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Her research focuses on the analysis and representation of chemical and bioactivity data, molecular modeling, and the development of predictive approaches for bioactive molecules. A central theme of her current work is understanding how molecular representation, data quality, and experimental context shape chemical and predictive spaces, with particular interest in bioactivity modeling and structure–property relationships. Her research has applications in food, pharmaceutical, and agrochemical sciences, as well as in the development of computational methodologies.

She has authored more than 100 scientific publications and book chapters and is the editor of the book *FoodInformatics*. She is currently Editor-in-Chief of the *Journal of Cheminformatics* and has been awarded one of Mexico's highest national recognitions for scientific achievement, Level III of the National System of Researchers (SNII).