

Supplementary Information

Thermodynamics of selective serotonin reuptake inhibitors partitioning into 1,2-dioleoyl-*sn*-glycero-3-phosphocholine bilayers

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Supporting Information

Addition spectra

In order to validate the interaction of either SSRIs and DOPC LUVs, a mathematical addition of the pure SSRI spectrum to the pure lipid spectrum was conducted. The results of the mathematical addition of either PAX or SER to DOPC liposomes were demonstrated in Fig. S1 and Fig. S2, respectively. Peak components were obtained by deconvolution of the addition spectra and presented in Table S1. The obtained results indicated that the addition spectra were different from the mixture spectra in terms of shape and vibrational frequency assignments.

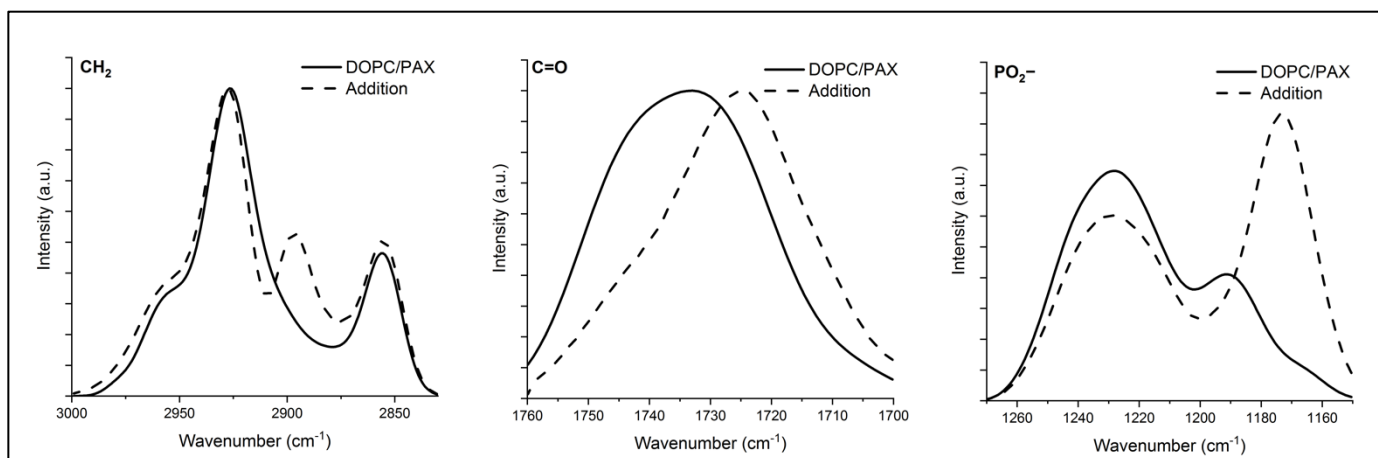


Figure S1. Normalized ATR-FTIR spectrum of mixture of DOPC and PAX (solid line) and addition spectrum (dash line) obtained by mathematical addition of pure DOPC and PAX.

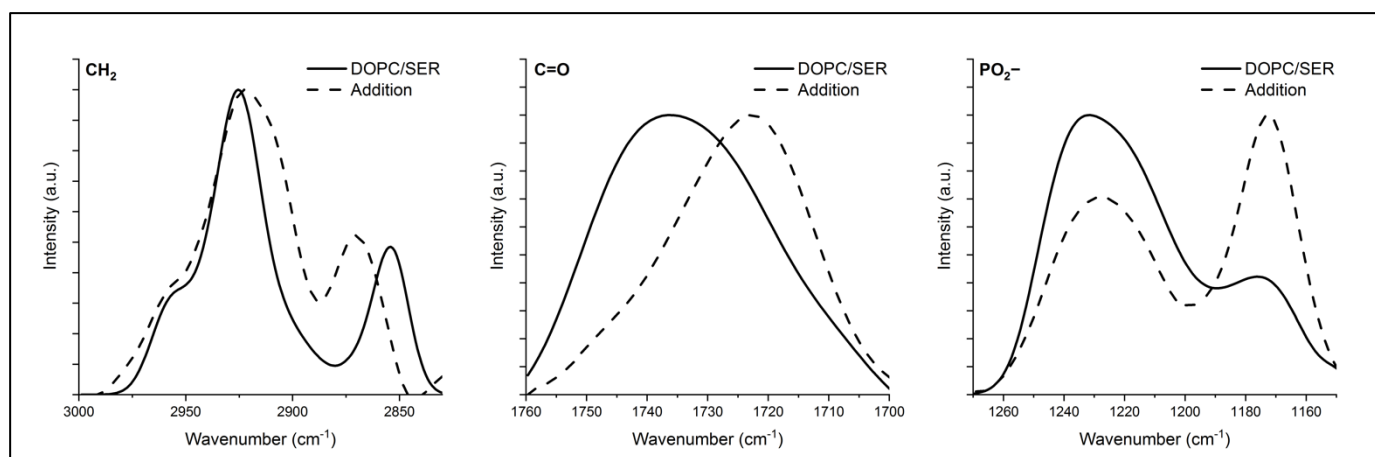


Figure S2. Normalized ATR-FTIR spectrum of mixture of DOPC and SER (solid line) and addition spectrum (dash line) obtained by mathematical addition of pure DOPC and SER.

Table S1. Vibrational frequency assignments of the CH₂, C=O and PO₂⁻ regions of the addition spectra.

Addition spectra	$\nu_s\text{CH}_2$ (cm ⁻¹)	$\nu_{as}\text{CH}_2$ (cm ⁻¹)	$\nu\text{C=O}_{\text{bonded}}$ (cm ⁻¹)	$\nu\text{C=O}_{\text{free}}$ (cm ⁻¹)	$\nu\text{PO}_2^-_{\text{free}}$ (cm ⁻¹)	$\nu\text{PO}_2^-_{\text{bonded}}$ (cm ⁻¹)
DOPC + PAX	2898	2927	1722	1729	1229	1171
DOPC + SER	2868	2923	1721	1734	1219	1173