

Supporting Information for

Evaluation of an Ion-Associate Phase Formed In Situ from the Aqueous Phase by Adding Benzethonium Chloride and Sodium Ethylbenzenesulfonate for Microextraction

Noriko Hata *, Akane Igarashi, Rie Yasui, Maho Matsushita, Nozomi Kohama, Tomoka Komiyama, Kazuto Sazawa, Hideki Kuramitz and Shigeru Taguchi

Major of Environmental and Analytical Chemistry, Graduate School of Science and Engineering (Science Div.), University of Toyama, 3190 Gofuku, Toyama 930-8555, Japan

* Correspondence: hata1000ko@gmail.com

Contents:

- Figure S1 Structures of organic ions constituting the ion-associate phase (IAP)
- Figure S2 Scheme for measuring percentage extraction
- Figure S3 Example of calibration curves for calculating percentage extraction

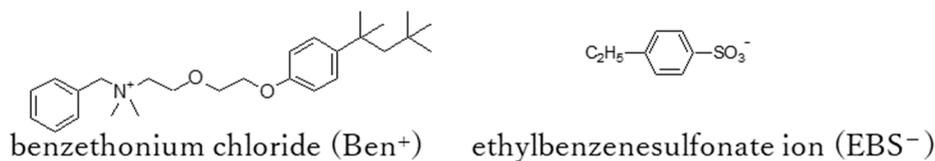


Figure S1 Structures of organic ions constituting the ion-associate phase (IAP)

3.3 Distribution coefficients for PAHs, estrogens, and pesticides

To evaluate the formed IAPs, the distribution coefficients for several environmental pollutants to IAPs consisting of BTC and TS^- or EBS^- ions were calculated and compared to the octanol-water distribution coefficients (K_{ow}). To determine the distribution coefficient, % E and V_{iap} must be determined. Calibration curves were obtained based on the peak area or peak height in the first and second extractions, and % E was calculated from the slopes of the curves. Let “ $Grad$ ” be the slope when % E is 100%; then, the following system of equations is obtained from the slopes, $Grad_1$ and $Grad_2$, of the first and second extraction calibration curves, respectively (**Figure S2, S3**).

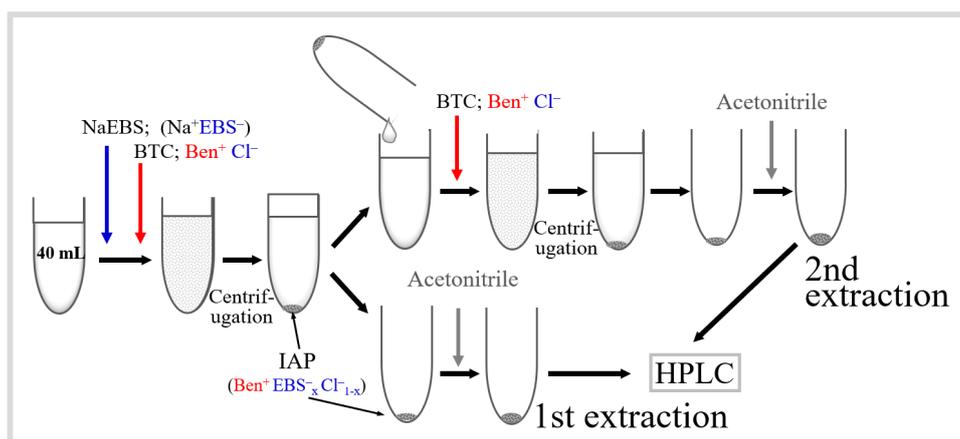


Figure S2 Scheme for measuring percentage extraction

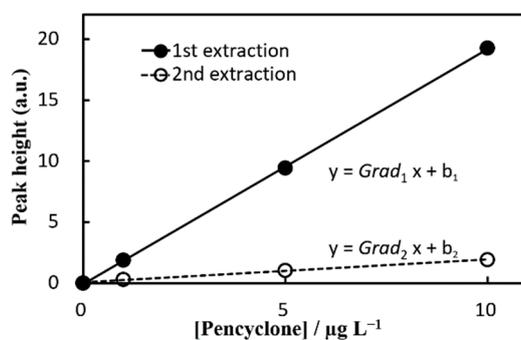


Figure S3 Example of calibration curves for calculating percentage extraction

$$Grad_1 = Grad \times \frac{\% E}{100} \quad (S1)$$

$$Grad_2 = \left(Grad \times \frac{100 - \% E}{100} \right) \times \frac{\% E}{100} \quad (S2)$$

Solving this system of equations yields % E .

$$\% E = \frac{Grad_1 - Grad_2}{Grad_1} \times 100 \quad (S3)$$

$$E = \frac{Grad_1 - Grad_2}{Grad_1} \quad (S4)$$