CM5239 Tutorial 3 – Molecular Descriptors and Lipinski's Rule

Below is a list of 30 essential drugs published by the World Health Organization (WHO). In this exercise, we would like to find out whether these drugs follow the Lipinski's rule of orally active drug (i.e., a molecule with a molecular mass less than 500 Da, no more than 5 hydrogen bond donors, no more than 10 hydrogen bond acceptors, and an octanol–water partition coefficient log P not greater than 5). We are going to use the DrugBank database to obtain the relevant descriptors' information (i.e., molar mass, numbers of hydrogen donors and hydrogen acceptors and log P value).

bupivacaine	amitriptyline	phenytoin
ketamine	cyclizine	diazepam
atropine	dexamethasone	phenobarbital
ephedrine	diazepam	albendazole
acetylsalicylic acid	fluoxetine	diethylcarbamazine
ibuprofen	metoclopramide	haloperidol
paracetamol	dexamethasone	spectinomycin
fentanyl	epinephrine	amikacin
morphine	hydrocortisone	amoxicillin
midazolam	carbamazepine	benzylpenicillin

The DrugBank database is a comprehensive, freely accessible, online database containing information on drugs & drug targets. As both a bioinformatics and a cheminformatics resource, DrugBank combines detailed drug (i.e., chemical, pharmacological and pharmaceutical) data with comprehensive drug target (i.e., sequence, structure, and pathway) information. The DrugBank Online website (https://go.drugbank.com/) is available to the public as a free-to-access resource. The latest release of the database (version 5.1.11, 3/1/2024) contains 16,579 drug entries including 2,766 approved small molecule drugs, 1,618 approved biologics (proteins, peptides, vaccines, and allergenics), 1345nutraceuticals and over 6,723 experimental (discovery-phase) drugs.

Tabulate the descriptors' details of the 30 drug molecules in an Excel file. Determine the percentage of compounds follows the Lipinski's rule of five. Plot the distribution of the descriptor values for all four types of molecular descriptors.