Electronic Supplementary Material (ESI) for RSC Advances.

Colorimetric and optical discrimination of halides by a simple chemosensor

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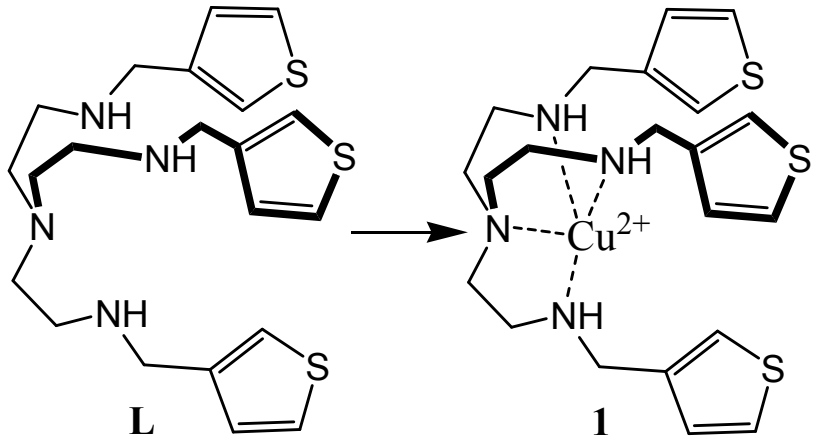

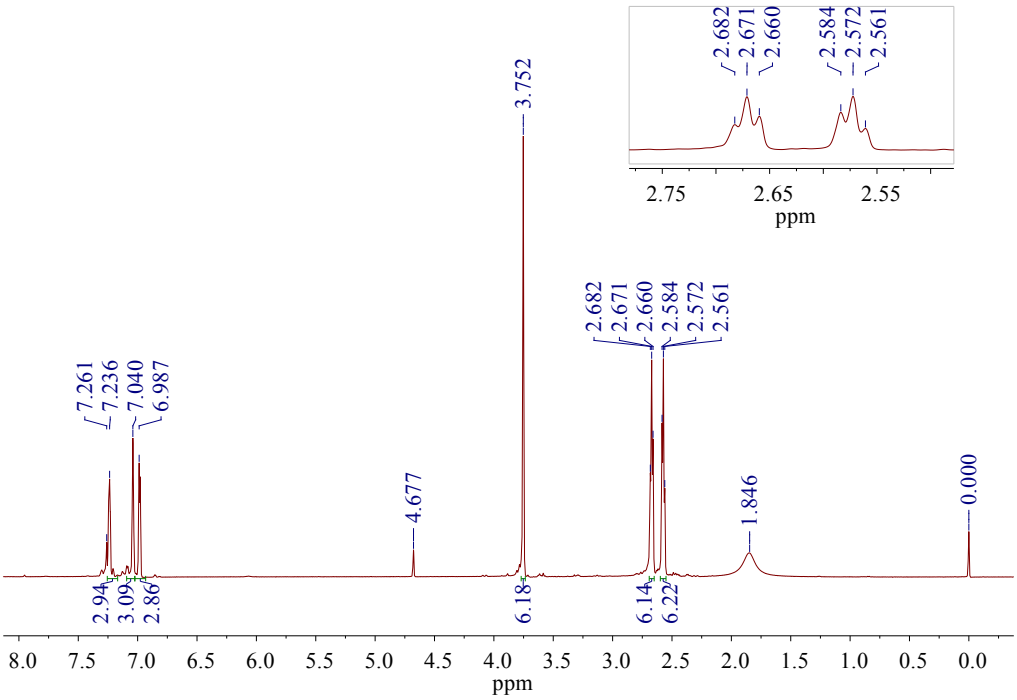

Fig S1: ^{1}H NMR spectrum of **L** in $CDCl_3$

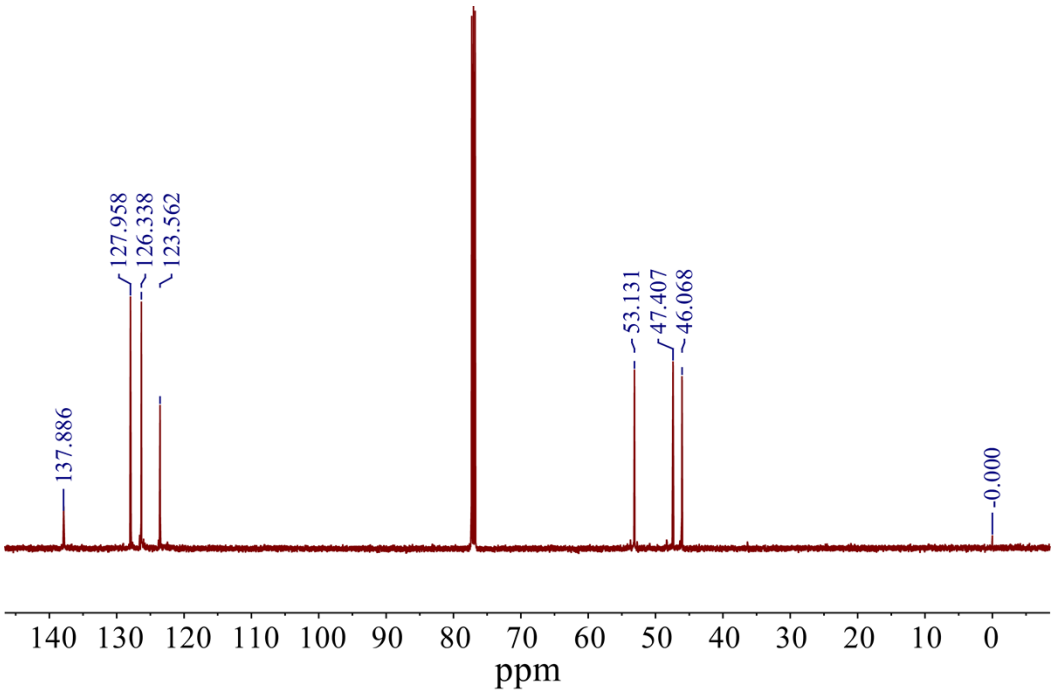

Fig S2: ^{13}C NMR spectrum of **L** in $CDCl_3$

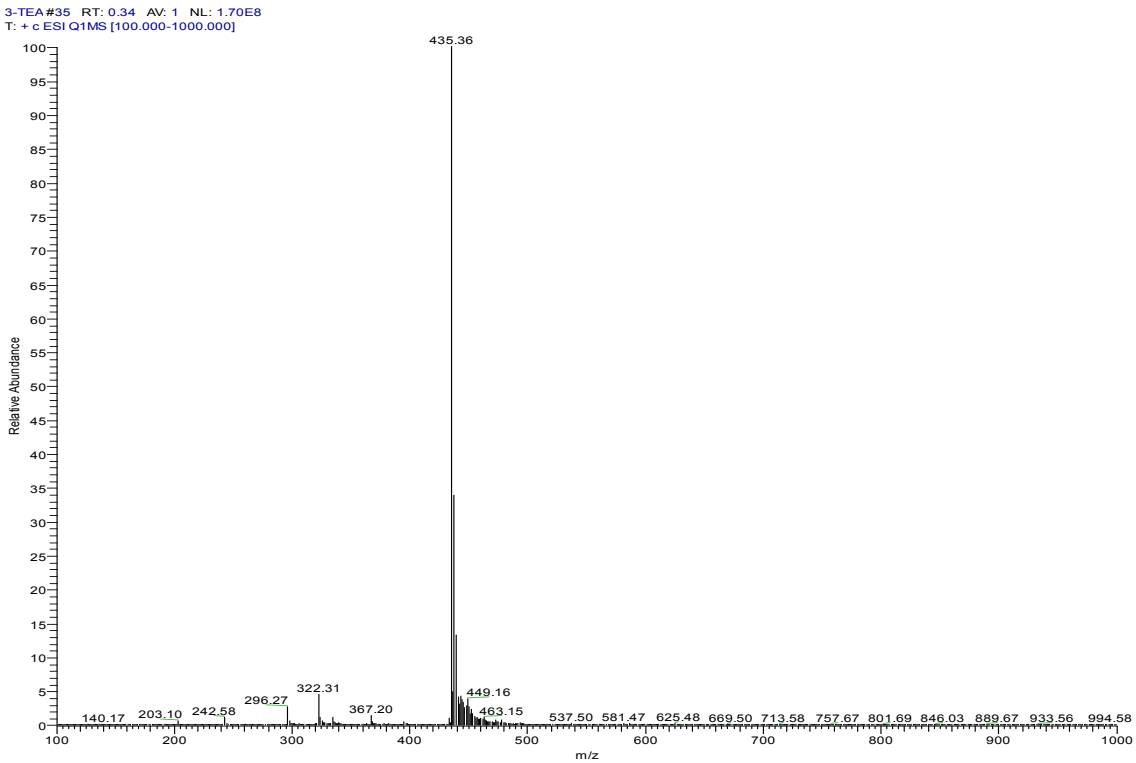

Fig. S3: Mass spectrum of **L**.

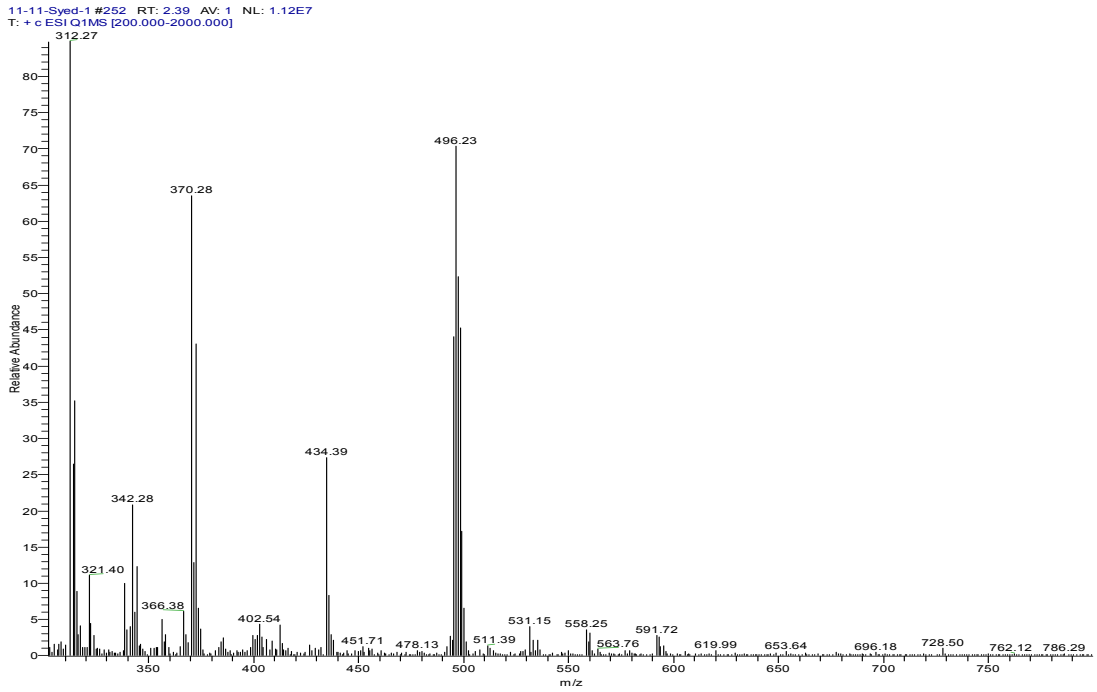

Fig. S4: Mass spectrum of **1**

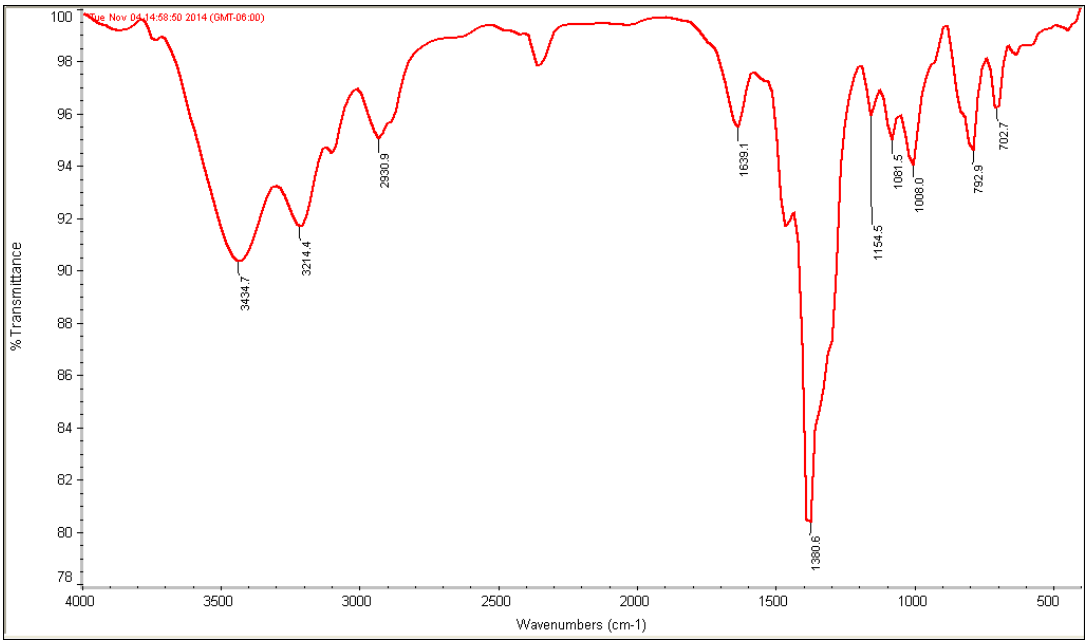

Fig. S5. IR spectrum of **1**.

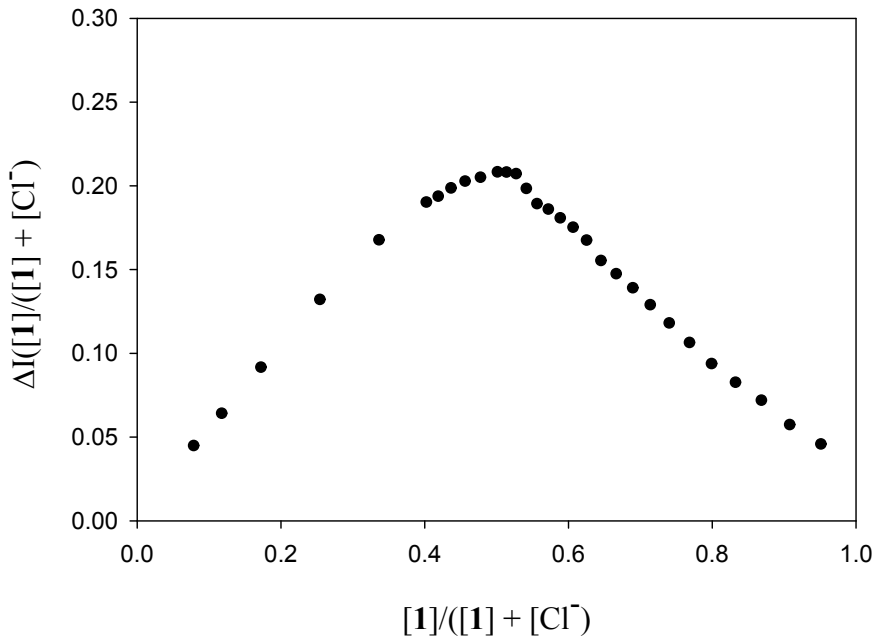

Fig. S6. Job plot analysis of **1** for the binding of chloride in CH_3CN. The change of the absorbance (ΔI) of **1** was determined from the titration plot as shown in Figure 5b.

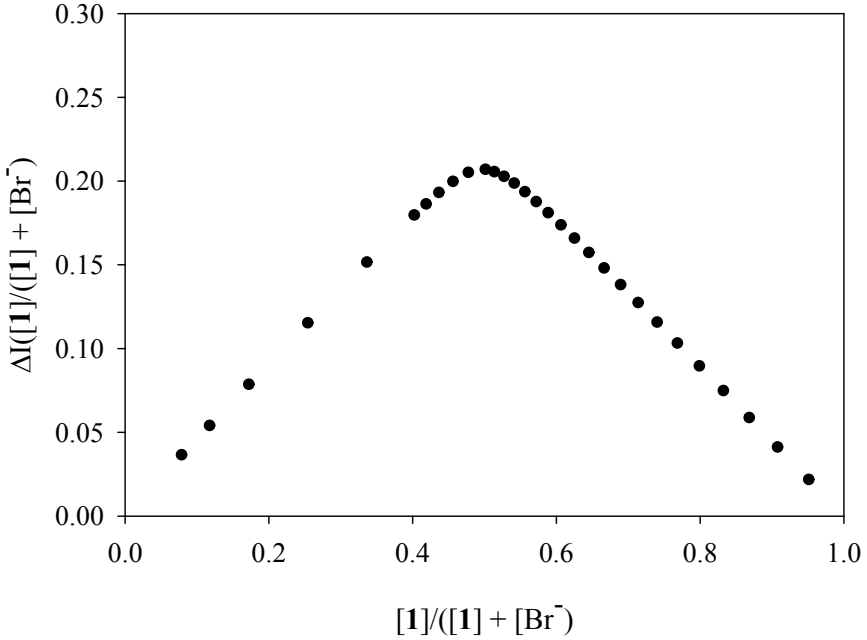

Fig. S7. Job plot analysis of **1** for the binding of bromide in CH_3CN. The change of the absorbance (ΔI) of **1** was determined from the titration plot as shown in Figure 5c.

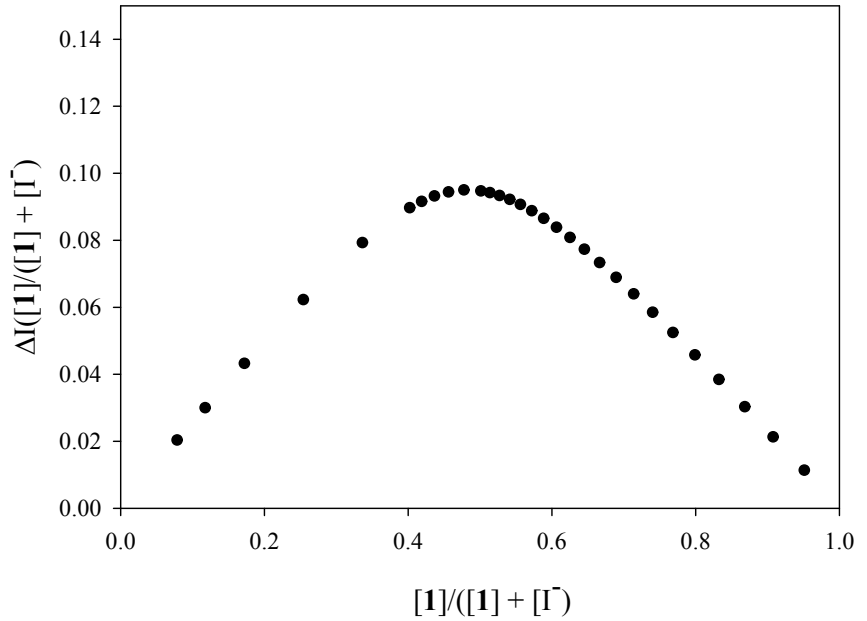

Fig. S8. Job plot analysis of **1** for the binding of iodide in CH_3CN. The change of the absorbance (ΔI) of **1** was determined from the titration plot as shown in Figure 5d.

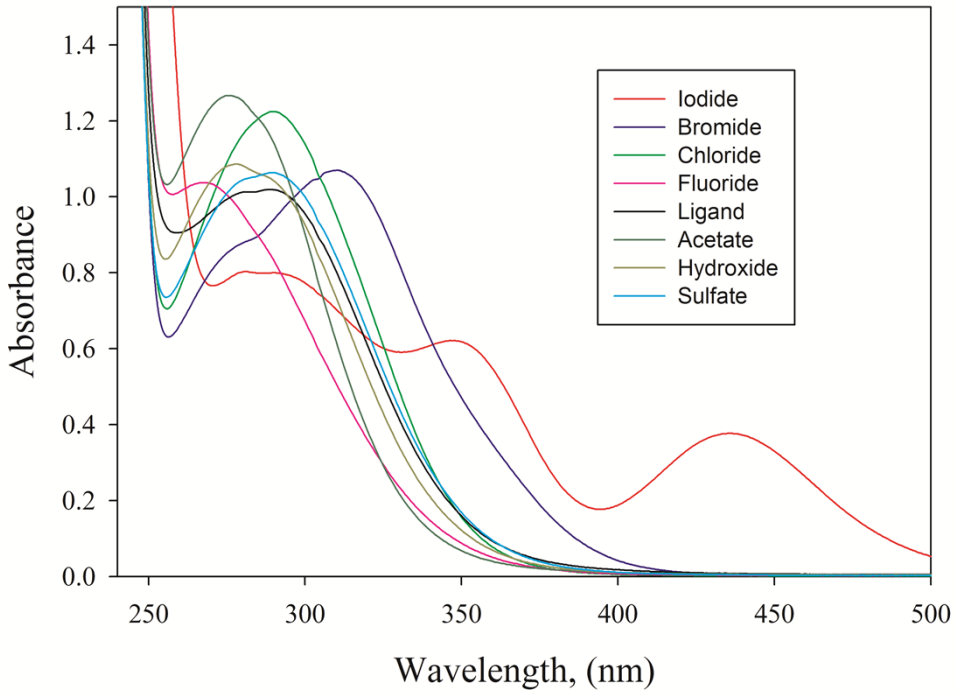

Fig. S9. Changes in absorbance of **1** (1 x 10^{-4} M) in the presence of one equivalent of different anions in CH_3CN at room temperature.

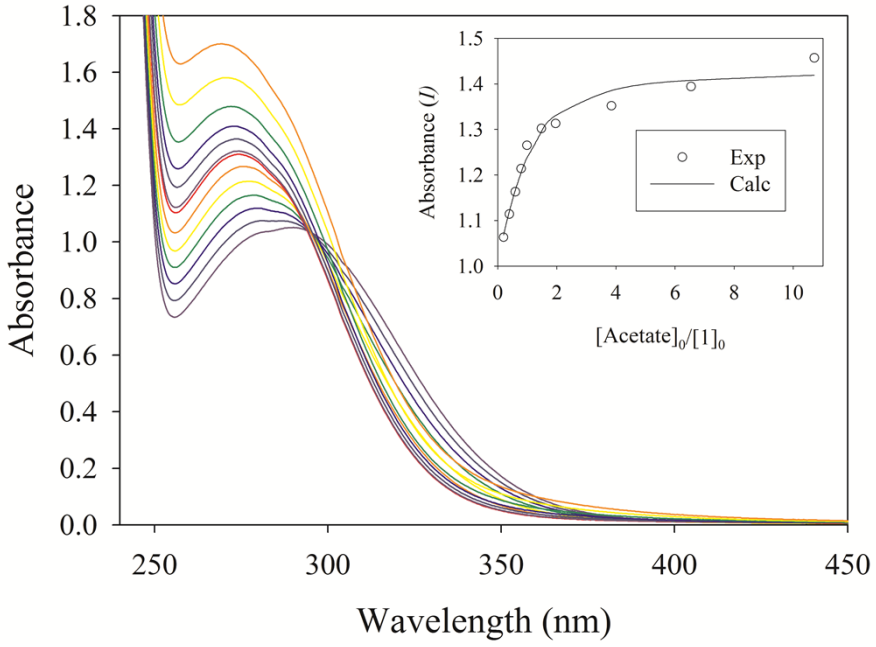

Fig. S10. Changes in absorption spectra of 1 (1 x 10^{-4} M) with an increasing amount of acetate in CH_3CN. The titration curve is shown in insets.

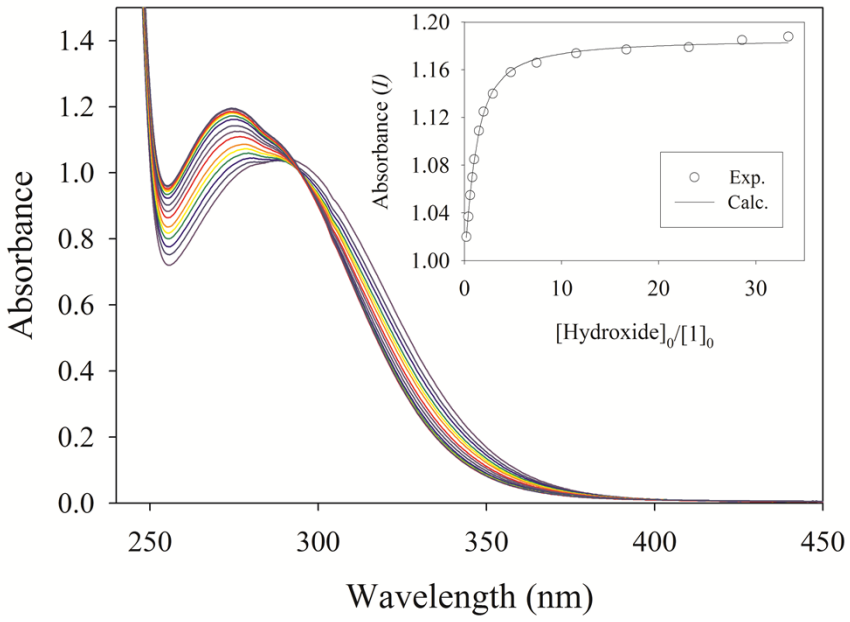

Fig. S11. Changes in absorption spectra of 1 (1 x 10^{-4} M) with an increasing amount of hydroxide in CH_3CN. The titration curve is shown in insets.

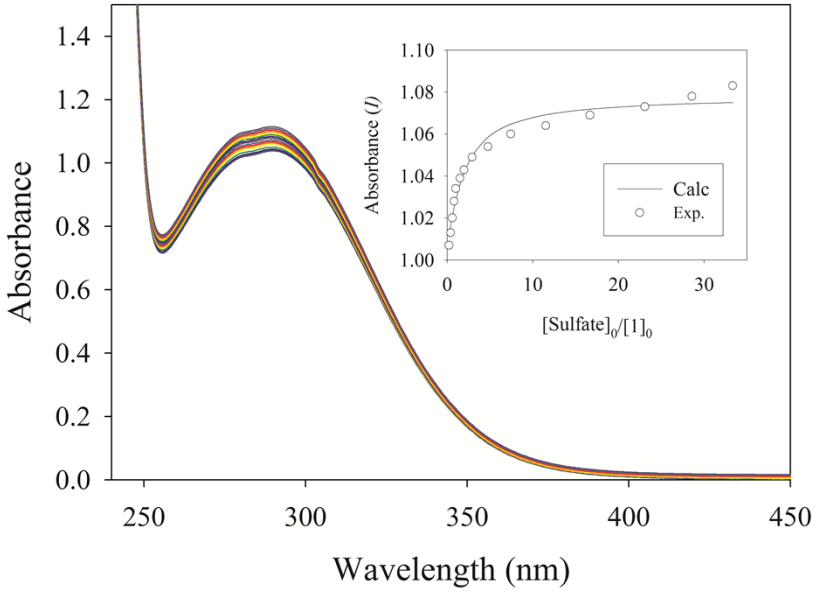

Fig. S12. Changes in absorption spectra of 1 (1 x 10^{-4} M) with an increasing amount of sulfate in CH_3CN. The titration curve is shown in insets.

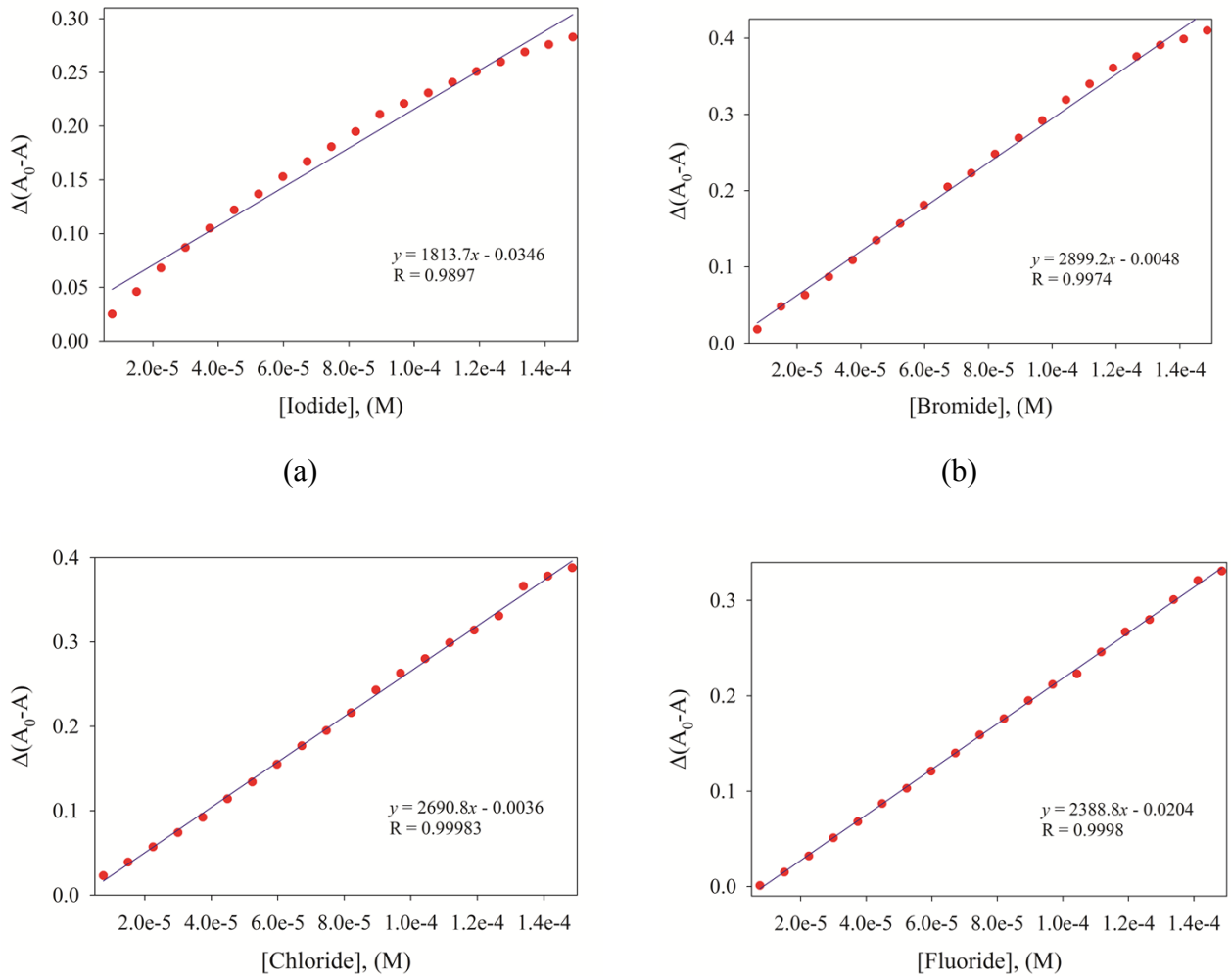

Fig. S13. Calibration plots using differences in absorbance against halide concentrations: iodide (a), bromide (b), chloride (c) and fluoride (d) in CH_3CN.

Table S1: Measurement of detection limit of the **1** for halides using UV-vis spectroscopy in 100% acetonitrile.

Vol. of **1** (μL)	Anion added (μL)	Total vol. (μL)	[**1**] M	[Anion] M	[Anion]/[**1**]	$\Delta(A_0\text{-}A)$			
						Br^-	Cl^-	F^-	I^-
2000	1	2001	1.50e-4	7.4963e-6	0.0500	0.0180	0.0230	0.0010	0.0250
2000	2	2002	1.50e-4	1.4985e-5	0.0999	0.0480	0.0390	0.0150	0.0460
2000	3	2003	1.50e-4	2.2466e-5	0.1498	0.0630	0.0570	0.0320	0.0680
2000	4	2004	1.50e-4	2.9940e-5	0.1996	0.0870	0.0740	0.0510	0.0870
2000	5	2005	1.50e-4	3.7406e-5	0.2494	0.1090	0.0920	0.0680	0.1050
2000	6	2006	1.50e-4	4.4865e-5	0.2991	0.1350	0.1140	0.0870	0.1220
2000	7	2007	1.50e-4	5.2317e-5	0.3488	0.1570	0.1340	0.1030	0.1370
2000	8	2008	1.50e-4	5.9761e-5	0.3984	0.1810	0.1550	0.1210	0.1530
2000	9	2009	1.50e-4	6.7198e-5	0.4480	0.2050	0.1770	0.1400	0.1670
2000	10	2010	1.50e-4	7.4627e-5	0.4975	0.2230	0.1950	0.1590	0.1810
2000	11	2011	1.50e-4	8.2049e-5	0.5470	0.2480	0.2160	0.1760	0.1950
2000	12	2012	1.50e-4	8.9463e-5	0.5964	0.2690	0.2430	0.1950	0.2110
2000	13	2013	1.50e-4	9.6870e-5	0.6458	0.2920	0.2630	0.2120	0.2210
2000	14	2014	1.50e-4	1.0427e-4	0.6951	0.3190	0.2800	0.2230	0.2310
2000	15	2015	1.50e-4	1.1166e-4	0.7444	0.3400	0.2990	0.2460	0.2410
2000	16	2016	1.50e-4	1.1905e-4	0.7937	0.3610	0.3140	0.2670	0.2510
2000	17	2017	1.50e-4	1.2643e-4	0.8428	0.3760	0.3310	0.2800	0.2600
2000	18	2018	1.50e-4	1.3380e-4	0.8920	0.3910	0.3660	0.3010	0.2690
2000	19	2019	1.50e-4	1.4116e-4	0.9411	0.3990	0.3780	0.3210	0.2760
2000	20	2020	1.50e-4	1.4851e-4	0.9901	0.4100	0.3880	0.3310	0.2830

Table S2: Limit of detection (LOD) was calculated using the linear regression of the calibration curve applying to the equation: $LOD=3\sigma/S$. Where, σ is the standard deviation of the absorbance and S is the slope of the calibration curve.

Anion	LOD, (M)
Fluoride	$3.01\text{x}10^{-6}$
Chloride	$5.24\text{x}10^{-6}$
Bromide	$9.72\text{x}10^{-6}$
Iodide	$15.6\text{x}10^{-6}$

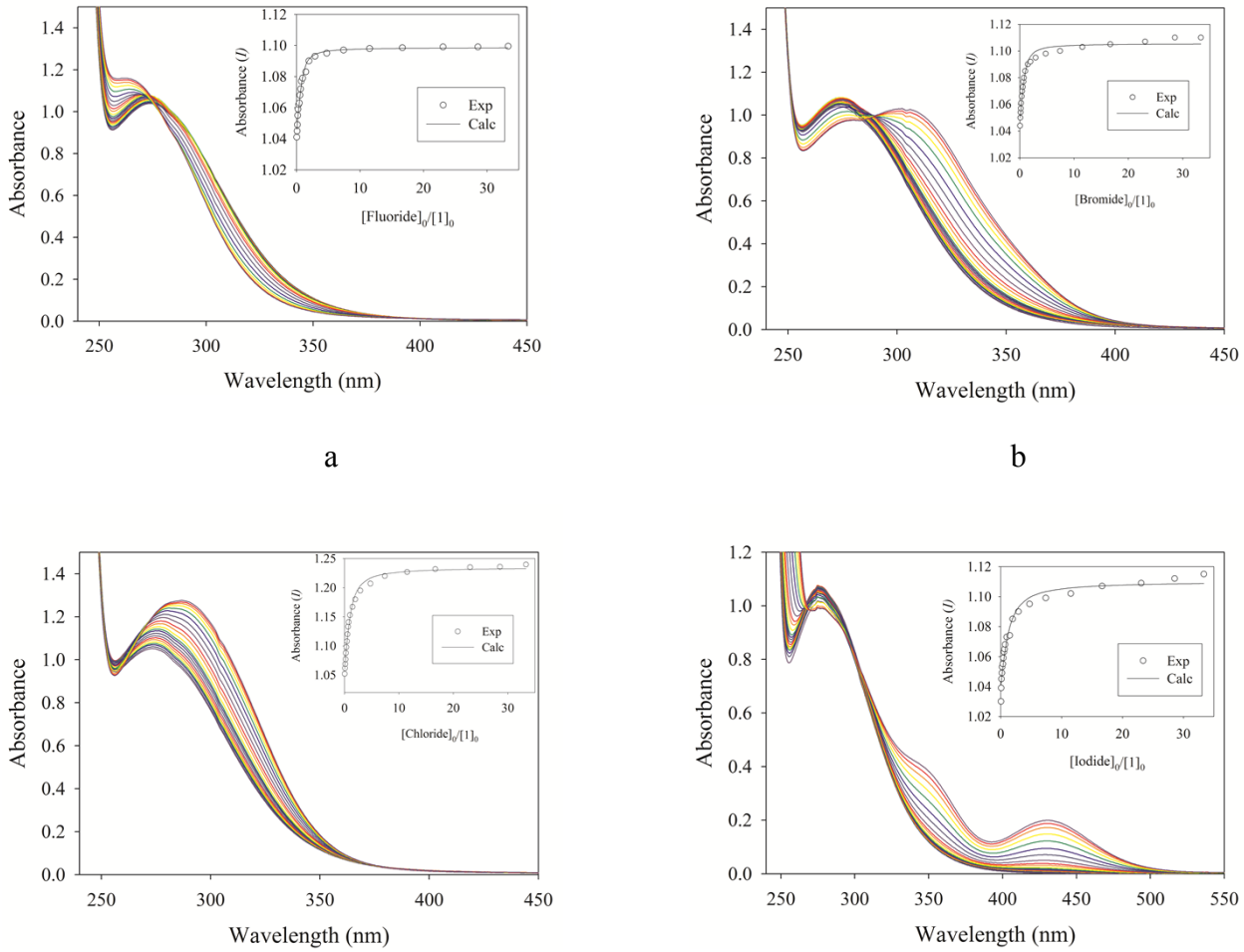

Fig. S14. Changes in absorption spectra of **1** (1 x 10^{-4} M) with an increasing amount of fluoride (a), bromide (b), chloride (c) and iodide (d) in 20% water in CH_3CN. The titration curves are shown in insets.

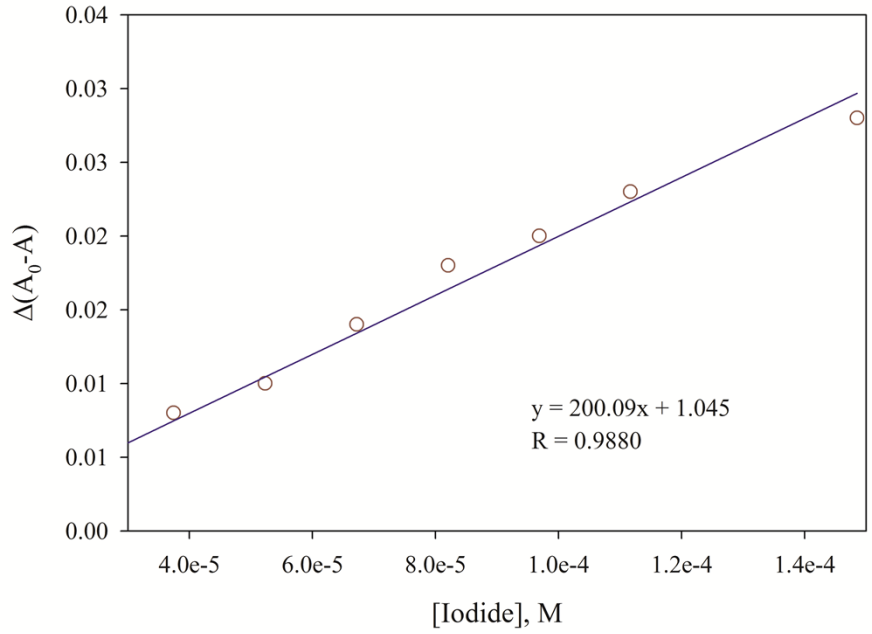

Fig. S15. Calibration plot using difference in absorbance against iodide concentration in 20% water in CH_3CN. Limit of detection for iodide (20% water in Acetonitrile) = 2.09×10^{-5} M

Table S3: Measurement of detection limit of **1** for iodide using UV-vis spectroscopy in 20% water in acetonitrile.

Vol. of **1** (μL)	Anion added (μL)	Total vol. (μL)	[**1**] M	[Iodide] (M)	[Iodide]/[**1**]	$\Delta(A_0-A)$
2000	4	2004	1.50e-4	2.9940e-5	0.1996	0.0040
2000	5	2005	1.50e-4	3.7406e-5	0.2494	0.0080
2000	7	2007	1.50e-4	5.2317e-5	0.3488	0.0100
2000	9	2009	1.50e-4	6.7198e-5	0.4480	0.0140
2000	11	2011	1.50e-4	8.2049e-5	0.5470	0.0180
2000	13	2013	1.50e-4	9.6870e-5	0.6458	0.0200
2000	15	2015	1.50e-4	1.1166e-4	0.7444	0.0230
2000	20	2020	1.50e-4	1.4851e-4	0.9901	0.0280

Table S4. Lowest ten excited states (eV) and oscillator strengths of all complexes

	Fluoride		**Chloride**		**Bromide**		**Iodide**	
State	E_{abs}/eV	Osc. strength	E_{abs}/eV	Osc. strength	E_{abs}/eV	Osc. strength	E_{abs}/eV	Osc. strength
1	1.4758	0.0030	1.2969	0.0028	1.2512	0.0026	1.2087	0.0023
2	1.4885	0.0031	1.3006	0.0028	1.2536	0.0025	1.2097	0.0023
3	1.9828	0.0001	1.9155	0.0000	1.8621	0.0000	1.8110	0.0000
4	1.9860	0.0001	1.9171	0.0000	1.8638	0.0000	1.8114	0.0000
5	3.4387	0.0000	3.4344	0.0000	3.3370	0.0006	2.7825	0.0003
6	3.4443	0.0000	3.4393	0.0000	3.3379	0.0006	2.7828	0.0003