

Acq. Data Name: PetterThorsen_030521_seq 1-6_ESI+_DI

Internal Sample Id:

Ionization Mode: ESI+

MS Calibration Name: PEG_ESI+_2000

Reduction History: Determine m/z[Peak Detect[Centroid,50,Area];Correct Base[5.0%]];Average(MS[1] 4.429..4.489)-1.0*Average(MS[1] 4.175..4.306);Correct Base[5.0%]

Experiment Date/Time: 5/3/2021 13:07:25

Orifice1 Volt Sweep: 23V

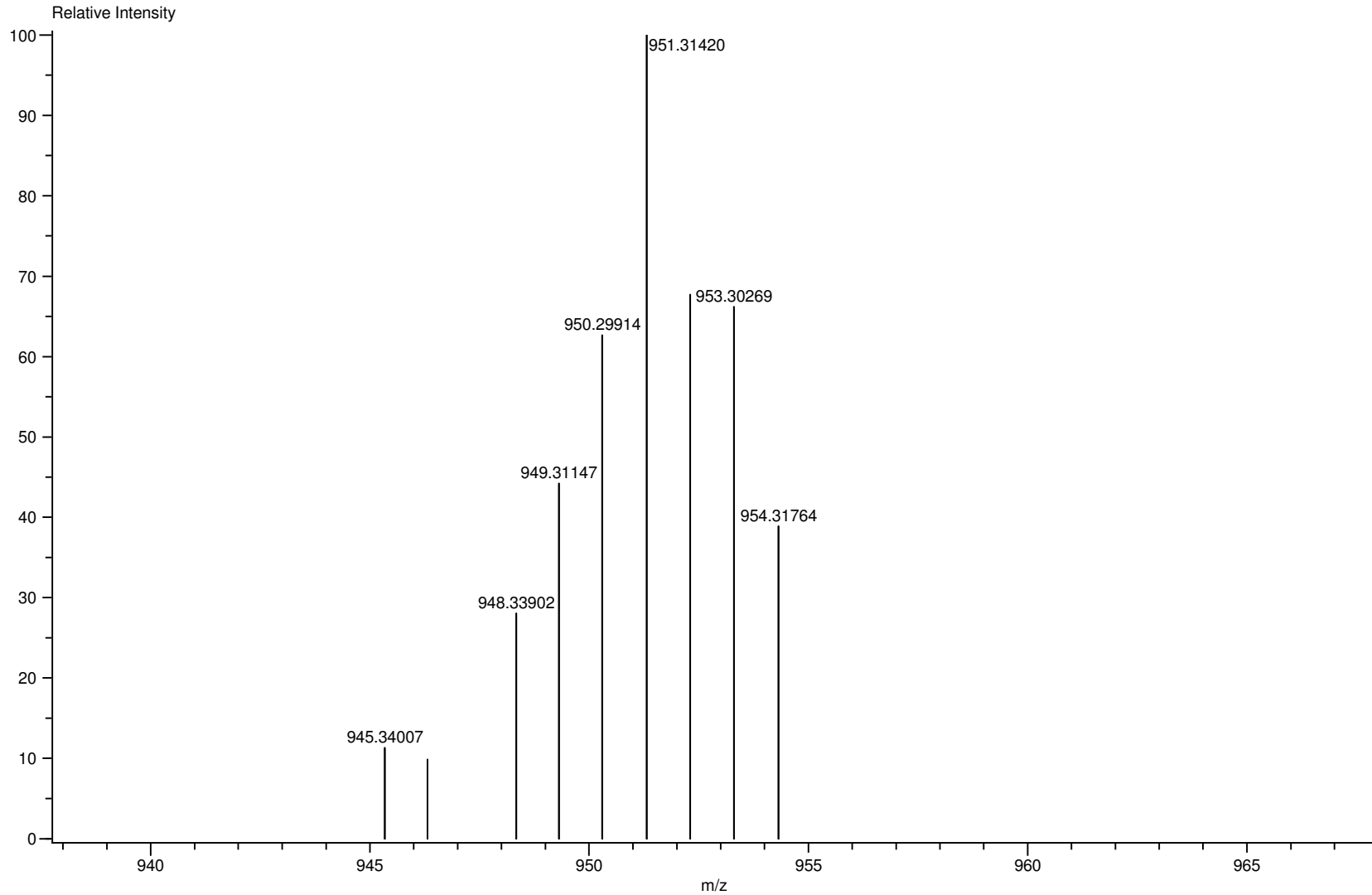
Acquired m/z Range: 30.0..2000.0

Spec. Record Interval: 0.6[s]

Ring Lens Volt: 11[V]

Time of Maximum: 4.449[min]

Operator Name: Accutof



Data:PetterThorsen_030521_seq 1-6_ESI+_DI

Sample Name:

Description:

Ionization Mode:ESI+

History:Determine m/z[Peak Detect[Centroid,50,Area];Correct Base[5.0%]];Average(MS[1] 4.429..4.489)-1.0*Avera...

Acquired:5/3/2021 13:07:25

Operator:Accutof

Mass Calibration data:PEG_ESI+_2000

Created:11/22/2021 9:20:05

Created by:Accutof

Charge number:1

Tolerance:5.00(mmu)

Unsaturation Number:-1.5 .. 40.0 (Fraction:Both)

Element:¹²C:57 .. 57, ¹H:0 .. 200, ¹⁴N:0 .. 4, ¹⁶O:0 .. 10, ⁹⁶Ru:0 .. 1, ⁹⁸Ru:0 .. 1, ⁹⁹Ru:0 .. 1, ¹⁰⁰Ru:0 .. 1, ¹⁰¹Ru:0 .. 1, ¹⁰²Ru:0 .. 1, ¹⁰⁴Ru:0 .. 1, ³²S:0 .. 1

Mass	Intensity	Calc. Mass	Mass Difference (ppm)	Possible Formula	¹² C	¹ H	¹⁴ N	¹⁶ O	⁹⁶ Ru	⁹⁸ Ru	⁹⁹ Ru	¹⁰⁰ Ru	
951.31420	162701.11	951.31459	-0.41	¹² C ₅₇ ¹ H ₅₈ ¹⁴ N ₁ ¹⁶ O ₄ ⁹⁹ Ru ₁ ³² S ₁	57	58	1	4			1		
		951.31334	0.91	¹² C ₅₇ ¹ H ₅₇ ¹⁴ N ₂ ¹⁶ O ₃ ¹⁰² Ru ₁ ³² S ₁	57	57	2	3					
		951.31571	-1.59	¹² C ₅₇ ¹ H ₅₇ ¹⁶ O ₇ ⁹⁸ Ru ₁	57	57		7		1			
		951.31592	-1.81	¹² C ₅₇ ¹ H ₅₉ ¹⁶ O ₅ ⁹⁶ Ru ₁ ³² S ₁	57	59		5	1				
		951.31217	2.13	¹² C ₅₇ ¹ H ₆₄ ⁹⁹ Ru ₁ ¹⁰⁴ Ru ₁	57	64						1	
		951.31634	-2.25	¹² C ₅₇ ¹ H ₅₆ ¹⁴ N ₁ ¹⁶ O ₆ ¹⁰¹ Ru ₁	57	56	1	6					
		951.31653	-2.45	¹² C ₅₇ ¹ H ₅₅ ¹⁴ N ₂ ¹⁶ O ₅ ¹⁰⁴ Ru ₁	57	55	2	5					
		951.31719	-3.15	¹² C ₅₇ ¹ H ₆₅ ¹⁰⁰ Ru ₁ ¹⁰² Ru ₁	57	65							1
		951.31073	3.65	¹² C ₅₇ ¹ H ₆₄ ¹⁰¹ Ru ₁ ¹⁰² Ru ₁	57	64							
951.31895	-4.99	¹² C ₅₇ ¹ H ₄₉ ¹⁴ N ₃ ¹⁶ O ₉ ³² S ₁	57	49	3	9							

¹⁰¹ Ru	¹⁰² Ru	¹⁰⁴ Ru	³² S	Unsaturation Number
			1	31.0
	1		1	32.0
				30.0
			1	30.0
		1		27.0
1				31.0
		1		32.0
	1			26.5
1	1			27.0
			1	36.0