Development of a Drug-Likeness Rule for Natural Products

Ahmed, Saadh (School: Northview High School)

Development of a Drug-likeness Rule for Natural Products Saadh Ahmed Northview High School, Johns Creek , GA, USA In the field of drug discovery, the first steps are crucial to the overall success of developing a marketable drug. Due to this, measures are taken to ensure that only compounds with the highest probability of being drug-like are selected to be taken into the next stages of drug development. During these phases, drug-likeness filters are used to reduce collections of compounds to only those that have the highest drug-like potential. However, it is during these stages that many compounds with excellent capacity of drug-likeness are overlooked. Natural products are often victims of initial screens as they tend to break these established rules, but hold considerable drug-like effects. To combat this issue, this research proposes a new series drug-likeness rules called the Natural Product Drug-likeness Rules. These rules were developed after analysis of a database that contains only drug-like natural compounds. 70 properties for each of the compounds were evaluated for patterns and commonalities within the database. Out of these 70 properties, 5 independent properties were selected for them being shared among 76% of the entire database and compiled into a new rule called the Primary NPDR. Two other variations of Natural Product Drug-likeness Rules were also created and successfully demonstrated high accuracy in drug-like compound selection. The Natural Product Drug-likeness Rules combine quantitative and qualitative screening techniques. These new rules outperform the most common drug-likeness rules when employed against natural products. The Natural Product Drug-likeness Rules have potential to open new opportunities for drug discovery of natural compounds.

Awards Won:
Second Award of $2,000
National Institute on Drug Abuse, National Institutes of Health &amp the Friends of NIDA: Third Award of $1,000