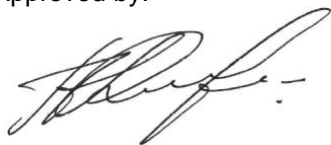


Name: 4-Isothiocyano-3,5-dimethylphenol
Lot#: GR-18-157
Test Date: 05/30/2023 (re-test date: 05/30/2028)
CAS No.: 1246818-00-7
MF: C₉H₉NOS
MW: 179.24
Appearance: Pale yellow needle like solid
Purity: 100% by HPLC (average of two sample preparations)
¹H-NMR: Conforms
MS-ESI (-) Conforms (shows peak at m/z = 178.03 [M-H]⁻)
Storage Store at -18°C in a dry place away from direct sunlight

Approved by:

Date: 05/30/2023



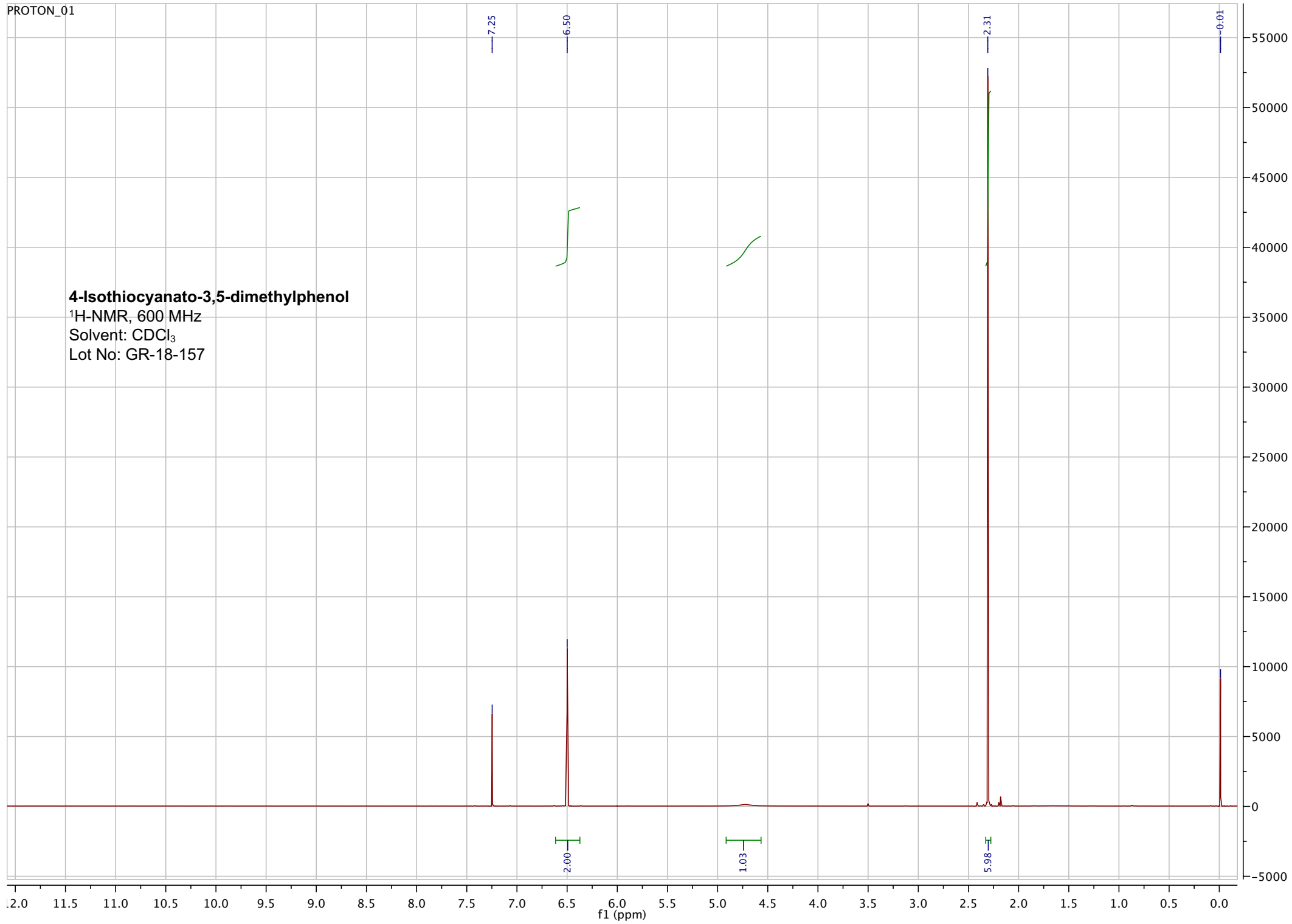
Viorica Rusu, QC/QA Manager

4-Isothiocyanato-3,5-dimethylphenol

¹H-NMR, 600 MHz

Solvent: CDCl₃

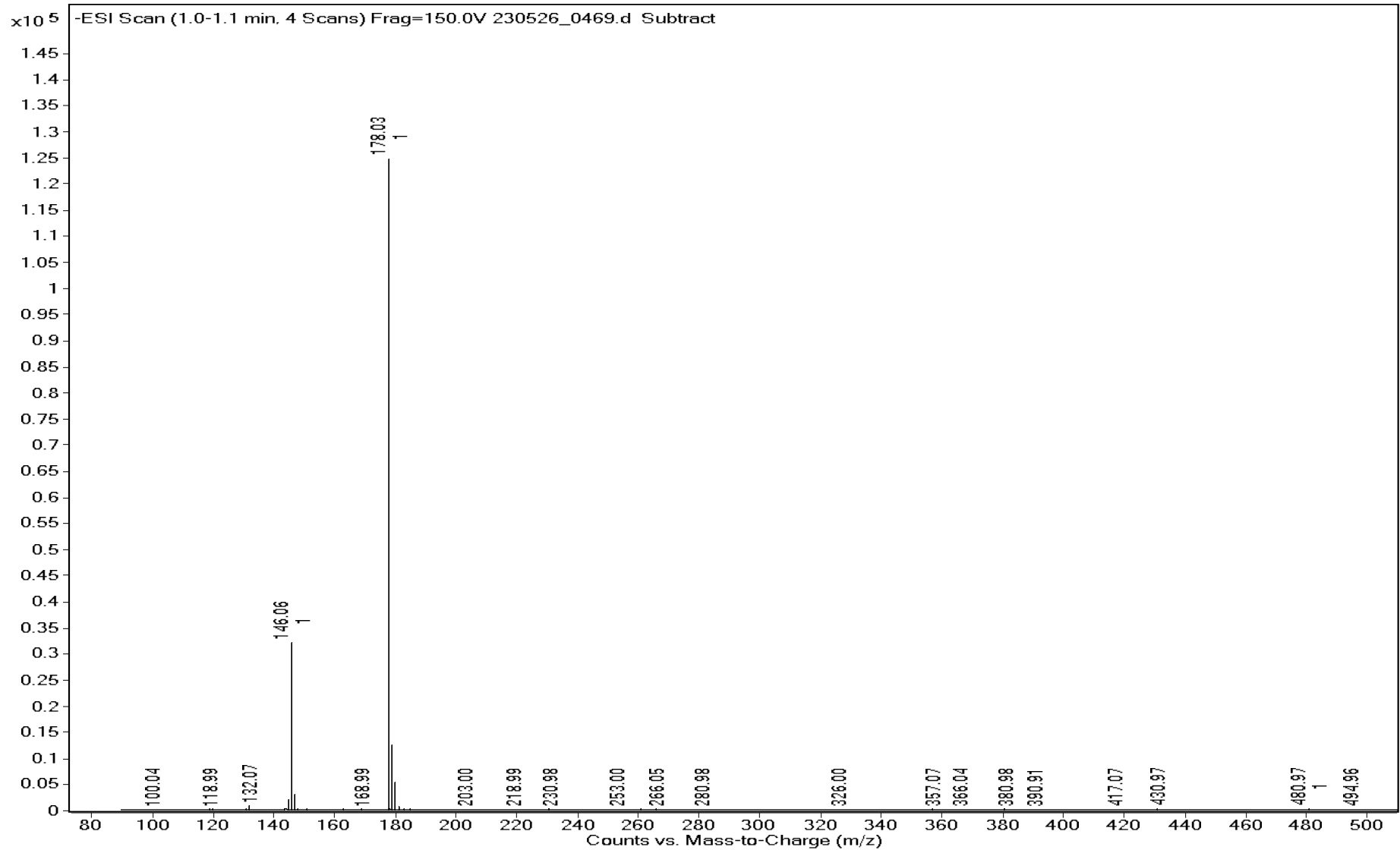
Lot No: GR-18-157



Sample Name GR-18-157
DA Method AIMS_Accurate_Mass.m
Comment ESI-

Data File 230526_0469.d
Instrument Agilent 6538 UHD

Acq Method HRMS_Negative.m
Acq Date, Time 29/05/2023 8:43:43 AM



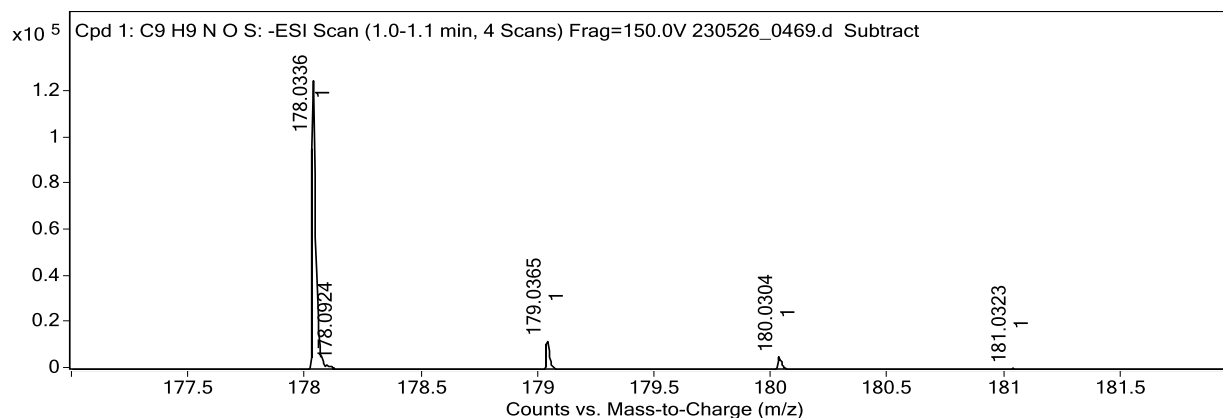
Sample Name	GR-18-157	Data File	230526_0469.d
Acq Method	HRMS_Negative.m	DA Method	AIMS_Accurate_Mass.m
Instrument	Agilent 6538 UHD	Acq Date, Time	29/05/2023 8:43:43 AM
Comment	ESI-		

Target Ion Species

Ion Species	m/z	Ionic Formula
(M-H) ⁻	178.0336	C ₉ H ₈ N O S

MFG Calculator Results

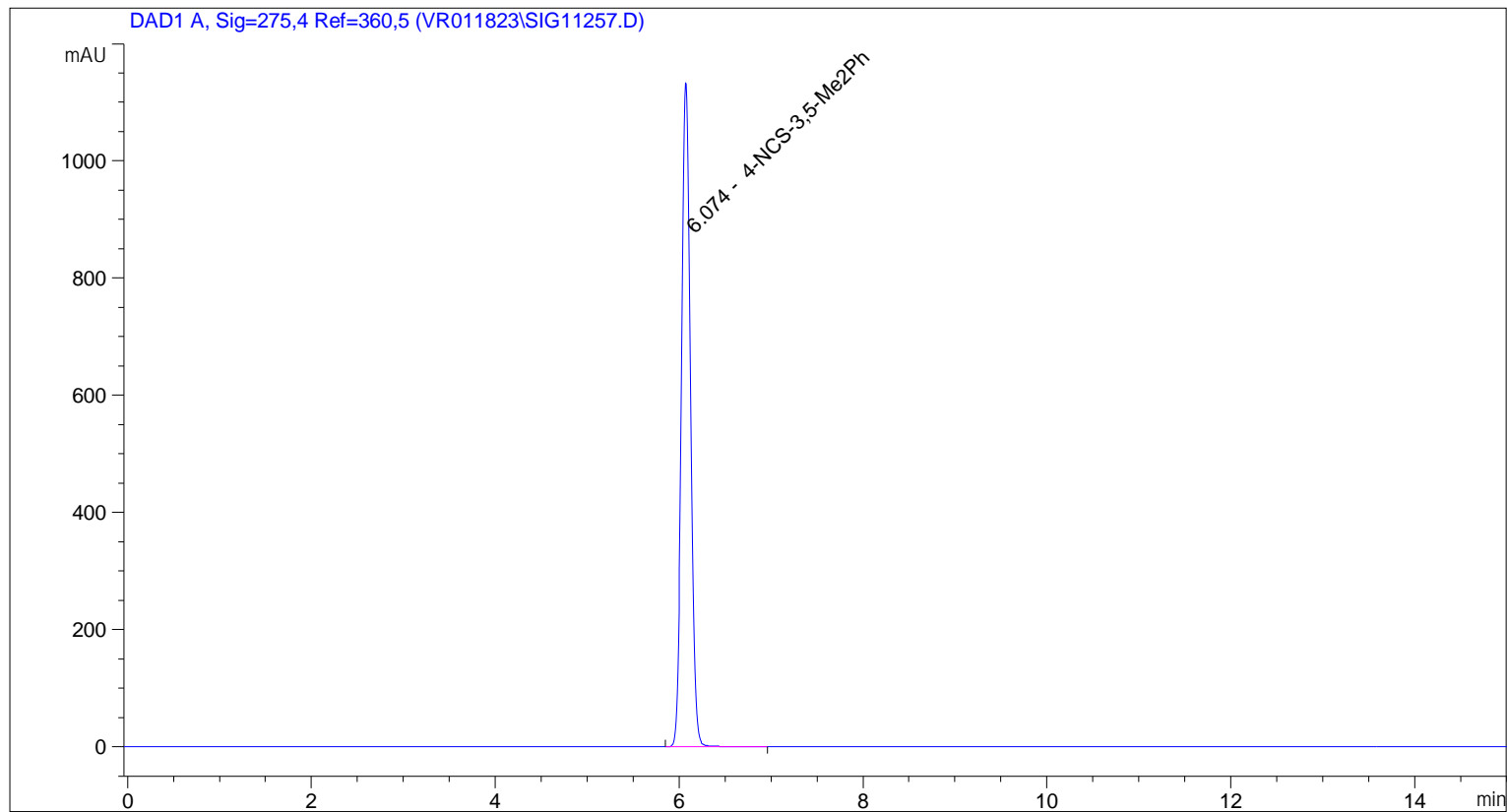
Target m/z	Ionic Formula	Calc m/z	+/- (mDa)	+/- (ppm)	DBE	MFG Score
178.0336	C ₉ H ₈ N O S	178.0332	0.4	2.2	6.0	98.52
178.0336	C ₅ H ₈ N O ₆	178.0357	-2.1	-11.8	2.0	64.18



Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (mDa)	Abund (%)	Calc Abund (%)	+/-
1	178.0336	178.0332	0.4	100.0	100.0	0.0
2	179.0365	179.0361	0.4	10.0	11.0	1.0
3	180.0304	180.0304	0.0	4.3	5.2	0.9
4	181.0323	181.0329	-0.6	0.5	0.5	0.0

=====
Acq. Operator : vrusu
Acq. Instrument : Instrument 1 Location : Vial 92
Injection Date : 5/30/2023 10:13:16 AM Inj Volume : 5.0 µl
Acq. Method : C:\CHEM32\1\METHODS\VR053023_157.M
Last changed : 5/30/2023 10:11:41 AM by vrusu
Analysis Method : C:\CHEM32\1\METHODS\VR053023_157PM.M
Last changed : 5/30/2023 10:54:23 AM by vrusu



=====
Area Percent Report
=====

Sorted By : Signal
Calib. Data Modified : 5/30/2023 10:52:15 AM
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

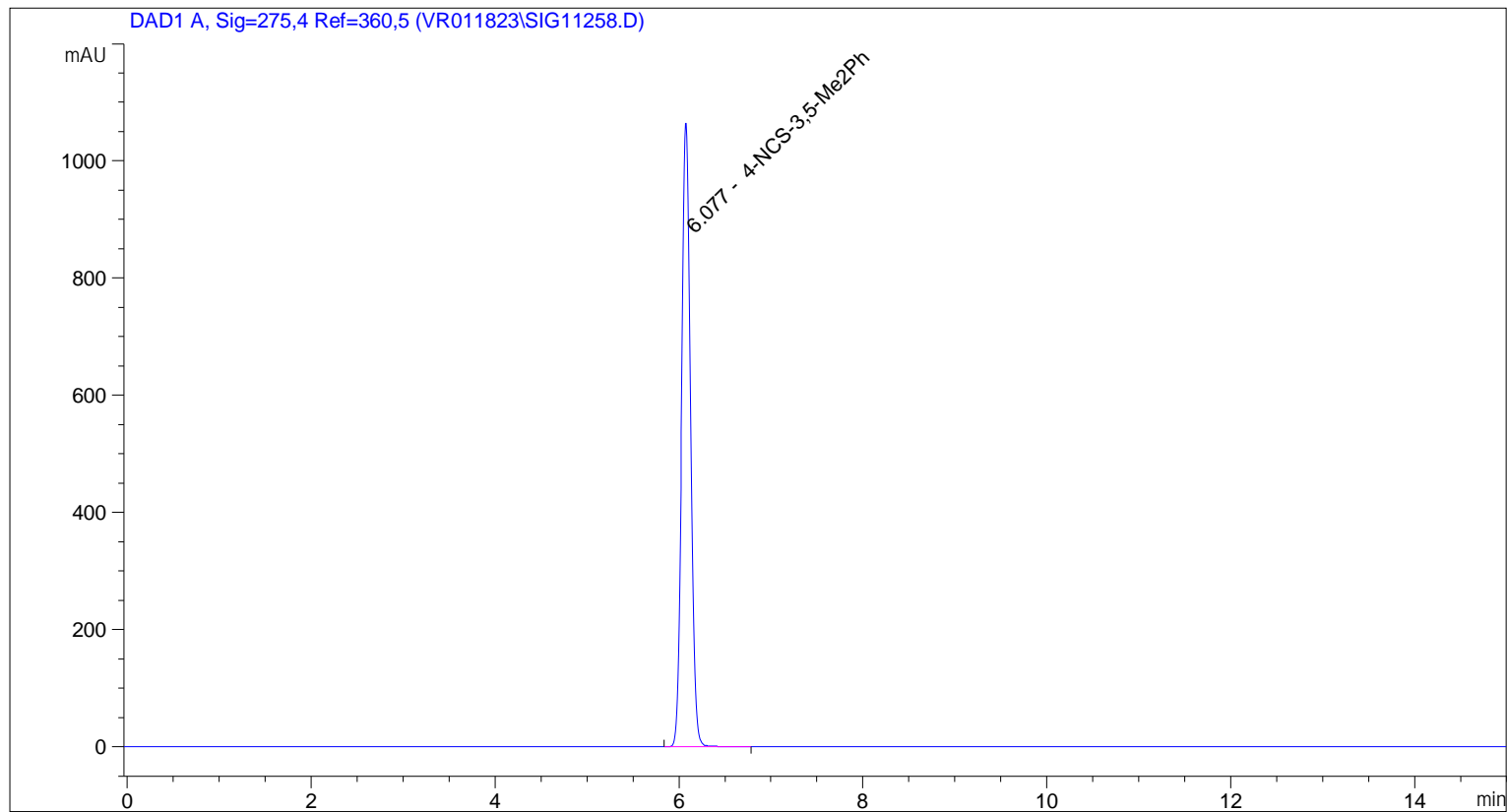
Signal 1: DAD1 A, Sig=275,4 Ref=360,5

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	6.074	BB	0.1064	7632.79688	100.0000	4-NCS-3,5-Me2Ph

Totals : 7632.79688

=====
*** End of Report ***

=====
Acq. Operator : vrusu
Acq. Instrument : Instrument 1 Location : Vial 93
Injection Date : 5/30/2023 10:31:11 AM Inj Volume : 5.0 µl
Acq. Method : C:\CHEM32\1\METHODS\VR053023_157.M
Last changed : 5/30/2023 10:29:30 AM by vrusu
Analysis Method : C:\CHEM32\1\METHODS\VR053023_157PM.M
Last changed : 5/30/2023 10:54:23 AM by vrusu



=====
Area Percent Report
=====

Sorted By : Signal
Calib. Data Modified : 5/30/2023 10:52:15 AM
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=275,4 Ref=360,5

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Area %	Name
1	6.077	BB	0.1043	7157.72070	100.0000	4-NCS-3,5-Me2Ph

Totals : 7157.72070

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*** End of Report ***