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Quantification of run order effect on chromatography - mass spectrometry profiling data

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Highlights

- OPLS was used for quantification of run order effect in XC-MS profiling studies.
- Presented approach does not use internal standards or quality control samples.
- OPLS analysis of run order effect can be applied for evaluation of data quality.
- Effectiveness of the data normalization can be quantified.
- Suggestions for the improvement of analytical protocols can be obtained.

Abstract

Chromatographic systems coupled with mass spectrometry detection are widely used in biological studies investigating how levels of biomolecules respond to different internal and external stimuli.