Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Noncovalent interactions of antitumor cycloplatinated complexes containing trifluoroacetate ligand as leaving group with bovine serum albumin. Implications for drug design

Marzieh Dadkhah Aseman,*[,a,†] Parisa Negaresh,[b,†] Zahra Shojaeifard,[b] Bahram Hemmateenejad,[b] and S. Masoud Nabavizadeh*[,b]

[a]*Department of Chemistry, Faculty of Sciences, Tarbiat Modares University, Tehran, Iran* [b]*Department of Chemistry, College of Sciences, Shiraz University, Shiraz, Iran,*

Table of Contents

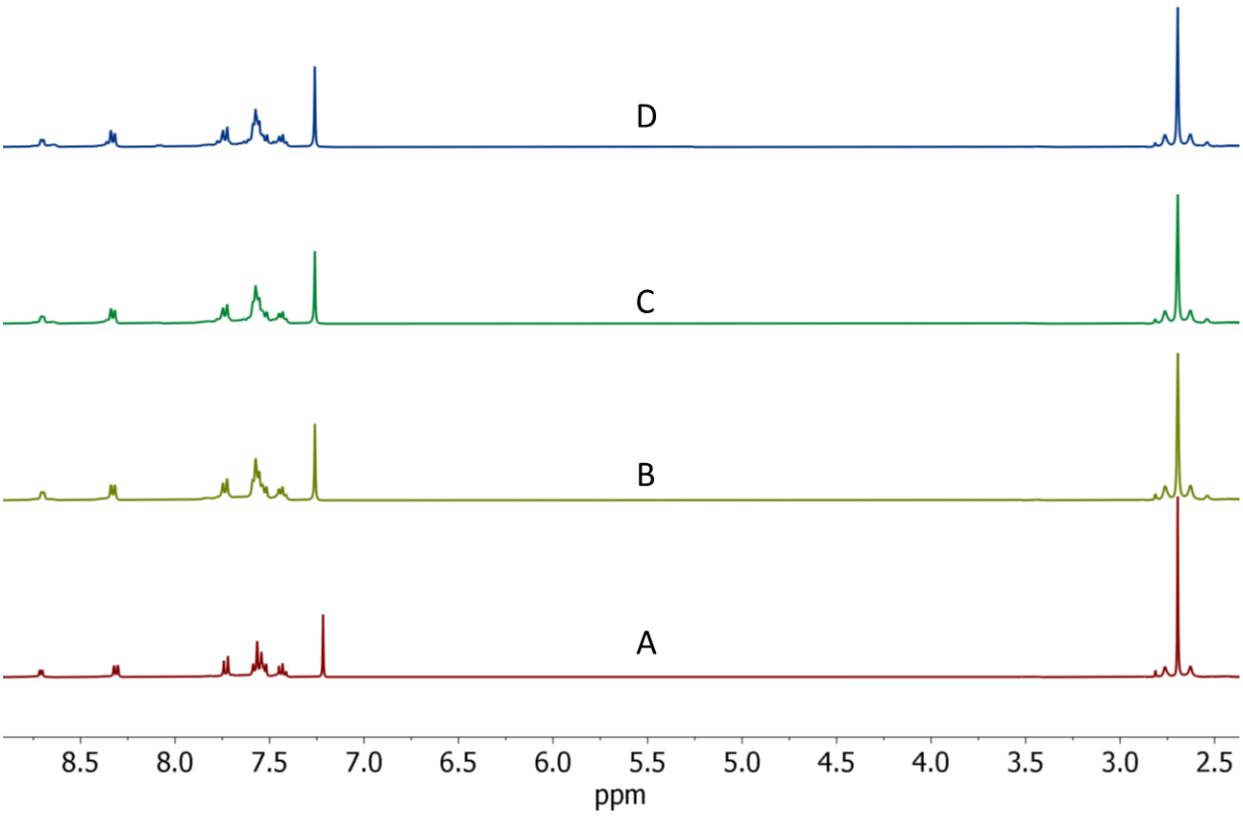


Figure S1. Changes in ^{1}H NMR spectrum of complex **1** (0.01 M) during its reaction with 10-fold excess of dimethyl sulfoxide-d^{6} (0.1 M) in $CDCl_3$. (A) Pure **1**, (B) 10 min (C) 1 h and (D) 24 h after addition of DMSO.

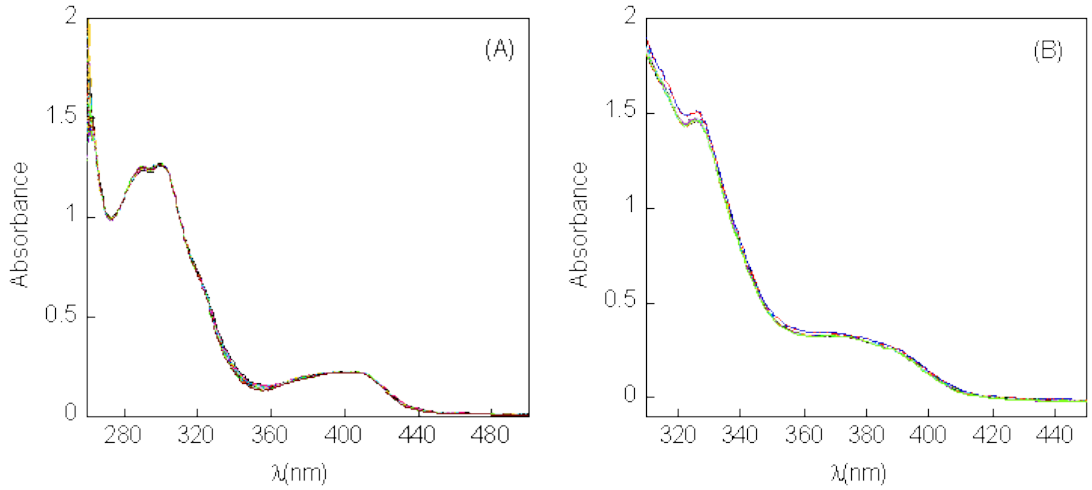


Figure S2. The changes in UV/Vis spectra of (A) complex **1** (3×10^{-4} M) and (B) complex **2** (3×10^{-4} M) in $CHCl_3$ after the addition of 10-fold excess of DMSO (3.0 mM).

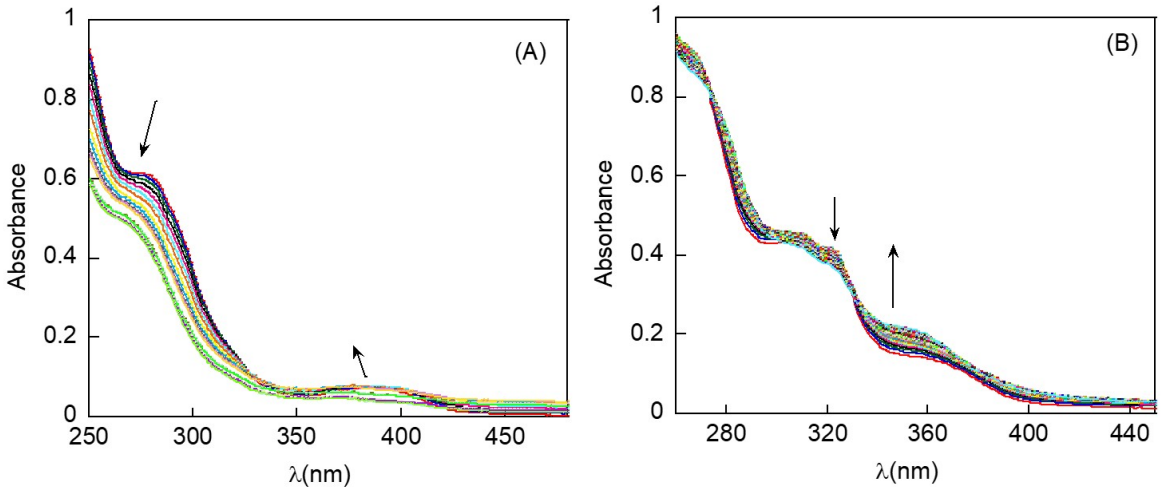


Figure S3. Changes in UV/Vis spectra of (A) complex **1** (90 μM) and (B) complex **2** (75 μM) in 10 % v/v DMSO/H_2O solution for 5 h.

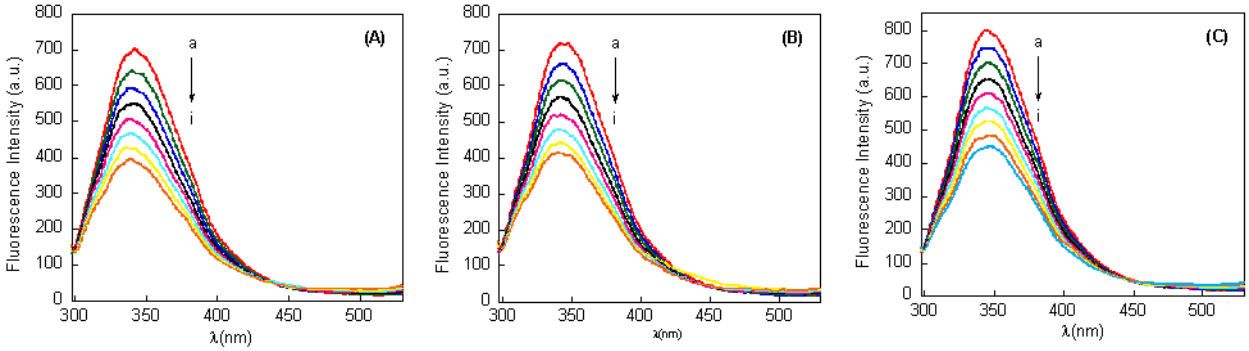


Figure S4. Changes in the fluorescence spectra of BSA upon titration with **1** at (A) 303 K, (B) 310 K and (C) 313 K. The concentration of BSA is 0.1 × 10^{-6} M and **1** concentration was varied from (a) 0.00 to (i) 0.15 × 10^{-6} M; pH 7.4 and λ_{ex}: 280 nm.

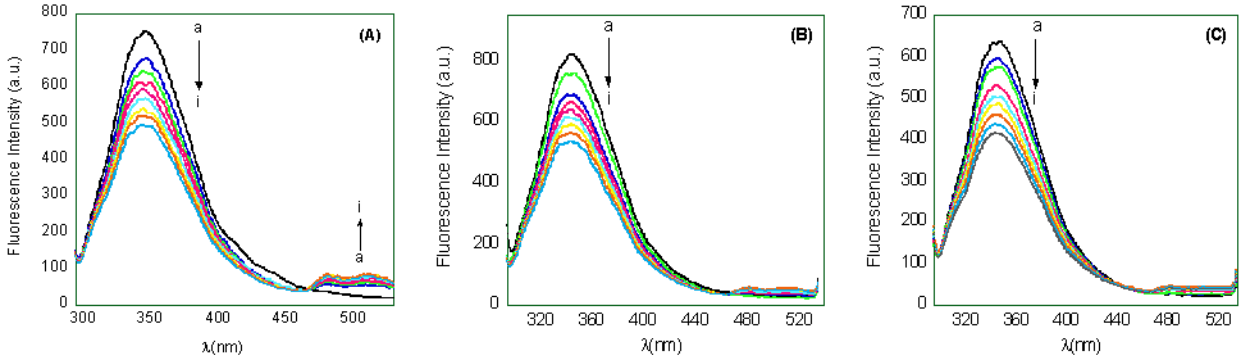


Figure S5. Changes in the fluorescence spectra of BSA upon titration with **2** at (A) 303 K, (B) 310 K and (C) 313 K. The concentration of BSA is 0.1 × 10^{-6} M and **2,** concentration was varied from (a) 0.00 to (i) 0.15 × 10^{-6} M; pH 7.4 and λ_{ex}: 280 nm.

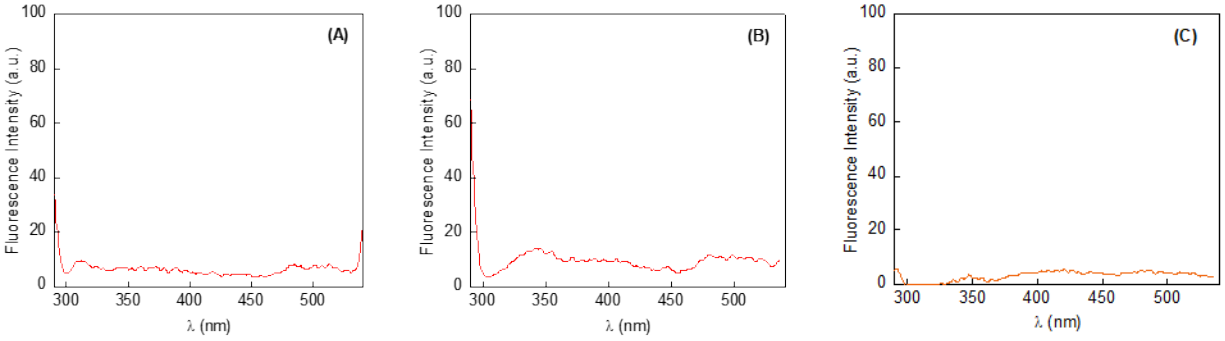


Figure S6. Fluorescence emission spectra of **2**, 0.15 μM(A) 1.5 μM,(B) and 2-phenylpyridine, 0.15 μM (C), T = 298 K, pH = 7.40, λex = 280 nm, in 0.1M Tris-HCl.

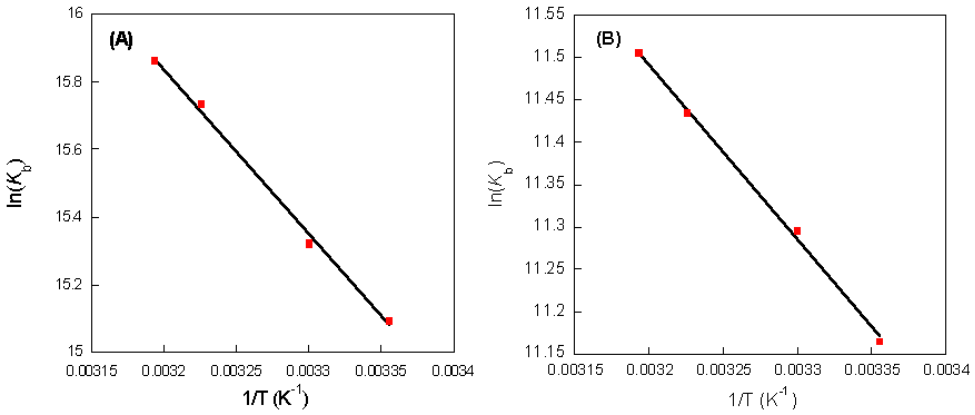


Figure S7. Van't Hoff plot obtained from the interaction between BSA and complex **1** (A) and **2** (B).

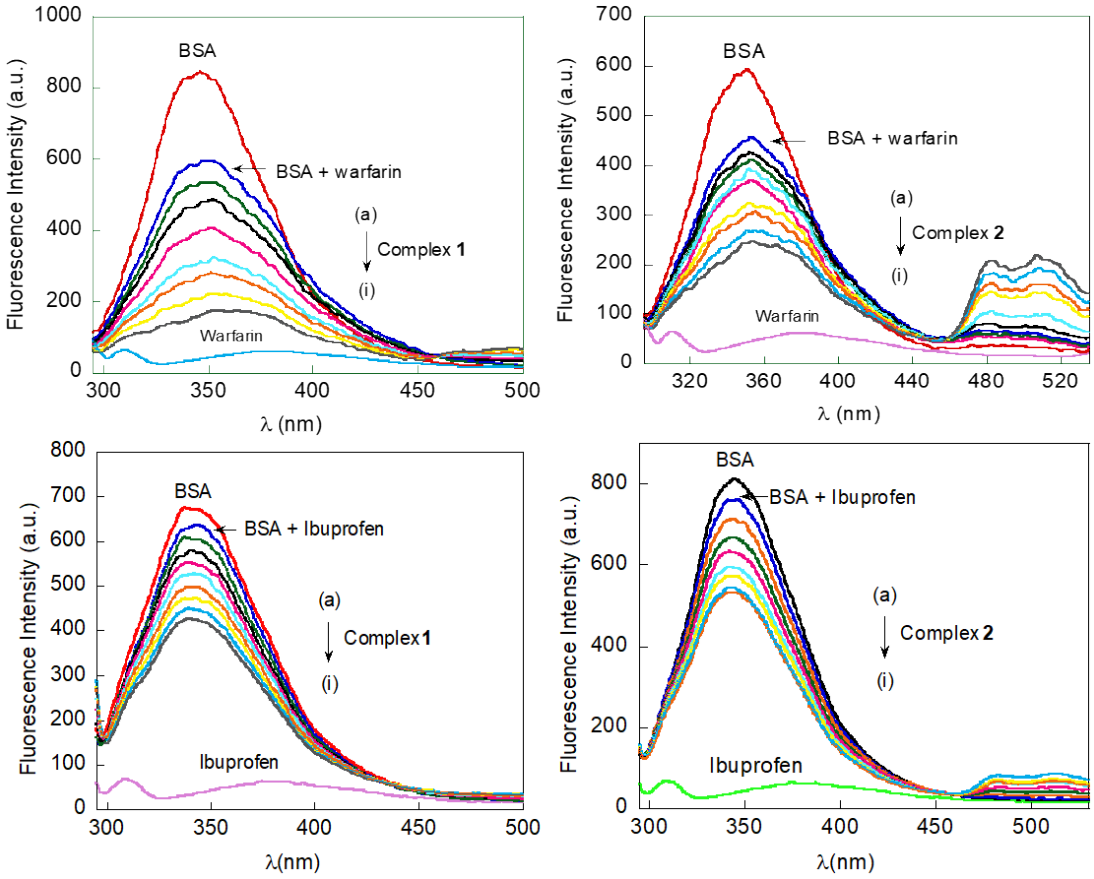


Figure S8. Effects of Pt(II) complexes **1** or **2**, on two BSA-site marker probes systems. [BSA] = [warfarin] = [ibuprofen] = 0.1 μM; the concentration of Pt(II) complexes was varying from 0.0 (a) to 0.15 (i) μM, λ_{ex} = 280 nm.

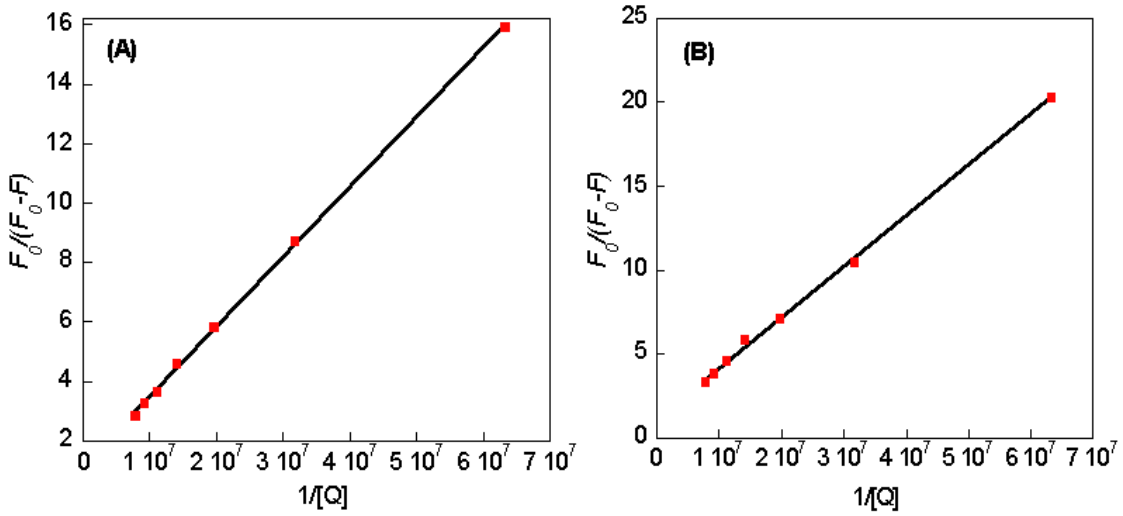


Figure S9. The modified Stern–Volmer plots of (A) BSA-warfarin and (B) BSA-ibuprofen in the presence of various concentration of Pt(II) complex **1**, at 310 K. λ_{ex} = 280 nm; pH = 7.4, [HSA] = [warfarin or ibuprofen] = 0.1 μM. **1** Concentration was from 0.0 to 0.15 μM.

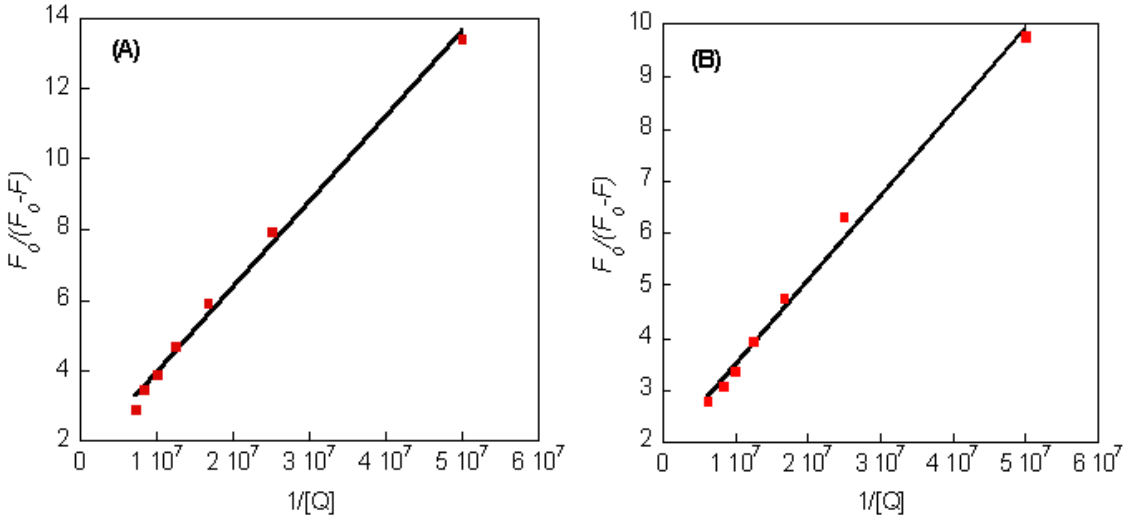


Figure S10. The modified Stern–Volmer plots of (A) BSA-warfarin and (B) BSA-ibuprofen in the presence of various concentration of Pt(II) complex **2**, at 310 K. λ_{ex} = 280 nm; pH = 7.4, [HSA] = [warfarin or ibuprofen] = 0.1 μM. **2** Concentration was from 0.0 to 0.15 μM.

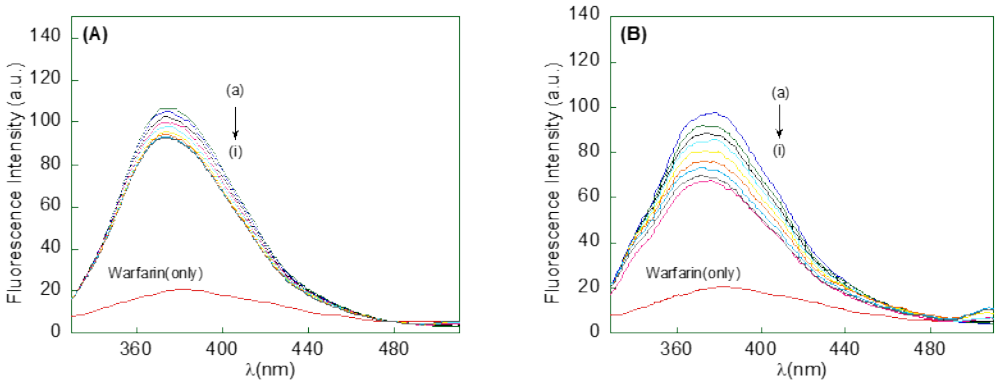
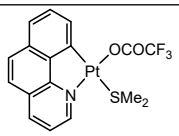
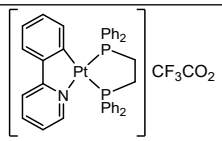
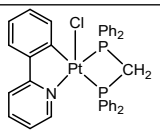
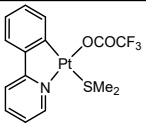
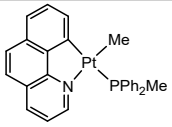
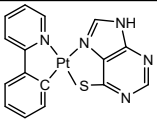
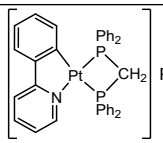
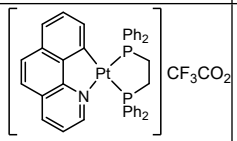
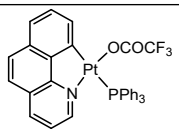
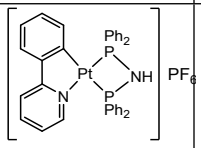
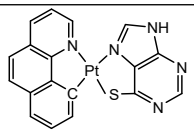
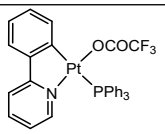
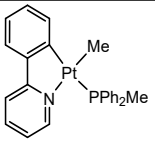
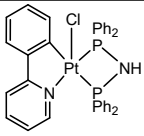


Figure S11. Effect of **1** (A) and **2** (B) to warfarin–BSA system (λex = 310 nm). [warfarin] = [BSA] = 0.1 μM; **1** and **2** concentrations were from (a) 0.0 to (i) 0.15 μM, λ_{ex} = 310 nm.

Table S1. List of cycloplatinated complexes and their Log K_b analyzed in this work

Comp	Structure	Log K_b	Comp	Structure	Log K_b	Comp	Structure	Log K_b
C1 = 1		6.55	**C6** Ref: 45		4.56	**C11** Ref: 48		5.51
C2 = 2		4.84	**C7** Ref: 47		5.16	**C12** Ref: 13		5.48
C3 Ref:46		0.11	**C8** Ref: 45		4.82	**C13** Ref: 49		7.02
C4 Ref:46		0.65	**C9** Ref: 13		5.78	**C14** Ref: 49		5.13
C5 Ref: 47		5.14	**C10** Ref: 48		5.47			

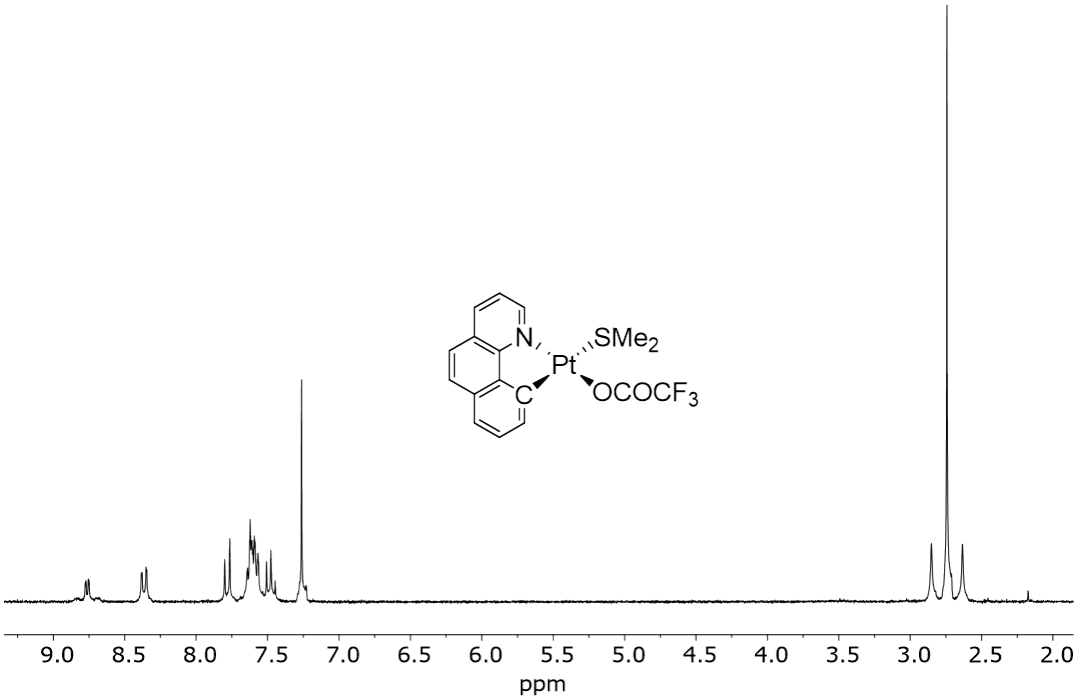


Figure S12. ^{1}H NMR of complex **1** in $CDCl_3$.

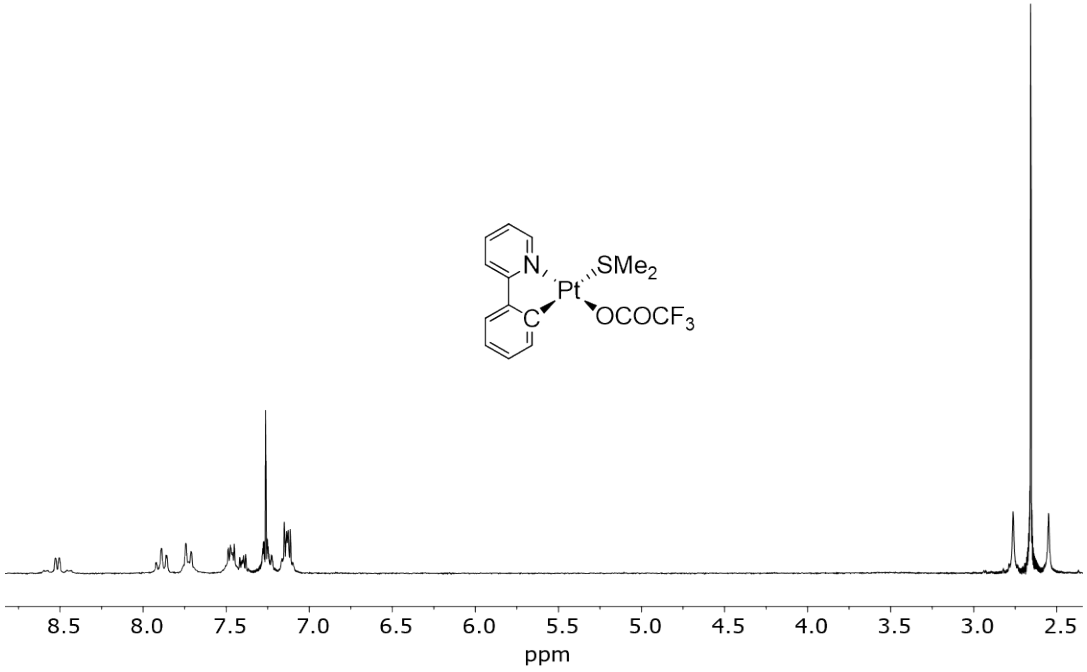


Figure S13. ^{1}H NMR of complex **2** in $CDCl_3$.

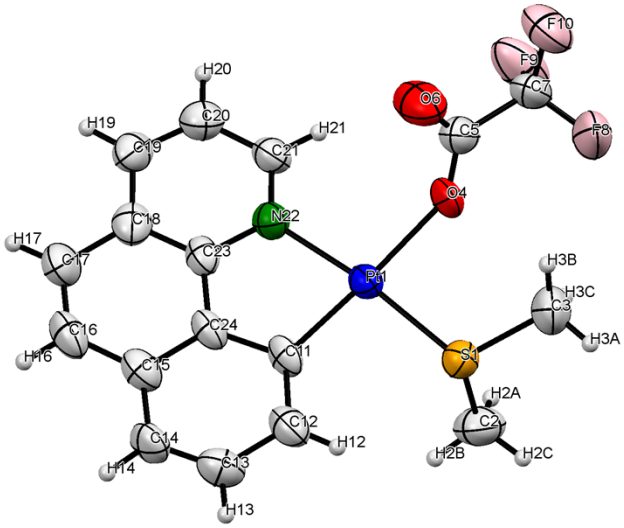


Figure S14. Structure of complex **1** (see ref. 42). Selected geometrical parameters (Å, °): Pt1–O4 2.113(5); Pt1–C11 1.972(8); Pt1–N22 2.062(8); Pt1–S1 2.263(3); O(4)–C(5) 1.265(17); O(6)–C(5) 1.223(15); N22–Pt1–O4 94.9(5); N22–Pt1–C11 82.0(6); O4–Pt1–S1 91.6(4); C11–Pt1–S1 91.5(5); S(1)–Pt(1)–N(22) 173.4(2); O(4)–Pt(1)–C(11) 176.8(8).

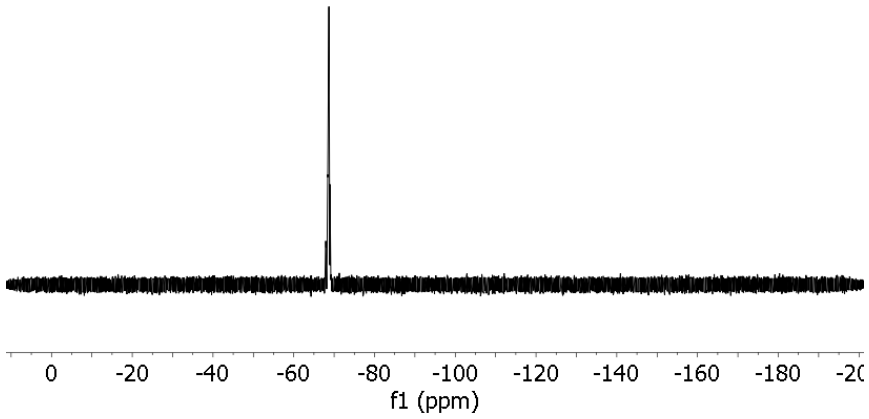


Figure S15. ^{19}F NMR of complex **2** in DMSO-d^6.

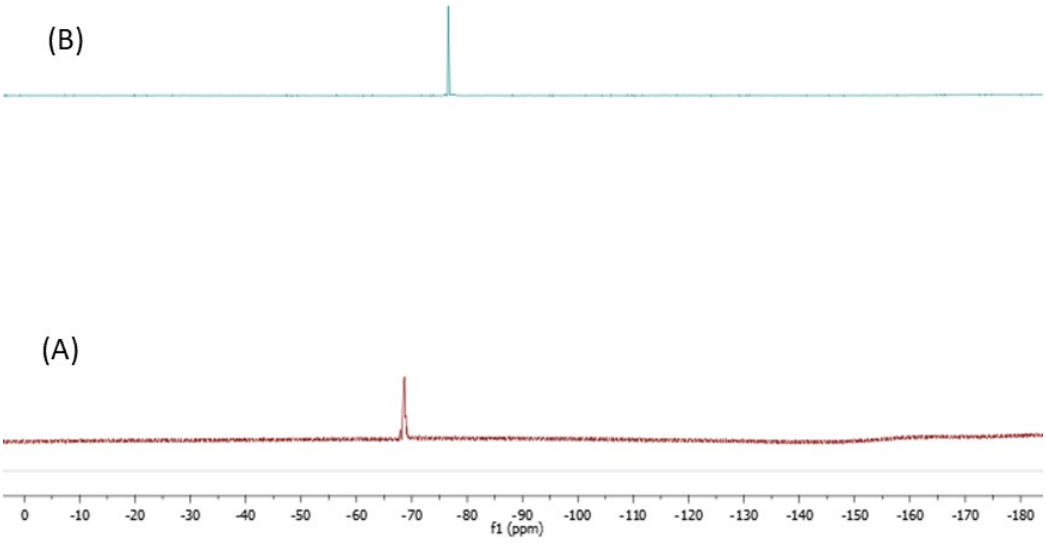


Figure S16. The changes in ^{19}F NMR spectrum of **2** (0.01 M) in DMSO (A) and in 10% DMSO/H_2O solution after (B) 2h.