

Figure legends

Fig. S1. The sequence alignment of the dimeric AbIDH2 with its homologous IDHs from *Azoarcus tolulyticus* (AtIDH, GenBank Accession WP_076602605.1) and *Acidovorax ebreus* (AeIDH, GenBank Accession WP_015913126.1) and two typical monomeric NADP-IDHs from *Azotobacter vinelandii* (AvIDH, GenBank Accession No. BAA11169.1) and *Corynebacterium glutamicum* (CgIDH, GenBank Accession No. WP_011013800.1). The residue numbering in the figure is based on AbIDH2 sequence. The conserved residues are shaded by black. The residues that involved in NADP⁺ binding are marked by red pentagram ★.

Fig. S2. The sequence alignment of the dimeric AbIDH2 with its homologous IDHs from *Azoarcus tolulyticus* (AtIDH, GenBank Accession WP_076602605.1) and *Acidovorax ebreus* (AeIDH, GenBank Accession WP_015913126.1) and two typical monomeric NADP-IDHs from *Azotobacter vinelandii* (AvIDH, GenBank Accession No. BAA11169.1) and *Corynebacterium glutamicum* (CgIDH, GenBank Accession No. WP_011013800.1). The residue numbering in the figure is based on AbIDH2 sequence. The conserved residues are shaded by black. The residues that involved in substrate binding are marked by red triangle ▲.

Fig. S3. (A), Overall AbIDH2 monomer structure is resolved into domain I and domain II. There are 12 α -helices and 7 β -strands in domain I, and 18 α -helices and 20 β -strands in domain II. (B), Superimposition of apo-AtIDH2 (purple) and apo-CgIDH (green, 2b0t) secondary structures. (C), Superimposition of apo-AtIDH2 (purple) and AvIDH-isocitrate (yellow, 1jtw) secondary structures. (D), Superimposition of apo-AtIDH2 (purple) and AvIDH-NADP⁺ (cyan, 1j1w) secondary structures.