

<b>Name:</b>	Dapagliflozin-D5
<b>Lot#:</b>	GR-19-199
<b>Test Date:</b>	12/04/2024 (re-test date: 12/04/2029)
<b>CAS No.:</b>	1204219-80-6
<b>MF:</b>	C <sub>21</sub> H <sub>20</sub> D <sub>5</sub> ClO <sub>6</sub>
<b>MW:</b>	413.90
<b>Appearance:</b>	White solid
<b>Purity:</b>	99.0% by HPLC (average of two sample preparations); 99.7% atom D
<b><sup>1</sup>H-NMR:</b>	Conforms (shows a trace of EtOAc)
<b>MS-ESI (+)</b>	Conforms (shows peaks at m/z = 431.20, 433.20 [M+NH <sub>4</sub> ] <sup>+</sup> ; 436.16, 438.15 [M+Na] <sup>+</sup> exhibits the expected pattern for mono-chloro compounds)
<b>Storage</b>	Store at -18°C in a dry place away from direct sunlight

Approved by:

Date: 12/20/2024



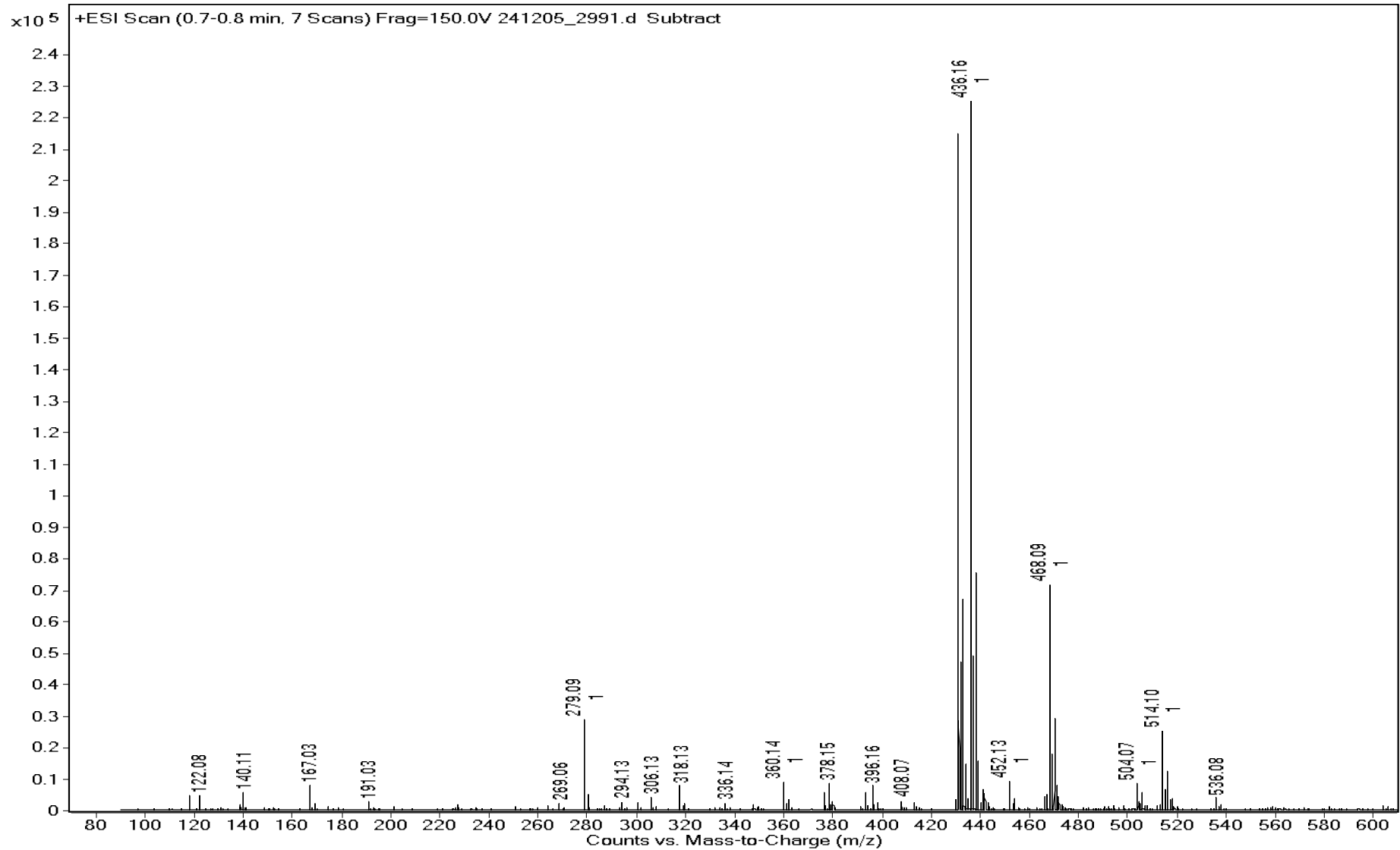
Viorica Rusu, QC/QA Manager

GR-19-199.1.1.1r  
1H-NMR using B600

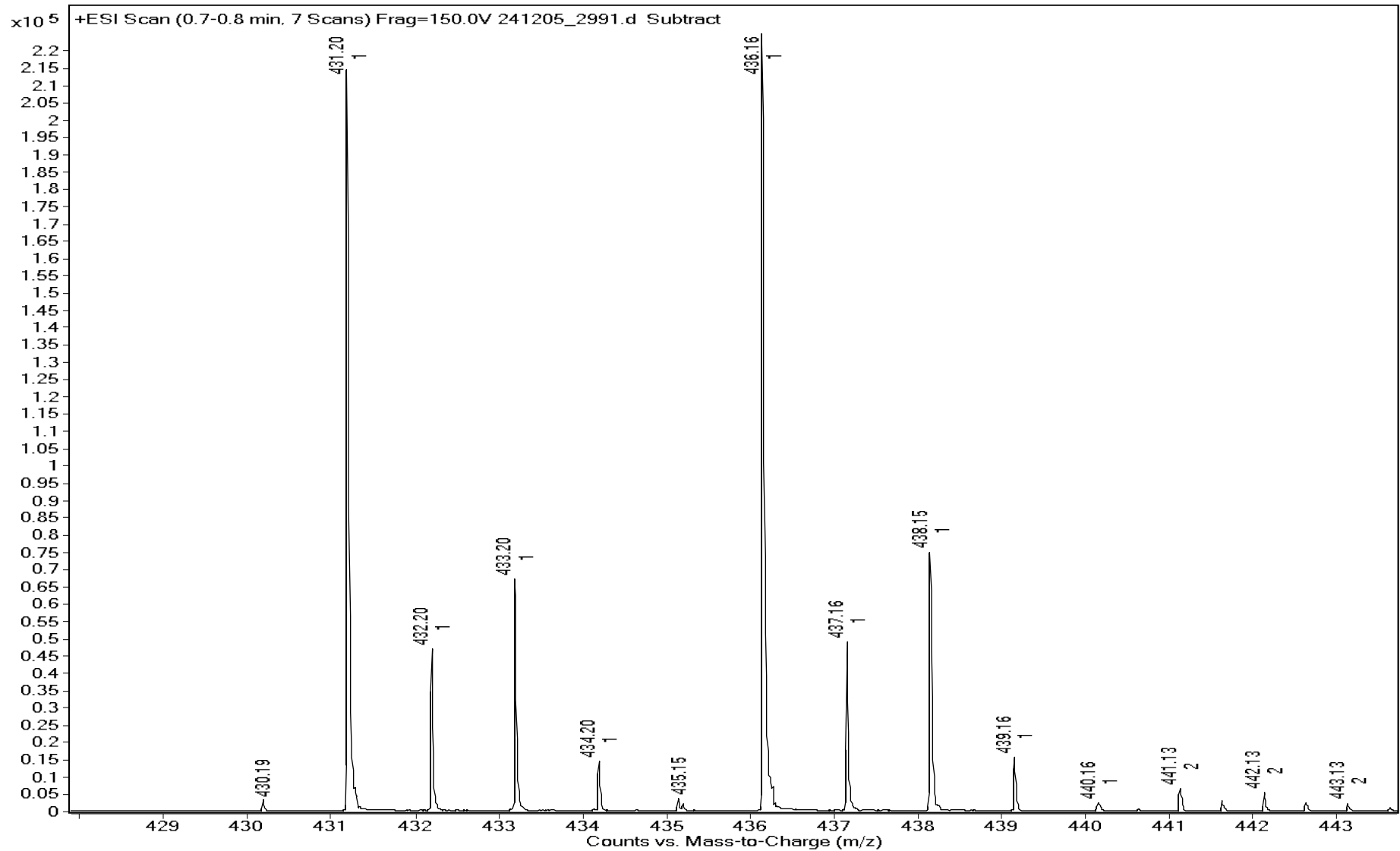
Dapagliflozin-D5  
1H-NMR, 600 MHz  
Solvent: DMSO-D6  
Lot No.: GR-19-199



<b>Sample Name</b>	GR-19-199	<b>Data File</b>	241205_2991.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>	05/12/2024 2:15:02 PM
<b>Comment</b>	ESI+				



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<b>Comment</b>	ESI+				



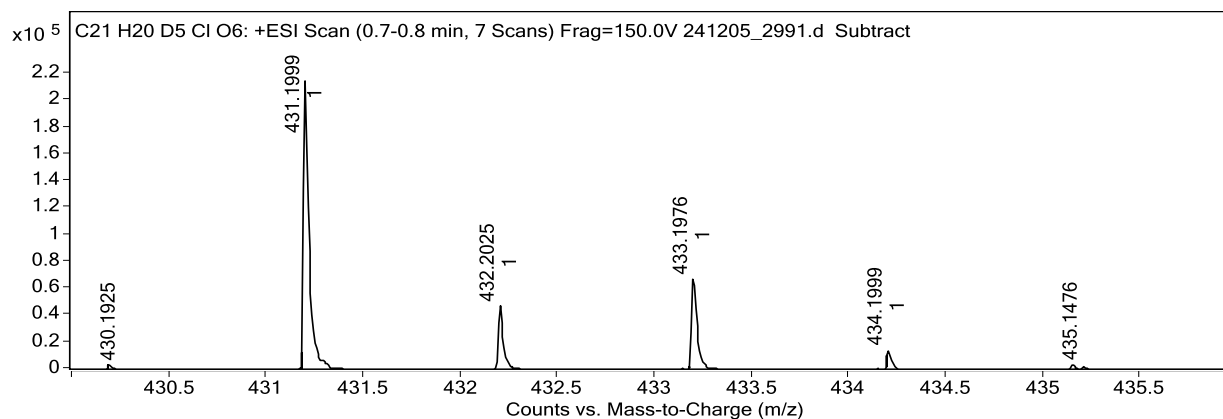
<b>Sample Name</b>	GR-19-199	<b>Data File</b>	241205_2991.d
<b>Acq Method</b>	HRMS.m	<b>DA Method</b>	AIMS_Accurate_Mass.m
<b>Instrument</b>	Agilent 6538 UHD	<b>Acq Date, Time</b>	05/12/2024 2:15:02 PM
<b>Comment</b>	ESI+		

### Target Ion Species

Ion Species	m/z	Ionic Formula
(M+NH4) <sup>+</sup>	431.1999	C21 H24 D5 C1 N O6

### MFG Calculator Results

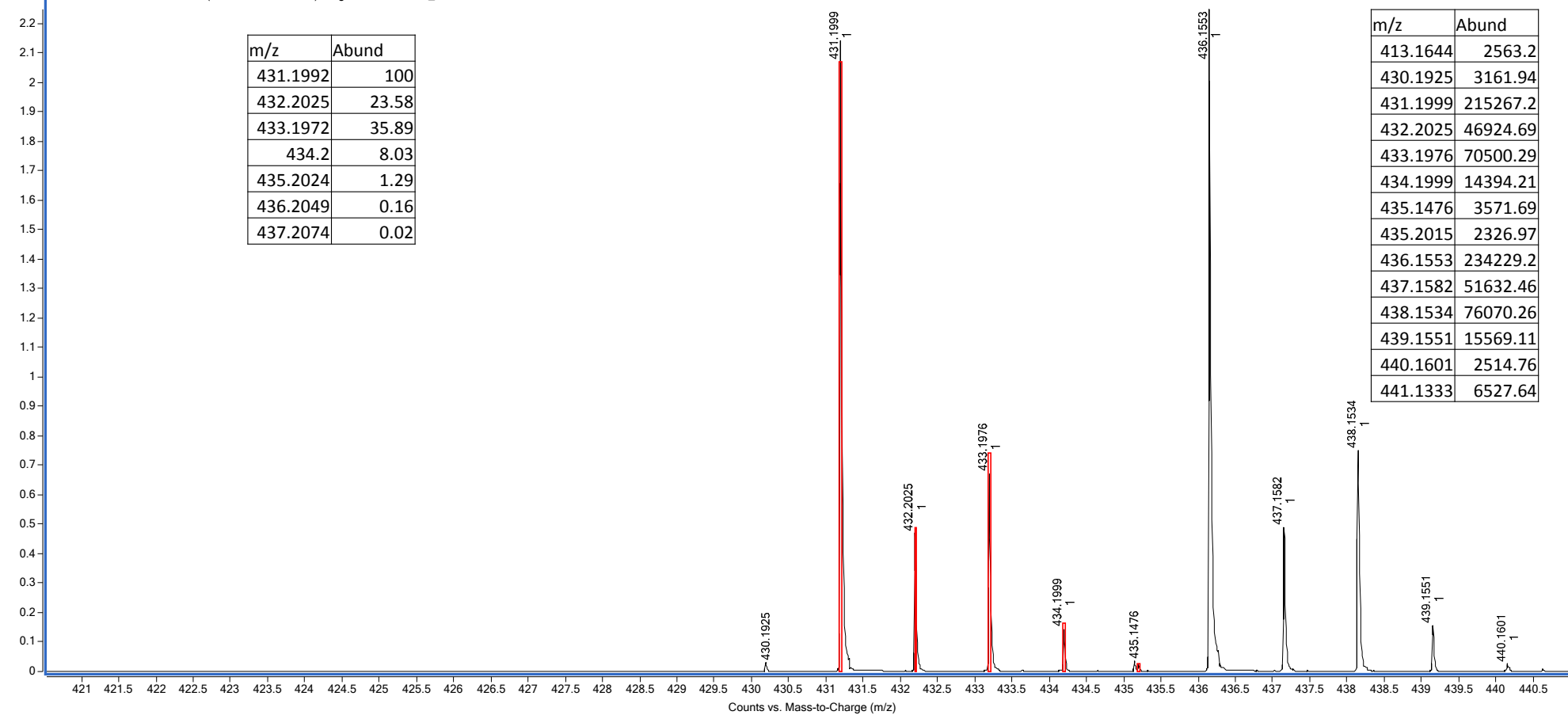
Target m/z	Ionic Formula	Calc m/z	+/- (mDa)	+/- (ppm)	DBE	MFG Score
431.1999	C21 H24 D5 C1 N O6	431.1992	0.7	1.6	9.0	97.93
431.1999	C22 H20 D5 C1 N5 O2	431.2005	-0.6	-1.4	14.0	96.64
431.1999	C18 H16 D5 C1 N11	431.1978	2.1	4.9	15.0	89.23
431.1999	C17 H20 D5 C1 N7 O4	431.1965	3.4	7.9	10.0	77.95
431.1999	C10 H24 D5 C1 N7 O9	431.2024	-2.5	-5.8	1.0	77.33
431.1999	C11 H20 D5 C1 N11 O5	431.2037	-3.8	-8.8	6.0	70.46



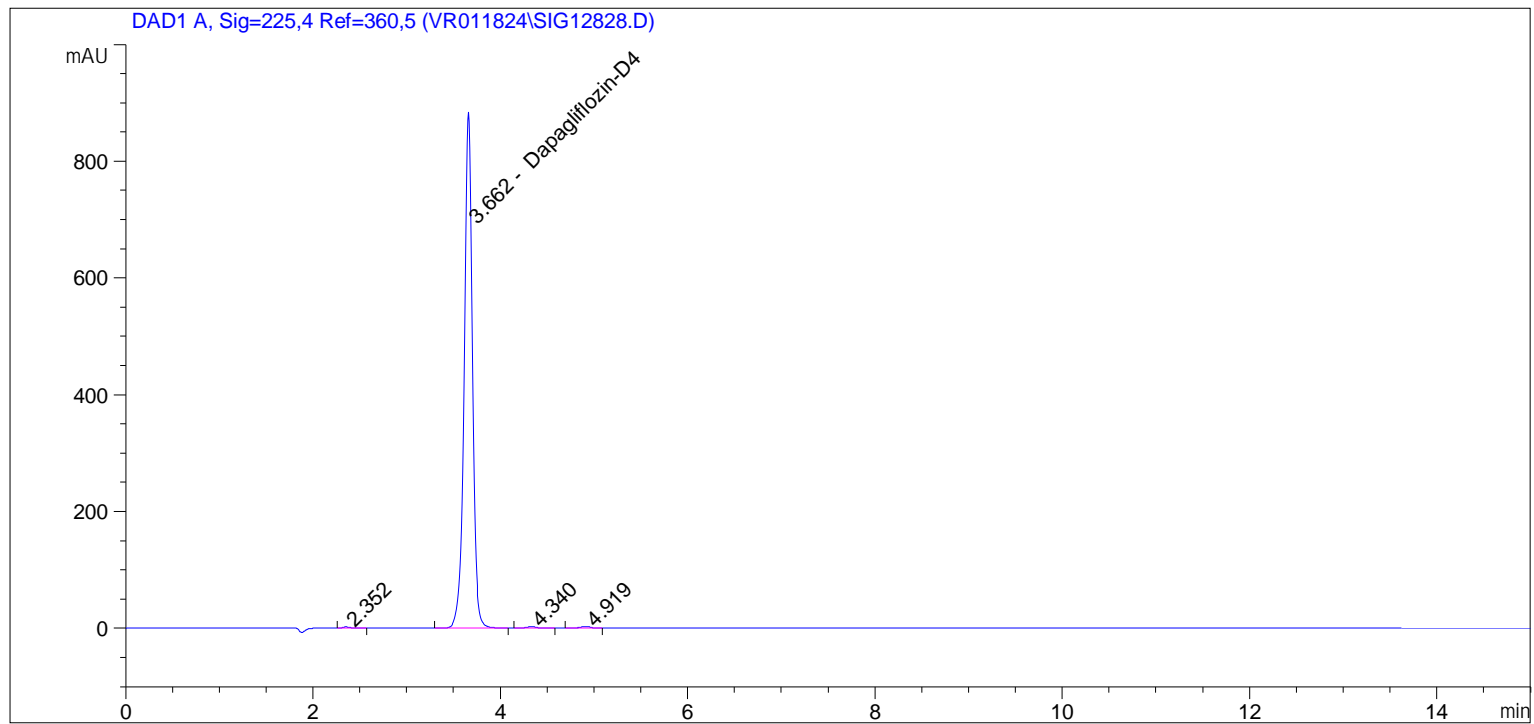
### Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (mDa)	Abund (%)	Calc Abund (%)	+/-
1	431.1999	431.1992	0.7	100.0	100.0	0.0
2	432.2025	432.2025	0.0	21.8	23.6	1.8
3	433.1976	433.1972	0.4	32.8	35.9	3.1
4	434.1999	434.2000	-0.1	6.7	8.0	1.3
5	435.2015	435.2024	-0.9	1.1	1.3	0.2

C21 H20 D5 Cl O6: +ESI Scan (0.7-0.8 min, 7 Scans) Frag=150.0V 241205\_2991.d Subtract



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Acq. Operator :  
Acq. Instrument : Instrument 1 Location : Vial 62  
Injection Date : 12/4/2024 10:21:57 AM Inj Volume : 5.0 µl  
Acq. Method : C:\CHEM32\1\METHODS\VR120424\_199.M  
Last changed : 12/4/2024 10:21:00 AM  
Analysis Method : C:\CHEM32\1\METHODS\VR120424\_199PM.M  
Last changed : 12/4/2024 11:02:09 AM by vrusu



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

Sorted By : Signal  
Calib. Data Modified : 12/4/2024 10:59:53 AM  
Multiplier: : 1.603e3  
Dilution: : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

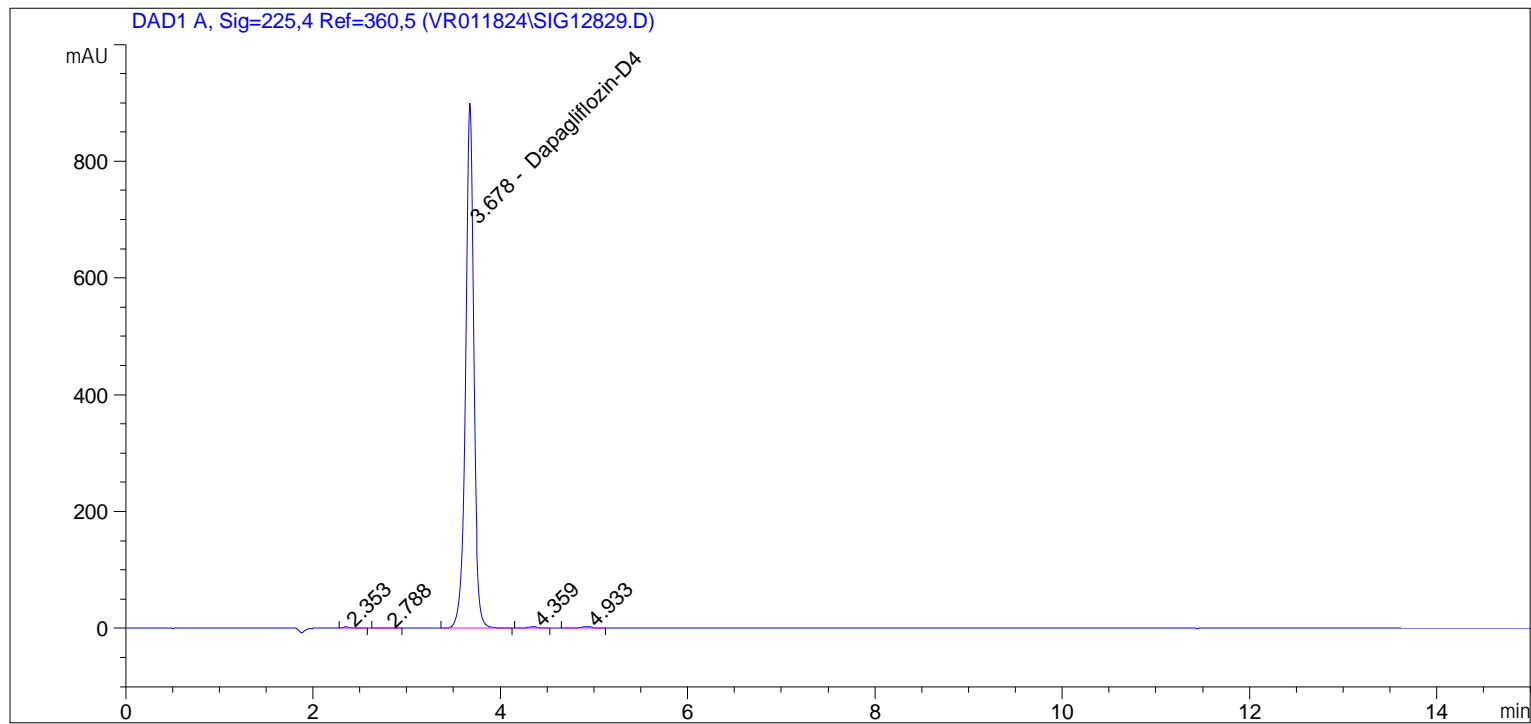
Signal 1: DAD1 A, Sig=225,4 Ref=360,5

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	2.352	BB	0.0788	10.66666	0.1983	?
2	3.662	BB	0.0923	5326.27441	99.0330	Dapagliflozin-D4
3	4.340	BB	0.1083	18.89725	0.3514	?
4	4.919	BB	0.1146	22.44587	0.4173	?

Totals : 5378.28419

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

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Acq. Operator :  
Acq. Instrument : Instrument 1 Location : Vial 63  
Injection Date : 12/4/2024 10:39:21 AM Inj Volume : 5.0 µl  
Acq. Method : C:\CHEM32\1\METHODS\VR120424\_199.M  
Last changed : 12/4/2024 10:38:23 AM  
Analysis Method : C:\CHEM32\1\METHODS\VR120424\_199PM.M  
Last changed : 12/4/2024 11:02:09 AM by vrusu



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

Sorted By : Signal  
Calib. Data Modified : 12/4/2024 10:59:53 AM  
Multiplier: : 1.603e3  
Dilution: : 1.0000  
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=225,4 Ref=360,5

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	2.353	BB	0.0744	10.03323	0.1832	?
2	2.788	BB	0.1070	3.14541	0.0574	?
3	3.678	BB	0.0903	5423.07129	99.0460	Dapagliflozin-D4
4	4.359	BB	0.1048	16.55560	0.3024	?
5	4.933	BB	0.1125	22.49872	0.4109	?

Totals : 5475.30424

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