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Name of thesis: Study on chemical composition and antioxidant activity of potential compounds from genus *Paederia* L. using computational chemistry methods.

Major: Organic chemistry **Code No:** 9 44 01 14

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Abstract: Two species of the genus *Paederia* L., including *Paederia lanuginosa* and *Paederia foetida*, were collected and identified in Quang Nam Province, Vietnam. The leaf extracts of the species exhibited significant DPPH radical scavenging activity, with IC_{50} values ranging from 2,95 μg/mL to 104 μg/mL. The ethyl acetate extract of *Paederia foetida* leaves showed the lowest IC_{50} value, comparable to ascorbic acid (2,67 μg/mL). Chemical components were also identified using GC–MS, revealing 55 compounds in the leaves of *Paederia lanuginosa* and 37 compounds in *Paederia foetida*, including biological compounds such as palmitic acid, phytol, vitamin E, oleic acid, linolenic acid, squalene, neophytadiene, campesterol, stigmasterol, and *β*–sitosterol. Additionally, 10 compounds were isolated from the extract of *Paederia lanuginosa* leaves, three of which (1-hexacosanol, phytol, and quercitrin) are reported for the first time from the genus *Paederia* L.. Five compounds (*β*–sitosterol, stigmasterol, arachidic acid, rutin, and linarin) were isolated for the first time from *Paederia lanuginosa*, while two others (kaempferol and quercetin) were previously reported.

Furthermore, the evaluation of 17 DFT methods for assessing the BDE (X–H) bonds (X = C, N, O, S) was also performed. The M06–2X method was identified as the most accurate and resource-efficient. Thus, this functional was then used to evaluate the antioxidant activities of phenolic compounds from *Paederia*, including cleomiscosins (cleomiscosin A, cleomiscosin B, cleomiscosin C), anthraquinones (1,3–dihydroxy–2,4–dimethoxy–9,10–anthraquinone, 2–hydroxy–1,4–dimethoxy–9,10–anthraquinone, 1–methoxy–2–methoxymethyl–3–hydroxy–9,10–anthraquinone, 1–hydroxy–2–hydroxymethyl–9,10–anthraquinone, 1–methyl–2,4–dimethoxy–3–hydroxyanthraquinone, 1–methoxy–3–hydroxy–2–ethoxymethylanthraquinone), feruloyl monotropeins (6'–*O*–*E*–feruloyl monotropein, 10'–*O*–*E*–feruloyl monotropein) and flavonoids (kaempferol, quercetin, quercitrin).

The results showed that the studied compounds exhibited good antioxidant activity in the polar environment. The overall rate constants for $HOO^{\bullet}$ radical scavenging reactions of cleomiscosins, feruloyl monotropein, and flavonoids range

from 10^6 to 10^8 M^{-1} s^{-1}, which was significantly higher than that of Trolox and comparable to ascorbic acid and resveratrol. The anthraquinones demonstrated exceptional $O_2^{\bullet-}$ radical scavenging activity, with rate constants that were within the same range. This capacity exceeded that of ascorbic acid by a factor of 10^3 to 10^5. In general, the antioxidant activity of these compounds is primarily attributed to their anionic and dianionic states in polar environments, particularly due to the –OH functional groups directly linked to their aromatic rings. This study represents the first published findings on the antioxidant activity of the aforementioned compounds.