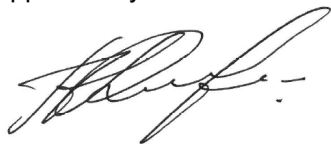


Name:	Tauroolithocholic Acid-D4
Lot#:	GR-19-077
Test Date:	02/07/2024 (re-test date: 02/07/2029)
CAS No.:	2410279-96-6
MF:	C ₂₆ H ₄₀ D ₄ NNaO ₅ S
MW:	509.71
Appearance:	White solid
Purity:	98.0% by HPLC; 99% atom D
¹H-NMR:	Conforms
MS-ESI (-)	Conforms (shows peak at m/z = 486.32 [M-Na] ⁻)
Storage	Store at -18°C in a dry place away from direct sunlight

Approved by:

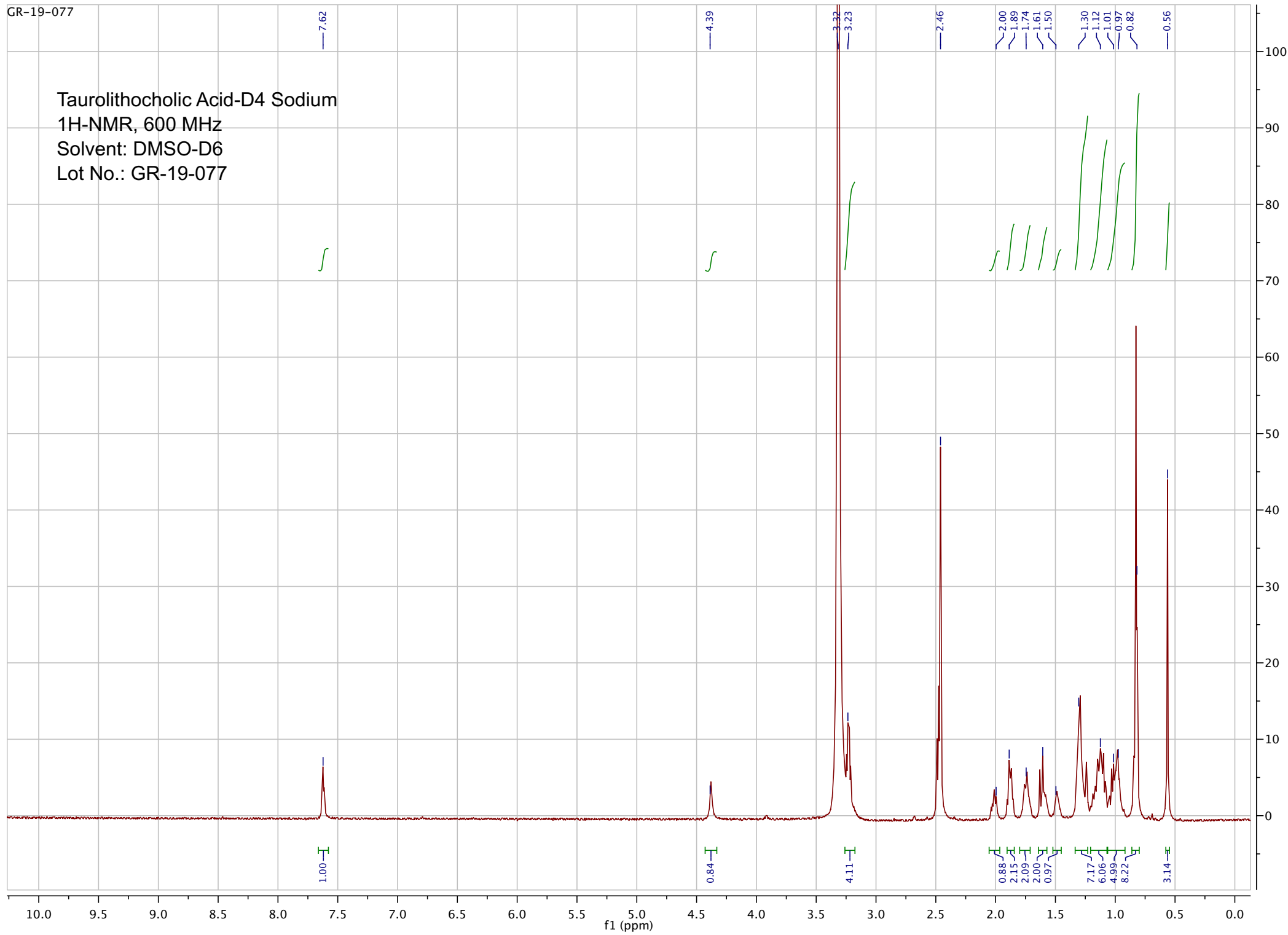
Date: 02/08/2024



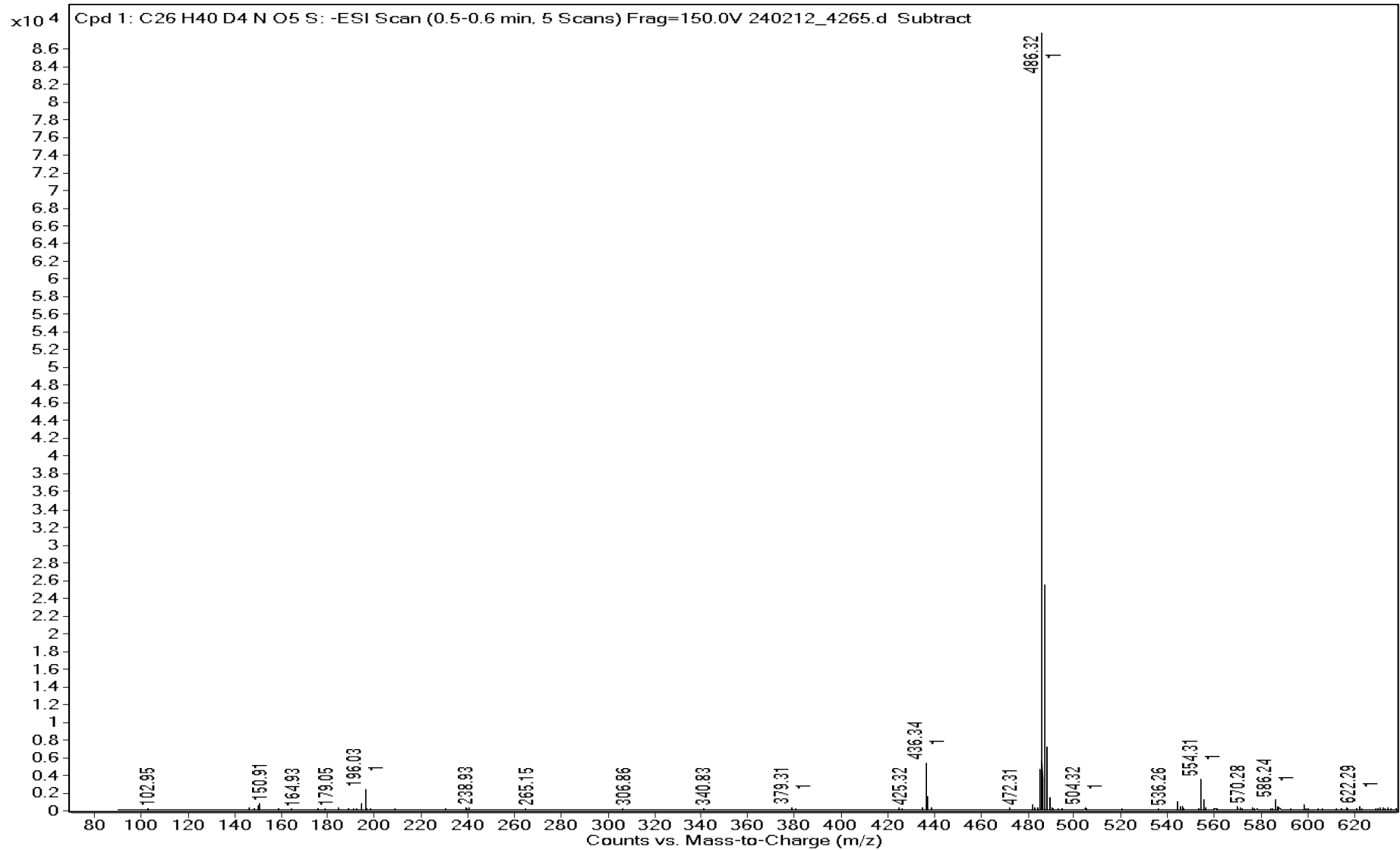
Viorica Rusu, QC/QA Manager

GR-19-077

Taurolithocholic Acid-D4 Sodium
1H-NMR, 600 MHz
Solvent: DMSO-D6
Lot No.: GR-19-077



Sample Name	GR-19-077	Data File	240212_4265.d	Acq Method	HRMS_Negative.m
DA Method	AIMS_Accurate_Mass.m	Instrument	Agilent 6538 UHD	Acq Date, Time	12/02/2024 1:58:09 PM
Comment	ESI-				



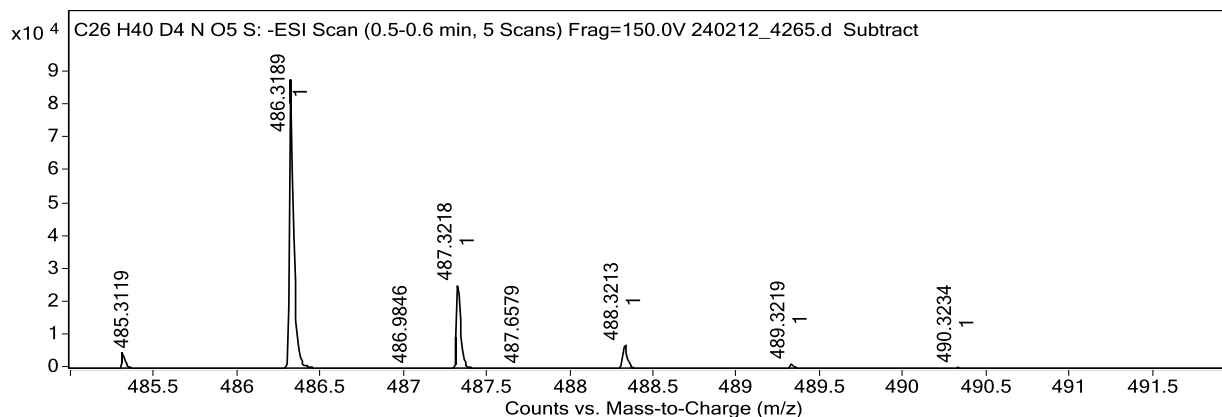
Sample Name	GR-19-077	Data File	240212_4265.d
Acq Method	HRMS_Negative.m	DA Method	AIMS_Accurate_Mass.m
Instrument	Agilent 6538 UHD	Acq Date, Time	12/02/2024 1:58:09 PM
Comment	ESI-		

Target Ion Species

Ion Species	m/z	Ionic Formula
M-	486.3189	C26 H40 [2H]4 N O5 S

MFG Calculator Results

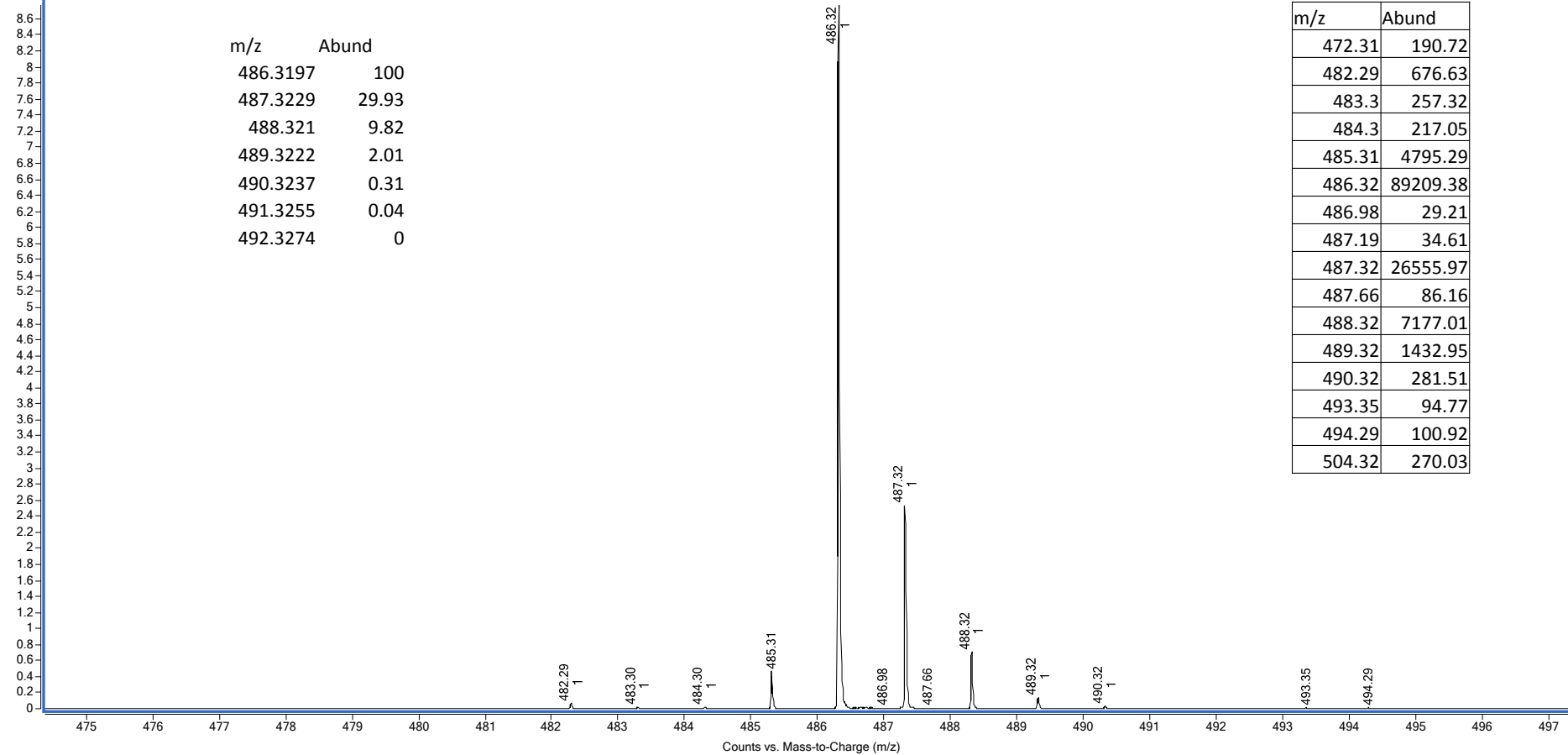
Target m/z	Ionic Formula	Calc m/z	+/- (mDa)	+/- (ppm)	DBE	MFG Score
486.3189	C26 H40 [2H]4 N O5 S	486.3197	-0.8	-1.6	5.5	97.68
486.3189	C27 H36 [2H]4 N5 O S	486.3210	-2.1	-4.3	10.5	90.67
486.3189	C22 H36 [2H]4 N7 O3 S	486.3170	1.9	3.9	6.5	89.39
486.3189	C21 H40 [2H]4 N3 O7 S	486.3157	3.2	6.6	1.5	76.52



Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (mDa)	Abund (%)	Calc Abund (%)	+/-
1	486.3189	486.3197	-0.8	100.0	100.0	0.0
2	487.3218	487.3229	-1.1	29.8	29.9	0.1
3	488.3213	488.3210	0.3	8.0	9.8	1.8
4	489.3219	489.3222	-0.3	1.6	2.0	0.4
5	490.3234	490.3237	-0.3	0.3	0.3	0.0

x10⁴ Cpd 1: C26 H40 D4 N O5 S: -ESI Scan (0.5-0.6 min, 5 Scans) Frag=150.0V 240212_4265.d Subtract



Sample Name: GR-09-093

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	2.545	BBA	0.1087	115.04021	2.0523	?

Uncalib. totals : 115.04021 2.0523

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*** End of Report ***

Sample Name: GR-09-093 spl-2

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	2.543	BBA	0.1053	113.88187	1.9523	?

Uncalib. totals : 113.88187 1.9523

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*** End of Report ***