

5th Symposium of Young Researchers on Pharmacognosy



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BOOK OF ABSTRACTS



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Composition decipherment of *Ficus pumila* var. *awkeotsang* and its potential on COVID-19 symptom amelioration and in silico prediction of SARS-CoV-2 interference

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The jelly derived from the achenes of *Ficus pumila* var. *awkeotsang* (FPAA) is a renowned beverage ingredient in Taiwan. In this study, the new compound ficumarin (**1**), derived from the twigs of *Ficus pumila* var. *awkeotsang* (FPAT), was elucidated with comprehensive spectroscopic data. It was proposed that the biosynthetic origin of the compound in question is the *p*-coumaroyl-CoA pathway. Alloxanthoxyletin, betulinic acid, and catechin were identified as the major and active constituents responsible for relieving neutrophilic inflammation by FPAT. Among the identified compounds, alloxanthoxyletin was found to interact with PRO350 and GLU377 of human INOSOX, exhibiting the highest potency. Furthermore, the capacity of the FPAT fraction and its coumarins to activate the Nrf2 pathway was confirmed. The analysis of LC-MS/MS data and feature-based molecular networking revealed that coumarins were the dominant and responsible components. Notably, alloxanthoxyletin was found to increase Nrf2 expression by up to $816.8 \pm 58\%$ due to its interaction with the VAL561, THR560 and VAL420 residues of the 5FNQ protein. The results of the simulation conducted using the COVID-19 Docking Server indicated that pyranocoumarins have the potential to interfere with the life cycle of SARS-CoV-2. Moreover, the findings indicated that FPAT exerts anti-inflammatory activity on neutrophils and activates Nrf2, suggesting that it may be developed as a complementary supplement for the treatment of patients with COVID-19.

References

[1] Hao-Chun Hu et al. *Journal of Food and Drug Analysis*. 2022, 30(3): 9.