Unexpected Differences Between Two Closely Related Bacterial P450 Camphor Monooxygenases

Vidhi C. Murarka, Dipanwita Batabyal[$], Jose A. Amaya, Irina F. Sevrioukova, Thomas L. Poulos*

Departments of Molecular Biology and Biochemistry, Pharmaceutical Sciences, and Chemistry, University of California, Irvine, California 92697-3900

*poulos@uci.edu

[$],Current address: Amgen Inc, Higher Order Structure, Attribute Sciences, Thousand Oaks, CA 91320

Figure S1 Sequence alignment of CYP101D1, P450tcu and P450cam. Sequence alignments were made the EMBL-EBI sequence analysis tools (http://europepmv/org/article/MED/3097693

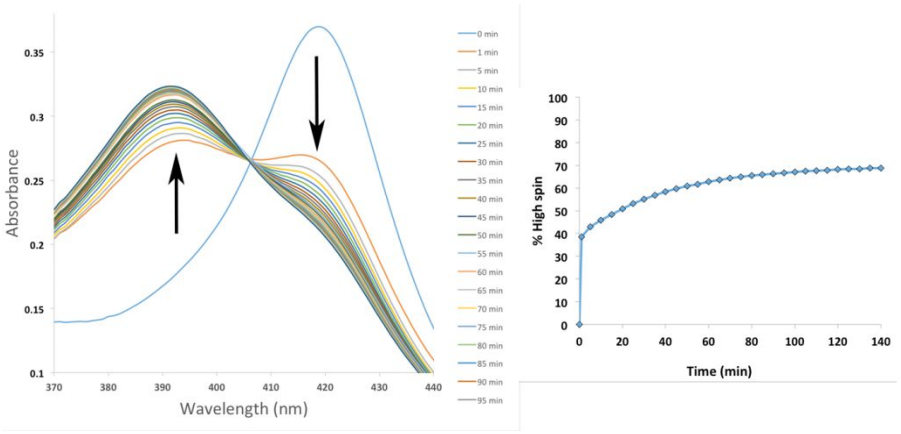

Figure S2 – Time dependent spectral changes after the addition of 1mM camphor. Since P450tcu does not undergo a full low- to high-spin transition, the expected spectral changes for 100% conversion were obtained from P450cam and used to estimate the per cent high-spin. P450tcu undergoes about 40% conversion within 1 minute followed by a slow conversion to about 70% high-spin with a half-life ≈25min.

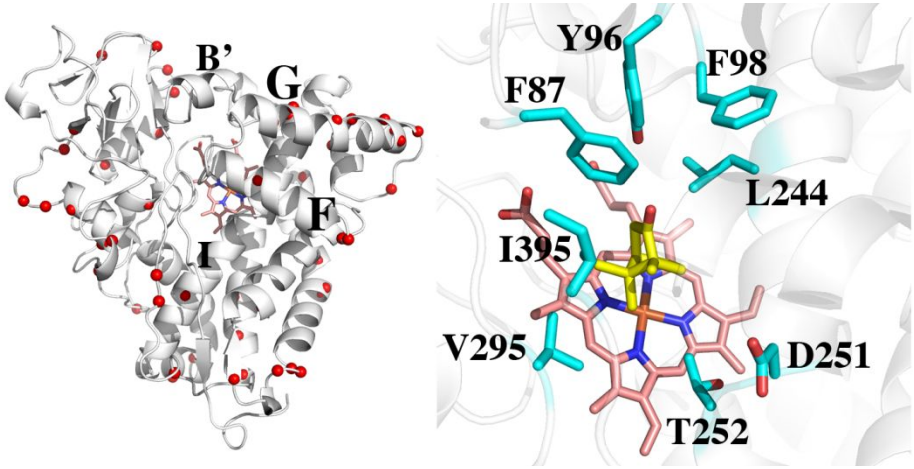

Figure S3 – Ribbon diagram of P450tcu with the location of sequence differences between P450tcu and P450cam highlighted as red spheres. A majority of the differences are located on or near the surface of the protein. The active site residues near the camphor are identical in both enzymes.

Table S1: Crystallographic Data Collection and Refinement Statistics

	P450tcu
PDB entry	6WPL
Space group	P 2_1 2_1 2_1
Resolution (Å)	2.1
Completeness (%)	95.64 (82.55)*
Number of unique reflections	22980 (1878)
R_{sym} *or* R_{merge}	0.0882 (0.6425)
R_{pim}	0.0882 (0.6425)
$I/\sigma(I)$	4.93 (2.42)
B factor (mean) (Å^2)	24.81
R_{work}	0.1934 (0.2424)
R_{free}	0.2468 (0.3128)
Root-mean-square deviation for bonds (Å)	0.008
Root-mean-square deviation for angles (deg)	1.07
Ramachandran favored (%)	96.53
Ramachandran allowed (%)	2.72
Ramachandran outliers (%)	0.74

Values in the () are for the highest resolution shell