DEPARTMENT OF CHEMISTRY AND ENVIRONMENTAL SCIENCE SEMINAR SERIES FALL 2019

DATE: WEDNESDAY, OCTOBER 30, 2019

LOCATION: TIERNAN HALL LECTURE 1 TIME: 1:00-2:20PM

GUEST SPEAKER

Dr. Dujuan Lu Manager/Global Leader-E&L SGS Life Sciences Fairfield, NJ

TOPIC

A Case Study to Investigate Fragmentation Mechanism of a Leachable from Secondary Packaging by GC-HRMS

ABSTRACT

Primary packaging components are those that are either in direct contact with the drug product or have the potential to be in direct contact. The common primary packaging includes vial, bottle, tube, syringe, and bag. These components may also include container liners and closures such as caps, stoppers and metering valves. Secondary packaging components are integral to the final marketed package but are not in direct contact with the drug product, such as pouches, labels, and cartons. Although this indirect contact decreases the possibility of migration, there is still a risk for leachables. Leachables derived from secondary packaging components are typically more volatile than those arising from primary packaging. This presentation will focus on a case study on fragmentation mechanism of a cyclic ester, which was found as a leachable from secondary packaging. During the GC-HRMS/FID analysis for volatile and semi-volatile organic compounds, the compound was originally shown as an unknown. By using the High Resolution Accurate Mass (HRAM) in both Electron Ionization (EI) and Chemical Ionization (CI) Modes, we were able to obtain the molecular ion information and chemical composition of this compound. Tandem mass spectrometric experiments by GC-MS/MS were also performed to obtain fragmentation information at different collision energies. We were able to successfully identify the unknown compound and have demonstrated that the current literature shows incorrect information on one of the major fragment ions. This presentation will show the importance of extractable studies on secondary packaging and that High Resolution Accurate Mass (HRAM) data can facilitate confident compound identification and unknown compound structure elucidation.

BIO

Dr. Lu serves as the manager for the extractables and leachables (E&L) team at the SGS Fairfield New Jersey facility as well as the global leader amongst the three centers of excellence for E&L testing. Before joining SGS, she worked at Fresenius Kabi as a research scientist, leading E&L projects to support transfusion and infusion medical device and parenteral products.

She has extensive pharmaceutical industry experience with more than 300 E&L projects on a broad range of packaging systems, including process materials, pharmaceutical finished packaging, and medical device. As a well-recognized E&L subject matter expert in the field, she is frequently presenting at various technical conferences and webinars as invited speakers. She has been chairing the E&L technical session at Pittcon since 2017. She has more than 10 years of experience in pharmaceutical analysis, specialized in trace analysis by LC/MS and GC/MS.

Dr. Dujuan Lu obtained her PhD in analytical chemistry from the University of Pittsburgh and BS in chemistry from Nanjing University. She has authored more than 10 peer-reviewed journal publications with more than 300 citations. She is serving as an expert reviewer for more than 10 prestigious journals in the field of analytical chemistry and pharmaceutical science.

> **Committee members:** Dr. Pier Champagne – pier.a.champagne@njit.edu Dr. Hao Chen - hao.chen.2@njit.edu