

Table S1. Chemical shifts of the compounds identified by ^1H NMR (700 MHz, 298K, TSP=1mM, D_2O sodium phosphate buffer 0.123M at pH 7.4). TSP was used as internal standard and referenced to chemical shift 0.000 ppm.

#	Molecule	^1H NMR Chemical shifts(ppm)
1	Formate	8.46 (s).
2	S-Adenosylhomocysteine	8.38 (s), 8.28 (s).
3	Oxypurinol	8.21 (s).
4	UDP-glucose	7.96 (d, $J = 8.4$ Hz).
5	Phenylalanine	7.43 (t, $J=7.2$ Hz), 7.34 (d, $J=7.6$ Hz).
6	Tyrosine	7.21-7.19 (m), 6.93-6.89 (m).
7	Glucose-1-phosphate	5.46 (dd, $J = 7.4, 3.5$ Hz).
8	Sucrose	5.42 (d, $J = 3.9$ Hz), 4.22 (d, $J = 8.8$ Hz), 4.06 (t, $J = 8.6$ Hz), 3.92 – 3.83 (m),
		3.69 (d, $J = 1.9$ Hz), 3.57 (dd, $J = 10.0, 3.9$ Hz), 3.48 (t, $J = 9.5$ Hz, 0H)
9	Glucose	5.24 (d, $J = 3.7$ Hz), 4.65 (d, $J = 8.0$ Hz).
10	Maltose	5.24 (d, $J = 3.7$ Hz), 4.65 (d, $J = 8.0$ Hz), 3.31 – 3.28 (m).
11	Trehalose	5.20 (d, $J = 3.7$ Hz).
12	Tartrate	4.35 (s).
13	Pyroglutamate	4.18 (dd, $J = 9.0, 5.8$ Hz), 2.51 (dtd, $J = 12.9, 9.1, 6.8$ Hz).
14	Gluconate	4.14 (d, $J = 3.7$ Hz).
15	Methanol	3.36 (s).
16	Dimethyl sulfone	3.16 (s).
17	Malonate	3.14 (s).
18	Ornithine	3.07-3.04 (m).
19	2-Oxoglutarate	3.01 (t, $J = 6.9$ Hz).
20	N,N-Dimethylglycine	2.92 (s).
21	Aspartate	2.82 (dd, $J = 17.5, 3.8$ Hz), 2.69 (dd, $J = 17.5, 8.7$ Hz).
22	Glutamate	2.35 (m), 2.14 (dddd, $J = 15.2, 8.4, 7.2, 4.8$ Hz), 2.07(m).
23	Acetone	2.24 (s).
24	Methionine	2.16 (s).
25	Homoserine	1.97 (dq, $J = 14.7, 7.6$ Hz).
26	Acetate	1.92 (s).
27	Alanine	1.49 (d, $J = 7.3$ Hz).
28	Threonine	1.33 (d, $J = 6.9$ Hz).
29	Lactate	1.33 (d, $J= 6.9$ Hz).
30	3-Hydroxy-3-methylglutarate	1.33 (s).
31	3-Hydroxyisovalerate	1.25 (s).
32	3-Hydroxybutyrate	1.21 (d, $J = 6.6$ Hz).
33	Ethanol	1.19 (t, $J = 7.1$ Hz).
34	3-hydroxyisobutyrate	1.07 (d, $J = 7.1$ Hz).
35	Valine	1.05 (d, $J = 7.1$ Hz), 1.00 (d, $J = 7.0$ Hz).
36	3-Methylglutarate	0.91 (d, $J = 6.6$ Hz).
37	Caprylate	0.87 (t, $J = 7.0$ Hz).