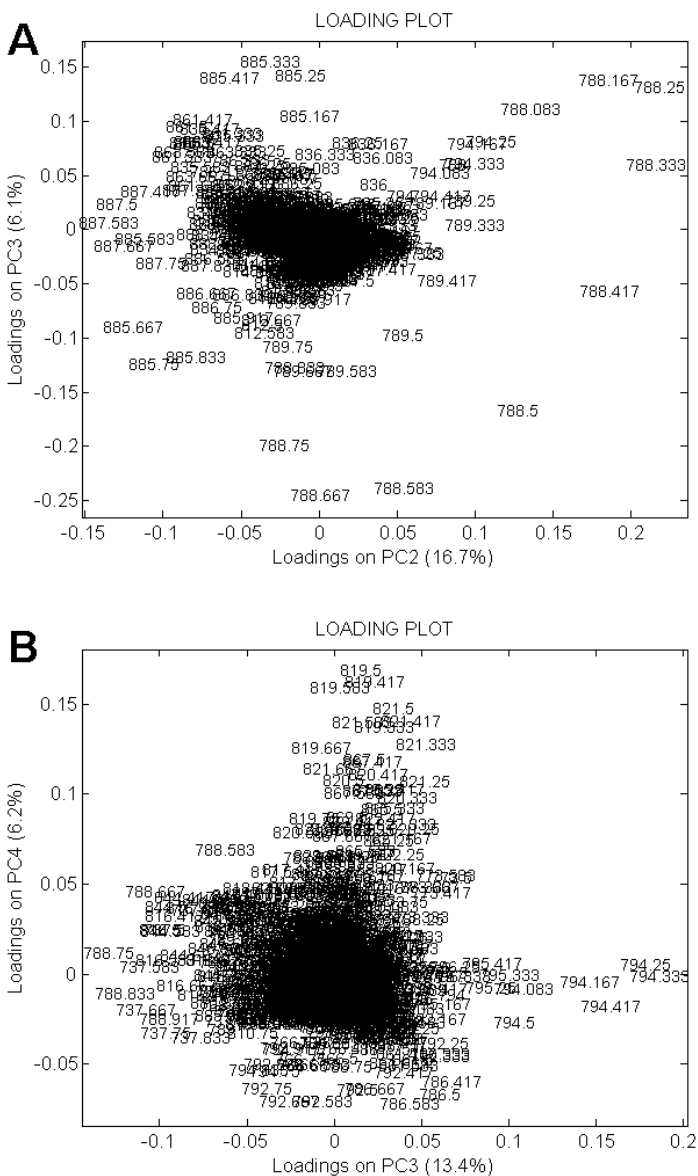


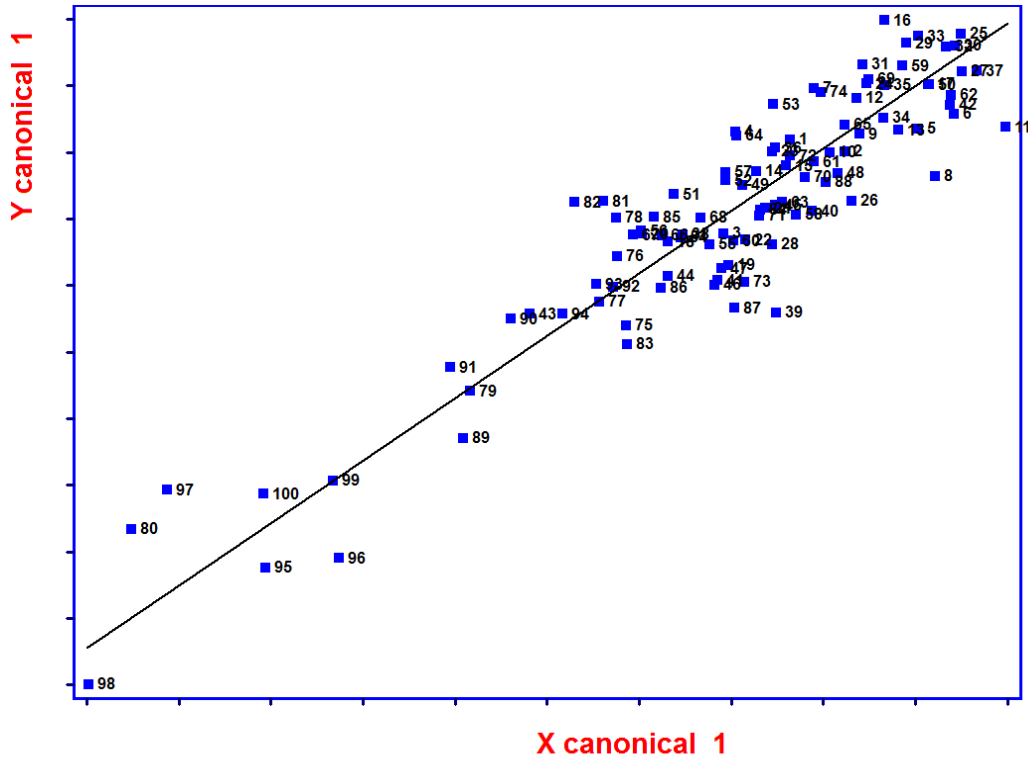
Supplemental Information

Differentiation of Prostate Cancer from Normal Tissue in Radical Prostatectomy Specimens by Desorption Electrospray Ionization and Touch Spray Ionization Mass Spectrometry

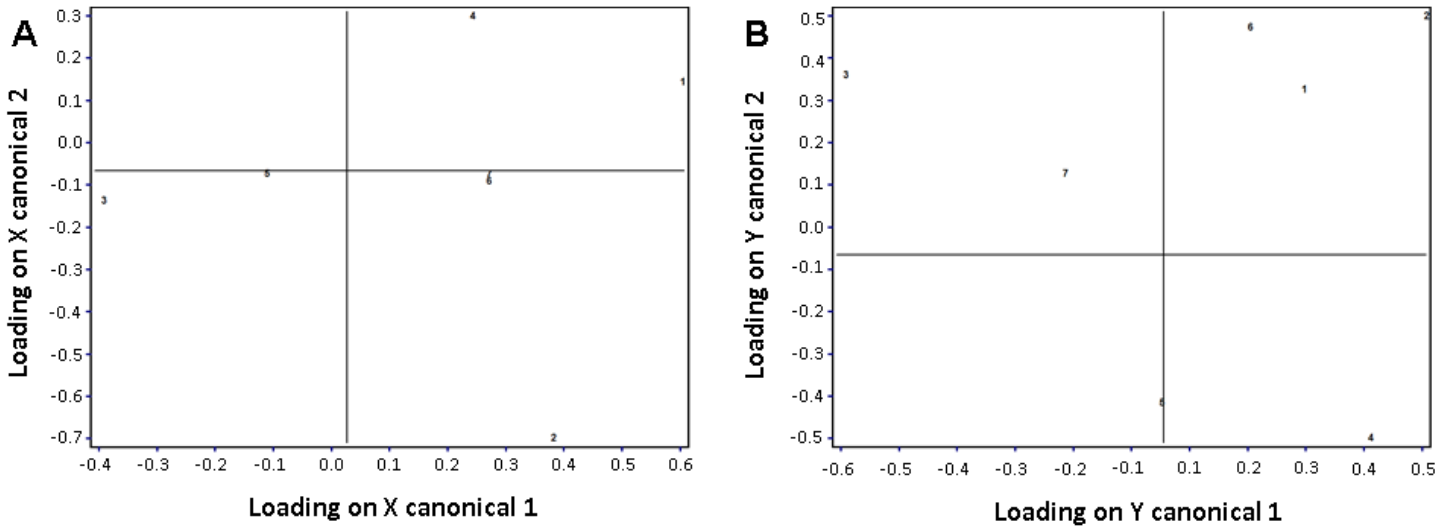
K.S. Kerian,^a A. K. Jarmusch,^a V. Pirro,^a M. O. Koch,^b T. A. Masterson,^b L. Cheng,^c and R. G. Cooks^a



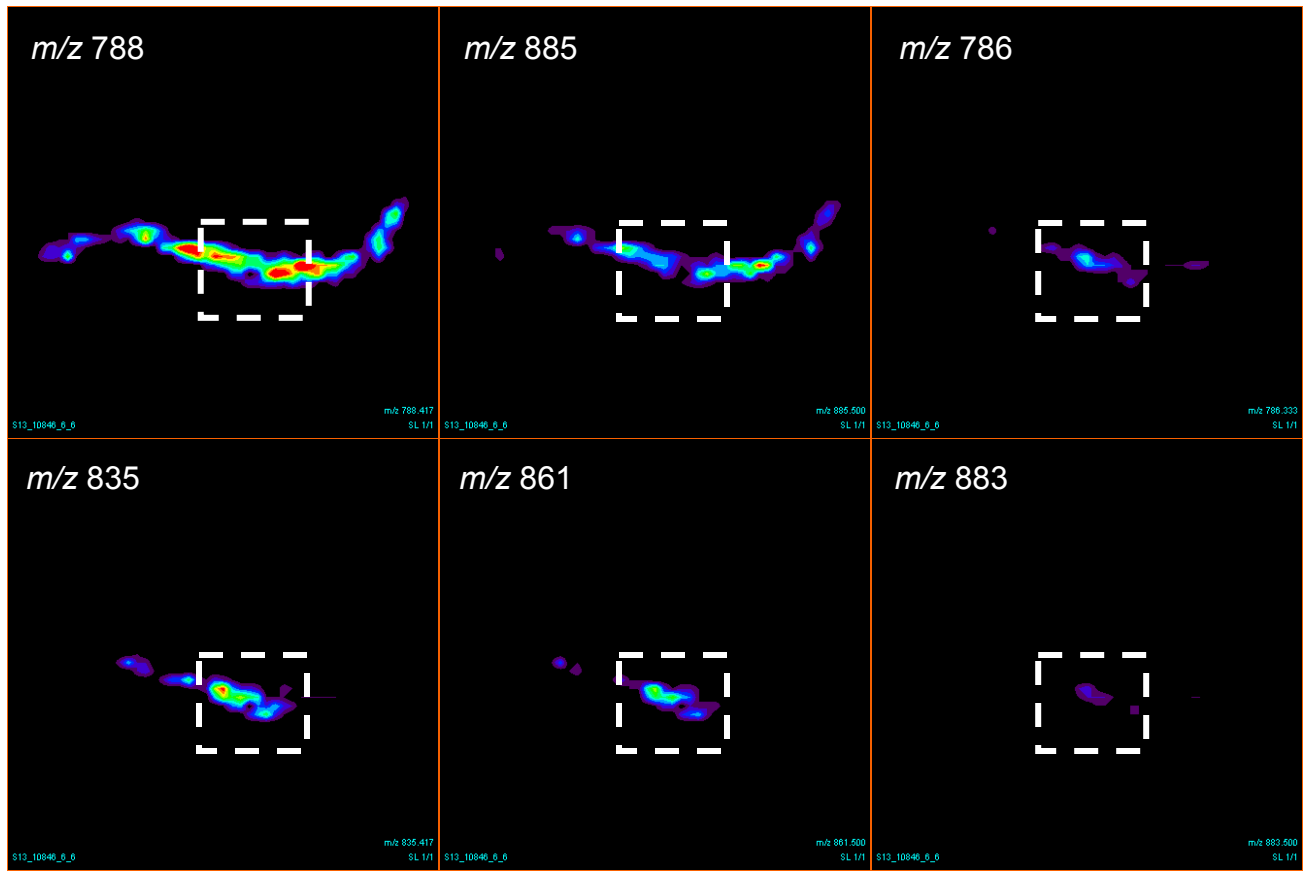
Supplemental Figure 1. (A) PC2 vs. PC3 DESI-MS loading plot displaying ions which contribute to the spread of samples in the score plot. (B) PC3 vs. PC4 TS-MS loading plot displaying ions which contribute to the spread of samples in the score plot. Variables are labeled as *m/z* values.



Supplemental Figure 2. CCA correlation plot between DESI (X) and TS (Y) with the first 3 correlation coefficient being equal to 0.94, 0.76, and 0.68.



Supplemental Figure 3. (A) CCA loading plot displaying greatest canonical variable contribution from the DESI principal components. (B) CCA loading plot displaying greatest canonical variable contribution from the TS principal components.



Supplemental Figure 4. DESI-MS ion images showing the relative distribution of ions m/z 788, 885, 786, 835, 861, and 883. The dashed white line is the region outlined by histopathology as tumor with ions correlating to tumor based on PCA (*i.e.* m/z 786, 835, 861, and 883) in high correlation to the outlined region.

Supplemental Table 1 – Targeted Data Set.

Patient #	Biopsy #	Sample # DESI:TS	Diagnosis	Gleason Score ^{a,b}
1	6	2:8	Tumor	(3+4)=7
2	3	6:3	Tumor	(3+4)=7
2	2	3:6	Normal	(3+4)=7
3	9	5:6	Tumor	(4+3)=7
3	7	6:3	Normal	(4+3)=7
4	3	6:4	Tumor	(4+3)=7
4	6	6:3	Tumor	(4+3)=7
4	9	5:7	Tumor	(4+3)=7
4	7	2:4	Normal	(4+3)=7
5	1	3:1	Normal	(4+5)=9
5	2	5:3	Normal	(4+5)=9
5	3	5:4	Normal	(4+5)=9
5	4	7:4	Normal	(4+5)=9
5	5	3:4	Normal	(4+5)=9
5	6	5:3	Tumor	(4+5)=9
5	7	6:3	Normal	(4+5)=9
5	8	2:7	Normal	(4+5)=9
5	9	5:4	Normal	(4+5)=9
6	1	5:2	Normal	(4+3)=7
6	2	5:3	Tumor	(4+3)=7
6	3	7:3	Normal	(4+3)=7
6	4	4:7	Tumor	(4+3)=7
6	5	4:6	Normal	(4+3)=7
6	6	3:7	Tumor	(4+3)=7
6	7	7:8	Tumor	(4+3)=7
6	8	8:6	Tumor	(4+3)=7
6	9	7:4	Tumor	(4+3)=7
6	10	5:4	Tumor	(4+3)=7
7	5	6:7	Normal	(4+3)=7
7	6	3:4	Normal	(4+3)=7
7	7	4:5	Normal	(4+3)=7
7	8	4:5	Normal	(4+3)=7
7	10	3:4	Normal	(4+3)=7
7	12	5:4	Tumor	(4+3)=7
7	14	3:4	Normal	(4+3)=7
8	2	6:5	Normal	(3+4)=7
8	3	5:6	Normal	(3+4)=7
8	4	6:7	Normal	(3+4)=7
8	5	3:4	Normal	(3+4)=7
8	6	5:6	Tumor	(3+4)=7
8	7	7:6	Normal	(3+4)=7
8	8	5:4	Normal	(3+4)=7
8	9	7:6	Tumor	(3+4)=7
8	10	5:4	Tumor	(3+4)=7
8	11	3:4	Normal	(3+4)=7
8	12	7:6	Normal	(3+4)=7
8	13	6:5	Normal	(3+4)=7
8	15	4:6	Normal	(3+4)=7
9	3	4:5	Normal	(3+4)=7
9	7	6:7	Normal	(3+4)=7

9	8	6:5	Normal	(3+4)=7
9	10	5:4	Normal	(3+4)=7
9	13	6:7	Normal	(3+4)=7
9	14	3:2	Normal	(3+4)=7
9	15	6:5	Normal	(3+4)=7
9	17	3:4	Tumor	(3+4)=7
10	1	7:6	Normal	(4+3)=7
10	2	5:6	Normal	(4+3)=7
10	3	6:5	Normal	(4+3)=7
10	4	4:3	Normal	(4+3)=7
10	5	6:7	Tumor	(4+3)=7
10	6	4:5	Normal	(4+3)=7
10	8	6:7	Normal	(4+3)=7
10	9	4:5	Normal	(4+3)=7
10	10	6:5	Normal	(4+3)=7
10	11	6:7	Normal	(4+3)=7
10	12	5:6	Normal	(4+3)=7
10	13	7:6	Normal	(4+3)=7
10	14	4:3	Normal	(4+3)=7
10	16	6:7	Normal	(4+3)=7
11	1	5:4	Normal	(4+5)=9
11	2	4:5	Normal	(4+5)=9
11	3	5:6	Normal	(4+5)=9
11	4	6:5	Normal	(4+5)=9
11	5	7:5	Tumor	(4+5)=9
11	7	6:5	Tumor	(4+5)=9
11	8	5:4	Normal	(4+5)=9
11	9	4:5	Tumor	(4+5)=9
11	10	5:4	Tumor	(4+5)=9
11	11	5:6	Normal	(4+5)=9
11	12	4:5	Normal	(4+5)=9
11	13	5:4	Normal	(4+5)=9
11	15	5:4	Normal	(4+5)=9
11	16	5:4	Normal	(4+5)=9
11	17	3:4	Normal	(4+5)=9
11	18	3:4	Normal	(4+5)=9
11	20	3:4	Tumor	(4+5)=9
11	21	4:3	Normal	(4+5)=9
11	22	6:5	Normal	(4+5)=9
11	23	6:5	Tumor	(4+5)=9
11	24	3:4	Normal	(4+5)=9
11	25	3:4	Normal	(4+5)=9
11	27	3:4	Normal	(4+5)=9
12	2	5:4	Normal	(4+3)=7
12	7	5:6	Normal	(4+3)=7
12	8	4:5	Normal	(4+3)=7
12	9	6:5	Normal	(4+3)=7
12	10	4:3	Normal	(4+3)=7
12	13	2:3	Normal	(4+3)=7
12	15	4:3	Normal	(4+3)=7

^aGleason score is based on the final pathology report per patient, first number is the primary score followed by the secondary score which sums to the overall Gleason score.

^bAccording to gross pathology reports, not the tissue sections analyzed by histopathology

Supplemental Table 1 – Evaluation Data Set.

Patient #	Biopsy #	Sample # TS	Diagnosis	Gleason Score ^{a,b}
1	6	4	Tumor	(3+4)=7
1	8	1	Normal	(3+4)=7
2	3	1	Tumor	(3+4)=7
2	3	1	Normal	(3+4)=7
2	2	1	Normal	(3+4)=7
3	9	3	Normal	(4+3)=7
3	7	2	Normal	(4+3)=7
3	7	2	Normal	(4+3)=7
4	6	1	Normal	(4+3)=7
4	6	1	Tumor	(4+3)=7
4	7	5	Normal	(4+3)=7
4	7	5	Normal	(4+3)=7
5	6	5	Tumor	(4+5)=9
6	6	1	Tumor	(4+3)=7
6	3	2	Normal	(4+3)=7
6	3	2	Normal	(4+3)=7
7	10	5	Normal	(4+3)=7
7	12	2	Normal	(4+3)=7
7	12	2	Tumor	(4+3)=7
8	9	4	Normal	(3+4)=7
8	9	4	Tumor	(3+4)=7
8	15	3	Normal	(3+4)=7
8	15	3	Normal	(3+4)=7
9	15	4	Normal	(3+4)=7
9	15	4	Normal	(3+4)=7
9	17	5	Normal	(3+4)=7
10	11	4	Normal	(4+3)=7
11	5	3	Normal	(4+5)=9
11	23	3	Normal	(4+5)=9
11	23	3	Normal	(4+5)=9
12	14	4	Normal	(4+3)=7
13	9	5	Normal	(3+4)=7
13	11	2	Normal	(3+4)=7
13	14	3	Normal	(3+4)=7
13	18	3	Normal	(3+4)=7
14	2	5	Normal	(4+3)=7
14	2	5	Normal	(4+3)=7
14	3	5	Normal	(4+3)=7
14	4	3	Normal	(4+3)=7
14	4	3	Normal	(4+3)=7
14	5	4	Normal	(4+3)=7
14	6	4	Normal	(4+3)=7
14	8	5	Normal	(4+3)=7
14	8	5	Normal	(4+3)=7
14	10	5	Normal	(4+3)=7
14	10	5	Normal	(4+3)=7
14	12	5	Normal	(4+3)=7
14	12	5	Normal	(4+3)=7
14	14	3	Normal	(4+3)=7

15	2	5	Normal	(3+4)=7
15	3	4	Normal	(3+4)=7
15	3	4	Normal	(3+4)=7
15	8	5	Normal	(3+4)=7
15	8	5	Normal	(3+4)=7
15	10	3	Normal	(3+4)=7
15	10	3	Normal	(3+4)=7
15	11	5	Normal	(3+4)=7
15	12	5	Normal	(3+4)=7
15	13	4	Normal	(3+4)=7
15	14	5	Normal	(3+4)=7
15	14	5	Normal	(3+4)=7
15	15	4	Normal	(3+4)=7
15	15	4	Normal	(3+4)=7
16	7	6	Normal	(4+3)=7
16	7	6	Normal	(4+3)=7
16	10	5	Normal	(4+3)=7
16	11	4	Normal	(4+3)=7
16	11	4	Normal	(4+3)=7
16	12	4	Normal	(4+3)=7
16	12	4	Normal	(4+3)=7
16	14	3	Normal	(4+3)=7
16	14	3	Normal	(4+3)=7
16	15	3	Normal	(4+3)=7
16	15	3	Normal	(4+3)=7
16	16	2	Normal	(4+3)=7
16	16	2	Normal	(4+3)=7
17	1	6	Normal	(3+4)=7
17	1	6	Normal	(3+4)=7
17	2	5	Normal	(3+4)=7
17	4	5	Normal	(3+4)=7
17	4	5	Normal	(3+4)=7
17	5	4	Normal	(3+4)=7
17	5	4	Normal	(3+4)=7
17	6	5	Normal	(3+4)=7
17	6	5	Normal	(3+4)=7
17	7	3	Normal	(3+4)=7
17	7	3	Normal	(3+4)=7
17	8	3	Normal	(3+4)=7
17	8	3	Normal	(3+4)=7
17	9	4	Normal	(3+4)=7
17	9	4	Normal	(3+4)=7
17	10	6	Normal	(3+4)=7
17	10	6	Normal	(3+4)=7
17	12	4	Normal	(3+4)=7
17	13	5	Normal	(3+4)=7
17	13	5	Normal	(3+4)=7
17	15	4	Normal	(3+4)=7
17	15	4	Normal	(3+4)=7
18	3	4	Tumor	(5+4)=9
18	4	2	Normal	(5+4)=9
18	7	4	Normal	(5+4)=9
18	7	4	Normal	(5+4)=9

18	10	4	Normal	(5+4)=9
18	10	4	Normal	(5+4)=9
18	11	3	Normal	(5+4)=9
18	11	3	Tumor	(5+4)=9
18	12	5	Normal	(5+4)=9
18	13	4	Normal	(5+4)=9
18	16	4	Normal	(5+4)=9
18	16	4	Normal	(5+4)=9

^aGleason score is based on the final pathology report per patient, first number is the primary score followed by the secondary score which sums to the overall Gleason score.

^bAccording to gross pathology reports, not the tissue sections analyzed by histopathology