**Supplementary information for**

# Modelling the effects of E/Z photoisomerization of a cyclocurcumin analogue on the properties of cellular lipid membranes

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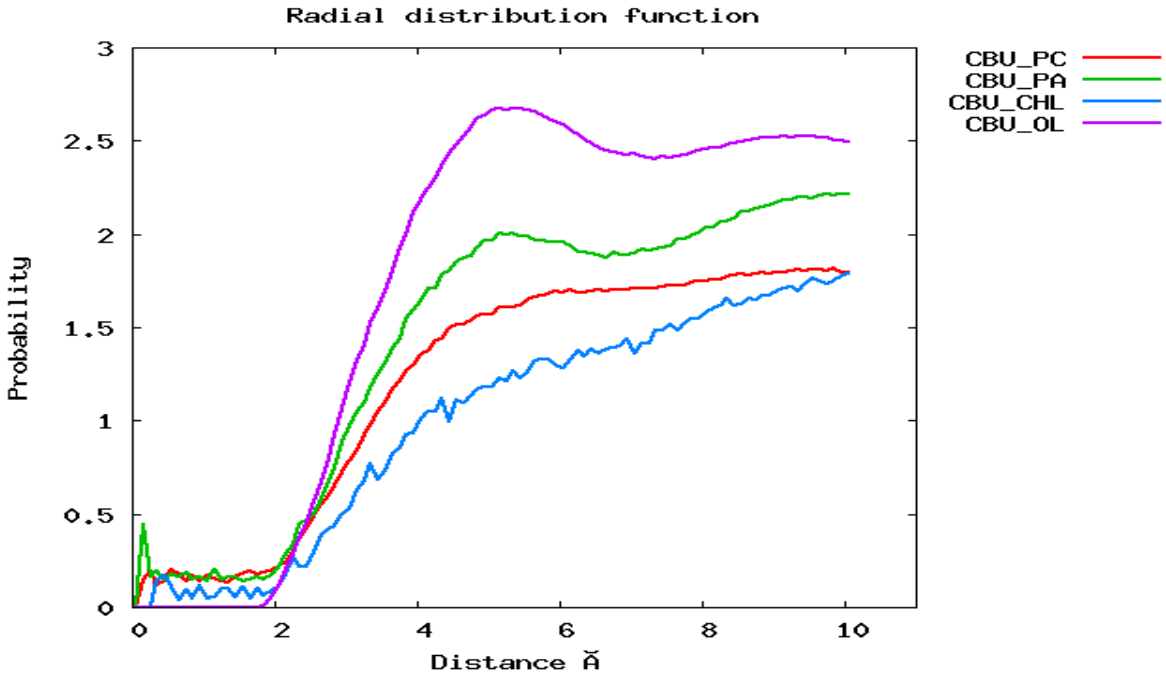



Figure S1. Radial distribution function between CCBu and different lipid moieities: PC are polar heads of DPPC and DOPC; PA is a hydrophobic part of DPPC lipid; OL is a hydrophobic chain of DOPC lipid; CHL is cholesterol.

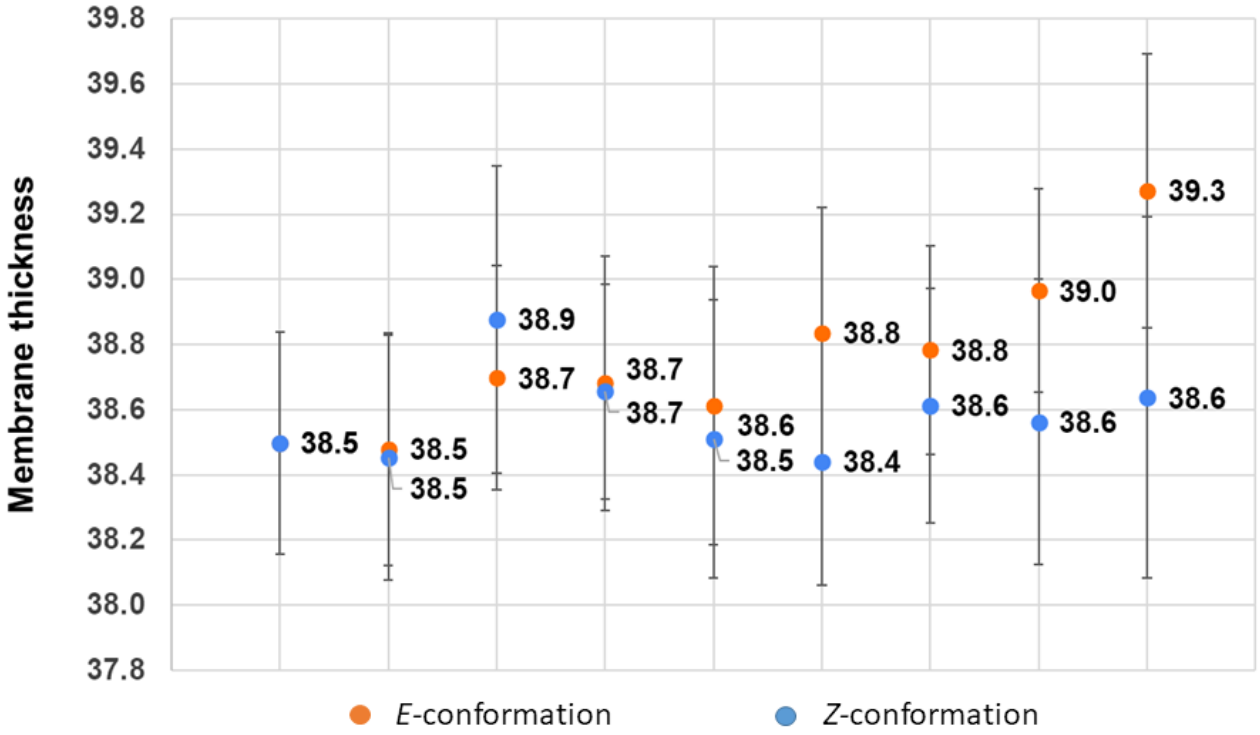



Figure S2. Average and standard deviation of the thickness in Å of the membrane composed of DPPC, DOPC and cholesterol.

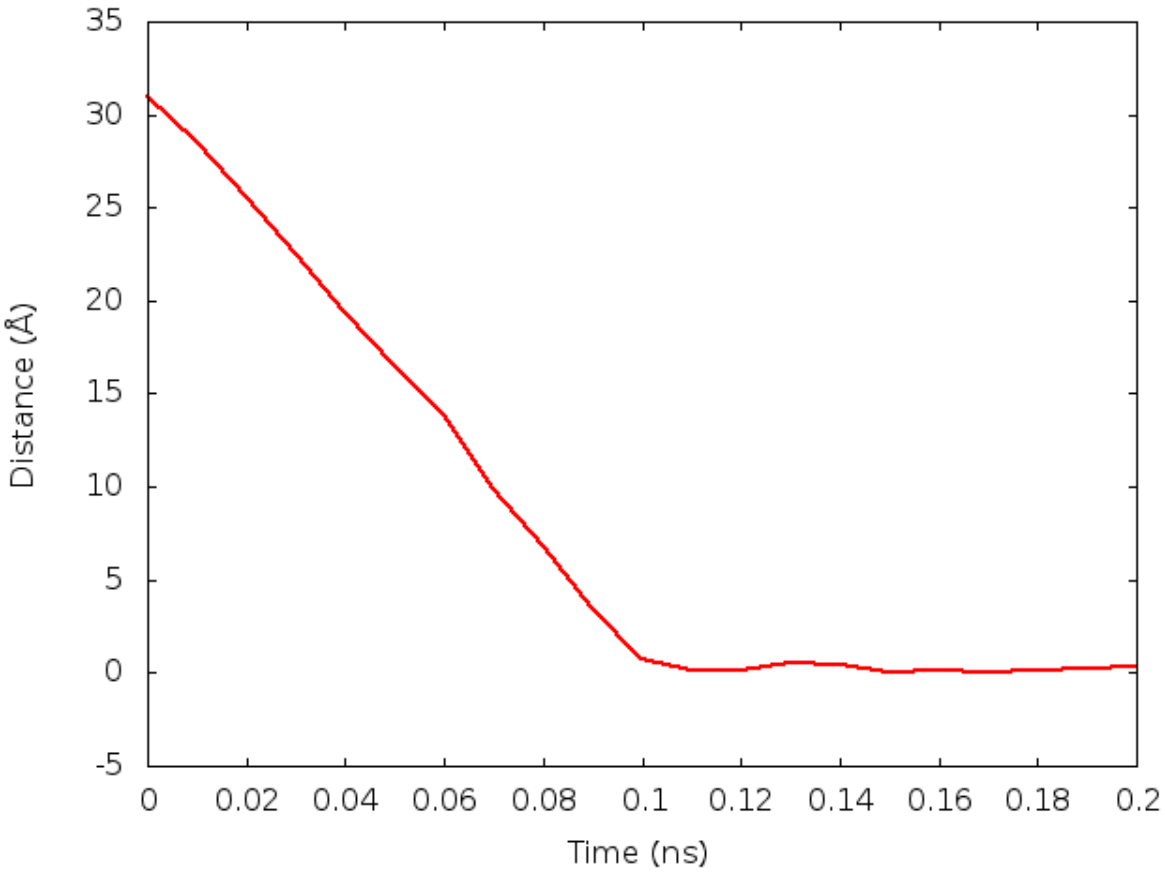



Figure S3. Evolution of the distance between 5 CCBu in E-conformation during the steered molecular dynamics.

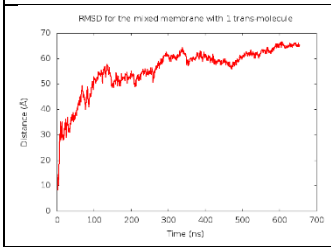
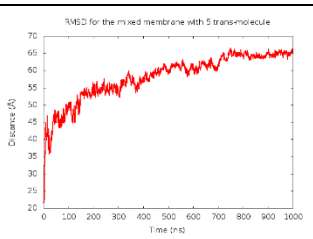
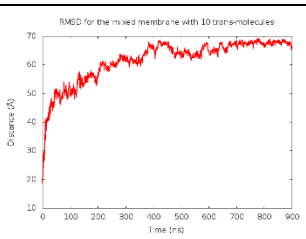
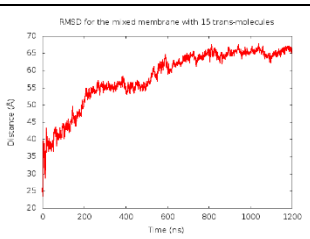
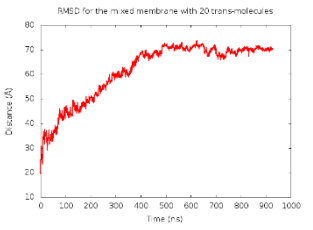
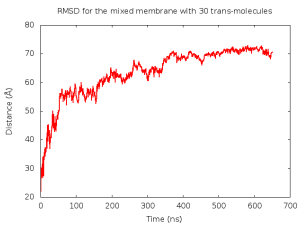
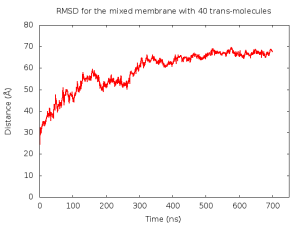
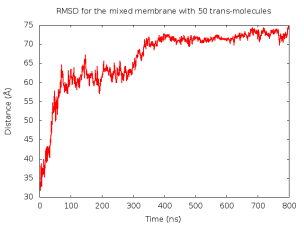
| RMSD for the DPPC, DOPC, cholesterol membrane | | | |
|---|---|---|---|
| 1 ***E***-CCBu (after 1000ns) | 5 ***E***-CCBu (after 1000ns) | 10 ***E***-CCBu (after 900ns) | 15 ***E***-CCBu (after 1200ns) |
|  |  |  |  |
| 20 ***E***-CCBu (after 1000ns) | 30 ***E***-CCBu (after 650ns) | 40 ***E***-CCBu (after 700ns) | 50 ***E***-CCBu (after 800ns) |
|  |  |  |  |

Figure S4. Time evolution of the RMSD for DPPC, DOPC and cholesterol for all constructed systems with different numbers of CCBu in E-conformation.

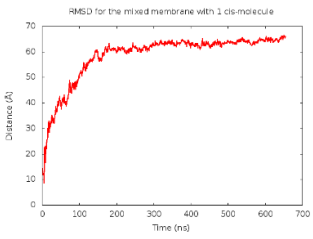
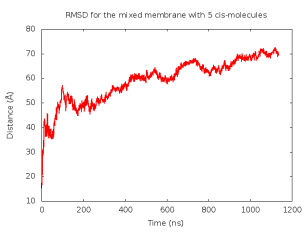
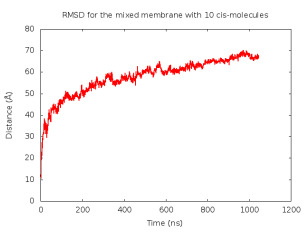
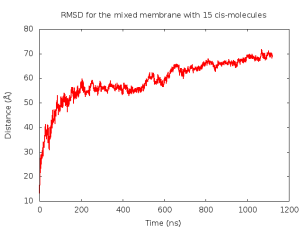
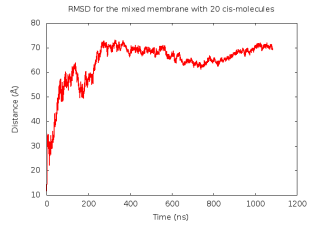
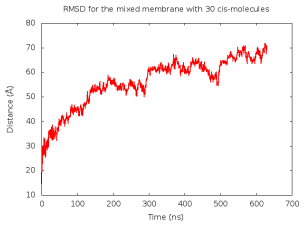
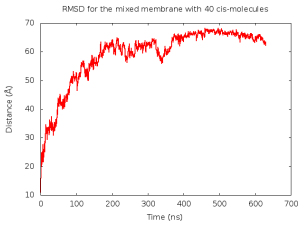
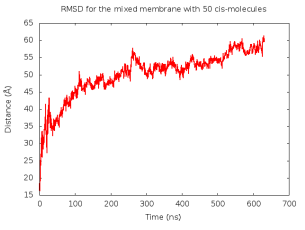
| RMSD for the DPPC, DOPC, cholesterol membrane | | | |
|---|---|---|---|
| 1 ***Z***-CCBu (after 1135ns) | 5 ***Z***-CCBu (after 1135ns) | 10 ***Z***-CCBu (after 1045ns) | 15 ***Z***-CCBu (after 1120ns) |
|  |  |  |  |
| 20 ***Z***-CCBu (after 1084ns) | 30 ***Z***-CCBu (after 630ns) | 40 ***Z***-CCBu (after 630ns) | 50 ***Z***-CCBu (after 630ns) |
|  |  |  |  |

Figure S5. Time evolution of the RMSD for DPPC, DOPC and cholesterol for all constructed systems with different numbers of CCBu in Z-conformation.

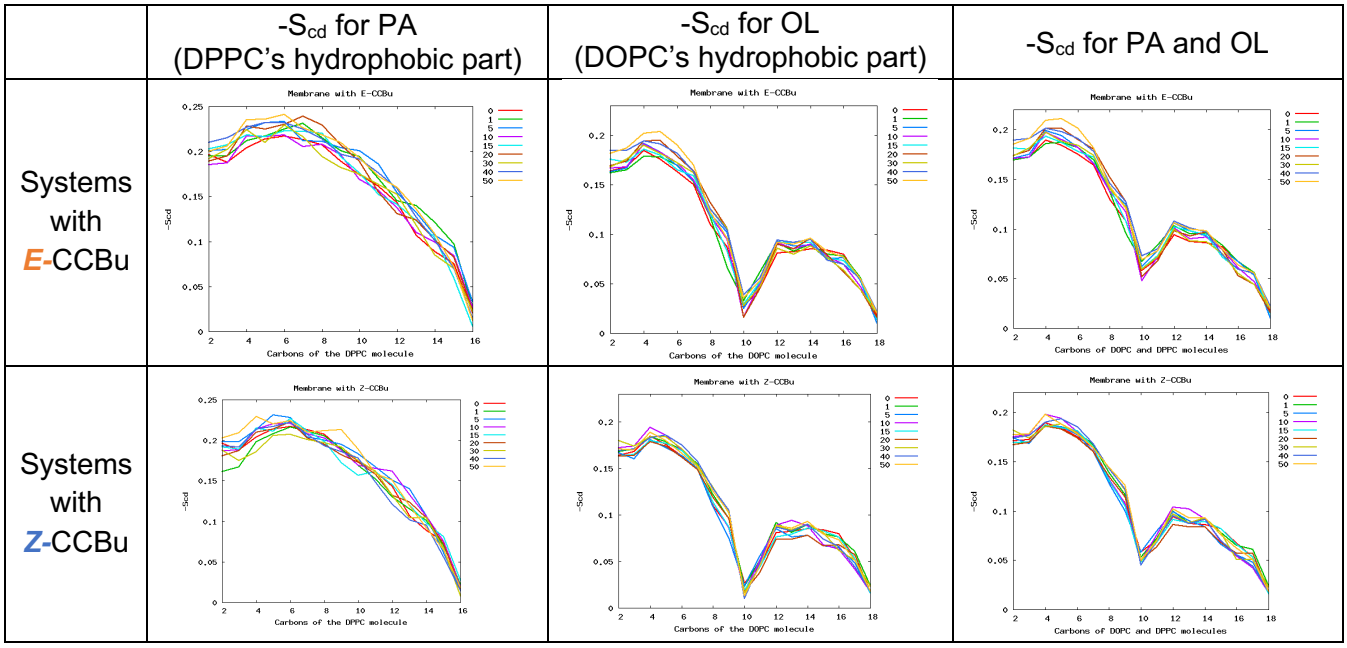
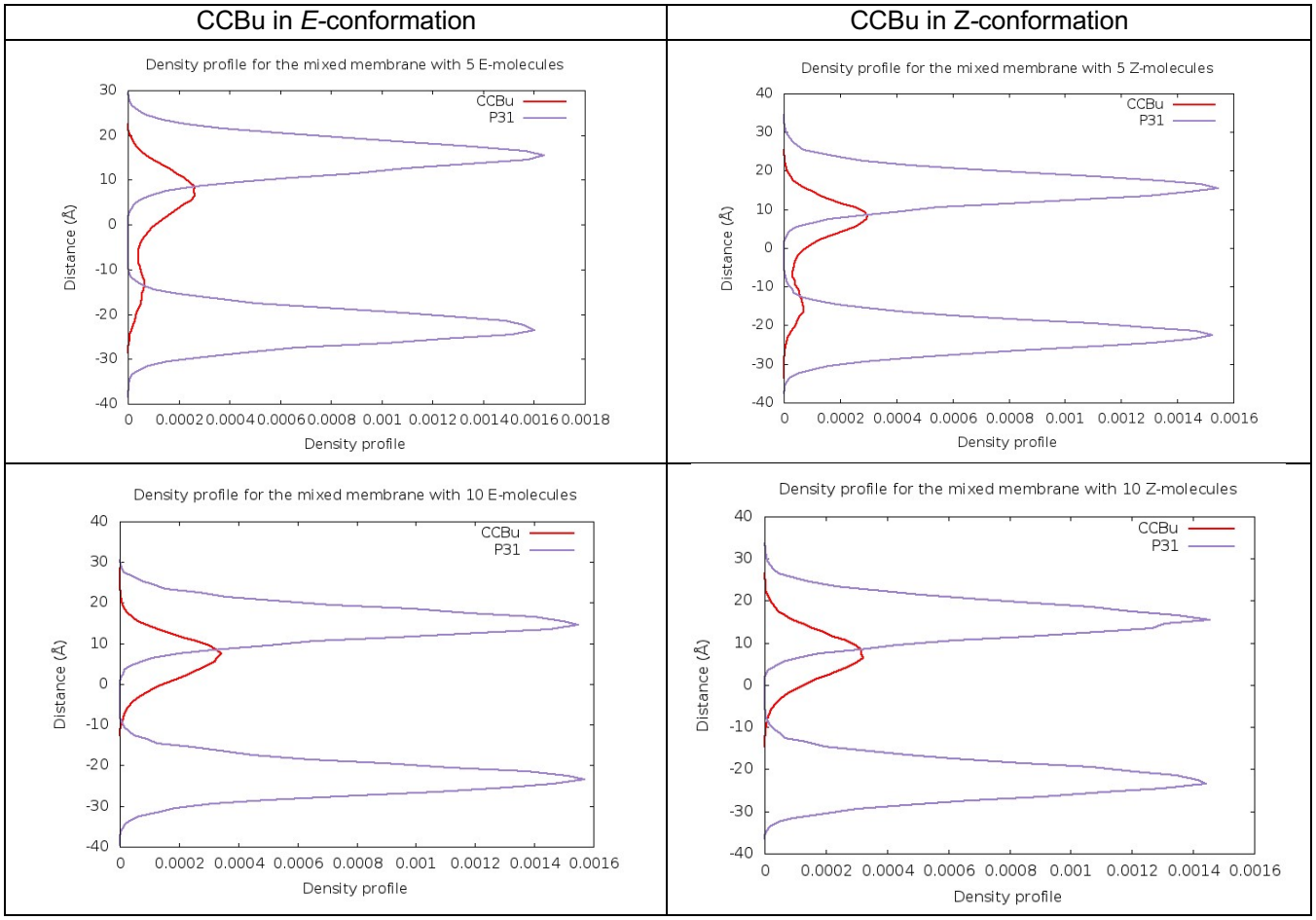



Figure S6. Deuterium order parameter ($-S_{cd}$) for PA (DPPC's hydrophobic tail), OL (DOPC's hydrophobic tail) and both of them for all constructed systems with different numbers of CCBu molecules in E- and Z-conformations.



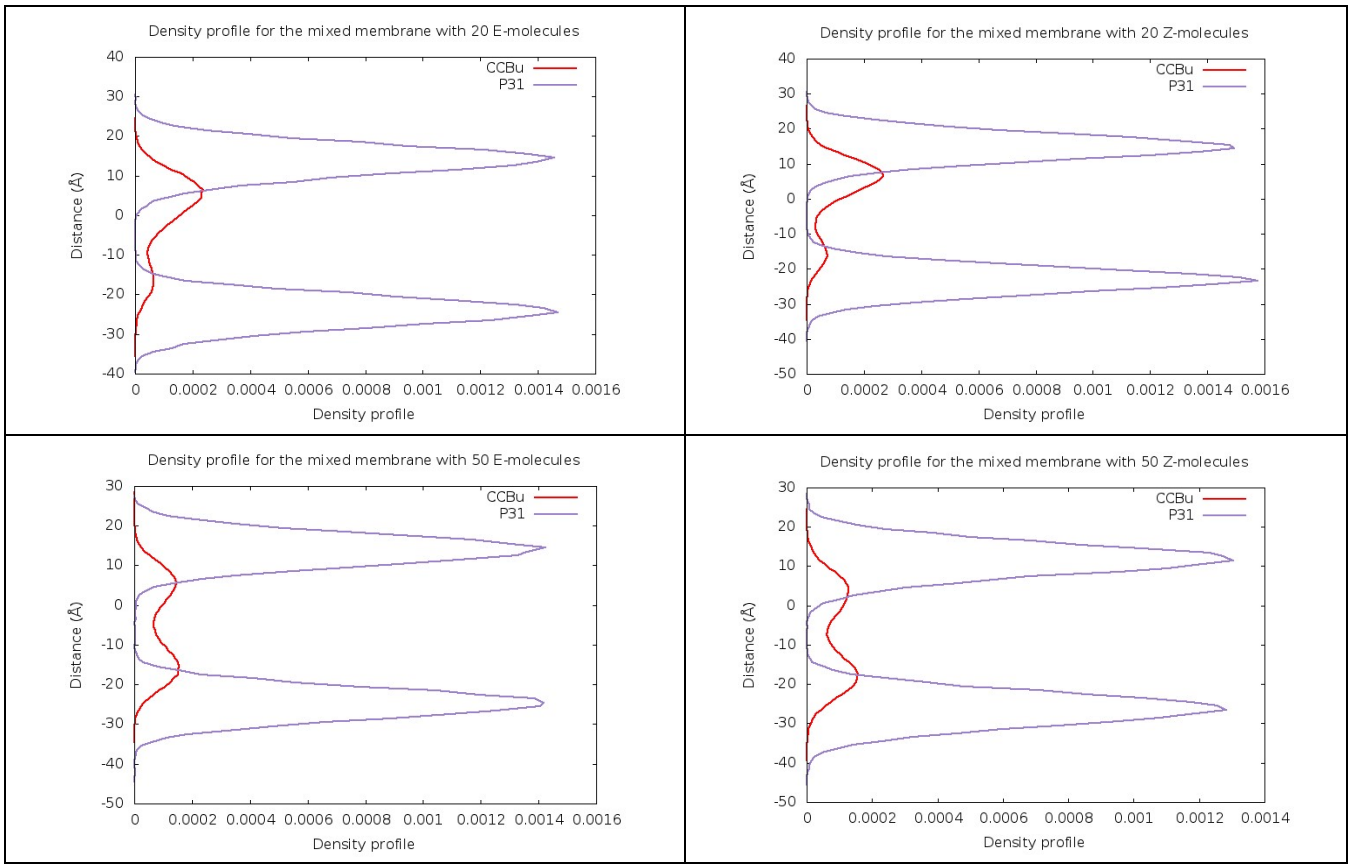



Figure S7. Normalized density profiles for CCBu in *E*- and *Z*-conformations for lipid bilayers containing 5, 10, 20, and 50 ligands where the red plot is a density for CCBu molecule and the purple plot is the density profile of phosphorus atom in the lipids polar heads.

**Force Field Parameters**

**Coordinates and Point RESP charges**

All compounds are described with Atom name; Atom type; X, Y, Z coordinates and RESP charges.

**E-CCBu**

| | | | | | |
|---|---|---|---|---|---|
| C1B | ca | -5.003 | -2.768 | -0.721 | -0.239554 |
| C2B | ca | -6.354 | -2.686 | -0.405 | 0.272242 |
| C3B | ca | -6.888 | -1.460 | 0.050 | 0.190995 |
| C4B | ca | -6.075 | -0.345 | 0.180 | -0.225953 |
| C5B | ca | -4.705 | -0.423 | -0.150 | -0.114296 |
| C6B | ca | -4.184 | -1.646 | -0.593 | -0.174799 |
| C7B | cc | -3.848 | 0.768 | -0.036 | 0.493676 |
| O1B | os | -2.518 | 0.447 | 0.000 | -0.311238 |
| C8B | cc | -1.562 | 1.429 | 0.099 | 0.483006 |
| C9B | cd | -1.912 | 2.738 | 0.191 | -0.670893 |
| C10B | c | -3.306 | 3.168 | 0.151 | 0.901030 |
| C11B | cd | -4.254 | 2.061 | 0.018 | -0.681997 |
| O2B | o | -3.655 | 4.350 | 0.219 | -0.645101 |
| C12B | ca | 2.282 | 0.996 | 0.022 | 0.048624 |
| O3B | oh | -7.157 | -3.775 | -0.524 | -0.563218 |
| O4B | os | -8.228 | -1.522 | 0.341 | -0.293945 |
| C13B | ca | 3.358 | 1.890 | -0.187 | -0.314286 |
| C14B | ca | 4.678 | 1.456 | -0.193 | 0.258286 |
| C15B | ca | 4.961 | 0.081 | 0.018 | 0.330382 |
| C16B | ca | 3.902 | -0.805 | 0.230 | -0.283542 |
| C17B | ca | 2.582 | -0.355 | 0.233 | -0.221286 |
| O5B | os | 5.765 | 2.253 | -0.389 | -0.336663 |
| O6B | os | 6.275 | -0.259 | -0.002 | -0.474312 |
| C18B | c3 | -8.875 | -0.342 | 0.798 | -0.125739 |
| C19B | c3 | 5.546 | 3.637 | -0.604 | 0.026521 |
| C20B | ce | -0.231 | 0.841 | 0.103 | -0.342579 |
| C21B | cf | 0.925 | 1.533 | 0.006 | -0.038913 |
| H1B | ha | -4.606 | -3.716 | -1.069 | 0.194953 |
| H2B | ha | -6.484 | 0.584 | 0.557 | 0.166619 |
| H3B | ha | -3.133 | -1.718 | -0.848 | 0.164719 |
| H4B | ha | -1.150 | 3.502 | 0.300 | 0.226795 |
| H5B | ha | -5.305 | 2.312 | -0.051 | 0.227206 |
| H6B | ho | -8.051 | -3.500 | -0.255 | 0.409175 |
| H7B | ha | 3.136 | 2.939 | -0.349 | 0.173244 |
| H8B | ha | 4.103 | -1.856 | 0.398 | 0.149378 |
| H9B | ha | 1.787 | -1.073 | 0.410 | 0.197761 |
| H10B | h1 | -9.921 | -0.611 | 0.951 | 0.107490 |
| H11B | h1 | -8.444 | 0.004 | 1.746 | 0.107490 |
| H12B | h1 | -8.808 | 0.460 | 0.053 | 0.107490 |
| H13B | h1 | 6.535 | 4.078 | -0.735 | 0.063969 |
| H14B | h1 | 4.946 | 3.816 | -1.507 | 0.063969 |
| H15B | h1 | 5.050 | 4.107 | 0.256 | 0.063969 |
| H16B | ha | -0.224 | -0.243 | 0.178 | 0.158621 |
| H17B | ha | 0.866 | 2.615 | -0.108 | 0.141473 |
| C22B | c3 | 6.635 | -1.625 | 0.201 | 0.306458 |
| H18B | h1 | 6.271 | -1.965 | 1.182 | 0.001941 |

| | | | | | |
|---|---|---|---|---|---|
| H19B | h1 | 6.164 | -2.253 | -0.569 | 0.001941 |
| C23B | c3 | 8.152 | -1.720 | 0.124 | -0.112489 |
| H20B | hc | 8.478 | -1.339 | -0.852 | 0.055166 |
| H21B | hc | 8.584 | -1.053 | 0.881 | 0.055166 |
| C24B | c3 | 8.663 | -3.152 | 0.329 | 0.096147 |
| H22B | hc | 8.215 | -3.813 | -0.427 | -0.015522 |
| H23B | hc | 8.321 | -3.527 | 1.304 | -0.015522 |
| C25B | c3 | 10.190 | -3.253 | 0.252 | -0.175700 |
| H24B | hc | 10.528 | -4.284 | 0.401 | 0.043882 |
| H25B | hc | 10.559 | -2.917 | -0.725 | 0.043882 |
| H26B | hc | 10.666 | -2.630 | 1.018 | 0.043882 |

**Z-CCBu**

| | | | | | |
|---|---|---|---|---|---|
| C1B | ca | 6.364 | -1.486 | -0.947 | -0.261883 |
| C2B | ca | 7.240 | -0.407 | -0.923 | 0.286293 |
| C3B | ca | 6.798 | 0.835 | -0.416 | 0.185719 |
| C4B | ca | 5.504 | 0.980 | 0.057 | -0.249740 |
| C5B | ca | 4.615 | -0.117 | 0.044 | -0.067866 |
| C6B | ca | 5.061 | -1.342 | -0.469 | -0.169670 |
| C7B | cc | 3.248 | 0.031 | 0.568 | 0.452886 |
| O1B | os | 2.427 | -0.988 | 0.169 | -0.355544 |
| C8B | cc | 1.110 | -1.028 | 0.563 | 0.614150 |
| C9B | cd | 0.592 | -0.063 | 1.363 | -0.671133 |
| C10B | c | 1.396 | 1.069 | 1.824 | 0.864095 |
| C11B | cd | 2.783 | 1.026 | 1.366 | 0.660296 |
| O2B | o | 0.949 | 1.966 | 2.544 | -0.633829 |
| C12B | ca | -2.044 | -1.791 | -0.178 | 0.020970 |
| O3B | oh | 8.509 | -0.540 | -1.389 | -0.562622 |
| O4B | os | 7.757 | 1.817 | -0.466 | -0.287542 |
| C13B | ca | -3.259 | -2.484 | 0.036 | -0.308653 |
| C14B | ca | -4.485 | -1.832 | 0.009 | 0.266331 |
| C15B | ca | -4.530 | -0.440 | -0.265 | 0.313400 |
| C16B | ca | -3.336 | 0.241 | -0.507 | -0.270120 |
| C17B | ca | -2.109 | -0.423 | -0.462 | -0.216038 |
| O5B | os | -5.694 | -2.425 | 0.221 | -0.336797 |
| O6B | os | -5.767 | 0.118 | -0.277 | -0.464959 |
| C18B | c3 | 7.426 | 3.108 | 0.027 | -0.133058 |
| C19B | c3 | -5.713 | -3.814 | 0.502 | 0.013403 |
| C20B | ce | 0.488 | -2.258 | 0.075 | -0.486439 |
| C21B | cf | -0.804 | -2.577 | -0.166 | 0.018797 |
| H1B | ha | 6.716 | -2.434 | -1.340 | 0.200816 |
| H2B | ha | 5.165 | 1.943 | 0.418 | 0.171521 |
| H3B | ha | 4.388 | -2.190 | -0.488 | 0.166696 |
| H4B | ha | -0.440 | -0.123 | 1.684 | 0.251707 |
| H5B | ha | 3.444 | 1.813 | 1.710 | 0.225551 |
| H6B | ho | 8.943 | 0.325 | -1.282 | 0.406071 |
| H7B | ha | -3.220 | -3.549 | 0.236 | 0.171459 |
| H8B | ha | -3.352 | 1.301 | -0.734 | 0.153447 |
| H9B | ha | -1.203 | 0.134 | -0.669 | 0.191766 |
| H10B | h1 | 8.324 | 3.716 | -0.094 | 0.109454 |

| | | | | | |
|---|---|---|---|---|---|
| H11B | h1 | 6.603 | 3.552 | -0.547 | 0.109454 |
| H12B | h1 | 7.150 | 3.068 | 1.088 | 0.109454 |
| H13B | h1 | -6.764 | -4.074 | 0.644 | 0.066103 |
| H14B | h1 | -5.304 | -4.401 | -0.331 | 0.066103 |
| H15B | h1 | -5.154 | -4.050 | 1.417 | 0.066103 |
| H16B | ha | 1.218 | -3.049 | -0.089 | 0.193890 |
| H17B | ha | -0.963 | -3.626 | -0.414 | 0.117896 |
| C22B | c3 | -5.886 | 1.517 | -0.538 | 0.291978 |
| H18B | h1 | -5.311 | 2.086 | 0.208 | 0.003779 |
| H19B | h1 | -5.472 | 1.748 | -1.530 | 0.003779 |
| C23B | c3 | -7.364 | 1.875 | -0.471 | -0.097664 |
| H20B | hc | -7.907 | 1.261 | -1.201 | 0.050846 |
| H21B | hc | -7.748 | 1.598 | 0.519 | 0.050846 |
| C24B | c3 | -7.621 | 3.364 | -0.739 | 0.094451 |
| H22B | hc | -7.223 | 3.633 | -1.727 | -0.014173 |
| H23B | hc | -7.063 | 3.969 | -0.010 | -0.014173 |
| C25B | c3 | -9.107 | 3.729 | -0.672 | -0.181897 |
| H24B | hc | -9.263 | 4.796 | -0.866 | 0.044961 |
| H25B | hc | -9.687 | 3.166 | -1.413 | 0.044961 |
| H26B | hc | -9.526 | 3.505 | 0.316 | 0.044961 |