Differential Diagnosis of Human Lung Tumors Using Surface Desorption Atmospheric Pressure Chemical Ionization Imaging Mass Spectrometry

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Supplementary Information

Table S1. Histological description of patients from 14 research subjects.

Figure S1. Tandem mass spectrometry (MS/MS) spectra of multiple potential biomarkers for distinguishing tumor and adjacent normal tissue using multivariate statistical analyses

Figure S2. PCA analysis of DAPCI-MSI data in the positive ion mode. (a) 3D plot of PCA score results for the differentiation of the tumor from adjacent normal lung tissue. (b) PCA loading results for the PCs

Figure S3. DAPCI-MS images of selected potential biomarkers using multivariate statistical analyses for the research subject A4 tissue section showing the spatial distributions of ions at (a) m/z 104.1 [C5H14NO]+, (b)175.2 [C6H15N4O2]+,(c) 184.2 [C5H15NO4p]+ ,(d) m/z 741.3 [SM(16:0)+K]+,(e) m/z 810.6 [PC(36:1)+Na]+,(f) m/z 826.6 [PC(36:1)+K]+,(g) m/z 834.6 [PC(38:3)+Na]+ ,(h)m/z 848.6 [PC(38:4)+K]+,and m/z 850.6 [PC(38:3)+K]+ (a) Light microscopy images of the H&E-stained sections are shown. (Scale bars)

**Table S1.** Histological description of patients from 14 research subjects.

Number	sex	Age	Tumor type	Histopathological grading
A1	Male	64	Squamous cell carcinoma	Moderate differentiated
A2	Male	47	Squamous cell carcinoma	Poorly differentiated
A3	Male	61	Squamous cell carcinoma	Moderate differentiated
A4	Male	73	Squamous cell carcinoma	Moderate differentiated
A5	Male	57	Squamous cell carcinoma	Moderate differentiated
A6	Male	63	Squamous cell carcinoma	Moderate differentiated
A7	Male	66	Squamous cell carcinoma	Moderate differentiated
A8	Male	61	Squamous cell carcinoma	Moderate differentiated
A9	Female	62	Squamous cell carcinoma	Moderate differentiated
A10	Male	59	Squamous cell carcinoma	Moderate differentiated
A11	Male	70	Squamous cell carcinoma	Moderate differentiated
A12	Male	48	Squamous cell carcinoma	Moderate differentiated
A13	Male	57	Squamous cell carcinoma	Moderate differentiated
A14	Male	61	Squamous cell carcinoma	Poorly differentiated

Figure S1.Tandem mass spectrometry (MS/MS) spectra of multiple potential biomarkers for distinguishing tumor and adjacent normal tissue using multivariate statistical analyses
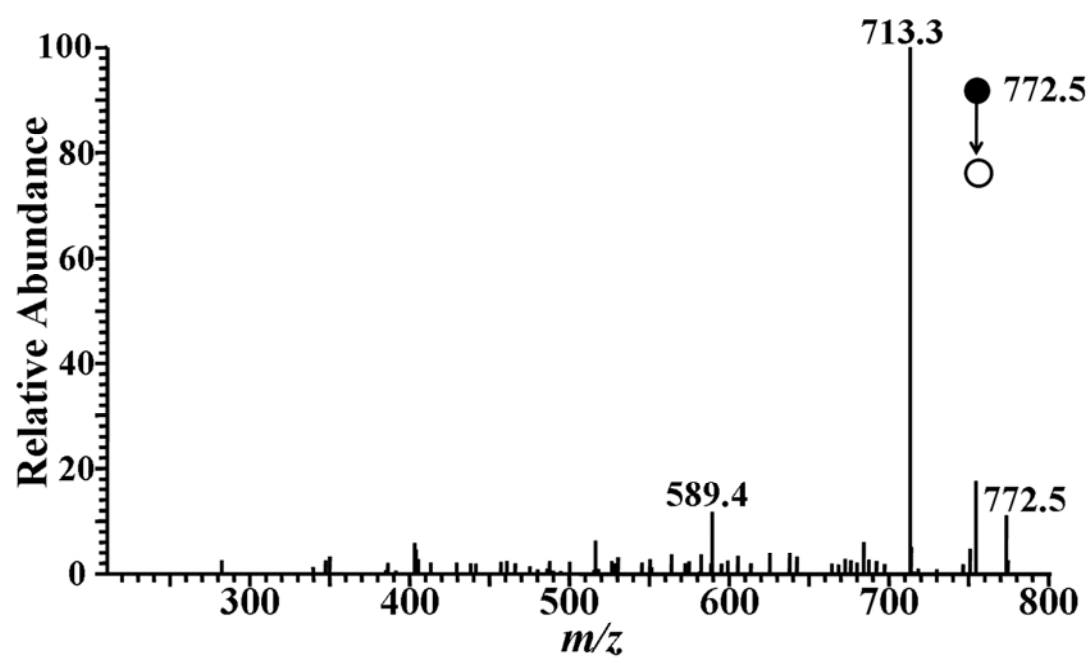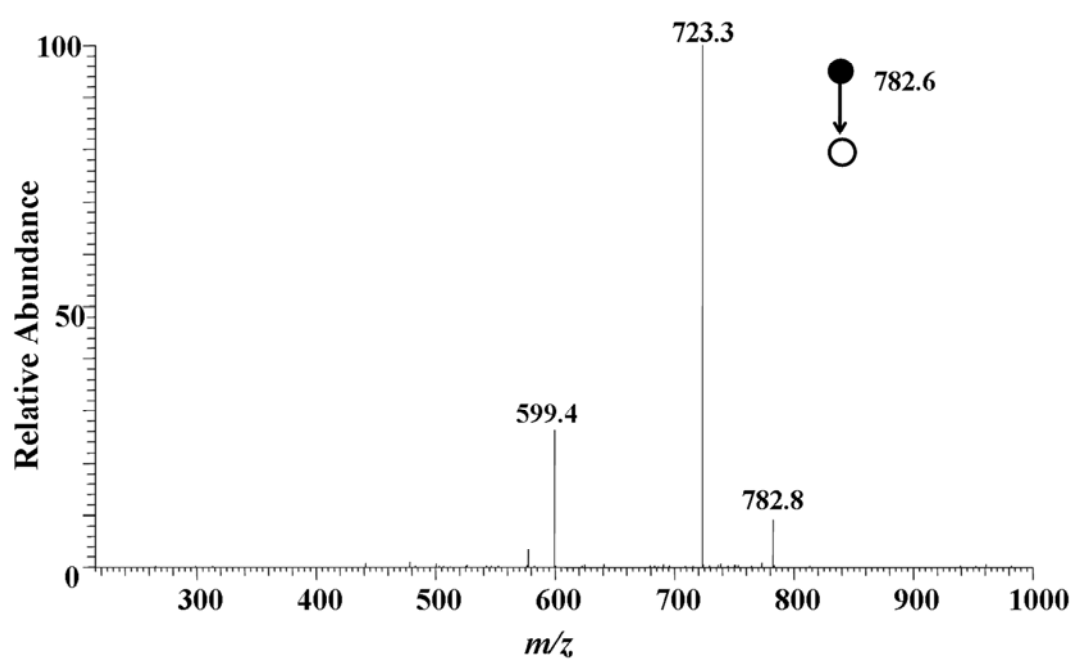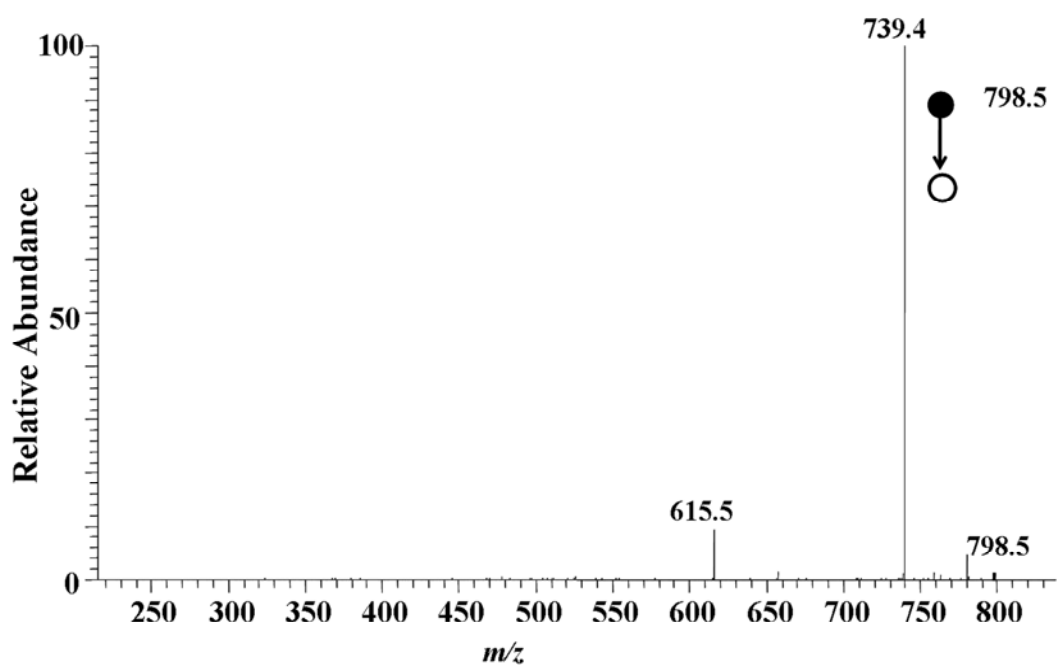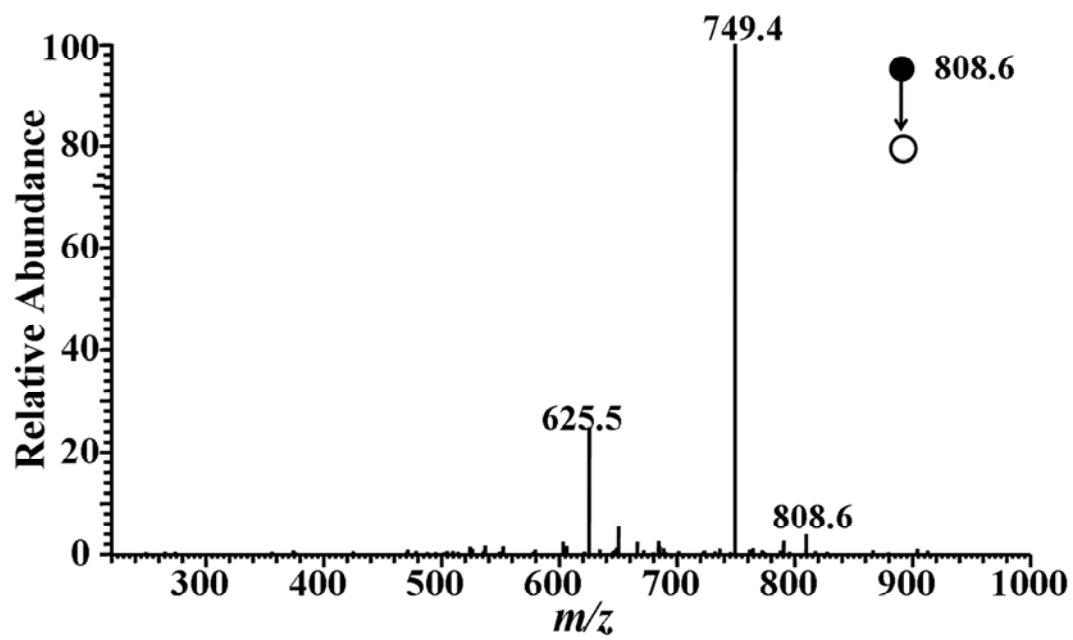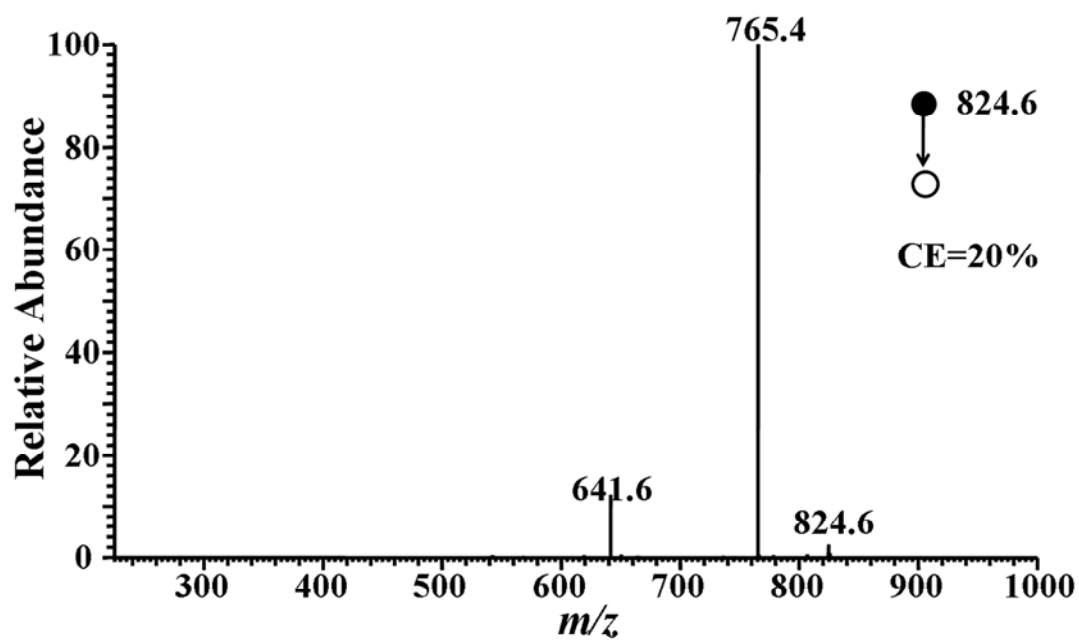
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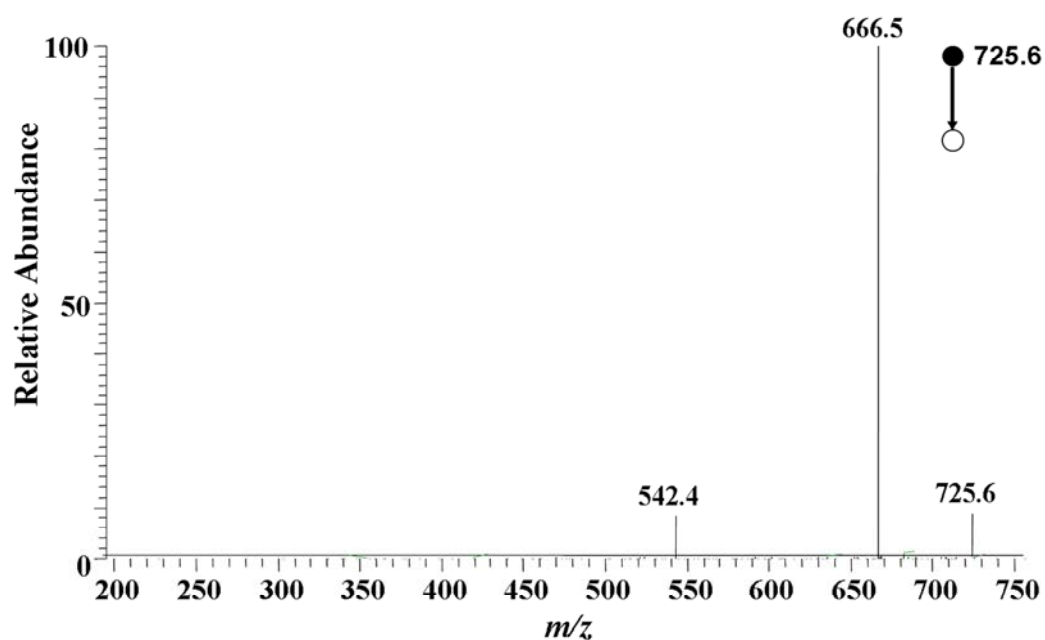
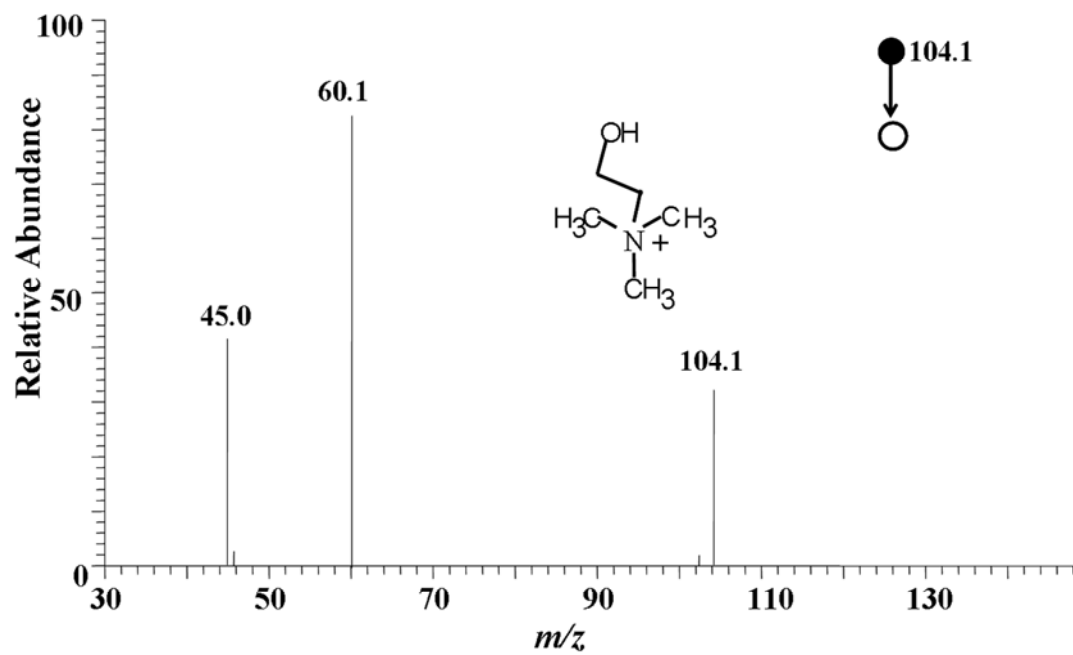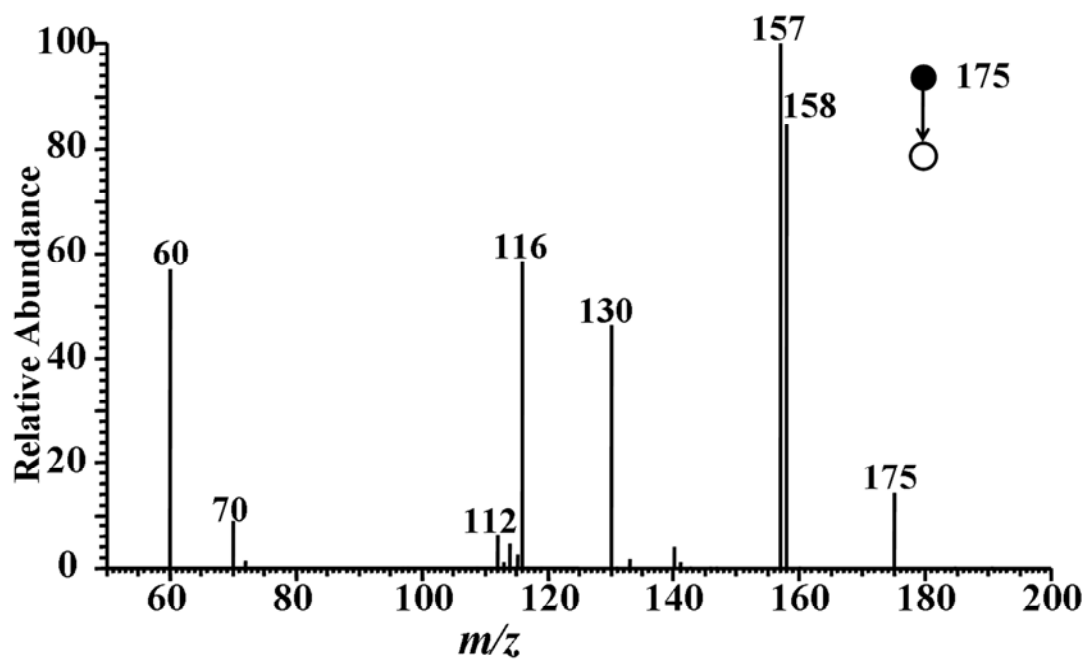(b) m/z 756.6
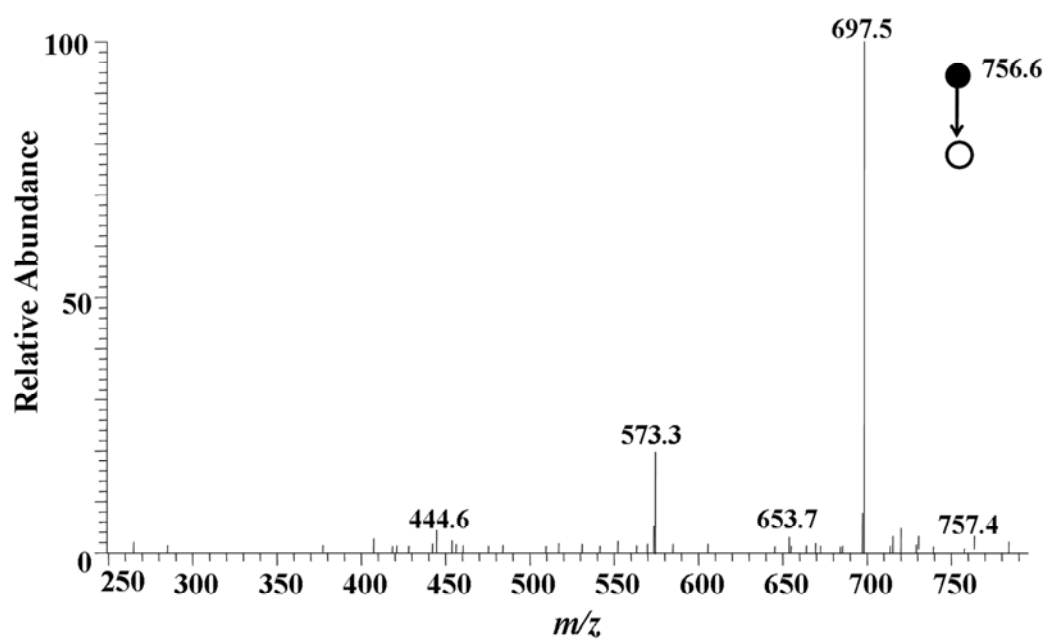
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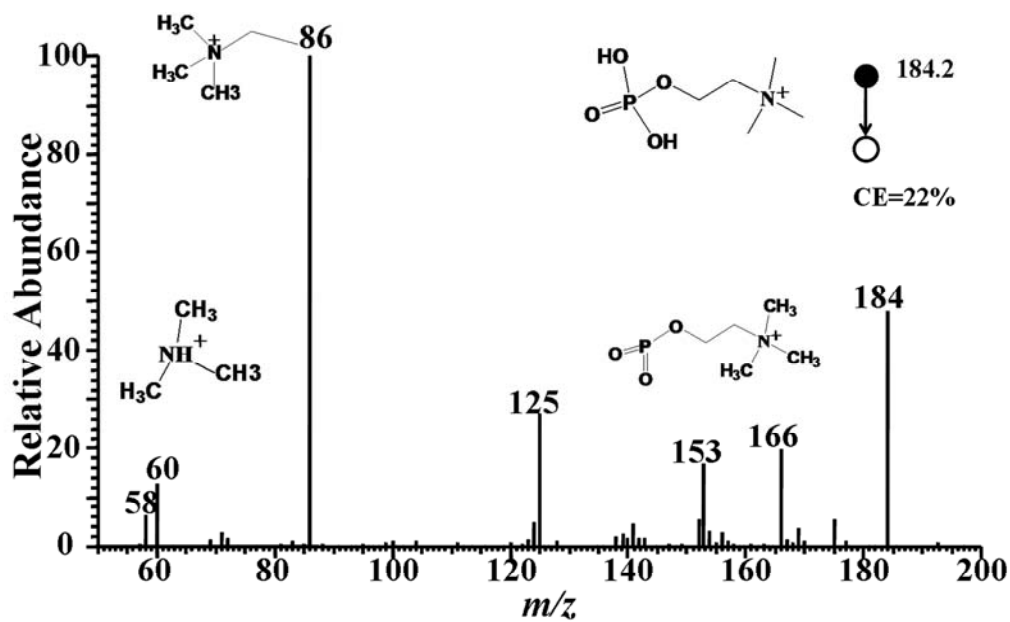(d) m/z 782.6

(e)m/z798.5

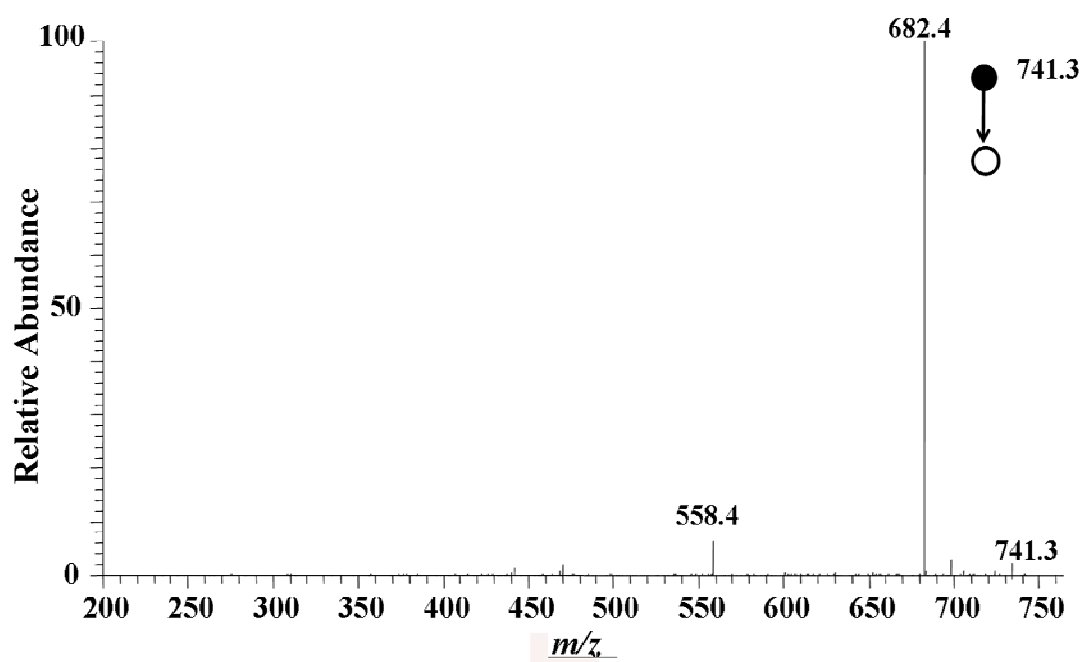(f) m/z 808.6

(g) m/z 824.6

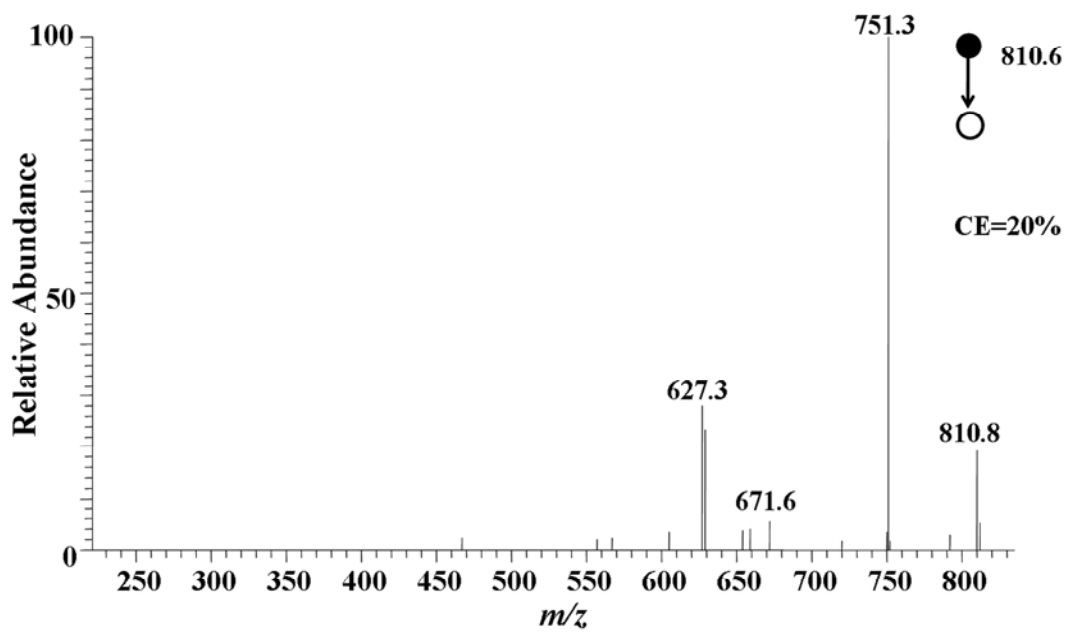

(f) m/z 104.1

(g) m/z 175.2

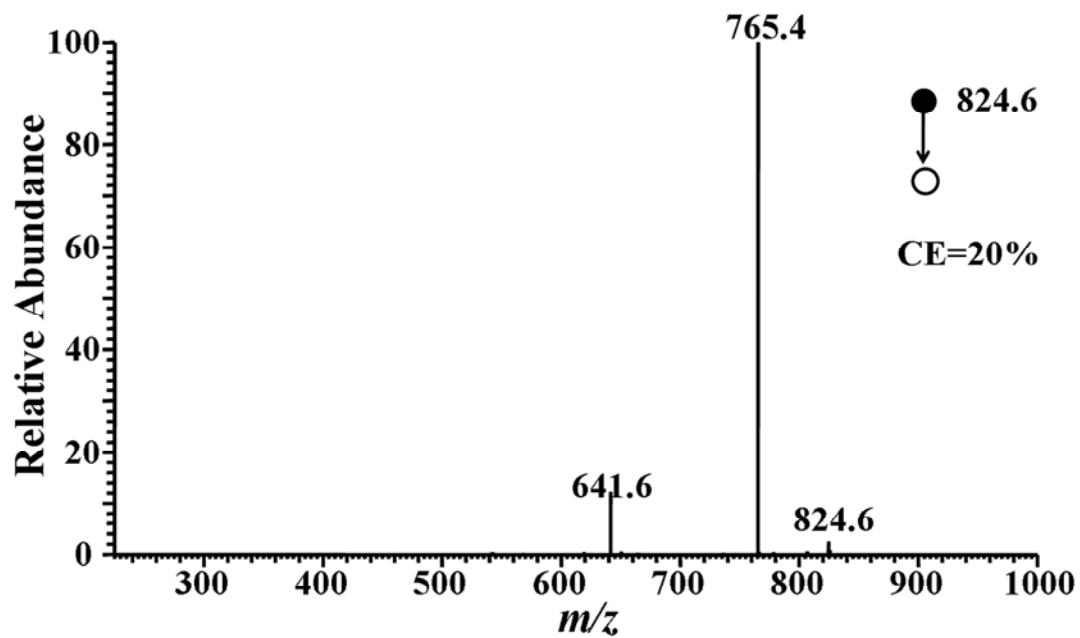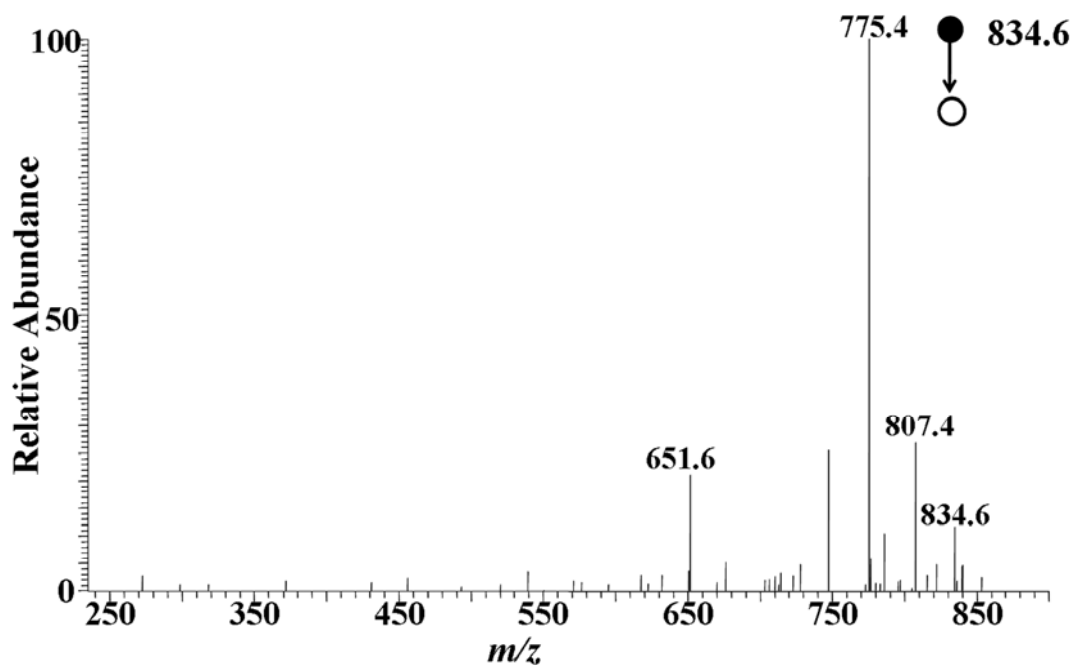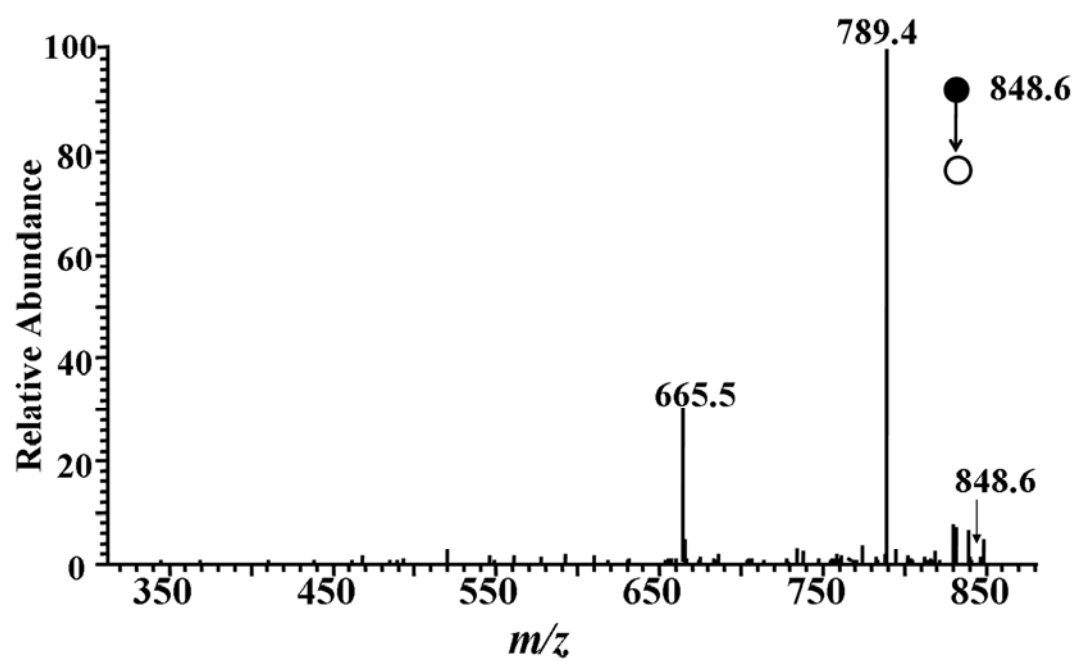(h) m/z 184.2

(I)   m/z 741.3

(J) m/z 810.6

(K) m/z 824.6
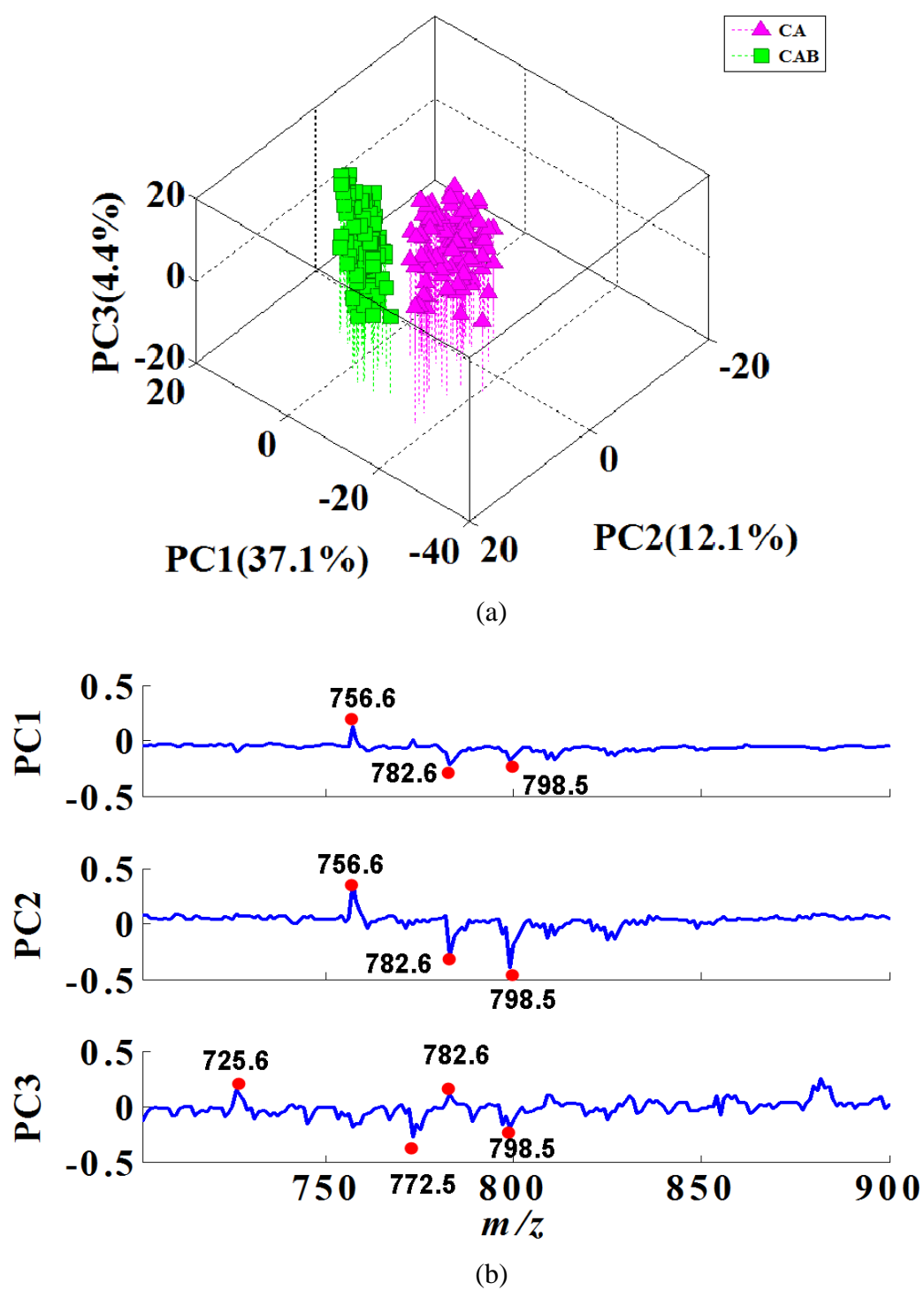

(L) m/z 834.6

(M) m/z 848.6

(a)

(b)

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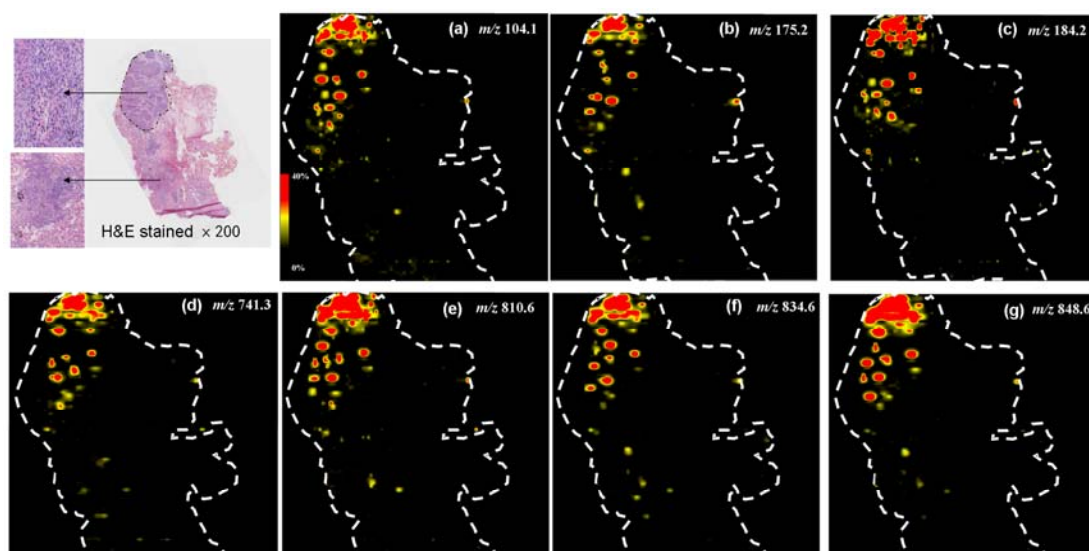
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