

# **KWOC – KHARAGPUR WINTER OF CODE**

A month long programme for introduction to open source community and providing a preface to budding developers to Google Summer Of Code 2018. Organized by students at Kharagpur Open Source Society (KOSS), IIT KHARAGPUR.

## **Participant Information**

My name is Shubham Gautam, currently studying Computer Science (2<sup>nd</sup> year) under the Dual Degree Programme at IIT KHARAGPUR.

## **Project Information**

**DEEPCHEM** (Mentored by Avijit Ghosh)

The project involved using Deep Learning to predict properties of Chemicals from their 3D structures.

The objective was to predict the properties of compounds using only the 3D structures. The property that was chosen for the project was Solubility of a compound.

The initial problem of the project was to create an extensive database of compounds, large enough to weed out any discrepancies. A database of around 4000 compounds was chosen, involving their name, formula, mol. weight, solubility and 3D structures.

Instead of manually copying each data element, code was used to create the database of 4000 compounds. Similarly the SDF files for the 3D structures were also fetched using code from the NIST database.

The second phase involved literature review and using the 3D structures to predict solubility by building a Deep neural network. Since my main programming languages are C and Java, and I got introduced to Deep learning through this project, my contribution to this project was limited and still under progress. The project is currently under heavy development.

Thanks to the people at Kharagpur Open Source Society for this opportunity and introducing me to the open source community, which was a great prep for GSoC.