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 CH\textsubscript{2}, C\textequiv O and PO\textsubscript{2}\textsuperscript{2−} regions of the addition spectra.

| Addition spectra | ν\textsubscript{CH\textsubscript{2}} (cm\textsuperscript{-1}) | ν\textsubscript{as CH\textsubscript{2}} (cm\textsuperscript{-1}) | ν\textequiv O\textsubscript{bonded} (cm\textsuperscript{-1}) | ν\textequiv O\textsubscript{free} (cm\textsuperscript{-1}) | νPO\textsubscript{2}\textsuperscript{−\textsubscript{free}} (cm\textsuperscript{-1}) | νPO\textsubscript{2}\textsubscript{−\textsubscript{bonded}} (cm\textsuperscript{-1}) |
|------------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| DOPC + PAX       | 2898            | 2927            | 1722            | 1729            | 1229            | 1171            |
| DOPC + SER       | 2868            | 2923            | 1721            | 1734            | 1219            | 1173            |