STRUCTURES OF SERINE HYDROXYMETHYLTRANSFERASE (SHMT) OF *YERSINIA PESTIS* AND *BACILLUS ANTHRACIS*

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Serine hydroxymethyltransferase (SHMT) is one of the three enzymes belonging to the folate cycle and converts serine in glycine by transferring a methylene group to tetrahydrofolate. Differently from the other enzymes of this cycle, (Dihydrofolate reductase and Thymidilate synthase) SHMT is little studied and has not been seen in literature as a target to chemoteraphy. In this work we propose *Yersinia pestis* and *Bacillus anthracis* SHMT (*Yp*SHMT and *Ba*SHMT) as potential targets for the design of selective plague and antraz chemotherapies. As no crystallographic structures of these enzymes are available in PDB, we suggest two theoretical low resolution models for each enzyme, one built by multiple alignment using, as templates, the crystallographic structures of SHMTs from *Escherichia coli* (*Ec*SHMT) and *Bacillus stearothermofillos* (*Bs*SHMT), and the other one built by single alignment using, as template, only *Ec*SHMT. All models were submitted to further steps of intensive optimization, validation and dynamics simulations in water. Superposition between the models of each enzyme showed that they are equivalent and further comparisons between their active sites with that of crystallographic Human serine hydroxymethyltransferase (*Hs*SHMT) revealed key differences that could be useful for the design of new selective inhibitors of *Yp*SHMT and *Ba*SHMT.

Keywords: serine hydroxymethyltransferase, homology modeling, *Yersinia pestis, Bacillus anthracis.*

Supported by: FRF/IME, CAPES/PRODEFESA, CNPq, FAPERJ.