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Crystal structure of dehydroquinate synthase from *Thermus thermophilus* HB8

Thermus thermophilus HB8 からの dehydroquinate synthase の結晶構造

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Dehydroquinate synthase (DHQS) is an NAD^+-dependent metalloenzyme catalysing five independent reactions in the shikimate pathway. The crystal structure of the dehydroquinate synthase from *Thermus thermophilus* (*Tt*DHQS) has been determined at 1.8 Å resolution (Fig. 1). It is the first structure of this enzyme from a thermophilic organism. A comparison of this structure with the reported crystal structure of *Aspergillus nidulans* enzyme[1] revealed their sharing similar homodimers of identically folded protomers with two domains. From a mapping of conserved residues onto a molecular surface model (Fig. 2), the conserved regions were located not only in the active site but also in the dimer interface, suggesting a biological importance of the dimeric state. Further comparison of molecular surface areas showed a negative correlation between accessible surface area of free subunit and the living temperature of source organism, indicating the contribution of the more compact molecular surface to the thermostability of *Tt*DHQS. On the other hand, the living temperature did not affect the dimer contact area. Taken together, the oligomeric state of this enzyme might be responsible for the catalytic function but it might not contribute to the thermostability.

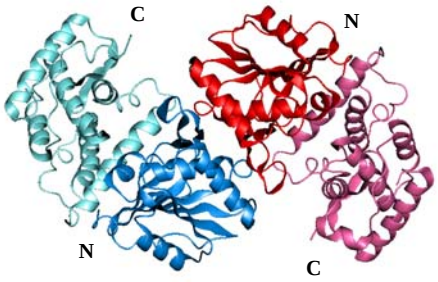

Fig. 1 Ribon diagram of the *Tt*DHQS dimer showing the chain A (N- and C-terminal domains: *blue* and *light blue*) and chain B (N- and C-terminal domains: *red* and *pink*).

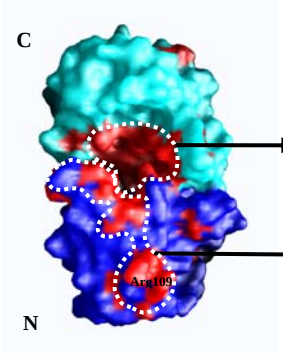

Fig. 2 Molecular surface of the *Tt*DHQS monomer. Red color denotes conserved residues. N- and C-terminal domains are colored blue and light blue, respectively. Active site region and dimer interface region are indicated by white dotted circles.

Reference

[1] Carpenter E., Hawkins A., Frost J., Brown K. *Nature*, 394, pp. 299–302 (1998)