[P15] Detection of Structural Alerts for Toxic Side Effects. A Case Study on Mutagenicity.

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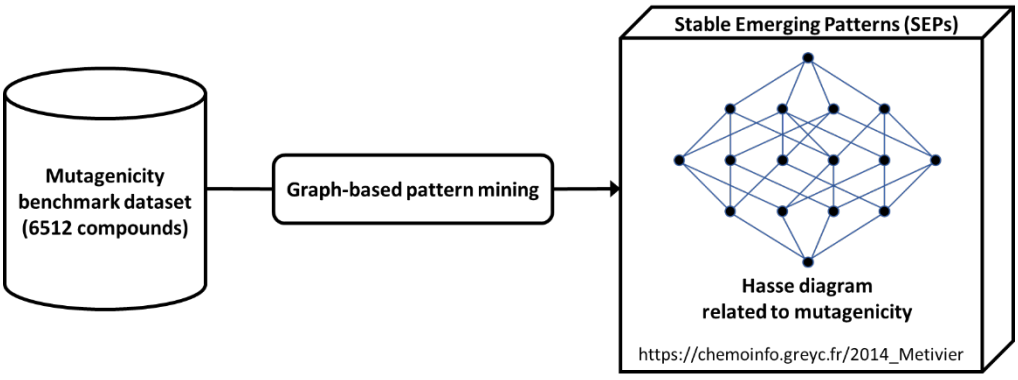
In the pharmaceutical industry, it is widely recognized that early safety evaluation of candidate molecules is needed before making significant investments of time and resources. To this aim, the concept of predictive toxicology, which includes the application of computer technologies to detect relationships that connect chemical structures and toxicological activities in large biological and chemical datasets, is extremely appealing.

The definition of structural alerts corresponds to one of the most interesting approach of predictive toxicology since it defines the key features of a molecule that are required to interact with a biological system and initiate a toxicology pathway. The evolution of artificial intelligence and data mining tools shorten the time and efforts needed to identify new structural alerts, sometimes beyond the limits of human perception.

The current work apply the emerging patterns methodology [1] that computes the conjunctions of molecular fragments whose frequency of occurrences in the dataset is sufficiently discriminative between the different classes of molecules (e.g. the mutagens and the non-mutagens). We rely on our original calculation method [2-3] to mine a benchmark mutagenicity dataset. Thanks to the background of Formal Concept Analysis [4], we are now able to select the most consistent emerging patterns, named the stable emerging patterns (SEPs) [5].

Moreover, we also provide an interactive visualization tool to easily explore and evaluate the structural alert candidates (https://chemoinfo.greyc.fr/2014_Metivier/).



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