

B36 Analysis of Anthraquinone Dyes by Electrospray Ionization Quadrupole-Time-of-Flight Tandem Mass Spectrometry (ESI-QTOF-MS/MS)

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After attending this presentation, attendees will understand how tandem mass spectrometry on a Quadrupole Time-of-Flight (QTOF) can provide structural elucidation of acid dyes extracted from fibers by specific key fragmentation patterns and how these data can be used to unambiguously identify commercial textile dyes.

This presentation will impact the forensic science community by providing an improved and faster analysis of dyed fiber by imparting a better understanding of the dye fragmentation pathways on a QTOF mass spectrometer for better identification compared to current methods.

In forensic analysis, textile fibers are frequently encountered as evidences in forensic crime scenes. Unambiguous identification and characterization of the dyes present in the fibers are of significance for forensic analysis. Several analytical methods such as Fourier Transform Infrared (FTIR), Ultraviolet/Visible (UV-Vis) spectroscopy, and Nuclear Magnetic Resonance (NMR) can be used for the identification of dyes; nevertheless, the low quantities of trace evidence found at crime scenes can hinder their analysis by these methodologies. Mass spectrometry offers an excellent option for analysis of trace evidence of dyes, due to its high sensitivity and versatility. In this sense, ESI-QTOF-MS/MS can be used for efficient identification and characterization of dyes.

This study is the first stage on the building of a mass spectrometry dye database from the recently donated Max Weaver dye library from Eastman® Chemicals, with approximately 100,000 dyes, to the College of Textiles in North Carolina State University. In this study, several sulfonated anthraquinone acid dyes containing the structure of 1-amino anthraquinone-2-sulfonate acid were analyzed by ESI-QTOF-MS/MS. A loss of 64amu was observed for all dyes and model compounds. This loss was confirmed to be SO₂ by high-resolution analysis. The unimolecular rearrangement and mechanisms of fragmentation triggered by Collision-Induced Disassociation (CID) were investigated by tracing the sulfur isotopes, ³²S and ³⁴S, as well as by exploring the functions of the ortho-amino group during the rearrangement. Also, it was found that the presence of different group functionalities (e.g., secondary or tertiary amines and thiols) attached to the anthraquinone structure have specific fragmentation pathways under similar CID conditions that can be used to identify them. For example, an anthraquinone having a secondary amine with an aromatic group attached to it (e.g., acid blue 25), can be distinguished from an anthraquinone having a secondary amine with an alkyl group attached to it (e.g., acid blue 62). The resultant fragmentation patterns could contribute to a dye database for identifying and fingerprinting unknown dyes with similar chemical structures and can be used for trace fiber evidence in forensic analysis.

Mass Spectrometry, Dyed Fibers, Trace Evidence