Supporting Information: Molecular Dynamics Simulations of the Interaction of Beta Cyclodextrin with a Lipid Bilayer

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1. The permeation and insertion of βCD molecule into the lipid bilayer

Figure S1. The initial structures of BCD1-BCD5 systems are presented in column (a), their distances of βCD from the bilayer center and the βCD tilt angle as a function of time are shown in column (b), and the last snapshots of each simulation, at 1 µs for BCD1-BCD4 systems and at 2 µs for BCD5 system are depicted in column (c).
2. Force field validation

**Table S1.** The structural properties of βCD in water from our MD simulation in comparison with the previous experimental and MD studies.\(^1\)\(^-\)\(^4\)

<table>
<thead>
<tr>
<th>properties</th>
<th>βCD in water</th>
<th>references</th>
</tr>
</thead>
<tbody>
<tr>
<td>cavity height (nm)</td>
<td>0.30±0.03</td>
<td>0.36(^a), 0.28(Glycam06)(^b),(^3), 0.35(Glycam04, Amber99SB, q4md-CD)(^b),(^3)</td>
</tr>
<tr>
<td>radial of gyration (nm)</td>
<td>0.60±0.01</td>
<td>0.6(^a),(^1), 0.6(^b),(^2)</td>
</tr>
<tr>
<td>1st rim diameter (nm)</td>
<td>1.07±0.29</td>
<td>1.01±0.08(^a),(^1), ~1.3(Glycam06)(^b),(^3), ~1.1(Glycam04, q4md-CD)(^b),(^3), ~1.2(Amber99SB)(^b),(^3)</td>
</tr>
<tr>
<td>2nd rim diameter (nm)</td>
<td>1.17±0.13</td>
<td>1.25±0.05(^a),(^1), ~1.35(Glycam06)(^b),(^3), ~1.3(Glycam04)(^b),(^3), ~1.25(Amber99SB, q4md-CD)(^b),(^3)</td>
</tr>
<tr>
<td>rmsd (nm)</td>
<td>0.24±0.02</td>
<td>0.19(Glycam06)(^b),(^3), 0.11(Glycam04)(^b),(^3), 0.15(Amber99SB)(^b),(^3), 0.13(q4md-CD)(^b),(^3), ~0.25(^b),(^4)</td>
</tr>
<tr>
<td>#intramolecular H-bonds</td>
<td>0-6</td>
<td>0-8(^b),(^4)</td>
</tr>
<tr>
<td>#H-bonds with waters</td>
<td>30-50</td>
<td>30-40(^b),(^4)</td>
</tr>
</tbody>
</table>

\(^a\)X-ray structure of βCD (entry code: BUVSEQ02)\(^1\)

\(^b\)MD data of βCD in solution at 298K using various force fields Glycam04\(^1\), Glycam04\(^3\), Amber99SB\(^2\), q4md-CD\(^3\), CHARMM22\(^2\) and GROMOS 53A6\(^6\)
3. The influence of the $\beta$CD on the lipid membrane properties

**Figure S2.** 2D-density maps on xy-plane of the phosphate groups, glycerol-ester groups, water and $\beta$CD molecule for all systems (BCD1-BCD5) compared to those of the POPC bilayer without $\beta$CD molecule (no $\beta$CD)
4. References


