Off-line LC×SFC-HRMS/MS method for the non-target analysis of depolymerised lignin

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Résumé

Lignin is an abundant natural polymer that is by far the largest natural resource for aromatic compounds. Nevertheless, approx. only 2% of it is commercialised while the rest is mainly burned to power the paper industry from where lignin is obtained by the fractionation of cellulose from lignocellulosic biomass. However, it has potential to be valorised more by isolating valuable aromatic compounds, by incorporating into materials (e.g., coatings, resins, thermoplastics), or used as biofuel. For making these valorisation processes efficient, thorough structural characterisation via a powerful chromatographic technique can be highly beneficial as the complex composition of lignin depends on the botanical origin, isolation and depolymerisation processes.

Therefore, in this study, an off-line comprehensive two-dimensional (2D) chromatography method combining liquid chromatography, supercritical fluid chromatography, and high-resolution mass spectrometry with fragmentation (LC×SFC-HRMS/MS) was developed. The implementation of a 1-aminoanthracene column in the second dimension enabled a good class separation of lignin monomers, dimers, trimers, and tetramers with additional separation based on the number of hydroxyl groups and steric effects. The pentafluorophenyl column in the first dimension additionally improved the separation based on hydrophobicity, thus the first 2D-LC plot demonstrating classification of lignin compounds was obtained. The comparison of the technique to 1D-SFC showed that the 2D-LC method is also superior for the separation of isomers, which is especially beneficial for lignin as 77% of the detected compounds had at least one isomer. Advanced data analysis methods (MS-DIAL, SIRIUS, and Feature-Based Molecular Network) were integrated into the non-target workflow to rapidly visualise and study the detected compounds.

The oral presentation, if selected, will be done by Eliise Tammekivi (postdoc) in English or by Karine Faure (researcher) in French, as suits the committee.

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