

POSTER PRESENTATION

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Learning antibacterial activity against *S. Aureus* on the Chimiothèque Nationale dataset

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“Chimiothèque Nationale” (CN) represents a library of synthetic and natural products from various French public laboratories. Recently, experimental screening for *S. Aureus* antibacterial activity of the part of this library has been performed by Dr J.-M. Paris and collaborators in Ecole des Mines (Paris, France). Here, experimental results of the screening have been used to build classification models using SMF descriptors and ISIDA modeling tools (Naïve Bayes (NB) and SVM modules). The dataset consisted in a large and structurally diverse set of 4563 compounds, 62 of which having a demonstrated antibacterial activity. In NB calculations, several variations of the algorithm were used. In particular, the *a priori* distribution of SMF descriptors was modeled using a binomial law, Bernoulli distributions or first order logic. SVM calculations were performed with an RBF kernel which parameters (C, γ) were optimized to maximize the balanced accuracy.

Both NB and SVM models were validated using external 5-fold cross validation, repeated three times on randomized data set. Additionally fifteen Y-randomizations were performed in order to check for chance correlation. Predictive performance of the models has been assessed by combination of *Precision* and *Recall* parameters: the models with *Precision* > 0.1 and *Recall* > 0.6 correspond to over 10-fold enrichment and, therefore, were considered as acceptable.

A consensus model was applied to estimate the antibacterial activity of 122 new compounds for the CN. All predictions were done blindly.

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