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Biophysical and Pharmacological Effects of Theobromine Using Computational and Thermodynamic Analysis SUNGJUN BAE, SEONG HO SHIN, JINWOOK JOSEPH SHIN, CRG-NJ (Choice Research Group) — Biophysical and pharmacological effects of theobromine in our bodies have not been studied in detail since it is biologically inert. Theobromine is an isomer of theophylline, which is a bitter alkaloid of the cacao plant, found in a number of foods including chocolate, leaves of the tea plant and nut. Theobromine is a heart stimulant and vasodilator, and it facilitates diuretic activity, instigating the body to naturally produce fat-burning hormones. Pharmaco-toxicological and clinical studies with Theobromine show that digestion of a substantial amount of the drug induces gene mutations in lower eukaryotes such as human as well as bacteria. In this paper, biophysical and pharmacokinetic modeling on the Theobromine and its derivatives is performed by computational and theoretical methods. This research utilizes computational programs and optimization theory that are capable of determining the physical and chemical properties of the molecules as well as the efficiencies of the fat burning abilities. Theoretical structure of each feasible molecules can be assessed to predict the efficiency of the molecule through analysis of the physical stability and thermodynamic activity.

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