

Supplemental Data Table S2. Tandem mass spectrometry operating conditions

Analyte	Precursor ion (m/z)	Product ion (m/z)	Dwell time (msec)	Cone voltage (V)	Collision energy (eV)
Ala	90.1	44.0	25	20	7
Arg	175.1	70.1	25	25	20
Cit	176.1	113.1	25	22	15
Gln + Lys	147.1	84.0	25	20	15
Glu	148.1	84.0	25	20	15
Gly	76.0	30.0	25	20	7
His	156.1	110.1	25	20	12
Leu + Ile	132.1	86.1	25	20	10
Met	150.1	104.1	25	20	10
Orn	133.1	70.1	25	20	15
Phe	166.1	120.1	25	22	12
Pro	116.1	70.0	25	25	13
Tyr	182.1	136.1	25	22	13
Val	118.1	72.1	25	20	10
ASA	291.1	70.1	5	47	30
SUAC	155.1	109.1	25	25	18
ADO	268.1	136.1	25	30	15
D-ADO	252.1	136.1	25	22	15
C0	162.1	103.1	25	35	18
C2	204.1	85.0	25	35	18
C3	218.1	85.0	25	35	18
C3DC + C40H	248.1	84.0	25	35	22
C4	232.2	85.0	25	35	19
C4DC + C50H	262.2	85.0	25	35	24
C5	246.2	85.0	25	35	21
C5:1	244.2	85.0	25	35	21
C5DC + C60H	276.1	85.0	25	35	24
C6	260.2	85.0	25	35	24
C6DC	290.2	85.0	25	35	24
C8	288.2	85.0	25	35	24
C8:1	286.2	85.0	25	35	24
C10	316.2	85.0	25	35	24
C10:1	314.2	85.0	25	35	24
C10:2	312.2	85.0	25	35	24
C12	344.3	85.0	25	40	23
C12:1	342.3	85.0	25	40	23
C14	372.3	85.0	25	40	25
C14OH	388.3	85.0	25	40	25

*(Continued to the next)***Supplemental Data Table S2.** Continued

Analyte	Precursor ion (m/z)	Product ion (m/z)	Dwell time (msec)	Cone voltage (V)	Collision energy (eV)
C14:1	370.3	85.0	25	40	25
C14:2	368.3	85.0	25	40	25
C16	400.3	85.0	25	46	25
C16OH	416.3	85.0	25	46	25
C16:1	398.3	85.0	25	46	25
C16:10H	414.3	85.0	25	46	25
C18	428.4	85.0	25	55	25
C18OH	444.4	85.0	25	55	25
C18:1	426.4	85.0	25	55	25
C18:10H	442.4	85.0	25	55	25
C18:2	424.3	85.0	25	55	25
C18:20H	440.3	85.0	25	55	25
C20	456.4	85.0	25	68	35
C22	484.4	85.0	25	68	35
C24	512.5	85.0	25	68	35
C26	540.5	85.0	25	68	35
C20:0-LPC	552.4	104.1	25	68	30
C22:0-LPC	580.4	104.1	25	68	30
C24:0-LPC	608.5	104.1	25	68	30
C26:0-LPC	636.5	104.1	25	68	30

Abbreviations: ASA, argininosuccinic acid; SUAC, succinylacetone; ADO, adenosine; D-ADO, 2'-deoxyadenosine; LPC, lysophosphatidylcholine; amino acids are abbreviated as three-letter symbols according to the International Union of Pure and Applied Chemistry (IUPAC) nomenclature.