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*Has received an application for a patent for a new and useful invention. The title and description of the invention are enclosed. The requirements of law have been complied with, and it has been determined that a patent on the invention shall be granted under the law.*

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**United States Patent**

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*David J. Kappas*

*Director of the United States Patent and Trademark Office*



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(12) **United States Patent**  
**Kopriva et al.**

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(54) **METHOD OF AND SYSTEM FOR BLIND EXTRACTION OF MORE PURE COMPONENTS THAN MIXTURES IN 1D AND 2D NMR SPECTROSCOPY AND MASS SPECTROMETRY COMBINING SPARSE COMPONENT ANALYSIS AND SINGLE COMPONENT POINTS**

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**G06K 9/00** (2006.01)  
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See application file for complete search history.

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(57) **ABSTRACT**

A computer-implemented data processing system for blind extraction of more pure components than mixtures recorded in 1D or 2D NMR spectroscopy and mass spectrometry. Sparse component analysis is combined with single component points (SCPs) to blind decomposition of mixtures data X into pure components S and concentration matrix A, whereas the number of pure components S is greater than number of mixtures X. NMR mixtures are transformed into wavelet domain, where pure components are sparser than in time domain and where SCPs are detected. Mass spectrometry (MS) mixtures are extended to analytical continuation in order to detect SCPs. SCPs are used to estimate number of pure components and concentration matrix. Pure components are estimated in frequency domain (NMR data) or m/z domain (MS data) by means of constrained convex programming methods. Estimated pure components are ranked using negentropy-based criterion.

**19 Claims, 23 Drawing Sheets**

