

Supplementary Information

Principal Component Analysis with Linear and Quadratic Discriminant Analysis for Identification of Cancer Samples Based on Mass Spectrometry

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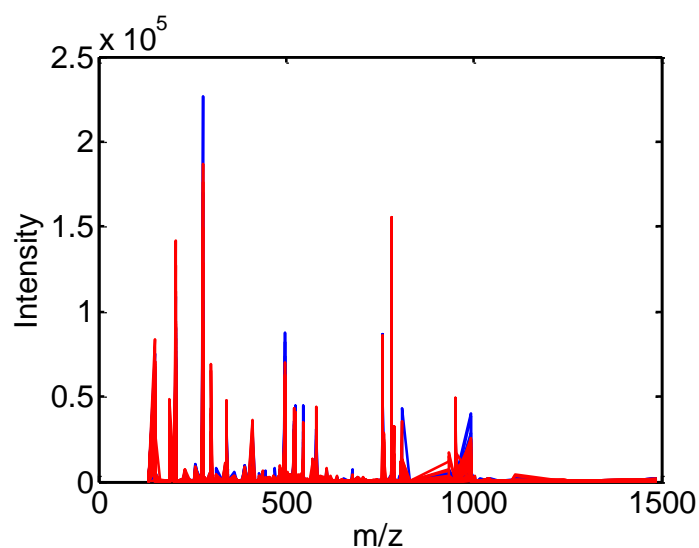


Figure S1. Raw spectra for healthy control (in blue) and ovarian cancer (in red) samples in data set 1.

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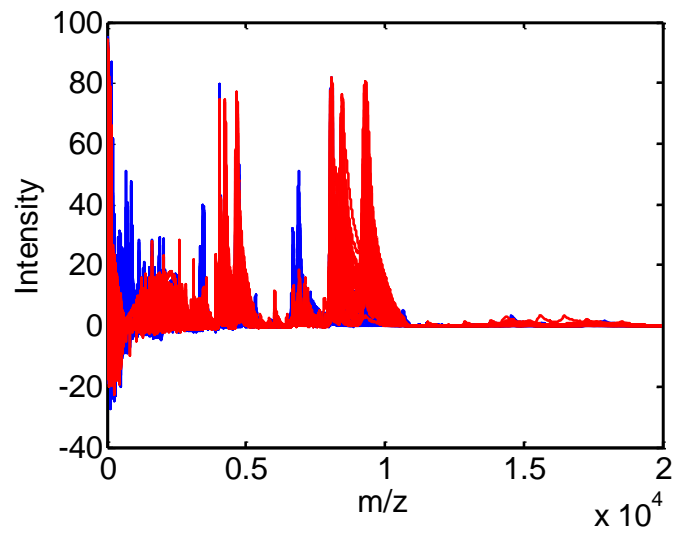


Figure S2. Raw spectra for healthy control (in blue) and prostate cancer (in red) samples in data set 2.

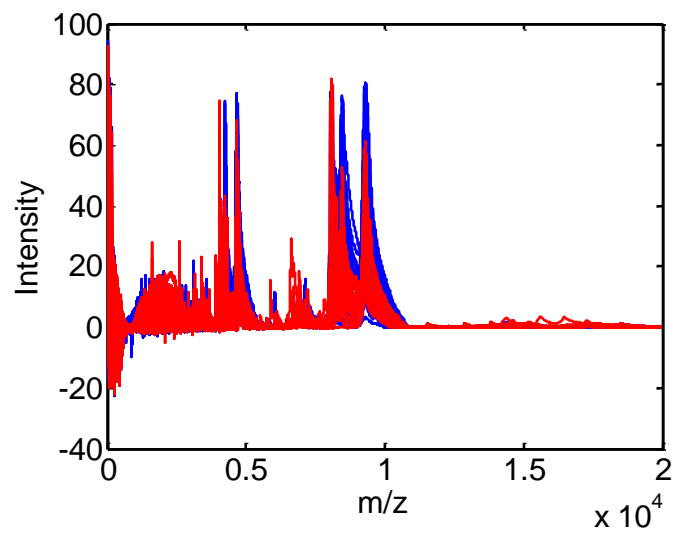


Figure S3. Raw spectra for low grade (PSA 4-10 ng mL^{-1} , in blue) and high grade (PSA > 10 ng mL^{-1} , in red) prostate cancer samples in data set 3.

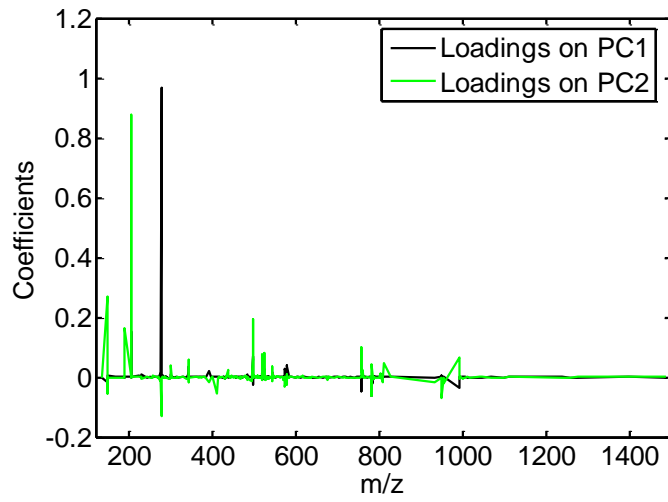


Figure S4. PCA loadings for data set 1: ovarian cancer.

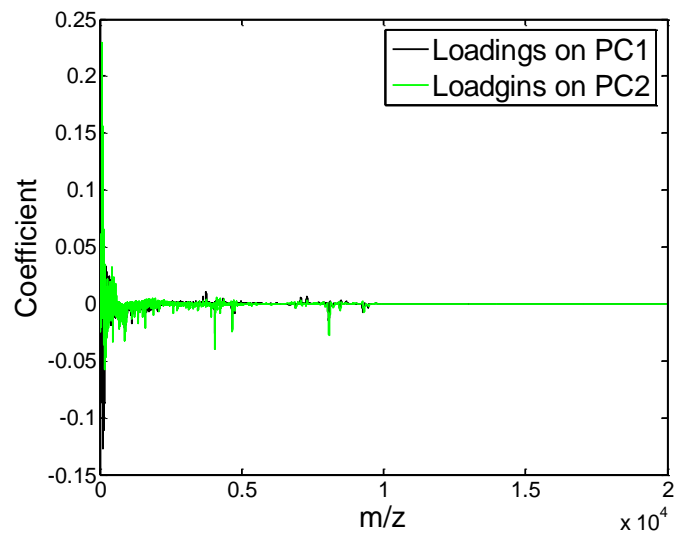


Figure S5. PCA loadings for data set 2: prostate cancer.

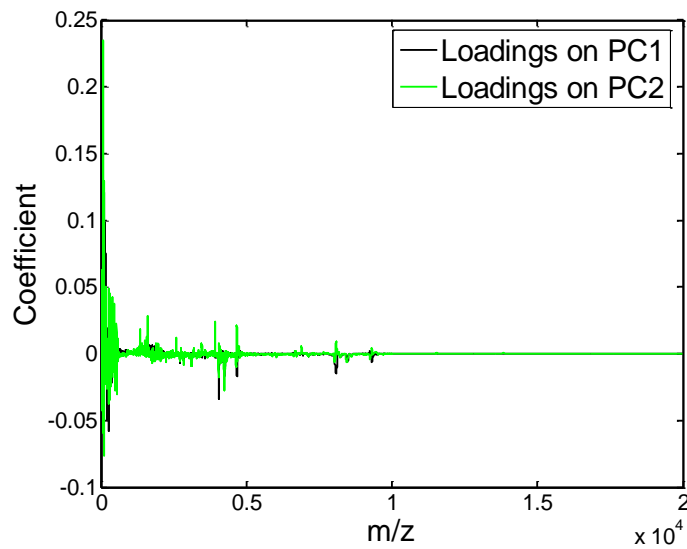


Figure S6. PCA loadings for data set 3: subtypes of prostate cancer.

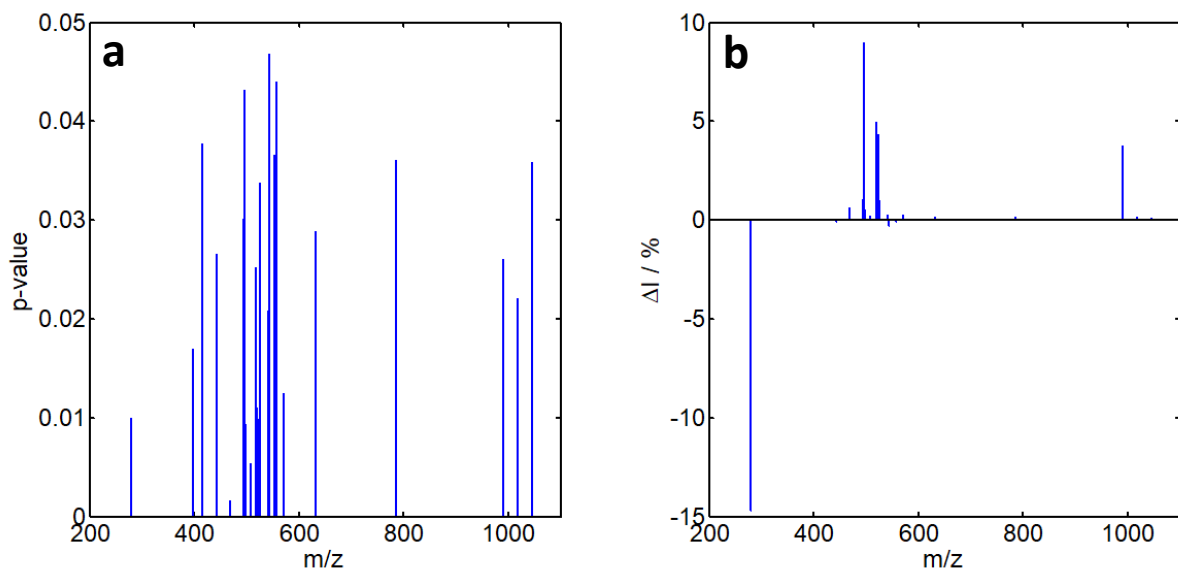


Figure S7. (a) Variables from data set 1 with significant p -value ($p < 0.05$); (b) variation between mean intensity (ΔI) of healthy control and ovarian cancer samples.

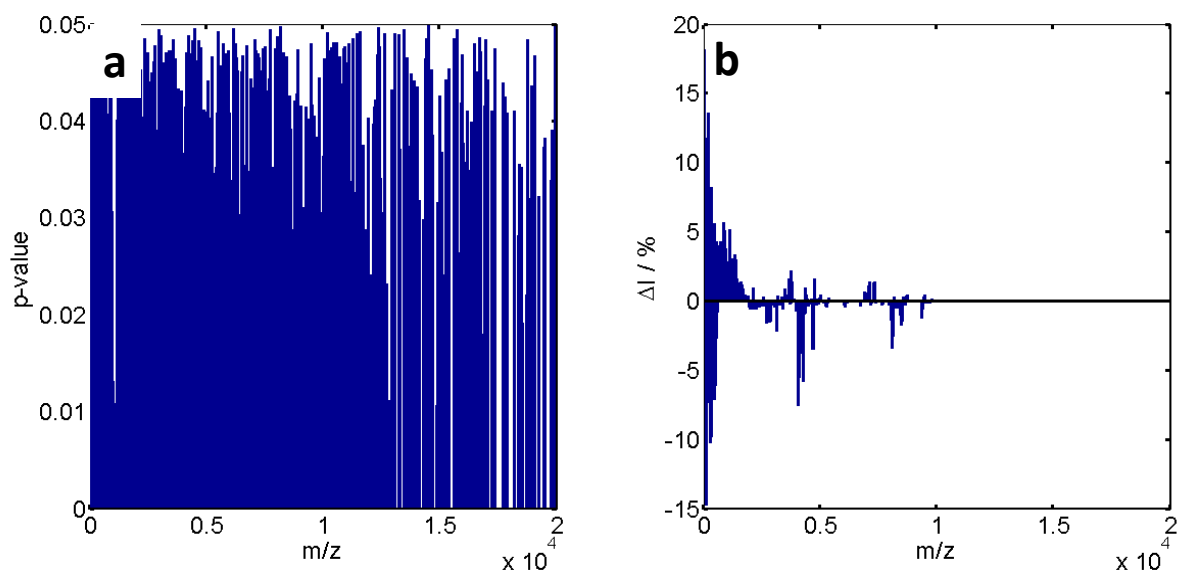


Figure S8. (a) Variables from data set 2 with significant p -value ($p < 0.05$); (b) variation between mean intensity (ΔI) of healthy control and prostate cancer samples.

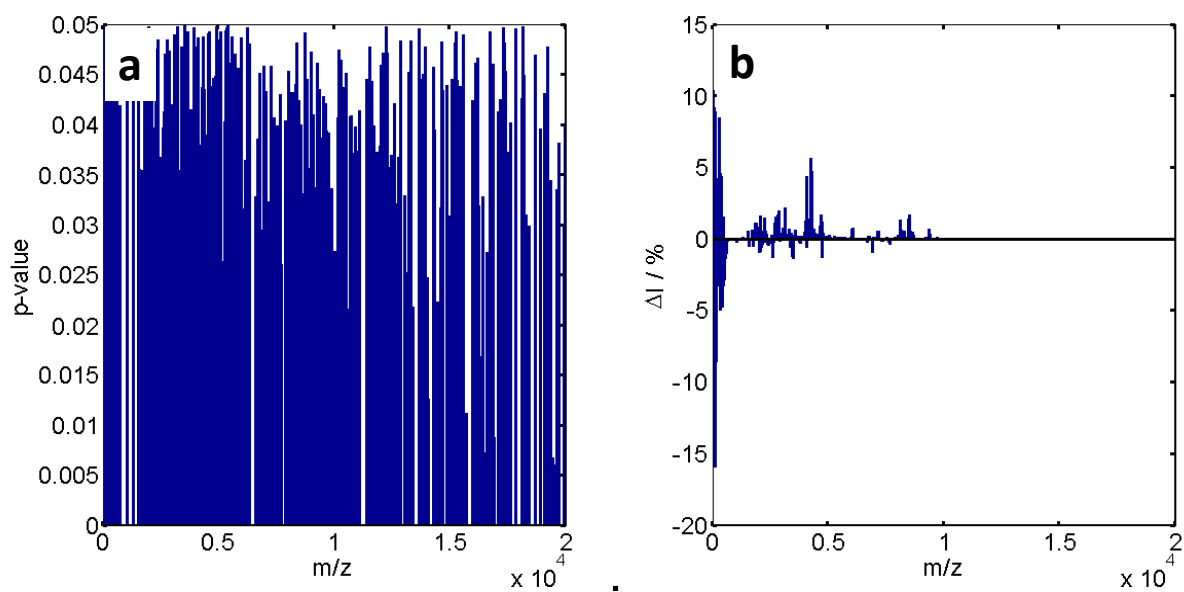


Figure S9. (a) Variables from data set 3 with significant p -value ($p < 0.05$); (b) variation between mean intensity (ΔI) of low grade and high grade prostate cancer samples.

Table S1. Explained variance in the 15 first PCs for data set 1: ovarian cancer

PC	Explained variance / %	Cumulative explained variance / %
1	25.25	25.25
2	13.86	39.11
3	12.07	51.18
4	11.37	62.55
5	7.71	70.26
6	4.71	74.97
7	3.65	78.62
8	3.33	81.95
9	2.31	84.26
10	2.08	86.33
11	1.34	87.67
12	1.28	88.95
13	1.10	90.06
14	0.98	91.04
15	0.88	91.92

Table S2. Explained variance in the 15 first PCs for data set 2: prostate cancer

PC	Explained variance / %	Cumulative explained variance / %
1	35.01	35.01
2	19.41	54.42
3	8.47	62.89
4	4.38	67.27
5	3.80	71.06
6	2.97	74.04
7	2.46	76.50
8	1.71	78.21
9	1.59	79.80
10	1.31	81.11
11	1.21	82.32
12	1.11	83.43
13	0.94	84.37
14	0.88	85.25
15	0.73	85.98

Table S3. Explained variance in the 15 first PCs for data set 3: subtypes of prostate cancer

PC	Explained variance / %	Cumulative explained variance / %
1	37.89	37.89
2	20.11	57.99
3	9.30	67.29
4	5.91	73.20
5	3.25	76.45
6	2.86	79.31
7	2.37	81.68
8	1.76	83.44
9	1.57	85.01
10	1.28	86.29
11	1.09	87.38
12	1.02	88.39
13	0.87	89.26
14	0.76	90.03
15	0.73	90.76