CLAIMS

1. A method for analyzing mixture components, comprising the steps of:

(1) separating mixture samples with constant concentration ratios using chromatographic techniques to obtain preliminary chromatograms;

(2) within any range of the preliminary chromatograms as obtained from step (1), carrying out a sampling as required, so as to obtain a series of spectra at different retention time, which is called the mixture spectra (i.e., a mixed spectra);

(3) using serial methods of the EM algorithms on the mixture spectra obtained from step (2) to calculate various reconstructed pure spectra and the corresponding pseudo concentrations;

wherein the pseudo concentration is the concentration that corresponds to the reconstructed pure spectra, which is calculated out when using EM algorithms to reconstruct the pure spectra;

for the analysis of a mixture sample containing unknown substances, one need to obtain as much information as possible on the components from the mixture spectra obtained in step (2) after multiple repeated calculation by using the serial methods of the EM algorithms under different parameters so as to get as many reconstructed pure spectra as possible; and

the different parameters refer to targeting different peaks, using different objective functions and penalty functions or using different optimization methods.

2. The method for analyzing mixture components according to claim 1, characterized in that the preliminary chromatogram obtained from step (1) include peaks of pure component and the overlapping peaks of the mixture.

3. The method for analyzing mixture components according to claim 2~~3~~, characterized in that for the overlapping peaks of the mixture, step (2) and step (3) are utilised for analysis.

4. The method for analyzing mixture components according to any one of claims 1 to 3, characterized in that any range of the preliminary chromatograms obtained in step (1) refers to a part of the preliminary chromatogram, or the whole preliminary chromatogram.

5. The method for analyzing mixture components according to any one of claims 1 to 3~~4~~, characterized in that in step (1), the chromatographic techniques are: gas chromatography (GC), liquid chromatography, or a combination of both.

6. The method for analyzing mixture components according to any one of claims 1 to 3~~5~~, characterized in that in step (1), preliminary chromatogram of the mixture ~~spectra~~ can be obtained by a detector after using chromatographic techniques to carry out separation.

7. The method for analyzing mixture components according to claim 6, characterized in that the detector can be selected from the group comprising one or a combination of MS, IR, UV, fluorescence, spectrophotometer and NMR detectors.

8. The method for analyzing mixture components according to any one of claims 1 to 3~~7~~, characterized in that in step (3), the serial methods of EM algorithms comprise one or a combination of BTEM, tBTEM or MREM methods.

9. The method for analyzing mixture components according to claim 8, characterized in that for each operation of the BTEM or tBTEM method, one reconstructed pure spectrum can be obtained; for each operation of the MREM method, multiple reconstructed pure spectra can be obtained.

~~10. The method for analyzing mixture components according to any one of claims 1 to 9, characterized in that for step (3), for the analysis of a mixture sample containing an unknown substance, repeated calculation using the serial methods of EM algorithms is carried out with~~

~~different parameters on the basis of the mixture spectra obtained in step (2) so as to get as many reconstructed pure spectra as possible.~~

10~~11~~. The method for analyzing mixture components according to any one of claims 1 to 3~~9~~, characterized in that in step (3), for analyzing if a mixture sample has a target compound/known compound, the target compound/known compound standard spectrum can be used as a reference for calculation using the serial methods of EM algorithms, reconstruction methods using different parameters can be used to obtain the target compound/known compound's reconstructed pure spectrum; during multiple reconstruction, if the reconstructed pure spectrum and the standard spectrum of the target compound/known compound are compared and found to be consistent, and the pseudo-concentration of the reconstructed pure spectrum is meaningful, the mixture contains the target compound/known compound; otherwise, the target compound/known compound is absent.

11~~12~~. The method for analyzing mixture components according to any one of claims 1 to~~-~~3~~11~~, characterized in that after finishing the step (3), the reconstructed pure spectra can be compared with the spectra found in a standard database to confirm their information; if the reconstructed pure spectrum is consistent with some spectrum in the standard database, the reconstructed pure spectrum can be confirmed to be the component as represented in the spectrum of the standard database.

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(1) separating mixture samples with constant concentration ratios using chromatographic techniques to obtain preliminary chromatograms;

(2) within any range of the preliminary chromatograms as obtained from step (1), carrying out a sampling as required, so as to obtain a series of spectra at different retention time, which is called the mixture spectra (i.e., a mixed spectra);

(3) using serial methods of the EM algorithms on the mixture spectra obtained from step (2) to calculate various reconstructed pure spectra and the corresponding pseudo concentrations;

wherein the pseudo concentration is the concentration that corresponds to the reconstructed pure spectra, which is calculated out when using EM algorithms to reconstruct the pure spectra;

for the analysis of a mixture sample containing unknown substances, one need to obtain as much information as possible on the components from the mixture spectra obtained in step (2) after multiple repeated calculation by using the serial methods of the EM algorithms under different parameters so as to get as many reconstructed pure spectra as possible; and

the different parameters refer to targeting different peaks, using different objective functions and penalty functions or using different optimization methods.

2. The method for analyzing mixture components according to claim 1, characterized in that the preliminary chromatogram obtained from step (1) include peaks of pure component and the overlapping peaks of the mixture.

3. The method for analyzing mixture components according to claim 2, characterized in that for the overlapping peaks of the mixture, step (2) and step (3) are utilised for analysis.

4. The method for analyzing mixture components according to any one of claims 1 to 3, characterized in that any range of the preliminary chromatograms obtained in step (1) refers to a part of the preliminary chromatogram, or the whole preliminary chromatogram.

5. The method for analyzing mixture components according to any one of claims 1 to 3, characterized in that in step (1), the chromatographic techniques are: gas chromatography (GC), liquid chromatography, or a combination of both.

6. The method for analyzing mixture components according to any one of claims 1 to 3, characterized in that in step (1), preliminary chromatogram of the mixture can be obtained by a detector after using chromatographic techniques to carry out separation.

7. The method for analyzing mixture components according to claim 6, characterized in that the detector can be selected from the group comprising one or a combination of MS, IR, UV, fluorescence, spectrophotometer and NMR detectors.

8. The method for analyzing mixture components according to any one of claims 1 to 3, characterized in that in step (3), the serial methods of EM algorithms comprise one or a combination of BTEM, tBTEM or MREM methods.

9. The method for analyzing mixture components according to claim 8, characterized in that for each operation of the BTEM or tBTEM method, one reconstructed pure spectrum can be obtained; for each operation of the MREM method, multiple reconstructed pure spectra can be obtained.

10. The method for analyzing mixture components according to any one of claims 1 to 3, characterized in that in step (3), for analyzing if a mixture sample has a target compound/known compound, the target compound/known compound standard spectrum can be used as a reference for calculation using the serial methods of EM algorithms, reconstruction methods using different

parameters can be used to obtain the target compound/known compound's reconstructed pure spectrum; during multiple reconstruction, if the reconstructed pure spectrum and the standard spectrum of the target compound/known compound are compared and found to be consistent, and the pseudo-concentration of the reconstructed pure spectrum is meaningful, the mixture contains the target compound/known compound; otherwise, the target compound/known compound is absent.

11. The method for analyzing mixture components according to any one of claims 1 to 3, characterized in that after finishing the step (3), the reconstructed pure spectra can be compared with the spectra found in a standard database to confirm their information; if the reconstructed pure spectrum is consistent with some spectrum in the standard database, the reconstructed pure spectrum can be confirmed to be the component as represented in the spectrum of the standard database.