RamanFest
Paris | FRANCE
November 09-10 2023

Nathan I. Hammer
Trevor J. Wolfe, Nicholas A. Kruse, Mohamed M. Radwan, Amira S. Wanas, Kalee, N. Sigworth, Mahmoud A. ElSohly
Department of Chemistry and Biochemistry, University of Mississippi, Oxford, MS 38677, USA
nhammer@olemiss.edu

A study of major cannabinoids via Raman spectroscopy and density functional theory

Cannabinoids, a class of molecules specific to the cannabis plant, are some of the most relevant molecules under study today due to their widespread use and varying legal status. Here, we present Raman spectra of a series of eleven cannabinoids and compare them to simulated spectra from density functional theory computations. The studied cannabinoids include three cannabinoid acids (Δ^9-THC acid, CBD acid, and CBG acid) and eight neutral ones (Δ^9-THC, CBD, CBG, CBDVA, CBDV, Δ^8-THC, CBN and CBC). All cannabinoids have been isolated from cannabis plant gown at the University of Mississippi. The data presented in this work represents the most resolved experimental and highest-level simulated spectra available to date for each cannabinoid. All cannabinoids displayed higher peak separation in the experimental spectra than CBGA, which is most likely attributable to physical composition of the samples. The overall agreement between the experimental and simulated spectra is good, however for certain vibrational modes, especially those in the –OH stretching region, deviations are observed due to hydrogen bonding, suggesting that the OH stretching region is a good probe for decarboxylation reactions in these and related species.

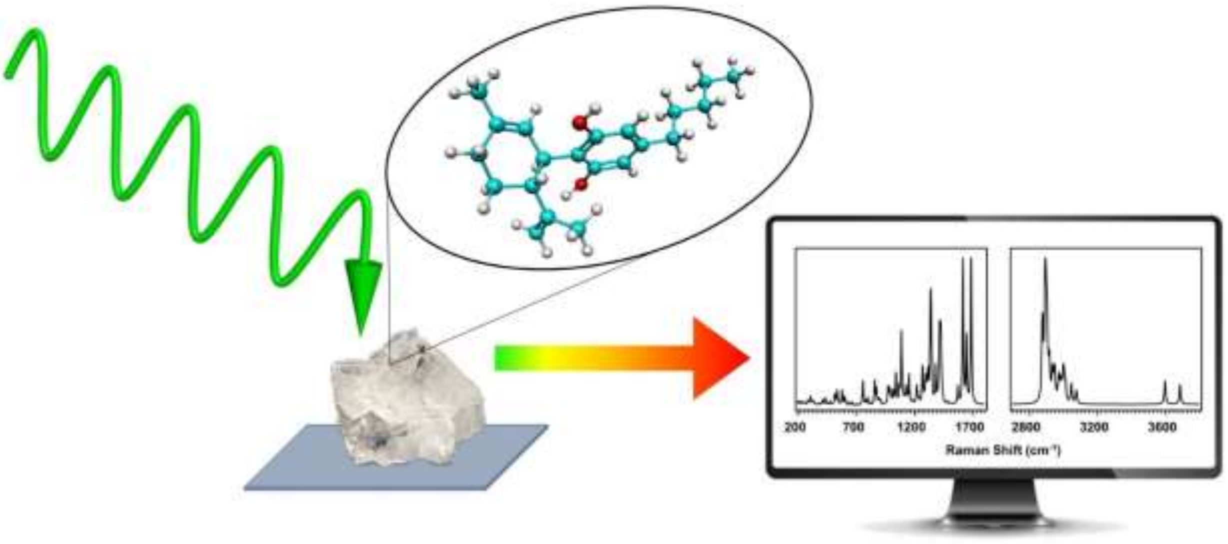

Figure 1: Raman spectroscopy and computational chemistry are used to study eleven major cannabinoids.