

Table S8 MS parameters for amino acid and acylcarnitines

Amino acids	Precursor Ion (m/z)	Product Ion (m/z)	Cone Voltage	Collision Energy
Glycine (Gly)	76	30.3	40	5
¹⁵ N, ²⁻¹³ C-Glycine (¹⁵ N, ²⁻¹³ C-Gly)	78	32.3	40	5
Alanine (Ala)	90	44.1	40	7
² H ₄ -Alanine (² H ₄ -Ala)	94	48.1	40	7
Proline (Pro)	115.9	70	50	10
¹³ C ₅ -Proline (¹³ C ₅ -Pro)	120.9	74	50	10
Valine (Val)	118	72	40	9
Threonine (Thr)	119.9	73.9	40	7
Serine (Ser)	105.8	60	40	6
² H ₈ -Valine (² H ₈ -Val)	126	80	40	9
Leucine/Isoleucine/ HydroxyProline (Leu/Ile/Pro-OH)	131.9	86	40	9
Aspartic acid (Asp)	133.8	87.8	40	7
Glutamic acid (Glu)	147.8	83.9	40	10
Asparagine (Asn)	132.9	73.9	40	10
² H ₃ -Leucine (² H ₃ -Leu)	134.9	89	40	9
Ornithine (Orn)	132.9 -46.50 -32.41	70	40	12
Lysine/Glutamine (Lys/Gln)	146.9	129.8	40	7
² H ₆ -Ornithine (² H ₆ -Orn)	138.9	76	40	12
Methionine (Met)	149.9 -25.78 -2.44	103.9	45	9
² H ₃ -Methionine (² H ₃ -Met)	152.9	106.9	45	9
Phenylalanine (Phe)	166 -26.81 16.19	120	45	11
¹³ C ₆ -Phenylalanine (¹³ C ₆ -Phe)	172	126	45	11
Arginine (Arg)	175 -43.08 -17.65	70	45	17
Histidine (His)	155.9	109.9	40	10
² H ₄ , ¹³ C-Arginine (² H ₄ , ¹³ C-Arg)	180	75	45	17
Citrulline (Cit)	176	112.9	45	13
² H ₂ -Citrulline (² H ₂ -Cit)	178	114.9	45	13
Tyrosine (Tyr)	182	135.9	45	12
¹³ C ₆ -Tyrosine (¹³ C ₆ -Tyr)	188	141.9	45	12

Acylcarnitines	Precursor Ion (m/z)	Product Ion (m/z)	Cone Voltage	Collision Energy
Free carnitine (C0)	160	102.9	60	15
² H ₉ - Free carnitine (² H ₃ -C0)	171	102.9	60	15
Acetylcarnitine (C2)	204	84.9	60	16
² H ₃ - Acetylcarnitine (² H ₃ -C2)	207	84.9	60	16
Propionylcarnitine (C3)	218	84.9	60	16
² H ₃ - Propionylcarnitine (² H ₃ -C3)	221	84.9	60	16
Butyrylcarnitine (C4)	232	84.9	60	17
Malonylcarnitine/3-Hydroxy-butyrylcarnitine (C3DC/C4OH)	248	84.9	60	17
² H ₃ -Butyrylcarnitine (² H ₃ -C4)	235	84.9	60	17
Isovalerylcarnitine (C5)	246.1	84.9	70	18
Tiglylcarnitine (C5:1)	244.1	84.9	70	18
Methylmalonyl/3-Hydroxy-isovalerylcarnitine (C4DC/C5OH)	262.1	84.9	70	18
² H ₉ -Isovalerylcarnitine (² H ₉ -C5)	255.1	84.9	70	18
Glutaryl/3-Hydroxy-hexanoylcarnitine (C5DC/C6OH)	276.1	84.9	70	20
Adipylcarnitine (C6DC)	290.1	84.9	70	20
² H ₆ -Adipylcarnitine (² H ₆ -C6DC)	282.1	84.9	70	20
Hexanoylcarnitine (C6)	260.1	84.9	65	18
² H ₃ -Hexanoylcarnitine (² H ₃ -C6)	263.1	84.9	65	18
Octanoylcarnitine (C8)	288.2	84.9	70	19
Octenoylcarnitine (C8:1)	286.2	84.9	70	19
² H ₃ -Octanoylcarnitine (² H ₃ -C8)	291.2	84.9	70	19
Decanoylcarnitine (C10)	316.2	84.9	75	20
Decenoylcarnitine (C10:1)	314.2	84.9	75	20
Decadienoylcarnitine (C10:2)	312.2	84.9	75	20
² H ₃ - Decanoylcarnitine (² H ₃ -C10)	319.2	84.9	75	20
Dodecanoylcarnitine (C12)	344.2	84.9	75	22
Dodecenoylcarnitine (C12:1)	342.2	84.9	75	22
² H ₃ - Dodecanoylcarnitine (² H ₃ -C12)	347.2	84.9	75	22
Tetradecanoylcarnitine (Myristoylcarnitine) (C14)	372.3	84.9	75	23
Tetradecenoylcarnitine	370.3	84.9	75	23

(C14:1)				
Tetradecadienoylcarnitine (C14:2)	368.3	84.9	75	23
3-Hydroxy- Tetradecanoylcarnitine (C14OH)	388.3	84.9	75	23
² H ₃ - Tetradecanoylcarnitine (² H ₃ -C14)	375.3	84.9	75	23
Hexadecanoylcarnitine (Palmitoylcarnitine) (C16)	400.3	84.9	75	25
Hexadecenoylcarnitine (C16:1)	398.3	84.9	75	25
3-Hydroxy- Hexadecanoylcarnitine (C16OH)	416.3	84.9	75	25
3-Hydroxy- Hexadecenoylcarnitine (C16:1OH)	414.3	84.9	75	25
² H ₃ - Hexadecanoylcarnitine (² H ₃ -C16)	403.3	84.9	75	25
Octadecanoylcarnitine (Stearoylcarnitine) (C18)	428.3	84.9	80	25
Octadecenoylcarnitine (Oleylcarnitine) (C18:1)	426.3	84.9	80	25
Octadecadienoylcarnitine (Linoleylcarnitine) (C18:2)	424.3	84.9	80	25
3-Hydroxy- Octadecanoylcarnitine (C18OH)	444.3	84.9	80	25
3-Hydroxy- Octadecenoylcarnitine (C18:1OH)	442.3	84.9	80	25
² H ₃ - Octadecanoylcarnitine (² H ₃ -C18)	431.3	84.9	80	25