

Gold(I) complexes bearing alkylated 1,3,5-triaza-7-phosphaadamantane ligands as thermoresponsive anticancer agents in colon cells

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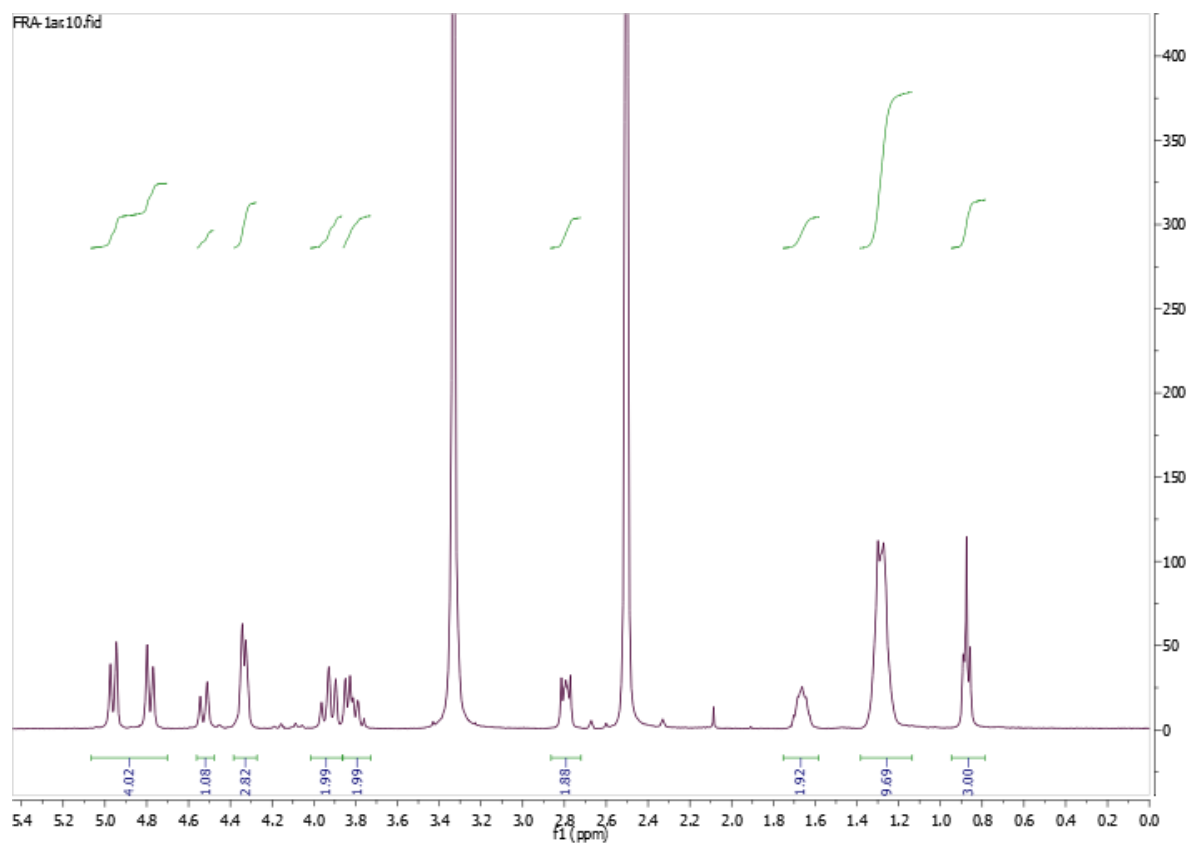


Figure S1. ^1H NMR spectrum of [PTA-CH₂-(CH₂)₆-CH₃]I (**La**)

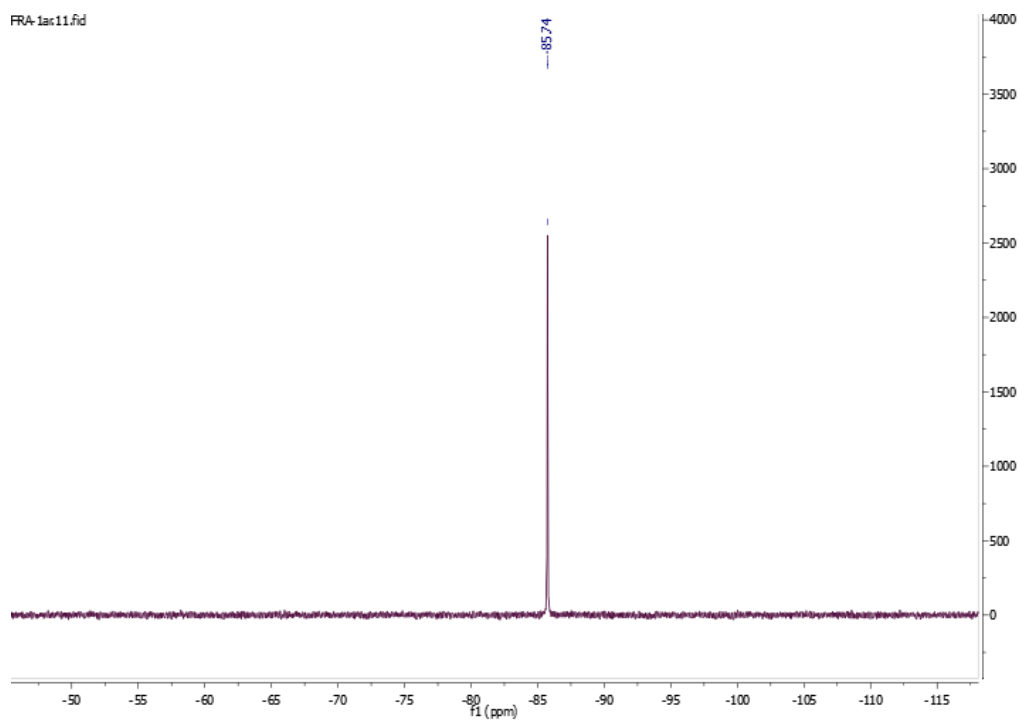


Figure S2. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of [PTA-CH₂-(CH₂)₆-CH₃]I (**La**)

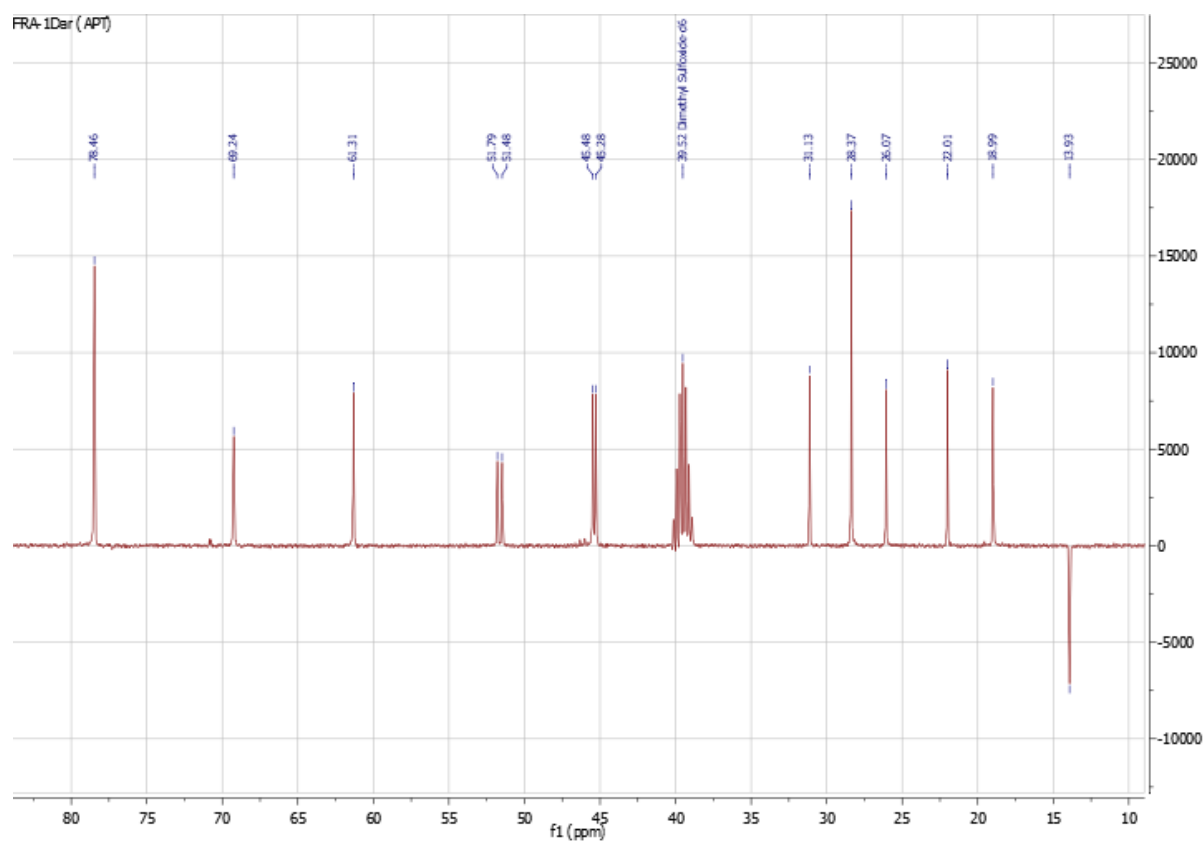


Figure S3. ^{13}C $\{^1\text{H}\}$ -APT spectrum of [PTA-CH₂-(CH₂)₆-CH₃]I (**La**) in dms0-d₆

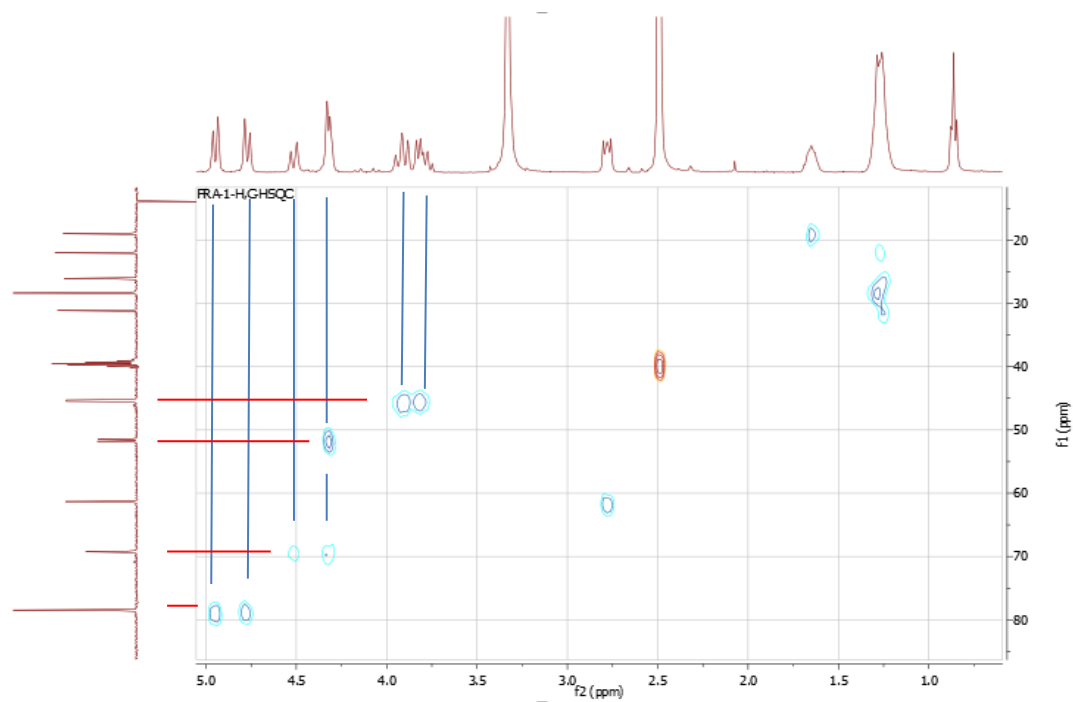


Figure S4. C,H-HSQC experiment of [PTA-CH₂-(CH₂)₆-CH₃]I (**La**) in dms0-d₆

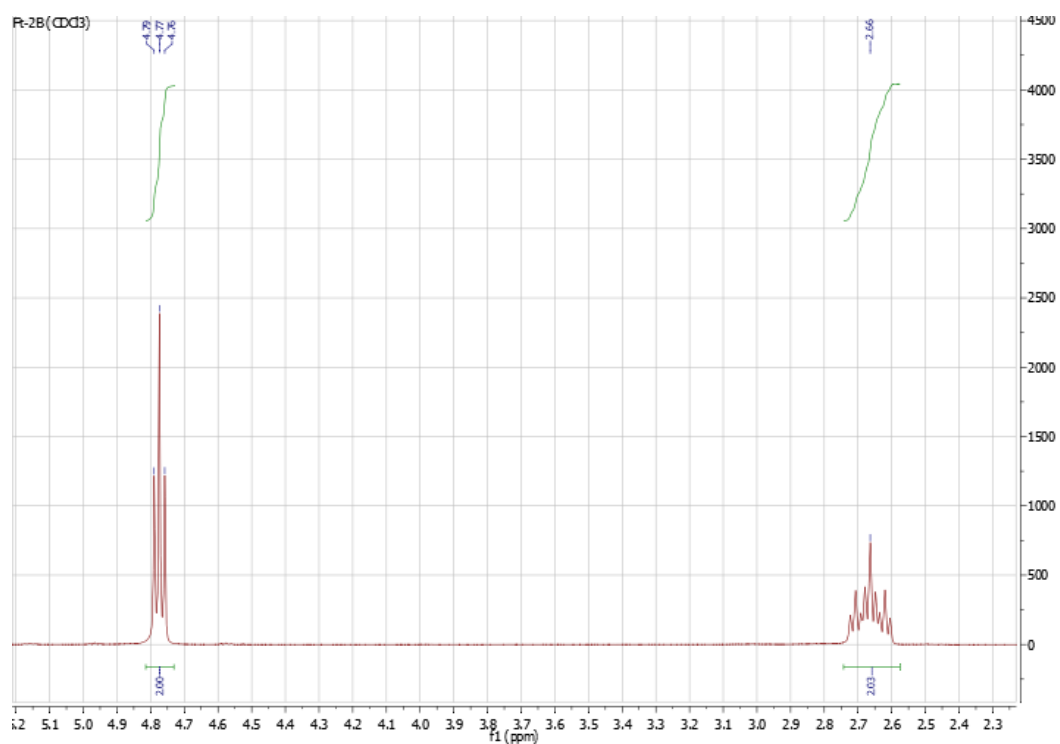


Figure S5. ¹H NMR spectrum of TfOCH₂CH₂(CF₂)₅CF₃ in CDCl₃

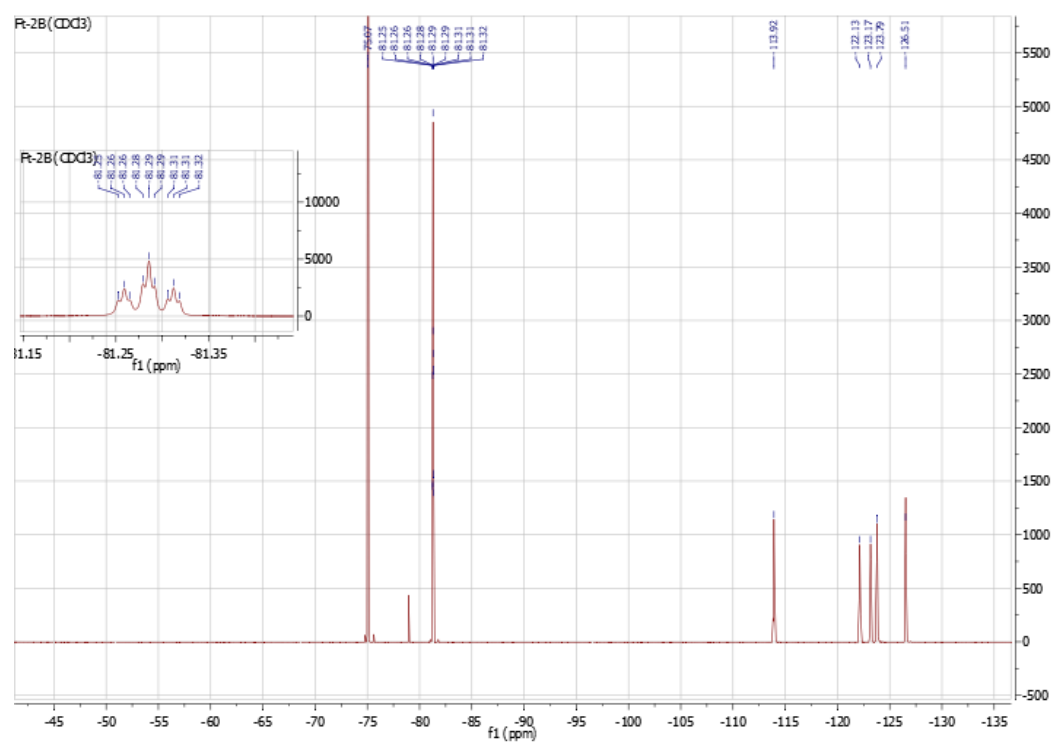


Figure S6. ¹⁹F {¹H} NMR spectrum of TfOCH₂CH₂(CF₂)₅CF₃ in CDCl₃

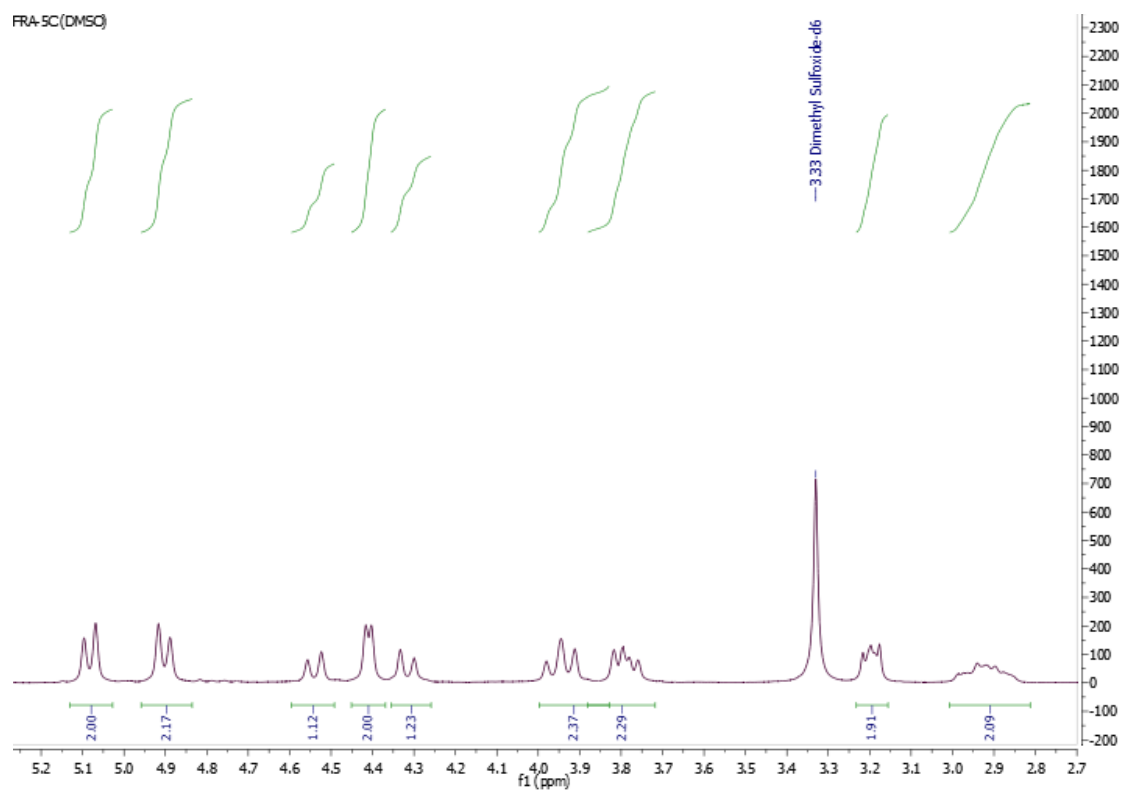


Figure S7. ^1H NMR spectrum of [PTA-CH₂CH₂(CF₂)₅CF₃]TfO (**Lb**) in dmsO-d₆

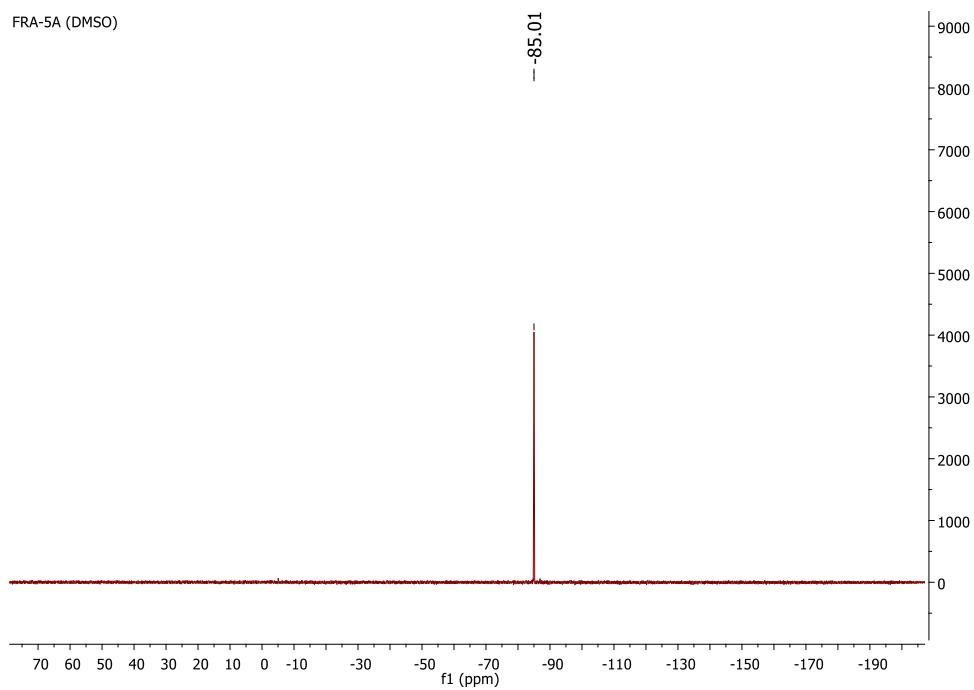


Figure S8. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of [PTA-CH₂CH₂(CF₂)₅CF₃]TfO (**Lb**) in dmsO-d₆

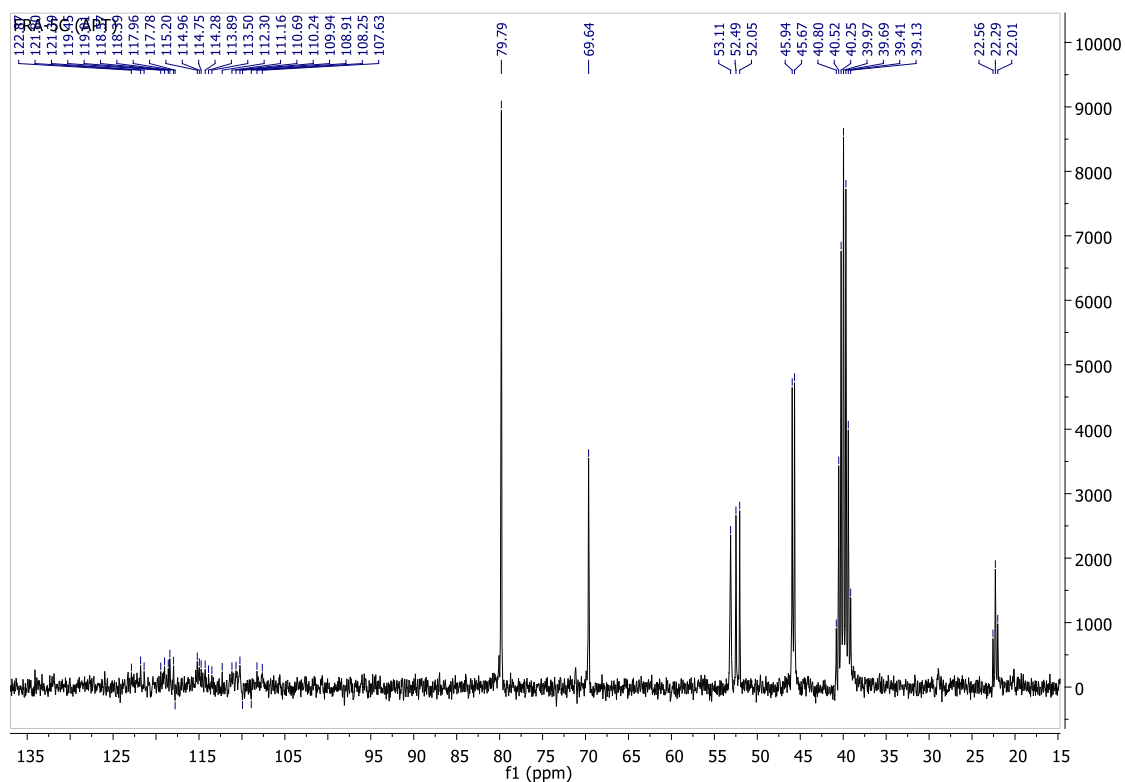


Figure S9. ^{13}C $\{^1\text{H}\}$ NMR spectrum of [PTA- $\text{CH}_2\text{CH}_2(\text{CF}_2)_5\text{CF}_3$]TfO (**Lb**) in dms0-d_6

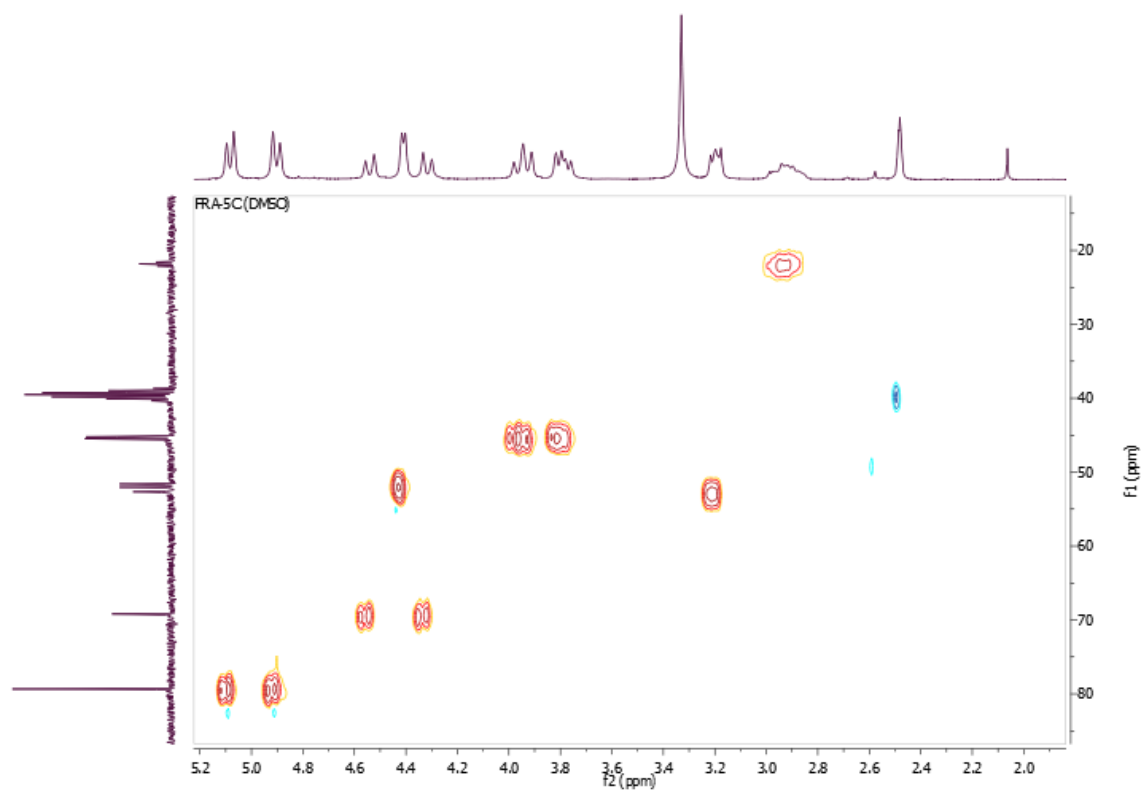


Figure S10. C,H-HSQC experiment of [PTA- $\text{CH}_2\text{CH}_2(\text{CF}_2)_5\text{CF}_3$]TfO (**Lb**) in dms0-d_6

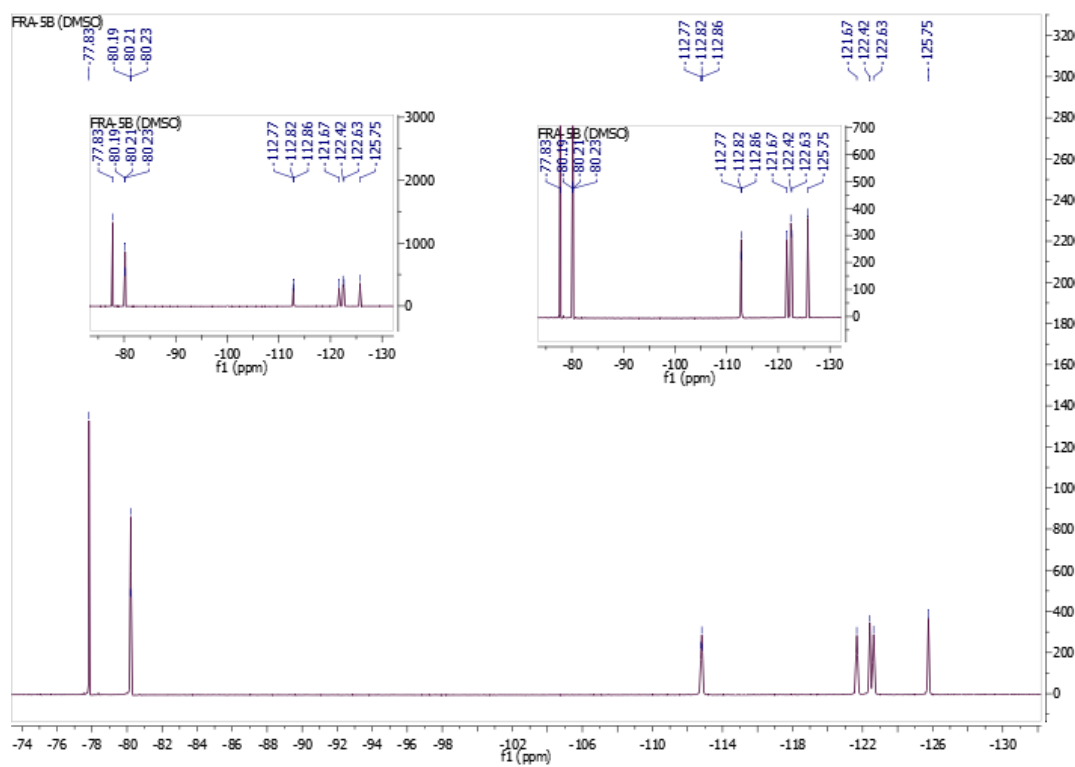


Figure S11. ^{19}F $\{^1\text{H}\}$ NMR spectrum of $[\text{PTA-CH}_2\text{CH}_2(\text{CF}_2)_5\text{CF}_3]\text{TfO}$ (**Lb**) in dms0-d_6

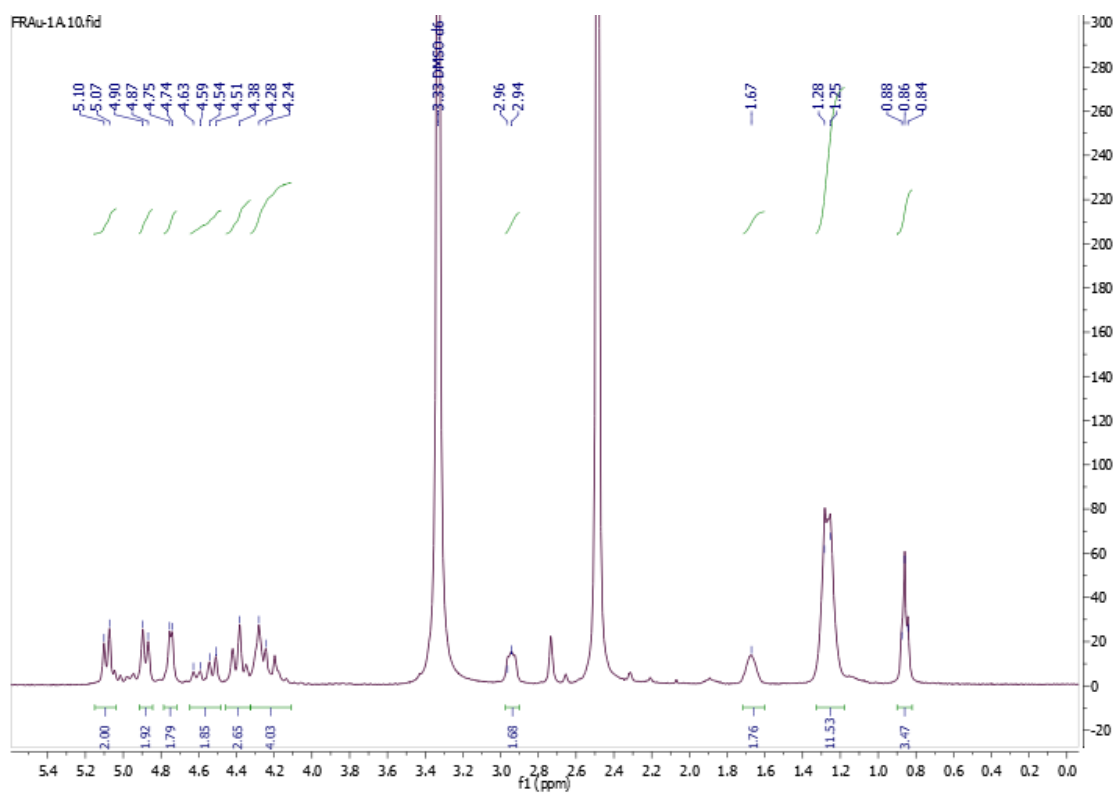


Figure S12. ^1H NMR spectrum of $[\text{AuCl(PTA-CH}_2(\text{CH}_2)_6\text{CH}_3)]\text{I}$ (**1a**) in dms0-d_6

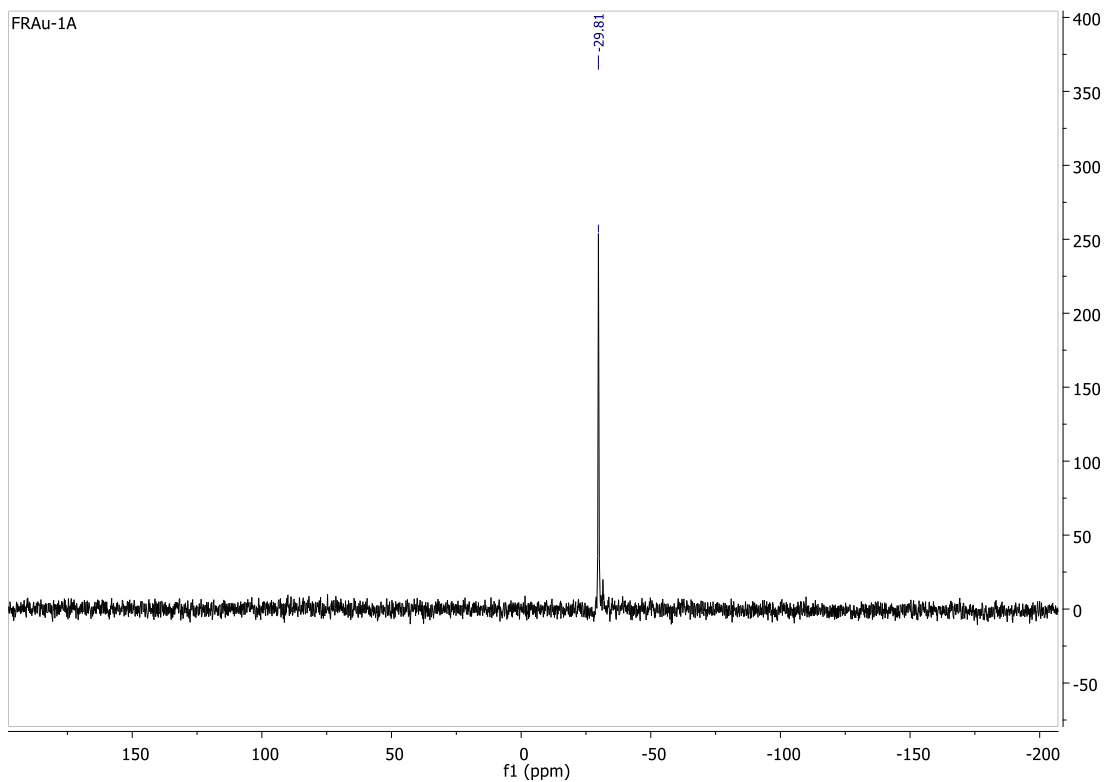


Figure S13. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of $[\text{AuCl}(\text{PTA}-\text{CH}_2(\text{CH}_2)_6\text{CH}_3)]\text{I}$ (**1a**) in $\text{dms0}-d_6$

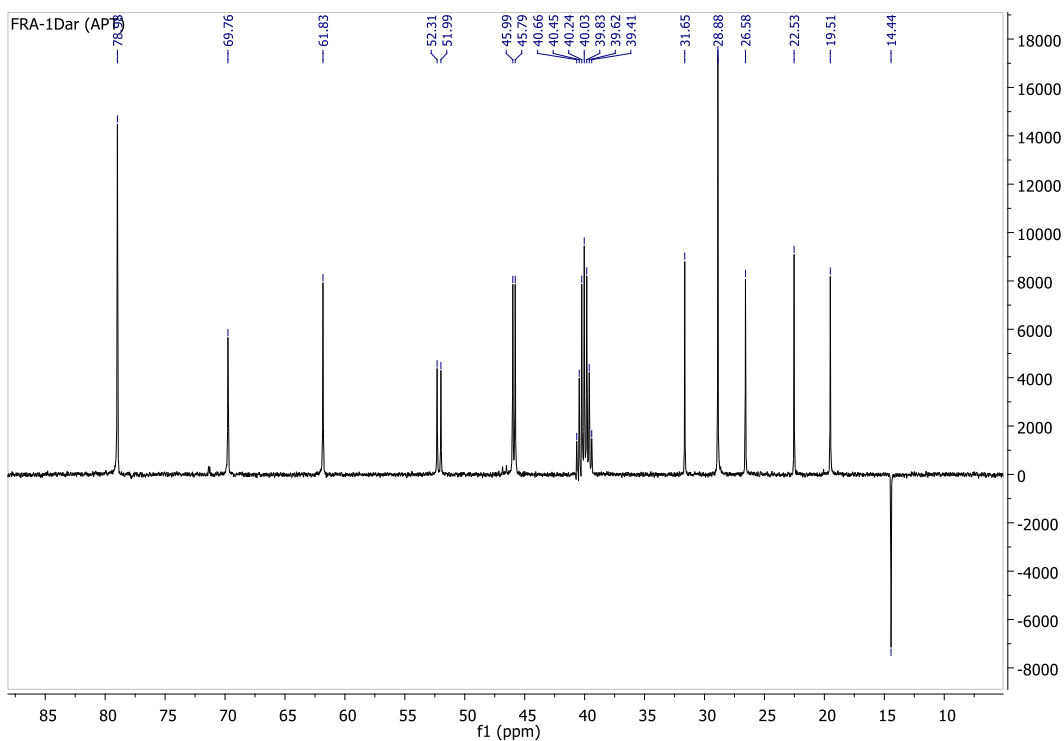


Figure S14. $^{13}\text{C}\{^1\text{H}\}$ -APT spectrum of $[\text{AuCl}(\text{PTA}-\text{CH}_2(\text{CH}_2)_6\text{CH}_3)]\text{I}$ (**1a**) in $\text{dms0}-d_6$

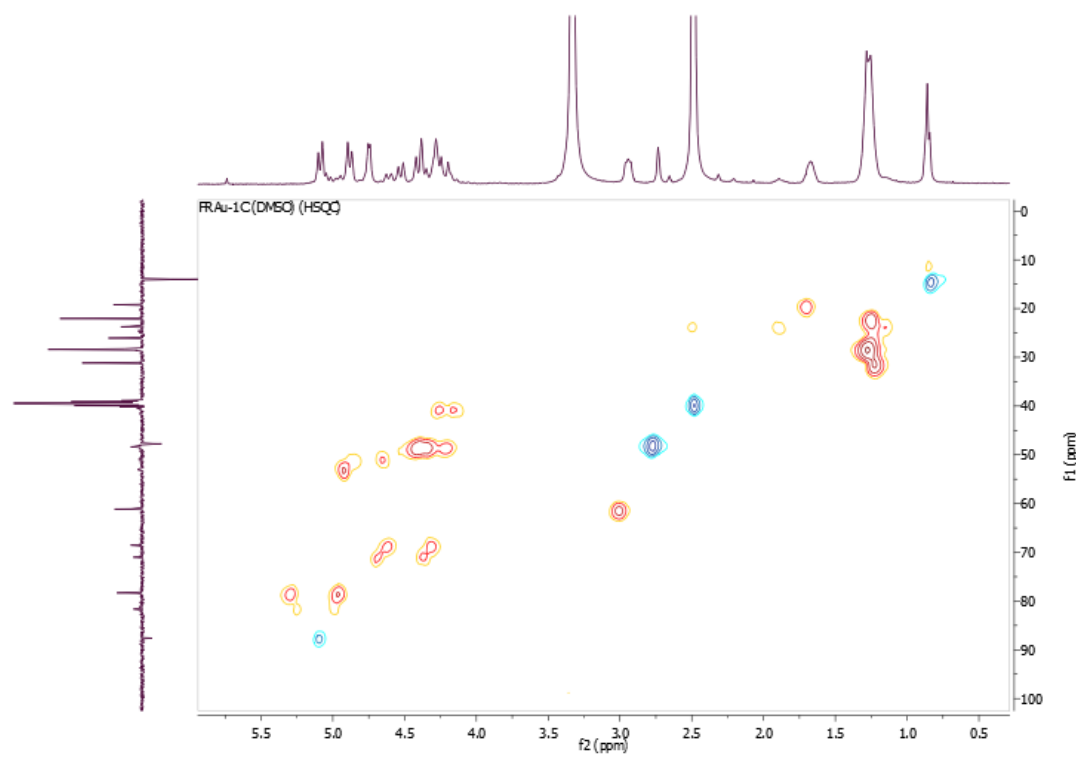


Figure S15. C,H-HSQC experiment of $[\text{AuCl}(\text{PTA}-\text{CH}_2(\text{CH}_2)_6\text{CH}_3)]\text{I}$ (**1a**) in dms0-d_6

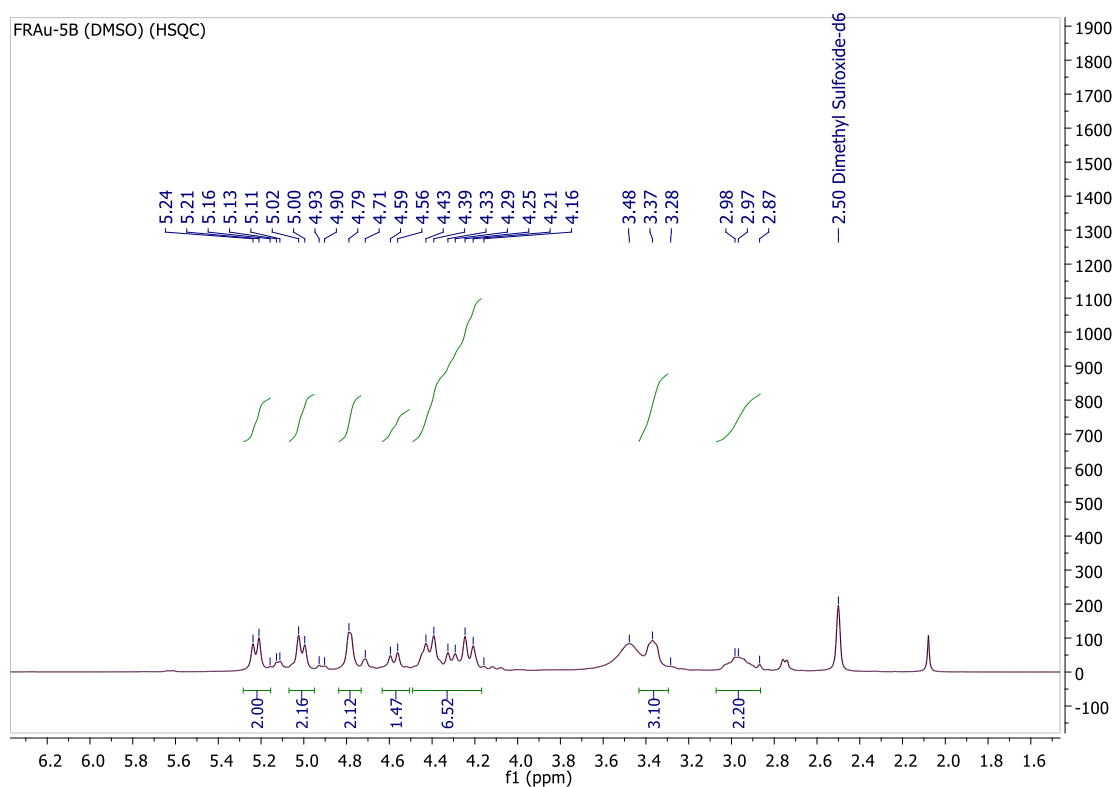


Figure S16 ^1H NMR spectrum of $[\text{AuCl}(\text{PTA}-\text{CH}_2\text{CH}_2(\text{CF}_2)_5\text{CF}_3)]\text{TfO}$ (**1b**) in dms0-d_6

Figure 6.25 IR spectrum of compound (**4**)

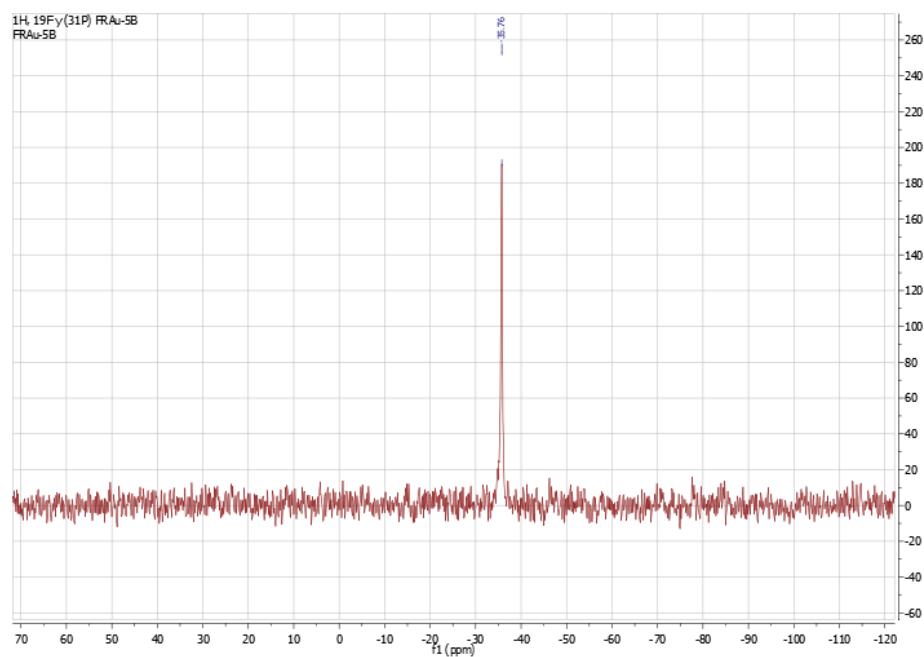


Figure S17. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of $[\text{AuCl}(\text{PTA}-\text{CH}_2\text{CH}_2(\text{CF}_2)_5\text{CF}_3)]\text{TfO}$ (**1b**) in $\text{dms0}-d_6$

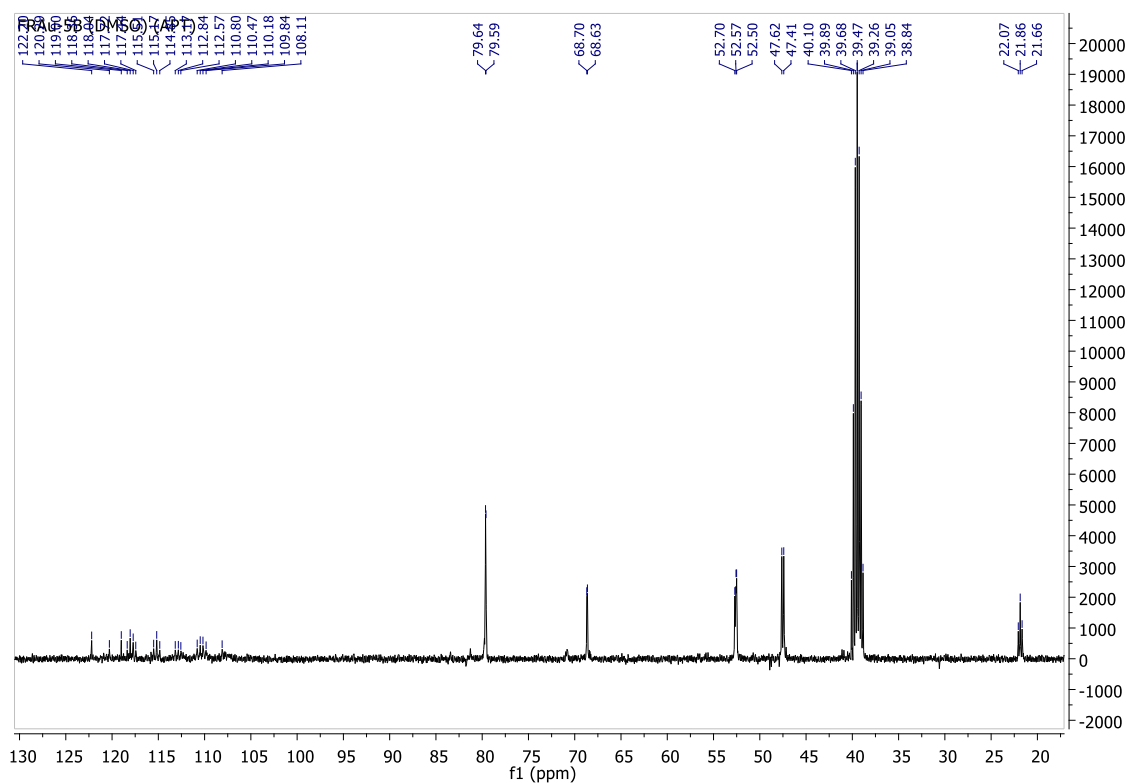


Figure S18. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $[\text{AuCl}(\text{PTA}-\text{CH}_2\text{CH}_2(\text{CF}_2)_5\text{CF}_3)]\text{TfO}$ (**1b**) in $\text{dms0}-d_6$

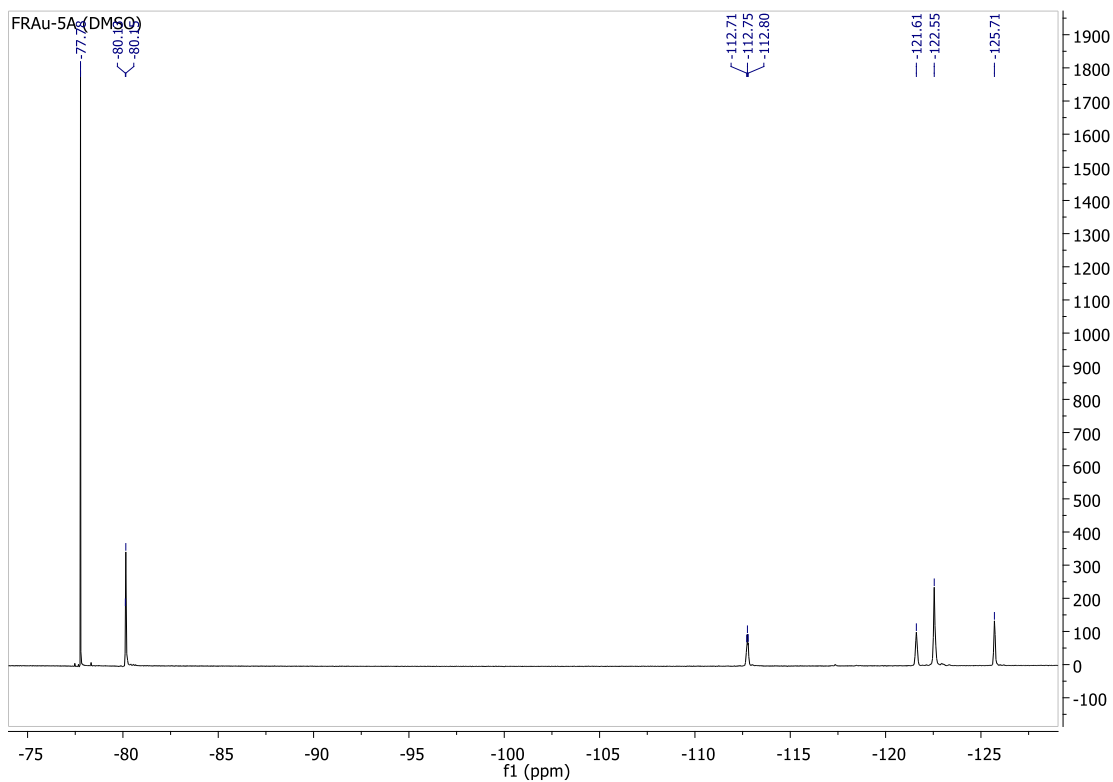


Figure S19. ^{19}F $\{^1\text{H}\}$ NMR spectrum of $[\text{AuCl}(\text{PTA-CH}_2\text{CH}_2(\text{CF}_2)_5\text{CF}_3)]\text{TfO}$ (**1b**) in dmsd-d_6

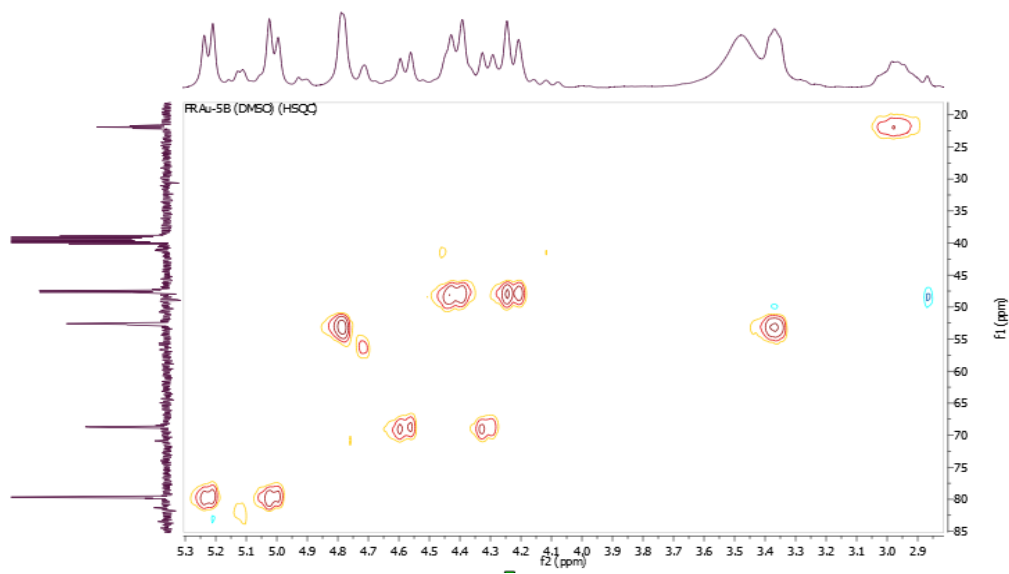


Figure S20. C,H-HSQC experiment of $[\text{AuCl}(\text{PTA-CH}_2\text{CH}_2(\text{CF}_2)_5\text{CF}_3)]\text{TfO}$ (**1b**) in dmsd-d_6

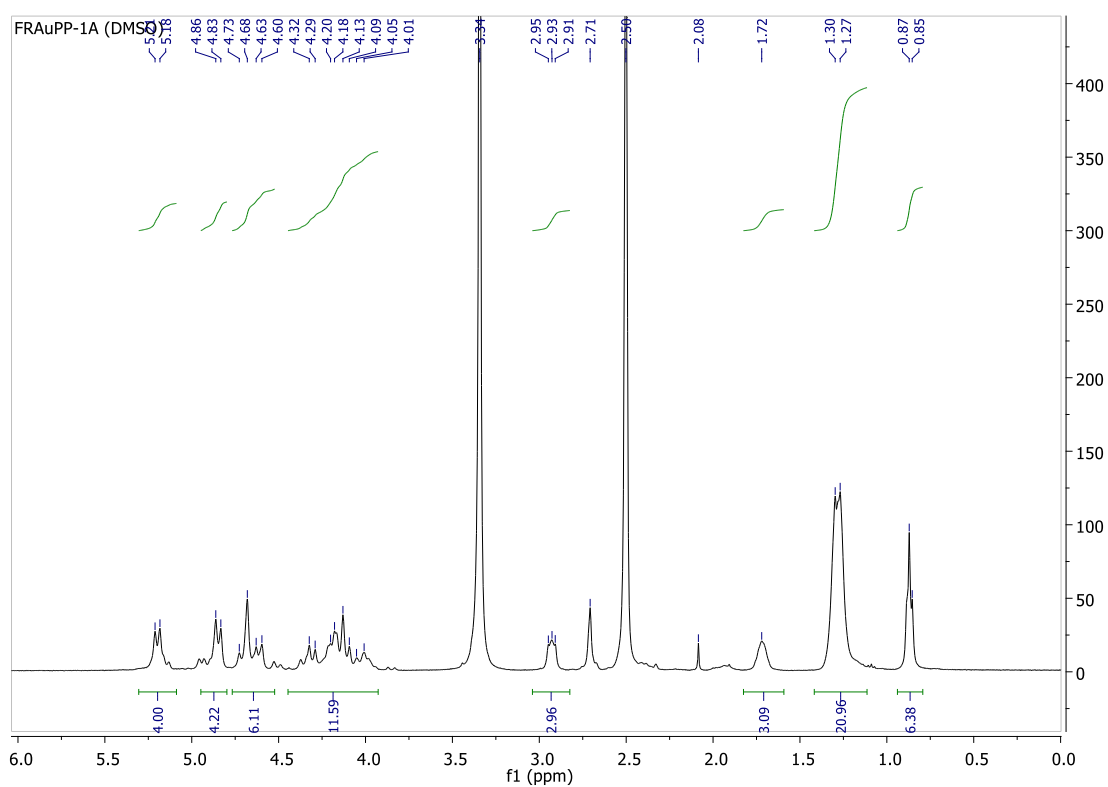


Figure S21 ^1H NMR spectrum of $[\text{AuCl}(\text{PTA-CH}_2(\text{CH}_2)_6\text{CH}_3)_2]\text{I}_2$ (**2a**) in dms0-d_6

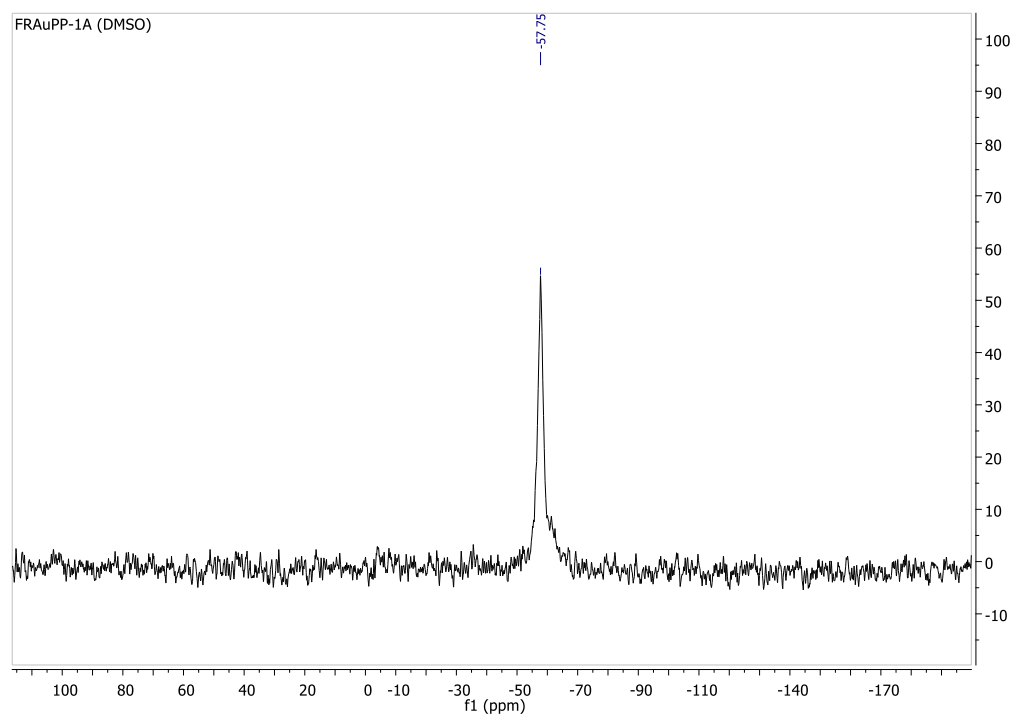


Figure S22. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of (**2a**) in dms0-d_6

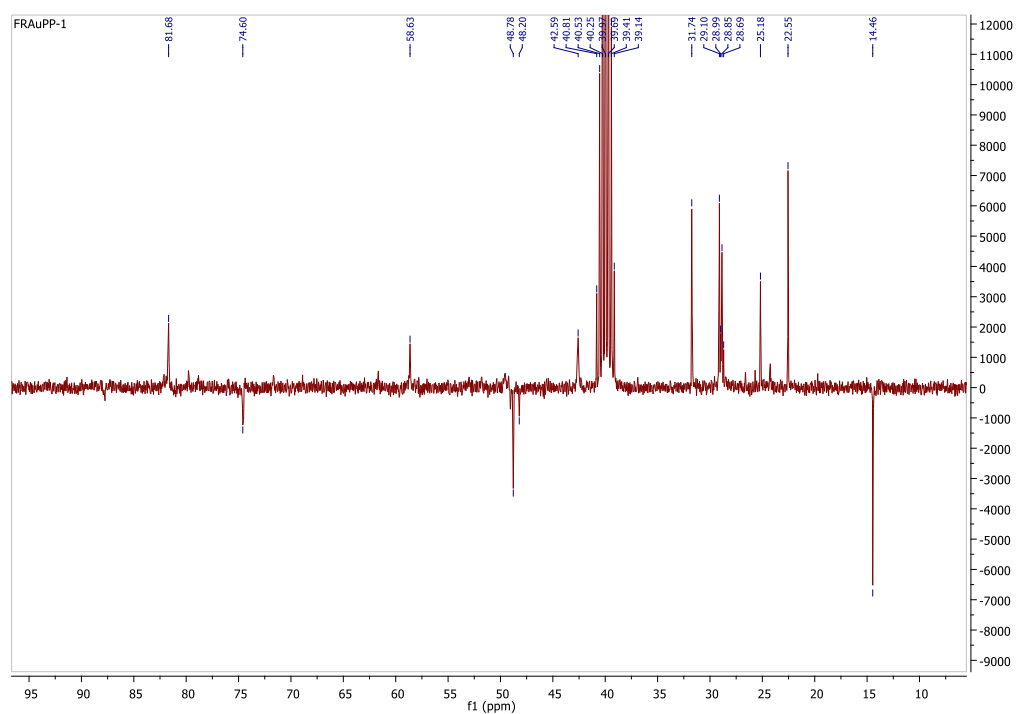


Figure S23. ^{13}C $\{^1\text{H}\}$ -APT spectrum of (**2a**) in dmsO-d_6

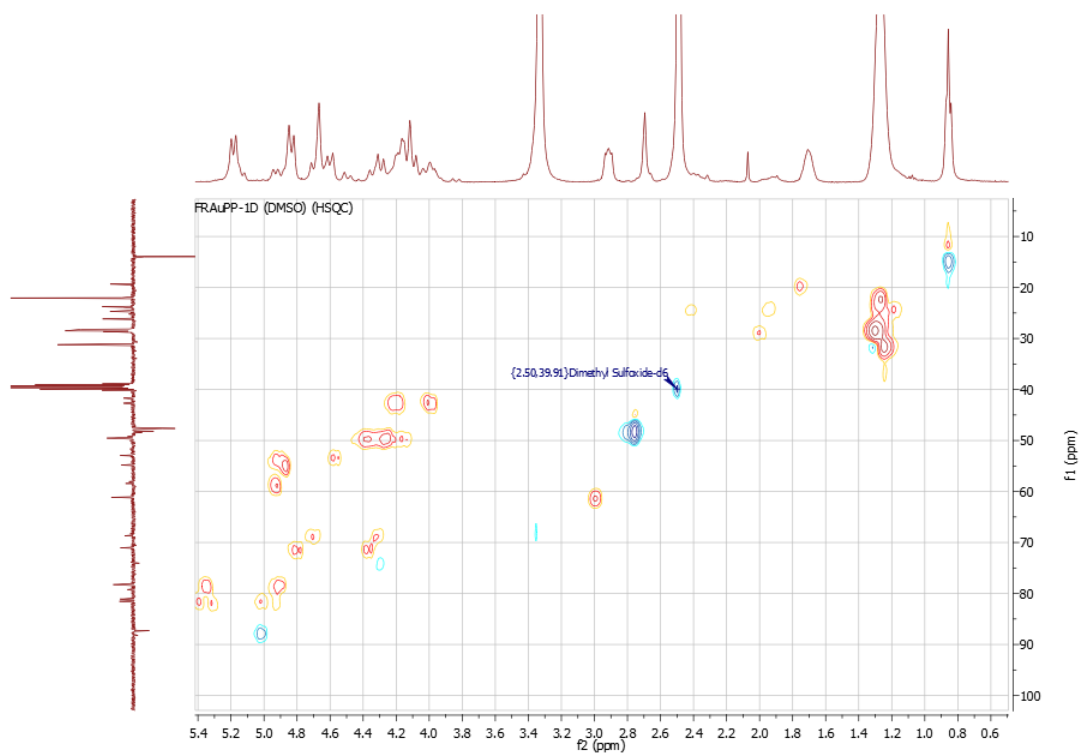


Figure S24. C,H-HSQC experiment of $[\text{AuCl}(\text{PTA-CH}_2(\text{CH}_2)_6\text{CH}_3)_2]\text{I}_2$ (**2a**) in dmsO-d_6

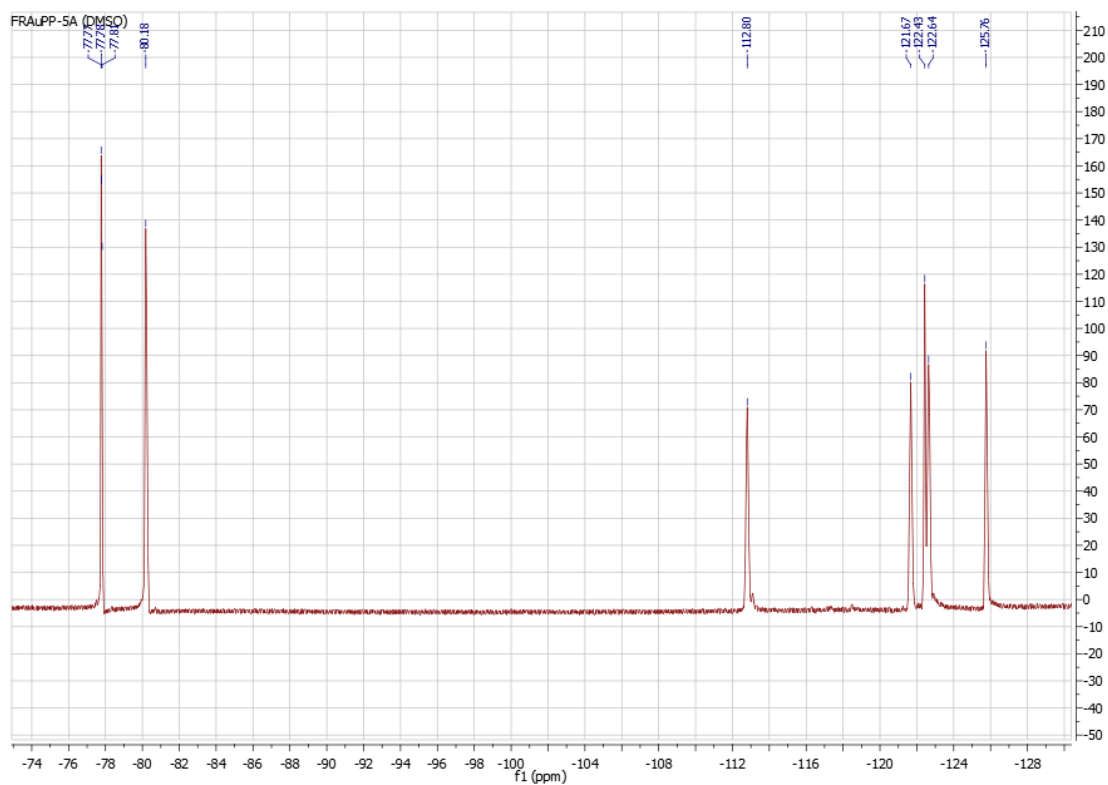


Figure S27. ^{19}F $\{^1\text{H}\}$ NMR of $[\text{AuCl}(\text{PTA}-\text{CH}_2\text{CH}_2(\text{CF}_2)_5\text{CF}_3)_2](\text{TfO})_2$ (**2b**) in $\text{dmsd}-d_6$

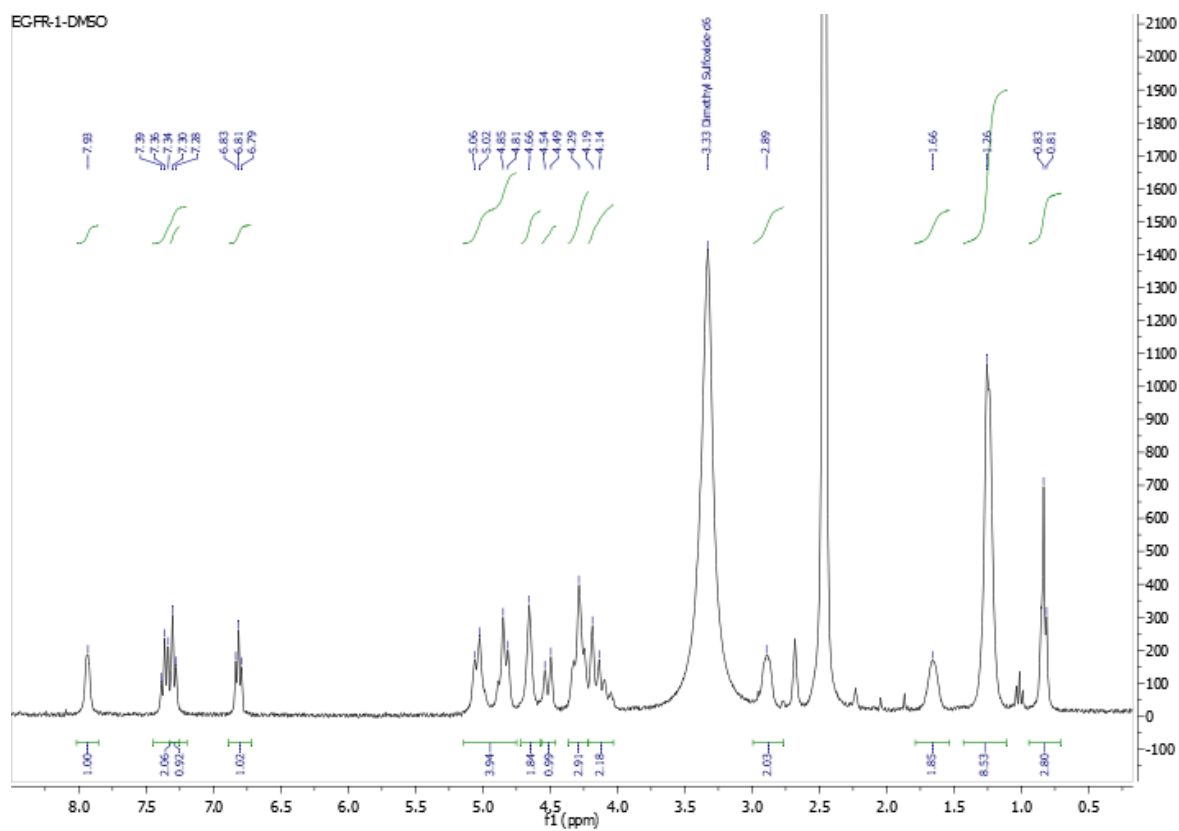


Figure S28. ^1H NMR spectrum of $[\text{Au}(\text{C}_5\text{H}_5\text{NS})(\text{PTA}-\text{CH}_2(\text{CH}_2)_6\text{CH}_3)]\text{I}$ (**3a**) in $\text{dmsd}-d_6$

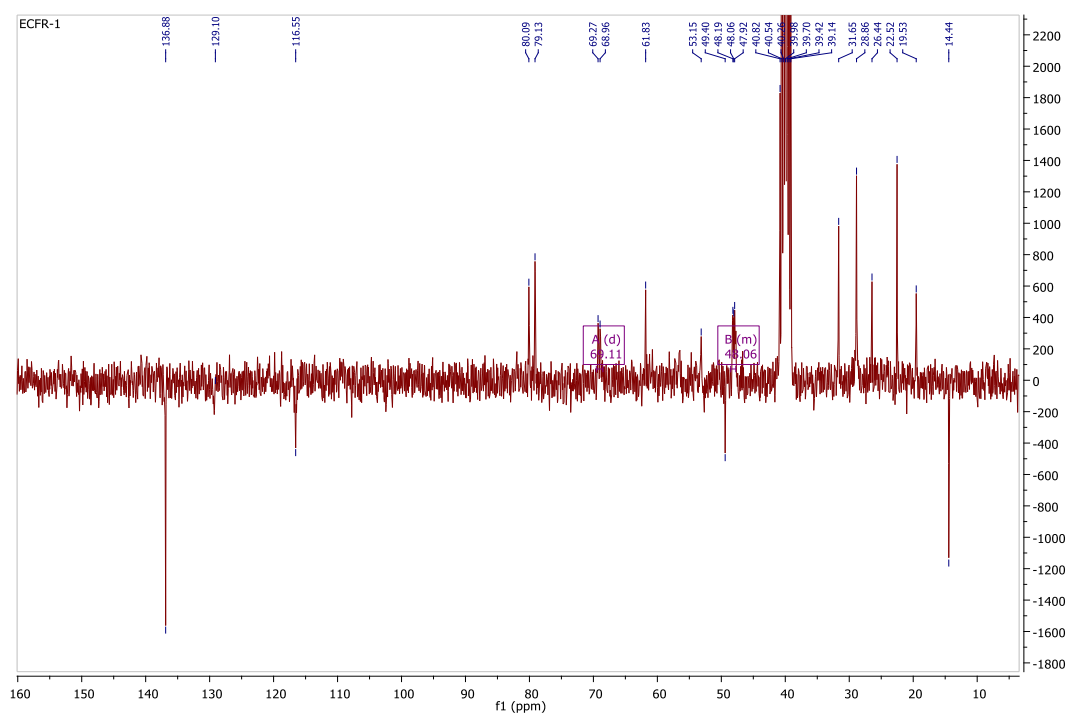


Figure S29. ^{13}C $\{^1\text{H}\}$ -apt NMR spectrum of $[\text{Au}(\text{C}_5\text{H}_5\text{NS})(\text{PTA}-\text{CH}_2(\text{CH}_2)_6\text{CH}_3)]\text{I}$ (**3a**) in $\text{dmsO}-d_6$

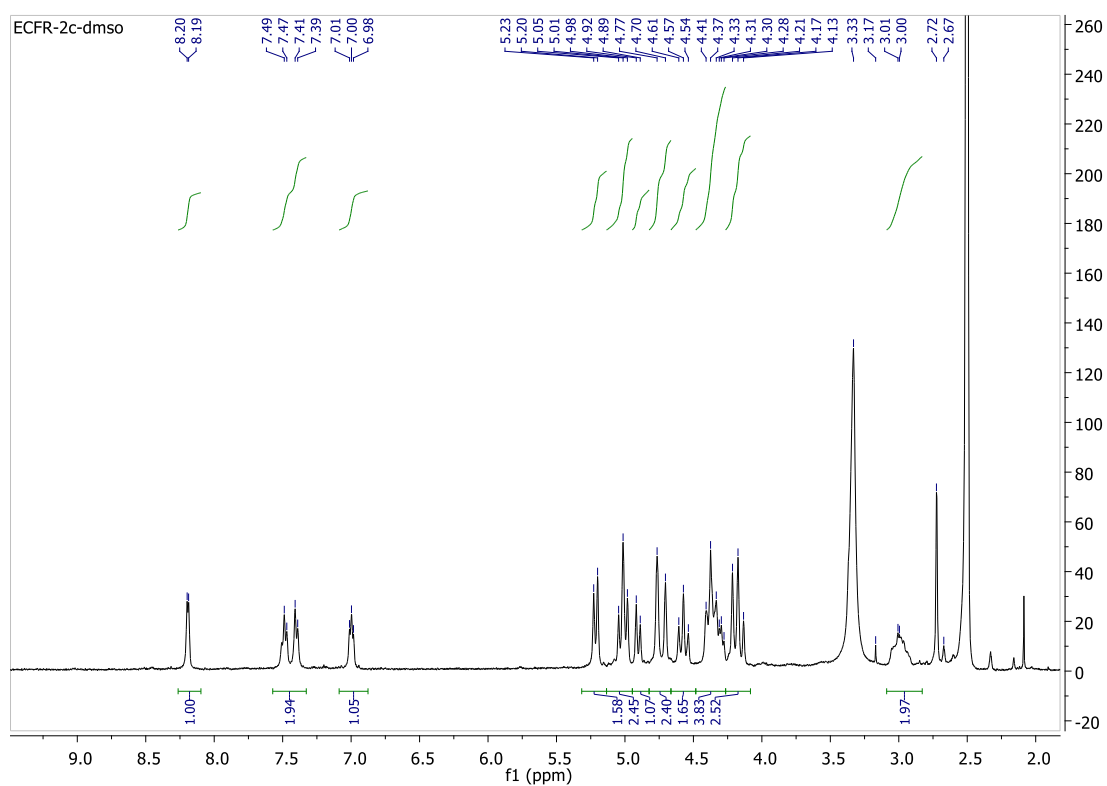


Figure S30. ^1H NMR spectrum of $[\text{Au}(\text{C}_5\text{H}_5\text{NS})(\text{PTA}-\text{CH}_2\text{CH}_2(\text{CF}_2)_5\text{CF}_3)]\text{TfO}$ (**3b**) in $\text{dmsO}-d_6$

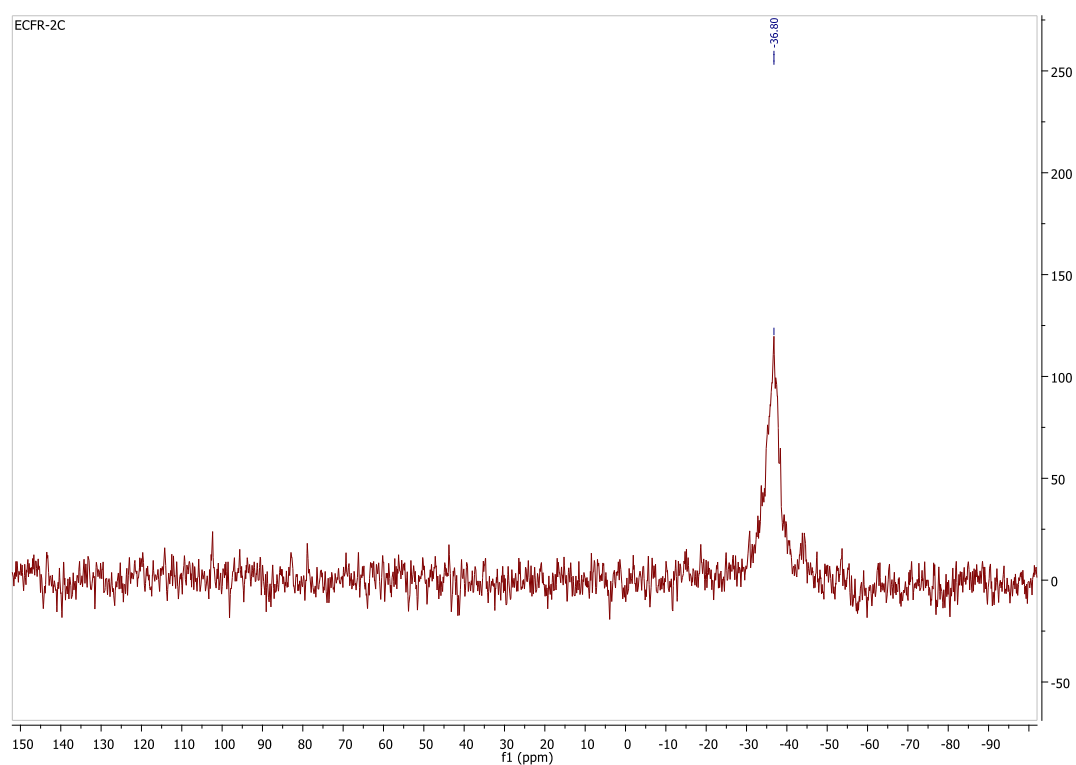


Figure S36. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **3b**

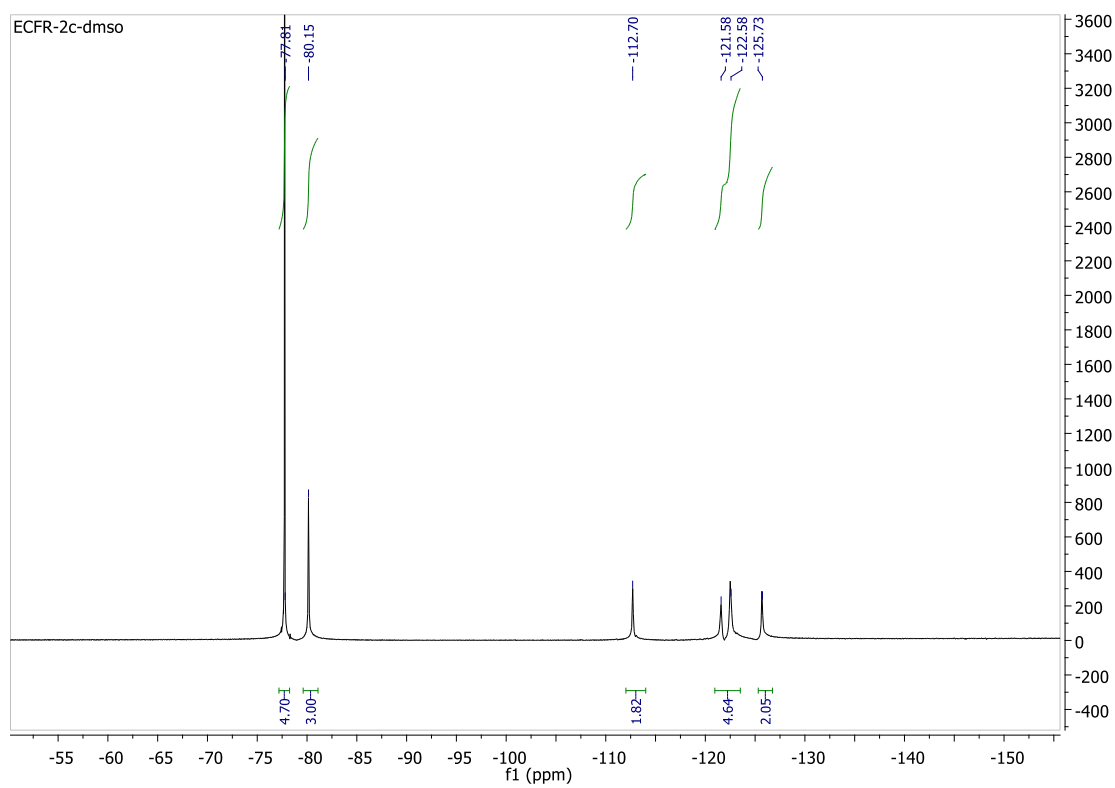


Figure S37. $^{19}\text{F}\{^1\text{H}\}$ NMR spectrum of **3b**

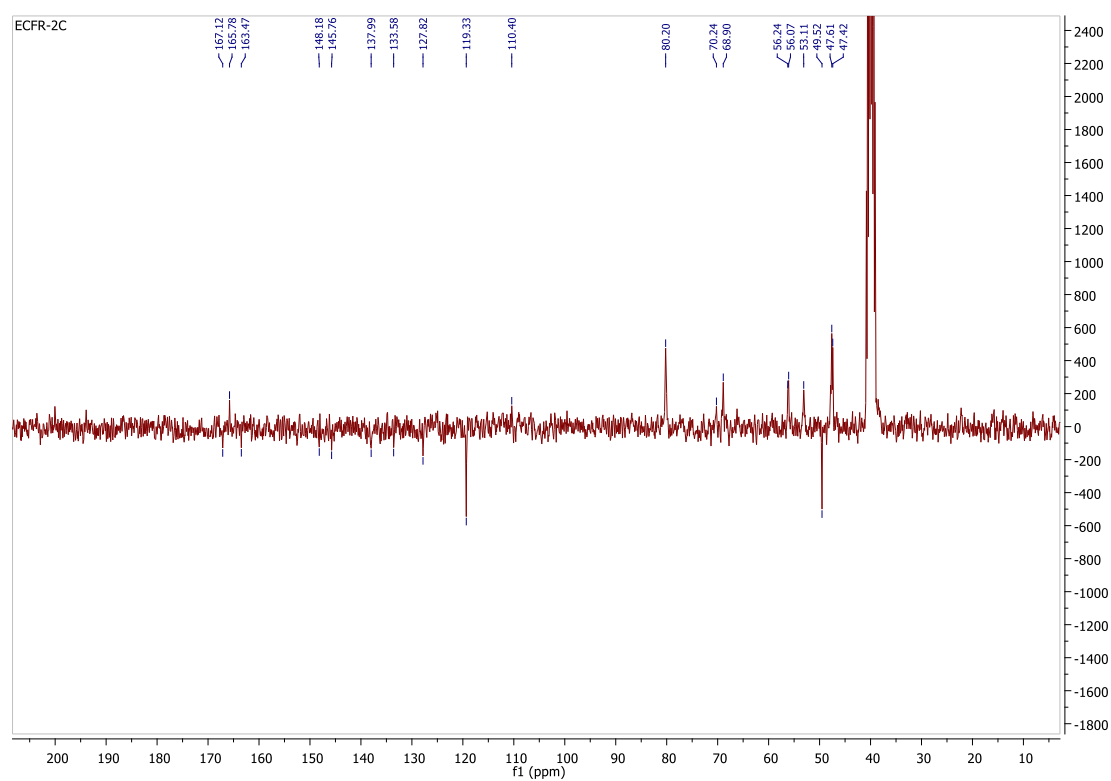
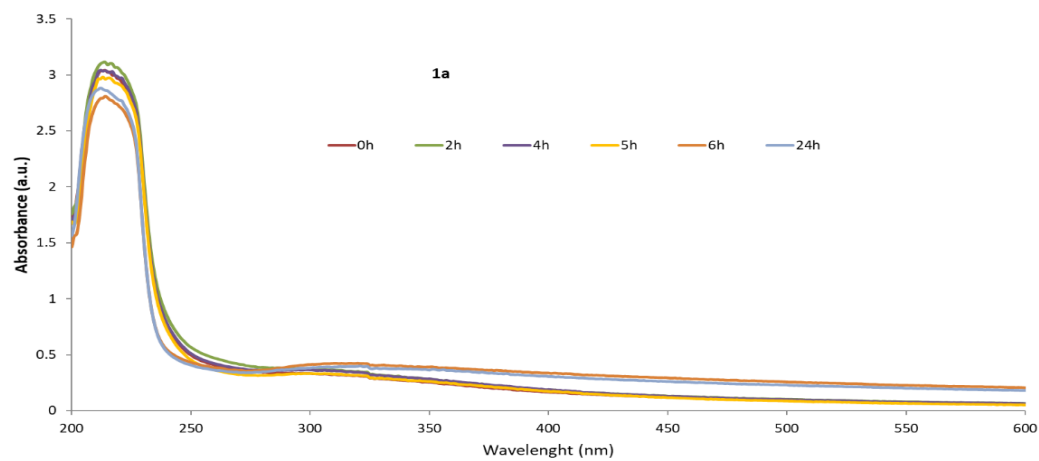
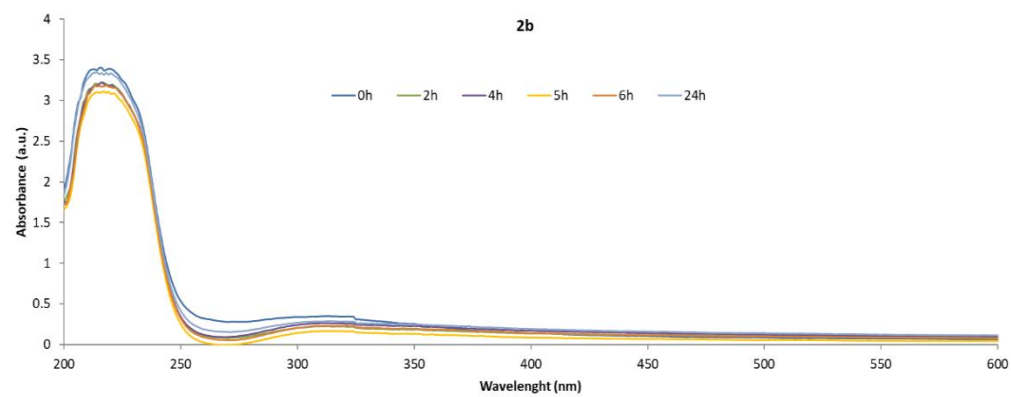
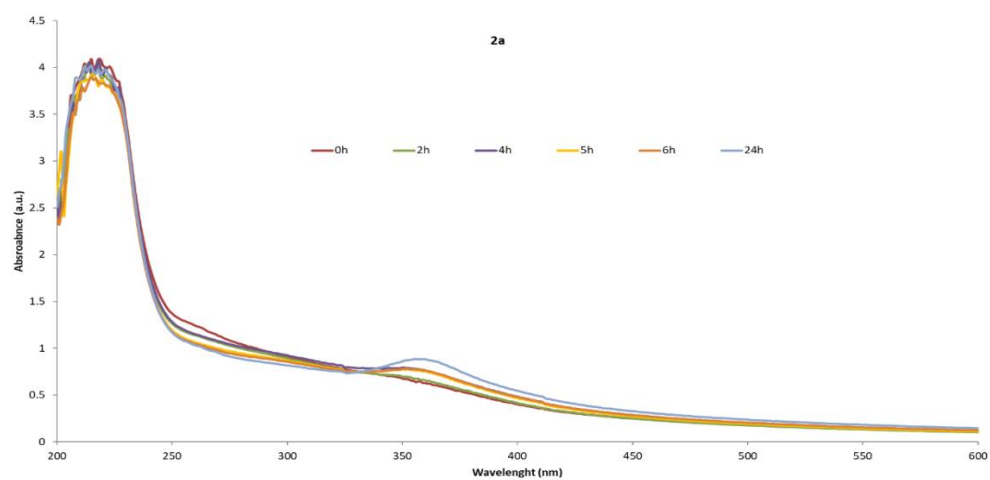
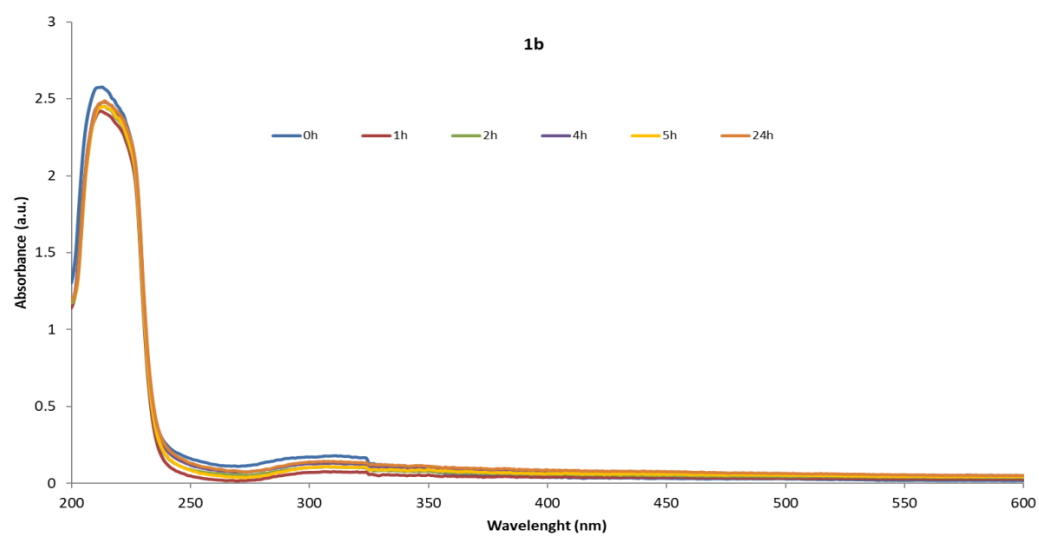


Figure S38. ^{13}C { ^1H }-apt NMR spectrum of **3b**





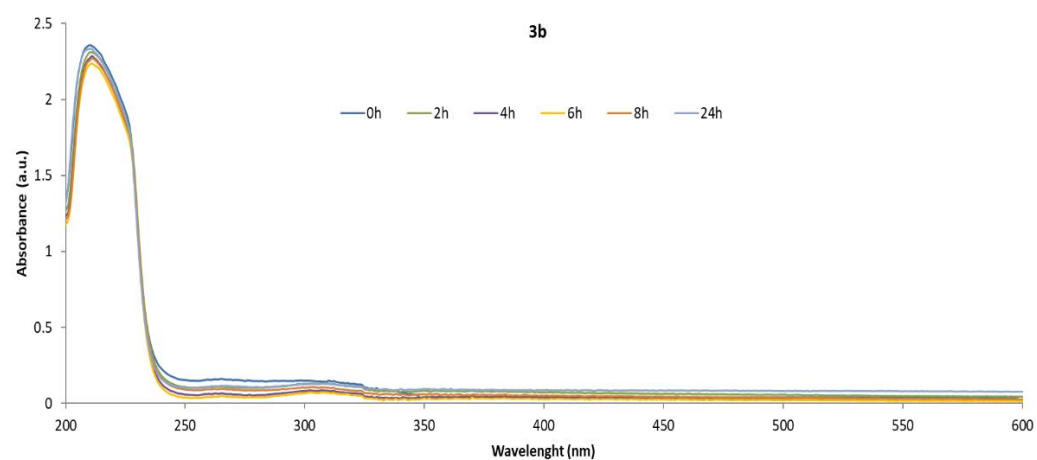
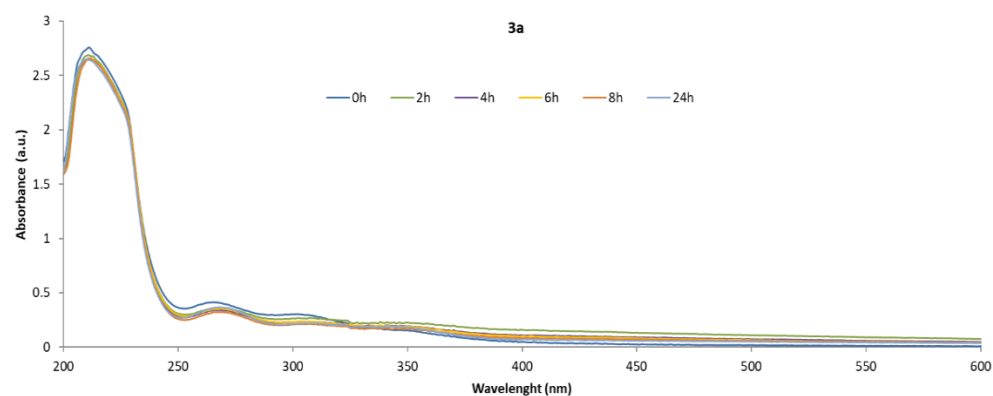


Figure S39. UV-Vis spectra of gold complexes recorded at different times for 24 h to test their stability under physiological conditions. [complex] = 30 μ M diluted in PBS at 37 $^{\circ}$ C.

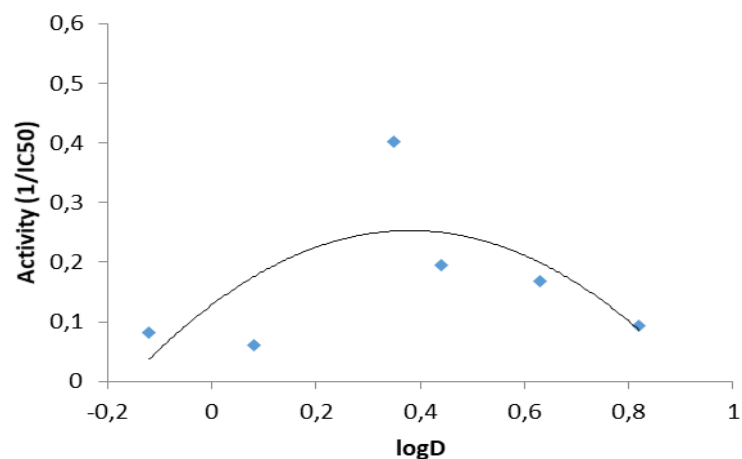


Figure S40. Correlation between cytotoxic activity of the complexes and logD_{7.4}. The activities are calculated as the inverse of IC₅₀ in Caco-2/PD7 cells.