An Artificial Neural Network Approach to Pre-screening of Large Chemical Datasets

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In this work we propose the use of artificial neural networks to predict the binding affinities of the compounds in a chemical database to a given receptor as a means to reduce the number of compounds before the docking step in the virtual screening pipeline. The neural networks are trained from nine parameters (molecular weight, octanol/water partition coefficient, etc.) describing compounds in a randomly chosen subset and the binding affinities of these compounds which have been previously computed with DOCK. The trained neural networks are then used to compute the binding energies of the remaining compounds in the database. This enables us to select an enriched subset of compounds for further screening at virtually no cost. Three different drug targets and ZINC compound database were used as the test system. The results show considerable improvement as compared to random screening with good accuracy.