Label-free Proteomics for Discovering Biomarker Candidates for Controlling Krypton Misuse in Castrated Horses (Geldings)

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SUPPORTING INFORMATION

Table S1. SRM acquisition parameters for detection of tryptic peptides of TFRC and their corresponding internal standard

Peptide	Precursor (m/z)	Charge state	Product (m/z)	Collision energy (eV)
Transferrin receptor protein 1 (TFRC)				
IFNVFGVIK	519.0	2+	233.2	32.7
HIFWGSGSHTLSALLEHLK	534.3	4+	380.2	95.3
LLWTDLR	916.6	1+	159.1	54.2
Internal standard				
SLHTLFGDELCK	473.9	3+	290.2	75.0

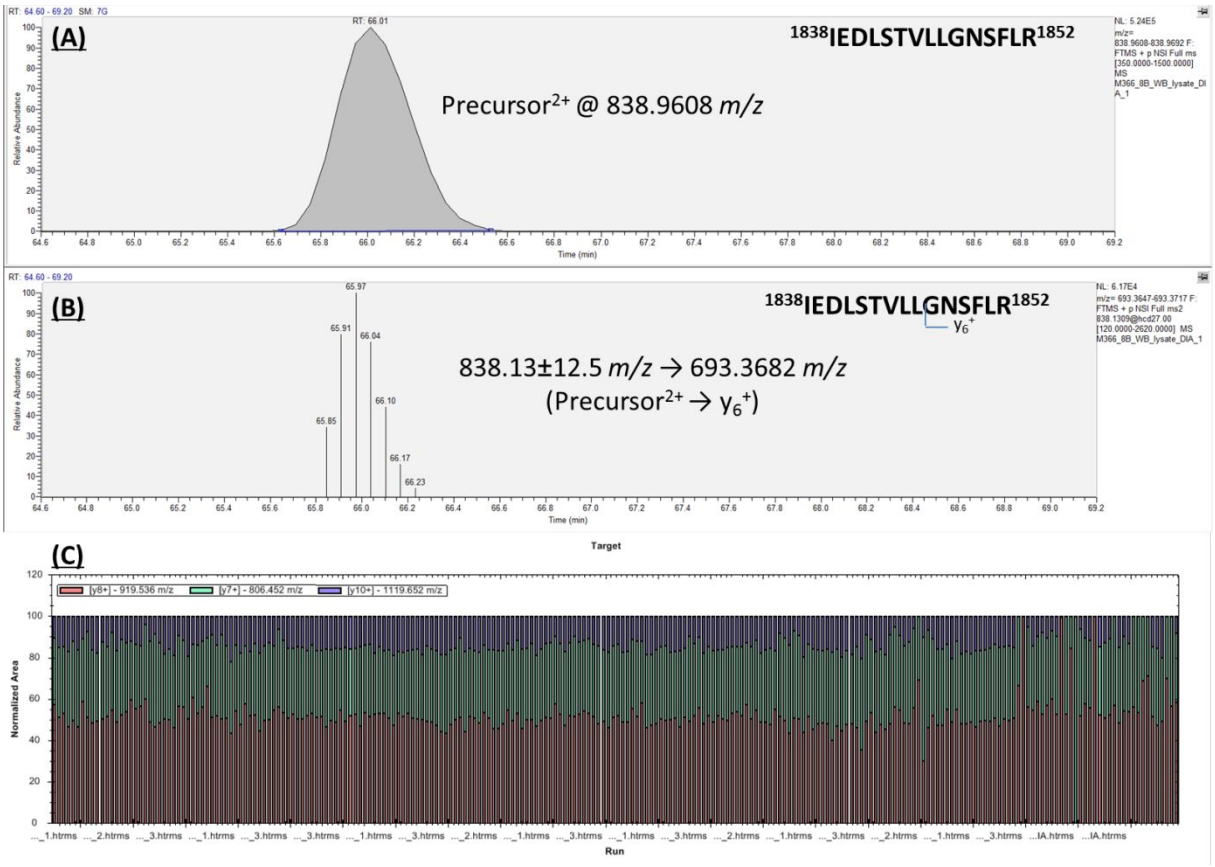

Figure S1. Data sampling across an example peak detected by DIA. (A) An extracted ion chromatogram of the precursor of a tryptic peptide of von Willebrand factor (VWF, Uniprot ID: F7BAT4). (B) The corresponding un-smoothed product ion chromatogram (precursor^{2+} → y_6^+) showing sufficient number of data point at MS2 level for accurate quantitation. (C) Three fragment ions were used to quantify the peptide. Consistent relative abundances of the ions between plasma samples suggested that the peptide can be consistently measured.

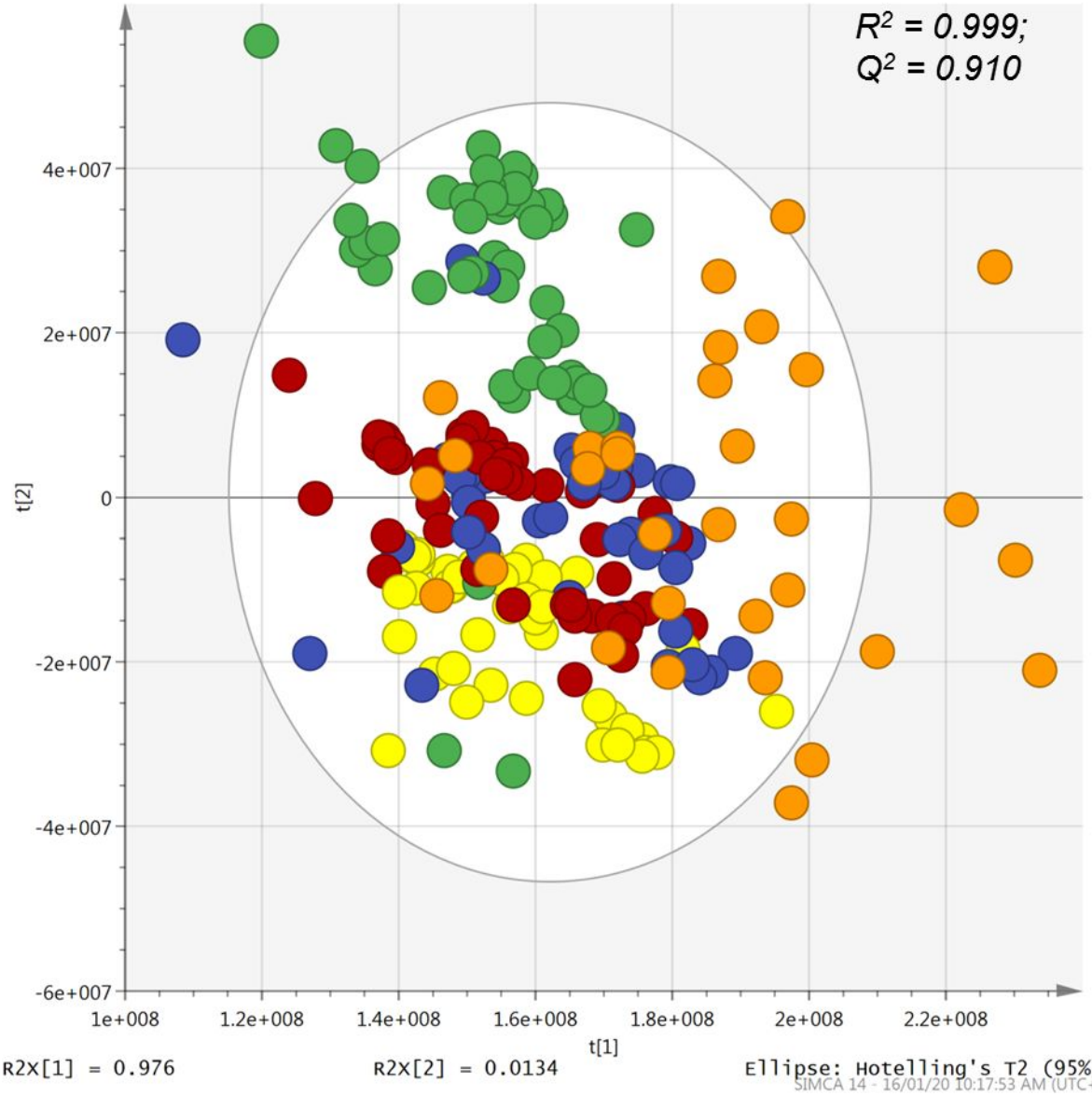

Figure S2. The un-supervised principal component analysis (PCA) of samples collected from the 4 geldings in trial and the 32 non-treated in-training thoroughbred geldings used for model validation. Raw LFQs were used in the analysis. Score plot showed no significant pre-existing difference between the two sample groups. Parameters of model performance were shown in the inset. Samples from the three Kr-administered geldings were individually labelled green, red and blue. Samples from the control gelding in the administration trial were labelled yellow.

Samples from the 32 non-treated in-training thoroughbred geldings for validation were labelled orange.