Generalized Likelihood Uncertainty Estimation (GLUE) methodology for optimization of extraction in natural products

ABSTRACT

Optimization process is an important aspect in the natural product extractions. Herein, an alternative approach is proposed for the optimization in extraction, namely, the Generalized Likelihood Uncertainty Estimation (GLUE). The approach combines the Latin hypercube sampling, the feasible range of independent variables, the Monte Carlo simulation, and the threshold criteria of response variables. The GLUE method is tested in three different techniques including the ultrasound, the microwave, and the supercritical CO2 assisted extractions utilizing the data from previously published reports. The study found that this method can: provide more information on the combined effects of the independent variables on the response variables in the dotty plots; deal with unlimited number of independent and response variables; consider combined multiple threshold criteria, which is subjective depending on the target of the investigation for response variables; and provide a range of values with their distribution for the optimization.

Keyword: Natural products extraction; Generalized Likelihood Uncertainty Estimation; Threshold criteria; Optimization of extraction; Ultrasound assisted extraction; Microwave assisted extraction; Supercritical CO₂ assisted extraction