

<b>Name:</b>	<b>Chenodeoxycholic Acid-D4</b>
<b>Lot#:</b>	GR-19-101
<b>Test Date:</b>	03/05/2024 (re-test date: 03/05/2029)
<b>CAS No.:</b>	99102-69-9
<b>MF:</b>	C <sub>24</sub> H <sub>36</sub> D <sub>4</sub> O <sub>4</sub>
<b>MW:</b>	396.60
<b>Appearance:</b>	White solid
<b>Purity:</b>	>97% by NMR; TLC – 1 spot (eluent 10% MeOH in DCM); >98% atom D
<b><sup>1</sup>H-NMR:</b>	Conforms
<b>MS-ESI (-)</b>	Conforms (shows peaks at m/z = 395.31 [M-H] <sup>-</sup> )
<b>Storage</b>	Store at -18°C in a dry place away from direct sunlight

Approved by:

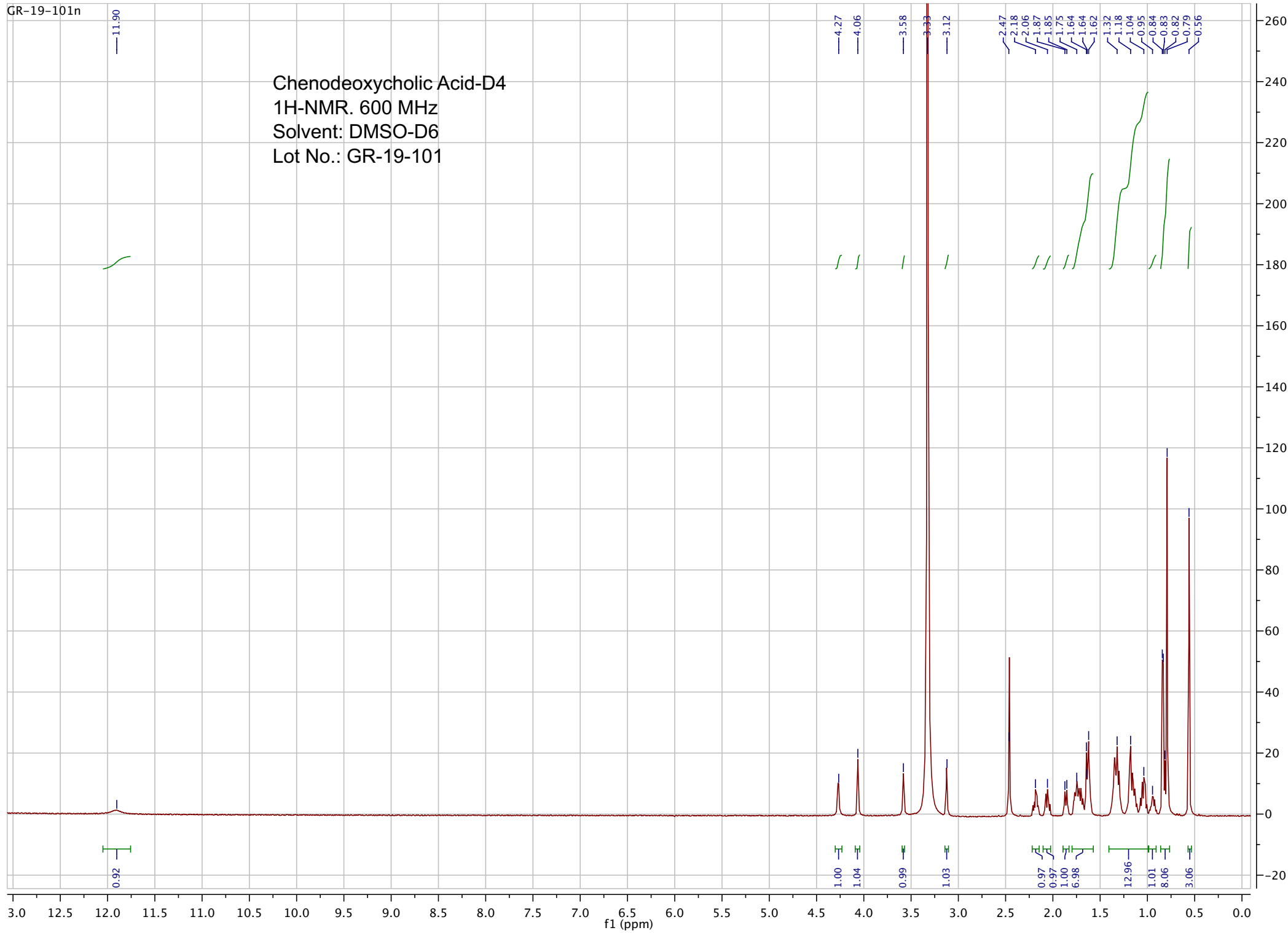
Date: 03/05/2024



Viorica Rusu, QC/QA Manager

GR-19-101n

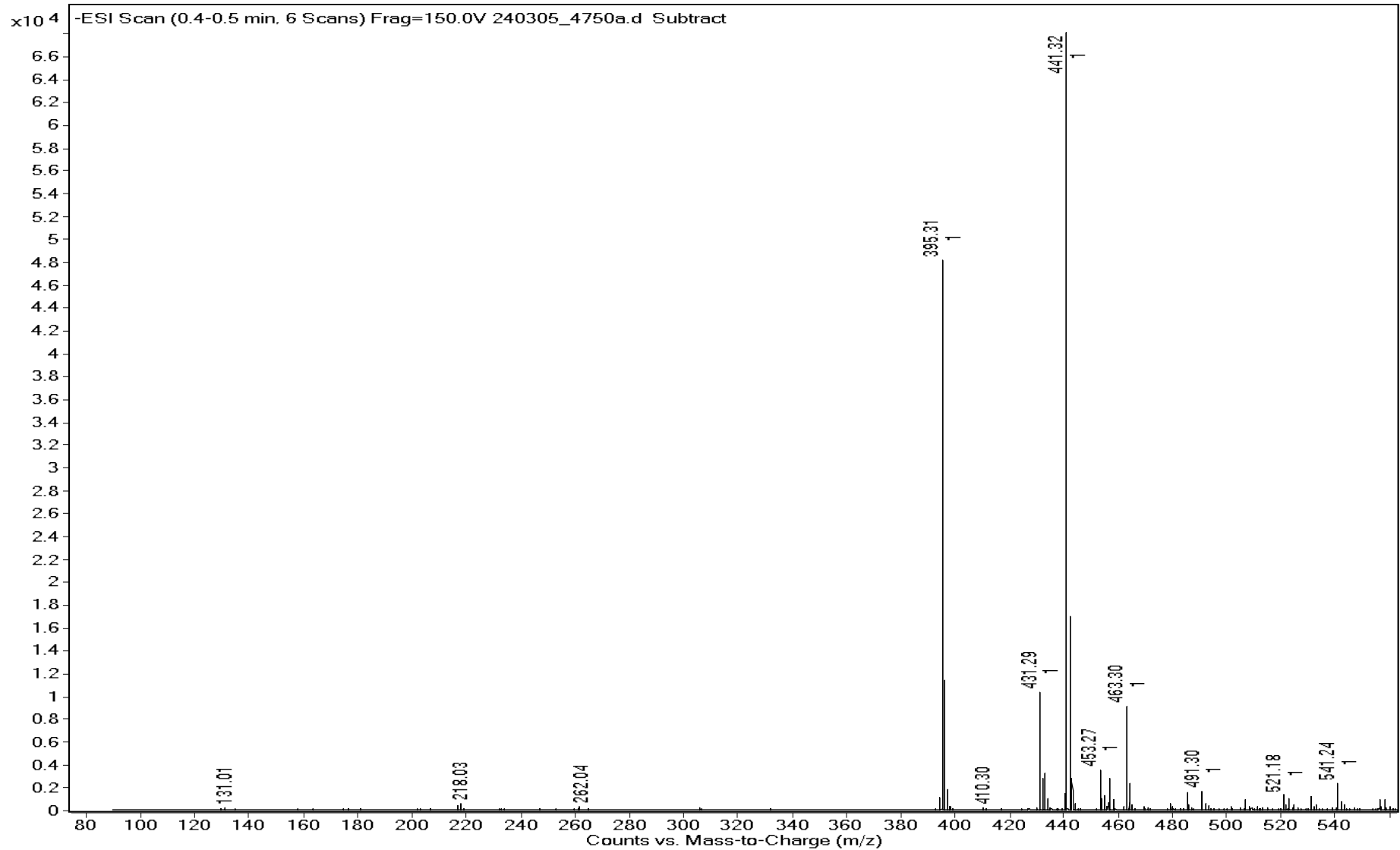
Chenodeoxycholic Acid-D4  
1H-NMR. 600 MHz  
Solvent: DMSO-D6  
Lot No.: GR-19-101



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



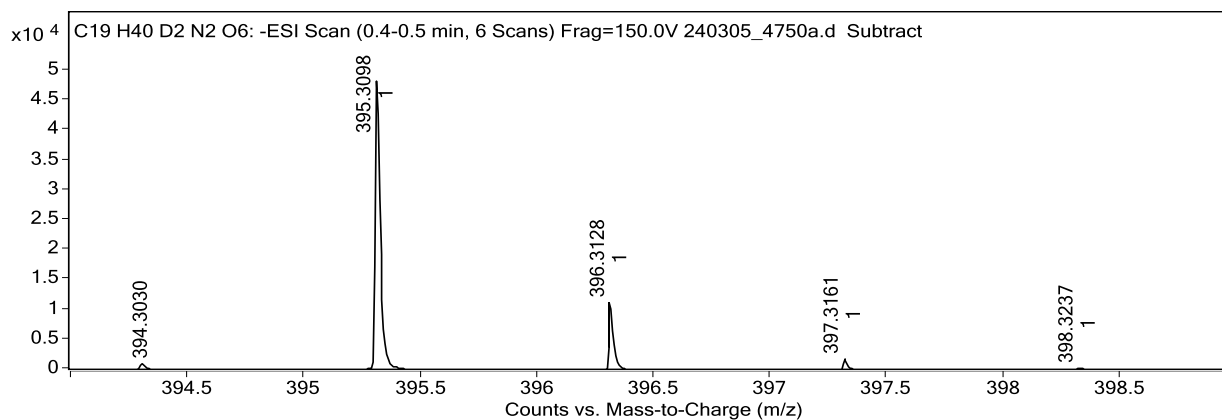
<b>Sample Name</b>	GR-19-101	<b>Data File</b>	240305_4750a.d
<b>Acq Method</b>	HRMS_Negative.m	<b>DA Method</b>	AIMS_Accurate_Mass.m
<b>Instrument</b>	Agilent 6538 UHD	<b>Acq Date, Time</b>	05/03/2024 5:10:24 PM
<b>Comment</b>	ESI-		

### Target Ion Species

Ion Species	m/z	Ionic Formula
(M-H) <sup>-</sup>	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

x10<sup>4</sup> -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

