Sabbatical Research:
Understanding Enzymes by Following Their Motions on a Computer

Enzymes are complex molecules and workhorses of Life. Many enzymes are drug targets, and accurate knowledge of enzymes’ structures, dynamics, and functions are needed to design and develop potent drug molecules with minimal side effects. During the one-year sabbatical leave, my research was focused on two main projects: i) understanding the role of enzyme motions in enhancing its catalytic power, and ii) investigating the role of host cell redox state on the binding of severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) to human cell surface receptor, angiotensin-converting enzyme 2. Both projects are conducted in collaboration with Dr. Hati and several undergraduate students. These studies resulted in four peer-reviewed publications.