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Full Schedule & My Itinerary

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Filter by Date

Topic Area

Session Type

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No **Upcoming Sessions Only**

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Eastern Standard Time (EST)

Event Itinerary

My Itinerary **2**

Analytical Development Relevant to Environmental Exposure and Effects (#27)

06:00pm - 10:00pm Eastern Standard Time (EST) - December 18, 2021 | Room: Virtual
Xing-Fang Li, Session Host; Prof. Dongchan Jang, Session Host
Topic Area: (01) Analytical
Session Type: Oral - Virtual

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Topic Area: (01) Analytical

Symposium Organizers: X. Li, S. Richardson, G. Jiang, S. F. Nakayama

Resolving identities of emerging per and polyfluoroalkyl substances isomers based on COSMO-RS derived retention factor and mass fragmentation patterns

Saturday

06:45pm - 07:15pm Eastern Standard Time (EST) - December 18, 2021 | Room: Virtual
Scott Simpson , Presenter; Mary Grace Guardian; Diana Aga
Topic Area: (01) Analytical
Session Type: Oral - Virtual

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Chromatographic retention times and mass spectrometral fragmentation of per- and polyfluoroalkyl substances (PFASs) standards were determined using the optimized parameters obtained for liquid chromatography with tandem high-resolution mass spectrometry (LC-HRMS) analysis. Characteristic fragment ions obtained at various collision energies (MS^2 fragmentation) were used for structural elucidation to predict the identities of newly discovered (emerging) PFASs detected in environmental samples. Moreover, the COnductor-like Screening MOdel for Realistic Solvents (COSMO-RS) was used to calculate the octanol-water partition coefficients (K_{ow}) and mean isotropic polarizabilities of known PFASs, and the values were plotted against their chromatographic retention factors (k) to obtain a multivariable regression model that can be used to predict k values of unknown PFASs. Retention factor values of different structural isomers of the unknown PFASs were calculated and compared to the experimental k. For all the unknown PFASs, the predicted k value for the isomer that matches the corresponding MS^2 fragmentation was found to be within 5% of the experimentally measured k value. This study demonstrates the applicability of a simple approach that combines the computationally-derived log K_{ow} and polarizabilities, experimentally-determined k va...

observed MS^2 fragmentation patterns, in assigning the structures of emerging PFASs at environmentally relevant conditions when no reference standards are available.

Hydrogen-rich systems: Materials chemistry for energy storage and delivery (#163)

01:00pm - 05:00pm Eastern Standard Time (EST) - December 21, 2021 | Room: Virtual

Godwin Severa, Session Host; Vitalie Stavila, Session Host

Topic Area: (12) Chemistry of Energy

Session Type: Oral - Virtual

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Topic Area: (12) Chemistry of Energy

Symposium Organizers: Z. Huang, M. Bowden, C. Yoon, T. HE, G. Severa

Tuesday

Search for molecular corks beyond carbon monoxide: A quantum mechanical study of N-heterocyclic carbene adsorption on Pd/Cu(111) and Pt/Cu(111) single atom alloys

04:05pm - 04:30pm Eastern Standard Time (EST) - December 21, 2021 | Room: Virtual

Scott Simpson , Presenter

Topic Area: (12) Chemistry of Energy

Session Type: Oral - Virtual

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