

Name:	Deoxycholic Acid-D4
Lot#:	GR-19-095
Test Date:	03/05/2024 (re-test date: 03/05/2029)
CAS No.:	112076-61-6
MF:	C ₂₄ H ₃₆ D ₄ O ₄
MW:	396.6
Appearance:	White solid
Purity:	>97% by NMR (contains 0.4% of the 3beta-isomer); TLC – 1 spot (eluent 10% MeOH in DCM); 99% atom D
¹H-NMR:	Conforms (shows a trace of Acetone)
MS-ESI (-)	Conforms (shows peaks at m/z = 395.31 [M-H] ⁻)
Storage	Store at -18°C in a dry place away from direct sunlight

Approved by:

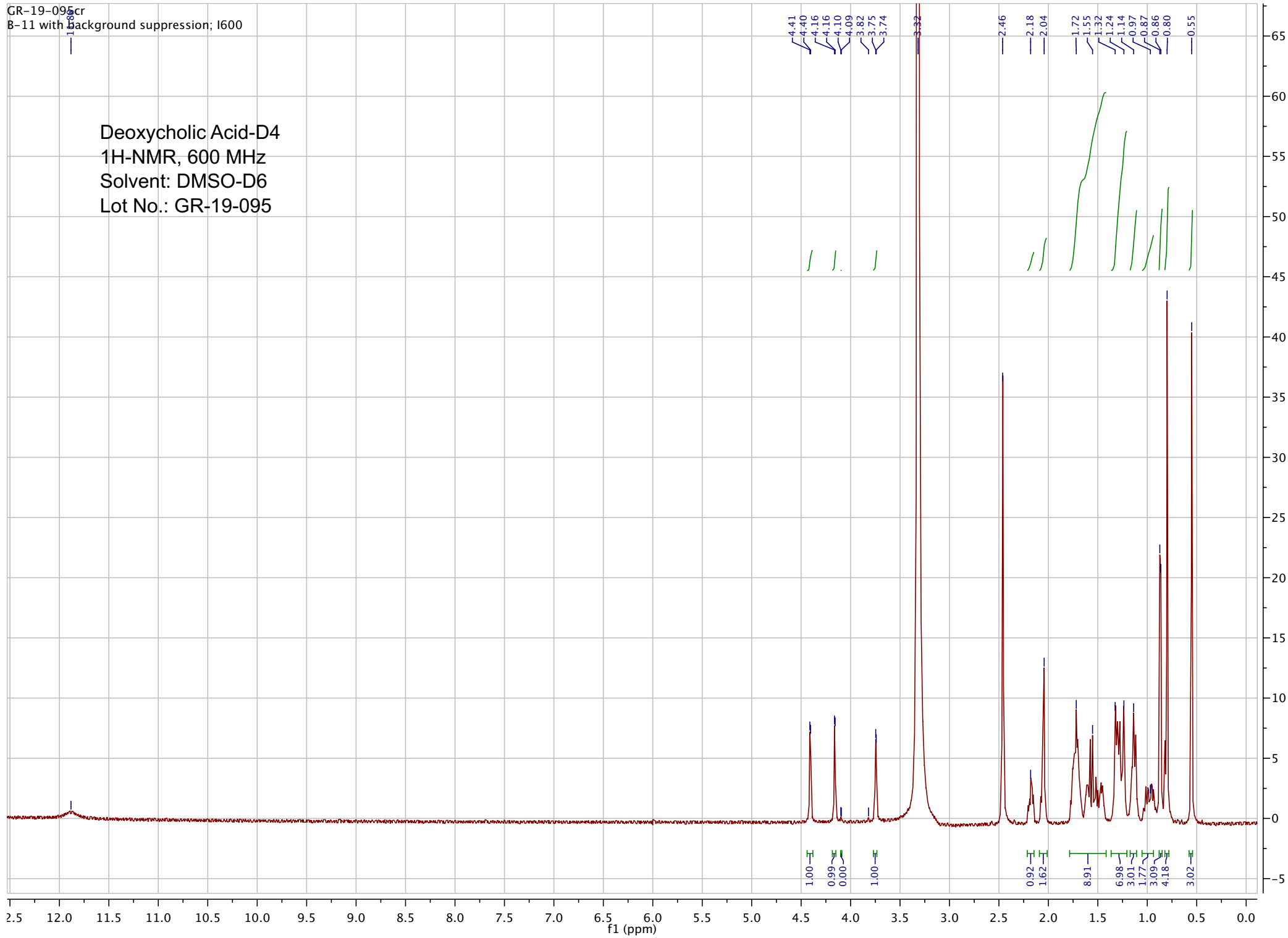
Date: 03/06/2024



Viorica Rusu, QC/QA Manager

GR-19-095cr
B-11 with background suppression; I600

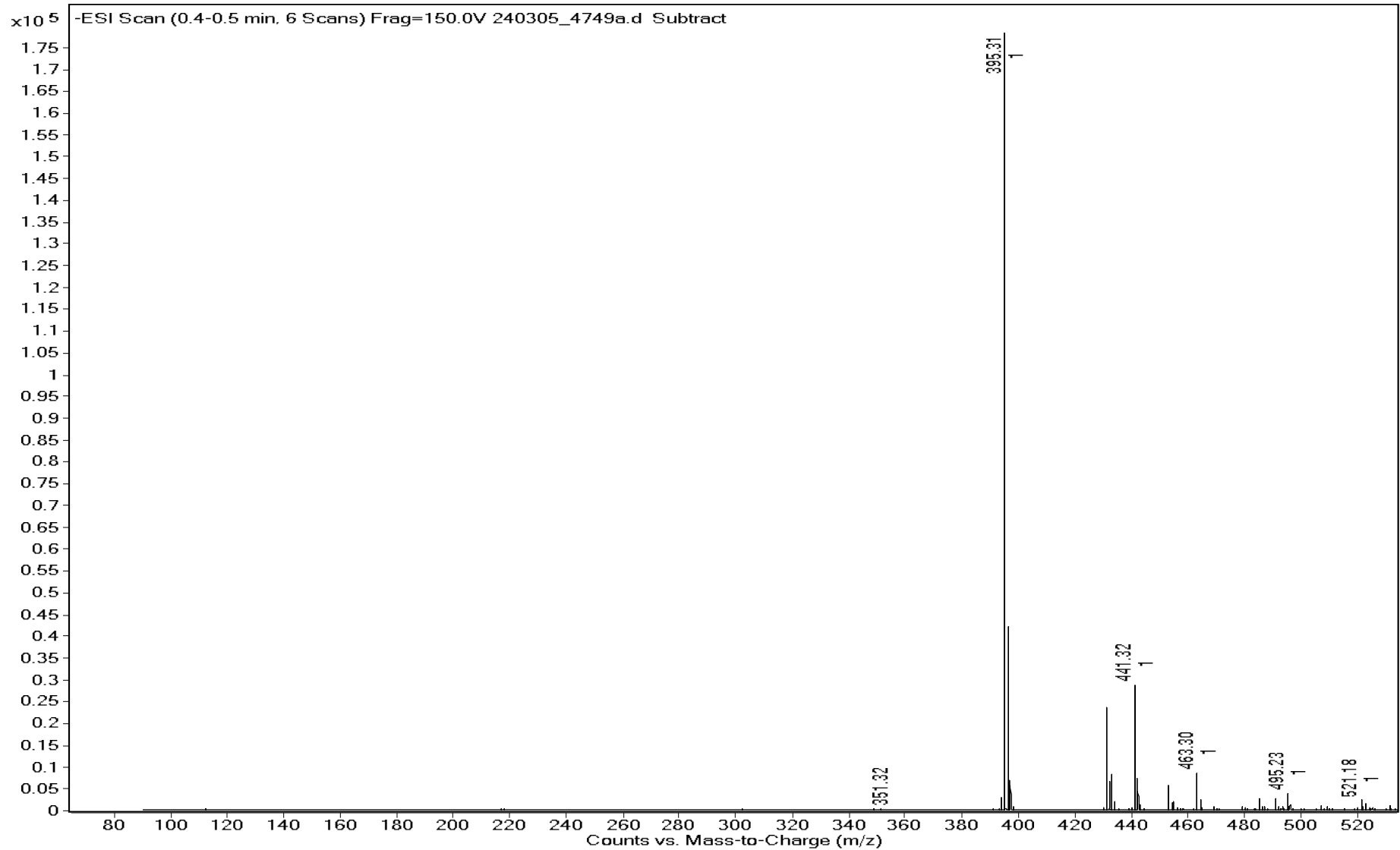
Deoxycholic Acid-D4
1H-NMR, 600 MHz
Solvent: DMSO-D6
Lot No.: GR-19-095



Sample Name GR-19-095
DA Method AIMS_Accurate_Mass.m
Comment ESI-

Data File 240305_4749a.d
Instrument Agilent 6538 UHD

Acq Method HRMS_Negative.m
Acq Date, Time 05/03/2024 5:21:54 PM



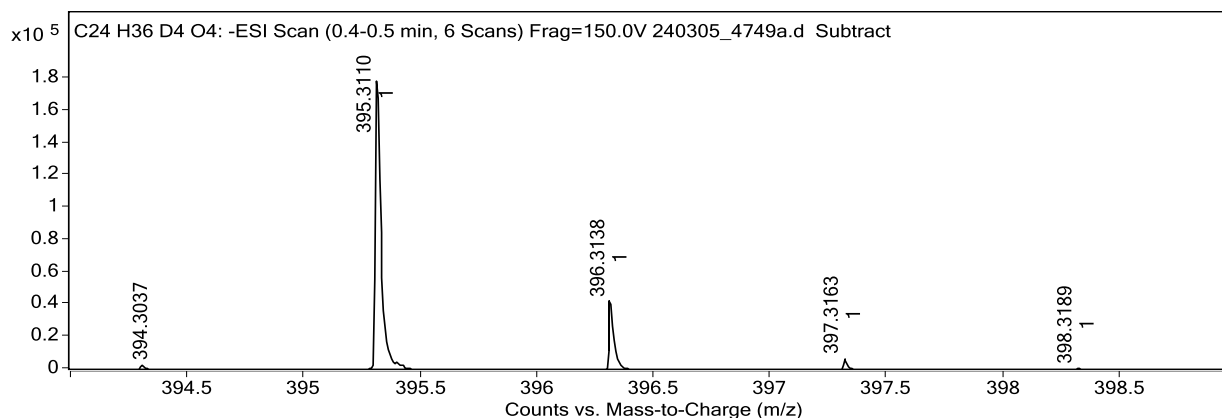
Sample Name	GR-19-095	Data File	240305_4749a.d
Acq Method	HRMS_Negative.m	DA Method	AIMS_Accurate_Mass.m
Instrument	Agilent 6538 UHD	Acq Date, Time	05/03/2024 5:21:54 PM
Comment	ESI-		

Target Ion Species

Ion Species	m/z	Ionic Formula
(M-H) ⁻	395.311	C24 H35 D4 O4

MFG Calculator Results

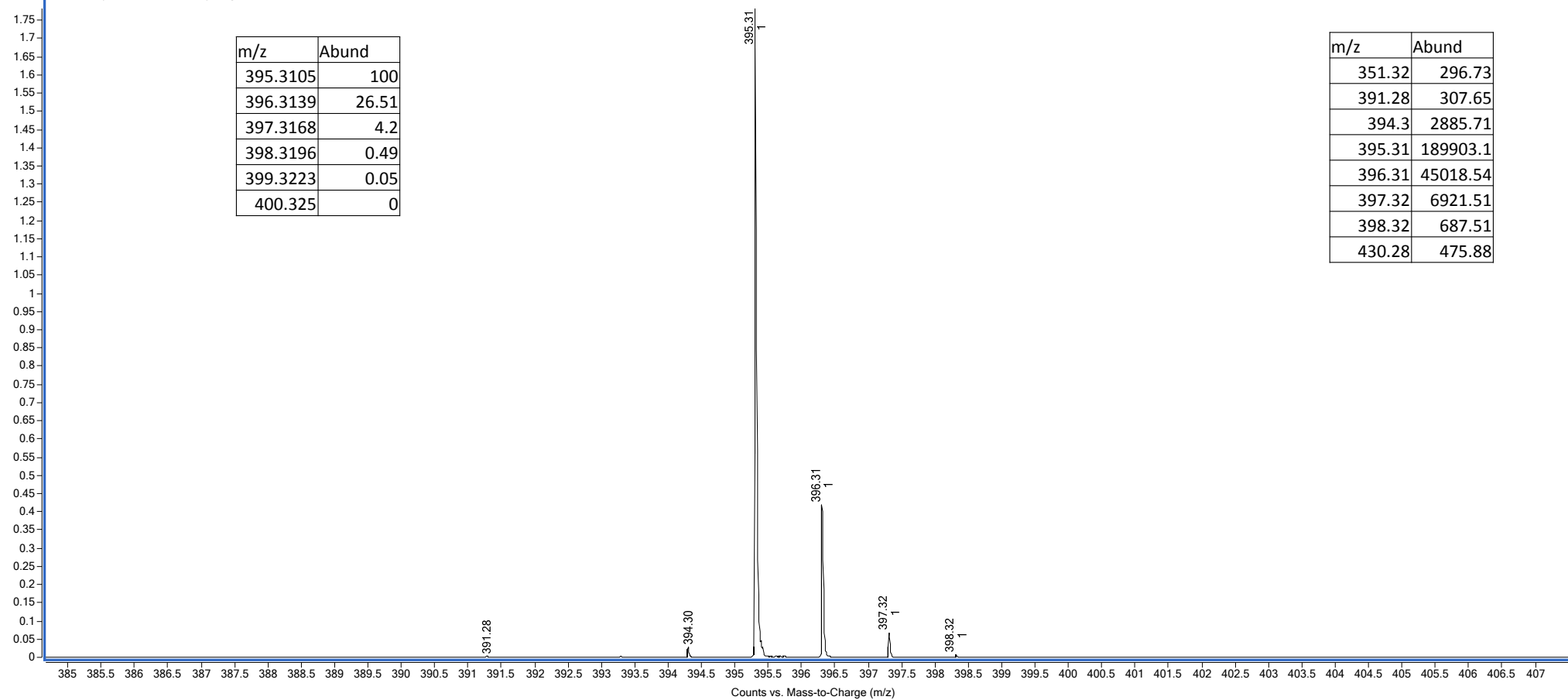
Target m/z	Ionic Formula	Calc m/z	+/- (mDa)	+/- (ppm)	DBE	MFG Score
395.3110	C20 H35 D2 N6 O2	395.3109	0.1	0.3	5.0	99.82
395.3110	C22 H35 D3 N3 O3	395.3107	0.3	0.8	5.0	99.16
395.3110	C24 H35 D4 O4	395.3105	0.5	1.3	5.0	97.79
395.3110	C19 H39 D2 N2 O6	395.3096	1.4	3.5	0.0	94.47
395.3110	C25 H31 D4 N4	395.3118	-0.8	-2.0	10.0	93.30
395.3110	C24 H39 D2 O4	395.3136	-2.6	-6.6	4.0	81.65
395.3110	C18 H31 D3 N9 O	395.3080	3.0	7.6	6.0	80.27
395.3110	C20 H31 D4 N6 O2	395.3078	3.2	8.1	6.0	79.22
395.3110	C14 H31 D4 N10 O3	395.3150	-4.0	-10.1	2.0	68.19
395.3110	C25 H35 D2 N4	395.3149	-3.9	-9.9	9.0	67.04



Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (mDa)	Abund (%)	Calc Abund (%)	+/-
1	395.3110	395.3105	0.5	100.0	100.0	0.0
2	396.3138	396.3139	-0.1	23.7	26.5	2.8
3	397.3163	397.3168	-0.5	3.6	4.2	0.6

x10⁵ -ESI Scan (0.4-0.5 min, 6 Scans) Frag=150.0V 240305_4749a.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
351.32	296.73
391.28	307.65
394.3	2885.71
395.31	189903.1
396.31	45018.54
397.32	6921.51
398.32	687.51
430.28	475.88