Supplementary Information

Acetate anion-triggered peroxygenation of non-native substrates by wild-type cytochrome P450s

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Figure S1. Carboxylate-Arg salt bridge of fungal unspecific peroxigenase (AaeUPO) from Agrocybe aegerita (PDB code: 2YOR, left, pink) and fungal Dye-decolorizing peroxidase (AauDyP) from Auricularia auricula-judae (PDB code: 4AUQ, right, orange). Cys-36, Arg-189 and Glu-196 of AaeUPO, Asp-168, His-304 and Arg-332 of AauDyP and Heme are represented as stick models. Solvent accessible surface is displayed by wireframe of PyMOL.

Figure S2. GC of the product mixture after oxidation of styrene by CYP152A1 WT (A), CYP152B1 WT (B), CYP152A1 G290F mutant (C) and CYP152B1 F288G mutant (D) in the presence of 1 M acetic acid. The retention time of styrene, products, and the internal standard were detected by authentic samples: styrene (3.6 min), (R)-styrene oxide (13.3 min, (R)-SO), (S)-styrene oxide (14.0 min, (S)-SO), phenylacetaldehyde (15.6 min, PAA), and 2-phenyl-2-propanol (33.4 min, IS).