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Supporting information for article:

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of D-3-hydroxybutyrate dehydrogenase**

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Tamotsu Yamamoto, Gota Kawai, Jiro Kondo and Akio Takénaka**

Structural insights into the catalytic reaction trigger and inhibition of D-3-hydroxybutyrate dehydrogenase

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Supplementary Data

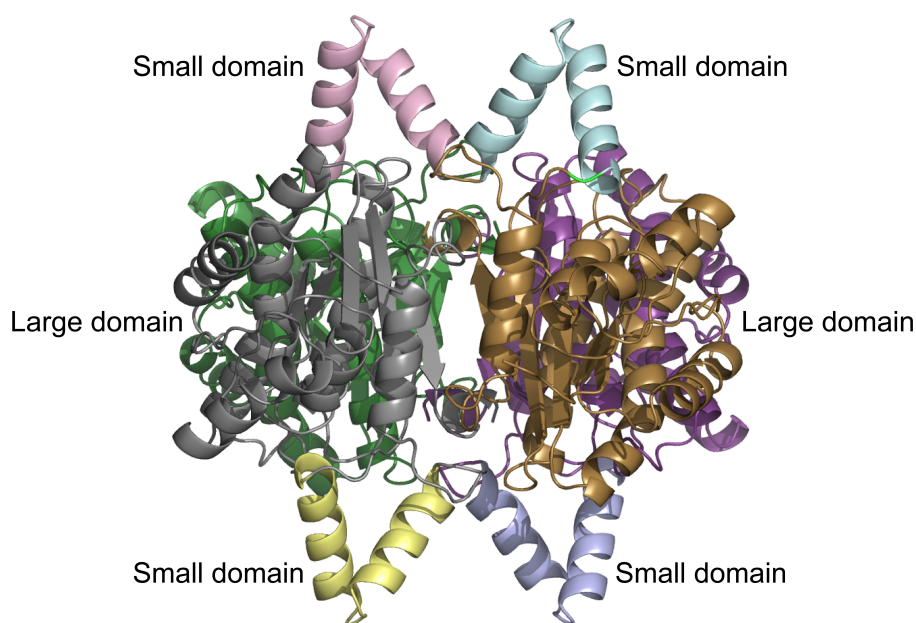


Fig. S1. A side view of HBDH tetramer. Two movable small domains are protruded on both sides (above and below) of the four large domains forming a tetramer.

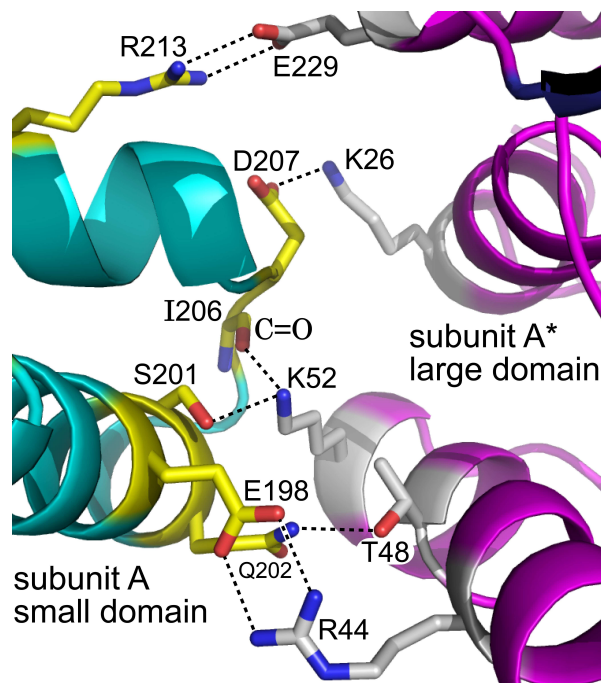


Fig. S2. Eight hydrogen bonds formed between the small domain of a tetramer and the large domain of another tetramer.

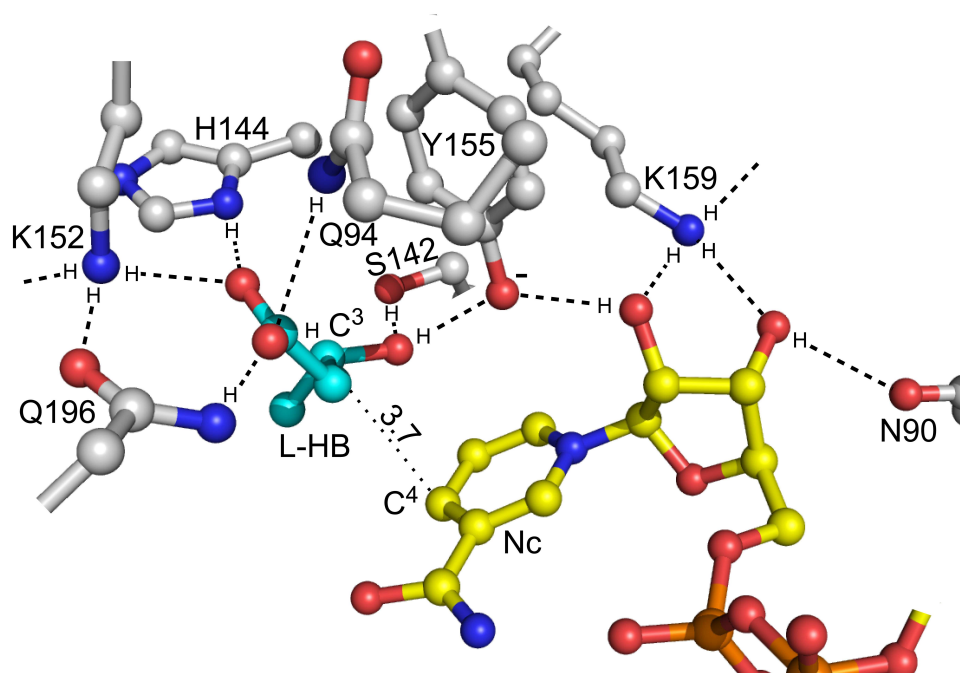


Fig. S3. Donor/acceptor relationship of hydrogen bonded network and postulated hydrogen atoms. L-form HB is bound in the active site of HBDH (PDB-ID 2ZTL). Due to the S configuration at C³, the C³ atom being separated at a distance of 3.7 Å from C⁴, and the attached H atom is located in the direction opposite of the target C⁴ atom of Nc.