HIGH RESOLUTION MASS SPECTROSCOPY FOR CHARACTERIZATION OF RESIN FROM GUAYULE (*PARTHENIUM ARGENTATUM*)

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Guayule (*Parthenium argentatum* A. Gray), a shrub native to the arid region of the U.S. southwest and Mexico belonging to the *Asteraceae* family, is a source of high quality, hypoallergenic natural rubber with applications in pharmaceutical, tire, and food industries. Production of rubber results in a substantial amount of resin-containing residues which contain a wide variety of secondary metabolites (sesquiterpene esters, triterpene alcohols, fatty acids, etc.). In order to enhance the economic viability of guayule as an industrial crop, value-added use of the residues is needed and has the potential to reduce gross rubber production costs as much as 26-49%. The main objective of this research is the characterization of guayule resin using rapid and accurate analytical techniques to identify compounds of potential commercial value. Guayule resin is inherently complex and includes many high-molecular-weight and non-volatile compounds that are not easy to observe using traditional chromatographic techniques (like GC-MS and HPLC). In this study, high-resolution Fourier Transform Ion Cyclotron Resonance Mass Spectroscopy (FT-ICR-MS) technique was used to characterize hundreds of compounds with over a wide range of molecular weights and degrees of aromaticity at higher levels of mass accuracy than other forms of mass spectrometry. The inherent high mass accuracy and resolution of FT-ICR MS allow for the detection and identification of thousands of compounds within a single mass spectrum and typically used to analyze complex mixtures such as petroleum, biofuels, dissolved organic matter, lipids, and proteins. Atmospheric pressure photoionization (APPI) is used to ionize both polar and non-polar compounds, especially aromatic species, for detection by mass spectrometry. Resin samples were diluted in 50:50 chloroform: methanol to 1 mg/ml stock solutions. Stock solutions were further diluted to 50 µg/ml in toluene for (+/-) APPI FT-ICR MS analysis. The obtained FTMS spectrum contained approximately 4500 peaks in the m/z range of 150-550. The major peaks correspond to m/z 199.11 ($C_{14}H_{14}O$), m/z 255.23 ($C_{16}H_{32}O_2$), m/z 279.23 ($C_{18}H_{32}O_2$), m/z 380.31 ($C_{27}H_{40}O$), m/z 396.30 ($C_{27}H_{40}O_2$), m/z 398.32 ($C_{27}H_{42}O_2$), m/z 407.26 ($C_{27}H_{36}O_3$), m/z 408.28 ($C_{27}H_{36}O_3$), m/z 421.35 ($C_{30}H_{44}O$), m/z 437.34 ($C_{30}H_{44}O_2$), m/z 439.36 ($C_{30}H_{46}O_2$), m/z 455.35 ($C_{30}H_{48}O_3$), m/z 469.33 ($C_{30}H_{46}O_4$), m/z 471.35 ($C_{30}H_{48}O_4$), m/z 473.36 ($C_{30}H_{50}O_4$), and m/z 379.26 ($C_{26}H_{36}O_2$), which most likely represent triterpenoids, steroids and fatty acids compounds discussed in literature. From these spectra, a comparison could be made with the groups of compounds in guayule resin identified in previous studies using other methods. The FT- MS data provides more information about new classes of compounds in the guayule resin for investigation of potential applications and improved chemical separation techniques.

Association for the Advancement of Industrial Crops, 31st Annual Meeting
~ Advancing the Adoption of Industrial Crops through Innovation and Technology ~
Tucson, Arizona – 8-11 September 2019.
https://aaic.org/

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