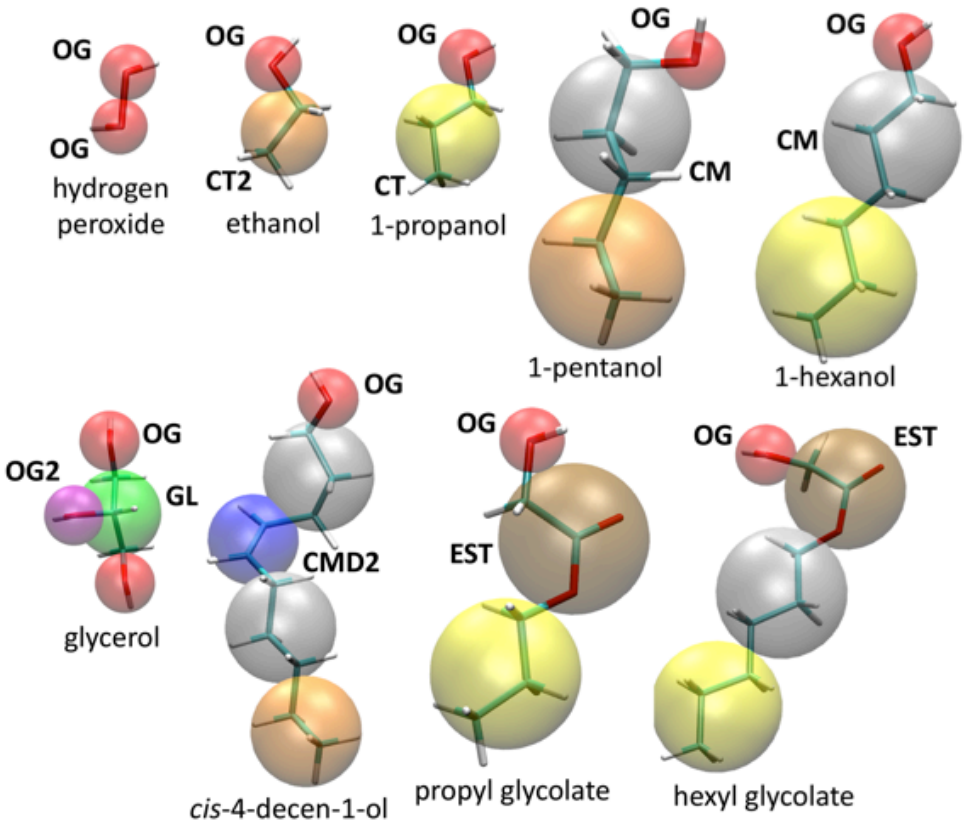
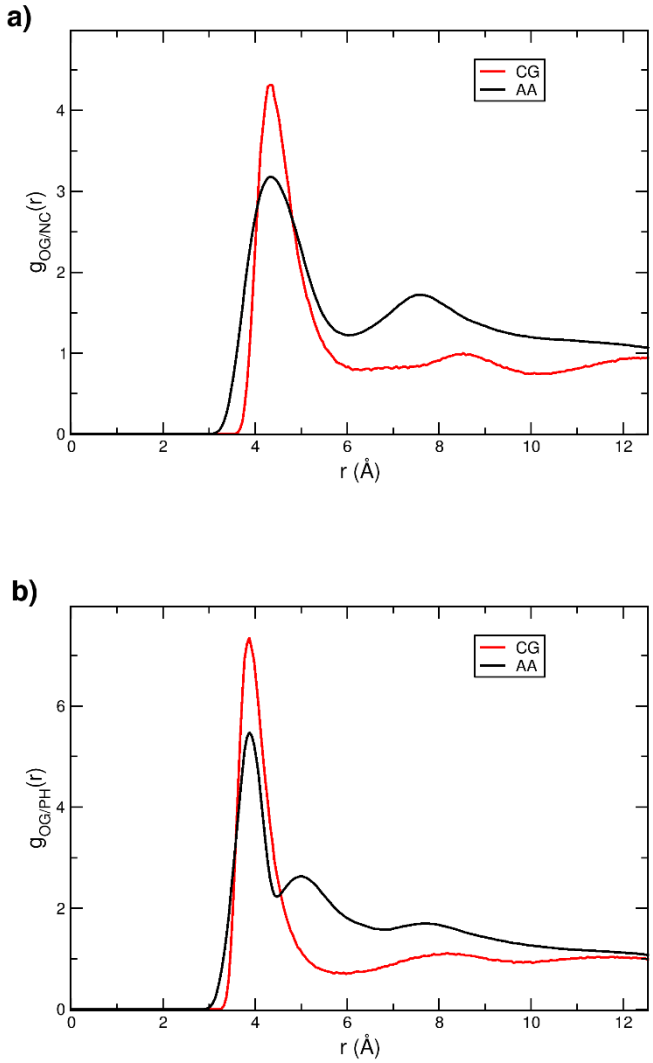
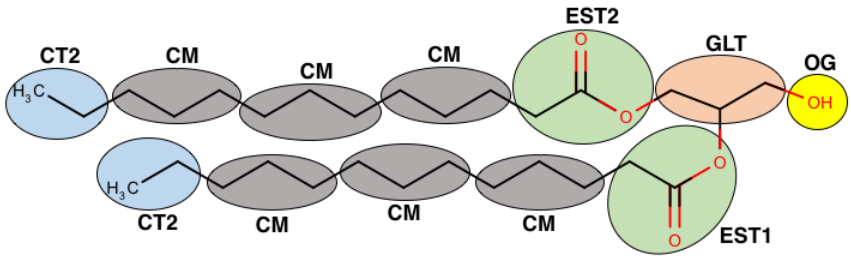


Supplementary Figure 1. All-atom (licorice) to coarse-grained (vdw) mapping for the compounds selected to derive the CG model for DAGs. New particles to account for the hydroxyl groups, named OG or OG2 depending on the chemical environment in which they are located, were introduced. In the case of glycerol, two different chemical environments in the vicinity of the OH groups, which strongly affects their CG bonded parameters, can be distinguished. For that reason, in this molecule, different names were given to the OG bead bound to C2 (OG2) and to those connected to the terminal carbons (OG) although their LJ parameters were adjusted to identical values.



Supplementary Figure 2. Comparison of all-atom and coarse-grained RDFs. (a) OG-NC and (b) OG-PH RDFs obtained from both all-atom (AA) and coarse-grained (CG) simulations. A DOPC/DOG mixed bilayer at an 85:15 molar ratio was employed as model system. An iterative protocol was used to tune the OG-NC and OG-PH coarse-grained non-diagonal LJ parameters until a consistent fit between both RDFs at short distances (maximizing the match in the location of the first peak) was found.



Supplementary Figure 3. All-atom to coarse-grained mapping for DLG.

Interaction	LJ type	ε (kcal mol^{-1})	σ (Å)
OG-OG	LJ9-6	0.3840	2.7850
OG-OG2	LJ9-6	0.3840	2.7580
OG-CT2	LJ9-6	0.3310	3.5470
OG-CT	LJ9-6	0.3840	3.6260
OG-CM	LJ9-6	0.2780	3.6340
OG-CMD2	LJ9-6	0.6970	3.4800
OG-GL	LJ9-6	0.2910	3.6945
OG-GLT	LJ9-6	0.2910	3.6945
OG-EST1	LJ9-6	0.2700	3.5825
OG-EST2	LJ9-6	0.2700	3.5825
OG-PH	LJ9-6	1.7133	3.3851
OG-NC	LJ9-6	0.5148	4.0397
OG-W	LJ12-4	0.7479	3.6580

Supplementary Table 1. Parameters corresponding to the Lennard Jones non-bonded interactions where the new OG bead was involved.

Compounds	Interaction	k_b (kcal mol^{-1} Å^{-2})	r_0 (Å)
H_2O_2	OG-OG	243.4977	1.5129
ethanol	OG-CT2	136.1780	1.8891
1-propanol	OG-CT	11.9654	2.5034
1-pentanol, 1-hexanol	OG-CM	13.5130	2.4662
glycerol	OG-GL	7.6443	2.3607
propyl and hexyl glycolate	OG-EST	106.2600	2.5354
DOG	OG-GLT	33.7103	2.1401

Supplementary Table 2. Bond stretching parameters corresponding to all bonded interactions in which the new OG bead was involved.

Compound	Interaction	Potential	k_θ (kcal mol^{-1} rad^{-2})	θ_0 (degree)
1-pentanol	OG-CM-CT2	sdk	4.470	153.290
1-hexanol	OG-CM-CT	sdk	2.874	158.846
glycerol	OG-GL-OG	sdk	3.620	142.557
glycerol	OG-GL-OG2	sdk	3.243	71.357
propyl glycolate	OG-EST-CT	sdk	0.852	176.582
hexyl glycolate	OG-EST-CM	sdk	0.858	179.970
DOG	OG-GLT-EST1	sdk	2.897	130.226
DOG	OG-GLT-EST2	sdk	5.943	112.856

Supplementary Table 3. Angle bending parameters corresponding to all bonded interactions in which the new OG bead was involved.

% DOG	Barrier (kcal mol^{-1})
5	1.14 ± 0.02
10	1.11 ± 0.01
15	1.05 ± 0.02
20	0.99 ± 0.02
30	0.86 ± 0.01

Supplementary Table 4. DOG flip-flop barriers calculated by Boltzmann inverting the populations obtained in the lateral density profiles.