

A metabolomic study of adipose tissue in mice with a disruption of the circadian system.

Supplementary Data

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Table S1. Parameters for validated models built considering LC-MS data for ASWAT. In the first part of the table, the ones obtained comparing control and *Ad-Arntl^{-/-}* mice are presented; in the second part all the validated models comparing the same genotype at different time points are shown.

Model	Description	Type	R ² X	R ² Y	Q ²
M1	Both genotypes at all time points	PCA	42.6%		23.3%
M2	Both genotypes and all time points	PLS-DA	42.5%	73.8%	56.6%
M4	Both genotypes at time T=0, classes assigned by genotype.	PLS-DA	58.2%	92.0%	71.5%
M5	Both genotypes at time T=6, classes assigned by genotype.	PLS-DA	20.3%	83.0%	46.8%
M6	Both genotypes at time T=12, classes assigned by genotype.	PLS-DA	29.9%	75.7%	62.2%
M7	Both genotypes at time T=18, classes assigned by genotype.	PLS-DA	23.7%	79.1%	51.0%
M11	Only <i>Ad-Arntl^{-/-}</i> mice at time T=0 and T=12, classes assigned by time.	PLS-DA	16.1%	81.0%	34.2%
M12	Only <i>Ad-Arntl^{-/-}</i> mice at time T=0 and T=18, classes assigned by time.	PLS-DA	16.4%	83.5%	50.0%

Table S2. Parameters for validated models built considering GC-FID data for ASWAT.

Model	Description	Type	R ² X	R ² Y	Q ²
M1	Both genotypes at all time points	PCA	46.2%		24.3%
M2	Both genotypes and all time points	PLS-DA	37.4%	90.4%	85.6%
M4	Both genotypes at time T=0, classes assigned by genotype.	PLS-DA	19.2%	90.9%	56.3%
M5	Both genotypes at time T=6, classes assigned by genotype.	PLS-DA	28.2%	82.3%	67.7%
M6	Both genotypes at time T=12, classes assigned by genotype.	PLS-DA	24.9%	91.1%	68.7%
M7	Both genotypes at time T=18, classes assigned by genotype.	PLS-DA	70.4%	98.6%	88.1%
M8	Only Ad- <i>Arntl</i> ^{-/-} mice at time T=0 and T=12, classes assigned by time.	PLS-DA	45.5%	77.2%	10.3%

Table S3. Parameters for validated models built considering LC-MS data for BAT.

Model	Description	Type	R²X (%)	R²Y (%)	Q² (%)
M1	Both genotypes and all time points.	PCA-X	38.4	-	23.1
M2	Both genotypes and all time points, classes assigned by genotype.	PLS-DA	35.7	74.1	45.5
M4	Both genotypes, only at T=0, classes assigned by genotype.	PLS-DA	52.7	99.0	84.2
M5	Both genotypes, only at T=6, classes assigned by genotype.	PLS-DA	36.2	67.2	43.7
M6	Both genotypes, only at T=12, classes assigned by genotype.	PLS-DA	53.2	99.2	72.0
M7	Both genotypes, only at T=18, classes assigned by genotype.	PLS-DA	26.4	76.9	49.1
M8	Both genotypes and all time points, classes assigned by time.	PLS-DA	27.1	9.35	3.29
M11	Both genotypes, at T=0 and T=6, classes assigned by time.	PLS-DA	48.2	90.0	52.4
M12	Only control mice, at T=0 and T=6, classes assigned by time.	PLS-DA	65.5	99.2	33.0
M13	Only Ad- <i>Arntl</i> ^{-/-} mice, at T=0 and T=6, classes assigned by time.	PLS-DA	47.4	98.7	63.3
M20	Both genotypes, at T=6 and T=12, classes assigned by time.	PLS-DA	37.7	72.8	37.4
M21	Only control mice, at T=6 and T=12, classes assigned by time.	PLS-DA	32.5	51.1	12.6
M24	Only control mice, at T=6 and T=18, classes assigned by time.	PLS-DA	29.2	55.0	17.9

Table S4. Parameters for validated models built considering GC-FID data for BAT.

Model	Description	Type	R²X (%)	R²Y (%)	Q² (%)
M1	Both genotypes and all time points.	PCA-X	76.5	-	47.2
M2	Both genotypes and all time points, classes assigned by genotype.	PLS-DA	52.0	87.0	75.4
M3	Both genotypes, only at T=0, classes assigned by genotype.	PLS-DA	28.5	76.3	32.5
M4	Both genotypes, only at T=6, classes assigned by genotype.	PLS-DA	43.8	94.9	63.7
M5	Both genotypes, only at T=12, classes assigned by genotype.	PLS-DA	75.6	90.7	78.4
M6	Both genotypes, only at T=18, classes assigned by genotype.	PLS-DA	56.2	92.2	73.0
M10	Both genotypes, at T=0 and T=6, classes assigned by time.	PLS-DA	41.1	48.0	40.3
M11	Only Ad- <i>Arntl</i> ^{-/-} mice, at T=0 and T=6, classes assigned by time.	PLS-DA	39.2	78.0	62.1
M12	Only control mice, at T=0 and T=6, classes assigned by time.	PLS-DA	53.3	35.2	19.7
M14	Only Ad- <i>Arntl</i> ^{-/-} mice, at T=0 and T=12, classes assigned by time.	PLS-DA	26.5	59.5	6.39
M16	Both genotypes, at T=0 and T=18, classes assigned by time.	PLS-DA	48.8	69.0	26.3
M17	Only Ad- <i>Arntl</i> ^{-/-} mice, at T=0 and T=18, classes assigned by time.	PLS-DA	29.9	50.3	21.2
M18	Only control mice, at T=0 and T=18, classes assigned by time.	PLS-DA	53.4	30.5	6.03

M19	Both genotypes, at T=6 and T=12, classes assigned by time.	PLS-DA	50.6	28.4	15.8
M20	Only Ad- <i>Arntl</i> ^{-/-} mice, at T=6 and T=12, classes assigned by time.	PLS-DA	57.2	49.0	36.5
M22	Both genotypes, at T=6 and T=18, classes assigned by time.	PLS-DA	45.8	68.0	50.7
M23	Only Ad- <i>Arntl</i> ^{-/-} mice, at T=6 and T=18, classes assigned by time.	PLS-DA	37.2	54.6	33.8
M24	Only control mice, at T=6 and T=18, classes assigned by time.	PLS-DA	54.2	79.4	31.1
M26	Only Ad- <i>Arntl</i> ^{-/-} mice, at T=12 and T=18, classes assigned by time.	PLS-DA	72.1	70.5	21.7

Table S5. Parameters for validated models built considering NMR spectroscopy data for BAT.

Model	Description	Type	R²X (%)	R²Y (%)	Q² (%)
M1	Both genotypes and all time points.	PCA-X	86.2	-	57.0
M4	Both genotypes and all time points, classes assigned by genotype.	PLS-DA	42.9	87.9	61.8
M6	Both genotypes, only at T=0, classes assigned by genotype.	PLS-DA	48.0	87.2	27.2
M7	Both genotypes, only at T=6, classes assigned by genotype.	PLS-DA	75.1	98.3	80.4
M8	Both genotypes, only at T=12, classes assigned by genotype.	PLS-DA	21.8	86.7	53.9
M9	Both genotypes, only at T=18, classes assigned by genotype.	PLS-DA	19.5	76.8	26.0
M10	Both genotypes and all time points, classes assigned by time.	PLS-DA	51.3	40.9	20.4
M11	Only Ad- <i>Arntl</i> ^{-/-} mice at all time points, classes assigned by time.	PLS-DA	30.3	17.8	7.43
M12	Only control mice at all time points, classes assigned by time.	PLS-DA	53.1	32.4	11.8
M16	Both genotypes, at T=0 and T=12, classes assigned by time.	PLS-DA	45.9	78.5	54.6
M17	Only Ad- <i>Arntl</i> ^{-/-} mice at T=0 and T=12, classes assigned by time.	PLS-DA	24.6	82.5	57.8
M18	Only control mice at T=0 and T=12, classes assigned by time.	PLS-DA	38.5	54.0	31.4
M19	Both genotypes, at T=0 and T=18, classes assigned by time.	PLS-DA	42.0	81.0	40.0

M20	Only Ad- <i>Arntl</i> ^{-/-} mice at T=0 and T=18, classes assigned by time.	PLS-DA	78.8	99.8	86.4
M21	Only control mice at T=0 and T=18, classes assigned by time.	PLS-DA	42.0	43.9	20.5
M22	Both genotypes, at T=6 and T=12, classes assigned by time.	PLS-DA	39.0	86.7	48.7
M23	Only Ad- <i>Arntl</i> ^{-/-} mice at T=6 and T=12, classes assigned by time.	PLS-DA	53.9	90.7	63.2
M24	Only control mice at T=6 and T=12, classes assigned by time.	PLS-DA	26.2	73.5	41.0
M25	Both genotypes at T=6 and T=18, classes assigned by time.	PLS-DA	30.5	66.0	60.3
M26	Only Ad- <i>Arntl</i> ^{-/-} mice at T=6 and T=18, classes assigned by time.	PLS-DA	50.5	91.8	56.9
M27	Only control mice at T=6 and T=18, classes assigned by time.	PLS-DA	58.1	97.4	68.6
M28	Both genotypes, at T=12 and T=18, classes assigned by time.	PLS-DA	44.8	82.0	66.7
M29	Only Ad- <i>Arntl</i> ^{-/-} mice at T=12 and T=18, classes assigned by time.	PLS-DA	69.8	99.9	90.0
M30	Only control mice at T=12 and T=18, classes assigned by time.	PLS-DA	53.3	88.2	61.6