

SUPPORTING INFORMATION FOR

Kinetics and Activation Parameters for Oxidations of Styrene by Compounds I from Cytochrome P450_{BM-3} (CYP102A1) Heme Domain and from CYP119

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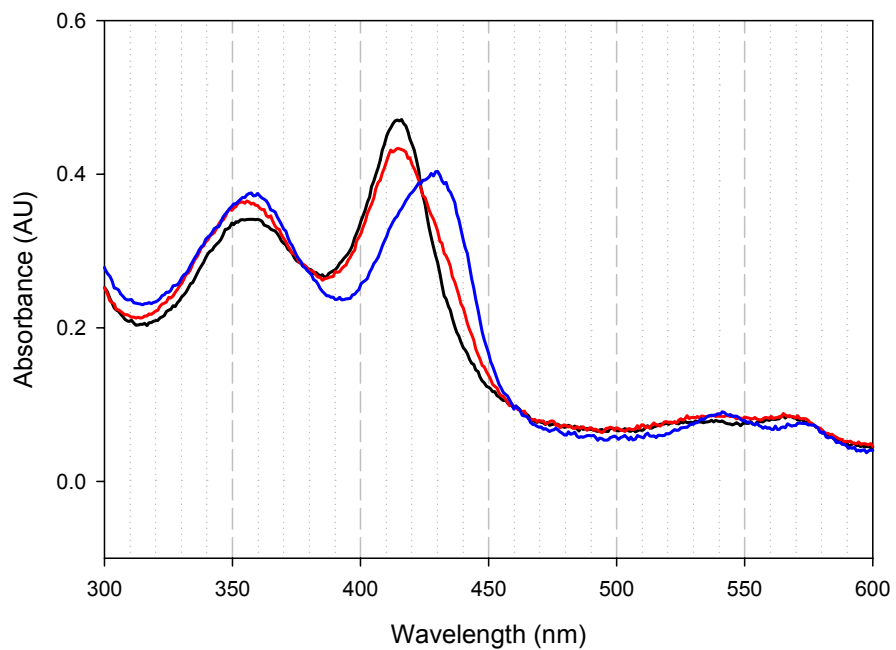


Figure S1. UV-visible spectra of CYP119 resting enzyme (black line), Compound II (blue line), and Compound I (red line).

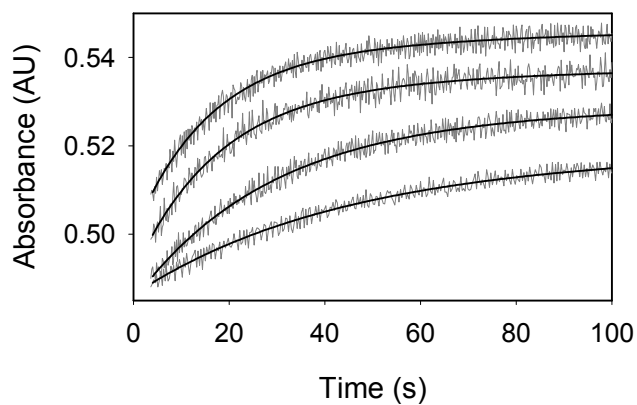


Figure S2. Representative kinetic traces monitored at 416 nm and fits for reactions of CYP119 Compound I with styrene at $-50\text{ }^{\circ}\text{C}$. The concentrations of styrene were, from the top, 6.5, 5.0, 2.0, and 1.0 mM.

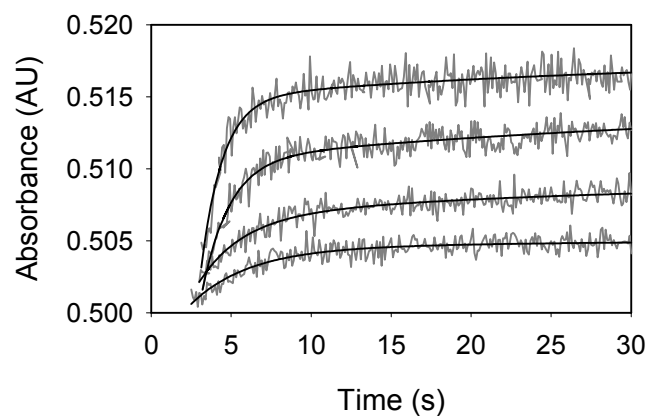


Figure S3. Representative kinetic traces monitored at 416 nm and fits for reactions of CYP102_{HD} Compound I with styrene at -20 °C. The concentrations of styrene were, from the top, 3.0, 2.0, 1.0, and 0.5 mM.

Table S1. Observed rate constants for reactions of styrene with CYP102_{HD} Compound I.

Temp (°C) ^b	[styrene] (mM)	k_{obs} (s ⁻¹) ^c
-35	0	<0.001
	1.0	0.10 ± 0.02
	2.0	0.14 ± 0.01
	4.0	0.16 ± 0.02
-30	0	0.0015 ± 0.0002
	0.5	0.13 ± 0.03
	1.0	0.18 ± 0.02
	2.0	0.25 ± 0.03
	4.0	0.30 ± 0.02
-20	0	0.0056 ± 0.0003
	0.5	0.28 ± 0.05
	1.0	0.36 ± 0.05
	2.0	0.59 ± 0.04
	3.0	0.74 ± 0.06
-10	0	0.025 ± 0.009
	0.25	0.21 ± 0.02
	0.5	0.43 ± 0.03
	1.0	0.73 ± 0.05

^aIn 1:1 solutions of glycerol and 100 mM potassium phosphate buffer (pH 7.4). ^b± 0.2 °C.

^cErrors are 1σ.

Table S2. Observed rate constants for reactions of styrene with CYP119 Compound I.

Temp (°C) ^b	[styrene] (mM)	k_{obs} (s ⁻¹) ^c
-50	0	0.0031 ± 0.0006
	1.0	0.024 ± 0.008
	2.0	0.035 ± 0.009
	3.0	0.046 ± 0.008
	5.0	0.058 ± 0.010
	6.0	0.063 ± 0.007
	6.5	0.064 ± 0.008
-35	0	0.023 ± 0.008
	1.0	0.142 ± 0.016
	2.0	0.24 ± 0.05
	3.0	0.30 ± 0.04
	4.0	0.37 ± 0.06
	6.0	0.44 ± 0.08
	6.5	0.47 ± 0.09
-25	0	0.077 ± 0.011
	1.0	0.312 ± 0.038
	2.0	0.517 ± 0.076
	3.0	0.680 ± 0.086

^aIn 1:1 solutions of glycerol and 100 mM potassium phosphate buffer (pH 7.4). ^b± 0.2 °C.

^cErrors are 1σ.

Table S3. Observed rate constants for reactions of benzyl alcohol- d_2 with CYP102_{HD}**Compound I.^a**

Temp (°C) ^b	[BA- d_2] (mM)	k_{obs} (s ⁻¹) ^c
-20	0	0.0056 ± 0.0003
	0.3	0.20 ± 0.02
	0.5	0.36 ± 0.05
	1.0	0.57 ± 0.05

^aThe substrate was C₆H₅CD₂OH (see ref 17 in text). Reactions were conducted in 1:1 solutions of glycerol and 100 mM potassium phosphate buffer (pH 7.4) as described in the Experimental Section of the text and in ref 17 of the text. ^b± 0.2 °C. ^cErrors are 1σ.
