

A Preliminary Study for Tunable Optical Assessment of Exhaled Breath Ammonia Based on Ultrathin Tetrakis(4-sulfophenyl)porphine Nanoassembled Films

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Table S1. Relationships between the concentrations of NH₄OH in the solution and the corresponding gas concentrations in the headspace.

| NH ₄ OH concentration in solution (ppm) | NH ₃ concentration in headspace (ppm) |
|--|--|
| 1 | 0.2 |
| 3 | 0.25 |
| 5 | 0.3 |
| 7 | 0.5 |
| 10 | 1 |
| 20 | 3 |
| 30 | 4.5 |
| 100 | 17 |
| 200 | 50 |
| 300 | 90 |
| 400 | 125 |
| 500 | 140 |
| 600 | 180 |
| 700 | 240 |
| 800 | 290 |
| 1000 | 360 |

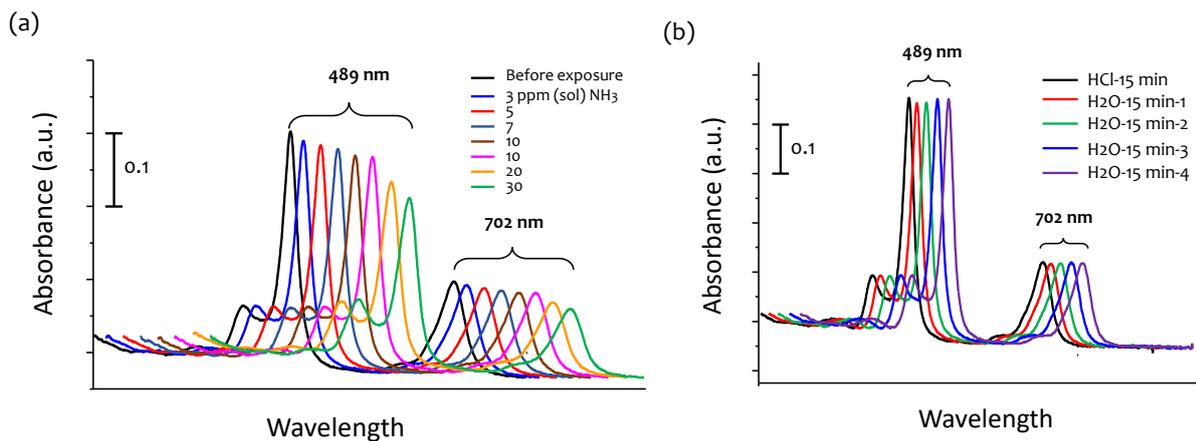


Figure S1. UV-vis spectra of the PDDA/TSPP film measured after (a) exposure to ammonia vapors produced by various concentrations of ammonia solutions and (b) continuous exposures to water vapor for 15 min each after HCl vapor treatment. The spectra are shifted horizontally for illustration purposes and convenience in reading the figures.

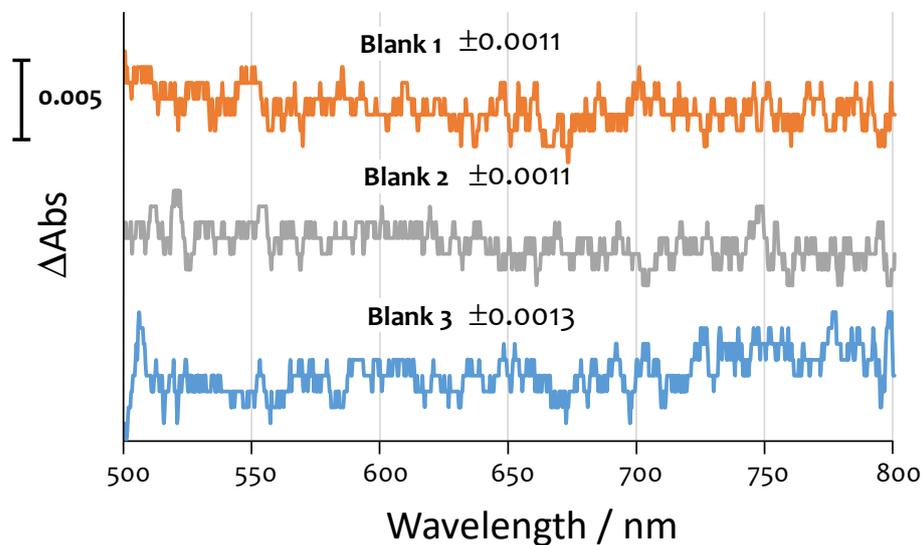


Figure S2. Difference absorption spectra of the three blank measurements before exposure to ammonia gas.

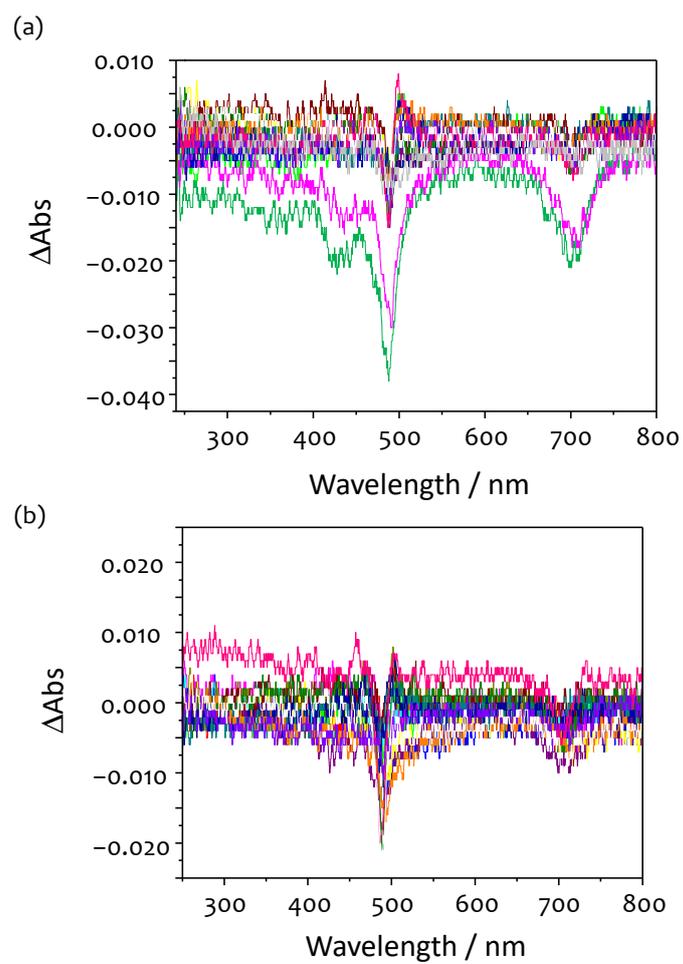


Figure S3. Difference absorption spectra of the PDDA/TSPP film measured for the selected breath samples collected from 20 volunteers (a) before lunch and (b) after lunch.