

# 2<sup>nd</sup> International Congress on Bacteriology & Infectious Diseases

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## How structural biology can help to understand antibiotic mechanism and resistance and contribute to discovery new anti-tuberculosis drugs

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Structural biology is one of the techniques that can be used to predict the interaction between proteins, such as enzymes and substrates. We also can use crystallography to design new inhibitors based in structure. One of the approaches which researches groups and pharmaceutical companies have been used the crystallography and its association with other biophysical techniques to design new drugs call fragment based drug discovery (FBDD). We have used this approach to identify new series of compounds that inhibits the enzyme dihydrofolate reductase (DHFR) from *M. tuberculosis*. We also have used crystallography to understand the reason why antifolate drugs; such as trimethoprim, which is a classical dihydrofolate reductase, does not have activity against *Mycobacterium tuberculosis*. We have identified residues of active site of DHFR which may decrease the affinity to trimethoprim and other antifolate drugs. We also describe a completely new structural movement of domains of DHFR which disturbs the interaction between DHFR and inhibitors. Based on this founds, we are applying the technique FBDD to identify compounds that might be leads in the development of new series of antibiotics against *M. tuberculosis*. Initially we have identified leads by biophysical methods and the crystallographic structures predicting its interactions were determined. In this talk we will show data about all our research on the enzyme DHFR from *M. tuberculosis*, including mechanism of low affinity effect of antifolate drugs until the start point of design of new inhibitors.

### Biography

Marcio Vinicius Bertacine Dias has completed his PhD at the age of 28 years from University of State of São Paulo- Brazil; and postdoctoral studies from University of Cambridge-UK, Department of Biochemistry. He is a Young Research Fellow at Laboratório Nacional de Biociências, CNPEM, a Brazil Federal Institute of Research. He has published about 20 papers in reputed journals.

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