Supporting Information

ESIPT-Active 8-Hydroxyquinoline Chemosensor for Highly Selective Detection of Diethyl Chlorophosphate and Molecular Logic Gate Applications

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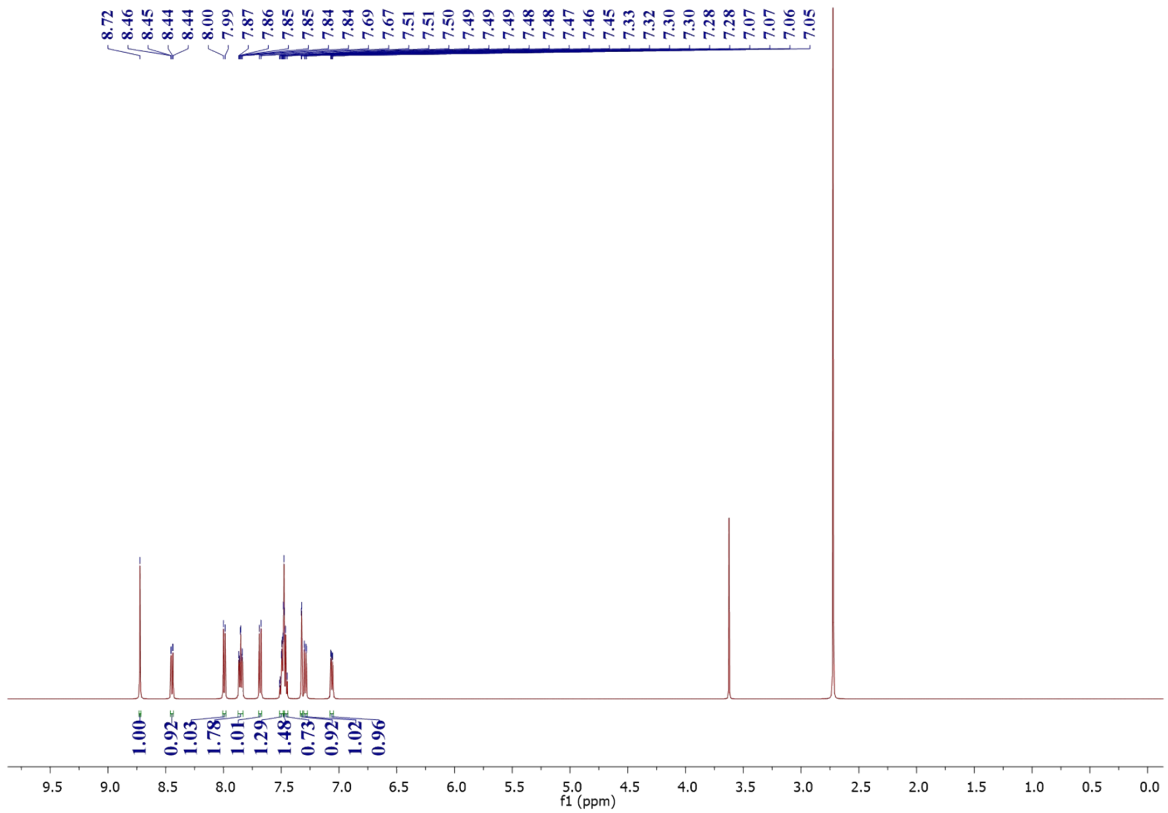


Figure S1: ^{1}H NMR spectrum of **HQHBI**.

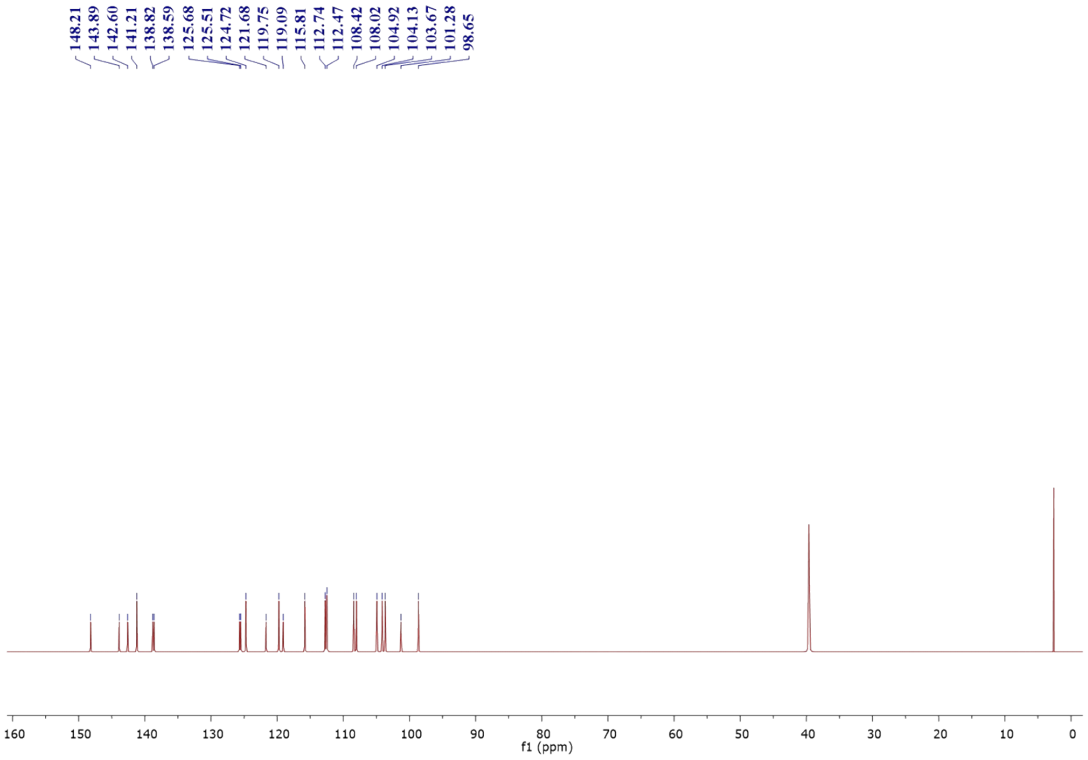


Figure S2: ^{13}C NMR spectrum of **HQHBI**.

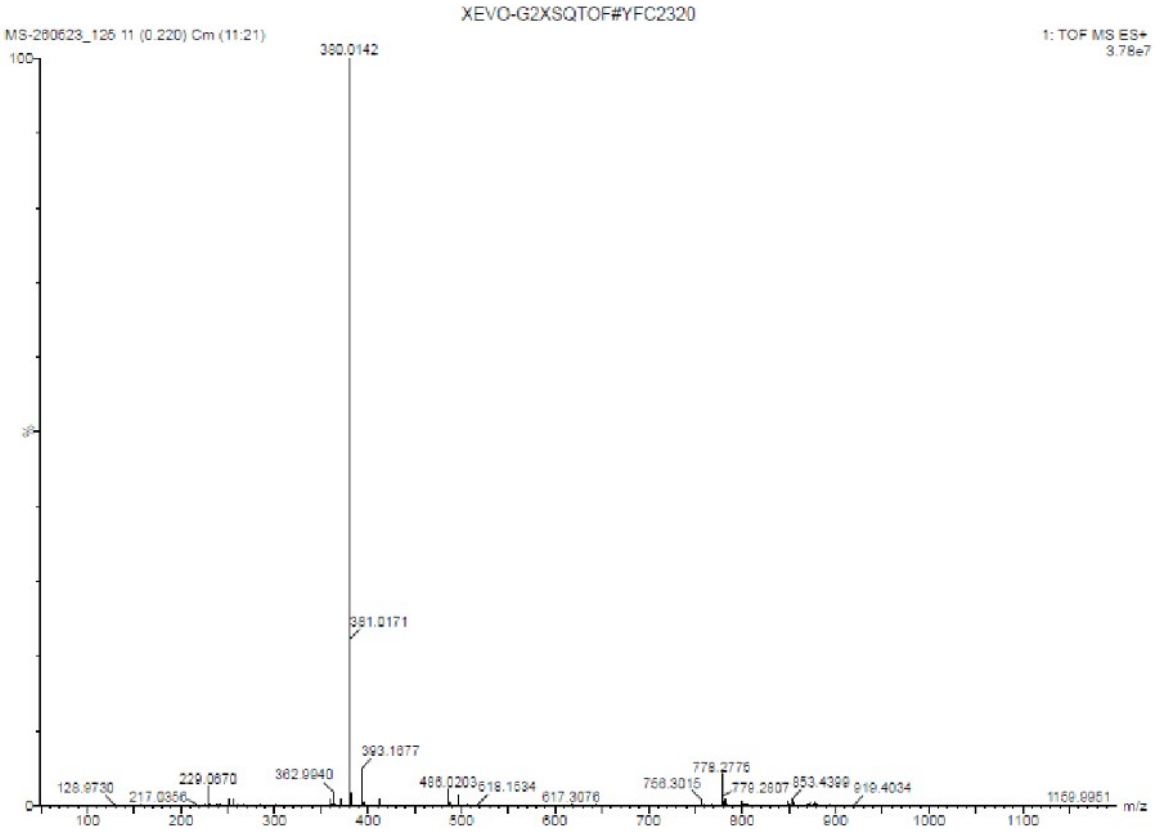


Figure S3: HRMS spectrum of **HQHBI**.

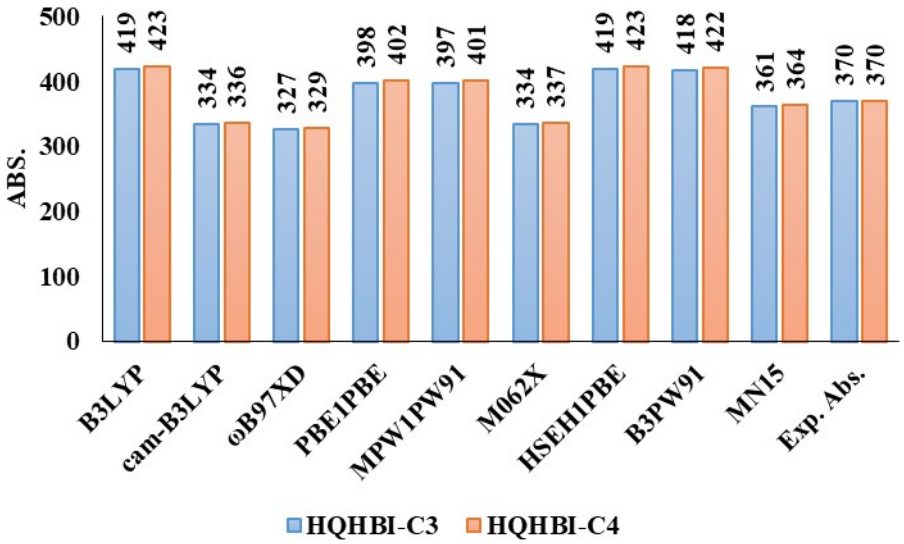


Figure S4: Comparison of calculated absorption spectra at different functional with experimental absorption spectra peak.

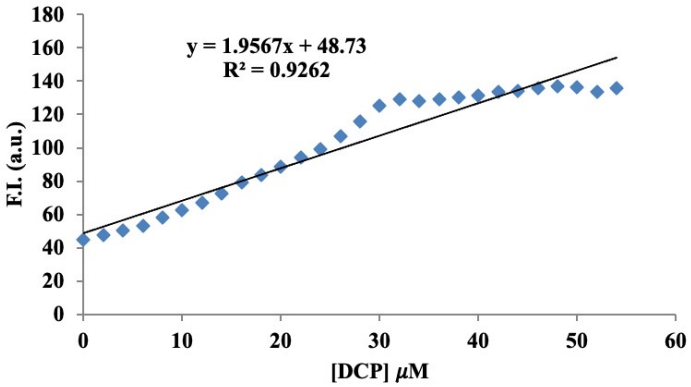


Figure S5: Plot for the determination of lowest detection limit of **HQHBI** (20 μM) with DCP in H_2O: CH_3CN, 1:1 [v/v].

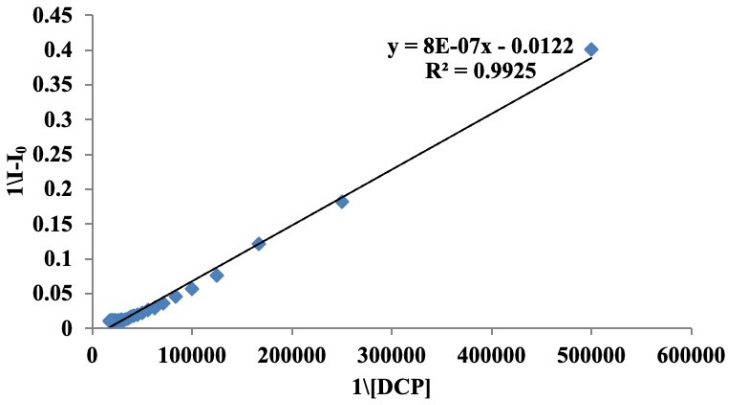


Figure S6: Benesi-Hildebrand plot for determination of binding constant of **HQHBI** (20 μM) with DCP in H_2O: CH_3CN, 1:1 [v/v].

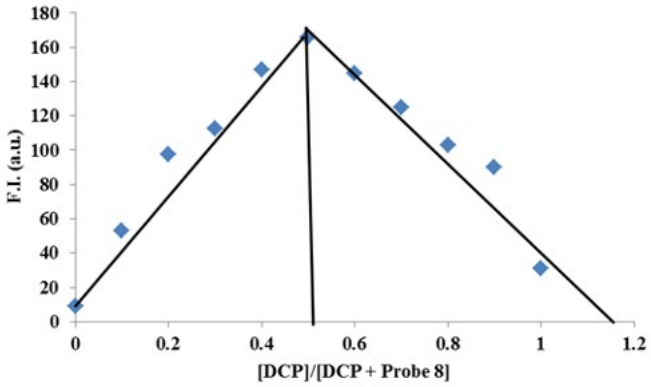
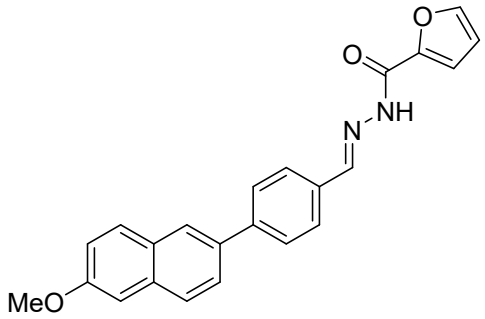
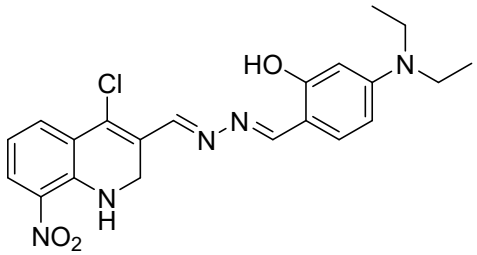
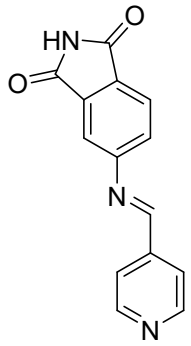
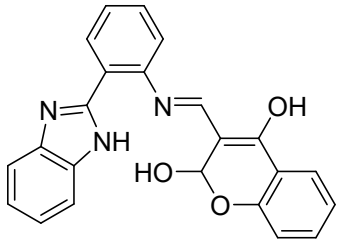
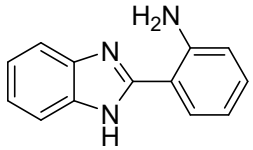
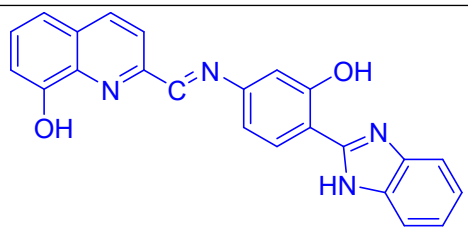


Figure S7: Job's Plot for **HQHBI** (20 μM) binding with DCP (20 μM) in H_2O: CH_3CN, 1:1 [v/v].

Table S1: Comparison with previously reported DCP sensors.

S. No.:	Structure	Solvent	Selectivity	Limit Of detection	References
1		CH_3CN	DCP	12.2 nM	1
2		DMF	DCP	1.5µM	2
3		CH_3CN	DCP	24 nM	3
4		CH_3CN	DCP	6.6 µM	4
5		CH_3CN	DCP	20.9 µM	5
6		H_2O: CH_3CN, 1:1 [v/v]	DCP	0.15 µM	This Work

1. S. Banerjee, P. Ghosh, A. Karak, D. Banik, and A. K. Mahapatra, A chemodosimetric chemosensor for the ratiometric detection of nerve agent-mimic DCP in solution and vapor phases, *Anal. Methods, 2025,**17**, 432-439.*
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3. X. Wen, T. Jiang, T. Liu, B. Zhao, X. Xu, H. Jeong, C. Fan, Y. Sun, J. Yoon, and Z. Lu, Schiff base-based turn-on fluorescent probe for rapid on-site detection of nerve agent simulants in solution and vapor, *Microchem. J.,* 2026, **224**, 117473.
4. N. Tohora, C. Debnath, S. Ahamed, J. Chourasia, M. Mahato, S. Ali, S. Lama, S. Pradhan, and S. K. Das, An efficient ESIPT-based ratio-/fluorimetric probe for rapid and sensitive detection of the sarin surrogate diethylchlorophosphate in solution and vapor phases, *Anal. Methods*, 2025,**17**, 2067-2075.
5. A. D. Jaiswal, J. Chourasia, S. Ahamed, N. Tohora, S. Lama, M. Mahato, U. Darnal, S. Ghanta, and S. K. Das, Decrypting the mechanistic aspect of a fluorochromic diethylcholorophosphate sensitive benzimidazole based probe: A combined spectroscopic and theoretical investigation, *Microchem. J.,* 2025, **212**, 113421.