

Table S2. Annotation information for metabolites. Chemical shift values for candidate HSQC peaks are from Human Metabolome Databases (HMDB) except for DHPS, DMSP, homarine, and β -1,3-glucan (see Methods for details). Confirmed peaks are shown in bold. Peaks overlapping with those of other compound(s) are indicated by asterisks. For the annotation confidence levels, see Methods.

Compounds	¹ H (ppm)	¹³ C (ppm)	Confidence level
2,3-dihydroxypropane-1-sulfonate (DHPS)	3.03, 3.11, 3.58, 3.69, 4.14	56.5, 56.5, 67.3, 67.3, 70.8	4
Dimethylsulfoniopropionate (DMSP)	2.73, 2.91, 3.44	34.1, 27.8, 43.4	4
Glycine	3.55	44.3	3
Proline	1.99, 2.07, 2.34, 3.32, 3.41, 4.13	26.5, 31.8, 31.7, 49, 49, 64	4
Glutamate	2.09, 2.34, 3.74*	29.8, 36.4, 57.6*	4
Glutamine	2.12*, 2.44, 3.76*	29.3*, 33.9, 57.2*	4
Alanine	1.49, 3.78	19.0, 53.6	4
Isoleucine	0.93, 1, 1.25, 1.45, 1.96, 3.65*	13.9, 17.4, 27.2, 27, 38.7, 62.5*	4
Valine	0.98, 1.03, 2.26, 3.6	19.4, 20.8, 31.9, 63.3	4
Betaine	3.25, 3.89*	55.9, 68.6*	3
Lysine	1.43*, 1.49*, 1.72, 1.88*, 3.02, 3.75*	24*, 24*, 29.2, 32.7*, 42.1, 57.5*	4
β -1,3-glucan	3.51*, 3.51*, 3.56, 3.73*, 3.78, 3.92*, 4.79	70.9*, 78.4*, 76.0, 63.4*, 86.9, 63.4*, 105.4	4
Arginine	1.68, 1.91, 3.24*, 3.76*	26.5, 30.5, 43.3*, 57.3*	4
Leucine	0.94, 0.96, 1.7*, 1.71, 3.74*	23.6, 24.8, 42.6*, 26.8, 56.2*	4
Acetate	1.91	26.1	3
Glycerol 3-phosphate	3.61*, 3.68*, 3.78, 3.82, 3.86*	65*, 65*, 67.6, 67.6, 74*	4
Guanosine	3.82*, 3.86*, 4.22*, 4.39*, 5.89, 7.98*	64.2*, 64.2*, 88.1*, 73.3*, 90.4, 140.6*	4
Uridine	3.8*, 3.91*, 4.12, 4.23*, 4.35, 5.89, 5.9, 7.86*	63.6*, 63.6*, 87.1, 72.1*, 76.5, 105.1, 92.1, 144.6*	4
Aspartate	2.71, 2.8, 3.91	39.3*, 39.5*, 55.1	4
Glucose	3.23, 3.4, 3.46, 3.52, 3.7, 3.72, 3.81, 3.82, 3.89, 4.63, 5.22	77, 72.5, 78.6, 74.3, 75.6, 63.5, 74.1, 63.3, 63.4, 98.7, 94.9	2
Homarine	4.37, 7.98, 8.04, 8.55, 8.72	49.3, 130.2, 129, 149.4, 148.6	4
Phosphorylcholine	3.2*, 3.57, 4.15	56.5*, 68.9, 60.6	4