Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Information

Evaluation of ferrocenyl phosphines as potent antimalarials targeting the Digestive vacuole Function of Plasmodium falciparum

Gowtham Subramanian[#1], Abdul Sadeer[#2], Kalyani Mukherjee[1], Tadayuki Kojima[2], Pallavi Tripathi[1], Renugah Naidu[1], Shan Wen Tay[2], Jia Hao Pang[2], Sumod A. Pullarkat[2] * and Rajesh Chandramohanadas [1]*

Table of Contents

I. Characterization data of Ferrocenyl-phosphine derivatives

O1: HP procedure of the respective enone produced orange-yellow precipitates. The reaction solvent was removed *via* cannula and solids washed with cold hexanes. Subsequently, the solids were dissolved in 5 mL non-degassed dichloromethane (DCM) and left to stir at ambient atmosphere for 24 h. Thereafter, the solvent was removed under reduced pressure and crude purified on SiO_2; silica gel column chromatography (DCM/E.A) to give FD1 as dull orange powder; yield: 98%. m.p. 191°C(decomp.); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 2.39 (s, 3H, - *Me*), 3.54 (s, 1H, Cp), 3.61 - 3.85 (m, 2H, - C*H2*), 3.89 (s, 1H, Cp), 3.92 (s, 5H, Cp), 4.11 (s, 1H, Cp), 4.23 (s, 1H, Cp), 4.42 (m, 1H, - C*H*PPh_2), 7.22 - 7.26 (m, 2H, - Ar), 7.28 – 7.34 (m, 2H, - Ar), 7.35 – 7.44 (m, 4H, - Ar), 7.47 – 7.55 (m, 2H, - Ar), 7.83 – 7.90 (m, 4H, - Ar). ^{31}P{^{1}H} NMR ($CDCl_3$, 161.6 MHz): δ 34.0 (s). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 21.8 (-*Me*), 34.2 (d, - *C*HPPh2, $^1J_{CP}$ = 67.0 Hz), 38.7(-CH_2), 67.2 (*m*-Cp), 67.7 (d, *o*-Cp, $^3J_{CP}$ = 1.6 Hz), 68.4 (*m*-Cp), 68.6 (5Cp), 70.3 (d, *o*-Cp, $^3J_{CP}$ = 2.0 Hz), 85.7 (*i*-Cp), 128.1 (d, 2 -*m* Ar, $^3J_{CP}$ = 11.5 Hz), 128.4(2 *m*-Ar), 128.6 (d, 2 *m*-Ar, $^3J_{CP}$ = 11.2 Hz), 129.5 (2 *o*-Ar), 131.5 (d, 2 *o*-Ar, $^2J_{CP}$ = 8.7 Hz), 131.5 (*p*-Ar), 131.6 (d, 2 *o*-Ar, $^2J_{CP}$ = 8.7 Hz), 131.6 (d, *i*-Ar, $^1J_{CP}$ = 95.0 Hz), 131.7 (d, *i*-Ar, $^1J_{CP}$ = 96.0 Hz), 131.9 (d, *p*-Ar, $^4J_{CP}$ = 3.1 Hz), 134.1 (*p*-Ar), 144.4 (*i*-Ar), 196.9 (d, *C*=O, $^3J_{CP}$ = 7.2 Hz). HRMS m/z (+ESI) $(M + H)^+$ calcd for C32H30O2P1Fe1: 533.1333, found: 533.1334.

O2: Similar procedure to O1; dull-orange powder; yield: 90%. m.p. 180°C(decomp.); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 3.50 – 3.58 (m, 1H, - C*H*), 3.62 (m, 1H, Cp), 3.73 - 3.86 (m, 1H, - C*H*), 3.90 (s, 1H, Cp), 3.98 (m, 1H, Cp), 4.06 – 4.12 (m, 6H, Cp), 4.52 (m, 1H, - C*H*PPh_2), 7.31 - 7.39 (m, 3H, - Ar), 7.43 – 7.58 (m, 6H, - Ar), 7.75 – 7.84 (m, 2H, - Ar), 7.86 – 7.94 (m, 2H, - Ar). ^{19}F{^{1}H} NMR ($CDCl_3$, 282.2 MHz): δ -62.99 (s), -58.41 (s). ^{31}P{^{1}H} NMR ($CDCl_3$, 161.6 MHz): δ 32.5 (s). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 35.7 (d, - *C*HPPh_2, $^1J_{CP}$ = 64.6 Hz), 43.9(-CH_2), 67.7 (*m*-Cp), 67.9 (*o*-Cp), 68.4 (*m*-Cp), 68.8 (5Cp), 69.9 (d, *o*-Cp, $^3J_{CP}$ = 1.7 Hz), 85.1 (*i*-Cp), 122.9 (q, *C*F_3, $^1J_{CF}$ = 273.2 Hz), 123.1 (q, *C*F_3, $^1J_{CF}$ = 273.9 Hz), 125.2(m, p-Ar), 127.0 (q, *m*-Ar, $^3J_{CF}$ = 3.9 Hz), 127.3 (q, *m*-Ar, $^3J_{CF}$ = 5.1 Hz), 128.1 (d, 2 -*m* Ar, $^3J_{CP}$ = 11.5 Hz), 128.8 (d, 2 -*m* Ar, $^3J_{CP}$ = 11.3 Hz), 129.7 (d, *i*-Ar, $^1J_{CP}$ = 97.7 Hz), 130.4 (d, *i*-Ar, $^1J_{CP}$ = 100.3 Hz), 131.5 (d, 2 *o*-Ar, $^2J_{CP}$ = 9.0 Hz), 132.0 (m, *p*-Ar), 132.3 (d, 2 *o*-Ar, $^2J_{CP}$ = 8.8 Hz), 132.4 (d, *p*-Ar, $^4J_{CP}$ = 2.2 Hz), 134.3 (q, 2 *m*-Ar, $^2J_{CF}$ = 33.0 Hz), 141.2 (*i*-Ar), 200.1 (s, *C*=O). HRMS m/z (+ESI) $(M + H)^+$ calcd for C33H26O2F6P1Fe1: 655.0924, found: 655.0927.

O3: Similar procedure to O1; dull-orange powder; yield: 90%. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 3.54 (s, 1H, Cp), 3.57 - 3.62 (dd, 2H, - *CH2*), 3.90 (s, 1H, Cp), 3.97 (s, 4H, Cp), 4.11 (s, 1H, Cp), 4.20 (s, 1H, Cp), 4.29 - 4.33 (m, 1H, - *CH*PPh_2), 6.50 - 6.52 (m, 1H, - furyl *CH*), 7.20 (d, 1H, - furyl *CH*), 7.29 – 7.46 (m, 5H, - Ar), 7.47 – 7.62 (m, 3H, - Ar), 7.79 – 7.92 (m, 2H, - Ar). ^{31}P{^{1}H} NMR ($CDCl_3$, 161.6 MHz): δ 33.9 (s).

O4: Similar procedure to O1; dull-orange powder; yield: 98%. m.p. 198°C(decomp.); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 3.52 (s, 1H, Cp), 3.62 - 3.71 (m, 2H, - C*H2*), 3.90 (s, 1H, Cp), 3.97 (s, 5H, Cp), 4.12 (s, 1H, Cp), 4.22 (s, 1H, Cp), 4.30 – 4.37 (m, 1H, - C*H*PPh_2), 7.07 - 7.14 (m, 1H, - thienyl C*H*), 7.28 – 7.46 (m, 6H, - Ar), 7.46 – 7.56 (m, 2H, - Ar), 7.62 (dd, 1H, $^3J_{HH}$ = 4.9 Hz, $^4J_{HH}$ = 0.7 Hz, - thienyl C*H*), 7.76 (dd, 1H, $^3J_{HH}$ = 3.7 Hz, $^4J_{HH}$ = 0.7 Hz, - thienyl C*H*), 7.82 – 7.91 (m, 2H, - Ar). ^{31}P{^{1}H} NMR ($CDCl_3$, 161.6 MHz): δ 33.5 (s). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 34.9 (d, - *C*HPPh_2, $^1J_{CP}$ = 67.3 Hz), 39.3(-CH_2), 67.3 (*m*-Cp), 67.6 (d, *o*-Cp, $^3J_{CP}$ = 2.3 Hz), 68.4 (*m*-Cp), 68.7 (5Cp), 70.2 (d, *o*-Cp, $^3J_{CP}$ = 2.1 Hz), 85.4 (*i*-Cp), 128.1 (d, 2 -*m* Ar, $^3J_{CP}$ = 11.7 Hz), 128.3 (thienyl Ar), 128.7 (d, 2 *m*-Ar, $^3J_{CP}$ = 11.4 Hz), 131.5 (d, 2 *i*-Ar, $^1J_{CP}$ = 96.9 Hz), 131.5 (d, 2 *o*-Ar, $^2J_{CP}$ = 8.9 Hz), 131.6 (d, *p*-Ar, $^4J_{CP}$ = 3.1 Hz), 131.7 (d, 2 *o*-Ar, $^2J_{CP}$ = 9.1 Hz), 131.9 (d, *p*-Ar, $^4J_{CP}$ = 2.6 Hz), 132.4 (thienyl Ar), 134.2 (thienyl Ar), 143.7 (thienyl Ar), 190.4 (d, *C*=O, $^3J_{CP}$ = 7.3 Hz).

O6: Similar procedure to O1; dull-orange oil; yield: 60%; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 2.03 (s, 3H, - C*H*$_3$), 3.00 – 3.40 (m, 2H, -C*H2*), 3.66 – 3.74 (m, 2H, -C*H2*), 3.96 (s, 5H, Cp), 4.12 – 4.15 (m, 1H, Cp), 4.32 – 4.35 (m, 1H, Cp), 4.78 – 4.84 (m, 1H, - C*H*$_2$), 3.57 (s, 1H, -Cp*H*), 3.92 (s, 1H, -Cp*H*), 4.00 – 4.30 (m, 8H, -Cp*H* & -C*H*PPh_2), 7.28 – 7.39 (m, 2H, - Ar), 7.39 – 7.54 (m, 6H, - Ar), 7.75 – 7.90 (m, 2H, - Ar). ^{31}P{^{1}H} NMR ($CDCl_3$, 161.6 MHz): δ 33.1 (s). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 1.0 (s, -Me), 30.1 (s, - *C*HPPh_2), 43.4 (s, -*C*H_2), 67.3 (*m*-Cp), 67.6 (*o*-Cp), 68.3 (*m*-Cp), 68.5 (5Cp), 69.9 (*o*-Cp), 85.4 (*i*-Cp), 125.2(m, p-Ar), 128.1 (m, 2 -*m* Ar), 128.6 (m, 2 -*m* Ar), 128.8, 129.0, 130.9, 129.7, 130.9, 131.6, 131.7, 131.8, 132.3, 141.2 (*i*-Ar), 205.7 (s, *C*=O).

O7: HP procedure gave a light purple solution. To the reaction vessel was added non-degassed DCM and left to stir under ambient atmospheric conditions for 24 h. The solvent was then removed under reduced pressure and crude purified on SiO_2; silica gel column chromatography (Hexane/E.A); orange-yellow; yield: 60%. m.p. 149°C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 1.18 (m, 6H, -*Me*), 1.29 (d, 6H, -*Me*), 3.73 (s, 1H, Cp), 3.97 – 4.00 (m, 2H, Cp), 4.05 (s, 5H, Cp), 4.07 (s, 1H, Cp), 4.32 (dd, 1H, $^3J_{HH}$ = 3.7 Hz, $^2J_{HP}$ = 20.0 Hz, -C*H*PPh2), 4.46 (dd, 1H, $^3J_{HH}$ = 3.6 Hz, $^3J_{HP}$ = 14.4 Hz, - C*H*), 4.95 (sep, 1H, $^3J_{HH}$ = 6.3 Hz, - C*H*), 5.08 (sep, 1H, $^3J_{HH}$ = 5.9 Hz, - C*H*), 7.27 - 7.35 (m, 2H, - Ar), 7.37 - 7.55 (m, 6H, - Ar), 7.71 - 7.81 (m, 2H, - Ar). ^{31}P{^{1}H} NMR ($CDCl_3$, 161.6 MHz): δ 30.5 (s). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 21.5 (-*Me*), 21.7 (-*Me*), 21.8 (-*Me*), 21.8 (-*Me*), 41.2 (d, - *C*HPPh$_2$, $^1J_{CP}$ = 67.1 Hz), 56.0 (d, - *C*H), 67.7 (-CH), 68.3 (-CH), 68.6 (d, *o*-Cp, $^3J_{CP}$ = 3.0 Hz), 67.0 (5 Cp), 69.3 (*m*-Cp), 70.0 (*m*-Cp), 69.3 (*o*-Cp), 85.0 (*i*-Cp), 127.7 (d, 2 -*m* Ar, $^3J_{CP}$ = 11.7 Hz), 128.3 (d, 2 *m*-Ar, $^3J_{CP}$ = 11.4 Hz), 131.2 (d, *p*-Ar, $^4J_{CP}$ = 2.6 Hz),131.5 (d, *p*-Ar, $^4J_{CP}$ = 2.5 Hz), 131.6 (d, *i*-Ar, $^1J_{CP}$ = 99.7 Hz), 131.9 (d, 2 *o*-Ar, $^2J_{CP}$ = 9.0 Hz), 132.7 (d, 2 *o*-Ar, $^2J_{CP}$ = 8.6 Hz), 134.7 (d, *i*-Ar, $^1J_{CP}$ = 95.9 Hz), 167.7 (d, *C*=O, $^3J_{CP}$ = 4.4 Hz), 168.2 (d, *C*=O, $^3J_{CP}$ = 4.4 Hz). HRMS m/z (+ESI) $(M + H)^+$ calcd for C32H36O5P1Fe1: 587.1650, found: 587.1652.

S1: HP procedure of the respective enone produced orange-yellow precipitates. The reaction solvent was removed *via* cannula and solids washed with cold hexanes. Thereafter, 1.2 equivalent of Sulphur was added and solids dissolved in 5 mL degassed DCM. The solution was left for 24 h. Thereafter, the solvent was removed under reduced pressure and crude purified on SiO_2; silica gel column chromatography (Hexane/E.A); orange powder; yield: 90%. m.p. 190°C(decomp.); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 2.40 (s, 3H, - *Me*), 3.38 (s, 1H, Cp), 3.61 - 3.80 (m, 2H, - C*H2*), 3.85 (s, 1H, Cp), 3.92 (s, 5H, Cp), 4.12 (s, 1H, Cp), 4.33 (s, 1H, Cp), 4.82 (m, 1H, - C*H*PPh$_2$), 7.22 - 7.24 (m, 2H, - Ar), 7.24 – 7.26 (m, 2H, - Ar), 7.28 – 7.43 (m, 6H, - Ar), 7.59 – 7.67 (m, 2H, - Ar), 7.87 – 7.92 (m, 2H, - Ar), 8.00 – 8.10 (m, 2H, - Ar). ^{31}P{^{1}H} NMR ($CDCl_3$, 161.6 MHz): δ 53.5 (s). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 21.7 (-*Me*), 35.9 (d, - *C*HPPh$_2$, $^1J_{CP}$ = 51.7 Hz), 39.6 (d, - *C*H$_2$, $^2J_{CP}$ = 4.6 Hz), 67.1 (*m*-Cp), 68.1 (d, *o*-Cp, $^3J_{CP}$ = 1.7 Hz), 68.2 (*m*-Cp), 68.6 (5Cp), 70.2 (d, *o*-Cp, $^3J_{CP}$ = 1.9 Hz), 85.3 (*i*-Cp), 127.9 (d, 2 -*m* Ar, $^3J_{CP}$ = 12.1 Hz), 128.3(2 *m*-Ar), 128.5 (d, 2 *m*-Ar, $^3J_{CP}$ = 11.5 Hz), 129.4 (2 *o*-Ar), 131.0 (d, *i*-Ar, $^1J_{CP}$ = 74.5 Hz), 131.2 (d, *i*-Ar, $^1J_{CP}$ = 79.4 Hz), 131.3 (d, *p*-Ar, $^4J_{CP}$ = 2.9 Hz), 131.6 (d, *p*-Ar, $^4J_{CP}$ = 2.9 Hz), 132.0(d, 2 *o*-Ar, $^2J_{CP}$ = 9.4 Hz), 132.2 (d, 2 *o*-Ar, $^2J_{CP}$ = 9.6 Hz), 134.0 (*p*-Ar), 144.4 (*i*-Ar), 196.8 (d, *C*=O, $^3J_{CP}$ = 7.9 Hz). HRMS m/z (+ESI) $(M + H)^+$ calcd for C32H30O1P1S1Fe1: 549.1104, found: 533.1107.

S2: Similar procedure to S1; orange powder; yield: 90%. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 3.45 – 3.49 (m, 1H, Cp), 3.86 - 3.98 (m, 2H, - C*H2*), 3.99 – 4.09 (m, 2H, Cp), 4.11(s, 5H, Cp), 4.79 – 4.87 (m, 1H, - C*H*PPh$_2$), 7.03 (s, 1H, - Ar), 7.30 – 7.55 (m, 6H, - Ar), 7.66 – 7.85 (m, 4H, -Ar), 8.08 – 8.19 (m, 2H, - Ar). ^{31}P{^{1}H} NMR ($CDCl_3$, 161.6 MHz): δ 53.4 (s). ^{19}F{^{1}H} NMR ($CDCl_3$, 282.2 MHz): δ -62.96 (s), -58.29 (s). ^{31}P{^{1}H} NMR ($CDCl_3$, 121.2 MHz): δ 53.4 (s). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 36.7 (d, - *C*HPPh$_2$, $^1J_{CP}$ = 49.5 Hz), 44.8 (d, -*C*H$_2$,$^2J_{CP}$ = 4.1 Hz), 67.5 (*m*-Cp), 68.3 (*o*-Cp), 68.4 (*m*-Cp), 68.7 (5Cp), 69.9 (*o*-Cp), 85.3 (*i*-Cp), 122.7 (q, *C*F$_3$, $^1J_{CF}$ = 273.4 Hz), 122.9 (q, *C*F$_3$, $^1J_{CF}$ = 273.9 Hz), 124.7 (m, p-Ar), 127.1 (q, *m*-Ar, $^3J_{CF}$ = 3.47 Hz), 127.3 (q, *m*-Ar, $^3J_{CF}$ = 4.9 Hz), 128.0 (d, 2 -*m* Ar, $^3J_{CP}$ = 12.0 Hz), 128.6 (d, 2 -*m* Ar, $^3J_{CP}$ = 11.5 Hz), 129.8 (d, *i*-Ar, $^1J_{CP}$ = 79.6 Hz), 130.1 (q, *m*-Ar, $^2J_{CF}$ = 33.4 Hz), 130.4 (d, *i*-Ar, $^1J_{CP}$ = 74.4 Hz), 131.6 (d, *p*-Ar, $^4J_{CP}$ = 2.7 Hz), 132.1 (d, *p*-Ar, $^4J_{CP}$ = 2.6 Hz), 132.6 (d, 2 *o*-Ar, $^2J_{CP}$ = 9.5 Hz), 134.0 (q, *m*-Ar, $^2J_{CF}$ = 33.6 Hz), 140.7 (*i*-Ar), 200.1 (d, *C*=O, $^3J_{CP}$ = 2.7 Hz).

S3: Similar procedure to S1; orange powder; yield: 90%. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 3.34 – 3.37 (m, 1H, Cp), 3.58 (dd, 2H, - C*H2*, $^3J_{CP}$ = 4.98 Hz, $^2J_{HH}$ = 1.98 Hz), 3.62 (d, 1H, -C*H2*, $^3J_{CP}$ = 5.00 Hz), 3.84 -3.88 (m, 1H, Cp), 3.96 (s, 5H, Cp), 4.12 – 4.15 (m, 1H, Cp), 4.29 - 4.32 (m, 1H, Cp), 4.66 – 4.73 (m, 1H, - C*H*PPh$_2$), 6.51 (dd, - furyl C*H*, $^2J_{HH}$ = 1.52 Hz, $^2J_{HH}$ =3.52 Hz), 7.23 (d, - furyl C*H*, $^2J_{HH}$ = 3.60 Hz), 7.28 - 7.35 (m, 2H, - Ar), 7.36 – 7.45 (m, 4H, - Ar), 7.58 (s, 1H, - thienyl C*H*), 7.61 – 7.69 (m, 2H, -Ar), 8.00 – 8.09 (m, 2H, -Ar). ^{31}P{^{1}H} NMR ($CDCl_3$, 161.6 MHz): δ 52.8 (s). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 36.3 (d, - *C*HPPh$_2$, $^1J_{CP}$ = 51.4 Hz), 39.3 (d, -*C*H$_2$, $^2J_{CP}$ = 4.6 Hz), 67.3 (*m*-Cp), 68.3 (*m*-Cp, o-Cp), 68.8 (5Cp), 70.1 (d, *o*-Cp, $^3J_{CP}$ = 1.6 Hz), 85.2 (*i*-Cp), 112.6 (furyl Ar), 118.1 (furyl Ar), 128.1 (d, 2 -*m* Ar, $^3J_{CP}$ = 11.8 Hz), 128.6 (d, 2 -*m* Ar, $^3J_{CP}$ = 11.6 Hz), 131.0 (d, *i*-Ar, $^1J_{CP}$ = 74.5 Hz), 131.1 (d, *i*-Ar, $^1J_{CP}$ = 79.2 Hz), 131.5 (d, 2 p-Ar, $^2J_{CP}$ = 2.8 Hz, overlap with i-Ar doublet), 131.8 (d, *p*-Ar, $^4J_{CP}$ = 2.8 Hz), 132.2 (d, o-Ar, $^2J_{CP}$ = 9.5 Hz), 132.4 (d, o-Ar, $^2J_{CP}$ = 9.8 Hz), 146.9 (furyl Ar), 152.4 (furyl Ar), 186.6 (d, *C*=O, $^3J_{CP}$ = 7.9 Hz).

S4: Similar procedure to S1; orange powder; yield: 90%. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 3.35 (s, 1H, Cp), 3.58 - 3.76 (m, 2H, - C*H2*), 3.87 (s, 1H, Cp), 3.97 (s, 5H, Cp), 4.14 (s, 1H, Cp), 4.31 (s, 1H, Cp), 4.68 – 4.76 (m, 1H, - C*H*PPh_2), 7.08 - 7.13 (m, 1H, - thienyl C*H*), 7.28 – 7.45 (m, 6H, - Ar), 7.60 – 7.69 (m, 3H, - 2Ar & - thienyl C*H*), 7.80 (m, 1H, - thienyl C*H*), 8.00 – 8.10 (m, 2H, - Ar). ^{31}P{^{1}H} NMR ($CDCl_3$, 161.6 MHz): δ 53.7 (s). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 36.7 (d, - *C*HPPh_2, $^{1}J_{CP}$ = 51.3 Hz), 40.1 (d, - *C*H2, $^{2}J_{CP}$ = 4.1 Hz), 67.2 (*m*-Cp), 68.1 (d, *o*-Cp, $^{3}J_{CP}$ = 1.4 Hz), 68.2 (*m*-Cp), 68.7 (5Cp), 70.1 (d, *o*-Cp, $^{3}J_{CP}$ = 1.7 Hz), 85.1 (*i*-Cp), 128.0 (d, 2 -*m* Ar, $^{3}J_{CP}$ =12.1 Hz), 128.3(thienyl Ar), 128.5 (d, 2 *m*-Ar, $^{3}J_{CP}$ = 11.5 Hz), 130.8 (d, 2 *i*-Ar, $^{1}J_{CP}$ = 74.4 Hz), 131.5 (d, 2 *i*-Ar, $^{1}J_{CP}$ = 80.0 Hz), 131.4 (d, *p*-Ar, $^{4}J_{CP}$ = 3.2 Hz), 131.7 (d, *p*-Ar, $^{4}J_{CP}$ = 2.8 Hz), 131.2 (d, 2 *o*-Ar, $^{2}J_{CP}$ = 8.9 Hz), 131.3 (d, 2 *o*-Ar, $^{2}J_{CP}$ = 10.0 Hz), 132.6 (thienyl Ar), 134.4 (thienyl Ar), 143.7 (thienyl Ar), 190.4 (d, *C*=O, $^{3}J_{CP}$ = 7.8 Hz).

S5: Similar procedure to S1; orange powder; yield: 90%. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 3.39 – 3.42 (m, 1H, Cp), 3.70 - 3.81 (m, 2H, - C*H2*), 3.87 – 3.90 (m, 1H, Cp), 3.98 (s, 5H, Cp), 4.14 -4.17 (m, 1H, Cp), 4.33 – 4.36 (m, 1H, Cp), 4.71 – 4.78 (m, 1H, - C*H*PPh_2), 7.28 – 7.38 (m, 6H, - Ar), 7.39 – 7.45 (m, 1H, - Ar), 7.46 – 7.52 (m, 1H, - Ar), 7.56 – 7.62 (m, 2H, - Ar), 7.63 – 7.72 (m, 3H, - 2Ar & - thienyl C*H*), 8.00 – 8.09 (m, 2H, - Ar). ^{31}P{^{1}H} NMR ($CDCl_3$, 161.6 MHz): δ 52.9 (s). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 36.3 (d, - *C*HPPh_2, $^{1}J_{CP}$ = 51.0 Hz), 39.3 (d, -*C*H_2, $^{2}J_{CP}$ = 4.4 Hz), 69.2 (*m*-Cp), 70.1 (*m*-Cp, o-Cp), 71.0(5Cp), 72.1 (*o*-Cp), 87.1 (*i*-Cp), 112.6 (furyl Ar), 113.9 (furyl Ar), 123.5 (Ar), 124.1 (Ar), 126.9 (Ar), 128.2 (d, 2 -*m* Ar, $^{3}J_{CP}$ = 12.0 Hz), 128.6 (d, 2 -*m* Ar, $^{3}J_{CP}$ = 11.3 Hz), 128.7 (Ar), 130.9 (d, *i*-Ar, $^{1}J_{CP}$ = 74.5 Hz), 131.0 (d, *i*-Ar, $^{1}J_{CP}$ = 79.9 Hz), 131.6 (d, p-Ar, $^{2}J_{CP}$ = 1.5 Hz), 131.7 (d, p-Ar, $^{2}J_{CP}$ = 1.6 Hz), 132.1 (d, o-Ar, $^{2}J_{CP}$ = 9.3 Hz), 132.5 (d, o-Ar, $^{2}J_{CP}$ = 9.7 Hz), 152.0 (furyl Ar), 155.8 (furyl Ar), 188.1 (d, *C*=O, $^{3}J_{CP}$ = 7.2 Hz).

S7: HP procedure gave a light purple solution. 1.2 equivalent of Sulphur was added to the crude and washed with degassed DCM. Thereafter, the solution was left to stir for 24 h. The solvent was then removed under reduced pressure and crude purified on SiO_2; silica gel column chromatography (Hexane/E.A); orange powder; yield: 60%. m.p. 145°C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 1.11 (d, 3H, $^{3}J_{HH}$ = 6.2 Hz, -*Me*), 1.20 (d, 3H, $^{3}J_{HH}$ = 6.3 Hz, -*Me*), 1.27 (d, 3H, $^{3}J_{HH}$ = 6.2 Hz, -*Me*), 1.31 (d, 3H, $^{3}J_{HH}$ = 6.3 Hz, - *Me*), 3.42 (s, 1H, Cp), 3.90 (s, 1H, Cp), 4.04 (s, 5H, Cp), 4.11 (s, 1H, Cp), 4.19 (s, 1H, Cp), 4.50 (dd, 1H, $^{3}J_{HH}$ = 3.6 Hz, $^{2}J_{HP}$ = 18.8 Hz, - C*H*PPh_2), 4.79 (dd, 1H, $^{3}J_{HH}$ = 3.6 Hz, $^{3}J_{HP}$ = 12.8 Hz, - C*H*), 4.87 (sep, 1H, $^{3}J_{HH}$ = 6.3 Hz, - C*H*), 5.10 (sep, 1H, $^{3}J_{HH}$ = 6.3 Hz, - C*H*), 7.27 - 7.32 (m, 2H, - Ar), 7.35 - 7.49 (m, 4H, - Ar), 7.55 - 7.64 (m, 2H, - Ar), 7.88 - 7.97 (m, 2H, - Ar). ^{31}P{^{1}H} NMR ($CDCl_3$, 161.6 MHz): δ 47.9 (s). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 21.5 (-*Me*), 21.7 (2 -*Me*), 21.8 (-*Me*), 42.3 (d, - *C*HPPh_2, $^{1}J_{CP}$ = 50.0 Hz), 56.4 (d, - *C*H, $^{2}J_{CP}$ = 2.2 Hz), 67.3 (-CH), 67.4 (-CH), 67.0 (*o*-Cp & 5 Cp), 69.5 (*m*-Cp), 70.1 (*m*-Cp), 70.7 (d, *o*-Cp, $^{3}J_{CP}$ = 1.7 Hz), 86.2 (*i*-Cp), 127.6 (d, 2 -*m* Ar, $^{3}J_{CP}$ = 12.0 Hz), 128.3 (d, 2 *m*-Ar, $^{3}J_{CP}$ = 12.0 Hz), 131.0 (d, *p*-Ar, $^{4}J_{CP}$ = 2.9 Hz), 131.1 (d, *p*-Ar, $^{4}J_{CP}$ = 2.9 Hz), 131.1 (d, *i*-Ar, $^{1}J_{CP}$ = 80.9 Hz), 132.0 (d, 2 *o*-Ar, $^{2}J_{CP}$ = 9.8 Hz), 133.2 (d, 2 *o*-Ar, $^{2}J_{CP}$ = 9.5 Hz), 134.6 (d, *i*-Ar, $^{1}J_{CP}$ = 78.5 Hz), 167.1 (d, *C*=O, $^{3}J_{CP}$ = 5.6 Hz), 168.5 (d, *C*=O, $^{3}J_{CP}$ = 4.9 Hz). HRMS m/z (+ESI) $(M + H)^+$ calcd for C32H36O4P1S1Fe1: 603.1421, found: 603.1423.

S8: Similar procedure to S7; orange powder; yield: 80%. ^{1}H NMR ($CDCl_3$, 300 MHz): δ 3.36 – 3.42 (m, 1H, Cp), 3.45 (s, 3H, - C*H3*), 3.81 (s, 3H, -C*H3*), 3.91 – 3.96 (m, 1H, Cp), 4.06 (s, 5H, Cp), 4.09 – 4.15 (m, 1H, Cp), 4.64 (dd, 1H, - C*H*PPh_2, $^{2}J_{CP}$ = 19.8 Hz, $^{3}J_{HH}$ = 3.54 Hz), 4.79 (dd, 1h, -C*H*<, $^{2}J_{CP}$ = 13.5 Hz, $^{3}J_{HH}$ = 3.5 Hz), 7.27 – 7.34 (m, 2H, - Ar), 7.35 – 7.51 (m, 4H), 7.52 – 7.63 (m, 2H, Ar), 7.81 – 7.95 (m, 2H, Ar). ^{31}P{^{1}H} NMR ($CDCl_3$, 161.6 MHz): δ 47.3 (s). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 43.6 (d, - *C*HPPh_2, $^{1}J_{CP}$ = 49.0 Hz), 52.4 (s, -O*Me*), 53.2 (s, -O*Me*), 55.4 (s, -*CH*), 68.4 (s, *o*-Cp), 68.4 (s, *m*-Cp), 68.5 (s, 5 Cp), 70.0 (*m*-Cp), 70.5 (s, *o*-Cp), 85.6 (*i*-Cp), 127.6 (d, 2 -*m* Ar, $^{3}J_{CP}$ = 12.0 Hz), 128.3 (d, 2 *m*-Ar, $^{3}J_{CP}$ = 12.0 Hz), 131.1 (d, *o*-Ar, $^{3}J_{CP}$ = 8.0 Hz), 131.7 (d, *o*-Ar, $^{3}J_{CP}$ = 10 Hz), 133.2 (d, *o*-Ar, $^{3}J_{CP}$ = 10 Hz), 133.9 (s, Ar), 134.7 (s, Ar), 167.9 (s, *C*=O), 169.1 (s, *C*=O).

G1: HP procedure of the respective enone produced orange-yellow precipitates. The reaction solvent was removed *via* cannula and solids washed with cold hexanes. Thereafter, 1 equivalent of ClAu.SMe_2 was added and solids dissolved in 5 mL degassed DCM. The solution was left for 24 h in absence of light. Thereafter, the solvent was removed under reduced pressure and crude purified on SiO_2; silica gel column chromatography (Hexane/E.A); brownish-orange powder; yield: 90%. m.p. 180°C(decomp.); ^{1}H NMR ($CDCl_3$, 400 MHz): δ 2.42 (s, 3H, - *Me*), 3.39 (s, 1H, Cp), 3.36 - 3.49 (m, 1H, - C*H*), 3.88 - 4.00 (m, 7H, - C*H & 6 Cp*), 4.19 (s, 1H, Cp), 4.36 (s, Cp), 4.65 – 4.74 (m, 1H, - C*H*PPh_2), 7.27 - 7.35 (m, 4H, - Ar), 7.35 – 7.50 (m, 6H, - Ar), 7.80 – 7.92 (m, 4H, - Ar). ^{31}P{^{1}H} NMR ($CDCl_3$, 161.6 MHz): δ 48.9 (s). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 21.9 (-*Me*), 34.6 (d, - *C*HPPh$_2$, $^1J_{CP}$ = 36.2 Hz), 41.7(d, - *C*H2, $^2J_{CP}$ = 12.0 Hz), 67.7 (d, *o*-Cp, $^3J_{CP}$ = 3.0 Hz), 67.8 (*m*-Cp), 68.8 (5 Cp), 69.2 (*m*-Cp), 70.4 (d, *o*-Cp), 86.9 (*i*-Cp), 128.1 (d, *i*-Ar, $^1J_{CP}$ = 80.1 Hz), 128.4 (2 *m*-Ar), 128.6 (d, *i*-Ar, $^1J_{CP}$ = 86.1 Hz), 128.7 (d, 2 *o*-Ar, $^2J_{CP}$ = 11.6 Hz), 129.3 (d, 2 *o*-Ar, $^2J_{CP}$ = 11.2 Hz), 129.7 (2 *o*-Ar), 132.0 (d, *p*-Ar, $^4J_{CP}$ = 2.5 Hz), 132.3 (d, *p*-Ar, $^4J_{CP}$ = 2.4 Hz), 132.3 (d, 2 -*m* Ar, $^3J_{CP}$ = 11.5 Hz), 133.7 (*p*-Ar), 134.3 (d, 2 *m*-Ar, $^3J_{CP}$ = 13.0 Hz), 134.6 (d, 2 *m*-Ar, $^3J_{CP}$ = 13.0 Hz), 145.0 (*i*-Ar), 196.0 (d, *C*=O, $^3J_{CP}$ = 9.1 Hz). HRMS m/z (+ESI) $(M + H)^+$ calcd for C32H30O1P1Cl1Fe1Au1: 749.0738, found: 749.0739.

G2: Similar procedure to G1; brownish-orange powder; yield: 89%. m.p. 178°C(decomp.); ^{1}H NMR (CDCl$_3$, 300 MHz): 3.45 (m, 1H, Cp), 3.53 - 3.92 (m, 2H, - C*H$_2$*), 4.01 (m, 1H, Cp), 4.12 (m, 5H, Cp), 4.21 (m, 2H, Cp), 4.70 (m, 1H, - C*H*PPh$_2$), 6.49 (s, 1H, - Ar), 7.34 – 7.69 (m, 8H, - Ar), 7.74 – 7.90 (m, 2H, - Ar), 7.92 – 8.06 (m, 2H, - Ar). ^{19}F{^{1}H} NMR (CDCl$_3$, 282.2 MHz): δ -62.83 (s), -58.25 (s). ^{31}P{^{1}H} NMR (CDCl$_3$, 161.6 MHz): δ 52.5 (s). ^{13}C NMR (CDCl$_3$, 100 MHz): δ 32.7 (d, - *C*HPPh$_2$, $^1J_{CP}$ = 34.6 Hz), 47.2(d, -*C*H$_2$, $^2J_{CP}$ = 12.7 Hz), 67.6 (d, *o*-Cp, $^3J_{CP}$ = 4.4 Hz), 68.1 (*m*-Cp), 68.8 (5Cp), 69.4 (*m*-Cp), 69.8 (d, *o*-Cp, $^3J_{CP}$ = 1.9 Hz), 86.8 (d, *i*-Cp, $^2J_{CP}$ = 7.3 Hz), 122.7 (q, *C*F$_3$, $^1J_{CF}$ = 273.4 Hz), 122.9 (q, *C*F$_3$, $^1J_{CF}$ = 274.2 Hz), 123.9(m, p-Ar), 127.5 (d, *i*-Ar, $^1J_{CP}$ = 74.3 Hz), 127.6 (m, *m*-Ar), 127.8 (m, *m*-Ar), 128.1 (d, *i*-Ar, $^1J_{CP}$ = 81.4 Hz), 128.9 (d, 2 *o*-Ar, $^2J_{CP}$ = 11.8Hz), 129.6 (d, 2 *o*-Ar, $^2J_{CP}$ = 11.1 Hz), 130.2 (q, *m*-Ar, $^2J_{CF}$ = 32.8 Hz), 132.4 (d, *p*-Ar, $^4J_{CP}$ = 2.5 Hz), 133.0 (d, *p*-Ar, $^4J_{CP}$ = 2.2 Hz), 134.4 (q, *m*-Ar, $^2J_{CF}$ = 33.0 Hz), 134.6 (d, 2 -*m* Ar, $^3J_{CP}$ = 13.3 Hz), 135.2 (d, 2 -*m* Ar, $^3J_{CP}$ = 13.8 Hz), 140.3 (s, *i*-Ar), 141.2 (*i*-Ar), 199.2 (d, *C*=O, $^3J_{CP}$ = 4.6 Hz). HRMS m/z (+ESI) $(M + H)^+$ calcd for C33H26O1P1Cl1Fe1Au1F6: 871.0329, found: 871.0333.

G3: Similar procedure to G1; brownish-orange powder; yield: 95%. m.p. 119°C(decomp.); ^{1}H NMR (CDCl$_3$, 400 MHz): δ 3.30 - 3.48 (m, 2H, Cp & C*H*), 3.74 - 3.88 (m, 1H, - C*H*), 3.95 (m, 1H, Cp), 3.98 (s, 5H, Cp), 4.21 (s, 1H, Cp), 4.36 (s, 1H, Cp), 4.53 – 4.64 (m, 1H, - C*H*PPh$_2$), 6.56 (m, 1H, - thienyl C*H*), 7.25 (m, 1H, - thienyl C*H*), 7.30 – 7.54 (m, 8H, - Ar), 7.46 – 7.56 (m, 2H, - Ar), 7.63 (m, 1H, - thienyl C*H*), 7.83 – 7.92 (m, 2H, - Ar). ^{31}P{^{1}H} NMR (CDCl$_3$, 161.6 MHz): δ 49.0 (s). ^{13}C NMR (CDCl$_3$, 100 MHz): δ 32.9 (d, - *C*HPPh$_2$, $^1J_{CP}$ = 35.6 Hz), 41.3 (d, -*C*H$_2$, $^2J_{CP}$ = 11.9 Hz), 67.6 (d, *o*-Cp, $^3J_{CP}$ = 4.4 Hz), 67.8 (*m*-Cp), 68.3 (5Cp), 69.2 (*m*-Cp), 70.1 (d, *o*-Cp, $^3J_{CP}$ = 1.9 Hz), 86.6 (d, *i*-Cp, $^2J_{CP}$ = 6.9 Hz), 112.8 (furyl Ar), 118.1 (furyl Ar), 127.8 (d, *i*-Ar, $^1J_{CP}$ = 72.5 Hz), 128.4 (d, *i*-Ar, $^1J_{CP}$ = 78.6 Hz), 128.7 (d, 2 *o*-Ar, $^3J_{CP}$ = 11.6 Hz), 129.2 (d, 2 *o*-Ar, $^3J_{CP}$ = 11.2 Hz), 132.1 (d, *p*-Ar, $^4J_{CP}$ = 2.7 Hz), 132.3 (d, *p*-Ar, $^4J_{CP}$ = 2.6 Hz), 134.4 (d, 2 *m*-Ar, $^2J_{CP}$ = 13.1 Hz), 134.6 (d, 2 *m*-Ar, $^2J_{CP}$ = 13.2 Hz), 147.1 (furyl Ar), 152.1 (furyl Ar), 185.6 (d, *C*=O, $^3J_{CP}$ = 8.9 Hz). HRMS m/z (+ESI) $(M + H)^+$ calcd for C29H26O2P1Cl1Fe1Au1: 725.0374, found: 725.0370.

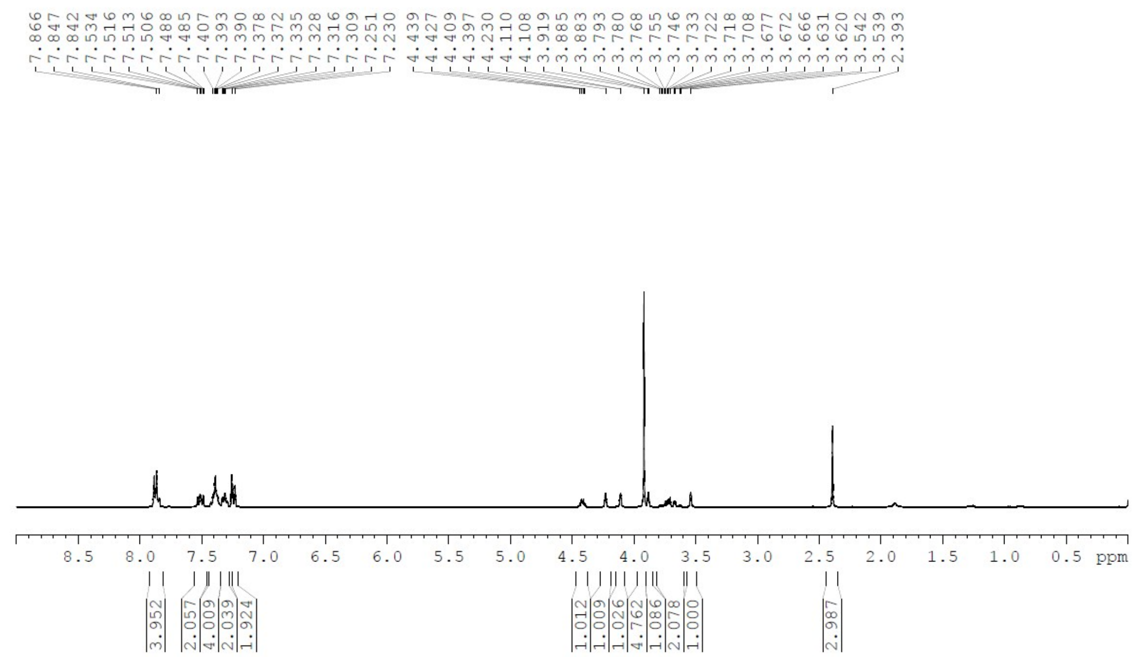
DS1: A Schlenk tube was charged with racemic catalyst (1.95 mg, 4×10^{-3} mmol), diarylphosphine (0.02 mmol) and anhydrous MeOH (1 ml). The clear yellow solution was further stirred at -60 °C for 10 minutes before the racemic ferrocenyl enone (0.04 mmol) in 1 ml of anhydrous MeOH was added. The resulting dark purple solution was stirred for 10 minutes followed by dropwise addition of NEt$_3$ (2.03 mg, 2.79 µL, 0.02 mmol) in anhydrous MeOH (0.5 ml). The resulting solution was stirred for 24 hours. Following that, sulphur (1.92 mg, 0.06 mmol) in degassed DCM (1 ml) was administered. The reaction mixture was then warmed to RT and stirred for another hour. The crude was then concentrated and purified via silica gel column chromatography (DCM: EA; 10: 1); Yellow oil; yield: 50%. ^{1}H NMR (CDCl$_3$, 500 MHz): δ 1.31 (m, 1H, -CH$_2$O*H*), 2.39 (s, 3H, -ArC*H$_3$*), 3.55 - 3.90 (m, 4H, -C*H$_2$*OH and -CH(PPh$_2$)C*H$_2$*), 3.91 (s, 5H, -Cp), 4.06 (m, 1H, -Cp), 4.25 (m, 1H, -Cp), 4.71 (m, 1H, -Cp), 4.93 (m, 1H, -C*H*PPh$_2$), 7.17 - 7.50 (m, 10H, -Ar), 7.92 (d, 2H, ^3J = 8.5 Hz, -Ar), 8.06 - 8.10 (m, 2H, -Ar). ^{13}C NMR (CDCl$_3$, 400 MHz): δ 21.7, 25.4, 32.2, 32.7, 41.9, 42.0, 58.8, 67.7, 67.8, 68.4, 68.8, 85.6, 88.6, 127.9, 128.0, 128.3, 128.7, 128.8, 129.2, 129.4, 129.5, 129.9, 131.3, 131.4, 131.8, 131.9, 132.0, 132.5, 132.6, 132.7, 133.6, 144.6, 196.9. ^{31}P{^{1}H} NMR (CDCl$_3$, 161.6 MHz): δ 54.4 (major diastereomer), 52.5(minor diastereomer). d.r (95:5). MS (m / z) = 577.05.

DS3: Similar procedure to DS1; yellow oil; yield: 50%. Bright yellow oil. ^{1}H NMR (CDCl$_3$, 500 MHz): 1.22 (m, 1H, -CH$_2$O*H*), 3.46 - 3.80 (m, 4H, -C*H$_2$*OH and -CH(PPh$_2$)C*H$_2$*), 3.96 (s, 5H, -Cp), 4.08 (m, 1H, -Cp), 4.26 (m, 1H, -Cp), 4.66 (m, 1H, -Cp), 4.84 (m, 1H, -C*H*PPh$_2$), 6.52 - 6.52 (m, 1H, -Ar), 7.20 - 8.10 (m, 12H, -Ar). δ ^{13}C NMR (CDCl$_3$, 125): δ 14.2, 21.1, 32.5 (d, - *C*HPPh$_2$, $^1J_{CP}$ = 52.5 Hz), 41.5 (d, -*C*H$_2$, $^2J_{CP}$ = 7.5 Hz), 58.7, 60.4 (s, 5Cp), 67.1, 67.7, 67.8, 68.5, 68.84, 69.0, 71.9, 72.8, 85.5, 88.53, 88.5, 112.4, 112.5, 117.9, 118.3, 127.9, 128.0, 128.1, 128.3, 128.4, 128.6, 128.7, 128.9, 129.5, 131.4, 131.42, 131.8, 131.9, 132.0, 132.1, 132.2, 132.5, 132.6, 132.7, 146.8, 152.1, 186.3 (d, *C*=O, $^3J_{CP}$ = 8.9 Hz). $^{31}P\{^1H\}$ NMR ($CDCl_3$, 400 MHz): δ 54.1 (major diastereomer). MS (m / z) = 554.93.

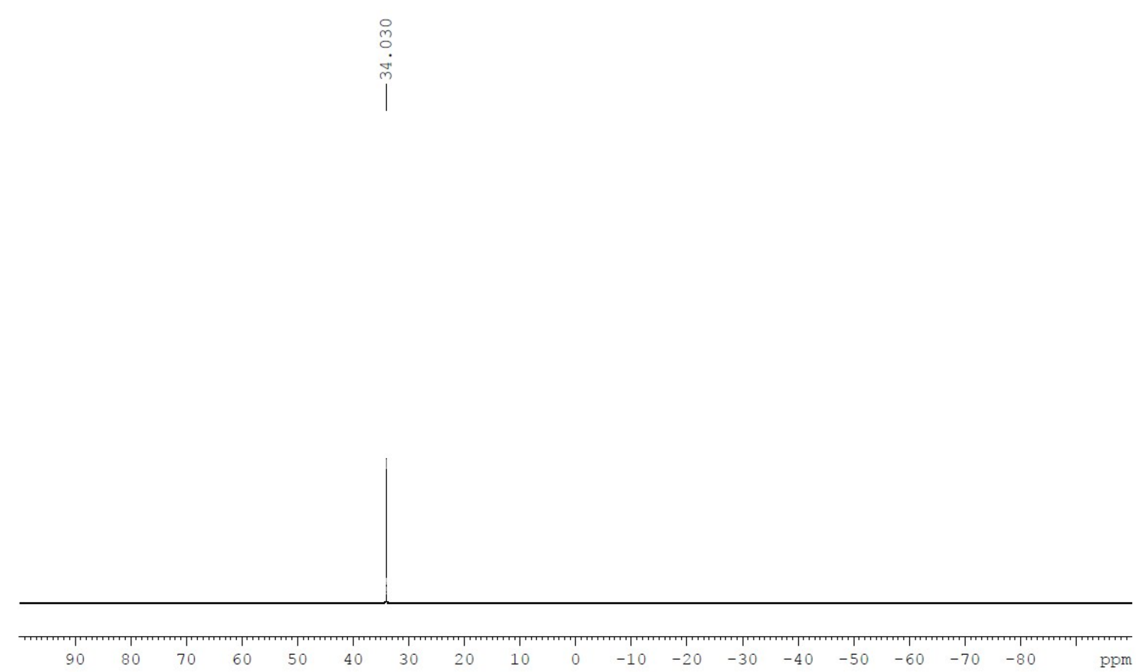
DS4: Similar procedure to DS1; yellow oil; yield: 50%. ^1H NMR ($CDCl_3$, 500 MHz): δ 1.19 (m, 1H, -CH_2OH), 3.50 - 3.82 (m, 4H, -CH_2OH and -CH(PPh_2)CH_2), 4.00 (s, 5H, -Cp), 4.06 (m, 1H, -Cp), 4.26 (m, 1H, -Cp), 4.68 (m, 1H, -Cp), 4.87 (m, 1H, -C*H*PPh_2), 7.09 - 8.09 (m, 13H, -Ar). δ ^{13}C NMR ($CDCl_3$, 75 MHz): δ 14.2, 21.1, 32.7, 33.3, 42.3, 42.4, 58.8, 60.4, 67.7, 67.8, 68.4, 68.5, 68.9, 69.0, 85.5, 88.6, 127.8, 128.0, 128.3, 128.6, 128.7, 128.8, 129.7, 131.4, 131.6, 131.9, 132.0, 132.1, 132.5, 132.6, 132.7, 134.4, 143.3, 190.1. $^{31}P\{^1H\}$ NMR ($CDCl_3$, 161.6 MHz): δ 54.1 (major diastereomer), δ 52.0 (minor diastereomer). (Diastereomeric ratio 96:4). MS (m / z) = 570.97.

II. ^{1}H, $^{31}P\{^{1}H\}$, $^{19}F\{^{1}H\}$ & ^{13}C Spectra of O1-7, S1-8, G1-3, DS1-4

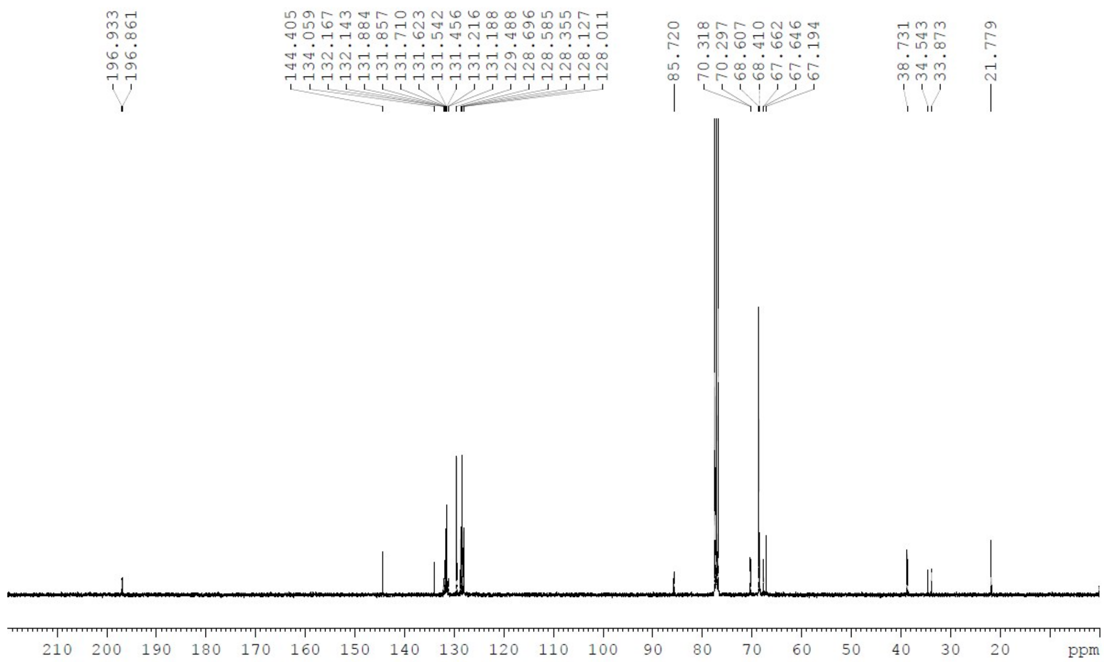
O1.
CDCl3
1H



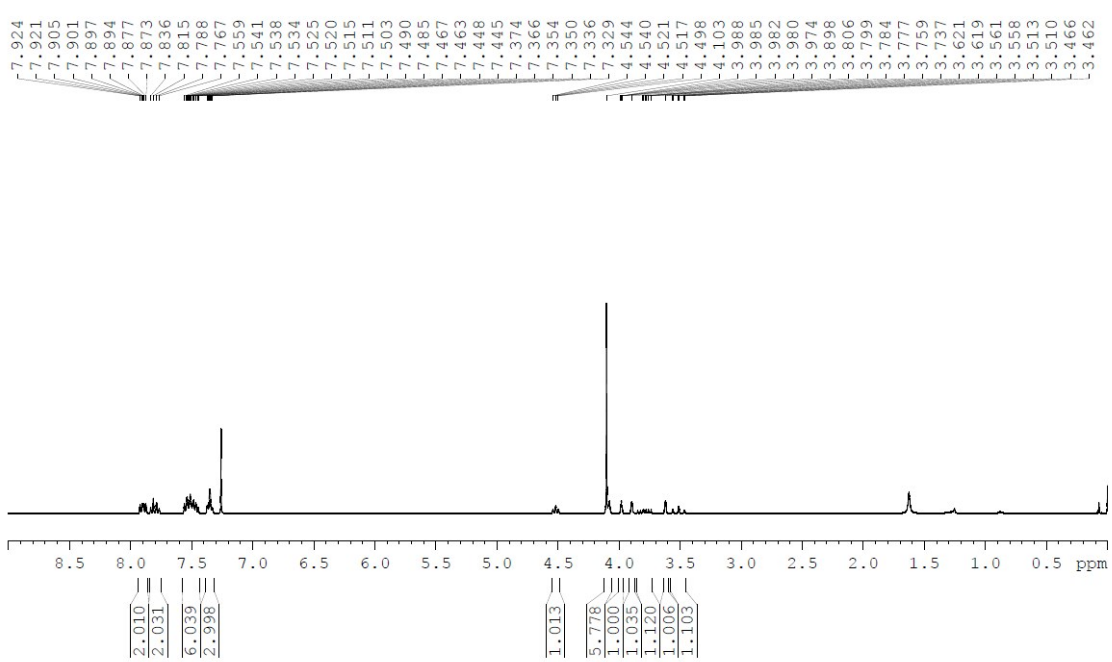
O1.
CDCl3
31P



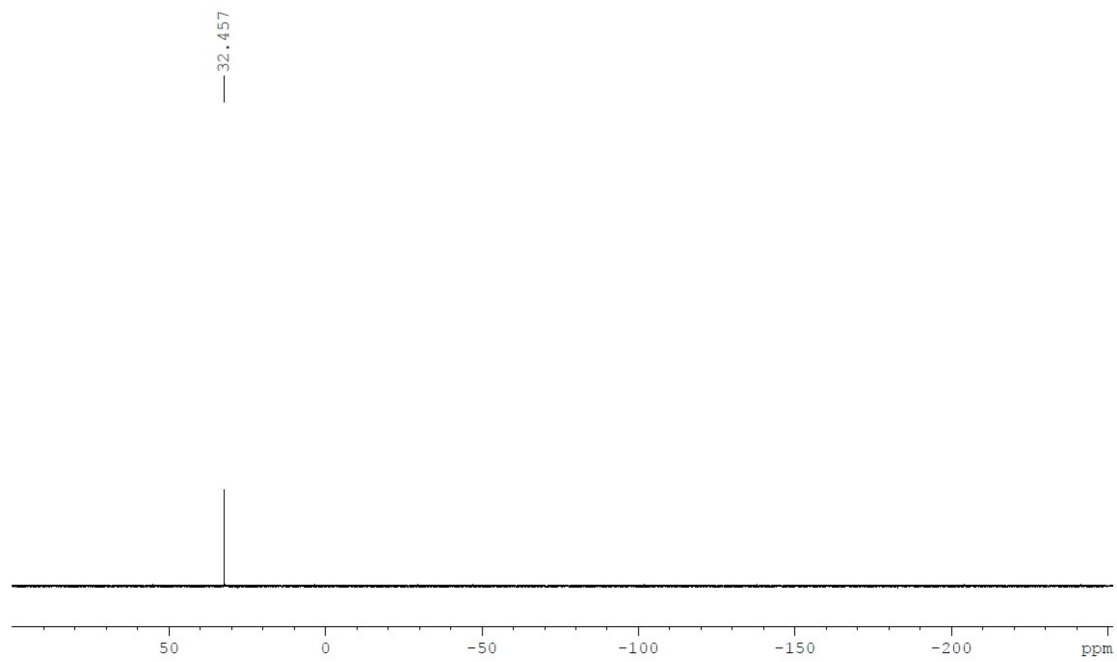
O1.
CDCl3
13C



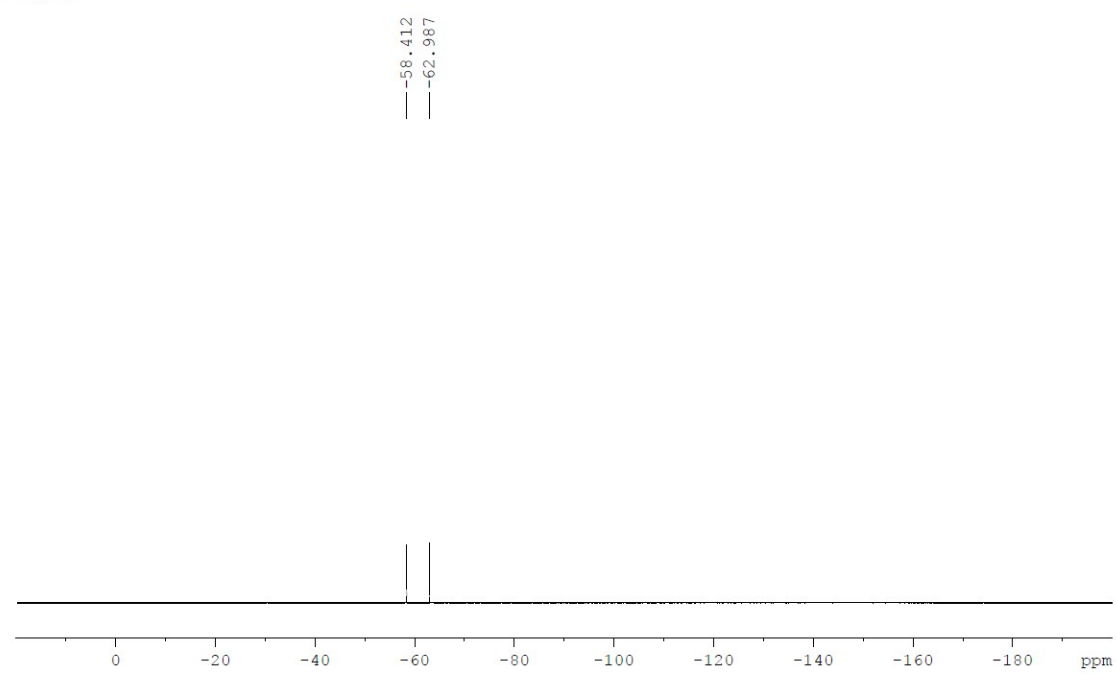
O2.
CDCl3
1H

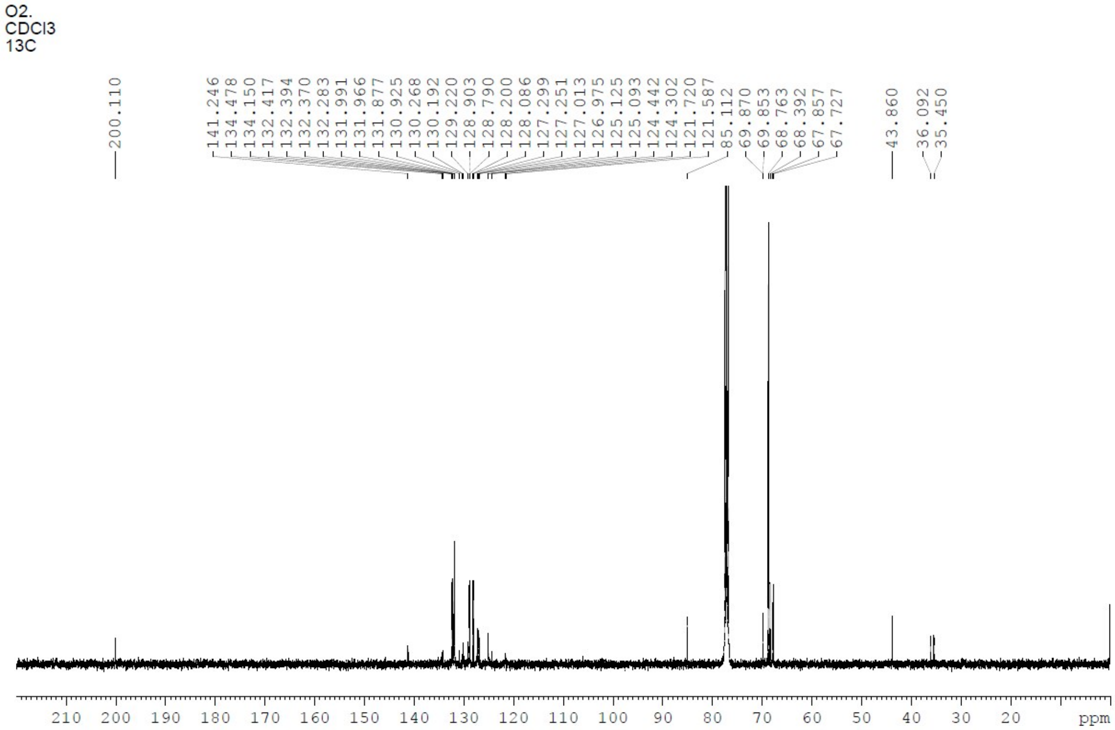


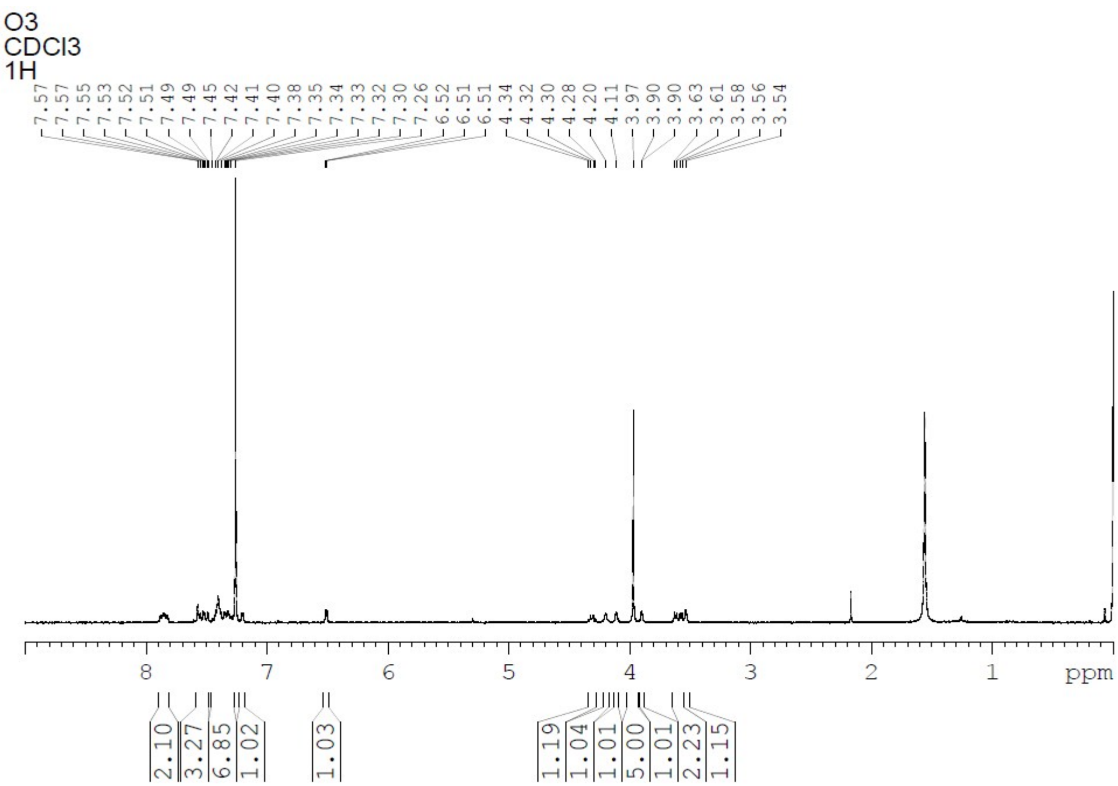
O2.
CDCl3
31P{1H}



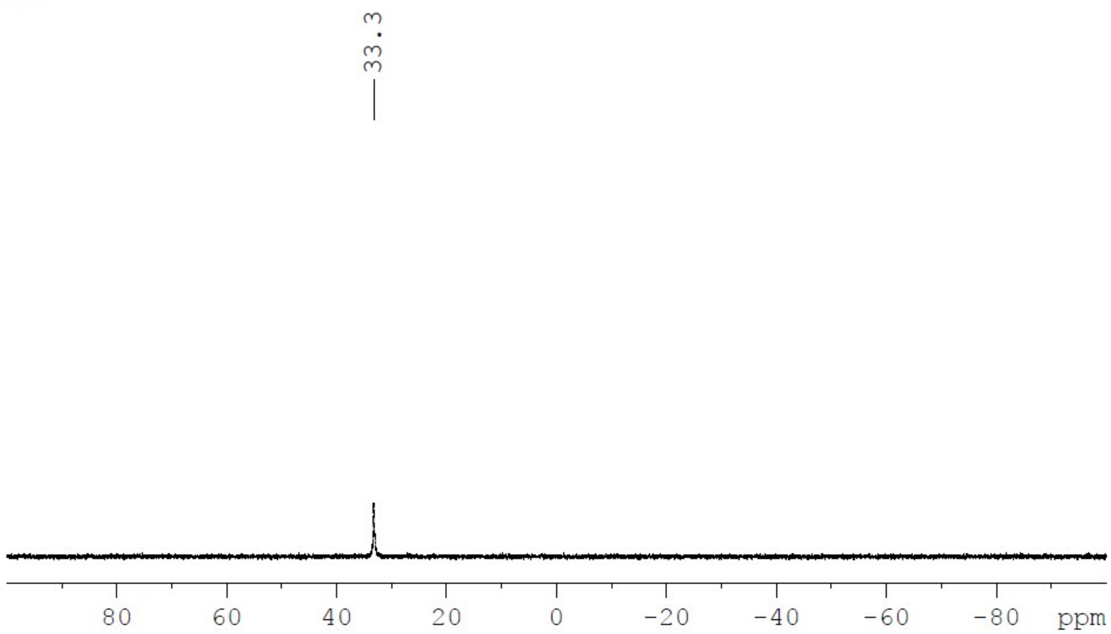
O2.
CDCl3
19F{1H}



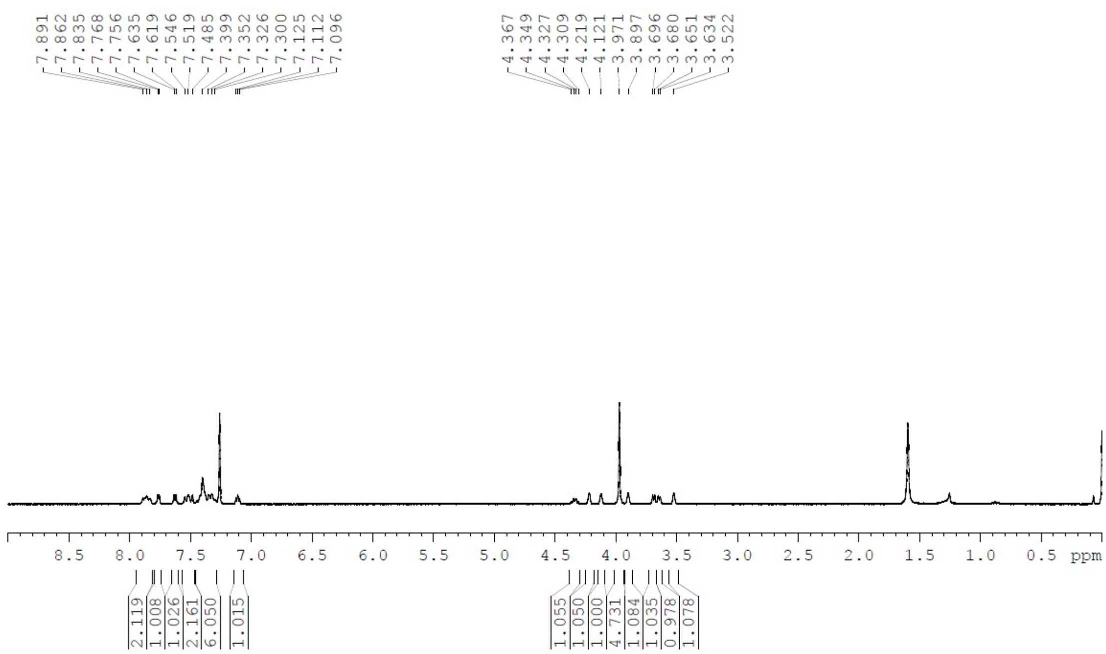

O2.
CDCl3
13C
200.110
141.246
134.478
134.150
132.417
132.394
132.370
132.283
131.991
131.966
131.877
130.925
130.268
130.192
129.220
128.903
128.790
128.200
128.086
127.299
127.251
127.013
126.975
125.125
125.093
124.442
124.302
121.720
121.587
85.112
69.870
69.853
68.763
68.392
67.857
67.727
43.860
36.092
35.450
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


O3
CDCl3
1H
7.57
7.57
7.55
7.53
7.52
7.51
7.49
7.49
7.45
7.42
7.41
7.40
7.38
7.35
7.34
7.33
7.32
7.30
7.26
6.52
6.51
6.51
4.34
4.32
4.30
4.28
4.20
4.11
3.97
3.90
3.90
3.63
3.61
3.58
3.56
3.54
8 7 6 5 4 3 2 1 ppm
2.10
3.27
6.85
1.02
1.03
1.19
1.04
1.01
5.00
1.01
2.23
1.15

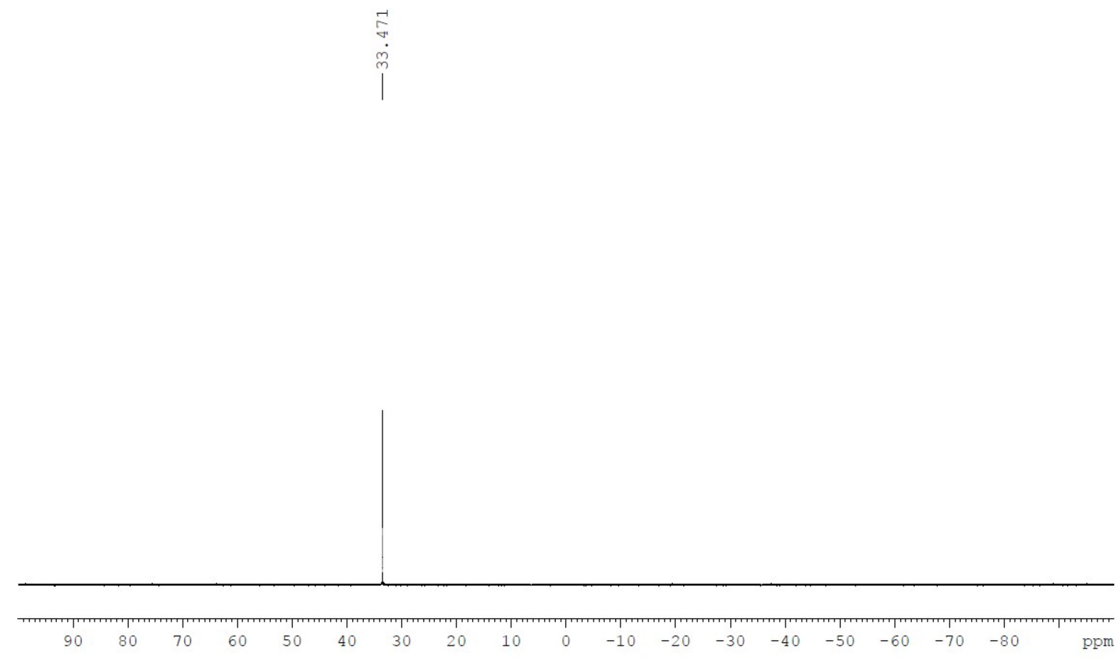
O3
CDCl3
31P



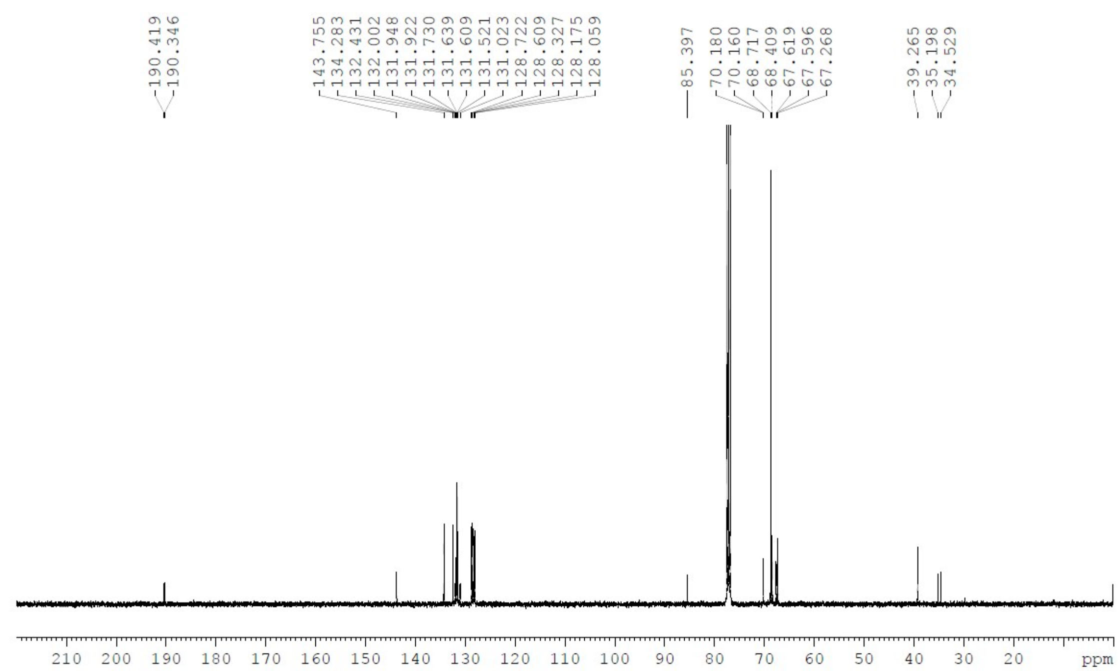
O4.
CDCl3
1H



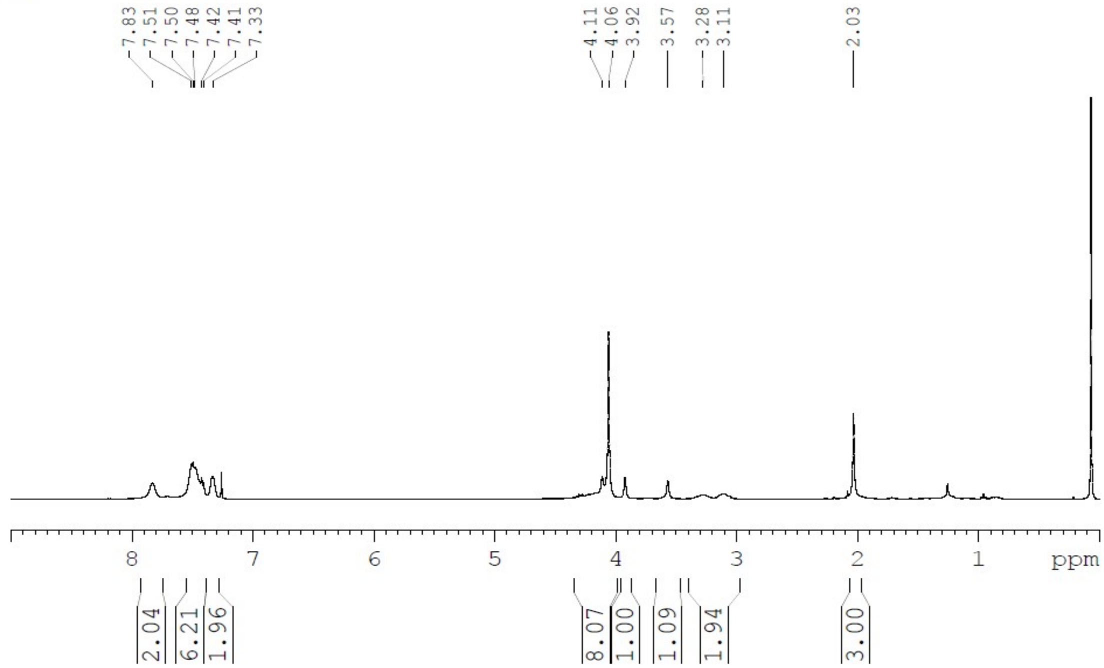
O4.
CDCl3
31P{1H}



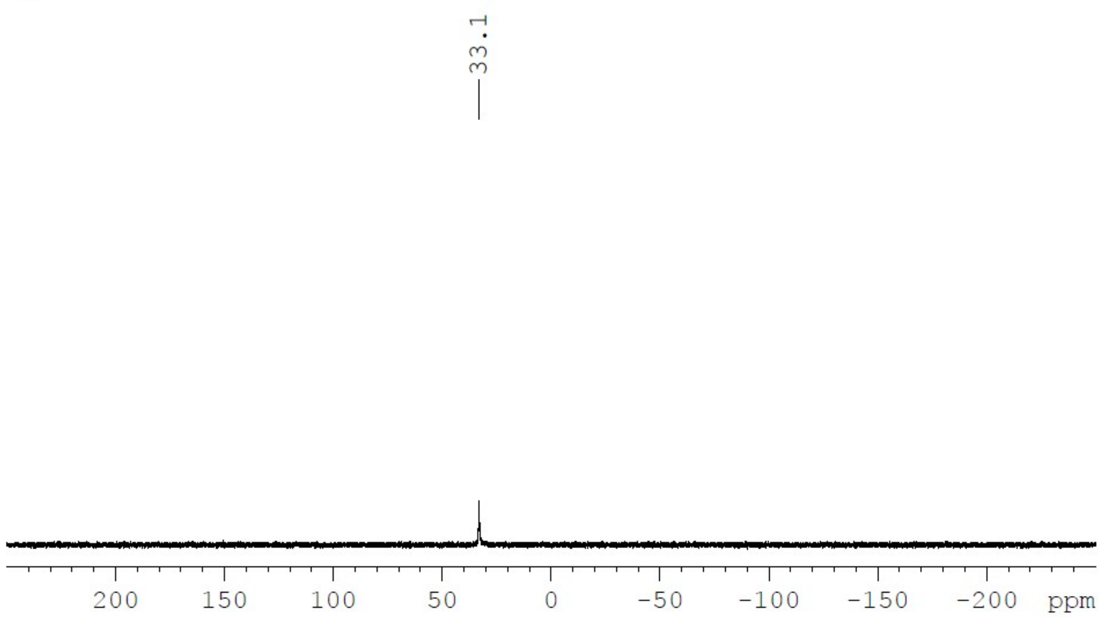
O4.
CDCl3
13C

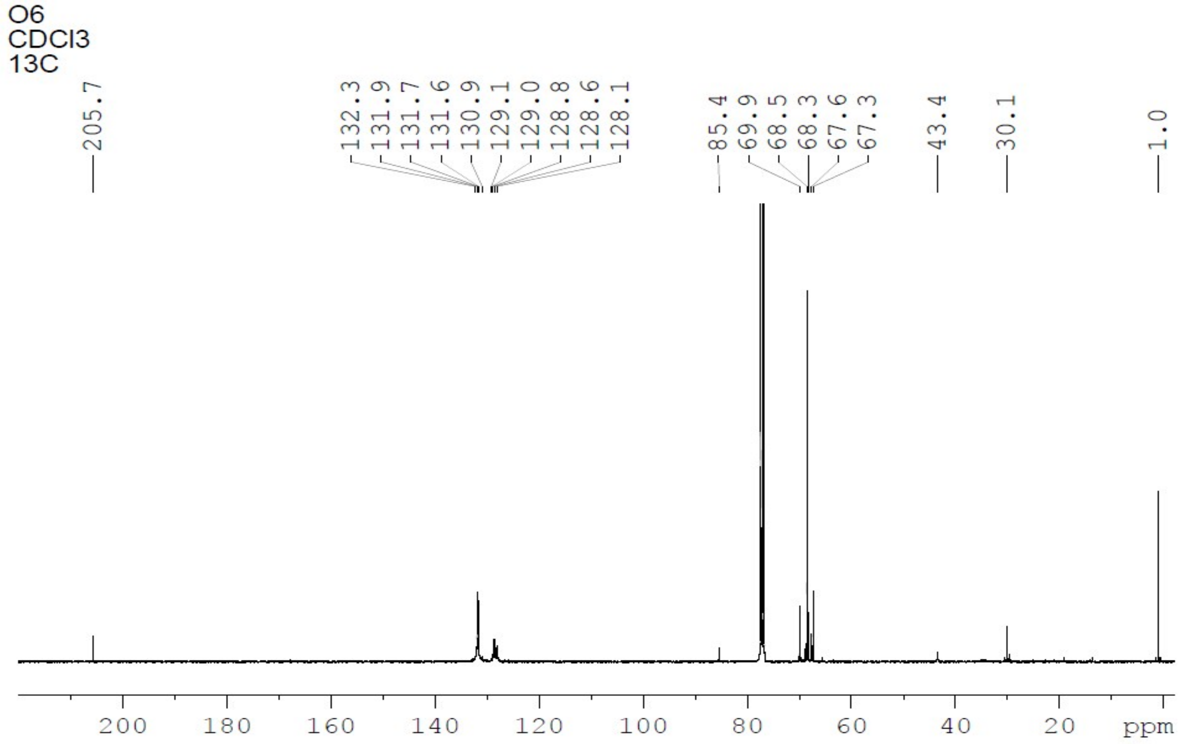


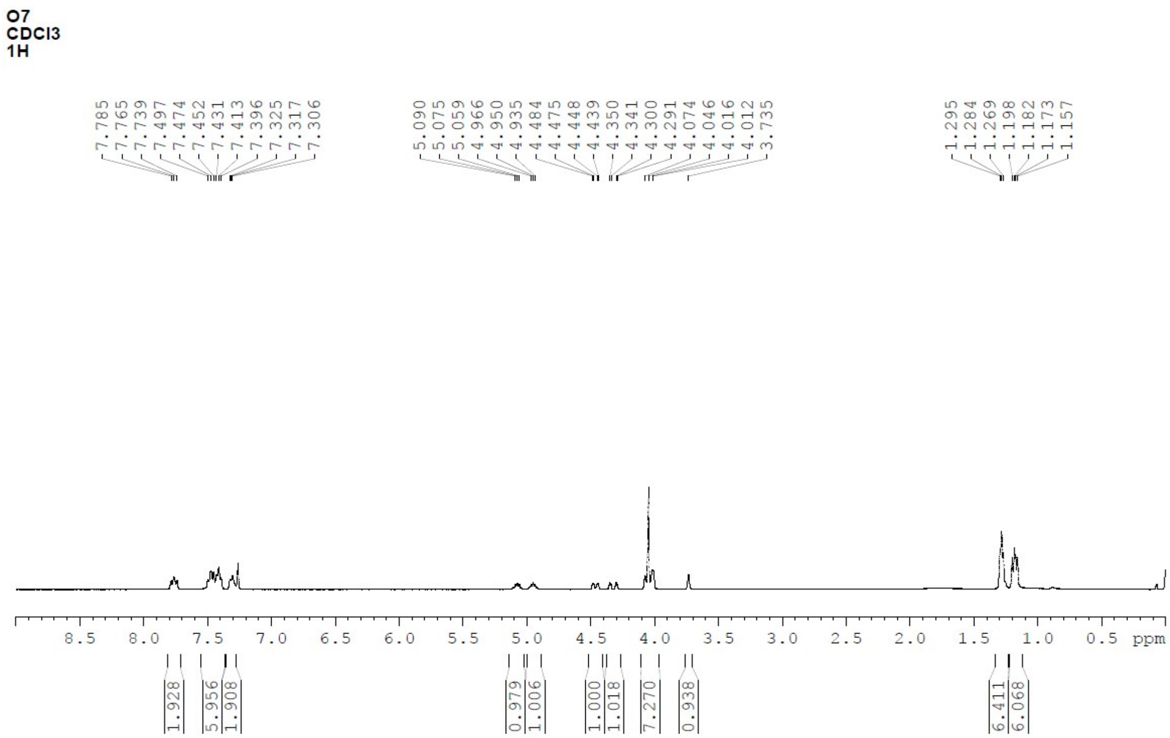
O6
CDCl3
1H



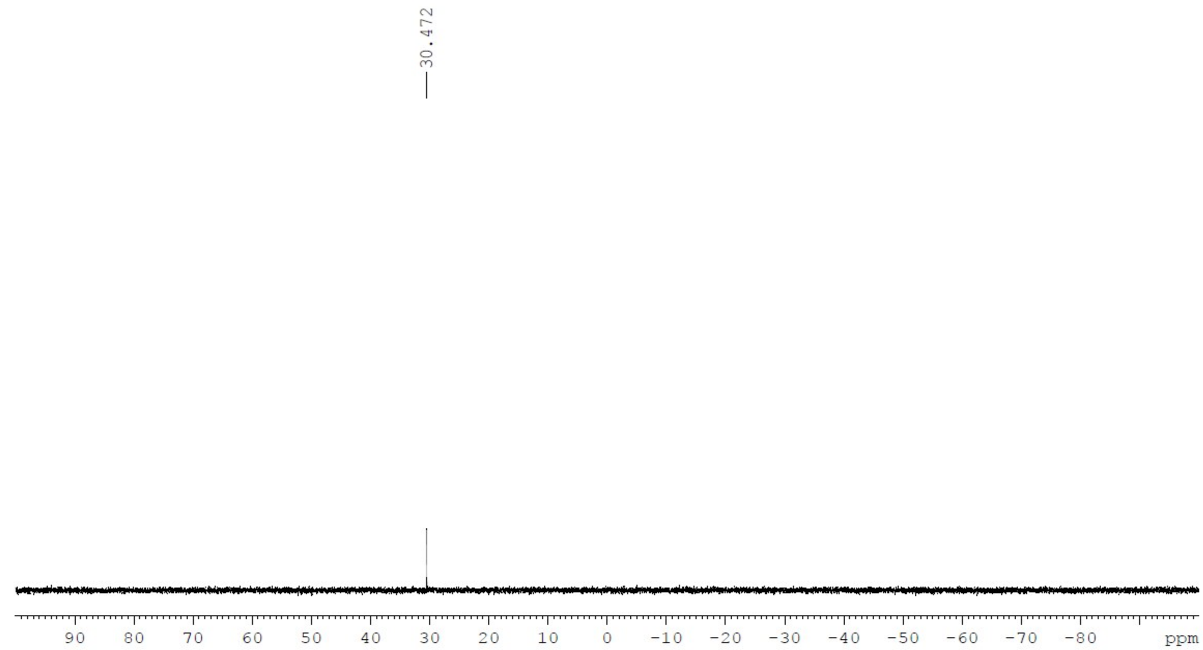
O6
CDCl3
31P



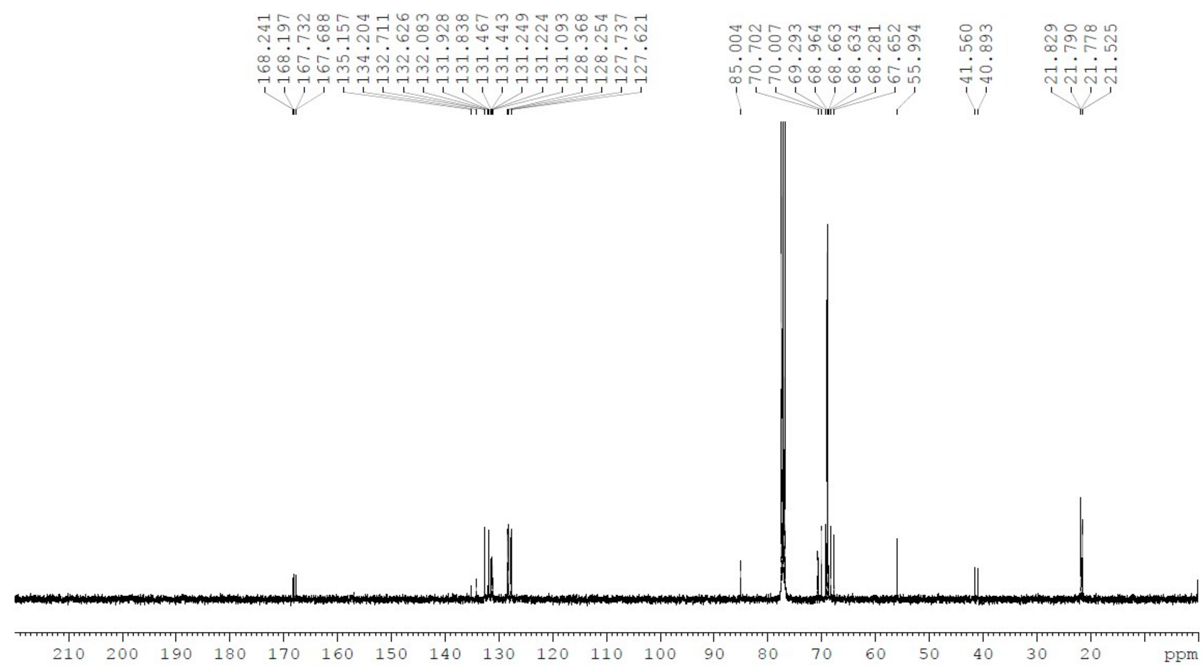

O6
CDCl3
13C
205.7
132.3
131.9
131.7
131.6
130.9
129.1
129.0
128.8
128.6
128.1
85.4
69.9
68.5
68.3
67.6
67.3
43.4
30.1
1.0
200
180
160
140
120
100
80
60
40
20
ppm


O7
CDCl3
1H
7.785
7.765
7.739
7.497
7.474
7.452
7.431
7.413
7.396
7.325
7.317
7.306
5.090
5.075
5.059
4.966
4.950
4.935
4.484
4.475
4.448
4.439
4.350
4.341
4.300
4.291
4.074
4.046
4.016
4.012
3.735
1.295
1.284
1.269
1.198
1.182
1.173
1.157
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.928
5.956
1.908
0.979
1.006
1.000
1.018
7.270
0.938
6.411
6.068

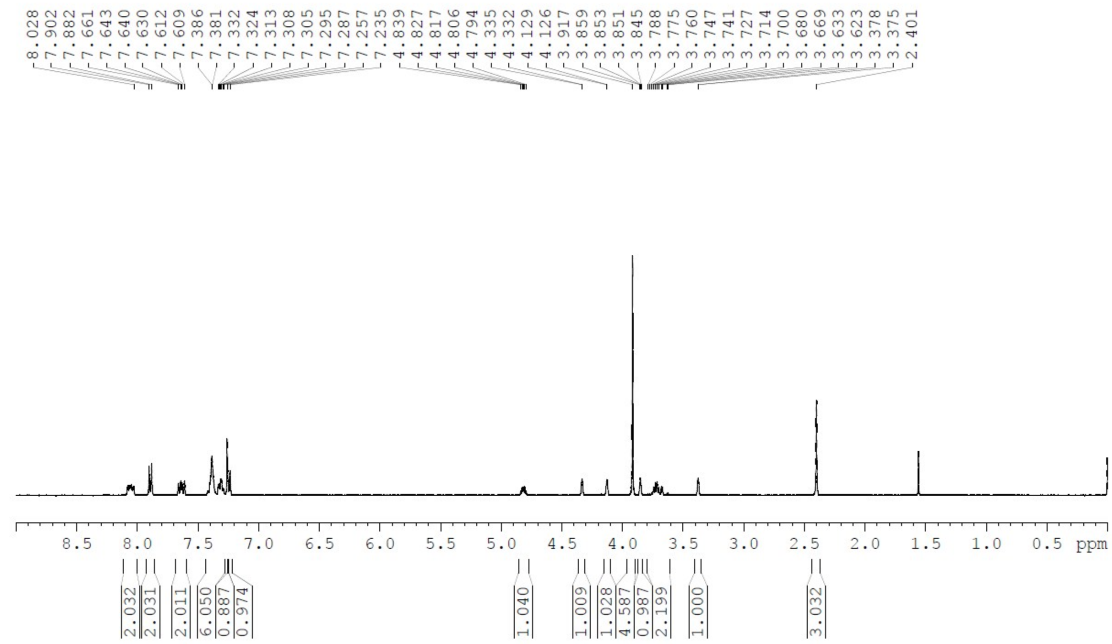
O7.
CDCl3
31P{1H}



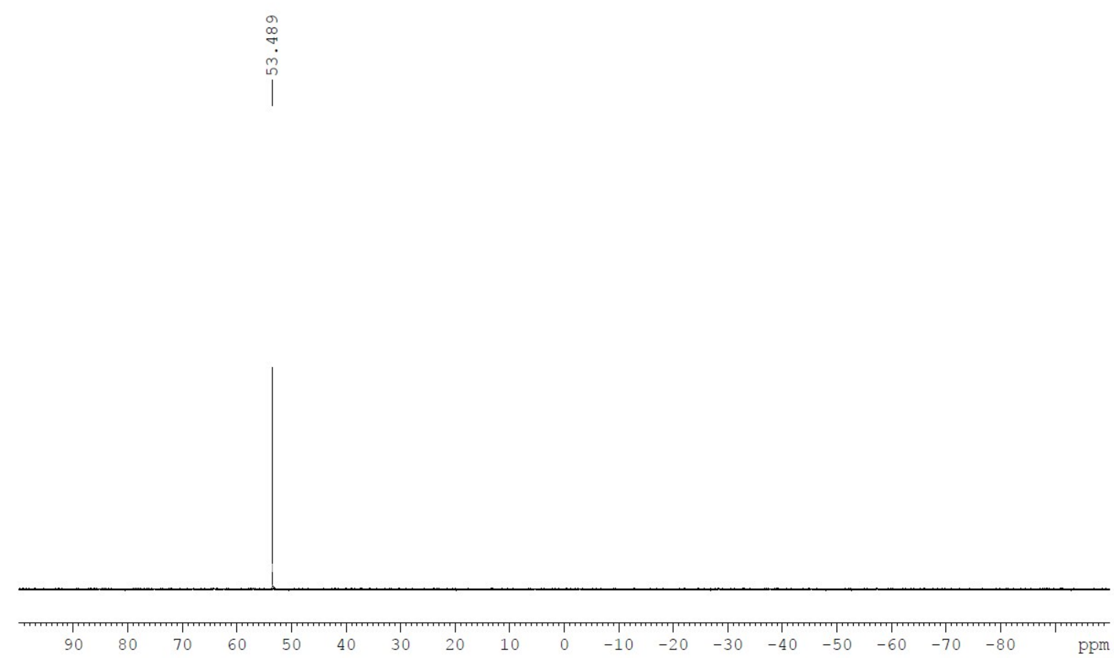
O7.
CDCl3
13C

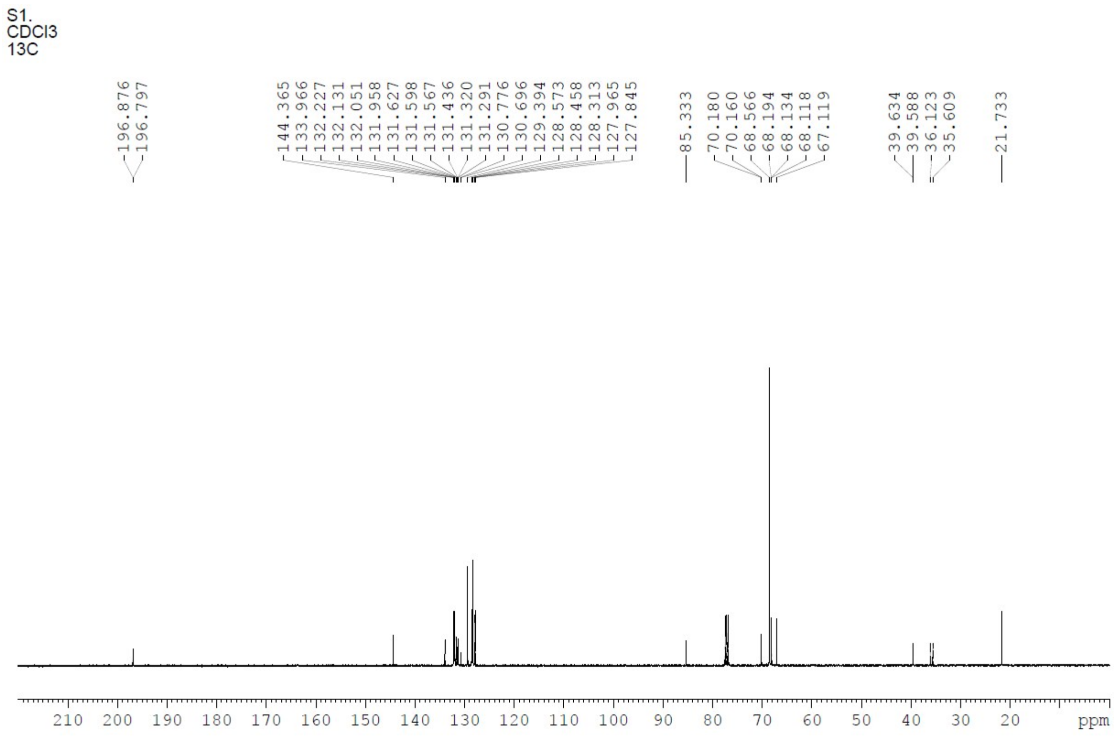


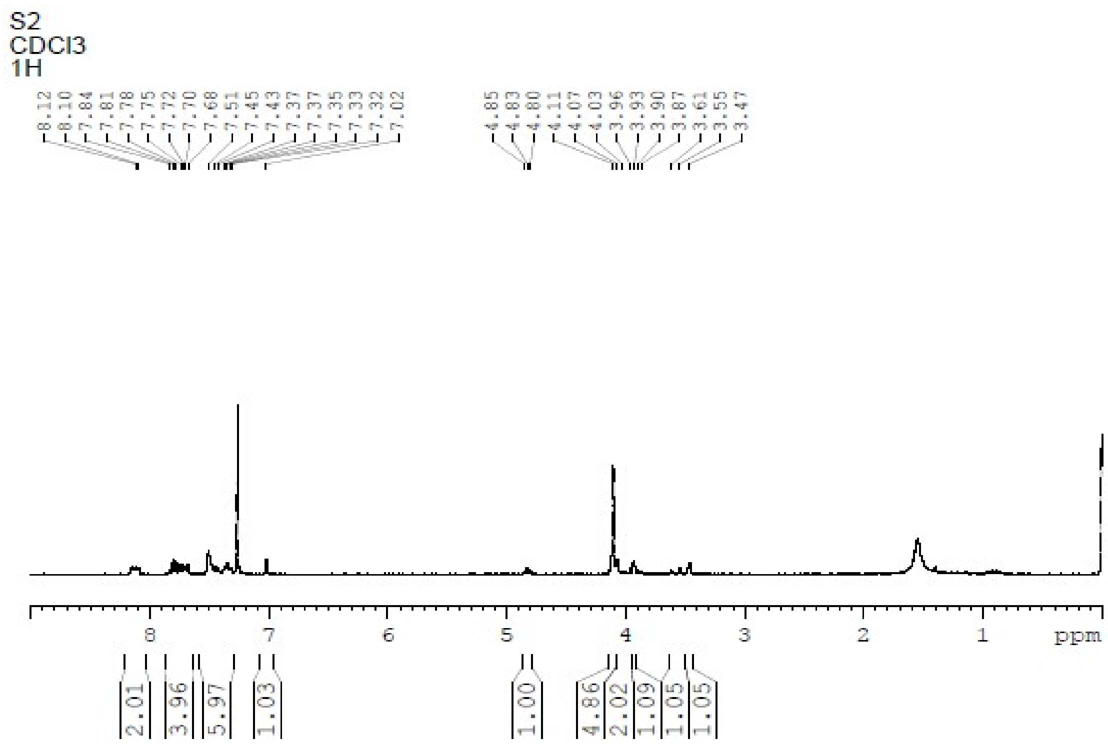
S1.
CDCl3
1H



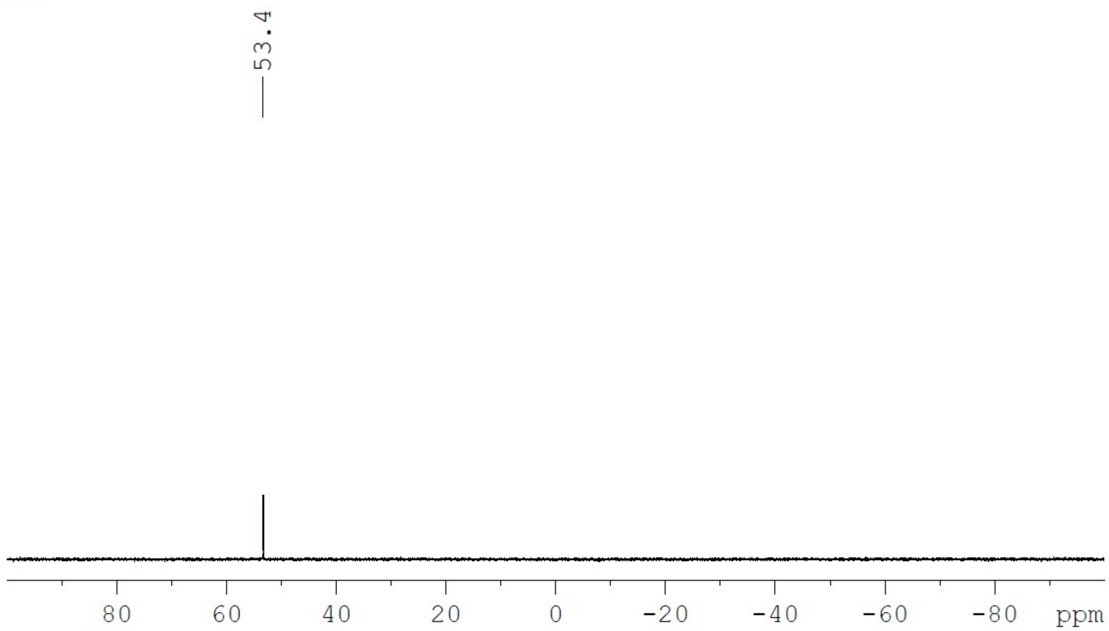
S1.
CDCl3
31P{1H}



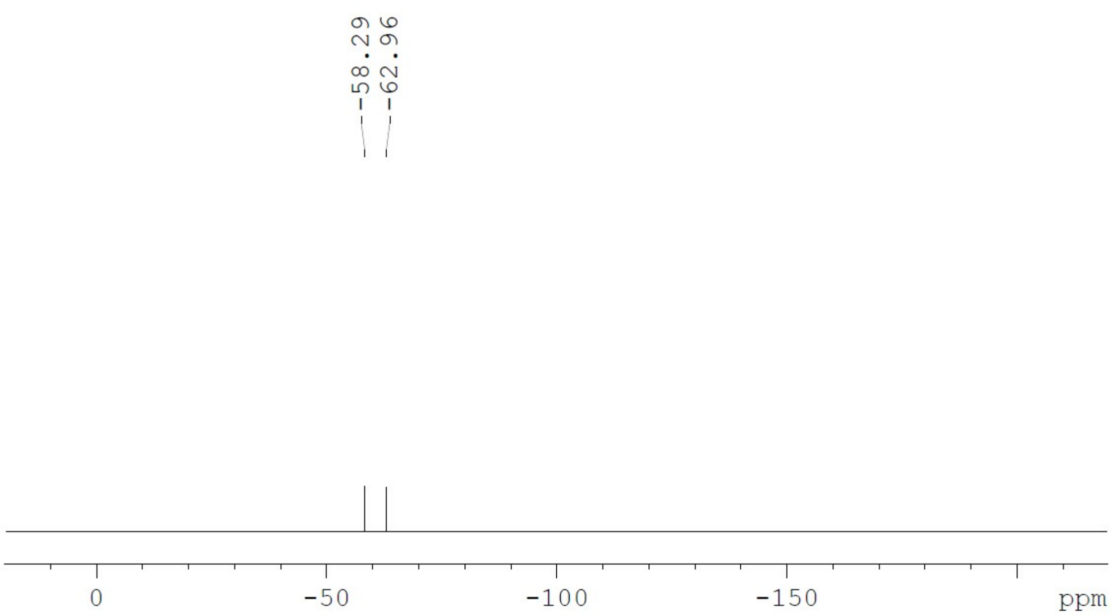

S1.
CDCl3
13C
196.876
196.797
144.365
133.966
132.227
132.131
132.051
131.958
131.627
131.598
131.567
131.436
131.320
131.291
130.776
130.696
129.394
128.573
128.458
128.313
127.965
127.845
85.333
70.180
70.160
68.566
68.194
68.134
68.118
67.119
39.634
39.588
36.123
35.609
21.733
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


S2
CDCl3
1H
8.12
8.10
7.84
7.81
7.78
7.75
7.72
7.70
7.68
7.51
7.45
7.43
7.37
7.35
7.33
7.32
7.02
4.85
4.83
4.80
4.11
4.07
4.03
3.96
3.93
3.90
3.87
3.61
3.55
3.47
8 7 6 5 4 3 2 1 ppm
2.01
3.96
5.97
1.03
1.00
4.86
2.02
1.09
1.05
1.05

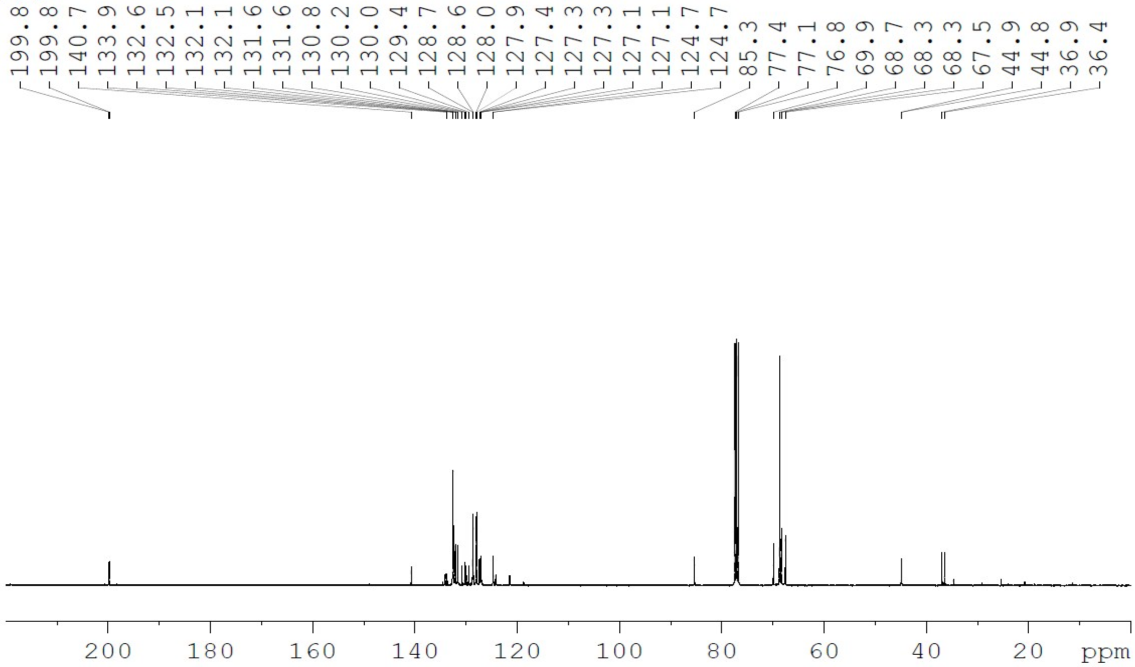
S2
CDCl3
31P



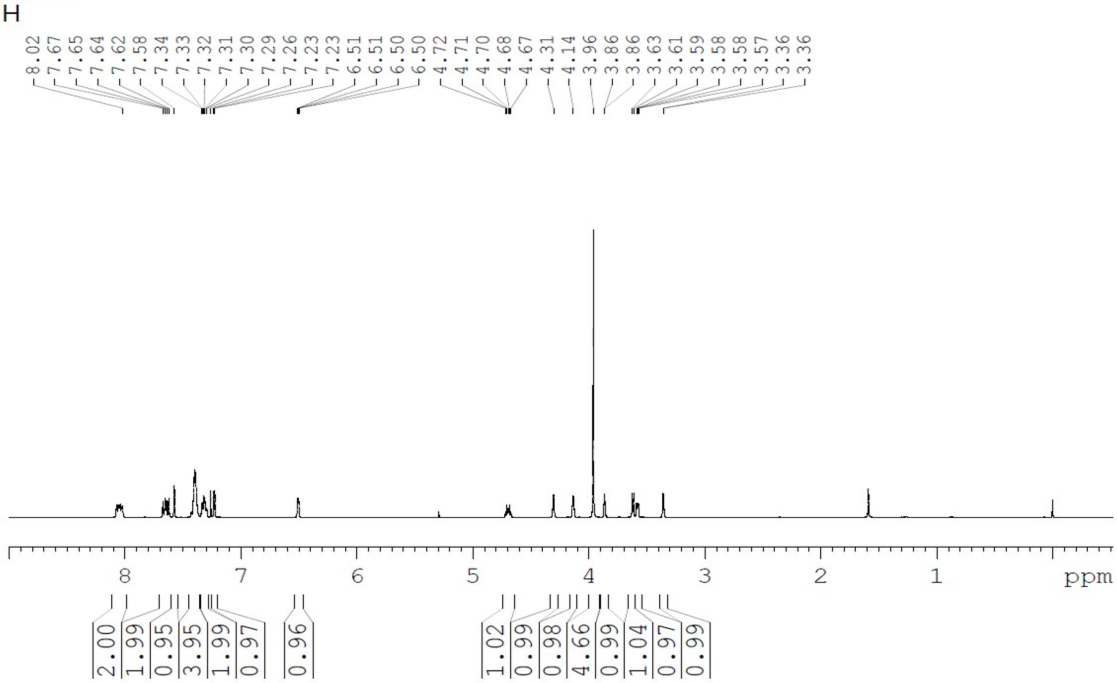
S2
CDCl3
19F



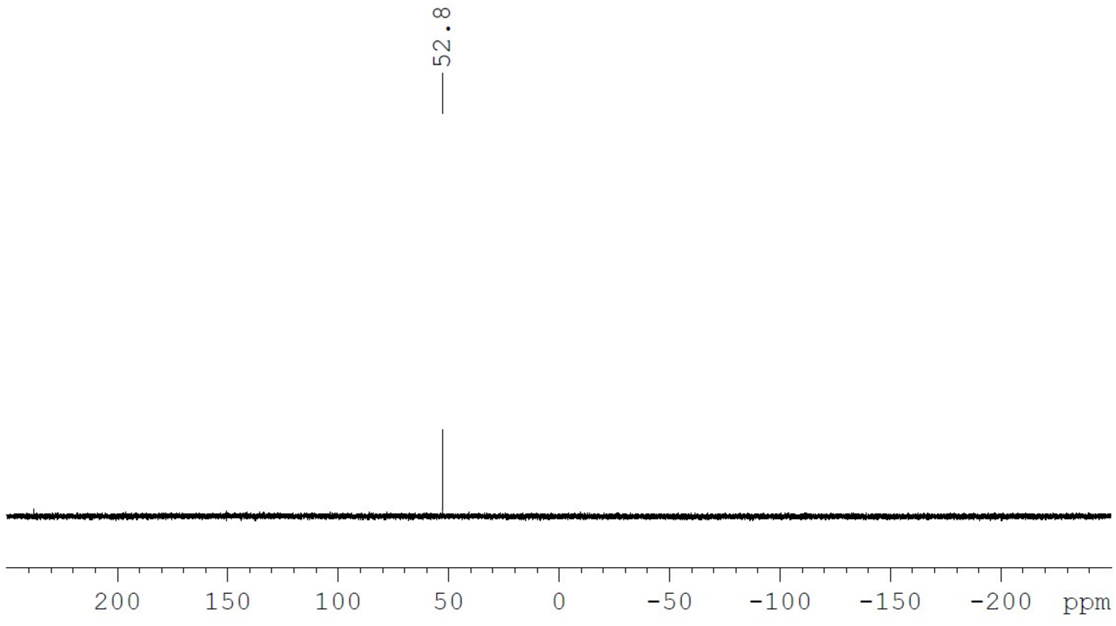
S2
CDCl3
13C



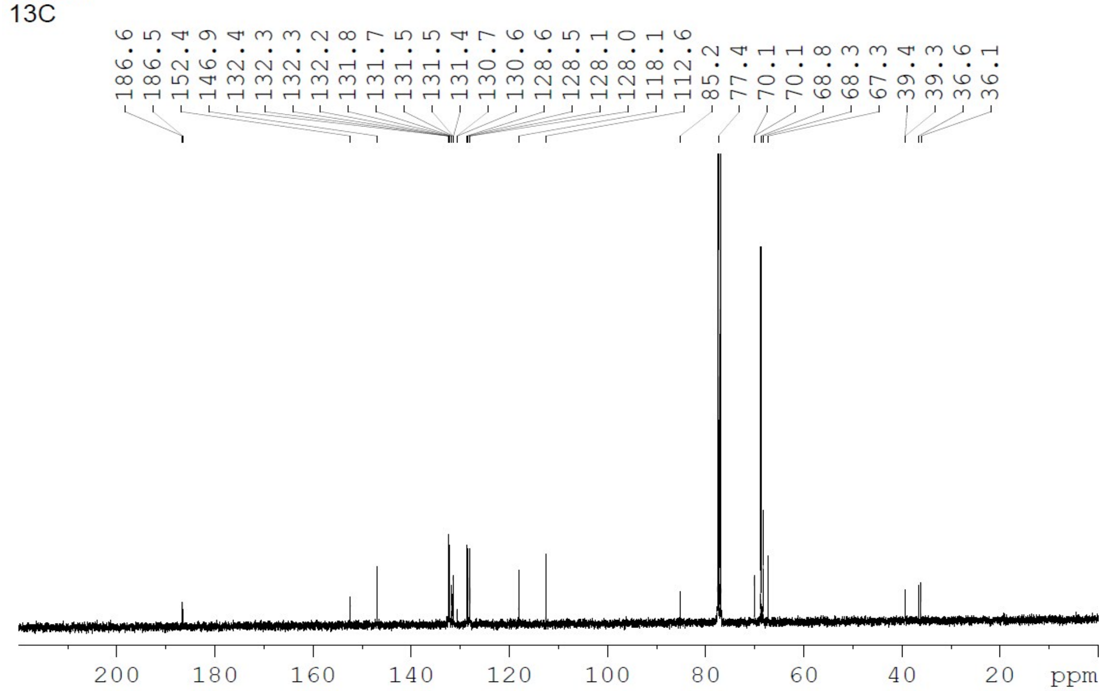
S3
CDCl3
1H



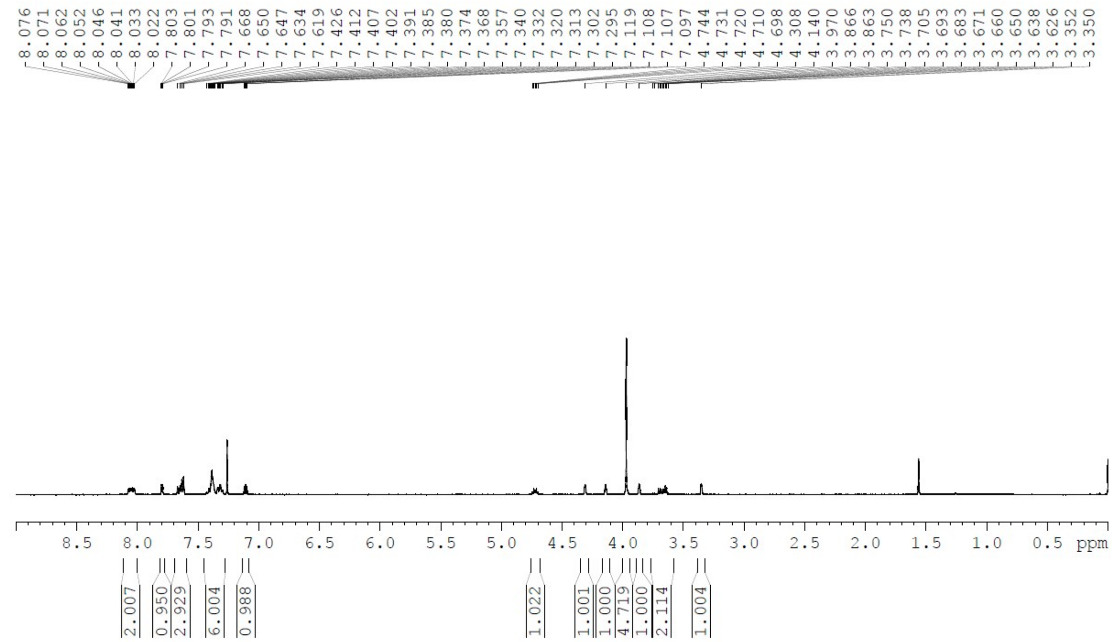
S3
CDCl3
31P



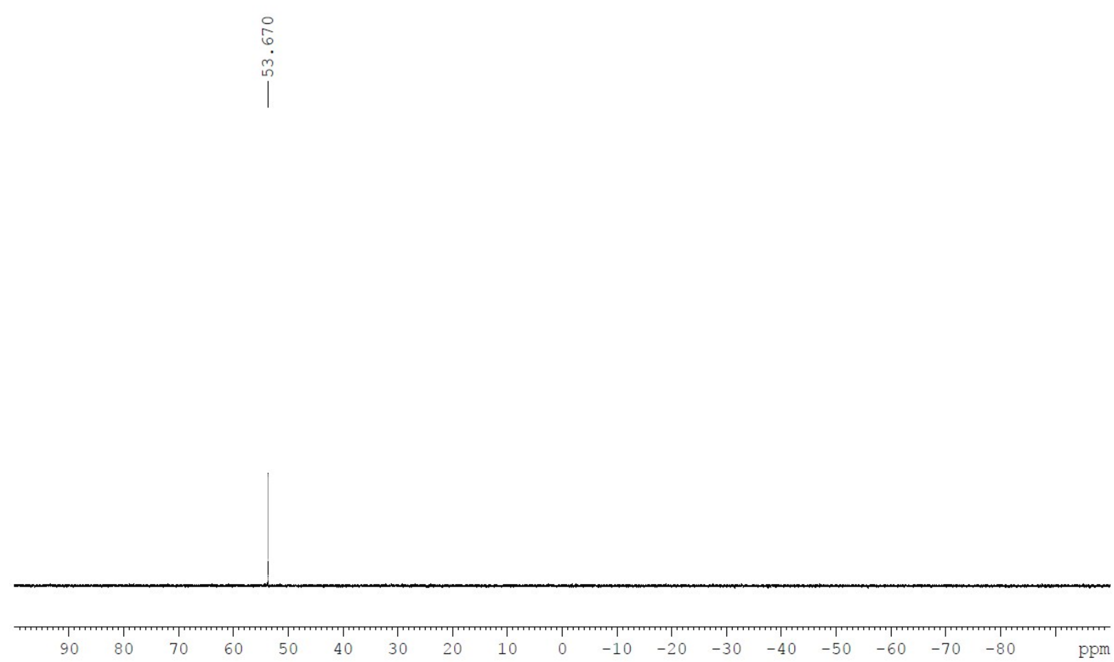
S3
CDCl3
13C



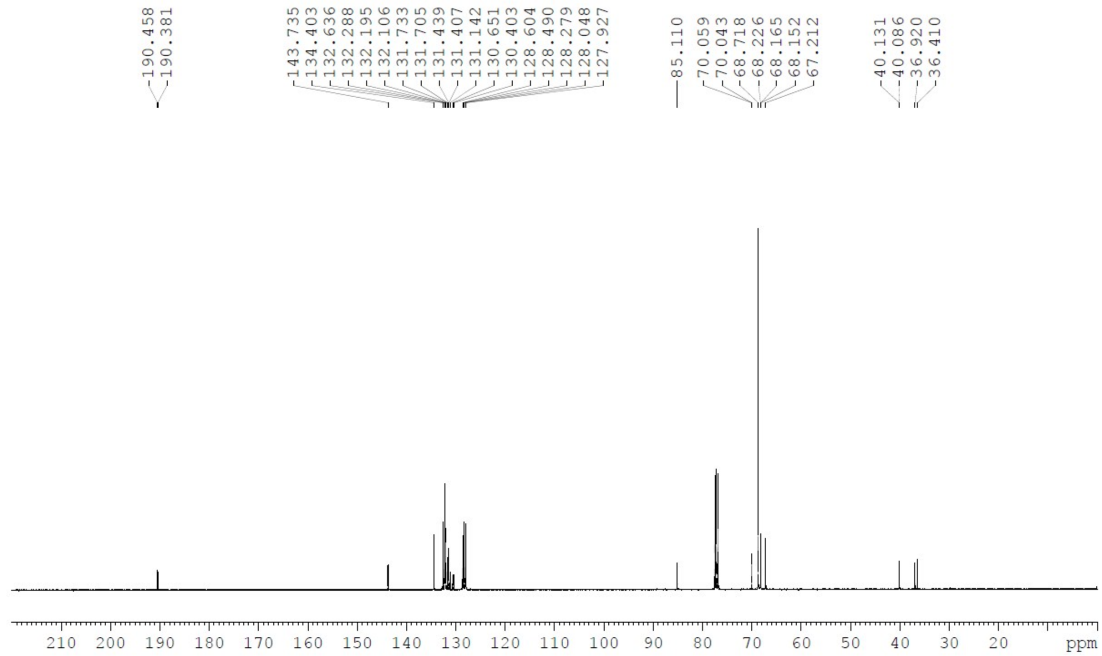
S4
CDCl3
1H



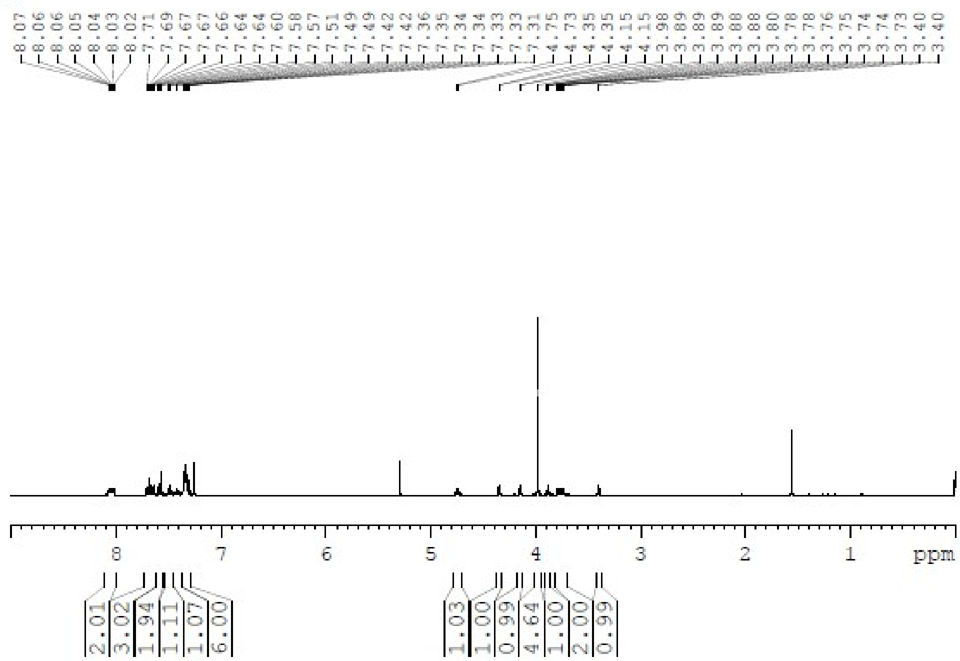
S4.
CDCl3
31P{1H}



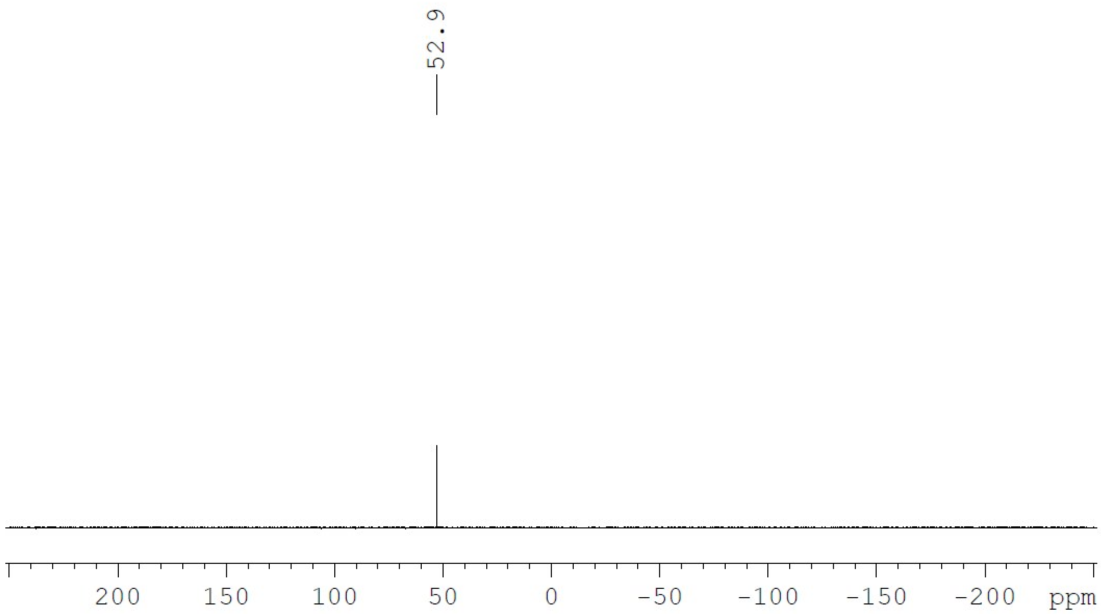
S4
CDCl3
13C



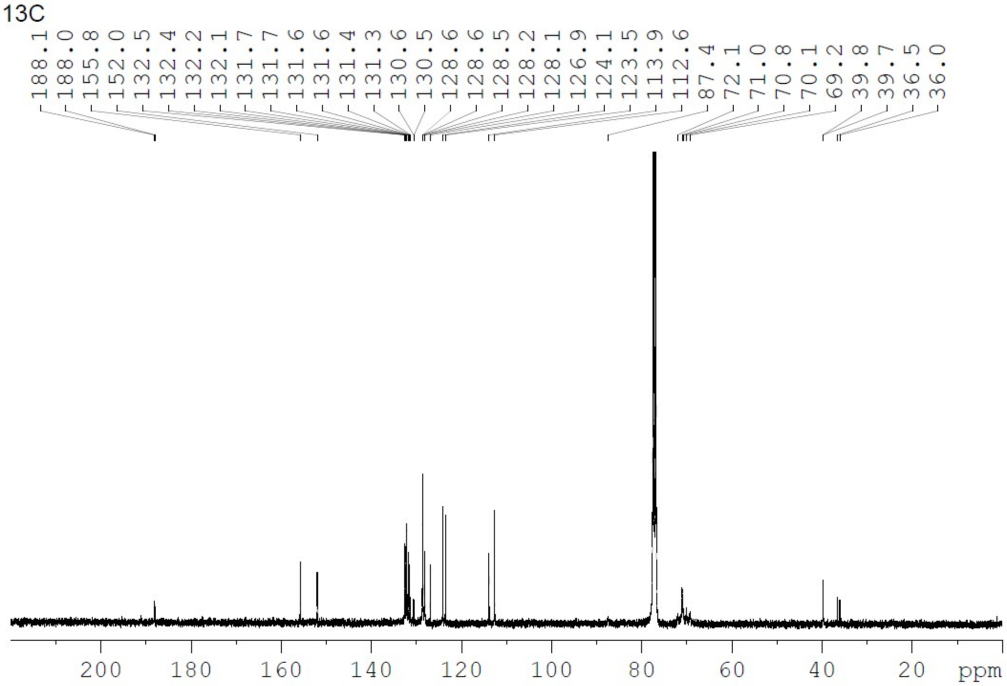
S5
CDCl3
1H

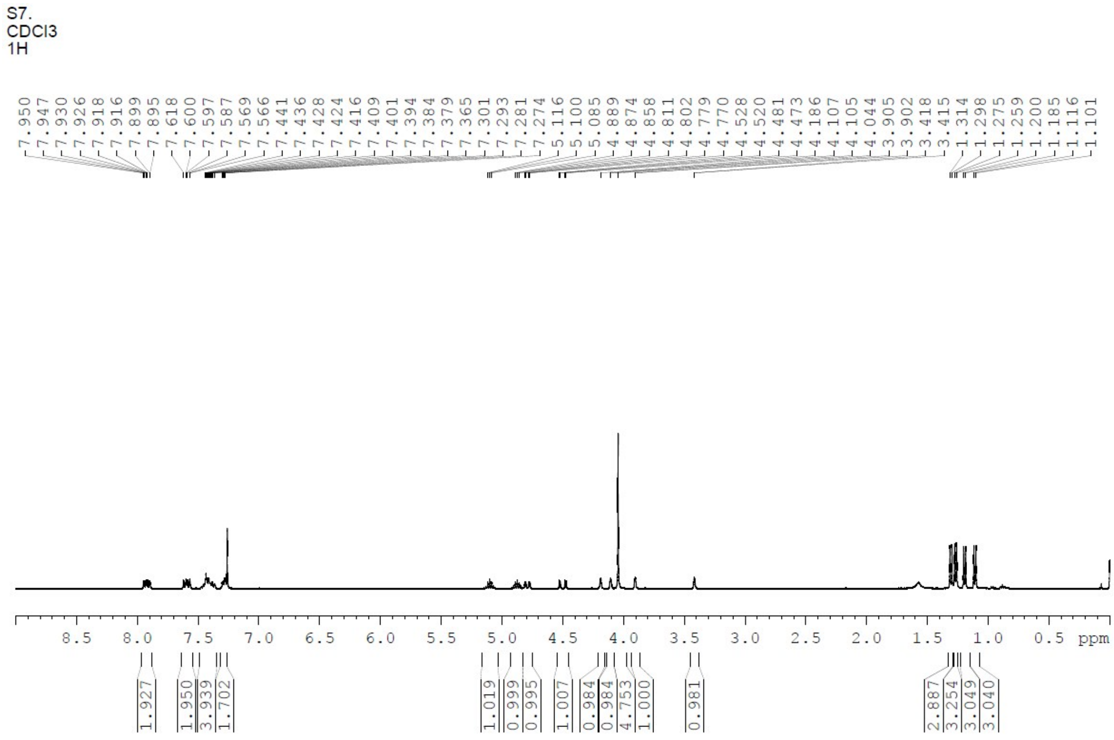


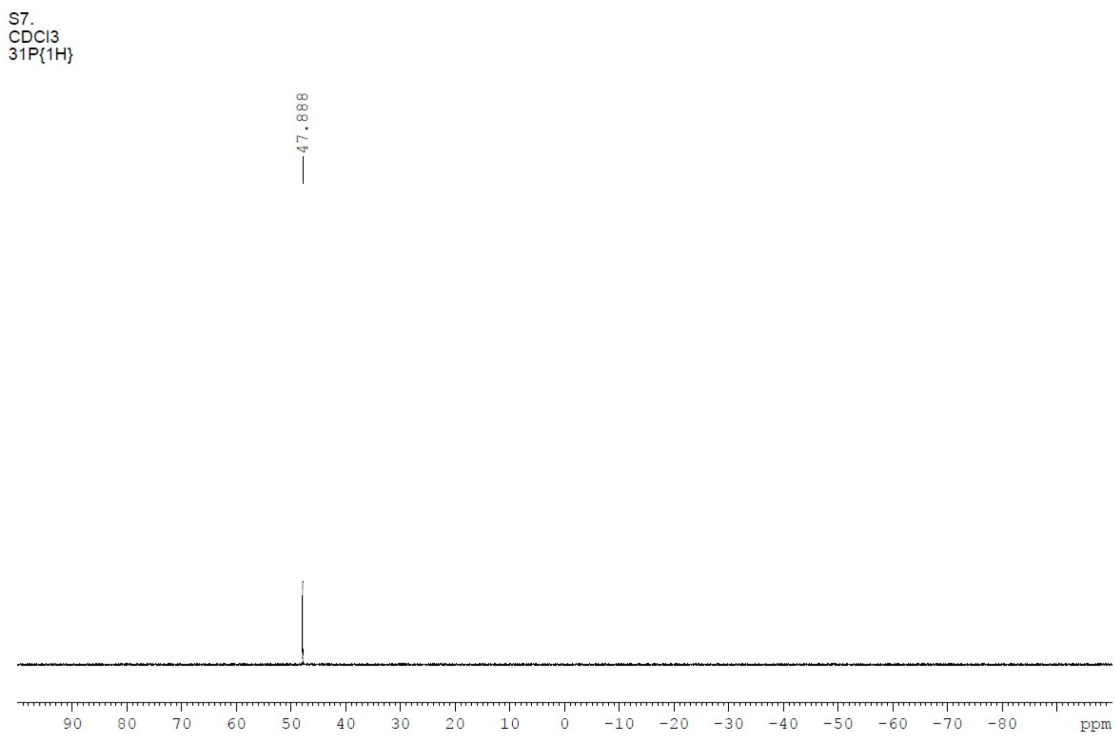
S5
31P
CDCl3

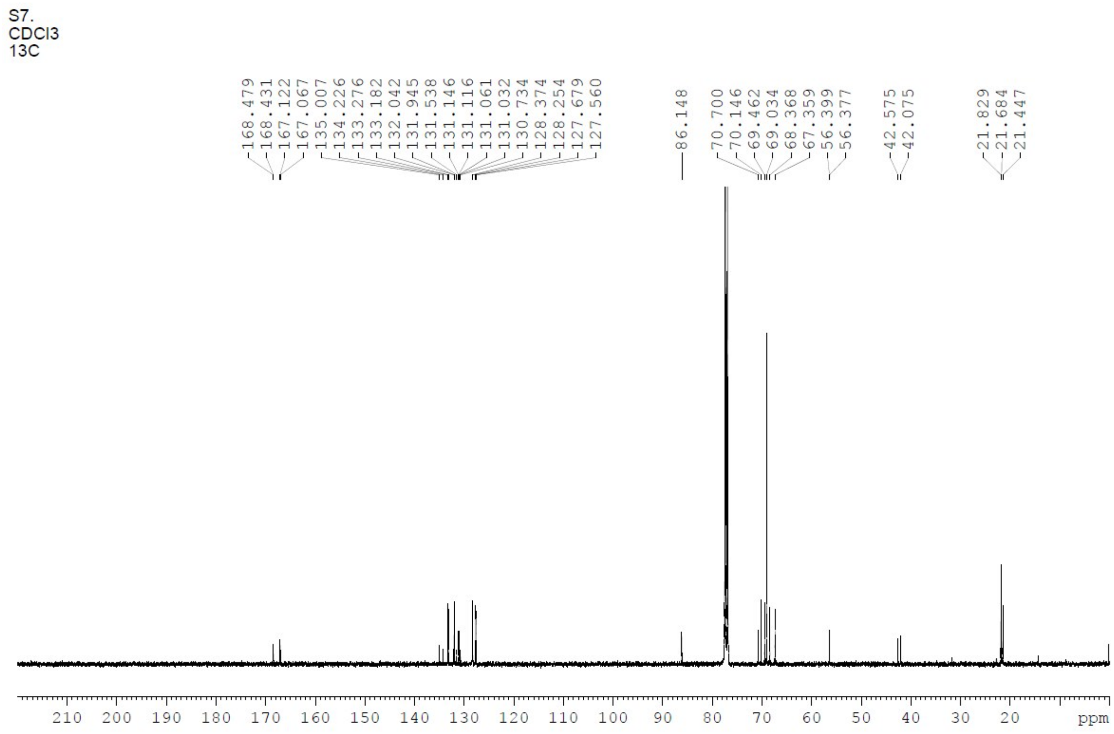


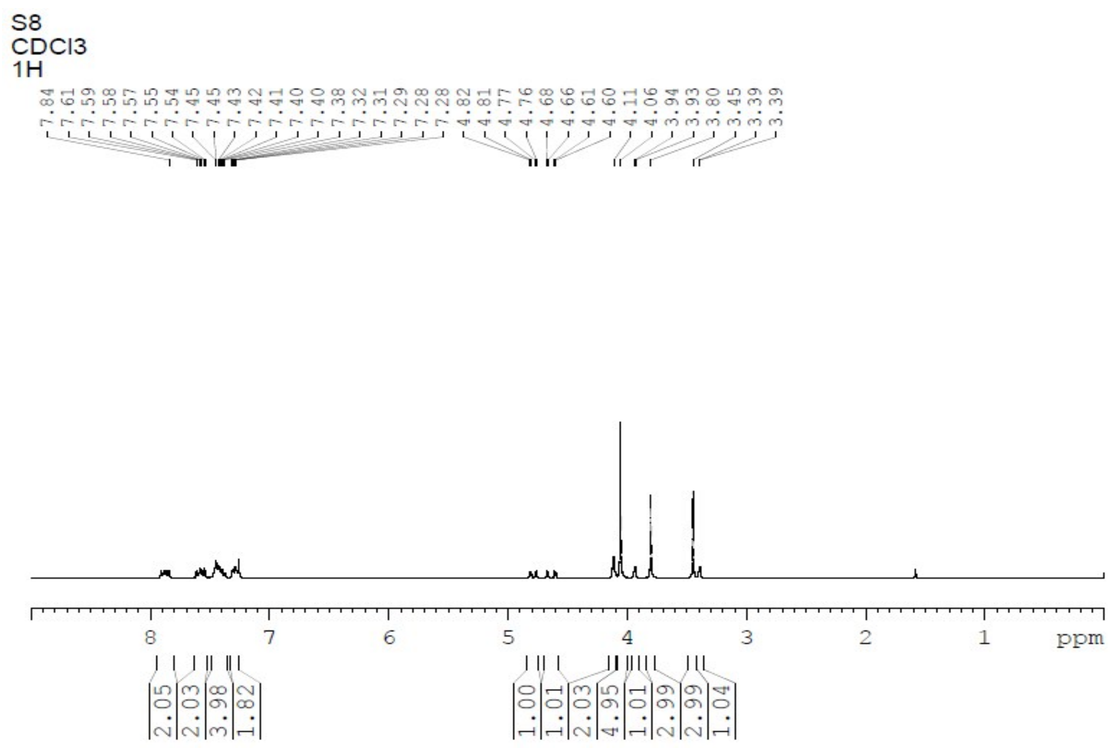
S5
CDCl3
13C

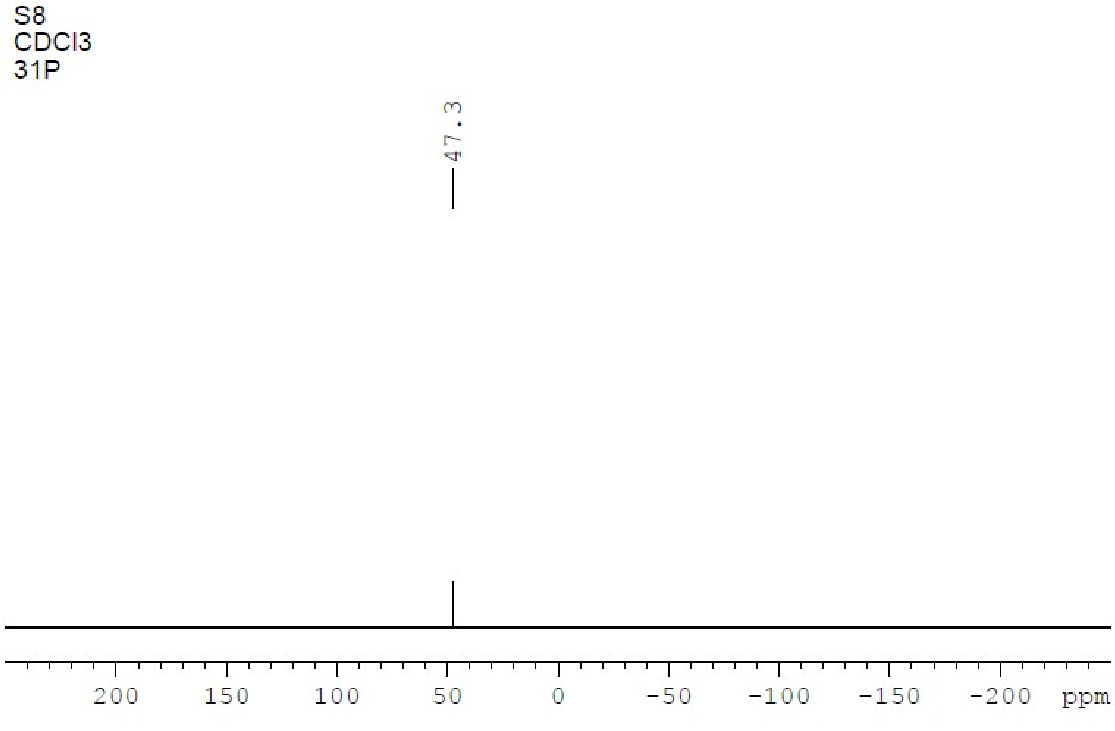


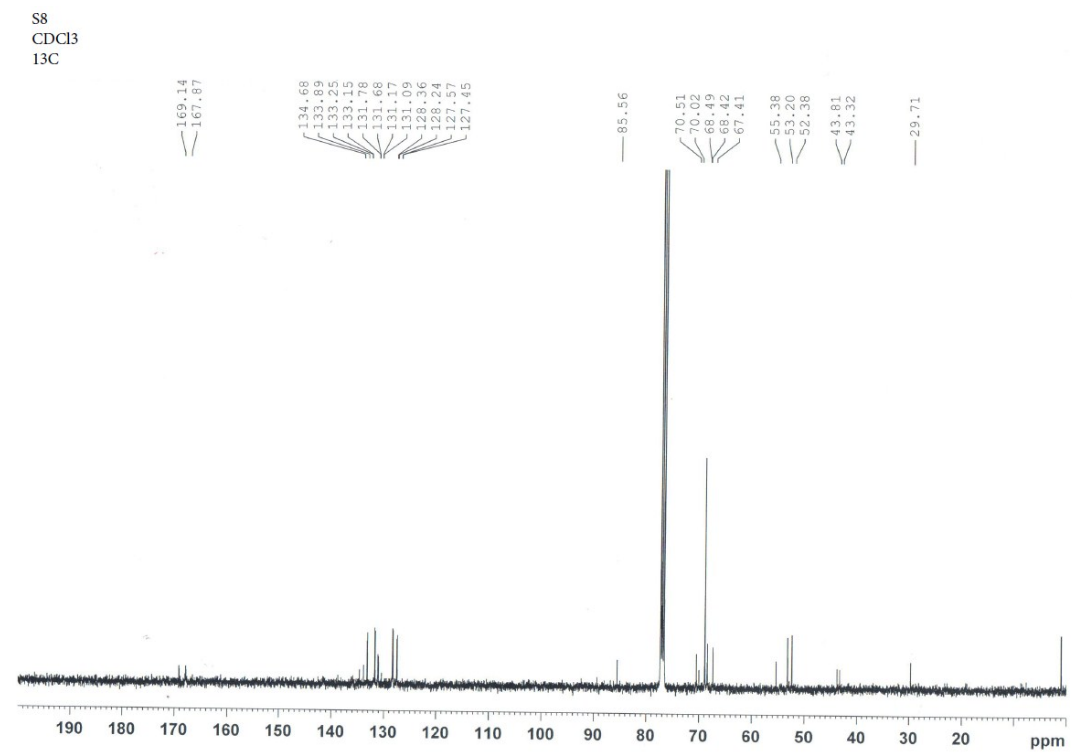

S7.
CDCl3
1H
7.950 7.947 7.930 7.926 7.918 7.916 7.899 7.895 7.618 7.600 7.597 7.587 7.569 7.566 7.441 7.436 7.428 7.424 7.416 7.409 7.401 7.394 7.384 7.379 7.365 7.301 7.293 7.281 7.274 5.116 5.100 5.085 4.889 4.874 4.858 4.811 4.802 4.779 4.770 4.528 4.520 4.481 4.473 4.186 4.107 4.105 4.044 3.905 3.902 3.418 3.415 1.314 1.298 1.275 1.259 1.200 1.185 1.116 1.101
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.927 1.950 3.939 1.702 1.019 0.999 0.995 1.007 0.984 0.984 4.753 1.000 0.981 2.887 3.254 3.049 3.040

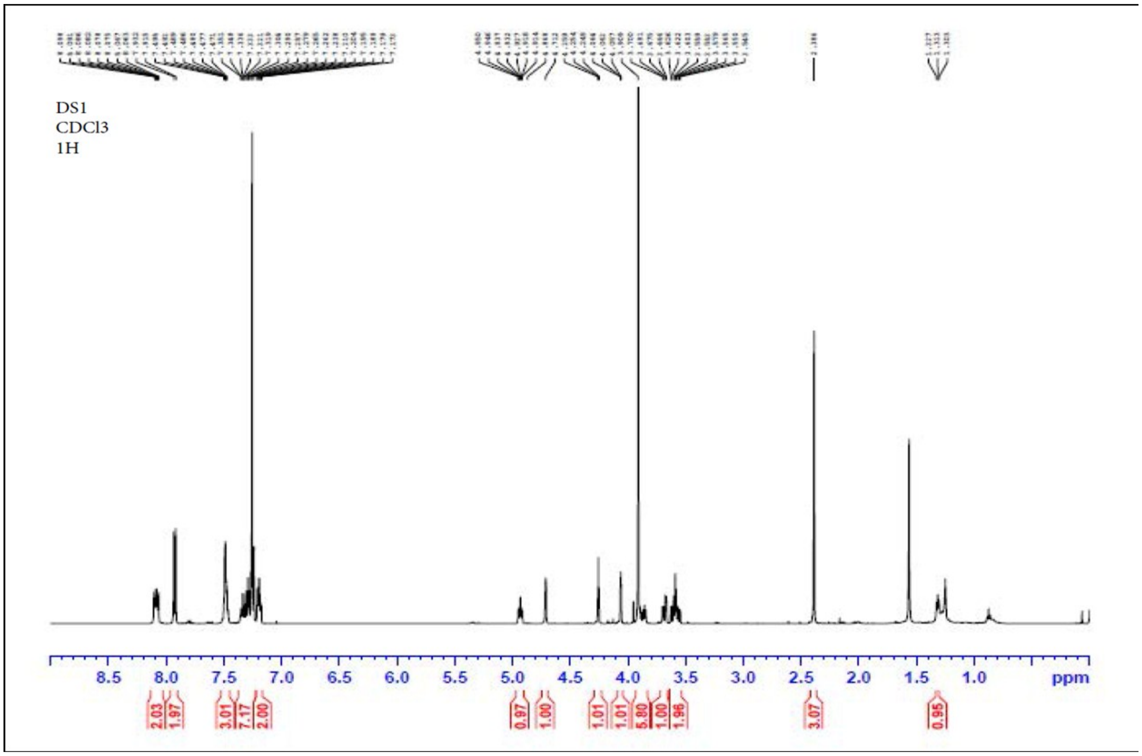

S7.
CDCl3
31P{1H}
47.888
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 ppm

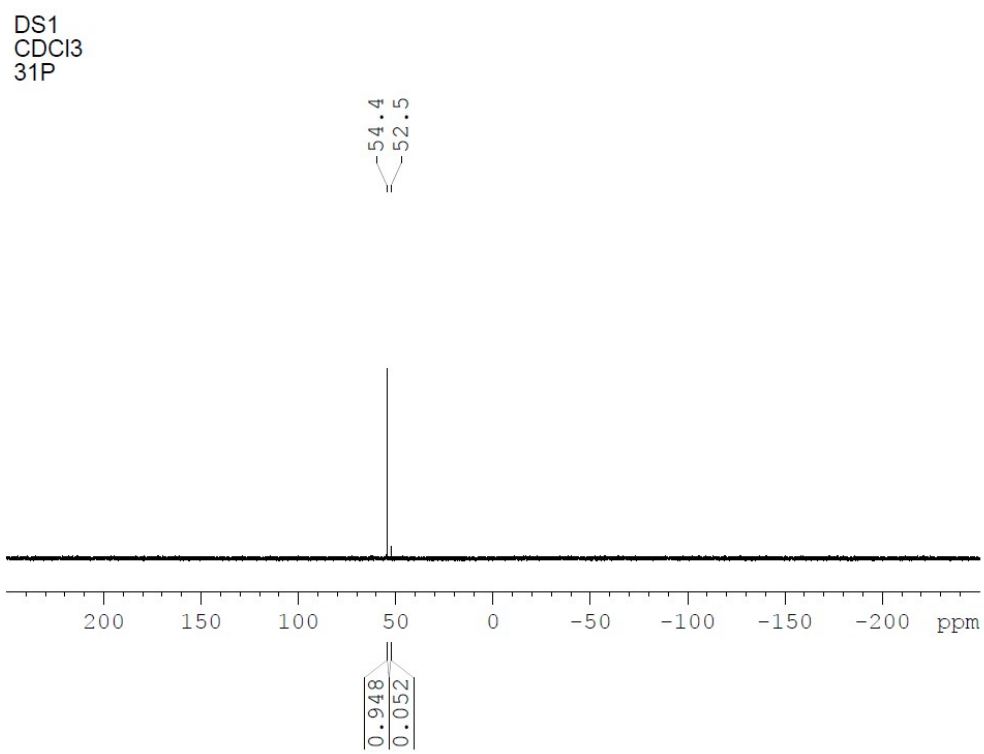

S7.
CDCl3
13C
168.479
168.431
167.122
167.067
135.007
134.226
133.276
133.182
132.042
131.945
131.538
131.146
131.116
131.061
131.032
130.734
128.374
128.254
127.679
127.560
86.148
70.700
70.146
69.462
69.034
68.368
67.359
56.399
56.377
42.575
42.075
21.829
21.684
21.447
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

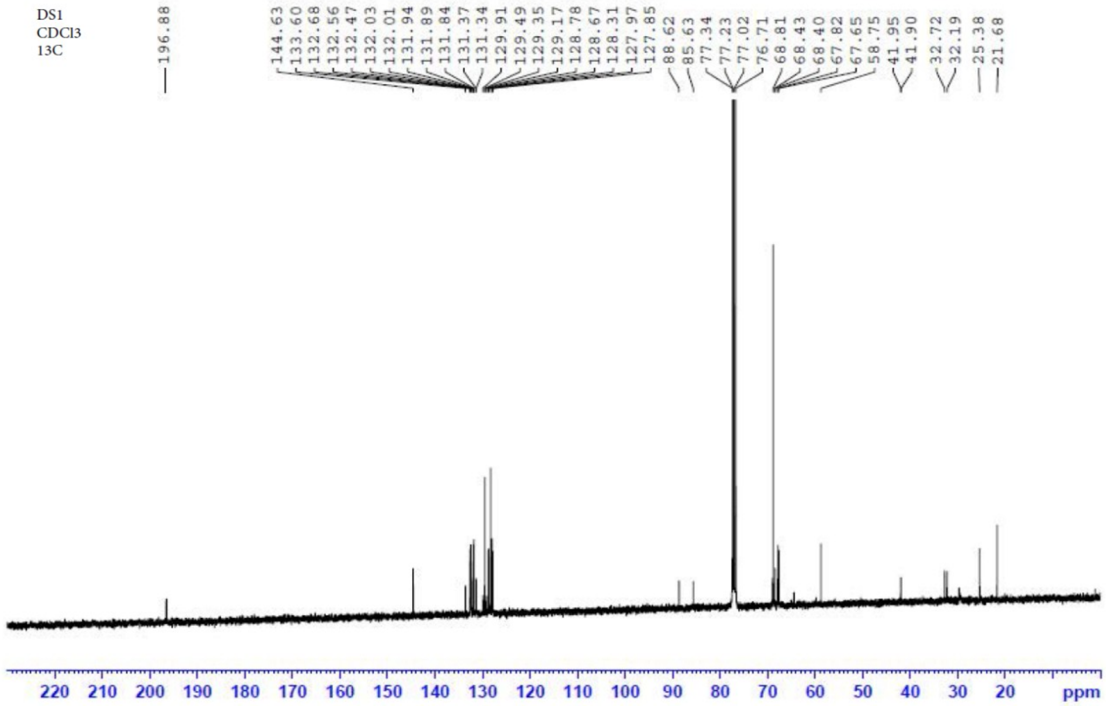

S8
CDCl3
1H
7.84
7.61
7.59
7.58
7.57
7.55
7.54
7.45
7.45
7.43
7.42
7.41
7.40
7.40
7.38
7.32
7.31
7.29
7.28
7.28
4.82
4.81
4.77
4.76
4.68
4.66
4.61
4.60
4.11
4.06
3.94
3.93
3.80
3.45
3.39
3.39
8 7 6 5 4 3 2 1 ppm
2.05
2.03
3.98
1.82
1.00
1.01
2.03
4.95
1.01
2.99
2.99
1.04

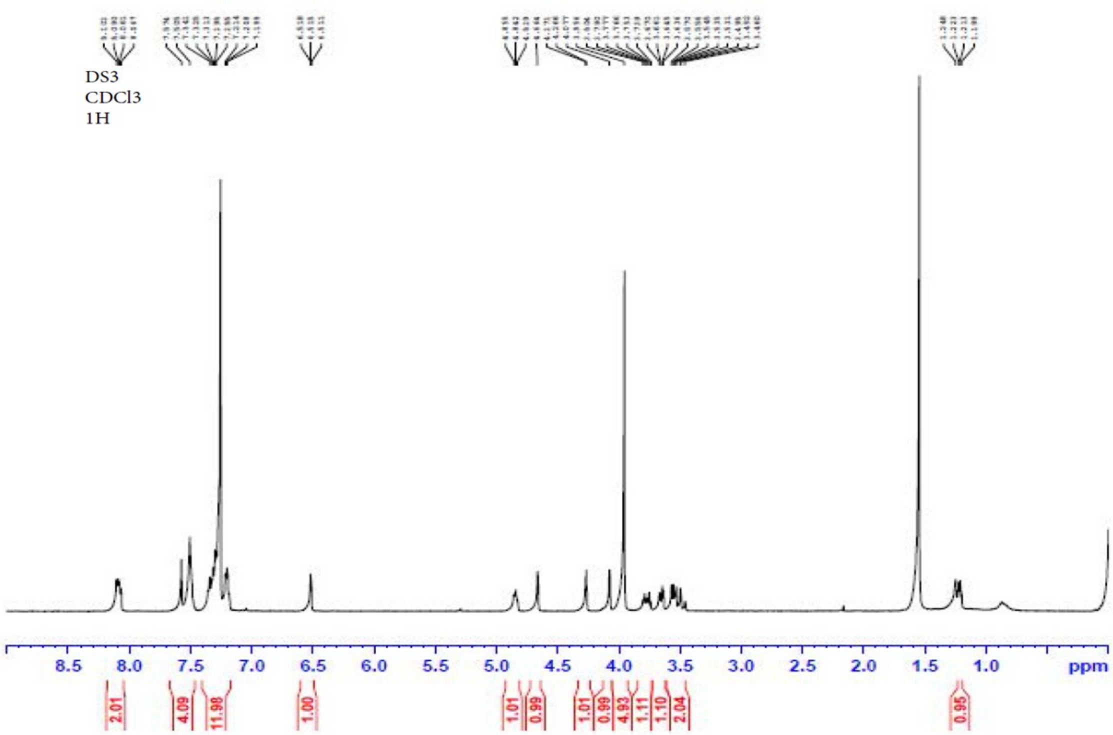

S8
CDCl3
31P
47.3
200 150 100 50 0 -50 -100 -150 -200 ppm

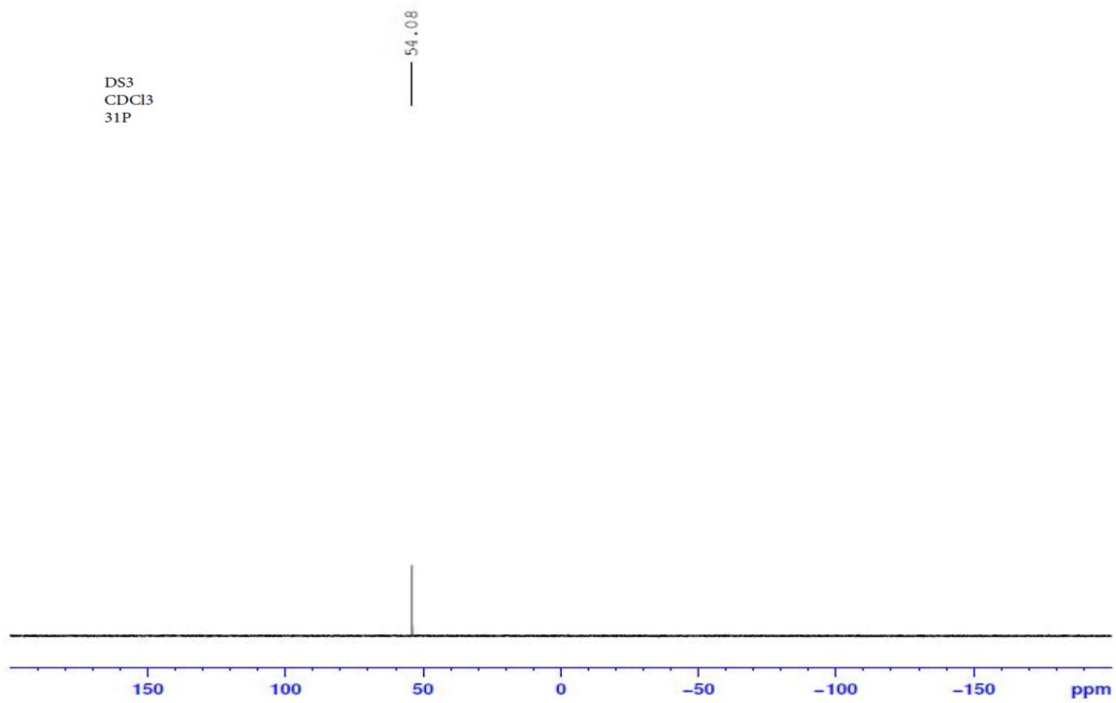

S8
CDCl3
13C
169.14
167.87
134.68
133.89
133.25
133.15
131.78
131.68
131.17
131.09
128.36
128.24
127.57
127.45
85.56
70.51
70.02
68.49
68.42
67.41
55.38
53.20
52.38
43.81
43.32
29.71
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

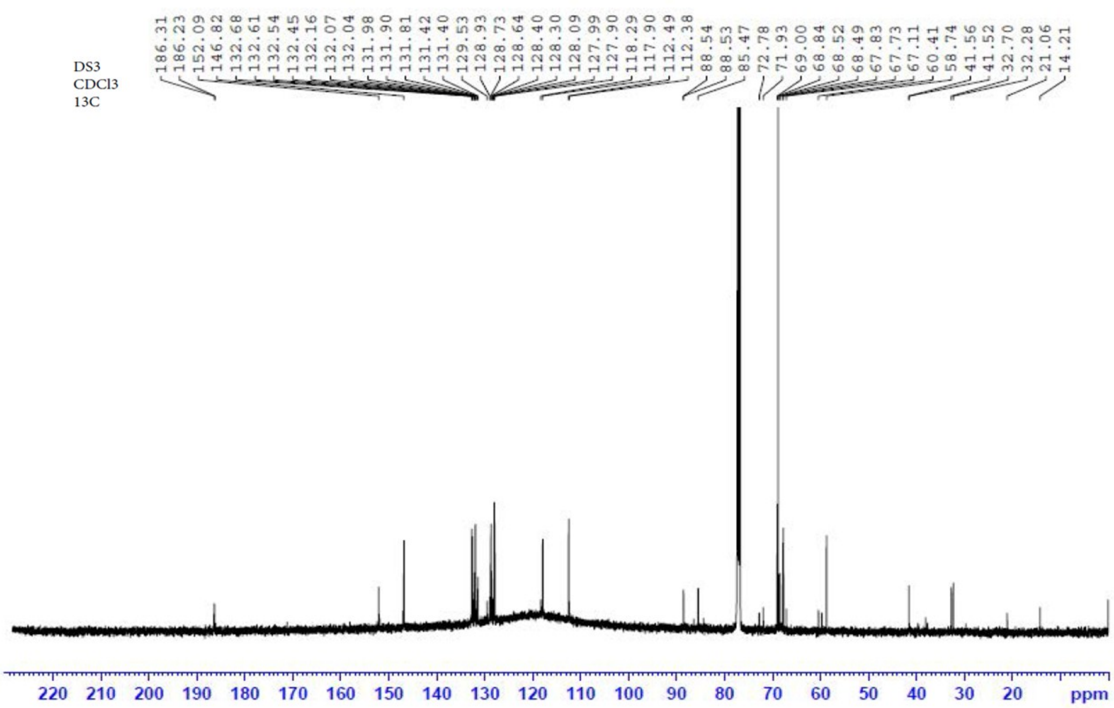

DS1
CDCl3
1H
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
2.03
1.97
3.01
7.17
2.00
0.97
1.00
1.01
1.01
5.80
1.00
1.96
3.07
0.95

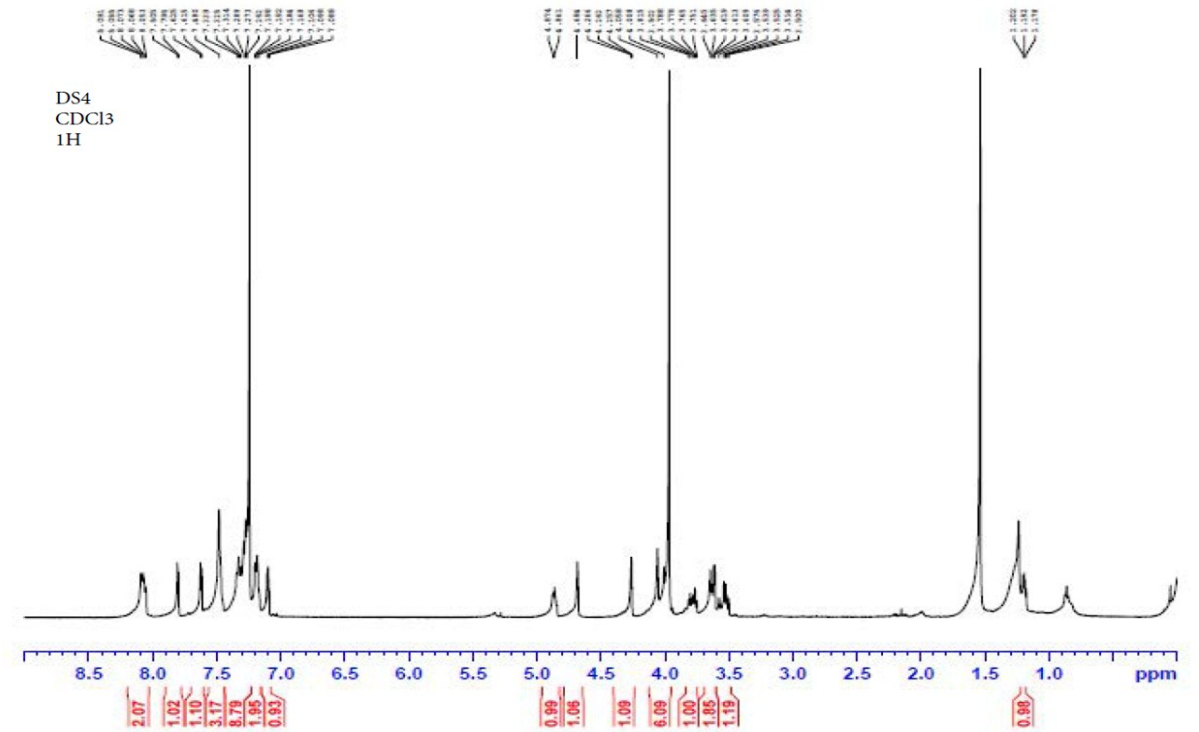

DS1
CDCl3
31P
54.4
52.5
200
150
100
50
0
-50
-100
-150
-200
ppm
0.948
0.052

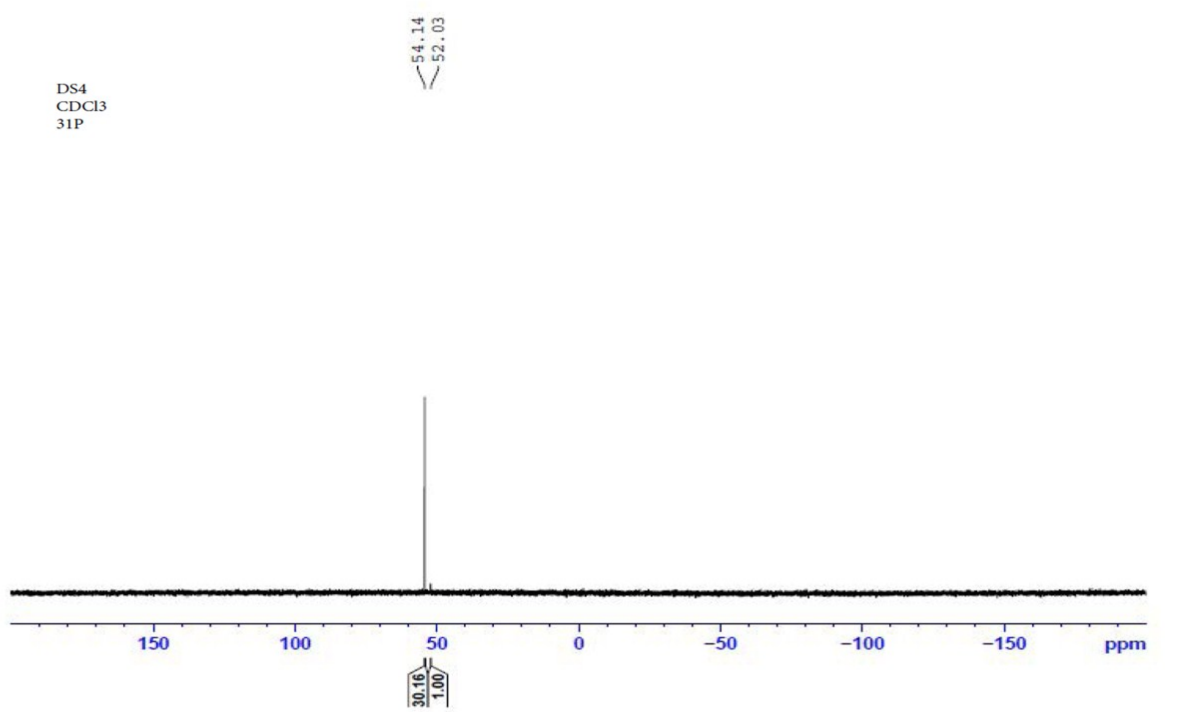

DS1
CDCl3
13C
196.88
144.63
133.60
132.68
132.56
132.47
132.03
132.01
131.94
131.89
131.84
131.37
131.34
129.91
129.49
129.35
129.17
128.78
128.67
128.31
127.97
127.85
88.62
85.63
77.34
77.23
77.02
76.71
68.81
68.43
68.40
67.82
67.65
58.75
41.95
41.90
32.72
32.19
25.38
21.68
ppm

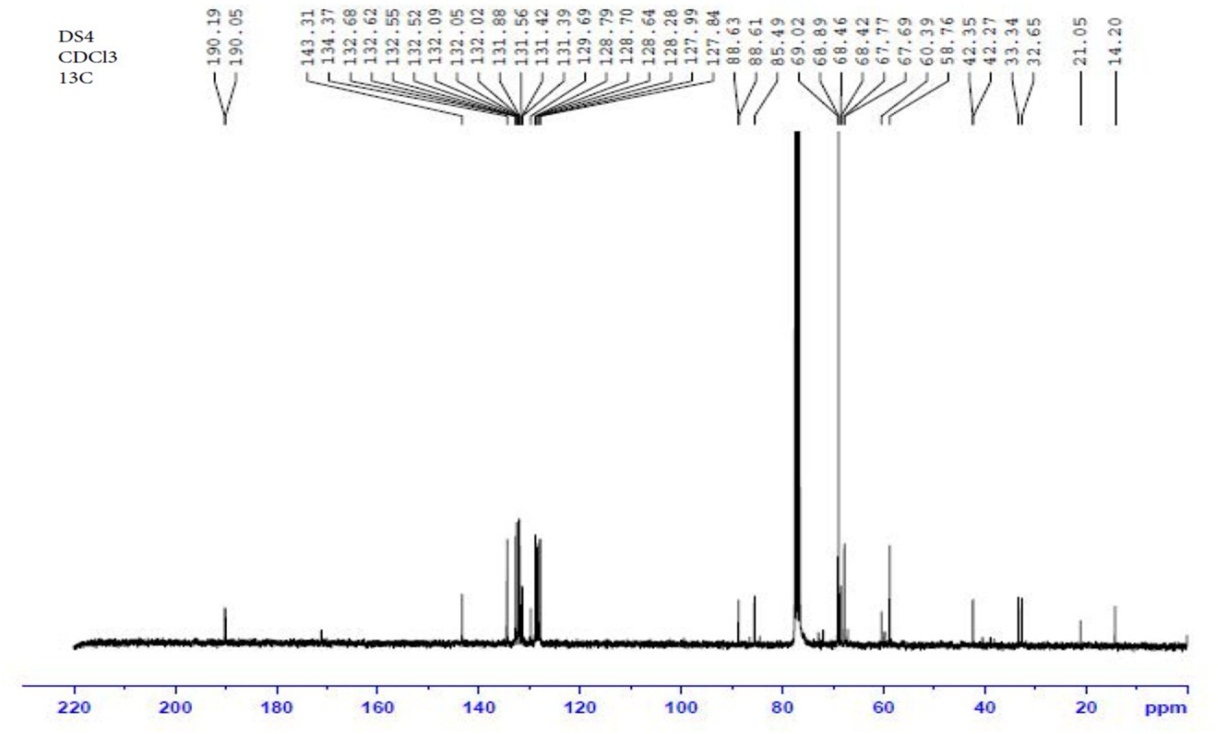

DS3
CDCl3
1H
ppm
2.01
4.09
11.98
1.00
1.01
0.99
1.01
0.99
4.93
1.11
1.10
2.04
0.95

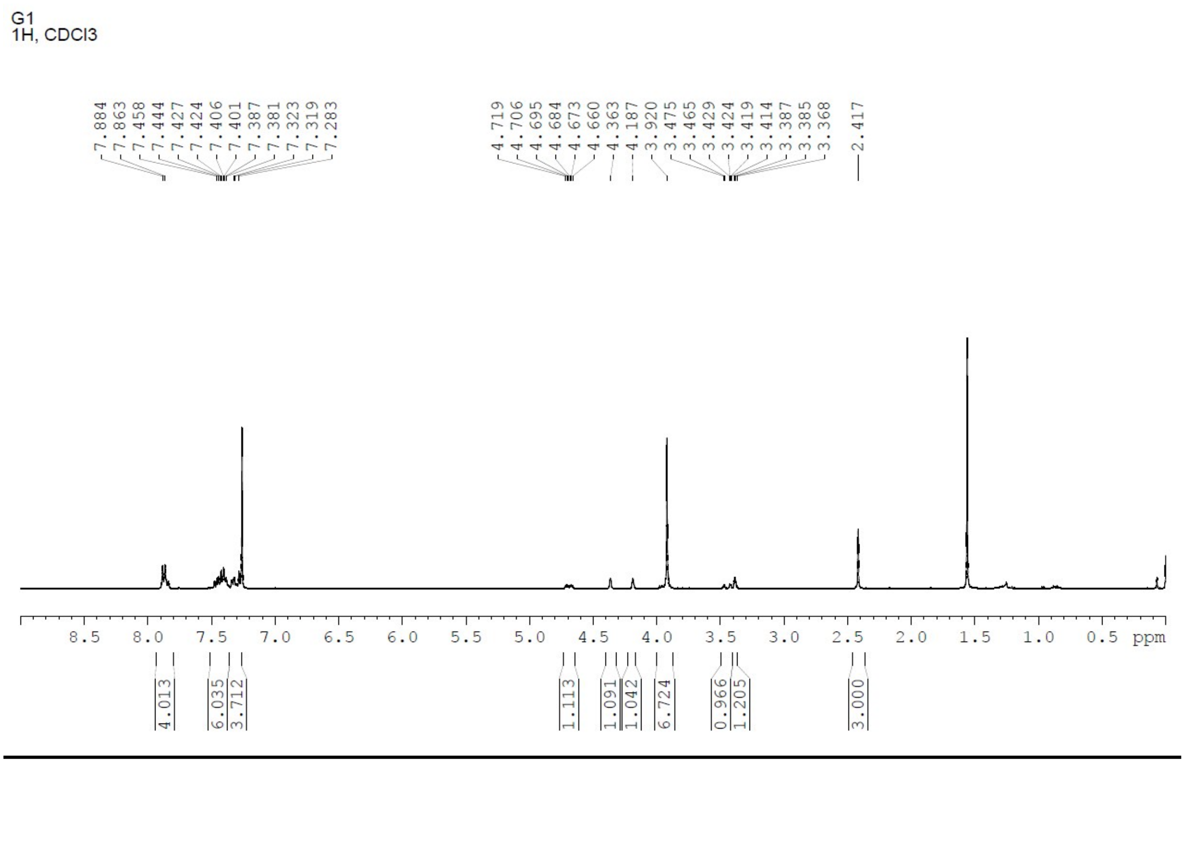

DS3
CDCl3
31P
54.08
150
100
50
0
−50
−100
−150
ppm


DS3
CDCl3
13C
186.31
186.23
152.09
146.82
132.68
132.61
132.54
132.45
132.16
132.07
132.04
131.98
131.90
131.81
131.42
131.40
129.53
128.93
128.73
128.64
128.40
128.30
128.09
127.99
127.90
118.29
117.90
112.49
112.38
88.54
88.53
85.47
72.78
71.93
69.00
68.84
68.52
68.49
67.83
67.73
67.11
60.41
58.74
41.56
41.52
32.70
32.28
21.06
14.21
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

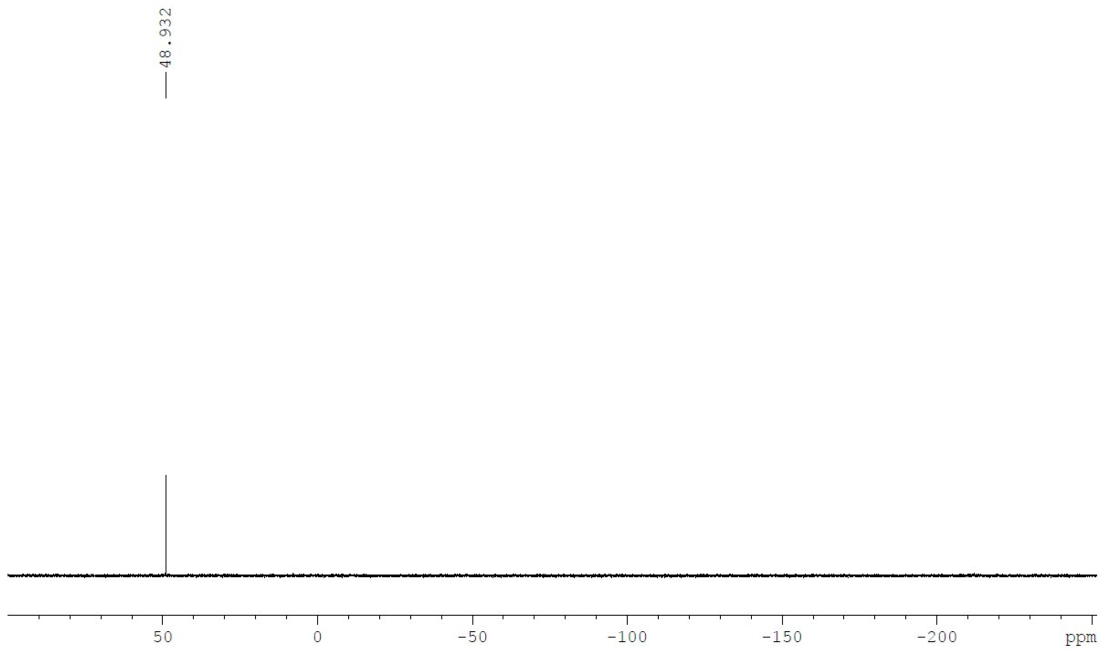

DS4
CDCl3
1H
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
2.07 1.02 1.10 3.17 8.79 1.95 0.93 0.99 1.06 1.09 6.09 1.00 1.85 1.19 0.98


54.14
52.03
DS4
CDCl3
31P
150 100 50 0 −50 −100 −150 ppm
30.16
1.00

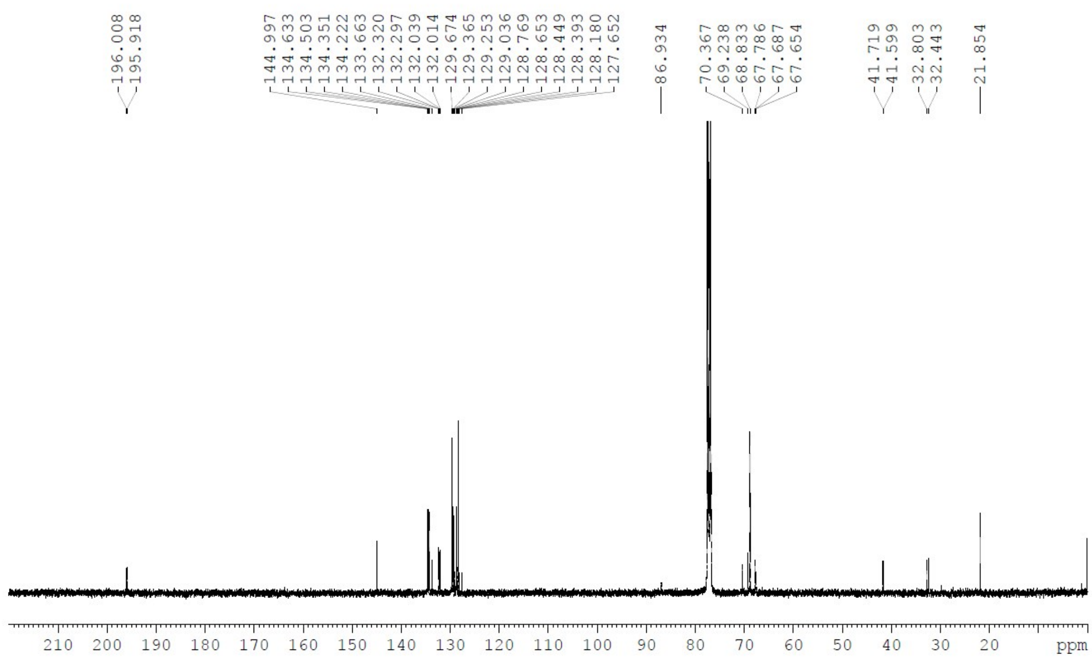

DS4
CDCl3
13C
190.19
190.05
143.31
134.37
132.68
132.62
132.55
132.52
132.09
132.05
132.02
131.88
131.56
131.42
131.39
129.69
128.79
128.70
128.64
128.28
127.99
127.84
88.63
88.61
85.49
69.02
68.89
68.46
68.42
67.77
67.69
60.39
58.76
42.35
42.27
33.34
32.65
21.05
14.20
220
200
180
160
140
120
100
80
60
40
20
ppm


G1
1H, CDCl3
7.884
7.863
7.458
7.444
7.427
7.424
7.406
7.401
7.387
7.381
7.323
7.319
7.283
4.719
4.706
4.695
4.684
4.673
4.660
4.363
4.187
3.920
3.475
3.465
3.429
3.424
3.419
3.414
3.387
3.385
3.368
2.417
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
4.013
6.035
3.712
1.113
1.091
1.042
6.724
0.966
1.205
3.000

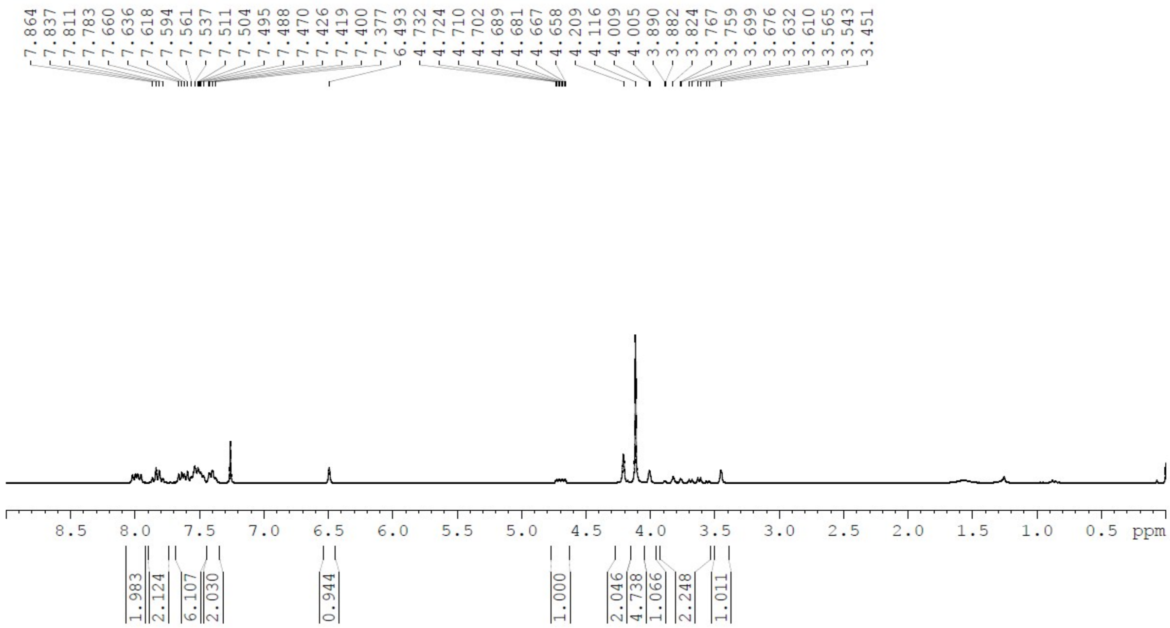
G1
31P, CDCl3



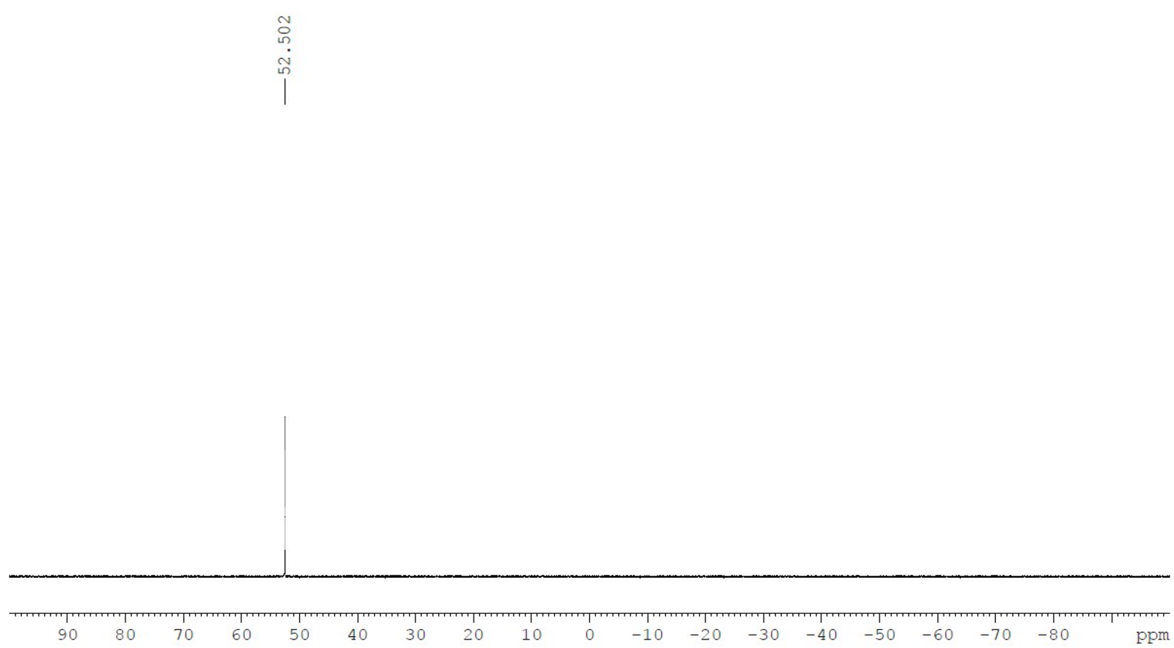
G1
CDCl3
13C



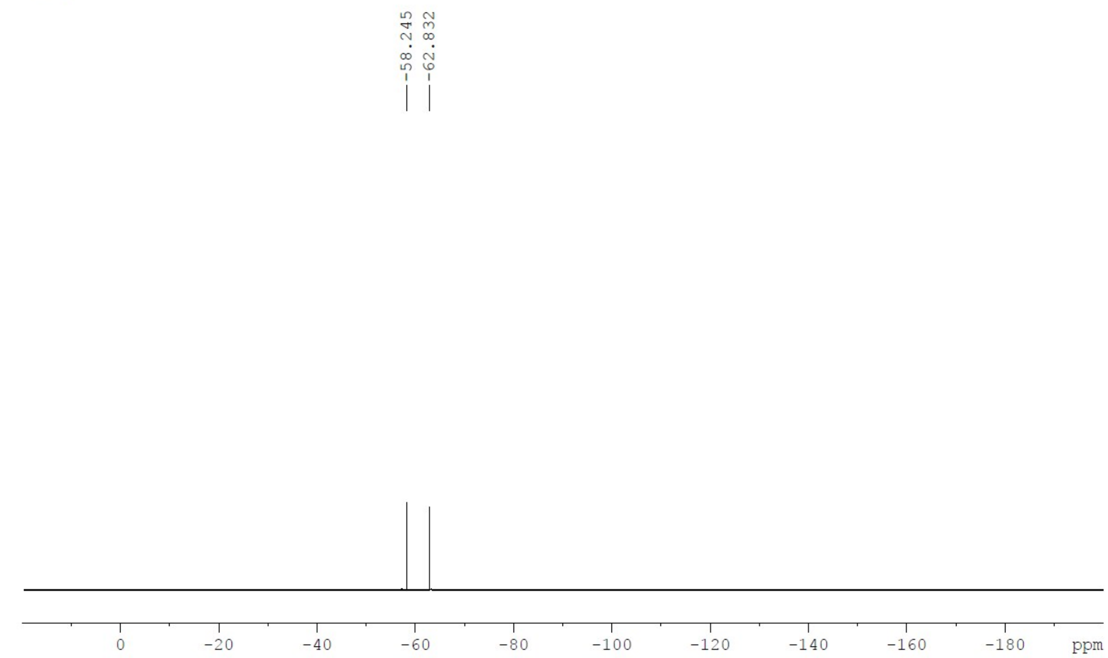
G2.
CDCl3
1H



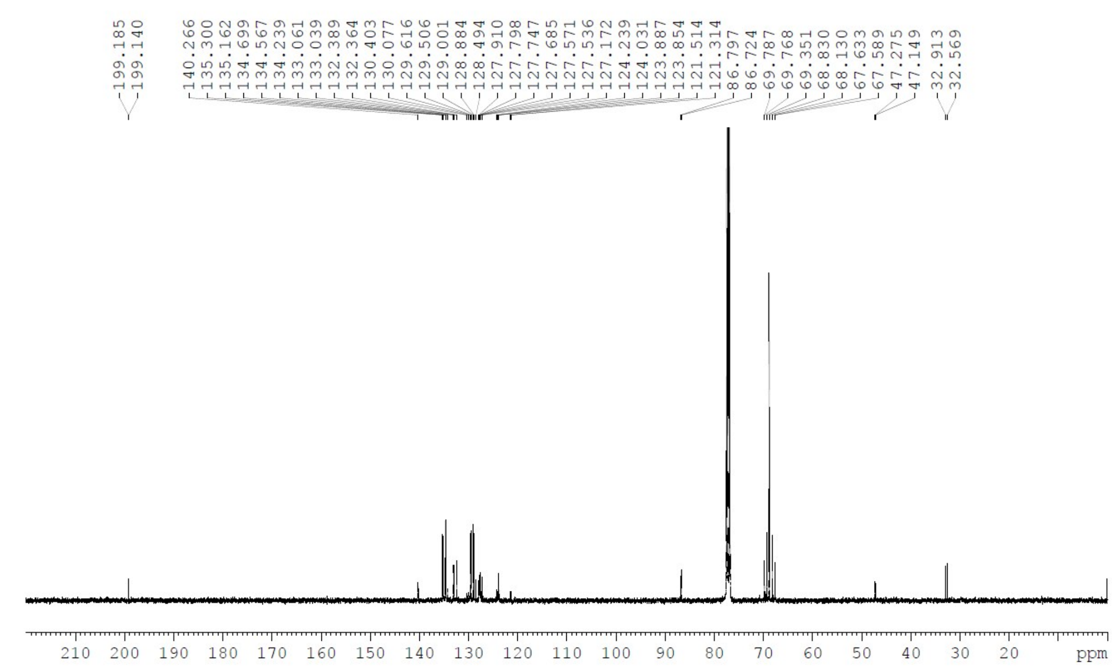
G2.
CDCl3
31P{1H}

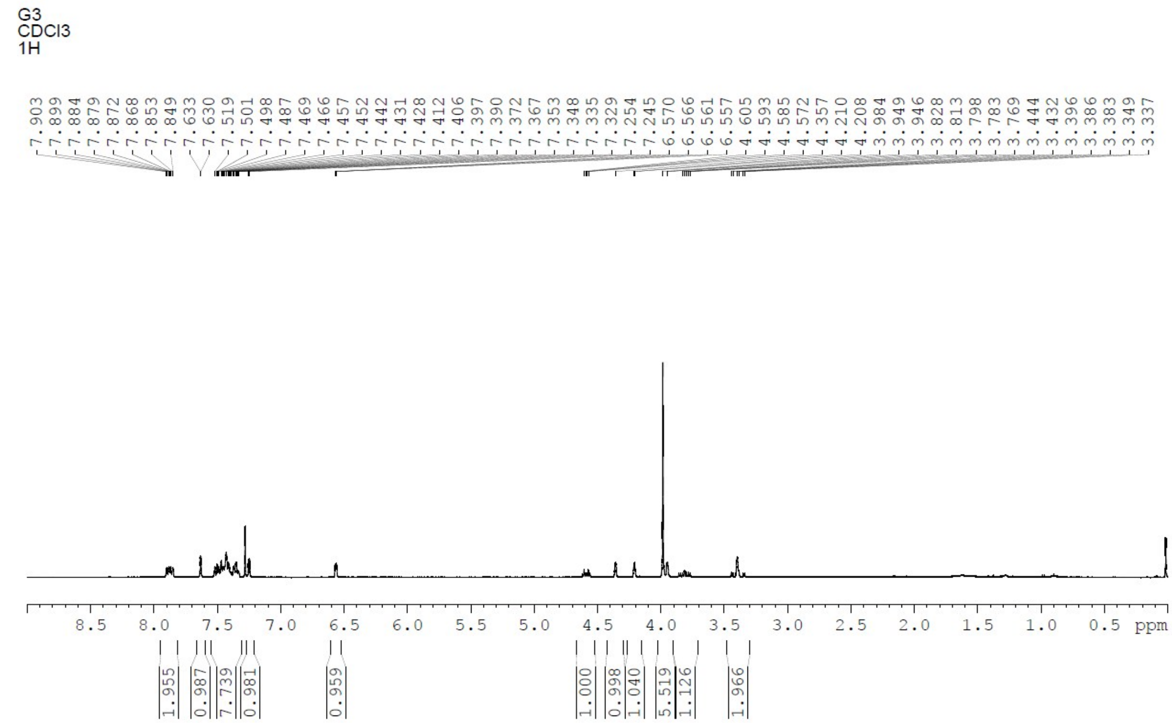


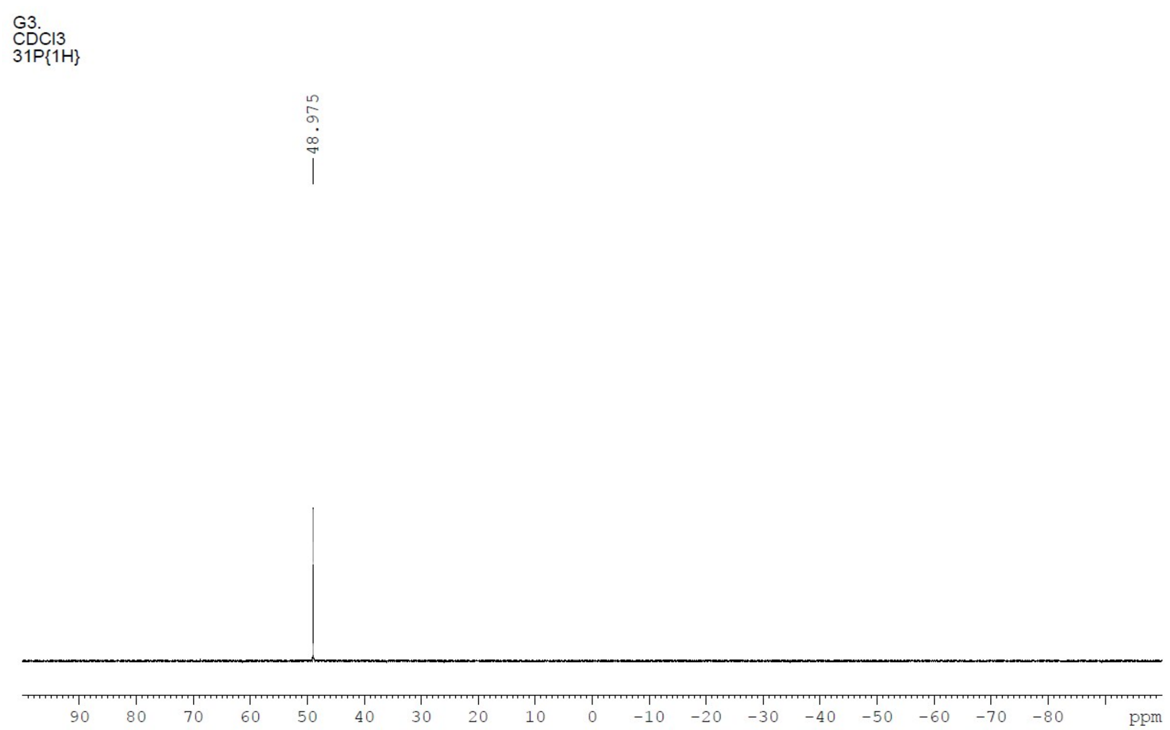
G2.
CDCl3
19F{1H}

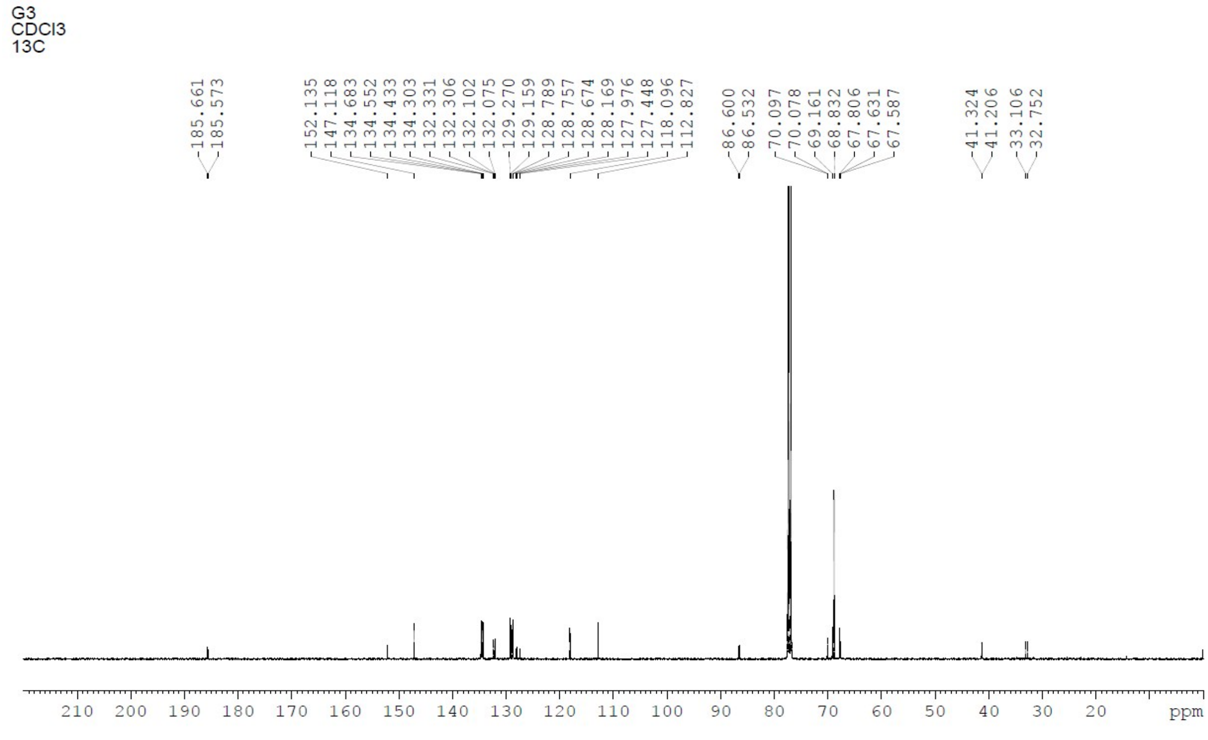


G2.
CDCl3
13C




G3
CDCl3
1H
7.903 7.899 7.884 7.879 7.872 7.868 7.853 7.849 7.633 7.630 7.519 7.501 7.498 7.487 7.469 7.466 7.457 7.452 7.442 7.431 7.428 7.412 7.406 7.397 7.390 7.372 7.367 7.353 7.348 7.335 7.329 7.254 7.245 6.570 6.566 6.561 6.557 4.605 4.593 4.585 4.572 4.357 4.210 4.208 3.984 3.949 3.946 3.828 3.813 3.798 3.783 3.769 3.444 3.432 3.396 3.386 3.383 3.349 3.337
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.955 0.987 7.739 0.981 0.959 1.000 0.998 1.040 5.519 1.126 1.966


G3.
CDCl3
31P{1H}
48.975
90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 ppm


G3
CDCl3
13C
185.661
185.573
152.135
147.118
134.683
134.552
134.433
134.303
132.331
132.306
132.102
132.075
129.270
129.159
128.789
128.757
128.674
128.169
127.976
127.448
118.096
112.827
86.600
86.532
70.097
70.078
69.161
68.832
67.806
67.631
67.587
41.324
41.206
33.106
32.752
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

Crystal Structure Report for G3

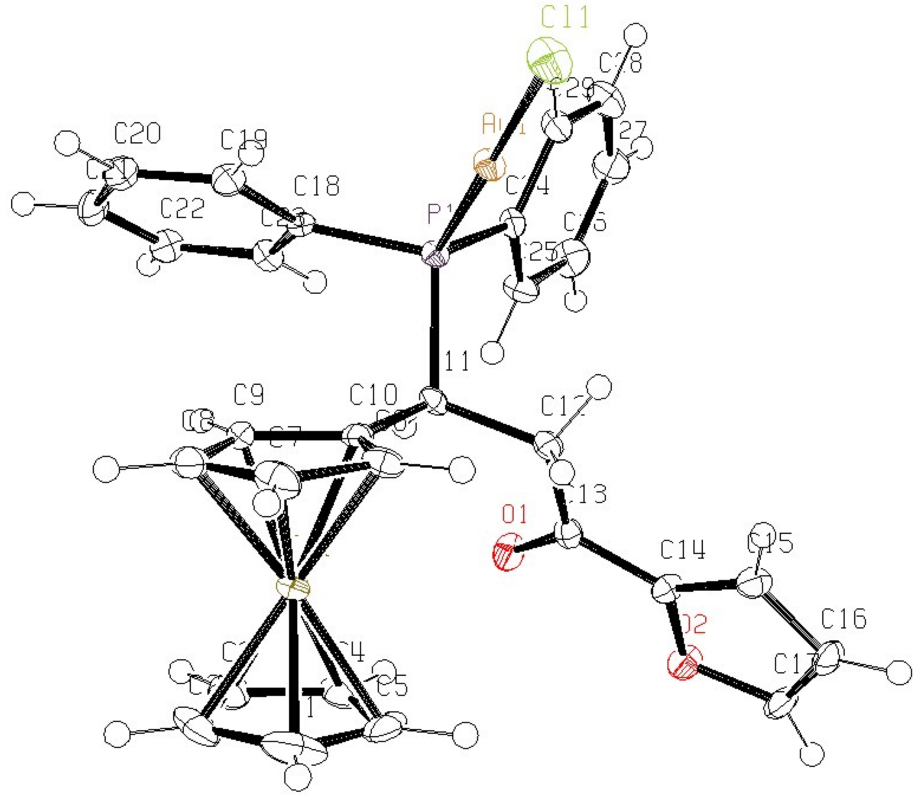


Figure 1. ORTEP of gold complex of **G3** with thermal ellipsoids drawn at the 50% probability level

Table 1. Sample and crystal data for G3.

Identification code	G3
Chemical formula	$C_{29}H_{25}AuClFeO_2P$
Formula weight	724.72 g/mol
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal size	0.020 x 0.040 x 0.100 mm
Crystal habit	orange block
Crystal system	monoclinic
Space group	P 1 21/c 1

Unit cell dimensions	a = 9.0226(2) Å	α = 90°
	b = 11.2002(2) Å	β = 96.9250(10)°
	c = 25.5416(6) Å	γ = 90°
Volume	2562.27(9) $Å^3$	
Z	4	
Density (calculated)	1.879 g/cm^3	
Absorption coefficient	6.477 mm^{-1}	
F(000)	1408	

Table 2. Data collection and structure refinement for G3.

Theta range for data collection	2.27 to 31.53°	
Index ranges	-13<=h<=13, -16<=k<=16, -37<=l<=37	
Reflections collected	34522	
Independent reflections	8538 [R(int) = 0.0622]	
Coverage of independent reflections	99.7%	
Absorption correction	Multi-Scan	
Max. and min. transmission	0.8810 and 0.5640	
Structure solution technique	direct methods	
Structure solution program	XT, VERSION 2014/5	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2017/1 (Sheldrick, 2017)	
Function minimized	Σ w(F_o^2 - F_c^2)^2	
Data / restraints / parameters	8538 / 0 / 316	
Goodness-of-fit on F^2	1.030	
Δ/σ_{max}	0.002	
Final R indices	6521 data; I>2σ(I)	R1 = 0.0386, wR2 = 0.0621
	all data	R1 = 0.0617, wR2 = 0.0708
Weighting scheme	w=1/[$\sigma^2(F_o^2)+(0.0169P)^2+3.8876P$] where P=($F_o^2+2F_c^2$)/3	
Largest diff. peak and hole	1.396 and -1.609 e$Å^{-3}$	
R.M.S. deviation from mean	0.198 e$Å^{-3}$	

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for G3.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
Au1	0.83846(2)	0.84284(2)	0.47177(2)	0.01478(4)

	x/a	y/b	z/c	U(eq)
C1	0.1629(6)	0.4717(5)	0.4439(2)	0.0406(13)
C2	0.0660(5)	0.5618(5)	0.4226(2)	0.0304(11)
C3	0.1051(5)	0.5918(4)	0.37261(19)	0.0248(10)
C4	0.2265(5)	0.5202(4)	0.3625(2)	0.0300(11)
C5	0.2616(5)	0.4450(4)	0.4070(2)	0.0389(14)
C6	0.4876(4)	0.6504(4)	0.46978(16)	0.0188(8)
C7	0.3720(5)	0.6869(4)	0.50000(18)	0.0249(10)
C8	0.2844(5)	0.7744(4)	0.47080(19)	0.0254(10)
C9	0.3436(4)	0.7927(3)	0.42250(18)	0.0189(9)
C10	0.4701(4)	0.7157(3)	0.42122(16)	0.0138(7)
C11	0.5747(4)	0.7170(3)	0.37960(16)	0.0139(8)
C12	0.6632(4)	0.6001(3)	0.37542(16)	0.0154(8)
C13	0.6053(4)	0.5244(3)	0.32832(16)	0.0147(8)
C14	0.6693(4)	0.4052(3)	0.32628(15)	0.0145(8)
C15	0.7727(4)	0.3434(4)	0.35862(16)	0.0181(8)
C16	0.7899(5)	0.2315(3)	0.33451(18)	0.0211(9)
C17	0.6961(5)	0.2310(3)	0.28980(18)	0.0227(9)
C18	0.5764(4)	0.9716(3)	0.38421(15)	0.0126(7)
C19	0.5408(4)	0.0332(3)	0.42876(16)	0.0178(8)
C20	0.4267(5)	0.1178(4)	0.42278(18)	0.0209(9)
C21	0.3518(5)	0.1428(4)	0.37336(17)	0.0203(9)
C22	0.3919(5)	0.0849(4)	0.32914(17)	0.0194(8)
C23	0.5030(4)	0.9986(3)	0.33483(16)	0.0159(8)
C24	0.8145(4)	0.8527(3)	0.33870(15)	0.0144(7)
C25	0.7650(5)	0.8105(4)	0.28828(17)	0.0201(9)
C26	0.8516(5)	0.8261(4)	0.24750(18)	0.0250(10)
C27	0.9870(5)	0.8841(4)	0.25668(19)	0.0259(10)
C28	0.0375(5)	0.9254(4)	0.30656(19)	0.0254(10)

	x/a	y/b	z/c	U(eq)
C29	0.9524(4)	0.9098(4)	0.34764(17)	0.0186(8)
Cl1	0.97890(11)	0.84359(10)	0.55232(4)	0.0250(2)
Fe1	0.28153(6)	0.61895(5)	0.42895(2)	0.01630(12)
O1	0.5147(3)	0.5612(2)	0.29272(11)	0.0199(6)
O2	0.6202(3)	0.3364(2)	0.28290(12)	0.0211(6)
P1	0.70238(10)	0.84546(9)	0.39305(4)	0.01203(18)

Table 4. Bond lengths (Å) for G3.

Au1-P1	2.2260(10)	Au1-Cl1	2.2825(11)
C1-C2	1.402(7)	C1-C5	1.406(8)
C1-Fe1	2.028(5)	C1-H1	1.0
C2-C3	1.406(6)	C2-Fe1	2.035(4)
C2-H2	1.0	C3-C4	1.406(6)
C3-Fe1	2.036(4)	C3-H3	1.0
C4-C5	1.420(7)	C4-Fe1	2.037(4)
C4-H4	1.0	C5-Fe1	2.030(4)
C5-H5	1.0	C6-C7	1.431(5)
C6-C10	1.432(5)	C6-Fe1	2.050(4)
C6-H6	1.0	C7-C8	1.414(7)
C7-Fe1	2.045(5)	C7-H7	1.0
C8-C9	1.417(6)	C8-Fe1	2.042(4)
C8-H8	1.0	C9-C10	1.435(5)
C9-Fe1	2.038(4)	C9-H9	1.0
C10-C11	1.504(5)	C10-Fe1	2.047(4)
C11-C12	1.545(5)	C11-P1	1.849(4)
C11-H11	1.0	C12-C13	1.513(5)
C12-H12A	0.99	C12-H12B	0.99
C13-O1	1.219(5)	C13-C14	1.458(5)
C14-C15	1.358(5)	C14-O2	1.378(5)
C15-C16	1.413(6)	C15-H15	0.95
C16-C17	1.337(6)	C16-H16	0.95
C17-O2	1.366(5)	C17-H17	0.95
C18-C23	1.385(5)	C18-C19	1.401(5)
C18-P1	1.811(4)	C19-C20	1.394(6)
C19-H19	0.95	C20-C21	1.386(6)
C20-H20	0.95	C21-C22	1.388(6)
C21-H21	0.95	C22-C23	1.387(5)
C22-H22	0.95	C23-H23	0.95
C24-C29	1.392(5)	C24-C25	1.394(6)
C24-P1	1.816(4)	C25-C26	1.386(5)
C25-H25	0.95	C26-C27	1.379(6)
C26-H26	0.95	C27-C28	1.380(6)
C27-H27	0.95	C28-C29	1.384(5)

C28-H28	0.95	C29-H29	0.95

Table 5. Bond angles (°) for G3.

P1-Au1-Cl1	179.00(4)	C2-C1-C5	108.0(5)
C2-C1-Fe1	70.1(3)	C5-C1-Fe1	69.8(3)
C2-C1-H1	126.0	C5-C1-H1	126.0
Fe1-C1-H1	126.0	C1-C2-C3	108.2(4)
C1-C2-Fe1	69.6(3)	C3-C2-Fe1	69.8(2)
C1-C2-H2	125.9	C3-C2-H2	125.9
Fe1-C2-H2	125.9	C4-C3-C2	108.5(4)
C4-C3-Fe1	69.8(3)	C2-C3-Fe1	69.8(3)
C4-C3-H3	125.8	C2-C3-H3	125.8
Fe1-C3-H3	125.8	C3-C4-C5	107.2(4)
C3-C4-Fe1	69.8(3)	C5-C4-Fe1	69.3(3)
C3-C4-H4	126.4	C5-C4-H4	126.4
Fe1-C4-H4	126.4	C1-C5-C4	108.2(4)
C1-C5-Fe1	69.7(3)	C4-C5-Fe1	69.8(3)
C1-C5-H5	125.9	C4-C5-H5	125.9
Fe1-C5-H5	125.9	C7-C6-C10	108.1(4)
C7-C6-Fe1	69.4(2)	C10-C6-Fe1	69.4(2)
C7-C6-H6	126.0	C10-C6-H6	126.0
Fe1-C6-H6	126.0	C8-C7-C6	108.1(4)
C8-C7-Fe1	69.6(3)	C6-C7-Fe1	69.7(2)
C8-C7-H7	125.9	C6-C7-H7	125.9
Fe1-C7-H7	125.9	C7-C8-C9	108.3(4)
C7-C8-Fe1	69.9(3)	C9-C8-Fe1	69.5(2)
C7-C8-H8	125.8	C9-C8-H8	125.8
Fe1-C8-H8	125.8	C8-C9-C10	108.5(4)
C8-C9-Fe1	69.8(2)	C10-C9-Fe1	69.8(2)
C8-C9-H9	125.8	C10-C9-H9	125.8
Fe1-C9-H9	125.8	C6-C10-C9	107.0(3)
C6-C10-C11	127.2(3)	C9-C10-C11	125.4(4)
C6-C10-Fe1	69.7(2)	C9-C10-Fe1	69.1(2)
C11-C10-Fe1	132.3(3)	C10-C11-C12	114.5(3)
C10-C11-P1	107.8(3)	C12-C11-P1	110.9(2)
C10-C11-H11	107.8	C12-C11-H11	107.8
P1-C11-H11	107.8	C13-C12-C11	113.5(3)
C13-C12-H12A	108.9	C11-C12-H12A	108.9
C13-C12-H12B	108.9	C11-C12-H12B	108.9
H12A-C12-H12B	107.7	O1-C13-C14	121.1(4)
O1-C13-C12	122.7(3)	C14-C13-C12	116.2(3)
C15-C14-O2	109.6(3)	C15-C14-C13	133.7(4)
O2-C14-C13	116.7(3)	C14-C15-C16	106.8(4)
C14-C15-H15	126.6	C16-C15-H15	126.6
C17-C16-C15	106.6(4)	C17-C16-H16	126.7
C15-C16-H16	126.7	C16-C17-O2	111.2(4)

C16-C17-H17	124.4	O2-C17-H17	124.4
C23-C18-C19	120.1(4)	C23-C18-P1	120.5(3)
C19-C18-P1	119.0(3)	C20-C19-C18	119.0(4)
C20-C19-H19	120.5	C18-C19-H19	120.5
C21-C20-C19	120.6(4)	C21-C20-H20	119.7
C19-C20-H20	119.7	C22-C21-C20	120.0(4)
C22-C21-H21	120.0	C20-C21-H21	120.0
C21-C22-C23	119.7(4)	C21-C22-H22	120.1
C23-C22-H22	120.1	C18-C23-C22	120.5(4)
C18-C23-H23	119.8	C22-C23-H23	119.8
C29-C24-C25	119.2(3)	C29-C24-P1	117.7(3)
C25-C24-P1	123.0(3)	C26-C25-C24	120.3(4)
C26-C25-H25	119.8	C24-C25-H25	119.8
C27-C26-C25	120.0(4)	C27-C26-H26	120.0
C25-C26-H26	120.0	C26-C27-C28	120.1(4)
C26-C27-H27	119.9	C28-C27-H27	119.9
C29-C28-C27	120.4(4)	C29-C28-H28	119.8
C27-C28-H28	119.8	C28-C29-C24	120.0(4)
C28-C29-H29	120.0	C24-C29-H29	120.0
C1-Fe1-C5	40.5(2)	C1-Fe1-C2	40.4(2)
C5-Fe1-C2	67.9(2)	C1-Fe1-C3	68.1(2)
C5-Fe1-C3	68.0(2)	C2-Fe1-C3	40.40(18)
C1-Fe1-C4	68.6(2)	C5-Fe1-C4	40.9(2)
C2-Fe1-C4	68.17(18)	C3-Fe1-C4	40.41(17)
C1-Fe1-C9	161.6(2)	C5-Fe1-C9	155.7(2)
C2-Fe1-C9	124.26(19)	C3-Fe1-C9	106.53(18)
C4-Fe1-C9	119.6(2)	C1-Fe1-C8	124.6(2)
C5-Fe1-C8	163.4(2)	C2-Fe1-C8	105.16(18)
C3-Fe1-C8	117.18(19)	C4-Fe1-C8	152.4(2)
C9-Fe1-C8	40.64(16)	C1-Fe1-C7	107.4(2)
C5-Fe1-C7	127.9(2)	C2-Fe1-C7	117.57(18)
C3-Fe1-C7	151.30(17)	C4-Fe1-C7	166.6(2)
C9-Fe1-C7	68.41(18)	C8-Fe1-C7	40.48(19)
C1-Fe1-C10	155.89(19)	C5-Fe1-C10	121.91(18)
C2-Fe1-C10	163.00(19)	C3-Fe1-C10	126.81(17)
C4-Fe1-C10	109.23(17)	C9-Fe1-C10	41.13(15)
C8-Fe1-C10	68.94(15)	C7-Fe1-C10	68.97(16)
C1-Fe1-C6	120.7(2)	C5-Fe1-C6	110.49(19)
C2-Fe1-C6	153.39(18)	C3-Fe1-C6	165.77(17)
C4-Fe1-C6	129.24(17)	C9-Fe1-C6	68.64(17)
C8-Fe1-C6	68.50(18)	C7-Fe1-C6	40.90(15)
C10-Fe1-C6	40.92(15)	C17-O2-C14	105.8(3)
C18-P1-C24	105.60(17)	C18-P1-C11	102.48(16)
C24-P1-C11	106.56(18)	C18-P1-Au1	113.12(13)
C24-P1-Au1	113.18(13)	C11-P1-Au1	114.90(13)

Table 6. Anisotropic atomic displacement parameters ($Å^2$) for G3.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2$

h k a* b* U_{12}]

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Au1	0.01354(7)	0.01924(7)	0.01092(7)	-0.00148(6)	-0.00114(5)	0.00056(6)
C1	0.036(3)	0.041(3)	0.042(3)	0.014(3)	-0.006(2)	-0.023(2)
C2	0.014(2)	0.045(3)	0.032(3)	-0.006(2)	-0.0001(19)	-0.010(2)
C3	0.019(2)	0.027(2)	0.025(3)	-0.0026(19)	-0.0080(18)	-0.0027(18)
C4	0.024(2)	0.035(3)	0.031(3)	-0.020(2)	0.002(2)	-0.011(2)
C5	0.025(2)	0.014(2)	0.072(4)	-0.010(2)	-0.020(3)	-0.0026(19)
C6	0.0173(19)	0.024(2)	0.0140(19)	-0.0007(17)	-0.0017(15)	-0.0070(17)
C7	0.023(2)	0.034(3)	0.019(2)	-0.0045(18)	0.0058(18)	-0.0081(19)
C8	0.022(2)	0.024(2)	0.032(3)	-0.0118(19)	0.011(2)	-0.0077(18)
C9	0.0130(18)	0.0133(18)	0.030(2)	-0.0046(17)	0.0010(17)	0.0003(16)
C10	0.0145(18)	0.0121(17)	0.0148(19)	-0.0028(14)	0.0015(15)	-0.0037(15)
C11	0.0097(17)	0.0169(19)	0.0145(19)	0.0021(15)	-0.0011(15)	-0.0002(15)
C12	0.0121(18)	0.0172(19)	0.016(2)	-0.0001(15)	-0.0033(15)	-0.0002(15)
C13	0.0139(18)	0.0161(18)	0.0145(19)	0.0021(15)	0.0032(15)	0.0007(15)
C14	0.0189(19)	0.0126(18)	0.0116(19)	0.0007(14)	-0.0001(15)	0.0000(15)
C15	0.0203(19)	0.0161(18)	0.0167(19)	0.0015(16)	-0.0032(16)	-0.0021(17)
C16	0.024(2)	0.0120(18)	0.026(2)	0.0038(16)	-0.0034(18)	0.0038(17)
C17	0.028(2)	0.0111(18)	0.027(2)	-0.0044(17)	-0.0015(19)	0.0014(17)
C18	0.0138(17)	0.0109(17)	0.0128(18)	-0.0014(14)	0.0007(15)	-0.0021(14)
C19	0.0187(19)	0.020(2)	0.014(2)	-0.0028(15)	0.0007(16)	-0.0009(16)
C20	0.021(2)	0.021(2)	0.021(2)	-0.0056(17)	0.0026(18)	-0.0007(17)
C21	0.020(2)	0.017(2)	0.023(2)	0.0014(16)	-0.0021(17)	0.0061(16)
C22	0.022(2)	0.019(2)	0.017(2)	0.0014(16)	-0.0006(17)	0.0000(17)
C23	0.0157(18)	0.0189(19)	0.0131(19)	0.0027(15)	0.0026(15)	-0.0002(16)
C24	0.0122(17)	0.0165(18)	0.0144(18)	-0.0003(15)	0.0016(14)	0.0017(15)
C25	0.0169(19)	0.024(2)	0.019(2)	-0.0028(16)	0.0006(17)	-0.0054(17)
C26	0.031(2)	0.029(2)	0.016(2)	-0.0026(18)	0.0070(19)	-0.0002(19)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C27	0.026(2)	0.025(2)	0.029(3)	0.0033(19)	0.010(2)	-0.0022(19)
C28	0.018(2)	0.033(2)	0.026(2)	0.0027(19)	0.0044(19)	-0.0037(19)
C29	0.0143(19)	0.025(2)	0.016(2)	-0.0035(16)	0.0016(16)	0.0003(16)
Cl1	0.0227(5)	0.0382(6)	0.0127(5)	-0.0030(4)	-0.0029(4)	0.0017(5)
Fe1	0.0130(3)	0.0157(3)	0.0201(3)	-0.0008(2)	0.0013(2)	-0.0027(2)
O1	0.0224(15)	0.0216(15)	0.0138(15)	-0.0026(11)	-0.0057(12)	0.0057(12)
O2	0.0243(15)	0.0181(14)	0.0184(15)	-0.0029(12)	-0.0073(12)	0.0015(13)
P1	0.0117(4)	0.0144(4)	0.0098(4)	-0.0003(4)	0.0004(4)	-0.0003(4)

Table 7. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for G3.

	x/a	y/b	z/c	U(eq)
H1	0.1615	0.4328	0.4791	0.049
H2	-0.0161	0.5989	0.4401	0.037
H3	0.0556	0.6541	0.3485	0.03
H4	0.2779	0.5215	0.3299	0.036
H5	0.3430	0.3839	0.4114	0.047
H6	0.5659	0.5889	0.4804	0.023
H7	0.3555	0.6556	0.5355	0.03
H8	0.1953	0.8157	0.4821	0.03
H9	0.3033	0.8493	0.3940	0.023
H11	0.5138	0.7311	0.3448	0.017
H12A	0.7692	0.6201	0.3731	0.018
H12B	0.6591	0.5528	0.4080	0.018
H15	0.8237	0.3703	0.3912	0.022
H16	0.8552	0.1689	0.3475	0.025
H17	0.6838	0.1657	0.2659	0.027
H19	0.5936	1.0176	0.4625	0.021
H20	0.4000	1.1588	0.4528	0.025
H21	0.2730	1.1995	0.3698	0.024
H22	0.3435	1.1043	0.2951	0.023
H23	0.5290	0.9577	0.3046	0.019
H25	0.6715	0.7709	0.2818	0.024
H26	0.8176	0.7967	0.2133	0.03
H27	1.0457	0.8958	0.2286	0.031
H28	1.1313	0.9647	0.3127	0.031
H29	0.9879	0.9381	0.3819	0.022