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Multivariate curve resolution of incomplete fused multiset data from chromatographic and spectrophotometric analyses for drug photostability studies

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Graphical abstract

Highlights

► A new MCR-ALS algorithm is proposed for the analysis of incomplete fused multiset. ► Resolution of the data allowed the description of amiloride kinetic photodegradation. ► The new MCR-ALS algorithm can be easily applied to other drugs and chemicals.

Abstract

An advanced and powerful chemometric approach is proposed for the analysis of incomplete multiset data obtained by fusion of hyphenated liquid chromatographic DAD/MS data with UV spectrophotometric data from acid-base titration and kinetic degradation experiments. Column- and row-wise augmented data blocks were combined and simultaneously processed by means of a new version of the multivariate curve resolution – alternating least squares (MCR-ALS) technique, including the simultaneous