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Ph.D. Student in Chemistry, admitted Autumn 2015

Research & Scholarship

CURRENT RESEARCH AND SCHOLARLY INTERESTS
Computational drug discovery

Publications

PUBLICATIONS

• Retrosynthetic Reaction Prediction Using Neural Sequence-to-Sequence Models *ACS CENTRAL SCIENCE*
  Liu, B., Ramsundar, B., Kawthekar, P., Shi, J., Gomes, J., Quang Luu 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-glucopyranose 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