

Table S1. Products formed from P450 oxidations of probe 1.^a

Isozyme	Exps. ^b	Yield of products in nmol			C/A ^c	M/P ^d	Conv. ^e	Rec ^f	Turnovers ^g
		Cyclic Alcohol	Acyclic Alcohol	Phenol					
2B1 ^h					4.0	2.0			
cam ⁱ					7.0	5.0			
2B4	4	75.5	11.6	15.3	6.5	5.7	15	57	171
Δ2B4	4	119.6	20.1	24.7	6.0	5.7	25	57	274
Δ2E1	4	36.1	3.9	9.0	9.3	4.4	7	50	82
Δ2B4 T302A	4	6.9	1.5	10.6	4.6	0.8	3	78	32
Δ2E1 T303A	4	23.6	2.8	49.1	8.4	0.5	11	75	126
Δ2E1 T303A ^j	4	23.6	2.8	21.0	8.4	1.3	8	75	79

^a0.66 μmol of substrate was used in all experiments. ^bNumber of experiments. ^cRatio of cyclic to acyclic alcohol. ^dRatio of methyl group oxidation products to phenyl group oxidation products.

^ePercent conversion of the probe. ^fPercent recovery of the probe. ^gNumber of enzyme turnovers.

^hData from ref 11. ⁱData from ref 12. ^jData considering only the phenol for which an authentic sample exists, the *para*-phenol.

Table S2. Products formed from P450 oxidations of probe 2.^a

Isozyme	Experiments	Yield of products in nmol		C/A ^b	Conv. ^c	Rec. ^d	Turnover ^e
		Cyclic Alcohol	Acyclic Alcohol				
2B1 ^f				4.0	13		280
2B4	4	12.9	2.1	6.1	3	58	25
2B4 ^g	2	10.1	1.5	6.7	1	69	20
Δ2B4	4	13.9	2.6	5.3	3	60	28
Δ2B4 ^g	2	9.0	1.5	6.0	1	64	18
Δ2E1	8	4.3	0.45	9.6	1	38	8
Δ2B4 T302A	4	8.2	3.4	2.4	3	49	22
Δ2B4 T302A ^f	3	4.9	1.8	2.7	1	56	11
Δ2E1 T303A	4	11.9	7.6	1.6	4	64	33

^a0.53 μmol of substrate was used in all experiments. ^bRatio of cyclic to acyclic alcohol. ^cPercent conversion of the probe. ^dPercent recovery of the probe. ^eNumber of enzyme turnovers. ^fData from ref 4. ^gCatalase and superoxide dismutase were omitted from the reaction mixture.

Table S3. Stability control reactions for oxidation products.

Enzyme	Substrate	Amount (nmol)	Experiment (percent recovery)		
			A ^a	B ^b	C ^c
Δ2B4					
	1A	67.5	78	70	79
	1C	67.5	84	97	93
	2A	29.3	89	104	124
	2C	23.1	106	92	93
Δ2B4 T302A					
	1A	67.5	81	78	81
	1C	67.5	85	89	109
	2A	29.3	91	117	109
	2C	23.1	107	114	96
Δ2E1					
	1A	67.5	67	79	99
	1C	67.5	89	101	107
	2A	29.3	84	102	101
	2C	23.1	89	93	112
Δ2E1 T303A					
	1A	67.5	78	93	87
	1C	67.5	83	91	96
	2A	29.3	88	97	115
	2C	23.1	108	98	118

^aThe enzyme system was fully competent. ^bThe P450 and reductase enzymes were omitted from the system. ^cThe NADPH was omitted from the system.

Table S4. Detailed results from P450 oxidations of probe 1.^a

Isozyme	Yield of products in nmol			C/A ^b	M/P ^c	Conv. ^d	Rec. ^e	Turnover ^f
	Cyclic Alcohol	Acyclic Alcohol	Phenol					
2B4	95.7	14.4	19.2	6.6	5.7	19	53	216
2B4	96.5	13.9	21.6	6.9	5.1	20	53	220
2B4	60.5	10.1	11.6	6.0	6.1	12	47	137
2B4	49.4	8.0	8.6	6.2	6.7	10	74	110
Δ2B4	113.2	17.3	24.7	6.5	5.3	23	53	259
Δ2B4	116.6	20.6	24.2	5.7	5.7	24	62	269
Δ2B4	124.0	22.3	23.8	5.6	6.1	26	61	284
Δ2B4	124.5	20.3	26.1	6.1	5.5	26	52	285
Δ2B4 T302A	7.3	1.5	10.5	4.9	0.8	3	75	32
Δ2B4 T302A	6.2	1.4	9.8	4.4	0.8	3	75	29
Δ2B4 T302A	5.6	1.4	10.4	4.0	0.7	3	77	29
Δ2B4 T302A	8.4	1.6	11.5	5.3	0.9	3	86	36
Δ2E1	46.7	4.7	11.9	9.9	4.3	10	64	106
Δ2E1	41.2	4.5	10.0	9.2	4.6	8	66	93
Δ2E1	28.9	3.3	7.2	8.8	4.5	6	46	66
Δ2E1	27.7	3.0	6.8	9.2	4.5	6	44	63
Δ2E1 T303A ^g	18.2	2.2	41.0 (16.3)	8.3	0.5 (1.3)	9 (6)	67	102 (61)
Δ2E1 T303A ^g	24.9	3.0	52.3 (22.4)	8.3	0.5 (1.2)	12 (6)	81	134 (84)
Δ2E1 T303A ^g	25.2	3.0	48.5 (21.9)	8.4	0.6 (1.3)	12 (8)	66	128 (84)
Δ2E1 T303A ^g	23.6	3.1	54.2 (23.2)	8.5	0.5 (1.2)	12 (6)	84	134 (88)

^a0.66 μmol of substrate was used in all experiments. ^bRatio of cyclic to acyclic alcohol. ^cRatio of methyl group oxidation products to phenyl group oxidation products. ^dPercent conversion of the probe. ^ePercent recovery of the probe. ^fNumber of enzyme turnovers. ^gNumbers in parentheses are data considering only the phenol for which an authentic sample exists, the *para*-phenol.

Table S5. Detailed results from P450 oxidations of probe 2.^a

Isozyme	Yield of products in nmol		C/A ^b	Conv. ^c	Rec. ^d	Turnover ^e
	Cyclic Alcohol	Acyclic Alcohol				
2B4	13.7	2.2	6.2	3	61	27
2B4	12.9	2.3	5.6	3	63	25
2B4	12.9	2.1	6.1	3	62	25
2B4	13.2	2.2	6.0	3	62	26
2B4 ^f	9.1	1.4	6.5	0.7	84	18
2B4 ^f	11.1	1.6	6.9	0.8	53	21
Δ2B4	14.8	2.7	5.5	3	57	29
Δ2B4	15.3	3.1	4.9	3	60	31
Δ2B4	14.5	2.9	5.0	3	55	29
Δ2B4	14.9	2.9	5.1	3	57	30
Δ2B4 ^f	10.0	1.7	5.9	0.8	59	20
Δ2B4 ^f	8.0	1.3	6.2	0.6	69	16
Δ2B4 T302A	8.5	3.5	2.4	3	48	20
Δ2B4 T302A	7.9	3.4	2.3	3	47	19
Δ2B4 T302A	8.1	3.2	2.5	3	46	19
Δ2B4 T302A	8.2	3.4	2.4	3	47	19
Δ2B4 T302A ^f	4.6	1.6	2.9	0.4	53	10
Δ2B4 T302A ^f	4.9	1.9	2.6	0.5	56	11
Δ2B4 T302A ^f	5.3	1.8	2.9	0.5	60	12
Δ2E1	2.1	0.26	8.1	0.5	23	4
Δ2E1	2.1	0.23	9.1	0.5	19	4
Δ2E1	2.2	0.26	8.5	0.5	21	4
Δ2E1	1.7	0.20	8.5	0.4	21	3
Δ2E1	6.1	0.69	8.8	1.0	55	11
Δ2E1	7.1	0.78	9.1	1.0	65	13
Δ2E1	7.5	0.66	11.4	1.0	54	14
Δ2E1	5.2	0.53	9.8	1.0	47	10
Δ2E1 T303A	12.1	7.7	1.6	4	64	33
Δ2E1 T303A	11.2	7.6	1.5	4	65	31
Δ2E1 T303A	12.7	8.0	1.6	5	60	35
Δ2E1 T303A	11.6	7.1	1.6	4	66	31

^a0.53 μmol of substrate was used in all experiments. ^bRatio of cyclic to acyclic alcohol. ^cPercent conversion of the probe. ^dPercent recovery of the probe. ^eNumber of enzyme turnovers. ^fCatalase and superoxide dismutase were omitted from the reaction mixture.