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

10 YEARS *of* EXCELLENCE

Invitation to M.Tech. Thesis Defense of Shubhra Agrawal: May 21, 2020 (Thursday): 11.00-12.00 IST

In Partial Fulfillment of the Requirements for the Degree of

M.Tech. CB

Shubhra Agrawal (MT16128)

Will defend her thesis

Title: "Tandem Mass Spectrometry workflow in El-MAVEN"

IIIT-D Faculty and Students are invited

Date: May 21, 2020 (Thursday)
Time: 11.00-12.00 IST
Place: Online (Google Meet)

Examiner:	**Internal:**	**Debarka Sengupta**
	External/Internal:	**Vibhor Kumar**
	Advisor:	**Ganesh Bagler(IIITD), Abhishek Jha (Elucidata)**

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Abstract

"Metabolomics, defined as the study of an organism's entire metabolic profile, is a direct read-out of the physiological changes at the cellular level and has the potential to positively inform drug-target discovery and biomarker identification. Mass Spectrometry is one of the most popular techniques used to measure the levels of metabolites present in biological samples. Tandem Mass Spectrometry, and more commonly, Data Dependent Acquisition (DDA) has become a trusted technique for metabolite identification and quantification due to its dependence on spectral pattern matching with existing libraries. Since existing mass spectrometry data processing tools are either vendor-specific or difficult to use, the DDA workflow has been added to El-MAVEN, an open-source mass spectrometry data processing tool, maintained by Elucidata. Spectral matching capabilities have been added as part of the targeted DDA workflow and algorithmic improvements have been made to the untargeted workflow for optimum results. Additional widgets and features have been added for a better user experience in data curation. The improvements have been validated against known standards using datasets obtained from Elucidata's partner labs."