Mechanisms of Herb-Drug Interactions Involving Cinnamon and Cytochrome P450 2A6: Focus on Time-dependent Inhibition by Cinnamaldehyde and 2-Methoxycinnamaldehyde

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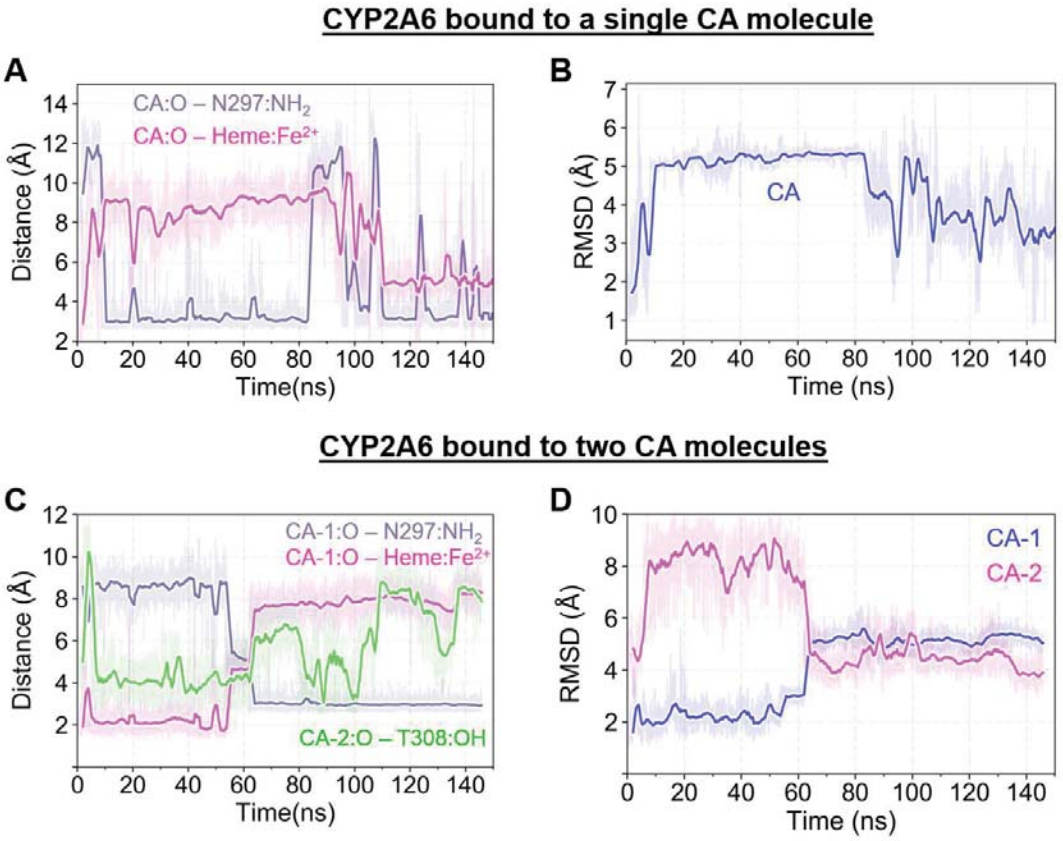

Supplemental Figure 2. Molecular interactions and stability of cinnamaldehyde (one and two copies) with the binding site of CYP2A6. A) The time evolution of critical interactions of one CA's carbonyl oxygen engaging in an H-bond interaction with the N297 side chain amino group as well as in close proximity to the heme iron. B) The RMSD changes in the single CA molecule within the binding site, indicating its dynamic nature. C) The presence of two CA molecules within the binding site stabilized the first docked structure in its position for a longer time period and allowed to engage in the expected interactions with N297. D) The RMSD plot indicates the stabilization effect of two CA molecules on each other after approximately 60 ns that led to stable interactions for the rest of the simulation time.