Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Interaction of aliphatic amino acids with zwitterionic and charged lipid membranes: hydration and dehydration phenomena

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Supporting Information

Figure S1: a) Normalized emission spectra of PRODAN in aqueous medium and in different lipid mediums (DPPC, DMPC and DOPC lipid bilayers) showing a blue shift in PRODAN−lipid bilayer systems as compared to PRODAN in aqueous solution; (b) representative time-resolved decay of PRODAN in different lipid bilayers collected at 440 nm.

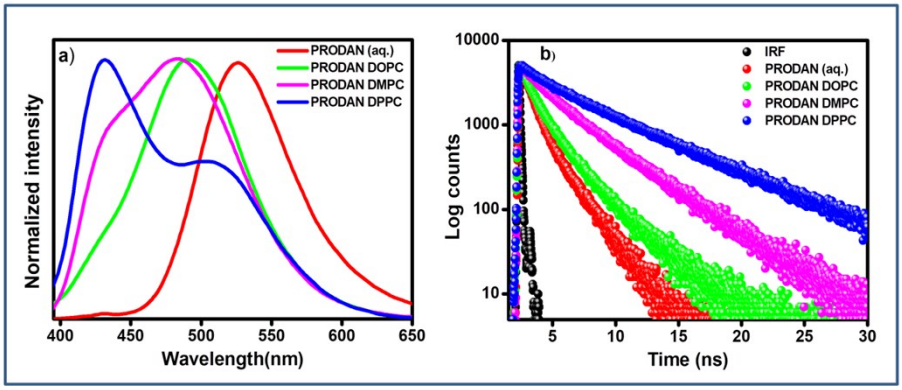

Figure S2: Steady state and corresponding time-resolved lifetime decay curves collected at 440 nm for DMPC-PRODAN upon interaction with L-aspartic acid (a-b) and L-glutamic acid (c-d).

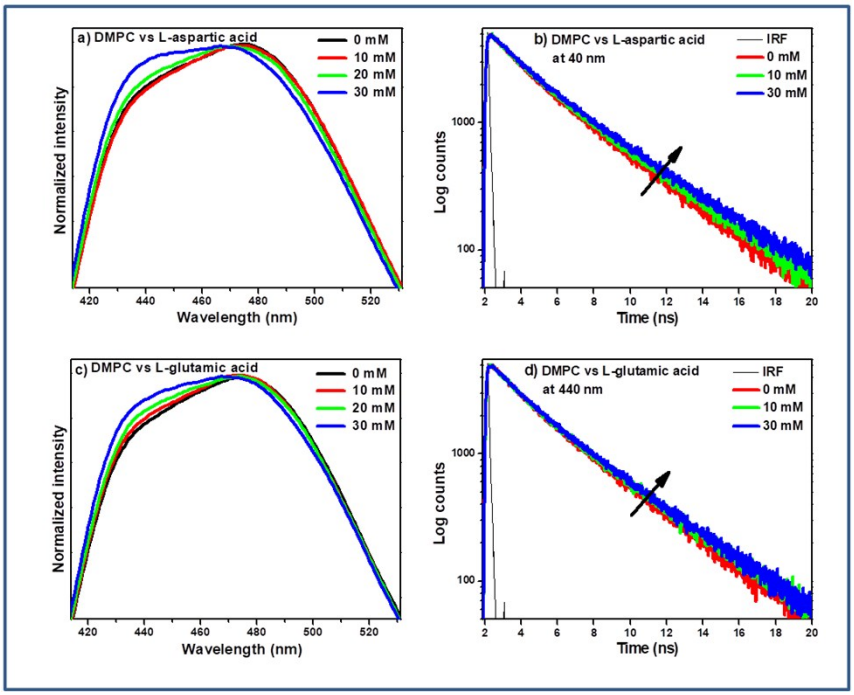

Figure S3: Steady state fluorescence spectra for interaction of negatively charged amino acids with positively charged lipid bilayer DMPC: DMTAP.

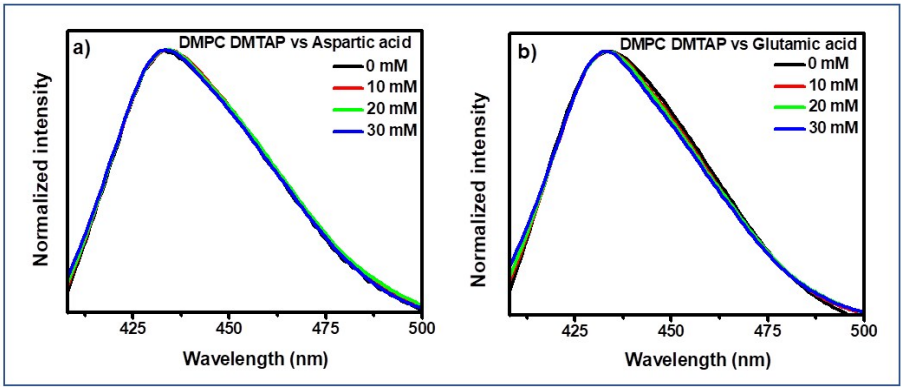

Figure S4: Plots of temperature-induced variation in the steady-state fluorescence spectra of PRODAN in a) negatively charged DMPC: DMPG bilayer, b) upon interaction with arginine, c) b) upon interaction with aspartic acid, d) area fraction ($A_{435\ nm}/A_{500\ nm}$) v/s temperature plot for DMPC: DMPG in the presence and absence of amino acids (from 10 °C to 40 °C) and e) first derivative of area (dA/dT) v/s temperature plot.

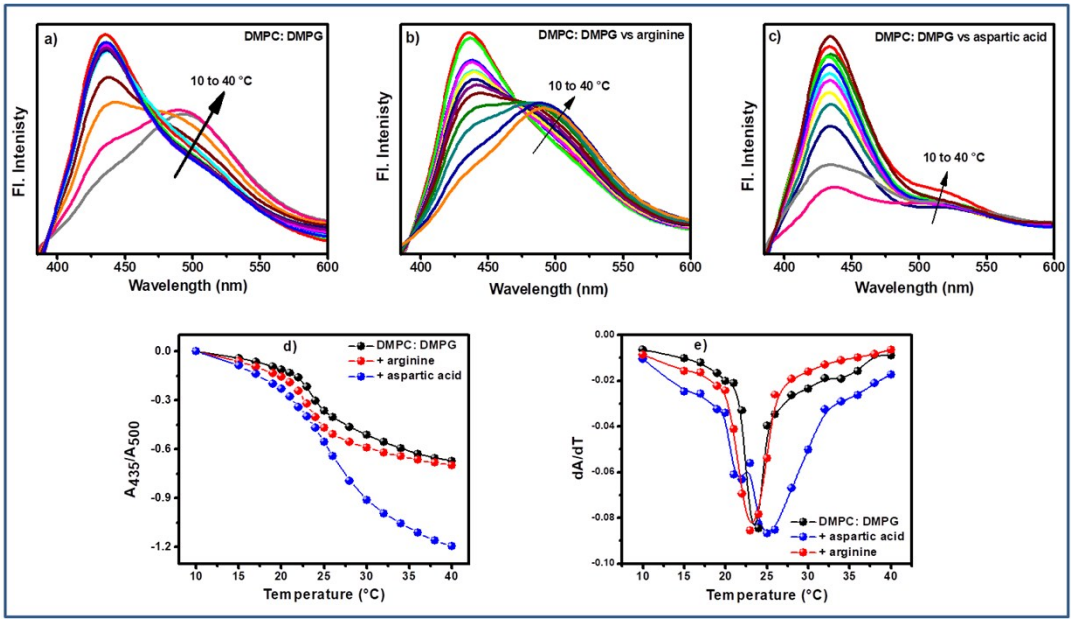

Figure S5: Steady state normalized fluorescence emission spectra (a), area fraction plot (b), time-resolved lifetime decay curves collected at 440 nm (c), and anisotropy plots at 440 nm (d) for DMPC-DMPG (prepared in HEPES buffer, pH = 7.0) upon interaction with L-aspartic acid.

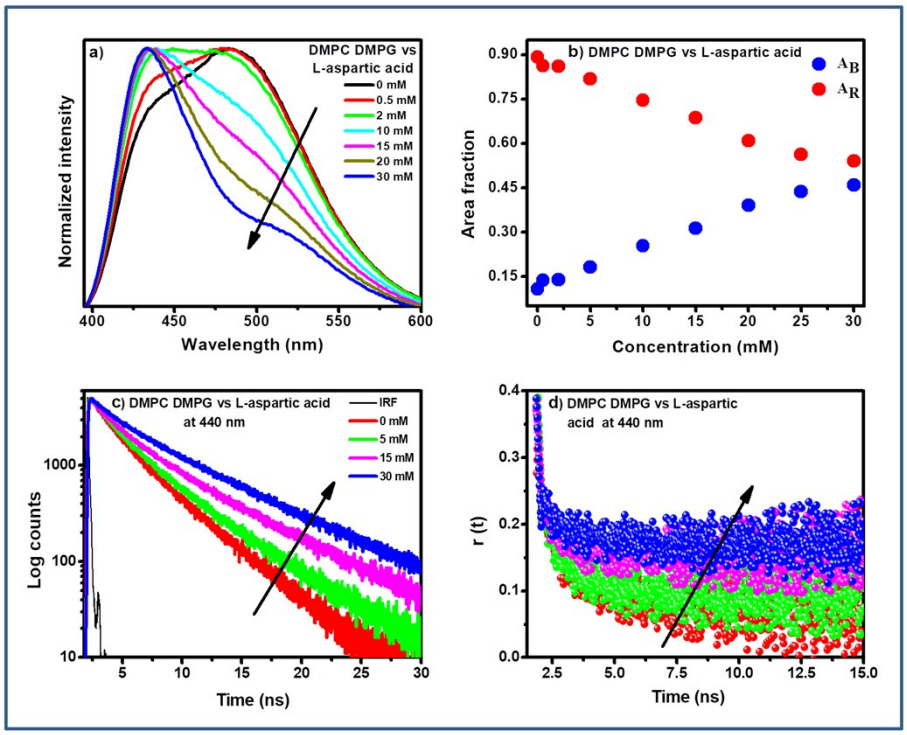

Figure S6: Steady state normalized fluorescence emission spectra (a), area fraction plot (b), time-resolved lifetime decay curves collected at 440 nm (c), and anisotropy plots at 440 nm (d) for DMPC-DMPG (prepared in HEPES buffer, pH = 7.0) upon interaction with L-glutamic acid.

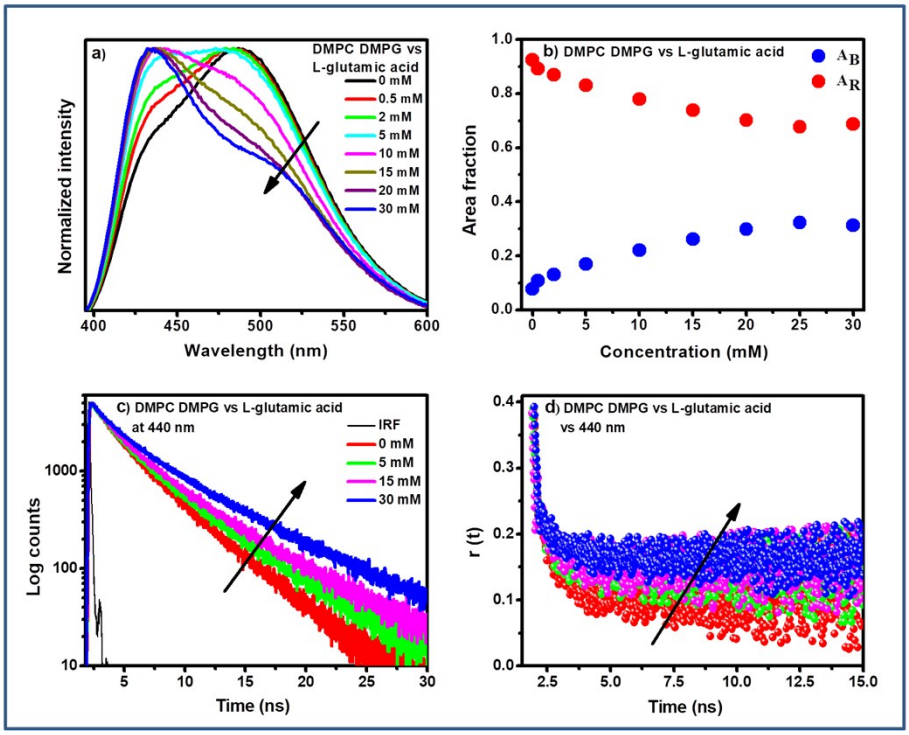

Figure S7: Steady state and corresponding time-resolved lifetime decay curves collected at 440 nm for DMPC-PRODAN upon interaction with L-lysine (a-b) and L-arginine (c-d).

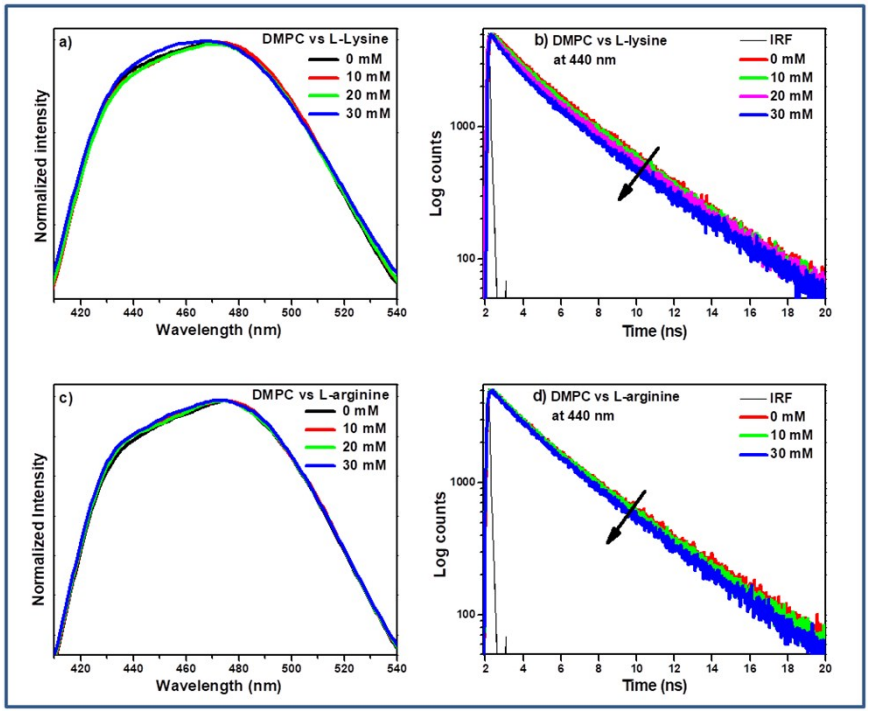

Figure S8: Steady state (a-b) and time resolved lifetime decay curves collected at 440 nm of L-lysine and L-arginine with DMPC: DMTAP.

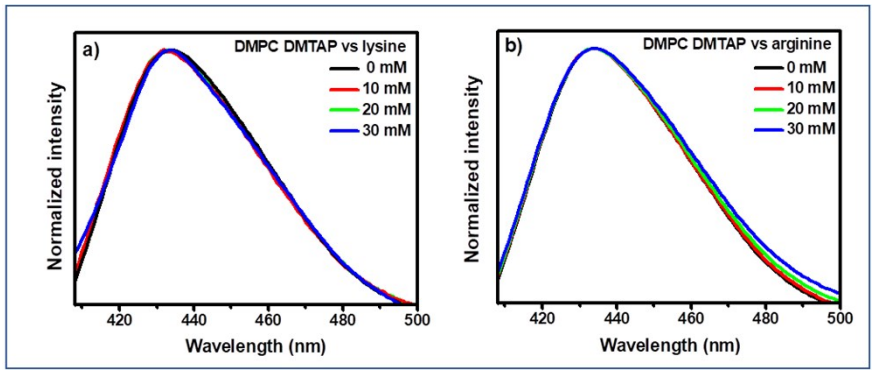

Figure S9: Steady state, corresponding area fraction plot (inset) and time-resolved lifetime decay curves collected at 440 nm for DMPC-DMPG upon interaction with L-lysine (a-b) and L-arginine (c-d). Upward arrows in emission spectra indicate an initial increase in peak at 440 nm, whereas downward arrows indicate a gradual decrease in the peak indicating fluidization of the bilayer.

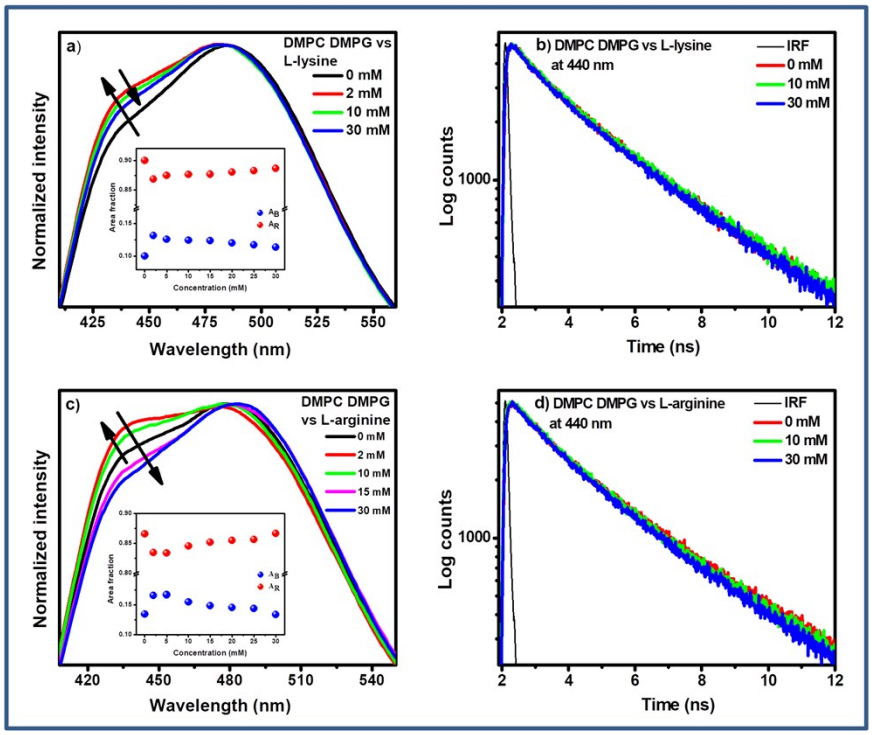

Figure S10: Comparison of emission curves for all maxima for L-amino acids with DMPC-PRODAN solutions prepared in Milli-Q water.

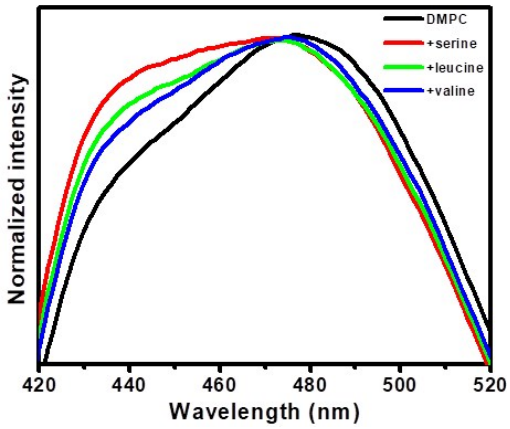

Figure S11: Steady state normalized fluorescence spectra (a-c) and corresponding area fraction plots for DMPC-PRODAN prepared in HEPES buffer (pH = 7.0) upon interaction with amino acids (d-f).

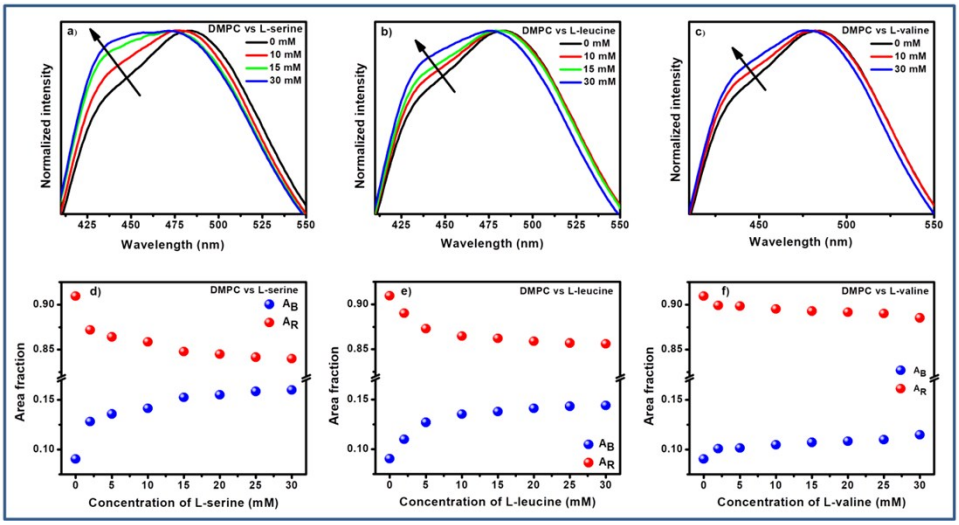

Figure S12: Binding of amino acids using confocal scanning laser microscopy (CLSM). Confocal, bright field and merged images for DMPC vesicles (a-c), DMPC + L-serine (d-f), Bars indicate 2 µm size.

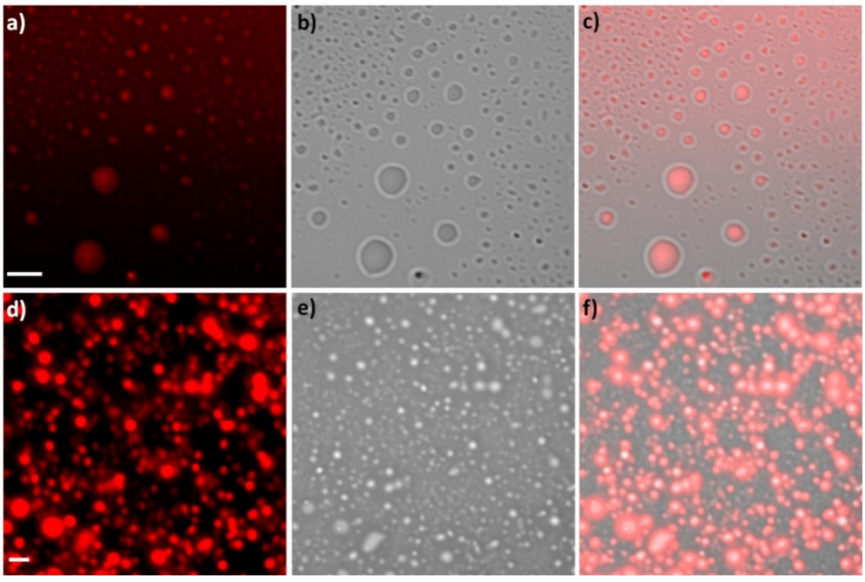

Figure S13: Steady state fluorescence emission and time-resolved lifetime decay curves collected at 440 nm (inset) for DMPC-PRODAN upon interaction with D-amino acids.

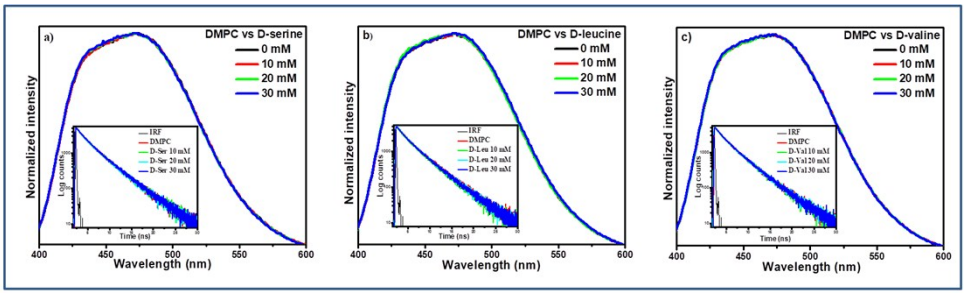

Figure S14: Steady state fluorescence emission (a-c), area fraction plots (d-f) and time-resolved lifetime decay curves collected at 440 nm (g-i) for DPPC-PRODAN upon interaction with L-amino acids.

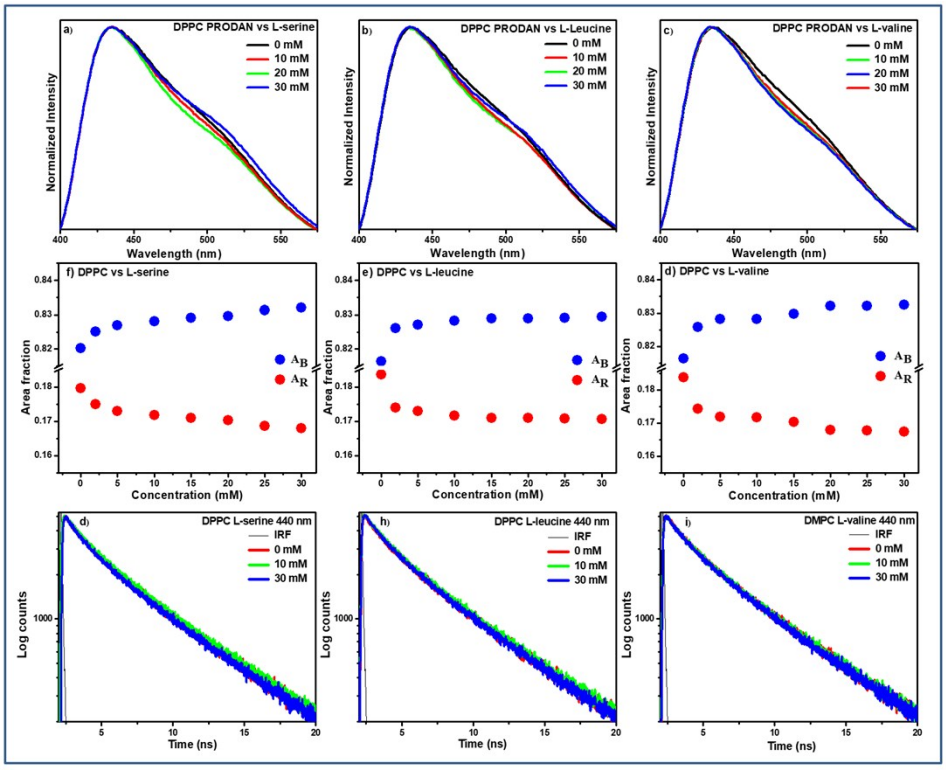

Figure S15: Steady state (a-c) and time resolved lifetime decay curves collected at 440 nm (d-f) of L-amino acids with DOPC.

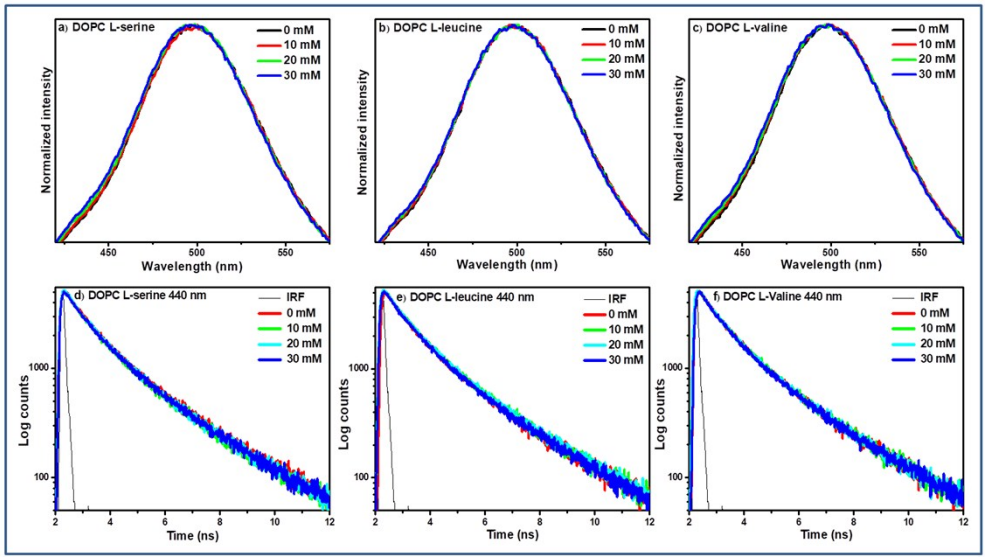

Table S1: Lifetime components, normalized amplitudes of lifetime components and average lifetime of PRODAN in different lipid mediums collected at 440 nm at 25 °C.[#]

Sample	τ_1 (ns)	τ_2 (ns)	a_1	a_2	$\langle\tau_{avg}\rangle$ (ns)	χ^2
PRODAN DOPC	**0.76**	**2.37**	**0.61**	**0.39**	**1.40**	**1.16**
PRODAN DMPC	**1.49**	**4.33**	**0.38**	**0.62**	**3.25**	**1.11**
PRODAN DPPC	**1.36**	**6.39**	**0.28**	**0.72**	**5.00**	**1.07**

[#]**Experimental error is within ±10%.**

Table S2: Lifetime components, normalized amplitudes of lifetime components, and average lifetime of PRODAN for DMPC: DMPC vesicles (prepared in Milli-Q water) upon interaction with L-aspartic acid and L-glutamic acid collected at 440 nm and 500 nm at 25 °C.[#]

DMPC: DMPG vs L-aspartic acid @440 nm, 25 °C								
Sample	**τ_1 (ns)**	**τ_2 (ns)**	**τ_3 (ns)**	**a_1**	**a_2**	**a_3**	**$<\tau_{avg}>$ (ns)**	**$\chi 2$**
0 mM	1.49	5.23	0.07	0.21	0.21	0.58	1.44	1.17
10 mM	1.32	6.12	0.02	0.04	0.04	0.93	0.29	1.10
20 mM	1.62	7.08	0.02	0.03	0.05	0.93	0.39	1.03
30 mM	2.59	7.78	0.01	0.01	0.04	0.95	0.36	1.06
DMPC: DMPG vs L-glutamic acid @440 nm, 25 °C								
0 mM	1.49	5.23	0.07	0.21	0.21	0.58	1.44	1.17
10 mM	1.30	5.91	0.03	0.07	0.07	0.86	0.52	1.13
20 mM	1.54	6.67	0.03	0.06	0.08	0.86	0.63	1.09
30 mM	2.03	7.50	0.02	0.03	0.11	0.85	0.92	1.02

[#]**Experimental error is within ±10%.**

Table S3: Lifetime components, normalized amplitudes of lifetime components, and average lifetime of PRODAN for DMPC: DMPC vesicles (prepared in HEPES buffer, pH =7.0) upon interaction with L-aspartic acid and L-glutamic acid collected at 440 nm and 500 nm at 25 °C.[#]

DMPC: DMPG vs L-aspartic acid @440 nm, 25 °C						
Sample	**τ_1 (ns)**	**τ_2 (ns)**	**a_1**	**a_2**	**$<\tau_{avg}>$ (ns)**	**χ^2**
0 mM	1.60	4.28	0.53	0.47	2.85	1.15
5 mM	1.84	5.09	0.56	0.44	3.26	1.21
15 mM	2.00	6.41	0.51	0.49	4.17	1.07
30 mM	2.30	7.61	0.40	0.60	5.50	1.10
DMPC: DMPG vs L-glutamic acid @440 nm, 25 °C						
0 mM	1.60	4.28	0.53	0.47	2.85	1.15
5 mM	1.83	5.08	0.57	0.43	3.21	1.16
15 mM	1.88	5.58	0.57	0.43	3.46	1.11
30 mM	1.88	6.49	0.50	0.50	4.18	1.11

[#]**Experimental error is within ±10%.**