Toxicity prediction model

-Topia Technologies

Goal

- To predict the toxicity of the novel molecules well in advance.
- Raise the warning before molecules are synthesized in laboratory.
- Give the analytical view of the critical organ based toxicity.
- Using the public and commercial data efficiently to predict the toxicity.

Screening the novel molecules

- For novel molecules limited information is available.
- With the help of model we have predicted the biological activity (IC50) value of the molecule.
- Furthermore, we can calculate the chemical properties using the descriptors/fingerprints, with the help of packages available in python.

List of toxicities screened

1. Carcinogenicity
2. Cardiotoxicity
3. Hepatotoxicity
4. Mutagenicity
5. Neurotoxicity
6. Nephrotoxicity

Data collection

- For Mutagenicity (Ames test), Carcinogenicity and Cardiotoxicity
  - From DataBank, commercial access of qualitative data
- For Hepatotoxicity, the data was considered from DILIst
- For neurotoxicity multiple parameters were considered for target including BBB, Amyloid Beta and AChE.
- For Nephrotoxicity the data from interleukin-8, SIDER and literature was combined

Results

1. Ames test (Mutagenicity) - 93.4%
2. Hepatotoxicity - 79.21%
3. Neurotoxicity - 81%
4. Nephrotoxicity - 85%
5. Carcinogenicity - 87.22%
6. Cardiotoxicity - 91.83% (Herg data)

Additional Information

- Prediction model for
- CYP450 enzyme
- synthesis accessibility score (SAS)
- Docking
- Tentative LD50