

# Electronic Polarization Effects on Membrane Translocation of Anti-cancer Drugs

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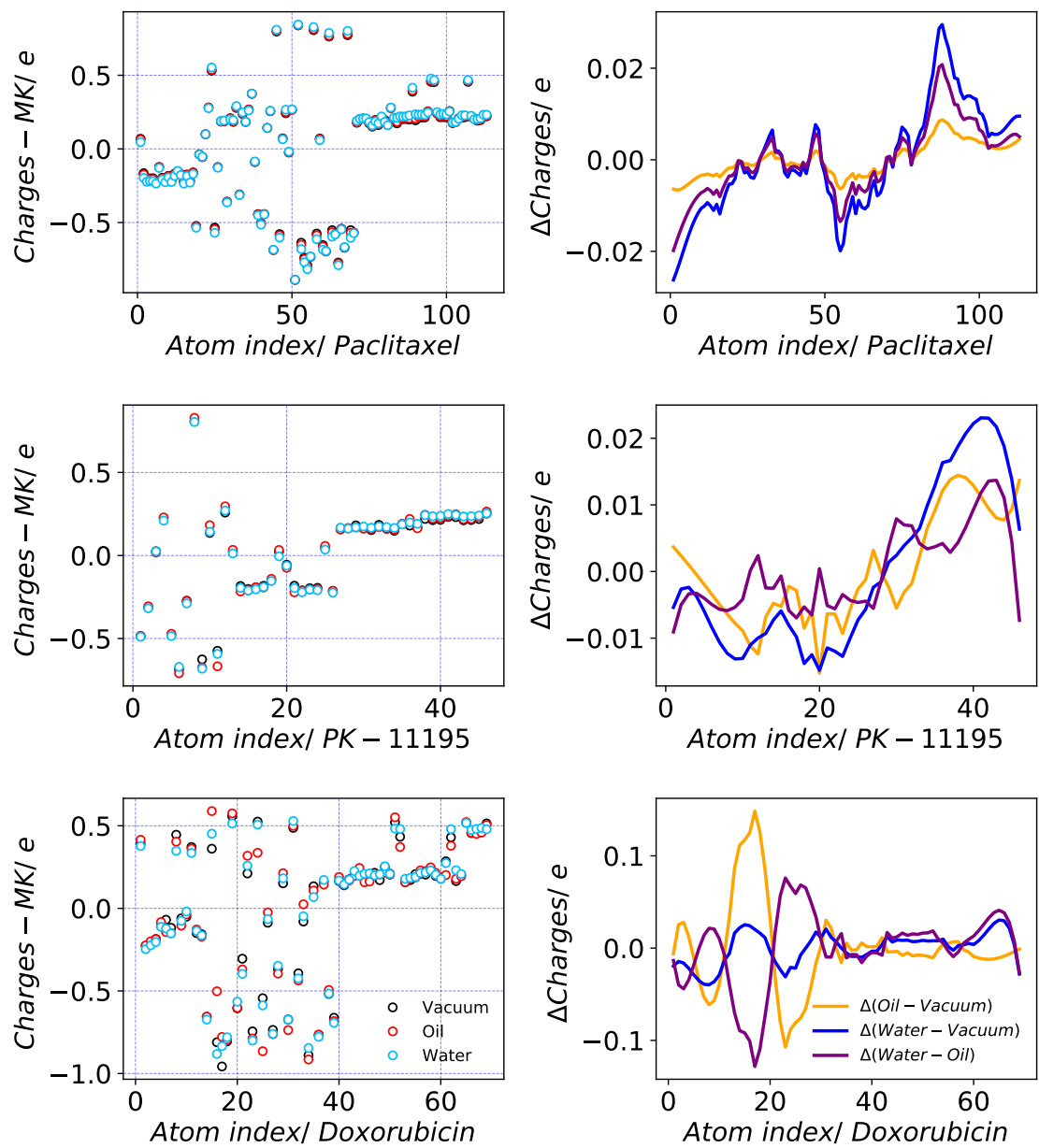


Figure S 1. MK charge distributions and their differences for the three drug molecules, obtained by DFT calculations.

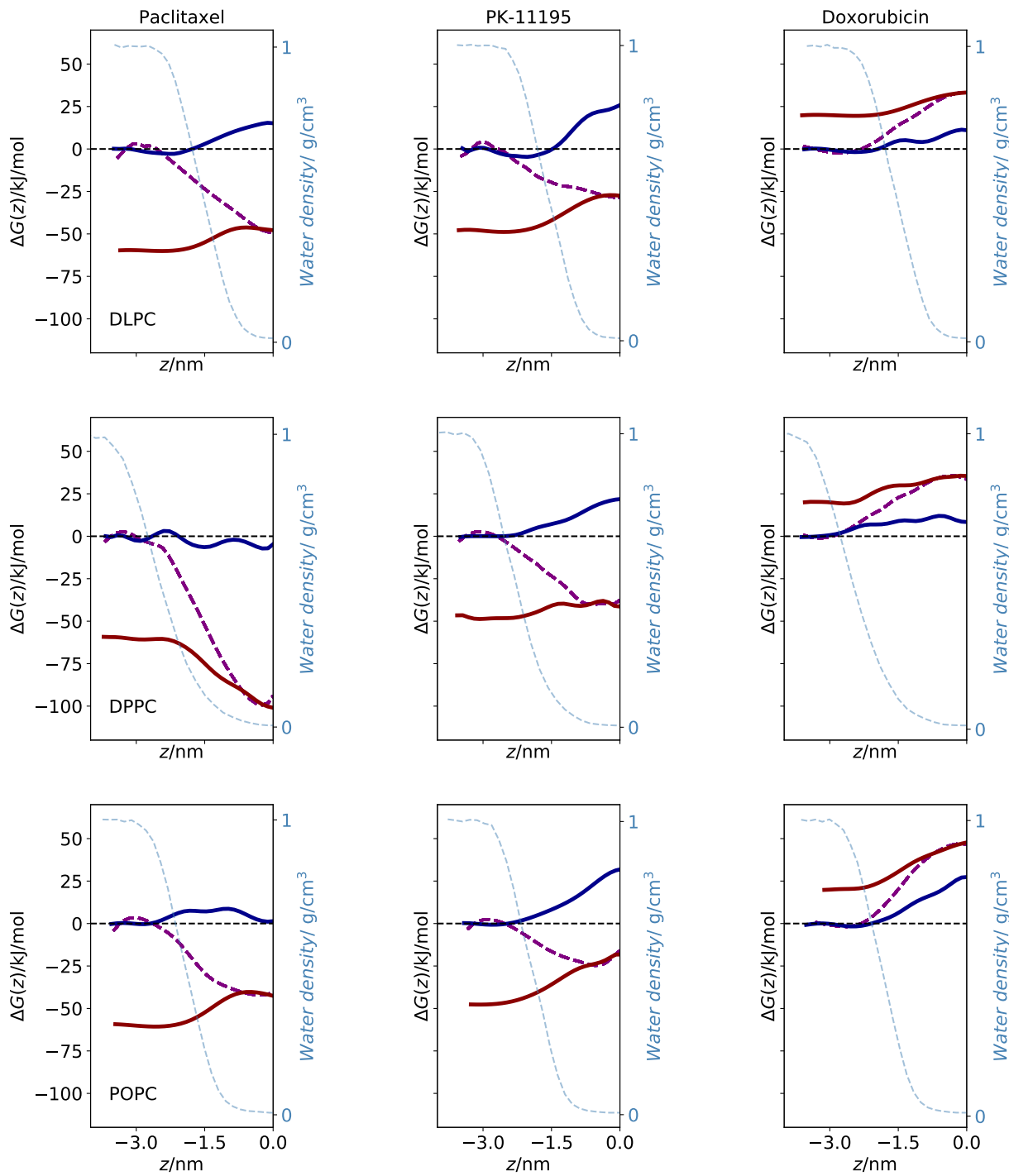


Figure S 2. Effective free energy of drug molecules when crossing the different lipid bilayers. Black circles show the *effective* free energy from the two-state SPFF model with MK charges.

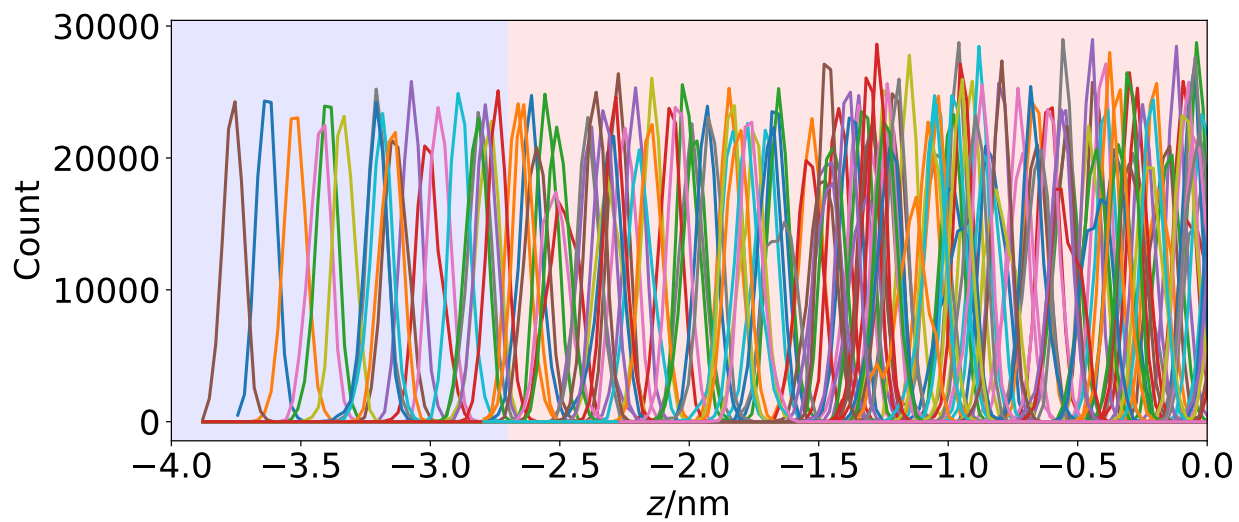


Figure S 3. The paclitaxel/DLPC corresponding umbrella histograms for upper and lower leaflet. The light blue color face is corresponded to the water medium and the light salmon color is related to DLPC membrane.

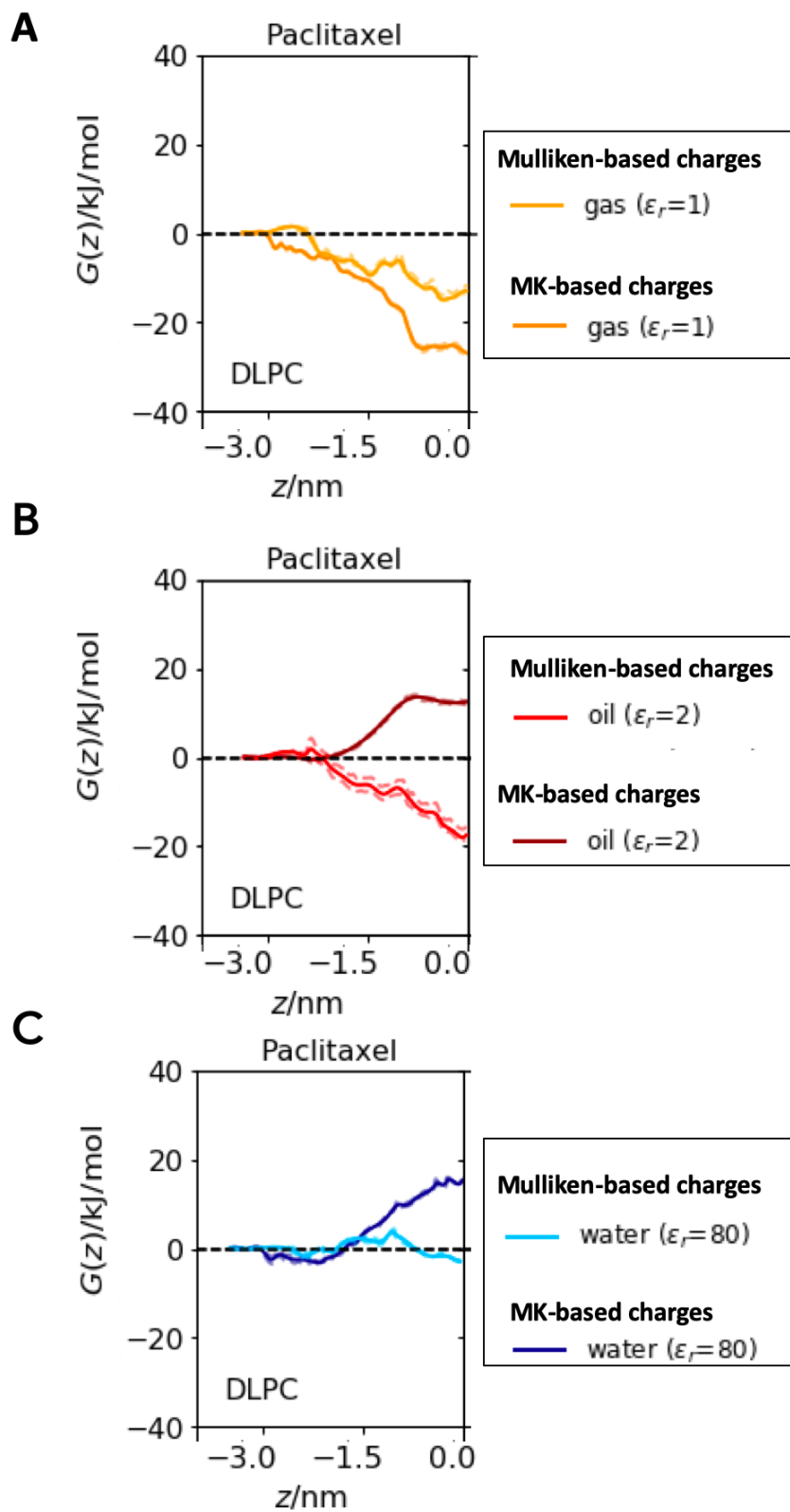


Figure S 4. Translocation free energies of paclitaxel from DLPC membrane are obtained using MK partial charges  $G_w(z)$  (dark blue),  $G_o(z)$  (dark red),  $G_g(z)$  (dark orange) and Mulliken charges  $G_w(z)$  (light blue),  $G_o(z)$  (light red), and  $G_g(z)$  (light orange).