

Effect of GM1 concentration change on plasma membrane: molecular
dynamics simulation and analysis

Yongkang Lyu, Shuo Chen, Yu Zhao, Hongxiu Yuan, Chenyang Zhang, Changzhe Zhang and
Qingtian Meng *

* Corresponding author. School of Physics and Electronics, Shandong Normal University, Jinan,
250014, People's Republic of China.

E-mail addresses: qtmeng@sdu.edu.cn

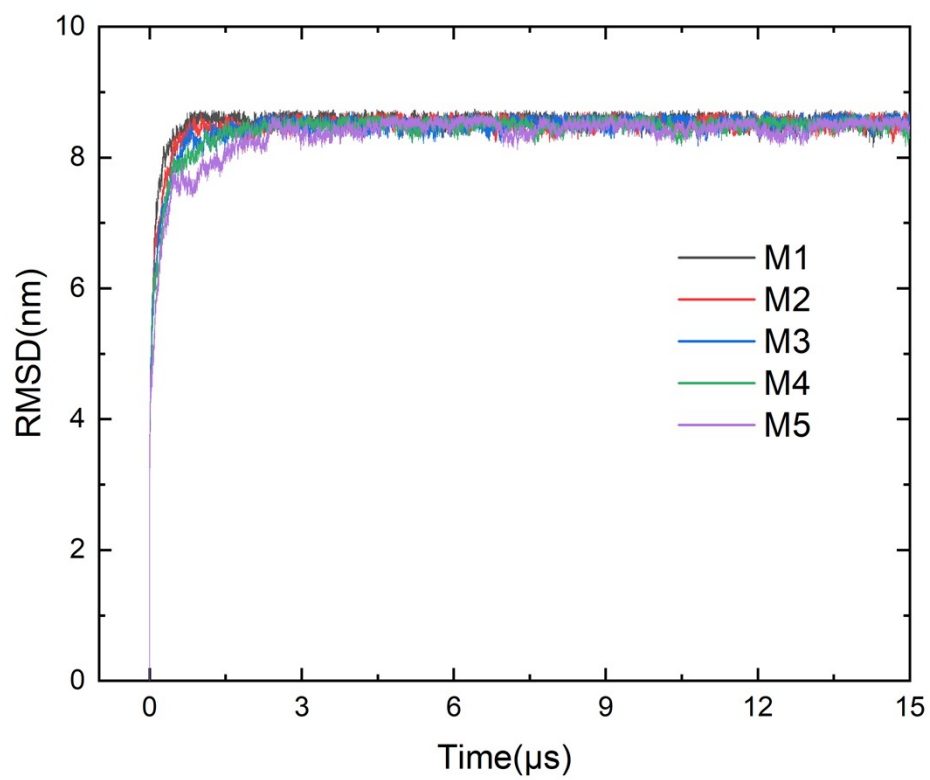


Fig. S1. RMSD of all the simulation systems.

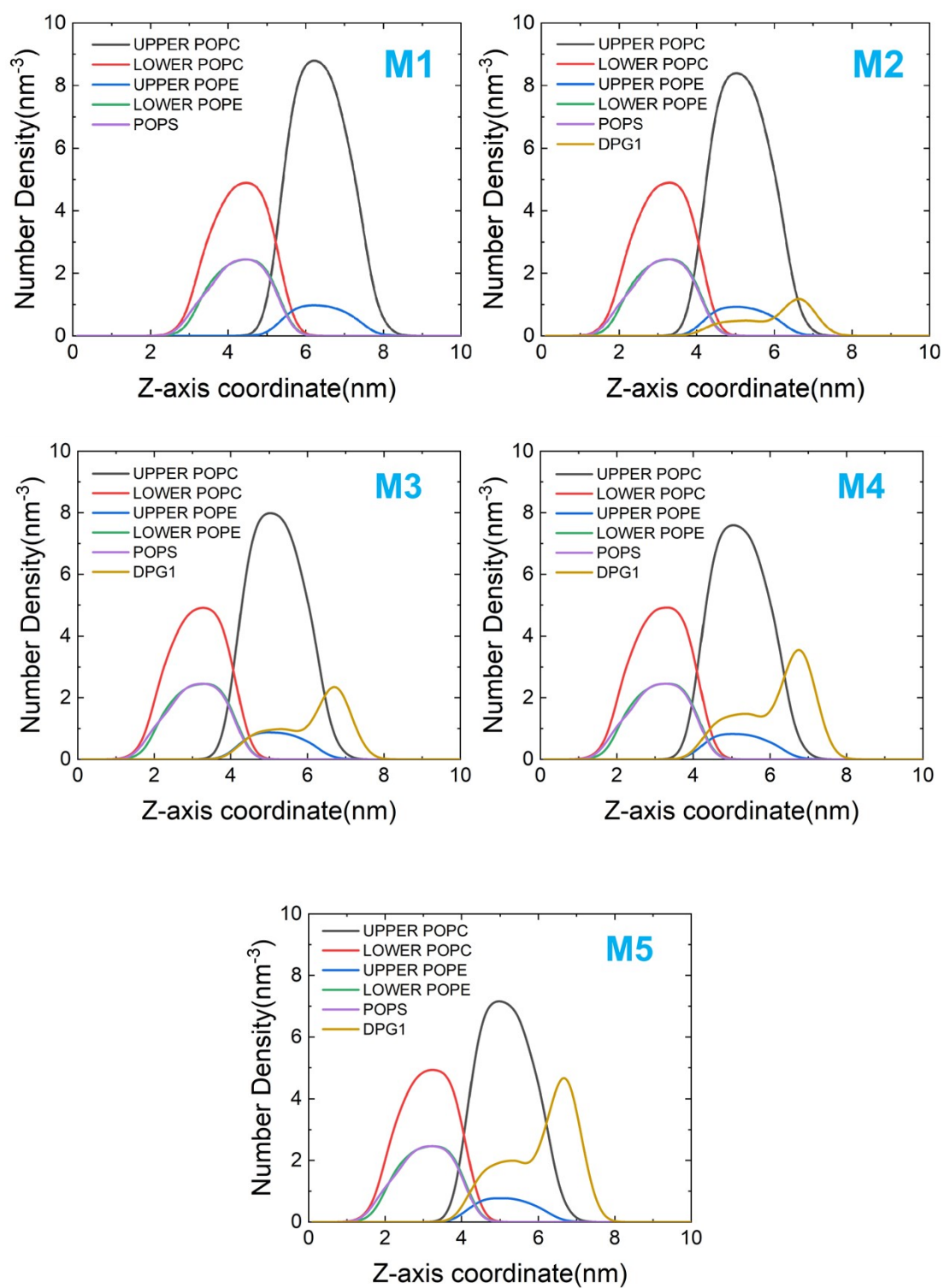


Fig. S2. Number density profiles of lipids measured along the membrane normal.

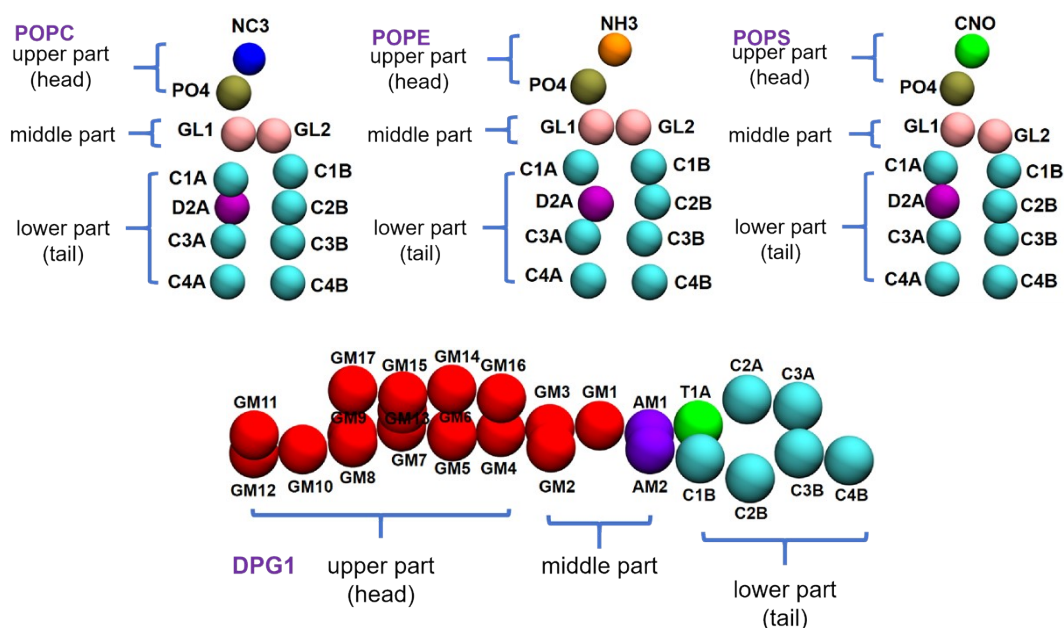


Fig. S3. Division of different regions of lipid molecules in the discussion of section 3.8. It should be noted that in lipidomics, the hydrophilic phosphate group is generally considered as the lipid head, and the hydrophobic alkyl chain as the lipid tail. The division here is a relatively arbitrary classification made for the convenience of discussion within the context of the main text.

Table. S1. The proportions of contacts between lipids in the two leaflets of membrane systems. The number in parentheses indicates the number of that item.

M2 UPPER	POPC	POPE	DPG1
POPC	76.6%(10015)	3.3%(429)	2.1%(274)
POPE	3.3%(429)	5.5%(719)	0.2%(32)
DPG1	2.1%(274)	0.2%(32)	12.3%(1606)

M2 LOWER	POPC	POPE	POPS
POPC	45.2%(4891)	6.1%(660)	6.2%(669)
POPE	6.1%(660)	19.5%(2109)	3.1%(333)
POPS	6.2%(669)	3.1%(333)	19.9%(2157)

M3 UPPER	POPC	POPE	DPG1
POPC	65.6%(9326)	2.7%(384)	3.8%(535)
POPE	2.7%(384)	4.8%(676)	0.4%(62)
DPG1	3.8%(535)	0.4%(62)	22.8%(3247)

M3 LOWER	POPC	POPE	POPS
POPC	45.2%(4912)	6.1%(664)	6.2%(675)
POPE	6.1%(664)	19.5%(2120)	3.1%(333)
POPS	6.2%(675)	3.1%(333)	19.9%(2164)

M4 UPPER	POPC	POPE	DPG1
POPC	56.0%(8646)	2.2%(340)	5.0%(775)
POPE	2.2%(340)	4.1%(630)	0.6%(91)
DPG1	5.0%(775)	0.6%(91)	32.1%(4947)

M4 LOWER	POPC	POPE	POPS
POPC	45.2%(4933)	6.1%(664)	6.2%(681)
POPE	6.1%(664)	19.5%(2126)	3.1%(339)
POPS	6.2%(681)	3.1%(339)	19.8%(2165)

M5 UPPER	POPC	POPE	DPG1
POPC	47.7%(7941)	1.8%(293)	6.0%(999)
POPE	1.8%(293)	3.6%(591)	0.7%(116)
DPG1	6.0%(999)	0.7%(116)	40.3%(6699)

M5 LOWER	POPC	POPE	POPS
POPC	45.3%(4956)	6.1%(671)	6.3%(686)
POPE	6.1%(671)	19.5%(2136)	3.1%(340)
POPS	6.3%(686)	3.1%(340)	19.8%(2175)

< 15%	15%~30%	> 30%
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Table. S2. 2D diffusion coefficients. The first two tables list the 2D diffusion rates of various lipids in the upper and lower leaflets of the membrane systems, while the last table shows that of the entire membrane, including both leaflets. The mathematical unit of the 2D diffusion coefficient is $10^{-7}\text{cm}^2\cdot\text{s}^{-1}$.

UPPER	M1	M2	M3	M4	M5
POPC	2.46±0.04	1.88±0.09	1.18±0.07	0.78±0.08	0.44±0.06
POPE	1.97±0.14	1.65±0.40	1.05±0.25	0.87±0.07	0.43±0.09
DPG1		0.99±0.13	0.70±0.18	0.44±0.09	0.26±0.06
LOWER	M1	M2	M3	M4	M5
POPC	2.46±0.54	2.21±0.11	2.18±0.60	2.11±0.35	1.72±0.00
POPE	2.35±0.05	2.34±0.21	1.97±0.19	1.86±0.08	1.73±0.16
POPS	2.46±0.24	2.32±0.73	2.36±0.21	2.14±0.37	2.00±0.14
BILAYER	M1	M2	M3	M4	M5
UPPER	2.41±0.05	1.76±0.03	1.14±0.04	0.69±0.08	0.38±0.06
LOWER	2.43±0.31	2.31±0.12	2.24±0.41	2.08±0.05	1.86±0.11