

Structural and Kinetic Properties of α -tocopherol in Phospholipid Bilayers, a Molecular Dynamics Simulation Study

Shan-Shan Qin, Zhi-Wu Yu*, and Yang-Xin Yu

Supporting Information

1. Force Field Deduction

1.1 The dihedral parameters

In order to ensure the R chirality of C15, C20, C25 and C30 in α -tocopherol, we first use improper dihedral parameters to keep the four chiral centers from flipping into S chirality. Then we deduce the proper dihedral parameters of CH1-CH2-CH2-CH2 and CH2-CH1-CH2-CH2, by calculating the stereo-energy of the two dihedrals from 0 to ± 180 degree every 15 degree apart, and fitting those energies to quantum chemistry calculation results, using Gaussian 98 at the 6-31G* level. And the two dihedral parameters can be directly used by other dihedrals in α -tocopherol tail. The fragments used to deduce dihedral parameters is shown in Figure S1 and Figure S2.

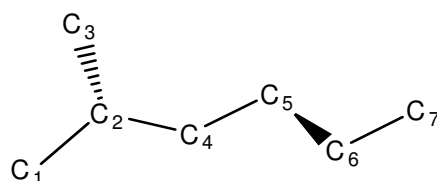


Figure S1. The fragment used to deduce C2-C4-C5-C6 dihedral parameters.

* To whom correspondence should be addressed. E-mail: yuzhw@tsinghua.edu.cn.

Angle (degree)	Quantum Energy(A.U.)	Relative Quantum Energy(kJ/mol)	MD Energy(kJ/mol)	Relative MD Energy(kJ/mol)	Torsional Energy(kJ/mol)
180	-274.3839128	0	3.976	0	0
165	-274.3830289	2.320169	4.378	0.402	1.918169
150	-274.3813772	6.655953	5.5	1.524	5.131953
135	-274.3792698	12.18772	3.273	-0.703	12.89072
120	-274.3792025	12.36454	11.394	7.418	4.946543
105	-274.3784538	14.32984	6.95	2.974	11.35584
90	-274.3808186	8.122225	3.22725	-0.74875	8.870975
75	-274.3780877	15.29078	9.98	6.004	9.28678
60	-274.3723236	30.42157	22.78	18.804	11.61757
45	-274.3761484	20.38145	19.63	15.654	4.727448
30	-274.3751322	23.0491	19.21	15.234	7.815101
15	-274.3709667	33.98353	17.45	13.474	20.50953
0	-274.3664689	45.7903	18.61	14.634	31.1563
-15	-274.3628372	55.32338	33.64	29.664	25.65938
-30	-274.3709059	34.14309	26.58	22.604	11.53909
-45	-274.3656056	48.0564	37.95	33.974	14.0824
-60	-274.3670367	44.29962	25.37	21.394	22.90562
-75	-274.3699247	36.71871	16.97	12.994	23.72471
-90	-274.3743598	25.07671	9.84	5.864	19.21271
-105	-274.3813772	6.655953	5.19	1.214	5.441953
-120	-274.3791332	12.54642	8.63	4.654	7.892424
-135	-274.3785637	14.04134	10.91	6.934	7.107338
-150	-274.3797512	10.92419	9.104	5.128	5.796195
-165	-274.3823582	4.080662	6.5	2.524	1.556662
-180	-274.3839128	0	3.976	0	0

The fitted result is:

$$E_{\text{Torsional}} = 83.2639(\cos\phi)^5 + 22.7450(\cos\phi)^4 - 94.3359(\cos\phi)^3 - 23.2166(\cos\phi)^2 + 26.5525(\cos\phi) + 14.6592$$

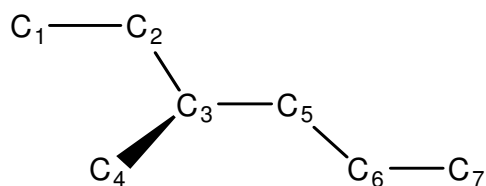


Figure S2. The fragment used to deduce C2-C3-C5-C6 dihedral parameters

Angle (degree)	Quantum Energy(A.U.)	Relative Quantum Energy(kJ/mol)	MD Energy(kJ/mol)	Relative MD Energy(kJ/mol)	Torsional Energy(kJ/mol)
180	-274.3825618	0	16.45	0	0
165	-274.37984	7.14601	23.4723	7.0223	0.12371
150	-274.37386	22.8465	36.81	20.36	2.4865
135	-274.36893	35.79021	47.82	31.37	4.420215
120	-274.36511	45.81962	58.04	41.59	4.229625
105	-274.36614	43.11536	56.67	40.22	2.89536
90	-274.37023	32.37706	48.72	32.27	0.107065
75	-274.37374	23.16156	36.99	20.54	2.62156
60	-274.37459	20.92988	28.5	12.05	8.879885
45	-274.37327	24.39554	25.66	9.21	15.18554
30	-274.37093	30.53921	27.78	11.33	19.20921
15	-274.36643	42.35396	33.04	16.59	25.76396
0	-274.36276	51.98955	38.32	21.87	30.11955
-15	-274.3608214	57.34341	41.87	25.42	31.92341
-30	-274.3709059	30.87165	28.96	12.51	18.36165
-45	-274.3788877	9.919416	19.5	3.05	6.869416
-60	-274.3650446	46.25744	36.7	20.25	26.00744
-75	-274.3701184	32.93878	25.9	9.45	23.48878
-90	-274.3717195	28.73587	19.72	3.27	25.46587
-105	-274.3771705	14.42707	13.78	-2.67	17.09707
-120	-274.3734915	24.08443	15.71	-0.74	24.82443
-135	-274.3771705	14.42707	13.8	-2.65	17.07707
-150	-274.3811664	3.937857	11.19	-5.26	9.197857
-165	-274.3837162	-2.75554	14.8624	-1.5876	-1.16794
-180	-274.3826665	0	16.45	0	0

$$E_{\text{Torsional}} = 37.9451(\cos\phi)^5 + 5.3846(\cos\phi)^4 - 28.0245(\cos\phi)^3 - 4.1356(\cos\phi)^2 + 6.5767(\cos\phi) + 13.2298$$

1.2 The force field for α -tocopherol in Gromacs format:

Atomtypes

name	bond_type	mass	charge	p_type	sigma	Epsilon
HO	HO	0	0	A	0.00E+00	0.00E+00
C3	C3	0	0	A	3.91E-01	6.69E-01
OS	OS	0	0	A	3.00E-01	7.11E-01
CT	CT	0	0	A	3.80E-01	2.09E-01

CB	CB	0	0	A	3.75E-01	4.60E-01
CA	CA	0	0	A	3.75E-01	4.60E-01
OH	OH	0	0	A	3.07E-01	8.80E-01
C2	C2	0	0	A	3.91E-01	4.94E-01
C1	C1	0	0	A	3.85E-01	3.35E-01

moleculetype

Name	nrexcl
VIT	3

atoms

nr	type	resnr	residue	atom	cgnr	charge	Mass
1	C2	1	VIT	CAJ	1	-0.149260	14
2	C2	1	VIT	CAT	2	0.099592	14
3	CB	1	VIT	CAX	3	-0.088009	12
4	CA	1	VIT	CAW	4	0.004509	12
5	C3	1	VIT	CBC	5	0.032485	15
6	CA	1	VIT	CBB	6	0.140251	12
7	OH	1	VIT	OBE	7	-0.527651	16
8	HO	1	VIT	HAA	8	0.397363	1
9	CA	1	VIT	CBA	9	-0.101017	12
10	C3	1	VIT	CAV	10	0.041773	15
11	CA	1	VIT	CAZ	11	0.035226	12
12	C3	1	VIT	CAU	12	0.024467	15
13	CB	1	VIT	CAY	13	0.015092	12
14	OS	1	VIT	OBD	14	-0.323149	16
15	CT	1	VIT	CAN	15	0.678142	12
16	C3	1	VIT	CAS	16	-0.107500	15
17	C2	1	VIT	CAR	17	-0.334848	14
18	C2	1	VIT	CAQ	18	0.201680	14
19	C2	1	VIT	CAA	19	-0.046655	14
20	C1	1	VIT	CAO	20	0.150445	13
21	C3	1	VIT	CAH	21	-0.111159	15
22	C2	1	VIT	CAM	22	-0.121733	14
23	C2	1	VIT	CAL	23	0.213581	14
24	C2	1	VIT	CAK	24	-0.227250	14
25	C1	1	VIT	CAI	25	0.272506	13
26	C3	1	VIT	CAF	26	-0.131782	15
27	C2	1	VIT	CAG	27	-0.036046	14
28	C2	1	VIT	CAE	28	0.041830	14
29	C2	1	VIT	CAD	29	-0.153113	14
30	C1	1	VIT	CAC	30	0.415516	13
31	C3	1	VIT	CAP	31	-0.159151	15
32	C3	1	VIT	CAB	32	-0.146140	15

bonds

ai	aj	funct	r	k
7	8	1	9.60E-02	4.63E+05
1	2	1	1.53E-01	2.59E+05
1	15	1	1.53E-01	2.59E+05
2	3	1	1.51E-01	2.65E+05
3	4	1	1.40E-01	3.92E+05
3	13	1	1.37E-01	4.35E+05
4	5	1	1.51E-01	2.65E+05
4	6	1	1.40E-01	3.92E+05
6	7	1	1.36E-01	3.77E+05
6	9	1	1.40E-01	3.92E+05
9	10	1	1.51E-01	2.65E+05
9	11	1	1.40E-01	3.92E+05
11	12	1	1.51E-01	2.65E+05
11	13	1	1.40E-01	3.92E+05
13	14	1	1.24E-01	4.02E+05
14	15	1	1.41E-01	2.68E+05
15	16	1	1.53E-01	2.59E+05
15	17	1	1.53E-01	2.59E+05
17	18	1	1.53E-01	2.59E+05
18	19	1	1.53E-01	2.59E+05
19	20	1	1.53E-01	2.59E+05
20	21	1	1.53E-01	2.59E+05
20	22	1	1.53E-01	2.59E+05
22	23	1	1.53E-01	2.59E+05
23	24	1	1.53E-01	2.59E+05
24	25	1	1.53E-01	2.59E+05
25	26	1	1.53E-01	2.59E+05
25	27	1	1.53E-01	2.59E+05
27	28	1	1.53E-01	2.59E+05
28	29	1	1.53E-01	2.59E+05
29	30	1	1.53E-01	2.59E+05
30	31	1	1.53E-01	2.59E+05
30	32	1	1.53E-01	2.59E+05

pairs

ai	aj	funct	r	k
4	8	1	0	0
8	9	1	0	0
1	4	1	0.35333	0.203
1	13	1	0.35333	0.203

1	18	1	0.36669	0.229
2	14	1	0.33335	0.285
2	16	1	0.36669	0.267
2	17	1	0.36669	0.229
2	5	1	0.36669	0.267
2	6	1	0.35333	0.203
2	11	1	0.35333	0.203
15	3	1	0.33997	0.203
3	7	1	0.32331	0.281
3	9	1	0.33997	0.18
3	12	1	0.35333	0.237
4	11	1	0.33997	0.18
4	14	1	0.31998	0.253
4	10	1	0.35333	0.237
5	13	1	0.35333	0.237
5	7	1	0.33667	0.371
5	9	1	0.35333	0.237
6	13	1	0.33997	0.18
6	12	1	0.35333	0.237
7	10	1	0.33667	0.371
7	11	1	0.32331	0.281
9	14	1	0.31998	0.253
10	12	1	0.36669	0.313
10	13	1	0.35333	0.237
11	15	1	0.33997	0.203
12	14	1	0.33335	0.333
13	16	1	0.35333	0.237
13	17	1	0.35333	0.203
14	18	1	0.33335	0.285
15	19	1	0.35333	0.229
16	18	1	0.36669	0.267
17	20	1	0.35779	0.218
18	21	1	0.36669	0.267
18	22	1	0.36669	0.229
19	23	1	0.36669	0.229
20	24	1	0.35779	0.218
21	23	1	0.36669	0.267
22	25	1	0.35779	0.218
23	26	1	0.36669	0.267
23	27	1	0.36669	0.229
24	28	1	0.36669	0.229
25	29	1	0.35779	0.218
26	28	1	0.36669	0.267
27	30	1	0.35779	0.218

28	31	1	0.36669	0.267
28	32	1	0.36669	0.267

angles

ai	aj	ak	funct	theta	Cth
6	7	8	1	1.13E+02	4.18E+02
1	2	3	1	1.14E+02	5.27E+02
1	15	14	1	1.10E+02	4.18E+02
1	15	16	1	1.10E+02	3.35E+02
1	15	17	1	1.10E+02	3.35E+02
2	1	15	1	1.10E+02	3.35E+02
2	3	4	1	1.20E+02	5.86E+02
2	3	13	1	1.20E+02	5.86E+02
3	4	5	1	1.20E+02	5.86E+02
3	4	6	1	1.20E+02	5.27E+02
3	13	11	1	1.17E+02	5.27E+02
3	13	14	1	1.25E+02	6.69E+02
4	3	13	1	1.17E+02	5.27E+02
4	6	7	1	1.20E+02	5.86E+02
4	6	9	1	1.20E+02	5.27E+02
5	4	6	1	1.20E+02	5.86E+02
6	9	10	1	1.20E+02	5.86E+02
6	9	11	1	1.20E+02	5.27E+02
7	6	9	1	1.20E+02	5.86E+02
9	11	12	1	1.20E+02	5.86E+02
9	11	13	1	1.20E+02	5.27E+02
10	9	11	1	1.20E+02	5.86E+02
11	13	14	1	1.25E+02	6.69E+02
12	11	13	1	1.20E+02	5.86E+02
13	14	15	1	1.17E+02	5.02E+02
14	15	16	1	1.10E+02	4.18E+02
14	15	17	1	1.10E+02	4.18E+02
15	17	18	1	1.10E+02	3.35E+02
16	15	17	1	1.10E+02	3.35E+02
17	18	19	1	1.10E+02	3.35E+02
18	19	20	1	1.10E+02	3.35E+02
19	20	21	1	1.10E+02	3.35E+02
19	20	22	1	1.10E+02	3.35E+02
20	22	23	1	1.10E+02	3.35E+02
21	20	22	1	1.10E+02	3.35E+02
22	23	24	1	1.10E+02	3.35E+02
23	24	25	1	1.10E+02	3.35E+02
24	25	26	1	1.10E+02	3.35E+02
24	25	27	1	1.10E+02	3.35E+02

25	27	28	1	1.10E+02	3.35E+02
26	25	27	1	1.10E+02	3.35E+02
27	28	29	1	1.10E+02	3.35E+02
28	29	30	1	1.10E+02	3.35E+02
29	30	31	1	1.10E+02	3.35E+02
29	30	32	1	1.10E+02	3.35E+02
31	30	32	1	1.10E+02	3.35E+02

dihedrals

i	j	k	l	func	C0	C1	C2	C3	C4	C5
4	6	7	8	3	7.5312	0	-7.5312	0	0	0
8	7	6	9	3	7.5312	0	-7.5312	0	0	0
1	2	3	4	3	0	0	0	0	0	0
1	2	3	13	3	0	0	0	0	0	0
1	15	14	13	3	1.60247	4.80742	0	-6.40989	0	0
1	15	17	18	3	1.95393	5.86178	0	-7.81571	0	0
2	1	15	14	3	1.95393	5.86178	0	-7.81571	0	0
2	1	15	16	3	1.95393	5.86178	0	-7.81571	0	0
2	1	15	17	3	1.95393	5.86178	0	-7.81571	0	0
2	3	4	5	3	29.288	0	-29.288	0	0	0
2	3	4	6	3	29.288	0	-29.288	0	0	0
2	3	13	11	3	45.6056	0	-45.6056	0	0	0
2	3	13	14	3	45.6056	0	-45.6056	0	0	0
15	1	2	3	3	15.8992	24.2672	-5.0208	-26.7776	0	0
3	4	6	7	3	30.334	0	-30.334	0	0	0
3	4	6	9	3	30.334	0	-30.334	0	0	0
3	13	11	9	3	29.288	0	-29.288	0	0	0
3	13	11	12	3	29.288	0	-29.288	0	0	0
3	13	14	15	3	8.7864	0	-8.7864	0	0	0
4	3	13	11	3	45.6056	0	-45.6056	0	0	0
4	3	13	14	3	45.6056	0	-45.6056	0	0	0
4	6	9	10	3	30.334	0	-30.334	0	0	0
4	6	9	11	3	30.334	0	-30.334	0	0	0
5	4	3	13	3	29.288	0	-29.288	0	0	0
5	4	6	7	3	30.334	0	-30.334	0	0	0
5	4	6	9	3	30.334	0	-30.334	0	0	0
6	4	3	13	3	29.288	0	-29.288	0	0	0
6	9	11	12	3	30.334	0	-30.334	0	0	0
6	9	11	13	3	30.334	0	-30.334	0	0	0
7	6	9	10	3	30.334	0	-30.334	0	0	0
7	6	9	11	3	30.334	0	-30.334	0	0	0
9	11	13	14	3	29.288	0	-29.288	0	0	0
10	9	11	12	3	30.334	0	-30.334	0	0	0
10	9	11	13	3	30.334	0	-30.334	0	0	0

11	13	14	15	3	8.7864	0	-8.7864	0	0	0
12	11	13	14	3	29.288	0	-29.288	0	0	0
13	14	15	16	3	1.60247	4.80742	0	-6.40989	0	0
13	14	15	17	3	1.60247	4.80742	0	-6.40989	0	0
14	15	17	18	3	1.95393	5.86178	0	-7.81571	0	0
15	17	18	19	3	14.6592	-26.5525	-23.2166	94.3359	22.7450	-83.2639
16	15	17	18	3	1.95393	5.86178	0	-7.81571	0	0
17	18	19	20	3	14.6592	-26.5525	-23.2166	94.3359	22.7450	-83.2639
18	19	20	22	3	13.2298	-6.5767	-4.1356	28.0245	5.3846	-37.9451
19	20	22	23	3	13.2298	-6.5767	-4.1356	28.0245	5.3846	-37.9451
20	22	23	24	3	14.6592	-26.5525	-23.2166	94.3359	22.7450	-83.2639
22	23	24	25	3	14.6592	-26.5525	-23.2166	94.3359	22.7450	-83.2639
23	24	25	27	3	13.2298	-6.5767	-4.1356	28.0245	5.3846	-37.9451
24	25	27	28	3	13.2298	-6.5767	-4.1356	28.0245	5.3846	-37.9451
25	27	28	29	3	14.6592	-26.5525	-23.2166	94.3359	22.7450	-83.2639
27	28	29	30	3	14.6592	-26.5525	-23.2166	94.3359	22.7450	-83.2639
28	29	30	32	3	13.2298	-6.5767	-4.1356	28.0245	5.3846	-37.9451
4	9	6	7	3	9.2048	0	-9.2048	0	0	0
3	13	4	2	2	0	1673.6	0	1673.6	3	13
4	3	6	5	2	0	1673.6	0	1673.6	4	3
6	4	9	7	2	0	1673.6	0	1673.6	6	4
9	6	11	10	2	0	1673.6	0	1673.6	9	6
11	9	13	12	2	0	1673.6	0	1673.6	11	9
13	14	11	3	2	0	1673.6	0	1673.6	13	14
4	6	9	11	2	0	1673.6	0	1673.6	4	6
6	9	11	13	2	0	1673.6	0	1673.6	6	9
9	11	13	3	2	0	1673.6	0	1673.6	9	11
11	13	3	4	2	0	1673.6	0	1673.6	11	13
13	3	4	6	2	0	1673.6	0	1673.6	13	3
15	1	14	16	2	35.3	836.8	35.3	836.8	15	1
20	19	21	22	2	35.3	836.8	35.3	836.8	20	19
25	26	27	24	2	35.3	836.8	35.3	836.8	25	26
30	29	31	32	2	35.3	836.8	35.3	836.8	30	29

2. Deuterium order parameter for lipids

The deuterium order parameters of *sn*-1 and *sn*-2 tail of all the phospholipids in four mixed systems and pure lipid bilayers over the last 40 ns of the 200 ns simulations have been calculated, and the results are listed in Table S1-S4.

Table S1. Deuterium order parameter of DPPC *sn*-1 and *sn*-2 acyl chain in mixed and pure bilayers.

α-tocopherol/DPPC						
	280 K		310 K		350 K	
*Atom	<i>sn</i>-1	<i>sn</i>-2	<i>sn</i>-1	<i>sn</i>-2	<i>sn</i>-1	<i>sn</i>-2
C2	0.185866	0.174439	0.181763	0.169935	0.161578	0.166443
C3	0.211723	0.184941	0.199816	0.176330	0.175167	0.168430
C4	0.206832	0.201947	0.193715	0.186689	0.169365	0.172986
C5	0.213468	0.204621	0.195141	0.186769	0.167211	0.168235
C6	0.209703	0.209454	0.190871	0.188812	0.161150	0.165683
C7	0.208582	0.206578	0.187078	0.185128	0.155876	0.158170
C8	0.196903	0.202095	0.176853	0.178535	0.145748	0.149664
C9	0.191733	0.196382	0.169366	0.170155	0.135772	0.139141
C10	0.176114	0.185818	0.154720	0.159027	0.120417	0.125475
C11	0.167275	0.177530	0.142475	0.148060	0.108075	0.113190
C12	0.150745	0.162103	0.126230	0.132592	0.092545	0.098560
C13	0.138536	0.150441	0.112880	0.119536	0.080497	0.085470
C14	0.117213	0.129655	0.093774	0.100096	0.064834	0.069618
C15	0.096442	0.108587	0.076207	0.081161	0.051024	0.054907
Pure DPPC						
	280 K		310 K		350 K	
*Atom	<i>sn</i>-1	<i>sn</i>-2	<i>sn</i>-1	<i>sn</i>-2	<i>sn</i>-1	<i>sn</i>-2
C2	0.203002	0.184418	0.173425	0.169145	0.158823	0.165009
C3	0.220609	0.184726	0.192643	0.174726	0.173759	0.166298
C4	0.216754	0.208922	0.187476	0.185463	0.168101	0.170995
C5	0.222309	0.207299	0.190610	0.182571	0.166432	0.164957
C6	0.218587	0.214346	0.185565	0.183308	0.159014	0.163531
C7	0.218920	0.213675	0.180768	0.178601	0.152586	0.155209
C8	0.211440	0.212006	0.167683	0.170841	0.140794	0.146450
C9	0.204626	0.208016	0.159100	0.162077	0.131078	0.135923
C10	0.192934	0.198141	0.142662	0.148238	0.116251	0.121937
C11	0.183875	0.190295	0.131390	0.137010	0.104791	0.110432
C12	0.168242	0.177040	0.115465	0.122079	0.090480	0.095897
C13	0.154792	0.163877	0.103294	0.110481	0.079153	0.084259
C14	0.132850	0.142849	0.085904	0.093777	0.064319	0.068895
C15	0.109298	0.119363	0.070110	0.076242	0.050915	0.054426

Note: * The carbon atoms in the *sn*-1 and *sn*-2 acyl chain are numbered from C=O to the tail end.

Table S2. Deuterium order parameter of POPC *sn*-1 and *sn*-2 acyl chain in mixed and pure bilayers.

α-tocopherol/POPC						
*Atom	280 K		310 K		350 K	
	<i>sn</i>-1	<i>sn</i>-2	<i>sn</i>-1	<i>sn</i>-2	<i>sn</i>-1	<i>sn</i>-2
C2	0.191023	0.161310	0.182127	0.168615	0.160921	0.158365
C3	0.211182	0.183854	0.202066	0.180529	0.178143	0.166858
C4	0.209853	0.186602	0.195321	0.180365	0.171841	0.163265
C5	0.211567	0.196445	0.196905	0.192448	0.170303	0.168969
C6	0.204968	0.182318	0.191590	0.178445	0.163035	0.154189
C7	0.202210	0.192962	0.185695	0.193795	0.157175	0.168005
C8	0.191154	0.162156	0.173114	0.160626	0.145587	0.137796
C9	0.186013	0.154897	0.165650	0.154557	0.136345	0.132331
C10	0.169684	0.118265	0.148679	0.119569	0.120400	0.104400
C11	0.161579	0.126164	0.138570	0.124686	0.109372	0.104733
C12	0.142036	0.149169	0.121757	0.147043	0.094883	0.123890
C13	0.130545	0.118409	0.109947	0.108115	0.083506	0.084880
C14	0.108705	0.125676	0.090920	0.115290	0.067594	0.090064
C15	0.091538	0.097424	0.074041	0.084035	0.053475	0.061582
		0.096945		0.083218		0.061229
		0.064888		0.053005		0.036457
Pure POPC						
*Atom	280 K		310 K		350 K	
	<i>sn</i>-1	<i>sn</i>-2	<i>sn</i>-1	<i>sn</i>-2	<i>sn</i>-1	<i>sn</i>-2
C2	0.173535	0.165962	0.168353	0.163526	0.159255	0.152293
C3	0.189455	0.183625	0.189760	0.174484	0.176744	0.163373
C4	0.180686	0.181600	0.181029	0.172014	0.171300	0.159651
C5	0.187016	0.189795	0.186648	0.182189	0.170628	0.166302
C6	0.187244	0.178577	0.180645	0.165953	0.164883	0.150539
C7	0.189080	0.191993	0.179950	0.180921	0.159815	0.165153
C8	0.184548	0.163606	0.168882	0.150078	0.148910	0.135614
C9	0.181534	0.155896	0.163280	0.144257	0.140298	0.130682
C10	0.170858	0.130260	0.148584	0.111449	0.124441	0.101121
C11	0.162643	0.139254	0.139417	0.115877	0.112436	0.102226
C12	0.146432	0.162480	0.121662	0.134271	0.096406	0.121279
C13	0.135423	0.131014	0.110260	0.099359	0.084974	0.086047
C14	0.113533	0.136858	0.091108	0.106871	0.069067	0.091123
C15	0.097259	0.107458	0.075662	0.078300	0.054407	0.063824
		0.105208		0.078089		0.063902
		0.071289		0.050606		0.038534

Note: * The carbon atoms in the *sn*-1 and *sn*-2 acyl chain are numbered from C=O to the tail end.

Table S3. Deuterium order parameter of DPPE *sn*-1 and *sn*-2 acyl chain in mixed and pure bilayers.

α-tocopherol/DPPE						
	280 K		310 K		350 K	
*Atom	<i>sn</i>-1	<i>sn</i>-2	<i>sn</i>-1	<i>sn</i>-2	<i>sn</i>-1	<i>sn</i>-2
C2	0.328091	0.320750	0.348310	0.348102	0.231837	0.239106
C3	0.332701	0.317774	0.364698	0.349367	0.249259	0.241973
C4	0.341574	0.336859	0.377709	0.371356	0.259757	0.261525
C5	0.344317	0.337428	0.383117	0.379876	0.265005	0.262140
C6	0.347312	0.344443	0.390378	0.391924	0.270690	0.271136
C7	0.345572	0.345481	0.395411	0.395196	0.272029	0.269021
C8	0.344417	0.345579	0.396288	0.398906	0.269572	0.269793
C9	0.343597	0.347397	0.396557	0.397903	0.265350	0.263747
C10	0.341997	0.347538	0.394482	0.398204	0.256136	0.257060
C11	0.341468	0.348418	0.391725	0.395782	0.244610	0.245741
C12	0.339232	0.348016	0.385269	0.393192	0.228061	0.232598
C13	0.334360	0.345857	0.374545	0.385782	0.206324	0.211563
C14	0.317467	0.334782	0.346904	0.366621	0.175926	0.183965
C15	0.277080	0.303481	0.296975	0.321742	0.136856	0.143871
Pure DPPE						
	280 K		310 K		350 K	
*Atom	<i>sn</i>-1	<i>sn</i>-2	<i>sn</i>-1	<i>sn</i>-2	<i>sn</i>-1	<i>sn</i>-2
C2	0.333195	0.319564	0.351835	0.359804	0.214300	0.216552
C3	0.346079	0.340153	0.366201	0.368216	0.232991	0.222496
C4	0.361040	0.358784	0.385298	0.385594	0.242626	0.244646
C5	0.370050	0.368201	0.395111	0.391485	0.248374	0.245130
C6	0.376920	0.374648	0.399556	0.397301	0.252949	0.254127
C7	0.380700	0.377111	0.399575	0.400205	0.253646	0.251991
C8	0.381837	0.376376	0.400087	0.400604	0.250887	0.251903
C9	0.380582	0.375460	0.398749	0.401461	0.244988	0.245275
C10	0.378869	0.374172	0.398848	0.400173	0.234445	0.238038
C11	0.374581	0.373864	0.398022	0.400254	0.222774	0.226493
C12	0.367909	0.371783	0.395492	0.399322	0.205762	0.212436
C13	0.356489	0.367484	0.386321	0.395752	0.185219	0.192424
C14	0.333869	0.352335	0.362117	0.378336	0.156819	0.166237
C15	0.289200	0.317171	0.310069	0.337319	0.122533	0.130132

Note: * The carbon atoms in the *sn*-1 and *sn*-2 acyl chain are numbered from C=O to the tail end.

Table S4. Deuterium order parameter of POPE *sn*-1 and *sn*-2 acyl chain in mixed and pure bilayers.

α-tocopherol/POPE						
*Atom	280 K		310 K		350 K	
	<i>sn</i>-1	<i>sn</i>-2	<i>sn</i>-1	<i>sn</i>-2	<i>sn</i>-1	<i>sn</i>-2
C2	0.281853	0.260688	0.261642	0.222891	0.219985	0.210584
C3	0.314066	0.300643	0.284975	0.252125	0.244864	0.227306
C4	0.332577	0.301931	0.291608	0.264792	0.252432	0.237796
C5	0.345768	0.319980	0.303885	0.282758	0.259826	0.254520
C6	0.352562	0.310974	0.312130	0.276850	0.263535	0.246471
C7	0.358347	0.330334	0.318937	0.302741	0.266508	0.271015
C8	0.359256	0.280278	0.319275	0.263261	0.262863	0.231713
C9	0.360719	0.265600	0.319289	0.249462	0.260726	0.219964
C10	0.354489	0.240604	0.312221	0.237790	0.250307	0.209881
C11	0.349591	0.260117	0.306948	0.254136	0.242805	0.218963
C12	0.336658	0.314625	0.294208	0.299435	0.227573	0.255798
C13	0.322831	0.295727	0.279494	0.269278	0.211120	0.213751
C14	0.291758	0.307613	0.248410	0.278749	0.181738	0.219914
C15	0.248057	0.277158	0.208508	0.237419	0.147636	0.172162
		0.265026		0.225241		0.162289
		0.196635		0.154133		0.101683
Pure POPE						
*Atom	280 K		310 K		350 K	
	<i>sn</i>-1	<i>sn</i>-2	<i>sn</i>-1	<i>sn</i>-2	<i>sn</i>-1	<i>sn</i>-2
C2	0.289070	0.266976	0.225816	0.218371	0.218669	0.210417
C3	0.316216	0.293563	0.249846	0.241466	0.241859	0.232434
C4	0.326417	0.294944	0.260205	0.254855	0.250729	0.239338
C5	0.339445	0.313547	0.268372	0.272729	0.259162	0.257225
C6	0.343460	0.302568	0.274438	0.262891	0.263372	0.245203
C7	0.351951	0.321691	0.279400	0.288197	0.267206	0.269304
C8	0.351684	0.275379	0.277152	0.244819	0.263699	0.228822
C9	0.354380	0.263941	0.276631	0.232752	0.261451	0.218299
C10	0.349561	0.236582	0.267493	0.221317	0.251742	0.203819
C11	0.347677	0.257575	0.261256	0.231905	0.243391	0.212900
C12	0.337265	0.314510	0.245385	0.270800	0.227392	0.248804
C13	0.326046	0.295856	0.228438	0.232184	0.209678	0.207392
C14	0.297689	0.307534	0.197773	0.239785	0.180705	0.214254
C15	0.256681	0.276620	0.161602	0.192974	0.146270	0.169220
		0.264445		0.182660		0.160585
		0.197512		0.116940		0.101464

Note: * The carbon atoms in the *sn*-1 and *sn*-2 acyl chain are numbered from C=O to the tail end.

3. Coordinates of atom O7 at 350 K

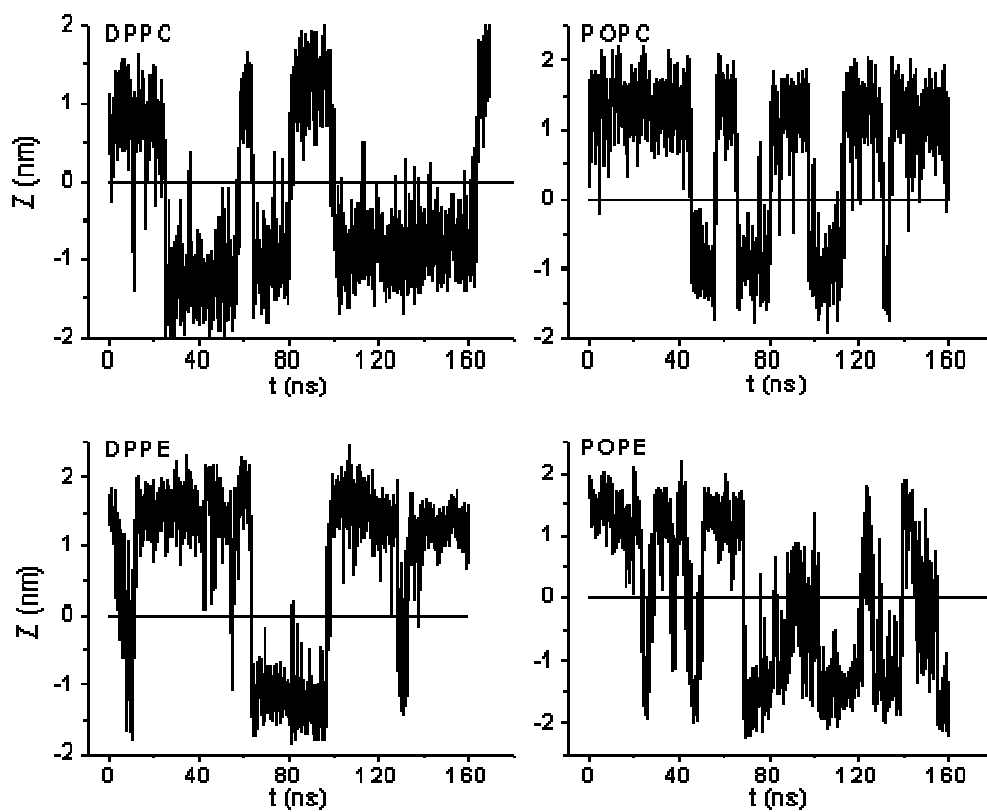


Figure S3. Coordinates of atom O7 in α -tocopherol in Z direction changing with time at 350 K in four α -tocopherol/lipid systems. $Z=0$ represents the bilayer center.