

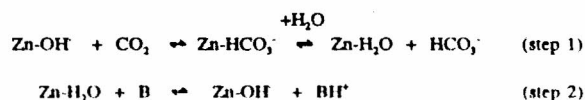
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MODELLING STUDY OF THE PARTIAL INHIBITION OF BOVINE
CARBONIC ANHYDRASE (BCA) II BY PYRIDOXAL PHOSPHATE (PLP)

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The molecular structure of BCA II was modelled by homology from the known structure of human carbonic anhydrase (Eriksson, Alwin Jones and Liljas, *PROTEINS: Structure Function and Genetics*, 4:274-282, 1989) using the facilities provided by the program WHAT IF (Vriend, *J Mol Graph* 8:52-55) that automatically performs the debump of eventual inter residue clashes and minimizes the molecular energy of the proposed model. To find a reasonable position for the PLP binding to BCAII three criteria were used: a) the experimental evidence for the binding at Lys 170 (Simoes, personal communication); b) analysis of the free space maps around the active site; c) analysis of the electrostatic potential maps of BCAII. The latter were calculated using the GRID program written by P.J. Goodford (MDL, West Way House, Elms Parade, Oxford OX2 9LL, England). A model for the inhibited enzyme was obtained from which it can be seen that PLL blocks the space around His 164, the residue believed to be responsible for the proton transfer needed to complete the enzymatic reaction:



B=buffer molecules (Poker and Sarkany, *Adv. Enzym.* 47:149-274, 1978) and in this way providing a reasonable mechanism for the partial inhibition experimentally observed.

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