Electronic Supplementary Information

Water soluble, optically active monofunctional Pd(II) and Pt(II) compounds: Promising adhesive and antimigratory effects on human prostate PC-3 cancer cells

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Selected characterization data:

Selected FRET DNA melting assay data:

Figure S1. ^{1}H NMR spectrum of **a** in $CDCl_3$

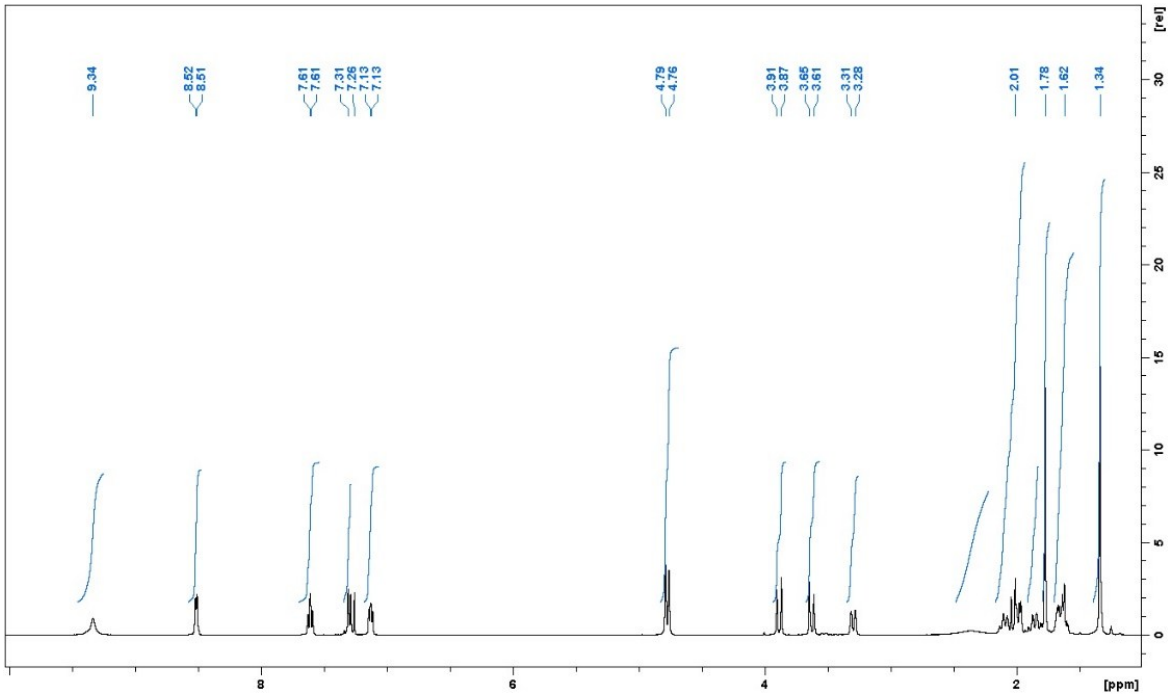


Figure S2. ^{1}H NMR spectrum of **a'** in $CDCl_3$

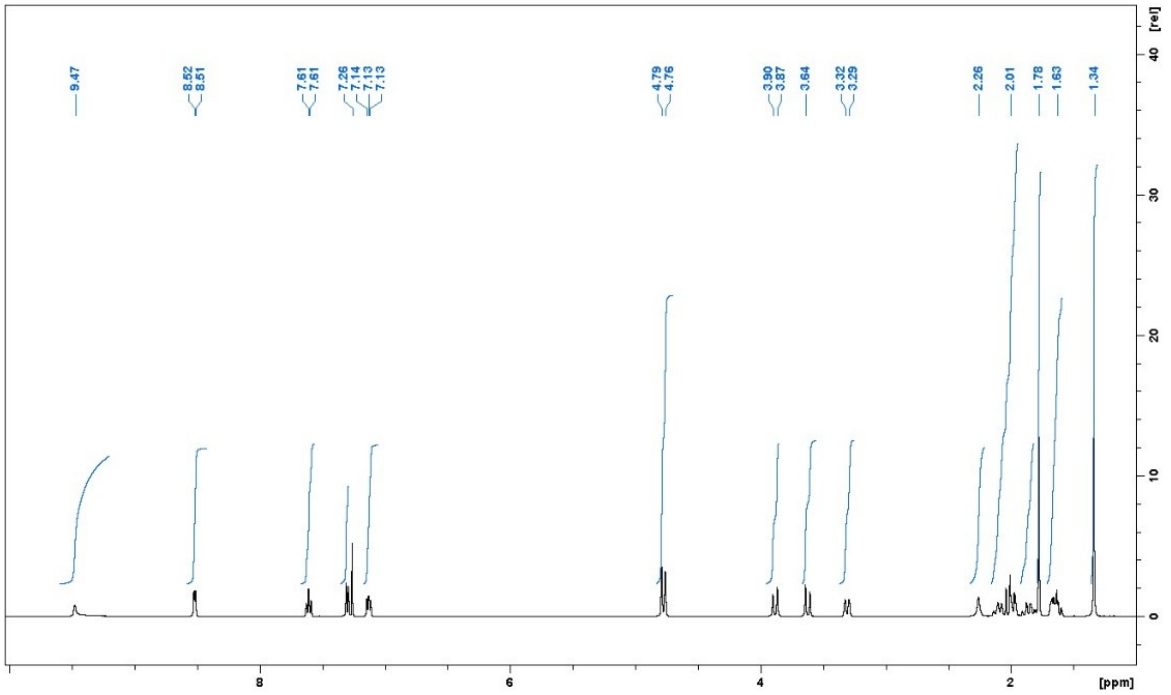


Figure S3. ^{1}H NMR spectrum of **1** in $CDCl_3$

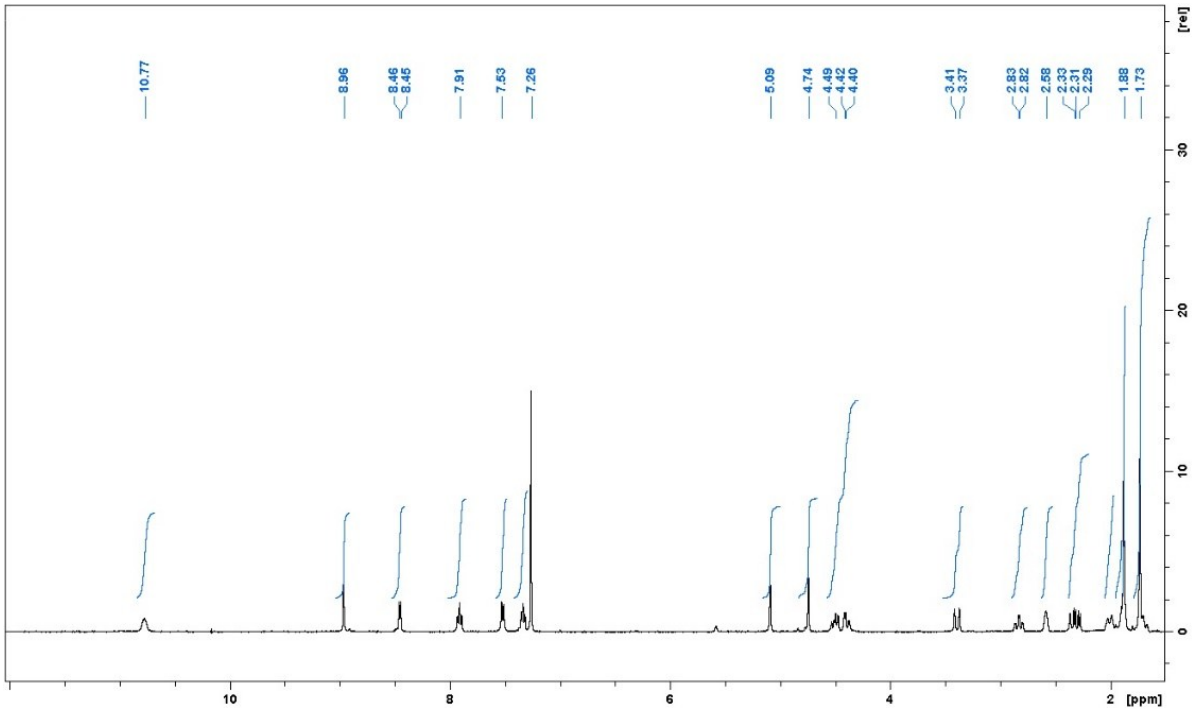


Figure S4. ^{1}H NMR spectrum of **1'** in $CDCl_3$

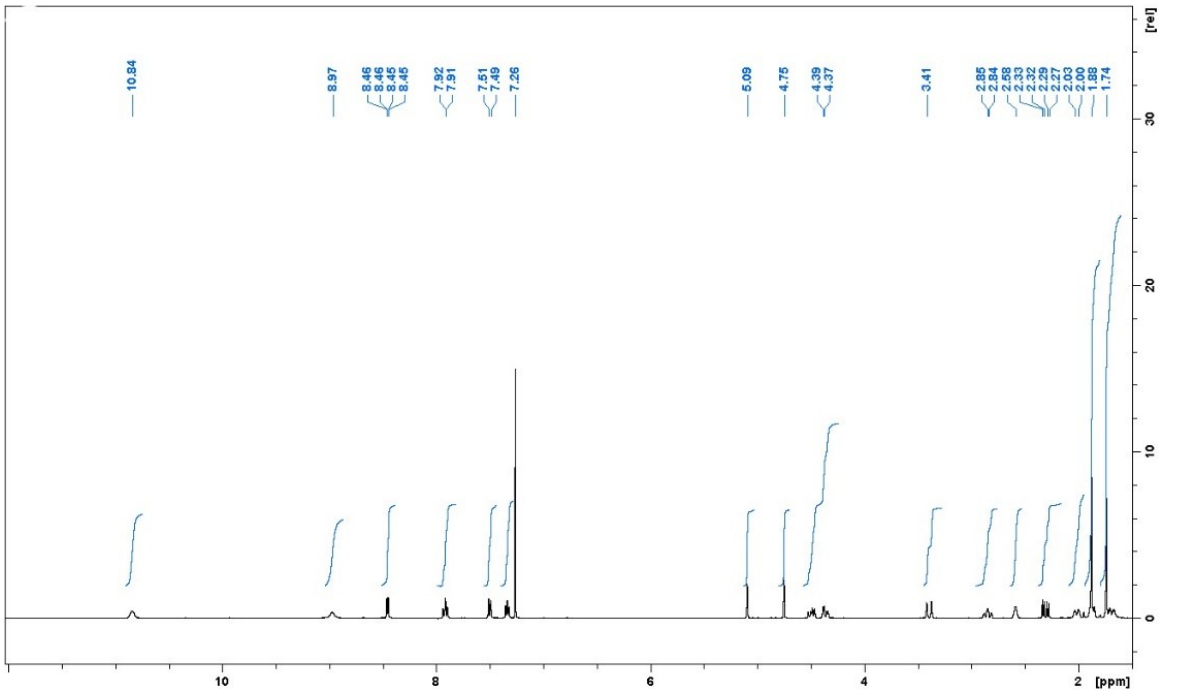


Figure S5. ^{13}C-^{1}H HSQC NMR spectrum of **1** in $CDCl_3$.

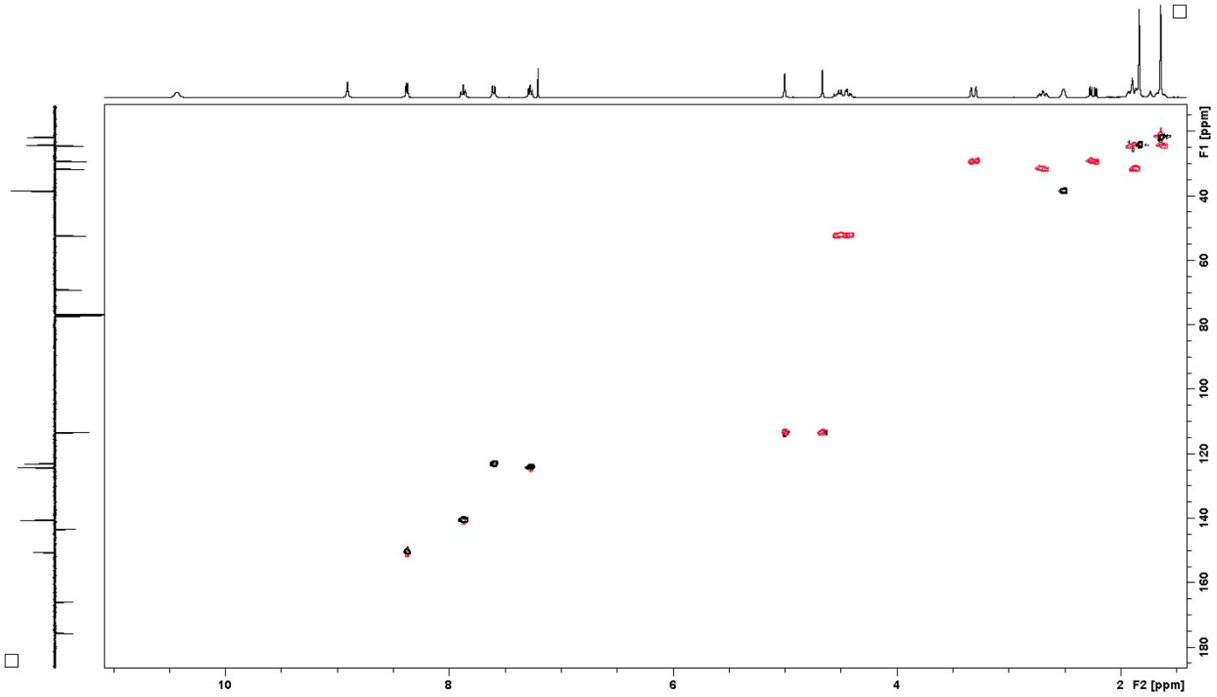


Figure S6. ^{13}C-^{1}H HMBC NMR spectrum of **1** in $CDCl_3$ (Assignment of =NO<u>H</u>)

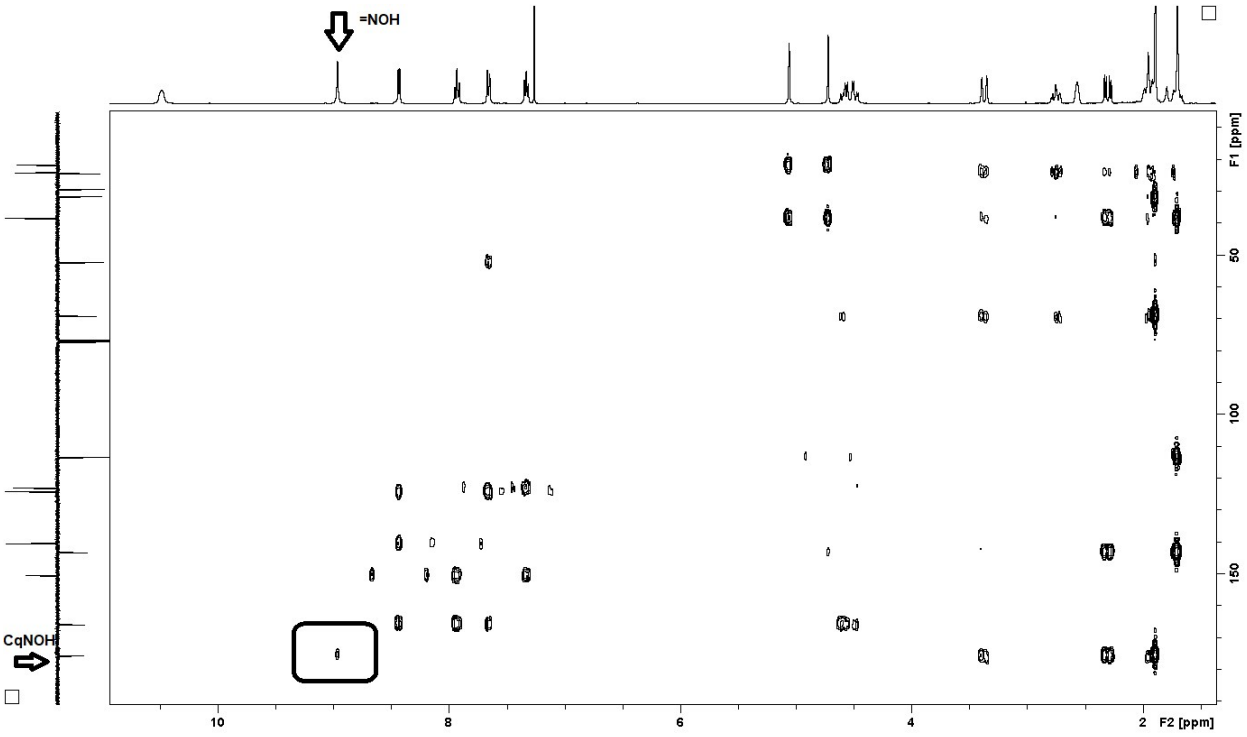


Figure S7. ^{15}N-^{1}H HMBC NMR spectrum of **1** in $CDCl_3$.

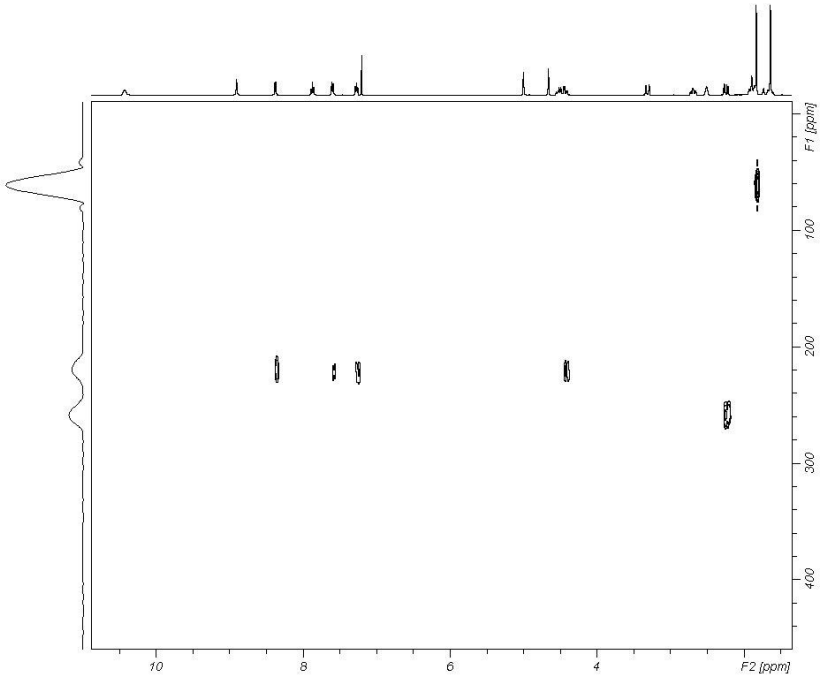


Figure S8. 2D NOESY NMR spectrum of **1** in $CDCl_3$

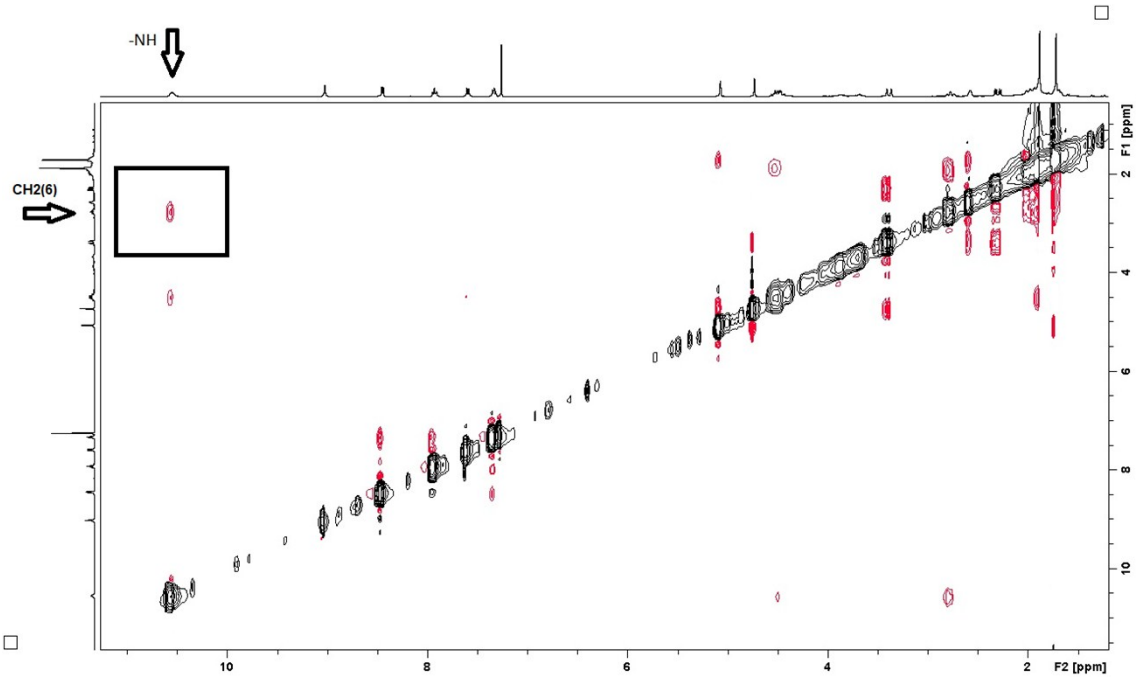


Figure S9. ^{1}H NMR spectrum of **2** in $CDCl_3$

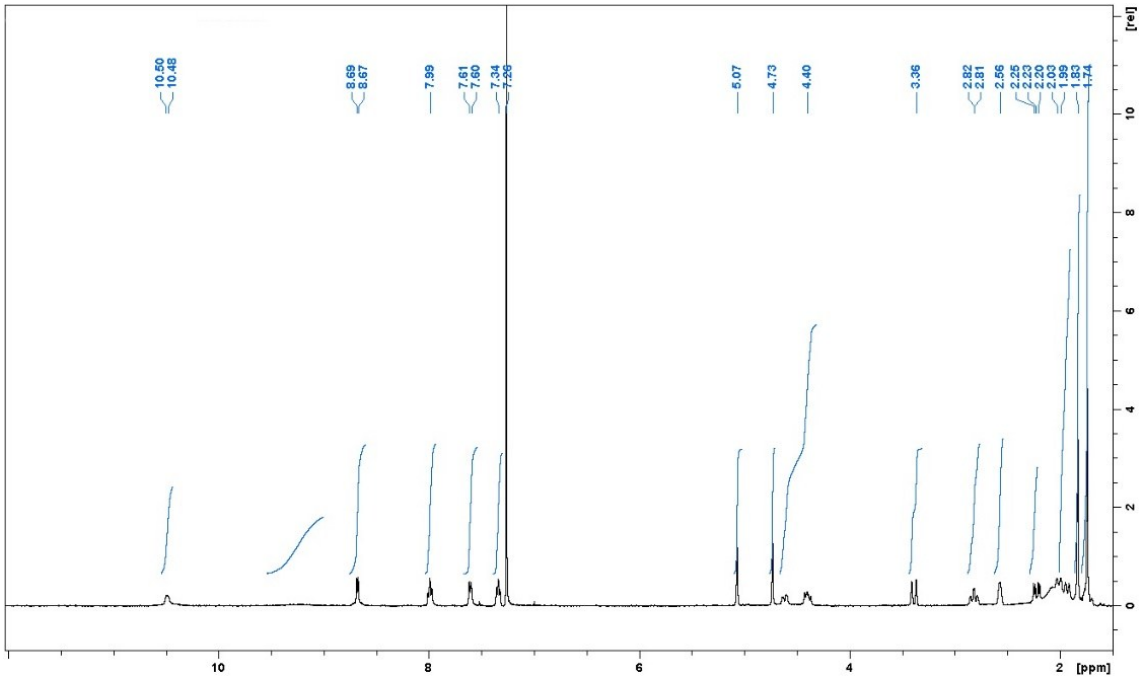


Figure S10. ^{1}H NMR spectrum of **2'** in $CDCl_3$

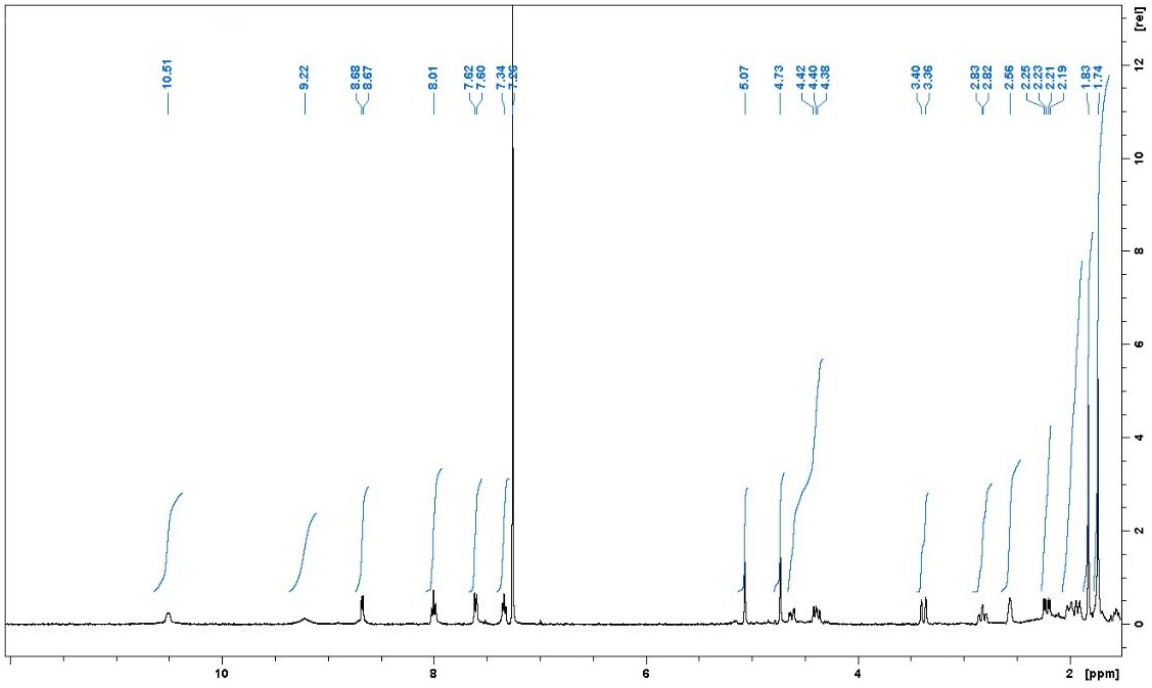


Figure S11. ^{13}C-^{1}H HSQC NMR spectrum of **2** in $CDCl_3$.

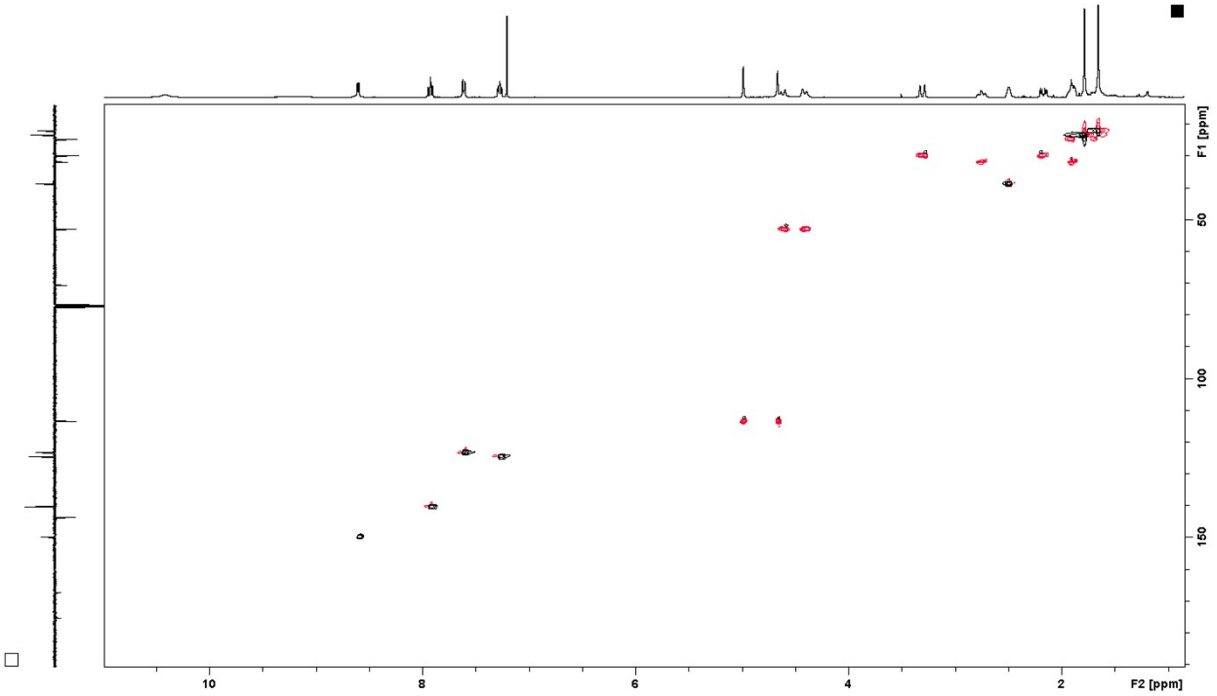


Figure S12. ^{15}N-^{1}H HMBC NMR spectrum of **2** in $CDCl_3$.

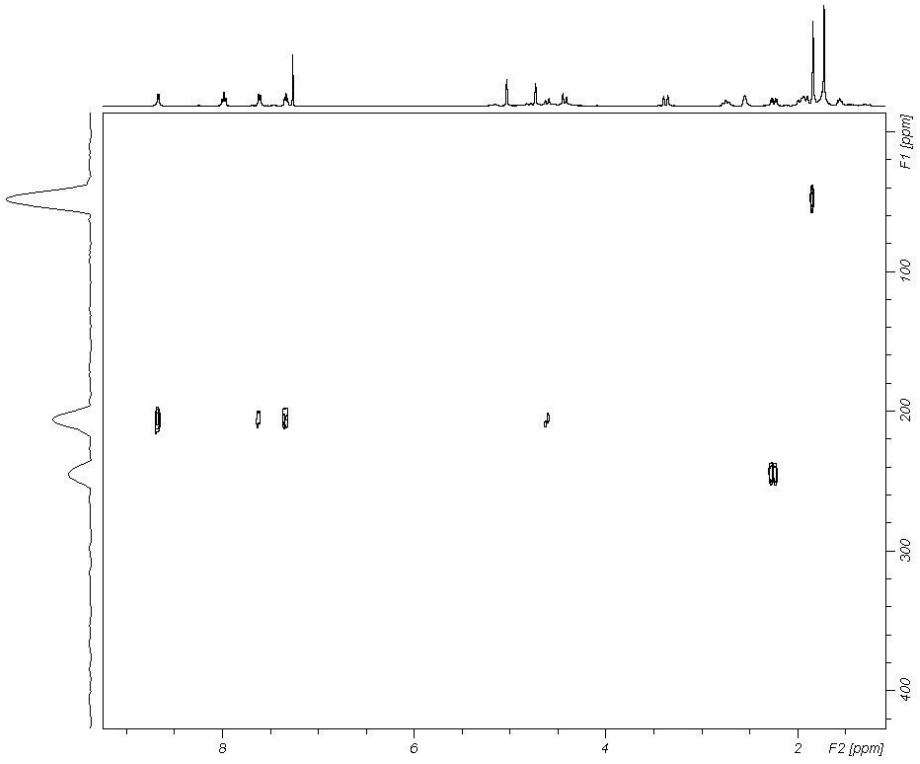


Figure S13. 2D NOESY NMR spectrum of **2** in $CDCl_3$

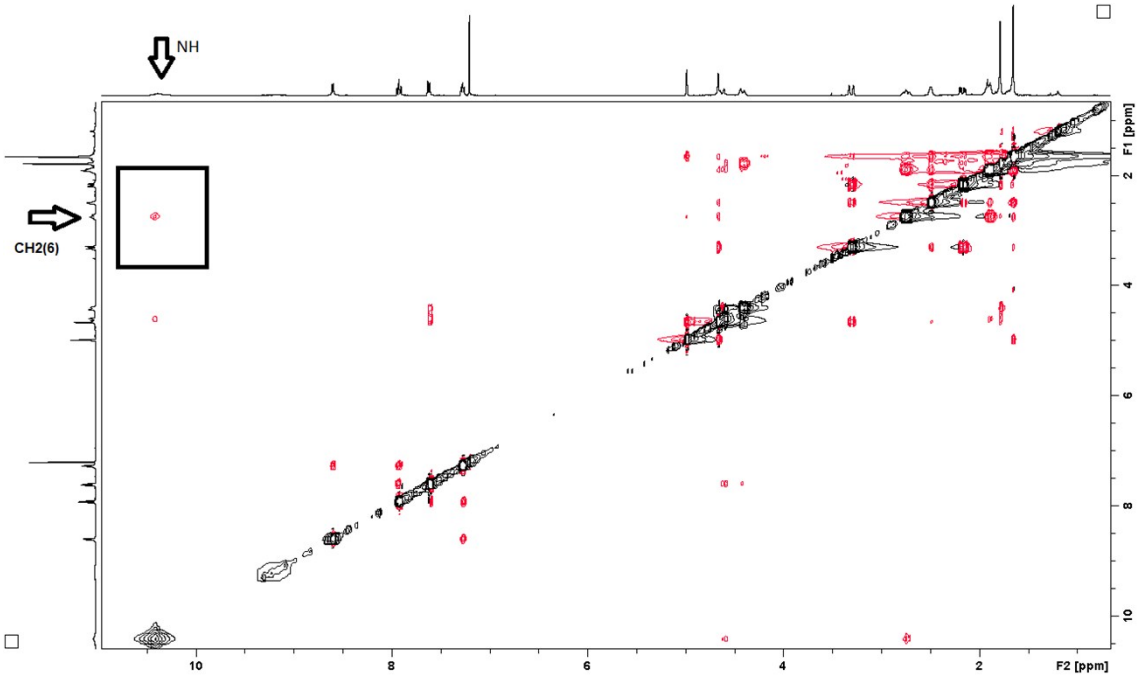


Figure S14. Comparison of UV-vis spectra of pro-ligand **a** and compound **1** in water or PBS.

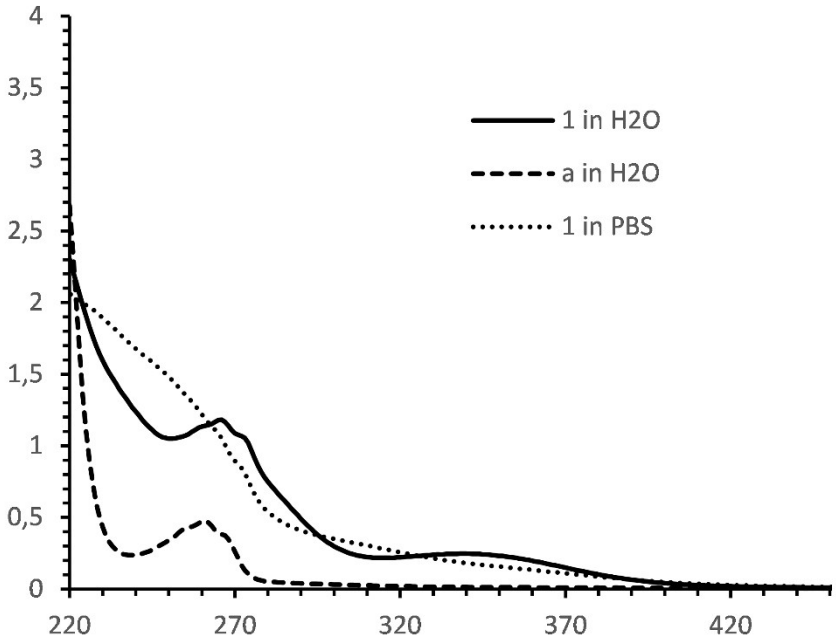


Figure S15. Comparison of UV-vis spectra of pro-ligand **a** and compound **2** in water or PBS.

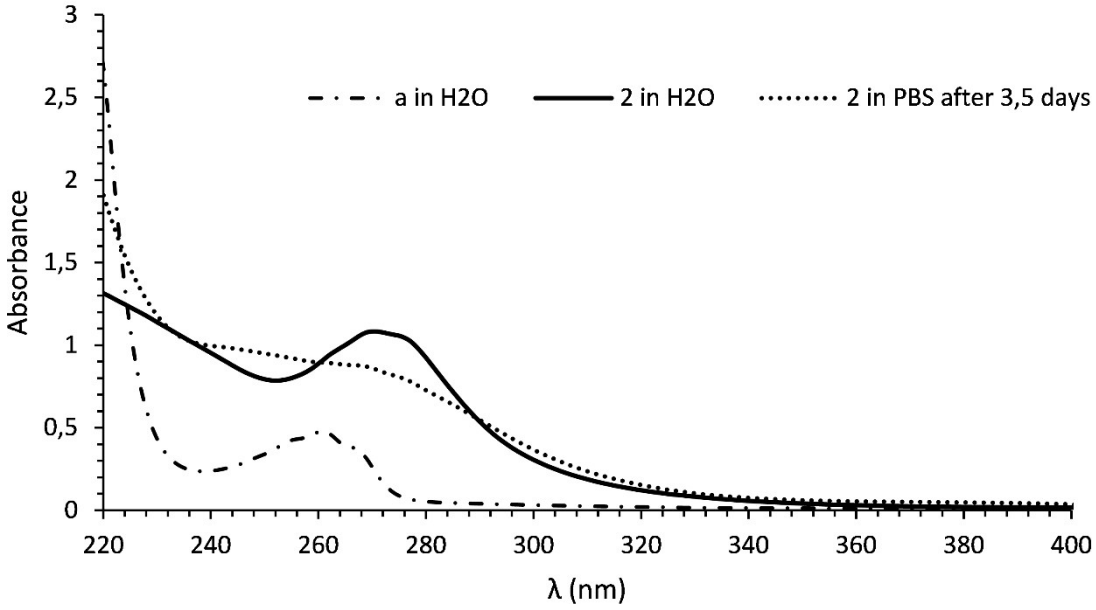


Figure S16. CD spectra of enantiomers **1** and **1'** in water solution.

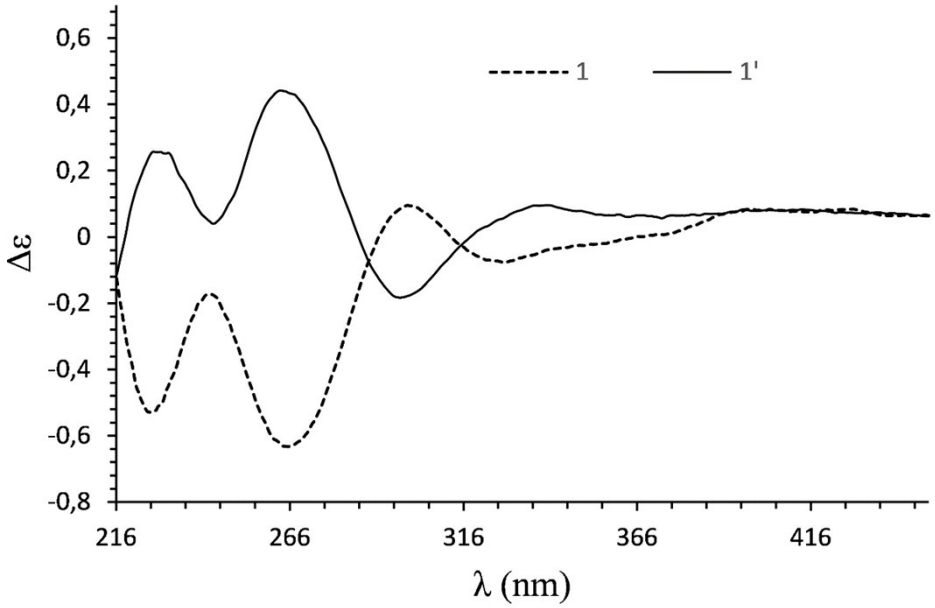


Figure S17. ^{1}H NMR spectrum of **3** in $CDCl_3$

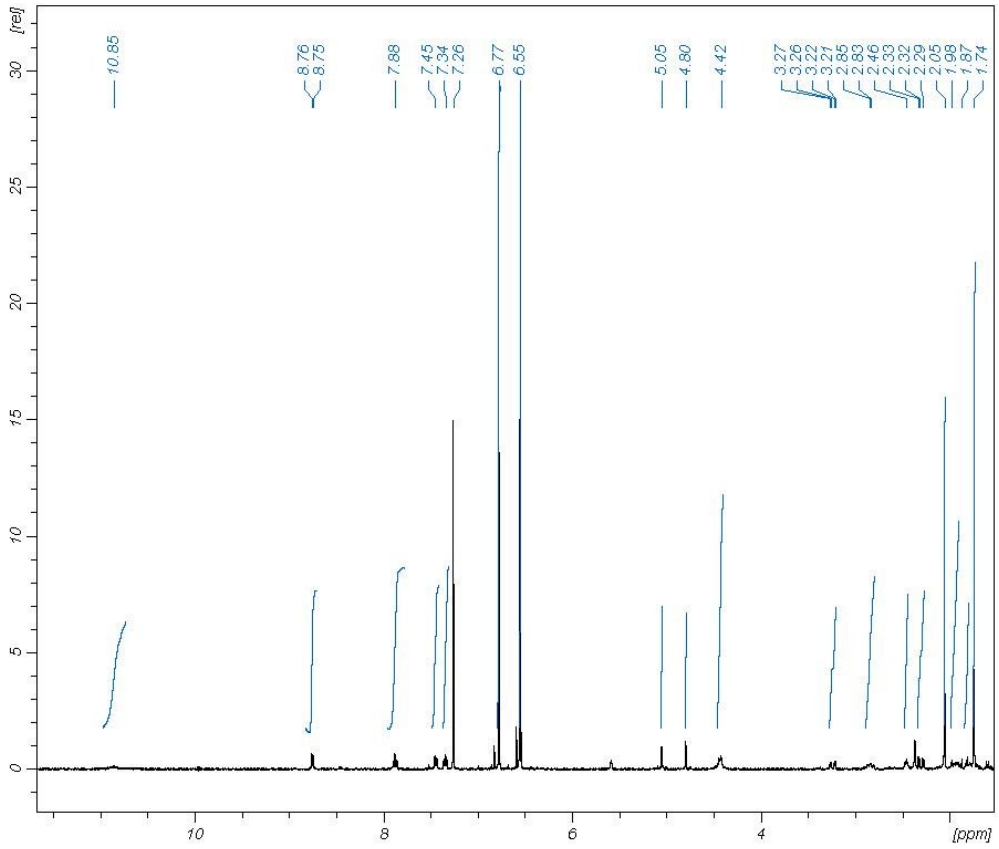


Figure S18. ^{13}C-APT NMR spectrum of **3** in $CDCl_3$.

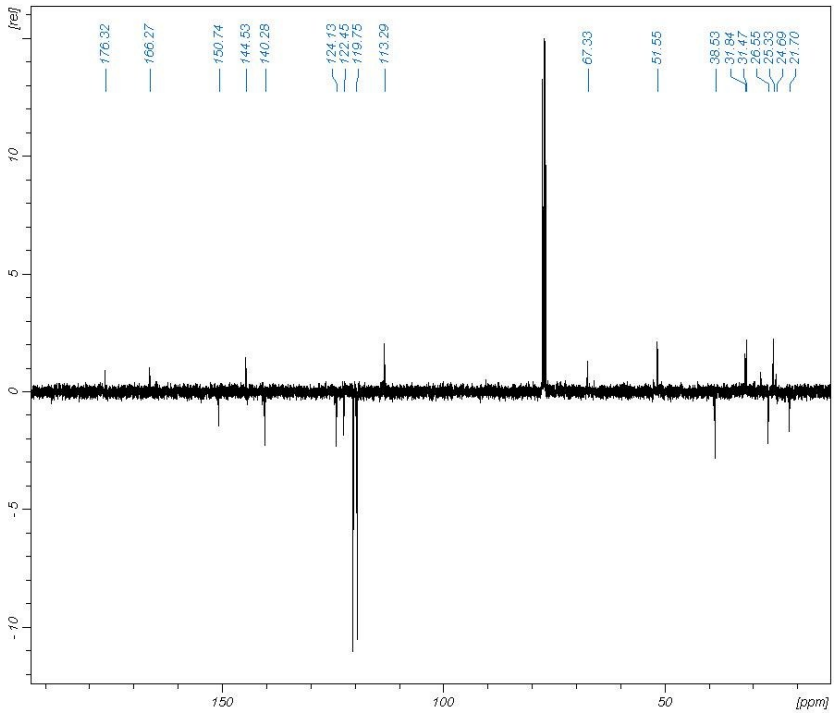


Figure S19. ^{15}N-^{1}H HMBC NMR spectrum of **3** in $CDCl_3$.

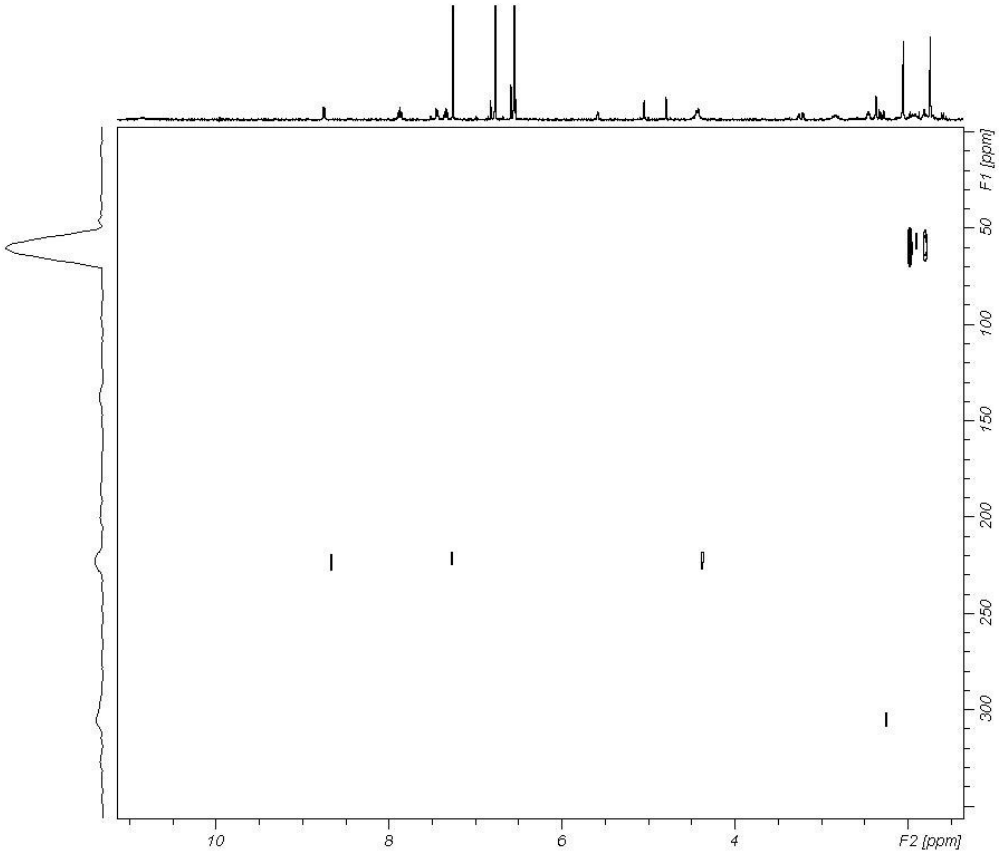


Figure S20. 2D NOESY NMR spectrum of **3** in $CDCl_3$

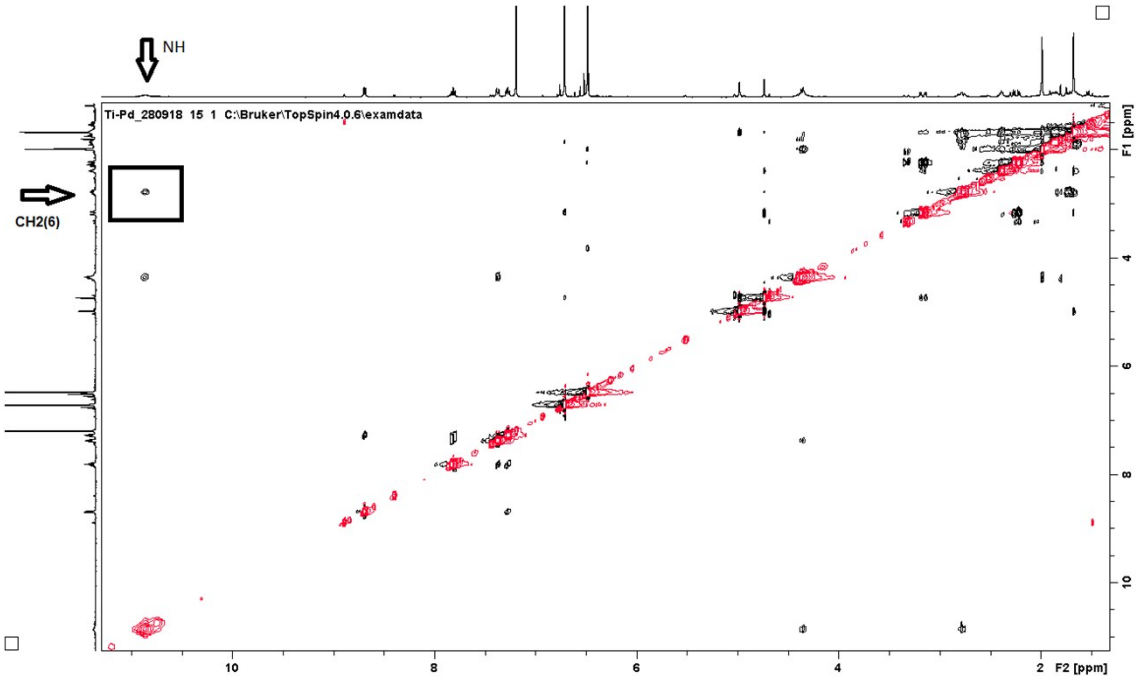


Figure S21. Time-dependent ^{1}H NMR spectra of **1** (10 mM) in water-d_2 (pH* = 2.3), with and without NaCl.

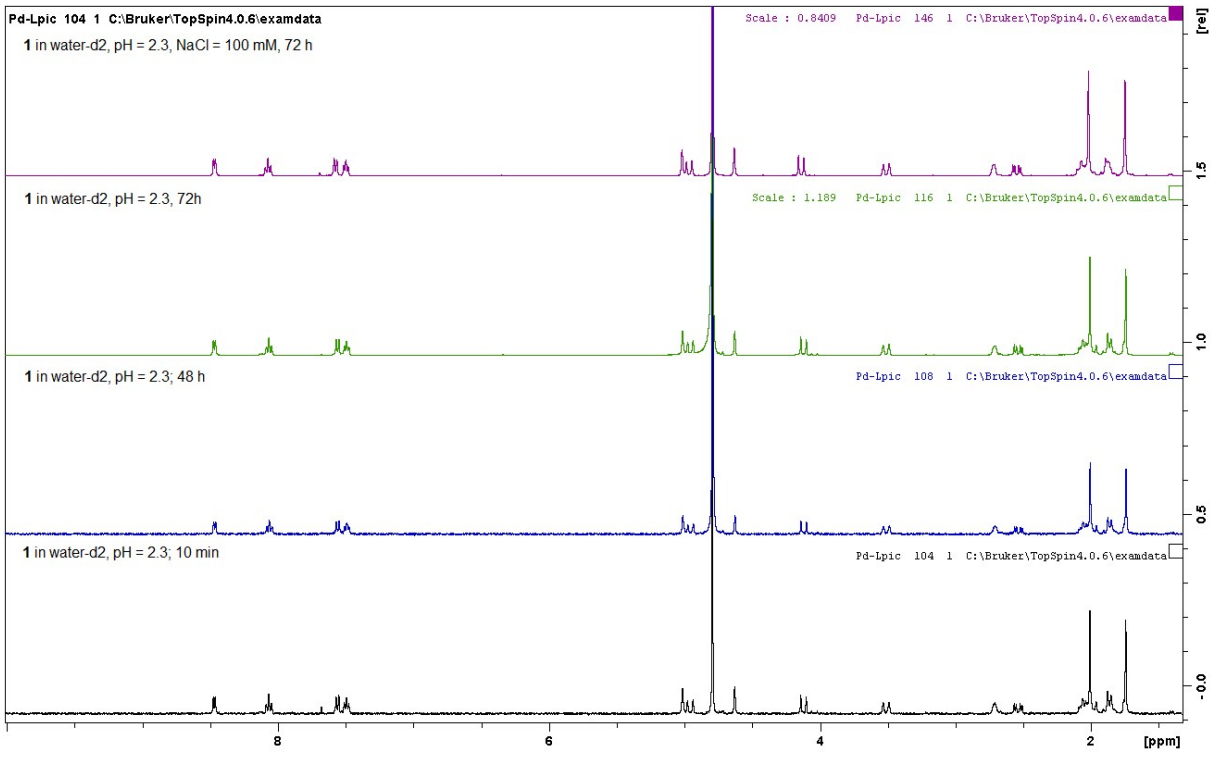


Figure S22. pH-dependent ^{1}H NMR spectra of **1** (10 mM) in water-d_2 and comparison with ^{1}H NMR of **1** (10 mM) in deuterated PBS.

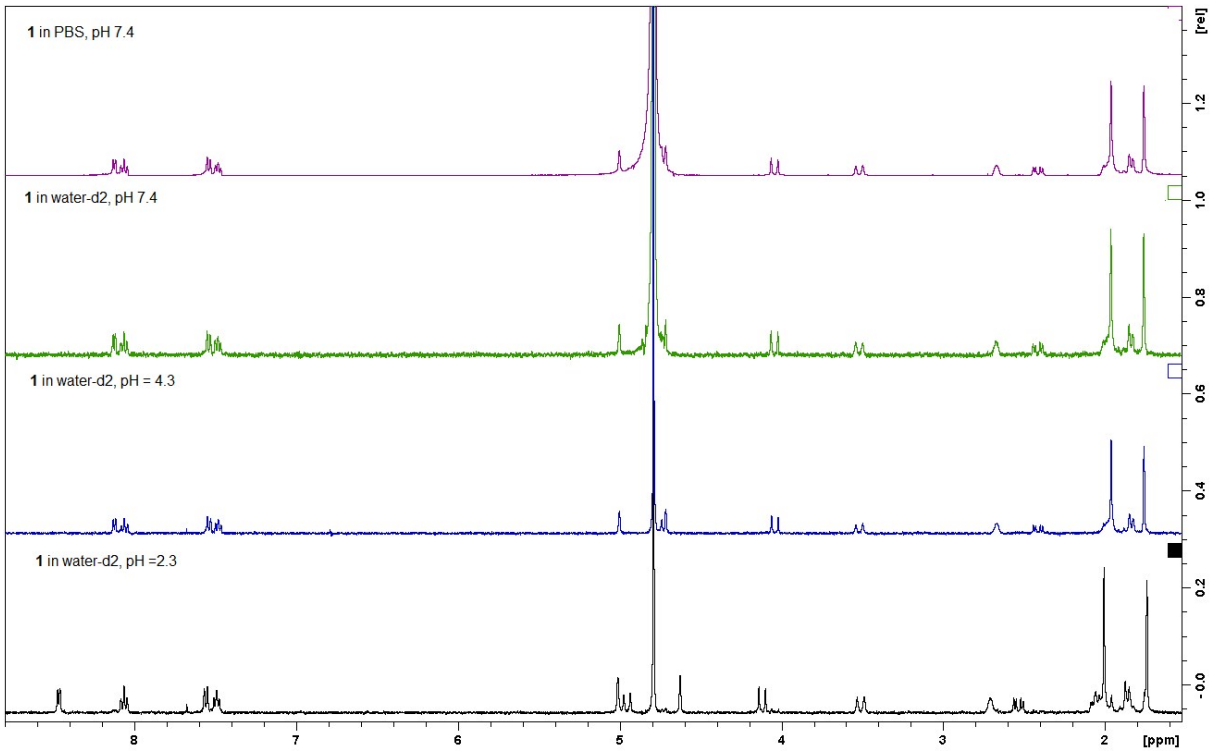


Figure S23. ^{1}H NMR spectrum of **1** in water-d_2 (pH* = 2.3).

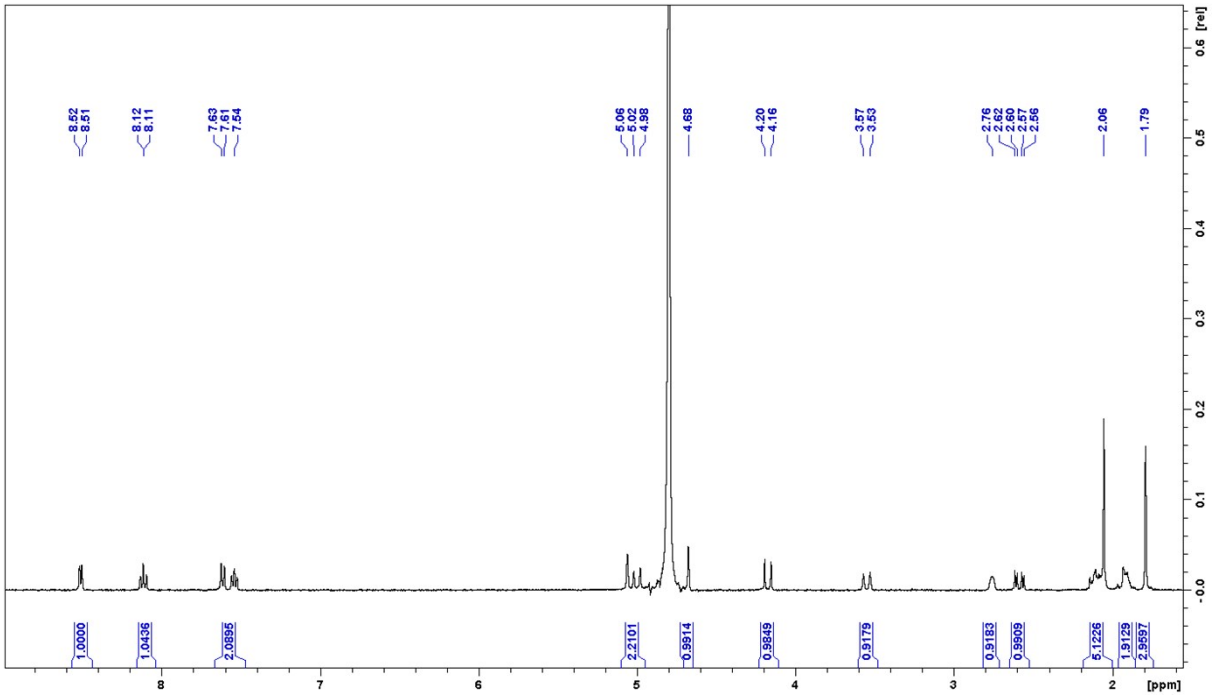


Figure S24. ^{13}C APT NMR spectrum of **1** (10 mM) in water-d_2 (pH* = 2.3).

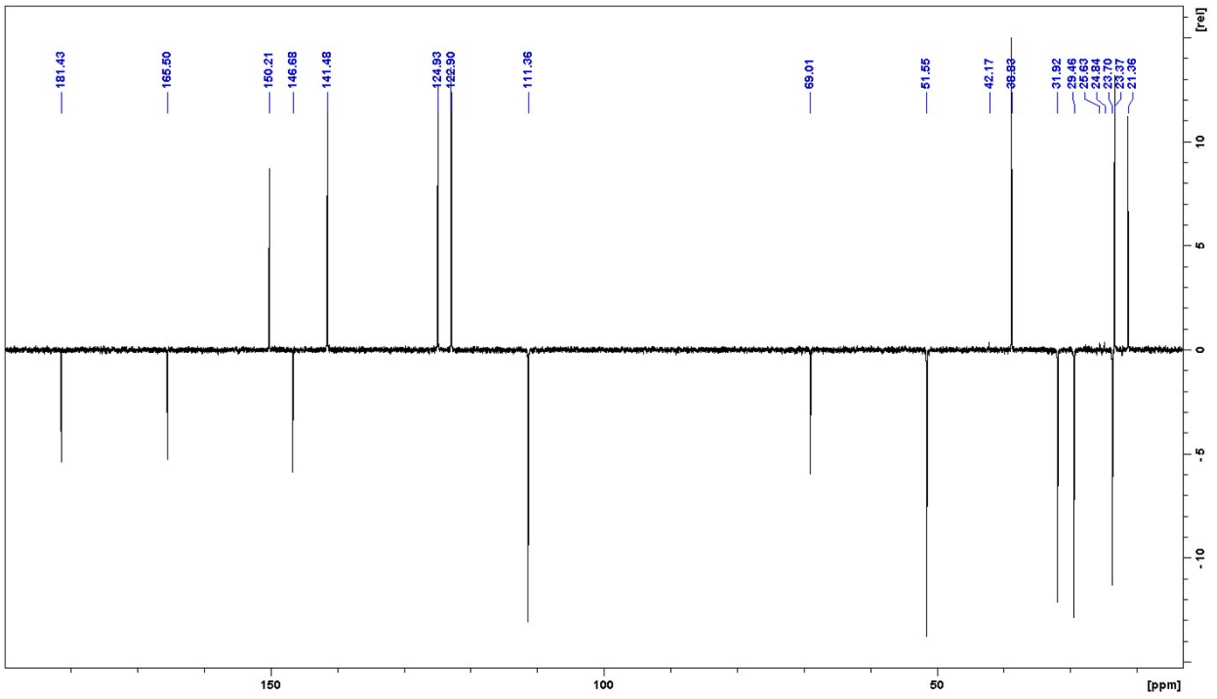


Figure S25. ^{15}N-^{1}H HMBC NMR spectrum of **1** (10 mM) in water-d_2 (pH* = 2.3).

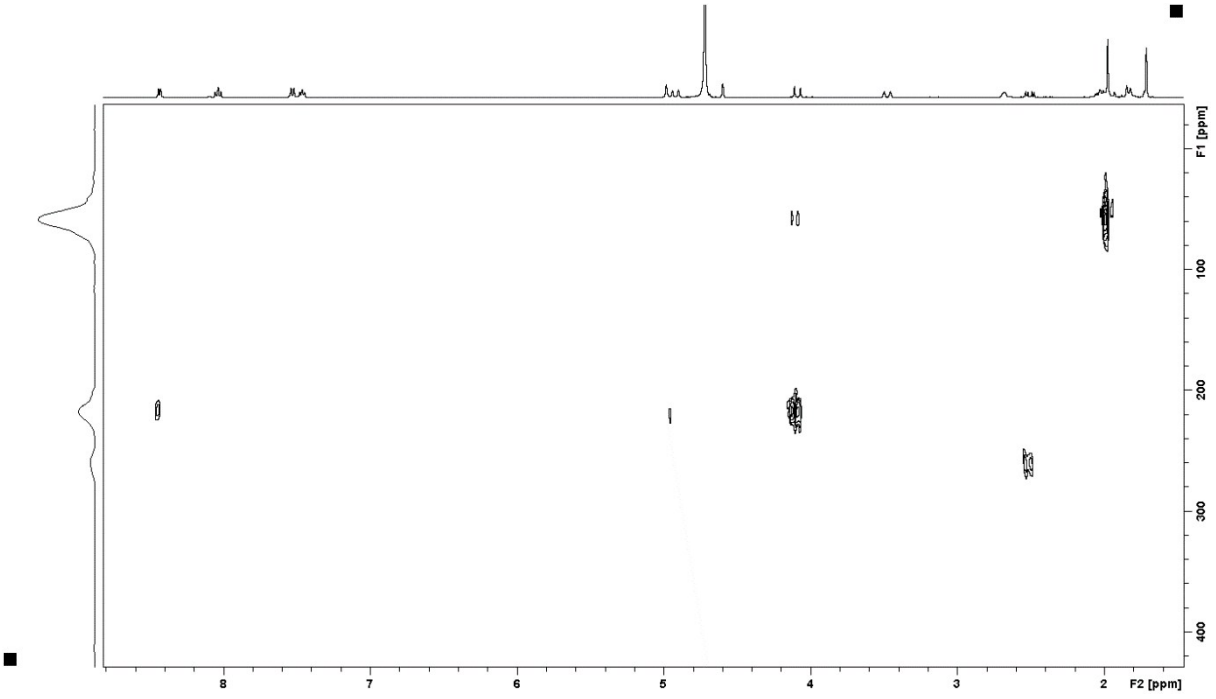
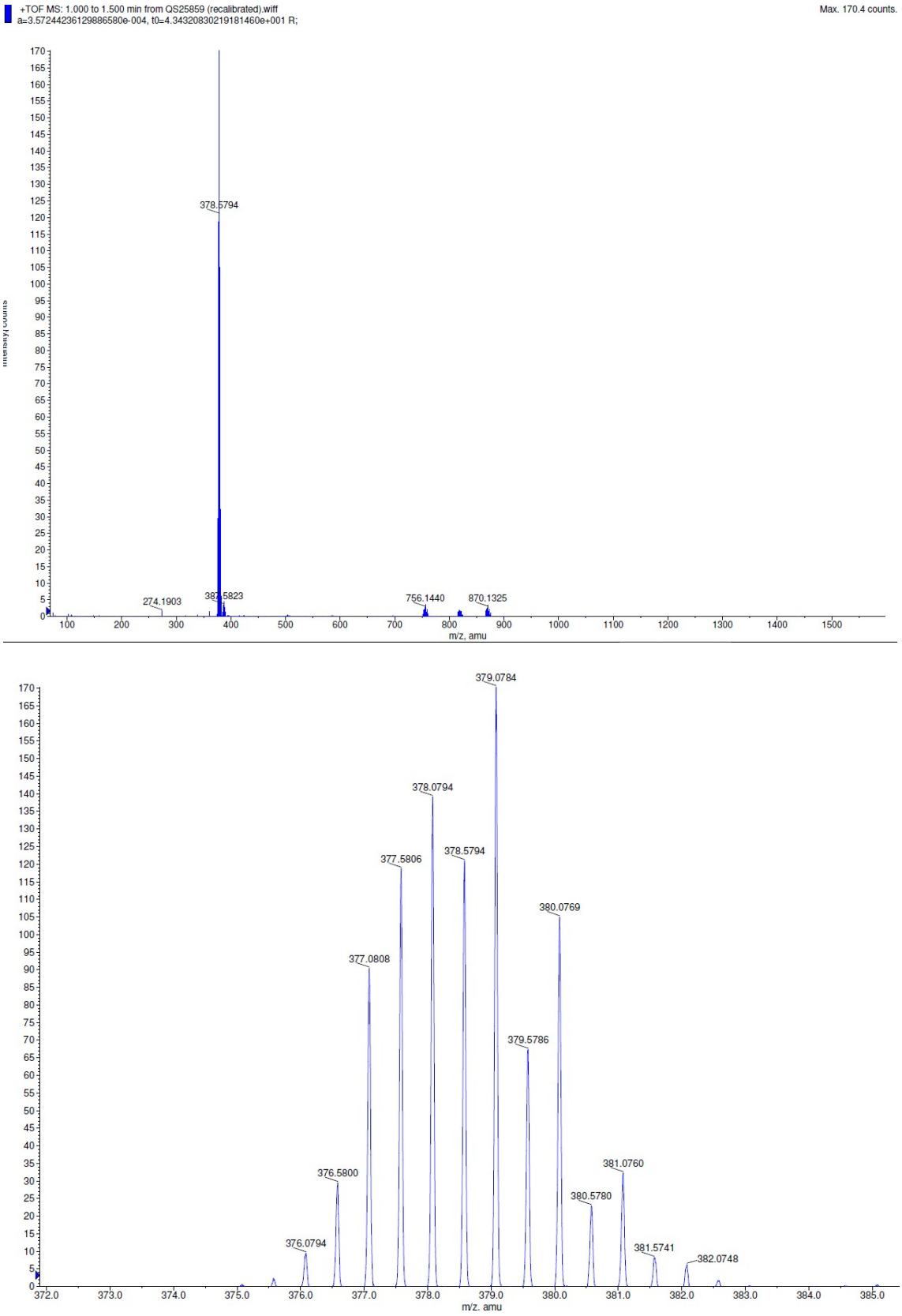


Figure S26. HR-ESI-MS spectrum of **1** (after pH = 7.4).



Pd1				
MASA TEORICA	MASA EXPERIMENTAL	ERROR (ppm)	ERROR (amu)	
376.0802	376.0794	2.1272	-0.0008	
376.5805	376.58	1.3277	-0.0005	
377.0804	377.0808	-1.0608	0.0004	
377.5805	377.5806	-0.2648	0.0001	
378.0801	378.0794	1.8515	-0.0007	
378.5806	378.5794	3.1697	-0.0012	
379.0802	379.0784	4.7483	-0.0018	
379.5812	379.5786	6.8497	-0.0026	
380.0804	380.0769	9.2086	-0.0035	

Figure S27. ^{1}H NMR of **1** in water-d_2 (pH* = 7.4).

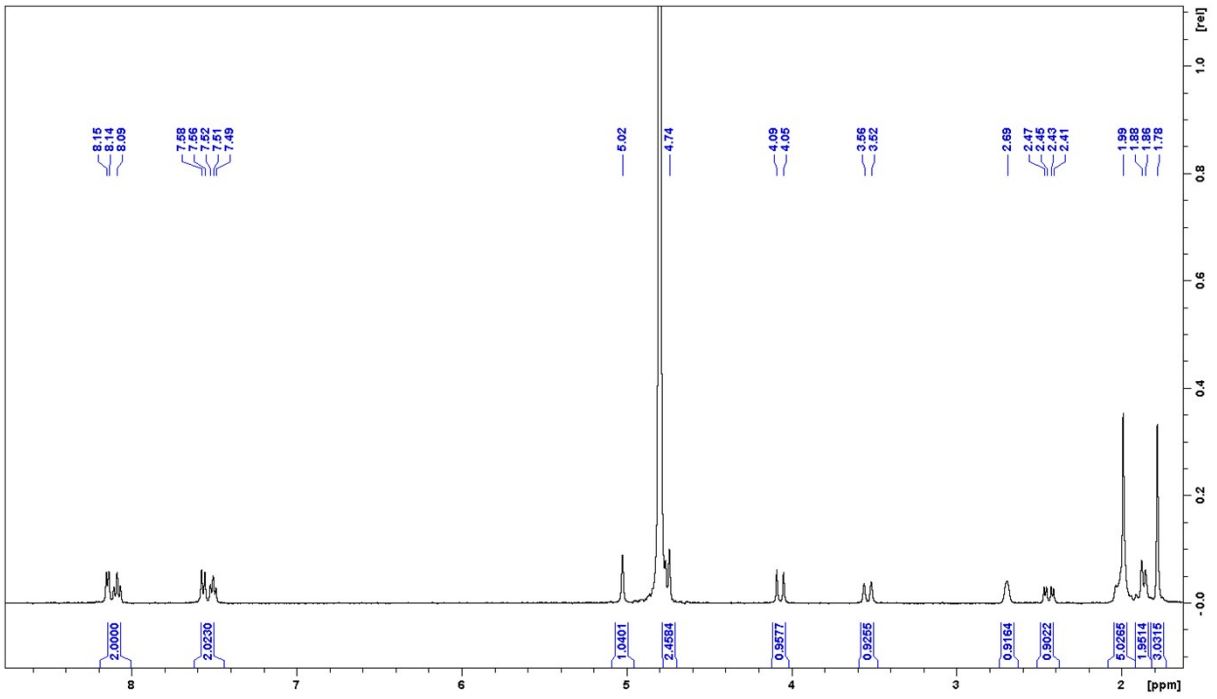


Figure S28. ^{13}C-^{1}H HSQC NMR spectrum of **1** in water-d_2 (pH* = 7.4).

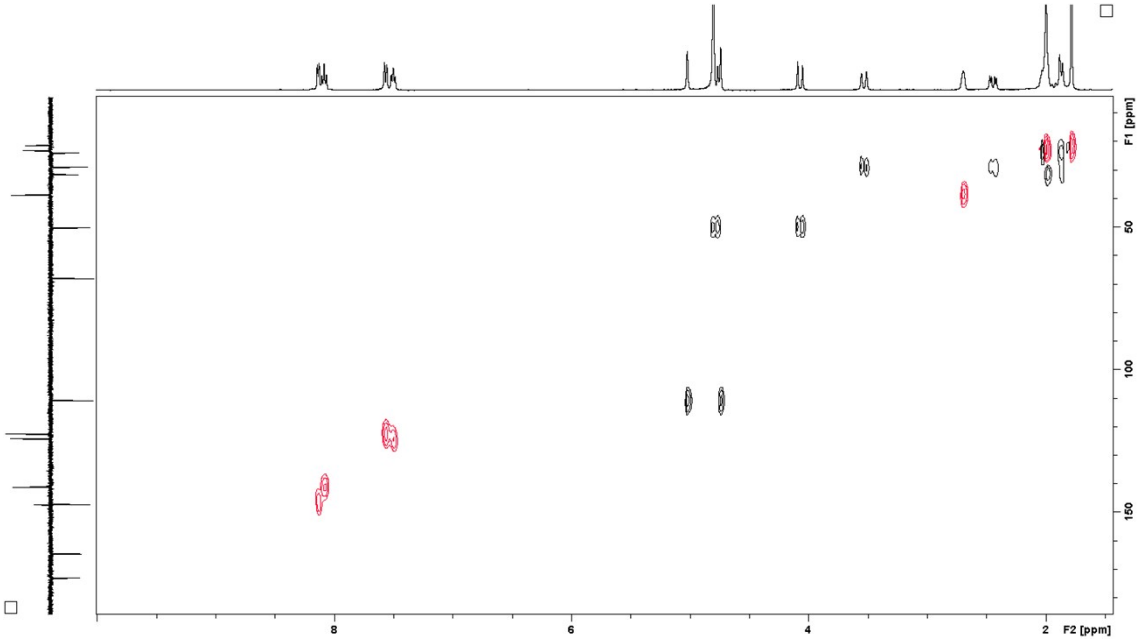


Figure S29. ^{15}N-^{1}H HMBC NMR spectrum of **1** in water-d_2 (pH* = 7.4).

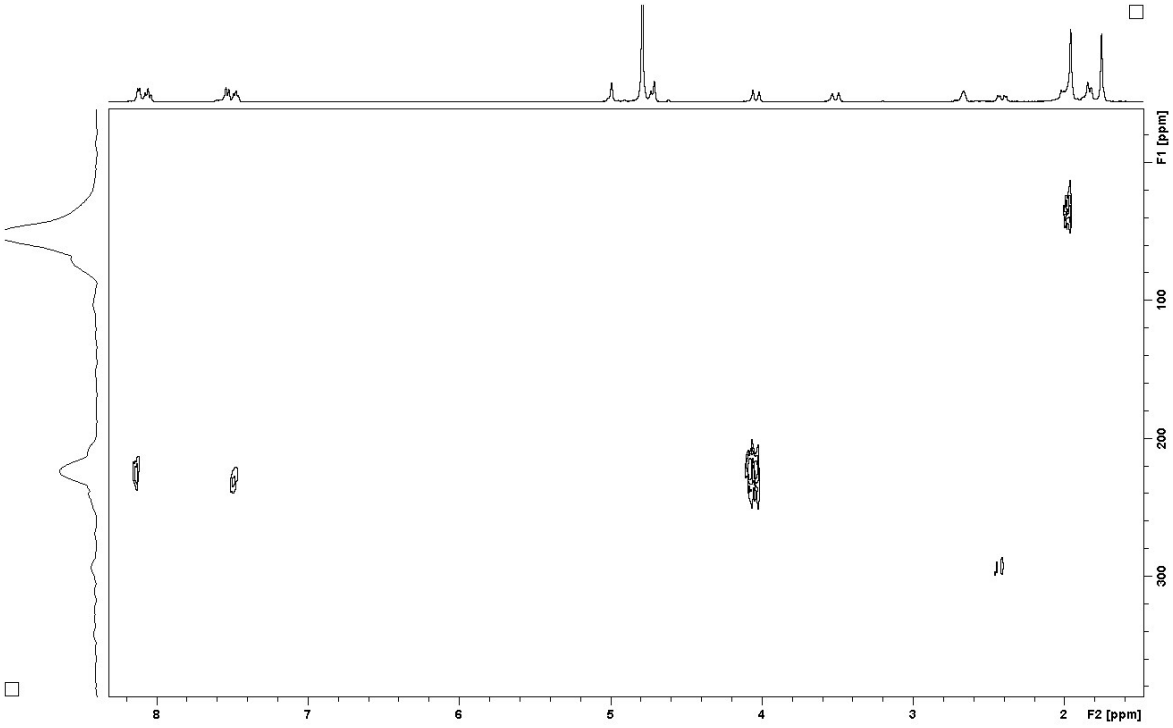


Figure S30. ^{1}H-^{1}H COSY NMR spectrum of **1** in water-d_2 (pH* = 7.4).

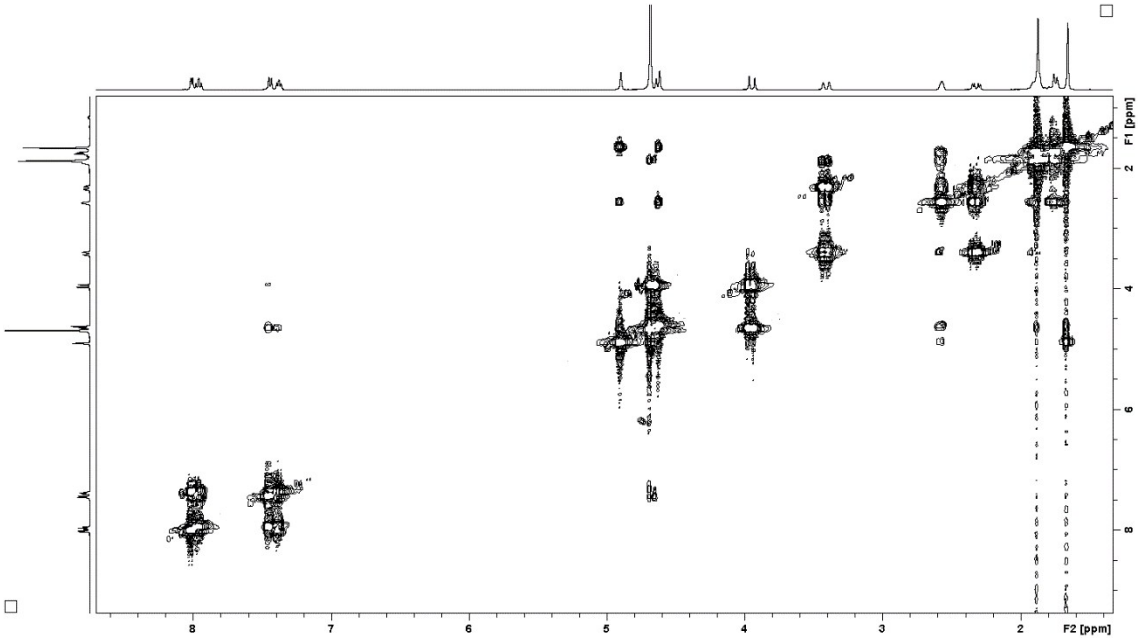


Figure S31. 2D NOESY NMR spectrum of **1** in water-d_2 (pH* = 7.4).

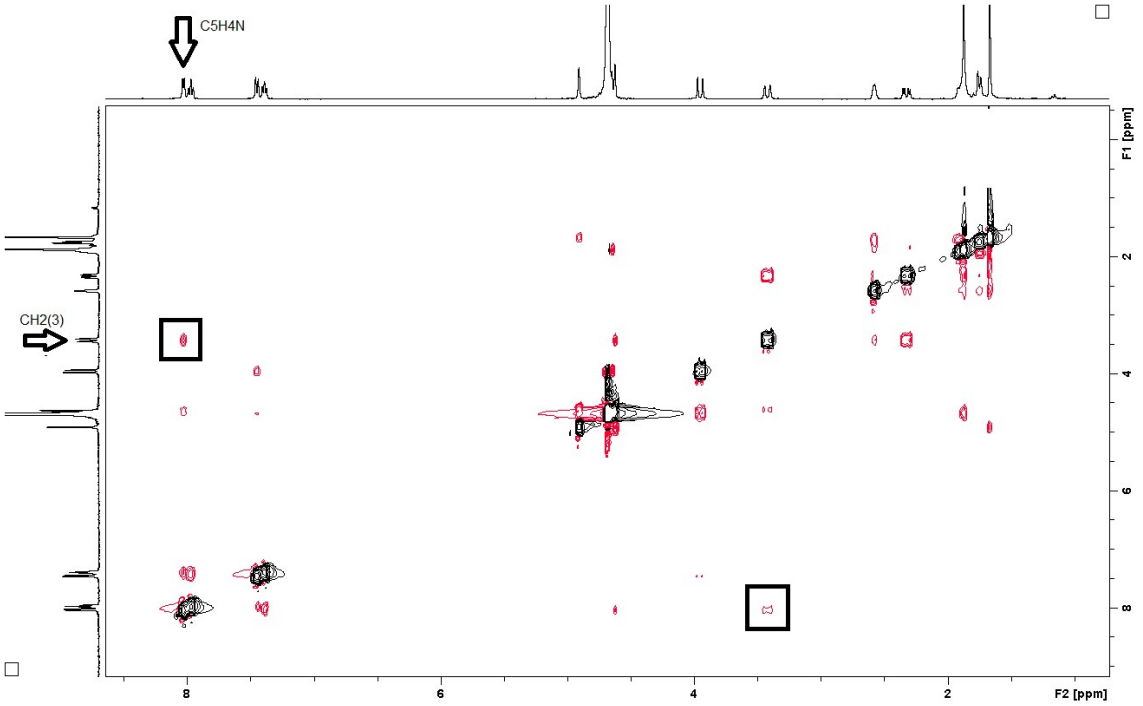


Figure S32. Time-dependent ^{1}H NMR spectra of **2** (10 mM) in water-d_2 at pH* = 3.0, with and without NaCl (100 mM).

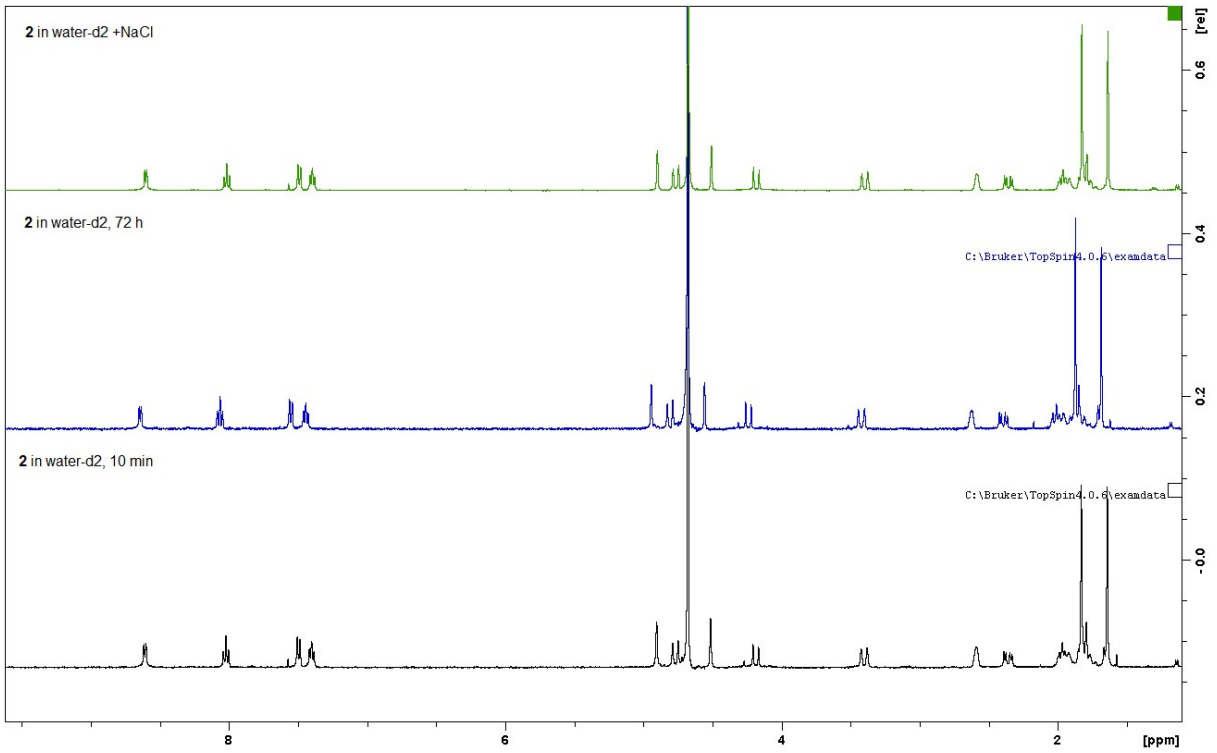


Figure S33. Time dependent ^{1}H NMR of **2** (10 mM) in PBS at pH* = 7.4.

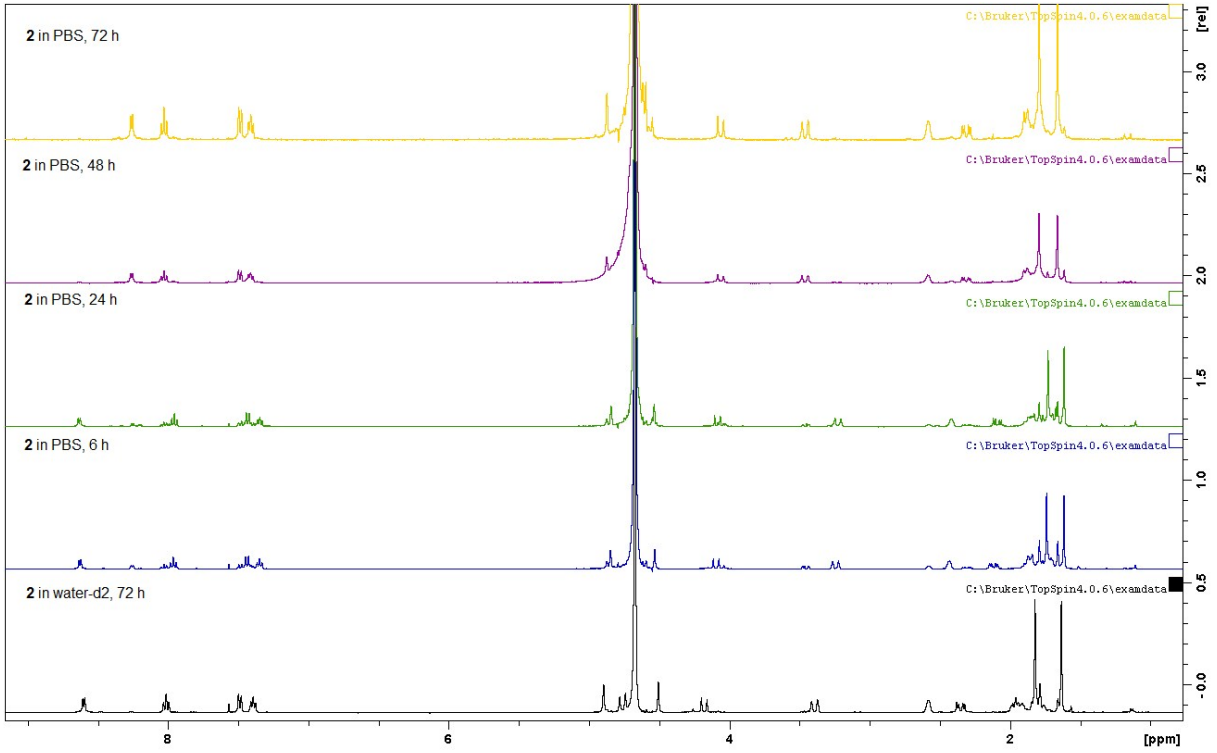


Figure S34. ^{1}H NMR spectrum of **2** (pH* = 3.0) in water-d_2

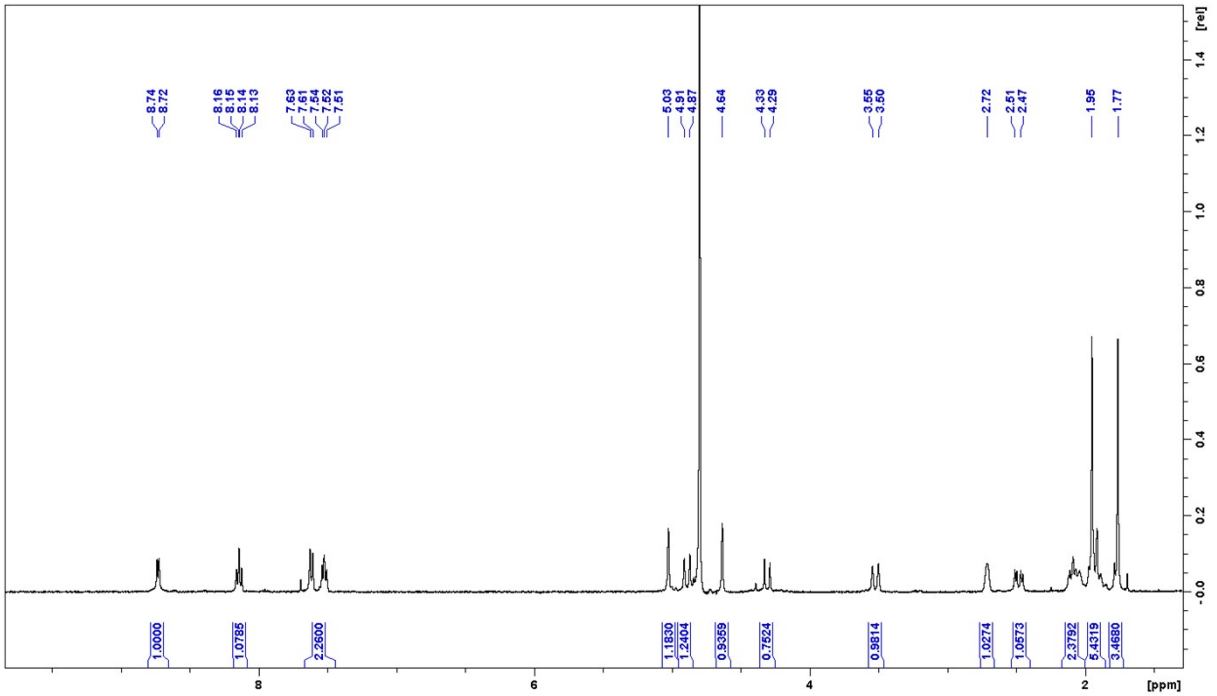


Figure S35. APT ^{13}C NMR spectrum of **2** (pH* = 3.0) in water-d_2

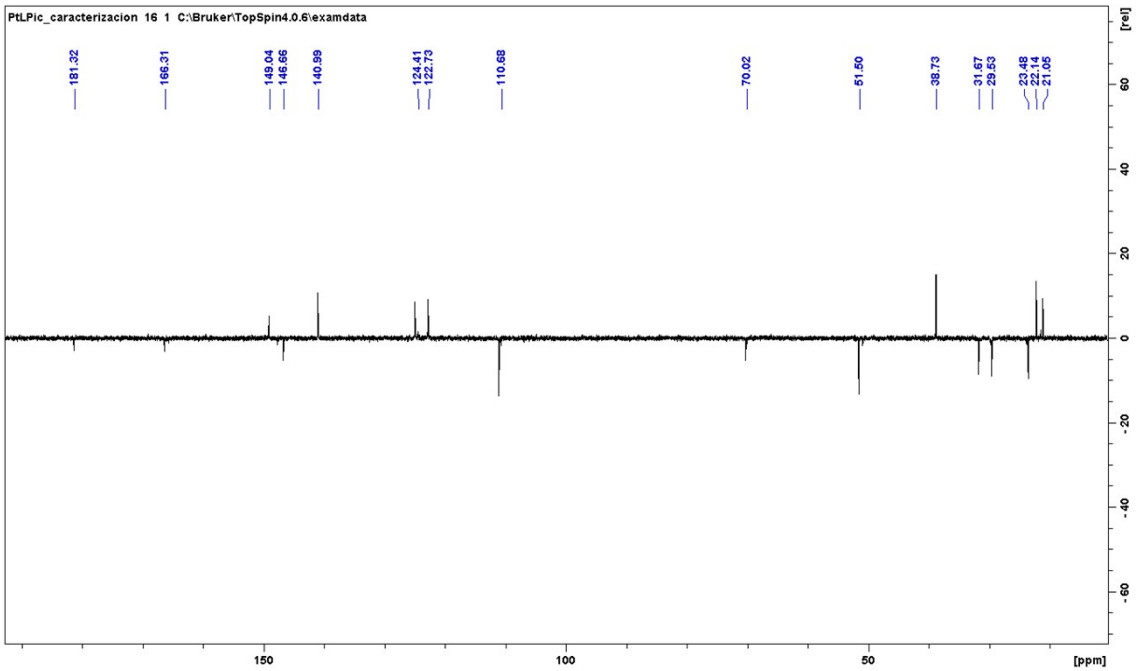
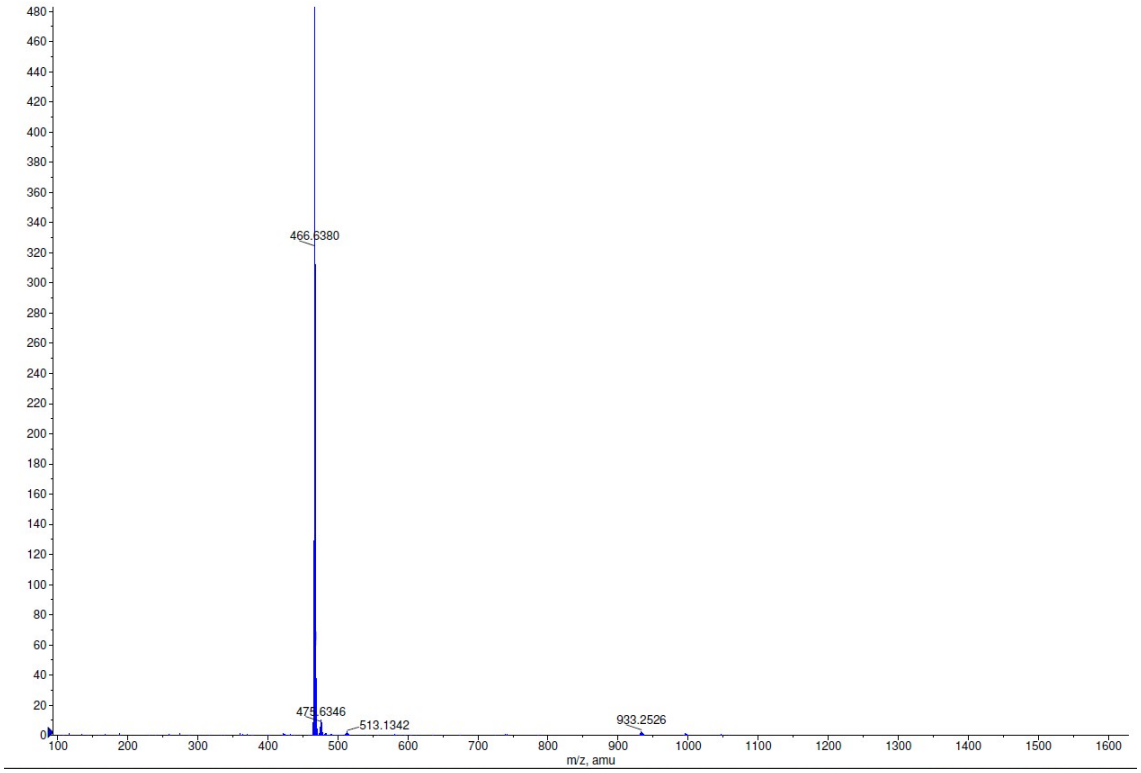
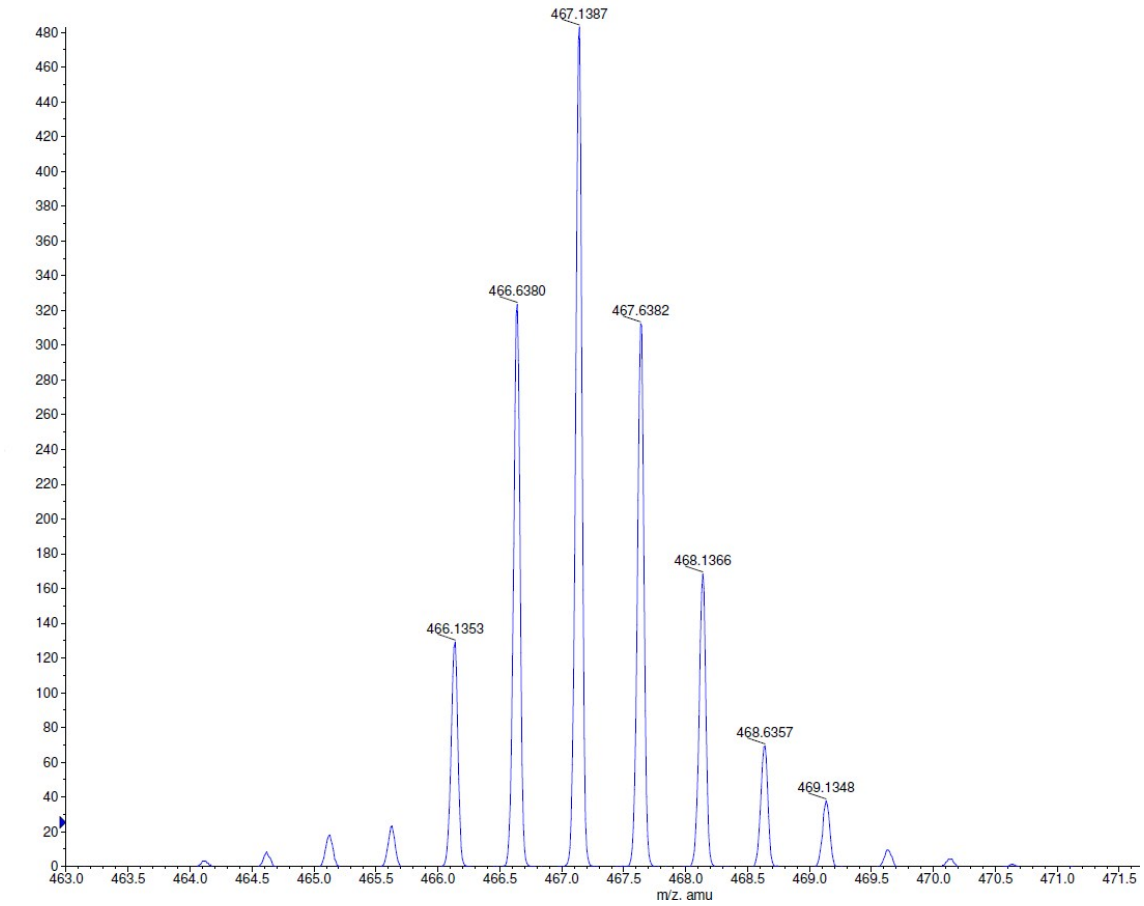


Figure S36. HR-ESI-MS spectrum of **2** (after pH* = 7.4, 72 h)





Pt1

MASA TEORICA	MASA EXPERIMENTAL	ERROR (ppm)	ERROR (amu)	
466.1385	466.1353	6.8649	-0.0032	
466.6396	466.638	3.4288	-0.0016	
467.1402	467.1387	3.2110	-0.0015	
467.641	467.6382	5.9875	-0.0028	
468.1415	468.1366	10.4669	-0.0049	
468.6424	468.6357	14.2966	-0.0067	

Figure S37. ^{1}H NMR spectrum of **2** in water-d_2 (pH* = 7.4, 72h).

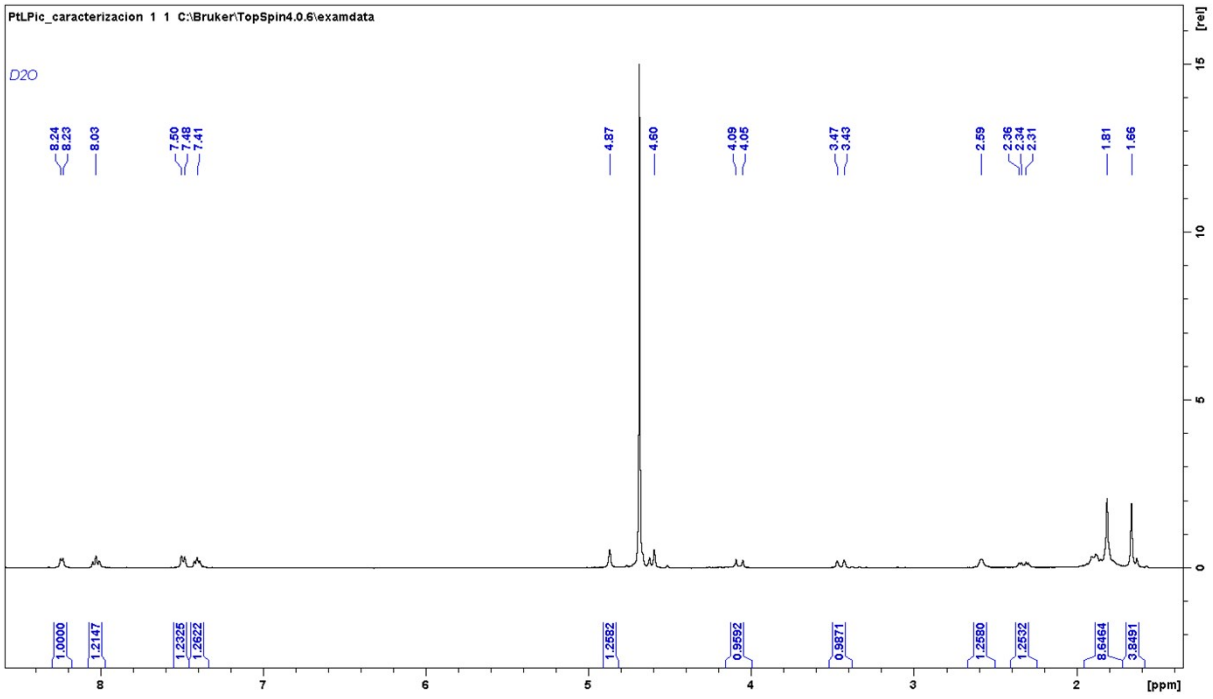


Figure S38. ^{13}C-^{1}H HSQC NMR spectrum of **2** in water-d_2 (pH* = 7.4, 72 h).

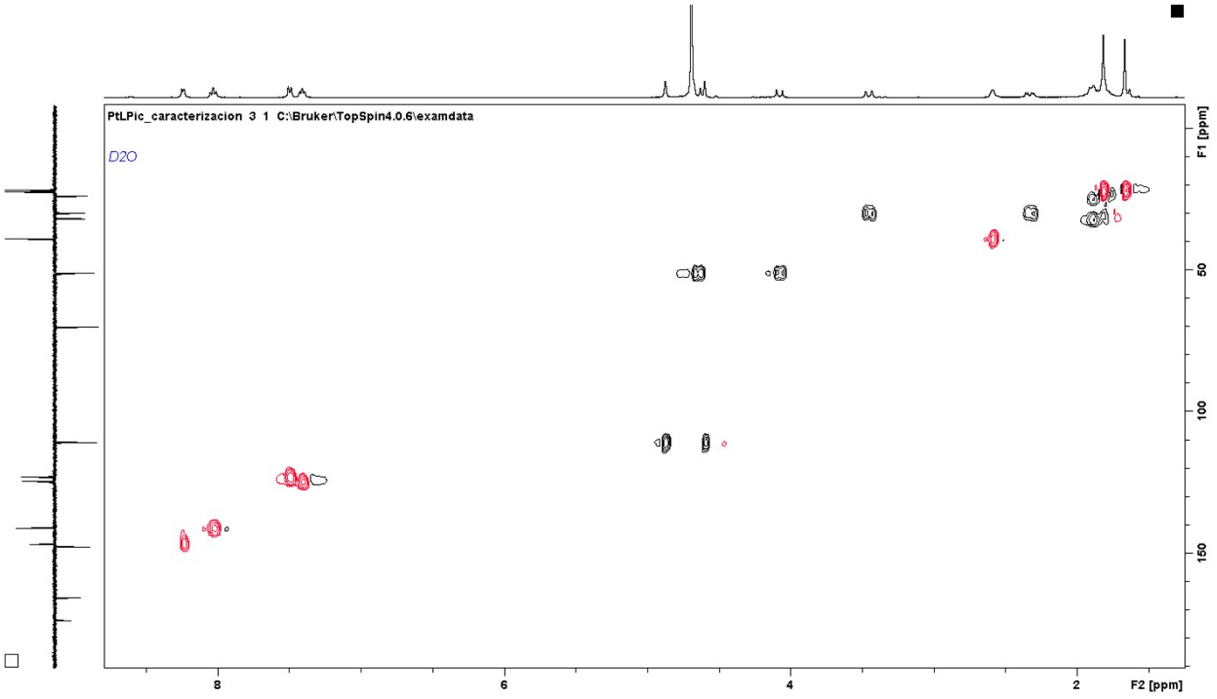


Figure S39. ^{15}N-^{1}H HMBC spectrum of **2** in water-d_2 (pH* = 7.4, 72 h).

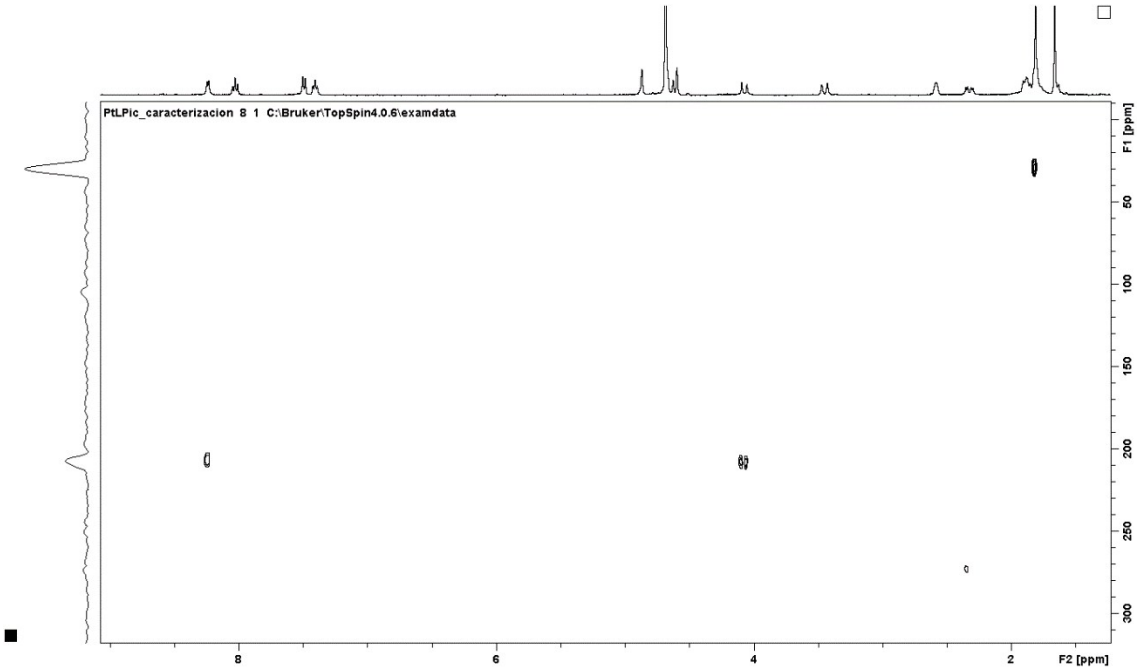


Figure S40. ^{1}H -^{1}H COSY spectrum of **2** in water-d_2 (pH* = 7.4, 72 h).

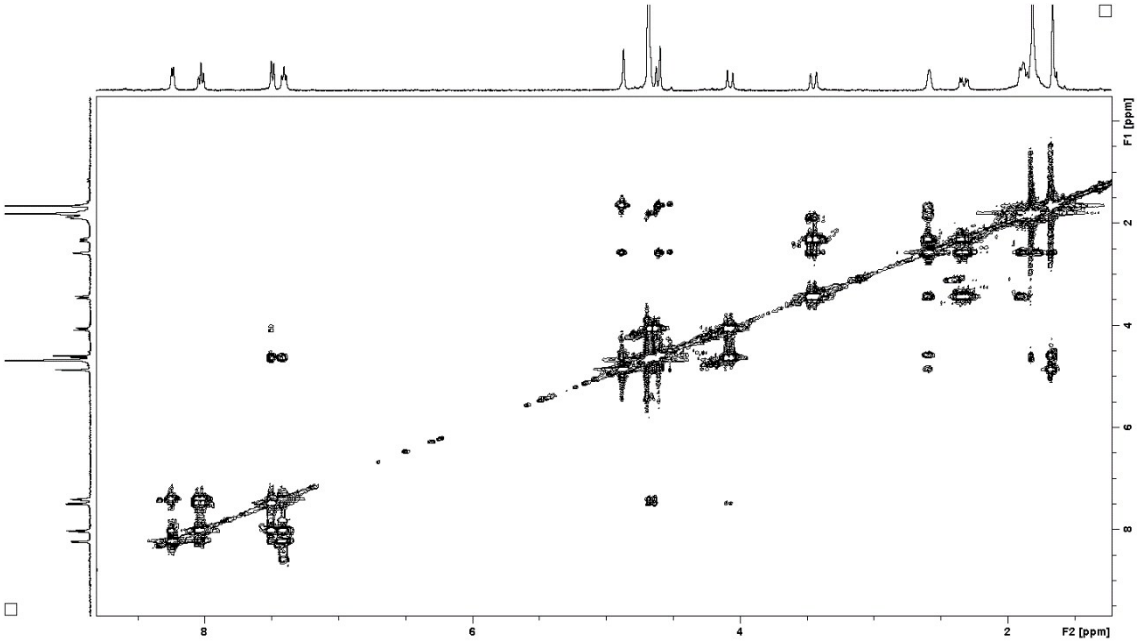


Figure S41. 2D NOESY NMR spectrum of **2** in water-d_2 (pH* = 7.4, 72h).

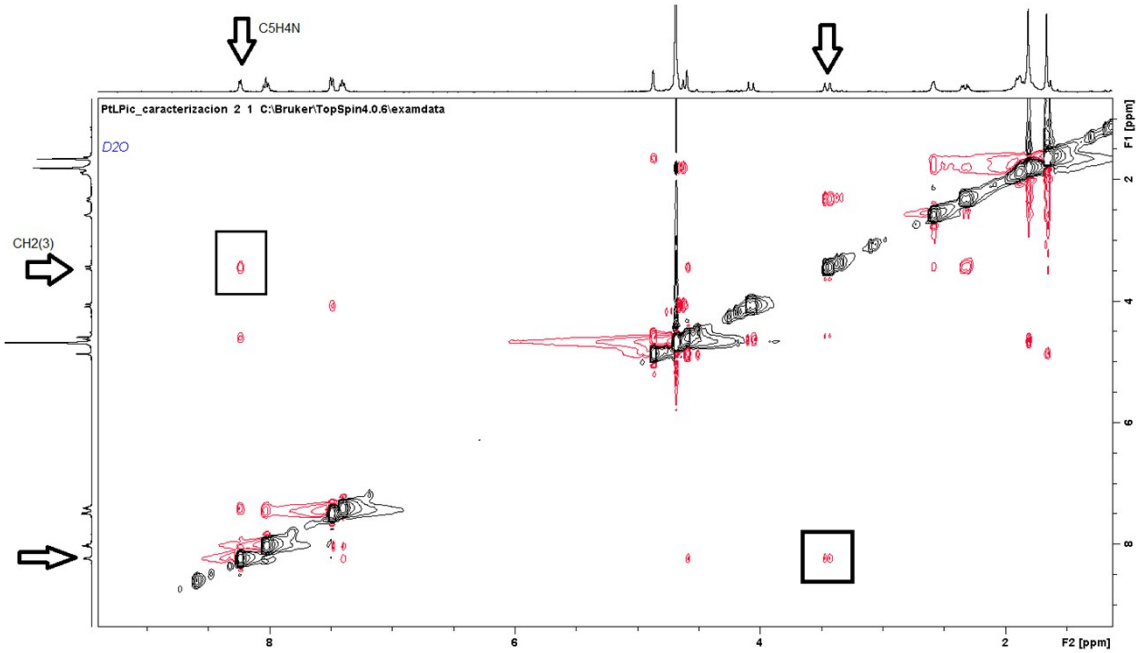
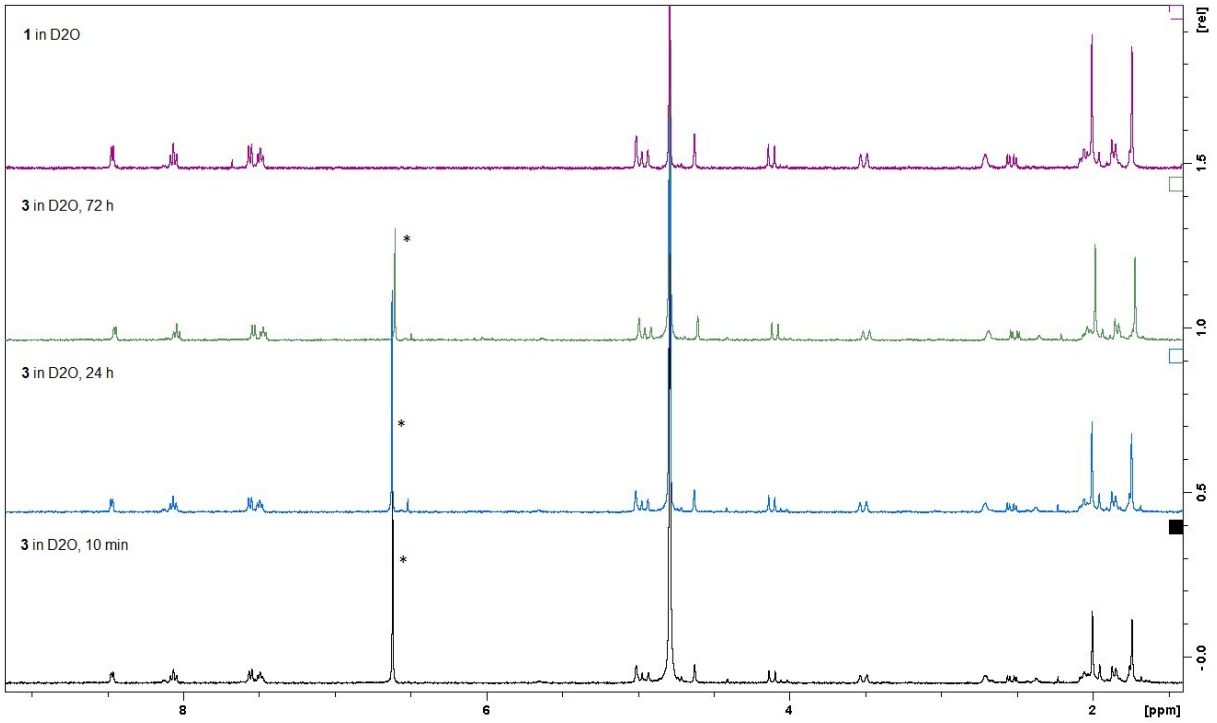


Figure S42. Time-dependent ^{1}H NMR spectra of **3** in water-d_2 (pH* 2.0)



(*) Singlet assigned to $[Cp_2Ti(OH)(H_2O)]^+$ according to reported data.

Figure S43. FRET DNA melting curves of A) **1**; B) **2**. The concentration of F10T is 0.2 μM. A titration was performed by using 1, 2, 3, 4, 5, 6, 7, 8, 9 or 10 μM concentration of tested compound.