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Title: Joint approximate diagonalization of eigenmatrices (JADE) as a high-throughput approach for analysis of hyphenated and comprehensive two-dimensional gas chromatographic data

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<AT>Joint;1; approximate diagonalization of eigenmatrices (JADE) as a high-throughput approach for analysis of hyphenated and comprehensive two-dimensional gas chromatographic data

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<ABS-HEAD>Highlights► JADE was developed for resolution of GC-MS and GC×GC-MS data ► JADE performance was compared with MILCA, MFICA and MCR-ALS ► JADE solutions are almost in the range of feasible solutions calculated by FACPACK ► JADE showed outperformance over existing method for gas chromatographic data ► Determination of PAHs in oil analyzed by GC×GC-MS is discussed as real case

<ABS-HEAD>Abstract
<ABS-P>The objective of the present work is development of joint approximate diagonalization of eigenmatrices (JADE) as a member of independent component analysis (ICA) family, for the analysis of gas chromatography-mass spectrometry (GC-MS) and comprehensive two-dimensional gas chromatography-mass spectrometry (GC×GC-MS) data to address incomplete separation problem occurred during the analysis of complex sample matrices. In this regard, simulated GC-MS and GC×GC-MS data sets with different number of components, different degree of overlap and noise were evaluated. In the case of simultaneous analysis of multiple samples, column-wise augmentation for GC-MS and column-wise super-augmentation for GC×GC-MS was used before JADE analysis. The performance of JADE was evaluated in terms of statistical parameters of lack of fit (LOF), mutual information (MI) and Amari index as well as analytical figures of merit (AFOMs) obtained from calibration curves. In addition, the area of feasible solutions (AFSs) was calculated by two different approaches of MCR-BANDs and polygon inflation algorithm (FACPACK). Furthermore, JADE performance was compared with multivariate curve resolution-alternating least squares (MCR-ALS) and other ICA algorithms of mean-field ICA (MFICA) and mutual information least dependent component analysis (MILCA). In all cases, JADE could successfully resolve the elution and spectral profiles in GC-MS and GC×GC-MS data with acceptable statistical and calibration parameters and their solutions were in AFSs. To check the applicability of JADE in real cases, JADE was used for resolution and quantification of phenanthrene and anthracene in aromatic fraction of heavy fuel oil (HFO) analyzed by GC×GC-MS. Surprisingly, pure elution and spectral profiles of target compounds were properly resolved in the presence of baseline and interferences using JADE. Once more, the performance of JADE was compared with MCR-ALS in real case. On this matter, the mutual information (MI) values were 1.01 and 1.13 for resolved profiles by JADE and MCR-ALS, respectively. In addition, LOD values (μg/mL) were respectively 1.36 and 1.24 for phenanthrene and 1.26 and 1.09 for anthracene using MCR-ALS and JADE which showed outperformance of JADE over MCR-ALS.
<KWD>Keywords: Independent component analysis; Joint approximate diagonalization of eigenmatrices; Comprehensive two-dimensional gas chromatography; Rotational ambiguity; Multivariate curve resolution.