

List of Metabolites and Carbon Species

Metabolites of Glucose									Currency Metabolites				
No. and Name	(compartment)	Index of carbon atoms							KEGG#	No. and Name	(compartment)	KEGG#	
1	D-Glucose	(c)	(1,1)	(1,2)	(1,3)	(1,4)	(1,5)	(1,6)	C00031	33	ATP	(c,m)	C00002
2	D-Glucose 6-phosphate	(c)	(2,1)	(2,2)	(2,3)	(2,4)	(2,5)	(2,6)	C00092	34	ADP	(c,m)	C00008
3	D-Fructose 6-phosphate	(c)	(3,1)	(3,2)	(3,3)	(3,4)	(3,5)	(3,6)	C00085	35	GTP	(c,m)	C00044
4	D-Fructose 1,6-bisphosphate	(c)	(4,1)	(4,2)	(4,3)	(4,4)	(4,5)	(4,6)	C00354	36	GDP	(c,m)	C00035
5	D-Glyceraldehyde 3-phosphate	(c)	(5,1)	(5,2)	(5,3)				C00118	37	FAD	(c,m)	C00016
6	Dihydroxyacetone phosphate	(c)	(6,1)	(6,2)	(6,3)				C00111	38	FADH2	(c,m)	C01352
7	1,3-Bisphospho-D-glycerate	(c)	(7,1)	(7,2)	(7,3)				C00236	39	NAD+	(c,m)	C00003
8	3-Phospho-D-glycerate	(c)	(8,1)	(8,2)	(8,3)				C00197	40	NADH	(c,m)	C00004
9	2-Phospho-D-glycerate	(c)	(9,1)	(9,2)	(9,3)				C00631	41	NADP+	(c,m)	C00006
10	Phosphoenolpyruvate	(c)	(10,1)	(10,2)	(10,3)				C00074	42	NADPH	(c,m)	C00005
11	Pyruvate	(c,m)	(11,1)	(11,2)	(11,3)				C00022	43	CoA	(c,m)	C00010
12	L-Lactate	(c)	(12,1)	(12,2)	(12,3)				C00186	44	Phosphate	(c,m)	C00009
13	Acetyl-CoA	(m)	(13,1)	(13,2)					C00024	45	H2O	(c,m)	C00001
14	Oxaloacetate	(m)	(14,1)	(14,2)	(14,3)	(14,4)			C00036	46	H+	(c,m)	C00080
15	CO2 including HCO3- C00288	(c,m)	(15,1)						C00011				
16	Citrate	(m)	(16,1)	(16,2)	(16,3)	(16,4)	(16,5)	(16,6)	C00158				
17	cis-Aconitate	(m)	(17,1)	(17,2)	(17,3)	(17,4)	(17,5)	(17,6)	C00417				
18	Isocitrate	(m)	(18,1)	(18,2)	(18,3)	(18,4)	(18,5)	(18,6)	C00311				
19	2-Oxoglutarate	(m)	(19,1)	(19,2)	(19,3)	(19,4)	(19,5)		C00026				
20	Succinyl-CoA	(m)	(20,1)	(20,2)	(20,3)	(20,4)			C00091				
21	Succinate	(m)	(21,1)	(21,2)					C00042				
22	Fumarate	(m)	(22,1)	(22,2)					C00122				
23	L-Malate	(m)	(23,1)	(23,2)	(23,3)	(23,4)			C00149				
24	L-Malate	(c)	(24,1)	(24,2)	(24,3)	(24,4)			C00149				
25	Oxaloacetate	(c)	(25,1)	(25,2)	(25,3)	(25,4)			C00036				
26	6-Phospho-D-glucono-1,5-lactone	(c)	(26,1)	(26,2)	(26,3)	(26,4)	(26,5)	(26,6)	C01236				
27	6-Phospho-D-gluconate	(c)	(27,1)	(27,2)	(27,3)	(27,4)	(27,5)	(27,6)	C00345				
28	D-Ribulose 5-phosphate	(c)	(28,1)	(28,2)	(28,3)	(28,4)	(28,5)		C00199				
29	D-Ribose 5-phosphate	(c)	(29,1)	(29,2)	(29,3)	(29,4)	(29,5)		C00117				
30	Sedoheptulose 7-phosphate	(c)	(30,1)	(30,2)	(30,3)	(30,4)	(30,5)	(30,6)	(30,7)	C00281			
31	D-Erythrose 4-phosphate	(c)	(31,1)	(31,2)	(31,3)	(31,4)			C00279				
32	D-Xylulose 5-phosphate	(c)	(32,1)	(32,2)	(32,3)	(32,4)	(32,5)		C00231				

Letters in parentheses, "c" and "m" indicate compartmentation of the metabolites: c, cytosolic; m, mitochondrial. Carbon atoms of currency metabolites were not numbered.