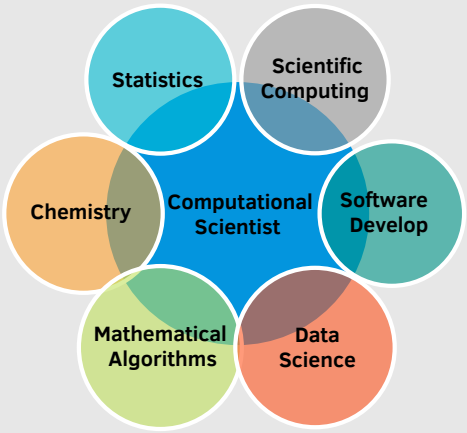
Yen Bui (Terri)

Computational Scientist

(816) 769 7048
yhb8r4@gmail.com
/in/yhbui
yhb8r4

Technical Skills

Overview



Programming

$0\ LOC \longrightarrow 5000\ LOC$

C • R • BASH • Shiny

Python • LaTeX

MySQL • Matlab • Fortran

Education

PhD, Theor. Phys. Chem. (GPA: 3.4)
Specialization: Computer Science
Purdue University
2013 - 2019 | West Lafayette, IN

BS., Chem. (GPA: 3.7)
Specialization: Chemistry
Rockhurst Universty
2009 - 2013 | Kansas City, MO

Experience

April 2019 - Present — **Sr. Scientist - PCD | Data Science & Informatics** — Merck Research Labs

- PI for collaboration between Merck and the Purdue Data Mine for full stack develop platforms for biometric and RFID platforms.
- Facilitated Merck-Data Carpentries engagement to deliver data science learning opportunities.
- Developed multiple data capture, processing, and visualization notebooks and ETL pipelines for characterization data.
- Responsible for interim digital strategy for centralization and standardization of lab data capture.
- Tools: AWS Cloud, Atlassian, JIRA, Confluence, Bitbucket, python, R programming, Shiny, Jupyter, bash, Databricks

Feb 2014 - March 2019 — **Graduate Research Assistant** — Slipchenko Research Group

- Obtained statistics and performed data analysis and visualization following large scale simulations to explain quantitative structure-activity relationships.
- Performed high performance scientific computations using various computational software packages to calculate structures and properties of molecules.
- Implemented mathematical algorithms in a portable software library called LIBEFP
- Tools: LIBEFP, VMD, Gromacs, Amber, Jupyter Notebook, RStudio, IQMol, QCHEM, GAMESS

Research Projects

Digital Sample Management RFID Lab Logistics Platform • **SFS-QR Dashboard:** 2D Barcoding System • **Merck-DC Engagement:** Learning & Development Opportunity • **MK Data Viz Tool:** Sterile Formulation Dashboard • **Merck-Purdue DataMine:** RFID & Biometrics • **SSI-EFP:** A benchmarking study using EFP, SAPT, and CCSD methods on the bFDB dataset • **EFPMD-MC:** An Implementation of the Monte Carlo Sampling Method • **P-EFP:** Extracting Pairwise Ligand-Fragment Components from Free Energies • **iSpiEFP:** A GUI and Database of EFP Parameters • **Umbrella Sampling with the EFP Method:** A Method for Decomposition of Binding Free Energies Calculations • **SMD-EFP:** A 'Steered' Study on Solvated Cation-pi Interactions • **CHARMM-LIBEFP:** Interfacting the LIBEFP API to the CHARMM Package

Presentations

2016 — **Midwest Theoretical Chemistry Conference (MTCC)** — Pittsburgh
Poster:"Bigger, Better, and Biologically Relevant: An EFP-SAPT benchmarking study on the bFDB database"

2019 — **American Chemical Society (ACS) National Meeting** — Orlando
Oral: "iSpiEFP: Automating the computational workbench"

2020 — **Joint Statistical Meetings (JSM)** — Philadelphia|Virtual
Panel: "Integrating Data Science and Statistics In Pharmaceutical Statistical Engineering and Research"

Honors | Distinctions

Merck Ways of Working • **William F. Epple Teaching Award** • **Eli Lilly Fellowship** • **Dean's Undergraduat Fellowship** • **UMKC SEARCH Grant 2012** • **Reva Servoss Chemistry Prize** • **Chancellor's Scholar** • **Dean's List (Fall 2009 - Spring 2013)** • **Regent's Scholarship**