

Electronic Supplementary Information

Metabolic stability of cells for extended metabolical measurements using NMR. A comparison between lysed and additionally heat inactivated cells.

G. Diserenst†, D. Hertigt†, M. Vermathen, B. Legeza, CE. Flück, JM. Nuoffer†† and P. Vermathen††

Table S1 Signal assignment of metabolites from fibroblast cell lines.

#	Chemical Shift	Compound	TOCSY
1	0.928 (t)	Isoleucine (Ile)	1.253, 1.447
2	0.950 (d)	Leucine (Leu)	1.702
3	0.976 (d)	Valine (Val)	2.265
4	1.000 (d)	Isoleucine (Ile)	1.969
5	1.031 (d)	Valine (Val)	2.265
6	1.174 (t)	Ethanol (EtOH)	3.627
7	1.242 (s)	Fatty Acid (FA)	
8	1.320 (d)	Lactic acid (Lac)	4.105
9	1.468 (d)	Alanine (Ala)	3.764
10	1.702 (m)	Leucine (Leu)	0.950
11	1.905 (s)	Acetate (Ac)	
12	1.969 (m)	Isoleucine (Ile)	1.000
13	2.060 (m)	Glutamate (Glu)	2.335
14	2.122 (m)	Glutamine (Gln)	3.780
15	2.150 (m)	Glutathione (GSH)	2.540, 3.777
16	2.333 (m)	Glutamate (Glu), Glutamine (Gln)	Glu 3.736
17	2.540 (m)	Glutathione (GSH)	2.150, 3.777
18	2.647 (t)	Methionine (Met)	
19	2.677 (d)	Citric Acid? (Cit)	
20	2.776 (d)	Citric Acid? (Cit)	
21	2.949 (dd)	Glutathione (GSH)	4.574
22	3.022 (s)	Creatine (Cre)	
23	3.030 (s)	Creatinine (Crein)	
24	3.199 (s)	Choline (Cho)	
25	3.208 (dd)	Glucose (Glc)	3.524
26	3.213 (s)	Posphocholine (PC)	
28	3.223 (s)	Glycerophosphocholine (GPC)	
29	3.249 (t)	Taurine (Tau)	3.403
30	3.267 (t)	Inositol (Ino)	3.524, 3.608, 4.045
31	3.403 (t)	Taurine (Tau)	3.249
32	3.459 (m)	Glucose (Glc)	
33	3.477 (m)	Glucose (Glc)	
34	3.497 (m)	Choline (Cho)	4.05
35	3.524	Inositol (Ino) (dd), Glucose (Glc) (dd)	Ino 3.267, Glc 3.730
36	3.582 (m)	Posphocholine (PC)	4.107
37	3.608 (t)	Inositol (Ino)	3.246, 3.524, 4.045
38	3.730-3.800	Alanine (Ala) (q), Glutamate (Glu) (dd), Glutamine (Gln) (t), Glutathione (GSH) (m), Glucose (Glc)	Ala 1.452, GSH 2.150 2.540, Gln 2.122

39	3.840 (m)	Glucose (Glc)	
40	3.900 (dd)	Glucose (Glc)	
41	3.924 (s)	Creatine (Cre)	
42	4.045	Choline (Cho) (m), Inositol (Ino) (t)	Ino 3.608, Cho 3.497
43	4.105 (q)	Lactic Acid (Lac)	1.320
44	4.183 (m)	Posphocholine (PC)	3.582
45	4.316 (m)	Glycerophosphocholine (GPC)	
46	4.574 (q)	Glutathione (GSH)	2.949
47	4.638	Glucose (Glc) (d), Glucose-6-P (Glc6P) (d)	
48	5.366 (s)	Phosphoenolpyruvate? (PEP)	5.179
49	5.605 (dd)	UDP Glucose (UDPGlc)	
50	5.788 (d)	Uracil (Ura)	7.525
51	5.970 (m)	UDP Glucose (UDPGlc)	
52	5.905 (2d)	Uridine (Urd)	7.886
53	5.950 (d)	CTP	
54	6.143 (d)	CTP	7.975
55	5.975 (m)	UMP / UDP	UMP 8.143, UDP 7.955
56	6.510 (s)	Fumaric acid (Fum)	
57	6.886 (d)	Tyrosine (Tyr)	7.177
58	7.177 (d)	Tyrosine (Tyr)	6.886
59	7.315 (m)	Phenylalanine (Phe)	
60	7.406 (m)	Phenylalanine (Phe)	
61	7.525 (d)	Uracil (Ura)	5.786
62	7.884 (d)	Uridine(Urd)	5.905
63	7.955	UDP-Glc (d), CTP (d), UDP (d)	
64	8.143 (d)	UMP	5.975
65	8.161 (s)	NAD	8.889, 9.113
66	8.182 (s)	Hypoxanthine? (HXan)	
67	8.202 (s)	Hypoxanthine? (HXan)	
68	8.223 (s)	Inosine(Ine)	
69	8.377 (s)	Inosine(Ine)	
70	8.471 (s)	NADH?	
71	8.255 (s)	AMP	
72	8.532 (s)	AMP	
73	8.160	1-Methyl Niacinamide? (1M-Niac) (t), NAD (s)	1M-Niac 8.889 8.97, NAD 8.889 9.113
74	8.889 (d)	1-Methyl Niacinamide (1M-Niac)?	8.160, 8.97
75	8.970 (d)	1-Methyl Niacinamide (1M-Niac)?	8.160, 8.889
76	9.290 (s)	1-Methyl Niacinamide (1M-Niac)?	
77	8.424 (s)	NAD	
78	8.889 (d)	NAD	8.160
79	9.113 (d)	NAD	8.160, 8.889
80	9.317 (s)	NAD	