

**Name:** Sonidegib-D4  
**Lot#:** GR-17-131  
**Test Date:** 04/14/2022 (re-test date: 04/14/2027)  
**CAS No.:** 956697-53-3 (unlabelled)  
**MF:** C<sub>26</sub>H<sub>22</sub>D<sub>4</sub>F<sub>3</sub>N<sub>3</sub>O<sub>3</sub>  
**MW:** 489.52  
**Appearance:** Light Purple Solid  
**Purity:** 97.4% by HPLC (average of two sample preparations); 99% atom D  
**<sup>1</sup>H-NMR:** Conforms (contains a trace of TMU)  
**MS-ESI (+)** Conforms (shows peak at m/z = 490.23 [M+H]<sup>+</sup>)  
**Storage** Store at -18°C in a dry place away from direct sunlight

Approved by:

Date: 04/21/2022



Viorica Rusu, QC/QA Manager

GR-17-131-CDCl3

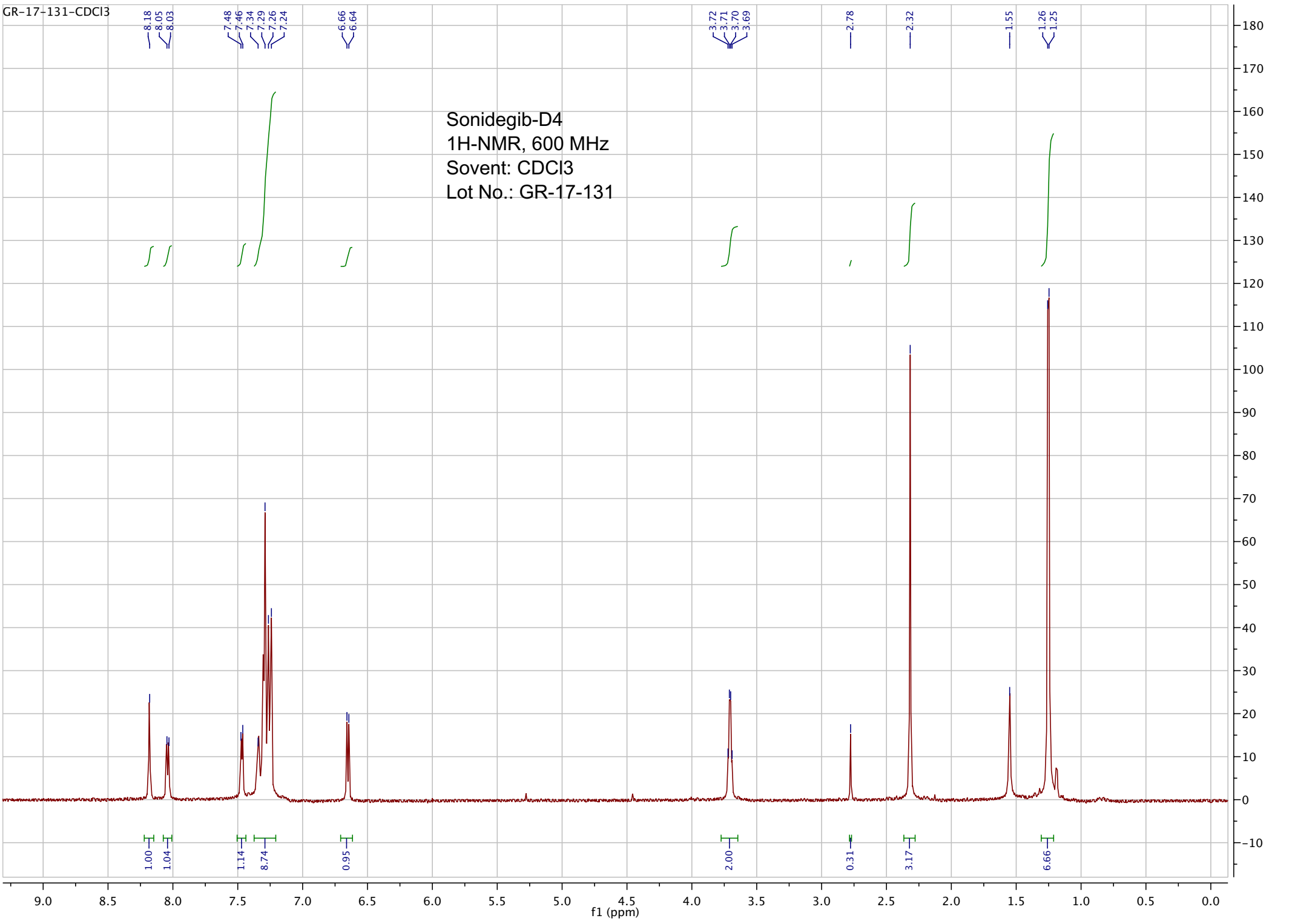
8.18  
8.05  
8.03  
7.48  
7.46  
7.34  
7.29  
7.26  
7.24  
6.66  
6.64

3.72  
3.71  
3.70  
3.69  
2.78  
2.32  
1.55  
1.26  
1.25

Sonidegib-D4  
1H-NMR, 600 MHz  
Solvent: CDCl3  
Lot No.: GR-17-131

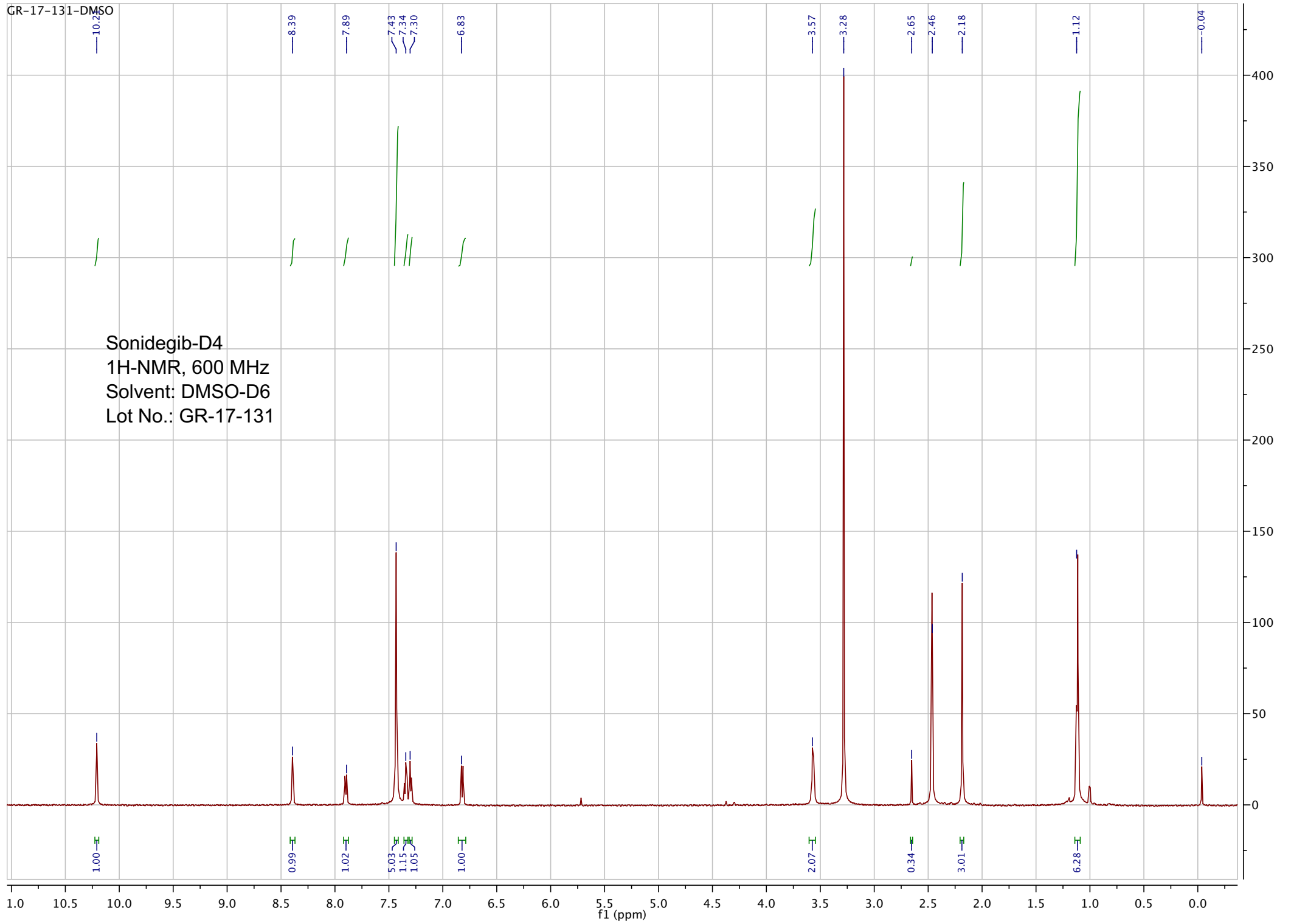
1.00  
1.04  
1.14  
8.74  
0.95

2.00  
0.31  
3.17  
6.66



GR-17-131-DMSO

Sonidegib-D4  
1H-NMR, 600 MHz  
Solvent: DMSO-D6  
Lot No.: GR-17-131

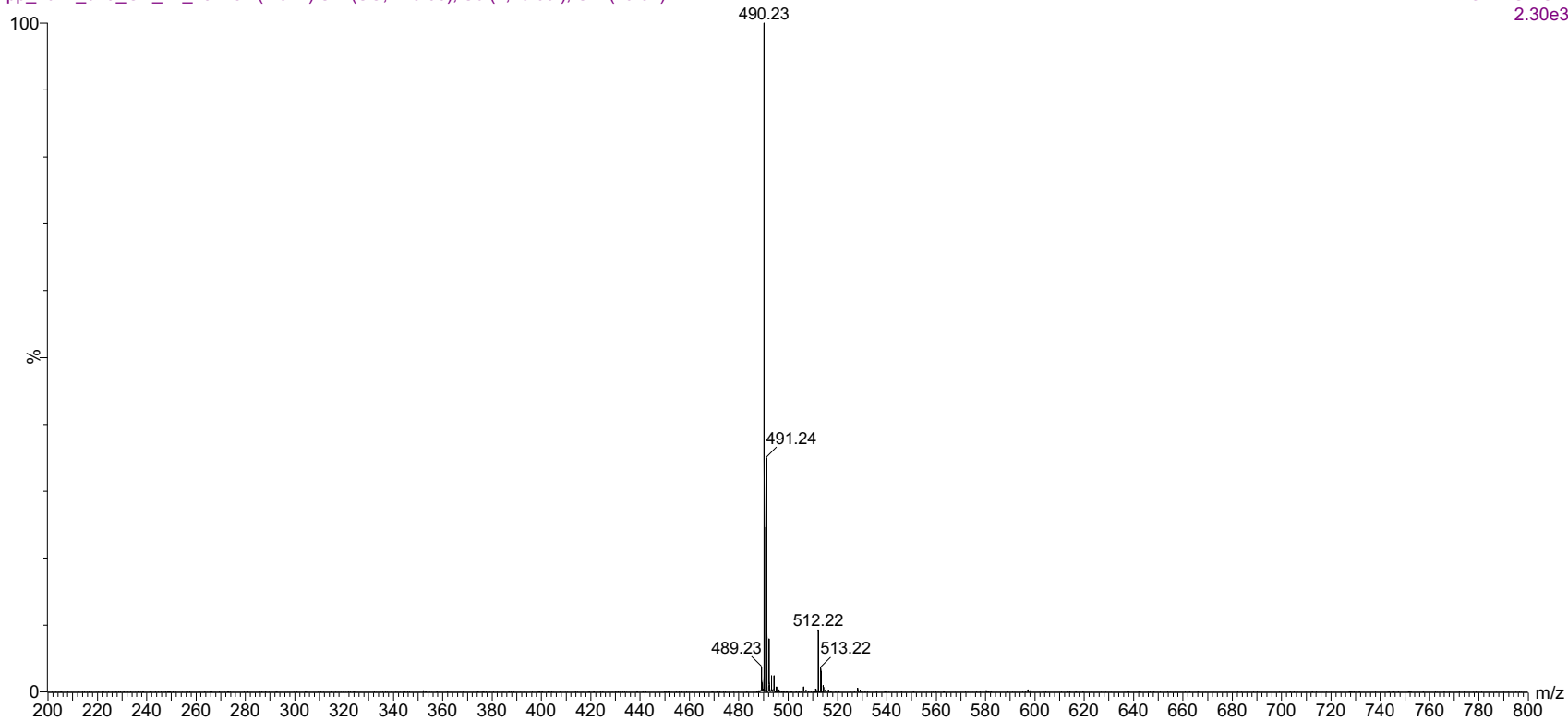


pp\_2022\_029\_GR\_17\_131 82 (1.571) Sm (SG, 2x5.00); Sb (2,10.00 ); Cm (79:84)

8.00000000

21-Apr-2022, 14:34:47

TOF MS ES+  
2.30e3



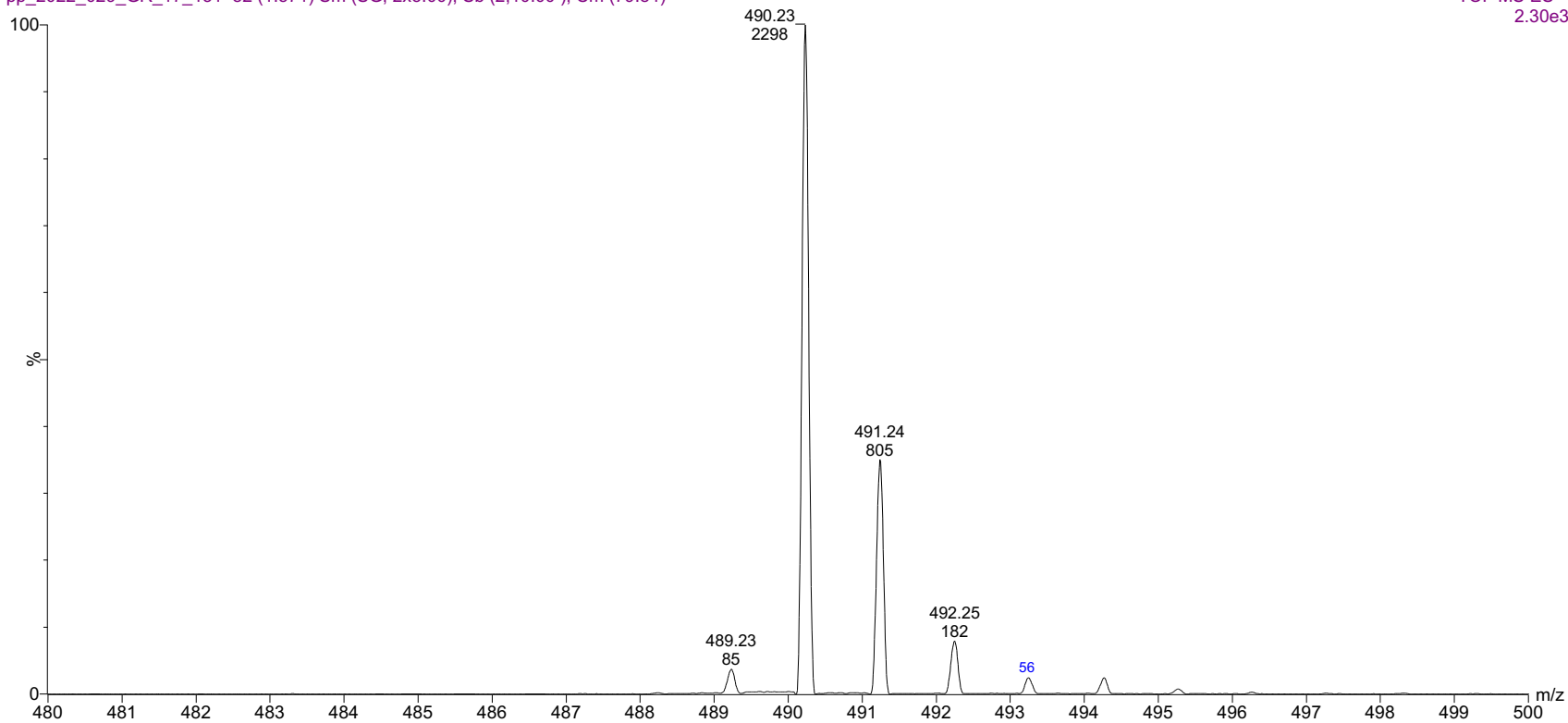
Raw ESI-MS spectrum for sample GR-17-131. Shows monoisotopic [M+H]<sup>+</sup> mass.

pp\_2022\_029\_GR\_17\_131 82 (1.571) Sm (SG, 2x5.00); Sb (2,10.00 ); Cm (79:84)

8.00000000

21-Apr-2022, 14:34:47

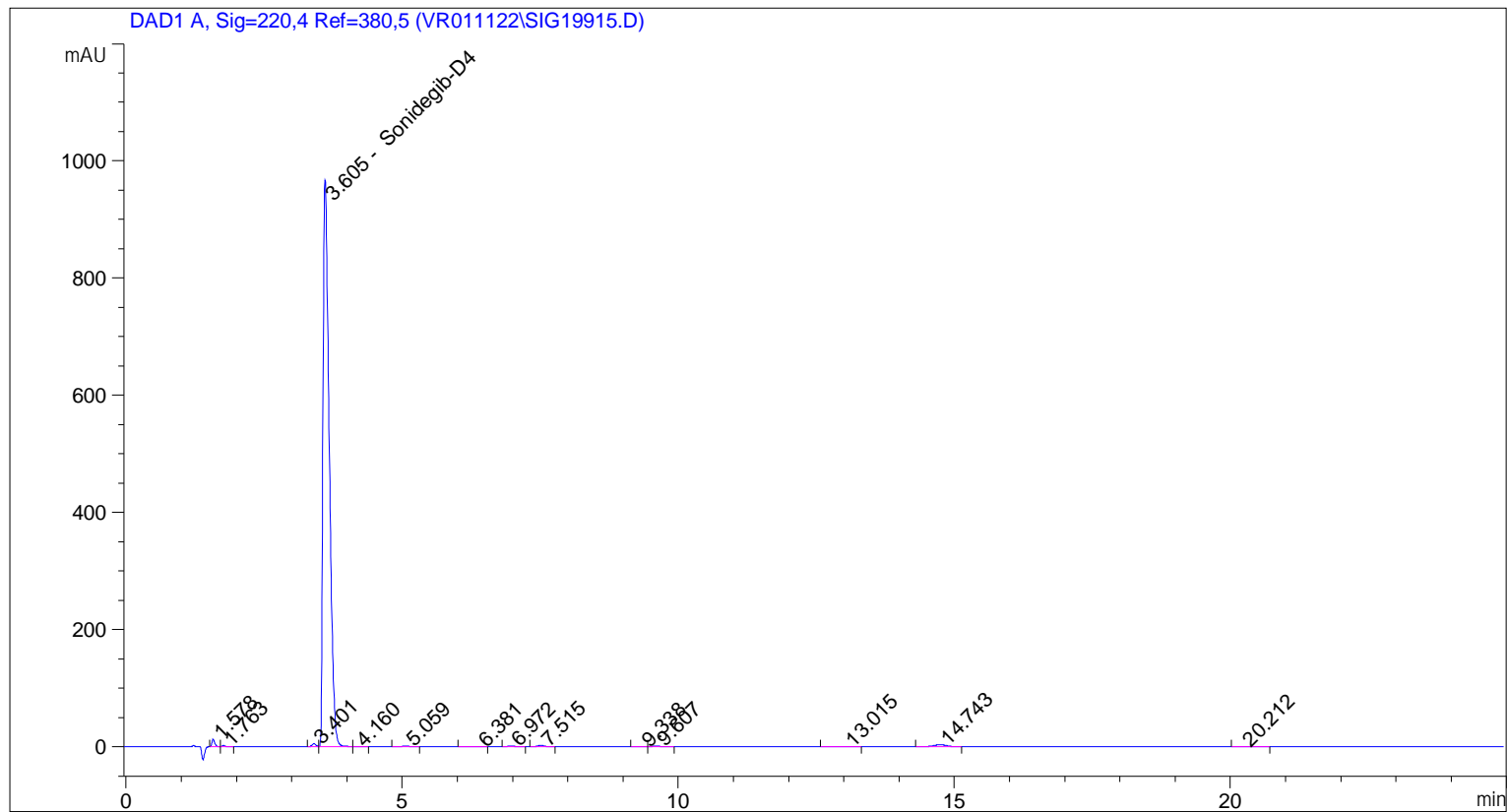
TOF MS ES+  
2.30e3



Expansion of above showing intensity labels.

```

=====
Acq. Operator   : vrusu
Acq. Instrument : Instrument 1                Location : Vial 21
Injection Date  : 4/13/2022 3:18:04 PM
                                           Inj Volume : 5.0 µl
Acq. Method    : C:\CHEM32\1\METHODS\VR041322_131.M
Last changed   : 4/13/2022 3:17:09 PM by vrusu
Analysis Method: C:\CHEM32\1\METHODS\VR041422_131PM.M
Last changed   : 4/14/2022 7:53:28 AM by vrusu
  
```



=====  
 Area Percent Report  
 =====

```

Sorted By      : Signal
Calib. Data Modified : 4/14/2022 7:43:40 AM
Multiplier:    : 1.0000
Dilution:     : 1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 1: DAD1 A, Sig=220,4 Ref=380,5

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	1.578	BV	0.0561	45.70100	0.5869	?
2	1.763	VV	0.0601	9.17529	0.1178	?
3	3.401	BV	0.0745	24.58860	0.3158	?
4	3.605	VV	0.1214	7586.98145	97.4365	Sonidegib-D4
5	4.160	VB	0.1121	2.29053	0.0294	?
6	5.059	BV	0.1158	10.82777	0.1391	?
7	6.381	BB	0.1662	1.76403	0.0227	?
8	6.972	BB	0.1137	10.71109	0.1376	?

Sample Name: GR-17-131

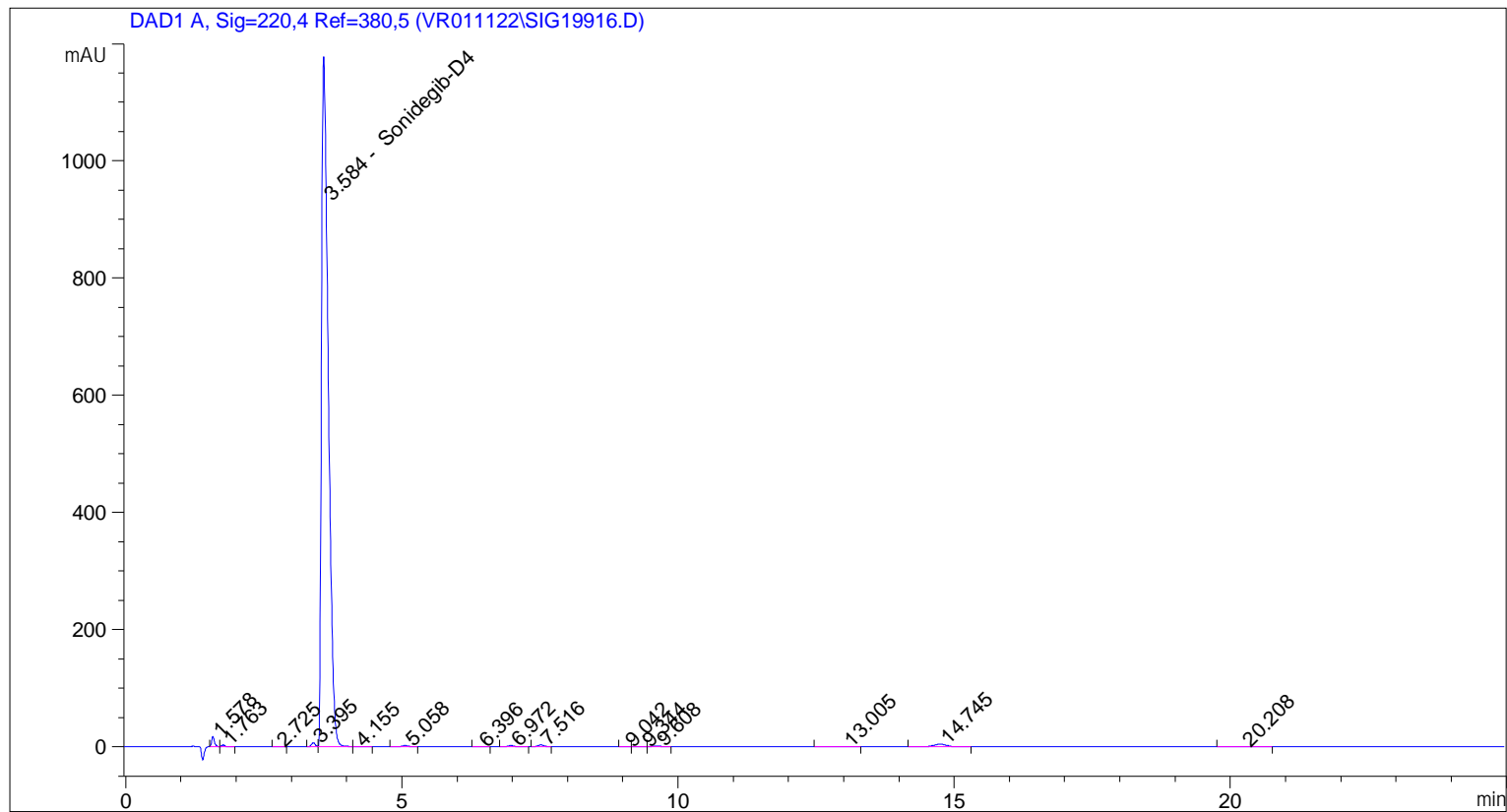
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
9	7.515	BB	0.1256	18.29251	0.2349	?
10	9.338	VV	0.1355	2.63524	0.0338	?
11	9.607	VB	0.1597	11.01834	0.1415	?
12	13.015	BB	0.2984	4.58527	0.0589	?
13	14.743	BB	0.2637	54.79403	0.7037	?
14	20.212	BB	0.3308	3.22866	0.0415	?

Totals : 7786.59380

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

```

=====
Acq. Operator   : vrusu
Acq. Instrument : Instrument 1                Location : Vial 22
Injection Date  : 4/13/2022 3:44:35 PM
                                           Inj Volume : 5.0 µl
Acq. Method     : C:\CHEM32\1\METHODS\VR041322_131.M
Last changed    : 4/13/2022 3:43:41 PM by vrusu
Analysis Method : C:\CHEM32\1\METHODS\VR041422_131PM.M
Last changed    : 4/14/2022 7:53:28 AM by vrusu
  
```



=====  
 Area Percent Report  
 =====

```

Sorted By           :      Signal
Calib. Data Modified :      4/14/2022 7:43:40 AM
Multiplier:         :      1.0000
Dilution:           :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 1: DAD1 A, Sig=220,4 Ref=380,5

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	1.578	BV	0.0557	61.52943	0.5962	?
2	1.763	VV	0.0583	11.62439	0.1126	?
3	2.725	VB	0.0993	1.10745	0.0107	?
4	3.395	BV	0.0734	32.33553	0.3133	?
5	3.584	VV	0.1314	1.00509e4	97.3870	Sonidegib-D4
6	4.155	VB	0.1172	3.17797	0.0308	?
7	5.058	VV	0.1162	15.21679	0.1474	?
8	6.396	BB	0.1011	1.21040	0.0117	?



Sample Name: GR-17-131 spl-2

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
9	6.972	VB	0.1206	14.61924	0.1417	?
10	7.516	BB	0.1240	23.84739	0.2311	?
11	9.042	VV	0.1222	1.26421	0.0122	?
12	9.344	VV	0.1286	3.54544	0.0344	?
13	9.608	VB	0.1587	14.37032	0.1392	?
14	13.005	BB	0.2944	6.53379	0.0633	?
15	14.745	BB	0.2580	73.43426	0.7115	?
16	20.208	BB	0.3691	5.86109	0.0568	?

Totals : 1.03206e4

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