Table S6 Transitions of derivatized amino acids: Retention time, collision potential, and precursor-product ion transition of $U^{12}C$ and $U^{13}C^{15}N$ isotopologues. Metabolite abbreviations are listed in Table S1.

Metabolite	Rentention time (min)	Collision (V)	^{12}C		$U^{13}C,^{15}N$	
			Q1	Q3	Q1	Q3
Ala	4,1	14	225,0	44,0	228,9	94,2
Arg	2,8	14	310,1	217,1	320,1	227,1
Asn	3,0	16	268,0	87,1	272,2	90,1
Asp	3,7	14	269,0	116,0	274,0	139,3
Cys	4,5	8	257,0	122,0	261,0	126,0
Gln	3,1	16	282,1	129,8	287,1	194,1
Glu	3,7	16	283,0	130,0	289,0	136,0
Gly	3,3	10	211,0	75,9	214,0	78,9
His	2,4	22	291,1	110,1	300,1	118,0
Ile	5,1	28	267,3	69,0	274,3	74,0
Leu	5,1	38	267,1	43,3	274,1	46,0
Lys	5,1	12	417,1	324,1	425,1	332,1
Met	4,8	18	285,1	104,0	291,1	108,0
Phe	5,1	26	301,1	136,0	311,1	136,0
Pro	4,1	24	251,0	136,0	257,0	136,0
Ser	3,2	16	241,1	60,0	245,1	63,0
Thr	4,0	18	255,0	74,0	259,0	77,0
Trp	5,0	28	340,1	146,0	-*	-*
Tyr	4,5	26	317,1	123,0	327,1	147,2
Val	4,8	18	253,0	136,0	259,0	136,0

*$U^{13}C,^{15}N$ Phe transition applied for correction