

Supplementary

Table S1:

Pulse shapes, durations etc.:

Pulse Shape	Duration in ms
Adiabatic half passage: hs_ex_500_400_100	4.652
Adiabatic full passage: oit_800_6500	3.4620
Block 90	0.096

Suppl table S2:*Composition of NADH, NAD⁺ and ATP phantoms in 200ml stackable cell culture bottle*

Metabolite	Concentration in mM	Additives	pH
NADH	0.875		6.0
	1.75	52.6 mM KCl, 42.3 mM MgCl ₂	6.0
	3.5		6.0
NAD ⁺	0.875		6.0
	1.75	52.6 mM KCl, 42.3 mM MgCl ₂	6.0
	3.5		6.0
ATP	18.0	52.6 mM KCl, 42.3 mM MgCl ₂ , 5 mM KH ₂ PO ₄	7.2

Suppl table S3: Fitting prior knowledge:

Fitting prior knowledge. From reference (53), various T_2 values within the 95% confidence interval were tested and the T_2 that resulted in the best fit (lowest residual) was chosen for further implementation. Furthermore, T_2 values for NADH and NAD^+ were assumed to be similar to the T_2 of ATP (28) and further optimization showed that a slightly shorter T_2 for NAD^+ resulted in a better fit (less residual) which is the basis for the prior knowledge as given in the table. The same prior knowledge was used for all in vivo measurements

Fitted Metabolite	Assumed T_2 in ms	Source	Relative Chemical Shift at 3T in Hz	Source
Pi	148	(53)	-258.5	(16)
GPE	44		-165.46	
GPC	28		-142.71	
PCr	334		0.0	
γ -ATP	62		128.23	
α -ATP	47		388.82	
NADH	42	Estimation	425.85	(15)
NAD^+	35	437.59		
β -ATP	55	(53)	835.0	(16)