Molecular characterization of prostate cancer with associated Gleason score using mass spectrometry imaging

Supplementary Data

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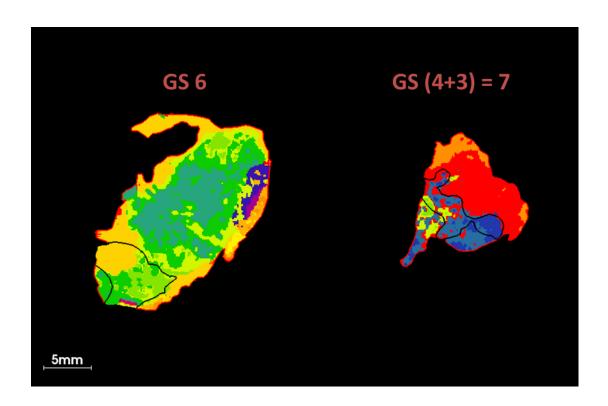
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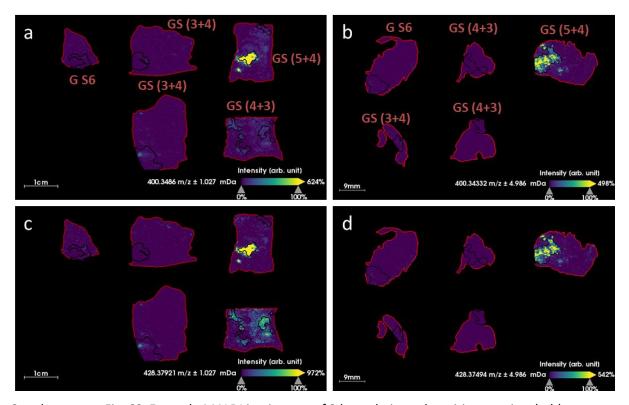
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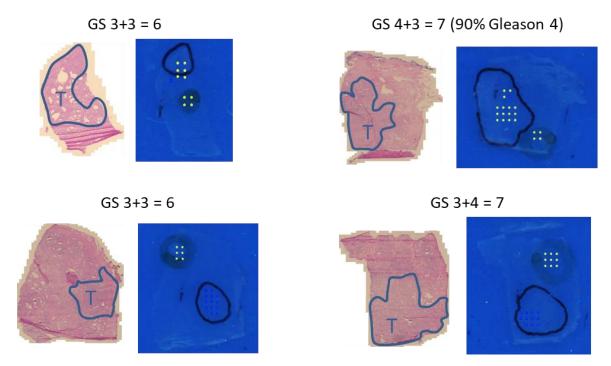
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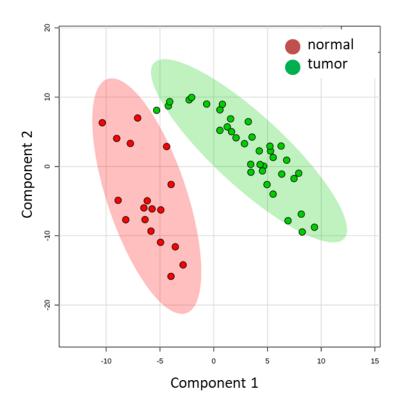
Supplementary Fig. S1. Segmentation map of a subset of lower Gleason tissue specimens, demonstrates regional differences between tumor and normal tissue, and between the two different Gleason grades.



Supplementary Fig. S2. Example MALDI ion images of 2 long chain acylcarnitine species, (a-b) palmitoylcarnitine (m/z 400.3433, Δ ppm = 2.9) and (c-d) stearoylcarnitine (m/z 428.3749, Δ ppm = 3.5); these are detected with high intensity in GS 9 specimens, low intensity in one specimen of GS (4+3) = 7 and in one very small region of one specimen of GS (3+4), and not detected at all in GS 6.



Supplementary Fig. S3. Annotated H&E and serial frozen sections of human prostate tissue, tumor regions are outlined in blue and marked 'T', and regions of normal epithelium were marked in green. Locations selected for LESA MS analysis are marked as yellow or blue spots over regions transferred from the H&E sections. The maximum number of points to fit within designated tumor or normal regions and spaced 1 mm apart, were selected and analyzed.



Supplemental Fig. S4 Scores plot from PLSDA multivariate analysis of LESA MS data from tumor and normal prostate tissue.

 $Supplementary\ Table\ 1.\ Pathological\ description\ of\ specimens\ used\ for\ MALDI\ MSI,\ cases\ were\ staged\ according\ to\ AJCC\ TNM\ 8^{th}\ edition.$

Specimen	рТ	pΝ	Extraprostatic extension	Seminal vesicles	Lymphovascular invasion	Resection margin
1	2	0	not detected	tumor-free	not detected	tumor-free
2	3a	0	present	tumor-free	present	focally positive
3	2	0	not detected	tumor-free	not detected	tumor-free
4	3b	0	present	both invaded	not detected	tumor-free
5	2	X	not detected	tumor-free	present	focally positive
6	3a	Х	present	tumor-free	present	tumor-free
7	3a	0	present	tumor-free	not detected	focally positive
8	3b	0	present	both invaded	present	positive
9	3a	Х	present	tumor-free	not detected	focally positive
10	2	0	not detected	tumor-free	not detected	tumor-free