The management of pharmaceutical screening projects is a key point in Research and Development of new drugs. To take the best decision, project managers have to extract the right information from huge quantity of experimental and structural data. Classical approaches involve database mining tools, well designed for experimental data, but not necessarily for structures of molecules.

In parallel, the use of chemical spaces based on molecular descriptors and mathematical tools allows to represent and compare molecules, facilitating the access to the chemical information. Classical design involves a physicochemical description of the molecules coupled with a principal component analysis (PCA) to extract the most informative dimensions. To become more universal, we propose the use of at least 3 chemical spaces, based respectively on a physicochemical, a topological and a pharmacophoric molecular description.

The condensation methods used for the chemical spaces can also be applied to experimental results. In this new data space, molecules were positioned depending on their experimental data profiles. Moreover, a global efficiency score, which correspond to the distance between a molecule of interest and an optimum profile of the project, represents a global scientific management approach.

In order to reduce even more all the information available into a unique representation, we propose to condense the 3 chemical spaces and the data space described above into a unique one by the use of Self Organized Map based on the PCA coordinates from these 4 spaces.

Practical illustration of the proposed approach will be given in the poster.