Supplementary Information for:

Micelle Maker: An Online Tool for Generating Equilibrated Micelles as Direct Input for Molecular Dynamics Simulations

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Table S1: Computational data calculated from MD simulations based on micelles generated with Micelle Maker, and corresponding experimental radii.[a]

Detergents	β-**OM**	β-**OG**	β-**NG**	β-**DM**
No. lipids	47	90	133	69
Salt c	0.1	0.1	0.1	0.1
Tail carbons	8	8	9	10
Rh	24±2	n.a.	n.a.	29±5
Rs	24.73±0.39	25.64±0.28	29.78±0.26	28.68±0.34
ROG	19.16±0.31	19.86±0.22	23.07±0.20	22.22±0.26
SASA	5631±277	9022±277	12133±430	7717±312
1st Ionshell	1.0±1.0	0.9±0.9	1.2±1.1	1.2±1.1
2nd Ionshell	2.6±1.5	2.5±1.5	3.4±1.8	3.1±1.7
l ratio	1.27±0.10	1.32±0.11	1.37±0.10	1.24±0.09
ecc	0.117±0.042	0.142±0.049	0.153±0.045	0.109±0.039
Dc_h	0.038±0.018	0.599±0.213	0.270±0.352	0.035±0.004
Dc_t	0.018±0.008	0.105±0.008	0.060±0.056	0.011±0.001
Detergents	**β-DDM**	**β-DDM**	**α-DDM**	**SDS**
No. lipids	98	110	98	62
Salt c	0.15	0.15	0.15	0.15
Tail carbons	12	12	12	12
Rh	33±5	n.a.	n.a.	n.a.
Rs	33.14±0.38	34.71±0.41	32.29±0.24	25.82±0.34
ROG	25.67±0.30	26.89±0.31	25.01±0.19	20.00±0.26
SASA	10365±391	11170±496	9231±416	9683±294
1st Ionshell	2.5±1.6	2.7±1.6	2.4±1.5	18.9±3.5
2nd Ionshell	6.2±2.3	6.7±2.4	6.0±2.3	34.5±3.5
l ratio	1.20±0.08	1.25±0.08	1.18±0.06	1.27±0.10
ecc	0.093±0.036	0.113±0.035	0.083±0.031	0.121±0.046
Dc_h	0.030±0.013	0.03±0.003	0.027±0.004	4.102±0.137
Dc_t	0.012±0.006	0.014±0.004	0.012±0.001	0.102±0.041

[a] **No. lipids:** Number of lipids. **Salt c:** Salt concentration in mol/l. **Rh:** Hydrodynamic radius in Å, experimentally determined by dynamic light scattering.[1] **Rs:** Effective micellar radius in Å, calculated by ROG * (5/3)^0.5.[2] **ROG:** Radius of gyration in Å calculated with CPPTRAJ. **SASA:** Solvent Accessible Surface Area in Å^2 calculated with CPPTRAJ, based on specified atoms using the linear combinations of pairwise overlaps (LCPO) algorithm of Weiser *et al*.[3] **1st and 2nd ion shells:** number of ions within 3.4 and 5.0Å of the micelle, respectively, using default cutoffs. **l:** Principle moments of inertia calculated with

CPPTRAJ, where the eigenvalues of the principle axes of each simulation frame are determined by diagonalization of the intertial matrix from the coordinates of the specified atoms. **l ratio:** I_{max}/I_{min}. **ecc:** Eccentricity calculated by 1 - (I_{min}/I_{avg}).[2] **Dc_h:** Diffusion coefficients for lipid head groups calculated with CPPTRAJ in $1x10^{-5}$ cm^2 /s using the Einstein relation. **Dc_t:** Diffusion coefficients for tails calculated with CPPTRAJ in $1x10^{-5}$ cm^2 using the Einstein relation. For a definition of lipid abbreviations, see either **Table S2** or **Table 1** of the main text.

Table S2: Summary of available experimental data for the mass, critical micelle concentration and aggregation numbers of the lipids that can be modelled by Micelle Maker at the time of publication.[a]

Lipid type	Mass [Da]	CMC [mM/L]	Aggregation number	Reference
Heptyl-α-D-glucopyranoside (α-HG)	278	n.a.	n.a.	n.a.
Heptyl-β-D-glucopyranoside (β-HG)	278	~70 (H_2O)	n.a.	4
Heptyl-α-D-maltopyranoside (α-HM)	443	n.a.	n.a.	n.a.
Heptyl-β-D-maltopyranoside (β-HM)	443	n.a.	n.a.	n.a.
Octyl-α-D-glucopyranoside (α-OG)	292	~10-21 (H_2O)	n.a.	5
Octyl-β-D-glucopyranoside (β-OG)	292	~18-20 (H_2O)/ 23.4 (0.1M NaCl)	~27-100/~90	5-8
Octyl-α-D-maltopyranoside (α-OM)	454	n.a.	n.a.	n.a.
Octyl-β-D-maltopyranoside (β-OM)	454	19.5 (100mM NaCl, 20mM HEPES pH7.5)	~47	5
Nonyl-α-D-glucopyranoside (α-NG)	306	n.a.	n.a.	n.a.
Nonyl-β-D-glucopyranoside (β-NG)	306	~6.5 (H_2O)/ ~6 (0.15M NaCl)/ 3.5(1M NaCl)	~133	4-5
Nonyl-α-D-maltopyranoside (α-NM)	469	n.a.	n.a.	n.a.
Nonyl-β-D-maltopyranoside (β-NM)	469	~6 (H_2O)	~55 (100mM NaCl, 20mM HEPES pH7.5)	5
Decyl-α-D-glucopyranoside (α-DG)	320	n.a.	n.a.	n.a.
Decyl-β-D-glucopyranoside (β-DG)	320	~2.2 (H_2O)/ ~2.3 (0.01M PO_4 Buffer)	n.a.	9-10
Decyl-α-D-maltopyranoside (α-DM)	483	~1.66 (H_2O)	n.a.	5
Decyl-β-D-maltopyranoside (β-DM)	483	~1.8 (H_2O)/ ~1.8 (0.15M NaCl)	~69	5, 11

Undecyl-α-D-glucopyranoside (α-UDG)	334	n.a.	n.a.	n.a.
Undecyl-β-D-glucopyranoside (β-UDG)	334	n.a.	n.a.	n.a.
Undecyl-α-D-maltopyranoside (α-UDM)	497	0.58 (H_2O)	n.a.	5
Undecyl-β-D-maltopyranoside (β-UDM)	497	~0.59 (H_2O)	~71 (100mM NaCl, 20mM HEPES pH7.5)	5
Dodecyl-α-D-glucopyranoside (α-DDG)	349	n.a.	n.a.	n.a.
Dodecyl-β-D-glucopyranoside (β-DDG)	349	~0.19 (H_2O)	n.a.	10
Dodecyl-α-D-maltopyranoside (α-DDM)	511	~0.152 (H_2O)	~90	12
Dodecyl-β-D-maltopyranoside (β-DDM)	511	~0.17 (H_2O)/ ~0.12 (0.2M NaCl)	~78-149/110-140	5, 7, 12
Sodium-dodecyl-sulfate (SDS)	288	1.2-7.1 (H_2O)	62-101	7

[a] n.a. = not available, no reference found

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