

Name:	Apalutamide-13C,D3
Lot#:	GR-19-167
Test Date:	08/08/2024 (re-test date: 08/08/2029)
CAS No.:	956104-40-8 (unlabeled)
MF:	C ₂₀ ¹³ CH ₁₂ D ₃ F ₄ N ₅ O ₂ S
MW:	481.45
Appearance:	White Solid
Purity:	98.7% by HPLC (average of two sample preparations); 99% atom ¹³ C, 99% atom D
¹H-NMR:	Conforms (shows 0.7% IPA)
MS-ESI (+)	Conforms (shows peak at m/z = 482.12 [M+H] ⁺)
Storage	Store at -18°C in a dry place away from direct sunlight

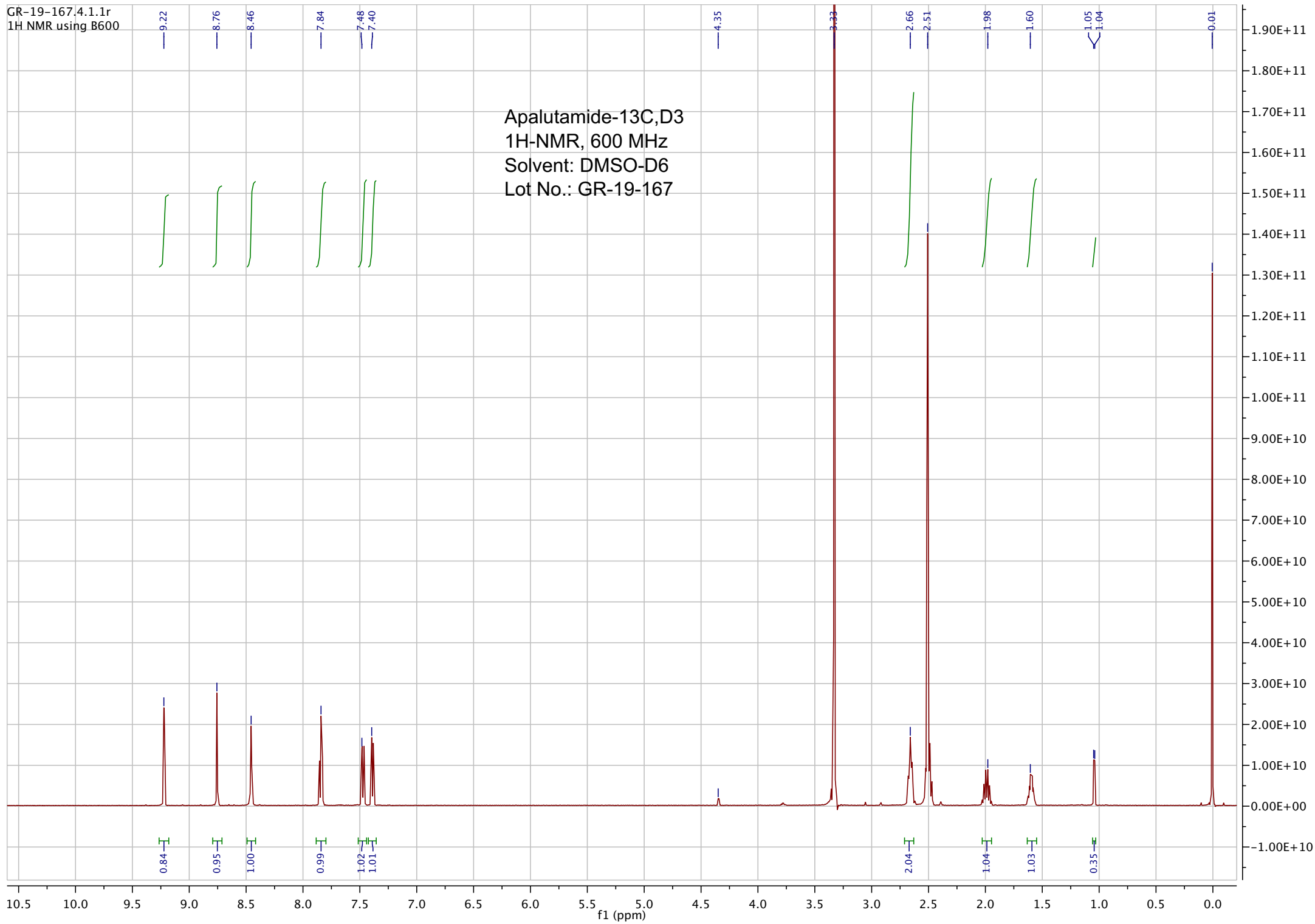
Approved by:

Date: 09/19/2024



Viorica Rusu, QC/QA Manager

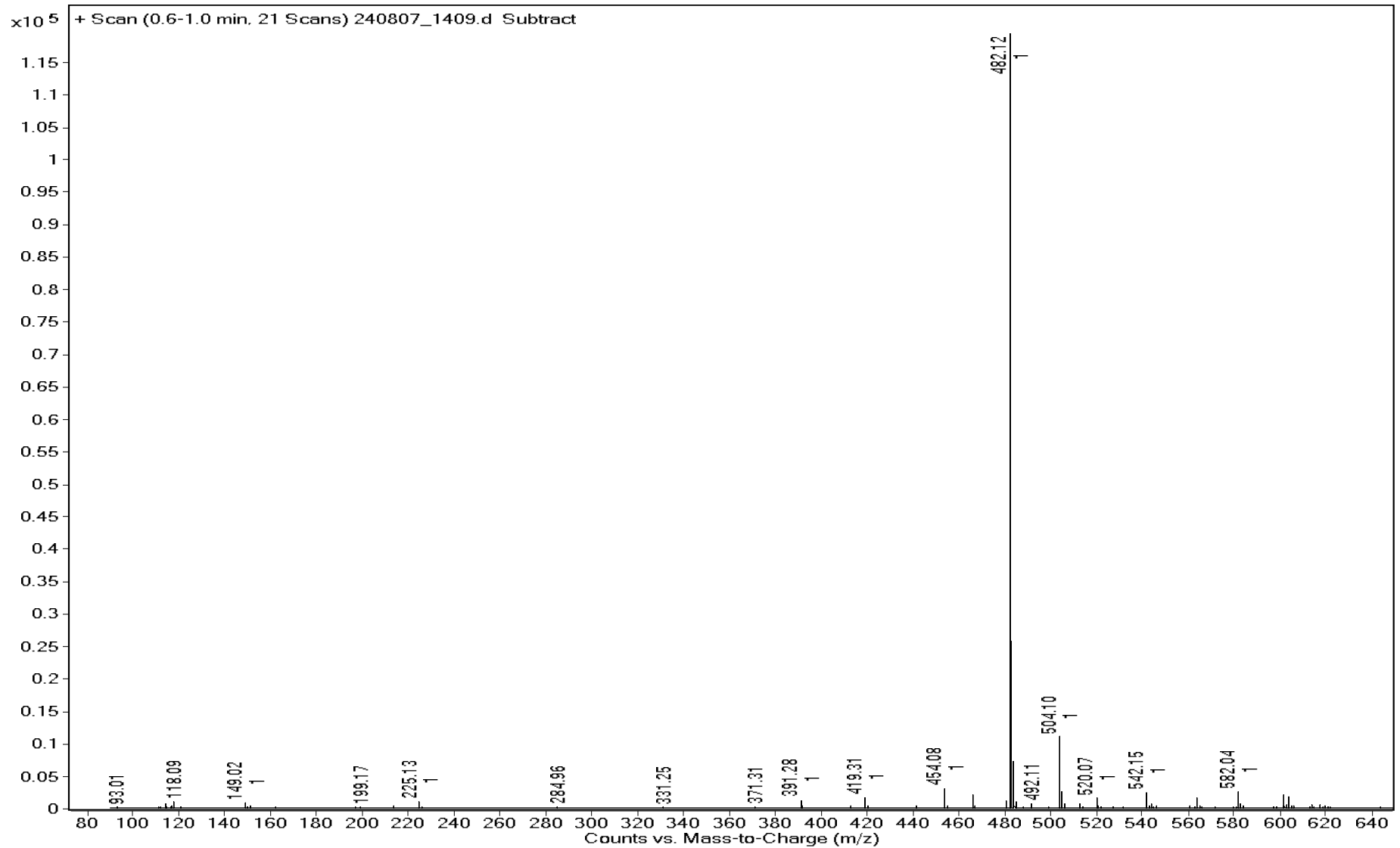
GR-19-167.4.1.1r
1H-NMR using B600



Sample Name GR-19-167
DA Method AIMS_Accurate_Mass.m
Comment ESI+

Data File 240807_1409.d
Instrument Agilent 6538 UHD

Acq Method HRMS.m
Acq Date, Time 07/08/2024 3:01:46 PM



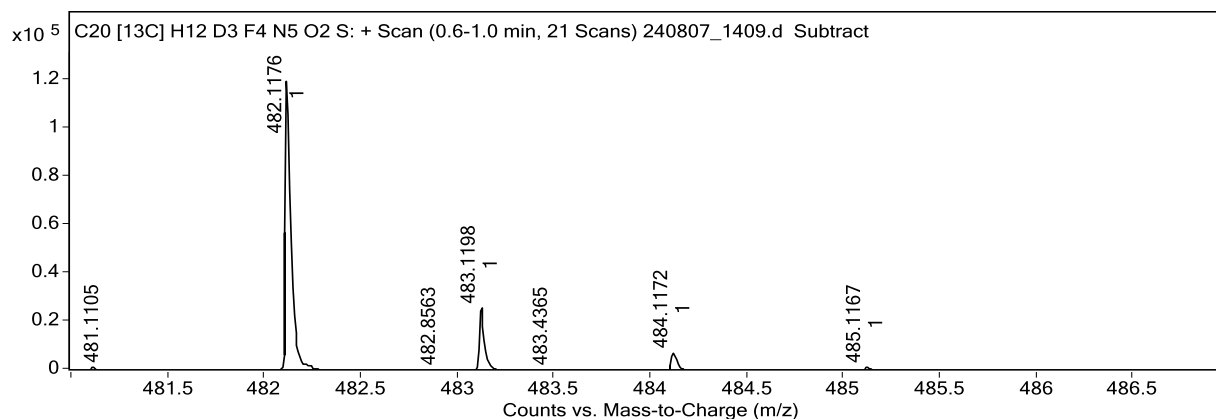
Sample Name	GR-19-167	Data File	240807_1409.d
Acq Method	HRMS.m	DA Method	AIMS_Accurate_Mass.m
Instrument	Agilent 6538 UHD	Acq Date, Time	07/08/2024 3:01:46 PM
Comment	ESI+		

Target Ion Species

Ion Species	m/z	Ionic Formula
(M+H) ⁺	482.1176	C ₂₀ [13C] H ₁₃ D ₃ F ₄ N ₅ O ₂ S

MFG Calculator Results

Target m/z	Ionic Formula	Calc m/z	+/- (mDa)	+/- (ppm)	DBE	MFG Score
482.1176	C ₂₀ [13C] H ₁₃ D ₃ F ₄ N ₅ O ₂ S	482.1177	-0.1	-0.2	15.0	97.41
482.1176	C ₁₉ [13C] H ₁₇ D ₃ F ₄ N ₆ O ₆ S	482.1164	1.2	2.5	10.0	95.72
482.1176	C ₁₁ [13C] H ₁₃ D ₃ F ₄ N ₇ O ₉	482.1162	1.4	2.9	7.0	86.13
482.1176	C ₁₅ [13C] H ₁₇ D ₃ F ₄ N ₁₁	482.1189	-1.3	-2.7	6.0	85.52
482.1176	C ₁₆ [13C] H ₁₃ D ₃ F ₄ N ₁₀	482.1202	-2.6	-5.4	11.0	78.40
482.1176	C ₂₈ [13C] H ₉ D ₃ F ₄ N ₃	482.1184	-0.8	-1.7	24.0	76.40
482.1176	C ₁₅ [13C] H ₁₃ D ₃ F ₄ N ₇ O ₄ S	482.1137	3.9	8.1	11.0	75.11
482.1176	C ₂₃ [13C] H ₉ D ₃ F ₄ N ₅ O ₂	482.1143	3.3	6.8	20.0	73.94
482.1176	C ₁₀ [13C] H ₁₇ D ₃ F ₄ N ₃ O ₁₃	482.1149	2.7	5.6	2.0	72.73
482.1176	C ₁₇ [13C] H ₉ D ₃ F ₄ N ₉ O ₃	482.1216	-4.0	-8.3	16.0	67.51



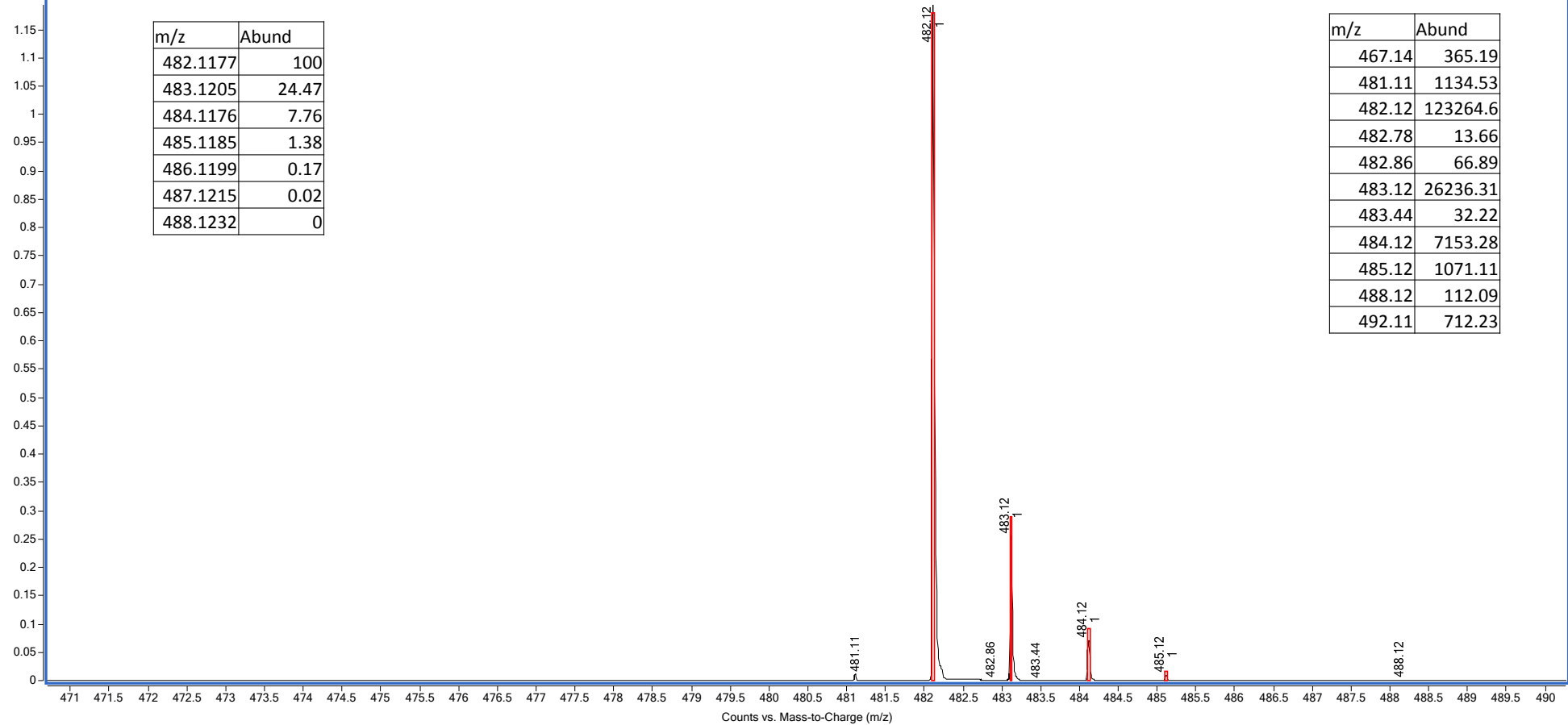
Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (mDa)	Abund (%)	Calc Abund (%)	+/-
1	482.1176	482.1177	-0.1	100.0	100.0	0.0
2	483.1198	483.1205	-0.7	21.3	24.5	3.2
3	484.1172	484.1176	-0.4	5.8	7.8	2.0
4	485.1167	485.1185	-1.8	0.9	1.4	0.5

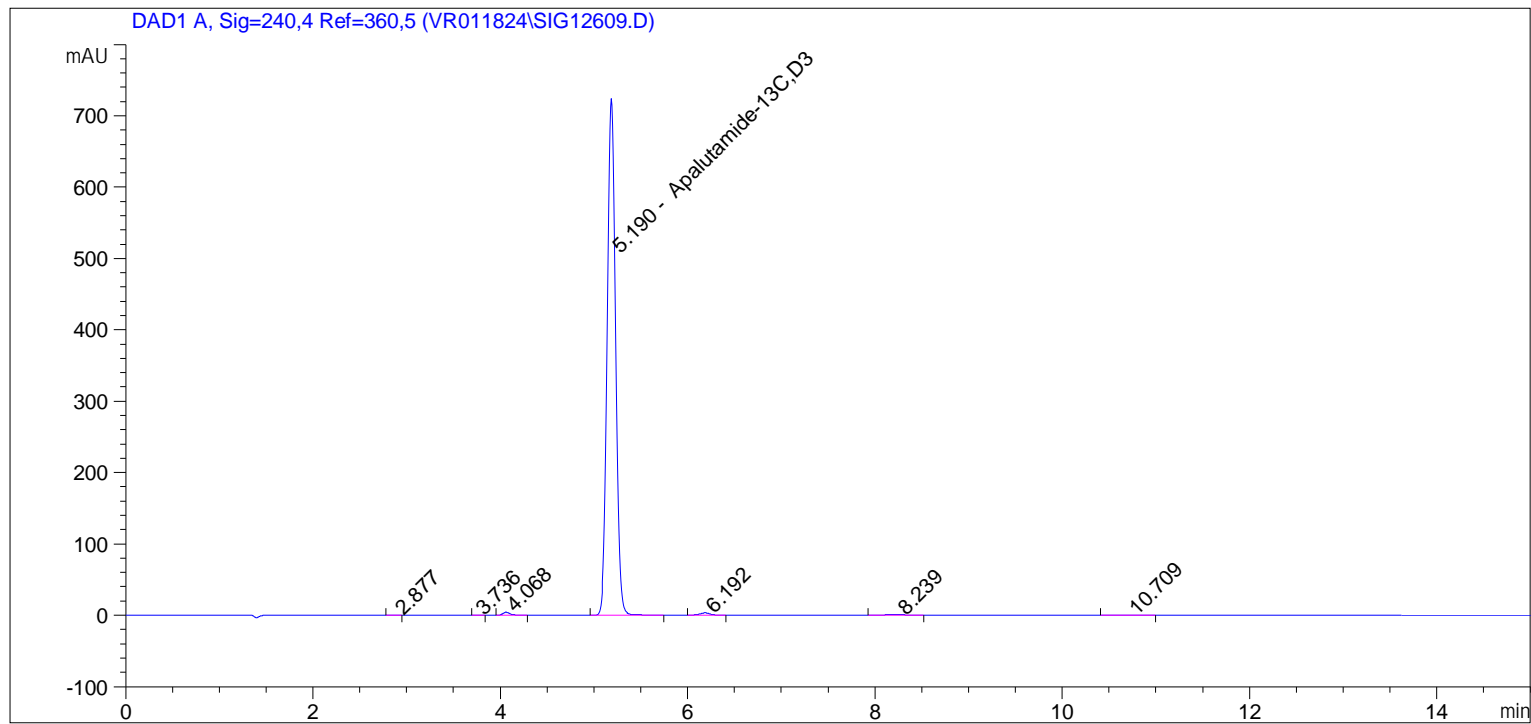
Cpd 1: C20 [13C] H12 D3 F4 N5 O2 S: + Scan (0.6-1.0 min, 21 Scans) 240807_1409.d Subtract

m/z	Abund
482.1177	100
483.1205	24.47
484.1176	7.76
485.1185	1.38
486.1199	0.17
487.1215	0.02
488.1232	0

m/z	Abund
467.14	365.19
481.11	1134.53
482.12	123264.6
482.78	13.66
482.86	66.89
483.12	26236.31
483.44	32.22
484.12	7153.28
485.12	1071.11
488.12	112.09
492.11	712.23



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Acq. Operator : vrusu
Acq. Instrument : Instrument 1 Location : Vial 9
Injection Date : 8/8/2024 9:20:18 AM Inj Volume : 5.0 µl
Acq. Method : C:\CHEM32\1\METHODS\VR080724_167.M
Last changed : 8/8/2024 9:19:12 AM by vrusu
Analysis Method : C:\CHEM32\1\METHODS\VR080824_167PM.M
Last changed : 8/8/2024 1:53:02 PM by vrusu



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Area Percent Report
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Sorted By : Signal
Calib. Data Modified : 8/8/2024 1:51:47 PM
Multiplier: : 1.603e3
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=240,4 Ref=360,5

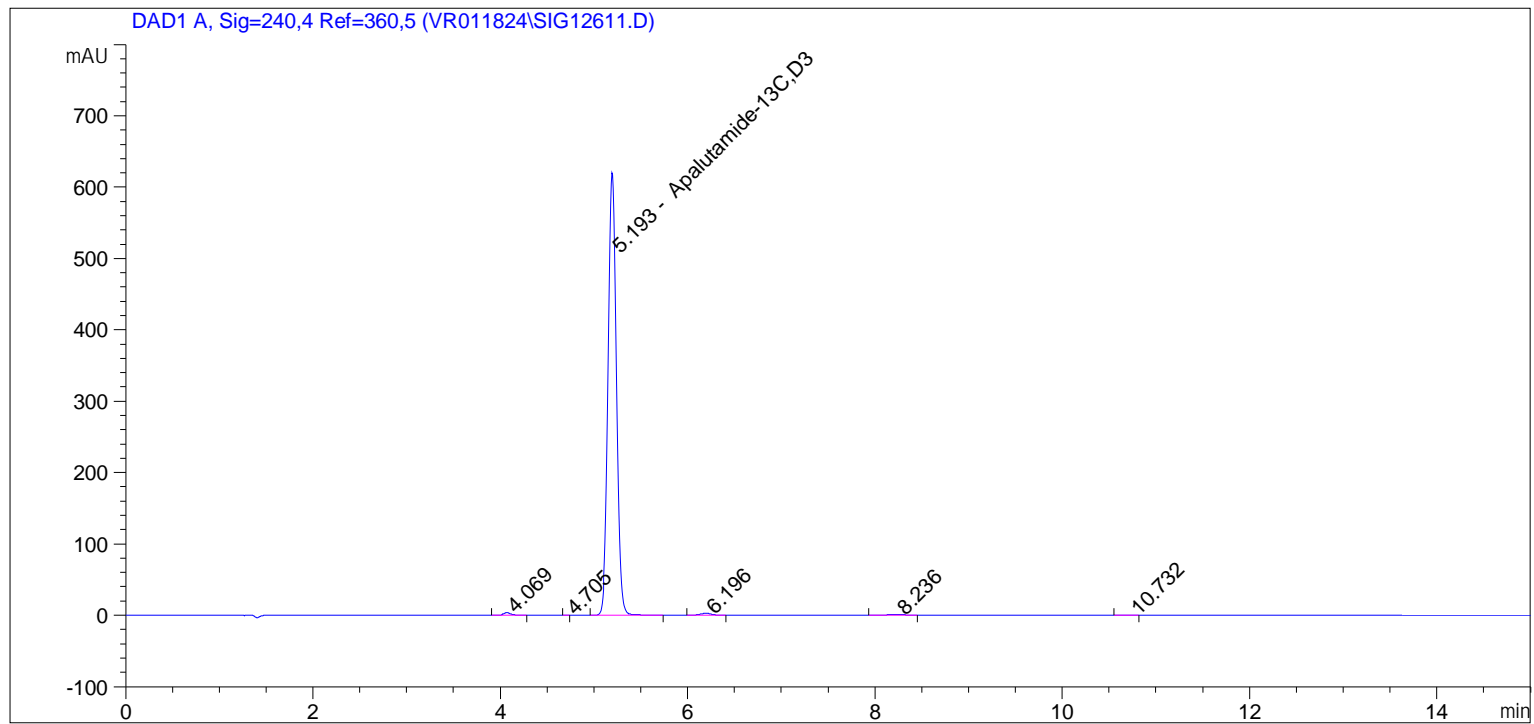
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	2.877	BB	0.0580	4.15770e-1	9.235e-3	?
2	3.736	BB	0.0428	2.10953e-1	4.686e-3	?
3	4.068	BB	0.0823	21.85640	0.4855	?
4	5.190	BB	0.0936	4438.89111	98.5990	Apalutamide-13C,D3
5	6.192	BB	0.1206	24.91293	0.5534	?
6	8.239	BB	0.1679	11.99821	0.2665	?
7	10.709	BB	0.2010	3.67972	0.0817	?

Totals : 4501.96509

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*** End of Report ***

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Acq. Operator : vrusu
Acq. Instrument : Instrument 1 Location : Vial 11
Injection Date : 8/8/2024 10:28:24 AM Inj Volume : 5.0 µl
Acq. Method : C:\CHEM32\1\METHODS\VR080724_167.M
Last changed : 8/8/2024 10:27:21 AM by vrusu
Analysis Method : C:\CHEM32\1\METHODS\VR080824_167PM.M
Last changed : 8/8/2024 1:53:02 PM by vrusu



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Area Percent Report
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Sorted By : Signal
Calib. Data Modified : 8/8/2024 1:51:47 PM
Multiplier: : 1.603e3
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=240,4 Ref=360,5

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	4.069	BB	0.0816	18.35318	0.4759	?
2	4.705	BB	0.0324	1.50919e-1	3.913e-3	?
3	5.193	BB	0.0955	3804.95752	98.6540	Apalutamide-13C,D3
4	6.196	BB	0.1193	21.53205	0.5583	?
5	8.236	BB	0.1810	10.27088	0.2663	?
6	10.732	BV	0.1256	1.60553	0.0416	?

Totals : 3856.87008