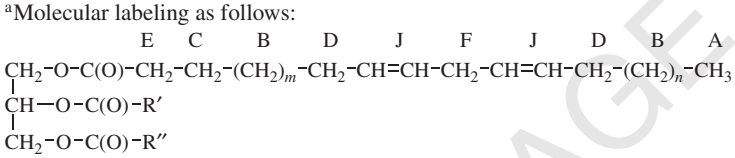
Appendix 3

Peak Assignments for Some Common Metabolites

Table 1. In vivo ^{1}H chemical shifts and estimated spin–lattice (T_1) and spin–spin (T_2) relaxation times of triglyceride fatty acid in human marrow and subcutaneous tissue measured at 7 T[1]

Chemical group[a]	δ (ppm)	T_1 (s)		T_2 (ms)	
		Marrow	Subcutaneous	Marrow	Subcutaneous
$-CH_3$ (A)	0.90[b]	1.16	1.08	74	67
$-(CH_2)_n-$ (B)	1.30	0.55	0.53	69	63
$-CH_2-CH_2-COO$ (C)	1.59	0.39	0.32	33	30
$-CH_2-CH=CH-CH_2-$ (D)	2.03	0.42	0.39	42	39
$-CH_2-COO$ (E)	2.25	0.44	0.40	60	55
$=CH-CH_2-CH=$ (F)	2.77	0.60	0.58	5	58
$-CH=CH-$ (J)	5.31				–

[a]Molecular labeling as follows:



[b]Used as a chemical shift reference.

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Table 2. In vivo ^{1}H chemical shifts (δ, relative to the creatine trimethyl resonance at 3.02 ppm) and relaxation times of lactate,[2] carnitine,[3] and acetyl-carnitine[3] in human skeletal muscle at 7 T

Moiety	δ (ppm)	T_1 (s)	T_2 (ms)
Lactate –CH–	4.09	1.7 ± 0.2[a]	109 ± 10[a]
–CH_3	1.31	1.2 ± 0.1[a]	–
Carnitine –$N(CH_3)_3$	3.20	1.07 ± 0.10[b]	109 ± 12[b]
		1.04 ± 0.12[a]	120 ± 13[a]
Acetyl-carnitine –$N(CH_3)_3$	3.17	0.90 ± 0.11[a]	129 ± 15[a]

[a]Measured after exercise
[b]Measured at rest.

Table 3. In vivo ^{1}H chemical shifts of amino acids and some other low-molecular-weight metabolites[4]

Moiety	Structure	δ (ppm)
Amino acids		
Neutral amino acids[a]	$\mathbf{CH_3}$–	0.9–1.0
Threonine	$\mathbf{CH_3}$–CH–	1.33
Alanine	$\mathbf{CH_3}$–CH–	1.49
Lysine/polyamines	H_3N^+–CH_2–$\mathbf{CH_2}$–CH_2–	1.71
N-Acetyl aspartate	$\mathbf{CH_3}$–COO–NH	2.03
Glutamate/glutamine	CH–$\mathbf{CH_2}$–CH_2–COO^-/–NH_3^+	2.17
Lysine	H_3N^+–$\mathbf{CH_2}$–CH_2–CH_2–	3.02
Alanine, glutamate, glutamine, and other amino acids	α-Protons –OOC–C**H**(R)–NH–	3.78
Other low-molecular-weight metabolites		
Lactate	$\mathbf{CH_3}$–CH–	1.33
Creatine	$\mathbf{CH_3}$–N–CH_2–COO^-	3.02
Phosphocreatine	$\mathbf{CH_3}$–N–CH_2–COO^-	3.02
Choline	$-N^+(\mathbf{CH_3})_3$	3.21
Phosphocholine	$-N^+(\mathbf{CH_3})_3$	3.23
Glycerophosphocholine	$-N^+(\mathbf{CH_3})_3$	3.24
Myo-inositol	–CH–C**H**(OH)–	3.25
Taurine	H_3N^+–$\mathbf{CH_2}$–CH_2–SO_3^-	3.25
Taurine	H_3N^+–CH_2–$\mathbf{CH_2}$–SO_3^-	3.43
Water	$\mathbf{H_2}O$, **H**OD	4.63

[a]Including valine, leucine, and isoleucine.
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Table 4. ^{31}P chemical shift (δ) and estimated apparent T_1 ($T_{1,app}$) of ^{31}P metabolites in human brain at rest at 7 T[5]

	δ (ppm)	$T_{1,app}$ (s)
Monophosphates		
Phosphoethanolamine (PE)	6.76 ± 0.05	6.33 ± 1.10
Phosphocholine (PC)	6.24 ± 0.02	4.31 ± 1.04
Extracellular inorganic phosphate (Pi^{ex})	5.24 ± 0.05	5.80 ± 1.07
Intracellular inorganic phosphate (Pi^{in})	4.82 ± 0.01	3.70 ± 0.46
Glycerophosphoethanolamine (GPE)	3.50 ± 0.01	6.79 ± 0.95
Glycerophosphocholine (GPC)	2.95 ± 0.01	5.82 ± 0.88
Phosphocreatine (PCr)	[0]	3.39 ± 0.17
Diphosphates		
Nicotinamide adenine dinucleotide (NAD)	−8.21 ± 0.04	2.07 ± 0.13
Uridine diphosphoglucose (UDPG)	−9.72 ± 0.04	2.95 ± 0.36
Triphosphates		
Adenosine triphosphate (γ-ATP)	−2.52 ± 0.01	1.70 ± 0.15
α-ATP	−7.56 ± 0.02	1.35 ± 0.14
β-ATP	−16.15 ± 0.05	1.13 ± 0.09

Table 5. ^{13}C chemical shifts, sorted by compound name

Shift	Compound	Shift	Compound	Shift	Compound
182.1	Acetate C1	72.5	α-Glucose C2	43.9	Malate C3
182.6	Acetate C1	73.2	α-Glucose C3	180.9	Malate C4
24.2	Acetate C2	73.8	α-Glucose C3	181.6	Malate C4
24.5	Acetate C2	73.9	α-Glucose C3	50.1	Methanol
24.6	Acetate C2	70.1	α-Glucose C4	31.4	Methionine C2
175	Acetoacetate C1	70.7	α-Glucose C4	55.1	Methionine C3
175.5	Acetoacetate C1	72.3	α-Glucose C5	30	Methionine C4
175.7	Acetoacetate C1	72.5	α-Glucose C5	15.2	Methionine S(CH_3)
54.2	Acetoacetate C2	72.6	α-Glucose C5	140.72	NAD C2
54.5	Acetoacetate C2	61.7	α-Glucose C6	134.68	NAD C3
210.9	Acetoacetate C3	61.8	α-Glucose C6	148.6	NAD C4
211	Acetoacetate C3	96.8	β-Glucose C1	129.6	NAD C5
30.5	Acetoacetate C4	97	β-Glucose C1	143.35	NAD C6
30.7	Acetoacetate C4	75.1	β-Glucose C2	166.22	NAD C7
30.5	Acetyl-CoA C2	75.2	β-Glucose C2	139.15	NADH C2
21.5	Acetylcarnitine –(CH_3)	75.3	β-Glucose C2	101.25	NADH C3
54.7	Acetylcarnitine –N(CH_3)$_3$	76.1	β-Glucose C3	22.86	NADH C4
176.3	Alanine C1	77	β-Glucose C3	106.22	NADH C5
176.7	Alanine C1	70.1	β-Glucose C4	125.12	NADH C6
51.5	Alanine C2	70.7	β-Glucose C4	173.62	NADH C7
51.7	Alanine C2	76.8	β-Glucose C5	148.29	Nicotinamide C2
51.9	Alanine C2	76.9	β-Glucose C5	129.7	Nicotinamide C3
17.3	Alanine C3	61.8	β-Glucose C6	137.04	Nicotinamide C4
17.4	Alanine C3	174.7	Glutamate C1	124.96	Nicotinamide C5

(*continued overleaf*)

Table 5. (*continued*)

Shift	Compound	Shift	Compound	Shift	Compound
34.8	β-Alanine C2	175.1	Glutamate C1	152.48	Nicotinamide C6
37.8	β-Alanine C3	55.2	Glutamate C2	170.79	Nicotinamide C7
55.8	Arginine C2	55.8	Glutamate C2	149.87	Nicotinate C2
28.9	Arginine C3	27.6	Glutamate C3	133.21	Nicotinate C3
25.5	Arginine C4	28.1	Glutamate C3	138.58	Nicotinate C4
41.8	Arginine C5	34.2	Glutamate C4	124.83	Nicotinate C5
157.7	Arginine C6	34.7	Glutamate C4	151.17	Nicotinate C6
175	Aspartate C1	181.4	Glutamate C5	173.85	Nicotinate C7
175.3	Aspartate C1	181.8	Glutamate C5	178.2	Oxaloacetate (hydrate) C1
52.7	Aspartate C2	174.2	Glutamine C1	99.5	Oxaloacetate (hydrate) C2
53.4	Aspartate C2	174.8	Glutamine C1	50	Oxaloacetate (hydrate) C3
37.4	Aspartate C3	55.2	Glutamine C2	181.9	Oxaloacetate (hydrate) C4
37.8	Aspartate C3	55.4	Glutamine C2	169.3	Oxaloacetate (keto) C1
178.3	Aspartate C4	27.2	Glutamine C3	201.5	Oxaloacetate (keto) C2
178.5	Aspartate C4	28.1	Glutamine C3	50.2	Oxaloacetate (keto) C3
160	Bicarbonate C1	31.8	Glutamine C4	175.9	Oxaloacetate (keto) C4
160.8	Bicarbonate C1	32	Glutamine C4	175.5	Oxaloacetate C1
161.8	Bicarbonate C1	177.8	Glutamine C5	204.7	Oxaloacetate C2
184	Butyrate C1	178.5	Glutamine C5	50	Oxaloacetate C3
19.4	Butyrate C3	91.3	Glyceraldehyde 3-P hydrate C1	169.4	Oxaloacetate C4
128.73	$=*CHCH_2*CH=$	74.9	Glyceraldehyde 3-P hydrate C2	57.2	Phenylalanine C2
27.95	$-CH_2*CH_2CH=CH-$	66	Glyceraldehyde 3-P hydrate C3	37.7	Phenylalanine C3
34.46	$-CH_2*CH_2CO-$	63.4	Glycerol 3-P C1	136.8	Phenylalanine C4
172.43	$-CH_2CH_2*CO-$	63.5	Glycerol 3-P C1	130.4	Phenylalanine C5
25.6	$-*CH_2CH_2CO-$	72.4	Glycerol 3-P C2	130	Phenylalanine C6
14.73	$*CH_3CH_2-$	65.8	Glycerol 3-P C3	128.6	Phenylalanine C7
32.76	$CH_3CH_2*CH_2CH_2-$	66	Glycerol 3-P C3	67.6	Phosphocholine (N)
130.25	$-CH=*CHCH_2CH_2-$	62.59	Glycerol C1,C3	59.1	Phosphocholine (O)
26.43	$-CH=CH*CH_2CH=CH-$	63.50	Glycerol C1,C3	55.1	Phosphocreatine (CH_2)
163.8	Carbamino group C1	63.6	Glycerol C1,C3	38.1	Phosphocreatine (CH_3)
45	Citrate (Mg^2 citrate) C2	69.74	Glycerol C2	174.2	Phosphoenolpyruvate C1
174.2	Citrate C1,C5	73	Glycerol C2	152.7	Phosphoenolpyruvate C2
179.7	Citrate C1,C5	73.3	Glycerol C2	102.1	Phosphoenolpyruvate C3
180	Citrate C1,C5	173.5	Glycine C1	41.8	Phosphoethanolamine (N)
44.1	Citrate C2,C4	42.6	Glycine C2	61.5	Phosphoethanolamine (O)
46.6	Citrate C2,C4	42.7	Glycine C2	179	2-Phosphoglycerate C1
46.8	Citrate C2,C4	100.5	Glycogen (1:4) C1	77.4	2-Phosphoglycerate C2
74.2	Citrate C3	74	Glycogen (1:4) C3	65.7	2-Phosphoglycerate C3
76	Citrate C3	77.7	Glycogen (1:4) C4	62.3	Proline C2
76.1	Citrate C3	61.4	Glycogen (1:4) C6	30	Proline C3
177.5	Citrate C6	72	Glycogen (1:4,1:6) C2	25	Proline C4
182.3	Citrate C6	99.2	Glycogen (1:6) C1	47.4	Proline C5
186.7	Citrate C6	73.5	Glycogen (1:6) C3	185.4	Propionate C1
174.5	2,3-Cyclopyrophosphoglycerate C1	70	Glycogen (1:6) C4	31.5	Propionate C2
78.6	2,3-Cyclopyrophosphoglycerate C2	67.9	Glycogen (1:6) C6	11	Propionate C3
70.1	2,3-Cyclopyrophosphoglycerate C3	72.2	Glycogen (1:6,1:4) C5	176.8	Propionylcarnitine C1

Table 5. (*continued*)

Shift	Compound	Shift	Compound	Shift	Compound
54.7	Cystine C2	177.3	Glycolate C1	9	Propionylcarnitine C3
40.6	Cystine C3	60.3	Glycolate C2	59.1	Pyroglutamate C2
65.1	DHAP (hydrate) C1	177.9	Glyoxylate C1	26.3	Pyroglutamate C3
96	DHAP (hydrate) C2	89.3	Glyoxylate C2	30.9	Pyroglutamate C4
67	DHAP (hydrate) C3	55.8	Histidine C2	177.6	Pyruvate (hydrate) C1
66.5	DHAP (keto) C1	29.7	Histidine C3	93.1	Pyruvate (hydrate) C2
212.6	DHAP (keto) C2	137.5	Histidine C6	26.3	Pyruvate (hydrate) C3
68.5	DHAP (keto) C3	117.5	Histidine C8	26.7	Pyruvate (hydrate) C3
67.4	Dioxane	180.5	β-Hydroxybutyrate C1	169.3	Pyruvate (keto) C1
52	EDTA (ac) C3	181.1	β-Hydroxybutyrate C1	205.4	Pyruvate (keto) C2
58.2	EDTA (en) C2	181.2	β-Hydroxybutyrate C1	27.6	Pyruvate (keto) C3
175.6	EDTA C1	47.3	β-Hydroxybutyrate C2	171.1	Pyruvate C1
58.6	Ethanol C1	47.6	β-Hydroxybutyrate C2	205.8	Pyruvate C2
17.4	Ethanol C2	65.7	β-Hydroxybutyrate C3	27.3	Pyruvate C3
18	Ethanol C2	66.6	β-Hydroxybutyrate C3	173.5	Serine C1
83.2	Formaldehyde (hydrate) C1	66.8	β-Hydroxybutyrate C3	57.4	Serine C2
171.4	Formate C1	22.7	β-Hydroxybutyrate C4	57.5	Serine C2
172.2	Formate C1	22.9	β-Hydroxybutyrate C4	61.4	Serine C3
65.4	α-Fructose 1,6-diP C1	56.7	Hypotaurine (N)	61.6	Serine C3
105.9	α-Fructose 1,6-diP C2	34.8	Hypotaurine (S)	63.6	D-Sorbitol C1
82.6	α-Fructose 1,6-diP C3	72.1	Inositol (myo) C1,C3	72.2	D-Sorbitol C2
77.8	α-Fructose 1,6-diP C4	73.3	Inositol (myo) C2	70.8	D-Sorbitol C3
82.9	α-Fructose 1,6-diP C5	73.6	Inositol (myo) C4,C6	72.1	D-Sorbitol C4
64.4	α-Fructose 1,6-diP C6	75.3	Inositol (myo) C5	74.1	D-Sorbitol C5
66.9	β-Fructose 1,6-diP C1	181	Isocitrate C1,C5	64	D-Sorbitol C6
102	β-Fructose 1,6-diP C2	38.5	Isocitrate C2	182.8	Succinate C1,C1′
76.9	β-Fructose 1,6-diP C3	49.9	Isocitrate C3	183.4	Succinate C1,C1′
75.1	β-Fructose 1,6-diP C4	74.6	Isocitrate C4	35	Succinate C2,C2′
80.6	β-Fructose 1,6-diP C5	60.7	Isoleucine C2	35.3	Succinate C2,C2′
65.3	β-Fructose 1,6-diP C6	37	Isoleucine C3	49	Taurine (N)
63.8	α-Fructose 6-P C1	25.7	Isoleucine C4	48.4	Taurine (N) (pH 6.5) C1
105.3	α-Fructose 6-P C2	15.8	Isoleucine CH_3 (4)	36.6	Taurine (S)
89.6	α-Fructose 6-P C3	12.2	Isoleucine CH_3 (5)	36.5	Taurine (S) (pH 6.5) C2
76.9	α-Fructose 6-P C4	170.7	α-Ketoglutarate C1	61.5	Threonine C2
81.4	α-Fructose 6-P C5	170.8	α-Ketoglutarate C1	67.3	Threonine C3
64.5	α-Fructose 6-P C6	206.3	α-Ketoglutarate C2	20.7	Threonine C4
63.75	β-Fructose 6-P C1	206.7	α-Ketoglutarate C2	94	a,a-Trehalose C1
102.5	β-Fructose 6-P C2	31.4	α-Ketoglutarate C3	94.4	a,a-Trehalose C1
76.2	β-Fructose 6-P C3	31.8	α-Ketoglutarate C3	72.2	a,a-Trehalose C2
75.4	β-Fructose 6-P C4	36.7	α-Ketoglutarate C4	73.3	a,a-Trehalose C2
80.9	β-Fructose 6-P C5	37	α-Ketoglutarate C4	73.5	a,a-Trehalose C3
65.3	β-Fructose 6-P C6	182	α-Ketoglutarate C5	73.7	a,a-Trehalose C3
175.3	Fumarate C1,C1′	182.7	α-Ketoglutarate C5	70.6	a,a-Trehalose C4
175.6	Fumarate C1,C1′	183.2	Lactate C1	70.9	a,a-Trehalose C4
136	Fumarate C2,C2′	183.5	Lactate C1	73	a,a-Trehalose C5
136.4	Fumarate C2,C2′	69.4	Lactate C2	61.5	a,a-Trehalose C6

(*continued overleaf*)

Table 5. (*continued*)

Shift	Compound	Shift	Compound	Shift	Compound
35.4	GABA C2	69.6	Lactate C2	61.7	a,a-Trehalose C6
24.6	GABA C3	21	Lactate C3	120.3	Tryptophan C10
40.4	GABA C4	21.3	Lactate C3	119.4	Tryptophan C11
180	Gluconate C1	55.3	Leucine C2	56	Tryptophan C2
75.9	Gluconate C2	41	Leucine C3	27.6	Tryptophan C3
72.3	Gluconate C3	25.3	Leucine C4	126	Tryptophan C5
75	Gluconate C4	22.2	Leucine CH_3	112.9	Tryptophan C8
73.2	Gluconate C5	55.7	Lysine C2	123	Tryptophan C9
64.3	Gluconate C6	31.2	Lysine C3	57.4	Tyrosine C2
93.2	α-Glucose 6-P C1	23.2	Lysine C4	36.7	Tyrosine C3
63.6	α-Glucose 6-P C6	27.3	Lysine C5	156.2	Tyrosine C4
96.8	β-Glucose 6-P C1	40.5	Lysine C6	131.8	Tyrosine C5
97	β-Glucose 6-P C1	180.4	Malate C1	116.8	Tyrosine C6
63.6	β-Glucose 6-P C6	182.1	Malate C1	127.6	Tyrosine C7
92.9	α-Glucose C1	71.2	Malate C2	61.6	Valine C2
93.1	α-Glucose C1	71.7	Malate C2	30.3	Valine C3
93.2	α-Glucose C1	43.4	Malate C3	19.2	Valine CH_3
72.3	α-Glucose C2				

Notes: The carbons are numbered from the terminal carboxyl group, i.e., acetate C1 refers to the carboxyl group and acetate C2 refers to the methyl group. Same for the amino acids: aspartate C1 refers to the α-carboxyl group while aspartate C4 refers to the δ-carboxyl group; glutamate C1 is the α-carboxyl while glutamate C5 is the ε-carboxyl group. The sugars use standard carbon nomenclature: glucose C1 is the aldehyde carbon and glucose C6 is the terminal CH_2OH carbon (same for fructose). Includes data from Refs. 6–11.

Table 5 was contributed by Mark Jeffrey, Craig Malloy and Dean Sherry of the University of Texas Southwestern Medical Center, Dallas, USA.

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