

Study lays foundations for future medicine design

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A study by the Computational Biochemistry Research Group of the Universitat Jaume I (UJI) of Castellón, Spain, shows that enzyme activity depends on electrostatic properties, as opposed to mechanical ones. The

scientists believe this result opens up new possibilities for the use of the enzymes in fields such as biomedicine for designing new medicines, or in biotechnology for producing environmentally friendly artificial enzymes for industrial processes. Results of this research have been published in the *Journal of the American Chemical Society*.

Data obtained with computational simulations by the research group headed by Physical Chemistry Professor Vicent Moliner coincide with experimental data obtained in other research groups in the United States, but have a different interpretation. "The study has allowed us to describe, on a molecular level, the activity of the important enzyme glycine N-methyltransferase, which is linked to degenerative processes such as dementia or Alzheimer's disease. The enzyme creates a localised electrical field which accelerates the chemical reactions that take place within living beings," explains Moliner.

"Understanding the basic principles of how enzymes work allows us to not only comprehend how living organisms function, but also to understand in depth the mechanism by which many diseases deteriorate or destroy them," says UJI group researcher Katarzyna Świderek.

More information: Katarzyna Świderek et al. Insights on the Origin of Catalysis on Glycine N-Methyltransferase from Computational Modeling, *Journal of the American Chemical Society* (2018). [DOI: 10.1021/jacs.7b13655](https://doi.org/10.1021/jacs.7b13655)

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