[S. Naik, V. Krajnák, and S. Wiggins. Support vector machines for learning reactive islands. Chaos: An Interdisciplinary Journal of Nonlinear Science, 31(10):103101, October 2021.](https://doi.org/10.1063/5.0062437)

We developed a machine learning approach based on trajectory data to discover structures in the phase space of a chemical reaction. We also verified the predictions of the learned model by comparing it with the results from dynamical systems analysis for a classical Hamiltonian. These structures, reactive islands, are pertinent for computing and understanding the structure of reactive and non-reactive trajectories and can be used to improve transition path sampling methods. Thus, this work presents a machine learning approach that leverages the phase space viewpoint of chemical reactions.