CLAIMS

1. A peak analyzing method using a computer to process three-dimensional data obtained by acquiring a series of first signal waveforms representing a relationship between a first parameter and a signal intensity for a given set of changing second parameters, and to separate overlapping peaks observed in a second signal waveform representing a relationship between the second parameter and the signal intensity into a plurality of individual peaks originating from different factors based on signal patterns observed in a dimension of the first parameter, wherein the peak analyzing method executes:

a singular value decomposition step configured to perform singular value decomposition on an input matrix expressing three-dimensional data to be processed, and to determine a first matrix representing a plurality of basis vectors related to the first parameter and a second matrix representing a plurality of weighting vectors related to the second parameter, where the first matrix and the second matrix have a lowered rank than the input matrix based on singular values obtained by the singular value decomposition;

a transformation matrix acquisition step configured to estimate characteristic orientations within a space spanned by the plurality of basis vectors by performing a geometric analysis on a trajectory defined by the plurality of weighting vectors in an SVD projection space whose number of dimensions is equal to the lowered rank given by a singular value decomposition process, and to determine a transformation matrix containing relevant information of the characteristic orientations; and

a peak separation step configured to deconvolute signal waveforms in the first matrix of the dimension of the first parameter by the transformation matrix, and to separate peaks in the second signal waveform in the second matrix by the transformation matrix .

2. The peak analyzing method according to claim 1, wherein the different factors are components in the sample, the first parameter is wavelength or mass-to-charge ratio, with the first signal waveform being a waveform spectrum or mass spectrum, and the second parameter is time, with the second signal waveform being a chromatogram.

3. The peak analyzing method according to claim 2, wherein the transformation matrix acquisition step includes estimation of the characteristics orientations corresponding to a single component based on a shape analysis of the trajectory within a time period in which only the single component is present.

4. The peak analyzing method according to claim 3, wherein the peak separation is carried out for a peak in which first, second and third components are mixed together, and under a condition that the peak includes a first time period in which only the first component is present, a second time period in which the first component and the second component only are mixed together, a third time period in which the three components are mixed together, a fourth time period in which the second component and the third component only are mixed together, as well as a fifth time period in which only the third component is present, the transformation matrix acquisition step includes estimation of the characteristic orientation corresponding to the second component from a line intersection between a plane defined by a section of the trajectory which corresponds to the first and second time periods , and a plane defined by a section of the trajectory which corresponds to the fourth and fifth time periods .

5. A peak analyzing method using a computer to process three-dimensional data obtained by acquiring a series of first signal waveforms representing a relationship between a

first parameter and a signal intensity for a given set of changing second parameters, and to ~~determine a purity of~~analyze a peak observed in a second signal waveform representing a relationship between the second parameter and the signal intensity, wherein the peak analyzing method executes:

a singular value decomposition step configured to perform singular value decomposition on an input matrix expressing three-dimensional data to be processed, and to determine a first matrix representing a plurality of basis vectors related to the first parameter and a second matrix representing a plurality of weighting vectors related to the second parameter, where the first matrix and the second matrix have a lowered rank than the input matrix based on singular values obtained by the singular value decomposition; and

a component number estimation step configured to estimate a number of components contributing to the peak from a behavior of a trajectory in an SVD projection space whose number of dimensions is equal to the lowered rank, and which is described by the plurality of weighting vectors.

6. The peak analyzing method according to claim 5, wherein the first parameter is wavelength or mass-to-charge ratio, with the first signal waveform being a waveform spectrum or mass spectrum, and the second parameter is time, with the second signal waveform being a chromatogram.

7. A waveform processing device configured to process three-dimensional data obtained by acquiring a series of first signal waveforms representing a relationship between a first parameter and a signal intensity for a given set of changing second parameters, and to separate overlapping peaks observed in a second signal waveform representing a relationship between the second parameter and the signal intensity into a plurality of individual peaks

originating from different factors based on signal patterns observed in a dimension of the first parameter, the waveform processing device comprising:

a singular value decomposition processor configured to perform singular value decomposition on an input matrix expressing three-dimensional data to be processed, and to determine a first matrix representing a plurality of basis vectors related to the first parameter and a second matrix representing a plurality of weighting vectors related to the second parameter, where the first matrix and the second matrix have a lowered rank than the input matrix based on singular values obtained by the singular value decomposition;

a transformation matrix acquirer configured to estimate characteristic orientations within a space spanned by the plurality of basis vectors by performing a geometric analysis on a trajectory defined by the plurality of weighting vectors in an SVD projection space whose number of dimensions is equal to the lowered rank given by a singular value decomposition process, and to determine a transformation matrix containing relevant information of the characteristic orientations; and

a peak separation calculator configured to deconvolute signal waveforms in the first matrix of the dimension of the first parameter by the transformation matrix, and to separate peaks in the second signal waveform in the second matrix by the transformation matrix.

8. The waveform processing device according to claim 7, wherein the different factors are components in the sample, the first parameter is wavelength or mass-to-charge ratio, with the first signal waveform being a waveform spectrum or mass spectrum, and the second parameter is time, with the second signal waveform being a chromatogram.

9. The waveform processing device according to claim 8, wherein the transformation matrix acquirer is configured to estimate the characteristics orientations

corresponding to a single component based on a shape analysis of the trajectory within a time period in which only the single component is present.

10. The waveform processing device according to claim 9, wherein the peak separation is carried out for a peak in which first, second and third components are mixed together, and under a condition that the peak includes a first time period in which only the first component is present, a second time period in which the first component and the second component only are mixed together, a third time period in which the three components are mixed together, a fourth time period in which the second component and the third component only are mixed together, as well as a fifth time period in which only the third component is present, the transformation matrix acquirer estimates the characteristic orientation corresponding to the second component from a line intersection between a plane defined by a section of the trajectory which corresponds to the first and second time periods, and a plane obtained by a section of the trajectory which corresponds to the fourth and fifth time periods.

11. A waveform processing device configured to process three-dimensional data obtained by acquiring a series of first signal waveforms representing a relationship between a first parameter and a signal intensity for a given set of changing second parameters,, and to ~~determine a purity of~~analyze a peak observed in a second signal waveform representing a relationship between the second parameter and the signal intensity, the waveform processing device comprising:

a singular value decomposition processor configured to perform singular value decomposition on an input matrix expressing three-dimensional data to be processed, and to determine a first matrix representing a plurality of basis vectors related to the first parameter

and a second matrix representing a plurality of weighting vectors related to the second parameter, where the first matrix and the second matrix have a lowered rank than the input matrix based on singular values obtained by the singular value decomposition; and

a component number estimator configured to estimate a number of components contributing to the peak from a behavior of a trajectory in an SVD projection space whose number of dimensions is equal to the lowered rank, and which is described by the plurality of weighting vectors .

12. The waveform processing device according to claim 11, wherein the first parameter is wavelength or mass-to-charge ratio, with the first signal waveform being a waveform spectrum or mass spectrum, and the second parameter is time, with the second signal waveform being a chromatogram.