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Supporting Material

Title: Interaction of Salicylate and a Terpenoid Plant Extract with Model

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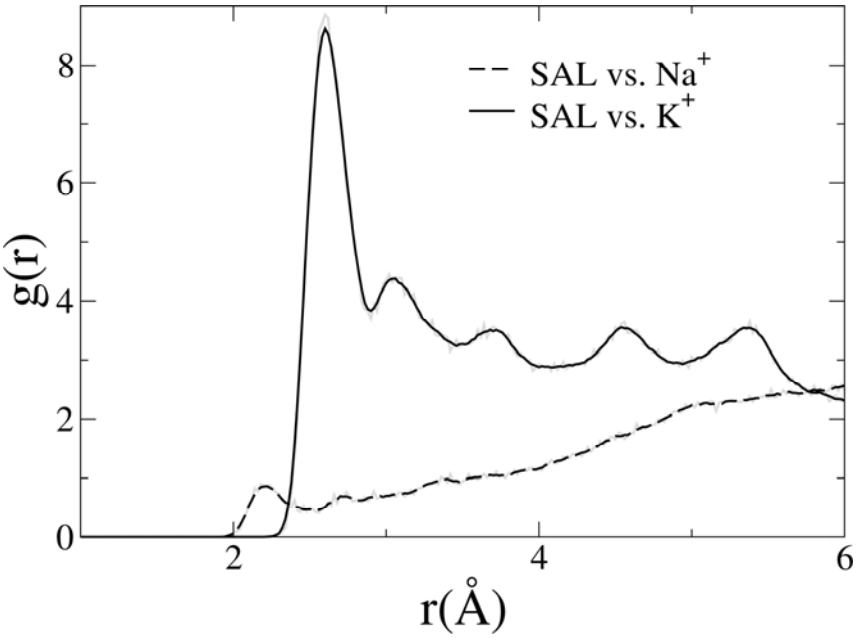

Figure S1: Radial pair correlation functions between cations and the SAL carboxyl group from the K20 and Na20 simulations. A 5-point average was taken over the original data (shown in light gray). K^+ ions are attracted to the interface after SAL binds to the lipid headgroups near the choline region. Na^+ ions, on the other hand, bind to the glycerol region, and cannot form ion-pairs with SAL.

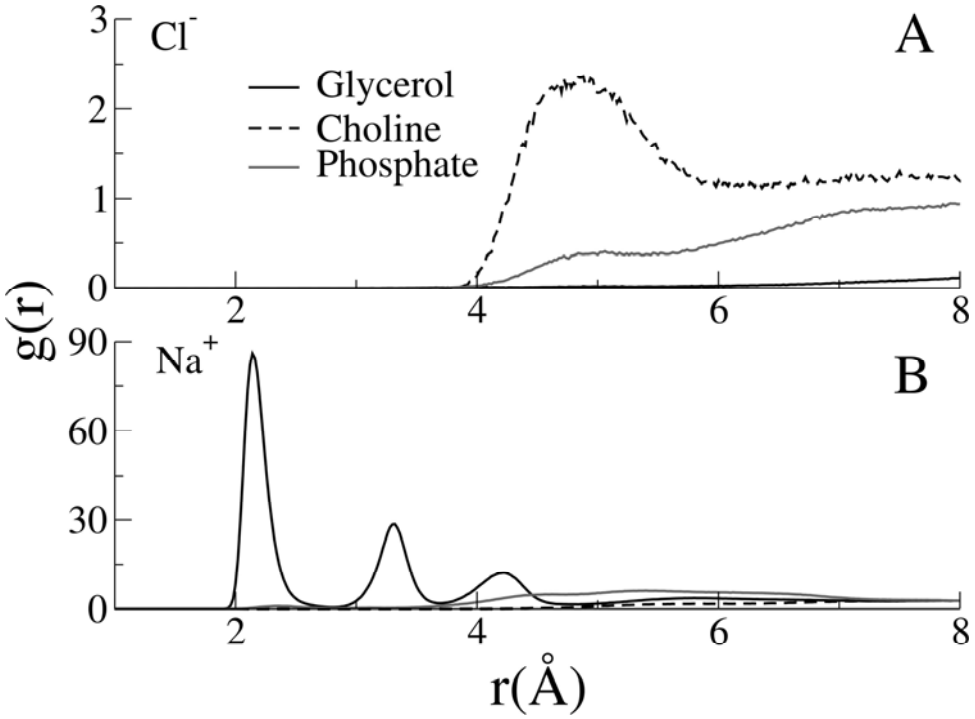

Figure S2: Radial distribution functions between the cations and various parts of the lipid headgroups. (A) Chloride ions do not interact specifically with any lipid part. (B) Na^+ ions bind deep into the headgroup region and interact with the glycerol backbone, and not the phosphate groups.