


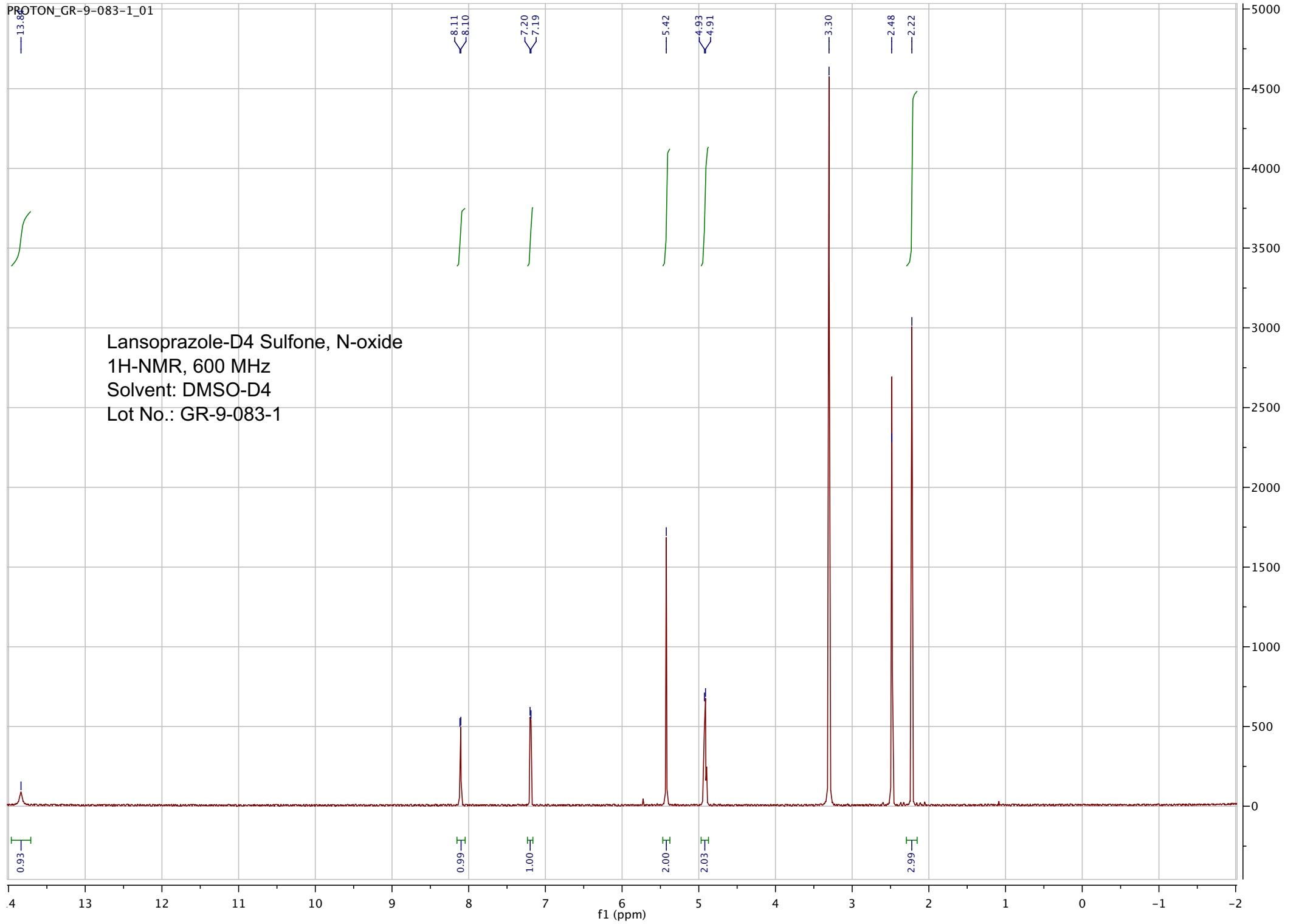
<b>Name:</b>	Lansoprazole-D4 Sulfone N-Oxide
<b>Lot#:</b>	GR-9-083-1
<b>Test Date:</b>	01/18/2022 (re-test date: 01/18/2027)
<b>CAS No.:</b>	1190009-70-1
<b>MF:</b>	C <sub>18</sub> H <sub>10</sub> D <sub>4</sub> F <sub>3</sub> N <sub>3</sub> O <sub>4</sub> S
<b>MW:</b>	405.38
<b>Appearance:</b>	White Solid
<b>Purity:</b>	99.0% by HPLC (average of two sample preparations); 99% atom D
<b><sup>1</sup>H-NMR:</b>	Conforms (shows a trace of DCM)
<b>MS-ESI (+)</b>	Conforms (shows peak at m/z = 406.10 [M+H] <sup>+</sup> )
<b>Storage</b>	Store at -18°C in a dry place away from direct sunlight

Approved by:

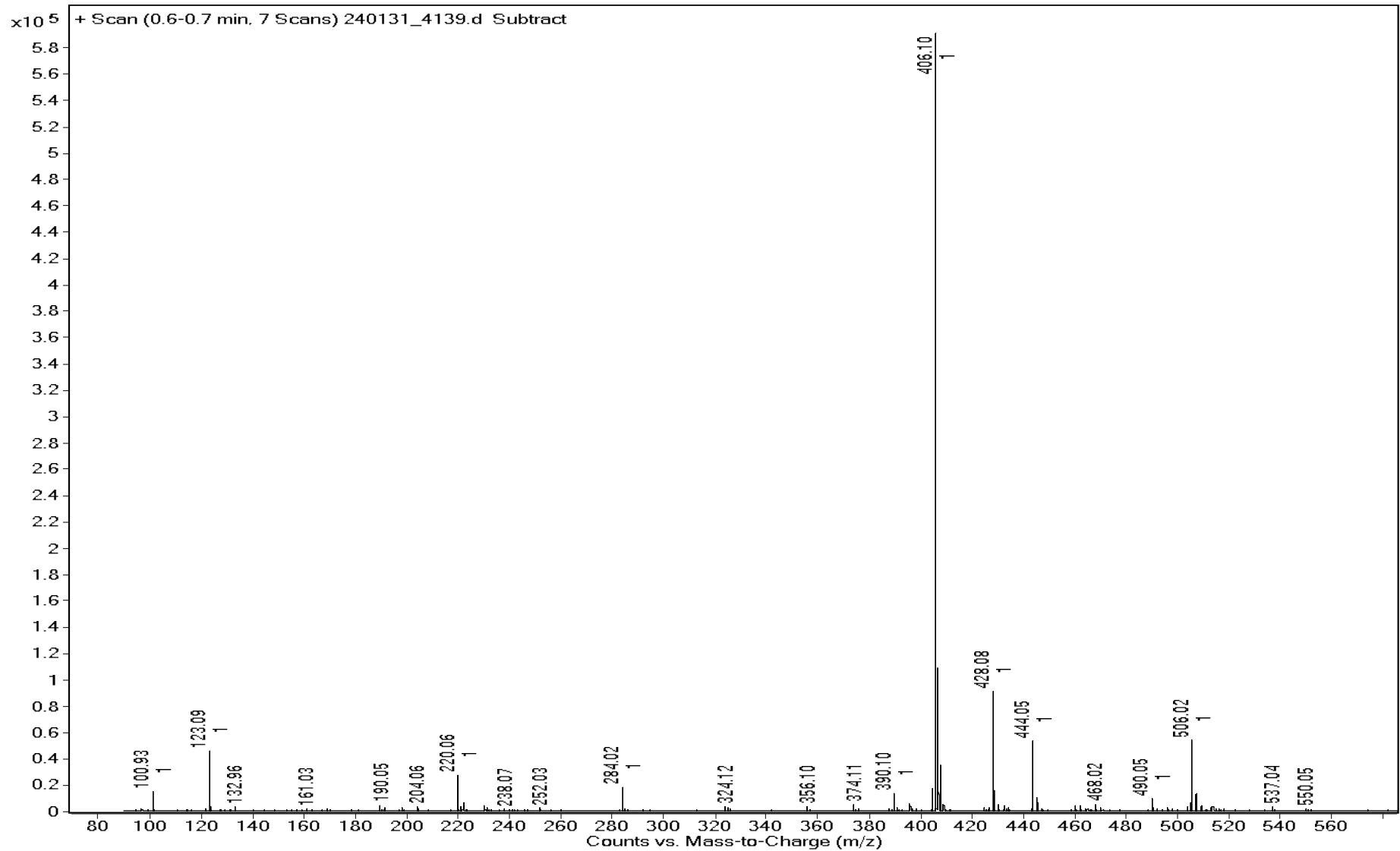
Date: 01/31/2024



Viorica Rusu, QC/QA Manager



<b>Sample Name</b>	GR-9-083-1	<b>Data File</b>	240131_4139.d	<b>Acq Method</b>	HRMS.m
<b>DA Method</b>	AIMS_Accurate_Mass.m	<b>Instrument</b>	Agilent 6538 UHD	<b>Acq Date, Time</b>	31/01/2024 12:40:10 PM
<b>Comment</b>	ESI+				



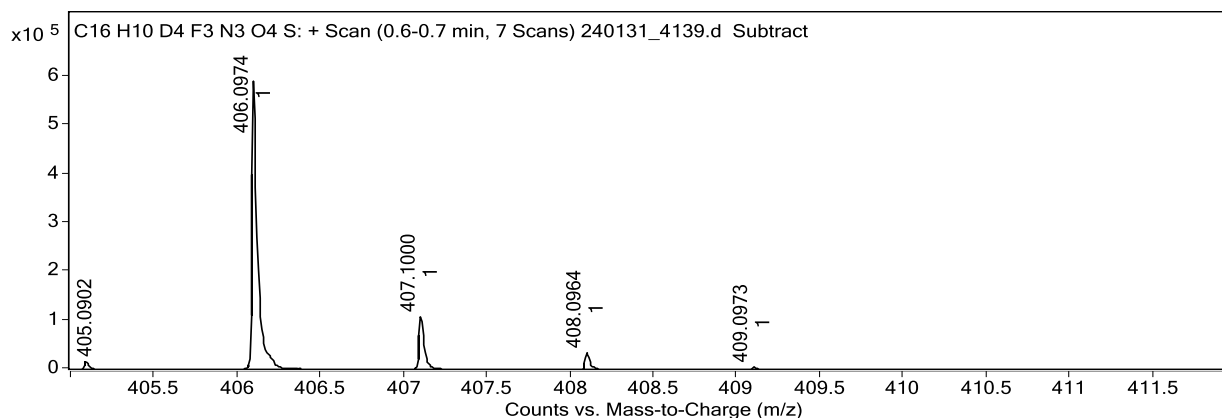
<b>Sample Name</b>	GR-9-083-1	<b>Data File</b>	240131_4139.d
<b>Acq Method</b>	HRMS.m	<b>DA Method</b>	AIMS_Accurate_Mass.m
<b>Instrument</b>	Agilent 6538 UHD	<b>Acq Date, Time</b>	31/01/2024 12:40:10 PM
<b>Comment</b>	ESI+		

### Target Ion Species

Ion Species	m/z	Ionic Formula
(M+H) <sup>+</sup>	406.0974	C16 H11 D4 F3 N3 O4 S

### MFG Calculator Results

Target m/z	Ionic Formula	Calc m/z	+/- (mDa)	+/- (ppm)	DBE	MFG Score
406.0974	C16 H11 D4 F3 N3 O4 S	406.0981	-0.7	-1.7	10.0	97.84
406.0974	C14 H11 D3 F3 N6 O3 S	406.0983	-0.9	-2.2	10.0	97.72
406.0974	C13 H15 D3 F3 N2 O7 S	406.0970	0.4	1.0	5.0	97.27
406.0974	C12 H11 D2 F3 N9 O2 S	406.0985	-1.1	-2.7	10.0	96.52
406.0974	C11 H15 D2 F3 N5 O6 S	406.0972	0.2	0.5	5.0	96.21
406.0974	C12 H7 D4 F3 N9 O2 S	406.0954	2.0	4.9	11.0	88.68
406.0974	C17 H7 D4 F3 N7 S	406.0994	-2.0	-4.9	15.0	88.22
406.0974	C10 H19 D2 F3 N O10 S	406.0958	1.6	3.9	0.0	85.66
406.0974	C25 H11 D3 F3 S	406.0951	2.3	5.7	18.0	76.59
406.0974	C11 H11 D4 F3 N5 O6 S	406.0941	3.3	8.1	6.0	74.46



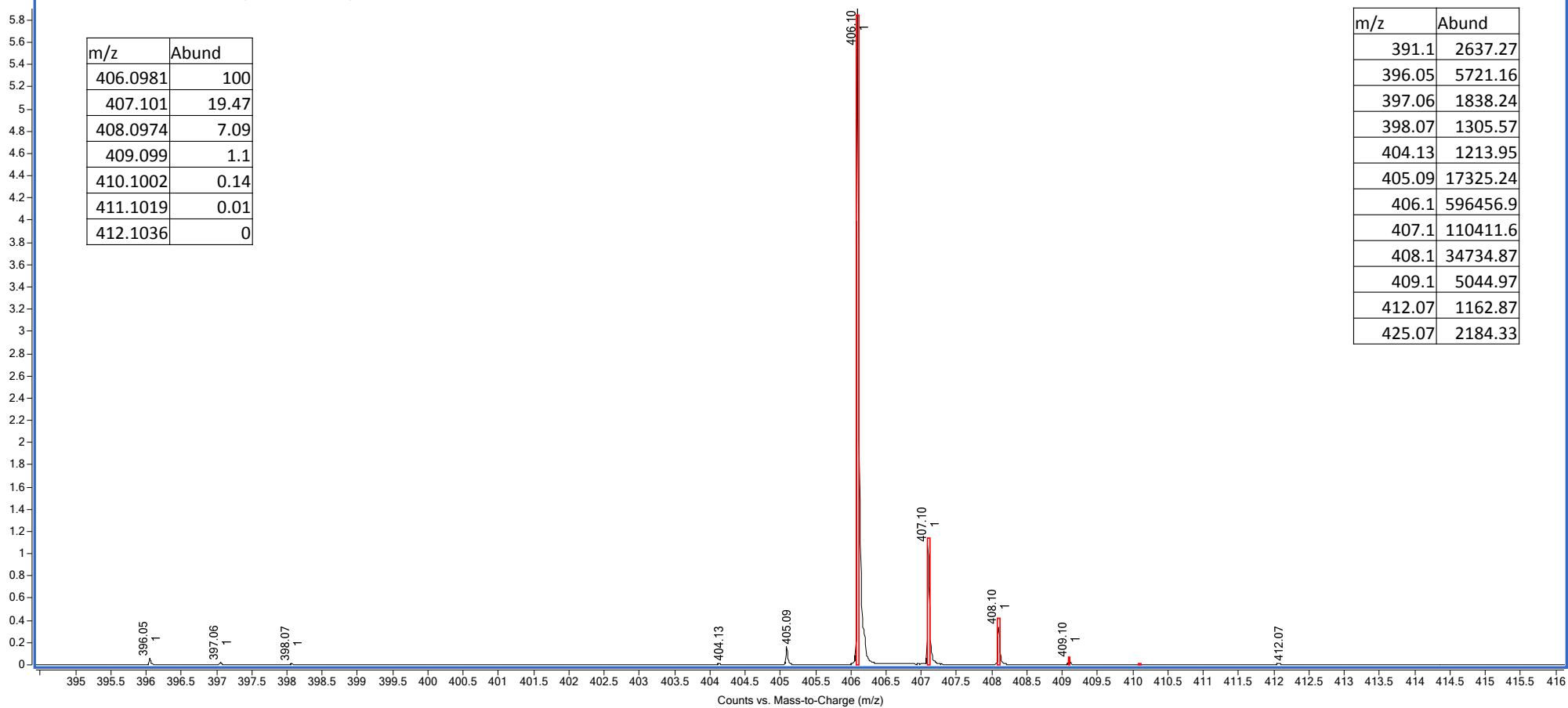
### Predicted Isotope Match Table

Isotope	m/z	Calc m/z	Diff (mDa)	Abund (%)	Calc Abund (%)	+/-
1	406.0974	406.0981	-0.7	100.0	100.0	0.0
2	407.1000	407.1010	-1.0	18.5	19.5	1.0
3	408.0964	408.0974	-1.0	5.8	7.1	1.3
4	409.0973	409.0990	-1.7	0.8	1.1	0.3
5	410.0979	410.1002	-2.3	0.1	0.1	0.0

x10<sup>5</sup> Cpd 1: C16 H10 D4 F3 N3 O4 S: + Scan (0.6-0.7 min, 7 Scans) 240131\_4139.d Subtract

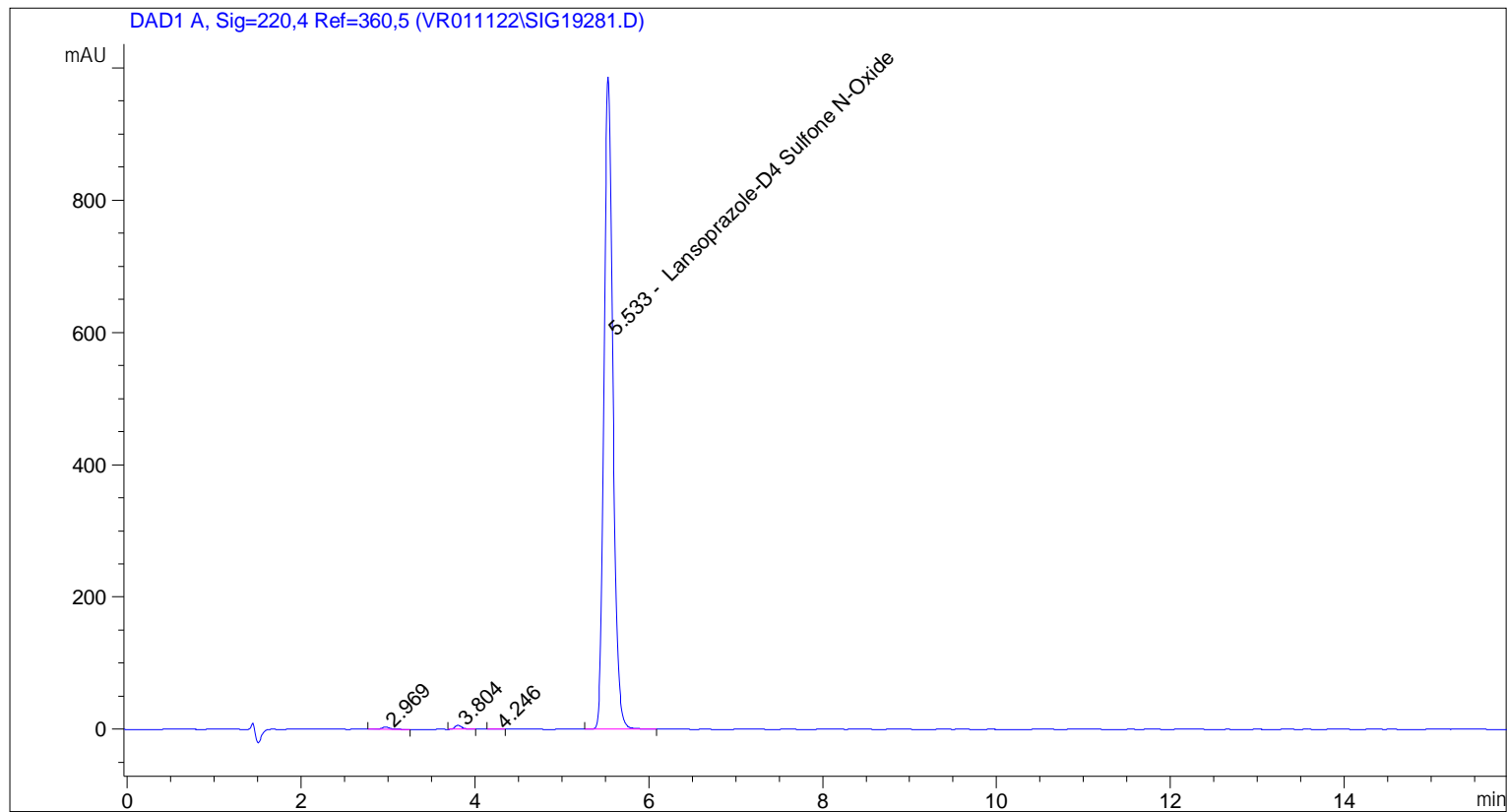
m/z	Abund
406.0981	100
407.101	19.47
408.0974	7.09
409.099	1.1
410.1002	0.14
411.1019	0.01
412.1036	0

m/z	Abund
391.1	2637.27
396.05	5721.16
397.06	1838.24
398.07	1305.57
404.13	1213.95
405.09	17325.24
406.1	596456.9
407.1	110411.6
408.1	34734.87
409.1	5044.97
412.07	1162.87
425.07	2184.33



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Acq. Operator   : vrusu
Acq. Instrument : Instrument 1                Location : Vial 7
Injection Date  : 1/18/2022 12:16:00 PM
                                           Inj Volume : 5.0 µl
Acq. Method     : C:\CHEM32\1\METHODS\VR011822_083.M
Last changed    : 1/18/2022 12:15:01 PM by vrusu
Analysis Method : C:\CHEM32\1\METHODS\VR011822_083PM.M
Last changed    : 1/18/2022 1:00:51 PM by vrusu
  
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 Area Percent Report  
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Sorted By           :      Signal
Calib. Data Modified :      1/18/2022 1:00:27 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	2.969	BB	0.1043	25.70057	0.3615	?
2	3.804	BB	0.0916	35.38663	0.4977	?
3	4.246	BB	0.0814	3.64113	0.0512	?
4	5.533	BB	0.1094	7045.65820	99.0897	Lansoprazole-D4 Sulfone N-Oxide

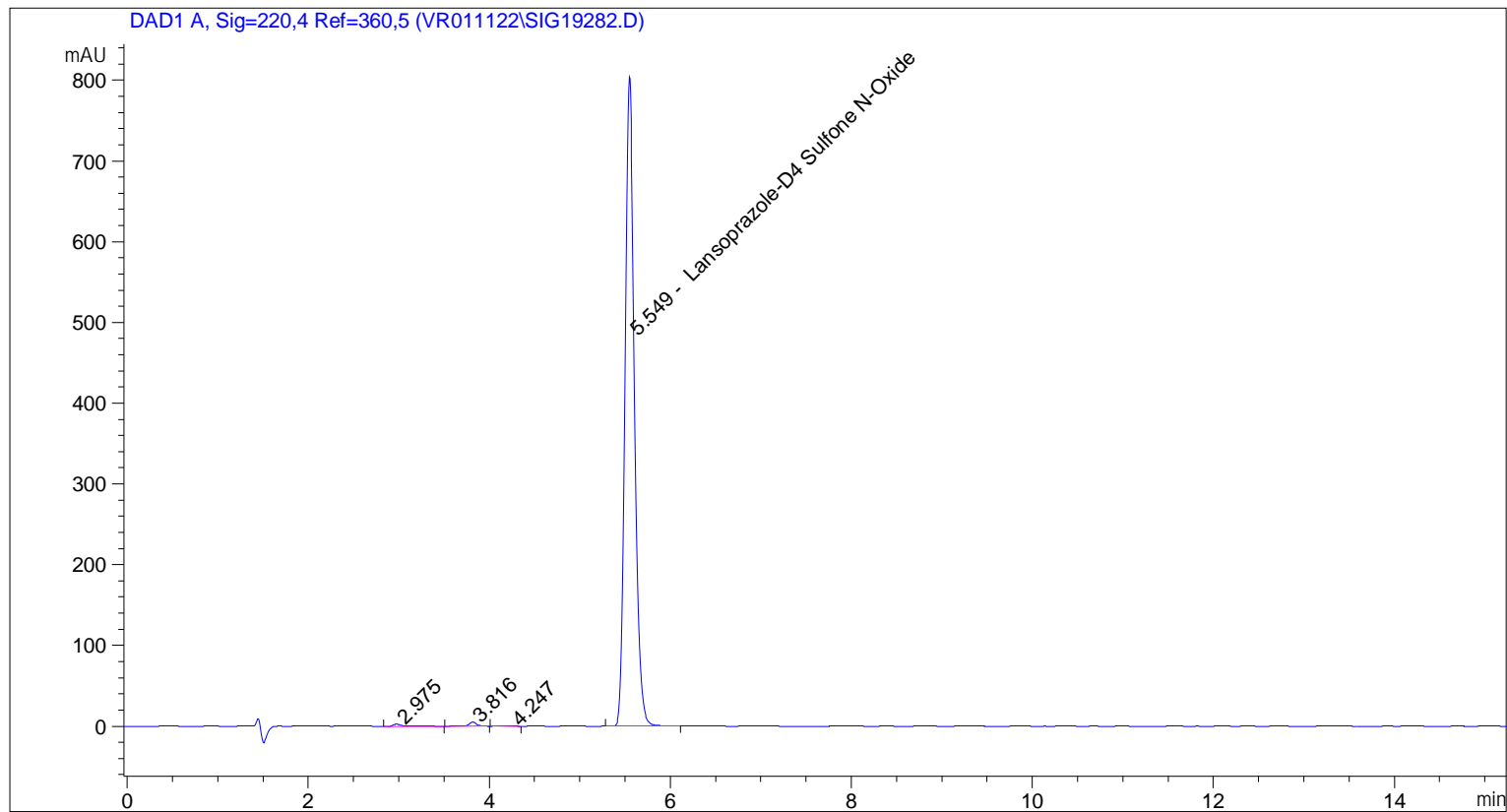
Totals : 7110.38653

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\*\*\* End of Report \*\*\*

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Acq. Operator   : vrusu
Acq. Instrument : Instrument 1                Location : Vial 8
Injection Date  : 1/18/2022 12:33:46 PM
                                           Inj Volume : 5.0 µl
Acq. Method     : C:\CHEM32\1\METHODS\VR011822_083.M
Last changed    : 1/18/2022 12:32:48 PM by vrusu
Analysis Method  : C:\CHEM32\1\METHODS\VR011822_083PM.M
Last changed    : 1/18/2022 1:00:51 PM by vrusu
  
```



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

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Sorted By           :      Signal
Calib. Data Modified :      1/18/2022 1:00:27 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	2.975	BB	0.1054	20.68172	0.3530	?
2	3.816	BB	0.0946	31.80345	0.5429	?
3	4.247	BB	0.1221	6.68907	0.1142	?
4	5.549	BB	0.1100	5799.34619	98.9899	Lansoprazole-D4 Sulfone N-Oxide

Totals : 5858.52043



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\*\*\* End of Report \*\*\*