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Notice for the PhD Viva Voce Examination

Ms Annika Maria Paul (Registration Number: 2071702), PhD scholar at the School of Sciences, CHRIST (Deemed to be University), Bangalore will defend her PhD thesis at the public viva-voce examination on Thursday, 12 December 2024 at 11.00 am in Room No. 044, Ground Floor, R & D Block, CHRIST (Deemed to be University), Bengaluru - 560029.

Title of the Thesis	:	**Screening of Plant-Based Bio-Active Metabolites as Potent Thrombin Inhibitors: *In Vitro* and *In Silico* Approach**
Discipline	:	**Botany**
External Examiner (Outside Karnataka)	:	**Dr Rita Kundu** Professor Department of Botany University of Calcutta 35, Ballygunge Circular Road, Kolkata - 700019 West Bengal
External Examiner (Within Karnataka)	:	**Dr B P Harini** Professor Department of Zoology Bangalore University Mysore Road, Jnana Bharathi Bengaluru – 560056 Karnataka
Supervisor	:	**Dr Anish Nag** Associate Professor Department of Life Sciences School of Sciences CHRIST (Deemed to be University) Bengaluru-560029 Karnataka

The members of the Research Advisory Committee of the Scholar, the faculty members of the Department and the School, interested experts and research scholars of all the branches of research are cordially invited to attend this open viva-voce examination.

Registrar

Place: Bengaluru
Date: 05 December 2024

ABSTRACT

The study aimed to optimize anti-thrombin phenolics and flavonoids from hydro- methanolic extracts of *Justicia adhatoda* L. (stem and flower: JAS, & JAF) and *Cordia dichotoma* G. (stem and fruit: CDS & CDF) through the response surface methodology (RSM). In the preliminary analysis, dried plant powder and unoptimized plant extracts showed considerable pharmacological activities, tested through the parameters like qualitative, microscopic, spectroscopic, chromatographic and fluorescence properties. The optimized stem and flower extracts of *J. adhatoda* exhibited substantial amounts of total phenolic content (TPC), total flavonoid content (TFC) and thrombin inhibition as 51.21±3.94 mg GAE (gallic acid equivalent)/g extract weight (EW), 21.32±1.59 mg QUE (quercetin equivalent)/g EW & 55.49±7.00 mg DAB (Dabigatran)/g EW and 132.58±6.28 mg GAE/g EW, 41.34±4.43 mg QUE/g EW and 116.51±16.75 mg DAB/g EW, respectively. The TPC, TFC and thrombin inhibition of *C. dichotoma* stem was found to be 16.77±1.72 mg GAE/g EW, 8.86±0.27 mg QUE/g EW, 45.68±2.88 mg DAB/g EW at the optimized extraction conditions. The optimized flower extract of *C. dichotoma* had TPC, TFC and thrombin inhibition values as 38.90±1.82 mg GAE/g EW,7.86±0.23 mg QUE/g EW, 37.50±1.57 mg DAB/g EW, respectively. The LC-MS and GC-MS analysis of the optimized extracts showed that the plant parts were dominated by phenolics, flavonoids and fatty acids, and the extracts were rich in antioxidant molecules.

The optimised extracts of JA and CD were rich in 33 and 50% of flavonoids and its derivatives, respectively. Polyphenols were detected as 12 and 6 % for JA and CD, respectively. Phytochemicals namely kaempferol 3-alpha-l-arabinopyranoside and kaempferol-3-oglucoside were found to be major compounds from JA and CD, respectively. Furthermore, GCMS study showed that the optimized extracts of JA and CD contained, 50 and 40% alkanes, respectively. All four extracts demonstrated significant antioxidant activities, with the range of 37.86 to 45.24 and 47.50 to 69.77 % at 50 µg /mL for DPPH, and ABTS radical scavenging assays, respectively. Finally, molecular docking study revealed that, majority of the identified compounds from JA and CD could activate and inhibit two thrombosis pathway proteins namely, tPA (tissue plasminogen factor) and PY21R (PY21 receptor), respectively. The docking studies between PY21 receptor and the identified compounds (through LC-Ms and GC-MS) revealed that, 1,2,3,6-tetragalloylglucose had the highest binding affinity (-9.93 Kcal mol-1) when compared to the control MRS2500 (-8.67 Kcal mol -1). In the case of tPA protein, Apigenin 7-O-(2G-rhamnosyl) gentiobioside showed the highest binding affinity (-10.06 Kcal mol-1) to that of the control drug 2,7-bis-(4-amidinobenzylidene)-cycloheptan-1-one (BABC) (-8.89 Kcal mol-1).

Keywords: Antioxidants, Thrombin, Docking, Flavonoids, Optimization

Publications:

1. Paul, A. M., & Anish, N. A. G. (2023). Phytochemical fingerprinting and evaluation of in silico anti-thrombotic properties of Justicia adhatoda L. and Cordia dichotoma Frost. *Notulae Scientia Biologicae*, *15*(3), 11625-11625. https://doi.org/10.55779/nsb15311625
2. Paul, A. M., & Nag, A. (2023). Antioxidant Phenolics of Justicia adhatoda L. and Cordia dichotoma Frost. Promote Thrombolytic Activity through Binding to a Serine Protease, Tissue Plasminogen Activator Protein. *Biomedical and Biotechnology Research Journal (BBRJ)*, *7*(4), 608-620. *DOI:* 10.4103/bbrj.bbrj_243_2