

Department of Chemistry Newsletter



July Issue, 2022

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Sylx Okanagan Nation Territory

Announcements

Congratulations to:



Dr. Thu-Thuy Dang for the Plant Journal–PSNA Early Career Award for outstanding early career scientists among members of the Phytochemical Society of North America.



Dr. Manjinder Kour (Szilagyi group) for the Best Poster Prize at World Association of Theoretical & Computational Chemists (WATOC) congress for her presentation entitled “Development of atomic-scale models for low temperature pyrite reduction reactions”.



Dr. Viki Kumar Prasad (DiLabio group) for the Best Poster Prize also at the WATOC congress for his presentation entitled “Development of atom-centered potentials for efficient and accurate electronic structure modeling of large molecular systems”, which was based on his PhD work.



Dr. Robert Szilagyi for the John R. Evans Leaders Fund (CFI-JELF) to set up a combined experimental and computational laboratory for structure/function studies of Fe–S clusters, nanoparticles, and mineral surfaces. With the new funding, Dr. Szilagyi can start equipping the laboratory with high-value instruments (glovebox, UV-vis, FTIR, compute servers, and chemical structure databases).

Chemical & environmental safety



Chemical and Environmental Safety News

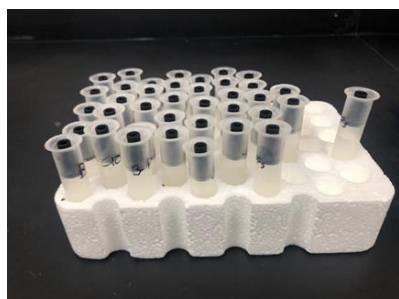
We are starting a new section for the Departmental Newsletter, where we wish to highlight a newsworthy event from the past month, provide information about any recent developments, as well as safety tips and reminders.

This month we are focusing on storage of samples, standards, and chemicals in shared fridges. A few years ago, we had an accident when irreplaceable lake samples were discarded from a fridge in SCI226 by a lab technician thinking they were CHEM461 samples from the previous term. This year, while cleaning out the fridge dedicated to teaching labs, precious research standards were thrown out. Again, the assumption was that these samples were left over CHEM461 labs from the previous term. They were stored adjacent to lot of samples from undergraduate courses labelled “Mary and Jon, part I”, “wine project”, and “1,2,3,4”. Given that the glycoside standards are needed by the second week of August, we are using departmental funds with the assistance of the Dean’s office to replenish the most essential ones that are commercially available. The rest of the thrown away samples will need to be custom synthesized pending on funding and personnel availability.

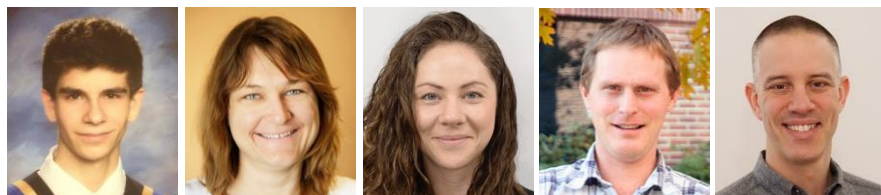
In order to avoid similar accidents, please review your lab’ policy and practice of storing research samples in shared freezers/fridges. As for the Teaching labs, please do not store research samples in any of the teaching dedicated fridges and particularly fridge/freezers FR#2 and FR#3. Please note that in SCI226 there is a brand-new fridge (FR#1) with extra space that can be a place to safely store research samples for a short term. FR#1 will never have teaching lab samples stored in it. It will be cleaned or maintained by lab technicians, but there is no chance of confusing anything in this fridge as discard. Furthermore, when placing teaching lab samples into the freezer, please use a container/Tupperware with your contact information (first and last name), content list, and date. Importantly, using teaching lab resources (space, chemicals, equipment, freezer/fridge space) needs to be cleared with the teaching lab manager.

If you have any research samples stored in any of the teaching lab freezers, please get in touch with the teaching lab manager for relocating them to FR#1. We need space for setting up for the fall courses and there are unlabelled samples (see photos) that needs our attention.

– Ieva Zigg, Michele Cannon, Robert Szilagy



Recent publications



James W. Favell*, Kerry L. Wilkinson*, **Ieva Zigg**, **Sarah M. Lyons**, Renata Ristic, Carolyn J. Puglisi, Eric Wilkes, Randell Taylor, Duane Kelly, Greg Howell, Marianne McKay, Lucky

Mokwena, Tim Plozza, Pei Zhang, AnhDuyen Bui, Ian Porter, Orrin Frederick, Jasha Karasek, Colleen Szeto, Bruce S. Pan, Steve Tallman, Beth Anne McClure, Hui Feng, Eric Hervé, Anita Oberholster, **Wesley F. Zandberg**[#], **Matthew Noestheden**[#] (2022). Correlating sensory assessment of smoke-tainted wines with inter-laboratory study consensus values for volatile phenols. *Molecules*. DOI: 10.3390/molecules27154892. (*: co-first authors; #: co-corresponding authors)



Yevgen Kovalenko, **Joshua Vander Weide**, Ricco Tindjau, **Wesley F. Zandberg**, Simone Diego Castellarin (2022). Timing and severity of crop load management influences technological maturity, terpene synthase expression and free terpene accumulation in Gewürztraminer grapes (*Vitis vinifera*). *Australian Journal of grape and Wine Research*. ([accepted](#))

New members



Erick Octavio Mora Hernández joining Dr. Thu-Thuy Dang's group (Plant BioCoRe). From Monterrey Institute of Technology & Higher Education (Tecnológico de Monterrey) in Mexico City (Mexico), Erick is a Mitacs Globalink student who works on alkaloid biosynthesis in plants.

Recent and upcoming events

Canadian Symposium on Theoretical & Computational Chemistry

Dr. Gino DiLabio co-organized the CSTCC, which was held on our campus from June 27th to July 1st. More than 80 students and PIs from across Canada and from international institutions participated in the event. **Dr. Robert Szilagy** gave a fantastic presentation of his research at the conference. The conference was more than four years in the making, with COVID delays. Members of the DiLabio group served as volunteers: **Greta Tödtmann** (International Undergraduate Research awardee), **Niamh Carbin** (Mitacs Globalink intern), and **Bhaves Gnanapareddy** were awesome, as was **Eduardo Montalvo Romero** (PhD student) who was the volunteer leader for the conference.

Several members of the Department presented at the symposium:

- **Dr. Robert Szilagyi** gave an invited talk entitled "Modelling Gas Adsorption on Porous Carbon Materials "
- **Eduardo Montalvo Romero** (DiLabio group) gave a 15-minute oral presentation entitled "The on-water effect in organic reactions".
- **Dr. Alireza Sadeghifar** (DiLabio group) presented a poster on "The pan-Canadian Computational Chemistry Course (PC3) Program: A collaborative approach to training graduate students in applied computational chemistry".
- **Dr. Viki Kumar Prasad** (DiLabio group) presented a poster entitled "Development of atom-centered potentials for efficient and accurate electronic structure modeling of large molecular systems".
- **Jessica Zarama** (Godin group) presented a poster titled "Combined experimental and computational study of the chemical reactivity and optical properties of carbon nitride (CN_x) and its analogues".



CANADIAN
ASSOCIATION OF
THEORETICAL
CHEMISTS

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CANADIENNE DES
CHIMISTES
THÉORICIENS

World Association of Theoretical Chemists Congress

UBC Okanagan's Department of Chemistry displayed an incredible démonstration de force with robust idea exchanges and excellent presentations by faculty and students at WATOC2020. **Dr. Gino DiLabio** co-organized the World Association of Theoretical Chemists Congress (WATOC 2020, as it had been planned for 2020). The congress was held at Canada Place in Vancouver from the 3rd to the 8th of July, 2022 with more than 800 participants from 52 countries.

At the congress,

- **Dr. DiLabio** gave an invited talk entitled "Atom-centered potentials: A cost-effective approach to improving computational chemistry methods".
- **Dr. Robert Szilagyi** gave an invited talk entitled "Modelling Gas Adsorption on Porous Carbon Materials ".
- **Greta Tödtmann** (DiLabio group) presented a poster on her summer project "Computational study of the PINOylation mechanism at benzylic C-H bonds".

At WATOC, **Dr. DiLabio** and partners presented **Dr. Sadeghifar's** poster above, and **Jessica Zarama** (Godin group) also presented her poster with the same title as at CSTCC. **Dr. Manjinder Kour** (Szilagyi group) and **Dr. Viki Kumar Prasad** (DiLabio group) for the **Best Poster Prize**.



Plant Biology 2022

Plant Biology 2022, the quadrennial joint meeting of the Canadian and American Societies of Plant Biologists, took place in Portland, Oregon (USA) from 9th to 13th of July. **Dr. Thu-Thuy Dang** was an invited speaker and chair for the session “Specialized metabolism”. **Dr. Lauren Erland** gave a talk received and received CSPB **Carl Douglas Award** for outstanding postdoctoral CSPB members.



PSNA 2022

At the annual meeting of the Phytochemical Society of North America from the 24th to the 28th of July in Blacksburg (Virginia, USA), **Dr. Thu-Thuy Dang** chaired the “Synthetic biology and metabolic engineering” session, and gave an invited talk to accept the Plant Journal–PSNA Early Career Award in the “Phytochemistry of functional foods and bioactive natural compounds” session.



We would like to acknowledge that the land on which we gather is the unceded territory of the Syilx (Okanagan) Peoples.

If you would like to contribute to, or have any suggestions for, our Department’s upcoming newsletter, please contact Thuy Dang (thuy.dang@ubc.ca).