

Pd(II)-complexes of a novel pyridinone based tripeptide conjugate: A solution and solid state study

András Ozsváth^a, Róbert Diószegi^a, Attila Csaba Bényei^b, Péter Buglyó^{a,*}

a) University of Debrecen, Department of Inorganic & Analytical Chemistry, Egyetem tér 1., 4032 Debrecen, Hungary

b) University of Debrecen, Department of Physical Chemistry, Egyetem tér 1., 4032 Debrecen, Hungary

buglyo@science.unideb.hu

Supporting information

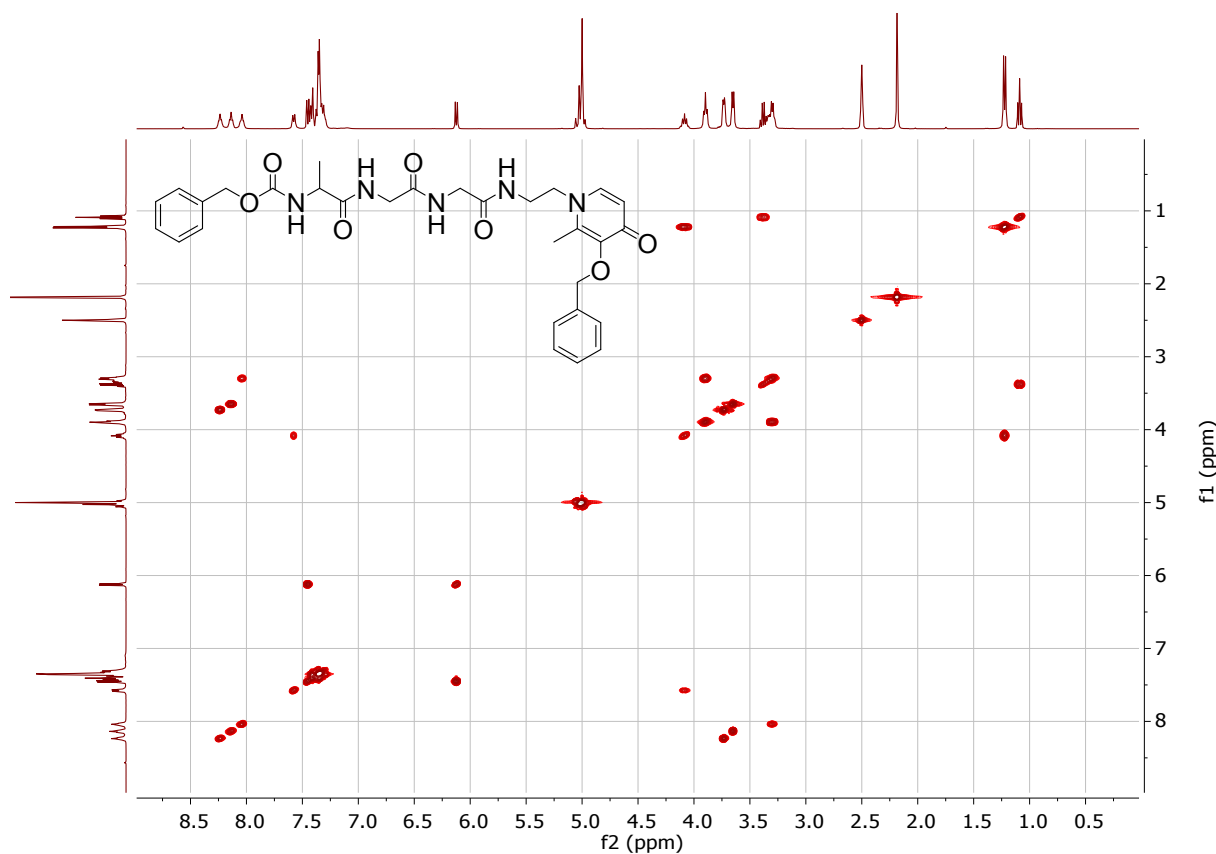


Figure S1. ¹H-¹H COSY spectrum of **1** in DMSO-d₆

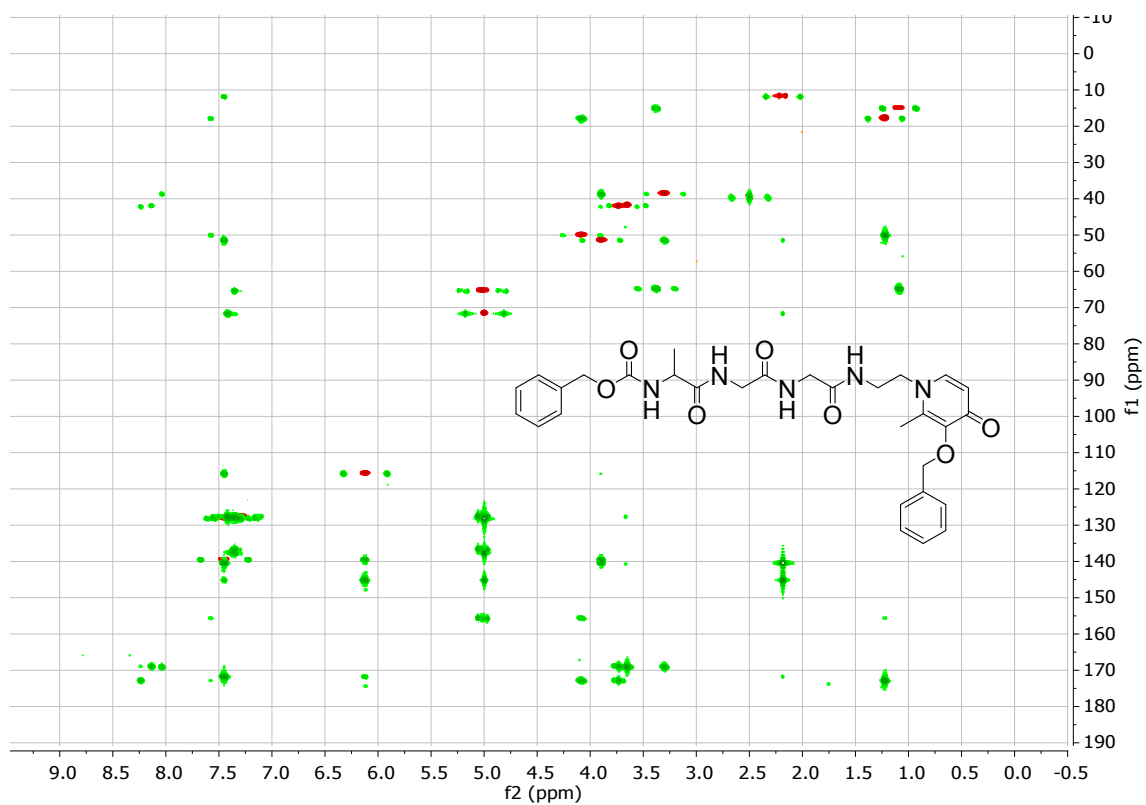


Figure S2. ^1H - ^{13}C HSQC (red) and ^1H - ^{13}C HMBC (green) spectra of **1** in DMSO-d_6

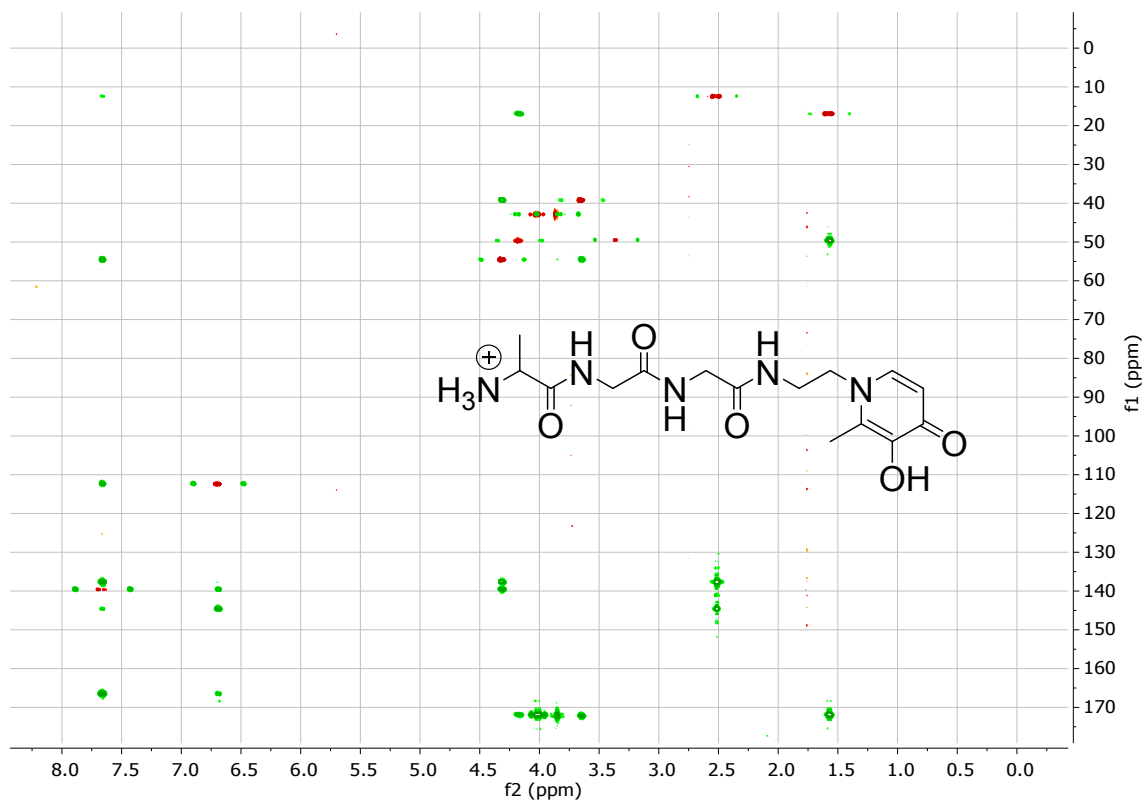


Figure S3. ^1H - ^{13}C HSQC (red) and ^1H - ^{13}C HMBC (green) spectra of **2** in D_2O

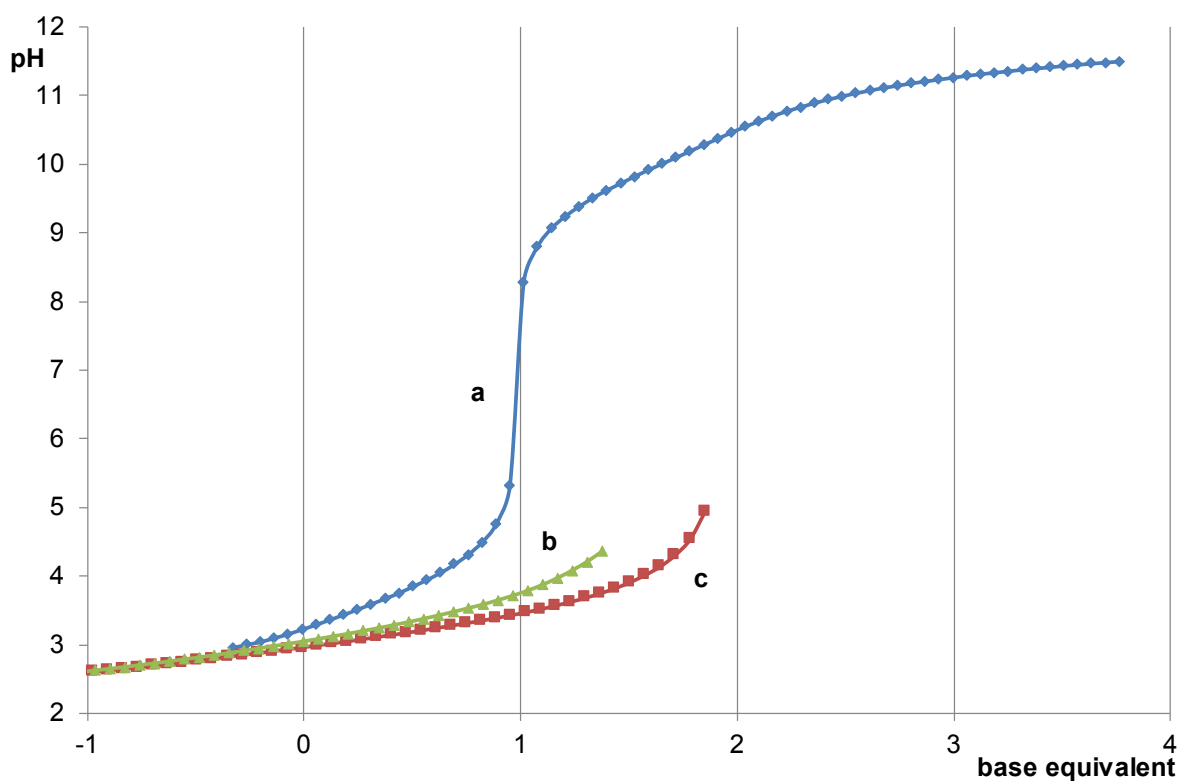


Figure S4. Representative titration curves of the H^+ –L1 (a) system and the Pd(II)–L1 systems at 1:2 (b) and 1:1 (c) metal ion to ligand ratios ($c_{\text{L1}} = 2.80 \text{ mM}$).

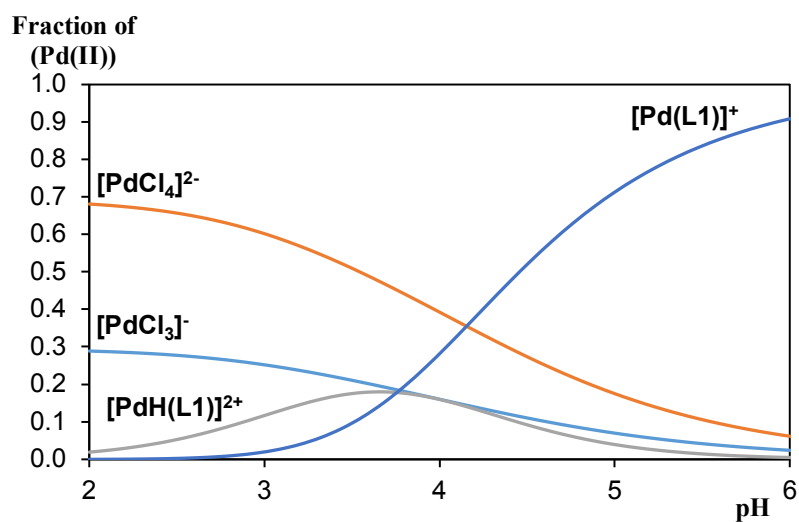


Figure S5. Concentration distribution curves for Pd(II)–L1 system at 1:1 metal ion to ligand ratio ($c_{\text{L1}} = 2.80 \text{ mM}$)

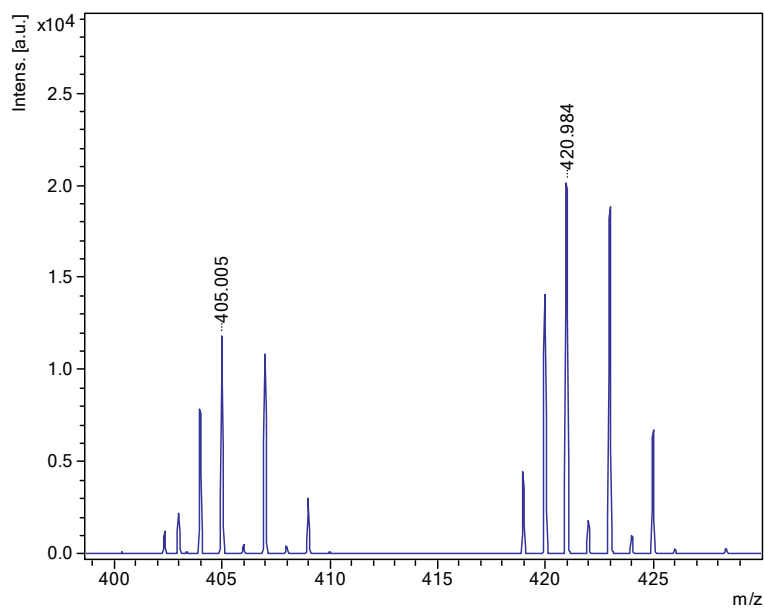


Figure S6. MALDI-MS spectrum of the precipitate obtained during the titration of Pd(II)L2 = 1:2 system

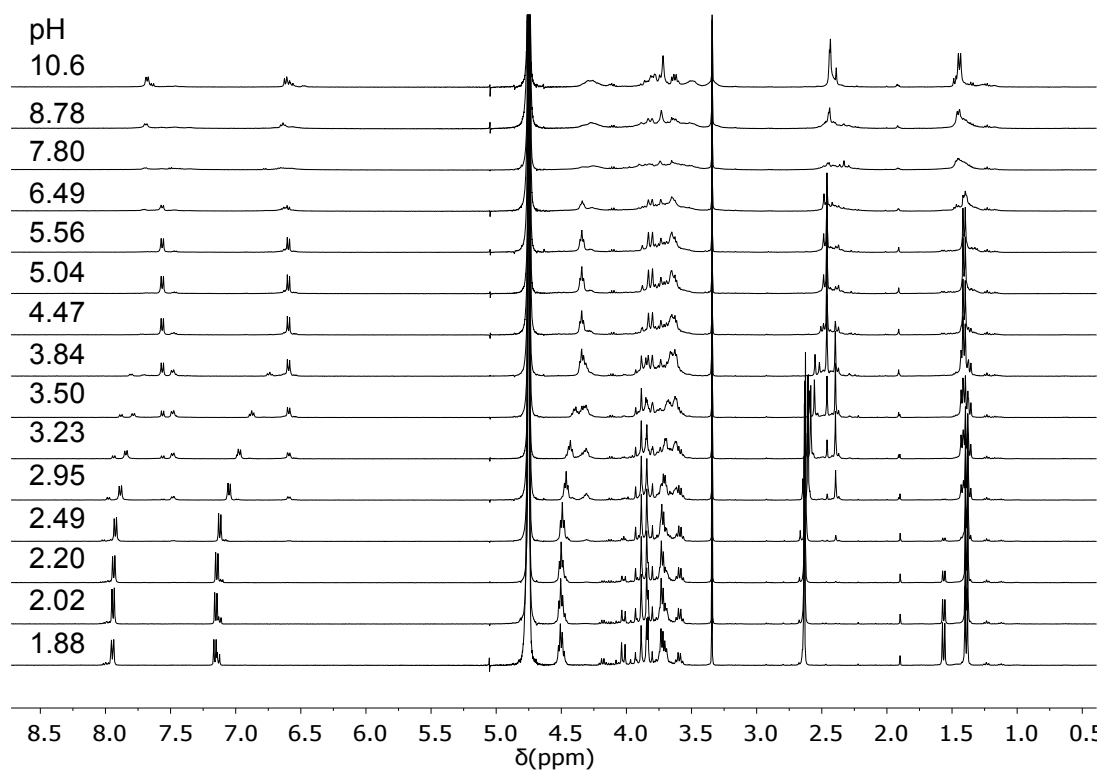


Figure S7. pH-dependent ^1H NMR spectra of the 2:1 Pd(II)–L2 sample, $c_{\text{L2}} = 5.0$ mM.

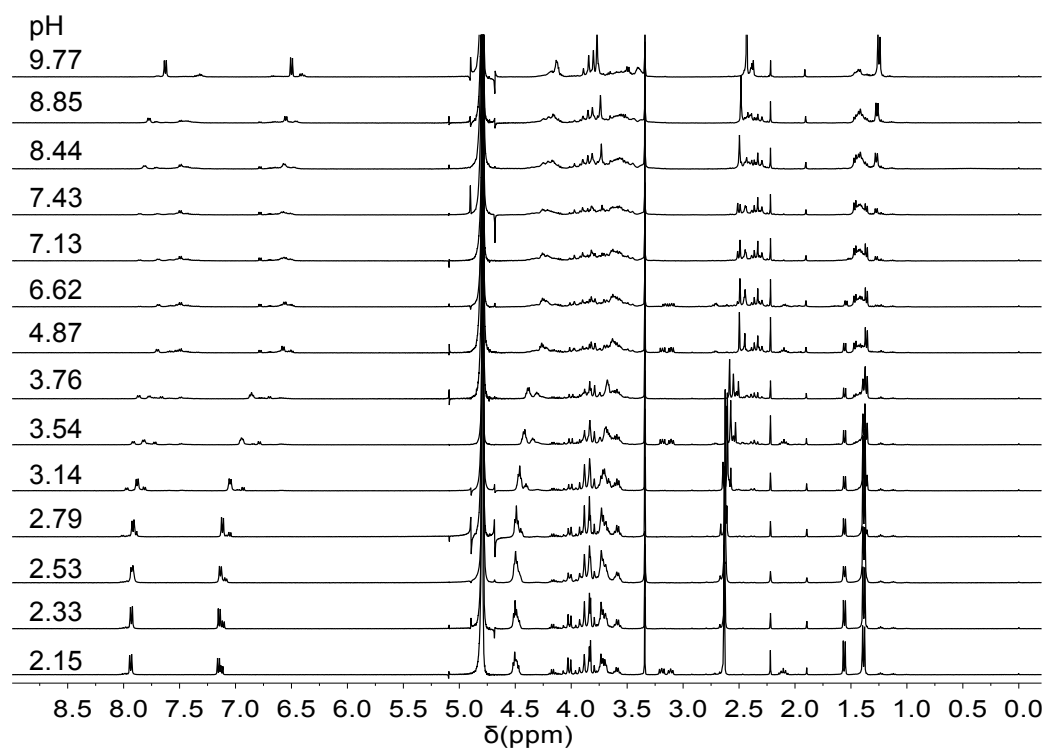


Figure S8. pH-dependent ^1H NMR spectra of the 1:1 Pd(II)–L2 sample, $c_{\text{L2}} = 5.0$ mM.

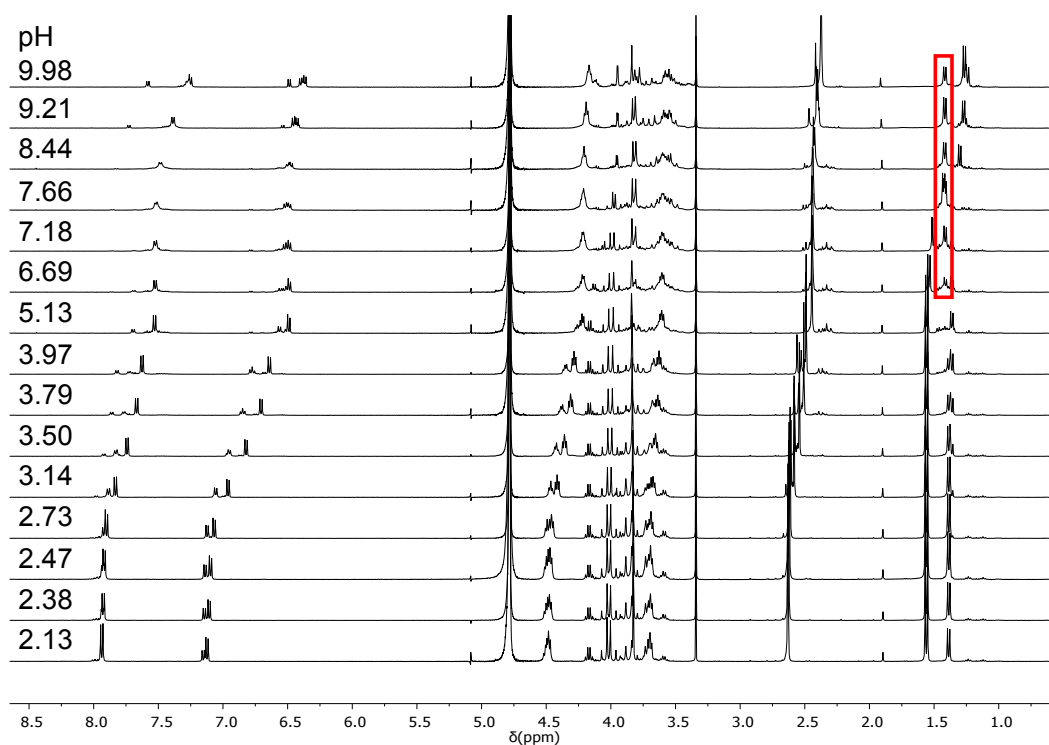


Figure S9. pH-dependent ^1H NMR spectra of the 1:2 Pd(II)–L2 sample, $c_{\text{L2}} = 5.0$ mM, A signals of the bis-complexes are highlighted

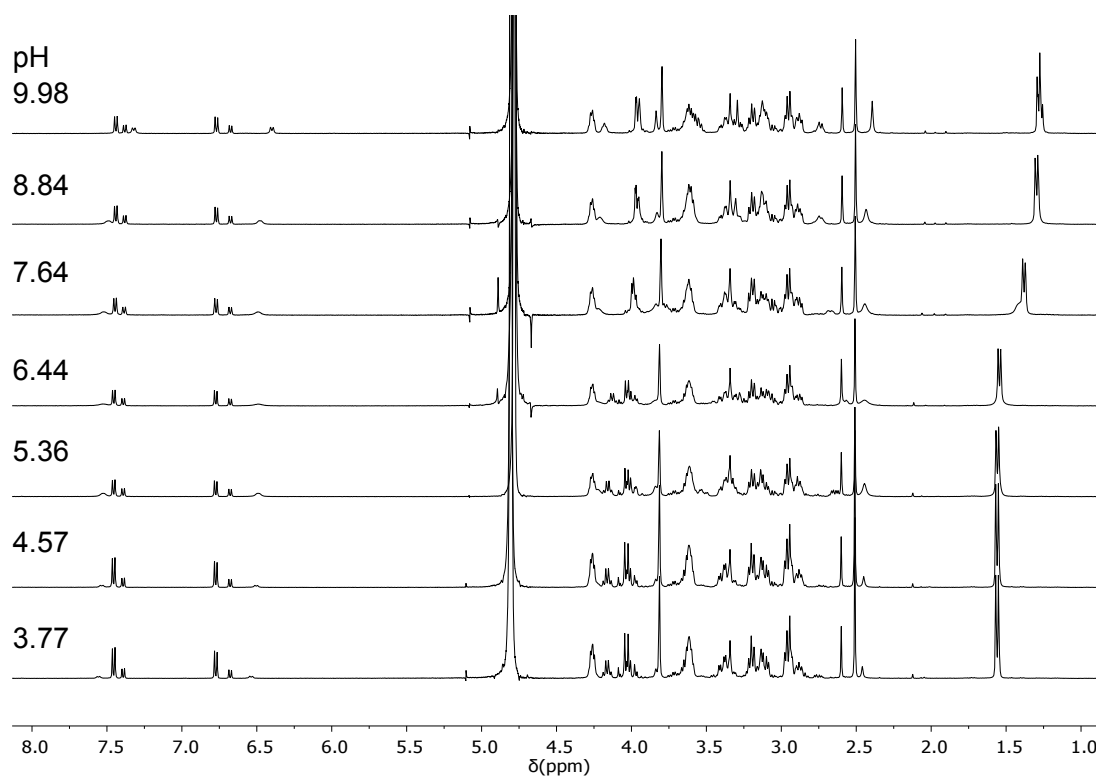


Figure S10. pH dependent ^1H NMR spectra of $[\text{Co}(\text{tren})\text{H}(\text{L2})]^{3+}$ in solution

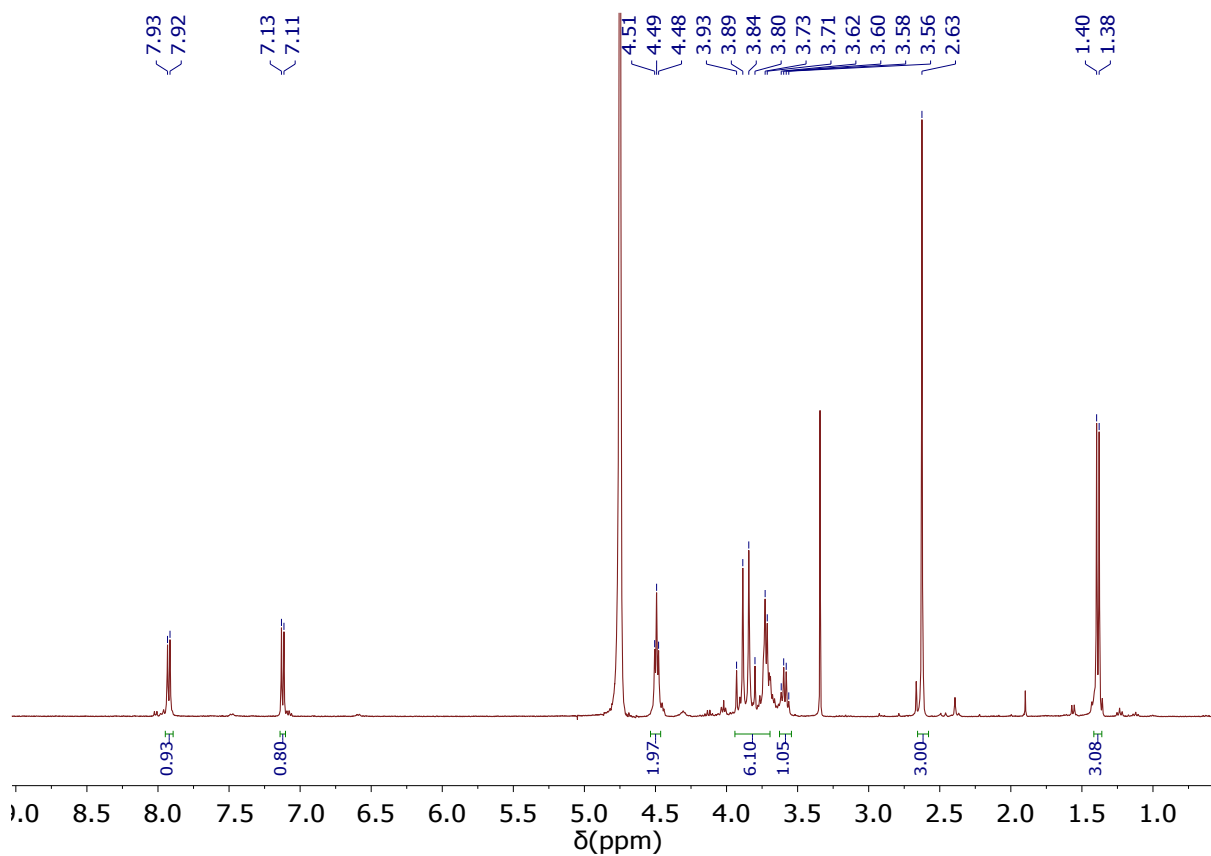


Figure S11. ^1H NMR spectrum of $[\text{PdH}(\text{L2})\text{Cl}_2] \cdot 2\text{H}_2\text{O}$ in D_2O .

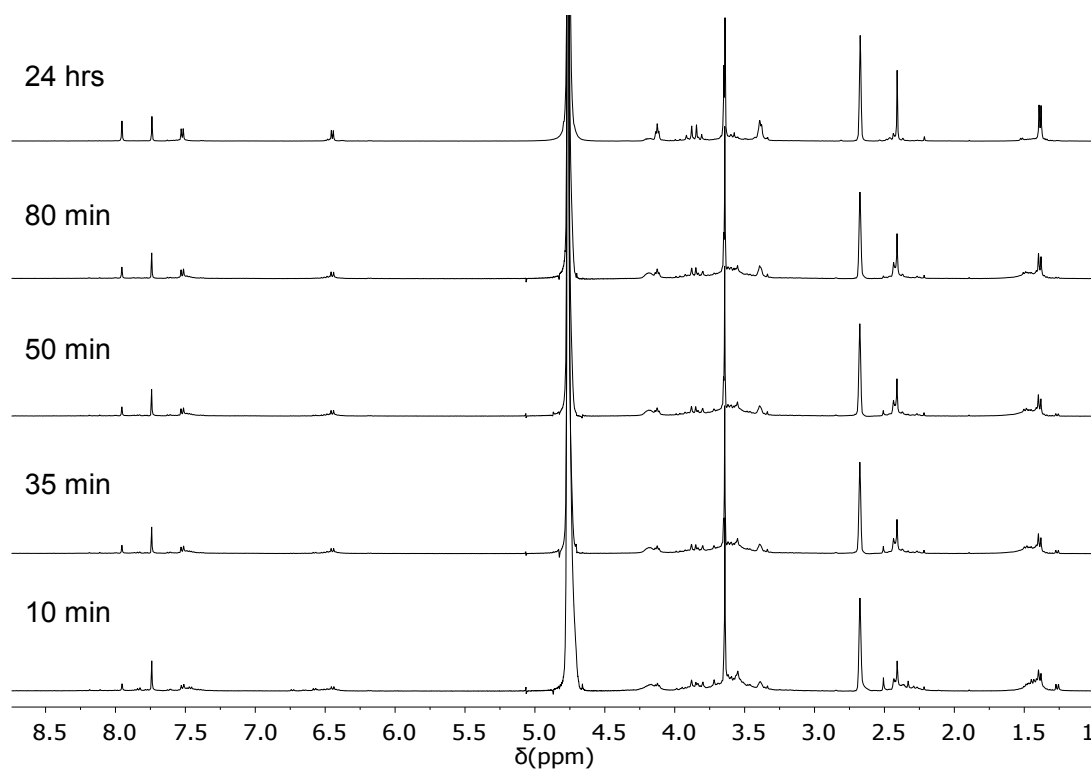


Figure S12. Time dependent ^1H NMR spectra of $[\text{PdH}(\text{L2})\text{Cl}_2] \cdot \text{H}_2\text{O}$ –9-MeG =1:4 system at $\text{pH} = 7.0$ ($c_{\text{M}} = 2.0 \text{ mM}$).