Table S1. Standard thermodynamic characteristics of monomer formation for 2-monoacyl-*sn*-glycerols

The number of carbon atoms in $C_nH_{2n+1}COO$ substituent	Enthalpy of formation $\Delta H^0_{298,mon}$, kJ/mol	Absolute entropy of formation $S^0_{298,mon}$, J/(mol·K)	Gibbs energy of formation $\Delta G^0_{298,mon}$, kJ/mol
n=6	−877.28	595.77 (635.97)*	−526.56 (−538.54)*
n=7	−899.98	626.83 (673.73)	−517.91 (−531.89)
n=8	−922.64	660.10 (713.70)	−509.88 (−525.85)
n=9	−945.32	689.39 (749.69)	−500.68 (−518.65)
n=10	−967.96	723.52 (790.52)	−492.89 (−512.85)
n=11	−990.60	753.22 (826.92)	−483.78 (−505.74)
n=12	−1013.35	785.83 (866.23)	−475.63 (−499.59)
n=13	−1036.01	813.04 (900.14)	−465.80 (−491.76)
n=14	−1058.69	844.98 (938.78)	−457.40 (−485.35)
n=15	−1081.27	875.87 (976.37)	−448.57 (−478.52)
n=16	−1103.87	913.84 (1021.04)	−441.88 (−473.83)
n=17	−1126.75	939.63 (1053.53)	−431.84 (−465.78)

*Data in parentheses corresponds to corrected values of the absolute entropy and Gibbs energy of formation with account for the free rotation term of the methylene units of the hydrophobic chain

Table S2. Clusterization thermodynamic parameters of formation for small assosiates of 2-monoacyl-*sn*-glycerol in the approximation of PM3 method calculated at 298 K

The number of carbon atoms in $C_nH_{2n+1}COO$ substituent	$\Delta H^{Cl}_{298,m}$, kJ/mol	$\Delta S^{Cl}_{298,m}$, J/(mol·K)	$\Delta G^{Cl}_{298,m}$, kJ/mol	The number of carbon atoms in $C_nH_{2n+1}COO$ substituent	$\Delta H^{Cl}_{298,m}$, kJ/mol	$\Delta S^{Cl}_{298,m}$, J/(mol·K)	$\Delta G^{Cl}_{298,m}$, kJ/mol
Dimer, p							
n=6	−38.72	−210.62	24.04	*n*=12	−60.04	−282.48	24.13
n=7	−36.75	−217.98	28.21	*n*=13	−67.91	−290.50	18.66
n=8	−39.49	−235.46	30.68	*n*=14	−70.46	−303.49	19.98
n=9	−47.09	−243.45	25.46	*n*=15	−78.50	−318.31	16.36
n=10	−49.74	−257.95	27.13	*n*=16	−81.22	−341.00	20.40
n=11	−57.59	−271.00	23.16	*n*=17	−88.65	−346.03	14.46
Dimer, s							
n=6	−38.72	−210.62	24.04	*n*=12	−69.77	−288.51	16.21
n=7	−40.10	−212.55	23.24	*n*=13	−71.21	−284.61	13.60
n=8	−49.02	−239.86	22.46	*n*=14	−80.19	−307.21	11.35
n=9	−50.40	−238.40	20.64	*n*=15	−81.82	−311.74	11.08
n=10	−59.45	−264.80	19.46	*n*=16	−90.96	−343.64	11.45
n=11	−60.93	−264.38	17.86	*n*=17	−91.97	−336.65	8.35

Tetramer							
n=6	−130.90	−744.36	90.92	*n*=12	−251.29	−978.56	40.32
n=7	−147.66	−777.52	84.04	*n*=13	−269.66	−1059.36	46.03
n=8	−170.36	−832.15	77.62	*n*=14	−292.81	−1106.96	37.06
n=9	−187.28	−839.95	63.02	*n*=15	−311.54	−1143.65	29.27
n=10	−210.62	−917.88	62.91	*n*=16	−335.18	−1222.42	29.10
n=11	−228.12	−924.36	47.34	*n*=17	−352.82	−1234.87	15.17
Hexamer, p							
n=6	−228.44	−1276.37	151.92	*n*=12	−436.47	−1804.75	101.34
n=7	−257.24	−1334.15	140.34	*n*=13	−466.88	−1776.07	62.39
n=8	−295.38	−1478.23	145.13	*n*=14	−509.38	−1865.46	46.53
n=9	−324.11	−1523.68	129.95	*n*=15	−540.57	−1923.10	32.51
n=10	−366.43	−1627.66	118.62	*n*=16	−583.53	−2047.37	26.59
n=11	−394.34	−1645.36	95.98	*n*=17	−613.04	−2078.97	6.49
Octamer							
n=6	−318.51	−1875.04	240.26	*n*=9	−457.58	−2158.96	185.79
n=7	−359.53	−1963.41	225.57	*n*=10	−521.71	−2325.48	171.29
n=8	−423.66	−2041.14	184.60	*n*=11	−557.73	−2321.12	133.96