Electronic Supplementary Material (ESI) for RSC Advances.

ELECTRONIC SUPPLEMENTARY INFORMATION

The Importance of Intramolecular Hydrogen Bonds on the Translocation of the Small Drug Piracetam through a Lipid Bilayer

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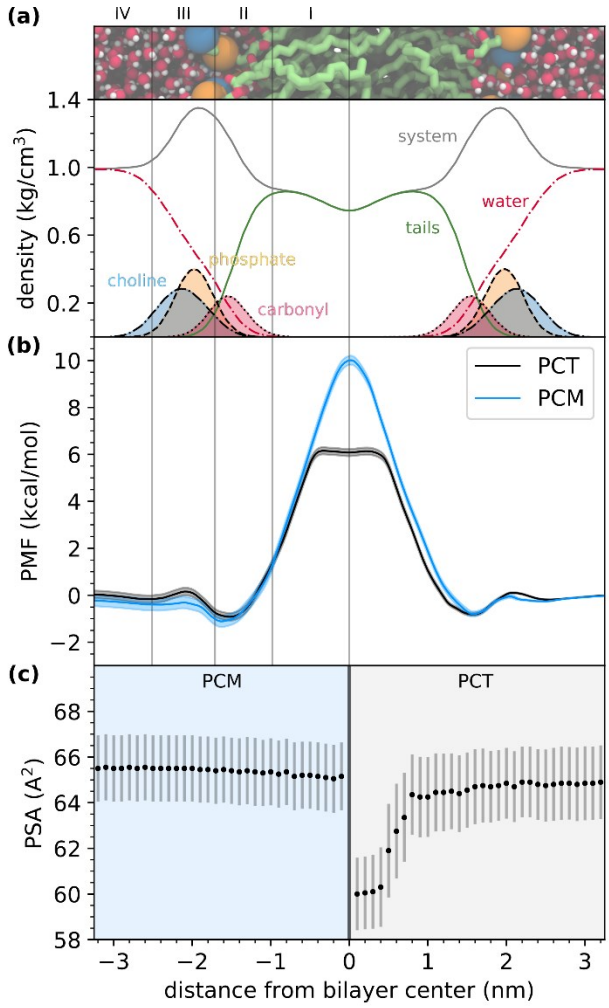

Figure S1. Energy and polar surface area (PSA) profiles of PCT and PCM in a DOPC hydrated bilayer model system. (a) representation of the hydrated bilayer system and partial density profiles for the different functional groups or molecules in the system. (b) unsymmetrized free energy profiles for the translocation of the two tested compounds (PCT, black and PCM, blue). (c) polar surface area (PSA) along the translocated distance. In the right (with a grey background), we show the results for PCT; and in the left (with a blue background), we show the results for PCM.

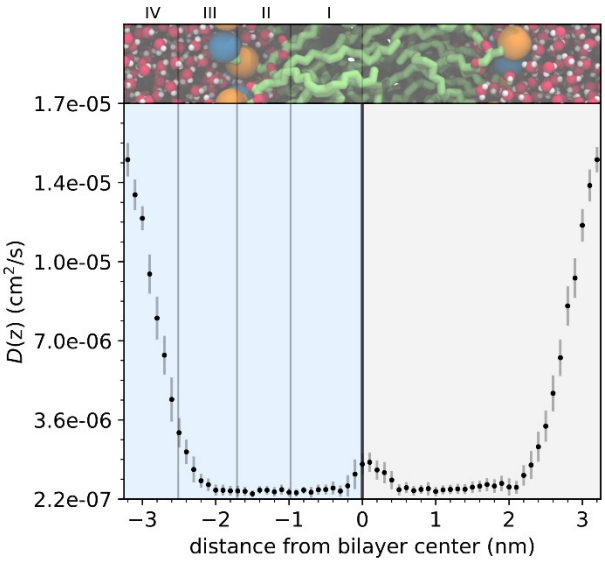

Figure S2. Diffusivity, *D*(z), profiles of PCT and PCM. In the right (with a grey background), we show the results for PCT; and in the left (with a blue background), we show the results for PCM.

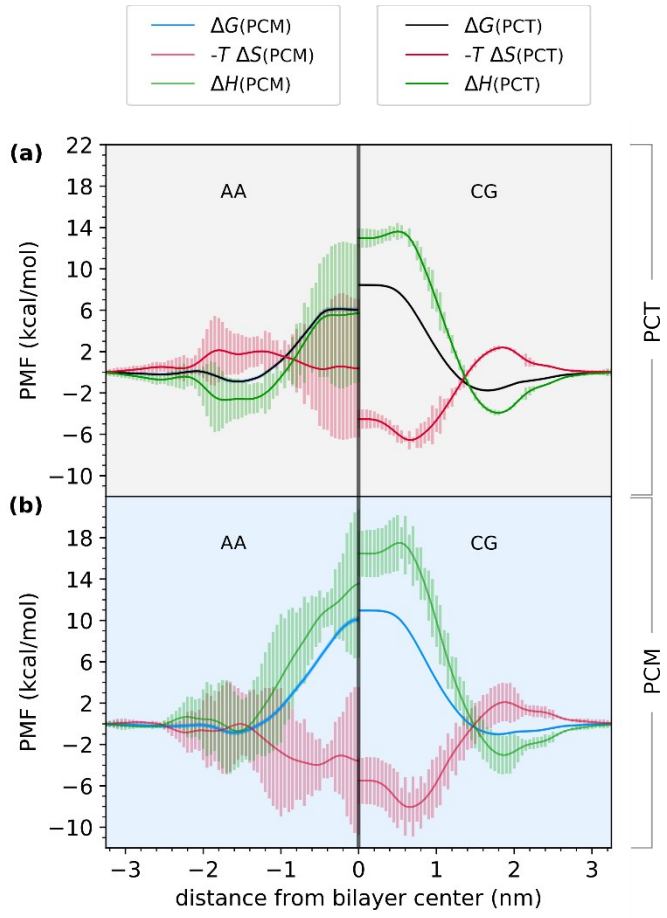

Figure S3. Thermodynamic profiles of PCT and PCM in a DOPC hydrated bilayer model system. (a) thermodynamic profiles of PCT derived from all-atom (left) and coarse-grained (right) MD simulations (Δ*G*, black; -*T*Δ*S*, red; Δ*H*, green). (b) thermodynamic profiles of PCM derived from all-atom (left) and coarse-grained (right) MD simulations (Δ*G*, blue; -*T*Δ*S*, red; Δ*H*, green). The energy profiles for PCT and PCM are shown with grey and blue backgrounds, respectively. Vertical bars represent the uncertainty of the estimates and were derived from the multiple determinations of entropy per system that were made (see Methods section for details). AA, all-atom MD simulations; CG, coarse-grained MD simulations.

CG topology files of PCT and PCM

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; Tristan Bereau (2014)

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  PCT           2

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  3     P3      1       PCT     P02     3       0     ; [H]N([H])C=O

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