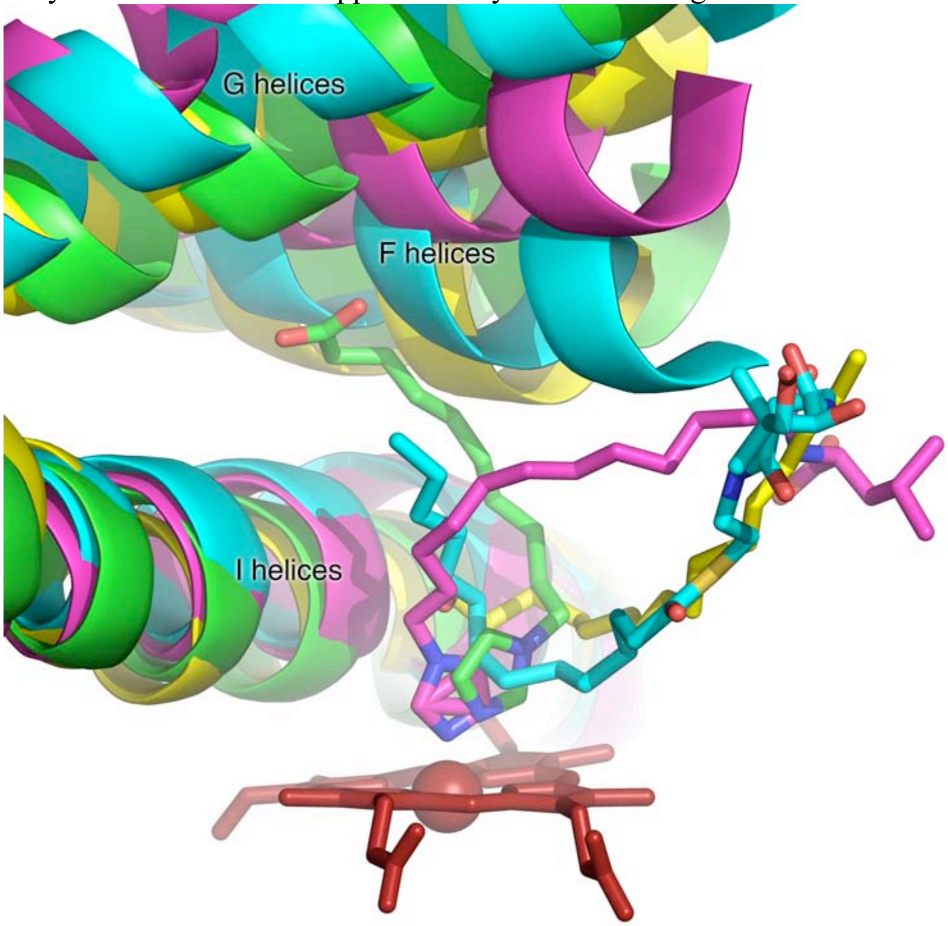
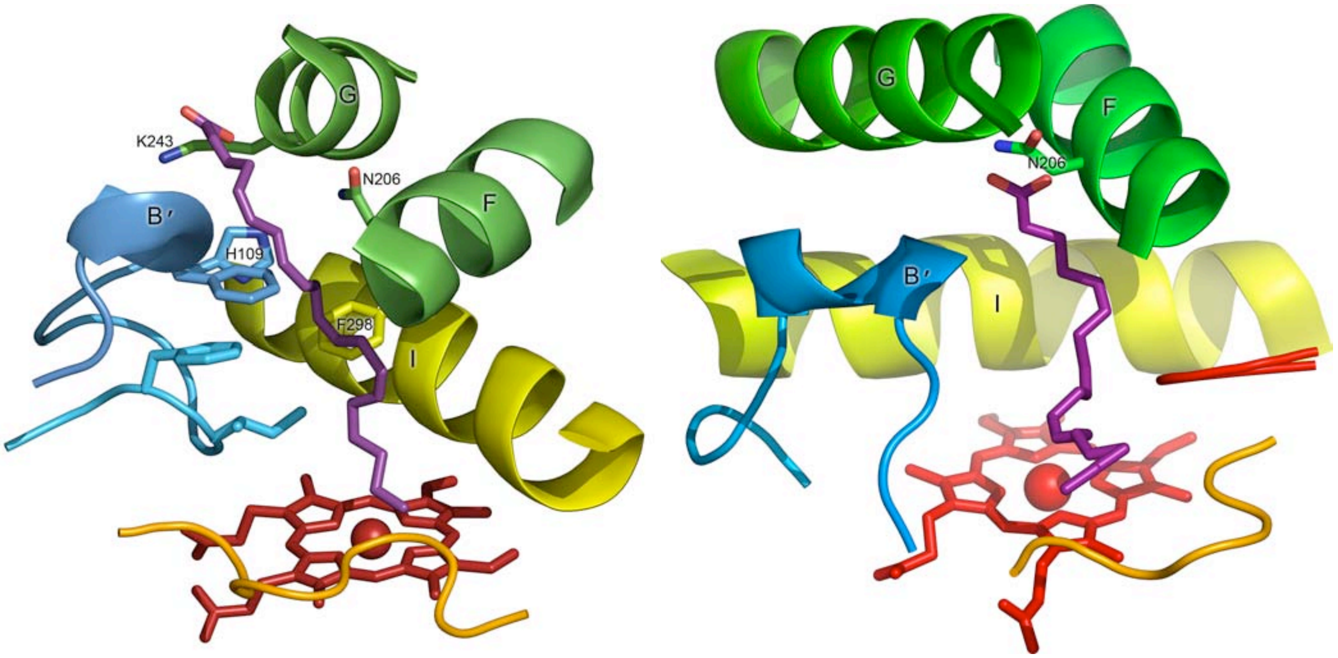
Supplemental Figures

Supplemental Figure 1. Comparison of fatty acid binding modes for CYP2E1 with ω-imidazolyl decanoic acid (green), BM3 with N-(12-imidazolyl-dodecanoyl)-L-leucine (magenta), BP450BioI with tetradecanoic acid (cyan) ligated to an acyl carrier protein (not shown), and BSbeta with palmitoleic acid (yellow). Structural alignment was accomplished using secondary structure matching of the entire enzymes. Orientation is approximately the same as figure 6.



Supplemental Figure 2. Arachidonic acid (purple sticks) docked into CYP2E1 in orientations generally consistent with A) oxidation at the terminal or subterminal positions to generate the experimentally observed 20-HETE or 19-HETE metabolites or B) oxidation at midchain unsaturated positions to generate EET metabolites.


A.

B.