Abstract

Understanding PFAS toxicity for Great Lakes fish: A computational approach

Nuno M.S. Almeida, Semiha Kevser Bali, Kyleen Hall, Rana Massoud, and Angela K. Wilson

Michigan State University, Department of Chemistry, East Lansing, MI 48864, U.S.A

Per- and polyfluoroalkyl substances (PFAS) are a family of compounds that are persistently among us in applications that range from firefight foam (AFFFs), to cookware, clothing, and even dental floss. Recently, PFAS have been implicated in multiple diseases by over activating or inhibiting protein functions, which can have atrocious impacts. On the human side there is more prevalent knowledge on how these chemicals affect different proteins and their up and downstream effects, however, in fish PFAS effects are not well known. In the Great Lakes, PFAS pollution has reached concerning levels, with the aquatic life impacted greatly. In this study, the binding of PFAS to fish proteins was studied through molecular dynamics (MD) simulations. The effects of the fluorinated carbon chain length and the functional group of PFAS were investigated. This work will help mitigating PFAS in fish and provide highly beneficial insight to the Great Lakes ecosystem.