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Shedding Light on Piper's Identity via Computational Mass Spectrometry

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Abstract

Morphological characteristics of *Piperrubro-venosum* hort. ex Rodigas bear a close resemblance to a plant identified as *Piper crocatum* Ruiz & Pav. in the literature. Hence, this study aimed to investigate whether both names describe the same species using data-dependent acquisition (DDA) LC-MS/MS analysis of methanol leaf extracts of *P. rubro-venosum* in positive and negative electrospray ionization modes. The data were analyzed using two computational mass spectrometry methods: spectral libraries search implemented in Global Natural Product Social (GNPS) molecular networking and molecular structure databases search implemented in SIRIUS. Classical molecular networking implied that the metabolites giving rise to two features with the highest intensities in the positive ionization chromatograms had distinct MS/MS spectra. De novo molecular formula

annotations and machine learning predictions in SIRIUS suggested that both features were sodiated precursor ions of neolignans. Based on the accurate mass of the precursor ions, the two features were annotated as crocatin A and B, which are bicyclooctanoid neolignans previously isolated in relatively large amounts from *P. crocatum* leaves. Based on the findings, it can be concluded that *P. crocatum* and *P. rubrovenosum* could be two names in the literature used to refer to one species of *Piper*. © 2022 Malaysian Institute of Chemistry. All rights reserved.

Author keywords

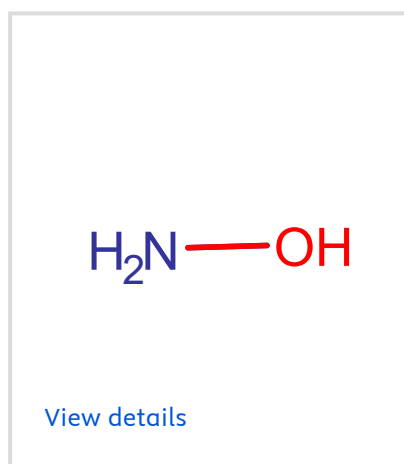
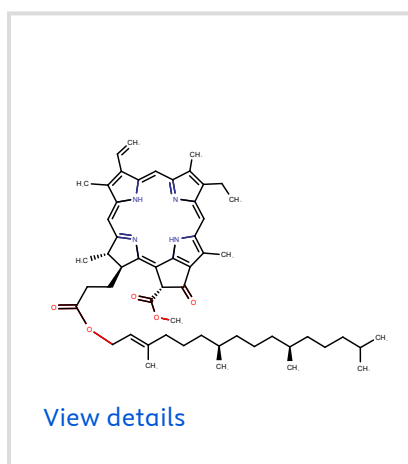
crocatin; GNPS; *Piper crocatum*; *Piper rubro-venosum*; SIRIUS

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Abstract

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