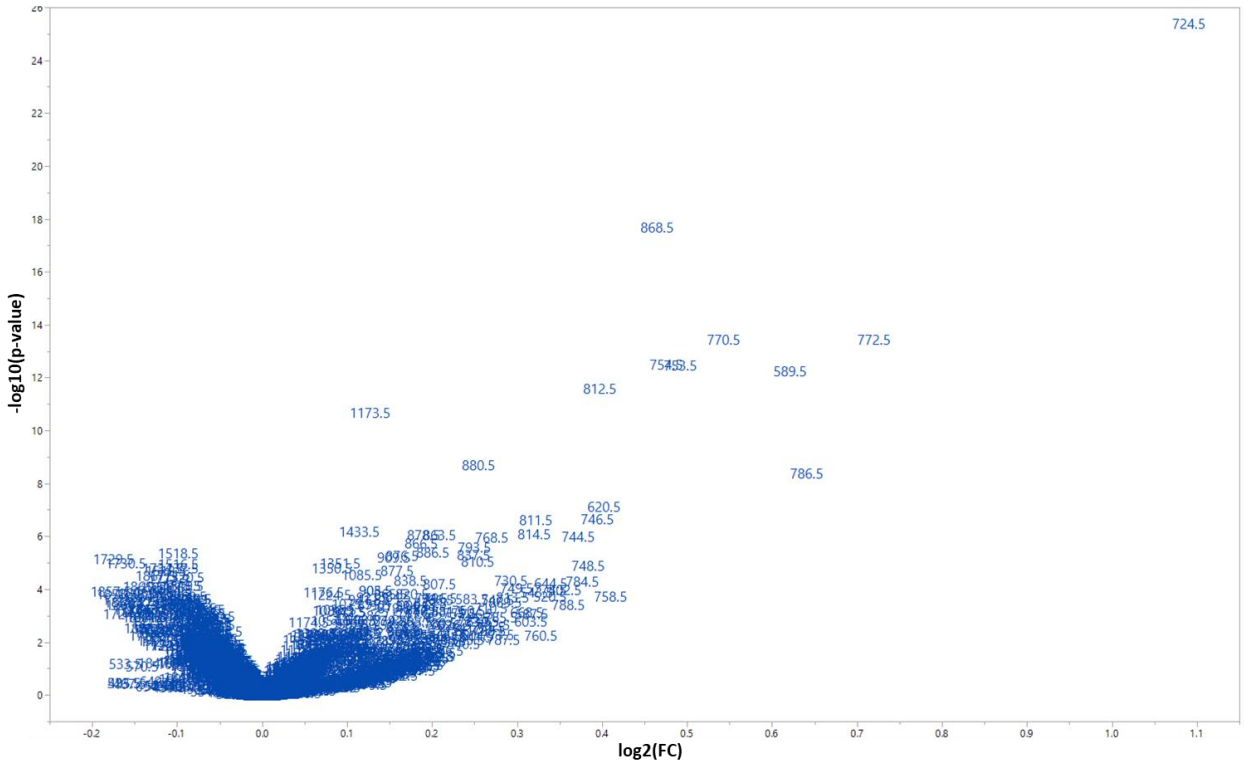
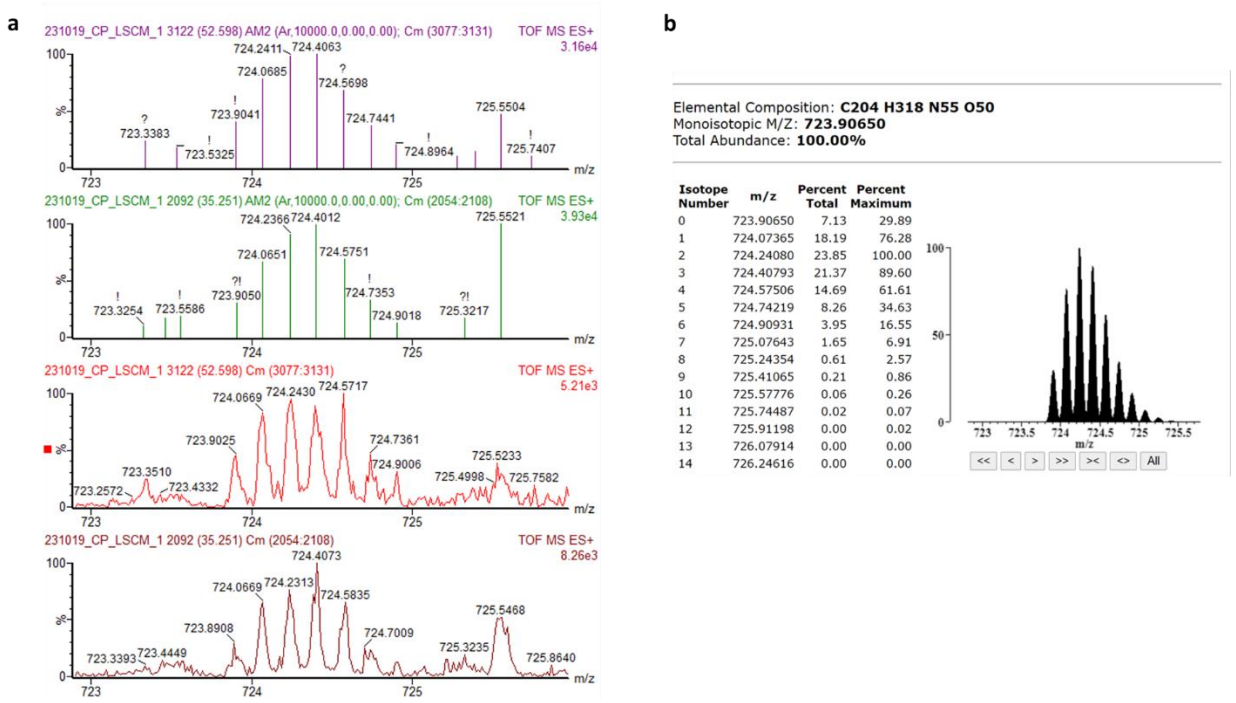


Supplementary Figure 1: Volcano plot representing the differential intensity of the mass bins as used for the pre-clinical mastitis detection. The fold change (FC) values and the p-values represent the comparisons of the relative intensities of each labelled mass bin between the control samples (lSCC and hSCC) and the pre-clinical mastitis samples collected up to 48 hours before the clinical event.



Supplementary Figure 2: The first isotopologue ion signal of the $[M+6H]^{6+}$ isracidin-containing peptide ion (RPKHPIKHQGLPQEVLNENLLRFFVAPFPEVFGKEKV; bovine alpha-S1-casein) is recorded at *m/z* 723.9 with an accuracy of <5ppm. **a.** Mass spectral raw data of two mastitis samples showing the isotopologue distribution of the $[M+6H]^{6+}$ isracidin-containing peptide ion (bottom two panels) and their corresponding centroided data (top two panels). **b.** Theoretical isotopologue distribution of the $[M+6H]^{6+}$ isracidin-containing peptide ion as obtained by the MS-Isotope function within ProteinProspector (prospector.ucsf.edu).