A quinazoline alkaloid isolation and its characterization by NMR experimental and GIAO-DFT data

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Abstract

In this work, we report the first time isolation of tryptanthrin from leaves *of Couroupita guianensis* and its structural assignment by ^{1}H, ^{13}C NMR chemical shift and Heteronuclear Multiple Bond Coherence (HMBC) calculations and experimental data. Couroupitine a is emerging as an important new therapeutic target for the treatment of cancer, neurological disorders, and other diseases that are characterized by pathological tryptophan metabolism.[1,2] The ^{13}C NMR spectrum in $CDCl_3$ showed a total of 15 carbon signals consistent with the proposed structure. Our results are in very good agreement with empirical data. So, we consider that EDF2/6-31G*//B3LYP/6-31G* empirical corrected NMR chemical shifts, using no scaling factors protocols, ^{1}H and ^{13}C calculations are useful tools to help structural elucidation of natural products.

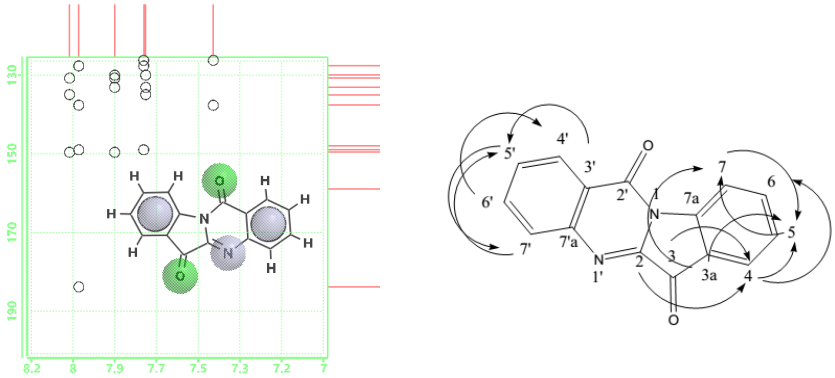

Figure 1. 2D [^{1}H,^{13}C]-HMBC spectrum for Couroupitine a and ^{1}H and ^{13}C correlation

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Keywords: Couroupitine a, EDF2/6-31G*, HMBC, spectroscopy