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Title: Metabolomic profiling of the phytochemical constituents of Carica papaya L. leaves and seeds by 1H NMR spectroscopy and multivariate statistical analysis

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Abstract: Extracts from the Carica papaya L. plant are widely reported to contain metabolites with antibacterial, antioxidant and anticancer activity. This study aims to analyze the metabolic profiles of papaya leaves and seeds in order to gain insights into their phytochemical constituents. We performed metabolite fingerprinting using 1D and 2D 1H NMR experiments and used multivariate statistical analysis to identify those plant parts that contain the most concentrations of metabolites of phytochemical value. Secondary metabolites such as phenyl propanoids, including flavonoids, were found in greater concentrations in the leaves as compared to the seeds. UPLC-ESI-MS verified the presence of significant metabolites in the papaya extracts suggested by the NMR analysis. Interestingly, the concentration of eleven secondary metabolites namely caffeic, cinnamic, chlorogenic, quinic, coumaric, vanillic, and protocatechuic acids, naringenin, hesperidin, rutin, and kaempferol, were higher in young as compared to old papaya leaves. The results of the NMR analysis were corroborated by estimating the total phenolic and flavonoid content of the extracts. Estimation of antioxidant activity in leaves and seed extracts by DPPH and ABTS in-vitro assays and antioxidant capacity in C2C12 cell line also showed that papaya extracts exhibit high antioxidant activity.

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