ABSTRACT

Metabolite Profilingand In Silico Study ofAffinity of Phytoestrogen Compounds in 96% Ethanol Extract N-Butanol Fraction of *M. crenata* C. PreslThrough Beta Estrogen Receptor

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Marsilea crentata C. Presl was known as one of plants contain phytoestrogen that can be used to overcome estrogen deficiency. The aim of this research was to identify metabolite profile and the metabolites affinity through they interaction with beta estrogen receptor in 96% ethanol extract n-butanol fraction of *Marsilea crenata* C. Presl leaves by in silico study. The metabolite profiling used UPLC-QToF-MS/MS with the MassLynx 4.1 to identify calculated mass and molecular formula, while the prediction of metabolite used Metfrag. Then, Pubchem and Chemspider used to confirm metabolite scientific publication. SwissADME was used to predict metabolite pharmacokinetic properties and it was screened by TPSA value, Blood Brain Barrier permeant (BBB permeant) and Human Intestinal Absorption (HIA). Selected metabolite was carried out by molecular docking to predict the affinity through beta estrogen receptor used PyRx with Autodock Vina. 11 metabolites identified in 96% ethanol extract n-butanol fraction of *Marsilea crenata* C. Presl was prepared by dicloromethane and 5-[6-(2H-tetrazol-5-yl)-2-naphthyl]-2H-tetrazole known as a major metabolite. While prepared by methanol, 26 metabolites identified and the major metabolite was [[4-[cyano(phenyl)methylidene]cyclohexa-2,5-dien-1-ylidene]amino] acetate. By this research, 15 metabolites predicted having agonist affinity with estrogen (17β-estradiol) through beta estrogen receptor (ERβ). Ethyl 5-phenyl-1H-pyrazole-3-carboxylate was a metabolite with high binding affinity, the value was -6.3.

Keywords: *Marsilea crenata* C. Presl, phytoestrogens, metabolite profiling, molecular docking.