Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

Transformations in Plasma Membranes of Cancerous Cells and Resulting Consequences for Cation Insertion Studied with Molecular Dynamics

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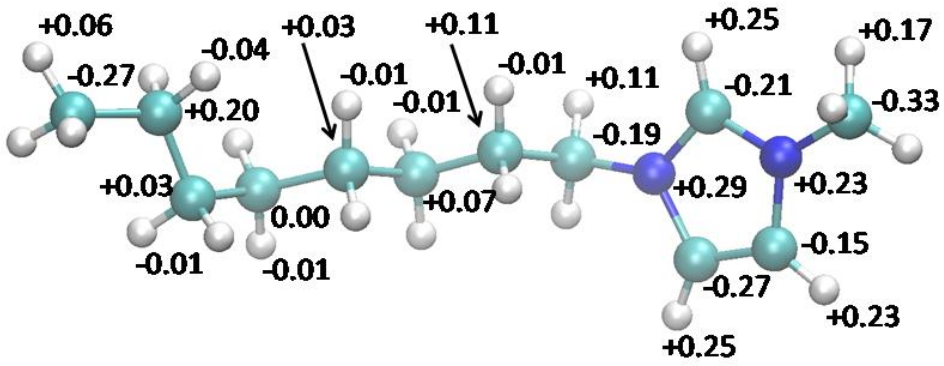

Figure S1: Atomic ESP partial charges of the $OMIM^+$ cation, derived from DFT with B3LYP functional and 6-311++g(d,p) basis set with PCM solvent model for water, which were used in the MM force field.

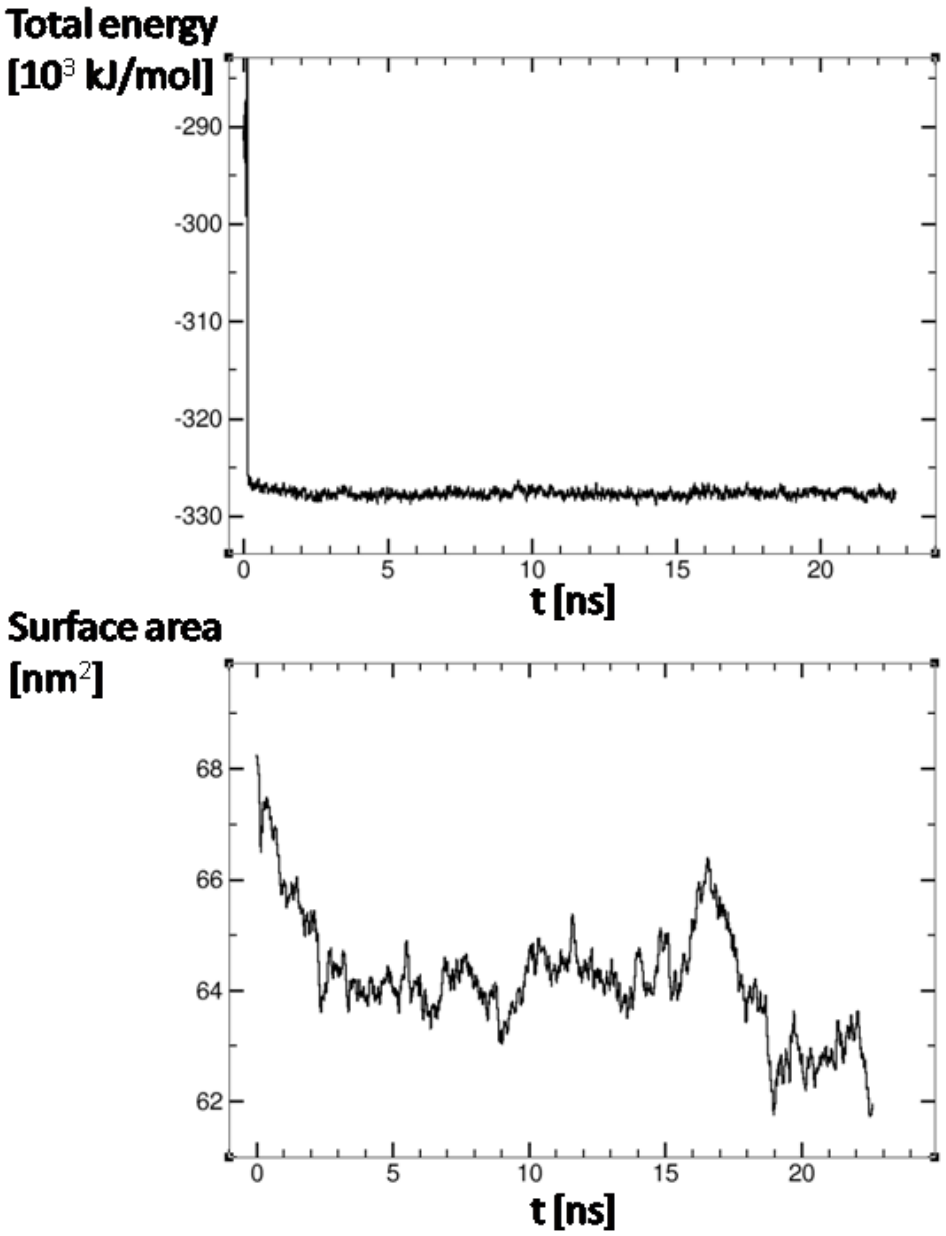

Figure S2: Total energy and membrane surface area of the membrane M-PC as a function of simulation time.

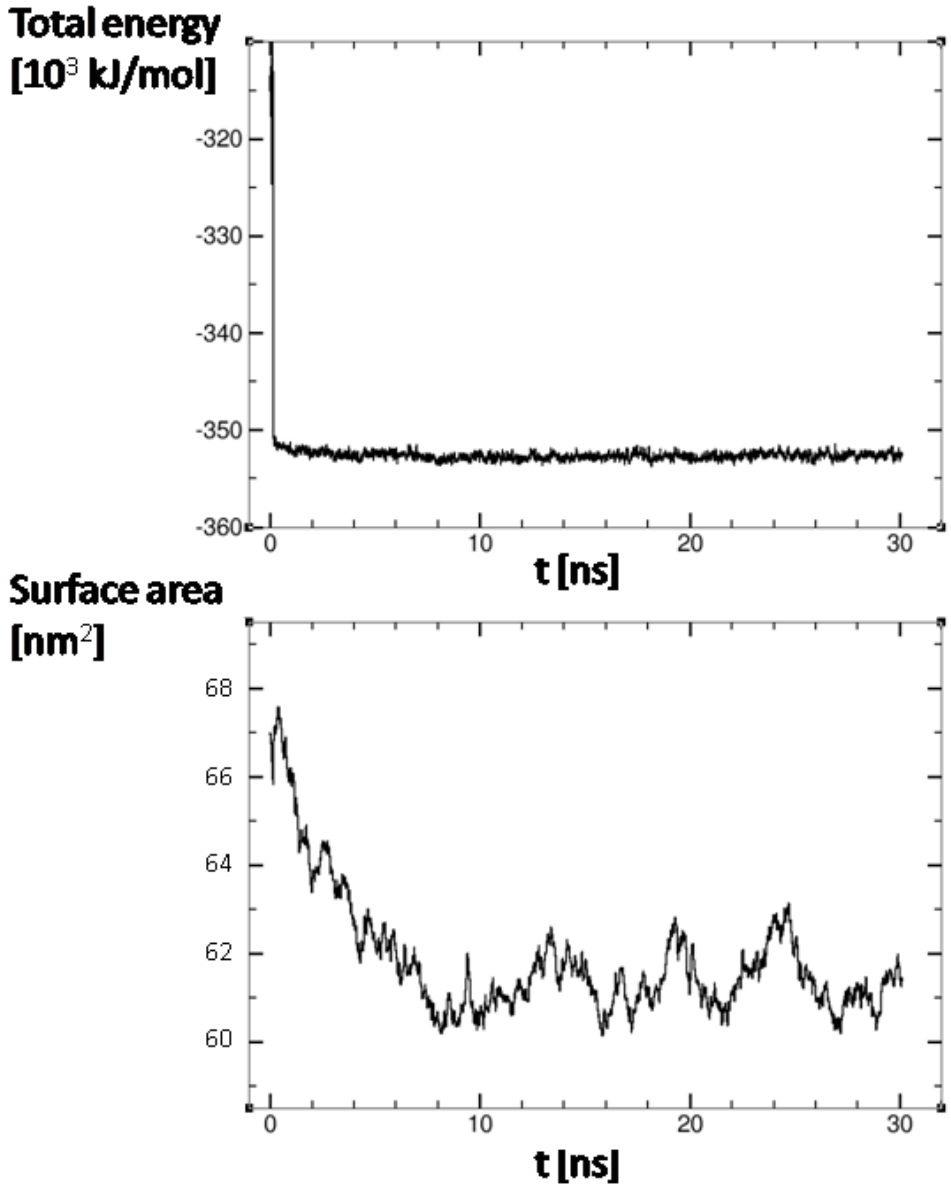

Figure S3: Total energy and membrane surface area of the membrane M-$PC_{0.8}S_{0.2}$ as a function of simulation time.

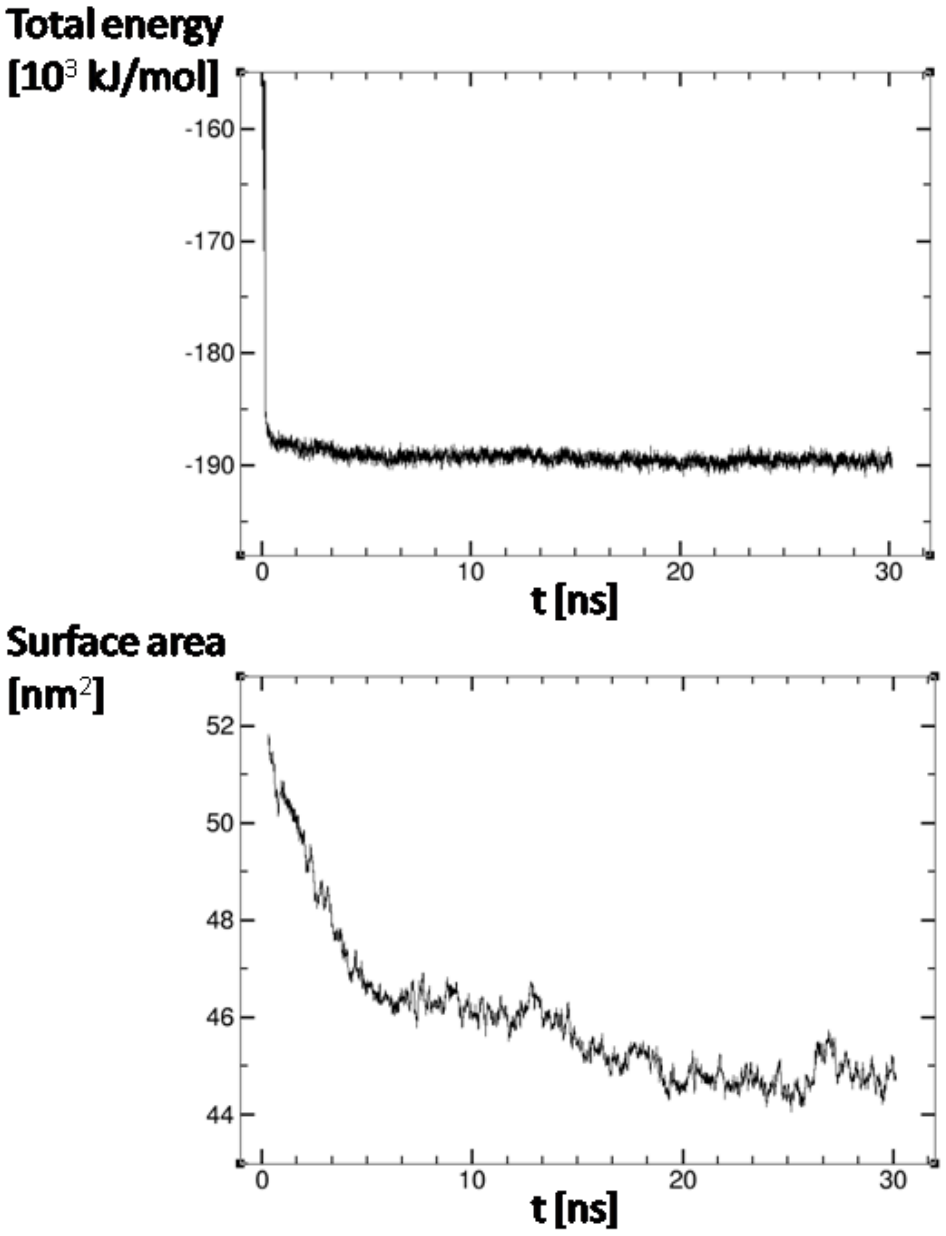

Figure S4: Total energy and membrane surface area of the membrane M-$PC_{0.66}Ch_{0.34}$ as a function of simulation time.

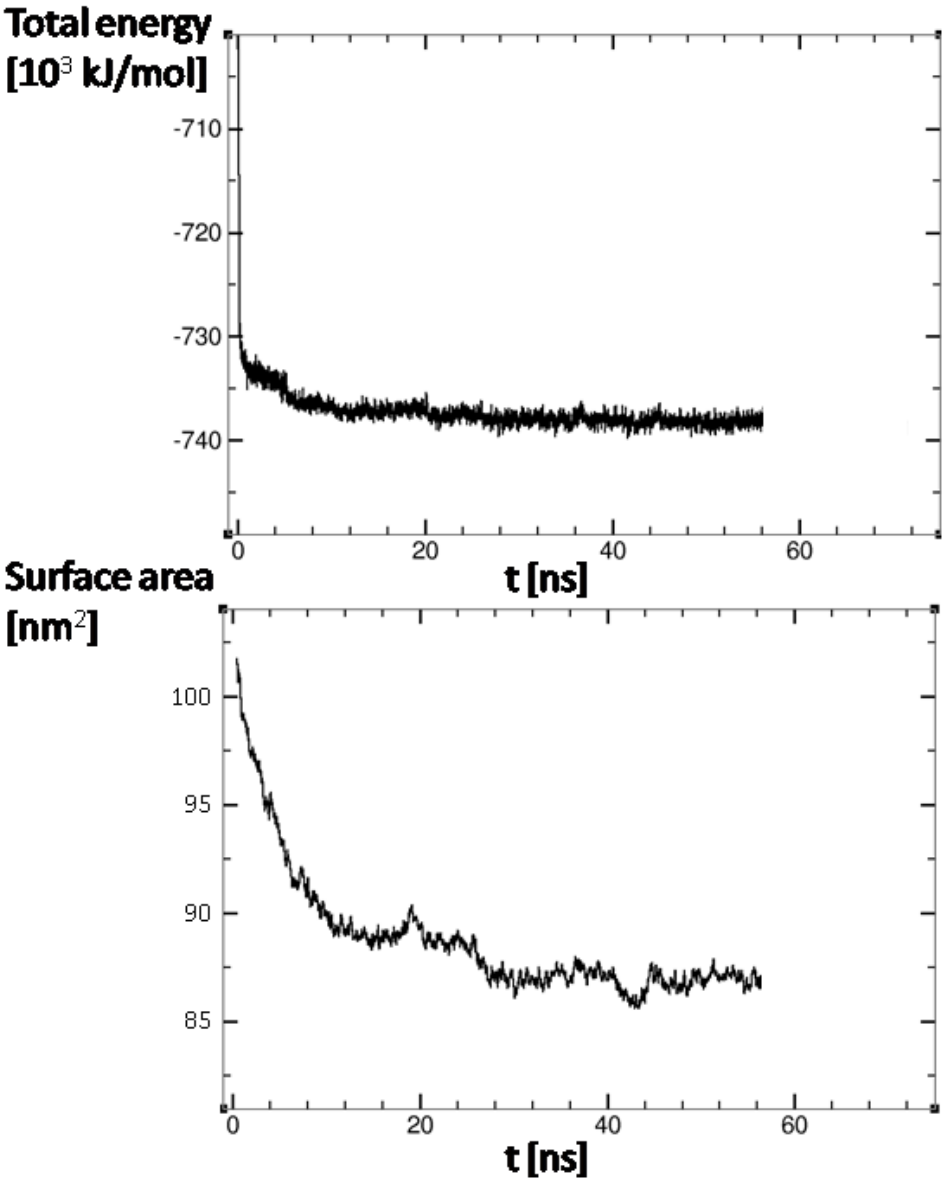

Figure S5: Total energy and membrane surface area of the membrane M-Eukar as a function of simulation time.

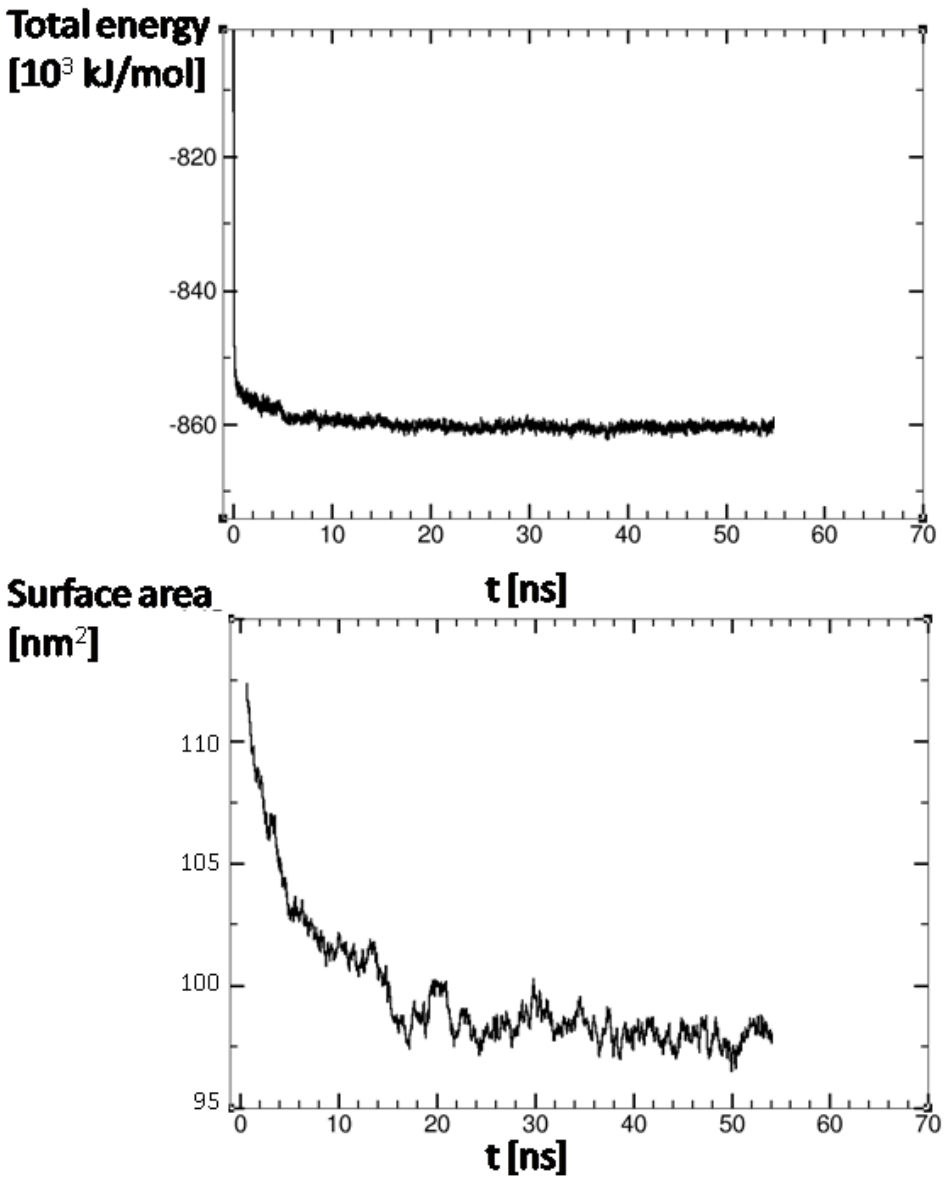

Figure S6: Total energy and membrane surface area of the membrane M-Cancer as a function of simulation time.

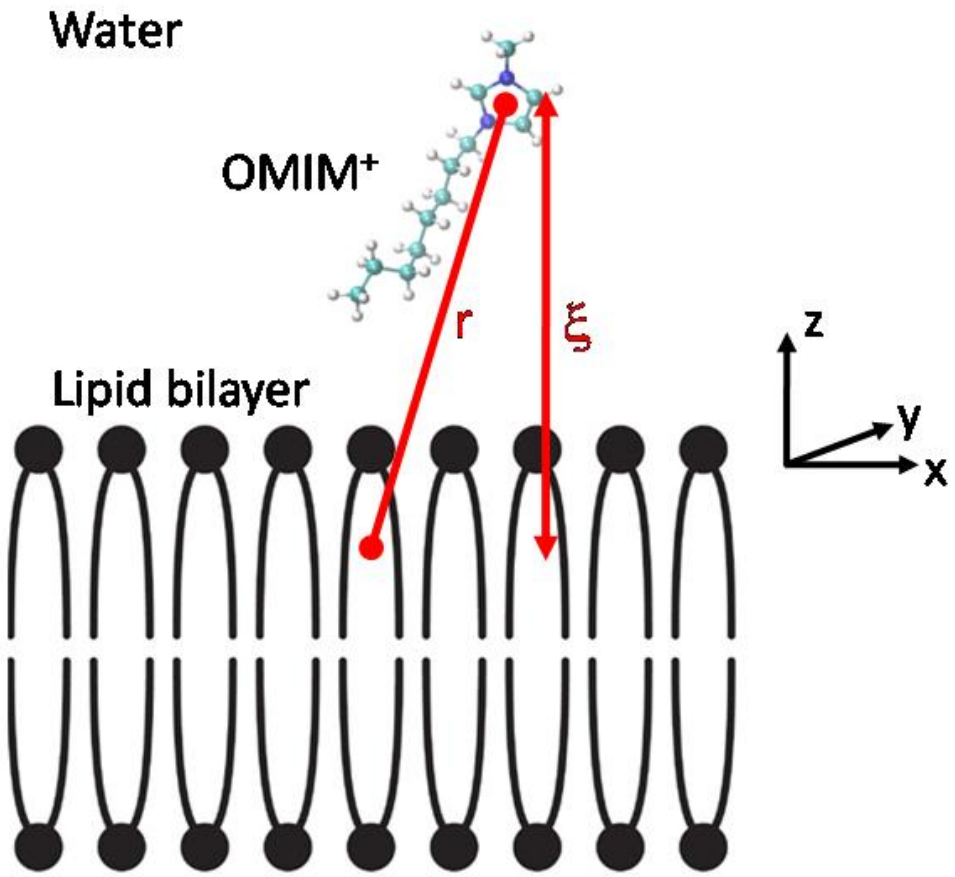

Figure S7: Definition of the reaction coordinate ξ, which was used to calculate the change in free energy for pulling the cation $OMIM^+$ from the membrane layer to the solvent phase. Distance *r* is defined as the distance between the center-of-masses of the $OMIM^+$ imidazole ring and the membrane layer into which the cation was inserted. Then ξ is defined as the projection of *r* onto the z-axis that is perpendicular to the membrane surface.

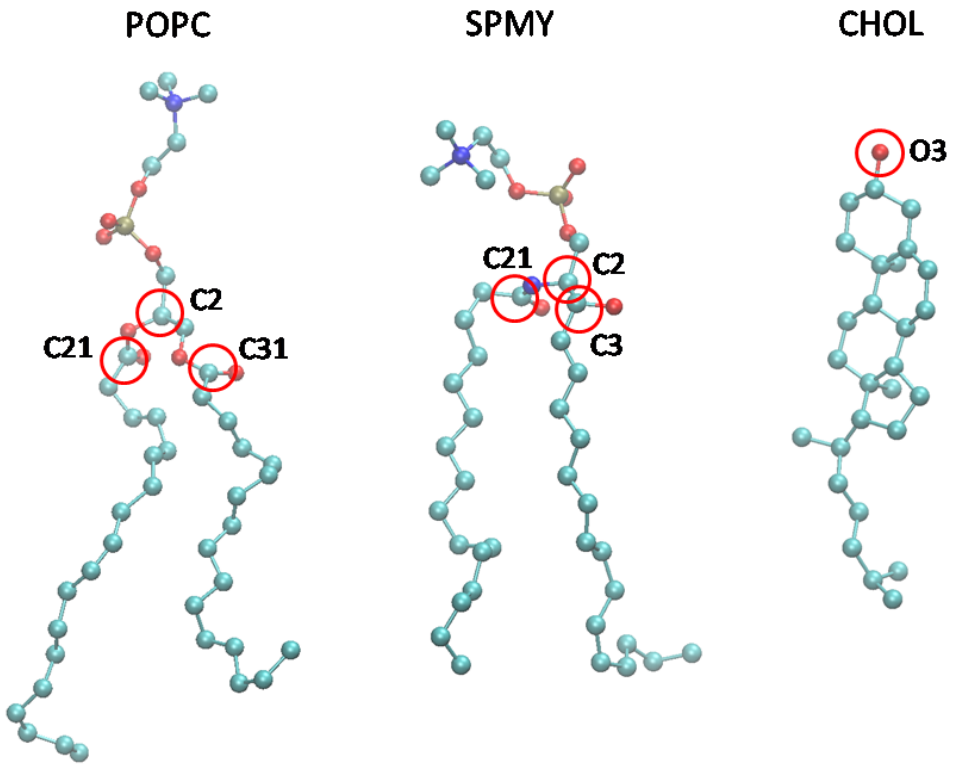

Figure S8: Atoms that were used to describe the extent of each compound to determine the average area size that lipids covered on the membrane surface. Atom names are given according to the nomenclature used in CHARMM. Atom selections for POPS and POPE are the same as for POPC. Hydrogen atoms are not displayed.

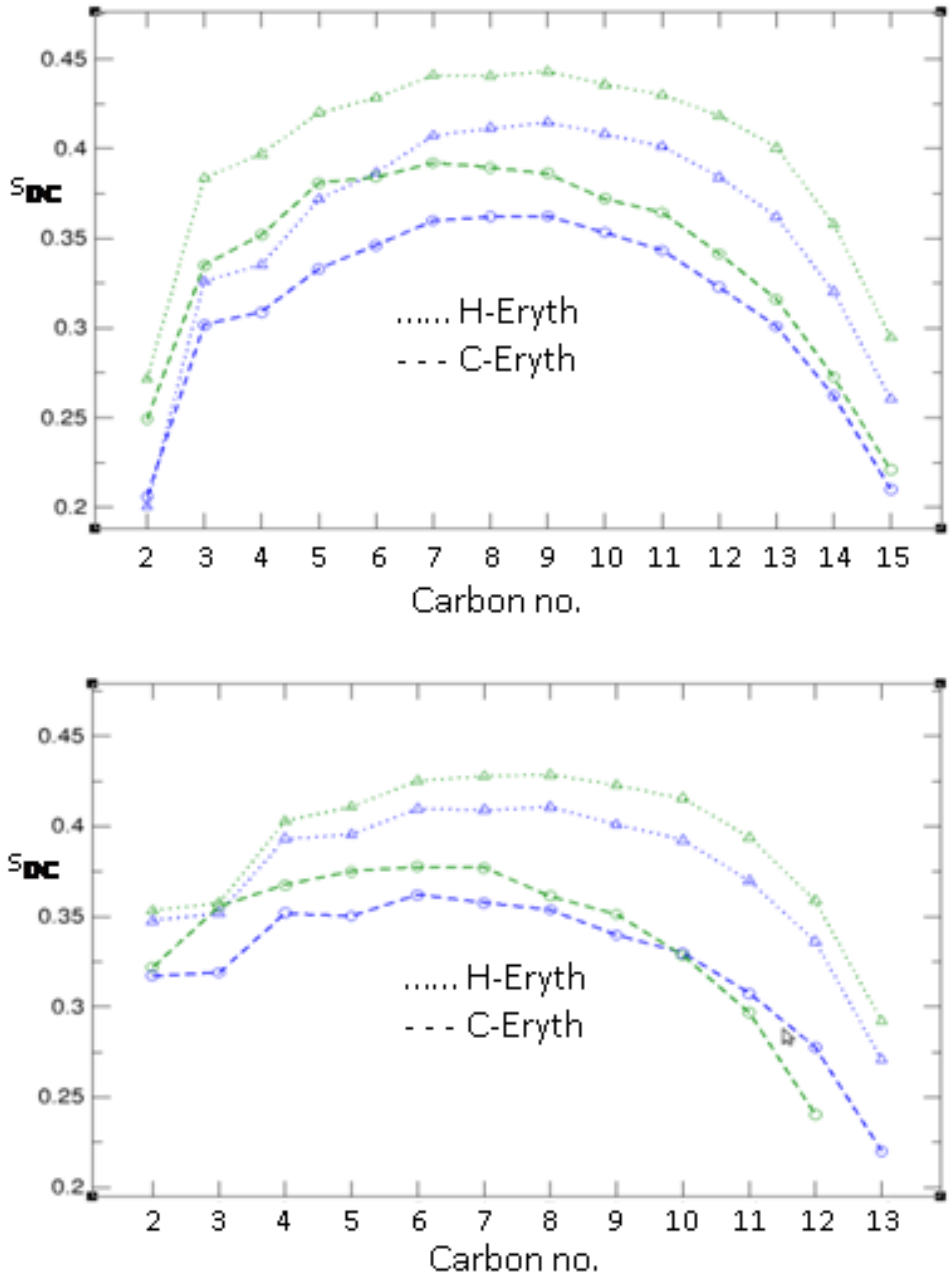

Figure S9: Comparison of deuterium order parameters of aliphatic chains in SPMY, the fatty acid (upper half) and sphingosine (lower half) in M-Eukar (dotted line) and M-Cancer (broken line). Values for the external layer are shown in blue and for the internal layer in green. Carbon atom numbers increase in the direction of the chain termini, with the highest number corresponding to $–CH_3$.

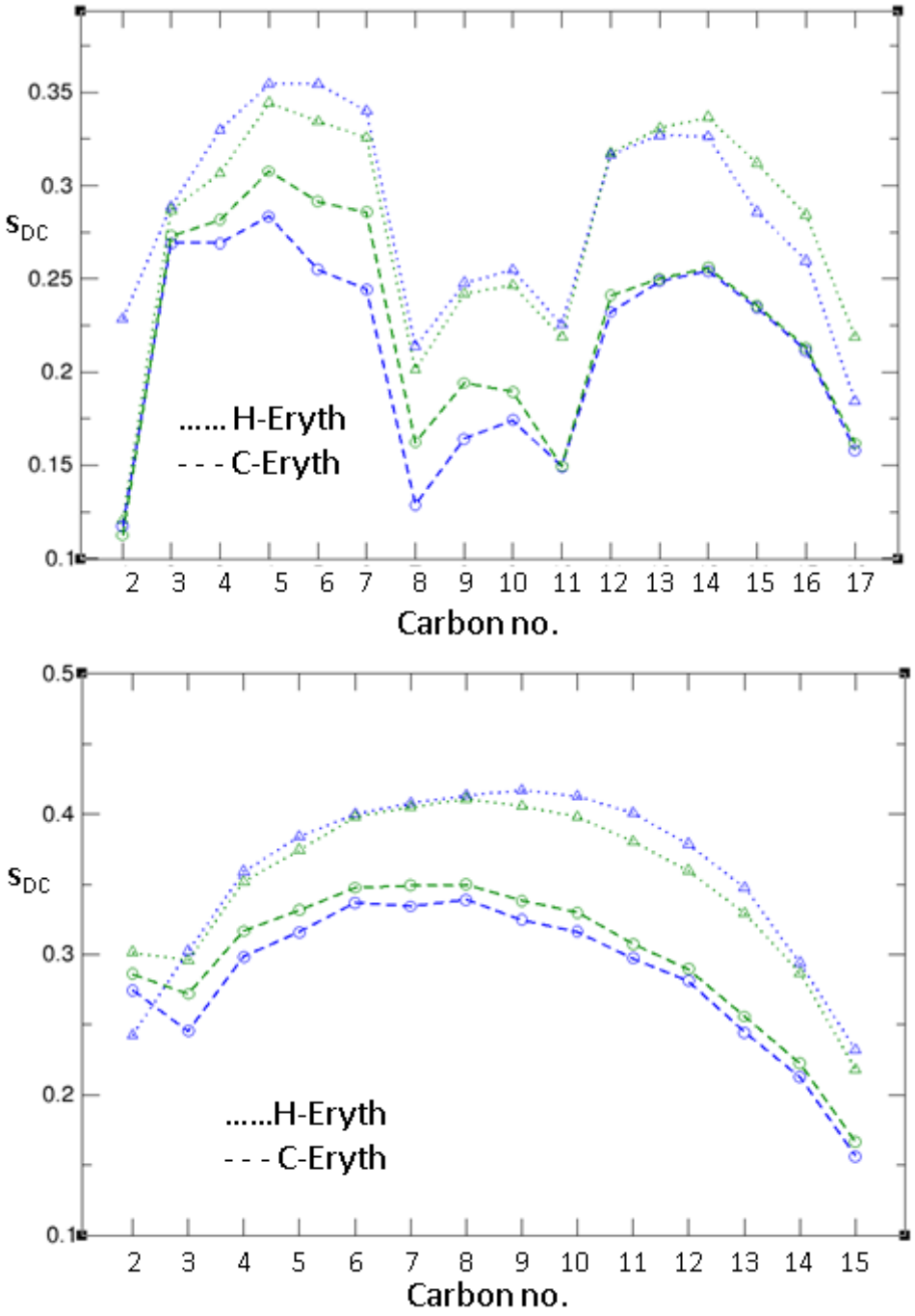

Figure S10: Comparison of deuterium order parameters for the two fatty acid chains of POPS, oleoyl (upper half) and palmitoyl (lower half) in M-Eukar (dotted line) and M-Cancer (broken line). Values for the external layer are shown in blue and for the internal layer in green. Carbon atom numbers increase in the direction of the chain termini, with the highest number corresponding to $-CH_3$.