

# Elucidating Novel Pathways for Prebiotic Glycine Synthesis: Merging Enhanced Sampling and Neural Network Atomic Potentials.

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Glycine has a central role in prebiotic chemistry inquiry as the simplest amino acid. While documented in meteorites<sup>1</sup>, glycine's presence in the interstellar medium poses a persistent enigma. Nevertheless, the presence of alternative amino acids in meteoritic samples, inexplicable within the confines of the generally admitted Strecker mechanism<sup>2</sup>, presents a compelling challenge<sup>3</sup>.

We engage computational modeling, rooted in quantum mechanics, to navigate the complex chemical landscape of this synthesis. We employed *ab initio* Molecular Dynamics (AIMD) calculations with enhanced sampling techniques alongside neural network potentials, enhancing simulation scalability and affordability beyond conventional bounds<sup>4</sup>.

This refined methodological framework<sup>5</sup>, called MLMD, allows us to identify and explore of an uncharted 'oxyglycolate path' for glycine synthesis. Building upon precedent investigations, our inquiry converges on two pivotal contributions: the unveiling of an unprecedented glycine synthesis route and the assertion of our new method as a potent instrument in probing chemical synthesis.

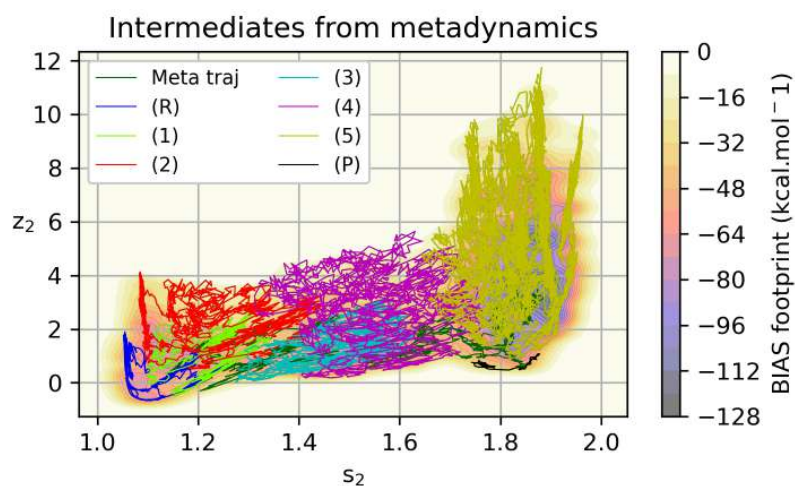


Figure 1. 2D graphics of the metadynamics trajectory that breaks toward glycine. The trajectory is colored with the initial set of intermediates out of the molecules observed during exploration of the chemical space.

**Keywords:** *ab initio* molecular dynamic; prebiotic chemistry; enhanced sampling; machine learning

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