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**Experimental Design and Molecular Dynamics in Herbal Plant Processing: A Review**

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**EXTENDED ABSTRACT**

Herbal plant currently has become significant and widely known due to its extensive sources of therapeutic phytochemicals agents. The practice of herbal plant as remedy has been adapted since thousands of years by ancient civilization such China, Mesopotamia, Egypt and India [1]. Unlike the modern drugs, treatment with herbal plant possess a range of therapeutic value and considered as safe since there is no or minimal side effect [2]. Previous study had proven that herbal plant able to treat ailment such as fever, antihypersensitive, diabetes, diarrhoea and even cancer [3]. Based on present-day scenario, the used of herbal plant as a therapeutic agent had increased mainly due to growing recognition and claim that herbal based product are safe, effective, non-toxic and minimal side effect as these remedies are in sync with nature. On the other side, the implementation of herbal plant in treating ailment seems to be a promising alternative for entire community as it is easily available, affordable and also cultural acceptability. Recently, World Health Organisation (WHO) estimated that more that 80% of the world population rely on herbal medicine for some part of their healthcare [2]. As for that, emerging for continous research and development for herbal plant is crucial as the demand increases throughout the year. In plant processing research, numerous experimental design has been practiced and implemented. There are various well known methods available in designing the experiment. Experimental designs are one of being frequently used for the optimization of different operating condition of various process and for improving the extraction performance, as well as achieving high extraction efficiency [4]. Application of experimental design is the most effective way to identify and optimize the significant factors and to achive a competent result by few experimental design trial. Hence, the experimental design can be design as an approach to solve the problem systematically and it is applied to collect data and to analyze data to obtain information rich results. Optimum and valid results with less number of experiments, time and resources are the primary objectives of applying the experimental design in herbal processing. In designing experiment using experimental design, investigators deliberately maneuver one or several predetermined factors to know their impact on experiment outcome. The computer simulation is a new evolving experimental tool that attracts scientist attention due to its ability to produce information at molecular level such as structure, dynamics, and thermodynamics of materials or biological systems. Moreover, computer simulation can also provide average prediction results for a new theory or process [5]. Recently, computer simulation, namely molecular dynamics simulation has been employed in various studies such as extraction, crystallization and membrane development [5-7]. This approach is ideally suitable to examine the intra and intermolecular interaction with different materials based on radial distribution function (RDF) analysis. Figure 1 illustrated the simulation of herbal plant processing. Hence, this article aim to review the up-to-date summary of the experimental design and molecular dynamics study implemented and available for various herbal plants processing.

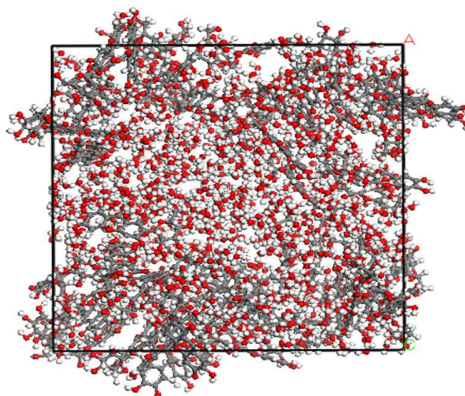


Fig. 1: Molecular dynamics simulation box of herbal plant bioactive compound in selected solvent system.

Keywords: Herbal plant; Experimental Design; Molecular Dynamics.

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#### References

- [1] Alebie, G., Urga, B., and Worku, A. (2017). Systematic review on traditional medicinal plants used for the treatment of malaria in Ethiopia: trends and perspectives. *Malar J.* 16(307): 1-13.
- [2] Te, M. (2013). The Expanding Market for Herbal, Medicinal and Aromatic Plants In Nigeria and the International Scene. *Medicinal & Aromatic Plants.* 02(06): 2-9.
- [3] Lay, M.M., Karsani, S.A., Banisalam, B., Mohajer, S., and Abd Malek, S.N. (2014). Antioxidants, phytochemicals, and cytotoxicity studies on *Phaleria macrocarpa* (Scheff.) Boerl seeds. *Biomed Res Int.* 2014:1-13.
- [4] Sharif, K.M., Rahman, M.M., Azmir, J., Mohamed, A., Jahurul, M.H.A., Sahena, F., and Zaidul, I.S.M. (2014). Experimental design of supercritical fluid extraction – A review. *Journal of Food Engineering.* 124(105-116).
- [5] Adam, F., A. B, S.H., Yusoff, M.M., and Tajuddin, S.N. (2014). Molecular Dynamic Simulation of the Patchouli Oil Extraction Process. *Journal of Chemical & Engineering Data.* 59(2): 183-188.
- [6] Schatschneider, B. and Chronister, E.L. (2008). Molecular dynamics simulations of temperature- and pressure-induced solid–solid phase transitions in crystalline para-terphenyl. *Molecular Simulation.* 34(10-15): 1159-1166.
- [7] Singh, A., Vanga, S.K., Orsat, V., and Raghavan, V. (2017). Application of molecular dynamic simulation to study food proteins: A review. *Crit Rev Food Sci Nutr.* 1-11.