

Accessory Publication

Recognition properties of flavin analogues with bile acid-based receptors: Role of steric effects in hydrogen bond based molecular recognition

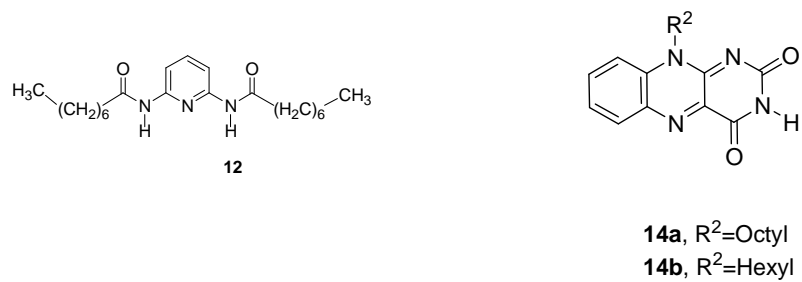
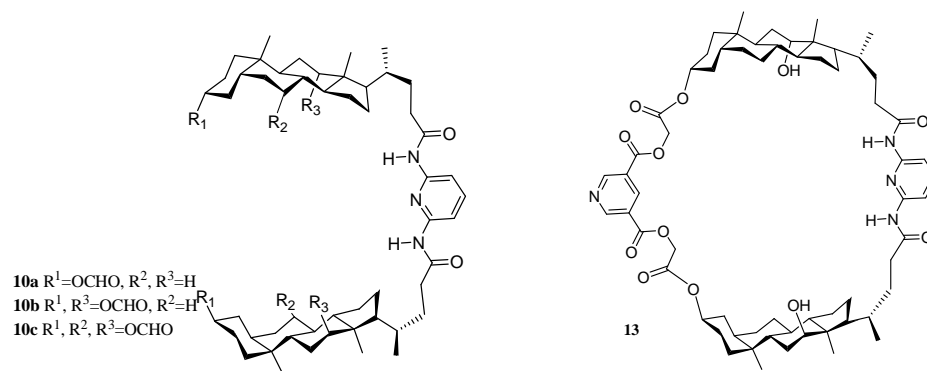
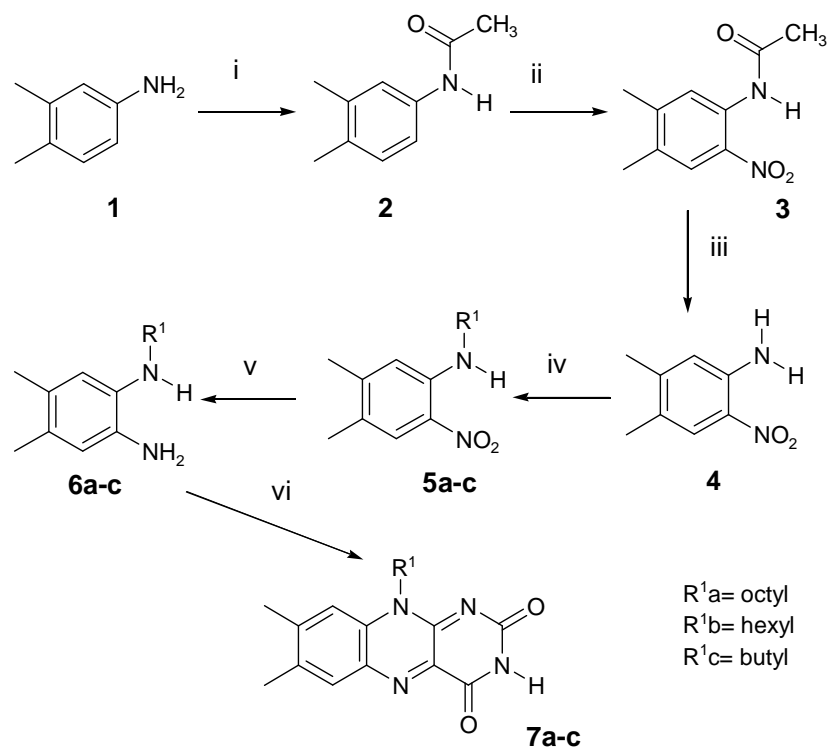
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Supplementary Information Available: X-ray data (CIF), NMR spectra, Job's plot data and binding isotherms are available in supplementary data.

Flavin Synthesis:



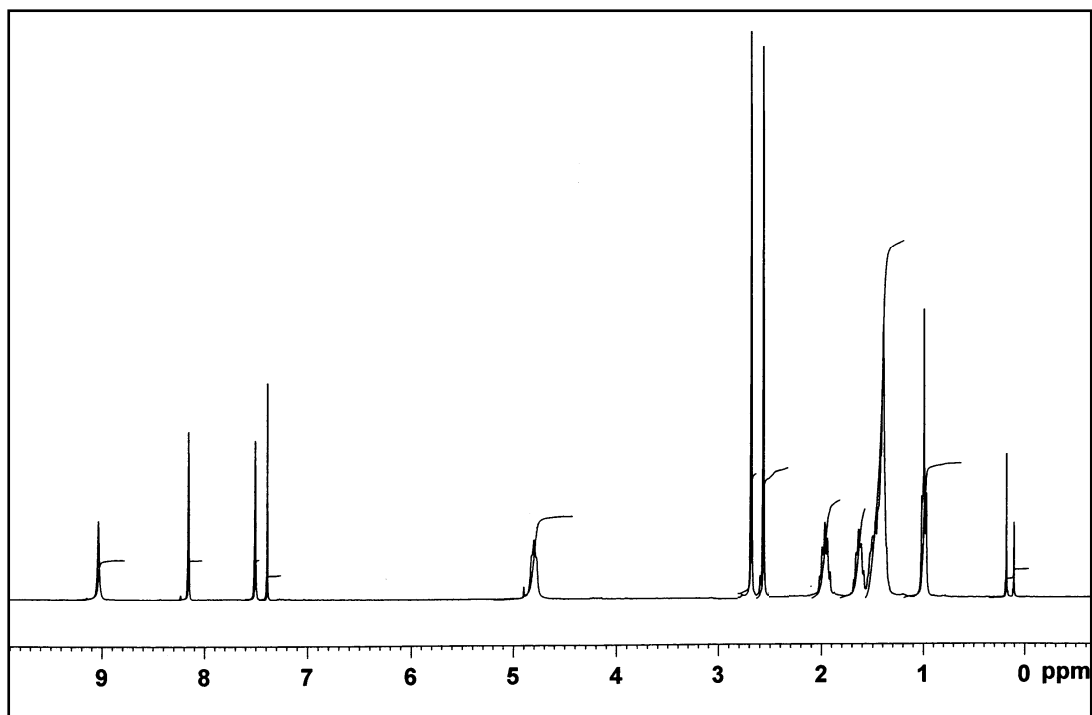


Figure S1: ^1H NMR spectrum of **7a**

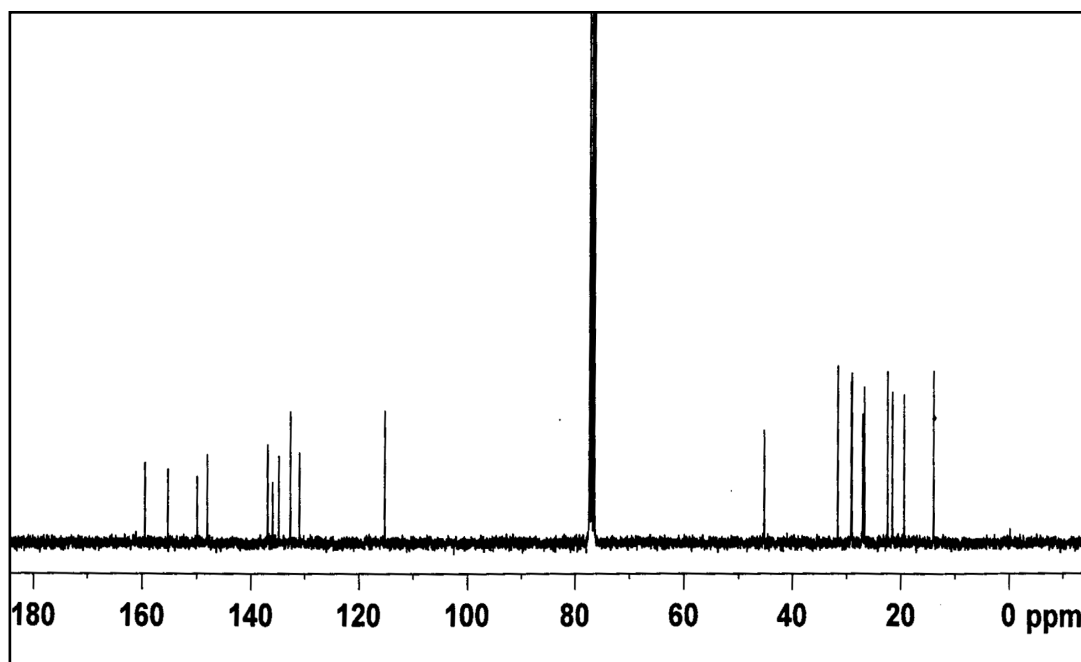


Figure S2: ^{13}C NMR spectrum of **7a**

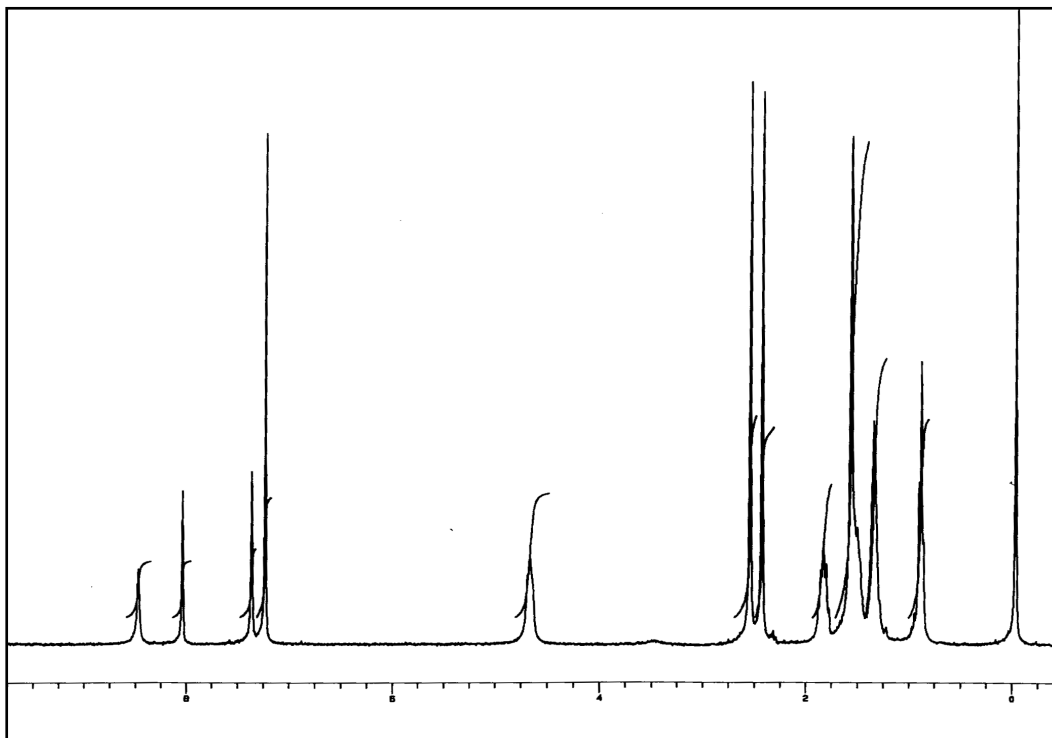


Figure S3: ^1H NMR spectrum of **7b**

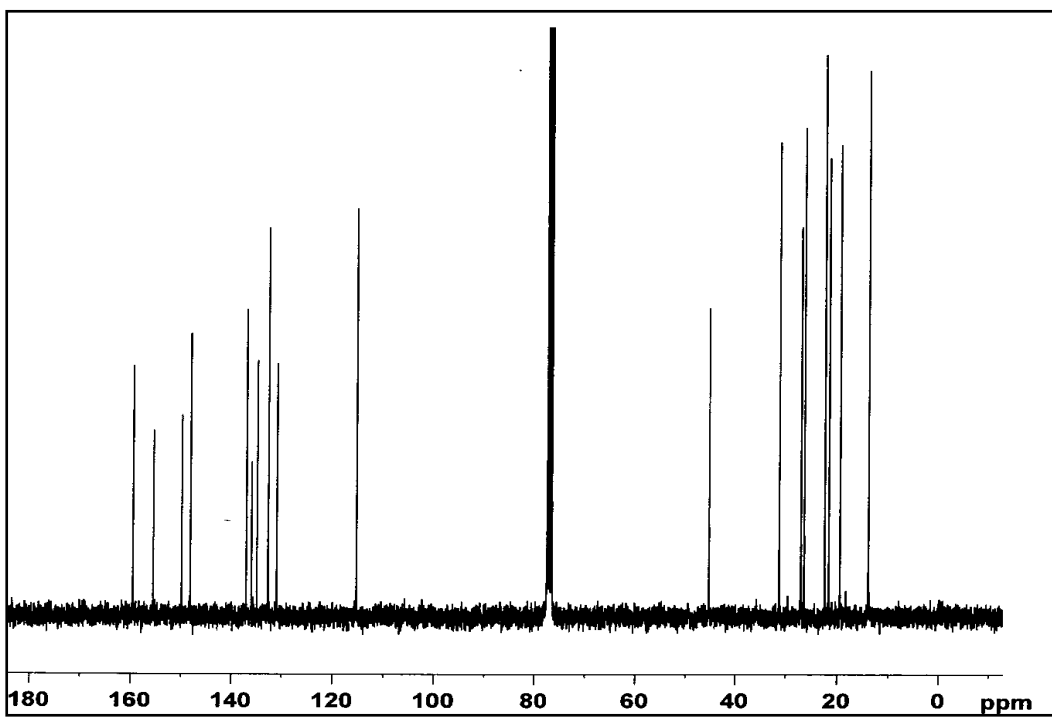
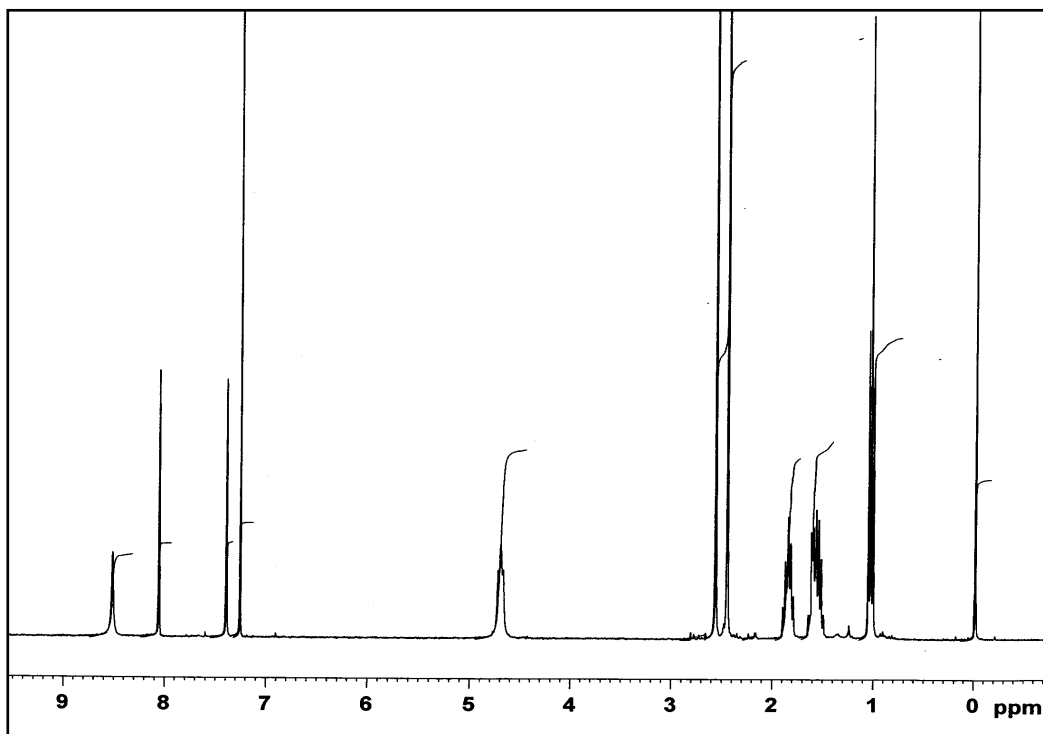
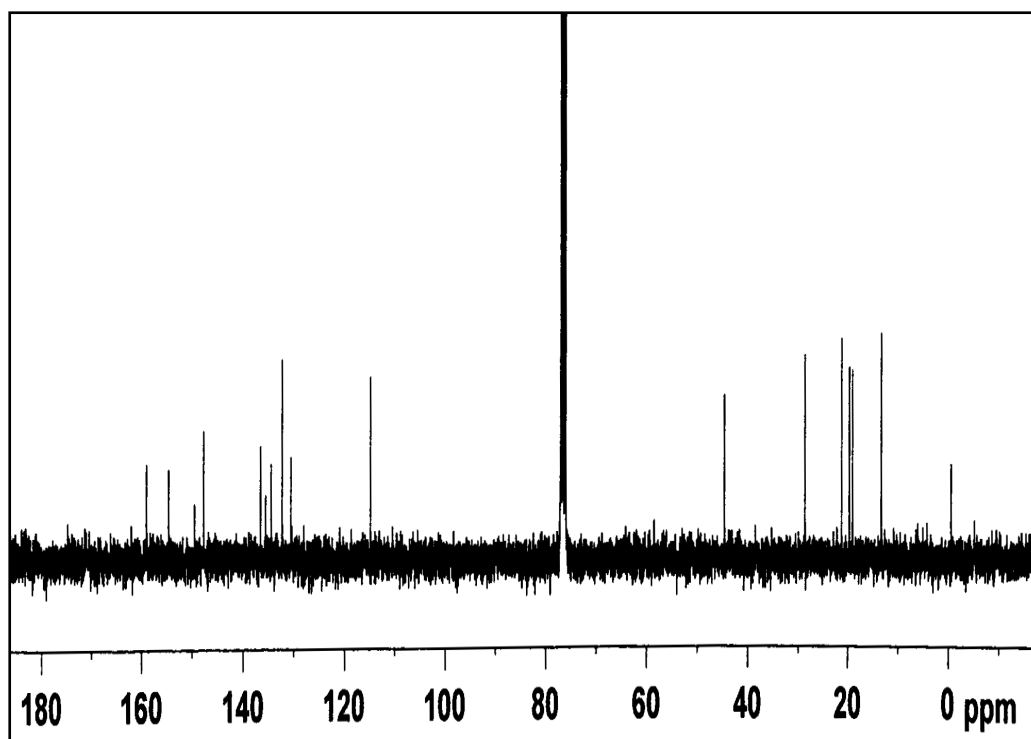


Figure S4: ^{13}C NMR spectrum of **7b**

Figure S5: ^1H NMR spectrum of 7cFigure S6: ^{13}C NMR spectrum of 7c

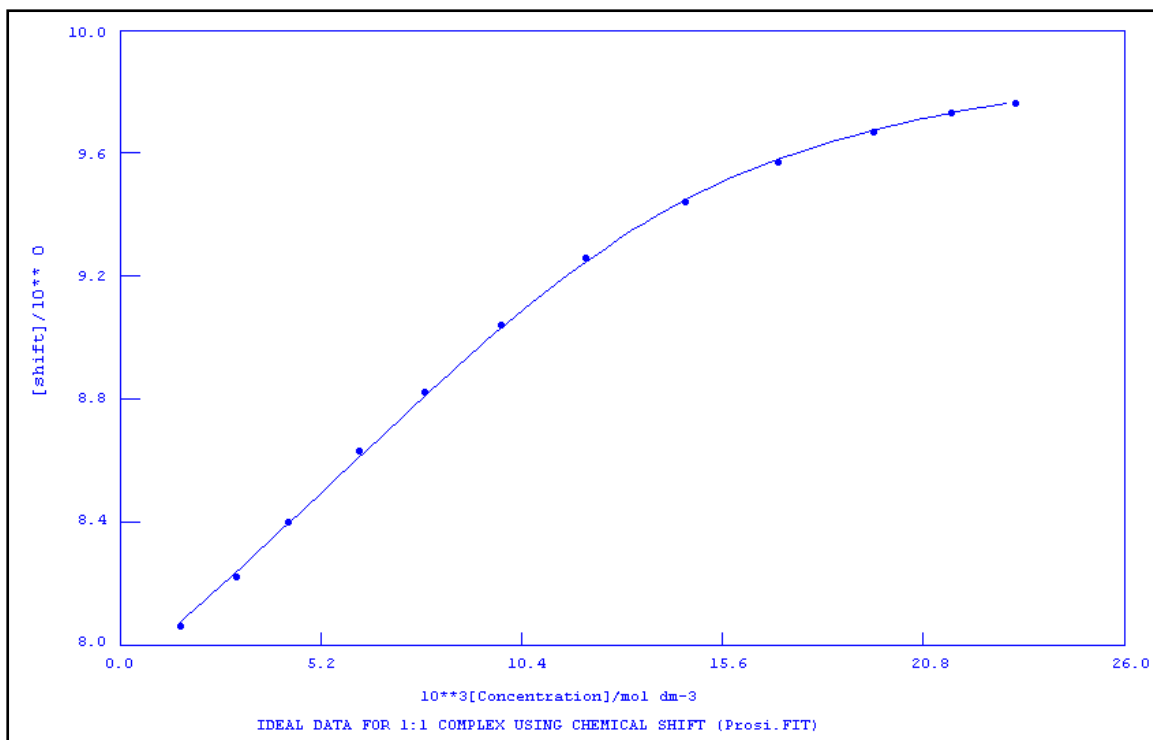


Figure S7: Binding isotherm for amide protons of **10a** with **7b**

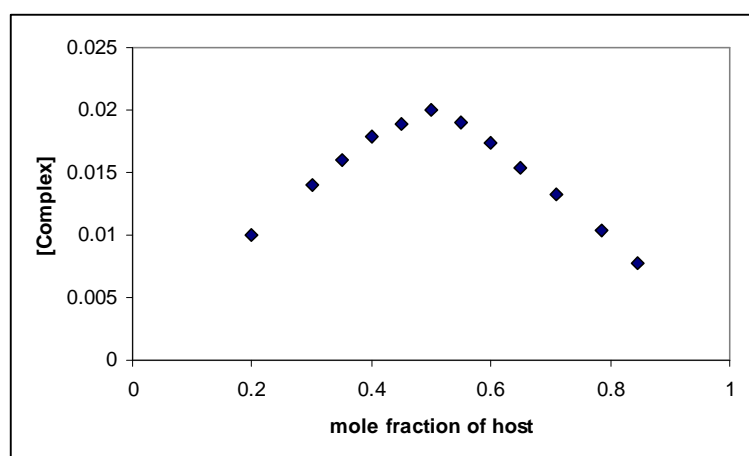


Figure S8: Job's plot showing 1:1 complex formation between **10a** and **7b**

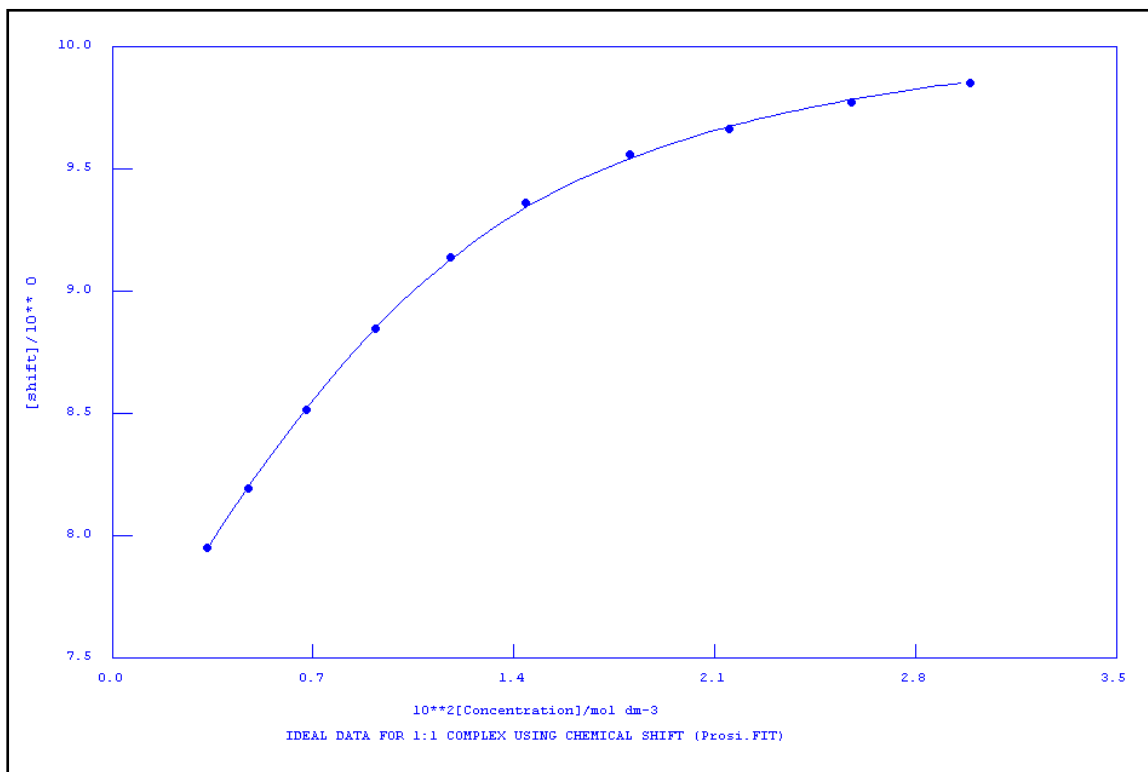


Figure S9: Binding isotherm for amide protons of **10b** with **7a**

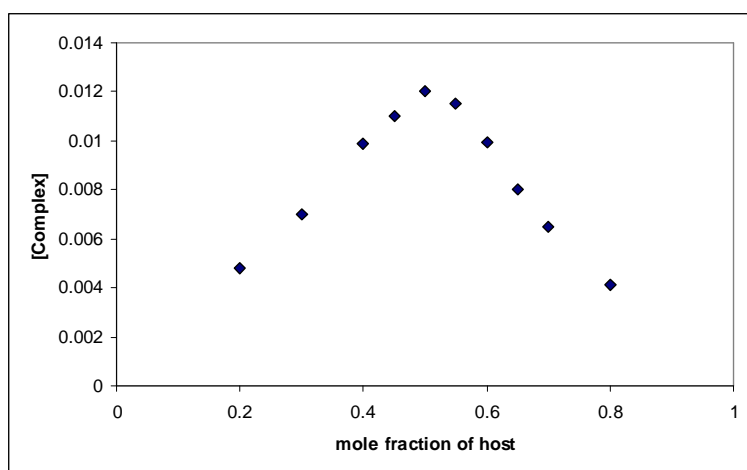


Figure S10: Job's plot showing 1:1 complex formation between **10b** and **7a**

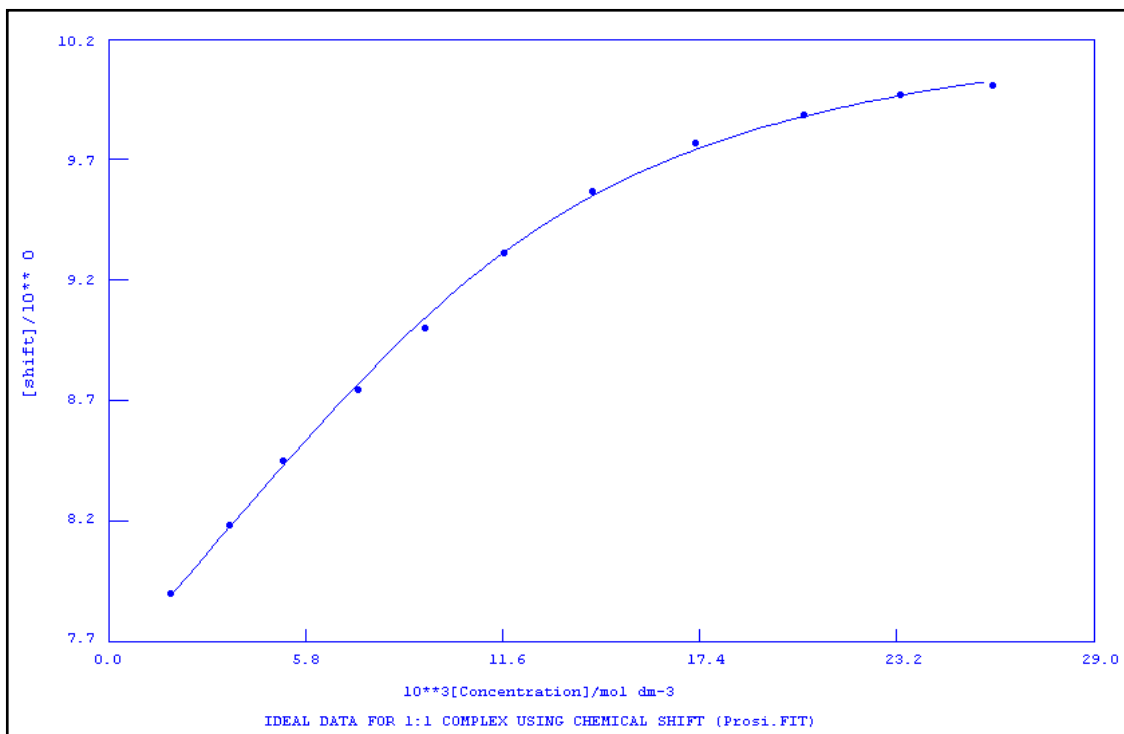


Figure S11: Binding isotherm for amide protons of **10c** with **7b**

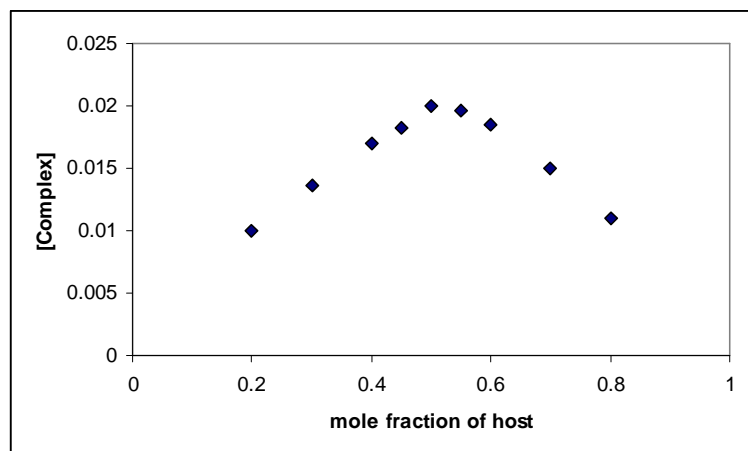


Figure S12: Job's plot showing 1:1 complex formation between **10c** and **7b**

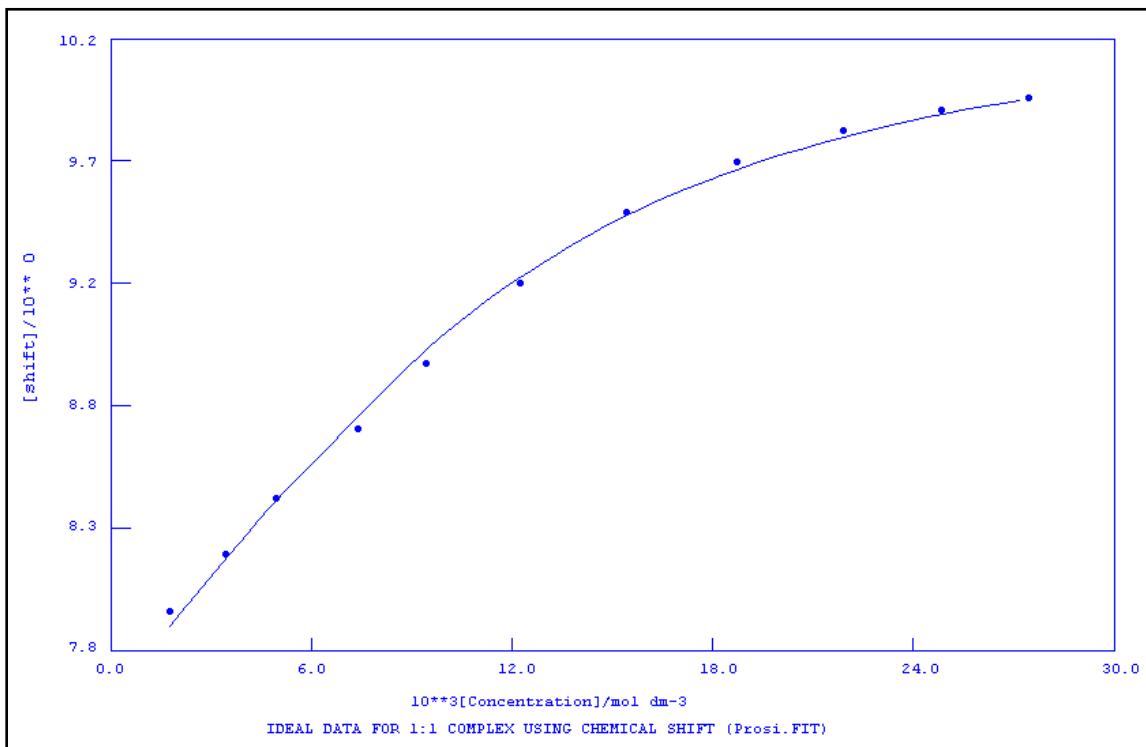


Figure S13: Binding isotherm for amide protons of **10c** with **7c**

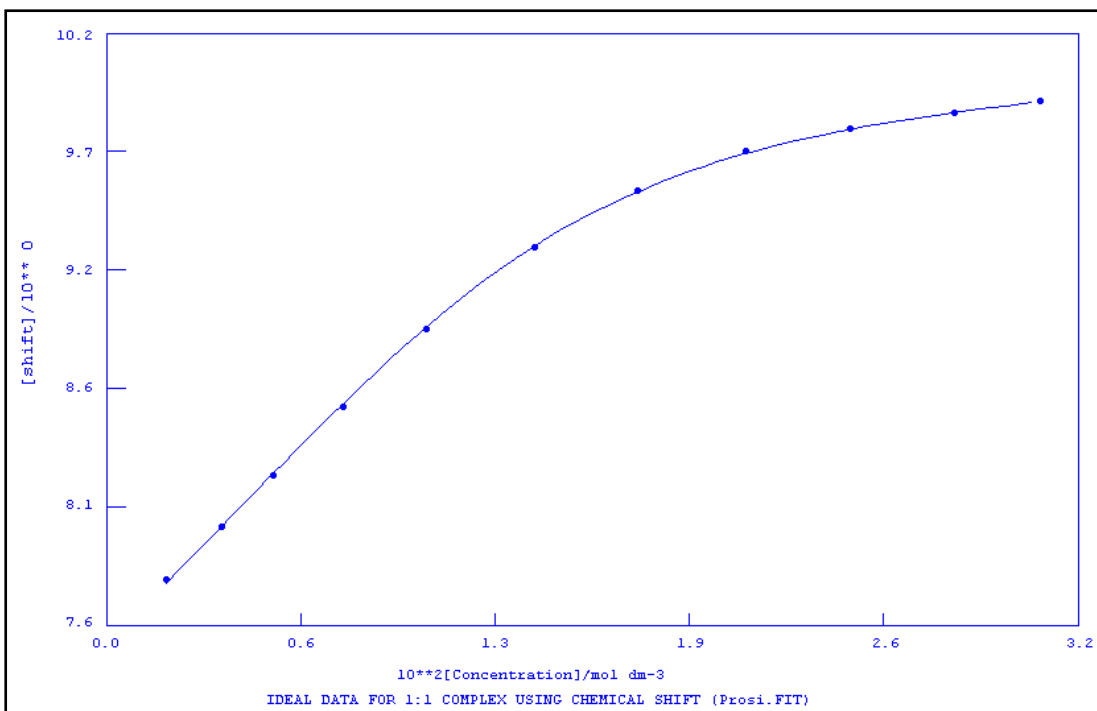


Figure S14: Binding isotherm for amide protons of **12** with **7b**

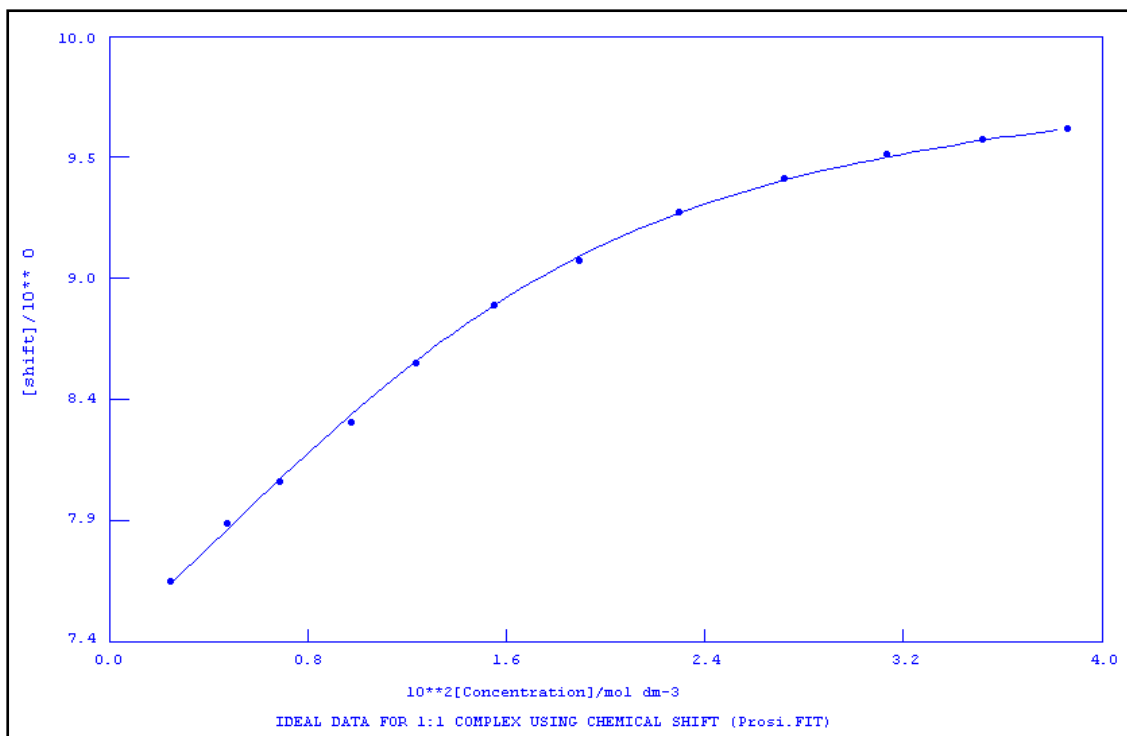


Figure S15: Binding isotherm for amide protons of **12** with **14a**

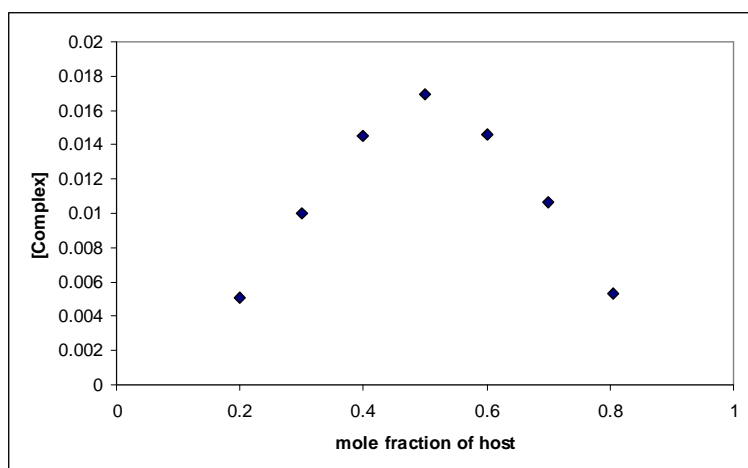


Figure S16: Job's plot showing 1:1 complex formation between **12** and **14a**

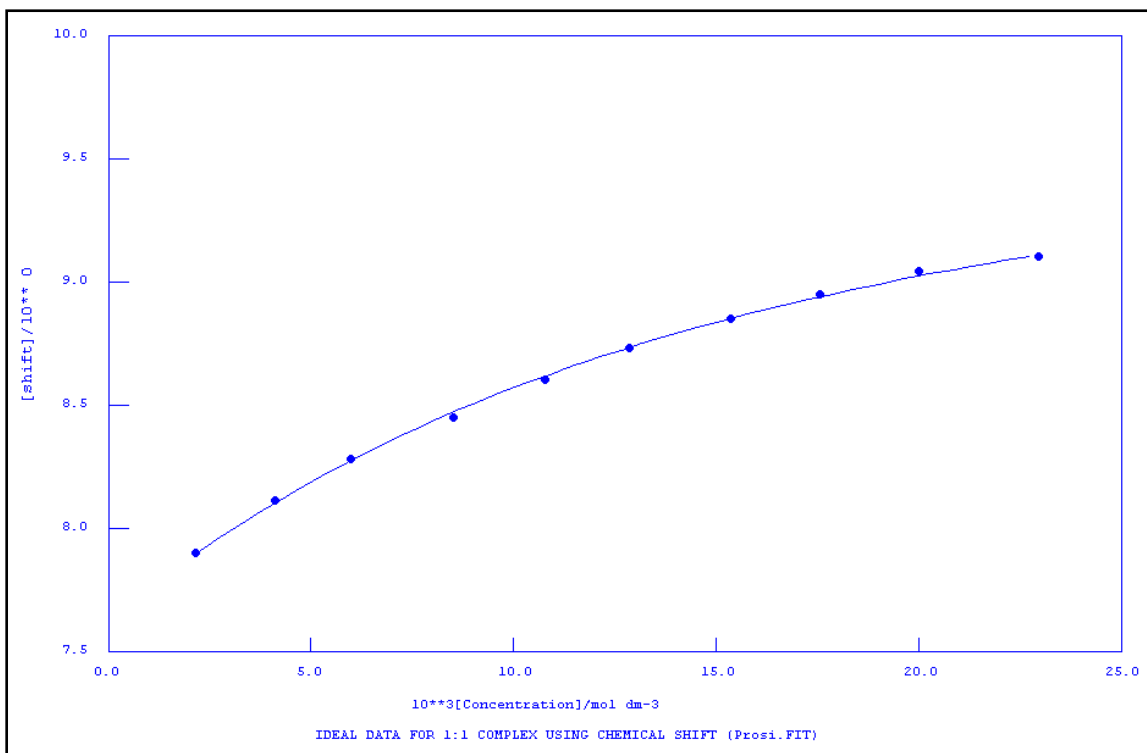


Figure S17: Binding isotherm for amide protons of **13** with **7a**

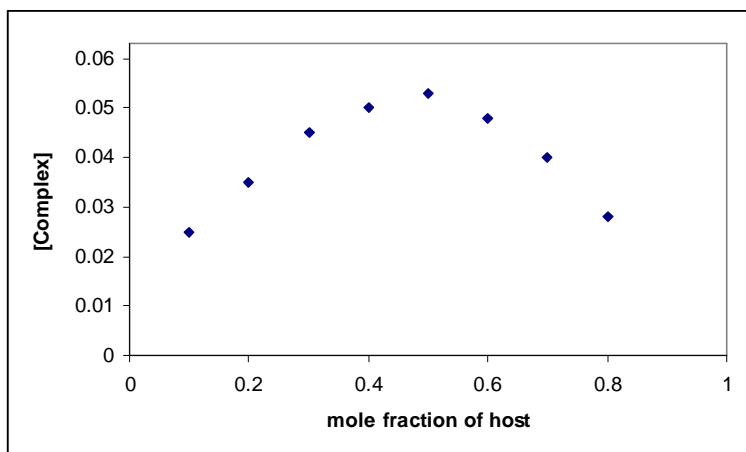


Figure S18: Job's plot showing 1:1 complex formation between **13** and **7a**