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# Monoamine oxidase B: Unveiling the catalytic mechanism through quantum chemical cluster approach

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The oxidative deamination mechanism of monoamine oxidase B is studied by means of density functional theory calculations. This enzyme catalyzes the oxidative deamination of neurotransmitters to yield a half-reduced flavine and a protonated imine byproduct. The quantum chemical cluster approach is employed to characterize transition states of two good substrates such as phenethylamine, benzylamine, and its para-nitro substituted counterpart which is a poor substrate for which experimental catalytic kinetic constants are available. Our results strongly suggest that this isoform can act using both mechanisms, contrary with what has been speculated for this enzyme. Also, the observed experimental kcat values reflect the preference that this isoform has for one mechanism over the other (polar nucleophilic vs. hydride transfer). According to our results, the better stabilized transition state, regarding their reactant complexes, determine the most probable mechanism for this isoform.

## Biography

Cristian Celis-Barros has completed his BSc major in chemistry at the age of 25 years from University of Chile and he is currently finishing his Master degree in chemistry from the Faculty of Chemical and Pharmaceutical Sciences at the same university. At present, he has been accepted to complete his PhD studies in Molecular Physical Chemistry. He has published 5 papers related with modeling of systems with molecules endowed of biological interest.

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