

¹H-NMR metabolomic profile of healthy and osteoarthritic canine synovial fluid before and after UC-II supplementation

Marzia Stabile^{1,* +}, Chiara Roberta Girelli^{2,+}, Luca Lacitignola¹, Rossella Samarelli³, Antonio Crovace¹, Francesco Paolo Fanizzi², and Francesco Staffieri¹

¹Section of Veterinary Clinics and Animal Production, Department of Emergency and Organ Transplantation, University of Bari, 70123, Bari, Italy

²Department of Biological and Environmental Sciences and Technologies, University of Salento, 73100 Lecce, Italy

³Section of Avian Pathology, Department of Veterinary Medicine, University of Bari, 70123, Bari, Italy

* marzia.stabile@uniba.it; Francesco.staffieri@uniba.it

⁺these authors contributed equally to this work

Supplementary information

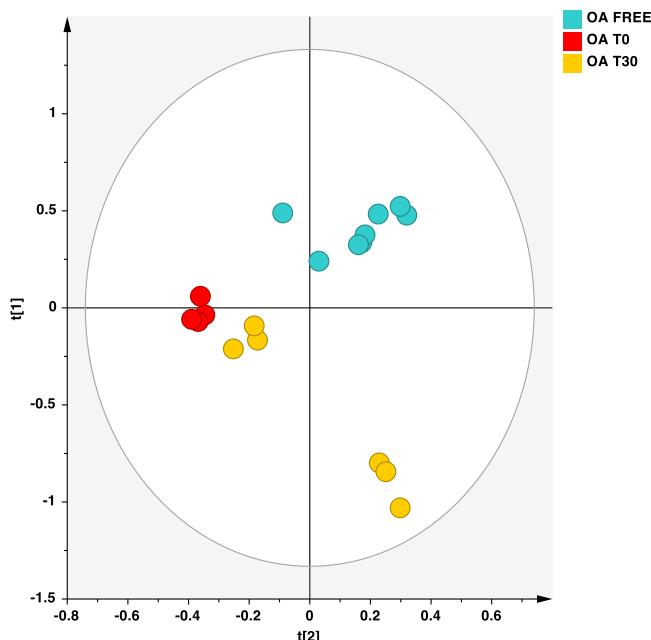


Figure S1. PCA $t[1]/t[2]$ scores plot of the whole SF samples data set. Three components give $R^2X=0.731$; $Q^2= 0.453$

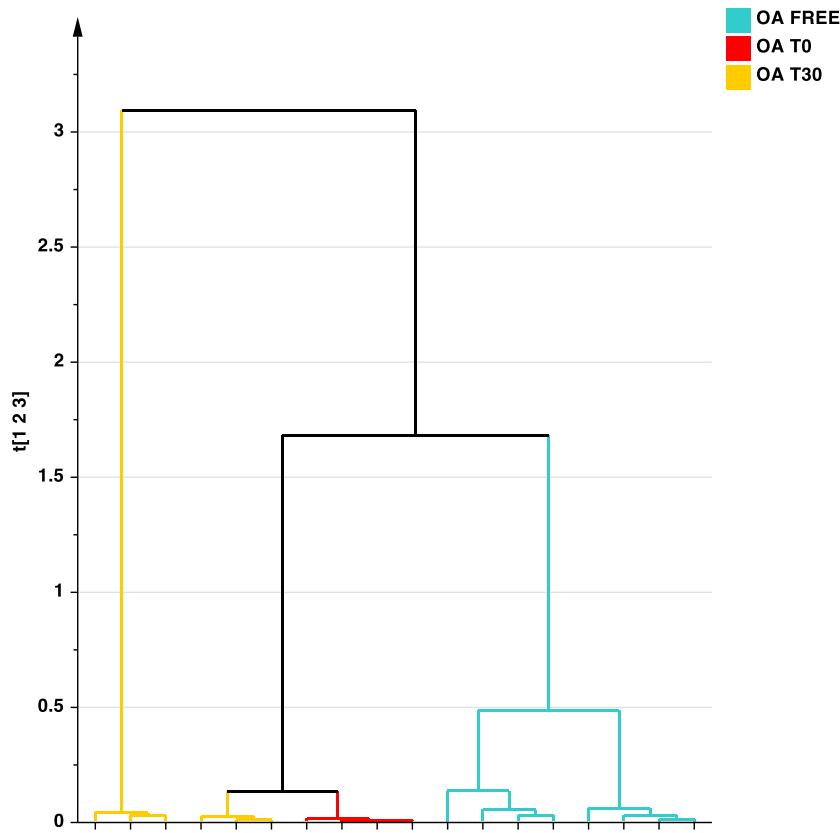


Figure S2. HCA dendrogram showing the clusters generated by hierarchical cluster analysis of the whole data set using Ward linkage criterion. Dendrograms are sorted by size.

Var ID (Primary)	M17.p(corr)[1]	M17.VIP[1+1+0]
creatine/creatinine (3.9 ppm)	-0.598987	2.55625
TMAO (3.26 ppm)	-0.634953	5.13238
citrate (2.7ppm)	0.961914	1.83663
citrate (2.54 ppm)	0.961048	1.82662
glutamine (2.1 ppm)	-0.920607	2.73875
β-OH-butyrate (1.18 ppm)	-0.795191	3.02273

Table S1 List of discriminating chemical descriptors (variables) with corresponding correlation coefficient (pcorr), and variable importance on the projection (VIP) for OA-T0 and OA-T30 SF samples OPLS-DA model

Var ID (Primary)	M22.p(corr)[1]	M22.VIP[1+1+0]
histidine (7.74 ppm)	-0.870006	0.816922
TMAO (3.26 ppm)	-0.63912	4.43003
glutamine (2.1 ppm)	-0.835927	2.67689
alanine (1.5 ppm)	-0.985323	2.41377
β-OH-butyrate (1.18 ppm)	-0.721501	2.15177
lactate (1.34 ppm)	0.616009	5.44766
lipids (0.86 ppm)	-0.95764	2.76259

Table S2 List of discriminating chemical descriptors (variables) with corresponding correlation coefficient (pcorr), and variable importance on the projection (VIP) for OA-FREE and OA- T0 SF samples OPLS-DA model

Var ID (Primary)	M37.p(corr)[1]	M37.VIP[1+1+0]
α-glucose (5.26 ppm)	-0.923619	2.29777
β-glucose (4.66 ppm)	-0.925983	2.10316
glutamine (2.1 ppm)	-0.94806	2.33689
alanine (1.5 ppm)	-0.917508	2.24029
lactate (1.34 ppm)	0.548916	2.96059
lipids (0.86 ppm)	-0.931488	2.26821

Table S3 List of discriminating chemical descriptors (variables) with corresponding correlation coefficient (pcorr), and variable importance on the projection (VIP) for OA-FREE and OA- T30 SF samples OPLS-DA model