International Conference on Innovations in Pharmacy and Biotechnology (ICIPB – 2022)
27th March, 2022, Vijayawada, Andhra Pradesh, India

CERTIFICATE NO : ICIPB /2022/ C0322302

SCREENING OF ACTIVE COMPOUNDS THROUGH BIOINFORMATICS SOFTWARE'S FOR ADME AND SOLUBILITY PROPERTIES.

Shivangi Gupta, Harmanpreet Meehnian

M. Tech, Department of Biotechnology,
Noida Institute of Engineering and Technology, Gr. Noida, (U.P)

ABSTRACT

Pharmaceutical industries face lots of issues due to its high cost and time taking process and chances of failure of drug is also high. By which for new drug discovery or novel discovery it takes long time and if it fails all money all process will waste. So, if we use bioinformatics it speeds up drug discovery process and we can analyse lot of compounds by using various software's at once it reduces time and cost. Log P, a well-known metric for evaluating a chemical compound's lipophilicity, was used in this research which is an important factor in lipnski rule of 5. Various software's use to mining the existing data for refine analysis. Active compounds, these are biologically active and already discovered compounds and present in databases having druglike properties but we don't know about its solubility or dissolution rate and pharmacological response. It is a major factor which is responsible for drug failure. So, we screened compounds by various software's, like ALOGPS 2.1 software for checking solubility of active compounds and then did statistical analysis of prediction value of active compound by discovery studio 2.1 software.

Keywords: Solubility, Drug Development, ADME Properties.