Supplementary Material (ESI) for *PCCP*

How does Proteinase 3 interact with lipid bilayers?

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Supplementary Material

Fig. A

Conformations along the MD simulations are compared against the X-ray structure of PR3 (PDB: 1fuj). The root mean square deviation (RMSd) between the backbone atoms of the MD-generated structures and the crystal structure is plotted along the simulation time. A) RMSd of a 40 ns long simulation of PR3 in water. B) PR3 bound to DMPC (200 ns, C) PR3 bound to DMPG (200 ns) and D) PR3 bound to an equimolar mixture of DMPC/DMPG (300 ns). For the simulations of membrane-bound PR3 the backbone RMSd is plotted for each copy of the enzyme, one in grey and the other one in black (one copy of PR3 is positioned on each leaflets, see Fig.1 of manuscript and Methods section).