Abstract

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LC–MS/MS-based chemometric analysis of phytochemical diversity in 13 Ficus spp.(Moraceae): Correlation to their in vitro antimicrobial and in silico quorum sensing inhibitory activities

Thirteen Ficus species, family Moraceae, were profiled via HPLC-ESI-MS/MS. About 35 metabolites were tentatively identified, for the first time, belonging to various classes including flavonoids (flavonols, flavanols, flavanonols, flavones, flavonones), flavonolignans, anthocyanins and hydroxycinnamic acids derivatives). We herein also report three species, viz. Ficus auriculata, Ficus lutea Vahl. and Ficus trigonata L., with promising antimicrobial activity for the management of the infectious diseases associated with the tested food-borne and spoilage microorganisms using agar well diffusion assay. The compositional variabilities existing among the studied species in correlation to their antimicrobial activities were explored using different chemometric tools. From the Orthogonal Projection to Latent Structures (OPLS) regression model, a correlation between the observed antimicrobial activity and the abundant Ficus