

## Chemical Shifts - Sorted By Compound Name

Shift	Compound	Shift	Compound	Shift	Compound
182.1	Acetate C1[d]	72.5	a-Glucose C2[c,g]	43.9	Malate C3[g]
182.6	Acetate C1[g]	73.2	a-Glucose C3[e]	180.9	Malate C4[g]
24.2	Acetate C2[d]	73.8	a-Glucose C3[g]	181.6	Malate C4[d]
24.5	Acetate C2[g]	73.9	a-Glucose C3[g]	50.1	Methanol[g]
24.6	Acetate C2[w]	70.1	a-Glucose C4[e]	31.4	Methionine C2[w]
175	Acetoacetate C1[e]	70.7	a-Glucose C4[c,g]	55.1	Methionine C3[w]
175.5	Acetoacetate C1[d]	72.3	a-Glucose C5[w]	30	Methionine C4[w]
175.7	Acetoacetate C1[g]	72.5	a-Glucose C5[c]	15.2	Methionine S(CH <sub>3</sub> )[w]
54.2	Acetoacetate C2[d]	72.6	a-Glucose C5[g]	140.72	NAD C2[g]
54.5	Acetoacetate C2[g]	61.7	a-Glucose C6[c]	134.68	NAD C3[g]
210.9	Acetoacetate C3[g]	61.8	a-Glucose C6[g]	148.6	NAD C4[g]
211	Acetoacetate C3[d]	96.8	b-Glucose C1[w]	129.6	NAD C5[g]
30.5	Acetoacetate C4[d]	97	b-Glucose C1[c,g]	143.35	NAD C6[g]
30.7	Acetoacetate C4[g]	75.1	b-Glucose C2[w]	166.22	NAD C7[g]
30.5	Acetyl-CoA C2[g]	75.2	b-Glucose C2[c]	139.15	NADH C2[g]
21.5	Acetylcarnitine - (CH <sub>3</sub> )[d]	75.3	b-Glucose C2[g]	101.25	NADH C3[g]
54.7	Acetylcarnitine - N(CH <sub>3</sub> ) <sub>3</sub> [d]	76.1	b-Glucose C3[e]	22.86	NADH C4[g]
176.3	Alanine C1[d]	77	b-Glucose C3[c]	106.22	NADH C5[g]
176.7	Alanine C1[g]	70.1	b-Glucose C4[e]	125.12	NADH C6[g]
51.5	Alanine C2[w]	70.7	b-Glucose C4[c,g]	173.62	NADH C7[g]
51.7	Alanine C2[g]	76.8	b-Glucose C5[c,w]	148.29	Nicotinamide C2[g]
51.9	Alanine C2[d]	76.9	b-Glucose C5[g]	129.7	Nicotinamide C3[g]
17.3	Alanine C3[d,g]	61.8	b-Glucose C6[c,g]	137.04	Nicotinamide C4[g]
17.4	Alanine C3[w]	174.7	Glutamate C1[e]	124.96	Nicotinamide C5[g]
34.8	b-Alanine C2[w]	175.1	Glutamate C1[d]	152.48	Nicotinamide C6[g]
37.8	b-Alanine C3[w]	55.2	Glutamate C2[d]	170.79	Nicotinamide C7[g]
55.8	Arginine C2[w]	55.8	Glutamate C2[w]	149.87	Nicotinate C2[g]
28.9	Arginine C3[w]	27.6	Glutamate C3[d]	133.21	Nicotinate C3[g]
25.5	Arginine C4[w]	28.1	Glutamate C3[w]	138.58	Nicotinate C4[g]
41.8	Arginine C5[w]	34.2	Glutamate C4[d]	124.83	Nicotinate C5[g]
157.7	Arginine C6[w]	34.7	Glutamate C4[w]	151.17	Nicotinate C6[g]
175	Aspartate C1[d]	181.4	Glutamate C5[e]	173.85	Nicotinate C7[g]
175.3	Aspartate C1[g]	181.8	Glutamate C5[d]	178.2	Oxaloacetate (hydrate) C1[g]
52.7	Aspartate C2[d]	174.2	Glutamine C1[e]	99.5	Oxaloacetate (hydrate) C2[g]
53.4	Aspartate C2[g]	174.8	Glutamine C1[d]	50	Oxaloacetate (hydrate) C3[g]
37.4	Aspartate C3[d]	55.2	Glutamine C2[d]	181.9	Oxaloacetate (hydrate) C4[g]

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37.8	Aspartate C3[g]	55.4	Glutamine C2[w]	169.3	Oxaloacetate (keto) C1[g]
178.3	Aspartate C4[d]	27.2	Glutamine C3[d]	201.5	Oxaloacetate (keto) C2[g]
178.5	Aspartate C4[g]	28.1	Glutamine C3[w]	50.2	Oxaloacetate (keto) C3[g]
160	Bicarbonate C1[e]	31.8	Glutamine C4[d]	175.9	Oxaloacetate (keto) C4[g]
160.8	Bicarbonate C1[d]	32	Glutamine C4[w]	175.5	Oxaloacetate C1[d]
161.8	Bicarbonate C1[g]	177.8	Glutamine C5[e]	204.7	Oxaloacetate C2[d]
184	Butyrate C1[e]	178.5	Glutamine C5[d]	50	Oxaloacetate C3[d]
19.4	Butyrate C3[e]	91.3	Glyceraldehyde 3-P hydrate C1[g]	169.4	Oxaloacetate C4[d]
128.73	=*CH-CH <sub>2</sub> <sup>-</sup> CH=[f]	74.9	Glyceraldehyde 3-P hydrate C2[g]	57.2	Phenylalanine C2[w]
27.95	-CH <sub>2</sub> <sup>-</sup> *CH <sub>2</sub> <sup>-</sup> CH=CH-[f]	66	Glyceraldehyde 3-P hydrate C3[g]	37.7	Phenylalanine C3[w]
34.46	-CH <sub>2</sub> <sup>-</sup> *CH <sub>2</sub> <sup>-</sup> CO-[f]	63.4	Glycerol 3-P C1[g]	136.8	Phenylalanine C4[w]
172.43	-CH <sub>2</sub> <sup>-</sup> CH <sub>2</sub> <sup>-</sup> *CO-[f]	63.5	Glycerol 3-P C1[w]	130.4	Phenylalanine C5[w]
25.6	-*CH <sub>2</sub> <sup>-</sup> CH <sub>2</sub> <sup>-</sup> CO-[f]	72.4	Glycerol 3-P C2[g]	130	Phenylalanine C6[w]
14.73	CH <sub>3</sub> <sup>-</sup> CH <sub>2</sub> <sup>-</sup> [f]	65.8	Glycerol 3-P C3[g]	128.6	Phenylalanine C7[w]
32.76	CH <sub>3</sub> <sup>-</sup> CH <sub>2</sub> <sup>-</sup> *CH <sub>2</sub> <sup>-</sup> CH <sub>2</sub> <sup>-</sup> [f]	66	Glycerol 3-P C3[w]	67.6	Phosphocholine (N)[w]
130.25	-CH=*CH-CH <sub>2</sub> <sup>-</sup> CH <sub>2</sub> <sup>-</sup> [f]	62.59	Glycerol C1,C3[f]	59.1	Phosphocholine (O)[w]
26.43	-CH=CH-*CH <sub>2</sub> <sup>-</sup> CH=CH-[f]	63.50	Glycerol C1,C3[d]	55.1	Phosphocreatine (CH <sub>2</sub> )[w]
163.8	Carbamino group C1[g]	63.6	Glycerol C1,C3[j]	38.1	Phosphocreatine (CH <sub>3</sub> )[w]
45	Citrate (Mg <sup>2+</sup> citrate) C2[d]	69.74	Glycerol C2[f]	174.2	Phosphoenolpyruvate C1[g]
174.2	Citrate C1,C5[j]	73	Glycerol C2[d]	152.7	Phosphoenolpyruvate C2[g]
179.7	Citrate C1,C5[g]	73.3	Glycerol C2[g]	102.1	Phosphoenolpyruvate C3[g]
180	Citrate C1,C5[d]	173.5	Glycine C1[g]	41.8	Phosphoethanolamine (N)[w]
44.1	Citrate C2,C4[j]	42.6	Glycine C2[w]	61.5	Phosphoethanolamine (O)[w]
46.6	Citrate C2,C4[d]	42.7	Glycine C2[j]	179	2-Phosphoglycerate C1[g]
46.8	Citrate C2,C4[g]	100.5	Glycogen (1:4) C1[c]	77.4	2-Phosphoglycerate C2[g]
74.2	Citrate C3[j]	74	Glycogen (1:4) C3[c]	65.7	2-Phosphoglycerate C3[g]

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76	Citrate C3[g]	77.7	Glycogen (1:4) C4[c]	62.3	Proline C2[w]
76.1	Citrate C3[d]	61.4	Glycogen (1:4) C6[c]	30	Proline C3[w]
177.5	Citrate C6[j]	72	Glycogen (1:4,1:6) C2[c]	25	Proline C4[w]
182.3	Citrate C6[g]	99.2	Glycogen (1:6) C1[c]	47.4	Proline C5[w]
186.7	Citrate C6[d]	73.5	Glycogen (1:6) C3[c]	185.4	Propionate C1[d]
174.5	<sup>2,3-</sup> Cyclopyrophosphogly cerate C1[g]	70	Glycogen (1:6) C4[c]	31.5	Propionate C2[d]
78.6	<sup>2,3-</sup> Cyclopyrophosphogly cerate C2[g]	67.9	Glycogen (1:6) C6[c]	11	Propionate C3[d]
70.1	<sup>2,3-</sup> Cyclopyrophosphogly cerate C3[g]	72.2	Glycogen (1:6,1:4) C5[c]	176.8	Propionylcarnitine C1[d]
54.7	Cystine C2[w]	177.3	Glycolate C1[d]	9	Propionylcarnitine C3[d]
40.6	Cystine C3[w]	60.3	Glycolate C2[d]	59.1	Pyroglutamate C2[w]
65.1	DHAP (hydrate) C1[g]	177.9	Glyoxylate C1[g]	26.3	Pyroglutamate C3[w]
96	DHAP (hydrate) C2[g]	89.3	Glyoxylate C2[g]	30.9	Pyroglutamate C4[w]
67	DHAP (hydrate) C3[g]	55.8	Histidine C2[w]	177.6	Pyruvate (hydrate) C1[g]
66.5	DHAP (keto) C1[g]	29.7	Histidine C3[w]	93.1	Pyruvate (hydrate) C2[g]
212.6	DHAP (keto) C2[g]	137.5	Histidine C6[w]	26.3	Pyruvate (hydrate) C3[d]
68.5	DHAP (keto) C3[g]	117.5	Histidine C8[w]	26.7	Pyruvate (hydrate) C3[g]
67.4	Dioxane	180.5	b-Hydroxybutyrate C1[e]	169.3	Pyruvate (keto) C1[g]
52	EDTA (ac) C3[d]	181.1	b-Hydroxybutyrate C1[d]	205.4	Pyruvate (keto) C2[g]
58.2	EDTA (en) C2[d]	181.2	b-Hydroxybutyrate C1[g]	27.6	Pyruvate (keto) C3[g]
175.6	EDTA C1[d]	47.3	b-Hydroxybutyrate C2[e]	171.1	Pyruvate C1[d]
58.6	Ethanol C1[g]	47.6	b-Hydroxybutyrate C2[d]	205.8	Pyruvate C2[d]
17.4	Ethanol C2[j]	65.7	b-Hydroxybutyrate C3[e]	27.3	Pyruvate C3[d]
18	Ethanol C2[g]	66.6	b-Hydroxybutyrate C3[d]	173.5	Serine C1[g]
83.2	Formaldehyde (hydrate) C1[g]	66.8	b-Hydroxybutyrate C3[g]	57.4	Serine C2[w]
171.4	Formate C1[g]	22.7	b-Hydroxybutyrate C4[d]	57.5	Serine C2[g]
172.2	Formate C1[w]	22.9	b-Hydroxybutyrate C4[g]	61.4	Serine C3[g]
65.4	a-Fructose 1,6-diP C1[g]	56.7	Hypotaurine (N)[w]	61.6	Serine C3[w]

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105.9	a-Fructose 1,6-diP C2[g]	34.8	Hypotaurine (S)[w]	63.6	D-Sorbitol C1[g]
82.6	a-Fructose 1,6-diP C3[g]	72.1	Inositol (myo) C1,C3[w]	72.2	D-Sorbitol C2[g]
77.8	a-Fructose 1,6-diP C4[g]	73.3	Inositol (myo) C2[w]	70.8	D-Sorbitol C3[g]
82.9	a-Fructose 1,6-diP C5[g]	73.6	Inositol (myo) C4,C6[w]	72.1	D-Sorbitol C4[g]
64.4	a-Fructose 1,6-diP C6[g]	75.3	Inositol (myo) C5[w]	74.1	D-Sorbitol C5[g]
66.9	b-Fructose 1,6-diP C1[g]	181	Isocitrate C1,C5[d]	64	D-Sorbitol C6[g]
102	b-Fructose 1,6-diP C2[g]	38.5	Isocitrate C2[d]	182.8	Succinate C1,C1` [d]
76.9	b-Fructose 1,6-diP C3[g]	49.9	Isocitrate C3[d]	183.4	Succinate C1,C1'[g]
75.1	b-Fructose 1,6-diP C4[g]	74.6	Isocitrate C4[d]	35	Succinate C2,C2` [d]
80.6	b-Fructose 1,6-diP C5[g]	60.7	Isoleucine C2[w]	35.3	Succinate C2,C2'[g]
65.3	b-Fructose 1,6-diP C6[g]	37	Isoleucine C3[w]	49	Taurine (N)[w]
63.8	a-Fructose 6-P C1[g]	25.7	Isoleucine C4[w]	48.4	Taurine (N) (pH 6.5) C1[a]
105.3	a-Fructose 6-P C2[g]	15.8	Isoleucine CH <sub>3</sub> (4)[w]	36.6	Taurine (S)[w]
89.6	a-Fructose 6-P C3[g]	12.2	Isoleucine CH <sub>3</sub> (5)[w]	36.5	Taurine (S) (pH 6.5) C2[a]
76.9	a-Fructose 6-P C4[g]	170.7	a-Ketoglutarate C1[g]	61.5	Threonine C2[w]
81.4	a-Fructose 6-P C5[g]	170.8	a-Ketoglutarate C1[d]	67.3	Threonine C3[w]
64.5	a-Fructose 6-P C6[g]	206.3	a-Ketoglutarate C2[d]	20.7	Threonine C4[w]
63.75	b-Fructose 6-P C1[g]	206.7	a-Ketoglutarate C2[g]	94	a,a-Trehalose C1[j]
102.5	b-Fructose 6-P C2[g]	31.4	a-Ketoglutarate C3[d]	94.4	a,a-Trehalose C1[j]
76.2	b-Fructose 6-P C3[g]	31.8	a-Ketoglutarate C3[g]	72.2	a,a-Trehalose C2[j]
75.4	b-Fructose 6-P C4[g]	36.7	a-Ketoglutarate C4[d]	73.3	a,a-Trehalose C2[j]
80.9	b-Fructose 6-P C5[g]	37	a-Ketoglutarate C4[g]	73.5	a,a-Trehalose C3[j]
65.3	b-Fructose 6-P C6[g]	182	a-Ketoglutarate C5[d]	73.7	a,a-Trehalose C3[j]
175.3	Fumarate C1,C1` [d]	182.7	a-Ketoglutarate C5[g]	70.6	a,a-Trehalose C4[j]
175.6	Fumarate C1,C1'[g]	183.2	Lactate C1[d]	70.9	a,a-Trehalose C4[j]
136	Fumarate C2,C2` [d]	183.5	Lactate C1[g]	73	a,a-Trehalose C5[j]
136.4	Fumarate C2,C2'[g]	69.4	Lactate C2[d]	61.5	a,a-Trehalose C6[j]
35.4	GABA C2[w]	69.6	Lactate C2[g]	61.7	a,a-Trehalose C6[j]

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24.6	GABA C3[w]	21	Lactate C3[d]	120.3	Tryptophan C10[w]
40.4	GABA C4[w]	21.3	Lactate C3[w]	119.4	Tryptophan C11[w]
180	Gluconate C1[h]	55.3	Leucine C2[w]	56	Tryptophan C2[w]
75.9	Gluconate C2[h]	41	Leucine C3[w]	27.6	Tryptophan C3[w]
72.3	Gluconate C3[h]	25.3	Leucine C4[w]	126	Tryptophan C5[w]
75	Gluconate C4[h]	22.2	Leucine CH <sub>3</sub> [w]	112.9	Tryptophan C8[w]
73.2	Gluconate C5[h]	55.7	Lysine C2[w]	123	Tryptophan C9[w]
64.3	Gluconate C6[h]	31.2	Lysine C3[w]	57.4	Tyrosine C2[w]
93.2	a-Glucose 6-P C1[g]	23.2	Lysine C4[w]	36.7	Tyrosine C3[w]
63.6	a-Glucose 6-P C6[g]	27.3	Lysine C5[w]	156.2	Tyrosine C4[w]
96.8	b-Glucose 6-P C1[w]	40.5	Lysine C6[w]	131.8	Tyrosine C5[w]
97	b-Glucose 6-P C1[g]	180.4	Malate C1[d]	116.8	Tyrosine C6[w]
63.6	b-Glucose 6-P C6[j]	182.1	Malate C1[g]	127.6	Tyrosine C7[w]
92.9	a-Glucose C1[w]	71.2	Malate C2[d]	61.6	Valine C2[w]
93.1	a-Glucose C1[c]	71.7	Malate C2[g]	30.3	Valine C3[w]
93.2	a-Glucose C1[g]	43.4	Malate C3[d]	19.2	Valine CH <sub>3</sub> [w]
72.3	a-Glucose C2[w]				