

Name: 3β-Ursodeoxycholic Acid
Lot#: GR-18-277
Test Date: 11/06/2023 (re-test date: 11/06/2028)
CAS No.: 78919-26-3
MF: C₂₄H₄₀O₄
MW: 392.58
Appearance: White solid
Purity: >97% by NMR; TLC – one spot (eluent EtOAc)
¹H-NMR: Conforms
MS-ESI (-) Conforms (shows peak at m/z = 391.29 [M-H]⁻)

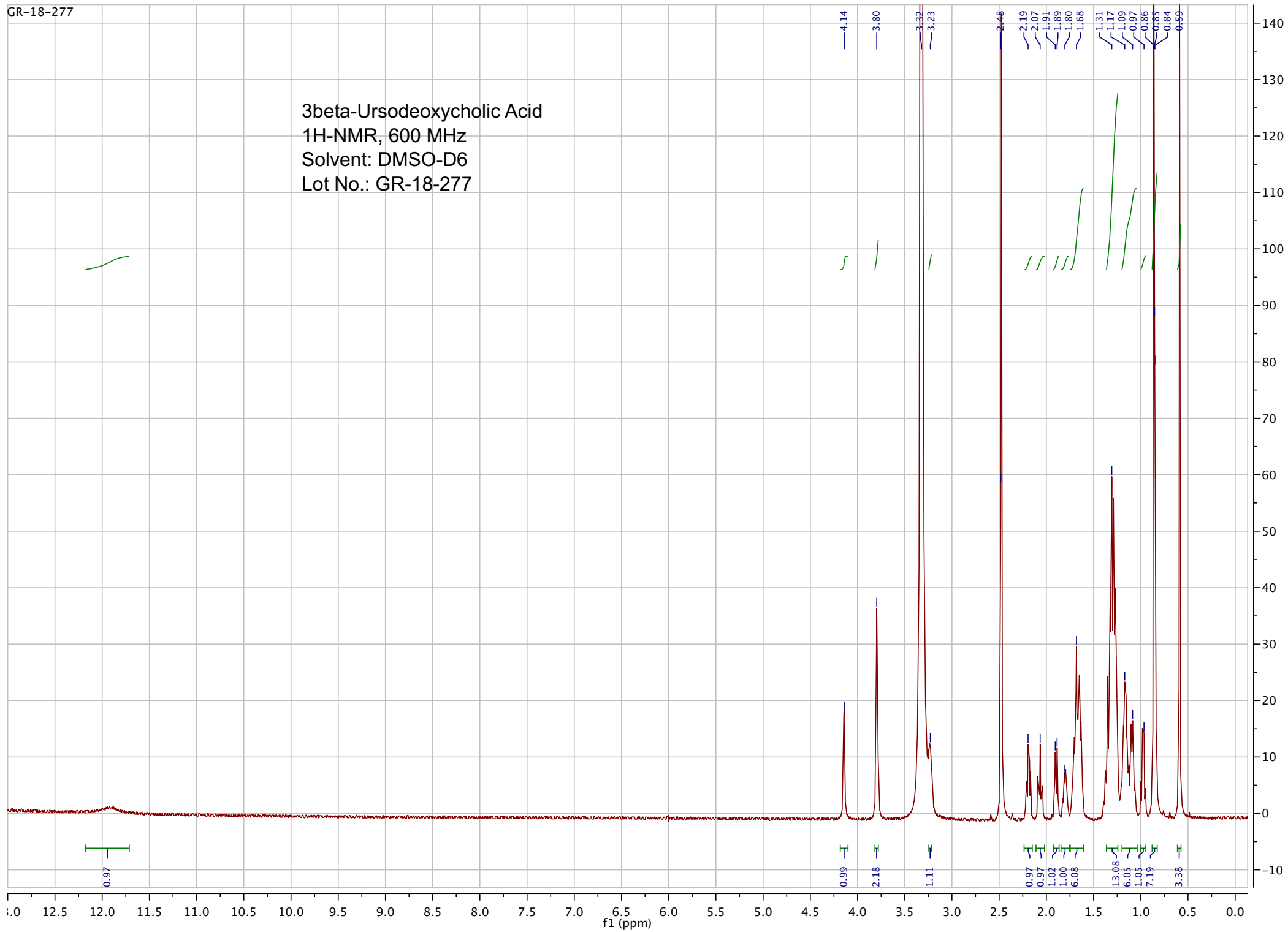
Approved by:

Date: 11/06/2023

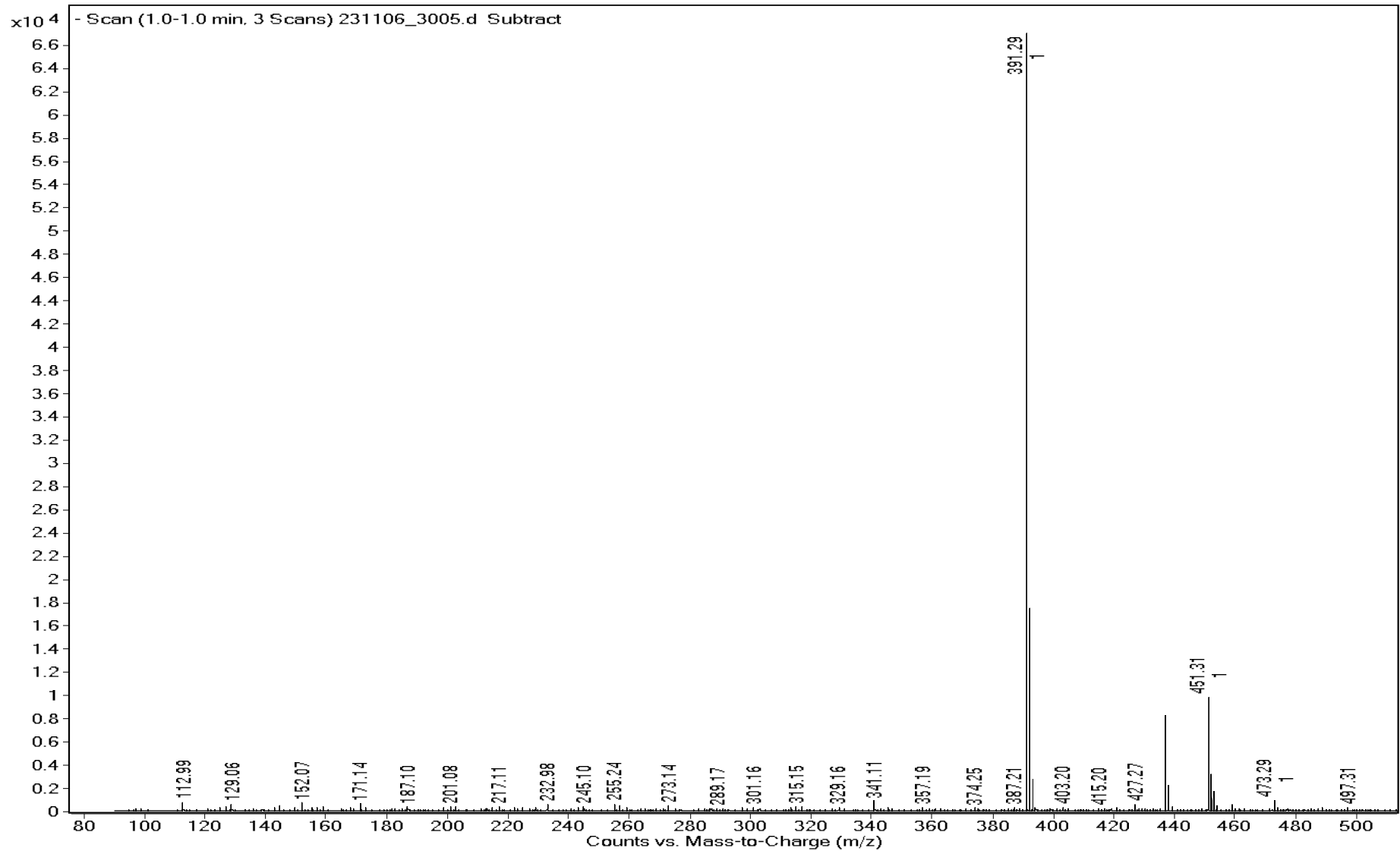


Viorica Rusu, QC/QA Manager

3beta-Ursodeoxycholic Acid
1H-NMR, 600 MHz
Solvent: DMSO-D6
Lot No.: GR-18-277



Sample Name	GR-18-277	Data File	231106_3005.d	Acq Method	HRMS.m
DA Method	AIMS_Accurate_Mass.m	Instrument	Agilent 6538 UHD	Acq Date, Time	06/11/2023 10:22:59 AM
Comment	ESI-				



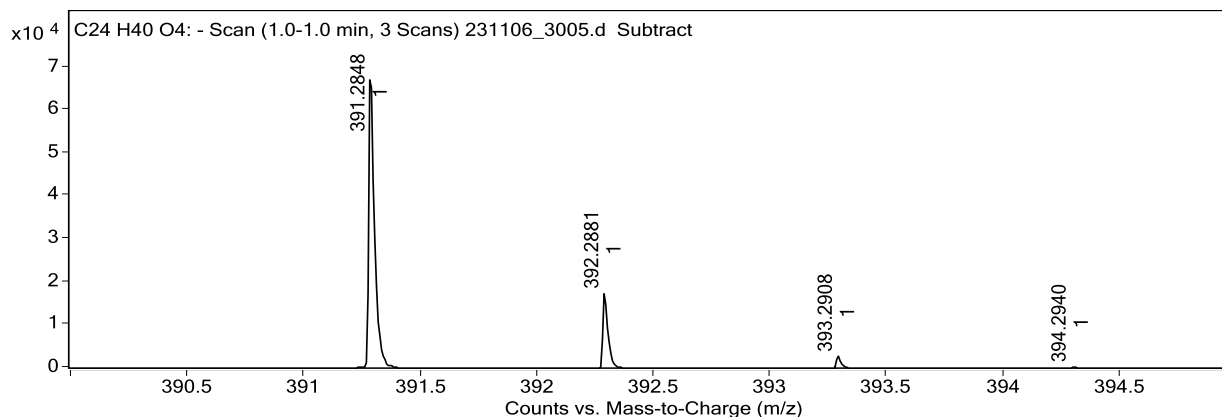
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Acq Method	HRMS.m	DA Method	AIMS_Accurate_Mass.m
Instrument	Agilent 6538 UHD	Acq Date, Time	06/11/2023 10:22:59 AM
Comment	ESI-		

Target Ion Species

Ion Species	m/z	Ionic Formula
(M-H) ⁻	391.2848	C ₂₄ H ₃₉ O ₄

MFG Calculator Results

Target m/z	Ionic Formula	Calc m/z	+/- (mDa)	+/- (ppm)	DBE	MFG Score
391.2848	C ₂₄ H ₃₉ O ₄	391.2854	-0.6	-1.5	5.0	98.53
391.2848	C ₂₅ H ₃₅ N ₄	391.2867	-1.9	-4.9	10.0	88.72
391.2848	C ₂₀ H ₃₅ N ₆ O ₂	391.2827	2.1	5.4	6.0	87.79
391.2848	C ₁₉ H ₃₉ N ₂ O ₆	391.2814	3.4	8.7	1.0	74.34



Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (mDa)	Abund (%)	Calc Abund (%)	+/-
1	391.2848	391.2854	-0.6	100.0	100.0	0.0
2	392.2881	392.2888	-0.7	24.9	26.6	1.7
3	393.2908	393.2917	-0.9	3.8	4.2	0.4