

Supplementary Data



Figure S1: The "proteinClass" node (in yellow) Serine protease is a level 1 protein class, and the node Protease is a level 2 protein class for the "UniprotInter" node Serine protease hepsin (colored in blue). They are linked by a relationship *memberOf* which indicates their belonging to a specific family.

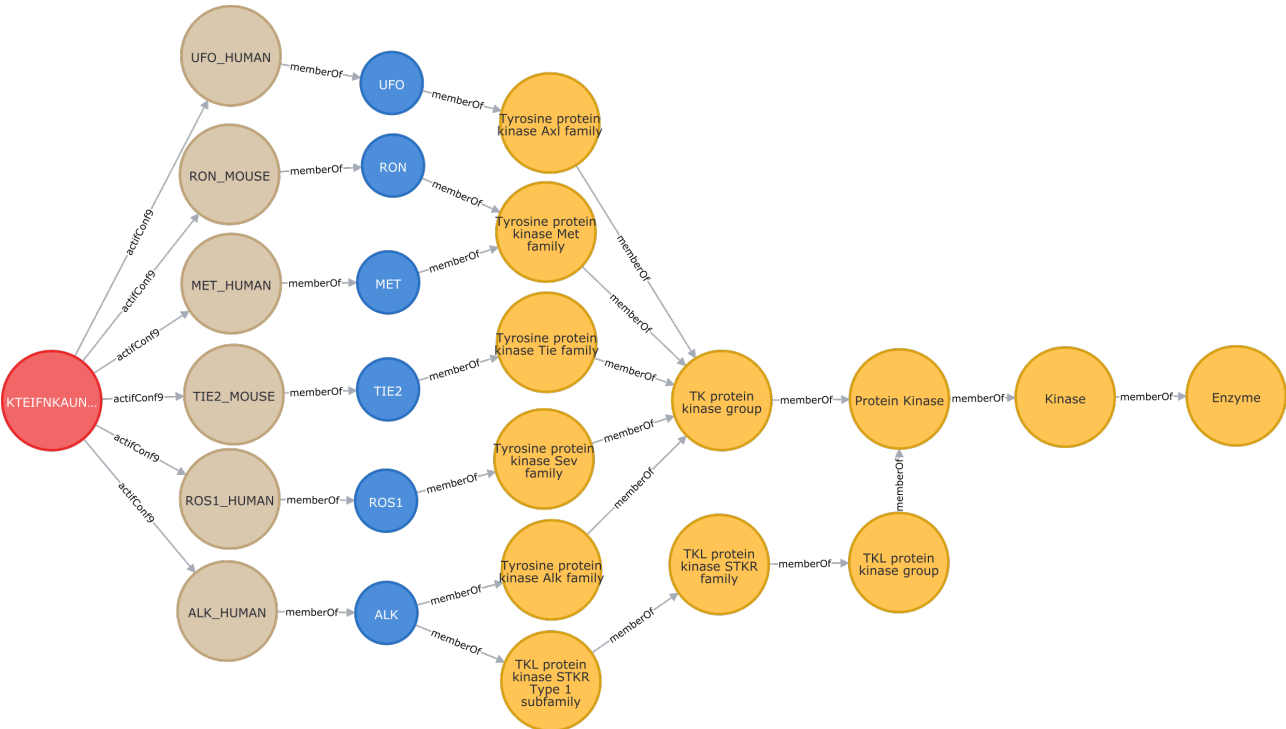


Figure S2: Example of network representation with crizotinib. 1 molecule, multiple targets hit in multiple protein classes in one main family.

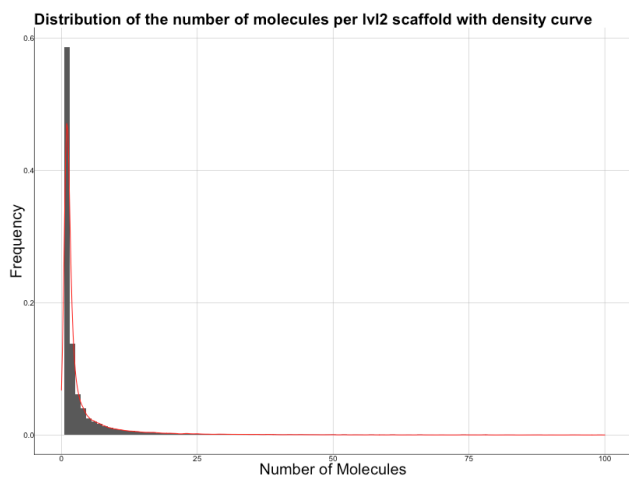


Figure S3: Repartition of the number of targets for each scaffold, with the repartition curve in red.

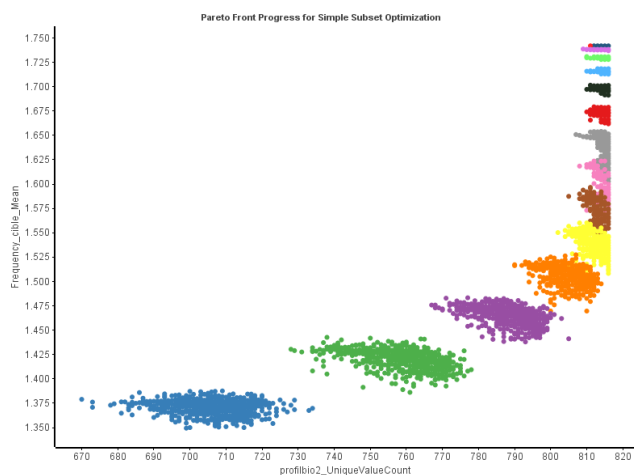


Figure S4: Overview of the 43th pareto front selection between the maximization of the different biological profiles (x axis) and the average number of times a UI is hit (y axis). Each iteration is of a different colour, each point equal 1 out of the 5000 molecules.

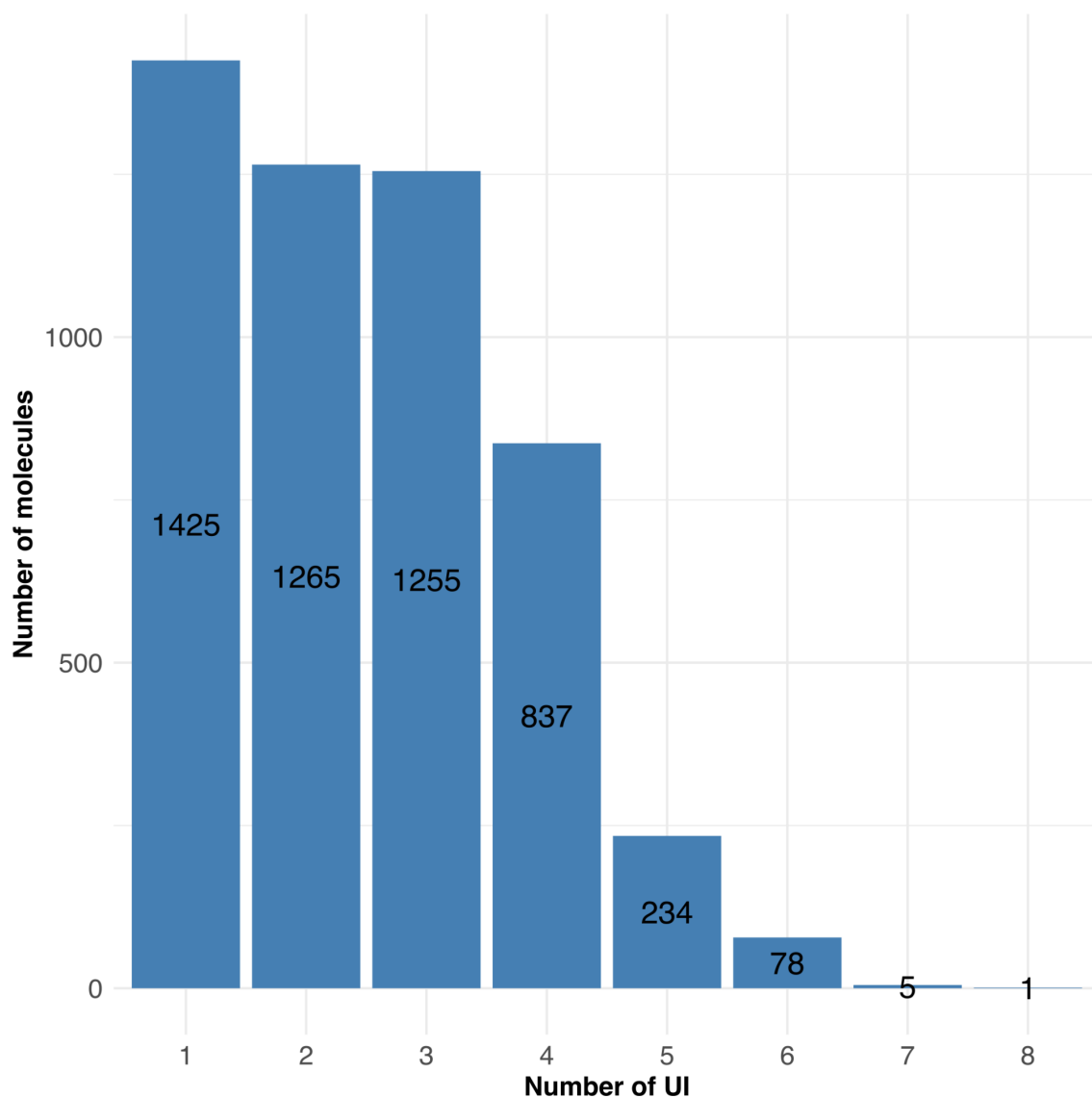


Figure S5: Bar chart of the number of UI targeted by the final selection of molecules