

Machine Learning Study of Metabolic Networks vs ChEMBL Data of Antibacterial Compounds

[Machine Learning Study of Metabolic Networks vs ChEMBL Data of Antibacterial Compounds - PubMed \(nih.gov\)](https://pubmed.ncbi.nlm.nih.gov/35671399/)

The screenshot shows a web browser displaying a PubMed article. The browser's address bar shows the URL: <https://pubmed.ncbi.nlm.nih.gov/35671399/>. The article title is "Machine Learning Study of Metabolic Networks vs ChEMBL Data of Antibacterial Compounds". The authors listed are Karel Diéguez-Santana, Gerardo M Casa-Rola-Martin, Roldan Torres, Bakhtiyor Rasulev, James R Green, and Humbert González-Díaz. The article is dated July 4, 2022, with a DOI of 10.1021/acs.molpharmaceut.2c00029. The abstract discusses the use of machine learning (ML) to predict antibacterial compounds based on metabolic network (MN) mutations and the interaction of AD vs MN. It mentions the use of the IPFTML (Information Fusion + Perturbation Theory) + Machine Learning (ML) algorithm on a dataset of 155,000 AD assays vs >40 MNs of multiple bacteria species. The abstract also mentions the use of linear discriminant analysis (LDA) and 17 ML models centered on the linear index and based on atoms to predict antibacterial compounds. The IPFTML-LDA model presented the following results for the training subset: specificity (Sp) = 76% out of 710,000 cases, sensitivity (Sn) = 70%, and Accuracy (Acc) = 73%. The same model also presented the following results for the validation subsets: Sp = 76%, Sn = 70%, and Acc = 73.1%. Among the IPFTML nonlinear models, the k nearest neighbors (KNN) showed the best results with Sn = 99.2%, Sp = 95.5%, Acc = 97.4%, and Area Under Receiver Operating Characteristic (AUROC) = 0.998 in training sets. In the validation series, the Random Forest had the best results: Sn = 93.96% and Sp = 87.02% (AUROC = 0.945). The IPFTML linear and nonlinear models regarding the ADs vs MNs have good statistical parameters, and they could contribute toward finding new metabolic mutations in antibiotic resistance and reducing time/costs in antibacterial drug research. The keywords are ChEMBL; antibacterial compounds; complex networks; information fusion; machine learning; multidrug-resistant; perturbation theory. The publication type is "Research Support, Non-U.S. Gov't". The browser's taskbar at the bottom shows the date and time as 10:18 a.m. on 14/07/2022, and the temperature as 21°C in Soleado.