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SUPPORTING MATERIAL:

Stabilization of DPPC Lipid Bilayers in the Presence of Co-Solutes: Molecular Mechanisms and Interaction Patterns

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Force Field Parameters

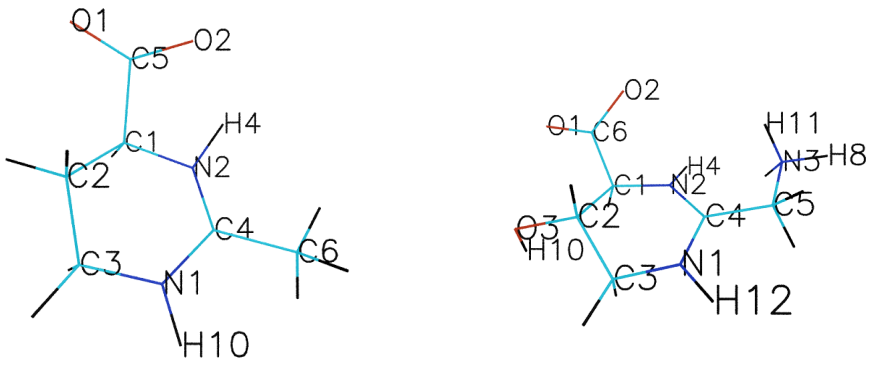

Figure 1: Structures of ectoine (left) and aminoectoine (right) with atom names.

Table 1: Partial charges of the MD simulations.

atom name	atom type	initial charge	penalty	final charge
ectoine				
C1	CG314	0.325	104.34	0.105
C2	CG321	-0.139	36.846	-0.14
C3	CG324	0.214	16.375	0.105
C4	CG2N2	0.663	5.392	0.636
C5	CG2O3	0.435	101.879	0.501
C6	CG331	-0.142	3.536	-0.191
N1	NG2P1	-0.658	5.948	-0.548
N2	NG2P1	-0.658	31.08	-0.548
O1	OG2D2	-0.76	8.256	-0.70
O2	OG2D2	-0.76	8.256	-0.70
amino-ectoine				
C1	CG314			0.140
C2	CG311			0.114
C3	CG324			0.214
C4	CG2N2			0.603
C5	CG324			0.285
C6	CG2O3			0.550
N1	NG2P1			-0.658
N2	NG2P1			-0.608
N3	NG3P3			-0.300
O1	OG2D2			-0.700
O2	OG2D2			-0.700
O3	OG311			-0.650
H4	HGP2			0.380
H8	HGP2			0.330
H10	HGP1			0.420
H11	HGP2			0.330
H12	HGP2			0.380

Table 2: Bond parameters with penalties from CGenFF program output for the potential $V_{bond} = K_b(b - b_0)^2$.

atoms	K_b (kcal/mol/Å^2)	b_0 (Å)	penalty
ectoine			
CG314 NG2P1	300.00	1.4530	4
amino-ectoine			
CG2N2 CG324	280.00	1.5000	7

Table 3: Angle parameters with penalties from CGenFF program output for the potential $V_{ang}(\alpha) = K_\alpha(\alpha - \alpha_0)^2$ and $V_{UB}(S) = K_{UB}(S - S_0)^2$.

atoms	Kα (kcal/mol/rad)	α_0 (deg)	K_{UB} (kcal/mol/Å)	S_0	penalty
ectoine					
CG2O3 CG314 NG2P1	50.00	107.00			25
CG321 CG314 NG2P1	67.70	110.00			4
NG2P1 CG314 HGA1	42.00	110.10			4
CG314 CG321 CG324	58.35	113.50	11.16	2.56100	17
CG2N2 NG2P1 CG314	62.30	120.00			1.1
CG2N2 NG2P1 CG324	62.30	120.00			0.5
CG314 NG2P1 HGP2	40.40	120.00			0.6
amino-ectoine					
CG324 CG2N2 NG2P1	52.00	118.50			17.9
CG314 CG311 CG324	53.35	111.00	8.00	2.56100	17
CG314 CG311 OG311	75.70	112.10			0.6
CG2O3 CG314 NG2P1	50.00	107.00			25
CG311 CG314 NG2P1	67.70	110.00			4.6
NG2P1 CG314 HGA1	42.00	110.10			4
CG2N2 CG324 NG3P3	43.70	110.00			11
CG2N2 CG324 HGA2	33.00	109.50	30.00	2.13000	7
CG311 CG324 NG2P1	67.70	110.00			0.6
CG2N2 NG2P1 CG314	62.30	120.00			1.1
CG2N2 NG2P1 CG324	62.30	120.00			0.5
CG314 NG2P1 HGP2	40.40	120.00			0.6

Table 4: Dihedral parameters including heavy atoms with penalties from CGenFF program output for the potential $V_{dihedral}(\delta) = K_\chi(1 + \cos(n(\chi - \delta)))$.

atoms	Kχ (kcal/mol)	n	δ (deg)	penalty
ectoine				
CG331 CG2N2 NG2P1 CG314	2.2500	2	180.00	82.1
CG331 CG2N2 NG2P1 CG324	2.2500	2	180.00	81.5
NG2P1 CG2N2 NG2P1 CG314	2.2500	2	180.00	5.6
NG2P1 CG2N2 NG2P1 CG324	2.2500	2	180.00	5
OG2D2 CG2O3 CG314 NG2P1	0.0000	6	180.00	25
CG2O3 CG314 CG321 CG324	0.1950	3	0.00	5.6
NG2P1 CG314 CG321 CG324	0.1950	3	0.00	21
CG2O3 CG314 NG2P1 CG2N2	0.0000	6	180.00	79.5
CG321 CG314 NG2P1 CG2N2	0.0000	6	180.00	4.5
CG314 CG321 CG324 NG2P1	0.1950	3	0.00	17
CG321 CG324 NG2P1 CG2N2	0.0000	6	180.00	0.5
amino-ectoine				
NG2P1 CG2N2 CG324 NG3P3	0.4000	1	0.00	39
CG324 CG2N2 NG2P1 CG314	2.2500	2	180.00	78.6
CG324 CG2N2 NG2P1 CG324	2.2500	2	180.00	78
NG2P1 CG2N2 NG2P1 CG314	2.2500	2	180.00	5.6
NG2P1 CG2N2 NG2P1 CG324	2.2500	2	180.00	5
OG2D2 CG2O3 CG314 NG2P1	0.0000	6	180.00	25
CG324 CG311 CG314 CG2O3	0.1950	3	0.00	9.6
CG324 CG311 CG314 NG2P1	0.1950	3	0.00	25
OG311 CG311 CG314 CG2O3	0.2000	3	0.00	1
OG311 CG311 CG314 NG2P1	0.2000	3	0.00	25
CG314 CG311 CG324 NG2P1	0.1950	3	0.00	21
OG311 CG311 CG324 NG2P1	0.2000	3	0.00	29
CG2O3 CG314 NG2P1 CG2N2	0.0000	6	180.00	79.5
CG311 CG314 NG2P1 CG2N2	0.0000	6	180.00	5.1
CG311 CG324 NG2P1 CG2N2	0.0000	6	180.00	1.1

Cumulative Number Distribution Functions for Co-Solutes

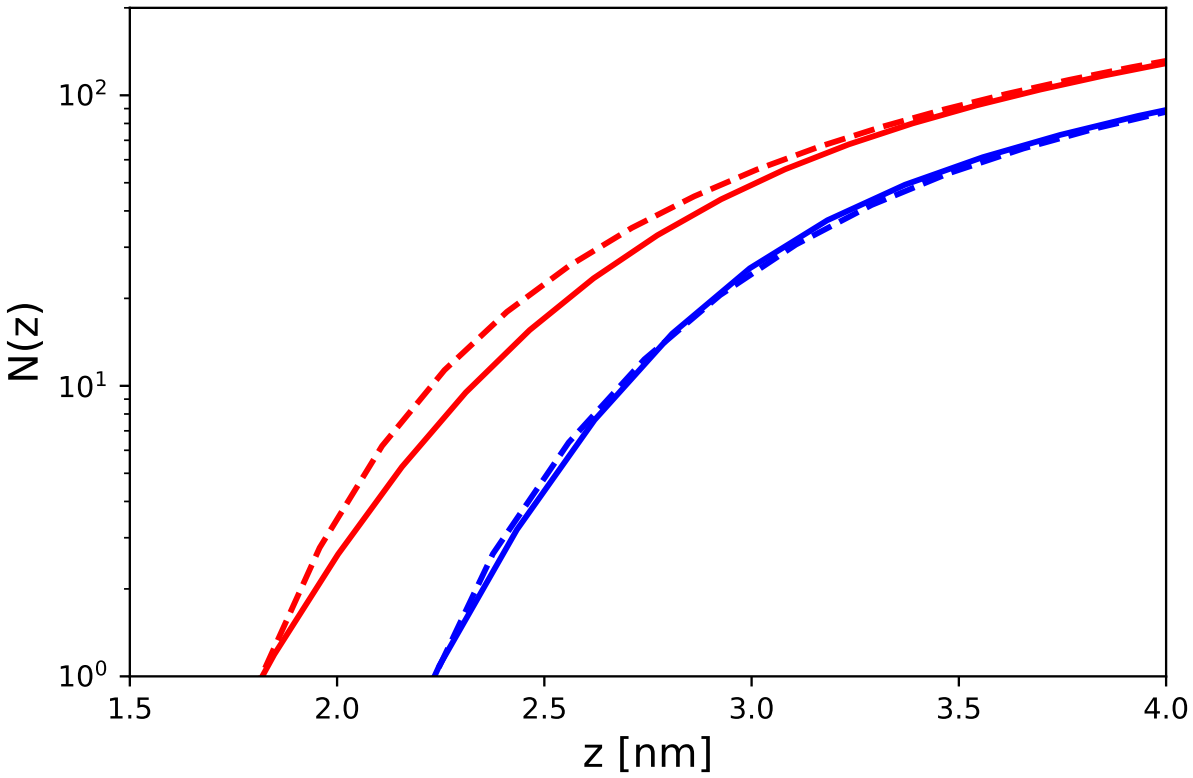

Figure 2: Cumulative number distribution functions $N((z)$ for ectoine (solid line) and amino ectoine (dashed line) for the gel (blue lines) and the fluid phase (red lines) in front of DPPC lipid bilayers at 300 K.

Preferential Binding Coefficients

Table 5: Preferential binding coefficients ν_{23} and differences of the preferential binding coefficients $\Delta\nu_{23}$ for DPPC lipid bilayers in the gel and the fluid phase in the presence of ectoine and amino ectoine, respectively.

Species	ν_{23} (gel)	ν_{23} (fluid)	$\Delta\nu_{23}$
Amino ectoine	-15.61 ± 0.32	-19.40 ± 0.11	-3.79 ± 0.43
Ectoine	-14.83 ± 0.12	-19.82 ± 0.07	-4.99 ± 0.06