

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%]];Smooth[3];Average(MS[1] 8.708..8.725)-1.0*Average(MS[1] 8.449..8.513);Correct Base[5....

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

Orifice1 Volt Sweep: 23V

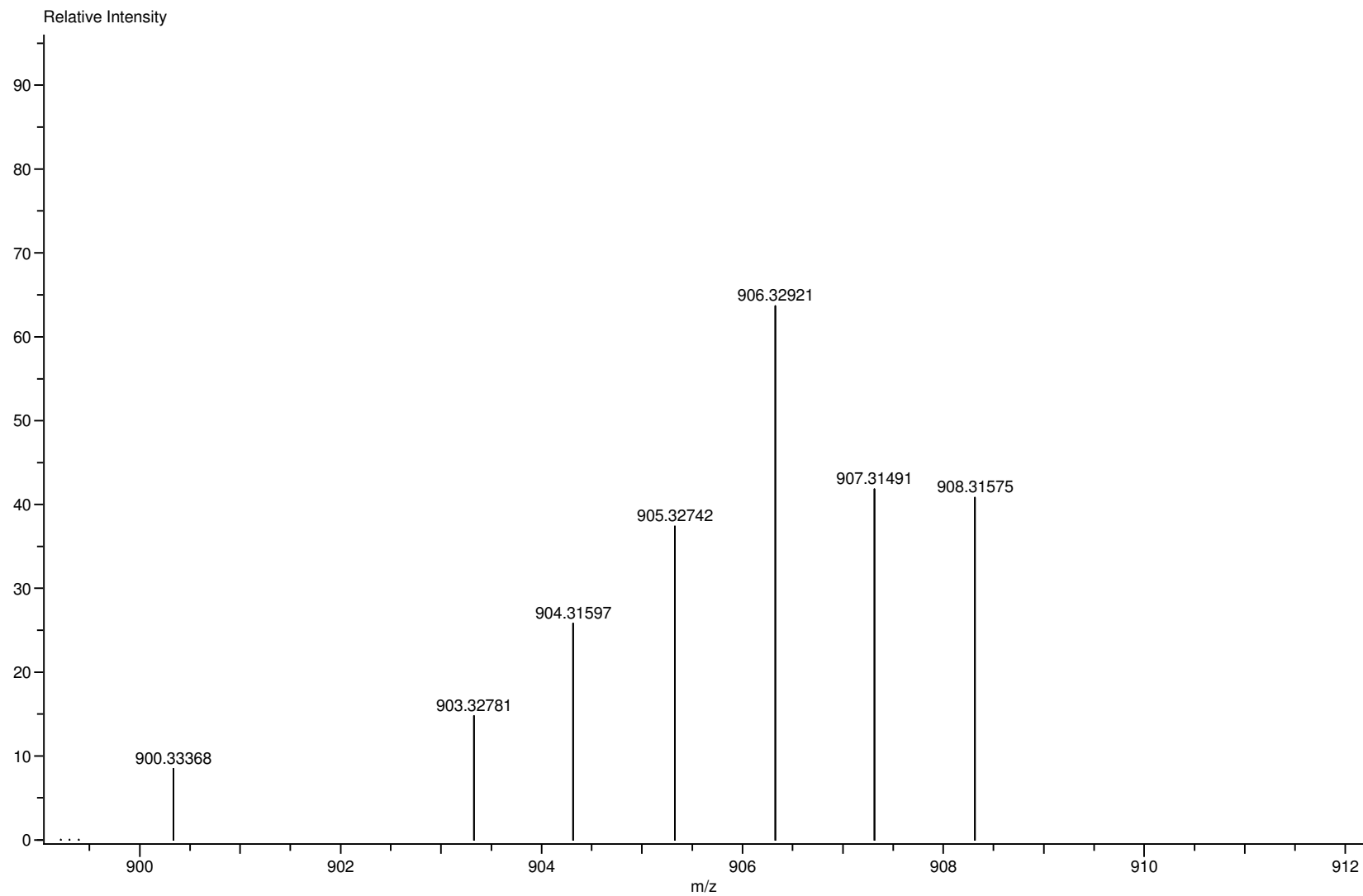
Acquired m/z Range: 30.0..2000.0

Spec. Record Interval: 0.6[s]

Ring Lens Volt: 11[V]

Time of Maximum: 8.714[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%]];Smooth[3];Average(MS[1] 8.708..8.725)...

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

Operator:Accutof

Mass Calibration data:PEG_ESI+_2000

Created:11/22/2021 9:32:09

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 .. 10, 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	¹⁰¹ Ru
906.32921	148513.44	906.32951	-0.34	¹² C ₅₇ ¹ H ₅₉ ¹⁶ O ₂ ⁹⁹ Ru ₁ ³² S ₁	57	59		2			1		
		906.32826	1.05	¹² C ₅₇ ¹ H ₅₈ ¹⁴ N ₁ ¹⁶ O ₁ ¹⁰² Ru ₁ ³² S ₁	57	58	1	1					
		906.32782	1.53	¹² C ₅₇ ¹ H ₄₈ ¹⁴ N ₁ ¹⁶ O ₁₀	57	48	1	10					
		906.33126	-2.27	¹² C ₅₇ ¹ H ₅₇ ¹⁶ O ₄ ¹⁰¹ Ru ₁	57	57		4					1
		906.33145	-2.47	¹² C ₅₇ ¹ H ₅₆ ¹⁴ N ₁ ¹⁶ O ₃ ¹⁰⁴ Ru ₁	57	56	1	3					
		906.32649	3.00	¹² C ₅₇ ¹ H ₅₂ ¹⁴ N ₅ ¹⁰⁰ Ru ₁	57	52	5						1
906.33387		906.33387	-5.14	¹² C ₅₇ ¹ H ₅₀ ¹⁴ N ₂ ¹⁶ O ₇ ³² S ₁	57	50	2	7					

¹⁰² Ru	¹⁰⁴ Ru	³² S	Unsaturation Number
		1	30.0
1		1	31.0
			34.5
			30.0
	1		31.0
			35.0
		1	35.0