

## **Binding Studies and Structure Determination of the Recombinantly Produced Type-II 3-Dehydroquinase Dehydratase from *Acinetobacter Baumannii***

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**Abstract :** Dehydroquinase (3-dehydroquinase dehydratase, DHQD, EC 4.2.1.10) is involved in shikimate pathway and catalyzes the conversion of dehydroquinase to dehydroshikimate. Shikimate pathway is important drug target as this pathway is absent in mammals. DHQD from *Acinetobacter baumannii* (AbDHQD) was cloned, expressed and purified to homogeneity. The binding studies showed that compounds quinic acid and citrazinic acid bound to AbDHQD at micromolar concentrations. AbDHQD was crystallized using 30% PEG-3350, 50mM tris-HCl, and 1.0M MgSO<sub>4</sub> at PH 8.0. Crystals of AbDHQD were stabilized by transferring them into reservoir solution to which 25% glycerol was added for data collection at 100K. The X-ray intensity data were collected to 2.0Å resolution. The crystals belong to monoclinic space group P21 with cell dimensions, a = 82.3, b = 95.3, c = 132.3Å and  $\beta = 95.7^\circ$ . The structure was solved with molecular replacement method and refined to Rcryst/Rfree factors of 0.200/0.232. The structures of 12 crystallographically independent molecules in the asymmetry unit were identical with r.m.s shifts for the C $\alpha$  atoms ranging from 0.3 Å to 0.8 Å. They formed a dodecamer with four trimers arranged in a tetrahedral manner. The classical lid adopted an open conformation although a sulfate ion was observed in the substrate binding site. As a result of which, the compounds quinic acid and citrazinic acid did not bind to AbDHQD.

**Keywords :** acinetobacter Bauman Nii, dehydroquinase dehydratase, dodecamer, open conformation

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