Protein Interactions: Computational Techniques

Assignment 1   (10 marks)

Submission date 30 sept 2024

- Select disease

- Identify target protein/enzyme in that disease pathway that can be inhibited

- From literature find 10 drugs or ligands reported to inhibit that target

- Calculate various descriptors for these drugs (use CHEMDES)

- Develop QSAR-regression 1 parameter or/and 2 parameters models

- Divide the data into training and validation set and check all the statistics

- Determine the ADME properties of these drugs you selected (SWISS ADME , pkCSM)

- Prepare a report with introduction /methodology / .Results /discussions/Conclusion