

<b>Name:</b>	<b>Secorapamycin</b>
<b>Lot#:</b>	GR-19-173
<b>Test Date:</b>	08/19/2024 (re-test date: 08/19/2026)
<b>CAS No.:</b>	147438-27-5; 148554-65-8 (Na salt)
<b>MF:</b>	C <sub>51</sub> H <sub>79</sub> NO <sub>13</sub>
<b>MW:</b>	914.20
<b>Appearance:</b>	White solid
<b>Purity:</b>	93.1% by HPLC
<b><sup>1</sup>H-NMR:</b>	Conforms
<b>MS-ESI (+)</b>	Conforms (shows peaks at m/z = 931.59 [M+NH <sub>4</sub> ] <sup>+</sup> , 936.55 [M+Na] <sup>+</sup> )
<b>Storage</b>	Store at -20°C in a dry place away from direct sunlight under nitrogen

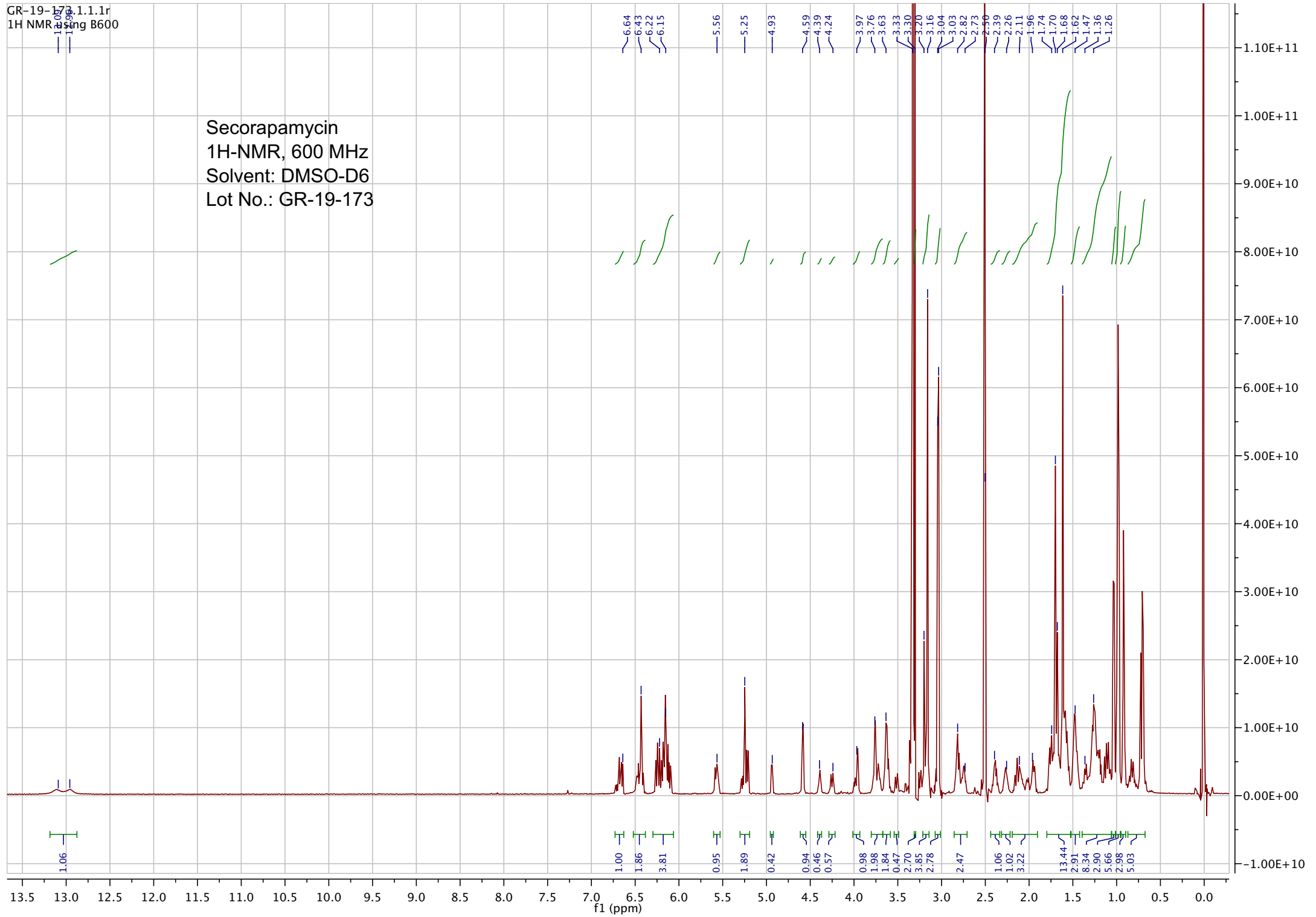
Approved by:

Date: 08/20/2024

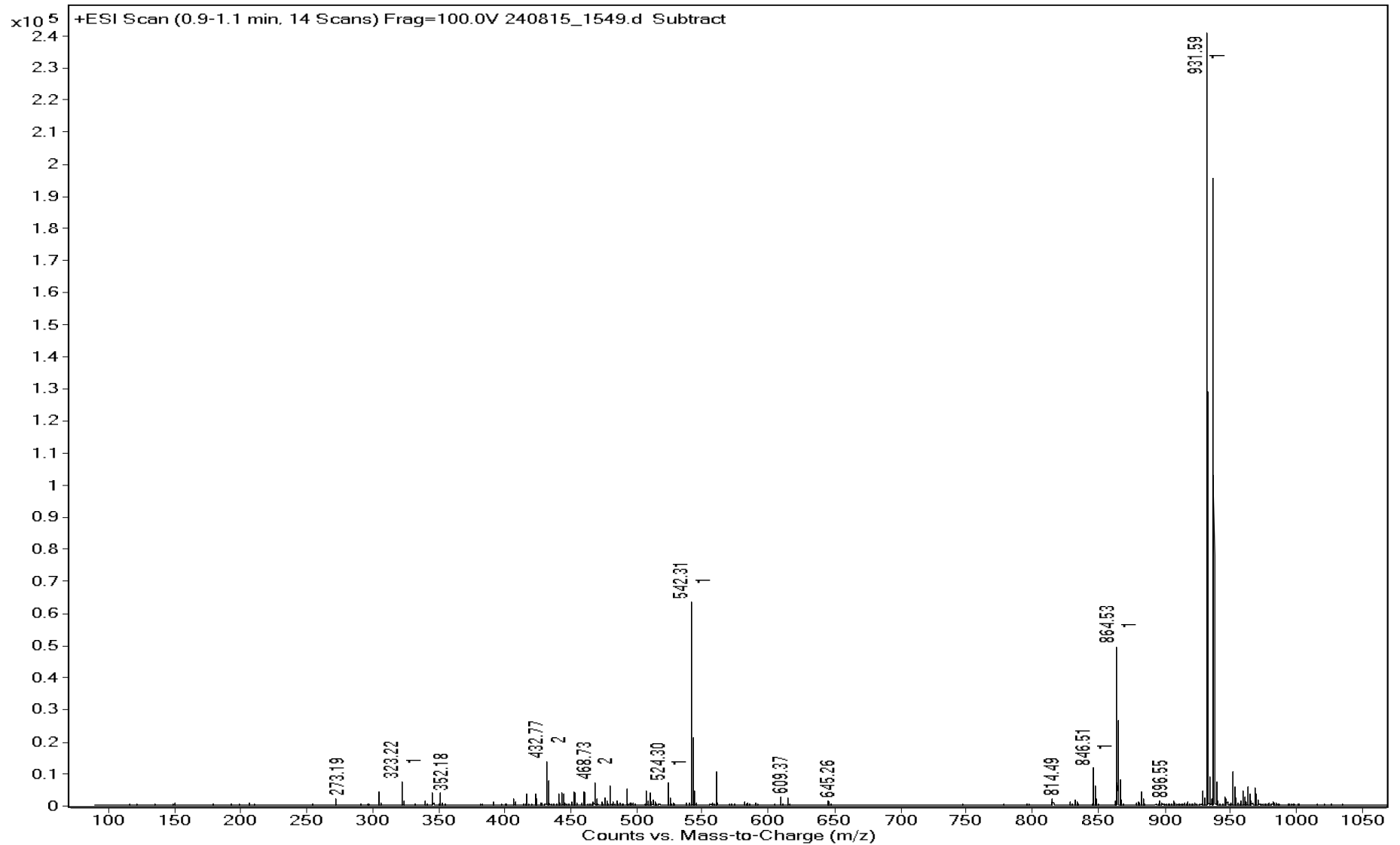
Viorica Rusu, QC/QA Manager

GR-19-173.1.1.1r  
1H NMR using B600

Secorapamycin  
1H-NMR, 600 MHz  
Solvent: DMSO-D6  
Lot No.: GR-19-173



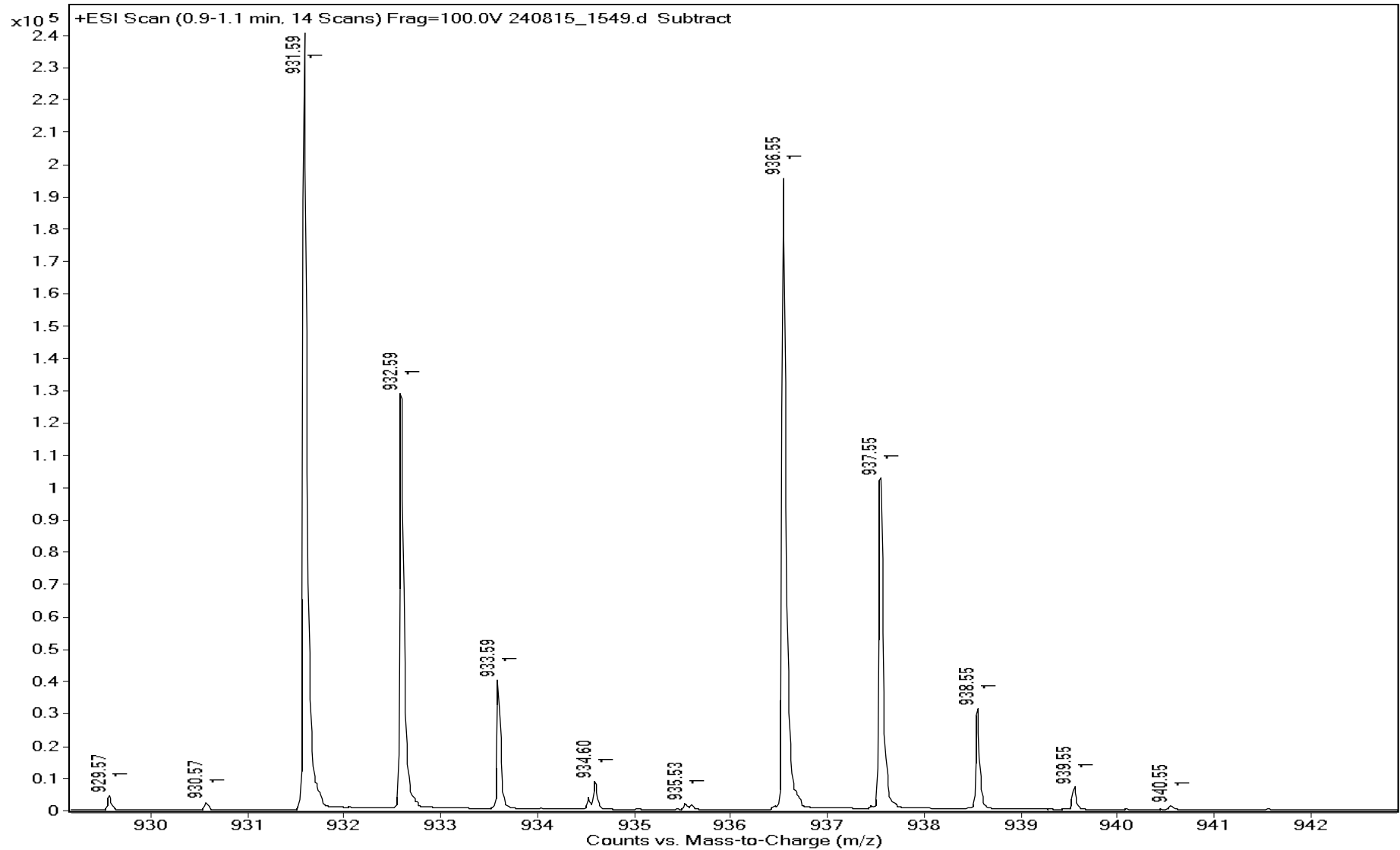
<b>Sample Name</b>	GR-19-173	<b>Data File</b>	240815_1549.d	<b>Acq Method</b>	HRMS.m
<b>DA Method</b>	AIMS_Accurate_Mass.m	<b>Instrument</b>	Agilent 6538 UHD	<b>Acq Date, Time</b>	15/08/2024 11:18:25 AM
<b>Comment</b>	ESI+				



**Sample Name** GR-19-173  
**DA Method** AIMS\_Accurate\_Mass.m  
**Comment** ESI+

**Data File** 240815\_1549.d  
**Instrument** Agilent 6538 UHD

**Acq Method** HRMS.m  
**Acq Date, Time** 15/08/2024 11:18:25 AM



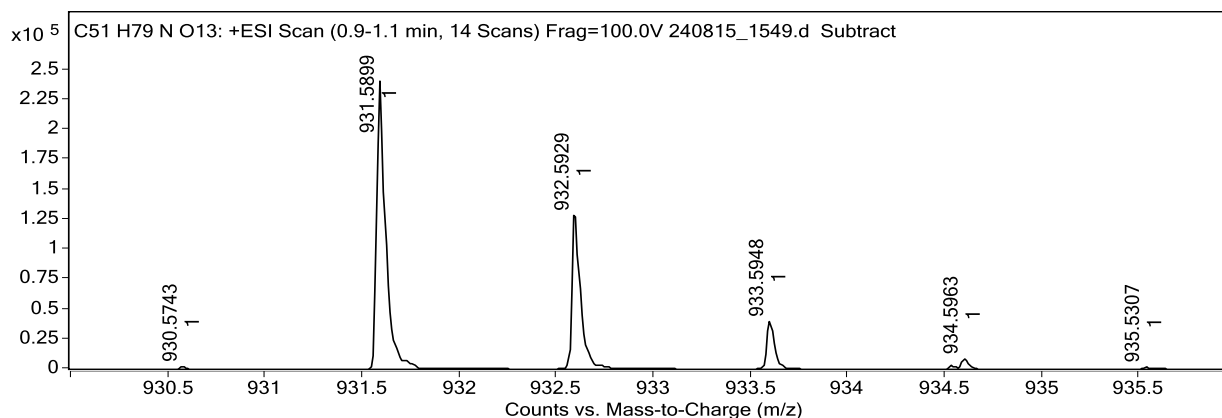
<b>Sample Name</b>	GR-19-173	<b>Data File</b>	240815_1549.d
<b>Acq Method</b>	HRMS.m	<b>DA Method</b>	AIMS_Accurate_Mass.m
<b>Instrument</b>	Agilent 6538 UHD	<b>Acq Date, Time</b>	15/08/2024 11:18:25 AM
<b>Comment</b>	ESI+		

### Target Ion Species

Ion Species	m/z	Ionic Formula
(M+NH4) <sup>+</sup>	931.5899	C51 H83 N2 O13

### MFG Calculator Results

Target m/z	Ionic Formula	Calc m/z	+/- (mDa)	+/- (ppm)	DBE	MFG Score
931.5899	C51 H83 N2 O13	931.5890	0.9	1.0	13.0	98.59
931.5899	C52 H79 N6 O9	931.5903	-0.4	-0.4	18.0	98.54
931.5899	C53 H75 N10 O5	931.5916	-1.7	-1.8	23.0	95.03
931.5899	C39 H87 N4 O20	931.5908	-0.9	-1.0	0.0	90.94
931.5899	C40 H83 N8 O16	931.5922	-2.3	-2.5	5.0	90.13
931.5899	C47 H79 N8 O11	931.5863	3.6	3.9	14.0	89.67
931.5899	C64 H75 N4 O2	931.5885	1.4	1.5	31.0	89.64
931.5899	C46 H83 N4 O15	931.5849	5.0	5.4	9.0	81.77
931.5899	C60 H71 N10	931.5858	4.1	4.4	32.0	80.76
931.5899	C57 H79 N4 O7	931.5943	-4.4	-4.7	22.0	79.98



### Predicted Isotope Match Table

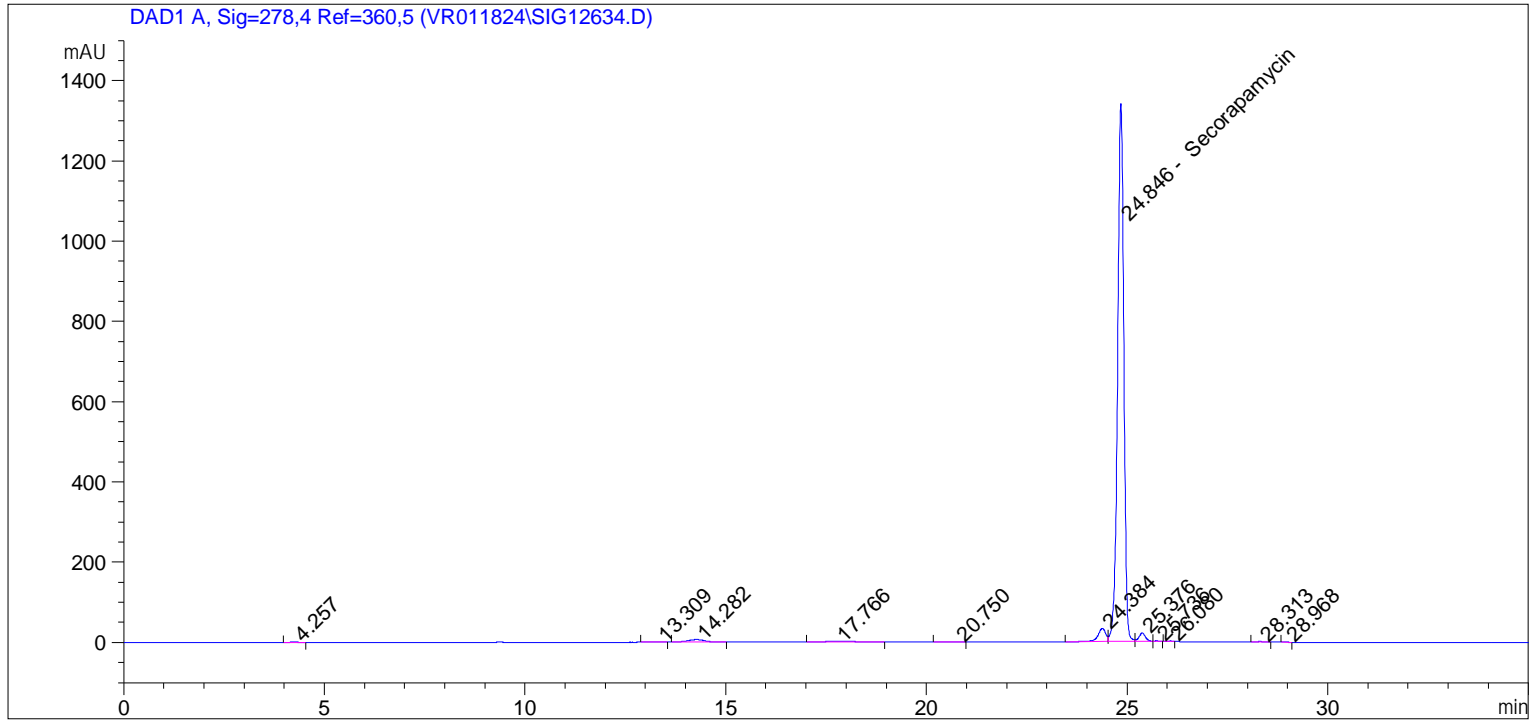
Isotope	m/z	Calc m/z	Diff (mDa)	Abund (%)	Calc Abund (%)	+/-
1	931.5899	931.5890	0.9	100.0	100.0	0.0
2	932.5929	932.5923	0.6	56.4	57.3	0.9
3	933.5948	933.5953	-0.5	16.7	18.8	2.1
4	934.5963	934.5981	-1.8	3.7	4.5	0.8

Sample Name: GR-19-173

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Acq. Operator   : vrusu
Acq. Instrument : Instrument 1
Injection Date  : 8/19/2024 3:45:56 PM
Location       : Vial 29
Inj Volume     : 10.0 µl
Acq. Method    : C:\CHEM32\1\METHODS\VR081924_173.M
Last changed   : 8/19/2024 3:44:49 PM by vrusu
Analysis Method: C:\CHEM32\1\METHODS\VR081924_173PM.M
Last changed   : 8/19/2024 5:06:21 PM by vrusu
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                          Area Percent Report
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Sorted By           :      Signal
Calib. Data Modified :      8/19/2024 5:04:55 PM
Multiplier          :      1.603e3
Dilution            :      1.0000
Use Multiplier & Dilution Factor with ISTDs

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Signal 1: DAD1 A, Sig=278,4 Ref=360,5

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	4.257	BB	0.1509	8.65267	0.0558	?
2	13.309	BB	0.2622	11.48524	0.0741	?
3	14.282	BB	0.3926	189.42458	1.2221	?
4	17.766	BB	0.6194	115.83710	0.7474	?
5	20.750	BB	0.3863	15.13999	0.0977	?
6	24.384	BV	0.2060	460.93024	2.9738	?
7	24.846	VV	0.1675	1.44276e4	93.0831	Secorapamycin
8	25.376	VB	0.1652	229.61497	1.4814	?
9	25.736	BB	0.1075	8.05809	0.0520	?
10	26.080	BB	0.1211	11.19458	0.0722	?
11	28.313	BB	0.1292	17.22145	0.1111	?

Sample Name: GR-19-173

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
12	28.968	BB	0.1061	4.53548	0.0293	?

Totals : 1.54997e4

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\*\*\* End of Report \*\*\*