

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 13 2016000005.d
Method FengPOSNEW.m
Sample Name 6-Chlorothieno(3,2-c)quinolin-4(5H)-one
Comment

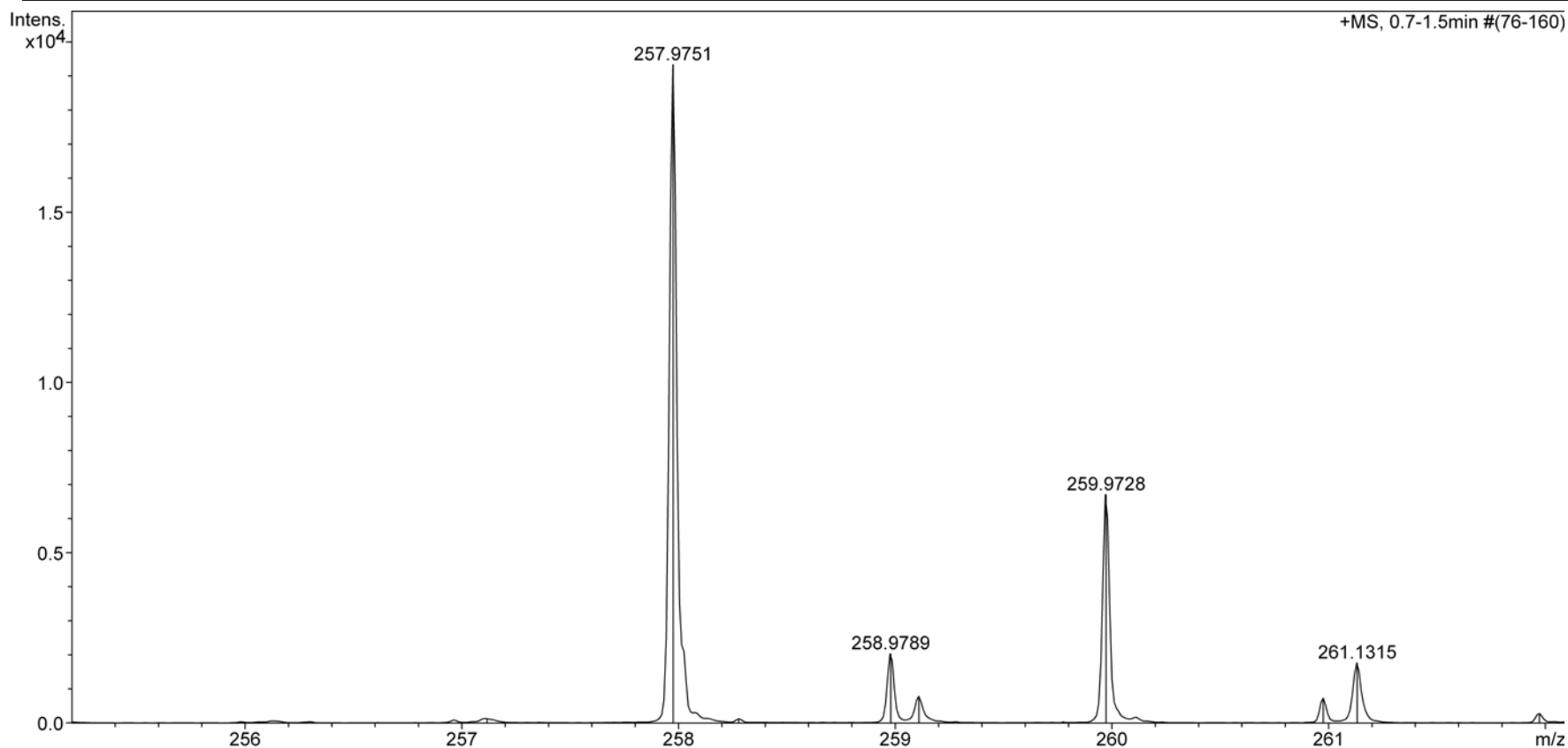
Acquisition Date 10/13/2016 11:25:36 AM

Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI Ion Polarity Positive
Scan Range n/a Capillary Exit 100.0 V
Scan Begin 50 m/z Hexapole RF 150.0 V
Scan End 2000 m/z Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdB	N Rule	e ⁻
C 11 H 6 Cl 1 N 1 Na 1 O 1 S 1	0.02	257.9751	-0.20	-14.54	8.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 13 2016000007.d
Method FengPOSNEW.m
Sample Name 8-Chlorothieno(3,2-c)quinolin-4(5H)-one
Comment

Acquisition Date 10/13/2016 11:44:06 AM

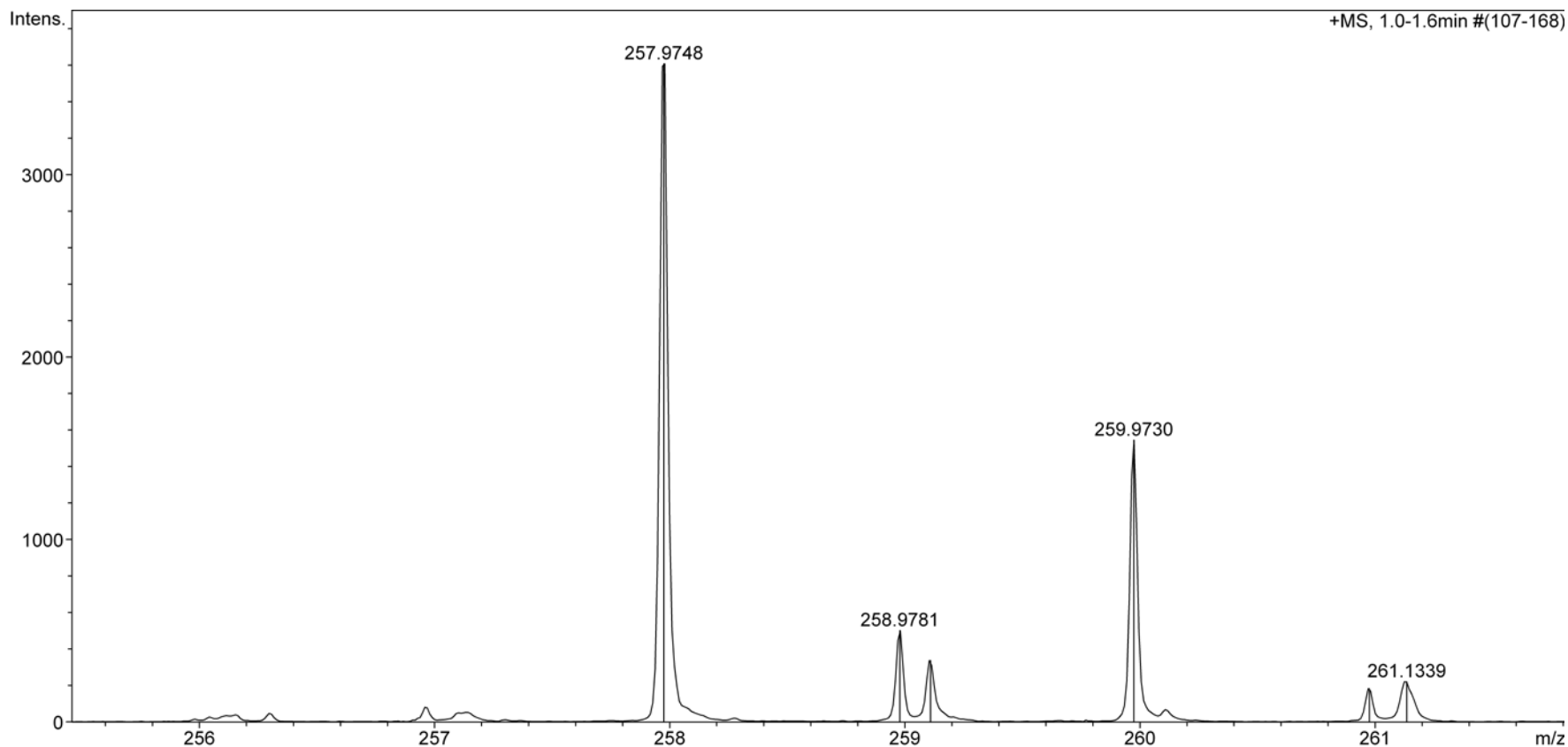
Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdB	N Rule	e ⁻
C 11 H 6 Cl 1 N 1 Na 1 O 1 S 1	0.03	257.9751	1.07	-0.15	8.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 13 2016000006.d
Method FengPOSNEW.m
Sample Name 8-Fluorothieno(3,2-c)quinolin-4(5H)-one
Comment

Acquisition Date 10/13/2016 11:35:23 AM

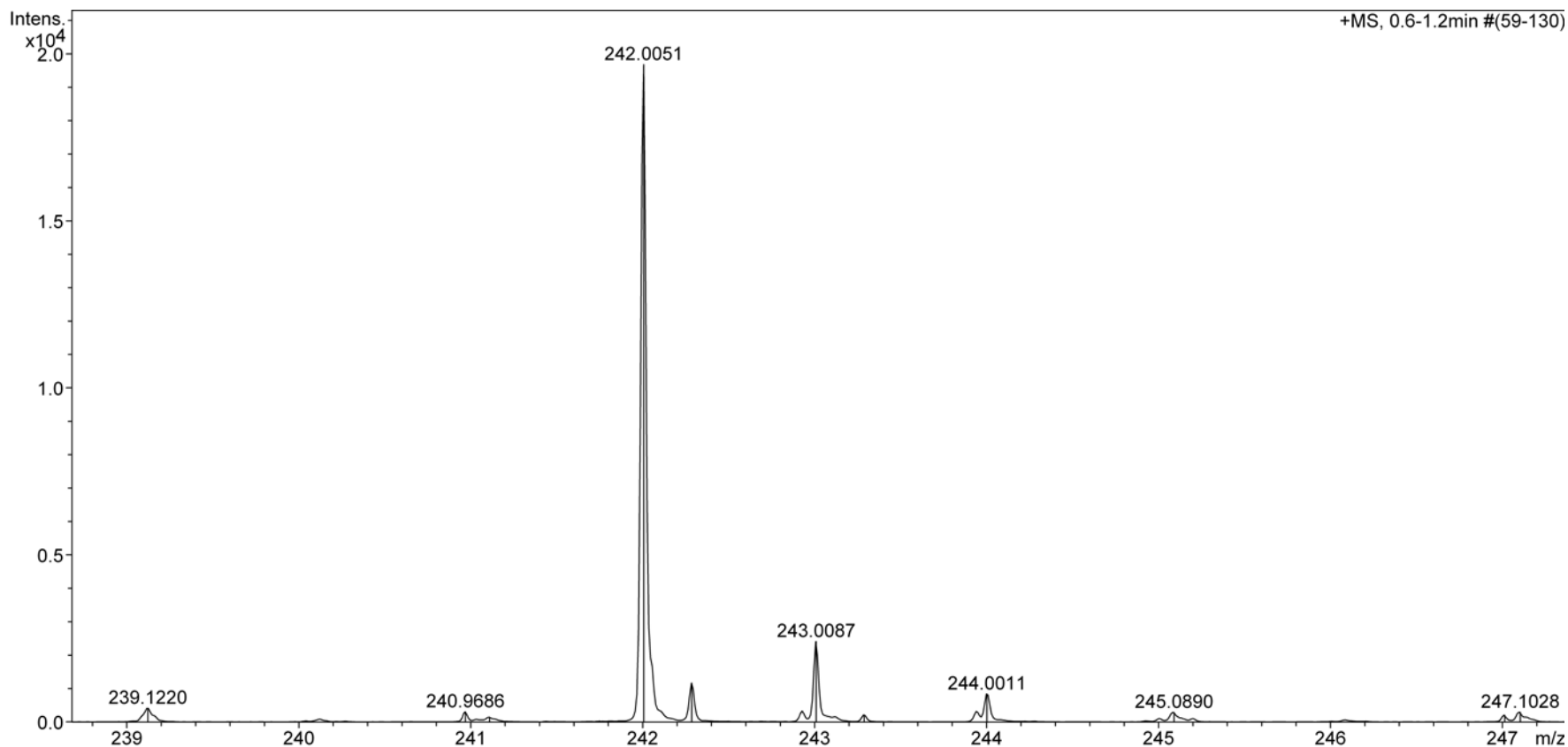
Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

	Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdB	N Rule	e ⁻
C 11 H 6 F 1 N 1 Na 1 O 1 S 1		0.01	242.0046	-2.12	-7.66	8.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 13 2016000009.d
Method FengPOSNEW.m
Sample Name 8-(Trifluoromethyl)thieno(3,2-c)quinolin-4(5H)-one
Comment

Acquisition Date 10/13/2016 12:00:46 PM

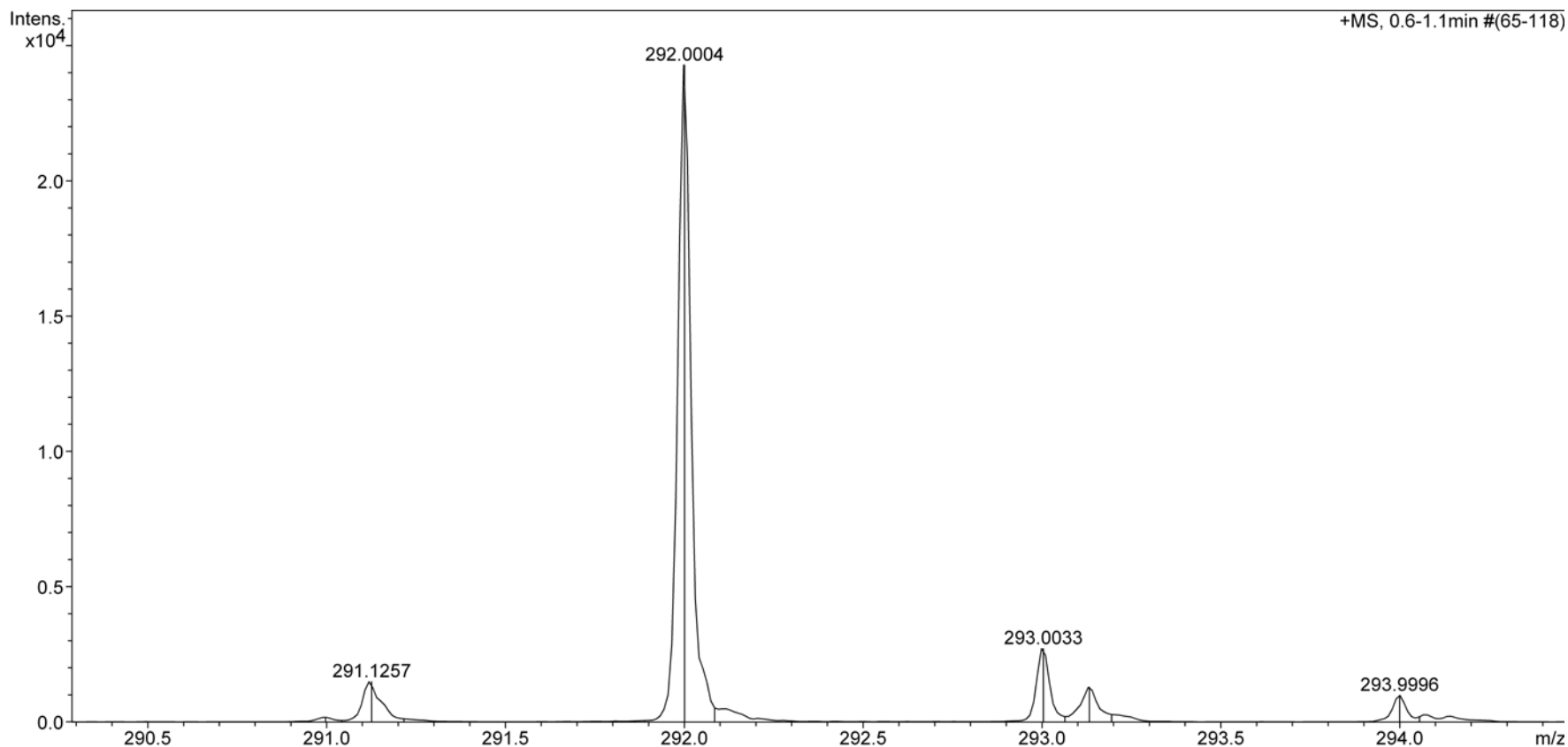
Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdb	N Rule	e ⁻
C 12 H 6 F 3 N 1 Na 1 O 1 S 1	0.02	292.0014	3.56	24.18	8.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 13 2016000010.d
Method FengPOSNEW.m
Sample Name 6-Methoxythieno(3,2-c)quinolin-4(5H)-one
Comment

Acquisition Date 10/13/2016 1:23:39 PM

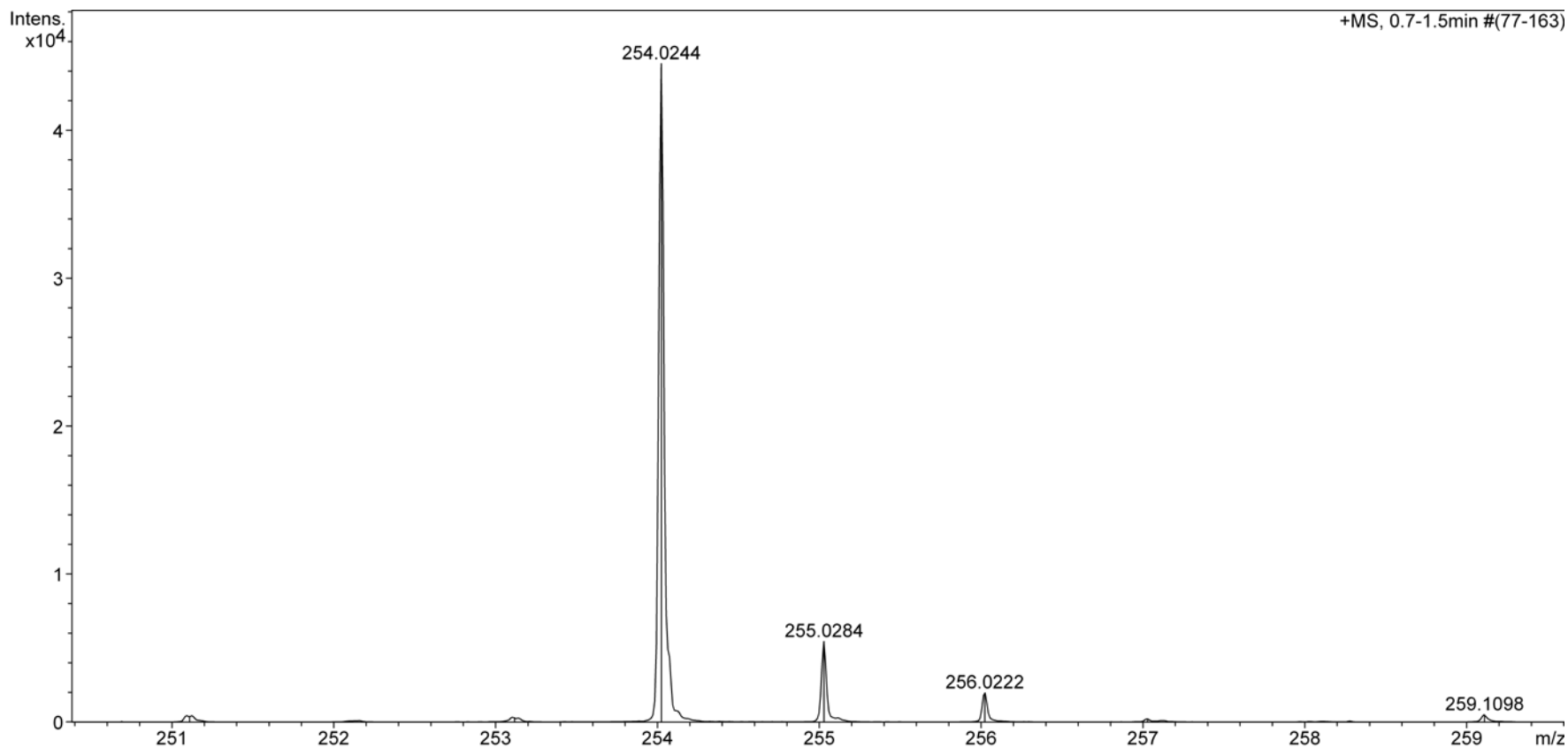
Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdb	N Rule	e ⁻
C 12 H 9 N 1 Na 1 O 2 S 1	0.01	254.0246	1.05	0.42	8.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 13 2016000011.d
Method FengPOSNEW.m
Sample Name 8-Methoxythieno(3,2-c)quinolin-4(5H)-one
Comment

Acquisition Date 10/13/2016 1:33:45 PM

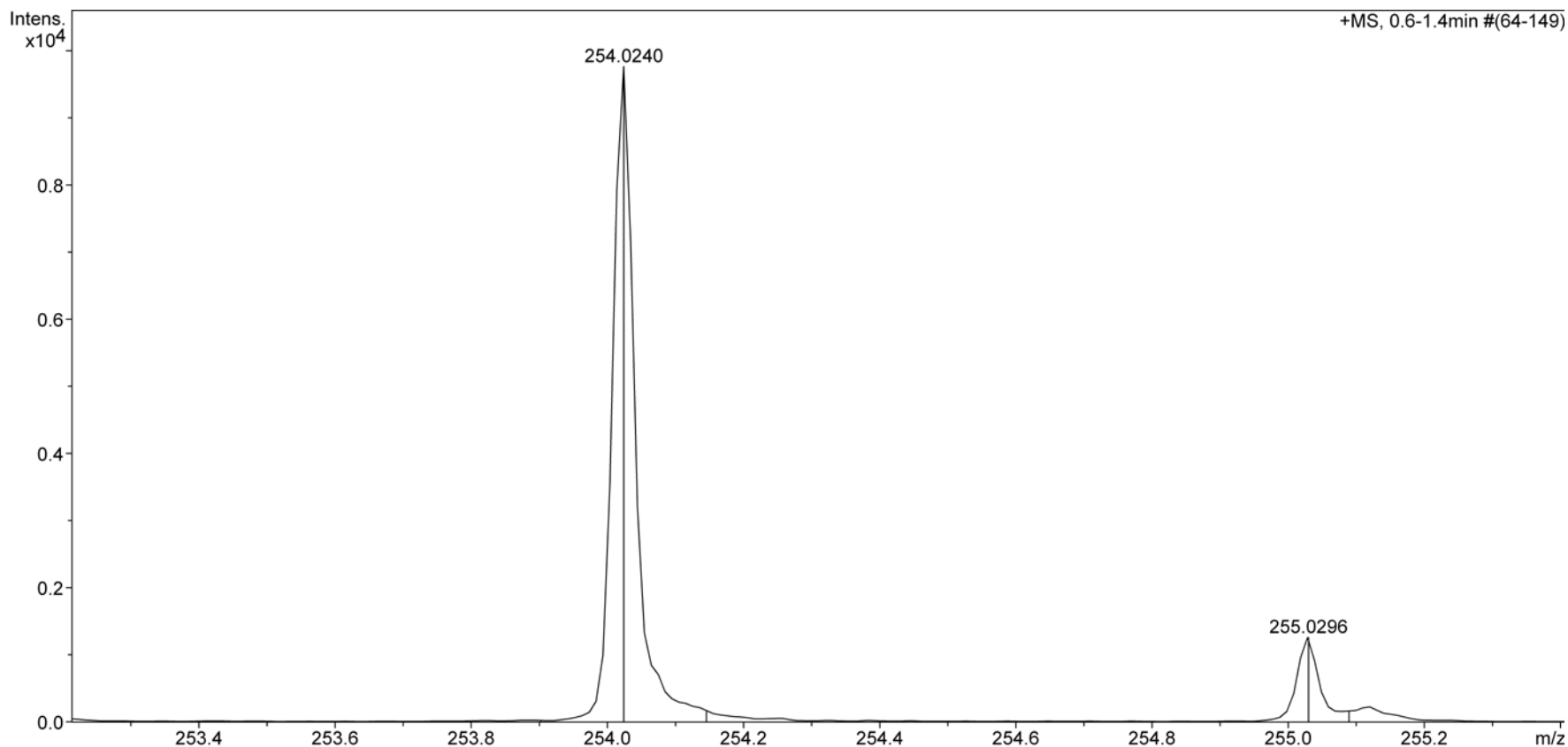
Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdb	N Rule	e ⁻
C 12 H 9 N 1 Na 1 O 2 S 1	0.01	254.0246	2.31	1.03	8.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 13 2016000008.d
Method FengPOSNEW.m
Sample Name 6-Methylthieno(3,2-c)quinolin-4(5H)-one
Comment

Acquisition Date 10/13/2016 11:51:42 AM

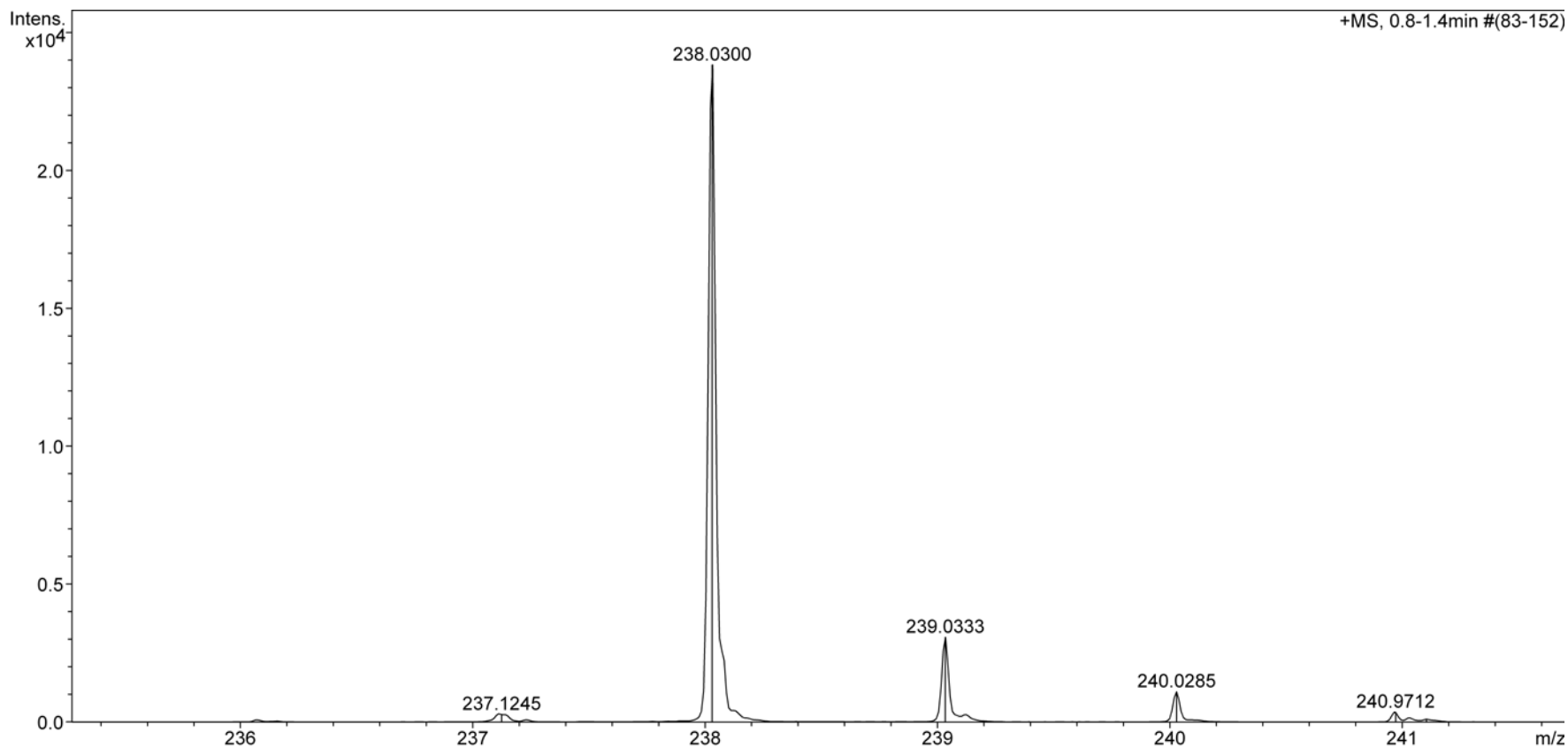
Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdB	N Rule	e ⁻
C 12 H 9 N 1 Na 1 O 1 S 1	0.01	238.0297	-1.19	2.68	8.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 13 2016000012.d
Method FengPOSNEW.m
Sample Name N-((4-Oxo-4,5-dihydrothieno(3,2-c)quinolin-8-yl)sulfonyl)aceta
Comment

Acquisition Date 10/13/2016 1:44:15 PM

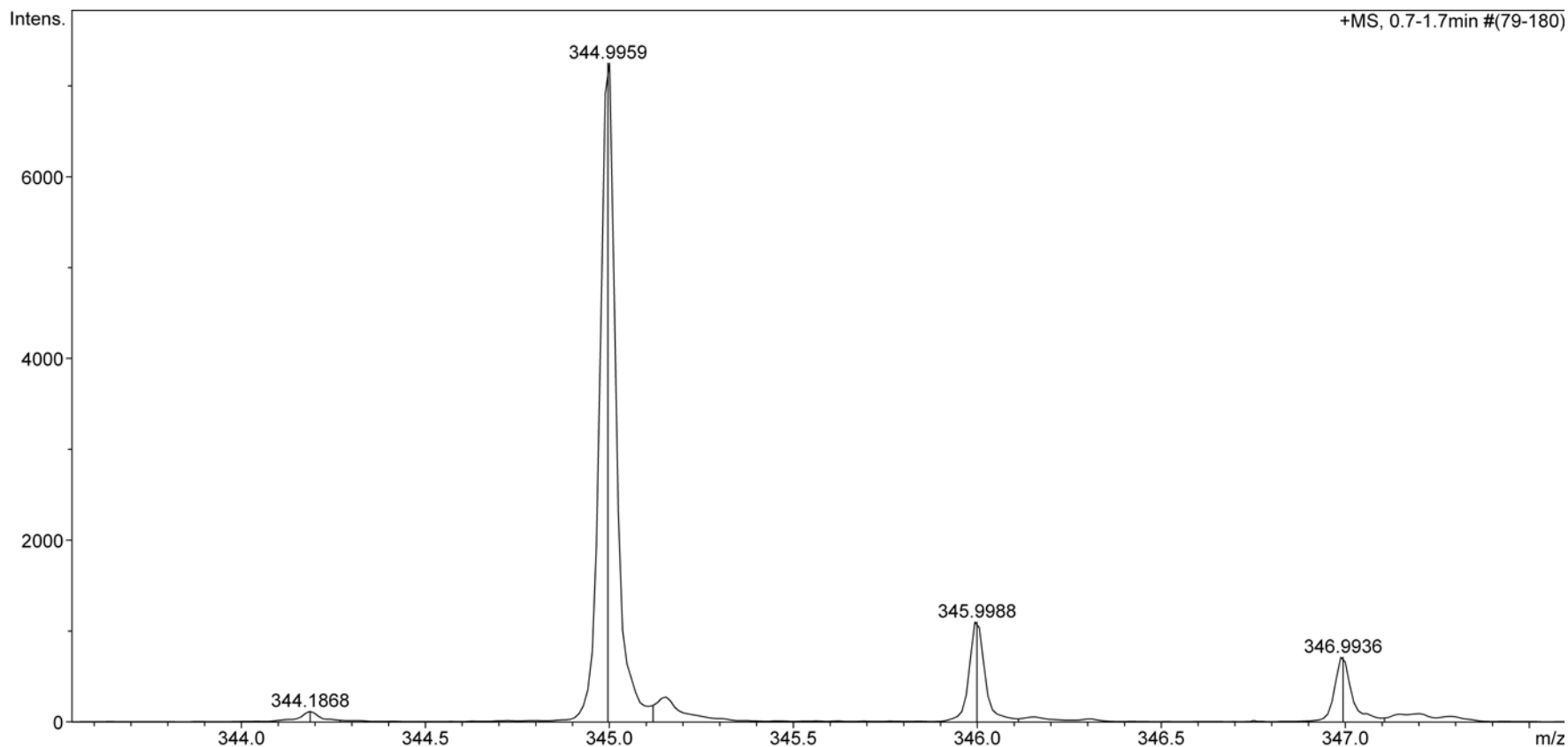
Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdB	N Rule	e ⁻
C 13 H 10 N 2 Na 1 O 4 S 2	0.01	344.9974	4.41	-12.89	9.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 13 2016000013.d
Method FengPOSNEW.m
Sample Name N,N-Diethyl-4-oxo-4,5dihydrothieno(3,2-c)qui-8-sulfonamide
Comment

Acquisition Date 10/13/2016 1:56:12 PM

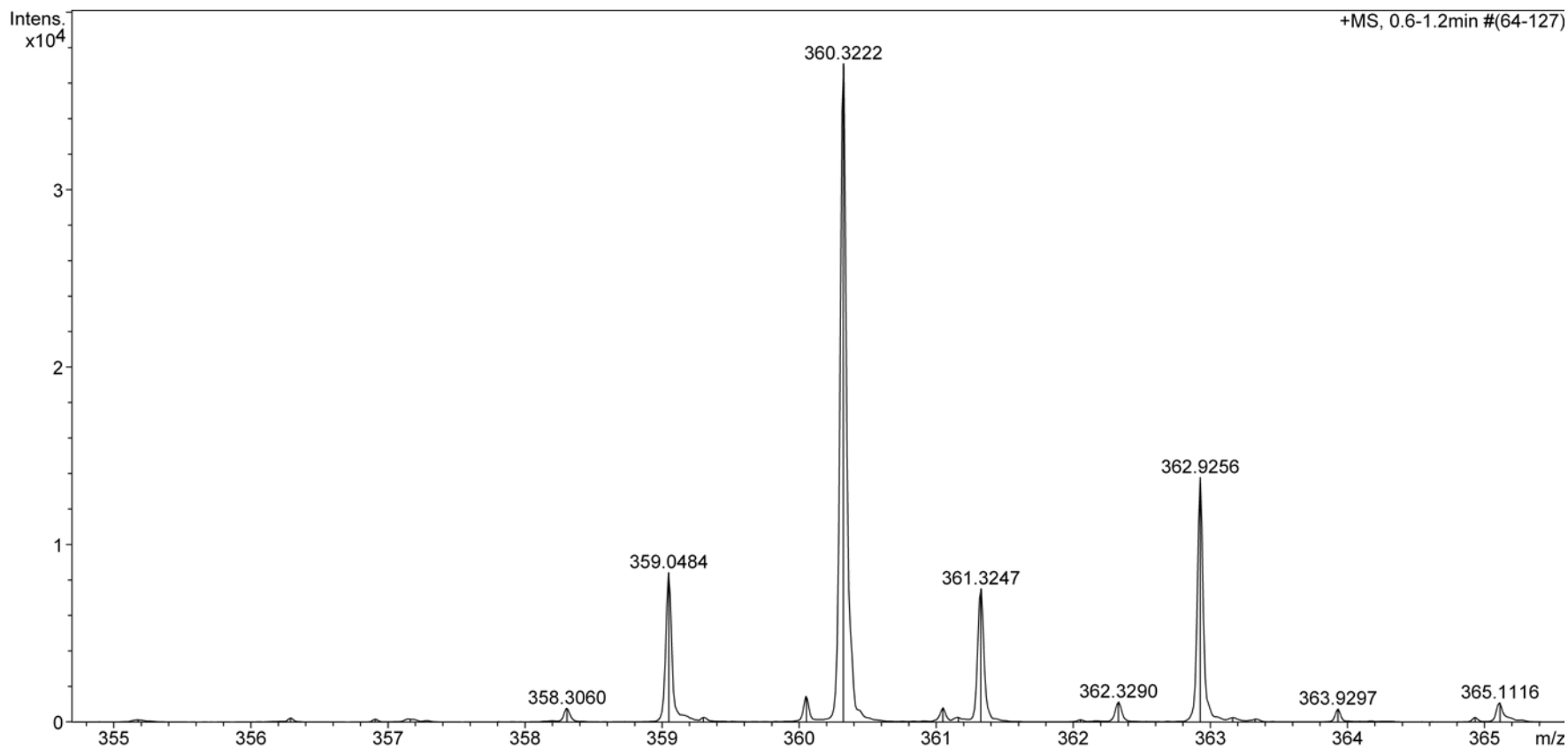
Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdB	N Rule	e ⁻
C 15 H 16 N 2 Na 1 O 3 S 2	0.01	359.0495	3.04	-5.58	8.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 13 2016000014.d
Method FengPOSNEW.m
Sample Name 2-Chlorothieno(3,2-c)quinolin-4(5H)-one
Comment

Acquisition Date 10/13/2016 2:09:33 PM

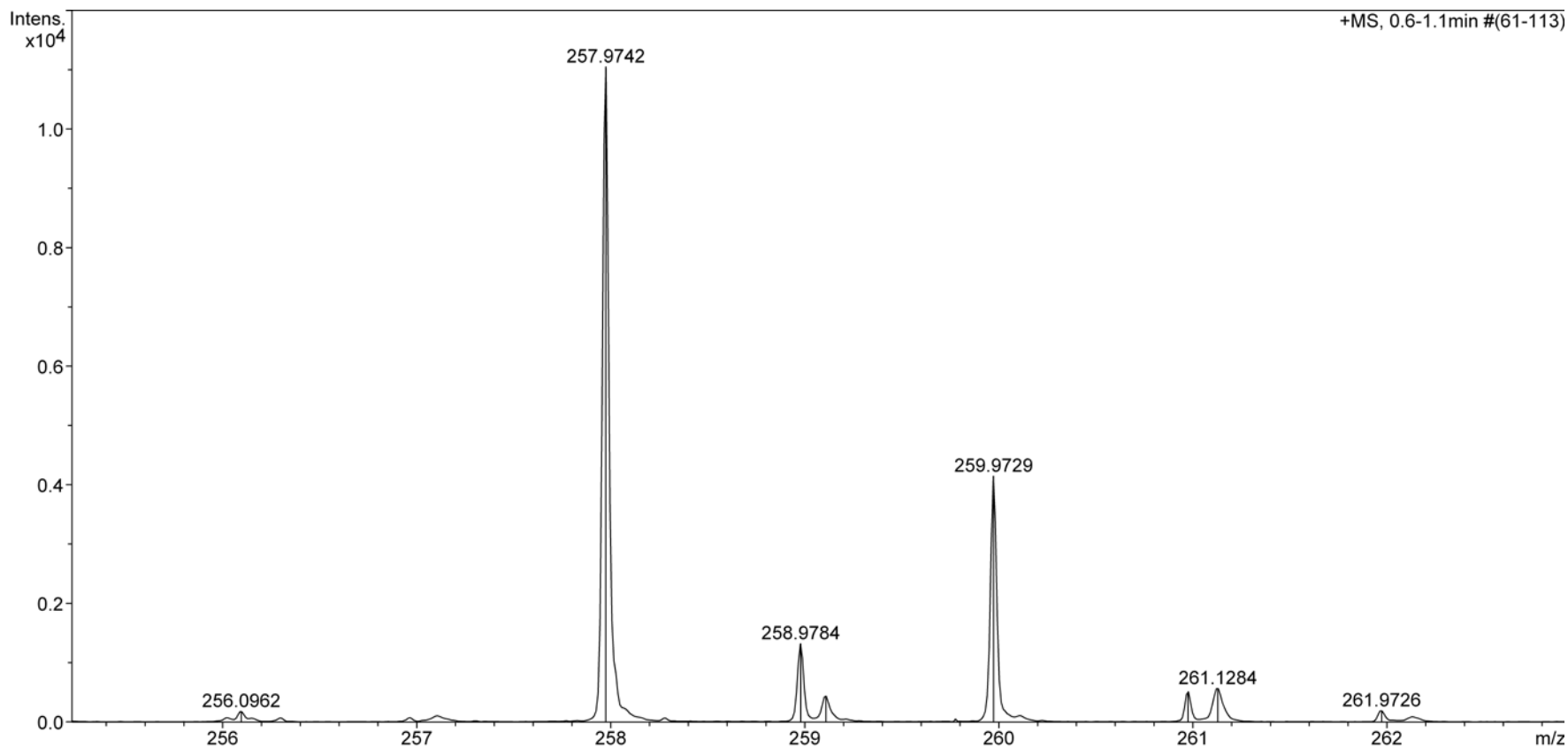
Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdB	N Rule	e ⁻
C 11 H 6 Cl 1 N 1 Na 1 O 1 S 1	0.01	257.9751	3.55	-8.79	8.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 13 2016000015.d
Method FengPOSNEW.m
Sample Name 2,6-Dichlorothieno(3,2-c)quinolin-4(5H)-one
Comment

Acquisition Date 10/13/2016 2:18:33 PM

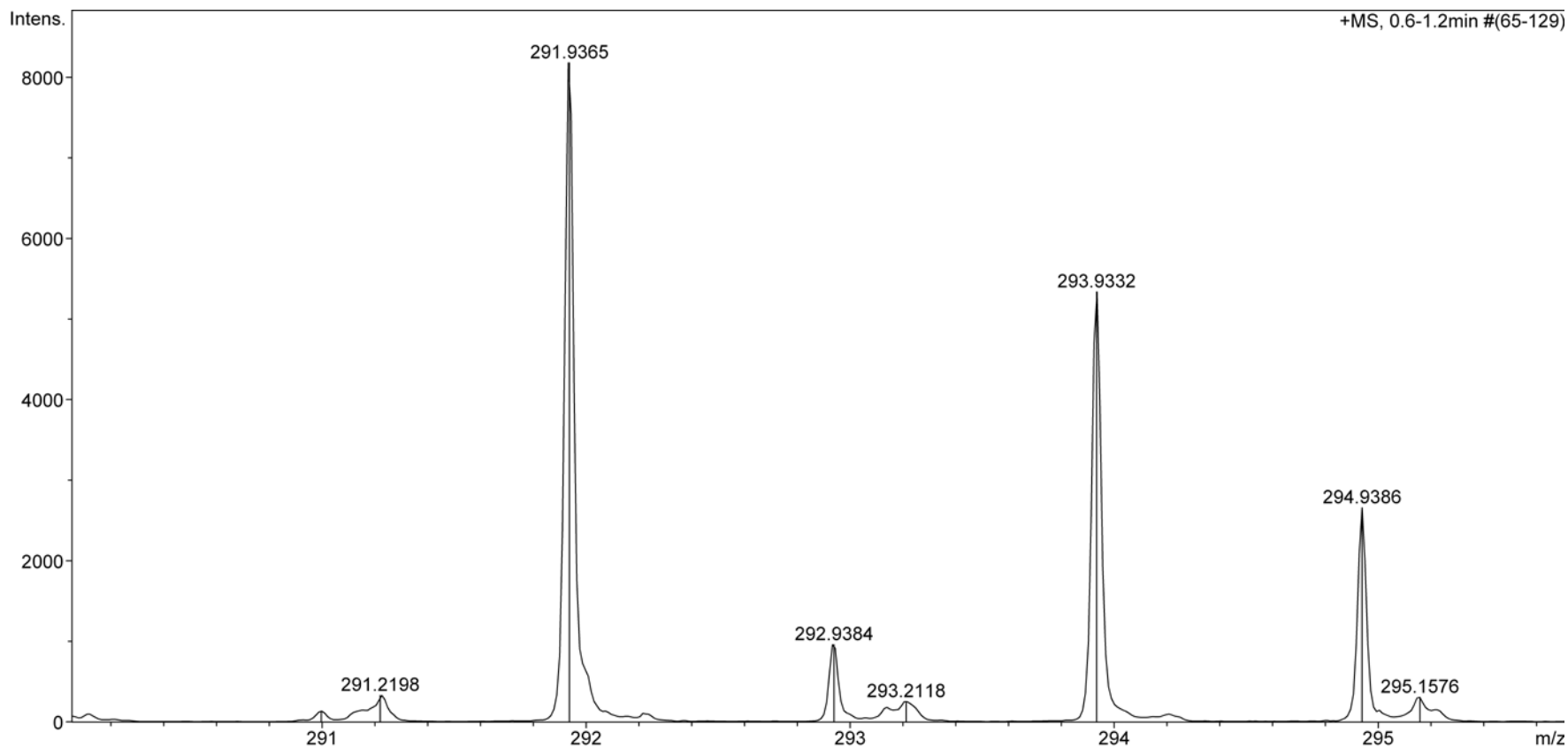
Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdB	N Rule	e ⁻
C 11 H 5 Cl 2 N 1 Na 1 O 1 S 1	0.10	291.9361	-1.17	-1.73	8.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 13 2016000016.d
Method FengPOSNEW.m
Sample Name 2,8-Dichlorothieno(3,2-c)quinolin-4(5H)-one
Comment

Acquisition Date 10/13/2016 2:27:01 PM

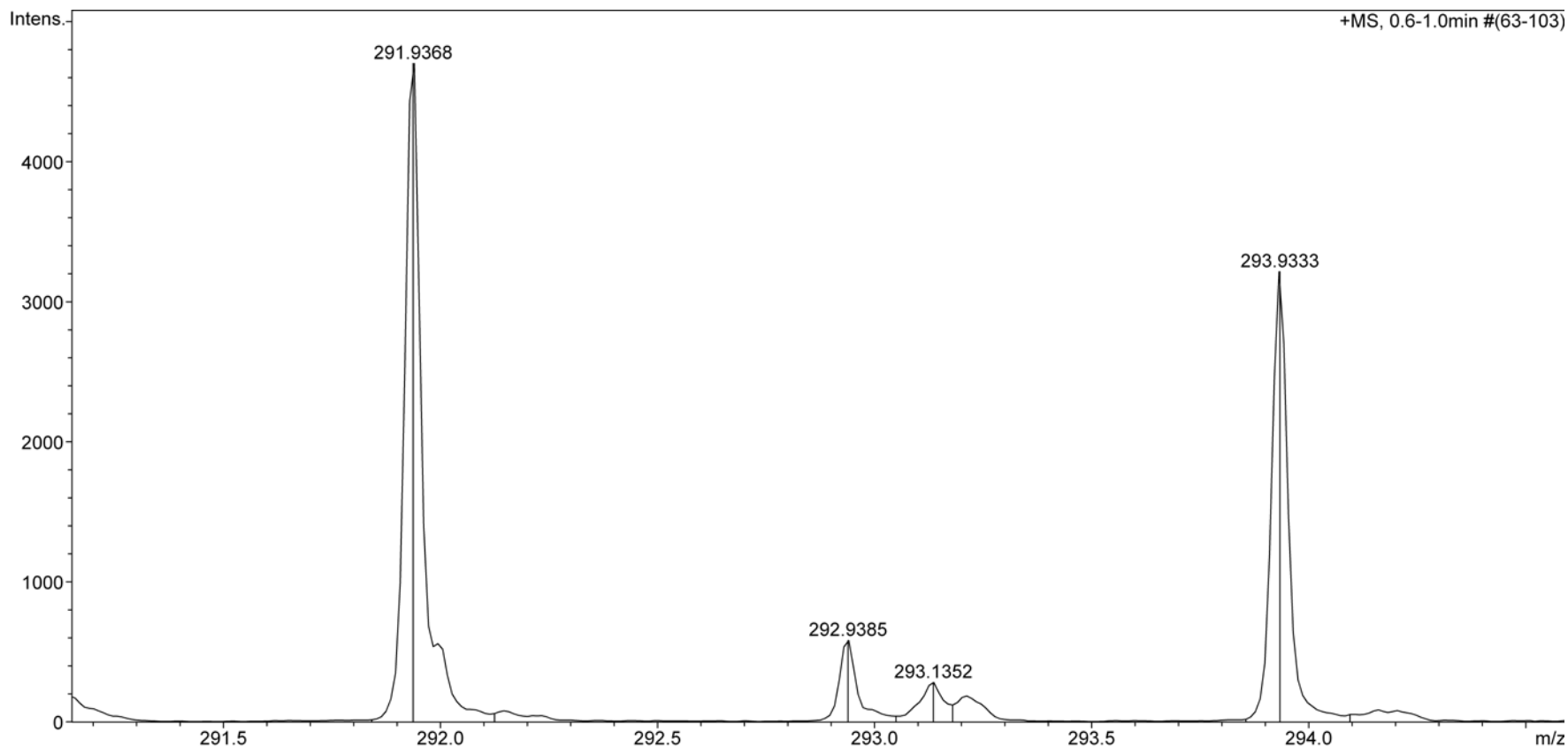
Operator Administrator
Instrument microTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdB	N Rule	e ⁻
C 11 H 5 Cl 2 N 1 Na 1 O 1 S 1	0.13	291.9361	-2.38	-3.10	8.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 13 2016000017.d
Method FengPOSNEW.m
Sample Name 2-Chloro-8-Fluorothieno(3,2-c)quinolin-4(5H)-one
Comment

Acquisition Date 10/13/2016 2:35:20 PM

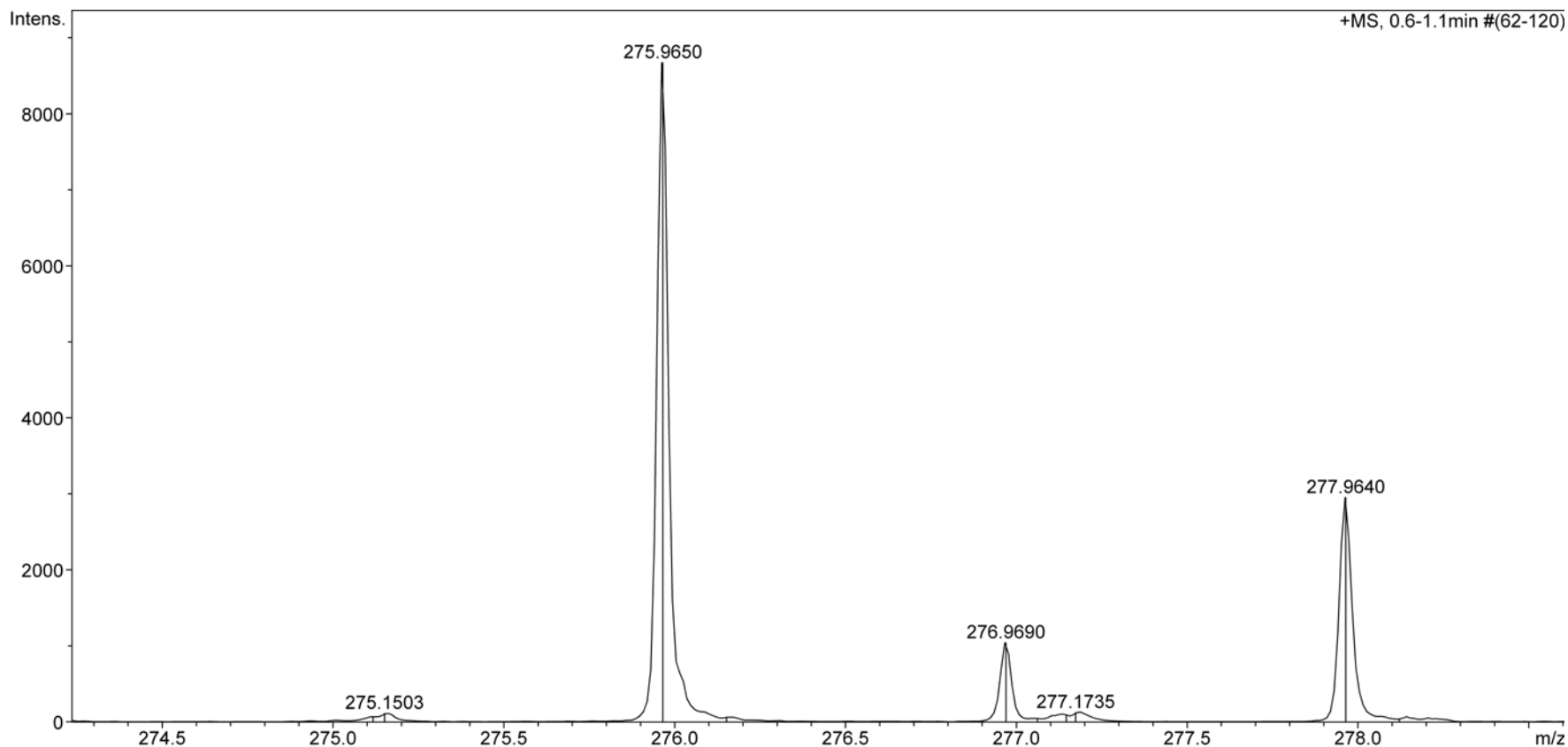
Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdB	N Rule	e ⁻
C 11 H 5 Cl 1 F 1 N 1 Na 1 O 1 S 1	0.02	275.9657	2.40	-0.32	8.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 13 2016000018.d
Method FengPOSNEW.m
Sample Name N-((2-Cl-4-oxo-4,5dihydrothieno(3,2-c)quin-8-yl)sulfonyl)acet
Comment

Acquisition Date 10/13/2016 2:45:27 PM

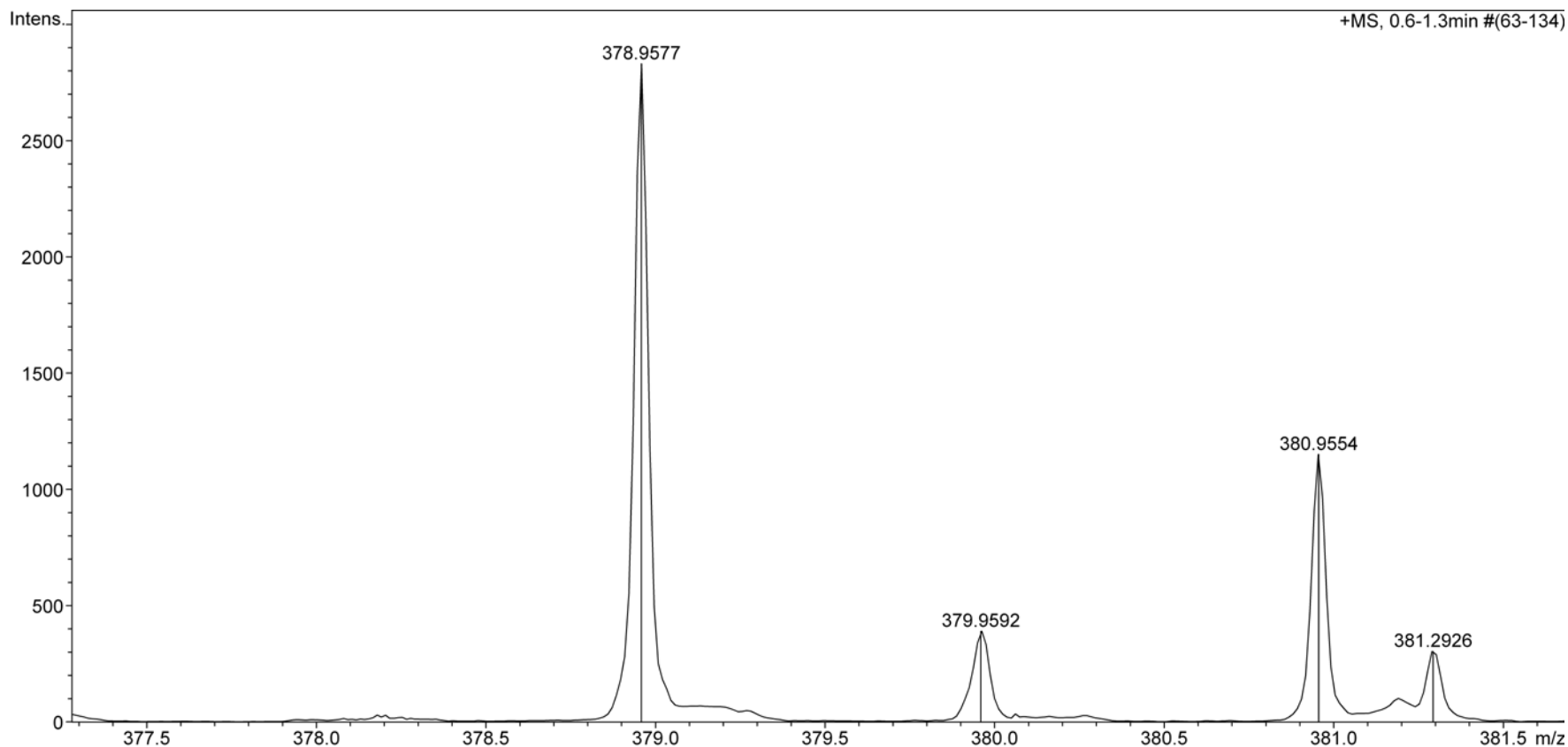
Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdB	N Rule	e ⁻
C 13 H 9 Cl 1 N 2 Na 1 O 4 S 2	0.02	378.9584	2.02	1.66	9.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 13 2016000019.d
Method FengPOSNEW.m
Sample Name 2-Cl-NN-di-4-oxo-4,5dihydrothieno(3,2-c)quin-8-sulfonamide
Comment

Acquisition Date 10/13/2016 2:55:24 PM

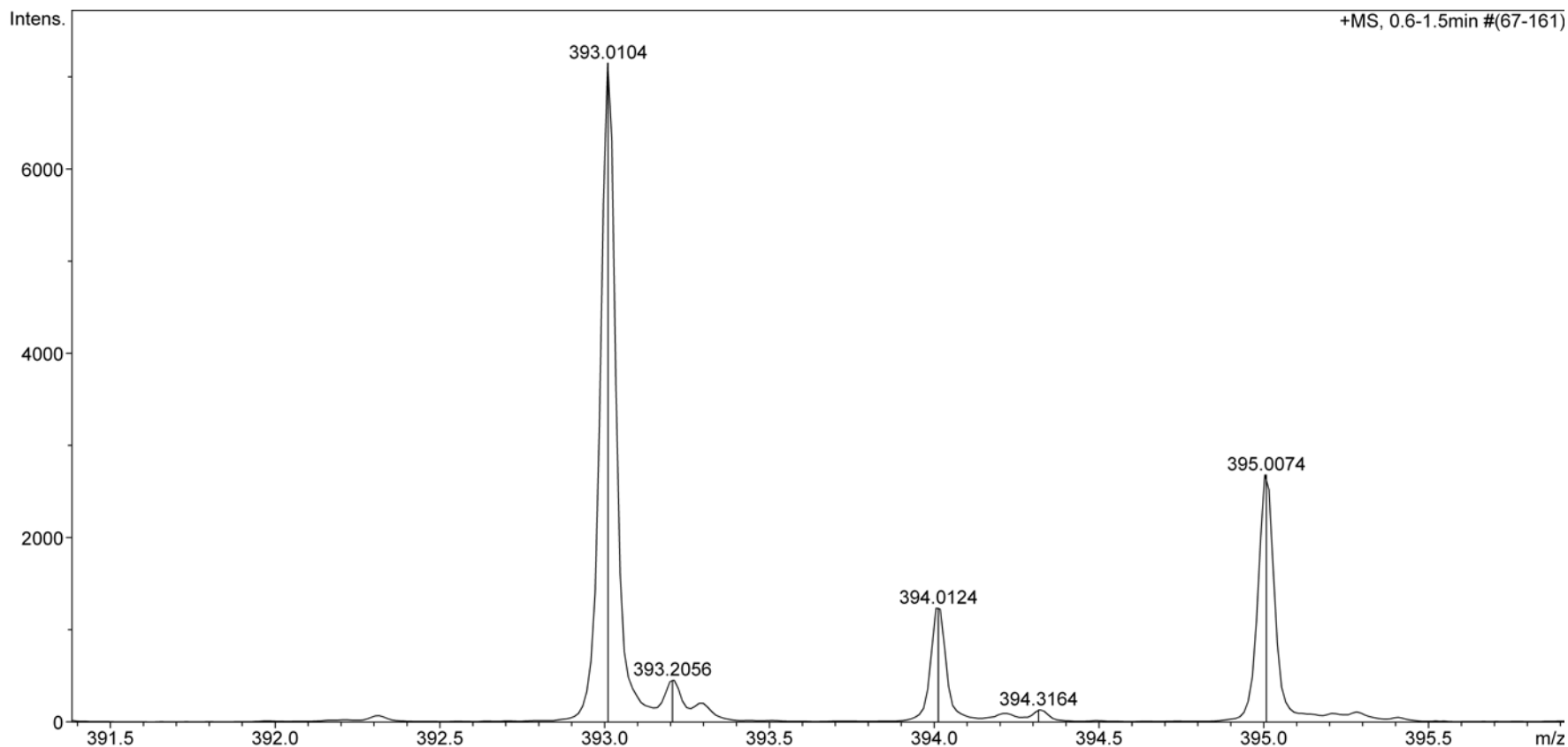
Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdB	N Rule	e ⁻
C 15 H 15 Cl 1 N 2 Na 1 O 3 S 2	0.03	393.0105	0.25	0.38	8.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 13 2016000020.d
Method FengPOSNEW.m
Sample Name 7-chlorobenzo(h)-1,6-naphthyridin-5(6H)-one
Comment

Acquisition Date 10/13/2016 3:06:21 PM

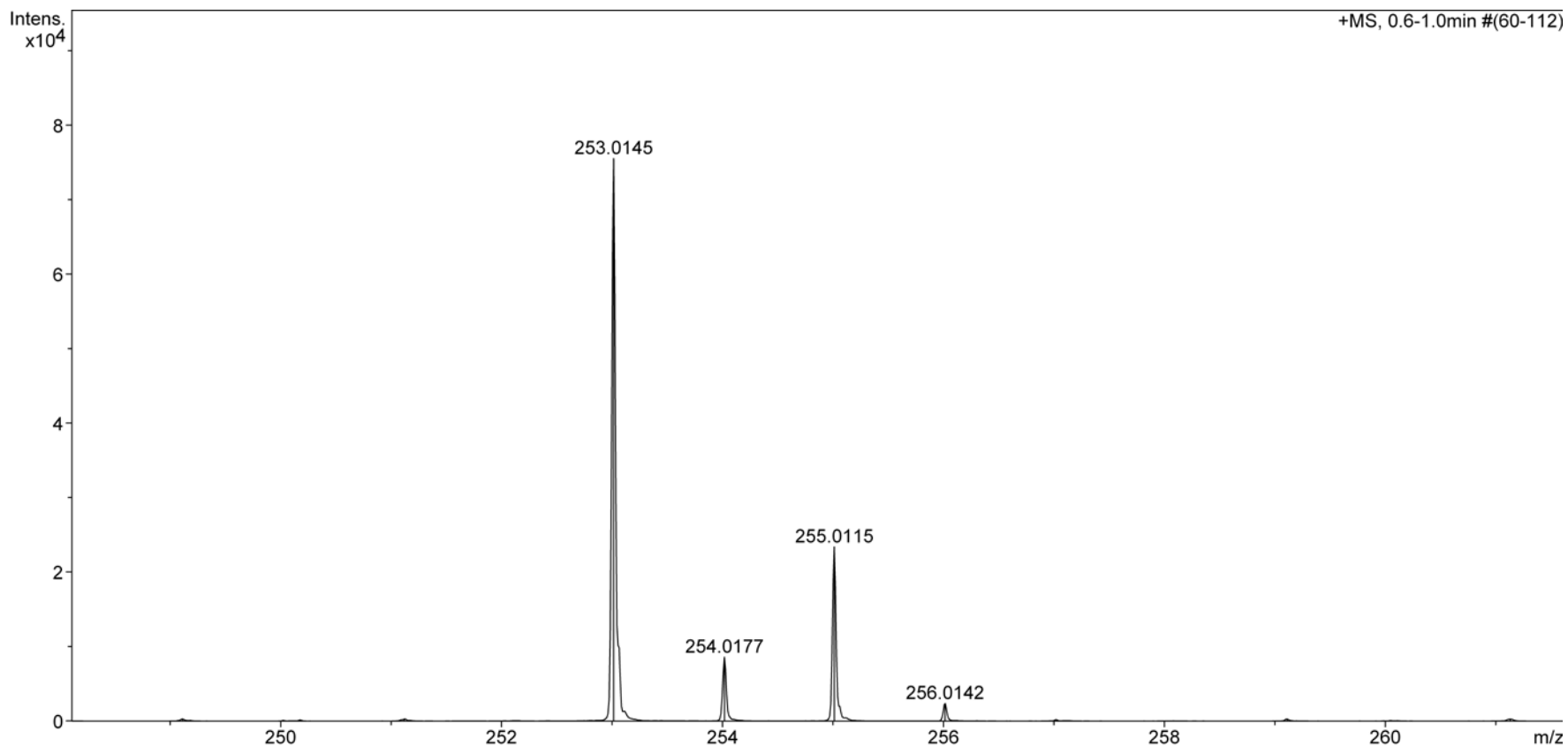
Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdb	N Rule	e ⁻
C 12 H 7 Cl 1 N 2 Na 1 O 1	0.02	253.0139	-2.27	-2.06	9.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 13 2016000023.d
Method FengPOSNEW.m
Sample Name 9-chlorobenzo(h)-1,6-naphthyridin-5(6H)-one
Comment

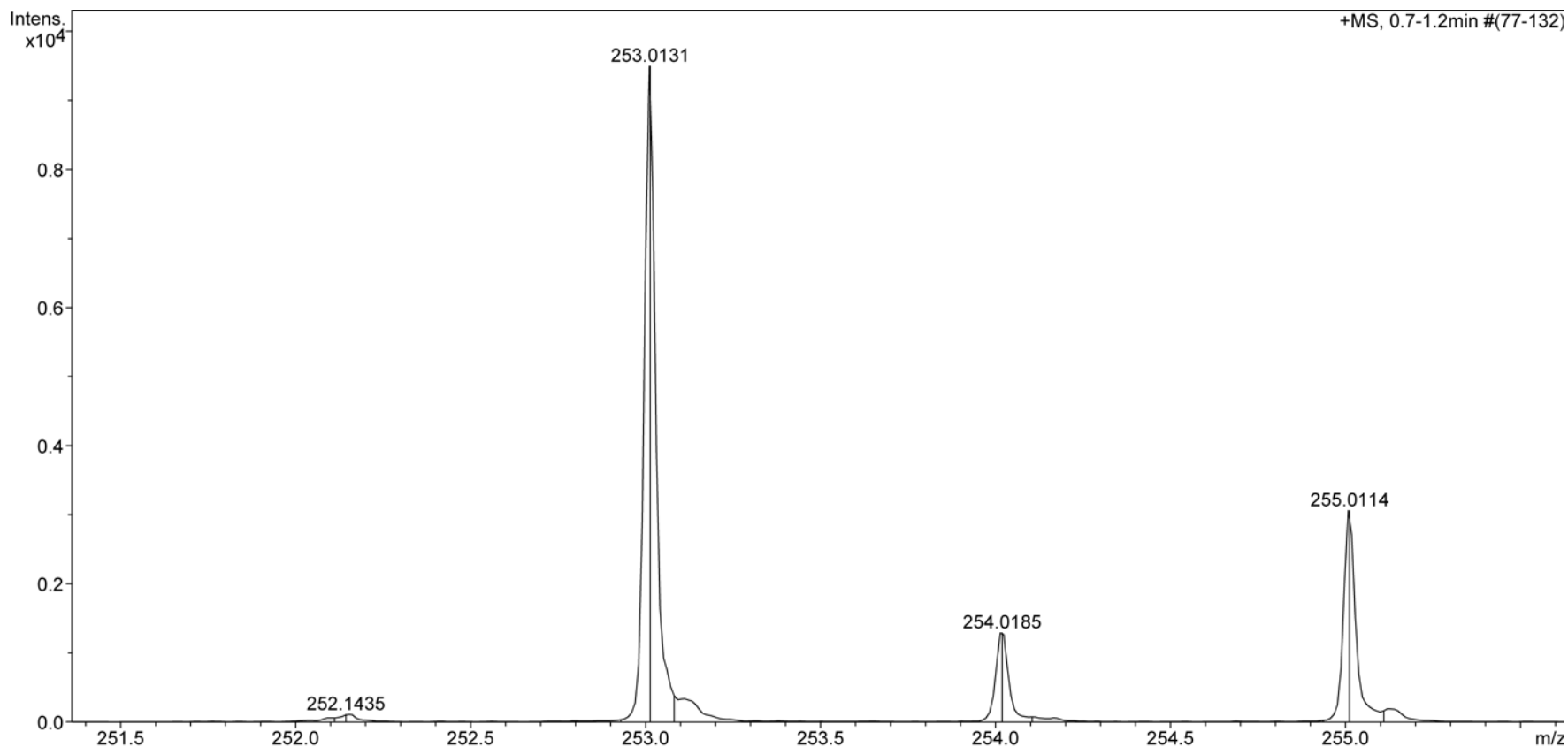
Acquisition Date 10/13/2016 3:26:42 PM

Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive
Scan Range	n/a	Capillary Exit	100.0 V
Scan Begin	50 m/z	Hexapole RF	150.0 V
Scan End	2000 m/z	Skimmer 1	50.0 V
		Hexapole 1	23.0 V

Set Corrector Fill	45 V
Set Pulsar Pull	400 V
Set Pulsar Push	400 V
Set Reflector	1300 V
Set Flight Tube	9000 V
Set Detector TOF	2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdb	N Rule	e ⁻
C 12 H 7 Cl 1 N 2 Na 1 O 1	0.00	253.0139	3.34	-1.89	9.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 13 2016000022.d
Method FengPOSNEW.m
Sample Name 9-fulorobenzo(h)-1,6-naphthyridin-5(6H)-one
Comment

Acquisition Date 10/13/2016 3:16:56 PM

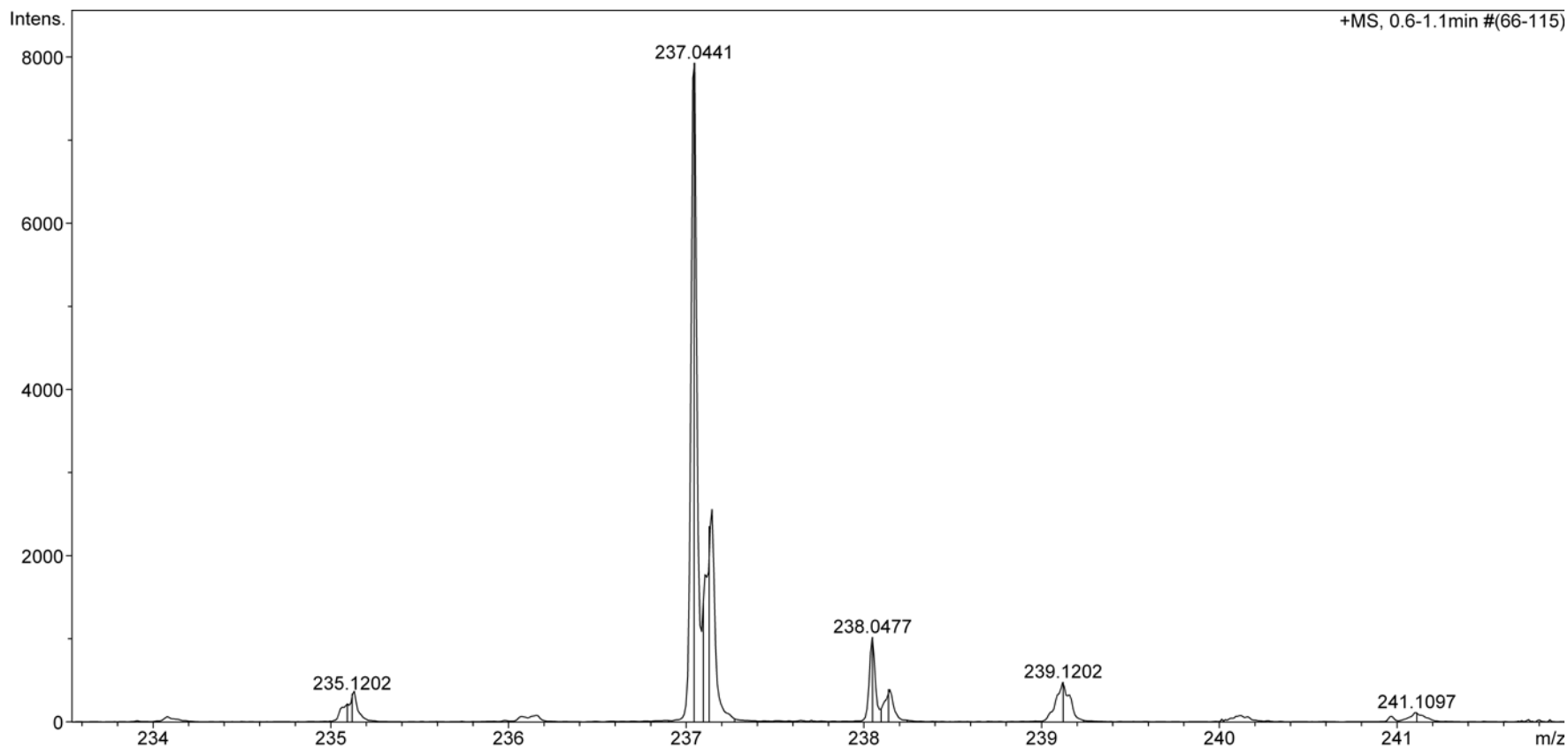
Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdb	N Rule	e ⁻
C 12 H 7 F 1 N 2 Na 1 O 1	0.01	237.0435	-2.79	-12.96	9.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 13 2016000024.d
Method FengPOSNEW.m
Sample Name 9-(Trifluoromethyl)benzo(h)-1,6-naphthyridin-5(6H)-one
Comment

Acquisition Date 10/13/2016 3:35:13 PM

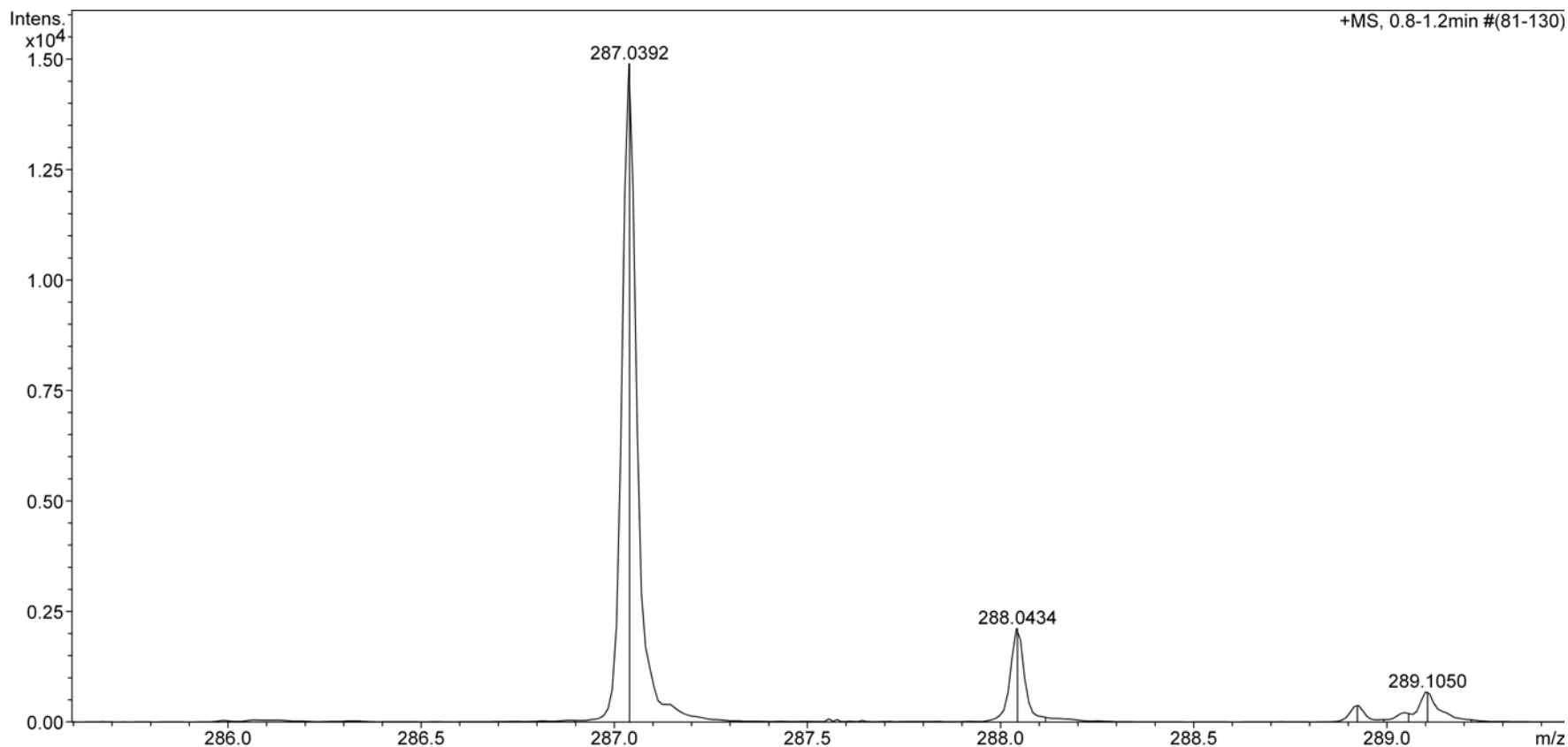
Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdb	N Rule	e ⁻
C 13 H 7 F 3 N 2 Na 1 O 1	0.01	287.0403	3.88	-2.12	9.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 13 2016000025.d
Method FengPOSNEW.m
Sample Name N-((5-oxo-5,6-dihydrobenzo(h)-1,6-naphthyridin-9-yl)sulfonyl
Comment

Acquisition Date 10/13/2016 3:44:42 PM

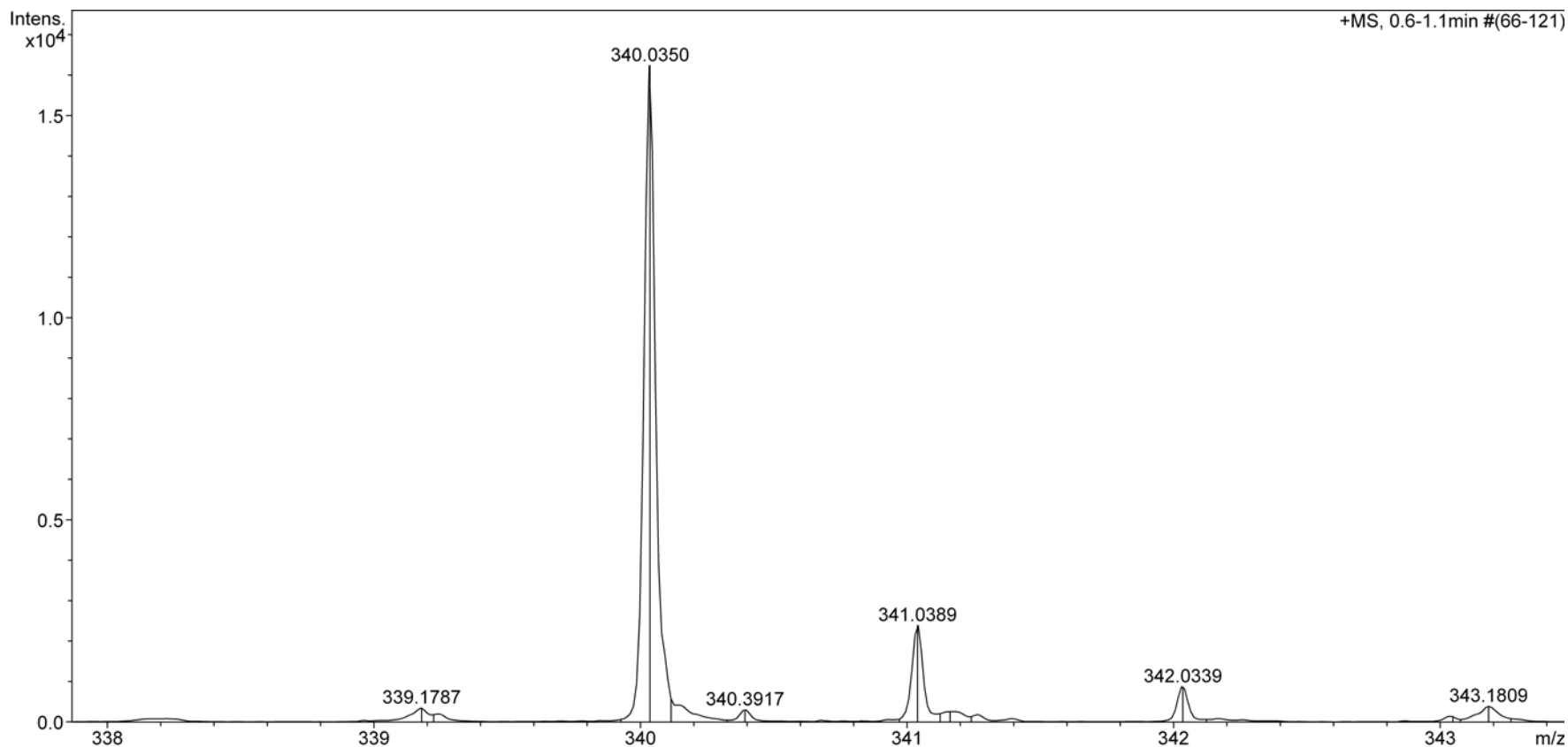
Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdB	N Rule	e ⁻
C 14 H 11 N 3 Na 1 O 4 S 1	0.01	340.0362	3.74	2.79	10.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 06 2016000003.d
Method FengPOSNEW.m
Sample Name 2-Chloro-N-Phenylthiophene-3-Carboxamide
Comment

Acquisition Date 10/6/2016 11:35:30 AM

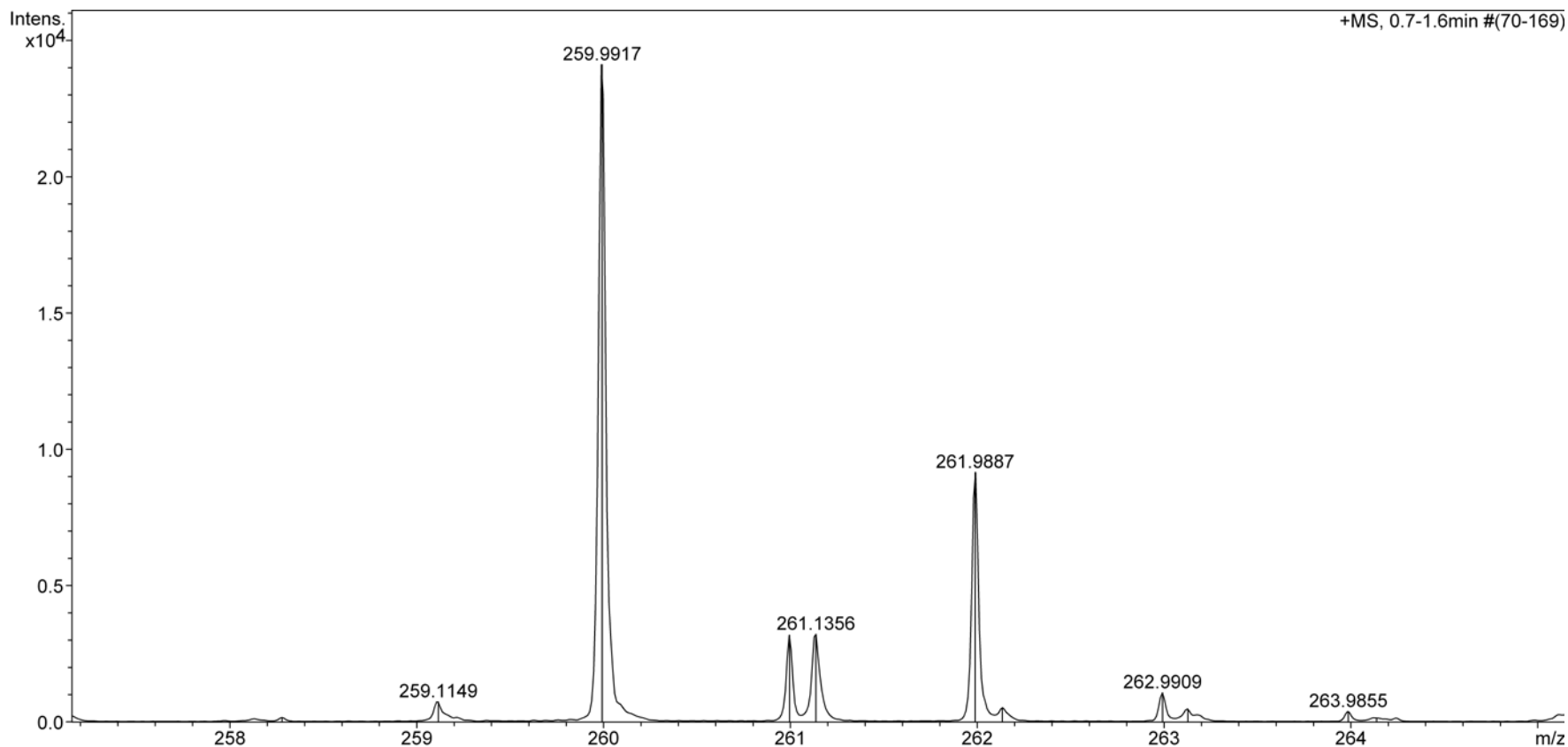
Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdB	N Rule	e ⁻
C 11 H 8 Cl 1 N 1 Na 1 O 1 S 1	0.00	259.9907	-3.82	-8.69	7.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 06 2016000004.d
Method FengPOSNEW.m
Sample Name 2-Chloro-N-(chlorophenyl)thiophene-3-carboxamide
Comment

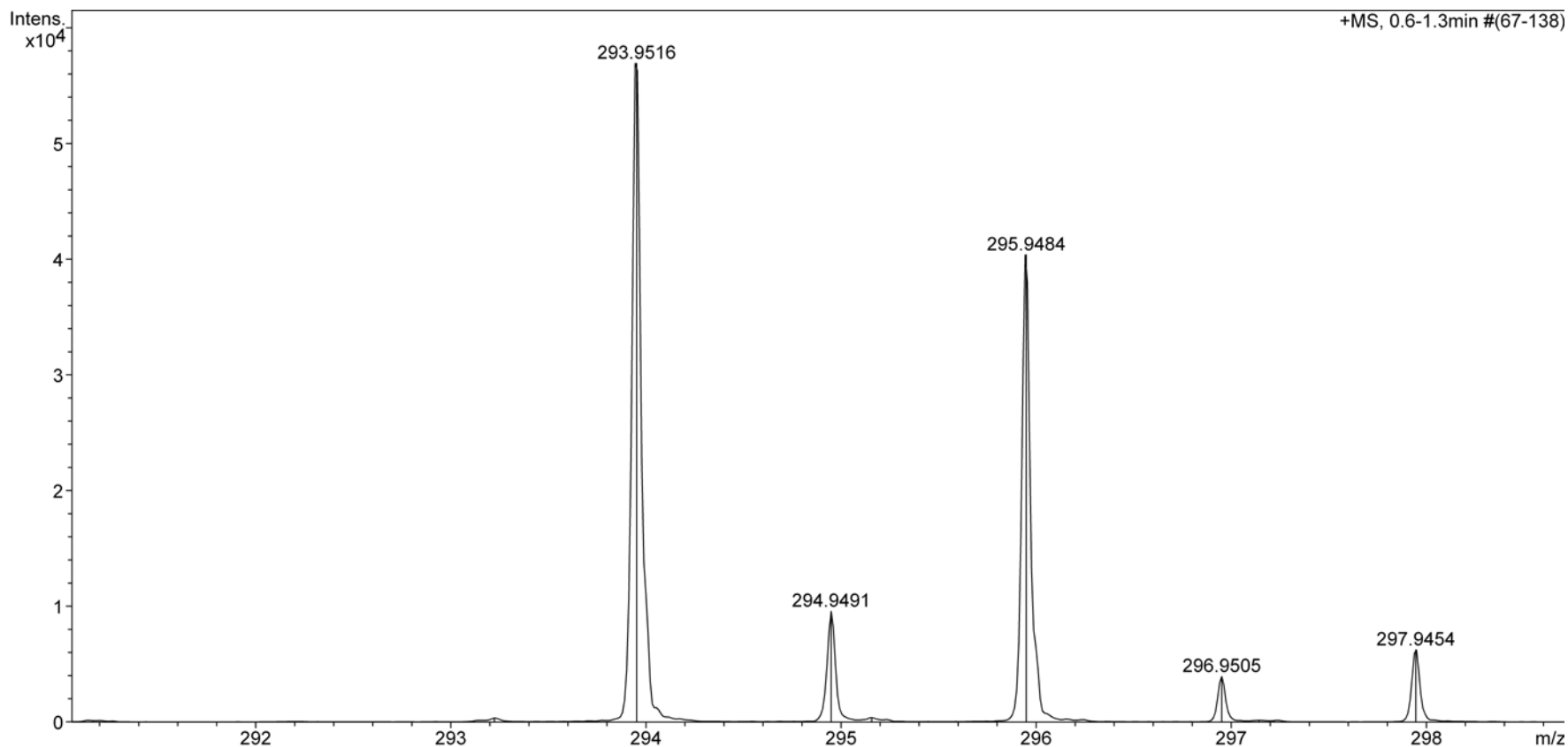
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Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdB	N Rule	e ⁻
C 11 H 7 Cl 2 N 1 Na 1 O 1 S 1	0.02	293.9518	0.69	2.65	7.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 06 2016000005.d
Method FengPOSNEW.m
Sample Name 2-Chloro-N-(4-chlorophenyl)thiophene-3-carboxamide
Comment

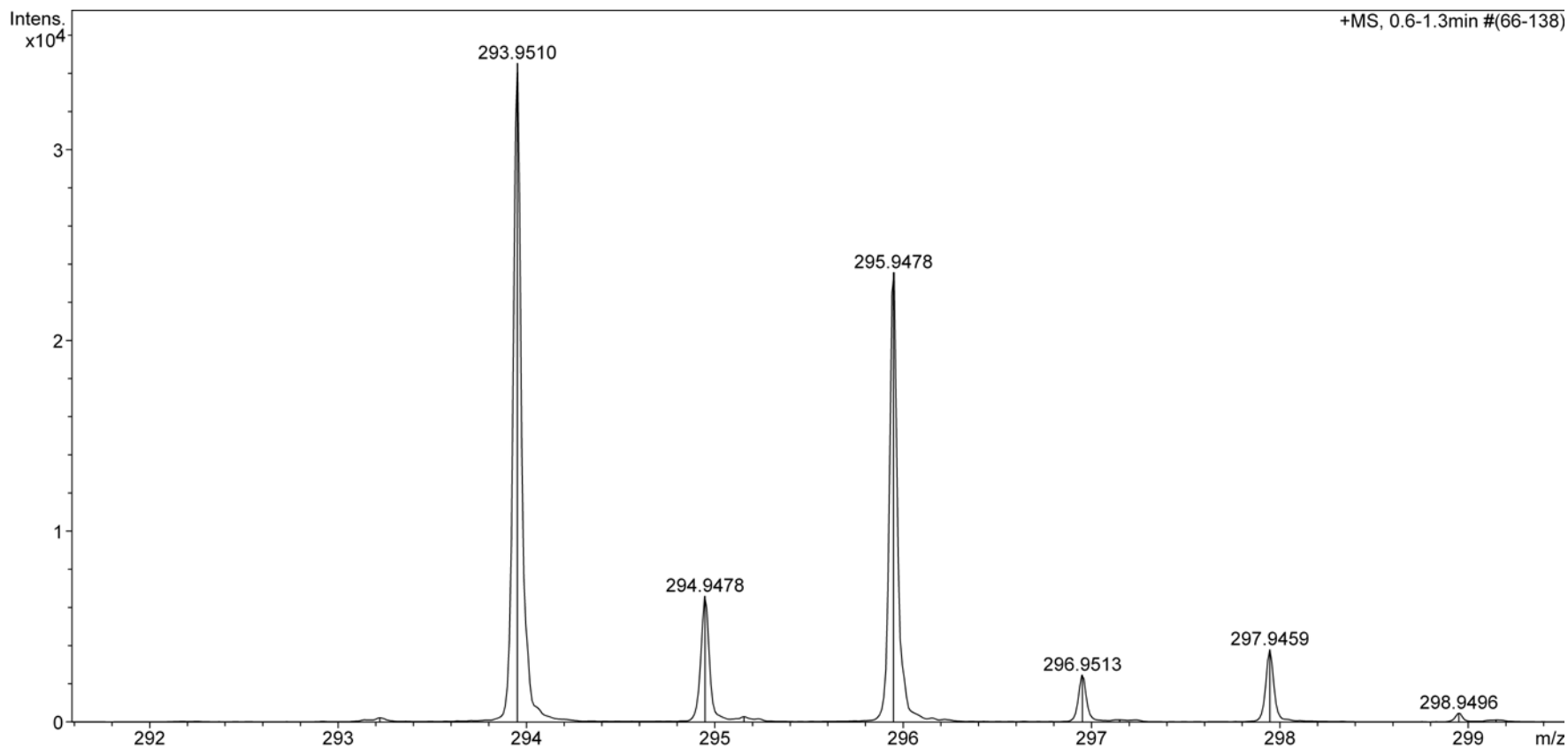
Acquisition Date 10/6/2016 1:29:11 PM
Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdB	N Rule	e ⁻
C 11 H 7 Cl 2 N 1 Na 1 O 1 S 1	0.03	293.9518	2.63	4.63	7.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 06 2016000006.d
Method FengPOSNEW.m
Sample Name 2-Chloro-N-(4-fluorophenyl)thiophene-3-carboxamide
Comment

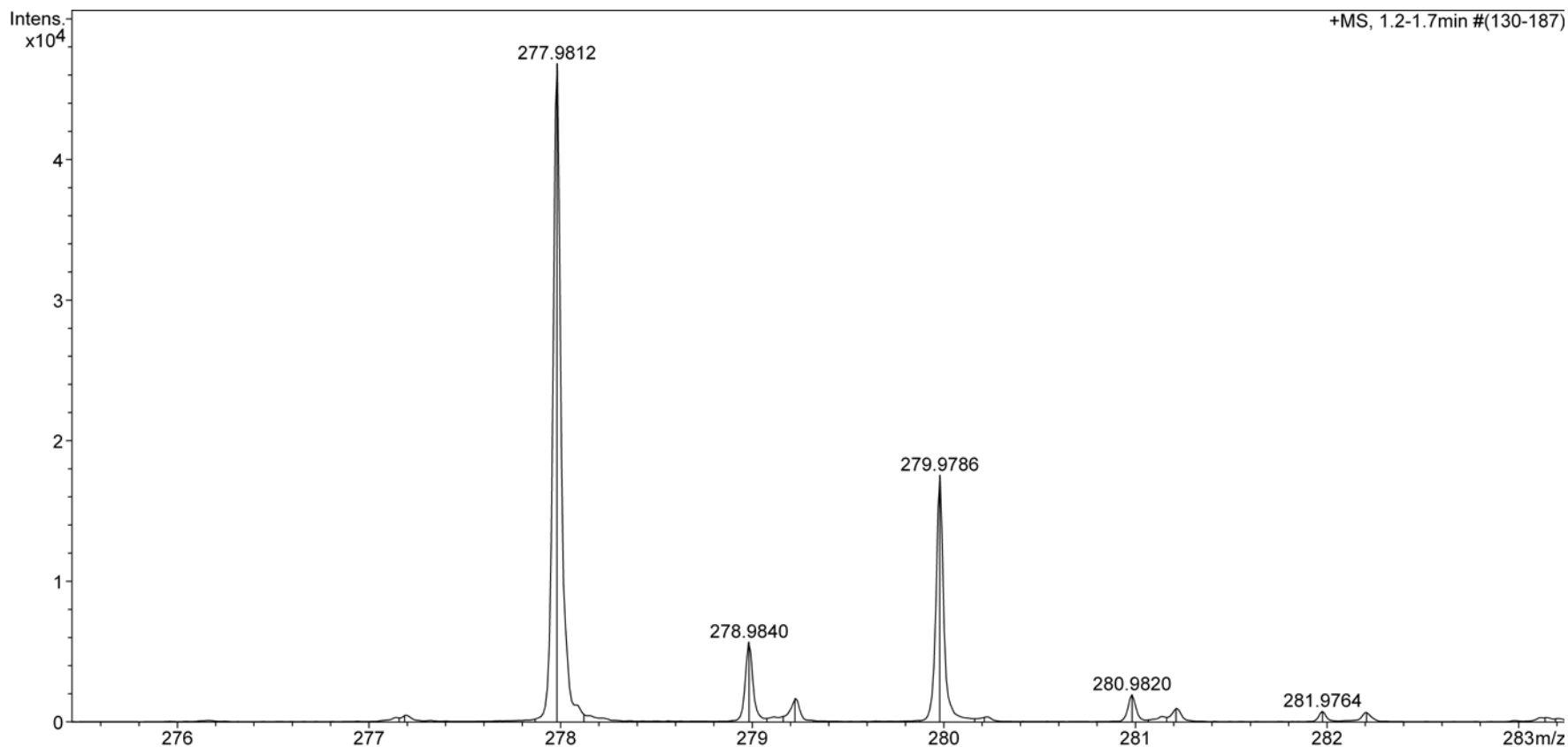
Acquisition Date 10/6/2016 1:38:24 PM
Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdB	N Rule	e ⁻
C 11 H 7 Cl 1 F 1 N 1 Na 1 O 1 S 1	0.01	277.9813	0.56	-3.35	7.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 06 2016000007.d
Method FengPOSNEW.m
Sample Name 2-Chloro-N-(4-(3Fmethyl)phenyl)thiophene-3-carboxamide
Comment

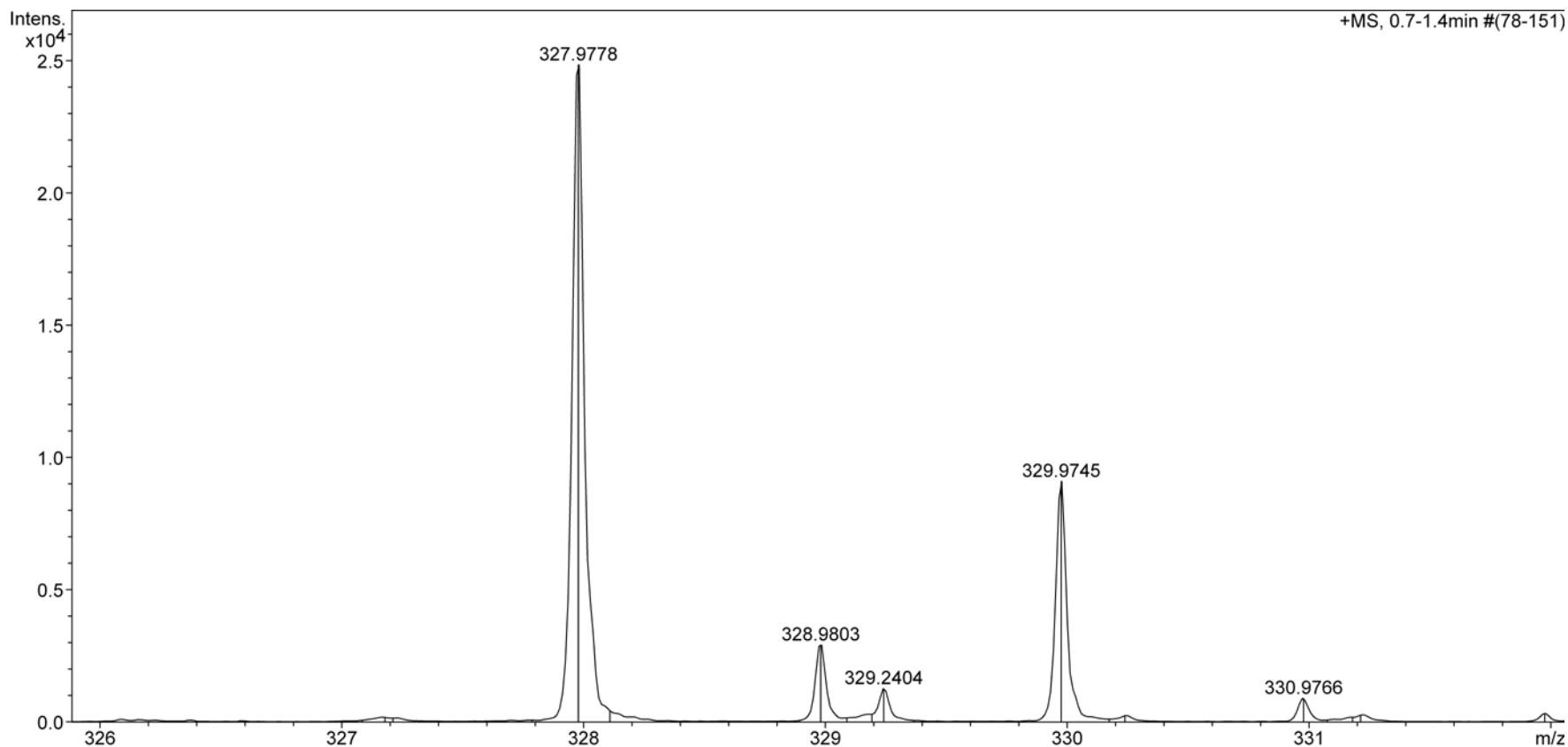
Acquisition Date 10/6/2016 1:49:28 PM
Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdB	N Rule	e ⁻
C 12 H 7 Cl 1 F 3 N 1 Na 1 O 1 S 1	0.01	327.9781	0.88	-5.39	7.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 06 2016000008.d
Method FengPOSNEW.m
Sample Name 2-Chloro-N-(2-methoxyphenyl)thiophene-3-carboxamide
Comment

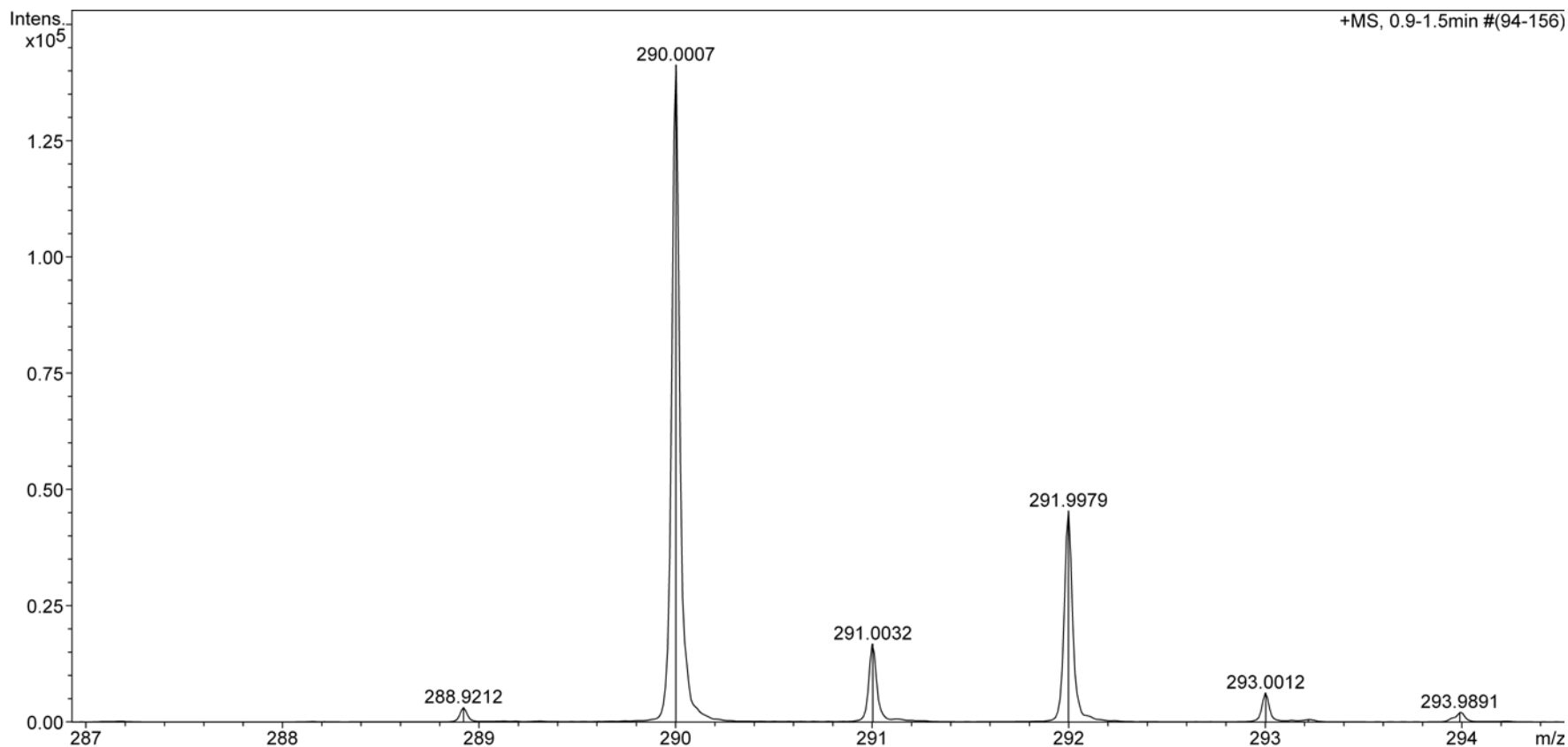
Acquisition Date 10/6/2016 1:58:53 PM
Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdB	N Rule	e ⁻
C 12 H 10 Cl 1 N 1 Na 1 O 2 S 1	0.03	290.0013	2.06	10.51	7.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 06 2016000009.d
Method FengPOSNEW.m
Sample Name 2-Chloro-N-(4-methoxyphenyl)thiophene-3-carboxamide
Comment

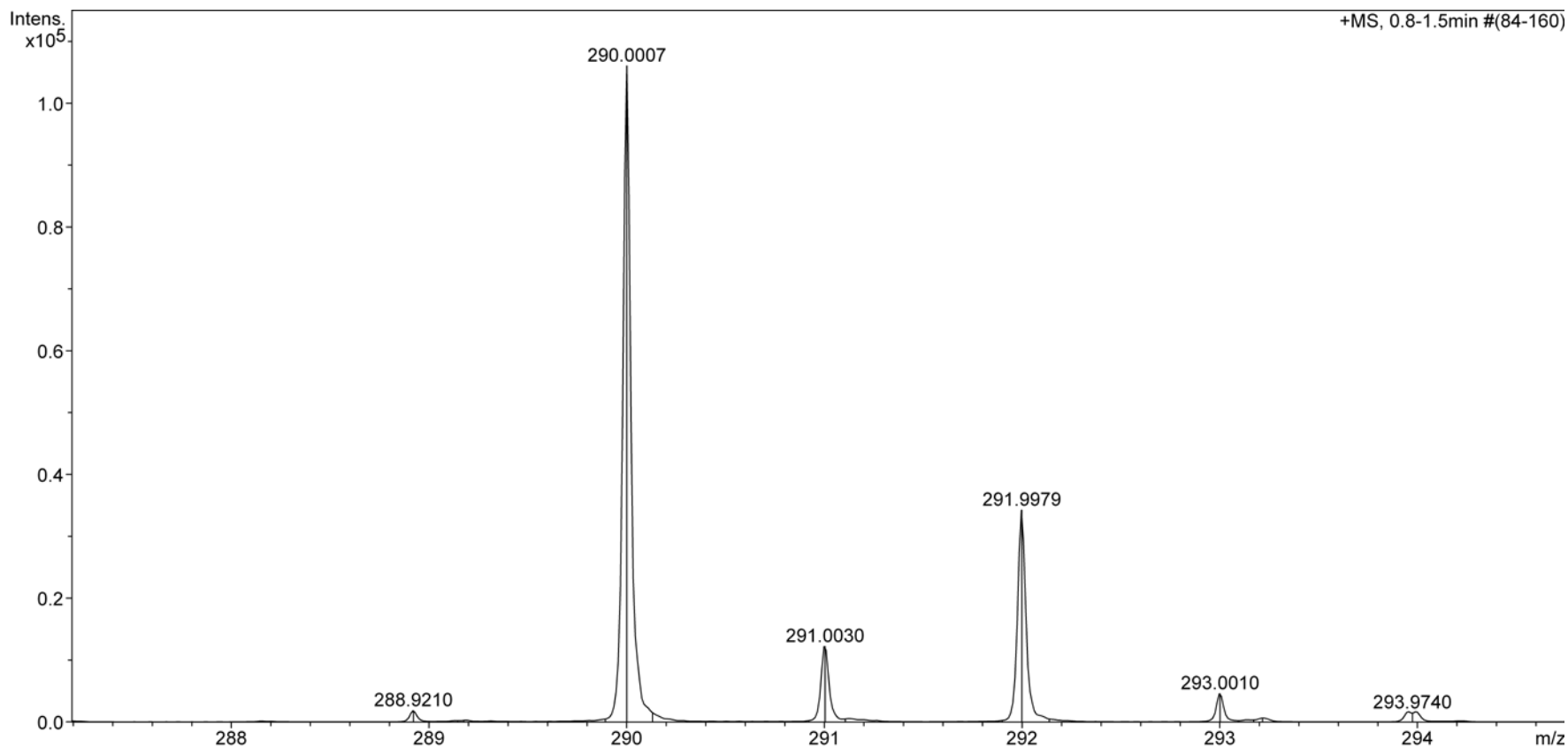
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Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdB	N Rule	e ⁻
C 12 H 10 Cl 1 N 1 Na 1 O 2 S 1	0.03	290.0013	2.17	12.45	7.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 06 2016000010.d
Method FengPOSNEW.m
Sample Name 2-Chloro-N-(o-tolyl)thiophene-3-carboxamide
Comment

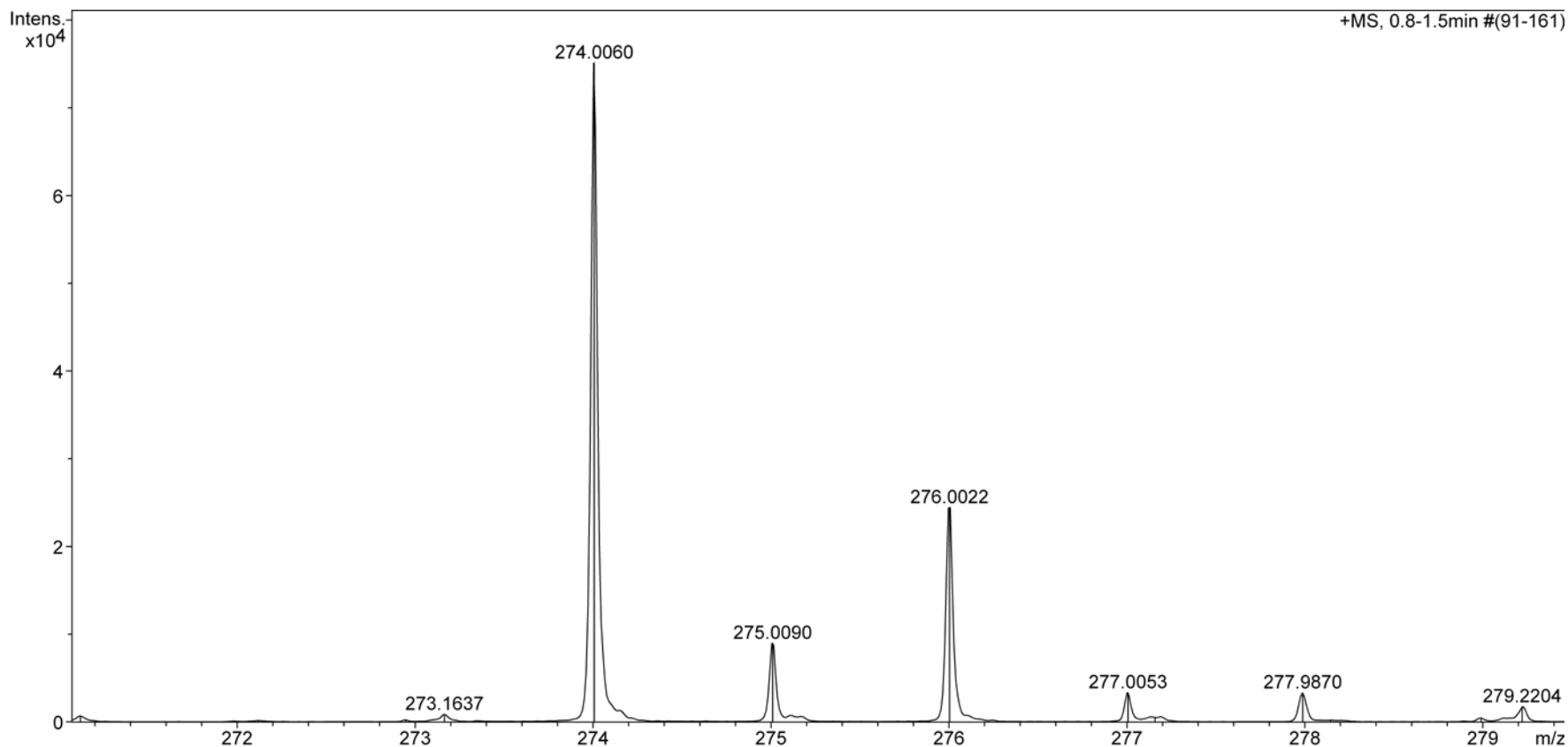
Acquisition Date 10/6/2016 2:15:38 PM
Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdB	N Rule	e ⁻
C 12 H 10 Cl 1 N 1 Na 1 O 1 S 1	0.03	274.0064	1.44	4.30	7.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 06 2016000011.d
Method FengPOSNEW.m
Sample Name N-(4-(N-Acetylsulfa)phenyl)-2-Chlothiophene-3-carboxamide
Comment

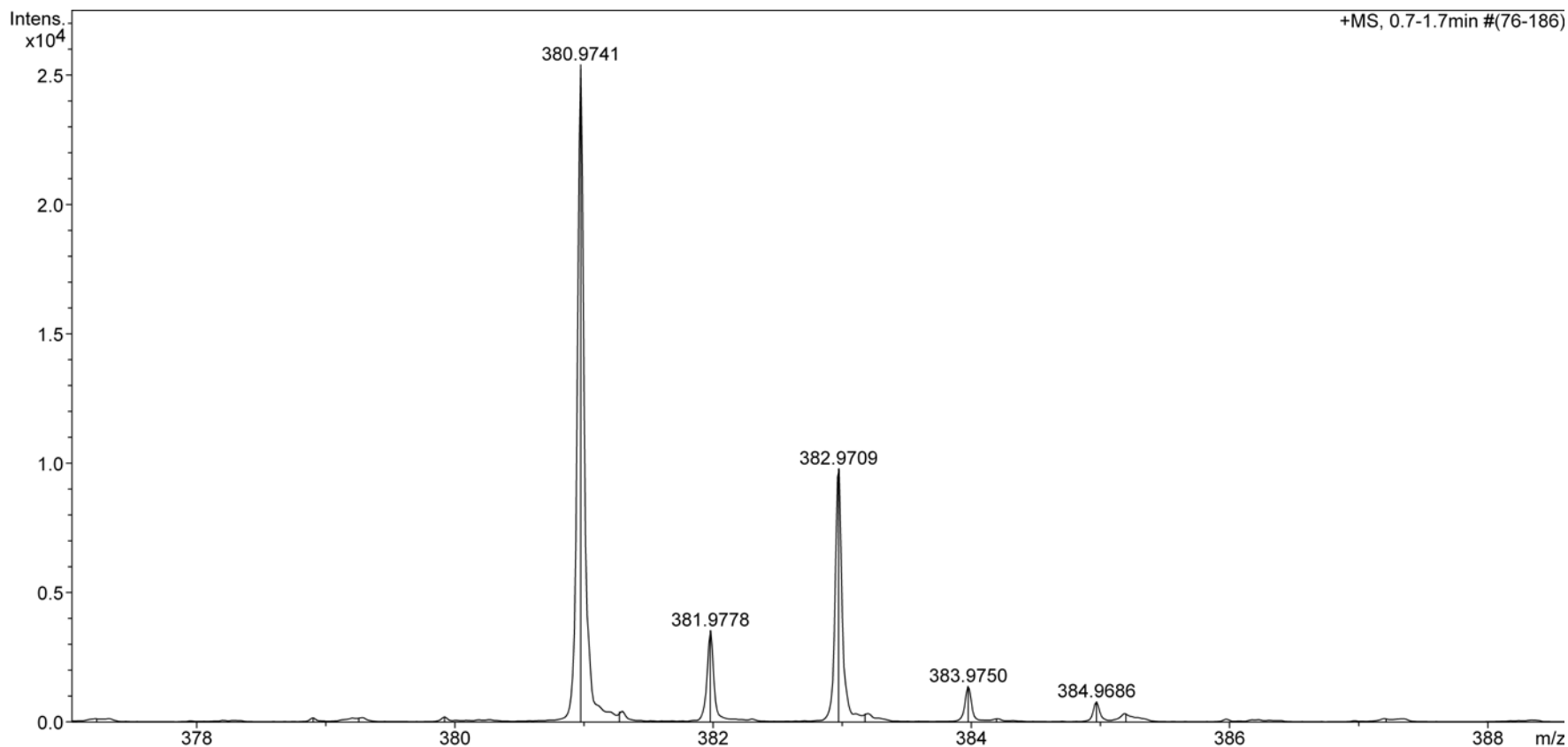
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Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdB	N Rule	e ⁻
C 13 H 11 Cl 1 N 2 Na 1 O 4 S 2	0.03	380.9741	0.03	-0.11	8.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 06 2016000012.d
Method FengPOSNEW.m
Sample Name 2-Cl-N-(4-(NN-diethylsulfamoyl)phenyl)thiophe-3-carboxamide
Comment

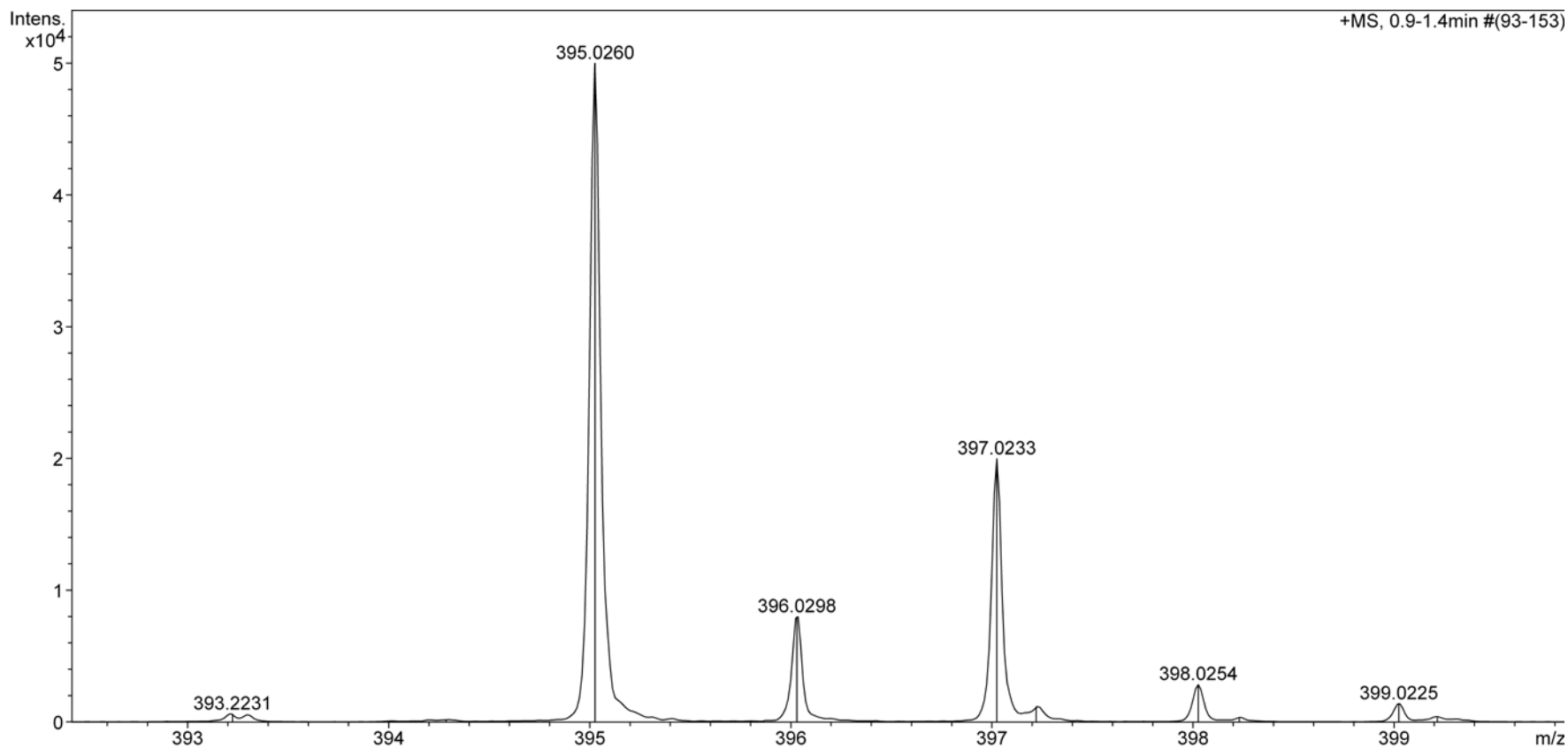
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Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdB	N Rule	e ⁻
C 15 H 17 Cl 1 N 2 Na 1 O 3 S 2	0.02	395.0261	0.39	-0.08	7.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 06 2016000013.d
Method FengPOSNEW.m
Sample Name 2,5-Dichloro-N-phenylthiophene-3-carboxamide
Comment

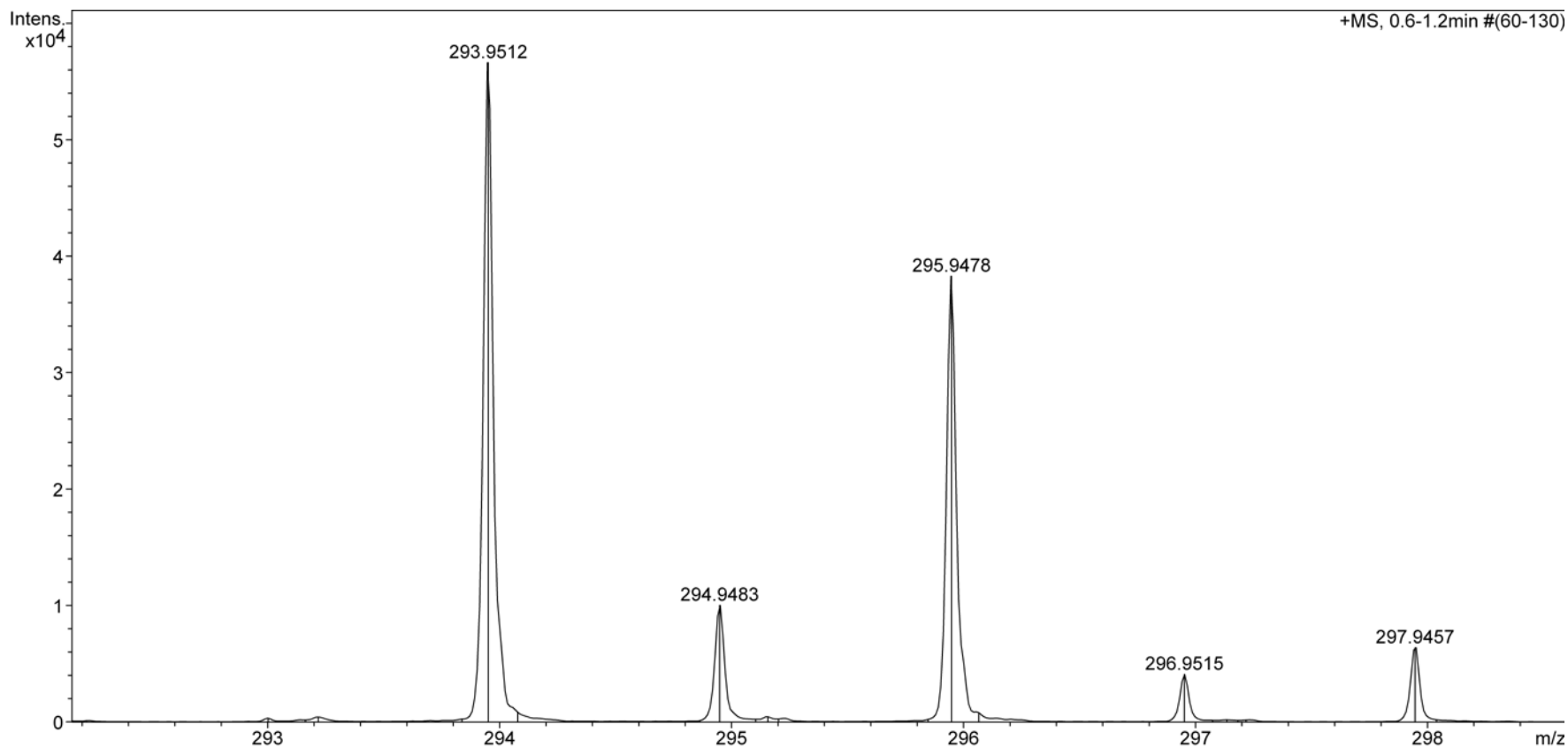
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Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdB	N Rule	e ⁻
C 11 H 7 Cl 2 N 1 Na 1 O 1 S 1	0.02	293.9518	2.04	4.13	7.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 06 2016000014.d
Method FengPOSNEW.m
Sample Name 2,5-Dichloro-N-(2-chlorophenyl)thiophene-3-carboxamide
Comment

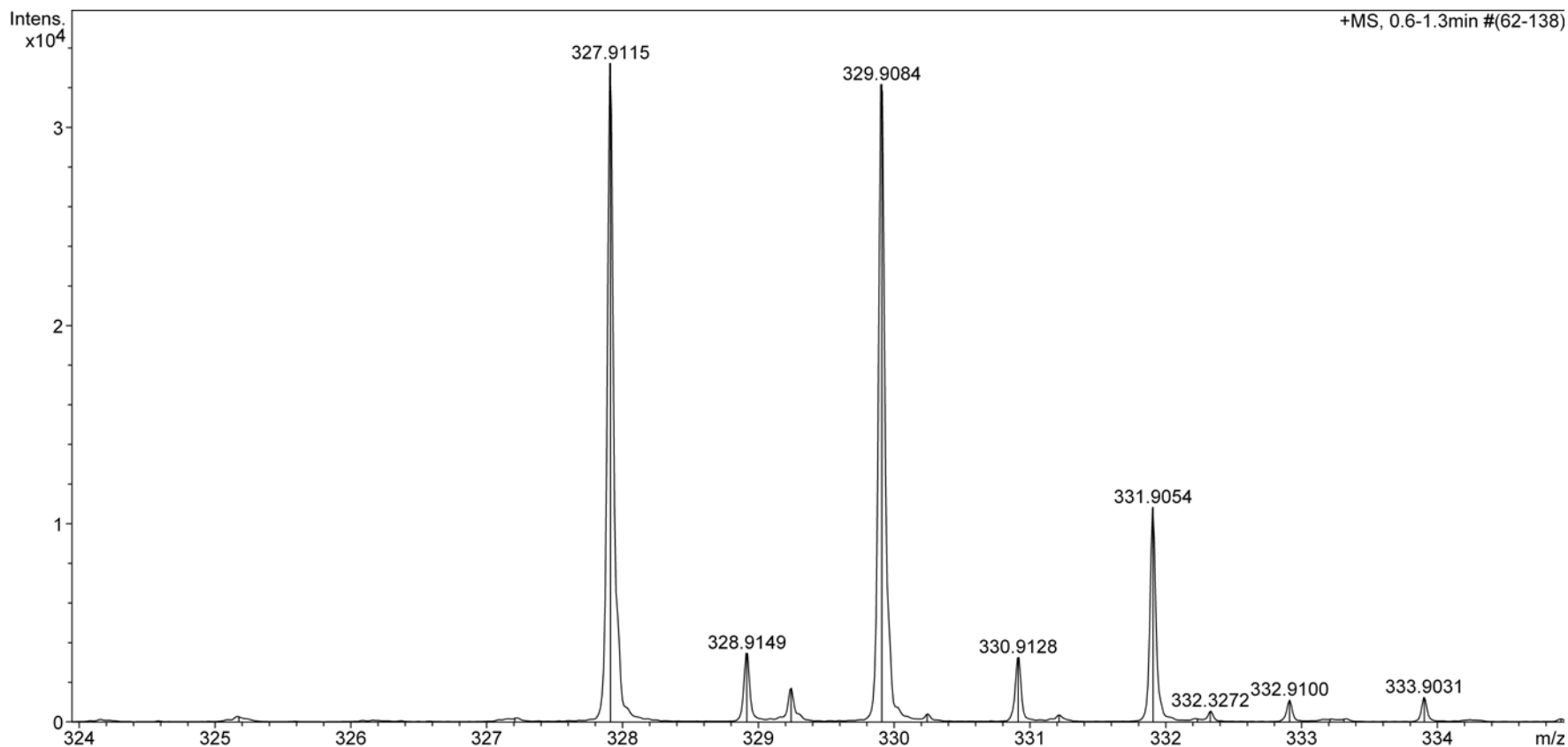
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Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdB	N Rule	e ⁻
C 11 H 6 Cl 3 N 1 Na 1 O 1 S 1	0.02	327.9128	4.07	3.89	7.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 06 2016000015.d
Method FengPOSNEW.m
Sample Name 2,5-Dichloro-N-(4-chlorophenyl)thiophene-3-carboxamide
Comment

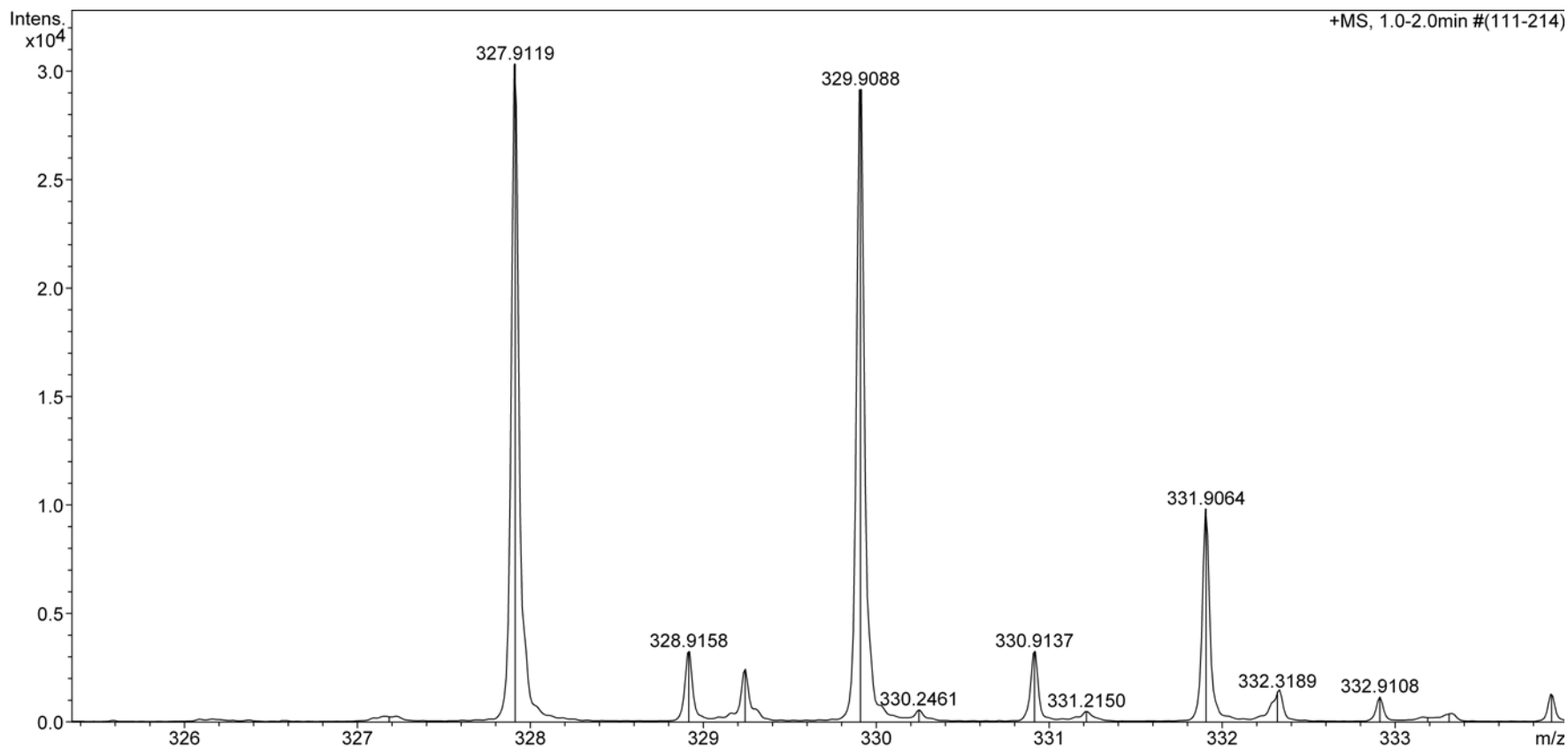
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Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdB	N Rule	e ⁻
C 11 H 6 Cl 3 N 1 Na 1 O 1 S 1	0.02	327.9128	2.62	2.18	7.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 06 2016000016.d
Method FengPOSNEW.m
Sample Name 2,5-Dichloro-N-(4-fluorophenyl)thiophene-3-carboxamide
Comment

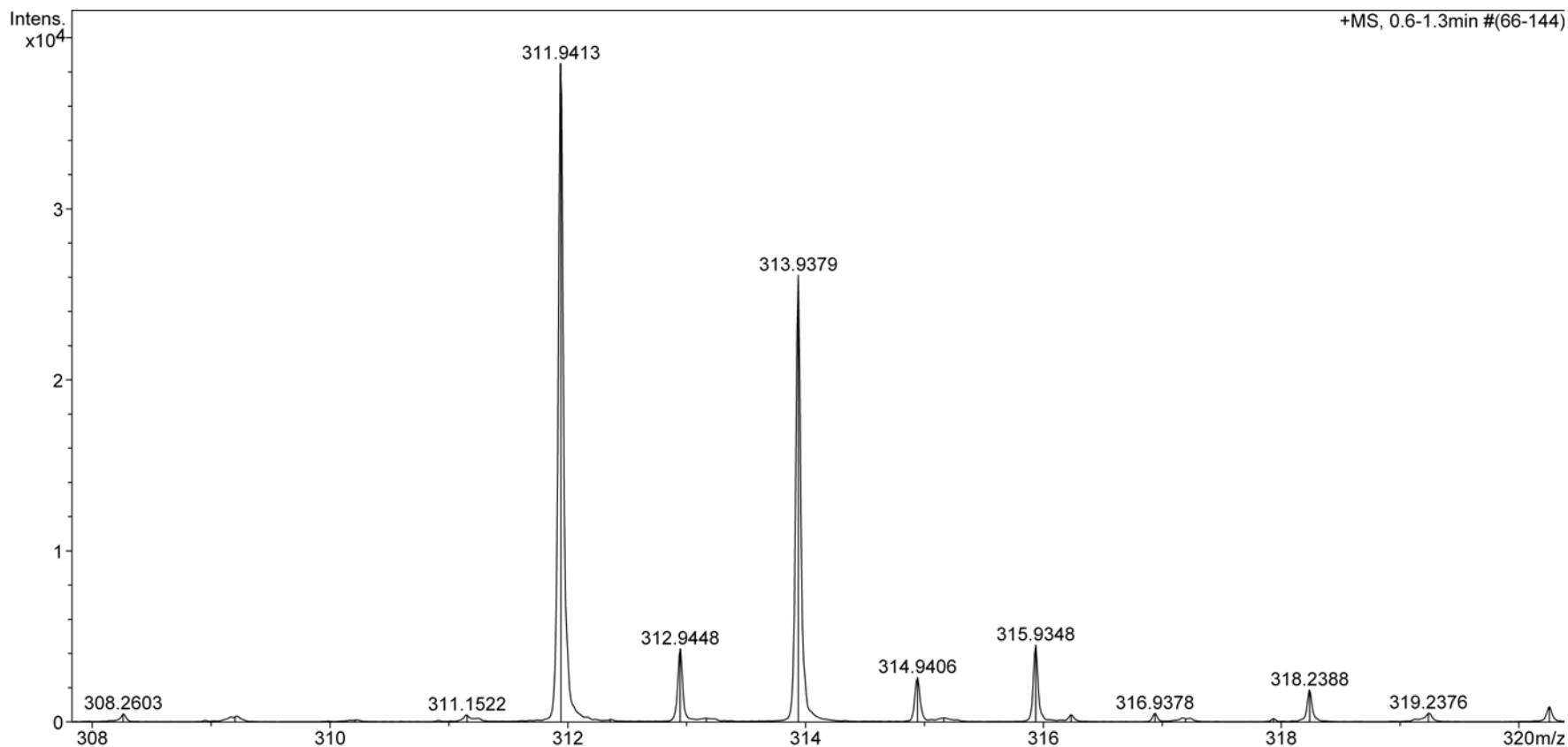
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Operator Administrator
Instrument microTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdB	N Rule	e ⁻
C 11 H 6 Cl 2 F 1 N 1 Na 1 O 1 S 1	0.02	311.9423	3.44	3.96	7.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 06 2016000017.d
Method FengPOSNEW.m
Sample Name N-(4-(N-Acetylsulfamoyl)phenyl)-2,5-DiClthiop3-carboxamide
Comment

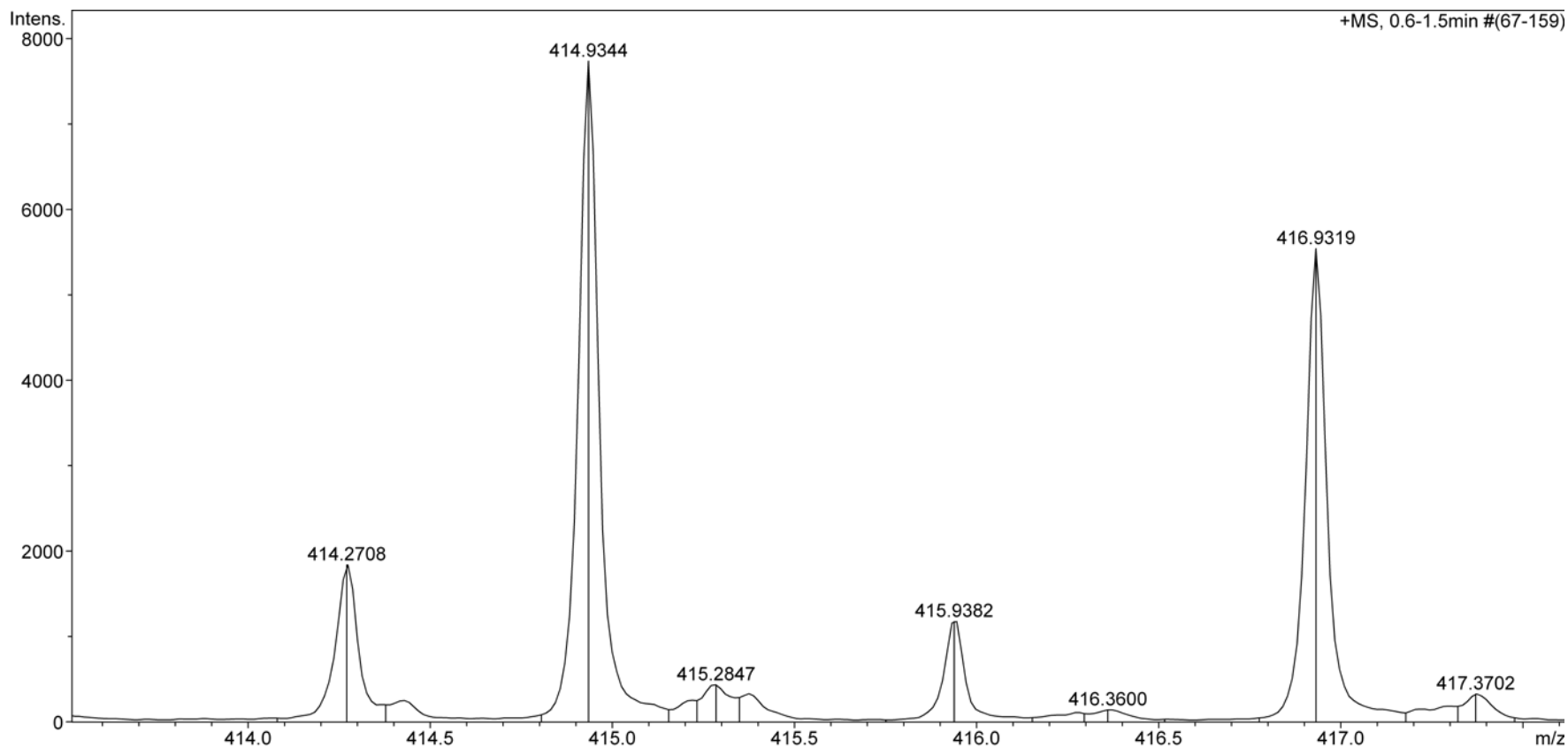
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Operator Administrator
Instrument microTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdB	N Rule	e ⁻
C 13 H 10 Cl 2 N 2 Na 1 O 4 S 2	0.02	414.9351	1.70	2.92	8.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 06 2016000018.d
Method FengPOSNEW.m
Sample Name 2,5-Dichloro-N-(4-(N,N-diethylsulfamoyl)ph-3-carboxamide
Comment

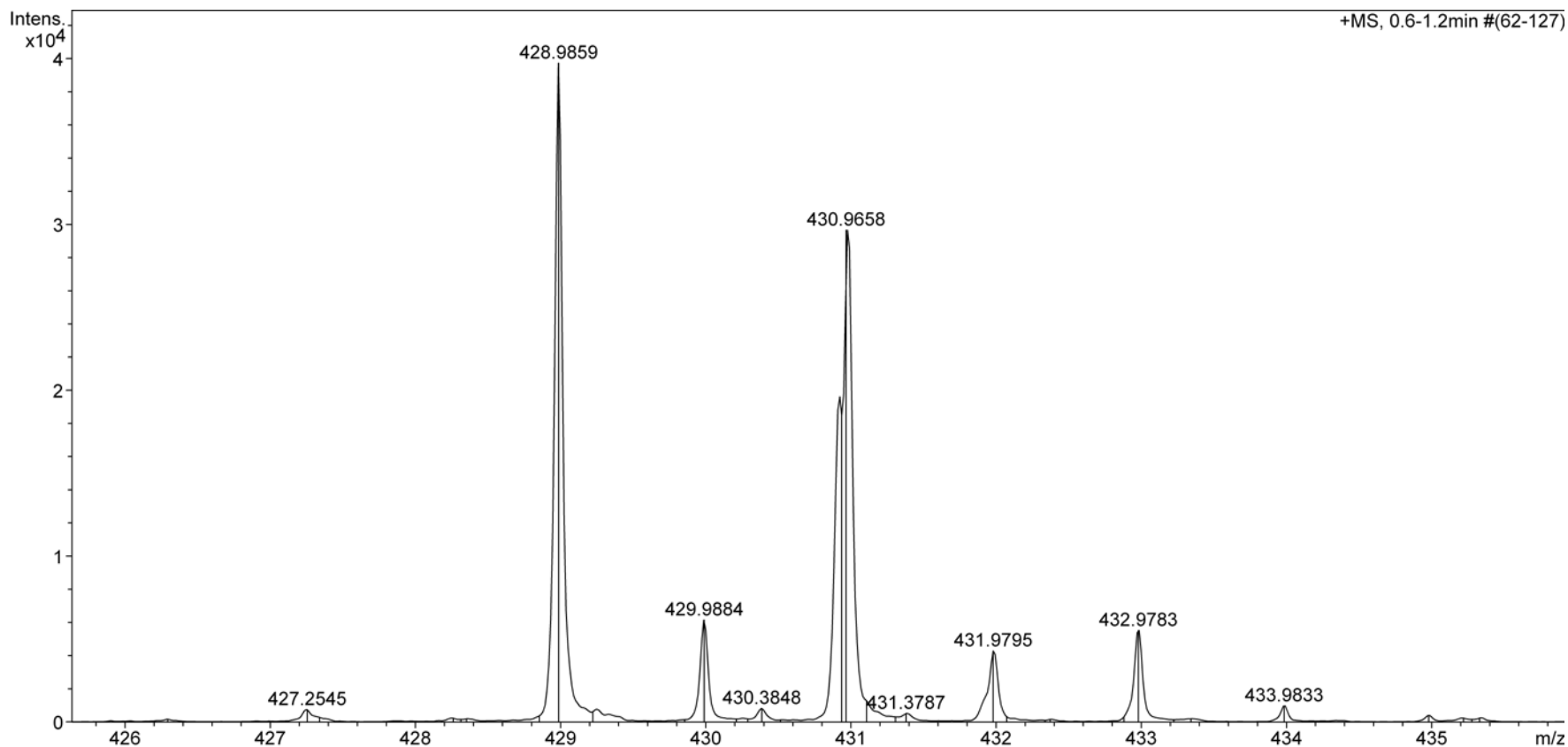
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Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdB	N Rule	e ⁻
C 15 H 16 Cl 2 N 2 Na 1 O 3 S 2	0.02	428.9872	2.95	17.16	7.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 13 2016000001.d
Method FengPOSNEW.m
Sample Name 2-Chloro-N-(2-chlorophenyl)nicotinamide
Comment

Acquisition Date 10/13/2016 10:46:50 AM

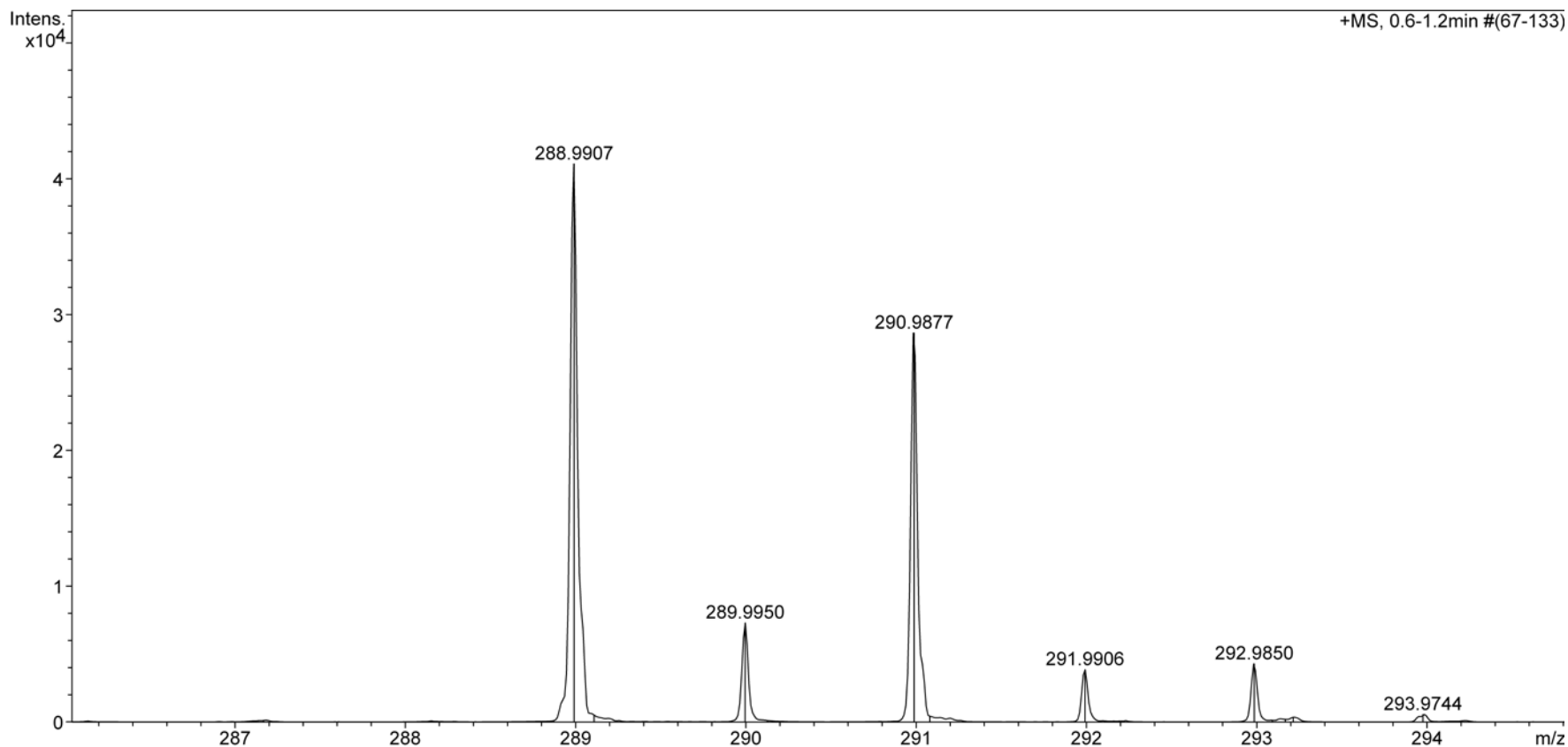
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Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdb	N Rule	e ⁻
C 12 H 8 Cl 2 N 2 Na 1 O 1	0.03	288.9906	-0.47	5.23	8.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 13 2016000002.d
Method FengPOSNEW.m
Sample Name 2-Chloro-N-(4-(trifluoromethyl)phenyl)nicotinamide
Comment

Acquisition Date 10/13/2016 10:57:35 AM

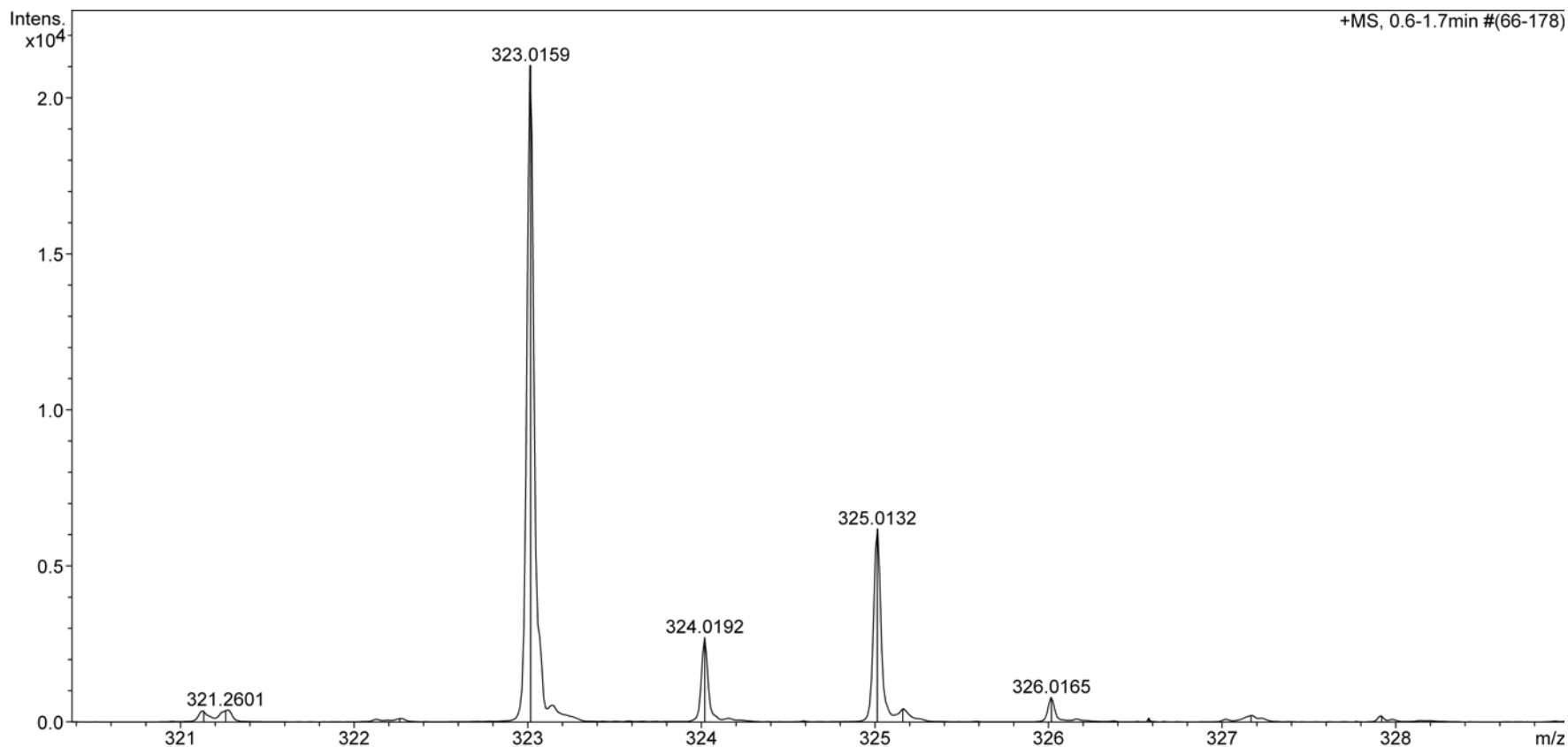
Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdB	N Rule	e ⁻
C 13 H 8 Cl 1 F 3 N 2 Na 1 O 1	0.02	323.0169	3.13	-4.18	8.50	ok	even

Mass Spectrum Molecular Formula Report

Analysis Info

Analysis Name D:\Data\Xiao\Oct 13 2016000003.d
Method FengPOSNEW.m
Sample Name N-(4-(N-Acetylsulfamoyl)phenyl)-2-chloronicotinamide
Comment

Acquisition Date 10/13/2016 11:06:46 AM

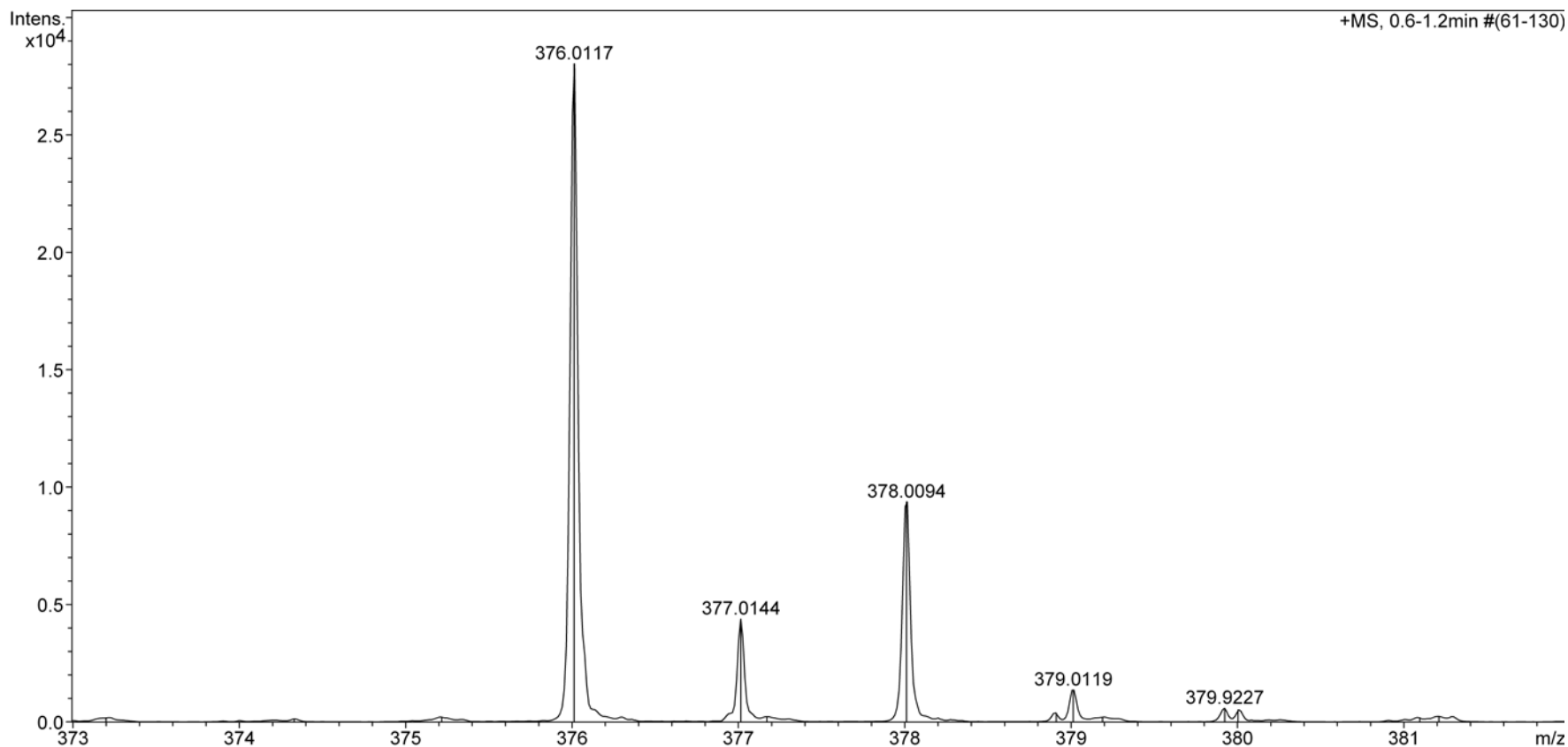
Operator Administrator
Instrument micrOTOF 57

Acquisition Parameter

Source Type ESI
Scan Range n/a
Scan Begin 50 m/z
Scan End 2000 m/z

Ion Polarity Positive
Capillary Exit 100.0 V
Hexapole RF 150.0 V
Skimmer 1 50.0 V
Hexapole 1 23.0 V

Set Corrector Fill 45 V
Set Pulsar Pull 400 V
Set Pulsar Push 400 V
Set Reflector 1300 V
Set Flight Tube 9000 V
Set Detector TOF 2200 V



Mass Spectrum Molecular Formula Report

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdB	N Rule	e ⁻
C 14 H 12 Cl 1 N 3 Na 1 O 4 S 1	0.03	376.0129	3.26	0.39	9.50	ok	even