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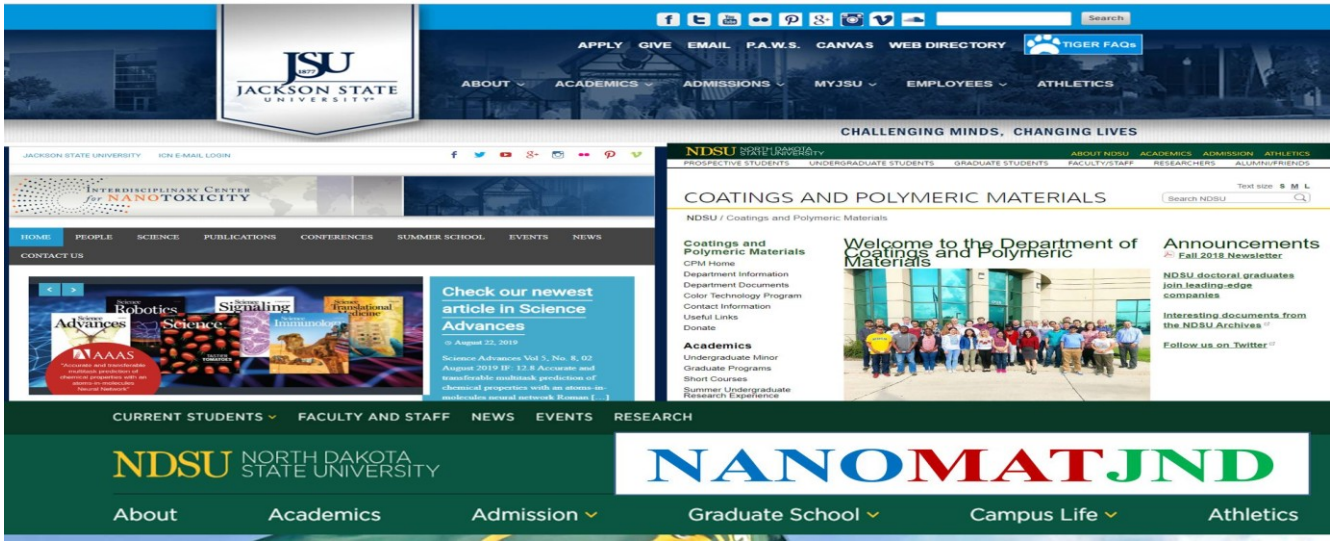

Predicting nanoparticles vs. bacteria with topological changes on metabolic networks

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Abstract

Nanoparticles may have anti-bacterial activity so they become interesting alternatives to drugs in a context of emergence of resistant bacteria. These bacteria have different metabolic networks. In a recent work we developed a information fusion perturbation-theory machine learning (IFPTML) model to predicting nanoparticles vs. bacteria with topological changes on metabolic networks. The dataset studied had 15 classes of nanoparticles (1-100 nm) with most cases in the range of 1-50 nm vs. >20 pathogenic bacteria species with different metabolic networks. The nanoparticles studied included metal nanoparticles of Au, Ag, and Cu; oxide nanoparticles of Zn, Cu, La, Al, Fe, Sn, Ti, Cd, and Si; and metal salt nanoparticles of CuI and CdS. We used the SOFT.PTML software (our own application) with a user-friendly interface for the IFPTML calculations and a control statistics package. Using SOFT.PTML, we found a random forest model with Sn and Sp = 98-99% in the training/validation series.

Ref: B. Ortega-Tenezaca, H. González-Díaz. IFPTML mapping of nanoparticle antibacterial activity vs. pathogen metabolic networks. Nanoscale 2021 Jan 7. doi: 10.1039/d0nr07588d.