

Table S7: MRM parameters for targeted analysis of charged hydrophilic metabolites. MRM: multiple reaction monitoring, m/z Q1: nominal mass to charge ratio of precursor ion (Quadrupole 1), m/z Q2: nominal mass to charge ratio of fragment ion (Quadrupole 2), RT: retention time, CE [V]: collision energy in Volts, DP [V]: declustering potential in Volts, CXP [V]: cell exit potential in Volts

Biocyc ID	m/z Q1	m/z Q3	Expected RT (min)	CE [V]	CXP [V]	DP [V]
2-PG	185	79	12.9	-20	-35	-25
G3P	185.1	96.7	13.2	-22	-7	-30
CPD-2961	275	79	13.1	-66	-5	-60
CIS-ACONITATE	173.1	84.9	13.4	-18	-5	-35
Adenosine	266.2	133.9	2.7	-12	-1	-70
ADENYLOSUCC	462.3	133.9	15.8	-62	-7	-85
ADP	426.2	78.9	13.2	-66	-3	-75
2-KETOGLUTARATE	145	101	10.7	-12	-13	-10
ALA	148	88.1	1.6	-8	-3	-20
AMP	346.2	78.8	8.9	-52	-3	-70
ARG	173.2	131	1.6	-18	-7	-50
L-ARGININO-SUCCINATE	289.3	271.3	2.7	-14	-15	-55
ASN	131.1	87.1	1.6	-16	-11	-75
L-ASPARTATE	132	88	1.9	-18	-13	-40
ATP	506.2	158.8	15.6	-38	-9	-80
CARBAMYUL-L-ASPARTATE	175.1	131.8	10	-16	-7	-25
CAMP	328.2	133.9	7.6	-36	-5	-125
CDP	402.2	78.9	12.8	-70	-5	-65
4-CYTIDINE-5-DIPHOSPHO-2-C	520.1	78.9	4.6	-108	-9	-120
2-PHOSPHO-4-CYTIDINE-5-DIPHOSPHO-2-C-MET	600	78.9	16	-126	-19	-115
CGMP	344.2	150	6.4	-34	-11	-70
CIT	191	87	14.1	-22	-15	-35
L-CITRULLINE	174.2	131	1.6	-18	-7	-35
CMP	322.2	79	7	-68	-5	-65
CTP	482.2	158.8	15.4	-36	-9	-85
Cytidine	242.2	108.9	1.8	-18	-5	-70
DIHYDROXY-ACETONE-PHOSPHATE	169.1	97	8.5	-14	-11	-35
DI-H-OROTATE	157.1	112.7	3.8	-10	-5	-40
CPD-4211	115.1	71	10.6	-12	-13	-5
TDP	401.2	78.8	13.1	-68	-3	-70
TMP	321.2	78.8	8.7	-58	-3	-65
TTP	481.2	158.7	15.4	-38	-9	-80
DEOXYXYLULOSE-5P	213	97	8.8	-16	-21	-5
ERYTHROSE-4P	199.1	96.8	6.1	-12	-5	-40
FAD	784.5	79	13.4	-130	-1	-60
FRUCTOSE-16-DIPHOSPHATE	339.1	96.9	15.1	-22	-11	-35
FUM	115.1	71	10.6	-12	-13	-5
CPD-448	259.1	240.8	6.7	-16	-15	-30
D-glucopyranose-6-phosphate	259.1	97	5.9	-18	-13	-65
GLUCOSAMINE-1P	258.2	78.9	2.7	-42	-1	-55
GAP	169	97	6.5	-12	-5	-30
GDP	442.2	78.9	12.9	-70	-3	-85
GLT	146	102	2.1	-18	-9	-80
GLYCEROL-3P	171.1	78.8	6.3	-24	-1	-45
GLN	145.1	108.9	1.6	-18	-5	-30
glucose	178.9	89	1.6	-12	-13	-50
GLY	74.1	74	1.6	-13	-3	-36
GMP	362.2	78.9	7.8	-66	-5	-65
GLUTATHIONE	306.3	143	4.7	-26	-7	-5
OXIDIZED-GLUTATHIONE	611.6	306.1	9.5	-34	-7	-35
GTP	522.2	158.8	15.4	-48	-9	-90
Guanosine	282.2	149.9	2.1	-26	-7	-80
HIS	154.2	93	1.8	-24	-3	-40
HYDROXY-METHYL-BUTENYL-DIP	261	79	13.3	-52	-9	-40
IMP	347.2	134.8	8.1	-38	-7	-70
THREO-DS-ISO-CITRATE	191.1	73	14.4	-28	-31	-45
L-LACTATE	89.1	42.9	3.8	-12	-5	-15
LYS	145.2	101	1.6	-14	-5	-65
MAL	133.1	115	9.9	-16	-5	-20
2C-METH-D-ERYTHRITOL-CYCLODIPHOSPHATE	277	79	10.9	-64	-37	-45
2-C-METHYL-D-ERYTHRITOL-4-PHOSPHATE	215	78.9	6.9	-56	-9	-40
MET	148.2	47	1.8	-24	-5	-45
NAD	662.4	540.1	5.5	-22	-15	-45
NADH	664.4	78.9	11.4	-124	-1	-100
NADP	742.4	620	13.4	-22	-17	-55
NADPH	744.4	79	16.3	-118	-3	-110
L-ORNITHINE	131.2	82.9	1.7	-20	-5	-60
PAN	218.2	88.1	7	-18	-5	-55
L-1-GLYCERO-PHOSPHORYLCHOLINE	242.2	167.9	2.3	-12	-9	-40
PHOSPHO-ENOL-PYRUVATE	167	78.8	13.9	-16	-9	-20
PHE	164.2	103	2.4	-24	-5	-55
PRO	114.1	86	1.6	-18	-3	-55
PRPP	389.1	176.8	16.8	-28	-9	-55
RIBOSE-5P	229.1	96.8	6.1	-20	-5	-35
D-RIBULOSE-15-P2	309.1	97	15.7	-20	-27	-35
RIBOSE-5P + XYLULOSE-5-PHOSPHATE	229.1	96.8	7.6	-18	-15	-45
D-SEDOHEPTULOSE-7-P	289.2	97	6.3	-22	-5	-50
ADENOSYL-HOMO-CYS	383.4	133.9	2.5	-36	-7	-80
SER	104.1	74	1.6	-16	-3	-20
SUC	117.1	73	9.9	-16	-7	-25
THR	118.1	73.9	1.6	-18	-3	-25
TRP	203.2	116.2	3.5	-22	-7	-50
TYR	180.2	118.9	1.9	-24	-5	-60
UDP	403.2	78.8	13.1	-68	-3	-75
CPD-12575	565.3	323	10.2	-36	-11	-125
UMP	323.2	79	7.8	-68	-5	-65
URIDINE	243.2	109.9	1.9	-22	-5	-65
UTP	483.1	158.8	15.5	-38	-9	-90
XANTHOSINE-5-PHOSPHATE	363.2	151.1	12.9	-36	-5	-60
D-SEDOHEPTULOSE-1-7-P2	369	97	16	-20	-27	-35