

Electrospray ionization tandem mass spectrometry (ESI-MS/MS) acquisition parameters for the analysis of whole blood amino acids (AAs) and acylcarnitines (ACs). MS/MS transitions for each analysed AA and AC, the optimal cone potential (V), and collision energy (eV) are shown for each analyte. The capillary potential was 3.5 kV.

Abbreviation	Full name	Transition	Cone potential	Collision energy
ALA	Alanine	90.2>44.3	40	6
ARG	Arginine	175.3>70.3	45	17
CIT	Citrulline	176.2>113.2	45	13
LYS-GLN	Lysine/Glutamine	147.2>130.2	40	12
GLU	Glutamic Acid	148.2>84.2	40	8
GLY	Glycine	76.2>30.3	40	5
LEU-ILE-PRO-OH	Leucine/Isoleucine/Hydroxyprolin	132.2>86.3	40	8
MET	Methionine	150.2>104.2	45	9
ORN	Ornithine	133.3>70.3	40	12
PHE	Phenylalanine	166.2>120.2	45	11
PRO	Proline	116.1>70.1	28	12
SA	Succinylacetone	155.1>109.1	24	22
TYR	Tyrosine	182.2>136.2	45	12
ADO	Adenosine	168.1>136.1	32	18
C0	Free Carnitine	162.2>103.2	60	14
C10:2	Decadienoylcarnitine	313.>85.2	75	19
C2	Acetylcarnitine	204.2>85.2	60	14
C3	Propionylcarnitine	218.2>85.2	60	15
C3DC-C4OH	Malonylcarnitine/3-Hydroxy-butyrylcarnitine	248.3>85.2	60	15
C4	Butyrylcarnitine	232.3>85.2	60	15
C4DC-C5OH	Methylmalonylcarnitine/3-Hydroxy-valerylcarnitine	262.2>85.2	70	16
C5	Valerylcarnitine	246.2>85.2	70	16
C5:1	Tiglylcarnitine	244.2>85.2	70	16
C5DC-C6OH	Glutaryl carnitine/3-Hydroxy-hexanoylcarnitine	276.3>85.2	70	20
C6	Hexanoylcarnitine	260.3>85.2	65	16
C6DC	Adipylcarnitine	282.3>85.2	70	20
C8	Octanoylcarnitine	288.3>85.2	75	18
C8:1	Octenoylcarnitine	286.3>85.2	75	18
C10	Decanoylcarnitine	316.3>85.2	75	19
C10:1	Decenoylcarnitine	314.3>85.2	75	19
C12	Dodecenoylcarnitine	344.4>85.2	75	22
C14:2	Tetradecadienoylcarnitine	368.4>85.2	75	23
C16	Hexadecanoylcarnitine (palmitoylcarnitine)	400.4>85.2	75	25
C16:1OH	3-Hydroxy-hexadecenoylcarnitine	414.4>85.2	75	25
C16OH	3-Hydroxy-hexadecanoylcarnitine	416.4>85.2	75	25
C18:1	Octadecenoylcarnitine (Oleylcarnitine)	426.4>85.2	80	25
C18:1OH	3-Hydroxy-octadecenoylcarnitine	442.4>85.2	80	25

Abbreviation	Full name	Transition	Cone potential	Collision energy
C18:2	Octadecadienoylcarnitine (Linoleoylcarnitine)	424.4>85.2	80	25
C18:2OH	3-Hydroxy-octadecadienoylcarnitine	440.3>85.0	56	28
C18OH	3-Hydroxy-octadecanoylcarnitine	444.4>85.2	80	25
C20	Eicosanoylcarnitine (Arachidoylcarnitine)	456.4>85.0	69	34
C22	Docosanoylcarnitine (Behenoylcarnitine)	484.4>85.0	69	34
C26	Hexacosanoylcarnitine (Cerotoylcarnitine)	540.5>85.0	69	34
C20:0-LPC	Tetracosanoylcarnitine (Lignoceroylcarnitine)	552.4>104.1	74	30
C24:0-LPC	C24:0 lysophosphatidylcholine	608.5>104.1	74	30
C26:0-LPC	C26:0 lysophosphatidylcholine	636.5>104.1	74	30