

Name:	Dapagliflozin-D5 Tetraacetate
Lot#:	GR-19-195
Test Date:	11/28/2024 (re-test date: 11/28/2029)
CAS No.:	461432-25-7 unlabeled
MF:	C ₂₉ H ₂₈ D ₅ ClO ₁₀
MW:	582.05
Appearance:	White solid
Purity:	98.7% by HPLC (average of two sample preparations); 99.7% atom D
¹H-NMR:	Conforms (shows a trace of MeOH)
MS-ESI (+)	Conforms (shows peaks at m/z = 599.24, 601.24 [M+NH ₄] ⁺ ; 604.20, 606.20 [M+Na] ⁺ exhibits the expected pattern for mono-chloro compounds)
Storage	Store at -18°C in a dry place away from direct sunlight

Approved by:

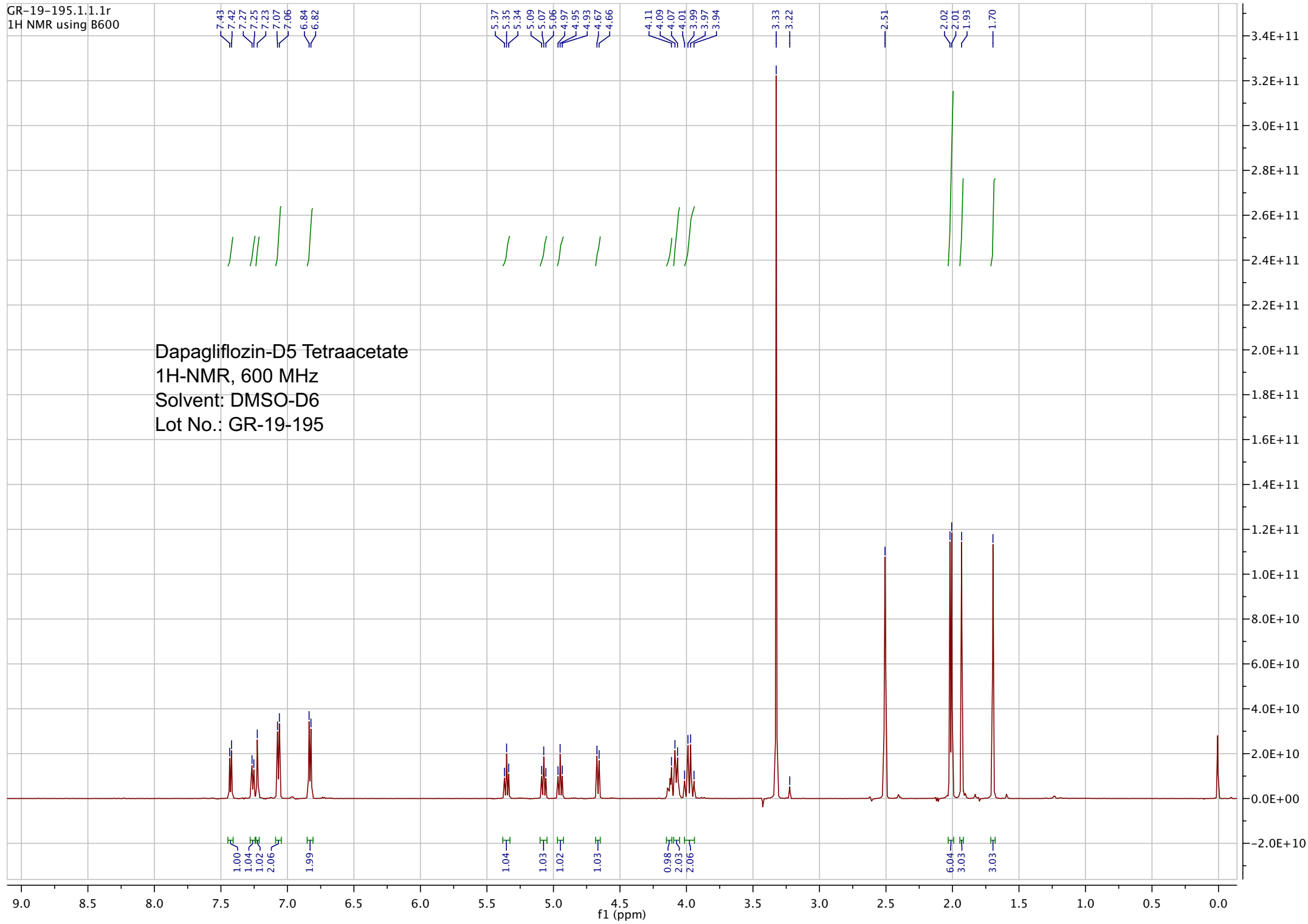
Date: 12/20/2024



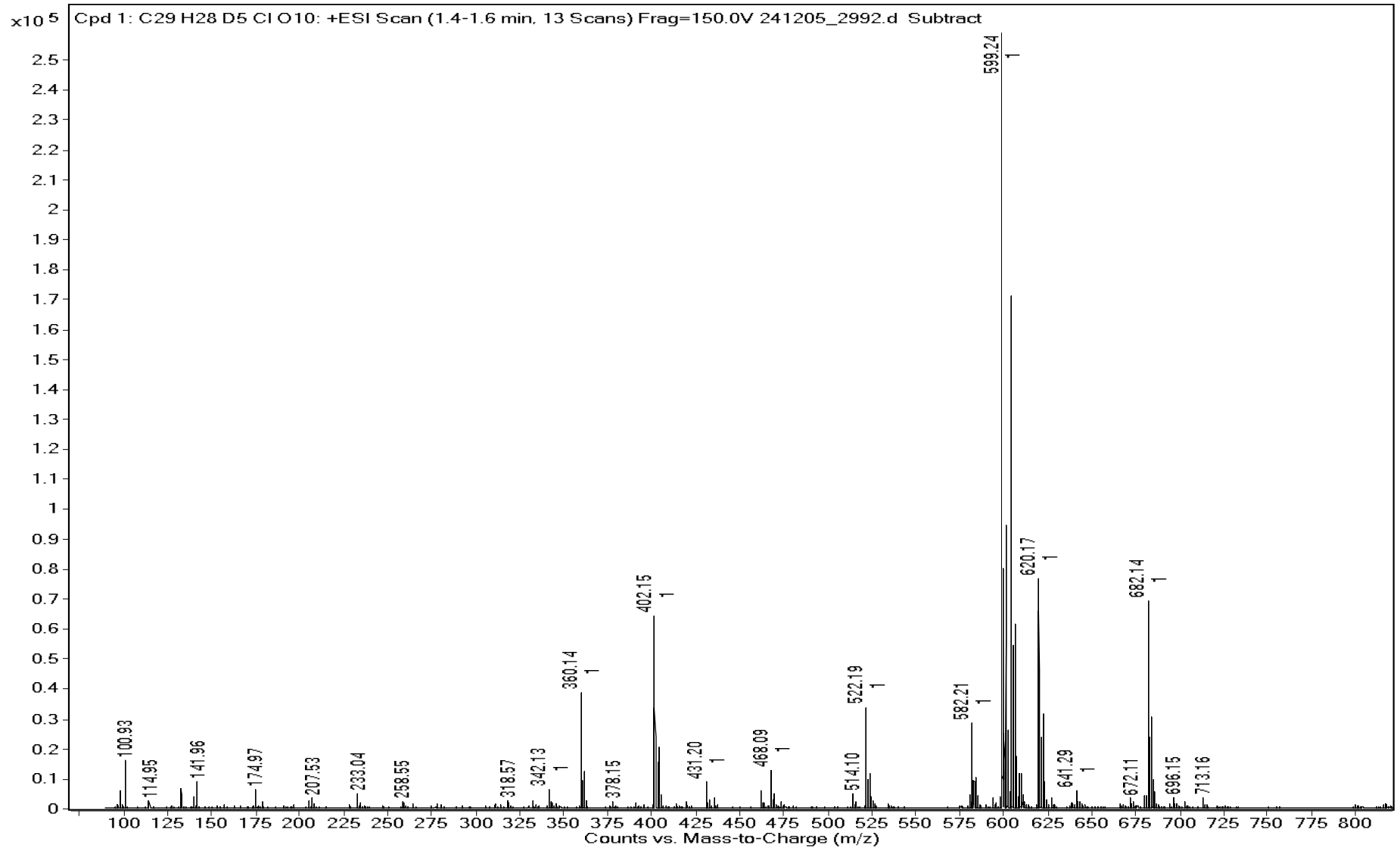
Viorica Rusu, QC/QA Manager

GR-19-195.1.1.1r
1H NMR using B600

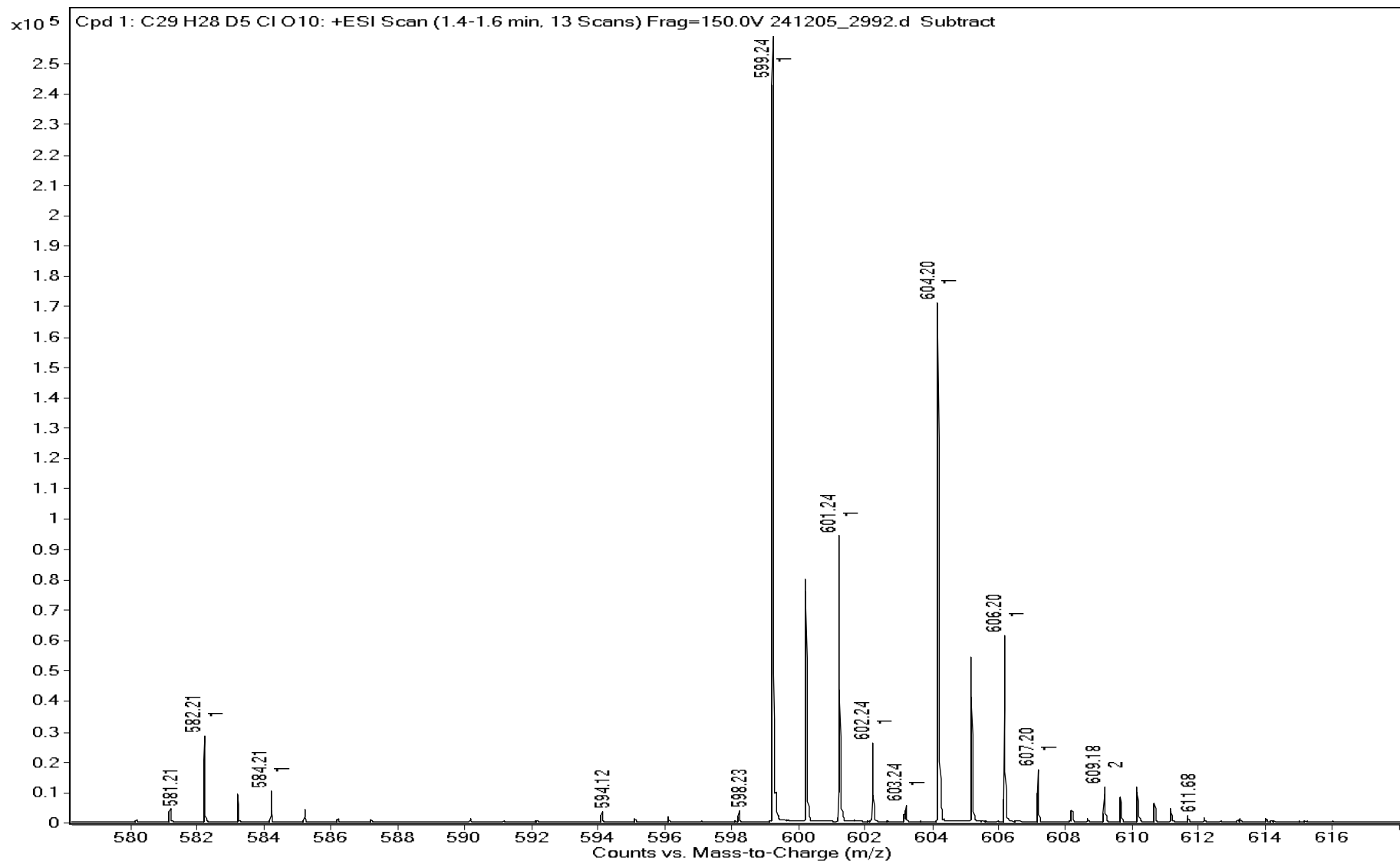
Dapagliflozin-D5 Tetraacetate
1H-NMR, 600 MHz
Solvent: DMSO-D6
Lot No.: GR-19-195



Sample Name	GR-19-195	Data File	241205_2992.d	Acq Method	HRMS.m
DA Method	AIMS_Accurate_Mass.m	Instrument	Agilent 6538 UHD	Acq Date, Time	05/12/2024 2:51:55 PM
Comment	ESI+				



Sample Name	GR-19-195	Data File	241205_2992.d	Acq Method	HRMS.m
DA Method	AIMS_Accurate_Mass.m	Instrument	Agilent 6538 UHD	Acq Date, Time	05/12/2024 2:51:55 PM
Comment	ESI+				



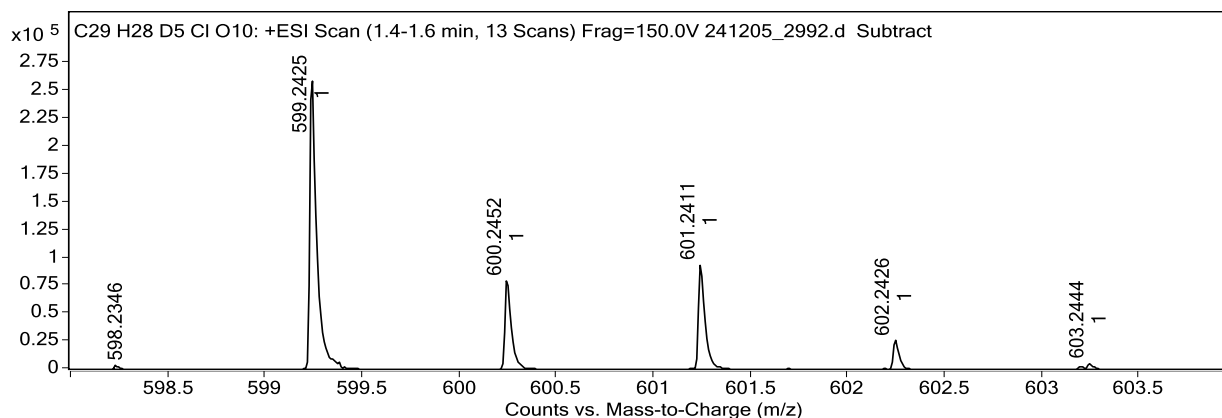
Sample Name	GR-19-195	Data File	241205_2992.d
Acq Method	HRMS.m	DA Method	AIMS_Accurate_Mass.m
Instrument	Agilent 6538 UHD	Acq Date, Time	05/12/2024 2:51:55 PM
Comment	ESI+		

Target Ion Species

Ion Species	m/z	Ionic Formula
(M+NH4) ⁺	599.2425	C29 H32 D5 C1 N O10

MFG Calculator Results

Target m/z	Ionic Formula	Calc m/z	+/- (mDa)	+/- (ppm)	DBE	MFG Score
599.2425	C30 H28 D5 C1 N5 O6	599.2428	-0.3	-0.5	18.0	98.82
599.2425	C29 H32 D5 C1 N O10	599.2414	1.1	1.8	13.0	97.96
599.2425	C31 H24 D5 C1 N9 O2	599.2441	-1.6	-2.7	23.0	93.51
599.2425	C26 H24 D5 C1 N11 O4	599.2401	2.4	4.0	19.0	90.62
599.2425	C17 H36 D5 C1 N3 O17	599.2433	-0.8	-1.3	0.0	85.20
599.2425	C18 H32 D5 C1 N7 O13	599.2446	-2.1	-3.5	5.0	84.18
599.2425	C25 H28 D5 C1 N7 O8	599.2387	3.8	6.3	14.0	80.85
599.2425	C19 H28 D5 C1 N11 O9	599.2460	-3.5	-5.8	10.0	79.47
599.2425	C35 H28 D5 C1 N3 O4	599.2468	-4.3	-7.2	22.0	71.70
599.2425	C24 H32 D5 C1 N3 O12	599.2374	5.1	8.5	9.0	69.59



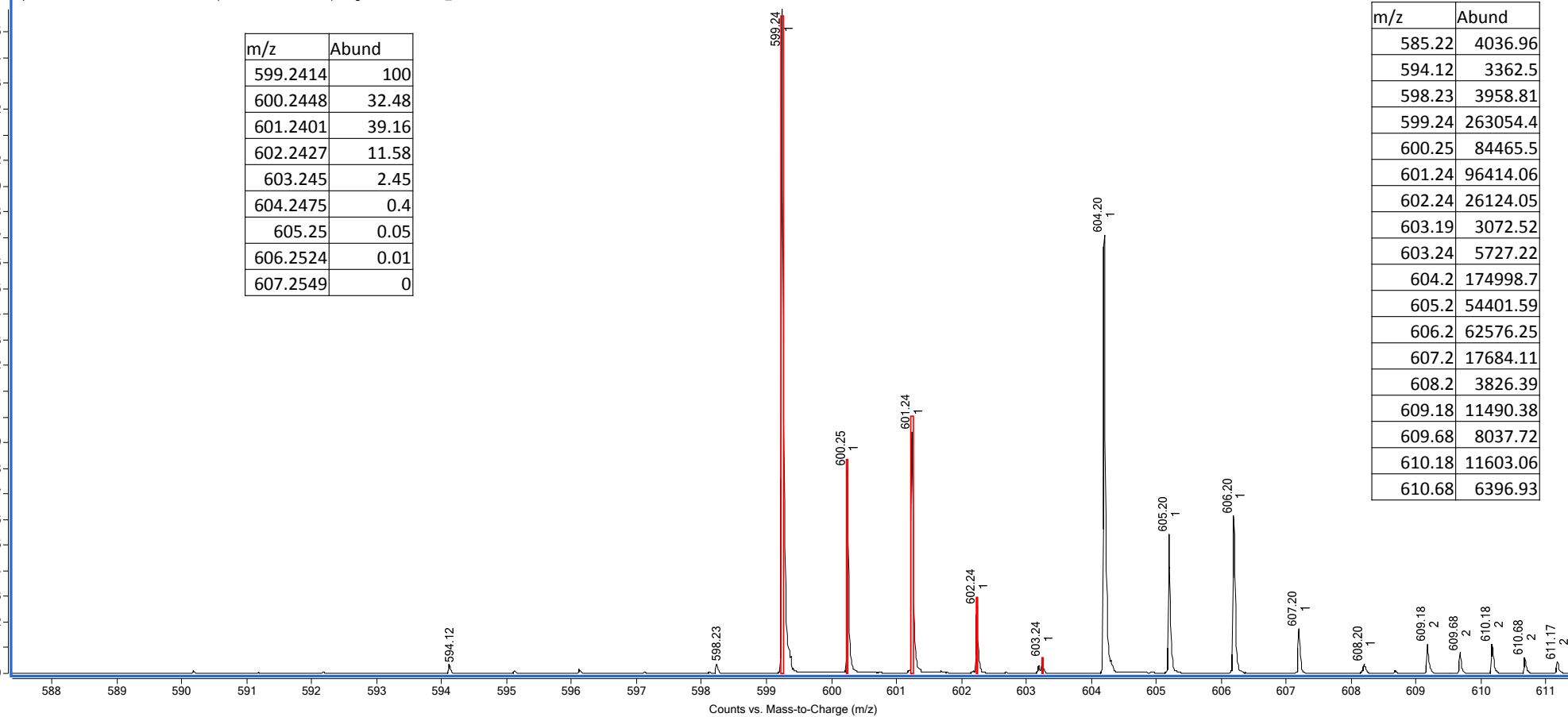
Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (mDa)	Abund (%)	Calc Abund (%)	+/-
1	599.2425	599.2414	1.1	100.0	100.0	0.0
2	600.2452	600.2448	0.4	32.1	32.5	0.4
3	601.2411	601.2401	1.0	36.7	39.2	2.5
4	602.2426	602.2427	-0.1	9.9	11.6	1.7
5	603.2444	603.2450	-0.6	2.2	2.5	0.3

x10⁵ Cpd 1: C29 H28 D5 Cl O10: +ESI Scan (1.4-1.6 min, 13 Scans) Frag=150.0V 241205_2992.d Subtract

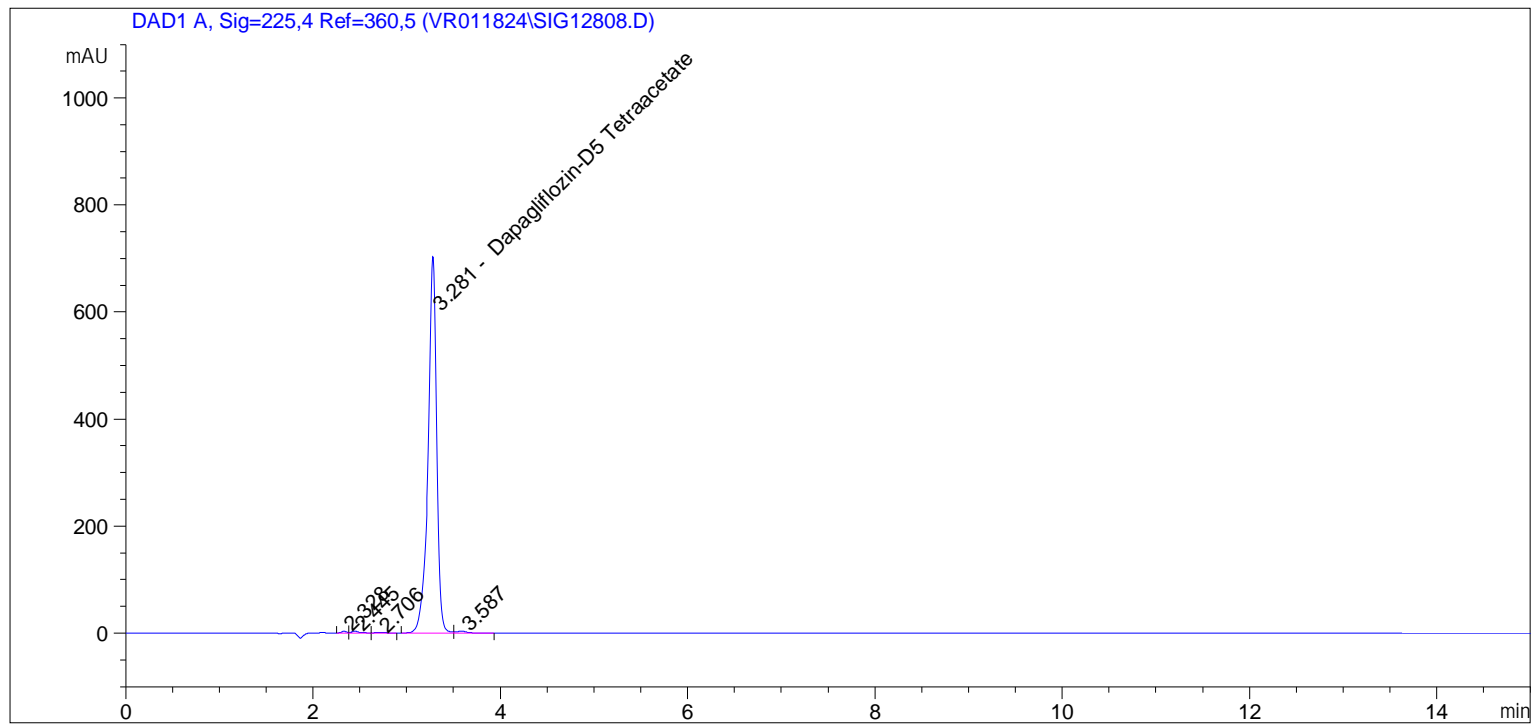
m/z	Abund
599.2414	100
600.2448	32.48
601.2401	39.16
602.2427	11.58
603.245	2.45
604.2475	0.4
605.25	0.05
606.2524	0.01
607.2549	0

m/z	Abund
585.22	4036.96
594.12	3362.5
598.23	3958.81
599.24	263054.4
600.25	84465.5
601.24	96414.06
602.24	26124.05
603.19	3072.52
603.24	5727.22
604.2	174998.7
605.2	54401.59
606.2	62576.25
607.2	17684.11
608.2	3826.39
609.18	11490.38
609.68	8037.72
610.18	11603.06
610.68	6396.93



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Acq. Operator   :
Acq. Instrument : Instrument 1                Location : Vial 49
Injection Date  : 11/28/2024 9:33:30 AM
                                           Inj Volume : 5.0 µl
Acq. Method     : C:\CHEM32\1\METHODS\VR112824_195.M
Last changed    : 11/28/2024 9:32:30 AM
Analysis Method  : C:\CHEM32\1\METHODS\VR112824_195PM.M
Last changed     : 11/28/2024 11:21:47 AM by vrusu
  
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 Area Percent Report
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Sorted By           :      Signal
Calib. Data Modified :      11/28/2024 11:20:56 AM
Multiplier:         :      1.603e3
Dilution:           :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
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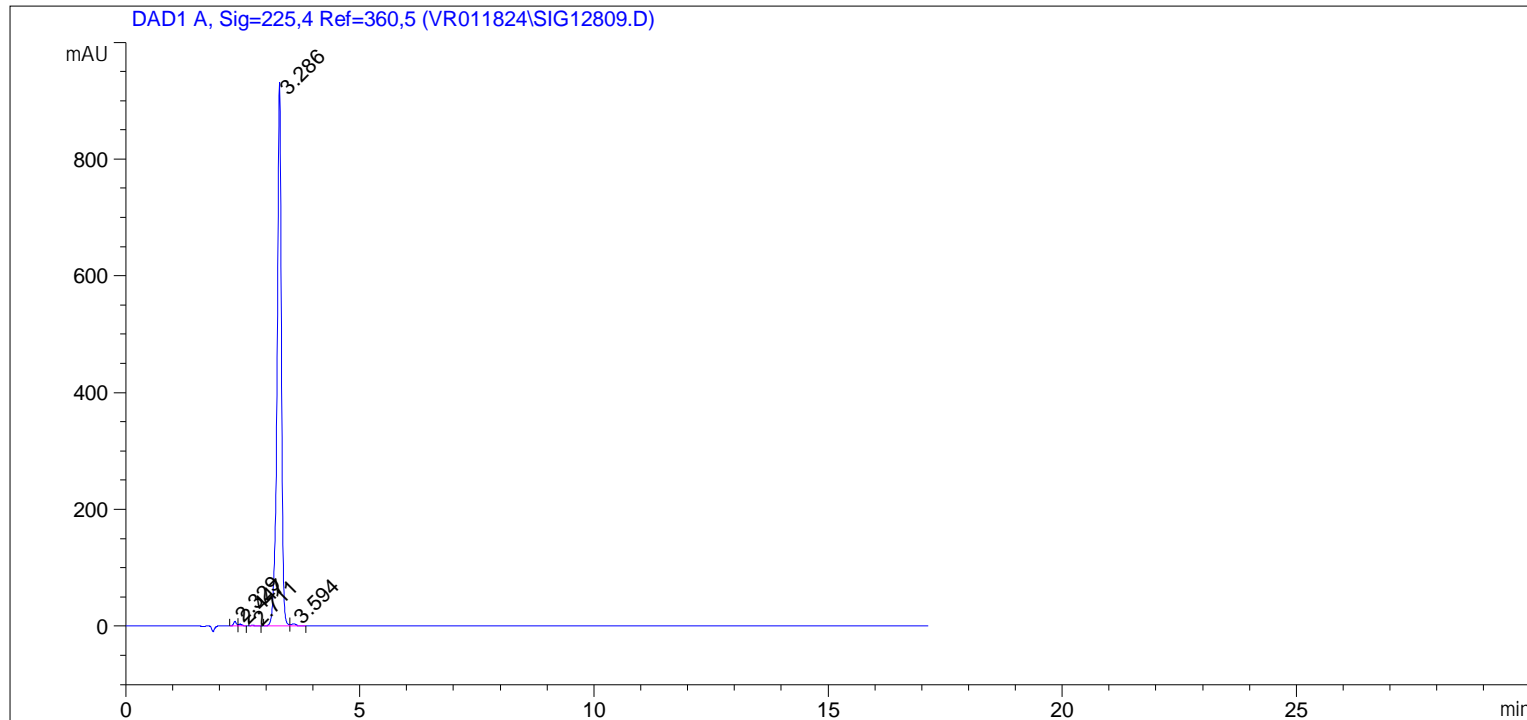
Signal 1: DAD1 A, Sig=225,4 Ref=360,5

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	2.328	BV	0.0640	12.46052	0.2751	?
2	2.445	VV	0.0785	18.27835	0.4035	?
3	2.706	VB	0.0866	7.84227	0.1731	?
4	3.281	BV	0.0939	4466.86816	98.6081	Dapagliflozin-D5 Tetraacetate
5	3.587	VB	0.1021	24.46958	0.5402	?

Totals : 4529.91888

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 *** End of Report ***

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Acq. Operator :
Acq. Instrument : Instrument 1 Location : Vial 50
Injection Date : 11/28/2024 10:07:23 AM Inj Volume : 5.0 µl
Acq. Method : C:\CHEM32\1\METHODS\VR112824_195.M
Last changed : 11/28/2024 10:06:26 AM
Analysis Method : C:\CHEM32\1\METHODS\VR121824_143PM.M
Last changed : 12/20/2024 9:58:33 AM by vrusu
(modified after loading)



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Area Percent Report
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Sorted By : Signal
Calib. Data Modified : 12/18/2024 4:03:46 PM
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	2.329	BV	0.0644	32.28525	0.5401	?
2	2.447	VB	0.0696	13.83801	0.2315	?
3	2.711	BB	0.0755	5.53436	0.0926	?
4	3.286	BV	0.0938	5899.77051	98.6982	?
5	3.594	VB	0.0976	26.15736	0.4376	?

Totals : 5977.58549

Sample Name: GR-19-195 spl-2

Signal 2: DAD1 A, Sig=240,4 Ref=360,5 not found

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	6.200		0.0000	0.00000	0.0000	Norethindrone Acetate-D6

Totals : 0.00000

1 Warnings or Errors :

Warning : Calibrated compound(s) not found

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*** End of Report ***