Hydrogen-bonding interactions in crown-(thio)urea complexes with anions, chemical warfare agents and simulants

Hannah Cave[1], Jayne A. Ede[2], Mark R. Sambrook[2], Howard Dodd[1], Flavia Fucassi[1], Alexander S. Cragg[1,3], Adam H. Lansley[1] and Peter J. Cragg[1]*

[1]School of Pharmacy and Biomolecular Sciences, Huxley Building, University of Brighton, Brighton BN2 4GJ, UK.

[2]CBR Division, Defence Science and Technology Laboratory (Dstl) Porton Down, Salisbury, SP4 0JQ, UK.

[3]School of Physical Sciences, University of Kent, Canterbury, CT2 7NH, UK

Email: Peter J. Cragg – P.J.Cragg@brighton.ac.uk

Supplementary Information

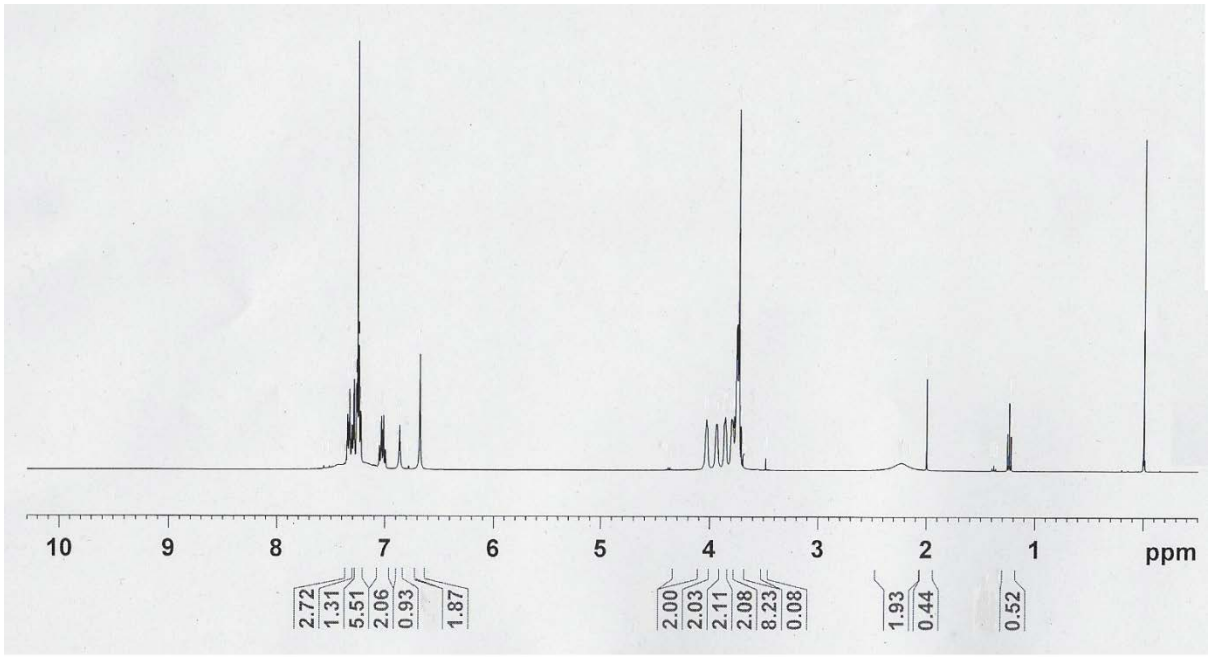

Figure S1. ^{1}H NMR for **1a**

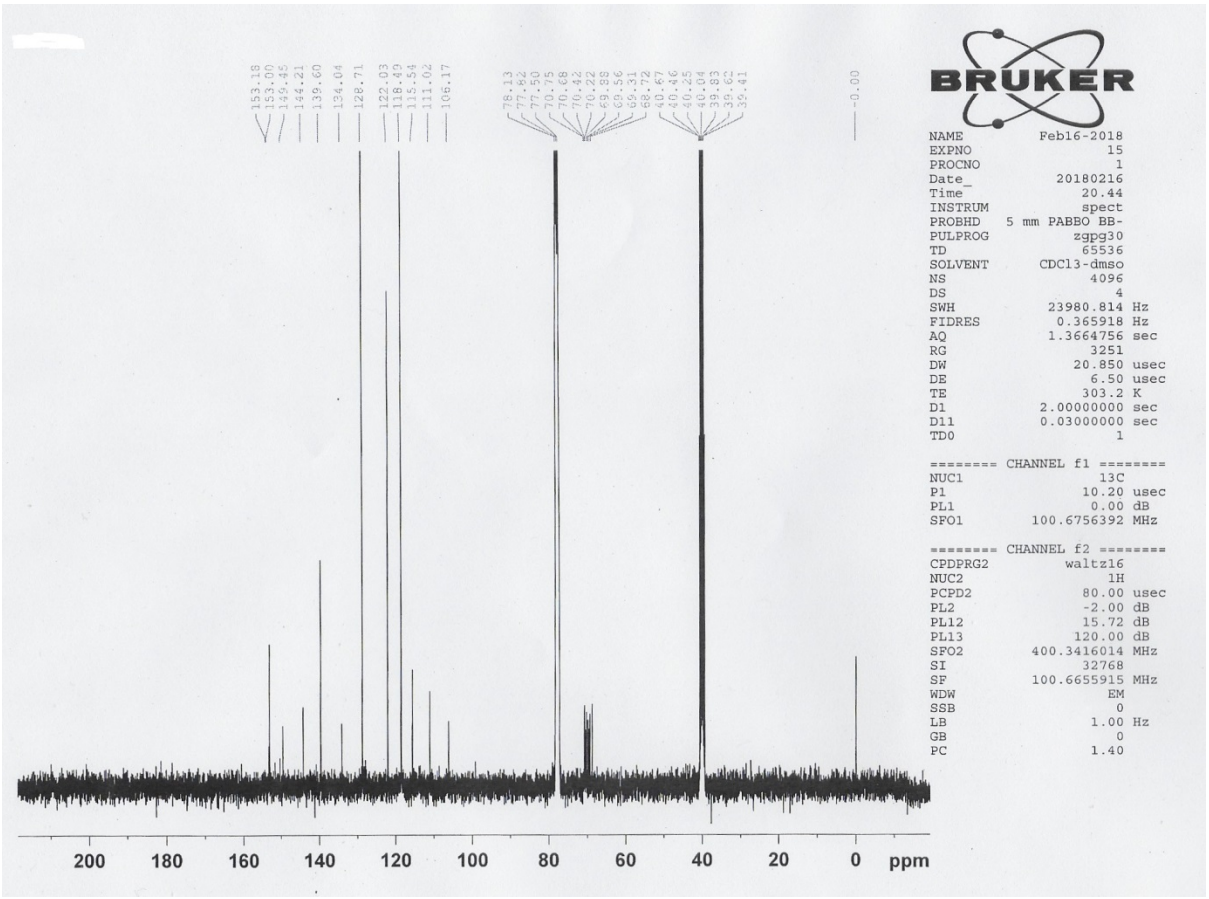

Figure S2. ^{13}C NMR for **1a**

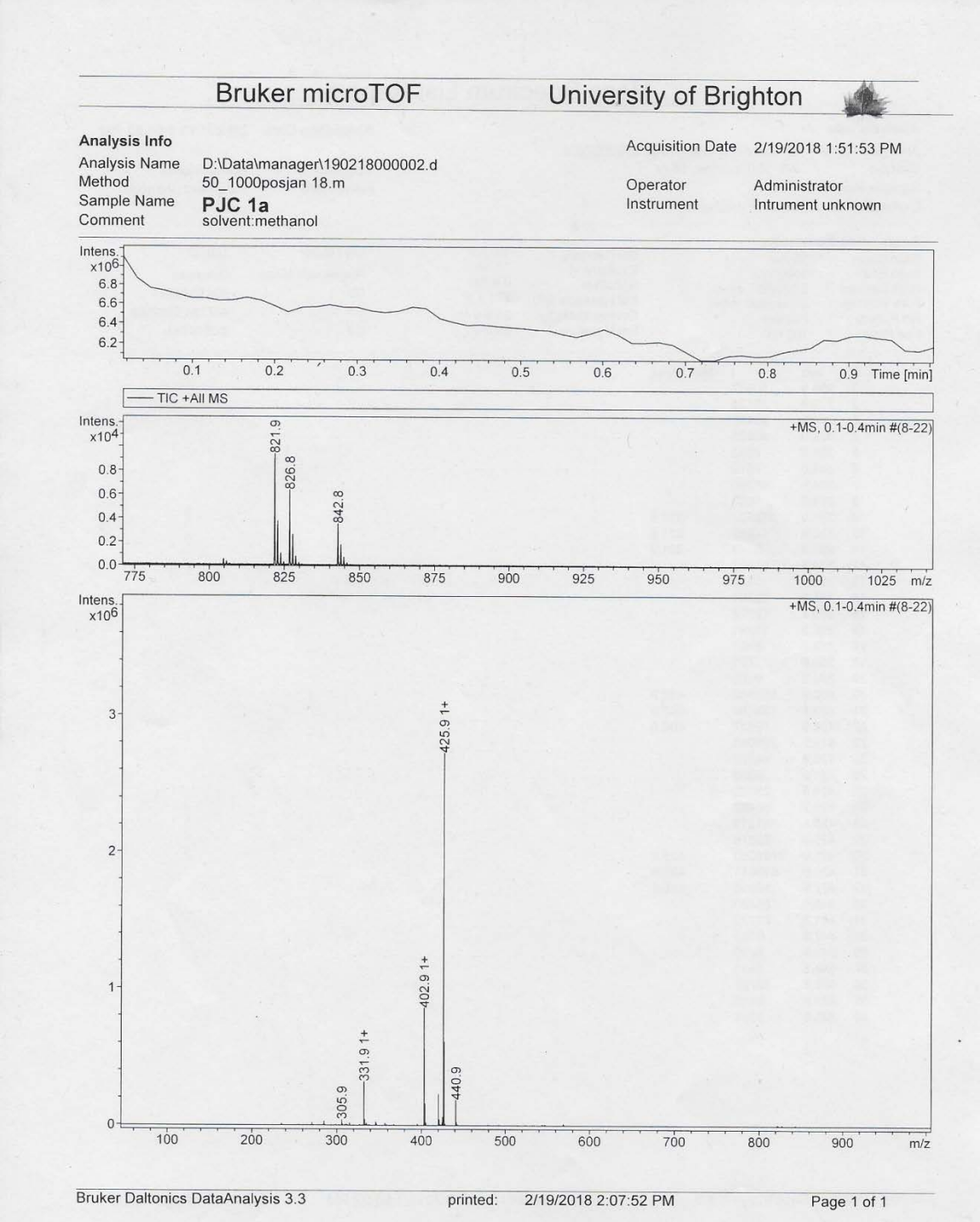

Figure S3. Mass spectrum for **1a**

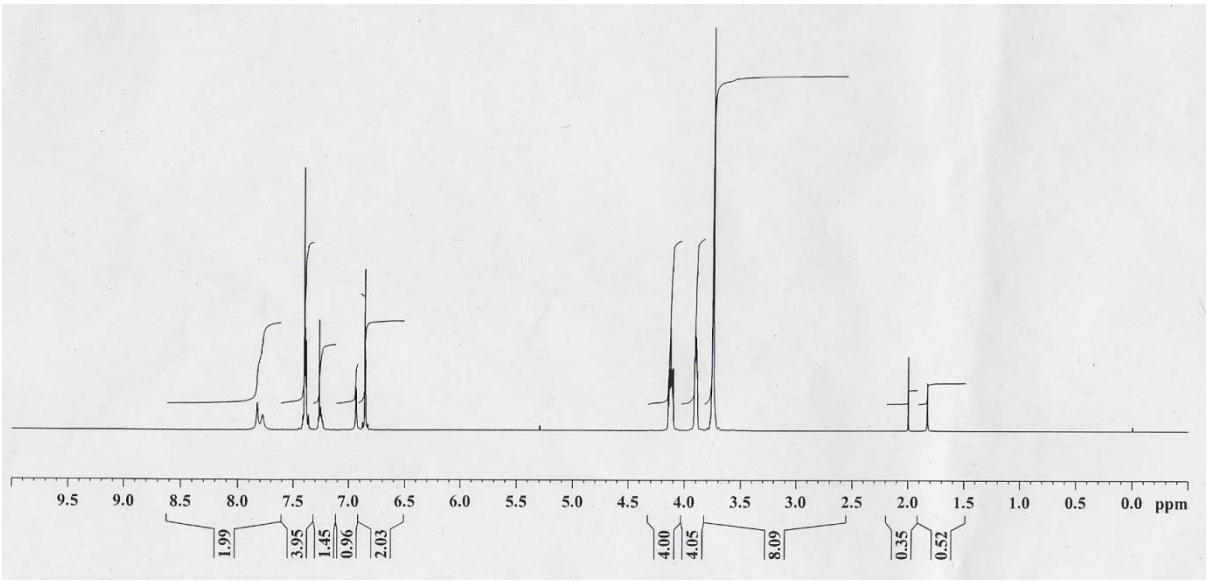

Figure S4. ^{1}H NMR for **1b**

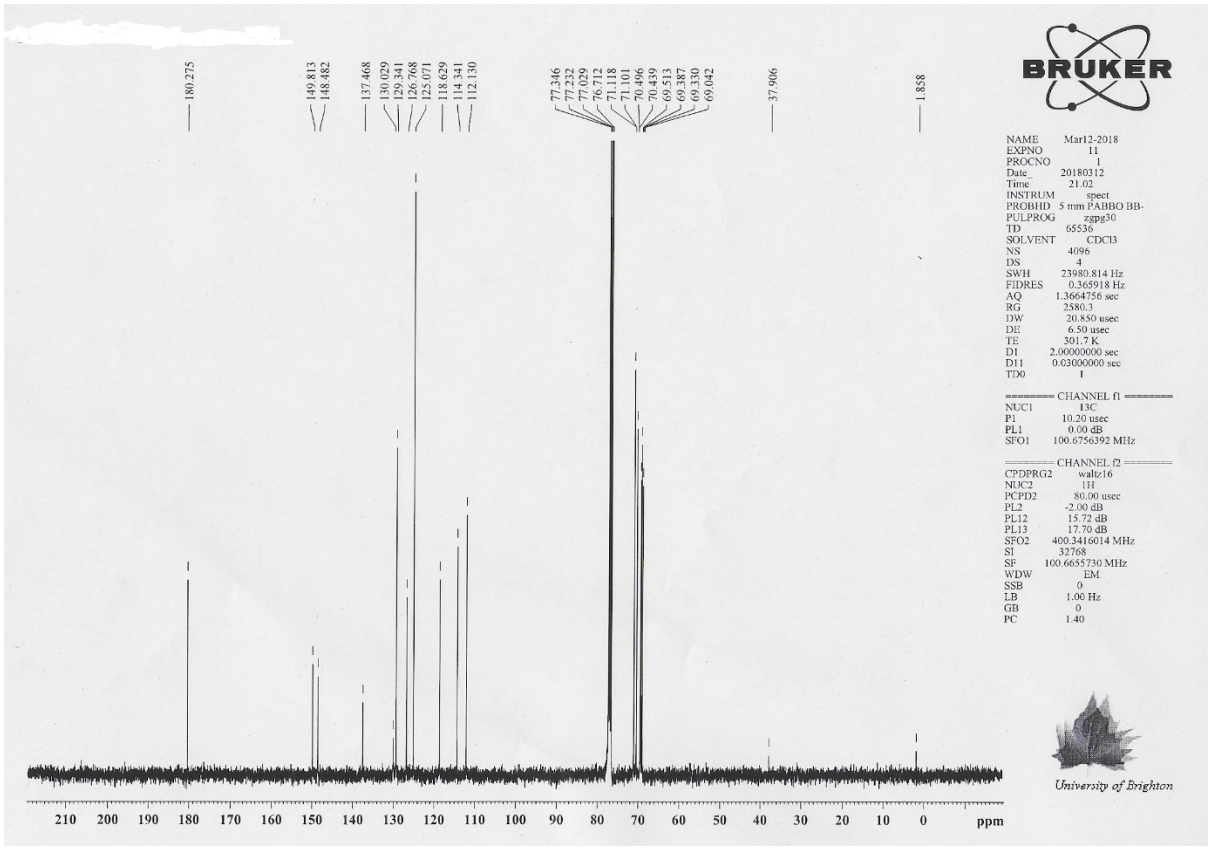

Figure S5. ^{13}C NMR for **1b**

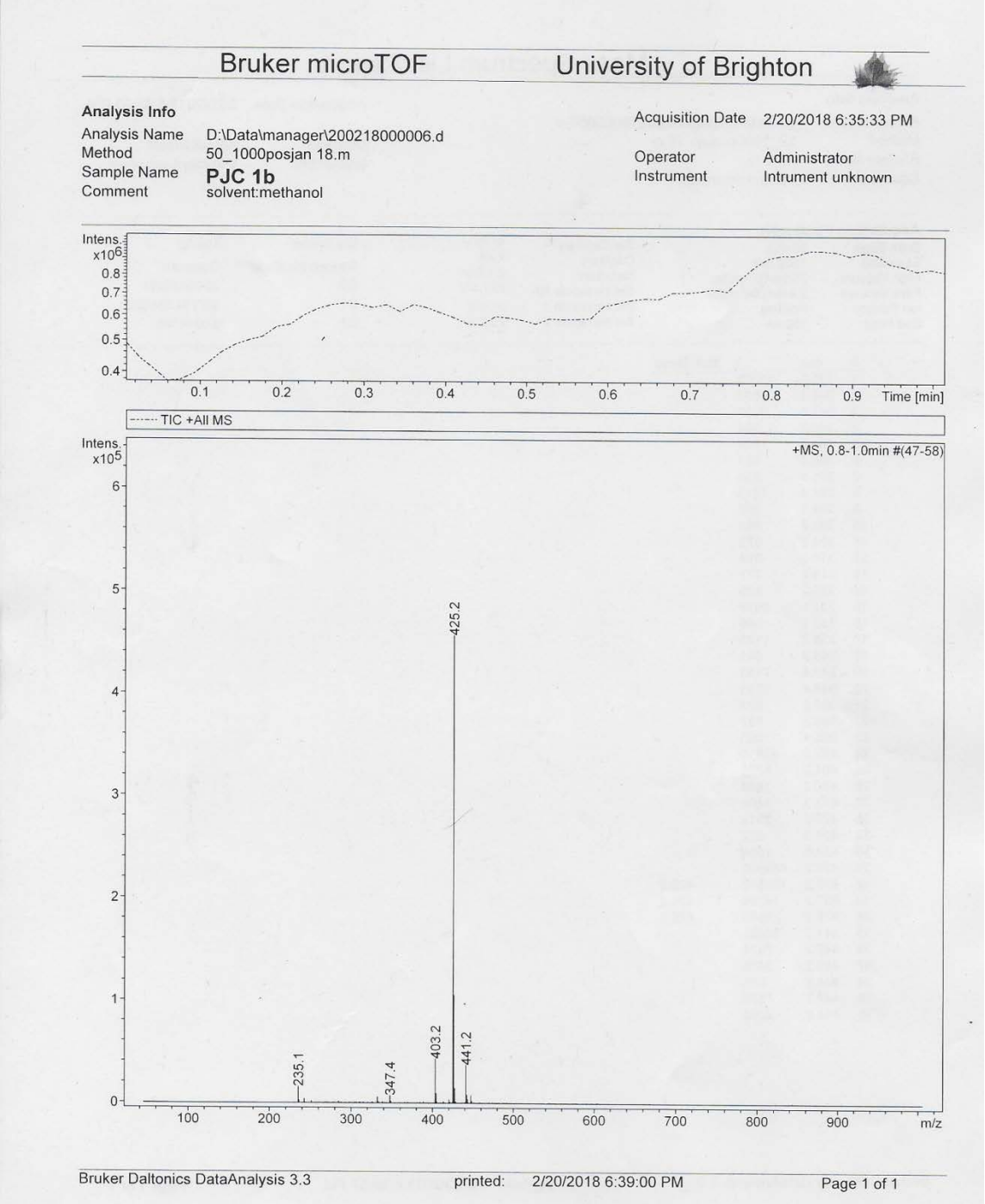

Figure S6. Mass spectrum for **1b**

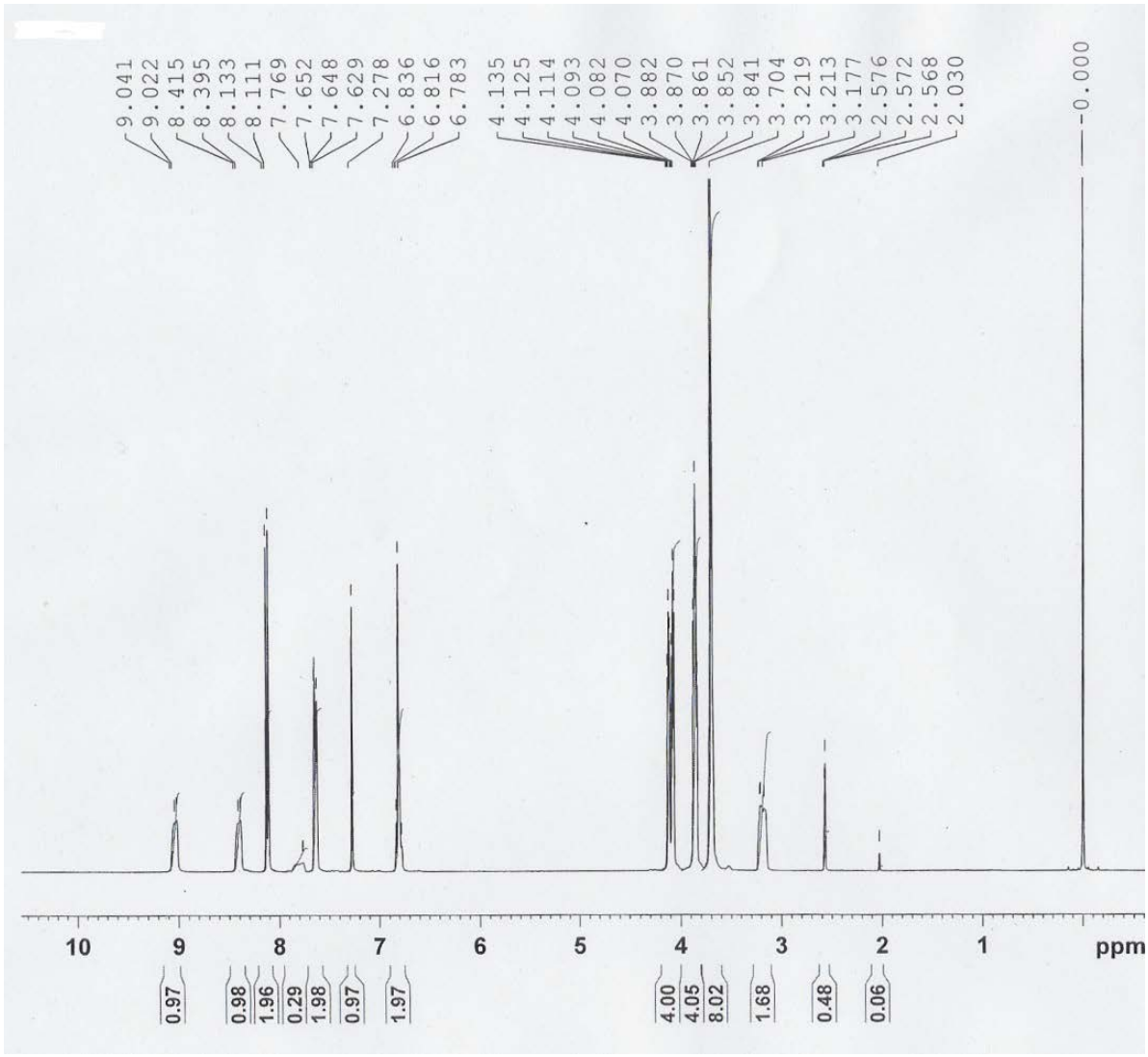

Figure S7. ^{1}H NMR for **1c**

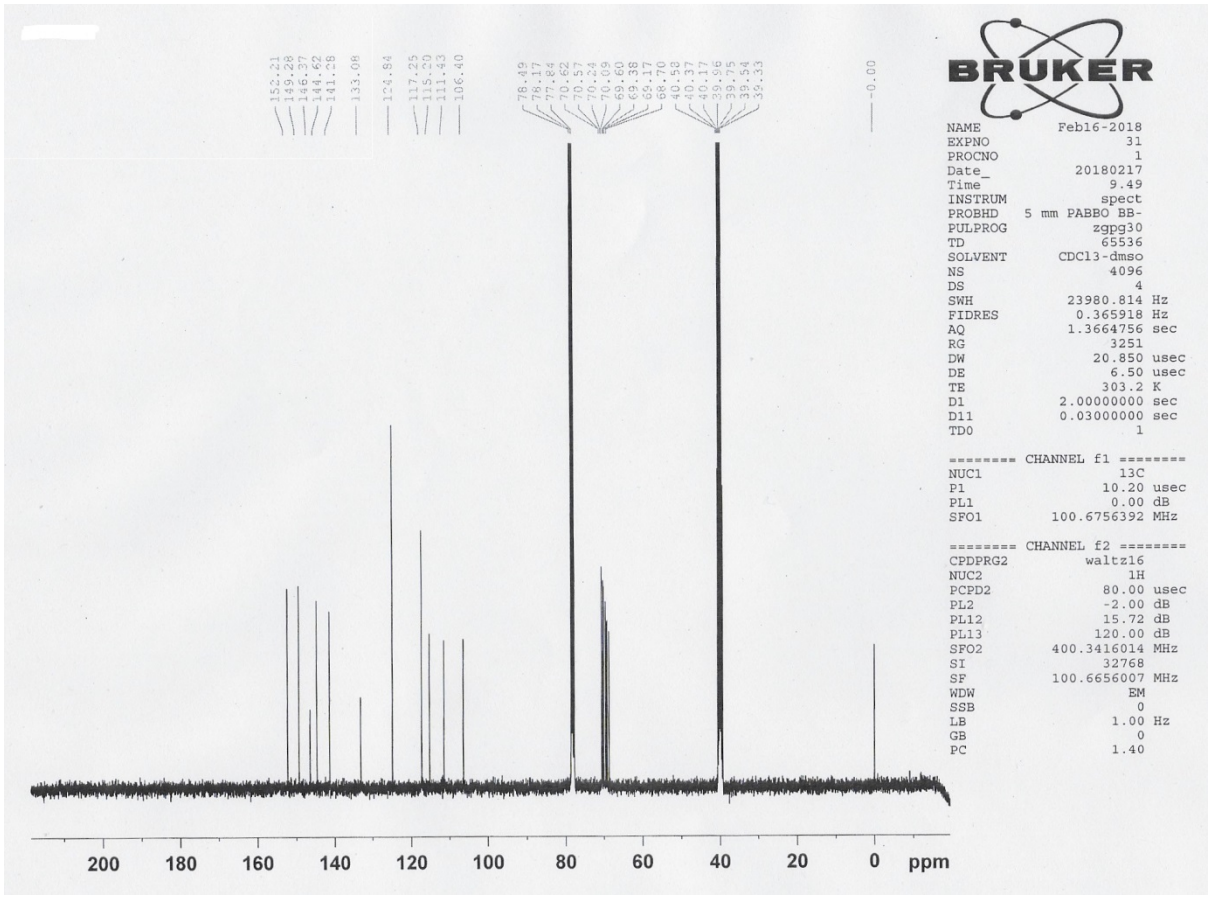

Figure S8. ^{13}C NMR for **1c**

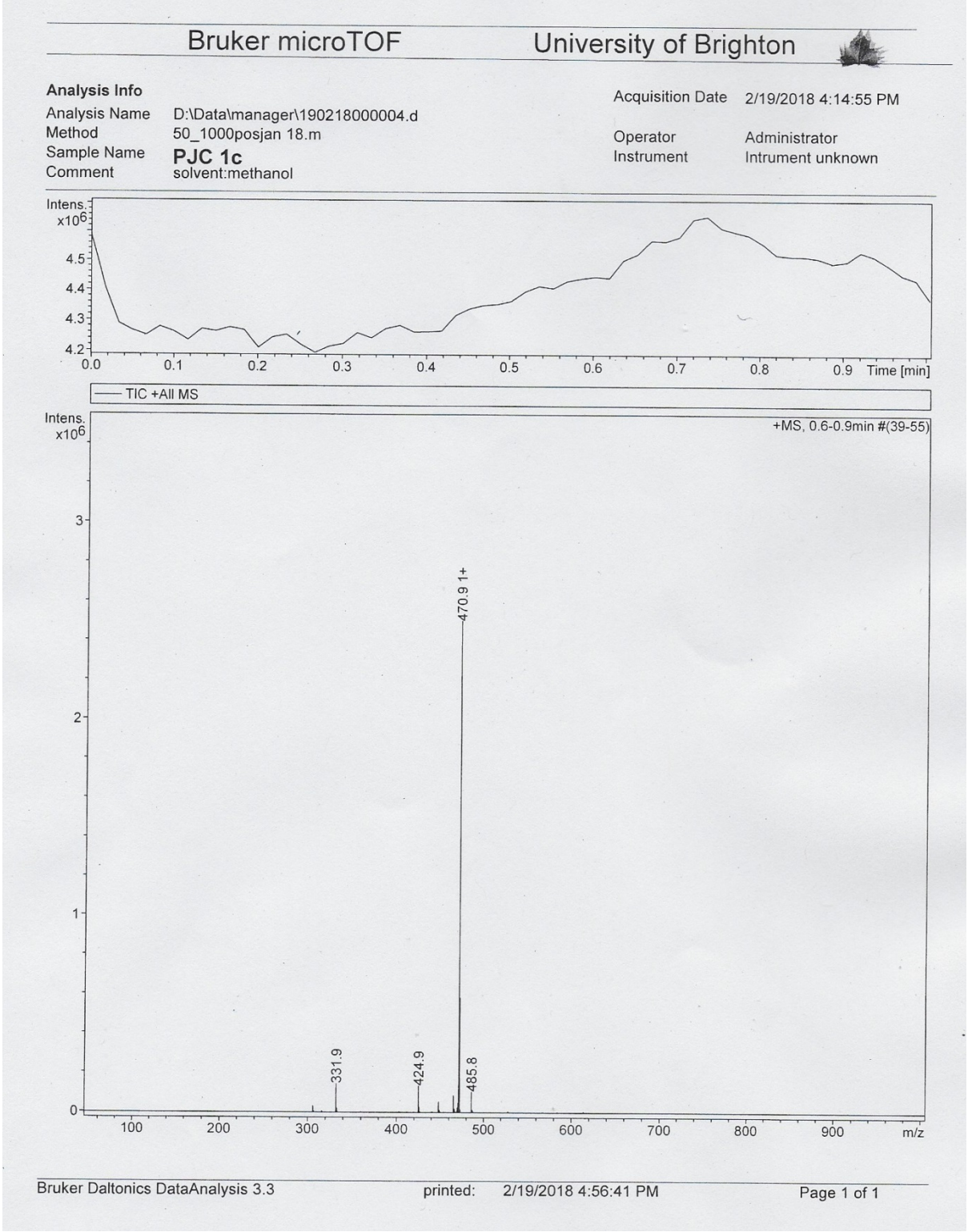

Figure S9. Mass spectrum for **1c**

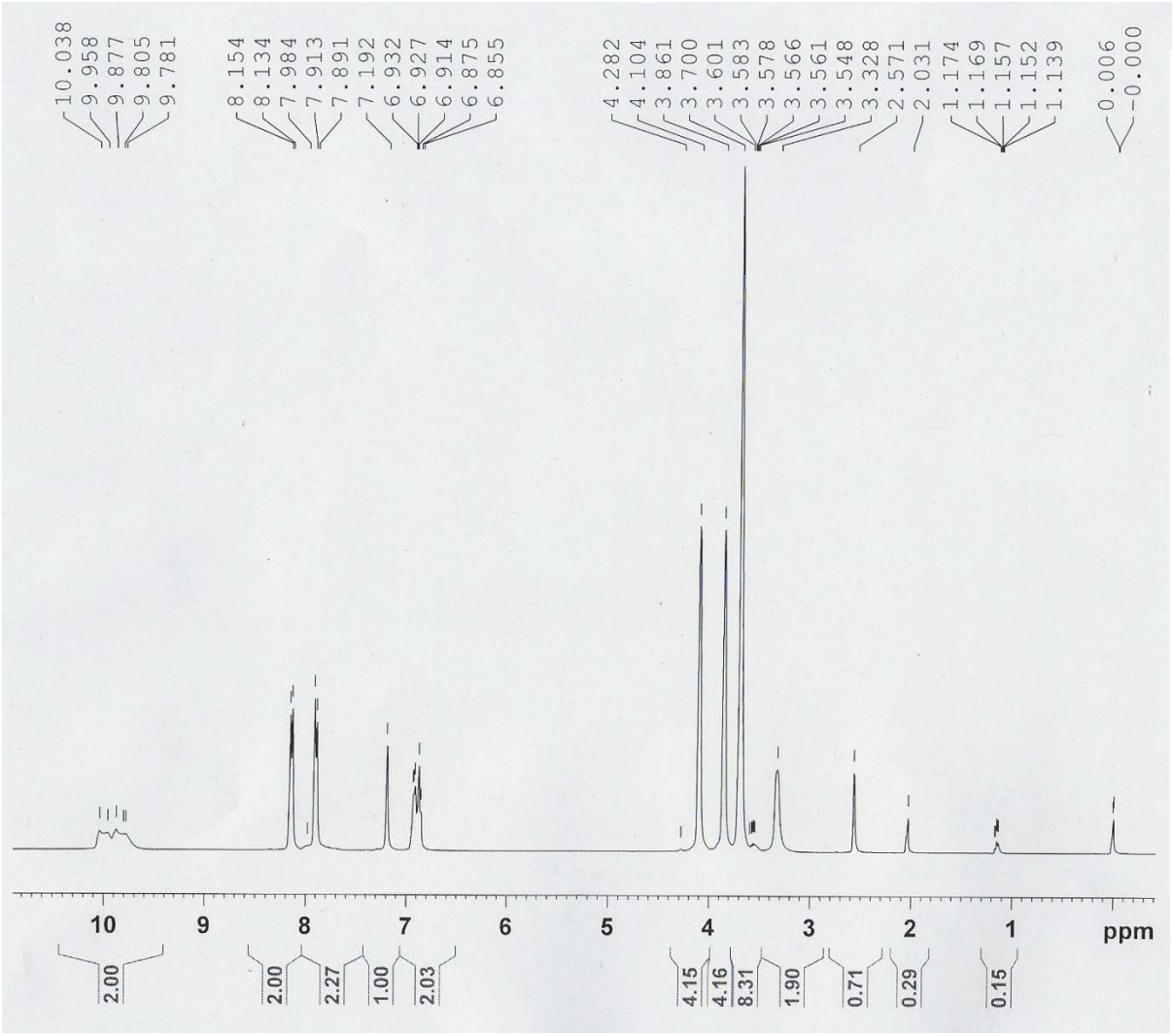

Figure S10. ^{1}H NMR for **1d**

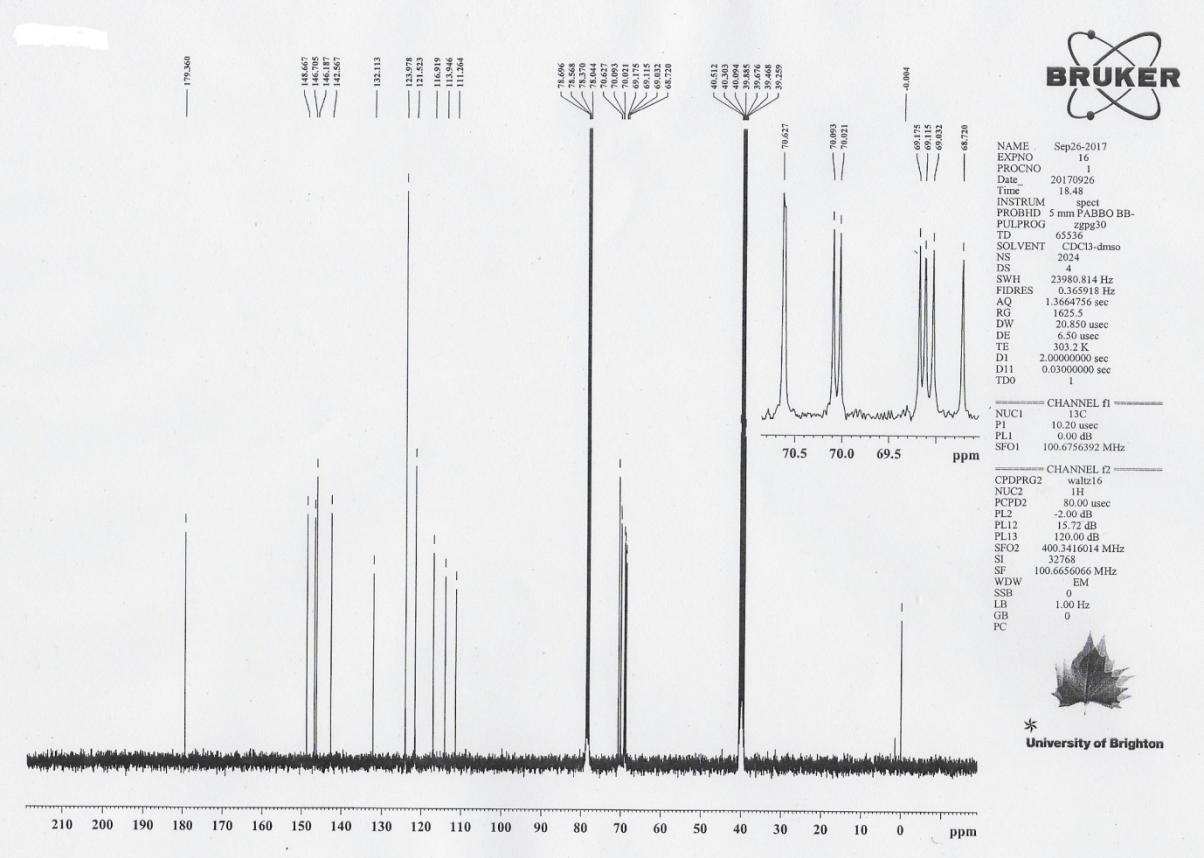

Figure S11. ^{13}C NMR for **1d**

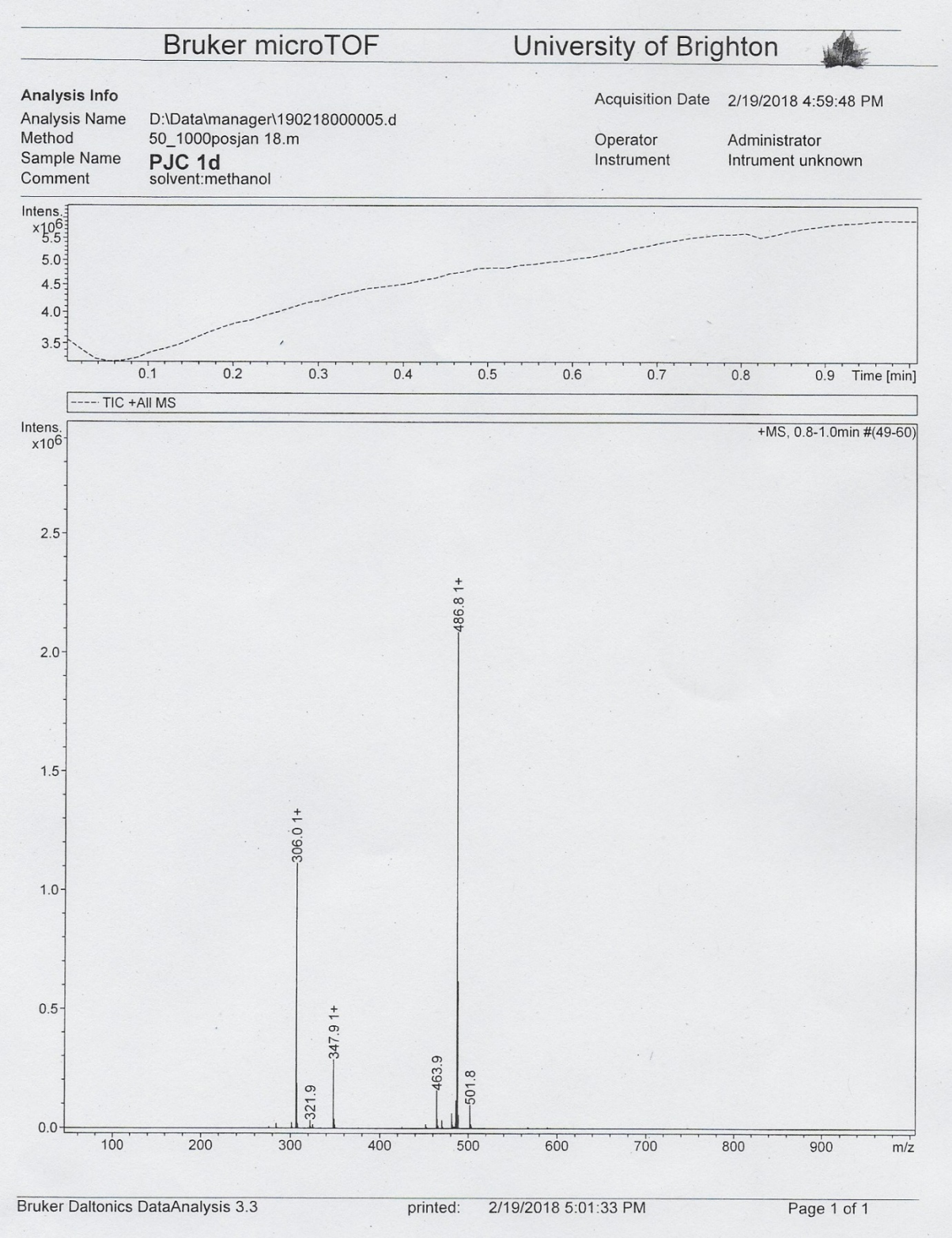

Figure S12. Mass spectrum for **1d**

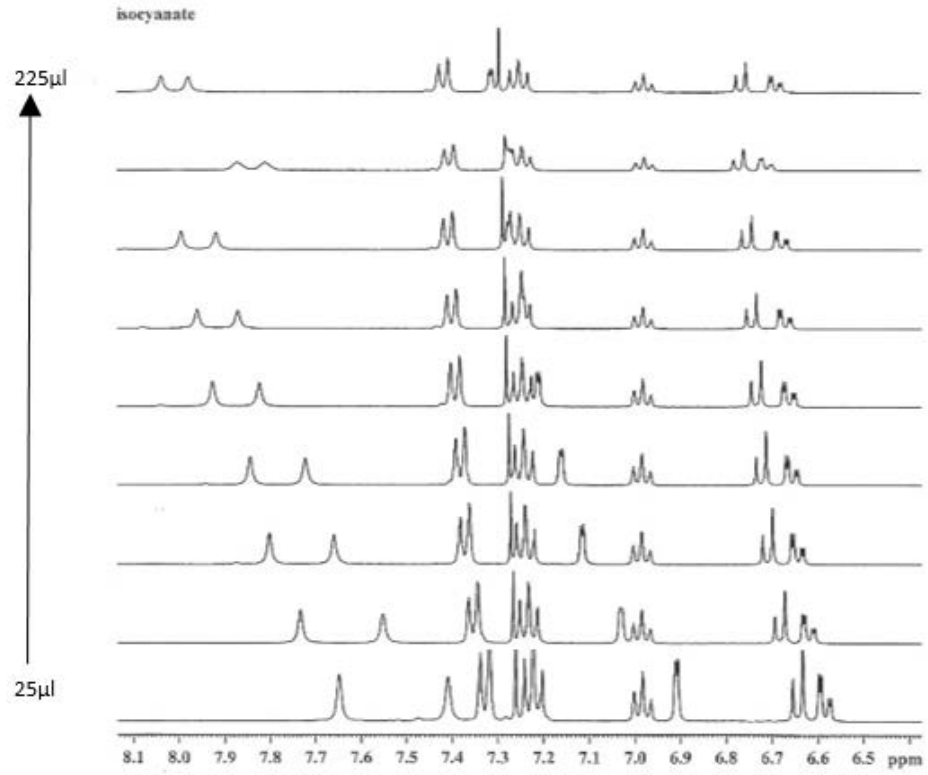

Figure S13. ^{1}H response of aromatic and urea protons to the sequential addition of DMMP to **1a**

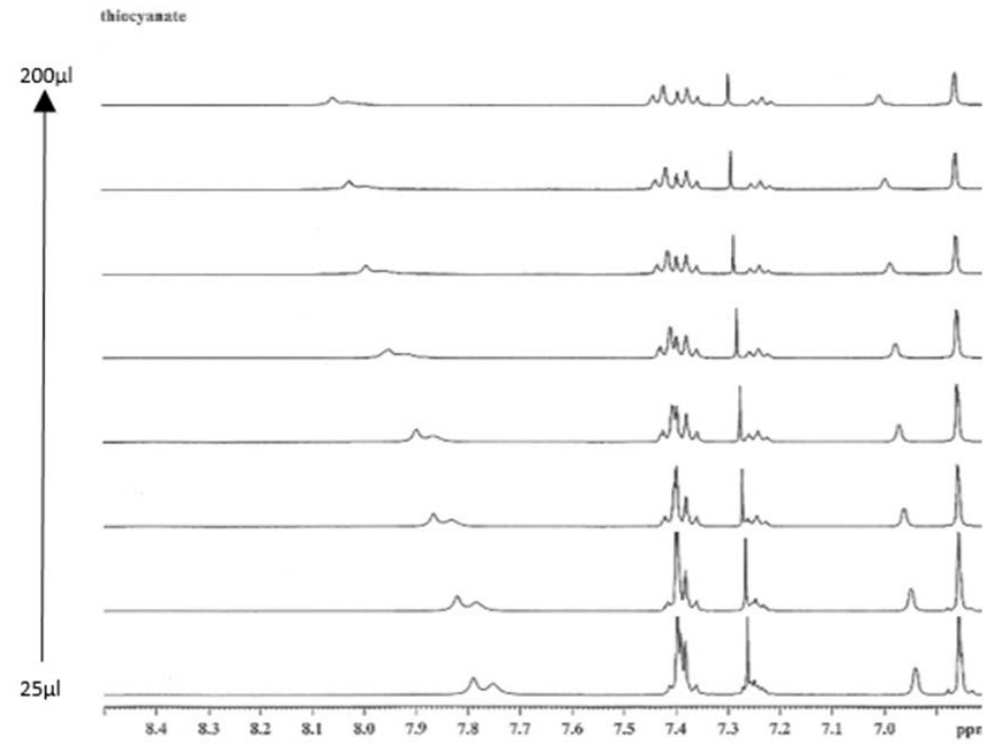

Figure S14. ^{1}H response of aromatic and urea protons to the sequential addition of DMMP to **1b**

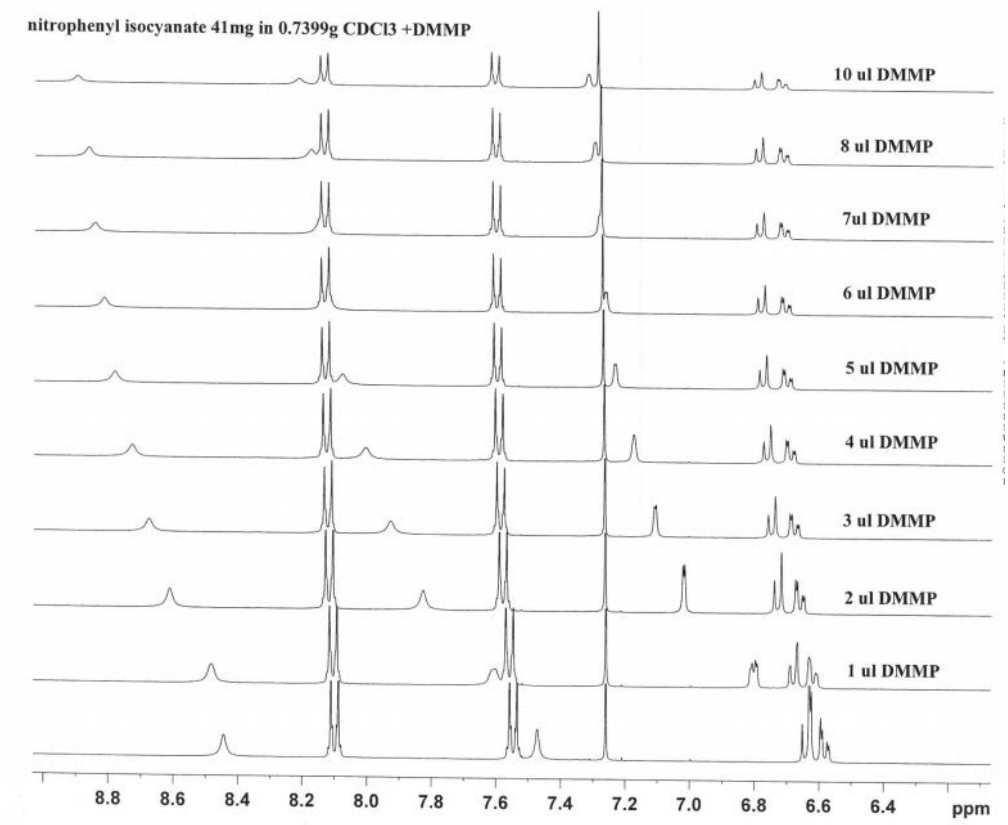

Figure S15. ^{1}H response of aromatic and urea protons to the sequential addition of DMMP to **1c**

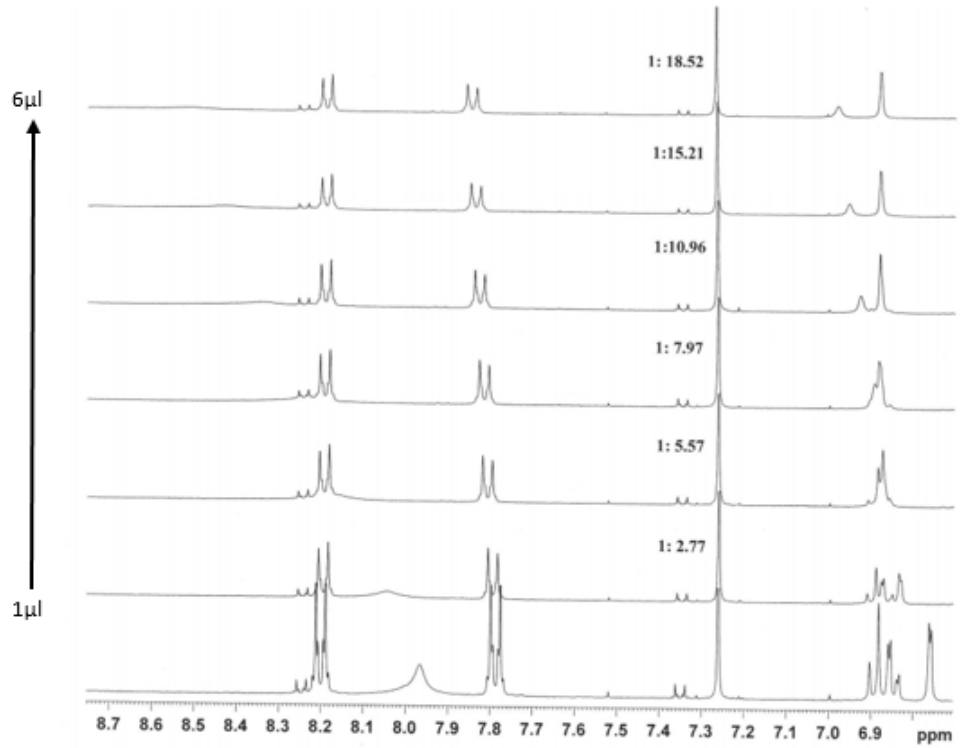

Figure S16. ^{1}H response of aromatic and urea protons to the sequential addition of DMMP to **1d**

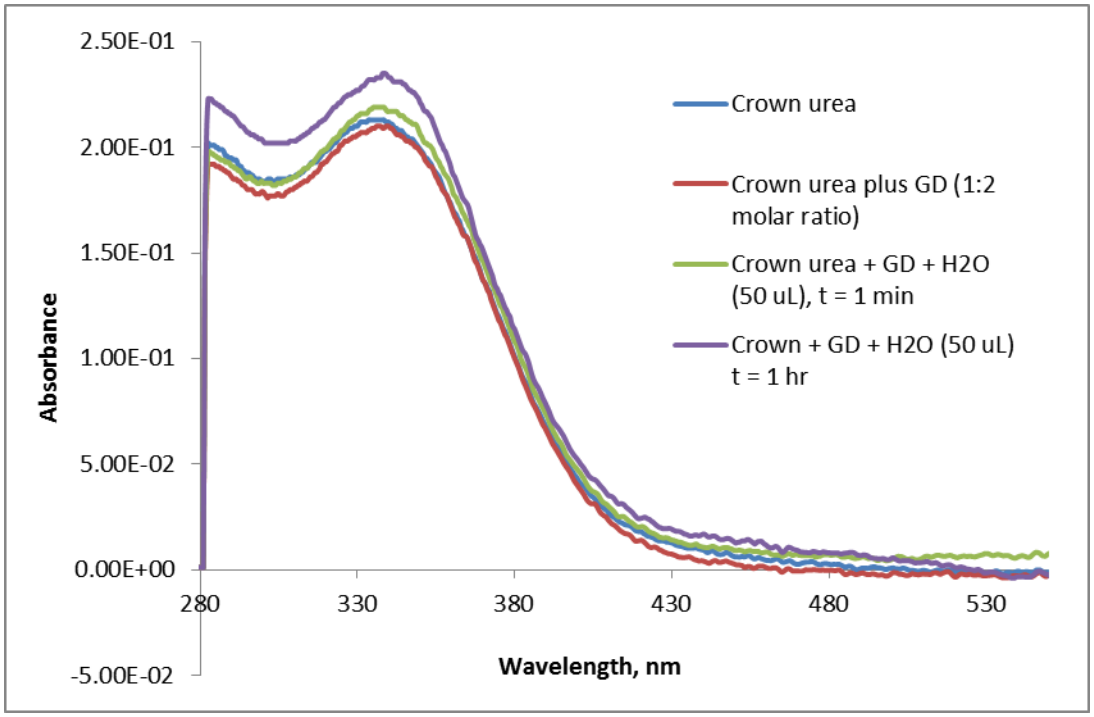

Figure S17. UV-visible spectra of **1c** with GD

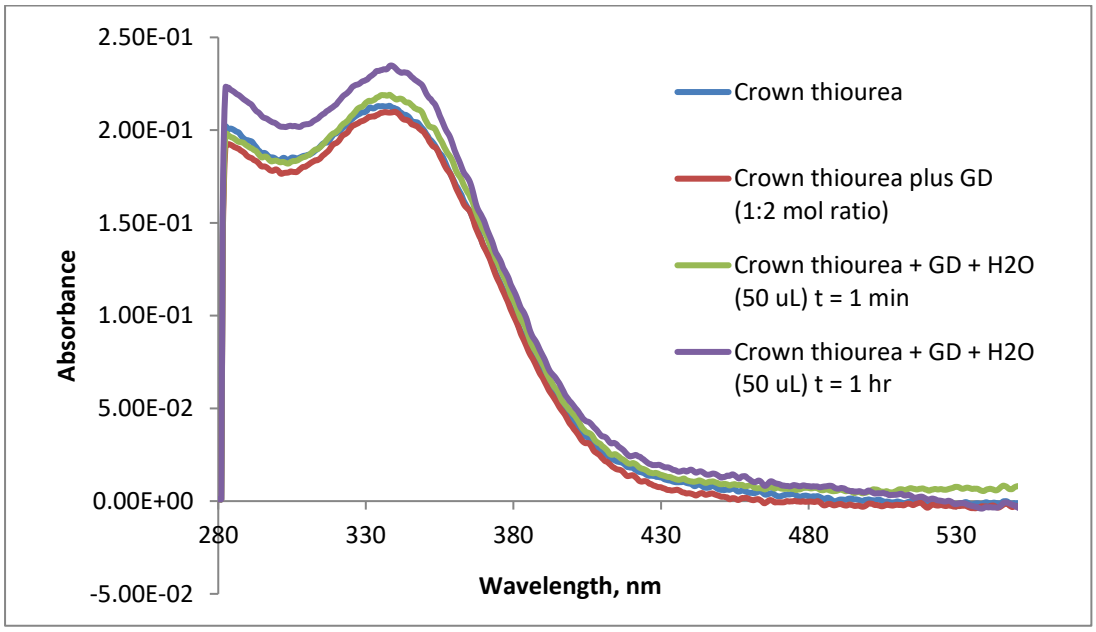

Figure S18. UV-visible spectra of **1d** with GD

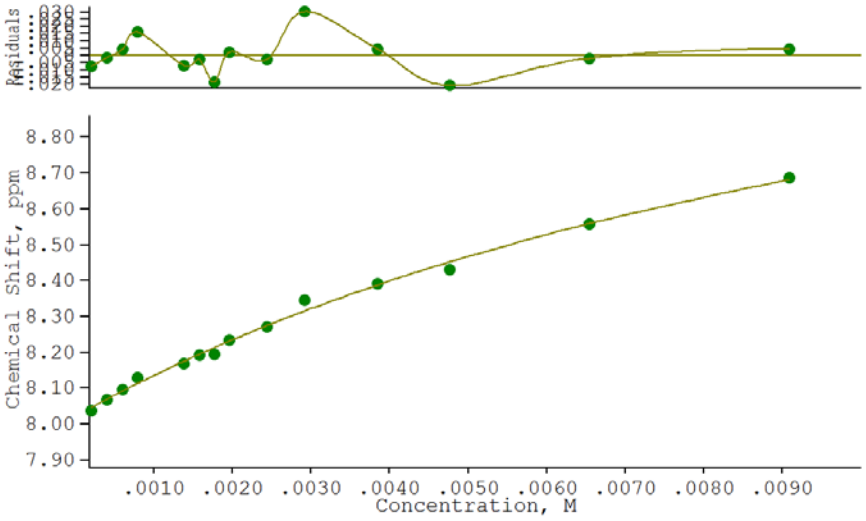

Figure S19. Data fitting for the addition of DIMP to **1c** ($CDCl_3$, 298 K) K_{assoc} = 85 ± 15 M^{-1}

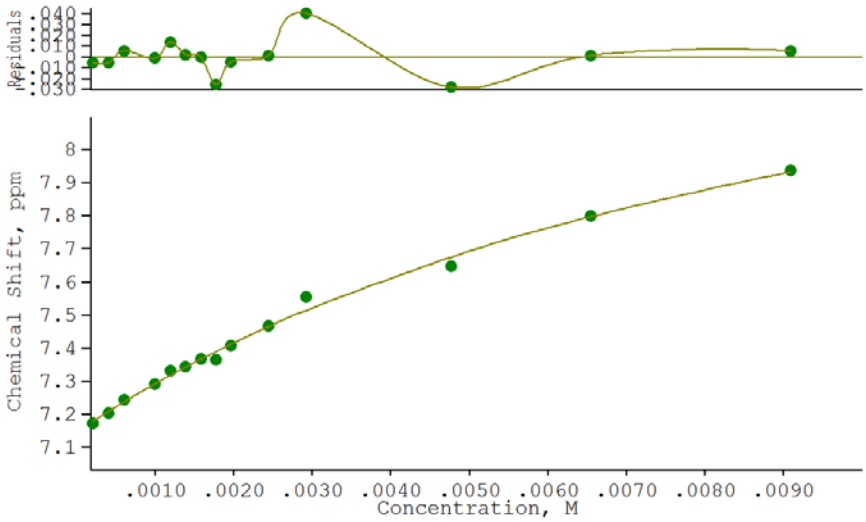

Figure S20. Data fitting for the addition of DIMP to **1c** ($CDCl_3$, 298 K) K_{assoc} = 107 ± 20 M^{-1}

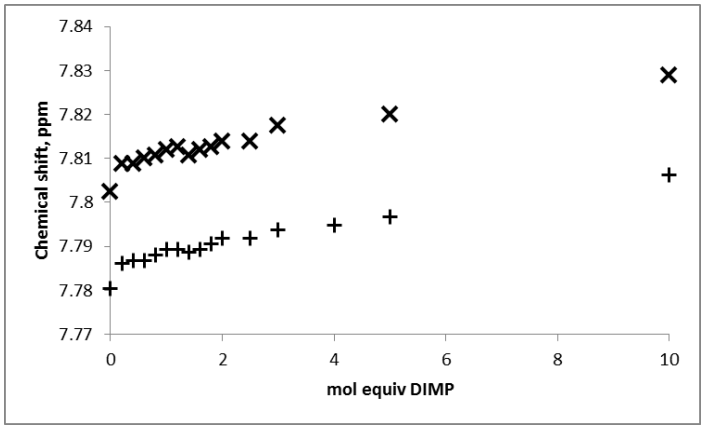

Figure S21. ^1H shifts of the two NH proton environments of **1d** upon addition of DIMP ($CDCl_3$, 298 K)

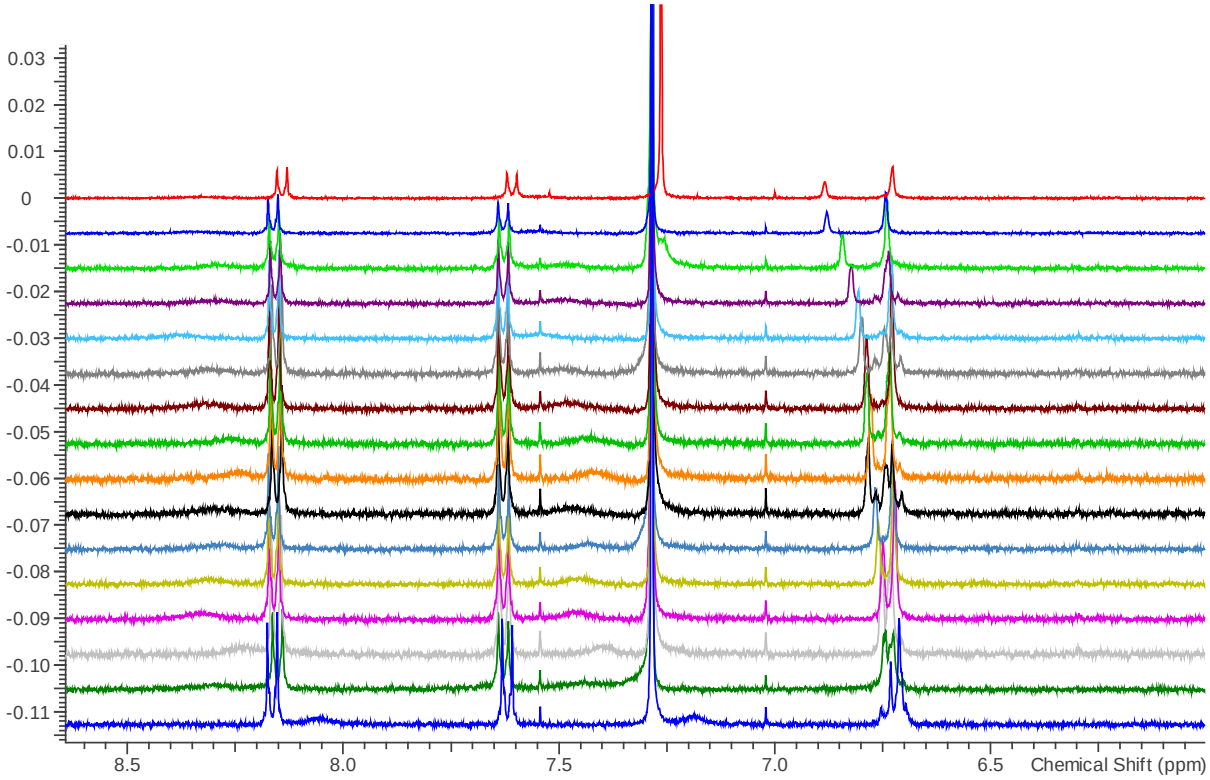

Figure S22. Sequential addition of GD to **1c** ($CDCl_3$, 298 K)

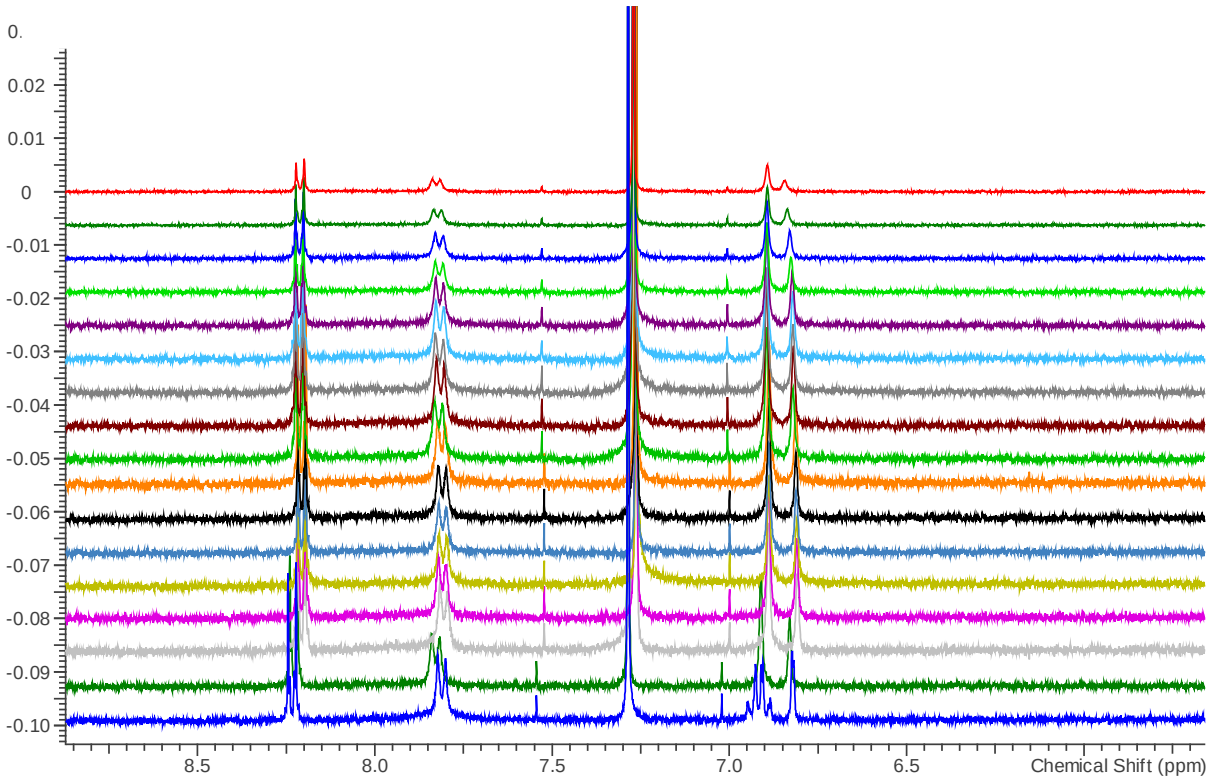

Figure S23. Sequential addition of GD to **1d** (298 K, $CDCl_3$)

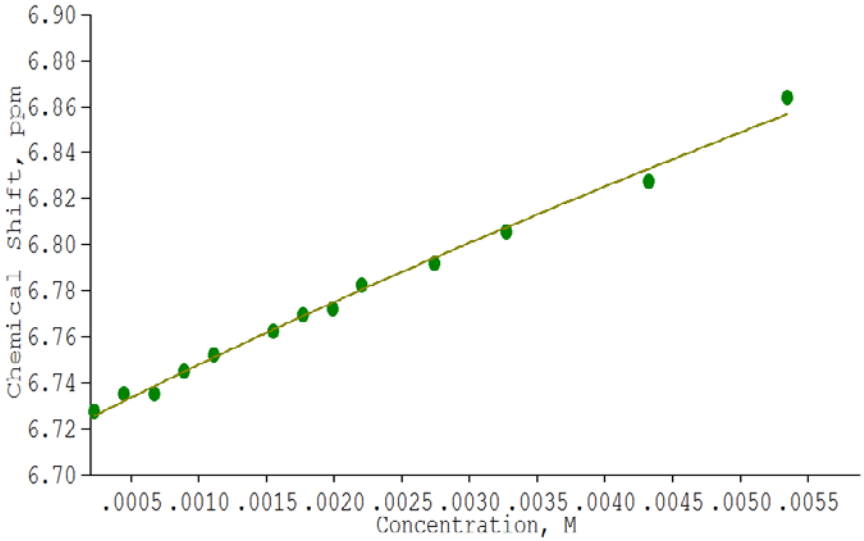

Figure S24. Data fitting for the addition of GD to **1c** ($CDCl_3$, 298 K). $K_{assoc} < 50\ M^{-1}$.