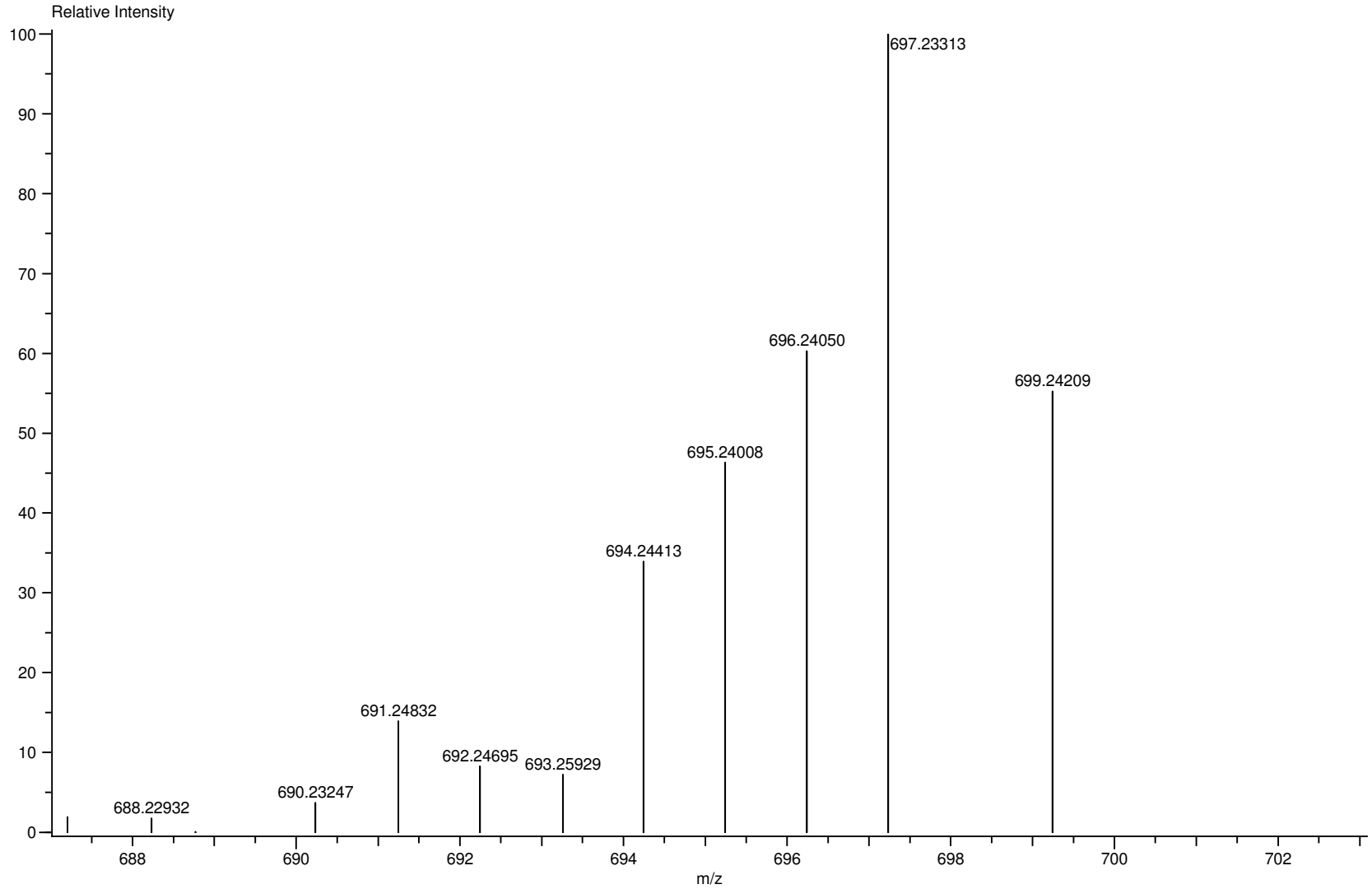
Acq. Data Name: PetterThorsen_030521_seq 1-6_ESi+_DI
Internal Sample Id:
Ionization Mode: ESI+
MS Calibration Name: PEG_ESI+_2000
Orifice1 Volt Sweep: 23V
Acquired m/z Range: 30.0..2000.0
Spec. Record Interval: 0.6[s]
Ring Lens Volt: 11[V]
Time of Maximum: 0.233[min]
Reduction History: Determine m/z[Peak Detect[Centroid,50,Area];Correct Base[5.0%]];Average(MS[1] 0.207..0.303)-1.0*Average(MS[1] 0.122..0.133);Correct Base[5.0%]
Experiment Date/Time: 5/3/2021 13:07:25
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] 0.207..0.303)-1.0*Avera...

Acquired:5/3/2021 13:07:25
Operator:Accutof
Mass Calibration data:PEG_ESI+_2000
Created:11/22/2021 9:53:18
Created by:Accutof

Charge number:1 Tolerance:5.00(mmu) Unsaturation Number:-1.5 .. 20.0 (Fraction:Both)
Element:^{12}C:35 .. 36, ^{1}H:0 .. 200, ^{14}N:0 .. 4, ^{16}O:0 .. 4, ^{96}Ru:0 .. 1, ^{98}Ru:0 .. 1, ^{99}Ru:0 .. 1, ^{100}Ru:0 .. 1, ^{101}Ru:0 .. 1, ^{102}Ru:0 .. 1, ^{104}Ru: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
697.23313	78010.10	697.23278	0.51	$^{12}C_{36}{}^{1}H_{43}{}^{14}N_{4}{}^{16}O_{4}{}^{102}Ru_{1}$	36	43	4	4					
		697.23270	0.63	$^{12}C_{35}{}^{1}H_{53}{}^{14}N_{2}{}^{96}Ru_{1}{}^{100}Ru_{1}$	35	53	2		1			1	
		697.23507	-2.77	$^{12}C_{35}{}^{1}H_{55}{}^{16}O_{1}{}^{102}Ru_{1}{}^{104}Ru_{1}$	35	55		1					
		697.23101	3.05	$^{12}C_{36}{}^{1}H_{54}{}^{16}O_{1}{}^{96}Ru_{1}{}^{99}Ru_{1}$	36	54		1	1		1		
		697.22975	4.85	$^{12}C_{36}{}^{1}H_{53}{}^{14}N_{1}{}^{96}Ru_{1}{}^{102}Ru_{1}$	36	53	1		1				
		697.23685	-5.33	$^{12}C_{36}{}^{1}H_{54}{}^{14}N_{1}{}^{98}Ru_{1}{}^{99}Ru_{1}$	36	54	1			1	1		

^{102}Ru	^{104}Ru	Unsaturation Number
1		18.0
		11.5
1	1	9.5
		11.0
1		12.0
		11.5