Supplementary Materials: Dinuclear Gold Complexes Supported by Wide Bite Angle Diphosphines for Preorganization-Induced Selective Dual-Gold Catalysis

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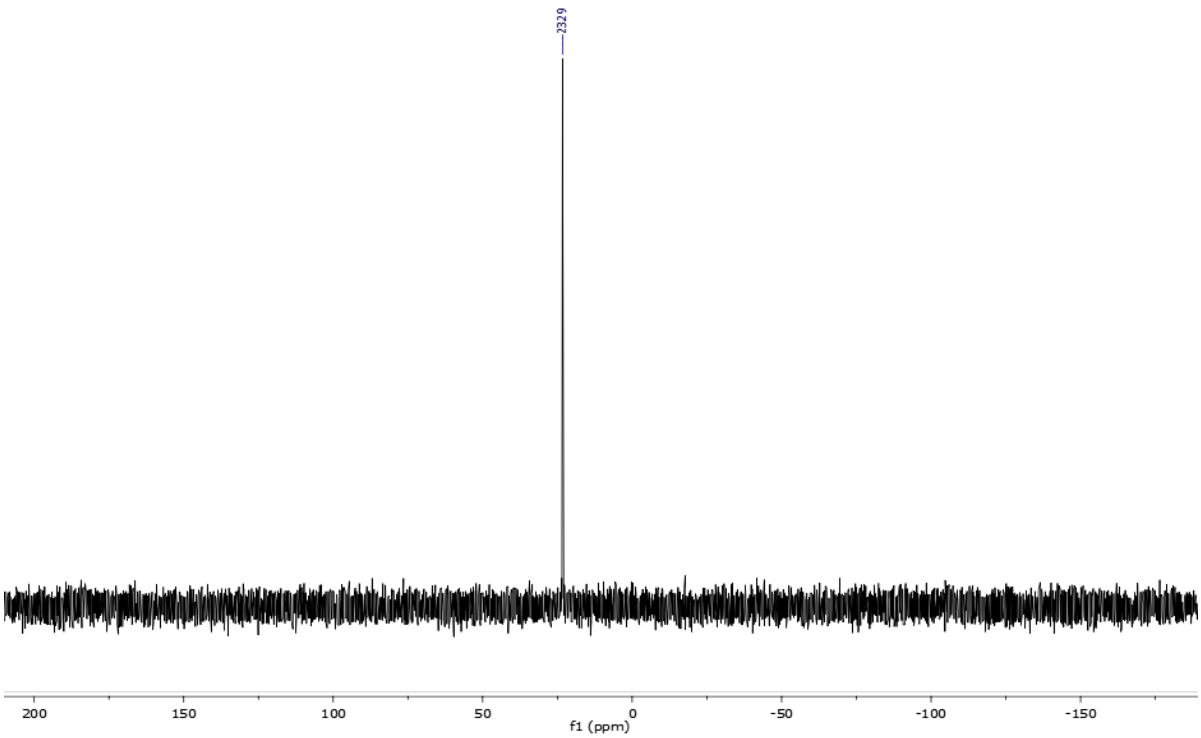

Figure S1. $^{31}P\{^{1}H\}$ NMR spectrum of complex **1** (CD_2Cl_2, 298 K, 202 MHz)

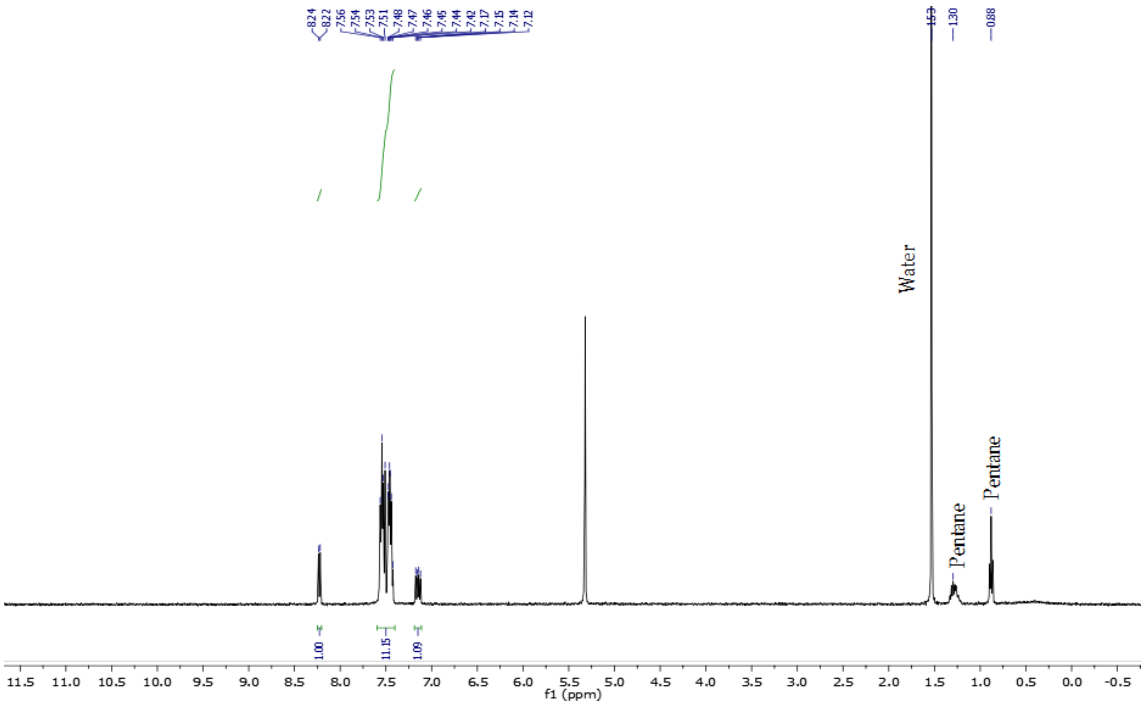

Figure S2. ^{1}H NMR spectrum of complex **1** (CD_2Cl_2, 298 K, 500 MHz)

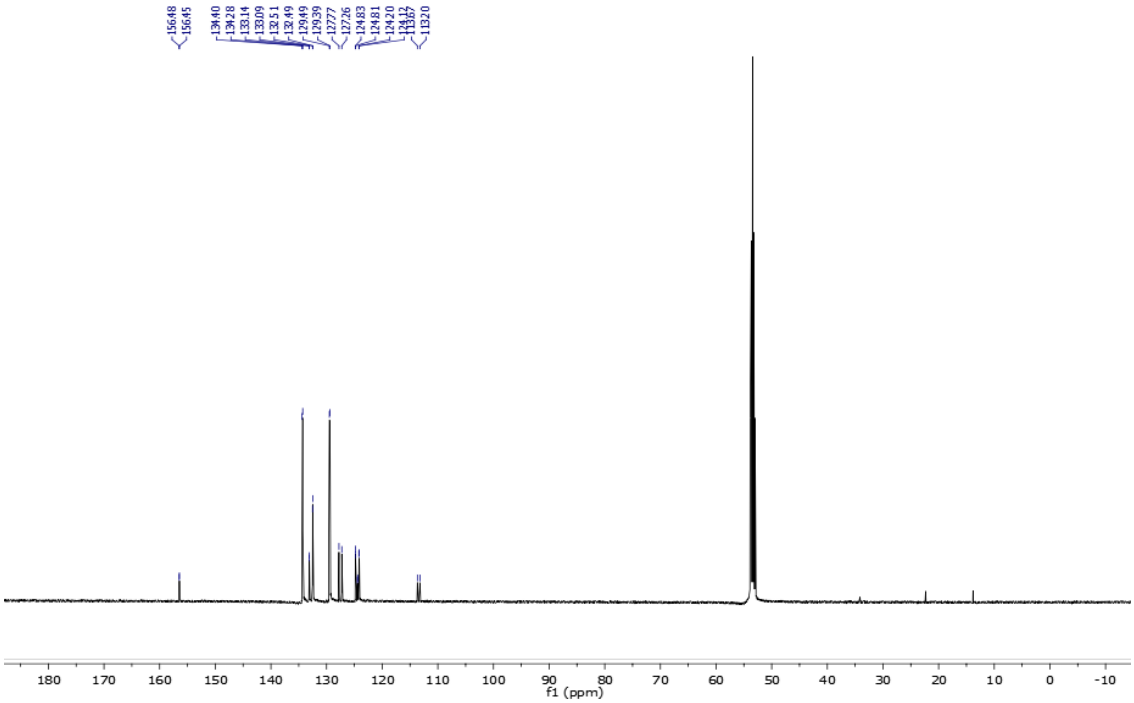

Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum of complex **1** (CD_2Cl_2, 298 K, 126 MHz)

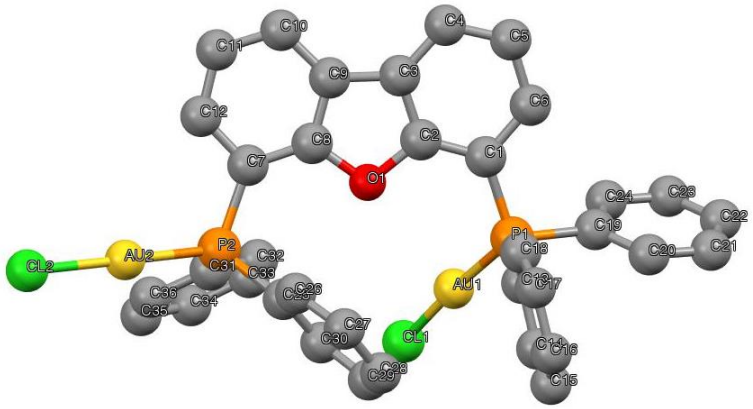

Figure S4. Connectivity plot of complex **1**

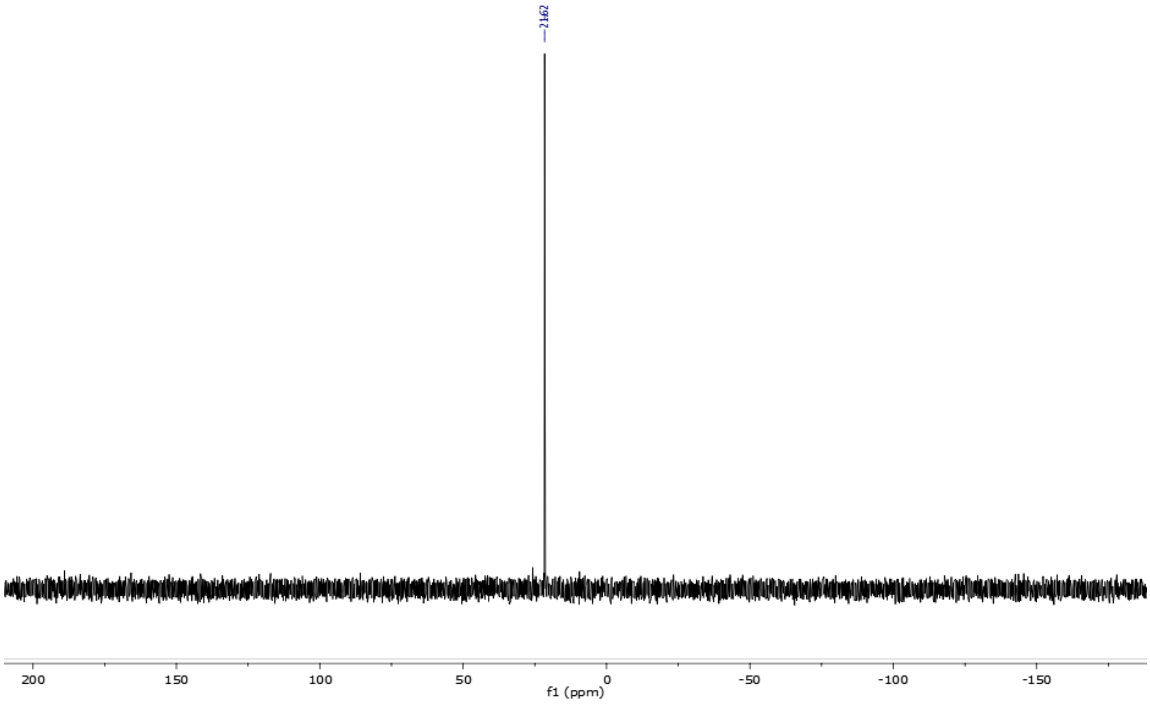

Figure S5. $^{31}P\{^{1}H\}$ NMR spectrum of complex **2** (CD_2Cl_2, 298 K, 162 MHz)

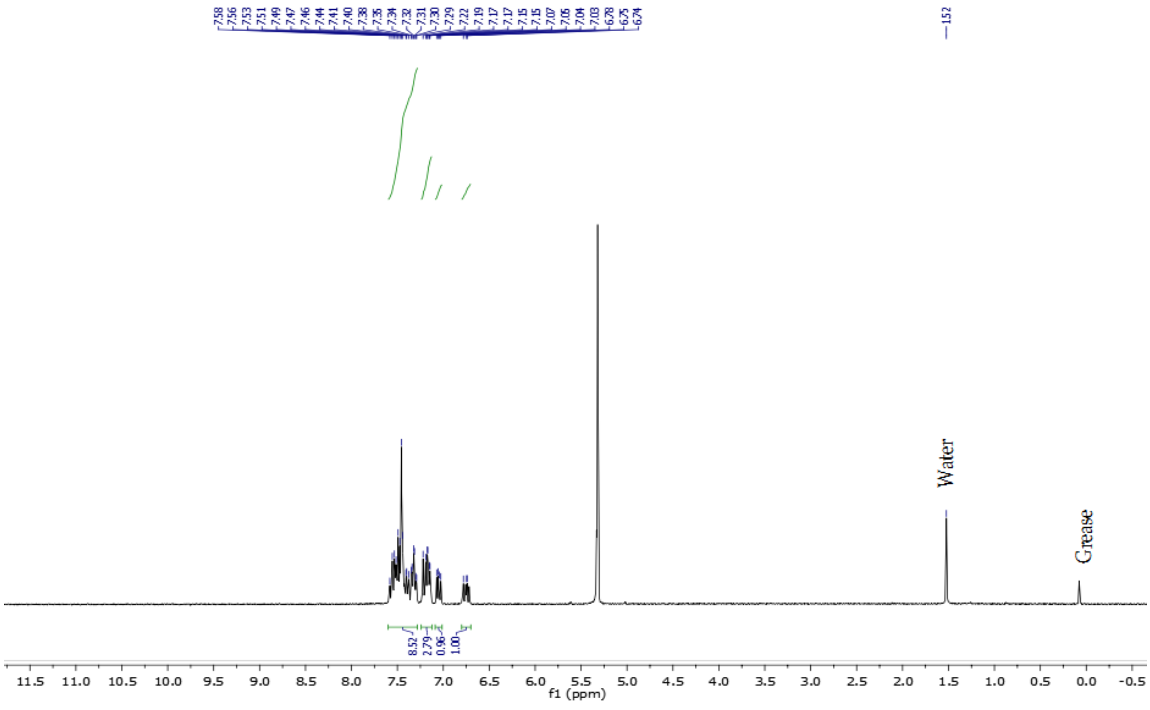

Figure S6. ^{1}H NMR spectrum of complex **2** (CD_2Cl_2, 298 K, 400 MHz)

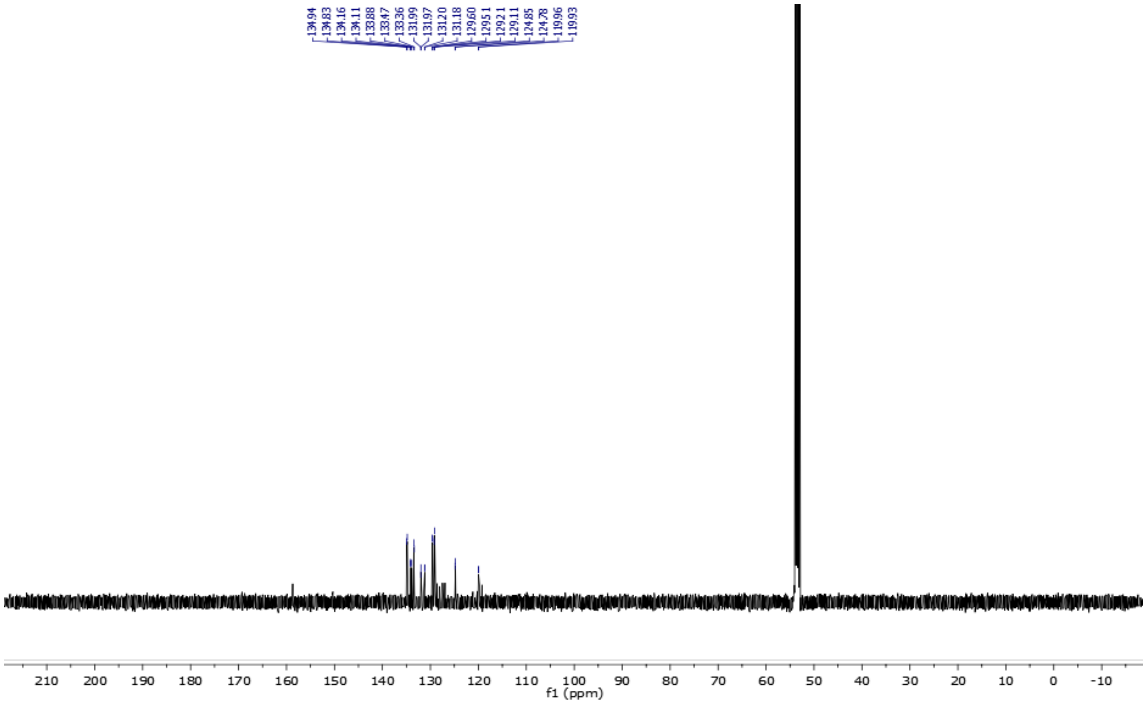

Figure S7. $^{13}C\{^{1}H\}$ NMR spectrum of complex **2** (CD_2Cl_2, 298 K, 101 MHz)

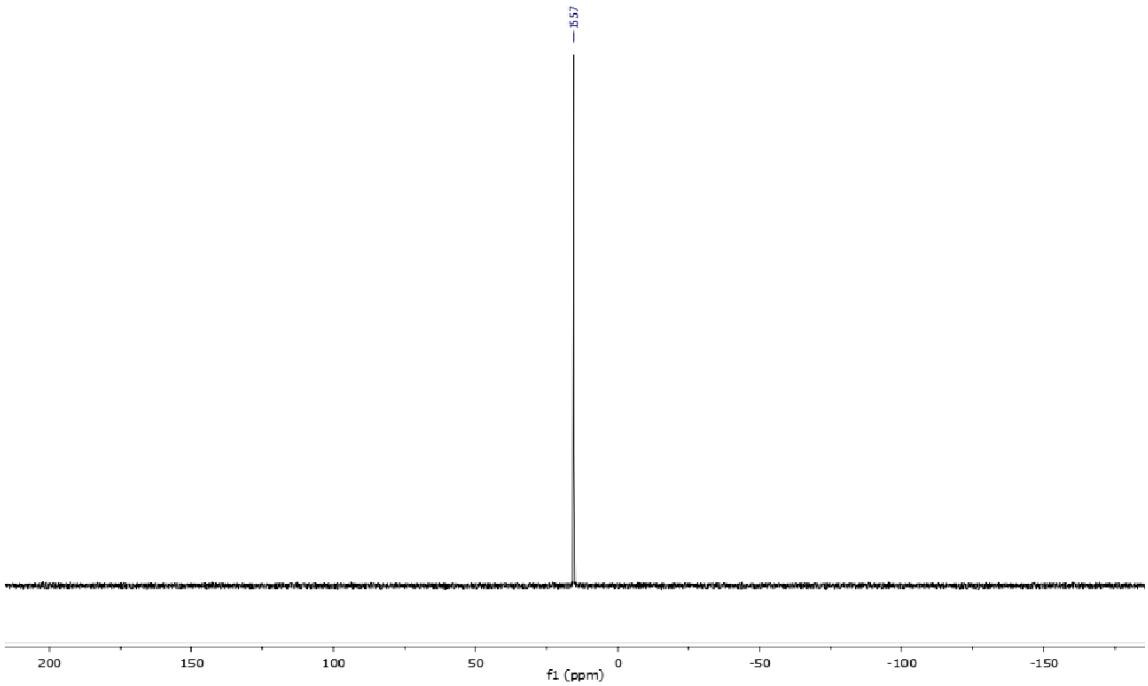

Figure S8. $^{31}P\{^{1}H\}$ NMR spectrum of complex **3** (CD_2Cl_2, 298 K, 121 MHz)

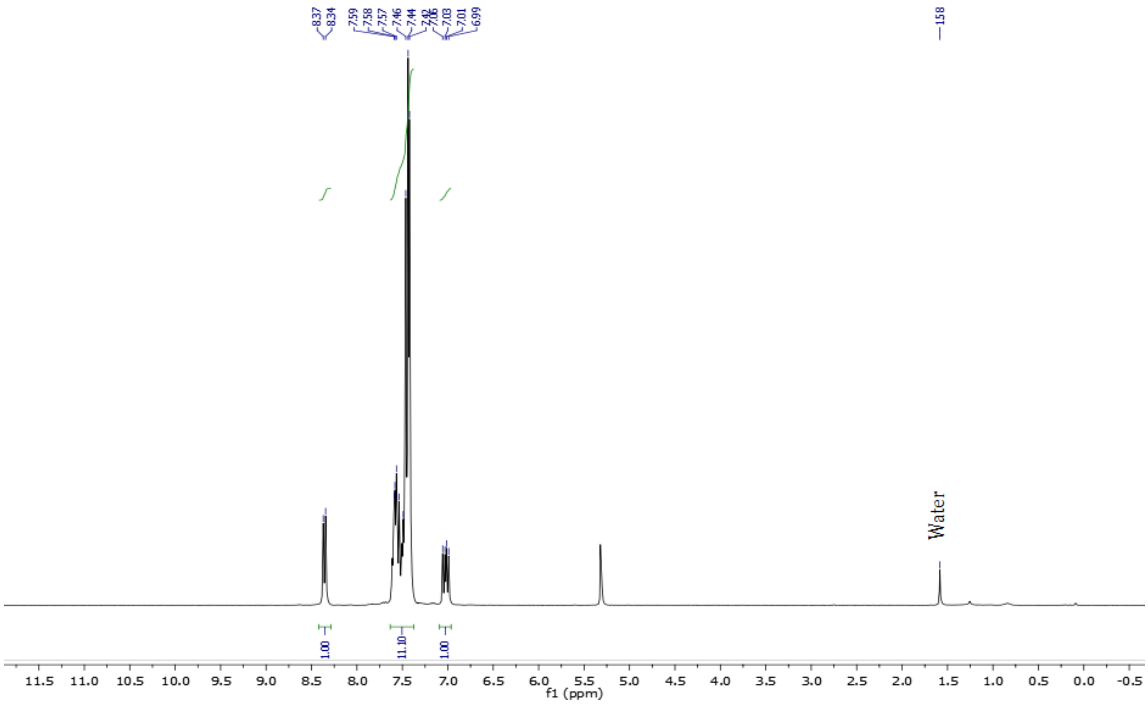

Figure S9. ^{1}H NMR spectrum of complex **3** (CD_2Cl_2, 298 K, 300 MHz)

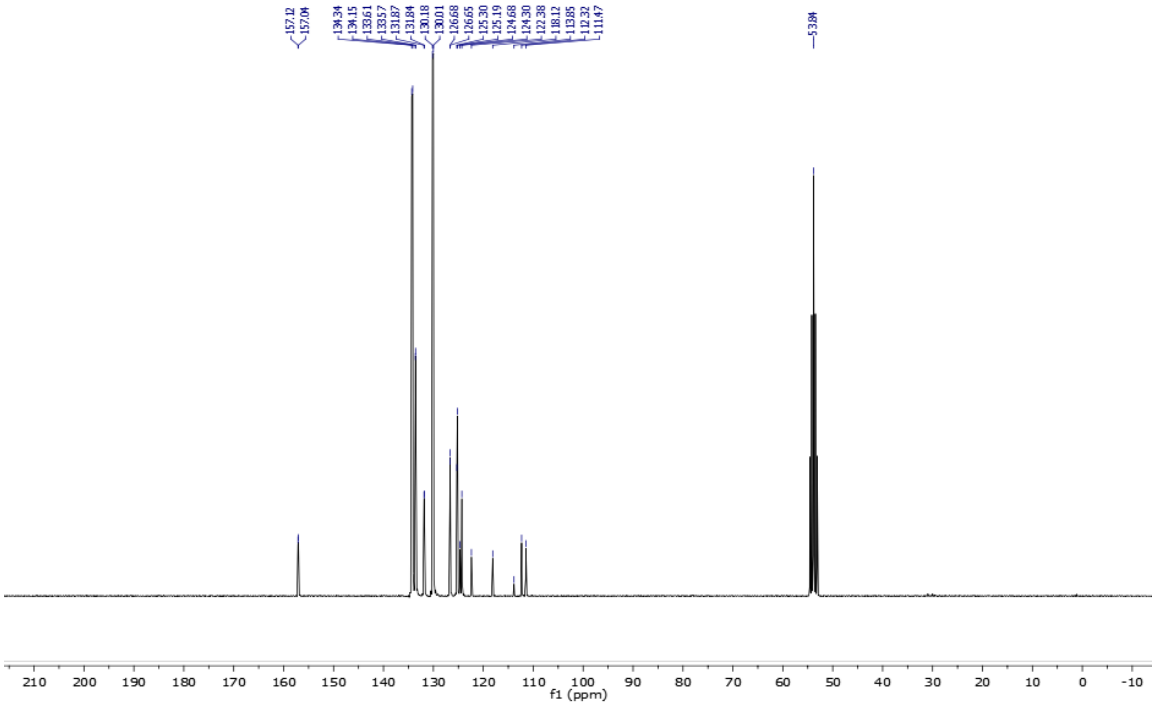

Figure S10. $^{13}C\{^{1}H\}$ NMR spectrum of complex **3** (CD_2Cl_2, 298 K, 75 MHz)

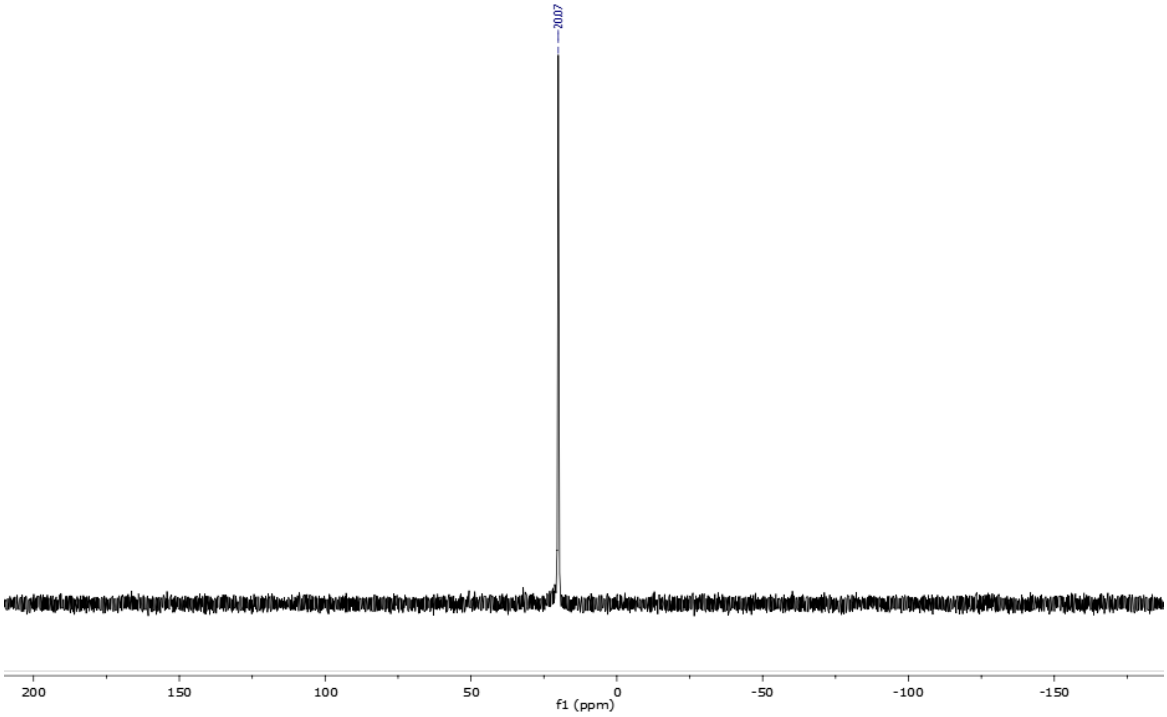

Figure S11. $^{31}P\{^{1}H\}$ NMR spectrum of complex **4** (CD_2Cl_2, 298 K, 121 MHz)

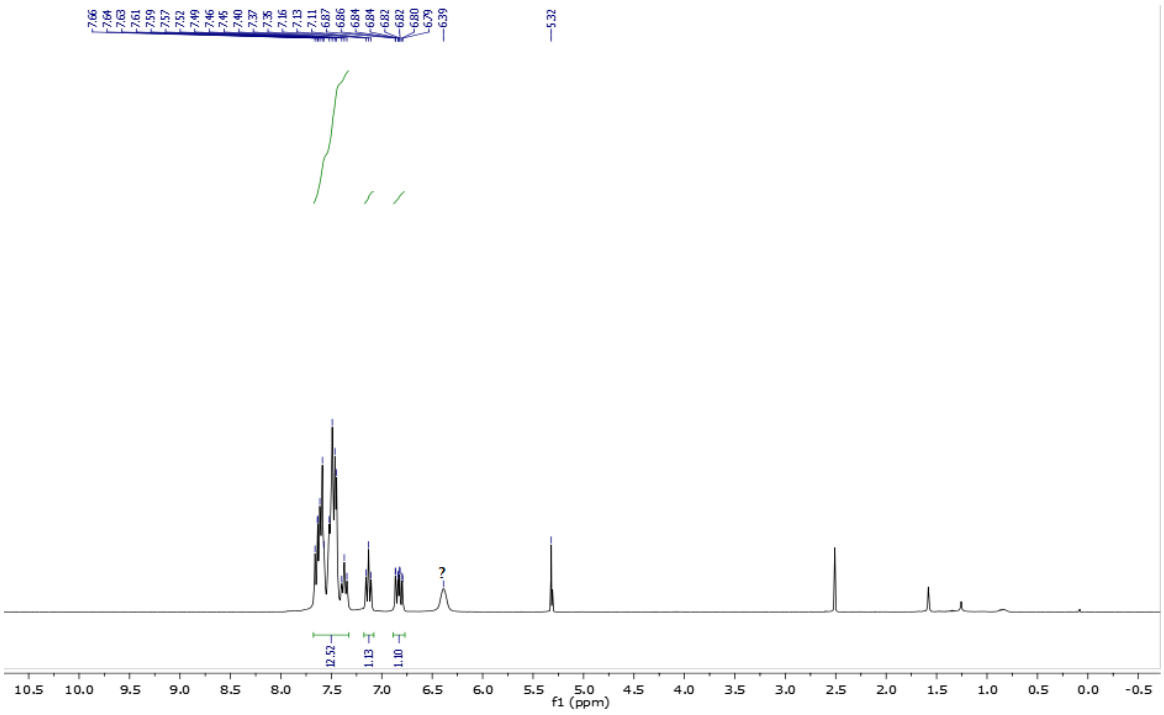

Figure S12. ^{1}H NMR spectrum of complex **4** (CD_2Cl_2, 298 K, 300 MHz)

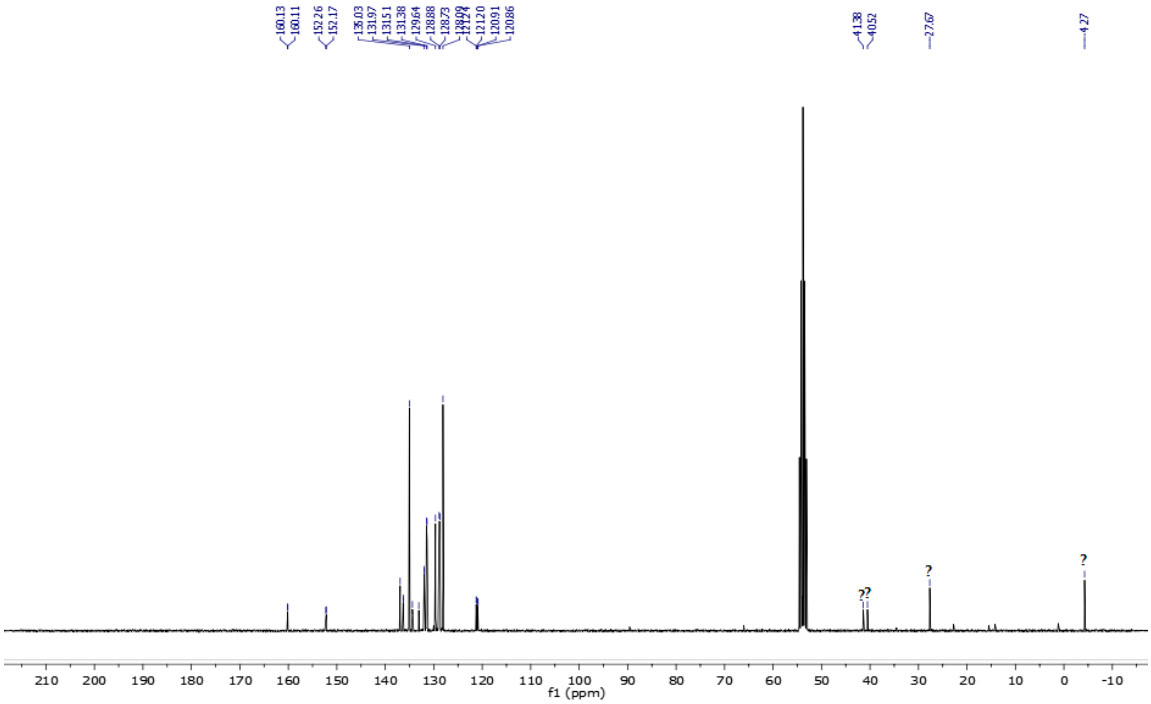

Figure S13. $^{13}C\{^{1}H\}$ NMR spectrum of complex **4** (CD_2Cl_2, 298 K, 75 MHz)

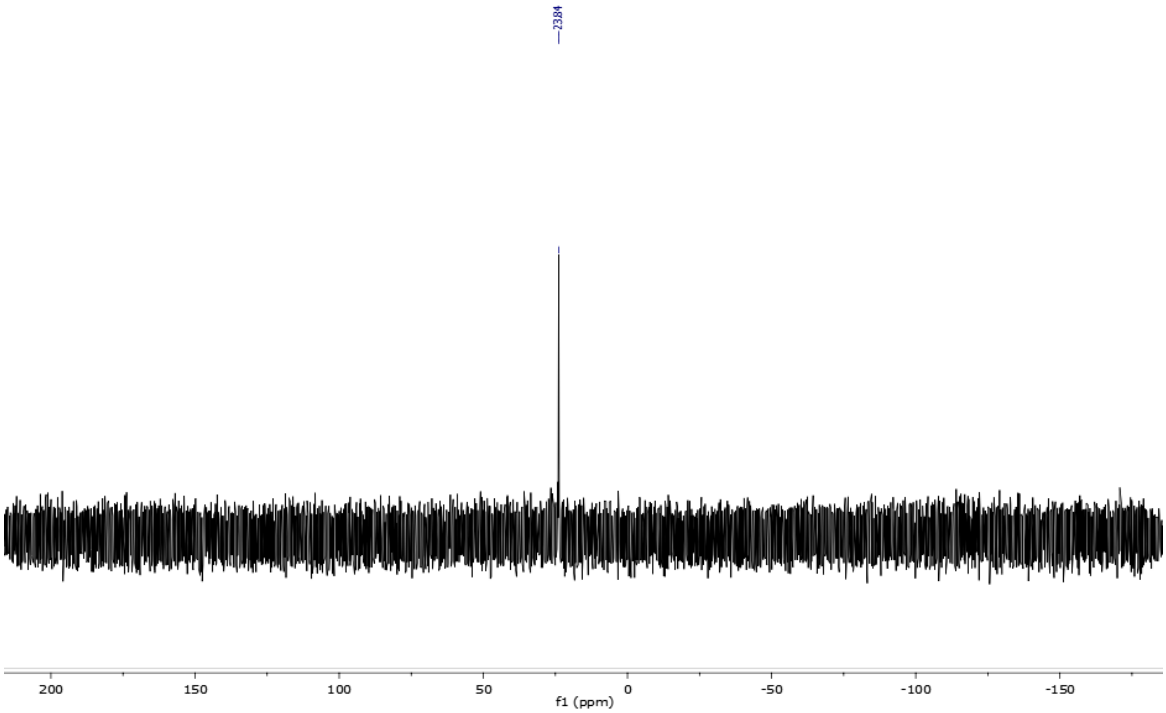

Figure S14. $^{31}P\{^{1}H\}$ NMR spectrum of complex **5** (CD_2Cl_2, 298 K, 162 MHz)

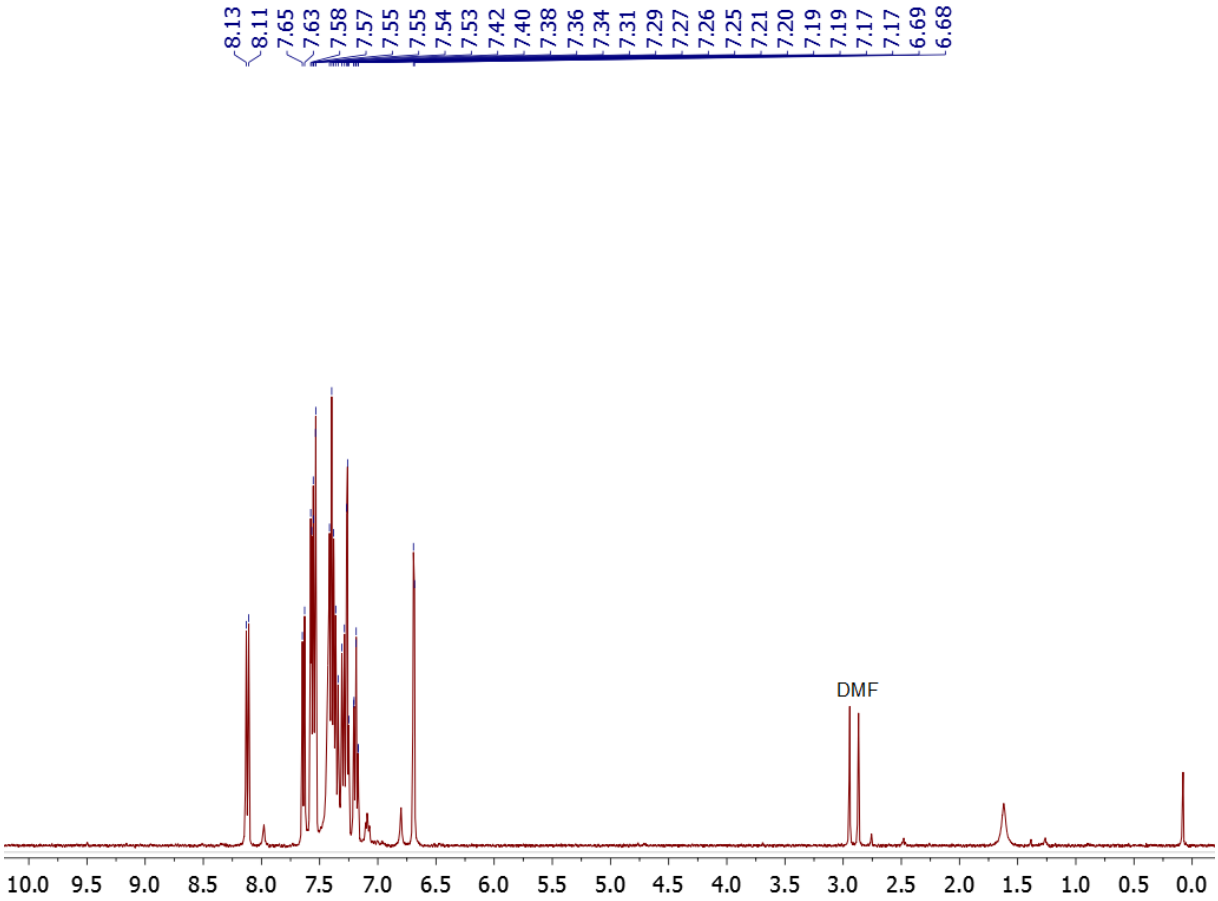

Figure S15. ^{1}H NMR spectrum of product **B** (98%) and **C** (2%) ($CDCl_3$, 298 K, 400 MHz), obtained by using complex **1** and two equivalents $AgSbF_6$.

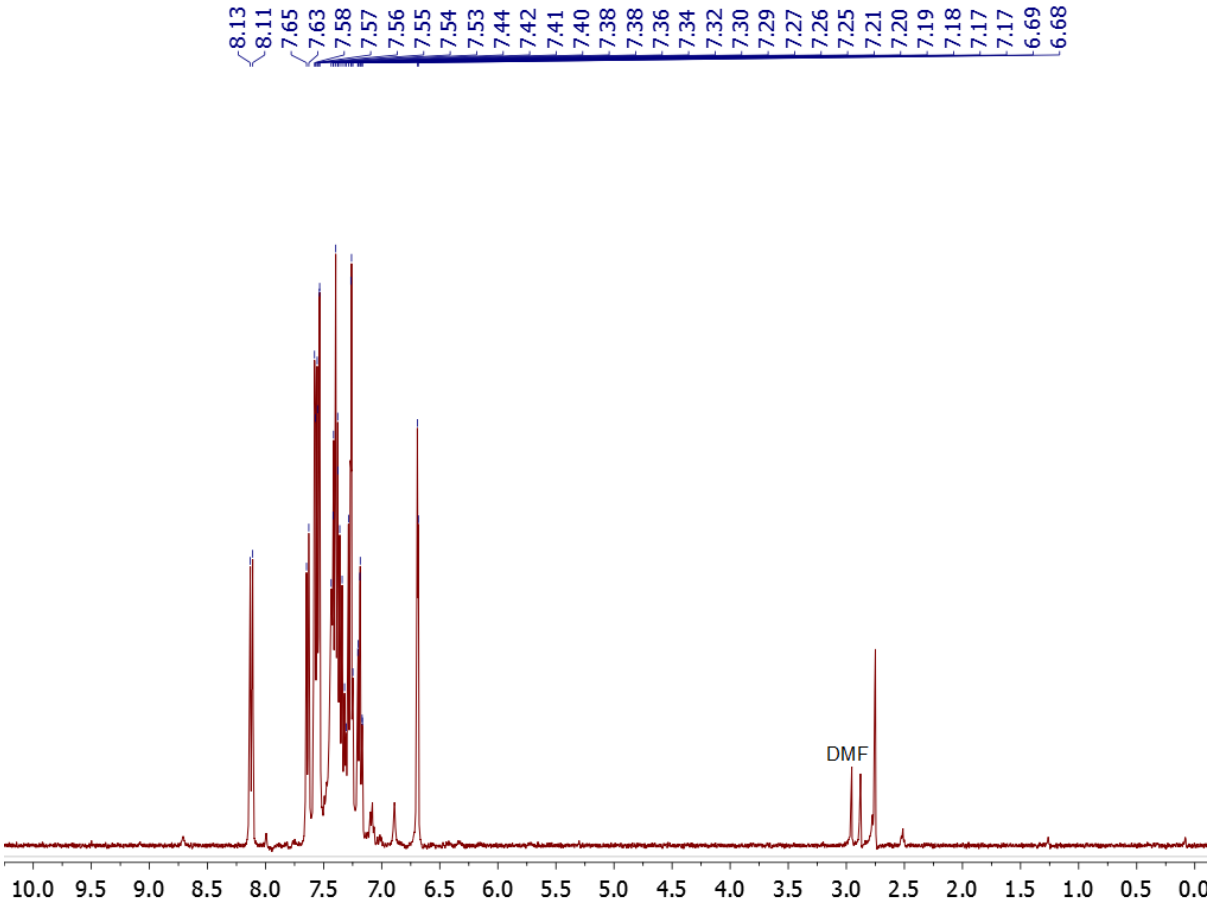

Figure S16. ^{1}H NMR spectrum of product **B** (100%) ($CDCl_3$, 298 K, 400 MHz), obtained by using complex **2** and two equivalents $AgSbF_6$.

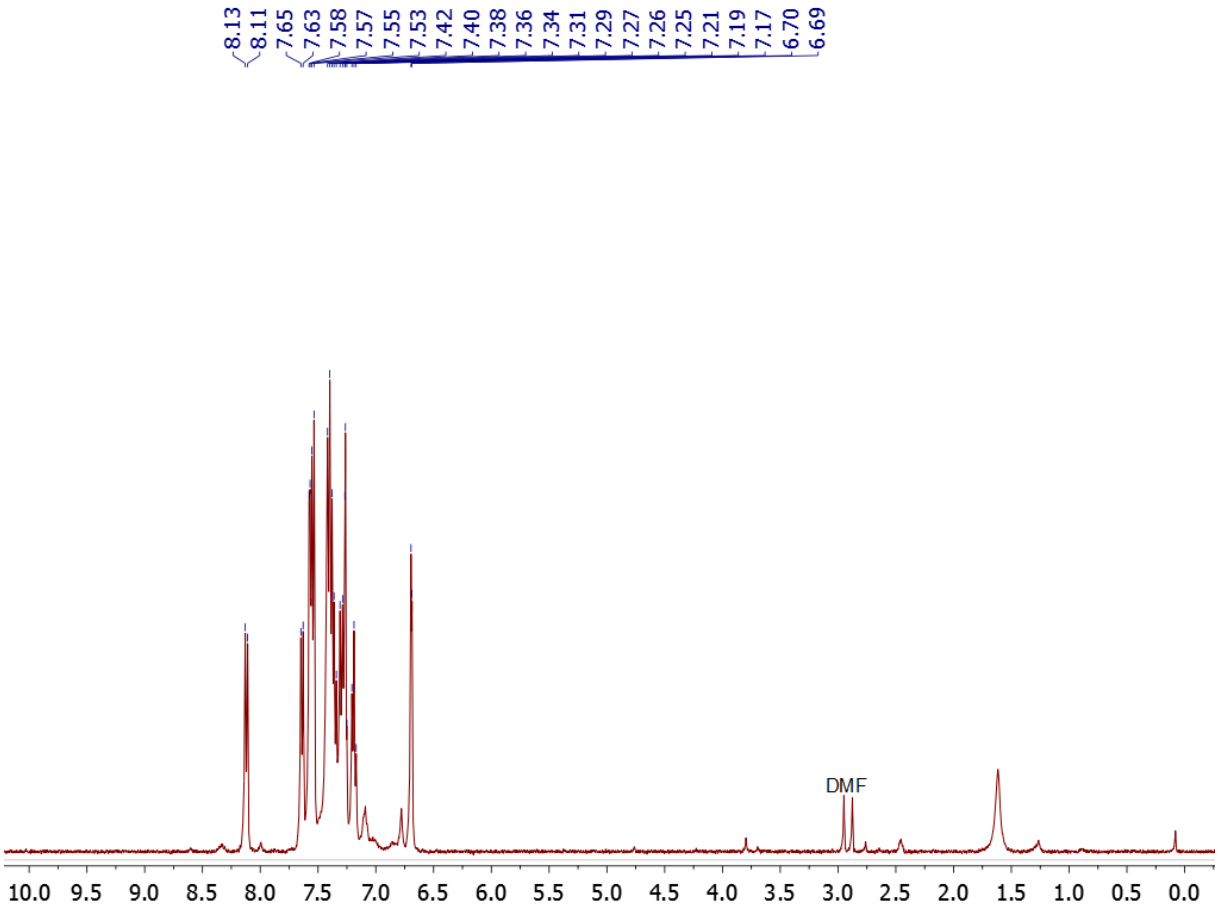

Figure S17. ^{1}H NMR spectrum of product **B** (97%) and **C** (3%) ($CDCl_3$, 298 K, 400 MHz), obtained by using complex **3** and one equivalent $AgSbF_6$.

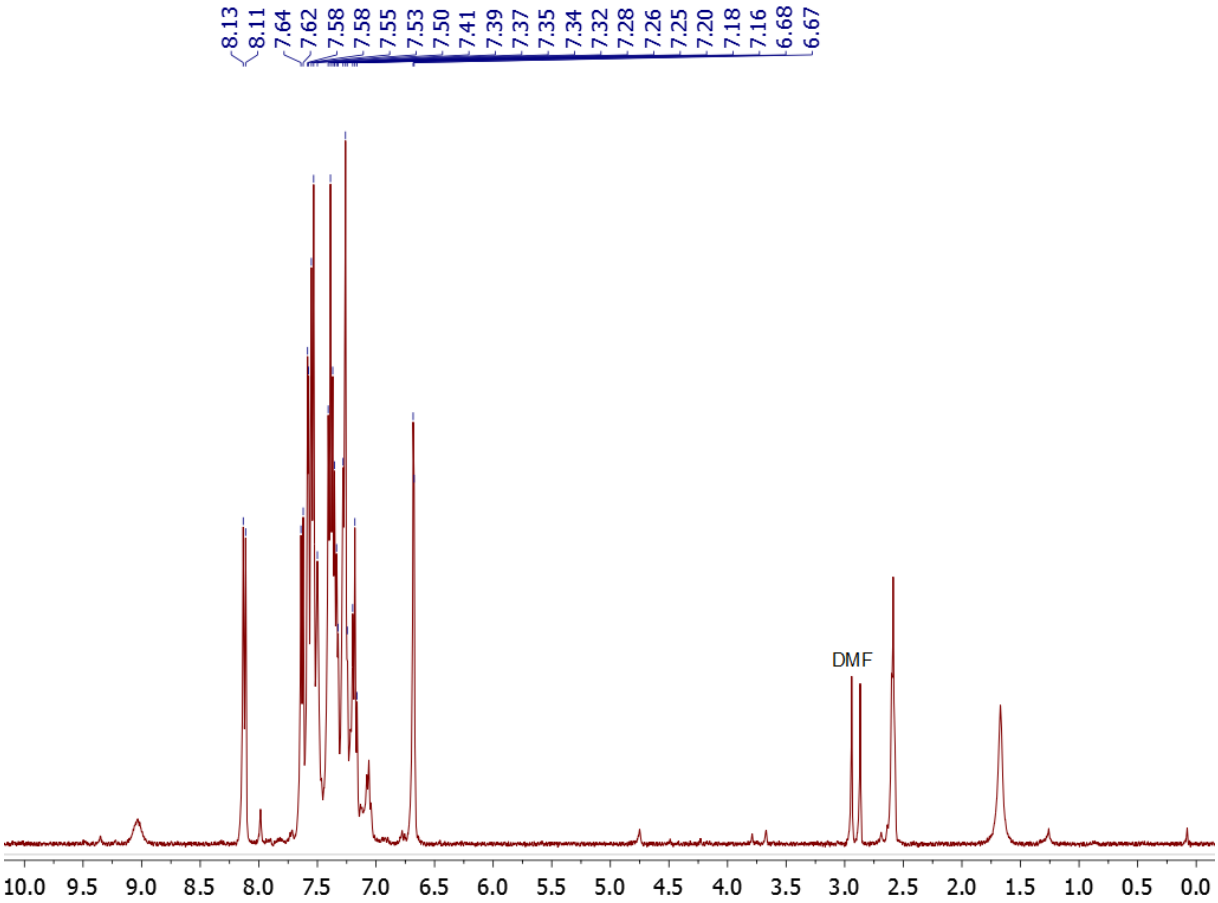

Figure S18. ^{1}H NMR spectrum of product **B** (95%) and **C** (5%) ($CDCl_3$, 298 K, 400 MHz), obtained by using complex **4** and one equivalent $AgSbF_6$.

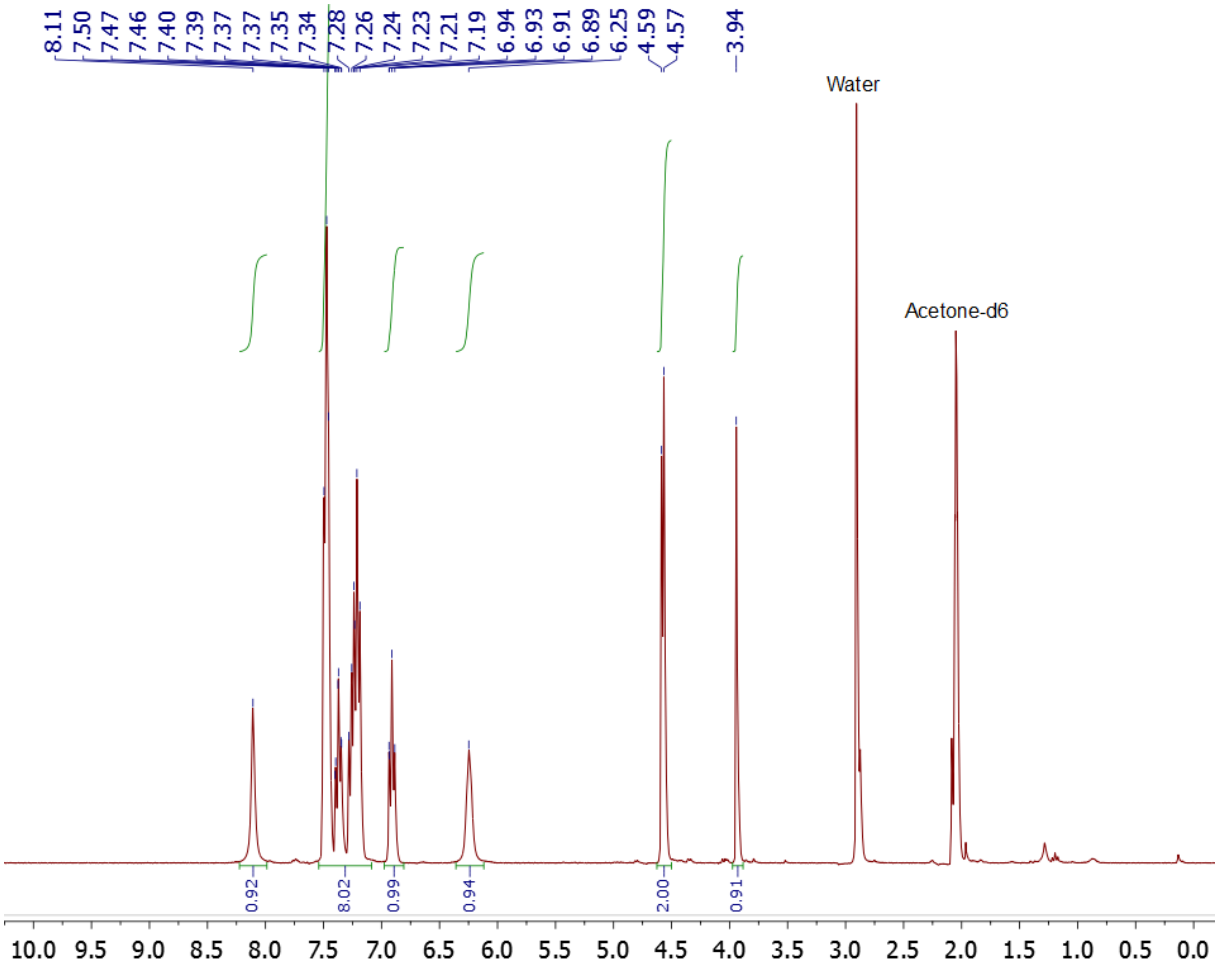

Figure S19. ^{1}H NMR spectrum of substrate **D** (acetone-d_6, 298 K, 300 MHz)

Spectral data for product **E**

^{1}H NMR (300 MHz, acetone-d_6, ppm): δ 8.30 (br s, 1H), 7.62–7.55 (m, 2H), 7.32–7.24 (m, 2H), 7.22–7.12 (m, 3H), 7.10–6.98 (m, 3H), 5.87 (d, *J* = 7.8 Hz, 1H), 4.92 (s, 2H).

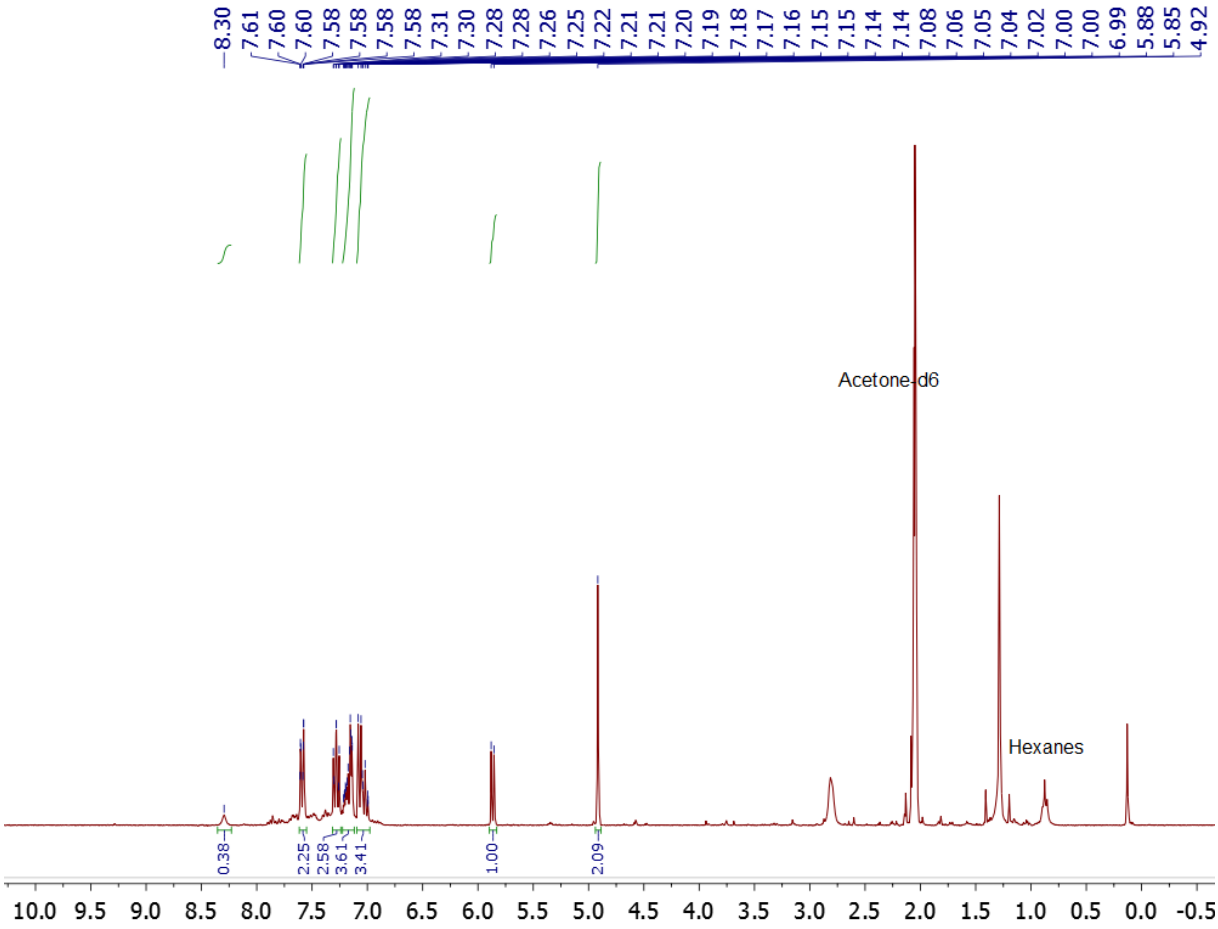

Figure S20. ^{1}H NMR spectrum of product **E** (acetone-d_6, 298 K, 300 MHz)

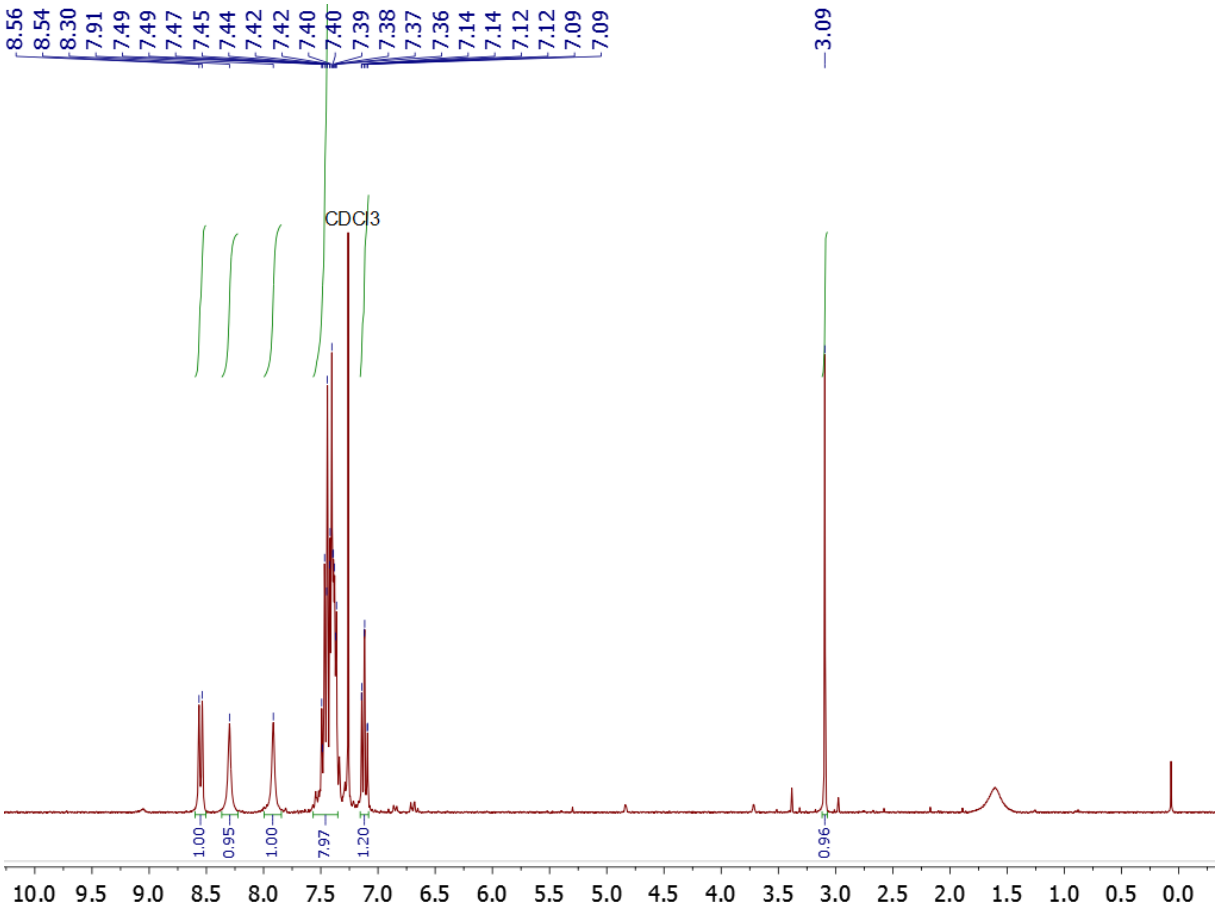

Figure S21. ^{1}H NMR spectrum of substrate **F** ($CDCl_3$, 298 K, 300 MHz)

Spectral data for product **G**

^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.80–6.94 (m, 9H), 5.68 (s, 1H), 5.23 (s, 1H).

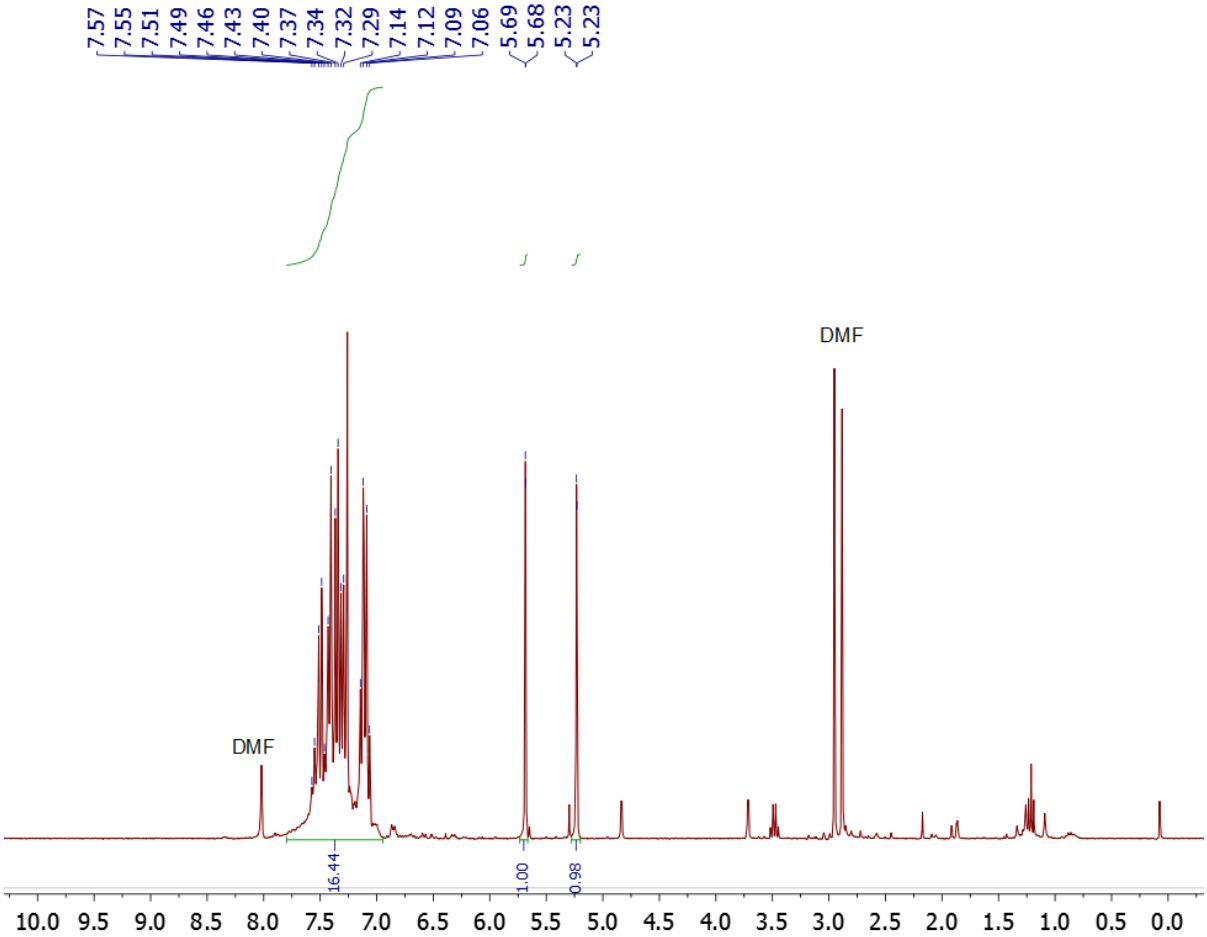

Figure S22. ^{1}H NMR spectrum of product **G** ($CDCl_3$, 298 K, 300 MHz)

Spectral data for product **H** (see ref S1)

^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 8.17 (br s, 1H), 7.65 (d, *J* = 7.8 Hz, 1H), 7.41 (d, *J* = 8.1 Hz, 1H), 7.24–7.18 (m, 2H), 7.12 (t, *J* = 7.4 Hz, 1H), 6.56 (s, 1H).

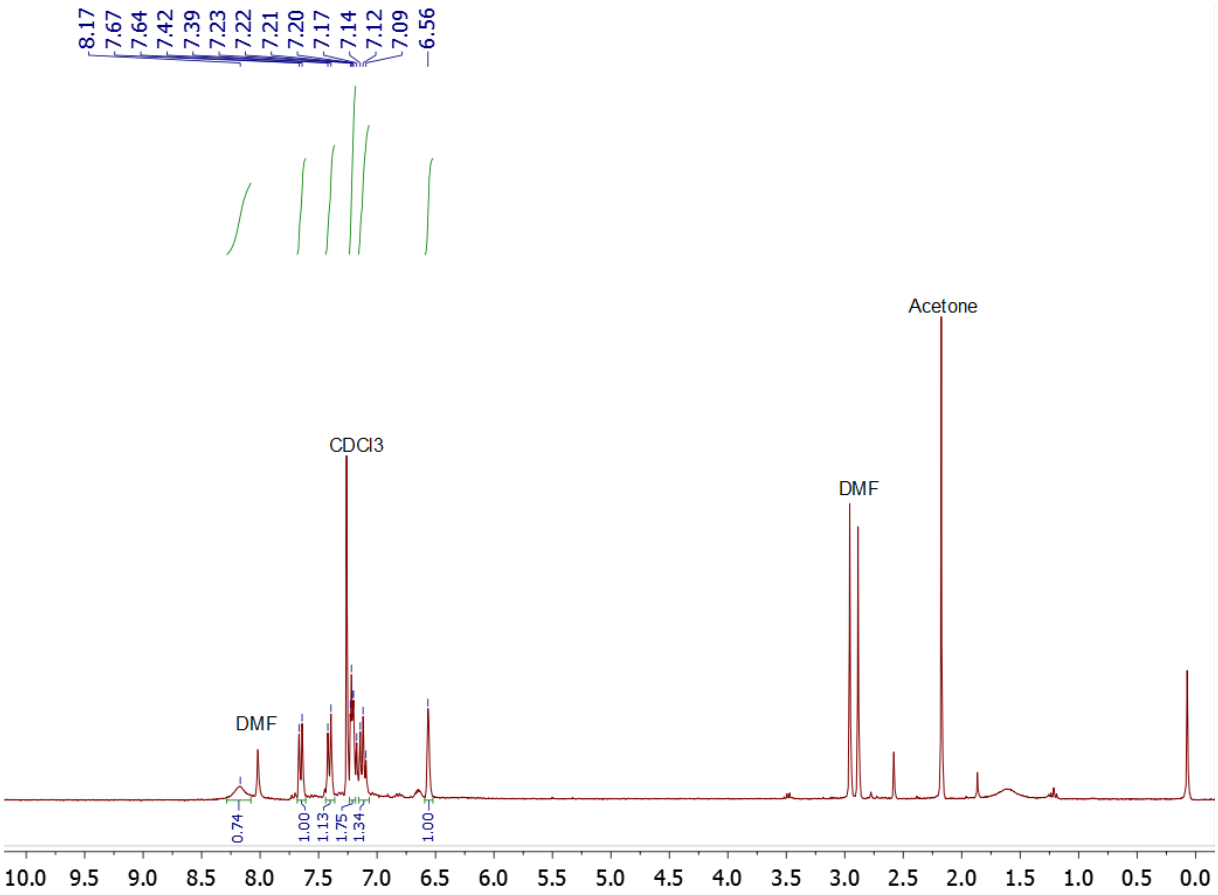

Figure S23. ^{1}H NMR spectrum of product **H** ($CDCl_3$, 298 K, 300 MHz)

References

S1 Kanchupalli, V.; Joseph, D.; Katukojvala, S. Pyridazine *N*-Oxides as Precursors of Metallocarbenes: Rhodium-Catalyzed Transannulation with Pyrroles. *Org. Lett.* **2015**, *17*, 5878–5881.