Xinhao Li

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Summary

3rd year Ph.D. student in Chemistry. Experienced in applying **machine learning** techniques and **cheminformatics** for solving chemistry problems, e.g. molecular activity/propriety prediction. Well-versed in programming languages including **Python** and **R**. Proficient skills in chemical data mining, curation, analysis, visualization, and modeling.

Research Interests by Keyworks

- Cheminformatics
- Computational Toxicology
- Machine Learning/Deep learning
- Big Data Mining, Analysis, Visulzation
- QSAR modeling
- Computer-Aided Drug Design
- Virtual Screening
- Software Development

Research

Graduate Research Assistant — Fourches Lab, NCSU
Advisor: **Denis Fourches** — *Aug 2017 - Current*

- Development of Novel Quantitative Structure-Property/Activity Relationship (**QSPR/QSAR**) Modeling Methodologies:
  - **MolPMoFiT**: An inductive transfer learning method for QSRR/QSAR modeling. MolPMoFiT pre-trained a universal molecular structure prediction model using one million bioactive molecules from ChEMBL and then fine-tuned it for various QSPR/QSAR tasks.
  - **Hierarchical QSAR**: An effective ensemble modeling method that Integrating binary/multi classification and regression models for predicting acute oral systemic toxicity.
- Software Development:
  - **CryptoChem**: A novel cryptographic and data storage method based on cheminformatics, machine learning, and big chemical data. Two independent software were developed: MOLWRITE and MOLREAD. MOLWRITE encrypts the text/image data into chemical message and MOLREAD decrypts the encoded chemical message back to text/image.

Education

PhD in Chemistry	**North Carolina State University**	Raleigh, NC	2017 – Current
MS in Chemistry	**Beijing University of Chemical Technology**	Beijing, China	2013 –2016
BS in Chemistry	**Beijing University of Chemical Technology**	Beijing, China	2009 –2013

Skills

- **Language:** English & Mandarin (native)
- **Programming Language:** Python & R
- **Cheminformatics Toolkits:** KNIME, RDKit, Schrodinger
- **Machine Learning Toolkits:** Pytorch, Keras, Scikit-Learn, Jyperter Notebook

Courses

- **deeplearning.ai:** Deep Learning Specialization

Publications

1. **Xinhao Li** and Denis Fourches. (2019): Inductive Transfer Learning for Molecular Activity Prediction: Next-Gen QSAR Models with MolPMoFiT. *ChemRxiv*.
2. **Xinhao Li**, Nicole Kleinstreuer and Denis Fourches. (2019): Hierarchical H-QSAR Modeling Approach for Integrating Binary/Multi Classification and Regression Models of Acute Oral Systemic Toxicity. *Chemical Research in Toxicology*. (Under Revision)
3. **Xinhao Li** and Jiaxi Xu. (2017): Effects of the Microwave Power on the Microwave-assisted Esterification. *Current Microwave Chemistry*. 158-162.
4. **Xinhao Li** and Jiaxi Xu. (2017): Identification of Microwave Selective Heating Effort in an Intermolecular Reaction with Hammett Linear Relationship as a Molecular Level Probe. *Current Microwave Chemistry*. 339-346.
5. **Xinhao Li** and Jiaxi Xu. (2016): Determination on temperature gradient of different polar reactants in reaction mixture under microwave irradiation with molecular probe. *Tetrahedron*. *35*, 5515-5520.
6. Shanyan Mo, **Xinhao Li** and Jiaxi Xu. (2014): In Situ-Generated Iodonium Ylides as Safe Carbene Precursors for the Chemoselective Intramolecular Buchner Reaction. *J. Org. Chem*. 19, 9186-9195.

Presentations

1. **NC State Chemistry Recruitment Weekend (March 2019, Raleigh, NC)**
   Xinhao Li, Denis Fourches. Hierarchical H-QSAR Modeling Method that Integrates Binary/Multi Classification and Regression Models for Predicting Acute Oral Systemic Toxicity. (**Poster**)
2. **American Chemical Society Conference (April 2019, Orlando, FL)**
   Xinhao Li, Denis Fourches. Hierarchical H-QSAR Modeling Method that Integrates Binary/Multi Classification and Regression Models for Predicting Acute Oral Systemic Toxicity. (**Poster**)
3. **"Innovations in Agriculture" Scientific Poster Session at BASF (May 2019, RTP, NC)**
   Xinhao Li, Denis Fourches. Hierarchical H-QSAR Modeling Method that Integrates Binary/Multi Classification and Regression Models for Predicting Acute Oral Systemic Toxicity. (**Poster**)
4. **NCSU/BASF Poster Session (Aug 2019, Raleigh, NC)**
   Xinhao Li, Denis Fourches**.** Transfer Learning for Molecular Property/Activity Prediction. (**Poster**)
5. **Triangle Machine Learning Day (Sep 2019, Durham, NC)**
   Xinhao Li, Denis Fourches**.** Transfer Learning for Molecular Property/Activity Prediction. (**Presentation** & **Poster**)

Awards

1. **CINF Scholarship for Scientific Excellence awarded by ACS CINF (2019 Spring)**