Exploring the Structural Basis of Substrate Preferences in Baeyer-Villiger Monooxygenases
INSIGHT FROM STEROID MONOOXYGENASE

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SUPPLEMENTAL DATA

Exploring the structural basis of substrate preferences in Baeyer-Villiger monooxygenases: insight from steroid monooxygenase

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Running Title: Steroid monooxygenase from Rhodococcus rhodochrous
SUPPLEMENTARY FIGURES

Figure S1. Quality of the final electron density with reference to the crystal structure of STMO bound to NADP⁺ (Table 1). The density was calculated with weighted 2Fo-Fc coefficients and is contoured at 1.3 σ level. Carbons are in purple, nitrogens in blue, oxygens in red, sulfurs in yellow, and phosphorous in orange.
Figure S2. Superposition of STMO (blue ribbon) and CHMO (green ribbon; open conformation; PDB entry 3GWF) active sites. FAD and NADP⁺ of STMO are depicted with yellow and orange carbons, respectively. The Cα atoms of the STMO residues targeted by mutagenesis are shown as blue spheres (Table 3).