

Electronic Supplementary Information

Amidothiourea based colorimetric receptors for basic anions: evidences of anion induced deprotonation of amide –NH proton and hydroxide induced anion... π interaction with the deprotonated receptors

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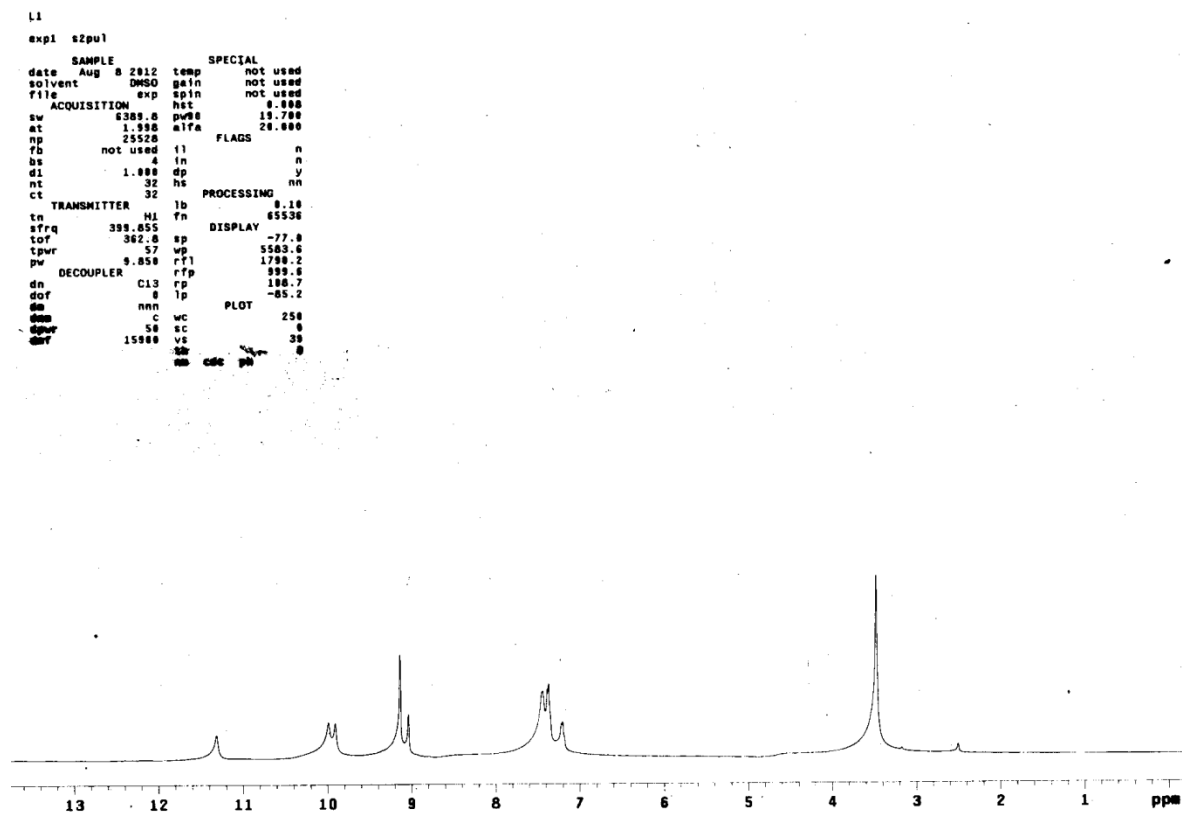


Fig.S1 ^1H -NMR spectrum of receptor L1 in d_6 -DMSO at 298K.

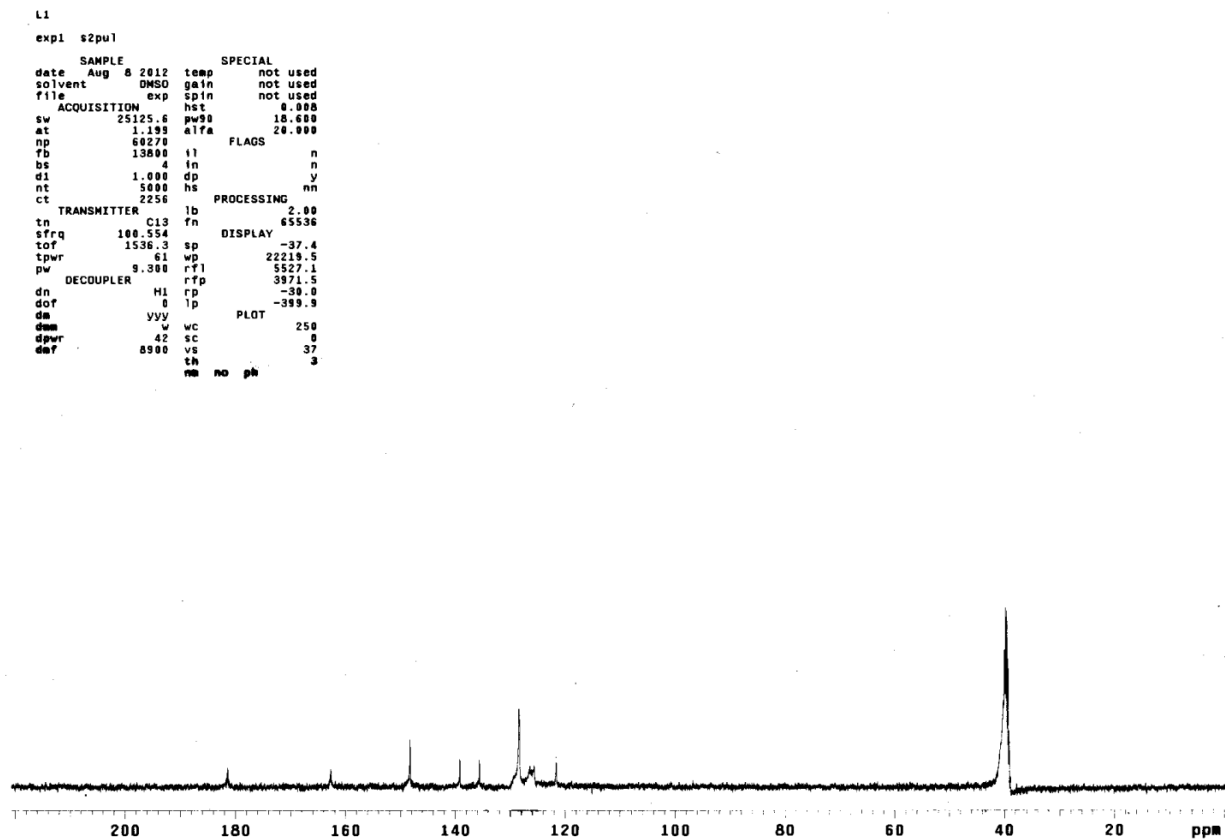


Fig.S2 ^{13}C -NMR spectrum of receptor L1 in d_6 -DMSO at 298K.

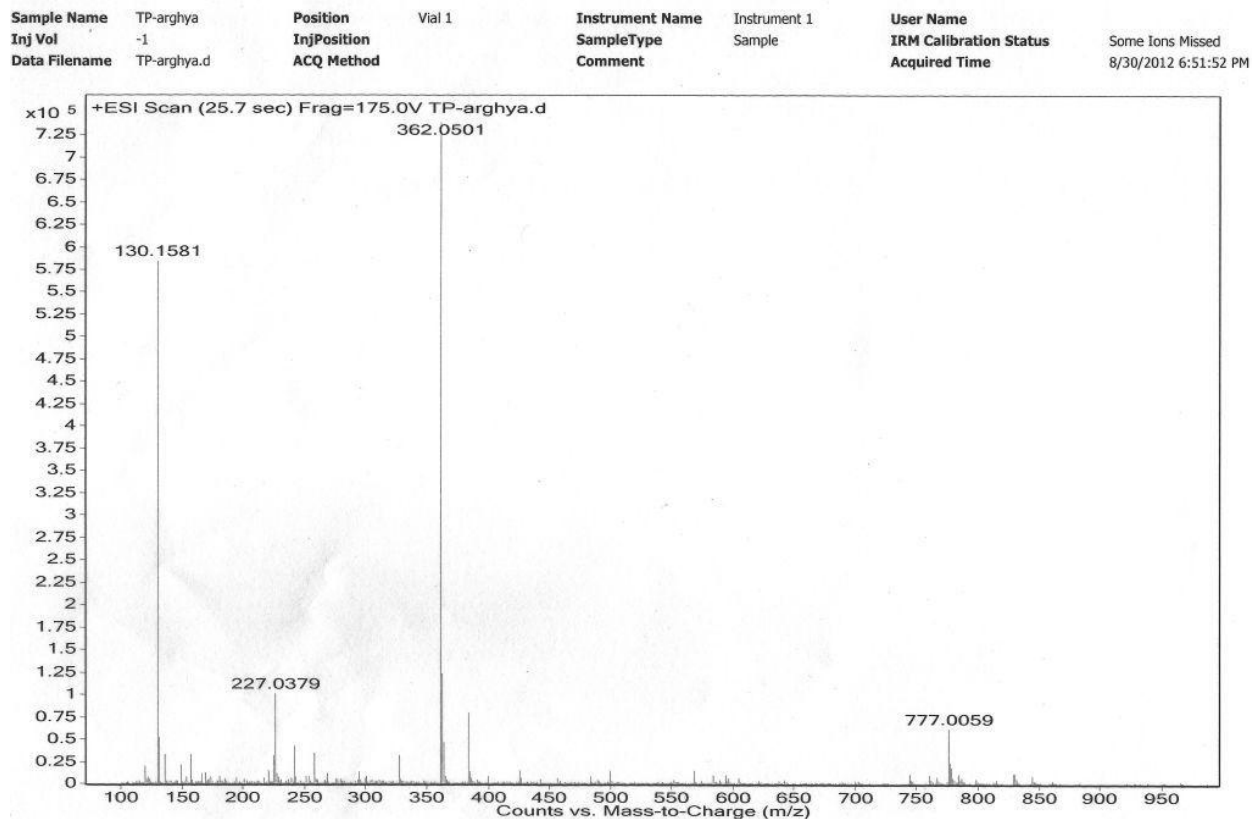


Fig.S3 Mass spectrum of receptor L1 in acetonitrile.

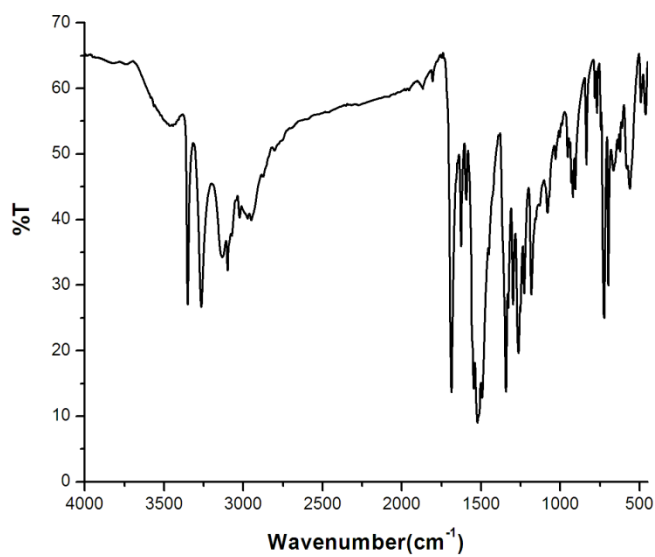


Fig.S4 IR spectrum of receptor L1.

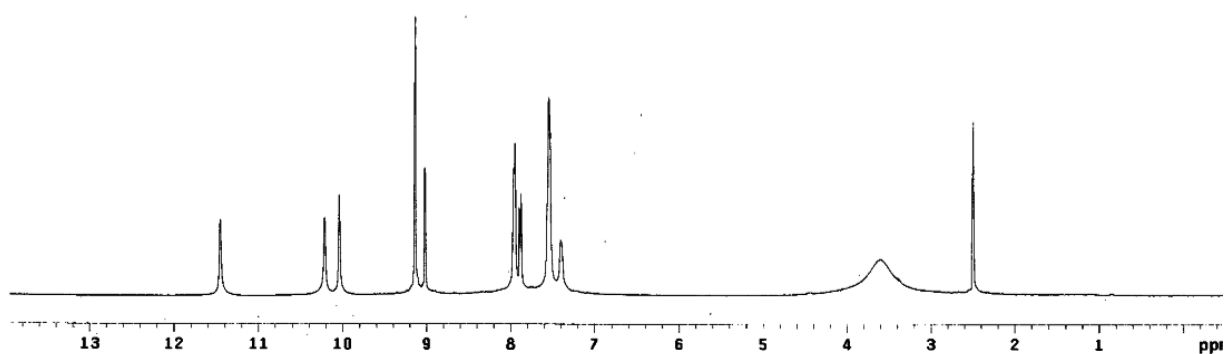


Fig.S5 ¹H NMR spectrum of receptor L2 in *d*₆-DMSO at 298K.

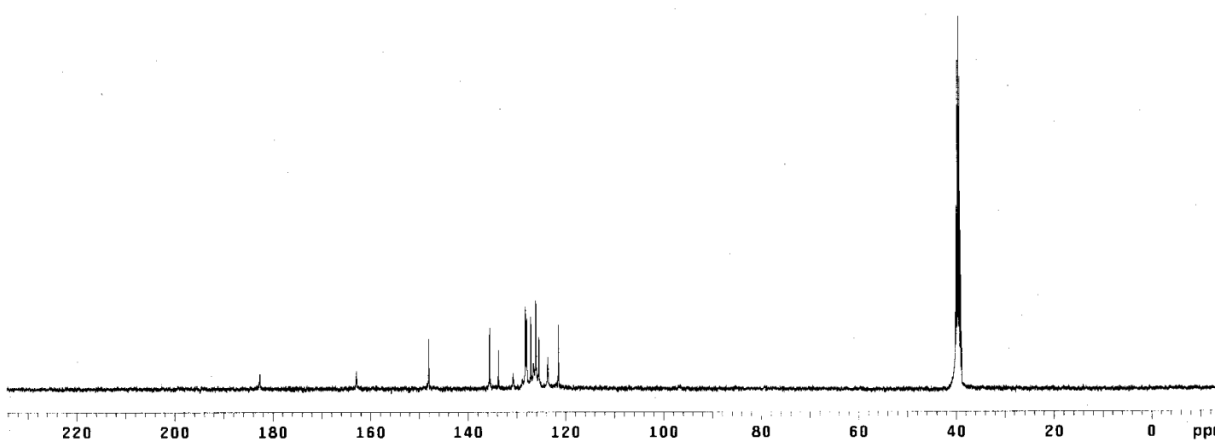


Fig.S6 ¹³C NMR spectrum of receptor L2 in *d*₆-DMSO at 298K.

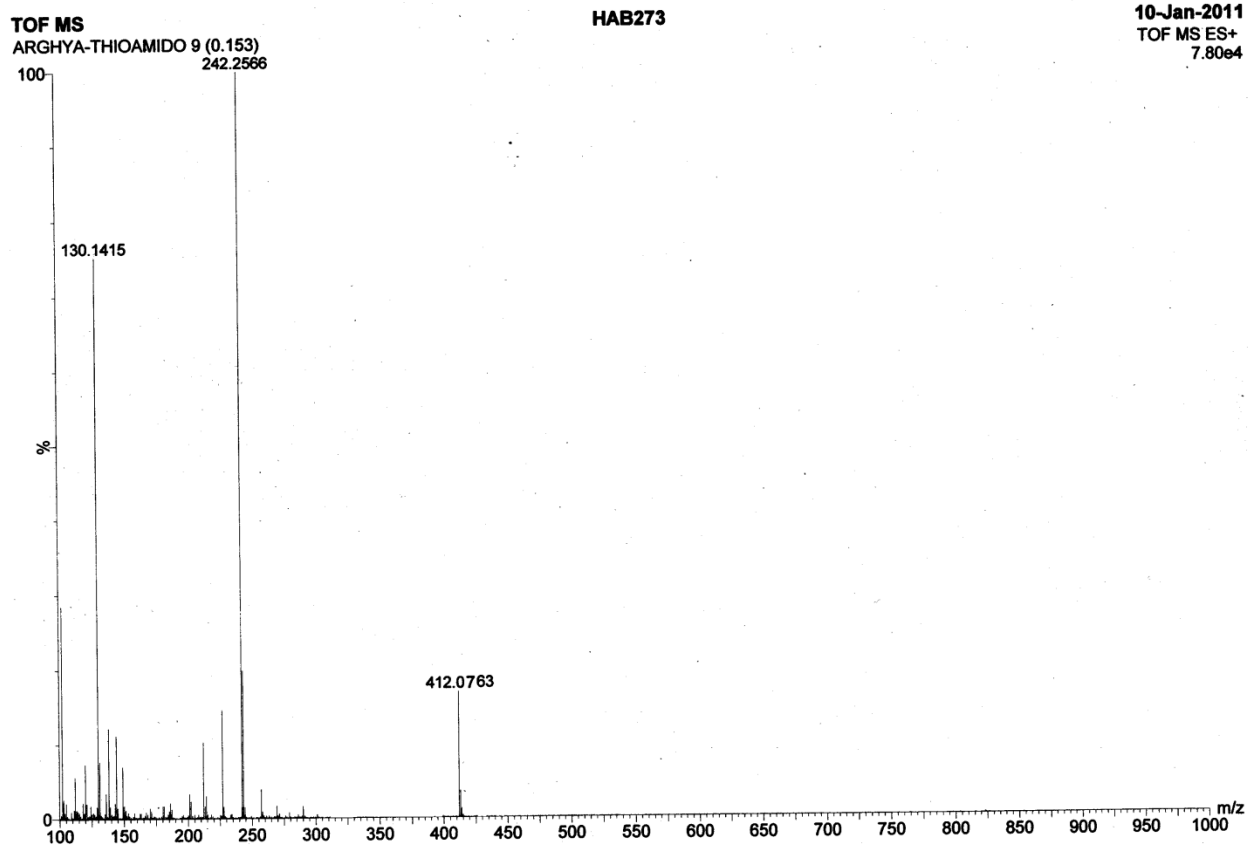


Fig. S7 ESI-Mass spectrum of receptor L2 in acetonitrile.

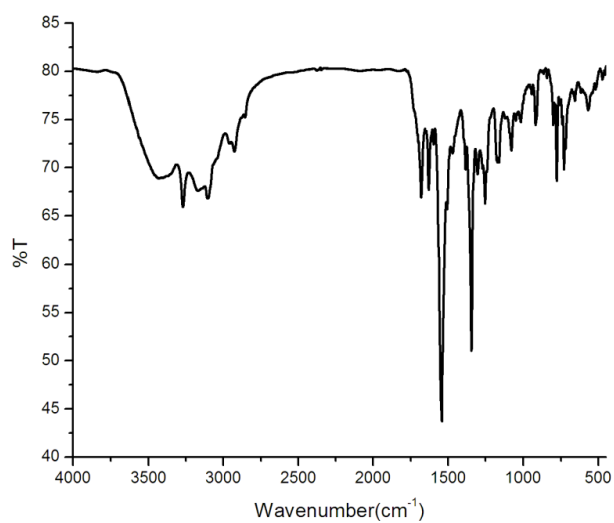


Fig.S8 IR spectrum of receptor L2.

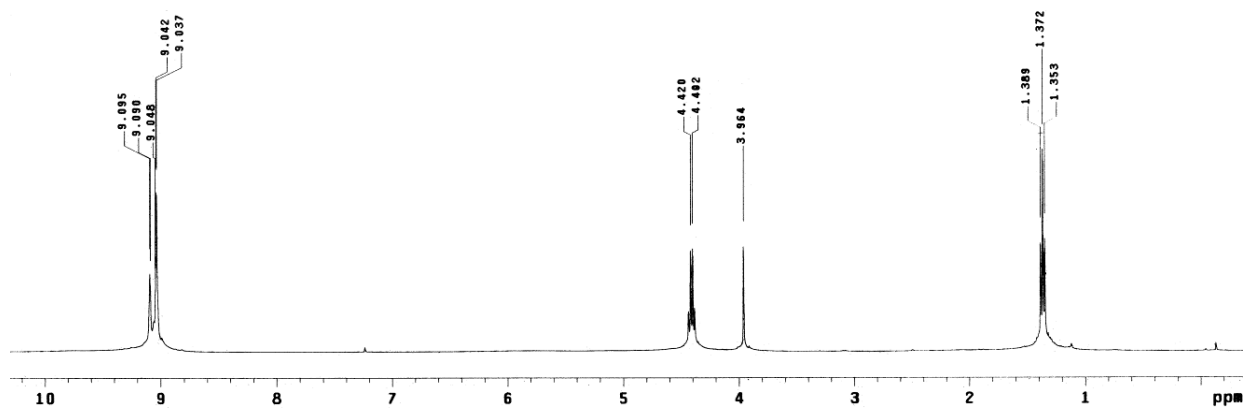


Figure S9. ^1H NMR spectrum of control receptor L_C in CDCl_3 at 298 K. (Figure reproduced from S. K. Dey and G. Das, *Chem. Commun.*, 2011, **47**, 4983–4985).

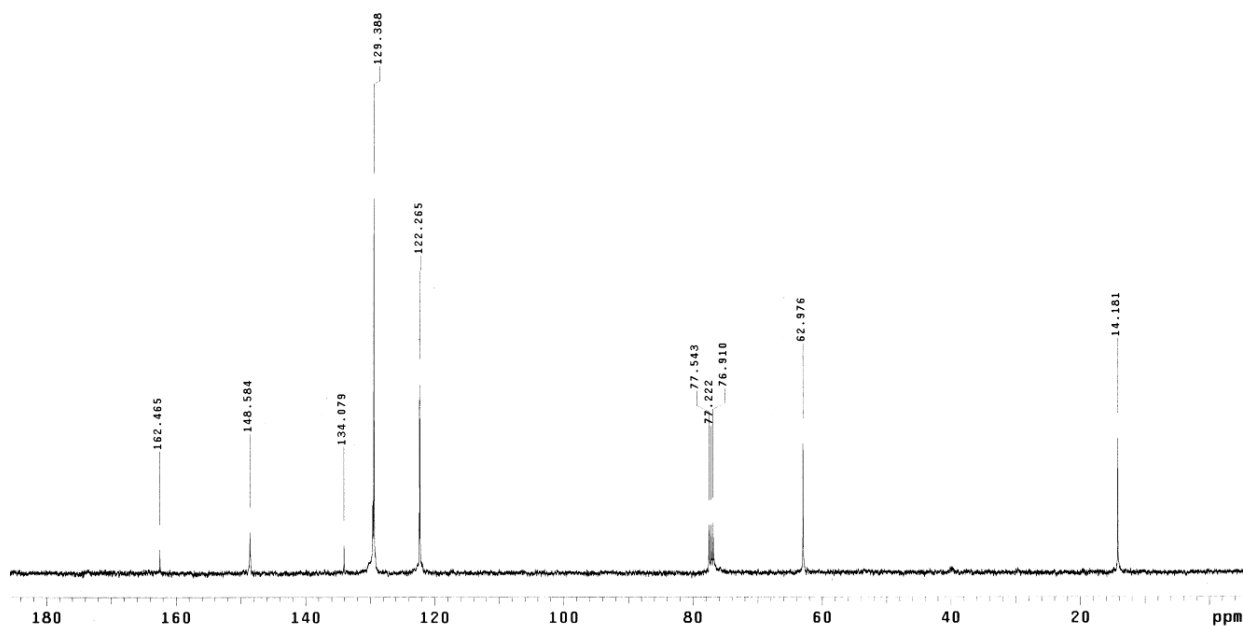


Fig.S10 ^{13}C NMR spectrum of control receptor L_C in CDCl_3 at 298K. (Figure reproduced from S. K. Dey and G. Das, *Chem. Commun.*, 2011, **47**, 4983–4985).

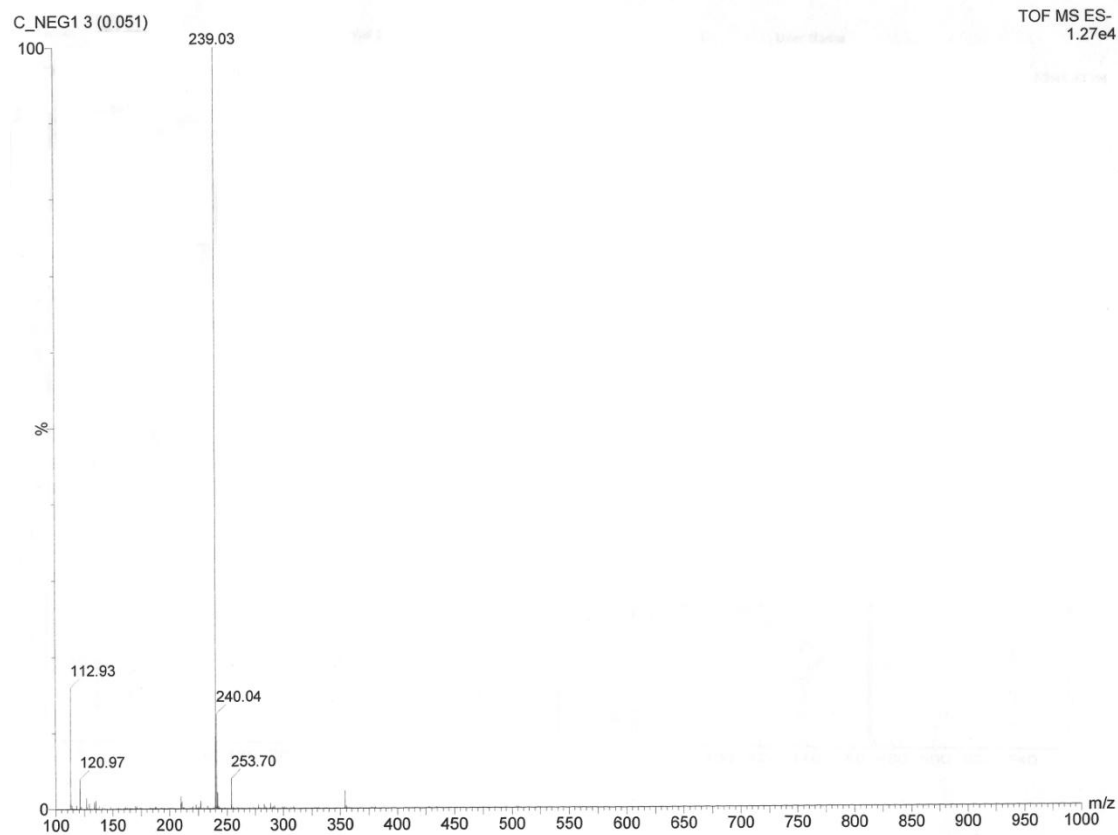


Fig. S11 ESI-Mass spectrum of receptor L_C in acetonitrile.

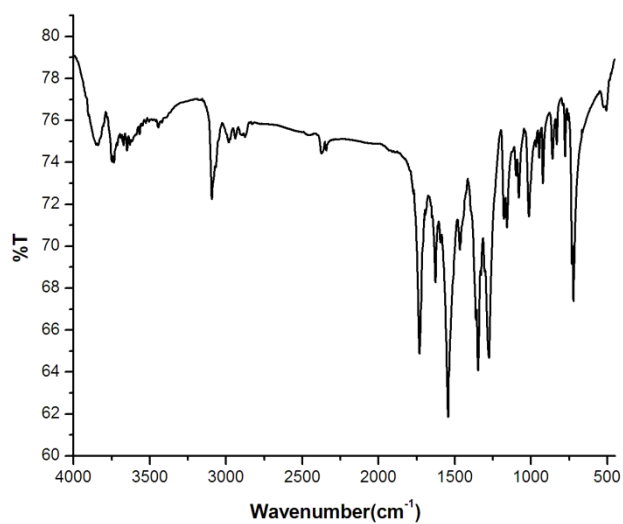


Fig.S12 IR spectrum of receptor L_C .

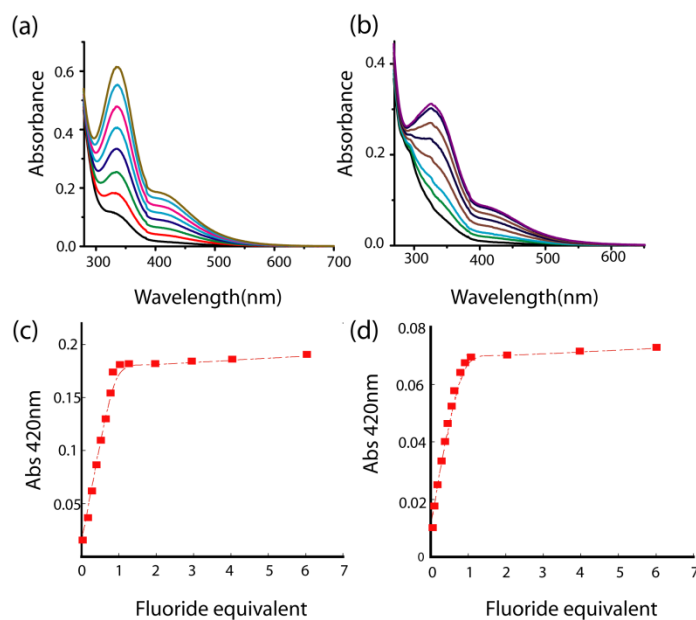


Fig.S13 a) UV-vis titration of the receptor L1 (4.0×10^{-5} M) in CH₃CN solution with standard solution of [n-Bu₄N]F. (b) The change of UV-vis spectra of the receptor L2 (3.4×10^{-5} M) in CH₃CN solution upon gradual addition of standard solution of [n-Bu₄N]F. (c) Relative change in the absorption spectra of L1 (4.0×10^{-5} M) at 420 nm upon addition of fluoride anions in CH₃CN. (d) Plot of the change in the absorption of L2 upon addition of fluoride in CH₃CN.

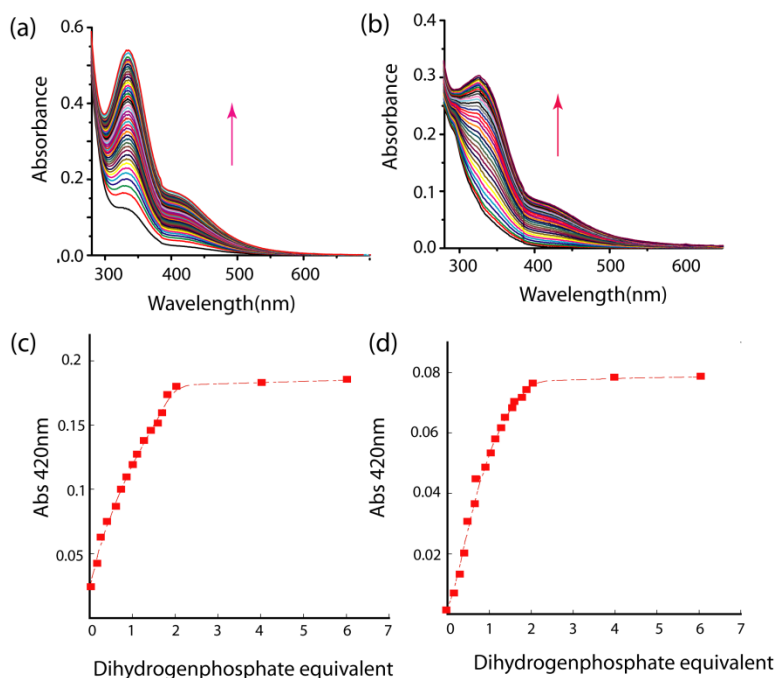


Fig. S14 a) UV-vis titration of the receptor L1 (4.0×10^{-5} M) in CH₃CN solution with standard solution of [*n*-Bu₄N]H₂PO₄. (b) The change of UV-vis spectra of the receptor L2 (3.4×10^{-5} M) in CH₃CN solution upon gradual addition of standard solution of [*n*-Bu₄N]H₂PO₄. (c) Relative change in the absorption spectra of L1 (4.0×10^{-5} M) at 420 nm upon addition of dihydrogenphosphate anions in CH₃CN. (d) Plot of the change in the absorption of L2 upon addition of di-hydrogenphosphate in CH₃CN.

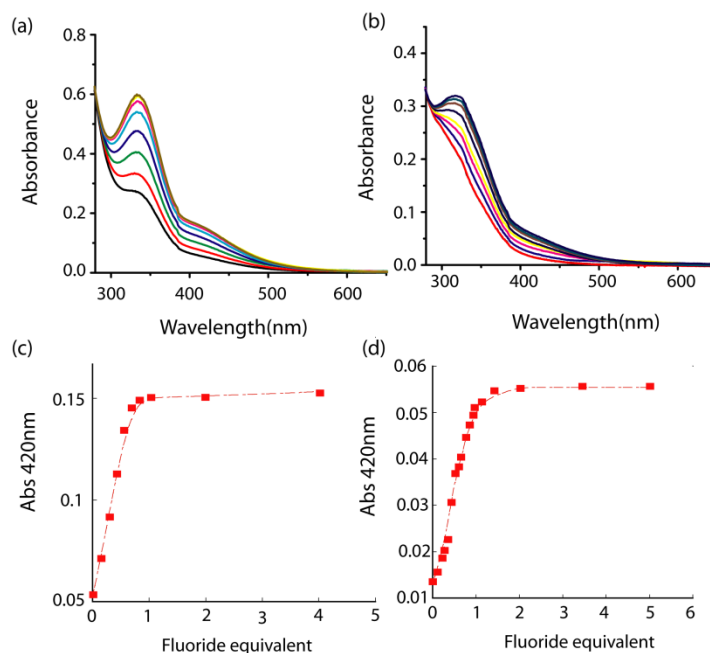


Fig. S15 a) UV-vis titration of the receptor L1(4.0×10^{-5} M) in DMSO-H₂O (5 : 1) (v/v) solution with standard solution of [n-Bu₄N]F. (b) The change of UV-vis spectra of the receptor L2 (3.4×10^{-5} M) in DMSO-H₂O (5 : 1) (v/v) solution upon addition of standard solution of [n-Bu₄N]F. (c) Relative change in the absorbance of L1 (4.0×10^{-5} M) at 420 nm upon addition of fluoride anions in DMSO-H₂O (5 : 1) (v/v). (d) Plot of the change in the absorbance at 420nm of L2 upon addition of fluoride in DMSO-H₂O (5 : 1) (v/v).

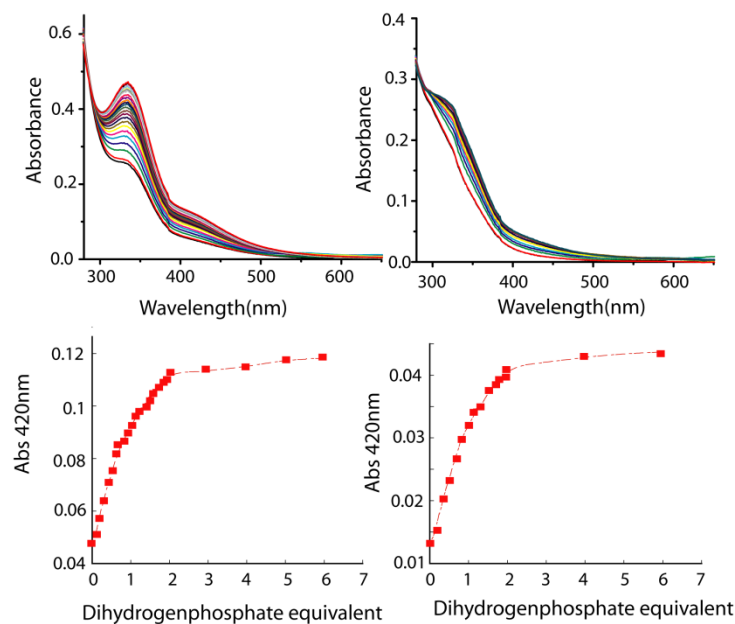


Fig. S16 a) UV-vis titration of the receptor L1 (4.0×10^{-5} M) in DMSO-H₂O (5 :1) (v/v) solution with standard solution of [n-Bu₄N]H₂PO₄. (b) The change of UV-vis spectra of the receptor L2 (3.4×10^{-5} M) in DMSO-H₂O (5 :1) (v/v) solution upon addition of standard solution of [n-Bu₄N]H₂PO₄. (c) Relative change in the absorbance of L1 (4.0×10^{-5} M) at 420 nm upon addition of di-hydrogenphosphate anions in DMSO-H₂O (5 :1) (v/v). (d) Plot of the change in the absorbance at 420nm of L2 upon addition of di-hydrogenphosphate in DMSO-H₂O (5 :1) (v/v).

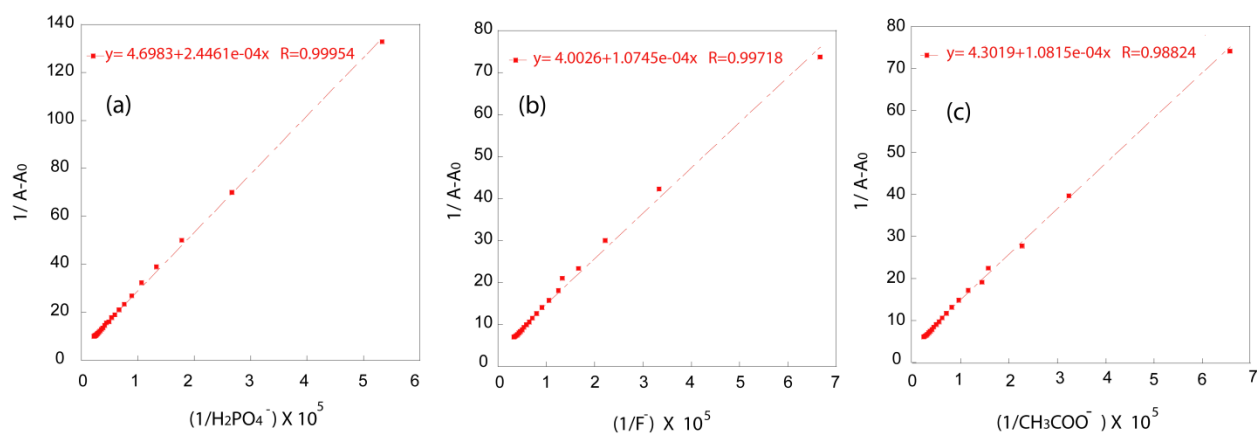


Fig. S17 Benesi-Hildebrand plots of L1 in CH₃CN with (a) Di-hydrogenphosphate, (b) Fluoride (c) Acetate.

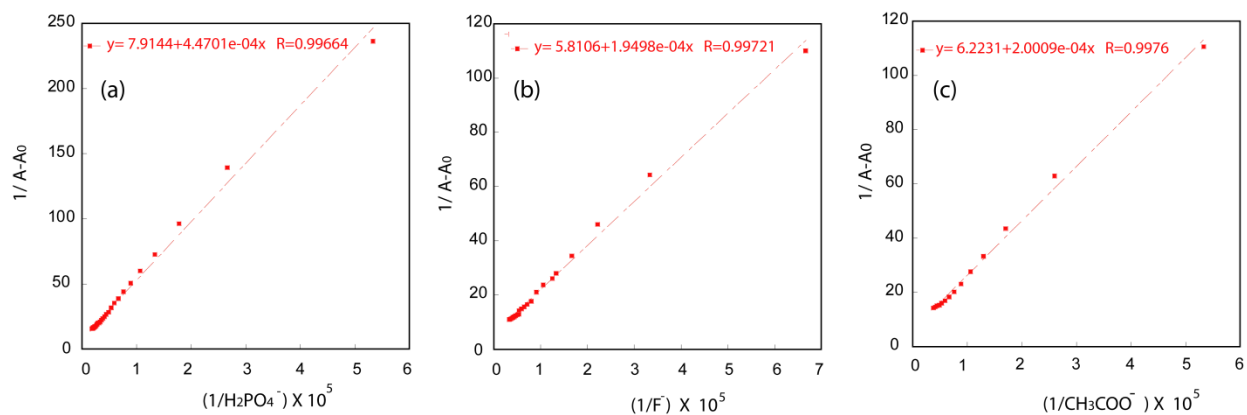


Fig. S18 Benesi–Hildebrand plots of L2 in CH₃CN with (a) Di-hydrogenphosphate, (b) Fluoride (c) Acetate.



Fig.S19. Hydroxide induce step-wise color changes observed for receptor L1.

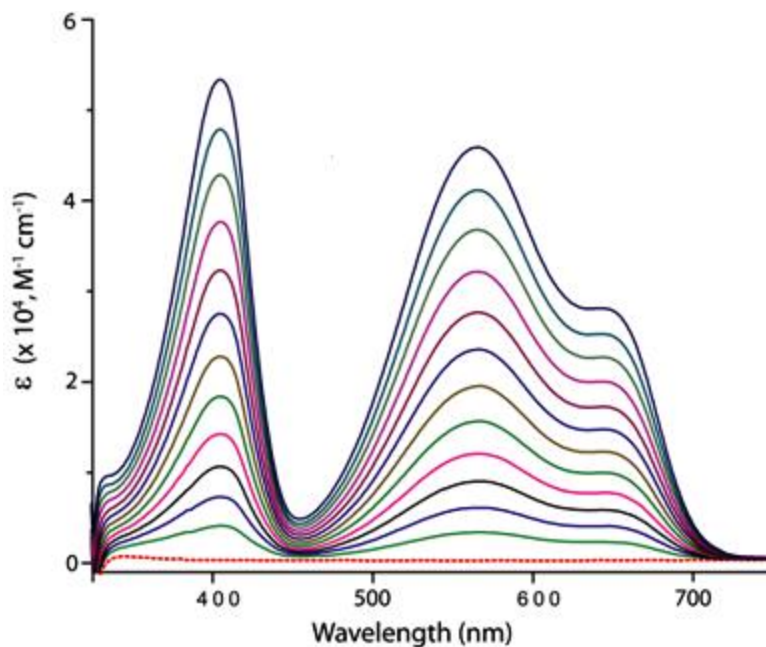


Figure S20. UV-Vis absorption titration of L_C ($10 \mu\text{M}$) in CH_3CN upon addition of standard hydroxide solution (10 mM). (Figure reproduced from S. K. Dey and G. Das, *Chem. Commun.*, 2011, **47**, 4983–4985).

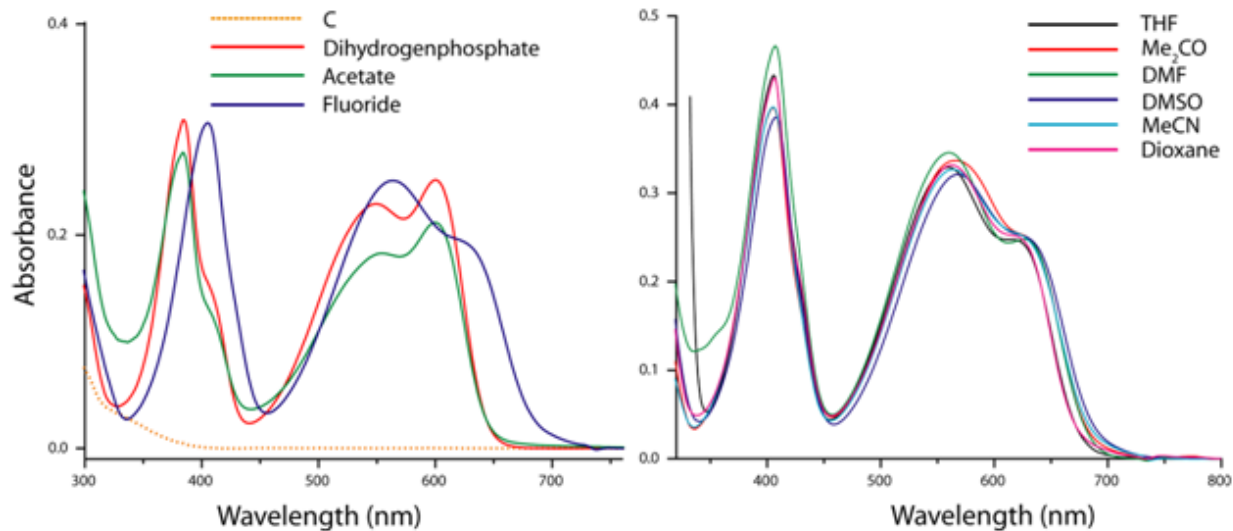


Figure S21. Changes in the UV-vis spectrum of L_C in acetonitrile solution upon addition of TBA salts of strongly basic anions such as, fluoride, acetate and dihydrogenphosphate anions (left) and no observable changes have been observed in the UV-vis spectrum of L_C in various aprotic solvents upon addition of TBAOH salt (right). (Figure reproduced from S. K. Dey and G. Das, *Chem. Commun.*, 2011, **47**, 4983–4985).

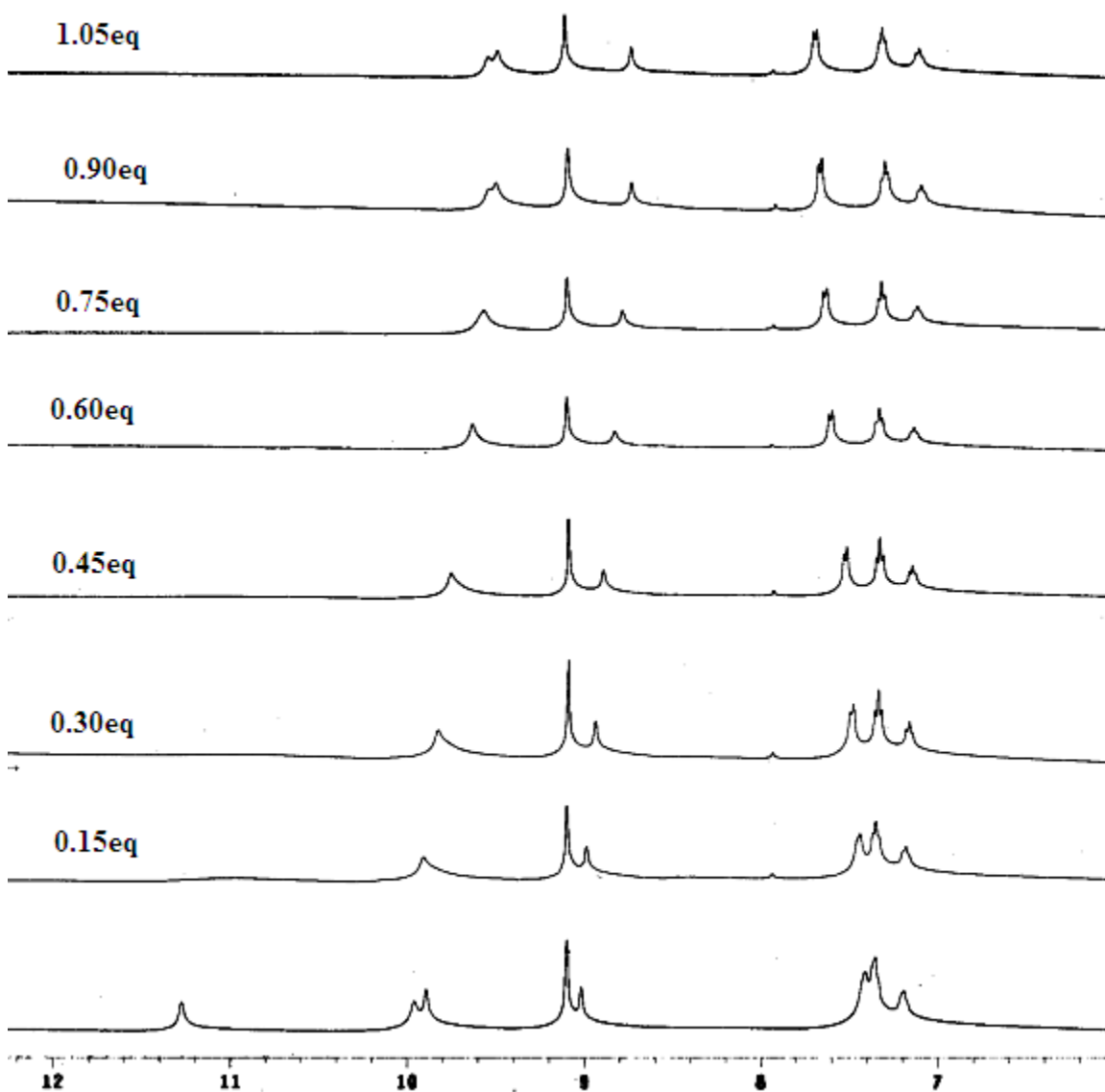


Fig. S22 Stack plot of the ¹H NMR spectra of receptor L1 in the presence of increasing amounts of [n-Bu₄N]F recorded in *d*₆-DMSO at 298 K.

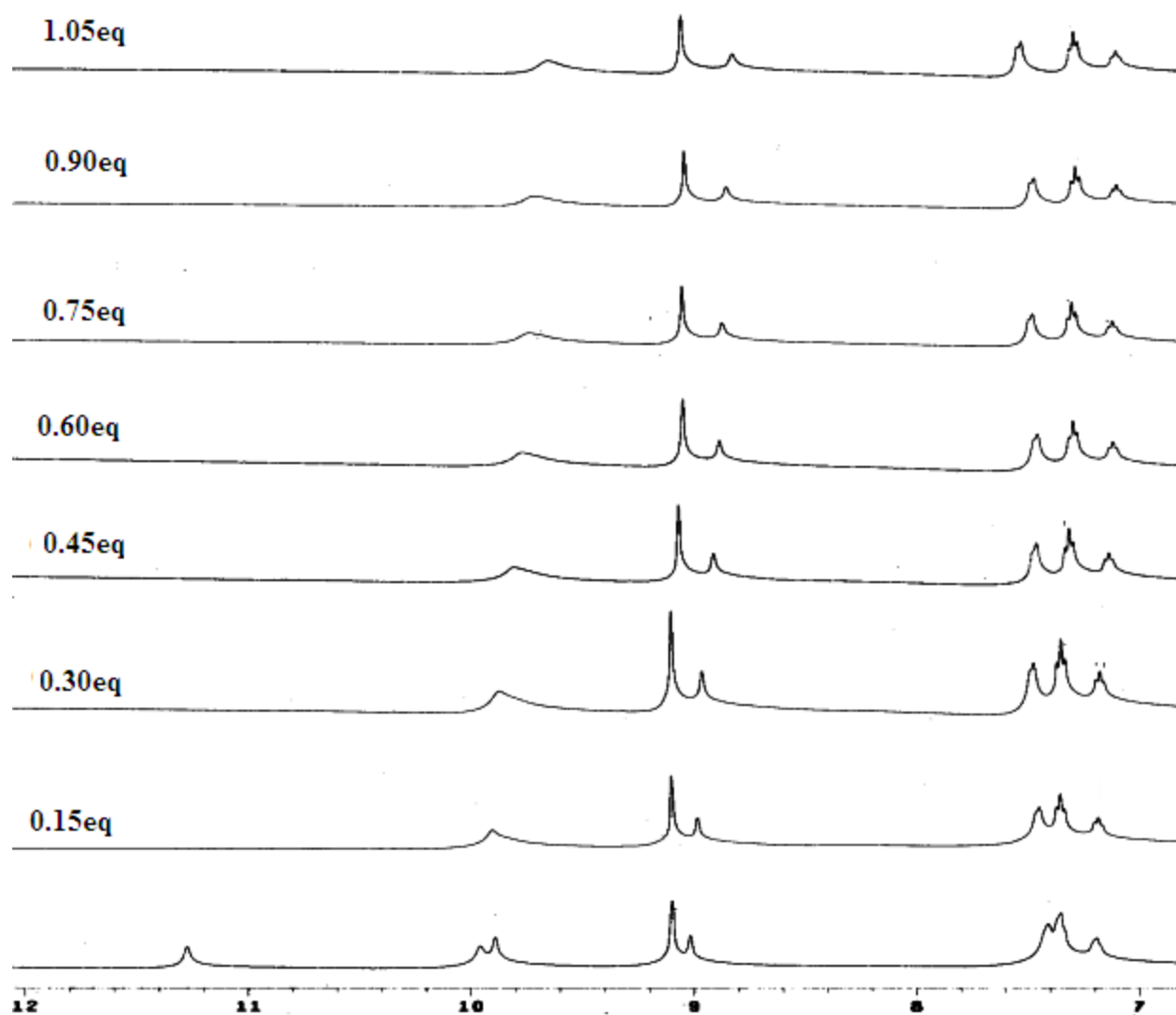


Fig. S23 Stack plot of the ¹H NMR spectra of receptor L1 in the presence of increasing amounts of [n-Bu₄N]H₂PO₄ recorded in *d*₆-DMSO at 298 K.

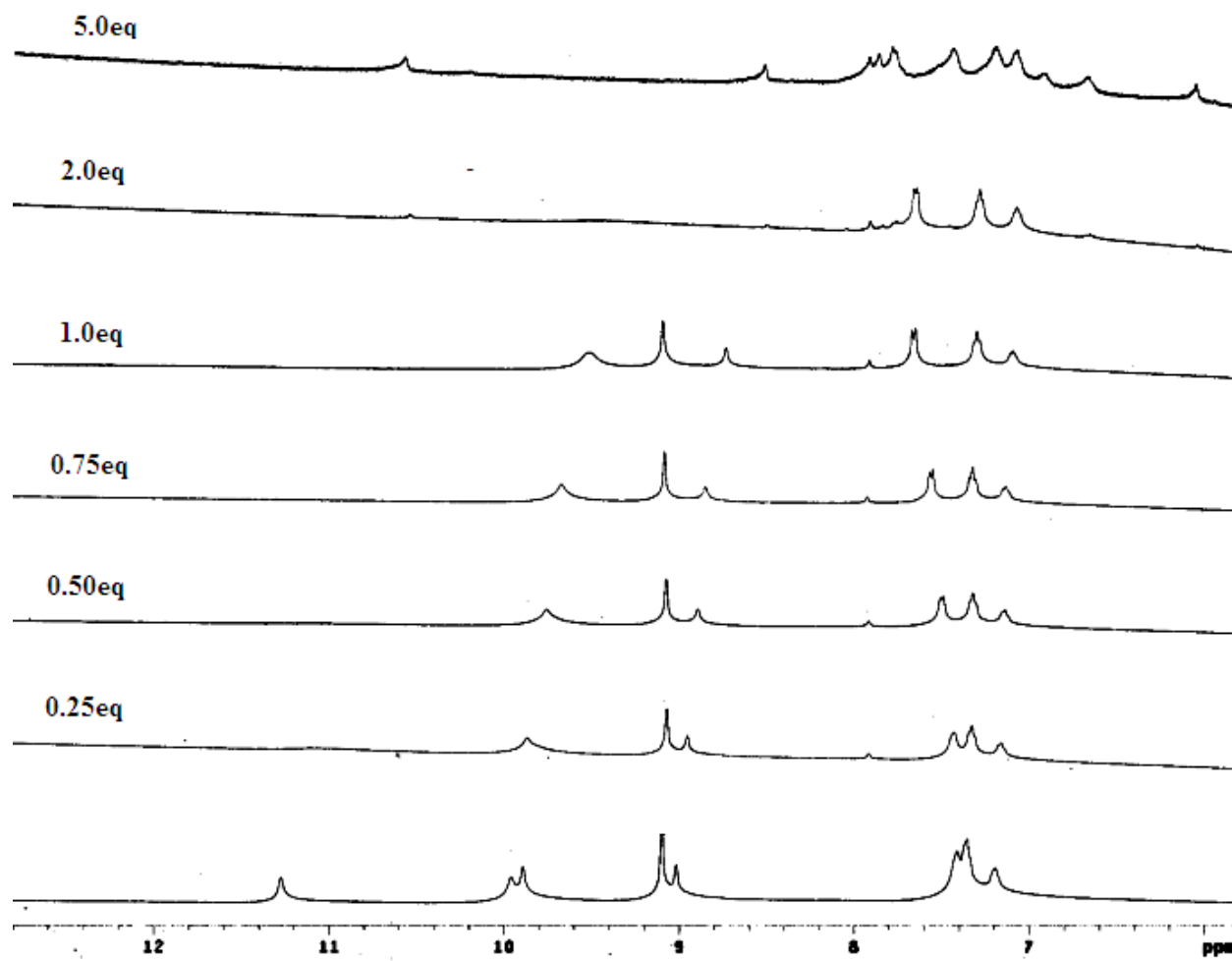


Fig. S24 Stack plot of the ^1H NMR spectra of receptor L1 in the presence of increasing amounts of $[n\text{-Bu}_4\text{N}]\text{OH}$ recorded in d_6 -DMSO at 298 K.

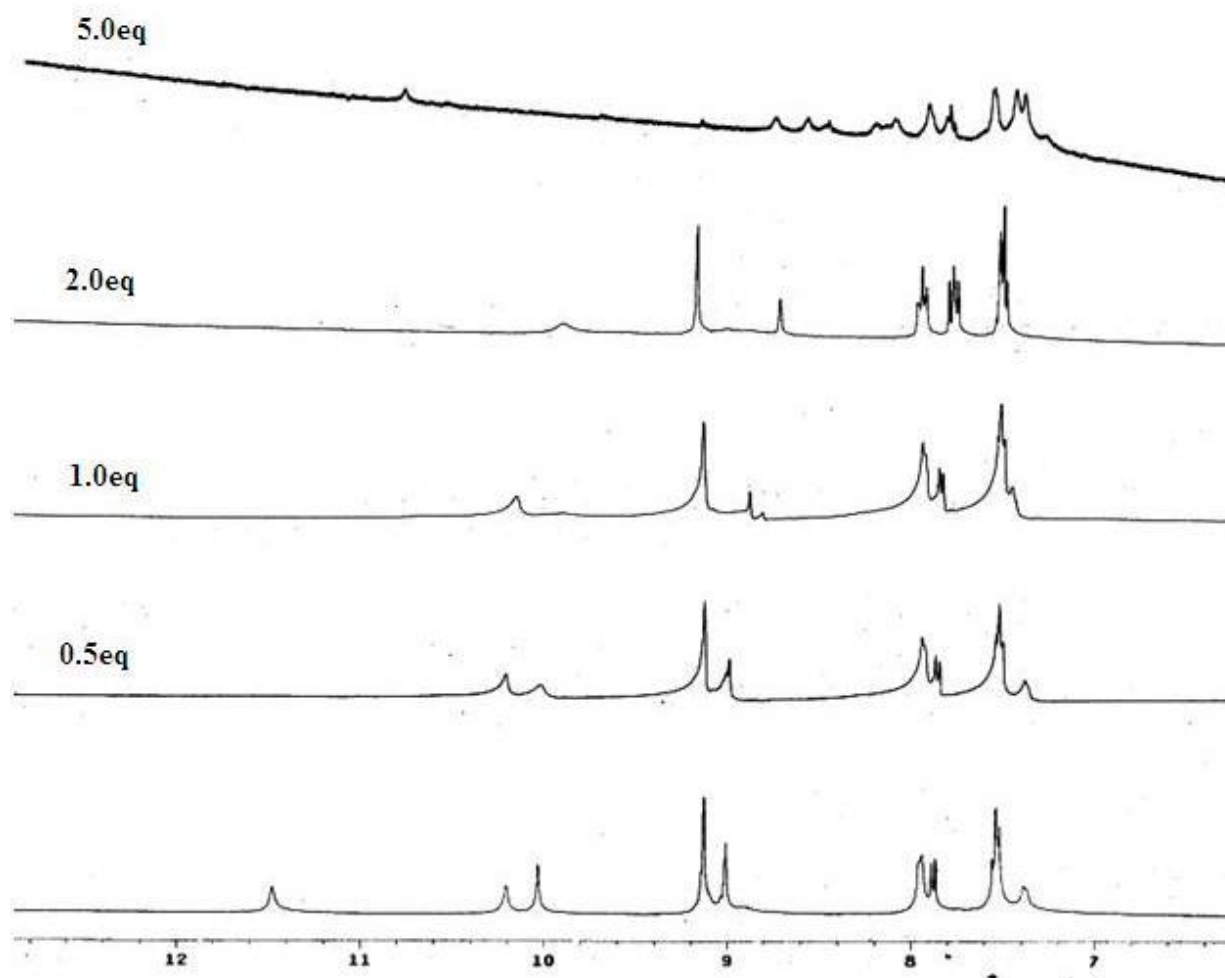


Fig. S25 Stack plot of the ^1H NMR spectra of receptor L2 in the presence of increasing amounts of $[\text{n-Bu}_4\text{N}]\text{OH}$ recorded in d_6 -DMSO at 298 K.

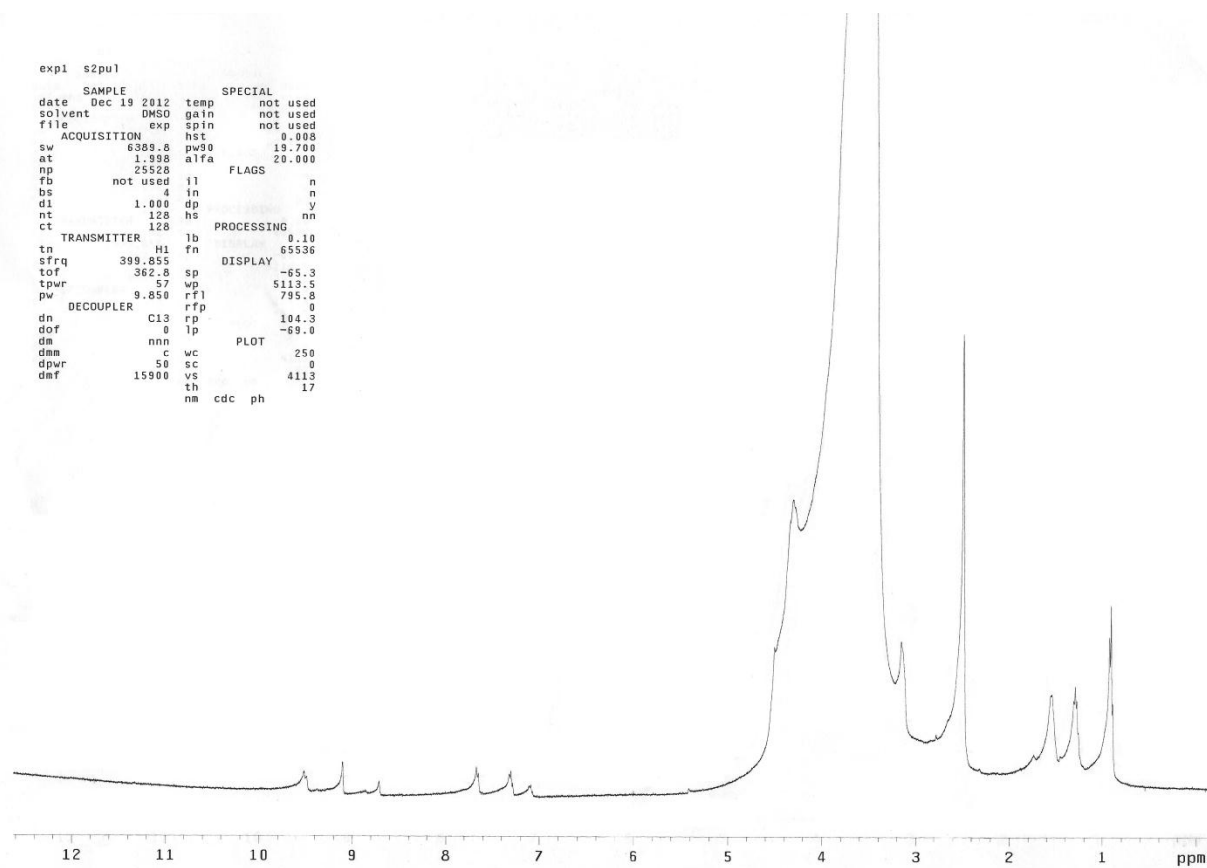


Fig.S26 ^1H -NMR spectrum of Salt 1 in d_6 -DMSO at 298K

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Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	AB-L-neg.d	ACQ Method		Comment		Acquired Time	12/21/2012 3:45:33 PM

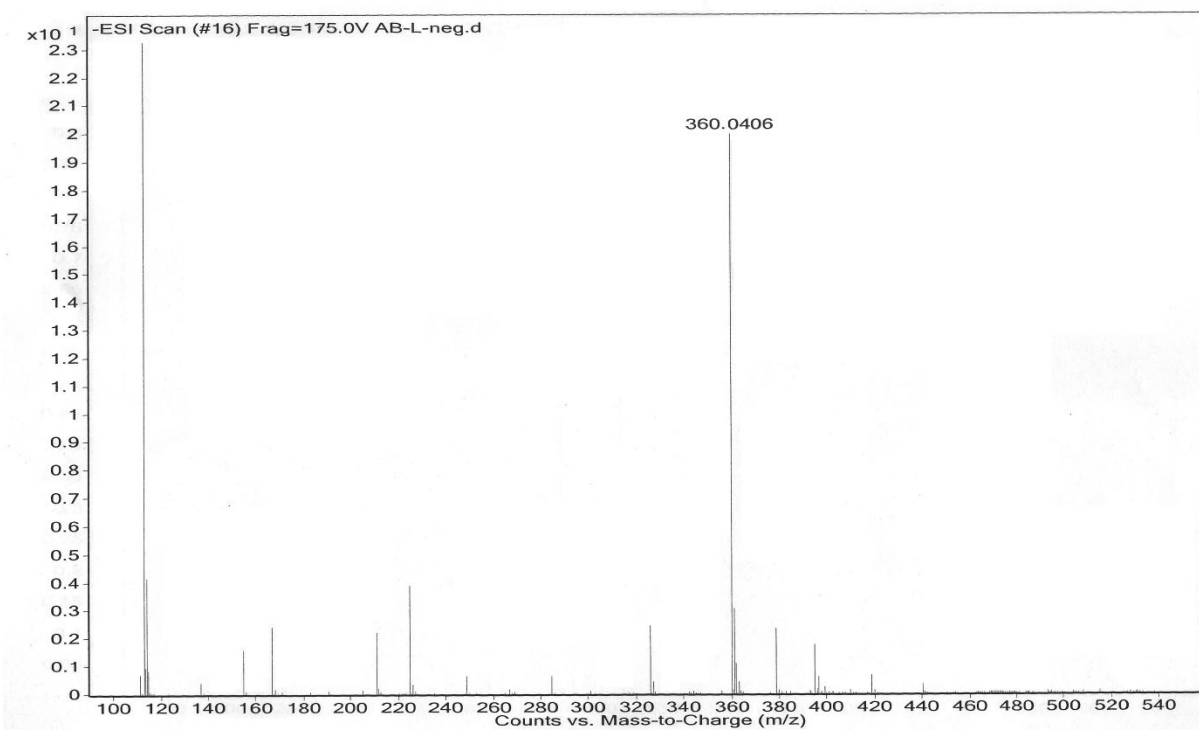


Fig.S27 Mass spectrum of Salt 1 in acetonitrile.

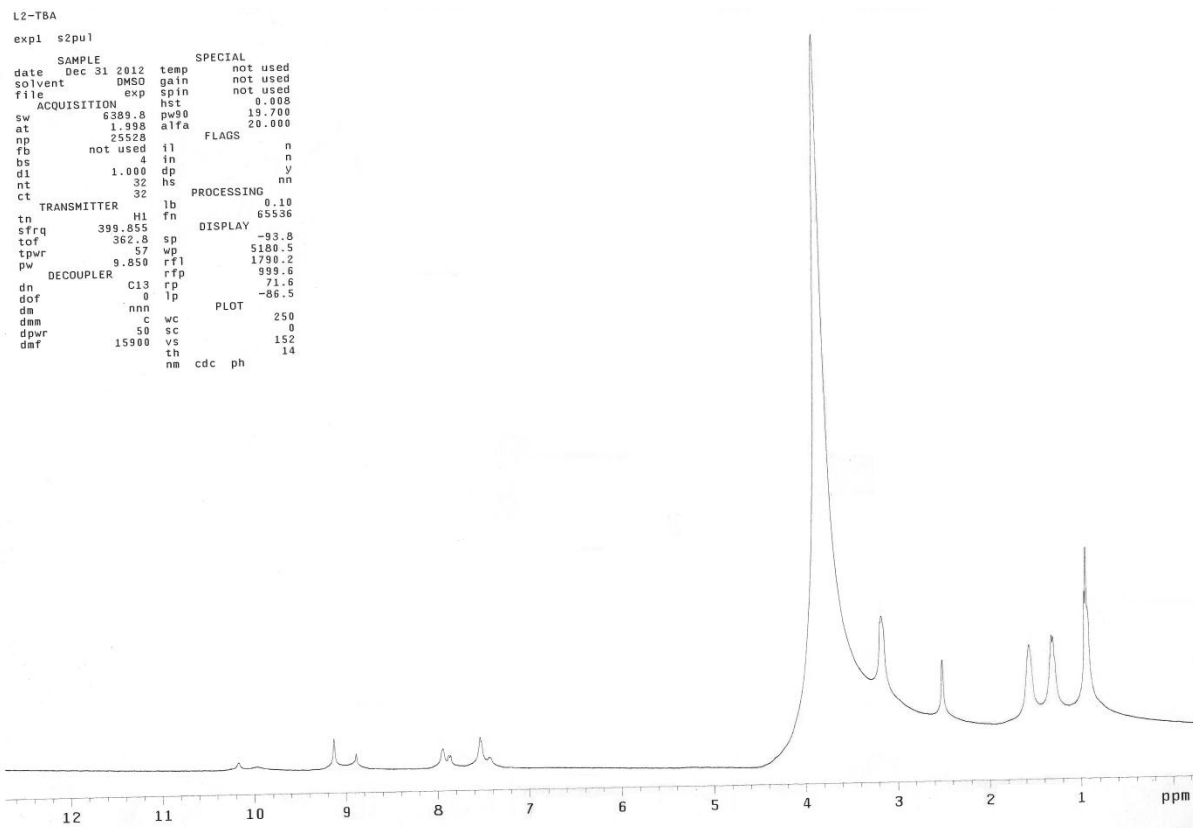


Fig.S28 ^1H -NMR spectrum of Salt 3 in d_6 -DMSO at 298K.

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Data Filename	TBA-L2-OAC.d	ACQ Method		Comment	Sample information is unavailable	Acquired Time	Unavailable

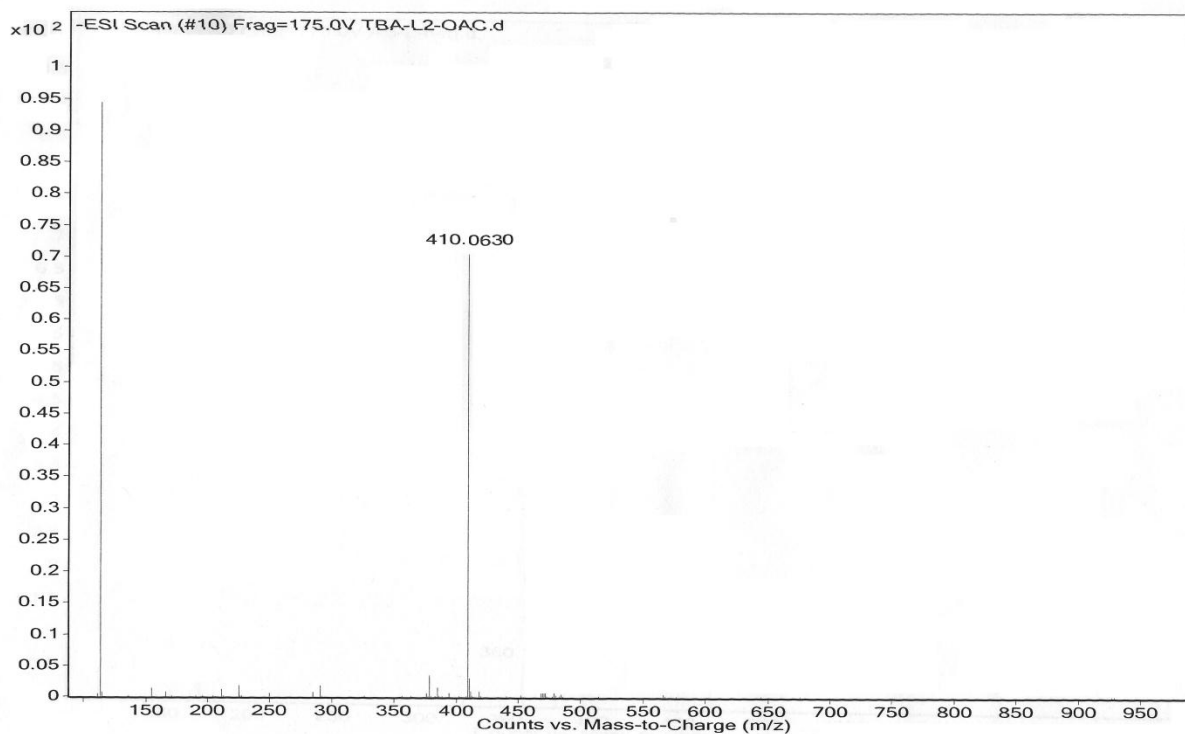


Fig.S29 Mass spectrum of Salt 3 in acetonitrile.