



Scientific Symposium

Untargeted screening methods in the 21st century - metabolomics vs extractable & leachable

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Abstract

Automated peak-picking algorithms have been around for more than 10 years, nowadays they are used widely in metabolomic studies. Several software tools, including platform based, multi-platform or open access, are now available to evaluate untargeted screenings with LC/MS and GC/MS. As a result, manual data evaluation has become outdated. Coupled with high-resolution mass spectrometry, these automated approaches enable the detection, identification, and semi-quantification of compounds previously undetectable. This includes distinguishing and accurately identifying co-eluting peaks in GC/MS.

Despite these advances, untargeted screenings for extractables and leachables are still often evaluated manually. Even the new USP chapter on system suitability tests (SSTs) in untargeted screening studies recommends a manual approach, emphasizing the need for peak separation.

We will demonstrate that automated peak picking can be effectively applied to extractable and leachable studies, even in complex matrices such as polysorbate.



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Free



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