Big data approach to predict chemical toxicity

The aim of the project is to develop a data-driven approach to predict successes and failures of clinical trials. Drug toxicity in humans is a major problem. Some promising small molecules that would efficiently kill tumor cells are frequently not able to get FDA approval or must be withdrawn from the market after approval due to severe toxicities.

Project includes:

> Application of machine learning, pharmacophore techniques for elucidation of structural features responsible for particular toxicity, drug network connectivity analysis, validation using molecular docking, exploring probable fragment- protein interaction.