

Analyte	Q1 (m/z)	Q3 (m/z)	Internal standard
ALA	90.0	44.0	² H ₄ -Ala
ARG	175.1	70.0	² H ₄ , ¹³ C-Arg
CIT	176.1	113.0	² H ₂ -Cit
LEU	132.1	86.0	² H ₃ -Leu
MET	150.0	104.0	² H ₃ -Met
ORN	133.1	70.0	² H ₂ -Orn
PHE	166.1	120.1	¹³ C ₆ -Phe
SUAC	155.0	142.1	¹³ C ₅ -SUAC
TYR	182.1	136.1	¹³ C ₆ -Tyr
VAL	118.05	72.0	² H ₈ -Val
C0	162.1	103.0	² H ₉ -C0
C2	204.1	85.0	² H ₃ -C2
C3DC+C4OH	248.1	85.0	² H ₃ -C4
C3	218.1	85.0	² H ₃ -C3
C4	232.1	85.0	² H ₃ -C4
C5	246.2	85.0	² H ₉ -C5
C5DC	276.2	85.0	² H ₃ -C5DC
C5OH	262.2	85.0	² H ₃ -C5OH
C6	260.2	85.0	² H ₃ -C8
C8	288.2	85.0	² H ₃ -C8
C10	316.2	85.0	² H ₉ -C12
C12	344.3	85.0	² H ₉ -C12
C14	372.3	85.0	² H ₉ -C14
C16	400.4	85.0	² H ₃ -C16
C16OH	416.4	85.0	² H ₃ -C16
C18	428.4	85.0	² H ₃ -C18
C18OH	444.4	85.0	² H ₃ -C18
Ado	268.2	136.1	¹³ C ₅ -Ado
dAdo	252.2	136.1	¹³ C ₅ -dAdo

S1: SRM transitions and associated internal standard for unlabeled analytes

Labeled standard	Q1 (m/z)	Q3 (m/z)	Concentration (μM)
D ₄ -Ala	94.0	48.0	2.5
D ₄ , ¹³ C-Arg	180.1	75.0	2.5
D ₂ -Cit	178.1	115.0	2.5
D ₃ -Leu	135.1	89.0	2.5
D ₃ -Met	153.0	107.0	2.5
D ₂ -Orn	135.1	72.0	2.5
¹³ C ₆ -Phe	172.1	126.1	2.5
¹³ C ₅ -SUAC	160.0	142.1	2.5
¹³ C ₆ -Tyr	188.1	142.1	2.5
D ₈ -Val	126.1	80.0	2.5
D ₉ -C0	165.1	103.0	0.76
D ₃ -C2	207.1	85.0	0.19
D ₃ -C3	221.1	85.0	0.038
D ₃ -C4	235.1	85.0	0.038
D ₉ -C5	255.2	85.0	0.038
D ₃ -C5DC	279.2	85.0	0.076
D ₃ -C5OH	265.5	85.0	0.038
D ₃ -C8	291.2	85.0	0.038
D ₉ -C12	353.3	85.0	0.038
D ₉ -C14	381.3	85.0	0.038
D ₃ -C16	403.4	85.0	0.076
D ₃ -C18	431.4	85.0	0.076
¹³ C ₅ -Ado	273.2	136.1	3.0
¹³ C ₅ -dAdo	257.2	136.1	3.0

S2: SRM transition and concentration associated with each internal standard