

Supporting Information

for

A facile synthetic route to benzimidazolium salts bearing bulky aromatic N-substituents

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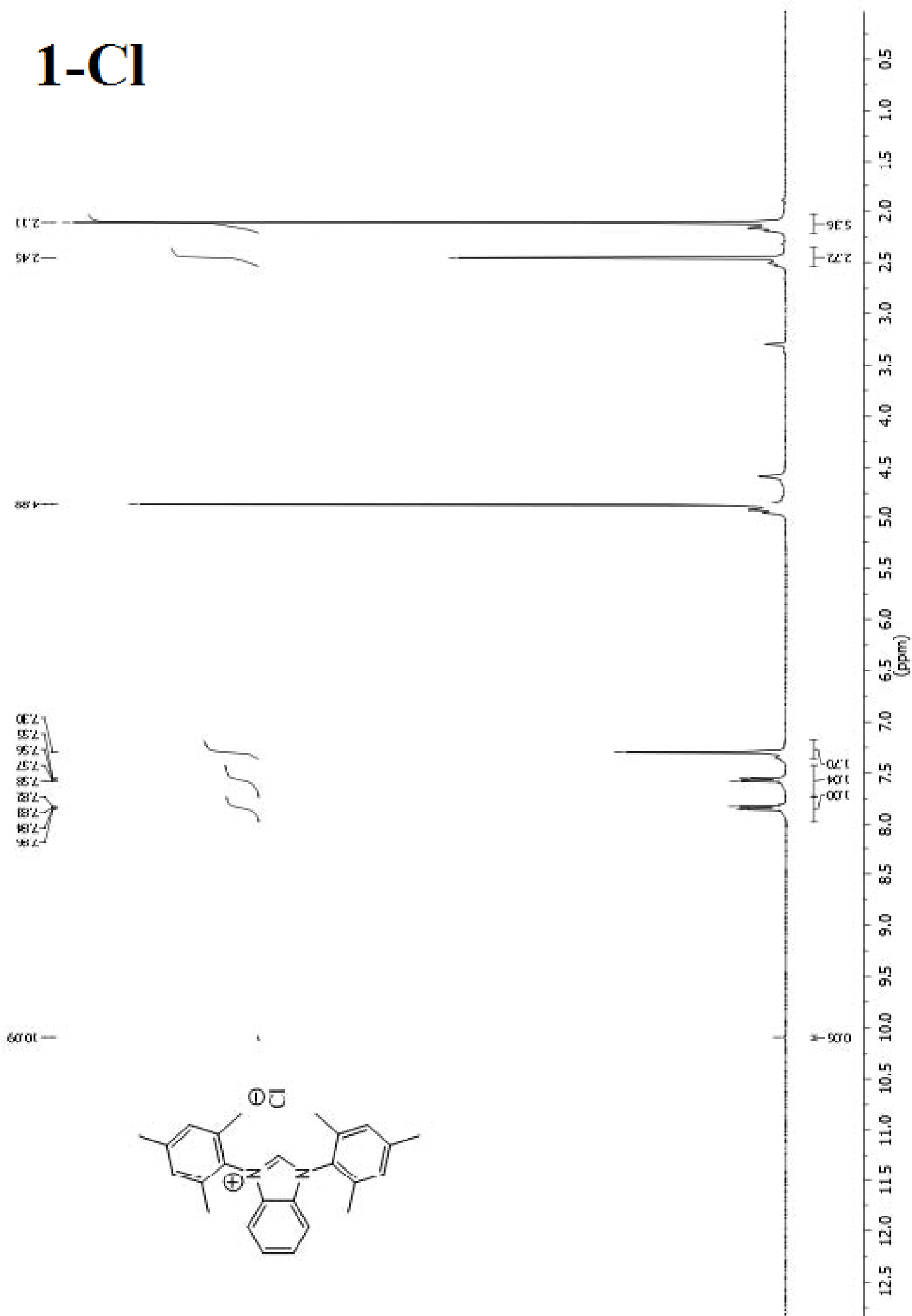
Email: Heinz Berke* - hberke@chem.uzh.ch

* Corresponding author

NMR and HRMS–ESI analyses

NMR analyses

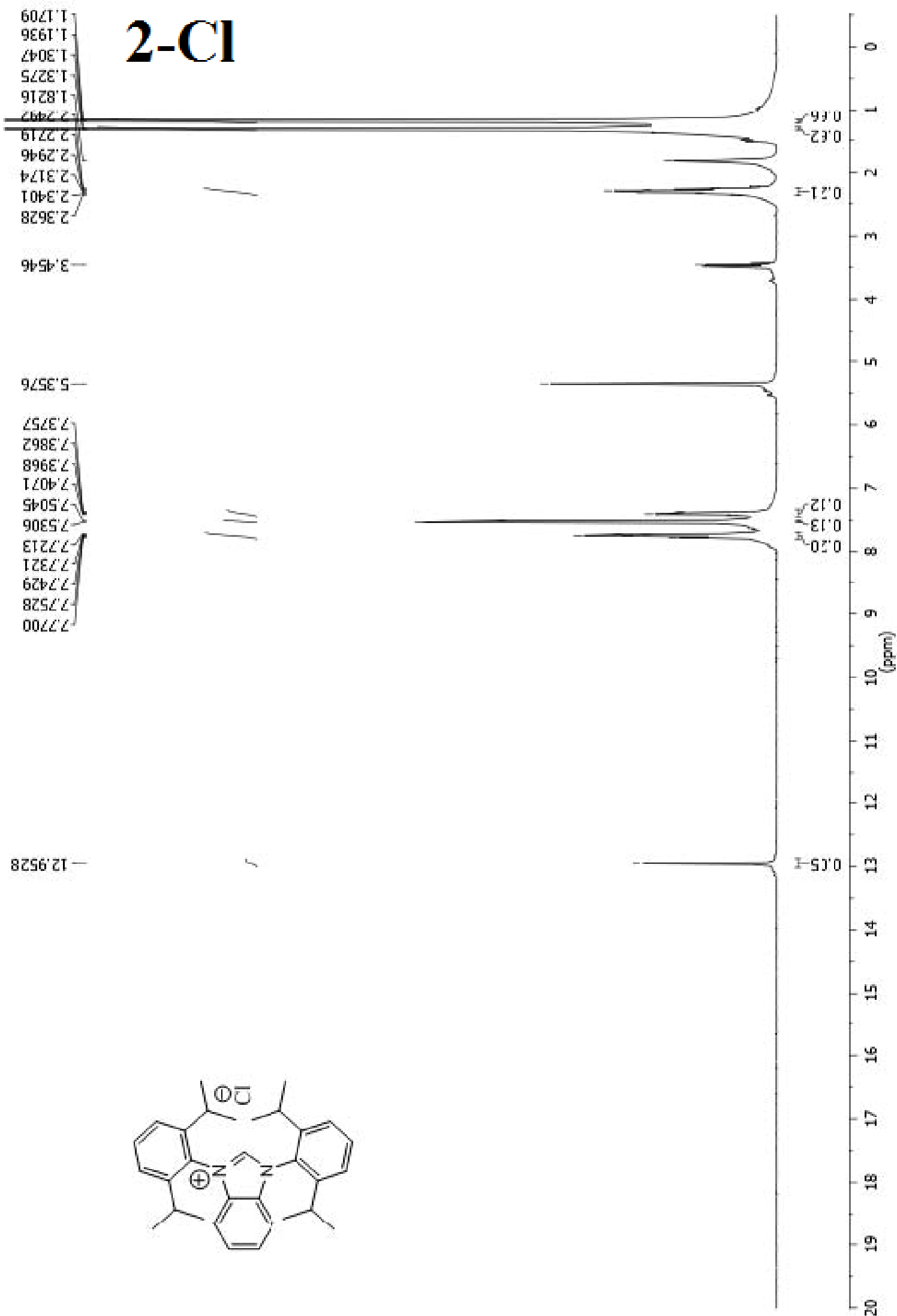
1-Cl



1-Cl



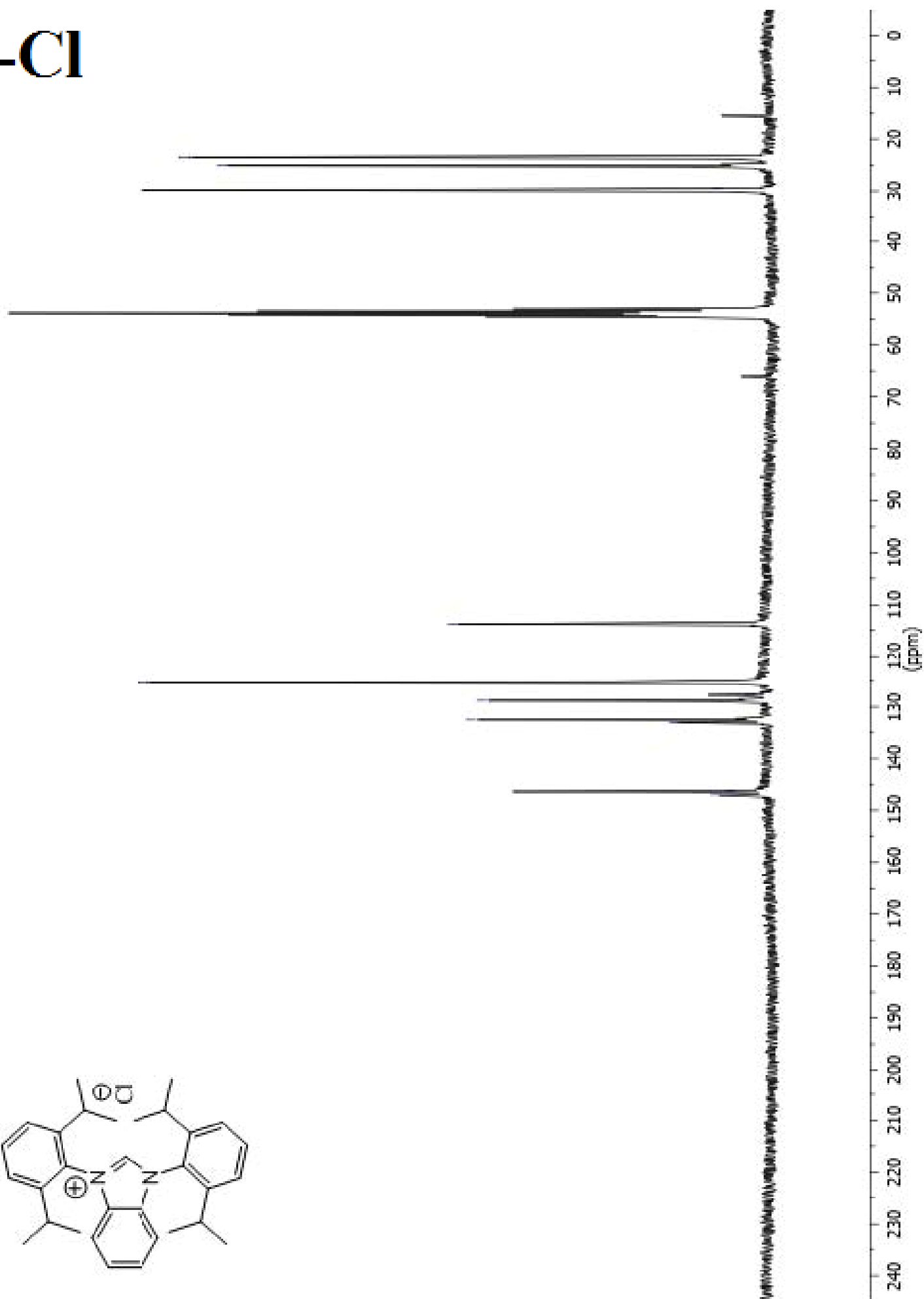
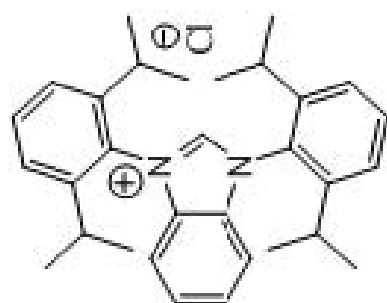
2-Cl



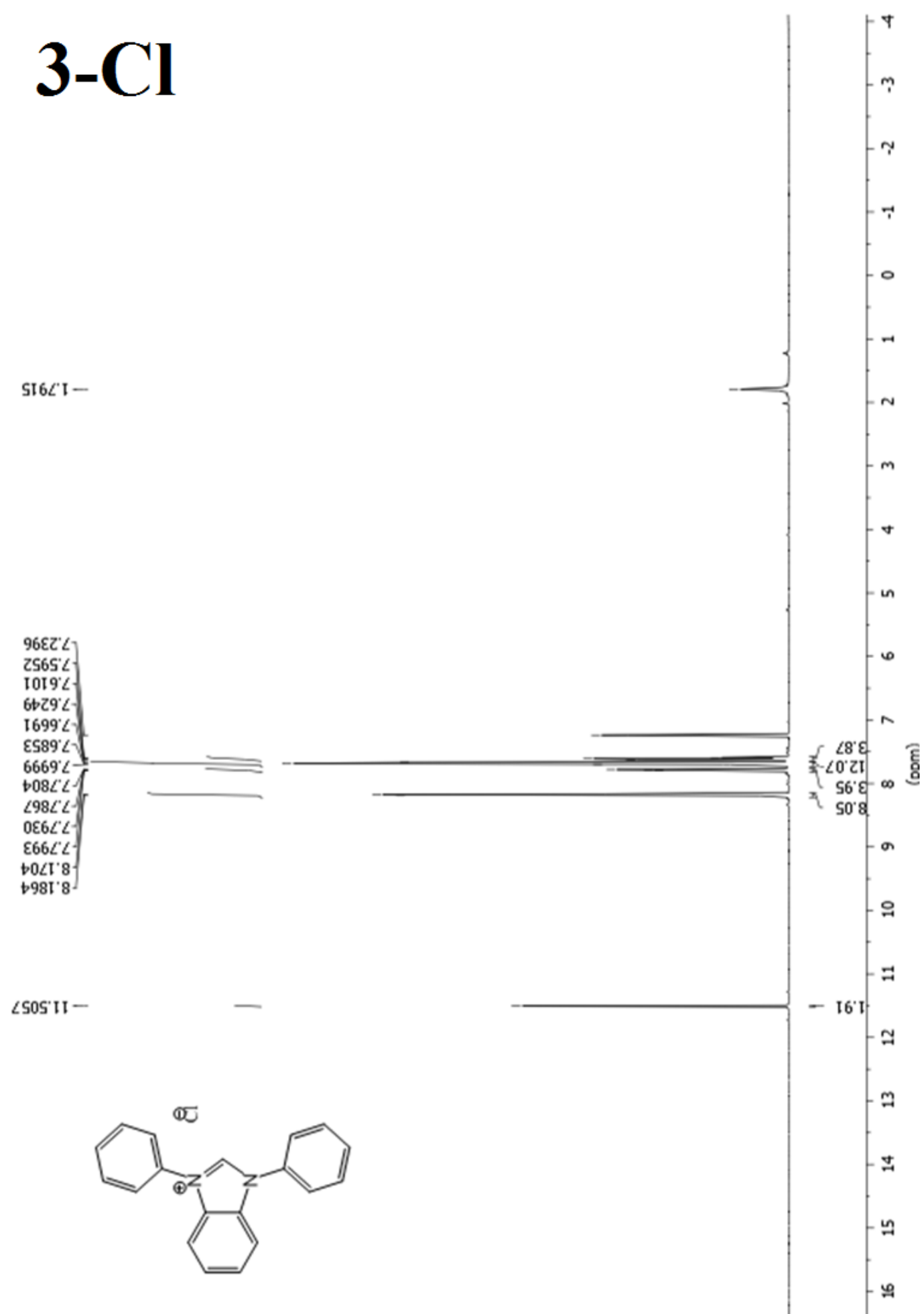
2-Cl

29.52
25.06
23.43

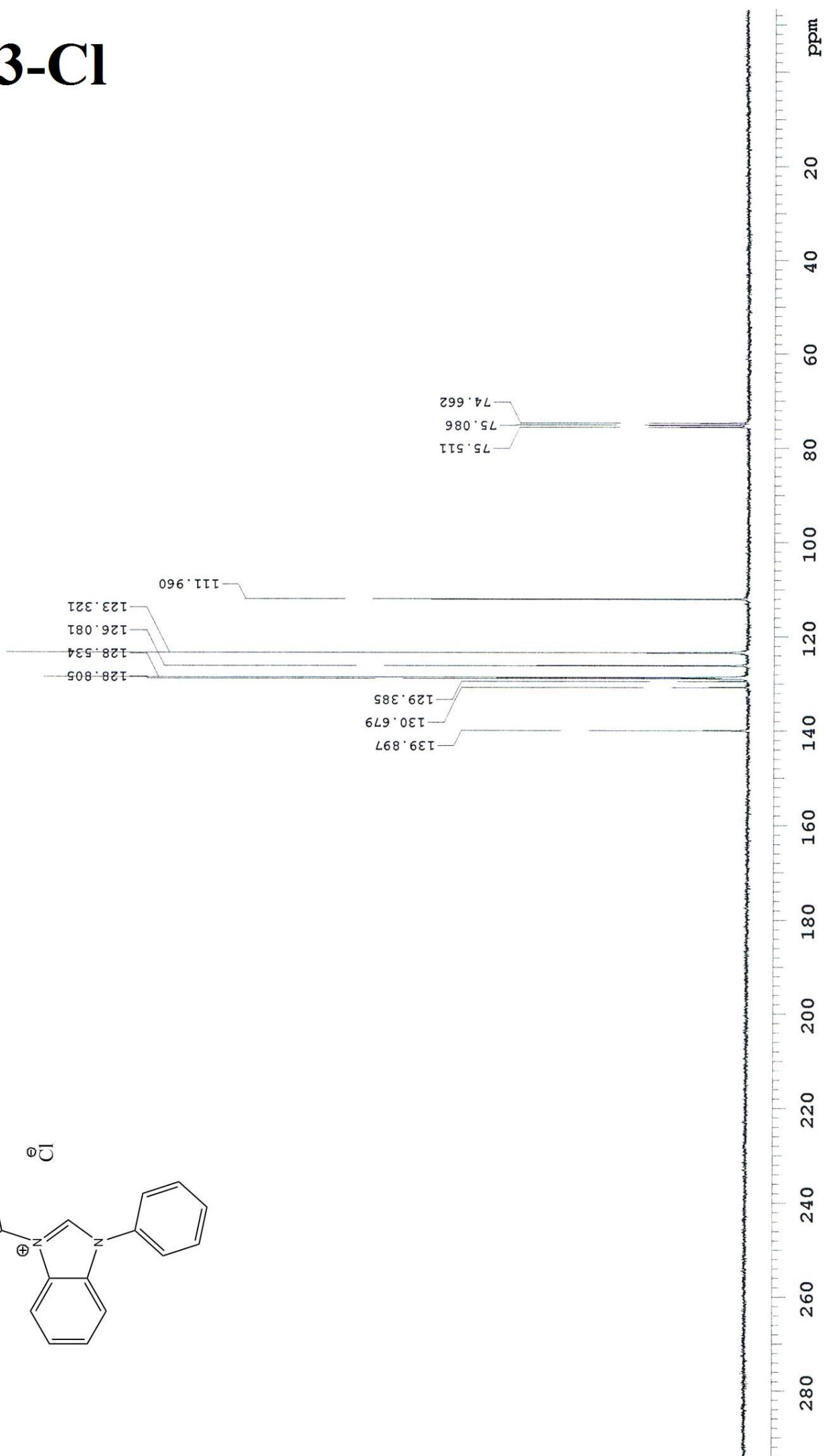
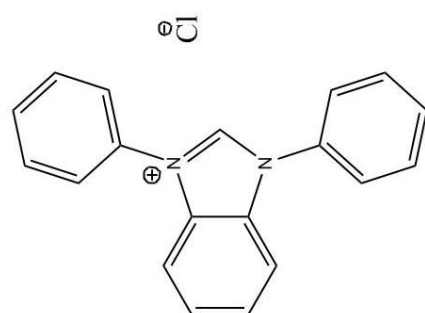
147.01
146.10
133.11
132.52
128.80
127.64
125.28
113.71



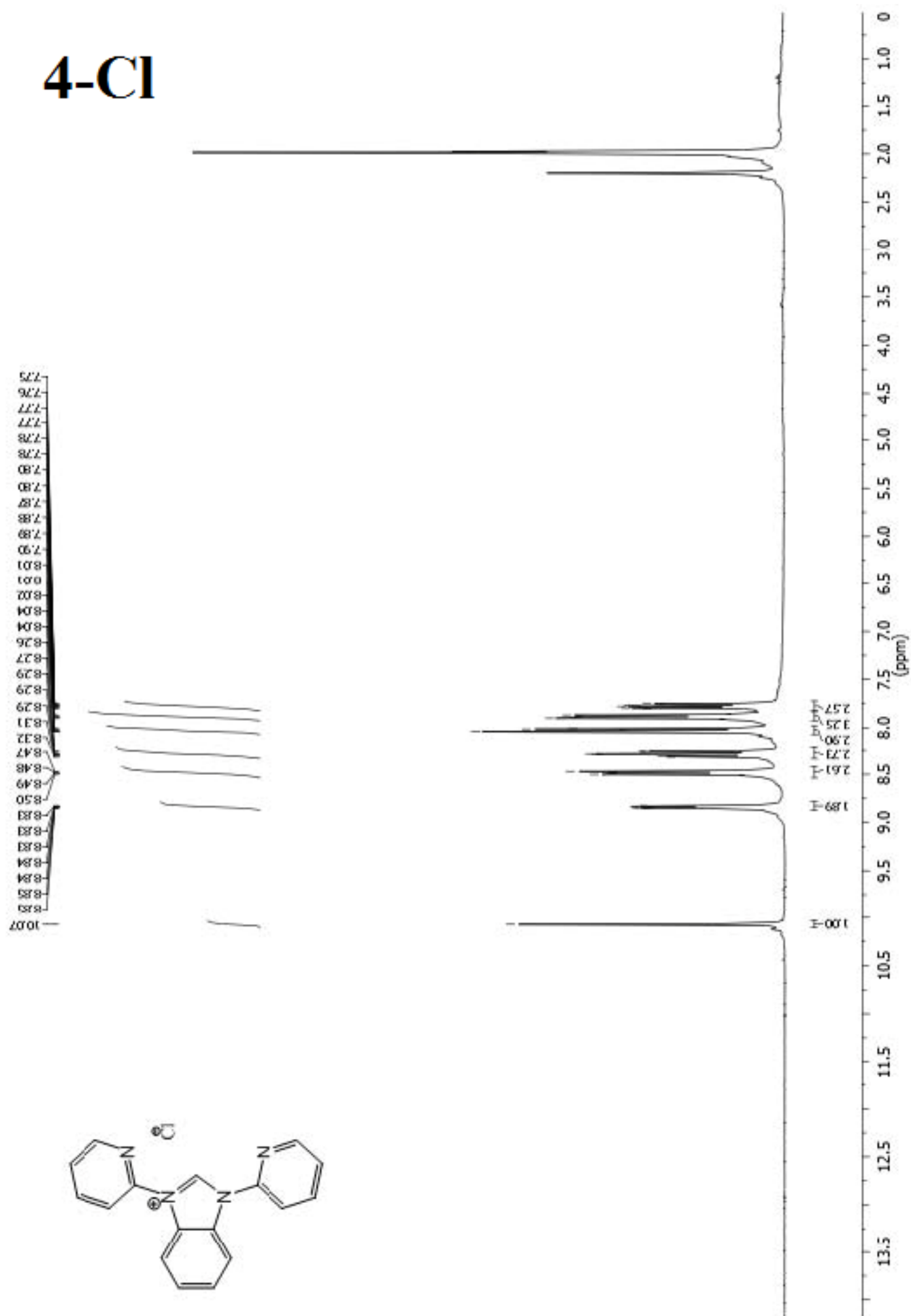
3-Cl



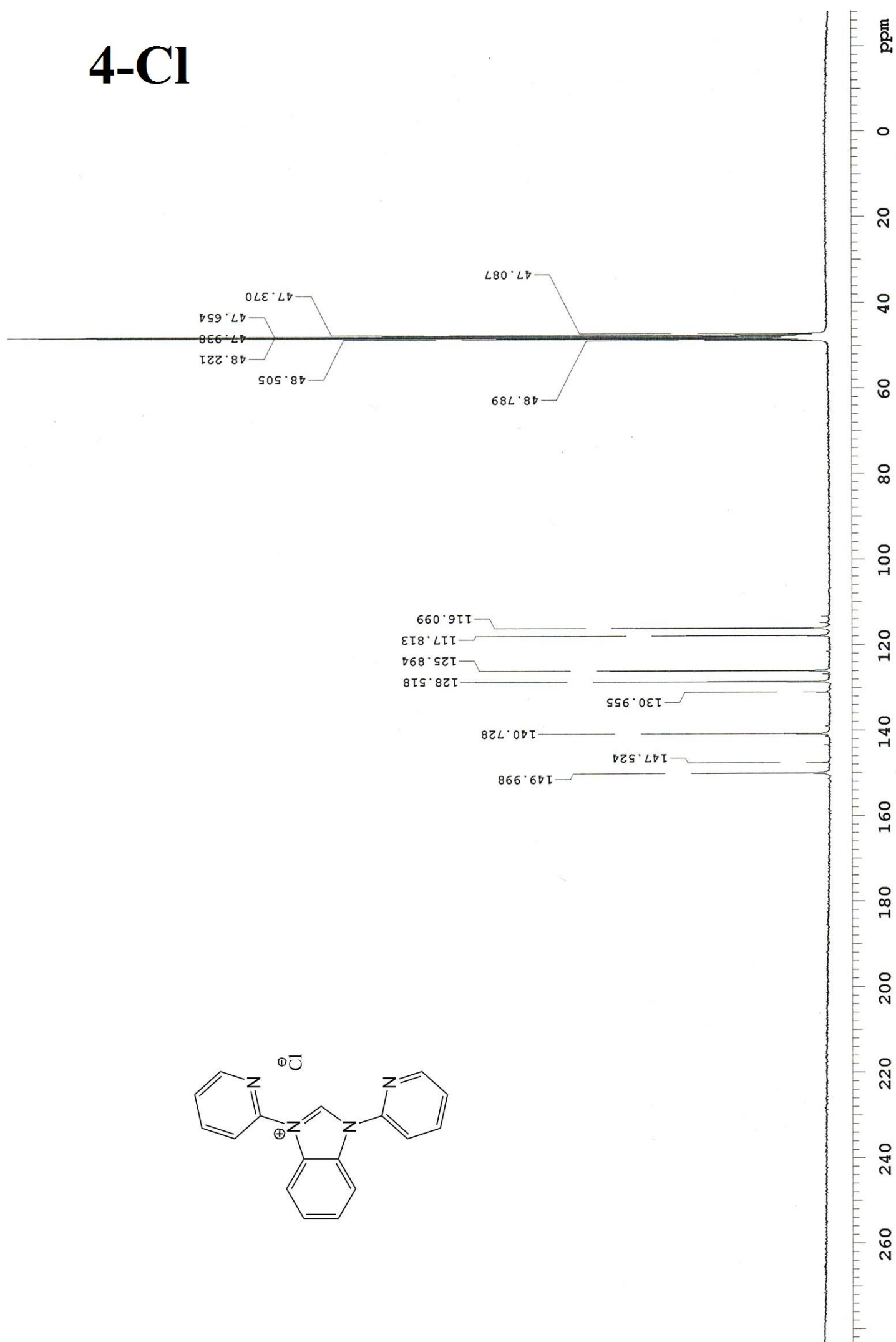
3-Cl



4-Cl

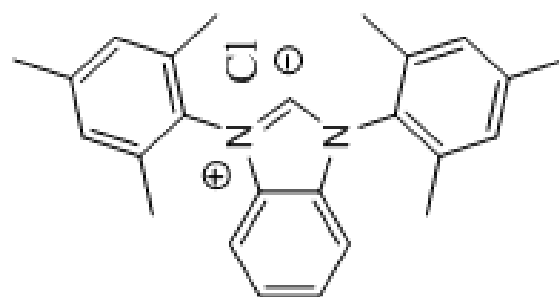


4-Cl

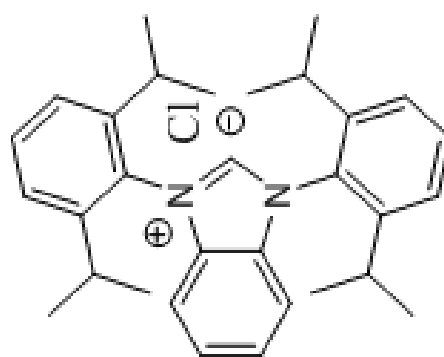


HRMS–ESI analyses

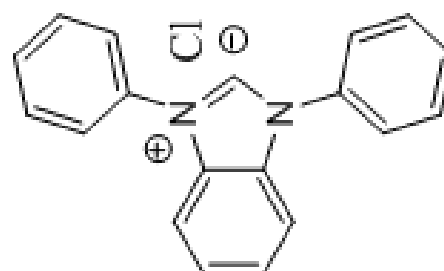
Sample Name



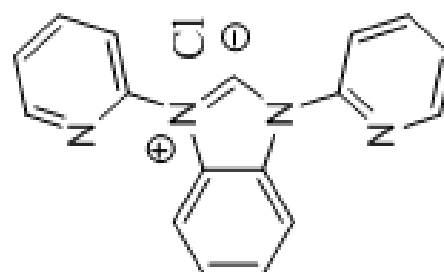
1-Cl = BIMes



2-Cl = BIPr



3-Cl = BPh



4-Cl = BPy

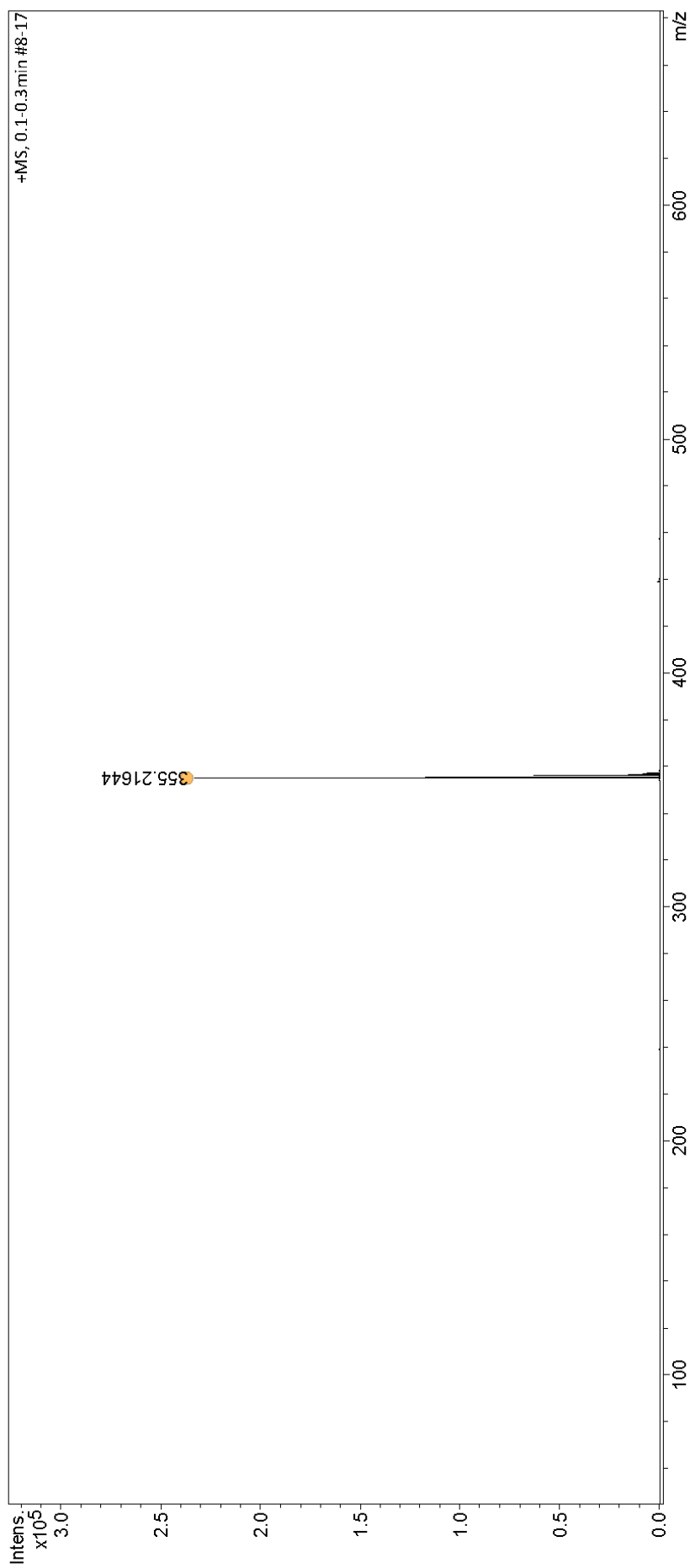
HR-ESI-MS (Bruker maXis)

Analysis Info

Analysis Name	D:\Data\Service\6404al\res.d	Acquisition Date	6/20/2014 9:40:15 AM
Method	tune_low_modified_09_01_14_pos.m	Operator	ust
Sample Name	BlMes	Instrument	maXis
Comment	Solvent: MeOH Client: Grieco		2555552.00033

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Scan Begin	50 m/z	Set Capillary	1500 V	Set Dry Heater	180 °C
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min



HR-ESI-MS (Bruker maXis)

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdB	e ⁻ Conf	N-Rule
355.21644	1	C ₂₅ H ₂₇ N ₂	355.21688	1.23	26.4	1	100.00	13.5	even	ok

HR-ESI-MS (Bruker maXis)

Analysis Info

Analysis Name D:\Data\Service\6404alhrs.d
Method tune_low_modified_09_01_14_pos.m
Sample Name BIMes
Comment Solvent: MeOH
Client: Grieco

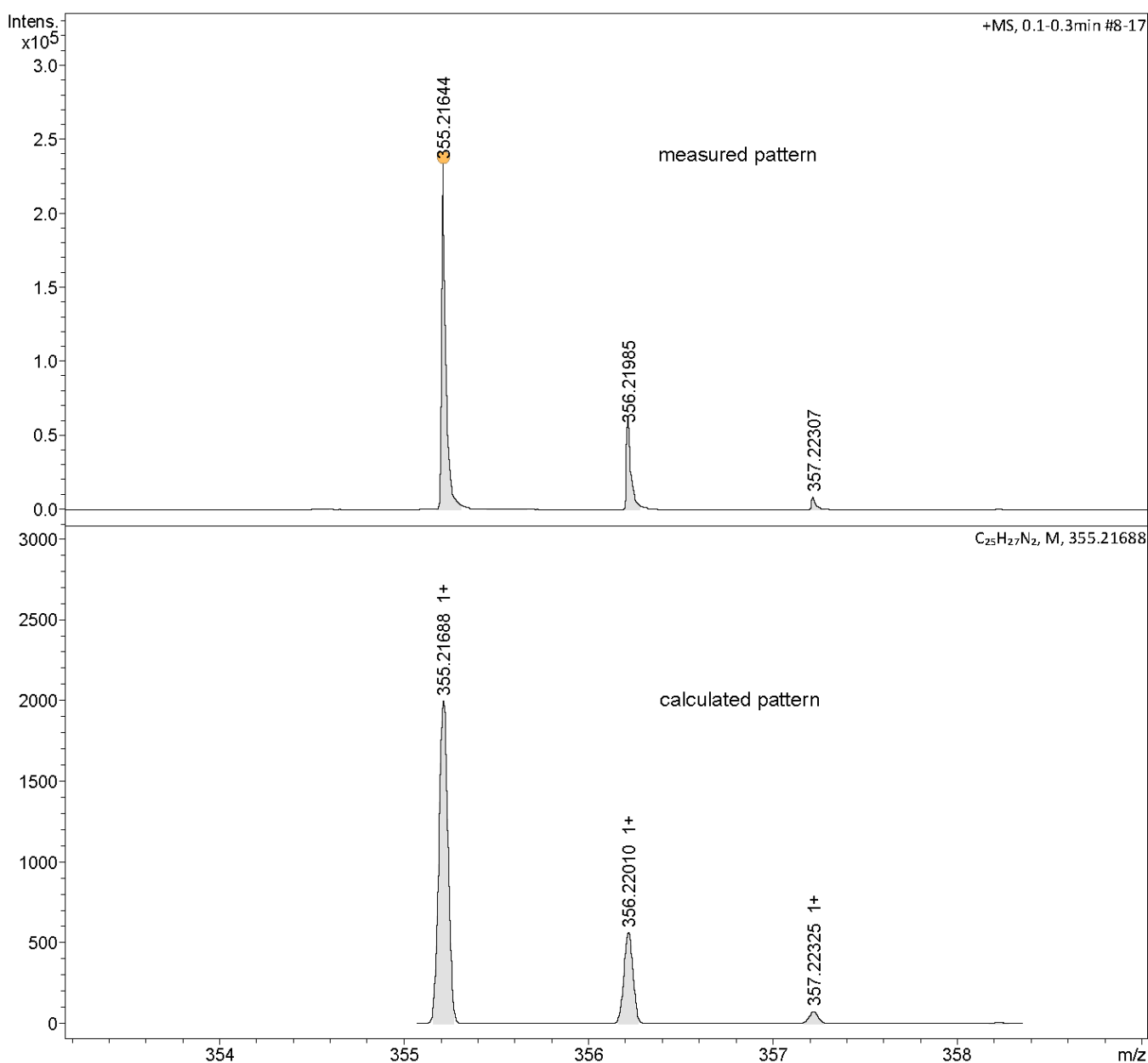
Acquisition Date 6/20/2014 9:40:15 AM

Operator ust

Instrument maXis 255552.00033

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Scan Begin	50 m/z	Set Capillary	1500 V	Set Dry Heater	180 °C
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min



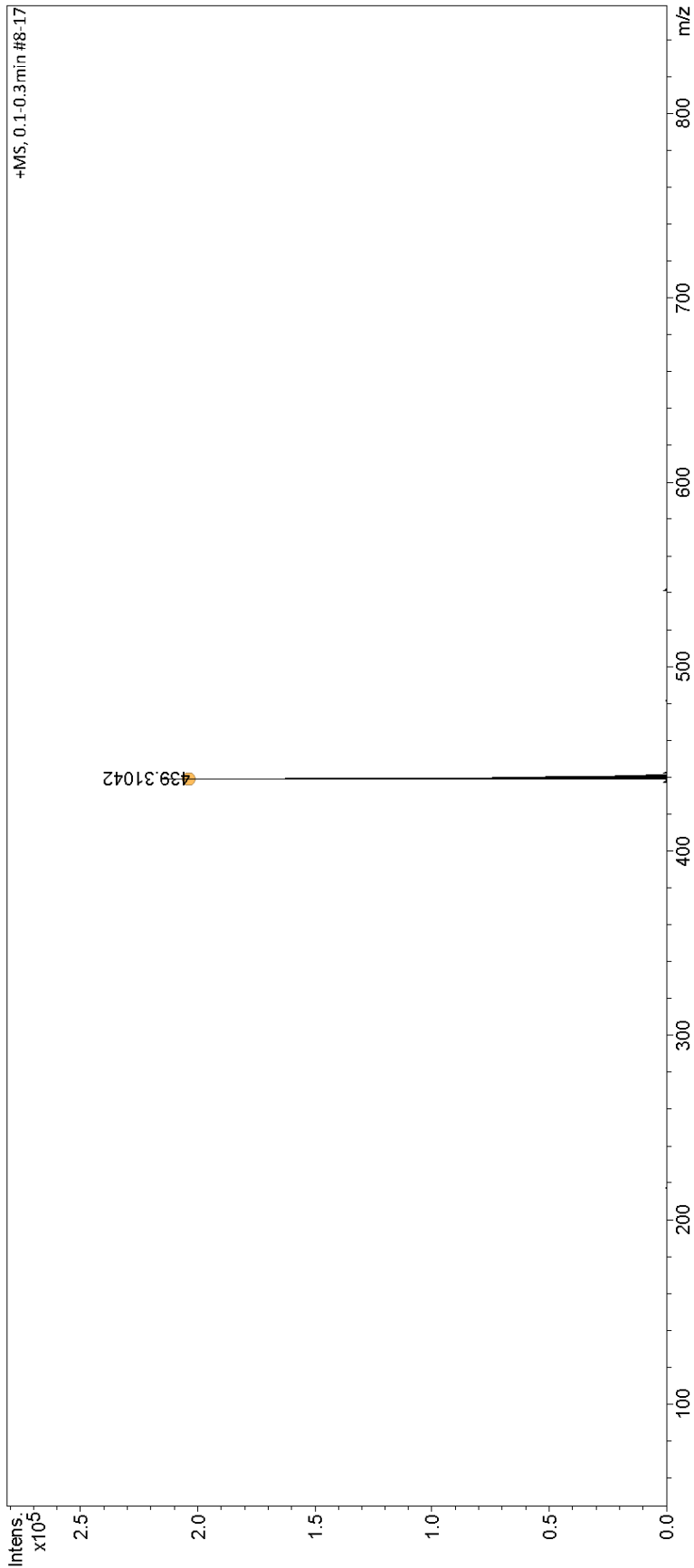
HR-ESI-MS (Bruker maXis)

Analysis Info

Analysis Name	D:\Data\Service\6403alres.d	Acquisition Date	6/20/2014 9:24:26 AM
Method	tune_low_modified_09_01_14_pos.m	Operator	ust
Sample Name	BIPr	Instrument	maXis
Comment	Solvent: MeOH		255552.00033
	Client: Grieco		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Scan Begin	50 m/z	Set Capillary	1500 V	Set Dry Heater	180 °C
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min



HR-ESI-MS (Bruker maXis)

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdB	e ⁻ Conf	N-Rule
439.31042	1	C31H39N2	439.31078	0.82	13.6	1	100.00	13.5	even	ok
	2	C16H35N14O	439.31128	1.96	83.9	2	9.22	6.5	even	ok
	3	C15H39N10O5	439.30994	-1.08	96.9	3	6.35	1.5	even	ok

HR-ESI-MS (Bruker maXis)

Analysis Info

Analysis Name D:\Data\Service\6403alhres.d
Method tune_low_modified_09_01_14_pos.m
Sample Name BIPr
Comment Solvent: MeOH
Client: Grieco

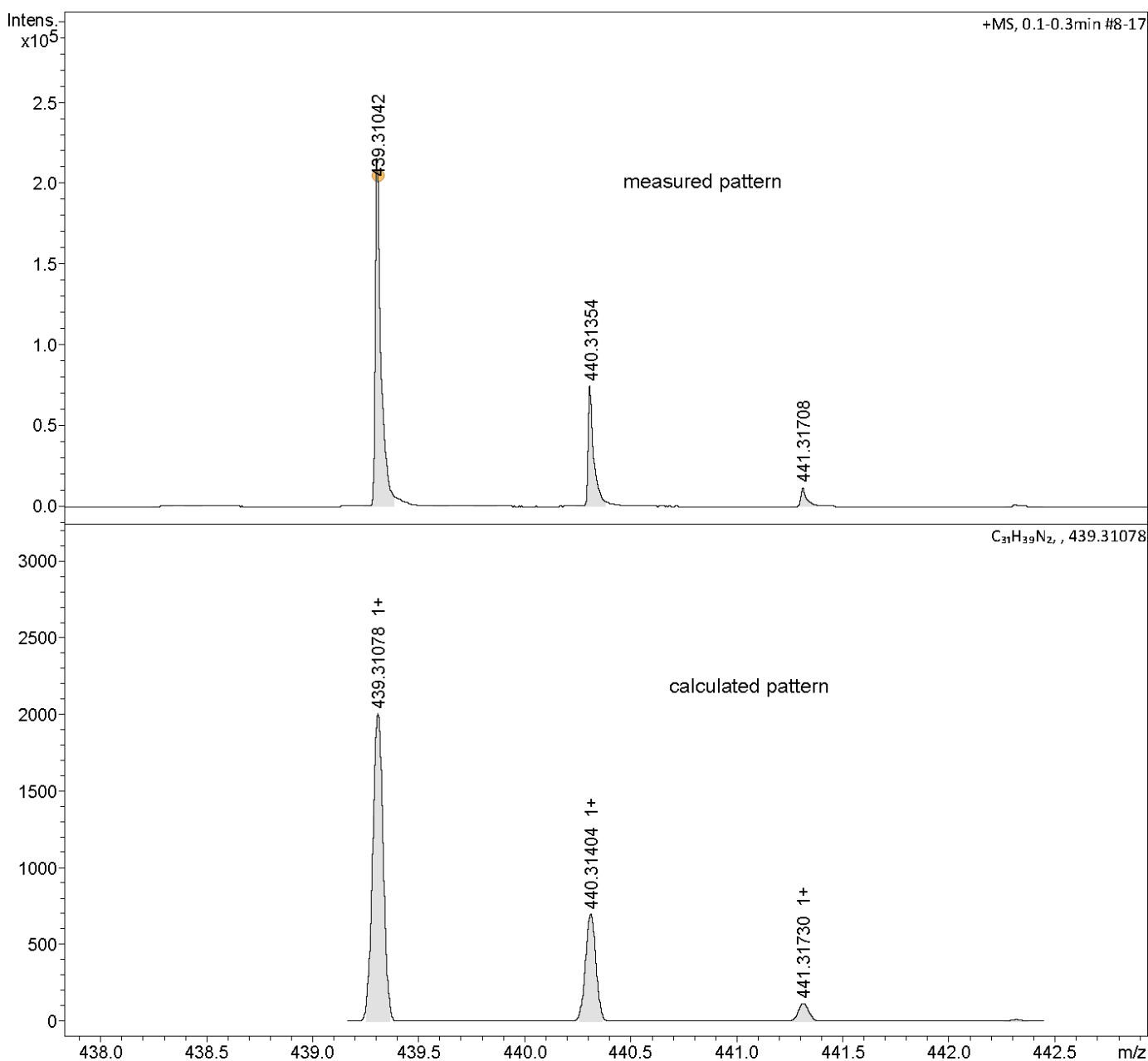
Acquisition Date 6/20/2014 9:24:26 AM

Operator ust

Instrument maXis 255552.00033

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Scan Begin	50 m/z	Set Capillary	1500 V	Set Dry Heater	180 °C
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min



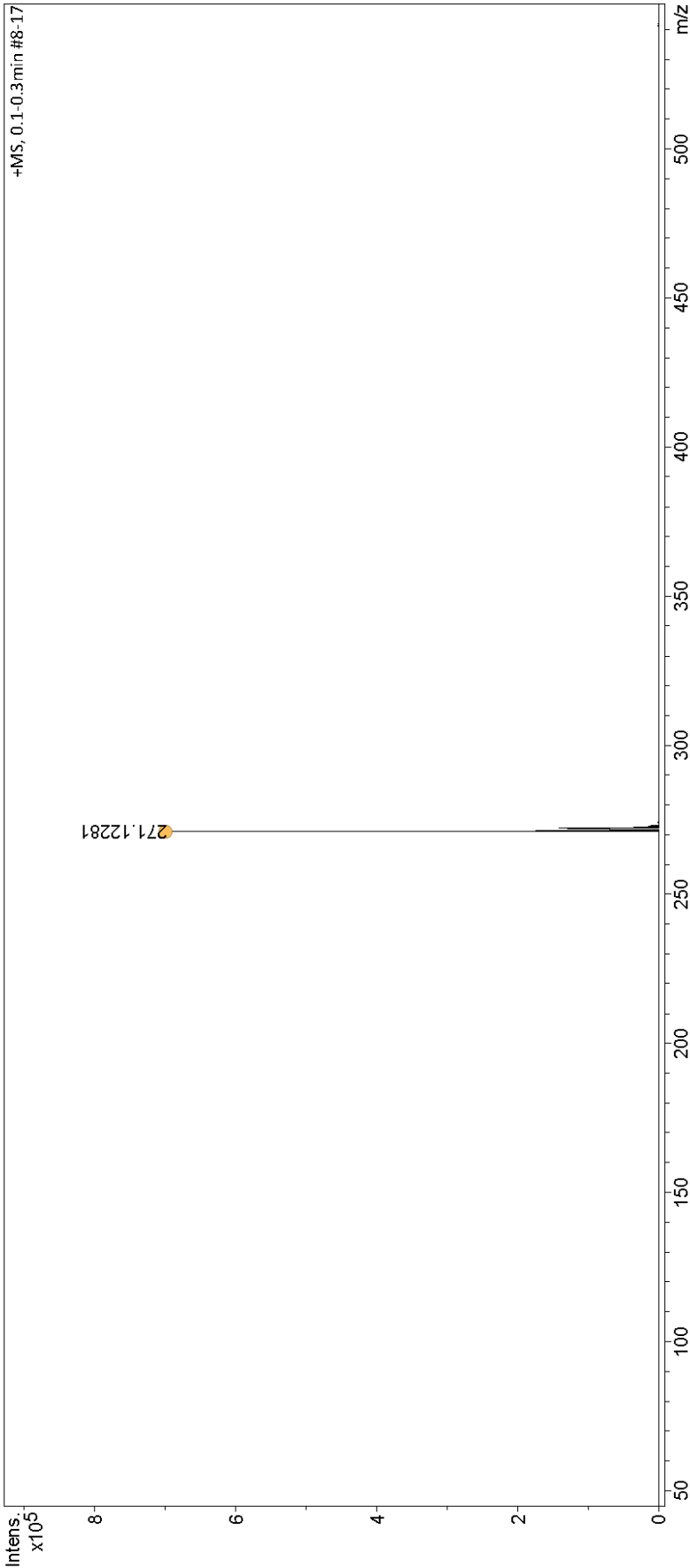
HR-ESI-MS (Bruker maXis)

Analysis Info

Analysis Name	D:\Data\Service\6513\alhrs.d	Acquisition Date	7/7/2014 5:02:28 PM
Method	tune_low_modified_09_01_14_pos.m	Operator	ust
Sample Name	BPh	Instrument	maXis
Comment	Solvent: MeOH/H2O 1:1		255552.00033
	Client: Grieco		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Scan Begin	50 m/z	Set Capillary	1000 V	Set Dry Heater	180 °C
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min



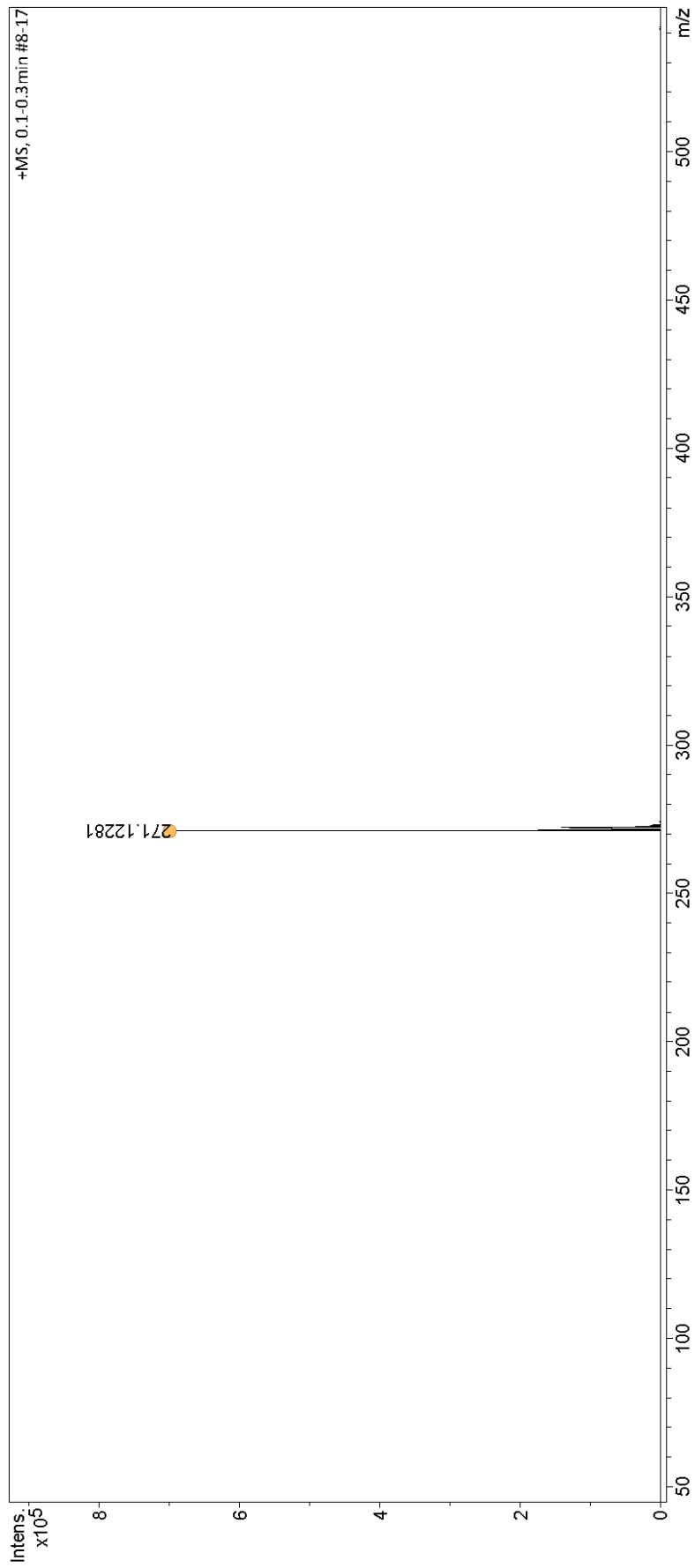
HR-ESI-MS (Bruker maXis)

Analysis Info

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Method	tune_low_modified_09_01_14_pos.m	Operator	ust
Sample Name	BPh	Instrument	maXis
Comment	Solvent: MeOH/H2O 1:1		255552.00033
	Client: Grieco		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Scan Begin	50 m/z	Set Capillary	1000 V	Set Dry Heater	180 °C
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min



HR-ESI-MS (Bruker maXis)

Analysis Info

Analysis Name D:\Data\Service\6513alhres.d
Method tune_low_modified_09_01_14_pos.m
Sample Name BPh
Comment Solvent: MeOH/H2O 1:1
Client: Grieco

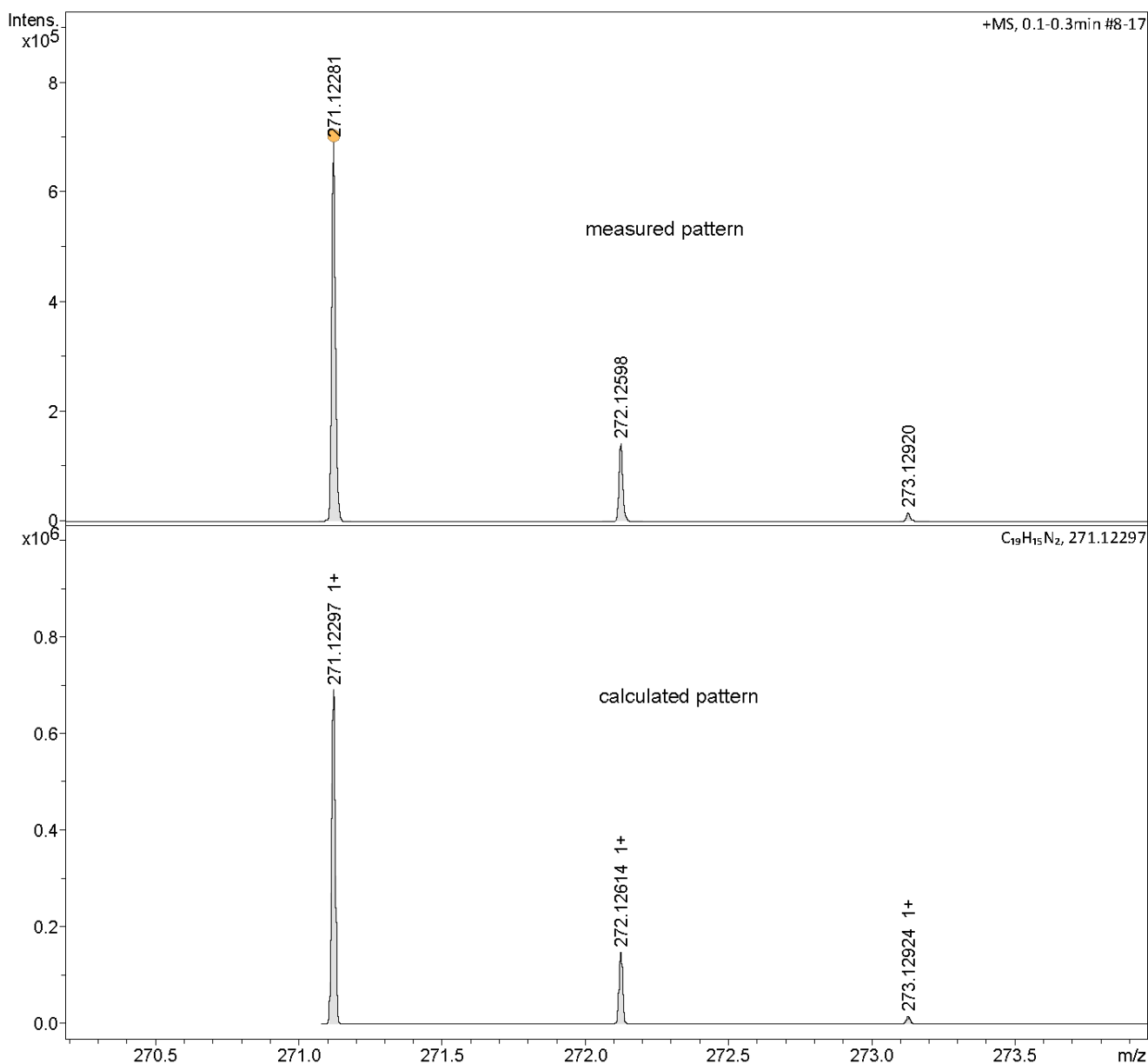
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Operator ust

Instrument maXis 255552.00033

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
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Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min



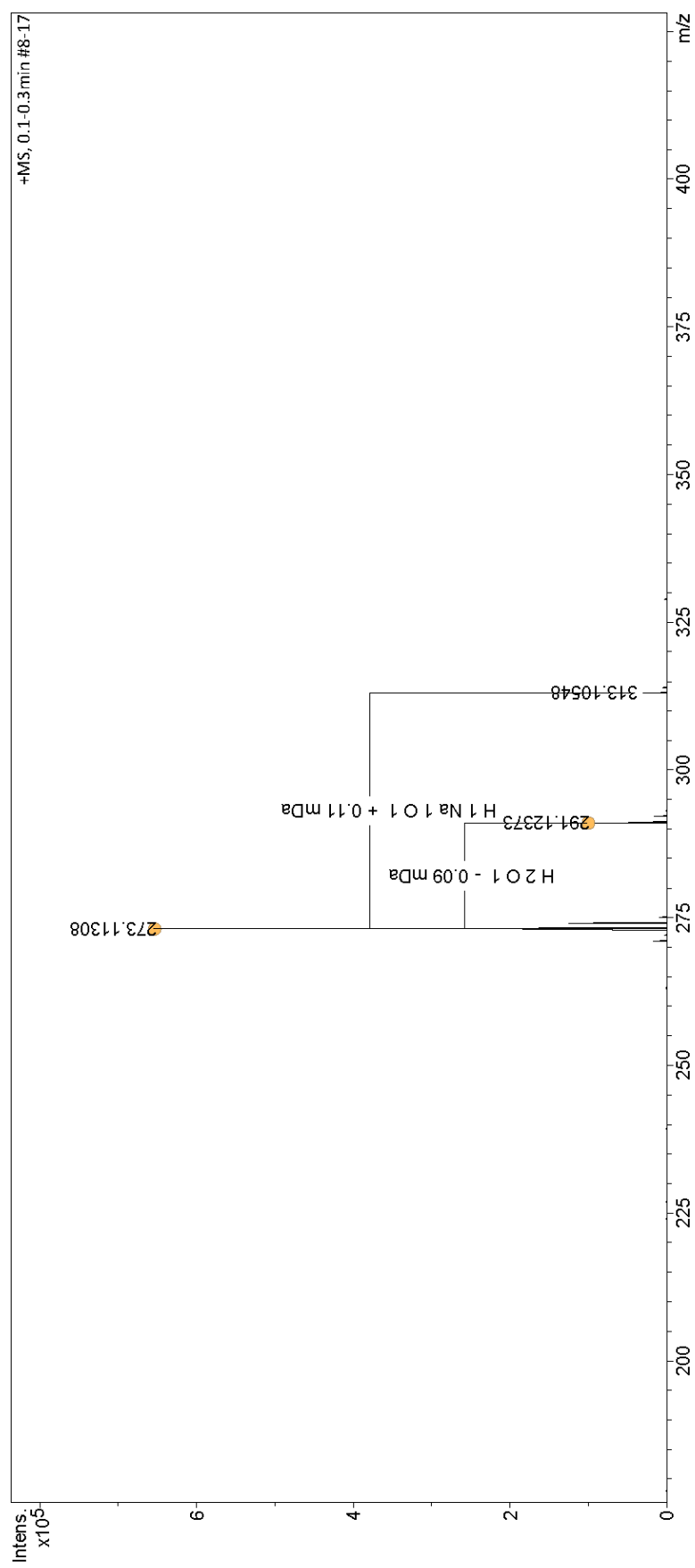
HR-ESI-MS (Bruker maXis)

Analysis Info

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Sample Name	BPY	Instrument	maXis
Comment	Solvent: MeOH/H2O 1:1		255552.00033
	Client: Grieco		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive
Scan Begin	50 m/z	Set Nebulizer	0.5 Bar
Scan End	3000 m/z	Set Capillary	1500 V
		Set End Plate Offset	-500 V
		Set Dry Heater	180 °C
		Set Dry Gas	4.0 l/min



HR-ESI-MS (Bruker maXis)

Analysis Info

Analysis Name D:\Data\Service\6514alhres.d
Method tune_low_modified_09_01_14_pos.m
Sample Name BPy
Comment Solvent: MeOH/H2O 1:1
Client: Grieco

Acquisition Date 7/7/2014 5:22:43 PM

Operator ust
Instrument maXis 255552.00033

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
Scan Begin	50 m/z	Set Capillary	1500 V	Set Dry Heater	180 °C
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min

