

Supplementary Information for the manuscript “Measuring Local pH at Interfaces from Molecular Tumbling: A Concept for Designing EPR-active pH-sensitive Labels and Probes”

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<u>Experimental data for potentiometric titration</u>	S1
<u>High resolution mass spectrometry and infrared spectroscopy data for:</u>	
3-tert-Butoxycarbonylamino-1-oxyl-2,2,5,5-tetramethylpyrrolidine-4-carboxylic acid (N-Boc POAC, 6)	S2
3-tert-Butoxycarbonylamino-4-hydroxymethyl-1-oxyl-2,2,5,5-tetramethylpyrrolidine 8	S6
3-Amino-4-hydroxymethyl-1-oxyl-2,2,5,5-tetramethylpyrrolidine 9	S8
3-Dimethylamino-4-hydroxymethyl-1-oxyl-2,2,5,5-tetramethylpyrrolidine 10	S11
Methanesulfonic acid (4-dimethylamino-1-oxyl-2,2,5,5-tetramethyl-pyrrolidin-3-yl)-methyl ester 11	S14
3-Bromomethyl-4-dimethylamino-1-oxyl-2,2,5,5-tetramethylpyrrolidine 13	S17
3-Dimethylamino-4-iodomethyl-1-oxyl-2,2,5,5-tetramethylpyrrolidine 14	S21
3-Azidomethyl-4-dimethylamino-1-oxyl-2,2,5,5-tetramethylpyrrolidine 15	S24
Adduct 16	S27
3-Dimethylamino-1-oxyl-2,2,5,5-tetramethyl-4-[2-(tetrahydropyran-2-yloxy)-ethoxymethyl]-pyrrolidine 17	S31
3-Dimethylamino-4-(2-hydroxy-ethoxymethyl)-1-oxyl-2,2,5,5-tetramethylpyrrolidine 18	S33
2-((4-(Dimethylamino)-1-oxyl-2,2,5,5-tetramethylpyrrolidin-3-yl)methoxy)ethyl methanesulfonate 19	S36
S-(2-((4-(dimethylamino)-1-oxyl-2,2,5,5-tetramethylpyrrolidin-3-yl)methoxy)ethyl) methanesulfonothioate 20	S39

(2-Bromoethyl)carbamic acid (4-dimethylamino-1-oxyl-2,2,5,5-tetramethylpyrrolidin-3-yl)-methyl ester 21	S46
(2-((Methylsulfonyl)thio)ethyl)carbamic acid (4-(dimethylamino)-1-oxyl-2,2,5,5-tetramethylpyrrolidin-3-yl)methyl ester 22	S50
Spin-labeled 1,2-dipalmitoyl-sn-glycero-3-phosphothioethanol (22-PTE)	S53
Spin-labeled 1,2-dipalmitoyl-sn-glycero-3-phosphothioethanol (20-PTE)	S42
Spin-labeled 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (23-DOPE)	S56
2-((2-Hydroxyethyl)-disulfaneyl)ethyl)carbamic acid (4-(dimethylamino)-1-oxyl-2,2,5,5-tetramethylpyrrolidin-3-yl)methyl ester 24	S60
3-(Dimethylamino)-4-((2-((2-hydroxyethyl)disulfaneyl)ethoxy)methyl)-2,2,5,5-tetramethylpyrrolidin-1-oxyl 25	S63
3-(2-Hydroxyethylamino)-1-oxyl-2,2,5,5-tetramethylpyrrolidine 26	S66

Experimental Electron Paramagnetic Resonance (EPR) spectra:

3-Dimethylamino-4-hydroxymethyl-1-oxyl-2,2,5,5-tetramethylpyrrolidine 10	S69
3-Dimethylamino-4-hydroxymethyl-1-oxyl-2,2,5,5-tetramethylpyrrolidine 10 in 50 mM NaCl solution	S70
3-Azidomethyl-4-dimethylamino-1-oxyl-2,2,5,5-tetramethylpyrrolidine 15	S71
Adduct 16	S72
3-Dimethylamino-4-(2-hydroxy-ethoxymethyl)-1-oxyl-2,2,5,5-tetramethylpyrrolidine 18	S73
[2-(2-Hydroxyethyl)disulfanyl]-ethyl]-carbamic acid 4-dimethylamino-1-oxyl-2,2,5,5-tetramethylpyrrolidin-3-ylmethyl ester 24	S74
3-Dimethylamino-4-[2-(2-hydroxyethyl)disulfanyl]-ethoxymethyl]-1-oxyl-2,2,5,5-tetramethylpyrrolidine 25	S75
3-(2-Hydroxyethylamino)-1-oxyl-2,2,5,5-tetramethylpyrrolidine 26	S76

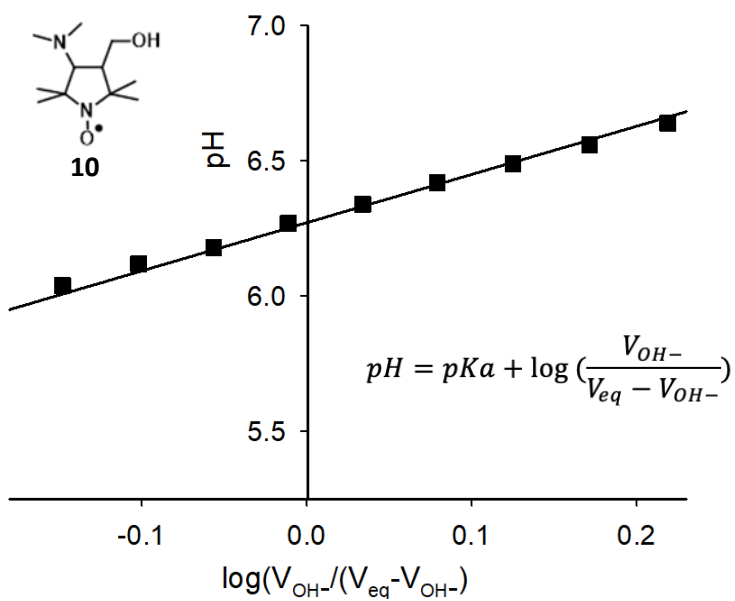


Figure S1. Determination of pK_a of dimethylamino nitroxide **10** by potentiometric titration. The linear fit gives $pK_a = 6.27 \pm 0.06$.

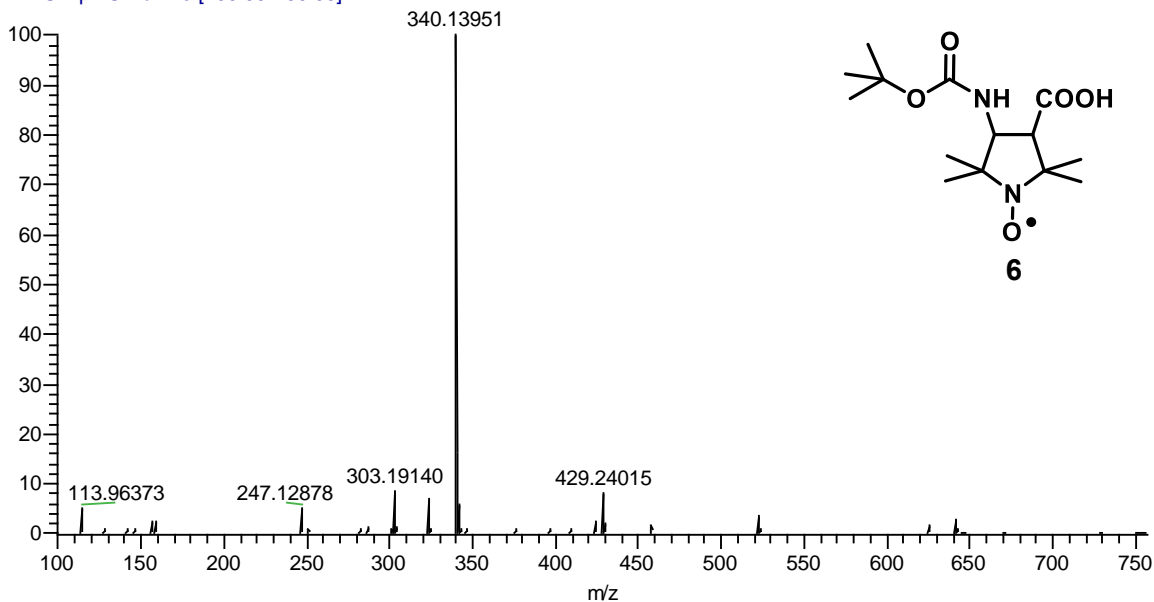
High resolution mass spectrometry and infrared spectroscopy data for 3-*tert*-Butoxycarbonyl-amino-1-oxyl-2,2,5,5-tetramethylpyrrolidine-4-carboxylic acid (*N*-Boc POAC, **6**)

Full Scan Positive Ion Mode

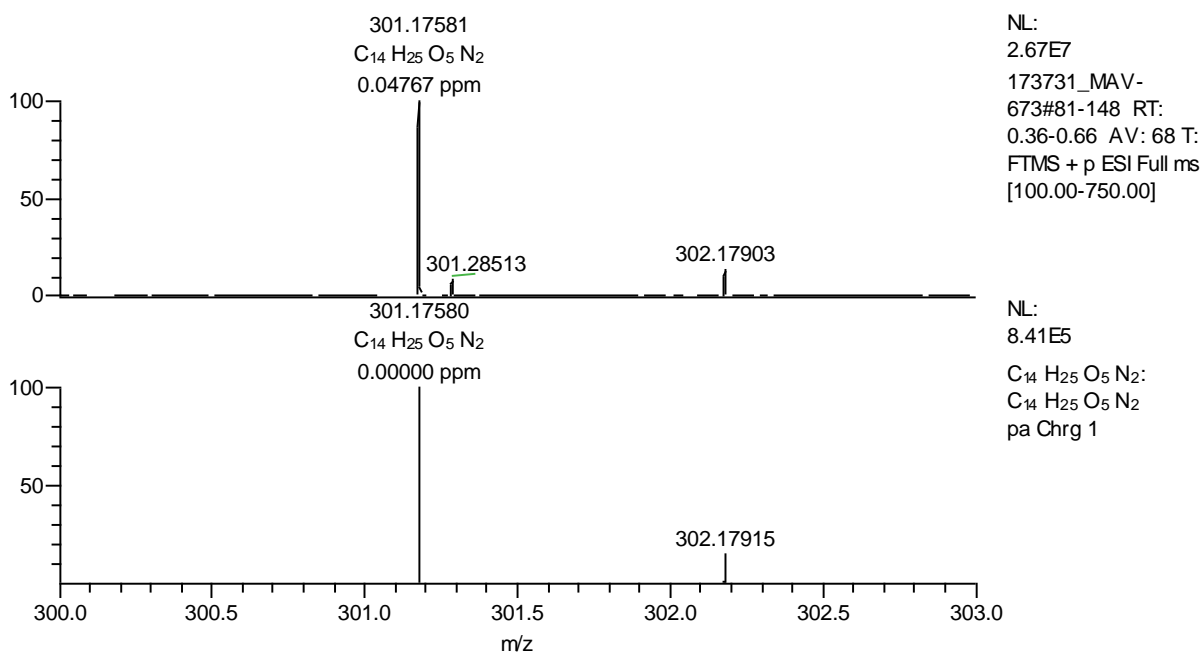
Sample	M _{Theoretical}	M _{Experimental}	ΔM (ppm)	Elemental Composition
	301.17580	301.17581	0.04767	C ₁₄ H ₂₅ N ₂ O ₅
	[M] ⁺	[M] ⁺		
	340.13951	340.13951	0.01073	[M]
	[M+K] ⁺	[M+K] ⁺		

173731_MAV-673 #81-148 RT: 0.36-0.66 AV: 68 NL: 2.55E9

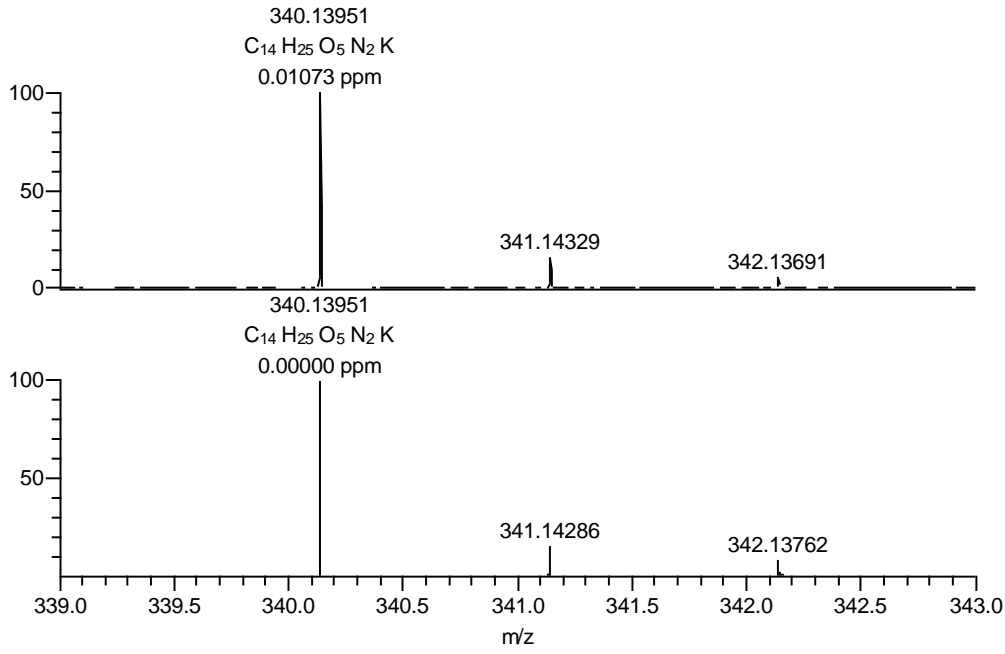
T: FTMS + p ESI Full ms [100.00-750.00]



Experimental and Theoretical Isotopic Distribution C₁₄H₂₅N₂O₅ [M]⁺

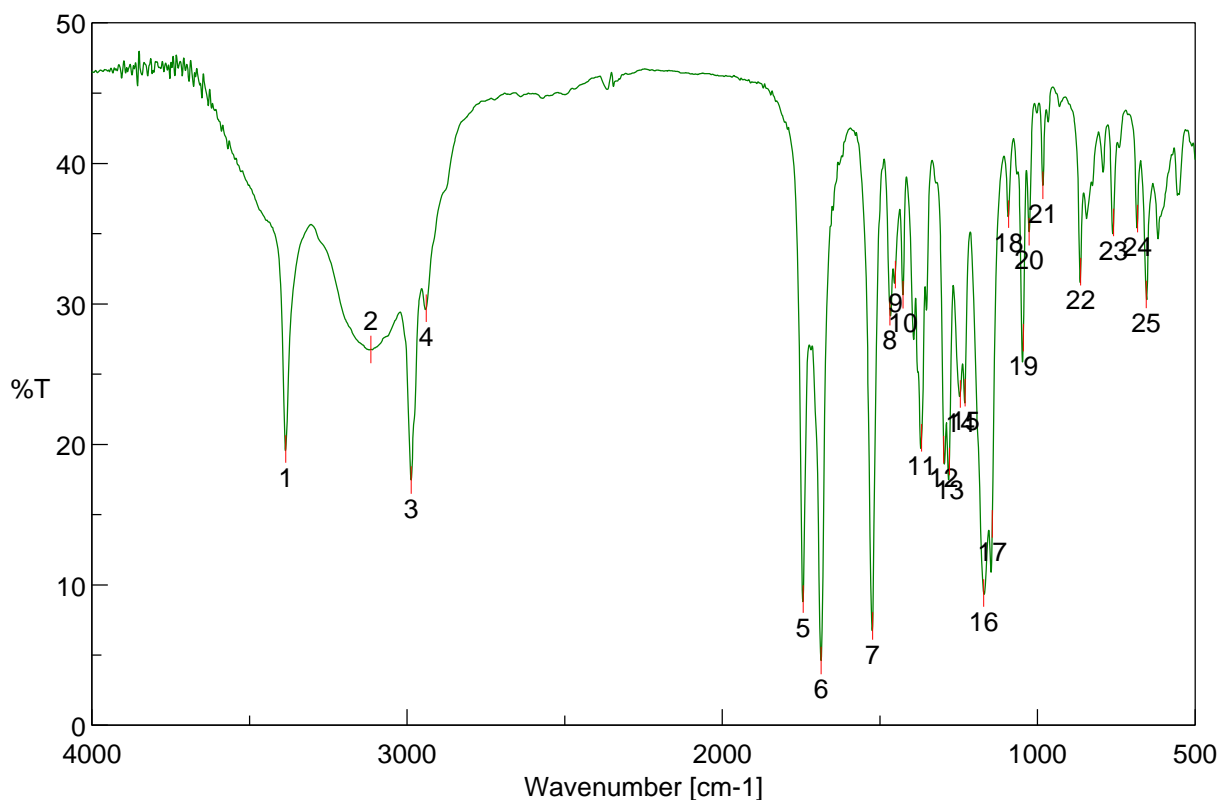


Experimental and Theoretical Isotopic Distribution C₁₄H₂₅N₂O₅K [M+K]⁺



NL:
2.55E9
173731_MAV-
673#81-148 RT:
0.36-0.66 AV: 68 T:
FTMS + p ESI Full ms
[100.00-750.00]

NL:
7.84E5
C₁₄ H₂₅ O₅ N₂ +K:
C₁₄ H₂₅ O₅ N₂ K₁
pa Chrg 1



[Comments]

Sample name
 Comment
 User
 Division
 Company Microsoft

[Detailed Information]

Creation date 8/28/2017 8:38 PM
 Data array type Linear data array
 Horizontal axis Wavenumber [cm-1]
 Vertical axis %T
 Start 499.473 cm-1
 End 4000.6 cm-1
 Data interval 0.964233 cm-1
 Data points 3632

[Measurement Information]

Model Name FT/IR-4100typeA
 Serial Number B096961016
 Measurement Date 8/28/2017 8:38 PM
 Light Source Standard
 Detector TGS
 Accumulation 20
 Resolution 4 cm-1
 Zero Filling On
 Apodization Cosine
 Gain Auto (4)
 Aperture Auto (7.1 mm)
 Scanning Speed Auto (2 mm/sec)
 Filter Auto (30000 Hz)

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
1	3384.46	19.6689	2	3114.47	26.7471

[Result of Peak Picking]

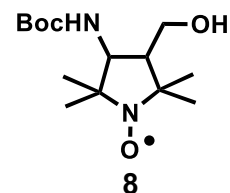
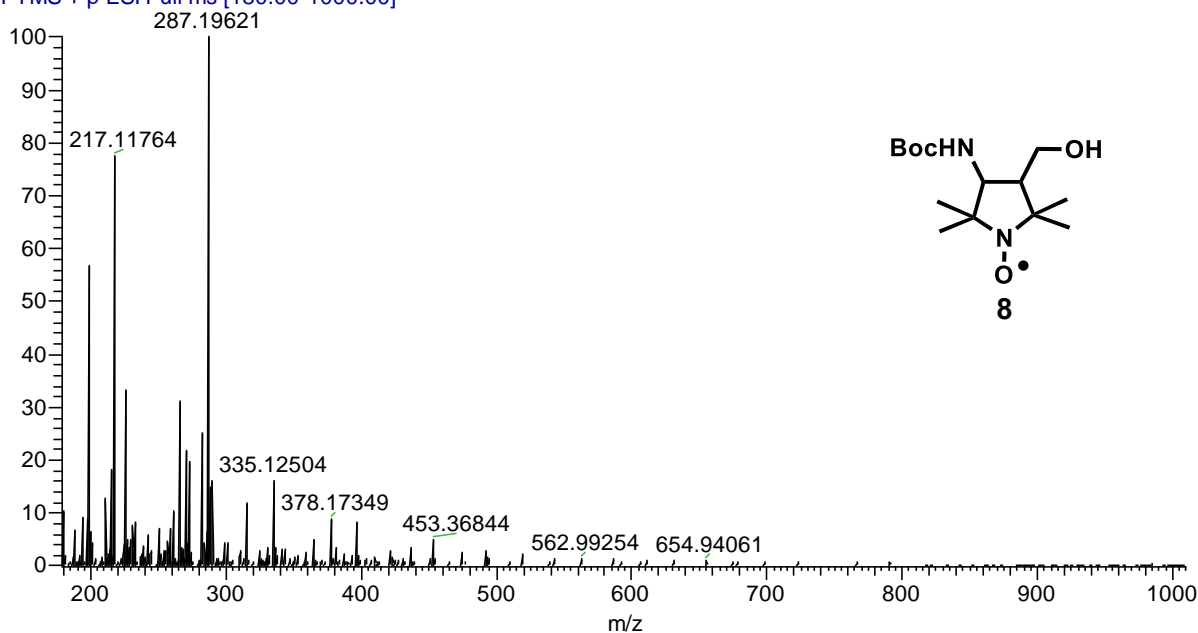
No.	Position	Intensity	No.	Position	Intensity
3	2987.2	17.4446	4	2938.98	29.6795
5	1743.33	8.98157	6	1686.44	4.6024
7	1523.49	7.06293	8	1468.53	29.4202
9	1451.17	32.084	10	1427.07	30.6492
11	1368.25	20.4632	12	1297.86	19.6115
13	1279.54	18.7646	14	1244.83	23.5722
15	1229.4	23.6632	16	1170.58	9.40426
17	1143.58	14.3182	18	1091.51	36.3771
19	1045.23	27.5855	20	1026.91	35.1315
21	983.518	38.4192	22	862.989	32.2784
23	758.852	35.78	24	682.677	36.0553
25	655.679	30.6668			

High resolution mass spectrometry and infrared spectroscopy data for 3-*tert*-Butoxycarbonyl-amino-4-hydroxymethyl-1-oxyl-2,2,5,5-tetramethylpyrrolidine **8**

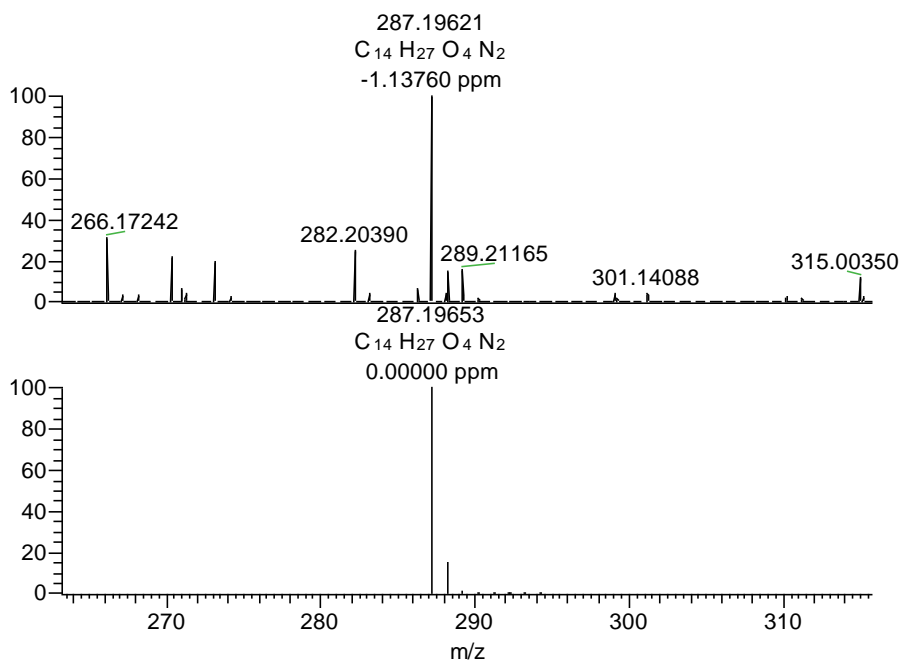
Full Scan Positive Ion Mode

Sample	M _{Theoretical}	M _{Experimental}	ΔM (ppm)	Elemental Composition
	287.19653	287.19621	-1.138	C ₁₄ H ₂₇ N ₂ O ₄
	[M] ⁺	[M] ⁺		

174163_MAV678b #49-63 RT: 0.36-0.44 AV: 15 SB: 57 0.01-0.19 , 0.80-1.01 NL: 9.07E6
T: FTMS + p ESI Full ms [180.00-1000.00]



Experimental and Theoretical Isotopic Distribution C₁₄H₂₇N₂O₄ [M+H]⁺



NL:
9.07E6
174163_MAV678b#49-63 RT:
0.36-0.44 AV: 15 SB: 57
0.01-0.19 , 0.80-1.01 T:
FTMS + p ESI Full ms
[180.00-1000.00]

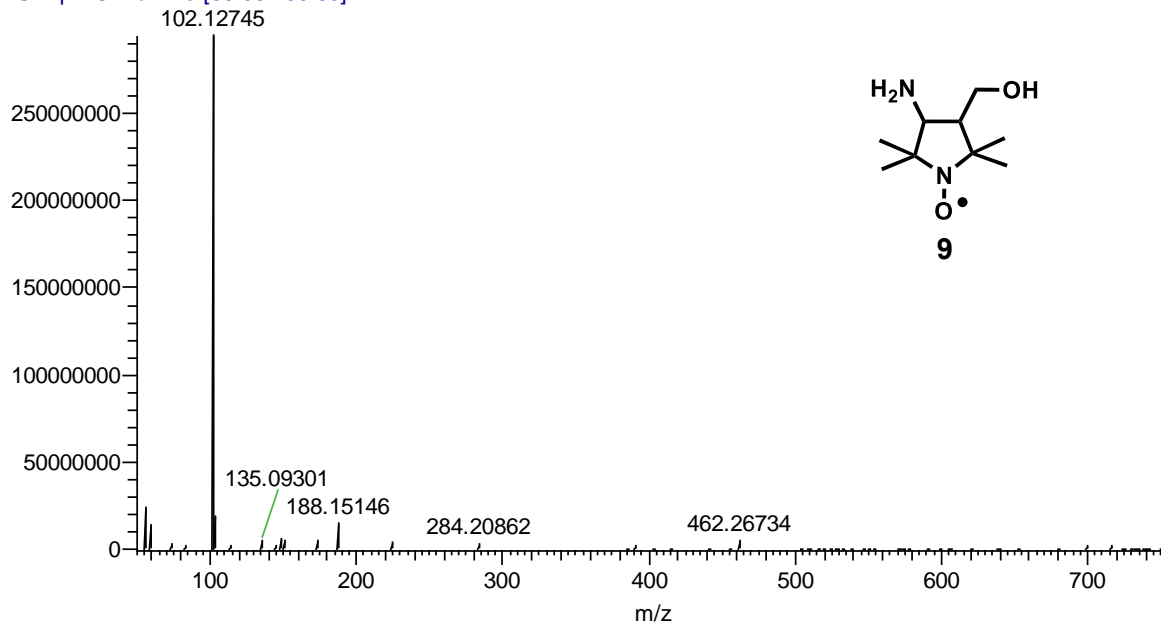
NL:
8.43E5
C₁₄ H₂₇ N₂ O₄:
C₁₄ H₂₇ N₂ O₄
pa Chrg 1

High resolution mass spectrometry and infrared spectroscopy data for 3-Amino-4-hydroxymethyl-1-oxyl-2,2,5,5-tetramethylpyrrolidine **9**

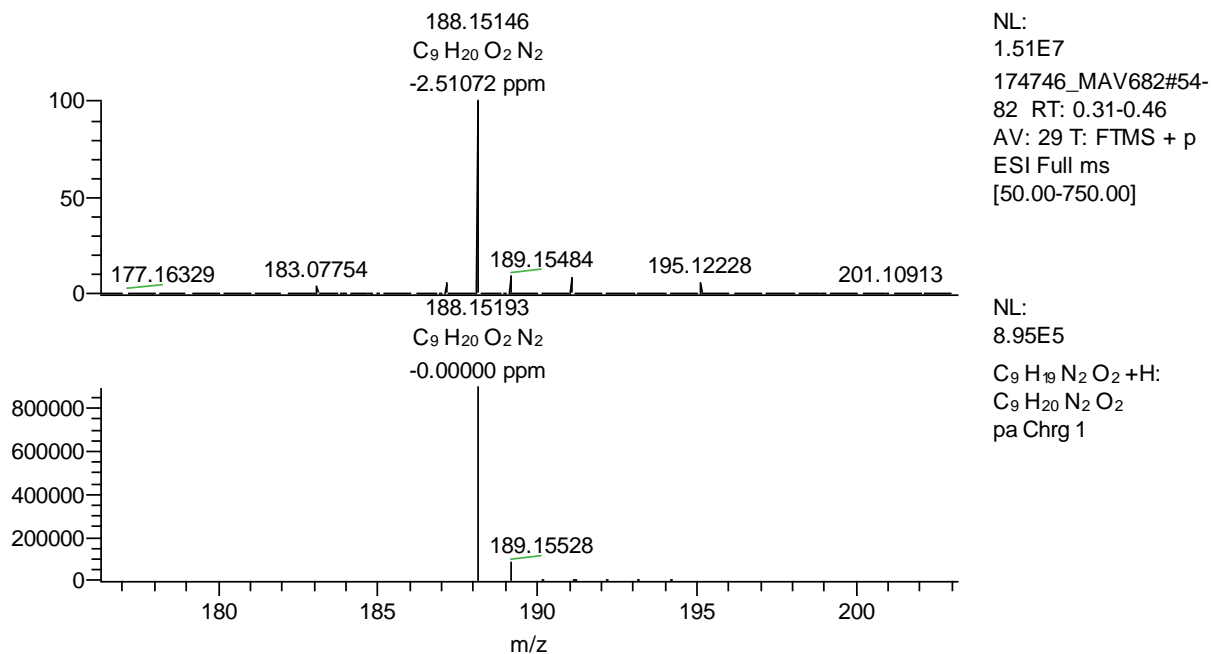
Full Scan Positive Ion Mode

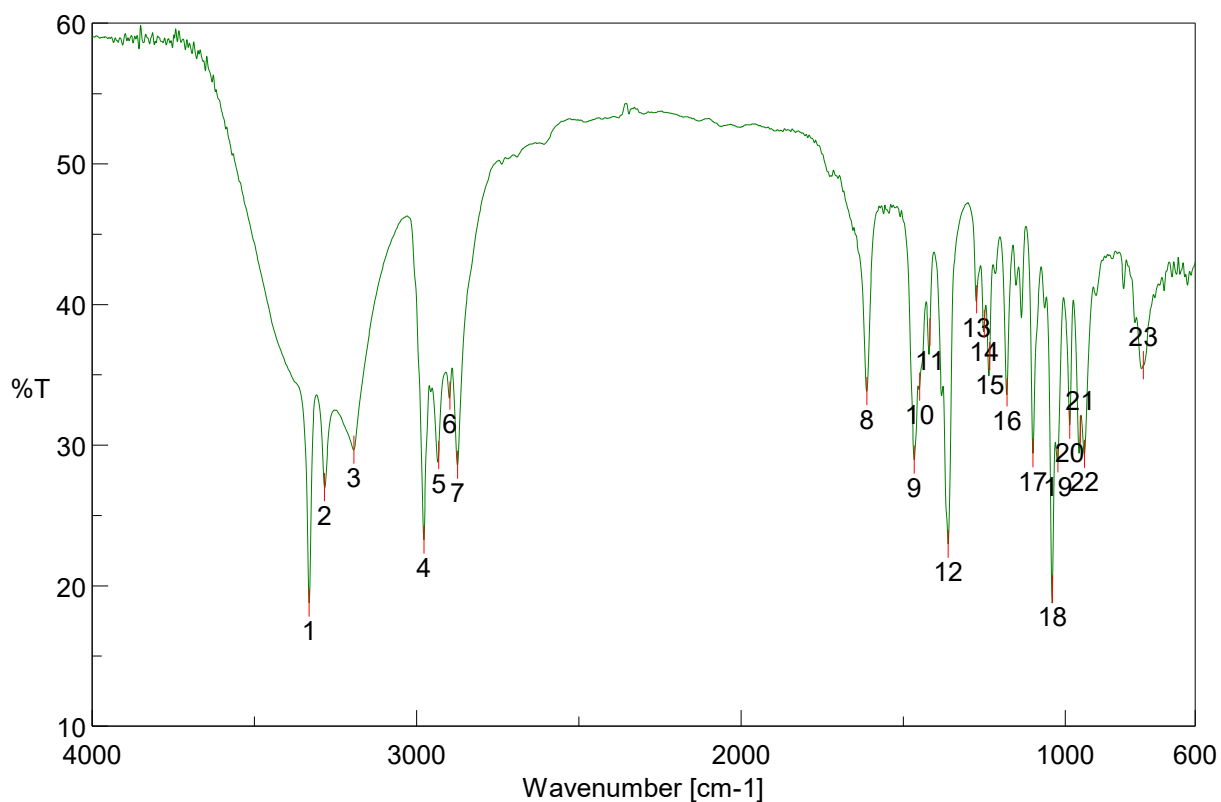
Sample	M _{Theoretical}	M _{Experimental}	ΔM (ppm)	Elemental Composition
	188.15193	188.15146	-2.511	C ₉ H ₁₉ N ₂ O ₂
	[M+H] ⁺	[M+H] ⁺		

174746_MAV682 #54-82 RT: 0.31-0.46 ,
T: FTMS + p ESI Full ms [50.00-750.00]



Experimental and Theoretical Isotopic Distribution for C₉H₁₉N₂O₂ [M+H]⁺





[Comments]

Sample name
 Comment
 User
 Division
 Company NCSU

[Detailed Information]

Creation date 9/23/2022 5:39 PM
 Data array type Linear data array
 Horizontal axis Wavenumber [cm-1]
 Vertical axis %T
 Start 0 cm-1
 End 7800.65 cm-1
 Data interval 0.964233 cm-1
 Data points 8091

[Measurement Information]

Model Name FT/IR-4100typeA
 Serial Number B096961016
 Measurement Date 9/23/2022 5:38 PM
 Light Source Standard
 Detector TGS
 Accumulation 8
 Resolution 4 cm-1
 Zero Filling On
 Apodization Cosine
 Gain Auto (4)
 Aperture Auto (7.1 mm)
 Scanning Speed Auto (2 mm/sec)
 Filter Auto (30000 Hz)

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
1	3331.43	18.776	2	3284.18	26.9994

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
3	3193.54	29.6562	4	2977.55	23.2732
5	2932.23	29.268	6	2897.52	33.515
7	2873.42	28.5947	8	1612.2	33.8309
9	1465.63	28.9515	10	1449.24	34.1503
11	1417.42	38.0088	12	1361.5	22.9733
13	1273.75	40.3531	14	1249.65	38.614
15	1233.25	36.3135	16	1180.22	33.7386
17	1100.19	29.424	18	1039.44	19.7724
19	1023.05	29.0425	20	986.411	31.4446
21	954.591	31.1062	22	941.092	29.3567
23	759.816	35.6806			

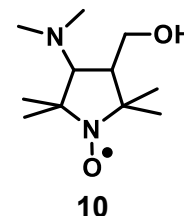
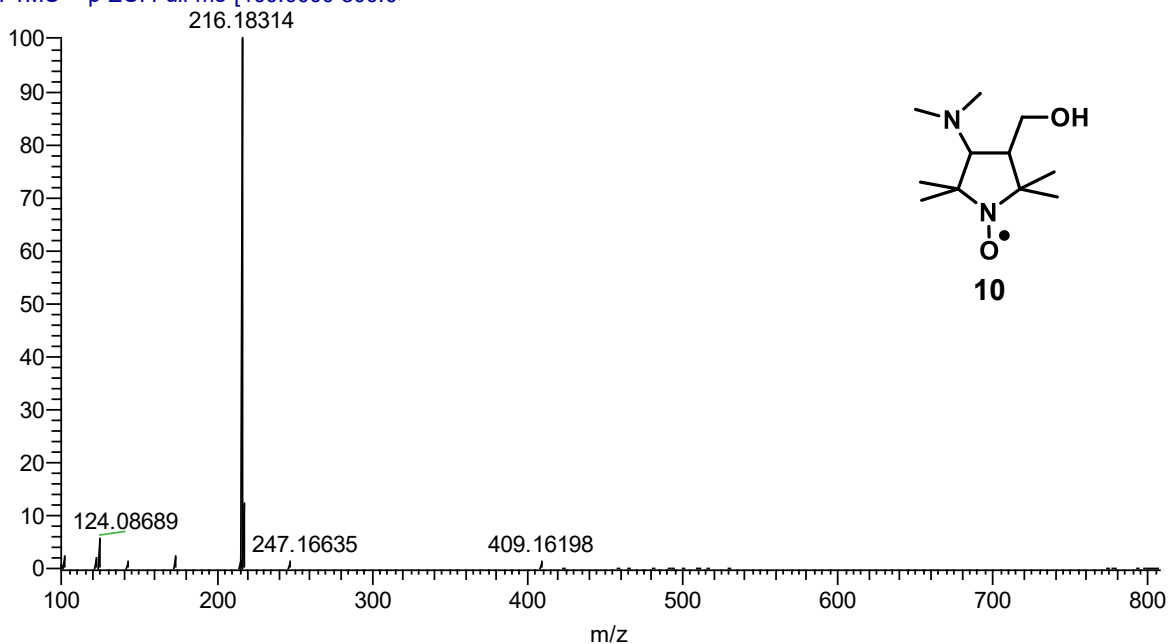
High resolution mass spectrometry and infrared spectroscopy data for 3-Dimethylamino-4-hydroxymethyl-1-oxyl-2,2,5,5-tetramethylpyrrolidine **10**

Full Scan Positive Ion Mode

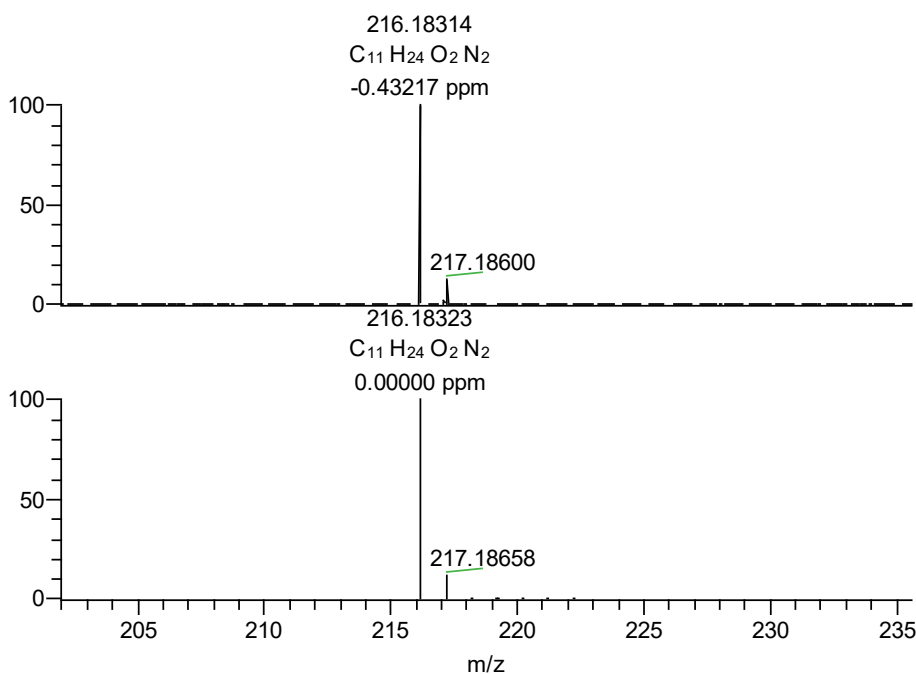
Sample	M _{Theoretical}	M _{Experimental}	ΔM (ppm)	Elemental Composition
	216.18323	216.18314	-0.432	C ₁₁ H ₂₃ N ₂ O ₂
	[M+H] ⁺	[M+H] ⁺		

192701_MAV_752 #46-73 RT: 0.26-0.40 AV: 28 NL: 5.35E8

T: FTMS + p ESI Full ms [100.0000-800.0]

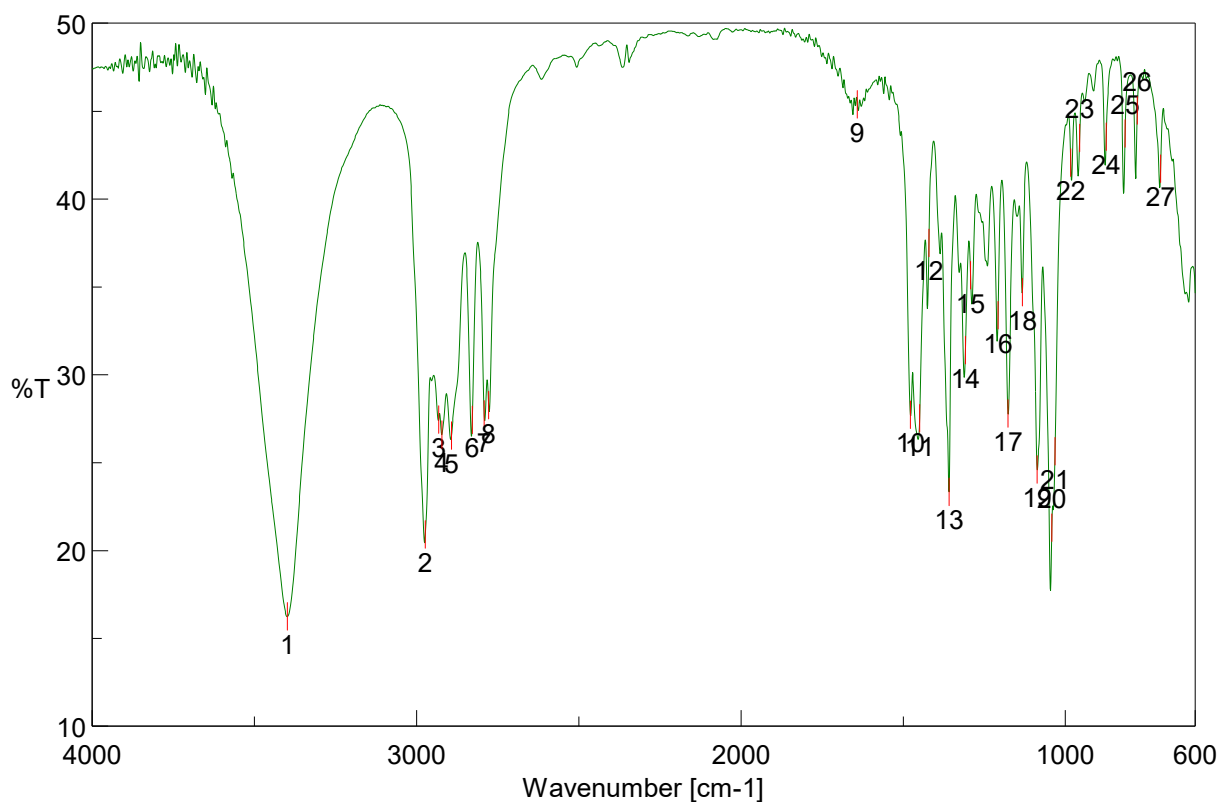


Experimental and Theoretical Isotopic Distribution C₁₁H₂₃N₂O₂ [M+H]⁺



NL:
5.35E8
192701_MAV_752#46-
73 RT: 0.26-0.40 AV:
28 T: FTMS + p ESI
Full ms
[100.0000-800.0000]

NL:
8.75E5
C₁₁H₂₃N₂O₂ +H:
C₁₁H₂₄N₂O₂
pa Chrg 1



[Comments]

Sample name
 Comment
 User
 Division
 Company NCSU

[Detailed Information]

Creation date 9/26/2022 7:26 PM
 Data array type Linear data array
 Horizontal axis Wavenumber [cm-1]
 Vertical axis %T
 Start 0 cm-1
 End 7800.65 cm-1
 Data interval 0.964233 cm-1
 Data points 8091

[Measurement Information]

Model Name FT/IR-4100typeA
 Serial Number B096961016
 Measurement Date 9/26/2022 7:26 PM
 Light Source Standard
 Detector TGS
 Accumulation 8
 Resolution 4 cm-1
 Zero Filling On
 Apodization Cosine
 Gain Auto (4)
 Aperture Auto (7.1 mm)
 Scanning Speed Auto (2 mm/sec)
 Filter Auto (30000 Hz)

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
1	3397.96	16.2407	2	2972.73	20.8991

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
3	2932.23	27.4441	4	2921.63	26.5851
5	2892.7	26.5285	6	2828.1	27.4237
7	2791.46	27.7268	8	2777.96	28.259
9	1641.13	45.374	10	1478.17	27.7189
11	1449.24	27.5218	12	1420.32	37.5005
13	1358.6	23.3198	14	1308.46	31.385
15	1292.07	35.6568	16	1207.22	33.3774
17	1177.33	27.7907	18	1132.97	34.6964
19	1087.66	24.6011	20	1042.34	21.2927
21	1031.73	25.6384	22	983.518	42.0692
23	956.52	43.4625	24	874.56	43.5401
25	815.742	43.7109	26	778.136	45.0303
27	706.783	41.7072			

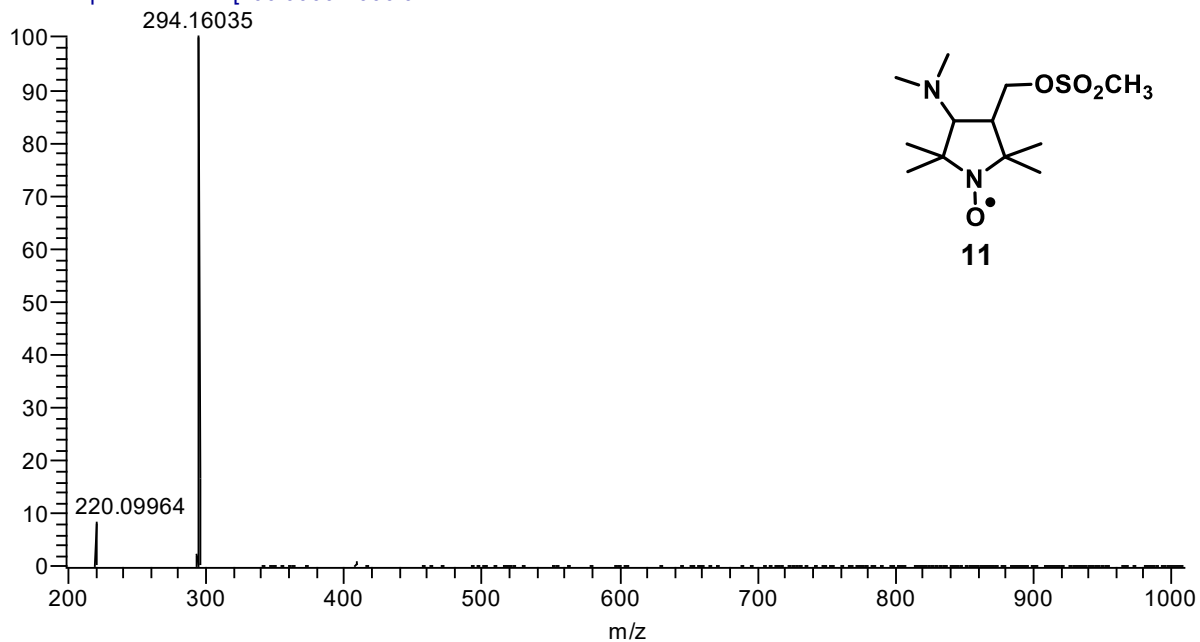
High resolution mass spectrometry and infrared spectroscopy data for Methanesulfonic acid (4-dimethylamino-2,2,5,5-tetramethylpyrrolidin-3-yl)-methyl ester **11**

Full Scan Positive Ion Mode

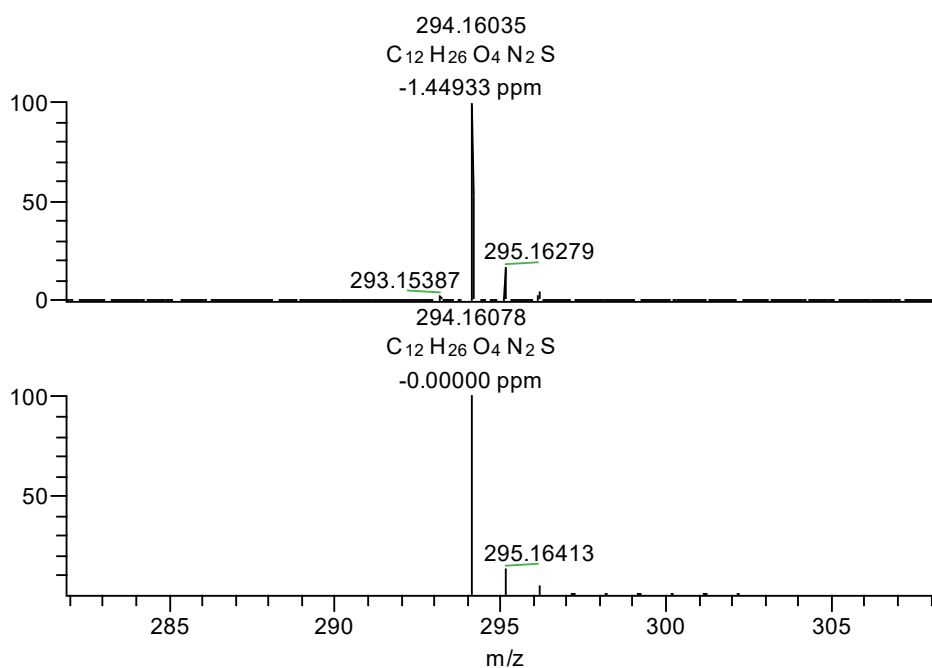
Sample	M _{Theoretical}	M _{Experimental}	ΔM (ppm)	Elemental Composition
	294.16078	294.16035	-1.450	C ₁₂ H ₂₅ N ₂ O ₄ S
	[M+H] ⁺	[M+H] ⁺		

200086_MAV-757 #48-70 RT: 0.29-0.40 AV: 23 NI: 7.54F8

T: FTMS + p ESI Full ms [200.0000-1000.C

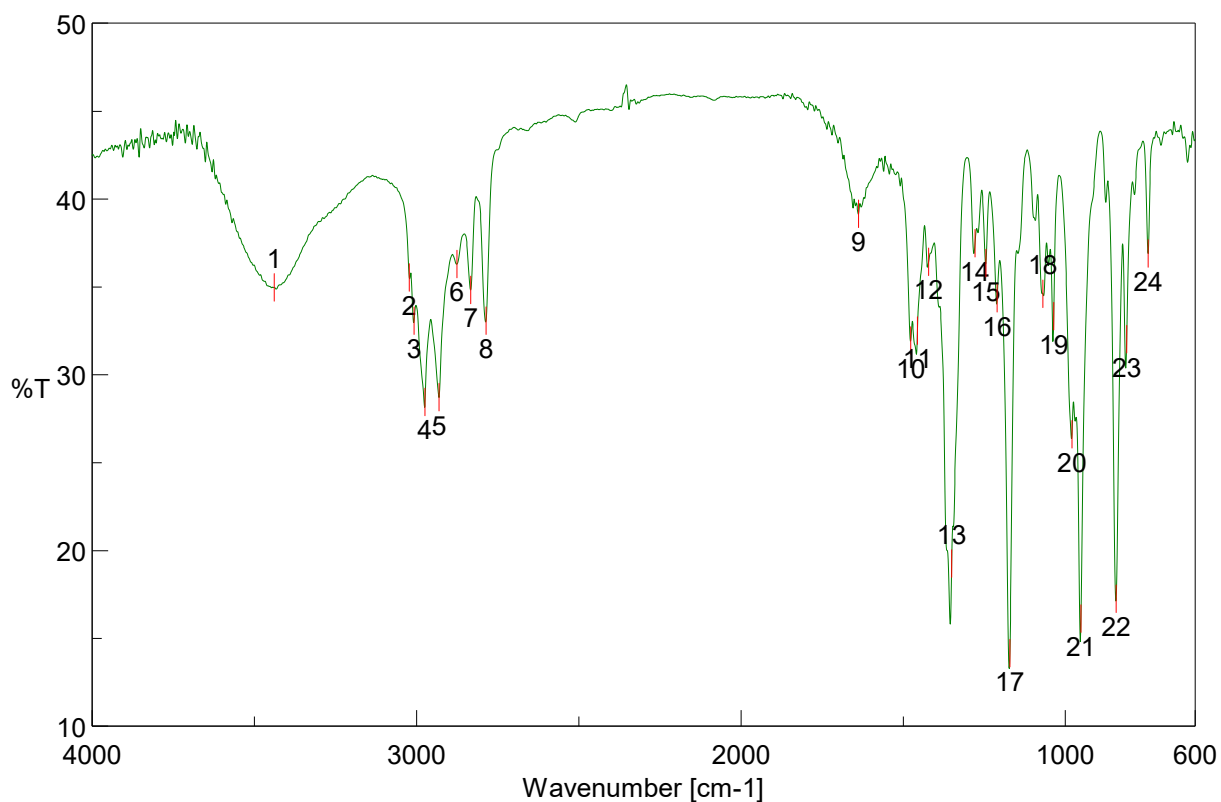


Experimental and Theoretical Isotopic Distribution C₁₂H₂₅N₂O₄S [M+H]⁺



NL:
7.54E8
200086_MAV-757#48-
70 RT: 0.29-0.40 AV:
23 T: FTMS + p ESI Full
ms
[200.0000-1000.0000]

NL:
8.18E5
C₁₂H₂₅N₂O₄S +H:
C₁₂H₂₆N₂O₄S₁
pa Chrg 1



[Comments]

Sample name
 Comment
 User
 Division
 Company NCSU

[Detailed Information]

Creation date 10/23/2019 7:10 PM
 Data array type Linear data array
 Horizontal axis Wavenumber [cm-1]
 Vertical axis %T
 Start 0 cm-1
 End 7800.65 cm-1
 Data interval 0.964233 cm-1
 Data points 8091

[Measurement Information]

Model Name FT/IR-4100typeA
 Serial Number B096961016
 Measurement Date 10/23/2019 7:09 PM
 Light Source Standard
 Detector TGS
 Accumulation 8
 Resolution 4 cm-1
 Zero Filling On
 Apodization Cosine
 Gain Auto (4)
 Aperture Auto (7.1 mm)
 Scanning Speed Auto (2 mm/sec)
 Filter Auto (30000 Hz)

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
1	3438.46	34.9667	2	3022.87	35.5319

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
3	3007.44	33.0638	4	2973.7	28.4482
5	2930.31	28.7203	6	2875.34	36.2855
7	2832.92	34.8097	8	2785.67	33.0599
9	1637.27	39.1536	10	1477.21	31.9328
11	1455.99	32.4972	12	1421.28	36.4136
13	1350.89	19.2438	14	1278.57	37.4737
15	1244.83	36.3434	16	1210.11	34.3344
17	1171.54	14.1508	18	1069.33	34.606
19	1035.59	33.3183	20	979.661	26.6071
21	951.698	16.1121	22	843.704	17.2465
23	810.92	32.0181	24	745.352	36.8897

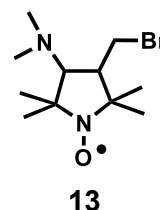
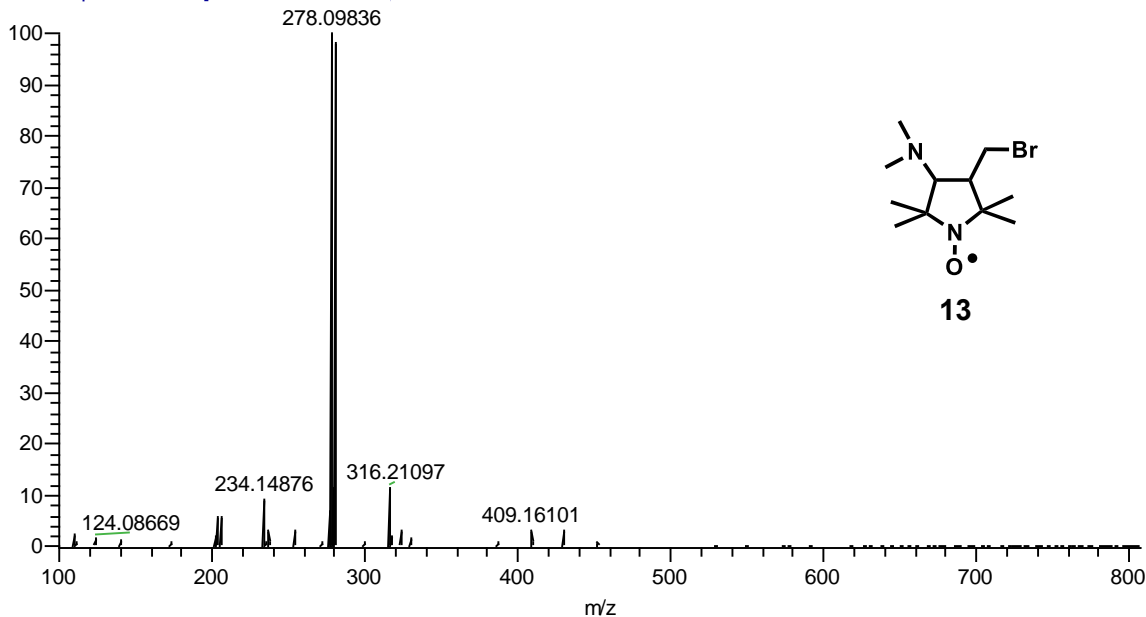
High resolution mass spectrometry and infrared spectroscopy data for 3-Bromomethyl-4-dimethylamino-1-oxyl-2,2,5,5-tetramethylpyrrolidine **13**

Full Scan Positive Ion Mode

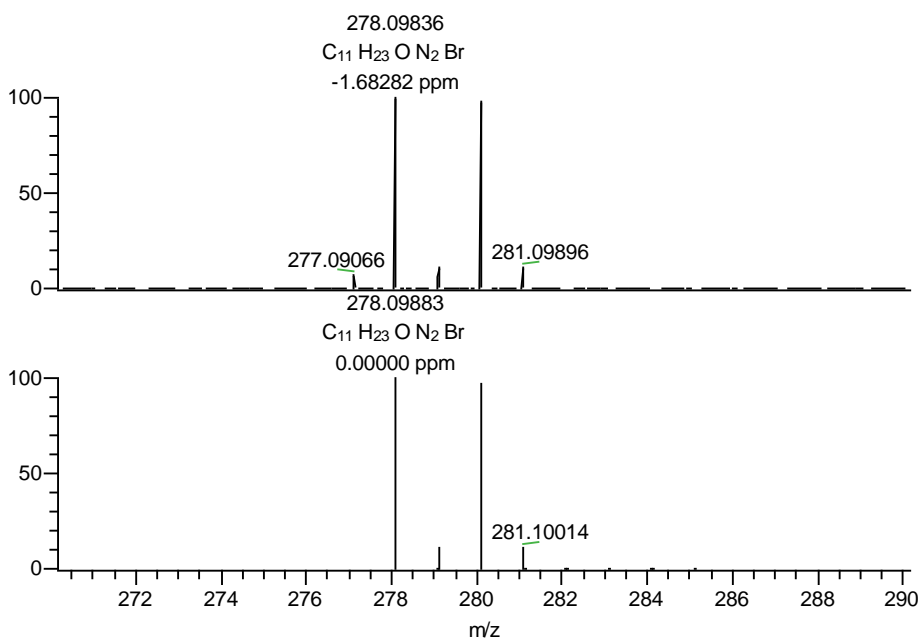
Sample	M _{Theoretical}	M _{Experimental}	ΔM (ppm)	Elemental Composition
	278.09883	278.09836	-1.683	C ₁₁ H ₂₂ BrN ₂ O
	[M+H] ⁺	[M+H] ⁺		
	280.09678	280.09573	-3.749	C ₁₁ H ₂₂ BrN ₂ O
	[M+H] ⁺	[M+H] ⁺		

210249_MAV809 #57-84 RT: 0.32-0.46 AV: 28 NL: 1.97E8

T: FTMS + p ESI Full ms [100.0000-800.0000]



Experimental and Theoretical Isotopic Distribution for C₁₁H₂₂BrN₂O [M+H]⁺



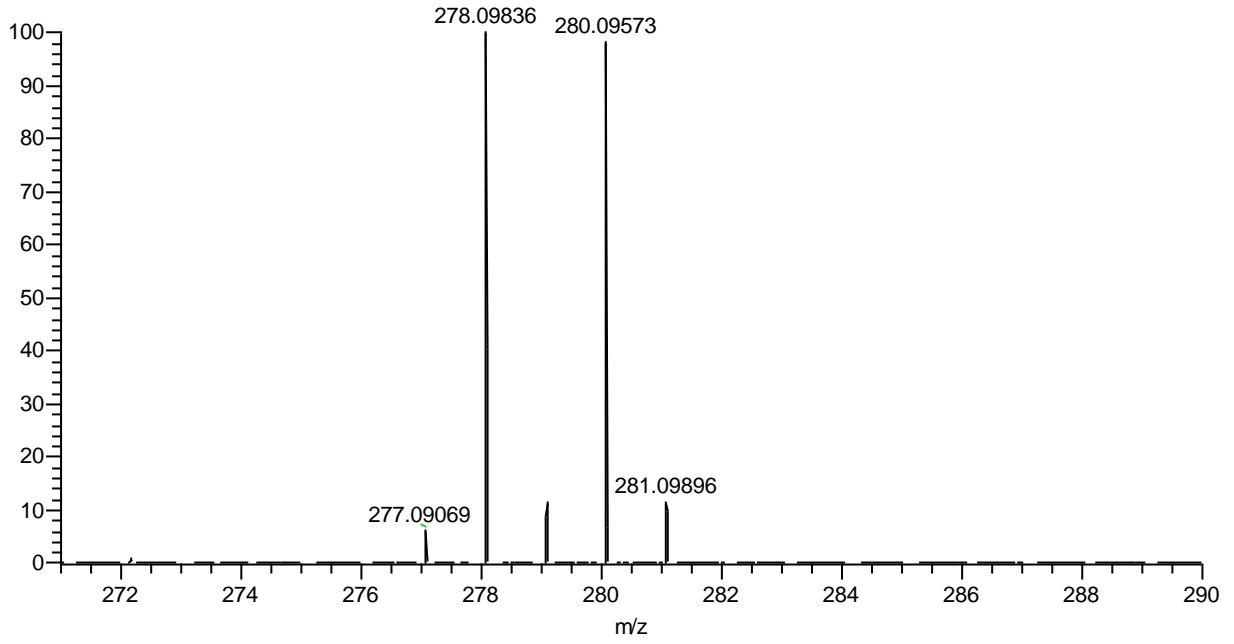
NL:
1.97E8
210249_MAV809#57-
84 RT: 0.32-0.46 AV:
28 T: FTMS + p ESI Full
ms
[100.0000-800.0000]

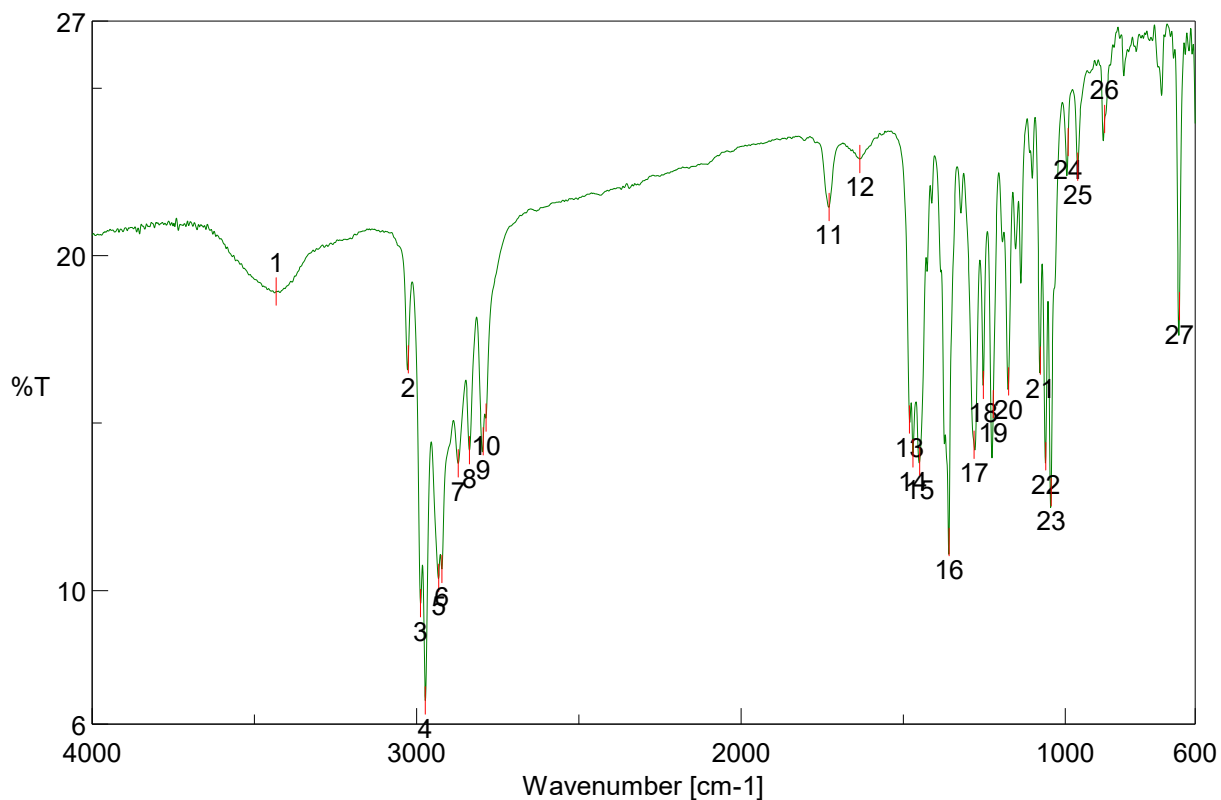
NL:
4.45E5
C₁₁H₂₂BrN₂O +H:
C₁₁H₂₃Br₁N₂O₁
pa Chrg 1

Scan 271 – 290 m/z

210249_MAV809 #58-84 RT: 0.32-0.46 AV: 27 NL: 2.03E8

T: FTMS + p ESI Full ms [100.0000-800.0000]





[Comments]

Sample name
 Comment
 User
 Division
 Company NCSU

[Detailed Information]

Creation date 10/21/2022 4:34 PM
 Data array type Linear data array
 Horizontal axis Wavenumber [cm-1]
 Vertical axis %T
 Start 0 cm-1
 End 7800.65 cm-1
 Data interval 0.964233 cm-1
 Data points 8091

[Measurement Information]

Model Name FT/IR-4100typeA
 Serial Number B096961016
 Measurement Date 10/21/2022 4:33 PM
 Light Source Standard
 Detector TGS
 Accumulation 8
 Resolution 4 cm-1
 Zero Filling On
 Apodization Cosine
 Gain Auto (8)
 Aperture Auto (7.1 mm)
 Scanning Speed Auto (2 mm/sec)
 Filter Auto (30000 Hz)

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
1	3432.67	18.9189	2	3025.76	16.8985

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
3	2988.16	9.61133	4	2972.73	6.70367
5	2932.23	10.3682	6	2921.63	10.6326
7	2871.49	13.7897	8	2836.77	14.1802
9	2794.35	14.4475	10	2785.67	15.1598
11	1728.87	21.4482	12	1633.41	22.884
13	1481.06	15.0992	14	1470.46	14.0911
15	1449.24	13.8488	16	1358.6	11.4343
17	1281.47	14.3484	18	1252.54	16.1364
19	1222.65	15.5551	20	1175.4	16.2356
21	1077.05	16.855	22	1060.66	13.9995
23	1044.26	12.9306	24	991.232	23.3845
25	962.305	22.6528	26	879.381	24.0753
27	647.965	18.4822			

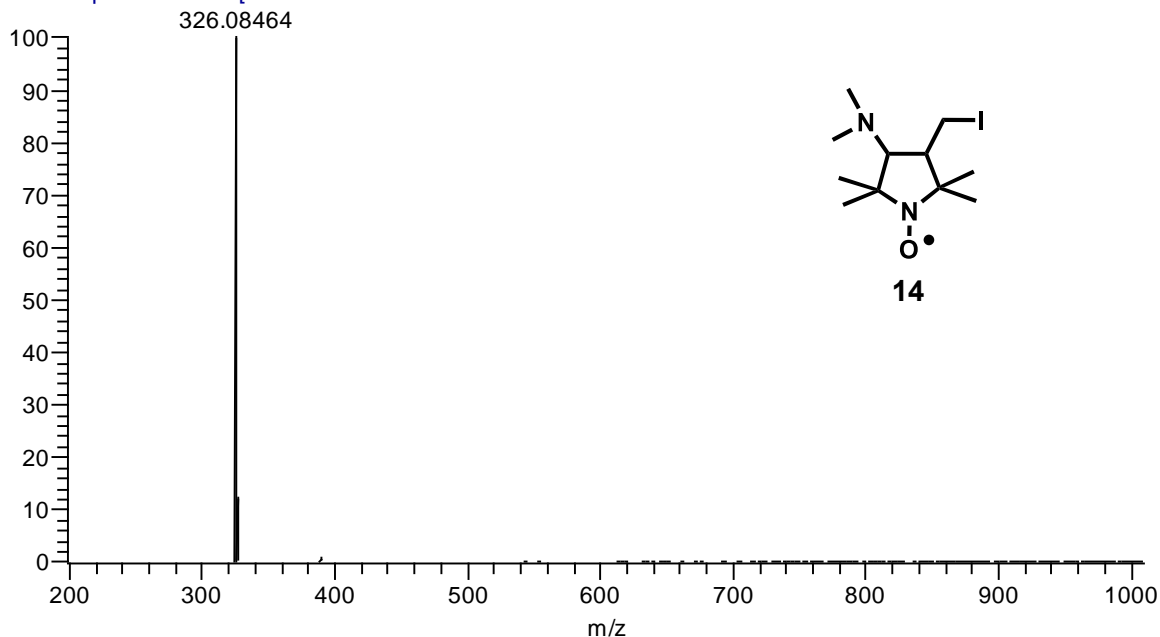
High resolution mass spectrometry and infrared spectroscopy data for 3-Dimethylamino-4-iodomethyl-1-oxyl-2,2,5,5-tetramethylpyrrolidine **14**

Full Scan Positive Ion Mode

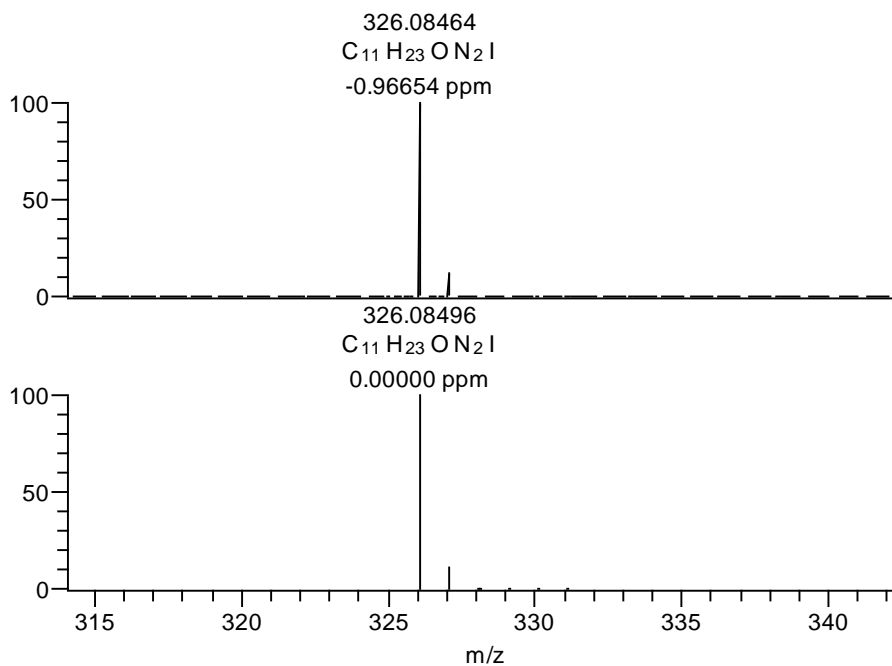
Sample	M _{Theoretical}	M _{Experimental}	ΔM (ppm)	Elemental Composition
	326.08496	326.08464	-0.967	C ₁₁ H ₂₂ IN ₂ O
	[M+H] ⁺	[M+H] ⁺		

210781_MAV821 #53-73 RT: 0.32-0.43 AV: 21 NI : 3.20F8

T: FTMS + p ESI Full ms [200.0000-1000.]

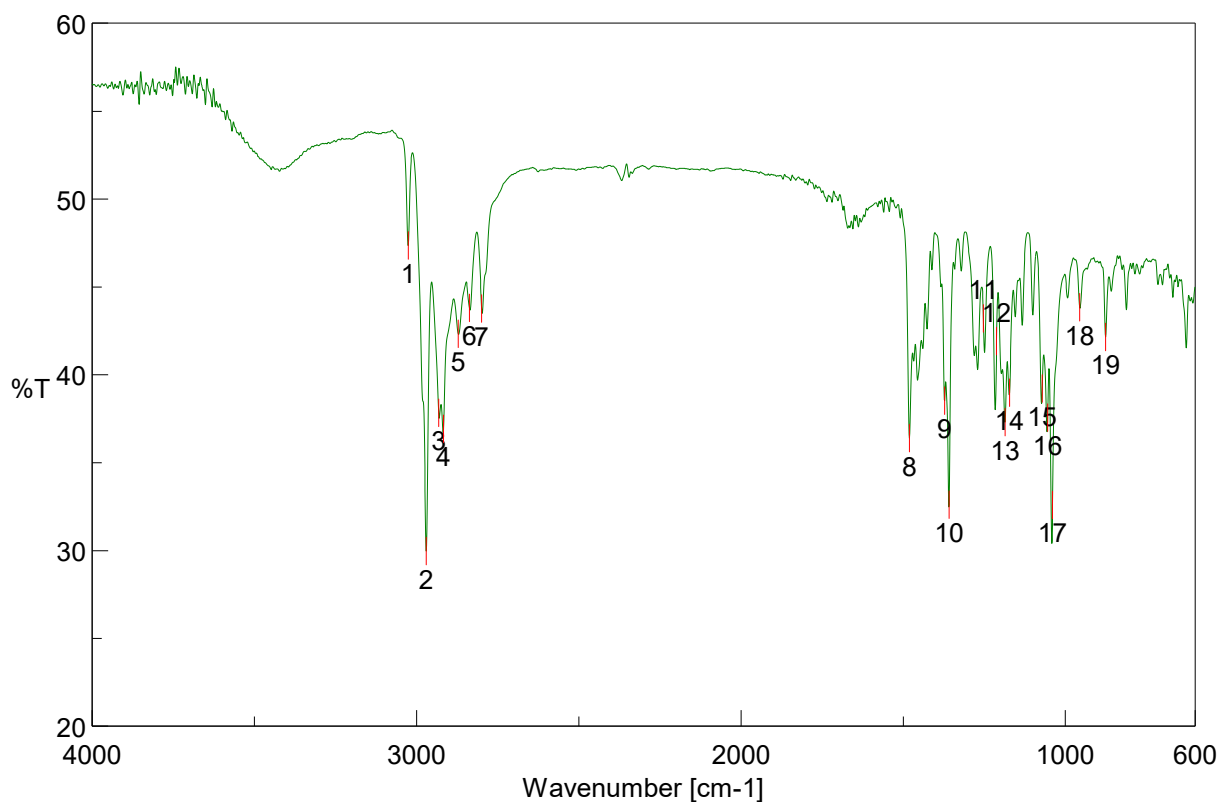


Experimental and Theoretical Isotopic Distribution for C₁₁H₂₂IN₂O [M+H]⁺



NL:
3.20E8
210781_MAV821#53-
73 RT: 0.32-0.43 AV:
21 T: FTMS + p ESI
Full ms
[200.0000-1000.0000]

NL:
8.77E5
C₁₁H₂₂IN₂O +H:
C₁₁H₂₃I₁N₂O₁
pa Chrg 1



[Comments]

Sample name
 Comment
 User
 Division
 Company NCSU

[Detailed Information]

Creation date 10/5/2022 7:43 PM
 Data array type Linear data array
 Horizontal axis Wavenumber [cm-1]
 Vertical axis %T
 Start 0 cm-1
 End 7800.65 cm-1
 Data interval 0.964233 cm-1
 Data points 8091

[Measurement Information]

Model Name FT/IR-4100typeA
 Serial Number B096961016
 Measurement Date 10/5/2022 7:43 PM
 Light Source Standard
 Detector TGS
 Accumulation 8
 Resolution 4 cm-1
 Zero Filling On
 Apodization Cosine
 Gain Auto (4)
 Aperture Auto (7.1 mm)
 Scanning Speed Auto (2 mm/sec)
 Filter Auto (30000 Hz)

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
1	3025.76	47.3521	2	2969.84	29.9548

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
3	2932.23	37.83	4	2916.81	36.9111
5	2871.49	42.3159	6	2836.77	43.7876
7	2799.17	43.7578	8	1481.06	36.3943
9	1372.1	38.5158	10	1358.6	32.6062
11	1252.54	43.1908	12	1212.04	41.9042
13	1186.01	37.2966	14	1172.51	38.9789
15	1071.26	39.2032	16	1054.87	37.5456
17	1039.44	32.5841	18	956.52	43.8363
19	876.488	42.14			

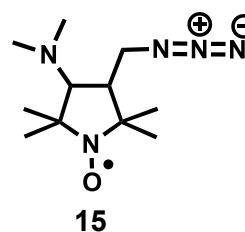
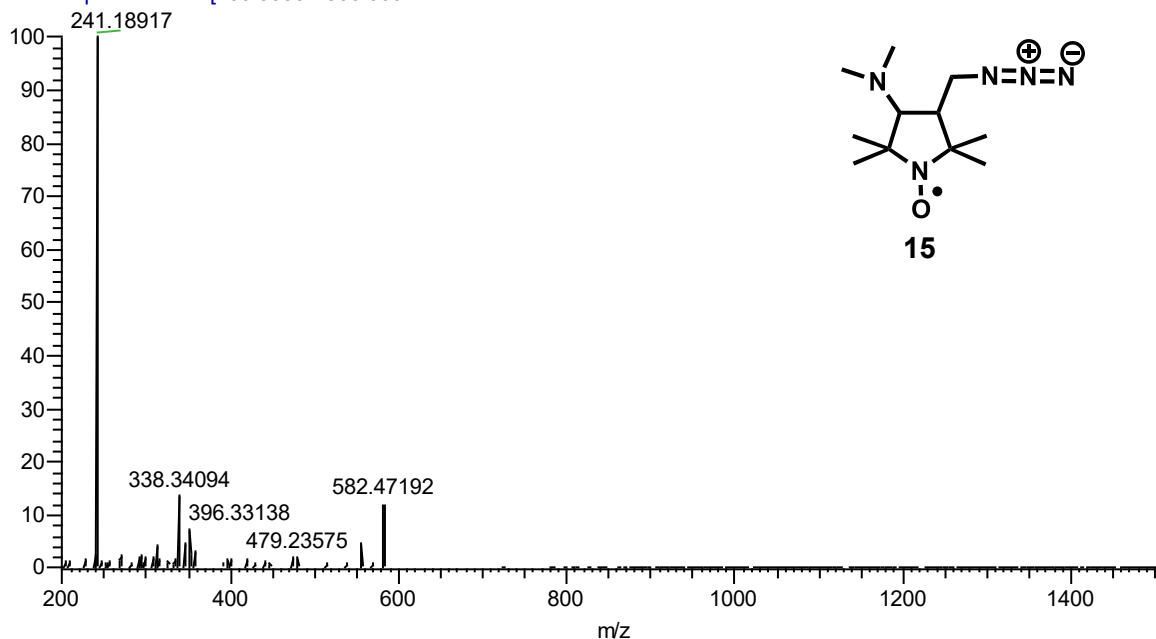
High resolution mass spectrometry and infrared spectroscopy data for 3-Azidomethyl-4-dimethylamino-1-oxyl-2,2,5,5-tetramethylpyrrolidine **15**

Full Scan Positive Ion Mode

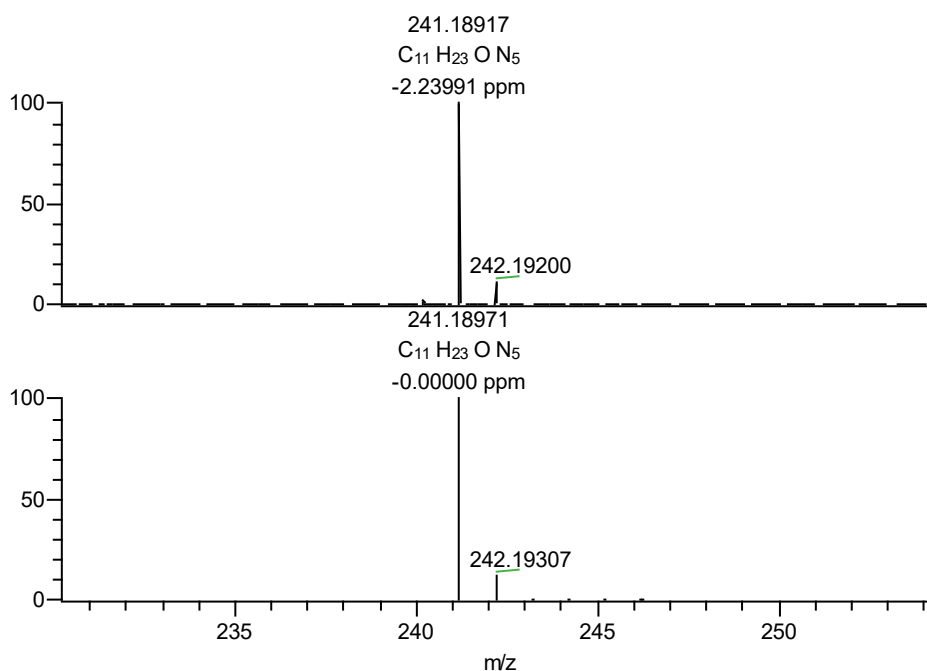
Sample	M _{Theoretical}	M _{Experimental}	ΔM (ppm)	Elemental Composition
	241.18971	241.18917	-2.240	C ₁₁ H ₂₂ N ₅ O
	[M+H] ⁺	[M+H] ⁺		

210442_MAV-808 #82-94 RT: 0.48-0.55 AV: 13 NL: 3.15E7

T: FTMS + p ESI Full ms [200.0000-1500.000]

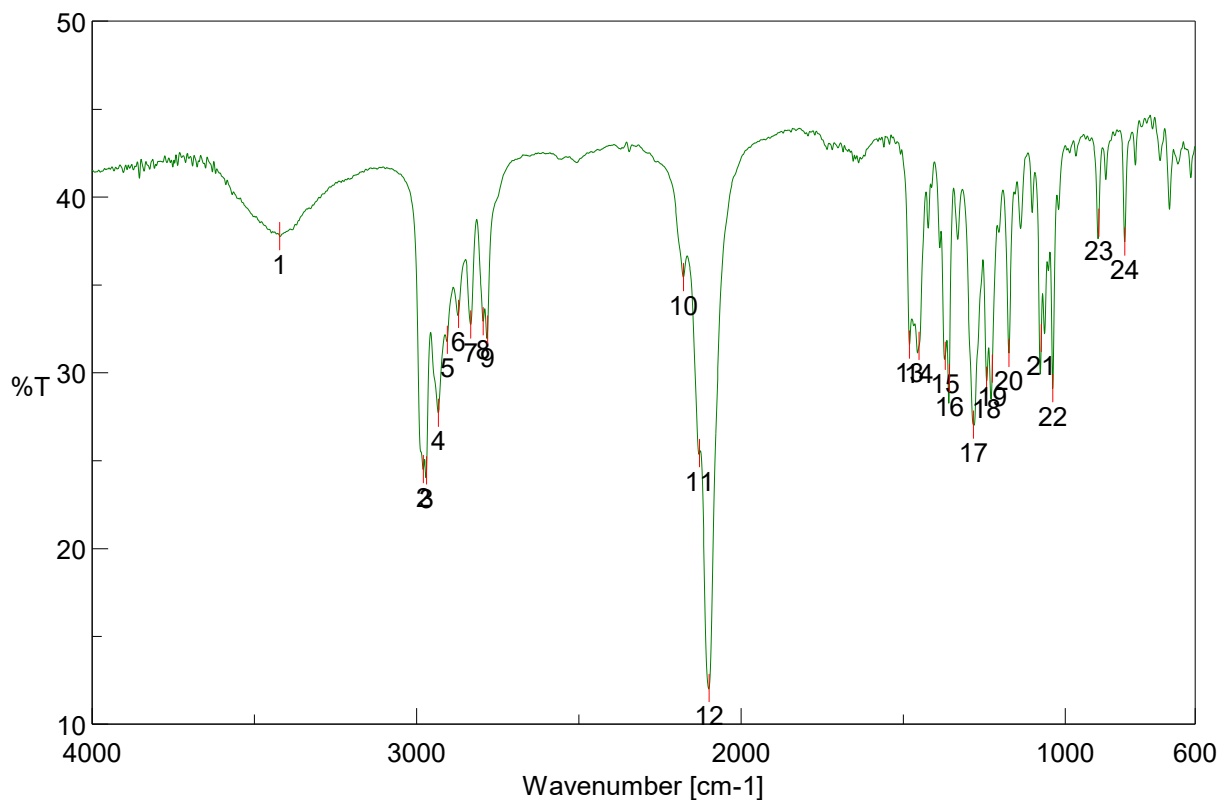


Experimental and Theoretical Isotopic Distribution for C₁₁H₂₂N₅O [M+H]⁺



NL:
3.15E7
210442_MAV-808#82-94 RT: 0.48-0.55 AV: 13 T: FTMS + p ESI Full ms [200.0000-1500.000]

NL:
8.68E5
C₁₁H₂₂N₅O +H:
C₁₁H₂₃N₅O₁
pa Chrg 1



[Comments]

Sample name
 Comment
 User
 Division
 Company NCSU

[Detailed Information]

Creation date 12/4/2020 1:12 PM
 Data array type Linear data array
 Horizontal axis Wavenumber [cm-1]
 Vertical axis %T
 Start 0 cm-1
 End 7800.65 cm-1
 Data interval 0.964233 cm-1
 Data points 8091

[Measurement Information]

Model Name FT/IR-4100typeA
 Serial Number B096961016
 Measurement Date 12/4/2020 1:12 PM
 Light Source Standard
 Detector TGS
 Accumulation 8
 Resolution 4 cm-1
 Zero Filling On
 Apodization Cosine
 Gain Auto (4)
 Aperture Auto (7.1 mm)
 Scanning Speed Auto (2 mm/sec)
 Filter Auto (30000 Hz)

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
1	3422.06	37.7615	2	2979.48	24.5035

[Result of Peak Picking]

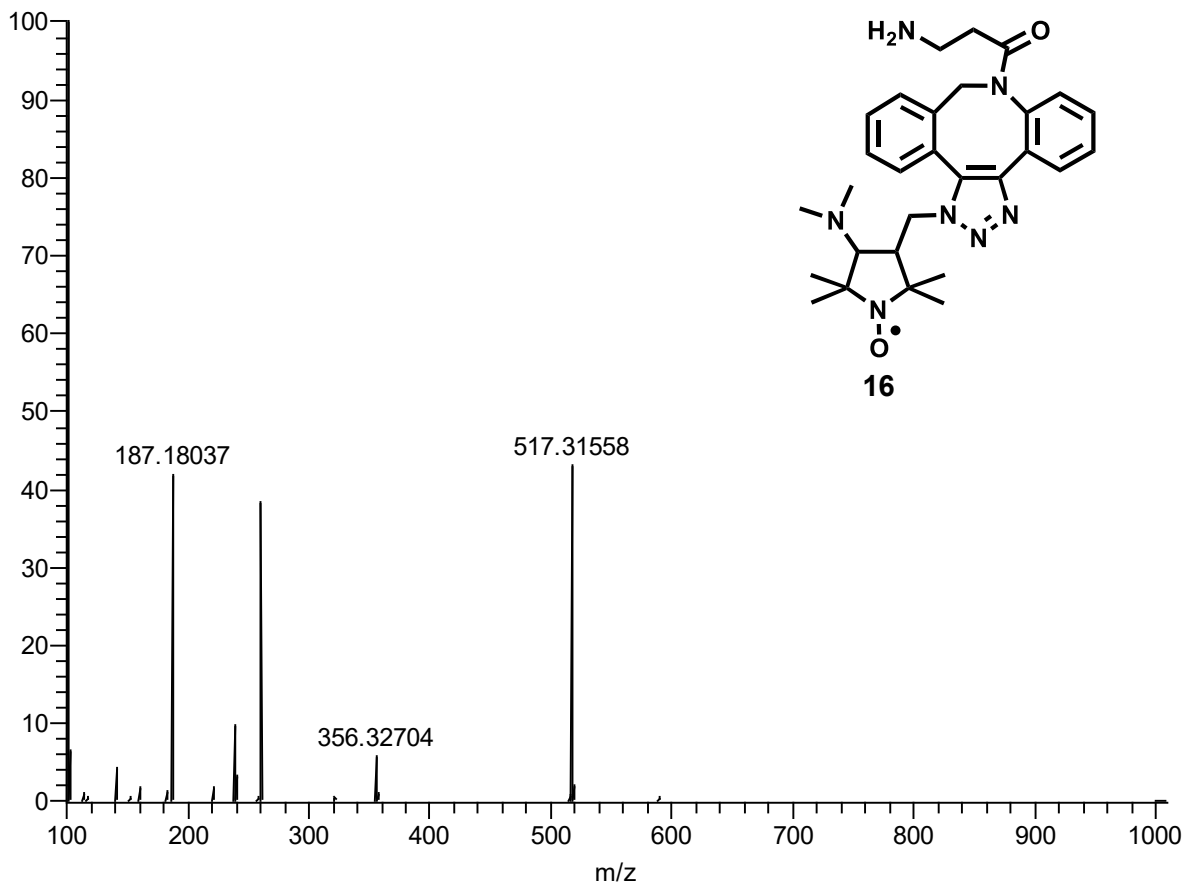
No.	Position	Intensity	No.	Position	Intensity
3	2968.87	24.4359	4	2933.2	27.7193
5	2905.24	31.8617	6	2870.52	33.35
7	2832.92	32.7414	8	2794.35	32.9133
9	2780.85	32.4474	10	2177.24	35.4262
11	2128.06	25.4213	12	2098.17	12.052
13	1481.06	31.5972	14	1451.17	31.5289
15	1370.18	30.9598	16	1357.64	29.6805
17	1283.39	27.0419	18	1242.9	29.5438
19	1225.54	30.2343	20	1174.44	31.1191
21	1074.16	31.9838	22	1038.48	29.1125
23	896.737	38.5219	24	816.706	37.4598

Full Scan Positive Ion Mode:

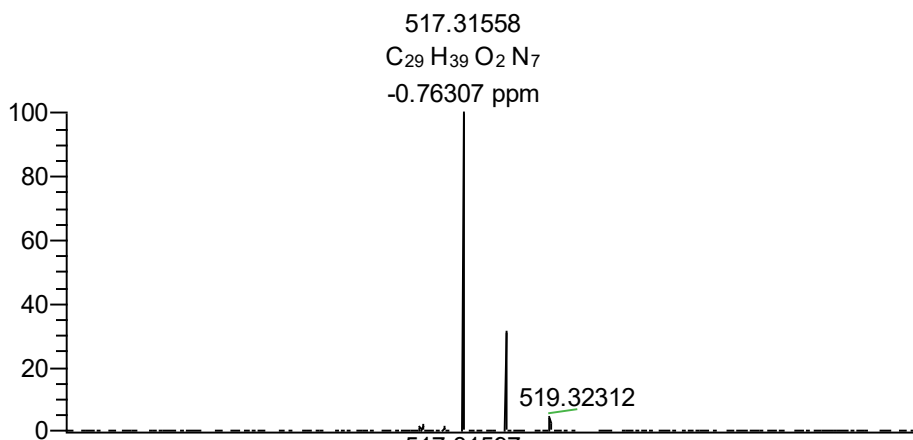
Sample	M _{Theoretical}	M _{Experimental}	ΔM (ppm)	Elemental Composition
	517.31597 [M+H] ⁺	517.31558 [M+H] ⁺	-0.76307	C ₂₉ H ₃₉ N ₇ O ₂

MAV-863 #169-681 RT: 0.77-3.08 AV: 513 NL: 1.33E9

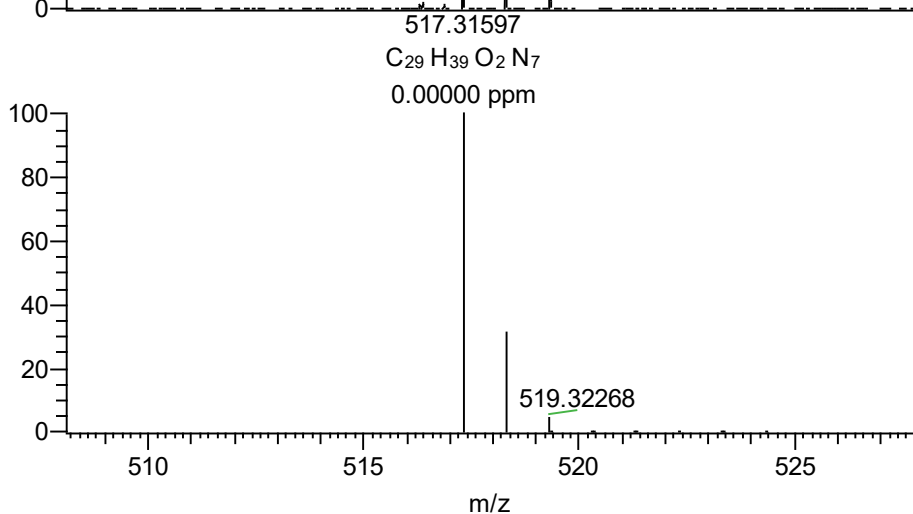
T: FTMS + p ESI Full ms [100.0000-1000.0000]



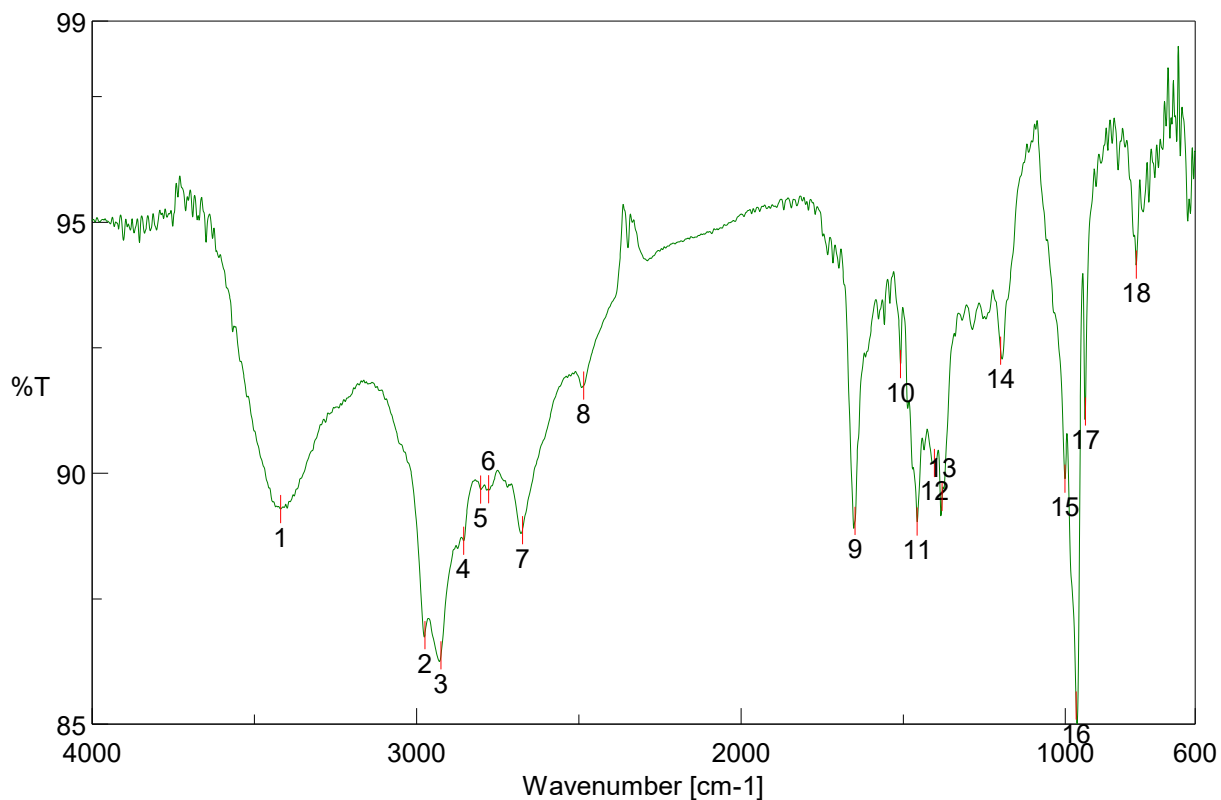
Experimental and Theoretical Isotopic Distribution [M+H]⁺



NL:
5.74E8
MAV-863#169-681
RT: 0.77-3.08 AV:
513 T: FTMS + p ESI
Full ms
[100.0000-1000.0000]



NL:
7.07E5
C₂₉ H₃₈ N₇ O₂ +H:
C₂₉ H₃₉ N₇ O₂
pa Chrg 1



[Comments]

Sample name
 Comment
 User
 Division
 Company NCSU

[Detailed Information]

Creation date 12/5/2022 5:44 PM
 Data array type Linear data array
 Horizontal axis Wavenumber [cm-1]
 Vertical axis %T
 Start 0 cm-1
 End 7800.65 cm-1
 Data interval 0.964233 cm-1
 Data points 8091

[Measurement Information]

Model Name FT/IR-4100typeA
 Serial Number B096961016
 Measurement Date 12/5/2022 5:44 PM
 Light Source Standard
 Detector TGS
 Accumulation 8
 Resolution 4 cm-1
 Zero Filling On
 Apodization Cosine
 Gain Auto (2)
 Aperture Auto (7.1 mm)
 Scanning Speed Auto (2 mm/sec)
 Filter Auto (30000 Hz)

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
1	3419.17	89.2848	2	2974.66	86.7732

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
3	2924.52	86.3688	4	2855.1	88.6506
5	2802.06	89.6719	6	2777.96	89.6747
7	2673.82	88.8634	8	2484.83	91.7437
9	1648.84	89.0495	10	1508.06	92.1679
11	1456.96	89.0346	12	1403.92	90.2019
13	1379.82	89.5218	14	1199.51	92.4348
15	1001.84	89.888	16	967.126	85.3681
17	938.199	91.2249	18	781.029	94.1504

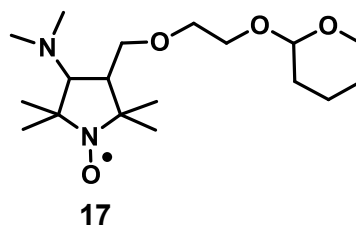
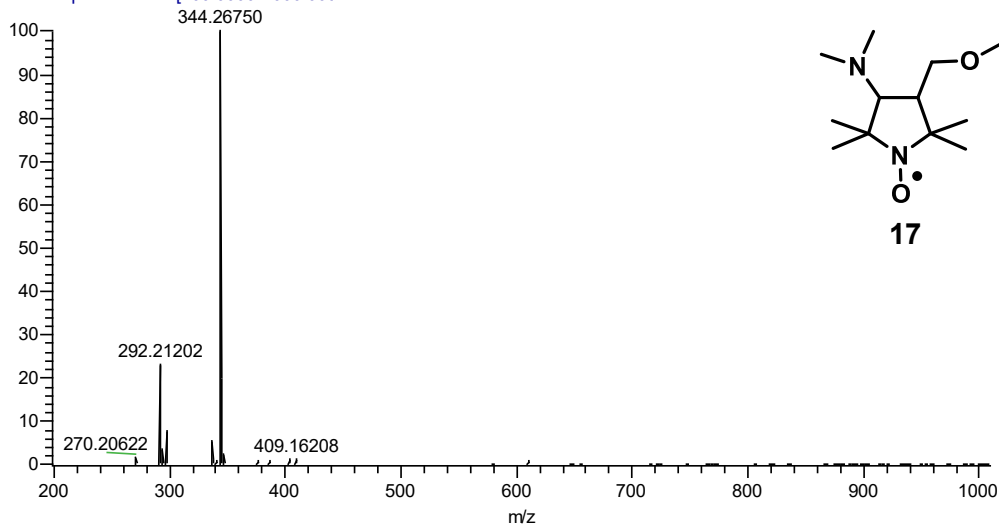
High resolution mass spectrometry and infrared spectroscopy data for 3-Dimethylamino-1-oxyl-2,2,5,5-tetramethyl-4-[2-(tetrahydropyran-2-yloxy)-ethoxymethyl]-pyrrolidine **17**

Full Scan Positive Ion Mode

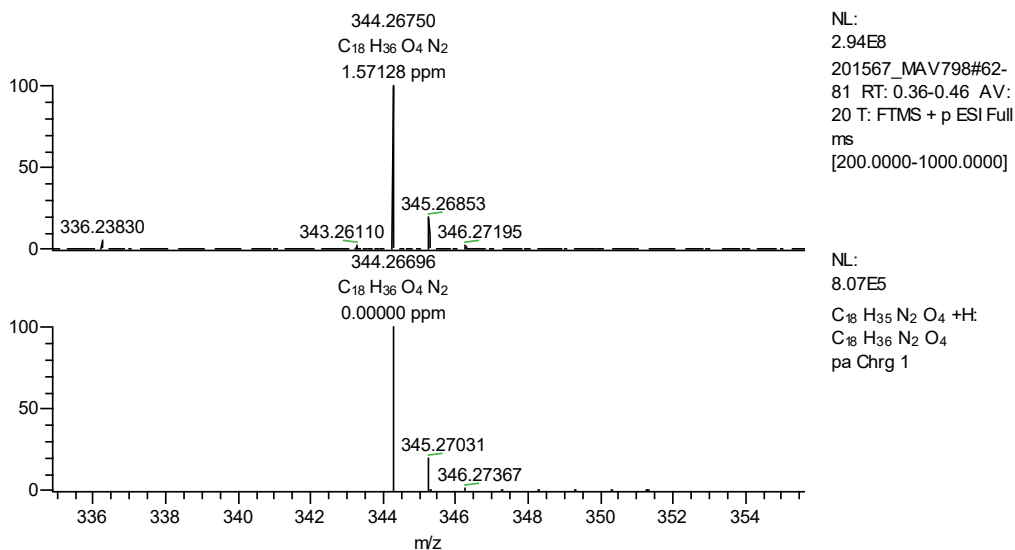
Sample	M _{Theoretical}	M _{Experimental}	ΔM (ppm)	Elemental Composition
	344.26696	344.26750	1.571	C ₁₈ H ₃₅ N ₂ O ₄
	[M+H] ⁺	[M+H] ⁺		

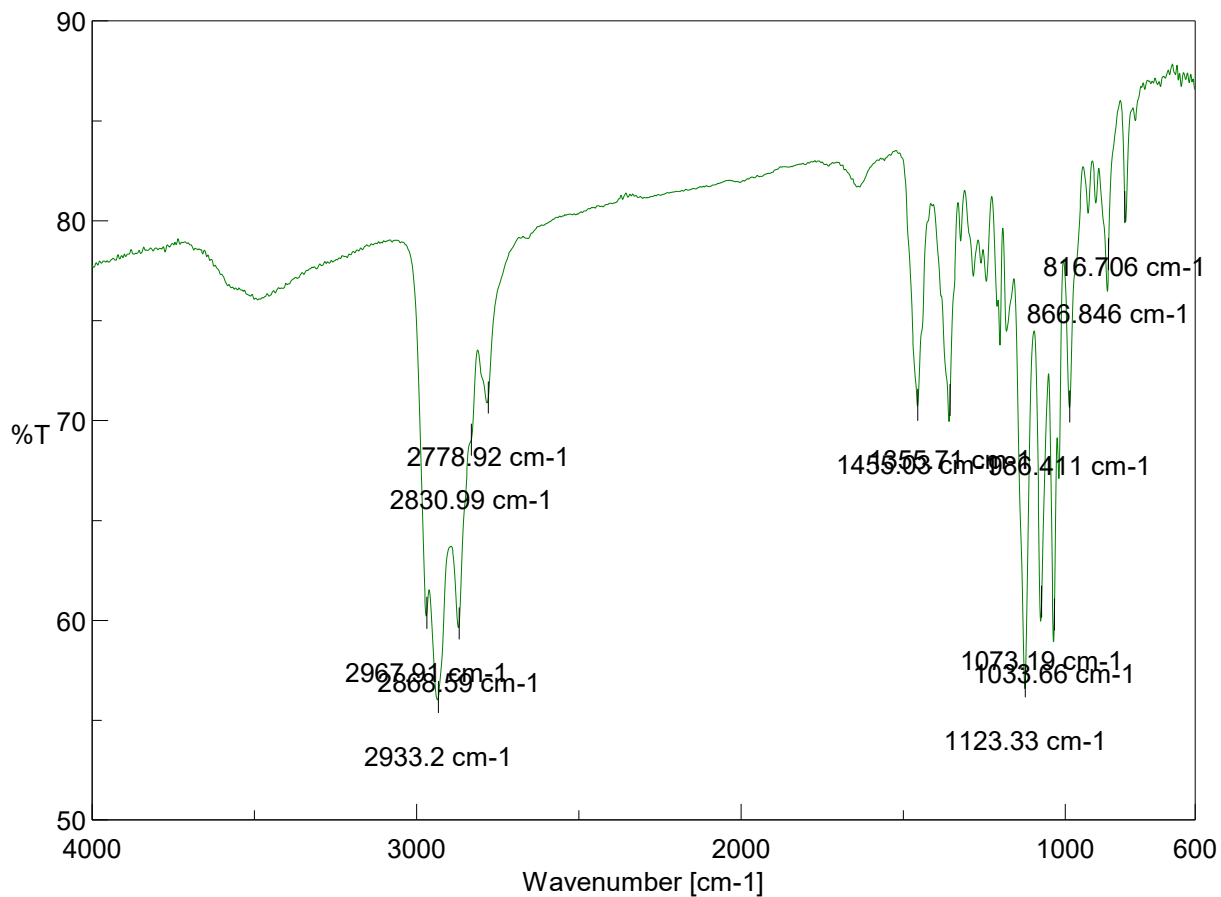
201567_MAV798 #62-81 RT: 0.36-0.46 AV: 20 NL: 2.94E8

T: FTMS + p ESI Full ms [200.0000-1000.0000]



Experimental and Theoretical Isotopic Distribution for C₁₈H₃₅N₂O₄ [M+H]⁺





[Comments]

Sample name
 Comment
 User
 Division
 Company

NCSU

MAV_798_neat_2.jws

[Detailed Information]

Creation date 10/22/2020 5:38 PM
 Data array type Linear data array
 Horizontal axis Wavenumber [cm-1]
 Vertical axis %T
 Start 0 cm-1
 End 7800.65 cm-1
 Data interval 0.964233 cm-1
 Data points 8091

[Measurement Information]

Model Name FT/IR-4100typeA
 Serial Number B096961016

Measurement Date 10/22/2020 5:34 PM

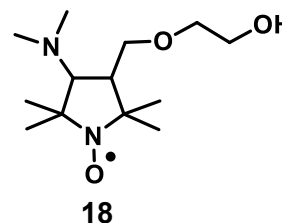
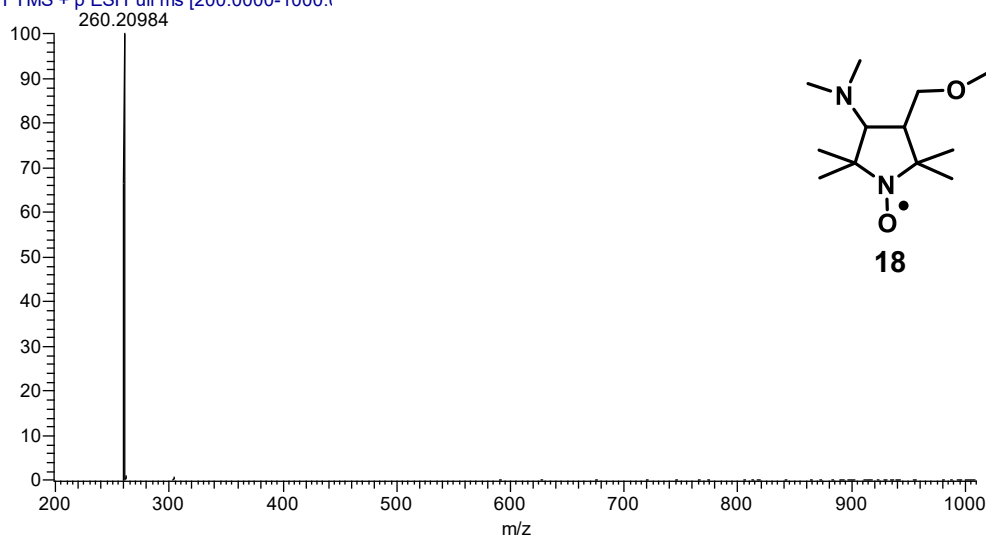
Light Source Standard
 Detector TGS
 Accumulation 8
 Resolution 4 cm-1
 Zero Filling On
 Apodization Cosine
 Gain Auto (2)
 Aperture Auto (7.1 mm)
 Scanning Speed Auto (2 mm/sec)
 Filter Auto (30000 Hz)

High resolution mass spectrometry and infrared spectroscopy data for 3-Dimethylamino-4-(2-hydroxy-ethoxymethyl)-1-oxyl-2,2,5,5-tetramethylpyrrolidine **18**

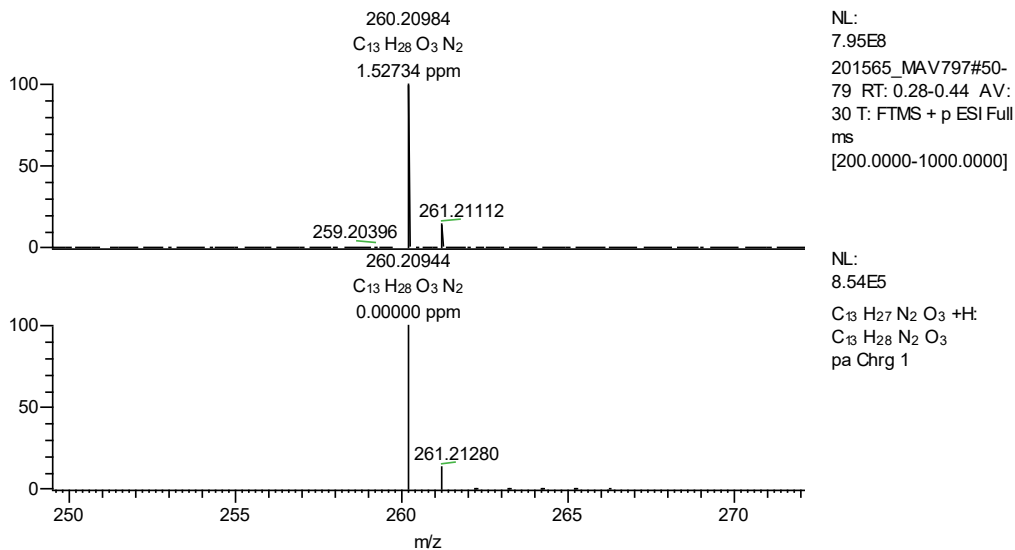
Full Scan Positive Ion Mode

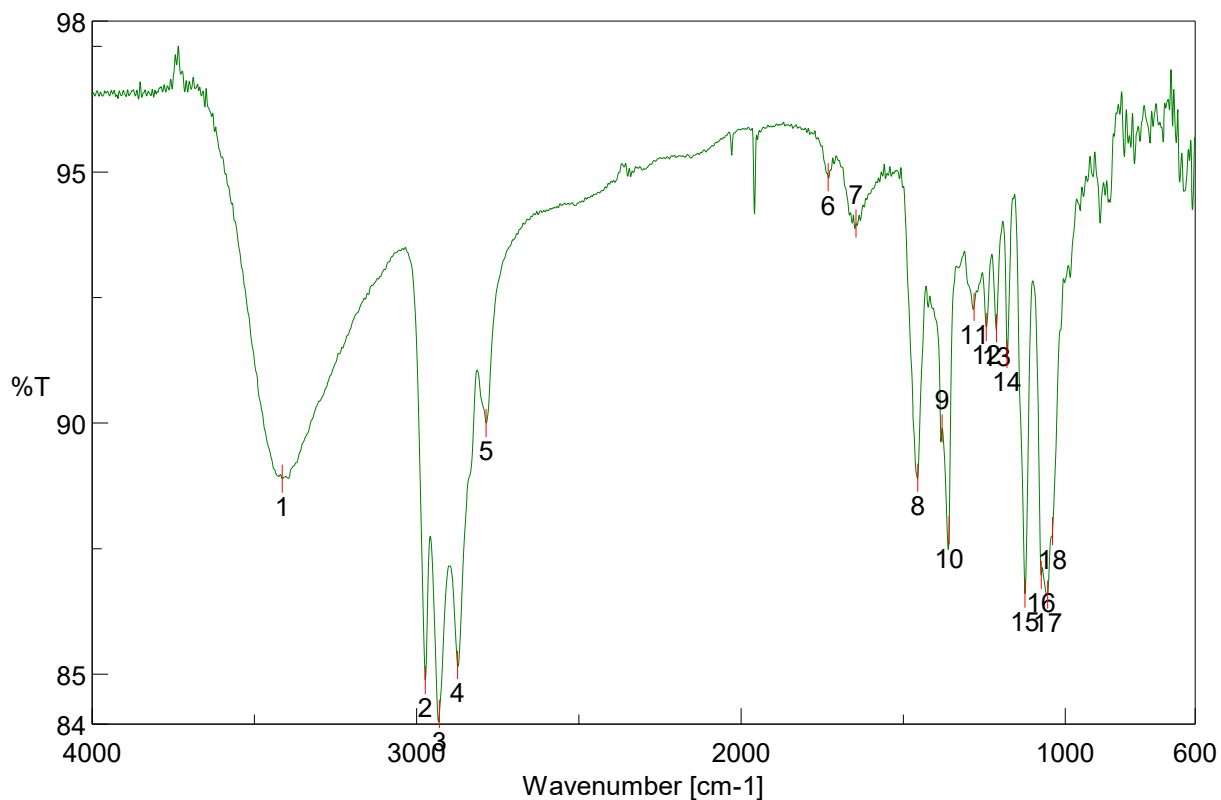
Sample	M _{Theoretical}	M _{Experimental}	ΔM (ppm)	Elemental Composition
	260.20944 [M+H] ⁺	260.20984 [M+H] ⁺	1.527	C ₁₃ H ₂₇ N ₂ O ₃

201565_MAV797 #50-79 RT: 0.28-0.44 AV: 30 NL: 7.95E8
T: FTMS + p ESI Full ms [200.0000-1000.0000]



Experimental and Theoretical Isotopic Distribution for C₁₃H₂₇N₂O₃ [M+H]⁺





[Comments]

Sample name
 Comment
 User
 Division
 Company NCSU

[Detailed Information]

Creation date 10/7/2022 5:11 PM
 Data array type Linear data array
 Horizontal axis Wavenumber [cm-1]
 Vertical axis %T
 Start 0 cm-1
 End 7800.65 cm-1
 Data interval 0.964233 cm-1
 Data points 8091

[Measurement Information]

Model Name FT/IR-4100typeA
 Serial Number B096961016
 Measurement Date 10/7/2022 5:10 PM
 Light Source Standard
 Detector TGS
 Accumulation 8
 Resolution 4 cm-1
 Zero Filling On
 Apodization Cosine
 Gain Auto (2)
 Aperture Auto (7.1 mm)
 Scanning Speed Auto (2 mm/sec)
 Filter Auto (30000 Hz)

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
1	3414.35	88.886	2	2972.73	84.878

[Result of Peak Picking]

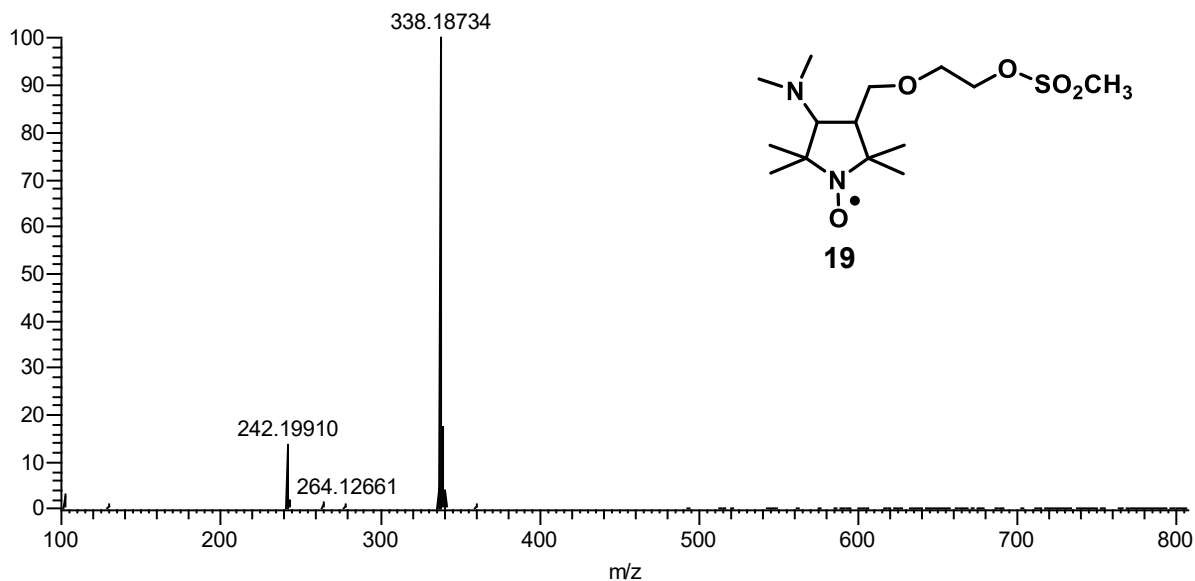
No.	Position	Intensity	No.	Position	Intensity
3	2929.34	84.2027	4	2873.42	85.177
5	2785.67	89.996	6	1731.76	94.8912
7	1645.95	93.9662	8	1455.03	88.9046
9	1379.82	89.8879	10	1358.6	87.8618
11	1281.47	92.3066	12	1243.86	91.9049
13	1212.04	91.8808	14	1180.22	91.3704
15	1124.3	86.6013	16	1074.16	86.9685
17	1054.87	86.5826	18	1039.44	87.8455

High resolution mass spectrometry and infrared spectroscopy data for 2-((4-(dimethylamino)-1-oxyl-2,2,5,5-tetramethylpyrrolidin-3-yl)methoxy)ethyl methanesulfonate **19**

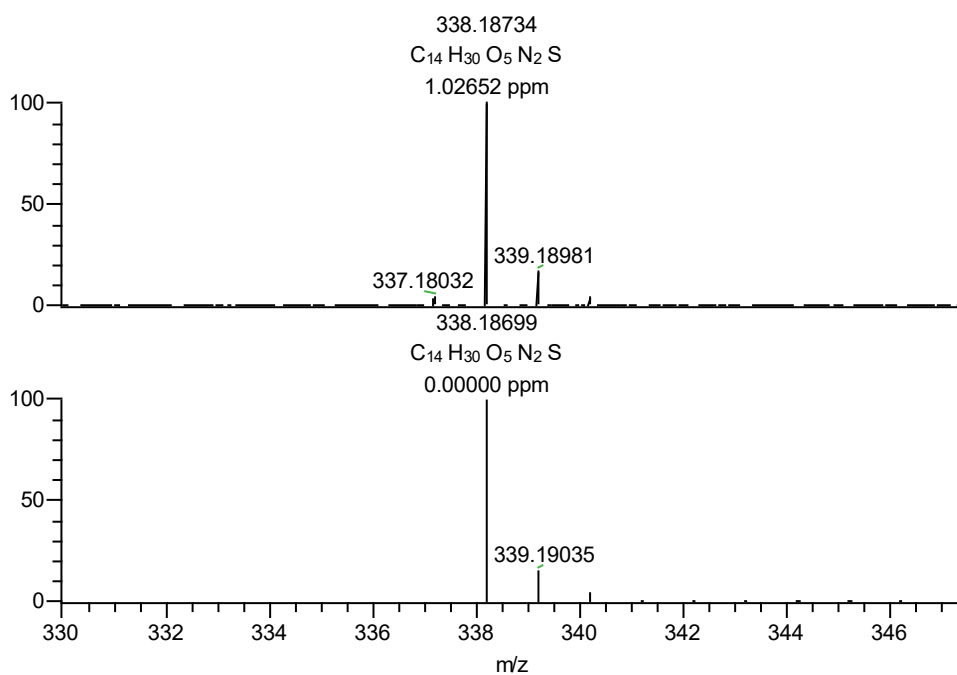
Full Scan Positive Ion Mode

Sample	M _{Theoretical}	M _{Experimental}	ΔM (ppm)	Elemental Composition
	338.18699	338.18734	1.027	C ₁₄ H ₂₉ N ₂ O ₅ S
	[M+H] ⁺	[M+H] ⁺		

201997_MAV-800 #41-78 RT: 0.25-0.44 AV: 38 NL: 1.40E9
T: FTMS + p ESI Full ms [100.0000-800.0000]

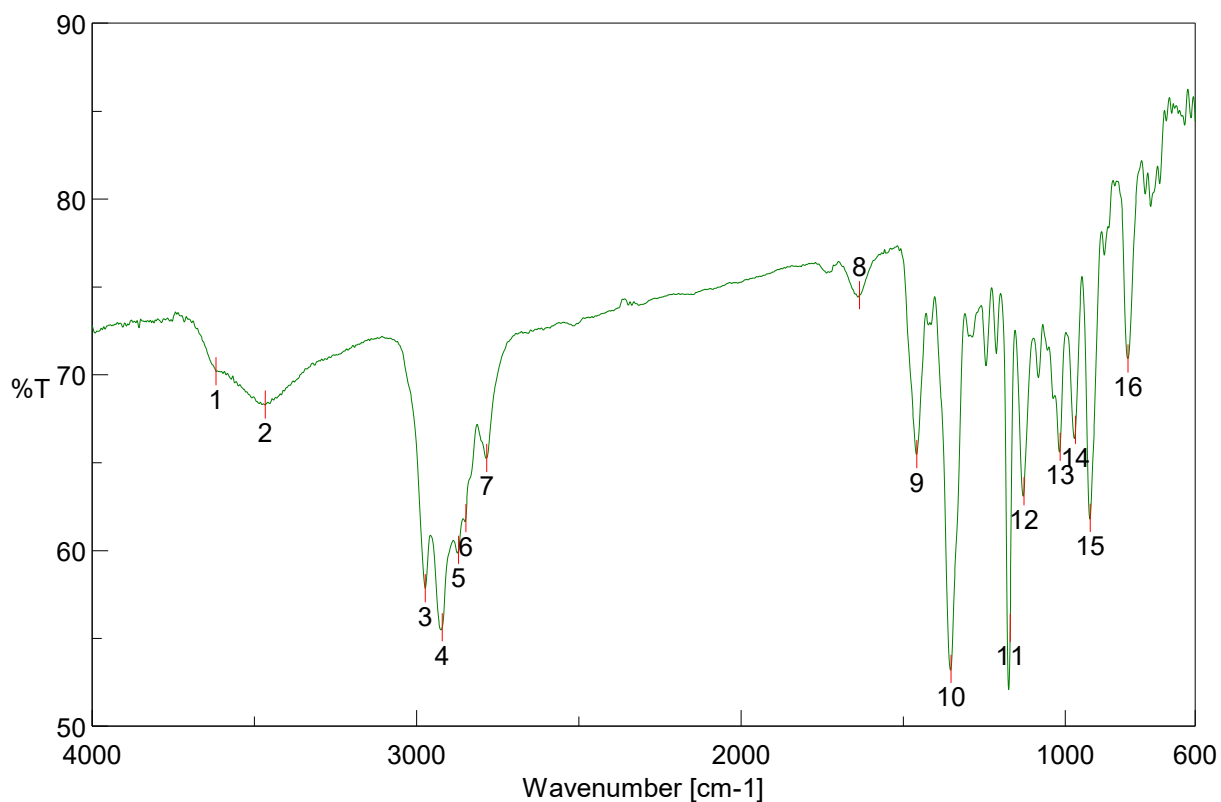


Experimental and Theoretical Isotopic Distribution for C₁₄H₂₉N₂O₅S [M+H]⁺



NL:
1.40E9
201997_MAV-800#41-
78 RT: 0.25-0.44 AV:
38 T: FTMS + p ESI Full
ms
[100.0000-800.0000]

NL:
7.98E5
C₁₄ H₂₉ N₂ O₅ S +H:
C₁₄ H₃₀ N₂ O₅ S₁
pa Chrg 1



[Comments]

Sample name
 Comment
 User
 Division
 Company NCSU

[Detailed Information]

Creation date 10/28/2020 12:18 PM
 Data array type Linear data array
 Horizontal axis Wavenumber [cm-1]
 Vertical axis %T
 Start 0 cm-1
 End 7800.65 cm-1
 Data interval 0.964233 cm-1
 Data points 8091

[Measurement Information]

Model Name FT/IR-4100typeA
 Serial Number B096961016
 Measurement Date 10/28/2020 12:18 PM
 Light Source Standard
 Detector TGS
 Accumulation 8
 Resolution 4 cm-1
 Zero Filling On
 Apodization Cosine
 Gain Auto (2)
 Aperture Auto (7.1 mm)
 Scanning Speed Auto (2 mm/sec)
 Filter Auto (30000 Hz)

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
1	3618.77	70.1974	2	3466.42	68.291

[Result of Peak Picking]

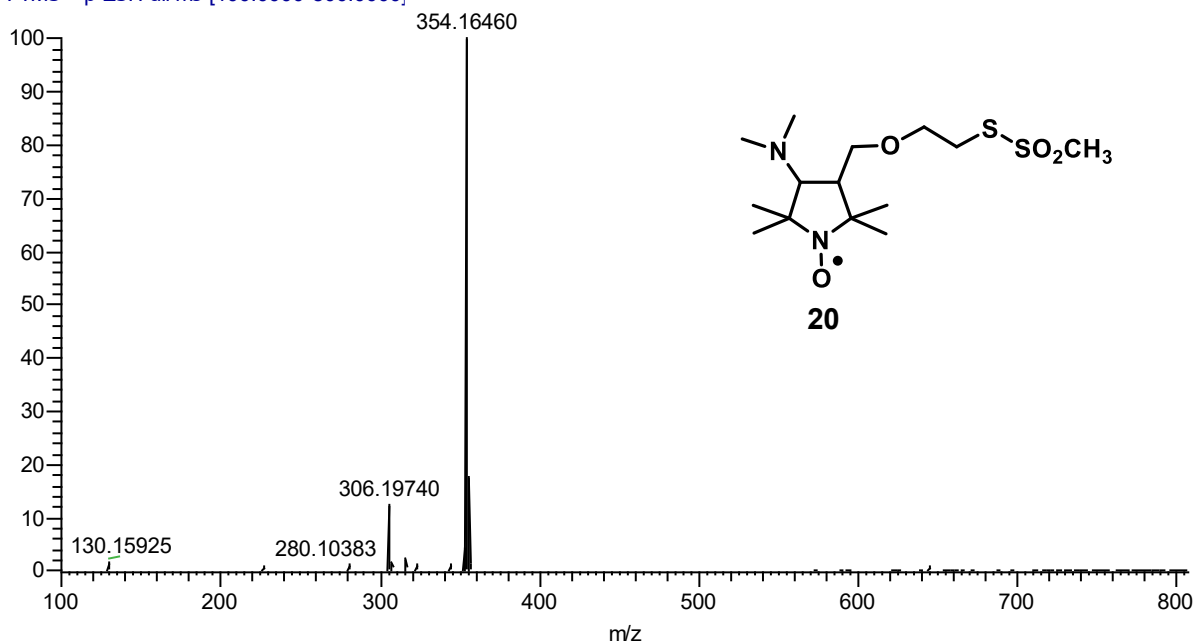
No.	Position	Intensity	No.	Position	Intensity
3	2972.73	57.8428	4	2920.66	55.6257
5	2870.52	60.0382	6	2848.35	61.8297
7	2783.74	65.2512	8	1634.38	74.5281
9	1457.92	65.4666	10	1352.82	53.2574
11	1170.58	55.5926	12	1128.15	63.3658
13	1016.3	65.8924	14	969.055	66.8618
15	923.736	61.8592	16	807.063	70.9281

High resolution mass spectrometry and infrared spectroscopy data for S-(2-((4-(dimethylamino)-1-oxyl-2,2,5,5-tetramethylpyrrolidin-3-yl)methoxy)ethyl) methanesulfonylthioate **20**

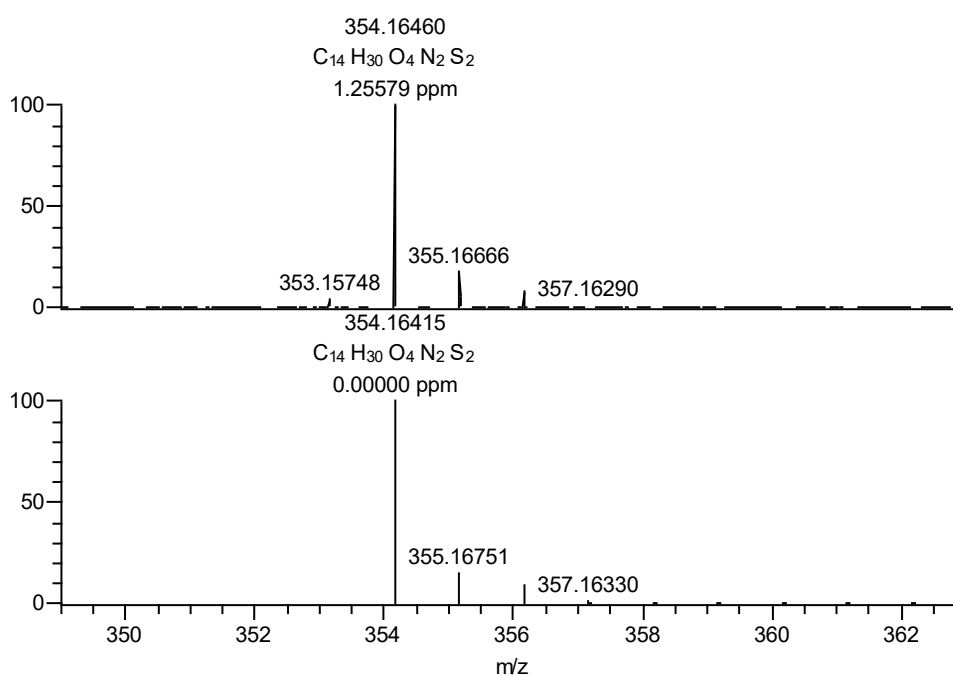
Full Scan Positive Ion Mode

Sample	M _{Theoretical}	M _{Experimental}	ΔM (ppm)	Elemental Composition
	354.16415	354.16460	1.256	C ₁₄ H ₂₉ N ₂ O ₄ S ₂
	[M+H] ⁺	[M+H] ⁺		

201999_MAV-801 #41-75 RT: 0.25-0.43 AV: 35 NL: 8.38E8
T: FTMS + p ESI Full ms [100.0000-800.0000]

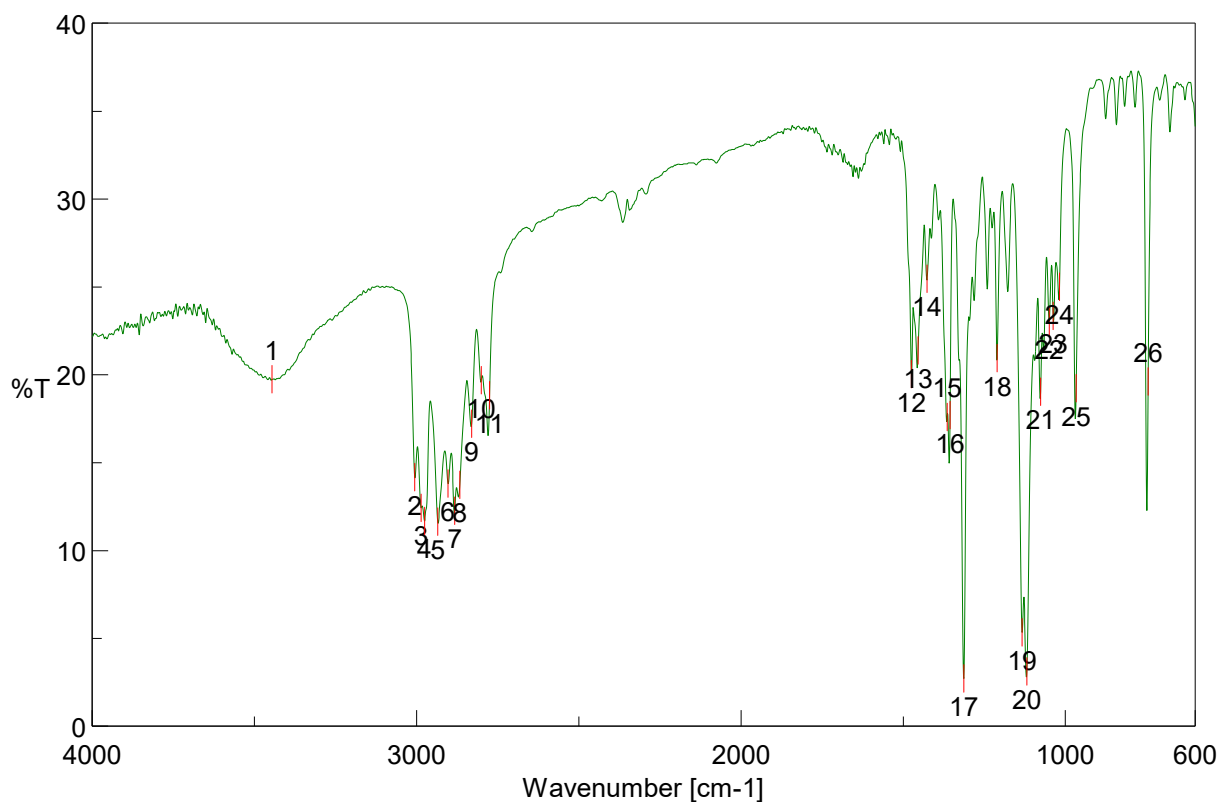


Experimental and Theoretical Isotopic Distribution for C₁₄H₂₉N₂O₄S₂ [M+H]⁺



NL:
8.38E8
201999_MAV-801#41-
75 RT: 0.25-0.43 AV:
35 T: FTMS + p ESI Full
ms
[100.0000-800.0000]

NL:
7.59E5
C₁₄ H₂₉ N₂ O₄ S₂ +H:
C₁₄ H₃₀ N₂ O₄ S₂
pa Chrg 1



[Comments]

Sample name
 Comment
 User
 Division
 Company NCSU

[Detailed Information]

Creation date 5/3/2021 5:27 PM
 Data array type Linear data array
 Horizontal axis Wavenumber [cm-1]
 Vertical axis %T
 Start 0 cm-1
 End 7800.65 cm-1
 Data interval 0.964233 cm-1
 Data points 8091

[Measurement Information]

Model Name FT/IR-4100typeA
 Serial Number B096961016
 Measurement Date 5/3/2021 5:27 PM
 Light Source Standard
 Detector TGS
 Accumulation 8
 Resolution 4 cm-1
 Zero Filling On
 Apodization Cosine
 Gain Auto (4)
 Aperture Auto (7.1 mm)
 Scanning Speed Auto (2 mm/sec)
 Filter Auto (30000 Hz)

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
1	3445.21	19.7408	2	3005.52	14.1668

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
3	2986.23	12.4228	4	2975.62	11.6685
5	2935.13	11.6297	6	2903.31	13.8028
7	2882.09	12.2527	8	2866.67	13.7305
9	2830.03	17.1978	10	2800.13	19.6884
11	2775.06	18.8241	12	1475.28	20.02
13	1454.06	21.3693	14	1426.1	25.4487
15	1364.39	17.5799	16	1355.71	17.6991
17	1313.29	2.71494	18	1210.11	20.9324
19	1133.94	5.33361	20	1118.51	3.10737
21	1076.08	19.0231	22	1050.05	23.0105
23	1037.52	23.3326	24	1018.23	24.9893
25	967.126	19.2327	26	745.352	19.6099

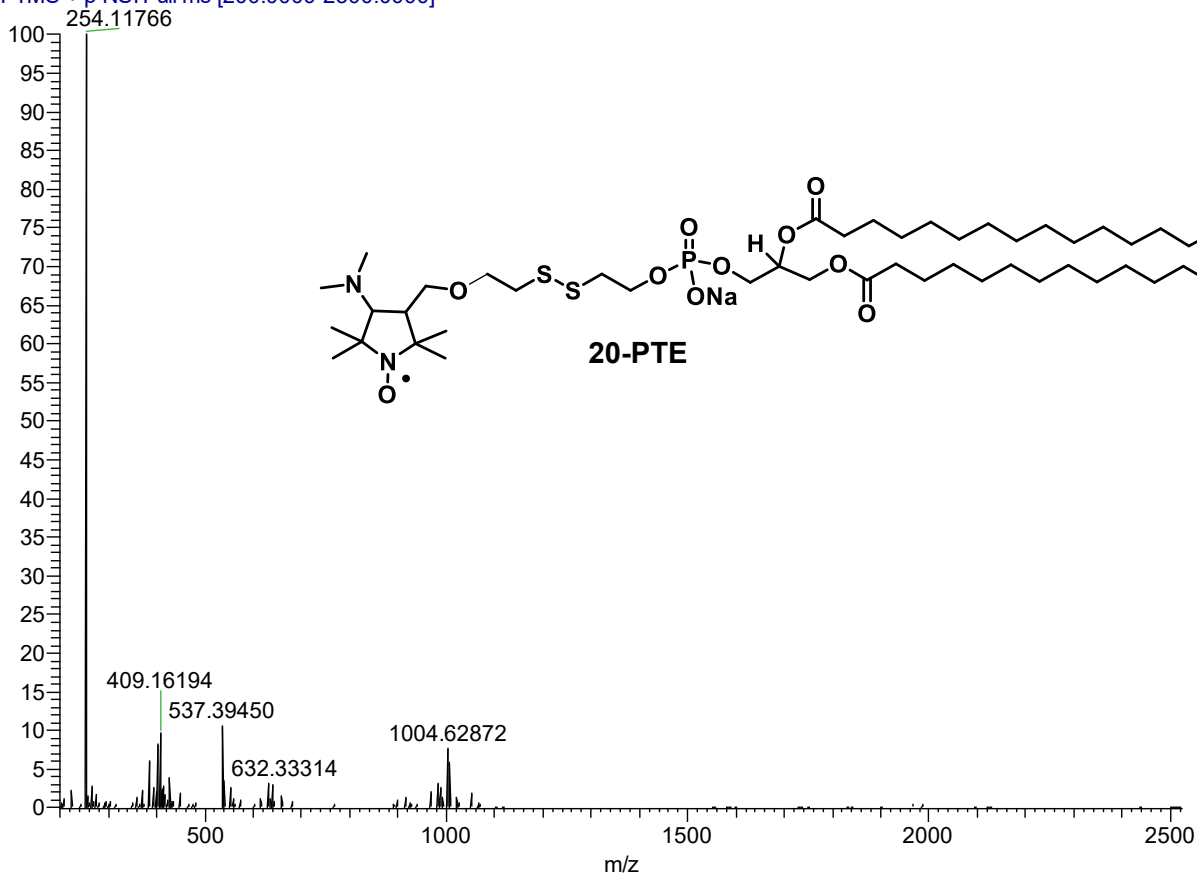
High resolution mass spectrometry and infrared spectroscopy data for spin-labeled 1,2-dipalmitoyl-*sn*-glycero-3-phosphothioethanol (**20-PTE**)

Full Scan Positive Ion Mode:

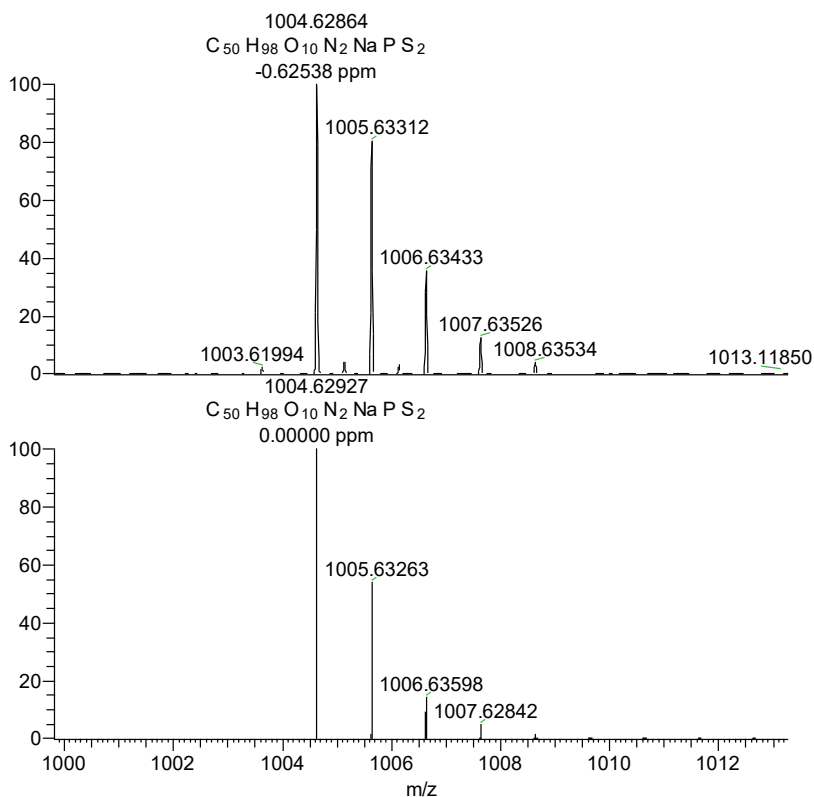
Sample	M _{Theoretical}	M _{Experimental}	ΔM (ppm)	Elemental Composition
	1004.62927 [M+H] ⁺	1004.62864 [M+H] ⁺	-0.62538	C ₅₀ H ₉₈ O ₁₀ N ₂ NaPS ₂
	1026.61122 [M+Na] ⁺	1026.61118 [M+Na] ⁺	-0.03024	C ₅₀ H ₉₇ O ₁₀ N ₂ Na ₂ PS ₂

2015_MAV-820_20221003134024 #142-285 RT: 0.74-1.48 AV: 144 NL: 1.21E9

T: FTMS + p NSI Full ms [200.0000-2500.0000]



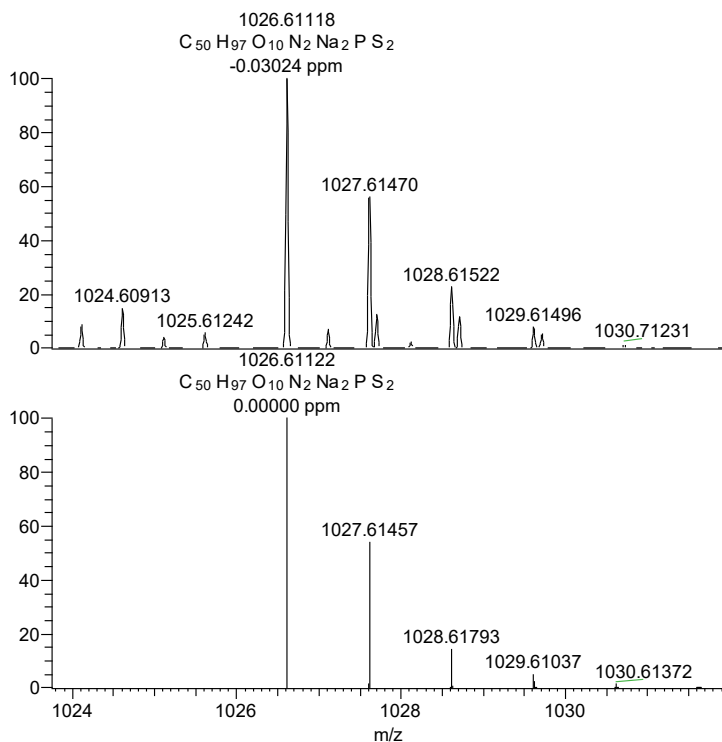
Experimental and Theoretical Isotopic Distribution [M+H]⁺



NL:
6.47E7
2015_MAV-
820_20221003134024#3-
385 RT: 0.03-2.00 AV: 383
T: FTMS + p NSI Full ms
[200.0000-2500.0000]

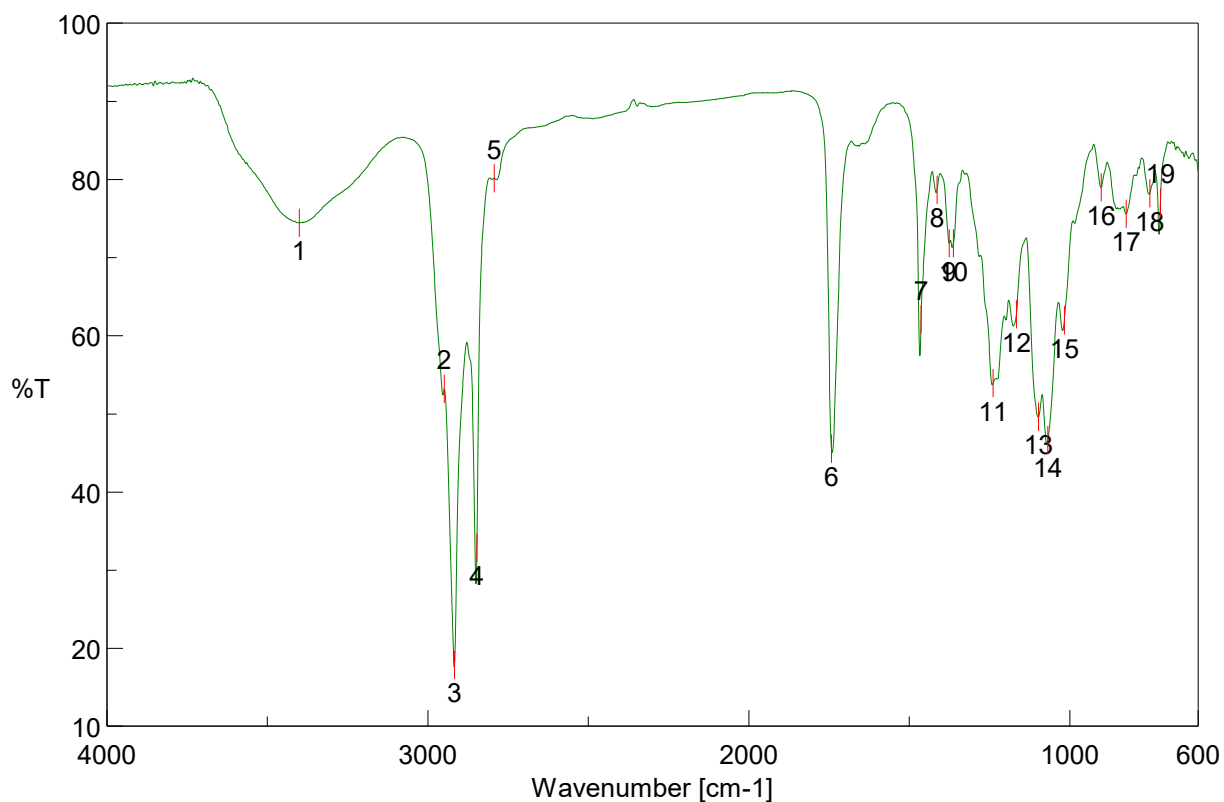
NL:
5.04E5
C₅₀H₉₇N₂NaO₁₀PS₂+H:
C₅₀H₉₈N₂Na₁O₁₀P₁S₂
pa Chrg 1

Experimental and Theoretical Isotopic Distribution [M+Na]⁺



NL:
9.46E6
2015_MAV-
820_20221003134024#3-385
RT: 0.03-2.00 AV: 383 T:
FTMS + p NSI Full ms
[200.0000-2500.0000]

NL:
5.04E5
C₅₀H₉₇N₂NaO₁₀PS₂+Na:
C₅₀H₉₇N₂Na₂O₁₀P₁S₂
pa Chrg 1



[Comments]

Sample name
 Comment
 User
 Division
 Company NCSU

[Detailed Information]

Creation date 9/26/2022 7:07 PM
 Data array type Linear data array
 Horizontal axis Wavenumber [cm-1]
 Vertical axis %T
 Start 0 cm-1
 End 7800.65 cm-1
 Data interval 0.964233 cm-1
 Data points 8091

[Measurement Information]

Model Name FT/IR-4100typeA
 Serial Number B096961016
 Measurement Date 9/26/2022 7:07 PM
 Light Source Standard
 Detector TGS
 Accumulation 8
 Resolution 4 cm-1
 Zero Filling On
 Apodization Cosine
 Gain Auto (2)
 Aperture Auto (7.1 mm)
 Scanning Speed Auto (2 mm/sec)
 Filter Auto (30000 Hz)

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
1	3400.85	74.4349	2	2948.63	53.1614

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
3	2916.81	17.8431	4	2847.38	32.8334
5	2793.38	80.1263	6	1742.37	45.5065
7	1463.71	62.0918	8	1413.57	78.6566
9	1375.96	71.8064	10	1362.46	71.831
11	1239.04	53.9045	12	1166.72	62.74
13	1097.3	49.5932	14	1068.37	46.6213
15	1017.27	61.9442	16	902.523	78.9726
17	824.42	75.5977	18	750.174	78.1889
19	717.39	77.0028			

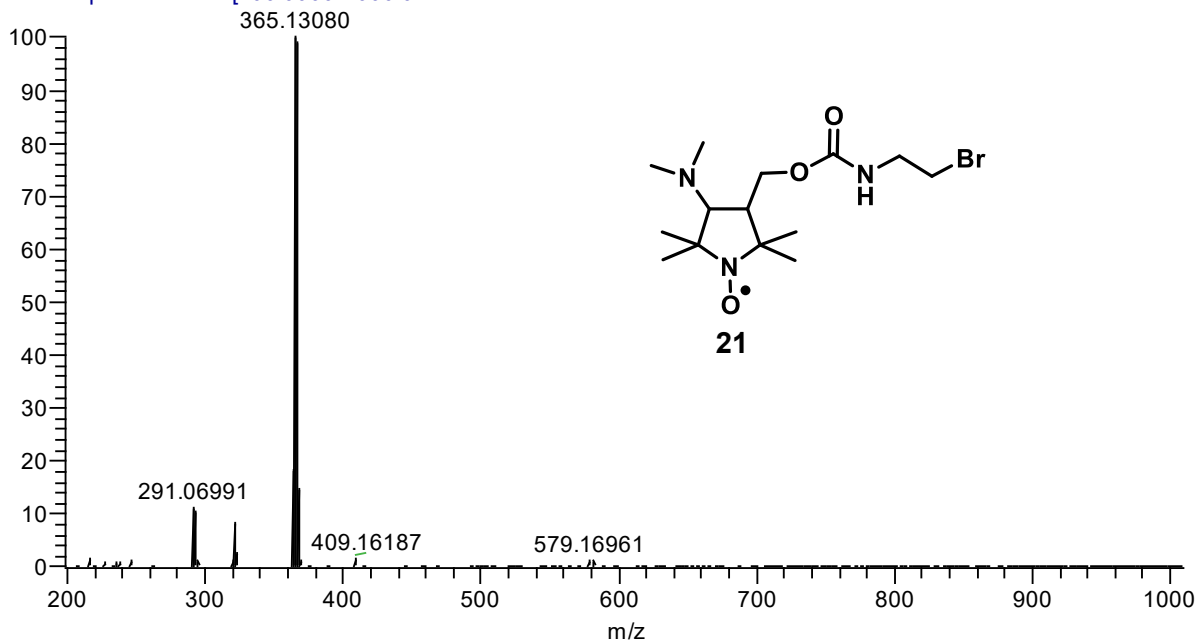
High resolution mass spectrometry and infrared spectroscopy data for (2-Bromoethyl)carbamic acid (4-dimethylamino-1-oxyl-2,2,5,5-tetramethylpyrrolidin-3-yl)methyl ester **21**

Full Scan Positive Ion Mode

365.13086 [M+H]⁺ 365.13080 [M+H]⁺ -0.162 C₁₄H₂₇BrN₃O₃

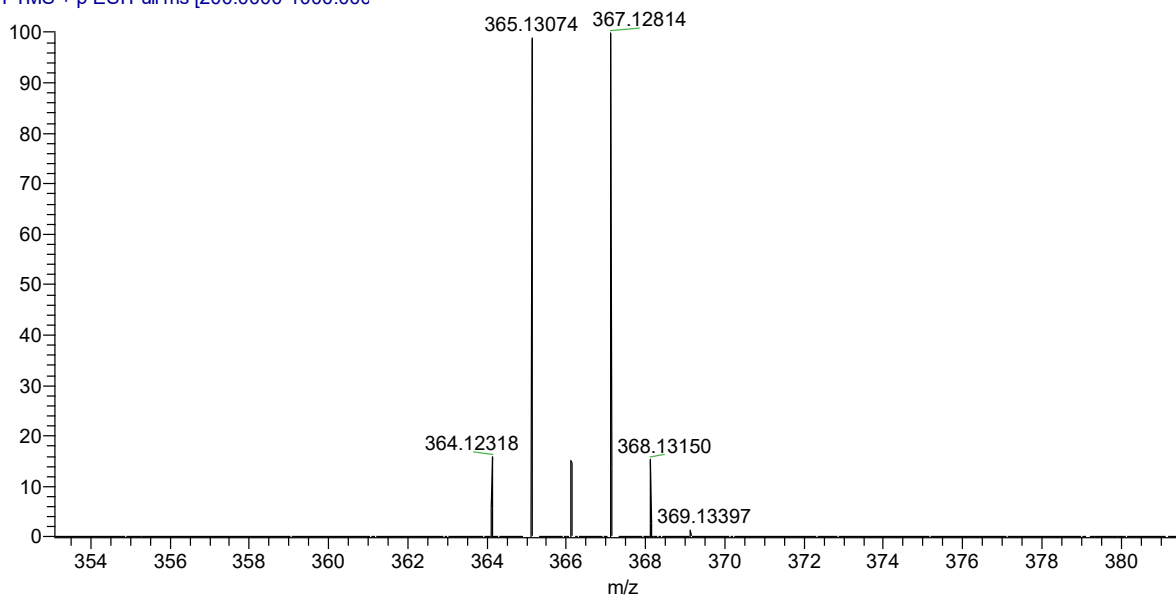
200088_MAV-760 #48-58 RT: 0.34-0.39 AV: 11 NI: 1 82F8

T: FTMS + p ESI Full ms [200.0000-1000.C

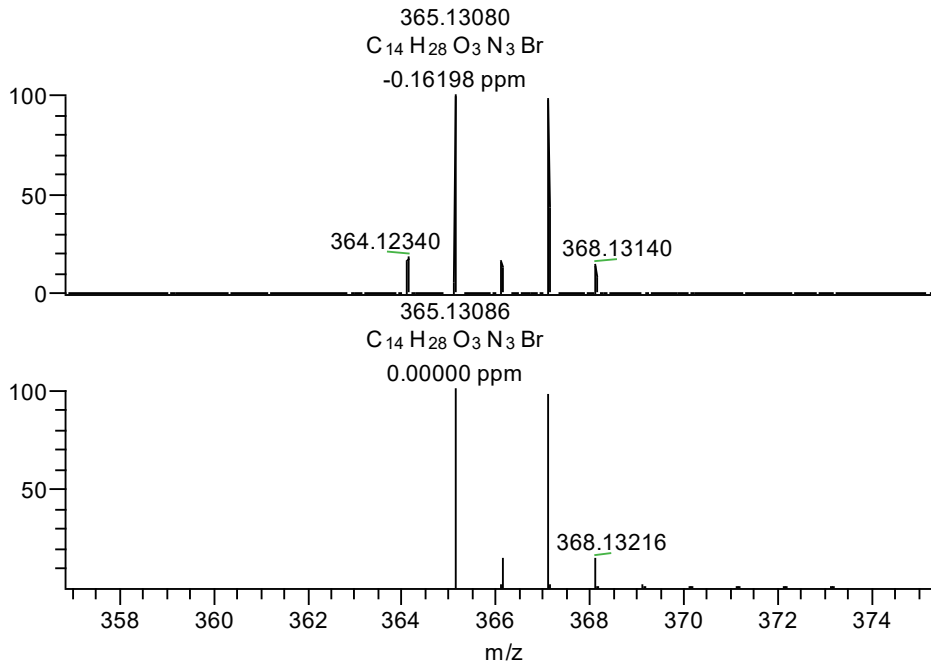


200088_MAV-760 #46-52 RT: 0.33-0.36 AV: 7 NL: 2.49E8

T: FTMS + p ESI Full ms [200.0000-1000.000

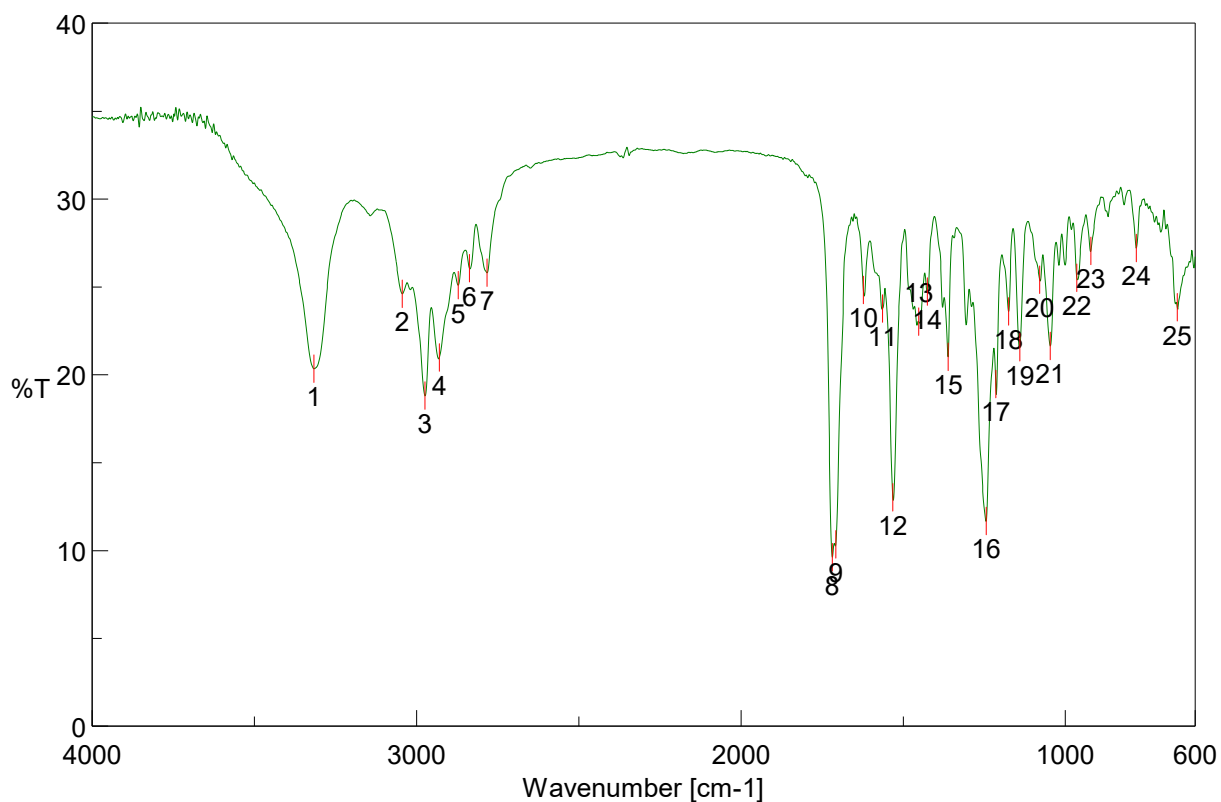


Experimental and Theoretical Isotopic Distribution $C_{14}H_{27}BrN_3O_3 [M+H]^+$



NL:
1.82E8
200088_MAV-760#48-
58 RT: 0.34-0.39 AV:
11 T: FTMS + p ESI Full
ms
[200.0000-1000.0000]

NL:
4.27E5
 $C_{14}H_{27}BrN_3O_3 + H$:
 $C_{14}H_{28}BrN_3O_3$
pa Chrg 1



[Comments]

Sample name
 Comment
 User
 Division
 Company NCSU

[Detailed Information]

Creation date 10/11/2022 2:06 PM
 Data array type Linear data array
 Horizontal axis Wavenumber [cm-1]
 Vertical axis %T
 Start 0 cm-1
 End 7800.65 cm-1
 Data interval 0.964233 cm-1
 Data points 8091

[Measurement Information]

Model Name FT/IR-4100typeA
 Serial Number B096961016
 Measurement Date 10/11/2022 2:05 PM
 Light Source Standard
 Detector TGS
 Accumulation 8
 Resolution 4 cm-1
 Zero Filling On
 Apodization Cosine
 Gain Auto (4)
 Aperture Auto (7.1 mm)
 Scanning Speed Auto (2 mm/sec)
 Filter Auto (30000 Hz)

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
1	3316	20.3333	2	3044.09	24.5964

[Result of Peak Picking]

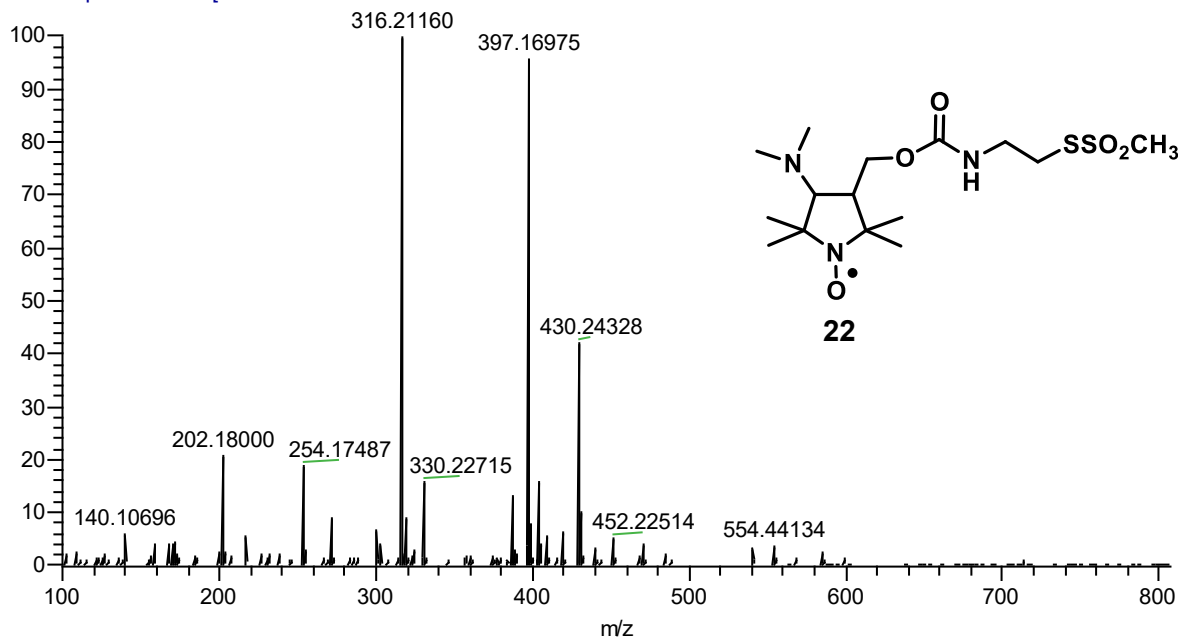
No.	Position	Intensity	No.	Position	Intensity
3	2974.66	18.8008	4	2929.34	20.9828
5	2871.49	25.0804	6	2836.77	26.0503
7	2782.78	25.7923	8	1718.26	9.61838
9	1707.66	10.3379	10	1622.8	24.8163
11	1563.99	23.7571	12	1532.17	13.025
13	1452.14	23.013	14	1425.14	24.7208
15	1361.5	21.0186	16	1243.86	11.664
17	1214.93	19.462	18	1175.4	23.588
19	1140.69	21.5649	20	1078.98	25.407
21	1047.16	21.6272	22	965.198	25.4993
23	921.807	27.0407	24	781.029	27.1928
25	655.679	23.8309			

High resolution mass spectrometry and infrared spectroscopy data for (2-((methylsulfonyl)thio)ethyl)carbamic acid (4-(dimethylamino)-1-oxyl-2,2,5,5-tetramethylpyrrolidin-3-yl)methyl ester **22**

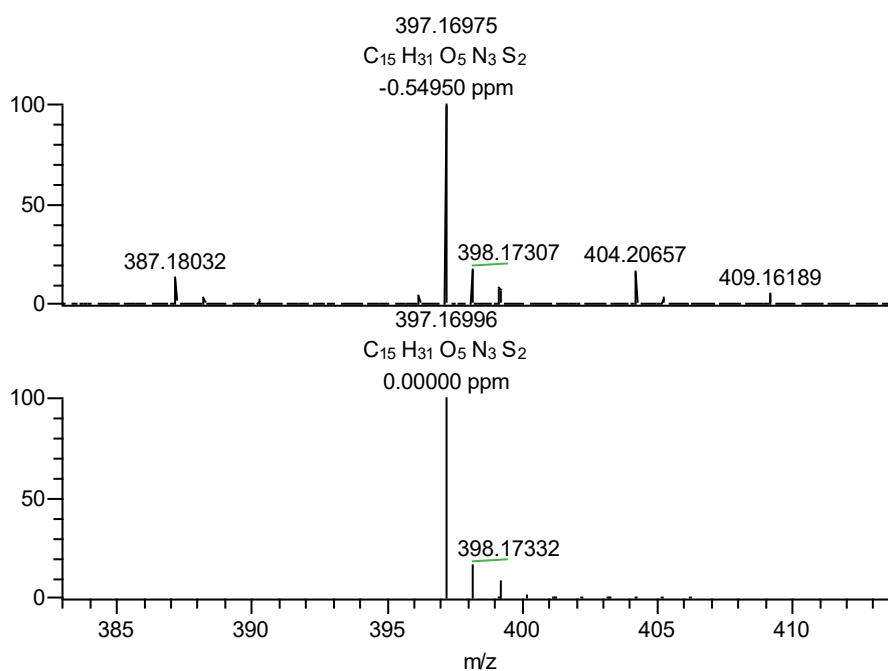
Sample	M _{Theoretical}	M _{Experimental}	ΔM (ppm)	Elemental Composition
	397.16996	397.16975	-0.550	C ₁₅ H ₃₀ N ₃ O ₅ S ₂
	[M+H] ⁺	[M+H] ⁺		

201610_MAV-763 #47-72 RT: 0.27-0.40 AV: 26 SB: 34 0.00-0.19 NL: 1.07E8

T: FTMS + p ESI Full ms [100.0000-800.0000]

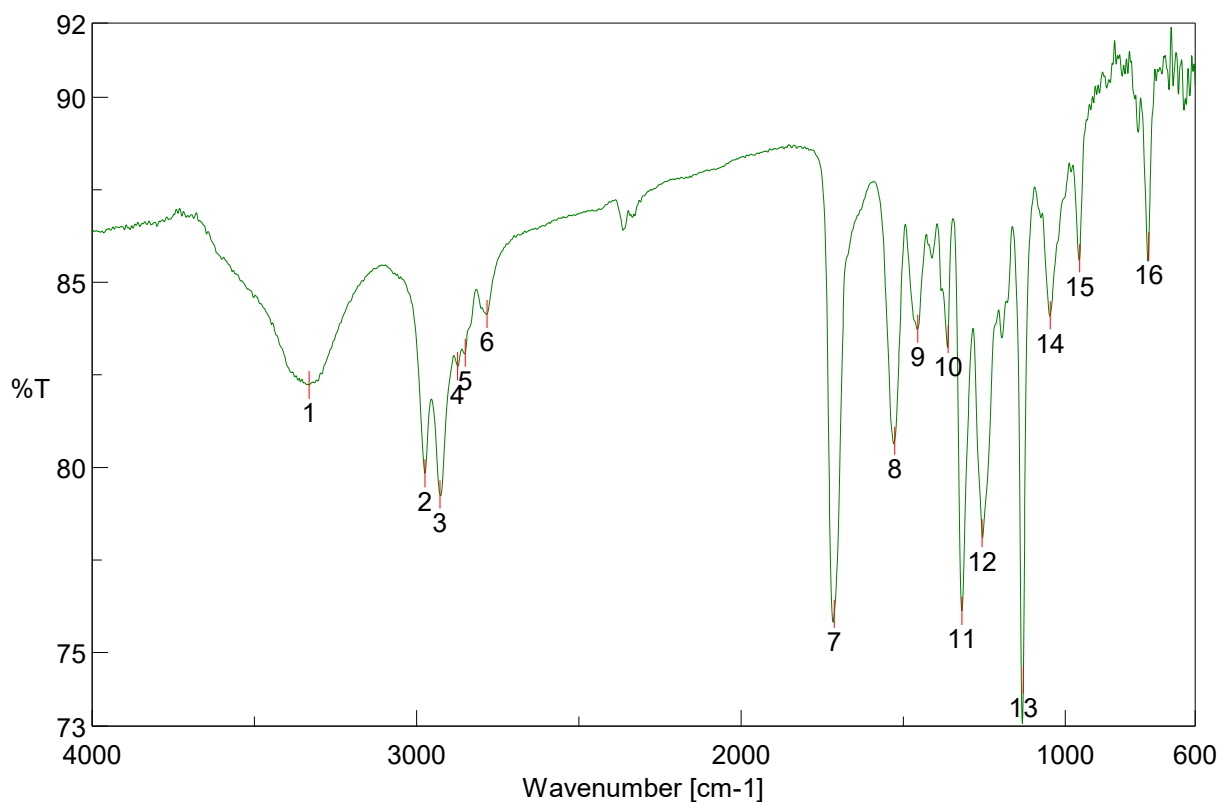


Experimental and Theoretical Isotopic Distribution for C₁₅H₃₀N₃O₅S₂ [M+H]⁺



NL:
 1.03E8
 201610_MAV-763#47-72
 RT: 0.27-0.40 AV: 26 SB:
 34 0.00-0.19 T: FTMS + p
 ESI Full ms
 [100.0000-800.0000]

NL:
 7.47E5
 C₁₅H₃₀N₃O₅S₂ +H:
 C₁₅H₃₁N₃O₅S₂
 pa Chrg 1



[Comments]

Sample name
 Comment
 User
 Division
 Company NCSU

[Detailed Information]

Creation date 10/12/2022 6:22 PM
 Data array type Linear data array
 Horizontal axis Wavenumber [cm-1]
 Vertical axis %T
 Start 0 cm-1
 End 7800.65 cm-1
 Data interval 0.964233 cm-1
 Data points 8091

[Measurement Information]

Model Name FT/IR-4100typeA
 Serial Number B096961016
 Measurement Date 10/12/2022 6:22 PM
 Light Source Standard
 Detector TGS
 Accumulation 8
 Resolution 4 cm-1
 Zero Filling On
 Apodization Cosine
 Gain Auto (2)
 Aperture Auto (7.1 mm)
 Scanning Speed Auto (2 mm/sec)
 Filter Auto (30000 Hz)

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
1	3331.43	82.218	2	2974.66	79.8324

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
3	2927.41	79.2577	4	2873.42	82.7303
5	2850.27	83.0937	6	2782.78	84.1349
7	1712.48	76.0352	8	1526.38	80.7102
9	1455.03	83.7415	10	1361.5	83.4605
11	1319.07	76.1133	12	1257.36	78.214
13	1130.08	74.2629	14	1047.16	84.1031
15	956.52	85.6395	16	743.424	85.9732

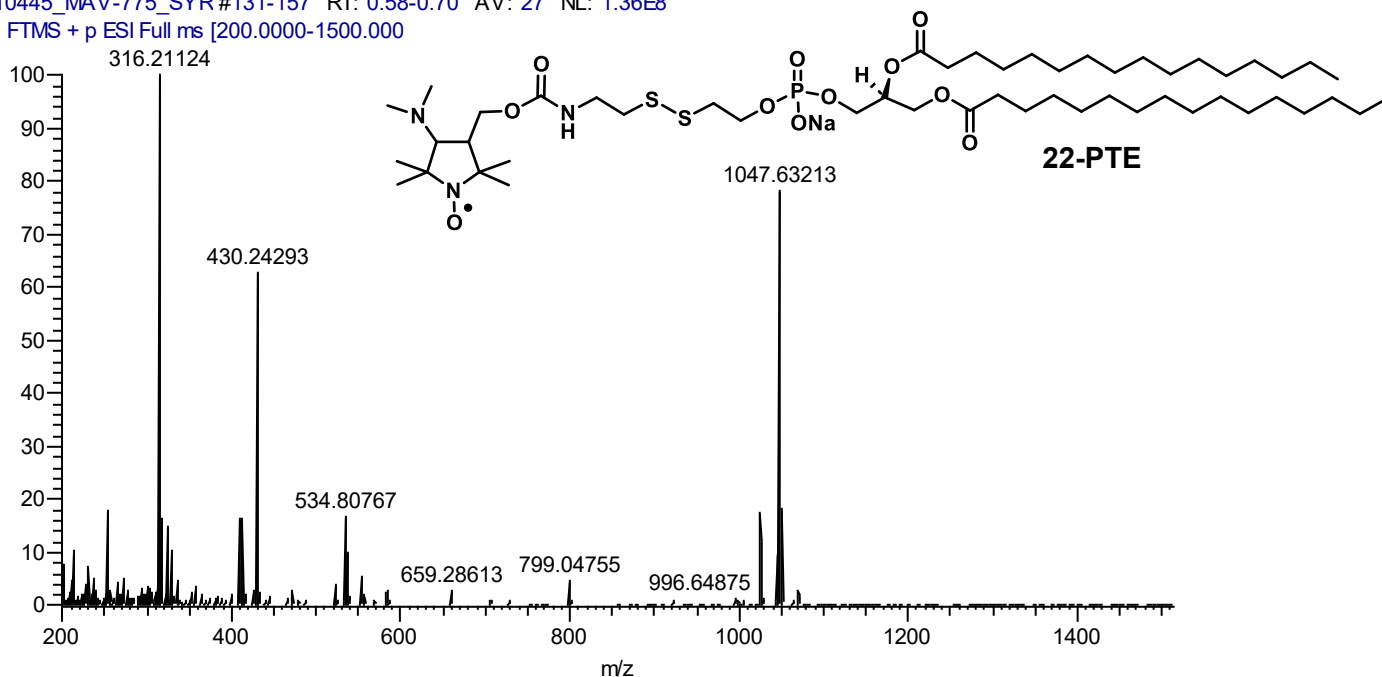
High resolution mass spectrometry and infrared spectroscopy data for spin-labeled 1,2-dipalmitoyl-*sn*-glycero-3-phosphothioethanol (**22-PTE**)

Full Scan Positive Ion Mode

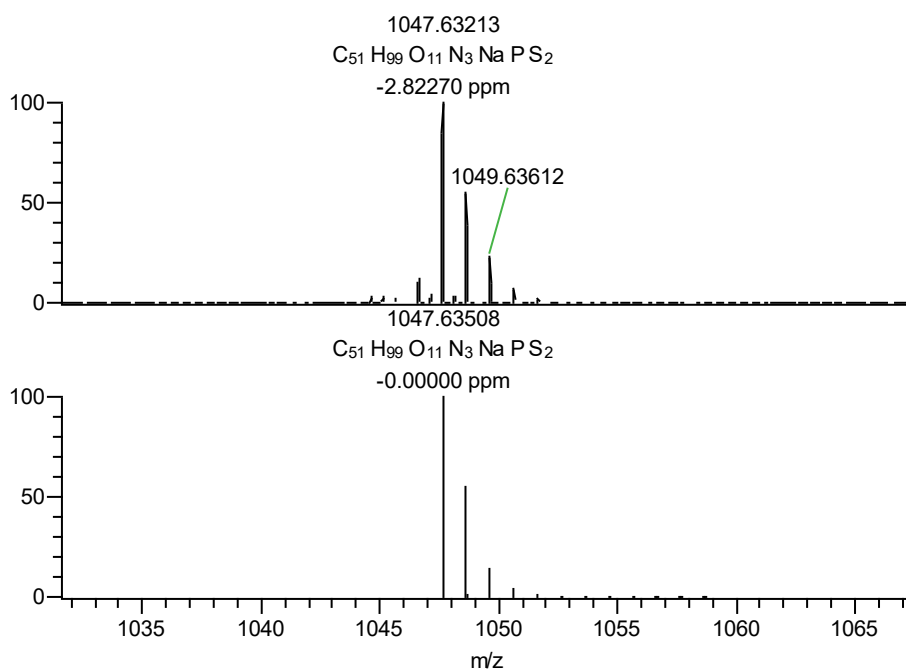
Sample	M _{Theoretical}	M _{Experimental}	ΔM (ppm)	Elemental Composition
	1047.63508	1047.63213	-2.823	C ₅₁ H ₉₈ N ₃ NaO ₁₁ PS ₂
	[M+H] ⁺	[M+H] ⁺		

210445_MAV-775_SYR#131-157 RT: 0.58-0.70 AV: 27 NL: 1.36E8

T: FTMS + p ESI Full ms [200.0000-1500.000]

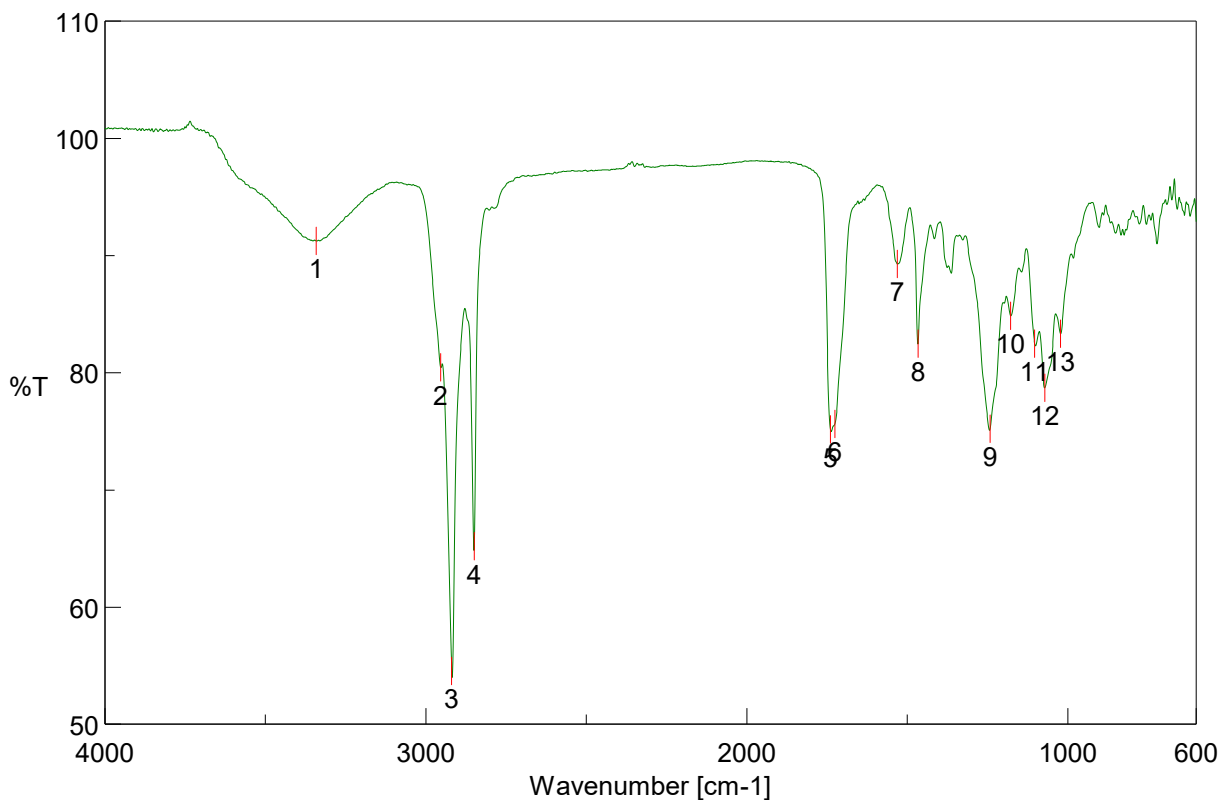


Experimental and Theoretical Isotopic Distribution for C₅₁H₉₈N₃NaO₁₁PS₂ [M+H]⁺



NL:
1.07E8
210445_MAV-
775_SYR#131-157 RT:
0.58-0.70 AV: 27 T: FTMS
+ p ESI Full ms
[200.0000-1500.0000]

NL:
4.96E5
C₅₁H₉₈N₃NaO₁₁PS₂ +H:
C₅₁H₉₉N₃Na₁O₁₁P₁S₂
pa Chrg 1



[Comments]

Sample name
 Comment
 User
 Division
 Company NCSU

[Detailed Information]

Creation date 10/7/2022 4:56 PM
 Date modified 10/7/2022 4:58 PM
 Data array type Linear data array
 Horizontal axis Wavenumber [cm-1]
 Vertical axis %T
 Start 0 cm-1
 End 7800.65 cm-1
 Data interval 0.964233 cm-1
 Data points 8091

[Measurement Information]

Model Name FT/IR-4100typeA
 Serial Number B096961016
 Measurement Date 10/7/2022 4:56 PM
 Light Source Standard
 Detector TGS
 Accumulation 8
 Resolution 4 cm-1
 Zero Filling On
 Apodization Cosine
 Gain Auto (2)
 Aperture Auto (7.1 mm)
 Scanning Speed Auto (2 mm/sec)
 Filter Auto (30000 Hz)

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
1	3342.03	91.2333	2	2954.41	80.4377

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
3	2919.7	54.5241	4	2849.31	65.1899
5	1739.48	75.1469	6	1725.98	75.6222
7	1531.2	89.2798	8	1466.6	82.4726
9	1241.93	75.1994	10	1178.29	84.8485
11	1103.08	82.4722	12	1071.26	78.7106
13	1023.05	83.3303			

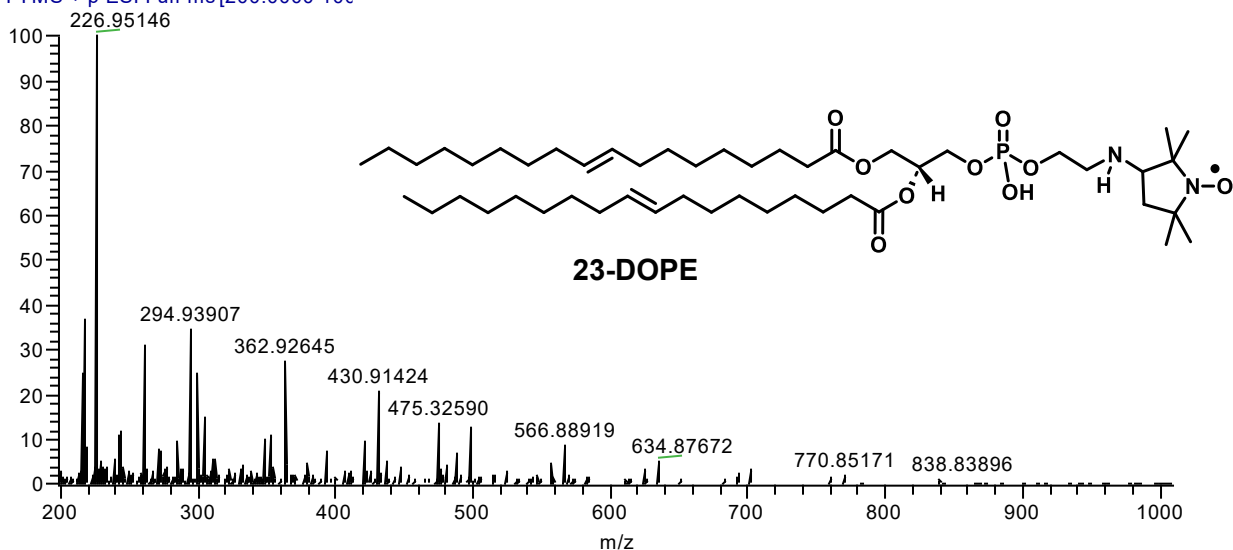
High resolution mass spectrometry and infrared spectroscopy data for spin-labeled 1,2-dioleoyl-*sn*-glycero-3-phosphoethanolamine (**23-DOPE**)

Full Scan Positive Ion Mode

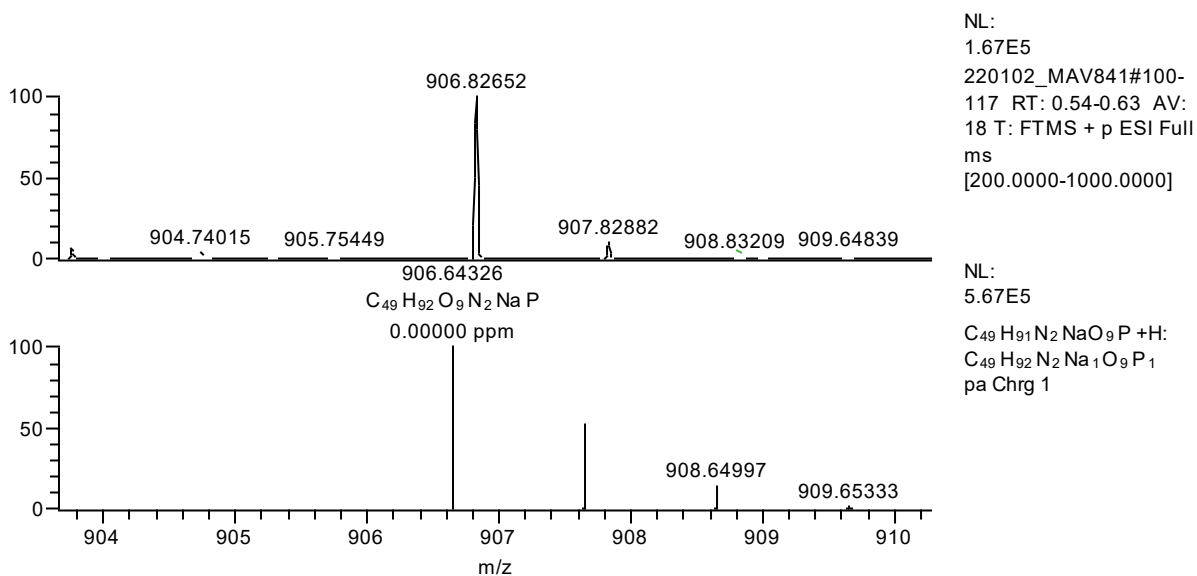
Sample	M _{Theoretical}	M _{Experimental}	ΔM (ppm)	Elemental Composition
	906.64326	-	-	C ₄₉ H ₉₁ N ₂ NaO ₉ P
	[M+H] ⁺	[M+H] ⁺		
	884.66132	-	-	C ₄₉ H ₉₂ N ₂ O ₉ P
	[M+H] ⁺	[M+H] ⁺		

220102_MAV841 #100-117 RT: 0.54-0.63 AV: 18 NL: 2.48E7

T: FTMS + p ESI Full ms [200.0000-1000.0000]

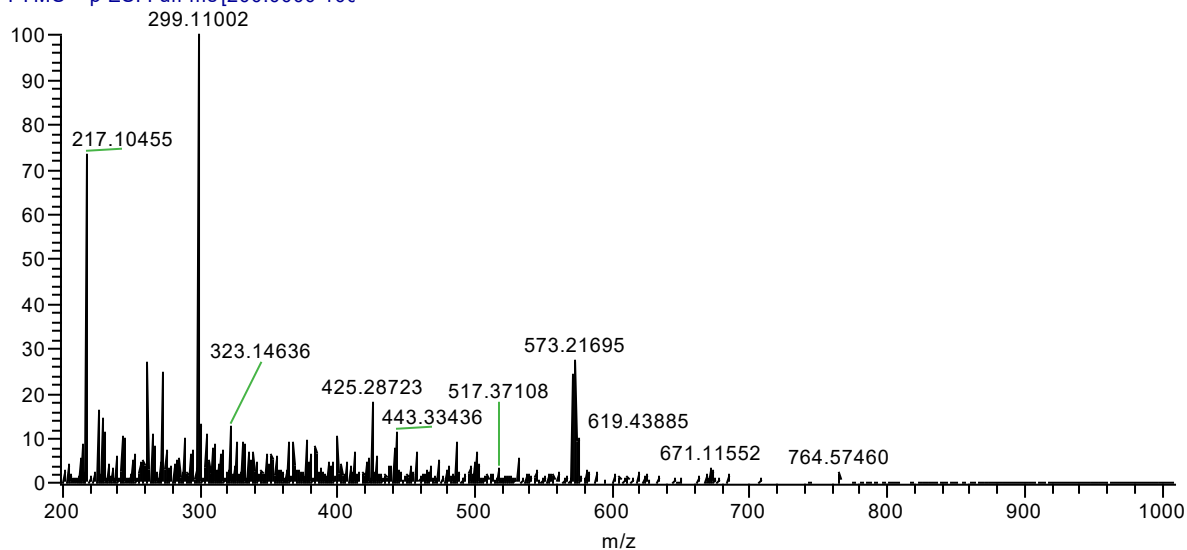


Experimental and Theoretical Isotopic Distribution for C₄₉H₉₁N₂NaO₉P [M+H]⁺

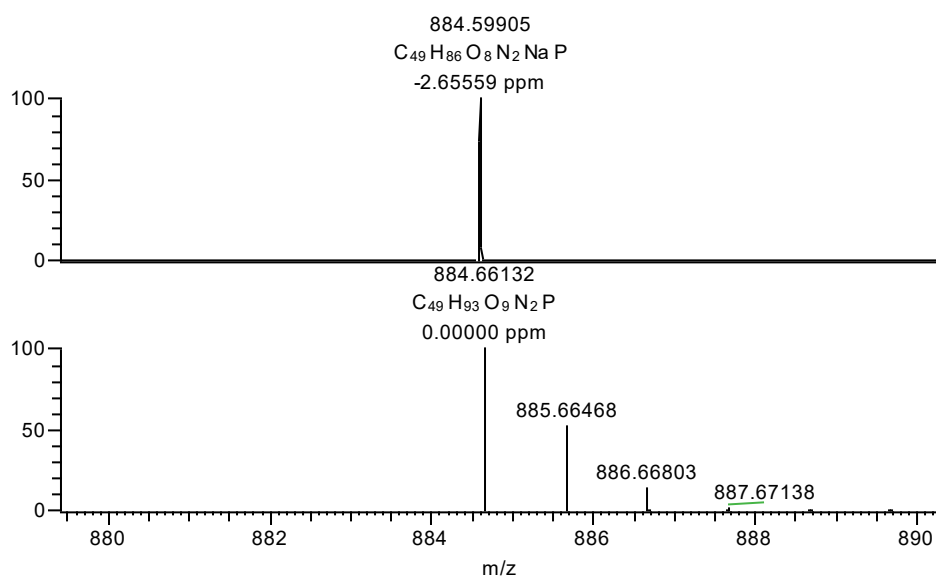


Full Scan Positive Ion Mode

220102_MAV841 #214-218 RT: 1.16-1.18 AV: 5 NL: 2.36E3
T: FTMS + p ESI Full ms [200.0000-1000.0000]

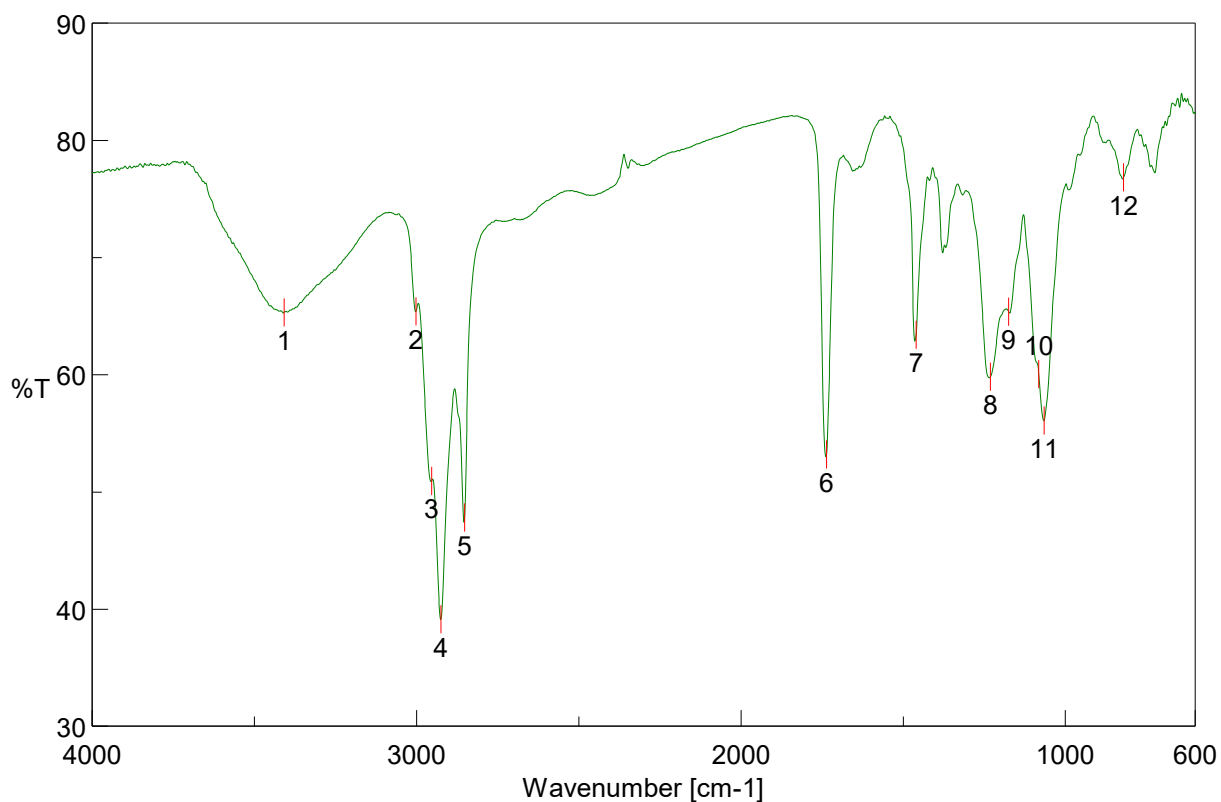


Experimental and Theoretical Isotopic Distribution for $C_{49}H_{92}N_2O_9P [M+H]^+$



NL:
2.36E3
220102_MAV841#214-
218 RT: 1.16-1.18 AV:
5 T: FTMS + p ESI Full
ms
[200.0000-1000.0000]

NL:
5.67E5
 $C_{49}H_{92}N_2O_9P + H$:
 $C_{49}H_{93}N_2O_9P_1$
pa Chrg 1



[Comments]

Sample name
 Comment
 User
 Division
 Company NCSU

[Detailed Information]

Creation date 6/1/2022 6:10 PM
 Data array type Linear data array
 Horizontal axis Wavenumber [cm-1]
 Vertical axis %T
 Start 0 cm-1
 End 7800.65 cm-1
 Data interval 0.964233 cm-1
 Data points 8091

[Measurement Information]

Model Name FT/IR-4100typeA
 Serial Number B096961016
 Measurement Date 6/1/2022 6:10 PM
 Light Source Standard
 Detector TGS
 Accumulation 8
 Resolution 4 cm-1
 Zero Filling On
 Apodization Cosine
 Gain Auto (2)
 Aperture Auto (7.1 mm)
 Scanning Speed Auto (2 mm/sec)
 Filter Auto (30000 Hz)

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
1	3408.57	65.3104	2	3001.66	65.4008

[Result of Peak Picking]

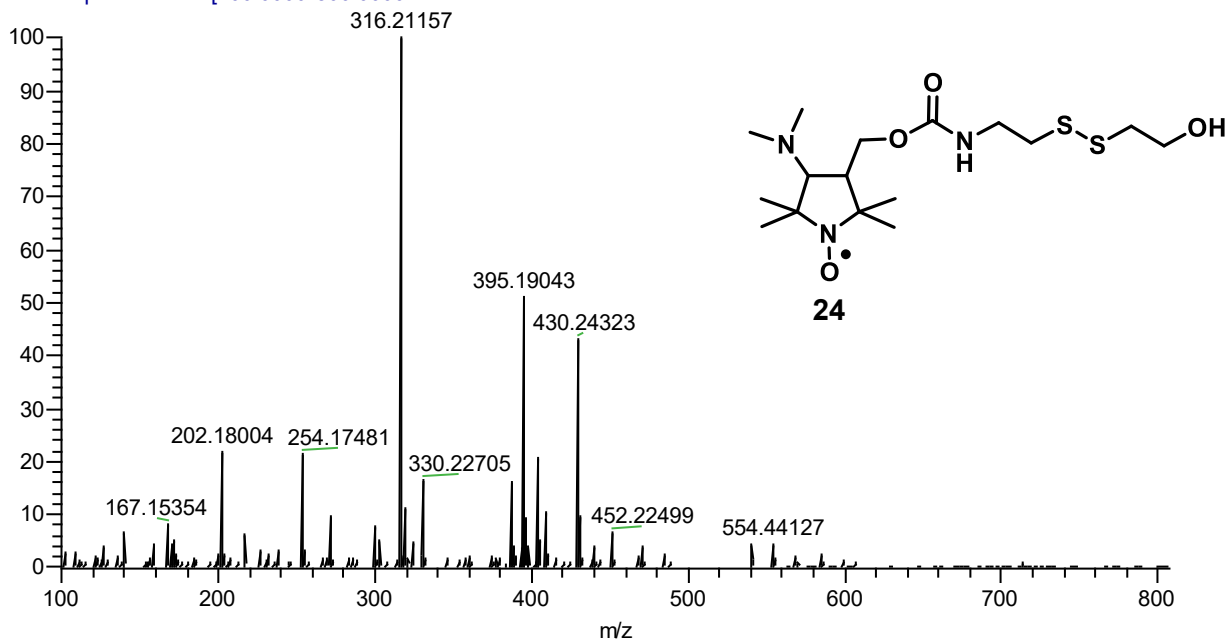
No.	Position	Intensity	No.	Position	Intensity
3	2953.45	50.9282	4	2924.52	39.1205
5	2852.2	47.8108	6	1736.58	53.1892
7	1459.85	63.4135	8	1231.33	59.8106
9	1175.4	65.3799	10	1081.87	60.0277
11	1065.48	56.0753	12	820.563	76.8461

High resolution mass spectrometry and infrared spectroscopy data for (2-((2-hydroxyethyl)-disulfaneyl)ethyl)carbamic acid (4-(dimethylamino)-1-oxyl-2,2,5,5-tetramethylpyrrolidin-3-yl)methyl ester **24**

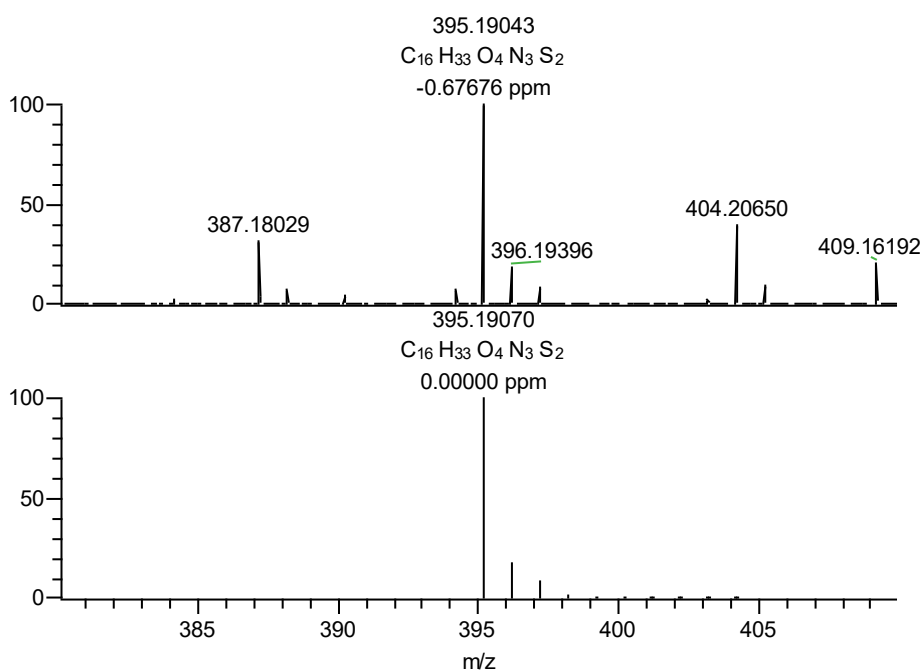
Sample	M _{Theoretical}	M _{Experimental}	ΔM (ppm)	Elemental Composition
	395.19070	395.19043	-0.677	C ₁₆ H ₃₂ N ₃ O ₄ S ₂
	[M+H] ⁺	[M+H] ⁺		

201608_MAV-765 #51-75 RT: 0.28-0.41 AV: 25 SB: 35 0.00-0.20 NL: 1.00E8

T: FTMS + p ESI Full ms [100.0000-800.0000]

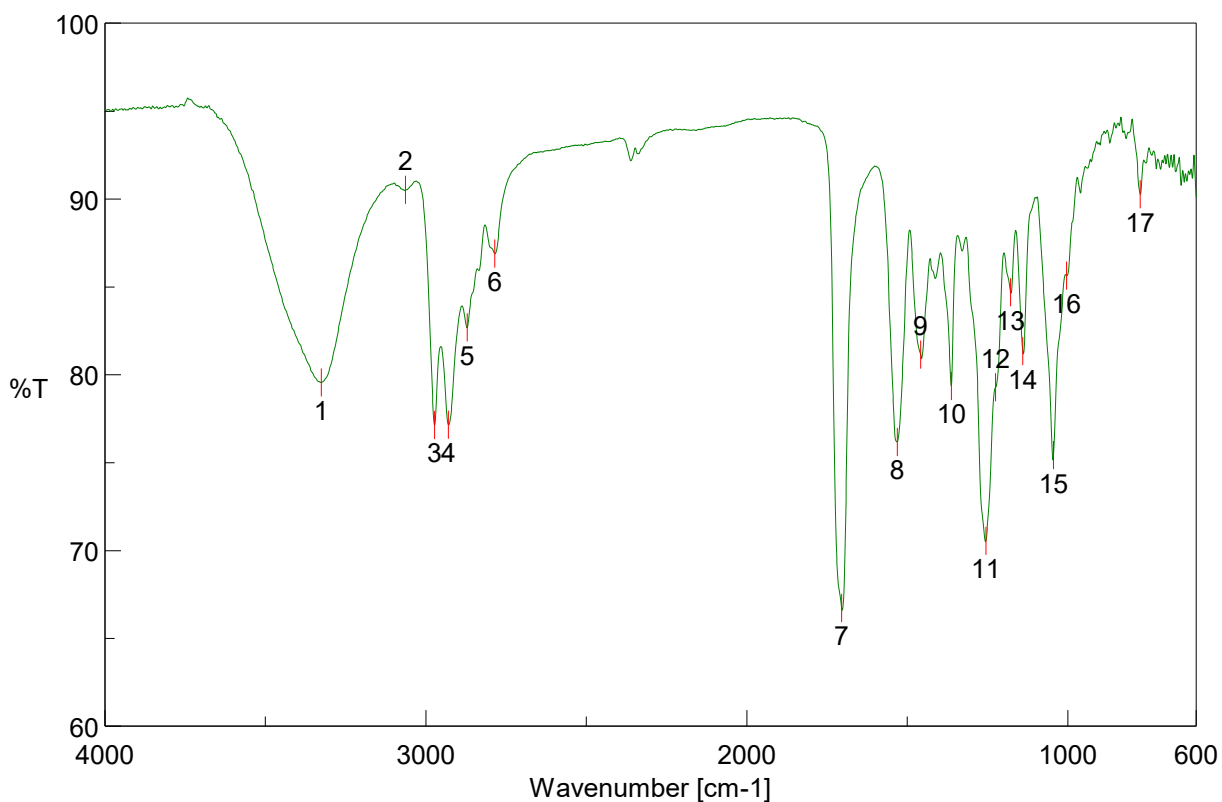


Experimental and Theoretical Isotopic Distribution for C₁₆H₃₂N₃O₄S₂ [M+H]⁺



NL:
5.13E7
201608_MAV-765#51-75
RT: 0.28-0.41 AV: 25 SB:
35 0.00-0.20 T: FTMS + p
ESI Full ms
[100.0000-800.0000]

NL:
7.40E5
C₁₆ H₃₂ N₃ O₄ S₂ +H:
C₁₆ H₃₃ N₃ O₄ S₂
pa Chrg 1



[Comments]

Sample name
 Comment
 User
 Division
 Company NCSU

[Detailed Information]

Creation date 10/11/2022 5:18 PM
 Data array type Linear data array
 Horizontal axis Wavenumber [cm-1]
 Vertical axis %T
 Start 0 cm-1
 End 7800.65 cm-1
 Data interval 0.964233 cm-1
 Data points 8091

[Measurement Information]

Model Name FT/IR-4100typeA
 Serial Number B096961016
 Measurement Date 10/11/2022 5:18 PM
 Light Source Standard
 Detector TGS
 Accumulation 8
 Resolution 4 cm-1
 Zero Filling On
 Apodization Cosine
 Gain Auto (2)
 Aperture Auto (7.1 mm)
 Scanning Speed Auto (2 mm/sec)
 Filter Auto (30000 Hz)

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
1	3325.64	79.5602	2	3063.37	90.5119

[Result of Peak Picking]

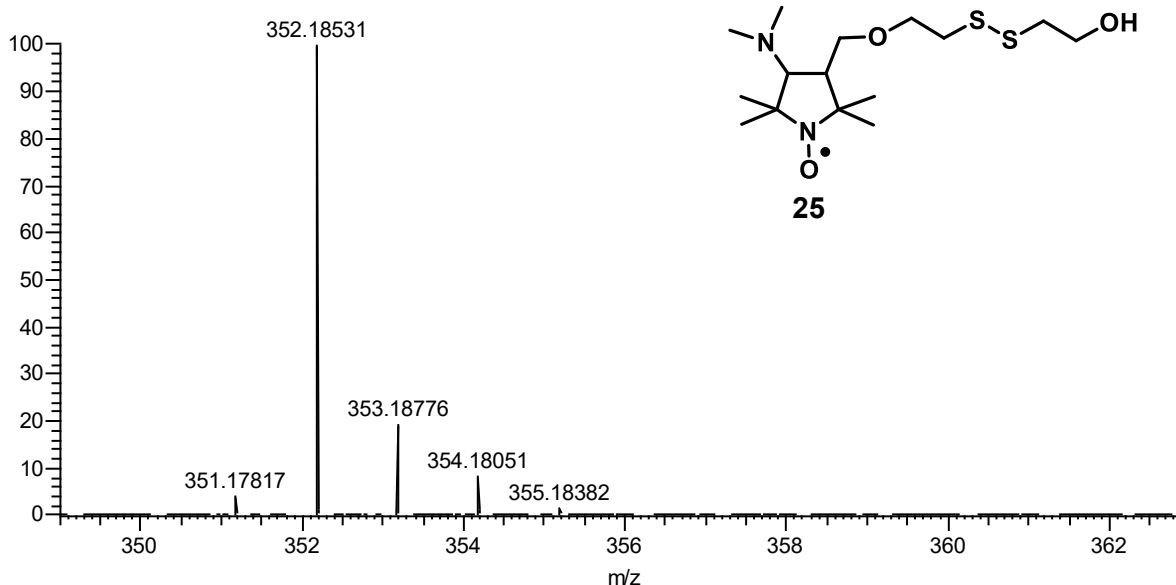
No.	Position	Intensity	No.	Position	Intensity
3	2972.73	77.1282	4	2930.31	77.151
5	2871.49	82.6807	6	2785.67	86.883
7	1704.76	66.7151	8	1531.2	76.1741
9	1458.89	81.1396	10	1362.46	79.3574
11	1255.43	70.5369	12	1225.54	79.2781
13	1178.29	84.6926	14	1140.69	81.3307
15	1044.26	75.4215	16	1003.77	85.6351
17	774.279	90.2606			

High resolution mass spectrometry and infrared spectroscopy data for 3-(dimethylamino)-4-((2-((2-hydroxyethyl)disulfaneyl)ethoxy)methyl)-2,2,5,5-tetramethylpyrrolidin-1-oxyl **25**

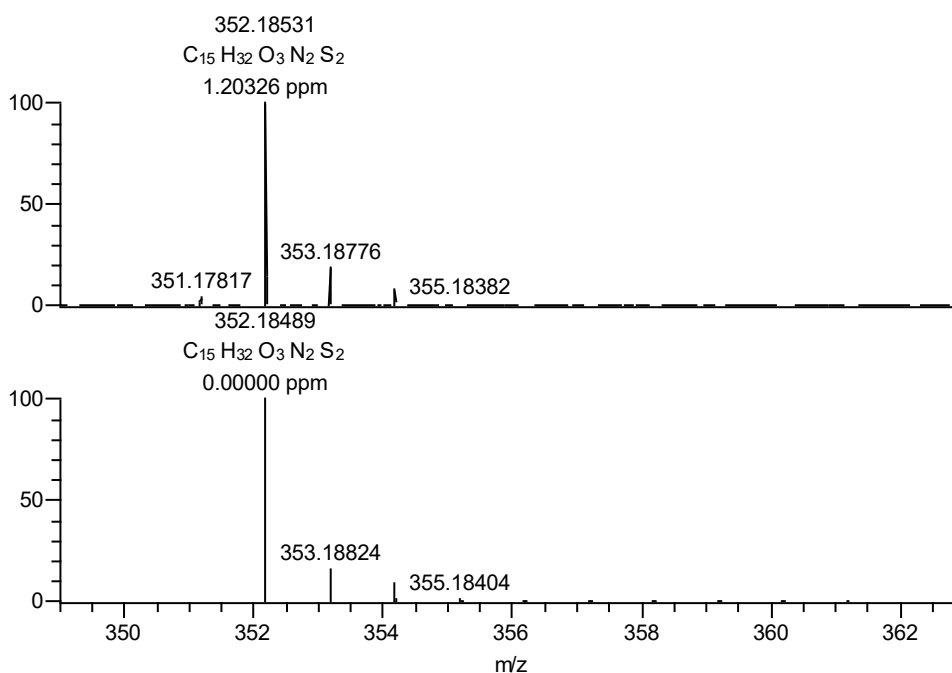
Full Scan Positive Ion Mode

Sample	M _{Theoretical}	M _{Experimental}	ΔM (ppm)	Elemental Composition
	352.18489	352.18531	1.203	C ₁₅ H ₃₁ N ₂ O ₃ S ₂
	[M+H] ⁺	[M+H] ⁺		

202001_MAV-803 #41-74 RT: 0.25-0.43 AV: 34 NL: 3.52E8
T: FTMS + p ESI Full ms [100.0000-800.0000]

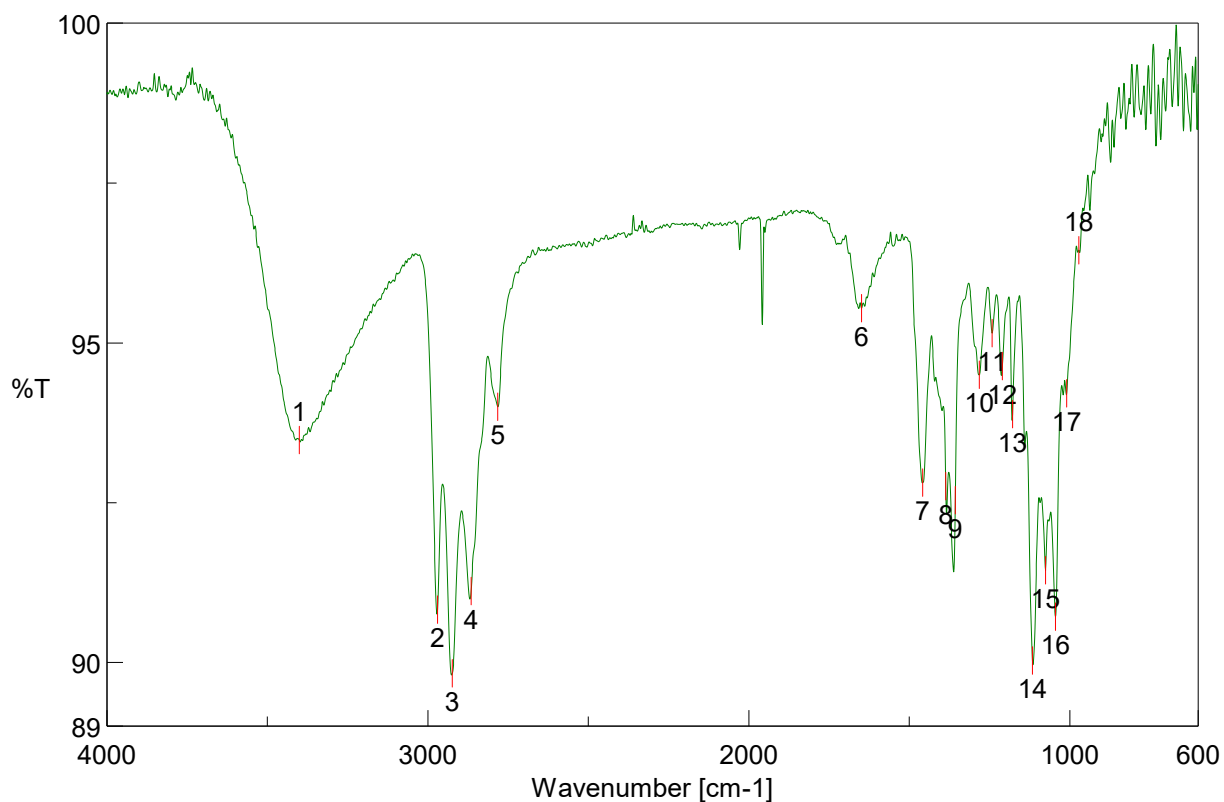


Experimental and Theoretical Isotopic Distribution for C₁₅H₃₁N₂O₃S₂ [M+H]⁺



NL:
3.52E8
202001_MAV-803#41-
74 RT: 0.25-0.43 AV:
34 T: FTMS + p ESI Full
ms
[100.0000-800.0000]

NL:
7.53E5
C₁₅H₃₁N₂O₃S₂ +H:
C₁₅H₃₂N₂O₃S₂
pa Chrg 1



[Comments]

Sample name
 Comment
 User
 Division
 Company NCSU

[Detailed Information]

Creation date 10/11/2022 5:48 PM
 Data array type Linear data array
 Horizontal axis Wavenumber [cm-1]
 Vertical axis %T
 Start 0 cm-1
 End 7800.65 cm-1
 Data interval 0.964233 cm-1
 Data points 8091

[Measurement Information]

Model Name FT/IR-4100typeA
 Serial Number B096961016
 Measurement Date 10/11/2022 5:37 PM
 Light Source Standard
 Detector TGS
 Accumulation 8
 Resolution 4 cm-1
 Zero Filling On
 Apodization Cosine
 Gain Auto (2)
 Aperture Auto (7.1 mm)
 Scanning Speed Auto (2 mm/sec)
 Filter Auto (30000 Hz)

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
1	3400.85	93.4741	2	2969.84	90.8233

[Result of Peak Picking]

No.	Position	Intensity	No.	Position	Intensity
3	2924.52	89.8238	4	2865.7	91.1106
5	2782.78	93.9991	6	1648.84	95.5389
7	1458.89	92.8094	8	1386.57	92.7568
9	1356.68	92.5361	10	1282.43	94.4963
11	1241.93	95.1489	12	1210.11	94.6337
13	1178.29	93.8808	14	1116.58	90.026
15	1076.08	91.4403	16	1044.26	90.7129
17	1009.55	94.2048	18	971.947	96.4464

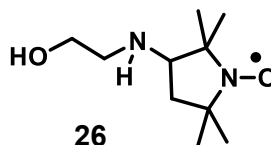
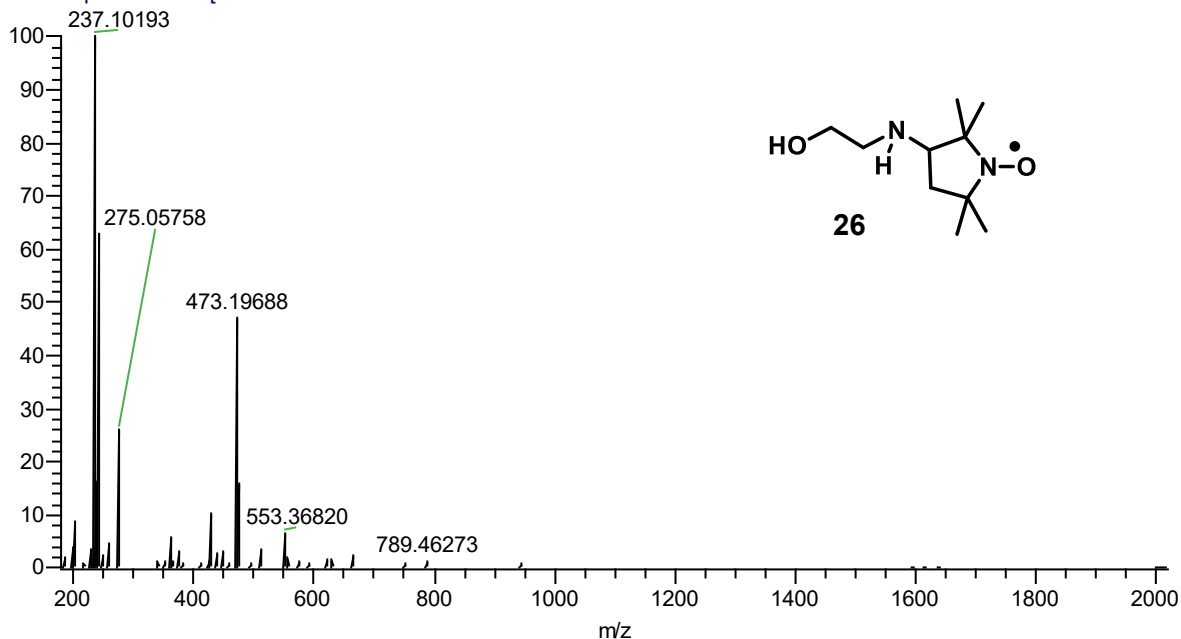
High resolution mass spectrometry and infrared spectroscopy data for 3-(2-Hydroxyethylamino)-1-oxyl-2,2,5,5-tetramethylpyrrolidine **26**

Full Scan Positive Ion Mode

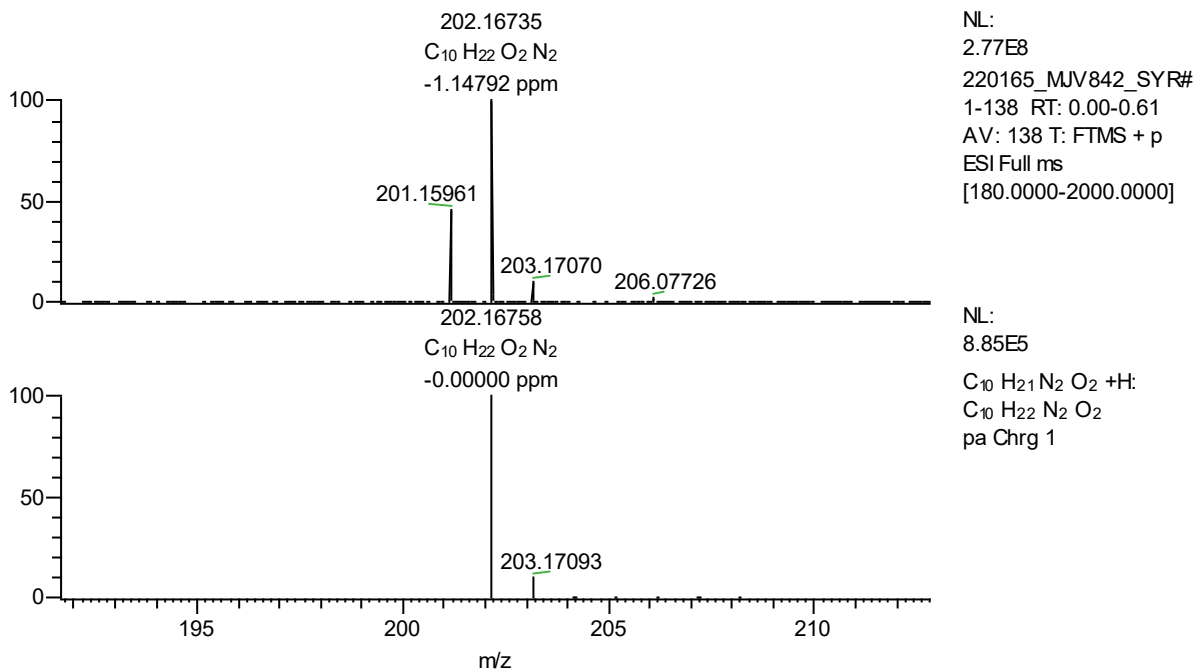
Sample	M _{Theoretical}	M _{Experimental}	ΔM (ppm)	Elemental Composition
	202.16758	202.16735	-1.148	C ₁₀ H ₂₁ N ₂ O ₂
	[M+H] ⁺	[M+H] ⁺		

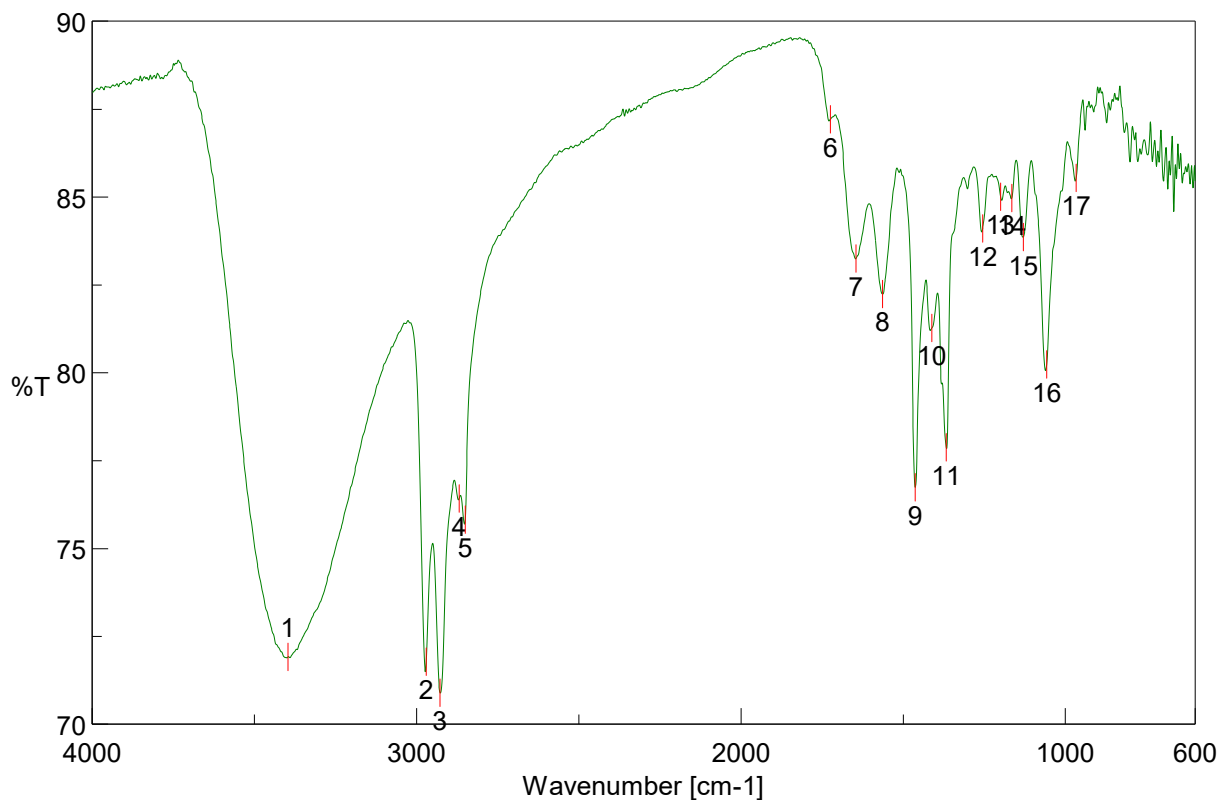
220165_MJV842_SYR#2-139 RT: 0.01-0.62 AV: 138 NL: 3.21E9

T: FTMS + p ESI Full ms [180.0000-2000.000]



Experimental and Theoretical Isotopic Distribution for C₁₀H₂₁N₂O₂ [M+H]⁺





[Comments]

Sample name
 Comment
 User
 Division
 Company NCSU

[Detailed Information]

Creation date 10/13/2022 6:52 PM
 Data array type Linear data array
 Horizontal axis Wavenumber [cm-1]
 Vertical axis %T
 Start 0 cm-1
 End 7800.65 cm-1
 Data interval 0.964233 cm-1
 Data points 8091

[Measurement Information]

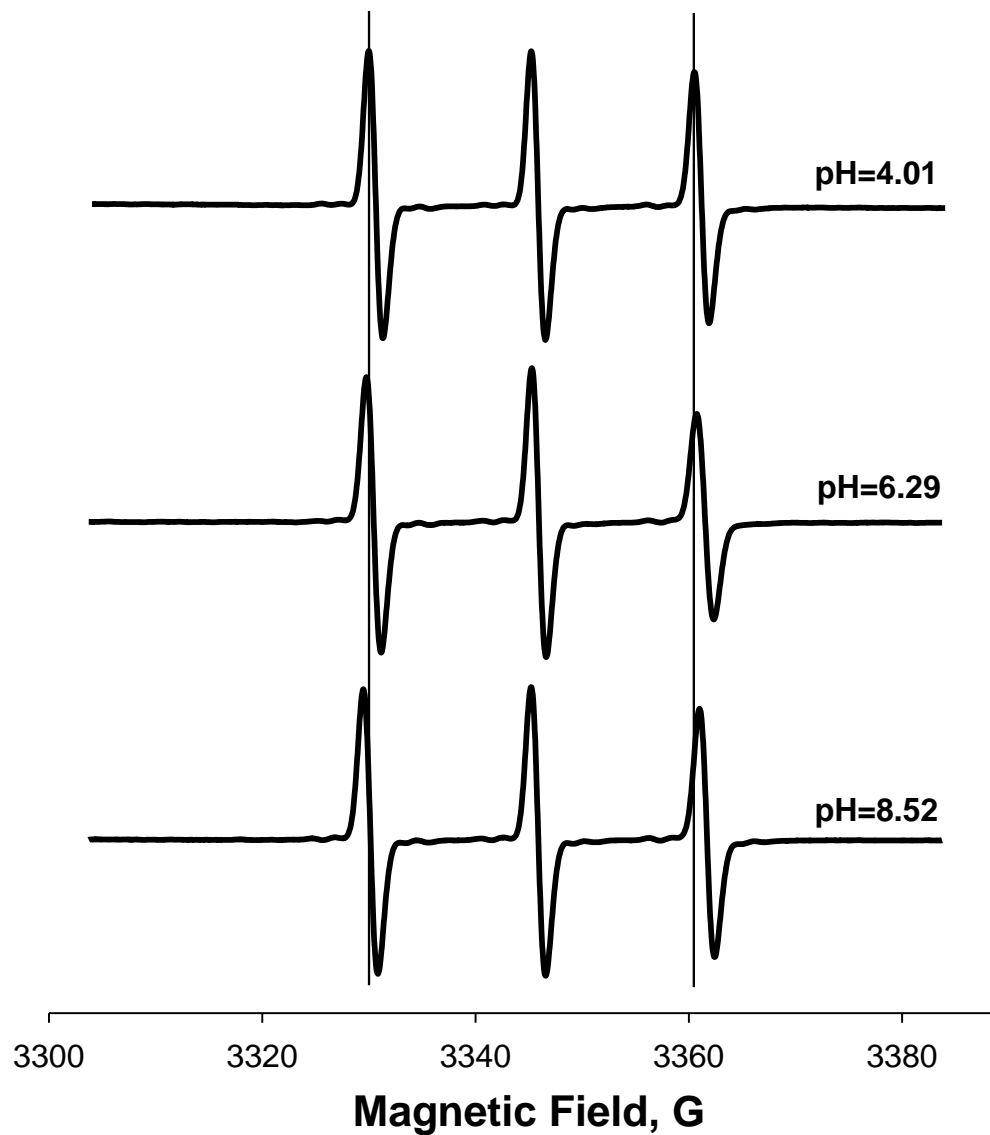
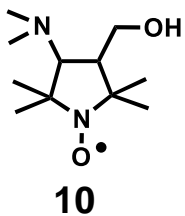
Model Name FT/IR-4100typeA
 Serial Number B096961016
 Measurement Date 10/13/2022 6:52 PM
 Light Source Standard
 Detector TGS
 Accumulation 8
 Resolution 4 cm-1
 Zero Filling On
 Apodization Cosine
 Gain Auto (2)
 Aperture Auto (7.1 mm)
 Scanning Speed Auto (2 mm/sec)
 Filter Auto (30000 Hz)

[Result of Peak Picking]

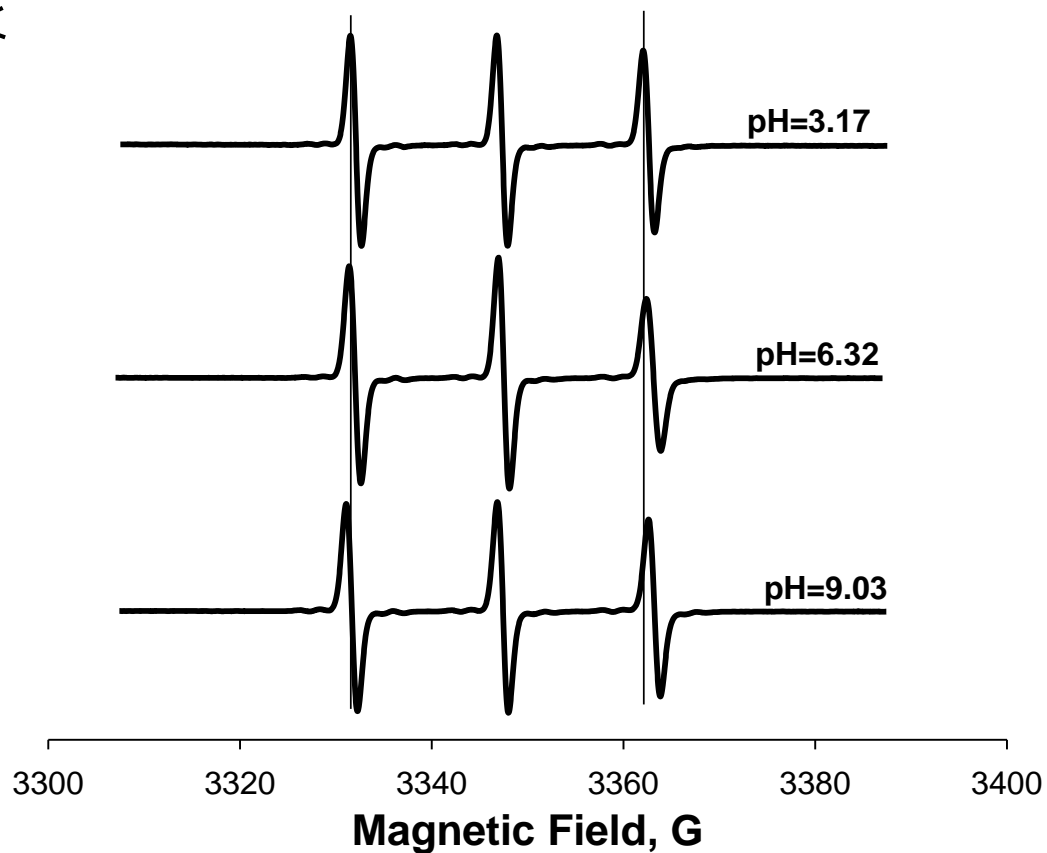
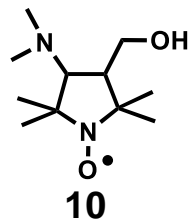
No.	Position	Intensity	No.	Position	Intensity
1	3396.03	71.9117	2	2969.84	71.7716

[Result of Peak Picking]

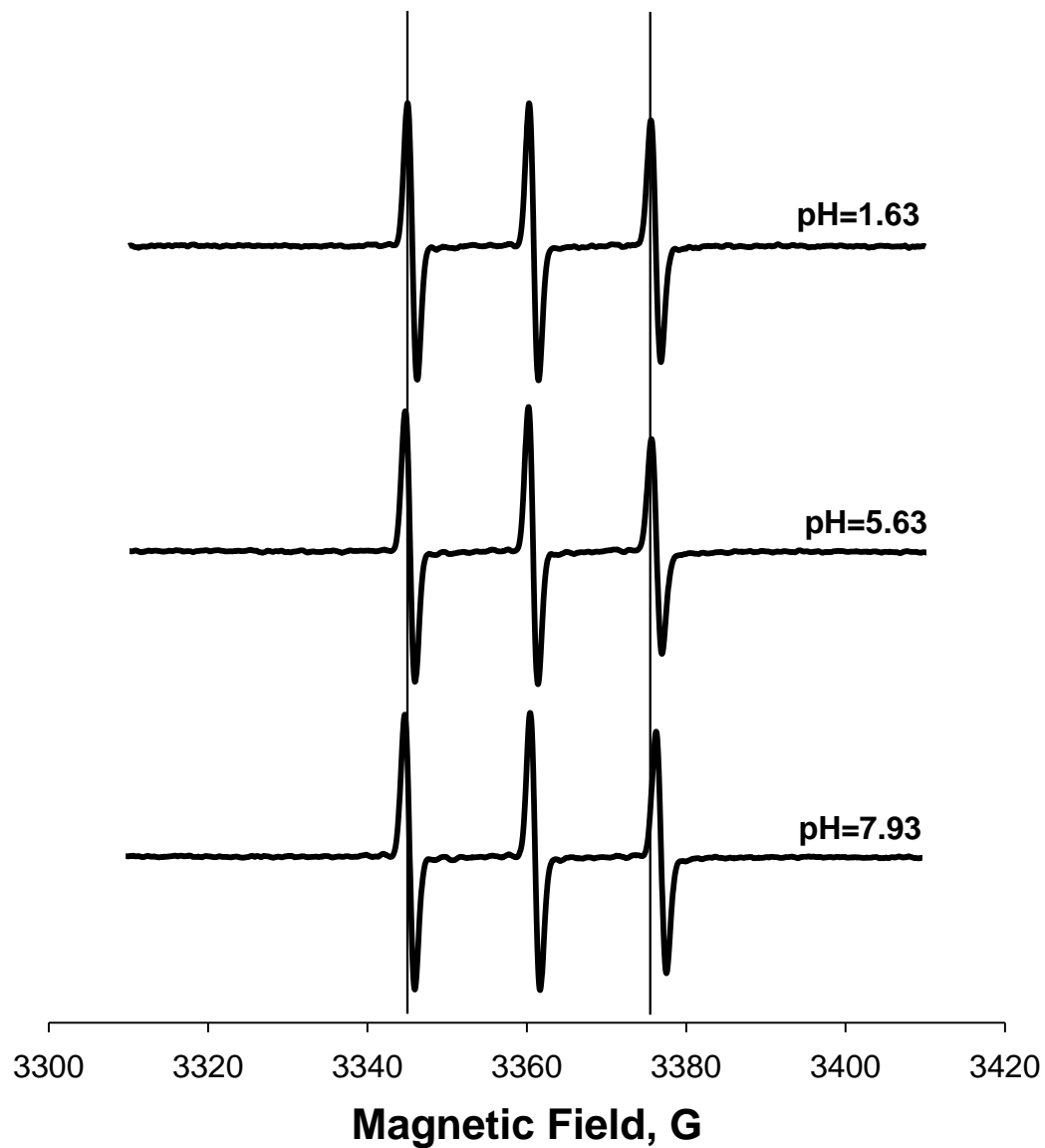
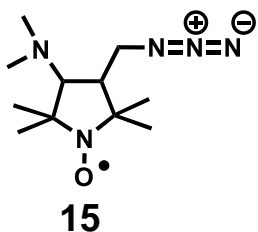
No.	Position	Intensity	No.	Position	Intensity
3	2927.41	70.8953	4	2868.59	76.4173
5	2850.27	75.8207	6	1724.05	87.2067
7	1645.95	83.2434	8	1563.99	82.2379
9	1462.74	76.738	10	1411.64	81.2661
11	1367.28	77.8776	12	1255.43	84.0989
13	1199.51	85.0005	14	1164.79	84.9654
15	1130.08	83.8567	16	1057.76	80.2344
17	967.126	85.5389			



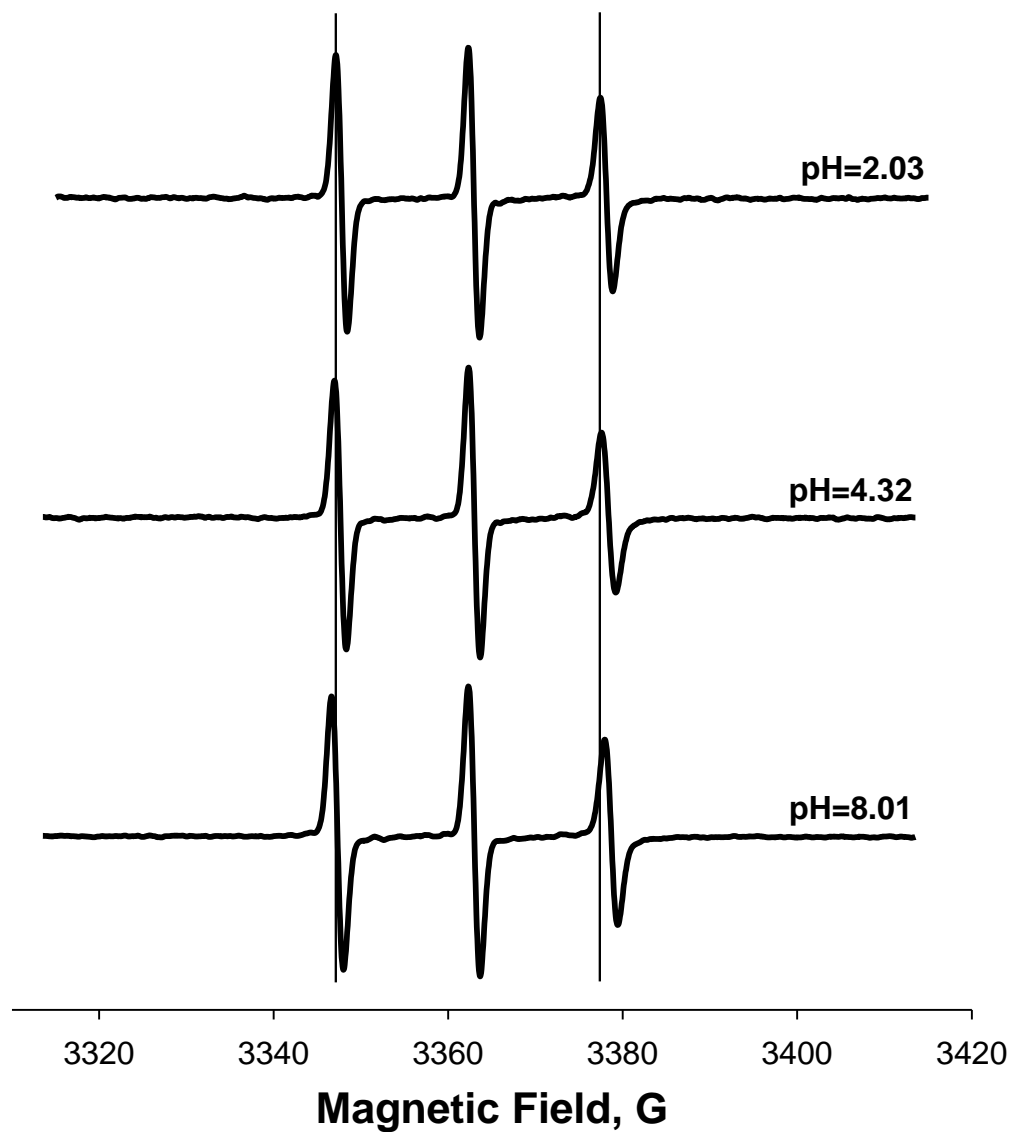
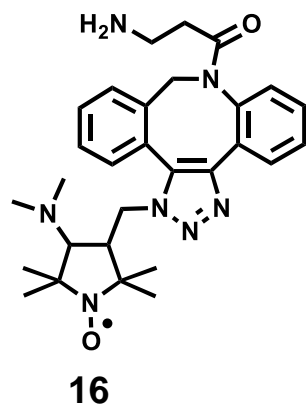
X-band (9.5 GHz) EPR spectra of the nitroxide **10** ($pK_a=6.25\pm 0.01$) in 50 mM phosphate buffer in fully protonated (pH=4.01) and non-protonated (pH=8.52) forms, and at pH=6.29 which is close to the pK_a value. Spectra were recorded at 17 °C. Vertical lines are shown as a guide for an eye.



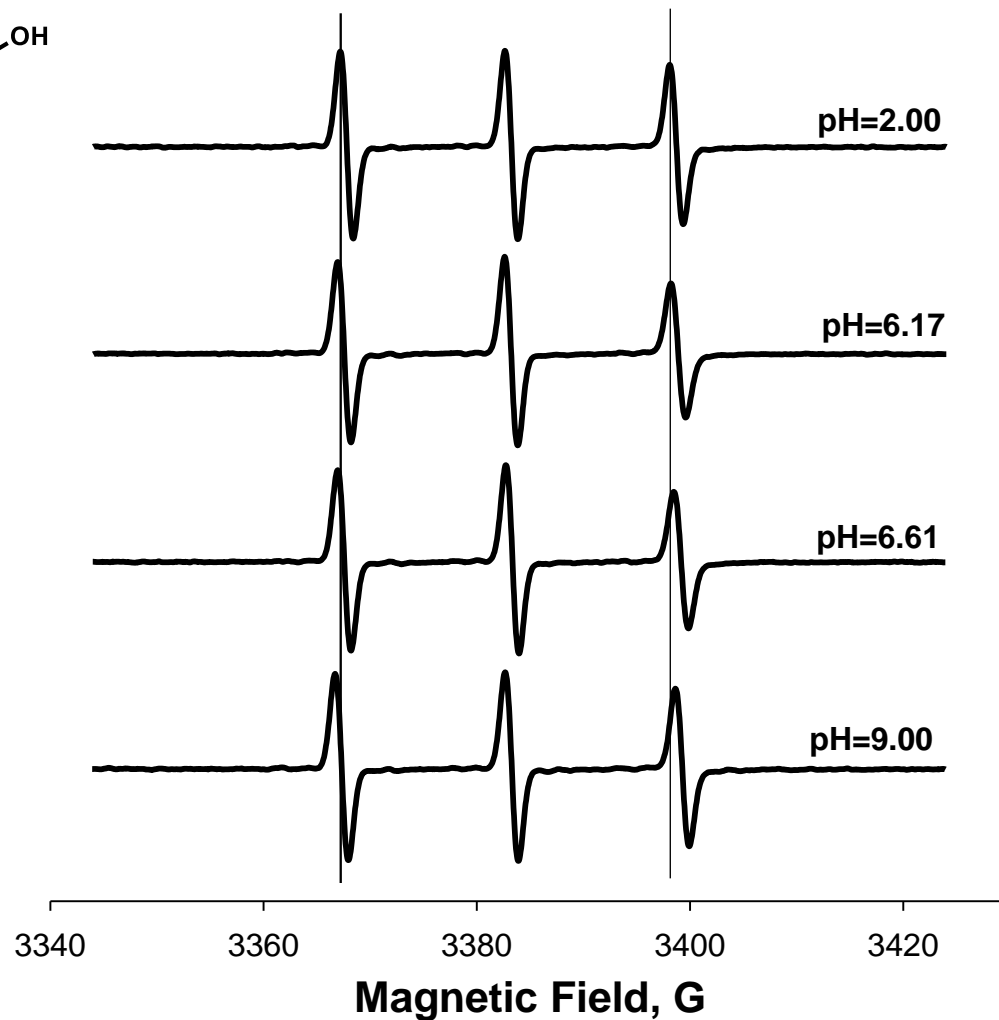
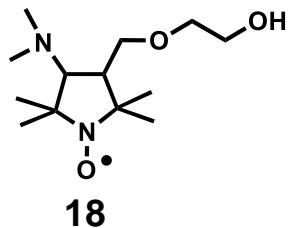
X-band (9.5 GHz) EPR spectra of the nitroxide **10** ($pK_a=6.25\pm 0.01$) in 50 mM NaCl solution in fully protonated (pH=3.17) and non-protonated (pH=9.03) forms, and at pH=6.32 which is close to the pK_a value. Spectra were recorded at 17 °C. Vertical lines are shown as a guide for an eye.



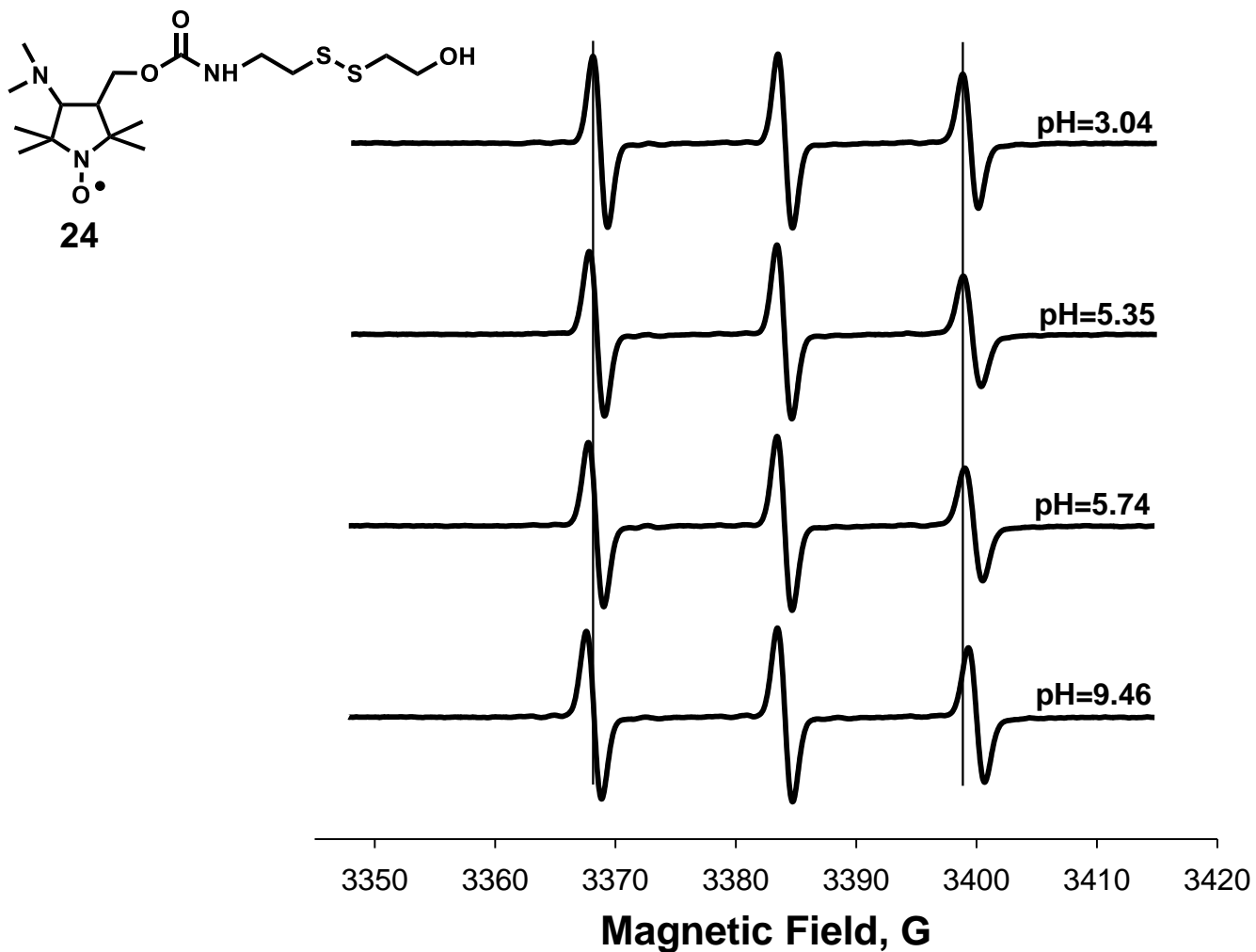
X-band (9.5 GHz) EPR spectra of the nitroxide **15** ($pK_a=5.80\pm 0.02$) in 50 mM phosphate buffer in fully protonated (pH=1.63) and non-protonated (pH=7.93) forms, and at pH=5.63 which is close to the pK_a value. Spectra were recorded at 17 °C. Vertical lines are shown as a guide for an eye.



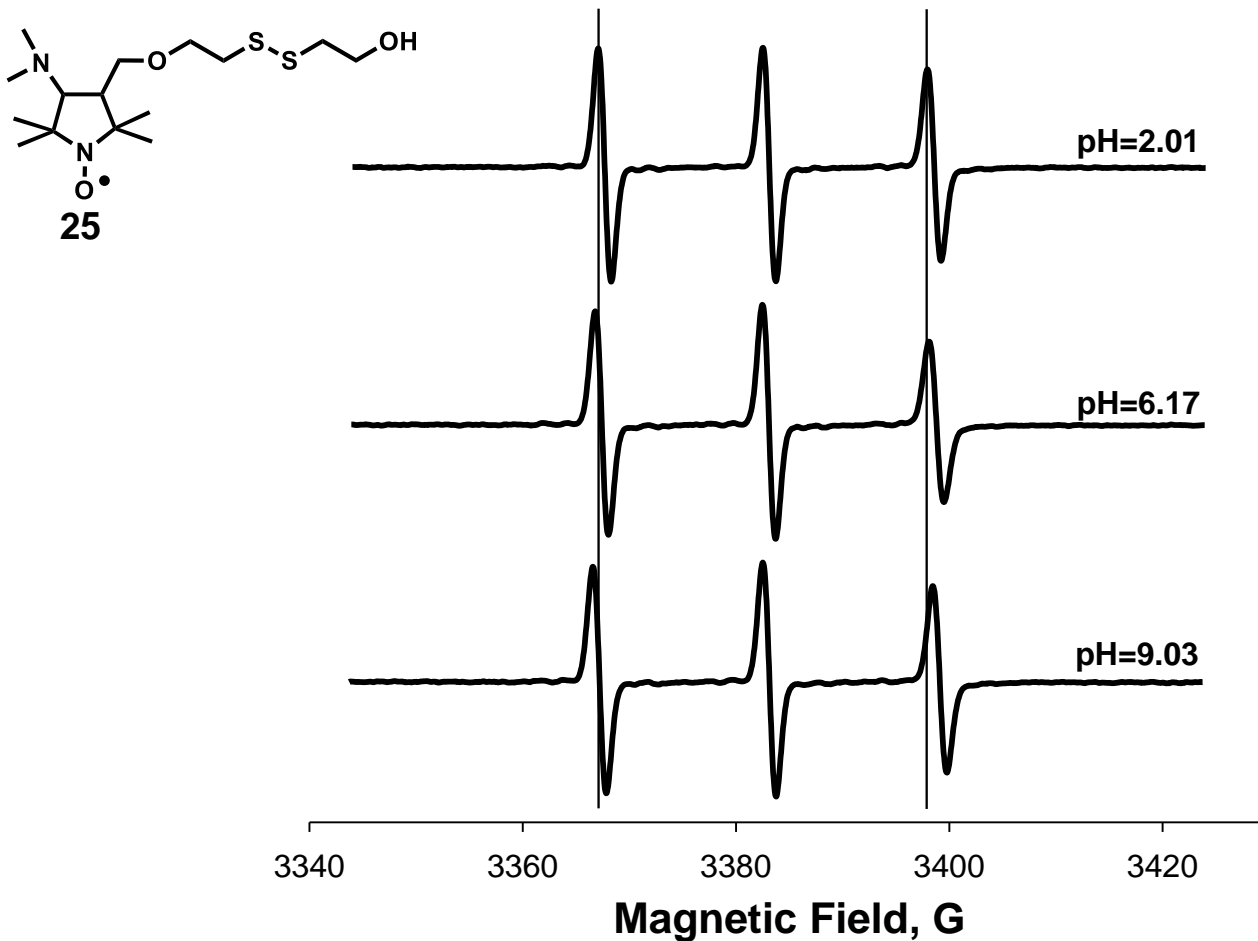
X-band (9.5 GHz) EPR spectra of the nitroxide **16** ($pK_a=4.44\pm 0.02$) in 50 mM phosphate buffer in fully protonated (pH=2.03) and non-protonated (pH=8.01) forms, and at pH=4.32 which is close to the pK_a value. Spectra were recorded at 17 °C. Vertical lines are shown as a guide for an eye. S72



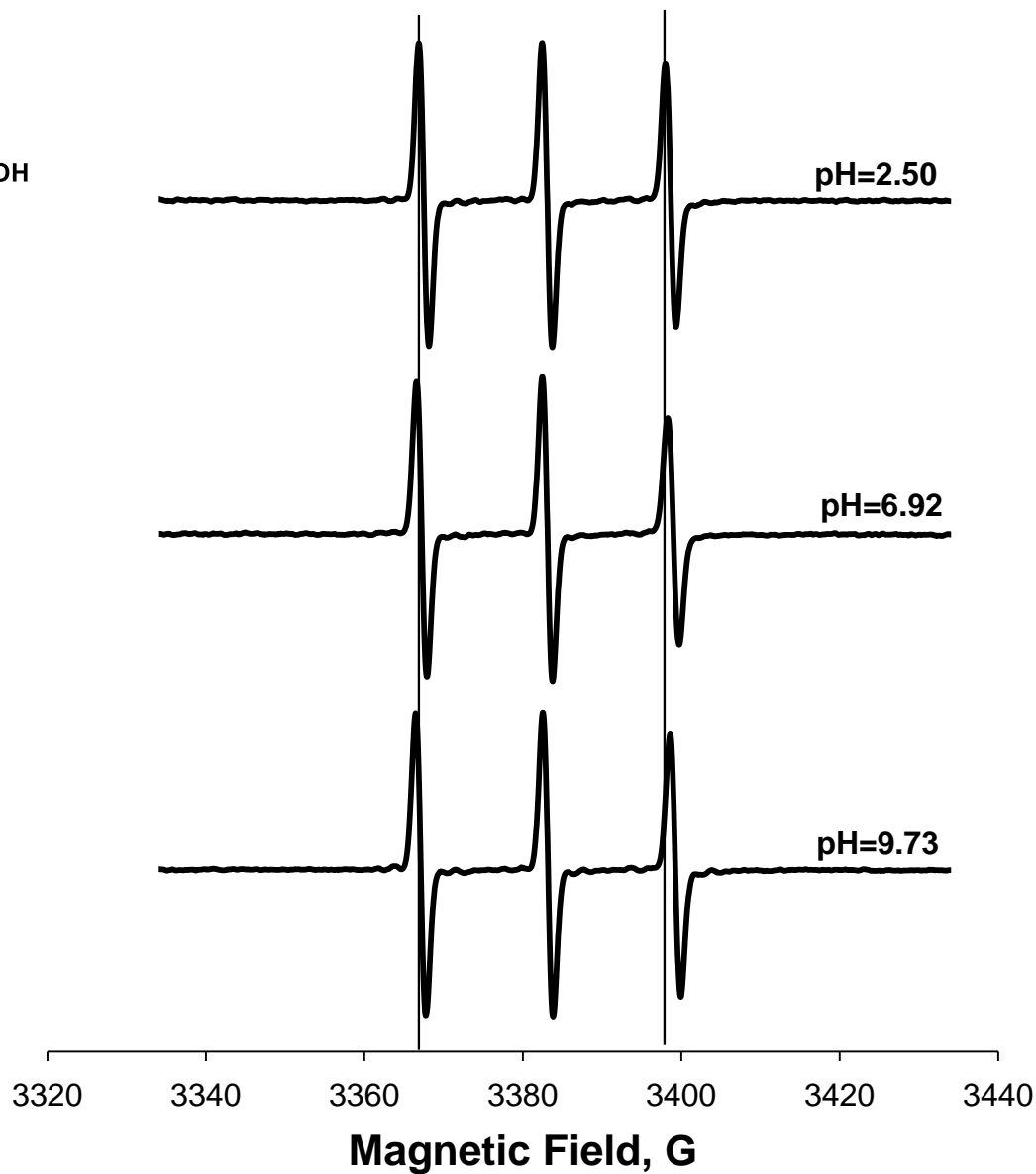
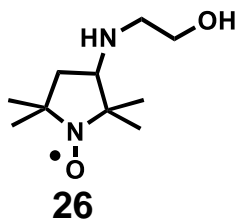
X-band (9.5 GHz) EPR spectra of the nitroxide **18** ($pK_a=6.39\pm 0.01$) in 50 mM phosphate buffer in fully protonated (pH=2.00) and non-protonated (pH=9.00) forms, and at pH=6.17 and pH=6.61 which are close to the pK_a value. Spectra were recorded at 17 °C. Vertical lines are shown as a guide for an eye.



X-band (9.5 GHz) EPR spectra of the nitroxide **24** ($pK_a=5.51\pm 0.03$) in 50 mM phosphate buffer in fully protonated (pH=3.04) and non-protonated (pH=9.46) forms, and at pH=5.35 and pH=5.74 which are close to the pK_a value. Spectra were recorded at 17 °C. Vertical lines are shown as a guide for an eye.



X-band (9.5 GHz) EPR spectra of the nitroxide **25** ($pK_a=6.22\pm 0.06$) in 50 mM phosphate buffer in fully protonated (pH=2.01) and non-protonated (pH=9.03) forms, and at pH=6.17 which is close to the pK_a value. Spectra were recorded at 17 °C. Vertical lines are shown as a guide for an eye.



X-band (9.5 GHz) EPR spectra of the nitroxide **26** ($pK_a=6.73\pm 0.01$) in 50 mM phosphate buffer in fully protonated (pH=2.50) and non-protonated (pH=9.73) forms, and at pH=6.92 which is close to the pK_a value. Spectra were recorded at 17 °C. Vertical lines are shown as a guide for an eye.