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Study on the Molecular Dynamics of Pain Relief Molecules NAYOON KIM, RICHARD KYUNG, CRG-NJ — In this project, the thermodynamic and stereochemical properties of several types of biochemical derivatives that can be used as a fever reducing agent were studied. We used the molecular editing software to model, optimize, and compare the resulting molecular optimization energies and activities of the molecules. This study used an open-source molecular editing program equipped with an auto-optimization feature, which determines the theoretical values of a certain structures atomic and chemical properties of the pharmaceutical products through the Density Functional Theory (DFT). This software allows users to build virtually any molecule and optimize its geometry according to various force field options. Optimization configuration energy was collected in order to compare each chemical compound's stability. It is observed that the less thermodynamic enthalpy needed to stabilize the compound, the more stable the compound is. Calculations show some compounds converge easily, which makes them suitable to use as biochemical compounds in fever reducing agents.

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