

Supplementary Material (ESI) for Organic and Biomolecular Chemistry
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Nitrophenylamide derivatives of pyrrole 2,5-diamides: structural behaviour, anion binding and colour change signaled deprotonation

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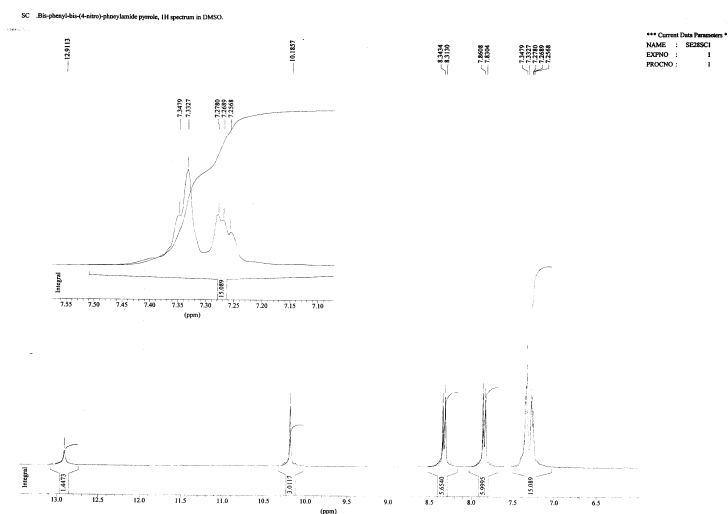


Figure S1 ^1H NMR of compound **2** in DMSO-d_6

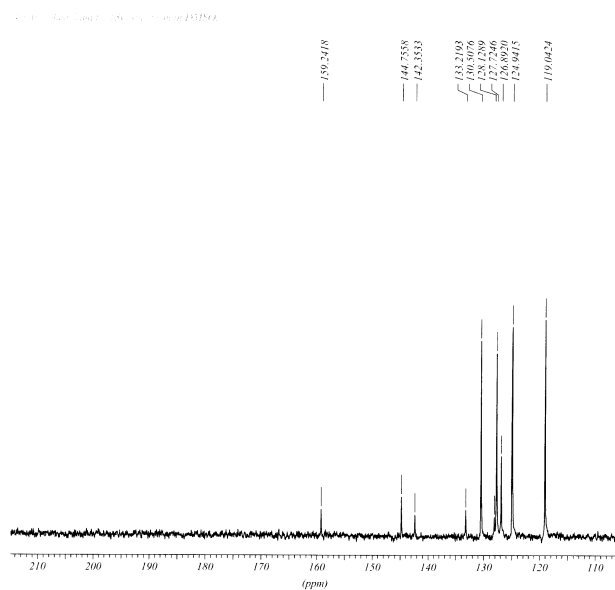


Figure S2 ^{13}C NMR of compound **2** in DMSO-d_6

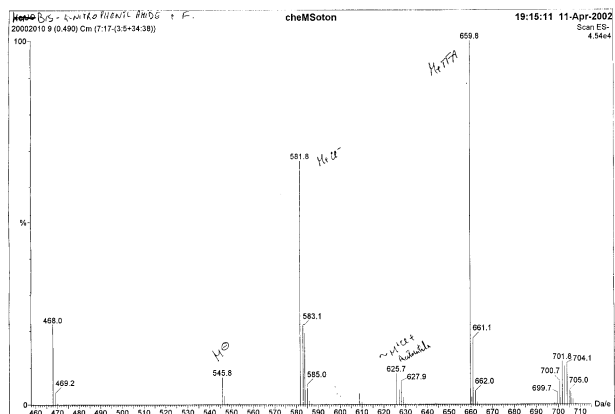


Figure S3 Negative Electrospray of compound **2** in the presence of TBAF

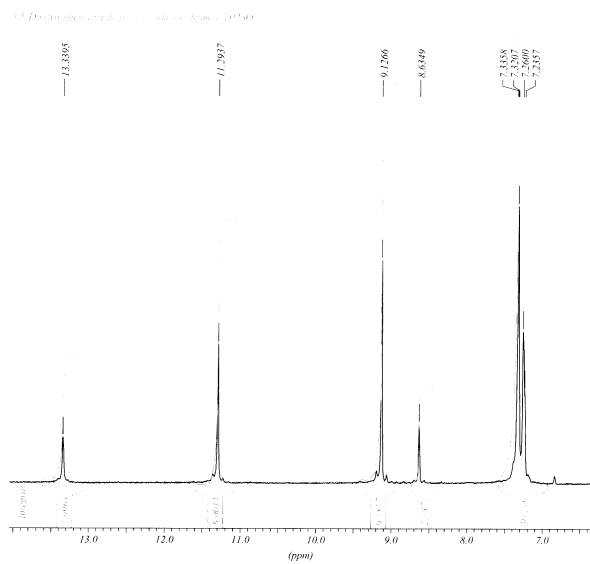


Figure S4 ¹H NMR of compound **3** in DMSO-d₆

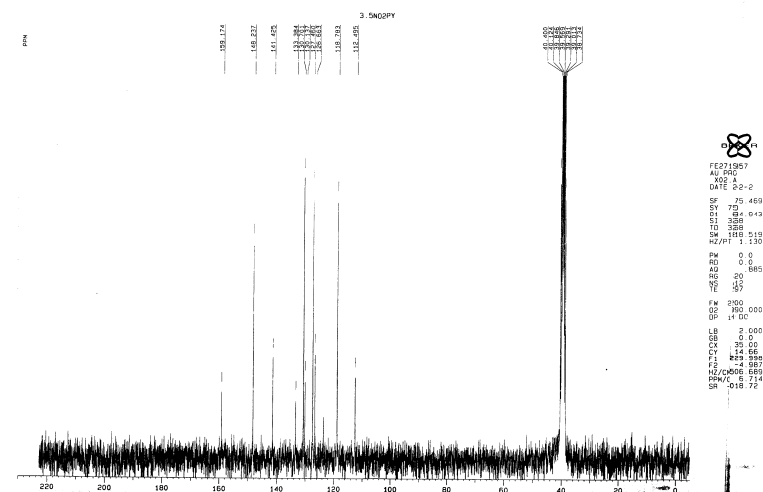


Figure S5 ^{13}C NMR of compound **3** in DMSO-d_6

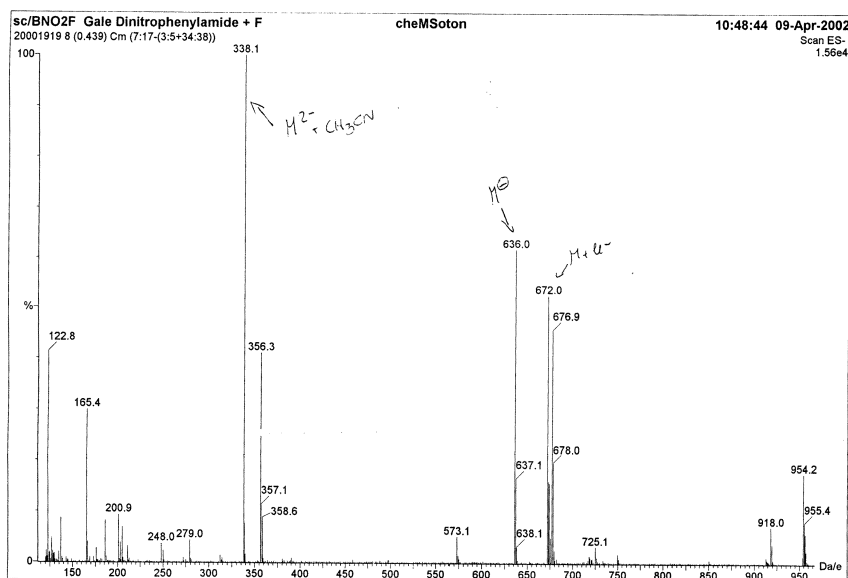


Figure S6 Negative electrospray of compound **3** in the presence of TBAF^- . Mass and UV/Vis spectroscopy support the idea that deprotonation may compete with the anion coordination process even though the pyrrole does not carry electron withdrawing groups. Negative electrospray mass spectrometry analysis 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.

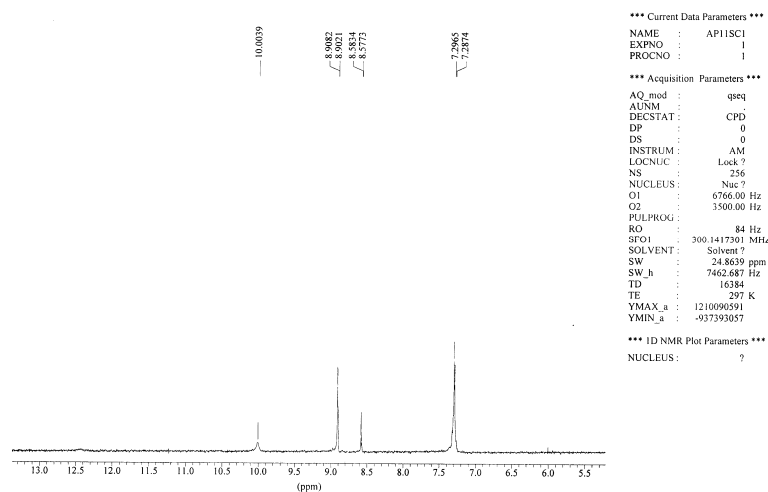


Figure S7 ^1H NMR spectrum of compound **3** in CD_3CN (sparingly soluble)

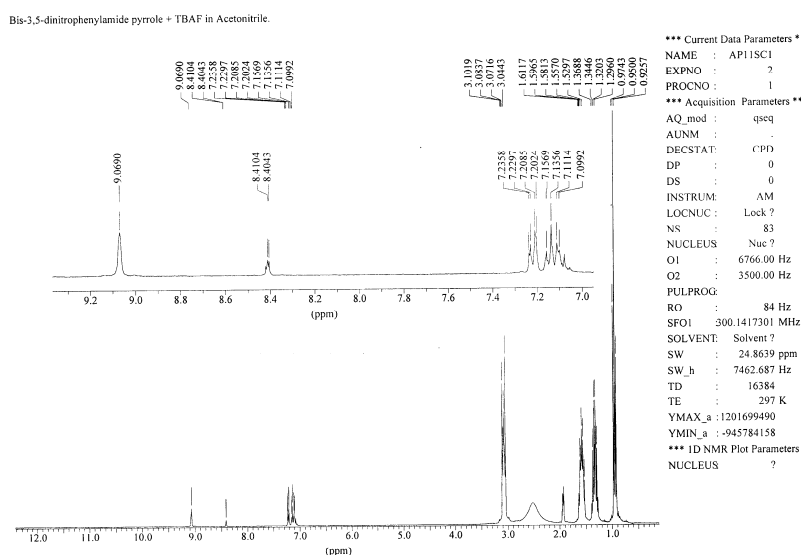
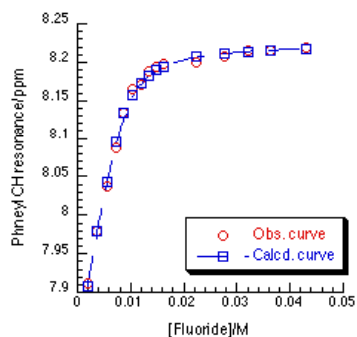
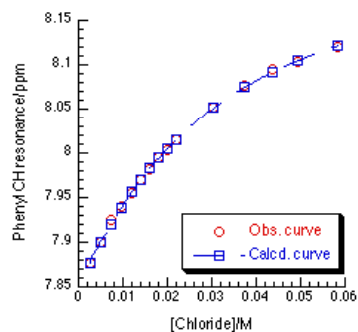


Figure S8 ^1H NMR spectrum of compound **3** in CD_3CN in the presence of TBAF

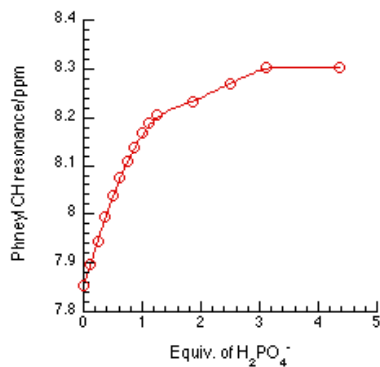
4-nitro-phenylamide pyrrole + TBAF in DMSO (0.5% water). Based on the phenyl CH resonance shift
 $K_1 = 1.24491E+03 \pm 1.135E+02$ (10.8%)



Titration of 4-nitro-phenylamide pyrrole with TBACl in DMSO (0.5%)
 $K_1 = 3.91757E+01 \pm 1.766E+00$ (4.5%)



4-nitro phenylamide pyrrole with H2PO4 in DMSO (0.5% water)



Titration of 4-nitro-phenylamide pyrrole with TBA Benzoate in DMSO (0.5% water).
 $K_1 = 4.15043E+03 \pm 2.244E+02$ (5.4%)

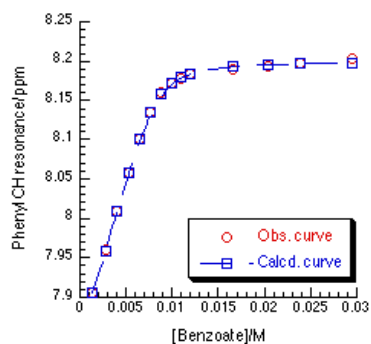
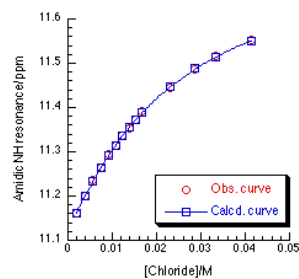
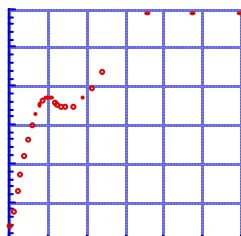
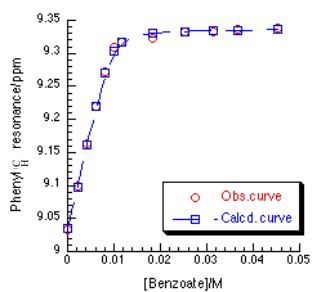


Figure S9 ^1H NMR titration curves with compound **2** and various anionic guests in DMSO- d_6 /0.5% water

**Bis-3,5-Dinitrophenylamide pyrrole with TBACl
in DMSO (0.5% water).**
K1 = 5.28118E+01 ± 1.981E+00 (3.7%)



**Titration of Bis-dinitrophenylamide pyrrole with
TBA Benzoate in DMSO (0.5% water)., based on the
shift of the aromatic protons.**
K1 = 4.21426E+03 ± 1.616E+02 (3.8%)



**3,5-dinitro phenylamide pyrrole
with TBA Benzoate in DMSO (0.5% water).
Based on the shift of the aromatic CH proton**

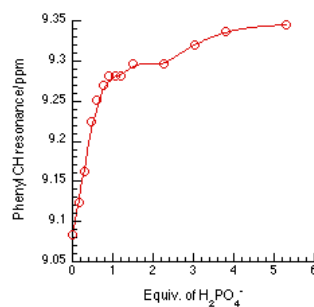


Figure S10 ¹H NMR titration curves with compound **3** and various anionic guests in DMSO-*d*₆/0.5% water.