Molecular graphs and drug discovery

Purpose: To develop and study molecular graphs for drug discovery.(see [1]).

Background: There are diseases or applications in biology which need a particular molecular.This can be possible with the help of machine learning and graph theory. We can model the huge molecular structures as graphs and with machine learning find similarities among the molecules.

Hypothesis: I have the necessary skills for this project and there are ways to improve these machine learning models and molecular graphs.

Research Plan: Machine learning with larger datasets is possible with the help of new software tools for dealing large datasets and improvement in processing power.
Aim 1 Model the molecule as graphs.
Aim 2 Using machine learning to find similarities between the of molecules and their graph structure.

Intellectual Merit: I'm a masters student from IISc Bangalore. I am doing masters in Computational and Data Sciences from CDS, IISc Bangalore. I am currently working in Bioinformatics Lab under the supervision of Dr.Debnath Pal.

Broader Impacts: This can be used to discover new molecules' properties and their functions.

References

[1] Duvenaud, D. K., Maclaurin, D., Iparraguirre, J., Bombarell, R., Hirzel, T., Aspuru-Guzik, A., & Adams, R. P. (2015). Convolutional networks on graphs for learning molecular fingerprints. In Advances in neural information processing systems (pp. 2224-2232). .