

# Unveiling the Antimicrobial, Anti-Biofilm, and Anti-Quorum-Sensing Potential of *Paederia foetida* Linn. Leaf Extract against *Staphylococcus aureus*: An Integrated In Vitro–In Silico Investigation

Sirijan Santajit <sup>1,2</sup>, Witawat Tunyong <sup>3</sup>, Dararat Horpet <sup>1</sup>, Asma Binmut <sup>1</sup>, Thida Kong-Ngoen <sup>3</sup>, Churaibhon Wisessaowapak <sup>4</sup>, Techit Thavorasak <sup>5</sup>, Pornpan Pumirat <sup>3</sup> and Nitaya Indrawattana <sup>3,6,\*</sup>

<sup>1</sup> Department of Medical Technology, School of Allied Health Sciences, Walailak University, Tha Sala 80160, Thailand; sirijan.sa@wu.ac.th (S.S.); pdararat@wu.ac.th (D.H.); abilmud@gmail.com (A.B.)

<sup>2</sup> Research Center in Tropical Pathobiology, Walailak University, Tha Sala 80160, Thailand

<sup>3</sup> Department of Microbiology and Immunology, Faculty of Tropical Medicine, Mahidol University, Bangkok 10400, Thailand; witawat.tun@mahidol.ac.th (W.T.); thida.kon@mahidol.ac.th (T.K.-N.); pornpan.pum@mahidol.ac.th (P.P.)

<sup>4</sup> Department of Medicine and Pharmacology, University of California, San Diego, CA 92093, USA; chwisessaowapak@health.ucsd.edu

<sup>5</sup> Center of Research Excellence in Therapeutic Proteins and Antibody Engineering, Department of Parasitology, Faculty of Medicine Siriraj Hospital, Mahidol University, Bangkok 10700, Thailand; techit.tha@mahidol.edu

<sup>6</sup> Siriraj Center of Research Excellence in Allergy and Immunology, Department of Research, Faculty of Medicine Siriraj Hospital, Mahidol University, Bangkok 10700, Thailand

\* Correspondence: nitaya.ind@mahidol.ac.th; Tel.: +66-2-354-9100 (ext. 1598)

**TableS1:** *In silico* ADMET prediction for flavonoid glycosides with anti-QS potential

Property	Isoquercetin (CID 5280804)#	Quercetin 3-galactoside (CID 5281643)	Quercetin 3-beta-D-glucoside (CID 44259136)	Kaempferol 3- $\alpha$ -D-galactoside (CID 44258736)	Kaempferol 3- $\alpha$ -D-glucoside (CID 44258798)
Solubility (LogS)	-4.2 log mol/L	-4.1 log mol/L	-3.27 log mol/L	-4.3 log mol/L	-4.3 log mol/L
Human Intestinal Absorption	Medium	Medium	Medium	Medium	Medium
Caco-2 Permeability	Low	Low	Low	Low	Low
Plasma Protein Binding (PPB)	95%	94%	69.89%	95%	95%
Blood-Brain Barrier (BBB)	Low	Low	Low	Low	Low
hERG Inhibition	Low risk	Low risk	Low risk	Low risk	Low risk
Hepatotoxicity	Low Risk	Low Risk	Low risk	Low Risk	Low Risk
LD50 (Acute Toxicity)	2500 mg/kg	2400 mg/kg	2110 mg/kg	2600 mg/kg	2600 mg/kg

---

**TableS2:** Physicochemical Properties and Bioavailability Parameters for Anti-QS Flavonoid Glycosides

Compound	MW (g/mol)#	LogP	H-Bond Donors	H-Bond Acceptors	Lipinski Violations	Bioavailability Score
Isoquercetin	464.38	1.08	8	12	1 (MW>500)	0.55
Quercetin 3-galactoside	464.38	1.04	8	12	1 (MW>500)	0.55
Quercetin 3- $\beta$ -D-glucoside	464.38	1.08	8	12	1 (MW>500)	0.55
Kaempferol 3- $\alpha$ -D-galactoside	448.38	0.45	8	11	0	0.55
Kaempferol 3- $\alpha$ -D-glucoside	448.38	0.45	8	11	0	0.55

---

MW: Molecular Weight

Lipinski Violations: Violations of Lipinski's rule of five.

---