Pt(IV) derivatives of [Pt(1*S*,2*S*-DACH)(5,6-dimehtyl-1,10-phenanthroline)]

Supporting Material

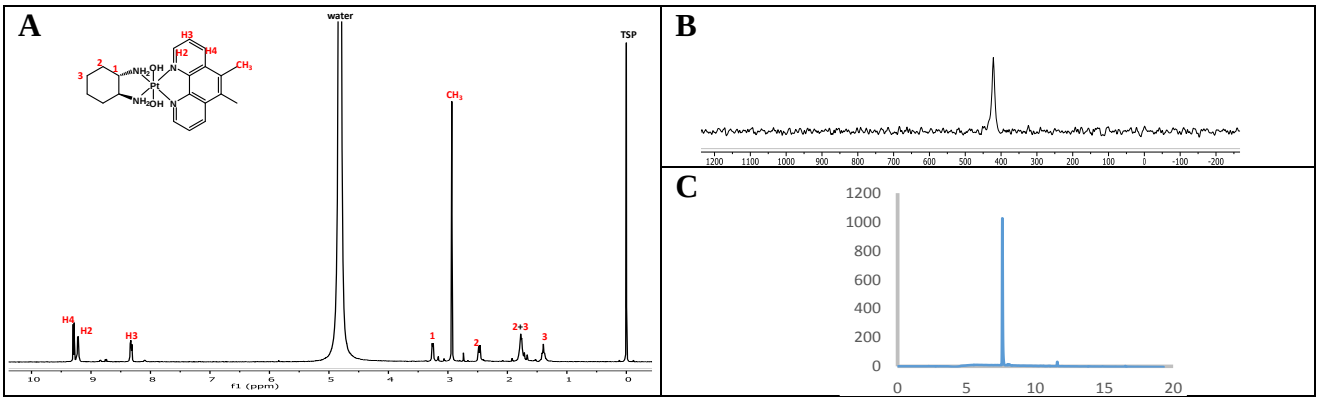

Figure S1. Complex **I**: A. ^{1}H and B. ^{195}Pt NMR spectra recorded in D_2O. C. HPLC chromatogram (0-90 % acetonitrile linear gradient over 30 min).

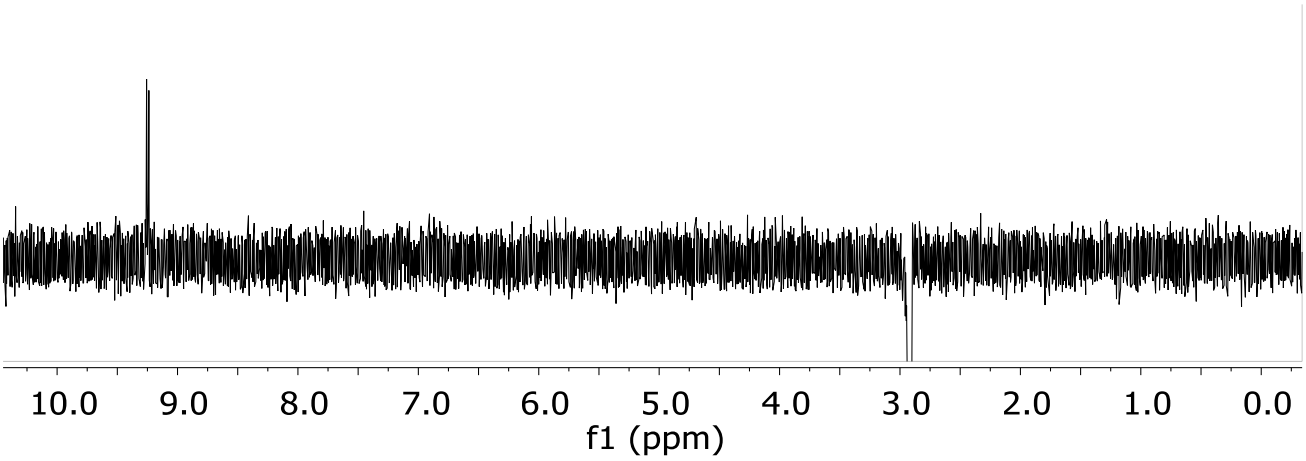

Figure S3. 1D NOESY irradiating the phenanthroline CH_3 (2.91 ppm) to identify H4 (9.25 ppm) of **II**.

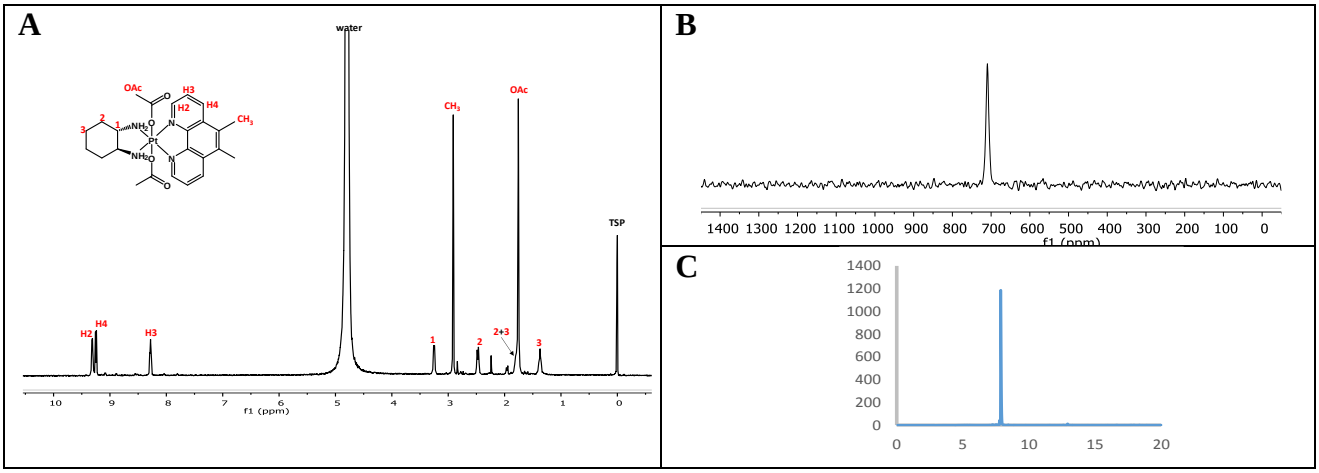

Figure S3. Complex **II**: A. ^{1}H and B. ^{195}Pt NMR spectra recorded in D_2O. C. HPLC chromatogram (0-90 % acetonitrile linear gradient over 20 min).

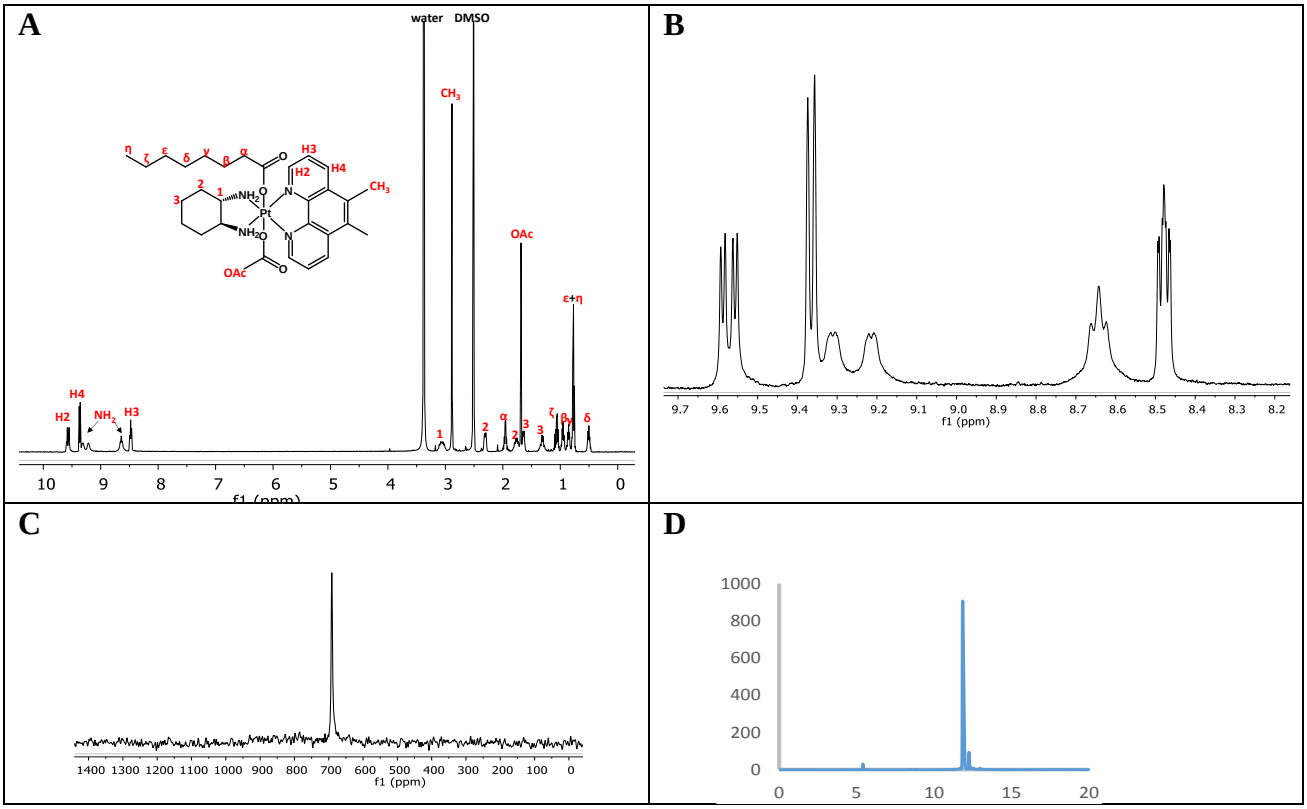

Figure S4. Complex **III**: A. ^{1}H with B. expansion of the aromatic area and C. ^{195}Pt NMR spectra recorded in DMSO-d_6. D. HPLC chromatogram (0-90 % acetonitrile linear gradient over 20 min).

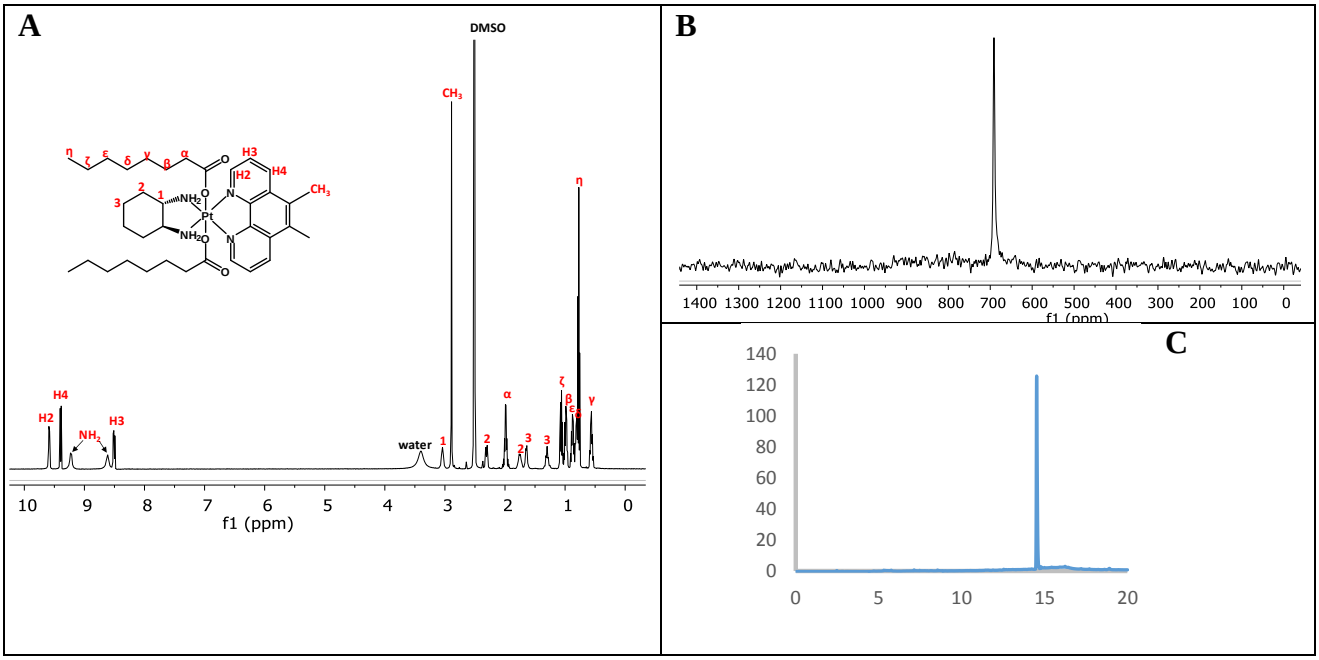

Figure S5. Complex **IV**: A. ^{1}H and B. ^{195}Pt NMR spectra recorded in DMSO-d_6. C. HPLC chromatogram (0-90 % acetonitrile linear gradient over 20 min).

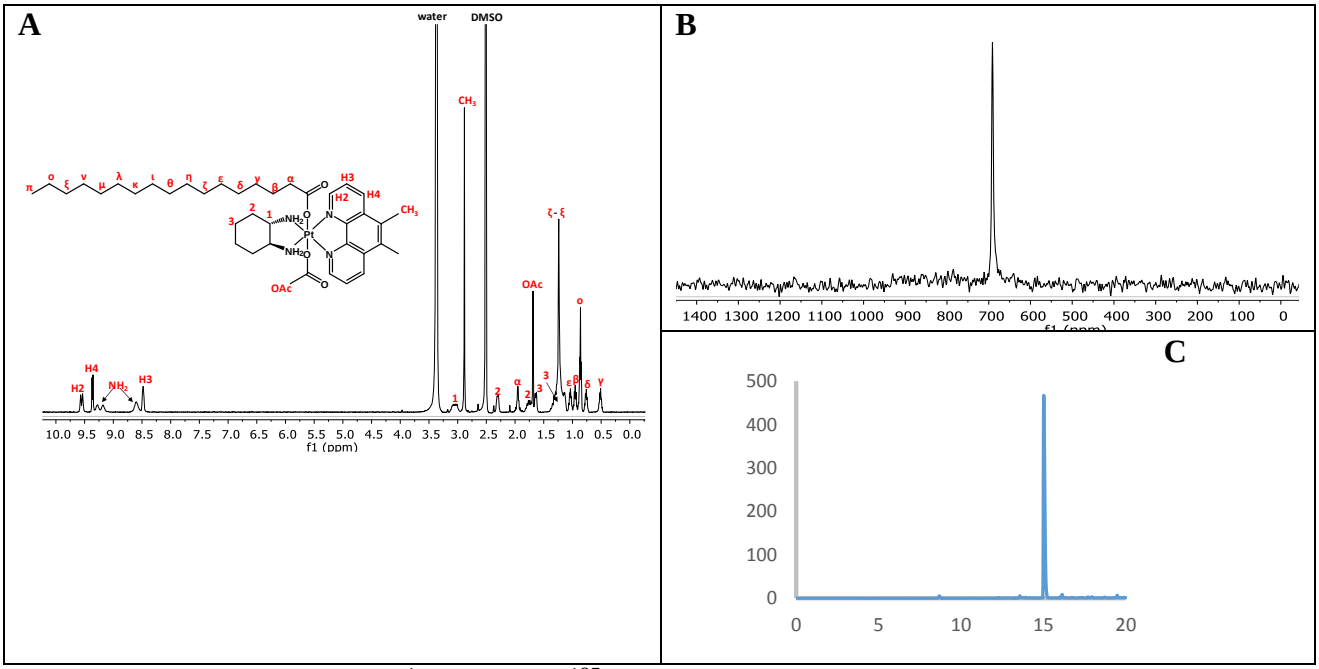

Figure S6. Complex **V**: A. ^{1}H and B. ^{195}Pt NMR spectra recorded in DMSO-d_6. C. HPLC chromatogram (0-90 % acetonitrile linear gradient over 20 min).

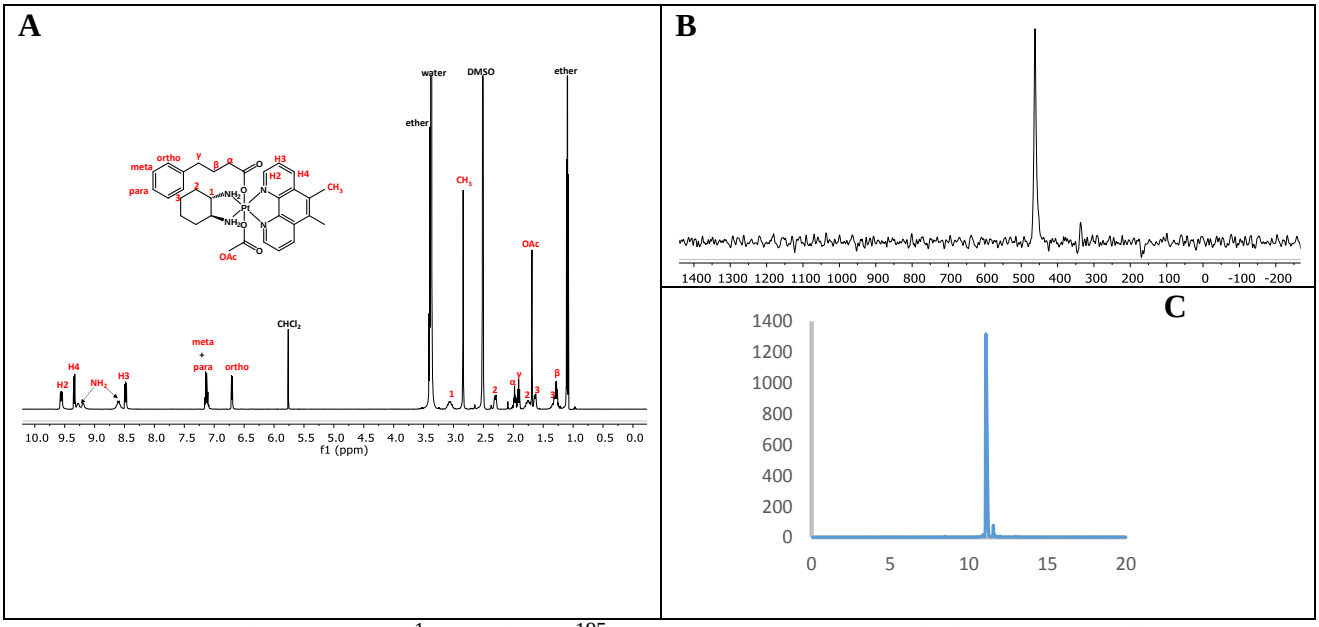

Figure S7. Complex **VI**: A. ^{1}H and B. ^{195}Pt NMR spectra recorded in DMSO-d_6. C. HPLC chromatogram (0-90 % acetonitrile linear gradient over 20 min).

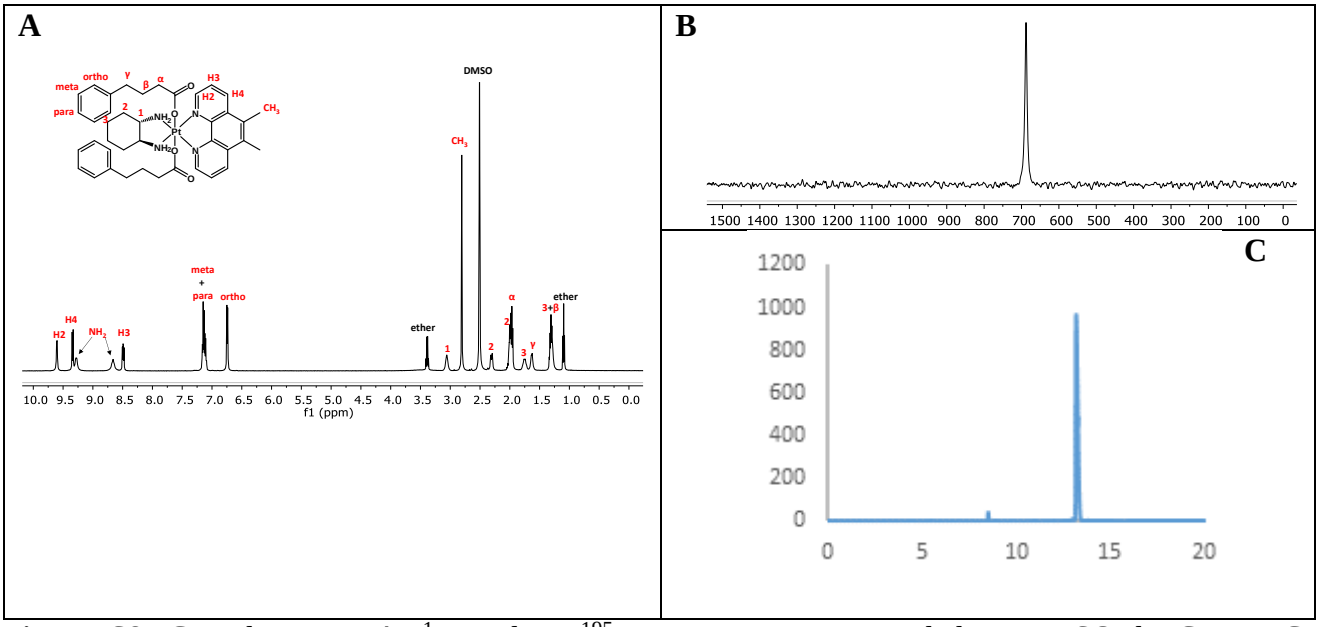

Figure S8. Complex **VII**: A. ^{1}H and B. ^{195}Pt NMR spectra recorded in DMSO-d_6. C. HPLC chromatogram (0-90 % acetonitrile linear gradient over 20 min).

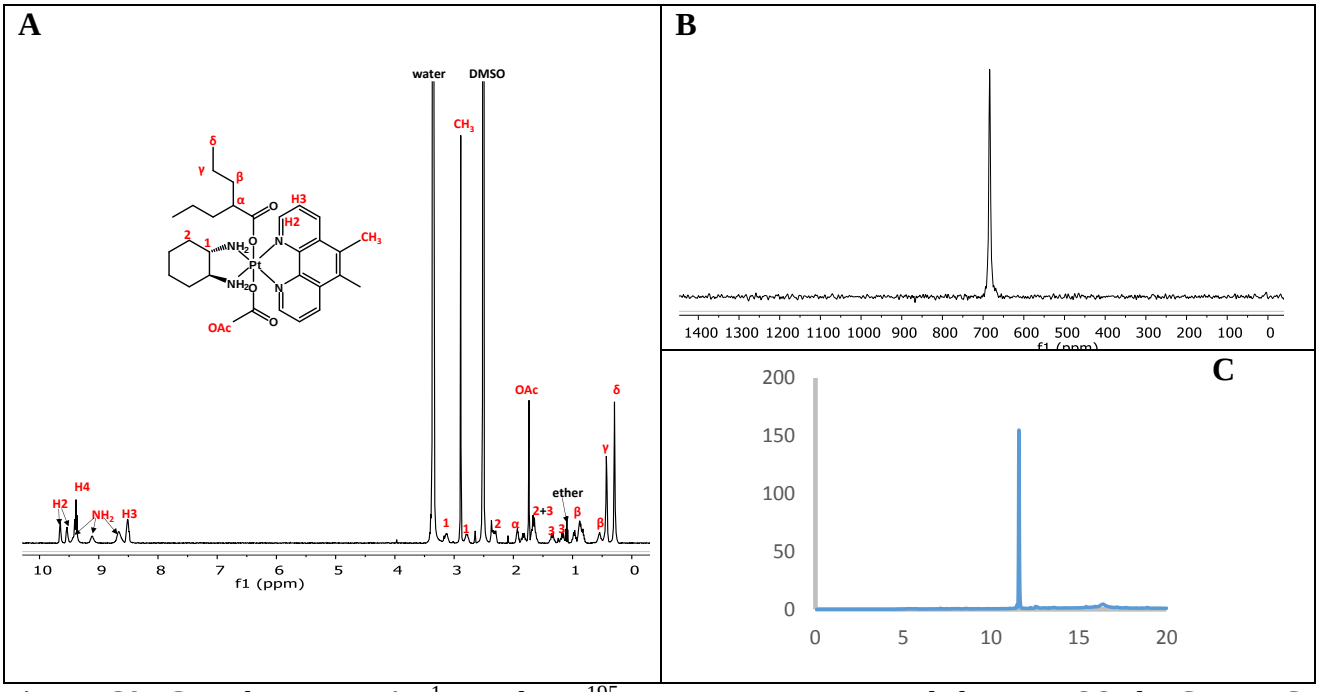

Figure S9. Complex **VIII**: A. ^{1}H and B. ^{195}Pt NMR spectra recorded in DMSO-d_6. C. HPLC chromatogram (0-90 % acetonitrile linear gradient over 20 min).

Table S1. ^{1}H NMR chemical shifts of free and coordinated acetate, octanoate, palmitate, phenylbutyrite and valproate ligands, and Δppm (chemical shift of free – chemical shift of coordinated ligand).

		α	β	γ	δ	ε	ζ	η	θ - ξ	ο
Acetate[a]	**free**	2.08								
	coordinated	1.76								
	Δppm	0.32								
Acetate[b]	**free**	1.98								
	coordinated[c]	1.70								
	Δppm	0.28								
Octanoate[b]	**free**	2.17	1.50	1.26				0.86		
	coordinated[d]	1.97	0.97	0.71	0.65	0.91	1.06	0.77		
	Δppm	0.20	0.53	0.55	0.51	0.35	0.20	0.13		
Palmitate[b]	**free**	2.18	1.48	1.24						0.86
	coordinated	1.95	0.95	0.51	0.76	1.03	1.24			0.86
	Δppm	0.23	0.53	0.73	0.48	0.21	0.00			
Phenylbutyrate[b]	**free**	2.22	1.81	2.60	/	7.19[f]	7.29[g]	7.18[h]		
	coordinated[e]	1.98	1.30	1.77	/	6.73[f]	7.15[g]	7.12[h]		
	Δppm	0.24	0.51	0.83	/	0.46	0.14	0.06		
Valproate[b]	**free**	2.21	1.41[i]	1.25	0.85					
	coordinated	1.93	0.76[i]	0.43	0.29					
	Δppm	0.28	0.65	0.82	0.56					

[a] Data from ^{1}H NMR spectra recorded in D_2O.

[b] Data from ^{1}H NMR spectra recorded in DMSO-d_6.

[c] Average of the chemical shift values of the acetate moieties of **III**, **V**, **VI** and **VIII**.

[d] Average of the chemical shift values of the octanoate moieties of **III** and **IV**.

[e] Average of the chemical shift values of the phenylbutyrate moieties of **VI** and **VII**.

[f] Corresponding to the protons in ortho position.

[g] Corresponding to the protons in meta position.

[h] Corresponding to the protons in para position.

[i] Average of the chemical shift values of the signals belonging to $C\beta H_2$ of **VIII**.

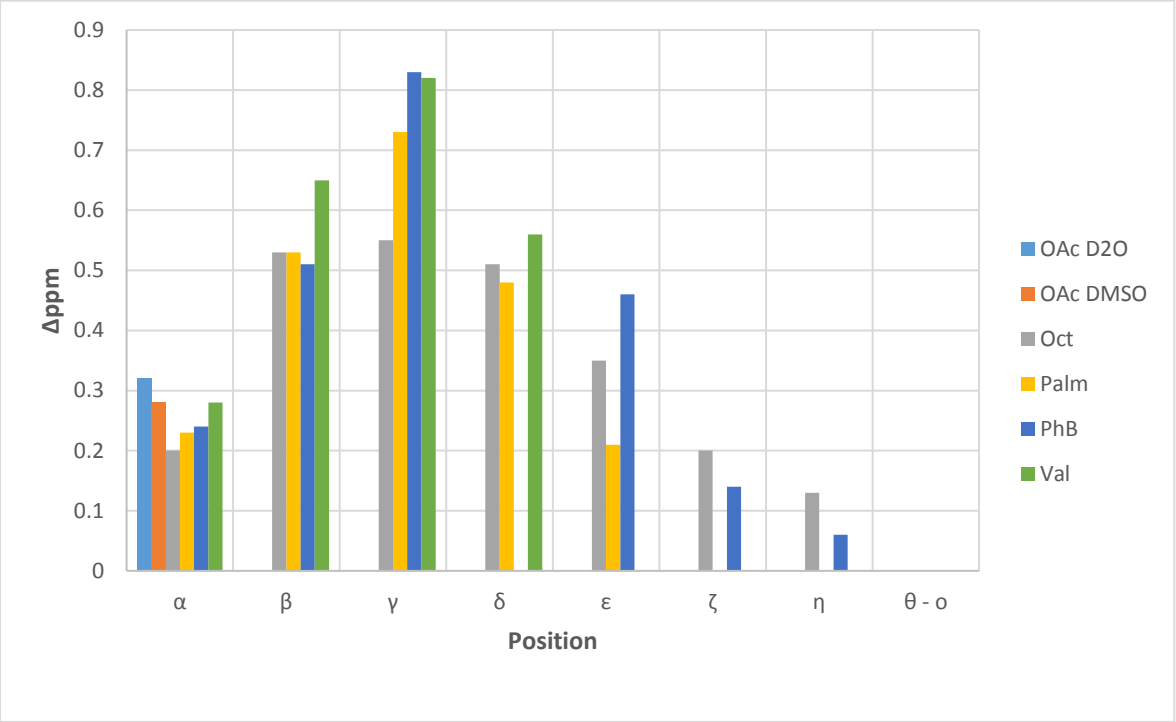

Figure S10. ^{1}H NMR Δppm ($\delta_{free\ ligand} - \delta_{coordinated\ ligand}$) *vs* the position of the groups of the *axial* ligands of **II**-**VIII**.