The Library

The Ocular Disease Library is held by ChemDiv, the leader in solutions for drug discovery. Founded by Dr. Alexander Ivashchenko in 1990, the company works with discovery of new drugs, drug candidates and leads for a range of specialities, like oncology, virology, immunology and cardiometabolic.

The library have over 13.000 compounds with 7 targets and 4 ocular diseases:

Age-Related Macular Degeneration (AMD) - Targets: Etinol-binding Protein 4 (RBP4), Factor D and VEGF pathway

Diabetic Macular Edema (DME) - Targets: Vascular Adhesion Protein-1 (VAP-1)

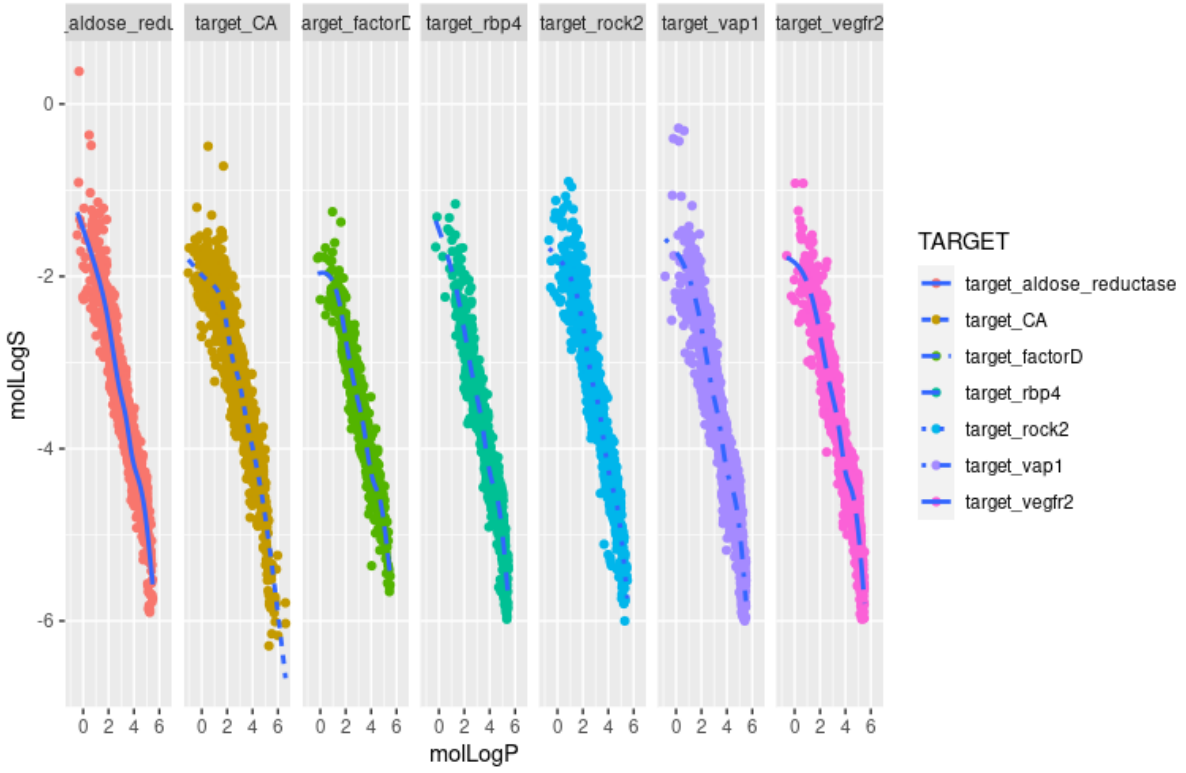
Cataract - Targets: Aldose Reductase

Glaucoma - Targets: Carbonic Anhydrase (CA) and ROCK II

Absorption

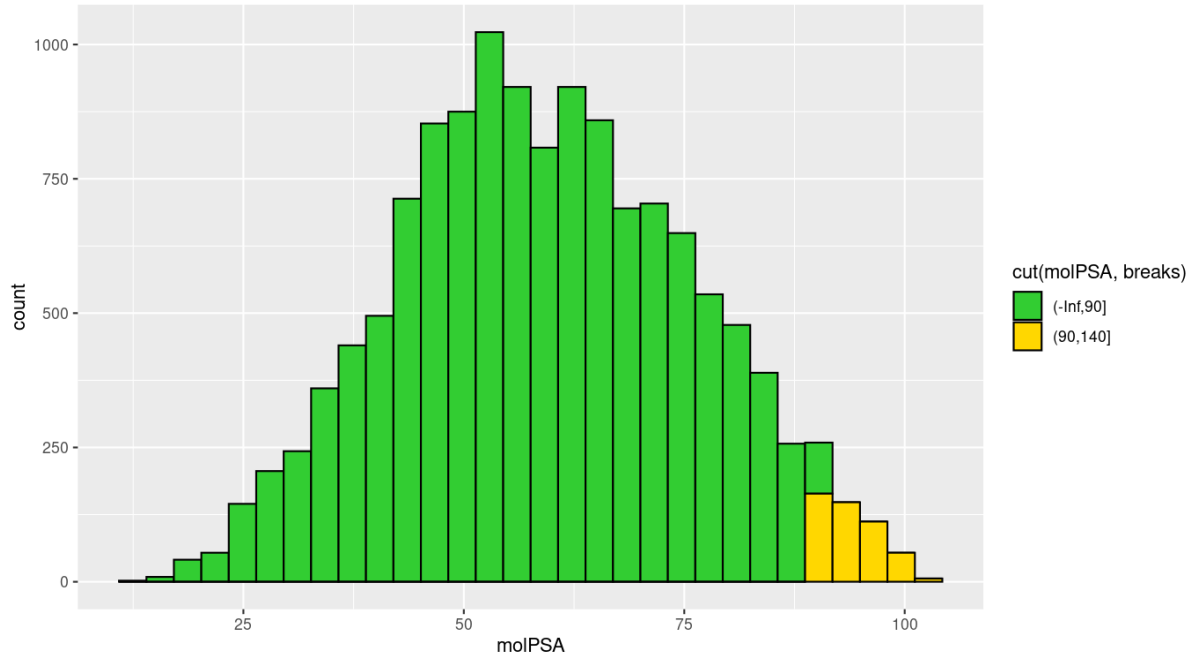
Mol Log P defines how easier the molecule is going to be absorbed by the membranes, with that said, bigger the log P, bigger the absorption.

The Log S is the solubility in water, to be effective, the medicine can't be too polar, in that case would be necessary a transporter protein to be absorbed. The graphic below shows when LogP grows the LogS goes down because higher the LogP, lowest its solubility.

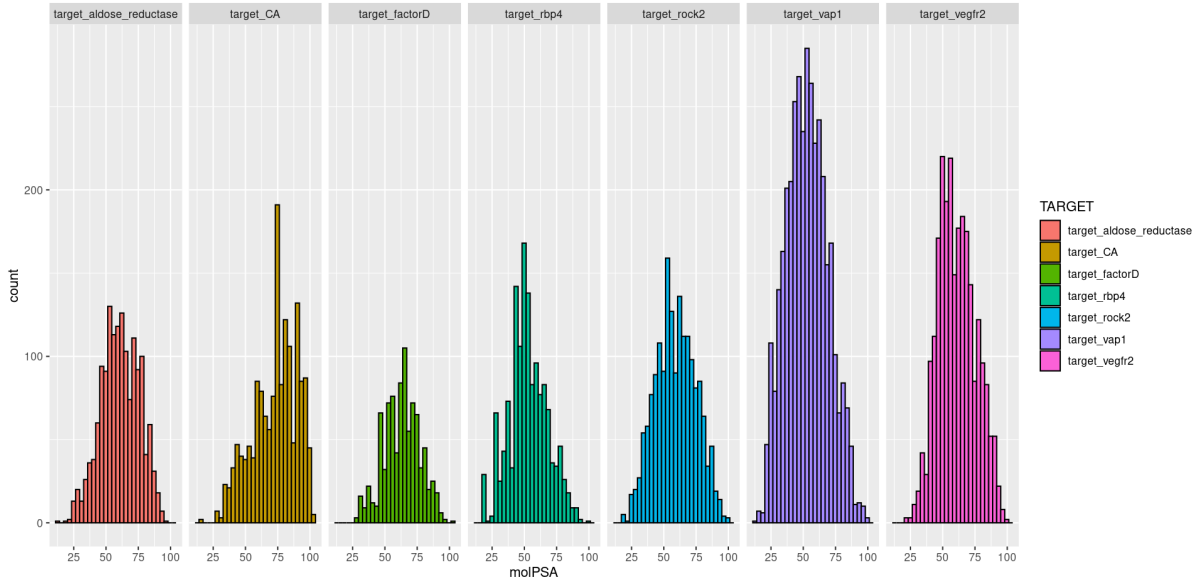


In the graphic we can notice that the points are grouped together with some outliers. But the graphic confirms that when Log P grows (less soluble) the Log S goes down (less soluble either).

The Polar Surface Area, this, like the Log S, has to be smaller to be well absorbed. For pharmacology the ideal is under 90 A². The graphics show there are few compounds over 90, so these molecules should be well absorbed.



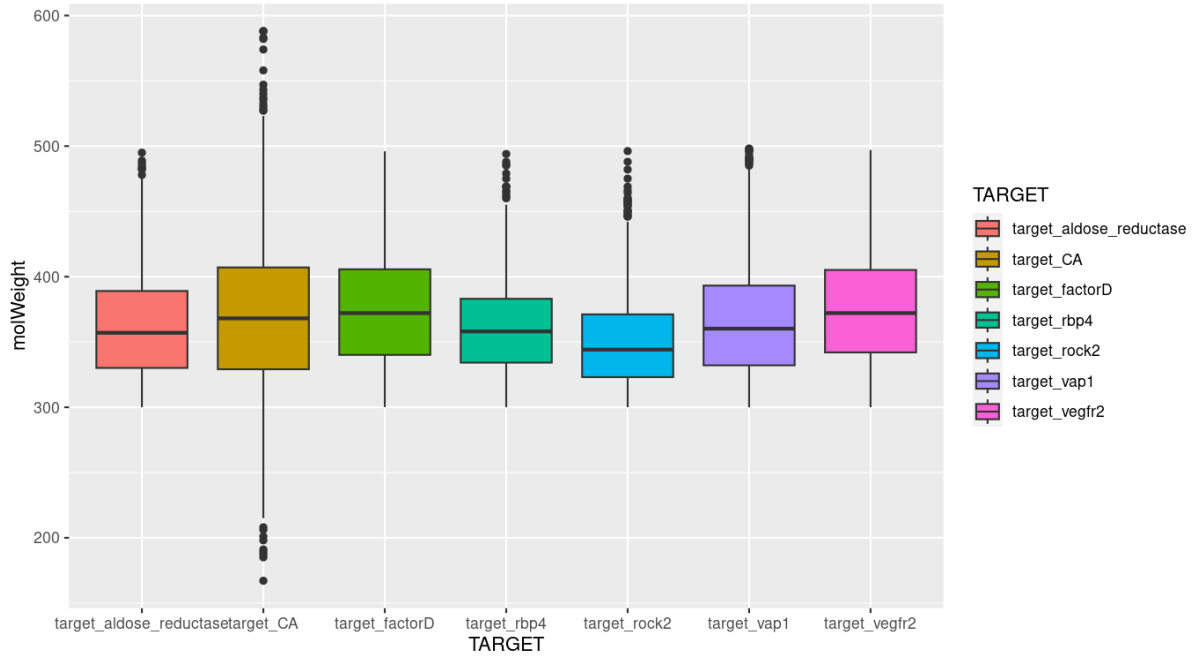
This graphic shows the mol PSA by target. It shows that Carbonic Anhydrase is the target that has the most molecules over 90 and Aldose Reductase has the lowest range of molecules over 90. The Vascular Adhesion Protein-1 has the most number of molecules under 90 and the Factor D the lowest.



Molecular Weight

The molecular weight can affect medications in several ways: it can influence the absorption, metabolism, distribution and excretion of the medicine, impact solubility, interact with the targets and

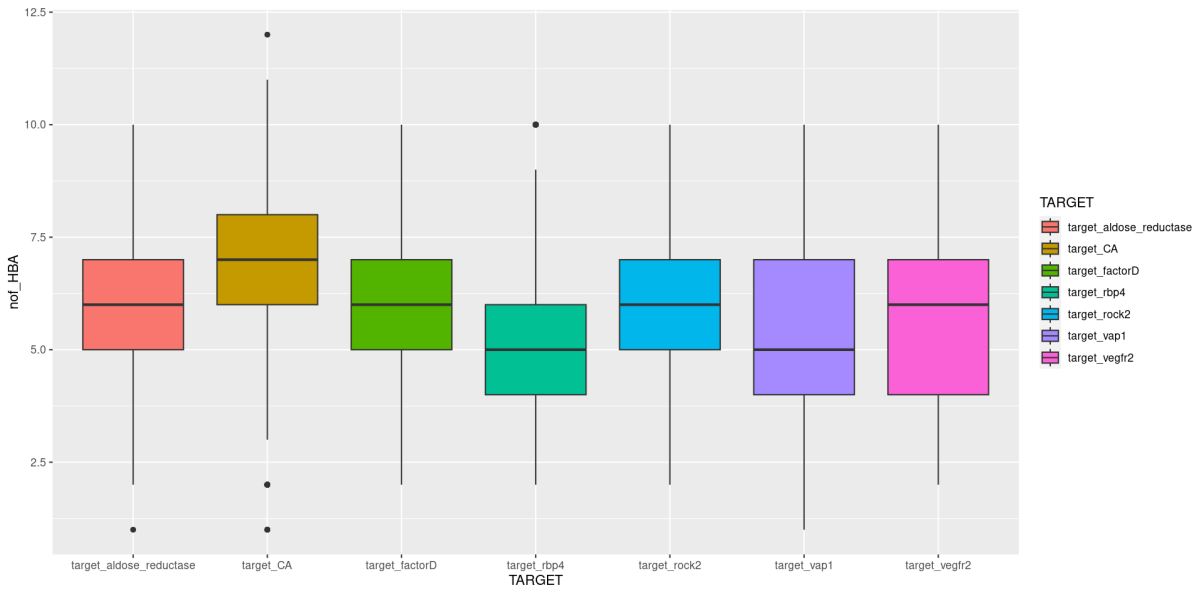
the formulation of the medicine. The higher the weight, the harder to work with it, lower the absorption and metabolism and the interaction with the targets.



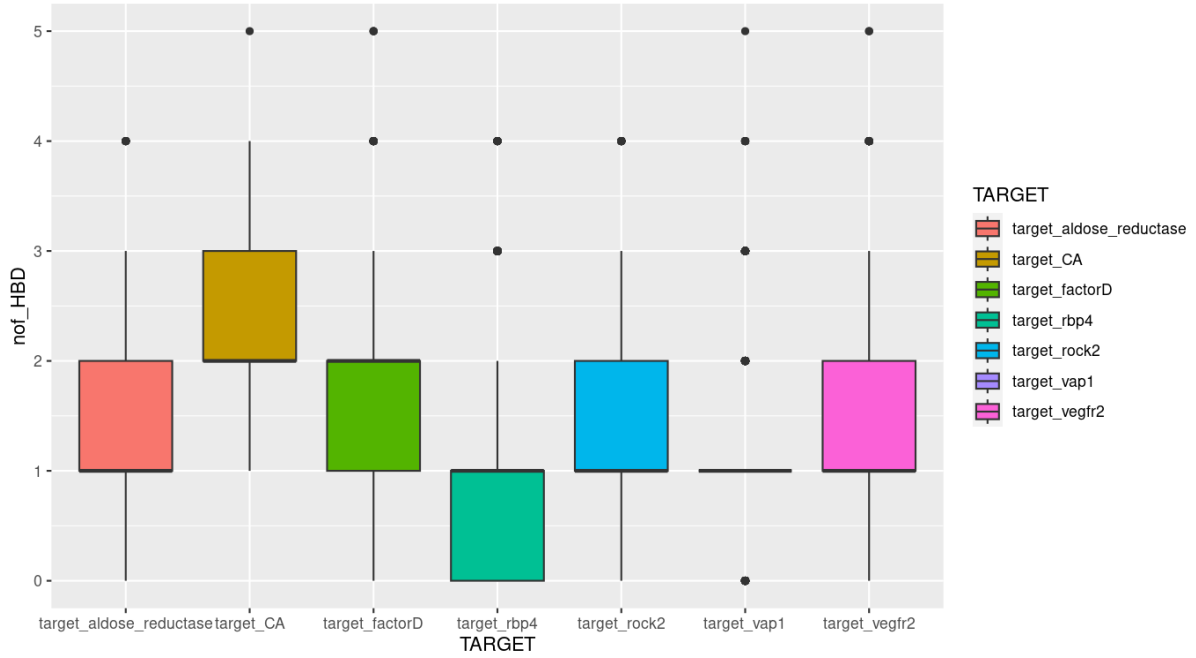
The graphic shows that The molecules are mostly between 300 and 400 g/mol with close medians, so, for these treatments, this should be the ideal weight. Over or below this could be hard to work with, that can be seeing some outliers that are way too much out of the range.

HBA e HBD

Hydrogen Bond Acceptor (HBA) is the number of acceptors for hydrogen bonds in a molecule, the interaction with the target can be increased when the HBA number is higher.



Hydrogen Bond Donor (HBD) is the number of donors for hydrogen bonds in a molecule, so it can form hydrogen bonds with the target too.



These two graphics show that our molecules have a tendency to create acceptor bonds and connect with the target. As we can see, Vascular Adhesion Protein-1 has only a line and some outliers in HBD, the data has little variability, that means the data for these are homogeneous.

Bibliography

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