Supplementary Information

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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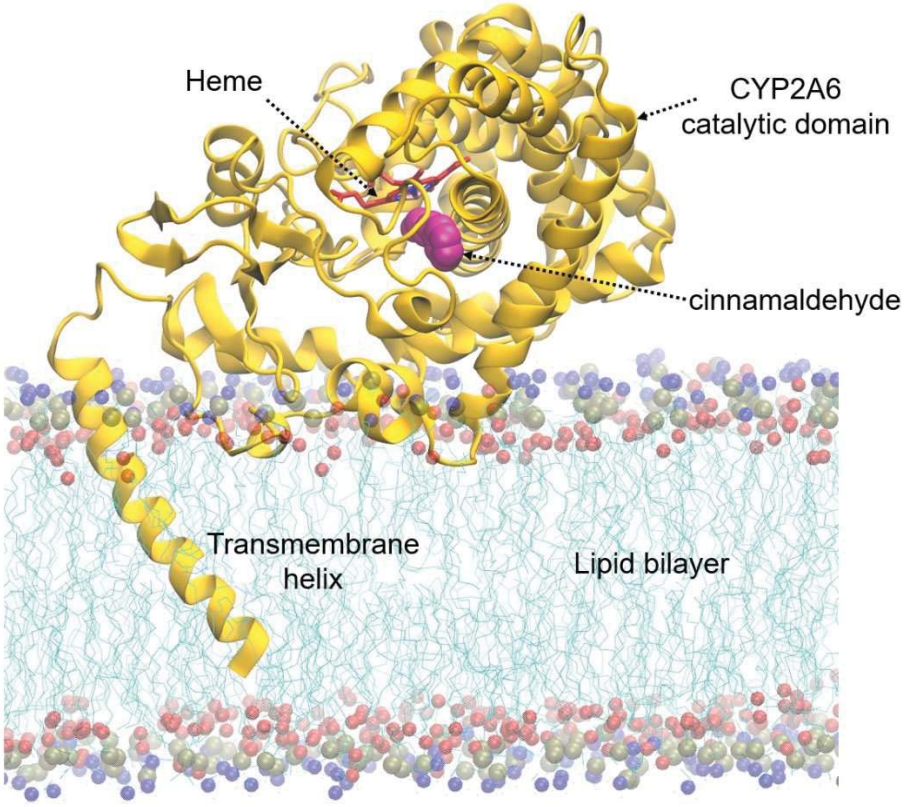
Drug Metabolism and Disposition-AR-2020-000087



Supplemental Figure 1. Simulated system of CYP2A6 bound to cinnamaldehyde in its native membrane environment. The catalytic domain of CYP2A6 is shown in its secondary structure representation (yellow) and is anchored by its transmembrane helix within the lipid bilayer made up of POPC lipids and cholesterol. The lipid headgroup choline nitrogen, phosphorus, and glyceryl oxygen atoms are shown in blue, olive, and red balls, respectively. The lipid alkyl tail is shown as cyan lines. The heme group within the catalytic binding site is shown as sticks (in red), and bound cinnamaldehyde is shown in van der Waals representation (in magenta). The lipid bilayer was padded with water molecules of 22.5 Å thickness on both sides (not shown here for clarity).