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## Supporting Information for

### Highly Selective and Sensitive Chromogenic Recognition of Sarin Gas Mimicking

#### Diethylchlorophosphate

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Fig. S2 <sup>13</sup>C NMR of our synthesized chemosensor HBD



Fig. S3 HRMS spectra of our developed HBD



Fig. S4 Fluorometric investigation of our probe HBD absence and presence of DCP.



**Fig. S5** Change in absorbance at 560 nm of **HBD** (black dots) and **HBD** in the presence of DCP at different pH (red dots)



Fig. S6 Spectrophotometric interference investigation of our probe HBD with the various metal ions.



Fig. S7 Spectrofluorometric interference investigation of our probe HBD with the various metal ions.



Fig. S8 Absorbance spectra of HBD upon sequential addition of DCP and TEA.



Fig. S9 <sup>1</sup>H NMR titration spectra of HBD in the absence and presence of DCP.



Fig. S10 HRMS spectra of phosphorylated product HBD-DCP.



Fig. S11 Absorbance spectra of HBD solution in different spiked and unspiked soil samples such as (a) sand, (b) field, and (c) clay soil, respectively.

**Table S1.** Comparison table of various chemosensors that have been introduced for the detection of DCP in the last few decades with our **HBD**.

| Sensors                               | Type of response             | Response<br>Time | Test kit                       | Detection<br>limit        | Detectio<br>n in<br>gaseous<br>phase | Ref. |
|---------------------------------------|------------------------------|------------------|--------------------------------|---------------------------|--------------------------------------|------|
| squaraine-<br>ethanolamine<br>adducts | Colorimetric                 | Not<br>available | Not<br>available               | 3.5µM                     | Not<br>available                     | 1    |
| Terpyridine<br>based                  | Colorimetric<br>fluorometric | Few<br>seconds   | vapor<br>test<br>Paper<br>test | 0.35 μM<br>and 0.30<br>μM | Yes                                  | 2    |
| thiourea-based<br>rhodamine           | Colorimetric fluorometric    | Not<br>available | No                             | 2 µM                      | No                                   | 3    |

| DASA-          | Colorimetric       | Within 2  | vapor     | 1mM            | Yes       | 4    |
|----------------|--------------------|-----------|-----------|----------------|-----------|------|
| Derived        | (On-off)           | minutes   | test      |                |           |      |
| Polymeric      |                    |           |           |                |           |      |
| Probe          |                    |           |           |                |           |      |
| bis-indolyl    | Colorimetric       | Few       | vapor     | 10.8 μM        | Yes       | 5    |
| based          |                    | minutes   | test      |                |           |      |
| chromogenic    |                    |           | Paper     |                |           |      |
| Pifunctional   | aalaumimatria      | Within 1  | lesi      | 0.2  mM        | Not       | 6    |
| azoaniline     | colourimente       | within 1  | mentione  | 0.2 11111      |           | ÷    |
| based          |                    | min       | d         |                | mentione  |      |
|                |                    |           | u<br>1 .  |                | d         | 7    |
| Polymer        | colorimetric       | Within    | polymeri  | 18.4 μM        | Yes       | /    |
| (BPAm-co-      |                    | few mins  | c film    |                |           |      |
| DMA-co-        |                    |           |           |                |           |      |
| MPDEA)         |                    |           |           |                |           |      |
| di-methyltin   | Fluorometric       | Almost 2  | Yes       | 0.023 and      | Yes       | 8    |
| derivative     | (turn-off)         | minutes   | (Spot     | 0.092 mM       |           |      |
|                |                    |           | Testing   |                |           |      |
|                | ON/OFF             | Earry     | Device)   | $0.1 \dots M$  | Vaa       | 9    |
| pyrene based   | UN/OFF             | Few       | Quartz    | 0.1 mM         | Y es      | ,    |
| fluorescent    | reversible         | minutes   | Vapor     |                |           |      |
| nolymeric      | fluorescence       |           | test      |                |           |      |
| probe          |                    |           | test      |                |           |      |
| benzothiazole- | Fluorometric       | Not       | Not       | 0.43 μM        | Not       | 10   |
| based          |                    | available | available | •              | available |      |
| Xanthene       | Colorimetric,fluor | Not       | Not       | 1.36 µM        | NA        | 11   |
|                | ometric (turnon)   | mentioned | mentione  | and 26 $\mu$ M |           |      |
|                |                    |           | d         | •              |           |      |
| Hydrazine      | Colorimetric       | Few       | Paper     | 0.30 µM        | Yes       | Our  |
| based          |                    | seconds   | test,     | •              |           | Work |
|                |                    |           | vapor     |                |           |      |
|                |                    |           | test      |                |           |      |

# References

- J. Zhao, M. Qin, J. You, K. Liu, L. Ding, T. Liu, J. Kong and Y. Fang, *Dye. Pigment.*, 2022, **197**, 109870.
- P. Zheng, Z. Cui, H. Liu, W. Cao, F. Li and M. Zhang, J. Hazard. Mater., 2021, 415, 125619.
- 3 S. Li, Y. Zheng, W. Chen, M. Zheng, H. Zheng, Z. Zhang, Y. Cui, J. Zhong and C.

Zhao, *Molecules*, , DOI:10.3390/MOLECULES24050827.

- 4 A. Balamurugan and H. Il Lee, *Macromolecules*, 2016, **49**, 2568–2574.
- 5 N. Dey, S. Jha and S. Bhattacharya, *Analyst*, 2018, **143**, 528–535.
- 6 M. Gupta and P. H. il Lee, Sensors Actuators B Chem., 2017, 242, 977–982.
- T. N. Annisa, S. H. Jung, M. Gupta, J. Y. Bae, J. M. Park and H. Il Lee, *ACS Appl. Mater. Interfaces*, 2020, **12**, 11055–11062.
- 8 N. Singh, K. Kumar, N. Srivastav, R. Singh, V. Kaur, J. P. Jasinski and R. J. Butcher, New J. Chem., 2018, 42, 8756–8764.
- 9 M. Gupta and H. Il Lee, *undefined*, 2017, **50**, 6888–6895.
- M. K. Das, T. Mishra, S. Guria, D. Das, J. Sadhukhan, S. Sarker, K. Dutta, A.
  Adhikary, D. Chattopadhyay and S. S. Adhikari, *New J. Chem.*, 2022, 47, 250–257.
- 11 K. C. Behera and B. Bag, Chem. Commun., 2020, 56, 9308–9311.