Yuanjun (Sherlock) Shi

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Education:

Yale University	New Haven, CT
Department of Chemistry	Sept, 2020 to present
Washington University in St. Louis	St. Louis, MO
Major: Biochemistry and Psychological & Brain Sciences	Sept, 2016 to May, 2020

Minor: Computer Science

Honors:

Dean's List (2016~2019)

Experience:

Academia

Summary Research experience   St. Louis, MO

Washington University BioSURF Program   May~Aug, 2018

• Studied the binding affinities of Farnesoid X receptor (FXR)-bound ligands at Dr. Ponder's lab. Obtained the optimized structures of the ligands at the lower MP2/6-311G (1d, 1p) level using Psi4 calculations and ran calculation at the higher MP2/aug-cc-pVTZ using the optimized structures to find the electrostatic parameters for the ligands.

Washington University SURA Program   May~Aug, 2019

• Participated in running dynamic simulations to model the binding of a series of organic ammonium guests to the cucurbituril(CB)-like clip host, which is a letter "C" like acyclic molecule with three repeating units. The results were submitted to the SAMPL7 blind prediction challenge.

Undergraduate Research Symposium Poster presentation

• Presented the summary poster of the results from summer 2018 research on prediction of binding affinities for FXR ligands.   St. Louis, MO

                                                                               Nov, 2018

• Presented the summary poster of the results from summer 2019 research on binding free energy simulations for the SAMPL7 Challenge.   St. Louis, MO

                                                                               Nov, 2019

Publication

• **Shi, Y**., Laury, M. L., Wang, Z., & Ponder, J. W. (2020). AMOEBA binding free energies for the SAMPL7 TrimerTrip host–guest challenge. *Journal of Computer-Aided Molecular Design*. doi:10.1007/s10822-020-00358-2

Contestant of ICPC Mid-Central 2017 contest (International Collegiate Programming Contest)

• Participated as a team of three (team name: Tungsten) and received 37th place in the mid-central region.

                                                                               Springfield, IL
                                                                               Nov 4th, 2017

Teaching experience

TA for Computer Science I

• Helped other students, such as debugging their code and answering their questions.   St. Louis, MO

• Also improved my knowledge of computer science through teaching others.   Sept~Dec, 2017

ArchHack experience

• Developed an app that analyzed data from Apple's built-in HealthKit to form a model based on long-term regularities in the person's behavior. It visualized the data for the users and generated alerts to the person's physician when there was an emergency.

<div align="right">St. Louis, MO
Nov, 2017</div>

Work

Summer Internship at Nanjing Engineering Institute of Aircraft Systems, Jingcheng. AVIC

- Did market research and statistical analysis of data for the marketing department.   Nanjing, China
<div align="right">June~Aug, 2017</div>