

Name:	Mesalazine-D3 HCl (5-Amino-2-hydroxybenzoic Acid-d3 Hydrochloride; 5-Aminosalicylic Acid-d3 Hydrochloride; 5-Aminosalicylic Acid-d3 Hydrochloride; Mesalamine-d3 HCl)
Lot#:	GR-19-223
Test Date:	02/03/2025 (re-test date: 02/03/2030)
CAS No.:	1346601-18-0
MF:	C ₇ H ₅ D ₃ ClNO ₃
MW:	192.61
Appearance:	Off-white solid
Purity:	99.9% by HPLC (average of two sample preparations); >98% atom D
¹H-NMR:	Conforms (shows a trace of acetone)
MS-ESI (+)	Conforms (shows peak at m/z = 157.07 [M _(free base) +H] ⁺)
Storage	Store at -18°C in a dry place away from direct sunlight

Approved by:

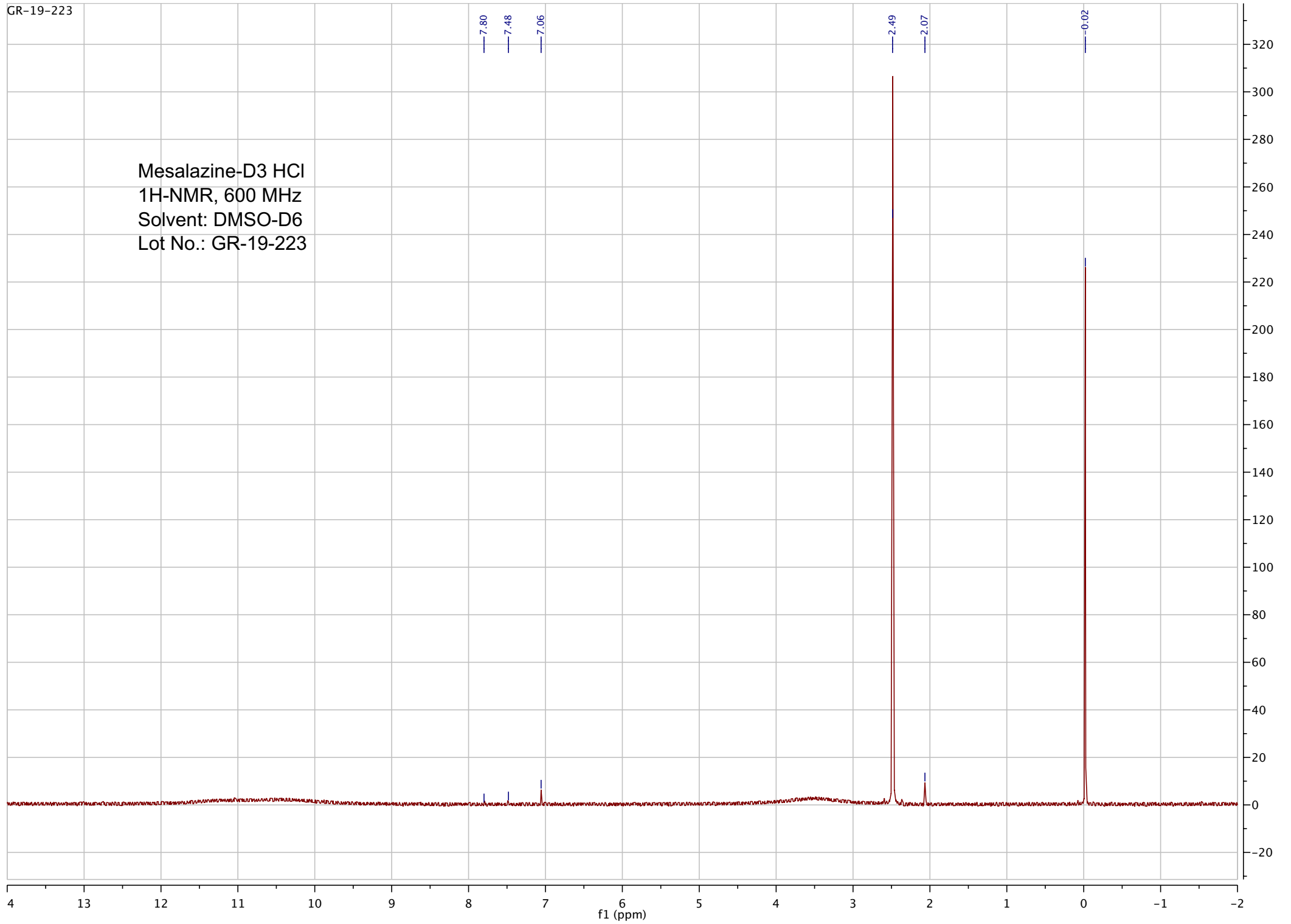
Date: 02/04/2025



Viorica Rusu, QC/QA Manager

GR-19-223

Mesalazine-D3 HCl
1H-NMR, 600 MHz
Solvent: DMSO-D6
Lot No.: GR-19-223



25.02.04.3588

MASS SPECTROMETRY

Sample Submission Form 2022-2023

The AIMS Mass Spectrometry Laboratory has no Biocontainment Level designation. All samples of biological origin must therefore be inactivated and free from pathogens.

Is sample of biological origin? Yes No

If yes, has sample been treated to inactivate pathogens? Yes No

Authorized Signature: *Archie*

P.I. Name: Expert Synthesis Solutions

Account: _____

Name: Ghenadie Rusu

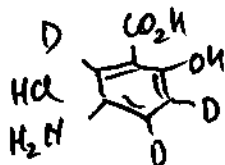
Email (Please type): grusu@esschemco.com

Sample ID: GR-19-223

Molecular Formula: C₇H₅D₃ClNO₂ Molecular Mass: 156.15 (free base)

Solubility: H₂O CH₃OH CH₂OH CH₂Cl₂ Other _____

Structure / Sample information:



Please, integrate the peaks at $M \pm 10$ Da

Thank you!

25.02.04.3588

Ionization/Analysis: EI ESI DART MALDI LC-MS

Polarity: + - GC-MS

Accurate Mass:



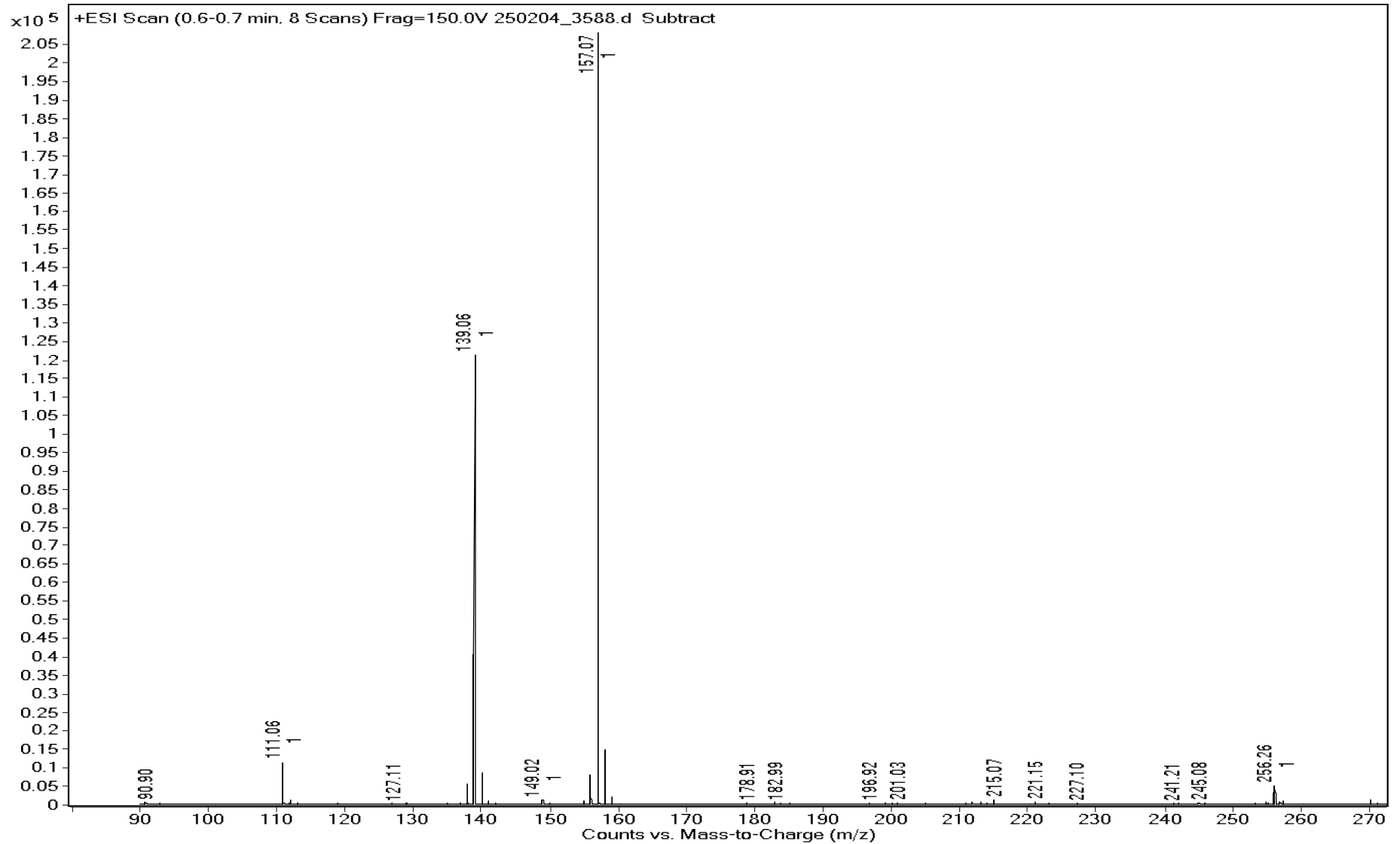
MASS SPECTROMETRY LABORATORY

uoft.me/AIMS

CHEMISTRY
UNIVERSITY OF TORONTO



Sample Name	GR-19-223	Data File	250204_3588.d	Acq Method	HRMS.m
DA Method	AIMS_Accurate_Mass.m	Instrument	Agilent 6538 UHD	Acq Date, Time	04/02/2025 10:35:26 AM
Comment	ESI+				



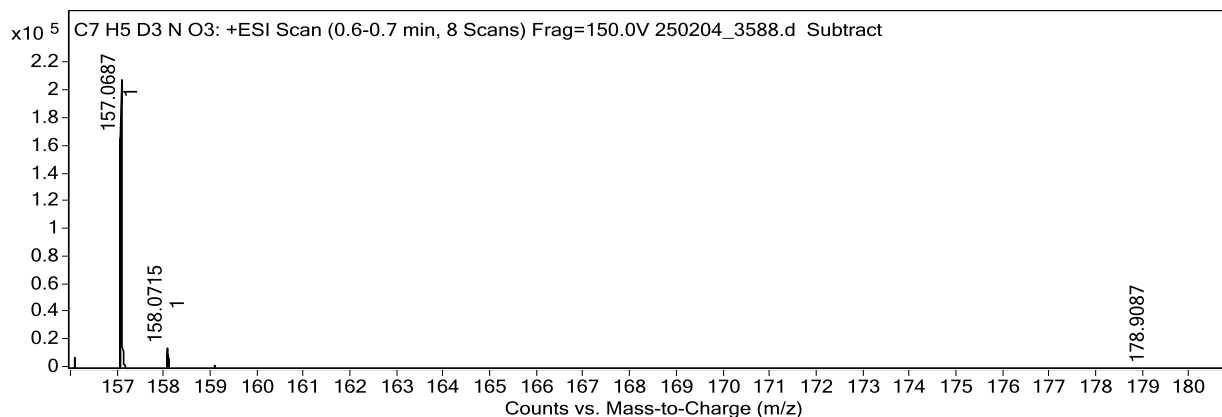
Sample Name	GR-19-223	Data File	250204_3588.d
Acq Method	HRMS.m	DA Method	AIMS_Accurate_Mass.m
Instrument	Agilent 6538 UHD	Acq Date, Time	04/02/2025 10:35:26 AM
Comment	ESI+		

Target Ion Species

Ion Species	m/z	Ionic Formula
M+	157.0687	C7 H5 [2H]3 N O3

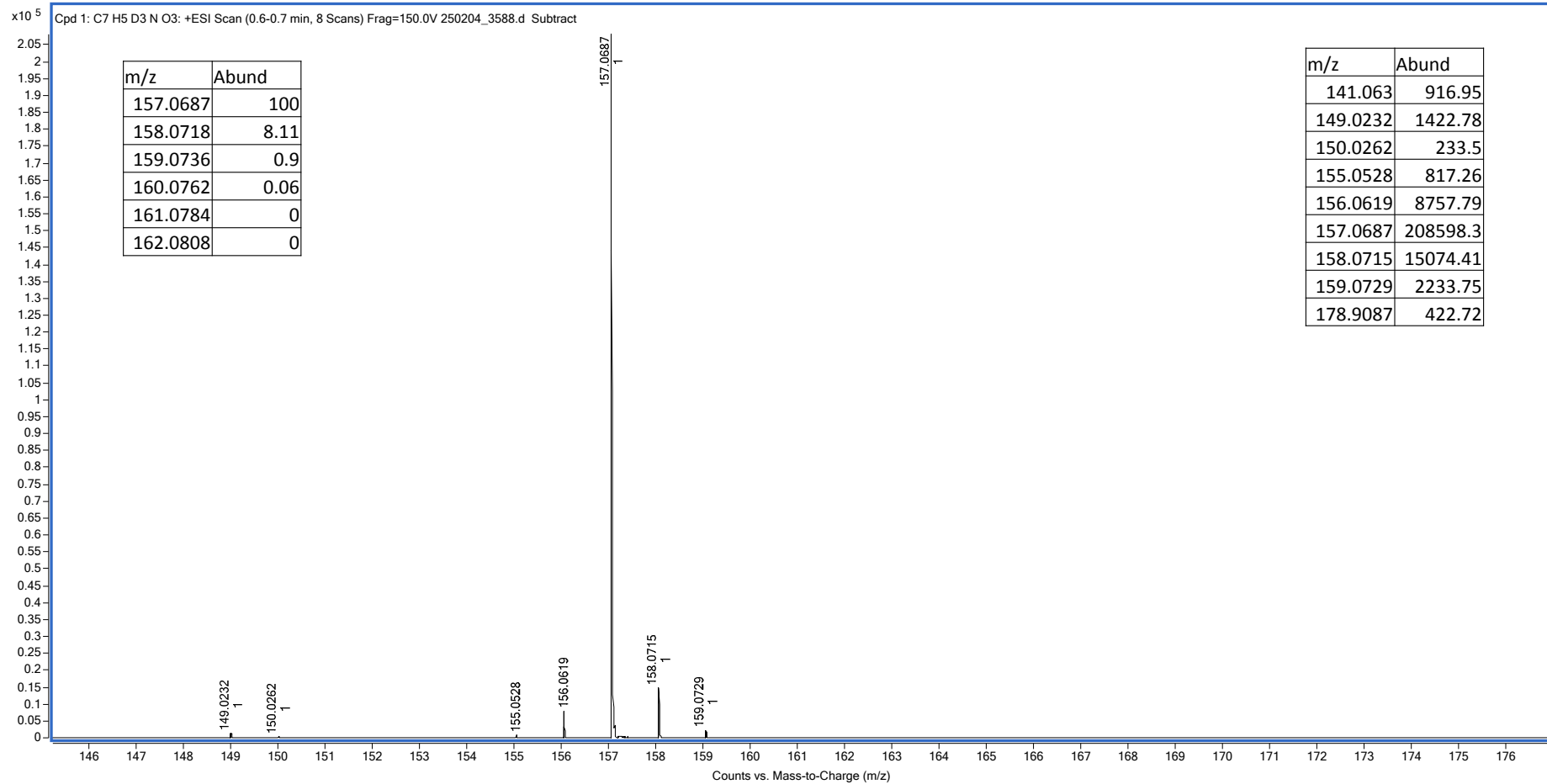
MFG Calculator Results

Target m/z	Ionic Formula	Calc m/z	+/- (mDa)	+/- (ppm)	DBE	MFG Score
157.0687	C7 H5 [2H]3 N O3	157.0687	0.0	0.0	4.5	99.59
157.0687	C5 H5 [2H]2 N4 O2	157.0689	-0.2	-1.3	4.5	98.91
157.0687	C2 H9 [2H] N3 O5	157.0678	0.9	5.7	-0.5	88.00
157.0687	H9 N6 O4	157.0680	0.7	4.5		77.35

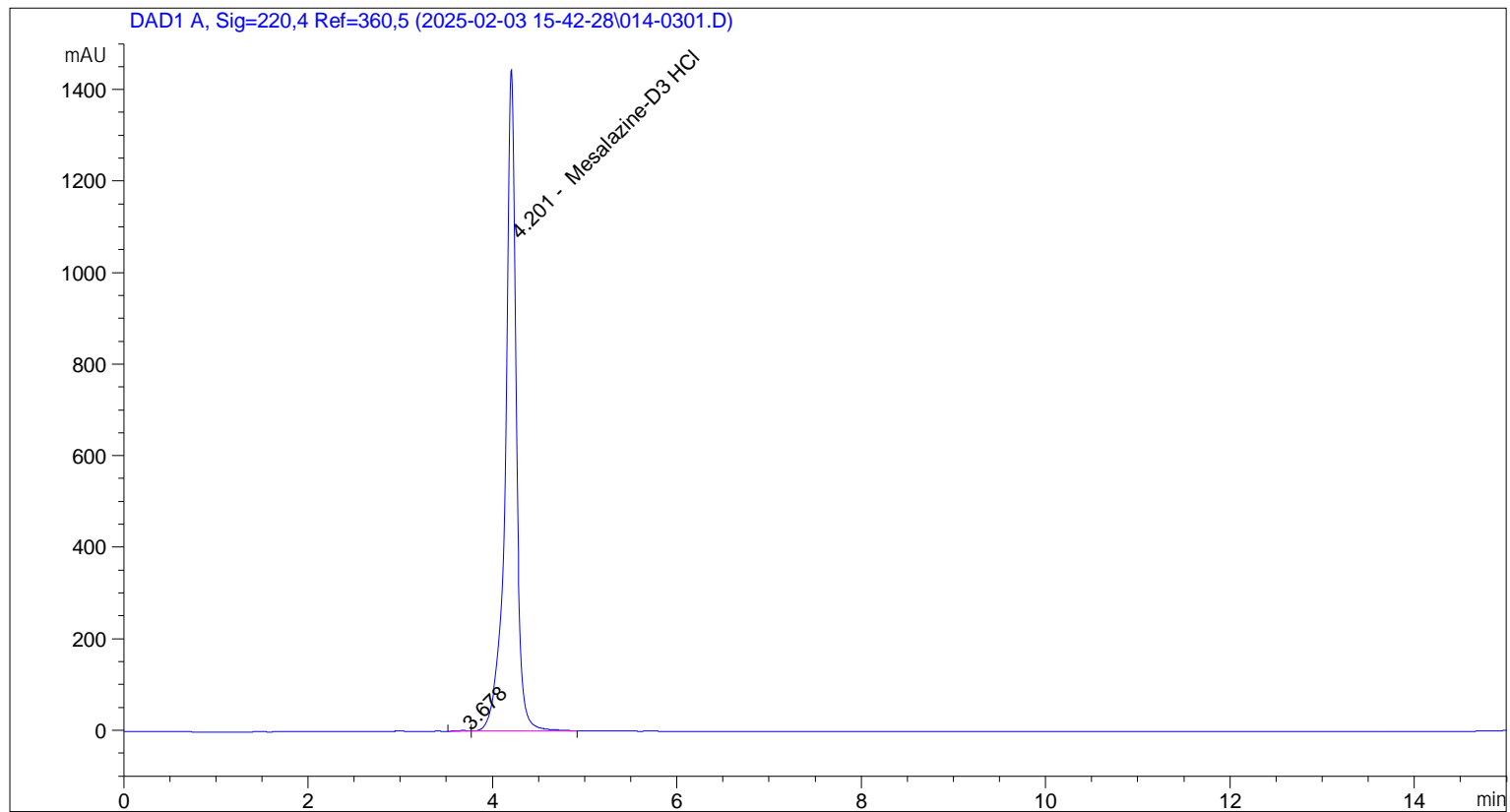


Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (mDa)	Abund (%)	Calc Abund (%)	+/-
1	157.0687	157.0687	0.0	100.0	100.0	0.0
2	158.0715	158.0718	-0.3	7.2	8.1	0.9
3	159.0729	159.0736	-0.7	1.1	0.9	-0.2



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Acq. Operator : vrusu Seq. Line : 3
Acq. Instrument : Instrument 1 Location : Vial 14
Injection Date : 2/3/2025 4:50:06 PM Inj : 1
 Inj Volume: 5.0 µl
Acq. Method : C:\CHEM32\1\DATA\2025-02-03 15-42-28\VR020325_223.M
Last changed : 2/3/2025 3:42:11 PM by vrusu
Analysis Method : C:\CHEM32\1\METHODS\VR020425_223PM.M
Last changed : 2/4/2025 8:05:38 AM
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Area Percent Report
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Sorted By : Signal
Calib. Data Modified : 2/4/2025 8:04:32 AM
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=220,4 Ref=360,5

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	3.678	BV	0.0868	10.05560	0.0866	?
2	4.201	VB	0.1175	1.16043e4	99.9134	Mesalazine-D3 HCl

Totals : 1.16143e4

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*** End of Report ***