

Structure and mechanism of benzaldehyde dehydrogenase from
Pseudomonas putida ATCC 12633, a member of the class 3 aldehyde
dehydrogenase superfamily

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Supporting material

Table S1. Primers employed to generate *Pp*BADH variants^a

Variant	Sequence of forward primer
E215D	5'-CCTGTCGTTCTAG <u>A</u> tCTCGGTGGTAAGTGCCC-3'
E215Q	5'-CCTGTCGTTCTA <u>c</u> AACTCGGTGGTAAGTGCCC-3'
E215L	5'-CCTGTCGTTCTA <u>ctc</u> CTCGGTGGTAAGTGCCC-3'
E337D	5'-CCTCTGATGTCCGAG <u>G</u> A _t CTTTTCGGCCCTATTC-3'
E337Q	5'-CCTCTGATGTCCGAG <u>c</u> AGCTTTTCGGCC-3'
E337L	5'-CCTCTGATGTCCGAG <u>ctc</u> CTTTTCGGCC-3'

^aThe mutated codon is underlined, and lowercase indicates a base change from wild-type.

Figure S2. (A) Overlay of the cofactors of *Pp*BADH (NADP⁺, PDB 5UCD) and *h*ALDH3 (NAD⁺, PDB 4L2O) highlighting the movement of Glu146 to avoid the clash with the additional phosphate of NADP⁺. (B) Overlay of the cofactors of *Pp*BADH (PDB 5UCD) and *Pa*BALDH (PDB 2WME) showing the similarity of mechanism used to hold the glutamic acid away from the phosphate. In both cases *Pp*BADH is in grey.

