

Name:	Estrone-3-Sulfate Sodium
Lot#:	GR-18-279
Test Date:	11/02/2023 (re-test date: 11/02/2026)
CAS No.:	438-67-5
MF:	C ₁₈ H ₂₁ NaO ₅ S
MW:	372.41
Appearance:	White solid
Purity:	99.9% by HPLC (average of two sample preparations)
¹H-NMR:	Conforms
MS-ESI (-)	Conforms (shows peak at m/z = 349.11 [M-Na] ⁻)
Storage	Store at -18°C in a dry place away from direct sunlight

Approved by:

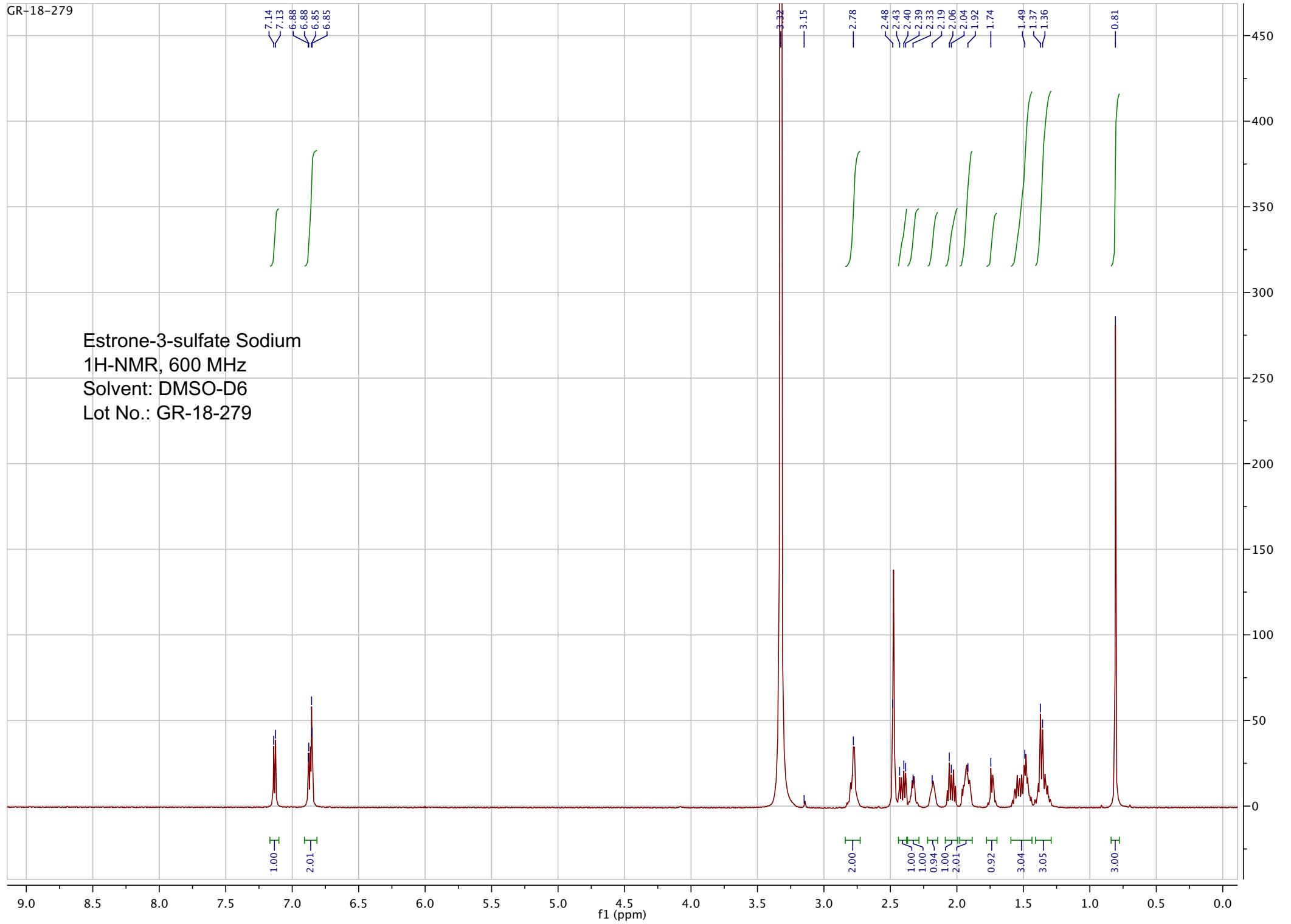
Date: 11/06/2023



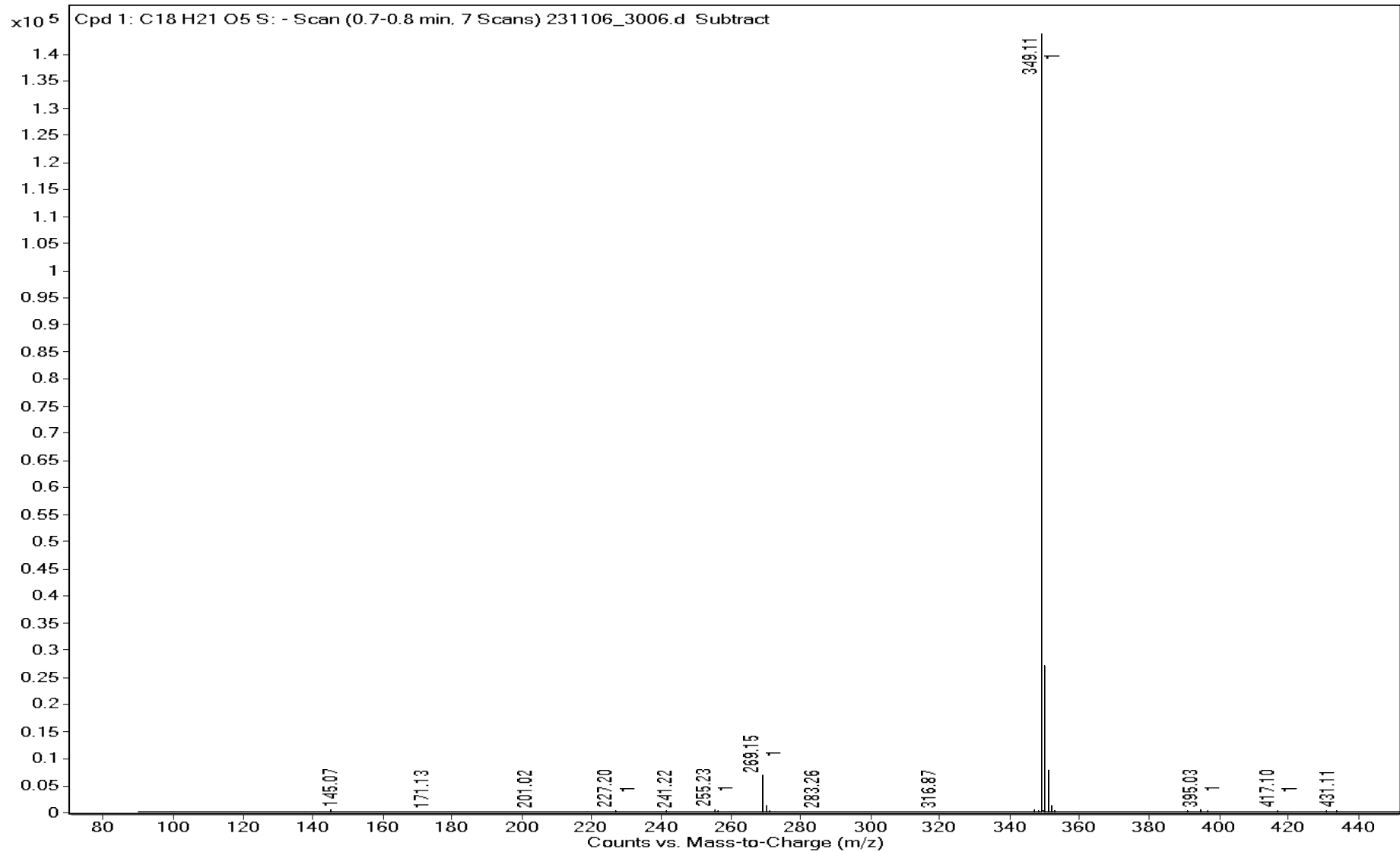
Viorica Rusu, QC/QA Manager

GR-18-279

Estrone-3-sulfate Sodium
1H-NMR, 600 MHz
Solvent: DMSO-D6
Lot No.: GR-18-279



Sample Name	GR-18-279	Data File	231106_3006.d	Acq Method	HRMS.m
DA Method	AIMS_Accurate_Mass.m	Instrument	Agilent 6538 UHD	Acq Date, Time	06/11/2023 10:38:27 AM
Comment	ESI-				



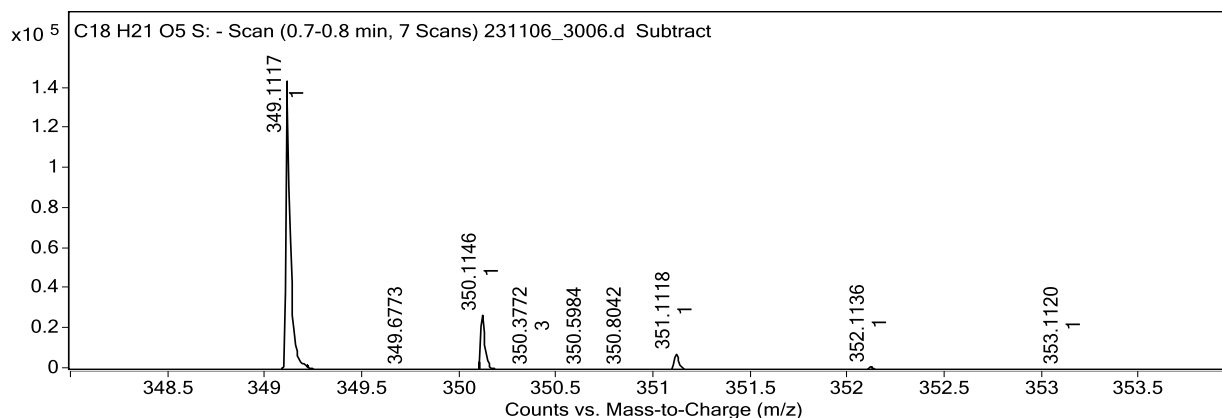
Sample Name	GR-18-279	Data File	231106_3006.d
Acq Method	HRMS.m	DA Method	AIMS_Accurate_Mass.m
Instrument	Agilent 6538 UHD	Acq Date, Time	06/11/2023 10:38:27 AM
Comment	ESI-		

Target Ion Species

Ion Species	m/z	Ionic Formula
M-	349.1117	C18 H21 O5 S

MFG Calculator Results

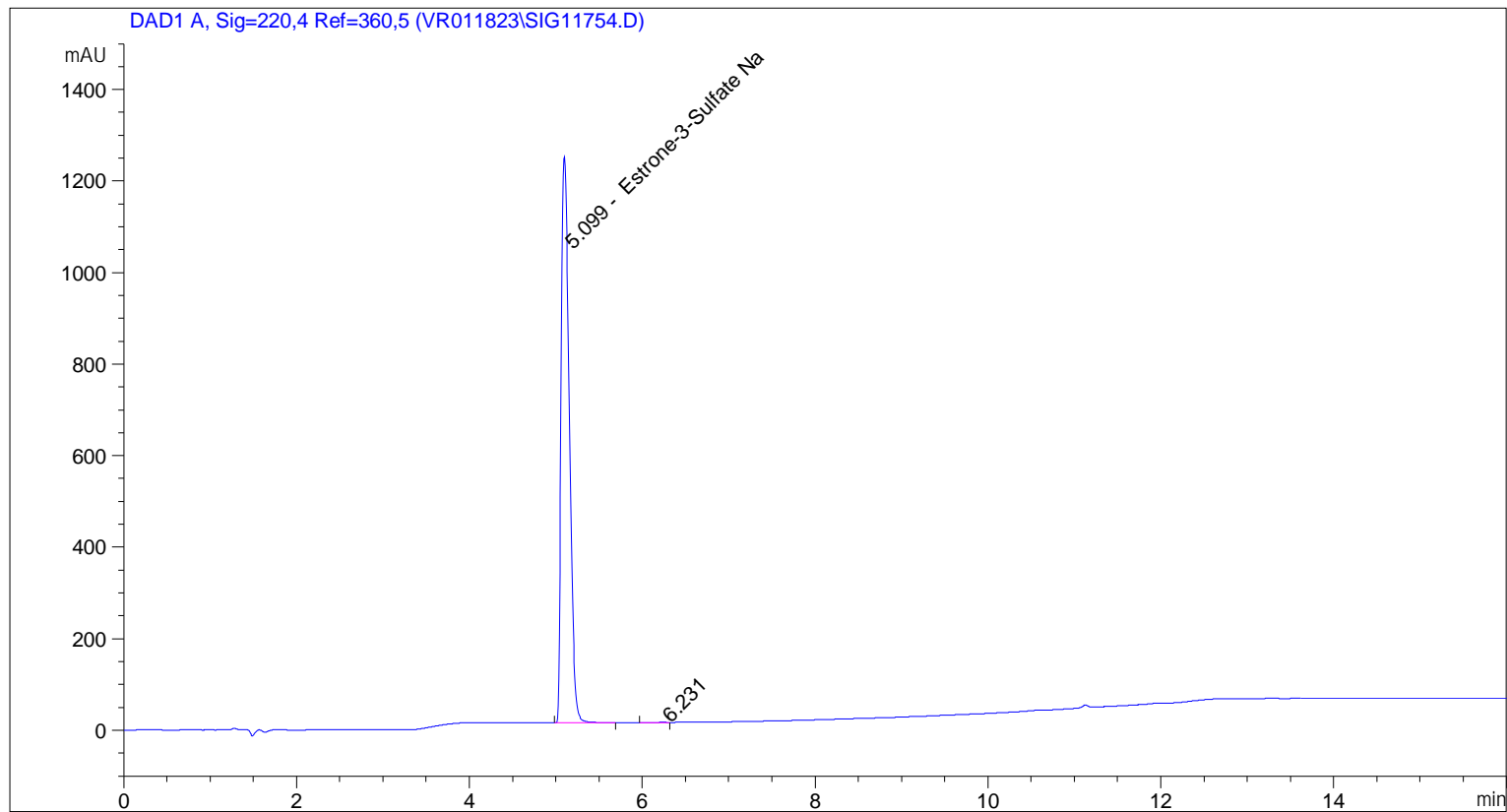
Target m/z	Ionic Formula	Calc m/z	+/- (mDa)	+/- (ppm)	DBE	MFG Score
349.1117	C18 H21 O5 S	349.1115	0.2	0.6	8.5	96.91
349.1117	C10 H17 N6 O8	349.1113	0.4	1.1	5.5	92.28
349.1117	C11 H13 N10 O4	349.1127	-1.0	-2.9	10.5	90.79
349.1117	C19 H17 N4 O S	349.1129	-1.2	-3.4	13.5	90.54
349.1117	C9 H21 N2 O12	349.1100	1.7	4.9	0.5	82.16
349.1117	C14 H17 N6 O3 S	349.1088	2.9	8.3	9.5	78.00
349.1117	C14 H21 O10	349.1140	-2.3	-6.6	4.5	77.85
349.1117	C22 H13 N4 O	349.1095	2.2	6.3	18.5	74.18
349.1117	C21 H17 O5	349.1081	3.6	10.3	13.5	65.93
349.1117	C15 H17 N4 O6	349.1154	-3.7	-10.6	9.5	65.61



Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (mDa)	Abund (%)	Calc Abund (%)	+/-
1	349.1117	349.1115	0.2	100.0	100.0	0.0
2	350.1146	350.1148	-0.2	17.7	20.7	3.0
3	351.1118	351.1114	0.4	5.0	7.5	2.5
4	352.1136	352.1132	0.4	0.8	1.2	0.4
5	353.1120	353.1144	-2.4	0.1	0.2	0.1

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Acq. Operator : vrusu
Acq. Instrument : Instrument 1 Location : Vial 21
Injection Date : 11/2/2023 10:42:24 AM Inj Volume : 5.0 µl
Acq. Method : C:\CHEM32\1\METHODS\VR110223_279.M
Last changed : 11/2/2023 10:41:07 AM by vrusu
Analysis Method : C:\CHEM32\1\METHODS\VR110223_279PM.M
Last changed : 11/2/2023 12:56:38 PM by vrusu



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Area Percent Report
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Sorted By : Signal
Calib. Data Modified : 11/2/2023 12:55:27 PM
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

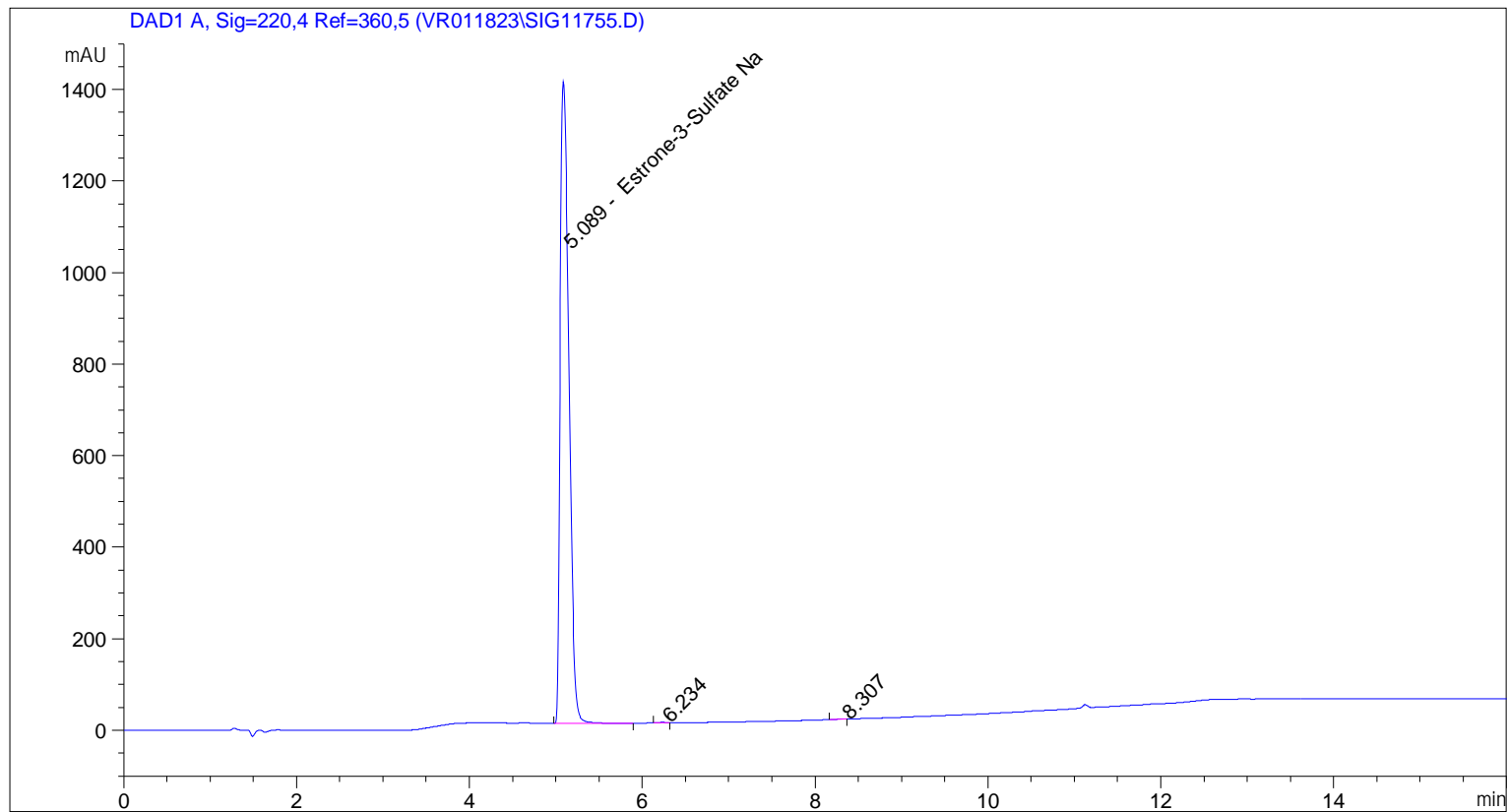
Signal 1: DAD1 A, Sig=220,4 Ref=360,5

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	5.099	BB	0.1063	8105.89453	99.9398	Estrone-3-Sulfate Na
2	6.231	BV	0.0688	4.88154	0.0602	?

Totals : 8110.77607

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*** End of Report ***

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Acq. Operator : vrusu
Acq. Instrument : Instrument 1 Location : Vial 22
Injection Date : 11/2/2023 11:04:20 AM Inj Volume : 5.0 µl
Acq. Method : C:\CHEM32\1\METHODS\VR110223_279.M
Last changed : 11/2/2023 11:03:20 AM by vrusu
Analysis Method : C:\CHEM32\1\METHODS\VR110223_279PM.M
Last changed : 11/2/2023 12:56:38 PM by vrusu



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Area Percent Report
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Sorted By : Signal
Calib. Data Modified : 11/2/2023 12:55:27 PM
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	5.089	BB	0.1164	9908.68945	99.8864	Estrone-3-Sulfate Na
2	6.234	BV	0.0664	6.64021	0.0669	?
3	8.307	BB	0.0667	4.62659	0.0466	?

Totals : 9919.95626