

Label ¹	Neutral Mass	Formula ²	Sample Retention Time (min)	Standard ³	Standard Retention Time	Ion (m/z) used for Sample Analyses ⁴	Additional ions ⁵	Largest MS/MS fragments ⁶
C5-Disaccharide (xylobiose) 1	282.0951	C10H18O9	11.4	Xylobiose	11.3	[NEG, H-] 281.0878	[POS, Na+] 305.0841; [NEG, Cl-] 317.0641	
C5-Disaccharide (xylobiose) 2	282.0951	C10H18O9	10.8	Xylobiose	10.7	[NEG, H-] 281.0878	[POS, Na+] 305.0841; [NEG, Cl-] 317.0641	
C12H22O10 (Rutinose) 1	326.1213	C12H22O10	12	Rutinose	11.7,12.1	[NEG, H-] 325.114	[POS, Na+] 349.1103	[NEG, 325.114 @ 20V] 163.0610, 103.0404; [POS, 349.1103 @ 20V] 149.0245
C12H22O10 (Rutinose) 2	326.1213	C12H22O10	11.6	Rutinose	11.7,12.1	[NEG, H-] 325.114	[POS, Na+] 349.1103	[NEG, 325.114 @ 20V] 163.0610, 103.0404; [POS, 349.1103 @ 20V] 149.0245
(C13H24O11)	356.1319	C13H24O11	10.8			[POS, NA+] 379.1198	[NEG, H-] 355.1246	[POS, 379.1121 @ 10V] 185.0417, 217.066
Sugar Alcohol 1 (Mannitol)	182.07904	C6H14O6	10.4	Mannitol	10.6	[NEG, H-] 181.0718	[POS, H+] 183.0863	[NEG, 181.073 @ 20V] 80.9166, 71.0136, 89.0235, 101.0241
Sugar Alcohol 2 (Xylitol)	152.06848	C5H12O5	8.8	Xylitol	8.9	[NEG, H-] 151.0613		[NEG, 151.063 @ 10V] 89.0231, 101.0234, 71.0147, 73.029
Sugar Alcohol 3 (Unk C5)	152.06848	C5H12O5	7.9			[NEG, H-] 151.0613		
Hexose 1 (Glucose/Galactose)	180.06339	C6H12O6	10.2	13C6-Glucose ISTD	10.2	[NEG, H-] 179.0565	[NEG, Cl-] 215.0324, [NEG, +Hac-H] 239.0778	
Hexose 2 (Glucose/Galactose)	180.06339	C6H12O6	10.8	13C6-Glucose ISTD	10.8	[NEG, H-] 179.0565	[NEG, Cl-] 215.0324, [NEG, +Hac-H] 239.0778	
(Hexose 3)	180.06339	C6H12O6	12			[NEG, H-] 179.0565	[NEG, Cl-] 215.0324, [NEG, +Hac-H] 239.0778	
(Hexose 4)	180.06339	C6H12O6	13.1			[NEG, H-] 179.0565	[NEG, Cl-] 215.0324, [NEG, +Hac-H] 239.0778	
(Hexose 5)	180.06339	C6H12O6	9.7			[NEG, H-] 179.0565	[NEG, Cl-] 215.0324, [NEG, +Hac-H] 239.0778	
Hexose 6 (Fructose)	180.06339	C6H12O6	9.1	Fructose	9	[POS, Na+] 203.0531	[NEG, H-] 179.0565; [NEG, Cl-] 215.0324 ;	
Hexose 7 (Mannose)	180.06339	C6H12O6	10.1	Mannose	10.4	[POS, Na+] 203.0531	[NEG, +Hac-H] 239.0778	
Trehalose	342.11622	C12H22O11	13.8	D-(+)-Trehalose	13.8	[NEG,+Hac-H] 401.1302	[NEG, H-] 341.1096; [NEG, Cl-] 377.0852; [NEG, Fragment] 179.0565; [POS, Na+] 365.1062; [POS, NH4+] 360.1507	
Sucrose	342.11622	C12H22O11	12.6	Sucrose	12.7	[NEG, H-] 341.1096	[NEG, Cl-] 377.0852; [NEG,+Hac-H] 401.1302	
Disaccharide 3 (Cellobiose/Maltose)	342.11622	C12H22O11	13.4	Cellobiose/Maltose	13.2,13.4	[NEG, H-] 341.1096	[NEG,+Hac-H] 401.1302; [NEG, Cl-] 377.0852; [POS, Na+] 365.1062; [POS, NH4+] 360.1507	
(Disaccharide 6)	342.11622	C12H22O11	15.8			[POS, Na+] 365.1062	[POS, NH4+] 360.1490	
Trisaccharide 1	504.169	C18H32O16	15.5			[NEG, H-] 503.162	[NEG, Cl-] 539.138; [NEG, +Hac-H] 563.1828; [POS, Na+] 527.1583; [POS, NH4+] 522.203	[NEG, 503.158 @ 20 V] 341.1074, 89.0238, 221.0667, 119.0371, 179.0555
Trisaccharide 2	504.169	C18H32O16	15	D-(+)-Raffinose	15	[NEG, H-] 503.162	[NEG, Cl-] 539.138; [NEG, +Hac-H] 563.1828; [POS, Na+] 527.1583; [POS, NH4+] 522.203	
Trisaccharide 3	504.169	C18H32O16	14.3			[POS, Na+] 527.1583	[NEG, Cl-] 539.138; [NEG, +Hac-H] 563.1828, [NEG, H-] 503.162, [POS, NH4+] 522.203	[POS, 527.1583 @ 20V] 185.0407, 201.0367, 111.9523, 467.6755
Trisaccharide 4	504.169	C18H32O16	13.7			[POS, Na+] 527.1583	[NEG, Cl-] 539.138; [NEG, +Hac-H] 563.1828, [NEG, H-] 503.162, [POS, NH4+] 522.203	
Trisaccharide 5	504.169	C18H32O16	14.9			[NEG, H-] 503.162	[NEG, Cl-] 539.138; [NEG, +Hac-H] 563.1828; [POS, Na+] 527.1583; [POS, NH4+] 522.203	
Trisaccharide 6	504.169	C18H32O16	13.1			[POS, Na+] 527.1583	[NEG, Cl-] 539.138; [NEG, +Hac-H] 563.1828, [NEG, H-] 503.162, [POS, NH4+] 522.203	
Tetrasaccharide 1 (Maltotetraose)	666.22186	C24H42O21	16	Maltotetraose	16	[NEG,H-] 665.2145	[POS, Na+] 689.2109; [POS, NH4+] 684.256; [NEG, Cl-] 701.191; [NEG, +Hac-H] 725.2357	
Tetrasaccharide 2 (Stachyose)	666.22186	C24H42O21	16.9	Stachyose	16.9	[NEG,H-] 665.2145	[POS, Na+] 689.2109; [POS, NH4+] 684.256; [NEG, Cl-] 701.191; [NEG, +Hac-H] 725.2357	[NEG, 665.2145 @40V] 89.025, 383.1175, 221.0661, 179.0565; [POS, 689.2109 @ 40V] 527.1577, 365.1028
Tetrasaccharide 3	666.22186	C24H42O21	16.3			[NEG,H-] 665.2145	[POS, Na+] 689.2109; [POS, NH4+] 684.256; [NEG, +Hac-H] 725.2357	
Tetrasaccharide 4	666.22186	C24H42O21	14.9			[NEG,H-] 665.2145	[POS, Na+] 689.2109; [POS, NH4+] 684.256	
Tetrasaccharide 6	666.22186	C24H42O21	14.5			[POS, Na+] 689.2109	[POS, fragment] 527.1582 ;[NEG, H-] 665.2145; [POS, NH4+] 684.256; [NEG, Cl-] 701.191; [NEG, +Hac-H] 725.2357	
Pentasaccharide 1	828.2747	C30H52O26	16.8	Maltopentose	17	[NEG, H-] 827.2663	[POS, Na+] 851.2637; [NEG, Cl-] 863.2437; [NEG, +Hac-H] 887.2885	[NEG, 827.2663 @ 40V] 383.1167, 323.0973, 647.1953, 131.0314

Pentasaccharide 2	828.2747	C30H52O26	17.8			[NEG, H-] 827.2663	[POS, Na+] 851.2637	[NEG, 827.2663 @ 40V] 383.1168, 179.0580, 647.1998, 443.099
Pentasaccharide 3	828.2747	C30H52O26	15.5			[NEG, H-] 827.2663	[POS, Na+] 851.2637	
Hexasaccharide 1	990.3275	C36H62O31	17.3	Maltohexose	17.3	[POS, NH4+] 1008.3619	[NEG, H-] 989.3202; [POS, Na+] 1013.3165; [NEG, H-H2O-] 971.3003	
Hexasaccharide 2	990.3275	C36H62O31	18.6			[POS, NH4+] 1008.3619	[NEG, H-] 989.3202; [POS, Na+] 1013.3165	
Tryptophan	204.08988	C11H12N2O2	9.3	L-Tryptophan, D-Tryptophan	9.4	[NEG, H-] 203.0826	[POS, H+] 205.0972	
L-Leucine	131.09463	C6H13NO2	8.8	L-Isoleucine	8.7	[NEG, H-] 130.0874	[POS, H+] 132.1022	
L-Isoleucine	131.09463	C6H13NO2	8.4	L-Leucine	8.4	[NEG, H-] 130.0874	[POS, H+] 132.1022	
Valine	117.07898	C5H11NO2	9.8	L-Valine	9.9	[NEG, H-] 116.0717	[POS, H+] 118.0864	
Phenylalanine	165.07898	C9H11NO2	8.4	L-Phenylalanine	8.5	[NEG, H-] 164.0717	[POS, H+] 166.0863	
(Sarcosine)	89.04768	C3H7NO2	11.5	Sarcosine	11.2	[POS, H+] 90.0551	[NEG, H-] 88.0403	
(N-acetyl-l-phenylalanine)	207.08954	C11H13NO3	4.4	N-Acetyl-L-Phenylalanine	4.5	[NEG, H-] 206.08226		
(4-aminobutanoate)	103.06333	C4H9NO2	12.6	4-Aminobutanoate	12.9	[POS, H+] 104.0706		
Proline	115.06333	C5H9NO2	9.4	L-Proline	9.3	[NEG, H-] 114.056	[POS, H+] 116.0707	
Tyrosine	181.07389	C9H11NO3	10.6	L-Tyrosine	10.5	[NEG, H-] 180.067	[POS, H+] 182.0813	
Deoxyguanosine	267.0968	C10H13N5O4	7.9	Deoxyguanosine	7.9	[POS, fragment] 151.0494	[POS, H+] 268.1031	
L-Carnitine	161.10519	C7H15NO3	10.4	L-Carnitine	10.5	[POS, H+] 162.1125	[POS, Na+] 184.0942	[POS 162.1125 @ 10V] 85.0244, 60.081, 65.025, 121.0465, 103.040
Acetylcarnitine	203.1158	C9H17NO4	7.8	O-Acetyl-L-carnitine	7.8	[POS, H+] 204.123	[POS, fragment] 162.113	[POS, 204.123 @ 10V] 85.0273, 145.0508
(C8H16N2O3)	188.11609	C8H16N2O3	8.6			[POS, H+] 189.1233		[POS, 189.1243 @ 10V] 130.0499, 85.0285, 60.0804
(N6-Acetyl-lysine)	188.11609	(C8H16N2O3)	10.4	N6-Acetyl-lysine	11	[POS, H+] 189.1233		[POS, 189.1243 @ 10V] 84.0797, 126.0903
Betaine	117.07898	C5H11NO2	7	betaine (glycine-betaine)	7.6	[POS, H+] 118.0864	[POS, NA+] 140.0682, [POS, fragment] 100.076	
(C8H16N2O3)2	188.11609	(C8H16N2O3)	9.5			[POS, H+] 189.1233		
Glutamine	146.06914	C5H10N2O3	13	L-Glutamine	13.2	[NEG, H-] 145.0618	[POS, H+] 147.0766	
Cytidine	265.067424	C9H13N3O5	8.2	Cytidine	8.2	[POS, H+] 266.0747	[POS, fragment] 112.0504	
Asparagine	132.1179	C4H8N2O3	13.1	L-Asparagine	13.2	[POS, H+] 133.1251		
Ectoine	142.0742	C6H10N2O2	9.6	Ectoine	9.9	[POS, H+] 143.0815		
Cytosine	111.04326	C4H5N3O	6.7	Cytosine	7.2	[POS, H+] 112.0505		
Deoxycytidine	227.09061	C9H13N3O4	6.6	Deoxycytidine	7.2	[POS, H+] 228.0979	[POS, fragment] 112.0504	
Adenine	135.0545	C5H5N5	5	Adenine	5.1	[POS, H+] 136.0618		
Inosine	268.08077	C10H12N4O5	7.9	Inosine	7.5	[POS, fragment] 137.0456		
Choline-O-Sulfate	183.056914	C5H13NO4S	6.1	Cholinesulfate	6.1	[POS, H+] 184.0642	[POS, fragment] 104.1076	[POS, 184.0642 @ 10V] 104.1073
Uridine	244.0695	C9H12N2O6	5.4	Uridine	5.6	[POS, H+] 245.0768	[NEG, H-] 243.0623	
Deoxyadenosine	251.1018	C10H13N5O3	4.2	2'-Deoxyadenosine	4.4	[POS, H+] 252.1095	[POS, fragment] 136.062	
Adenosine	267.09676	C10H13N5O4	5.1	Adenosine	5.3	[POS, H+] 268.1040		
Uracil	112.02728	C4H4N2O2	3.4	Uracil	3.8	[NEG, H-] 111.021		
Hypoxanthine	136.03851	C5H4N4O	5.7	Hypoxanthine	6.2	[POS, H+] 137.0458		
Deoxyuridine	228.07462	C9H12N2O5	3.6	Deoxyuridine	4	[NEG, H-] 227.0673	[NEG, fragment] 111.021	
Serine	105.0926	C3H7NO3	13.1	L-Serine	13.2	[NEG, H-] 104.036		
Guanosine	283.09167	C10H13N5O5	9.3	Guanosine	9.7	[POS, H+] 284.099		
(C6H11NO3)	145.0739	(C6H11NO3)	8.9			[POS, H+] 146.0812	[POS, fragment] 100.0756, [NEG, H-] 144.066	

Extraction Standards

Name	Neutral Mass	Formula	Retention Time (min)	Positive Ions	Negative Ions
ABMBA	228.9738	C8H8BrNO2	2.99	[POS, H+] 229.9811	[NEG, H-] 227.9666
UL-13C-Glucose	186.0814	[13C]6H12O6	10.2, 10.8	[POS, Na+] 209.0704	[NEG, H-] 185.25411
Internal Standards					
9-antracene carboxylic acid	222.068085	C15H10O2	3.11		[NEG, H-] 221.0608
d5-benzoic acid	127.068161	C7HD5O2	4.5		[NEG, H-] 126.0609

3,6-Dihydroxy-4-methylpyridazine	126.042931	C5H6N2O2	6.1	[POS, H+] 127.0503	[NEG, H-] 125.0357
4-(3,3-dimethyl-ureido)benzoic acid	208.084793	C10H12N2O3	6.7	[POS, H+] 209.0921	[NEG, H-] 207.0775
13C-15N-L-phenylalanine	175.106201	[13C]9H11[15N]O2	8.4	[POS, H+] 176.1135	[NEG, H-] 174.0989
d4 lysine	150.13063	C6H10D4N2O2	23.7	[POS, H+] 151.1379	[NEG, H-] 149.1233

1 - Corresponds to the label in the heat map

2 - Compound formulas are derived from compound if known, otherwise it was from a combination of isotope patterns, neutral losses, elution time and MS/MS if available

3 - Standards from the Northern Lab chemical library that were analyzed using the same column and gradient

4 - ions (m/z values) used for evaluating compounds across samples were selected based on their sensitivities and CV among replicate analyses

5 - Additional co-eluting ions that were used to confirm compound, neutral mass and type

6 - Selected MS/MS patterns observed on sample compounds that were present at sufficient abundance.