Grant Proposal

Name: Pathapati Abhishek

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Grant Title: To develop and study molecular graphs for drug discovery

Amount Requested: Two lakh and fifty thousand rupees (Rs 1,50,000)

Proposed Start Date: July 14, 2018

Duration: 2018/2019 Academic Year

1) Executive Summary

Purpose: To develop and study molecular graphs for drug discovery
Hypothesis: I have the necessary skills for this project and there are ways to improve these machine learning models and molecular graphs.
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

Background of the Project

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.

There are new drugs produced that are killing people and we don't the components in those drugs. It is like searching a needle in a haystack. But if we know what these drugs do we reverse engineer to find what these drugs' structure and be able to find an antidote. And save people from these deadly drugs.

With the help of machine learning and decrease in the cost of computing it is possible to combat these drugs with these modern tools.

3) Detailed Description of the Initiative

a) Project Theory

Goal of the Project	Project Activity	Expected Outcome or Impact
Goal #1: Build a the model that for molecular graphs	*a)* Implement the base line machine learning model *b)* Collect molecules and their properties i.e. build the dataset	Outcome is to understand the model and the properties of the molecule
Goal #2: Implemented proposed model is tested on different test cases	Implement collected datasets.	This should learn to identity properties of molecules from its molecular graph
Goal #3: Collecting more datasets and training the model for better outcomes	*a) Collecting more datasets and evaluating each output.*	Compare the model against the baseline on different datasets

b) Implementation Timeline

Goal	July	Aug.	Sept.	Oct.	Nov.	Dec.	Jan.	Feb.	March	April	May	June
#1	1a: Building A Model For Molecular Graphs		1b) Implement base line model									
#2							Implement machine learning model					
#3						3a: Evaluation			3a: Evaluation			
			Test it on different datasets and measure it against benchmark									

c) Budget

Budget Item	Sub-Total	Total Cost
Computing System	25000X2 i7 processor	50000
Harddisk	5000 X4 1Tb	20000
NvidiA GeForce GTX	80000X1 GPU	80000
Total Budget:		150000

4) Team

Name : Pathapati Abhishek
Qualification : M.Tech 1st year student
Experience : Machine Learning

5) Other Sources of Funding

We would also like to acknowledge the support from MHRD for the contingency and other resources necessary for the smooth delivery of the project.