

Table SIII. Acquisition parameters of metabolites as analyzed in the TBA method.

Compound name	Chemical formula	HMDB ID	Retention time (min)	Monoisotopic mass (amu)	Q1 mass (amu)	Q3 mass (amu)	Collision energy (eV)
Acetyl coenzyme A	C23H38N7O17P3S	HMDB0001206	24,0	809,13	808,10	408,00	36
N-Acetyl-D-galactosamine	C8H15NO6	HMDB0000212	1,5	221,09	220,10	119,00	0
N-Acetyl-D-galactosamine 6-phosphate	C8H16NO9P	HMDB0059626	14,2	301,06	300,00	97,00	16
N-Acetyl-D-galactosamine 6-phosphate	C8H16NO9P	HMDB0059626	14,2	301,06	300,00	79,00	36
N-Acetyl-D-glucosamine	C8H15NO6	HMDB0000215	1,5	221,09	220,10	59,00	20
N-Acetyl-D-glucosamine 1-phosphate	C8H16NO9P	HMDB0001367	14,0	301,06	300,00	97,00	18
N-Acetyl-D-glucosamine 1-phosphate	C8H16NO9P	HMDB0001367	14,0	301,06	300,00	79,00	48
N-Acetyl-D-glucosamine 6-phosphate	C8H16NO9P	HMDB0001062	13,8	301,06	300,00	97,00	16
N-Acetyl-D-glucosamine 6-phosphate	C8H16NO9P	HMDB0001062	13,8	301,06	300,00	79,00	36
N-Acetyl-D-mannosamine	C8H15NO6	HMDB0001129	1,5	221,09	220,10	59,00	0
N-Acetyl-D-mannosamine 6-phosphate	C8H16NO9P	HMDB0062500	14,5	301,06	300,10	87,10	9
N-Acetyl-D-mannosamine 6-phosphate	C8H16NO9P	HMDB0062500	14,5	301,06	300,10	78,90	41
N-Acetylneuraminic acid	C11H19NO9	HMDB0000230	7,0	309,11	308,10	169,90	10
N-Acetylneuraminic acid	C11H19NO9	HMDB0000230	7,0	309,11	308,10	87,00	14
N-Acetylneuraminic acid 9-phosphate	C13H21NO10	HMDB0000794	20,9	351,12	388,10	79,00	41
Adenine	C5H5N5	HMDB0000034	2,9	135,05	134,00	107,00	18
Adenine	C5H5N5	HMDB0000034	2,9	135,05	134,00	92,10	20
Adenosine 5-monophosphate	C10H14N5O7P	HMDB0000045	19,0	347,06	346,00	97,00	24
Adenosine 5-monophosphate	C10H14N5O7P	HMDB0000045	19,0	347,06	346,00	79,00	38
Adenosine 5-diphosphate	C10H15N5O10P2	HMDB0001341	22,0	427,03	426,00	328,00	16
Adenosine 5-diphosphate	C10H15N5O10P2	HMDB0001341	22,0	427,03	426,00	159,00	28
Adenosine 5-triphosphate	C10H16N5O13P3	HMDB0000538	23,2	507,00	506,00	408,10	22
Adenosine 5-triphosphate	C10H16N5O13P3	HMDB0000538	23,2	507,00	506,00	159,00	38
L-Arabinose	C5H10O5	HMDB0000646	3,0	150,05	149,00	89,10	4
L-Arabinose	C5H10O5	HMDB0000646	3,0	150,05	149,00	59,20	12
L-Arabitol	C5H12O5	HMDB0001851	1,5	152,07	151,00	89,00	12
L-Arabitol	C5H12O5	HMDB0001851	1,5	152,07	151,00	71,02	16
CDP-ribitol	C14H25N3O15P2	n.a.	20,5	537,08	536,10	322,00	20
CDP-ribitol	C14H25N3O15P2	n.a.	20,5	537,08	536,10	78,80	50
CMP-NeuNAc	C20H31N4O16P	HMDB0001176	20,5	614,15	613,14	321,90	20
CMP-NeuNAc	C20H31N4O16P	HMDB0001176	20,5	614,15	613,14	78,90	54
Cytidine	C9H13N3O5	HMDB0000089	1,8	243,09	242,10	109,00	8
Cytidine	C9H13N3O5	HMDB0000089	1,8	243,09	242,10	42,20	16
Cytidine 5-monophosphate	C9H14N3O8P	HMDB0000095	15,5	323,05	322,00	97,00	22
Cytidine 5-monophosphate	C9H14N3O8P	HMDB0000095	15,5	323,05	322,00	79,00	44
Cytidine 5-diphosphate	C9H15N3O11P2	HMDB0001546	21,0	403,02	402,01	158,92	24
Cytidine 5-diphosphate	C9H15N3O11P2	HMDB0001546	21,0	403,02	402,01	79,00	48
Cytidine 5-triphosphate	C9H16N3O14P3	HMDB0000082	23,0	482,98	482,00	158,80	40
Cytidine 5-triphosphate	C9H16N3O14P3	HMDB0000082	23,0	482,98	482,00	79,00	40
D-Erythrose 4-phosphate	C4H9O7P	HMDB0001321	14,0	200,01	199,00	97,00	14
D-Erythrose 4-phosphate	C4H9O7P	HMDB0001321	14,0	200,01	199,00	79,00	48
D-Fructose 1-phosphate	C6H12O6	HMDB0062538	14,0	180,06	259,00	97,00	14
D-Fructose 1-phosphate	C6H12O6	HMDB0062538	14,0	180,06	259,00	79,00	48
D-Fructose 6-phosphate	C6H13O9P	HMDB0000124	13,5	260,03	259,00	97,00	14
D-Fructose 6-phosphate	C6H13O9P	HMDB0000124	13,5	260,03	259,00	79,00	48
D-Fructose 1,6-bisphosphate	C6H14O12P2	HMDB0001058	20,3	340,00	338,90	241,01	12
D-Fructose 1,6-bisphosphate	C6H14O12P2	HMDB0001058	20,3	340,00	338,90	97,00	22
Galactitol	C6H14O6	HMDB0000107	1,4	182,08	181,07	101,00	13
Galactitol	C6H14O6	HMDB0000107	1,4	182,08	181,07	59,00	20
Galactonic acid	C6H12O7	HMDB0000565	4,0	196,06	195,10	129,00	11
Galactonic acid	C6H12O7	HMDB0000565	4,0	196,06	195,10	75,10	18
D-Galactose 1-phosphate	C6H13O9P	HMDB0000645	13,4	260,03	259,00	240,90	9
D-Galactose 1-phosphate	C6H13O9P	HMDB0000645	13,4	260,03	259,00	79,00	28
Glucose	C6H12O6	HMDB0000122	1,4	180,06	179,10	89,10	5
Glucose	C6H12O6	HMDB0000122	1,4	180,06	179,10	59,00	17
D-Glucose 1-phosphate	C6H13O9P	HMDB0001586	13,6	260,03	259,00	240,90	9
D-Glucose 1-phosphate	C6H13O9P	HMDB0001586	13,6	260,03	259,00	79,00	28
D-Glucose 6-phosphate	C6H13O9P	HMDB0001401	12,9	260,03	259,00	97,00	14
D-Glucose 6-phosphate	C6H13O9P	HMDB0001401	12,9	260,03	259,00	79,00	48
Glucuronic acid	C6H10O7	HMDB0000127	5,0	194,04	193,00	113,00	14
L-Glutamine	C5H10N2O3	HMDB0000641	1,4	146,07	145,10	127,00	7
L-Glutamine	C5H10N2O3	HMDB0000641	1,4	146,07	145,10	109,00	10
Glyceraldehyde 3-phosphate	C3H7O6P	HMDB0001112	14,0	170,00	169,00	97,00	4
Glyceraldehyde 3-phosphate	C3H7O6P	HMDB0001112	14,0	170,00	169,00	79,00	28
N-Glycolylneuraminic acid	C11H19NO10	HMDB0000833	6,0	325,10	324,09	116,00	13
N-Glycolylneuraminic acid	C11H19NO10	HMDB0000833	6,0	325,10	324,09	87,10	25
Guanine	C5H5N5O	HMDB0000132	3,0	151,05	150,00	133,02	12
Guanine	C5H5N5O	HMDB0000132	3,0	151,05	150,00	66,01	36
Guanosine	C10H13N5O5	HMDB0000133	8,8	283,09	282,10	150,00	17
Guanosine	C10H13N5O5	HMDB0000133	8,8	283,09	282,10	132,90	32
Mannitol	C6H14O6	HMDB0000765	14,0	182,08	181,10	71,00	22
D-Mannose	C6H12O6	HMDB0000169	1,4	180,06	179,10	89,00	4
D-Mannose	C6H12O6	HMDB0000169	1,4	180,06	179,10	59,20	16
D-Mannose 1-phosphate	C6H13O9P	HMDB0006330	13,5	260,03	259,00	79,00	28
D-Mannose 6-phosphate	C6H13O9P	HMDB0001078	13,1	260,03	259,00	97,00	14
D-Mannose 6-phosphate	C6H13O9P	HMDB0001078	13,1	260,03	259,00	79,00	48
Phosphoenolpyruvic acid	C3H5O6P	HMDB0000263	21,7	167,98	167,00	79,00	12
6-Phosphogluconic acid	C6H13O10P	HMDB0001316	14,0	276,02	275,00	79,00	50
5-Phosphoribosyl 1-pyrophosphate	C5H13O14P3	HMDB0000280	16,0	389,95	388,90	291,00	9
5-Phosphoribosyl 1-pyrophosphate	C5H13O14P3	HMDB0000280	16,0	389,95	388,90	177,00	25
5-Phosphoribosyl 1-pyrophosphate	C5H13O14P3	HMDB0000280	16,0	389,95	388,90	79,00	50
5-Phosphoribosylamine	C5H12NO7P	HMDB0001128	1,5	229	228,00	97,00	10
5-Phosphoribosylamine	C5H12NO7P	HMDB0001128	1,5	229	228,00	79,00	48

Pyruvic acid	C3H4O3	HMDB0000243	15,1	88,02	87,00	43,20	4
Ribitol	C5H12O5	HMDB0000508	1,5	152,07	151,10	89,20	9
Ribitol	C5H12O5	HMDB0000508	1,5	152,07	151,10	71,10	17
Ribitol 5-phosphate	C5H13O8P	n.a.	13,5	232,03	231,00	97,00	12
Ribitol 5-phosphate	C5H13O8P	n.a.	13,5	232,03	231,00	79,00	50
D-Ribose 5-phosphate	C5H11O8P	HMDB0001548	13,5	230,02	229,00	97,00	10
D-Ribose 5-phosphate	C5H11O8P	HMDB0001548	13,5	230,02	229,00	79,00	48
D-Ribose 1-phosphate	C5H11O8P	HMDB0001489	15,5	230,02	229,00	97,00	10
D-Ribose 1-phosphate	C5H11O8P	HMDB0001489	15,5	230,02	229,00	79,00	48
Ribulose 5-phosphate	C5H11O8P	HMDB0000618	14,5	230,02	229,01	97,00	14
Ribulose 5-phosphate	C5H11O8P	HMDB0000618	14,5	230,02	229,01	79,00	48
D-Sedoheptulose 7-phosphate	C7H15O10P	HMDB0001068	13,5	290,04	289,00	96,90	18
D-Sedoheptulose 7-phosphate	C7H15O10P	HMDB0001068	13,5	290,04	289,00	79,00	48
D-Sedoheptulose 1,7-bisphosphate	C7H16O13P2	HMDB0060274	21,2	370,01	369,00	97,00	14
D-Sedoheptulose 1,7-bisphosphate	C7H16O13P2	HMDB0060274	21,2	370,01	369,00	79,00	48
Sorbitol	C6H14O6	HMDB0000247	1,6	182,08	181,10	101,00	13
Sorbitol	C6H14O6	HMDB0000247	1,6	182,08	181,10	59,00	21
Trehalose	C12H22O11	HMDB0000975	1,5	342,12	341,00	89,01	12
UDP-GlcNAc	C17H27N3O17P2	HMDB0000290	20,8	607,08	606,07	385,10	28
UDP-GlcNAc	C17H27N3O17P2	HMDB0000290	20,8	607,08	606,07	282,20	30
Uridine	C9H12N2O6	HMDB0000296	4,0	244,07	243,10	200,00	6
Uridine	C9H12N2O6	HMDB0000296	4,0	244,07	243,10	110,00	12
Xylitol	C5H12O5	HMDB0002917	1,5	152,07	151,10	89,00	8
Xylitol	C5H12O5	HMDB0002917	1,5	152,07	151,10	71,00	8
D-Xylose	C5H10O5	HMDB0000098	4,0	150,05	149,05	89,02	4
D-Xylose	C5H10O5	HMDB0000098	4,0	150,05	149,05	71,01	4
D-Xylulose 5-phosphate	C5H11O8P	HMDB0000868	14,3	230,02	229,00	138,98	8
D-Xylulose 5-phosphate	C5H11O8P	HMDB0000868	14,3	230,02	229,00	79,00	36