

Supplementary Information

pMD-membrane: A method for ligand binding site identification in membrane-bound proteins

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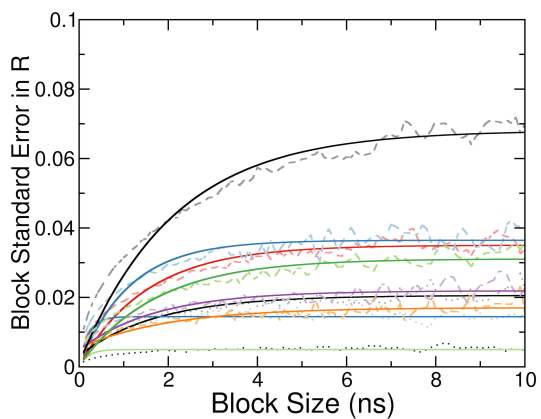
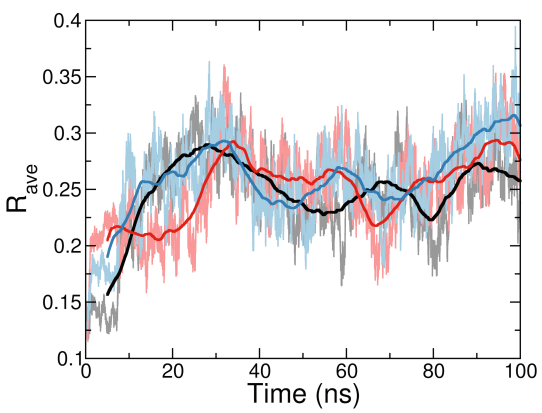


Figure S3: Convergence and sampling error. (Left) Time evolution of average probe occupancies calculated using equation 5 for simulations G12D mode 2 (black), G12D mode 1 (red) and G13D (blue). Bold lines indicate 5 ns-running average. (Right) Examples of the dependence of block standard errors (BSE) in R_i on block size. Shown here are just a few example curves for selected atoms illustrating atoms (see Methods in the main text for details).