Supporting Information

Drug Molecules Beyond Chemical Biology: Fluorescence and DFT-Based Investigation for Fluoride Ion Sensing and Traces Detection of Chloroform

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SI-1. Instruments and reagents

The fluorescence measurements of sensor **ECX** were executed by spectrofluorometer "Fluoromax-Plus-P-C" Horiba Scientific, USA while sensor **ECX** UV-*Vis.* absorption spectrum was recorded at UV-Vis. spectrophotometer. All chemicals and reagents including *N,N*-dimethylformamide (DMF), ethyl acetate (EtOAc), methanol (MeOH), tetrahydrofuran (THF), dimethyl sulfoxide(DMSO), dichloromethane (DCM), chloroform ($CHCl_3$), toluene and acetonitrile (ACN) were purchased from Daejung Chemicals & Metals (Korea), Alfa Aesar (UK), and Sigma Aldrich (USA), and utilized without purification.

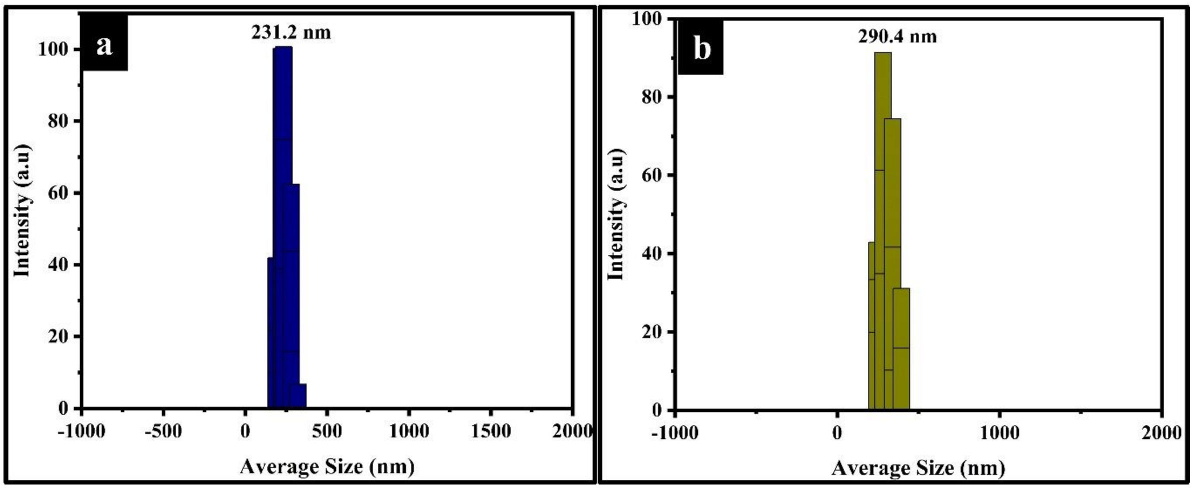

Figure S1: (a) DLS analysis of sensor **ECX** before addition of water and (b) after addition of water

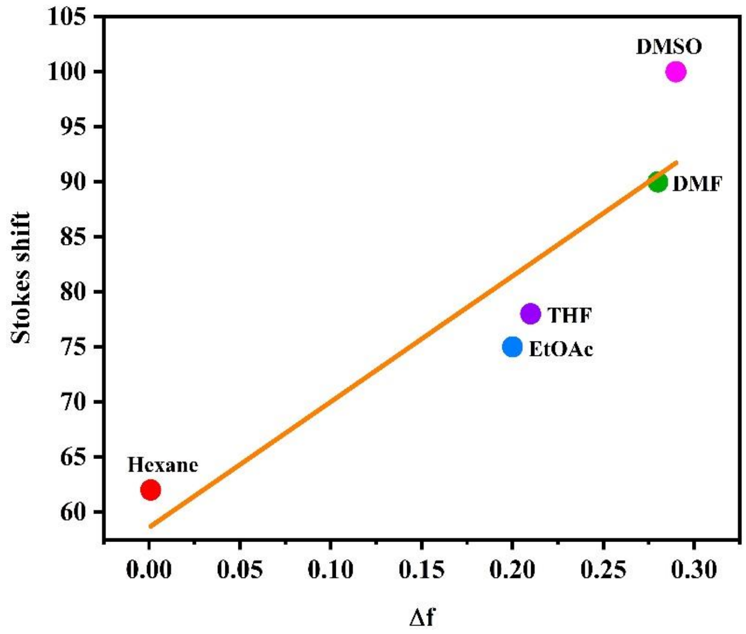

Figure S2: Lippert-Mataga plot of sensor **ECX** in different solvents

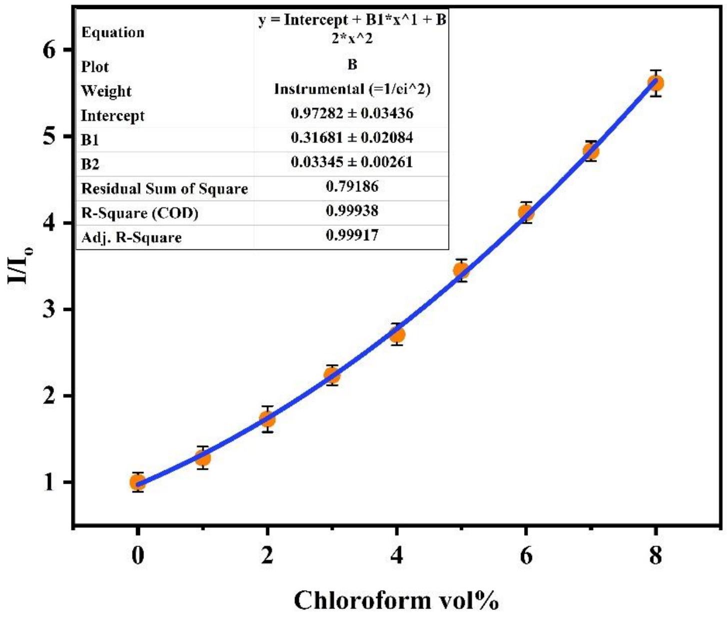

Figure S3: SV plot of **ECX** for increasing volume percentage of chloroform

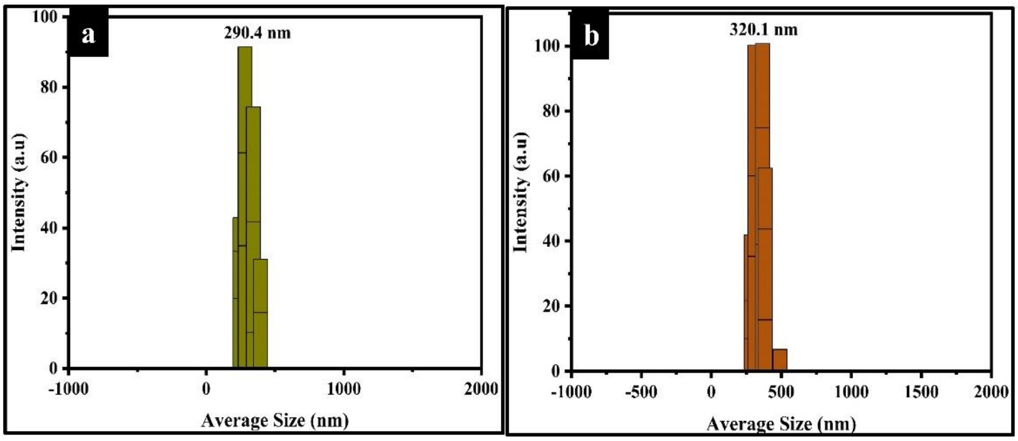

Figure S4: (a) DLS analysis of sensor **ECX** before addition and (b) after addition of F^-

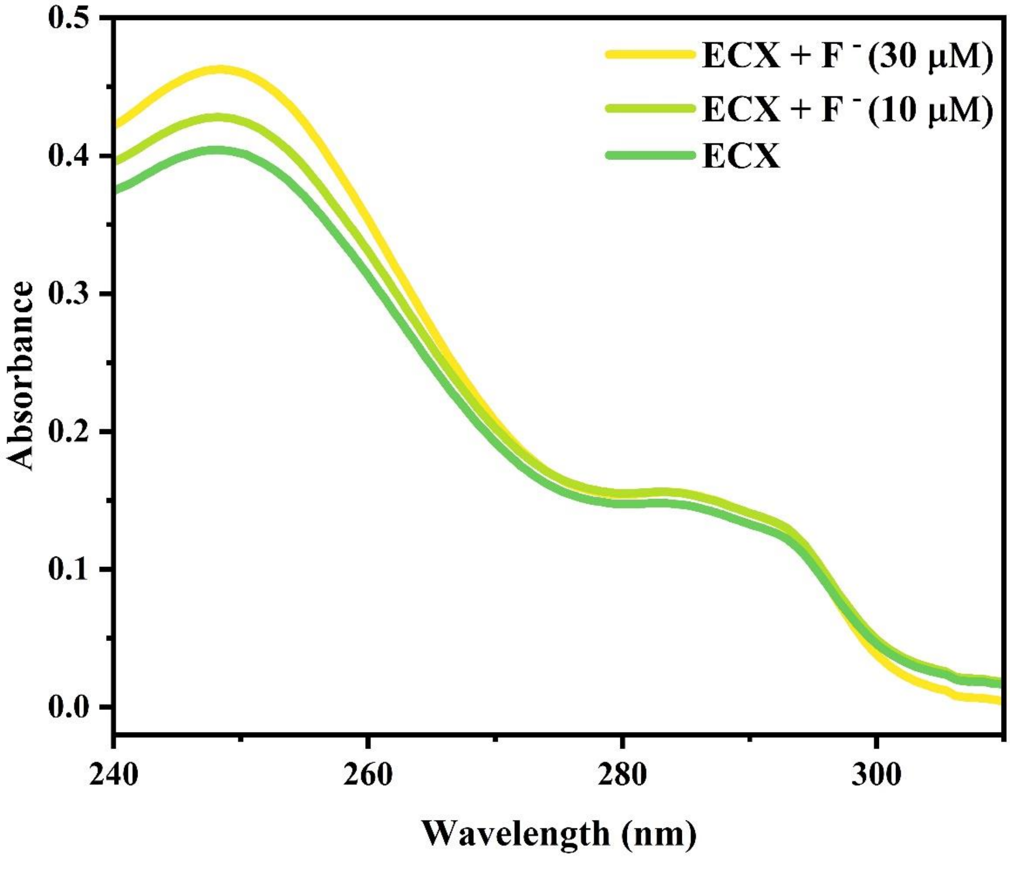

Figure S5: UV-*Vis.* absorbance spectrum of **ECX**-F^- complex

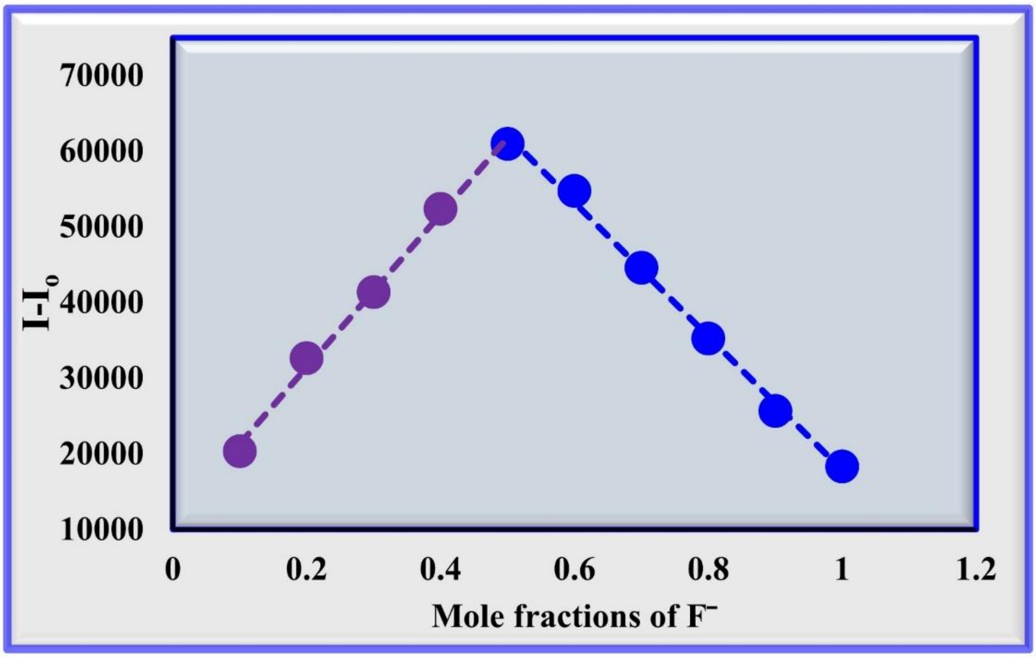

Figure S6: Job's plot of sensor **ECX**-F^- complex in DMF:water (1:4, v/v)

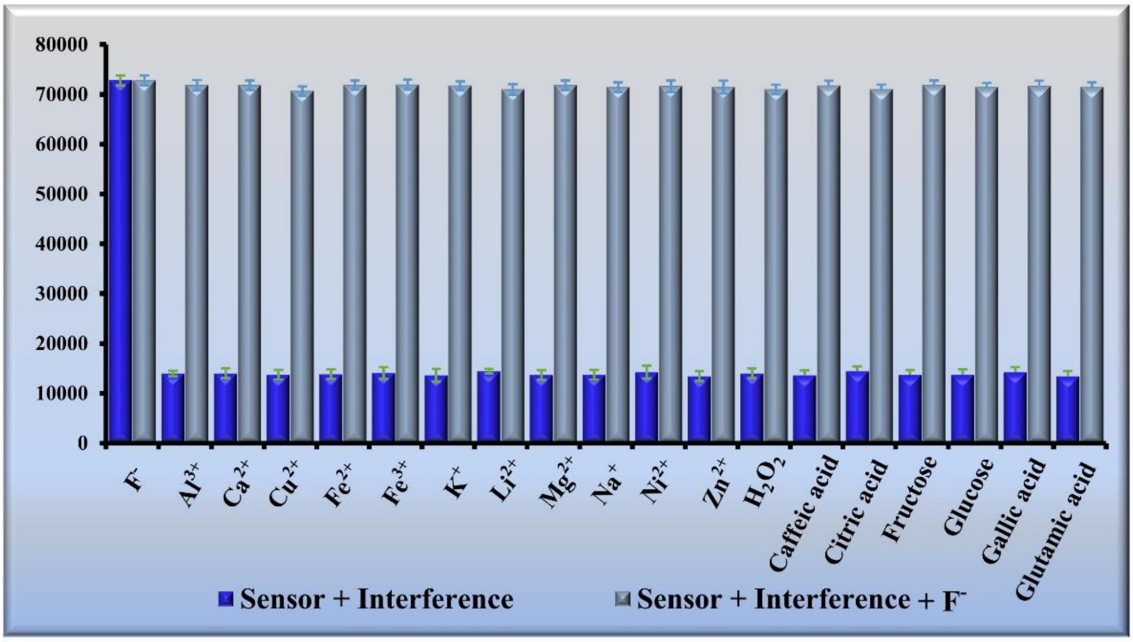

Figure S7: The emission response of sensor **ECX** towards F^- before and after addition of 100 µM of common interferences, cations and single molecules

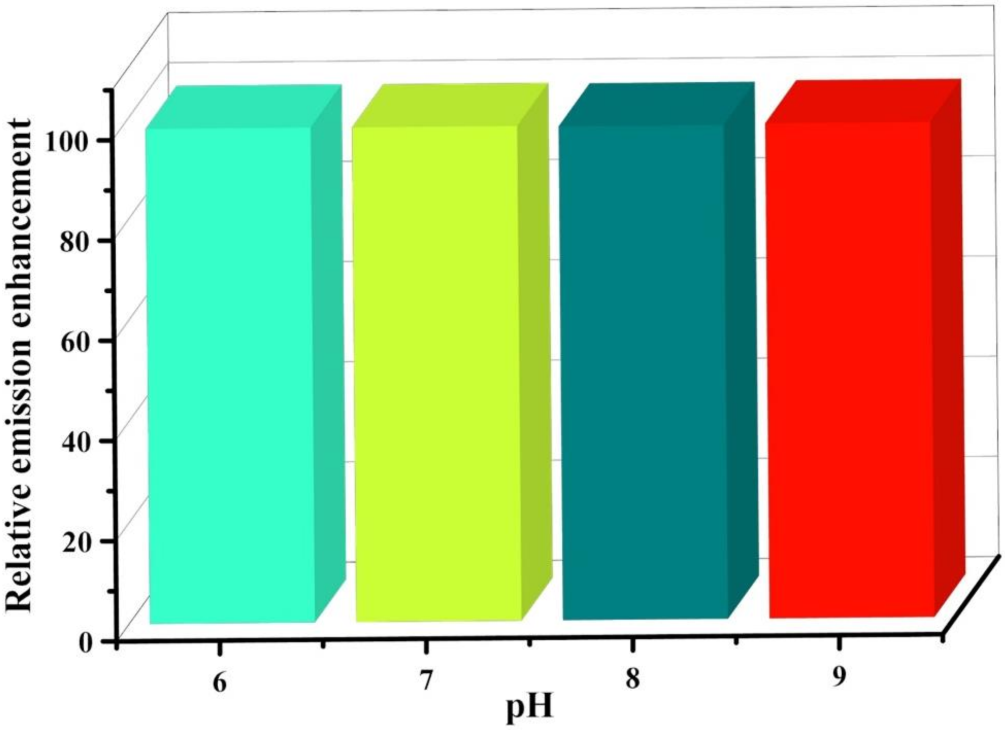

Figure S8: Effect of pH on the relative enhancement efficiency of sensor **ECX** towards F^-

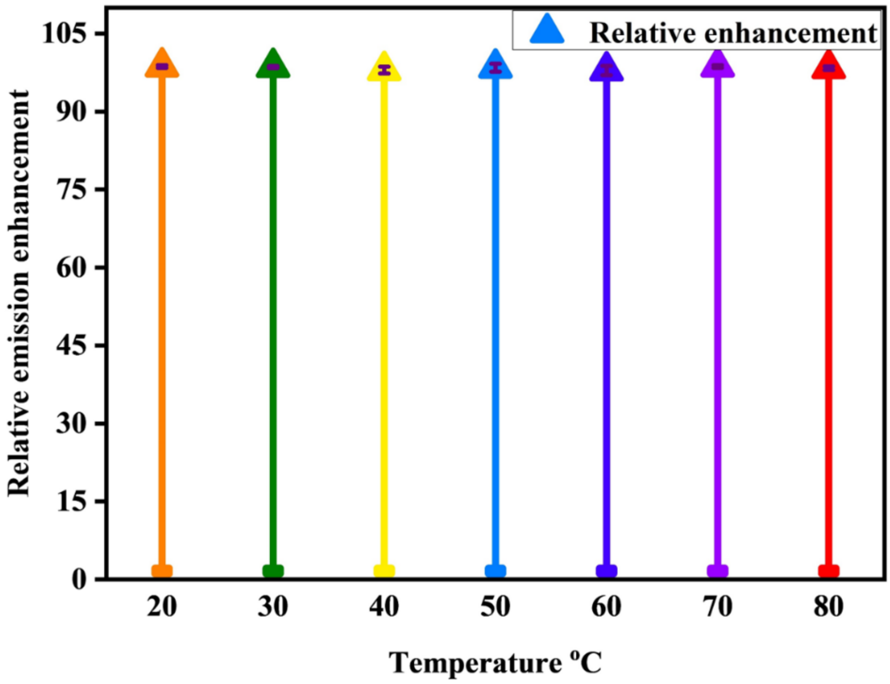

Figure S9: Effect of temperature on the relative enhancement efficiency of sensor **ECX** towards F^-

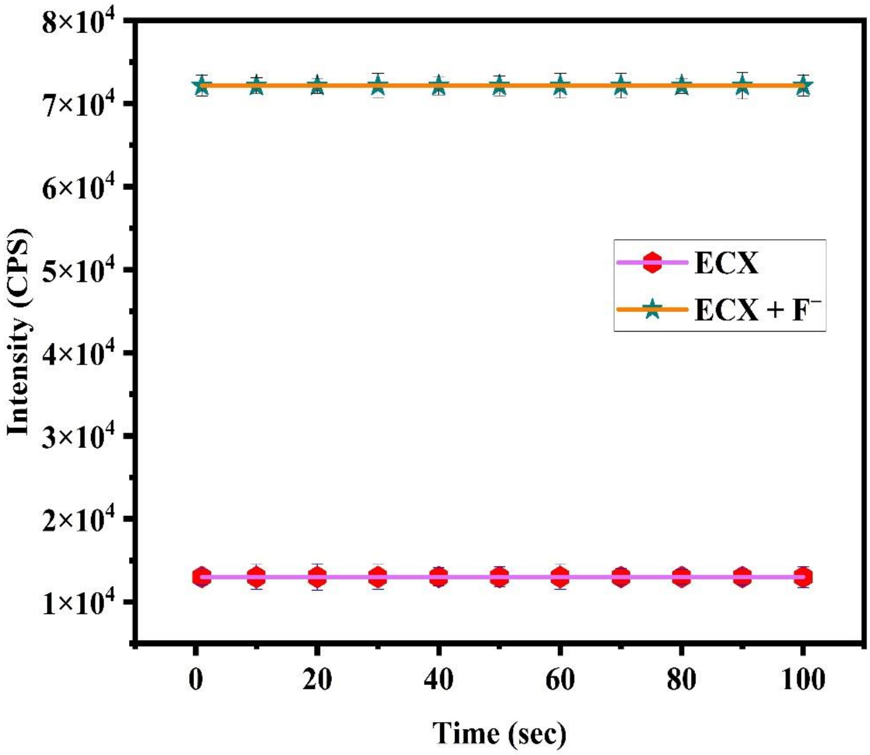

Figure S10: Photostability test of sensor **ECX** and **ECX**-F^- complex

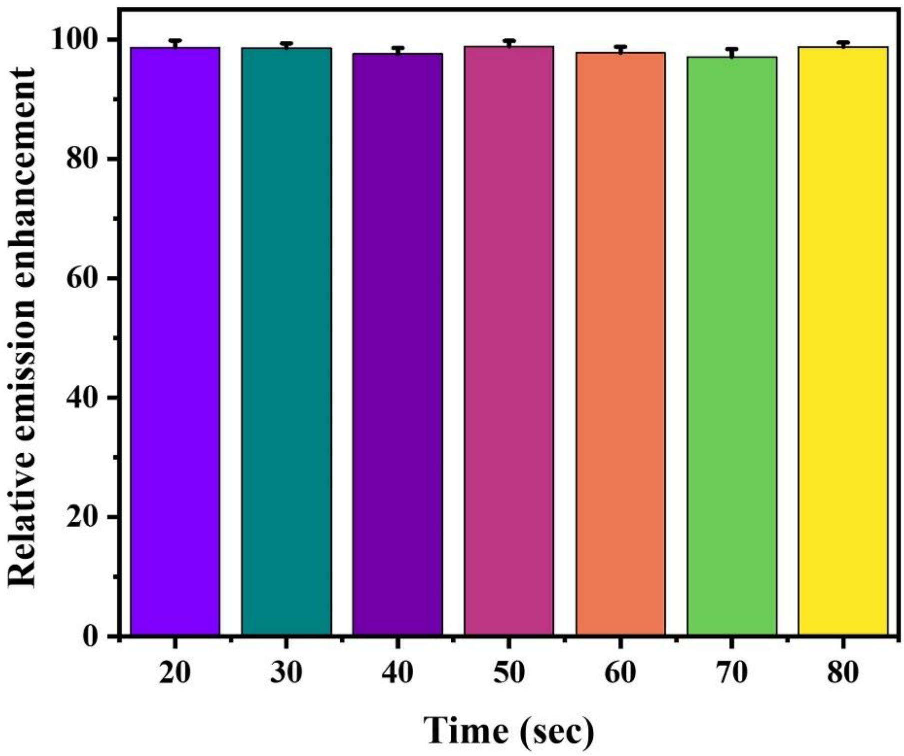

Figure S11: Effect of time on relative enhancement efficiency of sensor **ECX** towards F^-

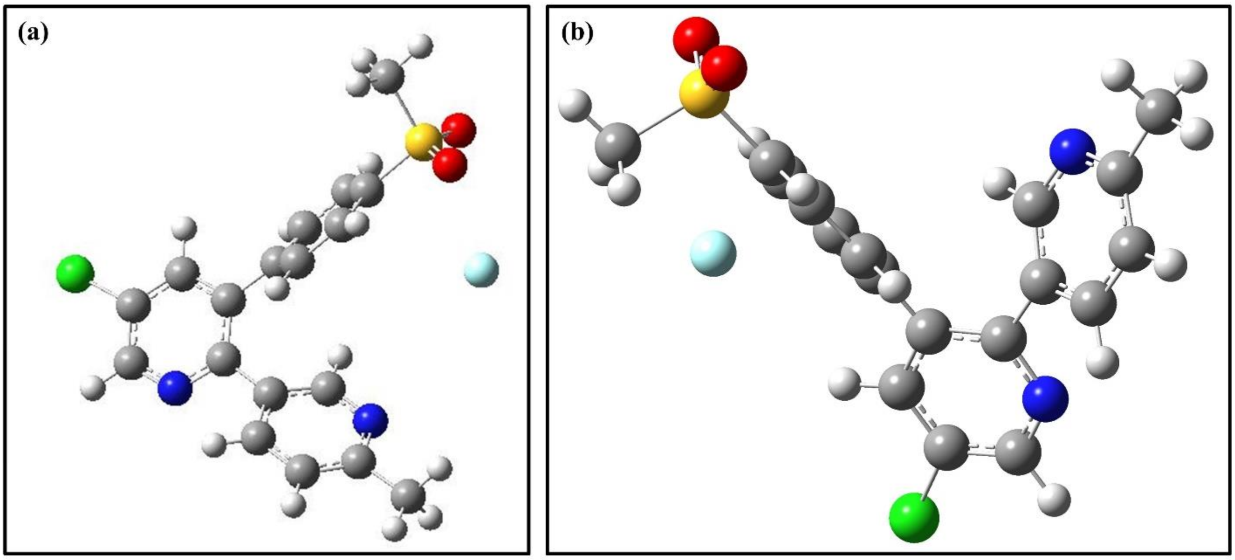

Figure S12: **ECX**-F⁻ complex interaction sites (a) I and (b) II

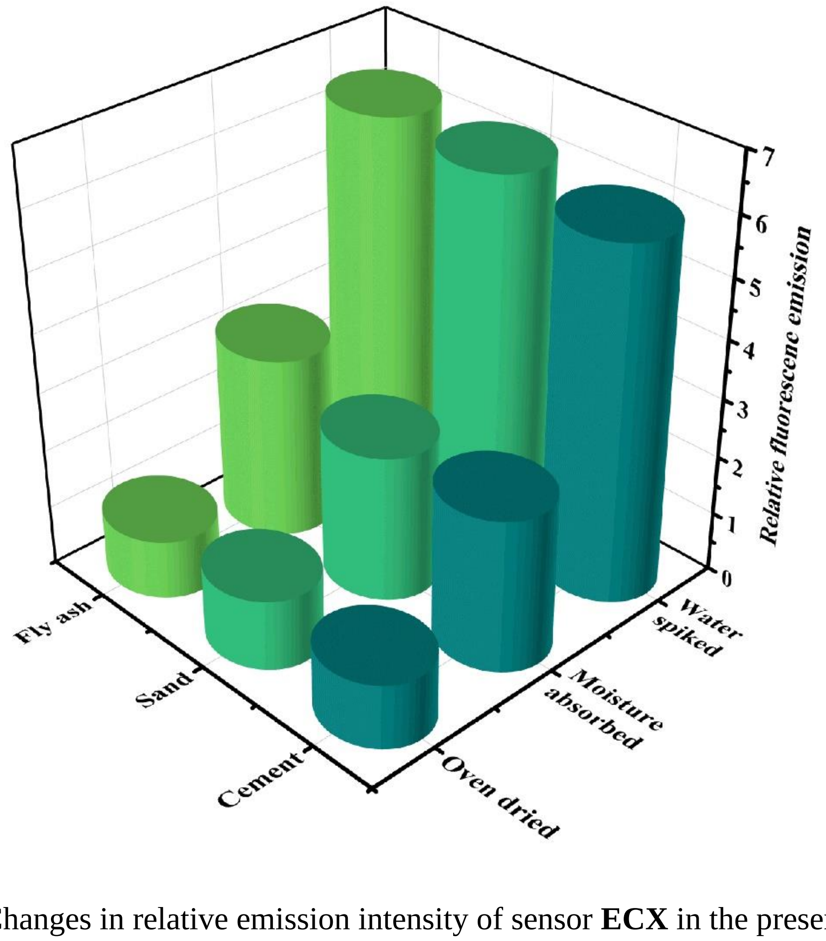

Figure S13: Changes in relative emission intensity of sensor **ECX** in the presence of various building materials

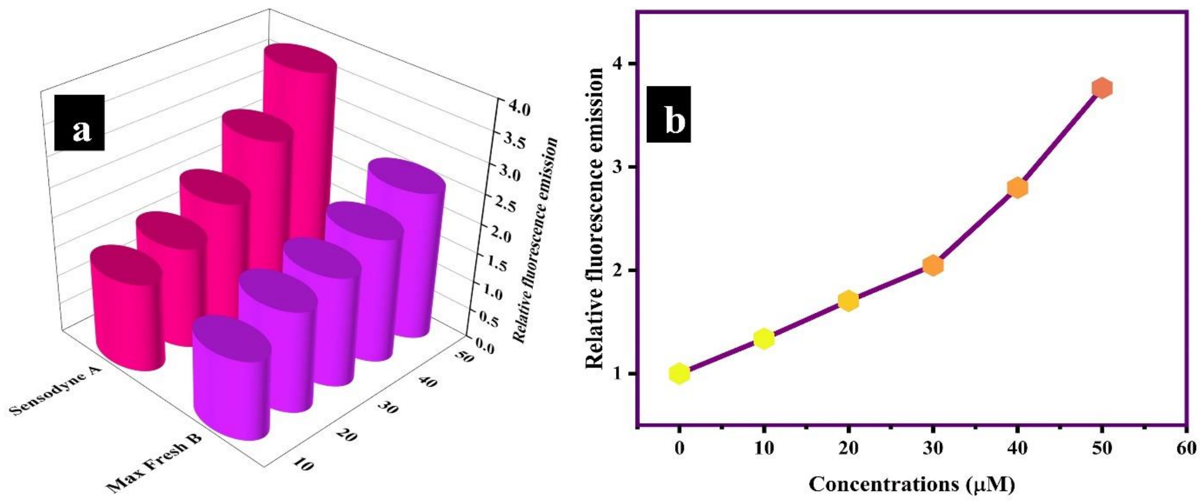

Figure S14: (a) Detection of F^- in toothpaste and (b) detection of F^- in water

Table 1 Comparison of probe **ECX** with previously reported sensors

S.No	Type of probes	Limit of Detection	References
1	Zr-based coordination polymer	1.55×10^{-6} mol L^{-1}	[1]
2	Quinoxaline-based chemosensor	3.1 µM	[2]
3	Thiosemicarbazone-based chemosensor	6.3×10^{-7} M	[3]
4	Loutonin-based probe	8.62×10^{-7} M	[4]
5	Tetraphenylethylene derived sensor	1.66×10^{-7} M	[5]
6	Protonated hemicryptophane capsule	570 nM	[6]
7	Biphenolic-dansyl derived sensor	18 µM	[7]
8	Fluorescent carbon dots (CDs)	49 µM	[8]
9	Curcumin coupled carbon dots	0.39 µM	[9]
10	**Etoricoxib**	**20 nM**	**This Study**

Table 2. Spike and recovery experiment for estimation of moisture in raw fly ash and sensing of fluoride in water by sensor **ECX**

Fly Ash			**Spiked Fluoride in Water**		
Spiked H_2O %	**Recovery (%)**	**RSD**	**Spiked (μM)**	**Recovery (%)**	**RSD**
0	00	00	0	00	00
2	97.2	1.62	10	99.5	1.54
4	96.9	1.80	20	99.3	1.43
6	97.5	1.36	30	98.8	1.78
8	97.1	1.23	40	99.2	1.34
10	96.9	1.36	50	99.1	1.48

References

1. L. Wang, X. Liu, Y. Zhu, J. Zhang and L. Zhu, *Polym. Bull.* 2024, **81**, 335-350.
2. G. A. Zalmi, S. E. Jadhav, H. A. Mirgane, B. R. Madje and S. V. Bhosale, *ChemistrySelect*. 2023, **8**, e202203380.
3. L. Yang, M. Li, S. Ruan, X. Xu, Z. Wang and S. Wang, *Spectrochim. Acta A Mol. Biomol. Spectrosc*. 2021, **255**, 119718.
4. D. Mohanasundaram, G. G. V. Kumar, S. K. Kumar, B. Maddiboyina, R. P. Raja, J. Rajesh and G. Sivaraman, *J. Mol. Liq.* 2020, **317**, 113913.
5. Y.-T. Zeng, S.-Y. Gao, K. Traskovskis, B. Gao and X.-K. Ren, *Dyes Pigments,* 2021, **193**, 109491.
6. Y. Lin, K. Du, M. R. Gau and I. J. Dmochowski, *Chem. Sci.* 2023, **14**, 291-297.
7. S. Mongkholkaew, A. Songsasen, W. Sirisaksoontorn and B. Wannalerse, *Supramol. Chem.* 2021, **33**, 151-159.
8. S. Liu, Z. Liu, Q. Li, H. Xia, W. Yang, R. Wang, Y. Li, H. Zhao and B. Tian, *Spectrochim. Acta A Mol. Biomol. Spectrosc*. 2021, **246**, 118964.
9. X. Zhang, X. Tan and Y. Hu, *J. Hazard. Mater.* 2021, **411**, 125184.

Complete reference for Gaussian 09

Gaussian 09, Revision D.01,M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega,J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo,R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma,V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.