

Abstract

The federally illegal psychoactive compound Δ -9-tetrahydrocannabinol (Δ -9-THC) is a structural isomer to the following: cannabidiol (CBD), cannabichromene (CBC), Δ -8-tetrahydrocannabinol (Δ -8-THC), and Δ -10-tetrahydrocannabinol (Δ -10-THC), which are all federally legal under US law. CBD and CBC are non-psychoactive structural isomers and show promise for treating chronic pain, inflammation, and other conditions. Δ -8-THC and Δ -10-THC are psychoactive and gaining popularity due to federal legality and with a few states criminalizing their sale. Differentiating these structures is challenging due to their isomeric nature. In this work, adduction of water molecules in a quadrupole ion trap mass spectrometer is utilized to differentiate between the aforementioned cannabinoid isomers using direct infusion mass spectrometry. Mass spectra of lithiated cannabinoids show two peaks of interest: a lithiated peak ($[M+Li]^+$) at m/z 321 and a water adduct peak ($[M+Li+H_2O]^+$) 18 mass-to-charge (m/z) units higher m/z 339. The mass spectra indicate that lithiated cannabinoids adduct water and do so on the millisecond timescale. Using this data, an unreacted fraction ($\frac{I_{321}}{I_{321}+I_{339}}$) was calculated for each cannabinoid. The unreacted fractions for Δ -8-THC, Δ -9-THC, Δ -10-THC, CBC, and CBD were measured in triplicate and are as follows: 0.315 ± 0.003 , 0.335 ± 0.003 , 0.195 ± 0.005 , 0.638 ± 0.001 , and 0.936 ± 0.003 , respectively.