

Table 1

N°	Metabolite	Group	¹ H chemical shift (ppm)
1	Taurine	-CH ₂ -NH ₃ ⁺	3.27
		-CH ₂ -SO ₃ ⁻	3.42
2	Aspartate	βCH ₂ (u)	2.69
		βCH ₂ (d)	2.81
		αCH	3.89
3	Serine	αCH	3.84
		βCH ₂ (u)	3.94
		βCH ₂ (d)	3.99
4	Acetate	CH ₃	1.92
5	N Acetyl Aspartate (NAA)	CH ₃	2.02
6	Isoleucine	δCH ₃	0.94
		γCH ₃	1.01
		γCH ₂	1.27
		αCH	3.68
		C4H	3.41
7	β-Glucose	C3H, C5H	3.48
		C6H(u)	3.76
		C6H(d)	3.89
		C1H	4.65
		CH ₂	3.56
8	Glycine	CH ₂	3.56
9	Valine	γCH ₃	0.99
		γ'CH ₃	1.04
		βCH	2.28
10	Lactate	CH ₃	1.33
		CH	4.12
11	Alanine	βCH ₃	1.48
		αCH	3.78
		C5H	3.27
12	myo-Inositol	C1H, C3H	3.53
		C4H, C6H	3.62
		C2H	4.05
		-CHOH-	4.02
13	Ascorbate	C4H	4.52
		CH ₂ -CONH	2.56
		CH ₂ -SH	2.95
14	Glutathione (GSH)	CH-NH ₂	3.79
		βCH ₂	2.09
		γCH ₂	2.34
15	Glutamate	αCH	3.76
		all Hs	3.34
		(α,β) CH ₂	2.41
17	Succinate	(α,β) CH ₂	2.41
18	Fumarate	all CH	6.52
19	Glutamine	βCH ₂	2.14
		γCH ₂	2.45
		αCH ₂	3.78
20	Arginine	γCH ₂ (u)	1.64
		γCH ₂ (d)	1.72
		βCH ₂	1.92
		δCH ₂	3.25
		αCH	3.78
21	Creatine	CH ₃	3.03
		CH ₂	3.94
22	Ethanolamine	-CH ₂ -NH ₃ ⁺	3.14
		CH ₂ OH	3.82
23	Choline	-N ⁺ -(CH ₃) ₃	3.22
		βCH ₂	3.54
		αCH	4.07
24	Glycerophosphocholine	-N ⁺ -(CH ₃) ₃	3.24
		αCH ₂ -OH	3.65
		βCH ₂ -OH and -CH ₂ -N ⁺	3.70
		CH ₂ -PO ₄ and CHO	3.92
		CH ₂ -PO ₄	4.33
25	Phosphorylcholine	-N ⁺ -(CH ₃) ₃	3.23
		βCH ₂	3.61
		αCH	4.16
26	Tyrosine	βCH ₂ (u)	3.06
		βCH ₂ (d)	3.20
		αCH	3.94
		orthoCH	6.89
		metaCH	7.18
27	Tryptophan	βCH ₂ (up)	3.31
		βCH ₂ (down)	3.49
		αCH	4.06
		CH-NH	7.32