

Name:	3β-Lithocholic Acid-D4
Lot#:	GR-19-075
Test Date:	02/14/2024 (re-test date: 02/14/2029)
CAS No.:	1534-35-6 (unlabeled)
MF:	C ₂₄ H ₃₆ D ₄ O ₃
MW:	380.60
Appearance:	White solid
Purity:	>97% by NMR; TLC – one spot (eluent EtOAc); 99% atom D
¹H-NMR:	Conforms
MS-ESI (-)	Conforms (shows peak at m/z = 379.32 [M-H] ⁻)
Storage	Store at -18°C in a dry place away from direct sunlight

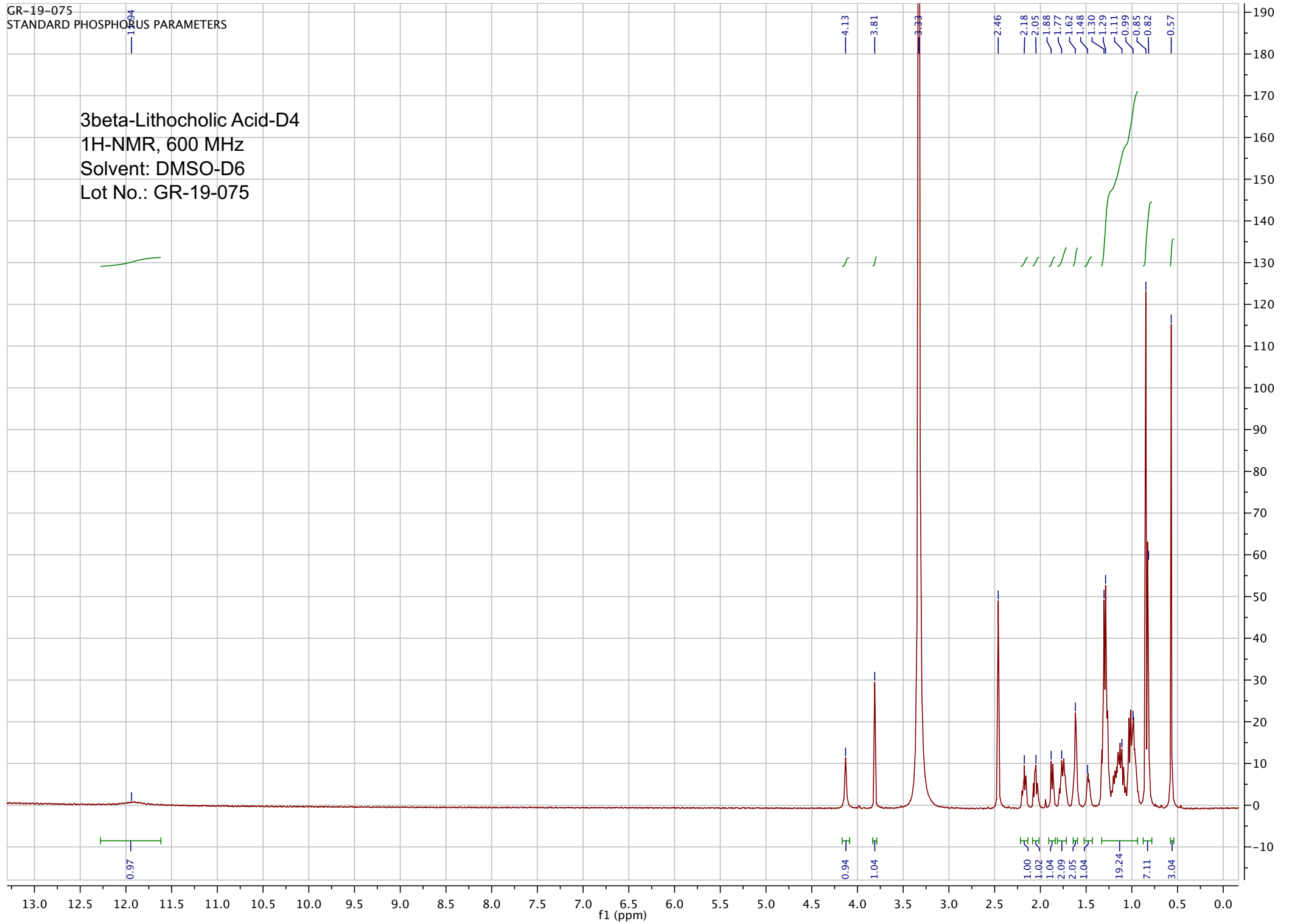
Approved by:

Date: 02/14/2024



Viorica Rusu, QC/QA Manager

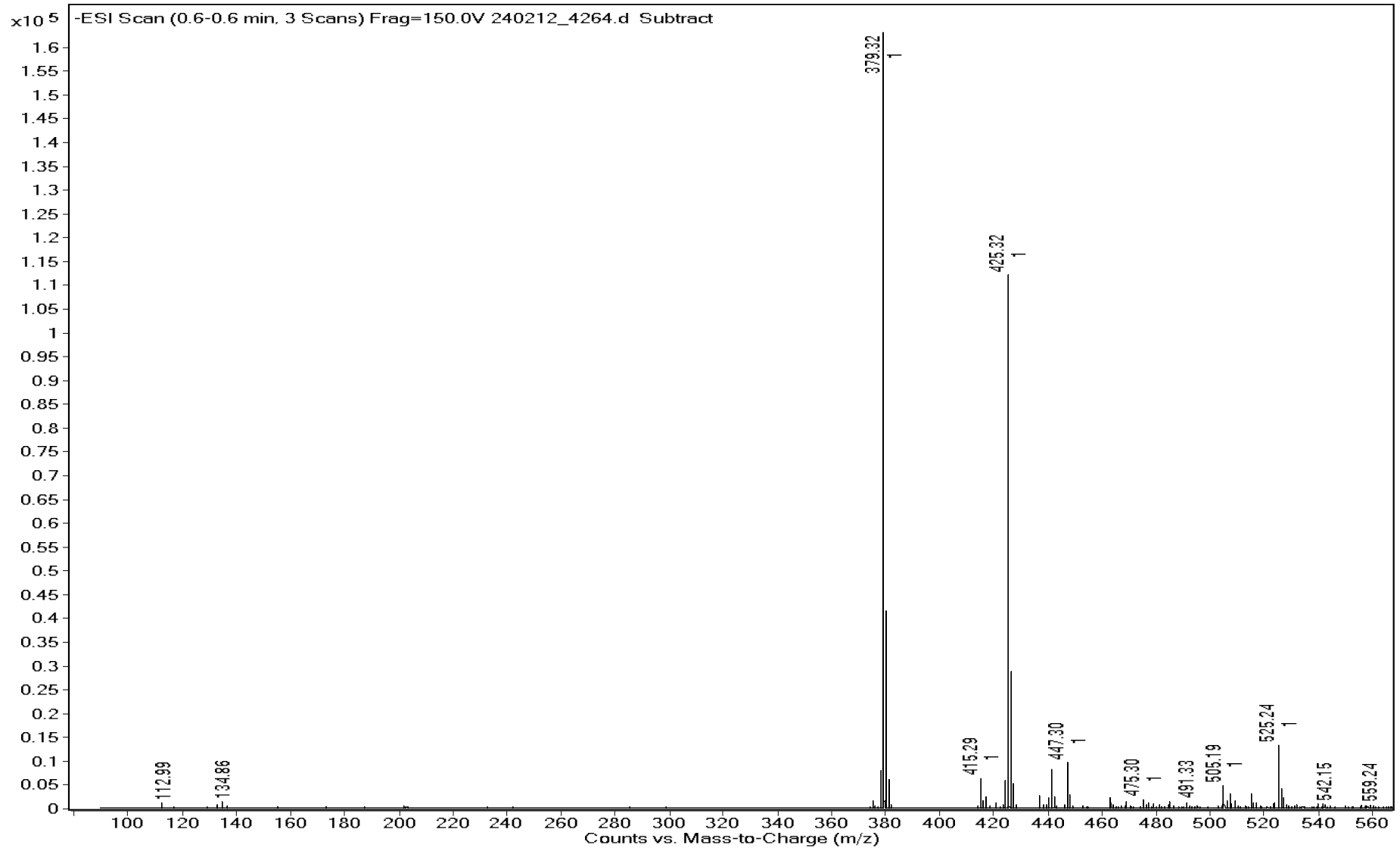
3beta-Lithocholic Acid-D4
1H-NMR, 600 MHz
Solvent: DMSO-D6
Lot No.: GR-19-075



Sample Name gr-19-075
DA Method AIMS_Accurate_Mass.m
Comment ESI-

Data File 240212_4264.d
Instrument Agilent 6538 UHD

Acq Method HRMS_Negative.m
Acq Date, Time 12/02/2024 1:15:56 PM



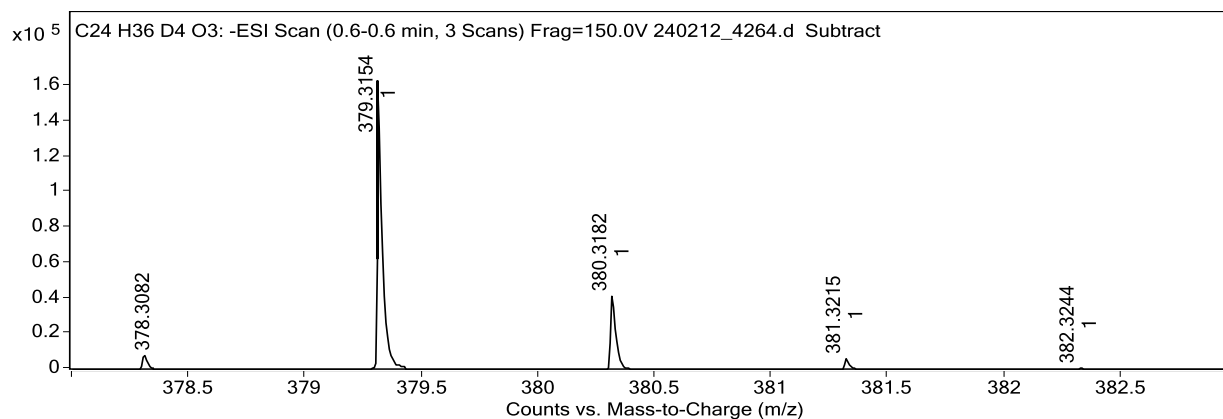
Sample Name	gr-19-075	Data File	240212_4264.d
Acq Method	HRMS_Negative.m	DA Method	AIMS_Accurate_Mass.m
Instrument	Agilent 6538 UHD	Acq Date, Time	12/02/2024 1:15:56 PM
Comment	ESI-		

Target Ion Species

Ion Species	m/z	Ionic Formula
(M-H) ⁻	379.3154	C ₂₄ H ₃₅ D ₄ O ₃

MFG Calculator Results

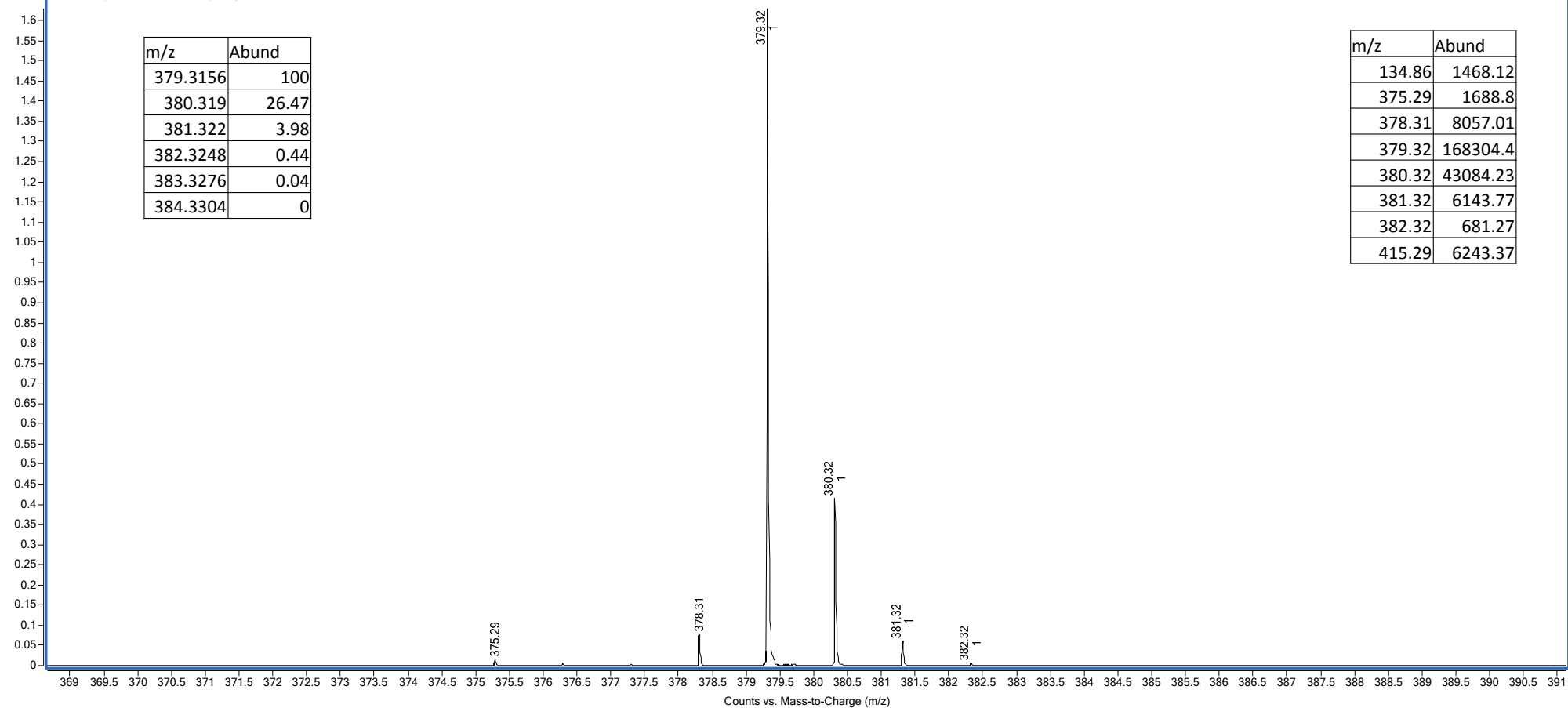
Target m/z	Ionic Formula	Calc m/z	+/- (mDa)	+/- (ppm)	DBE	MFG Score
379.3154	C ₂₄ H ₃₅ D ₄ O ₃	379.3156	-0.2	-0.5	5.0	99.19
379.3154	C ₂₀ H ₃₁ D ₄ N ₆ O	379.3129	2.5	6.6	6.0	84.93
379.3154	C ₁₉ H ₃₅ D ₄ N ₂ O ₅	379.3116	3.8	10.0	1.0	70.26



Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (mDa)	Abund (%)	Calc Abund (%)	+/-
1	379.3154	379.3156	-0.2	100.0	100.0	0.0
2	380.3182	380.3190	-0.8	25.6	26.5	0.9
3	381.3215	381.3220	-0.5	3.7	4.0	0.3

x10⁵ -ESI Scan (0.6-0.6 min, 3 Scans) Frag=150.0V 240212_4264.d Subtract



m/z	Abund
379.3156	100
380.319	26.47
381.322	3.98
382.3248	0.44
383.3276	0.04
384.3304	0

m/z	Abund
134.86	1468.12
375.29	1688.8
378.31	8057.01
379.32	168304.4
380.32	43084.23
381.32	6143.77
382.32	681.27
415.29	6243.37