

Electronic Supplementary Material (ESI) for Soft Matter.

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Supporting Information for Manuscript Entitled
Modulation of Partition and Localization of Perfume Molecules in Sodium
Dodecyl Sulfate Micelles

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Calculation of the fraction of perfume molecules incorporated into micelles

Assuming two sites of perfume molecule localization in the sample: Free molecules diffusing with D_f , the diffusion coefficient of the perfume molecules in D_2O , and molecules incorporated into the micelle, diffusing with D_M , the diffusion coefficient of the micelle in the mixture. However, the diffusion coefficient of surfactant alone D_s can be obtained from the diffusion results. Therefore, it is essential to note that surfactant diffusion coefficients D_s in micellar solutions are weighted averages of the monomer diffusion coefficient D_1 and the micellar diffusion coefficient D_M according to:

$$D_s = f_M D_M + f_1 D_1, \quad [1]$$

where f_M and f_1 are the fractions of surfactant present in micelles and as monomer in the aqueous phase, respectively. This equation holds for fast exchange between monomeric and micellar surfactant, which is typically the case in micellar solution. In this present study, the concentration of SDS (97.5 mM) was much larger than the critical micelle concentration. Thus compared to f_M , the monomer fraction f_1 can be neglected and D_s is equal to D_M .

The observed diffusion coefficient D of the perfume molecule then is a fast exchange average over these two sites, which is weighted by the fraction of molecules in either site. With f_p as the fraction of perfume molecules incorporated into the micelle, it is:

$$D = f_p D_M + (1 - f_p) D_f = D_f + f_p (D_M - D_f). \quad [2]$$

Thus,

$$f_p = \frac{D_f - D}{D_f - D_M}. \quad [3]$$

Table S1. The structural parameters of the SDS and SDS/perfume micelles from the SAXS data fitted with the ellipsoid model.

| Systems | R_a (Å) | R_b (Å) | $V_{\text{ellipsoid}}$ (Å³) | R_b/R_a | R_g (Å) | N_{agg} |
|-----------------------|-----------------------------|-----------------------------|--|-----------------------------|-----------------------------|------------------------------------|
| SDS | 15.0 | 21.0 | 2.8×10^4 | 1.40 | 12.9 | 58 |
| SDS/Ethyl Butyrate | 15.2 | 21.3 | 2.9×10^4 | 1.40 | 13.1 | 60 |
| SDS/Methyl Paraben | 15.6 | 21.7 | 3.1×10^4 | 1.39 | 13.4 | 64 |
| SDS/Methyl Salicylate | 16.2 | 22.5 | 3.4×10^4 | 1.39 | 13.9 | 72 |
| SDS/Anethole | 16.5 | 23.0 | 3.7×10^4 | 1.39 | 14.2 | 76 |
| SDS/Linalool | 16.1 | 23.2 | 3.6×10^4 | 1.44 | 14.1 | 76 |
| SDS/Piperitone | 16.1 | 22.5 | 3.4×10^4 | 1.40 | 13.8 | 71 |
| SDS/Carvone | 16.4 | 22.7 | 3.5×10^4 | 1.38 | 14.0 | 74 |
| SDS/Menthone | 16.2 | 22.1 | 3.3×10^4 | 1.36 | 13.7 | 69 |
| SDS/Menthol | 16.4 | 23.0 | 3.6×10^4 | 1.40 | 14.1 | 76 |
| SDS/Eucalyptol | 16.5 | 22.3 | 3.4×10^4 | 1.35 | 13.9 | 72 |
| SDS/Menthyl Acetate | 16.4 | 23.8 | 3.9×10^4 | 1.45 | 14.5 | 81 |
| SDS/Limonene | 16.2 | 23.3 | 3.7×10^4 | 1.44 | 14.2 | 77 |
| SDS/Pinene | 16.4 | 24.0 | 4.0×10^4 | 1.46 | 14.5 | 82 |