



Fig. S1 Percent viability values of high level nicotinamide concentration in normal condition. n=6

Table S1. Specific compound dependent MS parameters used in multiple reaction monitoring (MRM)

Measured Compound	Precursor ion	Fragment ion	Dwell (ms)	Fragmentor (V)	CE (V)
AcCoA	808.1	408	12	200	40
NADPH	744	408	10	240	40
NADP	742	620	10	100	10
NADH	664	346	10	200	20
NAD	662	540	10	80	20
ATP	506	408	12	135	20
ADP	426	159	12	100	20
AMP	346.1	97	12	100	20
IsoCIT	191	111	73	20	60
GLU	146.2	128	12	80	5
AKG	145	101	20	70	2
MAL	133	115	20	80	5
SUC	117.1	99	20	60	5
FUM	115.1	71	20	60	5
LA	89.1	70.9	20	60	5
PYR	87.1	43	20	60	2

Table S2. Linearity of calibration, limits of detection and relative standard deviation of three concentration levels of standards determined by the established HPLC/MS/MS method

Measured Compound	Linearity			Low		Medium		High	
	Range (ng/mL)	R <sup>2</sup>	LOD (ng/mL)	Spiked concentration	RSD%	Spiked concentration	RSD%	Spiked concentration	RSD%
				(ug/mL)	(ug/mL)	(ug/mL)	(ug/mL)	(ug/mL)	(ug/mL)
AcCoA	5-5000	0.9995	1	0.588	7%	1.18	5%	2.35	6%
NADPH	10-10000	0.9992	1	1.25	7%	2.51	8%	5.01	4%
NADP	15-10000	0.9997	5	0.586	6%	1.17	5%	2.35	4%
NADH	10-10000	0.9990	2	0.611	7%	1.22	7%	2.45	10%
NAD	50-10000	0.9982	5	1.26	4%	2.51	11%	5.03	5%
ATP	80-10000	0.9992	25	1.58	5%	3.17	9%	6.33	5%
ADP	80-10000	0.9987	25	1.58	3%	3.15	5%	6.30	7%
AMP	25-3000	0.9993	5	0.629	9%	1.26	5%	2.52	4%
IsoCIT	150-20000	0.9995	1	1.28	2%	2.56	4%	5.11	2%
GLU	250-25000	0.9992	5	1.51	3%	3.03	5%	6.05	3%
AKG	50-20000	0.9990	1	2.28	8%	4.57	3%	9.14	2%

MAL	50-20000	0.9992	1	1.35	3%	2.70	1%	5.40	2%
SUC	50-10000	0.9994	1	1.33	8%	2.67	3%	5.34	3%
FUM	50-8000	0.9982	10	0.736	4%	1.47	2%	2.95	3%
LA	100-10000	0.9989	1	0.626	6%	1.25	4%	2.50	4%
PYR	50-10000	0.9993	10	0.063	5%	0.125	6%	0.250	2%

