Supplementary Material: Protein-membrane interactions with a twist

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FIG. S1. Analysis of the internal dynamics of the cylinder for the two runs. The value of the angle α averaged along the last 500 frames of each trajectory is shown as a function of the nominal value of α . The dotted straight line passes through the origin with slope 1. Standard deviations (not shown) are equal to $\approx 5^{\circ}$ for all cases.



FIG. S2. Angle θ between the membrane normal and the cylinder axis plotted for different values of α for the second run of the MD simulations. The four panels correspond to different values of dwhile the colors correspond to different values of the cohesion parameter \tilde{w}_c .



FIG. S3. Positions of maxima in the distribution density of the angles θ describing the orientation of the cylinder inserted in the membrane for the second run of the MD simulations. For each trajectory, one or two such positions have been observed, corresponding to unimodel and bimodal distributions. (a,b,c) Histogram of maxima positions for the unique peak of the unimodal distribution (a) as well as for the smallest (b) and largest (c) peaks of the bimodal distribution. (d) Plot of the angle α together with the positions of the maxima θ_{p1} (black dots) and θ_{p2} (red dots) of each bimodal distribution. (e) Plot of θ_{p2} as a function of θ_{p1} .



FIG. S4. Central parts of the membrane surface (10x10 in scaled units) obtained by averaging the interpolated surfaces defined by the LI1 beads of the lipids of each monolayer of the membrane. The surfaces have been determined for the set of trajectories recorded with $\tilde{w}_c = 3$, and d = 2, and box sizes of $35 \cdot 35 \cdot 100\sigma^3$ and $40 \cdot 40 \cdot 100\sigma^3$. The reference height z = 0 is set to the mean height of the displayed surface.



FIG. S5. Central parts of the membrane surface (10x10 in scaled units) obtained by averaging the interpolated surfaces defined by the LI1 beads of the lipids of each monolayer of the membrane. The surfaces have been determined for the set of trajectories recorded with $\alpha = 20^{\circ}$, and d = 1, and box sizes of $35 \cdot 35 \cdot 100\sigma^3$ and $40 \cdot 40 \cdot 100\sigma^3$. The reference height z = 0 is set to the mean height of the displayed surface.



FIG. S6. Averaged scaled hydrophobic thickness of the membrane, h, as a function of α for the second run of the MD simulations. The four panels correspond to different values of d while the colors correspond to different values of the cohesion parameter \tilde{w}_c . The thickness was calculated as the difference of time-averaged z coordinates of the interpolated monolayers obtained from the positions of the LI1 beads and spatially averaged over a square of $5 \times 5 \sigma^2$ located at the center of the membrane where the cylinder is situated.

Scaled box size	$\tilde{w}_{\rm c} = 2$	$\tilde{w}_{\rm c} = 2.25$	$\tilde{w}_{\rm c} = 2.5$
$30 \cdot 30 \cdot 100$	37	46	62
$35 \cdot 35 \cdot 100$	36	49	60
$40 \cdot 40 \cdot 100$	35	48	69

TABLE S1. Torque τ obtained from the analysis of the simulations with d = 1 and $\alpha = 20^{\circ}$ for various box sizes. The torque is expressed in units of $k_{\rm B}T$.