

Mass Spectra

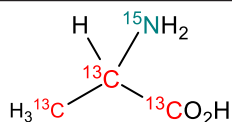
Stable Isotopes products

Stable Isotope Labeled Amino Acid Mix for Mass Spec - Product 909653

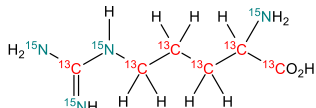
Component	Formula	Ionization mode	Precursor ion	Product ion 1	Product ion 2
Alanine- ¹³ C ₃ , ¹⁵ N	¹³ C ₃ H ₇ ¹⁵ NO ₂	+	94.1	47.1	
Arginine- ¹³ C ₆ , ¹⁵ N ₄	¹³ C ₆ H ₁₄ ¹⁵ N ₄ O ₂	+	185.1	75.1	64.1
Asparagine- ¹⁵ N ₂	C ₄ H ₈ ¹⁵ N ₂ O ₃	+	135.1	75.0	89.1
Aspartic acid- ¹³ C ₄ , ¹⁵ N	¹³ C ₄ H ₇ ¹⁵ NO ₄	+	139.1	77.0	92.0
Cystine-d ₄	C ₆ H ₈ d ₄ N ₂ O ₄ S ₂	+	245.1	122.0	154.0
Glutamic acid- ¹³ C ₅ , ¹⁵ N	C ₅ H ₁₀ ¹⁵ N ₂ O ₃	+	154.1	89.1	107.1
Glutamine- ¹⁵ N ₂	¹³ C ₅ H ₉ ¹⁵ NO ₄	+	149.1	131.0	85.0
Glycine- ¹³ C ₂ , ¹⁵ N	¹³ C ₂ H ₅ ¹⁵ NO ₂	+	79.0	32.0	
Histidine- ¹⁵ N ₃	C ₆ H ₉ ¹⁵ N ₃ O ₂	+	159.1	113.1	85.1
Isoleucine- ¹³ C ₆ , ¹⁵ N	¹³ C ₆ H ₁₃ ¹⁵ NO ₂	+	139.1	92.1	74.1
Leucine- ¹³ C ₆	¹³ C ₆ H ₁₃ NO ₂	+	138.1	91.1	
Lysine- ¹³ C ₆ , ¹⁵ N ₂	¹³ C ₆ H ₁₄ ¹⁵ N ₂ O ₂	+	155.1	90.1	137.1
Methionine- ¹³ C ₅ , ¹⁵ N	¹³ C ₅ H ₁₁ ¹⁵ NO ₂ S	+	156.1	109.1	138.0
Phenylalanine- ¹³ C ₉ , ¹⁵ N	¹³ C ₉ H ₁₁ ¹⁵ NO ₂	+	176.1	129.1	111.1
Proline- ¹³ C ₅ , ¹⁵ N	¹³ C ₅ H ₉ ¹⁵ NO ₂	+	122.1	75.1	46.0
Serine- ¹³ C ₃ , ¹⁵ N	¹³ C ₃ H ₇ ¹⁵ NO ₃	+	110.1	63.0	92.0
Threonine- ¹³ C ₄ , ¹⁵ N	¹³ C ₄ H ₉ ¹⁵ NO ₃	+	125.1	78.1	60.1
Tryptophan- ¹⁵ N ₂	C ₁₁ H ₁₂ ¹⁵ N ₂ O ₂	+	207.1	189.1	147.1
Tyrosine- ¹³ C ₉ , ¹⁵ N	¹³ C ₉ H ₁₁ ¹⁵ NO ₃	+	192.1	130.1	174.1
Valine- ¹³ C ₅ , ¹⁵ N	¹³ C ₅ H ₁₁ ¹⁵ NO ₂	+	124.1	77.1	59.1

Structures of Component Amino Acids - Product 909653

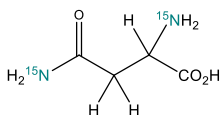
Alanine- $^{13}\text{C}_3, ^{15}\text{N}$



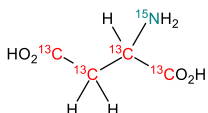
Arginine- $^{13}\text{C}_6, ^{15}\text{N}_4$



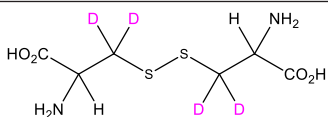
Asparagine- $^{15}\text{N}_2$



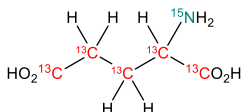
Aspartic acid- $^{13}\text{C}_4, ^{15}\text{N}$



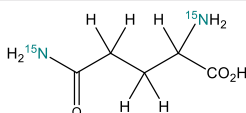
Cystine- d_4



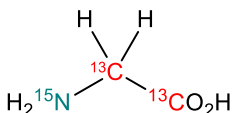
Glutamic acid- $^{13}\text{C}_5, ^{15}\text{N}$



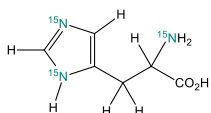
Glutamine- $^{15}\text{N}_2$



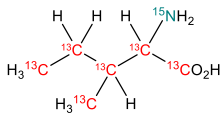
Glycine- $^{13}\text{C}_2, ^{15}\text{N}$



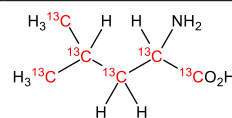
Histidine- $^{15}\text{N}_3$



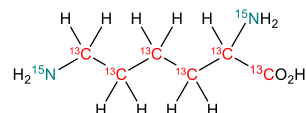
Isoleucine- $^{13}\text{C}_6, ^{15}\text{N}$



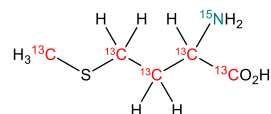
Leucine- $^{13}\text{C}_6$



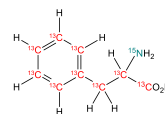
Lysine- $^{13}\text{C}_6, ^{15}\text{N}_2$



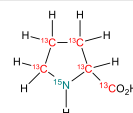
Methionine- $^{13}\text{C}_5, ^{15}\text{N}$



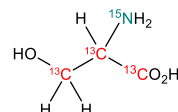
Phenylalanine- $^{13}\text{C}_9, ^{15}\text{N}$



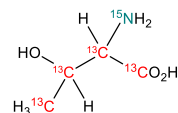
Proline- $^{13}\text{C}_5, ^{15}\text{N}$



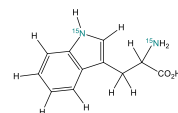
Serine- $^{13}\text{C}_3, ^{15}\text{N}$



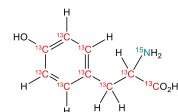
Threonine- $^{13}\text{C}_4, ^{15}\text{N}$



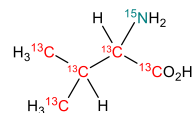
Tryptophan- $^{15}\text{N}_2$



Tyrosine- $^{13}\text{C}_9, ^{15}\text{N}$



Valine- $^{13}\text{C}_5, ^{15}\text{N}$



Alanine-¹³C₃, ¹⁵N

Labeled amino acid

	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	94.1		3	8			1	2			
Product ion											

Non labeled amino acid

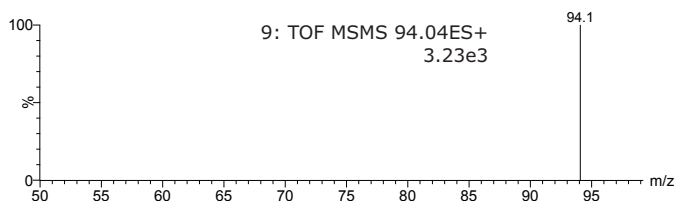
	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	90.1	3		8		1		2			
Product ion											

Experimental

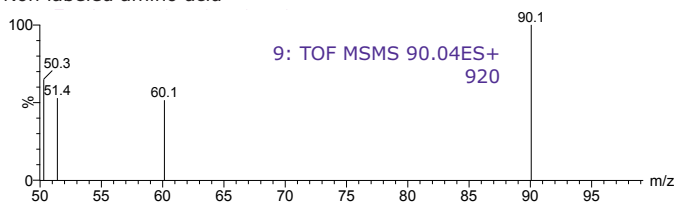
Instrument	XEVO-G2XSQTOF (waters)
Polarity	Positive
Analyzer	Resolution Mode
Capillary (kV)	2.0
Sampling Cone	40
Source Temperature (°C)	150
Source Offset	80
Desolvation Temperature (°C)	500
Cone Gas Flow (L/Hr)	50
Desolvation Gas Flow (L/Hr)	1000
Collision Energy Ramp (eV)	5-15
Lock spray	Leukine enkephalin
Calibration	Sodium formate

Spectrum

Labeled amino acid



Non labeled amino acid



Arginine-¹³C₆, ¹⁵N₄

Labeled amino acid

	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	185.1		6	15			4	2			
Product ion	122.1		5	10			1	2			
	75.1		4	8			1				
	64.1		1	6			3				

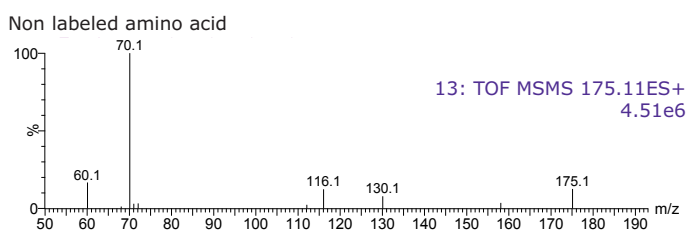
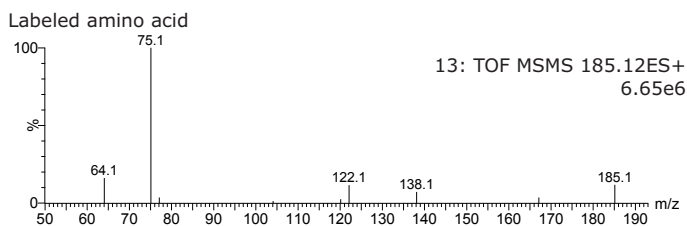
Non labeled amino acid

	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	175.1	6		15		4		2			
Product ion	116.1	5		10		1		2			
	70.1	4		8		1					
	60.1	1		6		3					

Experimental

Instrument	XEVO-G2XSQTOF (waters)
Polarity	Positive
Analyzer	Resolution Mode
Capillary (kV)	2.0
Sampling Cone	40
Source Temperature (°C)	150
Source Offset	80
Desolvation Temperature (°C)	500
Cone Gas Flow (L/Hr)	50
Desolvation Gas Flow (L/Hr)	1000
Collision Energy Ramp (eV)	10-35
Lock spray	Leukine enkephalin
Calibration	Sodium formate

Spectrum



Asparagine-¹⁵N₂

Labeled amino acid

	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	135.1	4		9			2	3			
Product ion	89.1	3		7			2	1			
	75.0	2		4			1	2			

Non labeled amino acid

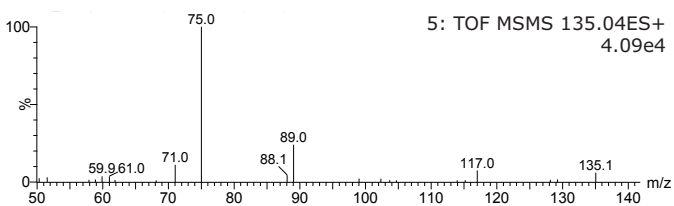
	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	133.1	4		9			2	3			
Product ion	87.1	3		7			2	1			
	74.0	2		4			1	2			

Experimental

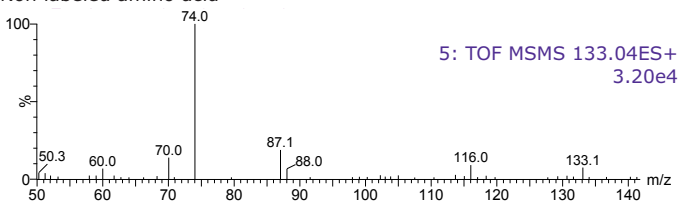
Instrument	XEVO-G2XSQTOF (waters)
Polarity	Positive
Analyzer	Resolution Mode
Capillary (kV)	2.0
Sampling Cone	40
Source Temperature (°C)	150
Source Offset	80
Desolvation Temperature (°C)	500
Cone Gas Flow (L/Hr)	50
Desolvation Gas Flow (L/Hr)	1000
Collision Energy Ramp (eV)	10-35
Lock spray	Leukine enkephalin
Calibration	Sodium formate

Spectrum

Labeled amino acid



Non labeled amino acid



Aspartic acid-¹³C₄, ¹⁵N

Labeled amino acid

	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	139.1		4	8			1	4			
Product ion	92.0		3	6			1	2			
	77.0		2	4			1	2			

Non labeled amino acid

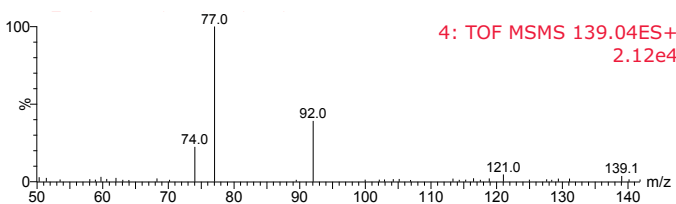
	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	134.0	4		8		1		4			
Product ion	88.0	3		6		1		2			
	74.0	2		4		1		2			

Experimental

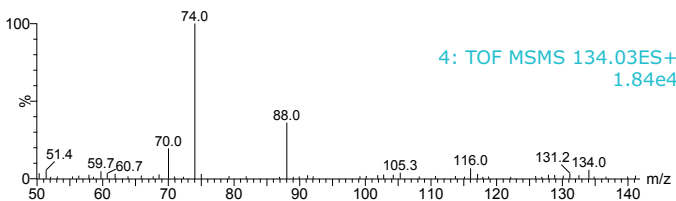
Instrument	XEVO-G2XSQTOF (waters)
Polarity	Positive
Analyzer	Resolution Mode
Capillary (kV)	2.0
Sampling Cone	40
Source Temperature (°C)	150
Source Offset	80
Desolvation Temperature (°C)	500
Cone Gas Flow (L/Hr)	50
Desolvation Gas Flow (L/Hr)	1000
Collision Energy Ramp (eV)	10-35
Lock spray	Leukine enkephalin
Calibration	Sodium formate

Spectrum

Labeled amino acid



Non labeled amino acid



Cystine-d₄

Labeled amino acid

	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	245.1	6		9	4	2		4			2
Product ion	154.0	3		4	2	1		2			2
	122.0	3		4	2	1		2			1

Non labeled amino acid

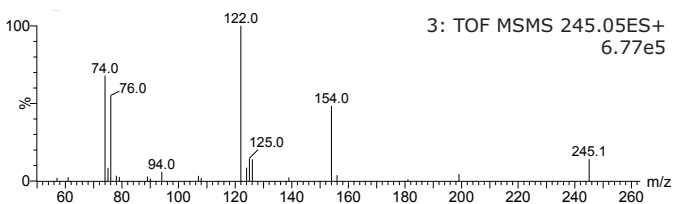
	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	241.0	6		13				4			2
Product ion	152.0	3		6				2			2
	120.0	3		6				2			1

Experimental

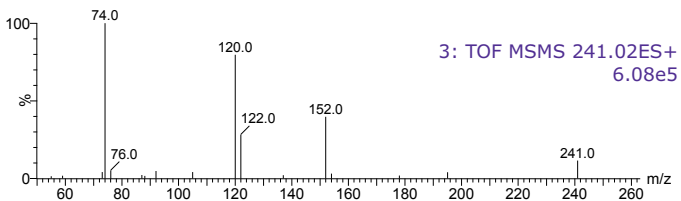
Instrument	XEVO-G2XSQTOF (waters)
Polarity	Positive
Analyzer	Resolution Mode
Capillary (kV)	2.0
Sampling Cone	40
Source Temperature (°C)	150
Source Offset	80
Desolvation Temperature (°C)	500
Cone Gas Flow (L/Hr)	50
Desolvation Gas Flow (L/Hr)	1000
Collision Energy Ramp (eV)	10-35
Lock spray	Leukine enkephalin
Calibration	Sodium formate

Spectrum

Labeled amino acid



Non labeled amino acid



Glutamic acid-¹³C₅,¹⁵N

Labeled amino acid

	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	154.1		5	10			1	4			
Product ion	136.1		5	8			1	3			
	107.1		4	8			1	2			
	89.1		4	6			1	1			

Non labeled amino acid

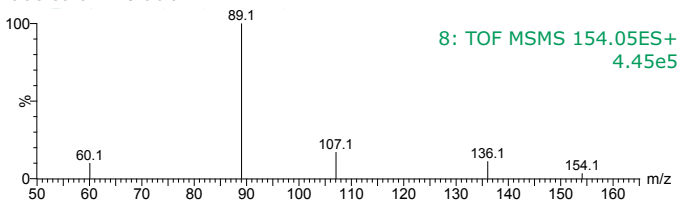
	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	148.1		5	10			1	4			
Product ion	130.1		5	8			1	3			
	102.1		4	8			1	2			
	84.0		4	6			1	1			

Experimental

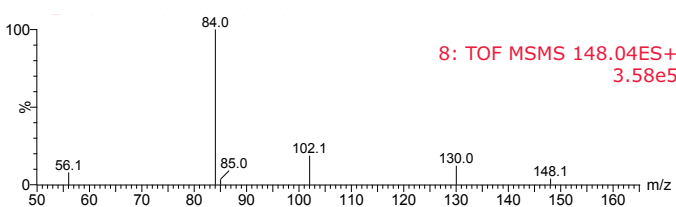
Instrument	XEVO-G2XSQTOF (waters)
Polarity	Positive
Analyzer	Resolution Mode
Capillary (kV)	2.0
Sampling Cone	40
Source Temperature (°C)	150
Source Offset	80
Desolvation Temperature (°C)	500
Cone Gas Flow (L/Hr)	50
Desolvation Gas Flow (L/Hr)	1000
Collision Energy Ramp (eV)	10-25
Lock spray	Leukine enkephalin
Calibration	Sodium formate

Spectrum

Labeled amino acid



Non labeled amino acid



Glutamine-¹⁵N₂

Labeled amino acid

	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	149.1	5		11			2	3			
Product ion	131.0	5		8			1	3			
	85.0	4		6			1	1			

Non labeled amino acid

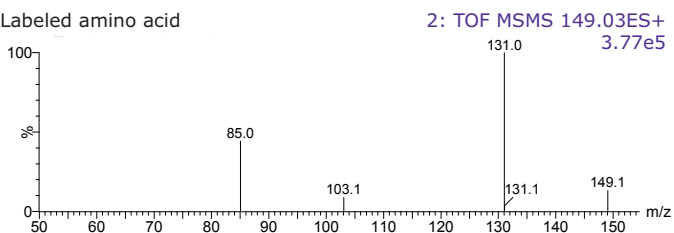
	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	147.1	5		11			2	3			
Product ion	130.1	5		8			1	3			
	84.0	4		6			1	1			

Experimental

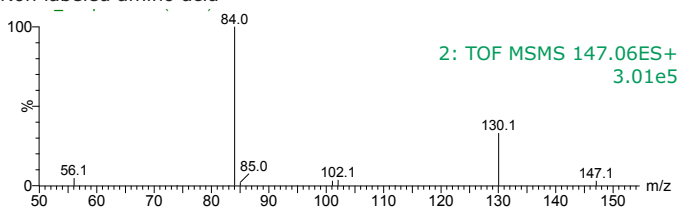
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Polarity	Positive
Analyzer	Resolution Mode
Capillary (kV)	2.0
Sampling Cone	40
Source Temperature (°C)	150
Source Offset	80
Desolvation Temperature (°C)	500
Cone Gas Flow (L/Hr)	50
Desolvation Gas Flow (L/Hr)	1000
Collision Energy Ramp (eV)	10-25
Lock spray	Leukine enkephalin
Calibration	Sodium formate

Spectrum

Labeled amino acid



Non labeled amino acid



Glycine-¹³C₂, ¹⁵N

Labeled amino acid

	m/z	C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	79.0		2	6			1	2			
Product ion											

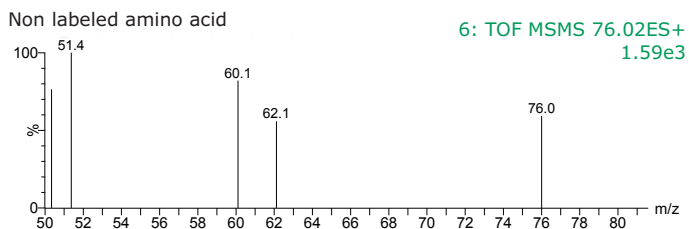
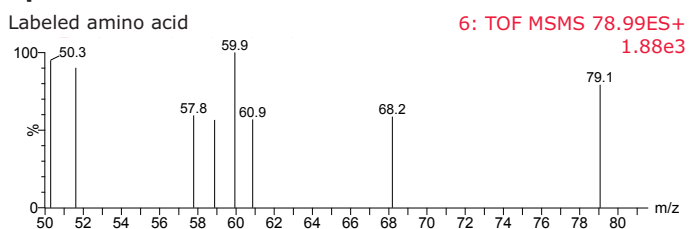
Non labeled amino acid

	m/z	C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	76.0	2		6		1		2			
Product ion											

Experimental

Instrument	XEVO-G2XSQTOF (waters)
Polarity	Positive
Analyzer	Resolution Mode
Capillary (kV)	2.0
Sampling Cone	5
Source Temperature (°C)	150
Source Offset	80
Desolvation Temperature (°C)	500
Cone Gas Flow (L/Hr)	50
Desolvation Gas Flow (L/Hr)	1000
Collision Energy Ramp (eV)	30
Lock spray	Leukine enkephalin
Calibration	Sodium formate

Spectrum



Histidine-¹⁵N₃

Labeled amino acid

	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	159.1	6		10			3	2			
Product ion	113.1	5		8			3				
	85.1	4		7			2				

Non labeled amino acid

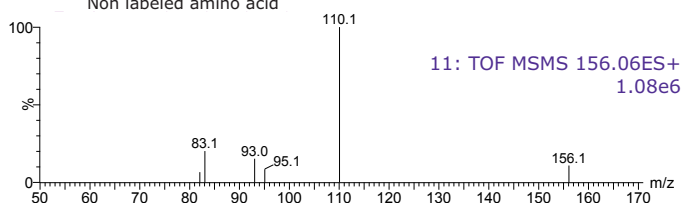
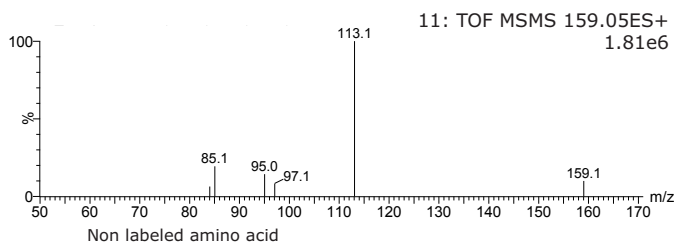
	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	156.1	6		10			3	2			
Product ion	110.1	5		8			3				
	83.1	4		7			2				

Experimental

Instrument	XEVO-G2XSQTOF (waters)
Polarity	Positive
Analyzer	Resolution Mode
Capillary (kV)	2.0
Sampling Cone	40
Source Temperature (°C)	150
Source Offset	80
Desolvation Temperature (°C)	500
Cone Gas Flow (L/Hr)	50
Desolvation Gas Flow (L/Hr)	1000
Collision Energy Ramp (eV)	10-25
Lock spray	Leukine enkephalin
Calibration	Sodium formate

Spectrum

Labeled amino acid



Isoleucine-¹³C₆, ¹⁵N

Labeled amino acid

	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	139.1		6	14			1	2			
Product ion	92.1		5	12			1				

Non labeled amino acid

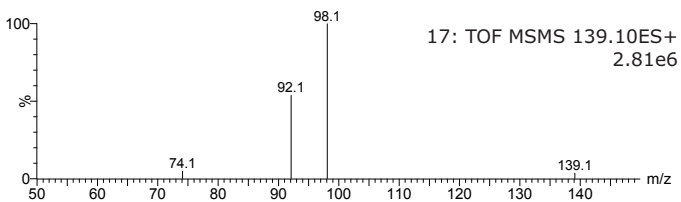
	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	132.1		6	14			1	2			
Product ion	86.1		5	12			1				

Experimental

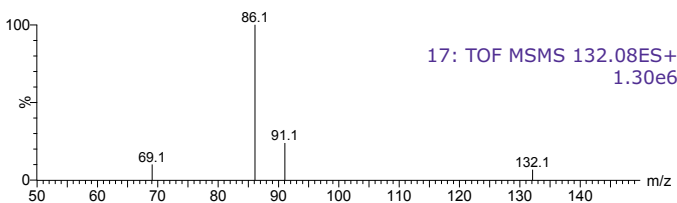
Instrument	XEVO-G2XSQTOF (waters)
Polarity	Positive
Analyzer	Resolution Mode
Capillary (kV)	2.0
Sampling Cone	20
Source Temperature (°C)	150
Source Offset	80
Desolvation Temperature (°C)	500
Cone Gas Flow (L/Hr)	50
Desolvation Gas Flow (L/Hr)	1000
Collision Energy Ramp (eV)	10-15
Lock spray	Leukine enkephalin
Calibration	Sodium formate

Spectrum

Labeled amino acid



Non labeled amino acid



Leucine-¹³C₆

Labeled amino acid

	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	138.1	6	14	1	2						
Product ion	91.1	5	12	1							

Non labeled amino acid

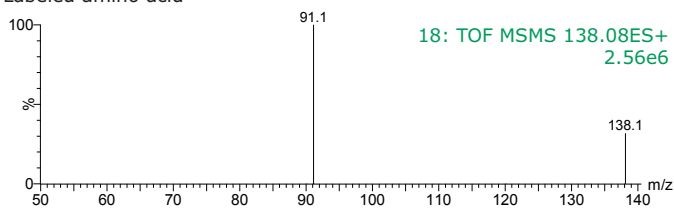
	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	132.1	6	14	1	2						
Product ion	86.1	5	12	1							

Experimental

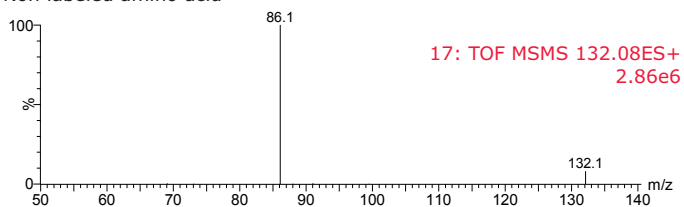
Instrument	XEVO-G2XSQTOF (waters)
Polarity	Positive
Analyzer	Resolution Mode
Capillary (kV)	2.0
Sampling Cone	20
Source Temperature (°C)	150
Source Offset	80
Desolvation Temperature (°C)	500
Cone Gas Flow (L/Hr)	50
Desolvation Gas Flow (L/Hr)	1000
Collision Energy Ramp (eV)	10-15
Lock spray	Leukine enkephalin
Calibration	Sodium formate

Spectrum

Labeled amino acid



Non labeled amino acid



Lysine-¹³C₆, ¹⁵N₂

Labeled amino acid

	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	155.1		6	15			2	2			
Product ion	137.1		6	12			1	2			
	90.1		5	10			1				

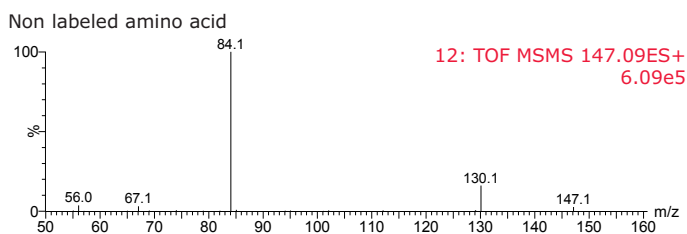
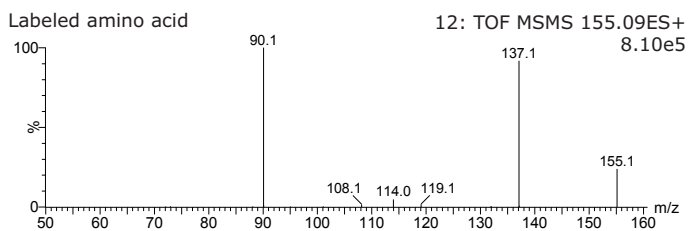
Non labeled amino acid

	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	147.1		6	15			2	2			
Product ion	130.1		6	12			1	2			
	84.1		5	10			1				

Experimental

Instrument	XEVO-G2XSQTOF (waters)
Polarity	Positive
Analyzer	Resolution Mode
Capillary (kV)	2.0
Sampling Cone	40
Source Temperature (°C)	150
Source Offset	80
Desolvation Temperature (°C)	500
Cone Gas Flow (L/Hr)	50
Desolvation Gas Flow (L/Hr)	1000
Collision Energy Ramp (eV)	10-25
Lock spray	Leukine enkephalin
Calibration	Sodium formate

Spectrum



Methionine-¹³C₅, ¹⁵N

Labeled amino acid

	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	156.1		5	12			1	2			1
Product ion	138.0		5	9				2			1
	109.1		4	10			1				1
	60.1		3	6			1				

Non labeled amino acid

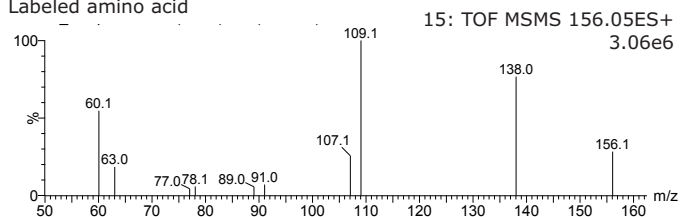
	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	150.1	5		12		1		2			1
Product ion	133.0	5		9				2			1
	104.1	4		10		1					1
	56.1	3		6		1					

Experimental

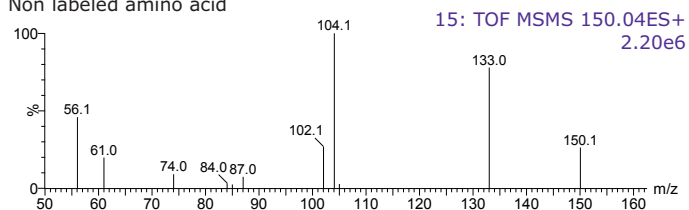
Instrument	XEVO-G2XSQTOF (waters)
Polarity	Positive
Analyzer	Resolution Mode
Capillary (kV)	2.0
Sampling Cone	20
Source Temperature (°C)	150
Source Offset	80
Desolvation Temperature (°C)	500
Cone Gas Flow (L/Hr)	50
Desolvation Gas Flow (L/Hr)	1000
Collision Energy Ramp (eV)	10-15
Lock spray	Leukine enkephalin
Calibration	Sodium formate

Spectrum

Labeled amino acid



Non labeled amino acid



Phenylalanine-¹³C₉, ¹⁵N

Labeled amino acid

	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	176.1		9	12			1	2			
Product ion	129.1		8	10			1				
	111.1		8	7							

Non labeled amino acid

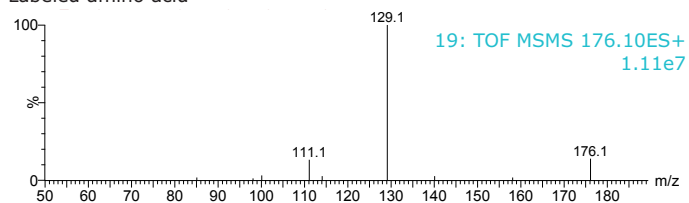
	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	166.1		9	12			1	2			
Product ion	120.1		8	10			1				
	103.1		8	7							

Experimental

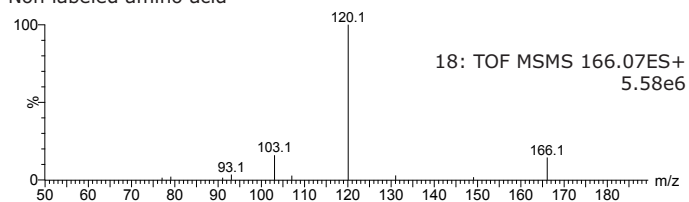
Instrument	XEVO-G2XSQTOF (waters)
Polarity	Positive
Analyzer	Resolution Mode
Capillary (kV)	2.0
Sampling Cone	40
Source Temperature (°C)	150
Source Offset	80
Desolvation Temperature (°C)	500
Cone Gas Flow (L/Hr)	50
Desolvation Gas Flow (L/Hr)	1000
Collision Energy Ramp (eV)	5-25
Lock spray	Leukine enkephalin
Calibration	Sodium formate

Spectrum

Labeled amino acid



Non labeled amino acid



Proline-¹³C₅, ¹⁵N

Labeled amino acid

	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	122.1		5	10			1	2			
Product ion	75.1		4	8			1				

Non labeled amino acid

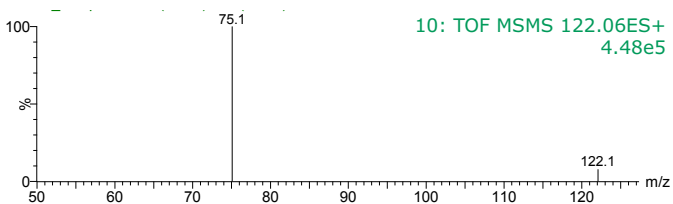
	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	116.1	5		10		1		2			
Product ion	70.1	4		8		1					

Experimental

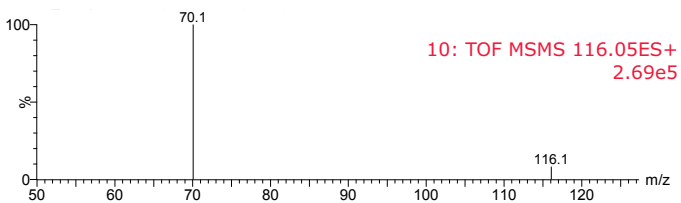
Instrument	XEVO-G2XSQTOF (waters)
Polarity	Positive
Analyzer	Resolution Mode
Capillary (kV)	2.0
Sampling Cone	40
Source Temperature (°C)	150
Source Offset	80
Desolvation Temperature (°C)	500
Cone Gas Flow (L/Hr)	50
Desolvation Gas Flow (L/Hr)	1000
Collision Energy Ramp (eV)	10-35
Lock spray	Leukine enkephalin
Calibration	Sodium formate

Spectrum

Labeled amino acid



Non labeled amino acid



Serine-¹³C₃, ¹⁵N

Labeled amino acid

	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	110.1		3	8			1	3			
Product ion	92.0		3	6			1	2			
	63.0		2	6			1	1			

Non labeled amino acid

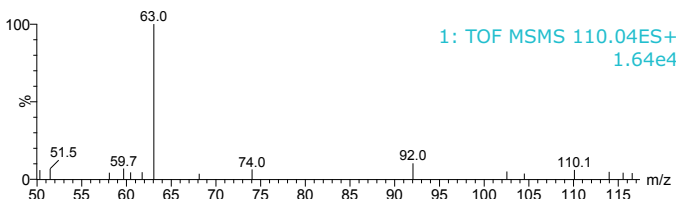
	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	106.0		3	8			1	3			
Product ion	88.0		3	6			1	2			
	60.0		2	6			1	1			

Experimental

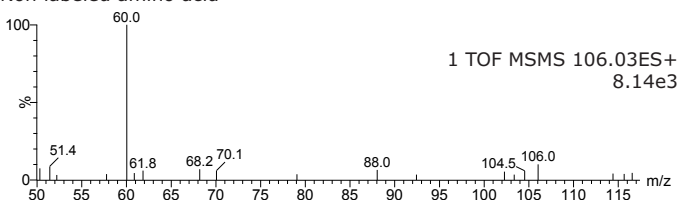
Instrument	XEVO-G2XSQTOF (waters)
Polarity	Positive
Analyzer	Resolution Mode
Capillary (kV)	2.0
Sampling Cone	40
Source Temperature (°C)	150
Source Offset	80
Desolvation Temperature (°C)	500
Cone Gas Flow (L/Hr)	50
Desolvation Gas Flow (L/Hr)	1000
Collision Energy Ramp (eV)	10-25
Lock spray	Leukine enkephalin
Calibration	Sodium formate

Spectrum

Labeled amino acid



Non labeled amino acid



Threonine-¹³C₄, ¹⁵N

Labeled amino acid

	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	125.1		4	10			1	3			
Product ion	107.1		4	8			1	2			
	78.1		3	8			1	1			
	60.1		3	6			1				

Non labeled amino acid

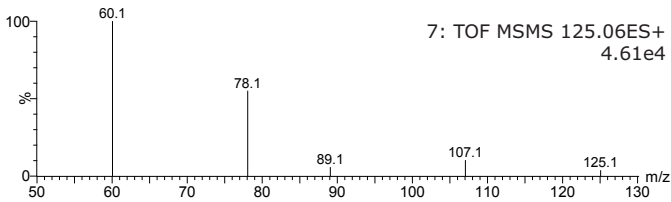
	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	120.1	4		10		1		3			
Product ion	102.1	4		8		1		2			
	74.1	3		8		1		1			
	56.1	3		6		1					

Experimental

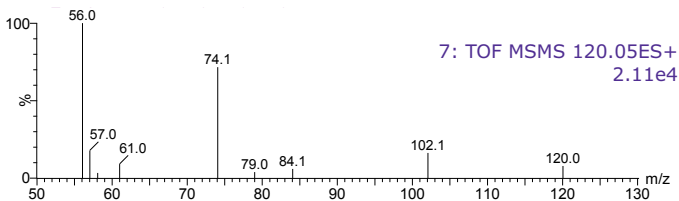
Instrument	XEVO-G2XSQTOF (waters)
Polarity	Positive
Analyzer	Resolution Mode
Capillary (kV)	2.0
Sampling Cone	40
Source Temperature (°C)	150
Source Offset	80
Desolvation Temperature (°C)	500
Cone Gas Flow (L/Hr)	50
Desolvation Gas Flow (L/Hr)	1000
Collision Energy Ramp (eV)	10-35
Lock spray	Leukine enkephalin
Calibration	Sodium formate

Spectrum

Labeled amino acid



Non labeled amino acid



Tryptophan-¹⁵N₂

Labeled amino acid

	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	207.1	11		13			2	2			
Product ion	189.1	11		10			1	2			
	147.1	9		8			1	1			

Non labeled amino acid

	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	205.1	11		13			2	2			
Product ion	188.1	11		10			1	2			
	146.1	9		8			1	1			

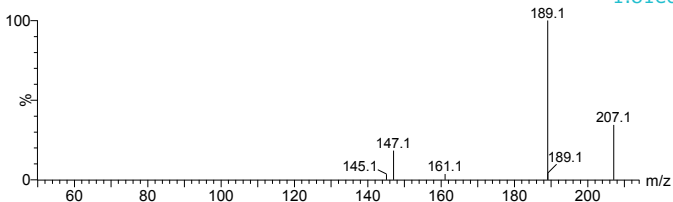
Experimental

Instrument	XEVO-G2XSQTOF (waters)
Polarity	Positive
Analyzer	Resolution Mode
Capillary (kV)	2.0
Sampling Cone	40
Source Temperature (°C)	150
Source Offset	80
Desolvation Temperature (°C)	500
Cone Gas Flow (L/Hr)	50
Desolvation Gas Flow (L/Hr)	1000
Collision Energy Ramp (eV)	5-15
Lock spray	Leukine enkephalin
Calibration	Sodium formate

Spectrum

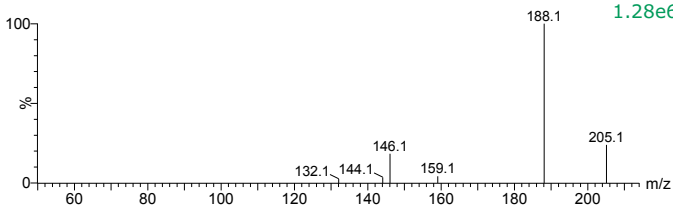
Labeled amino acid

20: TOF MSMS 207.05ES+
1.81e6



Non labeled amino acid

19: TOF MSMS 205.09ES+
1.28e6



Tyrosine-¹³C₉, ¹⁵N

Labeled amino acid

	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	192.1		9	12			1	3			
Product ion	174.1		9	9				3			
	130.1		7	7				2			
	98.1		7	7							

Non labeled amino acid

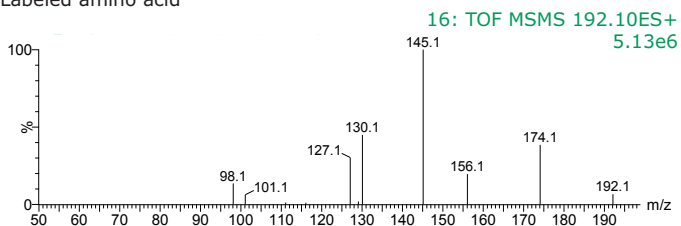
	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	182.1	9		12		1		3			
Product ion	165.1	9		9				3			
	123.0	7		7				2			
	91.1	7		7							

Experimental

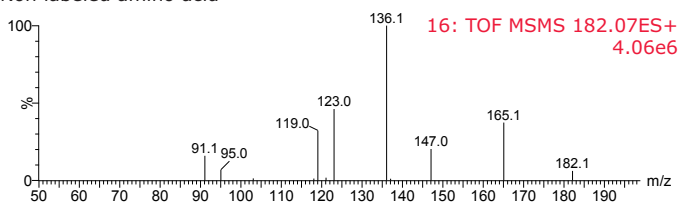
Instrument	XEVO-G2XSQTOF (waters)
Polarity	Positive
Analyzer	Resolution Mode
Capillary (kV)	2.0
Sampling Cone	40
Source Temperature (°C)	150
Source Offset	80
Desolvation Temperature (°C)	500
Cone Gas Flow (L/Hr)	50
Desolvation Gas Flow (L/Hr)	1000
Collision Energy Ramp (eV)	10-20
Lock spray	Leukine enkephalin
Calibration	Sodium formate

Spectrum

Labeled amino acid



Non labeled amino acid



Valine-¹³C₅,¹⁵N

Labeled amino acid

	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	124.1	5	12				1	2			
Product ion	77.1	4	10				1				
	59.1	4	7								

Non labeled amino acid

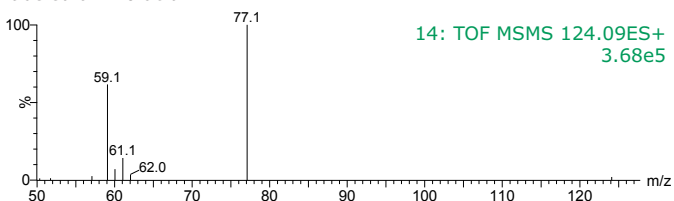
	m/z	Formula									
		C	¹³ C	H	D	N	¹⁵ N	O	¹⁸ O	P	S
Precursor ion	118.1	5		12		1		2			
Product ion	72.1	4		10		1					
	55.1	4		7							

Experimental

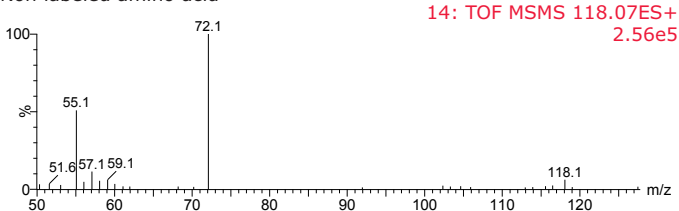
Instrument	XEVO-G2XSQTOF (waters)
Polarity	Positive
Analyzer	Resolution Mode
Capillary (kV)	2.0
Sampling Cone	40
Source Temperature (°C)	150
Source Offset	80
Desolvation Temperature (°C)	500
Cone Gas Flow (L/Hr)	50
Desolvation Gas Flow (L/Hr)	1000
Collision Energy Ramp (eV)	10-35
Lock spray	Leukine enkephalin
Calibration	Sodium formate

Spectrum

Labeled amino acid



Non labeled amino acid



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