Supporting Information

A New Type of Palladium–Pincer Complexes Generated via Hydrolytic Ring-Opening of Imidazole-2-ylidenes

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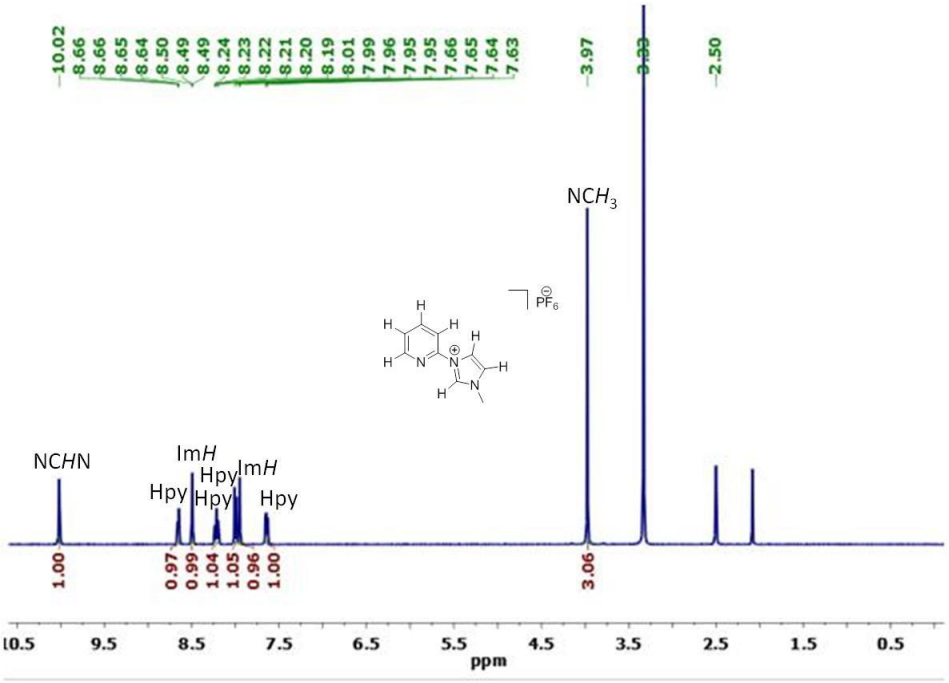

Figure S1. ^{1}H NMR spectrum of **[L$_1$H]PF$_6$** (400 MHz, DMSO-d_6, 300 K).

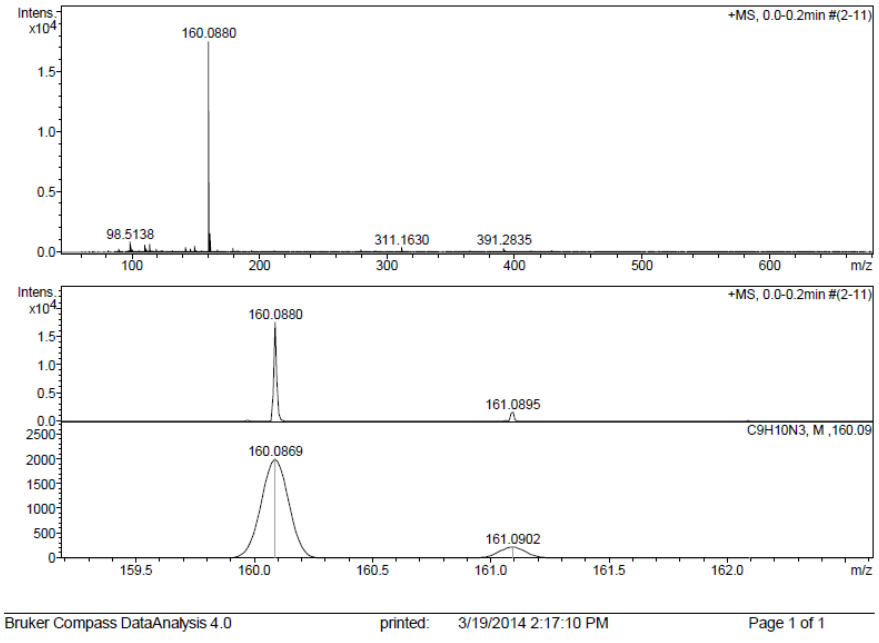

Figure S2. ESI-MS (positive ion mode) spectrum of **[L$_1$H]PF$_6$**.

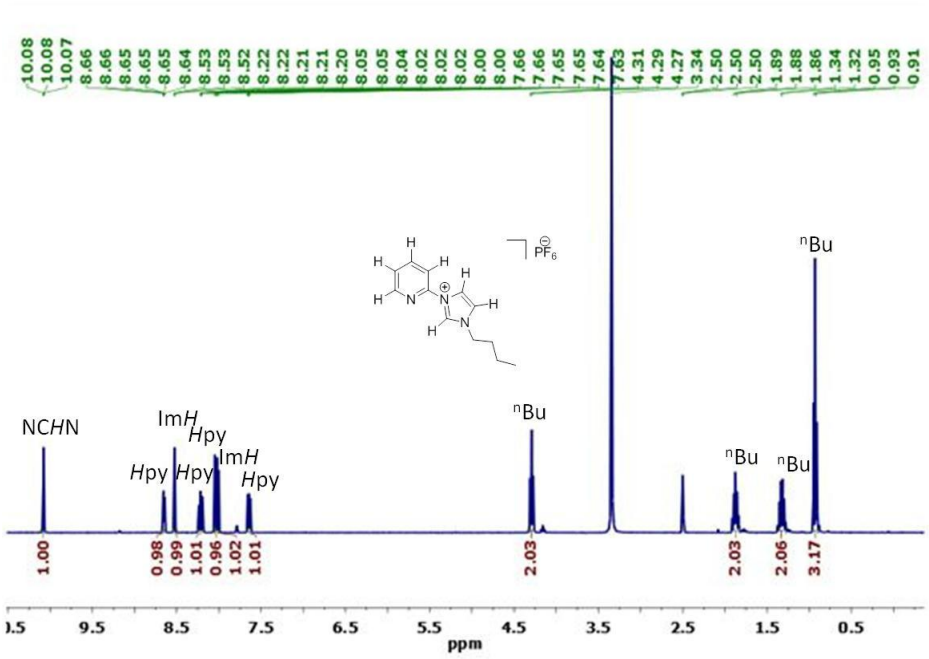

Figure S3. ^{1}H NMR spectrum of **[L$_2$H]PF$_6$** (400 MHz, DMSO-d_6, 300 K).

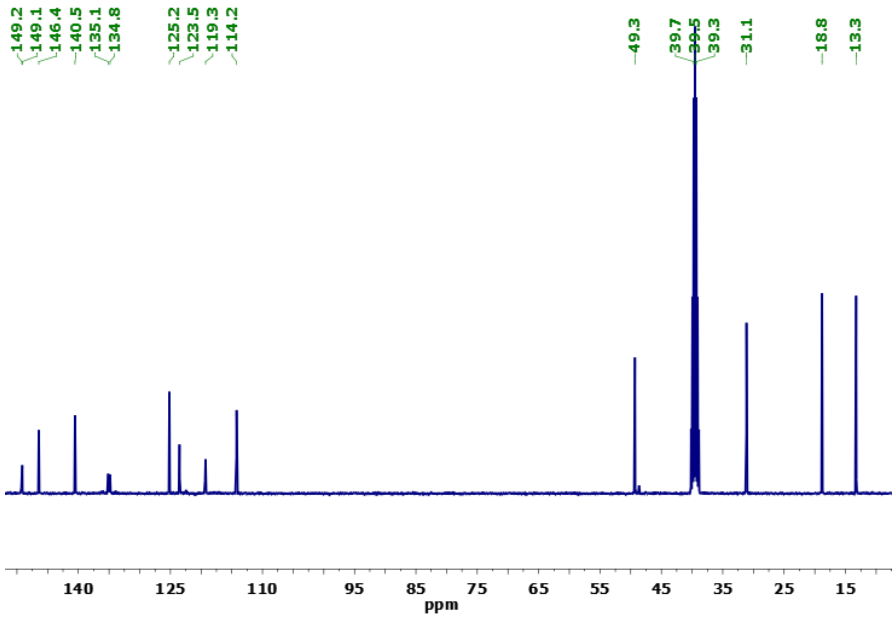

Figure S4. ^{13}C{^{1}H} NMR spectrum of **[L$_2$H]PF$_6$** (400 MHz, DMSO-d_6, 300 K).

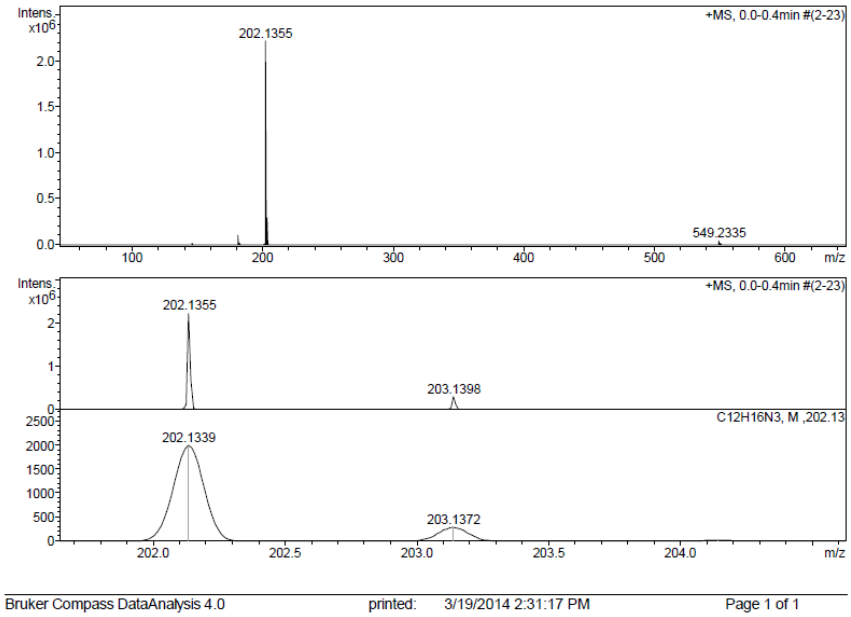

Figure S5. ESI-MS (positive ion mode) spectrum of **[L_2H]PF_6**.

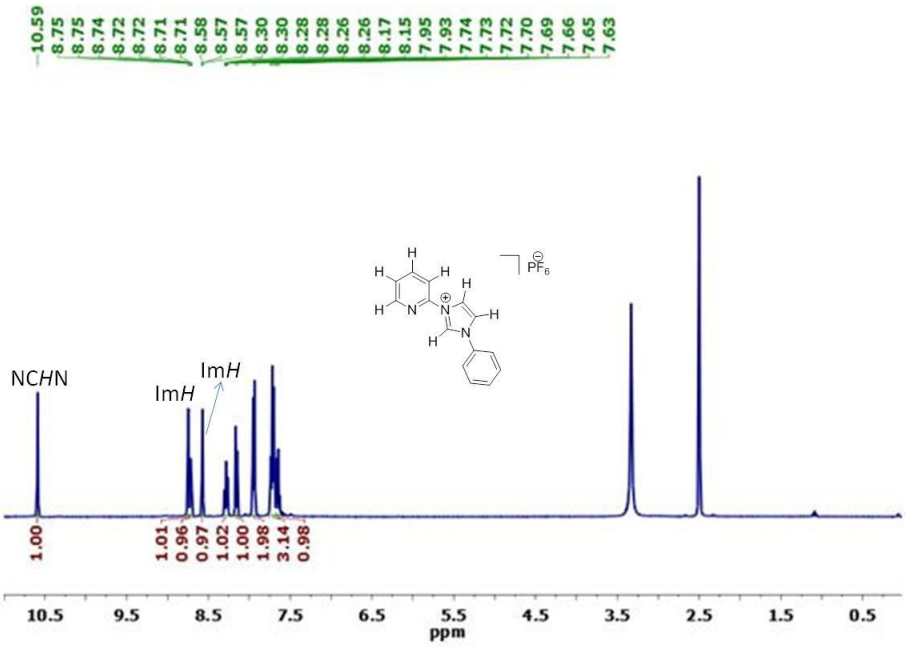

Figure S6. ^{1}H NMR spectrum of **[L_3H]PF_6** (400 MHz, DMSO-d_6, 300 K).

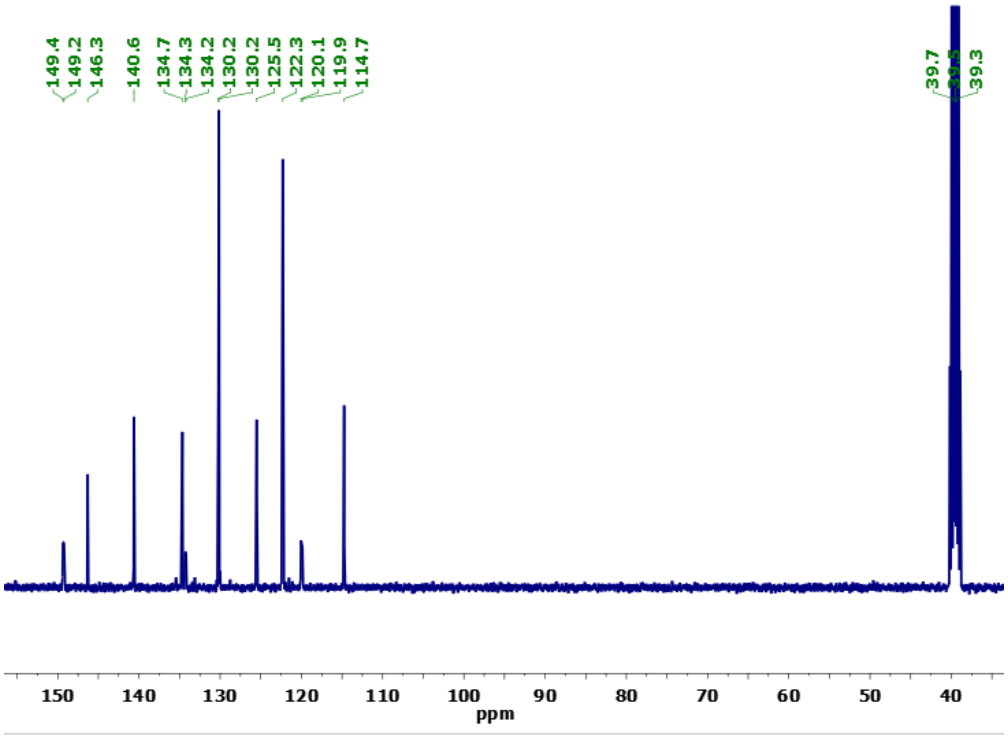

Figure S7. $^{13}C\{^{1}H\}$ NMR spectrum of **[L_3H]PF_6** (400 MHz, DMSO-d_6, 300 K).

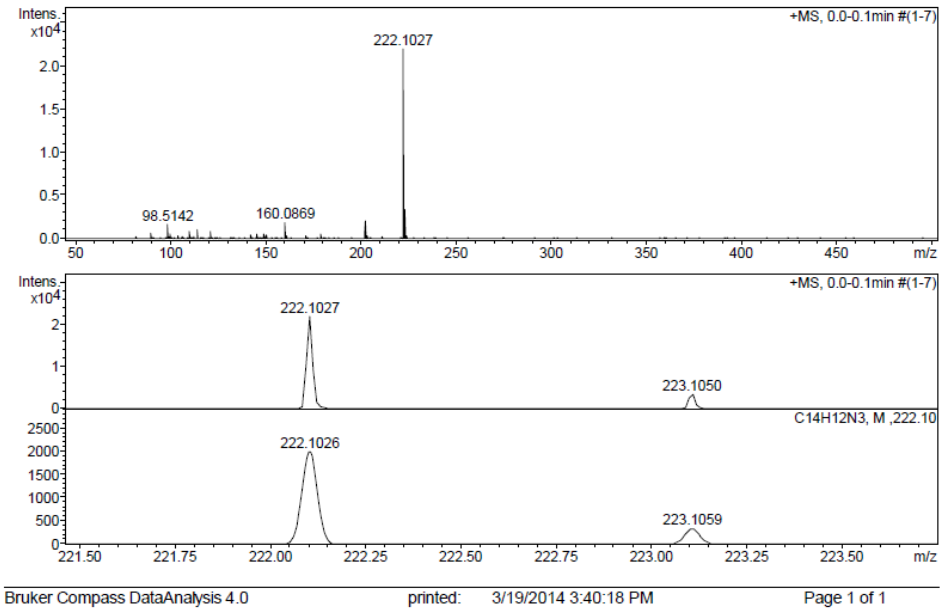

Figure S8. ESI-MS (positive ion mode) spectrum of **[L_3H]PF_6**.

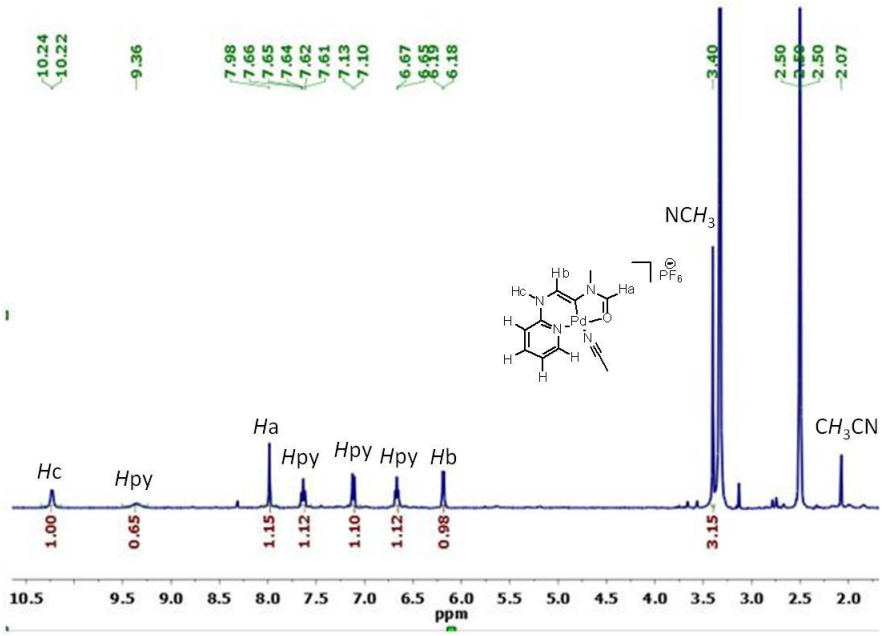

Figure S9. [1]H NMR spectrum of Complex **1** (400 MHz, DMSO-d_6, 300 K).

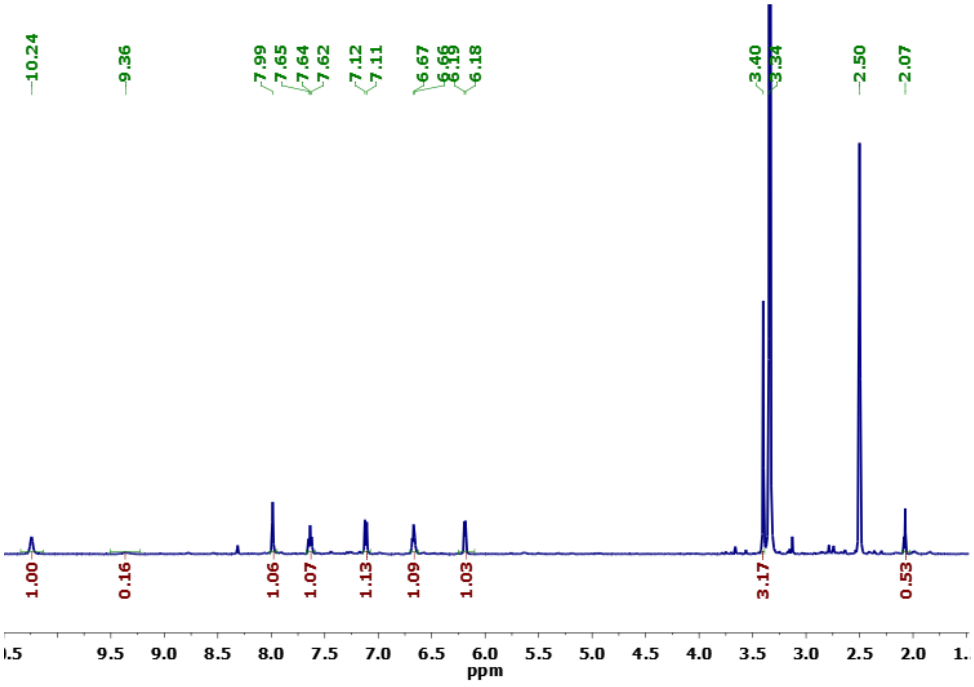

Figure S9a. [1]H NMR spectrum of Complex **1** (500 MHz, DMSO-d_6, 300 K) (recorded after 12 h) showing the decrease of intensity of the pyridyl C-H peak at 9.36 ppm due to H-D exchange with DMSO-d_6.

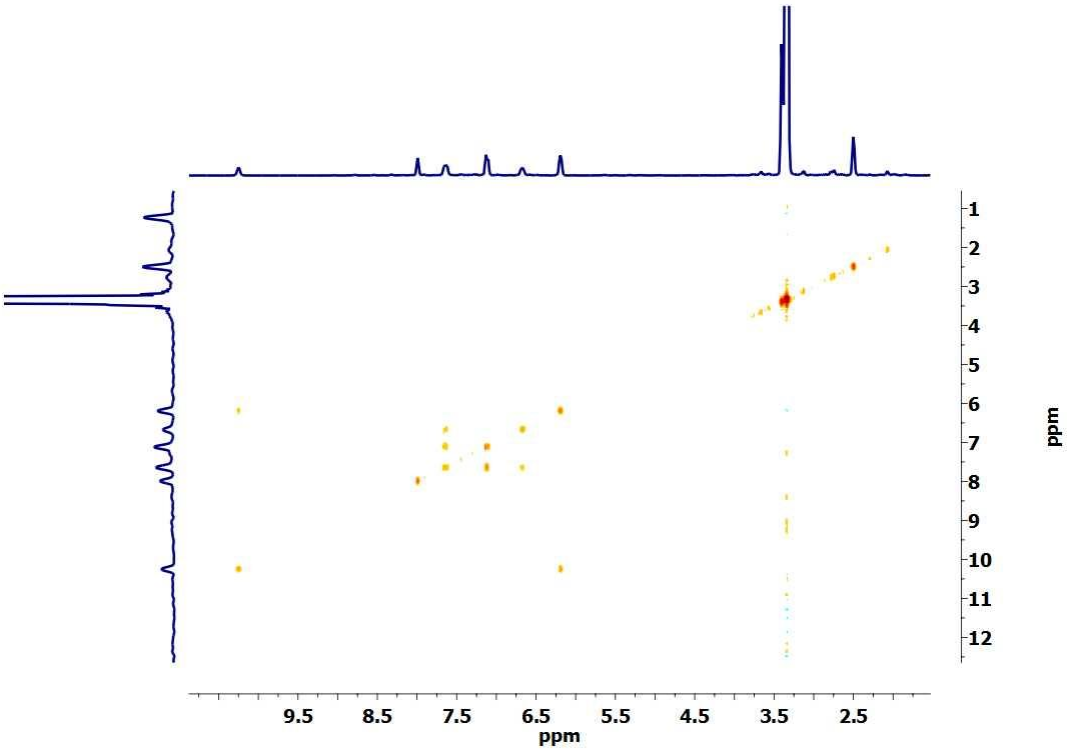

Figure S10. ^{1}H-^{1}H COSY NMR spectrum of Complex **1** (DMSO-d_6, 300 K).

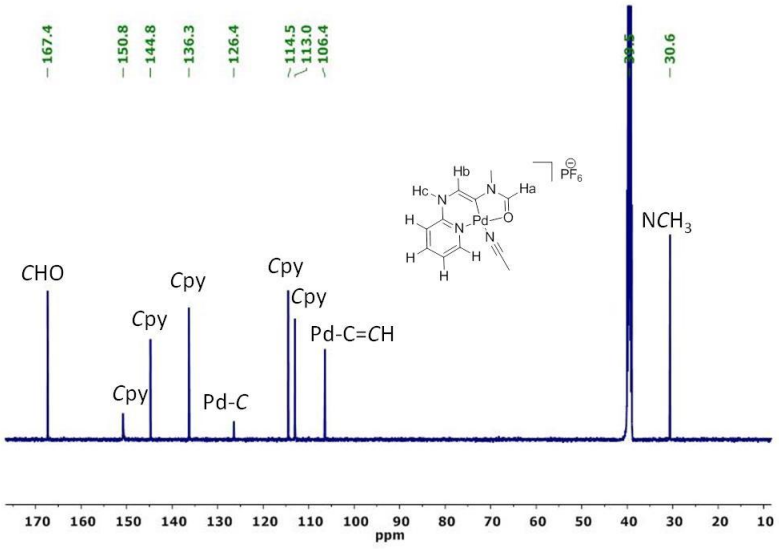

Figure S11. ^{13}C{^{1}H} NMR spectrum of Complex **1** (125 MHz, DMSO-d_6, 300 K).

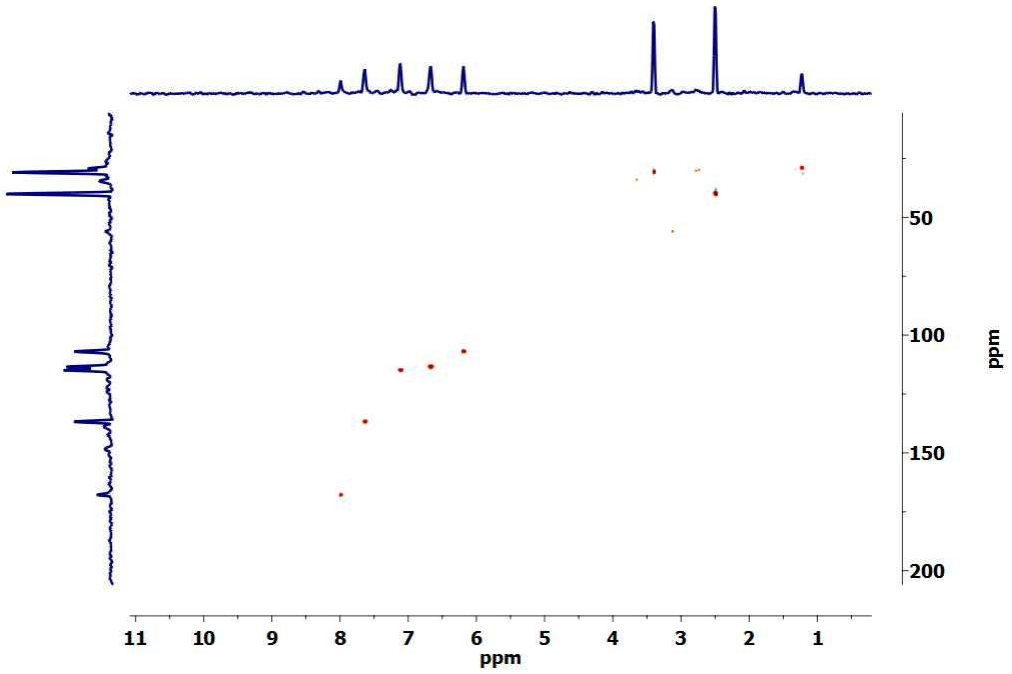

Figure S12. ^{1}H-^{13}C HSQC NMR spectrum of Complex **1** (DMSO-d_6, 300 K)

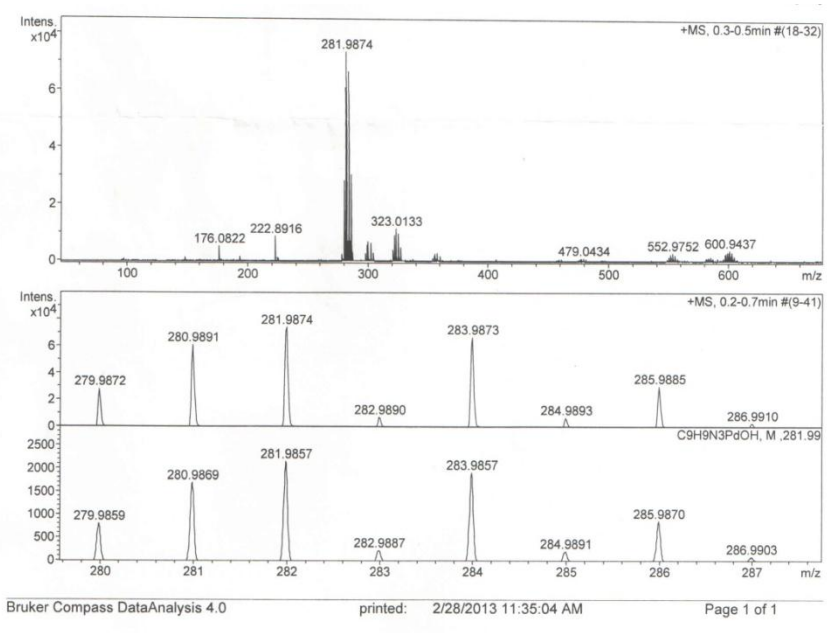

Figure S13. ESI-MS (positive ion mode) spectrum of Complex **1**.

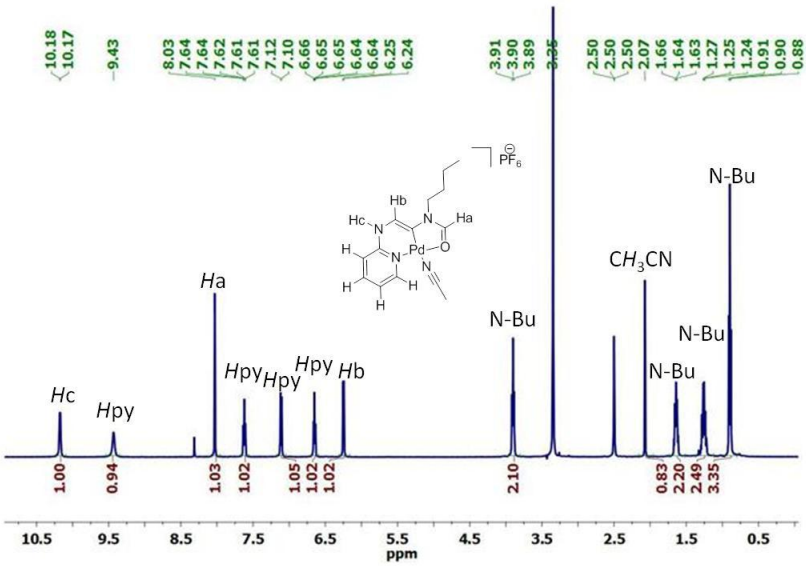

Figure S14. ^{1}H NMR spectrum of Complex **2** (500 MHz, DMSO-d_6, 300 K)

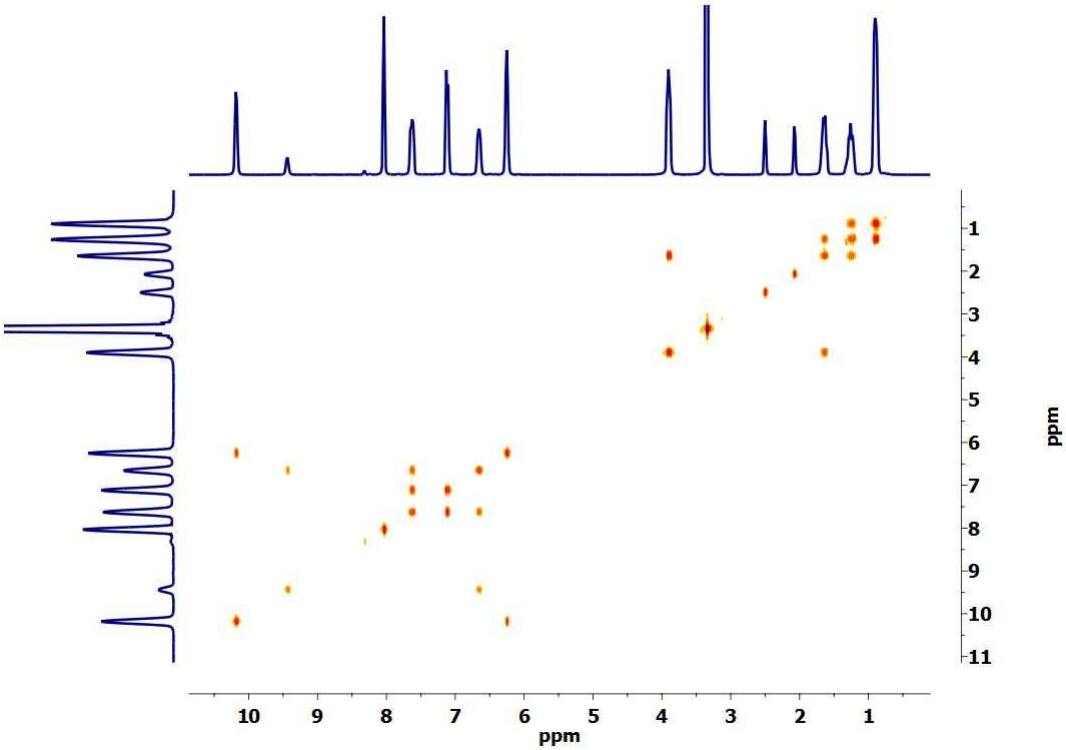

Figure S15. ^{1}H-^{1}H COSY NMR spectrum of Complex **2** (DMSO-d_6, 300 K).

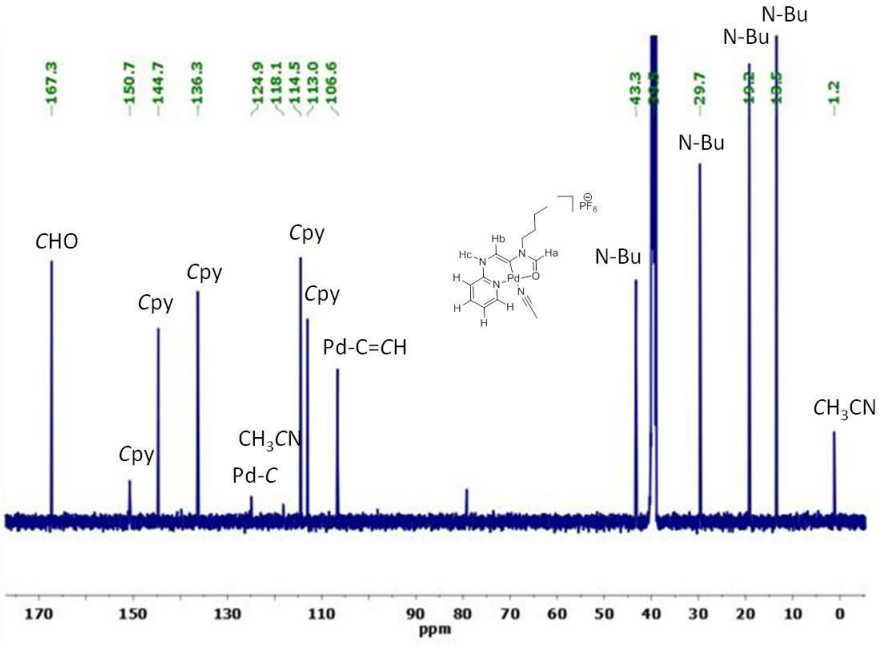

Figure S16. $^{13}C\{^{1}H\}$ NMR spectrum of Complex **2** (125 MHz, DMSO-d_6, 300 K).

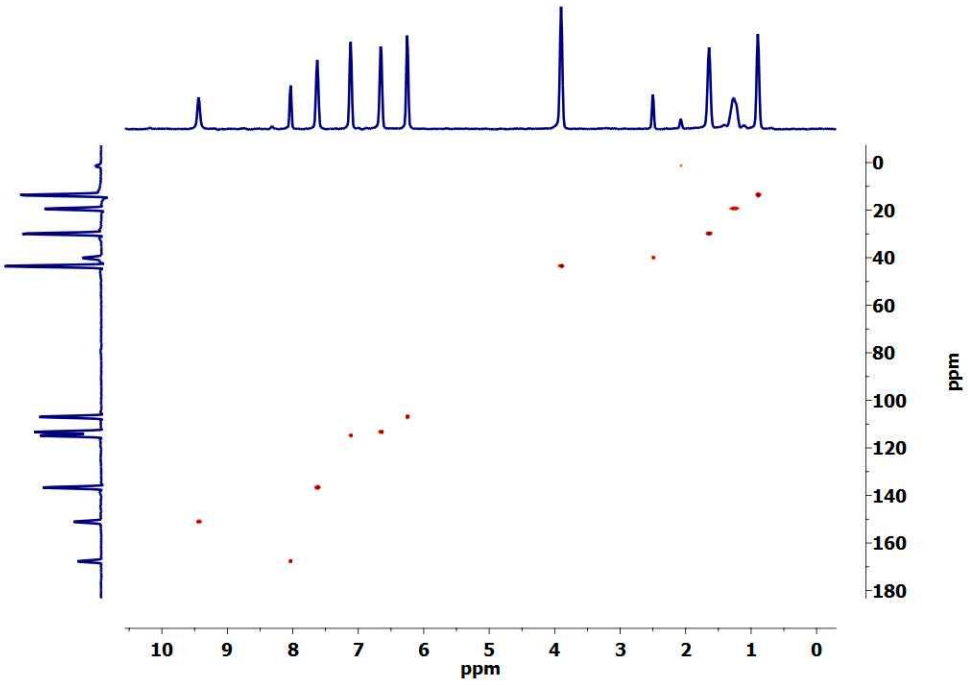

Figure S17. ^{1}H-^{13}C HSQC NMR spectrum of Complex **2** (DMSO-d_6, 300 K)

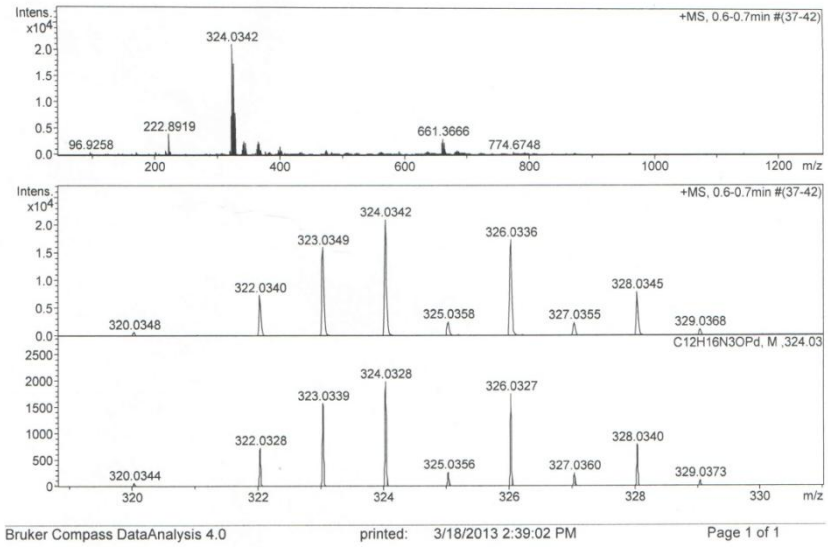

Figure S18. ESI-MS (positive ion mode) spectrum of Complex **2**.

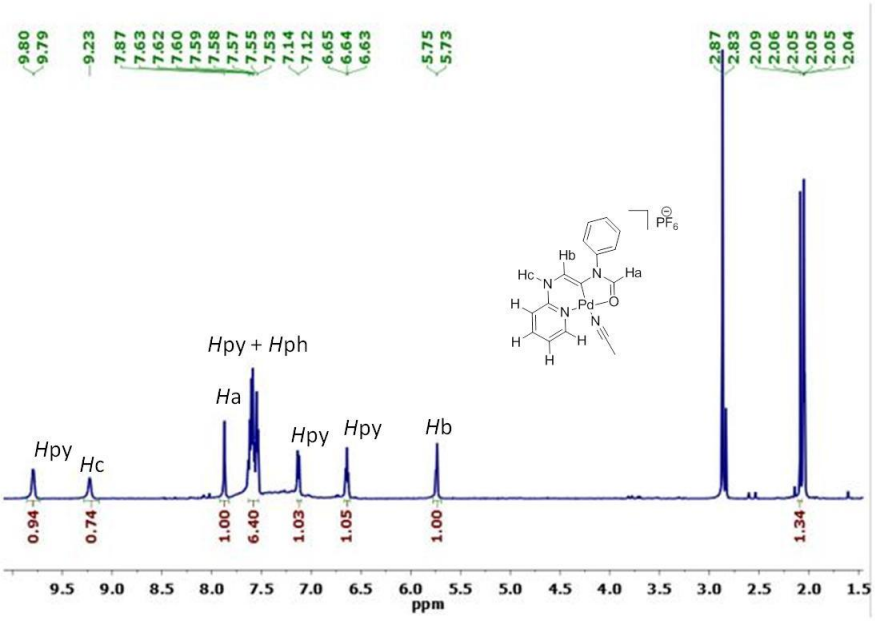

Figure S19. ^{1}H NMR spectrum of Complex **3** (500 MHz, acetone-d_6, 300 K).

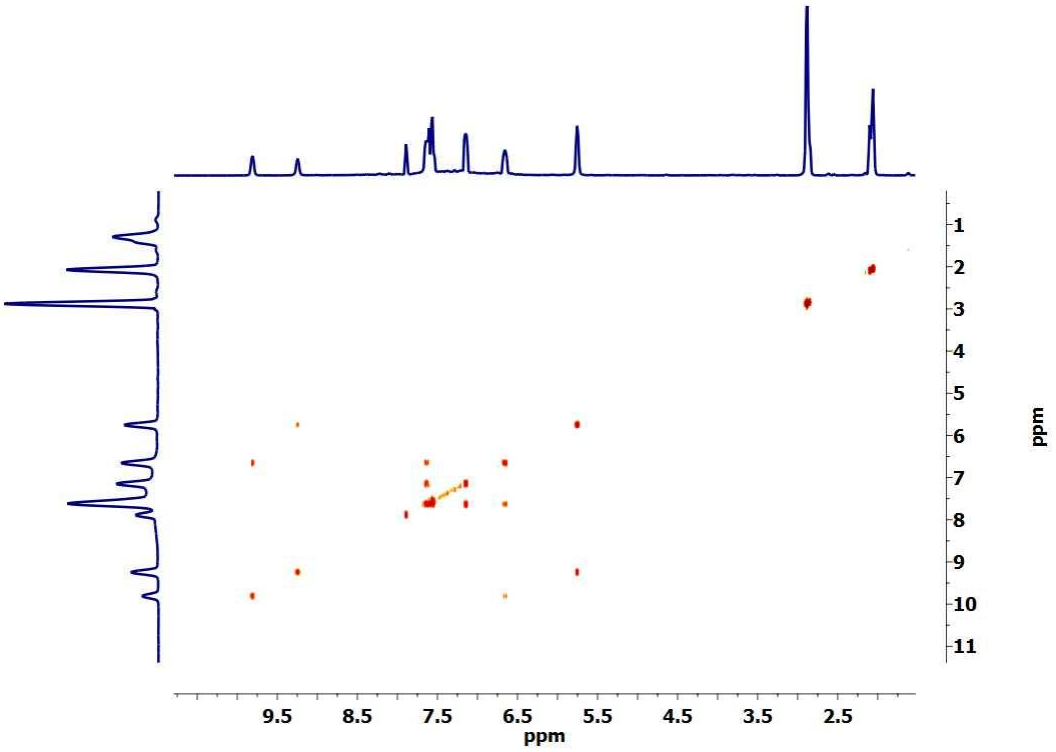

Figure S20. ^{1}H-^{1}H COSY NMR spectrum of Complex **3** (acetone-d_6, 300 K).

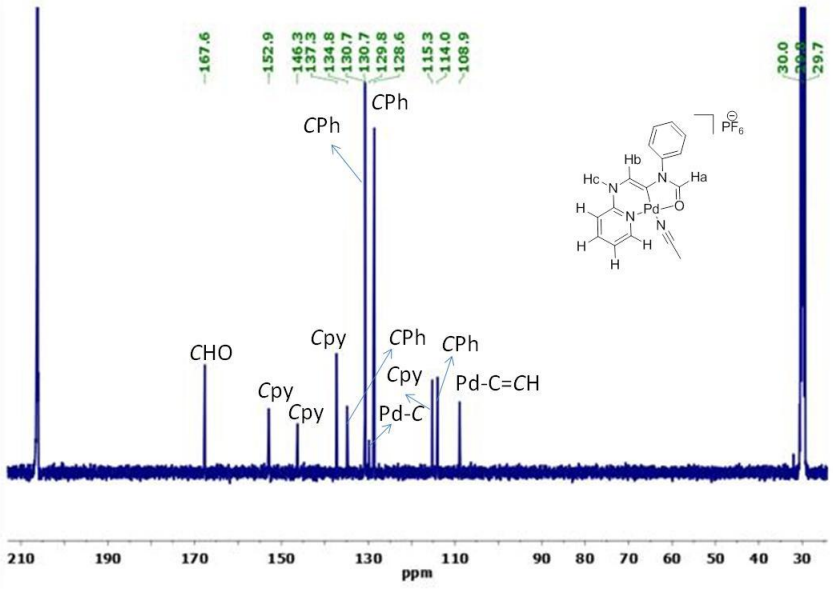

Figure S21. ^{13}C{^{1}H} NMR spectrum of Complex **3** (125 MHz, acetone-d_6, 300 K).

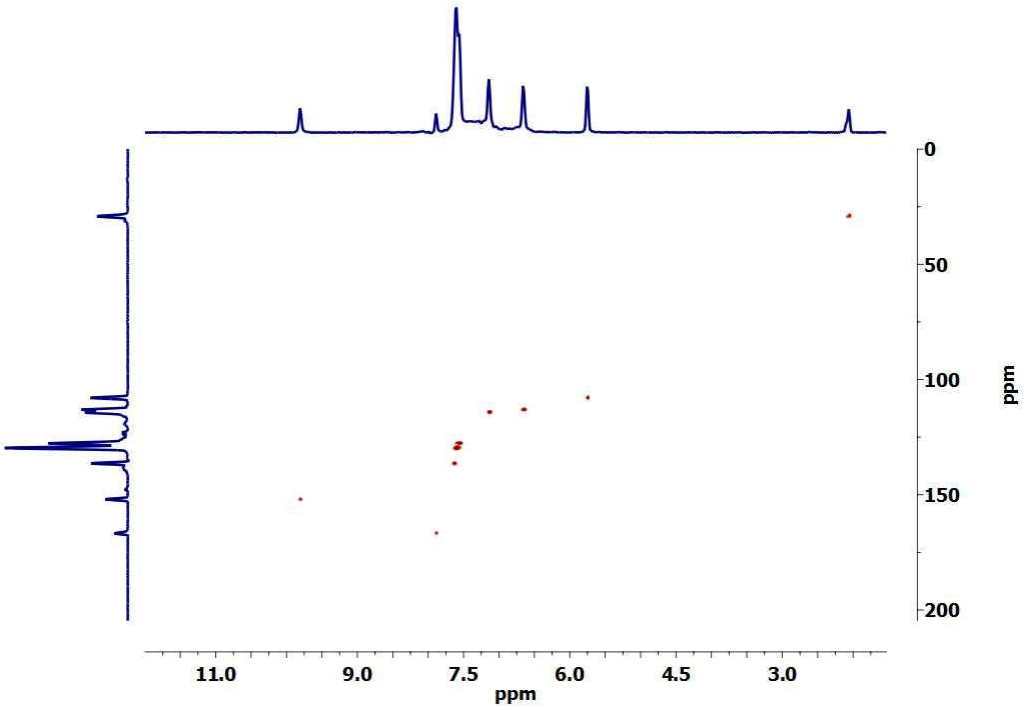

Figure S22. ^{1}H-^{13}C HSQC NMR spectrum of Complex **3** (acetone-d_6, 300 K)

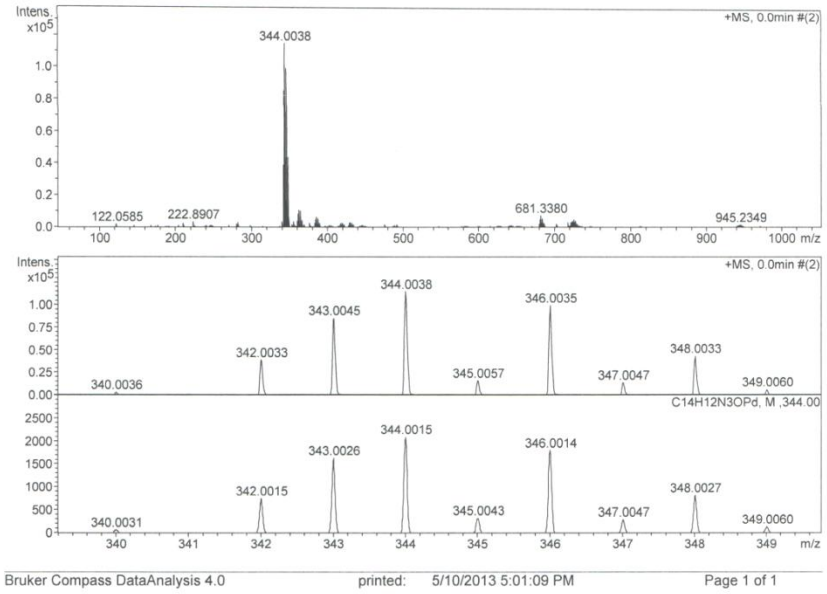

Figure S23. ESI-MS (positive ion mode) spectrum of Complex **3**.

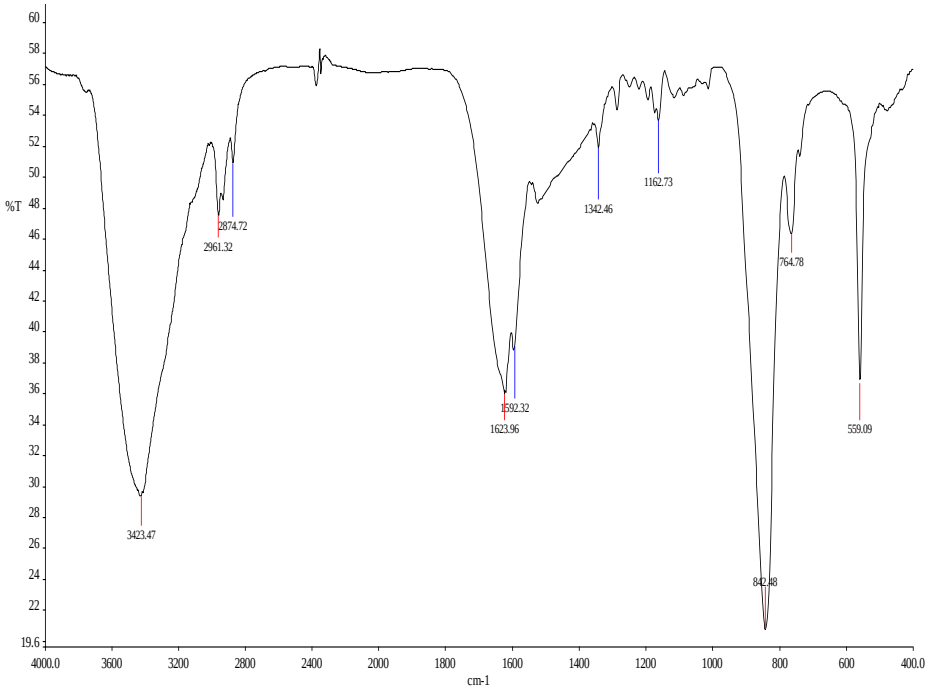

Figure S24. FT-IR spectrum of Complex **2** (KBr).

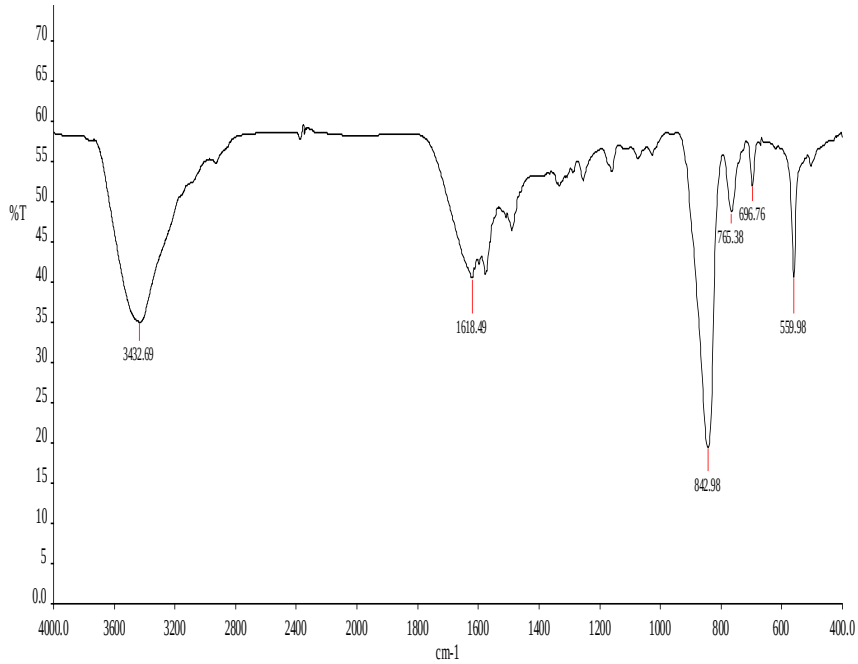

Figure S25. FT-IR spectrum of Complex **3** (KBr).