

Name:	3β-Chenodeoxycholic Acid-D4
Lot#:	GR-19-101B
Test Date:	04/22/2024 (re-test date: 04/22/2029)
CAS No.:	566-24-5 (unlabeled)
MF:	C ₂₄ H ₃₆ D ₄ O ₄
MW:	396.60
Appearance:	White solid
Purity:	>95% by NMR; TLC – one spot (eluent EtOAc); >98% atom D
¹H-NMR:	Conforms
MS-ESI (-)	Conforms (shows peaks at m/z = 395.31 [M-H] ⁻ and 441.32 [M+HCOOH-H] ⁻)
Storage	Store at -18°C in a dry place away from direct sunlight

Approved by:

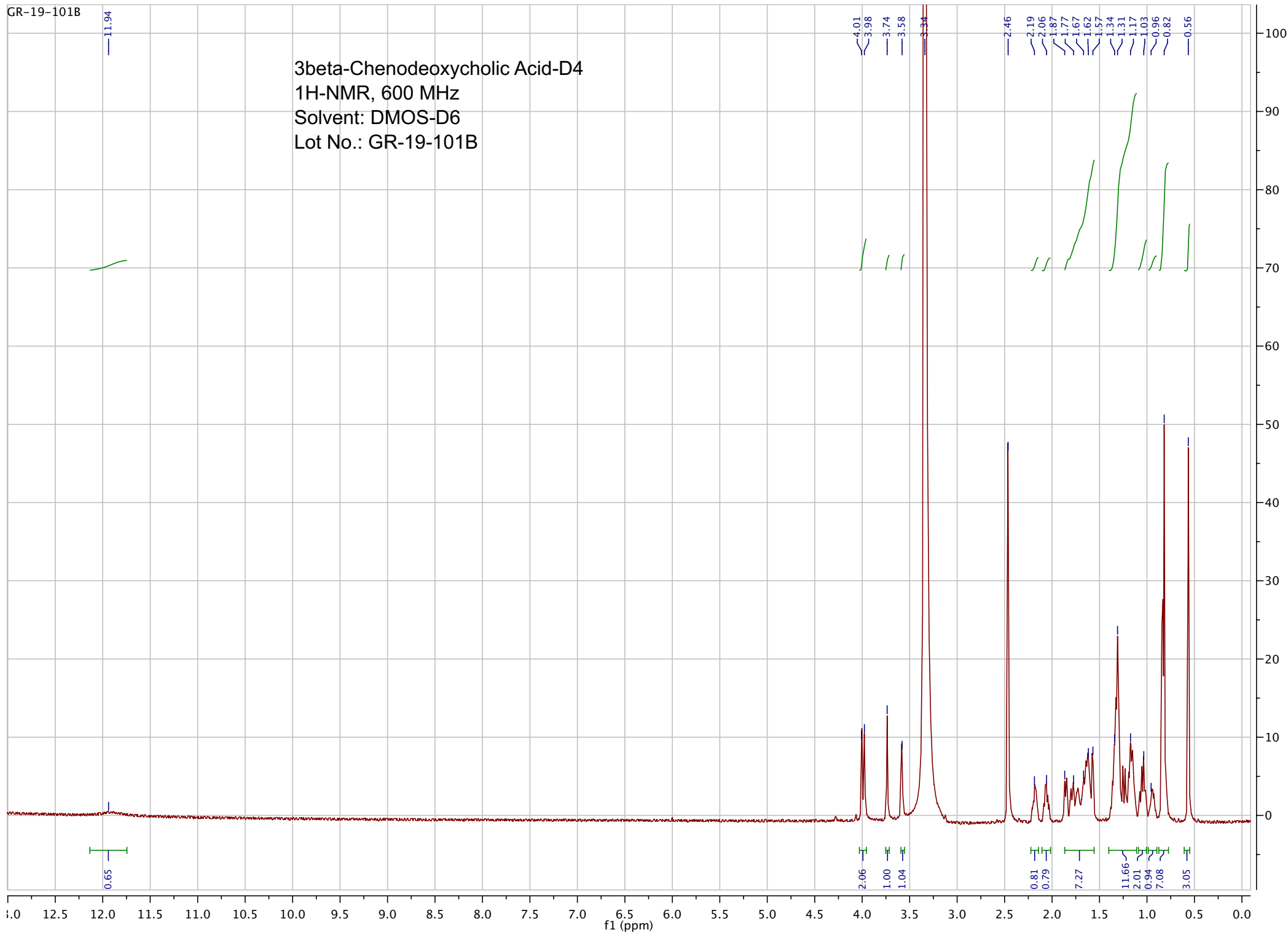
Date: 04/22/2024



Viorica Rusu, QC/QA Manager

GR-19-101B

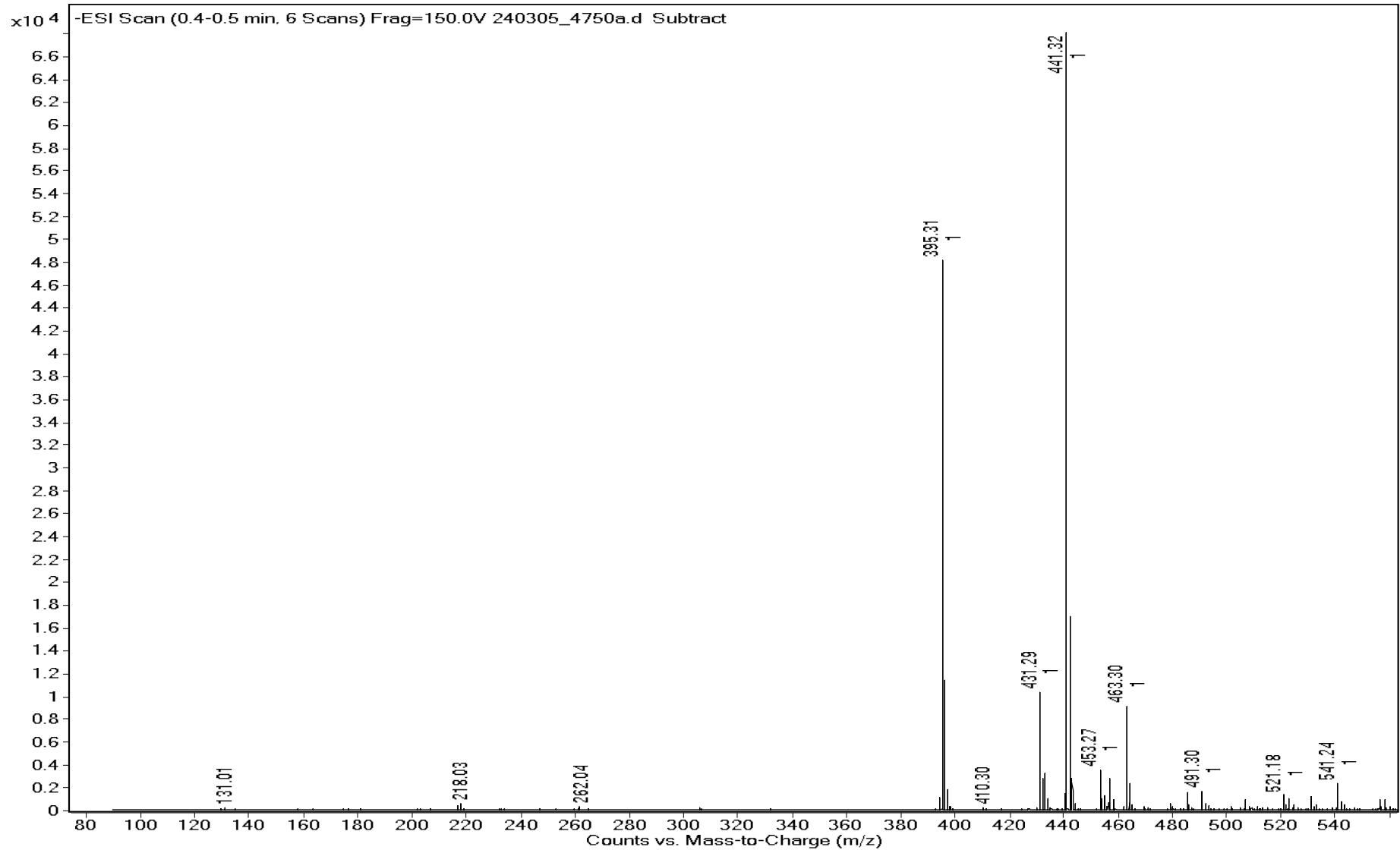
3beta-Chenodeoxycholic Acid-D4
1H-NMR, 600 MHz
Solvent: DMOS-D6
Lot No.: GR-19-101B



Sample Name GR-19-101
DA Method AIMS_Accurate_Mass.m
Comment ESI-

Data File 240305_4750a.d
Instrument Agilent 6538 UHD

Acq Method HRMS_Negative.m
Acq Date, Time 05/03/2024 5:10:24 PM



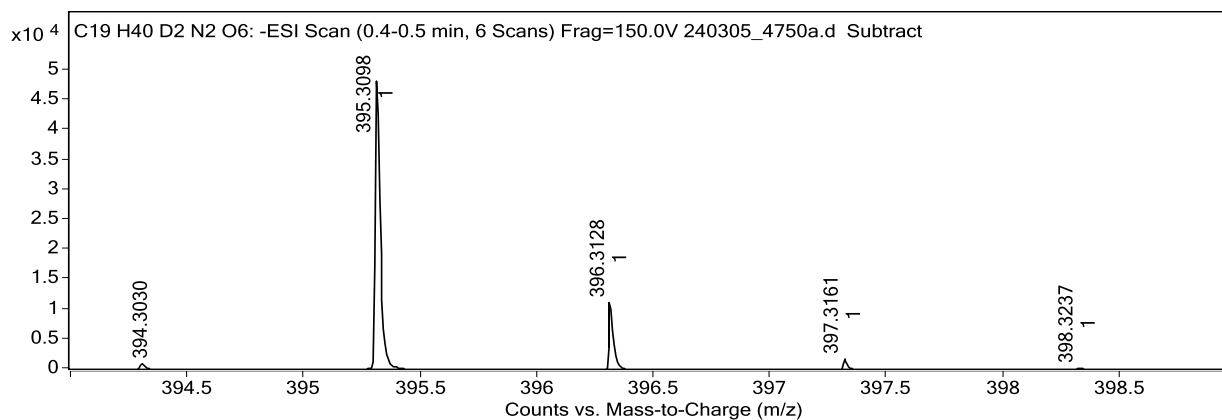
Sample Name	GR-19-101	Data File	240305_4750a.d
Acq Method	HRMS_Negative.m	DA Method	AIMS_Accurate_Mass.m
Instrument	Agilent 6538 UHD	Acq Date, Time	05/03/2024 5:10:24 PM
Comment	ESI-		

Target Ion Species

Ion Species	m/z	Ionic Formula
(M-H) ⁻	395.3098	C19 H39 D2 N2 O6

MFG Calculator Results

Target m/z	Ionic Formula	Calc m/z	+/- (mDa)	+/- (ppm)	DBE	MFG Score
395.3098	C19 H39 D2 N2 O6	395.3096	0.2	0.5	0.0	99.16
395.3098	C22 H35 D3 N3 O3	395.3107	-0.9	-2.3	5.0	97.27
395.3098	C20 H35 D2 N6 O2	395.3109	-1.1	-2.8	5.0	97.01
395.3098	C24 H35 D4 O4	395.3105	-0.7	-1.8	5.0	96.83
395.3098	C18 H31 D3 N9 O	395.3080	1.8	4.6	6.0	90.10
395.3098	C20 H31 D4 N6 O2	395.3078	2.0	5.1	6.0	89.35
395.3098	C25 H31 D4 N4	395.3118	-2.0	-5.1	10.0	85.63
395.3098	C17 H35 D3 N5 O5	395.3067	3.1	7.8	1.0	77.27
395.3098	C19 H35 D4 N2 O6	395.3065	3.3	8.3	1.0	77.02
395.3098	C15 H35 D2 N8 O4	395.3069	2.9	7.3	1.0	76.59



Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (mDa)	Abund (%)	Calc Abund (%)	+/-
1	395.3098	395.3096	0.2	100.0	100.0	0.0
2	396.3128	396.3128	0.0	23.5	22.0	-1.5
3	397.3161	397.3152	0.9	3.7	3.5	-0.2

x10⁴ -ESI Scan (0.4-0.5 min, 6 Scans) Frag=150.0V 240305_4750a.d Subtract

m/z	Abund
395.3105	100
396.3139	26.51
397.3168	4.2
398.3196	0.49
399.3223	0.05
400.325	0

m/z	Abund
262.04	300.54
394.3	1047.9
395.31	50374.3
396.31	11840.4
397.32	1861.92
398.32	315.56
410.3	182.24

