These compounds are synthetic analogues obtained during optimization programmes against different therapeutic targets (anti-HIV, anti-kinases, protein-protein interactions, phosphatase inhibitors...).

Targeted libraries have also been built from "scaffolds" with drug-like properties, such as purines and flavonoids. During the past 4 years, the Chemolibrary has grown steadily, and comprehends now over 8560 substances available in the form of microplates.

An important question concerning the Chemolibrary is the value of the compounds that comprise it. First, the results of screening carried out on the chimiothèque have shown that our collection is diverse enough to enable us to find active molecules against different therapeutic targets.

Insofar as the chemical library contains molecules that were designed to interact with the living, it is largely composed of heterocyclic compounds. Such compounds are known for their "drug-like properties".

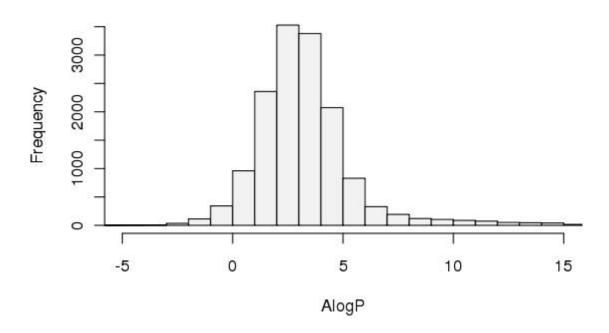
Finally, in a chemoinformatics analysis of the Chemolibrary, 80% and 65% of the compounds were found to be "drug-like" and "lead-like", respectively.

In conclusion, the analysis suggests that the chemical library contains a vast majority of compounds of great interest for research in drug discovery.

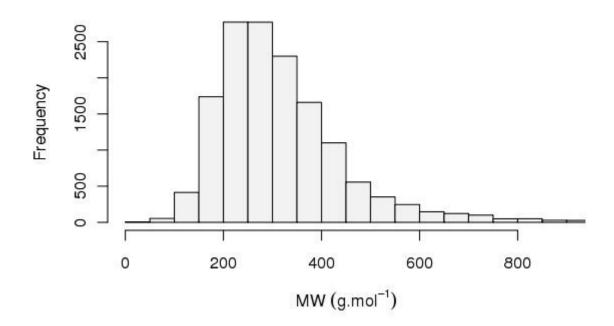
The electronic version (sdf file) may be freely obtained by writing to Claire Beauvineau (<u>claire.beauvineau@curie.fr</u>) and signing a Material Transfer Agreement (MTA). The compounds may be supplied either in plates or in powder, providing the signature of a MTA (not free of charge).

Physico-chemical Properties of the Chemical Library

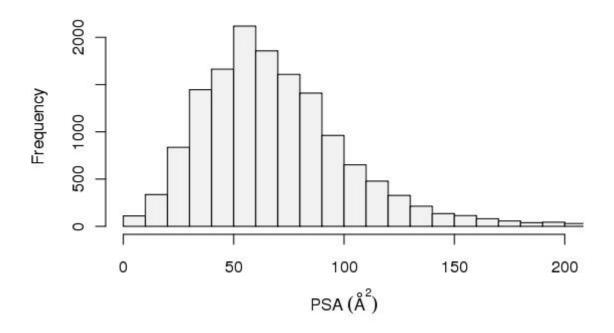
Octanol/water partition coefficient (AlogP)



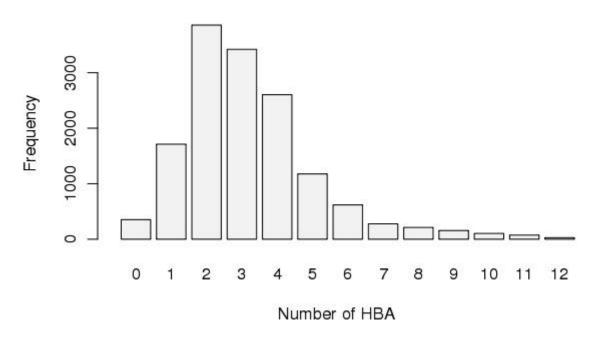
Molecular Weight



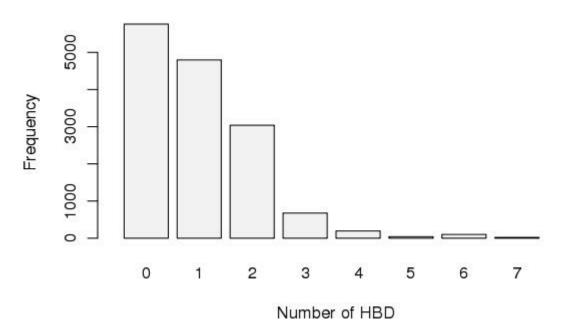
Polar Surface Area



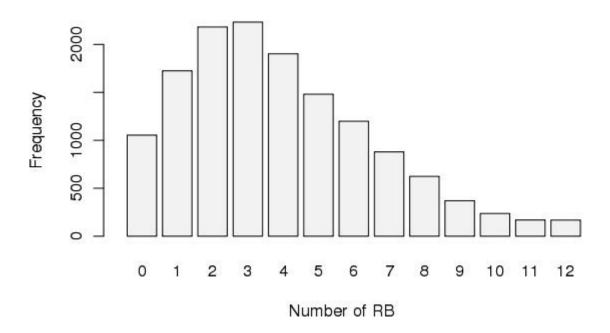
Hydrogen Bond Acceptor



Hydrogen Bond Donor



Rotatable Bond



Ring Count

