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High-performance reversed-phase liquid chromatography (RP HPLC) is one of the most widely used chromatographic techniques. Today, up to 60-80% of all chromatographic procedures are carried out using a RP HPLC. It is a consequence of its universality, relatively low costs and general simplicity of analytical procedures.

Optimization of RP HPLC separations is an important step in developing any analytical method. The most popular method, trial-and-error approach, has several disadvantages, like it requires a large number of preliminary experiments, it is time-consuming, it is often difficult to find the best conditions to carry out preliminary experiments. Very often in practice the software-based techniques are used to optimize the conditions of separations. They usually provide a theoretical chromatogram based on a series of preliminary experiments, and leads to separations often not achievable by trial-and-error approaches. However, these programs usually require large number of preliminary experiments to operate, which we believe may be lowered by the use of a Bayesian inference techniques.

In this project a general single statistical model will be proposed to describe the behavior of a large group of analytes in a chromatography column as a function of parameters that control its retention like temperature, the content and type of organic modifier, pH and column type, etc. Such a non-linear mixed effects model will allow researchers to better understand the impact of basic physicochemical parameters characterizing analyte on retention. This model and its parameters might also be used to predict the retention of the new analytes using Bayesian techniques, which combine an information from the previously analyzed compounds (a priori information) and any number of preliminary experiments.

The proposed project is innovative, as Bayesian inference methods are rarely used in chromatographic sciences. These study is important for better understanding the physical and analytical chemistry, as they allow for a more-thorough elucidation of analyte-stationary phase interactions in different mobile phase compositions. It will also provide the optimization strategy that will allow to get the desired quality of separation using a minimal number (we expect just one) of preliminary experiments.