

Supplementary Data – Morris et al. The Partitioning of Alcohols into the Aggregates of Gemini Amphiphiles from Diffusion NMR Experiments.

Supplementary Table 1. Structures of the m-s-m gemini amphiphiles used in the present
paper.

$C_{8}H_{17}N(CH_3)_2 - (CH_2)_8 - N(CH_3)_2C_{8}H_{17}Br_2$	8-4-8
$C_{8}H_{17}N(CH_3)_2 - (CH_2)_8 - N(CH_3)_2C_{8}H_{17}Br_2$	8-6-8
$C_{8}H_{17}N(CH_3)_2 - (CH_2)_8 - N(CH_3)_2C_{8}H_{17}Br_2$	8-8-8
$C_{10}H_{21}N(CH_3)_2 - (CH_2)_{10} - N(CH_3)_2C_{10}H_{21}Br_2$	10-4-10
$C_{10}H_{21}N(CH_3)_2 - (CH_2)_{10} - N(CH_3)_2C_{10}H_{21}Br_2$	10-6-10
$C_{10}H_{21}N(CH_3)_2 - (CH_2)_{10} - N(CH_3)_2C_{10}H_{21}Br_2$	10-10-10
$C_{12}H_{25}N(CH_3)_2 - (CH_2)_6 - N(CH_3)_2C_{12}H_{25}Br_2$	12-6-12
$C_{12}H_{25}N(CH_3)_2 - (CH_2)_8 - N(CH_3)_2C_{12}H_{25}Br_2$	12-8-12
$C_{12}H_{25}N(CH_3)_2 - (CH_2)_{10} - N(CH_3)_2C_{12}H_{25}Br_2$	12-10-12
$C_{12}H_{25}N(CH_3)_2 - (CH_2)_{12} - N(CH_3)_2C_{12}H_{25}Br_2$	12-12-12

Supplementary Information 2.

For the synthesis of the gemini surfactants used in this work, starting materials were purchased from either Sigma-Aldrich or TCI America, were the highest purity available, and used as received. Some of the gemini surfactants used in this work were prepared using the method described by Wettig and Verrall.^{1,2} As an example, the surfactant 12-6-12 was prepared by refluxing one equivalent of α,ω -dibromohexane with 2.1 molar equivalents of N,N-dimethyldodecylamine in 150 mL of HPLC-grade acetonitrile for 48 hours. After the solution was cooled, the solid material was collected by vacuum filtration and recrystallized several times from

acetonitrile, followed by a final recrystallization from an acetone/ethanol mixture. The yields obtained for the gemini surfactants using this methodology were better than 50%.

In some cases, the gemini surfactants were synthesized by our novel microwave method.³ For the synthesis of the surfactant 8-4-8, one equivalent of α,ω -butanedibromide and 2.1 equivalents of N,N-dimethyloctylamine were placed in 10.0 mL of acetonitrile in a 35 mL microwave reaction vessel. The reaction vessel was then placed in a CEM Discover microwave reactor set at 80°C at a maximum power of 30 W and stirred for 30 min following a 15 min ramp time. The reaction vessel has a pressure tolerance of 15 psi. After microwave irradiation was complete, the vessel was set in a freezer overnight; the resulting precipitate (the gemini surfactant) was vacuum-filtered and rinsed with a minimum of cold ethyl acetate. The crude surfactant was then placed in a vacuum desiccator for 24 h and was recrystallized in a minimum amount of boiling acetonitrile, cooled to room temperature and refrigerated for 2 days. The yields obtained for the gemini surfactants using this methodology were > 90%. Critical micelle concentration values obtained through conductivity measurements for all the gemini amphiphiles prepared in this work were in excellent agreement with the literature values where available.

- 1 S. Wettig and R. E. Verrall, Studies of the Interaction of Cationic Gemini Surfactants with Polymers and Triblock Copolymers in Aqueous Solution, *J Colloid Interface Sci*, 2001, **244**, 377–385.
- 2 X. Li, S. D. Wettig and R. E. Verrall, *J Colloid Interface Sci*, 2005, **282**, 466–477.
- 3 O. M. Singer, J. W. Campbell, J. G. Hoare, J. D. Masuda, G. Marangoni and R. D. Singer, Improved Green Synthesis and Crystal Structures of Symmetrical Cationic Gemini Surfactants, *ACS Omega*, 2022, **7**, 35326–35330.