

Supplementary information

Figure 7 data:

Enzyme origin	Enzyme	Substrate	Type of catalysis	k _{cat} /K _m (M ⁻¹ s ⁻¹)
Natural	Superoxide dismutase	Superoxide	Oxidoreductase	7.0 x 10 ⁹ ¹
Natural	Crotonase	2-trans-enoyl-CoA	Hydratase	2.8 x 10 ⁸ ²
Natural	Triose phosphate isomerase	Dihydroxyacetone phosphate and D-glyceraldehyde 3-phosphate	Isomerase	2.4 x 10 ⁸ ³
Natural	Fumarase	Fumarate	Hydratase	1.6 x 10 ⁸ ⁴
Natural	Ach esterase	Acetylcholine	Hydrolase	1.6 x 10 ⁸ ⁵
Natural	Human carbonic anhydrase	CO ₂	Hydratase	1.5 x 10 ⁸ ⁶
Natural	β lactamase	Cefoxitin	Hydrolase	1.0 x 10 ⁸ ⁷
Natural	P450 BM3	Palmitate	Oxidoreductase	6.0 x 10 ⁷ ⁸
Natural	Catalase	H ₂ O ₂	Oxidoreductase	4.0 x 10 ⁷ ⁹
Natural	Fumarate reductase	Fumarate	Oxidoreductase	2.1 x 10 ⁷ ¹⁰
Natural	P450 BM3	Myristate	Oxidoreductase	8.2 x 10 ⁶ ⁸
Natural	Horseradish peroxidase	H ₂ O ₂	Oxidoreductase	5.1 x 10 ⁶ ¹¹
Natural	Manganese peroxidase	H ₂ O ₂	Oxidoreductase	4.3 x 10 ⁶ ¹²
Natural	Xanthine oxidase	Xanthine	Oxidoreductase	1.9 x 10 ⁶ ¹³
Natural	Urease	Urea	Hydrolase	4.8 x 10 ⁵ ¹⁴
Natural	Indoleamine 2,3-dioxygenase	L-tryptophan	Oxidoreductase	2.0 x 10 ⁵ ¹⁵
Natural	Nitric oxide synthase	L-arginine	Oxidoreductase	1.8 x 10 ⁵ ¹⁶
Natural	Tryptophan 2,3 dioxygenase	L-trptophan	Oxidoreductase	1.7 x 10 ⁵ ¹⁷
Natural	Nitrogenase	Acetylane	Oxidoreductase	3.0 x 10 ⁴ ¹⁸
De novo scaffold/activity	di-Fe(III)-DF3 (phenol oxidase)	3,5-ditert-butyl-catechol	Oxidoreductase	100 ¹⁹
De novo scaffold/activity	MID1-zinc (carboxyesterase and phosphoesterase)	4-nitrophenyl acetate	Oxidoreductase	630 ²⁰
De novo scaffold/activity	S-836 (peroxidase)	H ₂ O ₂	Oxidoreductase	39 ²¹
De novo scaffold/activity	TRIL9CL23H	PNP acetate	Hydrolase	23 ²²
Natural scaffold/de novo activity	Diels alderase (DA2010)	4-carboxybenzyl trans-1,3-butadiene-1-carbamate and N,N-dimethylacrylamide	Diels alderase	*4.7 ²³
Natural scaffold/de novo activity	Diels alderase (CE6)	4-carboxybenzyl trans-1,3-butadiene-1-carbamate and N,N-dimethylacrylamide	Diels alderase	*87 ²³
Natural scaffold/de novo activity	Organophosphate (PT3)	Diethyl 7-hydroxycoumarinyl phosphate	Hydrolase	4.0 ²⁴
Natural scaffold/de novo activity	Organophosphate (PT3.3)	Diethyl 7-hydroxycoumarinyl phosphate	Hydrolase	9.8 x 10 ³ ²⁴
Natural scaffold/de novo activity	Kemp eliminase (KE70)	5-nitrobenzisoxazole	Kemp elimination	130 ²⁵
Natural scaffold/de novo activity	Kemp eliminase (R6 4/8B)	5-nitrobenzisoxazole	Kemp elimination	5.7 x 10 ⁴ ²⁵
Natural scaffold/de novo activity	AlleyCat	Benzisoxazole	Kemp elimination	5.8 ²⁶

*units are M⁻¹M⁻¹s⁻¹

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