

Name:	3β-Chenodeoxycholic Acid
Lot#:	GR-19-015
Test Date:	12/01/2023 (re-test date: 12/01/2028)
CAS No.:	566-24-5
MF:	C ₂₄ H ₄₀ O ₄
MW:	392.58
Appearance:	White solid
Purity:	>97% by NMR; TLC – one spot (eluent EtOAc)
¹H-NMR:	Conforms
MS-ESI (-)	Conforms (shows peaks at m/z = 391.29 [M-H] ⁻ and 437.29 [M+HCOOH-H] ⁻)
Storage	Store at 0-5°C in a dry place away from direct sunlight

Approved by:

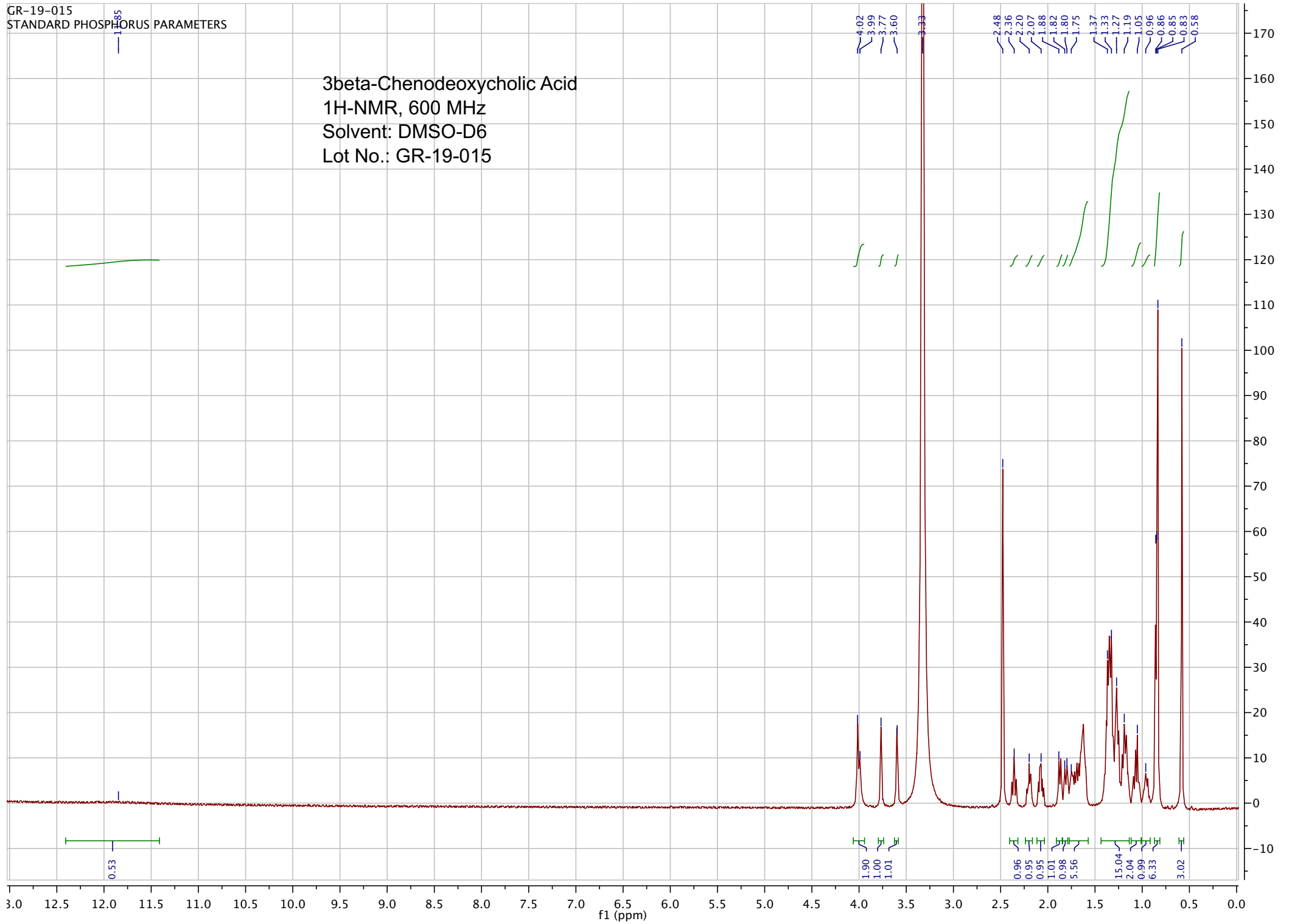
Date: 12/01/2023



Viorica Rusu, QC/QA Manager

GR-19-015
STANDARD PHOSPHORUS PARAMETERS

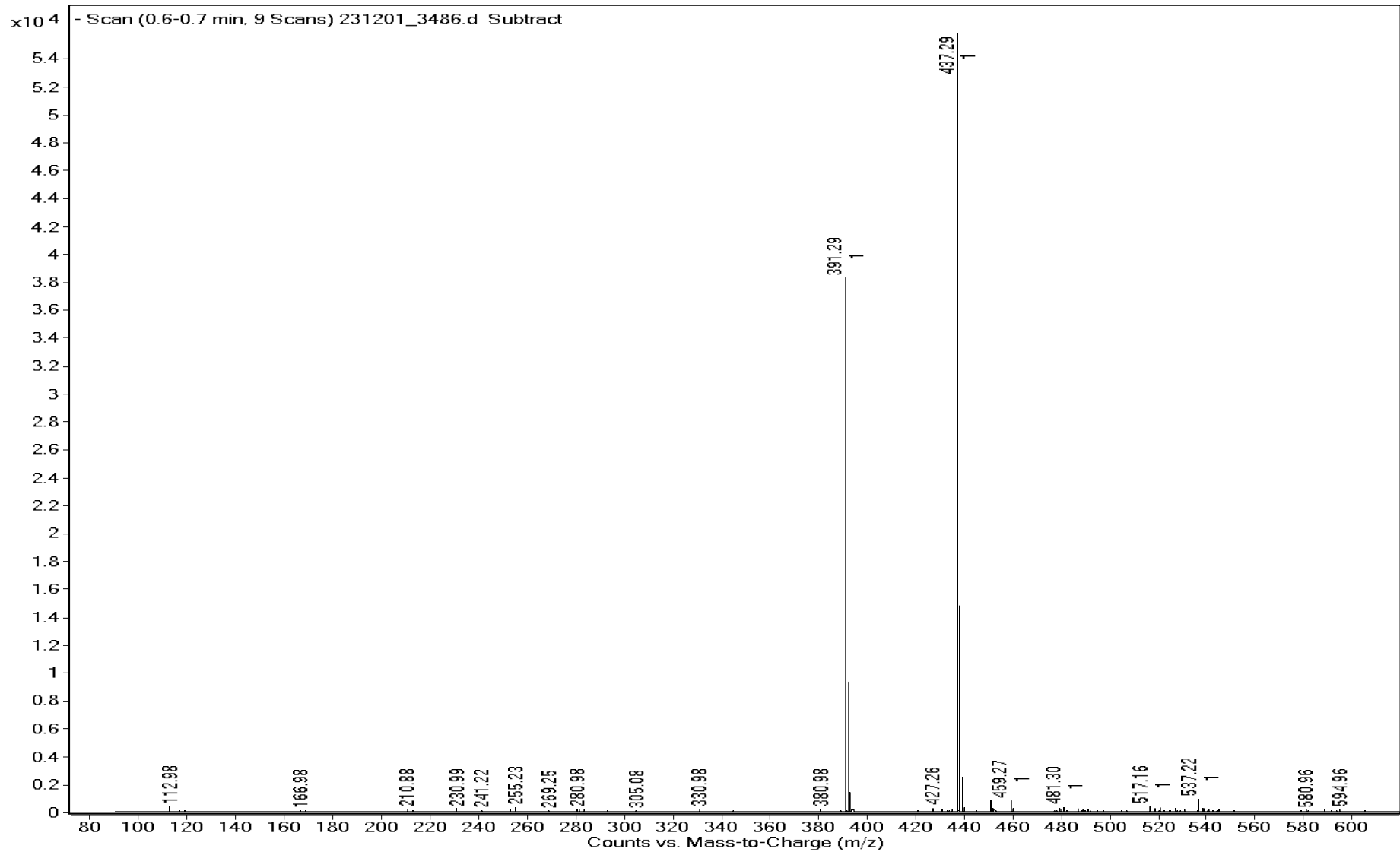
3beta-Chenodeoxycholic Acid
1H-NMR, 600 MHz
Solvent: DMSO-D6
Lot No.: GR-19-015



Sample Name GR-19-015
DA Method AIMS_Accurate_Mass.m
Comment ESI-

Data File 231201_3486.d
Instrument Agilent 6538 UHD

Acq Method HRMS_Negative.m
Acq Date, Time 01/12/2023 12:17:27 PM



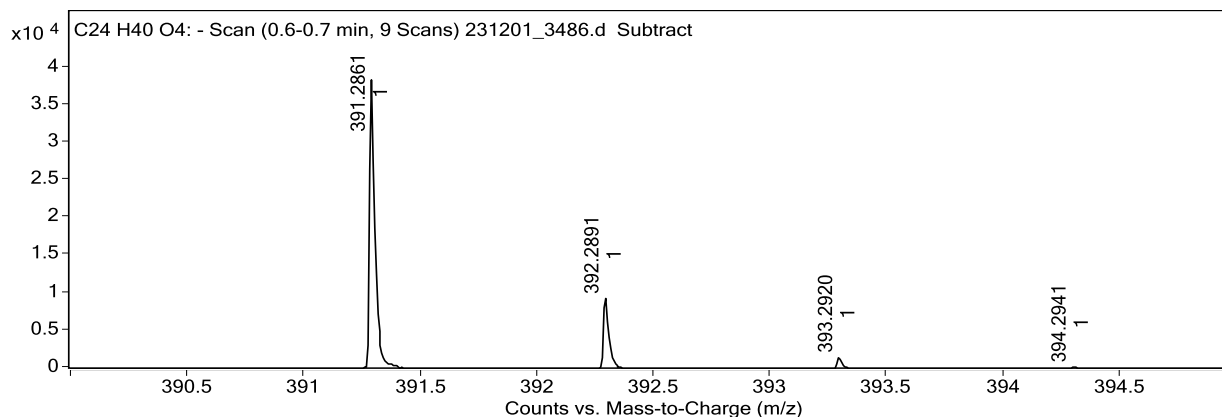
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Instrument	Agilent 6538 UHD	Acq Date, Time	01/12/2023 12:17:27 PM
Comment	ESI-		

Target Ion Species

Ion Species	m/z	Ionic Formula
(M-H) ⁻	391.2861	C ₂₄ H ₃₉ O ₄

MFG Calculator Results

Target m/z	Ionic Formula	Calc m/z	+/- (mDa)	+/- (ppm)	DBE	MFG Score
391.2861	C ₂₄ H ₃₉ O ₄	391.2854	0.7	1.8	5.0	98.11
391.2861	C ₂₅ H ₃₅ N ₄	391.2867	-0.6	-1.5	10.0	95.42
391.2861	C ₂₀ H ₃₅ N ₆ O ₂	391.2827	3.4	8.7	6.0	76.81
391.2861	C ₁₄ H ₃₅ N ₁₀ O ₃	391.2899	-3.8	-9.7	2.0	68.54



Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (mDa)	Abund (%)	Calc Abund (%)	+/-
1	391.2861	391.2854	0.7	100.0	100.0	0.0
2	392.2891	392.2888	0.3	24.5	26.6	2.1
3	393.2920	393.2917	0.3	3.8	4.2	0.4