Conformational analysis of cinnamic compound NGI27 using a combination of 2D NMR Spectroscopy and Molecular Dynamics studies

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NGI 27 is a novel cinnamic compound synthesized by our laboratory that could serve as a potential lead for various targets. Its conformational properties have been extensively studied using a combination of 2D NOESY experiments and molecular dynamics simulations. The conformation that explains both theoretical and experimental results is considered the most suitable for being used as the initial conformation in molecular docking studies in order to apply *in silico* rational drug design. The most important feature of this molecule as it is derived from the experimental results is its conformational flexibility and the absence of NOEs between the two aromatic rings. MD calculations have indicated that in the most possible conformation an orthogonality exists between the two aromatic rings that prohibits the spatial proximity between their aromatic protons. This conformation will serve as the starting point for the molecular docking experiments on different potential enzyme-targets, carrying hydrophobic cavities.

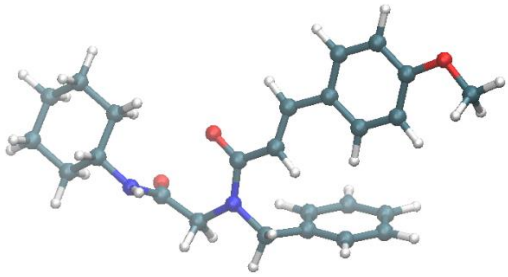

Figure 1: Conformation of NGI27 derived from molecular dynamics simulations.

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