

Name:	Oxo Dapagliflozin
Lot#:	GR-19-181
Test Date:	11/01/2024 (re-test date: 11/01/2029)
CAS No.:	2169998-23-4
MF:	C ₂₁ H ₂₃ ClO ₇
MW:	422.86
Appearance:	White solid
Purity:	98.7% by HPLC (average of two sample preparations)
¹H-NMR:	Conforms (shows a trace of ACM and Hexanes)
MS-ESI (+)	Conforms (shows peaks at m/z = 413.12 & 415.12 [M + H] ⁺ , shows the expected pattern for mono- chloro-compounds)
Storage	Store at 0-5°C in a dry place away from direct sunlight

Approved by:

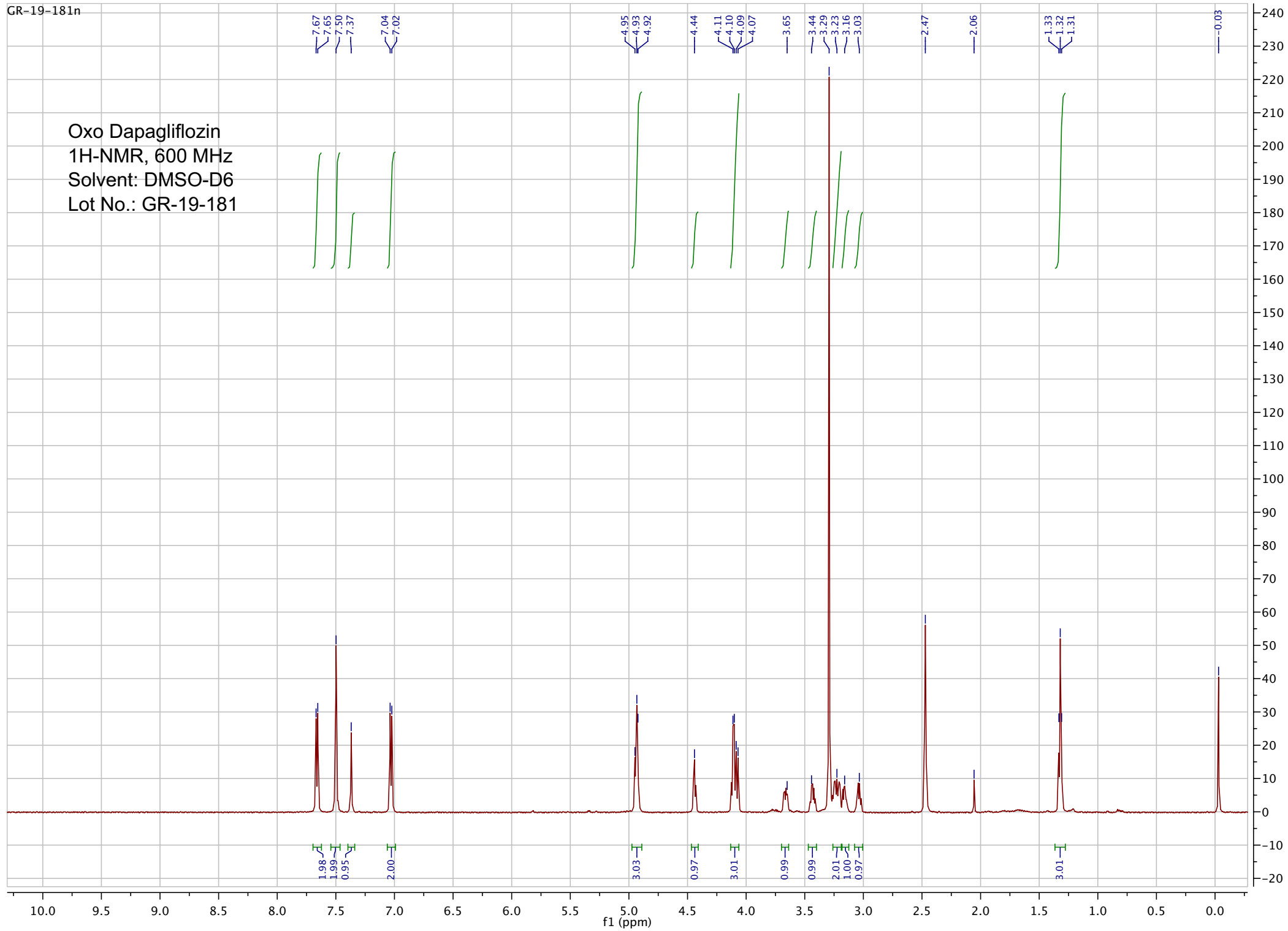
Date: 11/08/2024

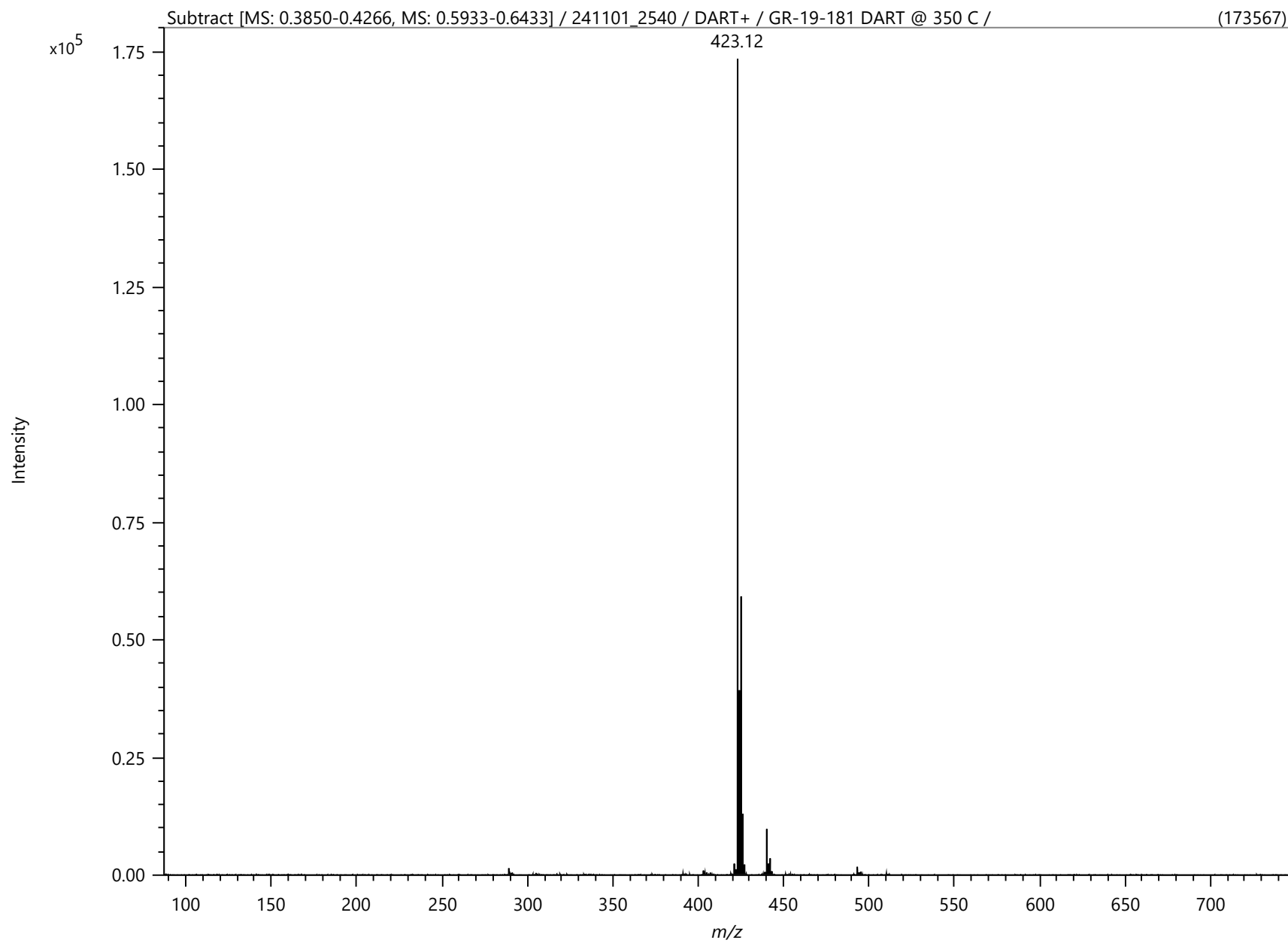


Viorica Rusu, QC/QA Manager

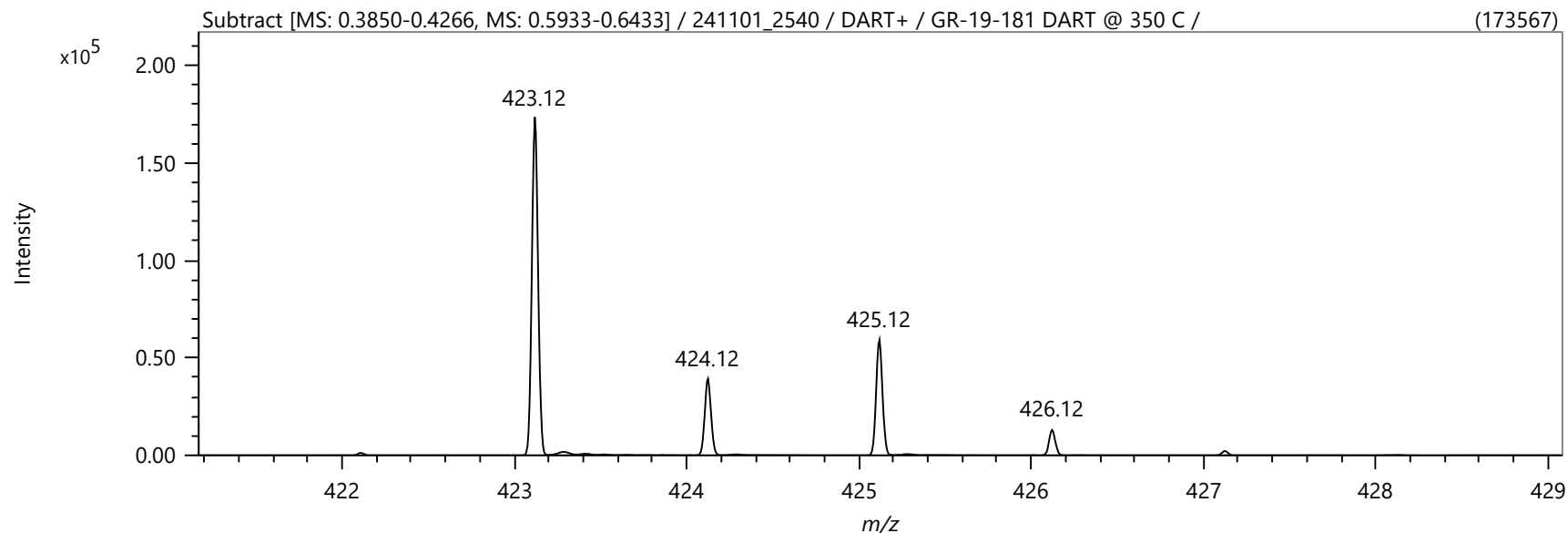
GR-19-181n

Oxo Dapagliflozin
1H-NMR, 600 MHz
Solvent: DMSO-D6
Lot No.: GR-19-181





Spectrum



Elemental Composition

Parameters

Tolerance: ±5.00 mDa
 Electron: Even
 Charge: +1
 DBE: -1.5 - 100.0

Elements Set 1:

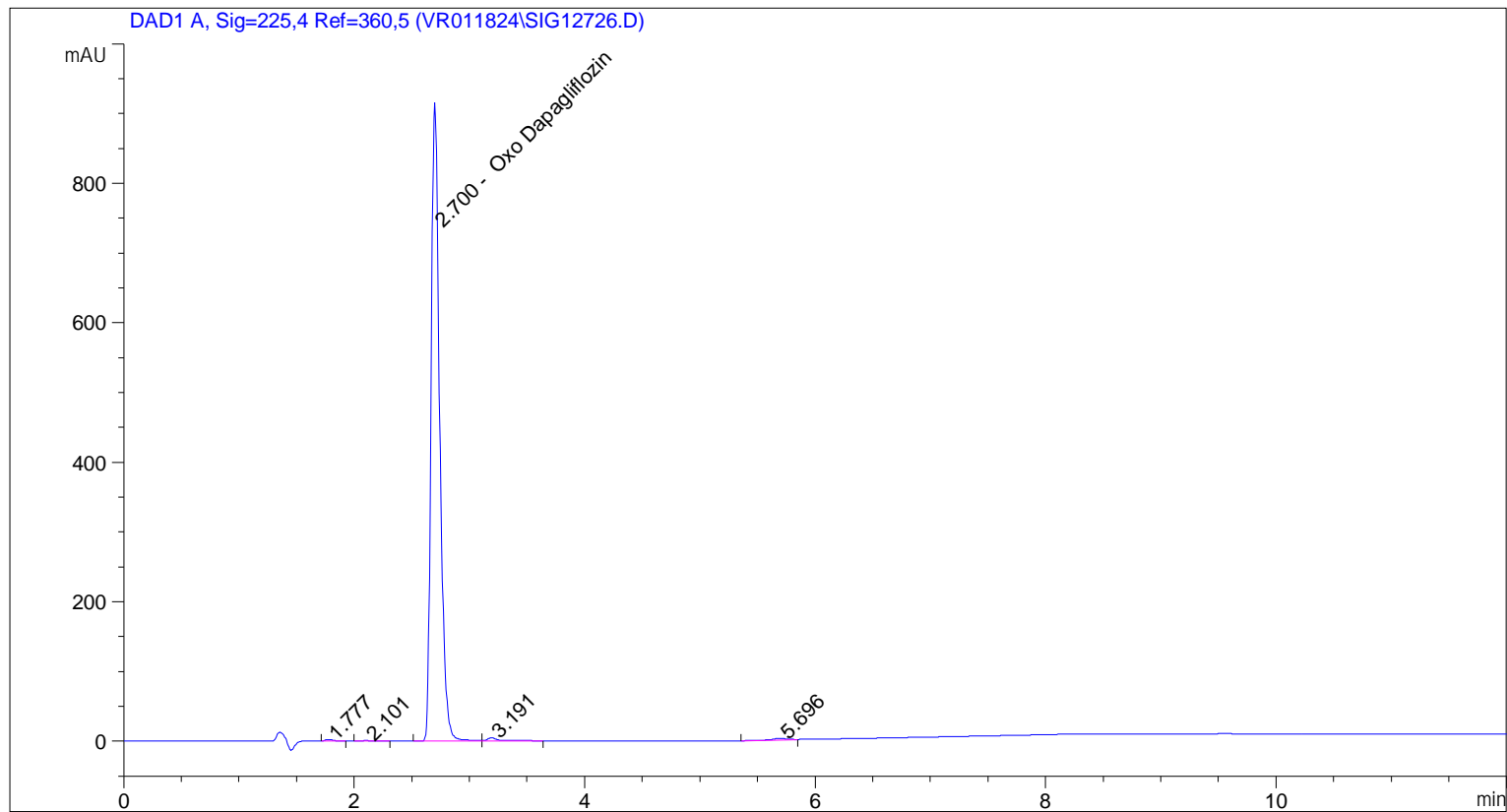
Symbol	C	H	O	N	Cl
Min	0	0	0	0	0
Max	100	200	20	10	1

Results

Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
423.12031	173567.34	C ₂₁ H ₂₄ O ₇ Cl	423.12051	-0.19	-0.46	9.5
		C ₁₀ H ₂₃ N ₄ O ₁₄	423.12053	-0.21	-0.51	1.5
		C ₂₃ H ₁₅ N ₆ O ₃	423.12001	0.30	0.71	19.5
		C ₁₈ H ₁₆ N ₁₀ O ₄ Cl	423.11916	1.15	2.73	15.5
		C ₂₂ H ₂₀ N ₄ O ₃ Cl	423.12184	-1.53	-3.62	14.5
		C ₁₁ H ₁₉ N ₈ O ₁₀	423.12187	-1.55	-3.67	6.5

Mass	Intensity	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
		C22 H19 N2 O7	423.11868	1.64	3.87	14.5
		C27 H19 O5	423.12270	-2.39	-5.64	18.5
		C6 H19 N10 O12	423.11784	2.47	5.84	2.5
		C17 H20 N6 O5 Cl	423.11782	2.49	5.89	10.5
		C10 H24 N6 O10 Cl	423.12370	-3.38	-7.99	1.5
		C34 H15	423.11683	3.49	8.24	27.5
		C28 H15 N4 O	423.12404	-3.72	-8.80	23.5
		C16 H24 N2 O9 Cl	423.11648	3.83	9.05	5.5
		C15 H23 N2 O12	423.12455	-4.24	-10.01	5.5
		C18 H15 N8 O5	423.11599	4.32	10.21	15.5
		C11 H20 N10 O6 Cl	423.12503	-4.72	-11.15	6.5

=====
Acq. Operator : vrusu
Acq. Instrument : Instrument 1 Location : Vial 97
Injection Date : 11/1/2024 2:47:07 PM Inj Volume : 5.0 µl
Acq. Method : C:\CHEM32\1\METHODS\VR110124_181.M
Last changed : 11/1/2024 2:46:03 PM by vrusu
Analysis Method : C:\CHEM32\1\METHODS\VR110124_181PM.M
Last changed : 11/1/2024 3:21:01 PM by vrusu



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

Sorted By : Signal
Calib. Data Modified : 11/1/2024 3:20:10 PM
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

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

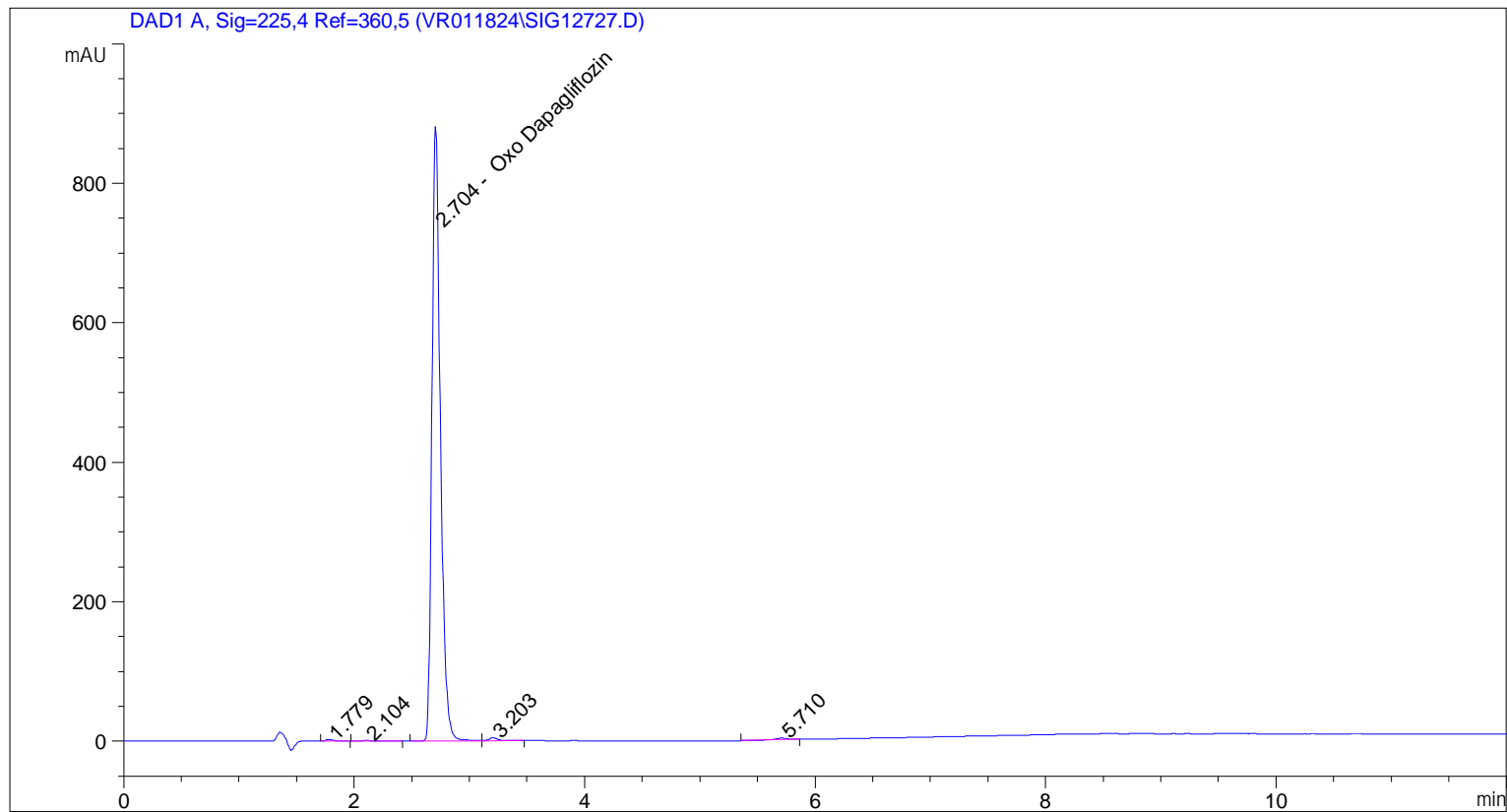
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	1.777	BB	0.0670	9.66673	0.2020	?
2	2.101	BB	0.0841	4.96235	0.1037	?
3	2.700	BV	0.0782	4725.23389	98.7249	Oxo Dapagliflozin
4	3.191	VB	0.0945	29.86704	0.6240	?
5	5.696	BB	0.1132	16.53574	0.3455	?

Totals : 4786.26574

=====

*** End of Report ***

=====
Acq. Operator : vrusu
Acq. Instrument : Instrument 1 Location : Vial 98
Injection Date : 11/1/2024 3:04:52 PM
Inj Volume : 5.0 µl
Acq. Method : C:\CHEM32\1\METHODS\VR110124_181.M
Last changed : 11/1/2024 3:03:45 PM by vrusu
Analysis Method : C:\CHEM32\1\METHODS\VR110124_181PM.M
Last changed : 11/1/2024 3:21:01 PM by vrusu



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

Sorted By : Signal
Calib. Data Modified : 11/1/2024 3:20:10 PM
Multiplier: : 1.0000
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	1.779	BB	0.0647	9.31263	0.2030	?
2	2.104	BB	0.0894	4.71602	0.1028	?
3	2.704	BV	0.0780	4531.79053	98.7686	Oxo Dapagliflozin
4	3.203	VB	0.0815	23.58955	0.5141	?
5	5.710	BB	0.1140	18.88358	0.4116	?

Totals : 4588.29231

=====

*** End of Report ***