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In silico research of herbal genomics through computational thermo-fluid dynamics for drug delivery system

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Evaluation of Molecular Dynamics (MD) can be investigated through the application of computational Structure-Based Drug Design (SBDD) for rapid genetic analysis of herbal medicines, such as agricultural functions, plant fingerprint and therapeutic effect. Analysis of SBDD is based from Arrhenius equation and developed by differential form of enthalpy and system volume. Development of kinetic reactions is necessary to investigate several processes performed in drug delivery system starting from general extraction, isolation of bioactive compounds and mass flux of herbal medicines resulting to catalytic reactions. This paper aimed to explore various determinants involved in free energy calculation and compare it with experimental results in order to observe various differences in drug delivery system, namely, controlled release, immediate release and sustained release herbal drug formulation. Factors such as pressure, using Kozeny-Carman and Burke-Plummer equation and temperature, based from Eyring-Polanyi equation can influence several attributes of drug delivery system. Hence, principles of mass transfer, fluid dynamics and thermodynamics can play key functions for better assessment of herbal medicines.

Biography

Zharama M Llarena has completed his BS Pharmacy degree at the University of Santo Tomas and has completed his MS Pharmacy major in Pharmaceutical Chemistry at the University of the Philippines Manila. He is currently pursuing his PhD from De La Salle University in Chemical Engineering. He has worked both in the pharmaceutical industry and academe as an Assistant Professor and Program Chair of the Pharmacy Department in colleges and universities in the Philippines.

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