

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%];Correct Base[5.0%];Average(MS[1] 2.060..2.660)

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

Orifice1 Volt Sweep: 23V

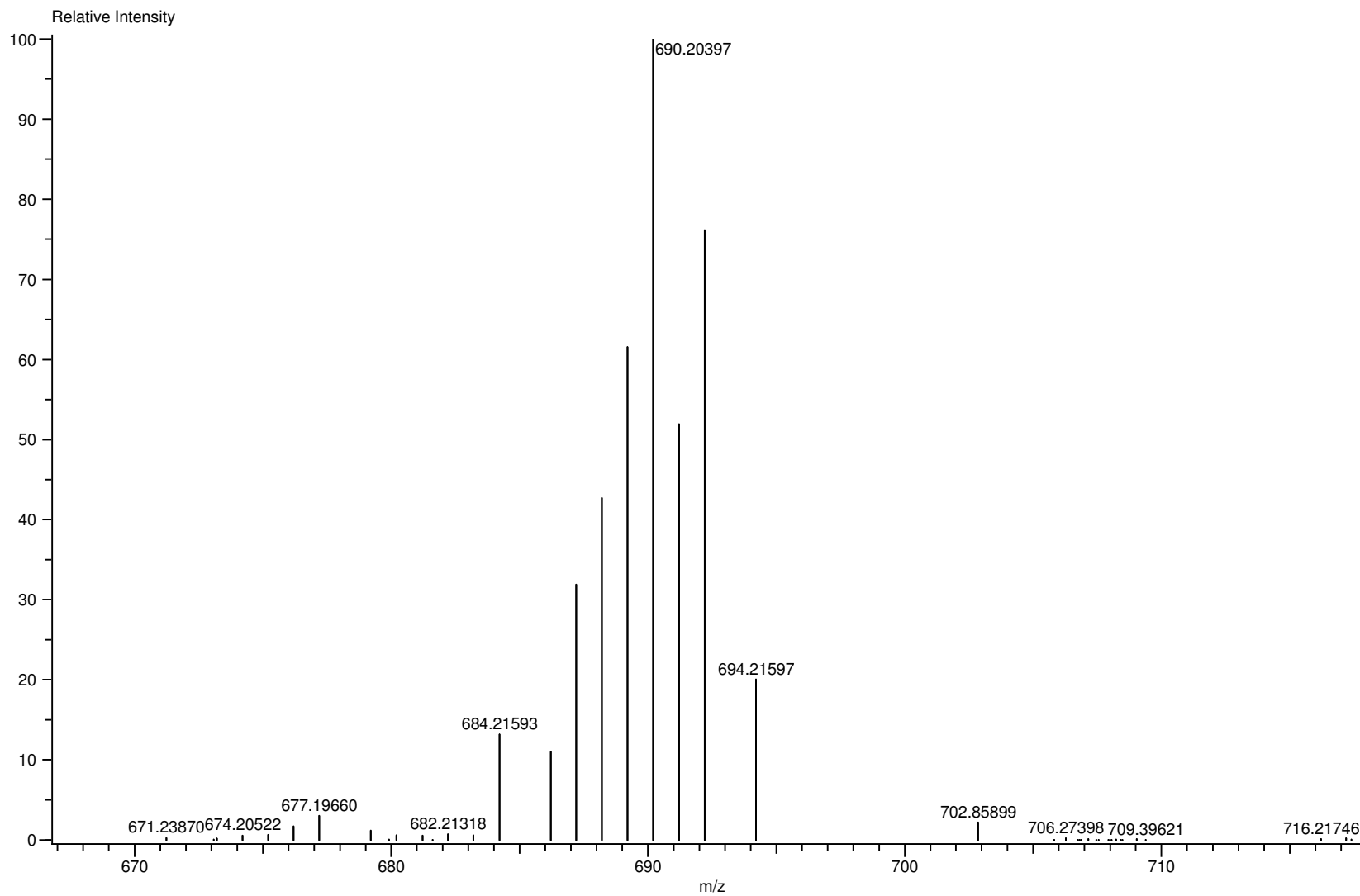
Acquired m/z Range: 30.0..2000.0

Spec. Record Interval: 0.6[s]

Ring Lens Volt: 11[V]

Time of Maximum: 2.321[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%]];Correct Base[5.0%];Average(MS[1] 2.0...

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

Operator:Accutof

Mass Calibration data:PEG_ESI+_2000

Created:11/22/2021 9:12:24

Created by:Accutof

Charge number:1

Tolerance:5.00(mmu)

Unsaturation Number:-1.5 .. 20.0 (Fraction:Both)

Element:¹²C:35 .. 35, ¹H:0 .. 200, ³⁵Cl:0 .. 1, ³⁷Cl:0 .. 1, ¹⁴N:0 .. 4, ¹⁶O:0 .. 4, ⁹⁶Ru:0 .. 1, ⁹⁸Ru:0 .. 1, ⁹⁹Ru:0 .. 1, ¹⁰⁰Ru:0 .. 1, ¹⁰¹Ru:0 .. 1, ¹⁰²Ru:0 .. 1, ¹⁰⁴Ru:0 .. 1

Mass	Intensity	Calc. Mass	Mass Difference (ppm)	Possible Formula	¹² C	¹ H	³⁵ Cl	³⁷ Cl	¹⁴ N	¹⁶ O	⁹⁶ Ru	⁹⁸ Ru	
690.20397	112431.83	690.20392	0.07	¹² C ₃₅ ¹ H ₅₁ ¹⁶ O ₁ ¹⁰¹ Ru ₁ ¹⁰² Ru ₁	35	51				1			
		690.20410	-0.20	¹² C ₃₅ ¹ H ₅₀ ¹⁴ N ₁ ¹⁰² Ru ₁ ¹⁰⁴ Ru ₁	35	50			1				
		690.20364	0.47	¹² C ₃₅ ¹ H ₄₃ ³⁵ Cl ₁ ¹⁴ N ₃ ¹⁶ O ₃ ¹⁰² Ru ₁	35	43	1		3	3			
		690.20490	-1.35	¹² C ₃₅ ¹ H ₄₄ ³⁵ Cl ₁ ¹⁴ N ₂ ¹⁶ O ₄ ⁹⁹ Ru ₁	35	44	1		2	4			
		690.20536	-2.02	¹² C ₃₅ ¹ H ₅₁ ¹⁶ O ₁ ⁹⁹ Ru ₁ ¹⁰⁴ Ru ₁	35	51					1		
		690.20056	4.93	¹² C ₃₅ ¹ H ₄₃ ³⁷ Cl ₁ ¹⁴ N ₃ ¹⁶ O ₃ ¹⁰⁰ Ru ₁	35	43		1	3	3			
		690.19945	6.55	¹² C ₃₅ ¹ H ₄₈ ³⁵ Cl ₁ ³⁷ Cl ₁ ¹⁶ O ₃ ¹⁰² Ru ₁	35	48	1	1			3		
		690.20851	-6.58	¹² C ₃₅ ¹ H ₄₃ ³⁵ Cl ₁ ³⁷ Cl ₁ ¹⁶ O ₃ ¹⁰¹ Ru ₁	35	49	1	1			3		
		690.20869	-6.84	¹² C ₃₅ ¹ H ₄₈ ³⁵ Cl ₁ ³⁷ Cl ₁ ¹⁴ N ₁ ¹⁶ O ₂ ¹⁰⁴ Ru ₁	35	48	1	1	1	2			
		690.20885	-7.08	¹² C ₃₅ ¹ H ₄₃ ³⁷ Cl ₁ ¹⁴ N ₄ ¹⁶ O ₂ ¹⁰² Ru ₁	35	43		1	4	2			

⁹⁹ Ru	¹⁰⁰ Ru	¹⁰¹ Ru	¹⁰² Ru	¹⁰⁴ Ru	Unsaturation Number
		1	1		11.5
			1	1	12.5
			1		16.0
1					15.0
1				1	11.5
	1				16.0
			1		11.5
		1			11.0
				1	12.0
			1		16.5