INDRAPRASTHA INSTITUTE *of* INFORMATION TECHNOLOGY **DELHI**

Invitation to M.Tech. Thesis Defense of Aditi Sharma: July 26, 2019 (Friday): 16.00-17.00 IST

In Partial Fulfillment of the Requirements for the Degree of
M.Tech CB

Aditi Sharma (MT17142)

Will defend her thesis

Title: "Prediction of sweetness using machine learning models"

IIIT-D Faculty and Students are invited

Date: July 26, 2019 (Friday)
Time: 16.00 – 17.00 IST
Place: CB Meeting Room (3rd Floor, R&D Building)

Examiner: **Internal:** **Vibhor Kumar**
 External/Internal: **GPS Raghava**
 Advisor: **Ganesh Bagler**

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Abstract

Taste percepts of small molecules are the emergent properties resulting out of their interaction with the gustatory receptors. In this thesis, we aim to investigate the sweetness of small molecules to correlate it with their molecular features and probe their interaction sweet receptors. We compiled a list of 647 manually curated molecules along with their experimentally reported sweetness. This dataset comprised of structurally diverse compounds with molecular weight ranging from 122.14 to 1287.62 Daltons and relative sweetness varying between 1 to $〚10〛^7$. Given the wide difference in relative sweetness, the prediction of sweetness based on their molecular features has been a longstanding challenge. We implemented regression models using Support Vector Regression, Random Forest and Decision Trees toward prediction of sweetness. We also modelled the structure of human sweet taste receptor (hSTR) structure to perform docking studies with sweet and bitter ligands.