

Siemens Competition

Math : Science : Technology

Regional Finalist

Names: Napasorn Kuprasertkul, Sumedha Mehta, Akash Wadawadigi

High School: Texas Academy of Math and Science

Mentor: Dr. William Acree

Project Title: *A Novel Methodology to Mimic Biological Properties using Ionic Liquids: An Extensive in Silico Study* (Biochemistry; Mathematics; Toxicology)

Chemistry-driven in silico methods were used to construct a methodology to elucidate ionic liquids (ILs) that simulate various biological barriers, using a predictive model known as the Abraham solvation parameter model. A PCA (principal component analysis) was performed on experimental data gathered from previous literature containing log P Abraham coefficient correlations of 673 ILs and 29 biological systems. The resulting scatter plot indicated which ILs had the most potential to successfully replace these systems during testing. The liquid, 1-(2-hydroxyethyl)-3-methylimidazolium tris(pentafluoroethyl)trifluorophosphate ([EtOHMIm]⁺[FAP]⁻) was found to simulate several partitioning systems in the human body. We formulated linear equations using log P values of [EtOHMIm]⁺[FAP]⁻ and barriers including the blood-brain, blood-liver, and blood-fat. It was found that the trio could be effectively mimicked by [EtOHMIm]⁺[FAP]⁻. The procedure was rerun for aquatic organisms to produce IL mimics for *Daphnia pulex*, *Carassius auratus*, and *Lepomis macrochirus*, proving our mechanism's versatility. Statistical analysis, employing test and training methods, produced standard deviation (SD), absolute average error (AAE) and average error (AE) values. Overall, this study resulted in computational data that could be further utilized to reduce the millions of dollars allocated to experimental biological testing, particularly drug testing, conducted on animals and humans.