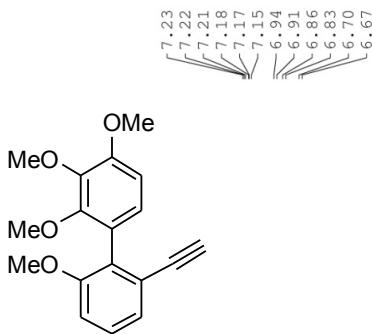
¹H NMR (300 MHz, CDCl₃) **20**



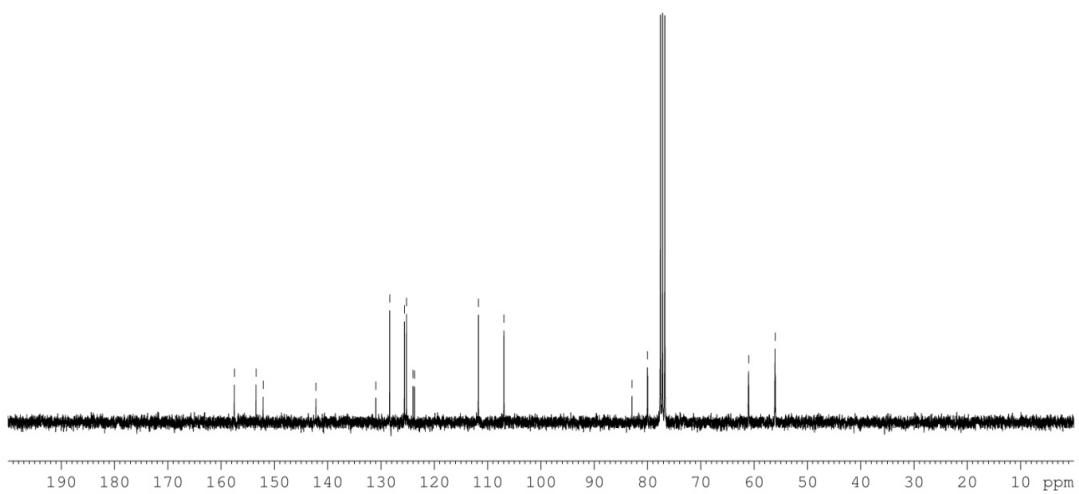
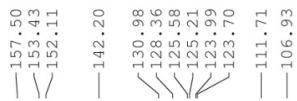
¹³C NMR (75 MHz, CDCl₃) **20**



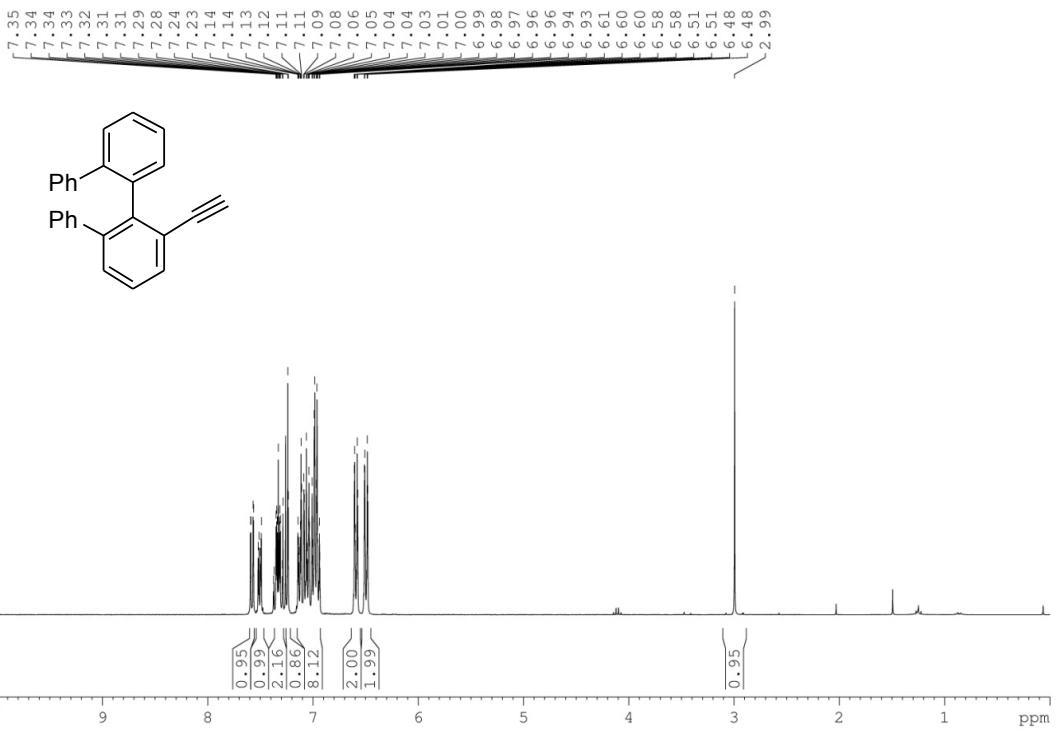
¹H NMR (300 MHz, CDCl₃) 21



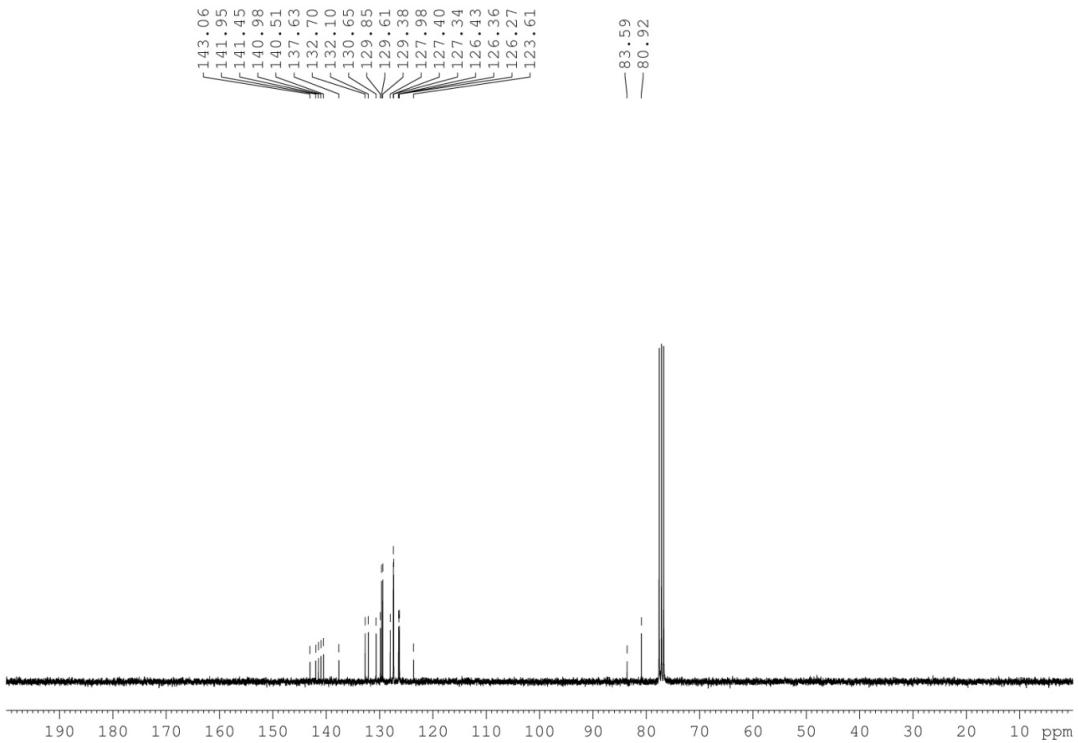
¹³C NMR (75 MHz, CDCl₃) 21



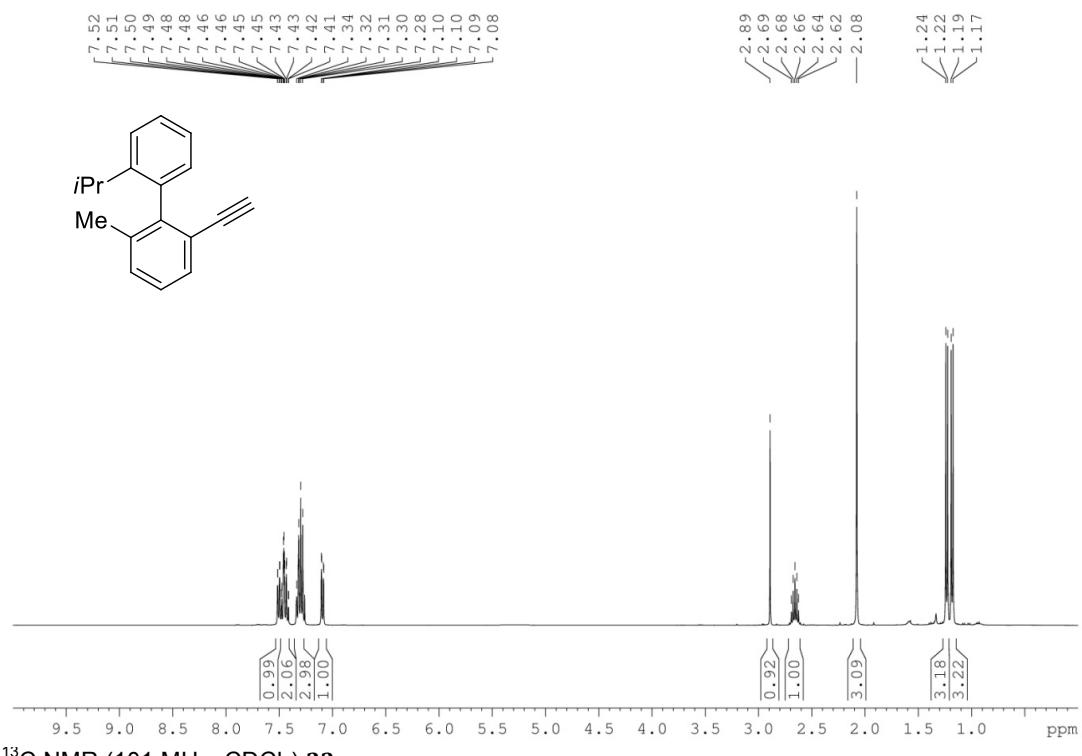
¹H NMR (300 MHz, CDCl₃) 22



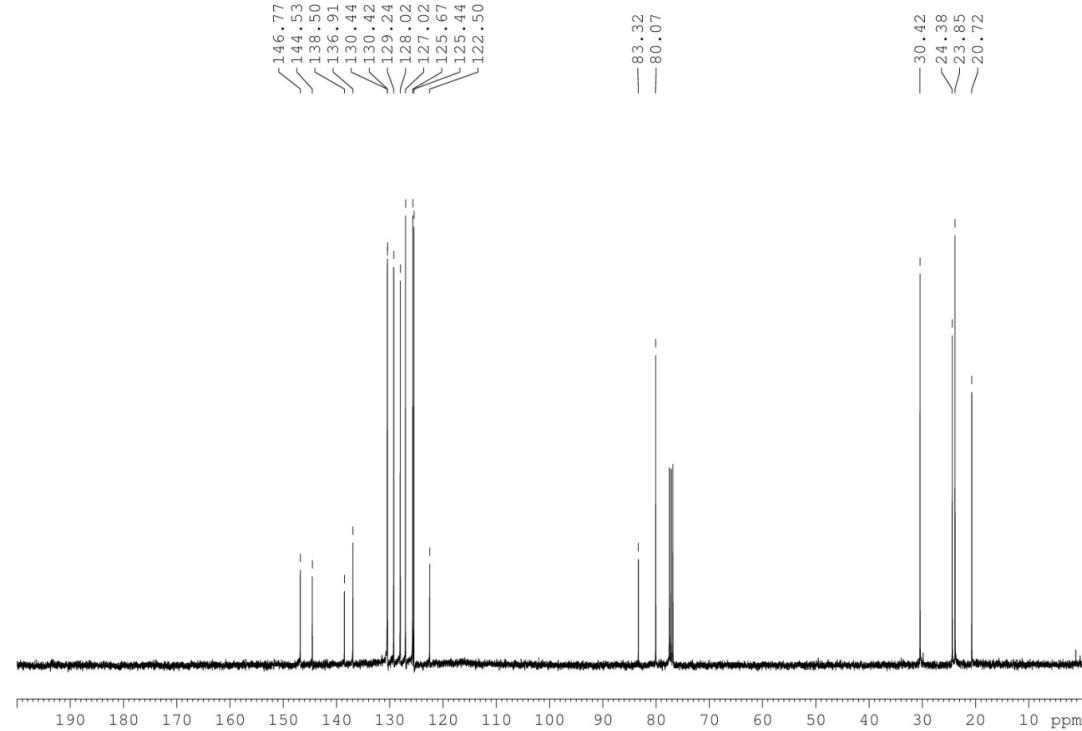
¹³C NMR (75 MHz, CDCl₃) 22



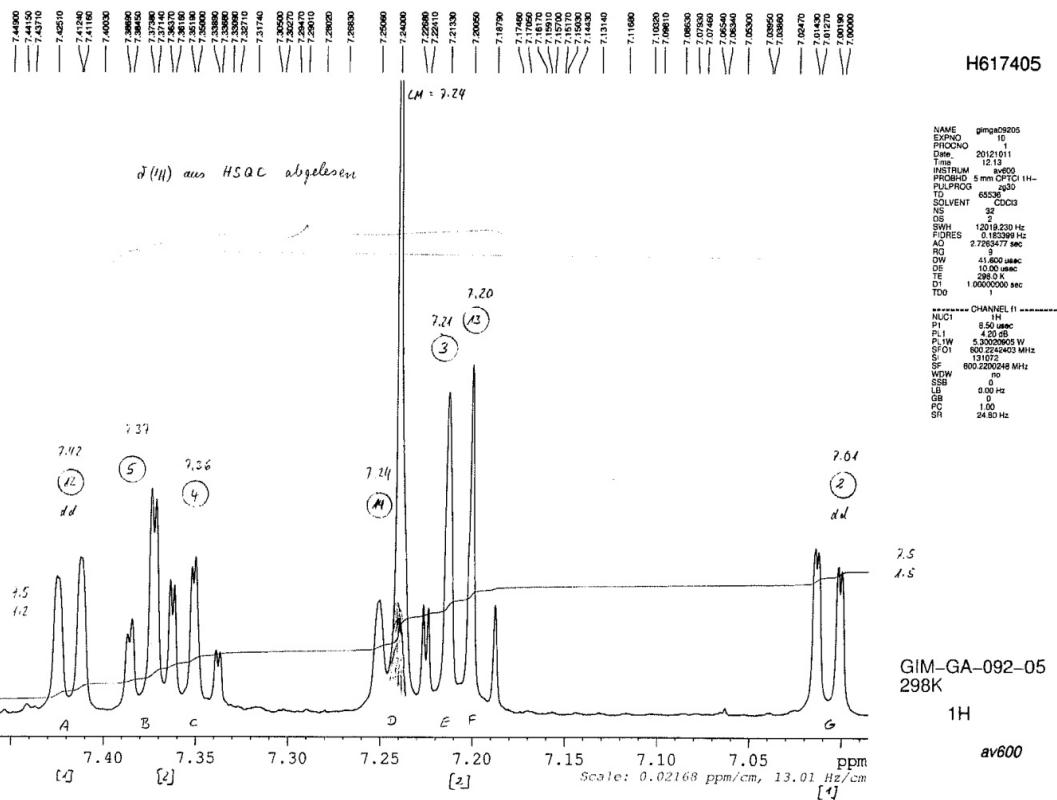
¹H NMR (400 MHz, CDCl₃) **23**



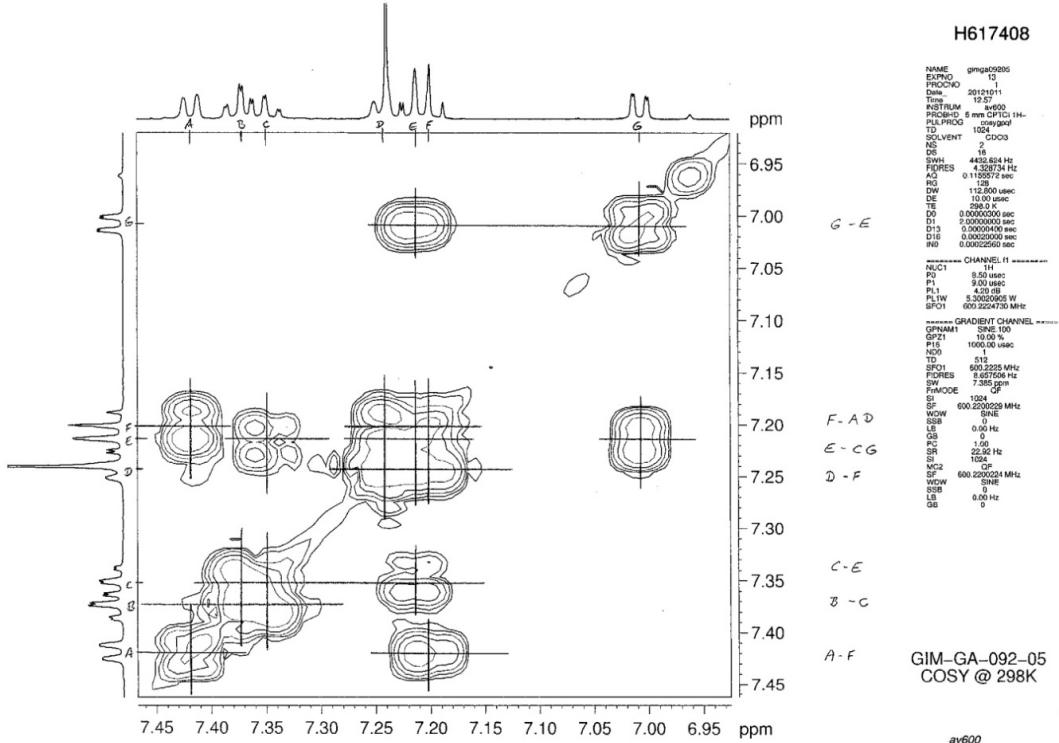
¹³C NMR (101 MHz, CDCl₃) **23**



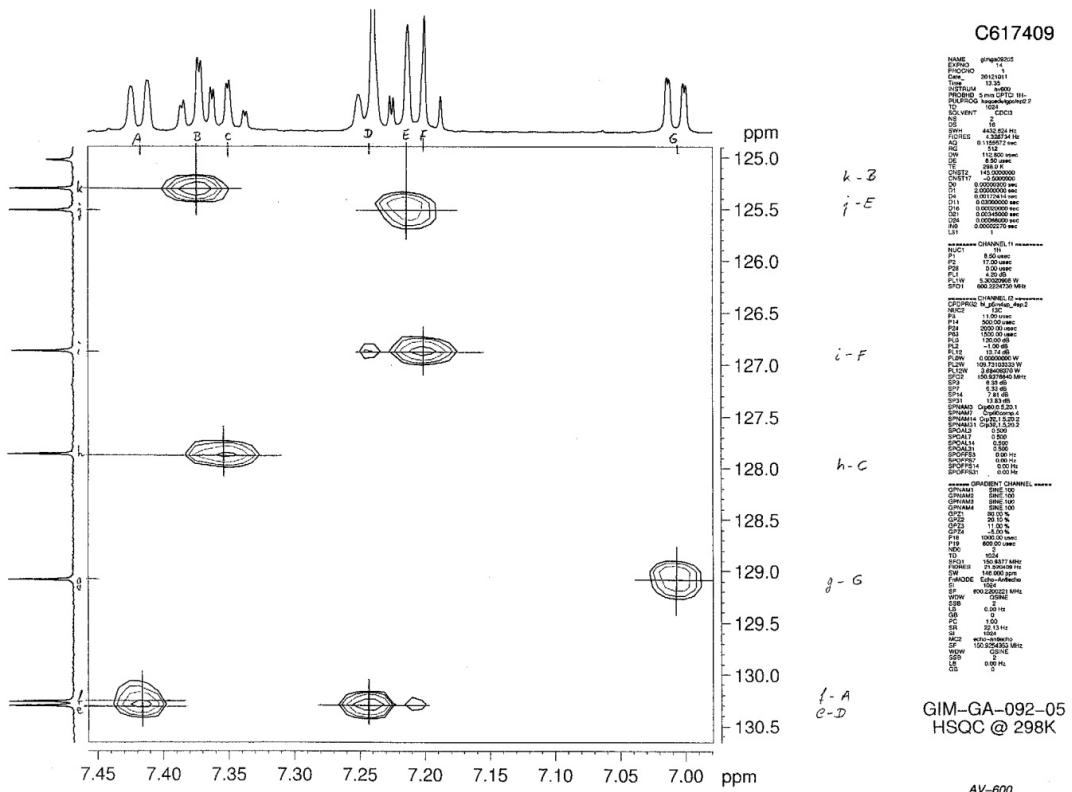
Select region for ^1H NMR (600 MHz, CDCl_3) 23



Select region for COSY (600 MHz, CDCl_3) 23



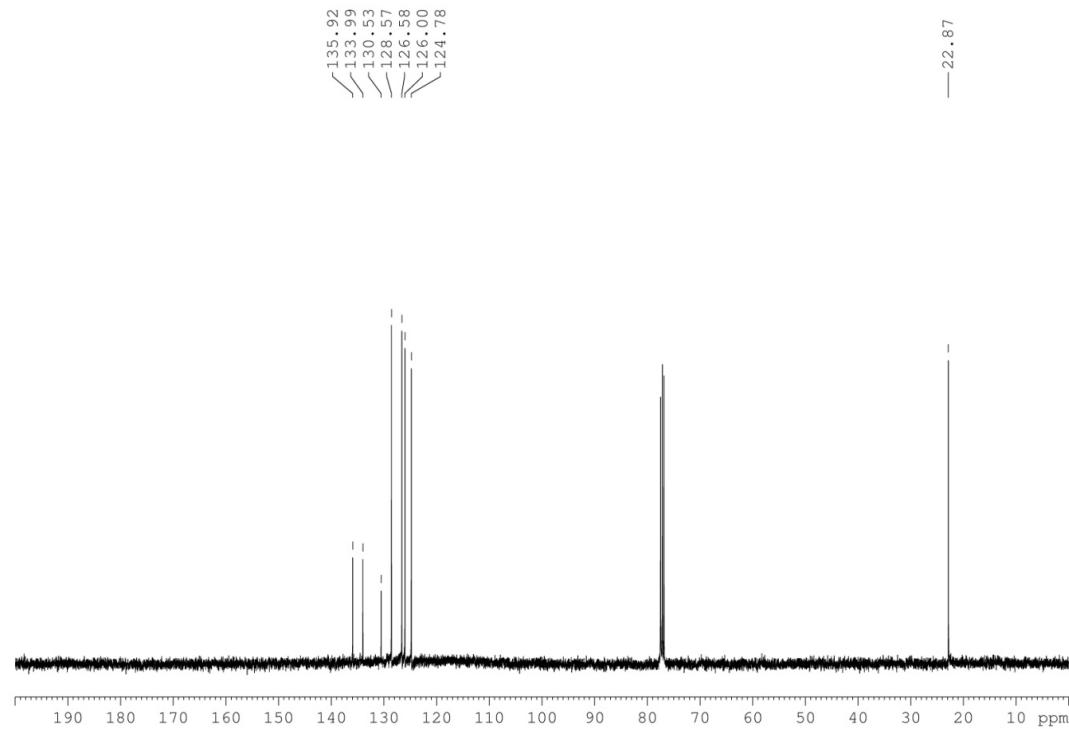
Select region for HSQC (600 MHz, CDCl_3) 23



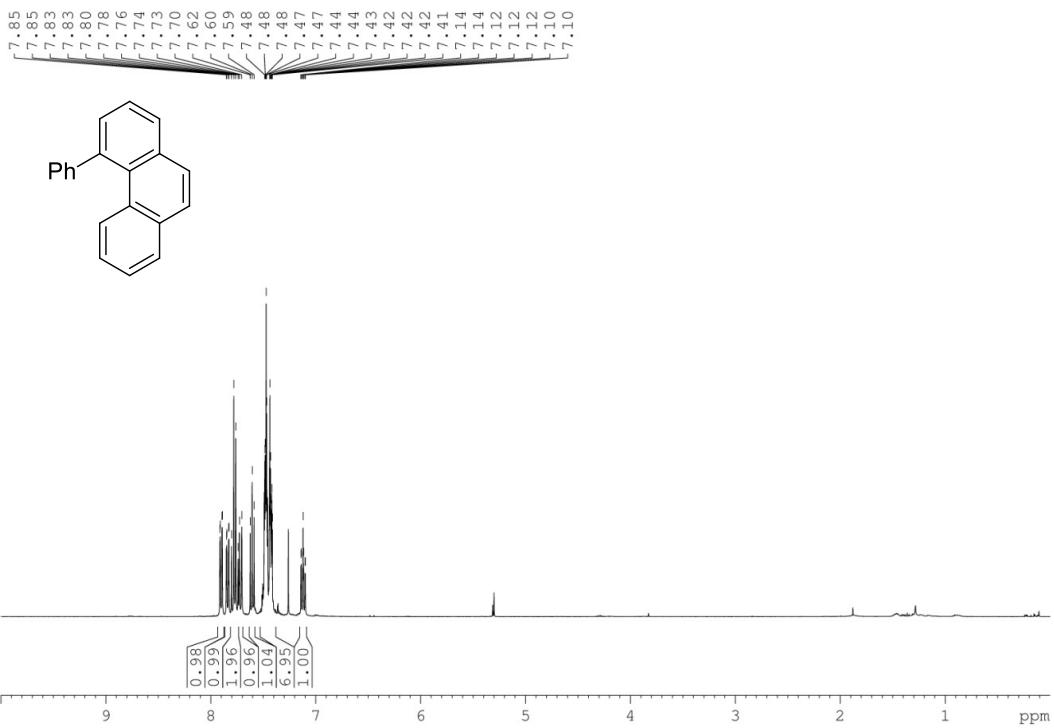
¹H NMR (400 MHz, CDCl₃) **8**



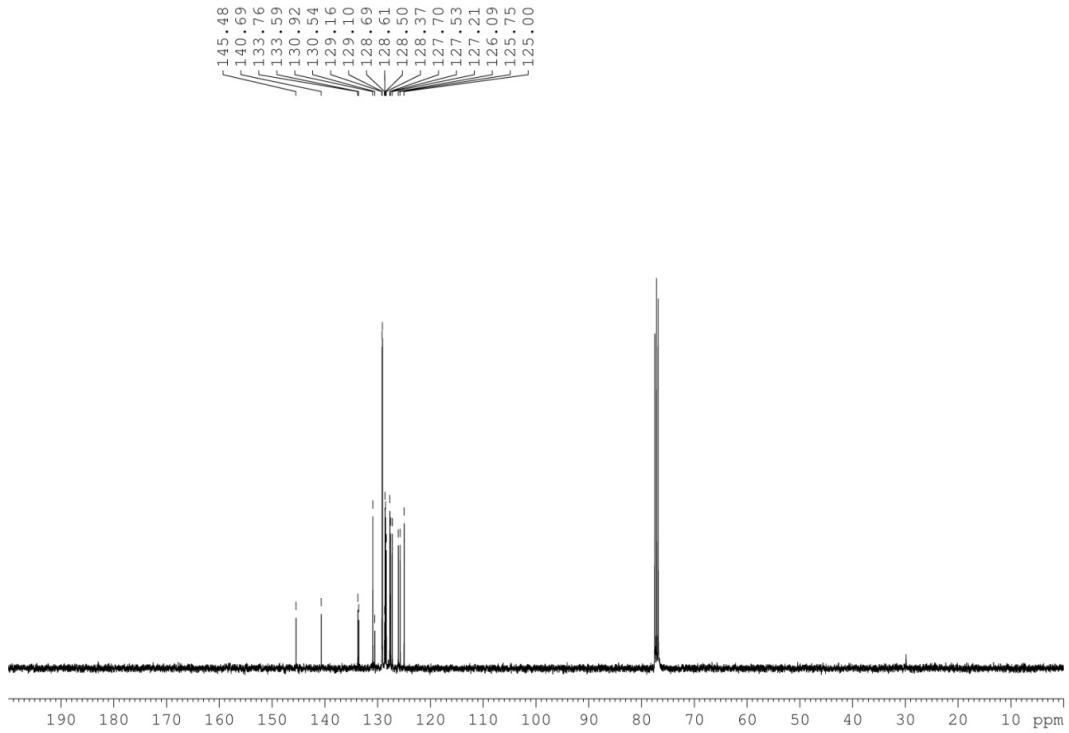
¹³C NMR (101 MHz, CDCl₃) **8**



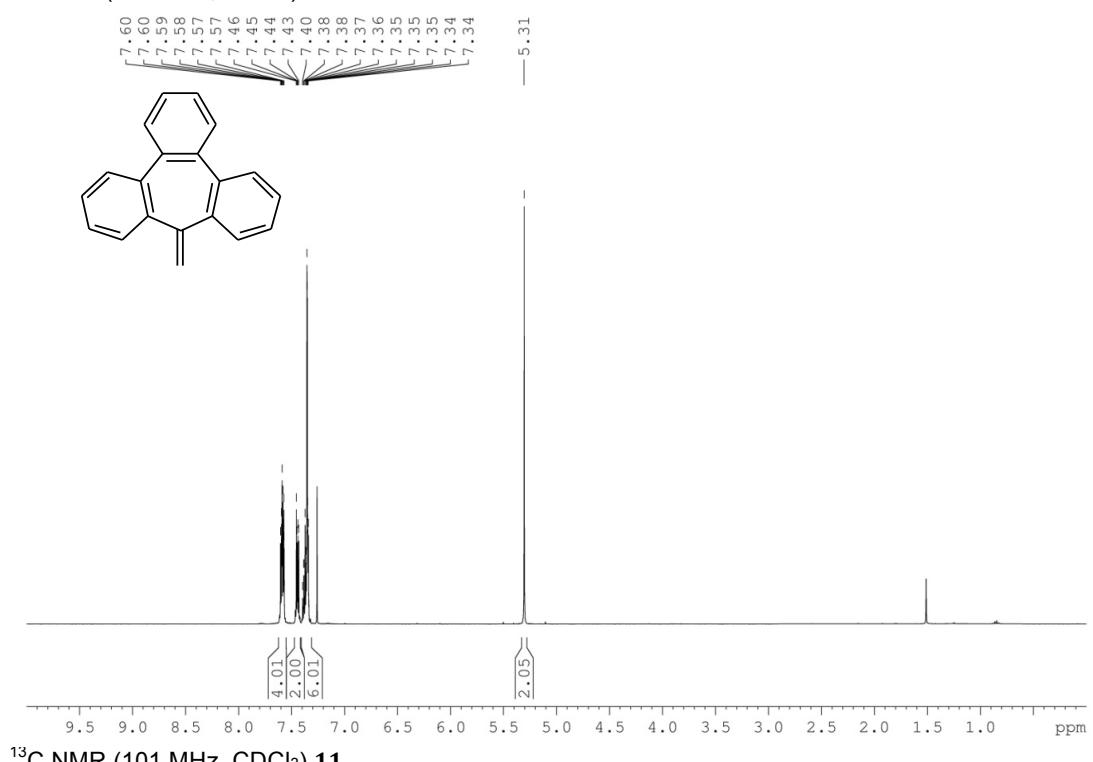
¹H NMR (400 MHz, CDCl₃) **10**



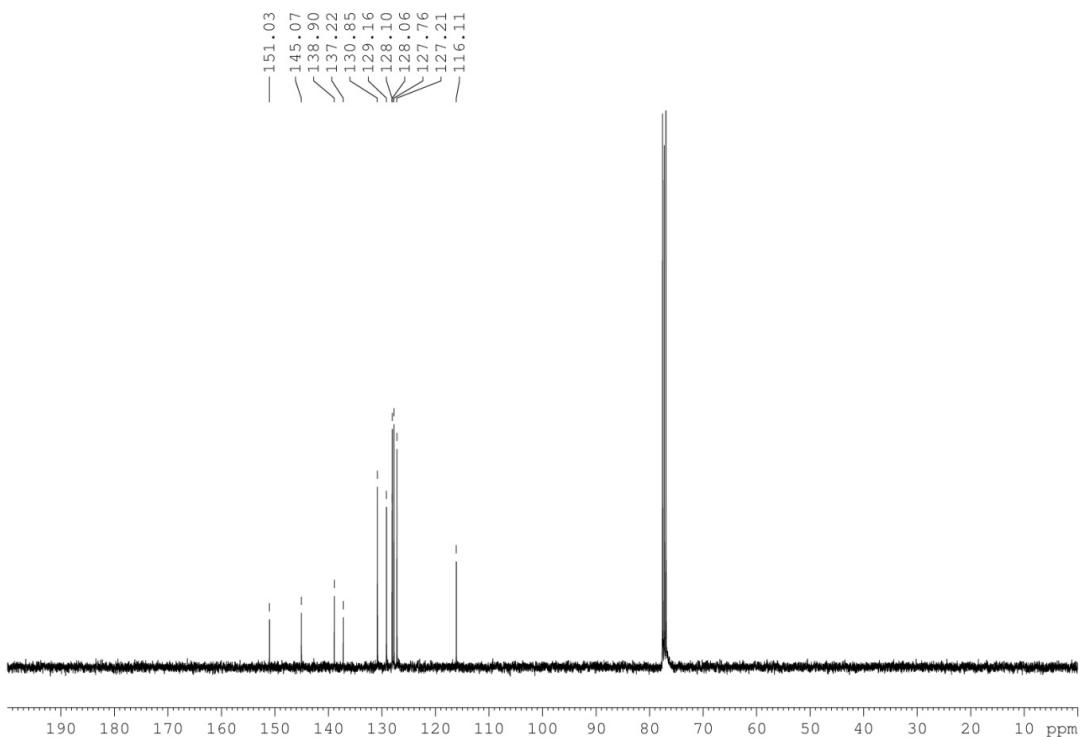
¹³C NMR (101 MHz, CDCl₃) **10**



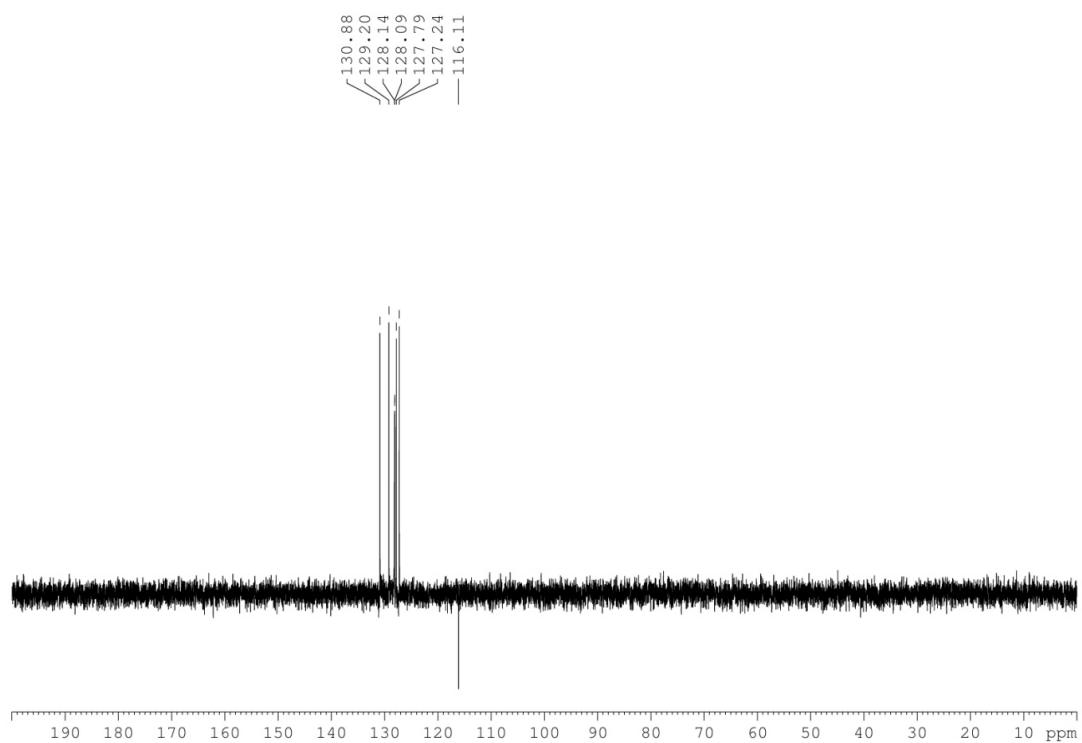
¹H NMR (400 MHz, CDCl₃) **11**



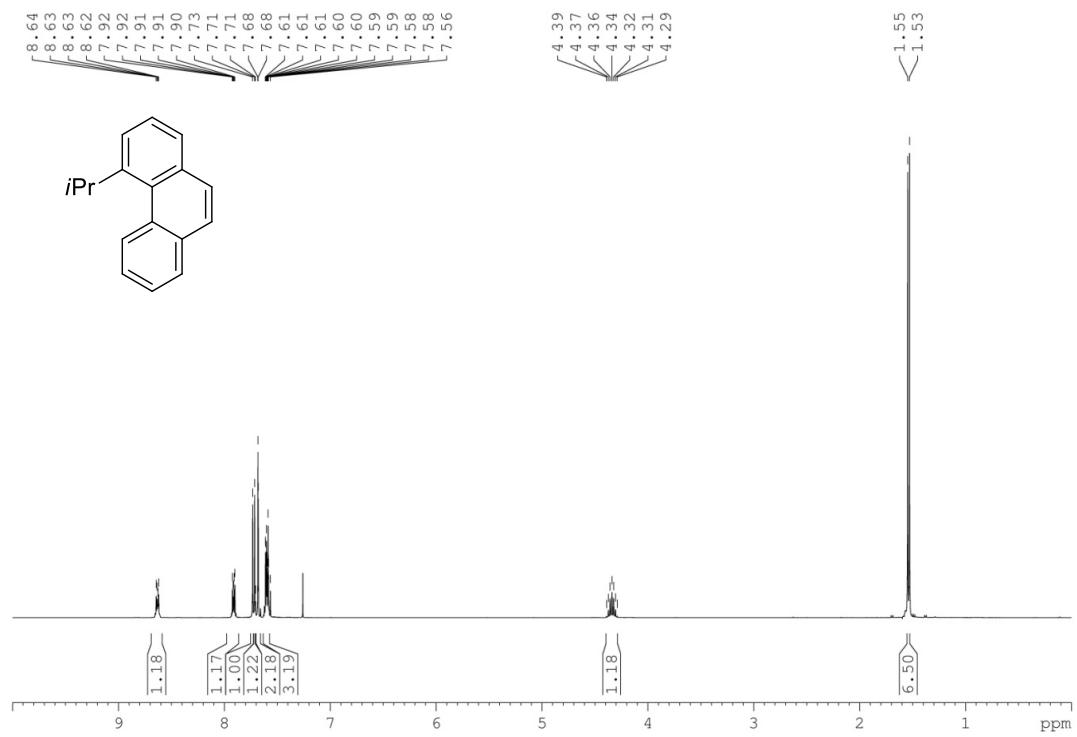
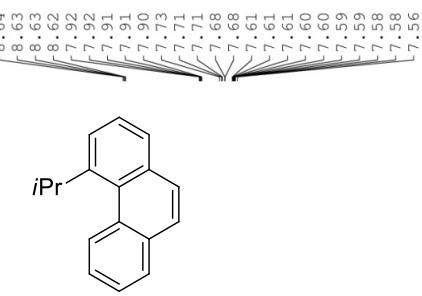
¹³C NMR (101 MHz, CDCl₃) **11**



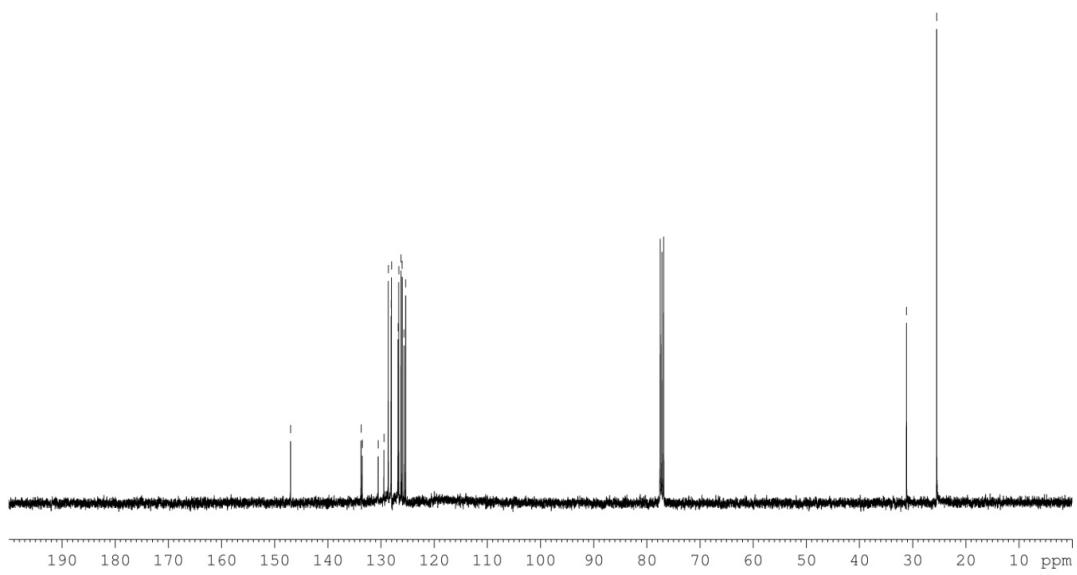
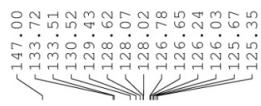
¹³C NMR [DEPT135] (101 MHz, CDCl₃) **11**



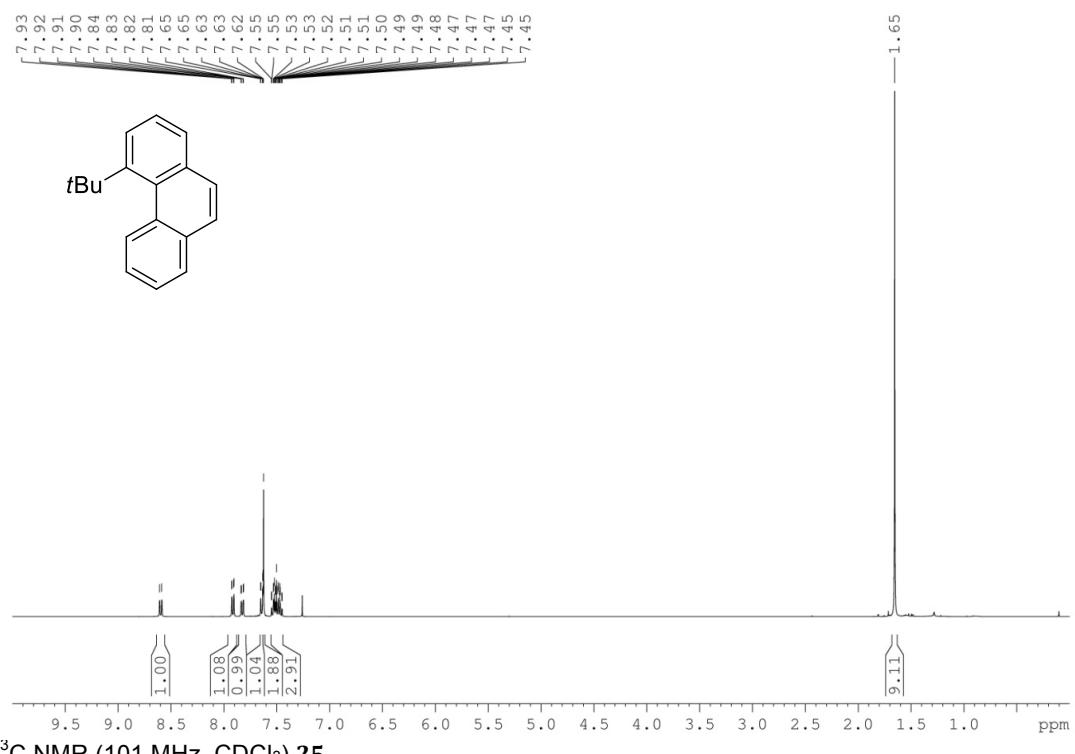
¹H NMR (400 MHz, CDCl₃) 24



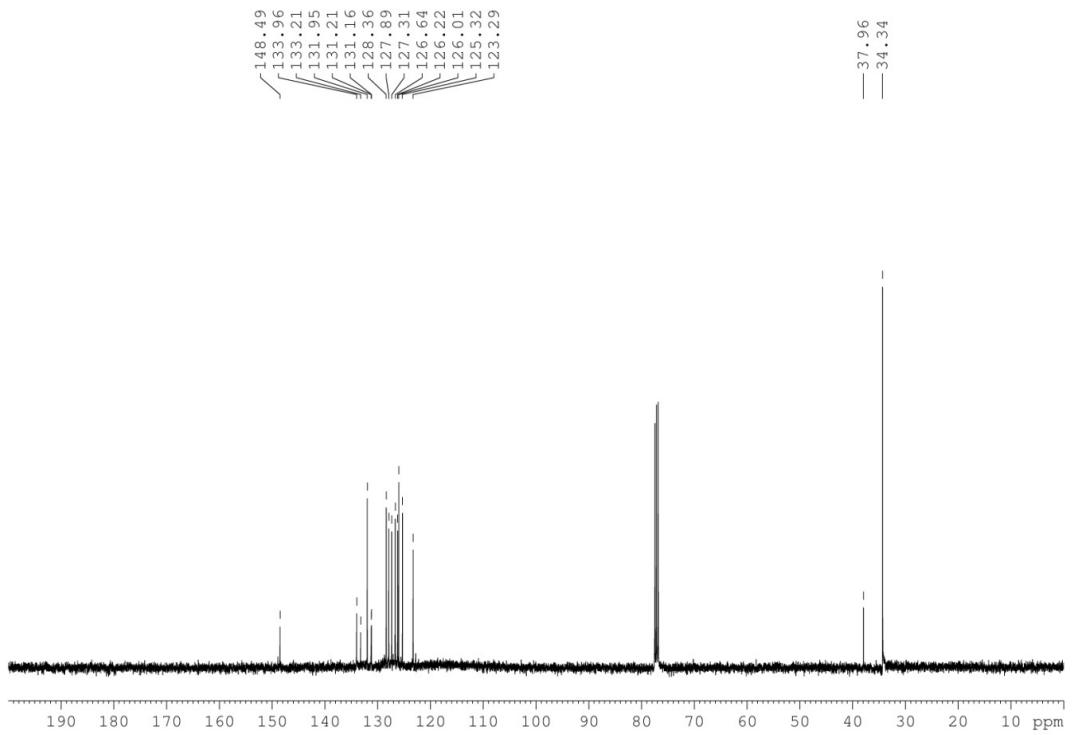
¹³C NMR (101 MHz, CDCl₃) 24



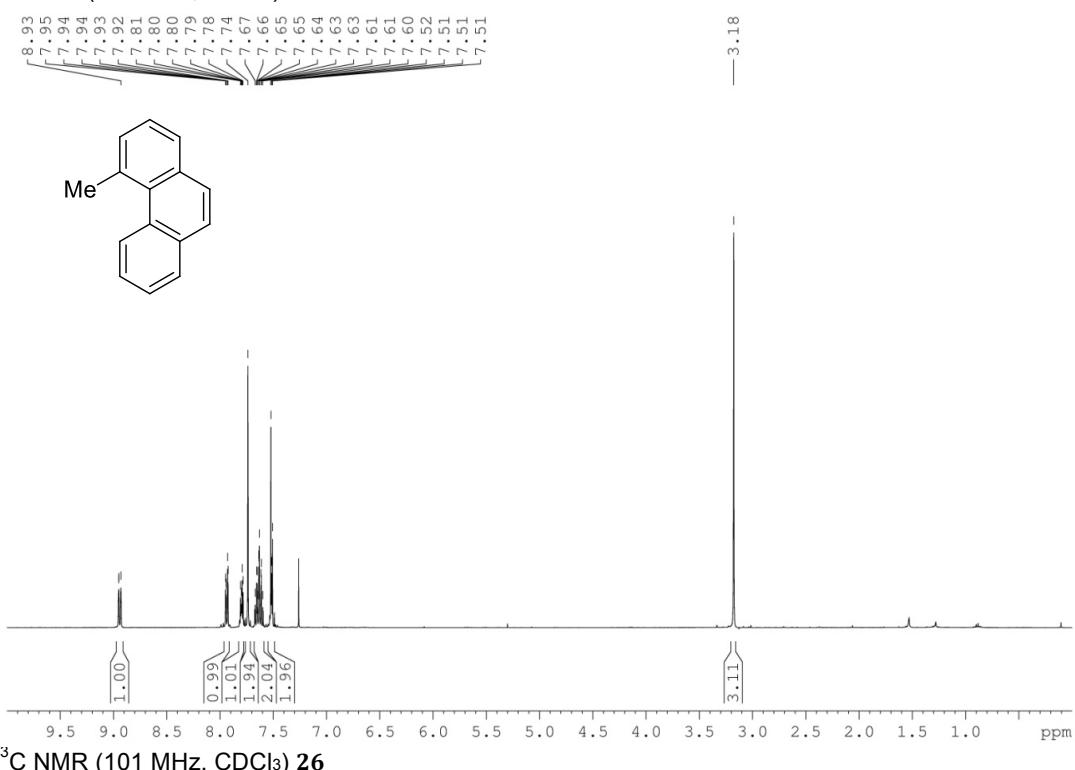
¹H NMR (400 MHz, CDCl₃) 25



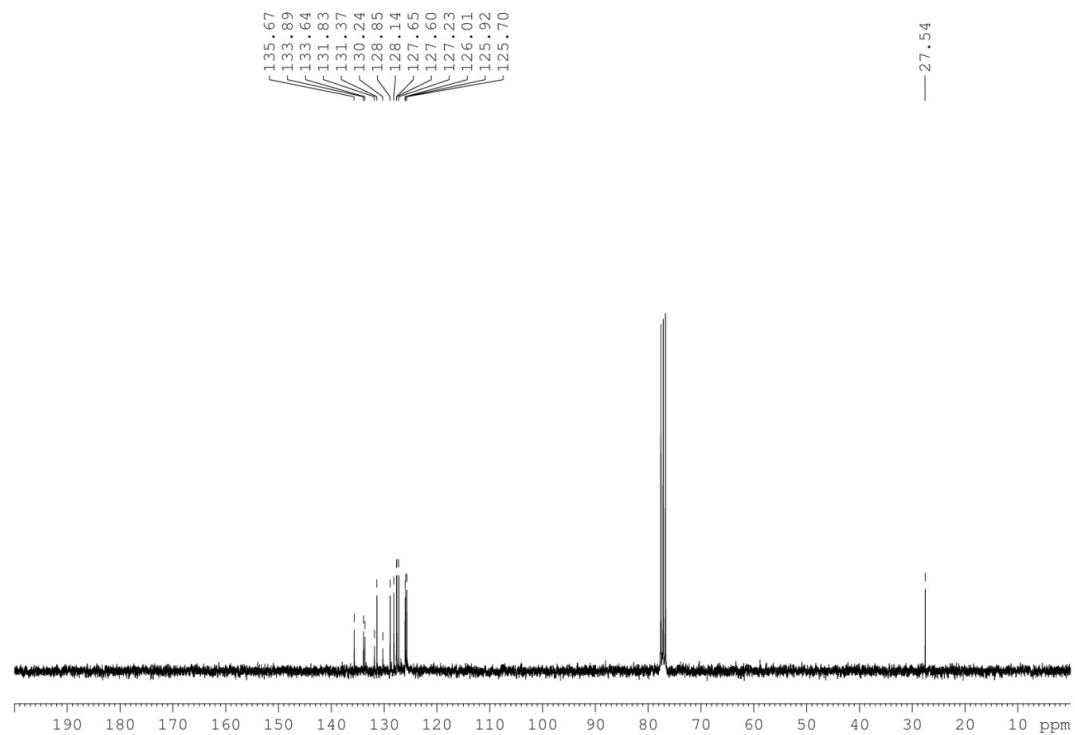
¹³C NMR (101 MHz, CDCl₃) 25



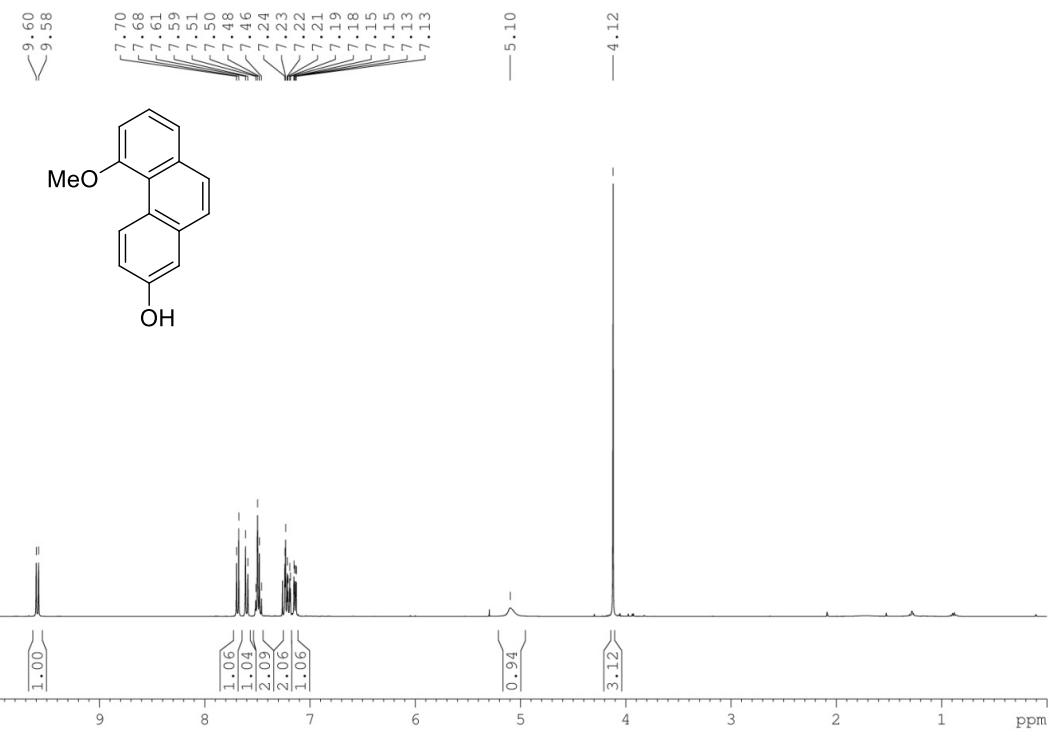
¹H NMR (400 MHz, CDCl₃) **26**



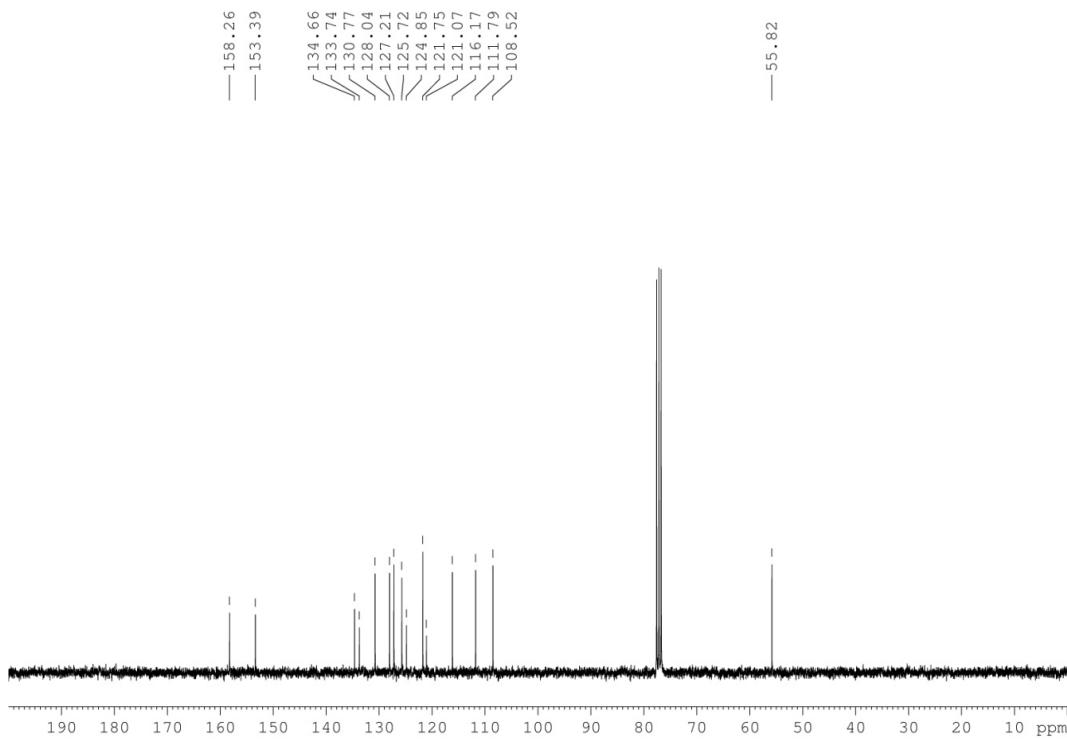
¹³C NMR (101 MHz, CDCl₃) **26**



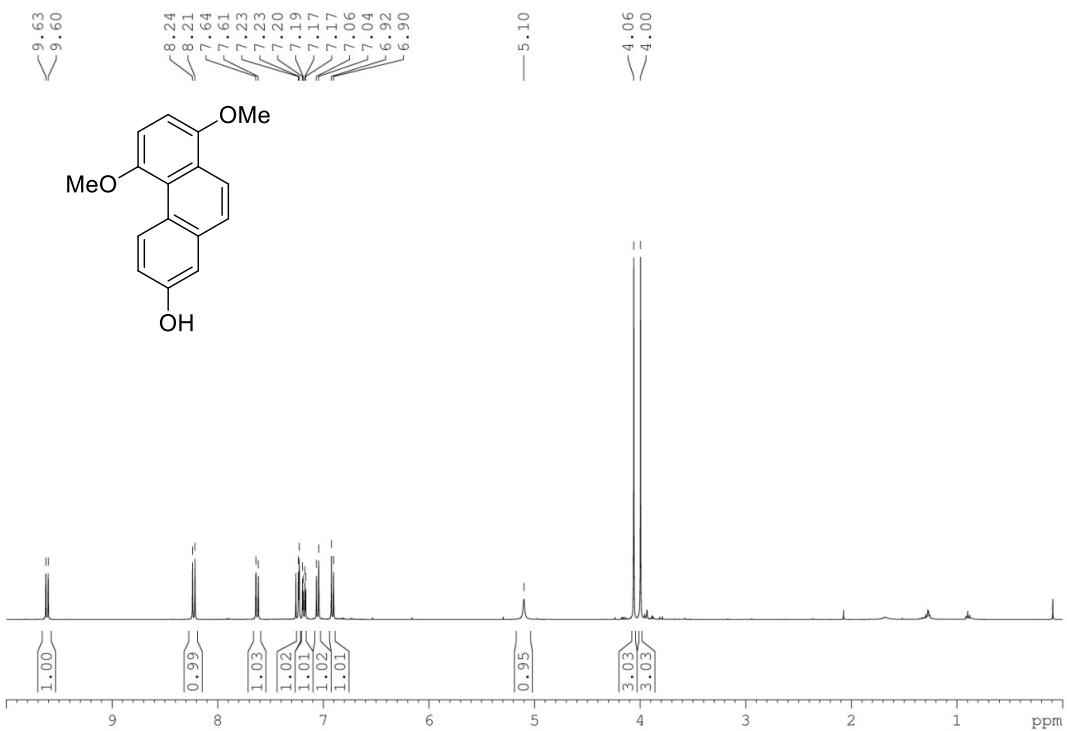
¹H NMR (400 MHz, CDCl₃) 27



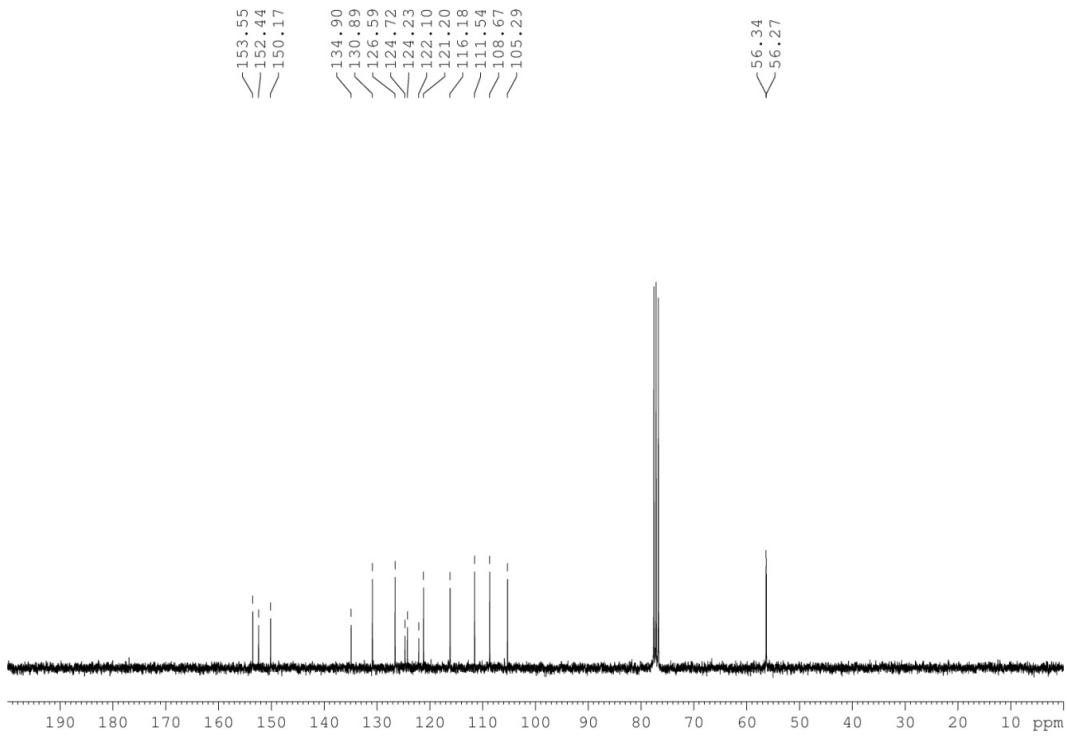
¹³C NMR (101 MHz, CDCl₃) 27



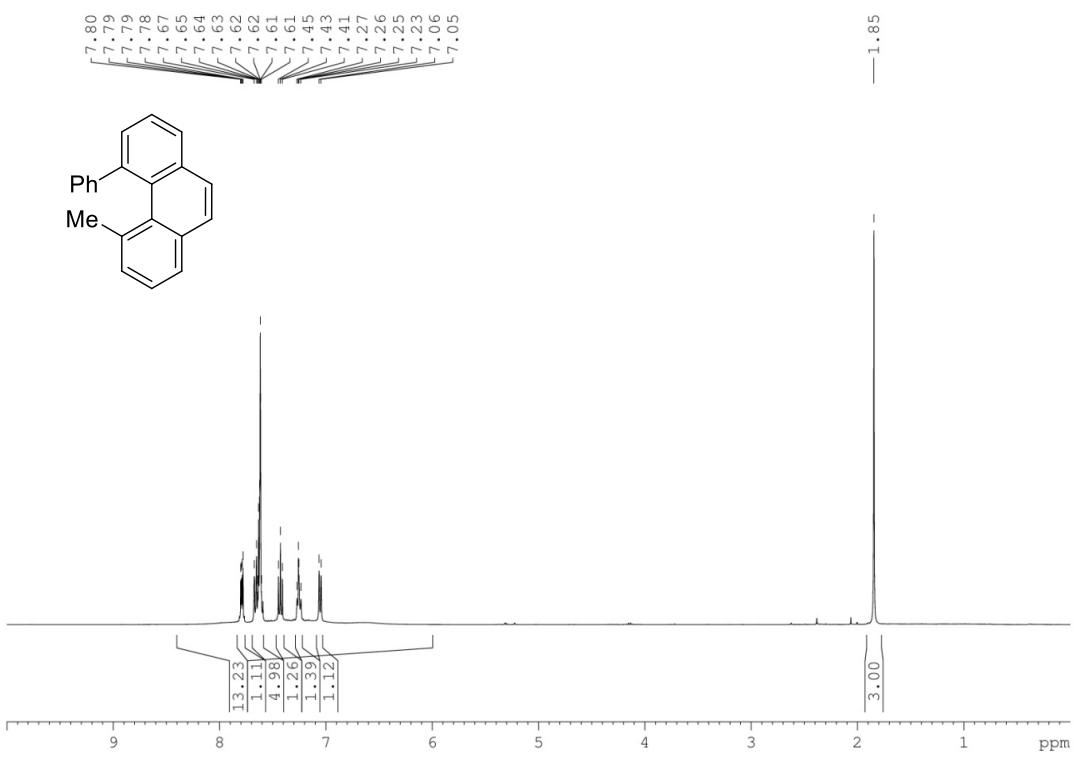
¹H NMR (400 MHz, CDCl₃) 28



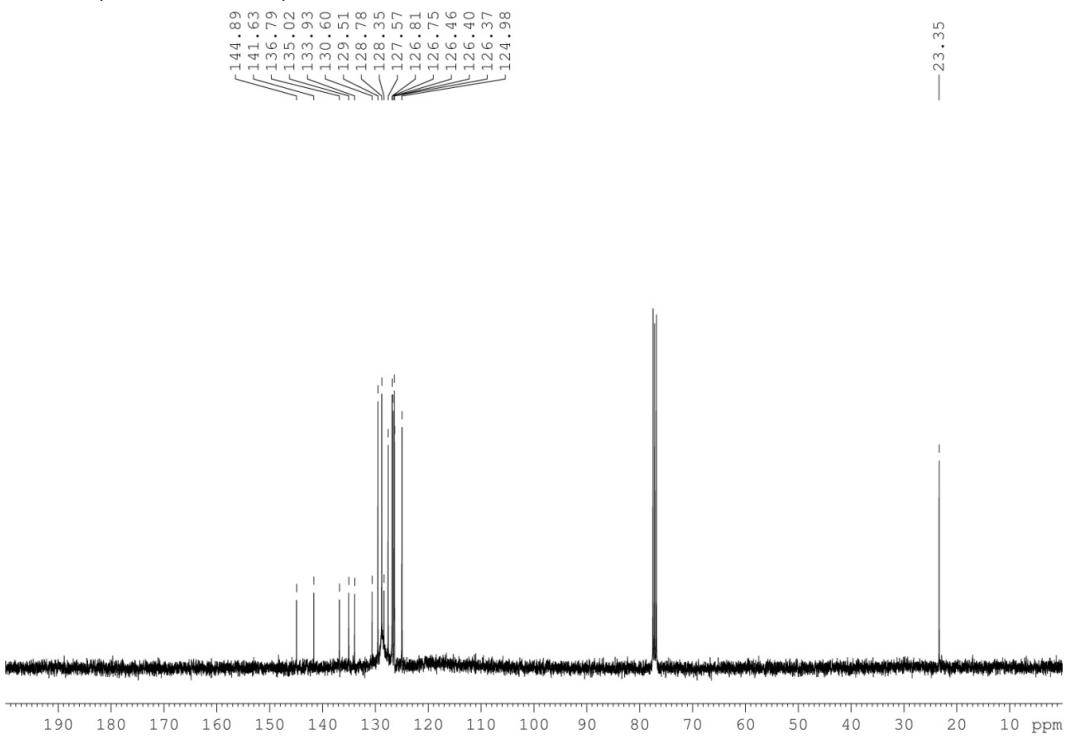
¹³C NMR (101 MHz, CDCl₃) 28



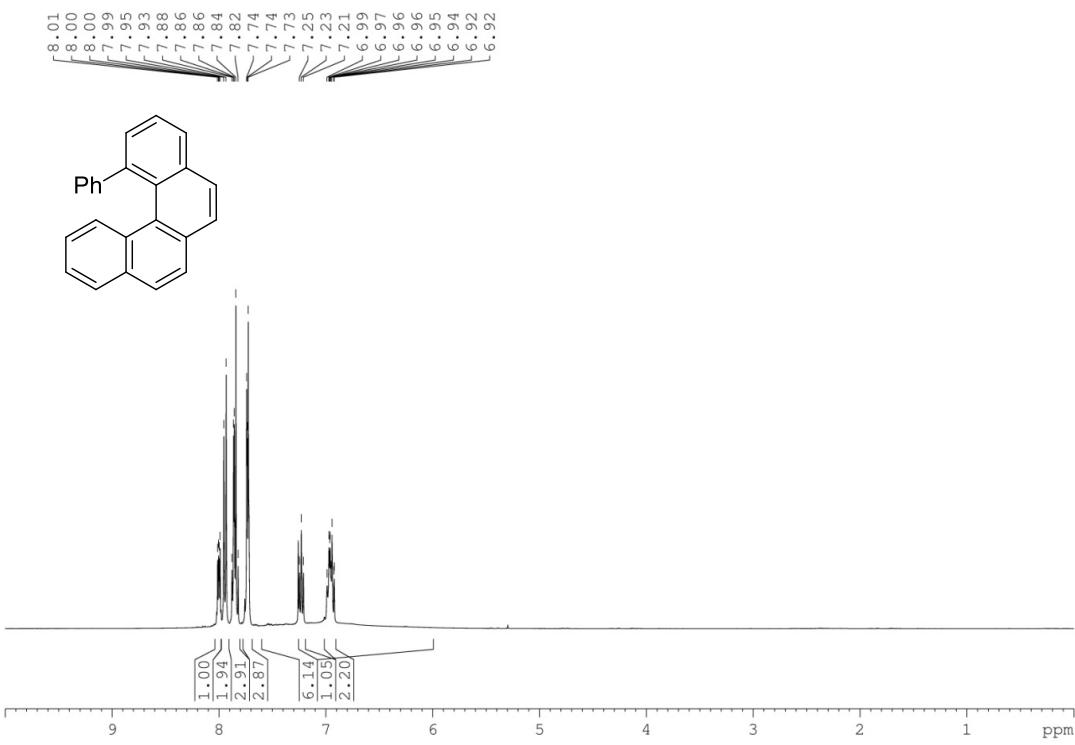
¹H NMR (400 MHz, CDCl₃) **29**



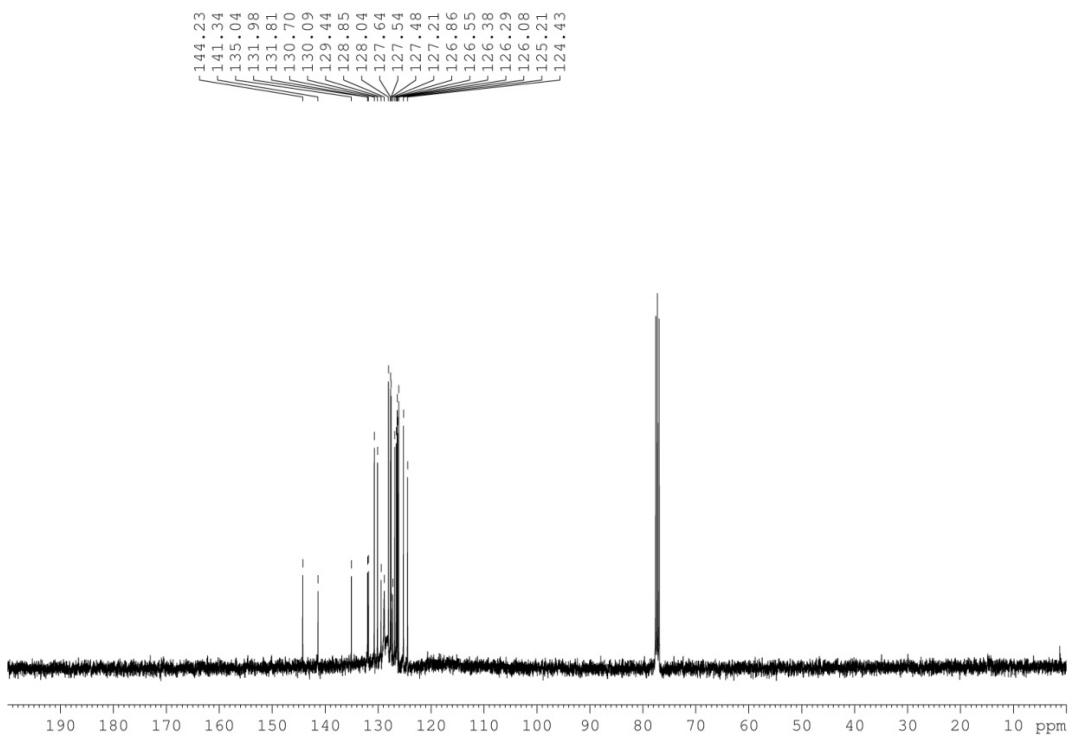
¹³C NMR (101 MHz, CDCl₃) **29**



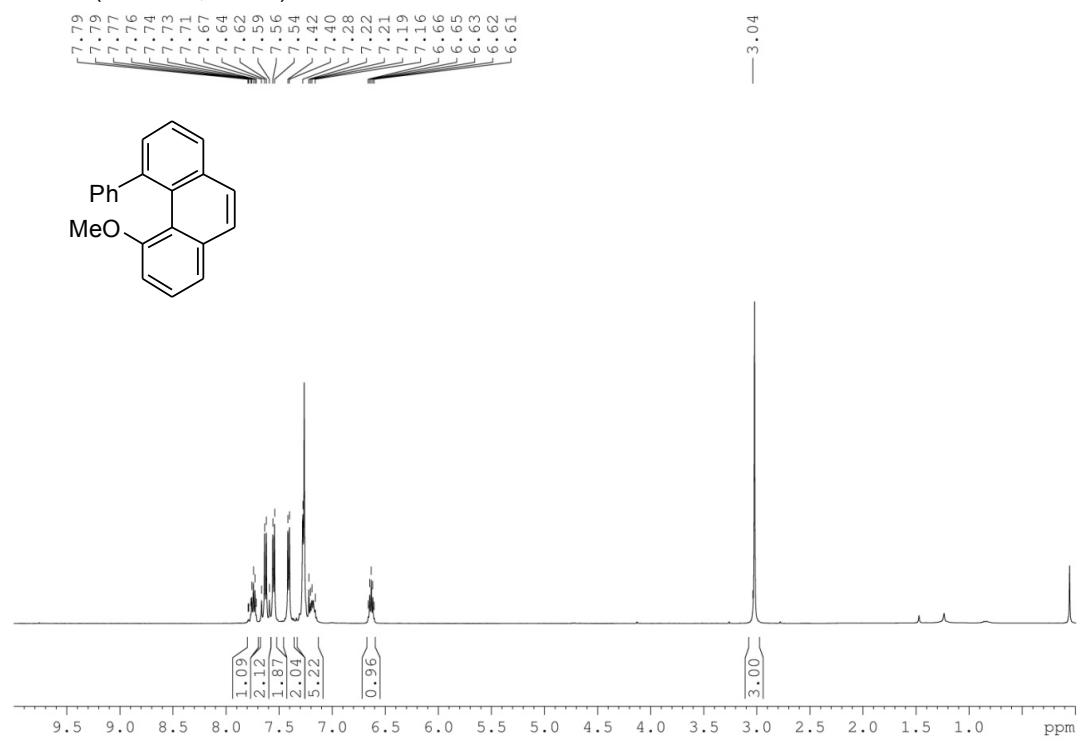
¹H NMR (400 MHz, CDCl₃) **30**



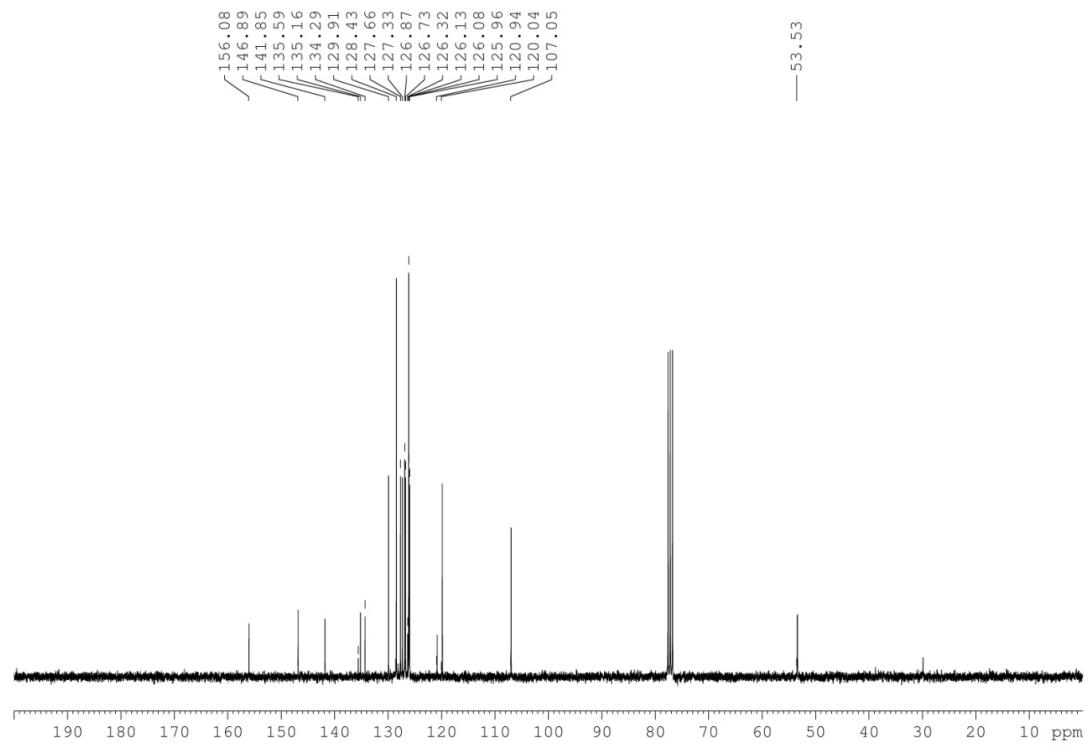
¹³C NMR (101 MHz, CDCl₃) **30**



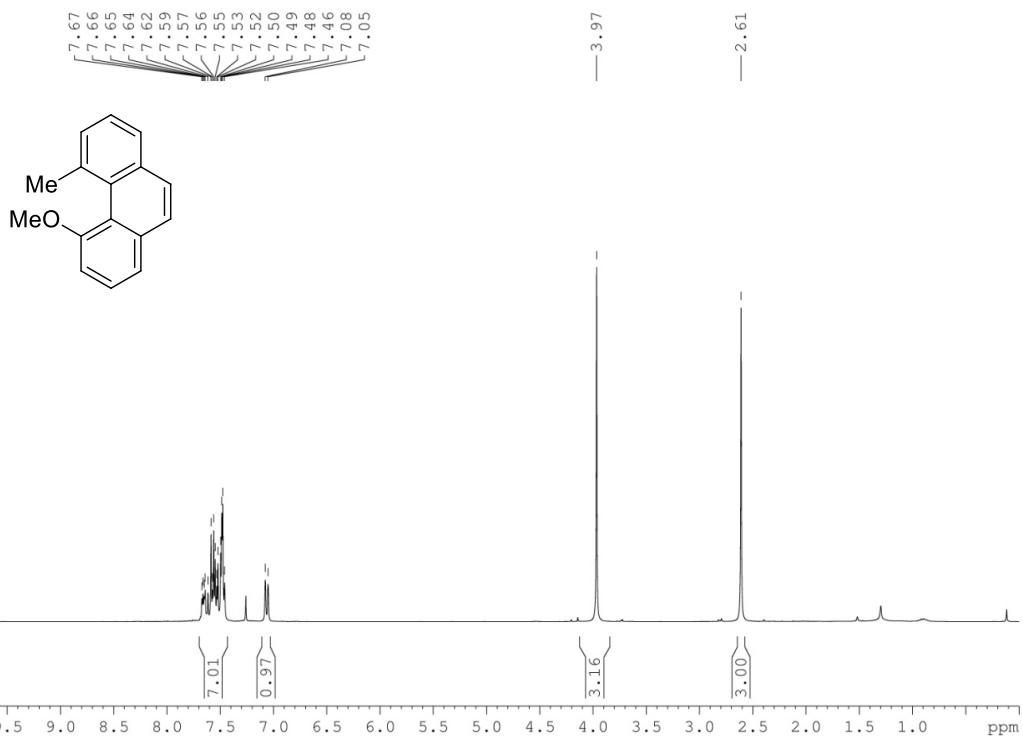
¹H NMR (300 MHz, CDCl₃) **31**



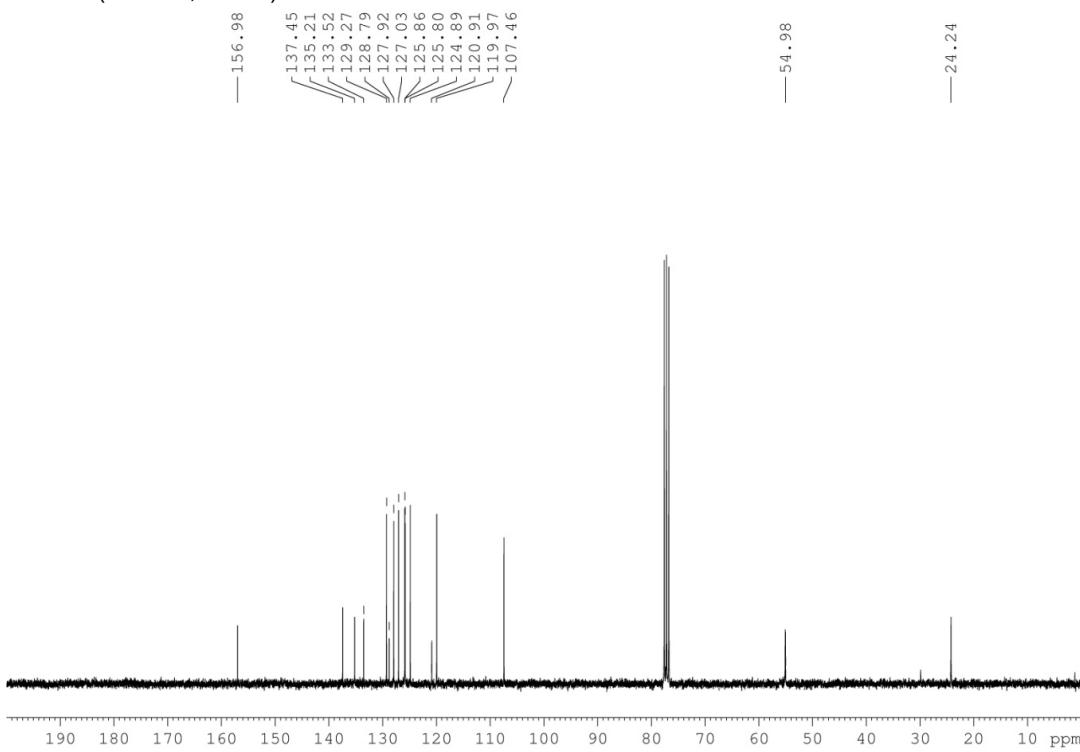
¹³C NMR (75 MHz, CDCl₃) **31**



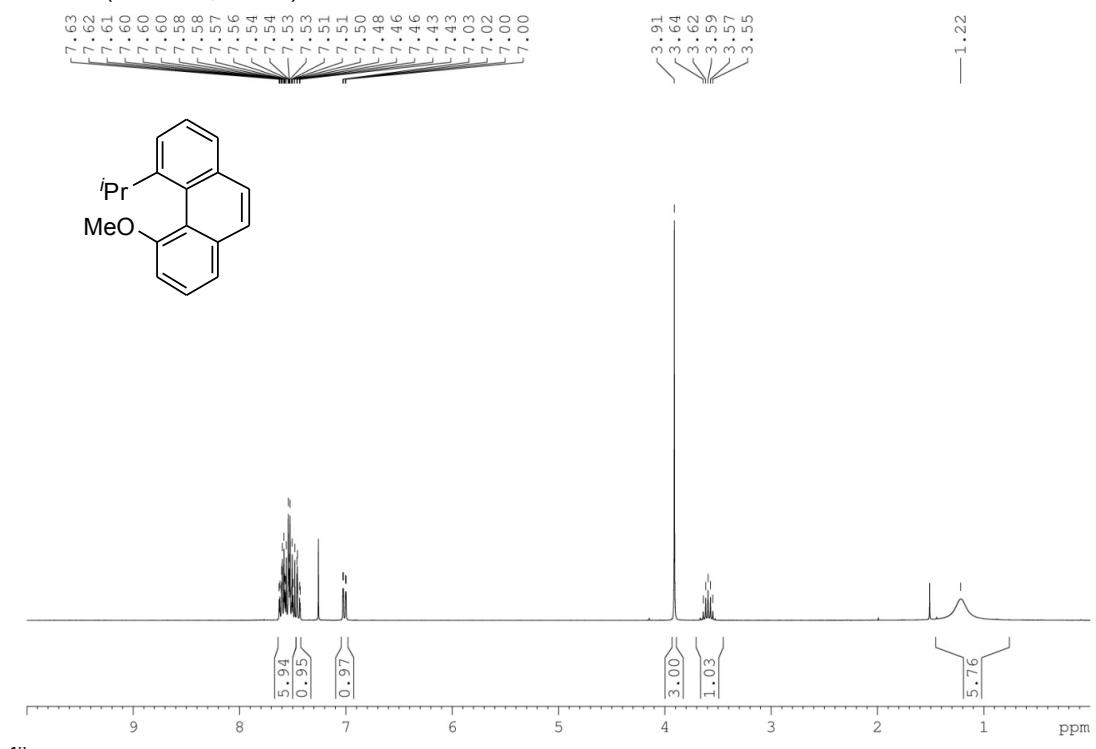
¹H NMR (300 MHz, CDCl₃) **32**



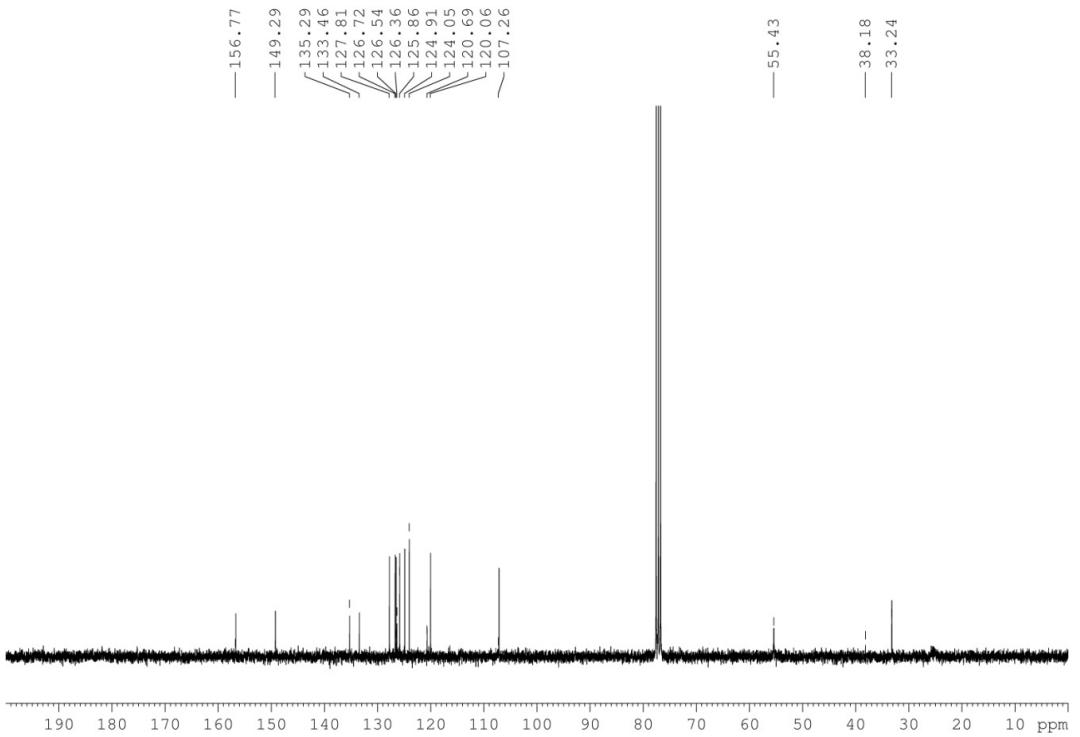
¹³C NMR (75 MHz, CDCl₃) 32



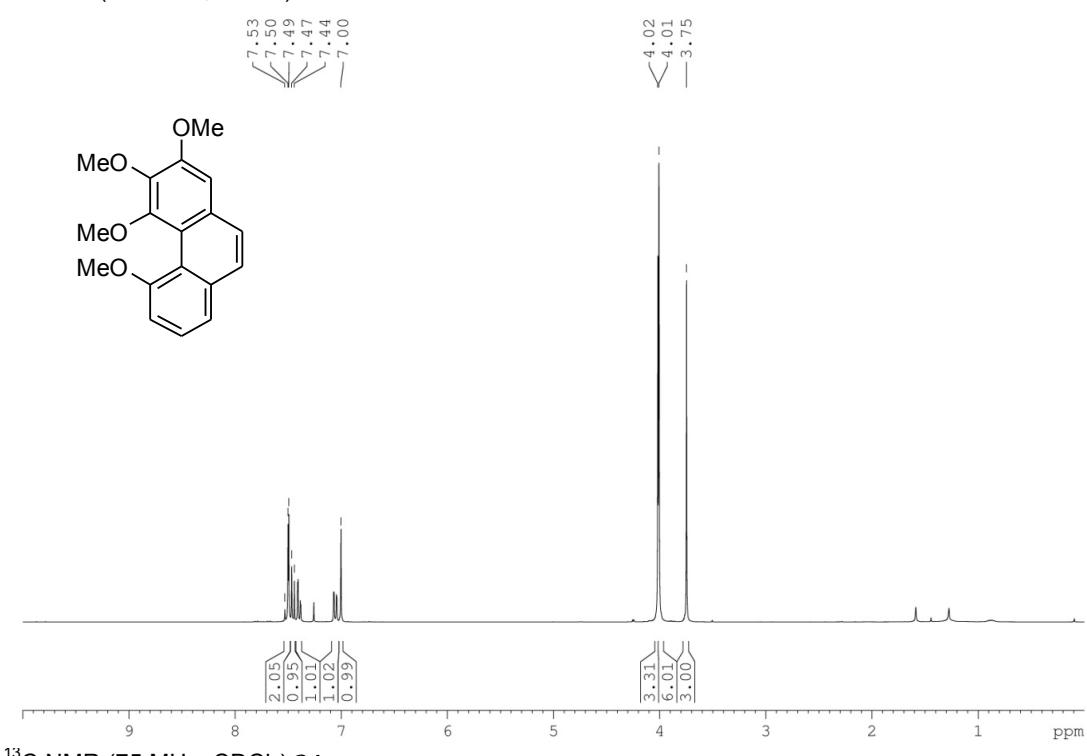
¹H NMR (300 MHz, CDCl₃) 33



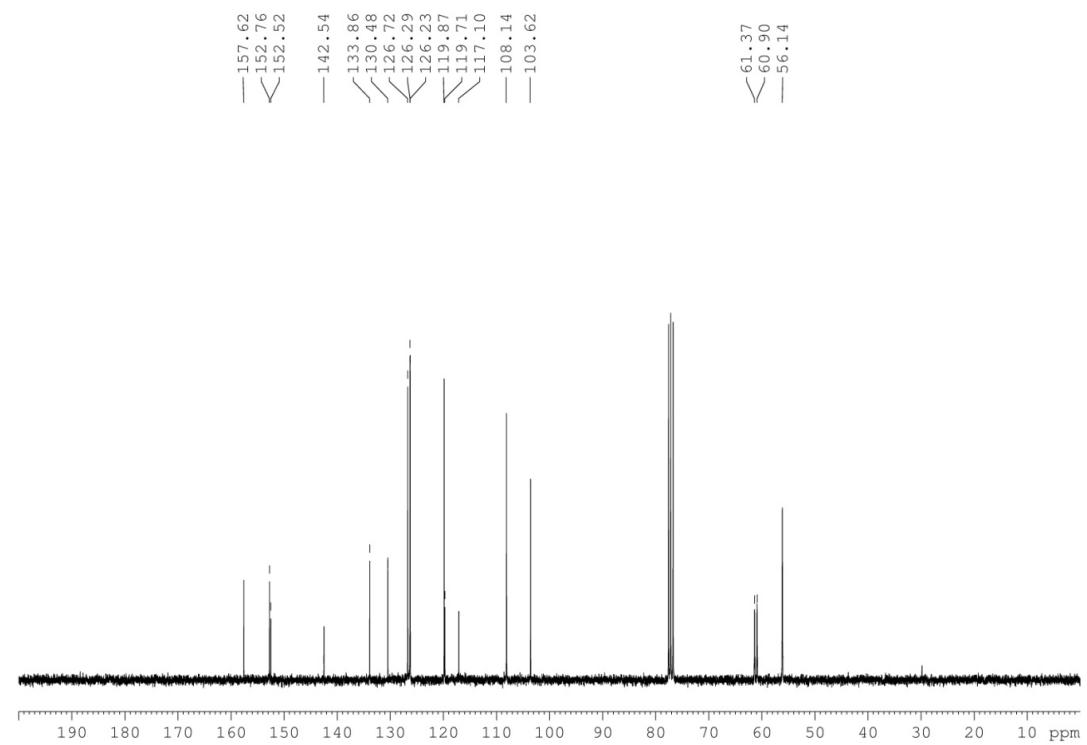
¹³C NMR (75 MHz, CDCl₃) 33



¹H NMR (300 MHz, CDCl₃) **34**



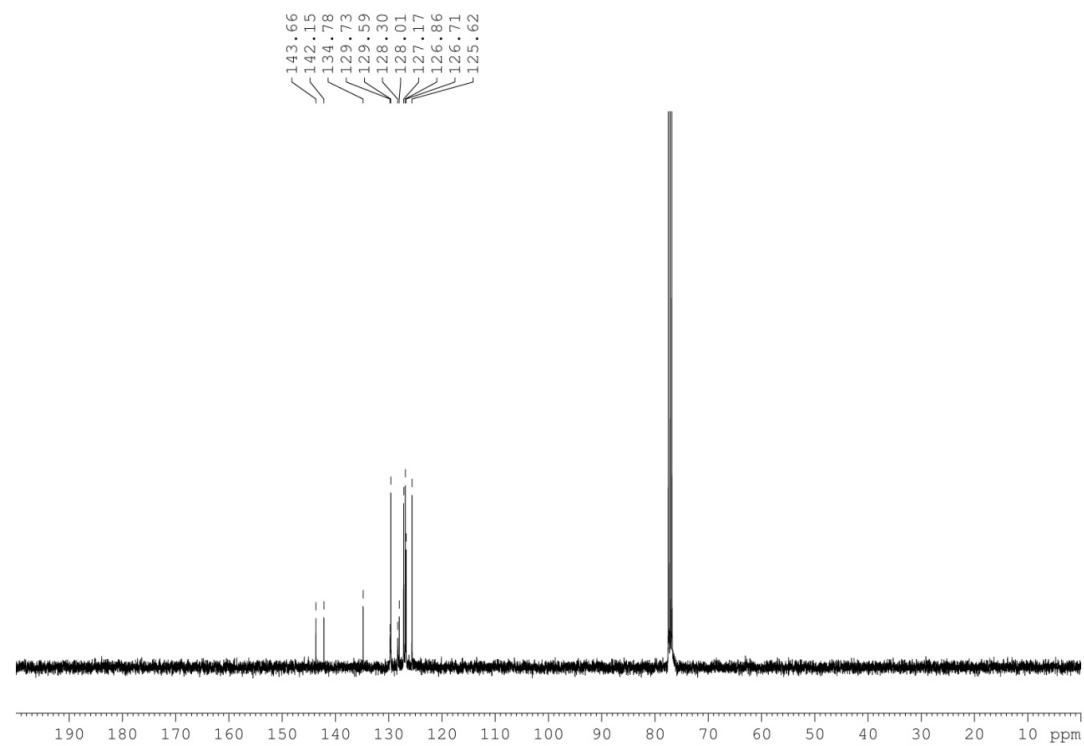
¹³C NMR (75 MHz, CDCl₃) **34**



¹H NMR (400 MHz, CDCl₃) 35



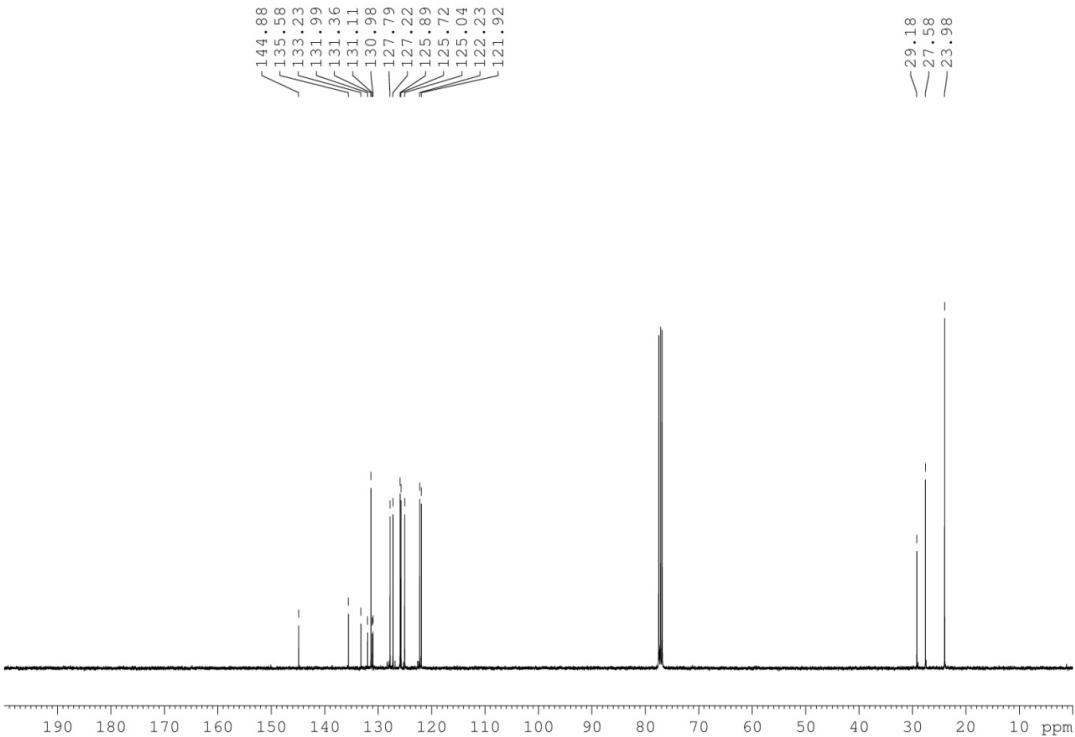
¹³C NMR (75 MHz, CDCl₃) 35



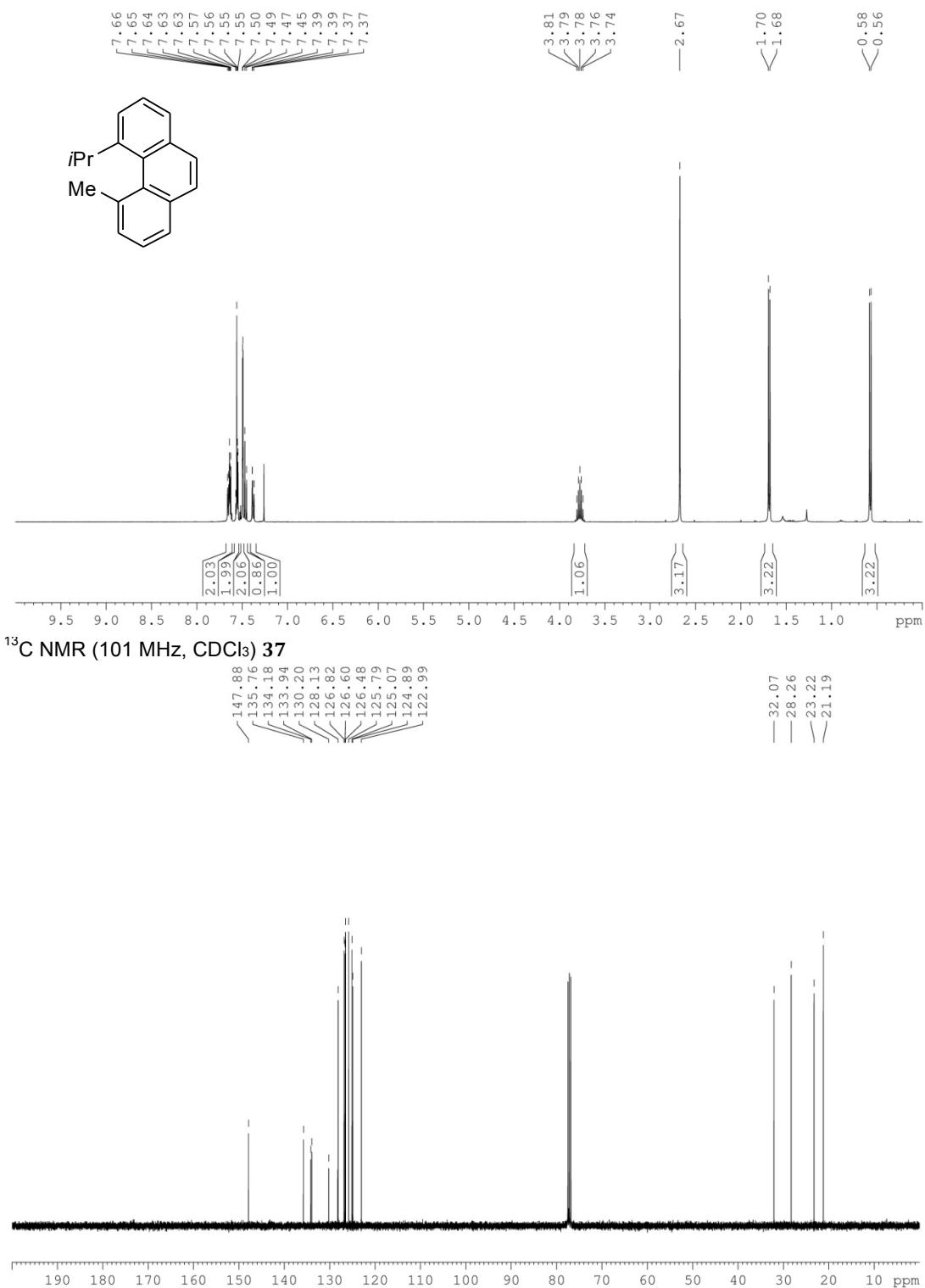
¹H NMR (400 MHz, CDCl₃) **36**



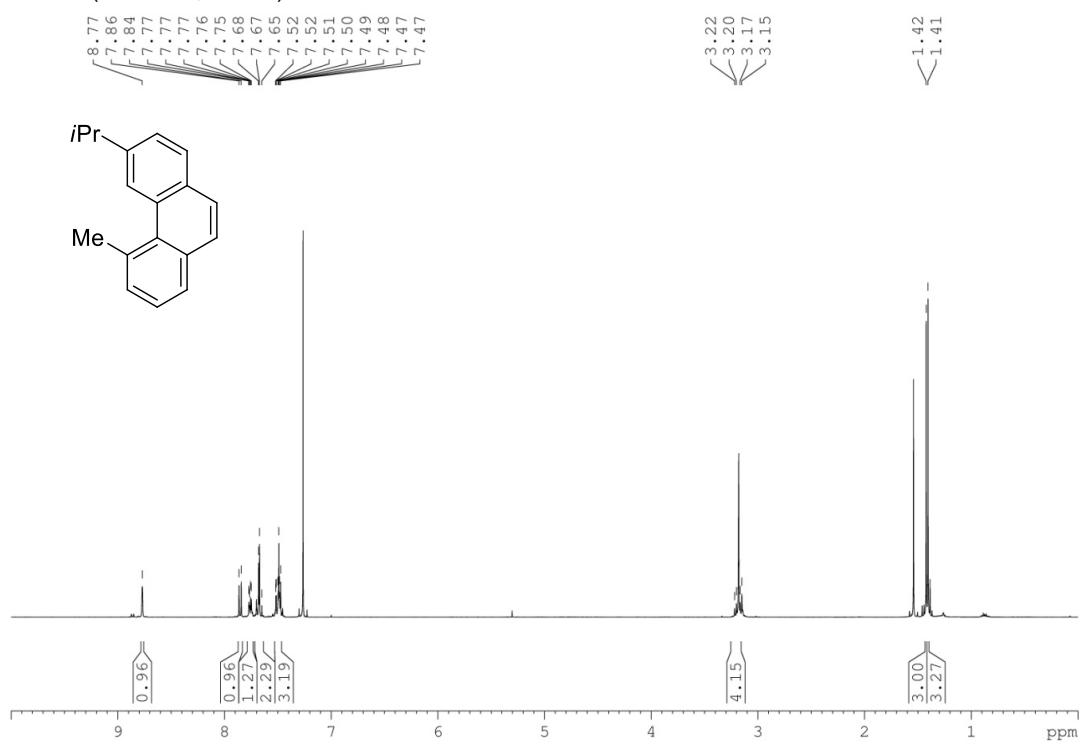
¹³C NMR (101 MHz, CDCl₃) **36**



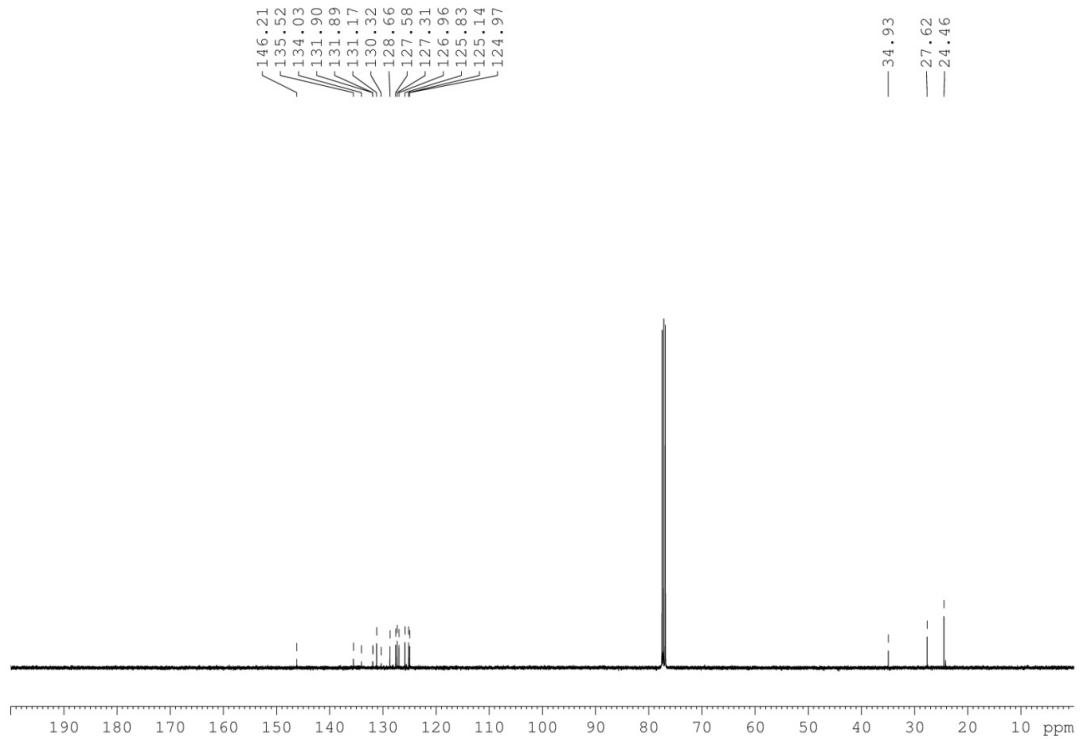
¹H NMR (400 MHz, CDCl₃) **37**



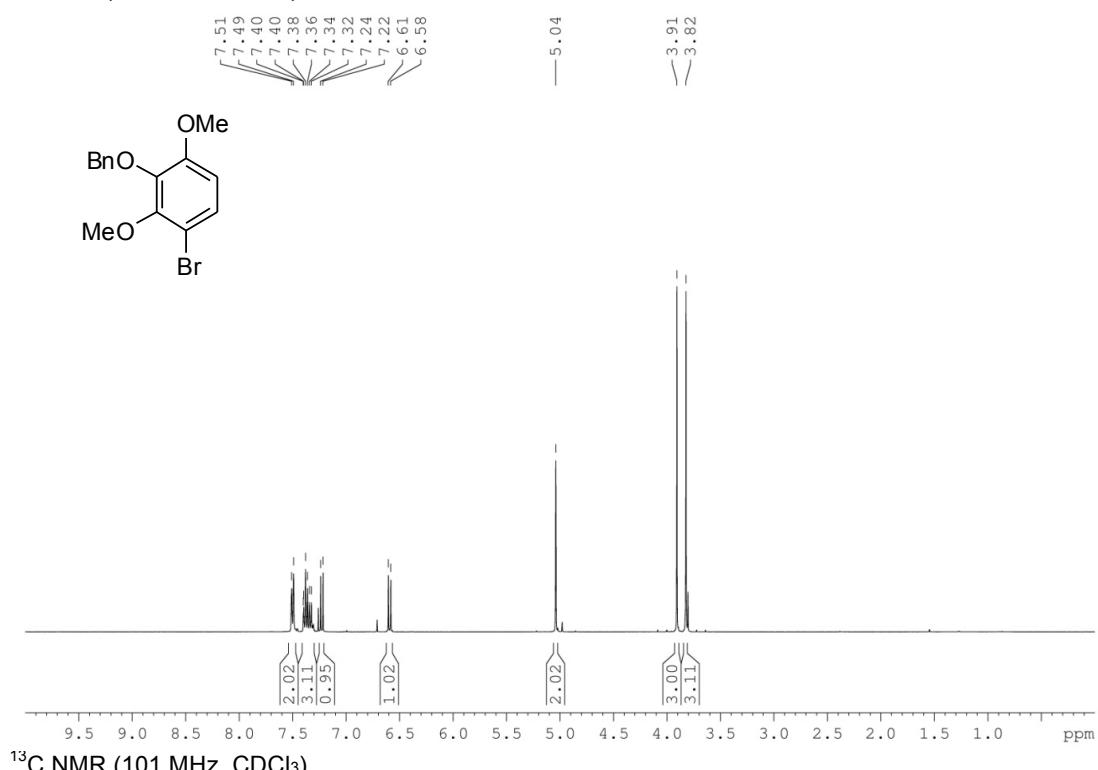
¹H NMR (300 MHz, CDCl₃) **38**



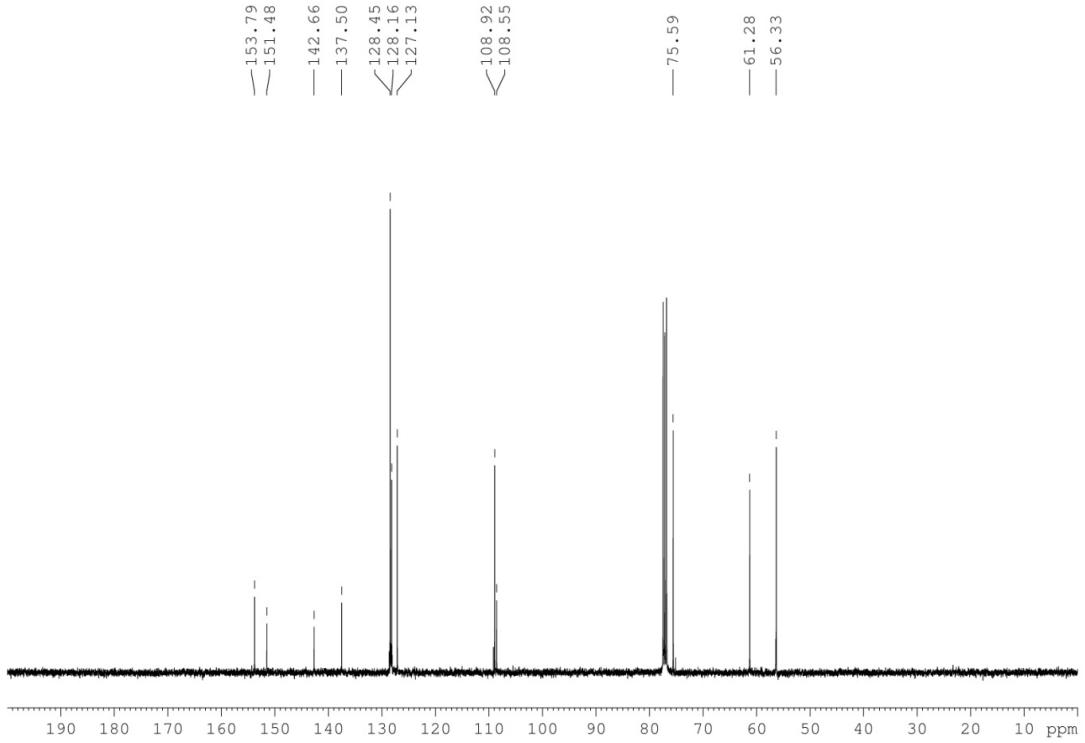
¹³C NMR (75 MHz, CDCl₃) **38**



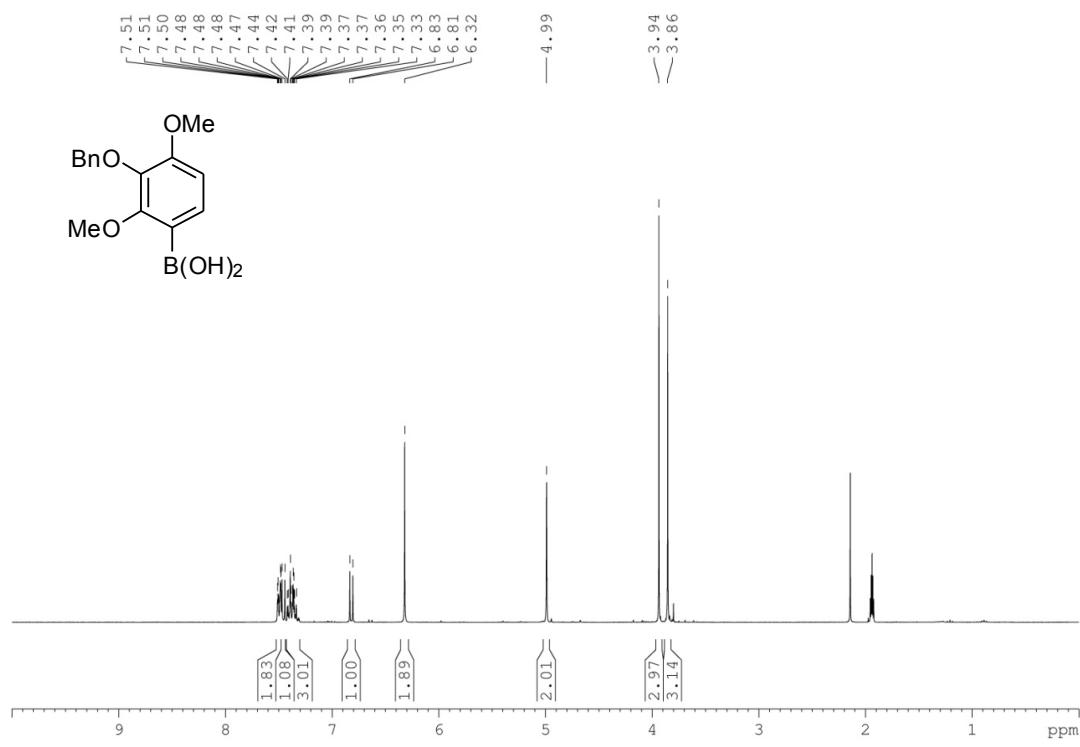
¹H NMR (400 MHz, CDCl₃)



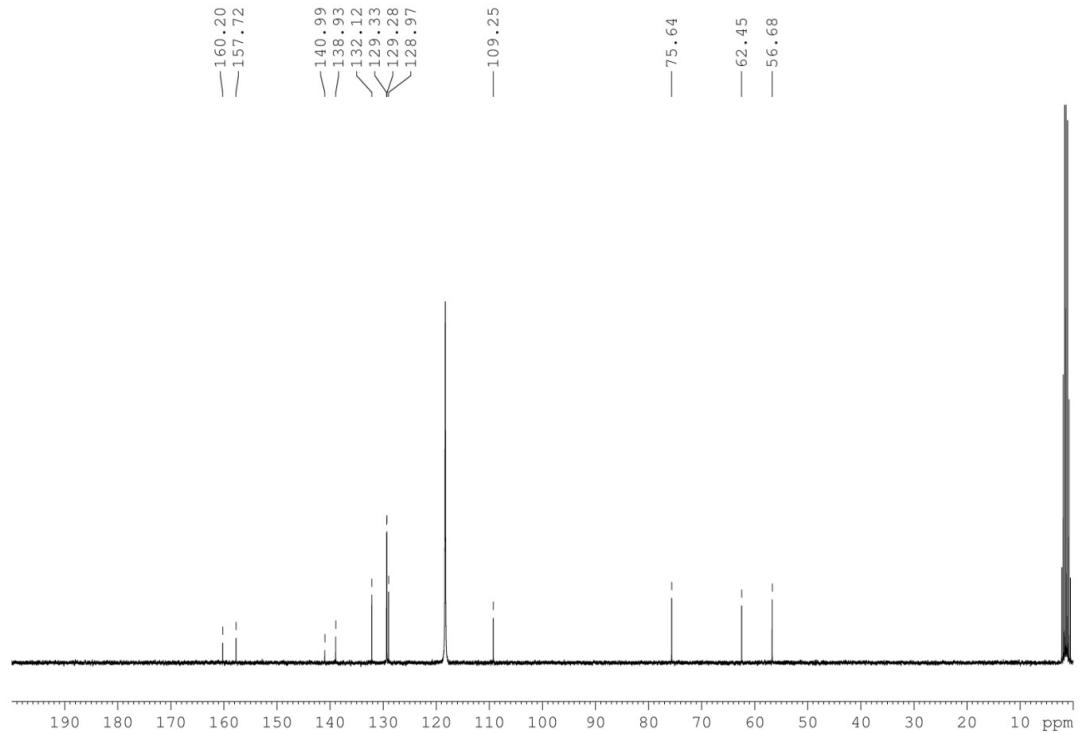
¹³C NMR (101 MHz, CDCl₃)



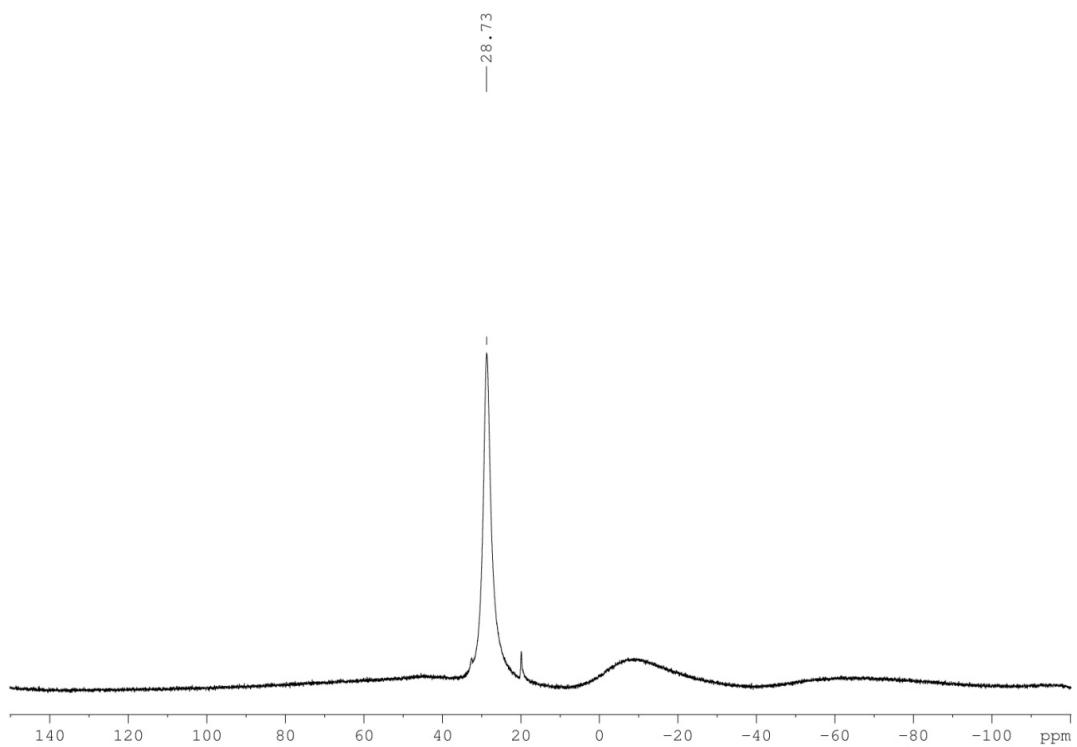
¹H NMR (300 MHz, CD₃CN) 42



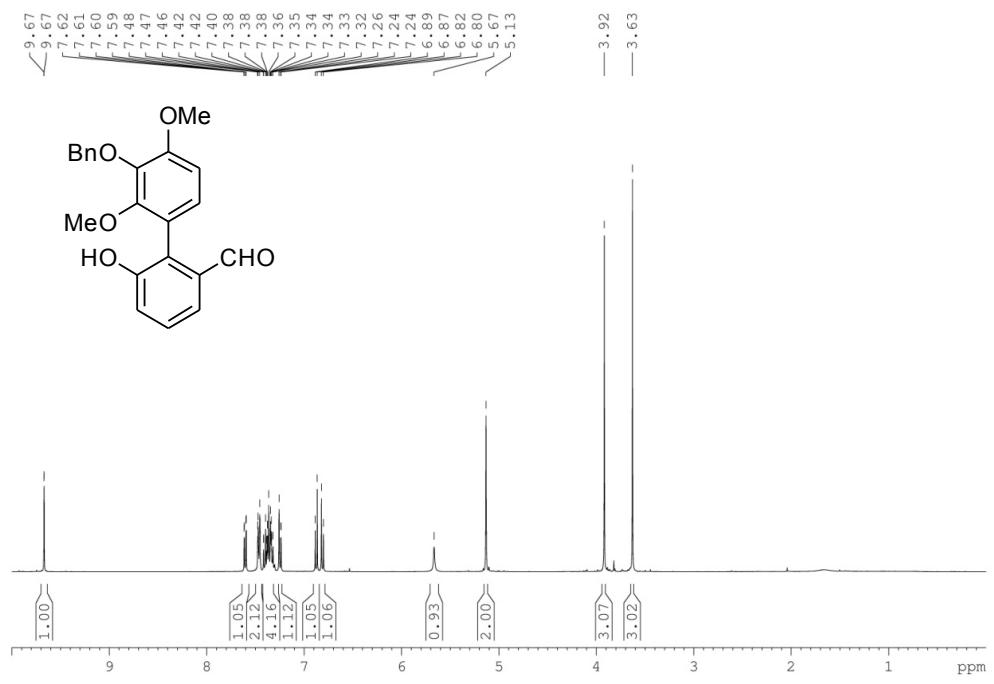
¹³C NMR (75 MHz, CD₃CN) 42



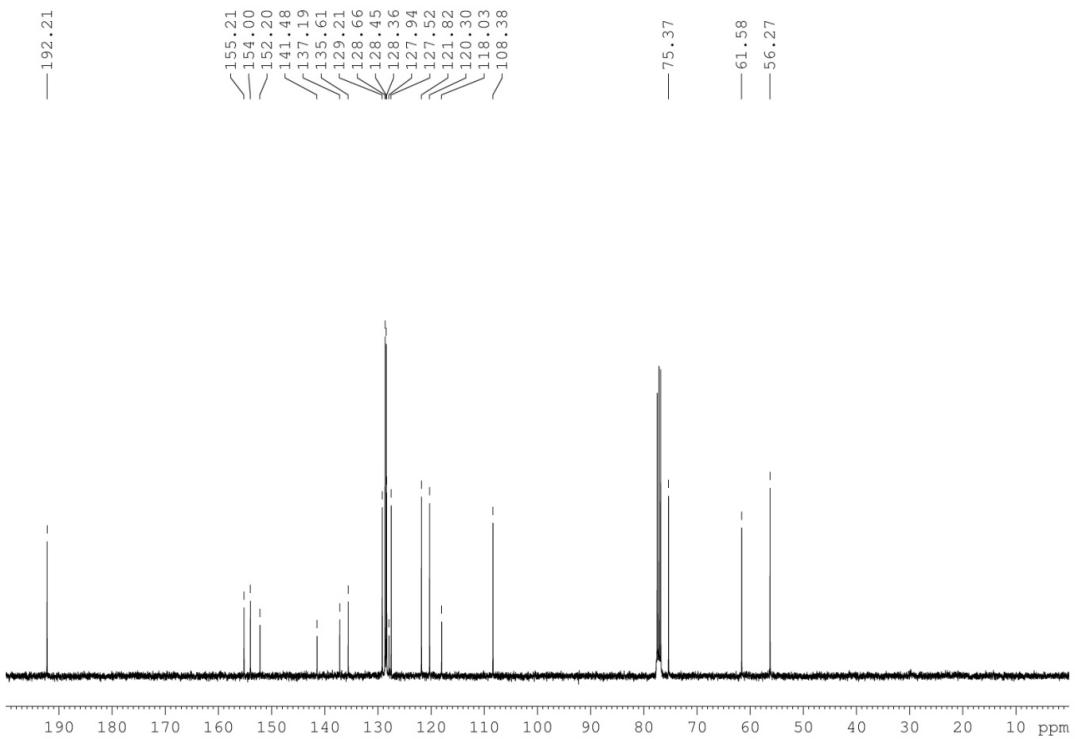
^{11}B NMR (96 MHz, CD_3CN) **42**



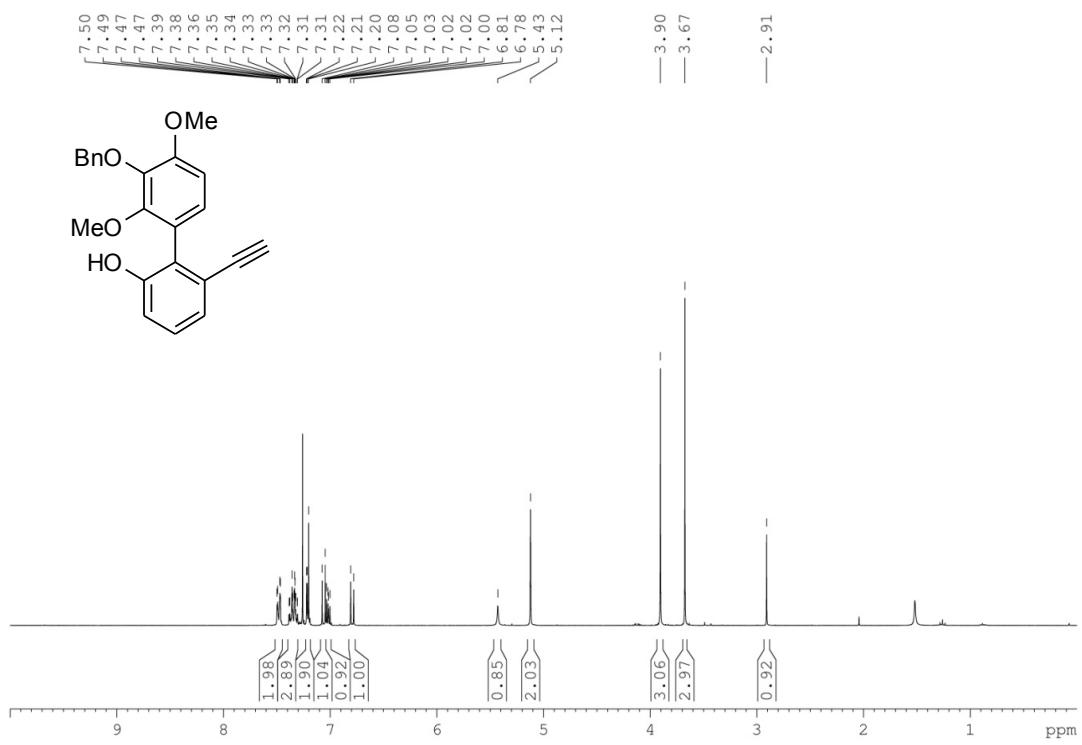
¹H NMR (400 MHz, CDCl₃) **43**



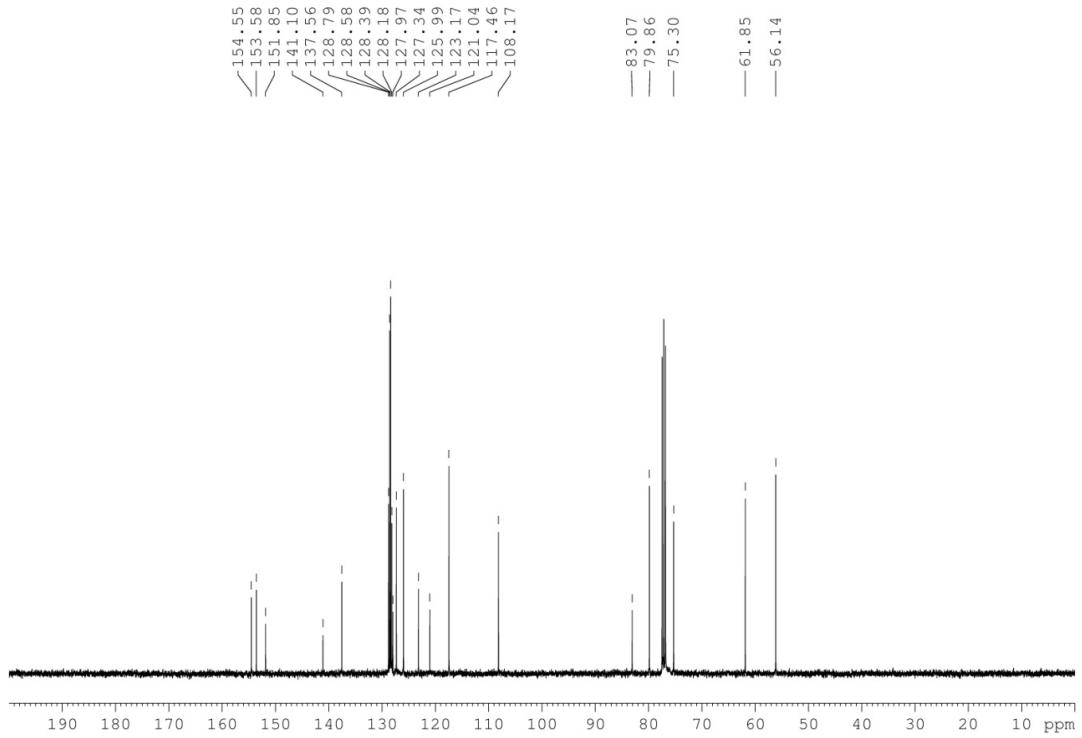
¹³C NMR (101 MHz, CDCl₃) **43**



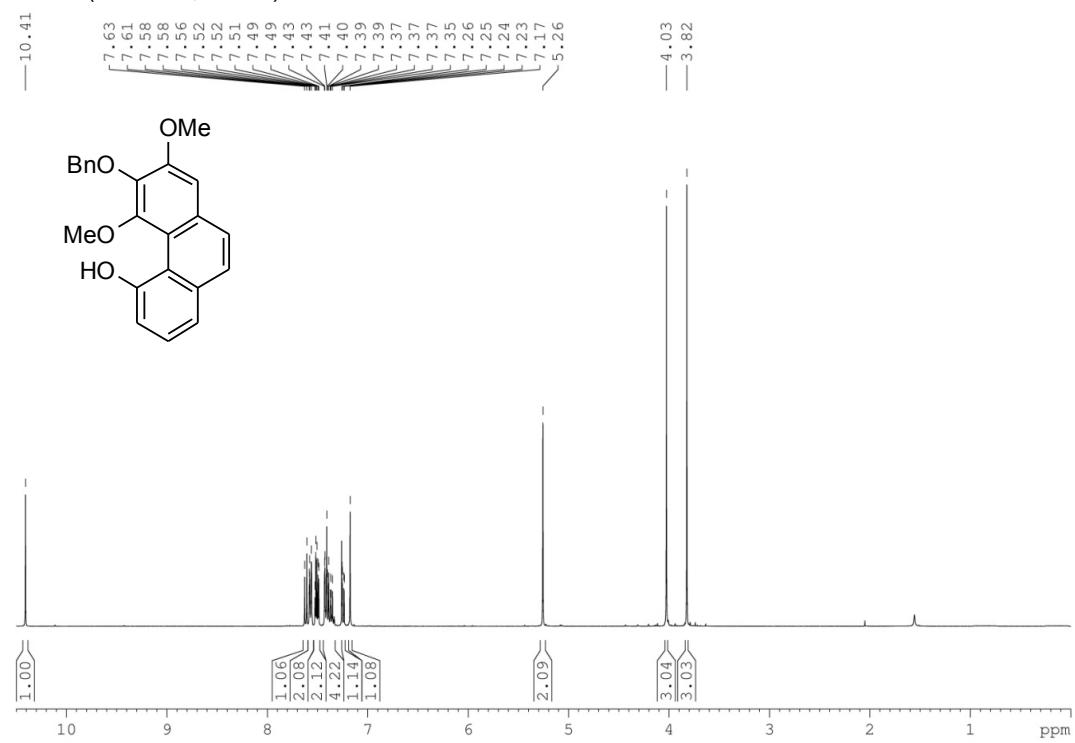
¹H NMR (400 MHz, CDCl₃) **44**



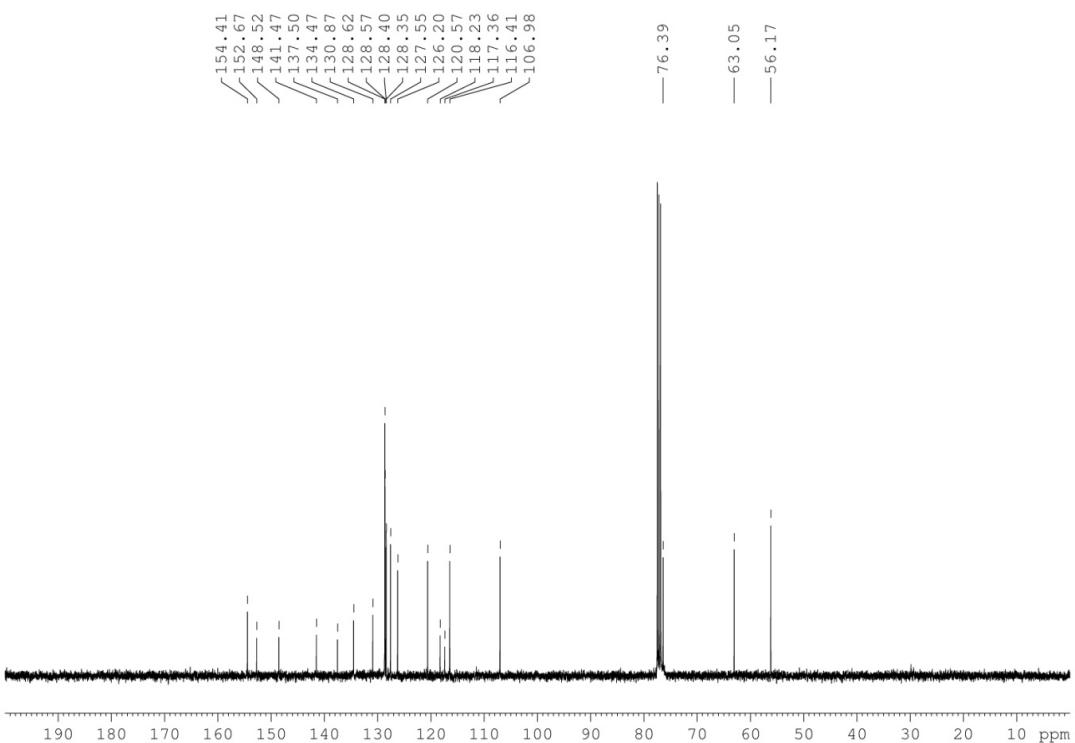
¹³C NMR (101 MHz, CDCl₃) **44**



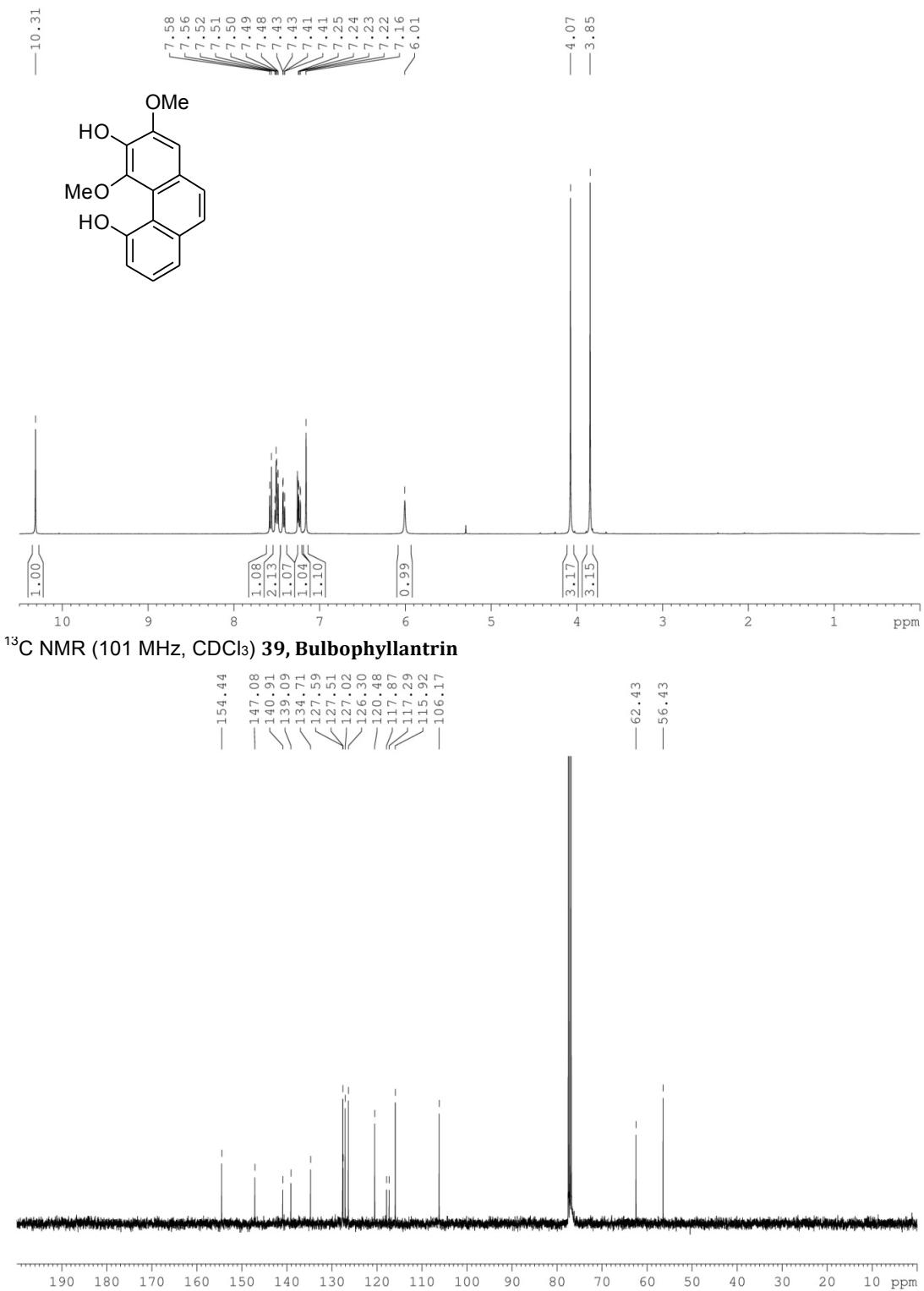
¹H NMR (400 MHz, CDCl₃) **45**



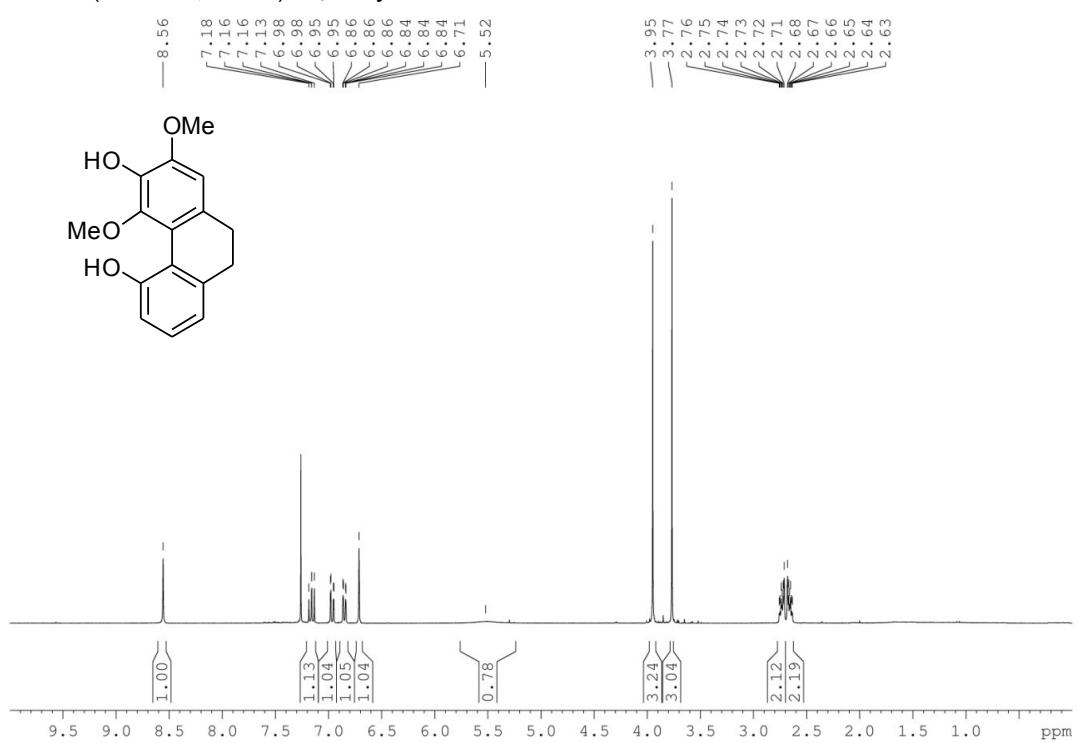
¹³C NMR (101 MHz, CDCl₃) **45**



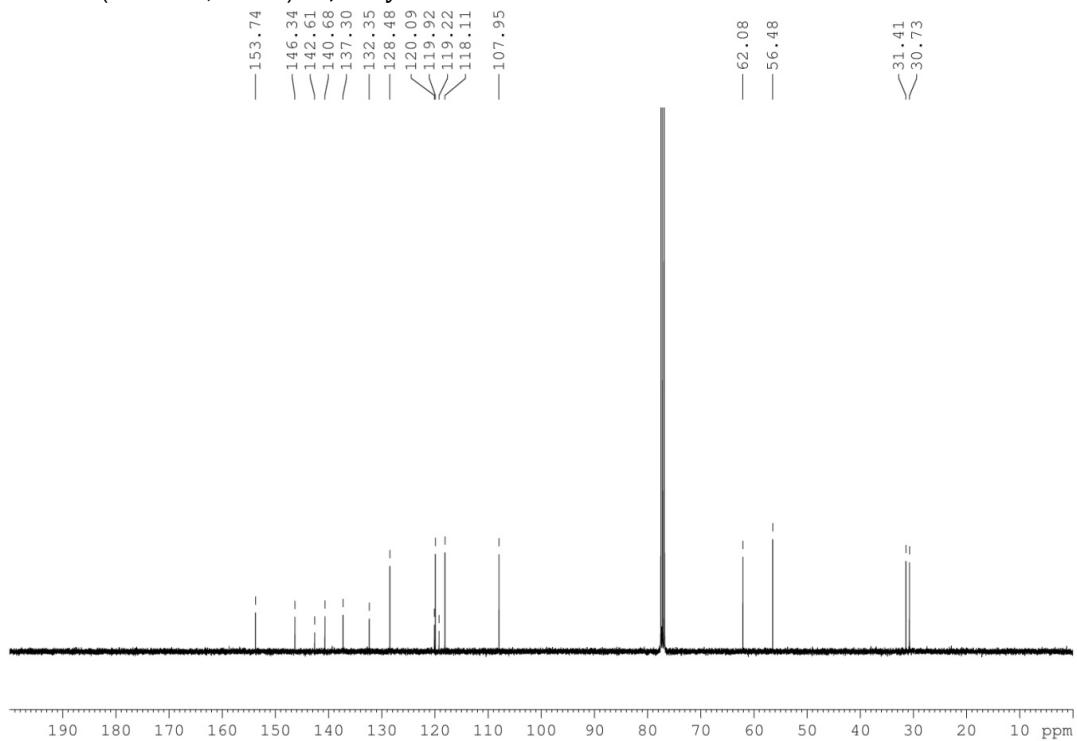
¹H NMR (400 MHz, CDCl₃) **39, Bulbophyllantran**



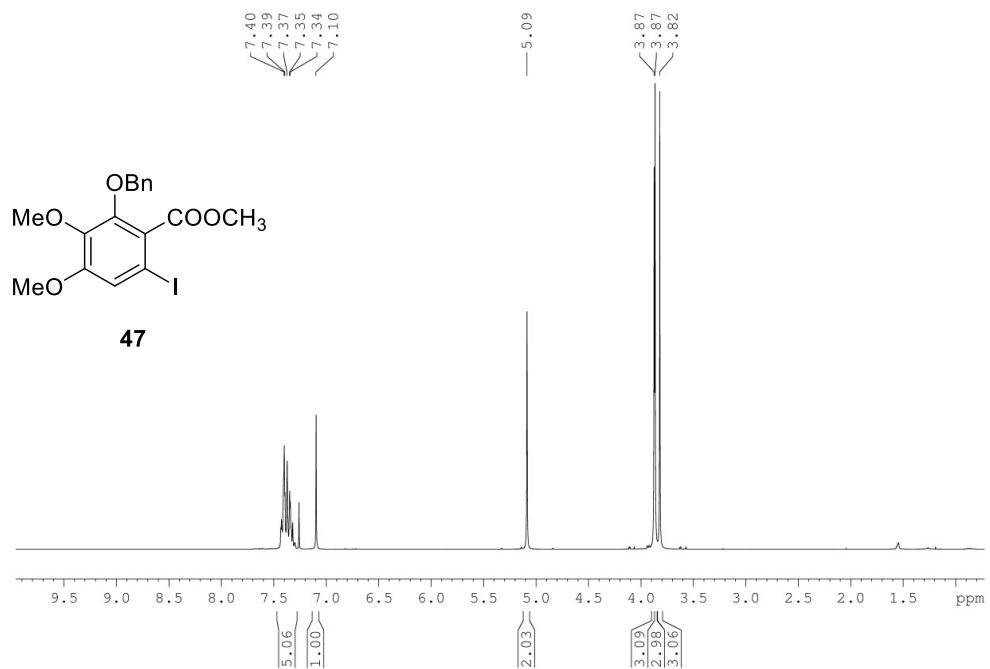
¹H NMR (400 MHz, CDCl₃) **40, Marylaurencinol A**



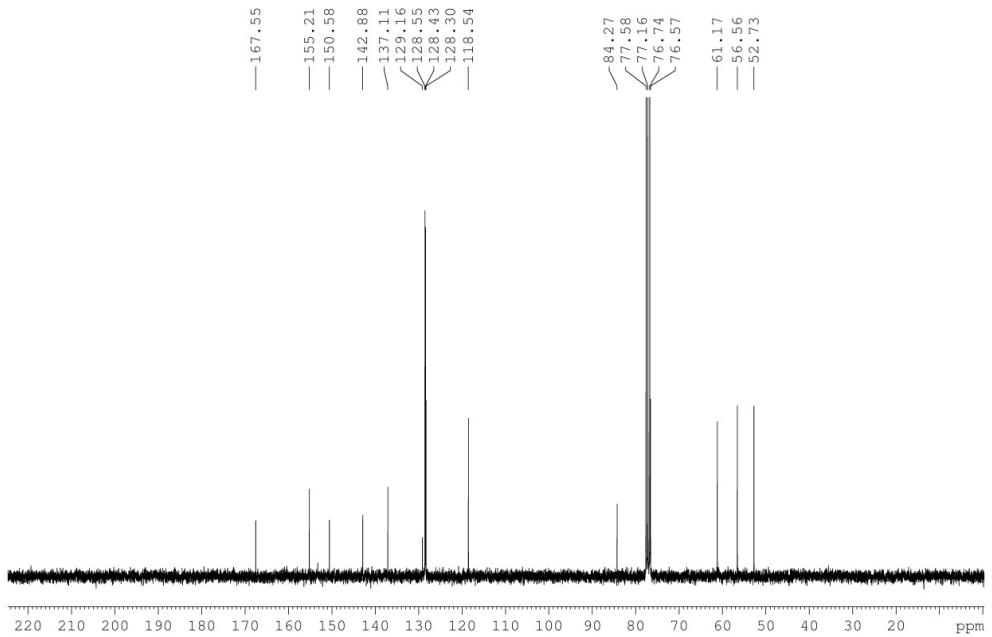
¹³C NMR (101 MHz, CDCl₃) **40, Marylaurencinol A**



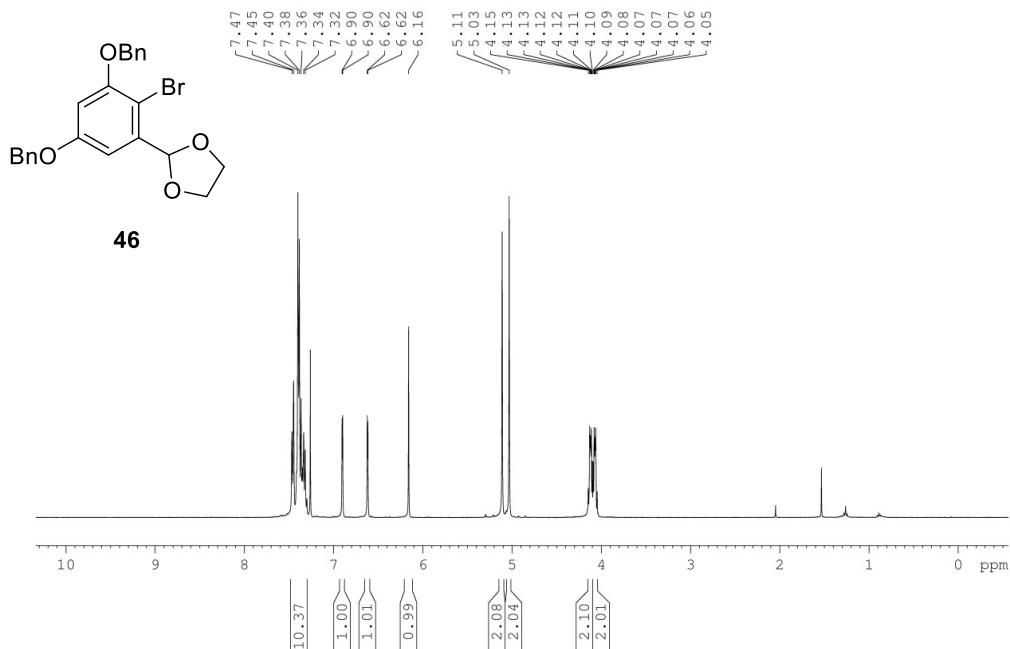
¹H NMR (300 MHz, CDCl₃) **47**



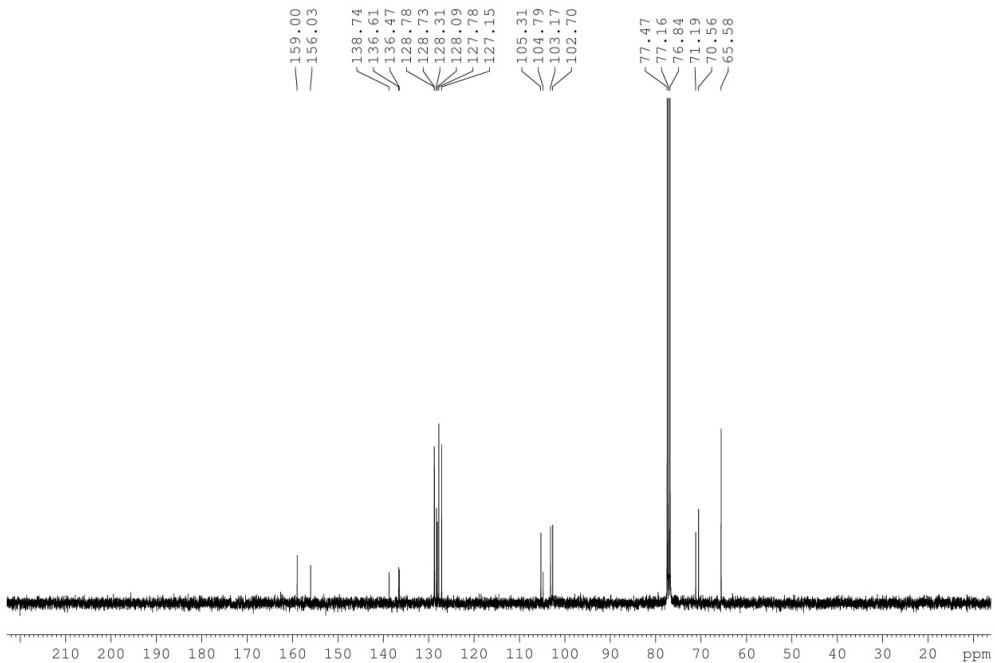
¹³C NMR (75 MHz, CDCl₃) **47**



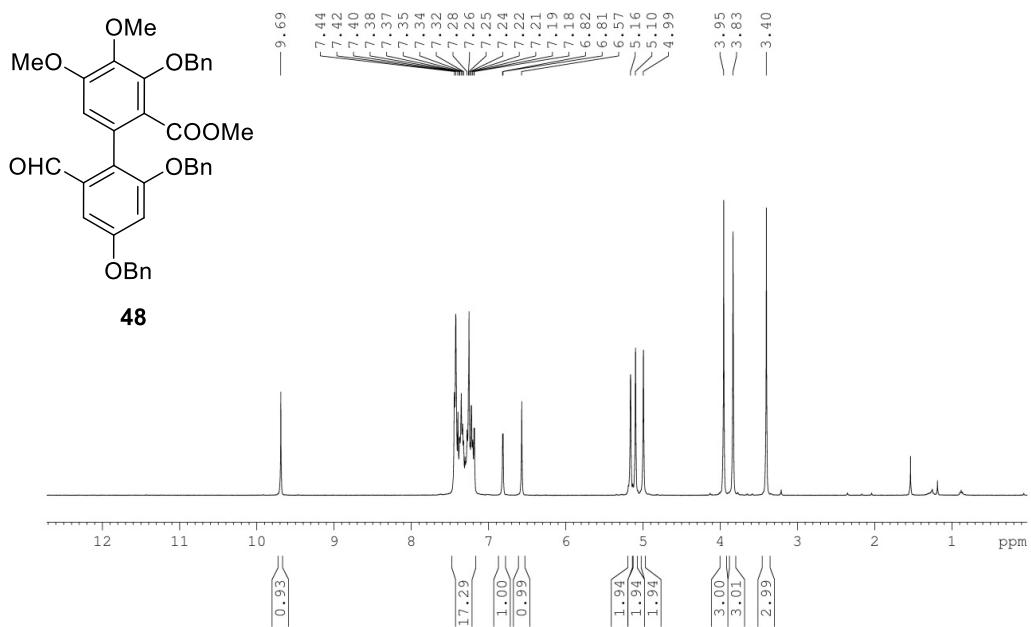
¹H NMR (400 MHz, CDCl₃) **46**



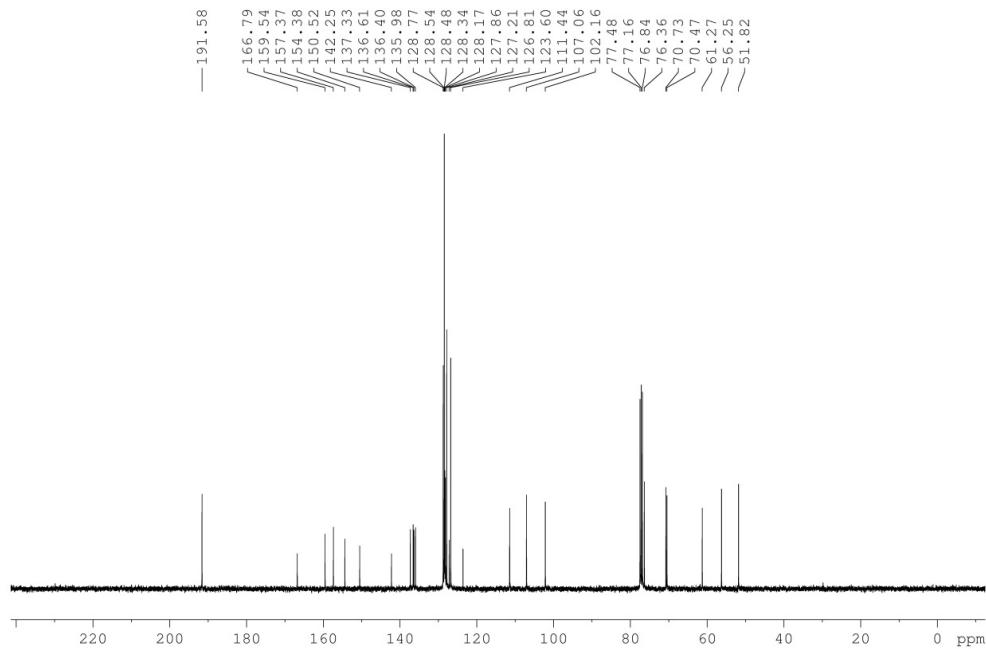
¹³C NMR (100 MHz, CDCl₃) **46**



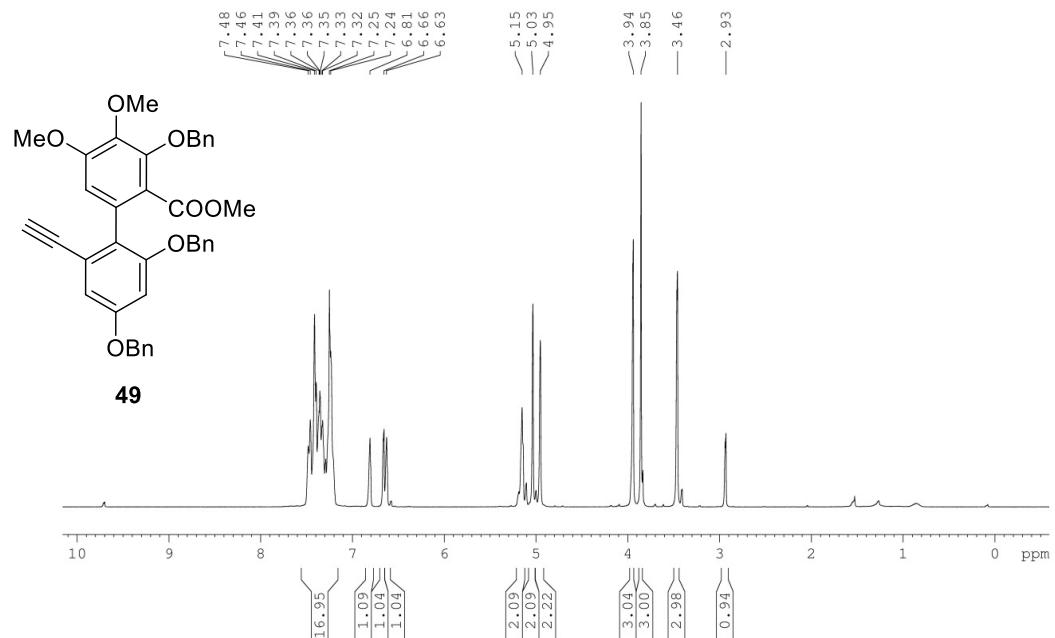
¹H NMR (400 MHz, CDCl₃) **48**



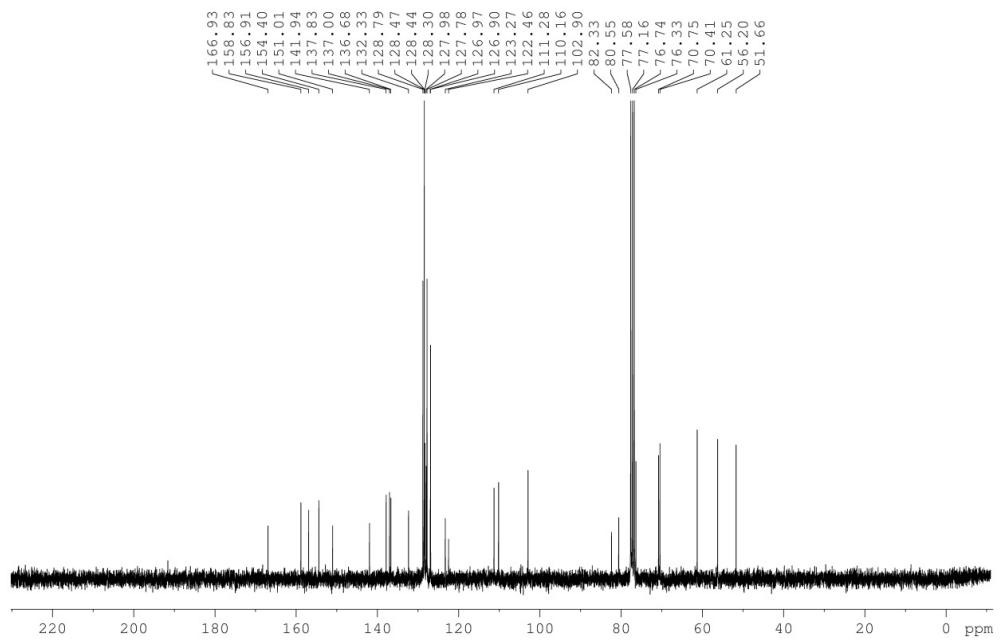
¹³C NMR (100 MHz, CDCl₃) **48**



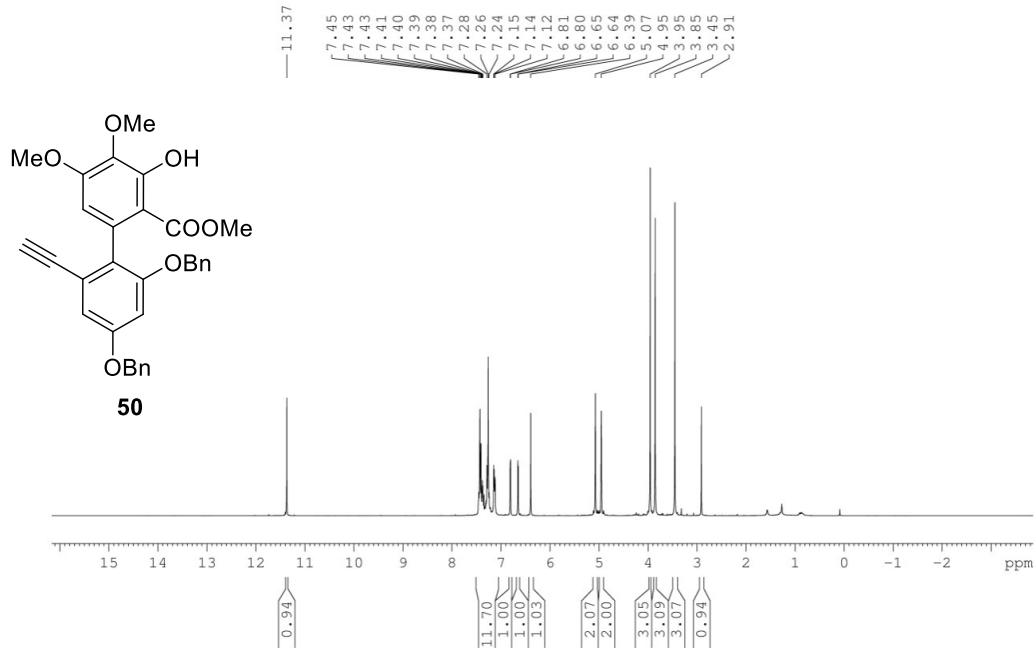
¹H NMR (300 MHz, CDCl₃) **49**



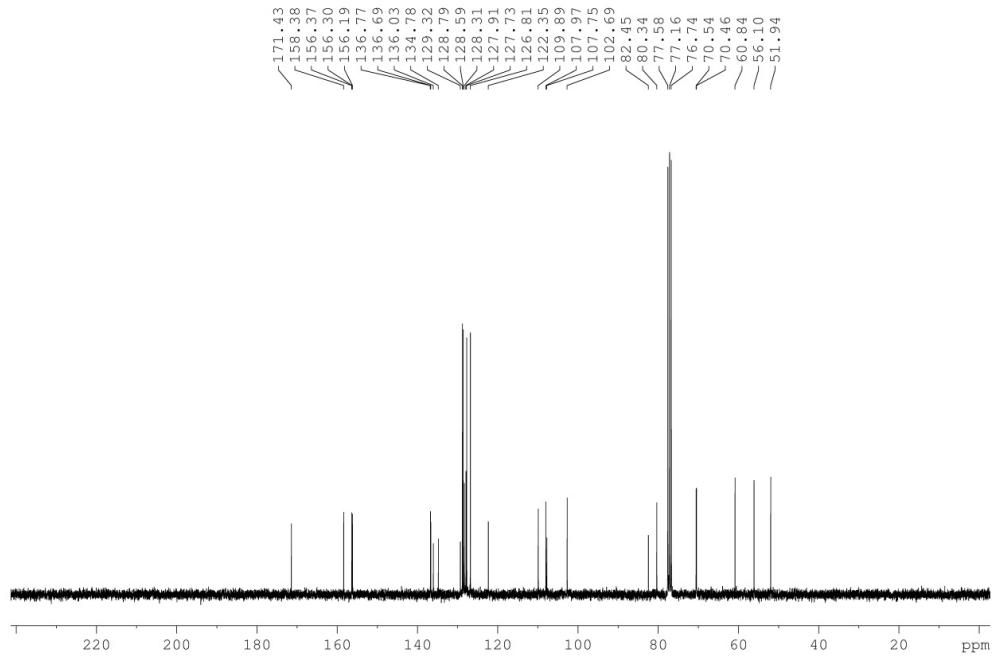
¹³C NMR (75 MHz, CDCl₃) **49**



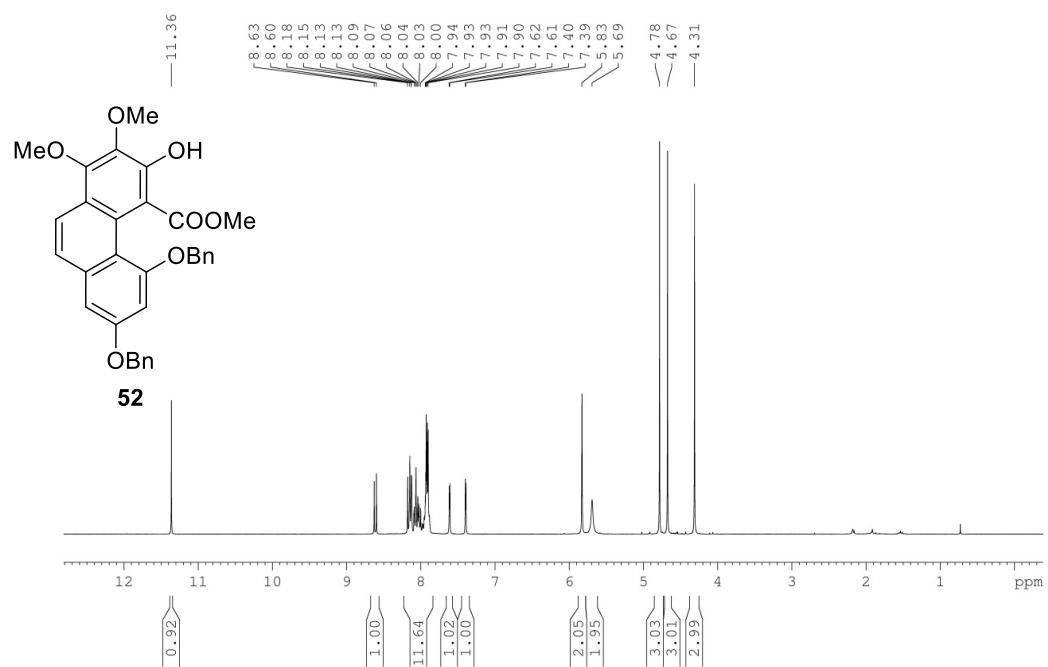
¹H NMR (300 MHz, CDCl₃) **50**



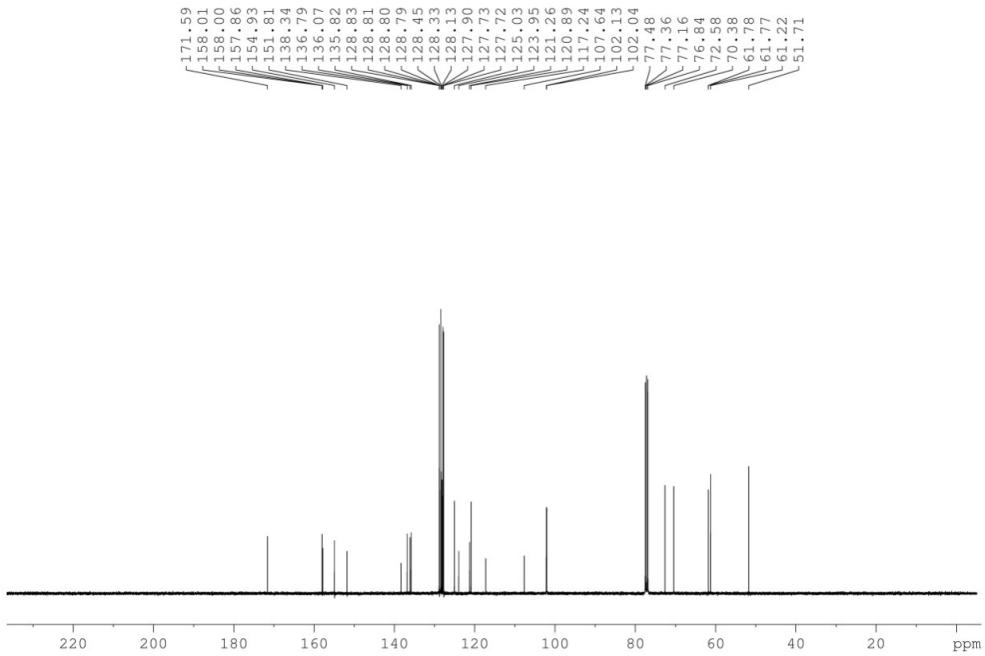
¹³C NMR (75 MHz, CDCl₃) 50



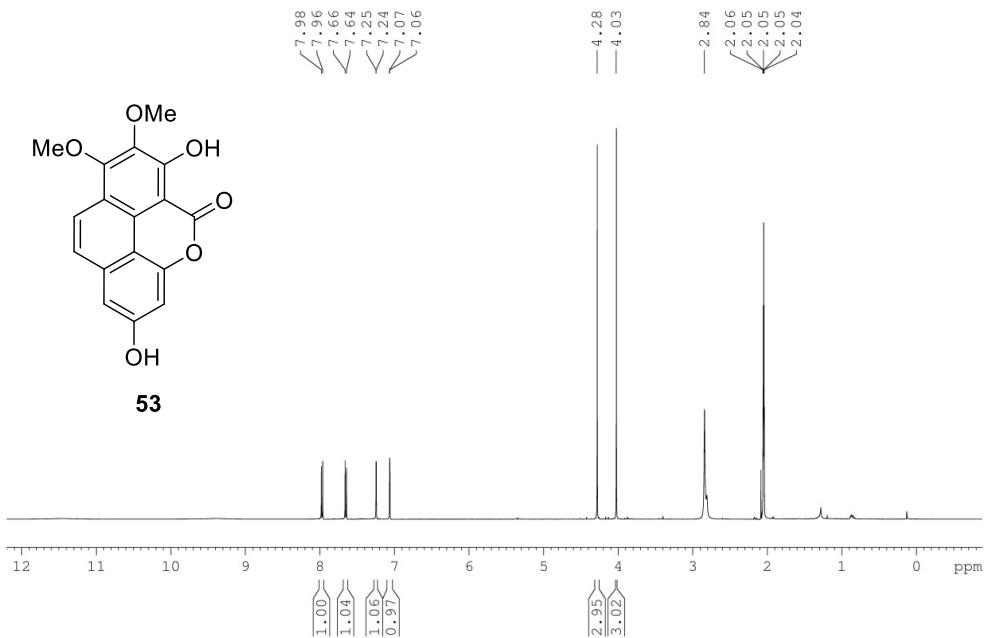
¹H NMR (300 MHz, CDCl₃) **52**



¹³C NMR (75 MHz, CDCl₃) **52**



¹H NMR (500 MHz, (CD₃)₂CO) **53**



¹³C NMR (125 MHz, (CD₃)₂CO) **53**

