University of Puerto Rico
Mayagüez Campus
Chemistry Department
Departmental Seminar

Friday, April 22th, 2016
Q -123
Abbott Room
11:30 AM

By

Nataly J. Galan-Freyle
Doctoral Candidate
UPRM-RUM

DETECTION OF ANALYTES IN COMPLEX MATRICES USING TUNABLE QUANTUM CASCADE LASER SPECTROSCOPY AND CHEMOMETRICS ANALYSIS

Available methods for detection and quantification of small amounts of analytes are costly and time-consuming. In addition, laborious sampling protocols can compromise the integrity of the analytes, specifically during sample collection, transport, and storage. In this study, development of simple, non-destructive, fast, low cost, and attractive methods of analysis based on tunable quantum cascade laser spectroscopy (QCLS), operating in the mid-infrared (MIR) region and coupled to chemometrics analysis was investigated. This technology was used for *in situ* detection, identification, and discrimination of multiple analytes under real world conditions. Detection of traces of emerging contaminants such as highly energetic materials (HEMs), petroleum and monitoring of active pharmaceutical ingredients (APIs) in formulations was demonstrated. Detection of multiple analytes was carried out on challenging matrices such as soils, pharmaceutical mixtures, food powder, makeup, fabrics, etc., which provides more realistic scenarios of potential applications. All these uses are vital for society because: (1) they can be applied in environmental monitoring; (2) in on-line control of pharmaceutical processes; and (3) in detection of explosives assisting in the task of deterring terrorist attacks. Various analytes were used in this study, including 2,4-dinitrotoluene (DNT), 2,4,6-trinitrotoluene (TNT), petroleum and ibuprofen (IBU). The methodology was capable of obtaining accurate evidence of the presence of the analytes at trace level on the mentioned complex matrices. With the additional assistance of chemometrics tools, in this study it was possible to confirm the presence of the various analytes in the matrices used.