Electronic Supplementary Information

Screening of Ferrocenyl-Phosphines Identifies Gold-Coordinated Derivative as a Novel Anticancer Agent for Hematological Malignancies

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I. Characterization data of Ferrocenyl-phosphine derivatives FD1-10

FD1: 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, $^{1}J_{CP}$ = 67.0 Hz), 38.7(-CH_2), 67.2 (*m*-Cp), 67.7 (d, *o*-Cp, $^{3}J_{CP}$ = 1.6 Hz), 68.4 (*m*-Cp), 68.6 (5Cp), 70.3 (d, *o*-Cp, $^{3}J_{CP}$ = 2.0 Hz), 85.7 (*i*-Cp), 128.1 (d, 2 -*m* Ar, $^{3}J_{CP}$ = 11.5 Hz), 128.4(2 *m*-Ar), 128.6 (d, 2 *m*-Ar, $^{3}J_{CP}$ = 11.2 Hz), 129.5 (2 *o*-Ar), 131.5 (d, 2 *o*-Ar, $^{2}J_{CP}$ = 8.7 Hz), 131.5 (*p*-Ar), 131.6 (d, 2 *o*-Ar, $^{2}J_{CP}$ = 8.7 Hz), 131.6 (d, *i*-Ar, $^{1}J_{CP}$ = 95.0 Hz), 131.7 (d, *i*-Ar, $^{1}J_{CP}$ = 96.0 Hz), 131.9 (d, *p*-Ar, $^{4}J_{CP}$ = 3.1 Hz), 134.1 (*p*-Ar), 144.4 (*i*-Ar), 196.9 (d, *C*=O, $^{3}J_{CP}$ = 7.2 Hz). HRMS m/z (+ESI) $(M + H)^+$ calcd for C32H30O2P1Fe1: 533.1333, found: 533.1334.

FD2: Similar procedure to FD1; 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, $^{3}J_{HH}$ = 4.9 Hz, $^{4}J_{HH}$ = 0.7 Hz, - thienyl C*H*), 7.76 (dd, 1H, $^{3}J_{HH}$ = 3.7 Hz, $^{4}J_{HH}$ = 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, $^{1}J_{CP}$ = 67.3 Hz), 39.3(-CH_2), 67.3 (*m*-Cp), 67.6 (d, *o*-Cp, $^{3}J_{CP}$ = 2.3 Hz), 68.4 (*m*-Cp), 68.7 (5Cp), 70.2 (d, *o*-Cp, $^{3}J_{CP}$ = 2.1 Hz), 85.4 (*i*-Cp), 128.1 (d, 2 -*m* Ar, $^{3}J_{CP}$ = 11.7 Hz), 128.3 (thienyl Ar), 128.7 (d, 2 *m*-Ar, $^{3}J_{CP}$ = 11.4 Hz), 131.5 (d, 2 *i*-Ar, $^{1}J_{CP}$ = 96.9 Hz), 131.5 (d, 2 *o*-Ar, $^{2}J_{CP}$ = 8.9 Hz), 131.6 (d, *p*-Ar, $^{4}J_{CP}$ = 3.1 Hz), 131.7 (d, 2 *o*-Ar, $^{2}J_{CP}$ = 9.1 Hz), 131.9 (d, *p*-Ar, $^{4}J_{CP}$ = 2.6 Hz), 132.4 (thienyl Ar), 134.2 (thienyl Ar), 143.7 (thienyl Ar), 190.4 (d, *C*=O, $^{3}J_{CP}$ = 7.3 Hz). HRMS m/z (+ESI) $(M + H)^+$ calcd for C29H26O2P1S1Fe1: 525.0741, found: 525.0742.

FD3: Similar procedure to FD1; 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, $^{1}J_{CP}$ = 64.6 Hz), 43.9(-*C*H_2), 67.7 (*m*-Cp), 67.9 (*o*-Cp), 68.4 (*m*-Cp), 68.8 (5Cp), 69.9 (d, *o*-Cp, $^{3}J_{CP}$ = 1.7 Hz), 85.1 (*i*-Cp), 122.9 (q, *C*F_3, $^{1}J_{CF}$ = 273.2 Hz), 123.1 (q, *C*F_3, $^{1}J_{CF}$ = 273.9 Hz), 125.2(m, p-Ar), 127.0 (q, *m*-Ar, $^{3}J_{CF}$ = 3.9 Hz), 127.3 (q, *m*-Ar, $^{3}J_{CF}$ = 5.1 Hz), 128.1 (d, 2 -*m* Ar, $^{3}J_{CP}$ = 11.5 Hz), 128.8 (d, 2 -*m* Ar, $^{3}J_{CP}$ = 11.3 Hz), 129.7 (d, *i*-Ar, $^{1}J_{CP}$ = 97.7 Hz), 130.4 (d, *i*-Ar, $^{1}J_{CP}$ = 100.3 Hz), 131.5 (d, 2 *o*-Ar, $^{2}J_{CP}$ = 9.0 Hz), 132.0 (m, *p*-Ar), 132.3 (d, 2 *o*-Ar, $^{2}J_{CP}$ = 8.8 Hz), 132.4 (d, *p*-Ar, $^{4}J_{CP}$ = 2.2 Hz), 134.3 (q, 2 *m*-Ar, $^{2}J_{CF}$ = 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.

FD4: 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, $^{1}J_{CP}$ = 51.7 Hz), 39.6 (d, - *C*H_2 , $^{2}J_{CP}$ = 4.6 Hz), 67.1 (*m*-Cp), 68.1 (d, *o*-Cp, $^{3}J_{CP}$ = 1.7 Hz), 68.2 (*m*-Cp), 68.6 (5Cp), 70.2 (d, *o*-Cp, $^{3}J_{CP}$ = 1.9 Hz), 85.3 (*i*-Cp), 127.9 (d, 2 -*m* Ar, $^{3}J_{CP}$ = 12.1 Hz), 128.3(2 *m*-Ar), 128.5 (d, 2 *m*-Ar, $^{3}J_{CP}$ = 11.5 Hz), 129.4 (2 *o*-Ar), 131.0 (d, *i*-Ar, $^{1}J_{CP}$ = 74.5 Hz), 131.2 (d, *i*-Ar, $^{1}J_{CP}$ = 79.4 Hz), 131.3 (d, *p*-Ar, $^{4}J_{CP}$ = 2.9 Hz), 131.6 (d, *p*-Ar, $^{4}J_{CP}$ = 2.9 Hz), 132.0(d, 2 *o*-Ar, $^{2}J_{CP}$ = 9.4 Hz), 132.2 (d, 2 *o*-Ar, $^{2}J_{CP}$ = 9.6 Hz), 134.0 (*p*-Ar), 144.4 (*i*-Ar), 196.8 (d, *C*=O, $^{3}J_{CP}$ = 7.9 Hz). HRMS m/z (+ESI) $(M + H)^+$ calcd for C32H30O1P1S1Fe1: 549.1104, found: 533.1107.

FD5: Similar procedure to FD4; orange powder; yield: 90%. m.p. 205°C(decomp.); ^{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). HRMS m/z (+ESI) $(M + H)^+$ calcd for C29H26O2P1S2Fe1: 557.0461, found: 557.0423.

FD6: 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.

FD7: 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, $^{3}J_{HH}$ = 3.7 Hz, $^{2}J_{HP}$ = 20.0 Hz, - C*H*PPh2), 4.46 (dd, 1H, $^{3}J_{HH}$ = 3.6 Hz, $^{3}J_{HP}$ = 14.4 Hz, - C*H*), 4.95 (sep, 1H, $^{3}J_{HH}$ = 6.3 Hz, - C*H*), 5.08 (sep, 1H, $^{3}J_{HH}$ = 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, $^{1}J_{CP}$ = 67.1 Hz), 56.0 (d, - *C*H), 67.7 (-CH), 68.3 (-CH), 68.6 (d, *o*-Cp, $^{3}J_{CP}$ = 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, $^{3}J_{CP}$ = 11.7 Hz), 128.3 (d, 2 *m*-Ar, $^{3}J_{CP}$ = 11.4 Hz), 131.2 (d, *p*-Ar, $^{4}J_{CP}$ = 2.6 Hz),131.5 (d, *p*-Ar, $^{4}J_{CP}$ = 2.5 Hz), 131.6 (d, *i*-Ar, $^{1}J_{CP}$ = 99.7 Hz), 131.9 (d, 2 *o*-Ar, $^{2}J_{CP}$ = 9.0 Hz), 132.7 (d, 2 *o*-Ar, $^{2}J_{CP}$ = 8.6 Hz), 134.7 (d, *i*-Ar, $^{1}J_{CP}$ = 95.9 Hz), 167.7 (d, *C*=O, $^{3}J_{CP}$ = 4.4 Hz), 168.2 (d, *C*=O, $^{3}J_{CP}$ = 4.4 Hz). HRMS m/z (+ESI) $(M + H)^+$ calcd for C32H36O5P1Fe1: 587.1650, found: 587.1652.

FD8: 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, $^{1}J_{CP}$ = 36.2 Hz), 41.7(d, - *C*H2, $^{2}J_{CP}$ = 12.0 Hz), 67.7 (d, *o*-Cp, $^{3}J_{CP}$ = 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, $^{1}J_{CP}$ = 80.1 Hz), 128.4 (2 *m*-Ar), 128.6 (d, *i*-Ar, $^{1}J_{CP}$ = 86.1 Hz), 128.7 (d, 2 *o*-Ar, $^{2}J_{CP}$ = 11.6 Hz), 129.3 (d, 2 *o*-Ar, $^{2}J_{CP}$ = 11.2 Hz), 129.7 (2 *o*-Ar), 132.0 (d, *p*-Ar, $^{4}J_{CP}$ = 2.5 Hz), 132.3 (d, *p*-Ar, $^{4}J_{CP}$ = 2.4 Hz), 132.3 (d, 2 -*m* Ar, $^{3}J_{CP}$ = 11.5 Hz), 133.7 (*p*-Ar), 134.3 (d, 2 *m*-Ar, $^{3}J_{CP}$ = 13.0 Hz), 134.6 (d, 2 *m*-Ar, $^{3}J_{CP}$ = 13.0 Hz), 145.0 (*i*-Ar), 196.0 (d, *C*=O, $^{3}J_{CP}$ = 9.1 Hz). HRMS m/z (+ESI) $(M + H)^+$ calcd for C32H30O1P1Cl1Fe1Au1: 749.0738, found: 749.0739.

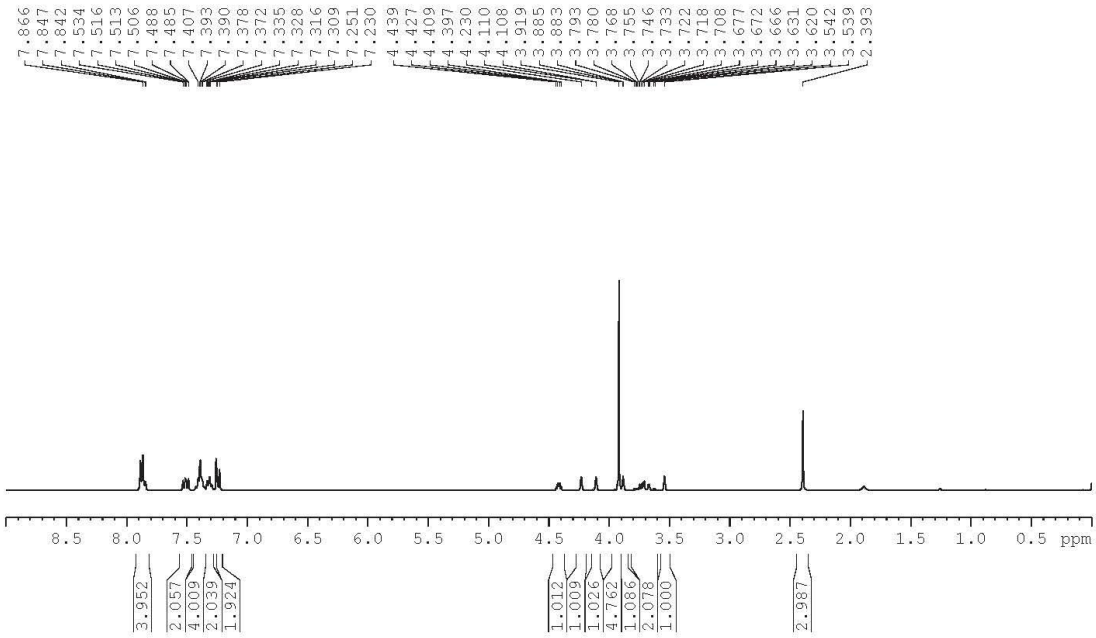
FD9: Similar procedure to FD8; brownish-orange powder; yield: 89%. m.p. 178°C(decomp.); ^{1}H NMR ($CDCl_3$, 300 MHz): 3.45 (m, 1H, Cp), 3.53 - 3.92 (m, 2H, - CH_2), 4.01 (m, 1H, Cp), 4.12 (m, 5H, Cp), 4.21 (m, 2H, Cp), 4.70 (m, 1H, - C*H*PPh_2), 6.49 (s, 1H, - Ar), 7.34 – 7.69 (m, 8H, - Ar), 7.74 – 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, $^{1}J_{CP}$ = 34.6 Hz), 47.2(d, -*C*H_2, $^{2}J_{CP}$ = 12.7 Hz), 67.6 (d, *o*-Cp, $^{3}J_{CP}$ = 4.4 Hz), 68.1 (*m*-Cp), 68.8 (5Cp), 69.4 (*m*-Cp), 69.8 (d, *o*-Cp, $^{3}J_{CP}$ = 1.9 Hz), 86.8 (d, *i*-Cp, $^{2}J_{CP}$ = 7.3 Hz), 122.7 (q, *C*F_3, $^{1}J_{CF}$ = 273.4 Hz), 122.9 (q, *C*F_3, $^{1}J_{CF}$ = 274.2 Hz), 123.9(m, p-Ar), 127.5 (d, *i*-Ar, $^{1}J_{CP}$ = 74.3 Hz), 127.6 (m, *m*-Ar), 127.8 (m, *m*-Ar), 128.1 (d, *i*-Ar, $^{1}J_{CP}$ = 81.4 Hz), 128.9 (d, 2 *o*-Ar, $^{2}J_{CP}$ = 11.8Hz), 129.6 (d, 2 *o*-Ar, $^{2}J_{CP}$ = 11.1 Hz), 130.2 (q, *m*-Ar, $^{2}J_{CF}$ = 32.8 Hz), 132.4 (d, *p*-Ar, $^{4}J_{CP}$ = 2.5 Hz), 133.0 (d, *p*-Ar, $^{4}J_{CP}$ = 2.2 Hz), 134.4 (q, *m*-Ar, $^{2}J_{CF}$ = 33.0 Hz), 134.6 (d, 2 -*m* Ar, $^{3}J_{CP}$ = 13.3 Hz), 135.2 (d, 2 -*m* Ar, $^{3}J_{CP}$ = 13.8 Hz), 140.3 (s, *i*-Ar), 141.2 (*i*-Ar), 199.2 (d, *C*=O, $^{3}J_{CP}$ = 4.6 Hz). HRMS m/z (+ESI) $(M + H)^+$ calcd for C33H26O1P1Cl1Fe1Au1F6: 871.0329, found: 871.0333.

FD10: Similar procedure to FD8; 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, $^{1}J_{CP}$ = 35.6 Hz), 41.3 (d, -*C*H_2 , $^{2}J_{CP}$ = 11.9 Hz), 67.6 (d, *o*-Cp, $^{3}J_{CP}$ = 4.4 Hz), 67.8 (*m*-Cp), 68.3 (5Cp), 69.2 (*m*-Cp), 70.1 (d, *o*-Cp, $^{3}J_{CP}$ = 1.9 Hz), 86.6 (d, *i*-Cp, $^{2}J_{CP}$ = 6.9 Hz), 112.8 (furyl Ar), 118.1 (furyl Ar), 127.8 (d, *i*-Ar, $^{1}J_{CP}$ = 72.5 Hz), 128.4 (d, *i*-Ar, $^{1}J_{CP}$ = 78.6 Hz), 128.7 (d, 2 *o*-Ar, $^{3}J_{CP}$ = 11.6 Hz), 129.2 (d, 2 *o*-Ar, $^{3}J_{CP}$ = 11.2 Hz), 132.1 (d, *p*-Ar, $^{4}J_{CP}$ = 2.7 Hz), 132.3 (d, *p*-Ar, $^{4}J_{CP}$ = 2.6 Hz), 134.4 (d, 2 *m*-Ar, $^{2}J_{CP}$ = 13.1 Hz), 134.6 (d, 2 *m*-Ar, $^{2}J_{CP}$ = 13.2 Hz), 147.1 (furyl Ar), 152.1 (furyl Ar), 185.6 (d, *C*=O, $^{3}J_{CP}$ = 8.9 Hz). HRMS m/z (+ESI) $(M + H)^+$ calcd for C29H26O2P1Cl1Fe1Au1: 725.0374, found: 725.0370.

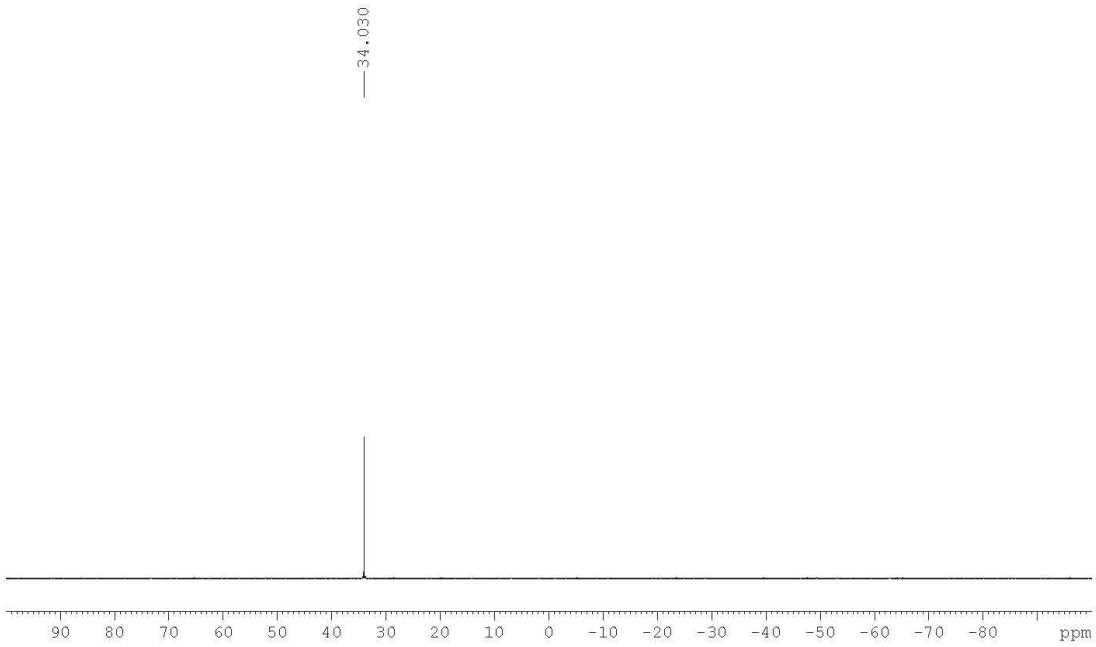
The solid gold complexes may be kept over a year under ambient conditions without signs of decomposition. The chemical structure of **FD10** has been verified by ^{1}H, ^{13}C NMR and HRMS. Since no other phosphine species was observed in the ^{31}P{^{1}H} NMR in DMSO, we find that the synthesized gold compound **FD10** is verifiably stable in the DMSO solution. While, we do not have absolute evidence of Gold(I) being leached in cytoplasmic environment as aggregates or nanoparticles, it might be a possible mechanism of action of the drug as Gold(I) complexes may undergo ligand exchange with biological ligands in cells.

II. ^{1}H, $^{31}P\{^{1}H\}$, $^{19}F\{^{1}H\}$ & ^{13}C Spectra of FD1-FD10 compounds

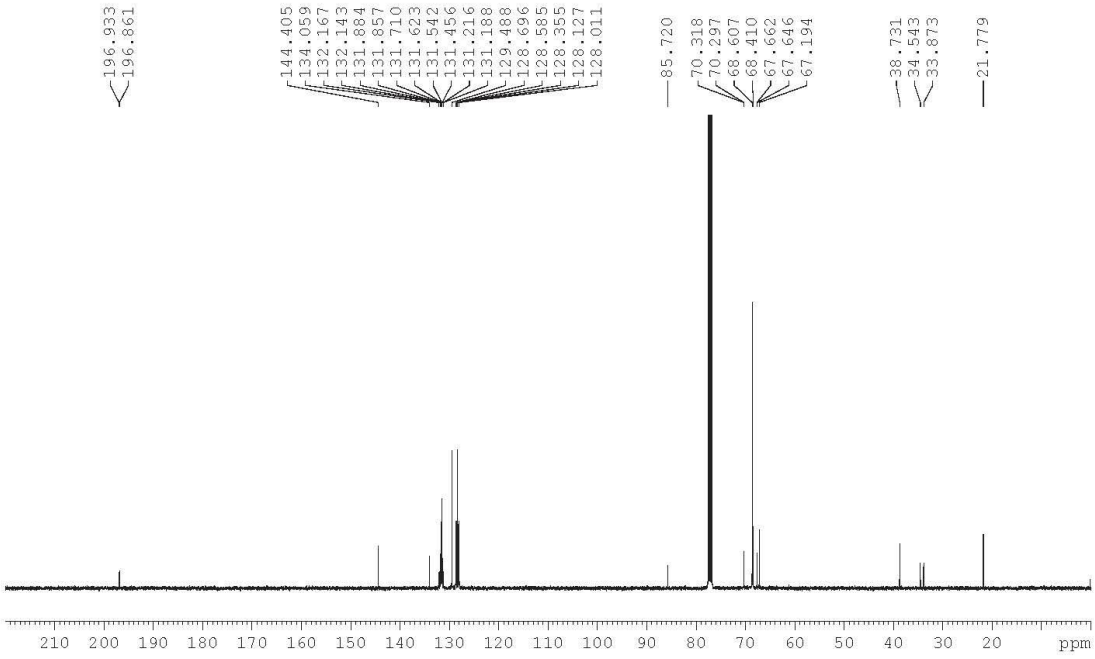
FD1.
CDCl3
1H



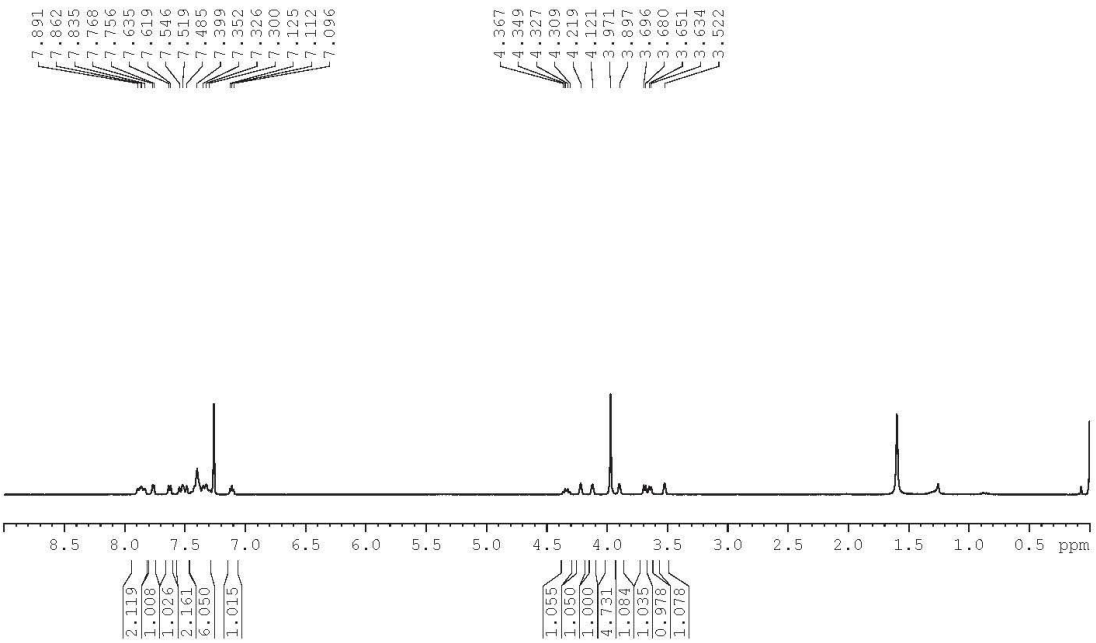
FD1.
CDCl3
31P



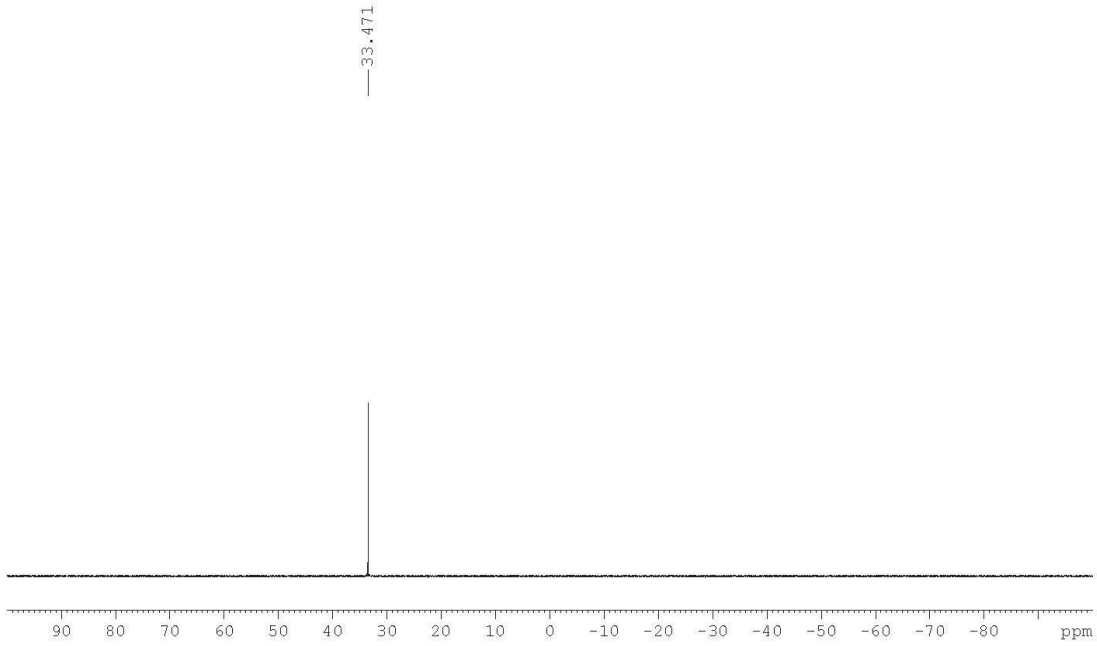
FD1.
CDCl3
13C



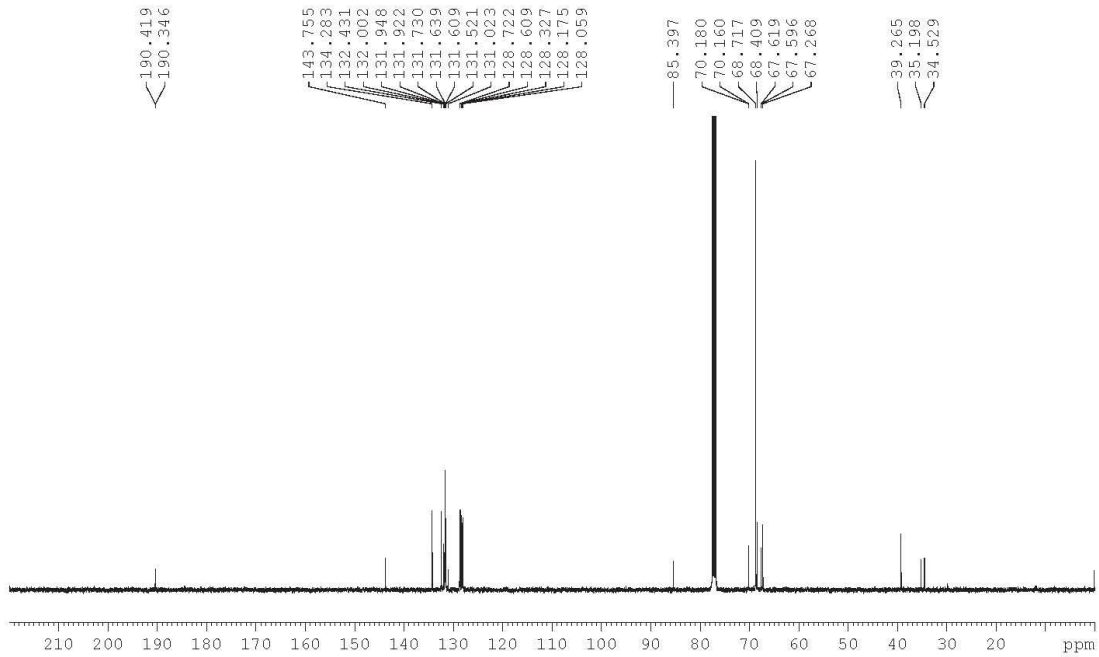
FD2.
CDCl3
1H



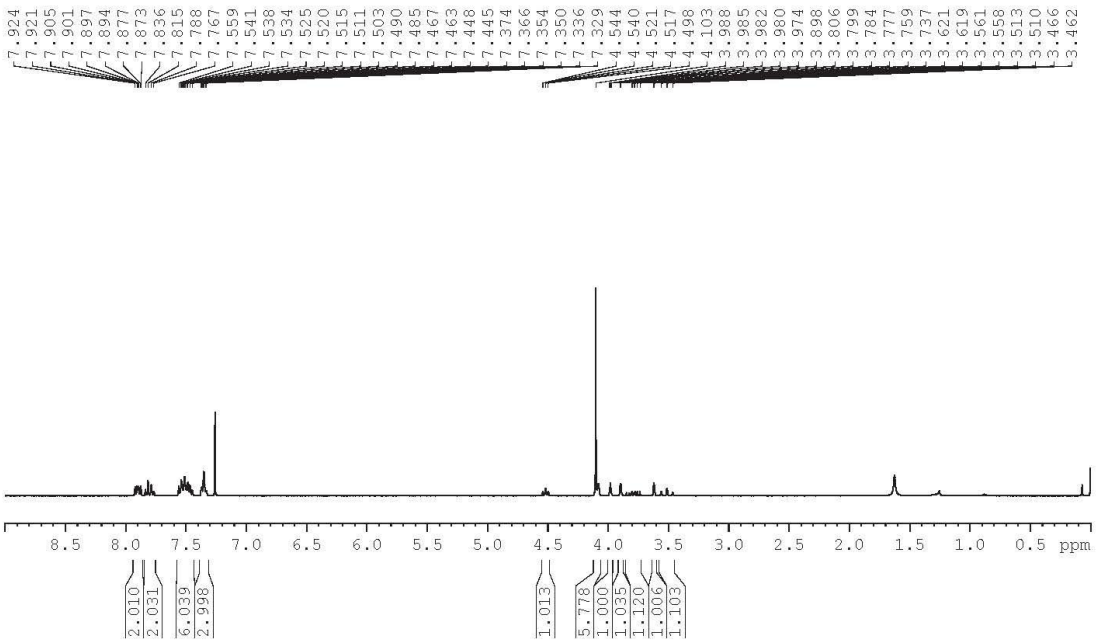
FD2.
CDCl3
31P{1H}



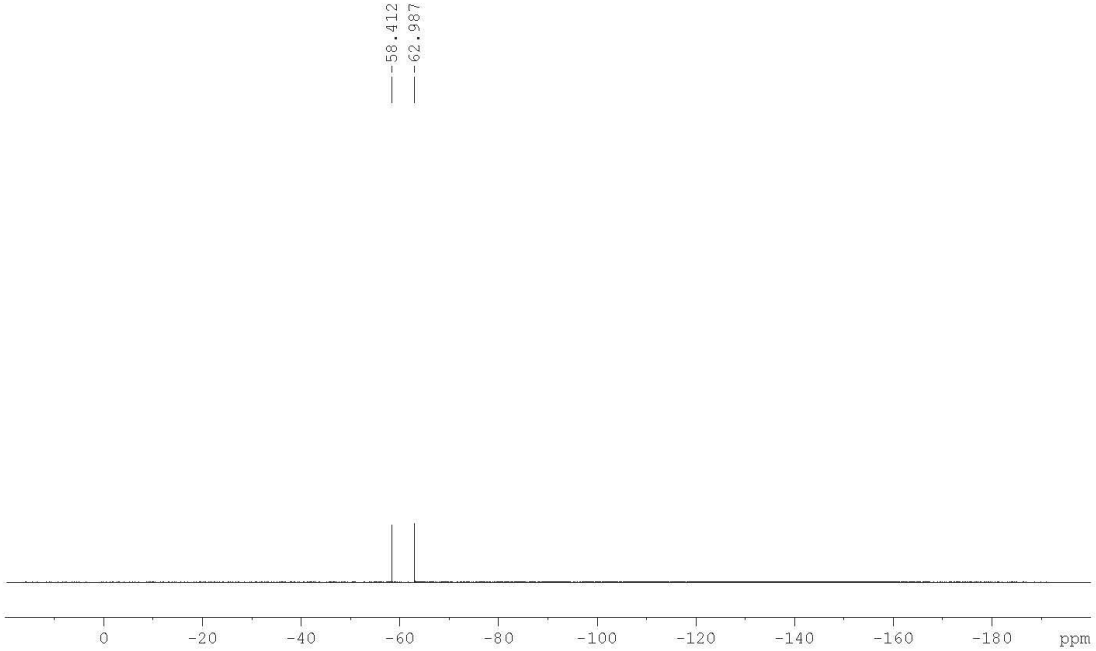
FD2.
CDCl3
13C



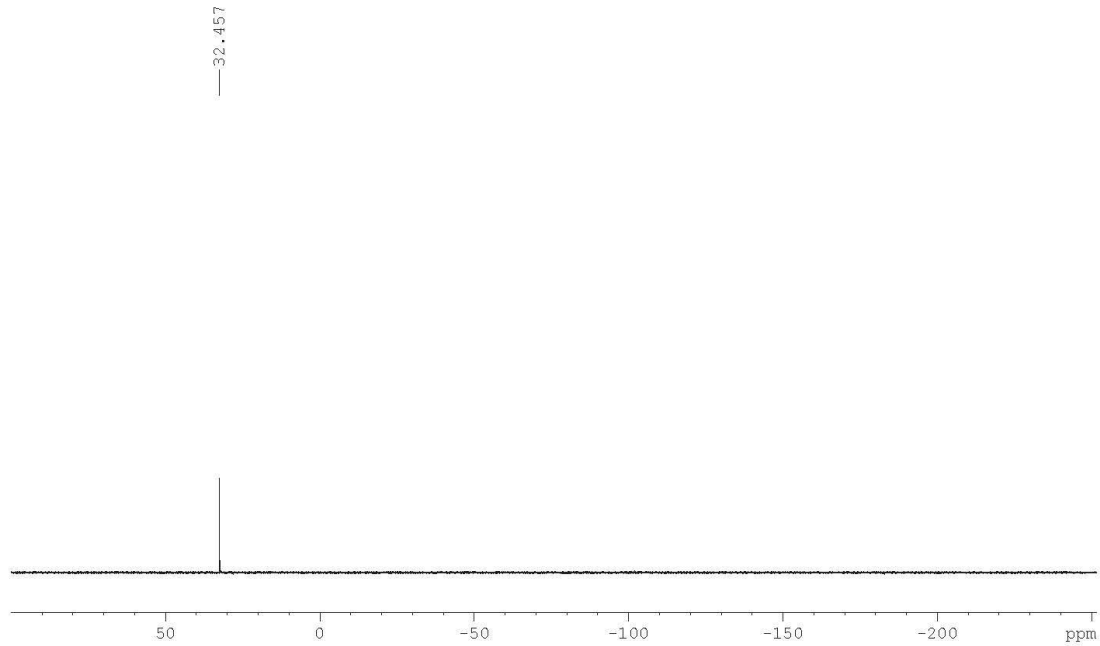
FD3.
CDCl3
1H



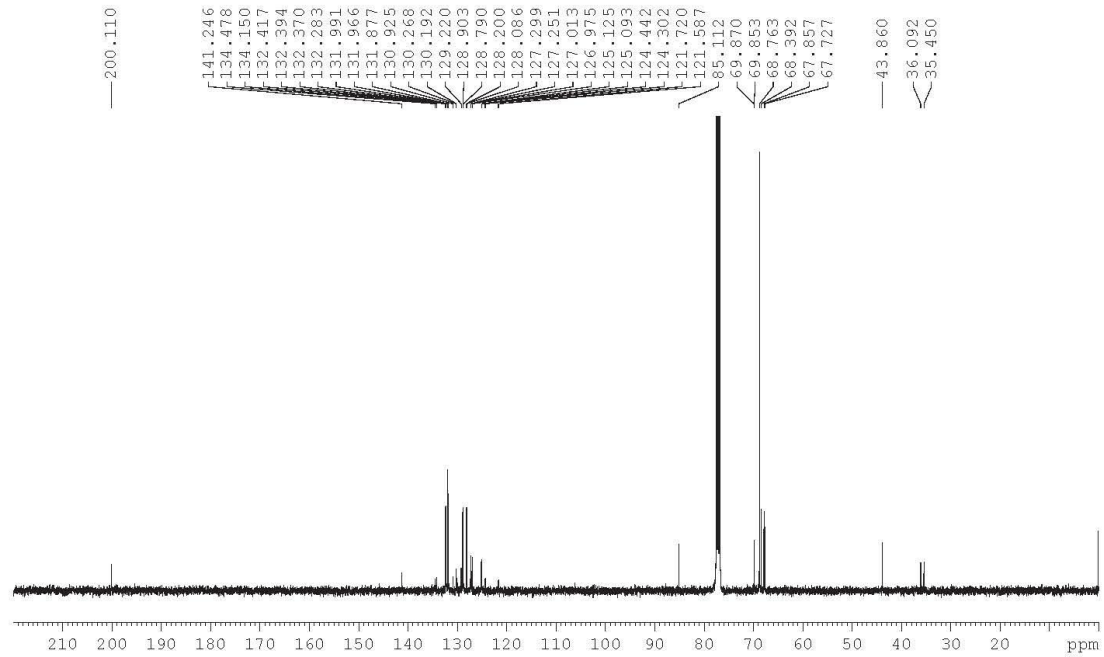
FD3.
CDCl3
19F{1H}



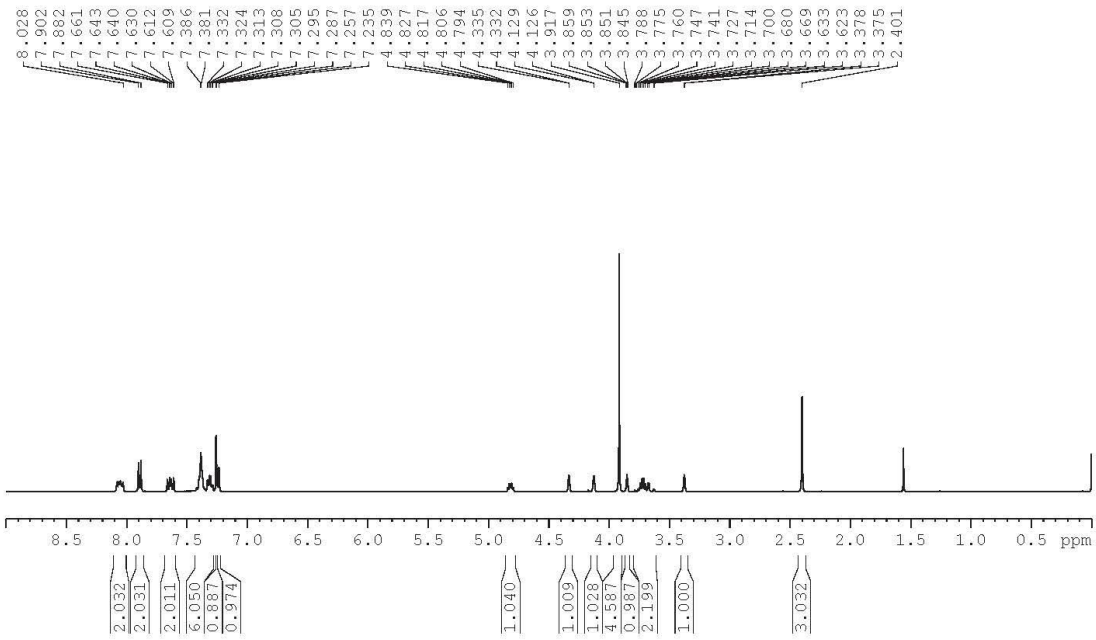
FD3.
CDCl3
31P{1H}



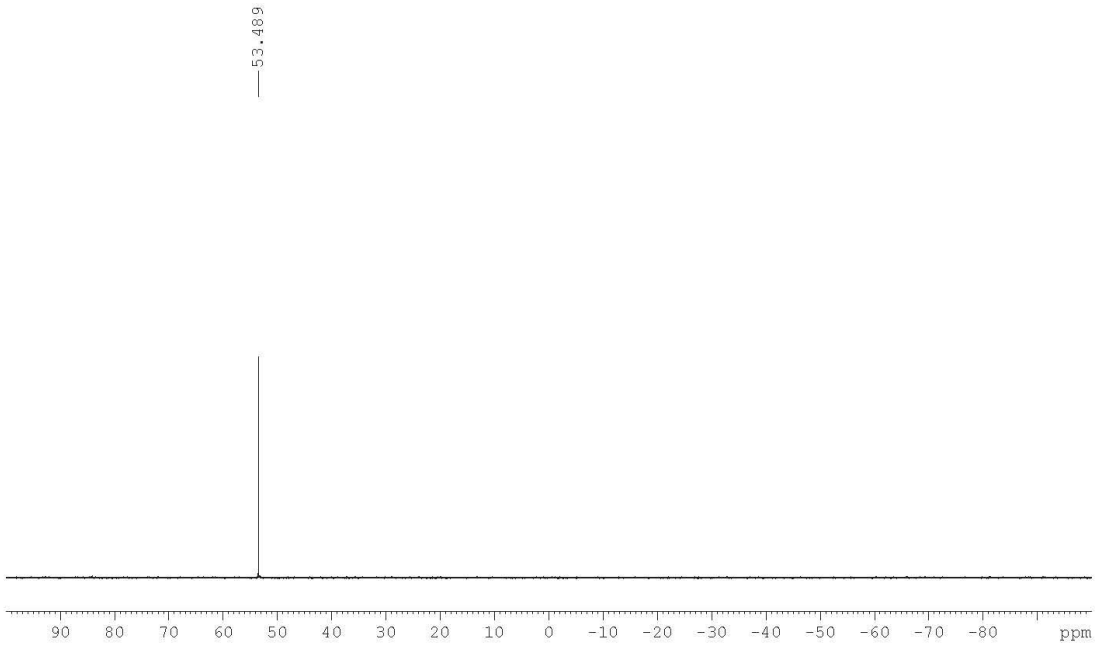
FD3.
CDCl3
13C



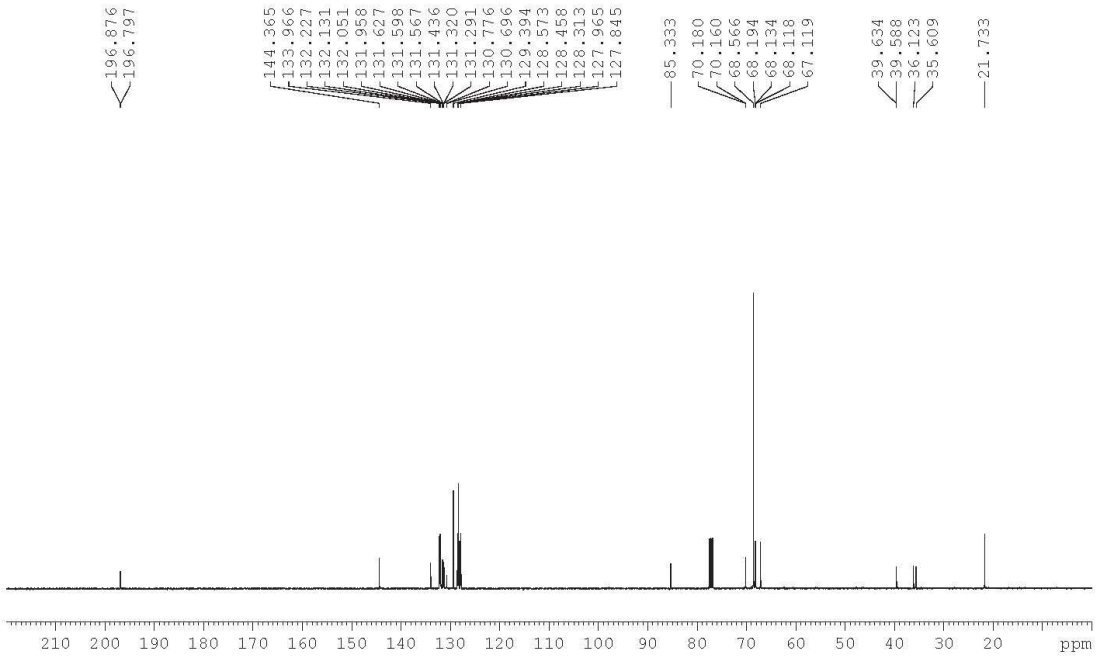
FD4.
CDCl3
1H



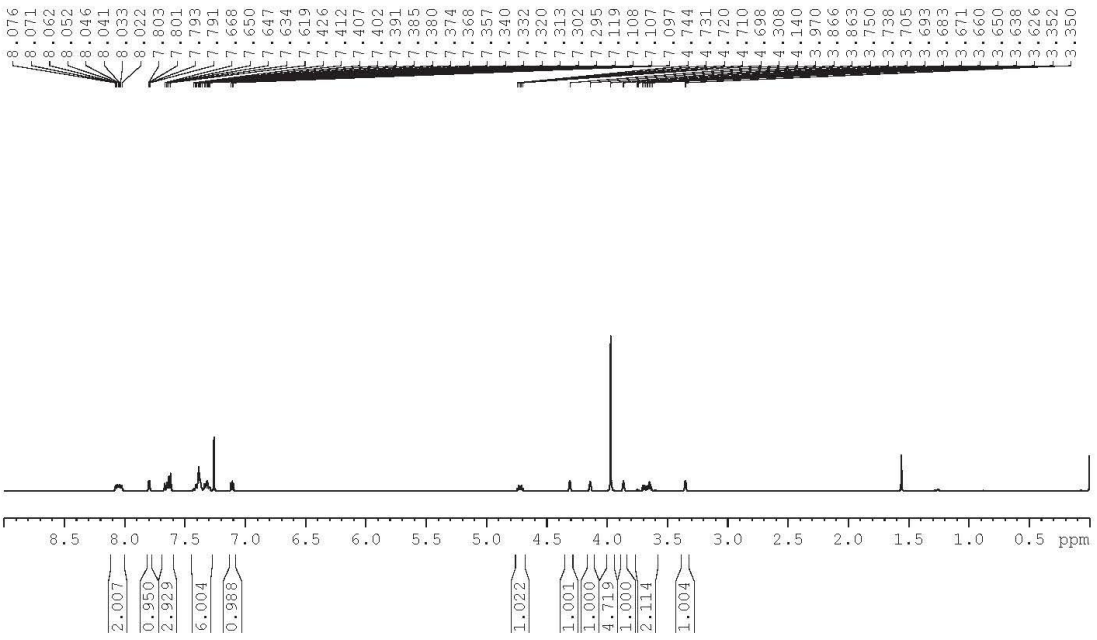
FD4.
CDCl3
31P{1H}



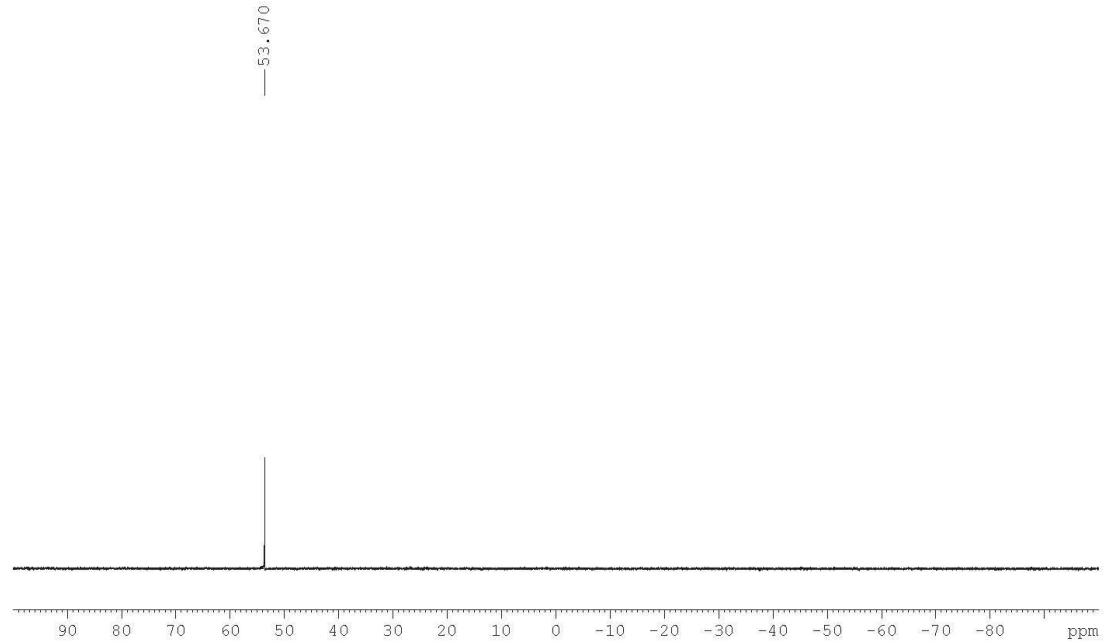
FD4.
CDCl3
13C



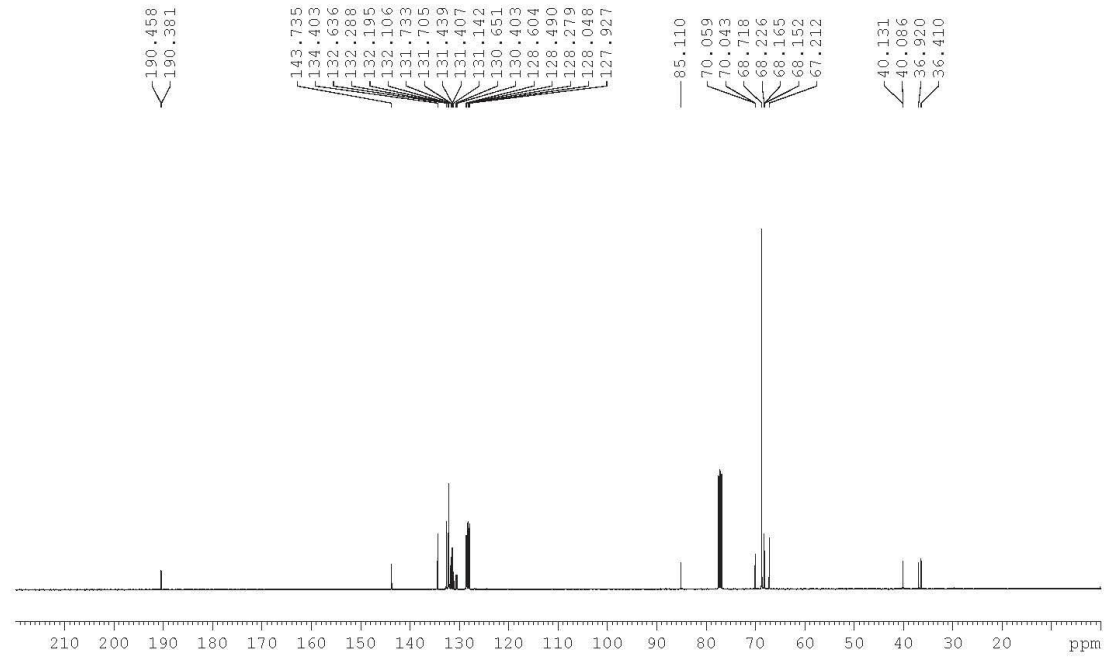
FD5
CDCl3
1H



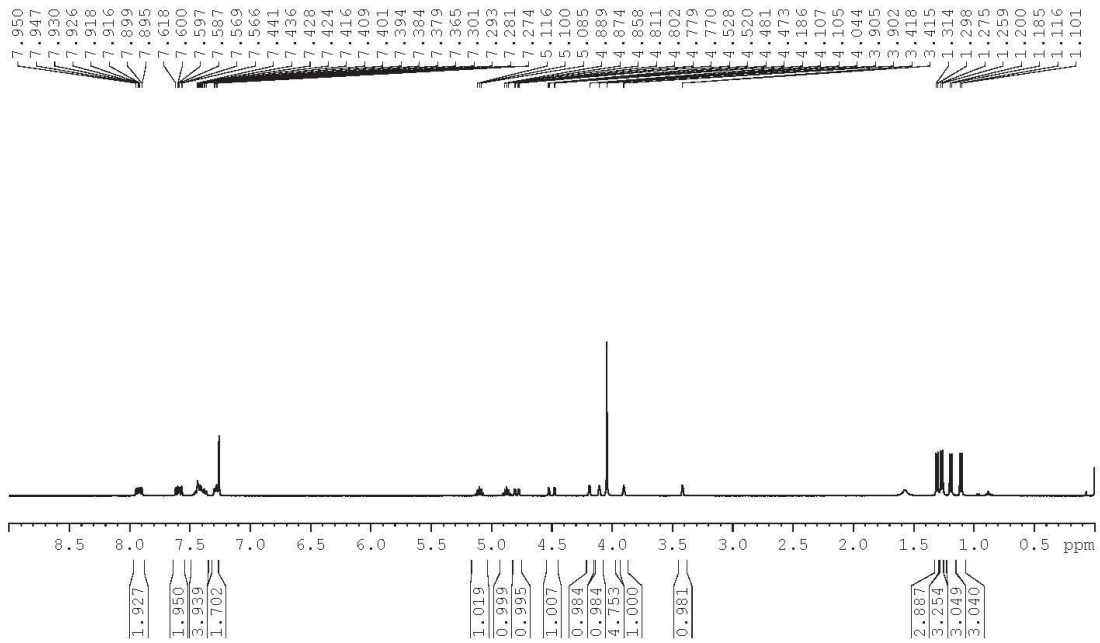
FD5.
CDCl3
31P{1H}



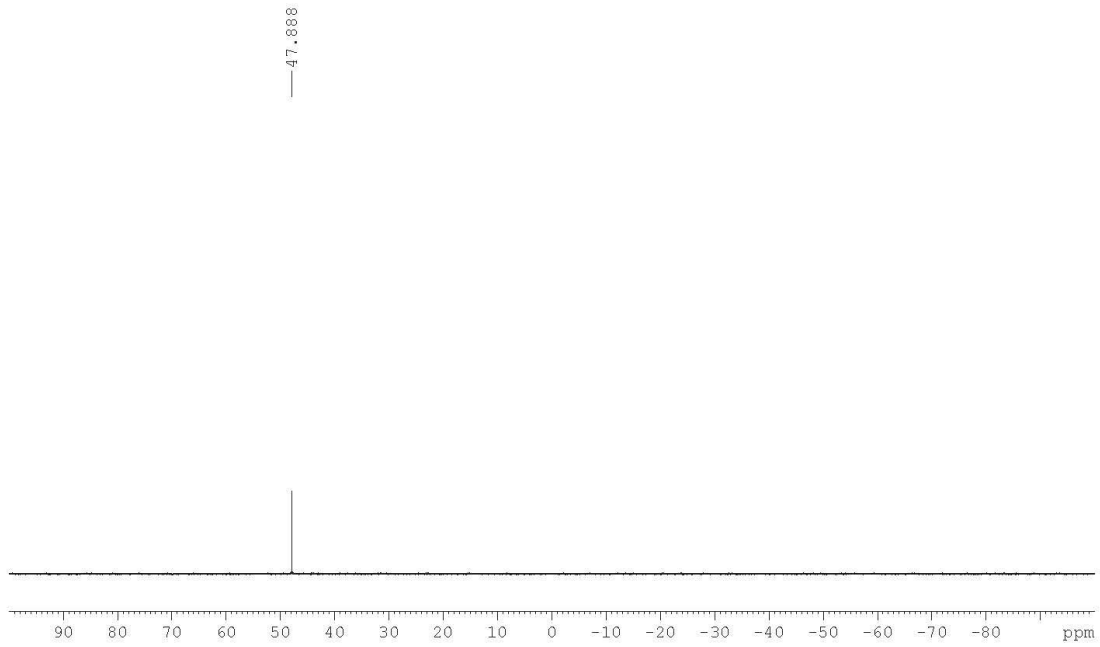
FD5
CDCl3
13C



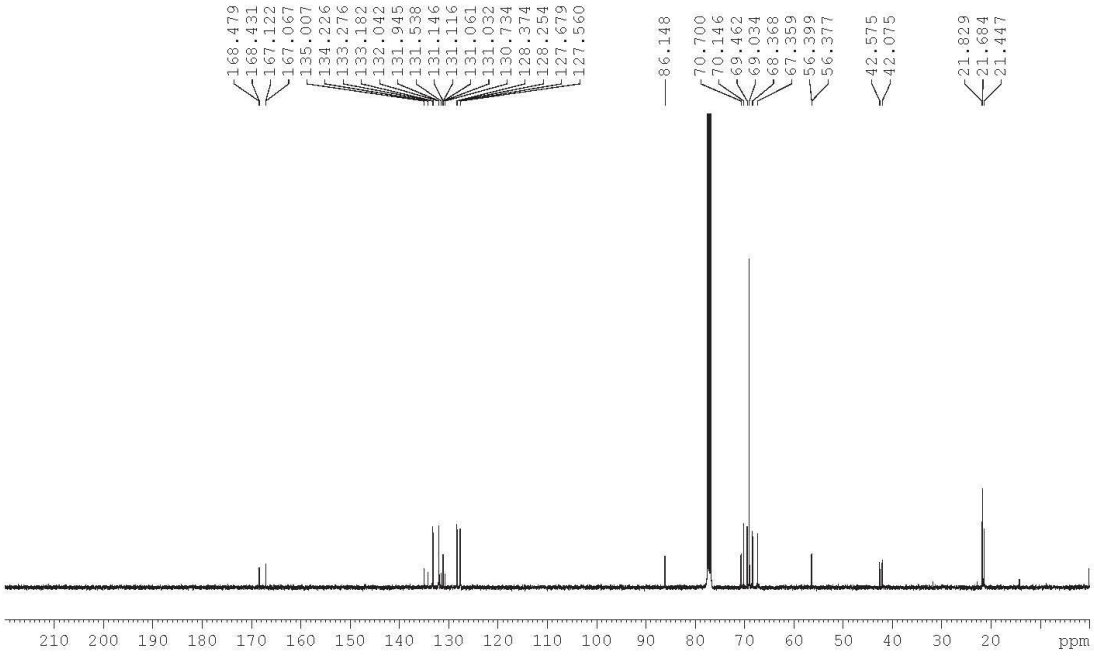
FD6.
CDCl3
1H



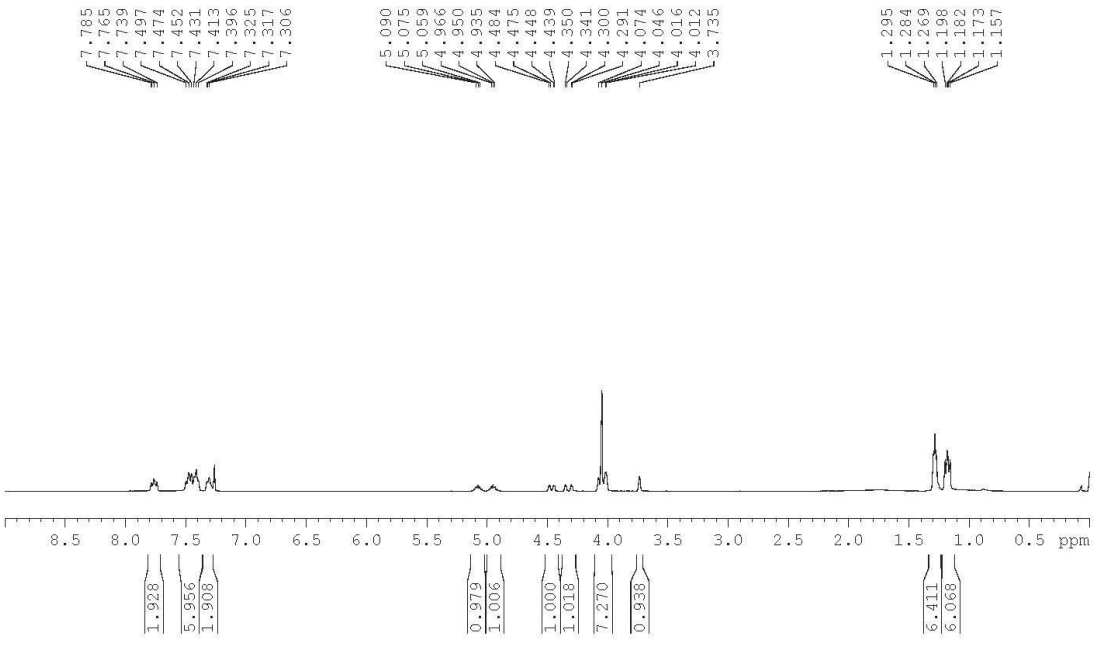
FD6.
CDCl3
31P{1H}



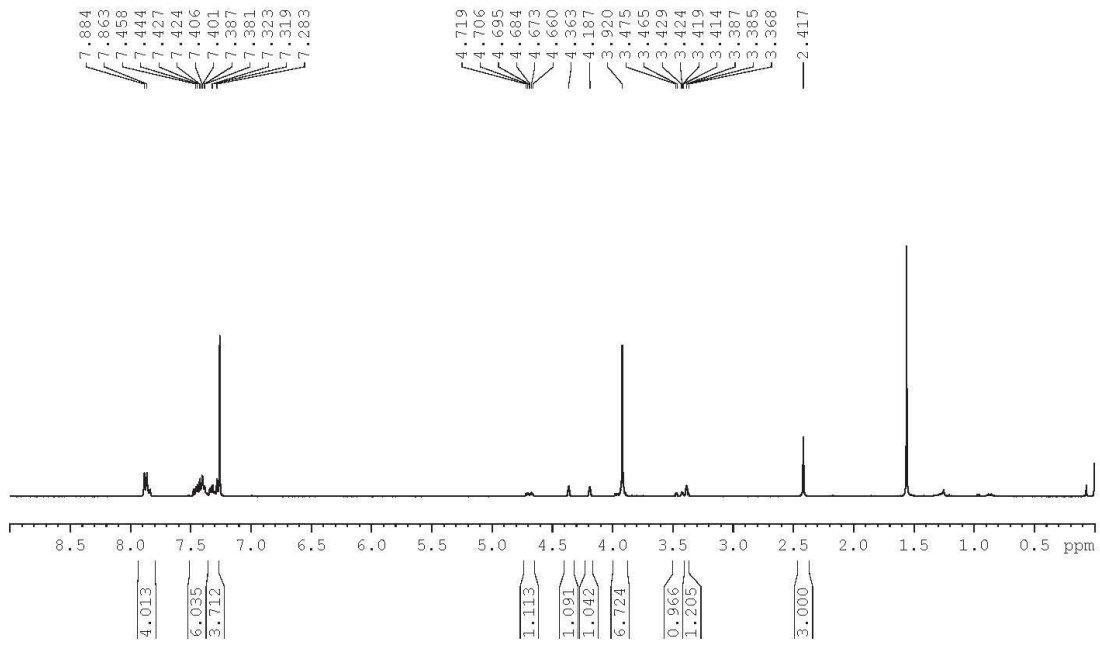
FD6.
CDCl3
13C



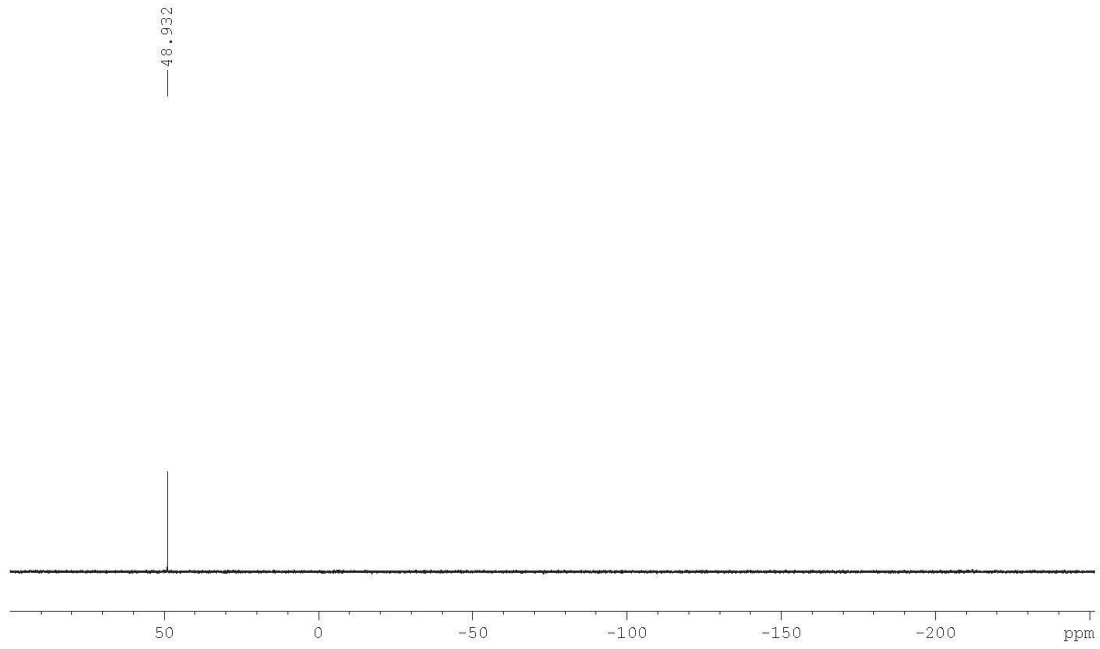
FD7.
CDCl3
1H



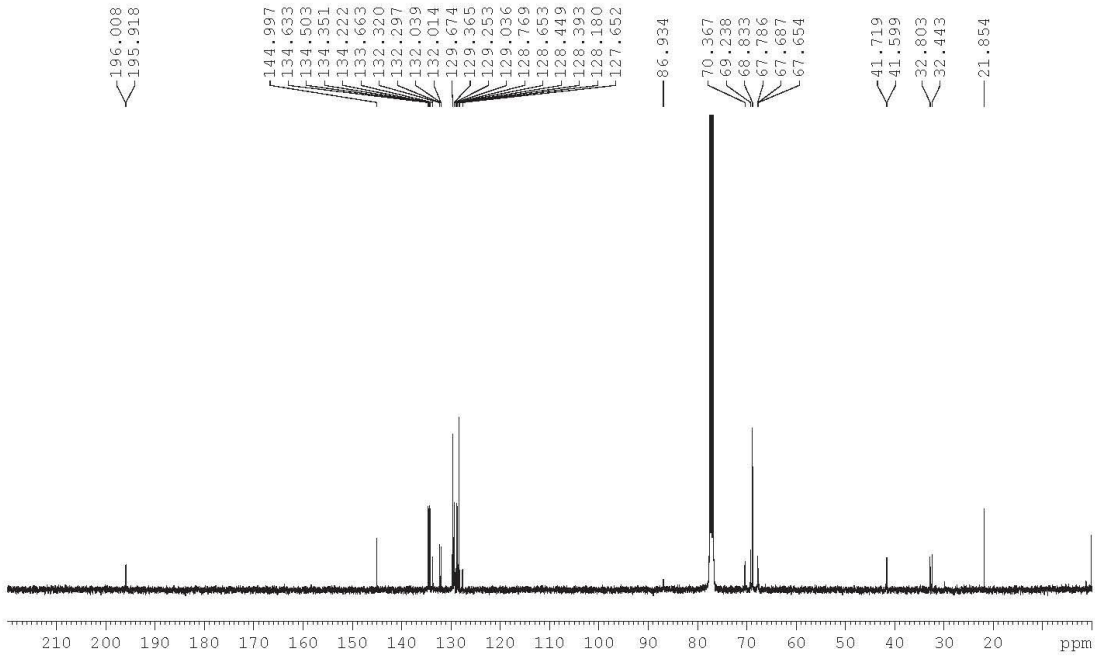
FD8
1H, CDCl3



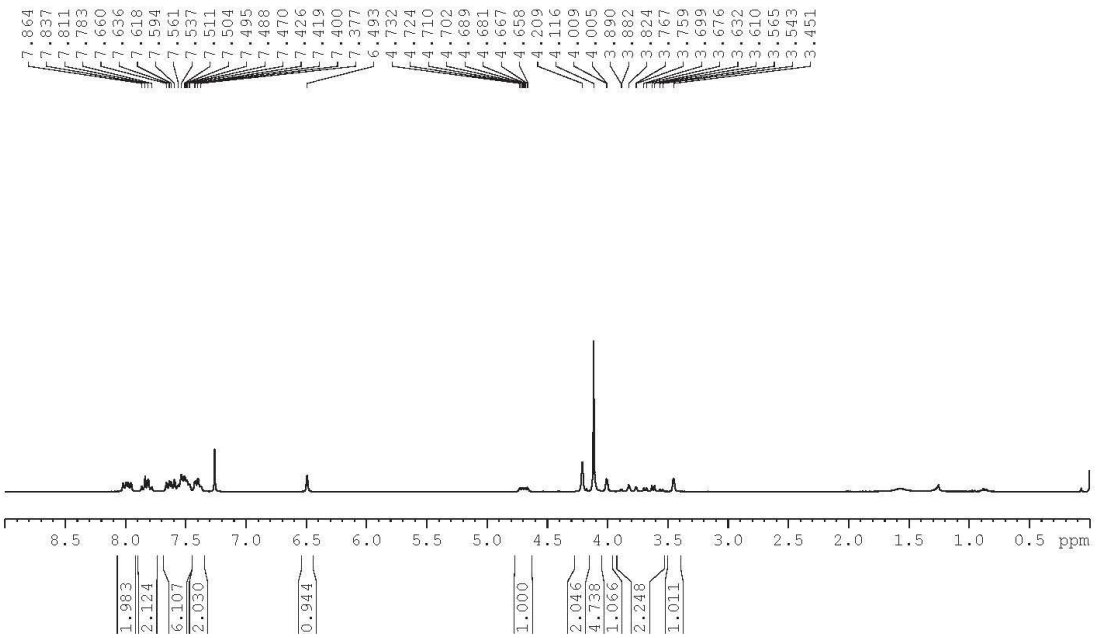
FD8
31P, CDCl3



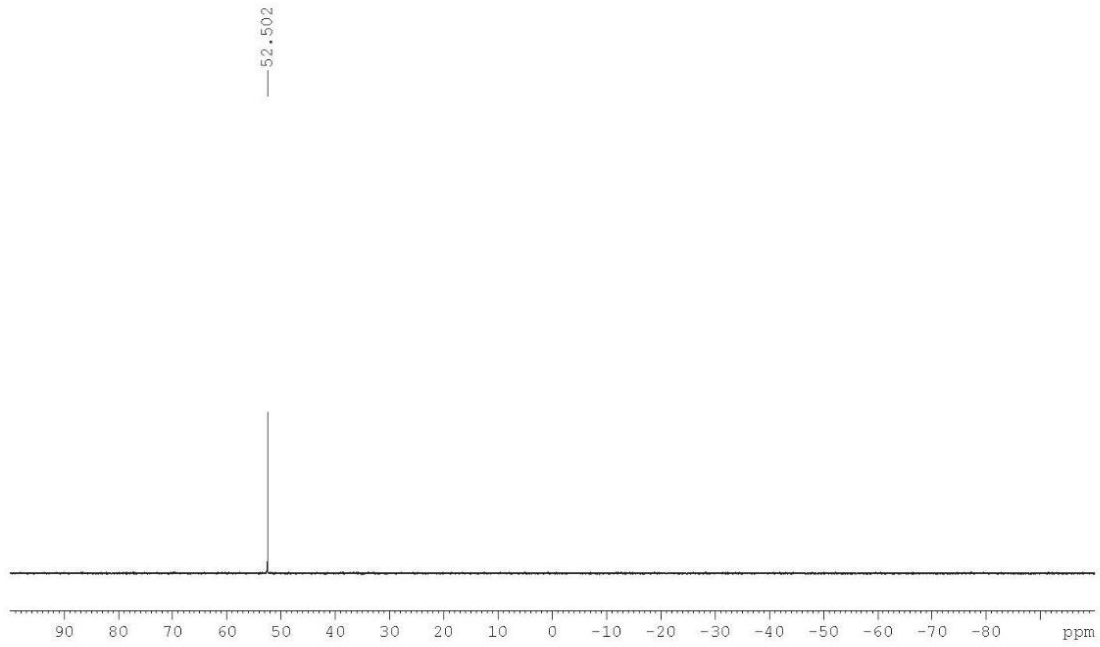
FD8.
CDCl3
13C



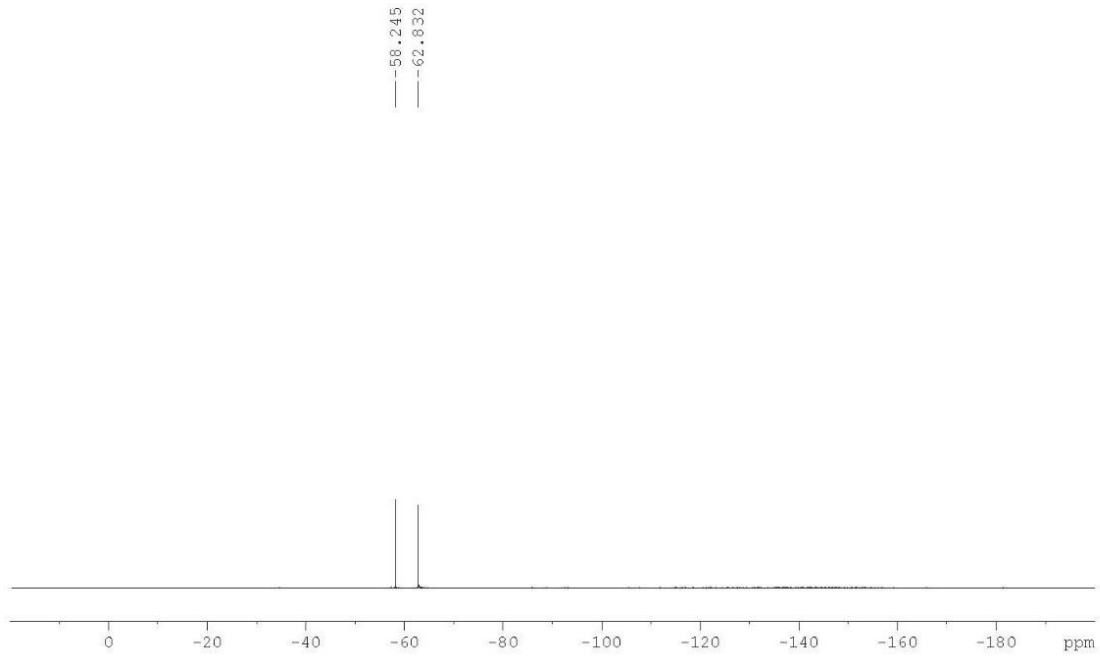
FD9.
CDCl3
1H



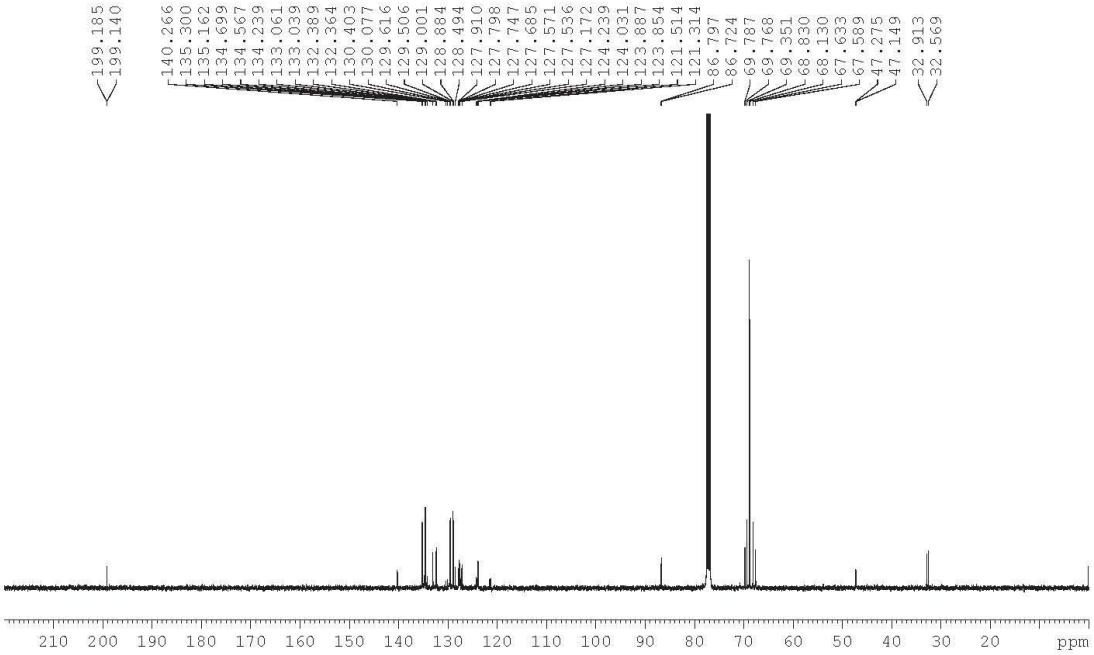
FD9.
CDCl3
31P{1H}



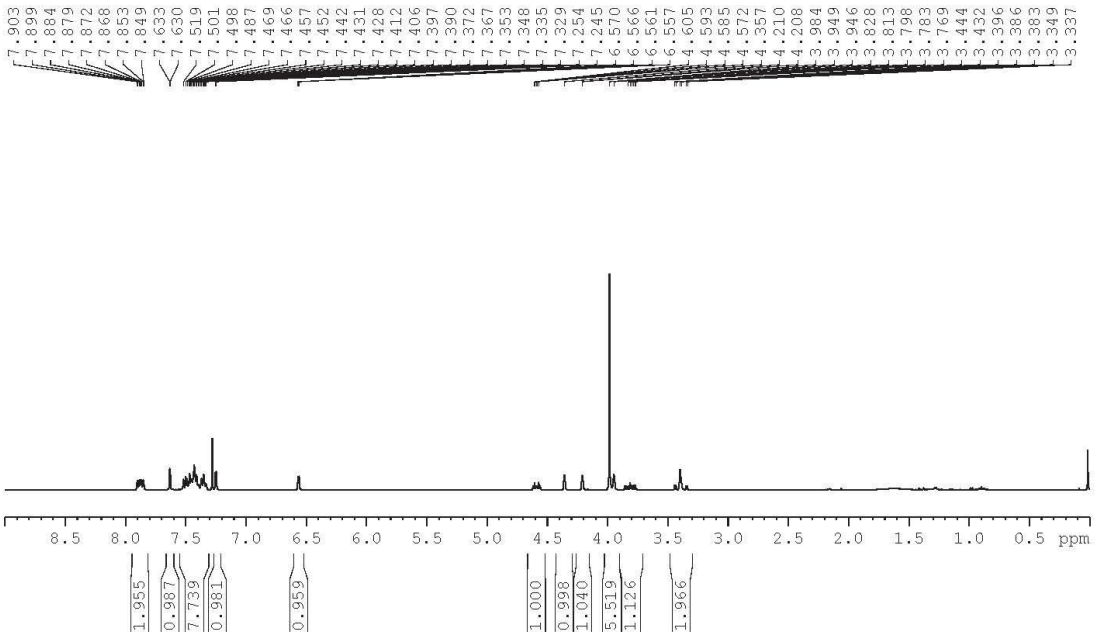
FD9.
CDCl3
19F{1H}



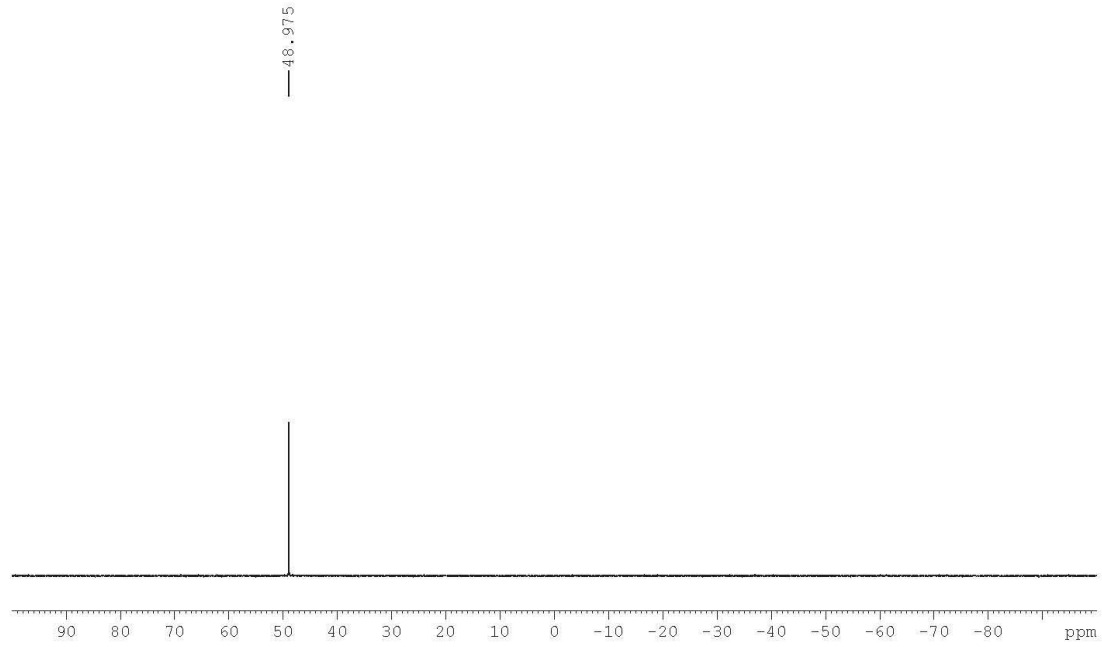
FD9.
CDCl3
13C



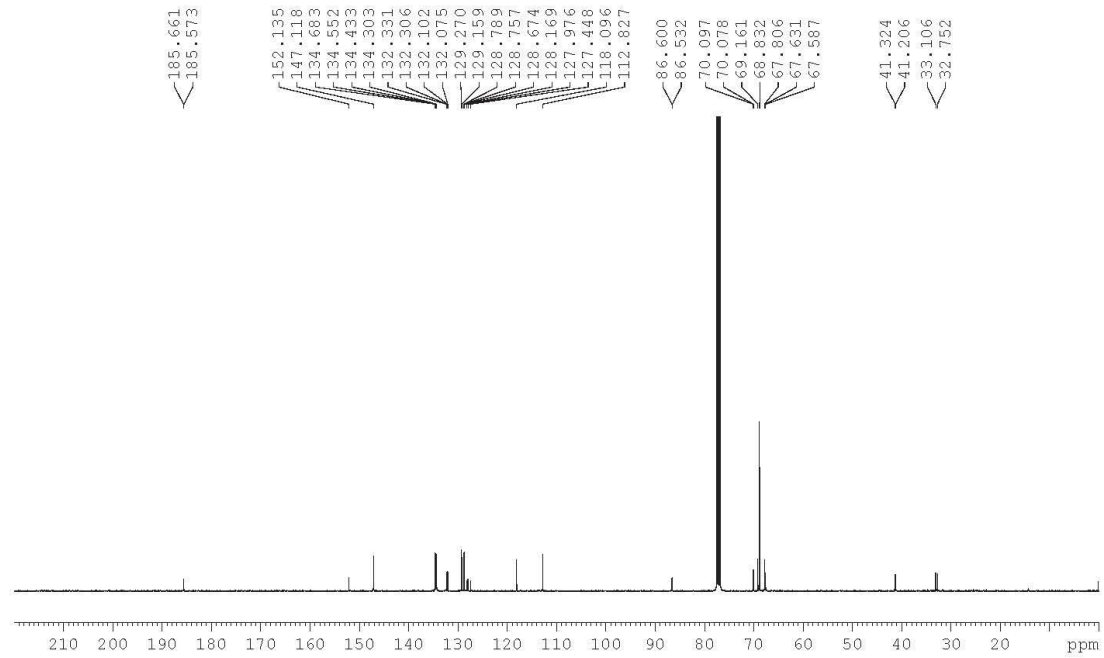
FD10.
CDCl3
1H



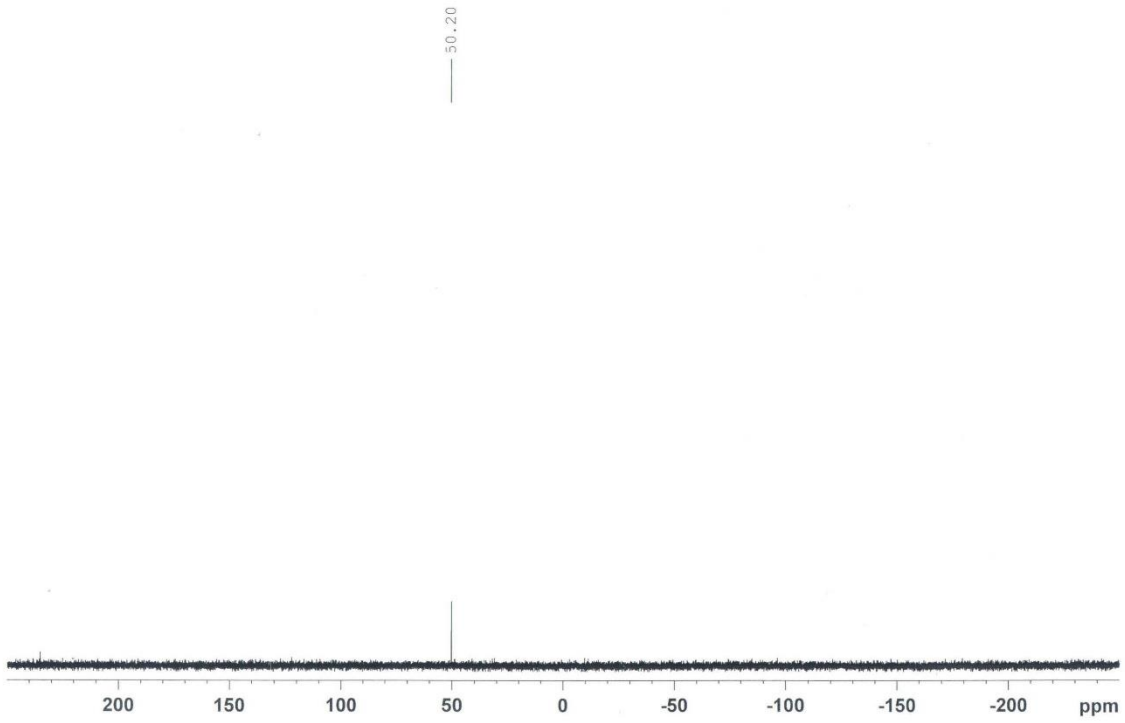
FD10.
CDCl3
31P{1H}



FD10.
CDCl3
13C



FD10
DMSO
31P{1H}



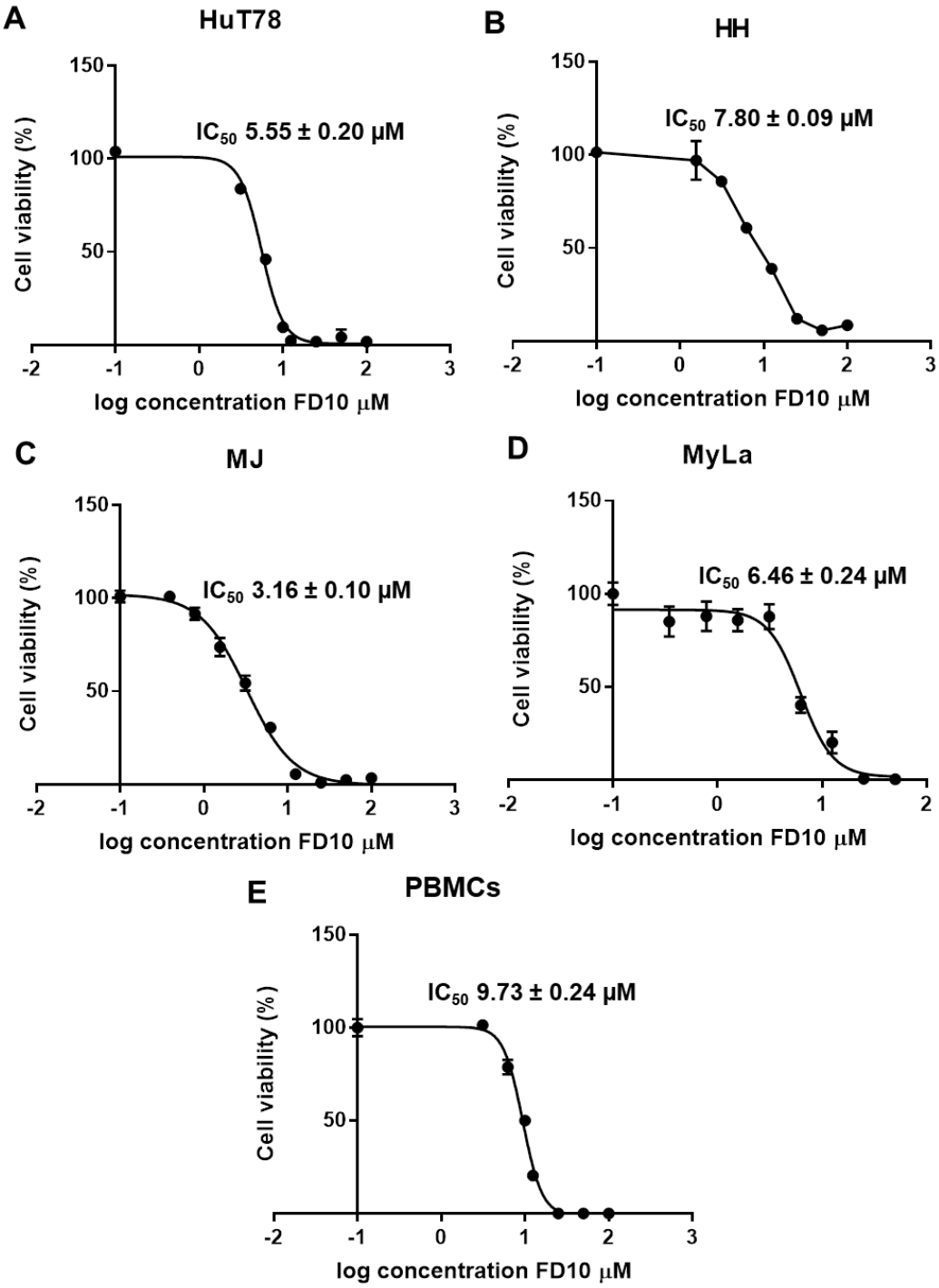


Figure S1. Cell viability graph indicating IC_{50} values of **FD10** in Hut78 **(A)**, HH **(B)**, MJ **(C)**, MyLa **(D)** and PBMCs **(E)**. Cells were treated with increasing concentrations of FD10 (1 – 100 µM) in triplicates for 24 h and cell viability percentage (%) was determined by MTS-based assay. Values were plotted using GraphPad Prism software and IC_{50} values were determines as indicated in the graphs. Data represents at least 3 independent experiments.