

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

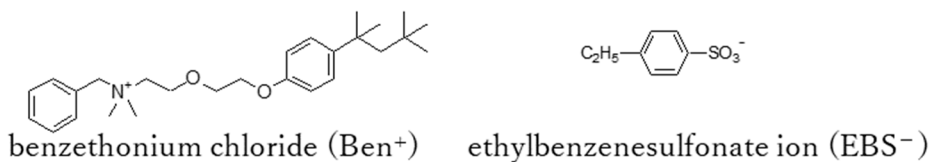
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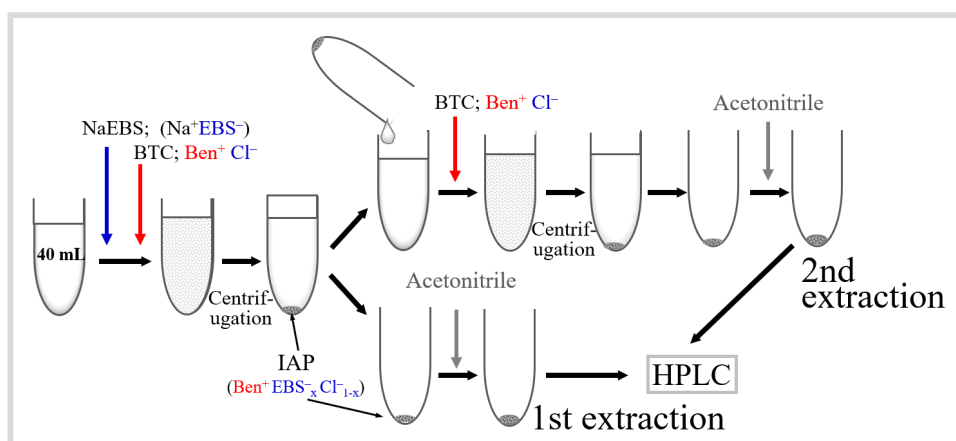
- Figure S1 Structures of organic ions constituting the ion-associate phase (IAP)
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- Figure S3 Example of calibration curves for calculating percentage extraction



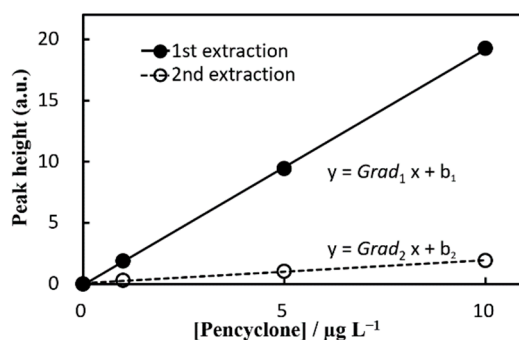
**Figure S1** Structures of organic ions constituting the ion-associate phase (IAP)

### 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  $\text{TS}^-$  or  $\text{EBS}^-$  ions were calculated and compared to the octanol-water distribution coefficients ( $K_{\text{ow}}$ ). To determine the distribution coefficient, %  $E$  and  $V_{\text{iap}}$  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 “ $\text{Grad}$ ” be the slope when %  $E$  is 100%; then, the following system of equations is obtained from the slopes,  $\text{Grad}_1$  and  $\text{Grad}_2$ , 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

$$\text{Grad}_1 = \text{Grad} \times \frac{\% E}{100} \quad (\text{S1})$$

$$\text{Grad}_2 = \left( \text{Grad} \times \frac{100 - \% E}{100} \right) \times \frac{\% E}{100} \quad (\text{S2})$$

Solving this system of equations yields %  $E$ .

$$\% E = \frac{\text{Grad}_1 - \text{Grad}_2}{\text{Grad}_1} \times 100 \quad (\text{S3})$$

$$E = \frac{\text{Grad}_1 - \text{Grad}_2}{\text{Grad}_1} \quad (\text{S4})$$