Development of a molecular docking exercise to elucidate principles of biophysical chemistry in the general chemistry laboratory

Clare E. O'Grady, Peter Talpey, and Adam W.Van Wynsberghe

Department of Chemistry, Hamilton College, Clinton, NY 13323

Computational chemistry has recently become one of the most active fields of chemistry, now serving as an essential supplement to organic synthesis, medicinal chemistry, chromatography, and many other areas of experimental chemistry. As the use of computational chemistry becomes more prevalent, undergraduate chemistry students need to be exposed to computational chemistry methods. However, several barriers, including cost and hesitation to add a new subject to a full syllabus, have hindered the insertion of computational chemistry into the undergraduate chemistry curriculum. We have developed a molecular docking exercise, intended for the general chemistry laboratory, which aims to elucidate principles of biophysical chemistry. This open-ended exploratory computational exercise will allow general chemistry students to explore the binding energies and interactions of hormones and hormones-mimics with their receptors, as well as design and test their own drug molecule with several receptors using software such as PyRx, VMD, and PRODRG. The exercise will utilize programs that are both easily accessible and inexpensive and will complement the students' previous knowledge as well as provide them with an introduction to both computational chemistry as well as some biomolecular, physical, and organic chemistry concepts.