Deep Belief Networks for Ligand-Based Virtual Screening of Drug Design(2016 6th International Workshop on Computer Science and Engineering (WCSE 2016)

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ABSTRACT
Virtual screening (VS) is a computational technique used in drug discovery. Virtual Screening process usually works by identifying structures that are most likely to bind the target of drug. Virtual screening is usually based on compound similarity or database docking. Thus, the identification for drug compounds based on structure classification still remain as a challenging task. The purpose of this research is to find a new approach for ligand-based virtual screening using machine learning technique. In this paper, the
classification has been done by using Deep Belief Networks (DBN) method. The data from Nicotinamide Adenine Dinucleotide (NAD) protein target family were used for training and testing the model. This research used four protein target classes from literature and two protein target classes from DUD-E docking website. Feature were obtained from molecular fingerprint descriptor. The experiments result show that DBN method outperform the existing pharmacophore approach.