

## STRUCTURE OF DIHYDROFOLATE REDUCTASE (DHFR) OF *BRUCELLA SUIIS*

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Dihydrofolate reductase (DHFR) is one of the three enzymes belonging to the folate cycle and works reducing dihydrofolate to tetrahydrofolate.

In this work we propose *Brucella Suis* DHFR (*Bs*DHFR) as a potential target for the design of selective chemotherapy of brucellosis, a known potential biological warfare agent. As no crystallography structure of this enzyme is available in PDB yet, we suggest one theoretical low resolution model for *Bs*DHFR, built by single alignment using, as template, the crystallographic structure of DHFR from *E. coli* (*Ec*DHFR). The model was submitted to further steps of intensive optimization, validation and dynamics simulations in water. Comparisons between its active site with that of crystallographic Human serine hydroxymethyltransferase (*Hs*DHFR) revealed key differences that could be useful for the design of new selective inhibitors of *Bs*DHFR.

Keywords: dihydrofolate reductase, homology modeling, *Brucella Suis*  
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