Bowen Liu
Ph.D. Student in Chemistry, admitted Autumn 2015

Research & Scholarship

CURRENT RESEARCH AND SCHOLARLY INTERESTS
Computational drug discovery

Publications

PUBLICATIONS

- Graph Convolutional Policy Network for Goal-Directed Molecular Graph Generation
  NEURAL INFORMATION PROCESSING SYSTEMS (NIPS). 2018

- Retrosynthetic Reaction Prediction Using Neural Sequence-to-Sequence Models
  ACS CENTRAL SCIENCE
  Liu, B., Ramsundar, B., Kawthekar, P., Shi, J., Gomes, J., Quang Lau Nguyen, Ho, S., Sloane, J., Wender, P., Pande, V.
  2017; 3 (10): 1103–13

- Is Multitask Deep Learning Practical for Pharma?
  Journal of chemical information and modeling
  2017; 57 (8): 2068–76

- Lighting up sugars: fluorescent BODIPY-gluco-furanose and -septanose conjugates linked by direct B-O-C bonds
  ORGANIC & BIOMOLECULAR CHEMISTRY
  Liu, B., Novikova, N., Simpson, M. C., Timmer, M. S., Stocker, B. L., Sohnel, T., Ware, D. C., Brothers, P. J.
  2016; 14 (23): 5205-5209