

Supplementary Information

Ratiometric Colorimetric Detection of Fluoride Ions using Schiff Base Sensor: Enhancing Selectivity and Sensitivity for Naked-Eye Analysis

Anusha A. Mahishi^{a§}, Sachin M. Shet^{b§}, Padmaja V Mane^a, Jingxian Yu^{c,d}, A. V. E. Sowrirraajan^e, Madhuprasad Kigga^{a*}, Mahesh P. Bhat^{f*}, Kyeong-Hwan Lee^{f,g,h,*}, Mahaveer D. Kurkuri^{a,*}

^a Centre for Research in Functional Materials (CRFM), JAIN (Deemed-to-be University), Jain Global Campus, Bengaluru 562112, India

^b Centre for Nano and Material Sciences, JAIN (Deemed-to-be University), Jain Global Campus, Bengaluru 562112, India

^c Guangxi Key Laboratory of Electrochemical and Magneto-chemical Functional Materials, College of Chemistry and Bioengineering, Guilin University of Technology, Guilin 541004, PR China

^d Department of Chemistry, School of Chemistry, Physics and Earth Sciences, The University of Adelaide, Adelaide, SA 5005, Australia

^e Fire and Combustion Research Center, Jain Deemed to be University, Kanakapura Road, Bangalore, India

^f Agricultural Automation Research Centre, Chonnam National University, Gwangju 61186, South Korea.

^g Department of Convergence Biosystems Engineering, Chonnam National University, Gwangju 61186, Republic of Korea.

^h BK21 Interdisciplinary Program in IT-Bio Convergence System, Chonnam National University, Gwangju 61186, Republic of Korea

*Corresponding author E-mail address: maheshbhat1306@gmail.com; khlee@jnu.ac.kr; madhuprasadab@gmail.com; mahaveer.kurkuri@jainuniversity.ac.in

§ Anusha A. Mahishi and Sachin M. Shet contributed equally

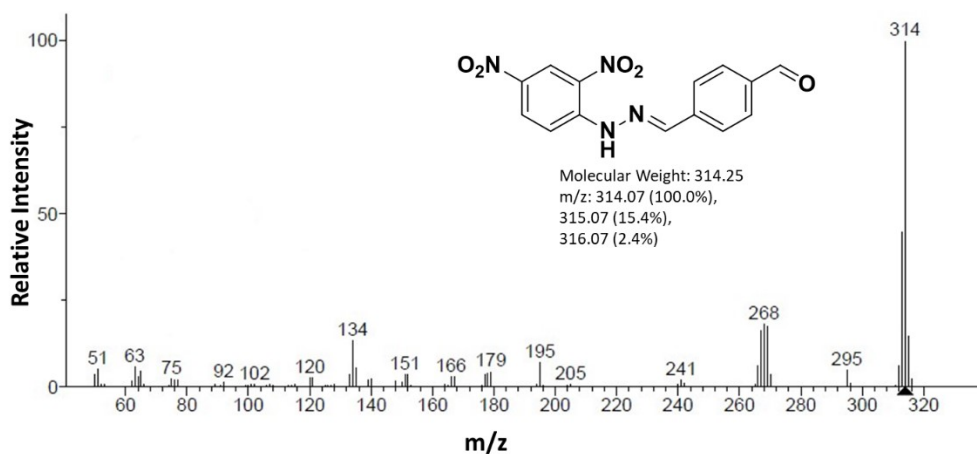


Fig. S1: GCMS spectrum of the receptor.

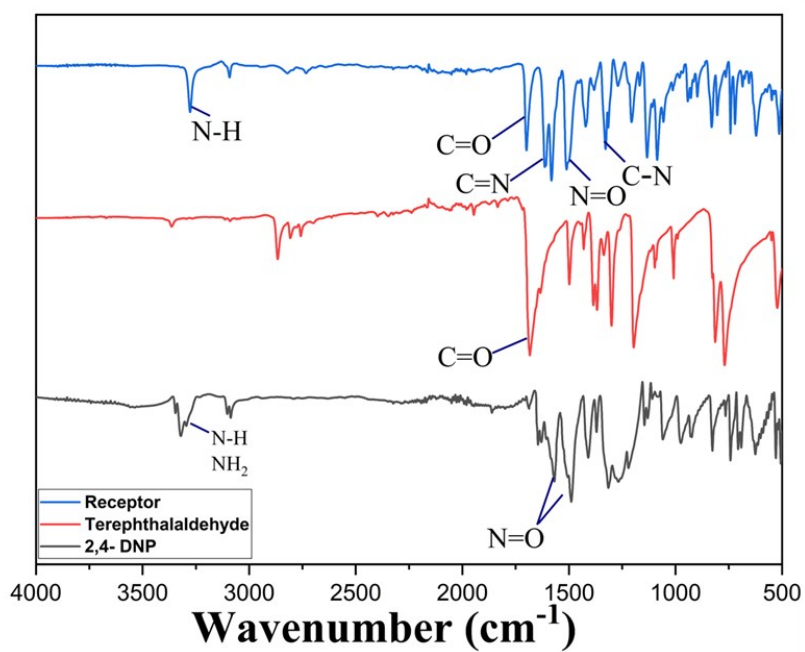


Fig. S2: FTIR spectra of 2,4-Dinitrophenylhydrazine, terephthalaldehyde, and receptor.

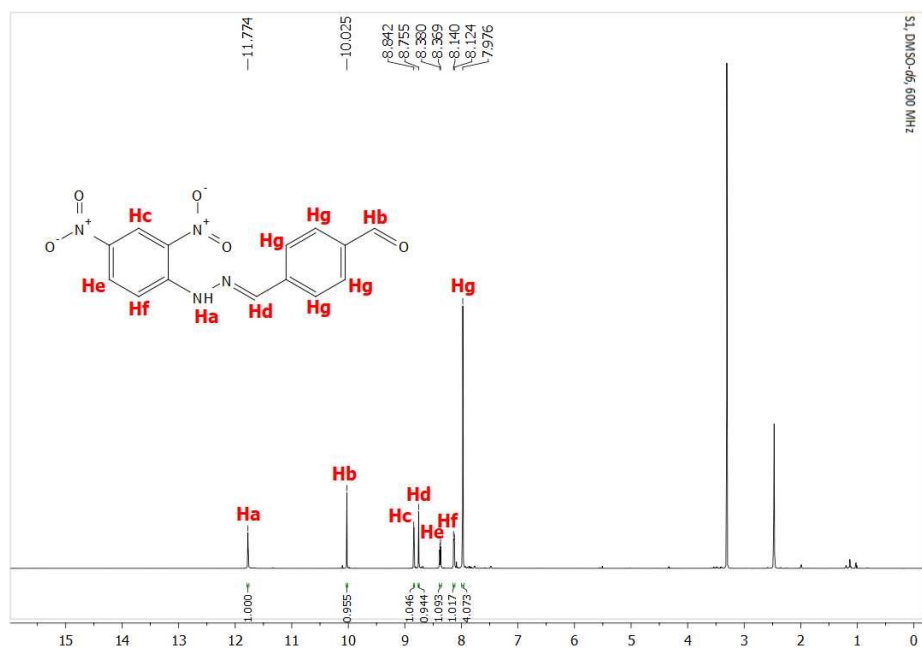


Fig. S3: ^1H NMR spectrum of the receptor.

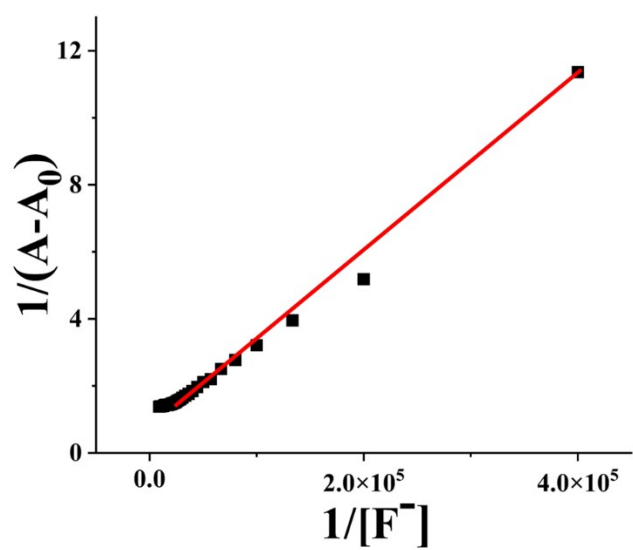


Fig. S4: Benesi–Hildebrand plot for receptor binding with F^- ions associated with absorbance change at 543 nm.

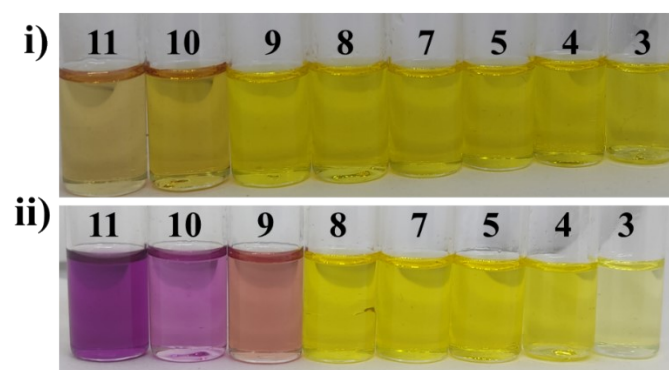


Fig. S5: pH studies for receptor from pH 3-11 (i) Visual color change observed for the receptor in mentioned pH, (ii) Visual color change observed for receptor + F^- in mentioned pH.

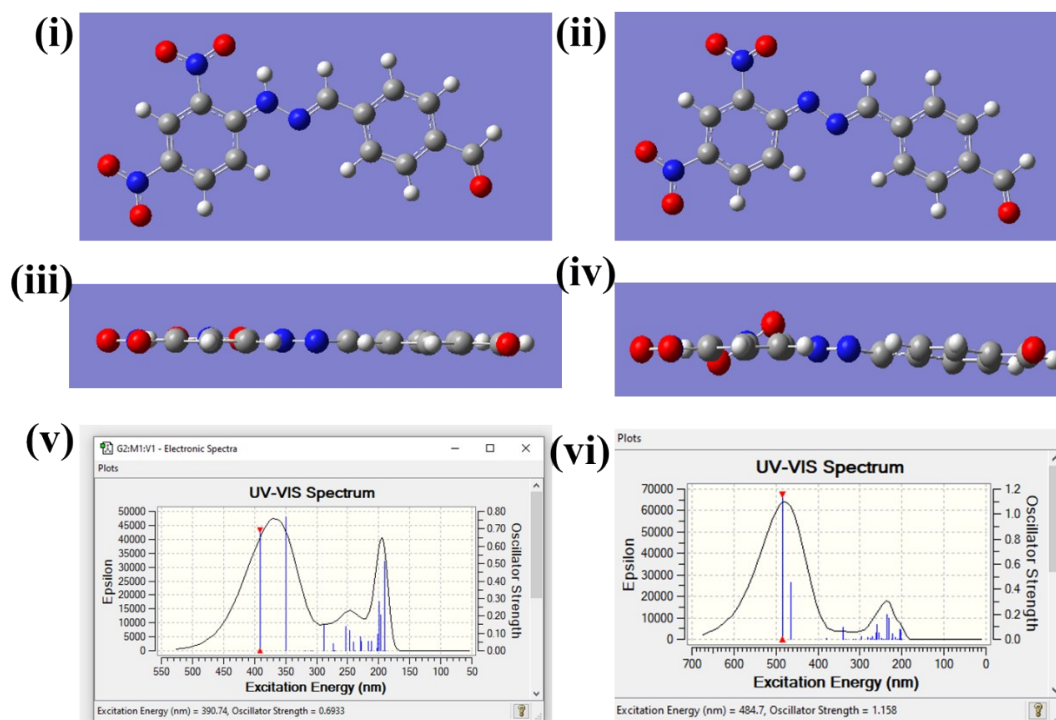


Fig. S6: Computational evidence, (i) 3D- front view of the receptor, (ii) 3D- front view of the deprotonated receptor, (iii) 3D- side view of the receptor, (iv) 3D- side view of the deprotonated receptor (v) Theoretically calculated UV-vis spectrum of the receptor, (vi) Theoretically calculated UV-vis spectrum of the deprotonated receptor.

Table S1: RGB% values obtained from the smartphone app for the color change after the addition of different anions.

Different anions	RGB%		
	Red %	Green%	Blue%
Receptor	68	98	28
F ⁻	71	1	78
Cl ⁻	87	99	33
Br ⁻	87	98	29
I ⁻	87	99	31
HSO ₄ ⁻	86	99	33
H ₂ PO ₄ ⁻	86	96	40
AcO ⁻	79	16	61

Table S2: RGB% values obtained from the smartphone app for the color change after the addition of various concentrations of F⁻ in TBA salt form.

Different equiv. addition of F ⁻	RGB%		
	Red %	Green%	Blue%
0	99	94	30
0.1	96	72	46
0.2	94	44	54
0.3	90	27	64
0.4	86	4	74
0.5	83	0	84
0.6	79	0	95

0.7	78	0	94
0.8	72	0	95
0.9	69	0	96
1	65	0	95

Table S3: RGB% values obtained from the smartphone app for the color change after the addition of different samples of F^- .

Different samples of F^-	RGB%		
	Red %	Green%	Blue%
Receptor	68	98	28
Receptor + 1 ppm NaF	86	53	44
Receptor + mouthwash (100 times diluted)	62	2	60
Receptor + 10 ppm NaF	48	0	59
