

Department of Chemistry

Graduate Student Seminar – Summer 2020

## Chemometric Analysis of Multidimensional Fluorescence Data Recorded from Benzo[a]pyrene Metabolites in Shpol'skii Like Matrixes

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The goal of the present study is to develop screening methodology for the analysis of metabolites of polycyclic aromatic hydrocarbons (PAH metabolites) in complex matrixes. The investigated metabolites include 1-Hydroxybenzo[a]pyrene, Benzo[a]pyrene-cis-4,5-dihydrodiol, Benzo[a]pyrene-r-7, t-8, t-9, c-10-tetrahydrotetrol (+/-) and Benzo[a]pyrene-r-7, t-8, t-9, t-10-tetrahydrotetrol (+/-). The analytical approach is based on Time-Resolved Laser-Induced Fluorescence Spectroscopy at liquid nitrogen (77K) and liquid helium (4.2K) temperatures. Multidimensional data formats - known as wavelength-time matrices (WTMs) and time-resolved excitation-emission matrices (TREEMs) - were recorded from frozen matrixes within the time domain of metabolites fluorescence decays (nanoseconds).<sup>1,2</sup> The information content of WTMs and TREEMs was processed with parallel factor analysis 2 (PARAFAC 2) and multivariate curve resolution-alternating least-squares (MCR-ALS). The performance of these two multi-way calibrations algorithms is then compared for the direct determination of the four metabolites in complex mixtures.

<sup>1</sup> The 71th Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy, Philadelphia, PA, March 2-5, 2020. Chemometric Analysis of Multidimensional Fluorescence Data Recorded from Benzo[a]pyrene Metabolites in Frozen Matrixes. Mohammadreza Chehelamirani, Anthony M. Santana and Andres D. Campiglia. Oral Presentation (5-17-3).

<sup>2</sup> Mohammadreza Chehelamirani, Anthony Santana and Andrés D. Campiglia\*; Shpol'skii Spectroscopy of Metabolites of Polycyclic Aromatic Hydrocarbons in Primary Alcohols at 77K and 4.2K; submitted to Analytical Methods, June 2020.