

Supplementary Material to

Dryfilm-ATR-FTIR analysis of urinary profiles as a point-of-care tool to evaluate aerobic exercise

Jaume Béjar Grimalt¹, Ángel Sánchez-Illana^{1*}, Miguel de la Guardia¹, Salvador Garrigues¹, Ignacio Catalá-Vilaplana², Jose Luis Bermejo-Ruiz³, Jose Ignacio Priego-Quesada^{2,4*}, David Pérez-Guaita¹

¹Department of Analytical Chemistry, University of Valencia, Burjassot, Spain

²Research Group in Sports Biomechanics (GIBD), Department of Physical Education and Sports, Universitat de València, Valencia, Spain.

³Department of Physical Education and Sports, Universitat de València, Valencia, Spain.

⁴Research Group in Medical Physics (GIFIME), Department of Physiology, Universitat de València, Valencia, Spain.

* Corresponding authors: angel.illana@uv.es, j.ignacio.priego@uv.es

Supplementary Table S1. Number of samples (N) of each time for the dry-film ATR analysis of urine samples.

	Pre (t = -2 h)	Post (t = 0 h)	Post2 (t = 2 h)	Post5 (t = 5 h)	Post11 (t = 11 h)	Post24 (t = 24 h)
N Experimental	14	14	13	14	14	14
N Control	-	4	7	4	5	7

Supplementary Table S2. Number of samples (N) of each time for the dry-film ATR analysis of urinary proteins.

	Pre (t = -2 h)	Post (t = 0 h)	Post2 (t = 2 h)	Post5 (t = 5 h)	Post11 (t = 11 h)	Post24 (t = 24 h)
N Experimental	5	9	11	9	10	12

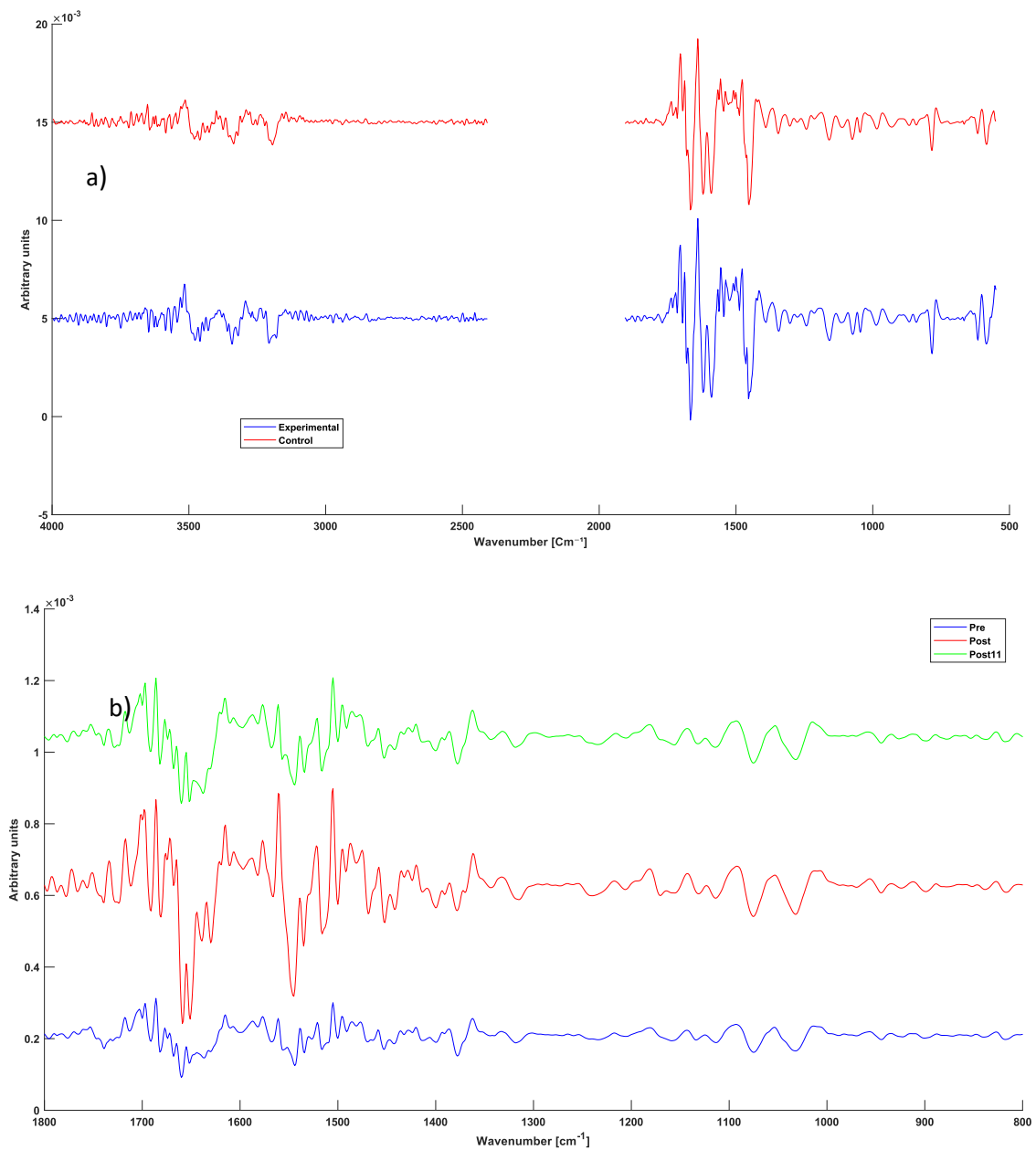


Figure SM1. a). Average second derivative IR spectra (lines) and standard deviation (shade) of the urine dry-films. b) Average Second derivative spectra from the protein extracts. Spectra have been shifted along the Y-axis in order to provide a better comparison.

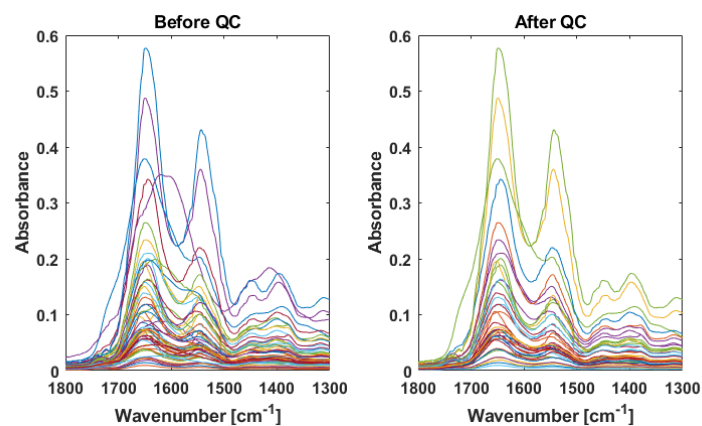


Figure SM2. Amide I and amide II bands in the IR spectra of protein extracts before and after the removal of samples with non-clear amide bands.

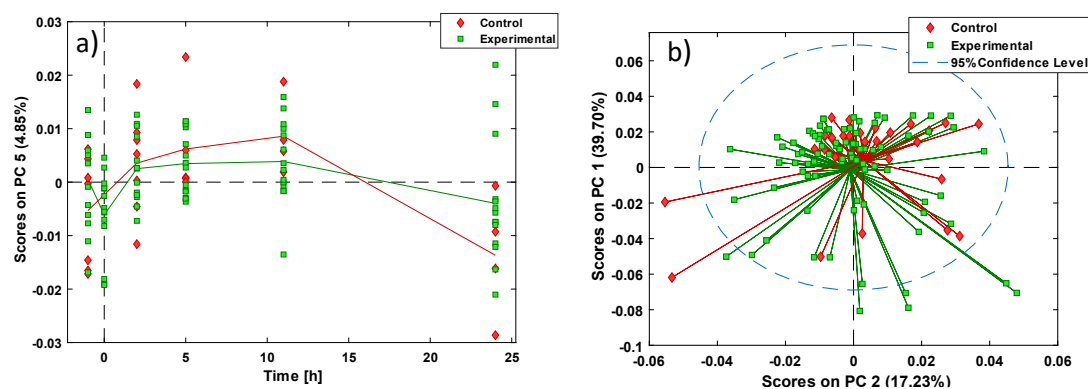


Figure SM3. Principal component analysis score plots of the urine dry films. a) PC5 vs. sampling time with a line connecting the mean score value for each time, b) PC1 vs. PC2.

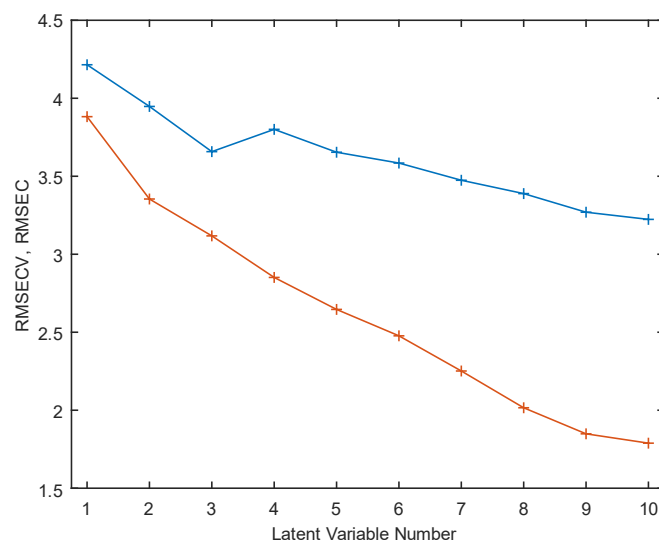


Figure SM4. RMSECV for the o-PLS using the samples from training group.

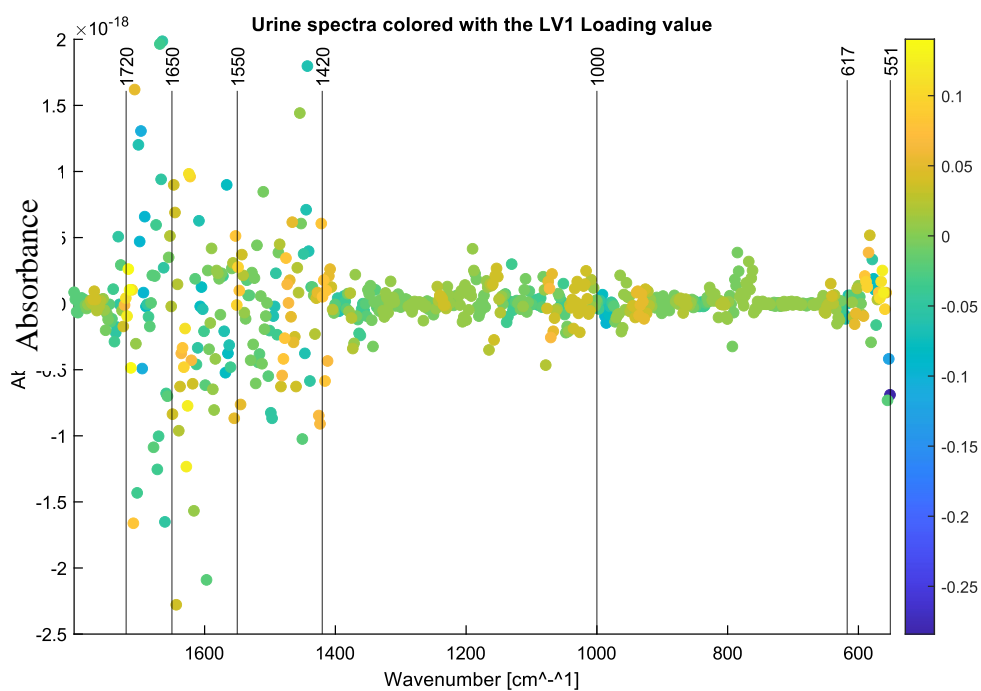


Figure SM5. Average spectrum of the dry films of urine after the second derivative. The color scale of the points indicates the values of the “component loading” (LV1 in the o-PLS).

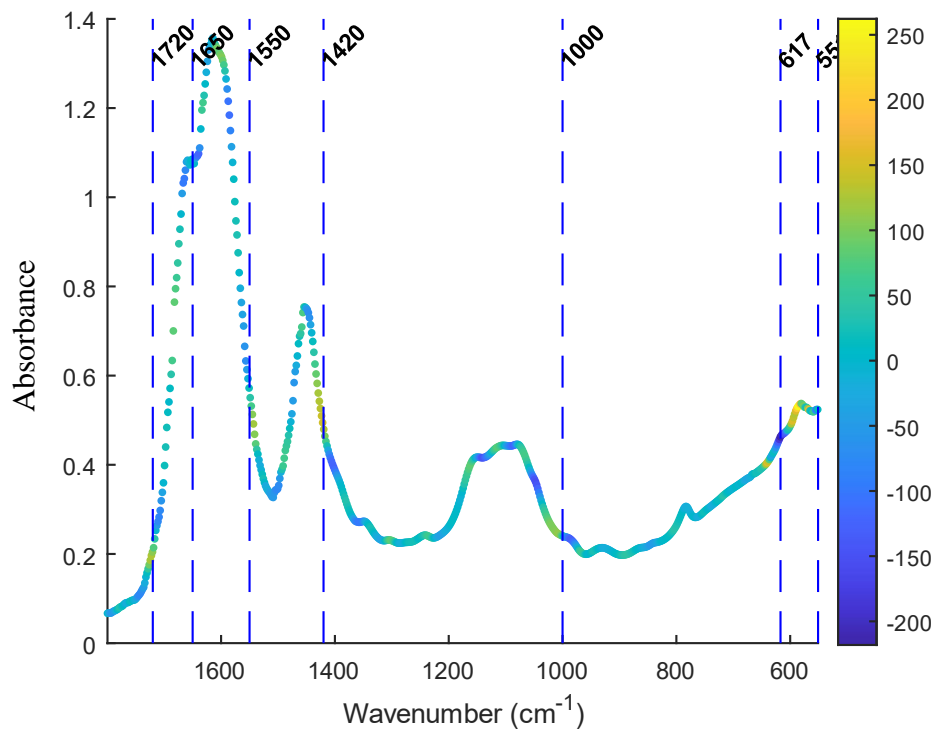


Figure SM6. Average spectrum of the dry film urine coloured with the o-PLS regression vector values.

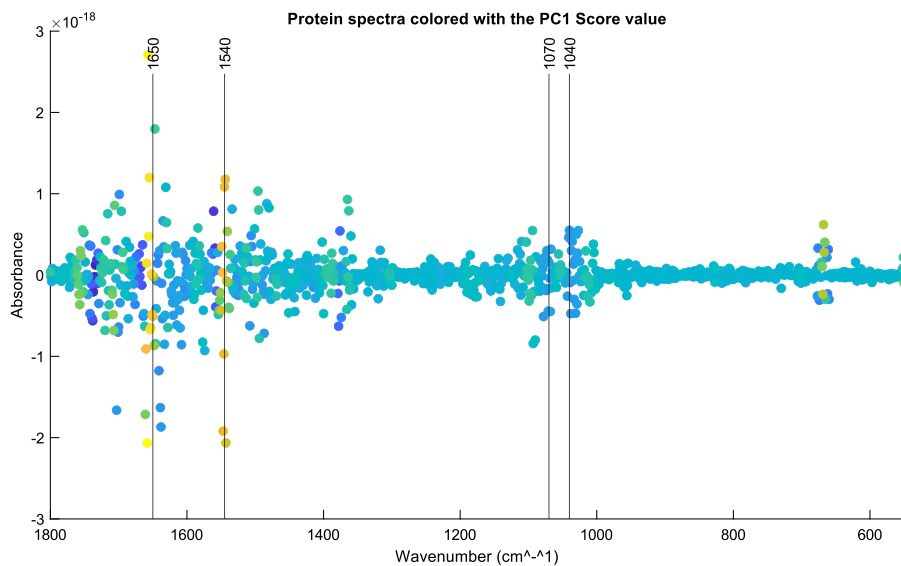


Figure SM7. Average spectrum of the protean extracts after the second derivative. The color scale of the points represents the values of the PC1 loading.