

Name:	Upadacitinib-D4 (major)
Lot#:	GR-17-087
Test Date:	03/24/2022 (re-test date: 03/24/2027)
CAS No.:	1310726-60-3 (unlabelled)
MF:	C ₁₇ H ₁₅ D ₄ F ₃ N ₆ O
MW:	384.39
Appearance:	Beige solid
Purity:	98.8% by HPLC (average of two sample preparations); >98% atom D
¹H-NMR:	Conforms
MS-ESI (+)	Conforms (shows peaks at m/z = 384.98 [M+H] ⁺ for D4 form and at m/z = 383.97 [M+H] ⁺ for D3 form)
Storage	Store at -18°C in a dry place away from direct sunlight

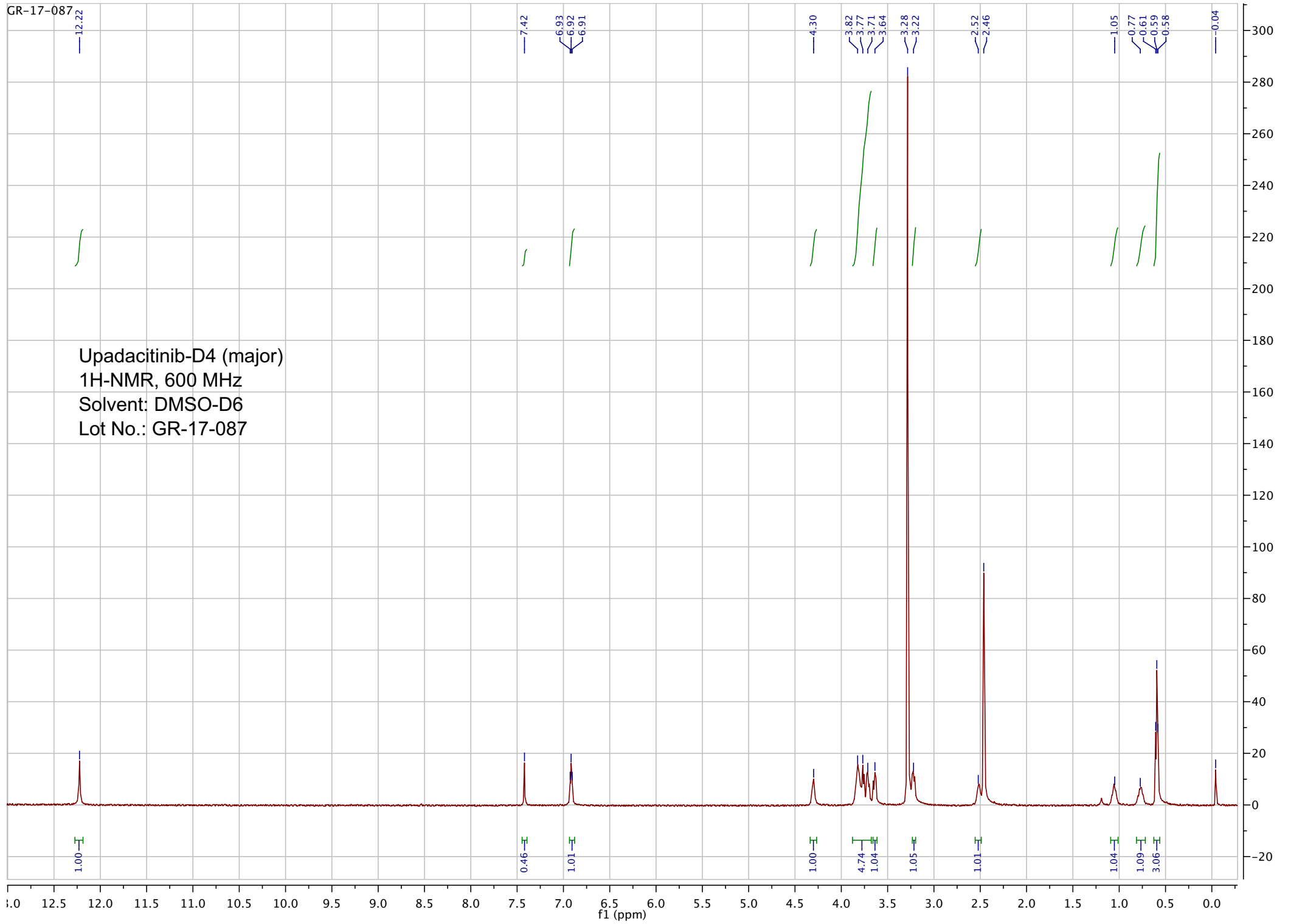
Approved by:

Date: 03/25/2022



Viorica Rusu, QC/QA Manager

GR-17-087

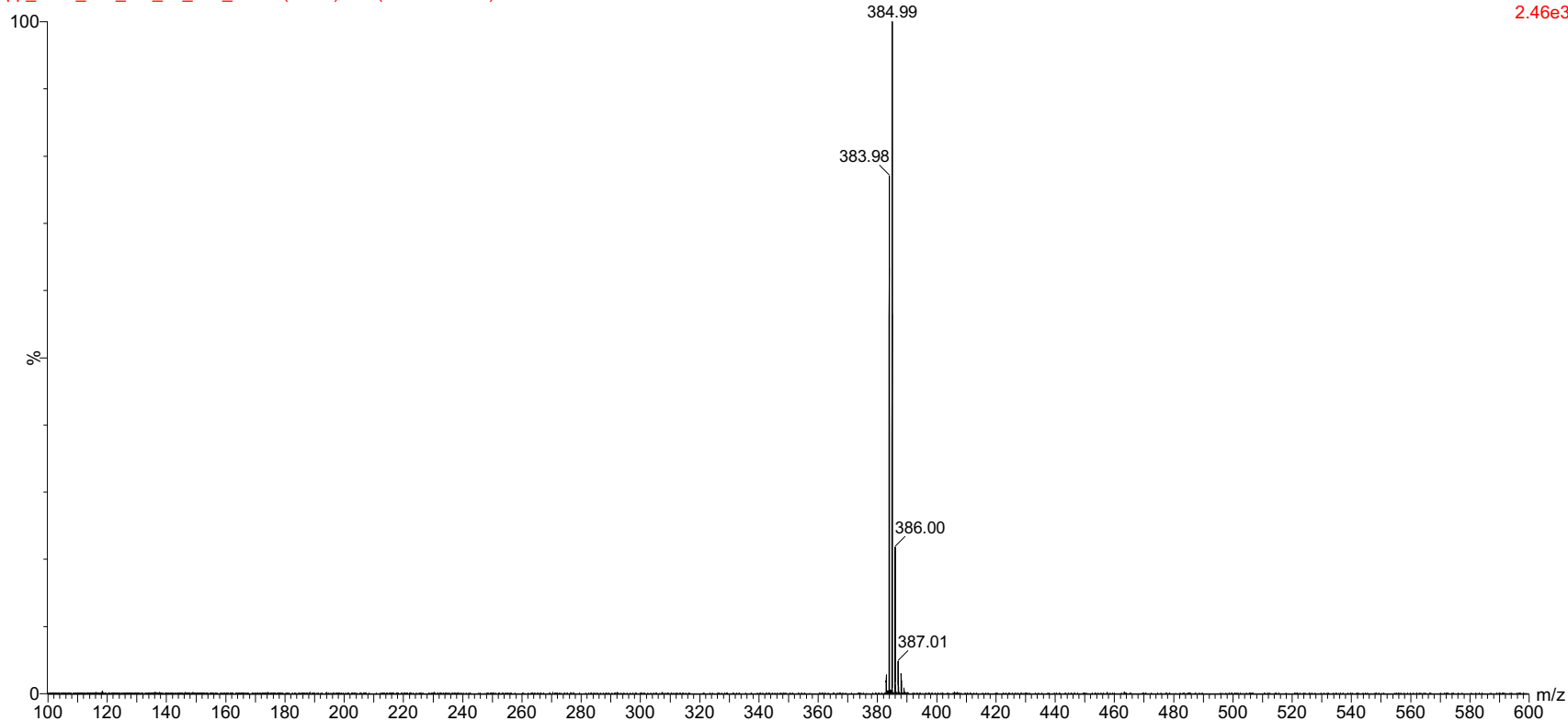


pp_2022_022_GR_17_087_1 167 (3.160) Cm (165:175-9:19)

8.00000000

25-Mar-2022, 10:15:26

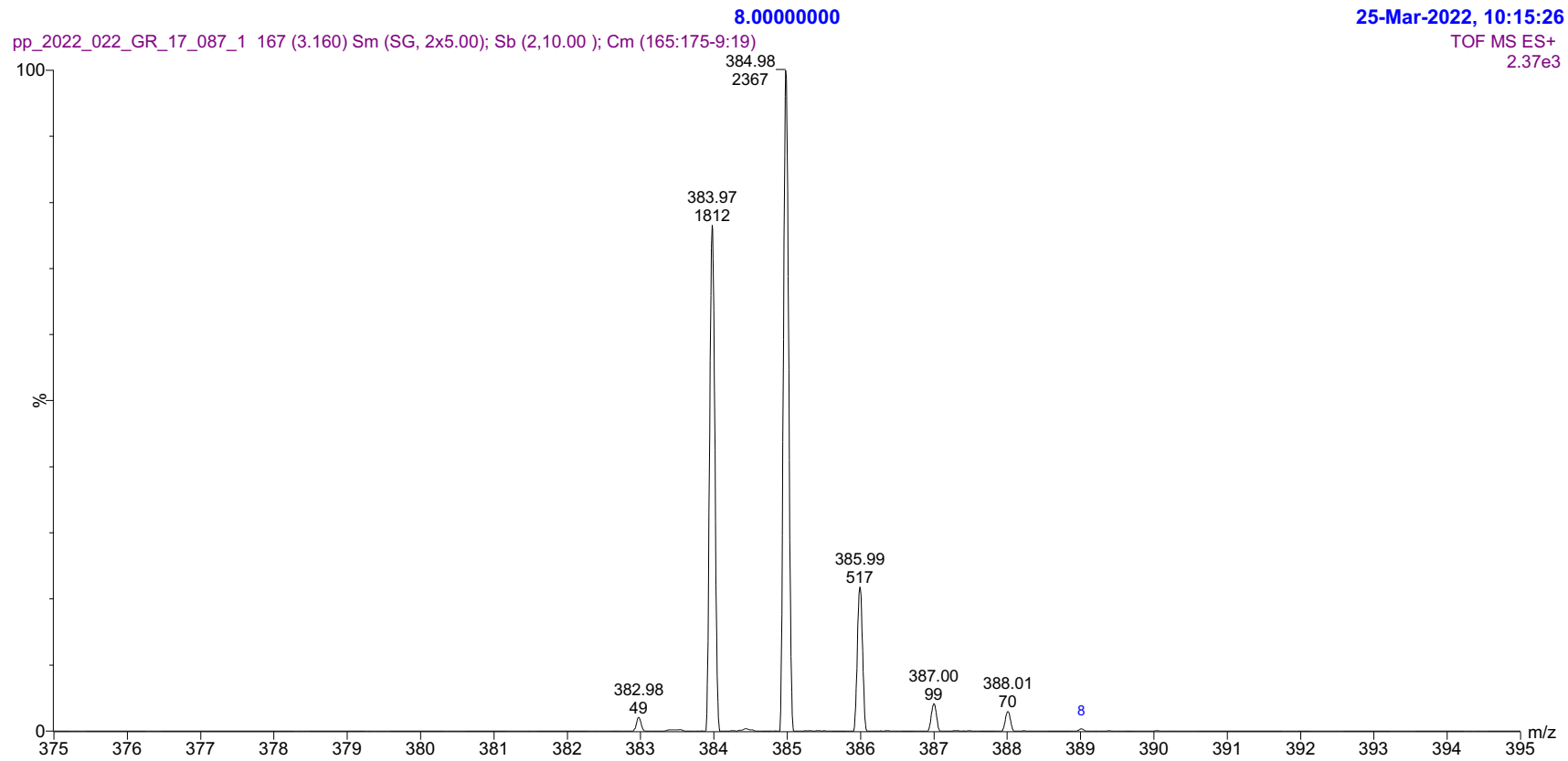
TOF MS ES+
2.46e3



ESI-MS spectrum for sample GR-17-087. Shows monoisotopic [M+H]⁺ mass.

25-Mar-2022, 10:15:26

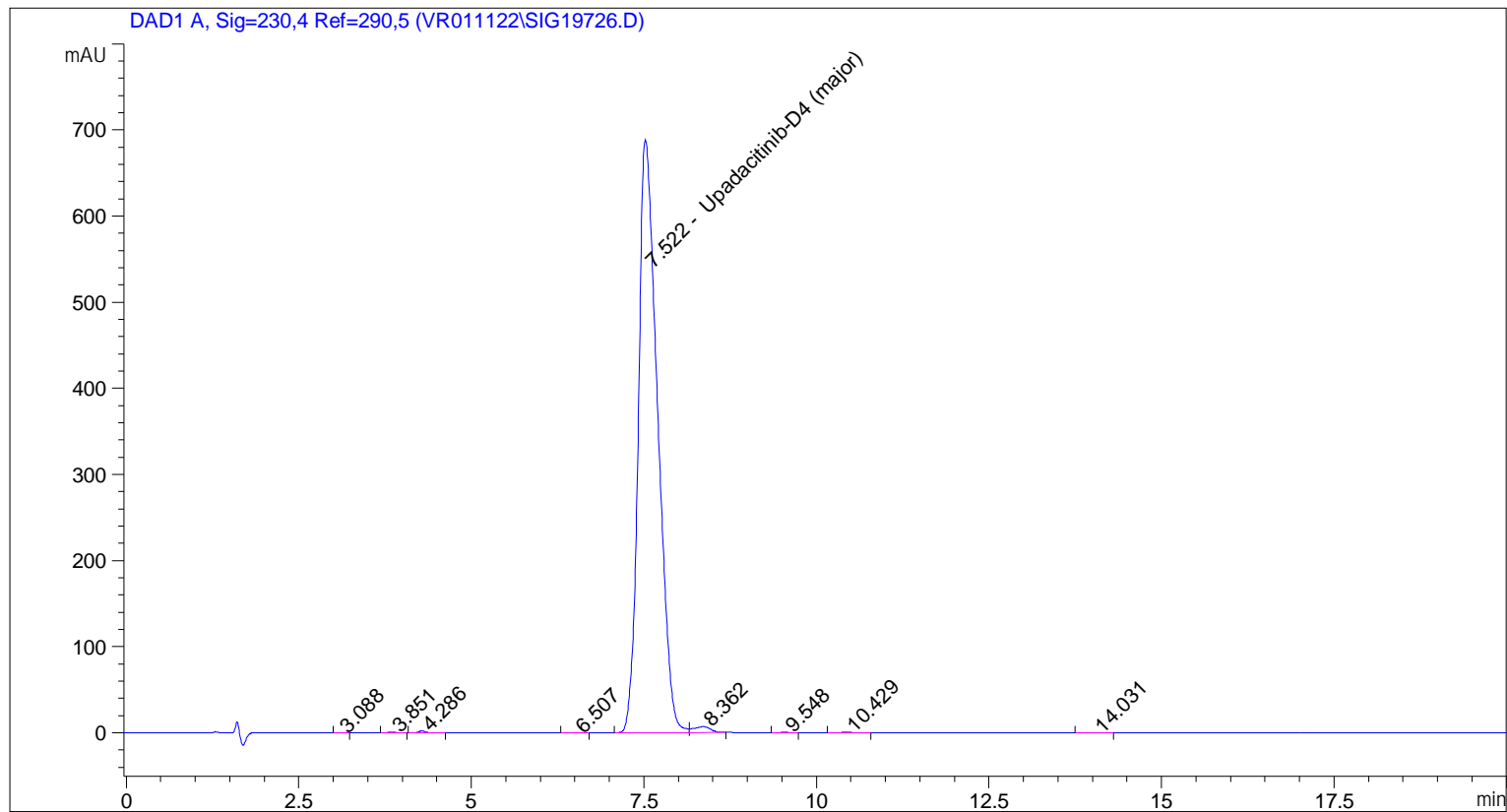
TOF MS ES+
2.37e3



Expansion of above showing intensity labels.

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=====
Acq. Operator   : vrusu
Acq. Instrument : Instrument 1                Location : Vial 4
Injection Date  : 3/24/2022 10:00:46 AM
                                           Inj Volume : 10.0 µl
Acq. Method     : C:\CHEM32\1\METHODS\VR032422_087.M
Last changed    : 3/24/2022 9:59:38 AM by vrusu
Analysis Method : C:\CHEM32\1\METHODS\VR032422_087PM.M
Last changed    : 3/25/2022 12:17:03 PM by vrusu
  
```



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 Area Percent Report
 =====

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Sorted By           :      Signal
Calib. Data Modified :      3/25/2022 12:16:52 PM
Multiplier:         :      1.0000
Dilution:           :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 1: DAD1 A, Sig=230,4 Ref=290,5

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	3.088	BB	0.0781	8.32939e-1	6.188e-3	?
2	3.851	BB	0.1192	4.99477	0.0371	?
3	4.286	BB	0.0959	14.73359	0.1095	?
4	6.507	BB	0.1494	3.02067	0.0224	?
5	7.522	BV	0.2914	1.33013e4	98.8194	Upadacitinib-D4 (major)
6	8.362	VB	0.2531	116.35950	0.8645	?
7	9.548	BB	0.1451	4.16842	0.0310	?
8	10.429	BB	0.1811	7.74012	0.0575	?

Sample Name: GR-17-087

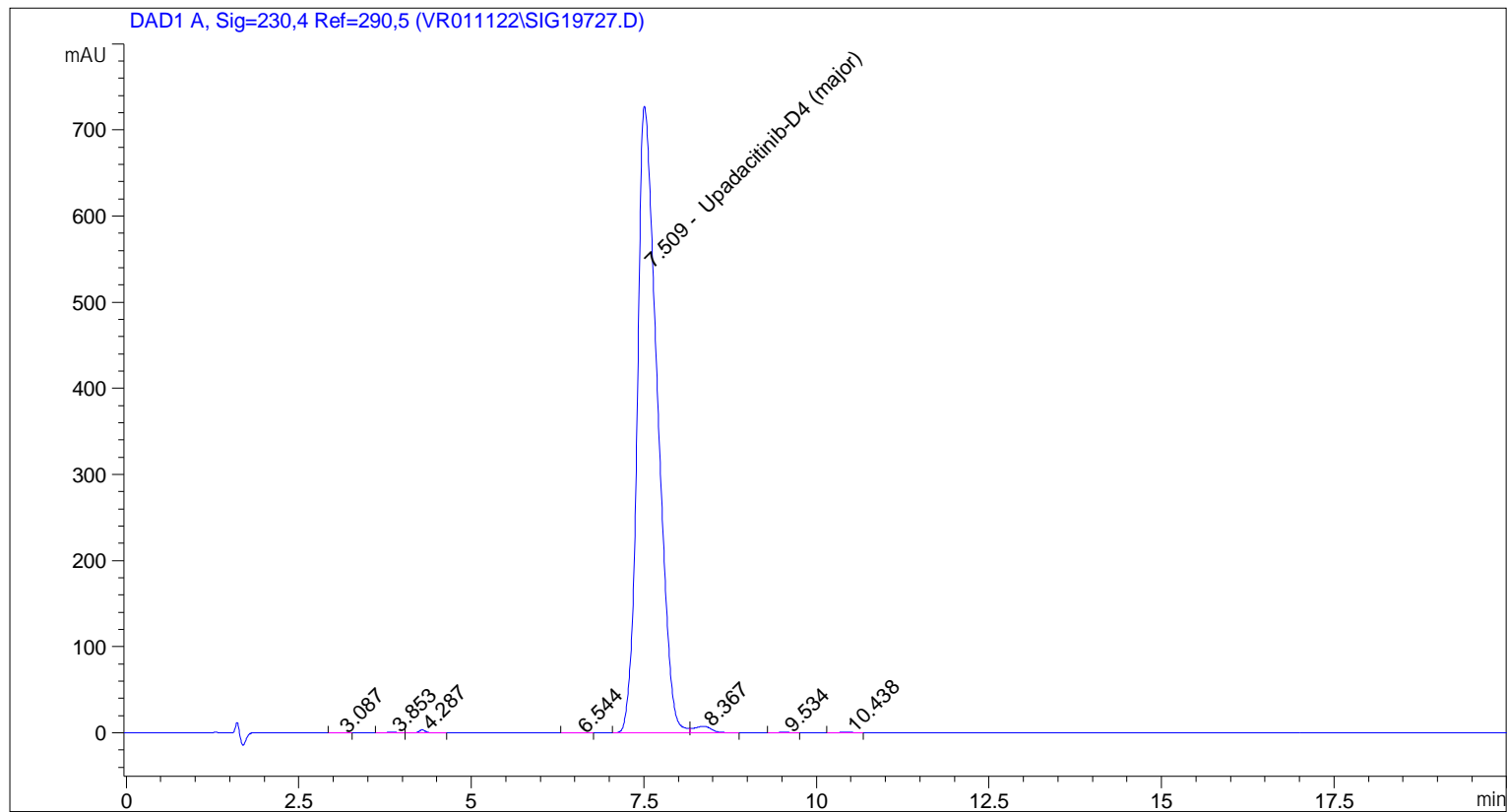
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
9	14.031	BB	0.2080	7.05633	0.0524	?

Totals : 1.34602e4

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*** End of Report ***

```

=====
Acq. Operator   : vrusu
Acq. Instrument : Instrument 1                Location : Vial 5
Injection Date  : 3/24/2022 10:23:35 AM
                                           Inj Volume : 10.0 µl
Acq. Method     : C:\CHEM32\1\METHODS\VR032422_087.M
Last changed    : 3/24/2022 10:22:30 AM by vrusu
Analysis Method : C:\CHEM32\1\METHODS\VR032422_087PM.M
Last changed    : 3/25/2022 12:17:03 PM by vrusu
  
```



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

```

Sorted By           :      Signal
Calib. Data Modified :      3/25/2022 12:16:52 PM
Multiplier:         :      1.0000
Dilution:           :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 1: DAD1 A, Sig=230,4 Ref=290,5

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	3.087	BB	0.1182	2.33698	0.0158	?
2	3.853	BB	0.1245	6.97489	0.0472	?
3	4.287	BB	0.1015	23.71740	0.1605	?
4	6.544	BB	0.1602	3.45274	0.0234	?
5	7.509	BV	0.3020	1.45841e4	98.6871	Upadacitinib-D4 (major)
6	8.367	VB	0.2651	138.03906	0.9341	?
7	9.534	BB	0.1822	8.08679	0.0547	?
8	10.438	BB	0.1883	11.40680	0.0772	?

Sample Name: GR-17-087 spl-2

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
Totals :				1.47781e4		

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*** End of Report ***