

Supplementary Materials

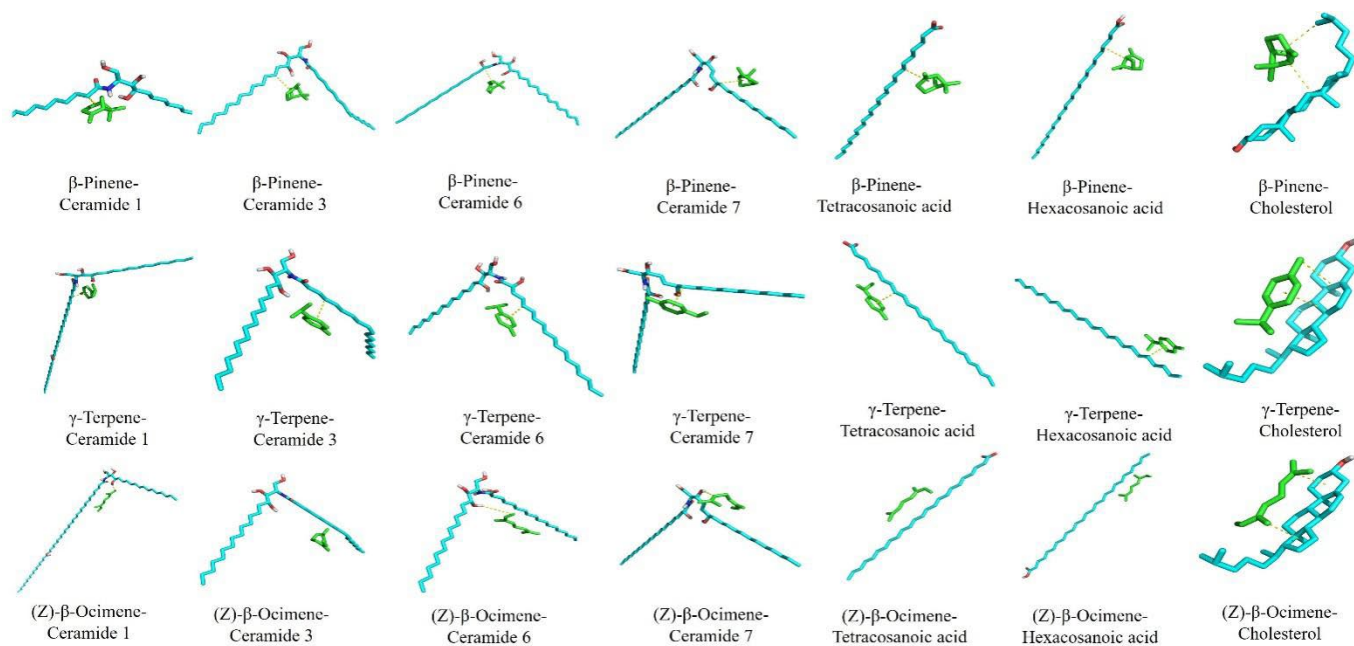


Figure S1a: Docking diagram of β -Pinene, γ -Terpinene and (Z)- β -Ocimene with lipid components in the skin lipid layer.

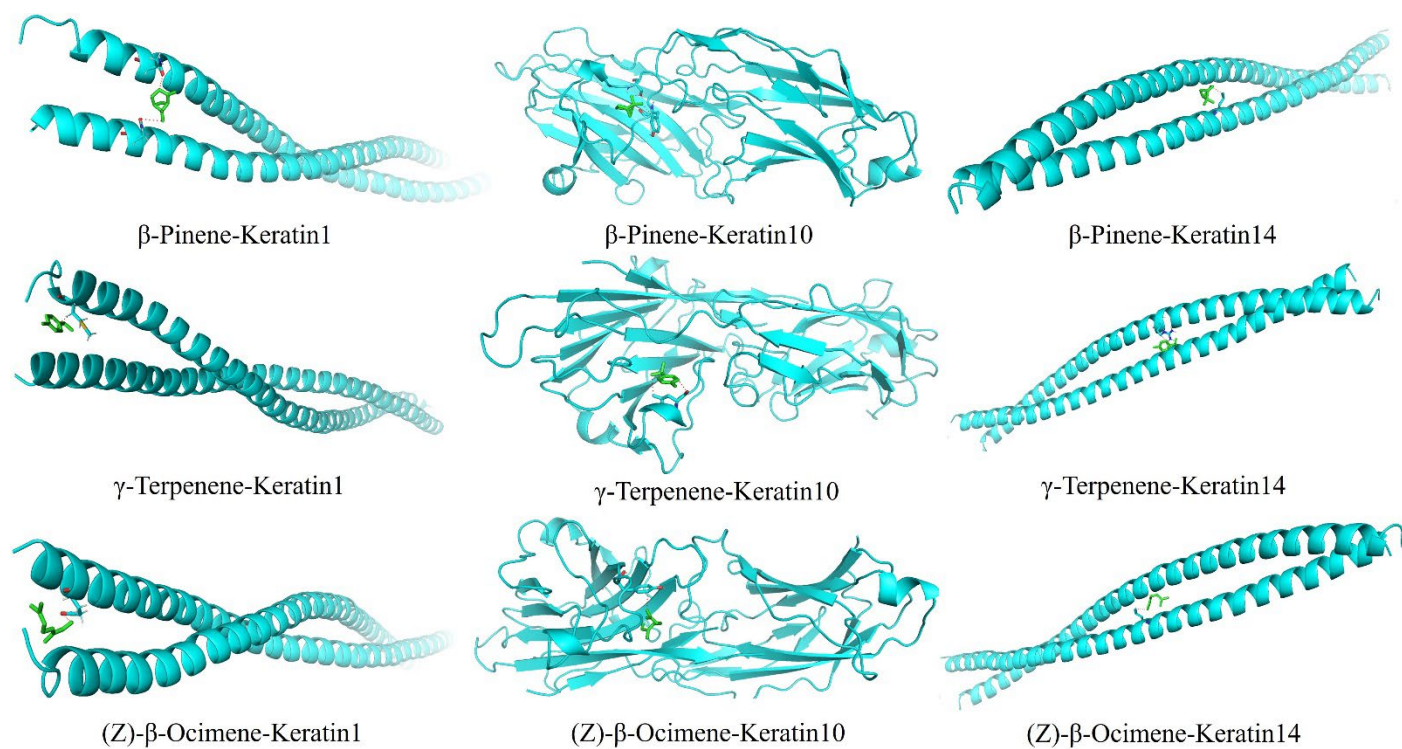


Figure S1b: Docking diagram of β -Pinene, γ -Terpinene and (Z)- β -Ocimene with keratins.

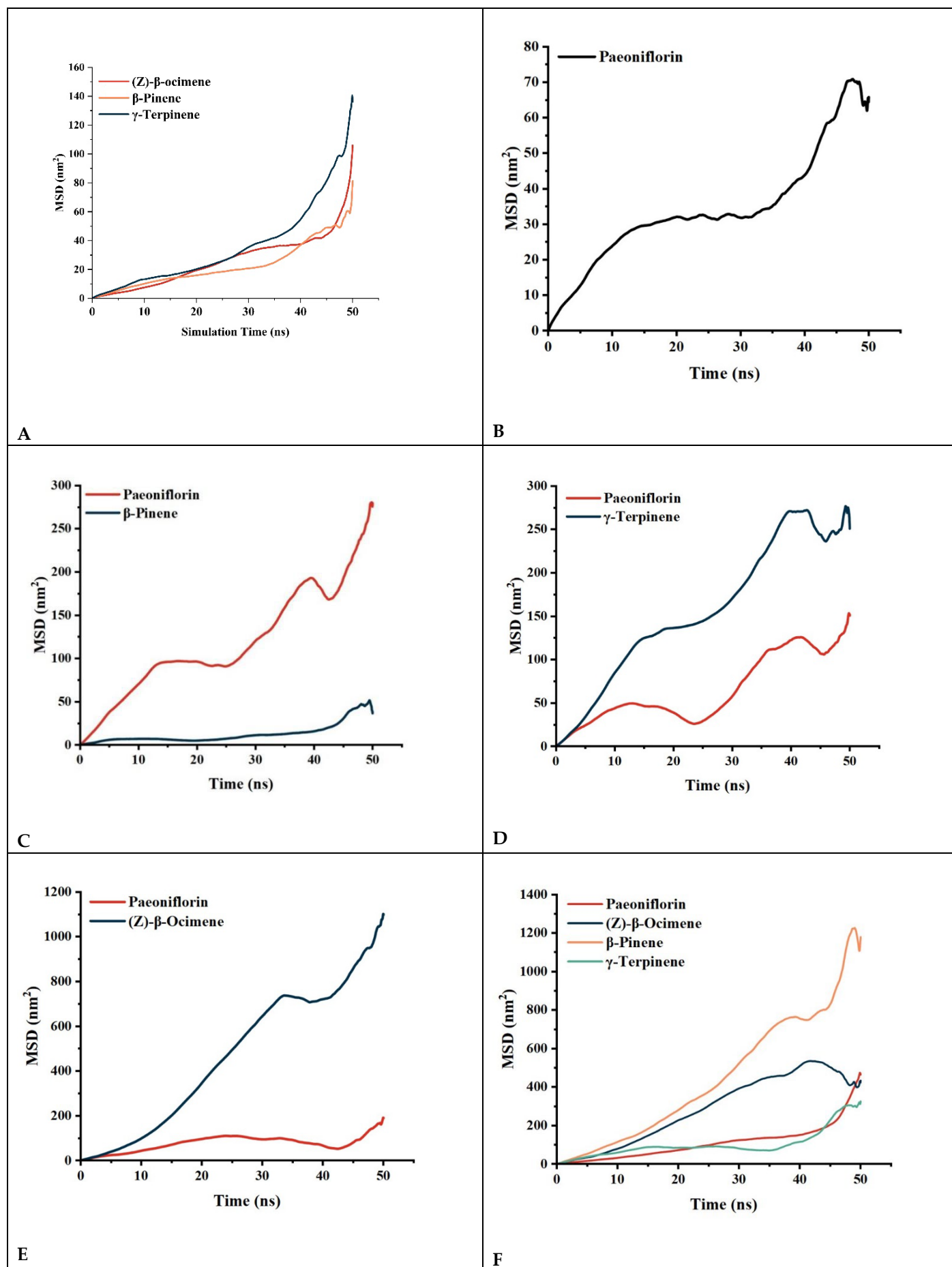


Figure S2: Mean square displacement (MSD) plots of terpenes from *Evodia rutaecarpa* volatile oil and paeoniflorin (PF)-terpene complexes in the lipid bilayer. (A) Individual motion trajectories of the terpene components (β -Pinene, γ -Terpinene and (Z)- β -Ocimene) in the lipid bilayer; (B) Paeoniflorin (PF) alone; (C) PF in combination with β -Pinene; (D) PF in combination with γ -Terpinene; (E) PF in combination with (Z)- β -Ocimene; (F) PF in combination with all three terpene components (β -Pinene, γ -Terpinene and (Z)- β -Ocimene). The MSD values are plotted as a function of simulation time. The slopes of the MSD curves correspond to the diffusion coefficients of the respective molecules or complexes.