Supplementary Material (ESI) for Organic and Biomolecular Chemistry

Nitrophenylamide derivatives of pyrrole 2,5-diamides: structural behaviour, anion binding and colour change signaled deprotonation

Salvatore Camiolo, Philip A. Gale,* Michael B. Hursthouse and Mark E. Light
Department of Chemistry, University of Southampton, Southampton, SO17 1BJ, UK.

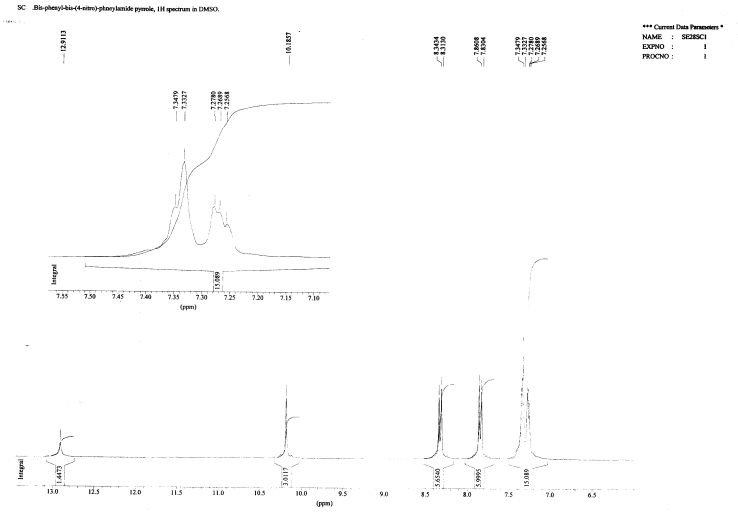


Figure S1 ^{1}H NMR of compound **2** in DMSO-d_6

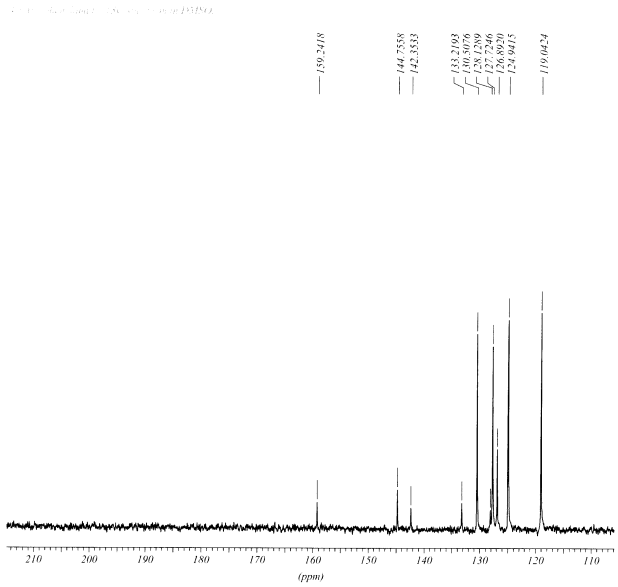


Figure S2 ^{13}C NMR of compound **2** in DMSO-d_6

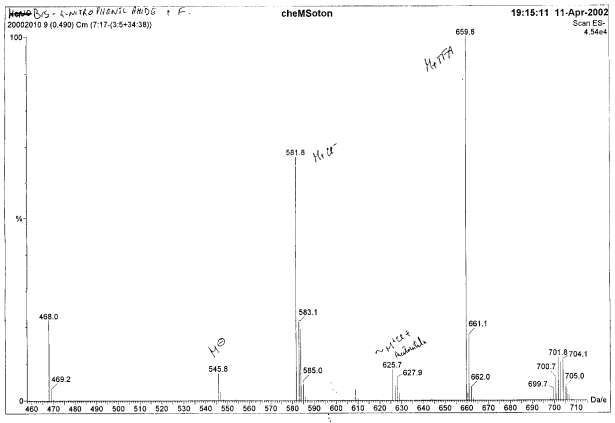


Figure S3 Negative Electrospray of compound **2** in the presence of TBAF

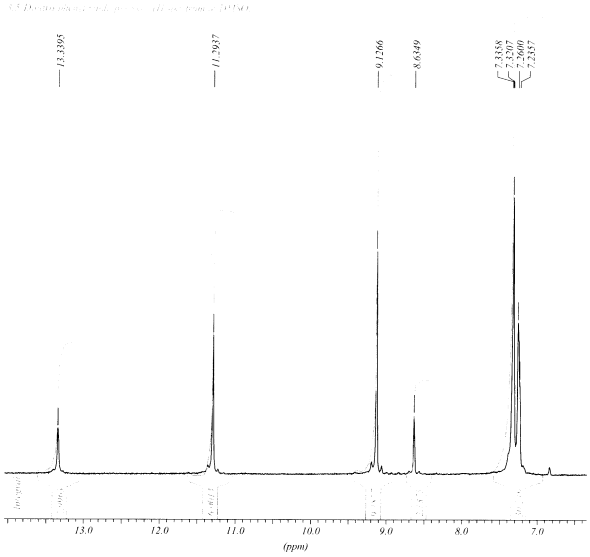


Figure S4 ^{1}H NMR of compound **3** in DMSO-d_6

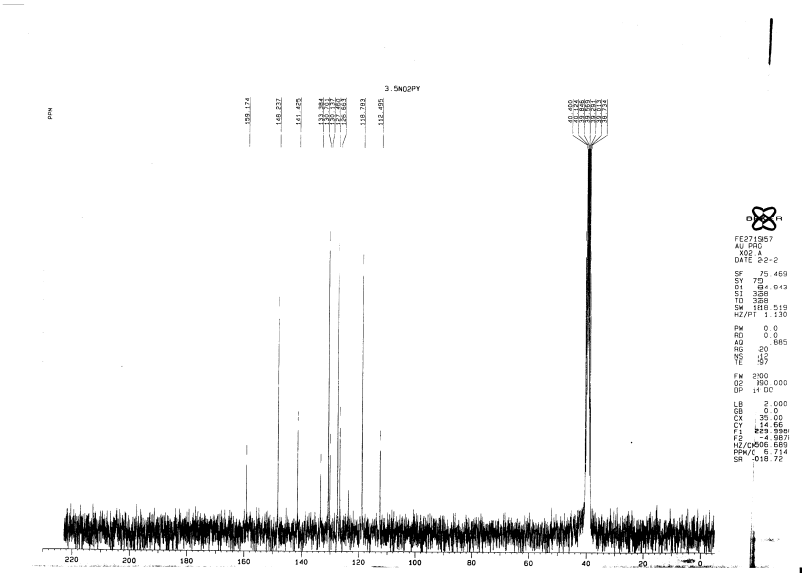


Figure S5 ^{13}C NMR of compound **3** in DMSO-d_6

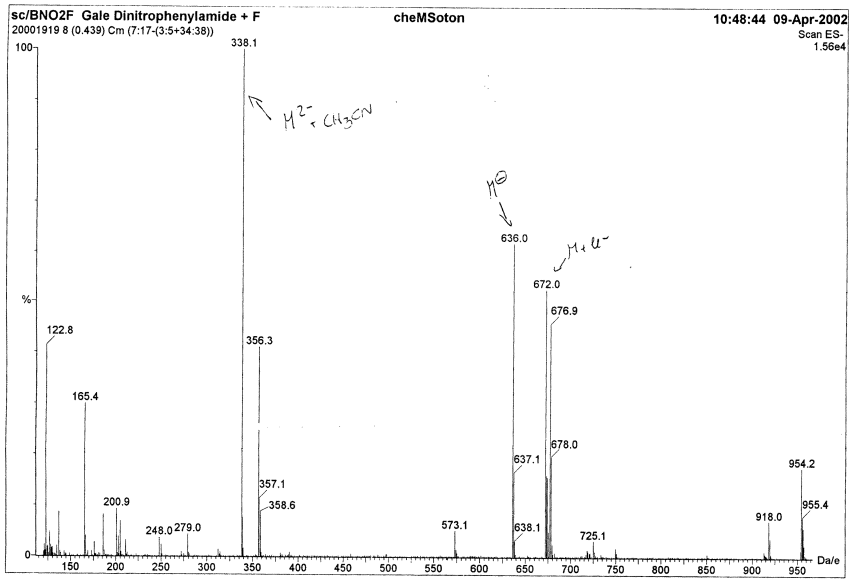


Figure S6 Negative electrospray of compound **3** in the presence of TBAF . Mass and UV/Vis spectroscopy support the idea that deprotonation may compete with the anion coordination process even though the pyrrole does not carry electron withdrawing groups. Negative electrospray mass spectrometry analysis carried out on receptor **3** in the presence of a variety of anionic species such as fluoride, chloride, benzoate and dihydrogenphosphate, showed that the M^- peak of the receptor is always present. However in the presence of an excess of fluoride the M^{2-} species was also observed.

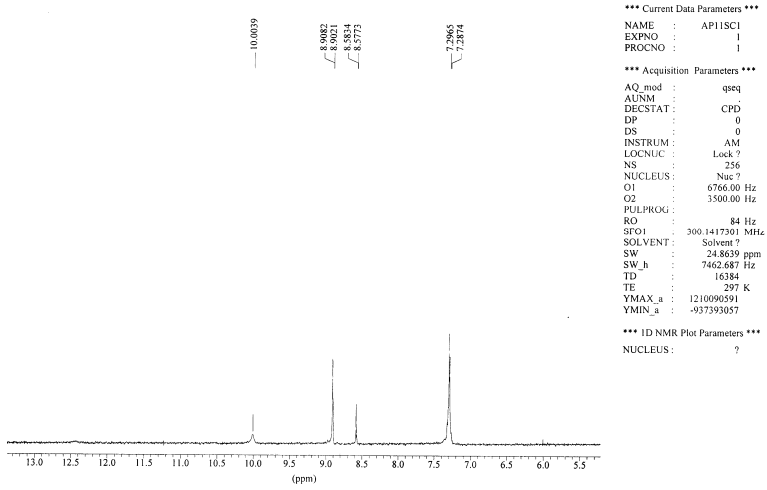


Figure S7 ^{1}H NMR spectrum of compound **3** in CD_3CN (sparingly soluble)

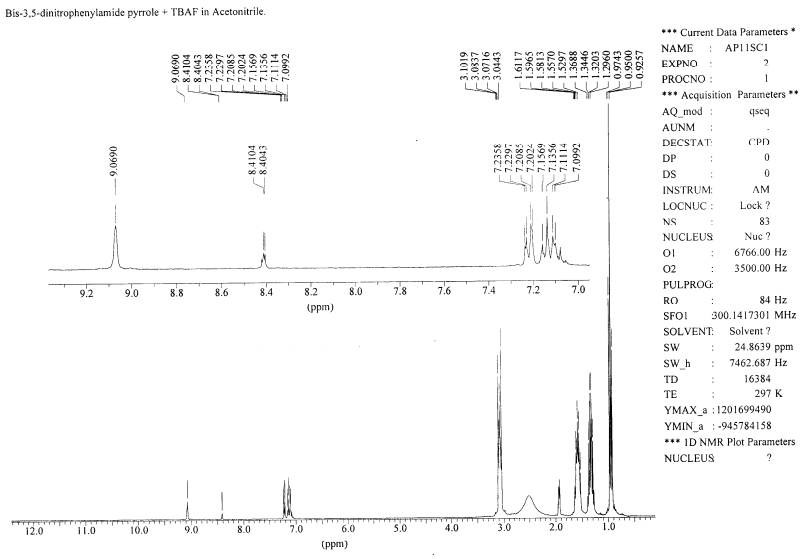


Figure S8 ^{1}H NMR spectrum of compound **3** in CD_3CN in the presence of TBAF

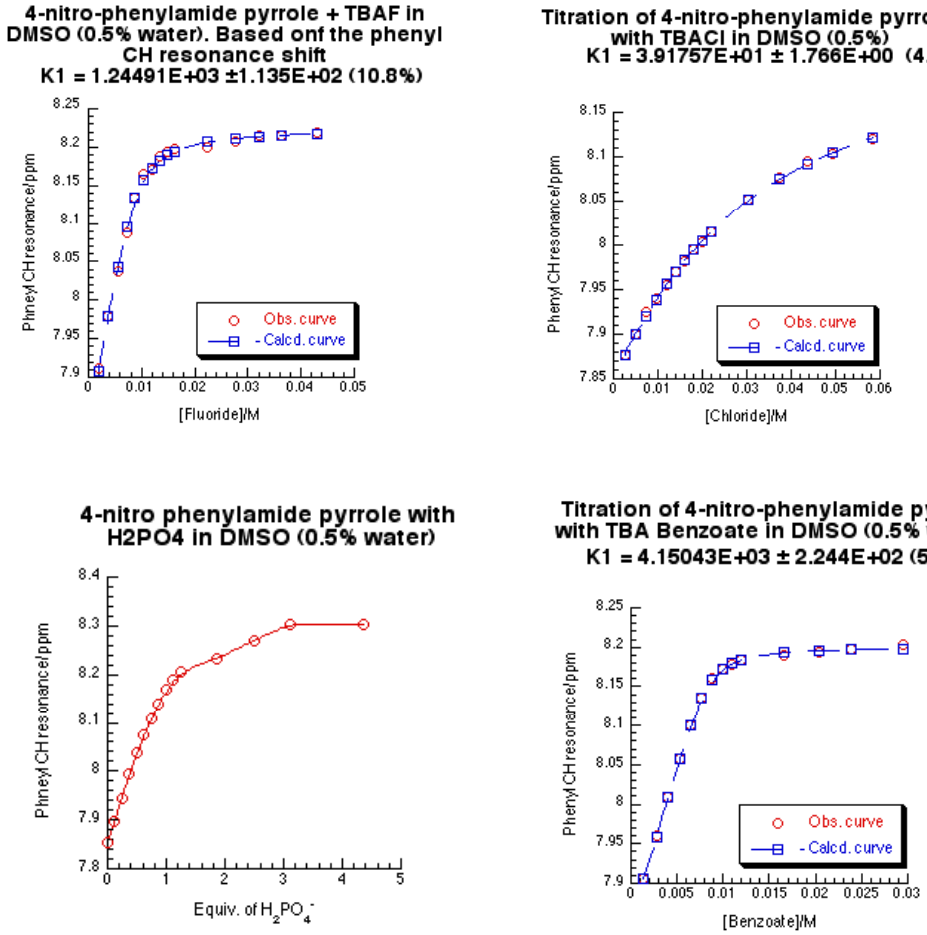
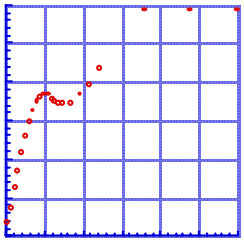
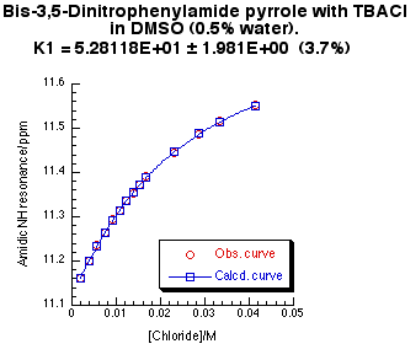
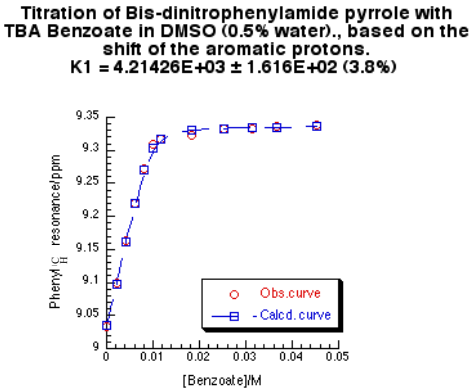


Figure S9 ^{1}H NMR titration curves with compound **2** and various anionic guests in DMSO-d_6/0.5% water







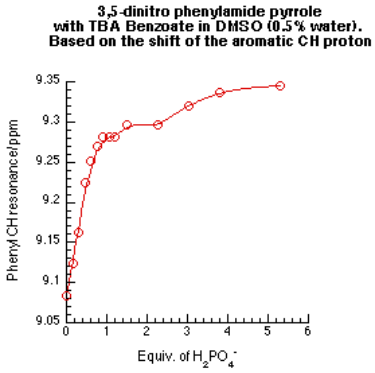


Figure S10 ^{1}H NMR titration curves with compound **3** and various anionic guests in DMSO-d_6/0.5% water.