



Jesús Israel Espinoza Castañeda graduated from the Autonomous University of Hidalgo in 2023, where he conducted research on the activation of metallic catalysts using Density Functional Theory (DFT) calculations. He is currently pursuing a Master's degree in Chemical Sciences at the Department of Pharmacy, National Autonomous University of Mexico (UNAM), and has been part of the DIFACQUIM Research Group since January 2024. As part of his Master's project, he is developing an open-source tool to automate the analysis of multiple structure-activity relationships. His research aims to streamline and enhance the efficiency of drug discovery processes by automating the analysis of structure-activity relationships.

Scientific interests: Chemoinformatics, drug discovery, software development, machine learning