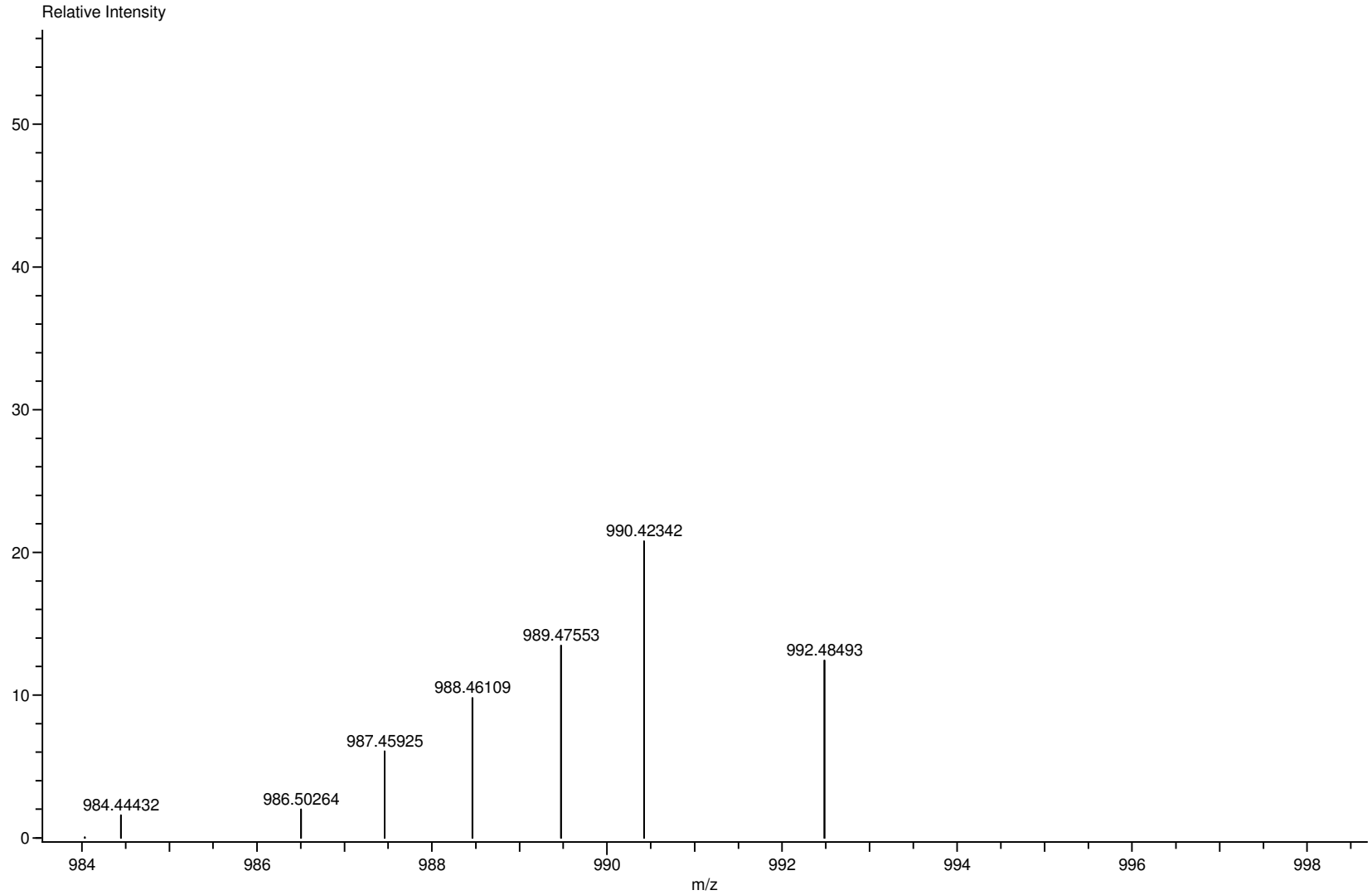
Acq. Data Name: PetterThorsen_030521_seq 1-6_ESi+_DI
Internal Sample Id:
Ionization Mode: ESI+
MS Calibration Name: PEG_ESI+_2000
Orifice1 Volt Sweep: 23V
Acquired m/z Range: 30.0..2000.0
Spec. Record Interval: 0.6[s]
Ring Lens Volt: 11[V]
Time of Maximum: 6.586[min]
Reduction History: Determine m/z[Peak Detect[Centroid,50,Area];Correct Base[5.0%]];Correct Base[5.0%];Average(MS[1] 6.578..6.593)
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%]];Correct Base[5.0%];Average(MS[1] 6.5...

Acquired:5/3/2021 13:07:25
Operator:Accutof
Mass Calibration data:PEG_ESI+_2000
Created:11/22/2021 9:26:54
Created by:Accutof

Charge number:1 Tolerance:5.00(mmu) Unsaturation Number:-1.5 .. 40.0 (Fraction:Both)
Element:^{12}C:63 .. 63, ^{1}H:0 .. 200, ^{14}N:0 .. 10, ^{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, ^{32}S: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
990.42342	65617.00	990.42341	0.00	$^{12}C_{63}{}^{1}H_{71}{}^{16}O_{2}{}^{99}Ru_{1}{}^{32}S_{1}$	63	71		2			1		
		990.42216	1.27	$^{12}C_{63}{}^{1}H_{70}{}^{14}N_{1}{}^{16}O_{1}{}^{102}Ru_{1}{}^{32}S_{1}$	63	70	1	1					
		990.42516	-1.77	$^{12}C_{63}{}^{1}H_{69}{}^{16}O_{4}{}^{101}Ru_{1}$	63	69		4					1
		990.42535	-1.95	$^{12}C_{63}{}^{1}H_{68}{}^{14}N_{1}{}^{16}O_{3}{}^{104}Ru_{1}$	63	68	1	3					
		990.42039	3.06	$^{12}C_{63}{}^{1}H_{64}{}^{14}N_{5}{}^{100}Ru_{1}$	63	64	5					1	

^{102}Ru	^{104}Ru	^{32}S	Unsaturation Number
		1	30.0
1		1	31.0
			30.0
	1		31.0
			35.0