

Supplement Material

**Human in vivo longevity is reflected in vitro by differential metabolism measured by
¹H-NMR profiling of cell culture supernatants**

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Table S1 Outlier identification: Characteristics of Spectroscopic Outliers

#	Sample ID	TSP line width	Water Suppression
89	Sample missing	-	-
91	Sample missing	-	-
109	50-24h	Acquisition failed	-
169	111-24h	OK (1.03 Hz)	FAIL
195	117-5d	FAIL (4.06 Hz)	OK
197	118-24h	FAIL (6.56 Hz)	OK
199	118-5d	FAIL (3.44 Hz)	OK
203	119-5d	FAIL (3.19 Hz)	OK
207	120-5d	OK (1.15 Hz)	FAIL
235	127-5d	OK (0.82 Hz)	FAIL
287	121-128-control-5d	FAIL (7.43 Hz)	OK
289	129-136-control-24h	FAIL (1.56 Hz)	FAIL

Visual inspection of the individual spectra during data processing was used to remove spectroscopic outliers. As parameter for shim quality, the half width of the TSP line was evaluated after processing without apodization. Water suppression quality was assessed by total height of the remaining water resonance and presence of shoulders at the base of the signal. A total of 10 datasets were removed prior to further analysis as summarized in table S1. Biological outliers were identified based on Hotelling's T2 range (above 99% T2 critical value) and distance of the observation in the training set to the X model plane values (> 2) (These parameters describe how well the data is located within model space).

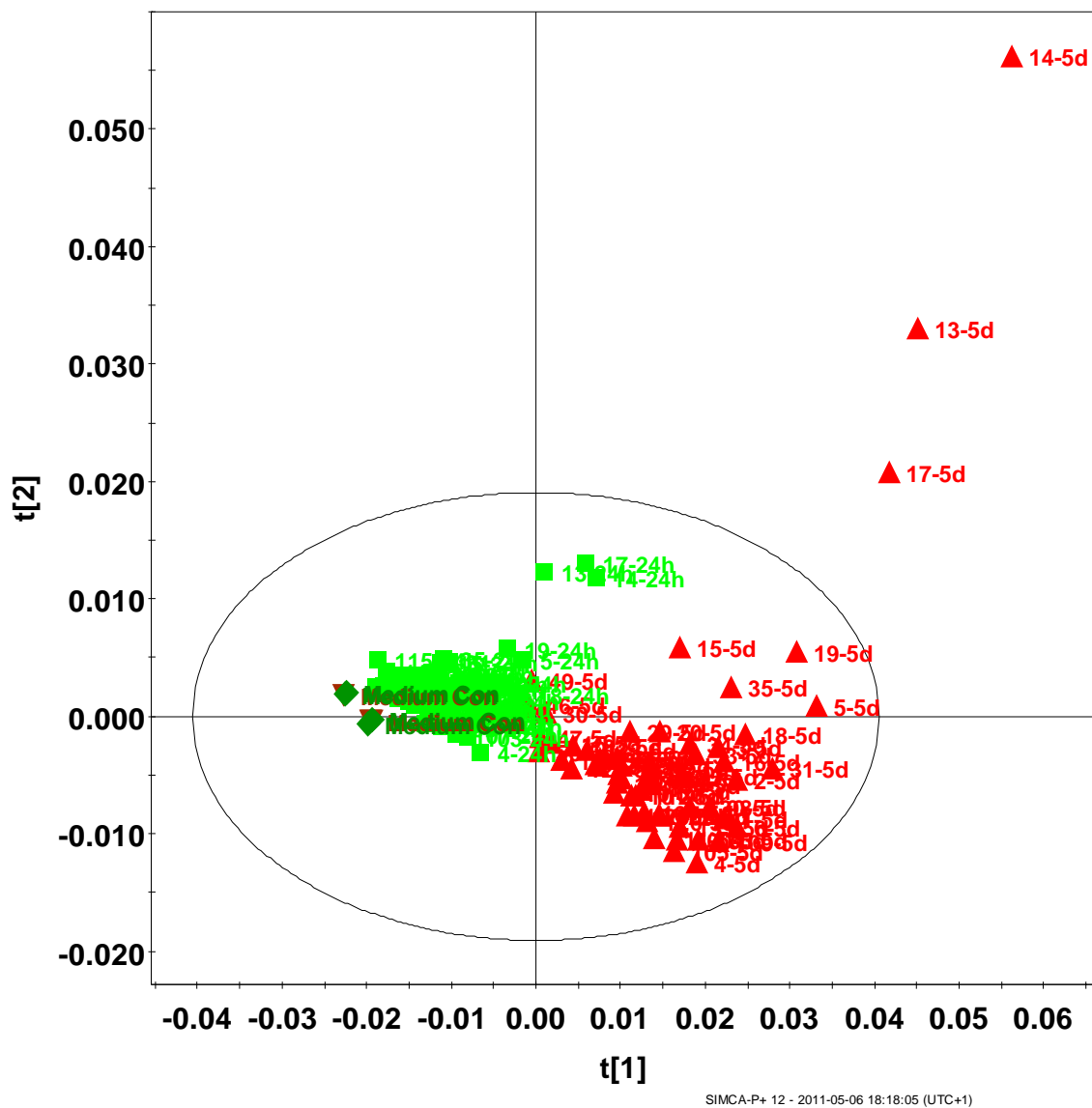


Figure S1 Scores plot of first two principal components from PCA model built from complete data set without scaling of variables. Data points are coloured according to fibroblast culture incubation duration of 24 hours (■) and five days (▲) as well as cell-free/serum-free medium (control medium) incubated for 24 hours (◆) and five days (▼).

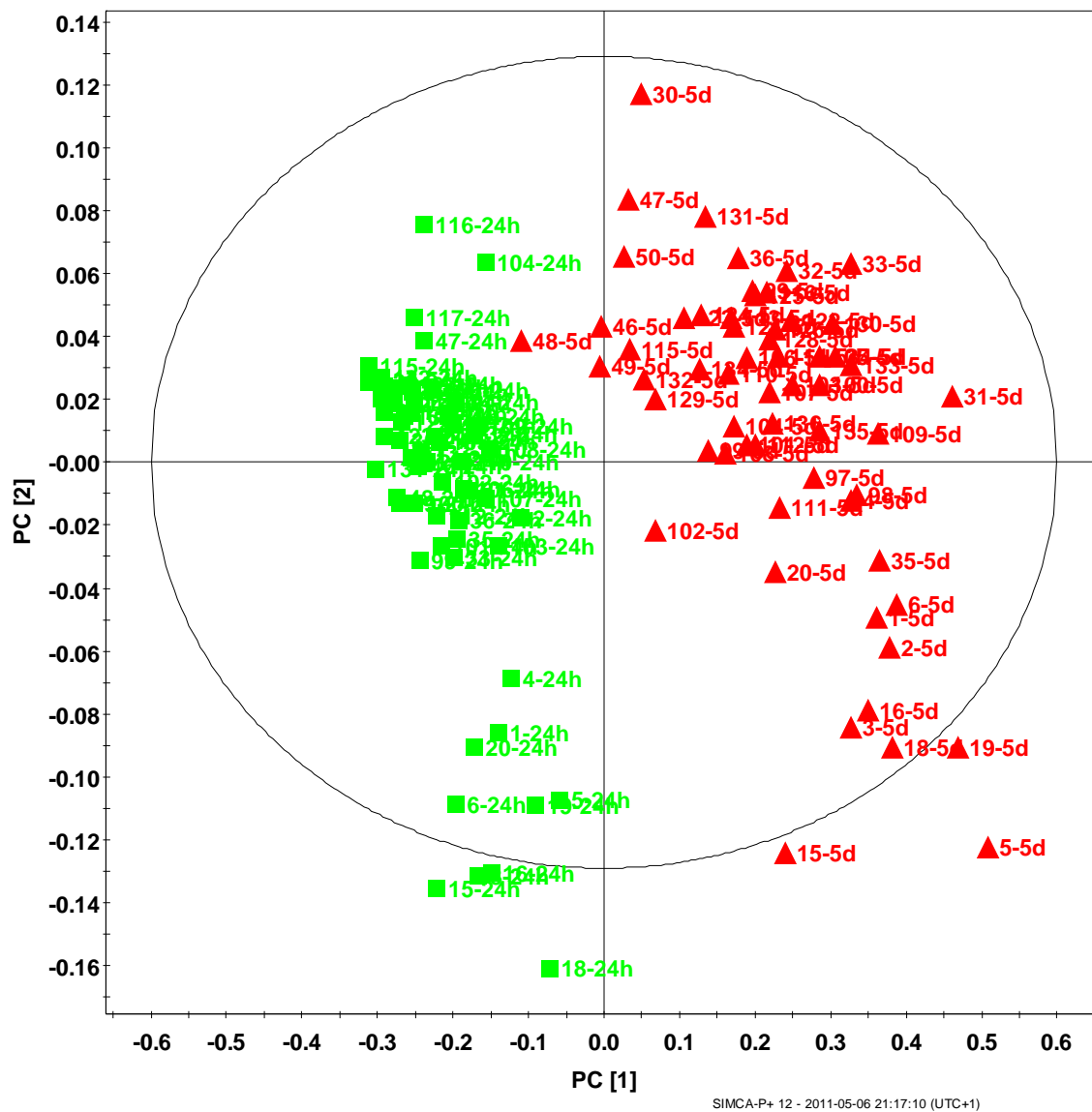


Figure S3 Scores plot of first two components from PLS-DA model built using time point as response variable. Data points are coloured according to fibroblast culture incubation duration of 24 hours (■) and five days (▲), respectively.

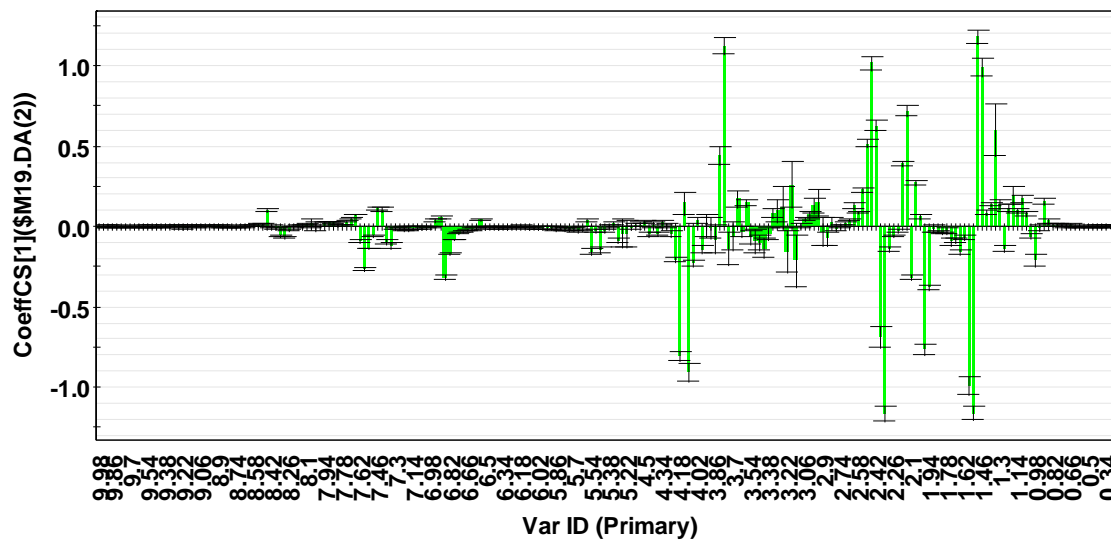


Figure S4 Coefficients plot for first component of PLS-DA model built using time point as response variable.

OSC Validation

For validation of the OSC filtering step, 59 datasets were generated using OSC filtering of the original data leaving out one of the 59 observations, such that each sample was omitted once (leave-one-out cross validation). For each dataset an independent PLS-DA two-class models was build using the 58 observations that were included in the filtering step followed by prediction of the response variable for the excluded observation using the respective model. The predicted values were then used for classification of the samples as summarized in Table S2. The overall correct classification of all samples was 62.7% with a 95% confidence interval for the proportion correctly identified of [0.5036, 0.7504] excluding the null hypothesis.

Table S2 Misclassification table for OSC leave-one-out cross validation

	Members	Correct	predicted	
			offspring	partner
offspring	28	60.7%	17	11
partner	31	64.5%	11	20
Total	59	62.7%	28	31