

Name:	Glycochenodeoxycholic Acid-D4
Lot#:	GR-19-115
Test Date:	05/06/2024 (re-test date: 05/06/2029)
CAS No.:	1201918-16-2
MF:	C ₂₆ H ₃₉ D ₄ NO ₅
MW:	453.65
Appearance:	Off-White solid
Purity:	>97% by NMR; TLC – one spot (eluent acetone); 99% atom D
¹H-NMR:	Conforms
MS-ESI (-)	Conforms (shows peak at m/z = 452.33 [M-H] ⁻)
Storage	Store at -18°C in a dry place away from direct sunlight

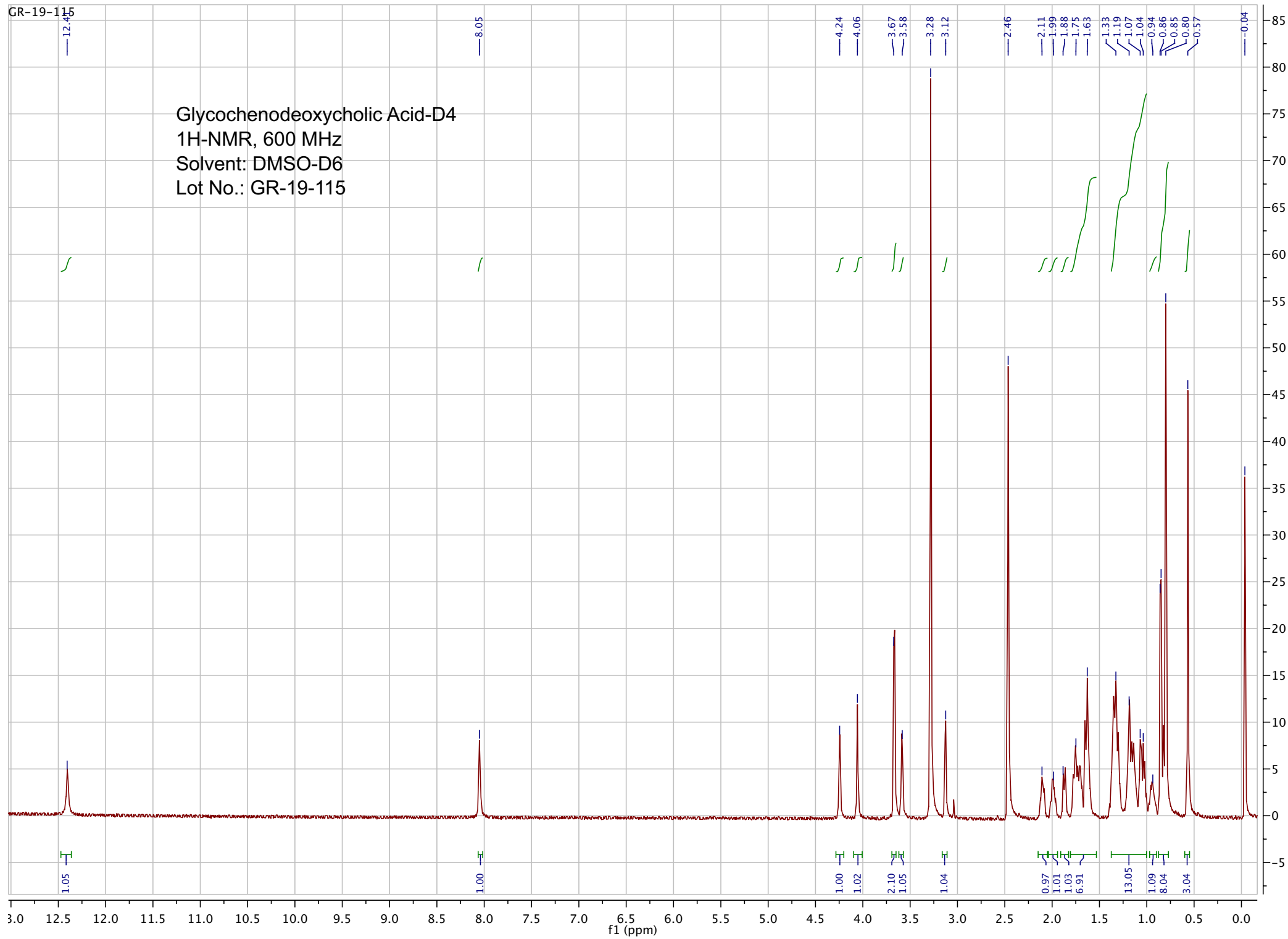
Approved by:

Date: 05/09/2024

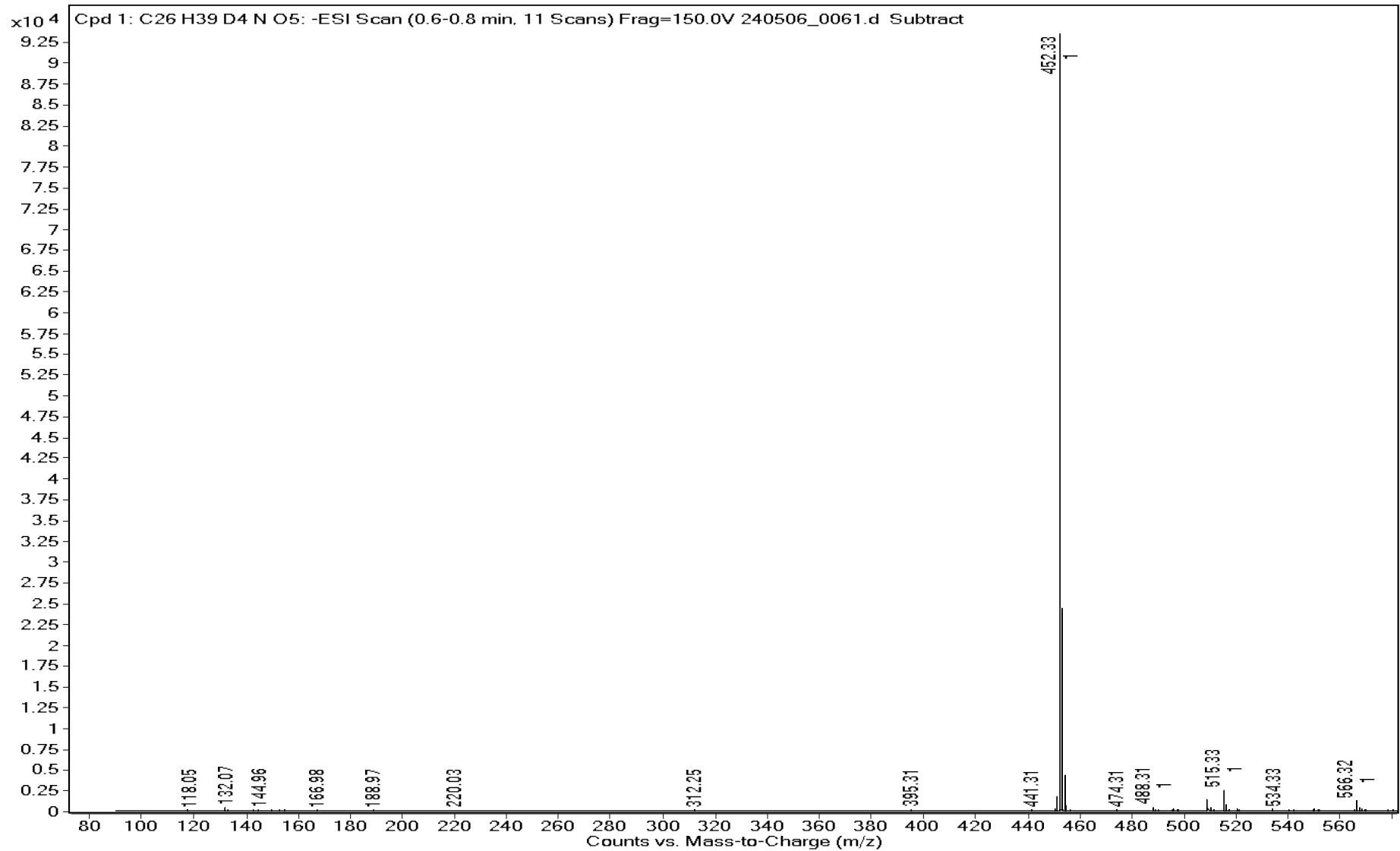


Viorica Rusu, QC/QA Manager

Glycochenodeoxycholic Acid-D4
1H-NMR, 600 MHz
Solvent: DMSO-D6
Lot No.: GR-19-115



Sample Name	GR-19-115	Data File	240506_0061.d	Acq Method	HRMS_Negative.m
DA Method	AIMS_Accurate_Mass.m	Instrument	Agilent 6538 UHD	Acq Date, Time	06/05/2024 12:34:17 PM
Comment	ESI-				



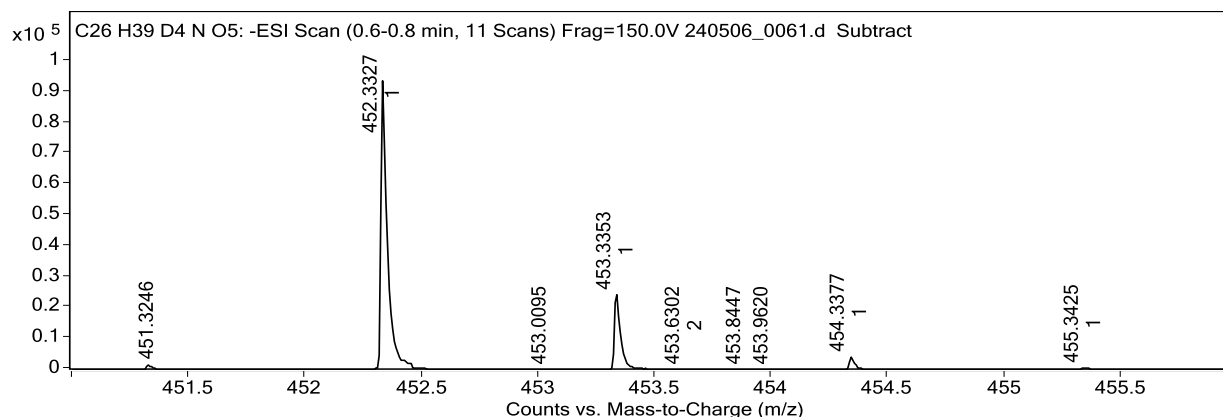
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Acq Method	HRMS_Negative.m	DA Method	AIMS_Accurate_Mass.m
Instrument	Agilent 6538 UHD	Acq Date, Time	06/05/2024 12:34:17 PM
Comment	ESI-		

Target Ion Species

Ion Species	m/z	Ionic Formula
(M-H) ⁻	452.3327	C26 H38 D4 N O5

MFG Calculator Results

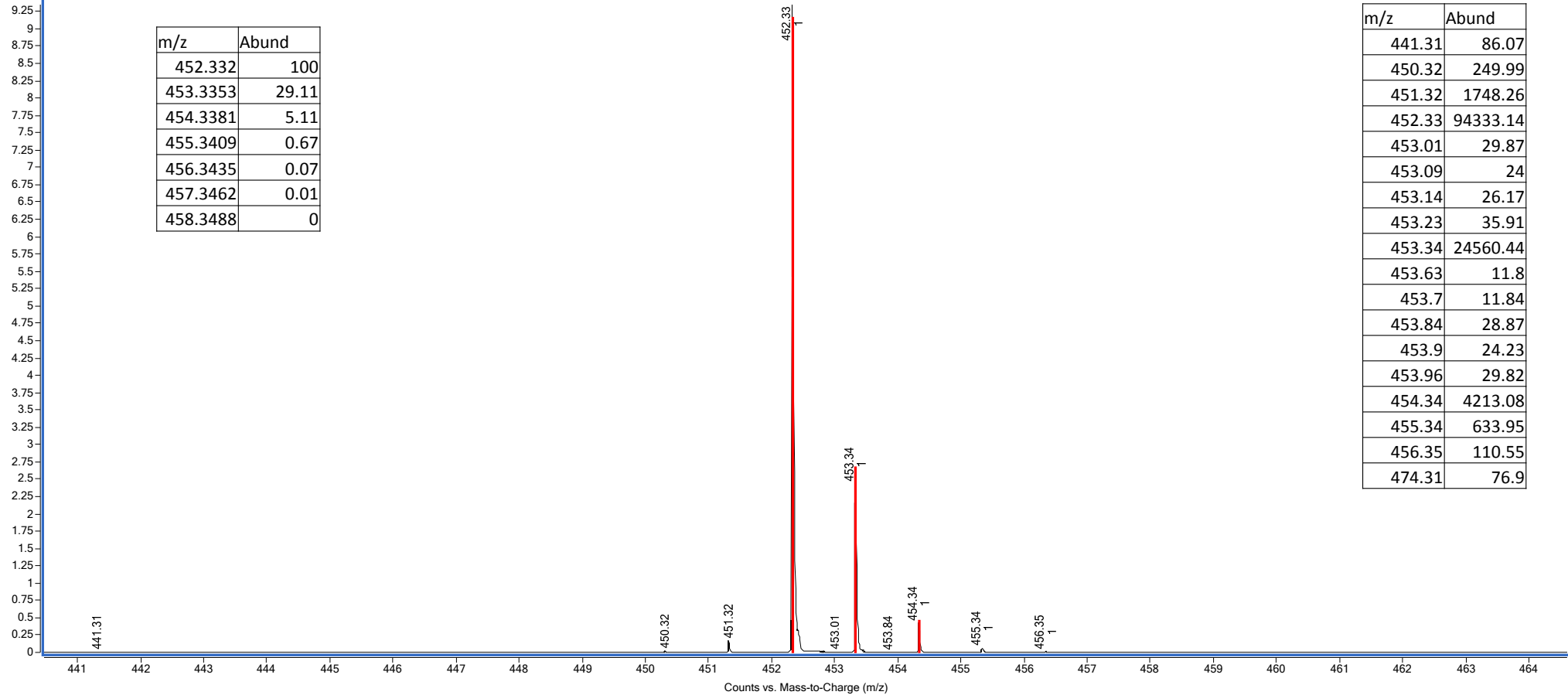
Target m/z	Ionic Formula	Calc m/z	+/- (mDa)	+/- (ppm)	DBE	MFG Score
452.3327	C26 H38 D4 N O5	452.3320	0.7	1.5	6.0	97.16
452.3327	C27 H34 D4 N5 O	452.3333	-0.6	-1.3	11.0	94.28
452.3327	C22 H34 D4 N7 O3	452.3293	3.4	7.5	7.0	79.37



Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (mDa)	Abund (%)	Calc Abund (%)	+/-
1	452.3327	452.3320	0.7	100.0	100.0	0.0
2	453.3353	453.3353	0.0	26.0	29.1	3.1
3	454.3377	454.3381	-0.4	4.5	5.1	0.6

x10⁴ Cpd 1: C26 H39 D4 N O5: -ESI Scan (0.6-0.8 min, 11 Scans) Frag=150.0V 240506_0061.d Subtract



m/z	Abund
452.332	100
453.3353	29.11
454.3381	5.11
455.3409	0.67
456.3435	0.07
457.3462	0.01
458.3488	0

m/z	Abund
441.31	86.07
450.32	249.99
451.32	1748.26
452.33	94333.14
453.01	29.87
453.09	24
453.14	26.17
453.23	35.91
453.34	24560.44
453.63	11.8
453.7	11.84
453.84	28.87
453.9	24.23
453.96	29.82
454.34	4213.08
455.34	633.95
456.35	110.55
474.31	76.9