NL MIND-BEST: AWEB SERVER FOR LIGANDS & PROTEINS DISCOVERY; THEORETIC-EXPERIMENTAL STUDY OF PROTEINS OF GIARDIA LAMBLIA

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There are many protein ligands and/or drugs described with very different affinity to a large number of target proteins or receptors. In this work, we selected Ligands or Drug-Target pairs (DTPs/nDTPs) of drugs with high affinity/non-affinity for different targets. Quantitative Structure-Activity Relationships (QSAR) models become a very useful tool in this context to substantially reduce time and resources consuming experiments. Unfortunately, most QSAR models predict activity against only one protein target and/or have not been implemented in the form of public web-server freely accessible online to the scientific community.To solve this problem, we developed a multi-target QSAR classifier using the MARCH-INSIDE technique to calculate structural parameters of drug and target plus one Artificial Neuronal Network (ANN) to seek the model.The best ANN model found is a Multi-Layer Perceptron (MLP) with profile MLP 20:20-15-1:1. This MLP classifies correctly 611 out of 678 DTPs (Sensitivity = 90.12%) and 3083 out of 3408 nDTPs (Specificity = 90.46%), corresponding to training Accuracy = 90.41%. The validation of the model was carried out by means of external predicting series. The model classifies correctly 310 out of 338 DTPs (Sensitivity = 91.72%) and 1527 out of 1674 nDTP (Specificity = 91.22%) in validation series, corresponding to total Accuracy = 91.30% for validation series (Predictability).We implemented the present model at web portal Bio-AIMS in the form of an online server called: **N**on-**L**inear **MARCH-INSIDE** **N**ested **D**rug-**B**ank **E**xploration & **S**creening **T**ool (**NL MIND-BEST**); which is located at URL: http://miaja.tic.udc.es/Bio-AIMS/NL-MIND-BEST.php. Finally, we illustrated the practical use of this server with one experiment. First, we report sampling, sample preparation, 2-DE, MALDI-TOF and -TOF/TOF MS, MASCOT search, MM/MD 3D structure modeling, and **NL MIND-BEST** prediction for different peptides of a new protein found in the proteome of the human parasite *Giardia,* which is promising for anti-parasite drug targets discovery.