Colorimetric and Fluorometric Turn-on Sensor for Selective Detection of Fluoride Ion: Sol-Gel Transition Studies and Theoretical Insights

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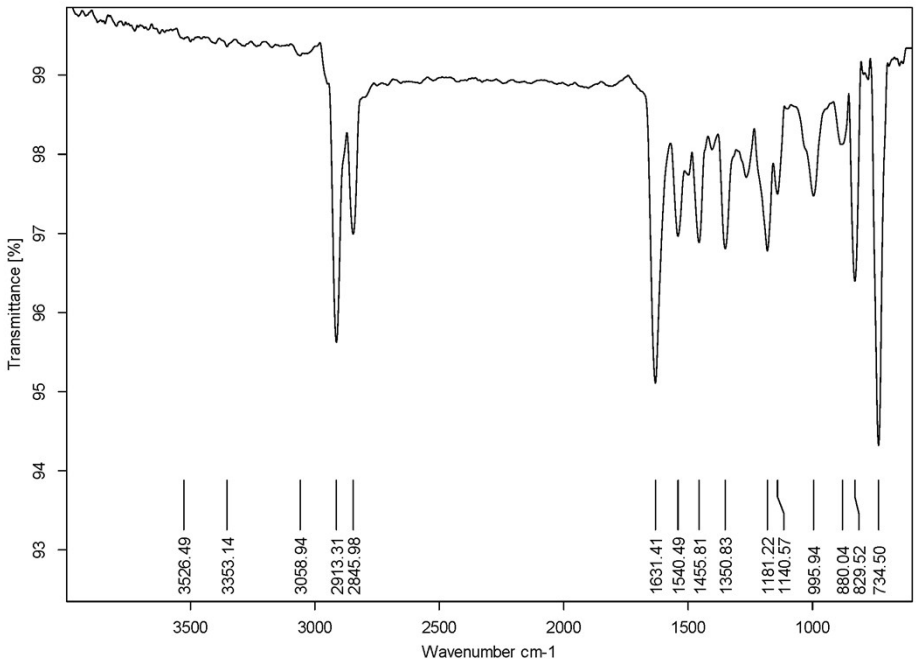

Fig. S1 FT-IR spectrum of receptor **R1**

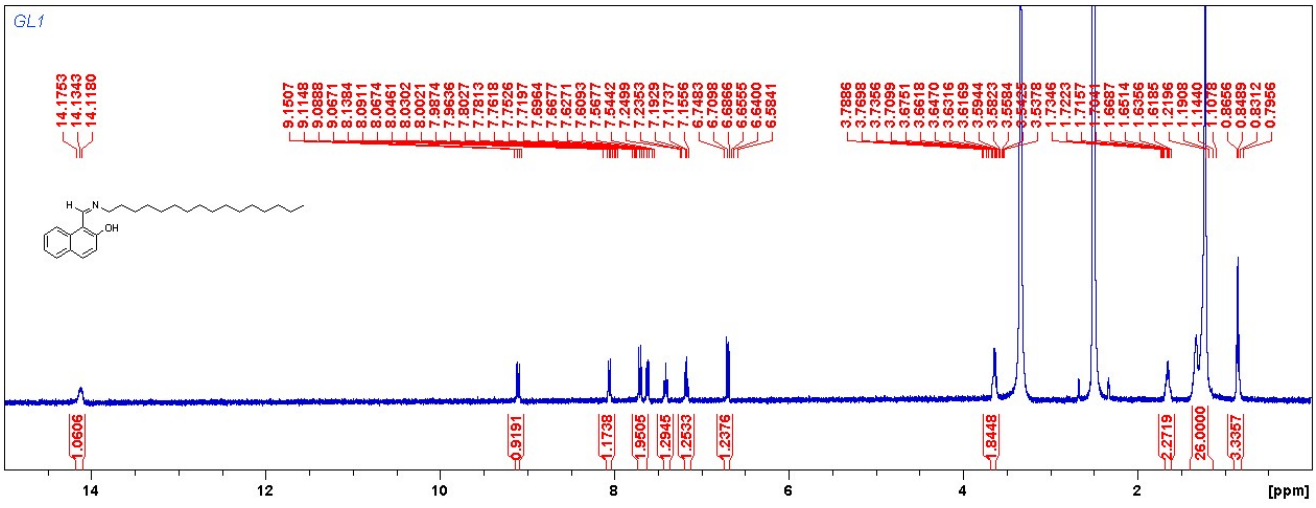

Fig. S2 ^{1}H-NMR spectrum of receptor **R1**

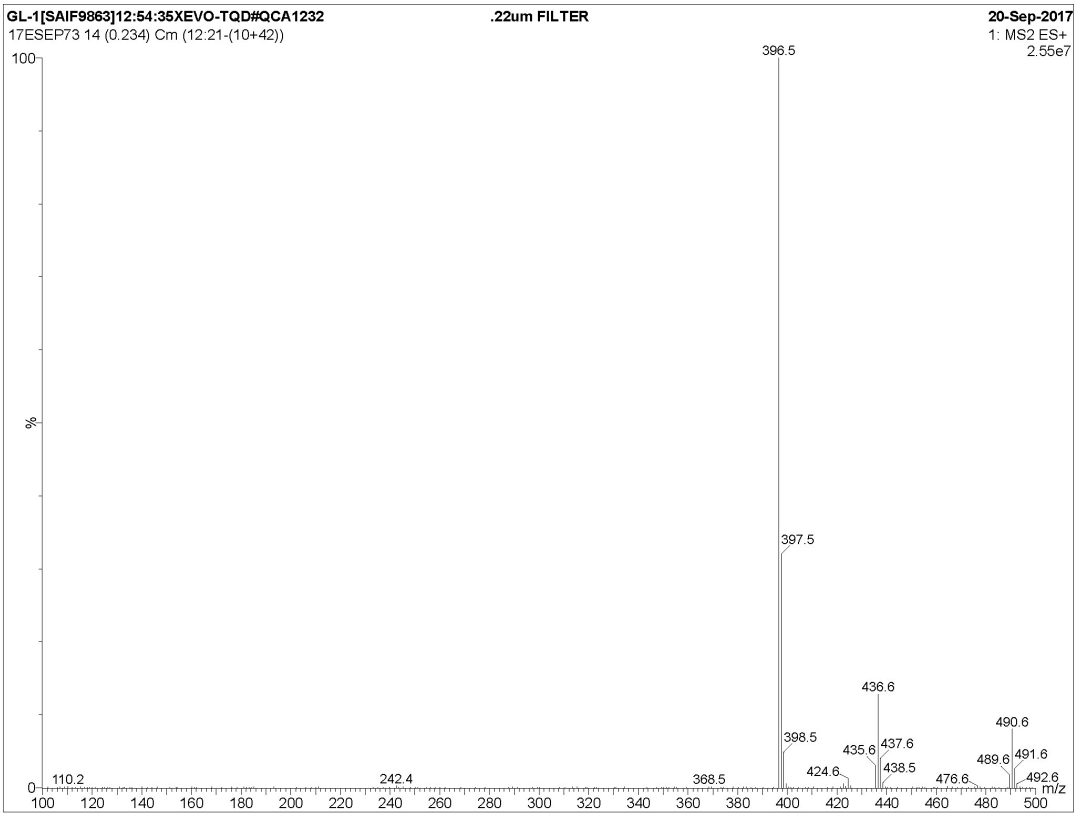

Fig. S3 ESI-MS spectrum of receptor **R1**

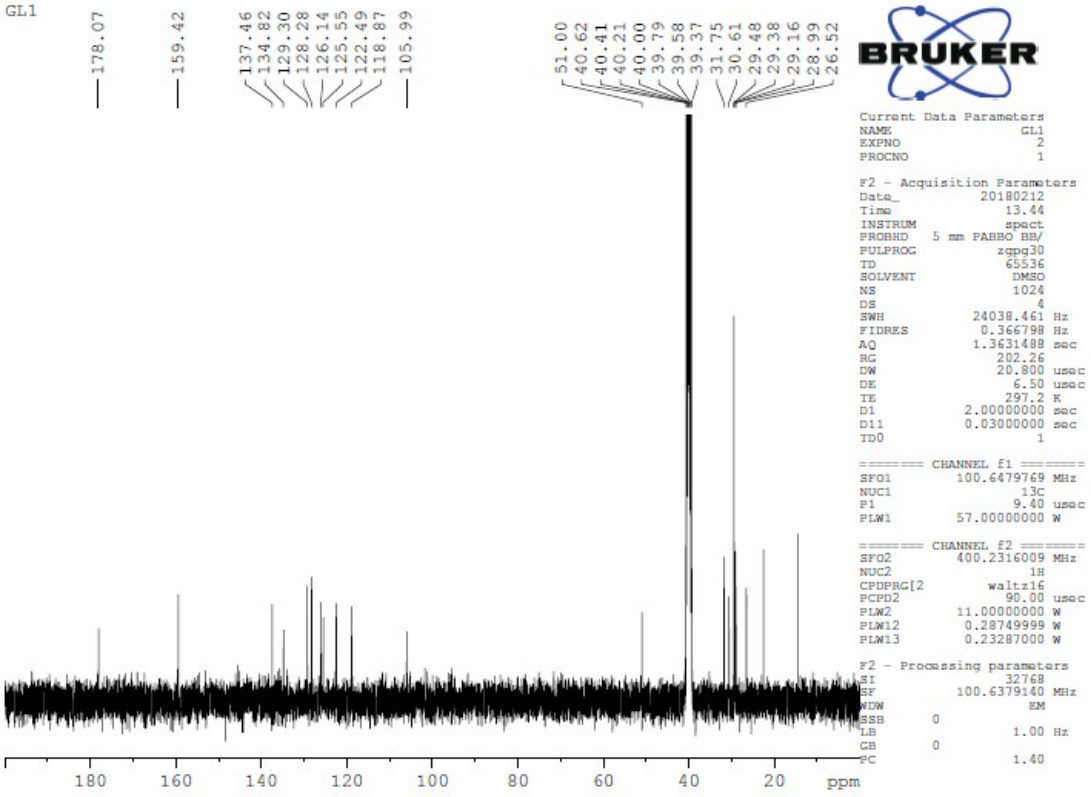

Fig. S4 ^{13}C NMR spectrum of receptor **R1**

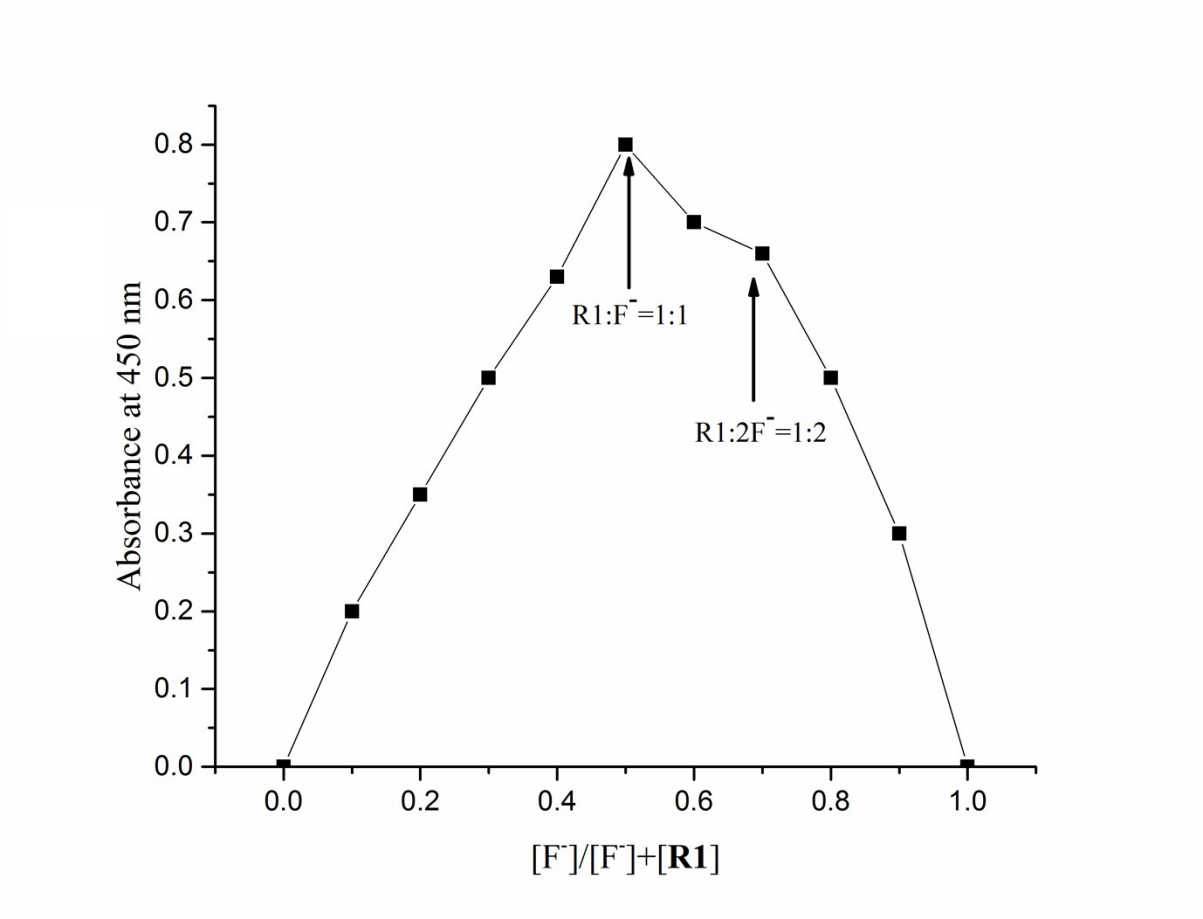

Fig. S5 Job's plot for **R1**-TBAF complex

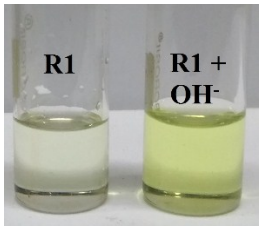

Fig. S6 Color change of **R1** with the addition of 2 equiv. of TBAOH

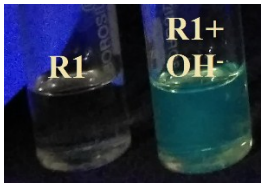

Fig. S7 Fluorometric response of **R1** with the addition of 2 equiv. of TBAOH

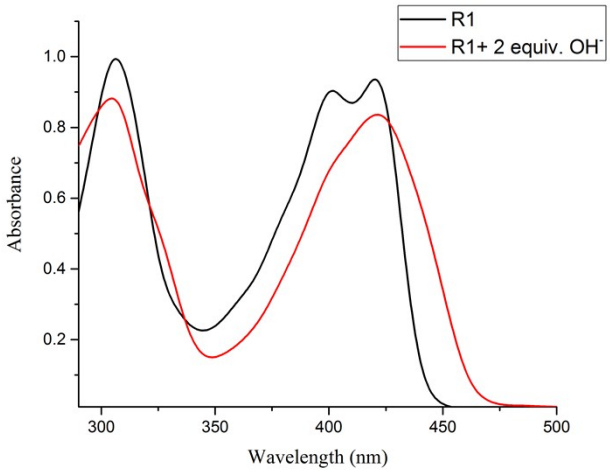

Fig. S8 UV-Vis spectra of **R1** with the addition of 2 equiv. of TBAOH

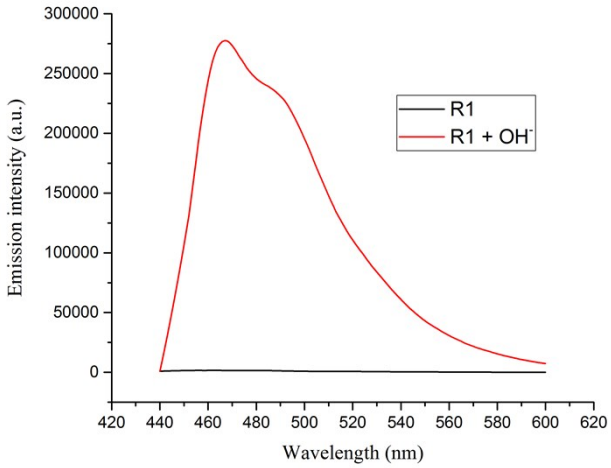

Fig. S9 PL spectra of **R1** with the addition of 2 equiv. of TBAOH

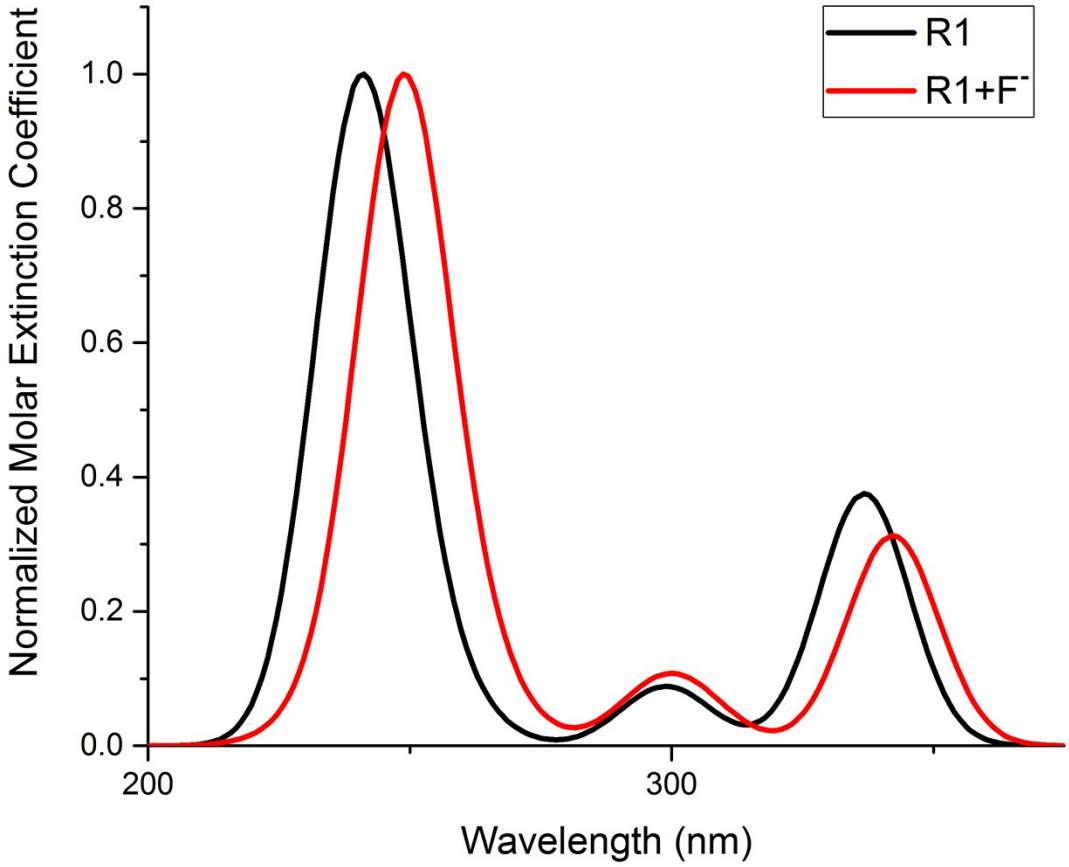

Fig. S10 DFT derived UV-Vis spectra of the **R1** and **R1**+ F^- complex

Table S1 Gelation properties of **R1**

Solvent	**State**
DMSO	G (26 mg/mL)
DMF	G (26 mg/mL)
Cyclohexane	S
Chloroform	S
Methanol	S
Acetonitrile	G (26 mg/mL)
n-Hexane	S
Diethyl ether	S
DCM	S
THF	S
DMF : H_2O (1:2 , v/v)	I
DMSO: H_2O (1:2 , v/v)	I
Propyl alcohol	S
Ethanol	S
Dioxane	S
S = solution; G = gel (minimum gelatination concentration); I = insoluble	

Calculation of binding constant from UV-Vis studies:

Binding constant has been calculated using Benesi-Hildebrand equation[1] as given below;

$$\mathbf{1/(A-A_o) = 1/(A_{max} - A_o) + 1/K\,[X^-]^n\,(A_{max} - A_o)}$$

where, A_0, A, A_{max} are the absorption considered in the absence of anion, at an intermediate, and at a concentration of saturation. K is binding constant, $[X^-]$ is concentration of anion and *n* is the stoichiometric ratio.

Calculation of Detection limit:

The limit of detection was found using this equation**.**[2]

$DL = C_L \times C_T$

C_L = Conc. of receptor; C_T = Conc. of Titrant at which change was observed.

References:

1. H. Benesi and H. Hildebrand, J. Am. Chem. Soc., 1948, 71, 2703–2707.
2. V. Bhalla, A. Gupta, M. Kumar., Chem. Commun., 2012, 48, 11862.