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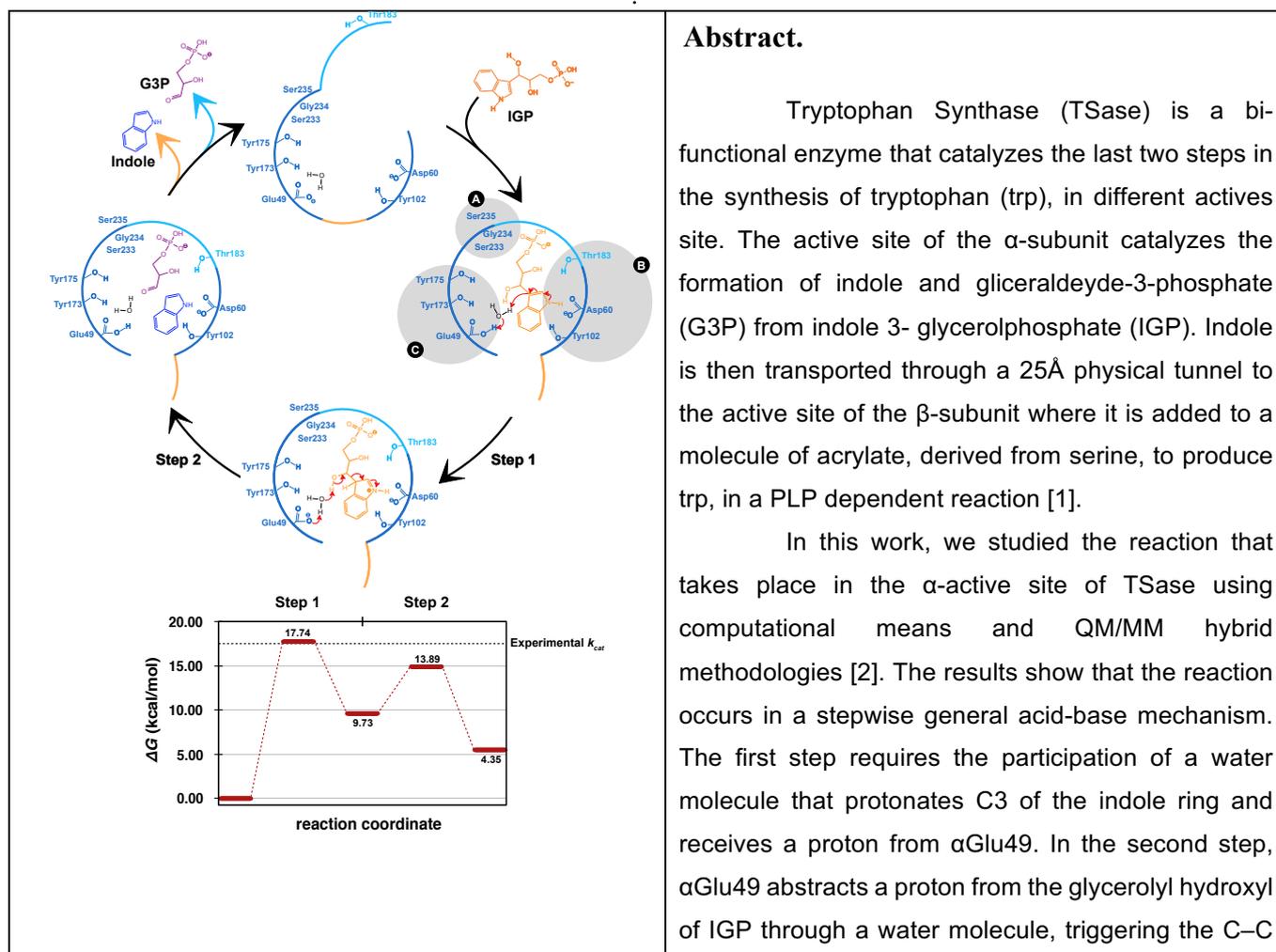
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## Computational studies addressed to the catalytic mechanism of the alpha sub-unit of Tryptophan Synthase

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bond cleavage to give indole and G3P. The rate-limiting step of this reaction is the first one that requires an activation free energy of 17.74 kcal/mol. This result agrees extremely well with the available experimental data that predicts reaction rate of 3.0-3.7 s<sup>-1</sup>, which corresponds to a free energy barrier of 17.37-17.50 kcal/mol.

The results obtained in this work provide important details about TSase that can now be used for the development of new transition state analogues inhibitors targeting TSase – an important drug target used in the treatment and prophylaxis of tuberculosis that is caused by the *Mycobacterium tuberculosis* pathogen.

## References

- [1] N. M. F. S. A. Cerqueira, P. A. Fernandes, M. J. Ramos, *J. Chem. Theory Comput.*, **2011**, 7, 1356-1368.  
[2] E. F. Oliveira, *et al.*, *J. Am. Chem. Soc.*, **2011**, 133, 15496-15505.