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QSPR model development to simplify compound identification in complex matrix analysis

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In order to assess and evaluate the toxicity of new products in a wide range of industrial settings (e.g., food and beverage, cosmeceutical industries), it is important to understand their chemical composition. Non-targeted screening of small molecules in complex matrices can be performed using various analytical techniques such as gas chromatography coupled to mass spectrometry. However, compound identification using a conventional mass spectral library search, e.g., NIST MSSearch, generally does not provide sufficient confidence regarding the proposed structures. The application of cheminformatics provides analytical chemists with tools to increase the accuracy for identifying compound structures, and to accelerate and standardize the identification process. QSPR (Quantitative Structure Property Relationship) models predict retention times and/or indices for all constituents potentially present in the complex matrix. These predicted retention times/indices enhance the level of confidence in the correct assignment of mass spectra to the right compounds. This poster presents QSPR models, which have been developed using different methodologies/algorithms and software tools, including ChromGenius (ACDLabs), RapidMiner, Dragon, and Pipeline Pilot. It describes the improvement afforded by such tools for elucidating the chemical composition of Reduced-Risk Products developed by Philip Morris.

Biography

Elyette Martin is a computational Chemistry Scientist at Philip Morris R&D in the chemoinformatics team. She received her PhD in Molecular Biology from the Strasbourg University (France) before working at the Institut de Recherche Servier, a French pharma company, in a Postdoctoral position. At Philip Morris, she manages the corporate chemical and spectral database and chemoinformatics development (properties calculation, development of QSAR models).

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