Bridging the Gap: Collaborative Tools for Chemoinformatics and Experimental Chemistry

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Effective usage of chemoinformatics tools requires a good amount of high-quality data, so the collaboration with the experimental and/or computational chemistry groups is paramount. In our work, we closely collaborate with a number of experimental chemistry groups. However, such collaboration also requires the development of tools that facilitate work on both ends: they should be easy to use and understand for experimentalists who might not have experience with coding or algorithms, but also correctly implement such algorithms and data analysis approaches. In this presentation, some tools that were developed in our group are shown and discussed. First, DOPtools is an open source Python library for QSPR modeling that includes full workflow from data preparation and descriptor calculation to model optimization and prediction. While the main functionality of the library is accessed via command line interface, the development of GUI is also undertaken to allow people unfamiliar with coding to use the main functionalities of the library in a visual format. Chromatography data analysis tools for chemistry robot systems are also developed and integrated with modeling. Finally, database solutions allow to facilitate the interaction between experimental groups and chemoinformatics groups in terms of data sharing and management.