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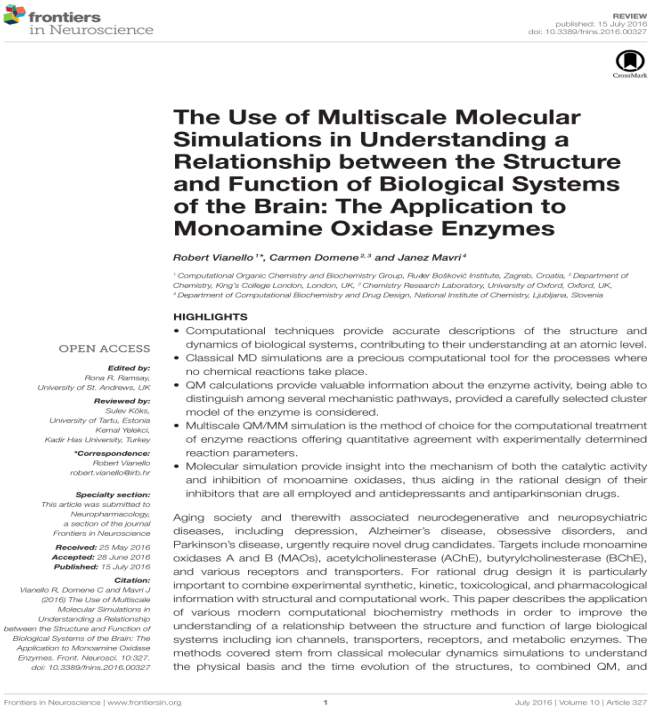

frontiers in Neuroscience

REVIEW
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The Use of Multiscale Molecular Simulations in Understanding a Relationship between the Structure and Function of Biological Systems of the Brain: The Application to Monoamine Oxidase Enzymes

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HIGHLIGHTS

- Computational techniques provide accurate descriptions of the structure and dynamics of biological systems, contributing to their understanding at an atomic level.
- Classical MD simulations are a precious computational tool for the processes where no chemical reactions take place.
- QM calculations provide valuable information about the enzyme activity, being able to distinguish among several mechanistic pathways, provided a carefully selected cluster model of the enzyme is considered.
- Multiscale QM/MM simulation is the method of choice for the computational treatment of enzyme reactions offering quantitative agreement with experimentally determined reaction parameters.
- Molecular simulation provide insight into the mechanism of both the catalytic activity and inhibition of monoamine oxidases, thus aiding in the rational design of their inhibitors that are all employed and antidepressants and antiparkinsonian drugs.

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Aging society and therewith associated neurodegenerative and neuropsychiatric diseases, including depression, Alzheimer's disease, obsessive disorders, and Parkinson's disease, urgently require novel drug candidates. Targets include monoamine oxidases A and B (MAOs), acetylcholinesterase (AChE), butyrylcholinesterase (BChE), and various receptors and transporters. For rational drug design it is particularly important to combine experimental synthetic, kinetic, toxicological, and pharmacological information with structural and computational work. This paper describes the application of various modern computational biochemistry methods in order to improve the understanding of a relationship between the structure and function of large biological systems including ion channels, transporters, receptors, and metabolic enzymes. The methods covered stem from classical molecular dynamics simulations to understand the physical basis and the time evolution of the structures, to combined QM, and

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