

Name:	Bictegravir-D4 Sodium
Lot#:	GR-18-173
Test Date:	06/13/2023 (re-test date: 06/13/2028)
CAS No.:	1807988-02-8 (unlabeled)
MF:	C ₂₁ H ₁₃ D ₄ F ₃ N ₃ NaO ₅
MW:	475.39
Appearance:	Pale yellow solid
Purity:	98.8% by HPLC (average of two sample preparations); >98% atom D
¹H-NMR:	Conforms
MS-DART (+)	Conforms (shows peak at m/z = 454.2 [M _(free acid) +H] ⁺)
Storage	Store at -18°C in a dry place away from direct sunlight

Approved by:

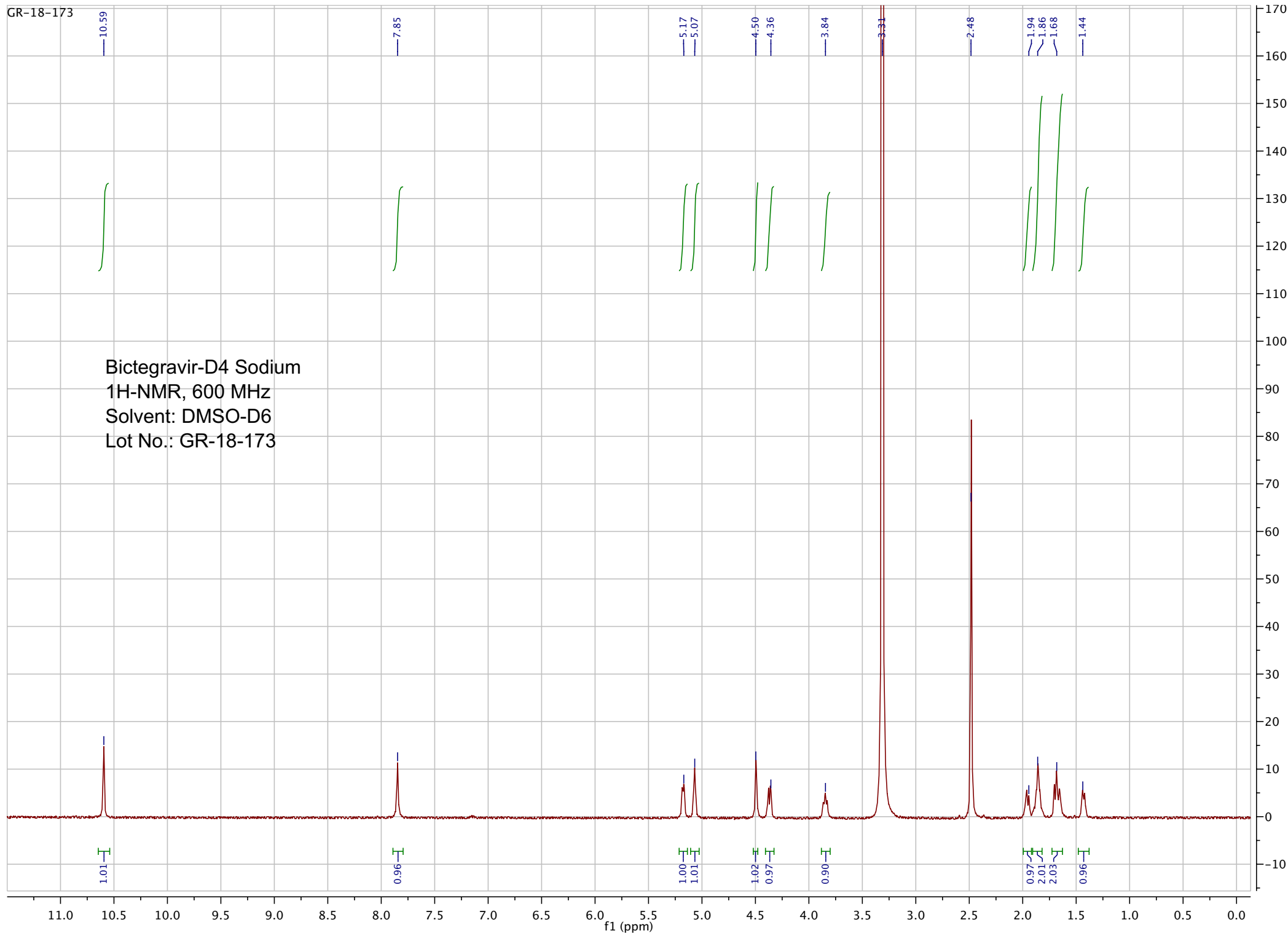
Date: 06/20/2023

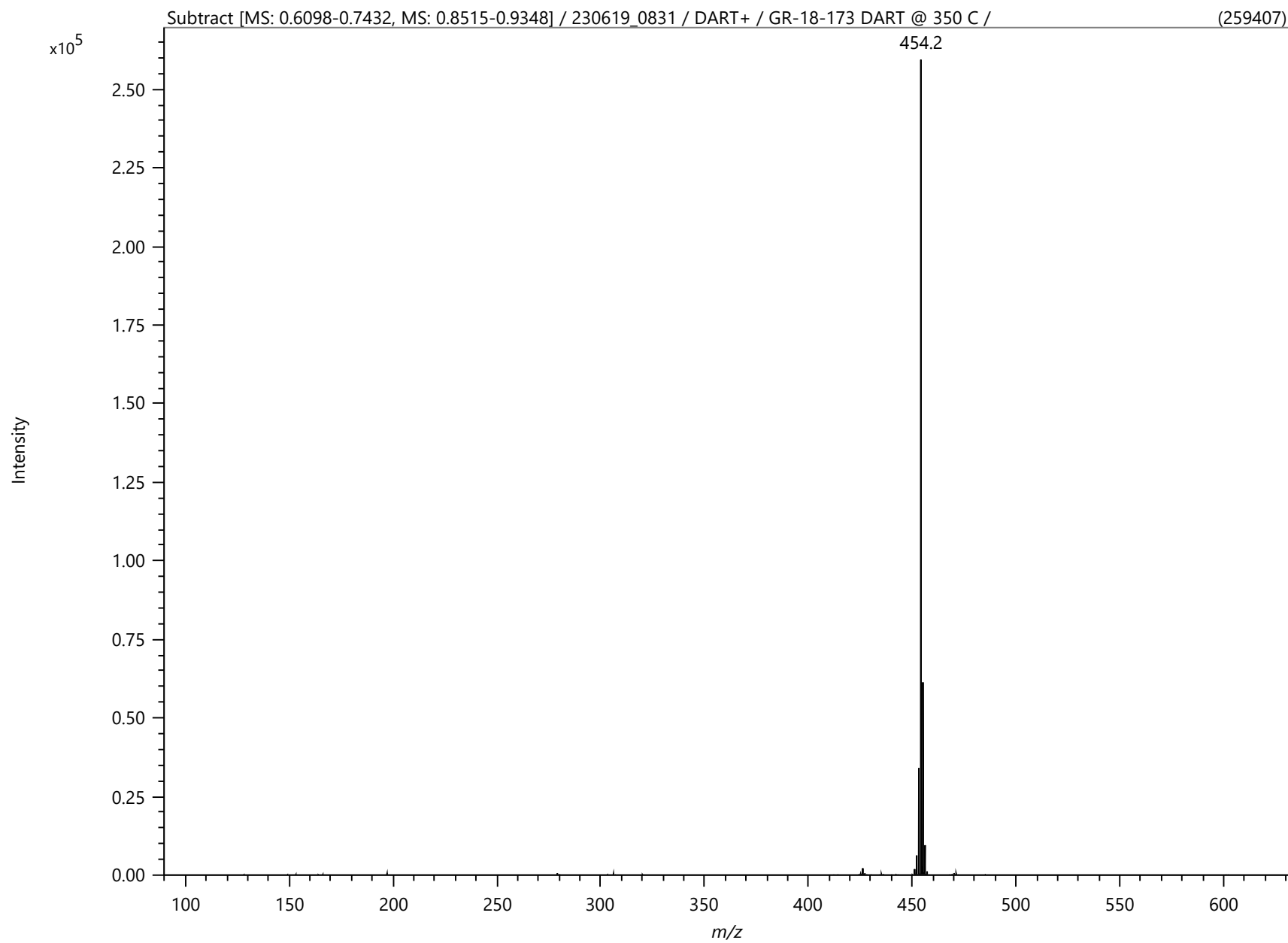


Viorica Rusu, QC/QA Manager

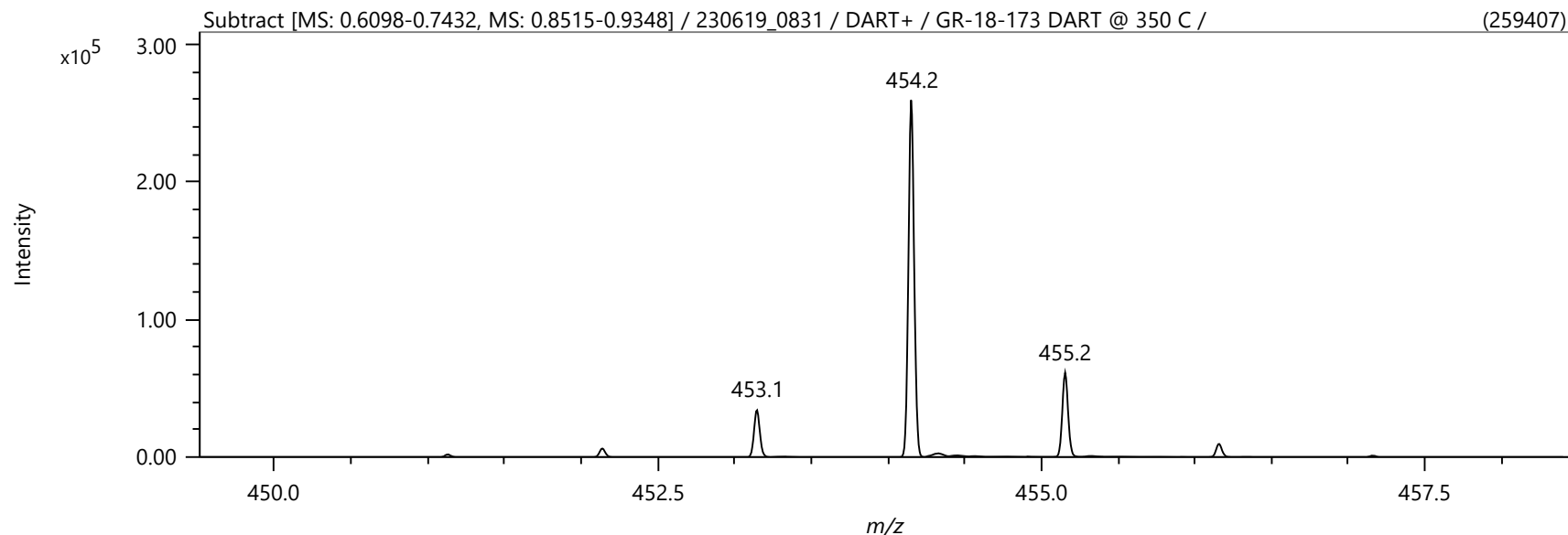
GR-18-173

Bictegravir-D4 Sodium
1H-NMR, 600 MHz
Solvent: DMSO-D6
Lot No.: GR-18-173





Spectrum



Elemental Composition

Parameters

Tolerance: ±10.00 mDa
 Electron: Even
 Charge: +1
 DBE: -1.5 - 100.0

Elements Set 1:

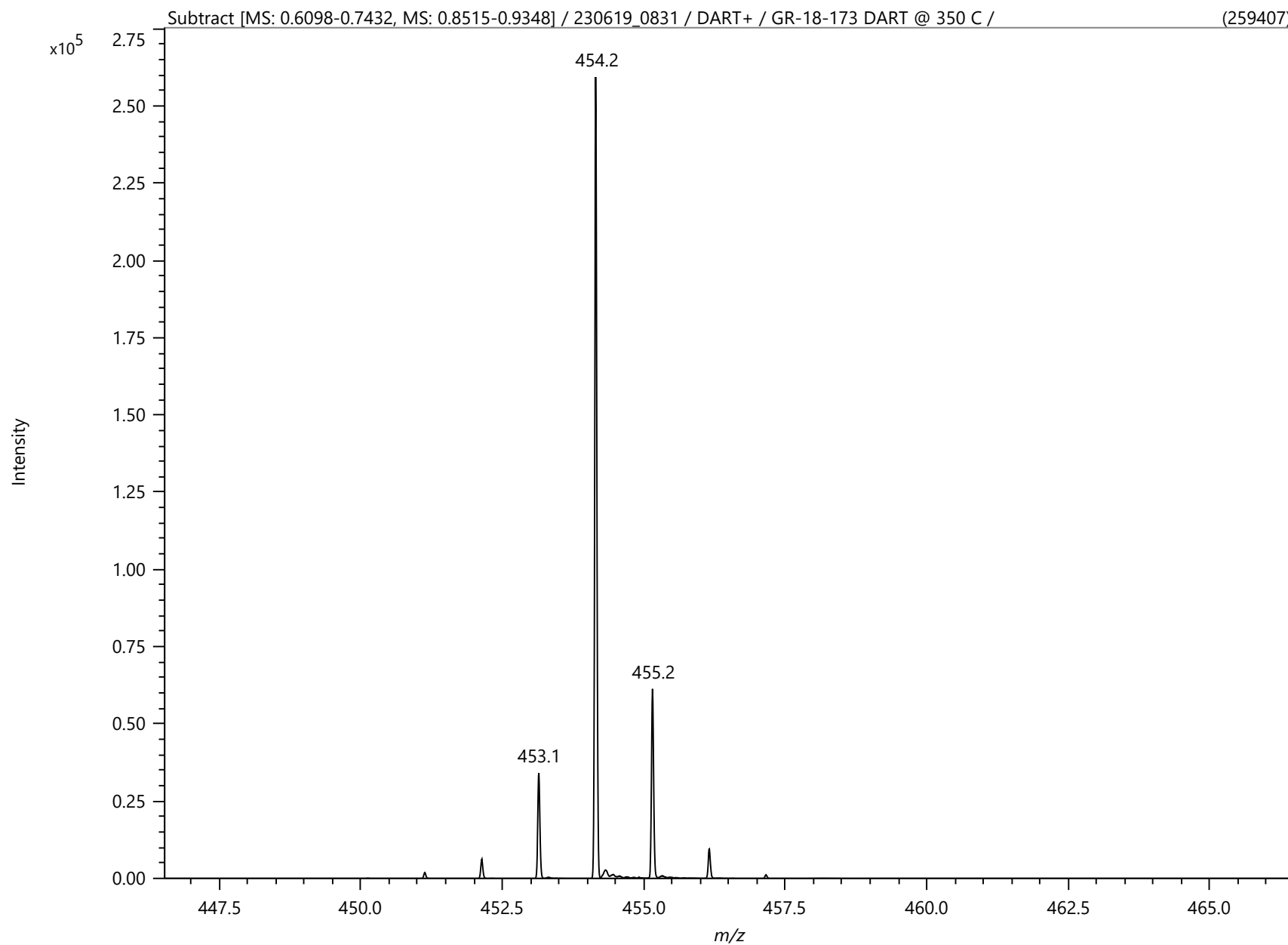
Symbol	C	H	O	N	F	D
Min	0	0	0	0	0	4
Max	100	200	20	10	3	4

Results

Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
454.15190	259406.89	C15 H17 N5 O10 F D4	454.15180	0.10	0.21	7.5
		C19 H12 N9 O5 D4	454.15200	-0.10	-0.22	16.5
		C11 H22 N O15 F2 D4	454.15161	0.29	0.64	-1.5
		C21 H15 N3 O5 F3 D4	454.15224	-0.34	-0.75	12.5
		C25 H10 N7 F2 D4	454.15243	-0.53	-1.17	21.5
		C6 H20 N7 O16 D4	454.15251	-0.61	-1.35	-1.5

Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
		C24 H14 N3 O4 F2 D4	454.15110	0.80	1.77	16.5
		C35 H12 N D4	454.15283	-0.93	-2.05	28.5
		C12 H18 N5 O11 F2 D4	454.15295	-1.05	-2.30	3.5
		C18 H16 N5 O9 D4	454.15066	1.24	2.73	11.5
		C16 H13 N9 O6 F D4	454.15314	-1.24	-2.73	12.5
		C14 H21 N O14 F D4	454.15047	1.43	3.16	2.5
		C22 H11 N7 O F3 D4	454.15358	-1.68	-3.69	17.5
		C27 H13 N3 O3 F D4	454.14995	1.95	4.29	20.5
		C32 H13 N O F D4	454.15398	-2.08	-4.57	24.5
		C9 H19 N5 O12 F3 D4	454.15409	-2.19	-4.82	-0.5
		C17 H11 N9 O3 F3 D4	454.14955	2.35	5.17	13.5
		C13 H14 N9 O7 F2 D4	454.15428	-2.38	-5.25	8.5
		C17 H20 N O13 D4	454.14932	2.58	5.67	6.5
		C23 H16 N3 O7 D4	454.15468	-2.78	-6.13	15.5
		C7 H18 N7 O13 F2 D4	454.14892	2.98	6.55	-0.5
		C30 H12 N3 O2 D4	454.14881	3.09	6.80	24.5
		C29 H14 N O2 F2 D4	454.15512	-3.22	-7.09	20.5
		C20 H10 N9 O2 F2 D4	454.14841	3.49	7.68	17.5
		C10 H15 N9 O8 F3 D4	454.15543	-3.53	-7.77	4.5
		C16 H15 N5 O7 F3 D4	454.14822	3.68	8.11	8.5
		C20 H17 N3 O8 F D4	454.15583	-3.93	-8.65	11.5
		C10 H17 N7 O12 F D4	454.14778	4.12	9.07	3.5
		C24 H12 N7 O3 D4	454.15602	-4.12	-9.07	20.5
		C26 H15 N O3 F3 D4	454.15626	-4.36	-9.60	16.5
		C23 H9 N9 O F D4	454.14727	4.63	10.20	21.5
		C11 H20 N5 O14 D4	454.15653	-4.63	-10.20	2.5
		C19 H14 N5 O6 F2 D4	454.14707	4.83	10.63	12.5
		C15 H19 N O11 F3 D4	454.14688	5.02	11.06	3.5
		C17 H18 N3 O9 F2 D4	454.15697	-5.07	-11.16	7.5
		C13 H16 N7 O11 D4	454.14664	5.26	11.59	7.5
		C21 H13 N7 O4 F D4	454.15716	-5.26	-11.59	16.5
		C9 H21 N3 O16 F D4	454.14644	5.46	12.01	-1.5
		C28 H11 N3 F3 D4	454.14637	5.53	12.19	21.5

Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
		C26 H8 N9 D4	454.14612	5.78	12.72	25.5
		C8 H21 N5 O15 F D4	454.15768	-5.78	-12.72	-1.5
		C22 H13 N5 O5 F D4	454.14593	5.97	13.14	16.5
		C12 H16 N9 O10 D4	454.15787	-5.97	-13.15	7.5
		C18 H18 N O10 F2 D4	454.14574	6.16	13.57	7.5
		C14 H19 N3 O10 F3 D4	454.15811	-6.21	-13.68	3.5
		C18 H14 N7 O5 F2 D4	454.15831	-6.41	-14.11	12.5
		C12 H20 N3 O15 D4	454.14530	6.60	14.53	2.5
		C28 H16 N O5 D4	454.15871	-6.81	-14.99	19.5
		C25 H12 N5 O4 D4	454.14479	7.11	15.66	20.5
		C9 H17 N9 O11 F D4	454.15901	-7.11	-15.66	3.5
		C21 H17 N O9 F D4	454.14459	7.31	16.09	11.5
		C15 H15 N7 O6 F3 D4	454.15945	-7.55	-16.62	8.5
		C11 H15 N7 O9 F3 D4	454.14419	7.71	16.97	4.5
		C25 H17 N O6 F D4	454.15985	-7.95	-17.50	15.5
		C5 H17 N9 O14 F D4	454.14376	8.14	17.93	-0.5
		C29 H12 N5 O D4	454.16004	-8.14	-17.93	24.5
		C6 H18 N9 O12 F2 D4	454.16016	-8.26	-18.18	-0.5
		C24 H16 N O8 D4	454.14345	8.45	18.61	15.5
		C16 H20 N3 O12 D4	454.16056	-8.66	-19.06	6.5
		C14 H14 N7 O8 F2 D4	454.14305	8.85	19.49	8.5
		C10 H19 N3 O13 F3 D4	454.14286	9.04	19.91	-0.5
		C22 H18 N O7 F2 D4	454.16099	-9.09	-20.02	11.5
		C8 H16 N9 O13 D4	454.14262	9.28	20.44	3.5
		C26 H13 N5 O2 F D4	454.16119	-9.29	-20.45	20.5
		C23 H11 N5 O2 F3 D4	454.14234	9.56	21.04	17.5
		C13 H21 N3 O13 F D4	454.16170	-9.80	-21.58	2.5
		C17 H13 N7 O7 F D4	454.14191	9.99	22.00	12.5
		C17 H16 N7 O8 D4	454.16189	-9.99	-22.01	11.5

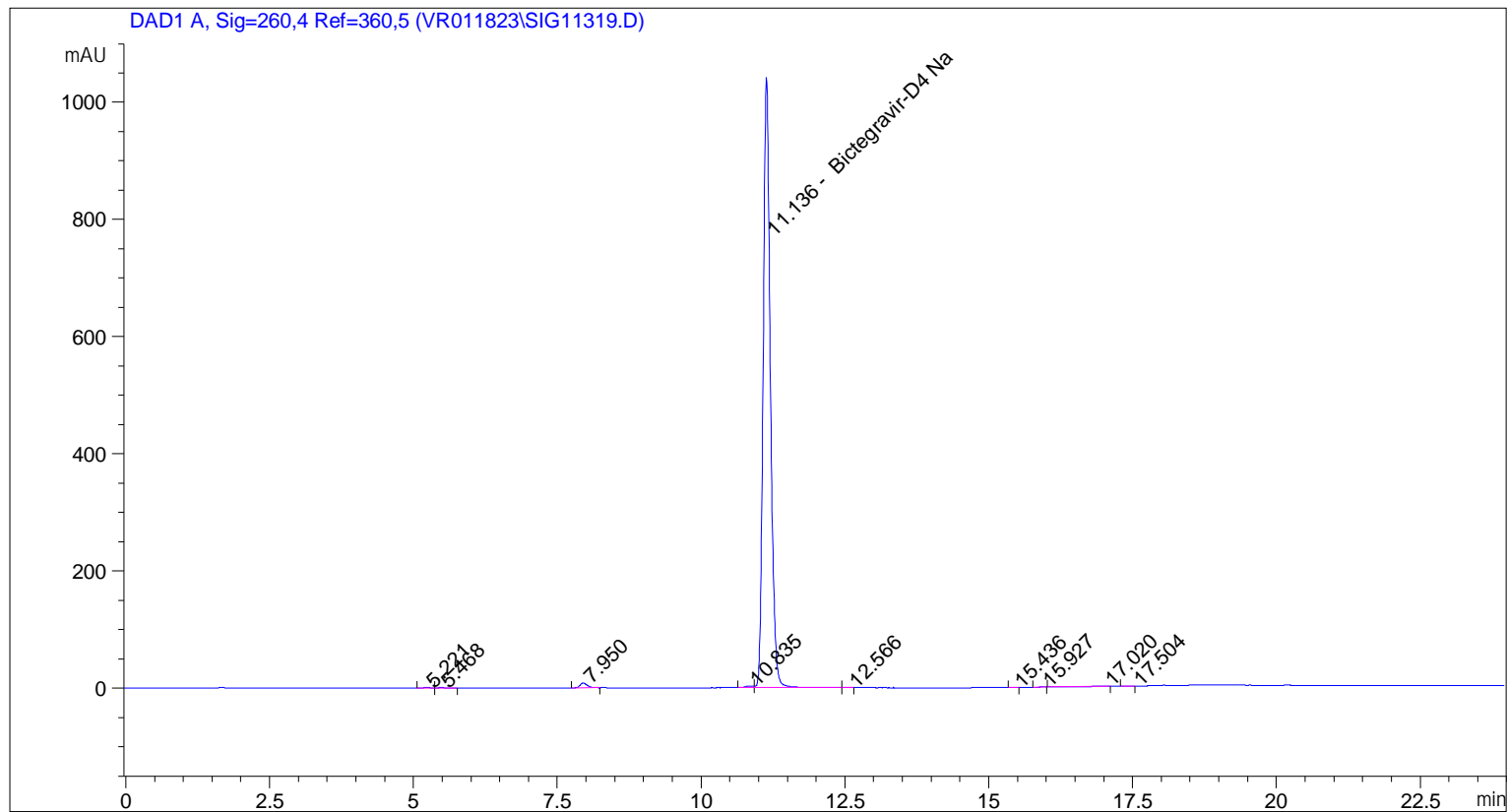


m/z	Area	Area%
449.0993	336.69	0.02
450.1227	975.91	0.05
451.131	13746.12	0.77
452.1381	43856.38	2.45
453.1459	238650.7	13.34
454.1519	1789446	100
454.323	39268.19	2.19
455.1553	426142.5	23.81
456.1581	68781.17	3.84
457.1604	8062.98	0.45
458.158	873.27	0.05
459.0206	93.03	0.01
460.0718	188.92	0.01
461.0583	171.15	0.01
461.4381	229.63	0.01
462.8436	108.9	0.01
463.3897	143.64	0.01
464.7369	142.86	0.01
466.1132	133.5	0.01

Calc. m/z	Abund
454.1522	100
455.1553	24.1841
456.1579	3.8269
457.1604	0.4545
458.1629	0.0438
459.1654	0.0036
460.1678	0.0002


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Acq. Operator   : vrusu
Acq. Instrument : Instrument 1                Location : Vial 36
Injection Date  : 6/12/2023 3:18:49 PM
                                           Inj Volume : 10.0 µl
Acq. Method     : C:\CHEM32\1\METHODS\VR061223_173.M
Last changed    : 6/12/2023 3:17:38 PM by vrusu
Analysis Method : C:\CHEM32\1\METHODS\VR061323_173PM.M
Last changed    : 6/13/2023 6:18:27 AM by vrusu
  
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 Area Percent Report
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Sorted By           :      Signal
Calib. Data Modified :      6/13/2023 6:17:34 AM
Multiplier:         :      1.0000
Dilution:           :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
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Signal 1: DAD1 A, Sig=260,4 Ref=360,5

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	5.221	BV	0.1160	1.50690	0.0164	?
2	5.468	VB	0.1193	1.26032	0.0137	?
3	7.950	BB	0.1298	70.23101	0.7623	?
4	10.835	BV	0.1395	25.43986	0.2761	?
5	11.136	VB	0.1320	9107.08691	98.8464	Bictegravir-D4 Na
6	12.566	BB	0.0934	7.73525e-1	8.396e-3	?
7	15.436	BB	0.0667	8.87191e-1	9.629e-3	?
8	15.927	BB	0.0749	1.01897	0.0111	?

Sample Name: GR-18-173

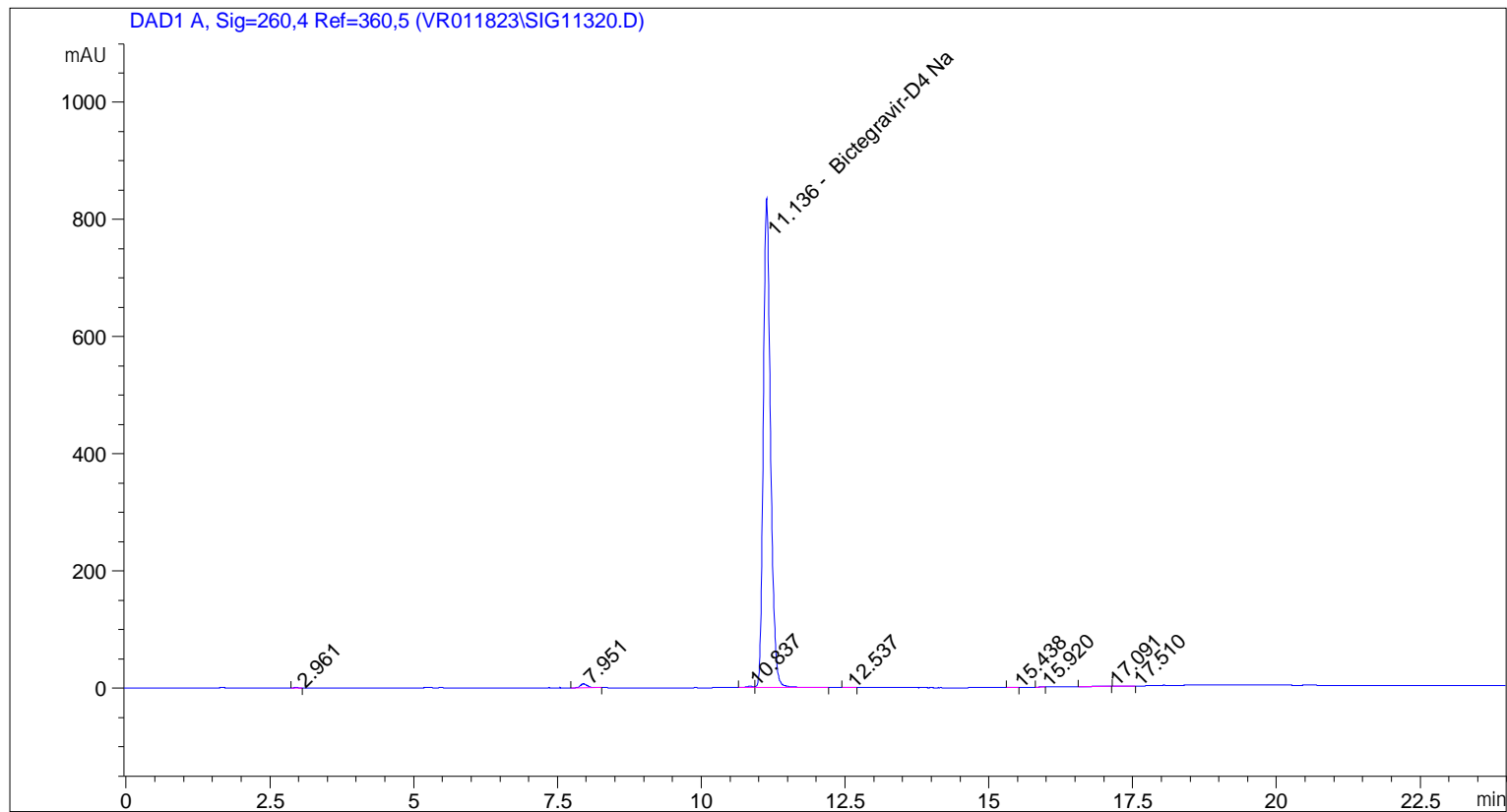
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
9	17.020	BB	0.1132	4.47625	0.0486	?
10	17.504	BB	0.1205	6.92041e-1	7.511e-3	?

Totals : 9213.37300

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*** End of Report ***

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Acq. Operator   : vrusu
Acq. Instrument : Instrument 1                Location : Vial 37
Injection Date  : 6/12/2023 3:46:55 PM
                                           Inj Volume : 10.0 µl
Acq. Method     : C:\CHEM32\1\METHODS\VR061223_173.M
Last changed    : 6/12/2023 3:45:27 PM by vrusu
Analysis Method : C:\CHEM32\1\METHODS\VR061323_173PM.M
Last changed    : 6/13/2023 6:18:27 AM by vrusu
  
```



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 Area Percent Report
 =====

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Sorted By           :      Signal
Calib. Data Modified :      6/13/2023 6:17:34 AM
Multiplier:         :      1.0000
Dilution:           :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 1: DAD1 A, Sig=260,4 Ref=360,5

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	2.961	BB	0.0829	5.73921e-1	7.766e-3	?
2	7.951	BB	0.1295	56.34686	0.7624	?
3	10.837	BV	0.1406	20.21201	0.2735	?
4	11.136	VB	0.1340	7307.08398	98.8703	Bictegravir-D4 Na
5	12.537	BB	0.0962	9.33647e-1	0.0126	?
6	15.438	BB	0.0748	8.04329e-1	0.0109	?
7	15.920	BB	0.0776	8.30901e-1	0.0112	?
8	17.091	BB	0.3974	2.58814	0.0350	?

Sample Name: GR-18-173 spl-2

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
9	17.510	BB	0.1679	1.19829	0.0162	?

Totals : 7390.57207

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*** End of Report ***