

Name:	24-Nor Tauroolithocholic Acid-D4 Sodium
Lot#:	GR-19-119
Test Date:	04/22/2024 (re-test date: 04/22/2029)
CAS No.:	NA
MF:	C ₂₅ H ₃₈ D ₄ NNaO ₅ S
MW:	495.68
Appearance:	White solid
Purity:	99.7% by HPLC (average of two sample preparations); >98% atom D
¹H-NMR:	Conforms
MS-ESI (-)	Conforms (shows peak at m/z = 472.30 [M-Na] ⁻)
Storage	Store at -18°C in a dry place away from direct sunlight

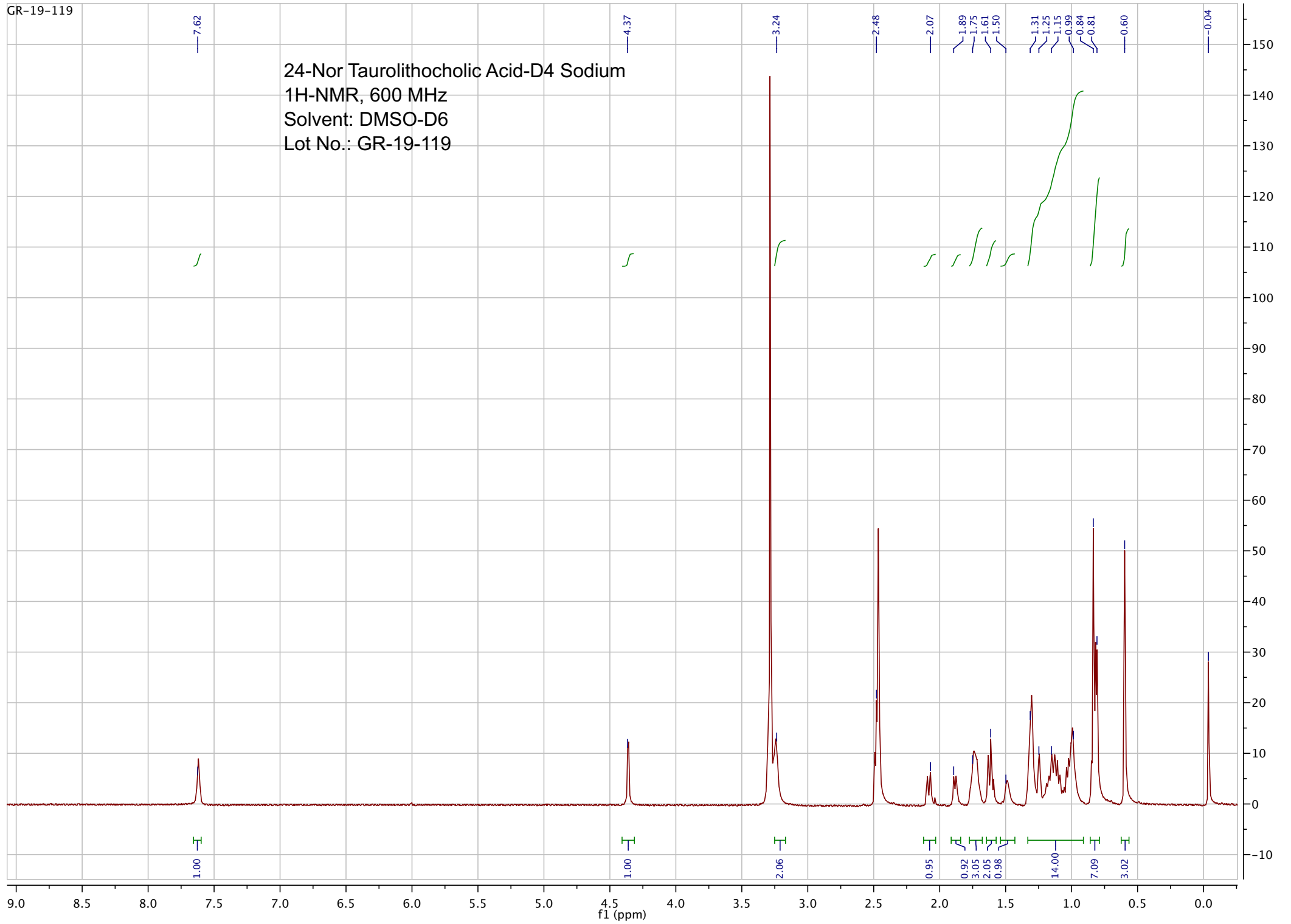
Approved by:

Date: 05/09/2024



Viorica Rusu, QC/QA Manager

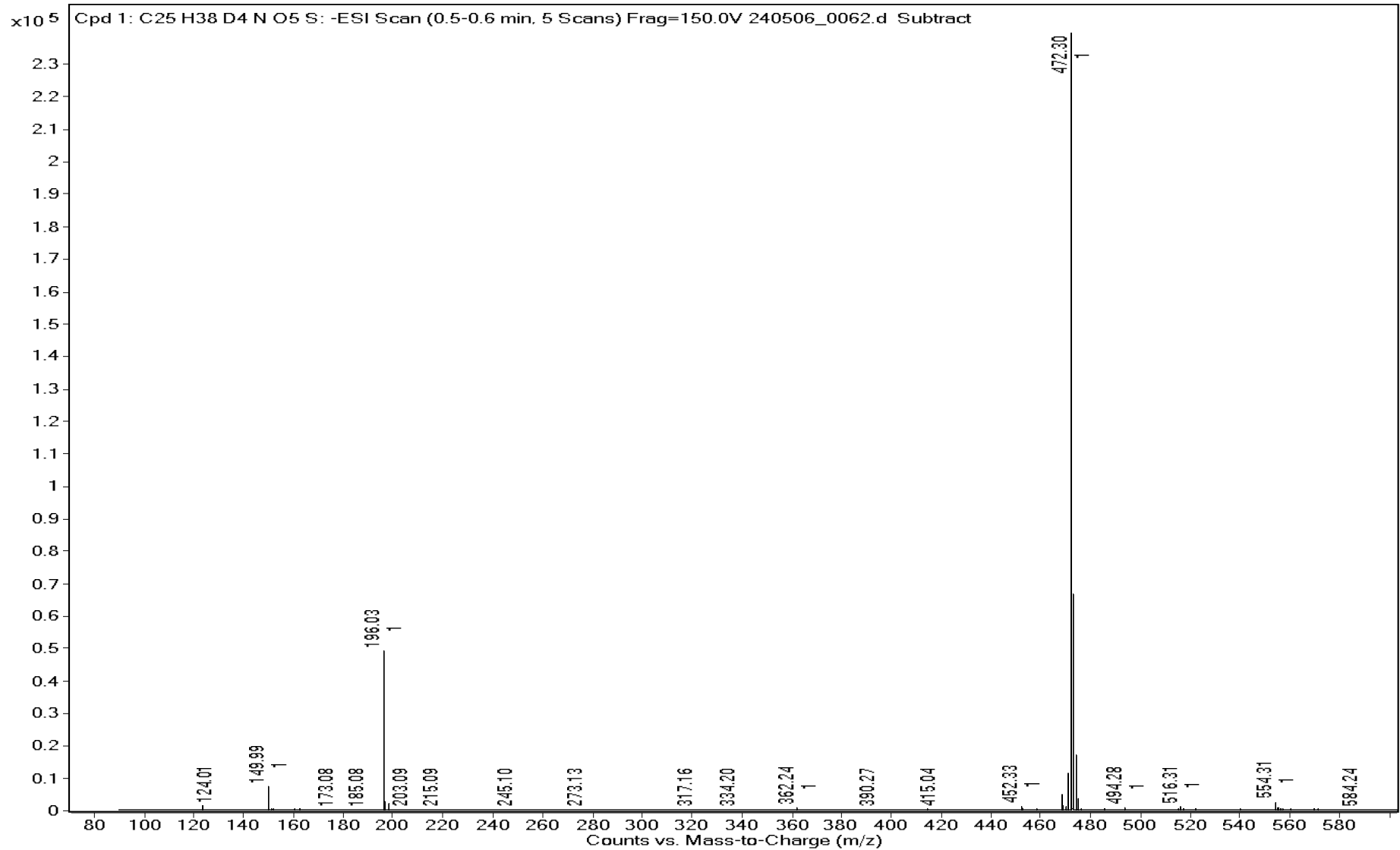
24-Nor Taurolithocholic Acid-D4 Sodium
1H-NMR, 600 MHz
Solvent: DMSO-D6
Lot No.: GR-19-119



Sample Name GR-19-119
DA Method AIMS_Accurate_Mass.m
Comment ESI-

Data File 240506_0062.d
Instrument Agilent 6538 UHD

Acq Method HRMS_Negative.m
Acq Date, Time 06/05/2024 12:51:47 PM



ESI-MS Report

Molecular Formula Generation (MFG)

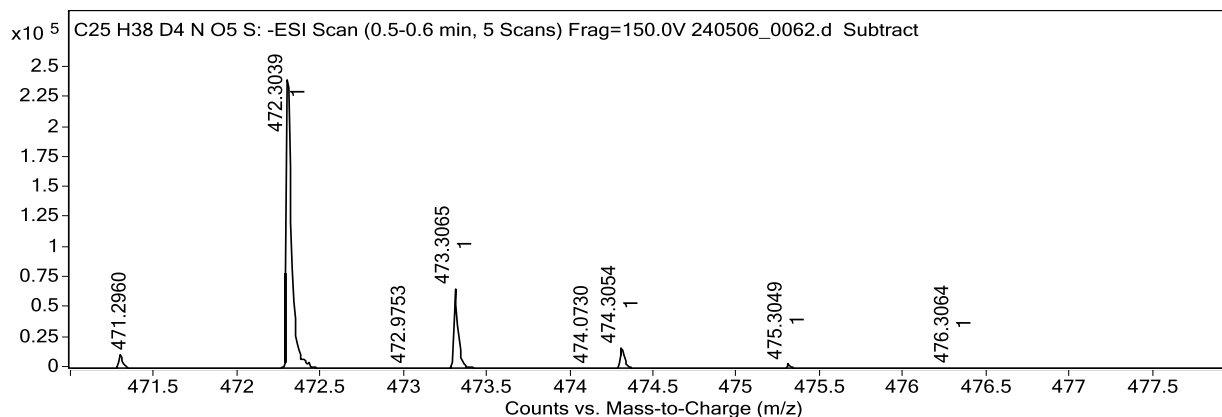
Sample Name	GR-19-119	Data File	240506_0062.d
Acq Method	HRMS_Negative.m	DA Method	AIMS_Accurate_Mass.m
Instrument	Agilent 6538 UHD	Acq Date, Time	06/05/2024 12:51:47 PM
Comment	ESI-		

Target Ion Species

Ion Species	m/z	Ionic Formula
M-	472.3039	C ₂₅ H ₃₈ [2H] ₄ N ₀₅ O ₅ S

MFG Calculator Results

Target m/z	Ionic Formula	Calc m/z	+/- (mDa)	+/- (ppm)	DBE	MFG Score
472.3039	C ₂₅ H ₃₈ [2H] ₄ N ₀₅ O ₅ S	472.3040	-0.1	-0.2	5.5	97.36
472.3039	C ₂₆ H ₃₄ [2H] ₄ N ₅ O ₅ S	472.3054	-1.5	-3.2	10.5	91.29
472.3039	C ₂₁ H ₃₄ [2H] ₄ N ₇ O ₃ S	472.3013	2.6	5.5	6.5	85.93
472.3039	C ₂₀ H ₃₈ [2H] ₄ N ₃ O ₇ S	472.3000	3.9	8.3	1.5	73.55



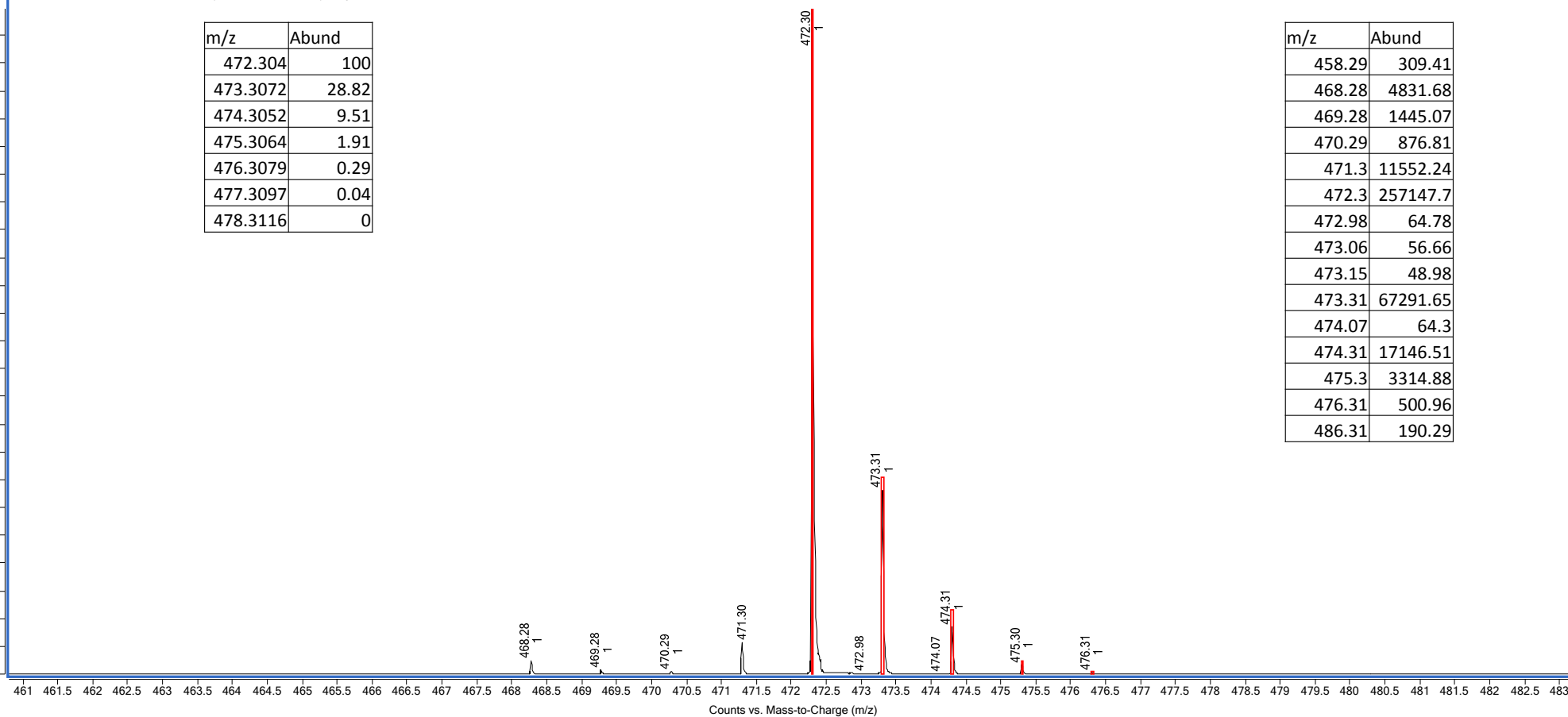
Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (mDa)	Abund (%)	Calc Abund (%)	+/-
1	472.3039	472.3040	-0.1	100.0	100.0	0.0
2	473.3065	473.3072	-0.7	26.2	28.8	2.6
3	474.3054	474.3052	0.2	6.7	9.5	2.8
4	475.3049	475.3064	-1.5	1.3	1.9	0.6
5	476.3064	476.3079	-1.5	0.2	0.3	0.1

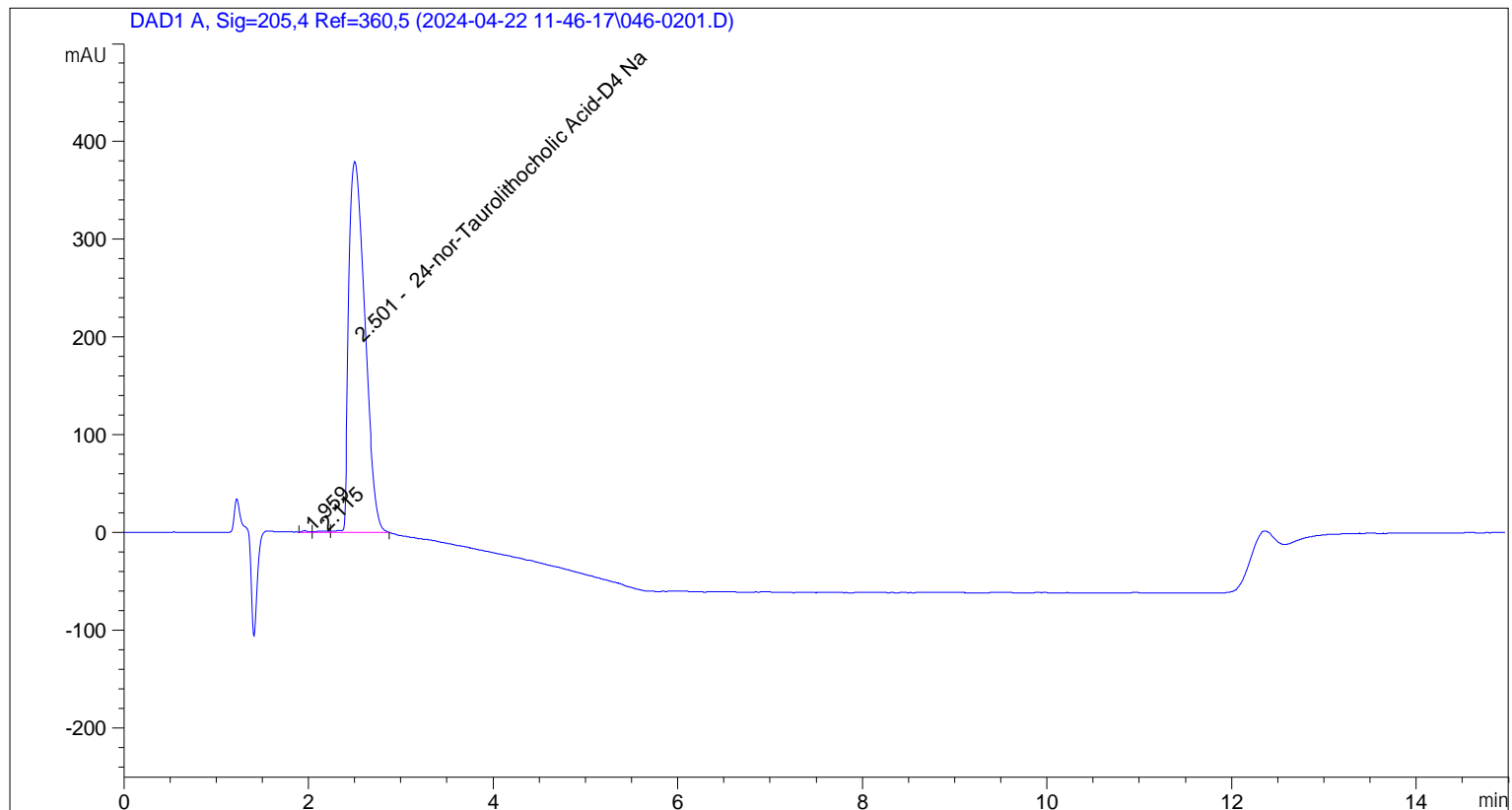
x10⁵ Cpd 1: C25 H38 D4 N O5 S: -ESI Scan (0.5-0.6 min, 5 Scans) Frag=150.0V 240506_0062.d Subtract

m/z	Abund
472.304	100
473.3072	28.82
474.3052	9.51
475.3064	1.91
476.3079	0.29
477.3097	0.04
478.3116	0

m/z	Abund
458.29	309.41
468.28	4831.68
469.28	1445.07
470.29	876.81
471.3	11552.24
472.3	257147.7
472.98	64.78
473.06	56.66
473.15	48.98
473.31	67291.65
474.07	64.3
474.31	17146.51
475.3	3314.88
476.31	500.96
486.31	190.29



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Acq. Operator : vrusu Seq. Line : 2
Acq. Instrument : Instrument 1 Location : Vial 46
Injection Date : 4/22/2024 12:03:50 PM Inj : 1
Inj Volume : 10.0 µl
Acq. Method : C:\CHEM32\1\DATA\2024-04-22 11-46-17\VR042224_119.M
Last changed : 4/22/2024 11:45:30 AM by vrusu
Analysis Method : C:\CHEM32\1\METHODS\VR042324_119PM.M
Last changed : 4/23/2024 9:03:16 AM by vrusu



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Area Percent Report
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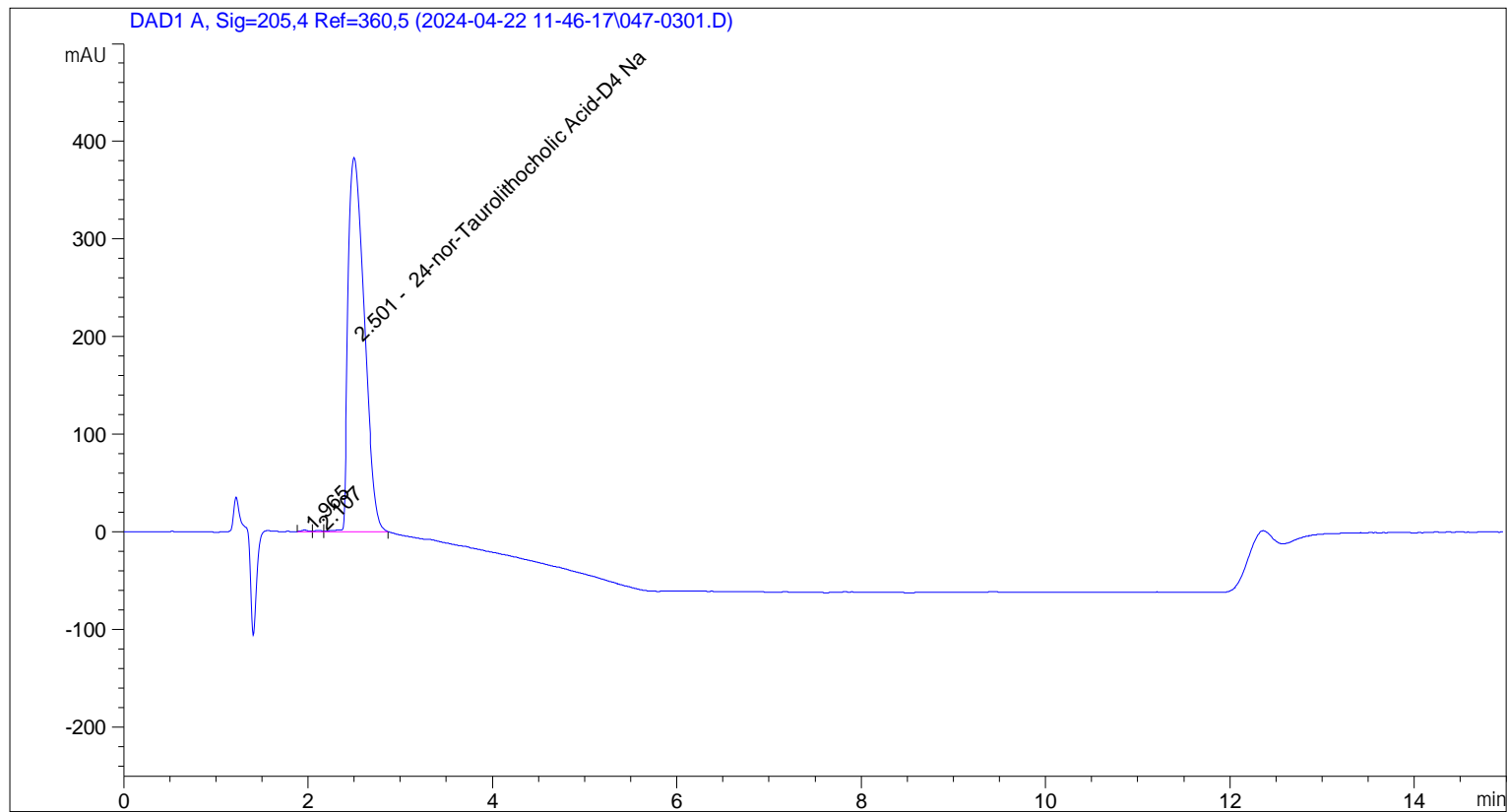
Sorted By : Signal
Calib. Data Modified : 4/23/2024 9:00:07 AM
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=205,4 Ref=360,5

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	1.959	BV	0.0602	5.89153	0.1284	?
2	2.115	VV	0.1211	10.01212	0.2181	?
3	2.501	VBA	0.1987	4574.02930	99.6535	24-nor-Tauro lithocholic Acid-D4 Na

Totals : 4589.93295

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Acq. Operator : vrusu Seq. Line : 3
Acq. Instrument : Instrument 1 Location : Vial 47
Injection Date : 4/22/2024 12:20:17 PM Inj : 1
Inj Volume : 10.0 µl
Acq. Method : C:\CHEM32\1\DATA\2024-04-22 11-46-17\VR042224_119.M
Last changed : 4/22/2024 11:45:30 AM by vrusu
Analysis Method : C:\CHEM32\1\METHODS\VR042324_119PM.M
Last changed : 4/23/2024 9:03:16 AM by vrusu



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Area Percent Report
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Sorted By : Signal
Calib. Data Modified : 4/23/2024 9:00:07 AM
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=205,4 Ref=360,5

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	1.965	BV	0.0632	7.12967	0.1527	?
2	2.107	VV	0.0697	5.70711	0.1222	?
3	2.501	VBA	0.2018	4656.49170	99.7251	24-nor-Tauroolithocholic Acid-D4 Na

Totals : 4669.32848