Supplementary Material

Oxidative conversion of N-substituted 3-aminopyrazoles to azopyrazoles using electrogenerated NaOCl as the mediator

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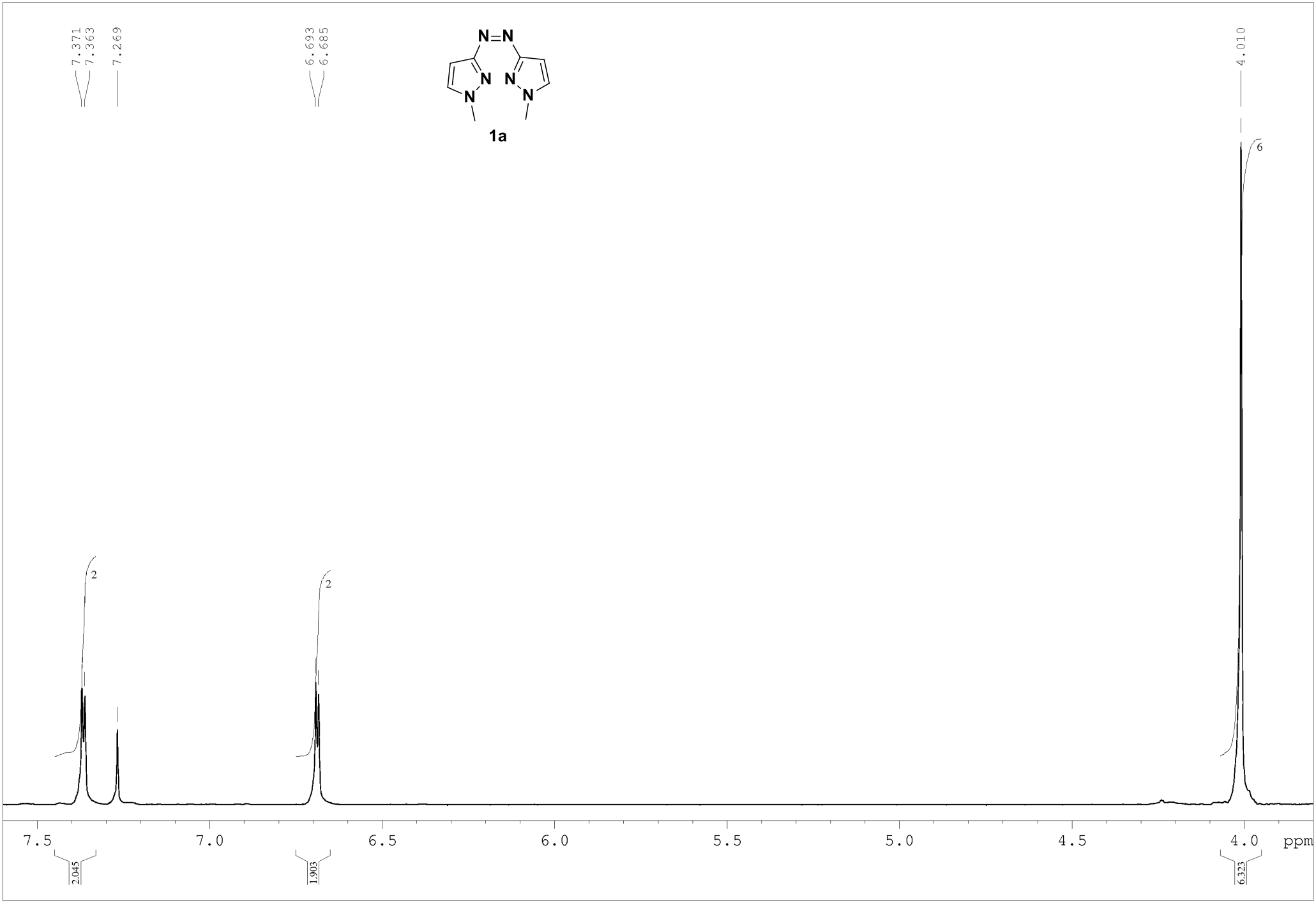
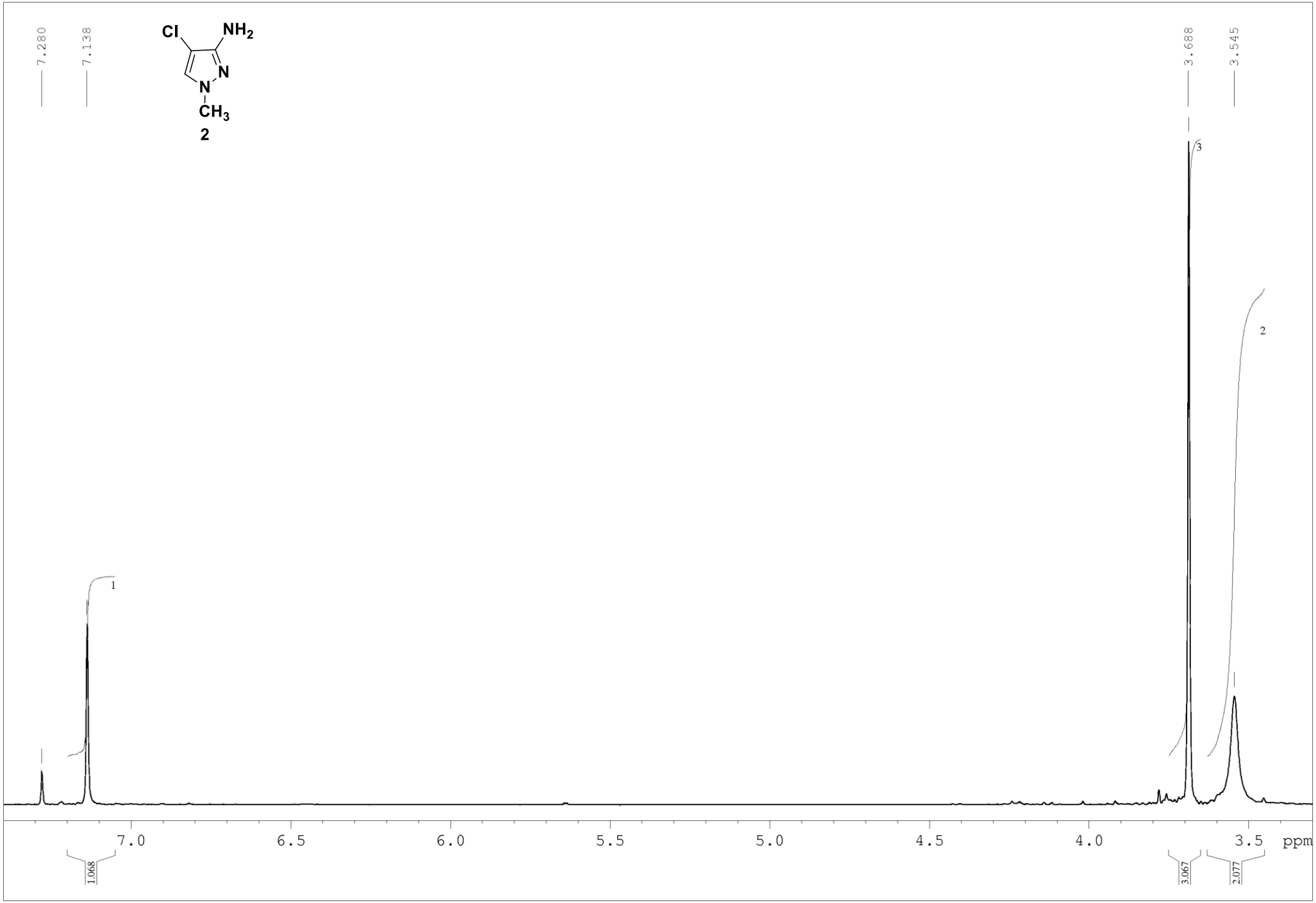
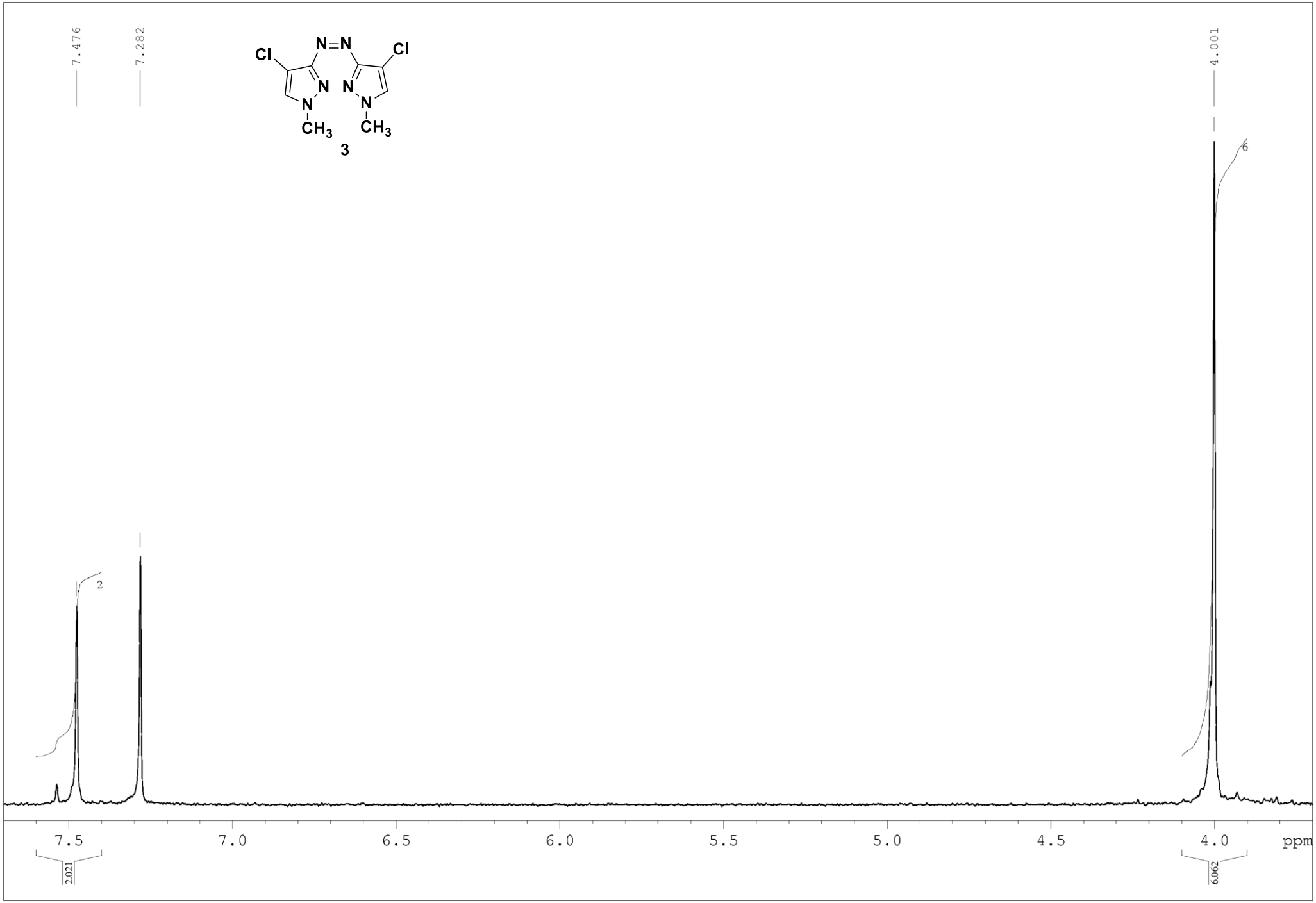
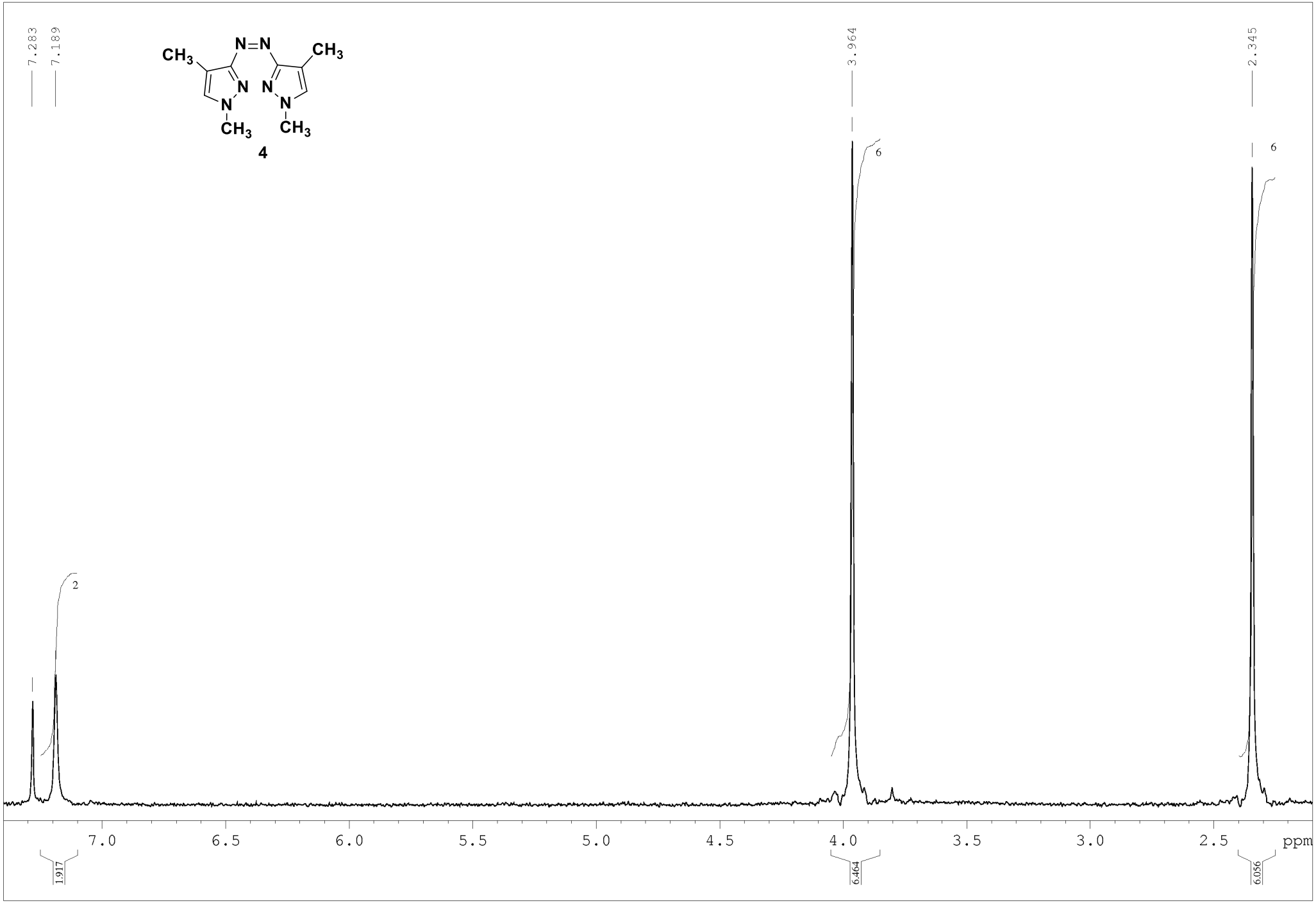
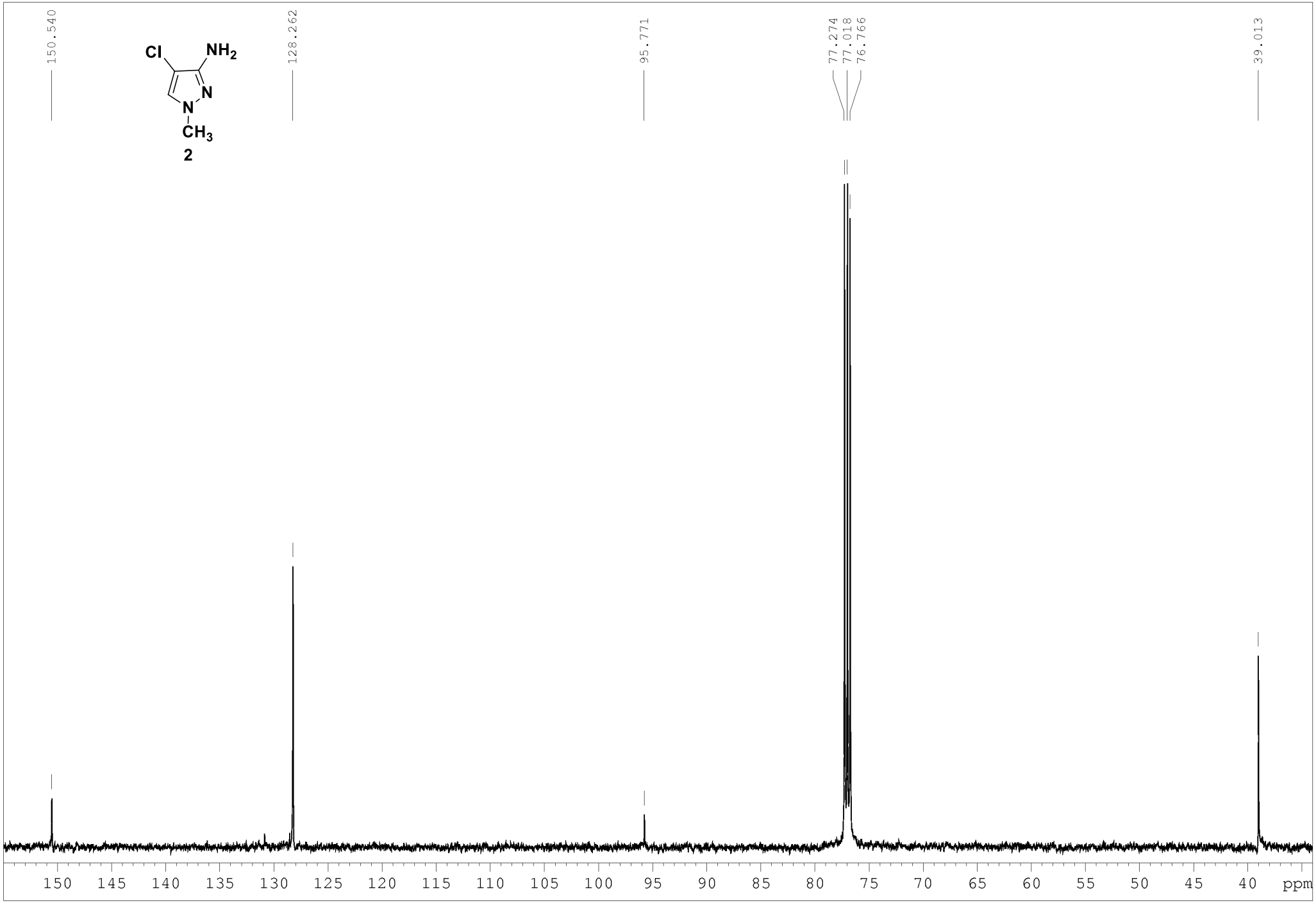

7.371
7.363
7.269
6.693
6.685
4.010
N=N
N
N
N
N
1a
2
2
6
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
ppm
2.045
1.903
6.323

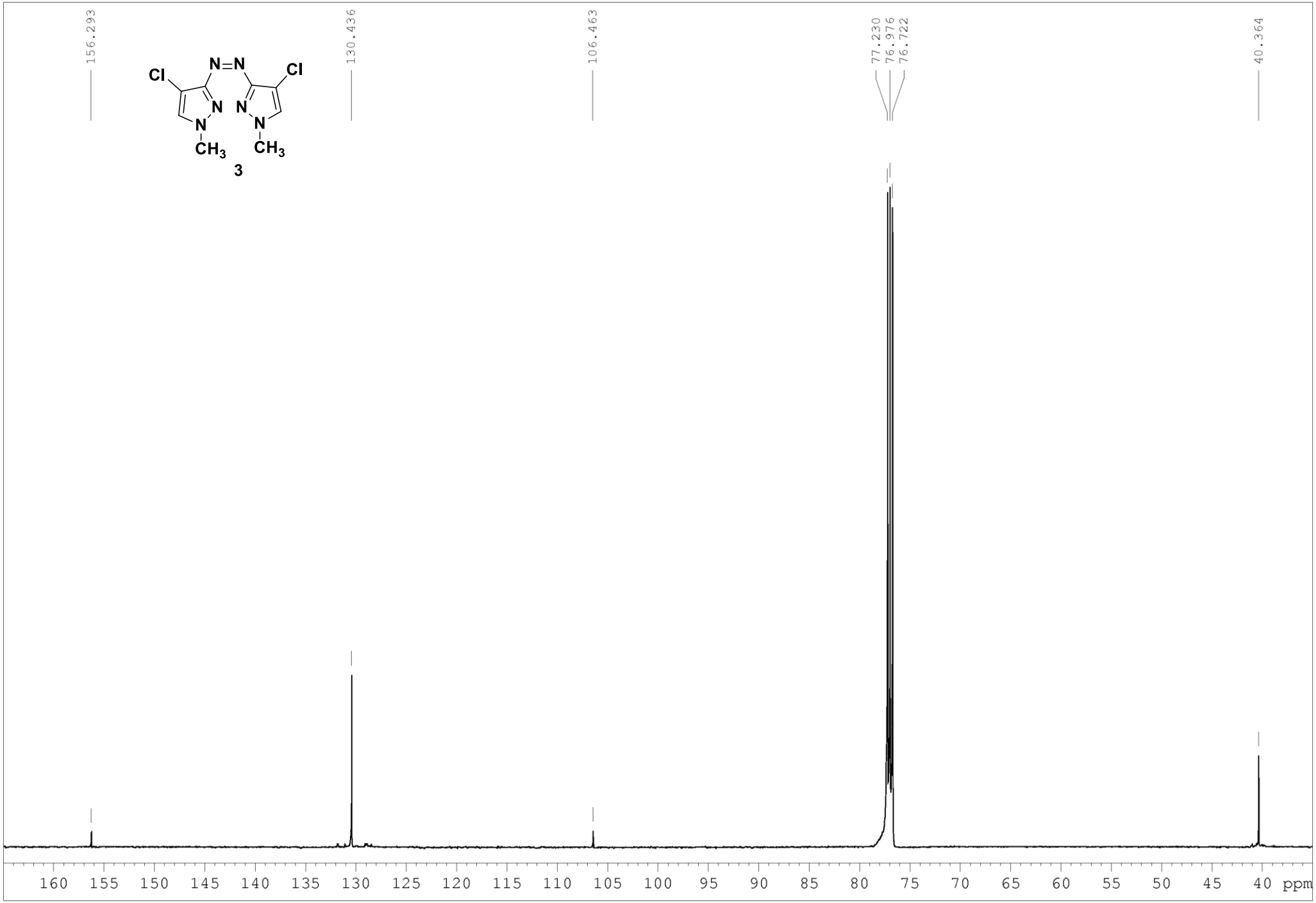

7.280
7.138
Cl
NH2
N
N
CH3
2
3.688
3.545
3
2
1
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
ppm
1.068
3.067
2.077

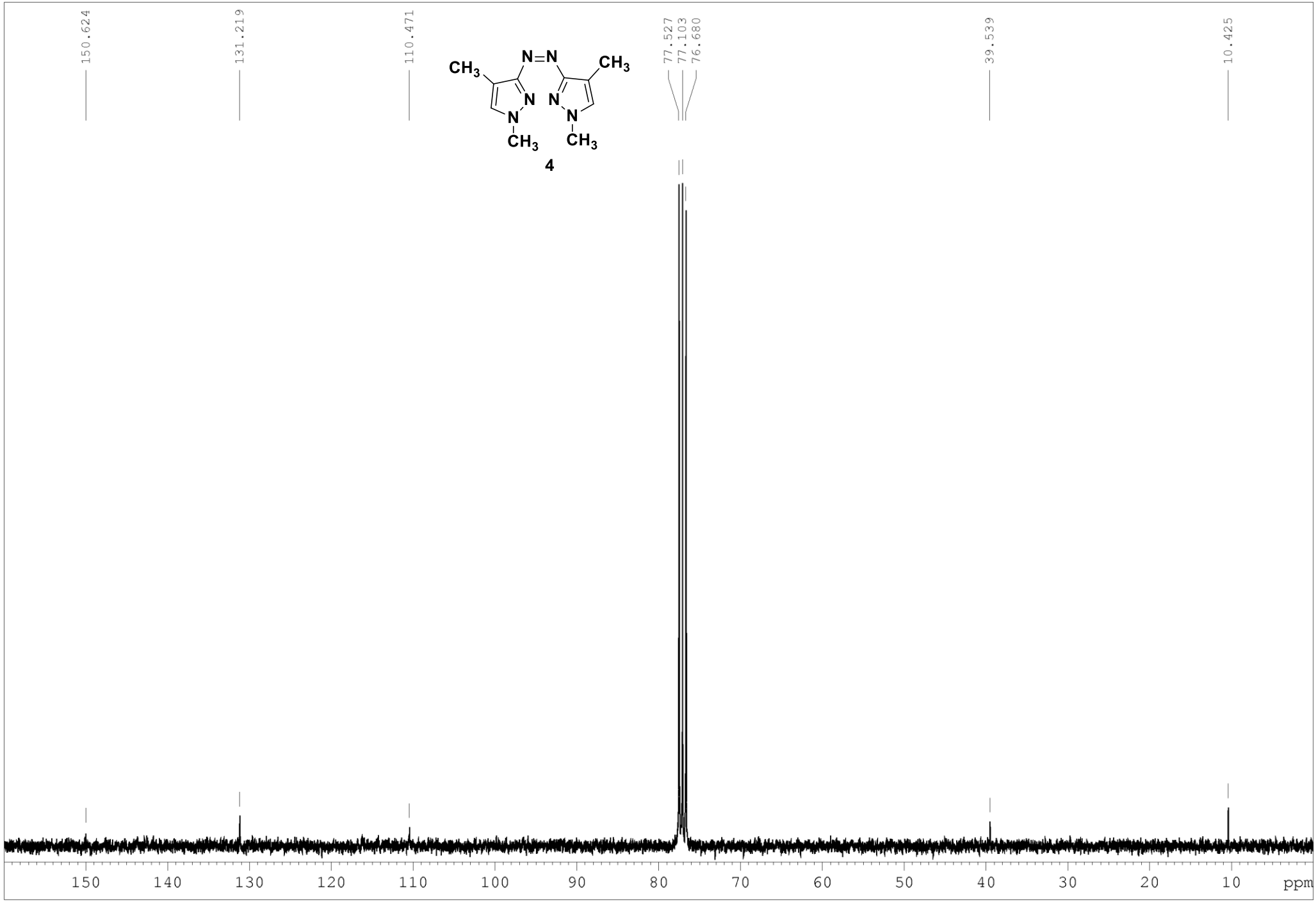

7.476
7.282
4.001
Cl
N=N
Cl
N
N
N
N
CH3
CH3
3
6
2
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
ppm
2.021
6.062


7.283
7.189
3.964
2.345
6
6
2
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
ppm
1.917
6.464
6.056

4


150.540
128.262
95.771
77.274
77.018
76.766
39.013
Cl
NH2
N
N
CH3
2
150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 ppm


156.293
130.436
106.463
77.230
76.976
76.722
40.364
Cl
N=N
Cl
N
N
N
N
CH3
CH3
3
160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 ppm


150.624
131.219
110.471
77.527
77.103
76.680
39.539
10.425
N=N
CH3
CH3
N
N
N
N
CH3
CH3
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

4

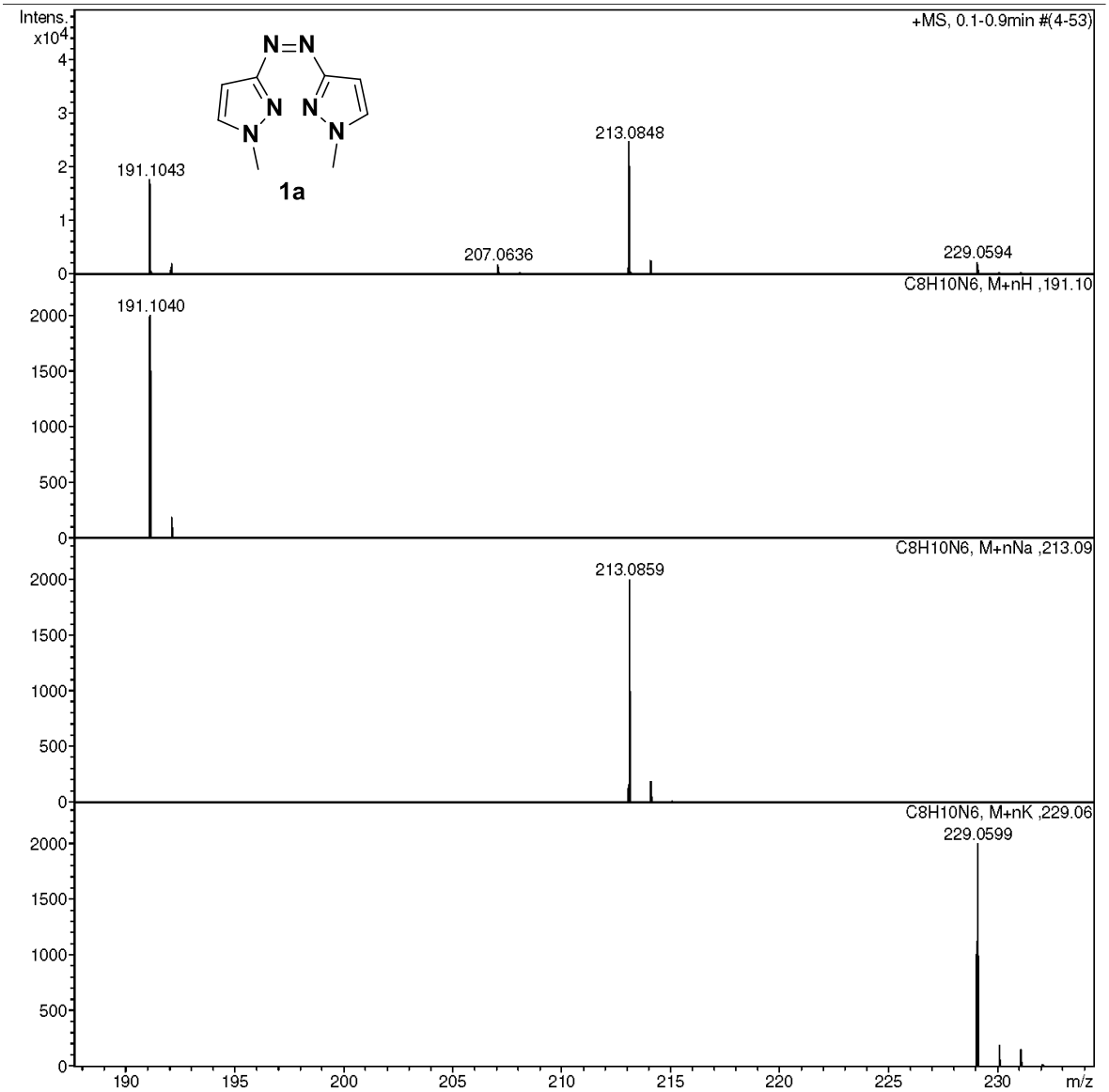
Display Report

Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2015\Sigacheva\0211026.d	Acquisition Date	11.02.2015 15:59:34
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/VAPP SIG-mass-011	Instrument / Ser#	micrOTOF 10248
Comment	C8H10N6 mw 190 clb added		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



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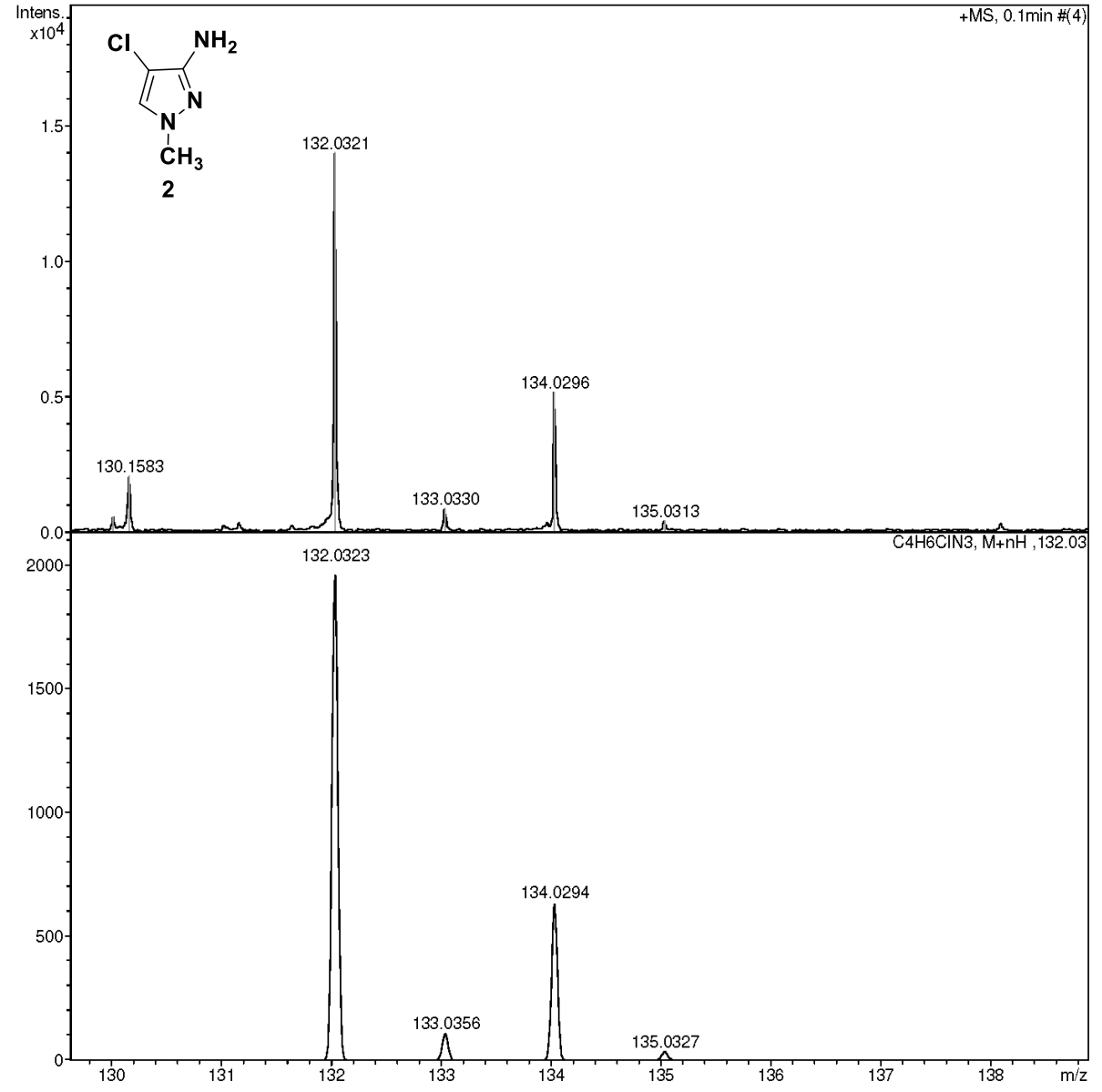
Analysis Info

Analysis Name	D:\Data\Kolotyrkina\2015\Sigachova\1022004.d	Acquisition Date	22.10.2015 10:16:24
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/VAPP sigmass016	Instrument / Ser#	micrOTOF 10248
Comment	C4H6ClN3 mw 131 calibrant added		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



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Display Report

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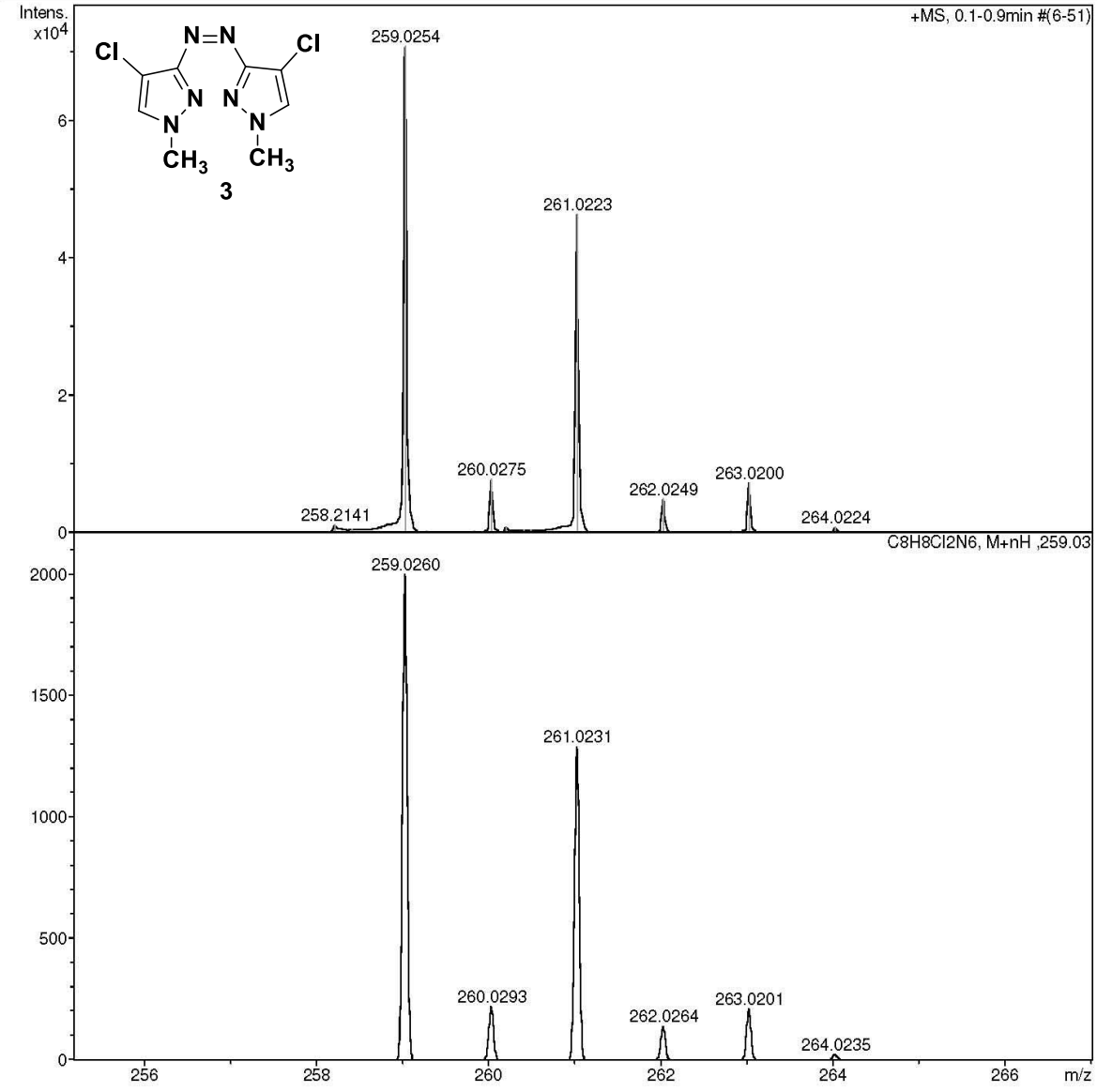
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/VAPP Sigmass025	Instrument / Ser#	micrOTOF 10248
Comment	C8H8Cl2N6 mwH 259.026 clb added		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



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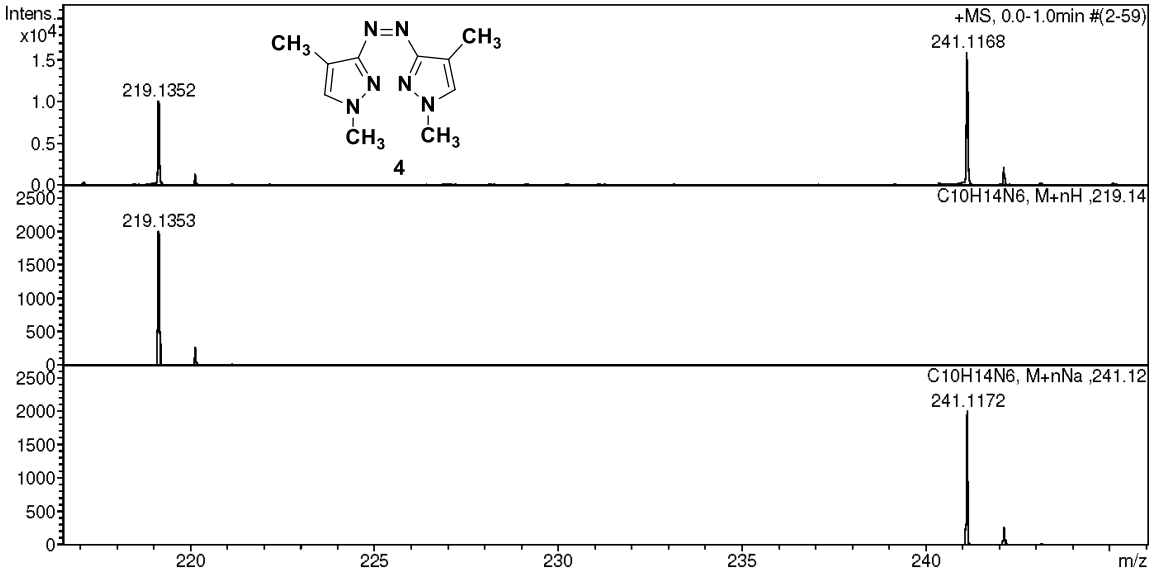
Analysis Info

Analysis Name	D:\Data\Chizhov\Egorov\Sigacheva\sigmass20_&clblow.d	Acquisition Date	14.03.2016 14:12:40
Method	tune_low.m	Operator	BDAL@DE
Sample Name	/VAPP Sigmass20	Instrument / Ser#	micrOTOF 10248
Comment	CH3CN 100 %, dil. 200, calibrant added		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



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