

Abstract Submitted
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Thermodynamical and Biochemical Analysis of Antipyretics Used for Fever Reducing Agents SEOJIN PARK, RICHARD KYUNG, Choice Research Group — Antipyretics are substances used in fever reducing agents. In this paper, thermodynamical and stereochemical aspects of several types of antipyretics that can be used as a fever reducing agent are studied. This research uses computational chemistry to calculate the thermodynamic stability of various fever reducing agents in order to identify whether the ingredients are of safe use for pharmaceutical products. The research uses the chemical software to find the optimized molecular geometry and calculate theoretical enthalpy of each compound models. The computer program uses DFT(Density Functional Theory) and UFF(Universal Force Field), which are used to optimize each model. The optimization configuration energy of all the molecules is collected in order to examine the relative stability of each chemical compound. It is known that the less thermodynamic enthalpy needed to stabilize the compound, the more stable the compound is. Calculations show that enthalpies of some compounds converge fast with significantly less thermodynamic enthalpy, indicating that they are relatively stable and are suitable to use as a biochemical compound in fever reducing agents.

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