ABSTRACT

IN SILICO STUDY OF FLAVONOIDS AND ALKALOIDS COMPOUNDS IN *Justicia gendarussa Burm. f.* FOR PHARMACOKINETIC PREDICTION

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Twelve flavonoid compounds were found in the n-butanol fraction of *Justicia gendarussa* Burm. f. The compounds have apigenin nuclei but only differ in the glycoside configuration attached to C-6 and C-8 as well as OH groups in glycosides. The objectives of this study were to determine the potency of 13 *Justicia gendarussa* Burm.f. compounds towards the pharmacokinetics parameters by *in silico* method using ACD/I-Lab Online, SwissADME Online, and pkCSM Online and to determine the Quantitative Structure-Activity Relationships between isolated *Justicia gendarussa* physicochemical properties with predicted parameters of pharmacokinetics using SPSS program. The results of pharmacokinetic studies of 13 *Justicia gendarussa* Burm. f. compounds, it was found that the compound with good pharmacokinetics potential was Justidrusamide D. When it was compared to the other compounds which had no Justidrusamide D, it was known that Justidrusamid had good absorption, distribution volume, blood brain barrier, binding protein. In addition, it also didn't affect nor inhibit drug absorption which was also absorbed by pgp substrates and has a high GI absorption that the drug could enter the blood vessels and circulated throughout the body easily. Justidrusamide D was also not metabolized by CYP1A2, CYP2C19, CYP2C9, CYP2D6, CYP3A4 enzymes so it would not affect the drug's action when it used in conjunction with drugs that were also metabolized by the same enzyme. In Quantitative Relation Structure-Activity test, there was a linear relationship between *in silico* pharmacokinetics parameters with hydrophobic, electronic, and steric parameters. It was known that the most influential parameter was the hydrophobic parameter. The correlation between pharmacokinetic parameters and logP stated that the higher the logP value was, the greater distribution volume, total clearance, intestinal absorption, DBP, and BBB would become.

Keywords: *Justicia gendarussa* Burm.f., *in silico*, Pharmakokinetic, Gendarusin, Justidrusamide, Amino-benzyl alcohols, QSAR