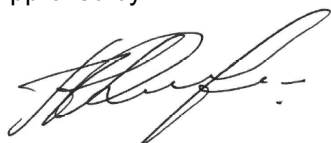


Name:	Methotrexate-D3
Lot#:	GR-18-233
Test Date:	07/26/2023 (re-test date: 07/26/2028)
CAS No.:	432545-63-6
MF:	C ₂₀ H ₁₉ D ₃ N ₈ O ₅
MW:	457.46
Appearance:	Orange solid
Purity:	99.5% by HPLC (average of two sample preparations); 99.5% atom D
NMR (¹H):	Conforms
MS-ESI (+)	Conforms (shows peak at m/z = 458.20 [M+H] ⁺)
Storage	Store at 0-5°C in a dry place away from direct sunlight

Approved by:

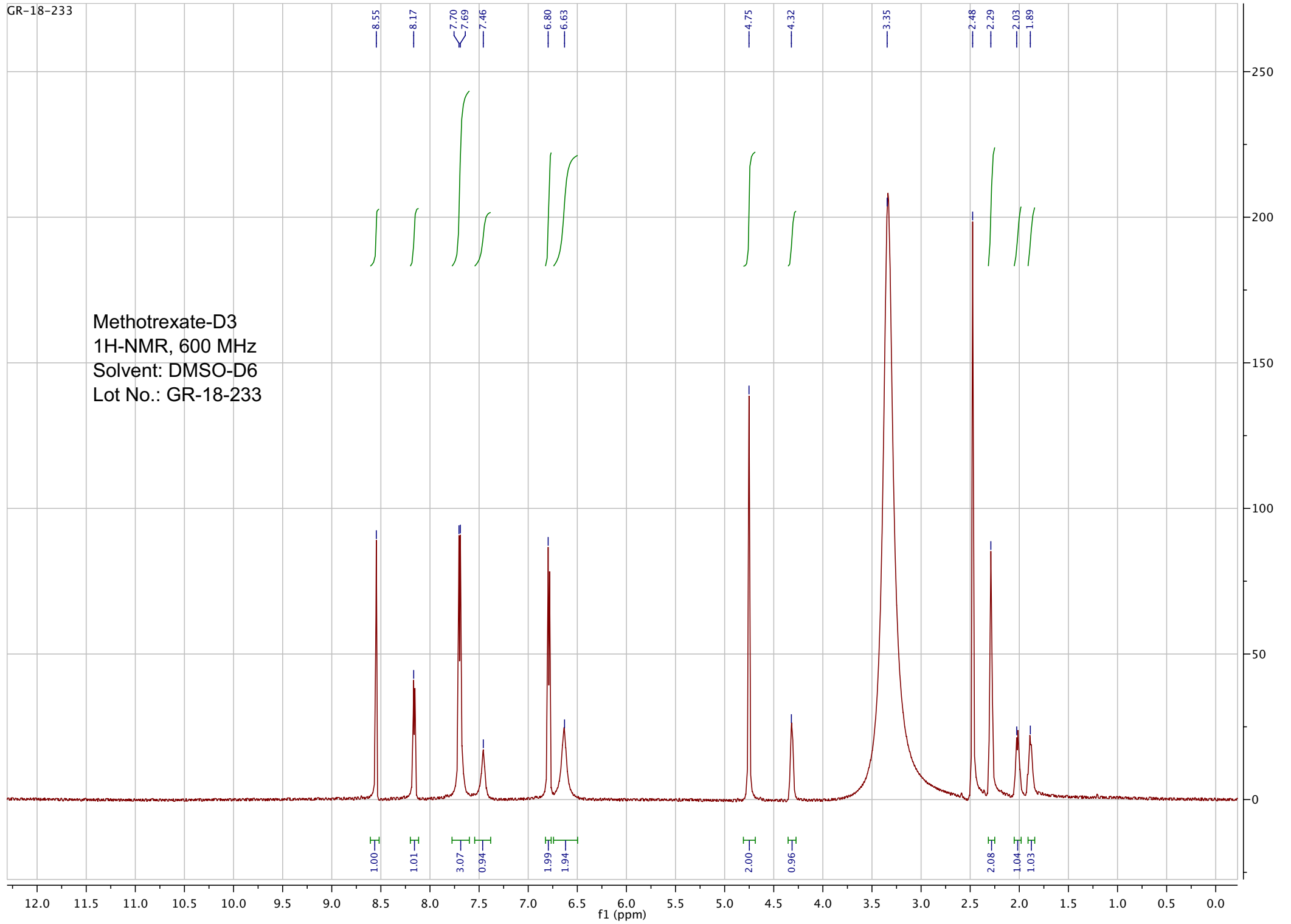
Date: 08/11/2023



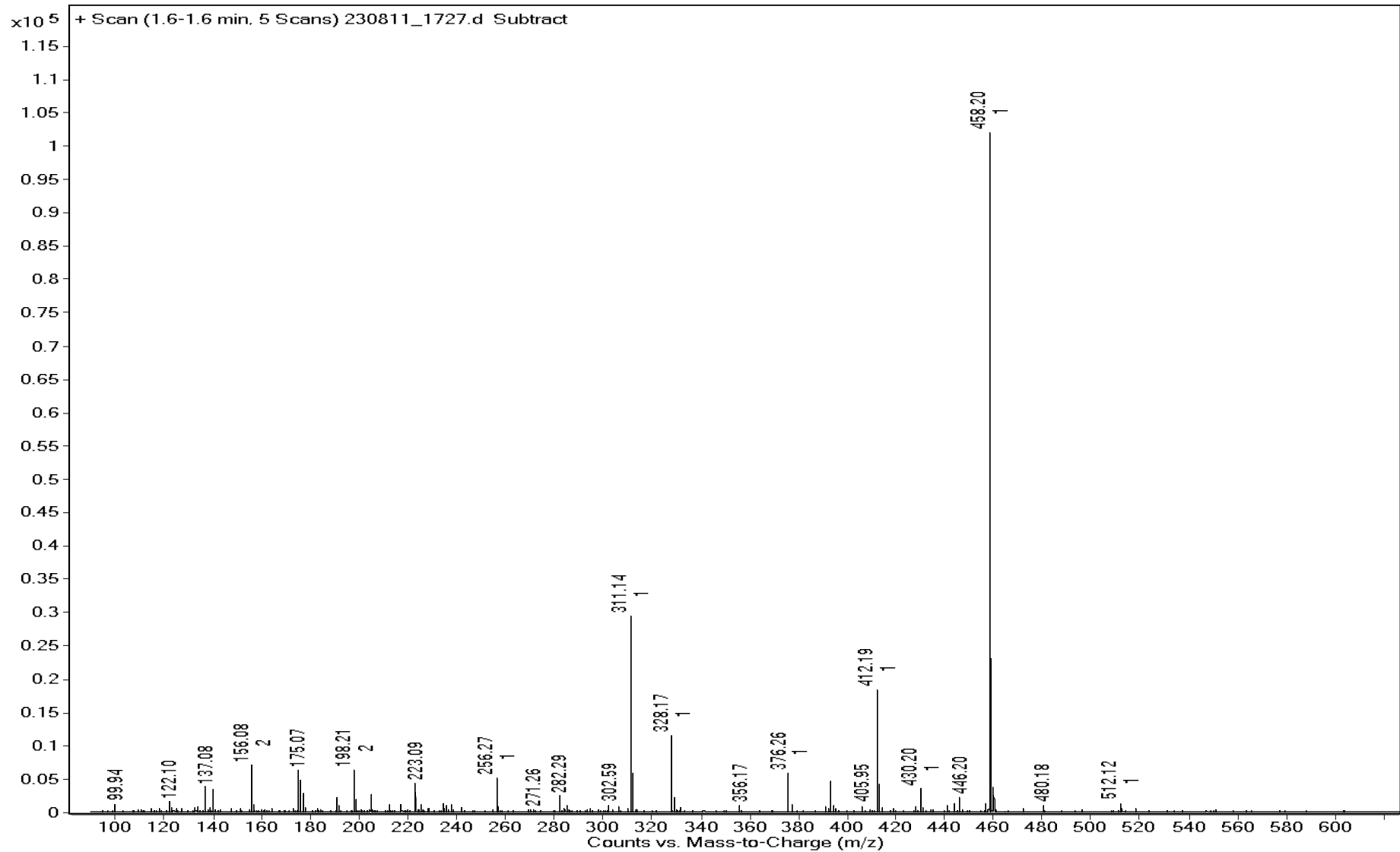
Viorica Rusu, QC/QA Manager

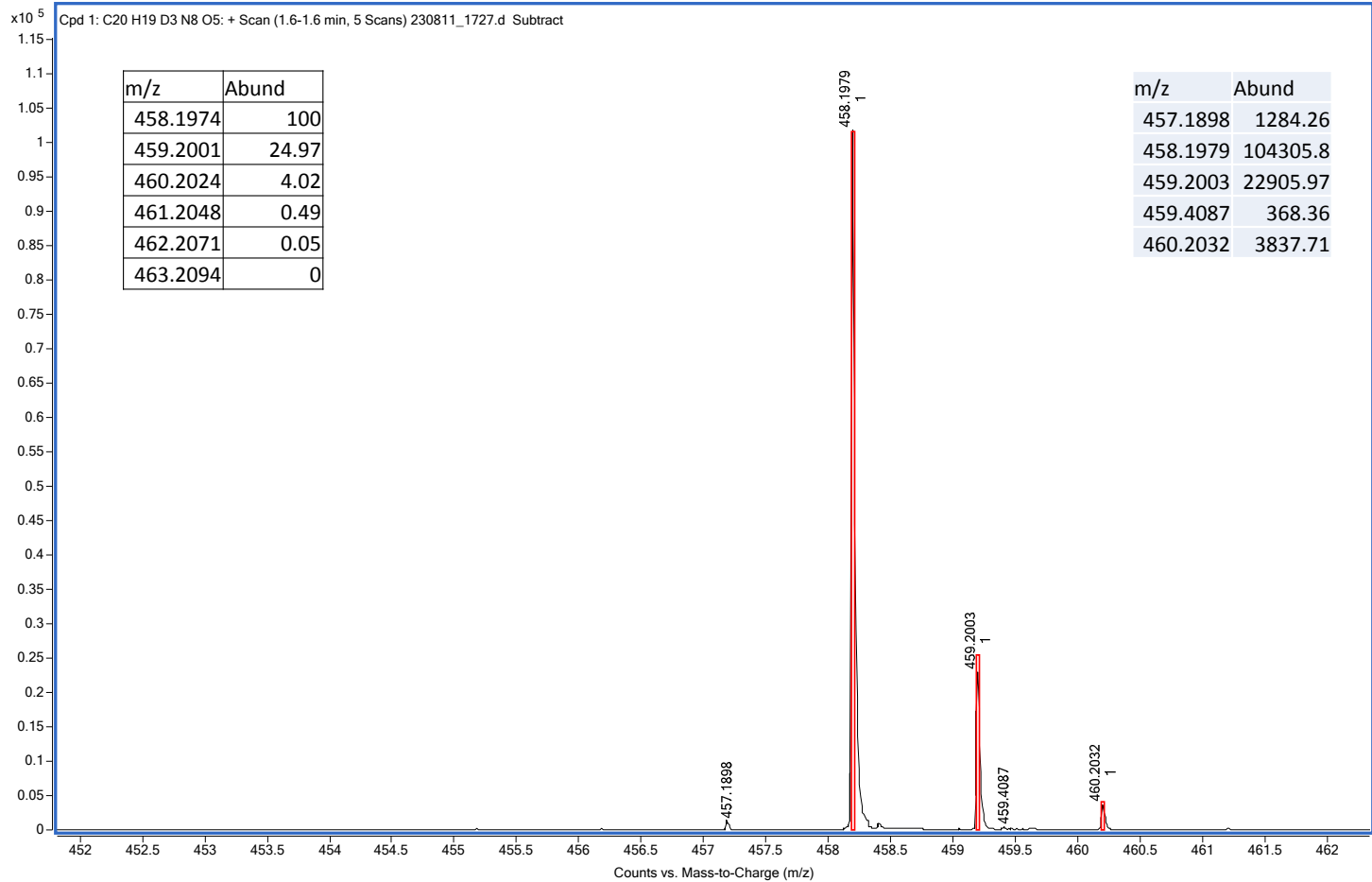
GR-18-233

Methotrexate-D3
1H-NMR, 600 MHz
Solvent: DMSO-D6
Lot No.: GR-18-233



Sample Name	GR-18-233	Data File	230811_1727.d	Acq Method	HRMS.m
DA Method	AIMS_Accurate_Mass.m	Instrument	Agilent 6538 UHD	Acq Date, Time	11/08/2023 11:19:27 AM
Comment	ESI+				





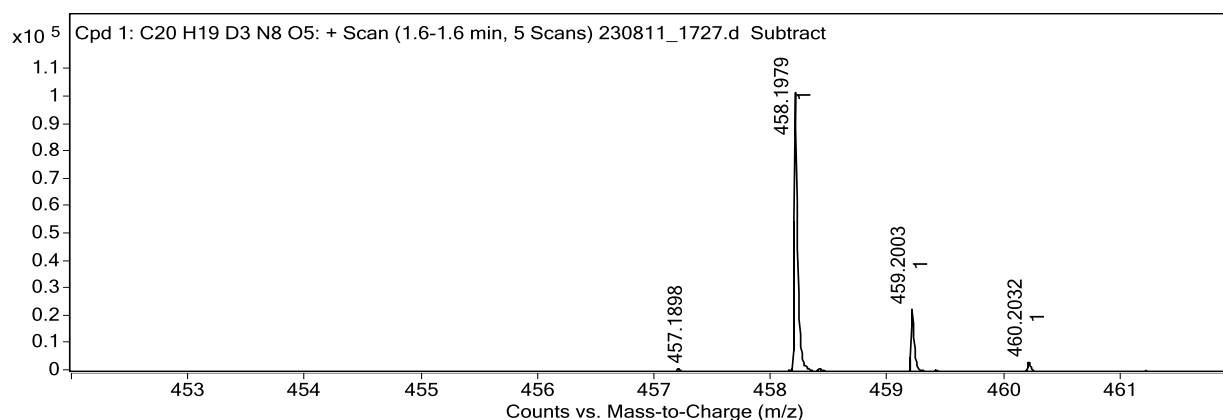
Sample Name	GR-18-233	Data File	230811_1727.d
Acq Method	HRMS.m	DA Method	AIMS_Accurate_Mass.m
Instrument	Agilent 6538 UHD	Acq Date, Time	11/08/2023 11:19:27 AM
Comment	ESI+		

Target Ion Species

Ion Species	m/z	Ionic Formula
(M+H) ⁺	458.1979	C ₂₀ H ₂₀ D ₃ N ₈ O ₅

MFG Calculator Results

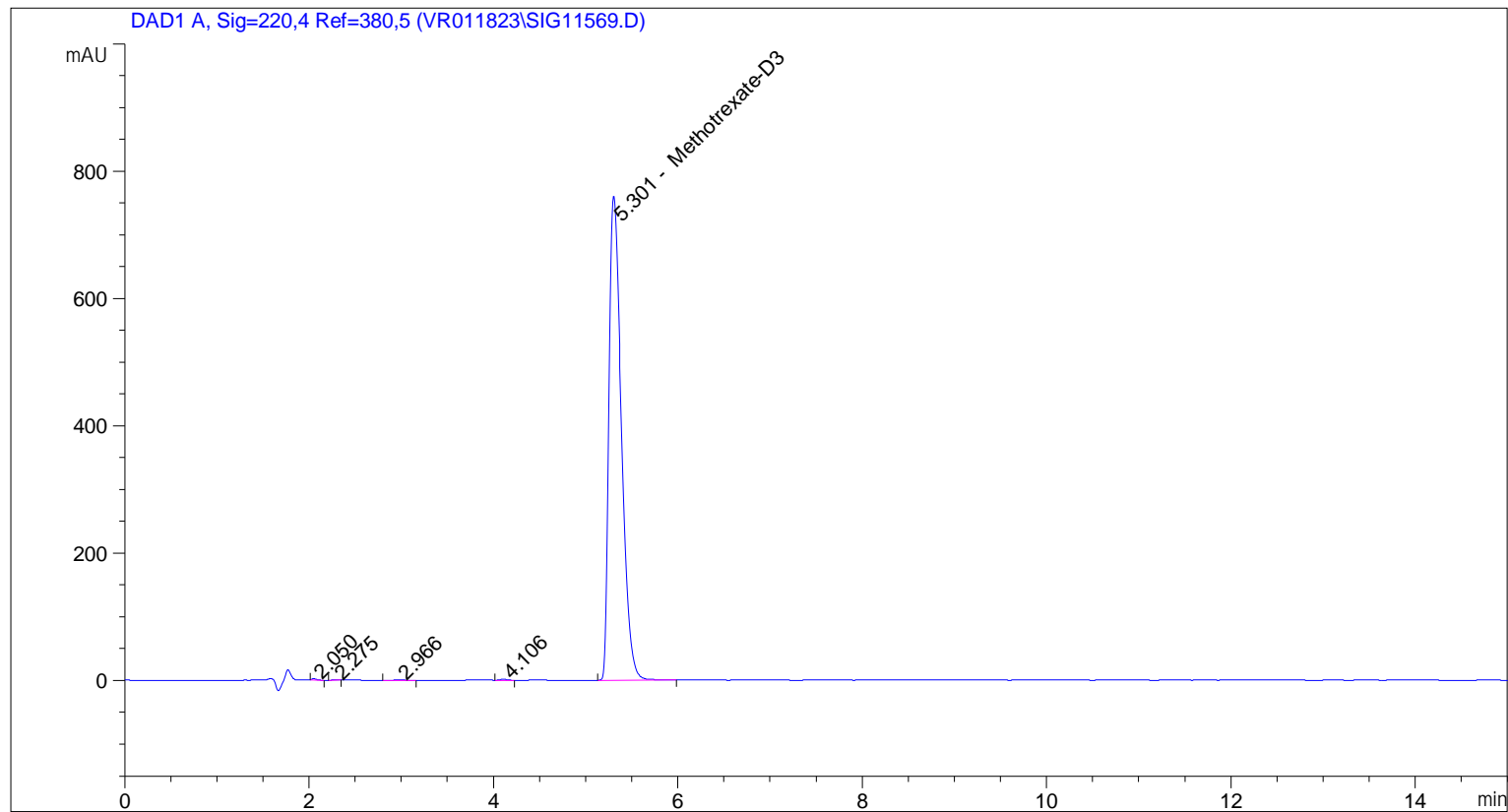
Target m/z	Ionic Formula	Calc m/z	+/- (mDa)	+/- (ppm)	DBE	MFG Score
458.1979	C ₂₀ H ₂₀ D ₃ N ₈ O ₅	458.1974	0.5	1.1	14.0	97.81
458.1979	C ₁₈ H ₃₂ D O ₁₃	458.1978	0.1	0.2	3.0	97.76
458.1979	C ₁₆ H ₃₂ N ₃ O ₁₂	458.1980	-0.1	-0.2	3.0	97.30
458.1979	C ₁₉ H ₂₈ D N ₄ O ₉	458.1992	-1.3	-2.8	8.0	95.18
458.1979	C ₂₁ H ₂₈ D ₂ N O ₁₀	458.1990	-1.1	-2.4	8.0	94.95
458.1979	C ₁₅ H ₂₄ D N ₁₀ O ₇	458.1965	1.4	3.1	9.0	94.79
458.1979	C ₁₇ H ₂₈ N ₇ O ₈	458.1994	-1.5	-3.3	8.0	94.72
458.1979	C ₁₇ H ₂₄ D ₂ N ₇ O ₈	458.1963	1.6	3.5	9.0	94.46
458.1979	C ₁₉ H ₂₄ D ₃ N ₄ O ₉	458.1961	1.8	3.9	9.0	93.24
458.1979	C ₂₀ H ₂₄ D N ₈ O ₅	458.2005	-2.6	-5.7	13.0	84.45



Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (mDa)	Abund (%)	Calc Abund (%)	+/-
1	458.1979	458.1974	0.5	100.0	100.0	0.0
2	459.2003	459.2001	0.2	22.0	25.0	3.0
3	460.2032	460.2024	0.8	3.7	4.0	0.3

=====
Acq. Operator : vrusu
Acq. Instrument : Instrument 1 Location : Vial 90
Injection Date : 7/26/2023 9:18:21 AM Inj Volume : 5.0 µl
Acq. Method : C:\CHEM32\1\METHODS\VR072623_233.M
Last changed : 7/26/2023 9:17:15 AM by vrusu
Analysis Method : C:\CHEM32\1\METHODS\VR072623_233PM.M
Last changed : 7/26/2023 10:21:49 AM by vrusu



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Area Percent Report
=====

Sorted By : Signal
Calib. Data Modified : 7/26/2023 10:20:06 AM
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=220,4 Ref=380,5

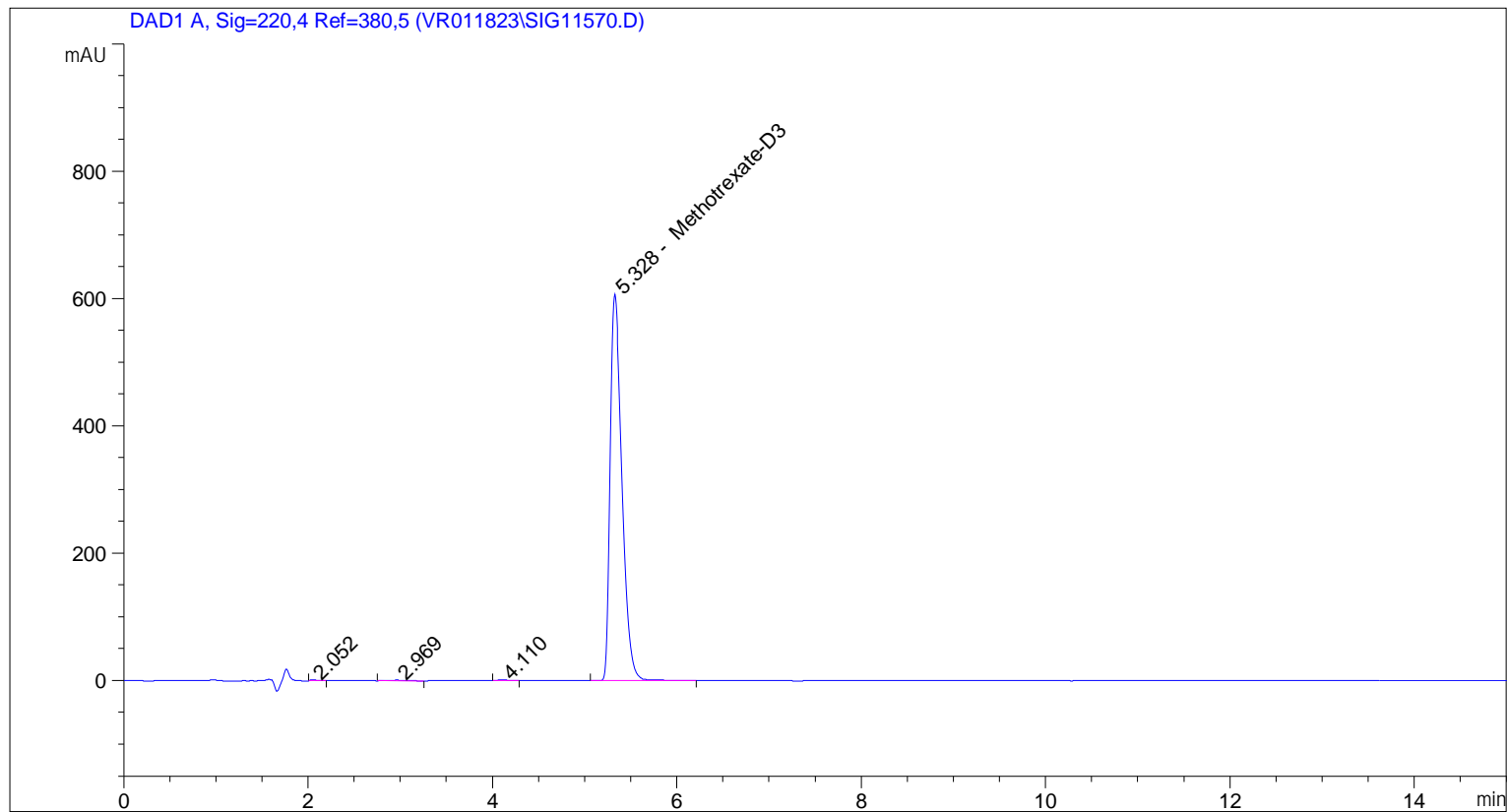
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	2.050	BB	0.0523	7.32441	0.1018	?
2	2.275	BB	0.0596	3.10587	0.0432	?
3	2.966	BB	0.0927	6.93150	0.0964	?
4	4.106	BB	0.0881	7.91235	0.1100	?
5	5.301	BB	0.1459	7166.68164	99.6486	Methotrexate-D3

Totals : 7191.95577

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*** End of Report ***

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Acq. Operator : vrusu
Acq. Instrument : Instrument 1 Location : Vial 91
Injection Date : 7/26/2023 9:35:38 AM Inj Volume : 5.0 µl
Acq. Method : C:\CHEM32\1\METHODS\VR072623_233.M
Last changed : 7/26/2023 9:34:36 AM by vrusu
Analysis Method : C:\CHEM32\1\METHODS\VR072623_233PM.M
Last changed : 7/26/2023 10:21:49 AM by vrusu



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Area Percent Report
=====

Sorted By : Signal
Calib. Data Modified : 7/26/2023 10:20:06 AM
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=220,4 Ref=380,5

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	2.052	BB	0.0632	7.97516	0.1460	?
2	2.969	BB	0.1354	11.20272	0.2050	?
3	4.110	BB	0.0981	9.31416	0.1705	?
4	5.328	BB	0.1405	5435.10889	99.4785	Methotrexate-D3

Totals : 5463.60092

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*** End of Report ***