

1 Supplemental Methods

2 Quantification of nucleotides

3 Clear supernatants were analyzed by means of LC-MS/MS with a 4000 QTrap (AB Sciex, Darmstadt,
4 Germany) and a Dionex UHPLC UltiMate 3000 (Thermo Fisher) or Prominence HPLC (Shimadzu,
5 Germany). The cell pellet was used for the quantitation of free fatty acids (see below).
6 For chromatographic separation of nucleotides, a ZIC pHILIC 5 μ M, 150 x 4.6 mm (Merck) was used with
7 acetonitrile/water with 5 mM ammonium acetate (95/5, v/v, pH 9.5) as solvent A and 5mM ammonium
8 acetate (pH 9.5) as solvent B. The separation of nucleotides was performed using a 500 μ L/min
9 flowrate and a linear gradient from 85% A which was maintained for 5 min to 50% A in 15 min.
10 Afterward the column was flushed and equilibrated to starting conditions. Ions were analyzed by MS
11 in the negative mode. The spray voltage was set to -4500 V at a source temperature of 450°C and using
12 nitrogen as collision gas. The parameters for the collision activated dissociation (CAD) were: -2, curtain
13 gas: 35 psi, ion source gas 1: 55 psi, ion source gas 2: 65 psi, entrance potential (EP) -10 V. The MRM
14 (multiple reaction monitoring) transition for each compound are listed in Table S1. The first MRM-
15 transition was used as quantifier the second as qualifier.

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17 *Table S1: MRM-transitions for quantitation of nucleotides.*

Compound	Quantifier/ Qualifier	Q ₁ (m/z)	Q ₃ (m/z)	Dwell Time (msec)	Decustering potential (V)	Collision Energy (V)	Cell Exit Potential (V)
ATP	Quantifier [M-H] ⁻	506.01	79.0	30	-70	-106	-7
	Qualifier [M-H] ⁻	506.01	158.9	30	-70	-50	
AMP	Quantifier [M-H] ⁻	346.02	78.9	30	-60	-56	-1
	Qualifier [M-H] ⁻	346.02	97.1	30	-60	-36	-5
ADP	Quantifier [M-H] ⁻	426.21	78.8	30	-50	-98	-1
	Qualifier [M-H] ⁻	426.21	133.9	30	-50	-36	-7
IMP	Quantifier [M-H] ⁻	347.03	78.9	30	-50	-66	-1
	Qualifier [M-H] ⁻	347.03	96.9	30	-50	-34	-5
Adenosin	Quantifier [M-H] ⁻	266.07	133.9	30	-35	-16	-1
	Qualifier [M-H] ⁻	266.07	106.8	30	-35	-52	-7
Guanosine	Quantifier [M-H] ⁻	282.05	150.0	30	-60	-26	-7
	Qualifier [M-H] ⁻	282.05	132.9	30	-60	-44	-7

	[M-H] ⁻						
GMP	Quantifier	362.07	78.8	30	-45	-60	-1
	[M-H] ⁻ Qualifier	362.07	210.9	30	-45	-26	-3
GDP	Quantifier	442.07	78.9	30	-50	-80	-1
	[M-H] ⁻ Qualifier	442.07	149.9	30	-50	-36	-1
GTP	Quantifier	522.02	78.9	30	-80	-118	-1
	[M-H] ⁻ Qualifier	522.02	158.7	30	-80	-48	-1
Guanin	Quantifier	149.96	132.9	30	-45	-20	-9
	[M-H] ⁻ Qualifier	149.96	65.9	30	-45	-42	-3
Adenin	Quantifier	134.05	106.9	30	-60	-24	-5
	[M-H] ⁻ Qualifier	134.05	92	30	-60	-28	-5
Hypoxanthin	Quantifier	134.97	91.8	30	-45	-24	-11
	[M-H] ⁻ Qualifier	134.97	64.8	30	-45	-40	-3
Xanthin	Quantifier	151.00	107.9	30	-55	-24	-7
	[M-H] ⁻ Qualifier	151.00	65.8	30	-55	-46	-3
Inosin	Quantifier	267.04	135	30	-70	-30	-5
	[M-H] ⁻ Qualifier	267.04	107.9	30	-70	-56	-4
¹⁵ N-AMP	IS [M-H] ⁻	350.9	79.0	30	-60	-56	-1
¹⁵ N-ATP	IS [M-H] ⁻	511.02	78.8	30	-70	-106	-3
¹⁵ N-GMP	IS [M-H] ⁻	367.02	78.8	30	-45	-60	-1
¹⁵ N-GTP	IS [M-H] ⁻	527.00	78.9	30	-80	-118	-1
¹³ C-Adenosin	IS [M-H] ⁻	271.06	133.9	30	-35	-16	-1

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23 Quantification of free fatty acids

24 The cell pellets were extracted with 1 mL acetonitrile/isopropanol/ammonium acetate buffer (55/45/5, v/v/v)
 25 and 50 μ L of internal standard solution. After vortexing, the samples were incubated overnight and centrifuged.
 26 The supernatant was dried under a nitrogen stream and dissolved in 50 μ L of extraction solution. Samples were
 27 subjected to LC-MS/MS using the setup above. Separation was performed using a 100 x 2.0 mm inner diameter,
 28 2.5 μ m Synergi Polar-RP 100 A column (Phenomenex, Aschaffenburg, Germany) with a 400 μ L/min flowrate and
 29 a linear gradient from 50% A (A: acetonitrile/isopropanol/water with 5 mM ammonia acetate (55/40/5, v/v/v,
 30 pH 5), B: 5 mM ammonia acetate (pH 5)) for 3 min to 100% A in 9 min which was maintained for 3 min. Afterward
 31 the column was equilibrated to starting conditions. Ions were analyzed by MS in the ESI negative mode. The ion
 32 spray voltage was set to -4500 V at a source temperature of 550°C and using nitrogen as collision gas. The
 33 parameters for the collision activated dissociation (CAD) were: medium, curtain gas: 25 psi, ion source gas 1: 55
 34 psi, ion source gas 2: 65, entrance potential (EP) -10 V. The MRM (multiple reaction monitoring) transition for
 35 each compound are listed in Table S2. The first MRM-transition was used as quantifier the second as qualifier.

36 *Table S2: MRM-transitions for quantitation of fatty acids.*

Compound	Quantifier/ Qualifier	Q ₁ (m/z)	Q ₃ (m/z)	Dwell Time (msec)	Declustering Potential (DP)	Collision Energy (CE)	Cell Exit Potential (CXP)
C12:0	Quantifier [M-H] ⁻	199.2	199.1	10	-70	-14	-1
	Qualifier [M-H] ⁻	199.1	154.9	10	-70	-16	-11
C14:0	Quantifier [M-H] ⁻	227.2	227.1	10	-85	-12	-15
	Qualifier [M-H] ⁻	227.2	138.8	10	-85	-20	-9
C15:0	Quantifier [M-H] ⁻	241.2	241.1	10	-80	-12	-15
	Qualifier [M-H] ⁻	241.2	197.0	10	-80	-20	-11
C16:0	Quantifier [M-H] ⁻	255.3	255.0	10	-80	-30	-9
	Qualifier [M-H] ⁻	255.3	166.7	10	-80	-26	-9
C16:1	Quantifier [M-H] ⁻	253.3	253.0	10	-85	-14	-17
	Qualifier [M-H] ⁻	253.3	208.9	10	-85	-34	-17
C18:0	Quantifier [M-H] ⁻	283.2	283.2	20	-60	-12	-13
	Qualifier [M-H] ⁻	283.1	283.1	20	-60	-22	-13
C18:1	Quantifier [M-H] ⁻	281.4	281.1	10	-100	-14	-17
	Qualifier [M-H] ⁻	281.4	96.8	10	-100	-38	-15
C18:2	Quantifier [M-H] ⁻	279.4	279.1	10	-85	-14	-7
	Qualifier [M-H] ⁻	279.4	96.7	10	-85	-36	-7
C18:3	Quantifier [M-H] ⁻	277.4	277.3	10	-80	-14	-7
	Qualifier [M-H] ⁻	277.4	58.7	10	-80	-24	-1

	[M-H] ⁻						
C20:0	Quantifier [M-H] ⁻	311.4	311.3	10	-90	-14	-9
	Qualifier [M-H] ⁻	311.4	182.8	10	-90	-50	-11
C20:4	Quantifier [M-H] ⁻	303.4	303.2	10	-80	-12	-11
	Qualifier [M-H] ⁻	303.4	259.2	10	-80	-20	-7
<i>d</i> ₅ -C3:0	IS [M-H] ⁻	78.1	78.0	10	-55	-6	-5
¹³ C ₂ -C6:0	IS [M-H] ⁻	117.0	116.6	10	-45	-6	-19
<i>d</i> ₃ -C12:0	IS [M-H] ⁻	202.3	202.3	10	-85	-26	-11
<i>d</i> ₂ -C18:1	IS [M-H] ⁻	283.4	283.3	10	-110	-18	-9
<i>d</i> ₃ -C18:0	IS [M-H] ⁻	286.3	286.3	10	-115	-16	-19
<i>d</i> ₃ -C20:0	IS [M-H] ⁻	314.5	314.3	10	-130	-16	-15