Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supplementary Material

Synthesis and Evaluation of Thiosemicarbazones Functionalized with Furyl Moieties as New Chemosensors for Anion Recognition

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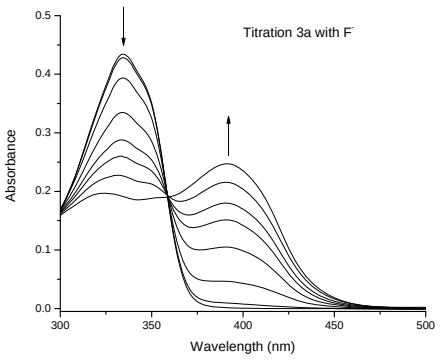
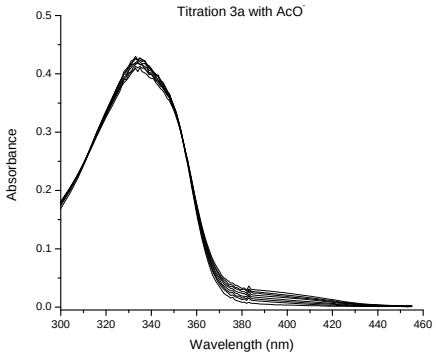
I. Characterization data of receptors 3a-f and 4 by ^{1}HNMR and IR

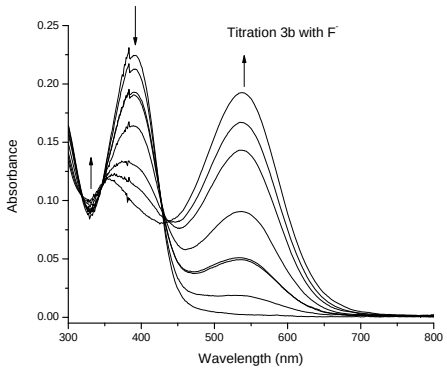
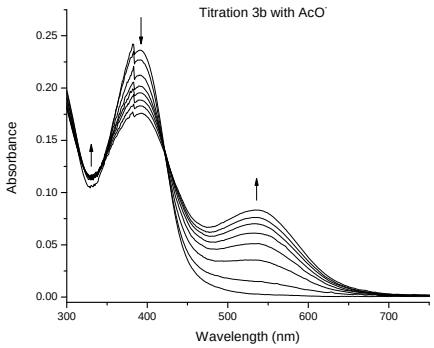
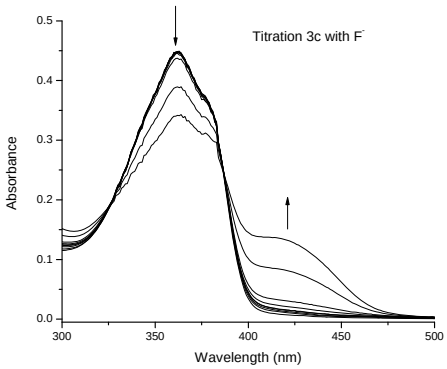
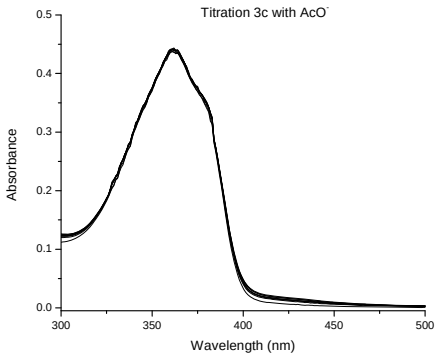
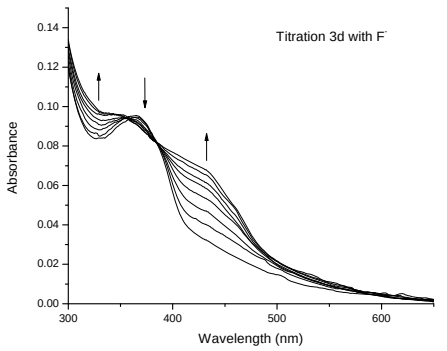
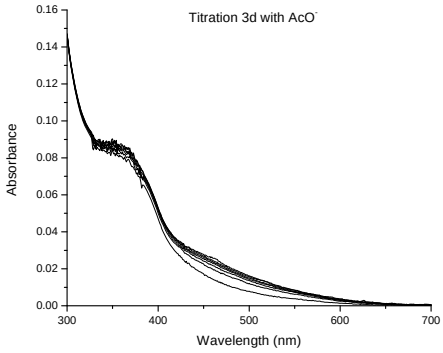
Table 1. Yields, ^{1}H NMR and IR data of furyl-thiosemicarbazone receptors **3a-f** and **4**.

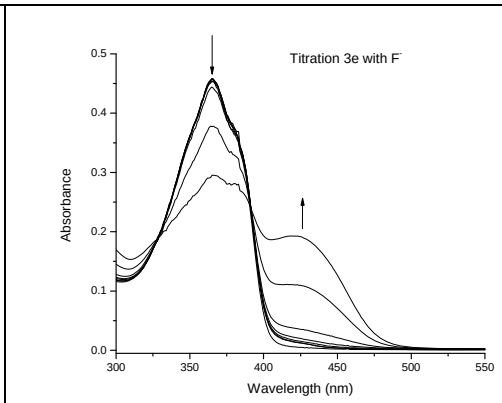
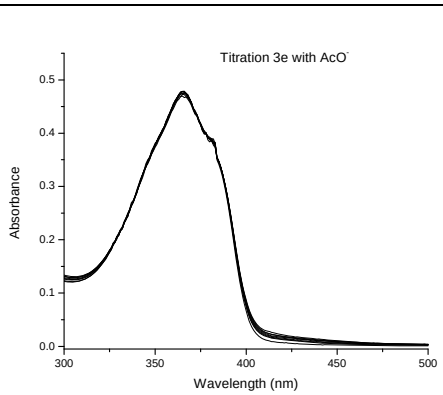
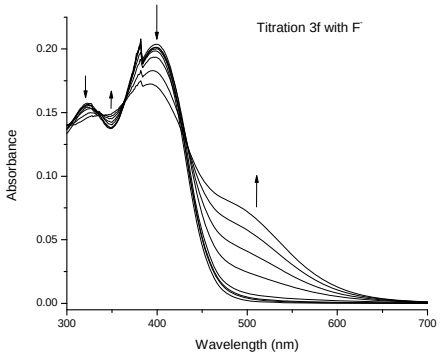
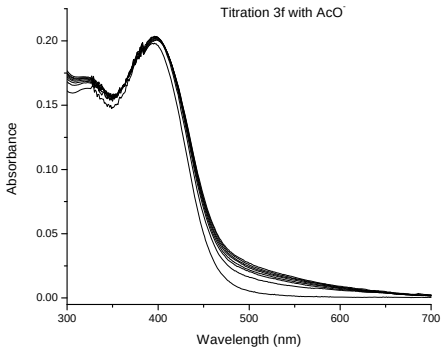
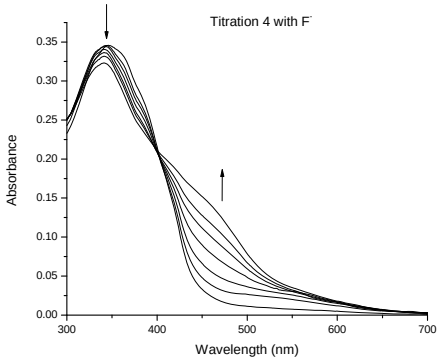
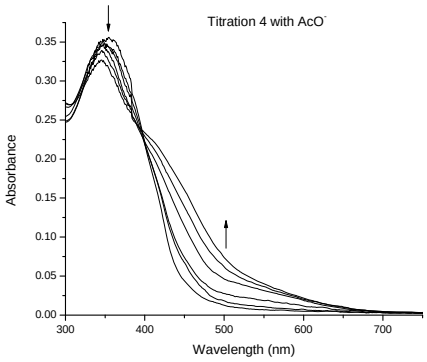
Formyl precursor	Receptor	Yield (%)	δ_H (ppm)[a]			IR[b] ν (cm^{-1})	
			(C*H*=N)	(C=N-N*H*)	(S=C-N*H*)	(CH=N)	(NH)
1a	**3a**	76	7.99	11.85	9.88	3132	3332
1b	**3b**	81	8.07	12.23	10.18	3135	3313
1c	**3c**	76	8.09	11.89	9.93	3147	3270
1d	**3d**	78	8.01	11.84	9.89	3133	3339
1e	**3e**	87	8.08	11.89	9.92	3143	3287
1f	**3f**	96	8.11	12.00	9.99	3135	3316
1g	**4**	90	8.10	11.86	10.15	3158	3322
			8.16	11.91	9.96	-	3300

[a] For the NH proton of the furyl-thiosemicarbazone receptors **3a-f** and **4** (300 or 400 MHz, DMSO-d_6). [b] IR recorded in Nujol.

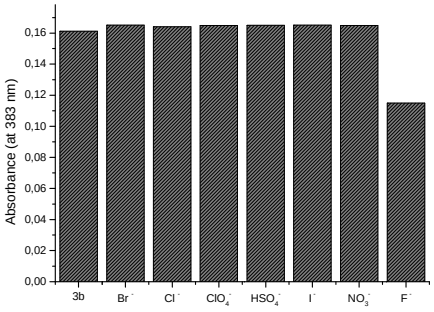
II. UV–Vis titration of receptors 3a-f and 4 (1.2×10^{-5} mol dm^{-3}) with fluoride (left) and acetate (rigth) anions (0 - 10 equiv.) in acetonitrile.

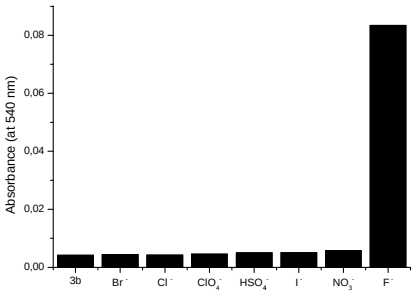
	Titration with Fluoride	Titration with Acetate
3a		

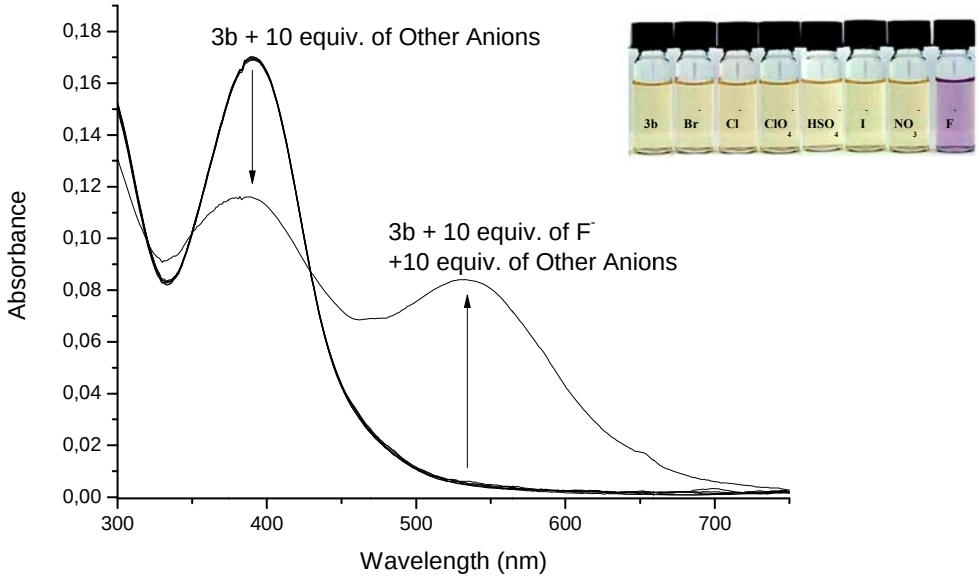
3b		
3c		
3d		

3e		
3f		
4		

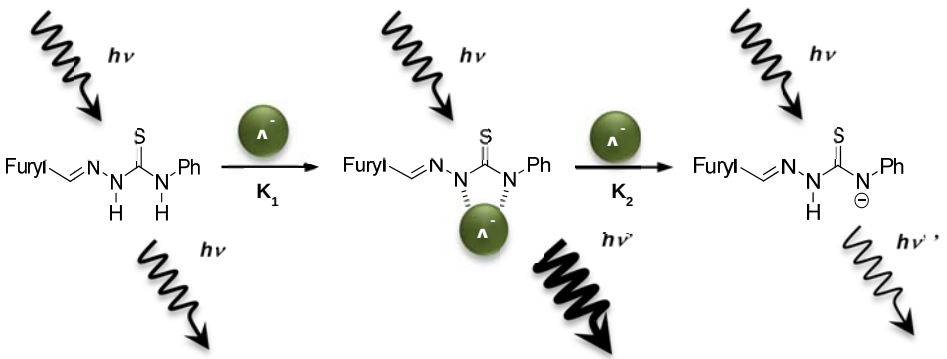
III. Study of selectivity of 3b (1 x 10-5 mol dm^{-3}) for F^- (10 equiv.) in presence of 10 equiv. of other anions (Br^-, Cl^-, ClO_4^-, HSO_4^-, I^- and NO_3^-) evaluated.







IV. Schematic representation of the dual coordination/deprotonation process for the interaction of thiosemicarbazone receptors with basic anions.



V. UV-Vis kinetic study of 3b (wavelength at 390 nm) with 10 equiv. of fluoride anion in acetonitrile, from 0 to 10 min of interaction.