Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

The Effect of POPC Acyl Chains Packing by Aromatic Amino Acid Methyl Esters Investigated by ATR-FTIR Combined with QM Calculations

Bo Peng,[a] Xiao-Yan Ding,[a] Chao Sun,[a] Wei Liu,[b] John Z. H. Zhang,[b,c] Xin Zhao*[a]

[a]Shanghai Key Laboratory of Magnetic Resonance, Department of Physics, School of Physics and Materials Science, East China Normal University, Shanghai 200062, P. R. China
[b]State Key Laboratory of Precision Spectroscopy, Department of Physics, School of Physics and Materials Science, East China Normal University, Shanghai 200062, P. R. China
[c]NYU-ECNU Center for Computational Chemistry at NYU Shanghai, Shanghai 200062, P. R. China

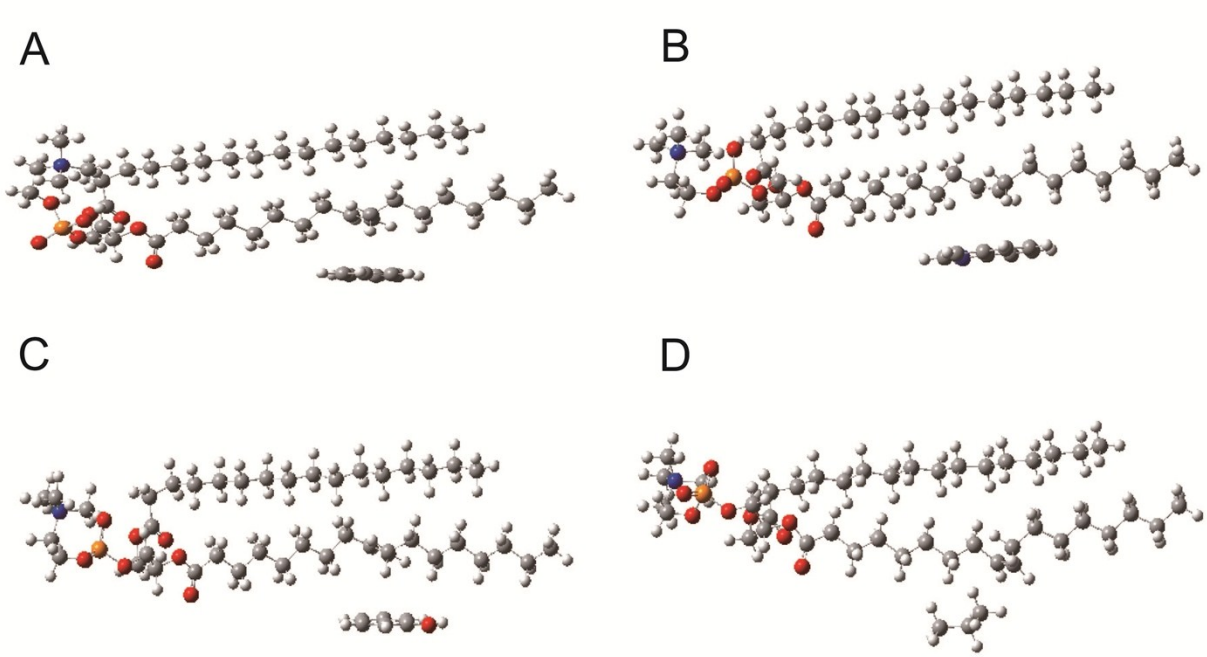

Fig. S1. Optimised geometries of study compounds determined by QM calculations at the ωB97X-D/6-31G (d,p) level. (A) benzene with POPC, (B) indole with POPC, (C) phenol with POPC, (D) propane with POPC. C (grey), H (white), O (red), N (blue), P (orange).

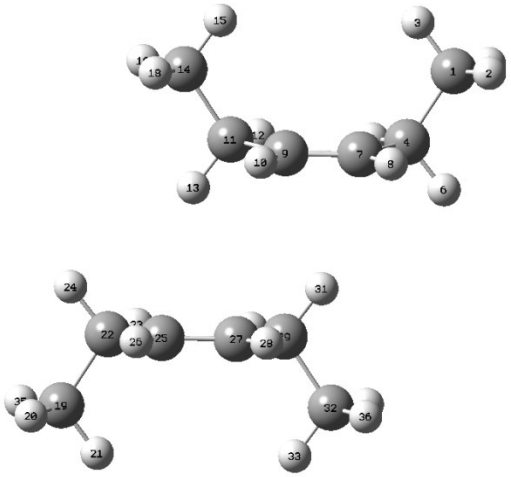

Fig. S2. Optimised geometry of 3-hexene with 3-hexene determined by QM calculations at the MP2/6-31G (d,p) level. C (grey), H (white).

Table S1. Important infrared group frequencies obtained by second derivative spectra of POPC bilayers and POPC bilayer–amino acid methyl ester complexes at a molar ratio of 10:1.

Frequencies(cm^{-1})					Assignments
POPC	POPC+Trp-OMe	POPC+Phe-OMe	POPC+Tyr-OMe	POPC+Leu-OMe	
3010	3007	3007	3008	3009	ν(=CH)
2961	2961	2961	2961	2961	$\nu_{as}(CH_3)$
2919	2921	2921	2922	2920	$\nu_{as}(CH_2)$
2883	2887	2886	2886	2885	$\nu_{s}(CH_3)$

2850	2852	2851	2852	2851	$\nu_s(CH_2)$
1735	1735	1735	1736	1735	ν(C=O),ester
1651	1646	1646	1646	1651	ν(C=C)
1465	1463	1464	1464	1465	$\delta_{as}(CH_2)$
1375	1375	1375	1375	1375	$\delta_s(^+N\text{-}CH_3)$
1241	1239	1240	1243	1241	$\nu_{as}(PO_2^-)$
1172	1170	1170	1172	1171	ν_{as}(C-O-C),ester
1091	1090	1091	1093	1091	$\nu_s(PO_2^-)$
1055	1054	1054	1055	1054	ν_s(C-O-C),ester
968	967	967	967	967	$\nu_{as}(C\text{-}N^+\text{-}C)$
919	919	919	919	919	$\nu_s(C\text{-}N^+\text{-}C)$

Table S2. Geometry parameters for 3-hexene–3-hexene complexes in 3.27 Å.

Atom symbol	x	y	z
C	-4.58372	0.718342	-0.169711
H	-4.947923	1.107442	0.781095
H	-4.81931	-0.344554	-0.20722
C	-3.074791	0.935575	-0.304061
H	-2.735609	0.55219	-1.266235
H	-2.868061	2.009813	-0.308085
C	-2.320124	0.294707	0.823052
H	-2.523506	0.711112	1.806423
C	-1.458464	-0.735024	0.751598
H	-1.017012	-1.084871	1.680597
C	-1.044939	-1.501348	-0.468427
H	-1.45655	-1.050612	-1.371585
H	0.043098	-1.449581	-0.556468
C	-1.476265	-2.967061	-0.386014
H	-2.561539	-3.045075	-0.329132
H	-1.13804	-3.527421	-1.257485
H	-5.128416	1.219231	-0.969784
H	-1.060508	-3.44306	0.502192
C	4.575579	-0.729956	-0.171621
H	4.940212	-1.11882	0.779115
H	4.816424	0.331655	-0.212047
C	3.065241	-0.939888	-0.301714
H	2.725583	-0.556838	-1.263864
H	2.853114	-2.013085	-0.302931
C	2.316585	-0.292853	0.825887
H	2.519932	-0.708483	1.809592
C	1.460283	0.74134	0.75438
H	1.022989	1.095402	1.68377
C	1.048401	1.507769	-0.466136
H	1.453649	1.051772	-1.369532

H	-0.040292	1.463898	-0.550583
C	1.491041	2.9704	-0.388779
H	2.577064	3.04032	-0.335866
H	1.154004	3.531186	-1.260434
H	5.115719	-1.235327	-0.971963
H	1.082022	3.451689	0.499701

Table S3. Geometry parameters for 3-hexene–3-hexene complexes in 3.47 Å.

Atom symbol	x	y	z
C	4.568627	-0.760412	-0.370868
H	5.005768	-1.166206	0.541443
H	4.824732	0.297175	-0.421593
C	3.04914	-0.942431	-0.373596
H	2.635596	-0.543306	-1.29955
H	2.817907	-2.011667	-0.366544
C	2.41135	-0.294678	0.819851
H	2.696108	-0.719552	1.779047
C	1.566708	0.751386	0.83104
H	1.217753	1.103009	1.798372
C	1.051344	1.527567	-0.343377
H	1.378974	1.079601	-1.281586
H	-0.040466	1.480649	-0.335479
C	1.496541	2.990464	-0.292189
H	2.582982	3.062605	-0.332145
H	1.085053	3.557381	-1.127118
H	5.029163	-1.266237	-1.219227
H	1.164526	3.463883	0.631913
C	-4.572441	0.751399	-0.369934
H	-5.010302	1.156586	0.542301
H	-4.824076	-0.307345	-0.418897
C	-3.053749	0.9399	-0.374614
H	-2.639536	0.541191	-1.30045
H	-2.827082	2.010112	-0.369319
C	-2.411891	0.296538	0.819029
H	-2.696346	0.722344	1.777895
C	-1.564114	-0.74698	0.830776
H	-1.212506	-1.095769	1.798167
C	-1.048591	-1.524004	-0.343014
H	-1.37682	-1.077291	-1.281612
H	0.043164	-1.476266	-0.335373
C	-1.492664	-2.9872	-0.290107
H	-2.57906	-3.060199	-0.329752
H	-1.080908	-3.554745	-1.124481

H	-5.036082	1.254067	-1.21848
H	-1.16011	-3.459312	0.63447

Table S4. Geometry parameters for 3-hexene–3-hexene complexes in 3.67Å.

Atom symbol	x	y	z
C	-4.523407	0.762328	-0.619573
H	-5.056887	1.177244	0.235599
H	-4.77865	-0.294259	-0.691212
C	-3.012051	0.936598	-0.454693
H	-2.500199	0.528744	-1.326068
H	-2.776514	2.004632	-0.429197
C	-2.514458	0.294629	0.806649
H	-2.905224	0.724971	1.725194
C	-1.678208	-0.752249	0.918888
H	-1.44228	-1.098702	1.921819
C	-1.031844	-1.534132	-0.185119
H	-1.260764	-1.097534	-1.157357
H	0.052323	-1.475235	-0.061417
C	-1.467037	-3.000749	-0.167985
H	-2.542127	-3.084108	-0.324224
H	-0.962738	-3.570643	-0.948192
H	-4.883763	1.264103	-1.517352
H	-1.232459	-3.463112	0.790935
C	4.532641	-0.759789	-0.610716
H	5.057736	-1.181994	0.246078
H	4.791103	0.296622	-0.672803
C	3.019545	-0.931446	-0.460058
H	2.516165	-0.516478	-1.332998
H	2.781135	-1.999044	-0.443769
C	2.512721	-0.296732	0.801261
H	2.899067	-0.730528	1.720064
C	1.672568	0.747	0.913614
H	1.429108	1.087442	1.916799
C	1.030283	1.532413	-0.190242
H	1.268188	1.103111	-1.163563
H	-0.054452	1.46827	-0.074461
C	1.458488	3.000945	-0.160991
H	2.534228	3.09026	-0.309246
H	0.956932	3.57334	-0.941134
H	4.899517	-1.256185	-1.508839
H	1.215102	3.456193	0.799134

Table S5. Geometry parameters for 3-hexene–3-hexene complexes in 3.87 Å.

Atom symbol	x	y	z
C	4.536047	-0.684306	-0.802232
H	5.152056	-1.070357	0.010068
H	4.748722	0.379153	-0.90564

C	3.050554	-0.906128	-0.510185
H	2.453033	-0.525791	-1.338266
H	2.854612	-1.980998	-0.45639
C	2.638274	-0.269932	0.78451
H	3.11171	-0.684847	1.670654
C	1.787634	0.756076	0.959147
H	1.61909	1.098343	1.977007
C	1.02986	1.50961	-0.092655
H	1.269565	1.133726	-1.087741
H	-0.039547	1.340393	0.057795
C	1.315861	3.010889	-0.032299
H	2.371508	3.210031	-0.214384
H	0.732806	3.552336	-0.776939
H	4.837552	-1.185895	-1.721788
H	1.064422	3.413694	0.948923
C	-4.55079	0.697782	-0.785891
H	-5.144191	1.116266	0.02702
H	-4.790834	-0.361927	-0.862768
C	-3.055766	0.88927	-0.522517
H	-2.482516	0.478786	-1.353436
H	-2.832408	1.959802	-0.492233
C	-2.637273	0.265305	0.77591
H	-3.110967	0.684977	1.6597
C	-1.777359	-0.75209	0.957611
H	-1.605272	-1.085089	1.978033
C	-1.014967	-1.510188	-0.087371
H	-1.236422	-1.128252	-1.08428
H	0.054374	-1.352955	0.078803
C	-1.318814	-3.008322	-0.035084
H	-2.374204	-3.194279	-0.231508
H	-0.732382	-3.554846	-0.773357
H	-4.855038	1.186392	-1.711191
H	-1.085232	-3.41647	0.94826