

Multiplatform investigation of plasma and tissue lipid signatures of breast cancer using mass spectrometry tools

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Supplementary information contains:

- A table with the summary of the type of samples collected for each breast cancer woman
- Supplementary Figures

Supplementary Table S1: Summary of the type of samples collected for each breast cancer woman

Subject #	Type of sample			Type
	plasma	biopsy	surgical specimen	NST ¹ / ST ²
1	yes	yes	yes	ST
2	yes	yes	yes	ST
3	yes	yes	yes	NST
4	yes	yes	yes	NST
5	yes	yes	yes	ST
6	yes	yes	no	ST
7	yes	yes	no	NST
8	yes	yes	no	NST
9	yes	yes	no	NST
10	yes	yes	no	NST
11	yes	yes	no	NST
12	yes	yes	no	ST
13	yes	yes	no	NST
14	yes	yes	no	ST
15	yes	no	yes	NST
16	yes	no	yes	NST
17	yes	no	yes	ST
18	yes	no	yes	NST
19	yes	no	yes	ST
20	yes	no	no	NST
21	no	yes	no	NST
22	no	yes	no	NST
23	no	no	yes	NST
24	no	no	yes	NST

¹ST: special type ductal carcinoma of the breast. ²NST: no special type.

Note: We included 24 women with breast cancer. From them, 20 women had blood samples collected and 23 had cancer breast tissue collected. Among women who had their tissue collected, 11 of them had only biopsy, 7 had only surgical specimens and 5 had biopsy and surgical specimens.

Supplementary Figures

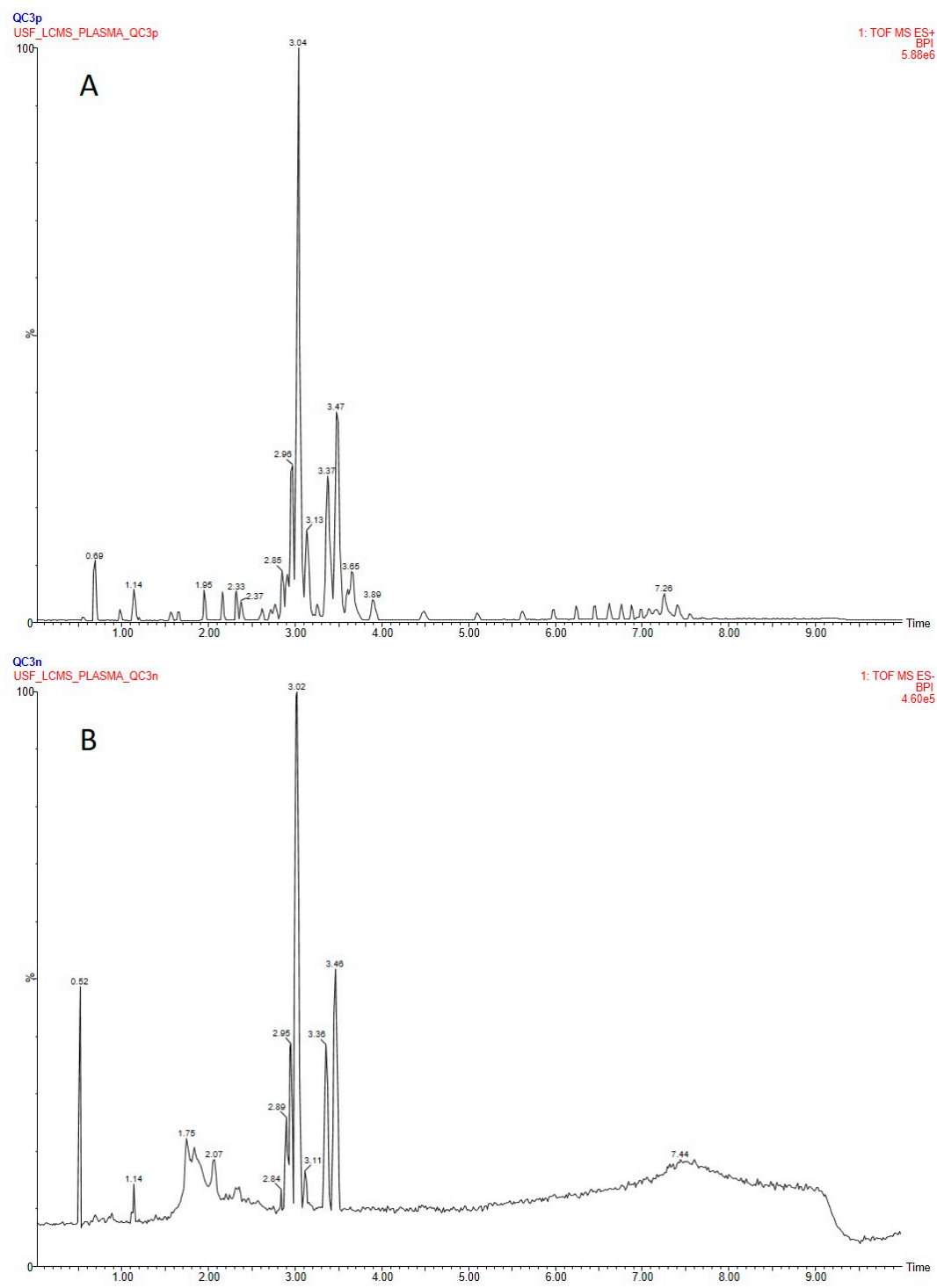


Figure S1: Base peak ion (BPI) chromatograms for a representative quality control (QC) sample acquired in (A) the positive ion mode and (B) the negative ion mode.

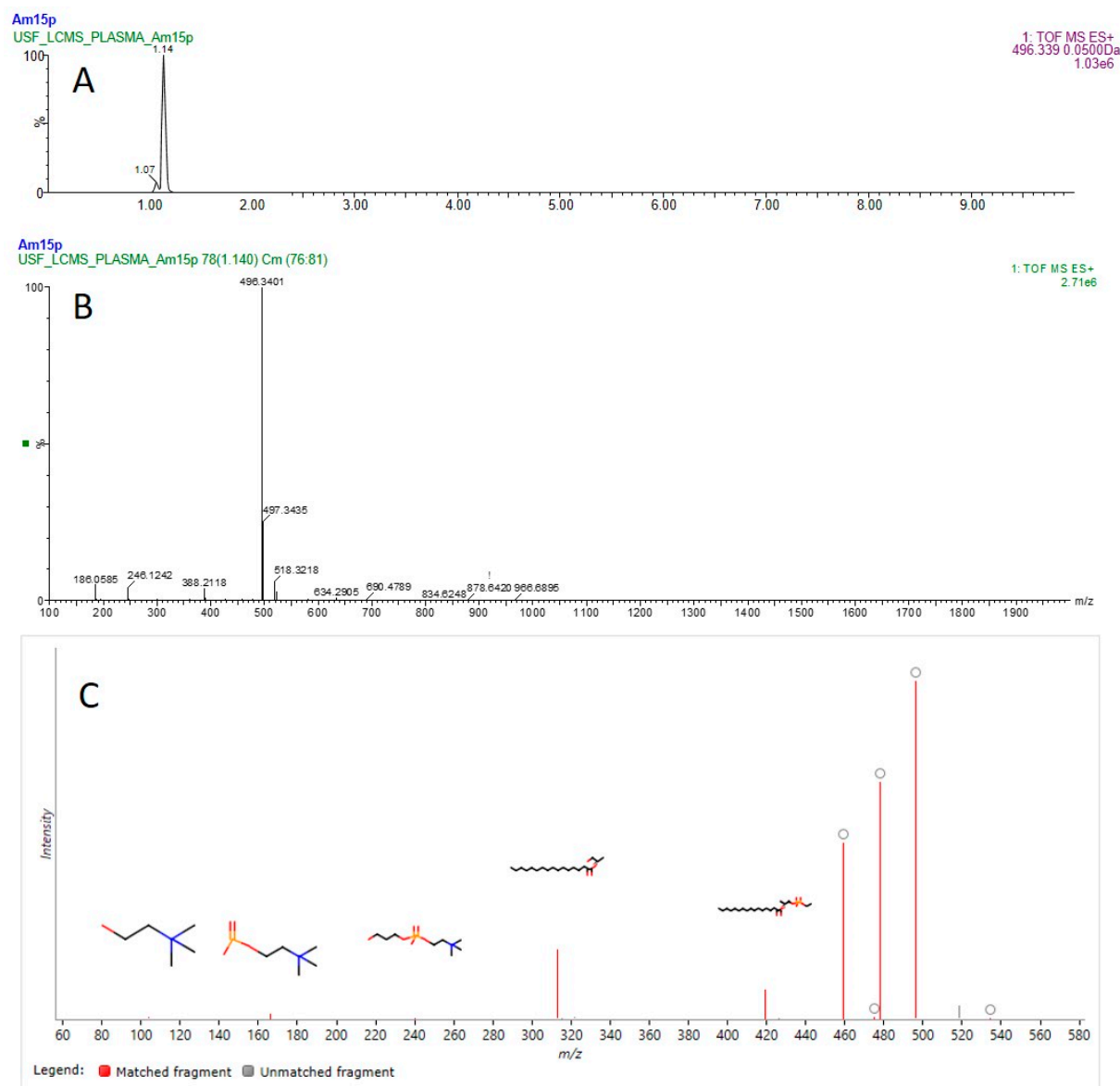


Figure S2: Data for one characteristic ion of healthy plasma samples observed in the positive ion mode. The LysoPC (16:0), observed as the $[M + H]^+$ adduct at m/z 496.3399. The extracted ion chromatogram (EIC) is shown in (A). The low-energy mass spectrum is shown in (B). The deconvoluted fragmentation spectrum obtained by Progenesis Q1 (Waters), showing the identifying fragments is shown in (C), where red signalizes the matched fragments, according to theoretical fragmentation.

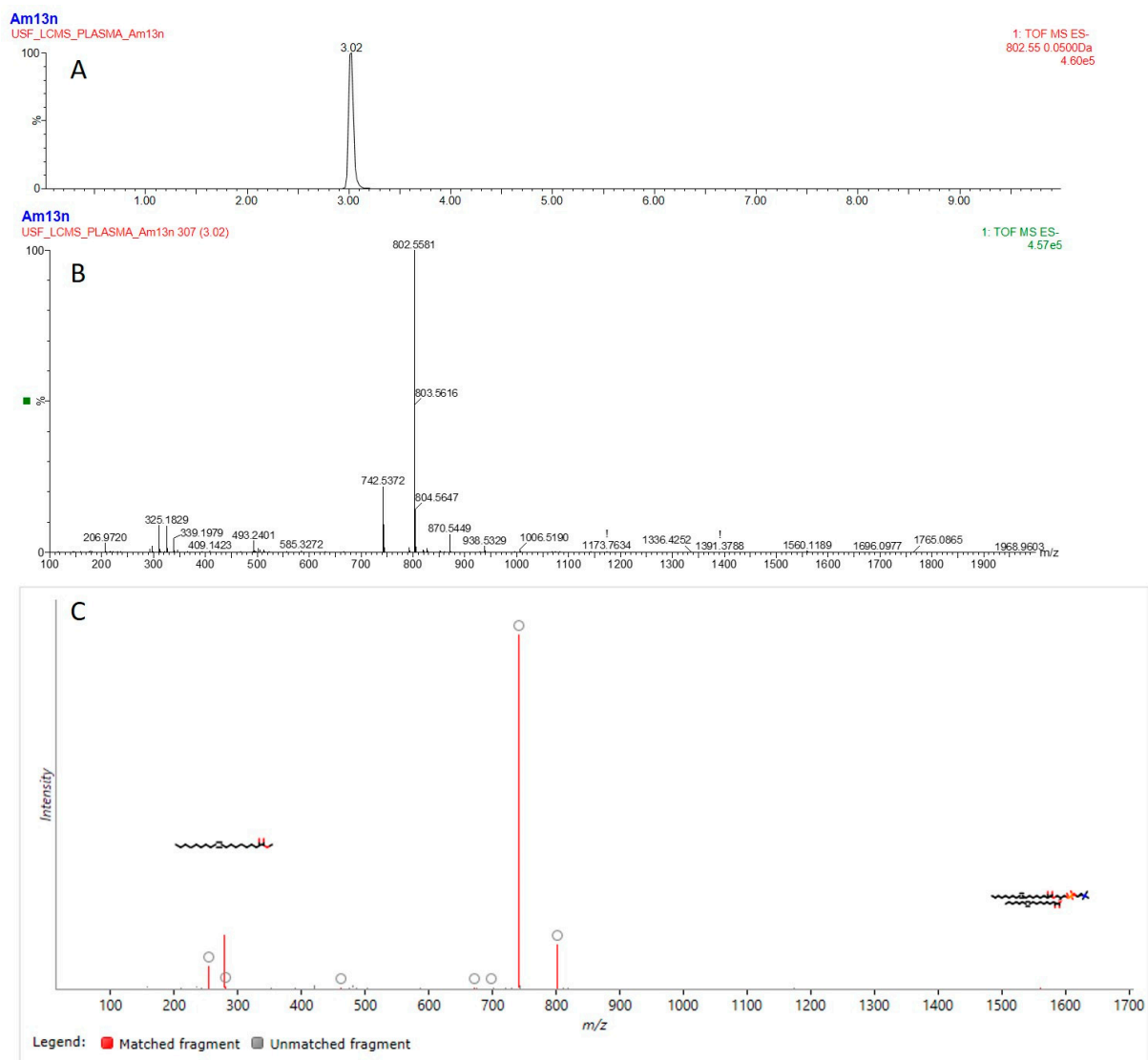


Figure S3: Data for one characteristic ion of cancer plasma samples observed in the negative ion mode. The PC(34:2)/PE-Nme(36:2), observed as the $[M + FA - H]^-$ adduct at m/z 802.5593. The extracted ion chromatogram (EIC) is shown in (A). The low-energy mass spectrum is shown in (B). The deconvoluted fragmentation spectrum obtained by Progenesis Q1 (Waters), showing the identifying fragments is shown in (C), where red signalizes the matched fragments, according to theoretical fragmentation.

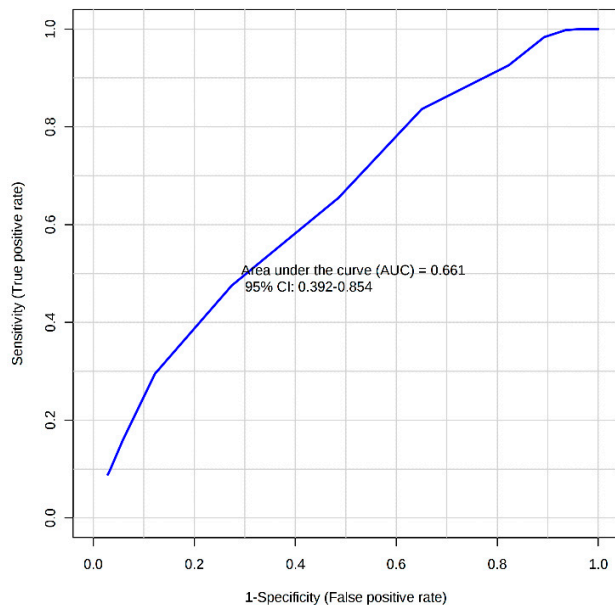


Figure S4: Receiver operator characteristics (ROC) curve for the support vector machine (SVM) model for differentiation among cancer and health status based on plasma lipids listed as molecular signatures for tissue differentiation using imaging mass spectrometry. A near to diagonal ROC curve represents an insufficient discriminatory power for the model. AUC is the area under the ROC curve and CI is the confidence interval.