Supporting Information

Breaking the regioselectivity rule for acrylate insertion in the Mizoroki-Heck reaction

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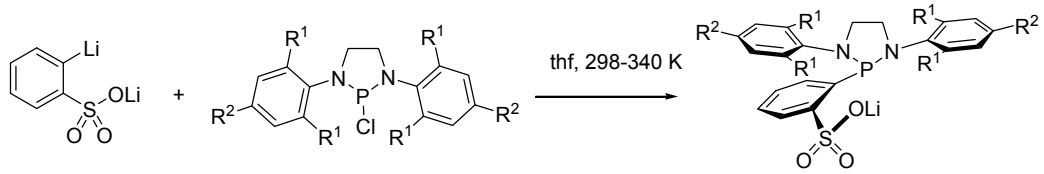
Materials and Experimental General Considerations

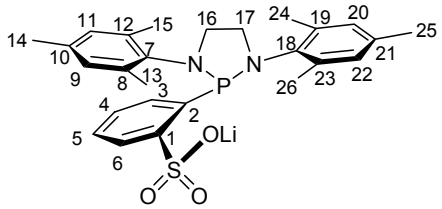
Unless noted otherwise, all manipulations of phosphorous halides or palladium complexes were carried out under an inert nitrogen or argon atmosphere using standard glovebox or Schlenk techniques. Methylene chloride, DMSO and pentane were destilled from calcium hydride, toluene and benzene from sodium, THF and diethyl ether from blue sodium/benzophenone ketyl, and methanol from activated (iodine) magnesium under argon prior to use. Acetone p.a. and methyl acrylate were degassed by repetitive freeze/thaw-cycles and used without further purification. All other solvents were commercial grade. 2,4,6-Trimethylaniline (98%) and 2,6-di(isopropyl)aniline (90%, technical grade) was purchased from Acros, and palladium(II)-chloride was obtained from Merck. Trichlorophosphine (99%) was purchased from Riedel-de Haën. Cyclooctadiene palladium methyl chloride ([(COD)PdMeCl]) (1) and 2-chloro-1,3-di(aryl)-1,3,2-diazaphospholidines (2) were synthesized according to literature procedures. All deuterated solvents were supplied by Eurisotop.
NMR spectra were recorded on a Varian Unity Inova 400, a Bruker Avance III DRX 400 or a Bruker Avance DRX 600 instruments. ^{1}H NMR spectra were referenced to residual protiated solvent signals. ^{13}C NMR spectra were referenced to the solvent signals, and ^{31}P NMR spectra to external 85% H_3PO_4. ^{1}H NMR spectra are reported as follows: chemical shift (δ ppm), multiplicity, coupling constant (Hz), and integration. Multiplicities are given as follows (or combinations thereof): s: singlet, d: doublet, t: triplet, sept: septet, m: multiplet, v[m]: virtual multiplet; br.: broad, v. br.: very broad. The identity of metal complexes and detailed NMR assignments were established by 2D NMR experiments (^{1}H-^{1}H gCOSY, ^{1}H-^{13}C gHSQC and ^{1}H-^{13}C gHMBC) in addition to 1D NMR experiments. NMR temperature calibration was performed using pure methanol (low temperature) or ethylene glycol (high temperature) samples.

Experimental Procedures

Ligand Synthesis



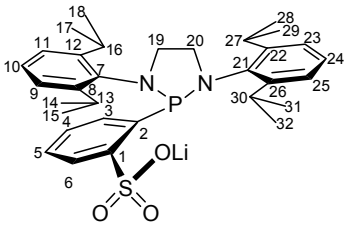
Lithium 2-(1,3-dimesityl-1,3,2-diazaphospholidin-2-yl)benzenesulfonate (L1a)



To a solution of benzenesulfonic acid (1582 mg, 10 mmol) in thf (35 mL) in a septum capped Schlenk tube was slowly added by syringe butyl lithium (14 mL 1.6 M pentane solution, 22.4 mmol) at 298 K under stirring. The formed suspension was stirred for 30 min at 298 K, then cannula transferred into a Schlenk frit, and filtrated. After washing with pentane (4 x 15 mL) the off-white powder was dried under high vacuum (10^{-3} mbar) to leave *o*-dilithiobenzenesulfonate•(0.75 THF) (2180 mg, 9.60 mmol, 96 %) which was used in the next step without further purification.

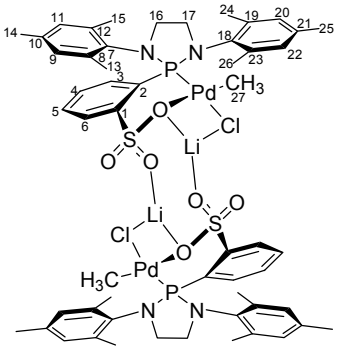
To *o*-dilithiobenzenesulfonate•(0.75 THF) (493 mg, 2.2 mmol) and 2-chloro-1,3-dimesityl-1,3,2-diazaphospholidine (742 mg, 2.06 mmol) in a 100 mL Schenk-tube was added THF (50 mL) and the resulting suspension was stirred for 4 hours at room temperature while a clear solution was obtained. The solvent was removed in vacuo (10^{-3} mbar), the remaining solid suspended in pentane (20 mL), and the suspension cannula transferred into a Schlenk-frit and washed with pentane (3 × 10 mL) to yield ligand **L1a** containing ca 0.2 equiv of THF (910 mg, 1.81 mmol, 87.8 %). ^{1}H NMR (400 MHz, 298K, methanol-d_4): δ 8.37 (d, $^{3}J_{HH}$ = 7.6 Hz, 1H, 6-H), 7.83 (m, 1H, 3-H), 7.49 (m, 1H, 5-H), 7.30 (m, 1H, 4-H), 6.70 (s br., 4H, 9-, 11-, 20-, and 22-H), 4.19 and 3.36 (m each, 2:2H, 16- and 17-H_2), 2.15 (s br., 18H, 13-, 14-, 15-, 24-, 25-, and 26-H_3). ^{13}C NMR (100 MHz, 298K, methanol-d_4): δ 149.51 (C_q, $^{2}J_{PC}$ = 26.8 Hz, C2), 148.70 (C_q, d, $^{1}J_{PC}$ = 77.4 Hz, C1), 141.86 (C_q, d, $^{2}J_{PC}$ = 16.5 Hz, C7 and C18), 138.94 and 138.94 (C_q each, C13, C15, C24, and C26), 135.68 and 135.66 (C_q each, C10 and C21), 134.60 (CH, C6), 129.73 (CH, d, $^{3}J_{PC}$ = 1.3 Hz, C4), 129.25 (CH, C5), 127.73 (CH, d, $^{2}J_{PC}$ = 2.0 Hz, C3), 53.37 (CH_2, d, $^{2}J_{PC}$ = 6.4 Hz, C16 and C17), 20.83, 20.76, and 20.72 (CH_3 each, C13, C14, C15, C24, C25, and C26). ^{31}P NMR (161 MHz, 298K, methanol-d_4): δ 86.81. Anal Calc (%) for $C_{26}H_{30}N_2O_3PSLi$•(0.2 C_4H_8O) (497.4): C: 64.72, H: 6.40, N: 5.63. Found C: 65.16, H 6.94, N 5.08.

Lithium 2-[1,3-di-(2,6-diisiopropyl)phenyl]-1,3,2-diazaphospholidin-2-yl) benzenesulfonate (L1b)



To *o*-dilithiobenzenesulfonate•(0.75 THF) (448 mg, 2 mmol) and 2-chloro-1,3-[di-(2,6-diisopropyl)phenyl]-1,3,2-diazaphospholidine (935 mg, 2.1 mmol) in a 20 mL Schenk-tube was added THF (10 mL) and the resulting suspension was heated under stirring to 340 K for 1 hour. The clear solution was cooled to room temperature and the solvent removed in vacuo (10^{-3} mbar). Diethyl ether (10 mL) was added to the remaining glassy solid and the mixture was sonicated for 20 min while a fine white precipitate formed. The white precipitate was cannula transferred into a Schlenk frit, washed with diethyl ether (2 × 5 mL) and pentane (2 × 10 mL), dried under high vacuum, and dissolved in hot benzene (50 mL). The resulting opaque mixture was filtrated through a pad of celite, and the solvent removed in vacuo. The remaining solid was triturated with pentane (10 mL) to yield ligand **L1b** containing 1 equiv of diethyl ether (1072 mg, 1.66 mmol, 82.8 %) after drying under vacuum. ^{1}H NMR (400 MHz, 298 K, CD_2Cl_2): δ 8.17 (d, $^{3}J_{HH}$ = 7.6 Hz, 1H, 6-H), 7.57 (m, 1H, 3-H), 7.37 (m, 1H, 5-H), 7.20 (m, 1H, 4-H), 7.09 (m, 4H, 9-, 11-, 23-, and 25-H), 6.91 (m, 2H, 10- and 24-H), 4.13 and 3.36 (m each, 2:2H each, 19- and 20-H_2), 3.68 (m, 2H, 13- and 16-H), 3.21 (m, 2H, 27- and 30-H), 1.32 and 1.21 (d each, $^{3}J_{HH}$ = 6.8 Hz, 6:6H, 14-, 15-, 17-, and 18-H), 1.03 and 0.29 (d each, $^{3}J_{HH}$ = 6.8 Hz, 6:6H, 28-, 29-, 31-, and 32-H). ^{13}C NMR (100 MHz, , 298 K, CD_2Cl_2): δ 152.0 (C_q, d, $^{2}J_{PC}$ = 28 Hz, C1), 148.74 and 148.72 (C_q each, C8 and C12), 147.7 (C_q, C22 and C26), 144.8 (C_q, d, $^{1}J_{PC}$ = 81 Hz, C2), 140.2 (C_q, d, $^{2}J_{PC}$ = 15.5 Hz, C7 and C21), 131.5 (CH, C6), 126.9 (CH, C4), 126.1 (CH, C5), 125.4 (CH, C5, C10, and C24), 123.2 (CH, C9 and C11), 122.9 (CH, C23 and C25), 54.6 (CH_2, d, $^{2}J_{PC}$ = 5.2 Hz, C19 and C20), 27.55 and 27.47 (CH each, C13 and C16), 27.2 (CH, C27 and C30), 24.9 (CH_3, C28 and C29), 23.8 and 23.6 (CH_3 each, C28, C29, C31, and C32), 23.75 and 23.72 (CH_3 each, C17 and C18). ^{31}P NMR (161 MHz, 298 K, CD_2Cl_2): δ 101.3. Anal Calc for $C_{32}H_{42}N_2O_3PSLi$•($C_4H_{10}O$) (646.8): C: 66.85, H: 8.10, N: 4.33. Found: C: 67.27, H: 8.42, N: 4.00.

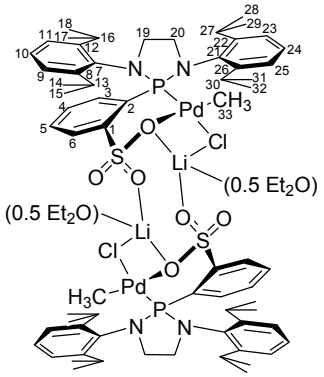
{(κ^2-*P,O*)-2-[1,3-dimesityl-1,3,2-diazaphospholidin-2-yl)benzenesulfonato]-palladium(II)-methyl} lithium chloride adduct 2a-LiCl



To ligand **L1a•(0.2 THF)** (408 mg, 0.82 mmol) and [(COD)PdMeCl] (214 mg, 0.81 mmol) in a 10 mL Schlenk tube was added methylene chloride (5 mL) and the resulting mixture was stirred for 10 min at 298K. The solvent was removed in vacuo to leave a glassy solid, which was dispersed in pentane and washed diethyl ether. A white powder of **2a-LiCl** containing traces of diethyl ether was isolated after dissolution of the crude reaction product in methylene chloride, precipitation with pentane, filtration, and drying under vacuum (440 mg, 0.665 mmol, 81 %). ^{1}H NMR (400 MHz, 298K, acetone-d_6): δ 8.32 (vt, *J* = 8.0 H, 1H, 6-H), 7.88 (m, 1H, 3-H), 7.67 (vt, *J* = 7.4 Hz, 1H 5-H), 7.55 (vt, *J* = 7.6 Hz, 1H, 4-H), 6.86 and 6.72 (s br. each, 2:2H, 9-, 11-, 20-, and 22-H), 4.03 and 3.90 (m each, 2:2H, 16- and 17-H_2), 2.65 and 1.78 (s br. each, 6:6H, 13-, 15-, 24- and 26-H_3), 2.20 (s, 6H, 14- and 25-H_3), 0.21 (s, 3H, Pd-CH_3). ^{13}C NMR (100 MHz, 298K, acetone-d_6): δ 147.94 (C_q, d, $^2J_{PC}$ = 17.5 Hz, C1), 140.90 (C_q, d, $^1J_{PC}$ = 26.7 Hz, C2), 139.92 (C_q, d, $^2J_{PC}$ = 8.5 Hz, C7 and C18), 137.62 (C_q br., C8, C12, C19, and C23), 136.07 (C_q, C10 and C21), 132.09 (CH, C6); 130.80, 130.65, and 130.61 (CH each, C4, C5, C9, C11, C20 and C22), 128.93 (CH, d, $^2J_{PC}$ = 6.8 Hz, C3), 52.49 (CH_2, C16 and C17), 21.34 (CH_3 br., C13, C15, C24, and C26), 20.74 (CH_3, C14 and C25), -7.12 (CH_3, Pd-CH_3). ^{31}P NMR (161 MHz, 298K, acetone-d_6): δ 82.56. Anal Calc for $C_{27}H_{33}N_2O_4PSPdLiCl$ (661.4): C: 49.03, H: 5.03, N: 4.24. Found: C: 49.81, H: 5.52, N: 4.25. Recrystallization yields **2a-LiCl•(acetone)** within 2 d after layering an acetone solution of **2a-LiCl** with pentane. Crystals of **2a-LiCl•(MeOH)** suitable for X-Ray diffraction were obtained by layering a methanol solution of **2a-LiCl** with pentane in an NMR tube.

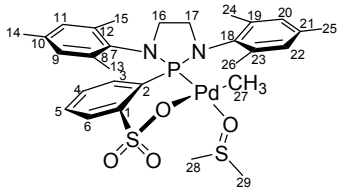
{(κ^2-*P,O*)-2-[1,3-di(2,6-diisopropyl)phenyl-1,3,2-diazaphospholidin-2-yl) benzenesulfonato]-palladium(II)-methyl} lithium chloride adduct [2b-LiCl•(0.5 Et$_2$O)/ 2b-LiCl•(2 THF)]

To ligand **L1b•(Et$_2$O)** (65 mg, 100 μmol) and [(COD)PdMeCl] (26 mg, 98 μmol) in a 10 mL Schlenk tube was added methylene chloride (5 mL) and the resulting mixture was stirred for 30 min at 298K. The solvent was removed in vacuo to leave a glassy solid, which was suspended in diethyl ether (7 mL). The mixture was transferred to a centrifugation vial and the solid separated by repeated centrifugation and extraction of the solid with diethyl ether (2 × 7 mL). After drying the solid under high vacuum (10^{-3} mbar) compound **2b-LiCl•(0.5 Et$_2$O)** was obtained as white microcrystalline material (70.5 mg, 45.9 mmol, 93.8 %) containing traces of methylene chloride. Different batches, however contained up to 1 equiv of diethyl ether per litihium depending on the time under high vacuum.



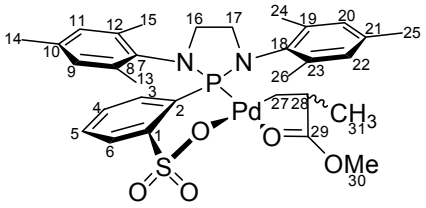
^{1}H NMR (400 MHz, 298K, acetone-d_6): δ 8.21 (vt, J = 8.2 Hz, 1H, 6-H), 7.90 (m, 1H, 3-H), 7.71 (vt, J = 7.3 Hz, 1H, 5-H), 7.58 (vt, J = 7.5 Hz, 1H, 4-H), 7.22 (m, 4H, 9-, 11-, 23-, and 25-H), 7.04 (m, 2H, 10- and 24-H), 4.21 and 3.93 (m each, 2:2H, 19- and 20-H$_2$), 3.77 and 2.96 (m each, 2:2H, 13-, 16-, 27-, and 30-H), 1.56, 137, 0.96, and 0.76 (d each, $^3J_{HH}$ = 6.8 Hz each, 6:6:6:6H, 14-, 15-, 17-, 18-, 28-, 29-, 31-, and 32-H$_3$), 0.22 (s br., 3H, Pd-CH$_3$). ^{13}C NMR (100 MHz, 298K, acetone-d_6): δ 148.23 and 147.80 (C$_q$ each, d each, $^3J_{PC}$ = 1.2 and 2.7 Hz, C8, C12, C22, and C26), 147.78 (C$_q$, d, $^2J_{PC}$ = 18.8 Hz, C1), 139.90 (C$_q$, d, $^1J_{PC}$ = 27.4 Hz, C2), 139.46 (C$_q$, d, $^2J_{PC}$ = 7.7 Hz, C7 and C21), 129.96 (CH br., C6), 129.90 (CH, d, $^3J_{PC}$ = 2.0 Hz, C4), 129.61 (CH, d, $^4J_{PC}$ = 5.0 Hz, C5), 129.29 (CH, d, $^2J_{PC}$ = 7.2 Hz, C3), 127.37, 127.36 and 125.04 (CH each, C9, C11, C23, and C25), 124.27 (CH, C10 and C24), 54.05 (CH$_2$, C19 and C20), 28.97 and 28.68 (CH each, C13, C16, C27, and C30), 26.20, 25.24, 24.25, and 23.23 (CH$_3$ each, C14, C15, C17, C18, C28, C29, C31, and C32), -7.54 (CH$_3$, d, $^2J_{PC}$ = 3.7 Hz, Pd-CH$_3$). ^{31}P NMR (161 MHz, 298K, acetone-d_6): δ 89.91. Anal Calc (%) for $C_{33}H_{45}N_2O_3PSPdLiCl•(0.5C_4H_{10}O)$ (766.6): C: 54.83, H: 6.57, N: 3.65. Found: C: 55.01, H: 6.78, N: 4.01. Crystals of **2b-LiCl•(2 THF)** suitable for X-ray diffraction analysis were obtained within 1d at 298K by layering a solution of 8 mg **2b-LiCl•(0.5 Et$_2$O)** in 60 μL THF with pentane (2 mL) in a NMR tube.

{[(κ^2-*P,O*)-2-(1,3-dimesityl-1,3,2-diazaphospholidin-2-yl)benzenesulfonato] palladium(II)-methyl-(κ-*O*)-dimethylsulfoxide} (2a-DMSO)



To a solution of **2a-LiCL•(acetone)** (84.3 mg, 59.9 μmol mmol) in methylene chloride (3 mL) was added DMSO (30.1 mg, 385 μmol). Addition of silvertetrafluoroborate (76.5 mg, 393 μmol) caused formation of a white precipitate which was filtered off by a syringe filter containing a celite plug after stirring for 3 h at 298K. After removal of all volatiles the resulting brown solid was suspended in pentane and sonicated. The insoluble light brown solid was filtered off and washed with pentane and diethyl ether, respectively, to yield **2a** which contains $LiBF_4$ by ^{19}F-NMR spectroscopy. Elemental analysis suggests a composition of ca **2a-DMSO•($LiBF_4$)** (yield: 80.6 mg, 104 μmol, 87 %). ^{1}H NMR (400 MHz, 298K, CD_2Cl_2): δ 7.98 (vt, *J* = 8.6 Hz, 1H, 6-H), 7.88 – 7.80 (m, 1H, 3-H), 7.50 (vt, *J* = 7.2 Hz, 1H, 5-H), 7.43 (vt, *J* = 7.6 Hz, 1H, 4-H), 6.77 (br, 4H, 9-, 11-, 20- and 22-H), 3.99 and 3.97 (s br. each, 2:2H, 16- and 17H_2),2.54 (s, 6H, DMSO-CH_3), 2.52 and 1.63 (br each, 6:6H, 13-, 15-, 24-, and 26-H_3), 2.16 (s, 6H, 14- and 25-H_3), 0.06 (s, 3H, Pd-CH_3). ^{31}P NMR (161 MHz, 298K, CD_2Cl_2): δ 89.85. ESI-MS: calc: 680.11 g mol^{-1}; Found: 603.2 (MH^+-DMSO), 625.0 (M+Na-DMSO)$^+$, 648.2 (M+HCOOH-DMSO)$^+$, 704.1 (M+$HNEt_3$-DMSO)$^+$. Anal Calc (%) for $C_{29}H_{39}N_2O_4PS_2Pd$•$LiBF_4$ (774.9): C, 44.95; H, 5.07; N, 3.62; Found: C, 46.14; H, 5.49; N, 3.68. Crystals of **2a-DMSO** suitable for X-ray diffraction were grown from a solution of **2a-DMSO•($LiBF_4$)** in benzene layered with pentane in an NMR-tube.

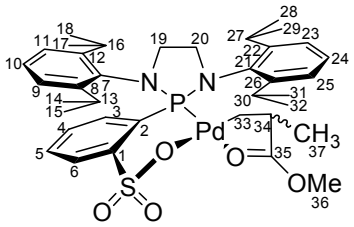
{[(κ^2-*P,O*)-2-(1,3-dimesityl-1,3,2-diazaphospholidin-2-yl)benzenesulfonato] palladium(II)-[(κ^2-*C,O*)-3-methoxy-2-methyl-3-oxopropyl]} (3a)



To a solution of **2a-LiCl•(acetone)** (200 mg, 284 μmol) in methylene chloride (5 mL) were added BHT (10 mg), methyl acrylate (MA; 190 mg, 2.2 mmol), and silver tetrafluoroborate (180 mg, 924 μmol). The reaction mixture was stirred for 2 h at 298 K in the dark and then filtered through a syringe filter to afford a yellow solution. Diethyl ether (20 mL) was added, the resulting precipitate separated by filtration and washed with diethyl ether (2 × 5 mL) and pentane (5 mL) to yield **3a** containing ca 1 equiv of $LiBF_4$ (by elemental analysis) as off-white solid after drying under high vacuum (187 mg, 239 μmol, 84.1%). ^{1}H NMR (400 MHz, 298K, CD_2Cl_2): δ 8.11 (vt, *J* = 8.6 Hz, 1H, 6-H), 7.97 (m, 1H, 3-H), 7.62 (vt, *J* = 7.5 Hz, 1H, 5-H), 7.54 (vt, *J* = 7.5 Hz, 1H, 4-H), 6.93 (br, 4H, 9-, 11-, 20- and 22-H), 3.91 (m, 4H, 16- and 17-H_2), 3.81 (s, 3H, 31-H_3), 2.65, 2.51, 1.85, and 1.72 (br. each, 3:3:3:3H, 13-, 15-, 24-, and 26-H_3), 2.35 (m, 1H, 28-H), 2.23 (s, 6H, 14- and 25-H_3), 1.39 (m, 1H, 27-H), 0.97 (m, 1H, 27-H), 0.87 (d, $^3J_{HH}$ = 7.0, 3H, 29-H_3). ^{13}C NMR (100 MHz, 298K, CD_2Cl_2): δ 189.77 (C_q, C29), 146.48 (C_q, d $^2J_{PC}$ = 20.0 Hz, C1), 139.38 (C_q, d, $^1J_{PC}$ = 36.8 Hz, C2), 138.99 and 138.90 (C_q each, C7 and C18), 138.34, and 138.26 (C_q each, C10 and C21), 136.89, 136.87, 136.63, and 136.61 (C_q each, C8, C12, C19, and C23), 131.47 (d, $^2J_{PC}$ = 1.5 Hz, C4), 131.37 (CH, $^2J_{PC}$ = 2.0 Hz, C6) 130.59 (CH, d, $^3J_{PC}$ = 5.7 Hz C5), 130.21 (CH each, C9, C11, C20 and C22) 128.48 (d, $2J_{PC}$= 7.8 Hz, C3), 55.55 (s, C30), 51.99 (CH_2, C16 and C17), 44.77 (CH, d, $^3J_{PC}$ = 2.4 Hz, C28), 21.05 (CH_3 br., C13, C14, C15, C24, C25, and C26) 20.98 (CH_2, d, $^2J_{PC}$ = 6.4 Hz, C27), 17.83 (CH_3, d, $^4J_{PC}$ = 2.5 Hz, C31). ^{31}P NMR (161 MHz, 298K, CD_2Cl_2): δ 85.67. Anal. Calcd. (%) for $C_{31}H_{39}N_2O_5PSPd$•$LiBF_4$ (782.9): C, 47.56; H, 5.02; N, 3.58; Found: C, 48.72; H, 5.35; N, 3.80. Crystals suitable for X-Ray diffraction were obtained by layering a methylene chloride solution of **3a** with pentane in a NMR tube.

A kinetic analysis of a solution obtained from **2a-LiCl•(acetone)** (21.8 mg, 29.8 μmol), methyl acrylate (115 mg, 1.34 mmol; 22.5 equiv vs palladium; ^{1}H and ^{31}P NMR recorded), and silver triflate (9.0 mg, 35 μmol) in methylene-chloride-d_2 after filtration reveals k_{obs} = 6.0 (±0.1) × 10^{-4} s^{-1} for the disappearance of the palladium methyl signal at 298 K.

{[(κ^2-*P,O*)-2-(1,3-di(2,6-diisopropyl)phenyl-1,3,2-diazaphospholidin-2-yl) benzenesulfonato]palladium(II)-[(κ^2-*C,O*)-3-methoxy-2-methyl-3-oxopropyl]} (3b)



To a solution of complex **2b-LiCl•(0.85 Et_2O)** (48 mg, 30.3 μmol) in methylene chloride-d_2 (350 μL) in a NMR tube (^{1}H and ^{31}P NMR recorded) was added methyl acrylate (115 mg, 1.34 mmol; 22 equiv vs palladium; ^{1}H and ^{31}P NMR recorded) and silver triflate (17.1 mg, 66.6 μmol) at 298K. The NMR tube was shaken for 2 min and then centrifuged, which resulted in the deposition of silver chloride. The solution was filtered through a syringe filter into a J. Young NMR tube, the syringe filter rinsed with additional methylene chloride-d_2 (120 μL), and the sample heated to 318 K in the NMR probe while continuously monitoring the reaction progress by ^{1}H NMR spectra. After complete consumption of the palladium methyl species (1 h at 318 K, k_{obs} = 4.8 (±0.1) × 10^{-4} s^{-1}), the J. Young tube was connected to a vacuum manifold and all volatiles were carefully removed at 243K to leave a highly viscous, sticky oil in the tube. Benzene (0.5 mL) was added, the tube was cooled to 273K (ice bath), and the frozen solvent (and residual volatiles) were removed by sublimation under vacuum. The sample thus obtained contains traces of methyl crotonate, methyl acrylate, and one not further identified ester apart from complex **3b** in ca 95 % NMR purity as was determined by 1- and 2D NMR experiments. Chemical shifts reported in the NMR assignment are based on the analysis of the crude reaction product obtained by the procedure reported here. Isolation of compound **3b** (40.6 mg, 52.5 μmol, 86.6%) was accomplished by crystallization after removing the solvent under vacuum, washing the residue with diethyl ether, redissolution of the residue in methylene chloride (85 μL) and layering pentane (1.5 mL) on top of the methylene chloride solution. ^{1}H NMR (600 MHz, 298K, CD_2Cl_2): δ 8.01 (m, 2H, 6- and 3-H), 7.63 (vt, *J* = 7.4 Hz, 1H, 5-H), 7.53 (vt, *J* = 7.7 Hz, 1H, 4-H), 7.28 and 7.24 (m each, 2:2H, 9-, 11-, 23-, and 25-H), 7.06 (m, 2H, 10- and 24-H), 4.20, 4.07 and 3.93 (m each, 1:1:2H, 19- and 20-H_2), 3.74 (s, 3H, 36-H_3), 3.72, 3.55, 2.88, and 2.73 (sept each, $^3J_{HH}$ = 6.8 Hz each, 1:1:1:1H, 13-, 16-, 27-, and 30-H), 2.48 (m, 1H, 34-H), 1.54, 1.51, 1.39, 1.38, 0.99, 0.98, 0.70, and 0.63 (d each, $^3J_{HH}$ = 6.8 Hz each, 3:3:3:3:3:3:3:3H, 14-, 15-, 17-, 18-, 28-, 29-,31-, and 32-H_3), 1.12 (m, 1H, 34-H), 0.77 (vt, *J* = 9.6 Hz, 34-H), 0.76 (d, $^3J_{HH}$ = 7.1 Hz, 3H, 37-H_3). ^{13}C NMR (150 MHz, 298K, CD_2Cl_2): δ 189.58 (C_q, br., C35), 149.29, 149.12, 148.10, and 147.85 (C_q each, d each, $^3J_{PC}$ = 1.2, 1.5, 1.8, and 2.2 Hz, C8, C12, C22, and C26), 147.52 (C_q br., d, $^2J_{PC}$ = 17.7 Hz, C1), 138.86 and 137.97 (C_q each, d each, $^2J_{PC}$ = 7.8 and 7.4 Hz, C7 and C21), 138.29 (C_q, d, $^1J_{PC}$ = 37.6 Hz, C2), 131.46 (CH, d, $^4J_{PC}$ = 1.5 Hz, C5), 130.17 (CH, C4), 130.13 (CH, d, $^2J_{PC}$ = 3.6 Hz, C3), 129.6 (CH, C6), 128.45, 125.56 and 125.45 (CH, C9, C11, C23, and C25), 125.16 (CH, C10 and C24), 55.62 (CH_3, C36), 54.72 and 54.11 (CH_2 each, C19 and C20), 44.65 (CH, C34), 29.69, 29.40, 29.38, and 29.36 (CH each, C13, C16, C27, and C30), 27.10, 26.90, 25.73, 25.67, 24.84, 24.71, 23.66, and 23.61 (CH_3 each, C14, C15, C17, C18, C28, C29, C31, and C32), 17.91 (CH_3 br.; C37), 17.86 (CH_2, d, $^2J_{PC}$ = 2.0 Hz, C33). ^{31}P NMR (161 MHz, 298K, CD_2Cl_2): δ 94.31. Anal Calc (%) for $C_{37}H_{51}N_2O_5PSPd$ (773.3): C: 57.47, H: 6.65, N 3.62. Found: C: 57.89, H: 6.97, N 3.41. Crystals suitable for X-ray analysis were obtained by layering a solution of 12 mg **3b** in methylene chloride (70 μL) with pentane (1.5 mL) in a NMR tube.

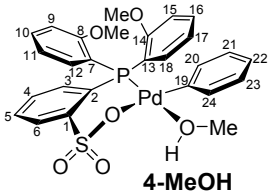
Methyl methacrylate

Thermolysis of isolated **3b** (16.3 mg, 21 μmol) in methylene chloride-d_2 solution (450 μL) in a J. Young NMR tube yields quantitatively methyl methacrylate after 16 h at 353 K according to ^{1}H NMR spectroscopy (residual protio-methylene chloride is used as internal reference).

{(κ^2-*P,O*)-[2-[di(2-anisyl)phosphin-2-yl]benzenesulfonato]palladium(II)-phenyl (methanol)} (4-MeOH)

[(DMSO)$_2$Pd(Ph)Cl]. In a 100 mL Schlenk tube palladium dichloride (887 mg, 5 mmol) was dissolved in DMSO (6 mL) at 383 K under stirring. After cooling to 298 K, diethyl ether was added (70 mL) under stirring, the resulting orange solid collected by filtration, washed with diethyl ether (4 × 10 mL), and dried under vacuum to yield [(DMSO)$_2$PdCl$_2$] (1.630 g, 4.89 mmol, 97.7 %). To a suspension of [(DMSO)$_2$PdCl$_2$] (334 g, 1 mmol) in a mixture of DMSO (3 mL) and THF (15 mL) in a 50 mL septum capped Schlenk tube was added tetraphenyl tin (215 mg, 503.3 μmol). The solution was stirred for 8 h at 298 K while the orange starting material dissolved and an orange-red solution containing some palladium black formed. The mixture was concentrated to ca 5 mL, DMSO (5 mL) was added and the resulting mixture filtered through a syringe filter into a 100 mL Schlenk flask. Removal of all volatiles under high vacuum (298 K, 10^{-3} mbar) gave a orange solid, which was dispersed in THF (15 mL) and cannula transferred into a Schlenk frit. The was solid filtered off, washed with THF (4 × 10 mL), and dried under vacuum to yield a white-grey powder of [(DMSO)$_2$Pd(Ph)Cl] which contains traces of palladium black (361.1 mg, 0.965 mmol, 96.5 %). **[(DMSO)$_2$Pd(Ph)Cl]**: ^{1}H NMR (400 MHz, 298K, DMSO-d_6): δ 7.18 (m, 2H, *ortho*-H, Ph), 6.96 (m, 2H, *meta*-H, Ph), 6.94 (m, 1H, *para*-H, Ph), 2.55 (s, 12H, 2 × DMSO-h_6). ^{13}C NMR (100 MHz, 298K, DMSO-d_6): δ 134.59 (CH, *ortho*-C, Ph) 126.97 (CH, *meta*-C, Ph), 123.82 (CH, *para*-C, Ph), 40.43 (CH_3, 2 × DMSO-h_6), *ipso*-C, Ph not detected. Anal Calc (%) for $C_{10}H_{17}O_2S_2ClPd$ (375.2): C: 32.01, H: 4.57. Found: C: 31.36, H 4.01.

4-MeOH. To sodium [di(2-anisyl)phosphinyl]benzene sulfonate (**L2**) (3) (42.4 mg, 100 μmol) and [(DMSO)$_2$Pd(Ph)Cl] (41.6 mg, 111 μmol) in a NMR tube was added CD_3OD (400 μL). The tube was shaken for 5 min at 298 K and centrifuged. ^{1}H and ^{31}P NMR monitoring indicated consumption of **L2** and formation of one new ^{31}P containing species in > 95 % NMR yield. Complex **4-MeOH** started to separate by crystallization after ca 10 min at 298 K. The solvent was removed in vacuo, the residue dissolved in methylene chloride (3 mL), and the solution filtrated. After removal of all volatiles the residue was recrystalized from refluxing methanol to yield **4-MeOH** (50.7 mg, 78.1 μmol, 78.1 %) containing traces of residual DMSO after 16h under high vacuum.



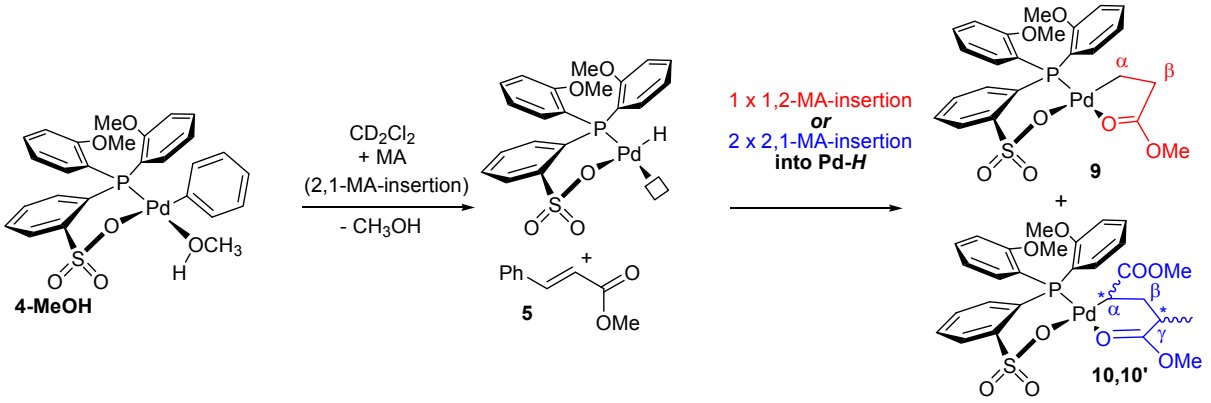
4-MeOH

^{1}H NMR (600 MHz, 298K, CD_3OD): δ 8.03 (ddd, $^3J_{HH}$ = 7.9, $^4J_{HH}$ = 1.2 and $^4J_{PH}$ = 4.7 Hz, 1H, 6-H), 7.78 (dd, $^3J_{HH}$ = 7.5 and $^3J_{PH}$ = 14.8 Hz, 2H, 12- and 18-H), 7.52 (m, 1H, 5-H), 7.49 (m, 1H, 3-H), 7.47 (m, 2H, 10- and 16-H), 7.39 (m, 1H, 4-H), 6.94 (m, 6H, 9-, 11-, 15-, 17-, 20-, and 24-H), 6.58 (m, 1H, 22-H), 6.53 (m, 2H, 21- and 23-H), 3.61 (s, 6H, 2 × OCH_3), 2.67 (s, 1.4H residual DMSO). ^{13}C NMR (150 MHz, 298K, CD_3OD): δ 161.60 (C_q, d, $^2J_{PC}$ = 1.1 Hz, C8 and C14), 148.05 (C_q, d, $^2J_{PC}$ = 14.3 Hz,

C1), 147.04 (C_q br., C19), 139.16 (C_q, d, $^2J_{PC}$ = 13.7 Hz, C12 and C18), 136.17 (CH, d, $^2J_{PC}$ = 2.8 Hz, C3), 135.23 (CH, d, $^3J_{PC}$ = 4.4 Hz, C20 and C24), 134.72 CH, d, $^4J_{PC}$ = 2.2 Hz, C10 and C16), 131.31 (CH, d, $^4J_{PC}$ = 2.5 Hz, C5), 129.84 (CH, d, $^3J_{PC}$ = 7.8 Hz, C4), 129.22 (C_q, d, $^1J_{PC}$ = 53.1 Hz, C2), 128.32 (CH, d, $^3J_{PC}$ = 8.3 Hz, C6), 127.65 (CH, d, $^4J_{PC}$ = 2.8 Hz, C21 and C23), 124.44 (CH, C22), 121.46 (CH, d, $^3J_{PC}$ =13.2 Hz, C11 and C17), 116.14 (C_q, d, $^1J_{PC}$ = 62.9 Hz, C7 and C13), 112.33 (CH, d, $^3J_{PC}$ = 4.7 Hz, C9 and C15), 55.53 (CH_3, 2 × OCH_3), 40.57 (CH_3, residual DMSO). ^{31}P NMR (161 MHz, 298K, CD_3OD): δ 17.97. Anal Calc (%) for $C_{27}H_{27}O_6PSPd$ (617.0): C: 52.56; H: 4.41. Found: C: 52.10; H: 4.23. Crystals of **4-MeOH•(MeOH)** suitable for X-ray diffraction analysis were grown from refluxing CD_3OD.

(*E*)-Methyl cinnamate (5) and methyl acrylate insertion products into palladium hydride (9 and 10,10')

To a solution of **4-MeOH** (14 mg, 22.7 μmol) in methanol-d_4 (400 μL) in a J. Young NMR tube was added methyl acrylate (45.5 mg, 529 μmol) and the sample was monitored by ^{1}H NMR spectroscopy periodically over a period of 2.5 h. After 61 min at 298 K consumption of **4-MeOH** was complete while formation of (*E*)-methyl cinnamate (**5**) and two products arising from insertion of methyl acrylate into (P^O)Pd(H) were observed. After removal of methanol-d_4 and excess methyl acrylate under vacuum, methyl cinnamate (**5**) was identified as solely organic product formed by insertion of methyl acrylate into the palladium methyl bond of **4-MeOH** after redissolution of the remaining material in methylene chloride-d_2. In addition, palladium complex **9** formed by 1,2-methyl acrylate insertion into (P^O)Pd(H) as well diastereomeric palladium complexes **10,10'** formed by two consecutive 2,1-methyl acrylate insertions into (P^O)Pd(H) were identified by 1- and 2-dimensional NMR experiments.



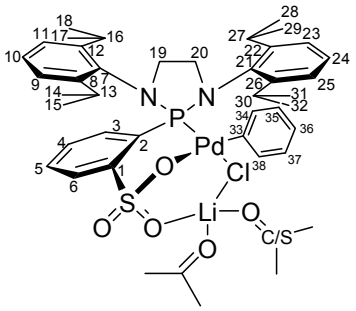
5: ^{1}H NMR (400 MHz, 298K, CD_2Cl_2): δ 7.68 (d, $^3J_{HH}$ = 16.1 Hz, 1H, PhC*H*=CH), 7.54 and 7.40 (m each, 2:3H, *ortho*-, *meta*-, and *para*-H, Ph), 6.46 (d, $^3J_{HH}$ = 16.1 Hz, 1H, PhCH=C*H*), 3.77 (s, 3H, OCH_3). ^{13}C NMR (100 MHz, 298K, CD_2Cl_2): δ 167.71 (Cq, CO_2Me), 145.09 (CH, Ph*C*H=CH), 135.00 (C_q, *ipso*-C, Ph), 130.83 (CH, *para*-C, Ph), 129.43 and 128.60 (CH each, *ortho*- and *meta*-C, Ph), 118.43 (CH, PhCH=*C*H), 52.08 (CH_3, OCH_3).

9: ^{1}H NMR (400 MHz, 298K, CD_2Cl_2, key resonances only): δ 1.95 and 1.27 (m each, 1:1H, β-H_2), 0.88 (t, $^3J_{HH}$ = 7.2 Hz 2H, α-H_2).

10 [**10'** (minor diastereomer) in ()]: ^{1}H NMR (400 MHz, 298K, CD_2Cl_2, key resonances only): δ .3.37 (3.22) (m, 1H, γ-H), 2.07 (1.92) (m, 1H, α-H), 1.27 and 1.00 (1.45 and 1.24) (m each, 1:1H, β-H_2), 1.17 (1.32) (d, $^3J_{HH}$ = 6.4 (7.2) Hz, γ-CH_3).

{(κ^2-*P,O*)-2-[1,3-di(2,6-diisopropyl)phenyl-1,3,2-diazaphospholidin-2-yl) benzenesulfonato]-palladium(II)-phenyl} lithium chloride adduct [6b-LiCl•(DMSO)]

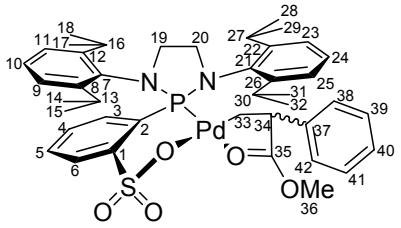
To **L1b•(Et_2O)** (65 mg, 100 μmol) and [$(DMSO)_2Pd(Ph)Cl$] (previous step; 39.8 mg, 106 μmol) in a NMR tube was added methylene chloride-d_2 (400 μL). The tube was shaken for 5 min at 298 K and then centrifuged. Monitoring of the solution by ^1H and ^{31}P NMR indicated consumption of **L1b•(Et_2O)** and formation of one new ^{31}P containing species in > 90 % NMR yield. The solution was filtrated, concentrated to dryness, and the resulting solid extracted with pentane (2 × 3 mL) to yield complex **6b-LiCl•(dmso)** after drying under vacuum (66.7 mg, 72 μmol, 72 %).



^1H NMR (600 MHz, 298K, acetone-d_6): δ 8.25 (vt, J = 8.7 Hz, 1H, 6-H), 7.90 (m, 1H, 3-H), 7.77 (vt, J = 7.7 Hz, 1H, 5-H), 7.66 (vt, J = 7.6 Hz, 1H, 4-H), 7.02 (br., 4H, 9-,11-,23-, and 25-H), 6.90 (br., 2H, 10-, and 24-H), 6.57 (v. br., 2H, 34- and 38-H), 6.28 (m, 1H, 36-H), 6.23 (br., 2H, 35-, and 37-H); 4.07, 3.74, and 2.98 (v. br.:br.: v. br., 4:2:2H, 13-, 16-, 27-, 30-H, and 19- and 20-H_2), 2.51 (s, 6H, DMSO), 1.66, 1.29, 1.12, and 0.83 (br.:d:d:br., $^3J_{HH}$ = 6.8 Hz, 6:6:6:6H, 14-, 15-, 17-, 18-, 28-, 29-, 31-, and 32-H_3). ^{13}C NMR (150 MHz, 298K, acetone-d_6): δ 148.4 (C_q, d br., $^2J_{PC}$ =18 Hz, C1), 147.9 and 147.45 (C_q each, C8, C12, C22, and C26), 137.2 (CH, C34 and C38), 136.8 (C_q br., d, $^1J_{PC}$ = 27 Hz, C2), 136.78 (C_q, C33), 135.8 (C_q br., C7 and C12), 130.4 (CH, d, $^3J_{PC}$ = 1.4 Hz, C4), 129.8 (CH br., C3), 129.46 (CH, d, $^4J_{PC}$ =5.0 Hz, C5), 128.7 (CH br., C6), 127.47 and 124.5 (CH each, C9, C11, C23, and C25), 125.26 (CH, d, $^4J_{PC}$ =3.9 Hz, C35 and C37), 123.8 (CH, C10 and C24), 121.7 (CH, C36), 54.7 (CH_2 br, C19 and C20), 40.18 (CH_3, DMSO), 29.46 and 28.79 (no correlation detected, C13, C16, C27, and C30), 27.24, 26.24, 23.32, and 21.74 (CH_3, C14, C15, C17, C18, C28, C29, C31, and C32). ^{31}P NMR (161 MHz, 298K, acetone-d_6): δ 88.95. Anal Calc (%) for $C_{43}H_{59}N_2O_5PS_2PdLiCl$ (927.87): C: 55.66; H: 6.41; N: 3.02. Found C: 55.99; H: 6.87; N: 2.55. Crystals of **6b-LiCl•(1.8 acetone, 0.2 DMSO)** suitable for X-ray diffraction analysis were grown from **6b-LiCl•(DMSO)** (12 mg) in acetone (60 μL) after layering with pentane.

{[(κ^2-*P,O*)-2-(1,3-di(2,6-diisopropyl)phenyl-1,3,2-diazaphospholidin-2-yl) benzenesulfonato]palladium(II)-[(κ^2-*C,O*)-3-methoxy-2-phenyl-3-oxopropyl]} (7b)

To a solution complex **6b-LiCl•(DMSO)** (38 mg, 41 μmol) in methylene chloride-d_2 in a NMR tube was added methyl acrylate (88 mg, 1.03 mmol, 25 equiv). The mixture was monitored by ^{1}H and ^{31}P NMR, then silver triflate (10.8 mg, 42 μmol, 1.02 equiv) was added and the tube was shaken for 2 min and centrifuged whereby silver chloride deposited. The resulting solution was monitored by ^{1}H and ^{31}P NMR at 318 K. Formation of complex **7b** (ca 90 % NMR yield by ^{1}H and ^{31}P NMR) together with methyl cinnamate (**5**) (ca 7% NMR yield) was complete after ca 25 min at 318 K. Isolation of complex **7b** was accomplished by filtration, removing all volatiles under vacuum, washing the residue with pentane (4 × 2 mL) and cold diethyl ether (1 mL, 243 K), and crystallization from methylene chloride (100 μL) after layering with pentane (1.5 mL) in a NMR tube (28.3 mg, 33.9 μmol, 82.6 %). The full NMR characterization was obtained from the crude reaction mixture, after filtration, removal of all volatiles and redissolution acetone-d_6.



^{1}H NMR (600 MHz, 298K, acetone-d_6): δ 8.22 (vt, *J* = 8.4 Hz, 1H, 6-H), 7.99 (m, 1H, 3-H), 7.69 (vt, J = 7.3 Hz, 1H, 5-H), 7.61 (vt, *J* = 7.5 Hz, 1H, 4-H), 7.20-6.96 (m, 11H, 9-11-, 23-25-, and 34-38-H), 4.24 and 3.98 (m each, 2:2H, 19- and 20-H_2), 3.75 (s, 3H, 36-H_3), 3.72, 3.63, 2.97, and 2.92 (sept each, $^3J_{HH}$ = 6.8 Hz, 1:1:1:1H, 13-, 16-, 27-, and 30-H), 3.72 (m, 1H, 34-H), 1.51, 1.36, 1.33, 0.96,0.92, 0.77, and 0.60 (d each, $^3J_{HH}$ = 6.8 Hz, 3:6:3:3:3:3:3H, 14-, 15-, 17-, 18-, 28-, 29-, 31-, and 32-H_3), 1.42 (m, 1H, 33-H), 1.16 (vt, *J* = 9.4 Hz, 1H, 33-H). ^{13}C NMR (150 MHz, 298K, acetone-d_6): δ 188.17 (C_q, d $^3J_{PC}$ = 3.0 Hz, C35), 149.92 (C_q, $^2J_{PC}$ = 28.5 Hz, C1), 149.30, 149.22, 148.08, and 148.03 (C_q each, d each, $^3J_{PC}$ = 2.6, 2.4, 3.6, and 3.9 Hz, C8, C12, C22, and C26), 139.97 (C_q, d, $^2J_{PC}$ = 2.4 Hz, C37), 139.26 and 139.22 (C_q each, d each, $^2J_{PC}$ = 11.4 Hz, C7 and C21), 138.71 (C_q, d, $^1J_{PC}$ = 60.6 Hz, C2), 131,4 (CH, d, $^3J_{PC}$ = 3.6 Hz, C4), 130.56 (CH, C6), 129.85 (CH, d, $^4J_{PC}$ = 7.5 Hz, C5), 129.53 (CH, d, $^2J_{PC}$ = 12.6 Hz, C3), 129.79, 129.20, 129.11, 129.00, 128.71, 128.39, 127.78, 125.89, 125.67, 125.29, and 125.17 (CH each, C9-C11, C23-C25, and C38-C42), 56.26 (CH, d, $^3J_{PC}$ = 3.8 Hz, C34), 55.66 (CH_3, C36), 54.57 and 54.44 (CH_2 each, C19 and C20), 29.53 and 29.41 (CH each, C13, C16, C27, and C30), 26.93, 26.90, 25.77, 25.67, 25.06, 24.57, 24.22, and 23,71 (CH_3 each, C14, C15, C17, C18, C28, C29, C31, and C32), 18.69 (CH_2, d, $^2J_{PC}$ = 7.7 Hz, C33). ^{31}P NMR (161 MHz, 298K, acetone-d_6): δ 91.22. Anal Calc (%) for $C_{42}H_{53}N_2O_5PSPd$ (835.35): C: 60.39; H: 6.39; N: 3.35. Found: C: 61.02; H: 6.81; N: 3.01.

(2-Phenyl)methyl acrylate (8)

A solution of **7b** (10.0 mg, 12 μmol) in 1,1,2,2-tetrachloroethane-d_2 (0.45 ml, residual protiated 1,1,2,2-tetrachloroethane was used as internal standard) was heated in a NMR tube at 363 K and occasionally monitored by ^{1}H NMR spectroscopy over 12 h. Consumption of **7b** was complete after 11 h at 363 K to give in quantitative NMR yield compound **8** identified by 1- and 2-D NMR experiments and by comparison to genuine **8** obtained by Wittig reaction of methyltriphenylphosphonium bromide and benzoyl methyl formate according to a literature procedure (4). ^{1}H NMR (400 MHz, 298K, 1,1,2,2-tetrachlorethane-d_2): δ 7.43-7.36 (m, 5H, Ph),6.35 and 5.93 (d each, $^2J_{HH}$ = 1.4 Hz each, 1:1H, C=CH_2), 3.86 (s, 3H, OCH_3). ^{13}C NMR (100 MHz, 298K, 1,1,2,2-tetrachlorethane-d_2): δ 167.38 (C_q, *C*O_2CH_3), 141.00 and 136.65 (C_q each, *ipso*-Ph and *C*=CH_2), 128.47 and 128.30 (CH each, *ortho*- and *meta*-C, Ph), 128.36 (CH, *para*-C, Ph), 127.33 (CH_2, C=*C*H_2), 52.50 (CH_3, OCH_3).

X-Ray Diffraction Analyses

X-Ray diffraction analyses were performed at 100 K on a STOE IPDS-II diffractometer equipped with a graphite-monochromated radiation source (λ = 0.71073 Å) and an image plate detection system. Crystals were mounted on a fine glass fiber with silicon grease. The selection, integration and averaging procedure of the measured reflex intensities, the determination of the unit cell dimensions and a least-squares fit of the *2θ* values as well as data reduction, LP-correction and space group determination were performed using the X-Area software package delivered with the diffractometer (5). A semiempirical absorption correction was performed. The structures were solved by the Patterson method (SHELXS-97) (6), completed with difference fourier syntheses, and refined with full-matrix least-square using SHELXL-97 (7) minimizing $\omega(F_0^2-F_c^2)^2$. Weighted *R* factor (wR_2) and the goodness of fit GooF are based on F^2. Except for complex **6b-LiCl•(1.8 acetone, 0.2 DMSO)**, all non-hydrogen atoms were refined with anisotropic displacement parameters. For complex **6b-LiCl•(1.8 acetone, 0.2 DMSO)**, positional and substitutional disordered solvent molecules were refined isotropically. All hydrogen atoms were treated in a riding model. Graphical output (Ortep plots) were created using ORTEP-3 V2.02 for Windows XP (8).

Table S1. X-Ray diffraction data of complexes **2a-DMSO**, **2a-LiCl•(MeOH), 2b-LiCl•(2 THF), 3a**, **3b**, **4-(MeOH)•(MeOH**), and **6b-LiCl•(acetone/DMSO)**

	2a-DMSO	**2a-LiCl•(MeOH)**	**2b-LiCl•(2 THF)**	**3a**	**3b**	**4-(MeOH)•(MeOH)**	**6b-LiCl•(acetone/DMSO)**
CCDC no.	792914	793498	792913	792915	792916	792918	792917
emp. formula	$C_{29}H_{39}N_2O_4PPdS_2$	$C_{56}H_{74}Cl_2Li_2N_4O_8P_2Pd_2S_2$	$C_{82}H_{122}Cl_2Li_2N_4O_{10}P_2Pd_2S_2$	$C_{31}H_{39}N_2O_5PPdS$	$C_{37}H_{51}N_2O_5PPdS$	$C_{28}H_{31}O_7PPdS$	$C_{43.79}H_{59}ClLiN_2O_5PPdS_{1.21}$
formula weight [g mol^{-1}]	681.11	1354.83	1747.48	689.07	773.23	648.96	912.03
temperature [K]	100 K	100 K	100 K	100 K	100 K	100 K	100 K
crystal system	Monoclinic	monoclinic	triclinic	orthorhombic	monoclinic	Triclinic	monoclinic
space group	*P21/c*	*C2/c*	*P-1*	*Pbca*	*P21/c*	*P-1*	*P21/c*
a [Å]	9.5065(6)	27.7024(15)	10.462(2)	15.1027(6)	13.2909(7)	8.2486(10)	16.9666(7)
b [Å]	21.7563(9)	10.5058(4)	12.917(3)	16.6125(5)	15.1835(10)	11.8255(14)	10.3382(3)
c [Å]	15.1499(10)	20.3957(12)	16.146(6)	24.1809(8)	22.0751(12)	15.613(2)	25.0043(10)
α [°]	90.00	90.00	101.91(2)	90.00	90.00	69.380(9)	90.00
β [°]	104.582(5)	100.256(5)	99.03(2)	90.00	121.621(4)	77.961(10)	91.511(3)
γ [°]	90.00	80.00	93.739(16)	90.00	90.00	77.384(10)	90.00
Volume [Å^3], *Z*	3032.5(3), 4	5841.0(5), 4	2097.8(9), 1	6066.8(4), 8	3793.4(4), 4	1376.4(3), 2	4384.3(3), 4
density [calc,g cm^{-3}]	1.492	1.541	1.383	1.509	1.354	1.566	1.382
abs coeff [mm^{-1}]	0.839	0.890	0.638	0.776	0.629	0.853	0.624
F(000)	1408	2784	916	2848	1616	664	1905
crystal size [mm^3]	0.15 x 0.133 x 0.1	0.24 x 0.1 x 0.1	0.5 x 0.4 x 0.3	0.4 x 0.277 x 0.08	0.35 x 0.24 x 0.12	0.45 x 0.23 x 0.04	0.48 x 0.33 x 0.18
θ range [°]	1.67 – 28.07	4.59 – 25.78	2.43 – 27.32	2.01 – 25.85	1.96 – 27.01	1.86 – 26.85	1.63 – 27.42
hkl-range	-12,12; -28,28; -19,18	-33,33;-12,12;-24,24	-13,13; -16,16; -20,20	-18,18; -20,19; -29,29	-16,16; -19,19; -27,26	-10,10; -14,14; -19,19	-21,21; -12,13; -32,32
no. of rflns collected	36387	35104	27982	69137	50973	18105	61077
no. of ind rflns, R_{int}	7279, 0.1045	5505, 0.1532	9362, 0.0632	5766/0.058	8092/0.0799	5791/0.1087	9893/0.0416
abs correction	Integration	integration	integration	integration	integration	integration	integration
weighting parameters a, b[A]	0.0355, 0	0.0428, 17.3928	0.0259, 0.9447	0.0216, 15.7103	0.0374, 0	0.0363, 9.7341	0.0348, 7.4081
GOF on F^2	0.980	1.123	1.029	1.135	0.967	1.089	1.021
R_1, wR_2 (all data)	0.0784/0.0836	0.0588/0.1143	0.0543/0.0672	0.0465/0.0785	0.0634/0.0754	0.0934/0.1590	0.0462/0.0892
R_1, wR_2 ($I > 2\sigma(I)$)	0.0447/0.0765	0.0477/0.1095	0.0349/0.0633	0.0365/0.0762	0.0380/0.0704	0.0620/0.1325	0.0357/0.0791
largest diff peak/hole [e/Å^3]	1.088/-0.828	1.480/-1.644	0.411/-0.770	1.346/-0.538	0.405/-0.586	1.236/-1.832	1.760/-1.115
remarks			positional disordered thf molecules		Positional disordered methyl group	positional disordered MeOH molecule	positional and substitutional disordered solvent molecules

[A]: weighting scheme: $w = 1/[\sigma^2(F_o^2) + (a \cdot P)^2 + b \cdot P)$, $P = [\max(F_o^2,0) + 2\,F_c^2]/3$.

Figure S1. ORTEP plot of complex **2a-DMSO**. Ellipsoids are shown with 50% probability. Hydrogen atoms are omitted for clarity.

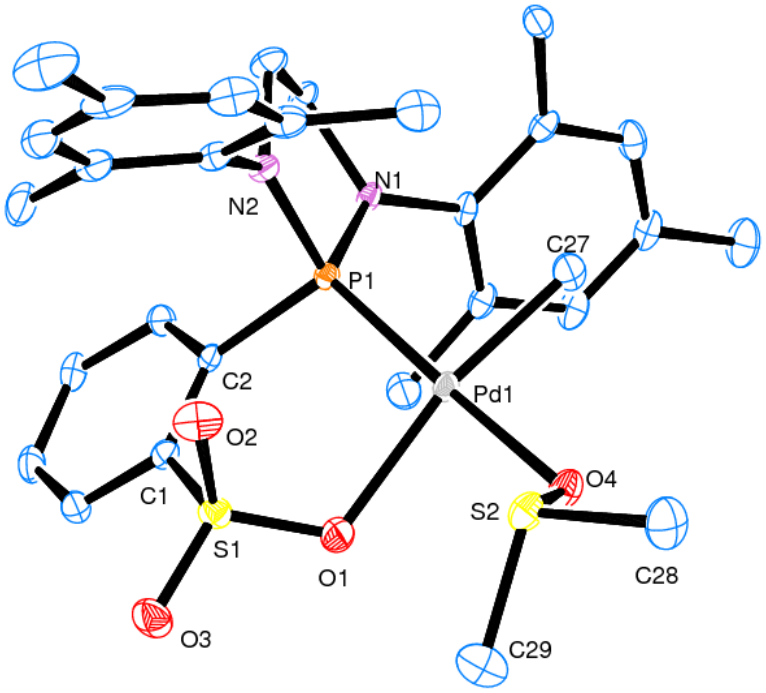


Figure S2. ORTEP plot of **2a-LiCl•(MeOH)**. Ellipsoids are shown with 50% probability. Hydrogen atoms are omitted for clarity.

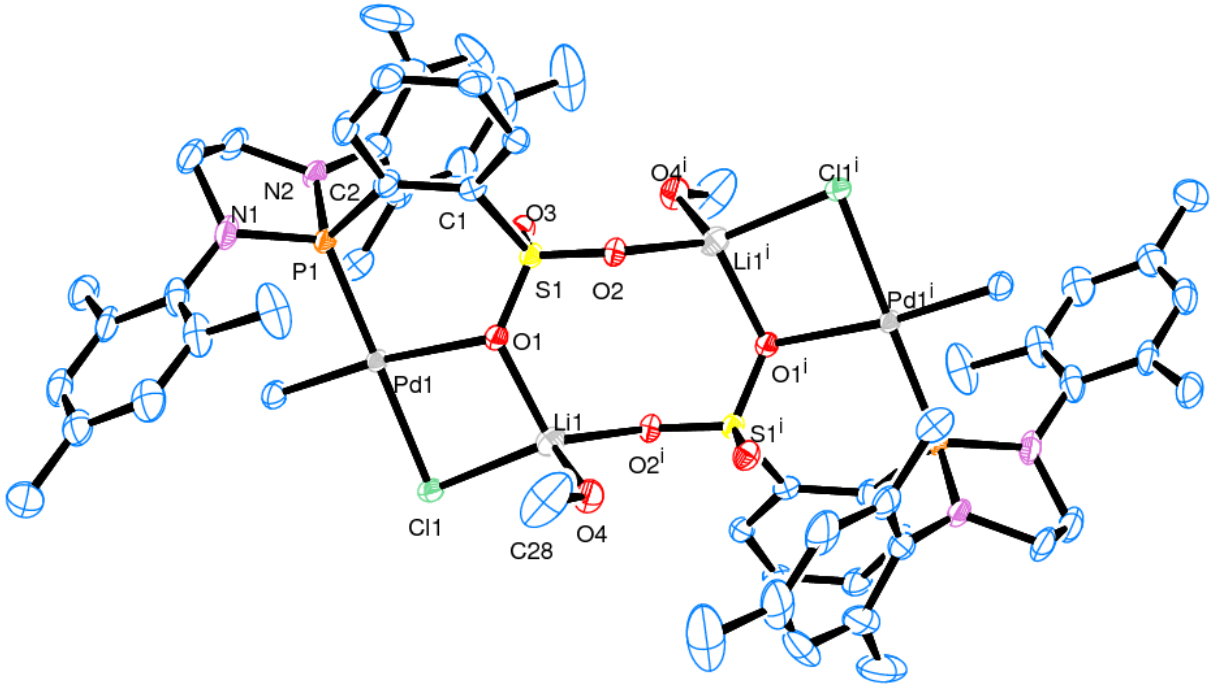


Figure S3. ORTEP plot of **2b-LiCl•(2 THF)**. Ellipsoids are shown with 50% probability. Hydrogen atoms as well as disordered THF molecules are omitted for clarity.

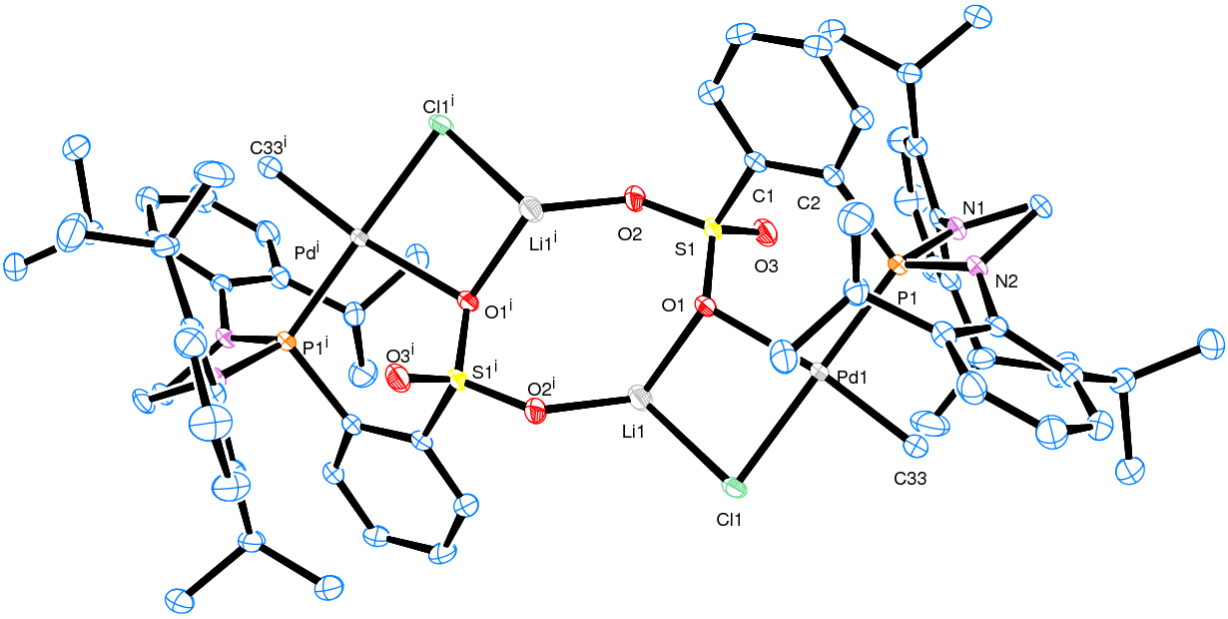


Figure S4. ORTEP plot of **3a**. Ellipsoids are shown with 50% probability. Hydrogen atoms are omitted for clarity.

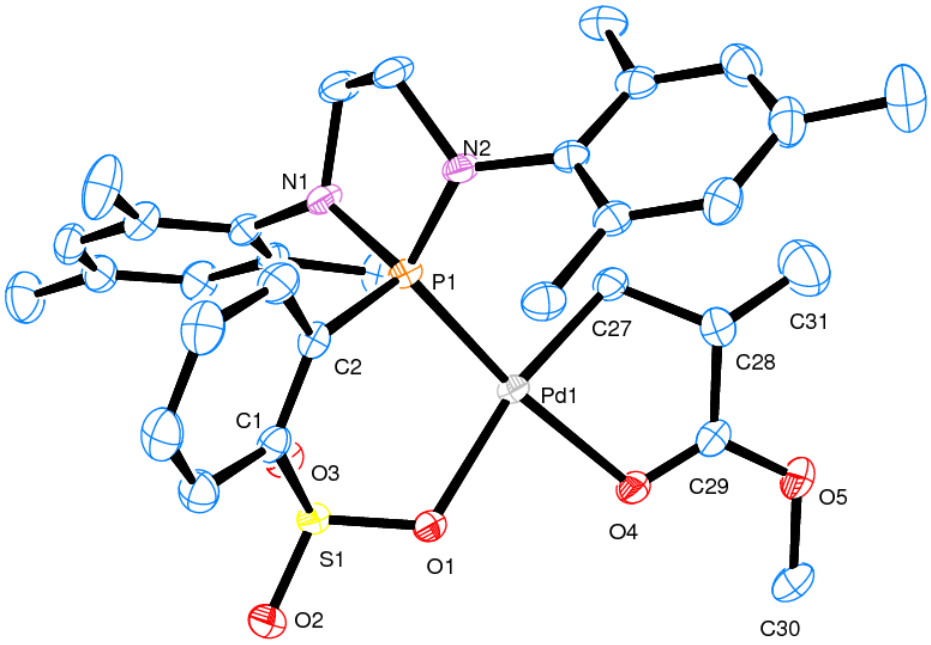


Figure S5. ORTEP plot of **3b**. Ellipsoids are shown with 50% probability. Hydrogen atoms as well as the disordered methyl position of C37 (C38) are omitted for clarity.

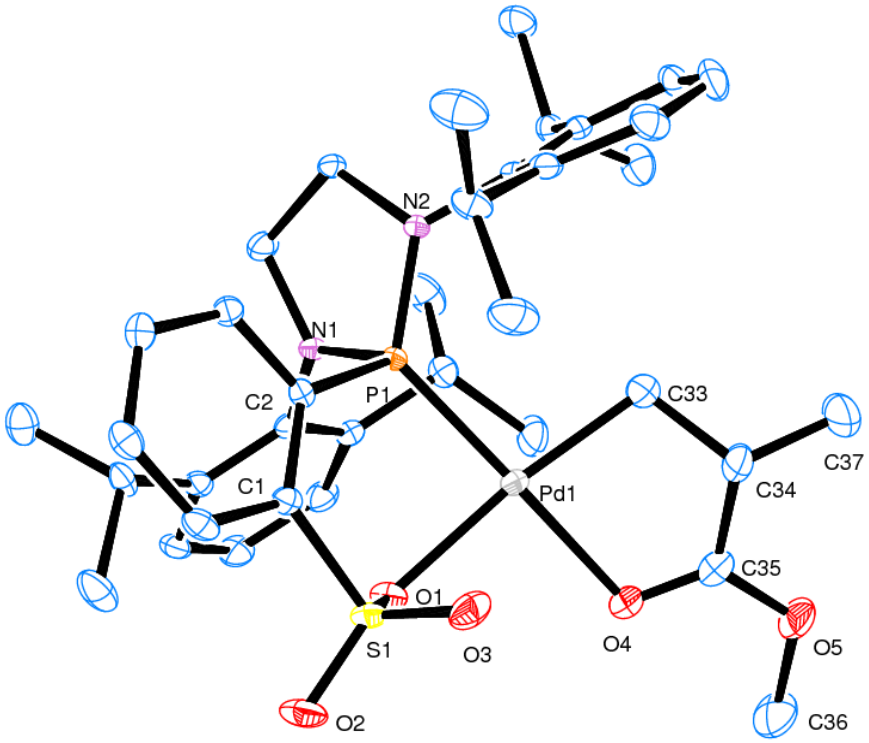


Figure S6. ORTEP plot of **6b-LiCl•(1.8 acetone, 0.2 dmso)**. Ellipsoids are shown with 50% probability. Hydrogen atoms as well as positional and substitutional disordered carbon and sulphur positions (O4, O5 are part of the acetone- and/or dmso-molecules, respectively) are omitted for clarity.

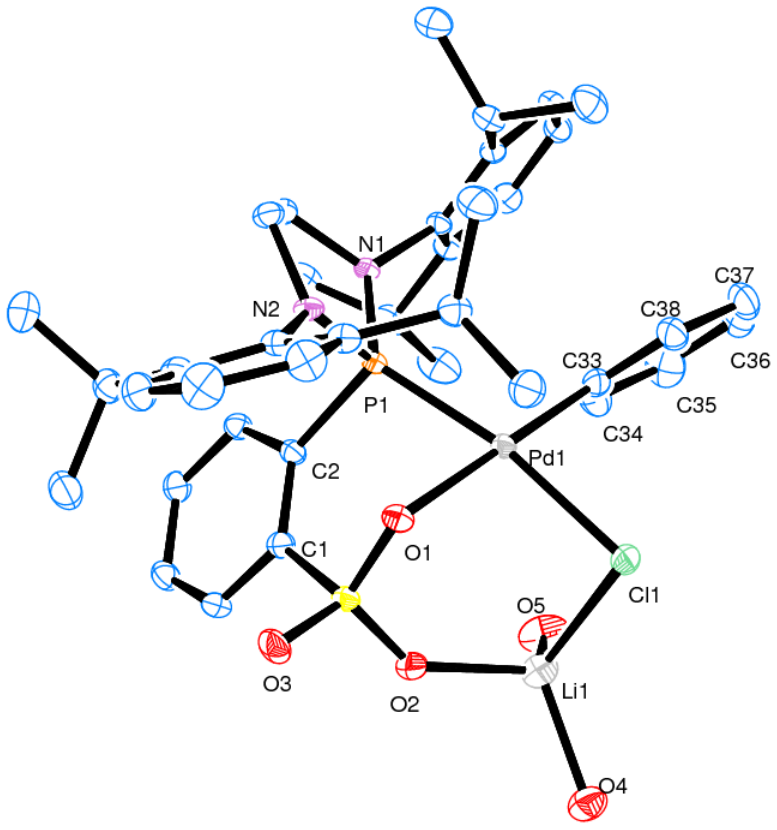
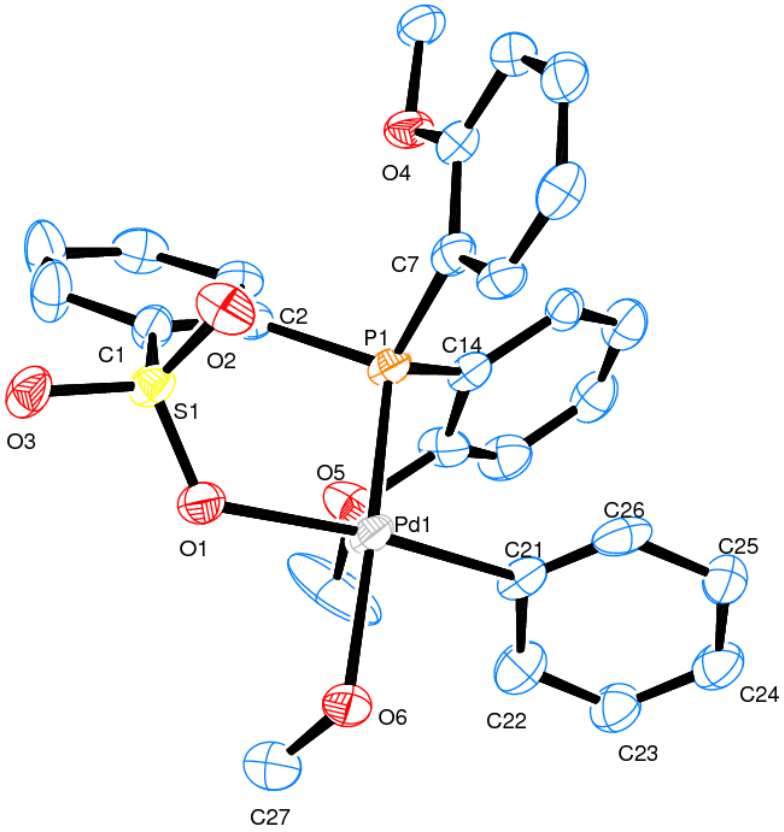


Figure S7. ORTEP plot of **4-(MeOH)•(MeOH)**. Ellipsoids are shown with 50% probability. Hydrogen atoms and one further MeOH molecule are omitted for clarity.



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(8) Faruggia LJ (2008) ORTEP-3 V2.02 for Windows XP, University of Glasgow, Scotland.

Figure S8: ^{1}H NMR (400 MHz, 298 K, acetone-d_6) of **2a-LiCl**

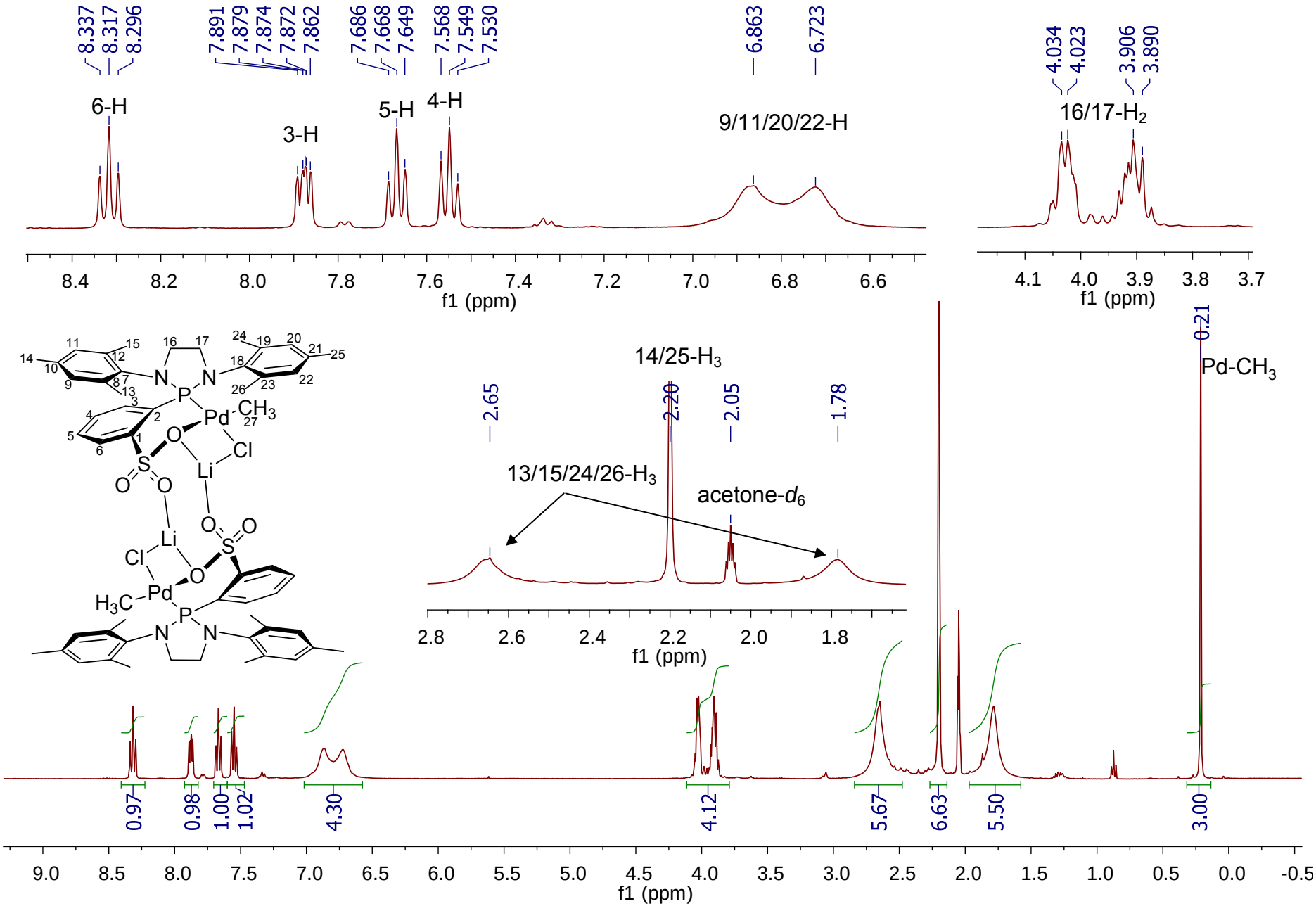


Figure S9: ^{13}C NMR (100 MHz, 298 K, acetone-d_6) of **2a-LiCl**

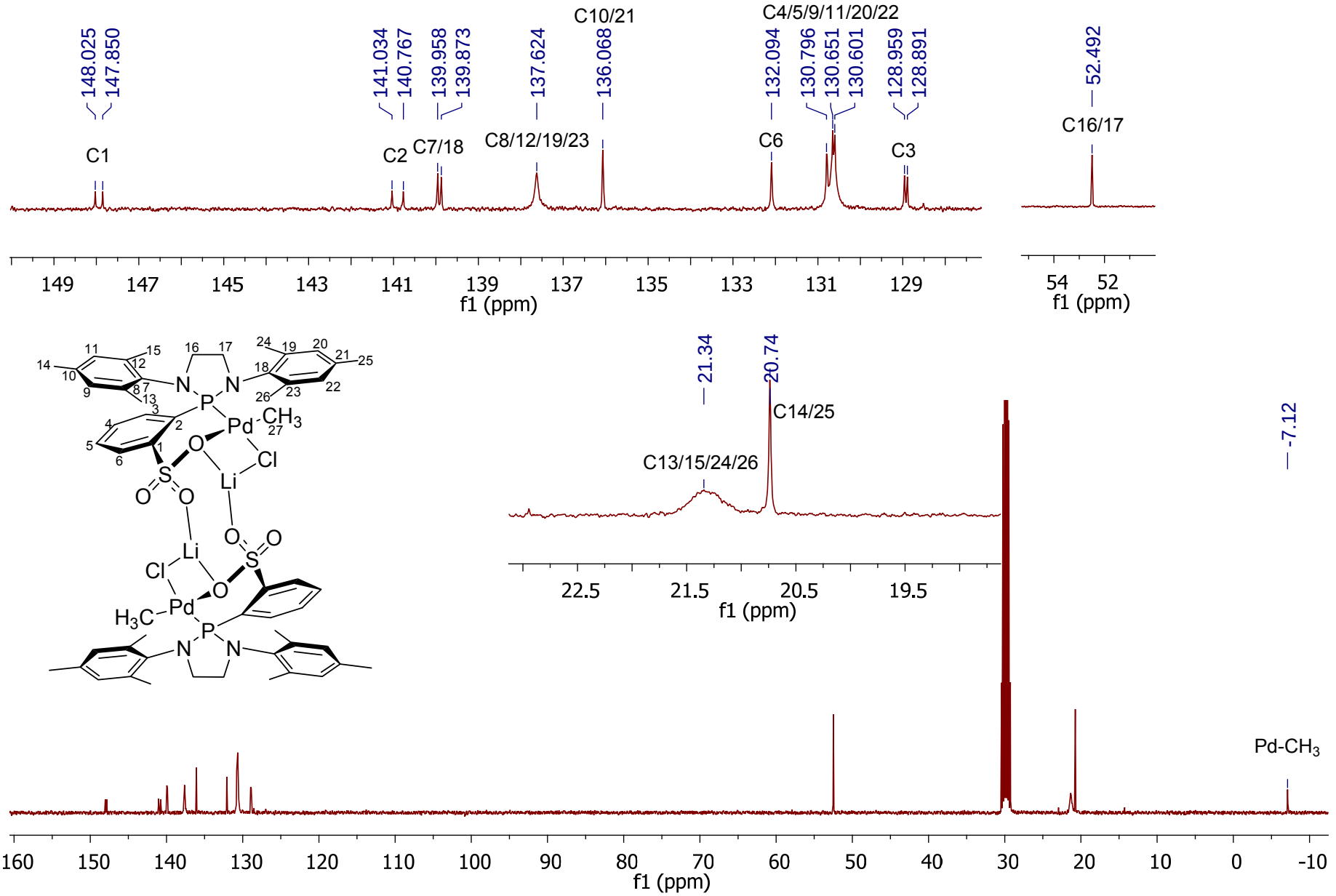


Figure S10: ^{31}P NMR (161 MHz, 298 K, acetone-d_6) of **2a-LiCl**

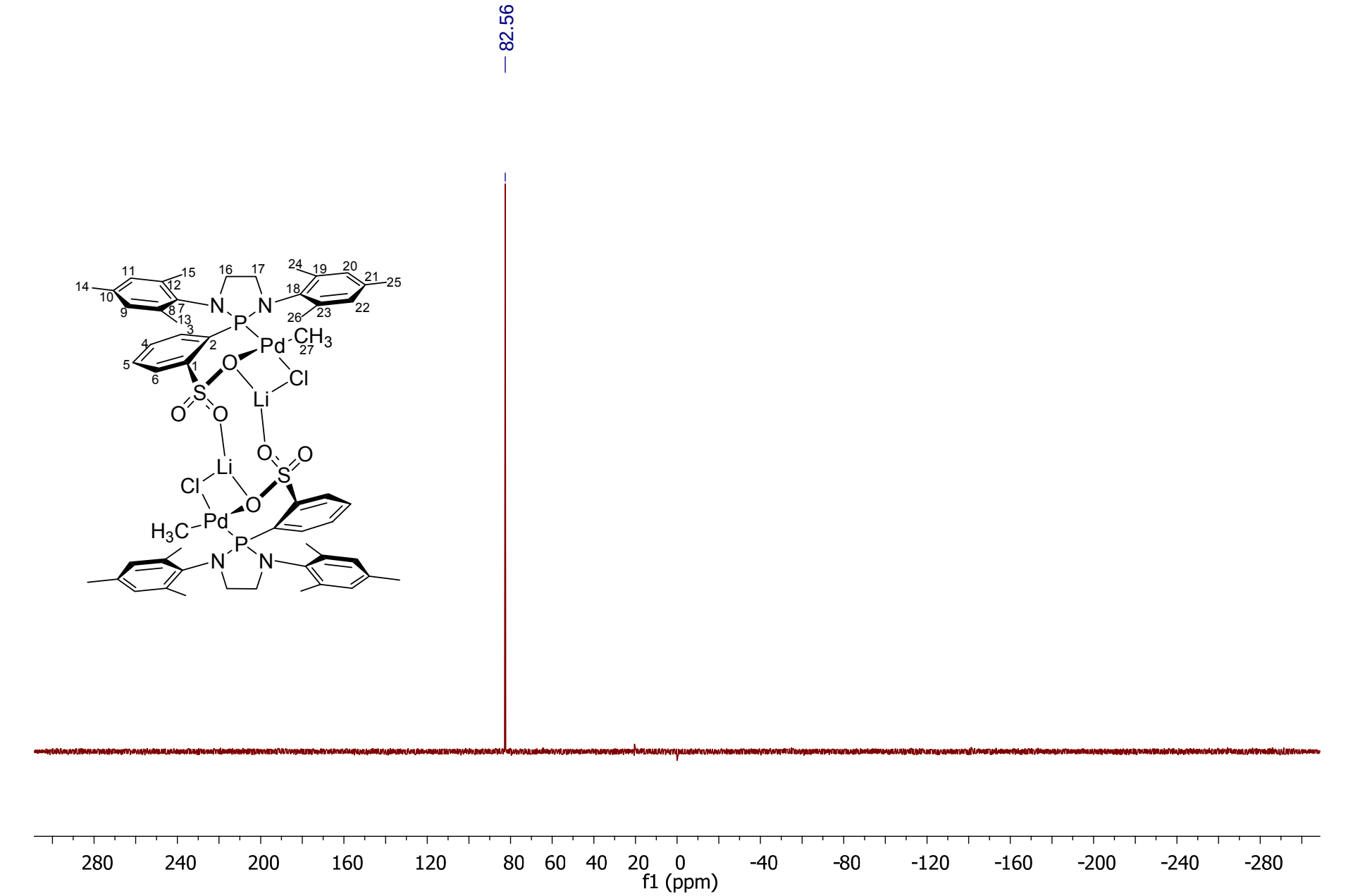


Figure S11: $^{1}H,^{1}H$ COSY NMR (400 MHz, 298 K, acetone-d_6) of **2a-LiCl**

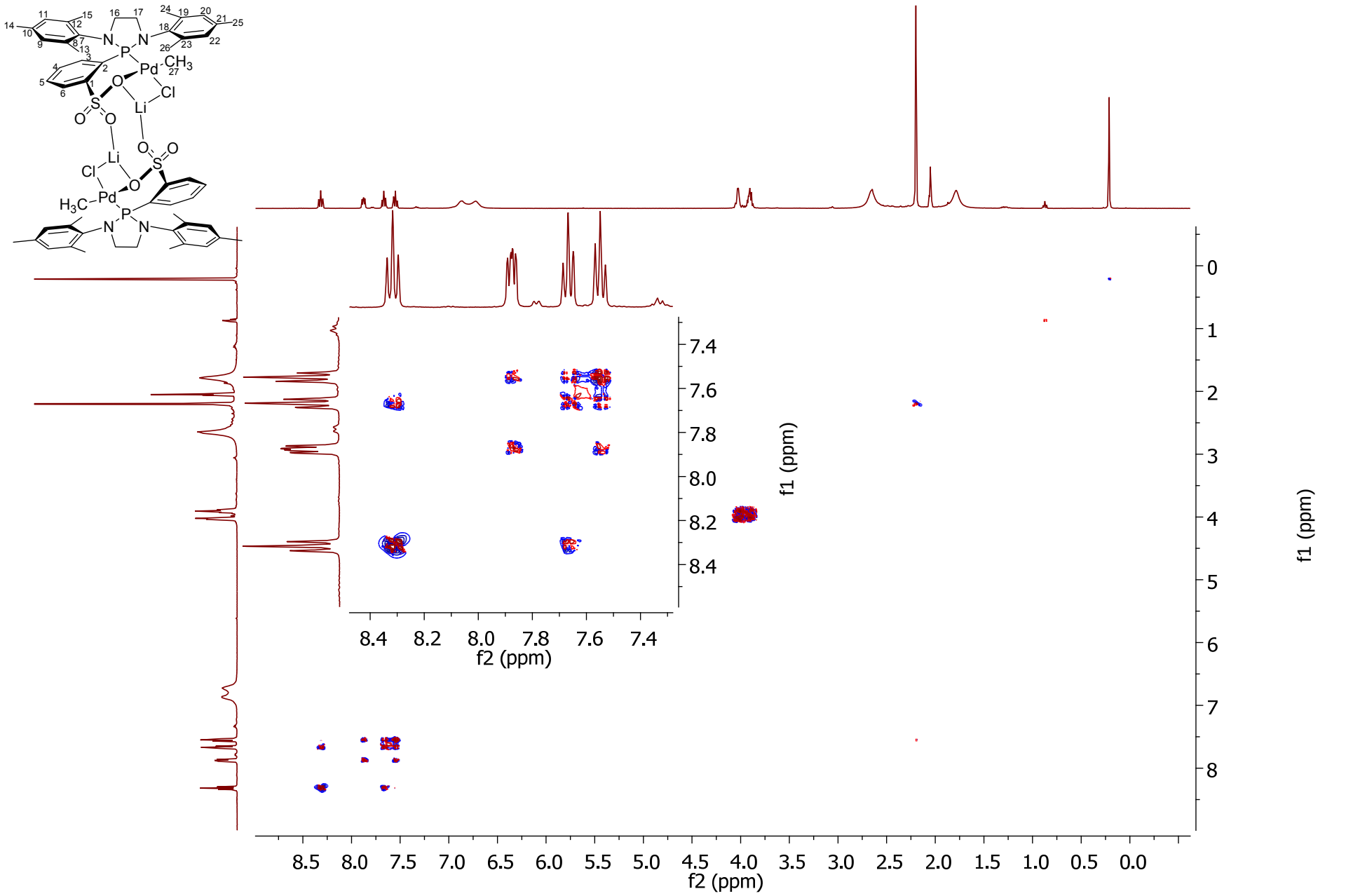


Figure S12: $^{1}H,^{13}C$ gHSQC NMR (400 MHz, 298 K, acetone-d_6) of **2a-LiCl** (CH and CH_3 red, CH_2 blue)

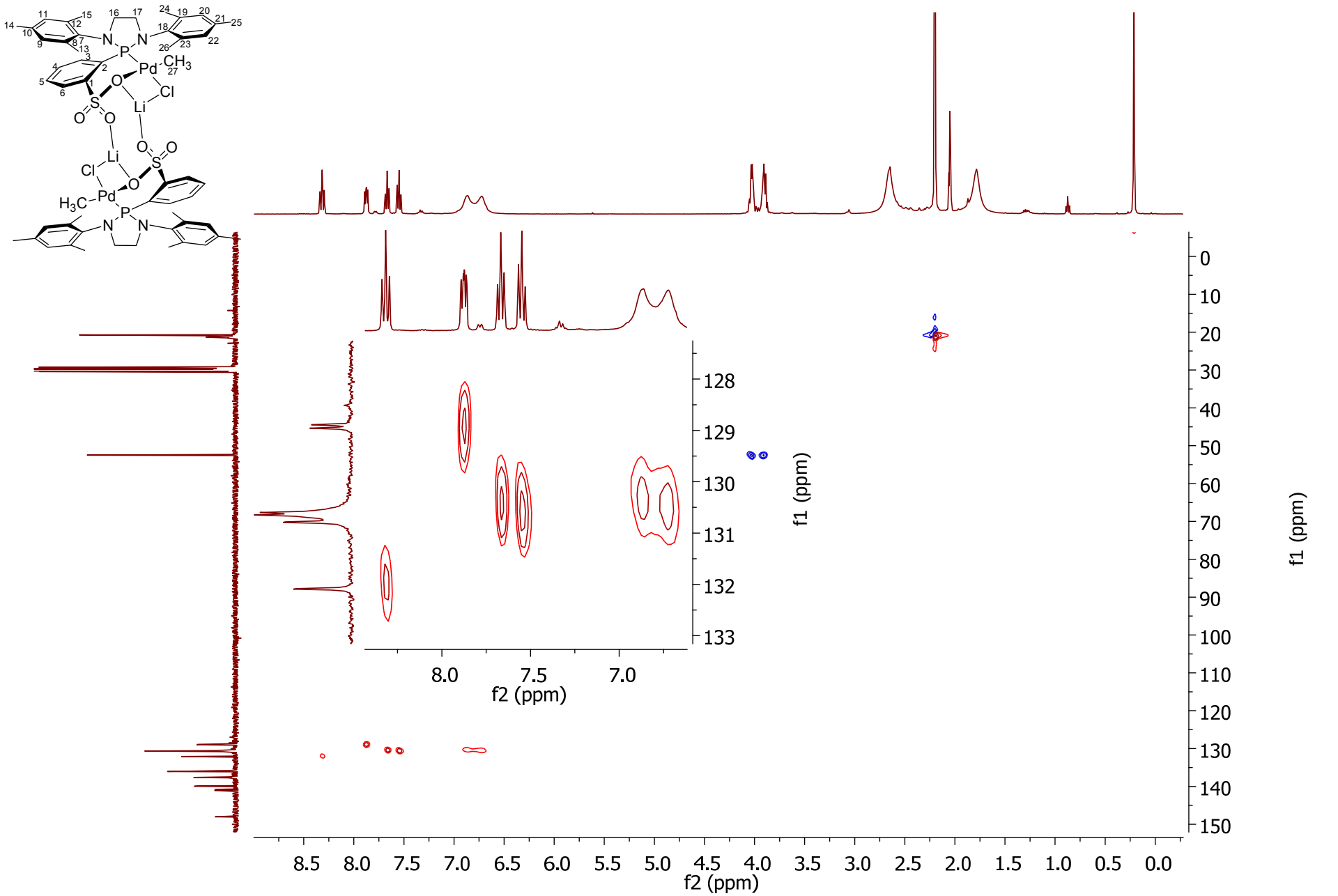


Figure S13: $^{1}H,^{13}C$ gHMBC NMR (400 MHz, 298 K, acetone-d_6) of **2a-LiCl**

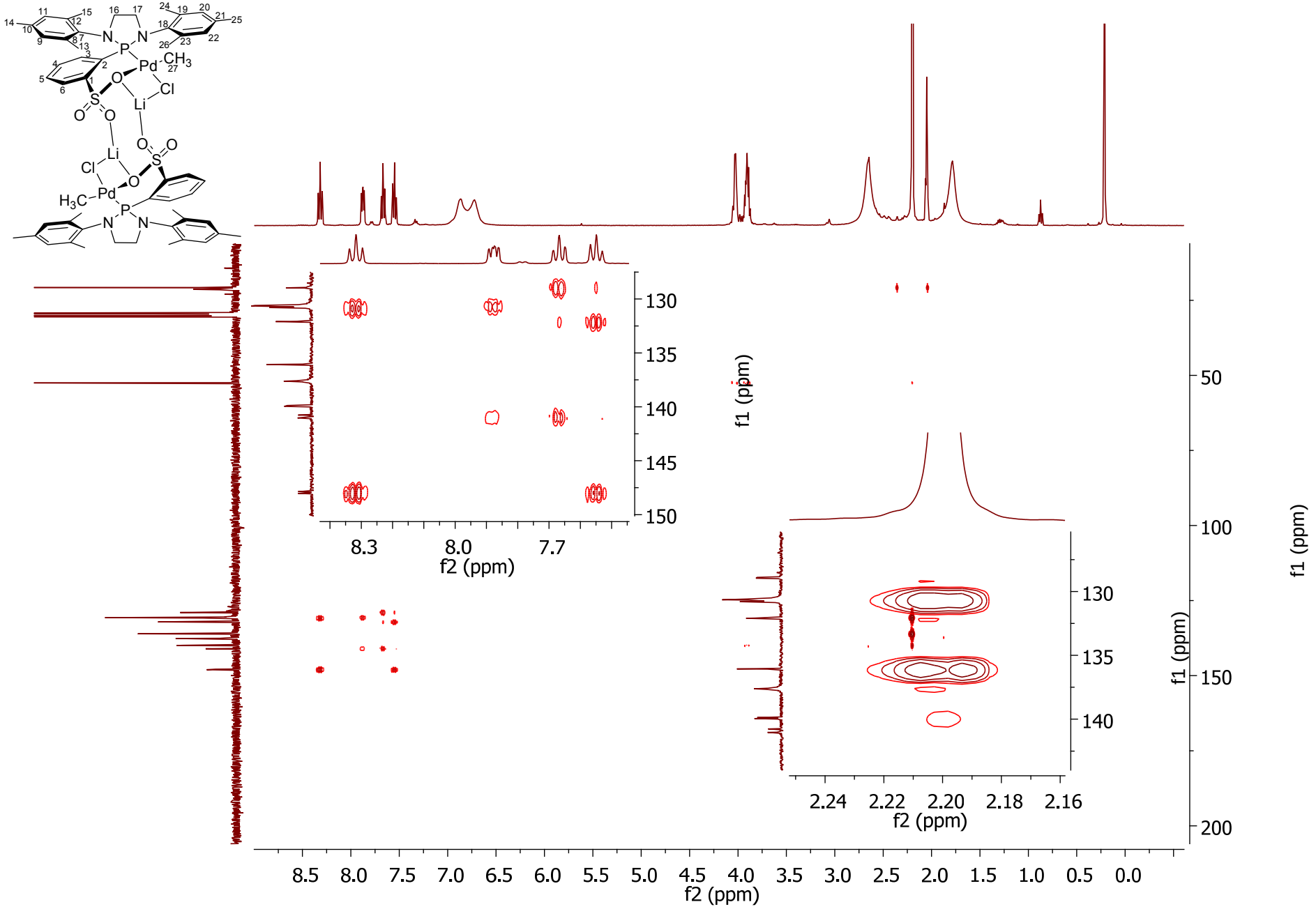


Figure S14: ^{1}H NMR (400 MHz, 298 K, acetone-d_6) of **2b-LiCl·(0.5 Et_2O)**

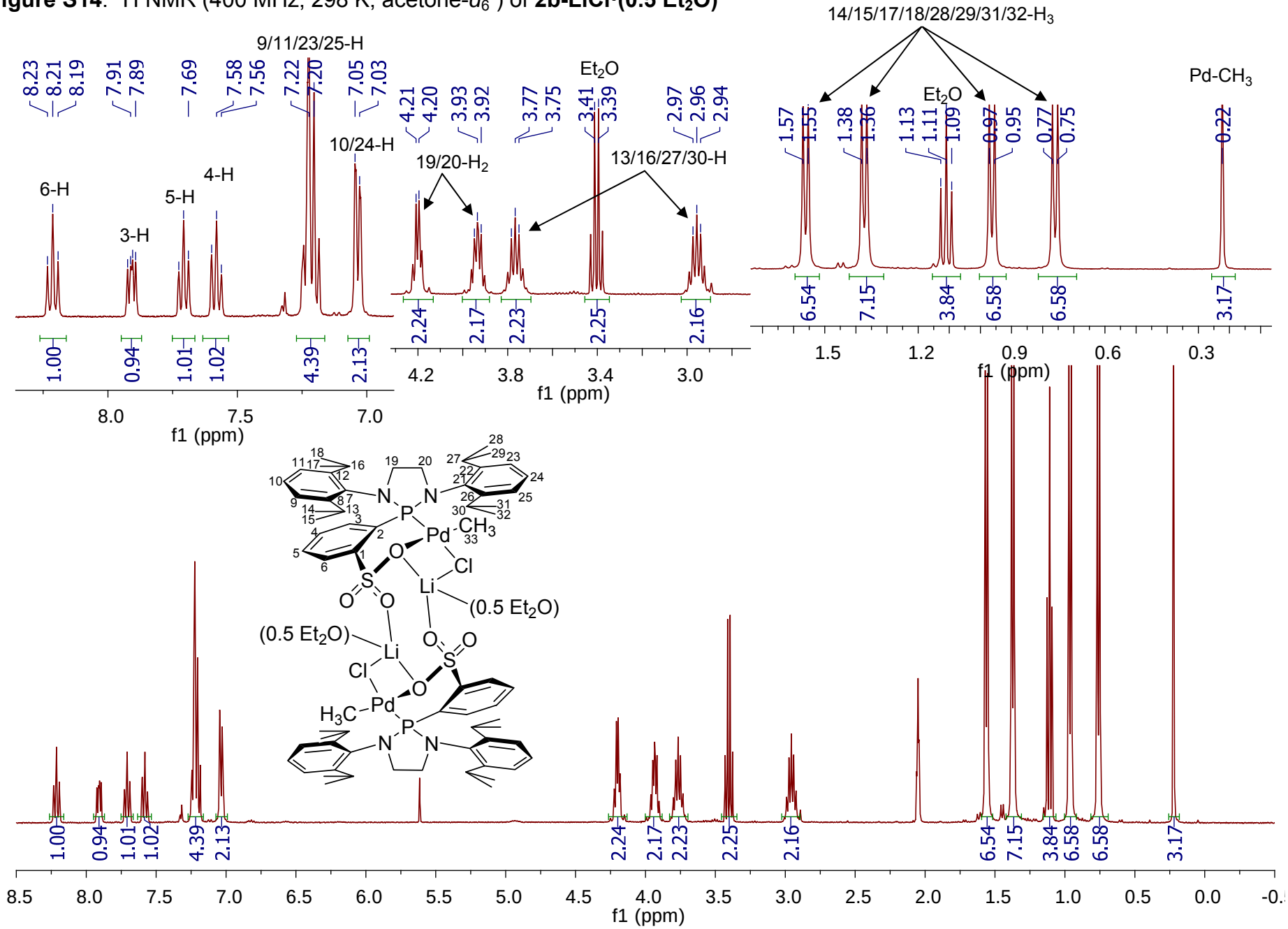


Figure S15: ^{13}C NMR (100 MHz, 298 K, acetone-d_6) of **2b-LiCl·(0.5 Et_2O)**

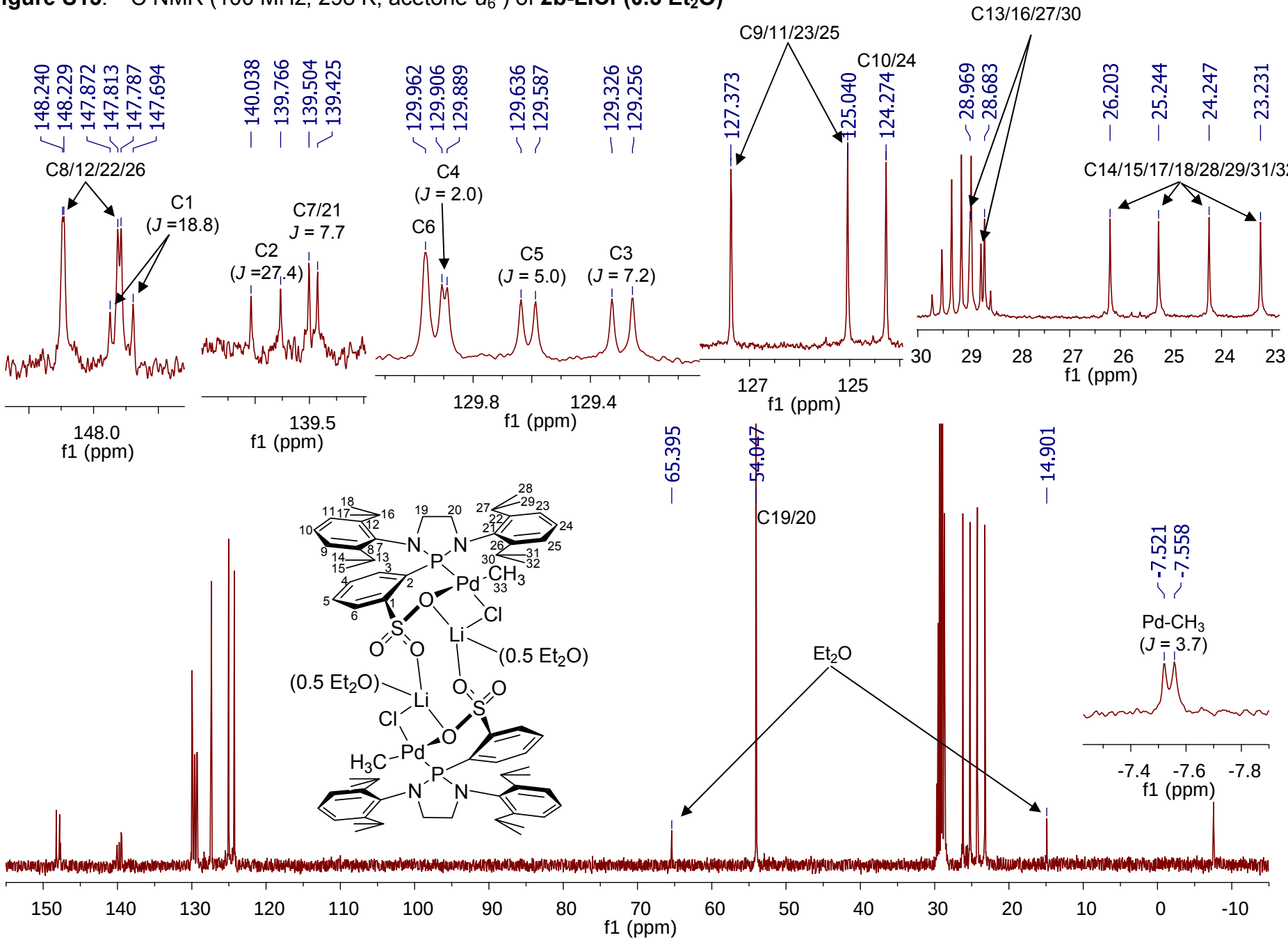


Figure S16: ^{31}P NMR (161 MHz, 298 K, acetone-d_6) of **2b-LiCl·(0.5 Et_2O)**

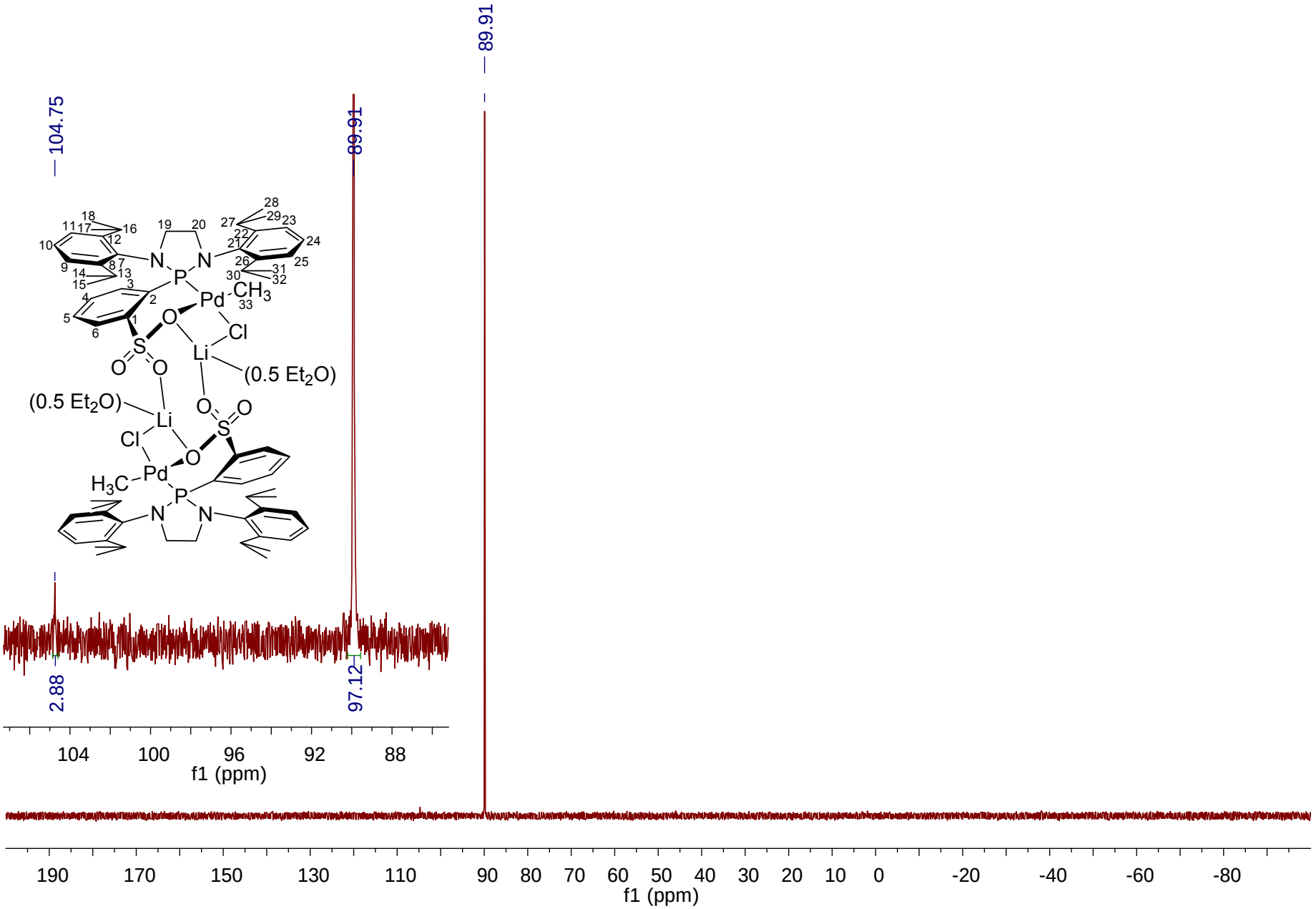


Figure S17: $^{1}H,^{1}H$ COSY NMR (400 MHz, 298 K, acetone-d_6) of **2b-LiCl·(0.5 Et_2O)**

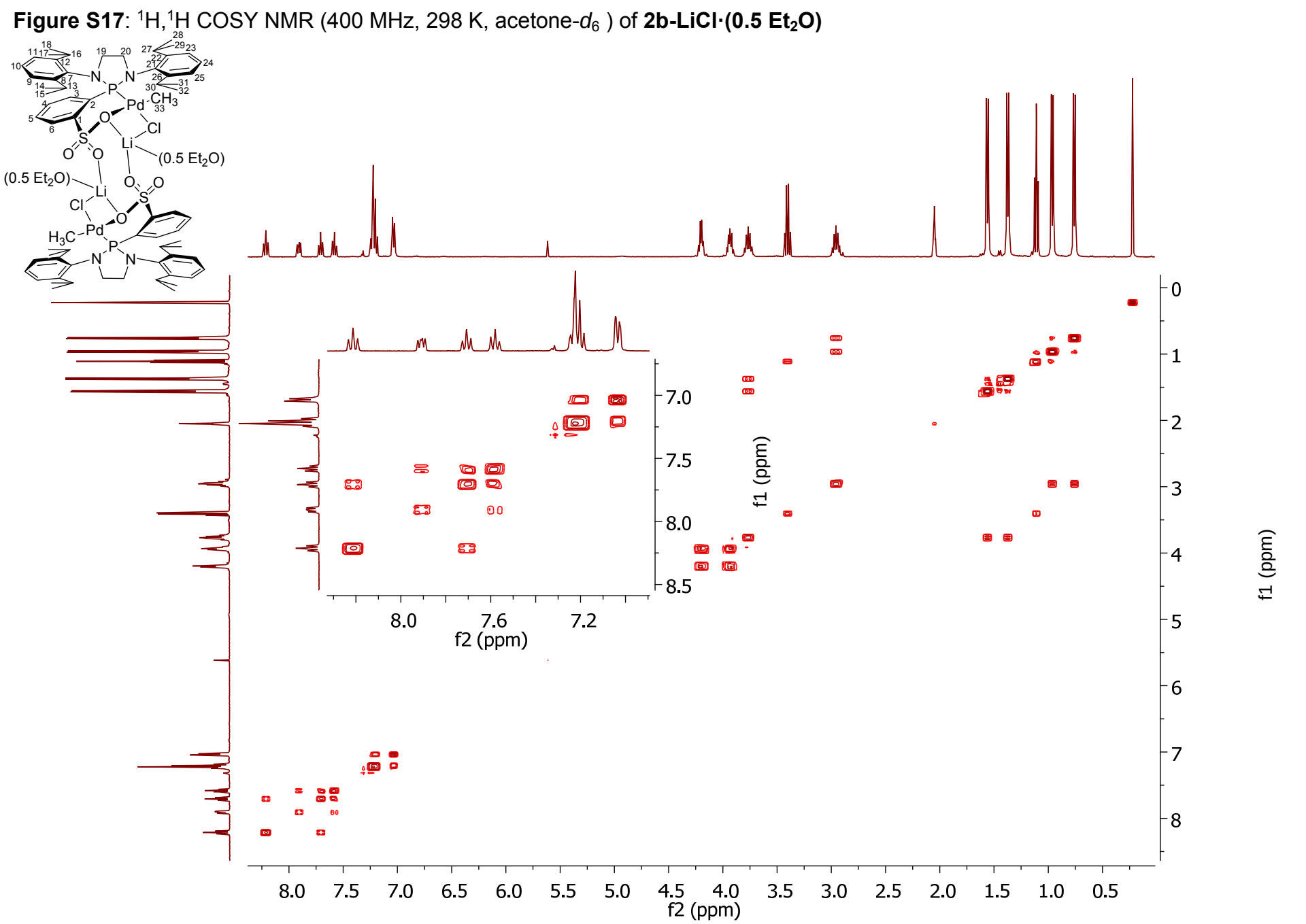
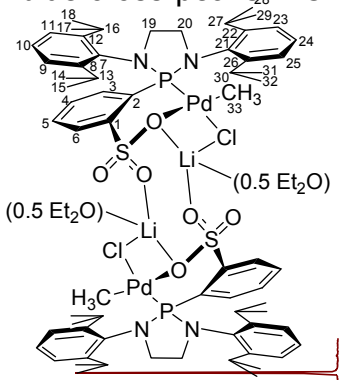


Figure S18: $^{1}H,^{1}H$ NOESY NMR (400 MHz, 298 K, acetone-d_6) of **2b-LiCl·(0.5 Et_2O)** (red cross-peaks: chemical exchange, blue cross-peaks: NOE)



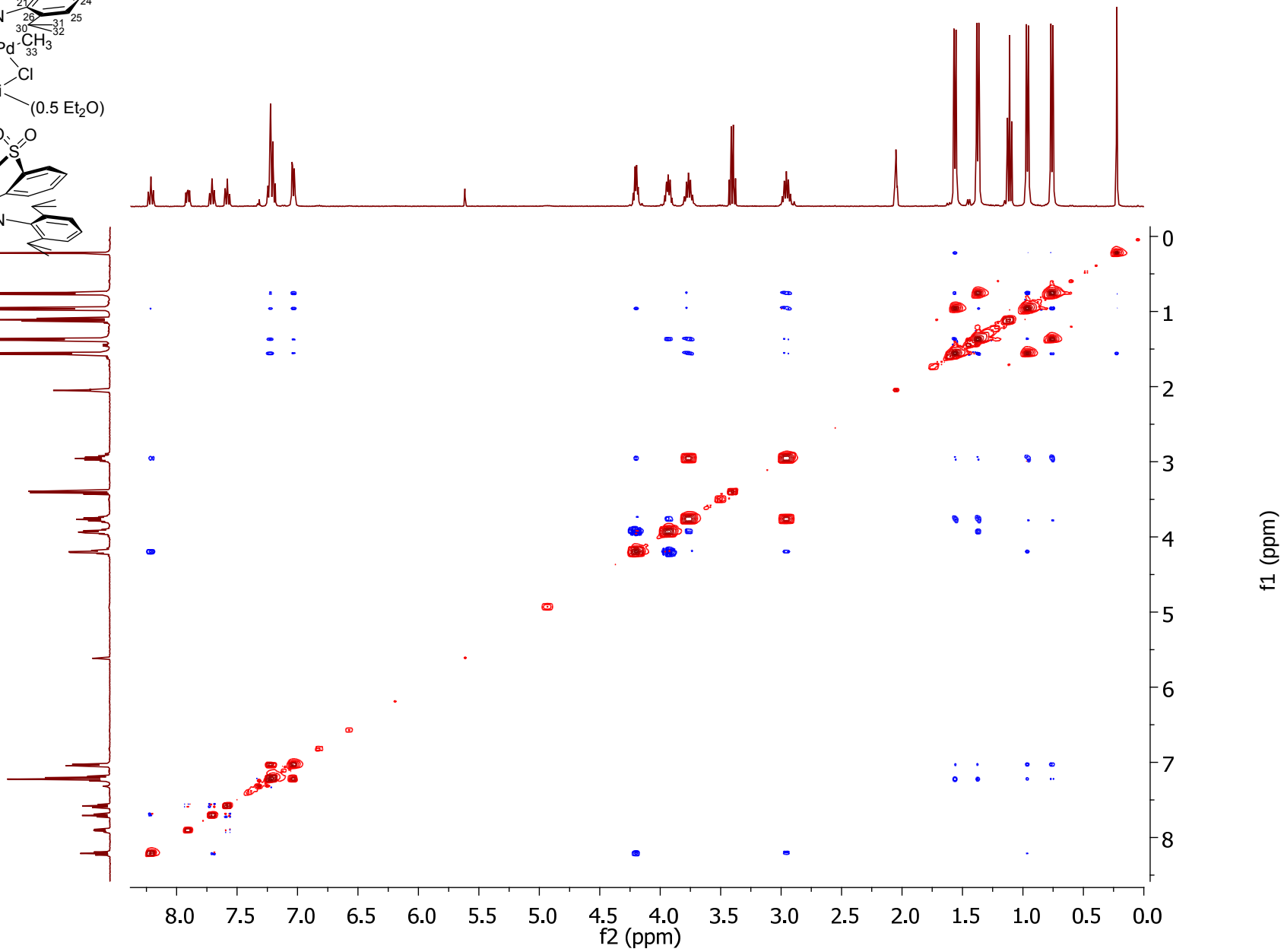


Figure S19: $^{1}H,^{13}C$ gHMQC NMR (400 MHz, 298 K, acetone-d_6) of **2b-LiCl·(0.5 Et_2O)**

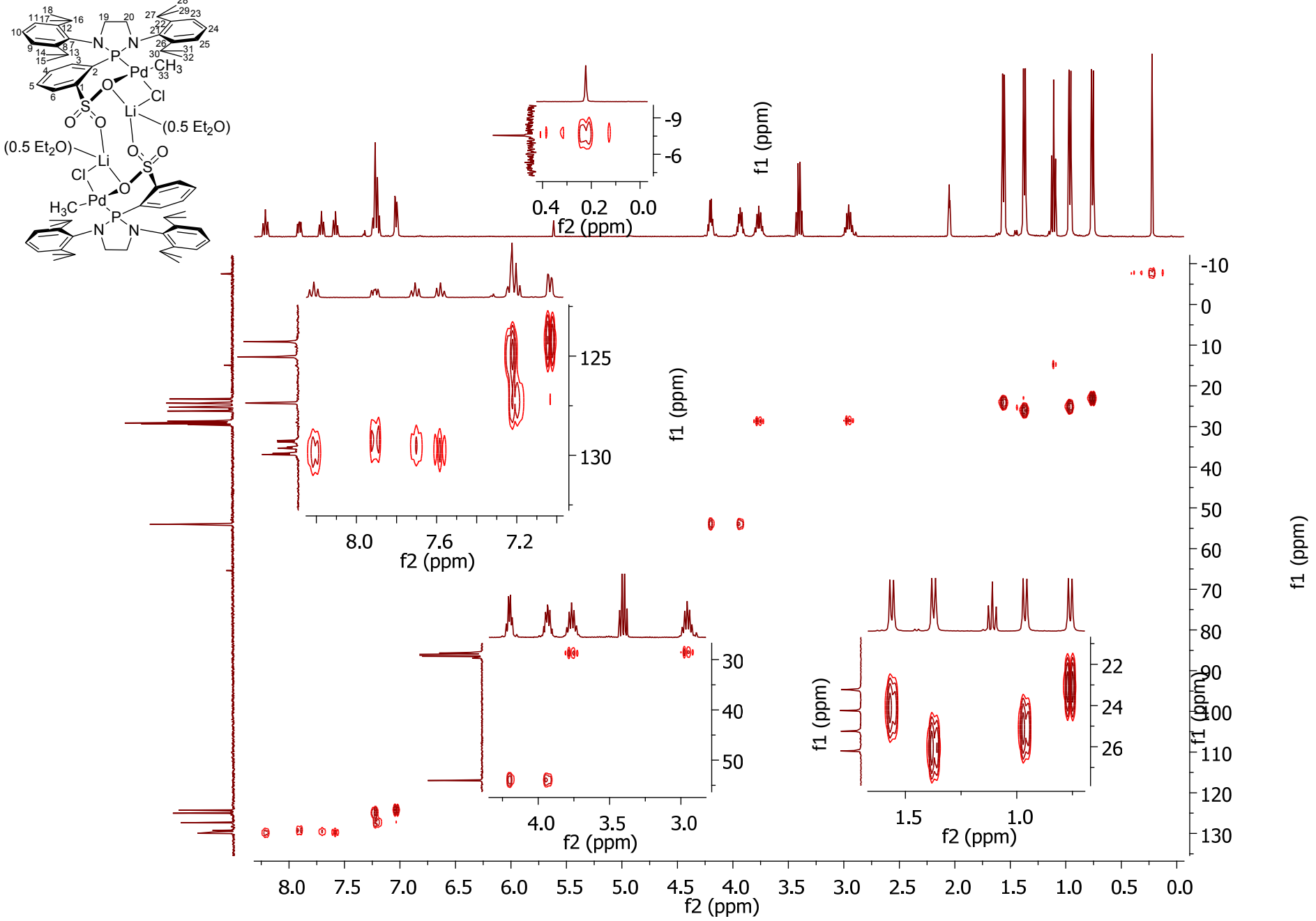


Figure S20: $^{1}H,^{13}C$ gHMBC NMR (400 MHz, 298 K, acetone-d_6) of **2b-LiCl·(0.5 Et_2O)**

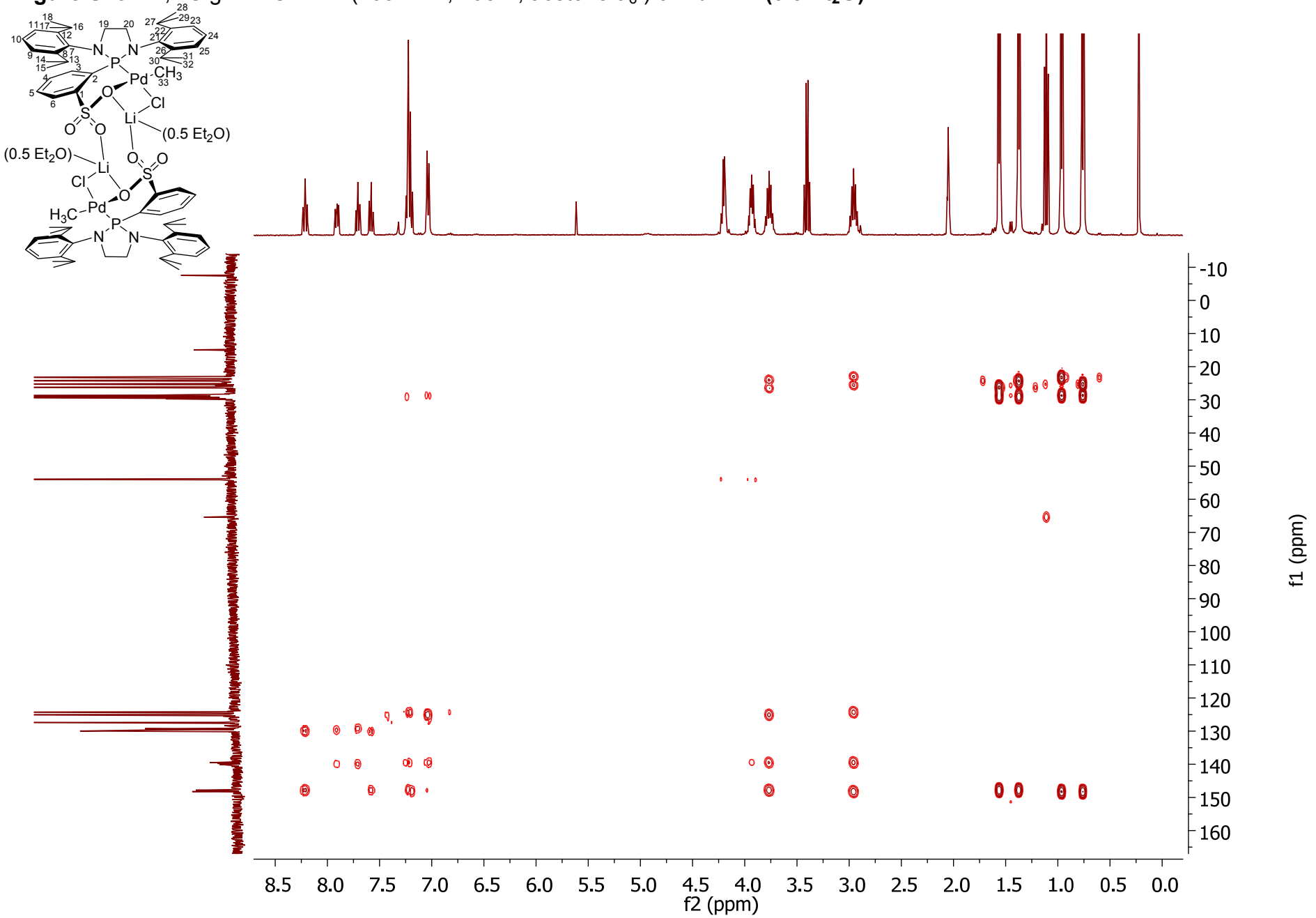


Figure S21: ^{1}H NMR (400 MHz, 298 K, methylene chloride-d_2) of crude **3a** after vaccum-removal of excess methyl acrylate

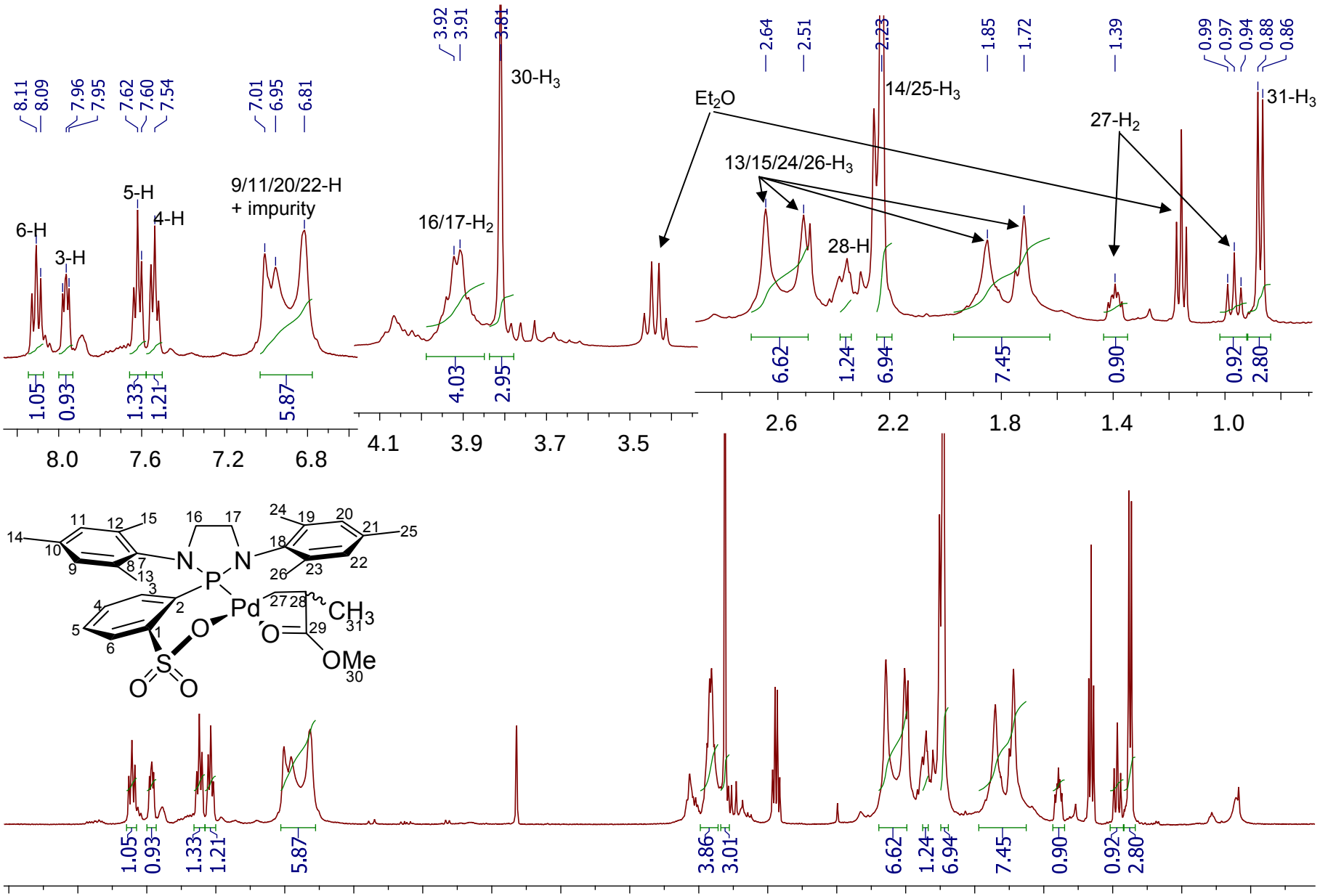


Figure S22: ^{13}C NMR (100 MHz, 298 K, methylene chloride-d_2) of crude **3a** after vaccum-removal of excess methyl acrylate

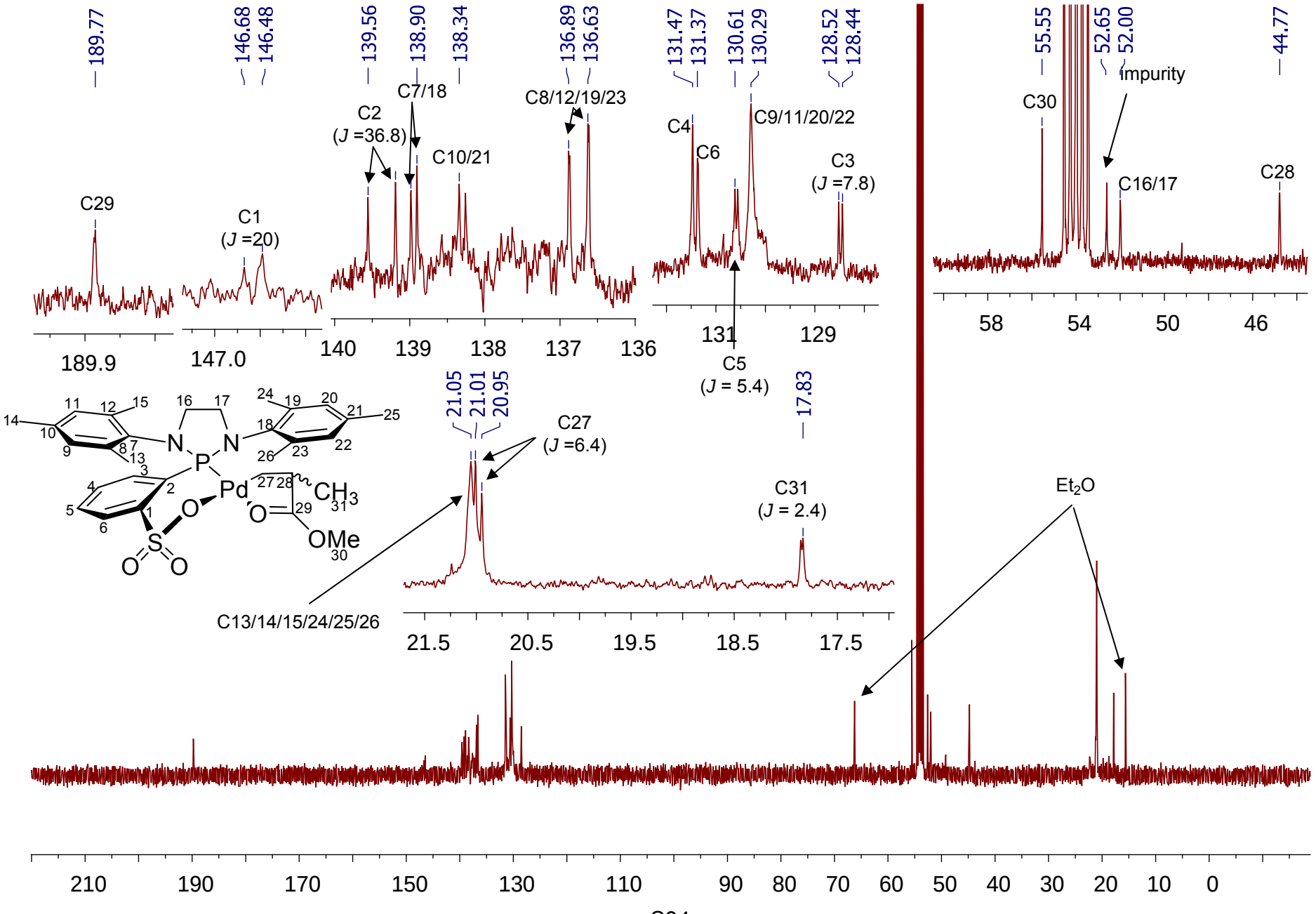


Figure S23: ^{31}P NMR (161 MHz, 298 K, methylene chloride-d_2) of crude **3a** after vaccum-removal of excess methyl acrylate

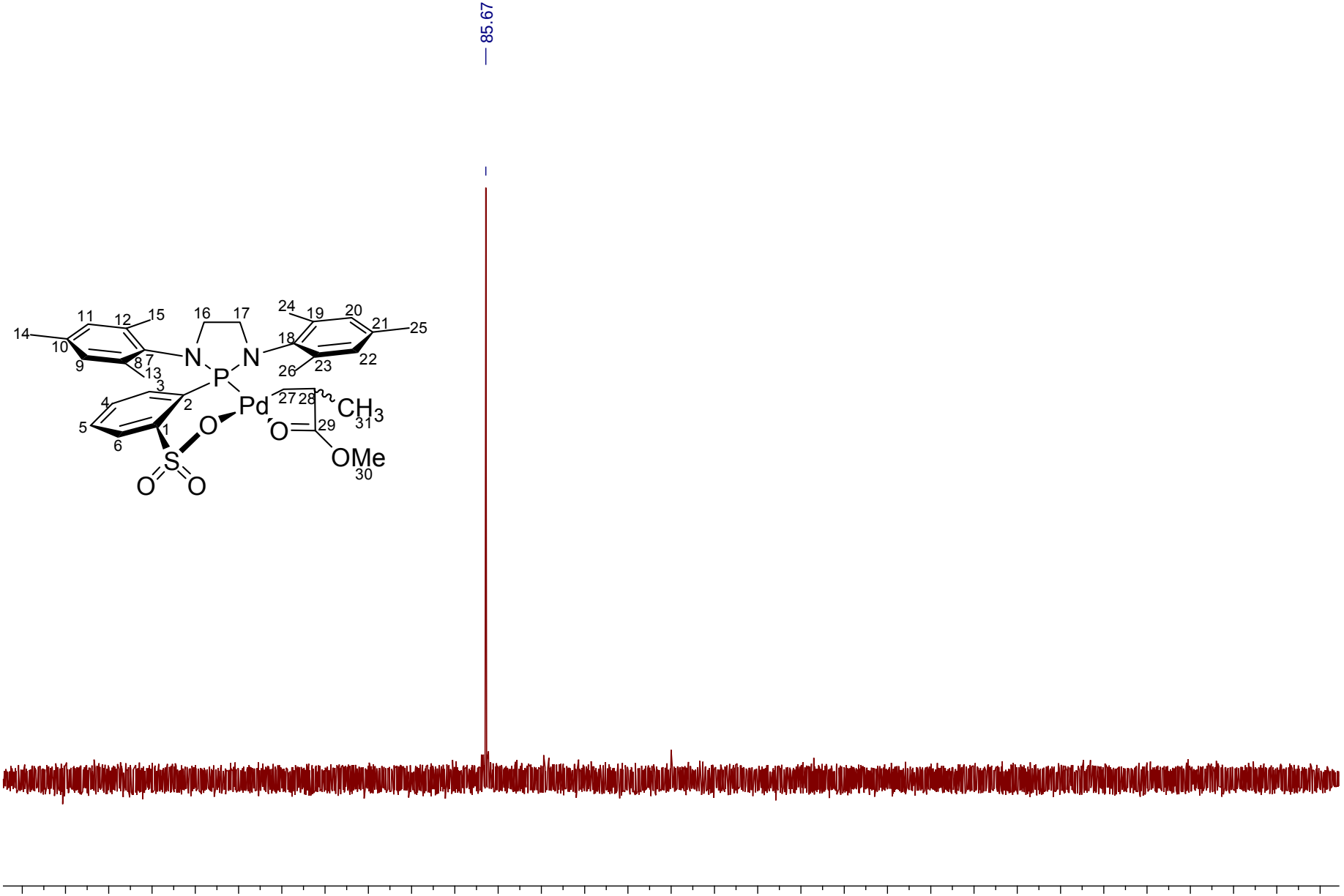


Figure S24: $^{1}H,^{1}H$ COSY NMR (400 MHz, 298 K, methylene chloride-d_2) of crude **3a** after vaccum-removal of excess methyl acrylate

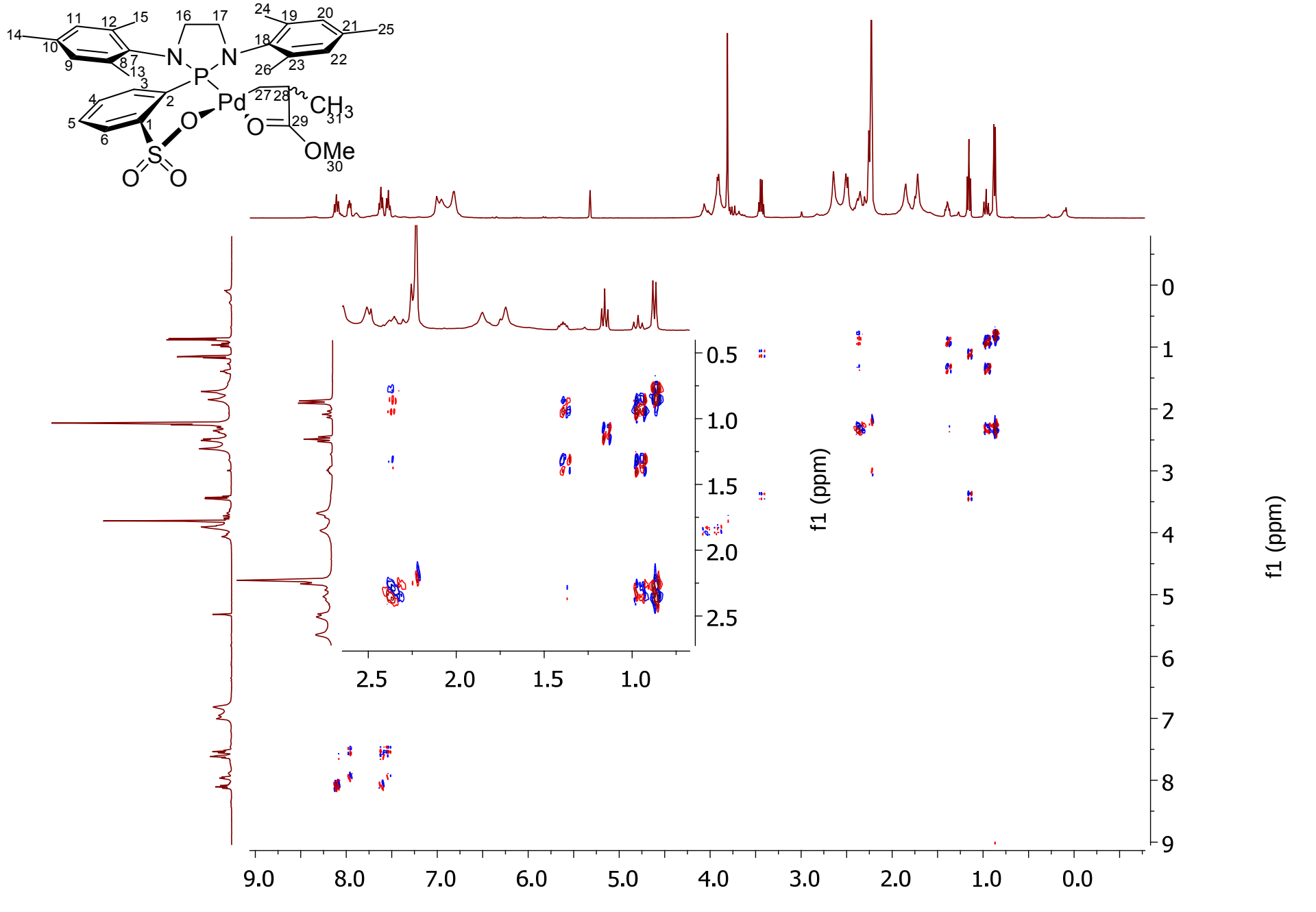


Figure S25: $^{1}H,^{13}C$ gHSQC NMR (400 MHz, 298 K, methylene chloride-d_2) of crude **3a** after vaccum-removal of excess methyl acrylate (CH and CH_3: red; CH_2: blue

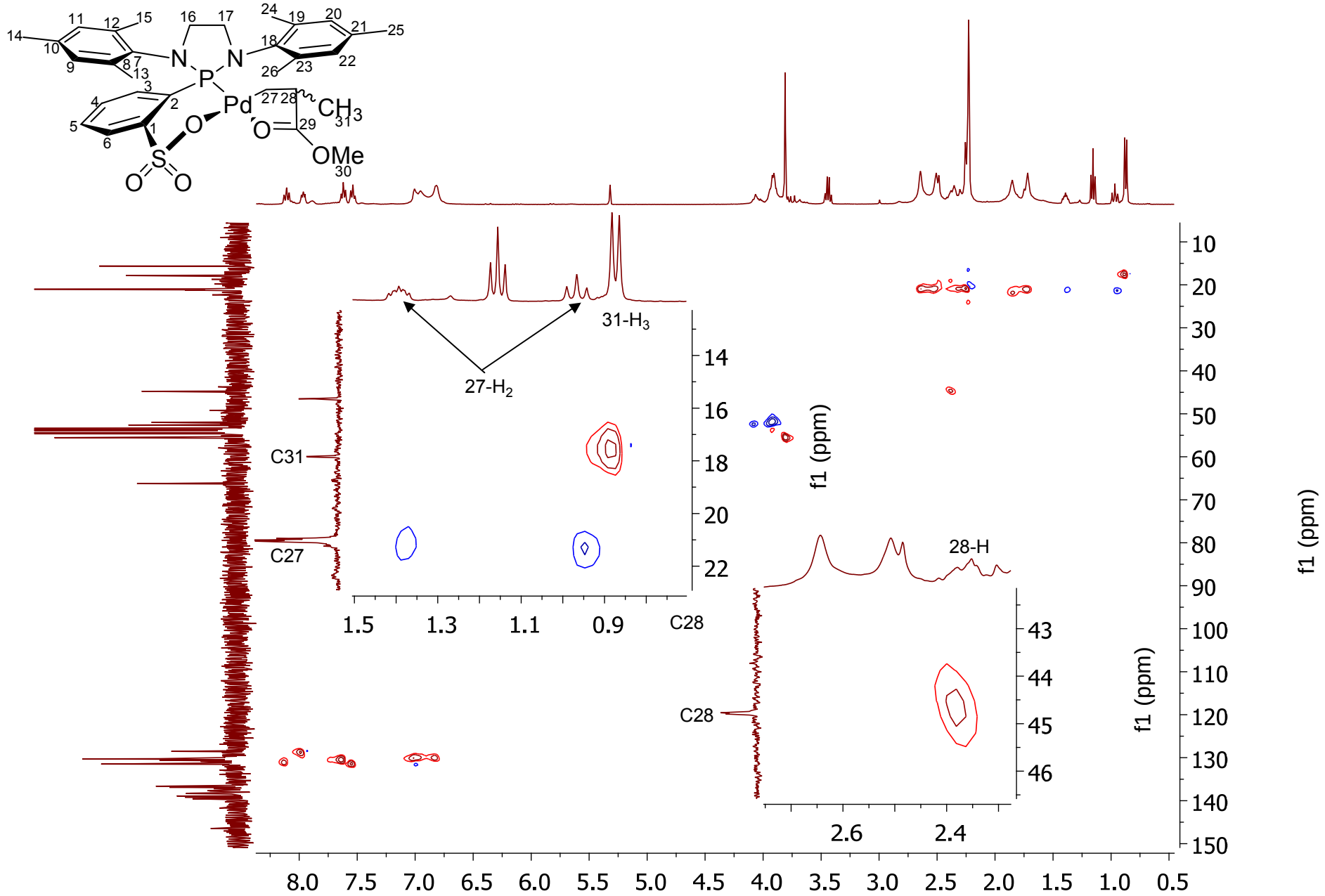


Figure S26: $^{1}H,^{13}C$ gHMBC NMR (400 MHz, 298 K, methylene chloride-d_2) of crude **3a** after vaccum-removal of excess methyl acrylate

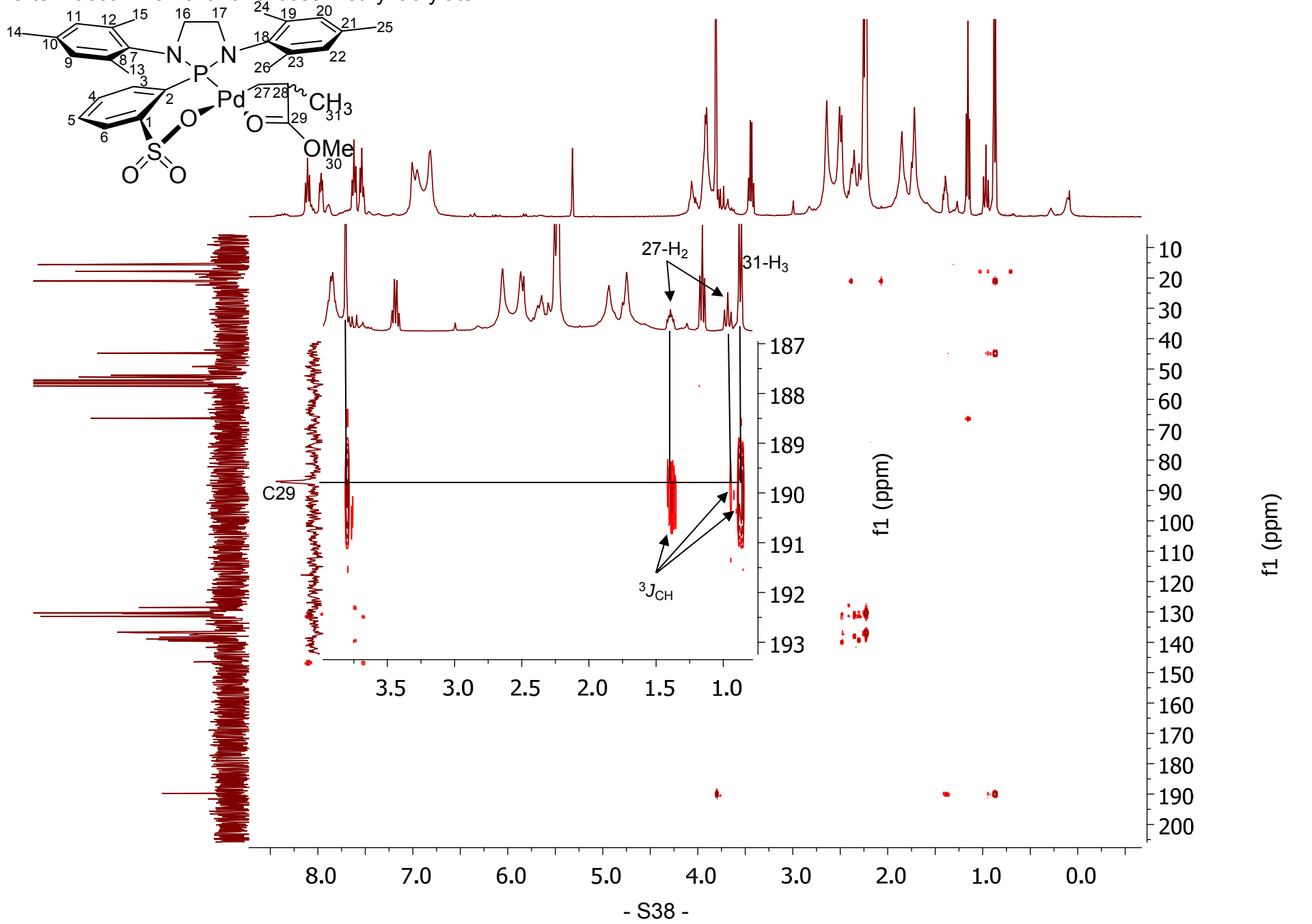


Figure S27: ^{1}H NMR (400 MHz, 298 K, methylene chloride-d_2) of crude **3b** after removal of of excess MA under vacuum

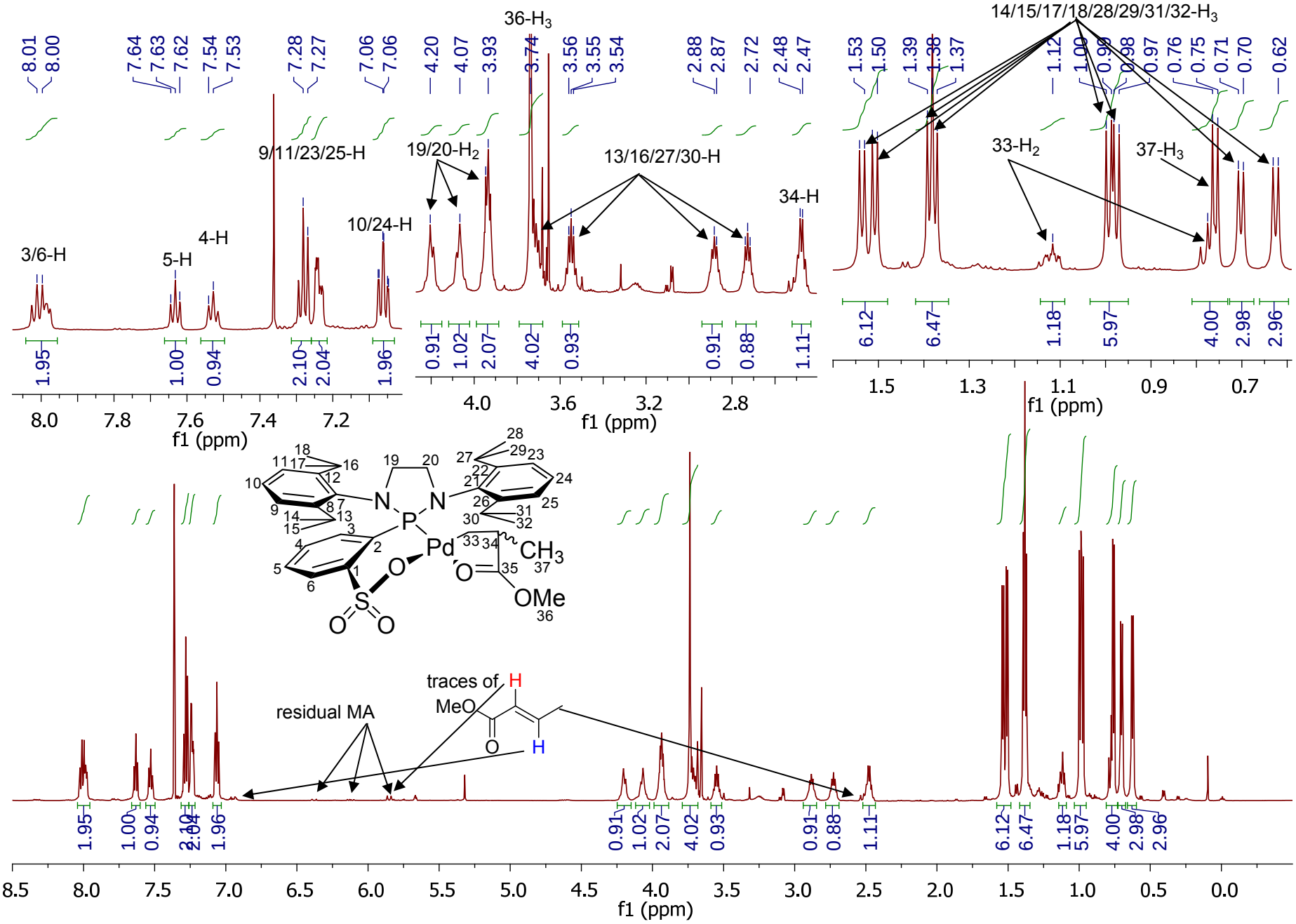


Figure S28: ^{13}C NMR (100 MHz, 298 K, methylene chloride-d_2) of crude **3b** after removal of of excess MA under vacuum

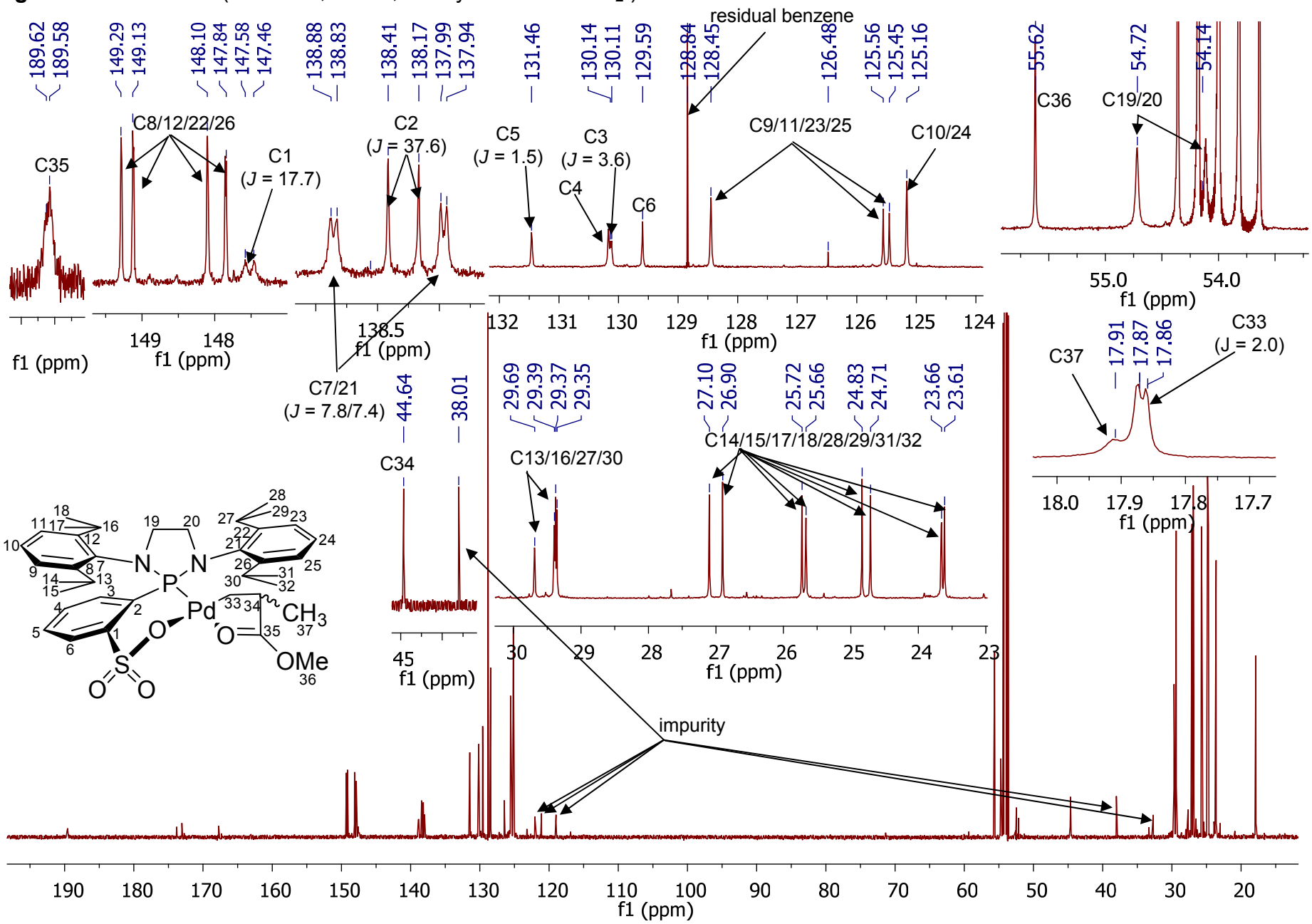


Figure S29: ^{31}P NMR (161 MHz, 298 K, methylene chloride-d_2) of crude **3b** after removal of of excess MA under vacuum

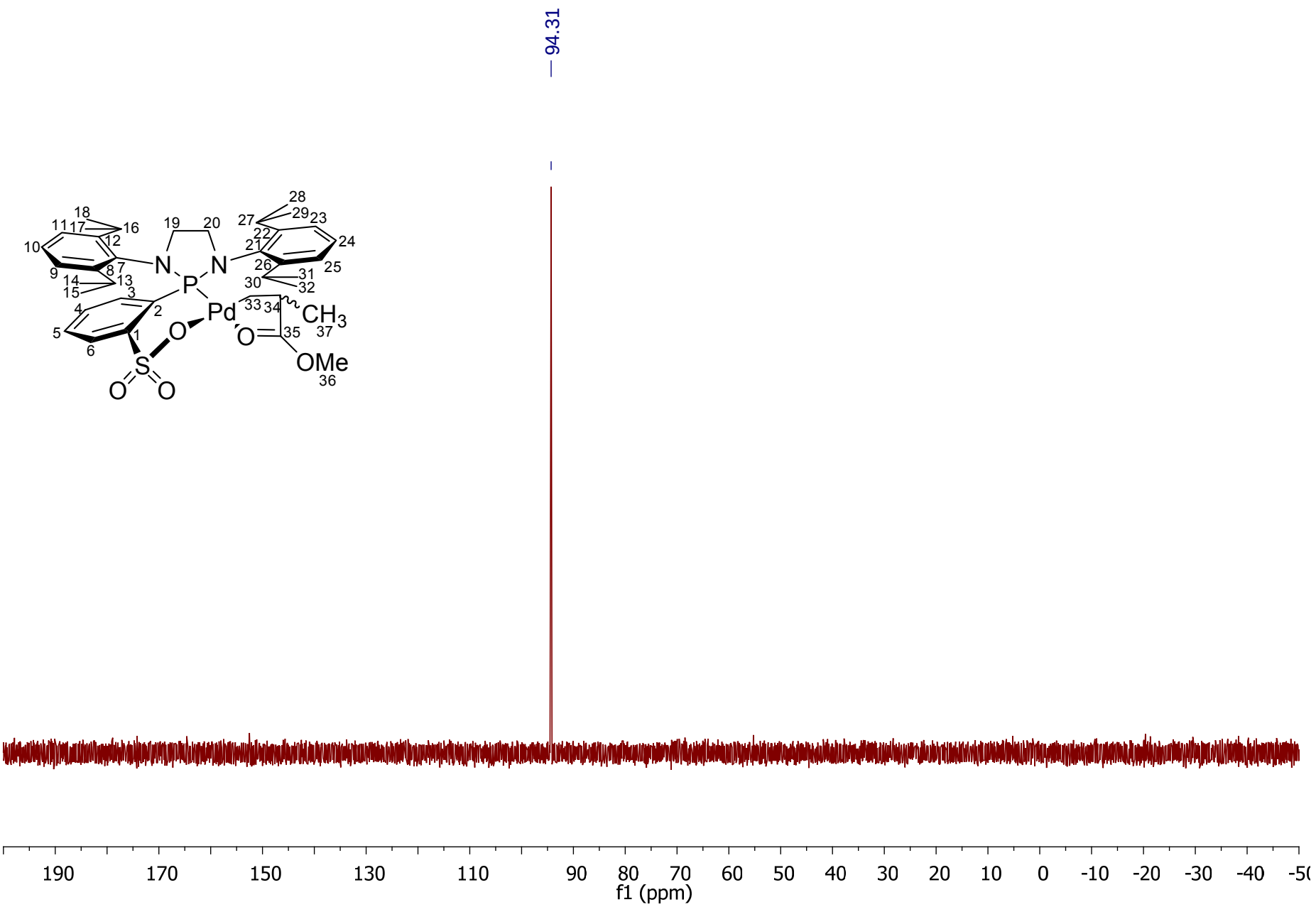


Figure S30: aliphatic region of $^{1}H,^{1}H$ COSY NMR (400 MHz, 298 K, methylene chloride-d_2) of crude **3b** after removal of of excess MA under vacuum

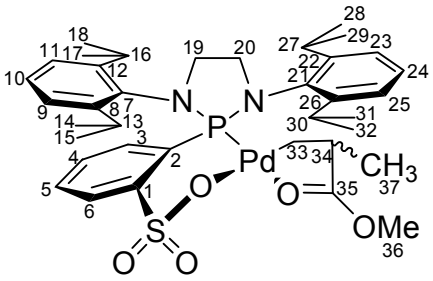
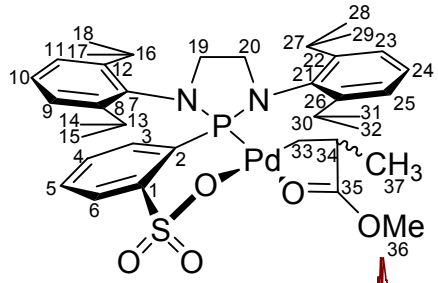
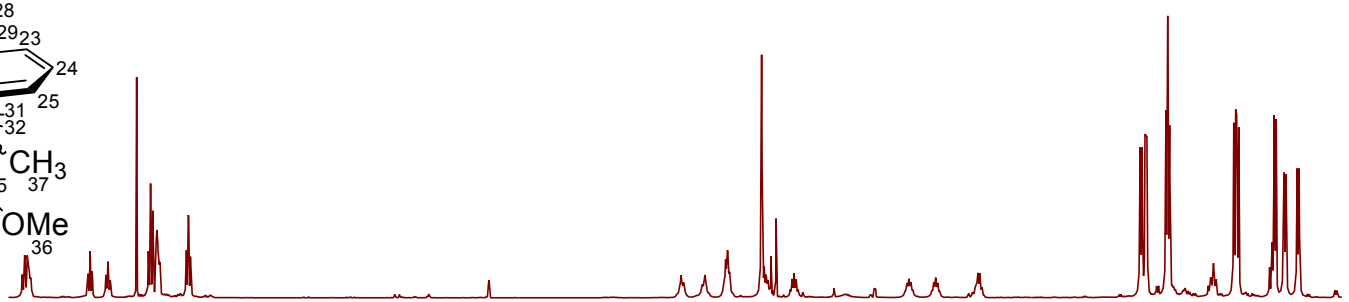


Figure S31: $^{1}H,^{13}C$ gHSQC NMR (400 MHz, 298 K, methylene chloride-d_2) of crude **3b** after removal of of excess MA under vacuum, CH and CH_3: red, CH_2: blue





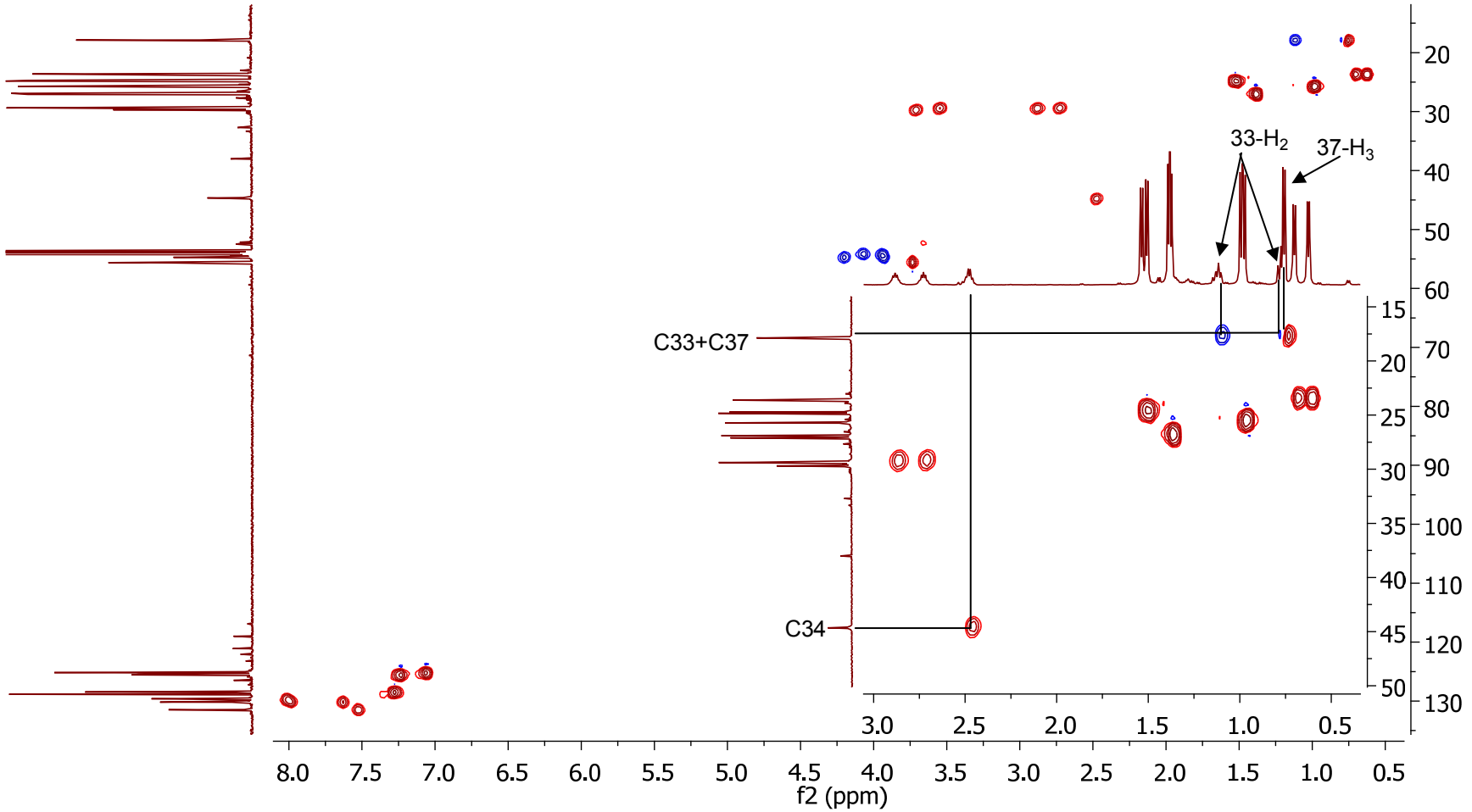


Figure S32: $^{1}H,^{13}C$ gHMBC NMR (400 MHz, 298 K, methylene chloride-d_2) of crude **3b** after removal of of excess MA under vacuum

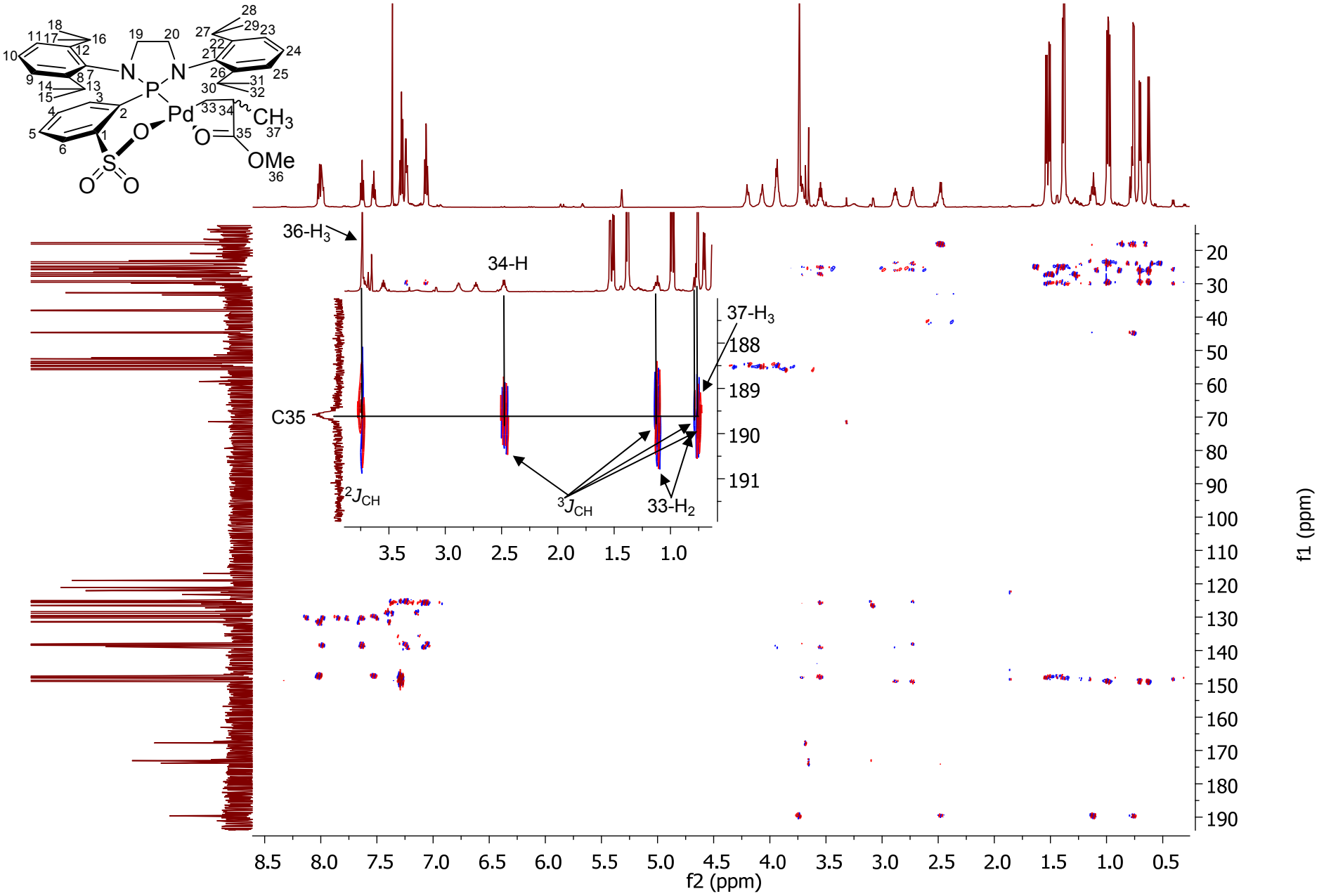


Figure S33: ^{1}H NMR (400 MHz, 298 K, methylene chloride-d_2) of X-Ray quality **3b** after washing with pentane

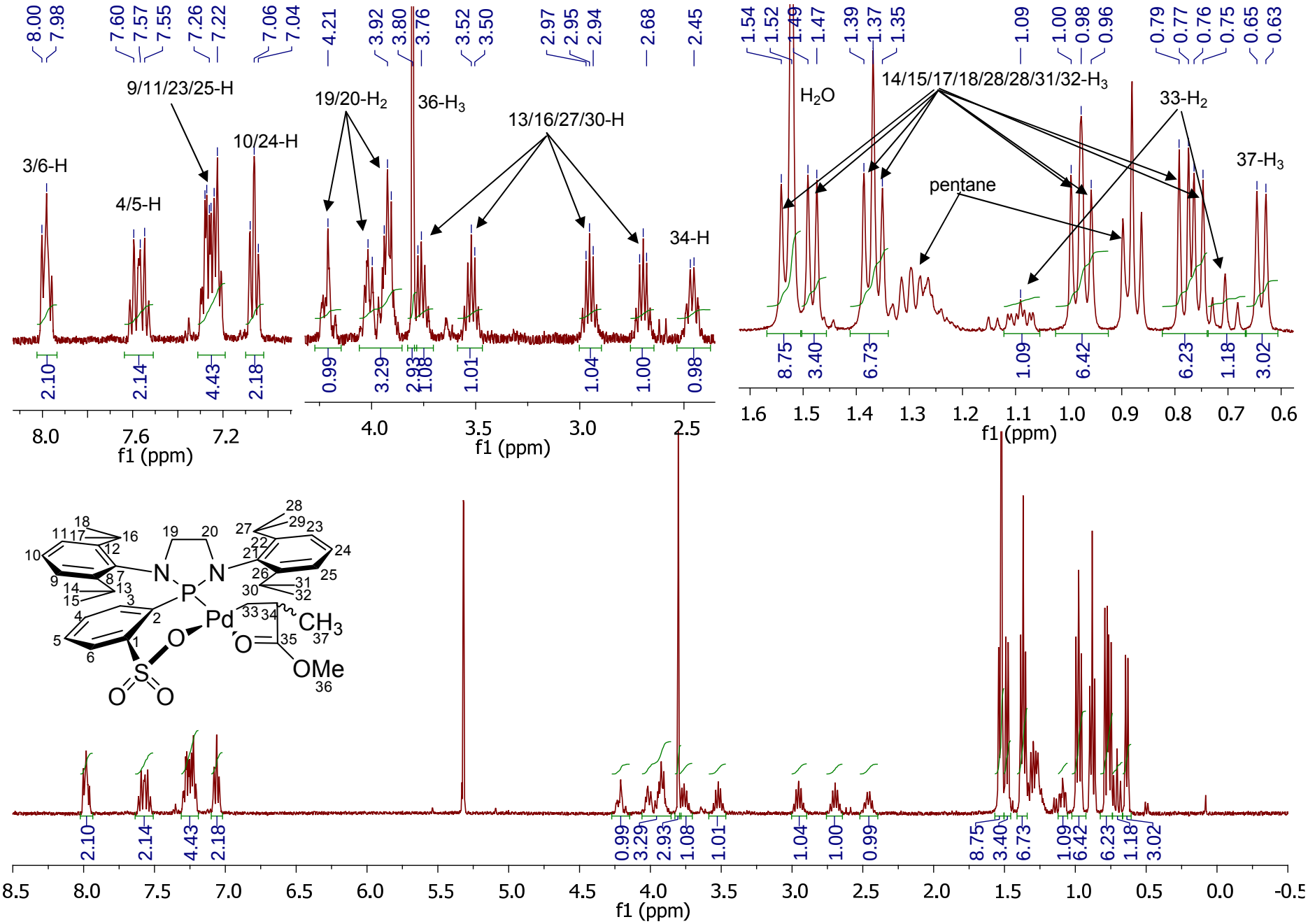


Figure S34: ^{1}H NMR (400 MHz, 298 K, CD_3OD) of **4-MeOH**

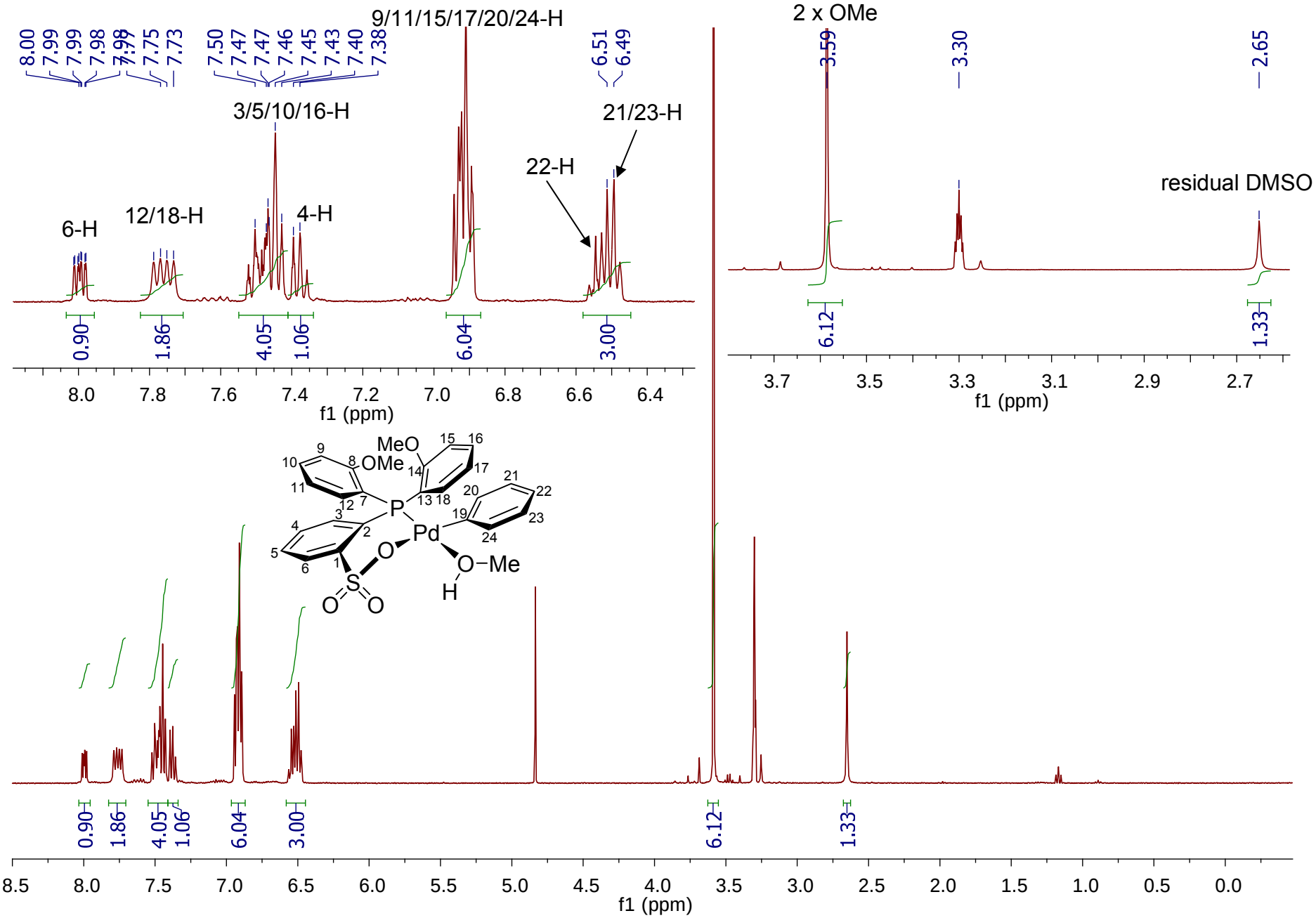


Figure S35: ^{13}C NMR (100 MHz, 298 K, CD_3OD) of **4-MeOH**

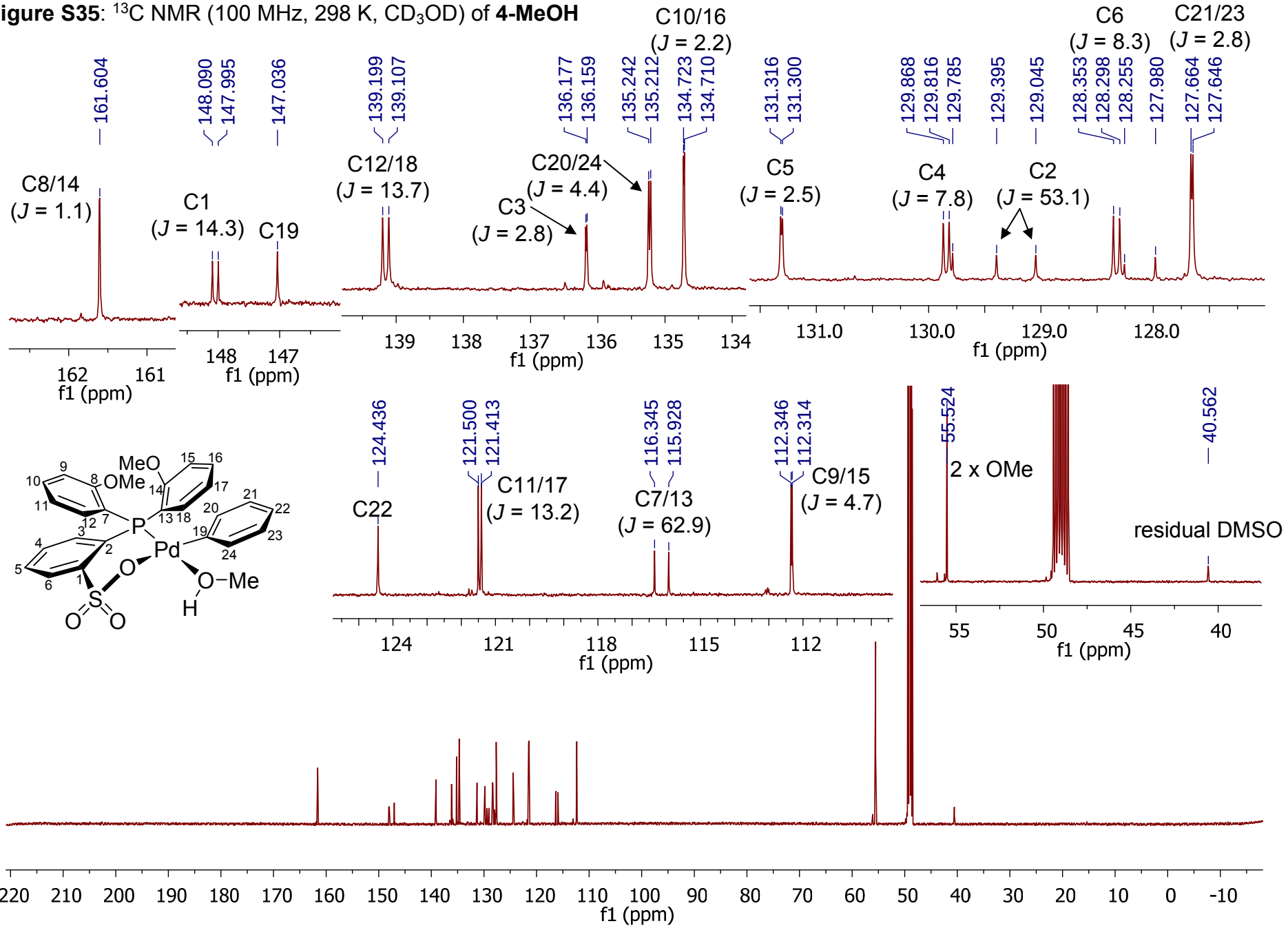


Figure S36: ^{31}P NMR (161 MHz, 298 K, CD_3OD) of **4-MeOH**

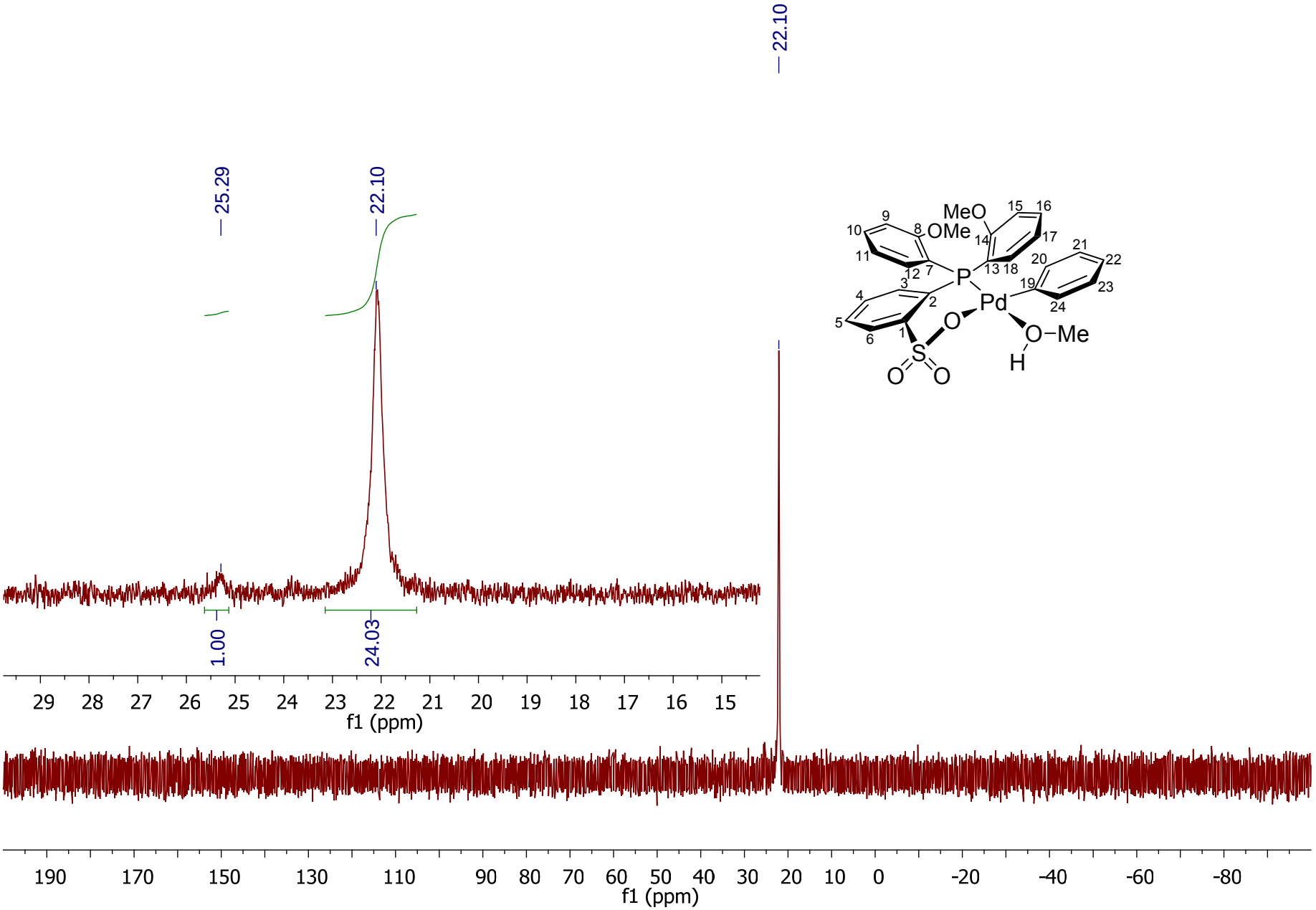


Figure S37: Reaction of complex **4-MeOH** and methyl acrylate in CD_3OD: Formation of methyl cinnamate (**5**) and complexes **9** and **10**,**10'** [^{1}H NMR (400 MHz, 298 K, CD_3OD)]

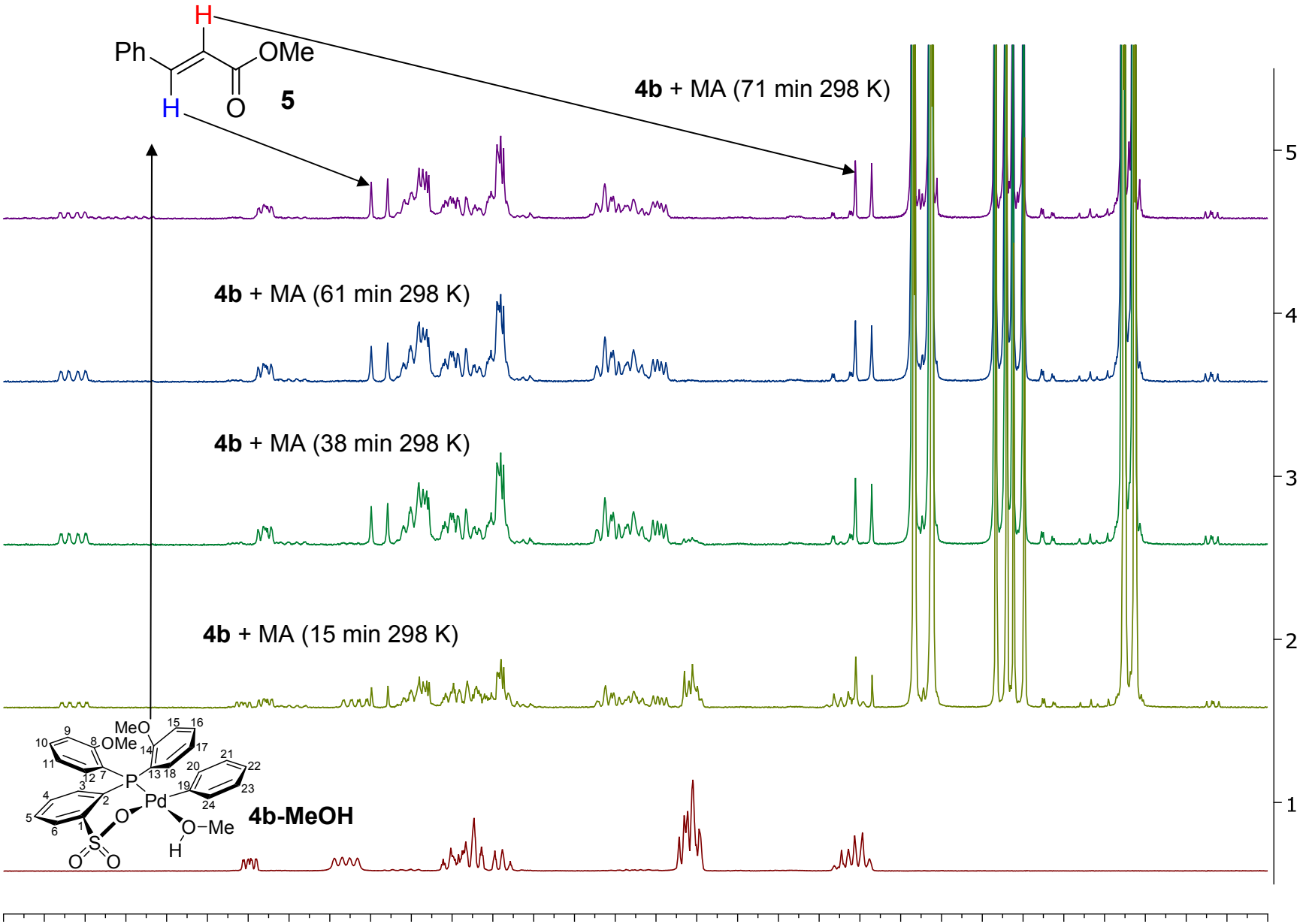


Figure S38: Reaction of complex **4-MeOH** and methyl acrylate in CD_3OD: Formation of methyl cinnamate (**5**) and complexes **9** and **10**,**10'** (sample after 2.5 reaction time, removal of volatiles and redissolution in CD_2Cl_2)

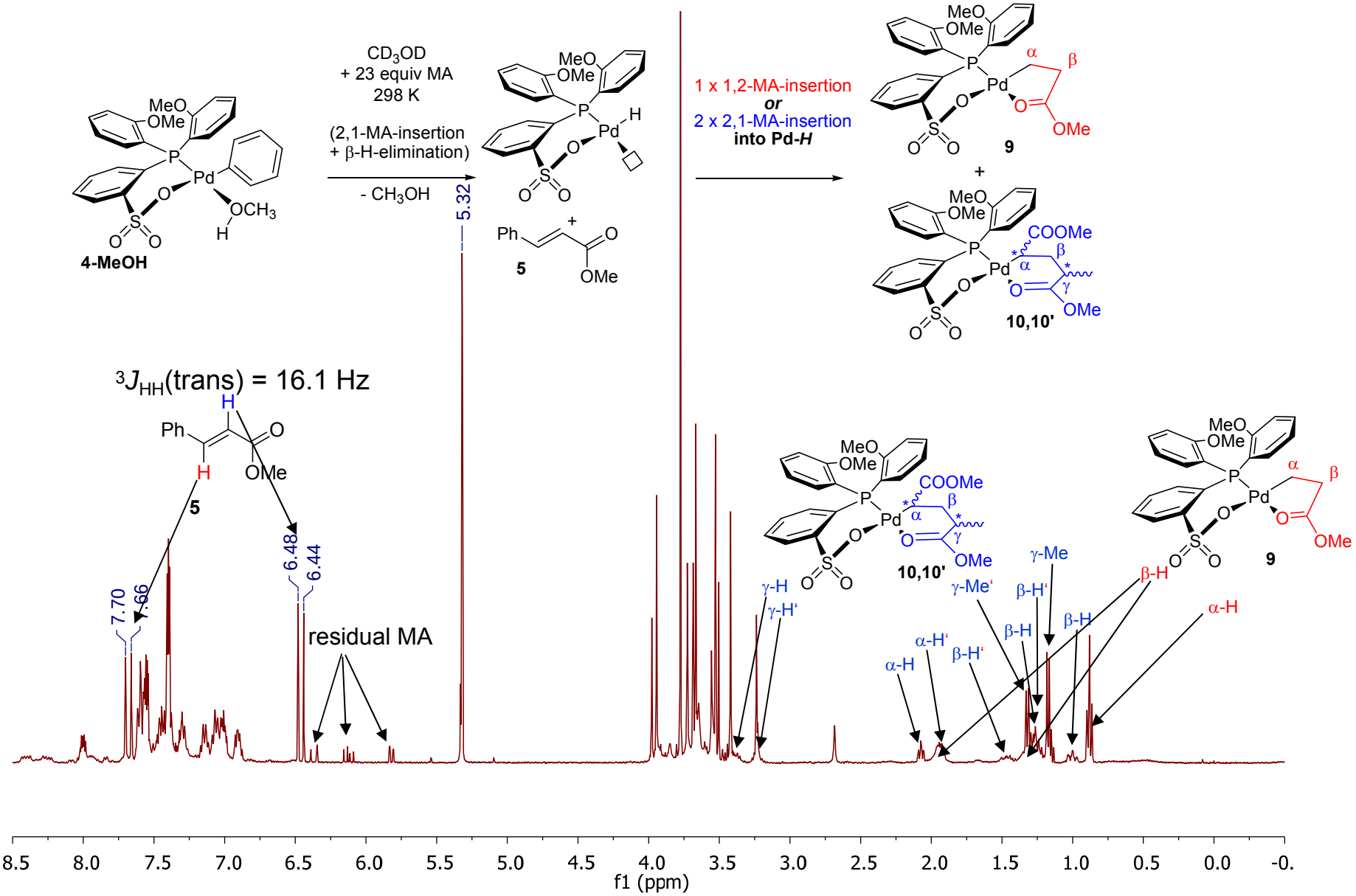


Figure S39: Reaction of complex **4-MeOH** and methyl acrylate in CD_3OD: Formation of methyl cinnamate (**5**) and complexes **9** and **10**,**10'** (sample after 2.5 reaction time, removal of volatiles and redissolution in CD_2Cl_2)

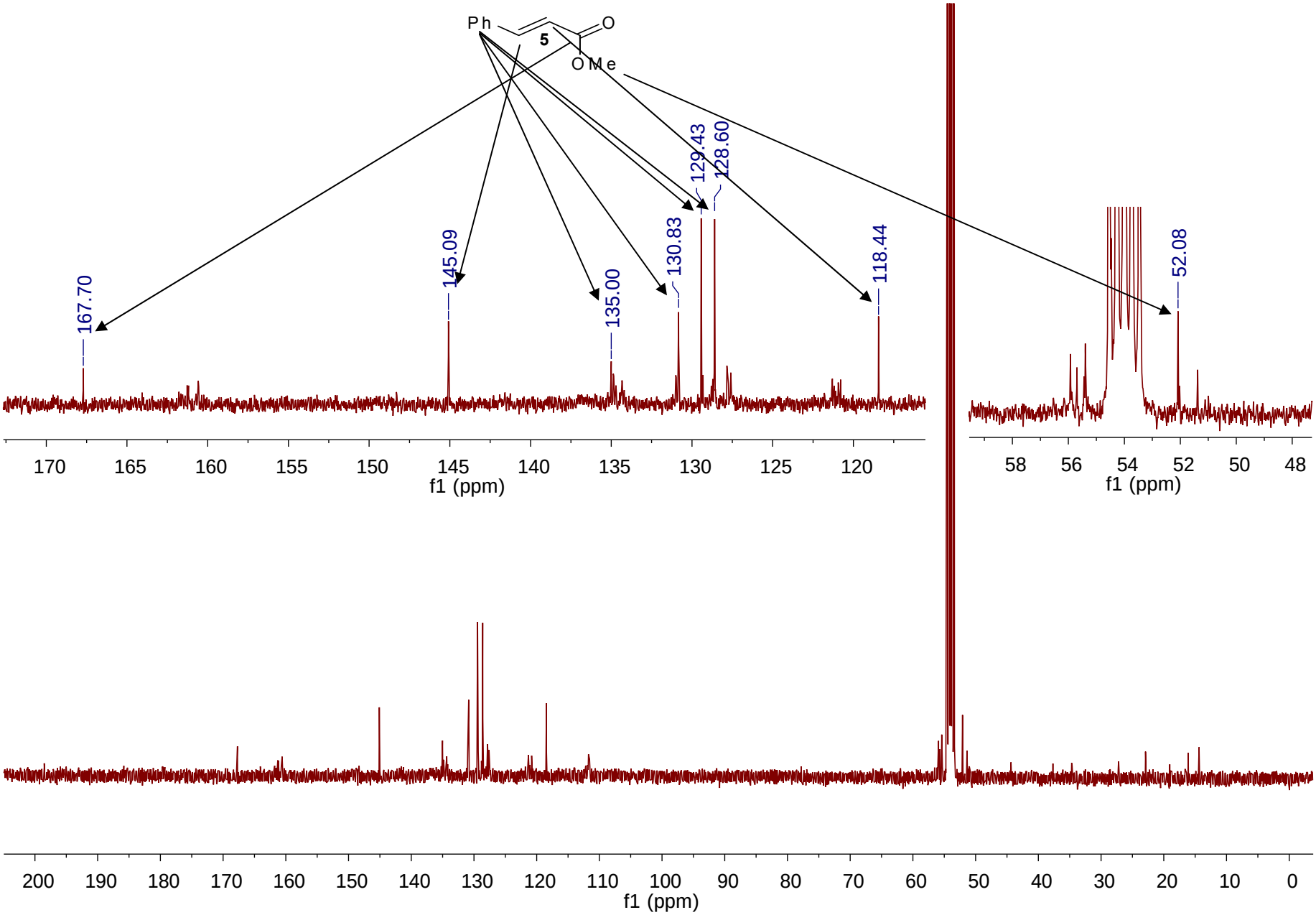


Figure S40: ^{1}H NMR (400 MHz, 298 K, acetone-d_6) of **6b-LiCl·(DMSO)**

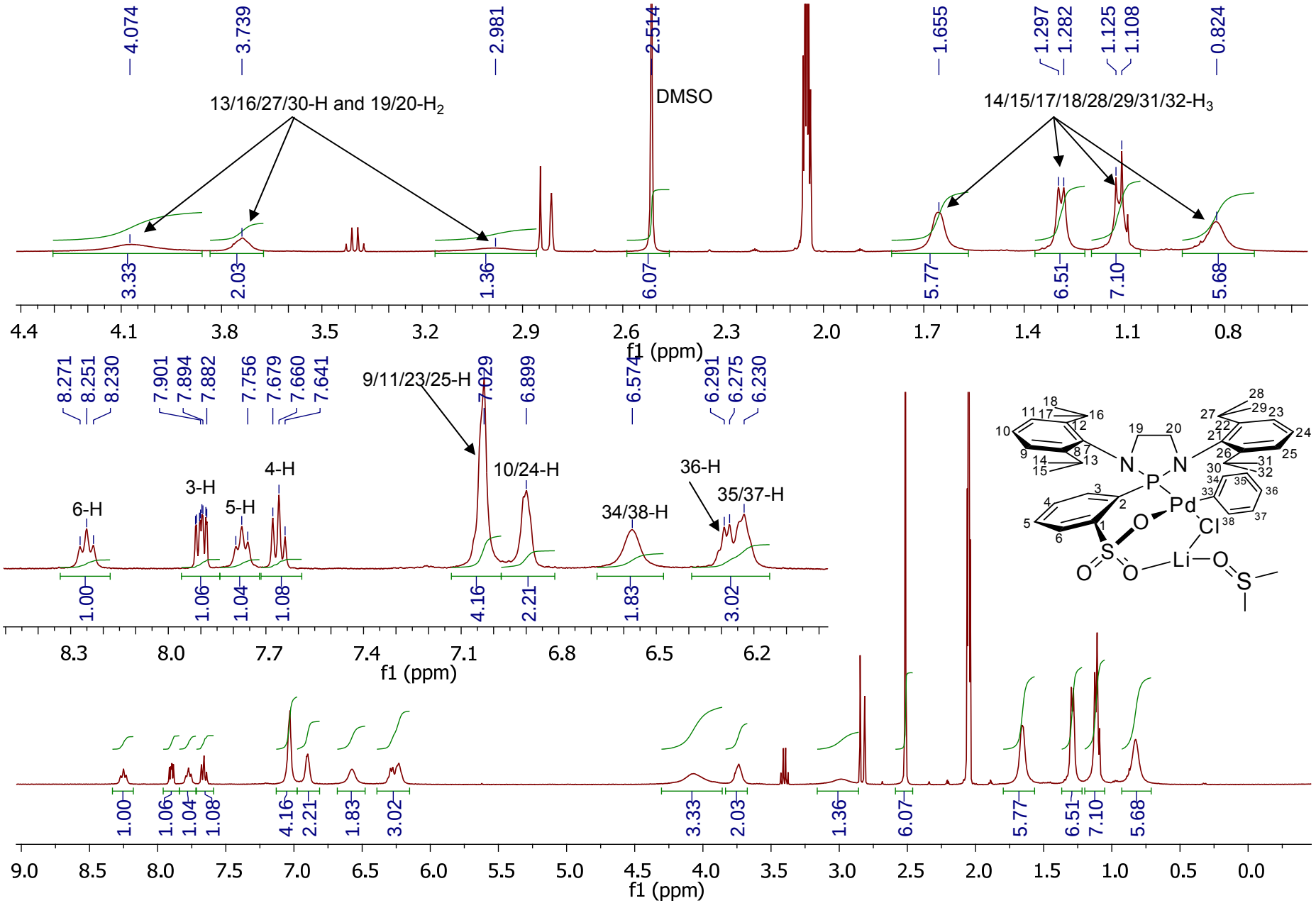


Figure S41: ^{13}C NMR (100 MHz, 298 K, acetone-d_6) of **6b-LiCl·(DMSO)**

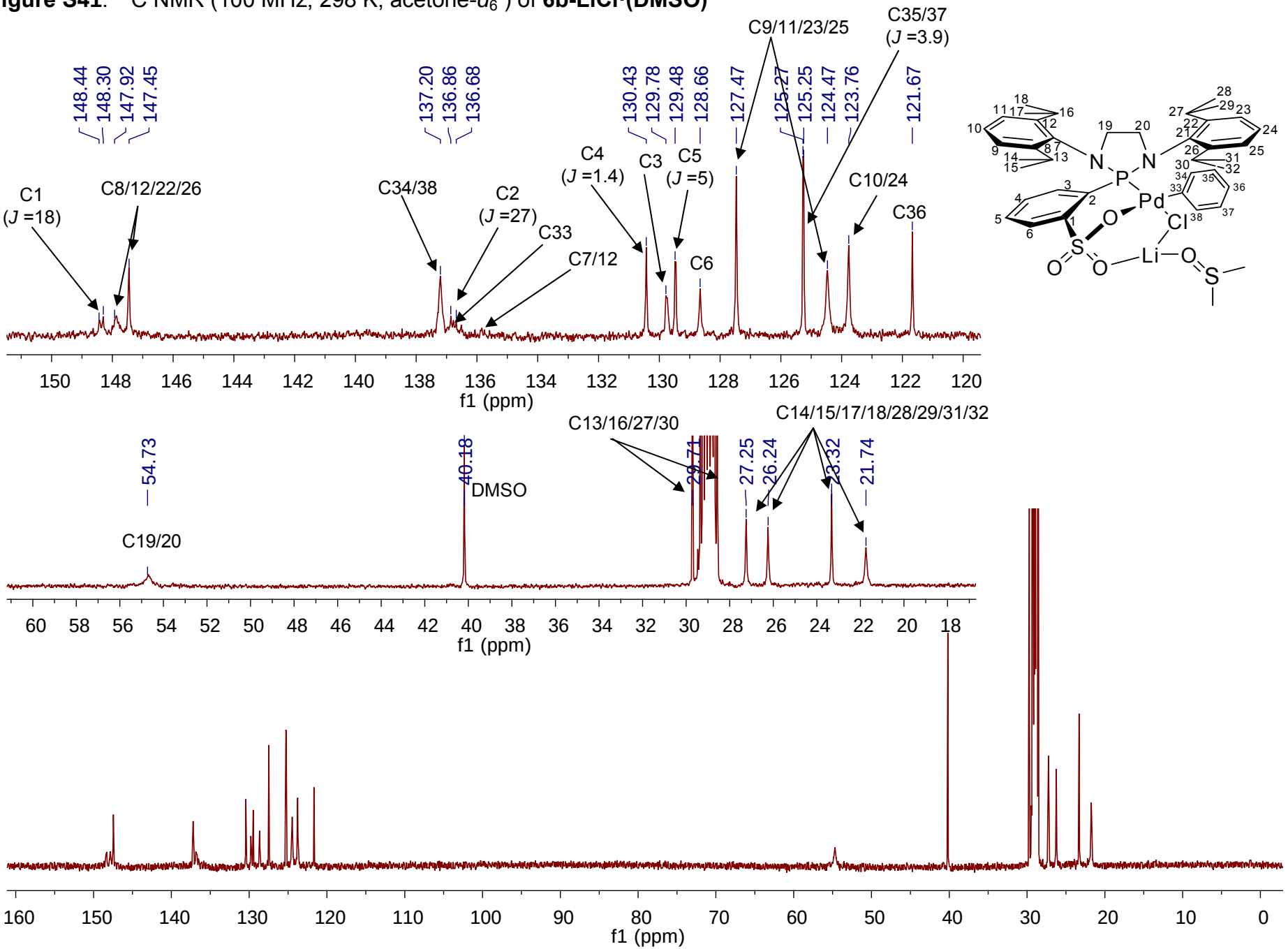


Figure S42: ^{31}P NMR (161 MHz, 298 K, acetone-d_6) of **6b-LiCl·(DMSO)**

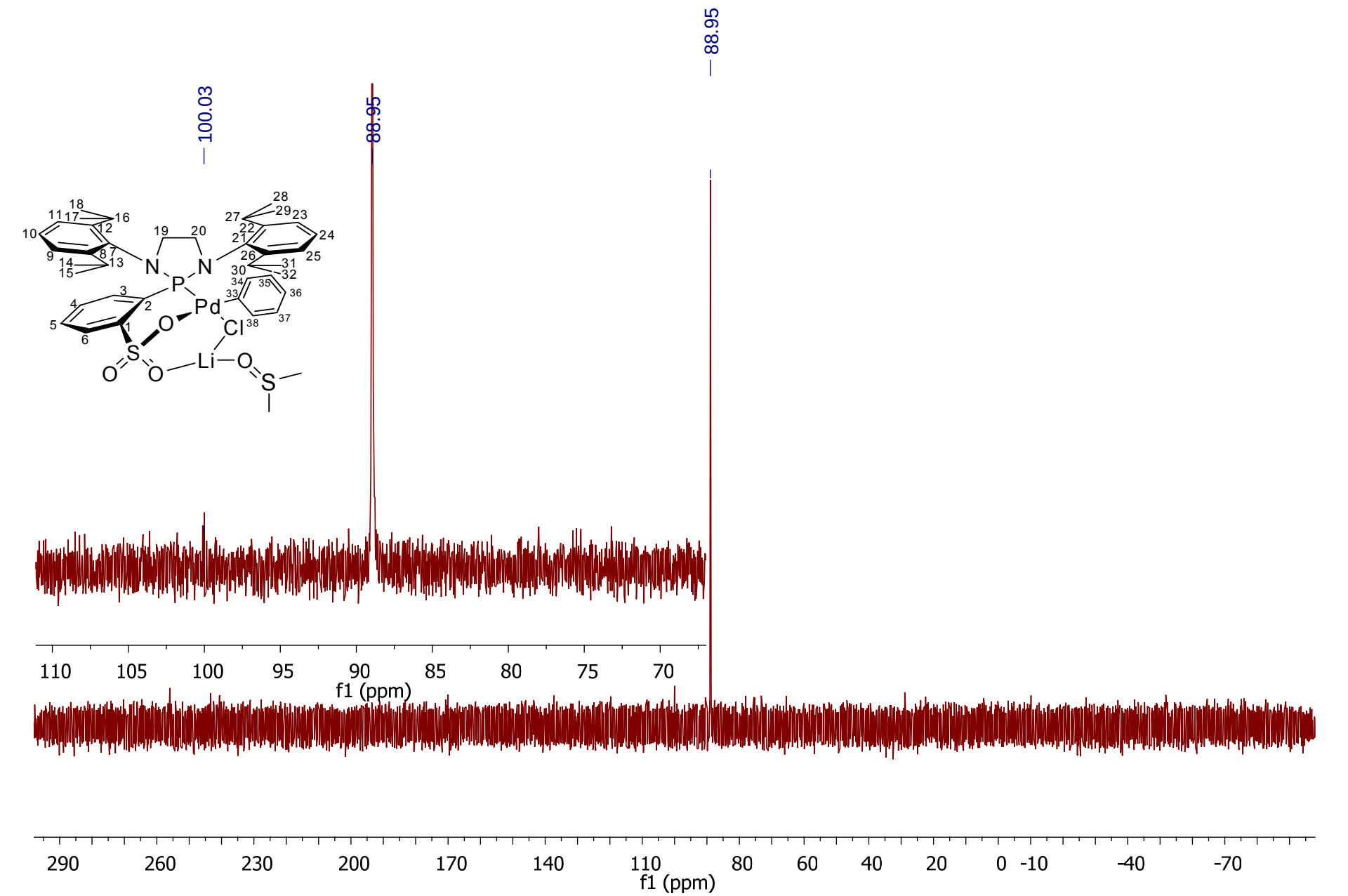


Figure S43: $^{1}H,^{13}C$ gHSQC NMR (400 MHz, 298 K, acetone-d_6) of **6b-LiCl·(DMSO)**

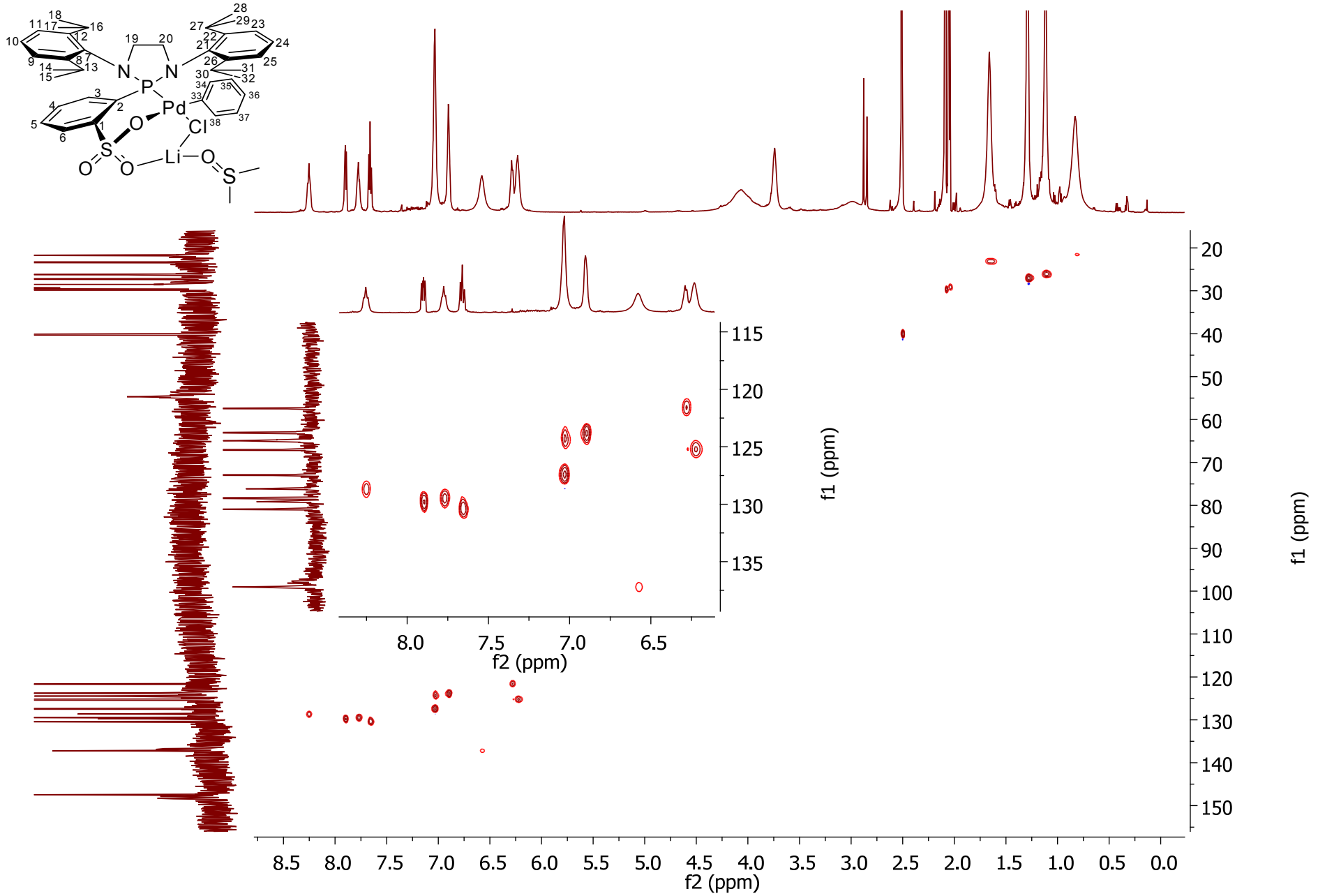


Figure S44: $^{1}H,^{13}C$ gHMBC NMR (400 MHz, 298 K, acetone-d_6) of **6b-LiCl·(DMSO)**

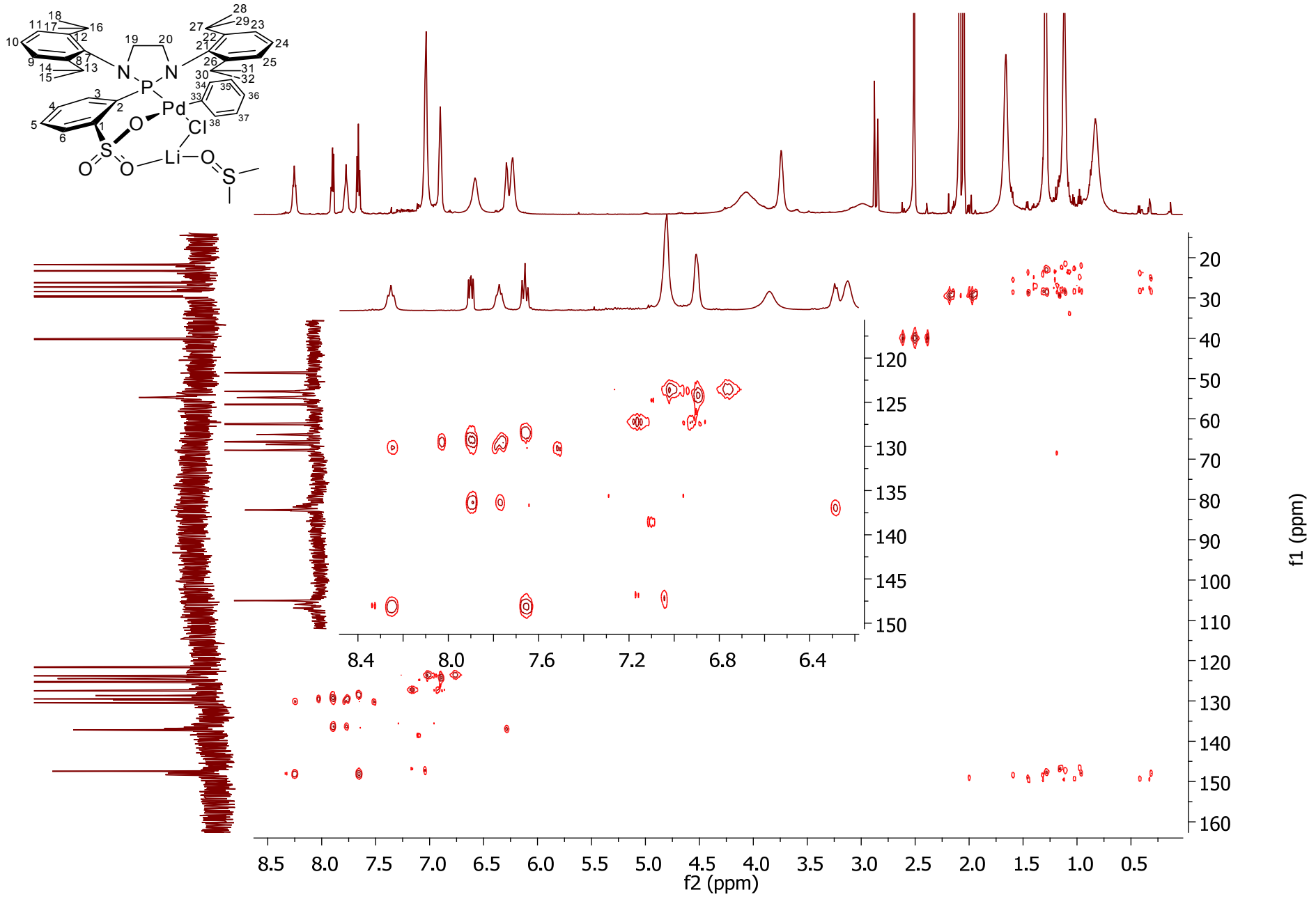


Figure S45: ^{1}H NMR (600 MHz, 298 K, acetone-d_6) of crude **7b** obtained from **6b-LiCl·(DMSO)**, 1.02 equiv AgOTf and 25 equiv methyl acrylate after 60 min at 318 K in methylene chloride-d_2 , removal of all volatiles under vacuum, and redissolution in acetone-d_6 (contains ca. 7 % methyl cinnamate)

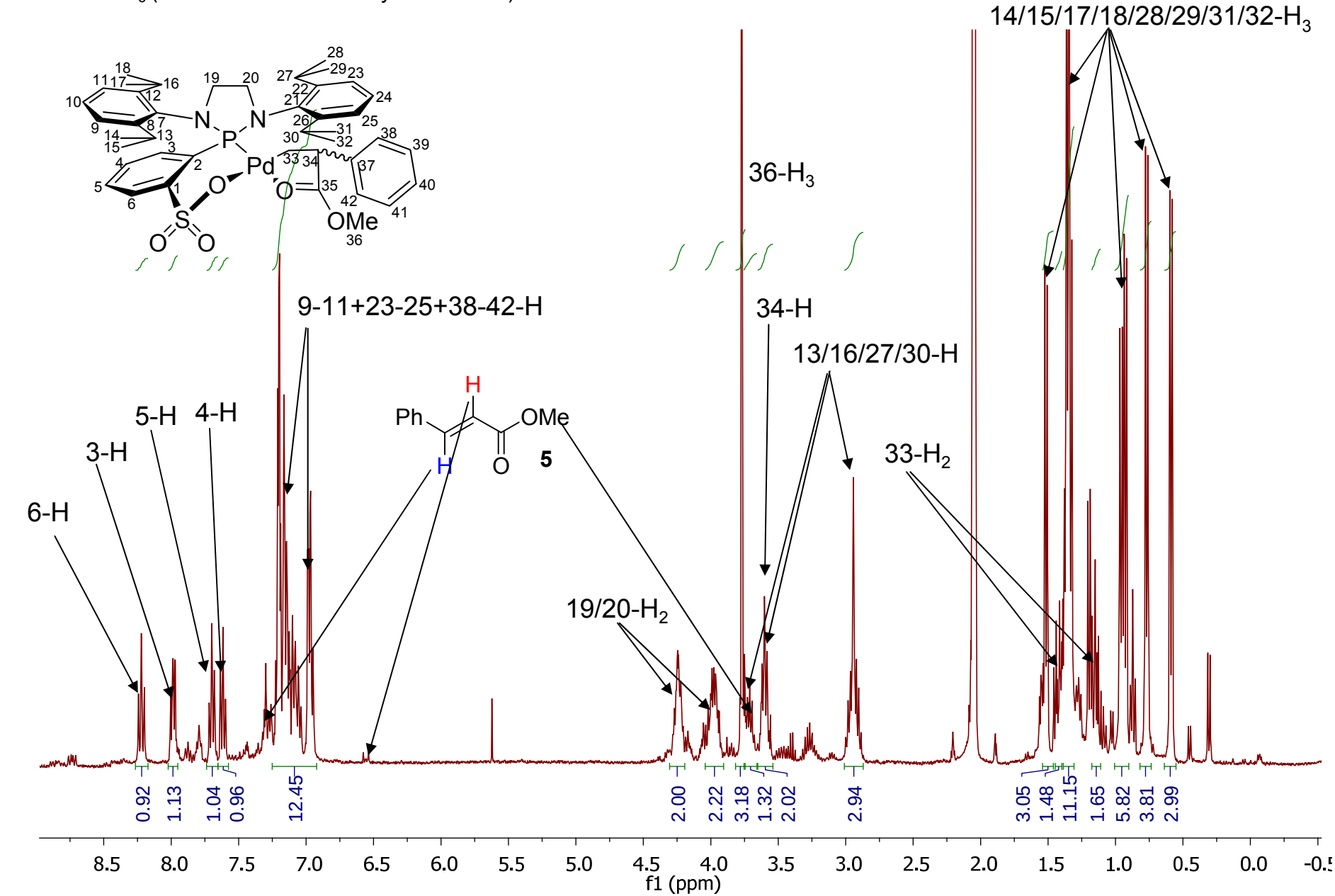


Figure S46: ^{13}C NMR (150 MHz, 298 K, acetone-d_6) of crude **7b** obtained from **6b-LiCl·(DMSO)**, 1.02 equiv AgOTf and 25 equiv methyl acrylate after 60 min at 318 K in methylene chloride-d_2 , removal of all volatiles under vacuum, and redissolution in acetone-d_6 (contains ca. 7 % methyl cinnamate)

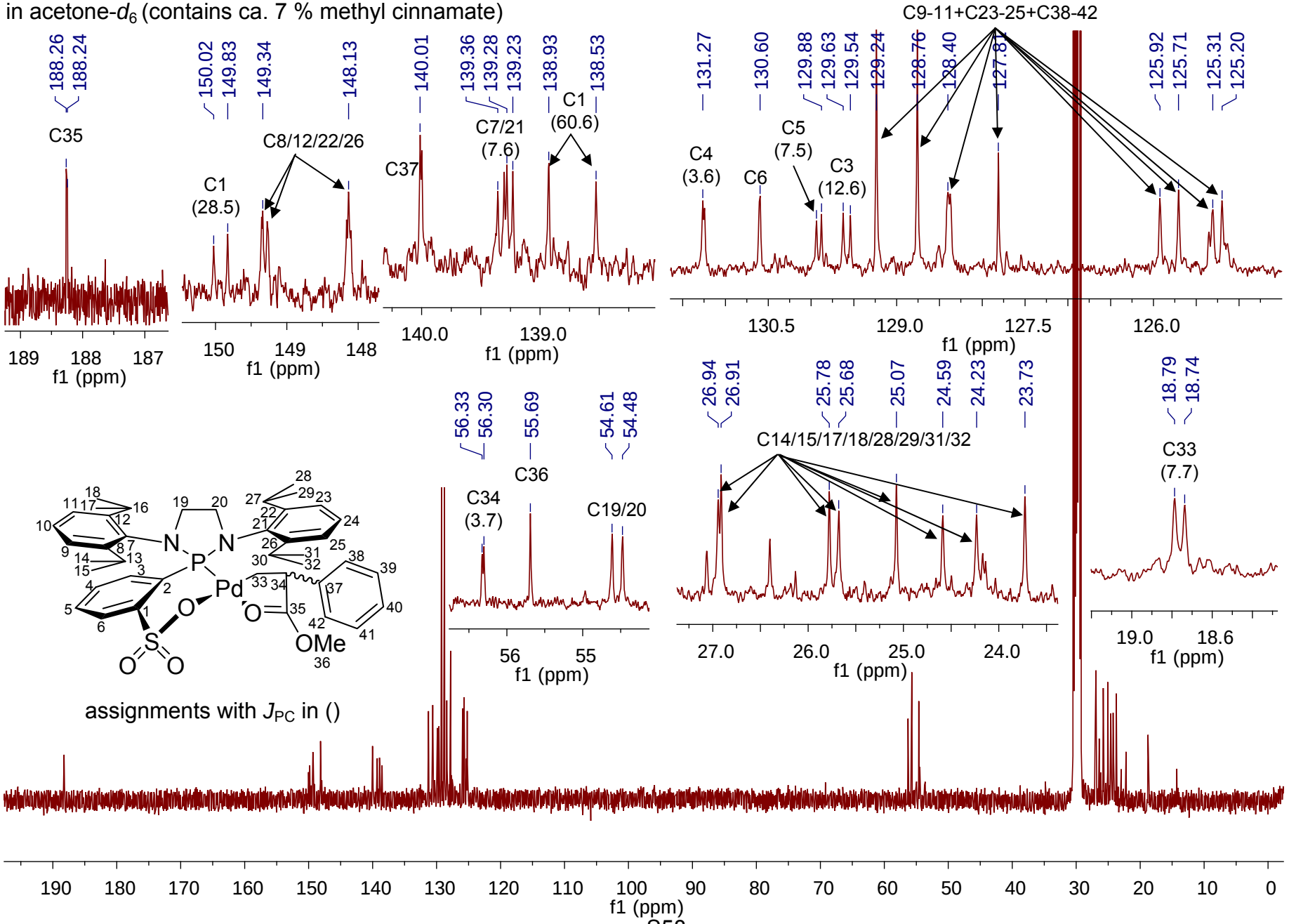


Figure S47: ^{31}P NMR (161 MHz, 298 K, acetone-d_6) of crude **7b** obtained from **6b-LiCl·(DMSO)**, 1.02 equiv AgOTf and 25 equiv methyl acrylate after 60 min at 318 K in methylene chloride-d_2 , removal of all volatiles under vacuum, and redissolution in acetone-d_6 (contains ca. 7 % methyl cinnamate)

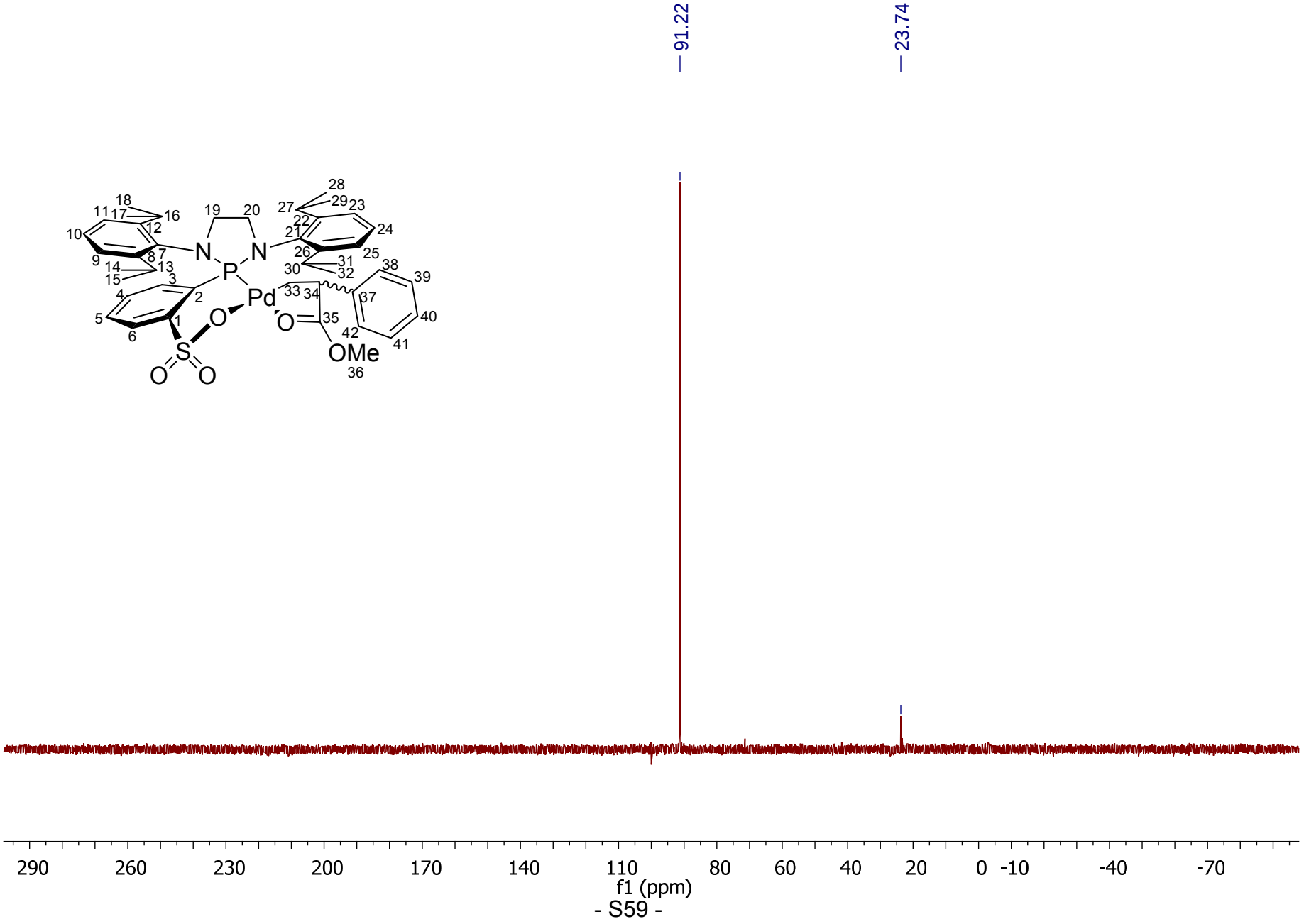


Figure S48: $^{1}H,^{13}C$ gHSQC NMR (600 MHz, 298 K, acetone-d_6) of crude **7b** obtained from **6b-LiCl·(DMSO)**, 1.02 equiv AgOTf and 25 equiv methyl acrylate after 60 min at 318 K in methylene chloride-d_2 , removal of all volatiles under vacuum, and redissolution in acetone-d_6 (contains ca. 7 % methyl cinnamate); CH and CH_3: red; CH_2: blue

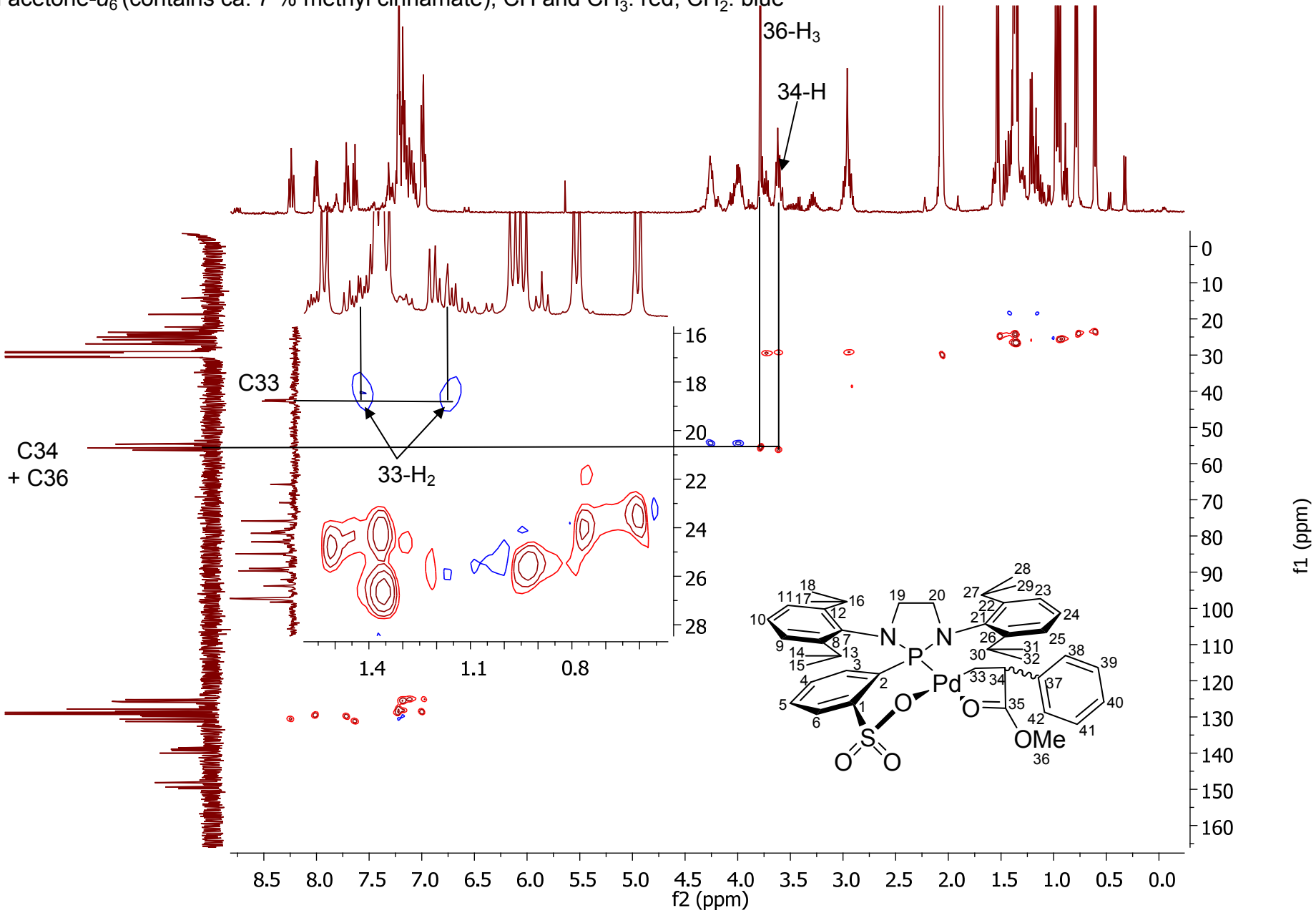


Figure S49: $^{1}H,^{13}C$ gHMBC NMR (600 MHz, 298 K, acetone-d_6) of crude **7b** obtained from **6b-LiCl·(DMSO)**, 1.02 equiv AgOTf and 25 equiv methyl acrylate after 60 min at 318 K in methylene chloride-d_2 , removal of all volatiles under vacuum, and redissolution in acetone-d_6 (contains ca. 7 % methyl cinnamate)

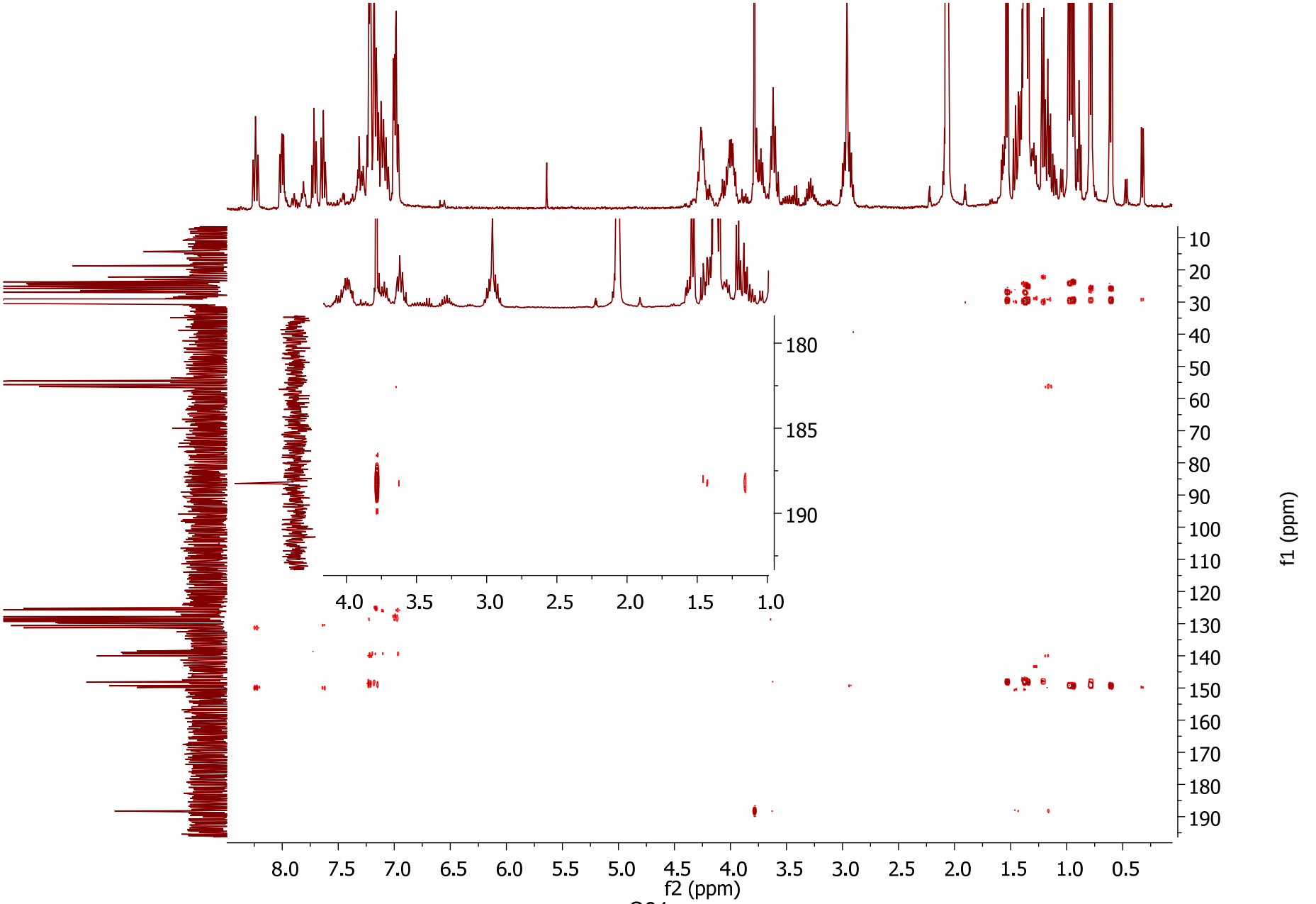


Figure S50: ^{1}H NMR (400 MHz, 298 K, 1,1,2,2-tetrachloroethane-d_2) of isolated **7b**

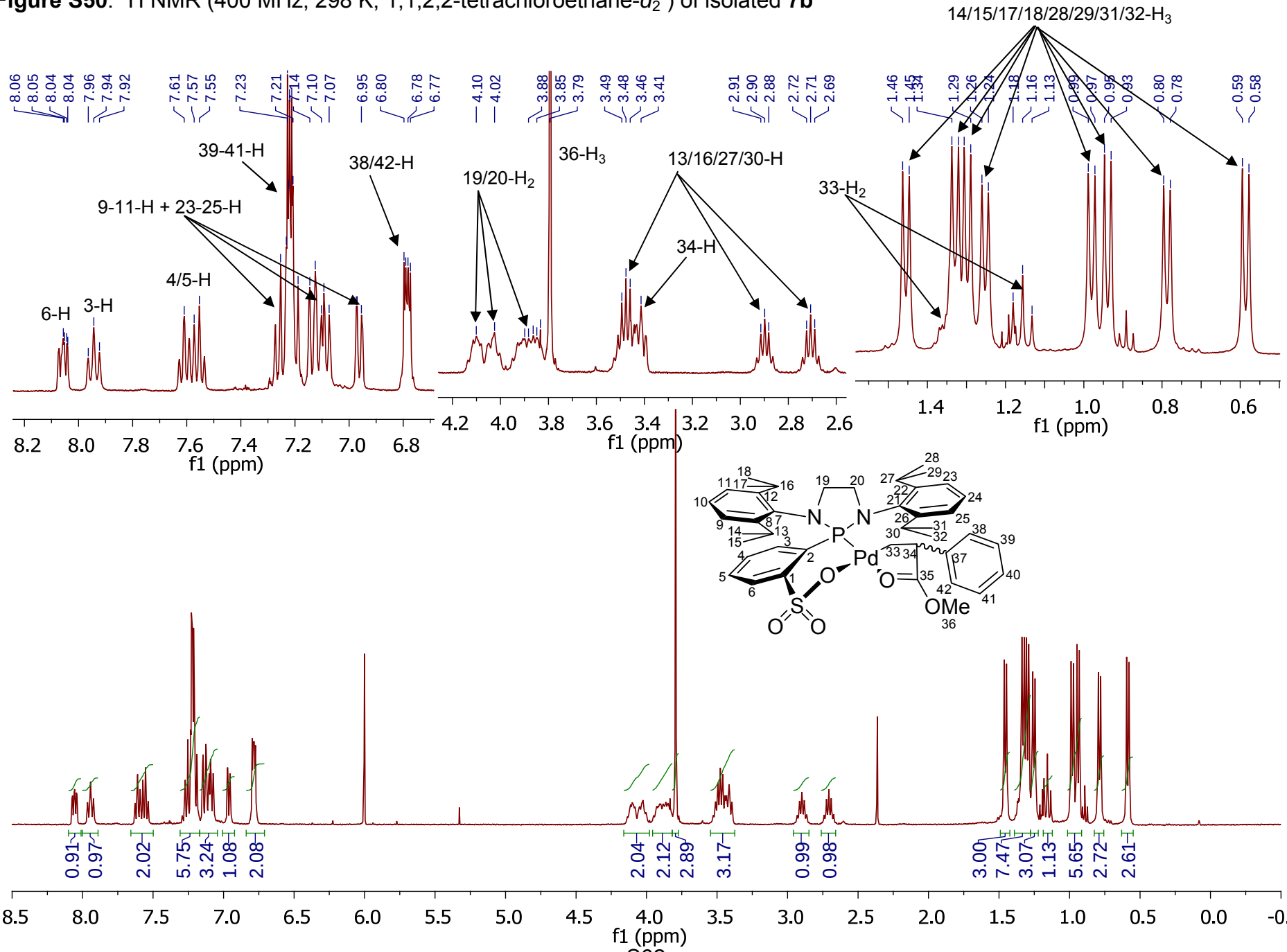


Figure S51: ^{13}C NMR (100 MHz, 298 K, 1,1,2,2-tetrachloroethane-d_2) of isolated **7b**

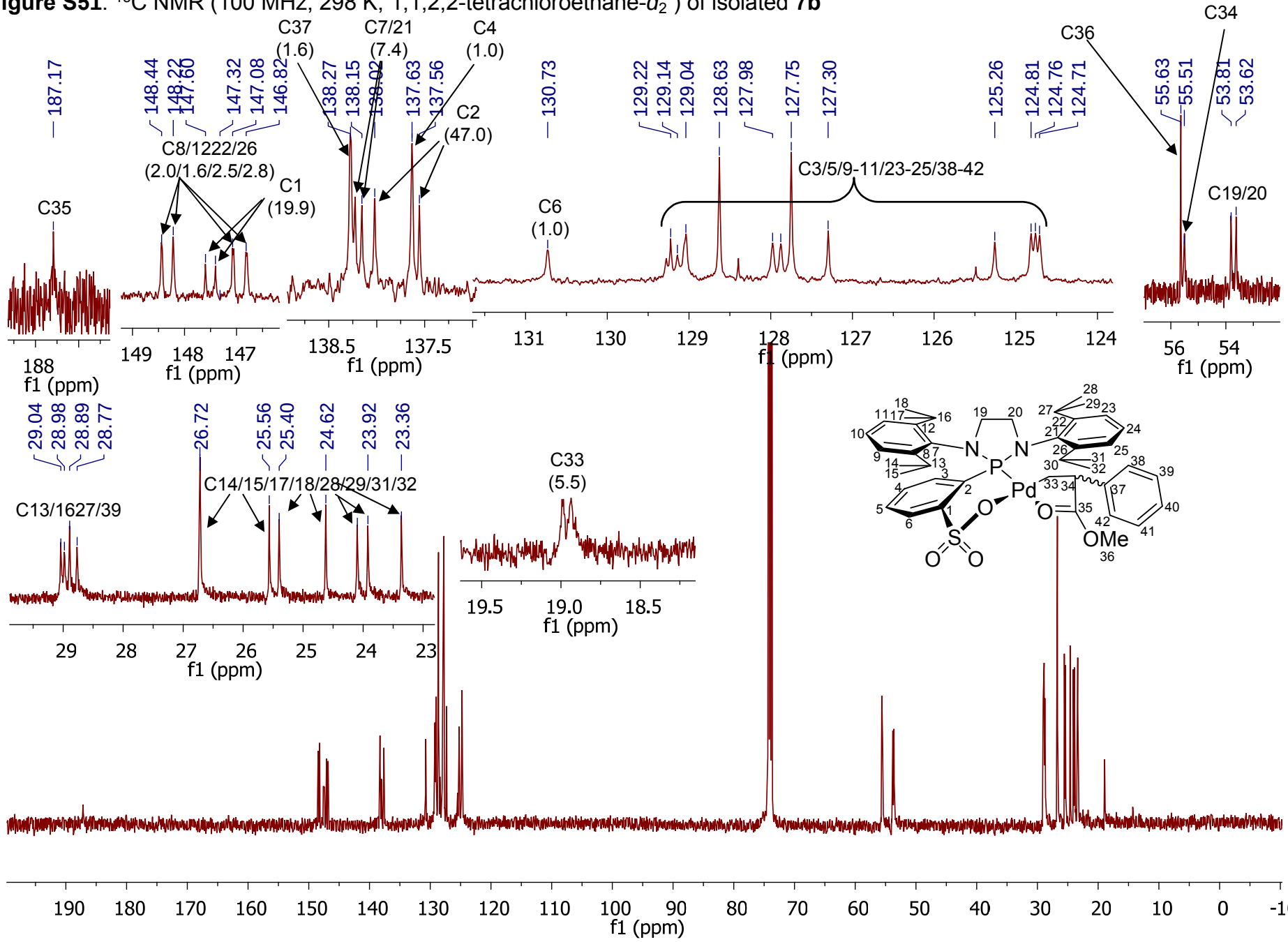


Figure S52: ^{31}P NMR (161 MHz, 298 K, 1,1,2,2-tetrachloroethane-d_2) of isolated **7b**

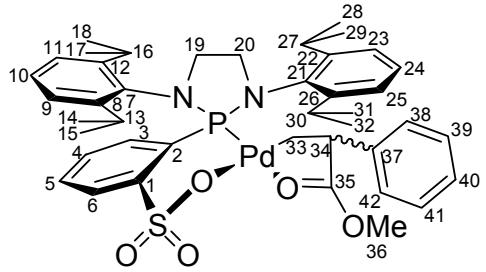


Figure S53: aliphatic region of the $^{1}H,^{1}H$ COSY NMR (400 MHz, 298 K, 1,1,2,2-tetrachloroethane-d_2) of isolated **7b**

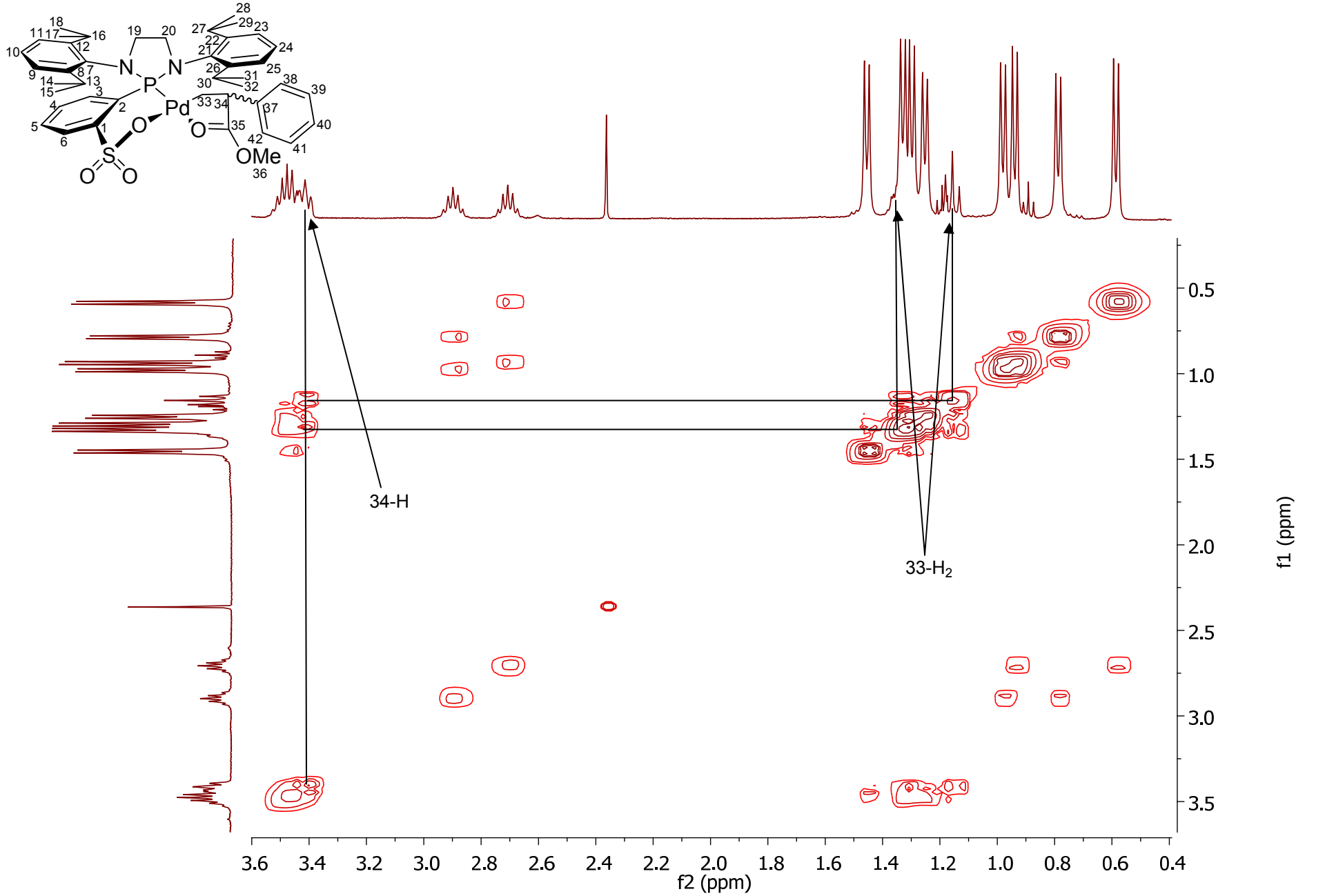


Figure S54: top line:[1]H NMR (400 MHz, 298 K, 1,1,2,2-tetrachloroethane-d_2) of isolated **7b**
middle line:[1]H NMR (400 MHz, 363 K, 1,1,2,2-tetrachloroethane-d_2) of isolated **7b** (after 5 min 363 K)
bottom line:[1]H NMR (400 MHz, 298 K, 1,1,2,2-tetrachloroethane-d_2) of isolated **7b** (after 12 h 363 K)

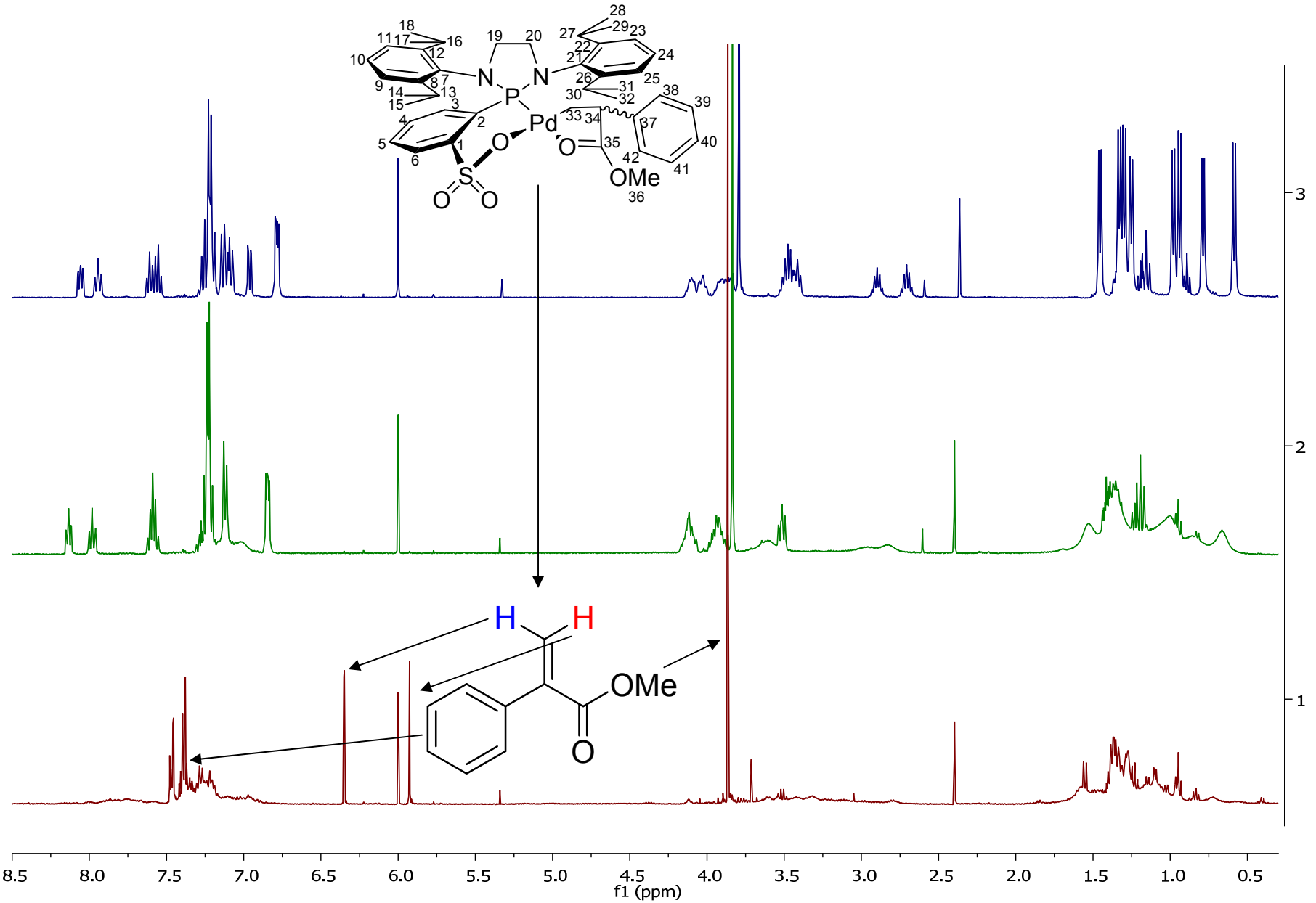


Figure S55: time dependent ^{1}H NMR spectra (400 MHz, 363 K, 1,1,2,2-tetrachloroethane-d_2, aromatic and olefinic region) indicating complete consumption of **7b** and formation of (2-phenyl)methyl acrylate after ca 11 h at 363 K

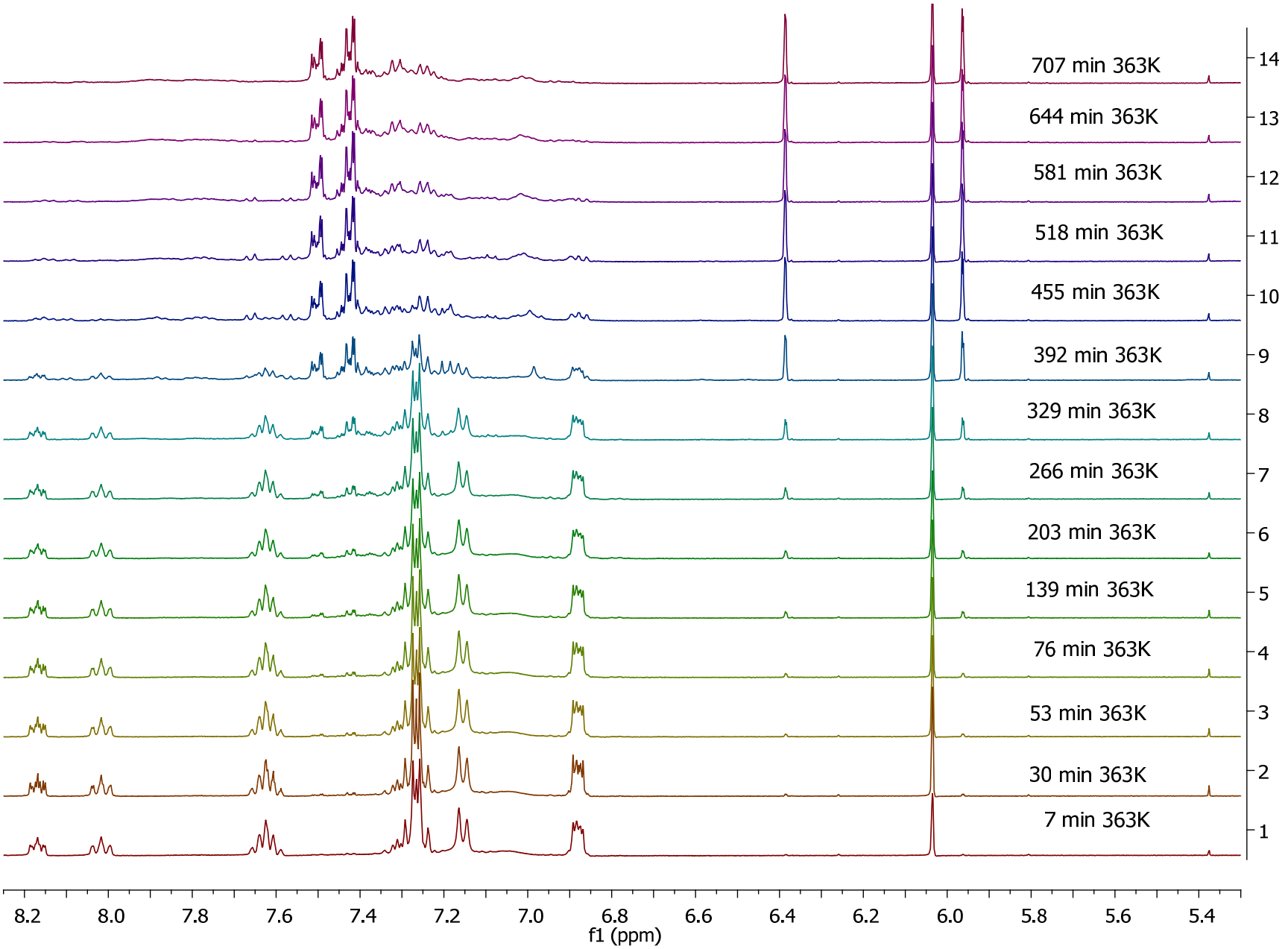


Figure S56: ^{1}H NMR (400 MHz, 298 K, 1,1,2,2-tetrachloroethane-d_2) of thermolyzed **7b** containing (2-phenyl)methyl acrylate (**8**)

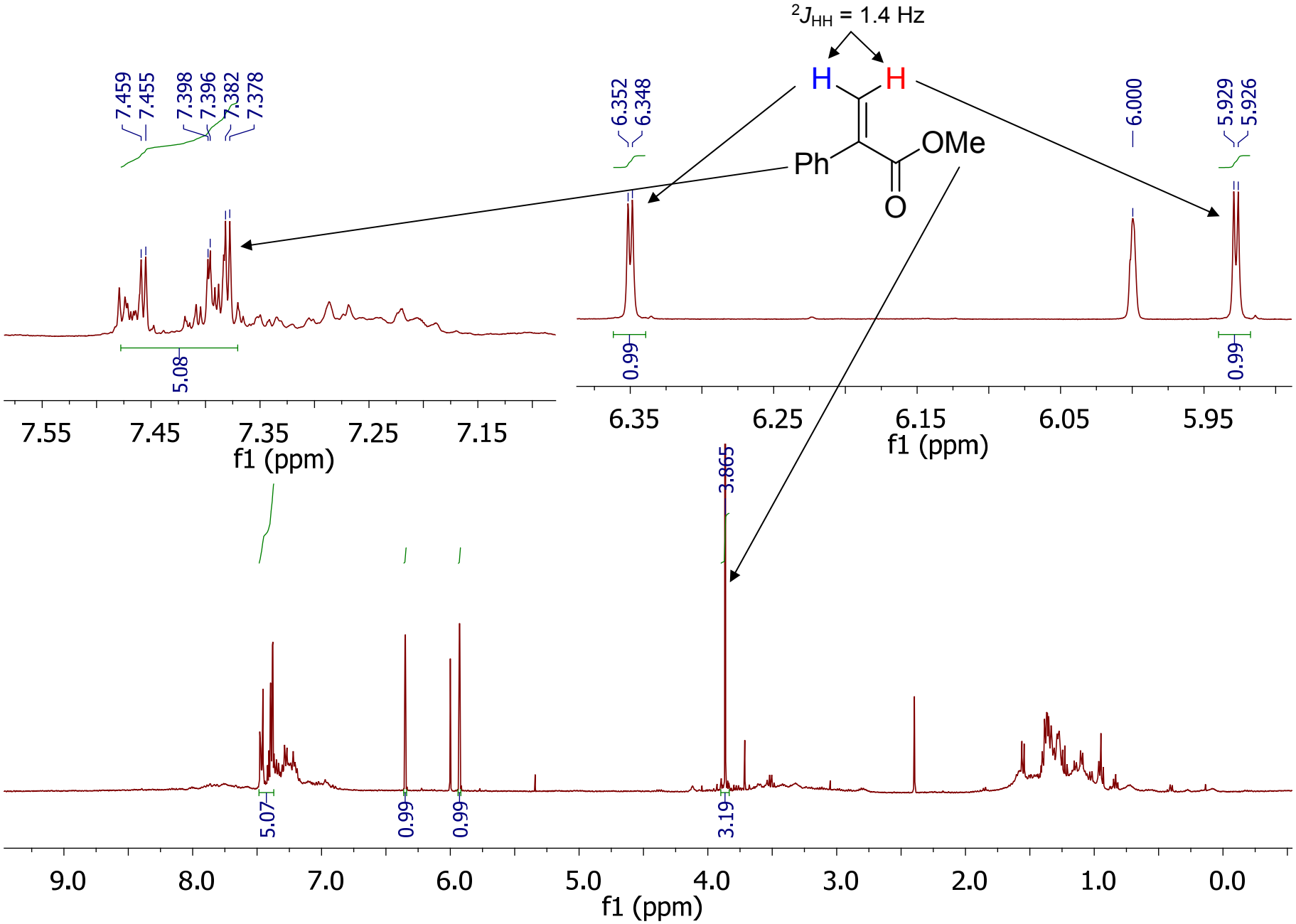


Figure S57: ^{13}C NMR (100 MHz, 298 K, 1,1,2,2-tetrachloroethane-d_2) of thermolyzed **7b** containing (2-phenyl)methyl acrylate (**8**)

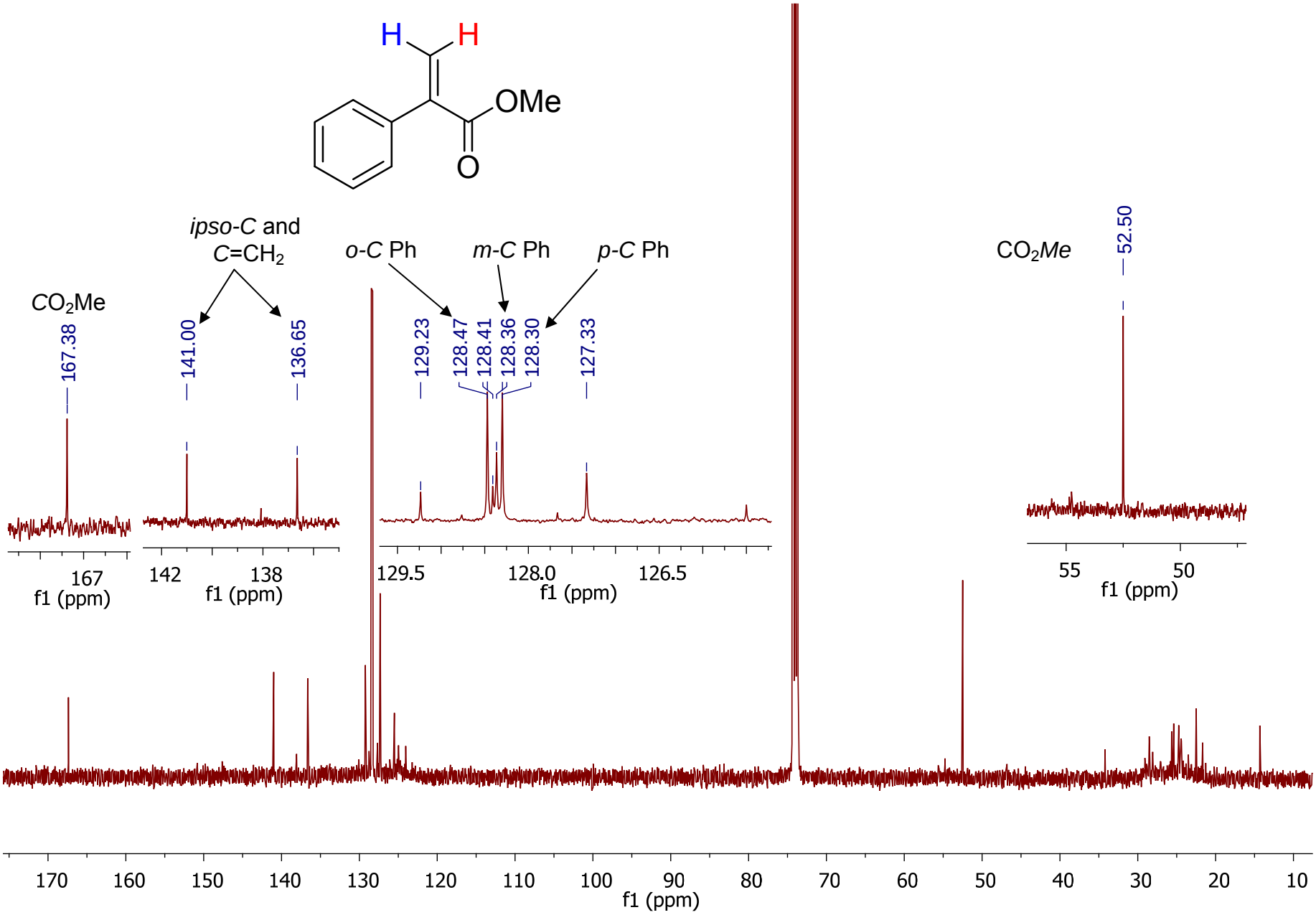


Figure S58: $^{1}H,^{13}C$ gHSQC NMR (400 MHz, 298 K, 1,1,2,2-tetrachloroethane-d_2) of thermolyzed **7b** containing (2-phenyl)methyl acrylate (**8**); CH and CH_3: red; CH_2: blue

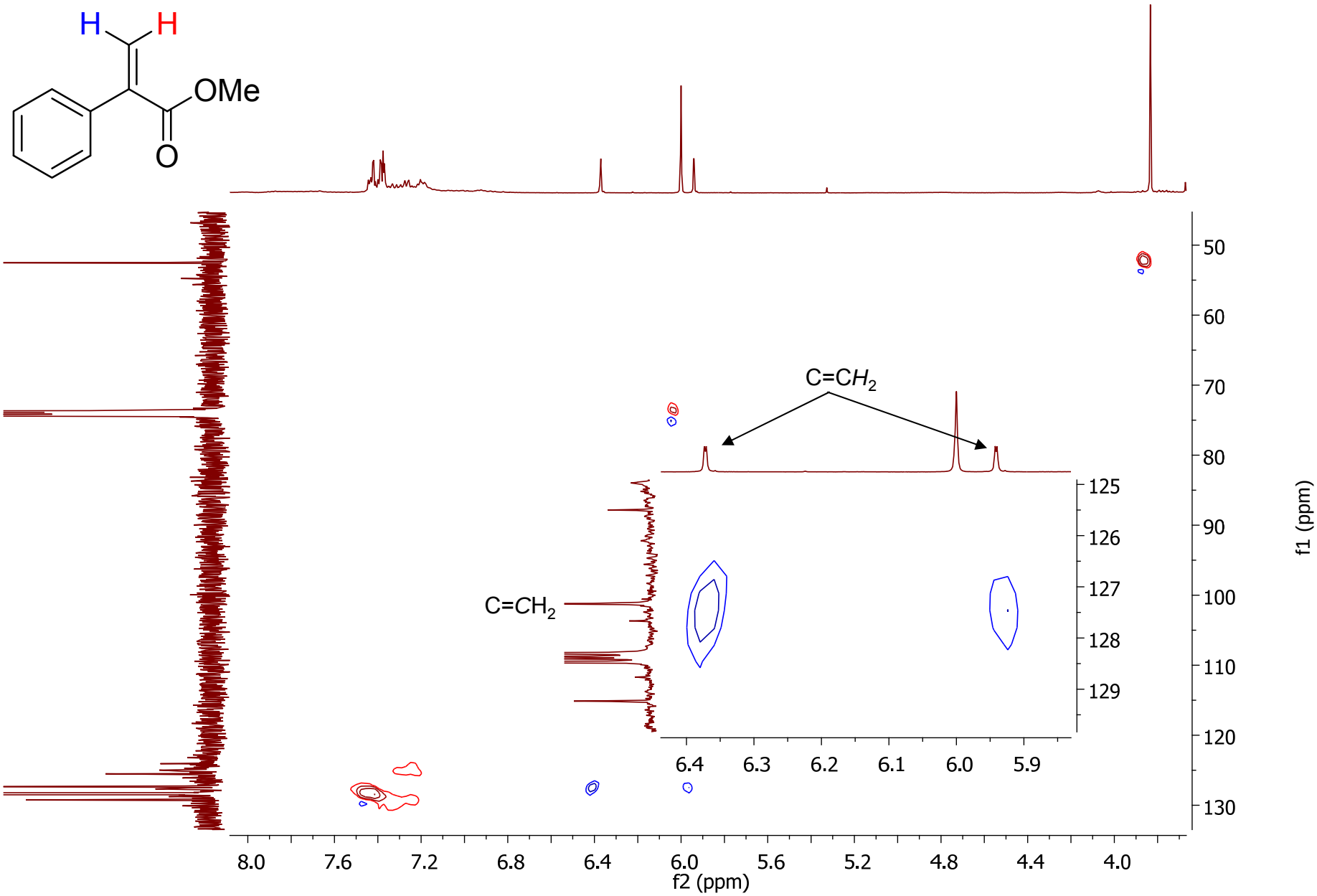
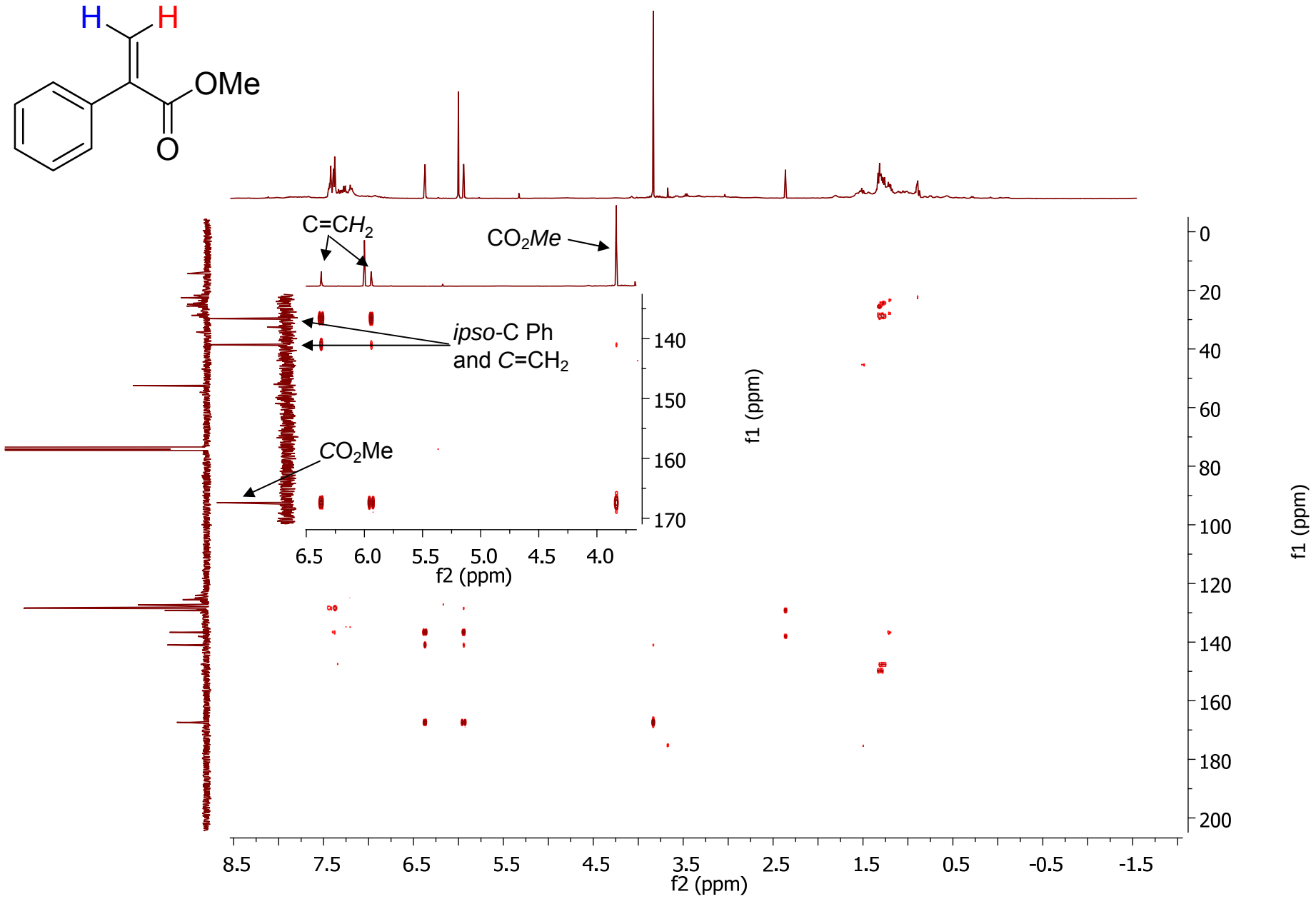


Figure S59: $^{1}H,^{13}C$ gHMBC NMR (400 MHz, 298 K, 1,1,2,2-tetrachloroethane-d_2) of thermolyzed **7b** containing (2-phenyl)methyl acrylate (**8**)



Theoretical Procedures and DFT results

Computational Details. The Amsterdam Density Functional (ADF) program (9,10) was used. The electronic configuration of the molecular systems was described by a triple-ζ STO basis set on Pd (ADF basis set TZV). Double-ζ STO basis sets, augmented by one polarization function, were used for main group atoms (ADF basis sets DZVP). The inner shells on Pd (including 3d), P and S (including 2p) C and O (1s), were treated within the frozen core approximation. Energies and geometries were evaluated using the local exchange-correlation potential by Vosko et al. (11), augmented in a self-consistent manner with Becke's (12) exchange gradient correction and Perdew's (13,14) correlation gradient correction (BP86 functional). The transition states were approached through a linear transit procedure starting from the coordination intermediates. The forming C-C bond was assumed as reaction coordinate during the linear transit scans. Full transition state searches were started from the maxima along the linear transit paths.

Topographic steric maps. The steric maps have been calculated for the phosphine sulfonato and diazaphospholidine sulfonato ligands in the DFT optimized geometry of the **1-DMSO**, **2a-DMSO** and **2b-DMSO** complexes. The points in space defining the steric map were located with the Samb*V*ca package developed by some of us (15). This program analyzes the first coordination sphere around the metal, which is the place where the reaction occurs. It is normally used to calculate the buried volume of a given ligand, which is a number that quantifies the amount of the first coordination sphere of the metal occupied by this ligand. We modified Samb*V*ca to understand how the ligand is distributed around the metal, which is the shape of the reactive pocket. We already introduced topographic steric maps to characterize Ru-complexes relevant to olefin metathesis (16), and Rh-complexes active in the asymmetric 1,4-addition of phenylboronic acid to 2-cyclohexenone (17).

To build the steric map, the complex under analysis has been placed with the Pd center at the origin, with the axis bisecting the S-Pd-P angle aligned along the z-axis, and with the S and P atoms in the xz plane at negative z values. After this alignment step the Me and DMSO groups have been removed (because they do not belong to the **1**, **2a** and **2b** ligands) and the first coordination sphere around the metal is analyzed. This sphere, of radius *R*, is sectioned by a regular 3D cubic mesh of spacing *s*, which defines cubic voxels *v*. The distance between the centre of each voxel with all the atoms in the ligand is tested to check if any of the atoms is within a van der Waals distance from the centre of the examined voxel. If no atom is within a van der Waals distance, the examined voxel is marked as a free voxel. Otherwise, the examined voxel is marked as buried.

After all the voxels in the first coordination sphere have been marked as free or buried, for each (x,y) point within the first coordination sphere the program scans the sphere from the top (i.e. away from the ligand) to find at which z value there is the first buried voxel. This procedure results in a surface, defined as $S(x,y) = z_B$, which represents the surface of the ligand that is exposed towards the incoming reactants. In other words, this $S(x,y) = z_B$ surface defines the shape of the reactive pocket. Positive values of z_B indicate that the ligands protrudes in the $z > 0$ half-sphere, which is the half-sphere where the reacting groups are placed. A schematic representation of the interaction surface between the complex and the substrate is shown in Figure S60.

Finally, the maps are a simple 2D isocontour representation of the surface of interaction $S(x,y) = z_B$. In this work, the radius R of the sphere around the metal center was set to 3.5 Å, while for the atoms we adopted the Bondi radii (18) scaled by 1.17, and a mesh of 0.1 Å was used to scan the sphere for buried voxels.

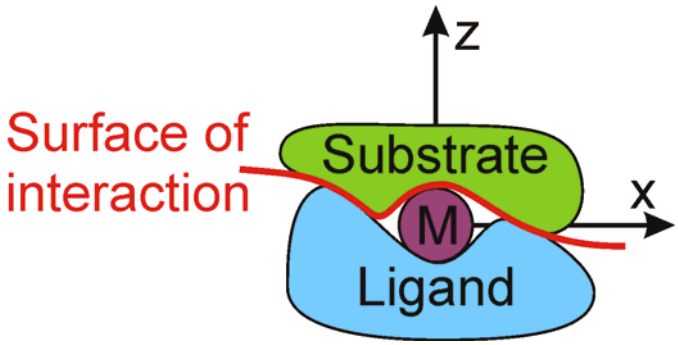


Figure S60. Schematic representation of the interaction surface between the substrate and the complex.

DFT Calculations of reaction pathways

fragment **1**

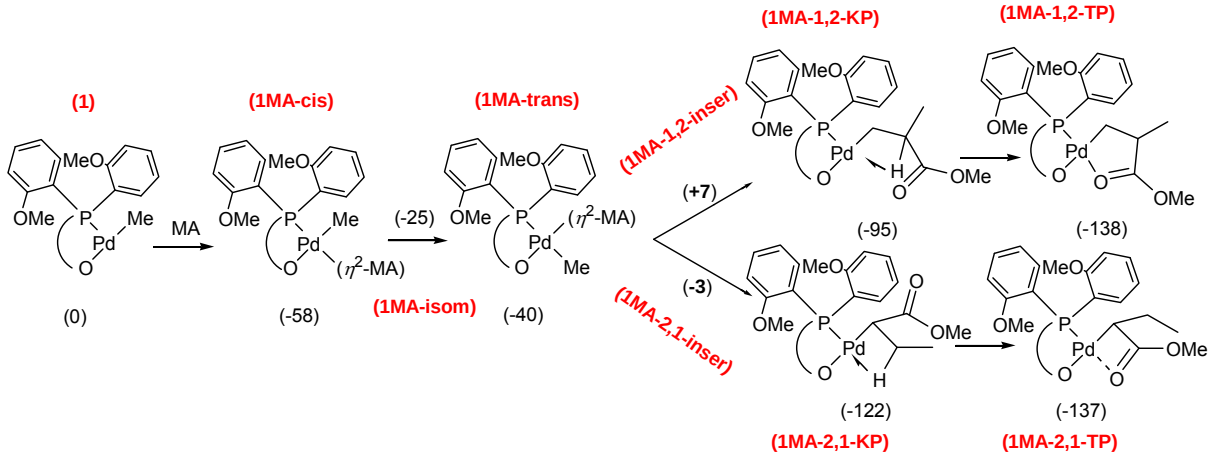


Figure S61. 2,1- and 1,2-insertion of methyl acrylate (MA) into the Pd methyl (Pd-Me) bond of fragment **1**. Energies in kJ mol^{-1}.

fragment **2a** (R = mesityl)

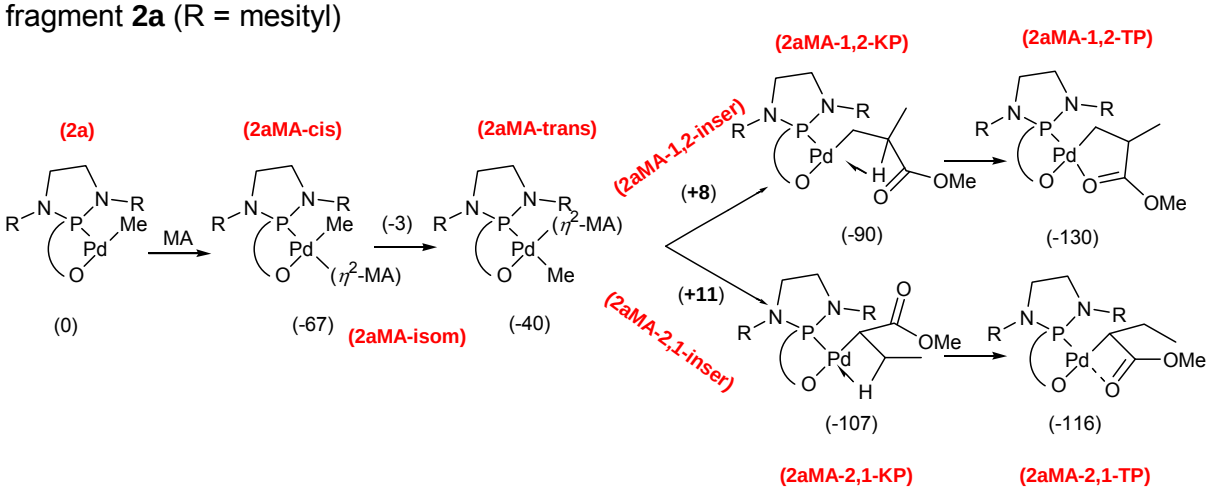


Figure S62. 2,1- and 1,2-insertion of methyl acrylate (MA) into the Pd methyl (Pd-Me) bond of fragment **2a**. Energies in kJ mol^{-1}.

fragment **2b** (R = 2,6-di(isopropyl)phenyl)

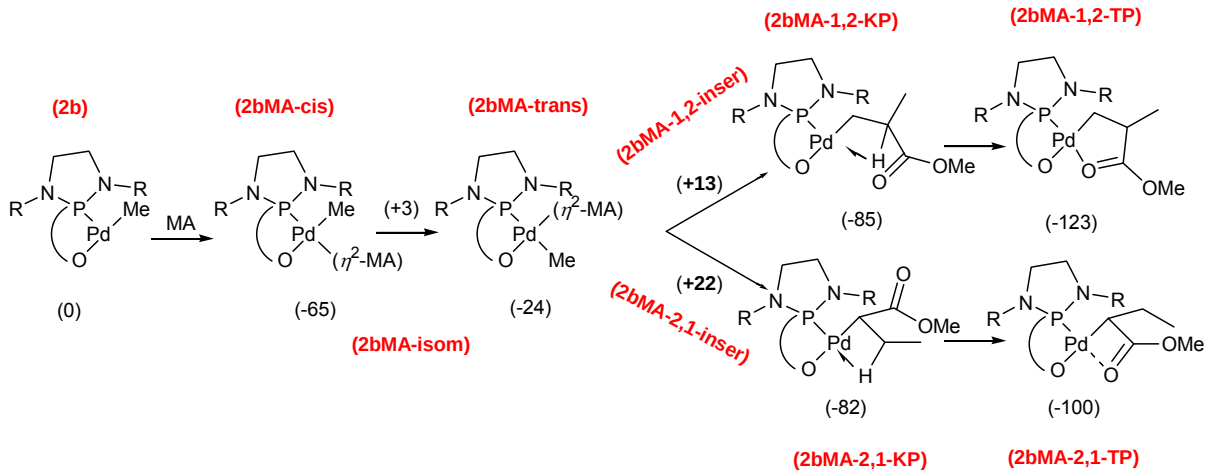


Figure S63. 2,1- and 1,2-insertion of methyl acrylate (MA) into the Pd methyl (Pd-Me) bond of fragment **2b**. Energies in kJ mol^{-1}.

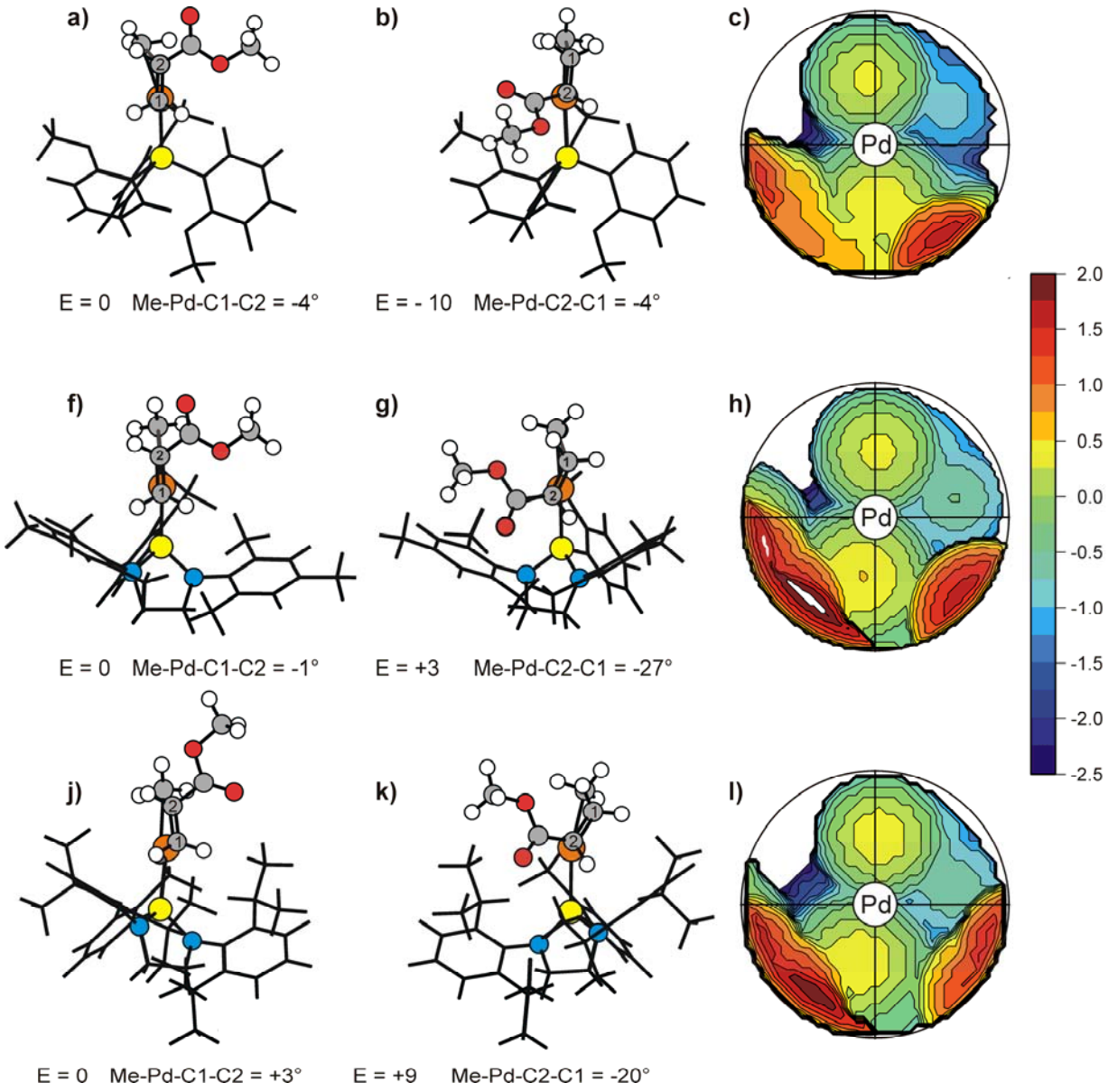
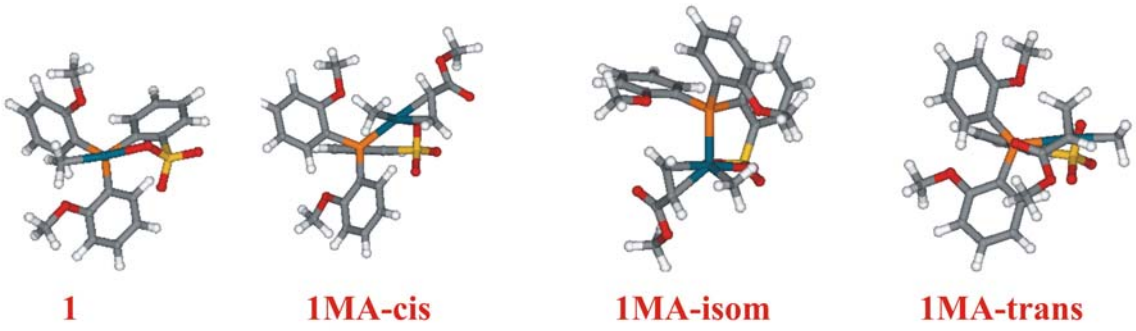
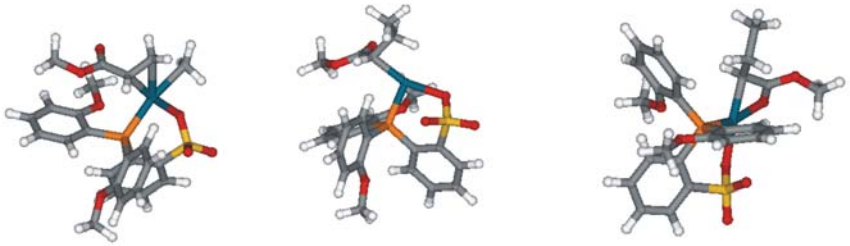


Figure S64. Geometry of the 1,2- (a, f, j) and 2,1-transition state (b, g, k) for methyl acrylate insertion into the Pd-Me bond of **1** (top line), **2a** (middle line), and **2b** (bottom line). Steric (c, g, l) maps of **1**, **2a** and **2b** with steric isocontour levels in Å.

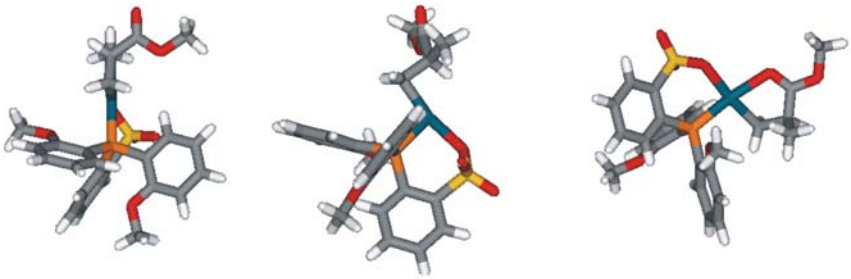
Cartesian coordinates and energies of the DFT structures



1 1MA-cis 1MA-isom 1MA-trans



1MA-2,1-inser 1MA-2,1-KP 1MA-2,1-TP



1MA-1,2-inser 1MA-1,2-KP 1MA-1,2-TP

1

E = -11.10574744 a.u.

Pd	0.00000	0.00000	0.00000
P	2.25186	0.00000	0.00000
C	3.10754	0.21885	1.60846
C	3.07913	-1.44587	-0.77222
C	2.82483	1.43493	-1.01576
C	2.91451	-0.70461	2.66095
O	2.14909	-1.79059	2.36968
C	1.86023	-2.71104	3.42763
H	1.20839	-3.47033	2.98388
H	2.78099	-3.18647	3.79791
H	1.33662	-2.20465	4.25188
C	3.51318	-0.48664	3.90318
H	3.36768	-1.19267	4.71744
C	4.29810	0.64750	4.10694
H	4.75360	0.80836	5.08458
C	4.49066	1.56781	3.08224
H	5.09039	2.46253	3.24333
C	3.89002	1.35265	1.84402
H	4.01939	2.08897	1.05219
C	2.61335	-1.91640	-2.02350

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O       1.61879  -1.19110  -2.59392
C       1.12139  -1.60781  -3.87181
H       0.34641  -0.88015  -4.13097
H       0.68534  -2.61555  -3.81154
H       1.92100  -1.58237  -4.62659
C       3.18539  -3.05293  -2.60046
H       2.83135  -3.42361  -3.56000
C       4.22464  -3.71547  -1.94747
H       4.66444  -4.59908  -2.41155
C       4.70153  -3.25513  -0.72363
H       5.52036  -3.76713  -0.21916
C       4.12351  -2.12600  -0.14319
H       4.49983  -1.75855   0.81175
C       3.95841   1.26531  -1.82225
H       4.47962   0.30807  -1.82886
C       4.43632   2.30659  -2.61443
H       5.32245   2.15022  -3.22984
C       3.78289   3.53443  -2.61320
H       4.15002   4.35513  -3.23078
C       2.65119   3.71714  -1.82195
H       2.11731   4.66757  -1.80442
C       2.16259   2.68181  -1.02476
S       0.69542   3.05214   0.00000
O       0.32496   4.42832  -0.31985
O       1.12019   2.73932   1.37004
O      -0.33362   2.05949  -0.52977
C      -0.10535  -2.01390   0.35996
H       0.79785  -2.62203   0.23939
H      -0.86255  -2.29288  -0.39718
H      -0.50103  -2.10157   1.38404

1MA-cis

E= -13.69111340 a.u.

Pd      0.00000   0.00000   0.00000
P       2.37872   0.00000   0.00000
C       3.06473   1.41306  -0.97540
C       2.43157   2.67146  -0.97730
S       0.93409   3.01069   0.00000
O      -0.09024   2.08800  -0.65758
O       1.26378   2.57675   1.36519
O       0.61546   4.41577  -0.23536
C       3.08348   0.02699   1.69409
C       3.11849  -1.47821  -0.80012
C       2.93704   3.70540  -1.76674
C       4.05579   3.49860  -2.56828
C       4.67523   2.25103  -2.58658
C       4.18230   1.21759  -1.79583
C       0.08212  -2.04447   0.39259
H       2.42505   4.66729  -1.73743
H       4.43971   4.31324  -3.18373
H       5.54736   2.07795  -3.21782
H       4.67545   0.24609  -1.81134
H       0.76455  -2.29426   1.21676
C      -2.29398  -0.01473   0.11555
H      -2.53070  -0.98692  -0.32522
C      -2.86323   1.18340  -0.56396
C      -1.78378   0.10253   1.38829
H      -1.73781   1.09353   1.84779
H      -1.64438  -0.76754   2.02919
H       0.44566  -2.50127  -0.53992
C       4.00376  -2.34204  -0.15409
C       4.48156  -3.48977  -0.78920
C       4.06463  -3.78174  -2.08411
C       3.16168  -2.94788  -2.74560
C       2.68055  -1.80497  -2.10470
H       4.32825  -2.11564   0.86118
H       5.17743  -4.14835  -0.27020
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H	4.43594	-4.67186	-2.59326
H	2.83698	-3.19732	-3.75367
O	1.77944	-0.94182	-2.64523
C	4.44957	0.26436	1.96240
C	4.90237	0.31390	3.28427
C	4.00936	0.12269	4.33639
C	2.66030	-0.11013	4.08722
C	2.20860	-0.14360	2.77098
O	5.26307	0.40566	0.88317
H	5.95161	0.50258	3.49966
H	4.37984	0.16596	5.36110
H	1.95788	-0.24092	4.90940
H	1.14912	-0.27644	2.56026
C	6.59429	0.88742	1.10692
H	7.01504	1.05458	0.11004
H	6.57210	1.83538	1.66315
H	7.19896	0.14134	1.64375
C	1.31573	-1.18832	-3.97858
H	0.62190	-0.37147	-4.19744
H	2.15394	-1.16689	-4.69027
H	0.79027	-2.15274	-4.03672
O	-3.05030	0.93387	-1.88852
O	-3.15436	2.22489	-0.01131
C	-3.57717	2.07243	-2.61581
H	-3.67197	1.73456	-3.65157
H	-4.55227	2.36175	-2.20476
H	-2.88120	2.91560	-2.53263
H	-0.93066	-2.40259	0.62481

1MA-isom

E= -13.67727321 a.u.

Pd	-1.274840	0.061542	0.500571
P	0.830411	-1.721757	0.390923
C	2.299808	-0.910653	-0.415657
C	2.433480	0.488671	-0.496241
S	1.183189	1.615384	0.176184
O	-0.023766	1.398113	-0.730515
O	0.870692	1.091600	1.532279
O	1.738082	2.958773	0.069756
C	1.567773	-2.283153	1.990461
C	0.731864	-3.274051	-0.604888
C	3.544585	1.062973	-1.115758
C	4.537586	0.254908	-1.662880
C	4.417294	-1.130224	-1.594738
C	3.306010	-1.703174	-0.981436
C	-2.706437	0.297606	-0.965649
H	3.613022	2.149956	-1.153251
H	5.405580	0.709402	-2.141889
H	5.191898	-1.771927	-2.015626
H	3.223351	-2.789519	-0.933931
H	-2.935618	1.370313	-0.976489
H	-2.145493	-0.018730	-1.851620
C	-2.636420	-1.077768	1.719262
H	-2.031257	-1.565834	2.484916
H	-3.242369	-1.719259	1.076556
C	-2.954180	0.277787	1.875881
H	-3.796676	0.738046	1.354738
C	-2.423484	1.025771	3.048338
H	-3.592311	-0.322010	-0.785966
C	1.083787	-4.540761	-0.139767
C	0.925394	-5.674149	-0.940995
C	0.406083	-5.540068	-2.224802
C	0.050398	-4.283274	-2.718647
C	0.212019	-3.154459	-1.914032
H	1.506766	-4.642763	0.859965
H	1.214236	-6.653906	-0.561316
H	0.277352	-6.416376	-2.861051

H	-0.348681	-4.193882	-3.726905
O	-0.086468	-1.883721	-2.305183
C	2.815389	-1.832282	2.430115
C	3.307693	-2.171063	3.690916
C	2.545949	-2.973039	4.532545
C	1.291341	-3.429210	4.126410
C	0.796712	-3.075625	2.870460
H	3.414173	-1.195442	1.780036
H	4.282213	-1.801362	4.008200
H	2.917318	-3.246553	5.520657
H	0.702088	-4.045461	4.801526
O	-0.424499	-3.468335	2.397351
C	-0.480490	-1.670293	-3.664887
H	-0.574276	-0.585049	-3.772938
H	0.289986	-2.042779	-4.356293
H	-1.445833	-2.155111	-3.875104
C	-1.220447	-4.314004	3.235148
H	-2.129614	-4.522411	2.662270
H	-0.696906	-5.258178	3.450373
H	-1.479471	-3.804997	4.175904
O	-1.777536	0.534573	3.956385
O	-2.758844	2.339607	2.963634
C	-2.196522	3.153116	4.023925
H	-2.541158	4.169980	3.817848
H	-2.555467	2.801845	4.998821
H	-1.102189	3.091663	3.991496

1MA-trans

E= -13.68447195 a.u.

Pd	0.00000	0.00000	0.00000
P	2.51266	0.00000	0.00000
C	3.18648	1.63943	-0.56592
C	2.42745	2.82315	-0.46482
S	0.67348	2.81588	0.00000
O	0.05495	2.00517	-1.12194
O	0.56474	2.02510	1.26848
O	0.25293	4.21011	0.05751
C	3.20330	-0.21488	1.69739
C	3.34183	-1.20400	-1.10596
C	2.97076	4.04785	-0.85402
C	4.25918	4.10967	-1.37718
C	4.99882	2.94065	-1.53057
C	4.46663	1.71921	-1.12530
C	-2.06084	0.32811	0.08855
H	2.35501	4.94130	-0.75425
H	4.67486	5.07100	-1.68121
H	5.99764	2.97581	-1.96661
H	5.04829	0.80831	-1.25073
H	-2.21541	1.14530	-0.62486
H	-2.66104	-0.55743	-0.15216
C	-0.38130	-1.92780	-0.84468
H	0.52496	-2.29375	-1.33567
H	-1.27723	-1.83619	-1.46160
C	-0.48940	-2.06809	0.54988
H	-1.46567	-2.03277	1.03959
C	0.56178	-2.79050	1.31174
H	-2.20555	0.65412	1.12810
C	4.57754	-0.22122	2.03231
C	4.97362	-0.33031	3.36895
C	4.01782	-0.40484	4.38050
C	2.66256	-0.36986	4.07305
C	2.27052	-0.27335	2.73982
O	5.45947	-0.12777	1.00184
H	6.02890	-0.34160	3.63132
H	4.34760	-0.47663	5.41759
H	1.91031	-0.39934	4.86051

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H       1.21066  -0.21331   2.49847
C       4.12508  -2.27070  -0.66638
C       4.62661  -3.21020  -1.56729
C       4.34229  -3.08527  -2.92438
C       3.53962  -2.04229  -3.38940
C       3.02568  -1.11389  -2.48215
H       4.33212  -2.37941   0.39629
H       5.23299  -4.03972  -1.20476
H       4.73536  -3.81121  -3.63713
H       3.30954  -1.96619  -4.45034
O       2.19247  -0.09157  -2.81154
C       1.85390   0.10705  -4.18778
H       1.19711   0.98235  -4.19578
H       2.75537   0.30870  -4.78511
H       1.32058  -0.76751  -4.58970
C       6.84848   0.00717   1.32115
H       7.35979   0.12413   0.36008
H       7.01854   0.89706   1.94472
H       7.22644  -0.89261   1.82930
O       0.17361  -2.95319   2.60900
O       1.60829  -3.21731   0.85762
C       1.11750  -3.70535   3.41124
H       0.66138  -3.77268   4.40320
H       1.26609  -4.70208   2.97698
H       2.07865  -3.17865   3.45429

 1MA-2,1-inser

E= -13.67046549  a.u.

Pd      0.00000   0.00000   0.00000
P       2.37377   0.00000   0.00000
C       3.08774   1.43951  -0.92804
C       2.47543   2.70726  -0.89898
S       0.92867   3.00877   0.00000
O      -0.02741   2.04493  -0.71381
O       1.17716   2.60090   1.38814
O       0.56215   4.39608  -0.27135
C       3.02277   3.76949  -1.61944
C       4.16853   3.58259  -2.38681
C       4.76515   2.32557  -2.44474
C       4.22788   1.26496  -1.72110
H       2.51832   4.73452  -1.57333
H       4.58626   4.41816  -2.94990
H       5.65238   2.16468  -3.05799
H       4.70414   0.28651  -1.77040
C       3.09074   0.04614   1.69311
C       3.14867  -1.44575  -0.82601
H      -2.25175  -1.94295   0.00887
C      -1.56421  -1.49716   0.72979
C      -0.22434  -1.99637   0.68583
H      -1.98361  -1.26656   1.71070
C       0.05837  -3.03004  -0.34603
C      -2.20934   0.44407   0.00273
H      -2.16224   0.67450  -1.06887
H       0.32526  -2.12223   1.62316
H      -3.16122  -0.02720   0.24988
H      -2.03322   1.32477   0.63083
C       4.46305   0.25488   1.95958
C       4.91433   0.34214   3.28004
C       4.01347   0.22456   4.33615
C       2.65789   0.02933   4.09114
C       2.20954  -0.04557   2.77530
O       5.28517   0.33707   0.88099
H       5.96862   0.50669   3.49077
H       4.38272   0.29894   5.35951
H       1.94872  -0.03762   4.91515
H       1.14469  -0.13583   2.56890
C       4.05603  -2.30397  -0.20478
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C       4.57948  -3.40737  -0.88072
C       4.18540  -3.65965  -2.19162
C       3.25170  -2.83874  -2.82464
C       2.72612  -1.73702  -2.14473
H       4.36099  -2.10902   0.82268
H       5.29670  -4.05964  -0.38268
H       4.59811  -4.51148  -2.73425
H       2.93921  -3.05862  -3.84374
O       1.81734  -0.87484  -2.66398
C       1.19435  -1.21304  -3.91111
H       0.47405  -0.41099  -4.09782
H       1.93576  -1.23865  -4.72326
H       0.67066  -2.17529  -3.82159
C       6.62847   0.78797   1.09216
H       7.05760   0.90330   0.09138
H       6.63283   1.75727   1.61092
H       7.21005   0.04619   1.65976
O      -0.48701  -3.11824  -1.43590
O       0.96478  -3.92630   0.12630
C       1.19568  -5.05723  -0.74765
H       1.98879  -5.63561  -0.26502
H       0.27533  -5.64947  -0.83916
H       1.51050  -4.71344  -1.73886

1MA-2,1-KP

E = -13.71546890  a.u.

Pd      0.00000   0.00000   0.00000
P       2.30597   0.00000   0.00000
C       2.94310   1.44173  -0.97388
C       2.29790   2.69474  -0.95077
S       0.77670   2.99532   0.00000
O      -0.19702   2.02971  -0.68454
O       1.07946   2.58674   1.37792
O       0.40125   4.38309  -0.25425
C       2.79203   3.75019  -1.71786
C       3.91165   3.57209  -2.52518
C       4.53786   2.32956  -2.57674
C       4.05657   1.27501  -1.80648
H       2.26601   4.70389  -1.67496
H       4.28530   4.40373  -3.12392
H       5.40435   2.17506  -3.22047
H       4.55601   0.30774  -1.84962
C       3.05090   0.07042   1.67544
C       3.05898  -1.45184  -0.82667
H      -1.90913  -0.28750   0.12571
C      -1.91744  -1.33385   0.62727
C      -0.52592  -1.88576   0.72117
H      -2.50371  -1.90639  -0.11086
C      -0.19752  -2.99103  -0.21063
C      -2.64326  -1.15258   1.96048
H      -2.03815  -0.56073   2.66167
H      -0.14387  -2.05730   1.73523
H      -2.83814  -2.13584   2.41472
H      -3.60404  -0.63758   1.82125
C       4.41929   0.33510   1.90838
C       4.89551   0.44485   3.21828
C       4.02457   0.28823   4.29431
C       2.67463   0.02744   4.08073
C       2.19952  -0.06641   2.77586
O       5.21202   0.44333   0.81003
H       5.94603   0.65525   3.40556
H       4.41324   0.38185   5.30891
H       1.98910  -0.07687   4.92072
H       1.13732  -0.21405   2.59035
C       3.99523  -2.28624  -0.21353
C       4.50319  -3.40373  -0.87664
C       4.06191  -3.69734  -2.16424
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C	3.10013	-2.90141	-2.78617
C	2.59223	-1.78194	-2.12174
H	4.33411	-2.05976	0.79687
H	5.24328	-4.03627	-0.38683
H	4.45923	-4.56294	-2.69637
H	2.75044	-3.15526	-3.78501
O	1.66161	-0.94156	-2.63519
C	0.98602	-1.32895	-3.84150
H	0.25766	-0.53423	-4.02826
H	1.69262	-1.38632	-4.68237
H	0.46809	-2.28649	-3.69023
C	6.53857	0.95591	0.98859
H	6.94041	1.08332	-0.02194
H	6.51014	1.92797	1.50142
H	7.16459	0.24493	1.54819
O	-0.69555	-3.16625	-1.31581
O	0.72434	-3.82622	0.34381
C	1.05848	-4.97484	-0.46991
H	1.81339	-5.52211	0.10247
H	0.16423	-5.59097	-0.63365
H	1.46220	-4.65257	-1.43631

1MA-2,1-TP

E= -13,72149122 a.u.

C	4.10550	1.22622	-1.76727
C	2.97770	1.41836	-0.96053
C	2.35563	2.68263	-0.94851
C	2.88472	3.72586	-1.70886
C	4.01710	3.52384	-2.49307
C	4.62265	2.27017	-2.52870
P	2.28485	0.00000	0.00000
C	2.96820	-1.48607	-0.83577
C	3.79804	-2.41277	-0.20076
C	4.20121	-3.58151	-0.84820
C	3.76751	-3.83145	-2.14681
C	2.92921	-2.92883	-2.80247
C	2.52238	-1.76219	-2.15142
O	1.69683	-0.83099	-2.69162
C	1.22464	-1.02698	-4.03044
S	0.83636	3.01522	0.00000
O	0.47694	4.40160	-0.28756
Pd	0.00000	0.00000	0.00000
O	-2.18156	-0.59704	0.21515
C	-1.62769	-1.47183	0.93280
O	-2.08370	-1.79664	2.15628
C	-3.21877	-1.00811	2.61220
O	-0.15563	2.04773	-0.65036
C	-0.35532	-2.04529	0.50298
H	-0.41072	-2.41801	-0.53168
C	3.03130	0.02655	1.67520
C	4.41983	0.14903	1.90667
C	4.90564	0.21656	3.21569
C	4.02128	0.16872	4.29171
C	2.65032	0.06408	4.07849
C	2.16757	0.00567	2.77432
H	1.09505	-0.02424	2.58749
O	1.15120	2.63943	1.38454
O	5.21625	0.16927	0.80576
H	5.97259	0.31253	3.40323
H	4.41742	0.22579	5.30617
H	1.95682	0.05173	4.91826
H	4.13451	-2.21981	0.81756
H	4.85278	-4.28927	-0.33640
H	4.07848	-4.73954	-2.66474
H	2.59522	-3.14176	-3.81591
H	2.37896	4.69086	-1.67586
H	4.42053	4.34692	-3.08423

H	5.50076	2.10003	-3.15240
H	4.58346	0.24772	-1.79825
H	0.58880	-0.16152	-4.23916
H	2.06611	-1.05229	-4.73824
H	0.63532	-1.95248	-4.10460
C	0.44463	-2.91774	1.43579
H	-3.43806	-1.38382	3.61547
H	-2.94967	0.05432	2.63766
H	-4.07264	-1.15511	1.94097
C	-0.12829	-4.34086	1.52802
H	1.47996	-2.98075	1.06660
H	0.48113	-2.46909	2.44072
H	0.48473	-4.95875	2.20161
H	-1.15821	-4.32576	1.91338
H	-0.13639	-4.82285	0.53818
C	6.60621	0.46387	0.98987
H	7.03092	0.51086	-0.01809
H	6.73251	1.43430	1.49109
H	7.10559	-0.33111	1.56386

1MA-1,2-inser

E= -13,66670678 a.u.

Pd	-1.210578	0.762863	0.160249
P	0.899332	1.486117	-0.549308
C	2.246775	0.343145	0.001267
C	2.040641	-1.050085	0.044106
S	0.474919	-1.820500	-0.474649
O	-0.515601	-1.267154	0.551746
O	0.217914	-1.295181	-1.822271
O	0.657268	-3.259633	-0.304056
C	3.050568	-1.891648	0.512866
C	4.259828	-1.363064	0.955512
C	4.463581	0.014851	0.935202
C	3.463598	0.859268	0.461743
H	2.857762	-2.964402	0.526352
H	5.041046	-2.030127	1.322297
H	5.404854	0.437493	1.288122
H	3.630868	1.935943	0.445374
C	1.033053	1.721831	-2.365780
C	1.378810	3.115152	0.163702
H	-3.621107	2.164676	1.339777
C	-3.226112	1.950649	0.344224
C	-2.041467	2.661487	-0.044415
C	-4.344001	1.760981	-0.638150
H	-1.581532	3.325105	0.695206
C	-3.175054	-0.115859	0.915760
H	-2.646896	-0.360538	1.846949
H	-1.964862	3.003852	-1.079859
H	-4.228987	0.092192	1.108850
H	-3.062189	-0.885315	0.141166
C	2.251751	1.978473	-3.032842
C	2.273057	2.107386	-4.424756
C	1.092541	1.986557	-5.154889
C	-0.114238	1.728673	-4.512380
C	-0.132186	1.586587	-3.127060
O	3.353744	2.115365	-2.249362
H	3.207956	2.300237	-4.945966
H	1.127459	2.088199	-6.240096
H	-1.032900	1.613266	-5.085660
H	-1.061962	1.335992	-2.618065
C	1.645617	4.240279	-0.618307
C	1.915608	5.479450	-0.034036
C	1.917310	5.598783	1.352038
C	1.637654	4.495008	2.159152
C	1.358703	3.259577	1.571341
H	1.641821	4.149867	-1.704303

H	2.125954	6.342917	-0.664521
H	2.133096	6.559138	1.821815
H	1.634061	4.606615	3.241574
O	1.049030	2.133324	2.266963
C	1.089234	2.183838	3.697634
H	0.849142	1.168855	4.028457
H	2.094027	2.461156	4.048943
H	0.342513	2.892032	4.086332
C	4.632313	2.161787	-2.894277
H	5.368548	2.151974	-2.083955
H	4.774336	1.278867	-3.533846
H	4.743929	3.084137	-3.483743
O	-3.908811	1.716967	-1.920122
O	-5.513496	1.664479	-0.308498
C	-4.963504	1.539631	-2.899504
H	-4.454628	1.512567	-3.866708
H	-5.496951	0.600622	-2.710310
H	-5.668246	2.378219	-2.848067

1MA-1,2-KP

E= -13.70537910 a.u.

Pd	-0.915735	0.544577	0.551349
P	0.947839	1.475747	-0.376709
C	2.437599	0.439394	-0.027240
C	2.356599	-0.967321	0.036729
S	0.801616	-1.893663	-0.215389
O	-0.058598	-1.409013	0.950434
O	0.284041	-1.427053	-1.510736
O	1.151239	-3.304348	-0.070786
C	3.499958	-1.713132	0.327924
C	4.715353	-1.080578	0.573971
C	4.794713	0.309218	0.539015
C	3.662746	1.061587	0.241276
H	3.405700	-2.798435	0.364295
H	5.599531	-1.677140	0.802398
H	5.739881	0.812950	0.743878
H	3.728979	2.148619	0.214803
C	0.835591	1.723424	-2.192001
C	1.335150	3.127401	0.322965
H	-2.916447	0.347118	1.146065
C	-3.297761	1.350385	0.748177
C	-2.100129	2.211112	0.394721
C	-4.222856	1.061494	-0.432942
H	-1.786347	2.936090	1.159185
C	-4.072623	1.927366	1.932202
H	-2.159574	2.672093	-0.600460
C	1.918617	2.173692	-2.981021
C	1.770571	2.294176	-4.365836
C	0.559282	1.964887	-4.970510
C	-0.512238	1.509974	-4.208554
C	-0.360824	1.383795	-2.830521
O	3.060514	2.492931	-2.317376
H	2.598866	2.639793	-4.979937
H	0.463743	2.060285	-6.052629
H	-1.452825	1.232310	-4.682265
H	-1.170192	0.980920	-2.224749
C	1.320267	4.296214	-0.440732
C	1.504855	5.546381	0.151599
C	1.706797	5.631756	1.525913
C	1.708239	4.481896	2.316576
C	1.509622	3.233329	1.723834
H	1.157605	4.230830	-1.516263
H	1.491229	6.445983	-0.462923
H	1.859901	6.602073	1.999668
H	1.856621	4.566470	3.391159
O	1.457572	2.060549	2.404996

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C        1.664172     2.082374     3.822081
H        1.591891     1.037477     4.138533
H        2.662195     2.476860     4.063312
H        0.887410     2.680789     4.320133
C        4.228957     2.781853    -3.094806
H        5.036516     2.918810    -2.368435
H        4.468055     1.940290    -3.760573
H        4.096076     3.705916    -3.676956
O       -3.381615     1.781389     3.088545
O       -5.158951     2.463558     1.841386
C       -4.043699     2.347744     4.249476
H       -3.388217     2.118449     5.093904
H       -4.162173     3.430625     4.123287
H       -5.029683     1.886183     4.380177
H       -4.713258     1.992332    -0.749716
H       -3.644592     0.651460    -1.271870
H       -5.004518     0.338551    -0.160036

1MA-1,2-TP
E= -13.72162971 a.u.

Pd      -1.094080     0.609645     0.147993
P        0.899377     1.482015    -0.503550
C        2.328337     0.468436     0.088955
C        2.248829    -0.937389     0.152277
S        0.762045    -1.864038    -0.355598
O       -0.285255    -1.351581     0.626490
O        0.496794    -1.428128    -1.733786
O        1.071745    -3.272514    -0.117978
C        3.330903    -1.673002     0.638445
C        4.484952    -1.029053     1.075497
C        4.561943     0.361212     1.034167
C        3.490584     1.102200     0.544348
H        3.235488    -2.758394     0.671373
H        5.322225    -1.615772     1.455862
H        5.458316     0.874104     1.384347
H        3.557446     2.189206     0.511868
C        1.050420     1.668072    -2.324964
C        1.216836     3.163240     0.172653
C       -2.100083     2.388681    -0.212350
C        2.249872     2.041915    -2.971385
C        2.299811     2.109359    -4.366878
C        1.168416     1.805902    -5.121522
C       -0.016884     1.427053    -4.499482
C       -0.061956     1.351356    -3.110096
O        3.302774     2.345140    -2.166906
H        3.220411     2.392755    -4.871863
H        1.226728     1.859188    -6.209240
H       -0.895173     1.166333    -5.088573
H       -0.964603     1.006486    -2.608928
C        1.341723     4.290356    -0.641627
C        1.471676     5.567863    -0.093451
C        1.476040     5.723534     1.289127
C        1.336797     4.616766     2.127908
C        1.195667     3.341354     1.576759
H        1.333359     4.170252    -1.724904
H        1.571976     6.432632    -0.748823
H        1.584724     6.714719     1.731101
H        1.334174     4.755961     3.207068
O        1.025427     2.208960     2.306176
C        1.075702     2.303454     3.733849
H        0.949300     1.277985     4.094290
H        2.048640     2.697297     4.063977
H        0.261634     2.938309     4.114145
C        4.585691     2.518088    -2.780295
H        5.292145     2.635764    -1.952096
H        4.853339     1.630989    -3.372145
H        4.603563     3.419471    -3.411131
C       -3.266836     2.421137     0.784551
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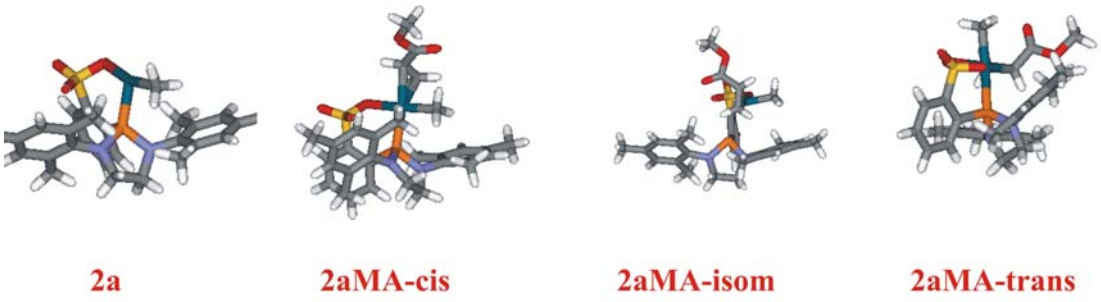
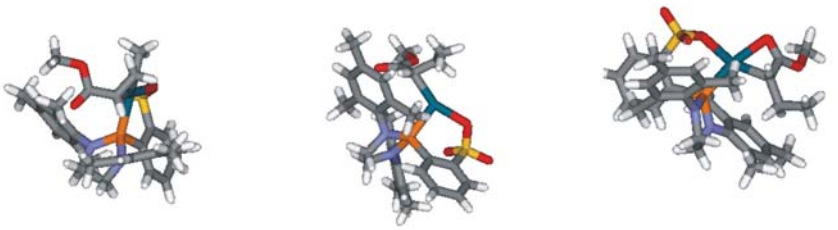
H	-1.491140	3.299725	-0.118572
H	-2.472166	2.311685	-1.248825
C	-2.824232	2.861483	2.194410
H	-4.058402	3.114716	0.442187
C	-3.848564	1.037921	0.873812
O	-5.158707	0.980616	1.128473
O	-3.157831	0.016949	0.748305
C	-5.704040	-0.368173	1.244421
H	-6.770485	-0.224341	1.435081
H	-5.535552	-0.915095	0.310093
H	-5.216482	-0.894907	2.072244
H	-3.672971	2.875524	2.895082
H	-2.048531	2.180176	2.575743
H	-2.396000	3.872878	2.135098



2a 2aMA-cis 2aMA-isom 2aMA-trans



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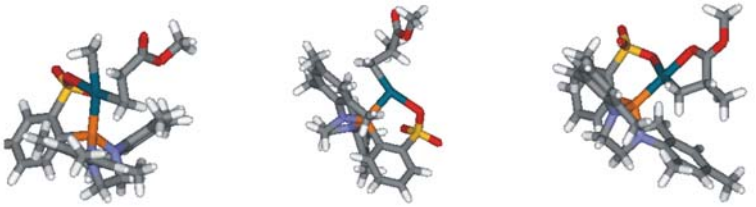

2aMA-1,2-inser 2aMA-1,2-KP 2aMA-1,2-TP

2a

E= -14.81496393 a.u.

Pd	-0.893071	0.202937	0.485598
P	1.306687	0.299404	0.087396
N	2.068867	0.876309	-1.329199
N	2.176271	-1.177194	0.048132
C	2.071928	1.325344	1.451112
C	3.340451	0.964059	1.923647
H	3.827455	0.070172	1.542065
C	3.989605	1.718630	2.896291
H	4.977253	1.414635	3.244808
C	3.372441	2.849324	3.424316
H	3.874055	3.445618	4.187534
C	2.101996	3.210071	2.985883
H	1.584022	4.079818	3.391343
C	1.449949	2.457970	2.007728
S	-0.208575	3.008938	1.498810
O	-0.508080	4.197843	2.290230
O	-0.112064	3.140277	0.035874
O	-1.068360	1.817178	1.912334
C	-1.256478	-1.396767	-0.745838
C	3.379733	-1.062301	-0.801677

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C        3.062707    -0.048297    -1.898189
C        1.785682     2.071294    -2.079330
C        1.617141    -2.462115     0.369341
C        2.598852     3.204820    -1.913131
C        2.360555     4.318666    -2.719883
C        1.345607     4.338369    -3.676542
C        0.557968     3.197569    -3.820204
C        0.763170     2.058165    -3.041066
C        3.688301     3.267139    -0.881488
H        2.988666     5.202949    -2.588996
C        1.102314     5.561460    -4.515110
H       -0.241973     3.187892    -4.563403
C       -0.125249     0.864243    -3.225709
C        1.301433    -2.769315     1.711117
C        0.776042    -4.026795     2.011639
C        0.577140    -5.007328     1.038479
C        0.886348    -4.677418    -0.276945
C        1.379270    -3.419779    -0.638325
C        1.517766    -1.791165     2.828857
H        0.531347    -4.250789     3.052478
C        0.059824    -6.370216     1.404242
H        0.714705    -5.412727    -1.066392
C        1.582622    -3.152269    -2.104370
H        4.234961    -0.708529    -0.201814
H        3.649104    -2.044302    -1.205572
H        2.670760    -0.530861    -2.811701
H        3.964750     0.517428    -2.182837
H        4.478250     3.963990    -1.195291
H        3.281830     3.625435     0.079174
H        4.144425     2.287219    -0.690978
H        0.448621    -0.070326    -3.298332
H       -0.809952     0.762583    -2.370436
H       -0.727669     0.963107    -4.138879
H        0.410292     5.347504    -5.340575
H        0.662608     6.366105    -3.904950
H        2.040877     5.941285    -4.944986
H        1.422382    -2.097226    -2.352867
H        2.594464    -3.430148    -2.445020
H        0.870276    -3.745762    -2.694598
H        1.326748    -2.271684     3.797788
H        2.546439    -1.406605     2.831511
H        0.848427    -0.919510     2.757257
H       -0.188240    -6.955859     0.508871
H        0.815574    -6.932346     1.975700
H       -0.843532    -6.299706     2.027841
H       -2.275071    -1.111470    -1.073633
H       -0.621053    -1.561529    -1.621069
H       -1.268309    -2.290703    -0.102695
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2aMA-cis

E= -17.40401140 a.u.

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C        1.643032    -3.546232    -0.448887
C        1.746424    -2.476619     0.467286
C        1.356742    -2.678610     1.811192
C        0.897005    -3.936244     2.203922
C        0.833095    -5.019473     1.327420
C        1.211561    -4.795797     0.008148
N        2.239289    -1.195037     0.046329
C        3.482169    -1.068526    -0.742609
C        3.169672    -0.125071    -1.898678
N        2.164078     0.818354    -1.389069
C        1.963621     2.058832    -2.088137
C        2.814847     3.149192    -1.837043
C        2.604543     4.338378    -2.538512
C        1.578996     4.476743    -3.472458
C        0.767798     3.371023    -3.720738
C        0.946445     2.160300    -3.052028
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C	3.919839	3.099404	-0.819534
C	1.338570	5.788007	-4.165942
C	0.025301	1.015216	-3.343136
C	1.431600	-1.596841	2.849396
C	0.383785	-6.373519	1.800316
C	1.929376	-3.417383	-1.920205
P	1.329602	0.263340	0.006317
C	2.014029	1.340518	1.372574
C	3.267033	1.053755	1.928144
C	3.820881	1.865021	2.913517
C	3.123026	2.981092	3.369976
C	1.865305	3.270298	2.849431
C	1.311096	2.455689	1.861724
S	-0.345417	2.850020	1.244902
O	-1.164708	1.664046	1.737038
Pd	-1.017282	0.048825	0.194725
C	-0.971547	-1.531256	-1.154869
O	-0.738810	4.105750	1.874811
O	-0.201087	2.811087	-0.225943
H	3.818328	0.175529	1.599630
H	4.800612	1.621599	3.326349
H	3.554406	3.622510	4.139448
H	1.286738	4.127510	3.195087
H	3.258359	5.189024	-2.332217
H	-0.037705	3.450911	-4.453580
H	0.598978	-4.074897	3.245645
H	1.144793	-5.614470	-0.712095
H	4.290694	-0.645102	-0.122972
H	3.815142	-2.053766	-1.085403
H	2.790573	-0.672962	-2.781312
H	4.068888	0.429634	-2.211157
H	4.764501	3.726409	-1.139663
H	3.564486	3.482545	0.151467
H	4.289648	2.081307	-0.648553
H	0.567749	0.065922	-3.446594
H	-0.702330	0.893833	-2.525649
H	-0.533765	1.191710	-4.272084
H	0.709504	5.658915	-5.056854
H	0.823632	6.488027	-3.488492
H	2.283523	6.256144	-4.476875
H	1.759254	-2.398377	-2.284067
H	2.966386	-3.700166	-2.168767
H	1.266883	-4.086407	-2.487412
H	1.165960	-2.001211	3.835514
H	2.443744	-1.175672	2.916226
H	0.746985	-0.759600	2.644736
H	0.211045	-7.054740	0.956485
H	1.146258	-6.830275	2.451385
H	-0.548610	-6.303975	2.379570
H	-1.931229	-1.495637	-1.687814
H	-0.133313	-1.425662	-1.850105
H	-0.879226	-2.461226	-0.577078
C	-2.780748	-0.953390	1.230462
C	-3.323259	0.049147	0.463771
H	-3.408467	1.067919	0.849227
C	-4.053113	-0.263275	-0.790847
H	-2.873007	-1.990893	0.903637
H	-2.465219	-0.754881	2.255532
O	-4.524661	0.881543	-1.352957
O	-4.221931	-1.375102	-1.263932
C	-5.269435	0.678510	-2.577212
H	-5.579688	1.678137	-2.893073
H	-4.630387	0.207044	-3.333463
H	-6.137903	0.036078	-2.387233

2aMA-isom

E= -17,37955034 a.u.

Pd	0.027832	0.106784	0.142248
P	0.008201	0.112924	3.058218
N	0.976057	0.076223	4.525095
N	-0.769071	-1.355061	3.538104
C	0.882792	-1.194541	5.259451
C	-0.486520	-1.767577	4.922630
H	-0.508045	-2.863526	4.997659
H	-1.254772	-1.378381	5.614458
H	1.693515	-1.890890	4.971241
H	0.983229	-1.004781	6.341851
C	2.136374	0.871446	4.814662
C	-1.245885	-2.309915	2.586331
C	3.336412	0.719839	4.095902
C	3.435892	-0.159518	2.883729
C	4.472235	1.419116	4.516738
H	5.401106	1.291541	3.956356
C	4.458685	2.249059	5.635422
C	5.694504	2.981113	6.079142
C	3.254705	2.393785	6.325894
C	2.092678	1.728865	5.933701
C	0.822951	1.957990	6.703359
C	-0.446545	-3.408288	2.204061
C	0.944770	-3.601604	2.734972
C	-0.959944	-4.337212	1.296883
C	-2.237652	-4.209544	0.750744
C	-2.779081	-5.247957	-0.191729
C	-3.004496	-3.109697	1.134562
C	-2.535805	-2.157209	2.043378
C	-3.406087	-0.996050	2.427682
H	2.785375	-1.038847	2.968546
H	4.468018	-0.510437	2.743550
H	3.145280	0.394891	1.976946
H	5.734376	3.985747	5.628177
H	6.605037	2.443058	5.781354
H	5.711617	3.103505	7.171371
H	3.215855	3.045370	7.201809
H	1.033272	2.483041	7.645424
H	0.303621	1.019986	6.943670
H	0.126711	2.573739	6.113718
H	1.473322	-2.644785	2.825367
H	0.942351	-4.070741	3.732866
H	1.527801	-4.255853	2.072026
H	-0.336506	-5.187011	1.007116
H	-3.259103	-6.065330	0.371272
H	-1.978851	-5.691836	-0.800797
H	-3.531929	-4.822512	-0.869147
H	-4.007773	-2.988007	0.719416
H	-3.390416	-0.833851	3.514682
H	-4.443873	-1.168868	2.111580
H	-3.066323	-0.054933	1.965219
C	-1.166953	1.514781	3.535541
C	-1.895705	1.449626	4.729572
H	-1.767287	0.591370	5.385384
C	-2.762467	2.467296	5.113988
H	-3.314961	2.387111	6.050944
C	-2.905091	3.596886	4.310412
H	-3.567180	4.409661	4.610863
C	-2.200038	3.686394	3.115175
H	-2.297610	4.552788	2.461158
C	-1.349881	2.650056	2.724047
S	-0.598924	2.801140	1.080032
O	0.815646	2.369455	1.190500
O	-0.869115	4.155875	0.616675
O	-1.385403	1.742715	0.294805
C	-1.398900	-0.812984	-1.036811
H	-1.369382	-0.317671	-2.015749
H	-1.209600	-1.892055	-1.091773
H	-2.315136	-0.572745	-0.485234
C	1.479225	-1.483063	-0.147908

C	1.441792	-0.706753	-1.307712
H	0.898239	-1.035269	-2.195974
H	0.967627	-2.446410	-0.111980
H	2.278198	-1.305221	0.573821
C	2.415883	0.398704	-1.509132
O	2.146693	1.047334	-2.671912
O	3.317225	0.692735	-0.742849
C	2.983671	2.205610	-2.913036
H	2.620866	2.627848	-3.854197
H	2.870302	2.920501	-2.089595
H	4.033520	1.899836	-2.995091

2aMA-trans

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C	0.819126	-4.028656	1.904110
C	0.521303	-4.942435	0.891918
C	0.768314	-4.553943	-0.422376
N	2.239885	-1.142444	0.018617
C	3.467586	-1.048229	-0.793541
C	3.237070	0.038688	-1.846728
N	2.184267	0.922534	-1.326714
C	1.911148	2.127566	-2.056980
C	2.690889	3.277365	-1.847178
C	2.434653	4.412299	-2.623246
C	1.435956	4.436936	-3.594261
C	0.684876	3.277367	-3.790870
C	0.907673	2.122854	-3.042717
C	3.774526	3.338671	-0.808343
C	1.153755	5.678688	-4.392385
C	0.059920	0.910175	-3.278653
C	1.689424	-1.855825	2.783472
C	-0.020011	-6.307449	1.211758
C	1.478710	-2.954972	-2.194831
P	1.370247	0.340142	0.079593
C	2.197466	1.324643	1.451713
C	3.484197	1.003730	1.900290
C	4.130888	1.775315	2.861911
C	3.496676	2.891634	3.402756
C	2.205577	3.215014	2.996525
C	1.561123	2.435256	2.036728
S	-0.156476	2.825922	1.634059
O	-0.904202	1.646865	2.226106
Pd	-1.178898	0.420368	0.322033
C	-1.721978	-1.323024	-0.950402
O	-0.457889	4.114351	2.243996
O	-0.232186	2.733970	0.139308
H	3.993994	0.130349	1.500346
H	5.134753	1.501817	3.189260
H	4.000872	3.503908	4.151250
H	1.672539	4.068842	3.415815
H	3.038372	5.307201	-2.455665
H	-0.098683	3.268820	-4.551872
H	0.624901	-4.302039	2.943908
H	0.518076	-5.237384	-1.237150
H	4.330283	-0.785027	-0.159011
H	3.690438	-2.020913	-1.249077
H	2.929333	-0.394627	-2.816886
H	4.164780	0.609628	-2.023276
H	4.576756	4.019185	-1.127912
H	3.370616	3.717545	0.145526
H	4.212594	2.354789	-0.601537
H	0.662701	-0.002193	-3.389491
H	-0.625225	0.748089	-2.434615
H	-0.549346	1.025871	-4.184500
H	0.835353	5.429813	-5.414615

H	0.345654	6.262049	-3.922061
H	2.040589	6.323774	-4.456485
H	1.375541	-1.876840	-2.367659
H	2.466677	-3.260641	-2.578946
H	0.722363	-3.471177	-2.802807
H	1.552431	-2.376467	3.740909
H	2.725591	-1.494625	2.729914
H	1.041339	-0.964929	2.797034
H	-0.542730	-6.741752	0.348776
H	0.799546	-6.991330	1.486988
H	-0.722281	-6.272401	2.056316
C	-2.889892	-1.189358	-1.857757
H	-0.792909	-1.605538	-1.446107
C	-1.905043	-1.602582	0.411641
C	-3.158433	1.021851	0.551302
H	-1.133864	-2.138162	0.969895
H	-2.923227	-1.648032	0.805577
H	-3.324330	1.040709	1.634515
H	-3.075509	2.033678	0.129899
H	-3.853153	0.377285	0.004704
O	-2.472253	-1.097863	-3.154257
O	-4.065132	-1.196674	-1.530828
C	-3.551641	-0.996658	-4.113073
H	-3.065778	-0.959795	-5.092359
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2aMA-2,1-inser

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C	0.748159	-3.877342	2.135145
C	0.682191	-4.942939	1.238268
C	1.145144	-4.718559	-0.054397
N	2.255436	-1.144581	0.082612
C	3.505867	-1.008050	-0.691983
C	3.219555	-0.019891	-1.816273
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C	2.682664	3.276760	-1.809153
C	2.390124	4.418071	-2.559408
C	1.390151	4.430593	-3.531499
C	0.696466	3.246357	-3.769682
C	0.955431	2.083535	-3.044922
C	3.753901	3.349546	-0.759133
C	1.039773	5.687757	-4.276305
C	0.144776	0.856695	-3.324521
C	1.354958	-1.576836	2.853059
C	0.152338	-6.283878	1.662474
C	2.005617	-3.339310	-1.925681
P	1.361049	0.330249	0.083993
C	2.125036	1.331902	1.479195
C	3.376414	0.977306	1.998008
C	3.991581	1.738029	2.988437
C	3.354898	2.867928	3.496550
C	2.097149	3.222625	3.018035
C	1.489420	2.463436	2.018022
S	-0.148200	2.948689	1.433673
O	-0.990403	1.730052	1.823359
Pd	-1.025900	0.135983	0.313043
C	-1.382465	-1.708545	-0.742409
O	-0.536706	4.131942	2.195150
O	-0.007576	3.050653	-0.027890
H	3.877770	0.080433	1.642989
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  H         0.393755   -4.019071    3.158694
  H         1.082832   -5.522569   -0.791148
  H         4.314521   -0.618290   -0.051940
  H         3.829538   -1.982979   -1.068532
  H         2.844472   -0.532052   -2.721987
  H         4.131007    0.533812   -2.096164
  H         4.529843    4.071762   -1.050780
  H         3.327065    3.682299    0.201635
  H         4.229721    2.377082   -0.580385
  H         0.687233   -0.070867   -3.114895
  H        -0.762095    0.858039   -2.697879
  H        -0.168962    0.834773   -4.377732
  H         0.622526    5.460231   -5.267206
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  H         1.916897    6.335234   -4.411876
  H         1.795553   -2.331386   -2.299199
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  C        -3.258509    0.386147    0.589220
  H        -2.453061   -2.073136    1.100693
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  H        -3.922699   -0.168250    1.258116
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  H        -3.708104    0.566482   -0.391472
  C        -1.551910   -1.683755   -2.213443
  H        -0.556432   -2.351994   -0.434044
  O        -0.760571   -2.173109   -3.004708
  O        -2.713804   -1.080844   -2.601734
  C        -2.943855   -1.110978   -4.030472
  H        -3.868688   -0.548177   -4.187012
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2aMA-2,1-KP

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C         1.153953   -4.487132   -0.291047
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C         3.576840   -0.819502   -0.410142
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C         1.828101    2.016661   -2.121839
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C         0.696940    2.756569   -4.118822
C         0.853626    1.805029   -3.112811
C         3.580370    3.515182   -1.034478
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C        -0.039209    0.603513   -3.090204
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P	1.369256	0.448479	0.252137
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C	3.267485	3.168394	3.566630
C	2.075770	3.551863	2.956540
C	1.490341	2.740969	1.986125
S	-0.087592	3.270061	1.268419
O	-1.039164	2.181897	1.765796
Pd	-0.879564	0.297186	0.730129
C	-1.540762	-1.619339	0.163886
O	-0.407636	4.566633	1.856502
O	0.123611	3.179393	-0.184956
H	3.732166	0.188841	2.017501
H	4.782701	1.637171	3.706249
H	3.721266	3.807901	4.324647
H	1.571415	4.480922	3.223894
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H	4.362554	-0.429004	0.257165
H	3.916215	-1.794833	-0.778374
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H	4.196428	0.840607	-1.670231
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H	3.146851	4.291929	-0.382488
H	3.807347	2.656014	-0.392743
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H	-0.581854	0.508644	-4.040135
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H	0.444077	5.578440	-5.054514
H	2.186531	5.535033	-5.409633
H	1.602059	-1.718744	-2.115431
H	2.846288	-2.978439	-2.302867
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H	1.389391	-2.368180	3.967014
H	2.734439	-1.540836	3.150210
H	1.089560	-0.922380	2.977337
H	-0.145844	-6.743626	0.378865
H	1.324953	-7.020693	1.334887
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C	-2.619604	-1.334232	1.169492
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H	-3.255299	-1.745003	3.211953
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H	-0.840597	-2.418872	0.424593
O	-3.016350	-0.935988	-1.551052
O	-1.303092	-2.322765	-2.123071
C	-3.453252	-1.005014	-2.927108
H	-4.324680	-0.346158	-2.986008
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2aMA-2,1-TP

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C	1.277244	-5.077141	1.598399
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N	2.196605	-1.224263	-0.014998
C	3.297432	-1.046852	-0.986349
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C	1.014782	-6.437337	2.181125
C	2.000858	-3.625418	-1.814181
P	1.273149	0.229100	0.112898
C	2.215312	1.315173	1.316254
C	3.540824	1.001195	1.643393
C	4.299199	1.832009	2.462640
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C	1.647286	2.466353	1.890097
S	-0.115158	2.847901	1.691760
O	-0.740553	1.578894	2.277979
Pd	-0.911365	0.047743	0.757936
C	-1.800588	-1.330517	-0.617271
O	-0.380347	4.015997	2.525938
O	-0.339024	2.948071	0.240388
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H	5.329370	1.562611	2.698746
H	4.329401	3.656722	3.618044
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H	4.132097	1.927020	-1.042075
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H	1.712474	-2.666967	-2.259134
H	3.044811	-3.836019	-2.103642
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H	1.513762	-1.913306	3.905091
H	2.646656	-1.035971	2.856971
H	0.903620	-0.762014	2.710820
H	0.682026	-7.145249	1.409652
H	1.930860	-6.846178	2.638069
H	0.243913	-6.395559	2.963657
C	-2.691435	-1.575669	0.513088
O	-3.023039	-0.599110	1.234655
O	-3.023194	-2.841460	0.805690
H	-2.219702	-0.550195	-1.270287
C	-1.177064	-2.481092	-1.357324
C	-3.736328	-3.012701	2.062664
H	-3.908026	-4.089385	2.144445
H	-3.120771	-2.646344	2.892228
H	-4.683567	-2.461880	2.034871
C	-2.154119	-3.131694	-2.349504

H	-0.304766	-2.110053	-1.914101
H	-0.811809	-3.231324	-0.639856
H	-1.674001	-3.971102	-2.875689
H	-3.040371	-3.518112	-1.825363
H	-2.491543	-2.405006	-3.105038

2aMA-1,2-inser

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C	-0.869817	4.015090	-2.106500
C	-0.708156	5.026299	-1.159275
C	-0.975719	4.709764	0.170195
N	-2.128445	1.159968	-0.058728
C	-3.337658	1.045744	0.779787
C	-3.011986	0.063769	1.898618
N	-1.997977	-0.855703	1.360482
C	-1.785281	-2.072339	2.092371
C	-2.675855	-3.147904	1.938278
C	-2.497597	-4.283221	2.733044
C	-1.466367	-4.381428	3.664815
C	-0.599235	-3.296411	3.799371
C	-0.743366	-2.140796	3.032577
C	-3.790039	-3.138469	0.930239
C	-1.275384	-5.629041	4.480844
C	0.231368	-1.012286	3.195628
C	-1.508808	1.725568	-2.863744
C	-0.281305	6.409868	-1.561472
C	-1.528874	3.163891	2.037303
P	-1.236334	-0.317104	-0.089069
C	-2.075941	-1.348288	-1.410315
C	-3.339121	-0.993167	-1.898281
C	-4.004835	-1.789715	-2.826349
C	-3.409857	-2.957934	-3.296720
C	-2.139593	-3.312664	-2.851571
C	-1.477254	-2.514936	-1.919381
S	0.188619	-2.988696	-1.399745
O	1.020243	-1.817376	-1.921005
Pd	1.078960	-0.112173	-0.545935
C	1.434043	1.551876	0.692265
O	0.512995	-4.231325	-2.093060
O	0.126328	-2.988817	0.072612
H	-3.811644	-0.073406	-1.561657
H	-4.990900	-1.491719	-3.184731
H	-3.928161	-3.586574	-4.021856
H	-1.633803	-4.206962	-3.217297
H	-3.187694	-5.121046	2.609561
H	0.214899	-3.348590	4.525750
H	-0.650113	4.227218	-3.155297
H	-0.818392	5.466950	0.942041
H	-4.183403	0.664397	0.183564
H	-3.627587	2.032352	1.158315
H	-2.632483	0.577153	2.801451
H	-3.909332	-0.503786	2.194880
H	-4.636856	-3.744004	1.283979
H	-3.442182	-3.568657	-0.024061
H	-4.153524	-2.127498	0.709557
H	-0.269445	-0.034970	3.160368
H	0.976748	-1.033568	2.385463
H	0.763481	-1.091344	4.153721
H	-0.894738	-5.395044	5.485093
H	-0.548520	-6.298564	3.993022
H	-2.218407	-6.181744	4.591832
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H	-2.547045	3.349938	2.417210
H	-0.850348	3.819502	2.600965

H	-1.300020	2.177853	-3.842577
H	-2.534122	1.331529	-2.878827
H	-0.835452	0.862306	-2.749091
H	0.192310	6.941047	-0.724455
H	-1.152571	7.002981	-1.884339
H	0.431077	6.382209	-2.397721
C	2.734078	1.425599	0.124388
C	3.196500	-0.118312	-1.383853
H	3.015855	2.162499	-0.630249
C	3.912675	1.042597	0.966146
H	4.129839	0.445750	-1.351213
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H	3.328846	-1.147445	-1.029692
H	1.294923	1.251512	1.732922
H	0.825593	2.388275	0.341817
O	3.564968	0.317735	2.054988
O	5.055009	1.375450	0.699735
C	4.681335	-0.045669	2.905976
H	4.243799	-0.635947	3.715502
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H	5.409960	-0.635956	2.337953

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C	1.077267	-4.081201	2.240925
C	0.859940	-5.056549	1.266206
C	0.892822	-4.652534	-0.065773
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C	3.229367	-1.063118	-0.703492
C	2.912473	-0.059099	-1.809395
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C	1.582812	1.986403	-2.114087
C	2.329416	3.173146	-2.048405
C	2.065608	4.180729	-2.979928
C	1.089845	4.045234	-3.965355
C	0.364398	2.853957	-4.009416
C	0.599630	1.818382	-3.105523
C	3.381327	3.405349	-1.005138
C	0.806395	5.157221	-4.935875
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C	1.659558	-1.785174	3.032200
C	0.637060	-6.495684	1.638013
C	1.145903	-2.985390	-1.897948
P	1.259319	0.399995	0.251226
C	2.208446	1.373600	1.540110
C	3.447913	0.900090	1.989581
C	4.198603	1.606828	2.925341
C	3.711520	2.801558	3.447342
C	2.468782	3.276169	3.037363
C	1.719209	2.573168	2.094116
S	0.113699	3.270291	1.606536
O	-0.867031	2.213235	2.100674
Pd	-0.954809	0.500675	0.767967
C	-1.766279	-1.131481	-0.200466
O	-0.029121	4.528533	2.333092
O	0.179932	3.308622	0.135075
H	3.830657	-0.047550	1.620310
H	5.162872	1.214384	3.250353
H	4.292689	3.360117	4.181938
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H	2.645026	5.105333	-2.926047
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H        3.819798     0.495697    -2.102096
H        4.210982     3.998654    -1.415967
H        2.947863     3.964380    -0.159735
H        3.783864     2.468815    -0.599490
H        0.418877    -0.251339    -3.710973
H       -0.483473     0.174510    -2.240023
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H        0.037109     5.834241    -4.530440
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H        0.895724    -1.928489    -2.043285
H        2.101760    -3.181033    -2.412583
H        0.379960    -3.590478    -2.403962
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H        2.693448    -1.413286     3.017163
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H        0.093183    -7.034273     0.849919
H        1.604788    -7.004660     1.781925
H        0.070663    -6.589416     2.574845
C       -3.107316    -0.449026    -0.024157
C       -3.644780     0.219132    -1.289073
C       -4.158652    -1.372784     0.598967
H       -2.997934     0.362653     0.778962
H       -4.548600     0.806183    -1.072180
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H       -3.908809    -0.551300    -2.027041
H       -1.495272    -1.316928    -1.245961
H       -1.585869    -2.009485     0.436706
O       -5.085870    -1.856454    -0.019281
O       -3.922734    -1.567777     1.915661
C       -4.900180    -2.414783     2.576880
H       -4.586605    -2.448654     3.623518
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C        0.326122    -4.906801     1.321425
C        0.631181    -4.663595    -0.012868
N        1.916614    -1.149782     0.052070
C        3.188764    -1.171997    -0.697839
C        3.381658     0.222056    -1.332668
N        2.080707     0.900322    -1.290412
C        1.778752     1.893955    -2.282732
C        2.000168     3.263742    -2.049795
C        1.714567     4.171158    -3.076620
C        1.248344     3.766222    -4.325133
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C        1.345116     1.457309    -3.552783
C        2.535090     3.790542    -0.752980
C        0.925367     4.766779    -5.399121
C        1.220285     0.000399    -3.884999
C        1.130740    -1.540191     2.877963
C       -0.118683    -6.265252     1.785750
C        1.319087    -3.286733    -1.944749
P        1.203031     0.419341     0.100384
C        2.083659     1.280405     1.511961
C        3.396728     0.878939     1.813615
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C	1.533976	2.335551	2.274183
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O	-0.969827	1.612931	2.184479
Pd	-1.020656	0.656190	0.229600
C	-1.408025	-0.297556	-1.565964
O	-0.426029	3.744954	3.311140
O	-0.285909	3.571857	0.811943
H	3.827461	0.013627	1.319287
H	5.177787	1.183331	2.980612
H	4.203954	3.100098	4.257324
H	1.832963	3.766627	3.830072
H	1.876755	5.234524	-2.886247
H	0.743101	2.050648	-5.524829
H	0.225188	-3.993841	3.265697
H	0.491512	-5.460355	-0.747582
H	4.031607	-1.424995	-0.031241
H	3.158817	-1.937726	-1.481291
H	3.708524	0.138369	-2.379562
H	4.151347	0.800322	-0.789521
H	3.120804	4.704079	-0.928450
H	1.699905	4.038050	-0.077362
H	3.175428	3.060939	-0.240837
H	0.949860	-0.576325	-2.998392
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H	2.173207	-0.400715	-4.272155
H	1.044100	4.329295	-6.400208
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H	1.575894	5.649673	-5.330928
H	1.192115	-2.255230	-2.284892
H	2.326794	-3.621130	-2.246328
H	0.598246	-3.912195	-2.490739
H	0.924658	-1.962406	3.870982
H	2.148268	-1.126638	2.887824
H	0.435999	-0.697004	2.734227
H	-0.478207	-6.875226	0.945644
H	0.719502	-6.805452	2.255691
H	-0.926020	-6.193237	2.528193
C	-2.865178	-0.782853	-1.492785
C	-3.004639	-2.114810	-0.728567
H	-3.278357	-0.921322	-2.509611
C	-3.678298	0.258938	-0.780495
H	-4.055925	-2.436695	-0.676585
H	-2.423185	-2.891857	-1.245814
H	-2.604755	-2.017814	0.292367
H	-1.278423	0.482414	-2.334273
H	-0.744746	-1.147191	-1.774085
O	-4.941842	0.390651	-1.186626
O	-3.213867	0.932883	0.150441
C	-5.715688	1.397397	-0.463876
H	-6.698982	1.390869	-0.940592
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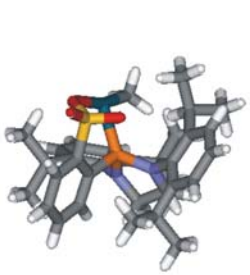

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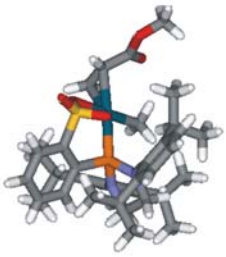

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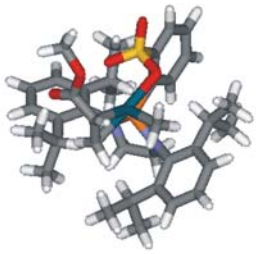

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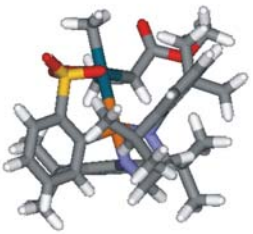

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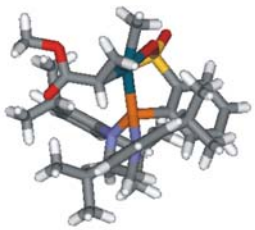

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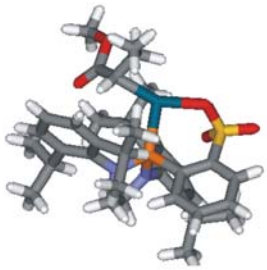

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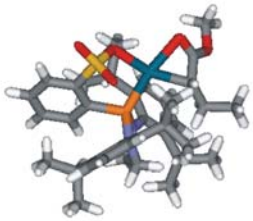

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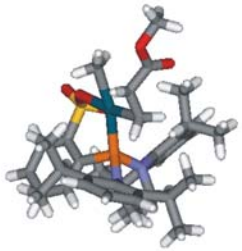

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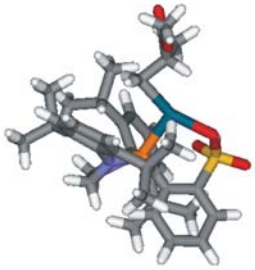

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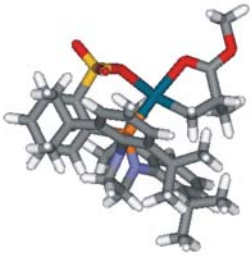

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C	0.920583	-4.008557	2.094230
C	0.897577	-5.057663	1.188882
C	1.272066	-4.813313	-0.124197
N	2.232025	-1.181816	0.004681
C	3.472486	-1.030534	-0.785403
C	3.136852	-0.102165	-1.943831

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C	1.970796	2.084713	-2.151049
C	2.954428	3.092982	-2.044849
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H	3.833110	-2.006253	-1.117618
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H	2.039781	-2.339340	-2.280042
C	3.273485	-4.106362	-2.441212
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C	0.102969	-1.616276	3.648968
C	2.607630	-1.957994	3.756119
H	1.548291	-0.700436	2.398320
H	0.139769	-0.755572	4.332997
H	-0.767966	-1.488828	2.988982
H	-0.054799	-2.521000	4.256546
H	2.688828	-1.167677	4.518632
H	2.494212	-2.926430	4.270521
H	3.547252	-1.994526	3.183538
H	1.005419	-3.686879	-3.976191
H	0.764908	-5.052050	-2.869670
H	-0.154570	-3.548615	-2.624704
H	3.516207	-3.906749	-3.496907
H	4.129318	-3.797207	-1.822432
H	3.171242	-5.196278	-2.317819
H	5.089300	3.984604	0.550023
H	4.450730	5.095646	-0.684358
H	3.325690	4.256053	0.411287
H	6.330480	2.708510	-1.300301
H	5.430347	2.043043	-2.694120
H	5.645419	3.795354	-2.532974
H	-2.301910	0.853005	-3.070792

H	-1.654838	2.193265	-2.063656
H	-1.857250	2.398977	-3.821121
H	-0.737520	-0.325901	-4.747906
H	-0.209328	1.230605	-5.434812
H	1.000166	0.097694	-4.793732
H	-2.065455	-1.241245	-1.311344
H	-0.344263	-1.593292	-1.711710
H	-1.081699	-2.371678	-0.262092

2bMA-cis

E= -20.96104395 a.u.

C	1.746584	-3.597843	-0.423820
C	1.763267	-2.527063	0.514204
C	1.354732	-2.771105	1.849244
C	0.959942	-4.061935	2.216042
C	0.990212	-5.119474	1.319523
C	1.388339	-4.875964	0.013809
N	2.233838	-1.216430	0.124362
C	3.522368	-1.066794	-0.583574
C	3.258977	-0.178274	-1.789474
N	2.199401	0.761995	-1.385752
C	2.093394	1.978043	-2.156235
C	3.103227	2.958949	-2.035891
C	3.051598	4.081013	-2.868372
C	2.031811	4.247104	-3.795071
C	1.041411	3.278752	-3.899181
C	1.052970	2.136367	-3.096813
C	4.256062	2.856033	-1.053305
H	2.004834	5.132107	-4.431838
C	-0.038332	1.103374	-3.287558
C	1.405311	-1.726040	2.948698
H	0.700398	-6.122831	1.633436
C	2.069021	-3.461451	-1.905663
P	1.333981	0.252162	0.020402
C	1.989341	1.363938	1.382966
C	3.198292	1.063378	2.024769
C	3.707515	1.881880	3.028754
C	3.006965	3.018417	3.424078
C	1.792499	3.324361	2.818456
C	1.285309	2.506933	1.808614
S	-0.316873	2.935689	1.085854
O	-1.215318	1.821675	1.601384
Pd	-1.026209	0.078962	0.206828
C	-0.972302	-1.596199	-1.016718
O	-0.683411	4.245039	1.613916
O	-0.093226	2.799906	-0.370783
H	3.742071	0.160237	1.759865
H	4.653429	1.622712	3.506075
H	3.401866	3.664507	4.209170
H	1.214158	4.201993	3.109574
H	3.824683	4.844848	-2.779805
H	0.237097	3.412665	-4.622491
H	0.644271	-4.244504	3.242391
H	1.393926	-5.697827	-0.701999
H	4.270353	-0.587792	0.070486
H	3.915351	-2.047113	-0.863710
H	2.942146	-0.760192	-2.673646
H	4.166442	0.377382	-2.063794
C	4.273546	4.045773	-0.083621
H	4.102690	1.952823	-0.446179
C	5.608838	2.734384	-1.774211
C	0.234873	0.233436	-4.523916
H	-0.027041	0.448789	-2.409750
C	-1.435588	1.732715	-3.357895
H	2.128491	-2.393886	-2.143531
C	3.408453	-4.129758	-2.267370
C	0.963400	-4.044217	-2.803425

C	0.205890	-1.785355	3.903464
C	2.718643	-1.865842	3.734918
H	1.390997	-0.728416	2.497486
H	-1.938123	-1.610586	-1.539273
H	-0.137790	-1.532813	-1.723744
H	-0.862794	-2.479293	-0.372426
C	-2.770283	-0.823576	1.348077
C	-3.342946	0.081244	0.486315
H	-3.441966	1.133367	0.763319
C	-4.104379	-0.380354	-0.701046
H	-2.851431	-1.892640	1.140570
H	-2.449208	-0.503784	2.340204
O	-4.684743	0.680273	-1.323577
O	-4.221044	-1.536750	-1.072554
C	-5.504478	0.322839	-2.461970
H	-5.880293	1.271700	-2.854078
H	-4.903064	-0.204022	-3.212242
H	-6.328791	-0.326285	-2.140565
H	2.808347	-1.062011	4.482393
H	2.745154	-2.835949	4.258652
H	3.592736	-1.828256	3.067598
H	0.200732	-0.893524	4.547544
H	-0.742310	-1.819051	3.349644
H	0.248493	-2.666357	4.562464
H	3.664691	-3.936157	-3.320967
H	4.244043	-3.787618	-1.638461
H	3.335413	-5.220742	-2.132829
H	1.170851	-3.792968	-3.855477
H	0.922522	-5.141564	-2.729554
H	-0.026485	-3.647523	-2.538450
H	5.057489	3.904622	0.677072
H	4.484564	4.986945	-0.615677
H	3.303699	4.153290	0.423748
H	6.419363	2.575748	-1.045360
H	5.621776	1.903789	-2.497160
H	5.835570	3.655826	-2.333666
H	-2.201690	0.942709	-3.331780
H	-1.597064	2.412517	-2.509274
H	-1.580452	2.296919	-4.292883
H	-0.536983	-0.546217	-4.624505
H	0.223530	0.847622	-5.439402
H	1.219612	-0.254876	-4.465199

2bMA-isom

E= -20,935103 a.u.

Pd	0.170544	0.093200	0.006014
P	0.082321	0.105209	3.032991
N	1.038485	0.043552	4.503979
N	-0.721063	-1.357853	3.490861
C	0.795032	-1.146616	5.332021
C	-0.562269	-1.699445	4.911760
H	-0.609834	-2.787324	5.042045
H	-1.371492	-1.266027	5.524682
H	1.590743	-1.900333	5.180367
H	0.795621	-0.873056	6.400910
C	2.220504	0.808142	4.811373
C	-1.266214	-2.309754	2.564662
C	3.462986	0.527865	4.194150
C	3.657334	-0.585174	3.180459
C	4.590524	1.258883	4.583585
H	5.549396	1.052076	4.109134
C	4.522192	2.232472	5.570831
H	5.415297	2.788439	5.858810
C	3.307529	2.482449	6.193638
C	2.151699	1.784258	5.835131
C	0.874468	2.086002	6.591043
C	-0.551284	-3.495248	2.260490

C	0.783576	-3.840318	2.898417
C	-1.120017	-4.418604	1.377066
C	-2.358127	-4.190911	0.792369
H	-2.782752	-4.920730	0.101557
C	-3.058982	-3.031483	1.104131
C	-2.542847	-2.083890	1.992402
C	-3.394413	-0.891889	2.393496
H	3.251532	3.236559	6.979490
H	-0.579979	-5.336946	1.143945
H	-4.036055	-2.862835	0.652630
C	-1.137015	1.501041	3.496462
C	-1.835003	1.459989	4.712278
H	-1.683078	0.623237	5.388569
C	-2.724877	2.460076	5.089874
H	-3.250834	2.386192	6.042813
C	-2.929945	3.556140	4.256565
H	-3.608672	4.357656	4.550575
C	-2.272565	3.617974	3.032884
H	-2.434146	4.446729	2.343491
C	-1.400273	2.596671	2.649627
S	-0.764714	2.685920	0.955775
O	0.694857	2.416729	1.003201
O	-1.201150	3.965843	0.410887
O	-1.469807	1.490539	0.305362
C	-1.111257	-0.952381	-1.217133
H	-1.374535	-0.235672	-2.005389
H	-0.659614	-1.872508	-1.605534
H	-1.943107	-1.158791	-0.535064
C	1.825975	-1.218971	-0.504085
C	1.629838	-0.311981	-1.547127
H	1.102066	-0.600481	-2.459125
H	1.467407	-2.244605	-0.601574
H	2.613761	-1.024887	0.225273
C	2.399305	0.960887	-1.621066
O	1.869141	1.758609	-2.581283
O	3.346320	1.255919	-0.915010
C	2.428633	3.096309	-2.608697
H	1.905756	3.605348	-3.423070
H	2.235089	3.587610	-1.646859
H	3.508726	3.049290	-2.793272
C	1.004483	1.741108	8.082971
C	0.435179	3.542531	6.396127
H	0.093547	1.447380	6.163846
C	4.431145	-0.111105	1.944973
C	4.378149	-1.778777	3.831803
H	2.661875	-0.921497	2.852300
C	0.621329	-4.958367	3.945323
C	1.850441	-4.253481	1.875904
H	1.153984	-2.938297	3.403349
C	-4.404554	-0.446698	1.332518
C	-4.118439	-1.202312	3.715306
H	-2.730554	-0.036558	2.569567
H	4.536066	-0.931742	1.218201
H	3.935728	0.733198	1.447390
H	5.452974	0.201710	2.210657
H	4.482386	-2.604515	3.110463
H	5.389487	-1.483626	4.156498
H	3.841530	-2.148333	4.718862
H	-0.518599	3.727163	6.915260
H	1.182954	4.240477	6.806011
H	0.301723	3.773465	5.327809
H	0.035611	1.873626	8.590550
H	1.336654	0.701501	8.230791
H	1.736347	2.395983	8.582230
H	-4.685662	-0.321720	4.055592
H	-4.821470	-2.040688	3.575573
H	-3.410134	-1.488395	4.505986
H	-4.890586	0.482113	1.666906
H	-3.918561	-0.233790	0.369666

H	-5.198399	-1.194404	1.177869
H	2.803234	-4.453055	2.390058
H	1.565706	-5.174760	1.344486
H	2.018499	-3.465963	1.130503
H	1.566503	-5.120316	4.487242
H	-0.167199	-4.733868	4.678720
H	0.343967	-5.905008	3.453644

2bMa-trans

E= -20.94548671 a.u.

C	1.247939	-3.338874	-0.825741
C	1.583029	-2.408820	0.200985
C	1.326009	-2.750334	1.553534
C	0.656834	-3.944816	1.843682
C	0.291672	-4.833859	0.845430
C	0.617585	-4.534901	-0.471696
N	2.169746	-1.130306	-0.114786
C	3.423188	-0.989575	-0.876882
C	3.202031	0.143123	-1.879675
N	2.196535	1.050373	-1.304168
C	1.893908	2.232790	-2.073201
C	2.664527	3.404256	-1.896882
C	2.435958	4.495897	-2.740620
C	1.482906	4.448522	-3.748023
C	0.722927	3.298452	-3.906518
C	0.901846	2.188414	-3.076764
C	3.726536	3.551966	-0.825943
H	1.321231	5.308937	-4.398448
C	-0.014410	1.000058	-3.277337
C	1.804583	-1.923577	2.731232
H	-0.225777	-5.762317	1.089771
C	1.594166	-3.145605	-2.295913
P	1.350952	0.383594	0.055571
C	2.212670	1.258671	1.492758
C	3.489768	0.879229	1.932164
C	4.104836	1.501987	3.014040
C	3.453439	2.532021	3.689268
C	2.191283	2.937026	3.269666
C	1.580612	2.307480	2.184043
S	-0.074534	2.847661	1.708441
O	-0.963109	1.734079	2.223582
Pd	-1.216640	0.520510	0.312170
C	-1.825168	-1.325456	-0.836699
O	-0.297582	4.145324	2.333237
O	-0.061752	2.796809	0.209233
H	4.017085	0.066105	1.439151
H	5.096135	1.175070	3.331130
H	3.928926	3.020251	4.540771
H	1.660708	3.749234	3.767223
H	3.016856	5.407401	-2.598679
H	-0.038888	3.264474	-4.684973
H	0.444158	-4.188246	2.885520
H	0.357613	-5.246681	-1.254596
H	4.268544	-0.751345	-0.210242
H	3.673093	-1.926770	-1.383528
H	2.846833	-0.251855	-2.849918
H	4.144284	0.686537	-2.062980
C	-2.975948	-1.284120	-1.773147
H	-0.891612	-1.693186	-1.263805
C	-2.045042	-1.442304	0.542617
C	-3.163557	1.231403	0.466124
H	-1.303788	-1.941381	1.170732
H	-3.072449	-1.411173	0.914380
H	-3.398211	1.244296	1.536383
H	-2.990581	2.243808	0.073997
H	-3.851914	0.634310	-0.139387
O	-2.561798	-1.597881	-3.039416

O	-4.140356	-1.055124	-1.493458
C	-3.613828	-1.573408	-4.033345
H	-3.127622	-1.844248	-4.975335
H	-4.400446	-2.291969	-3.773437
H	-4.050335	-0.568056	-4.096729
C	0.657887	-1.331267	3.559949
C	2.758385	-2.740367	3.619065
H	2.387474	-1.090347	2.333806
H	3.206292	-2.085505	4.382960
H	2.230245	-3.552470	4.143201
H	3.566780	-3.192314	3.023577
H	1.064675	-0.734059	4.391284
H	0.017446	-0.665082	2.962871
H	0.026102	-2.125936	3.990089
C	2.837762	-3.982515	-2.659204
C	0.454960	-3.516495	-3.258222
H	1.815424	-2.081974	-2.460839
H	0.751167	-3.264504	-4.288409
H	0.247597	-4.597340	-3.237341
H	-0.479785	-2.987058	-3.030152
H	3.169070	-3.765057	-3.686965
H	3.680331	-3.811696	-1.972503
H	2.592551	-5.055576	-2.600090
C	-1.478593	1.458938	-3.268540
C	0.311508	0.221840	-4.560507
H	0.128974	0.317028	-2.428074
H	-0.318742	-0.678242	-4.626900
H	0.125374	0.841606	-5.452712
H	1.367665	-0.088030	-4.588371
H	-2.144498	0.592603	-3.320843
H	-1.701959	2.033441	-2.357743
H	-1.701412	2.100383	-4.134599
C	5.116421	3.778476	-1.441158
C	3.375498	4.699199	0.135284
H	3.751311	2.620197	-0.243260
H	4.075094	4.713757	0.985670
H	3.443960	5.673454	-0.375876
H	2.350685	4.597711	0.520045
H	5.879797	3.840894	-0.649840
H	5.394009	2.970527	-2.135768
H	5.142908	4.724051	-2.006462

2bMA-2,1-inser

E= -20,92796908 a.u.

C	1.599121	-3.478923	-0.651076
C	1.675987	-2.444619	0.327783
C	1.280385	-2.726199	1.662889
C	0.783722	-3.995167	1.975494
C	0.713452	-5.006701	1.028507
C	1.139190	-4.741915	-0.264247
N	2.167950	-1.132575	-0.010703
C	3.435101	-0.966709	-0.751023
C	3.146710	-0.016068	-1.898257
N	2.134004	0.928846	-1.405107
C	1.984058	2.125838	-2.195188
C	2.967089	3.137051	-2.100940
C	2.891977	4.228109	-2.970454
C	1.874192	4.336284	-3.909403
C	0.912176	3.338690	-3.987414
C	0.950784	2.222478	-3.147635
C	4.104138	3.100690	-1.096252
H	1.829786	5.198062	-4.576423
C	-0.129092	1.173832	-3.297592
C	1.491700	-1.758293	2.813320
H	0.339030	-5.995133	1.297312
C	1.999061	-3.328861	-2.113357
P	1.275399	0.360209	-0.010958

C	2.079315	1.366168	1.374392
C	3.290246	0.965007	1.953370
C	3.898311	1.716121	2.956305
C	3.298507	2.885048	3.417287
C	2.082954	3.291349	2.876413
C	1.484471	2.541196	1.865773
S	-0.108408	3.073564	1.218216
O	-1.033888	1.968392	1.727493
Pd	-1.068059	0.099121	0.616123
C	-1.561045	-1.723155	-0.394404
O	-0.427927	4.356139	1.834854
O	0.055857	3.002309	-0.243470
H	3.756364	0.033058	1.645586
H	4.842410	1.375667	3.383801
H	3.770274	3.474577	4.204284
H	1.574534	4.192390	3.221675
H	3.644347	5.014469	-2.903713
H	0.110781	3.423179	-4.722105
H	0.475318	-4.203209	2.999622
H	1.088528	-5.532165	-1.012886
H	4.208771	-0.526830	-0.100018
H	3.809625	-1.934629	-1.092403
H	2.776833	-0.542977	-2.797998
H	4.056272	0.534173	-2.182249
C	4.060930	4.325595	-0.170025
H	3.967949	2.210853	-0.465675
C	5.475336	3.006294	-1.785518
C	-0.073168	0.496962	-4.675057
H	0.043153	0.393307	-2.543790
C	-1.510976	1.787238	-3.030690
H	2.110967	-2.261418	-2.330088
C	3.333000	-4.047010	-2.395433
C	0.930972	-3.844951	-3.090800
C	0.365724	-1.756185	3.853088
C	2.839583	-2.069147	3.487585
H	1.545417	-0.739707	2.419549
C	-2.384812	-1.810574	0.760015
C	-2.984375	0.023463	1.837948
H	-2.014834	-2.381422	1.614420
H	-3.458447	-1.855003	0.586514
H	-3.625423	-0.732184	2.294540
H	-2.431672	0.573660	2.606881
H	-3.555504	0.679510	1.170114
C	-2.187623	-1.533041	-1.728326
H	-0.640189	-2.307179	-0.437049
H	0.541614	-0.948229	4.579061
H	-0.612318	-1.577577	3.384067
H	0.317980	-2.700202	4.417457
H	3.061332	-1.323272	4.267181
H	2.809988	-3.067266	3.955658
H	3.662683	-2.073490	2.756743
H	1.257368	-3.639569	-4.122733
H	0.792275	-4.933204	-3.003791
H	-0.033180	-3.344440	-2.933874
H	3.685312	-3.821173	-3.414343
H	4.127000	-3.777190	-1.681954
H	3.195950	-5.138062	-2.319949
H	4.809686	4.224396	0.631550
H	4.284724	5.249054	-0.727835
H	3.066889	4.439396	0.285383
H	6.276997	2.931126	-1.033450
H	5.545366	2.136203	-2.456934
H	5.668555	3.904637	-2.393281
H	-2.280006	1.003596	-3.041732
H	-1.528408	2.298015	-2.057426
H	-1.772488	2.523665	-3.808231
H	-0.802826	-0.324585	-4.718369
H	-0.303700	1.215798	-5.478014
H	0.928291	0.084642	-4.874668

O	-3.485409	-1.126877	-1.642582
O	-1.631196	-1.763329	-2.790632
C	-4.186469	-1.083703	-2.908129
H	-5.207454	-0.779425	-2.659971
H	-3.719590	-0.356775	-3.582138
H	-4.172280	-2.074772	-3.379304

2bMA-2,1-KP

E= -20.96759175 a.u.

C	1.763376	-3.251822	-0.600204
C	1.851248	-2.303794	0.456091
C	1.468458	-2.686569	1.769861
C	0.882559	-3.938901	1.971243
C	0.727993	-4.842790	0.927587
C	1.200741	-4.504373	-0.330621
N	2.346492	-0.962423	0.244079
C	3.628531	-0.697403	-0.440464
C	3.356091	0.283474	-1.577037
N	2.182091	1.084465	-1.188275
C	1.839322	2.118374	-2.135358
C	2.617551	3.295841	-2.177554
C	2.395457	4.207488	-3.212538
C	1.426497	3.982316	-4.182597
C	0.648660	2.835432	-4.111192
C	0.835961	1.891652	-3.097121
C	3.657935	3.639962	-1.129056
H	1.266522	4.706894	-4.981909
C	-0.117399	0.720338	-3.032015
C	1.830542	-1.852768	2.988080
H	0.266599	-5.815888	1.101017
C	2.324769	-3.041196	-1.998950
P	1.382439	0.475443	0.211734
C	2.107239	1.514946	1.606577
C	3.275928	1.104511	2.260813
C	3.853857	1.870271	3.270660
C	3.264707	3.068986	3.659077
C	2.087517	3.485291	3.043689
C	1.510502	2.717814	2.032565
S	-0.048397	3.295056	1.316905
O	-1.025618	2.213581	1.769979
Pd	-0.898989	0.343295	0.694009
C	-1.682035	-1.556318	0.183712
O	-0.348500	4.582610	1.934279
O	0.174871	3.243710	-0.137467
H	3.735047	0.156567	2.001806
H	4.765071	1.518370	3.756115
H	3.710908	3.672518	4.450397
H	1.587221	4.407971	3.338469
H	2.986367	5.122911	-3.250327
H	-0.130327	2.666203	-4.855089
H	0.564182	-4.224270	2.972793
H	1.113218	-5.224435	-1.143258
H	4.347962	-0.246009	0.261672
H	4.067688	-1.629386	-0.802619
H	3.154131	-0.227043	-2.536454
H	4.226726	0.941835	-1.723761
C	-2.747136	-1.139592	1.151832
C	-2.791964	-1.892318	2.478782
H	-3.730049	-1.113702	0.656272
H	-2.641453	-0.012218	1.412700
H	-3.503264	-1.425294	3.174642
H	-3.106222	-2.932074	2.301971
H	-1.805002	-1.909963	2.955847
C	-2.057112	-1.793298	-1.231563
H	-0.982365	-2.329317	0.523479
O	-3.343449	-1.413009	-1.511516
O	-1.334040	-2.305849	-2.071396

C	-3.780557	-1.723713	-2.855414
H	-4.815848	-1.373205	-2.908351
H	-3.159367	-1.203875	-3.594249
H	-3.719405	-2.805303	-3.030742
C	5.066860	3.744087	-1.734005
C	3.289960	4.948970	-0.410998
H	3.655486	2.839945	-0.372967
H	3.966950	5.119071	0.440741
H	3.382356	5.809174	-1.093713
H	2.253484	4.918068	-0.047079
H	5.808221	3.950166	-0.946148
H	5.362503	2.823395	-2.260957
H	5.115240	4.568575	-2.463464
C	-1.515820	1.261063	-2.689569
C	-0.125401	-0.115733	-4.317525
H	0.200669	0.054755	-2.217406
H	-0.735128	-1.018669	-4.169446
H	-0.540899	0.450870	-5.165725
H	0.893563	-0.431213	-4.590919
H	-2.228116	0.447608	-2.507971
H	-1.472592	1.902879	-1.796044
H	-1.905770	1.874329	-3.518717
C	3.715057	-3.702095	-2.117151
C	1.432374	-3.580842	-3.125606
H	2.417767	-1.962920	-2.170245
H	4.190326	-3.433425	-3.074119
H	4.398473	-3.433239	-1.297563
H	3.605265	-4.798425	-2.088449
H	1.835525	-3.250169	-4.095605
H	1.426421	-4.681742	-3.141011
H	0.403318	-3.221380	-3.022391
H	1.722076	-0.789179	2.745881
C	0.969581	-2.110072	4.227461
C	3.307004	-2.124483	3.333516
H	1.225086	-1.377248	5.007203
H	-0.102719	-2.009857	4.011899
H	1.145890	-3.111785	4.649466
H	3.635995	-1.482910	4.166307
H	3.430645	-3.178404	3.634201
H	3.966161	-1.953646	2.469325

2bMA-2,1-TP

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C	1.964260	-3.669908	-0.325178
C	1.908919	-2.477275	0.466386
C	1.701584	-2.605032	1.867723
C	1.560604	-3.878091	2.430146
C	1.661720	-5.033885	1.676462
C	1.871988	-4.910560	0.312429
N	2.098520	-1.177315	-0.135404
C	3.117384	-0.949261	-1.184658
C	2.413329	-0.137304	-2.250982
N	1.609775	0.850381	-1.510949
C	1.490326	2.187710	-2.048128
C	2.632282	3.022489	-2.107391
C	2.512818	4.286036	-2.693573
C	1.304239	4.732648	-3.206814
C	0.193794	3.900641	-3.155333
C	0.263071	2.623304	-2.594920
C	4.002136	2.616167	-1.595328
H	1.227744	5.727245	-3.647771
C	-0.958749	1.728400	-2.670477
C	1.720819	-1.459292	2.864273
H	1.579590	-6.016196	2.142274
C	2.136084	-3.747630	-1.843253
P	1.168041	0.275984	0.058628
C	2.150674	1.390593	1.214626

C	3.492684	1.089933	1.487284
C	4.250202	1.876198	2.349308
C	3.678130	2.987609	2.961443
C	2.339539	3.286637	2.731186
C	1.574489	2.491908	1.876272
S	-0.201087	2.842242	1.775098
O	-0.769807	1.546888	2.360512
Pd	-0.961617	0.028450	0.836150
C	-1.863204	-1.345924	-0.522853
O	-0.452978	3.982218	2.651053
O	-0.496770	2.974083	0.340025
H	3.946392	0.200192	1.055949
H	5.289630	1.611126	2.546543
H	4.267070	3.612831	3.633856
H	1.847660	4.125294	3.225135
H	3.386897	4.935873	-2.736158
H	-0.752281	4.252028	-3.564905
H	1.401942	-3.954629	3.505203
H	1.942965	-5.813374	-0.292655
H	3.964883	-0.369400	-0.782811
H	3.518669	-1.888885	-1.555371
H	1.770889	-0.779067	-2.883174
H	3.124457	0.385014	-2.903156
C	0.535455	-1.476215	3.838343
C	3.053192	-1.451320	3.631258
H	1.653971	-0.506607	2.334630
C	-2.615027	-1.712626	0.674443
O	-2.990947	-0.797413	1.452582
O	-2.763849	-3.016684	0.953222
H	-2.401241	-0.570394	-1.090773
C	-1.232334	-2.409602	-1.376998
C	-3.321539	-3.309874	2.264277
H	-3.342217	-4.401580	2.323322
H	-2.679655	-2.887547	3.045630
H	-4.330447	-2.889502	2.347320
H	0.525250	-0.544704	4.423335
H	-0.418772	-1.539989	3.295982
H	0.594718	-2.319636	4.543967
H	3.123869	-0.551931	4.262687
H	3.130765	-2.340315	4.278806
H	3.912586	-1.467031	2.944135
C	1.168824	-4.742696	-2.510584
H	1.903607	-2.766669	-2.275318
C	3.572887	-4.159129	-2.226792
H	1.198292	-4.607230	-3.603200
H	1.456967	-5.784894	-2.307514
H	0.136865	-4.603983	-2.168253
H	3.709510	-4.123853	-3.319431
H	4.348429	-3.536361	-1.756400
H	3.759745	-5.192680	-1.894507
C	4.997214	2.387607	-2.746682
C	4.569412	3.645687	-0.609078
H	3.887405	1.674429	-1.045266
H	5.490540	3.258973	-0.145060
H	4.824679	4.586692	-1.120800
H	3.842787	3.874308	0.183802
H	5.954915	2.008085	-2.355459
H	4.619798	1.672606	-3.494013
H	5.199039	3.332525	-3.275719
C	-2.269044	2.476144	-2.396839
C	-1.008069	1.032513	-4.041673
H	-0.850435	0.957319	-1.897068
H	-1.878876	0.360447	-4.105642
H	-1.097552	1.781350	-4.846273
H	-0.095895	0.446803	-4.233069
H	-3.104179	1.761167	-2.332637
H	-2.208310	3.034675	-1.452647
H	-2.513076	3.177195	-3.210707
H	-0.467971	-1.948108	-2.021546

H	-0.722917	-3.141359	-0.732336
C	-2.279150	-3.113754	-2.256469
H	-1.810807	-3.868702	-2.905805
H	-3.032018	-3.617493	-1.632757
H	-2.797622	-2.390222	-2.904686

2bMA-1,2-inser

E= -20,93132191 a.u.

C	-1.588096	3.563359	0.537691
C	-1.623630	2.514446	-0.426757
C	-1.271952	2.803209	-1.769237
C	-0.972125	4.122905	-2.124937
C	-1.028520	5.162526	-1.208867
C	-1.327517	4.868985	0.114070
N	-2.075878	1.204581	-0.037219
C	-3.354470	1.068806	0.690038
C	-3.102957	0.106744	1.838612
N	-2.061905	-0.826707	1.382907
C	-1.905968	-2.001244	2.204483
C	-2.854597	-3.042667	2.101623
C	-2.779758	-4.108246	3.000829
C	-1.795229	-4.158893	3.979950
C	-0.865935	-3.131253	4.067019
C	-0.904954	-2.039575	3.195036
C	-3.948666	-3.059357	1.051372
H	-1.748979	-5.002343	4.670056
C	0.148389	-0.961193	3.341605
C	-1.252593	1.774035	-2.882926
H	-0.830395	6.188969	-1.519337
C	-1.775986	3.357783	2.034745
P	-1.243723	-0.314318	-0.049666
C	-2.084852	-1.284083	-1.432084
C	-3.271294	-0.826818	-2.021833
C	-3.909225	-1.551769	-3.025203
C	-3.358980	-2.746694	-3.481137
C	-2.162318	-3.203291	-2.938015
C	-1.533839	-2.482098	-1.923714
S	0.028804	-3.105150	-1.266938
O	1.018836	-2.038993	-1.728170
Pd	1.076293	-0.230378	-0.495487
C	1.463010	1.523380	0.591812
O	0.282432	-4.390140	-1.910871
O	-0.160553	-3.067085	0.194336
H	-3.694147	0.127952	-1.719460
H	-4.835822	-1.171503	-3.456953
H	-3.854058	-3.317449	-4.268011
H	-1.691796	-4.124587	-3.282960
H	-3.502720	-4.921099	2.924639
H	-0.088737	-3.175121	4.830852
H	-0.716910	4.340540	-3.162186
H	-1.335920	5.673454	0.850046
H	-4.136802	0.657559	0.031281
H	-3.700701	2.046288	1.034308
H	-2.770666	0.628003	2.755930
H	-4.021652	-0.447218	2.083078
C	-3.865094	-4.323376	0.181967
H	-3.789701	-2.197565	0.388523
C	-5.347237	-2.936513	1.678055
C	0.076147	-0.273089	4.712943
H	-0.052795	-0.200471	2.574153
C	1.547990	-1.538600	3.084455
H	-1.826347	2.279668	2.226900
C	-3.061679	4.021268	2.560370
C	-0.571242	3.886655	2.832733
C	0.066903	1.778963	-3.667371
C	-2.448427	1.980749	-3.825561
H	-1.348656	0.775268	-2.446595

C	2.724781	1.409546	-0.058318
C	3.187171	-0.325783	-1.343707
H	2.912968	2.070417	-0.907474
C	3.928279	1.160887	0.803771
H	1.431504	1.287561	1.659414
H	0.785020	2.303393	0.238247
O	3.918096	0.685625	1.922780
O	5.054252	1.582568	0.168041
H	0.075926	0.945537	-4.385675
H	0.926633	1.658541	-2.992023
H	0.203590	2.713226	-4.234288
H	-2.504363	1.161580	-4.559080
H	-2.350831	2.932612	-4.373159
H	-3.395425	2.017969	-3.266266
H	-0.687945	3.632527	3.897956
H	-0.493997	4.982214	2.758928
H	0.374565	3.457004	2.473949
H	-3.222352	3.767718	3.619937
H	-3.957291	3.724557	1.994113
H	-2.984986	5.117742	2.484804
H	-4.551140	-4.240512	-0.675770
H	-4.150989	-5.218034	0.758276
H	-2.842916	-4.475560	-0.192775
H	-6.116061	-2.894972	0.890164
H	-5.444409	-2.036931	2.305757
H	-5.565080	-3.806728	2.317716
H	2.307002	-0.743592	3.073854
H	1.571809	-2.070516	2.121737
H	1.819789	-2.260954	3.871884
H	0.826092	0.531002	4.778290
H	0.284285	-0.988325	5.524577
H	-0.920864	0.156861	4.896821
H	3.380259	-1.260839	-0.803916
H	4.092420	0.268683	-1.465524
H	2.685638	-0.476370	-2.307841
C	6.275992	1.371513	0.920226
H	7.077015	1.739292	0.273197
H	6.401500	0.303825	1.136506
H	6.239417	1.932627	1.861416

2bMA-1,2-KP

E= -20.96879131 a.u.

C	1.267009	-3.429461	-0.440719
C	1.470435	-2.409954	0.530019
C	1.219344	-2.693322	1.895240
C	0.849199	-3.991842	2.261002
C	0.736449	-5.013009	1.329078
C	0.936833	-4.718183	-0.012304
N	1.986467	-1.128985	0.122451
C	3.202721	-1.046243	-0.711021
C	2.944880	0.003100	-1.793903
N	1.890722	0.903170	-1.296192
C	1.507826	1.997374	-2.156866
C	2.156846	3.246577	-2.044313
C	1.761279	4.284940	-2.891540
C	0.772641	4.103063	-3.848720
C	0.188429	2.852225	-3.996575
C	0.548417	1.781735	-3.172744
C	3.312763	3.493430	-1.094700
H	0.465892	4.931997	-4.487906
C	-0.051219	0.419176	-3.467830
C	1.365046	-1.680171	3.014012
H	0.481802	-6.025952	1.642665
C	1.347285	-3.208190	-1.944366
P	1.235251	0.415222	0.219191
C	2.249778	1.335022	1.518256
C	3.463188	0.797998	1.972780

C	4.251363	1.464703	2.906533
C	3.834203	2.687615	3.423114
C	2.610415	3.217249	3.026165
C	1.818800	2.548781	2.091810
S	0.195232	3.263801	1.711199
O	-0.740624	2.210282	2.290966
Pd	-0.946616	0.572885	0.862308
C	-1.885265	-0.869212	-0.267030
O	0.116994	4.532126	2.430447
O	0.138380	3.293870	0.237066
H	3.786000	-0.179395	1.626234
H	5.188849	1.014932	3.236676
H	4.447678	3.217421	4.153037
H	2.233929	4.153636	3.438975
H	2.235412	5.261096	-2.791752
H	-0.565365	2.702967	-4.769681
H	0.671145	-4.208227	3.314568
H	0.812942	-5.506322	-0.755512
H	4.073400	-0.749227	-0.105116
H	3.431644	-2.024032	-1.143718
H	2.617000	-0.467342	-2.735929
H	3.866337	0.570589	-2.000982
C	-3.184968	-0.256791	0.218598
C	-3.834027	0.742960	-0.738424
C	-4.191952	-1.331071	0.643573
H	-2.970560	0.289932	1.200734
H	-4.716786	1.206454	-0.274574
H	-3.122910	1.538694	-0.997035
H	-4.160181	0.229156	-1.652738
H	-1.725675	-0.791723	-1.347211
H	-1.651614	-1.866252	0.131650
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O	-3.846176	-1.902734	1.817607
C	-4.763190	-2.939546	2.260576
H	-4.362549	-3.286298	3.216426
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H	3.935541	4.858816	0.474161
H	3.359663	5.679888	-0.989343
H	2.182397	4.921913	0.115465
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H	-1.817985	0.975289	-4.631922
C	2.508113	-3.985130	-2.590259
C	0.025705	-3.591617	-2.630862
H	1.493188	-2.136399	-2.127339
H	0.076379	-3.354656	-3.704822
H	-0.173538	-4.670538	-2.539077
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C	2.600186	-1.989362	3.874027
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H	3.507567	-2.073129	3.256416
H	0.195758	-0.748375	4.588234
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H	-0.060752	-2.505882	4.464341

2bMA-1,2-TP

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C	0.173539	-3.808612	1.993785
C	0.089783	-4.843977	1.076164
C	0.565154	-4.631168	-0.208899
N	1.882282	-1.117087	0.015949
C	3.208623	-1.067643	-0.639661
C	3.411838	0.372195	-1.164246
N	2.078464	0.978532	-1.268813
C	1.797415	2.008308	-2.239907
C	2.111369	3.363494	-1.990473
C	1.762022	4.316757	-2.952926
C	1.155225	3.954479	-4.146854
C	0.927863	2.611246	-4.419285
C	1.249292	1.620440	-3.487896
C	2.909749	3.814548	-0.783047
H	0.876081	4.717149	-4.875036
C	1.105163	0.163559	-3.889281
C	0.878763	-1.572181	2.801791
H	-0.345600	-5.803826	1.356140
C	1.533801	-3.307069	-2.067412
P	1.153257	0.448097	0.080588
C	2.018987	1.286500	1.524541
C	3.267582	0.806558	1.954194
C	4.013489	1.468816	2.925974
C	3.510462	2.623123	3.516012
C	2.245878	3.081472	3.158015
C	1.498714	2.427177	2.177504
S	-0.171836	3.077762	1.854032
O	-1.029718	1.844083	2.086213
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C	-1.505261	-0.488583	-1.414828
O	-0.397450	4.108786	2.864597
O	-0.170116	3.484906	0.438362
H	3.652726	-0.128144	1.558661
H	4.981268	1.067006	3.228397
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H	1.798420	3.949329	3.643293
H	1.970157	5.367536	-2.755510
H	0.490798	2.327442	-5.375944
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H	3.260608	-1.770007	-1.475202
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H	4.063162	0.944192	-0.479897
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C	2.828529	-4.103308	-2.318457
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C	-2.900960	-1.093195	-1.193760
C	-2.869094	-2.381592	-0.347320
H	-3.377085	-1.330623	-2.164481
C	-3.752588	-0.082267	-0.480639
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H	-2.260793	-3.140865	-0.859799
H	-2.406184	-2.188269	0.632322
H	-1.513954	0.258595	-2.224487
H	-0.775475	-1.277543	-1.637495

O	-5.060832	-0.139226	-0.732255
O	-3.277257	0.731313	0.325282
C	-5.868662	0.821449	0.016254
H	-6.893975	0.647755	-0.319175
H	-5.760707	0.635396	1.090642
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H	0.772981	-3.613684	-4.077025
H	0.254467	-4.867346	-2.938470
H	-0.504382	-3.256953	-2.882728
H	3.181214	-3.966213	-3.352979
H	3.636405	-3.814434	-1.629732
H	2.642647	-5.178181	-2.162494
C	-0.429616	-1.367873	3.575533
C	2.021335	-1.970898	3.749434
H	1.137844	-0.594932	2.387602
H	2.170738	-1.191685	4.513116
H	1.788292	-2.920431	4.259158
H	2.965857	-2.110469	3.201423
H	-0.314099	-0.529592	4.278287
H	-1.256552	-1.116841	2.895973
H	-0.708717	-2.261072	4.156294
C	4.405331	3.886938	-1.149498
C	2.452321	5.160215	-0.208122
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C	2.380536	-0.311190	-4.612933
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H	2.717157	5.995189	-0.876092
H	1.368637	5.163592	-0.032948
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MA
E= -2,563445 a.u.

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