

Synthesis of Novel Quinazolinone Analogues for Quorum Sensing Inhibition

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Supplementary figures for the HMBC spectrum of compound 6b

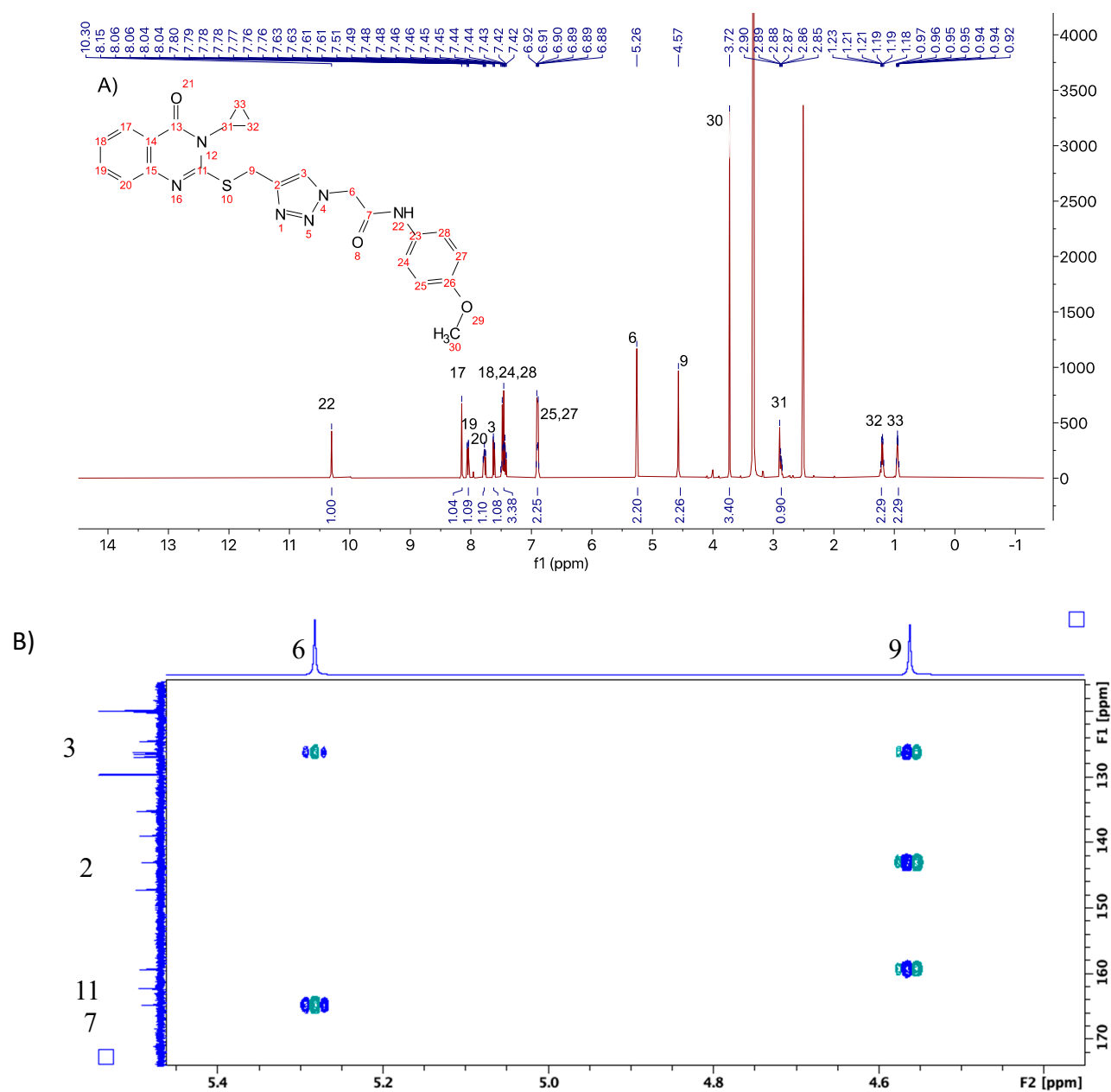
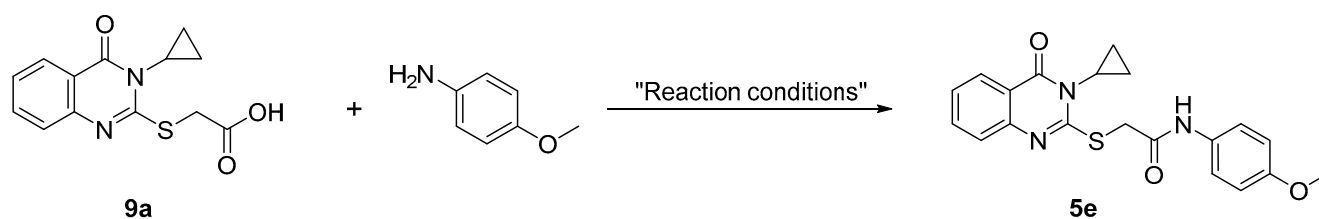


Figure S1. (A) ^1H NMR spectrum of compound **6b**. (B) Key ^1H : ^{13}C HMBC correlations in compound **6b**.

Supplementary scheme and table for optimization of reaction condition in the synthesis of compound 5e



Scheme S1. Synthesis of quinazolinone-based amide **5e**.

Table S1: Reaction conditions attempted for the synthesis of quinazolinone-based amide **5a**.

Entry	Reagents	Solvents	Reaction temperature	Reaction time (h)	Yield (%)
1	SOCl ₂ , Et ₃ N	DCM	Reflux	1	5
2	EDC-HCl, DIPEA	ACN:DMF (1:1)	r.t.	12	4
3	EDC-HCl, DIPEA	ACN:DMF (1:1)	50 °C	12	4
4	DCC, DMAP	DCM	r.t.	18	2
5	HATU, Et ₃ N	DMF	r.t.	12	64

Supplementary table for percentage growth inhibition of *P. aeruginosa* induced by test compounds

Table S2: Percentage growth inhibition of *P. aeruginosa* induced by test compounds at 100, 50 and 25 μM . (All measurements were performed in triplicate with \pm standard deviation from mean.)

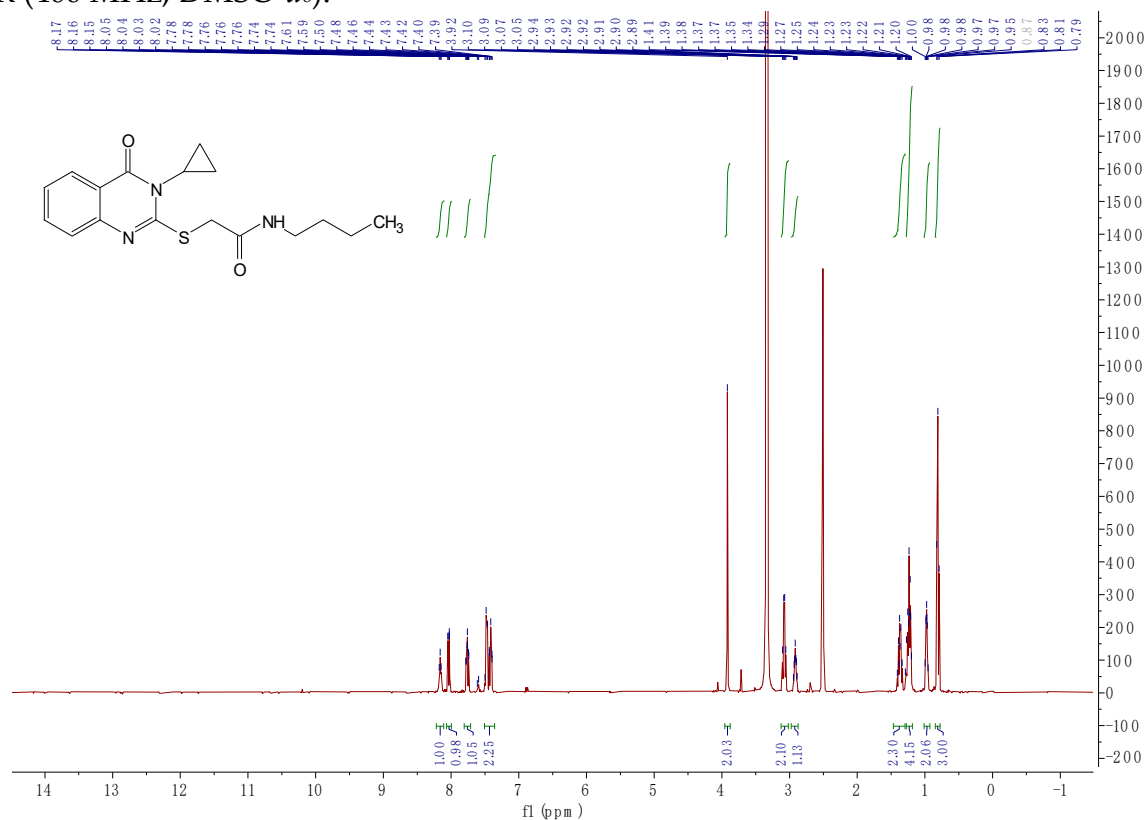
Compound	Concentration		
	100 μM	50 μM	25 μM
5a	0	0	0
5b	0	0	0
5c	0	0	0
5d	10.4 \pm 4.1	4.5 \pm 1.8	8.9 \pm 3.7
5e	0	0	0
5f	0.5 \pm 0.7	0	0
5g	0	0.4 \pm 2.1	3.1 \pm 2.1
5h	0	0	0
5i	1.2 \pm 4.1	0.2 \pm 2.0	0.2 \pm 3.1
5j	16.8 \pm 2.3	7.9 \pm 8.2	5.8 \pm 3.0
5k	0	0	0
6a	NT	NT	0
6b	0	1.0 \pm 7.6	1.0 \pm 2.4
6c	0	0.4 \pm 8.4	0
6d	7.2 \pm 6.2	3.6 \pm 3.6	0
6e	10.9 \pm 4.7	0	0

0 = no growth inhibition; NT = Not tested

^1H NMR and ^{13}C NMR spectra of synthesized compounds

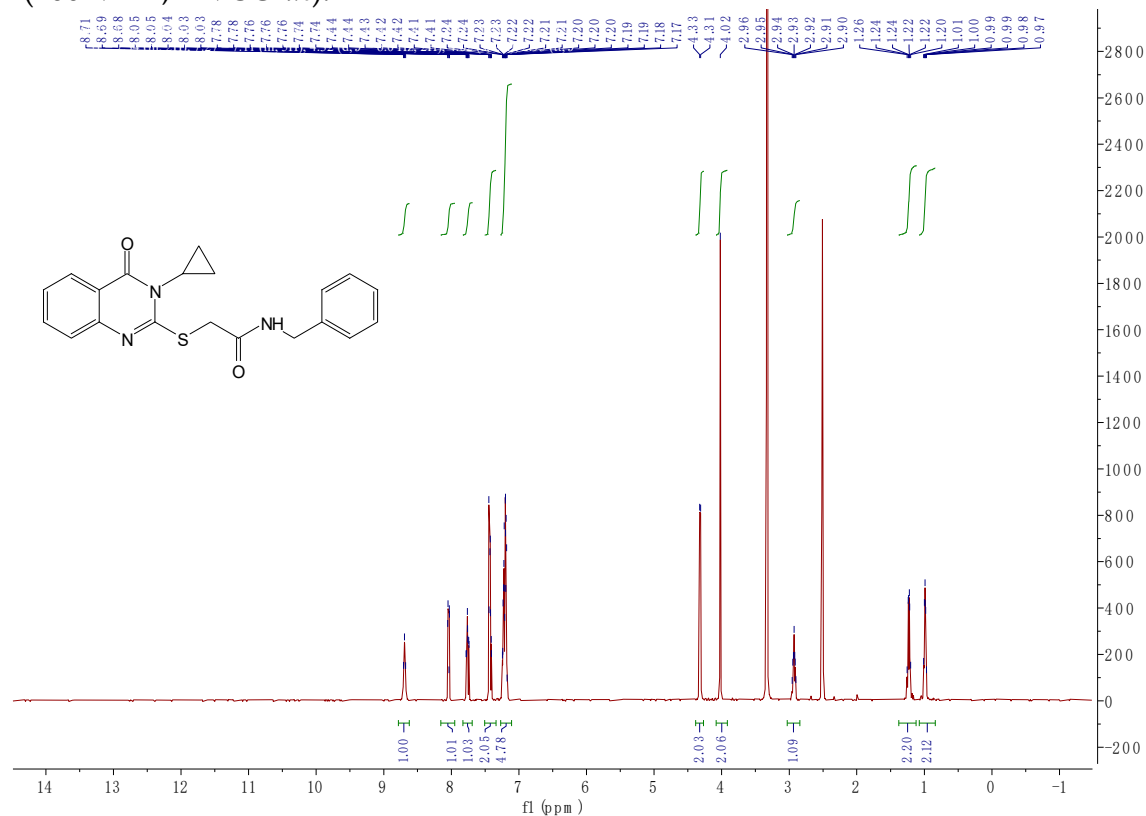
N-Butyl-2-((3-cyclopropyl-4-oxo-3,4-dihydroquinazolin-2-yl)thio)acetamide (5a)

^1H NMR (400 MHz, $\text{DMSO}-d_6$):

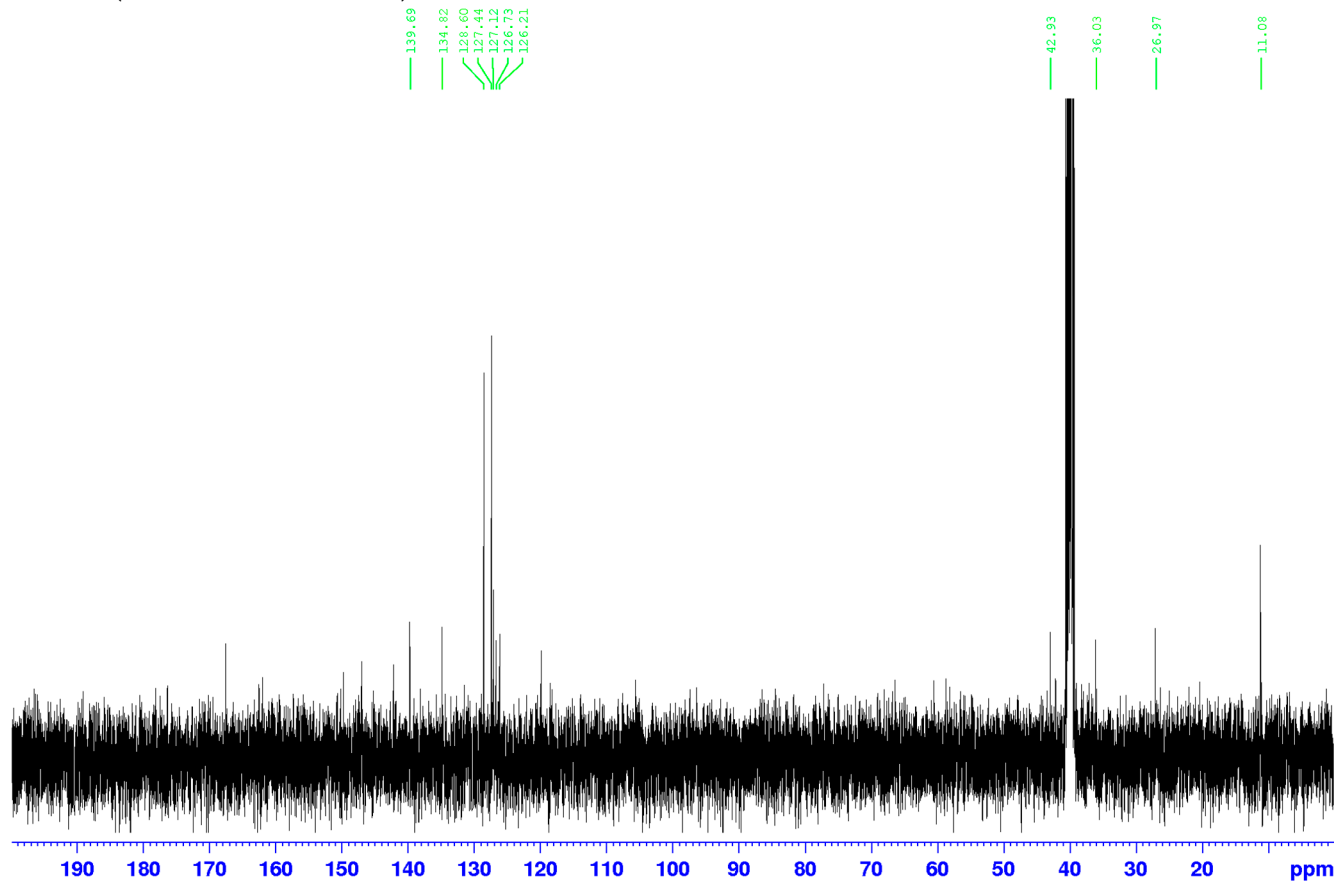


N-Benzyl-2-((3-cyclopropyl-4-oxo-3,4-dihydroquinazolin-2-yl)thio)acetamide (**5b**)

^1H NMR (400 MHz, $\text{DMSO}-d_6$):

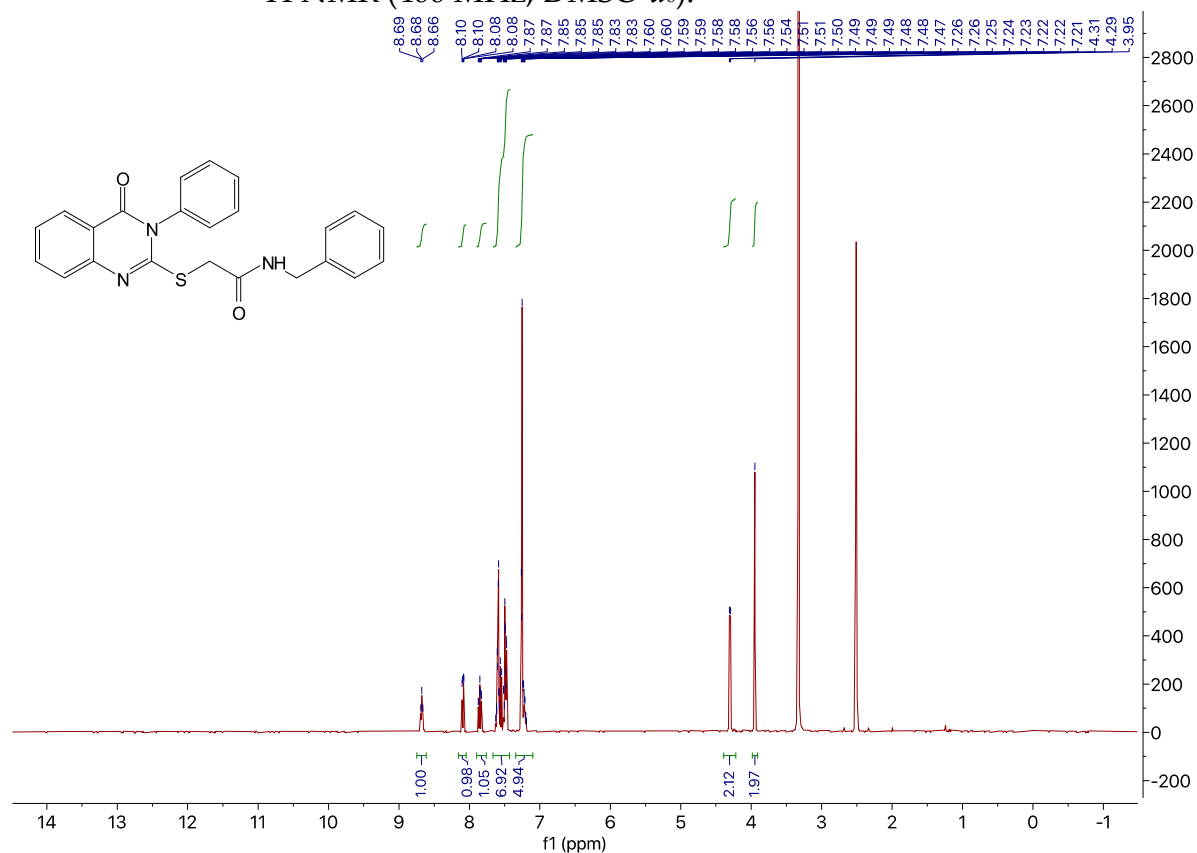


^{13}C NMR (100 MHz, $\text{DMSO}-d_6$):

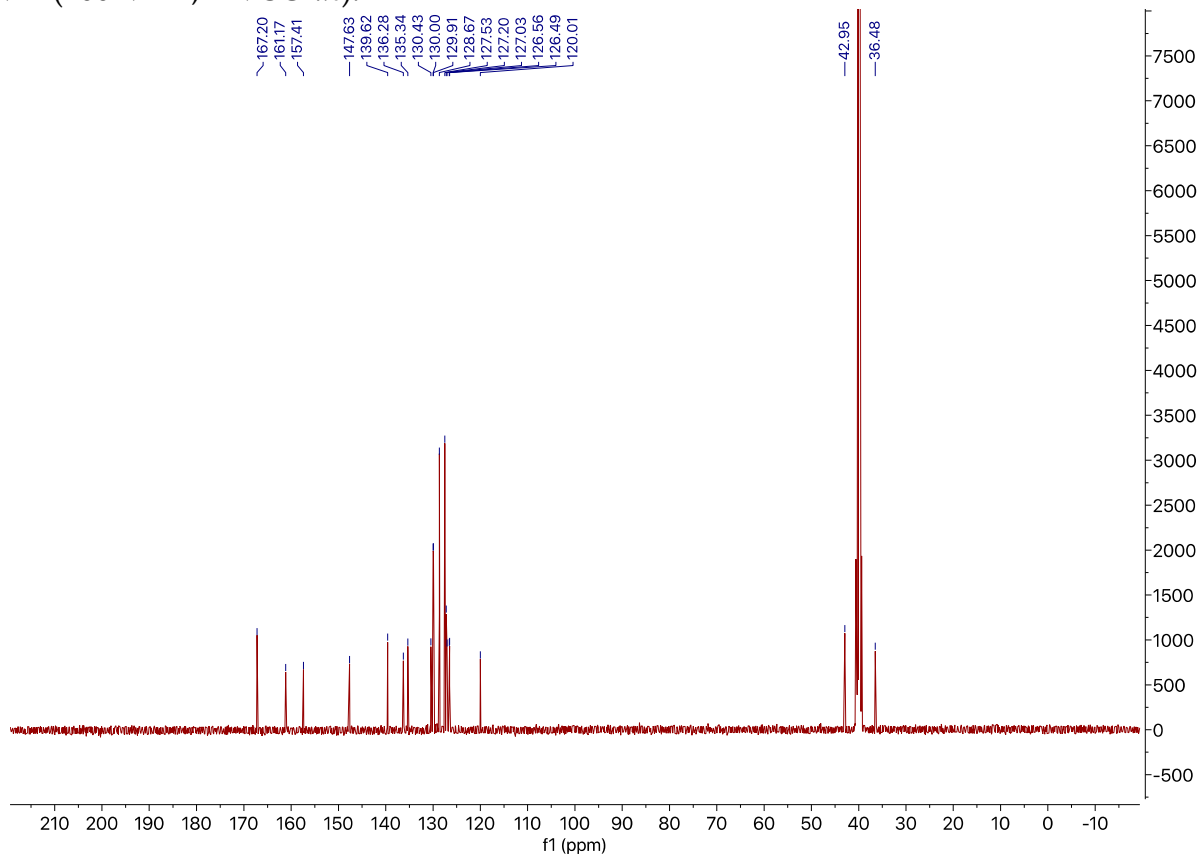


N-Benzyl-2-((4-oxo-3-phenyl-3,4-dihydroquinazolin-2-yl)thio)acetamide
(5c)

^1H NMR (400 MHz, $\text{DMSO}-d_6$):

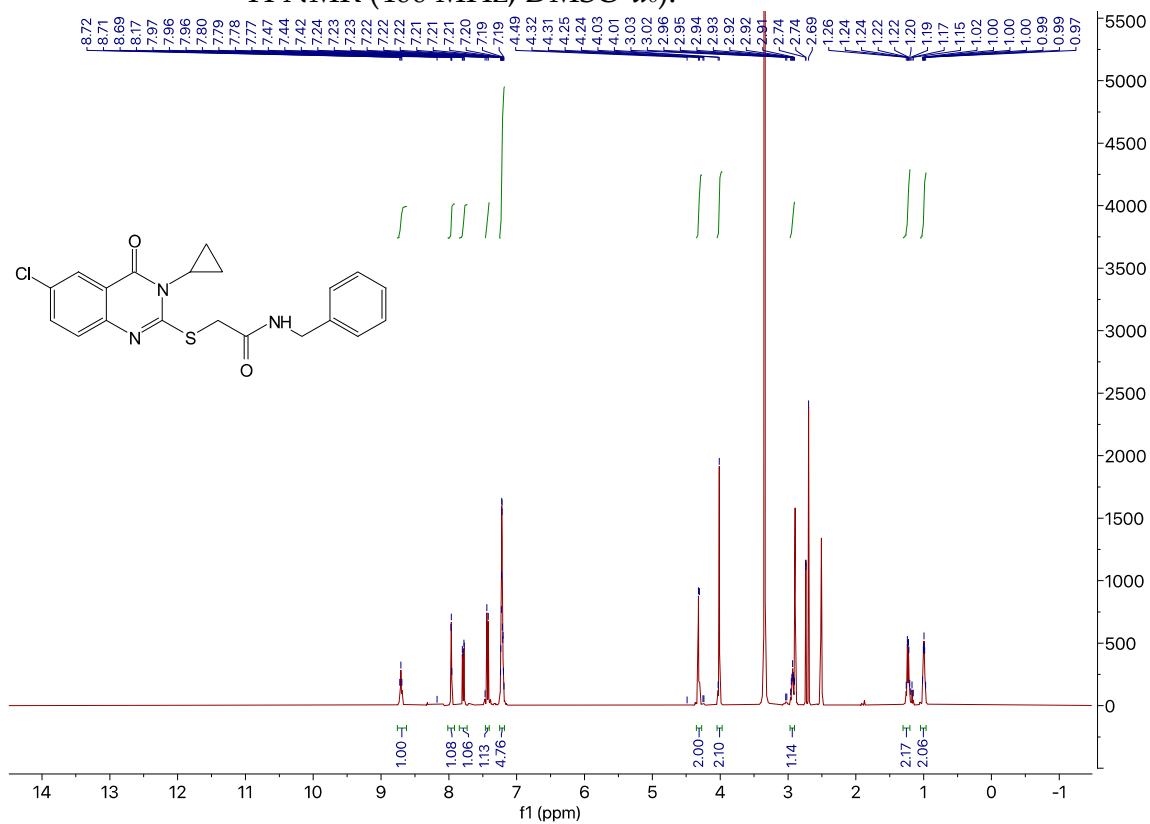


^{13}C NMR (100 MHz, $\text{DMSO}-d_6$):

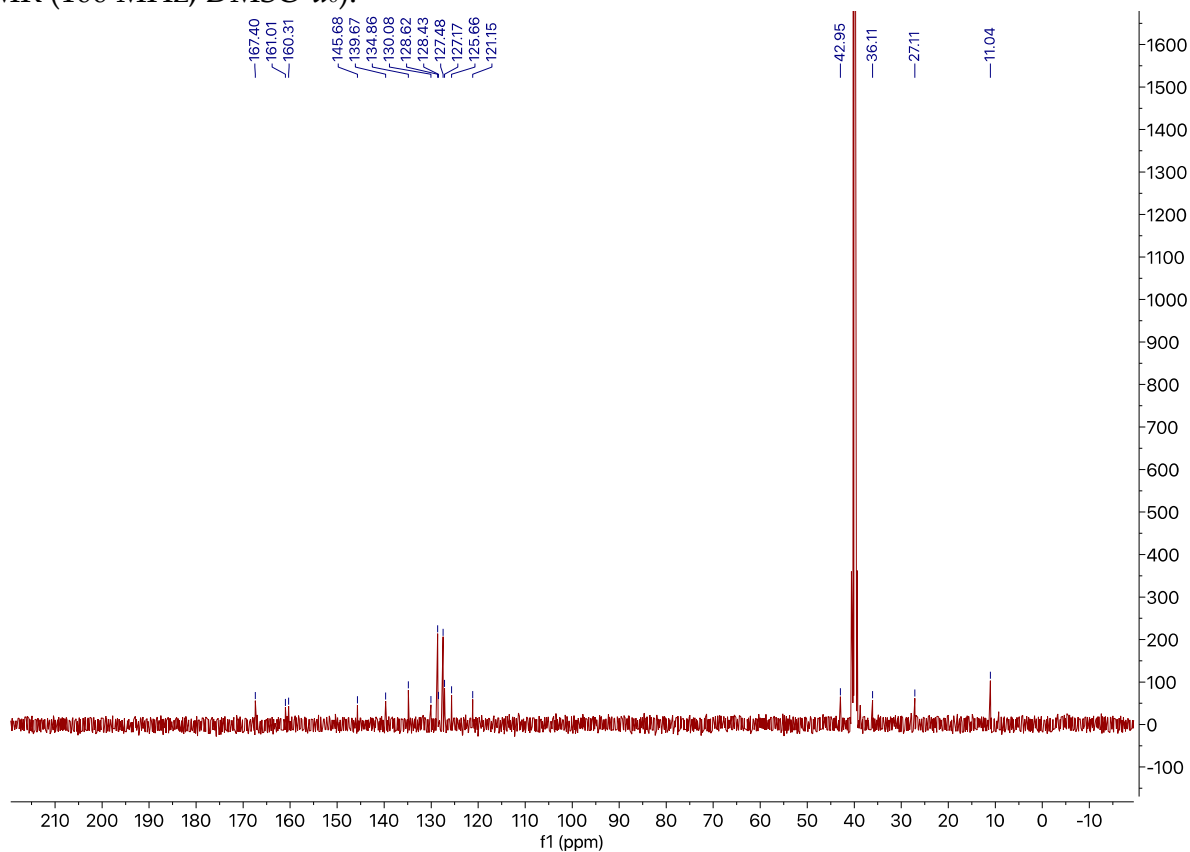


N-Benzyl-2-((6-chloro-3-cyclopropyl-4-oxo-3,4-dihydroquinazolin-2-yl)thio)acetamide (**5d**)

^1H NMR (400 MHz, $\text{DMSO}-d_6$):

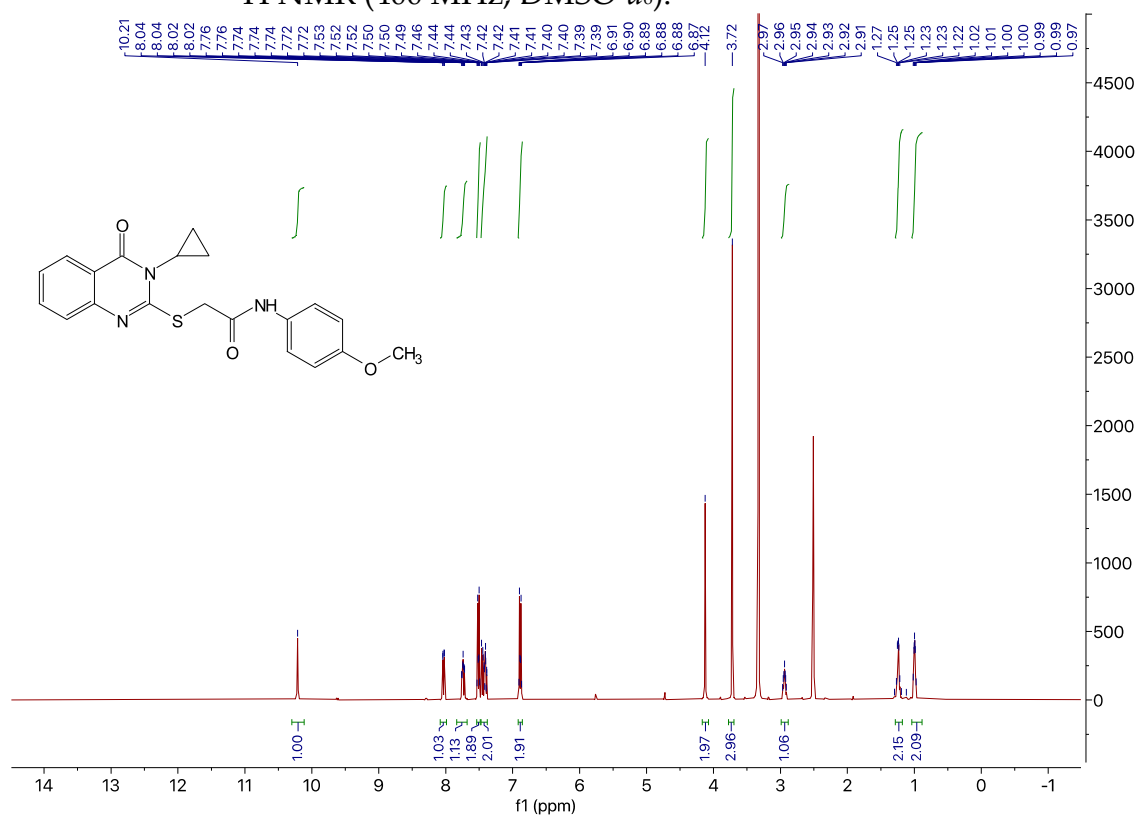


^{13}C NMR (100 MHz, $\text{DMSO}-d_6$):

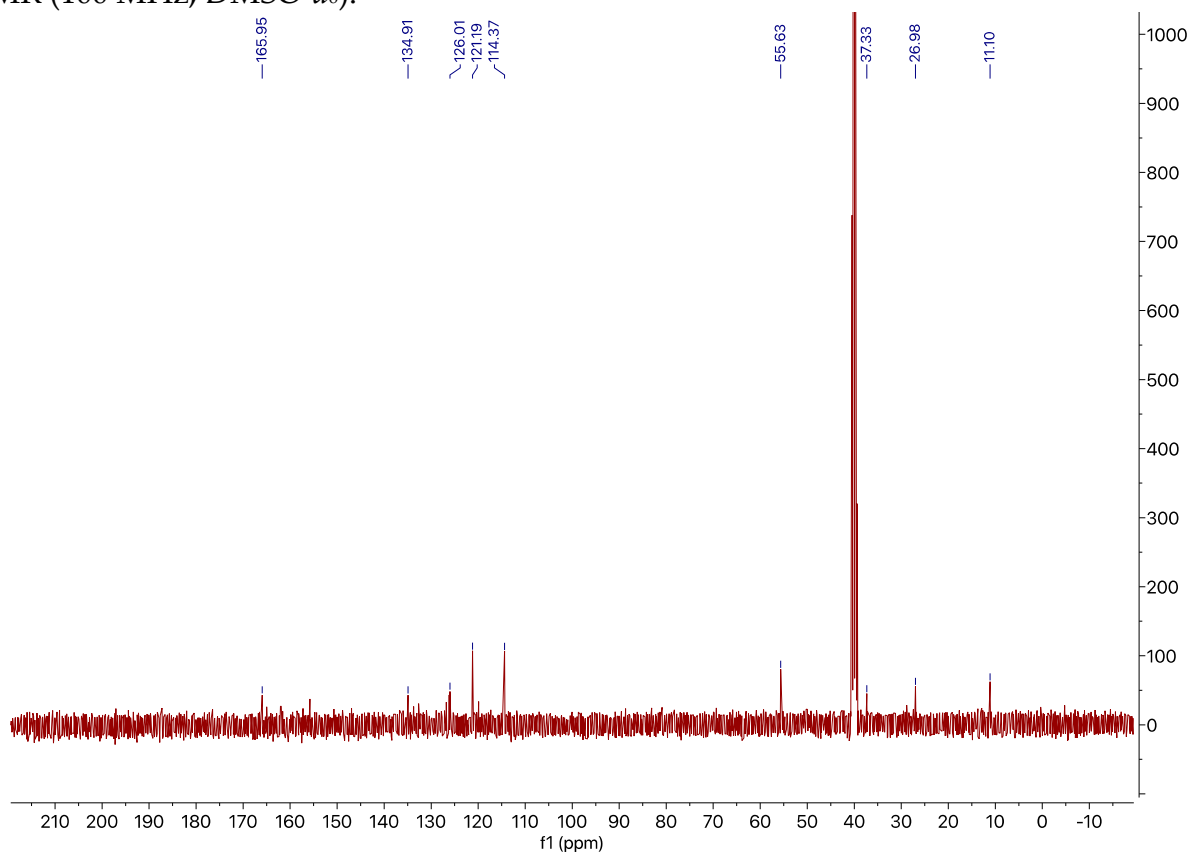


2-((3-Cyclopropyl-4-oxo-3,4-dihydroquinazolin-2-yl)thio)-N-(4-methoxyphenyl)acetamide (**5e**)

^1H NMR (400 MHz, $\text{DMSO}-d_6$):

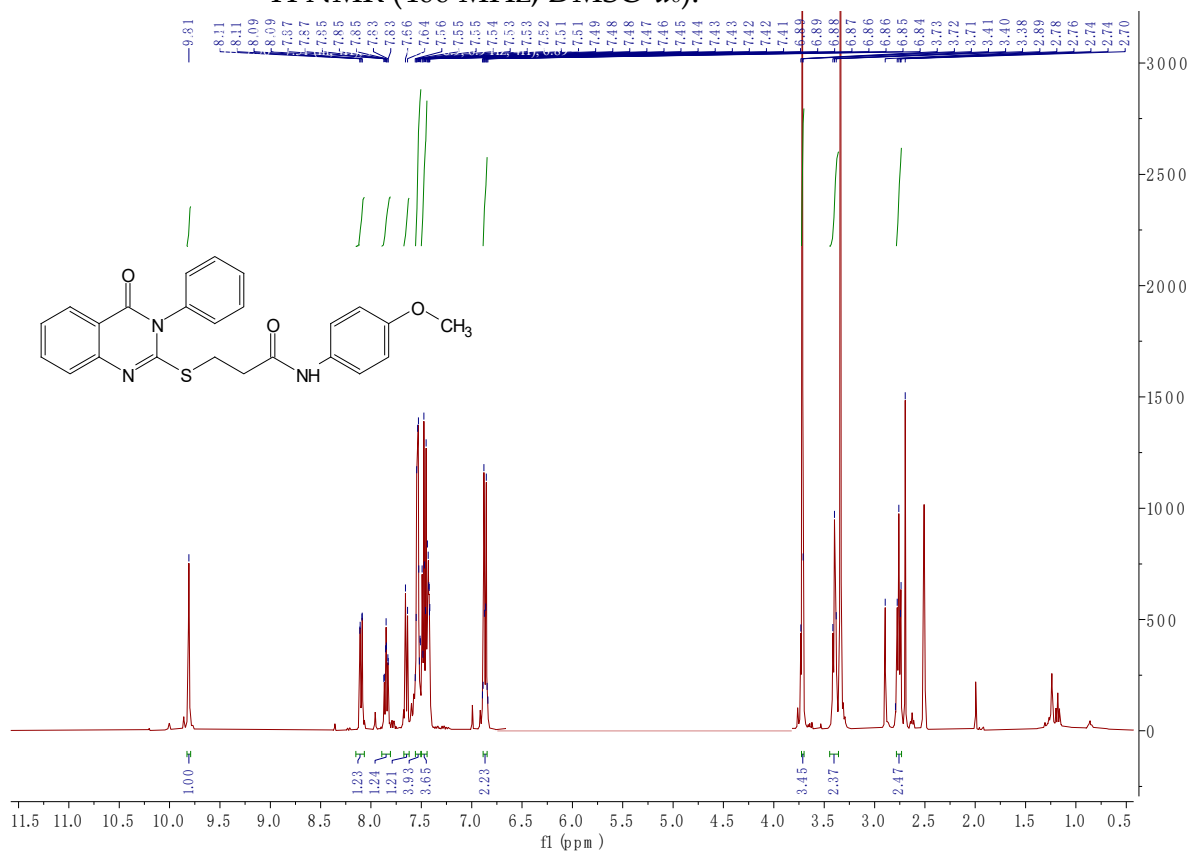


^{13}C NMR (100 MHz, $\text{DMSO}-d_6$):

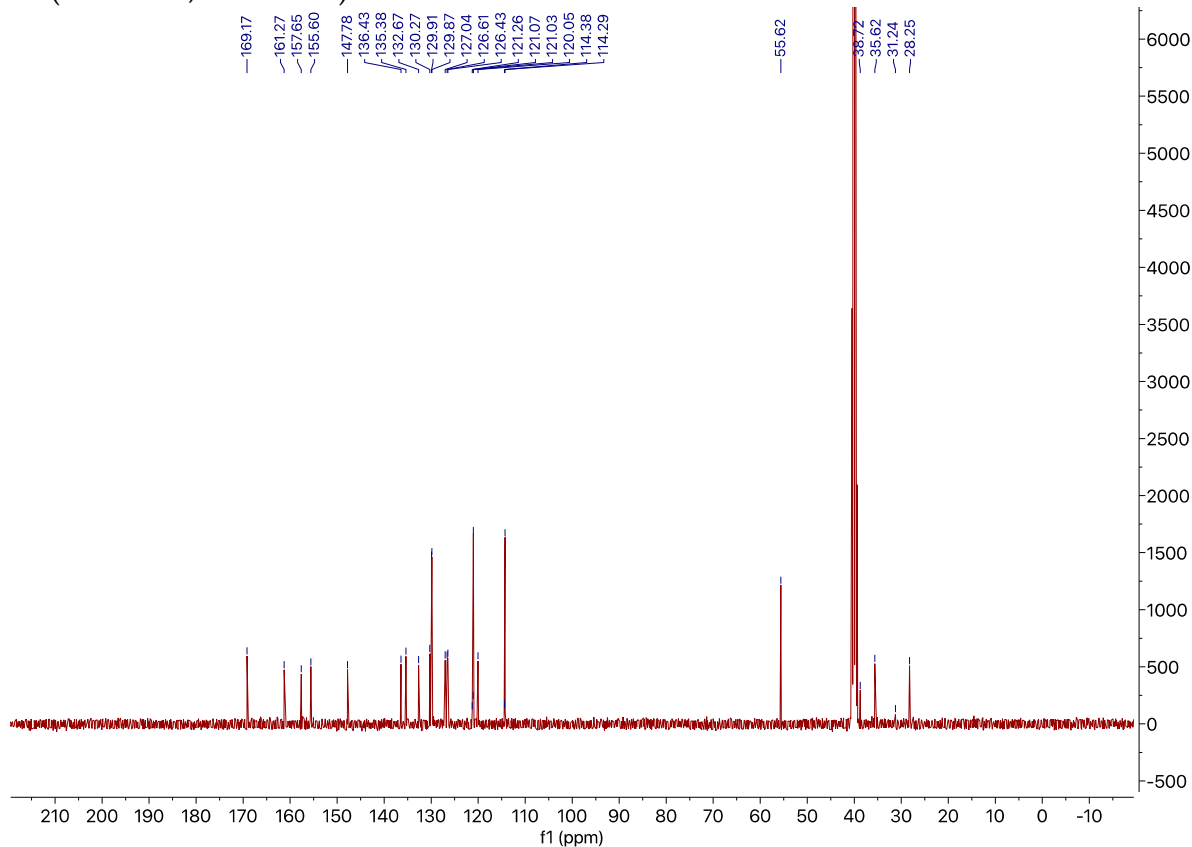


N-(4-Methoxyphenyl)-3-((4-oxo-3-phenyl-3,4-dihydroquinazolin-2-yl)thio)propanamide (**5f**)

^1H NMR (400 MHz, $\text{DMSO}-d_6$):

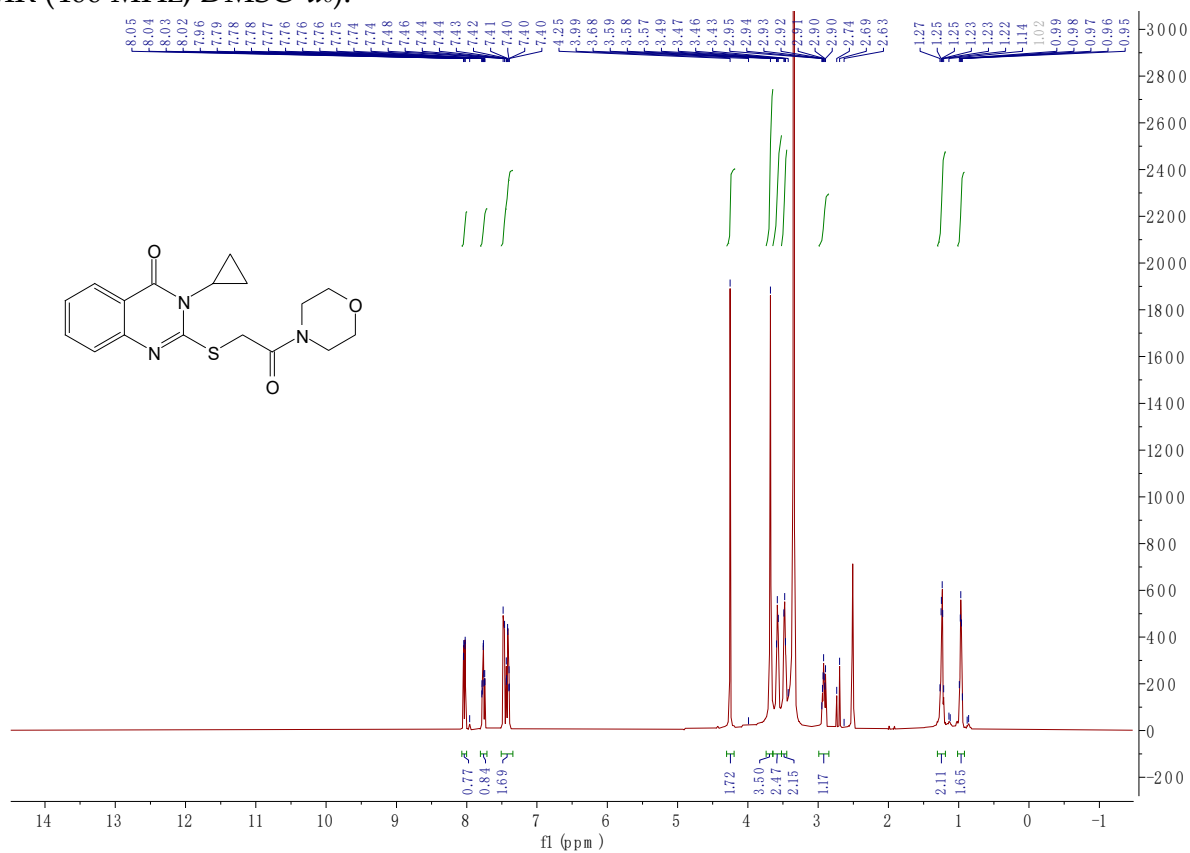


^{13}C NMR (100 MHz, $\text{DMSO}-d_6$):

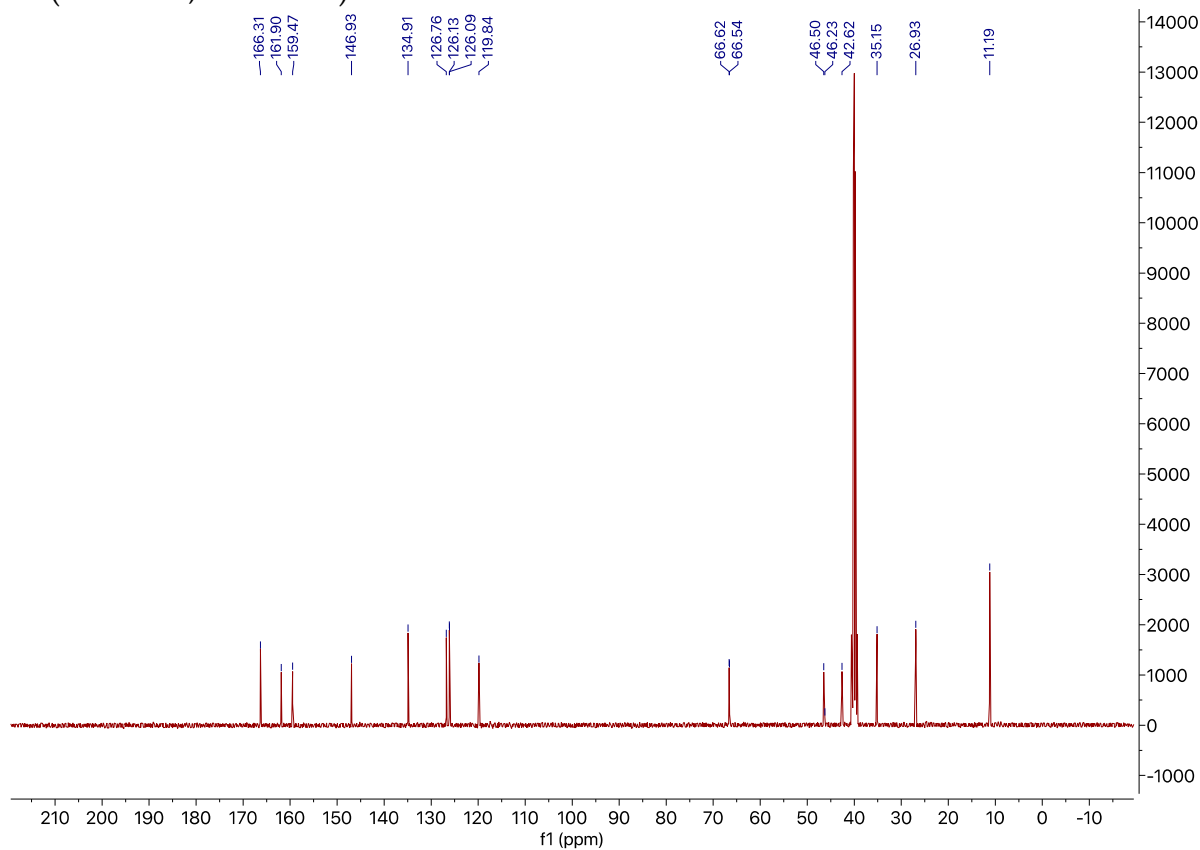


3-Cyclopropyl-2-((2-morpholino-2-oxoethyl)thio)quinazolin-4(3H)-one (**5g**)

^1H NMR (400 MHz, $\text{DMSO}-d_6$):

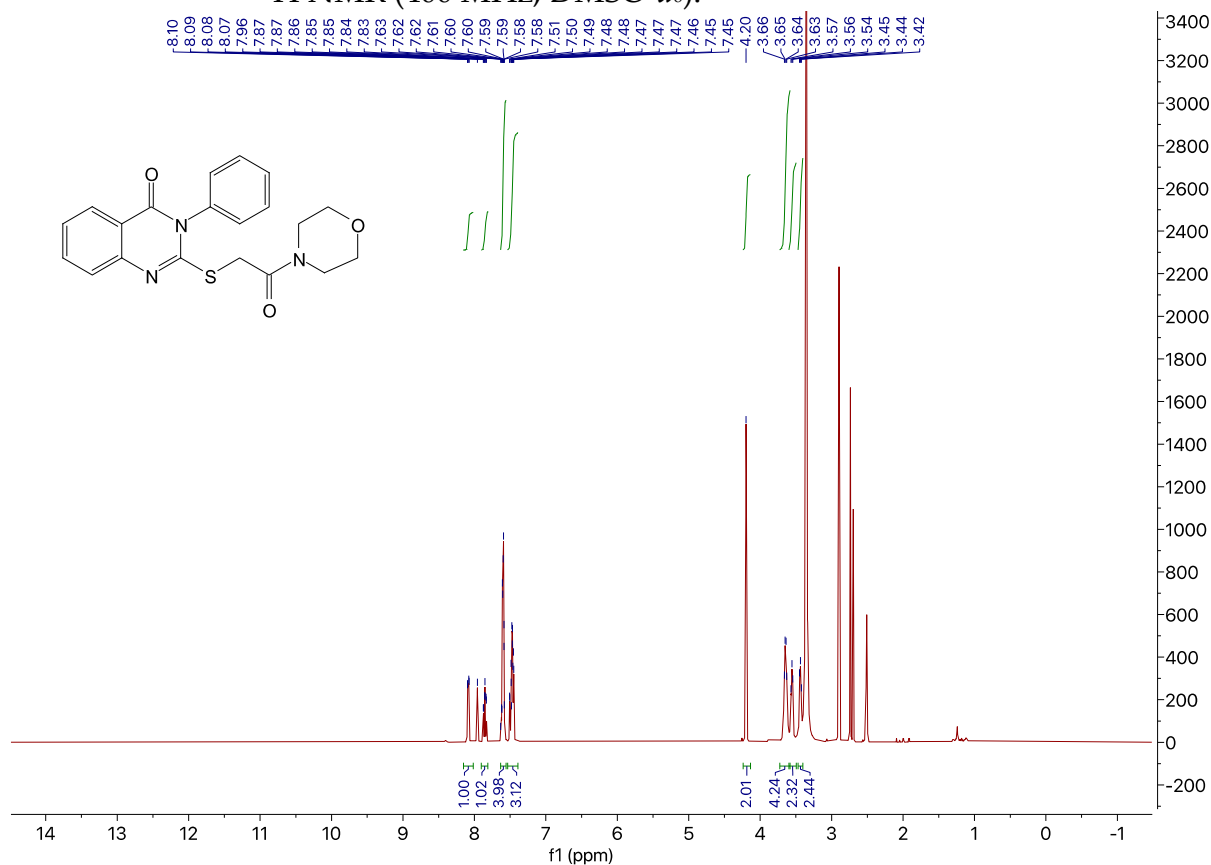


^{13}C NMR (100 MHz, $\text{DMSO}-d_6$):

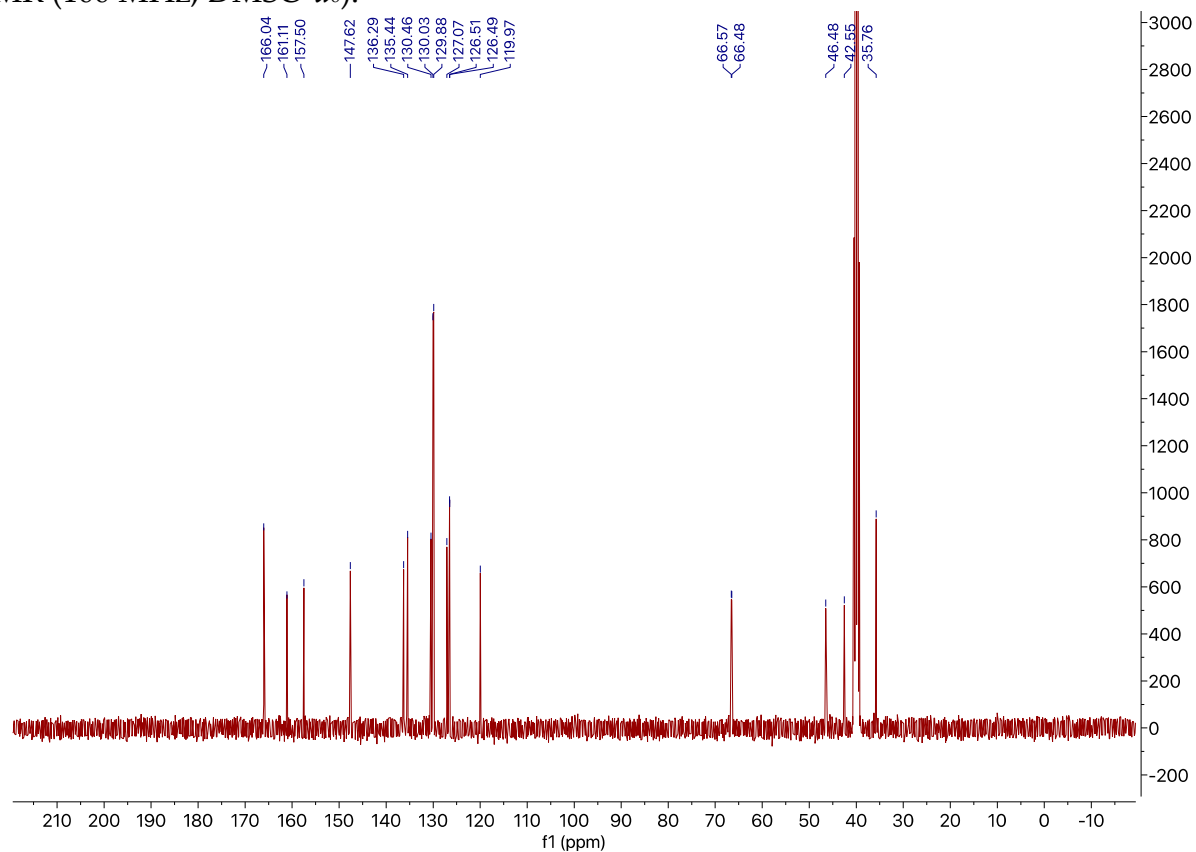


2-((2-Morpholino-2-oxoethyl)thio)-3-phenylquinazolin-4(3H)-one (**5h**)

^1H NMR (400 MHz, $\text{DMSO}-d_6$):

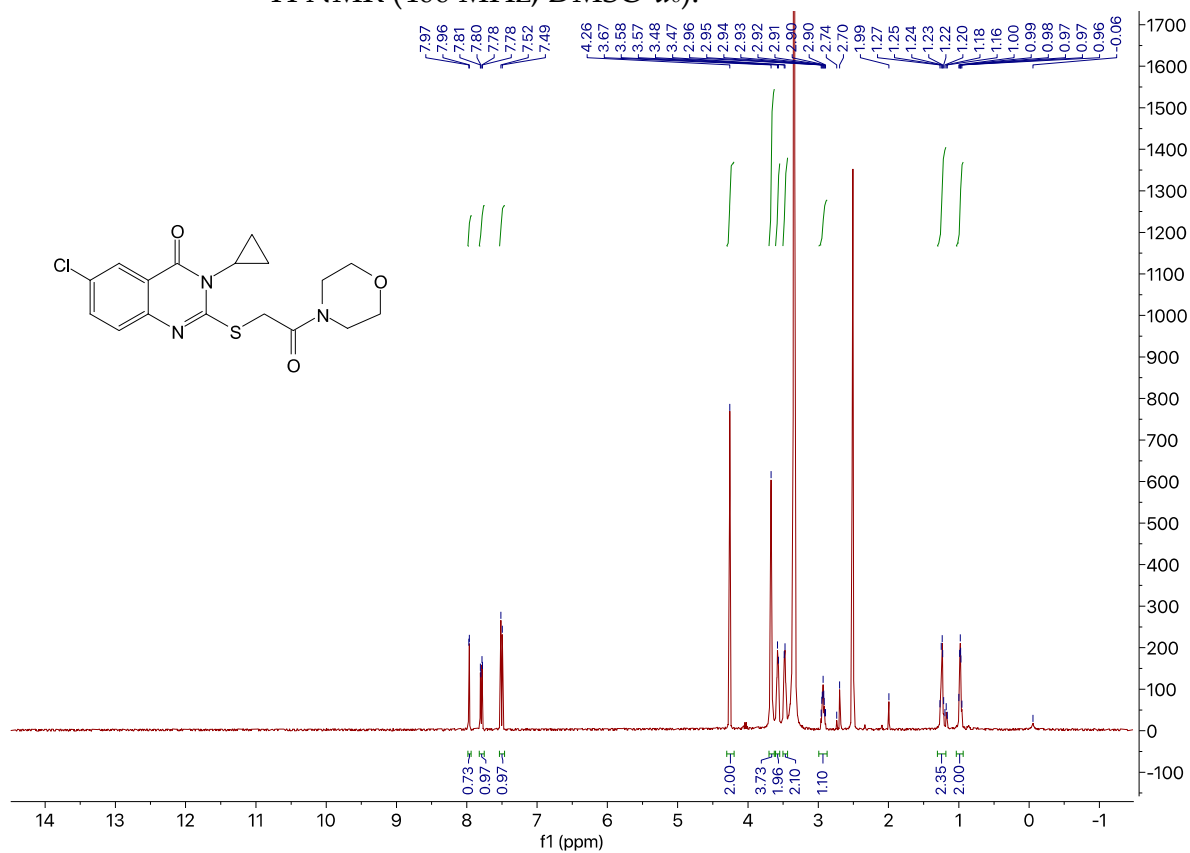


^{13}C NMR (100 MHz, $\text{DMSO}-d_6$):

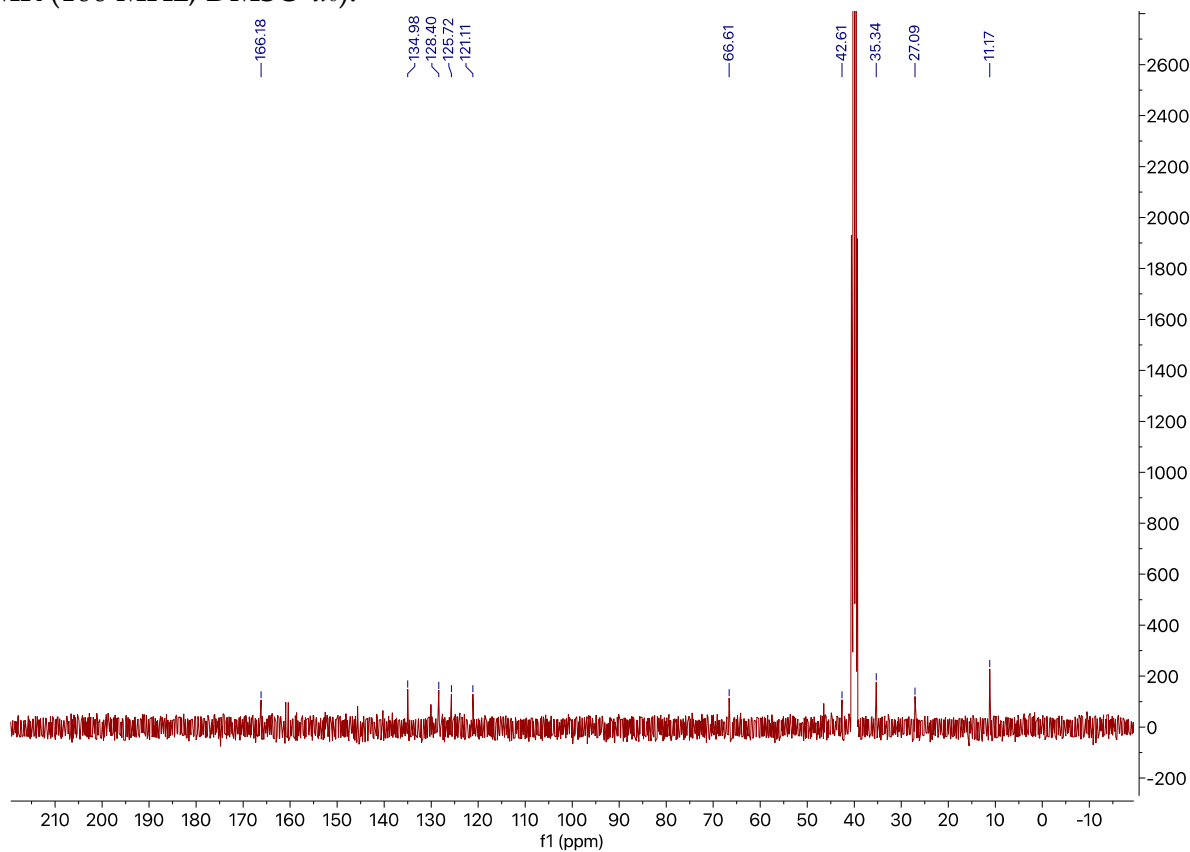


2-((2-Morpholino-2-oxoethyl)thio)quinazolin-4(3H)-one (**5i**)

^1H NMR (400 MHz, $\text{DMSO}-d_6$):

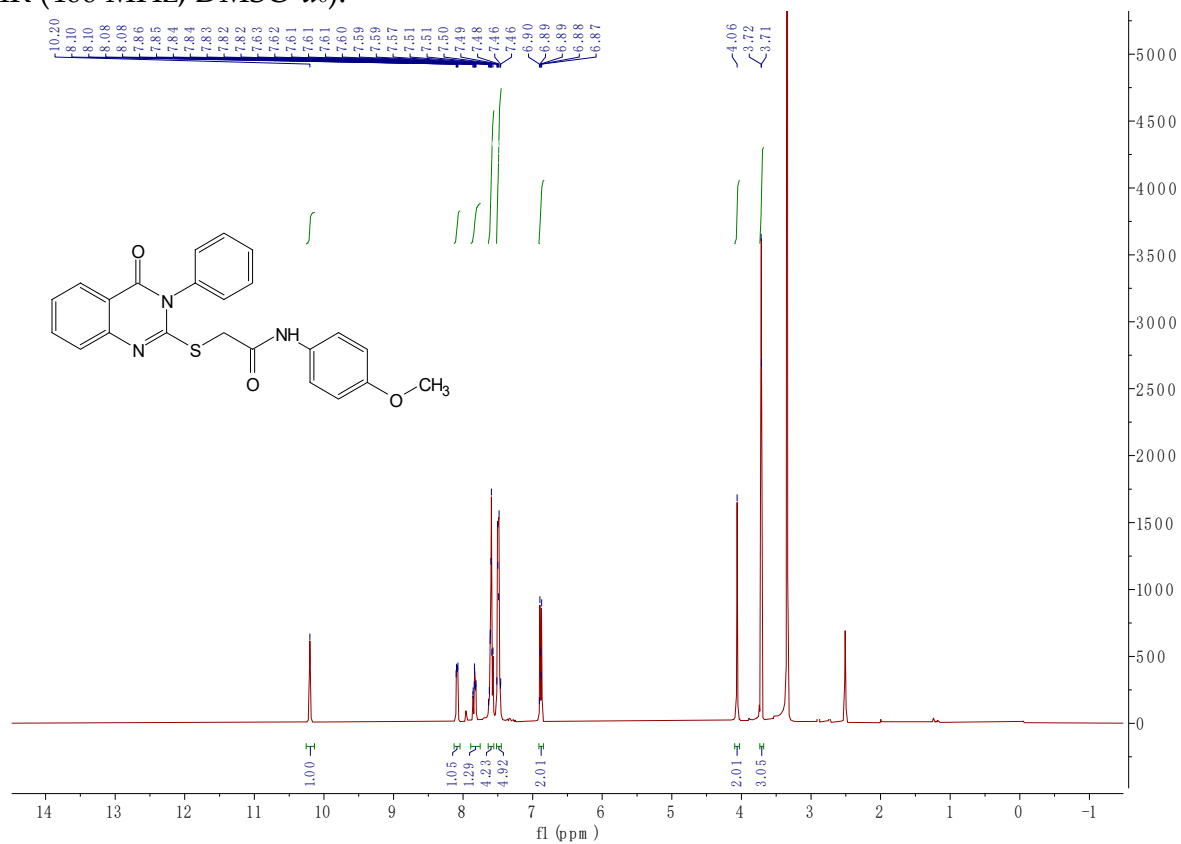


^{13}C NMR (100 MHz, $\text{DMSO}-d_6$):

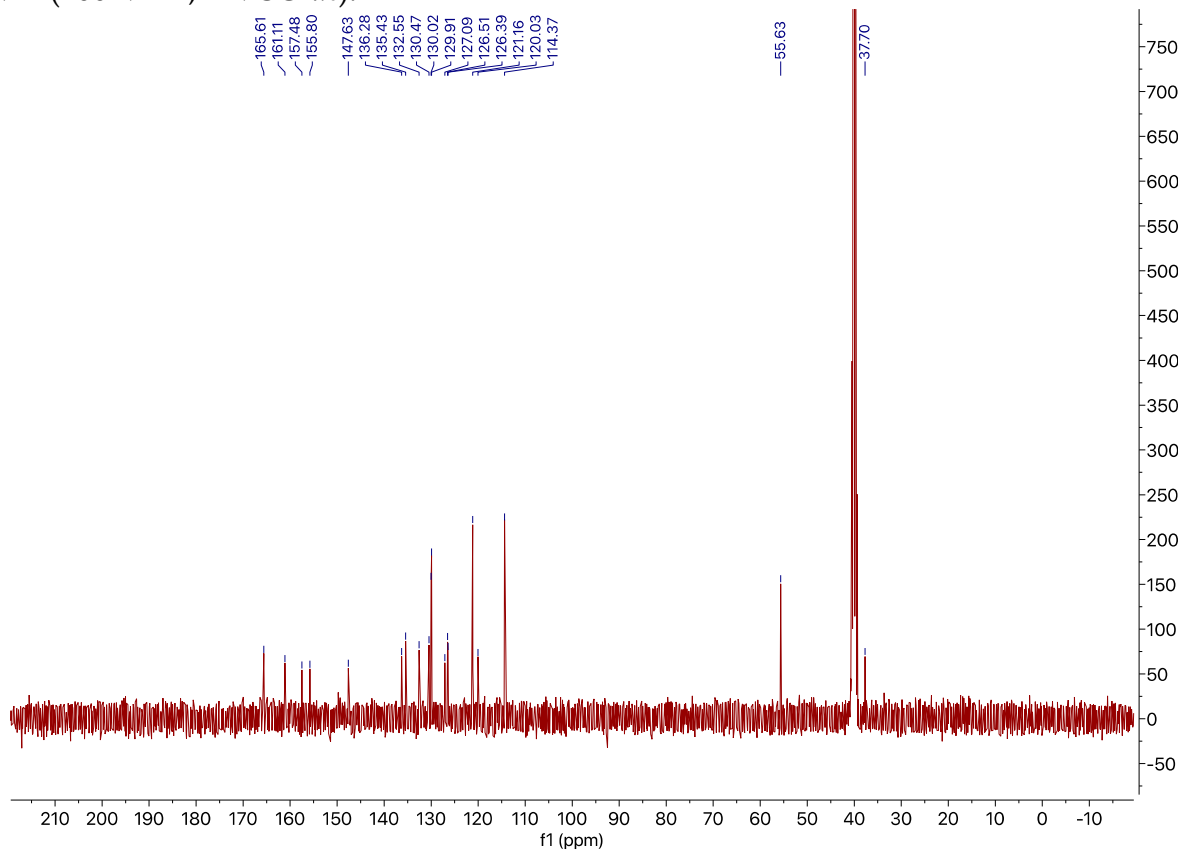


N-(4-Methoxyphenyl)-2-((4-oxo-3-phenyl-3,4-dihydroquinazolin-2-yl)thio)acetamide (**5j**)

^1H NMR (400 MHz, $\text{DMSO}-d_6$):

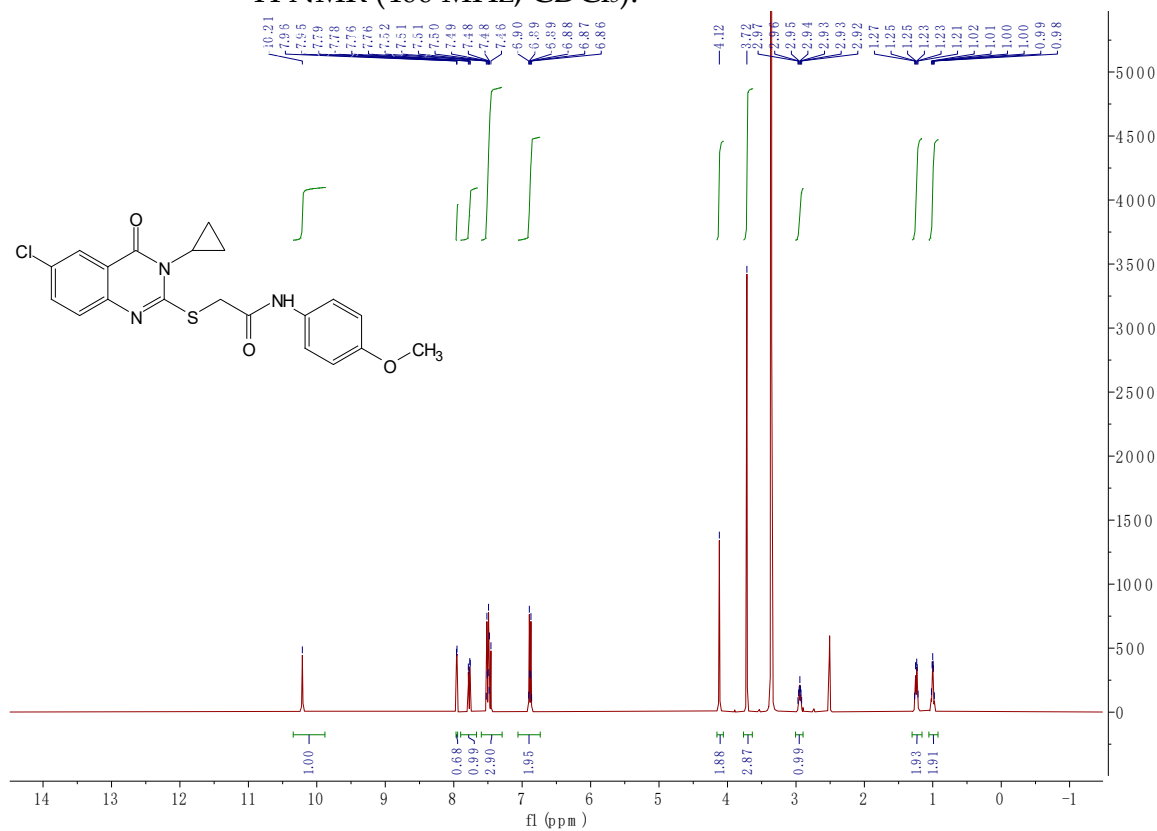


^{13}C NMR (100 MHz, $\text{DMSO}-d_6$):

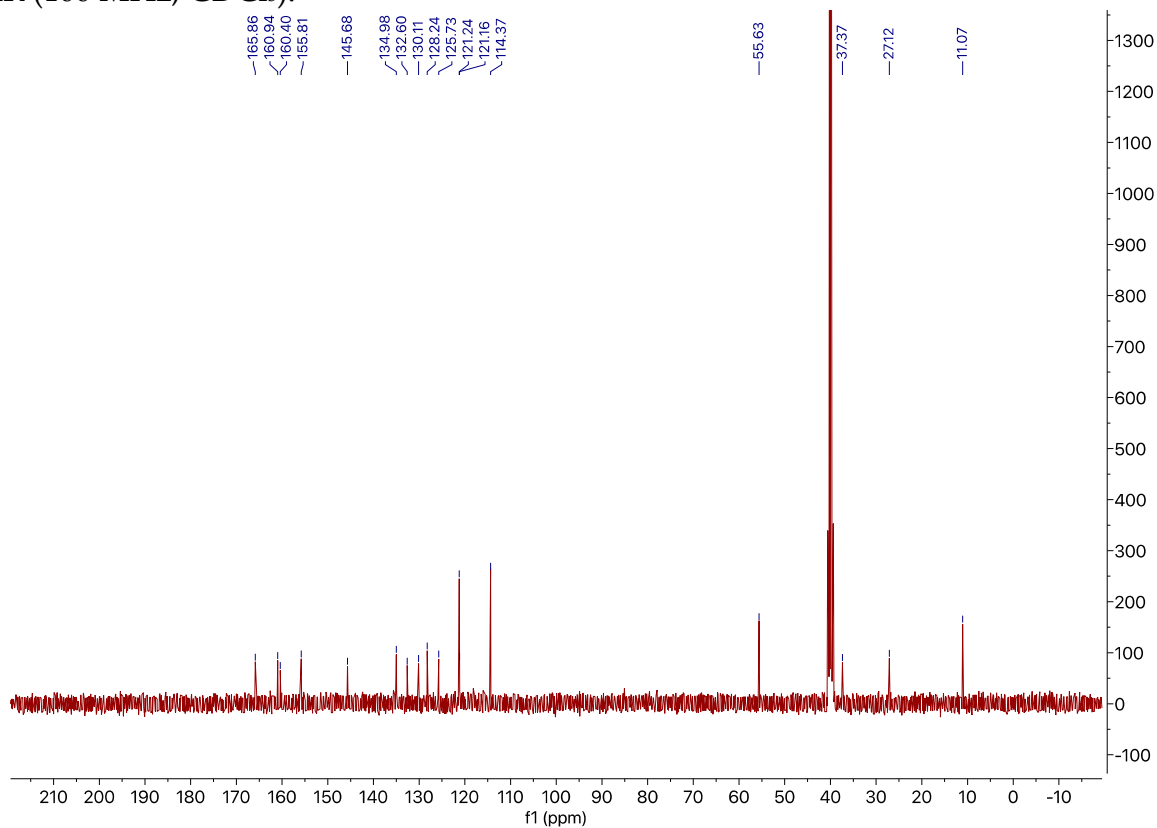


2-((6-Chloro-3-cyclopropyl-4-oxo-3,4-dihydroquinazolin-2-yl)thio)-N-(4-methoxyphenyl)acetamide (**5k**)

^1H NMR (400 MHz, CDCl_3):

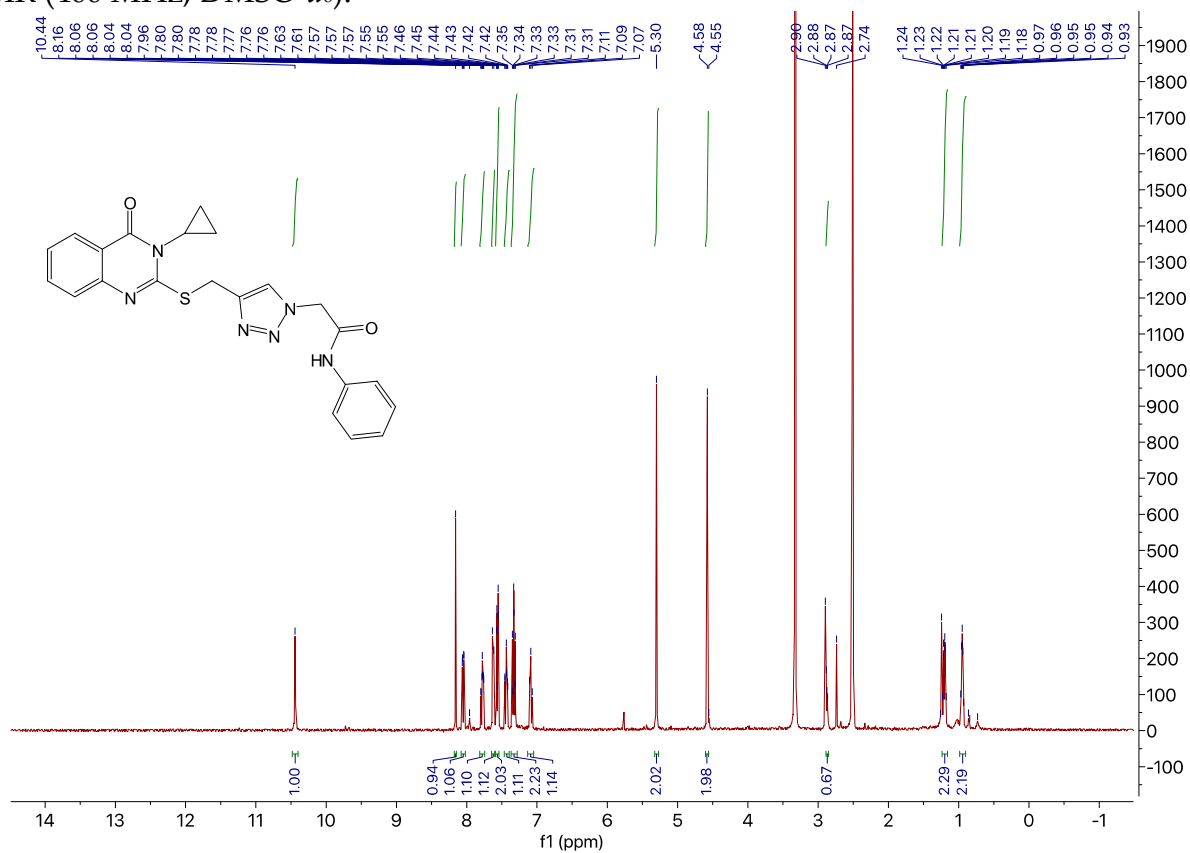


^{13}C NMR (100 MHz, CDCl_3):

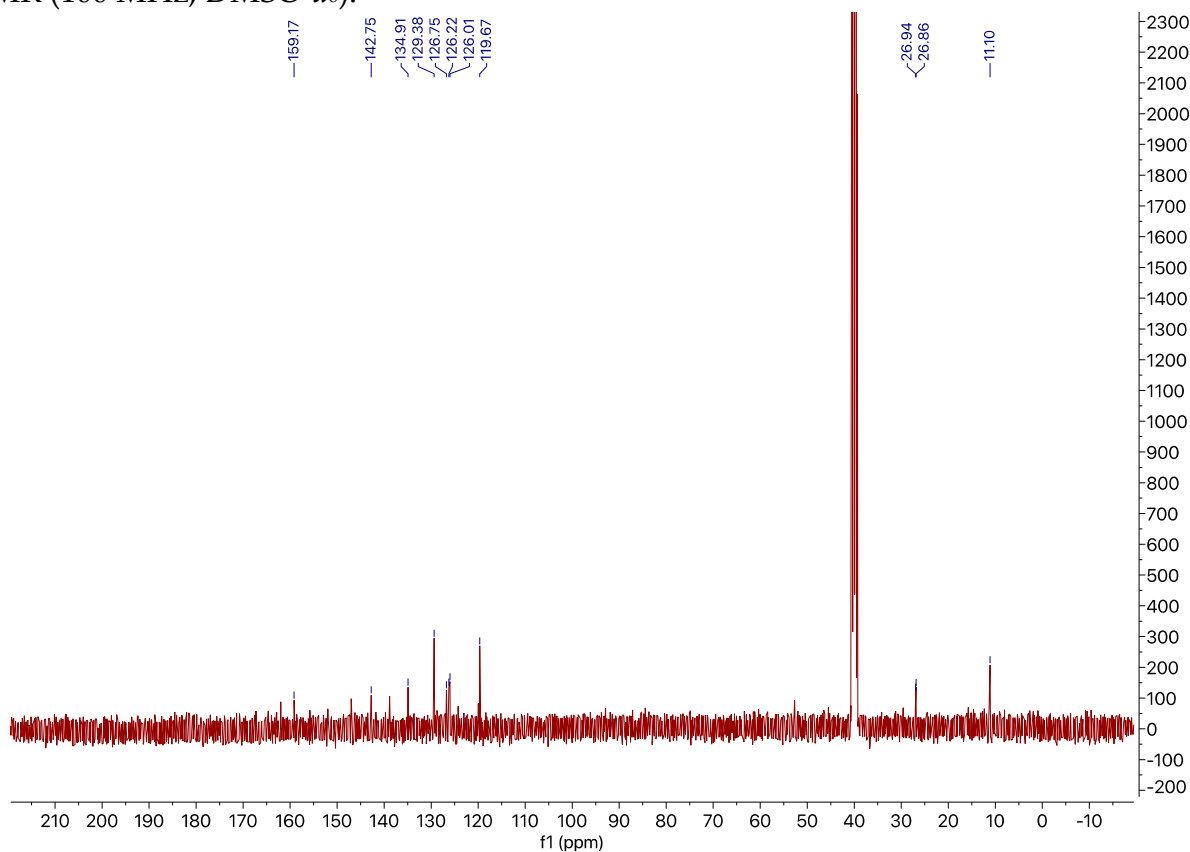


2-(4-(((3-Cyclopropyl-4-oxo-3,4-dihydroquinazolin-2-yl)thio)methyl)-1H-1,2,3-triazol-1-yl)-N-phenylacetamide (**6a**)

^1H NMR (400 MHz, $\text{DMSO}-d_6$):

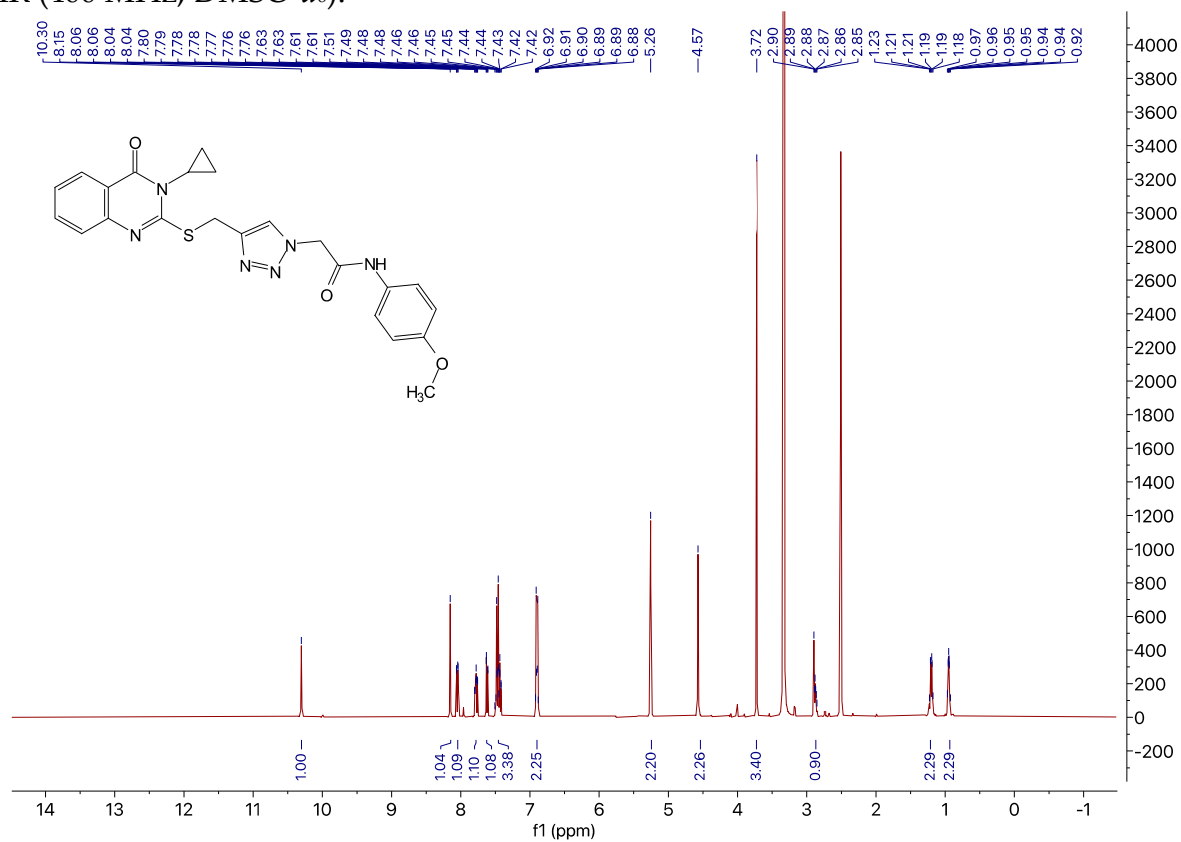


^{13}C NMR (100 MHz, $\text{DMSO}-d_6$):

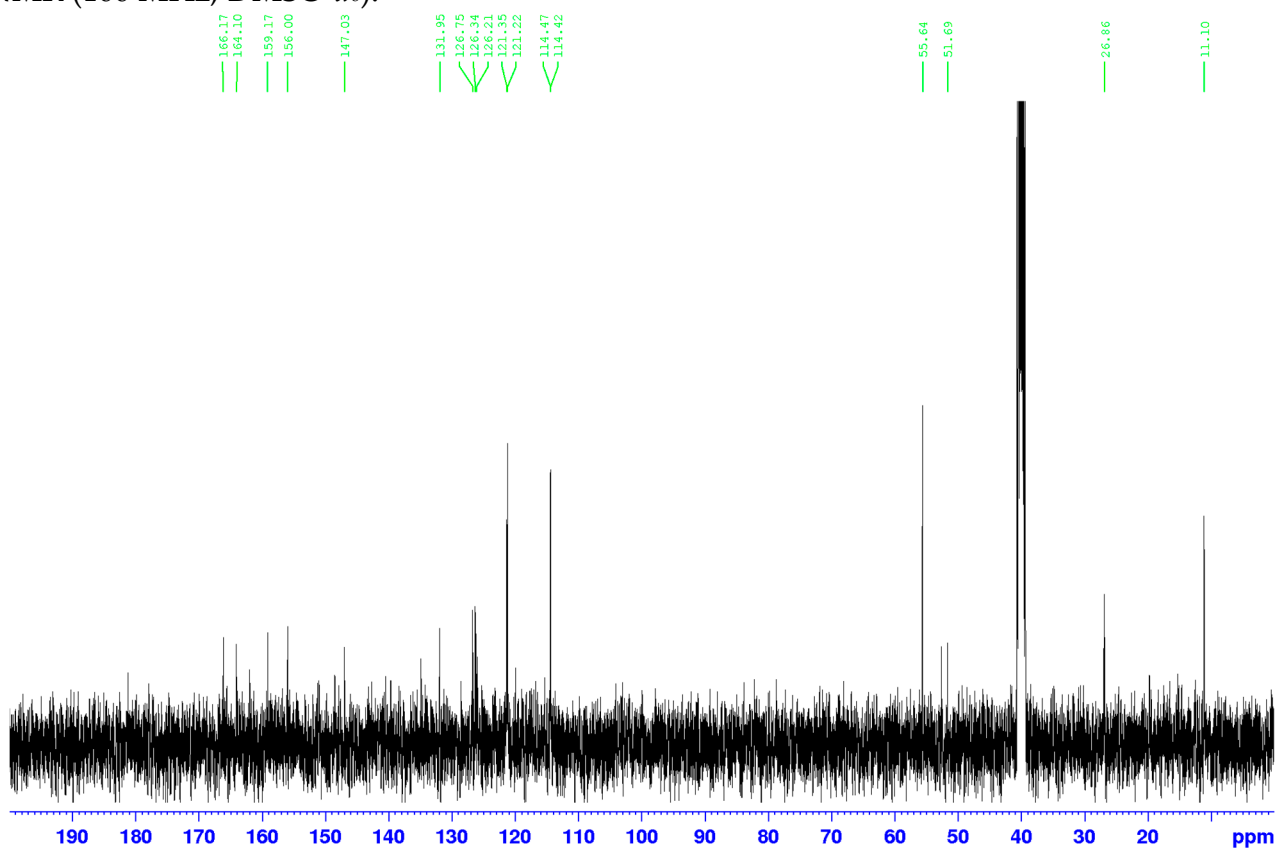


2-(4-(((3-Cyclopropyl-4-oxo-3,4-dihydroquinazolin-2-yl)thio)methyl)-1H-1,2,3-triazol-1-yl)-N-(4-methoxyphenyl)acetamide (**6b**)

^1H NMR (400 MHz, $\text{DMSO}-d_6$):

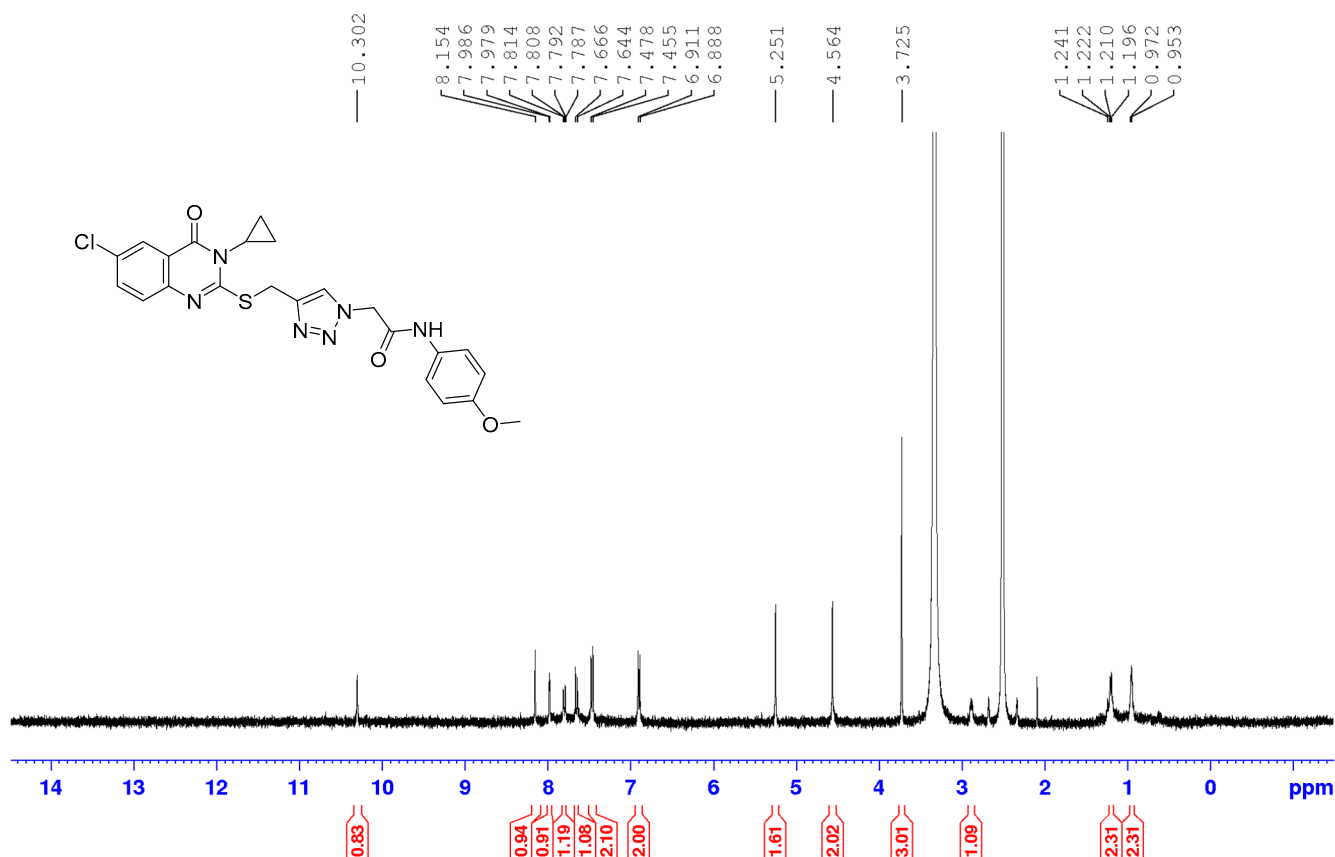


^{13}C NMR (100 MHz, $\text{DMSO}-d_6$):

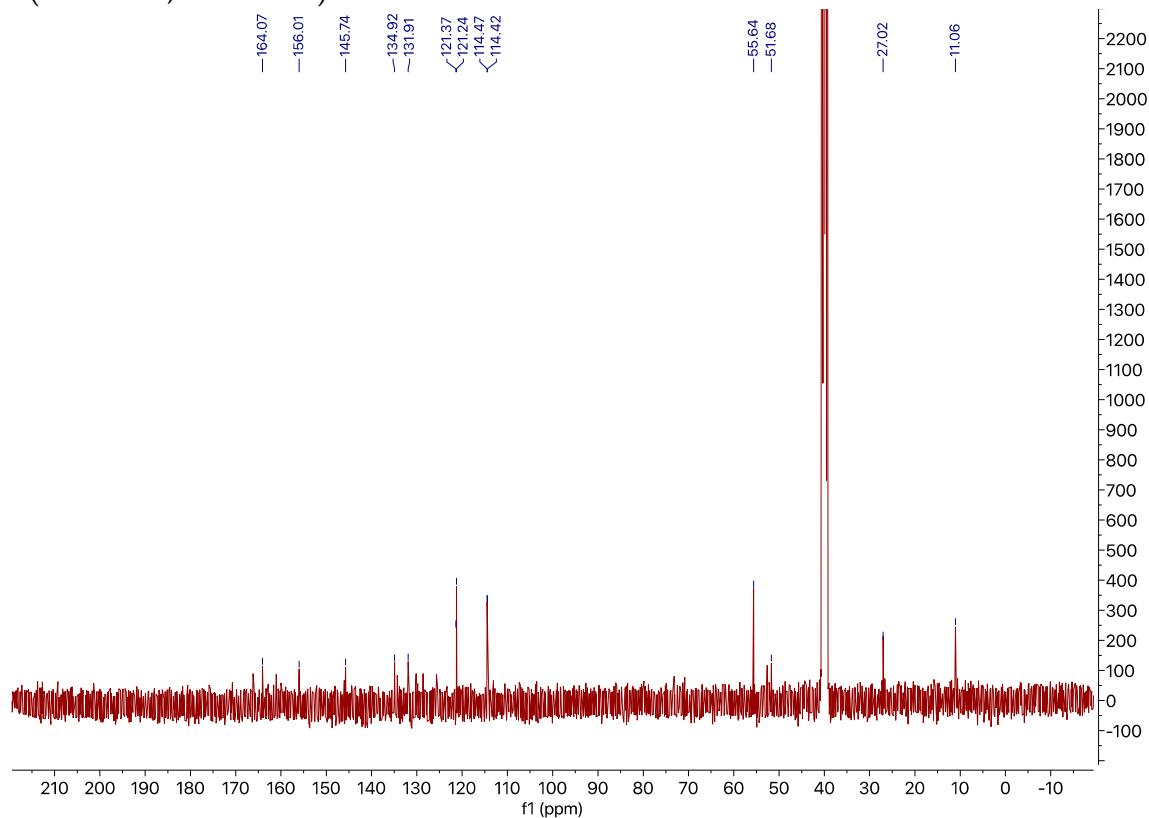


2-(4-(((6-Chloro-3-cyclopropyl-4-oxo-3,4-dihydroquinazolin-2-yl)thio)methyl)-1H-1,2,3-triazol-1-yl)-N-(4-methoxyphenyl)acetamide (**6c**)

^1H NMR (400 MHz, $\text{DMSO}-d_6$):

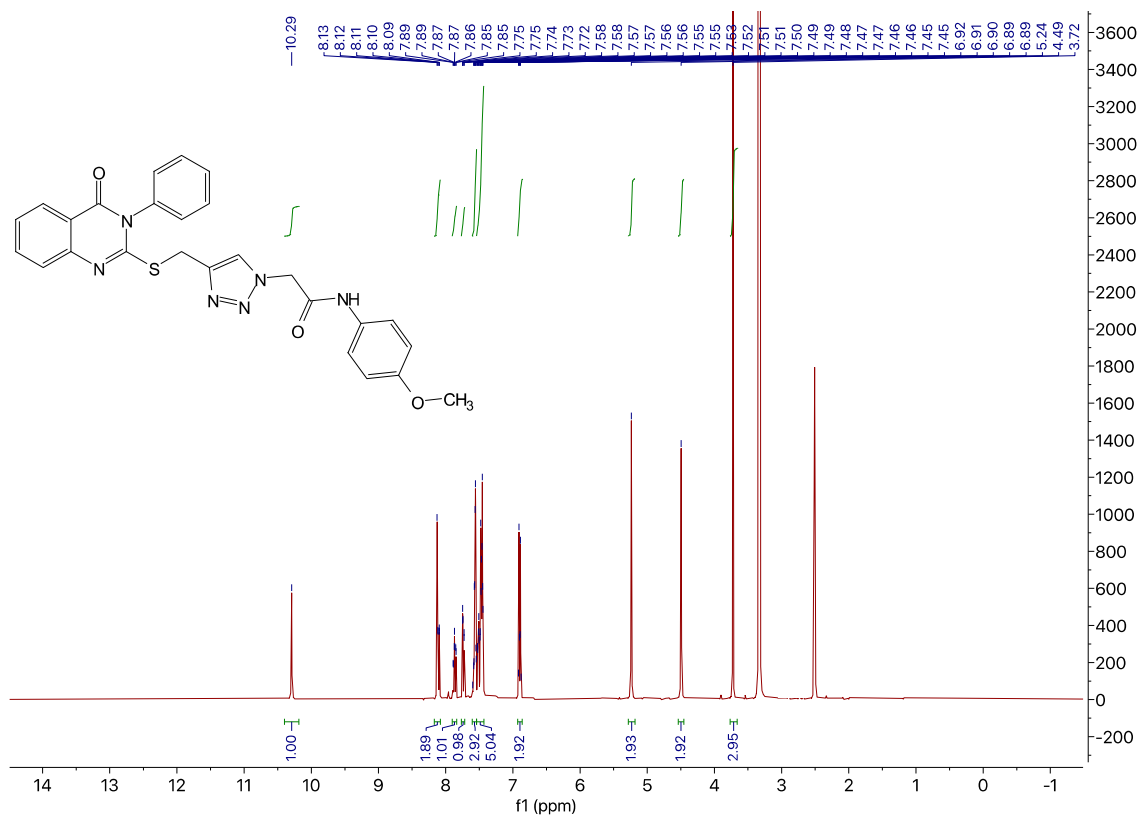


^{13}C NMR (100 MHz, $\text{DMSO}-d_6$):

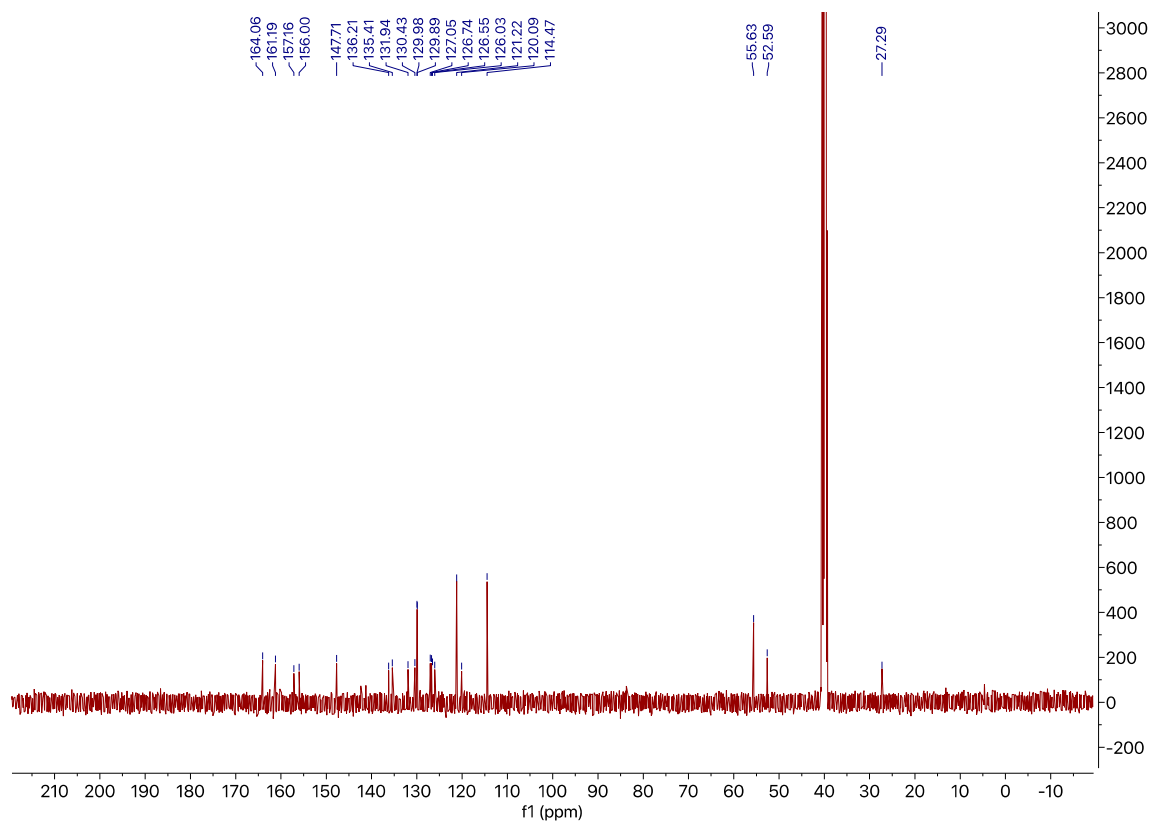


N-(4-Methoxyphenyl)-2-(4-(((4-oxo-3-phenyl-3,4-dihydroquinazolin-2-yl)thio)methyl)-1*H*-1,2,3-triazol-1-yl)acetamide (**6d**)

^1H NMR (400 MHz, $\text{DMSO-}d_6$):

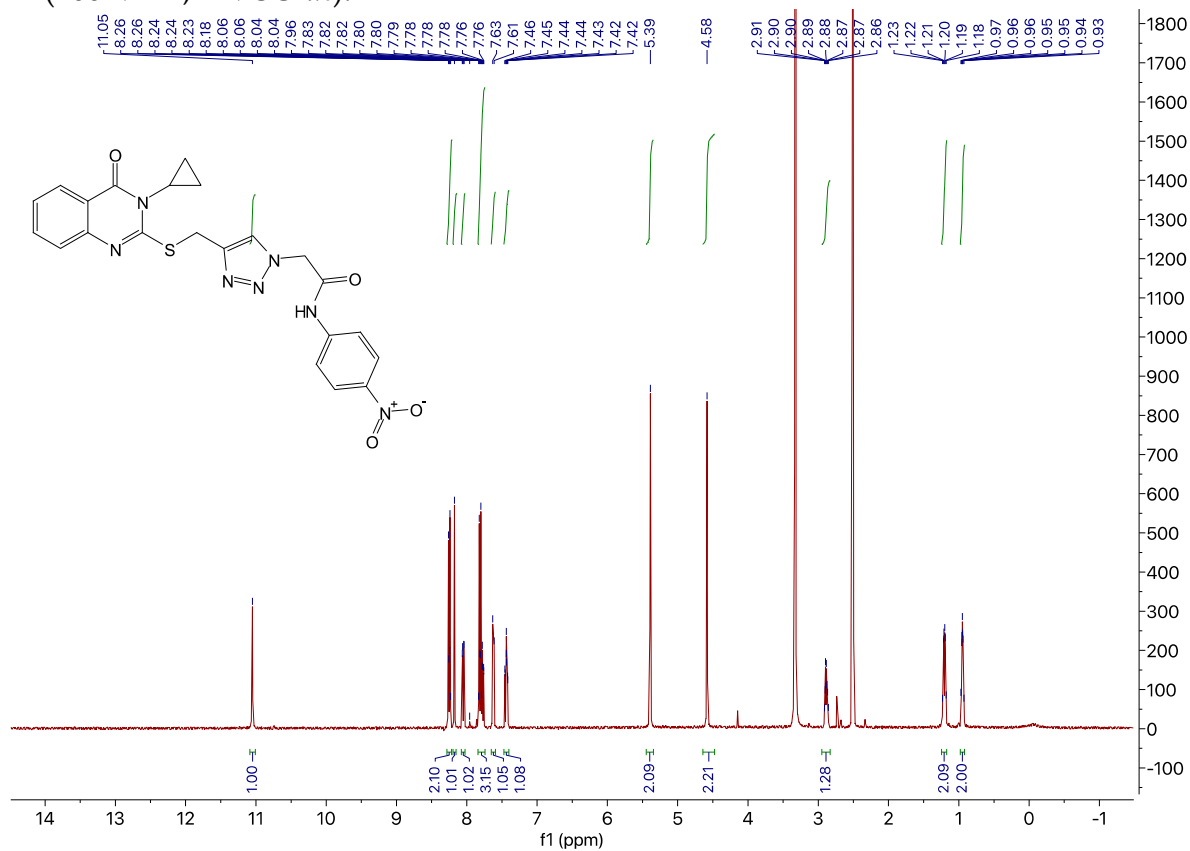


^{13}C NMR (100 MHz, $\text{DMSO-}d_6$):

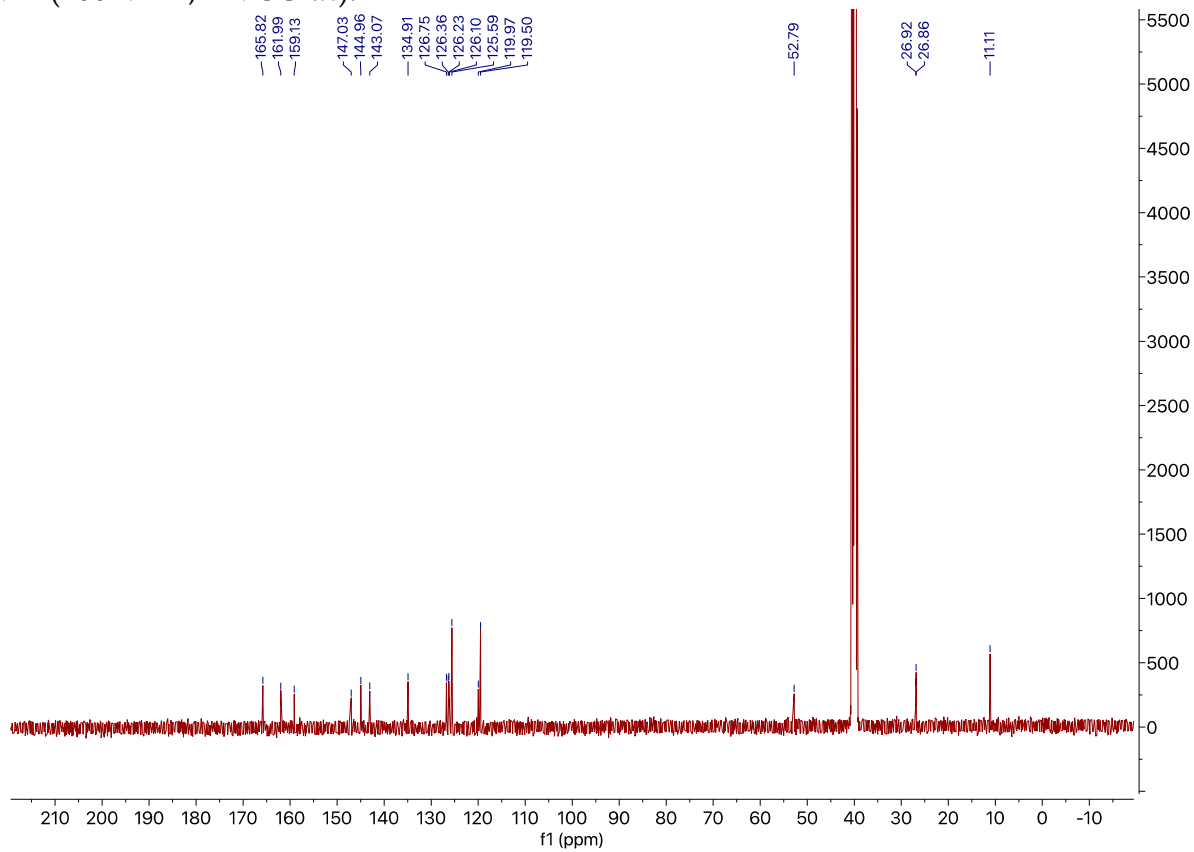


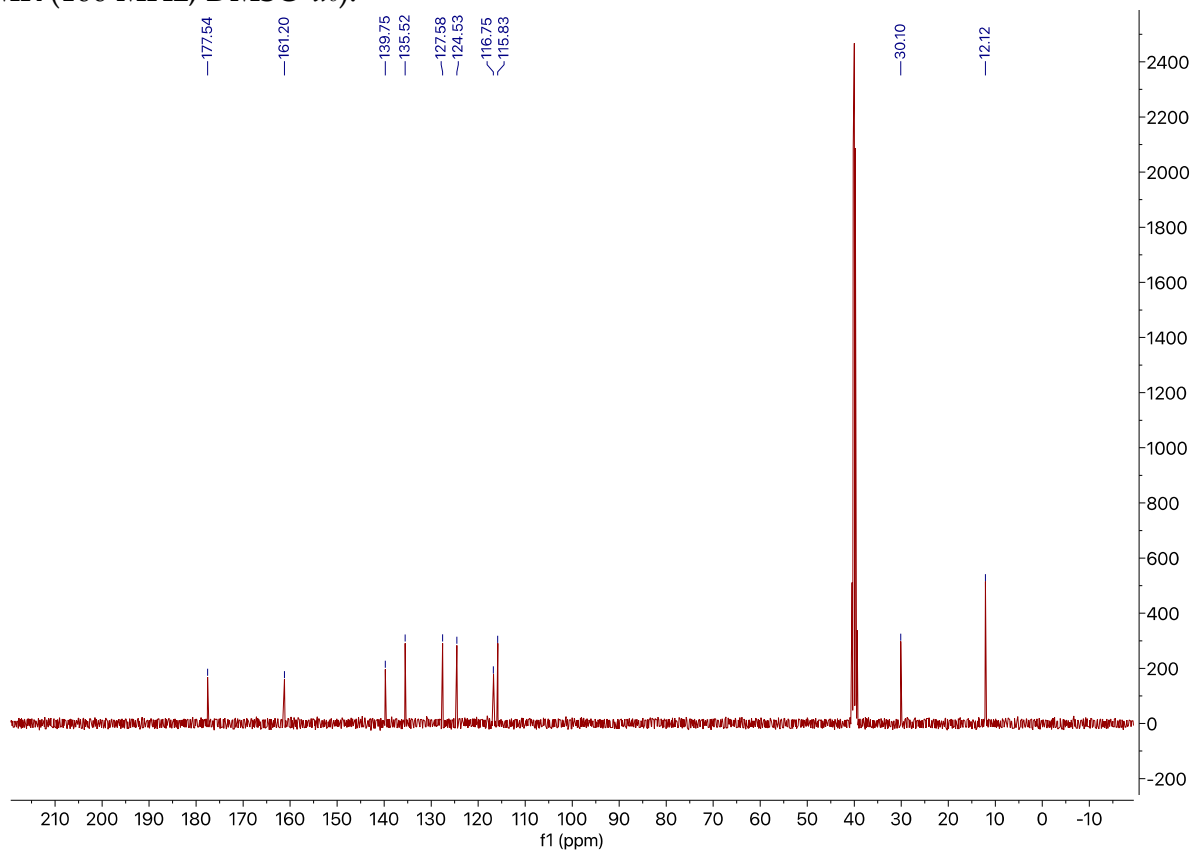
2-(4-(((3-Cyclopropyl-4-oxo-3,4-dihydroquinazolin-2-yl)thio)methyl)-1H-1,2,3-triazol-1-yl)-N-(4-nitrophenyl)acetamide (**6e**)

^1H NMR (400 MHz, $\text{DMSO}-d_6$):



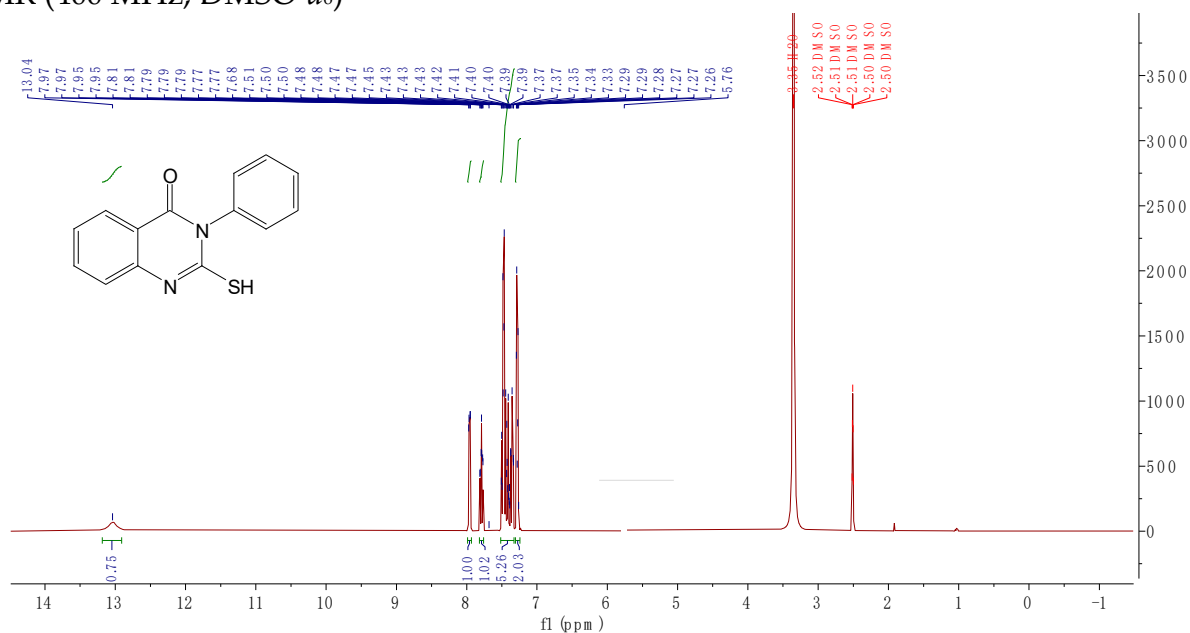
^{13}C NMR (100 MHz, $\text{DMSO}-d_6$):



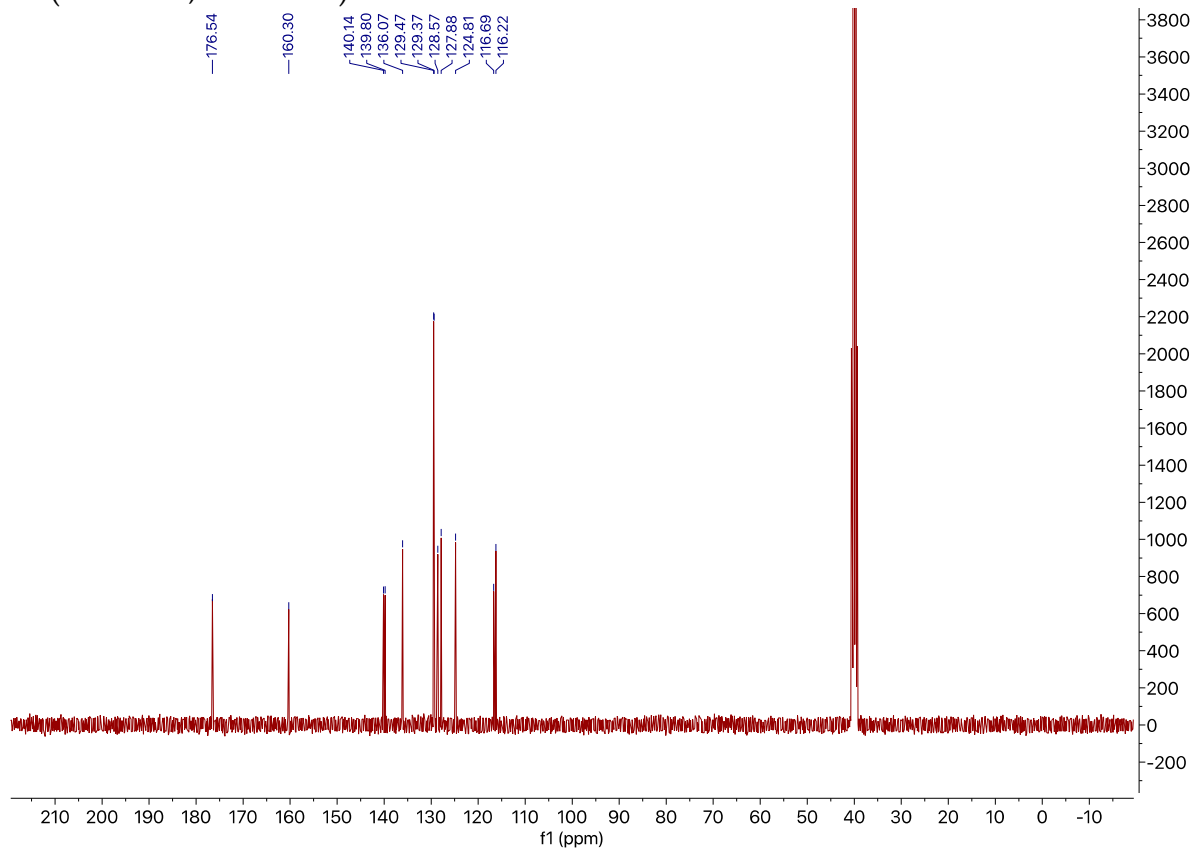
¹H NMR (400 MHz, DMSO-*d*₆)

2-Mercapto-3-phenylquinazolin-4(3H)-one (8b)

^1H NMR (400 MHz, $\text{DMSO}-d_6$)

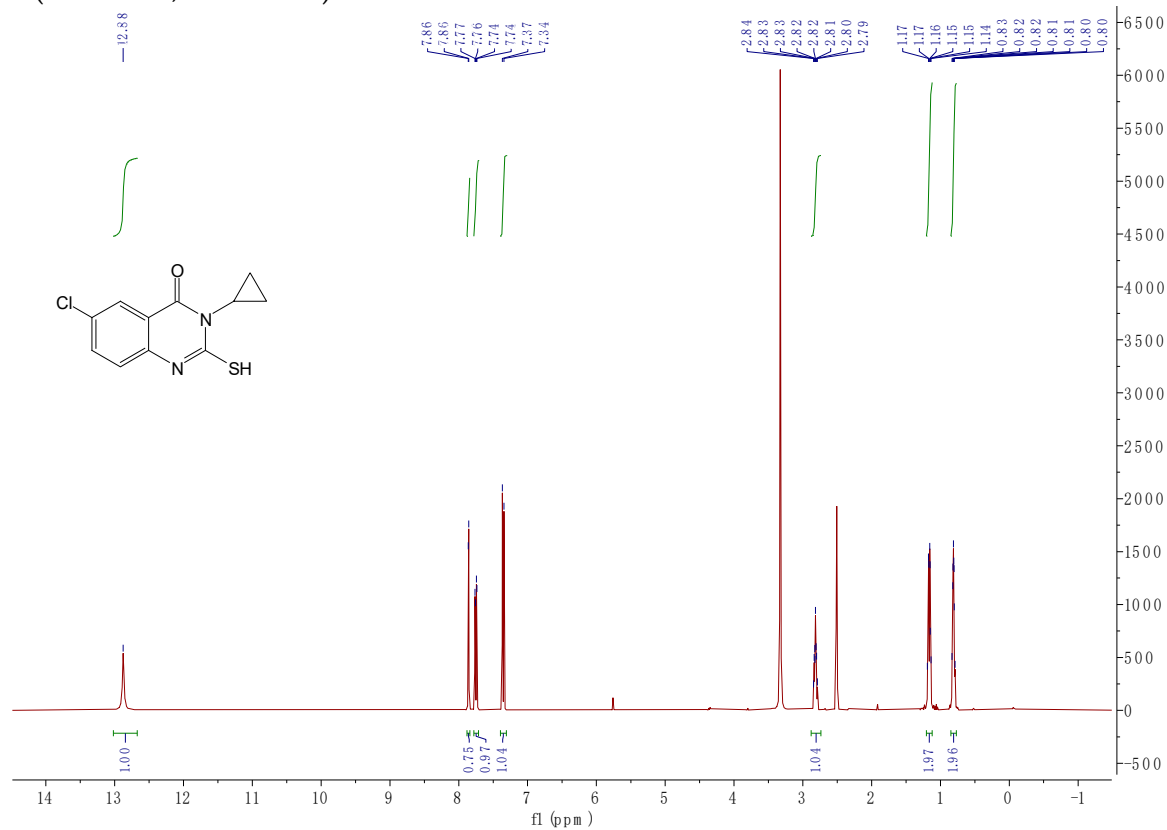


^{13}C NMR (100 MHz, $\text{DMSO}-d_6$):

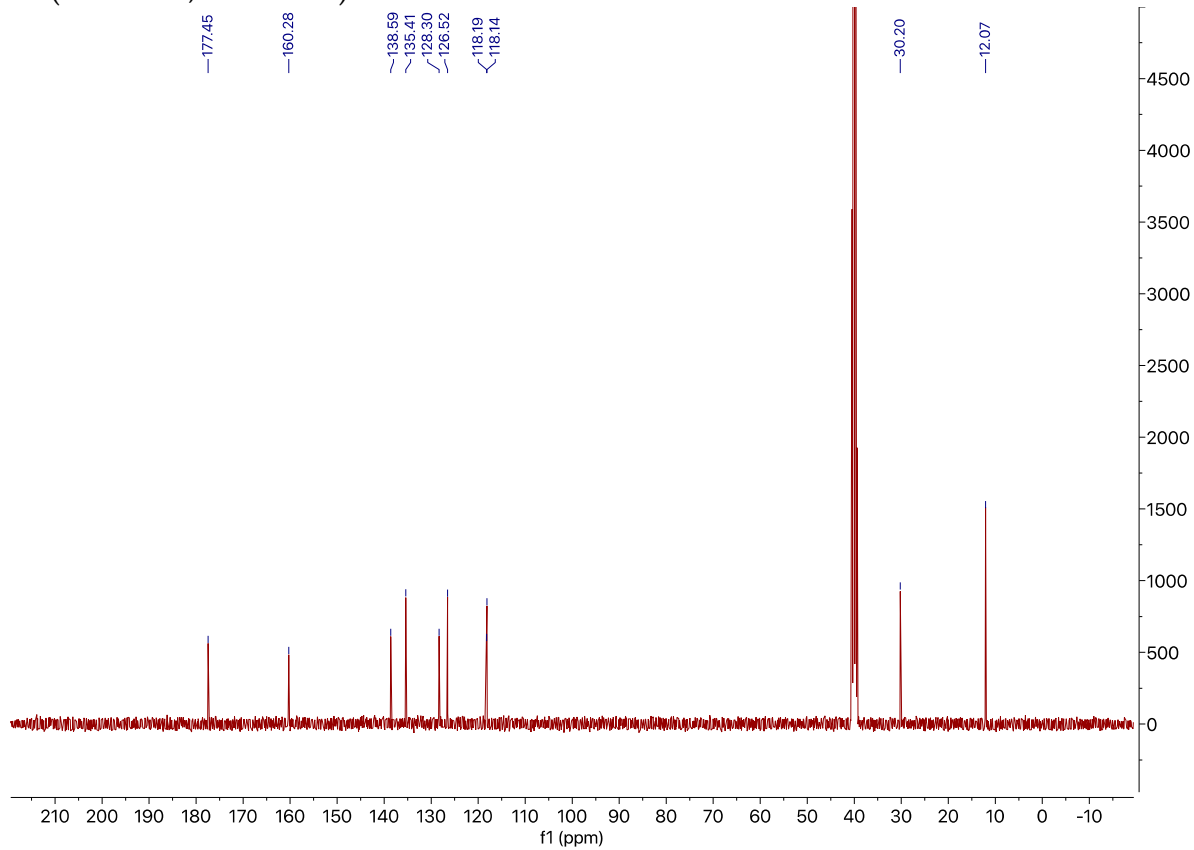


6-Chloro-3-cyclopropyl-2-mercaptoquinazolin-4(3H)-one (8c)

^1H NMR (400 MHz, $\text{DMSO-}d_6$)

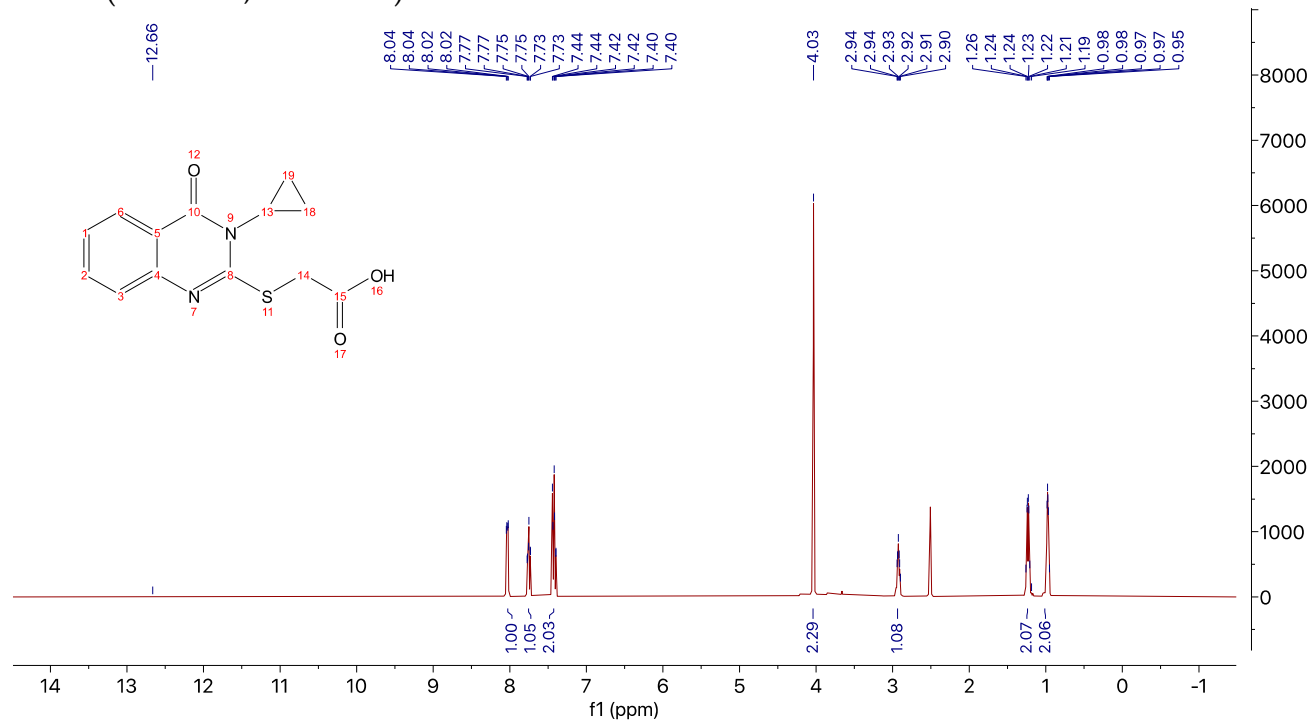


^{13}C NMR (100 MHz, $\text{DMSO-}d_6$):

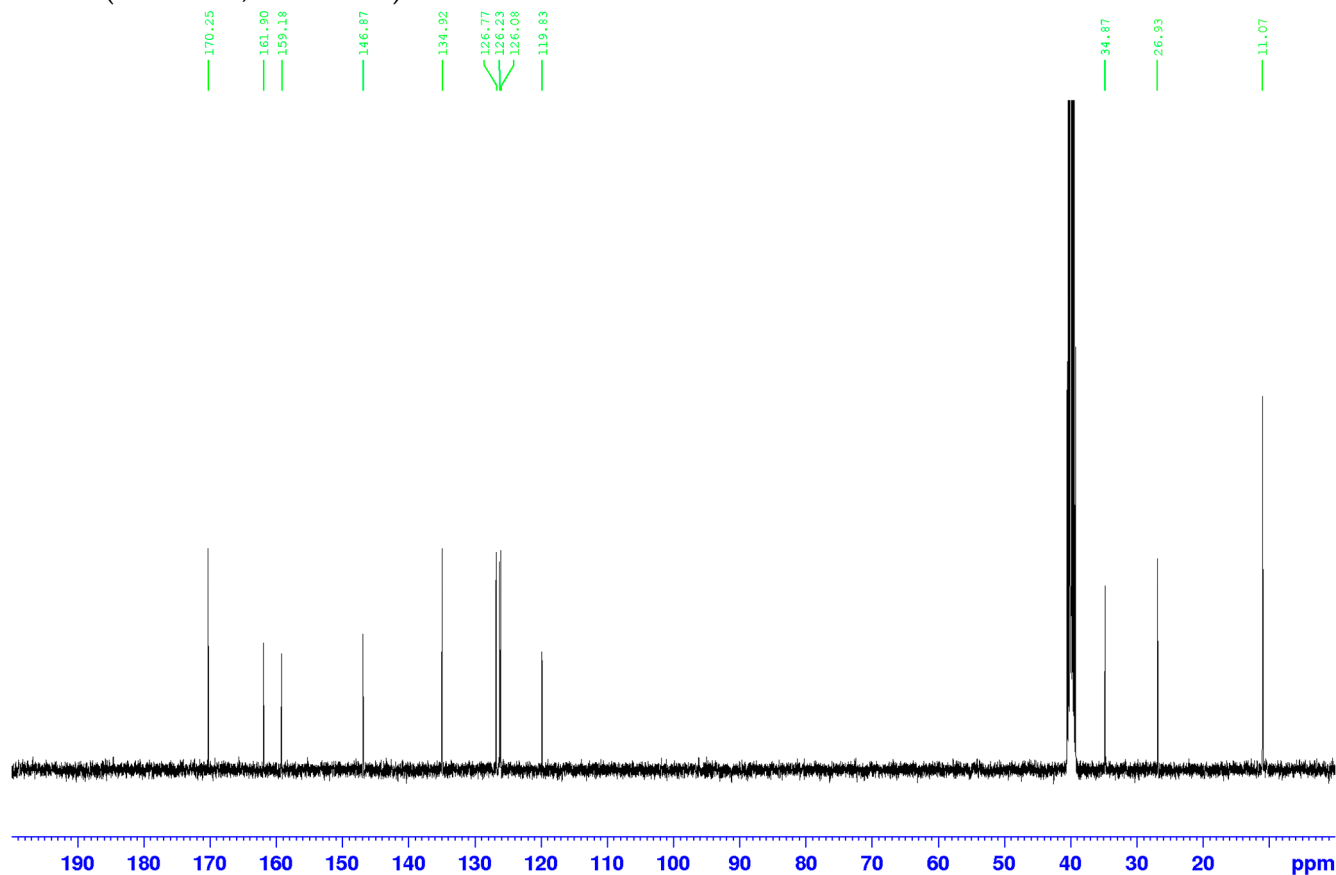


2-((3-Cyclopropyl-4-oxo-3,4-dihydroquinazolin-2-yl)thio)acetic acid (**9a**)

^1H NMR (400 MHz, $\text{DMSO}-d_6$):

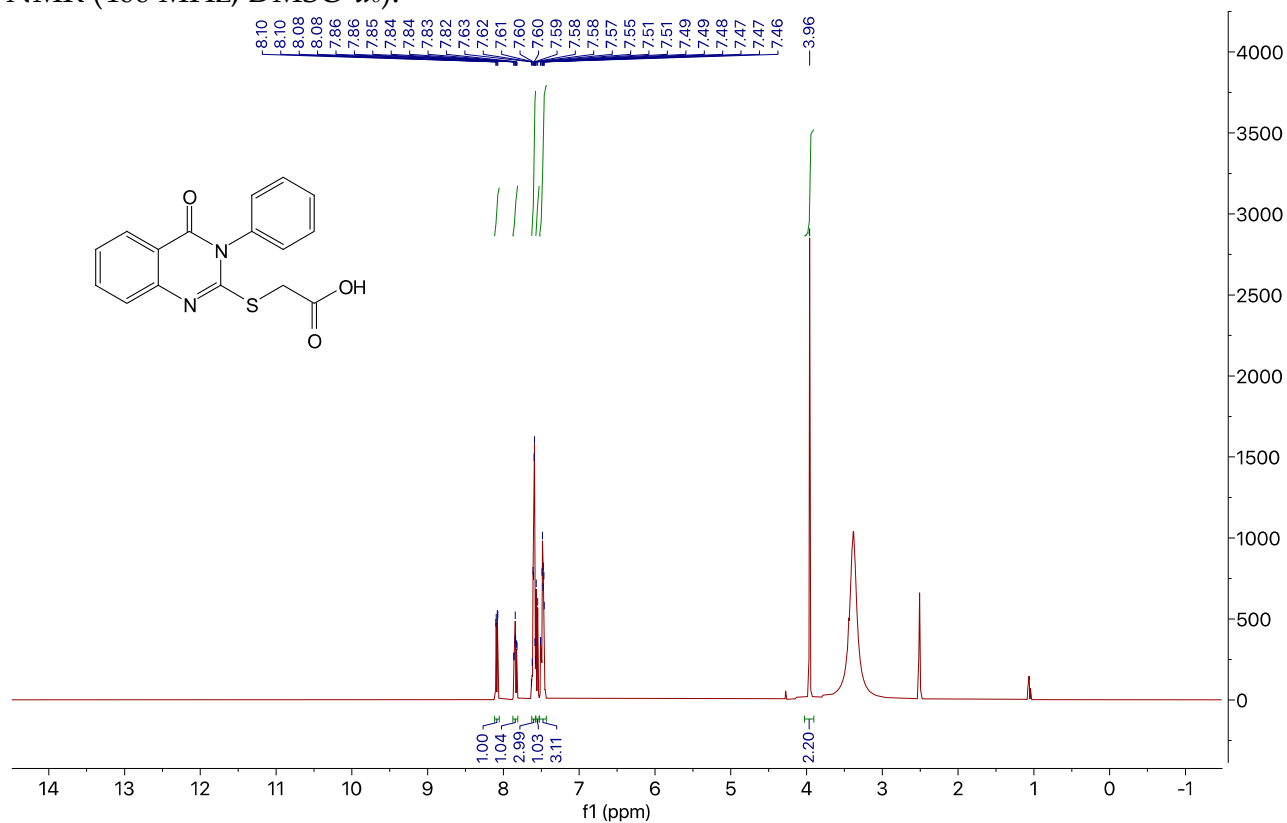


^{13}C NMR (100 MHz, $\text{DMSO}-d_6$):

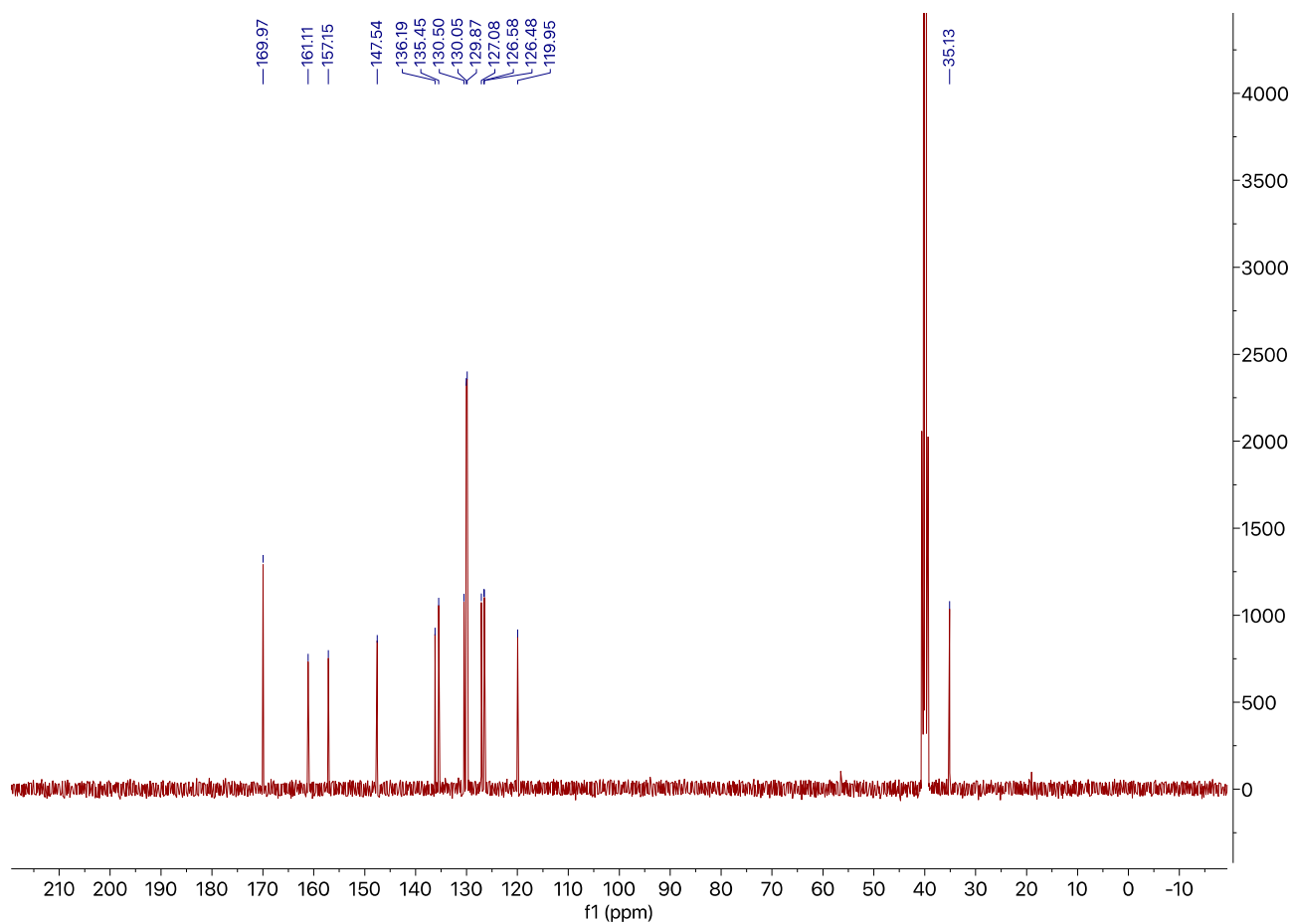


2-((4-Oxo-3-phenyl-3,4-dihydroquinazolin-2-yl)thio)acetic acid (**9b**)

^1H NMR (400 MHz, $\text{DMSO}-d_6$):

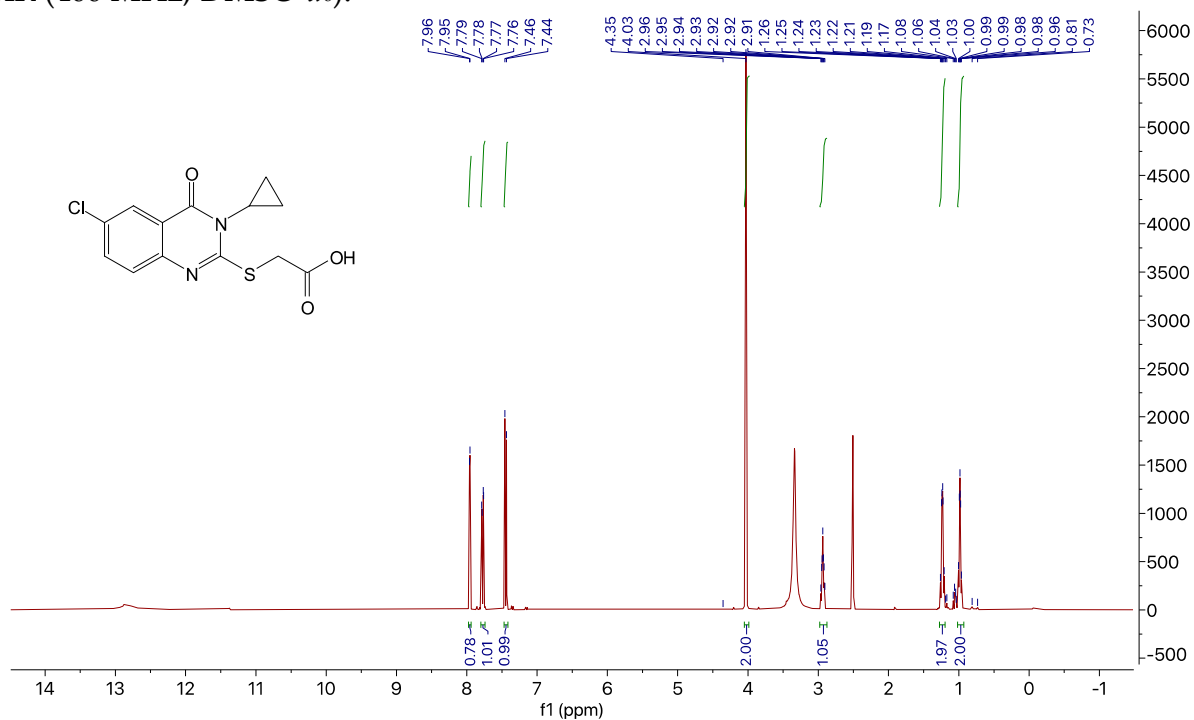


^{13}C NMR (100 MHz, $\text{DMSO}-d_6$):

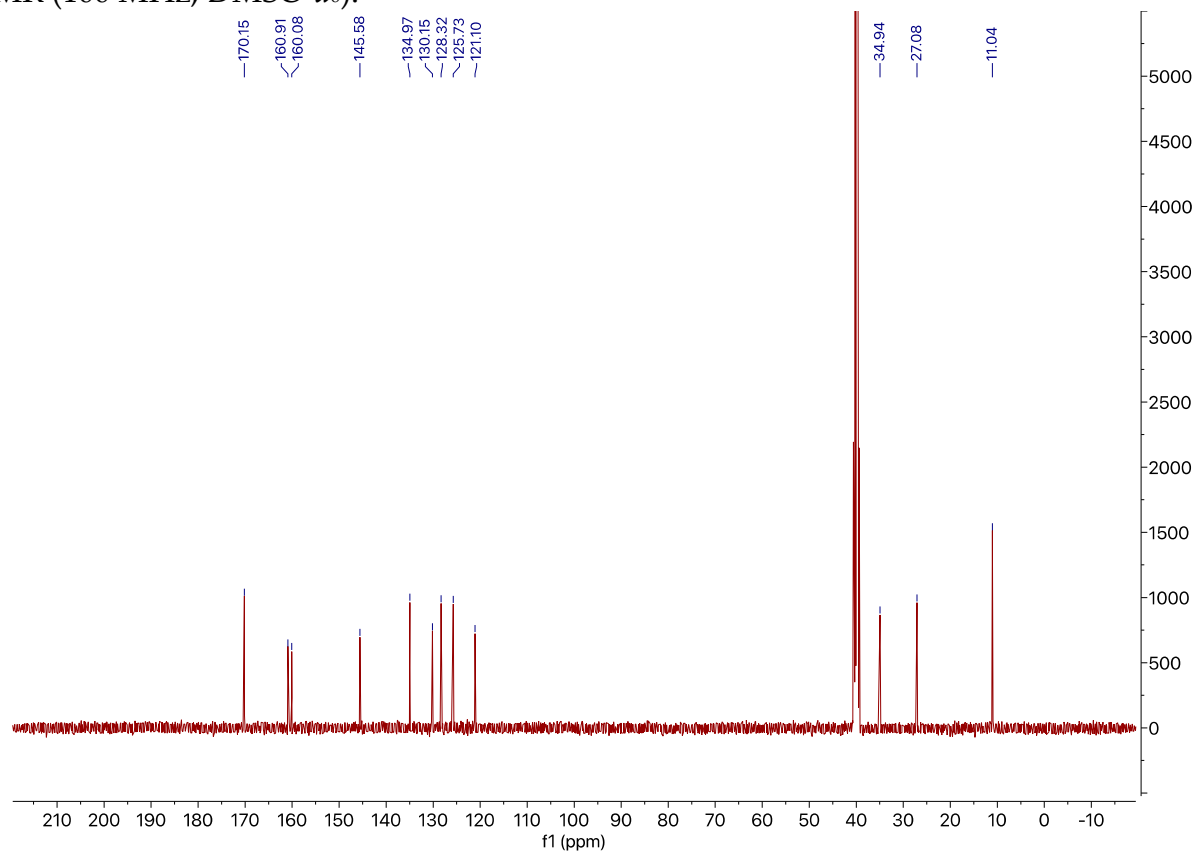


2-((6-Chloro-3-cyclopropyl-4-oxo-3,4-dihydroquinazolin-2-yl)thio)acetic acid (**9c**)

¹H NMR (400 MHz, DMSO-*d*₆):

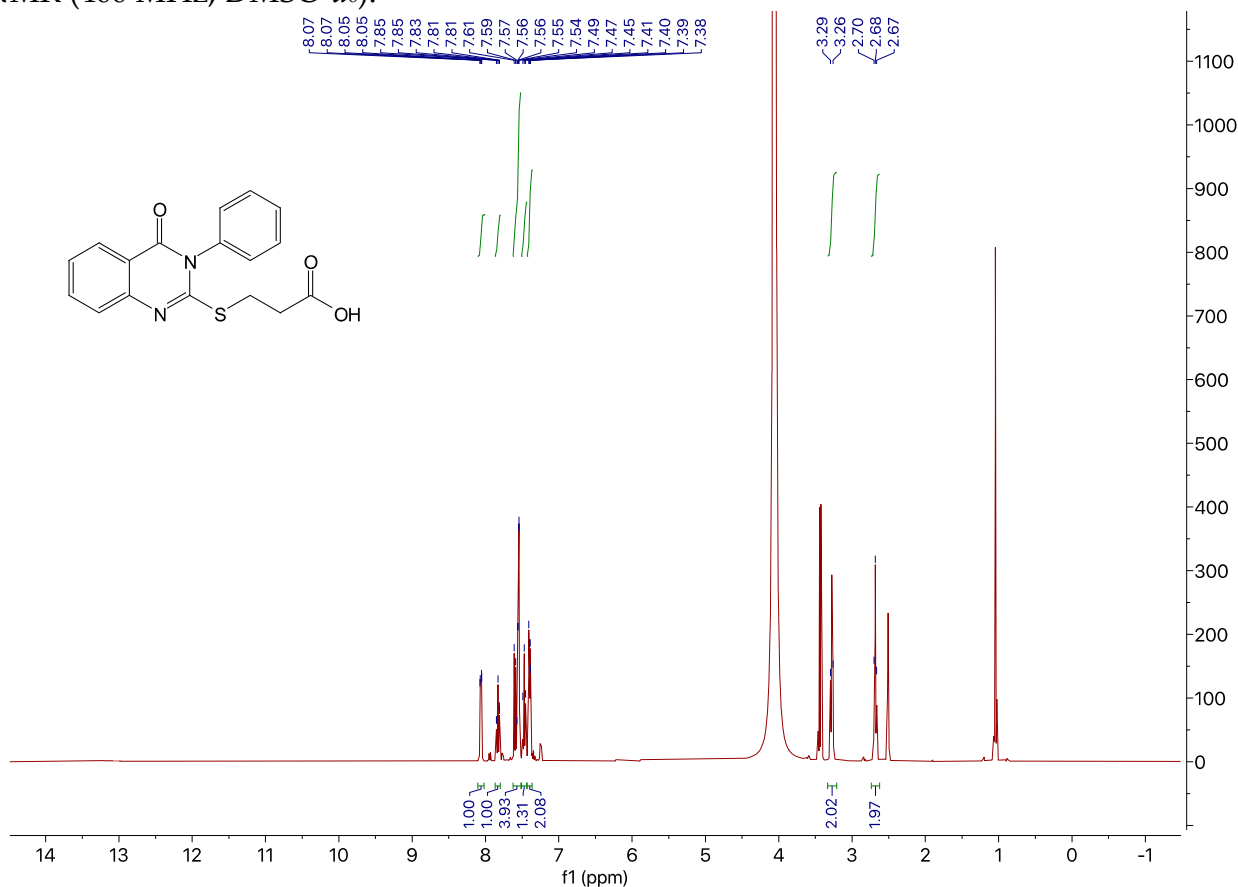


^{13}C NMR (100 MHz, $\text{DMSO}-d_6$):

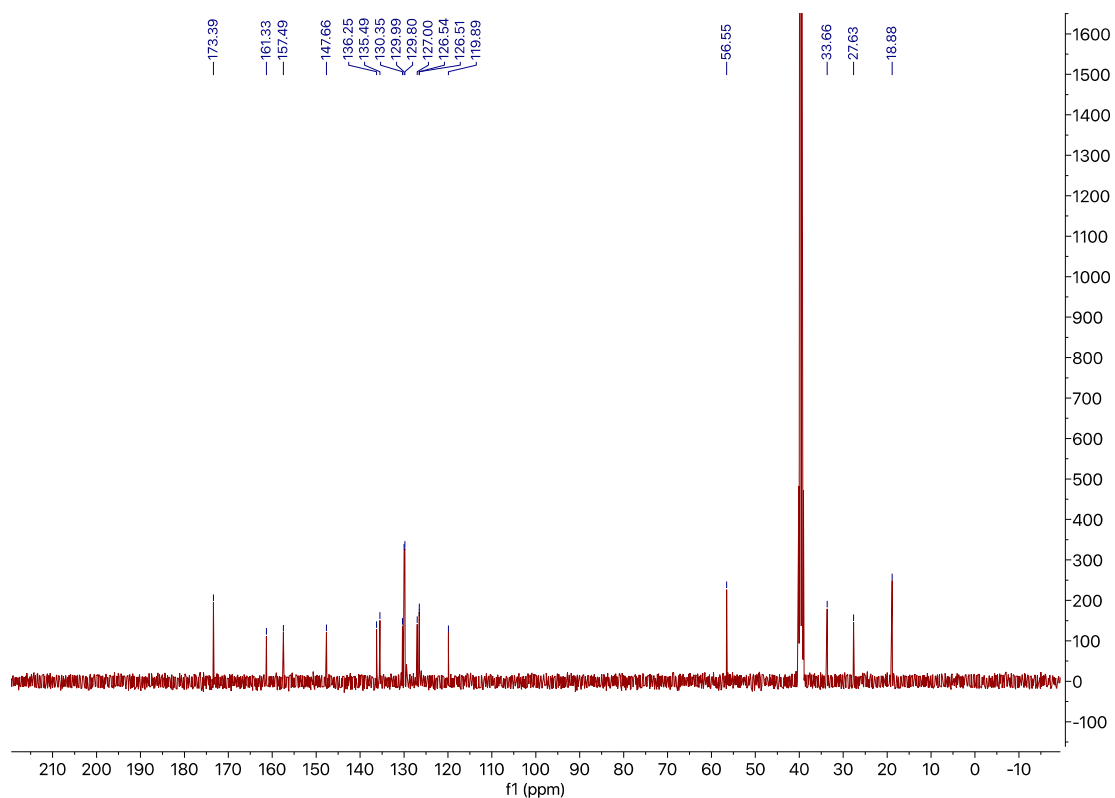


3-((4-Oxo-3-phenyl-3,4-dihydroquinazolin-2-yl)thio)propanoic acid (**9d**)

^1H NMR (400 MHz, $\text{DMSO}-d_6$):

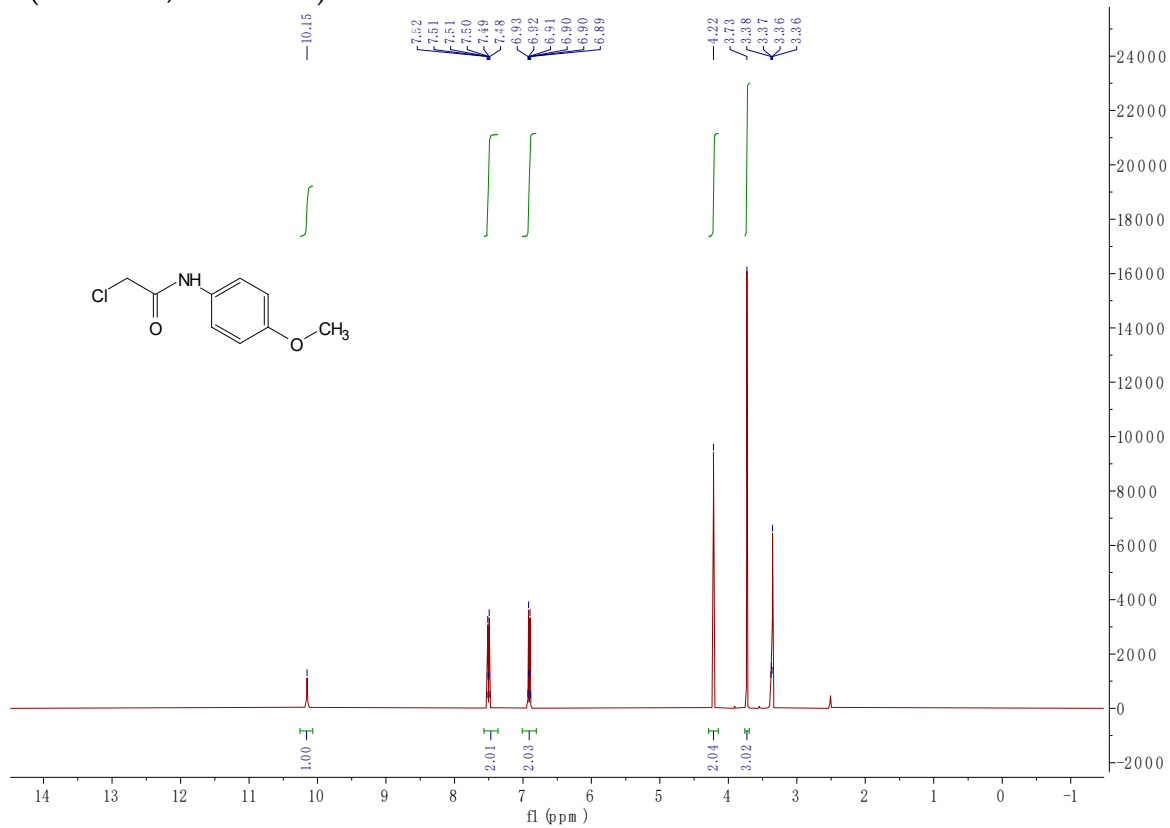


^{13}C NMR (100 MHz, $\text{DMSO}-d_6$):

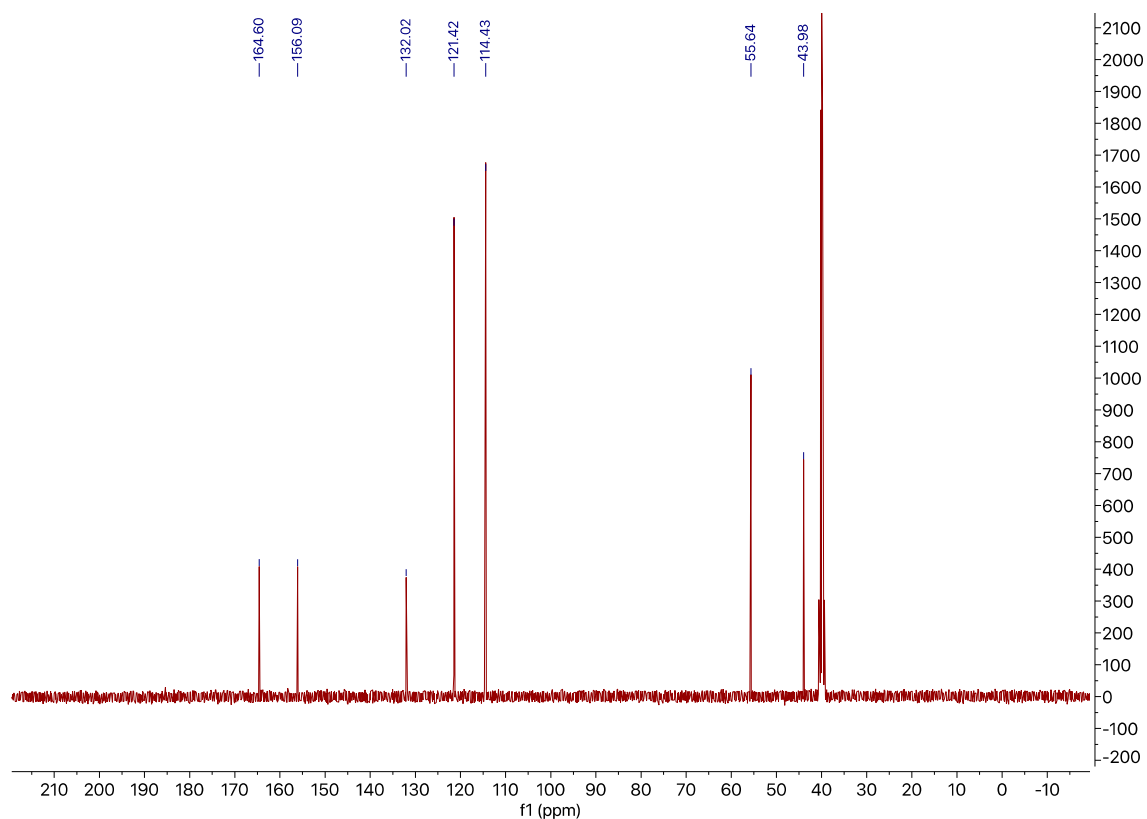


2-Chloro-*N*-(4-methoxyphenyl)acetamide (**12**)

^1H NMR (400 MHz, $\text{DMSO}-d_6$):

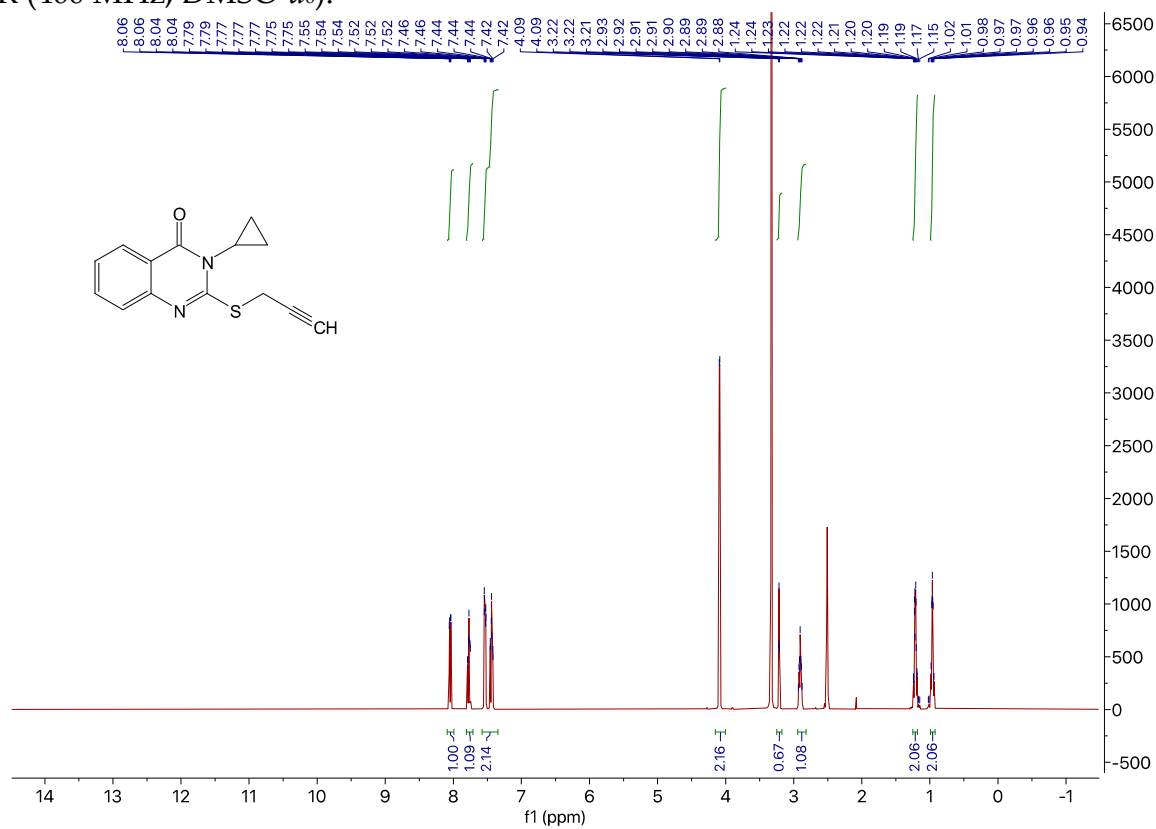


^{13}C NMR (100 MHz, $\text{DMSO}-d_6$):

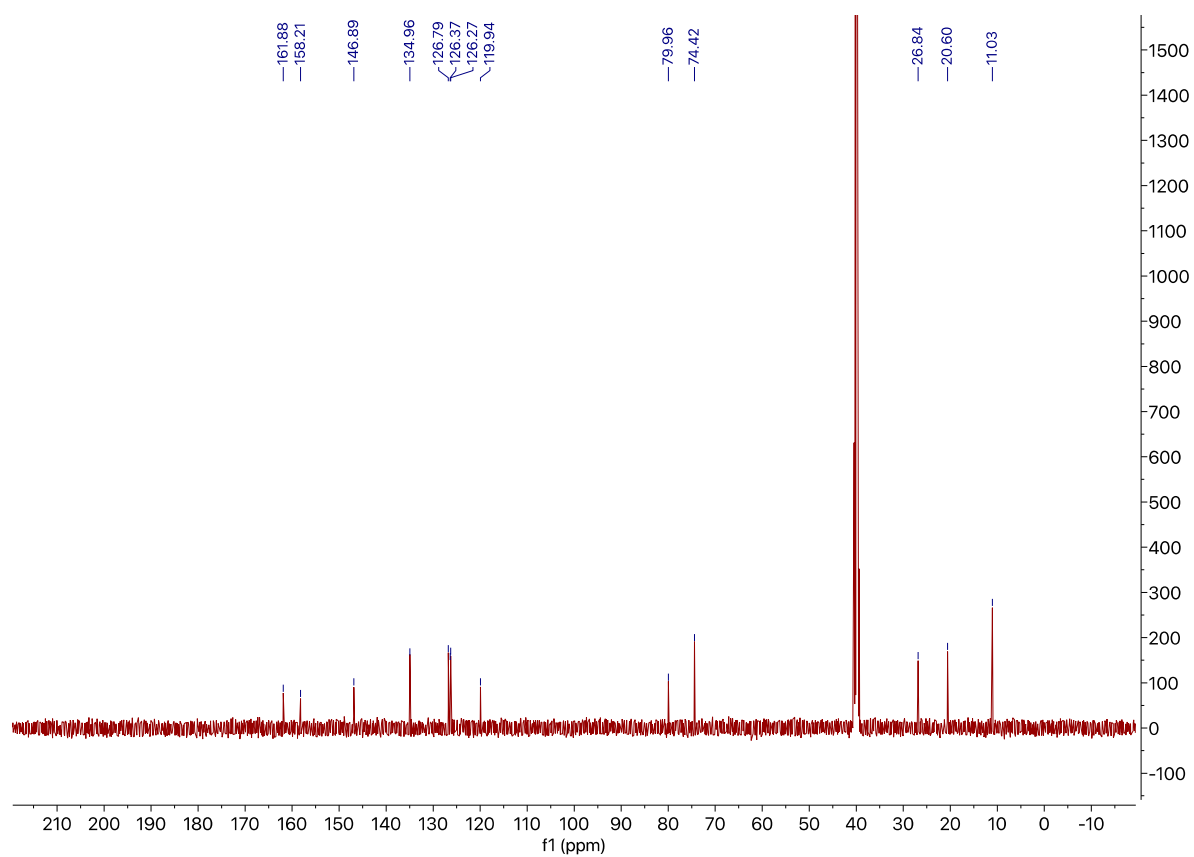


3-Cyclopropyl-2-(prop-2-yn-1-ylthio)quinazolin-4(3H)-one (13a)

¹H NMR (400 MHz, DMSO-*d*₆):

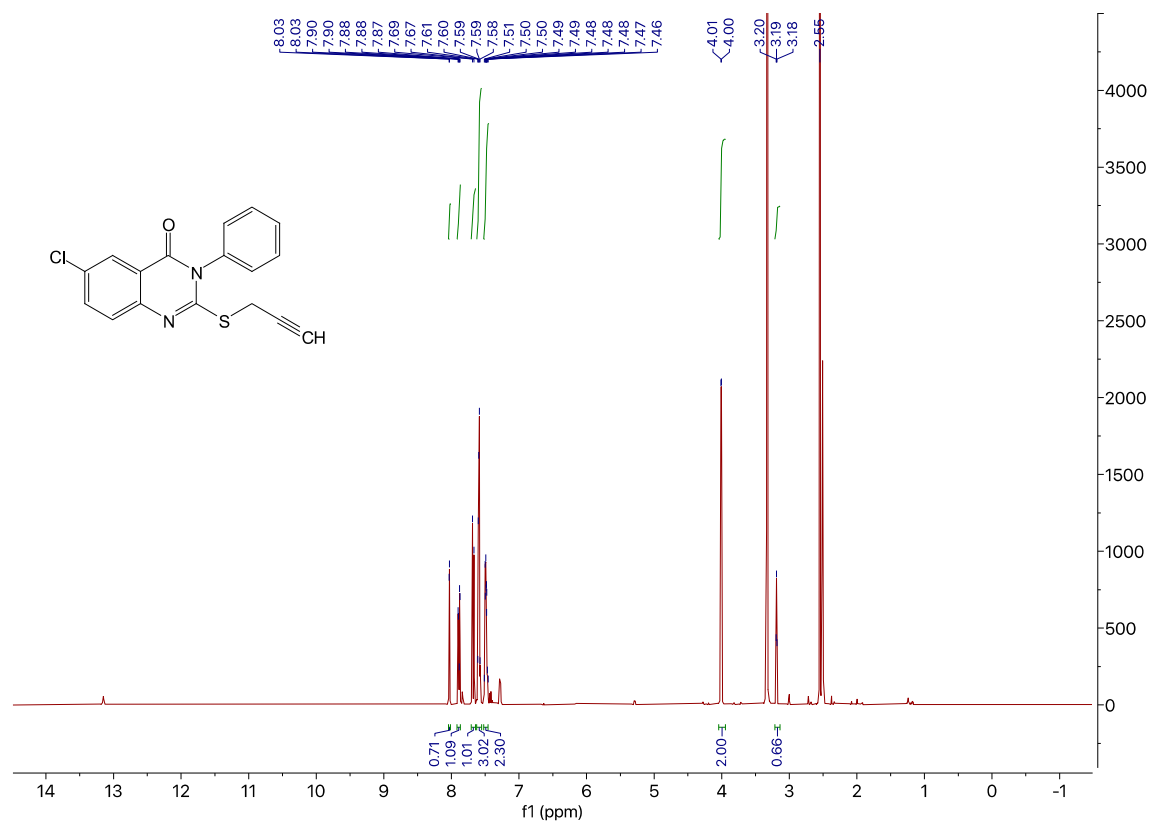


¹³C NMR (100 MHz, DMSO-*d*₆):

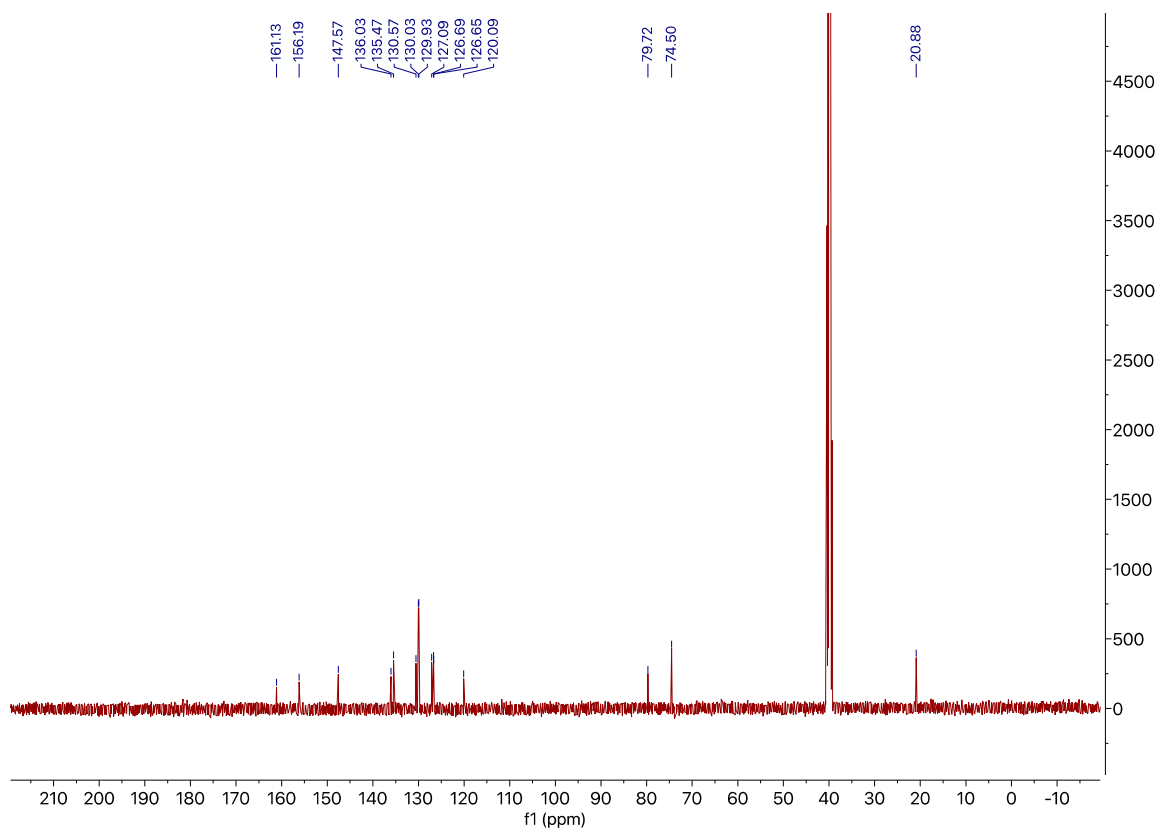


3-Phenyl-2-(prop-2-yn-1-ylthio)quinazolin-4(3H)-one (**13b**)

^1H NMR (400 MHz, $\text{DMSO}-d_6$):

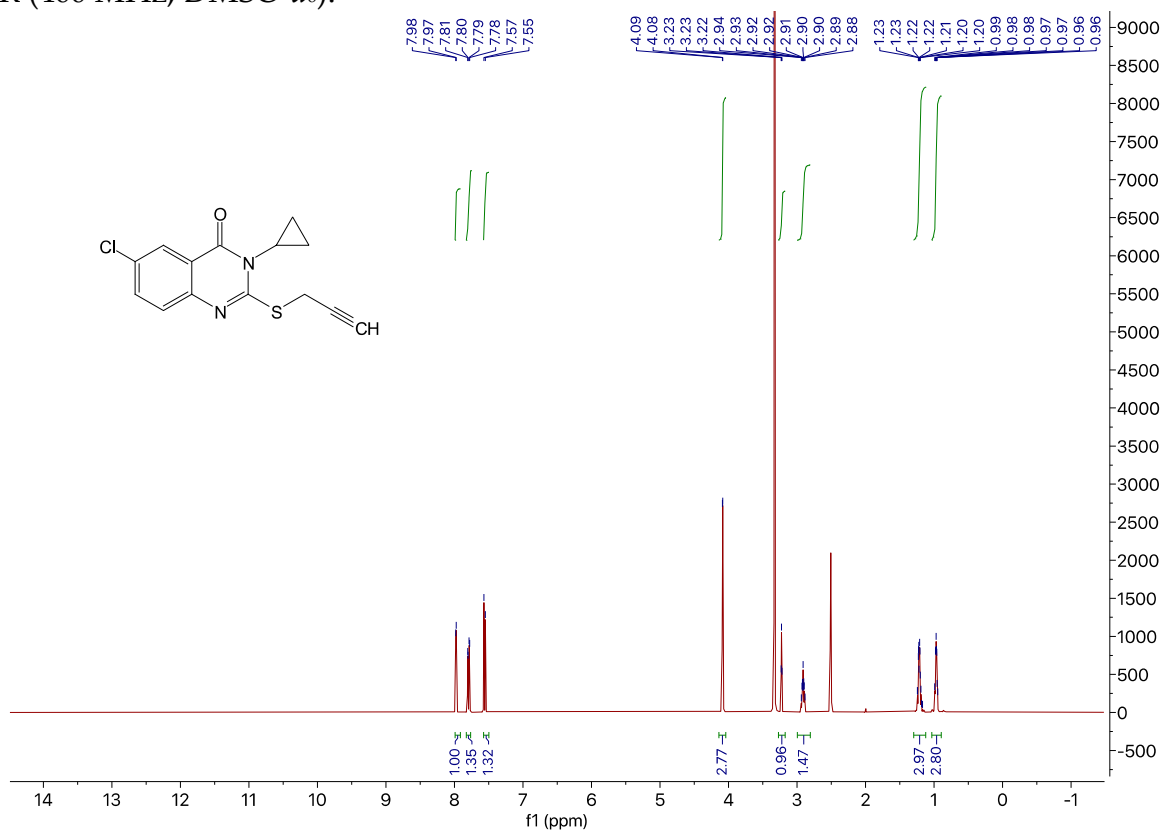


^{13}C NMR (100 MHz, $\text{DMSO}-d_6$):

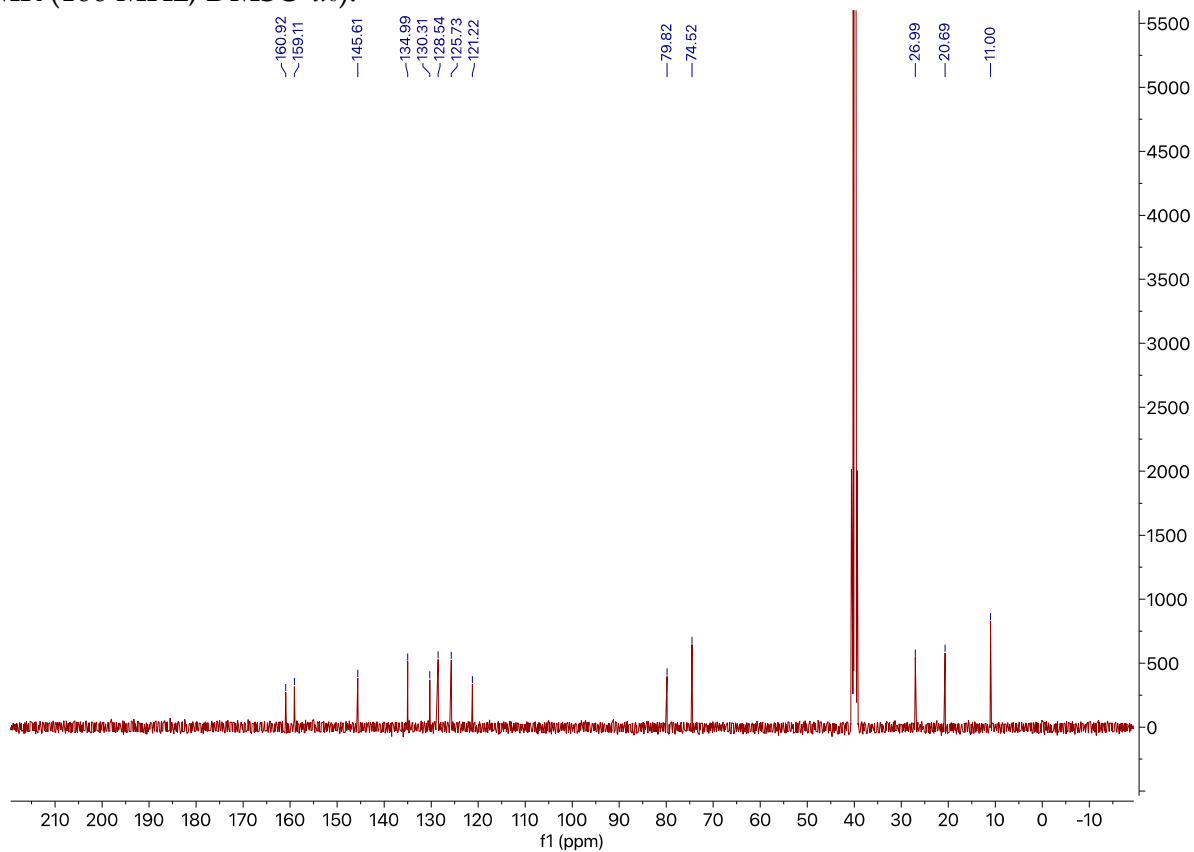


6-Chloro-3-cyclopropyl-2-(prop-2-yn-1-ylthio)quinazolin-4(3*H*)-one (**13c**)

^1H NMR (400 MHz, $\text{DMSO}-d_6$):

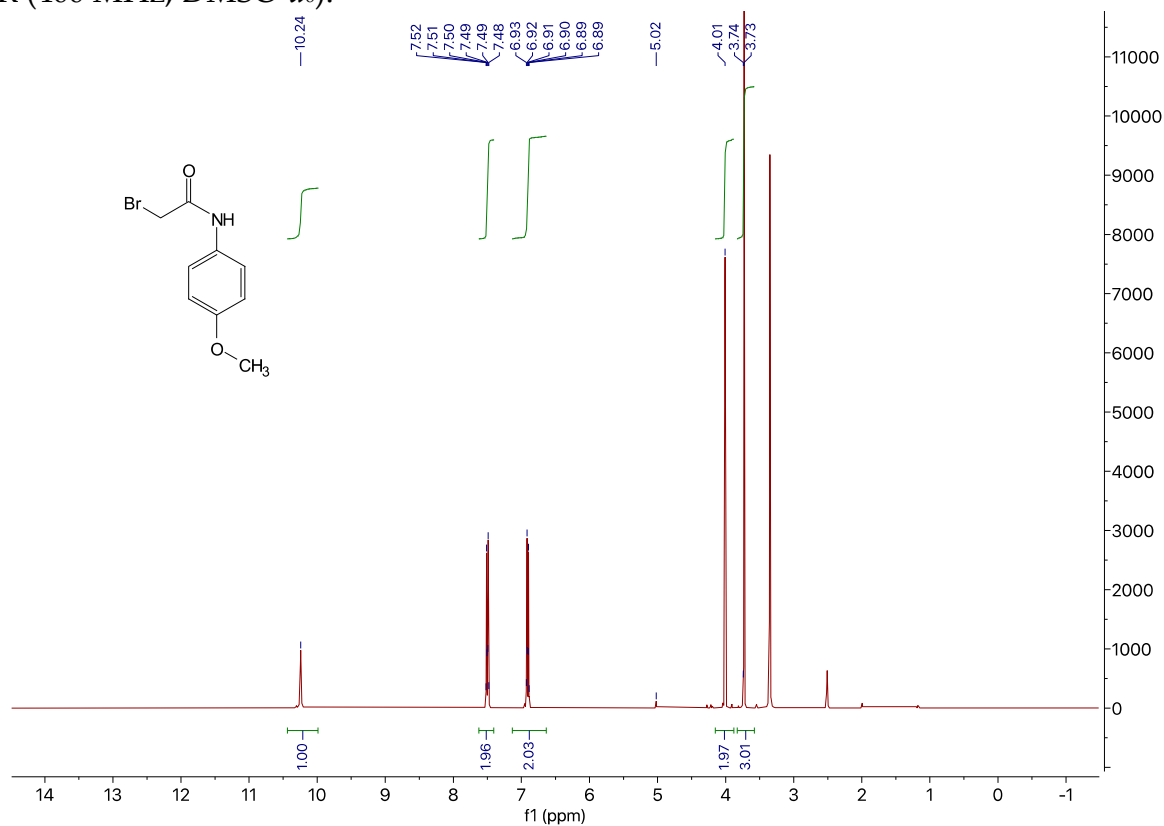


^{13}C NMR (100 MHz, $\text{DMSO}-d_6$):

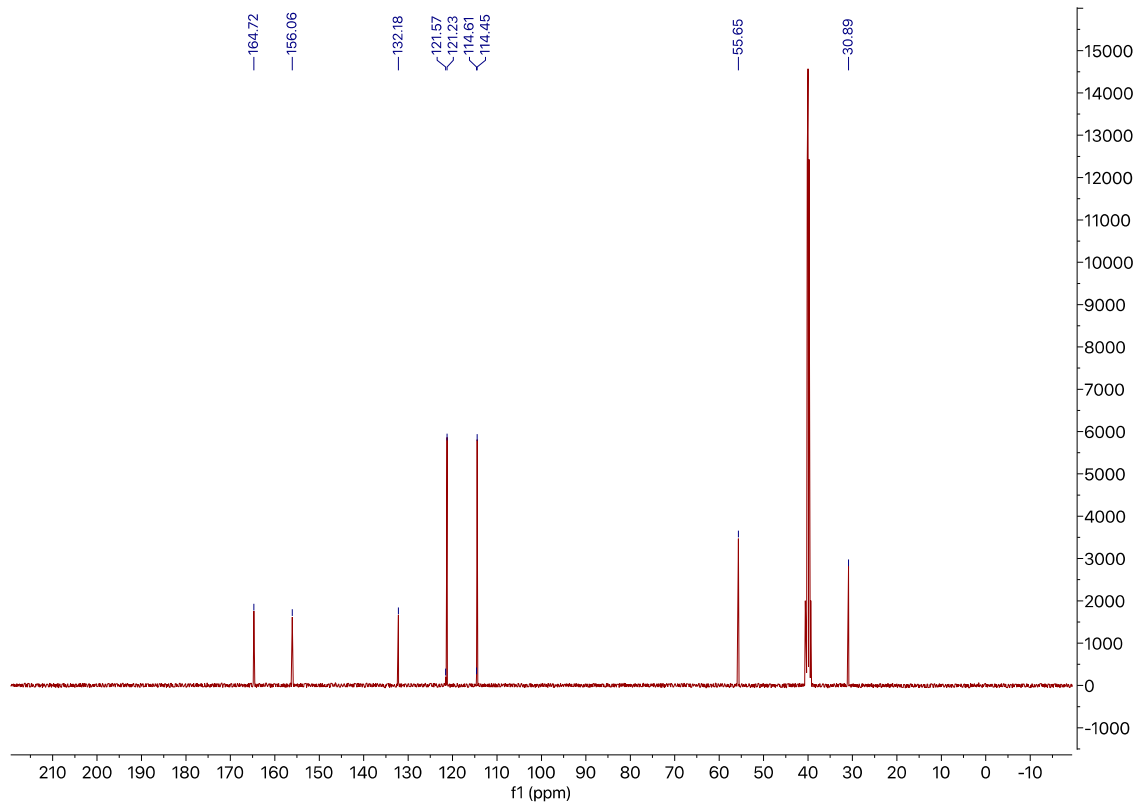


2-Bromo-*N*-(4-methoxyphenyl)acetamide (**15a**)

^1H NMR (400 MHz, $\text{DMSO}-d_6$):

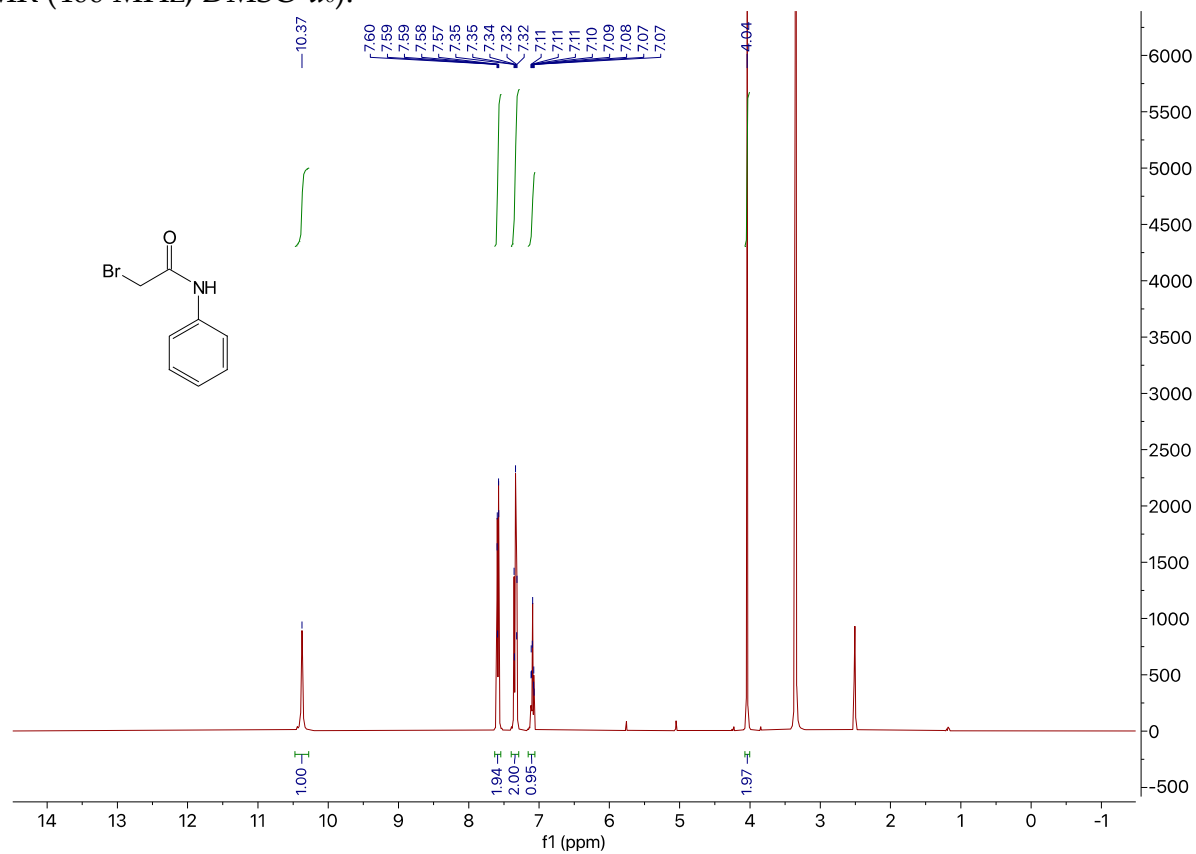


^{13}C NMR (100 MHz, $\text{DMSO}-d_6$):

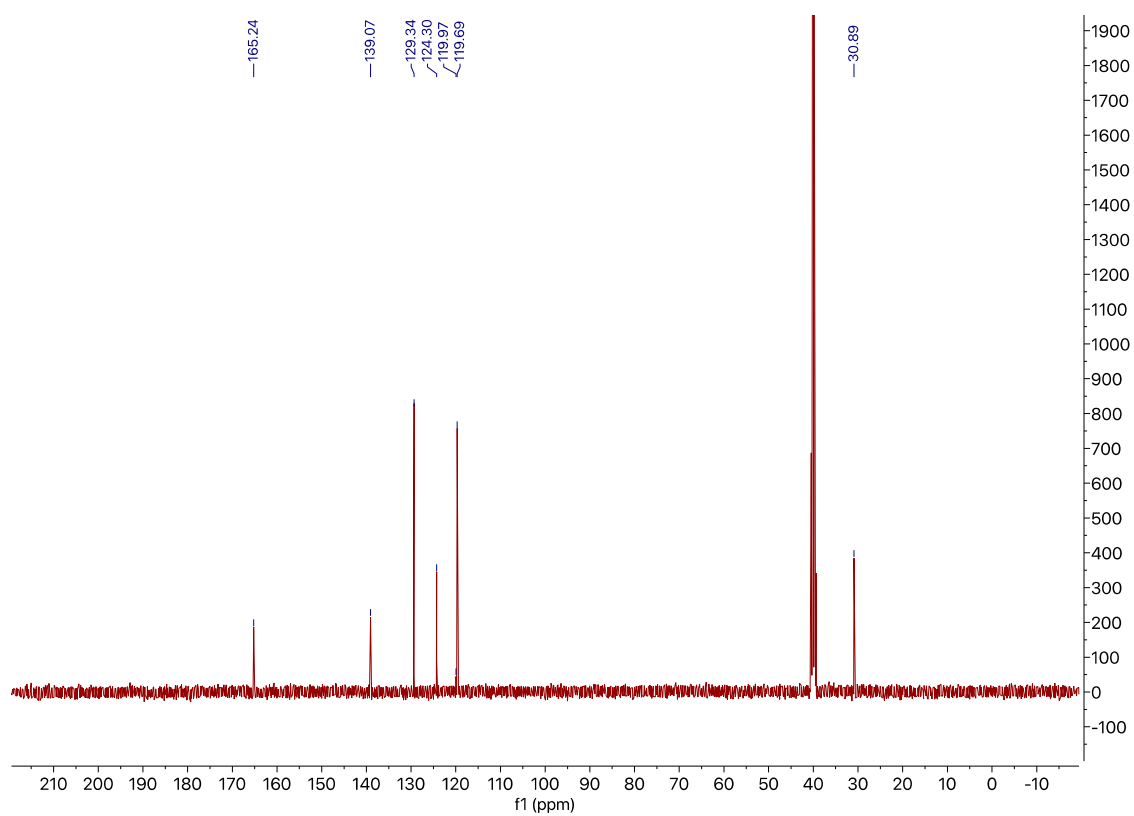


2-Bromo-*N*-phenylacetamide (**15b**)

^1H NMR (400 MHz, $\text{DMSO}-d_6$):

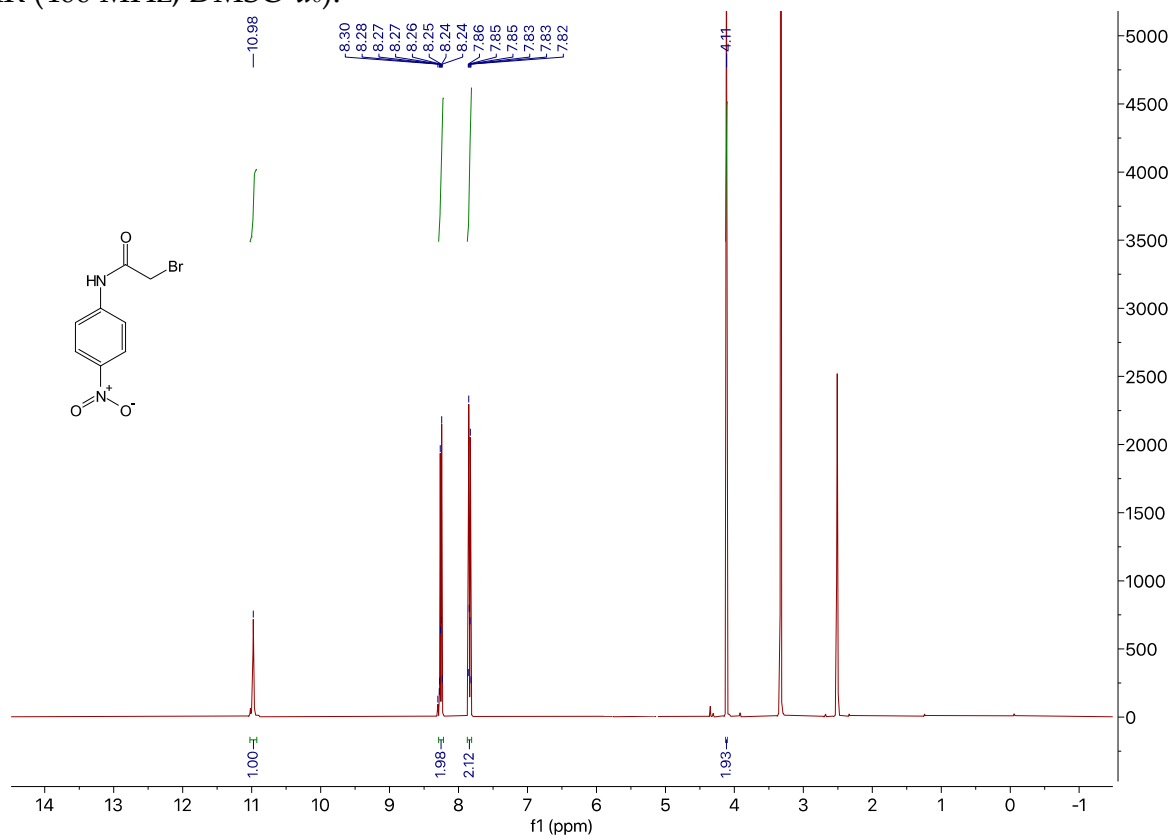


^{13}C NMR (100 MHz, $\text{DMSO}-d_6$):

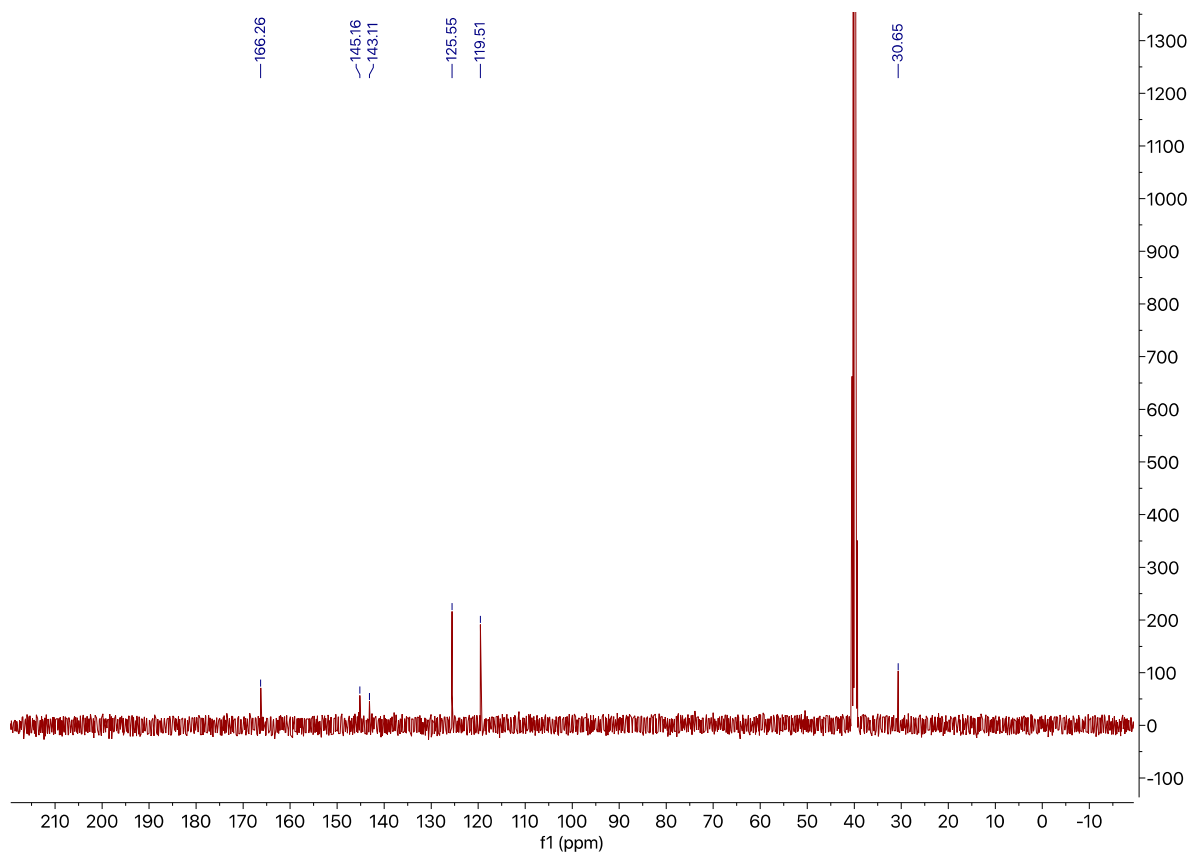


2-Bromo-N-(4-nitrophenyl)acetamide (**15c**)

^1H NMR (400 MHz, $\text{DMSO}-d_6$):



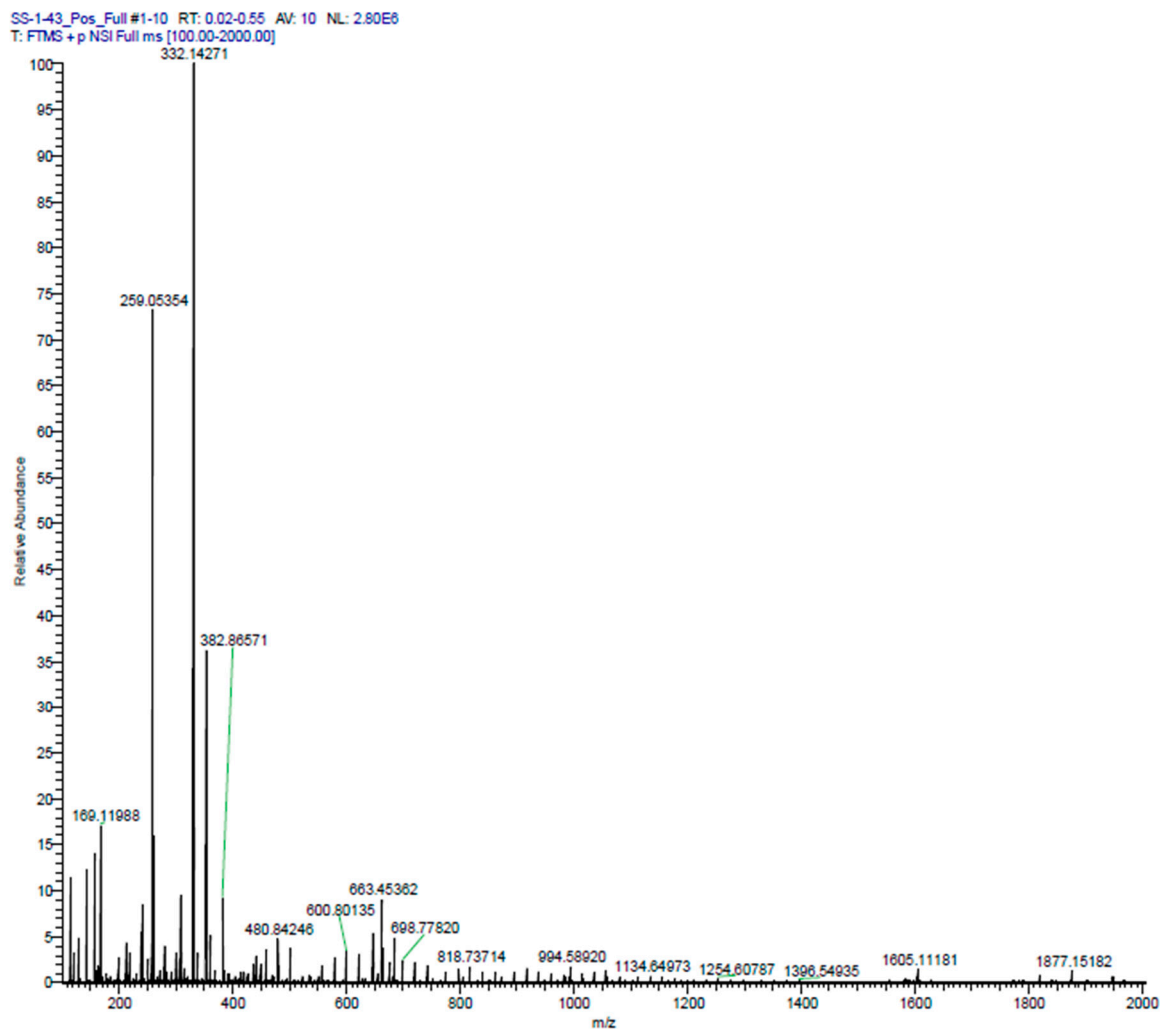
^{13}C NMR (100 MHz, $\text{DMSO}-d_6$):



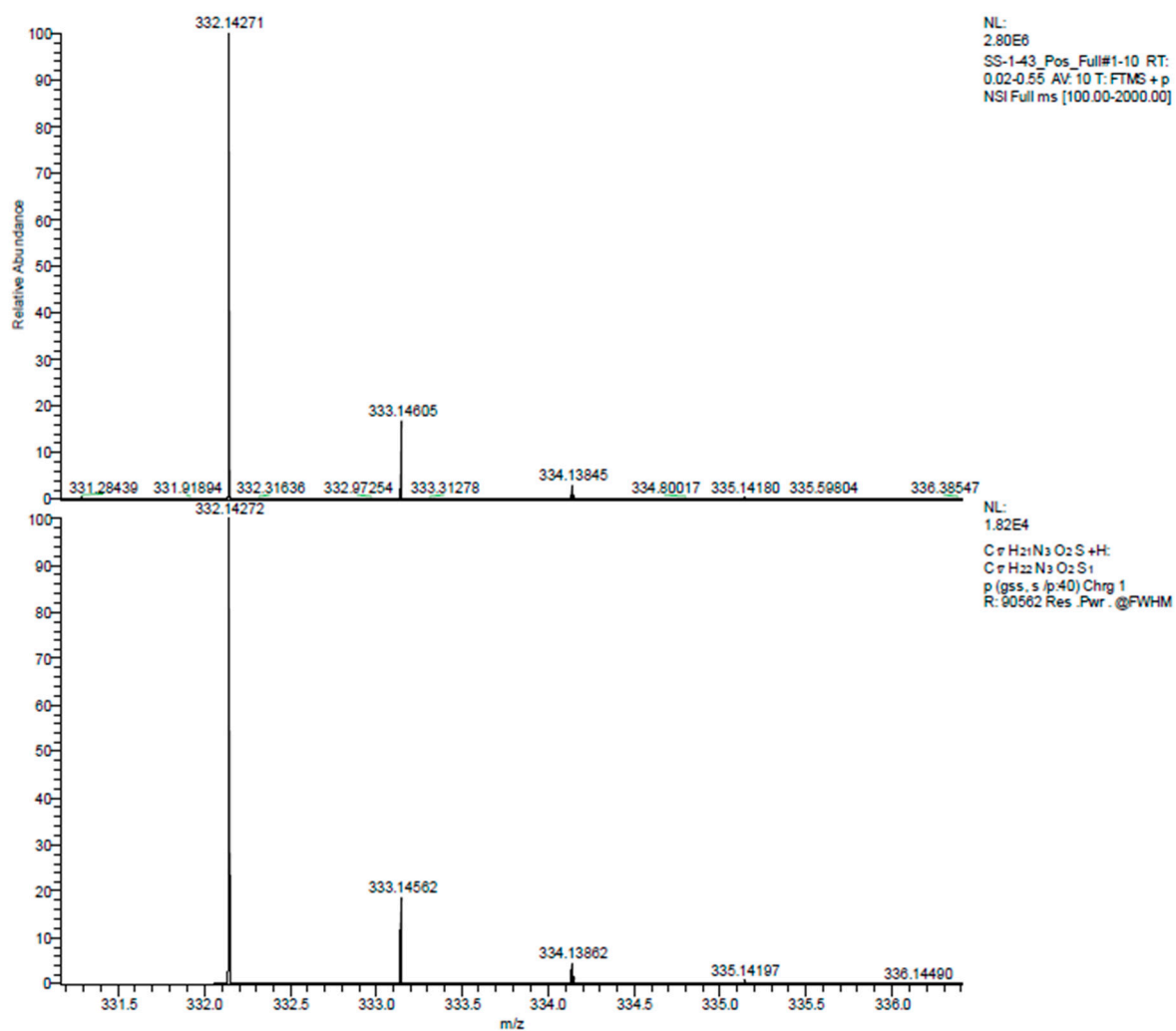
High resolution mass spectra (HRMS) of synthesised compounds

N-Butyl-2-((3-cyclopropyl-4-oxo-3,4-dihydroquinazolin-2-yl)thio)acetamide (**5a**)

Full spectrum



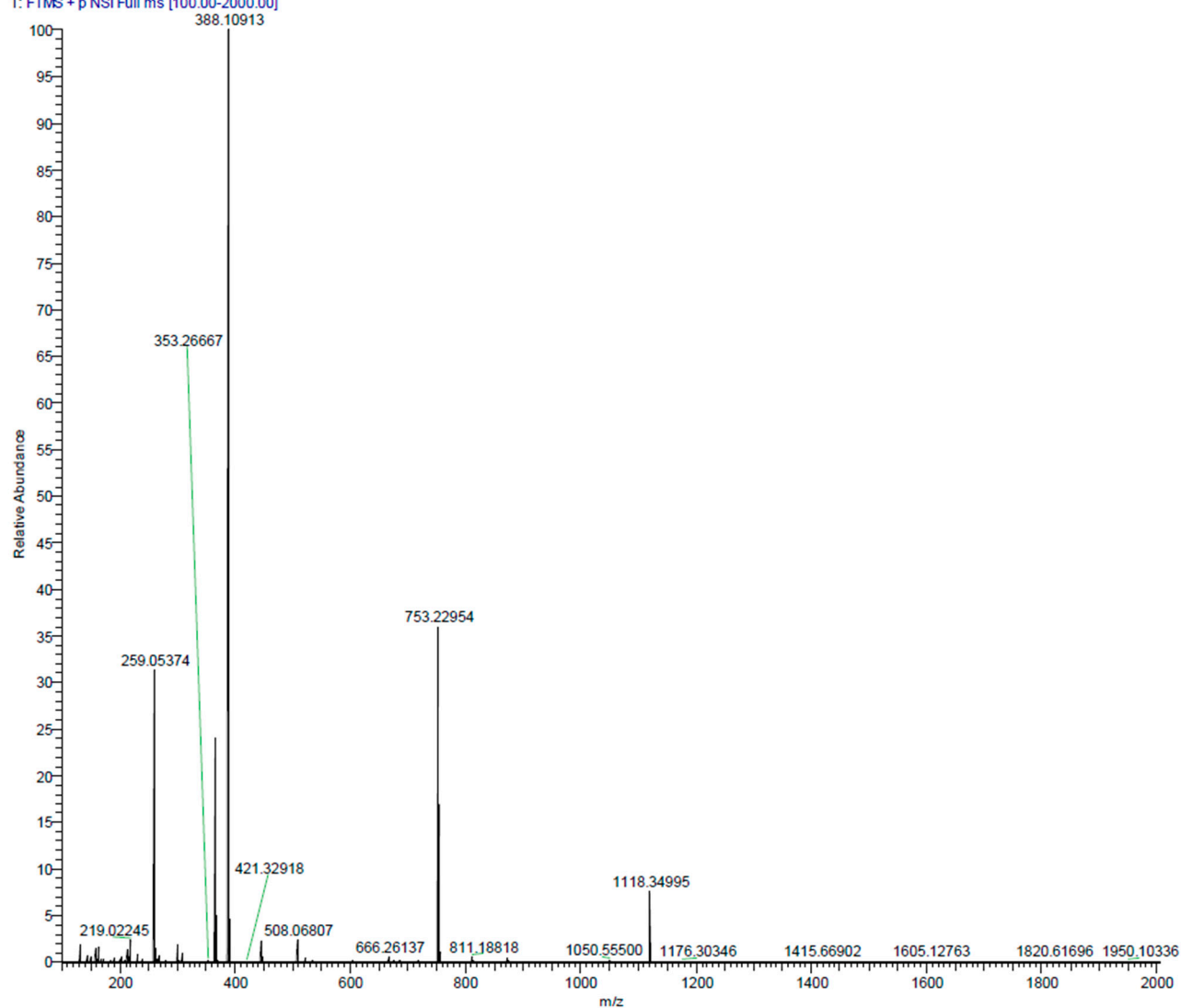
Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)



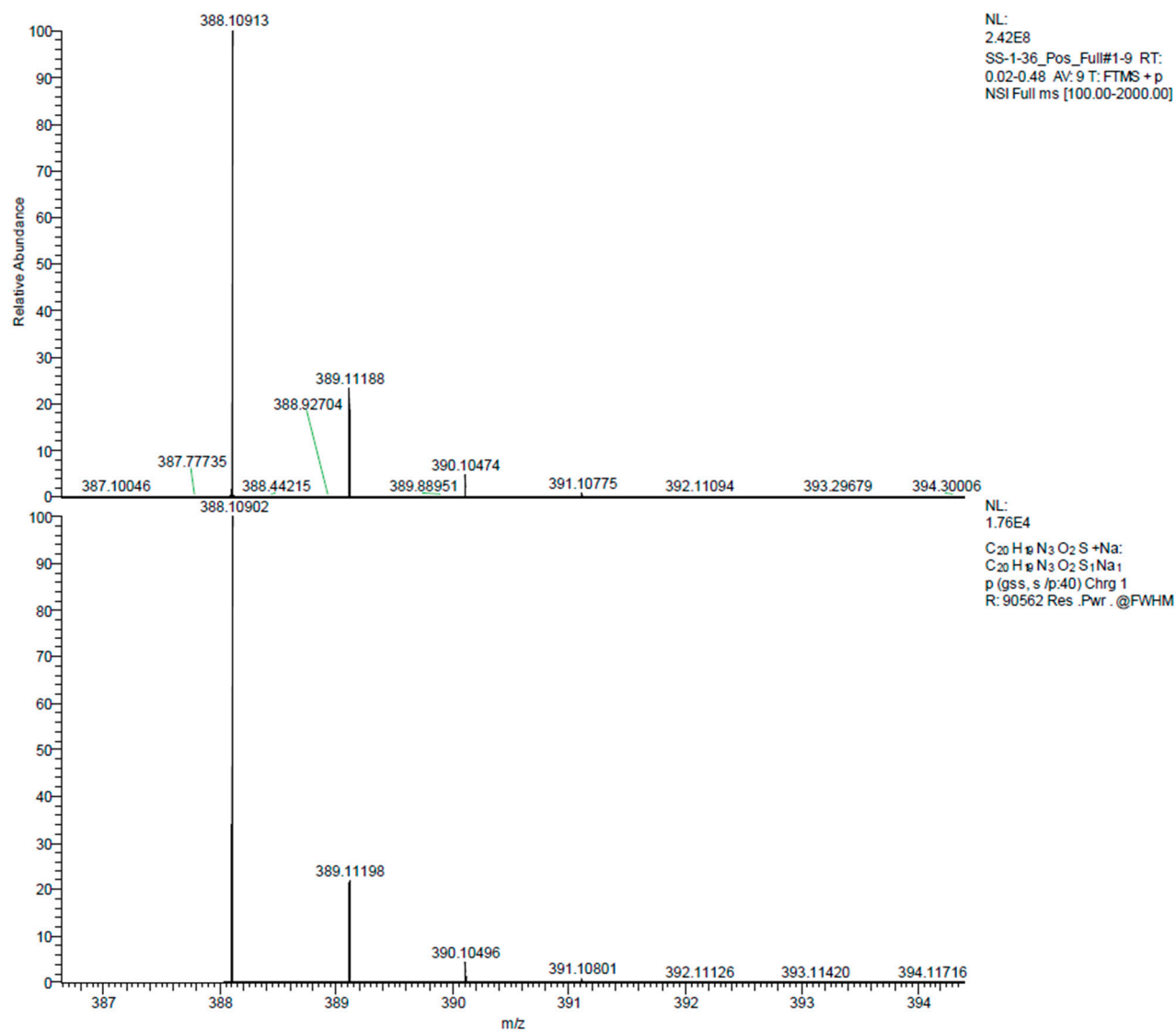
N-Benzyl-2-((3-cyclopropyl-4-oxo-3,4-dihydroquinazolin-2-yl)thio)acetamide (**5b**)

Full spectrum

SS-1-36_Pos_Full #1-9 RT: 0.02-0.48 AV: 9 NL: 2.42E8
T: FTMS + p NSI Full ms [100.00-2000.00]



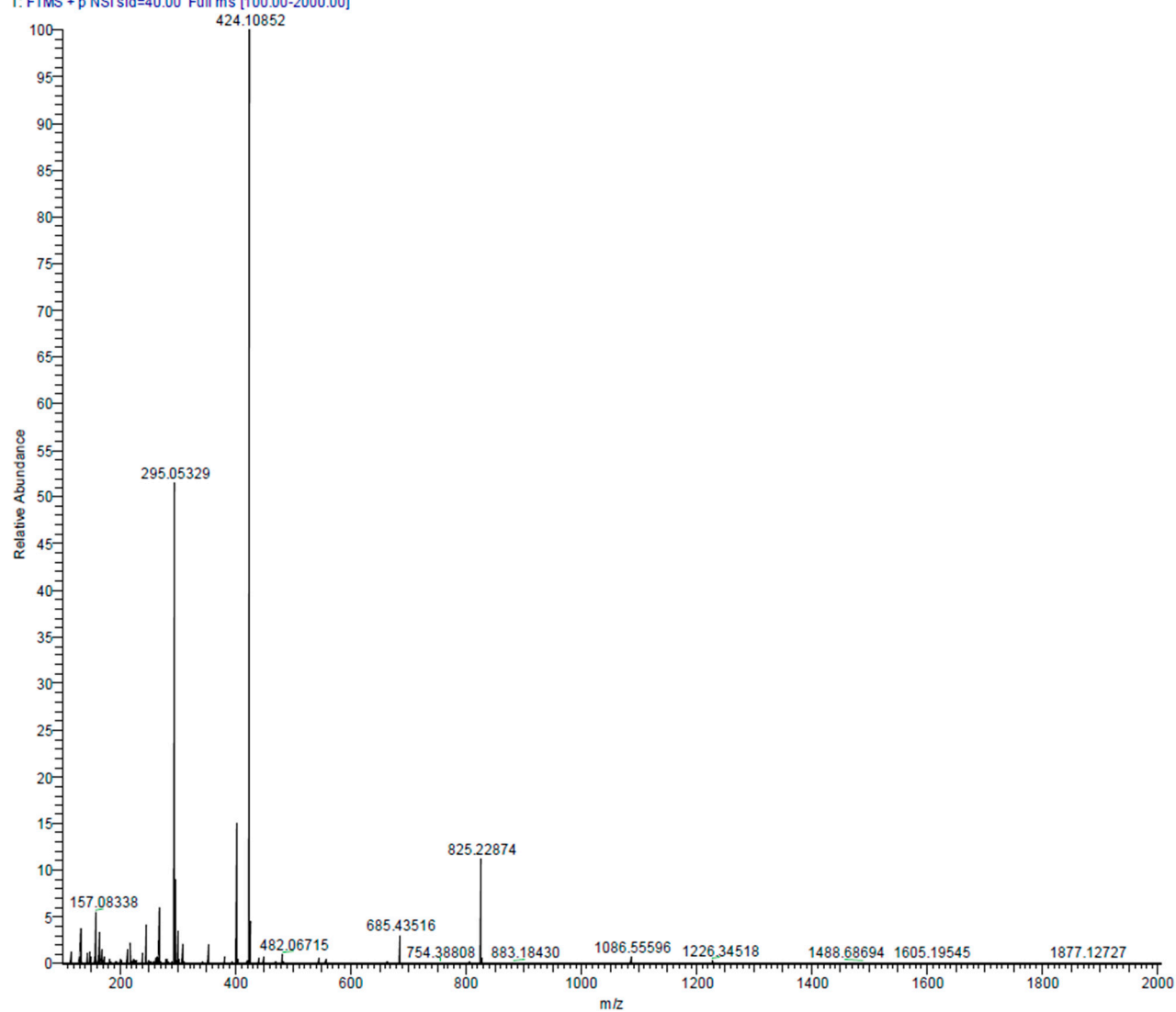
Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)



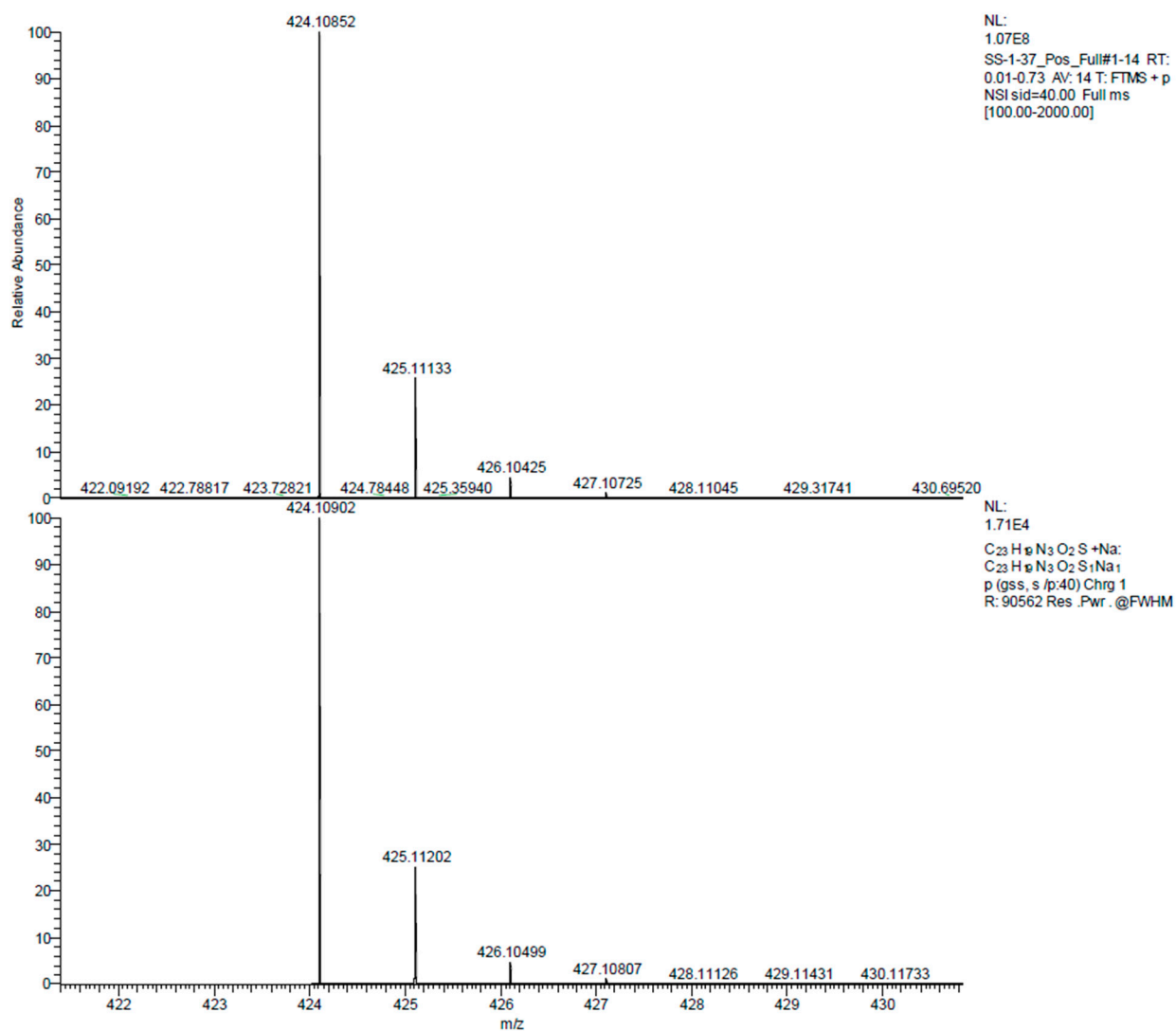
N-Benzyl-2-((4-oxo-3-phenyl-3,4-dihydroquinazolin-2-yl)thio)acetamide (**5c**)

Full spectrum

SS-1-37_Pos_Full #1-14 RT: 0.01-0.73 AV: 14 NL: 1.07E8
T: FTMS + p NSI sid=40.00 Full ms [100.00-2000.00]



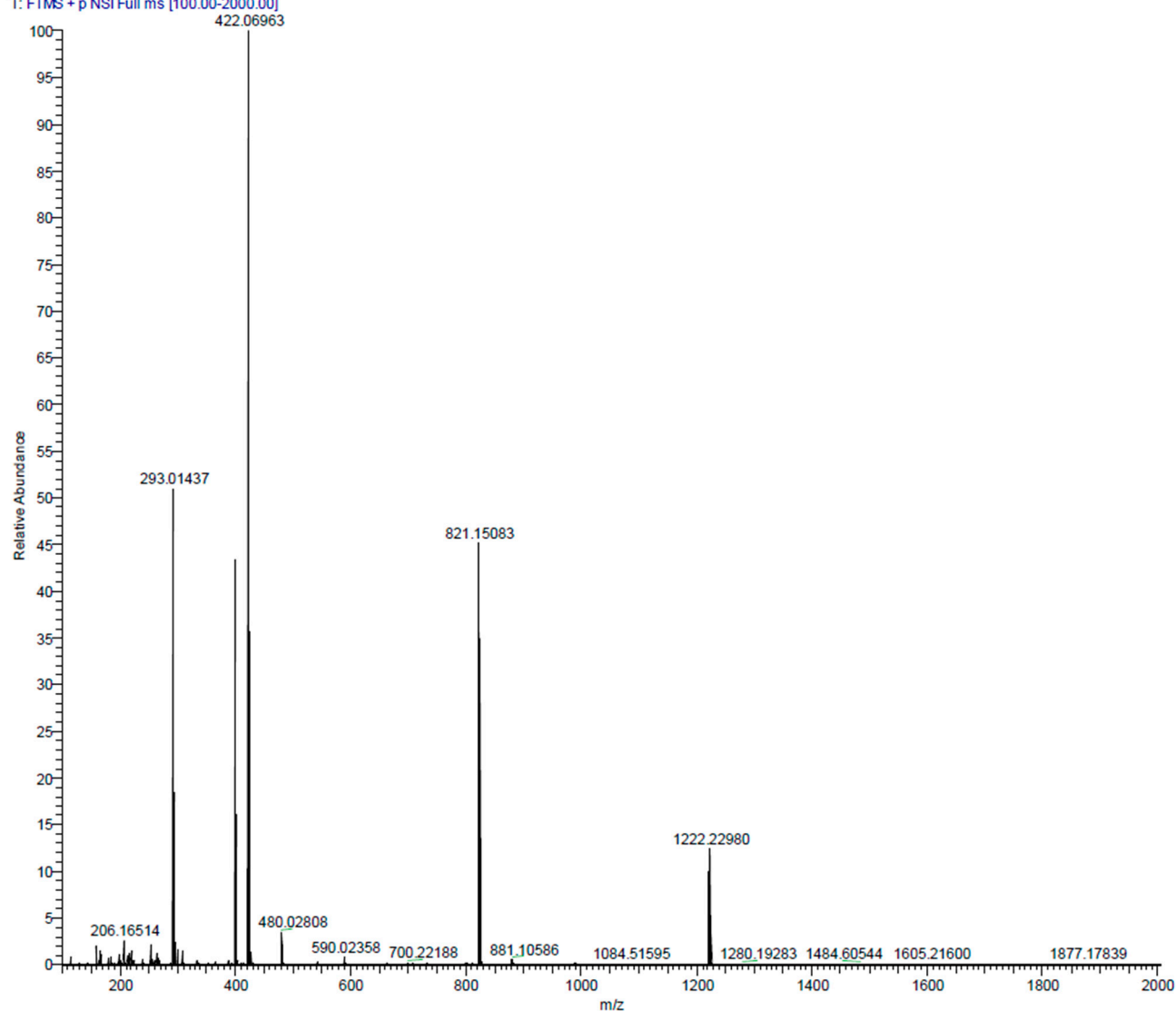
Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)



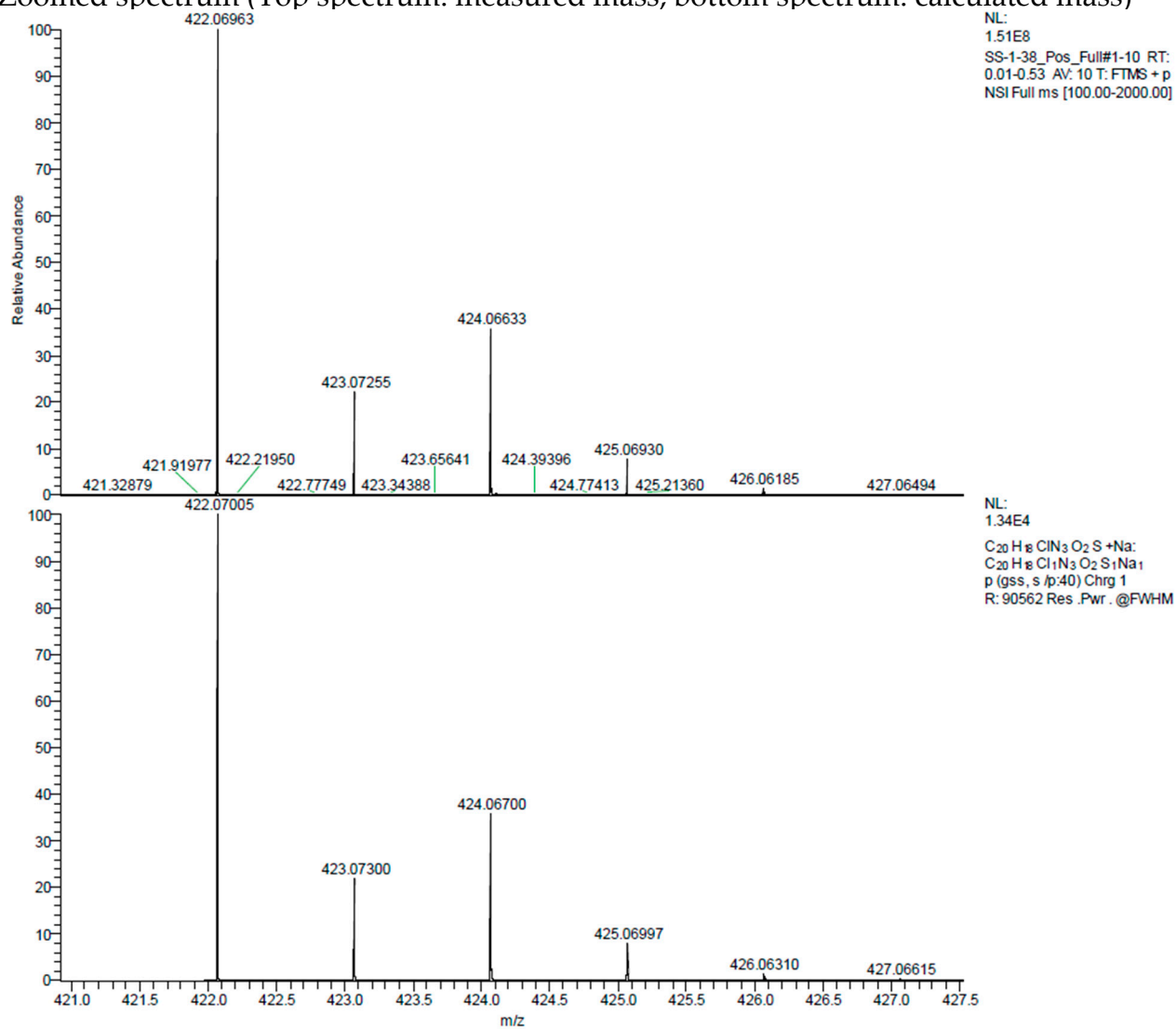
N-Benzyl-2-((6-chloro-3-cyclopropyl-4-oxo-3,4-dihydroquinazolin-2-yl)thio)acetamide (**5d**)

Full spectrum

SS-1-38_Pos_Full #1-10 RT: 0.01-0.53 AV: 10 NL: 1.51E8
T: FTMS + p NSI Full ms [100.00-2000.00]



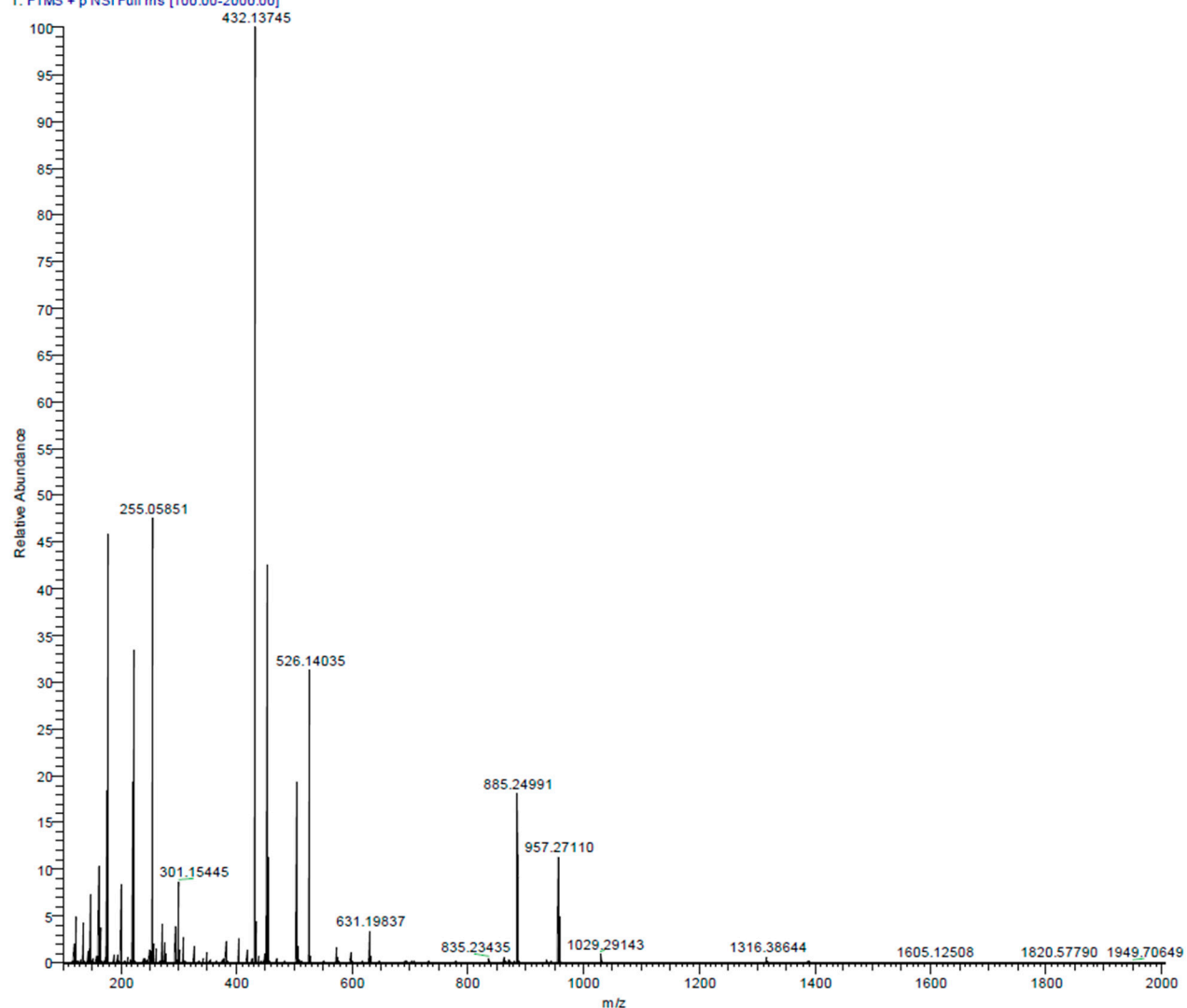
Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)



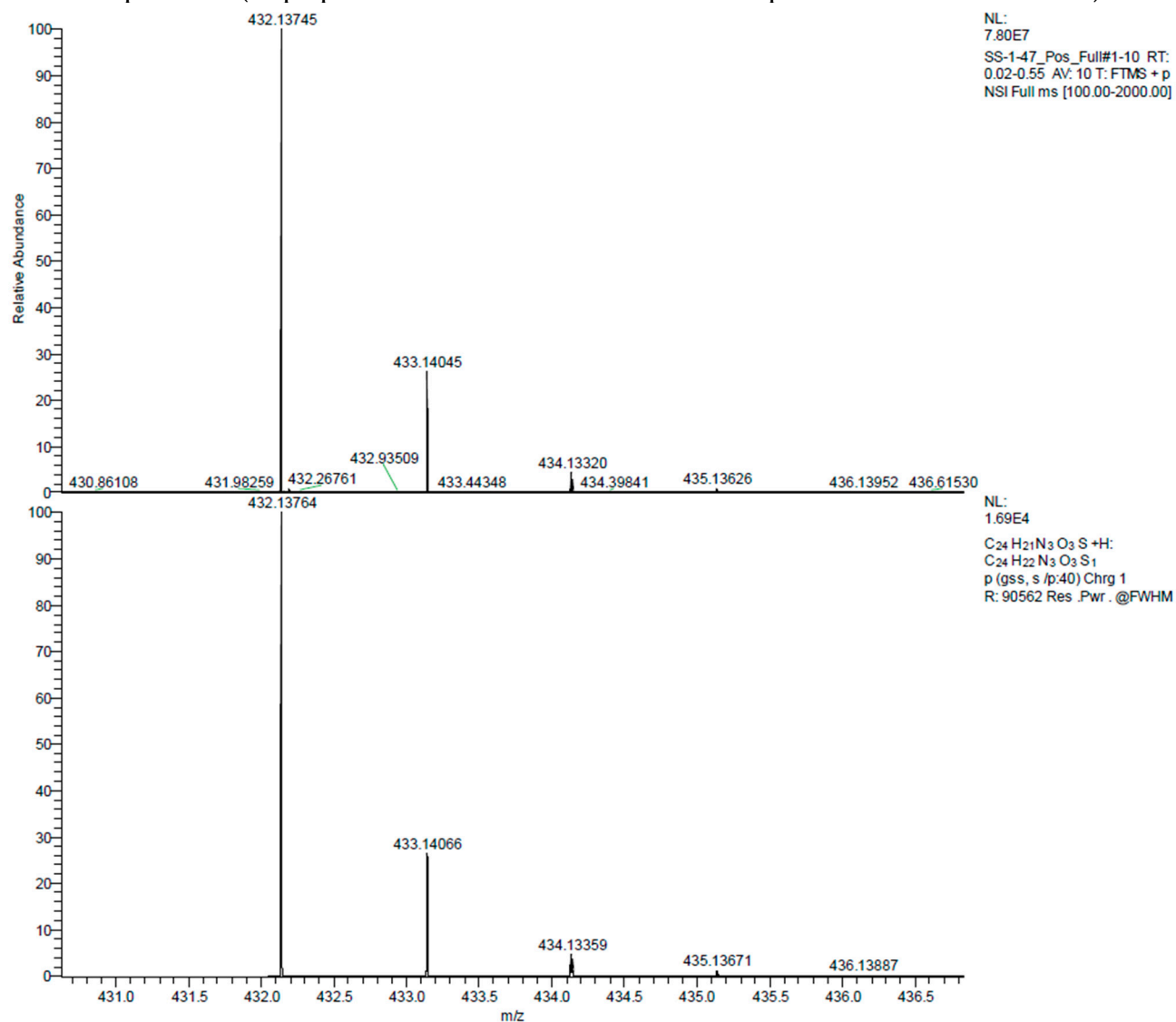
N-(4-Methoxyphenyl)-3-((4-oxo-3-phenyl-3,4-dihydroquinazolin-2-yl)thio)propenamide (**5f**)

Full spectrum

SS-1-47_Pos_Full #1-10 RT: 0.02-0.55 AV: 10 NL: 7.80E7
T: FTMS + p NSI Full ms [100.00-2000.00]



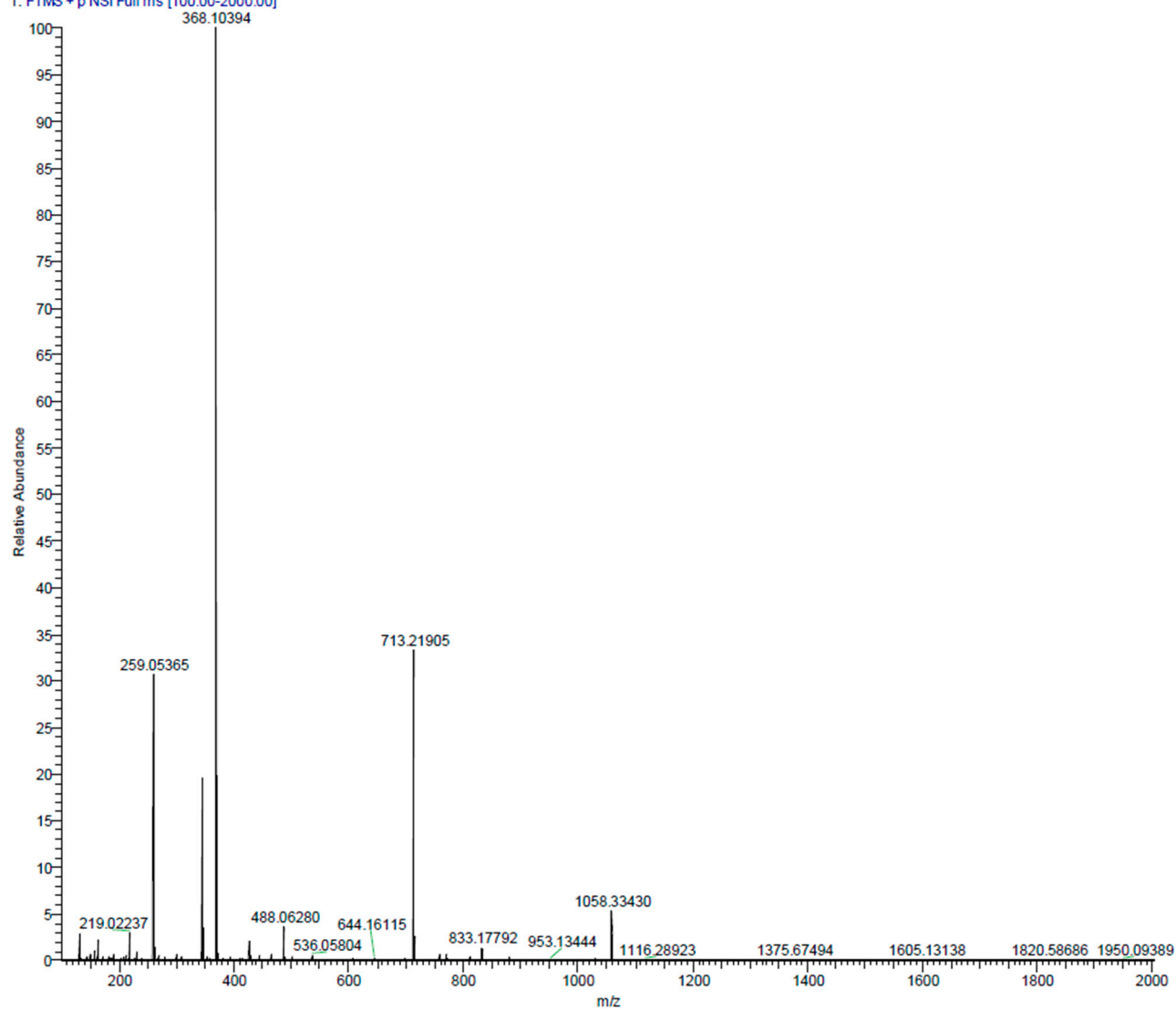
Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)



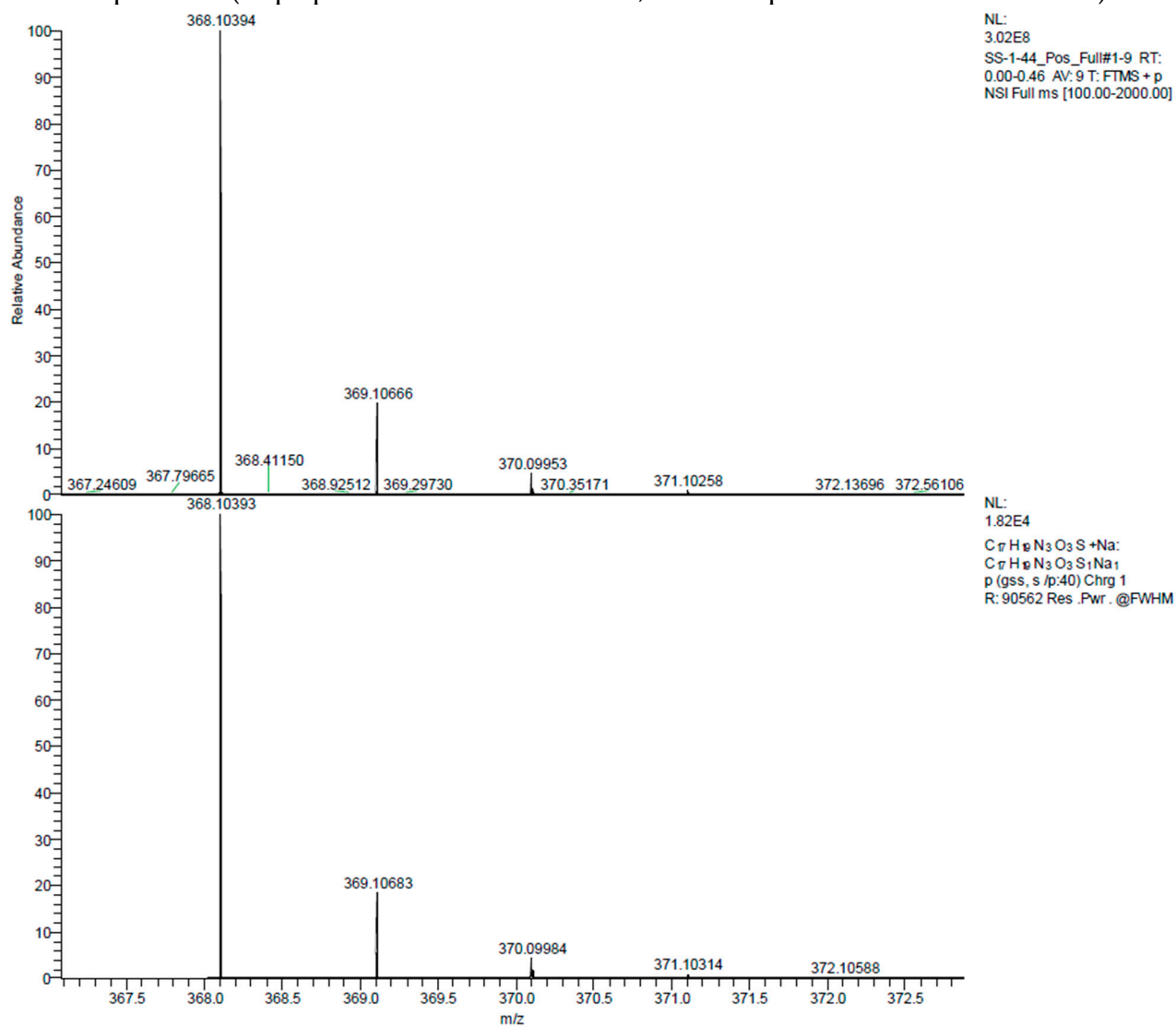
3-Cyclopropyl-2-((2-morpholino-2-oxoethyl)thio)quinazolin-4(3H)-one
(5g)

Full spectrum

SS-1-44_Pos_Full #1-9 RT: 0.00-0.46 AV: 9 NL: 3.02E8
T: FTMS + p NSI Full ms [100.00-2000.00]



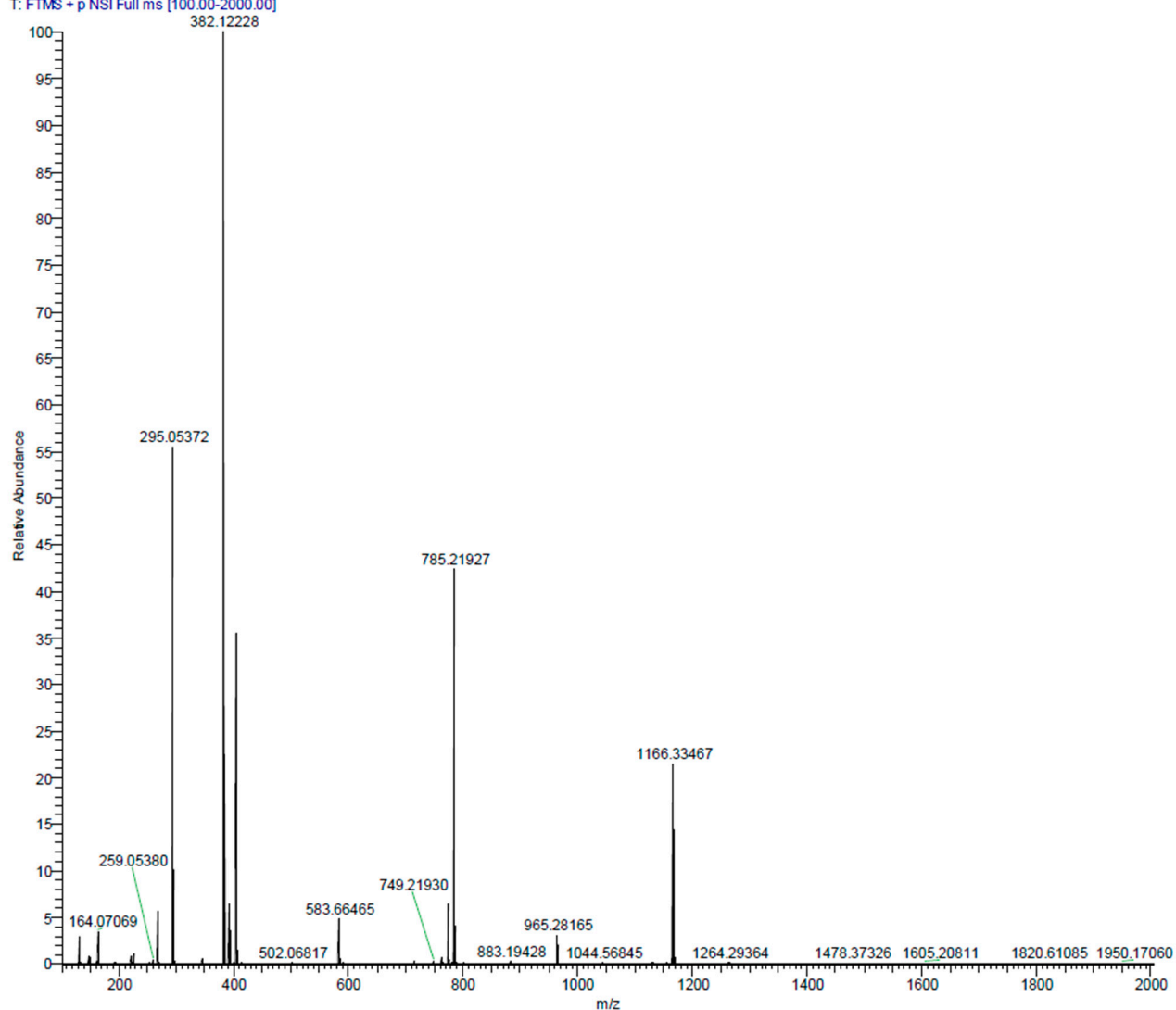
Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)



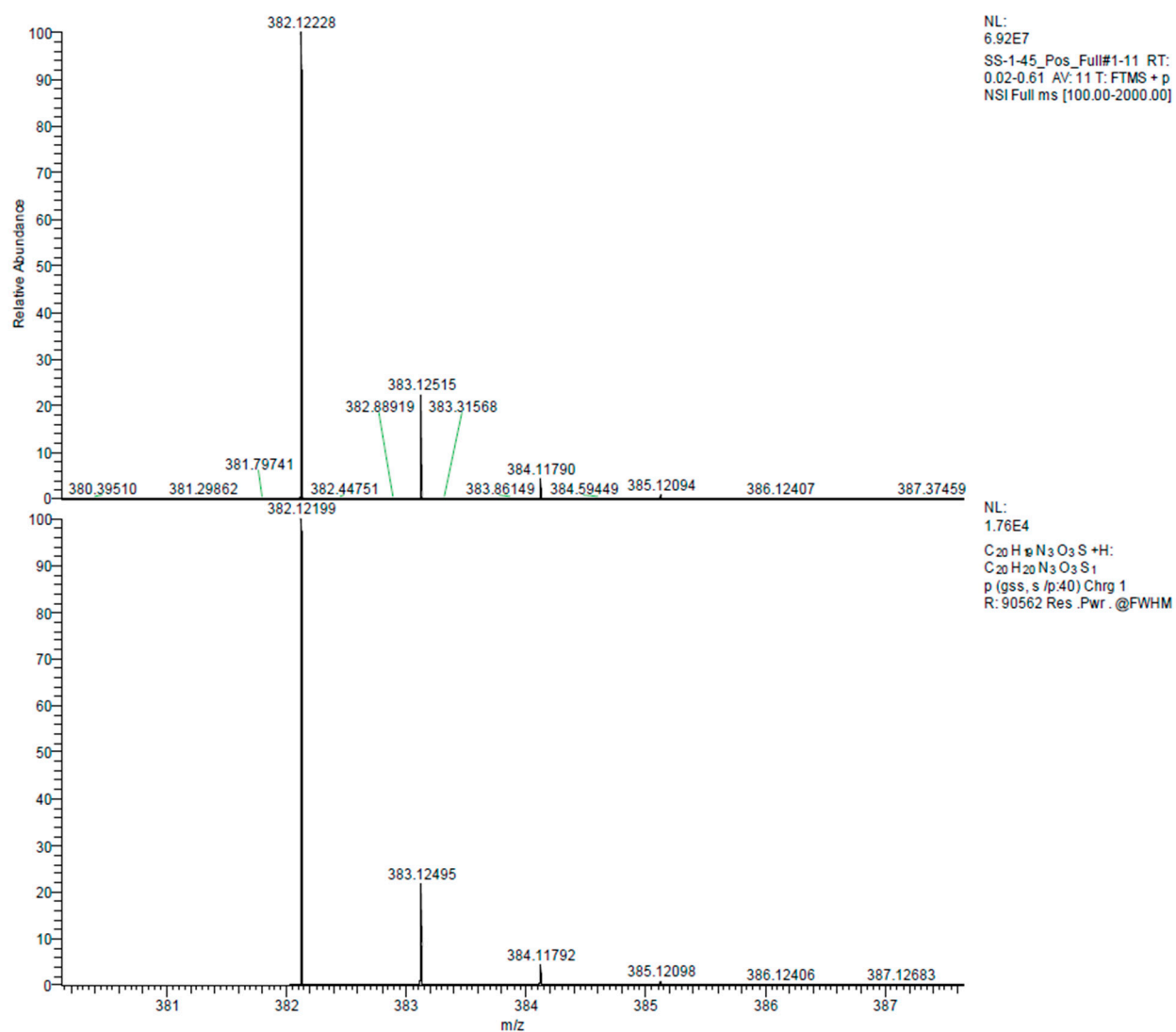
2-((2-Morpholino-2-oxoethyl)thio)-3-phenylquinazolin-4(3H)-one (**5h**)

Full spectrum

SS-1-45_Pos_Full #1-11 RT: 0.02-0.61 AV: 11 NL: 6.92E7
T: FTMS + p NSI Full ms [100.00-2000.00]



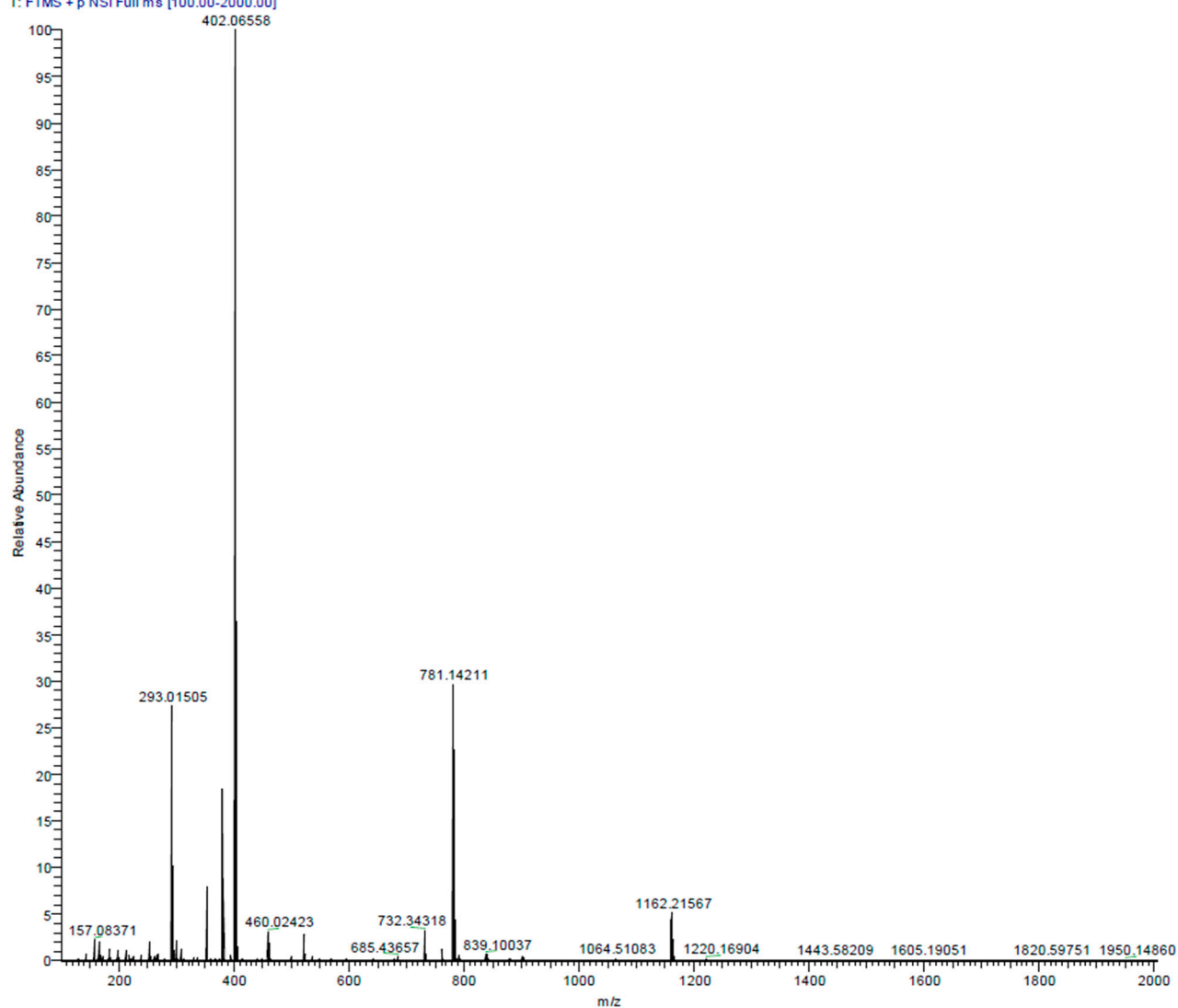
Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)



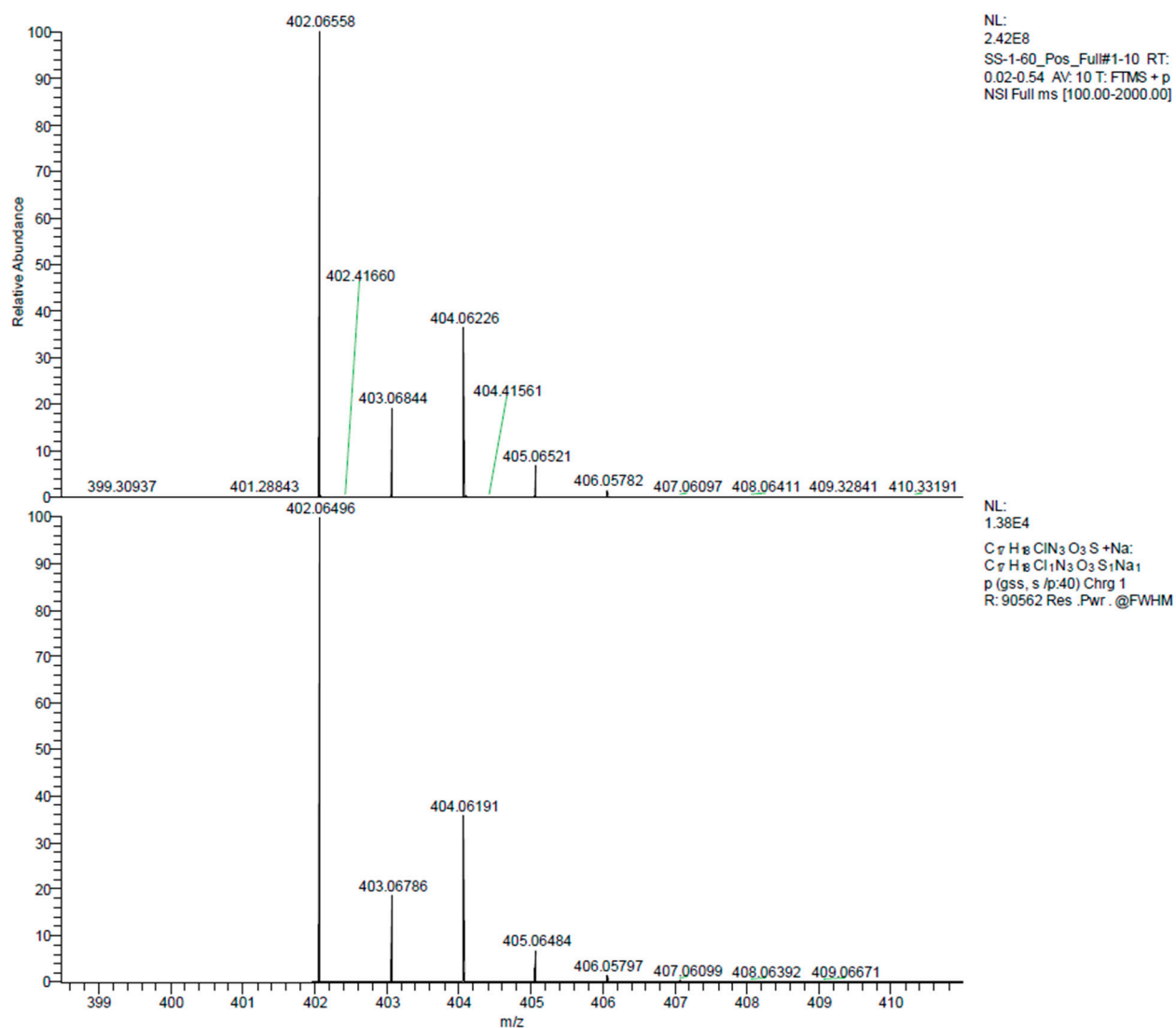
2-((2-Morpholino-2-oxoethyl)thio)quinazolin-4(3H)-one (**5i**)

Full spectrum

SS-1-60_Pos_Full #1-10 RT: 0.02-0.54 AV: 10 NL: 2.42E8
T: FTMS + p NSI Full ms [100.00-2000.00]



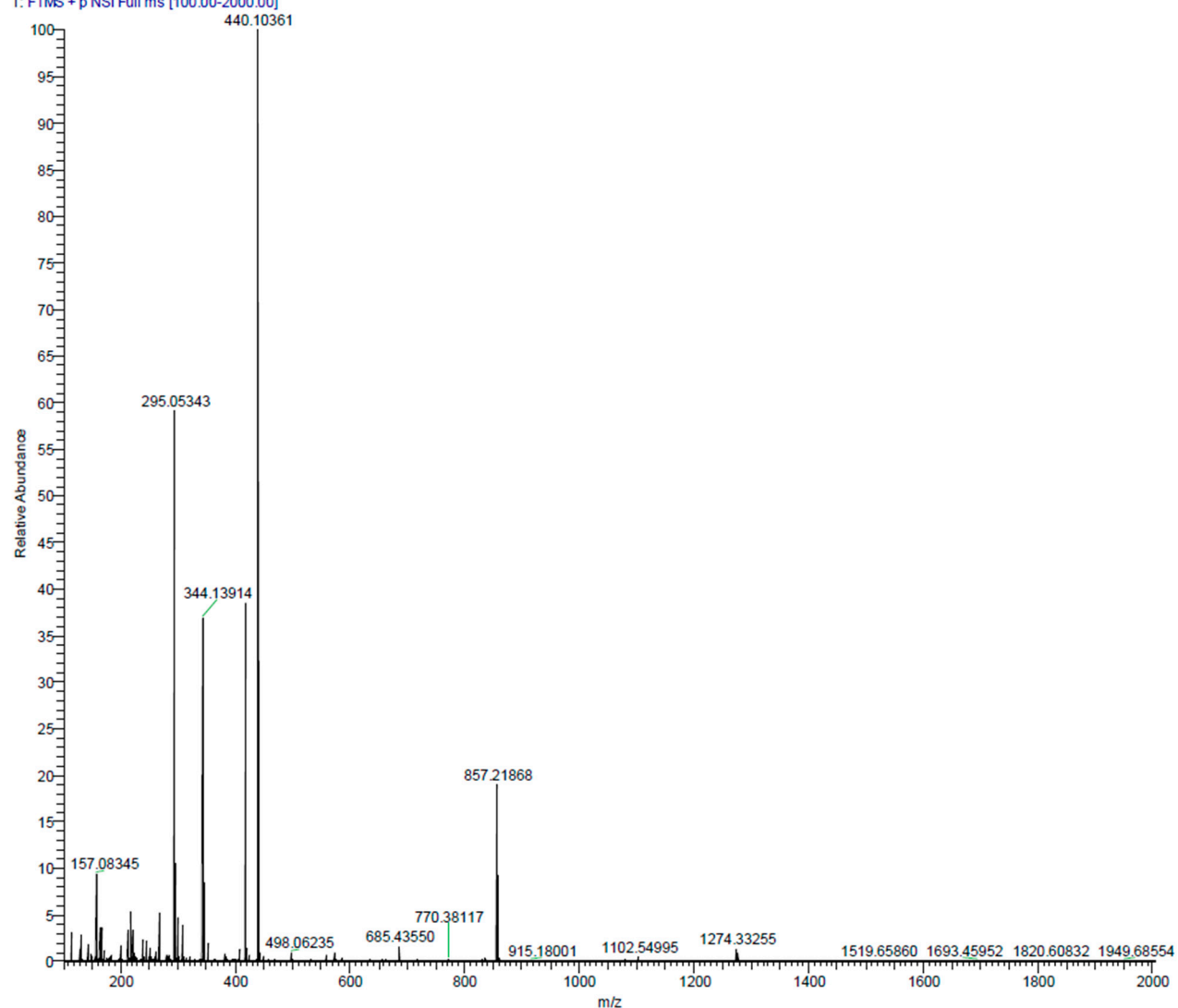
Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)



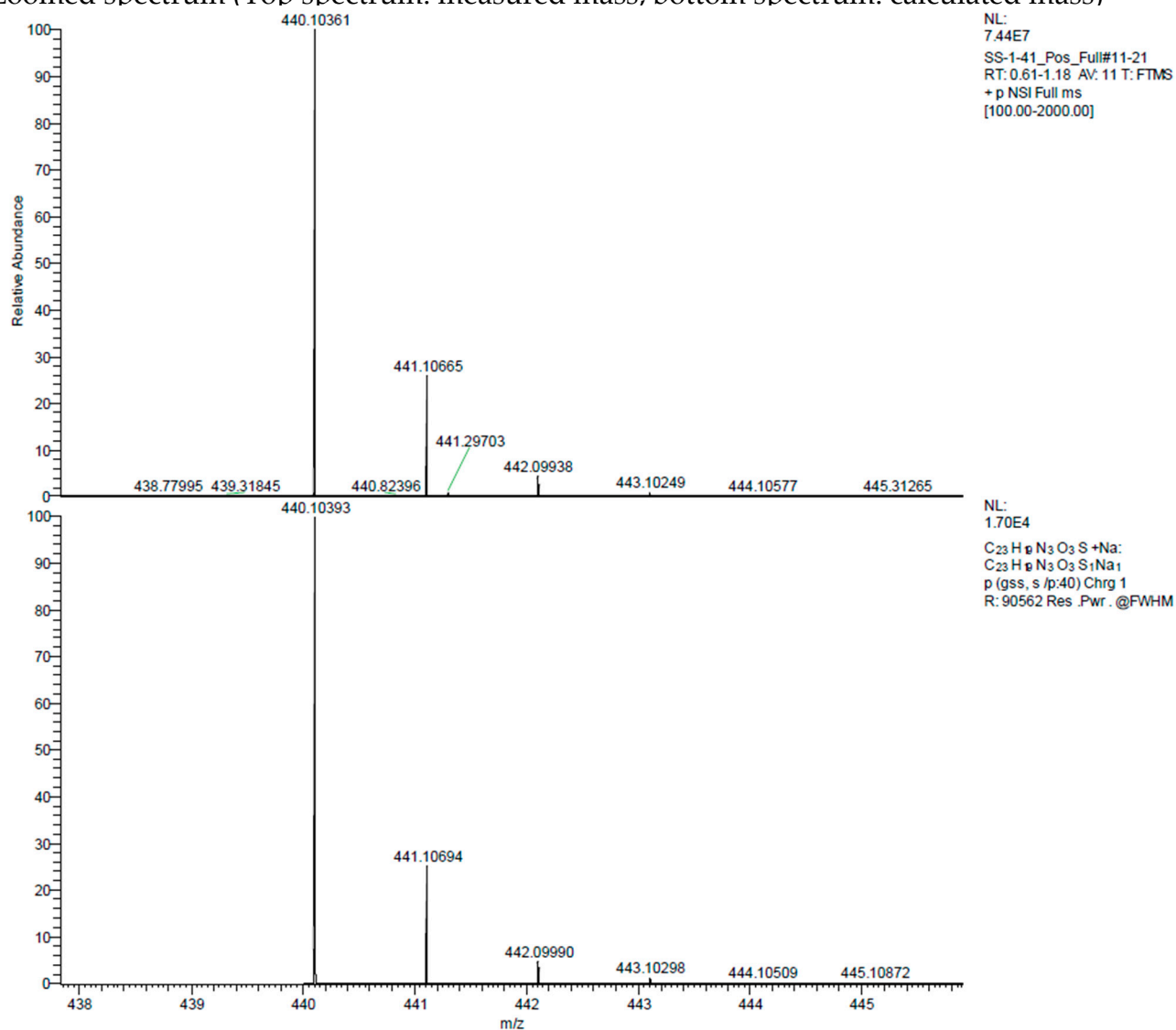
N-(4-Methoxyphenyl)-2-((4-oxo-3-phenyl-3,4-dihydroquinazolin-2-yl)thio)acetamide (**5j**)

Full spectrum

SS-1-41_Pos_Full #11-21 RT: 0.61-1.18 AV: 11 NL: 7.44E7
T: FTMS + p NSI Full ms [100.00-2000.00]



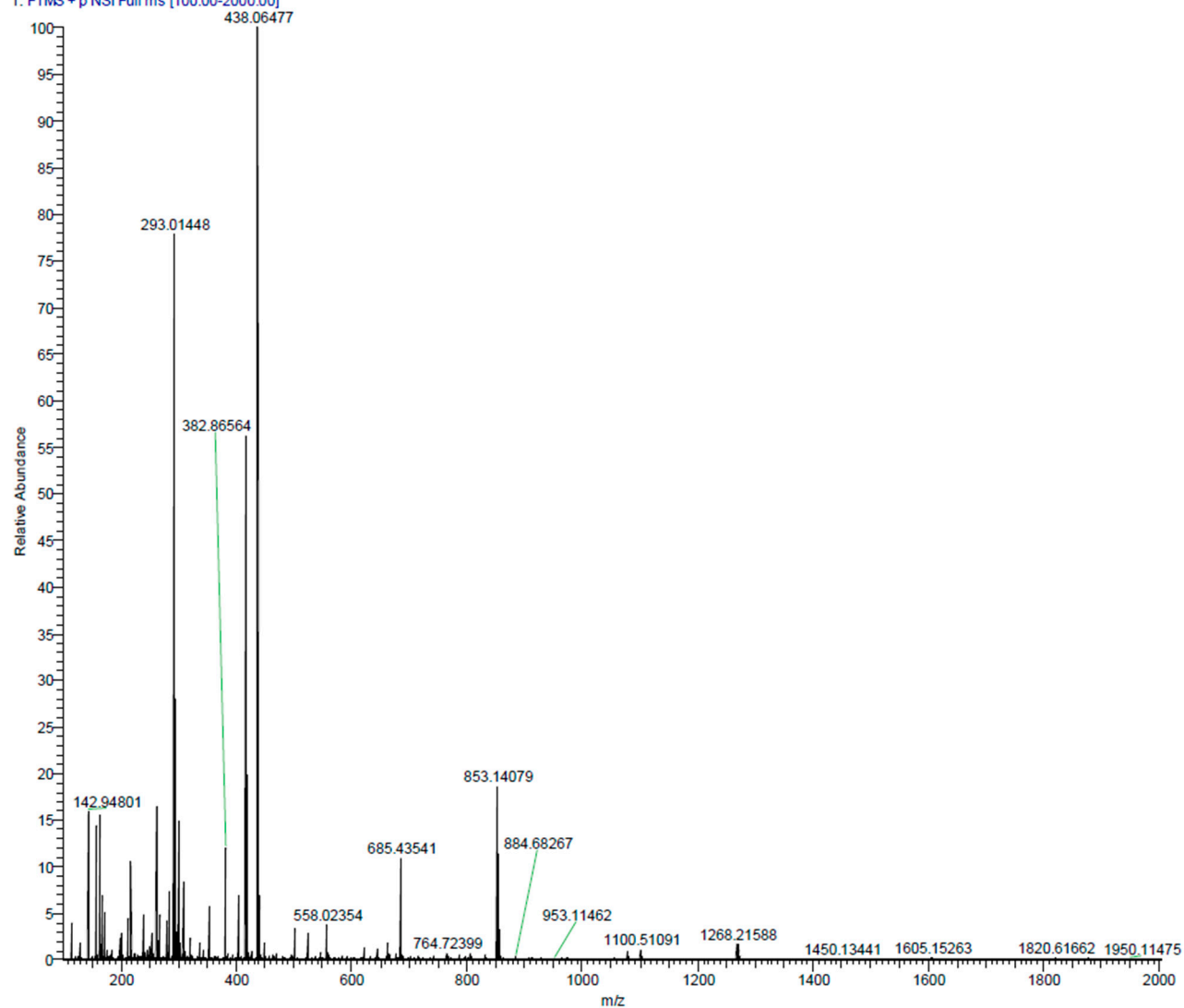
Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)



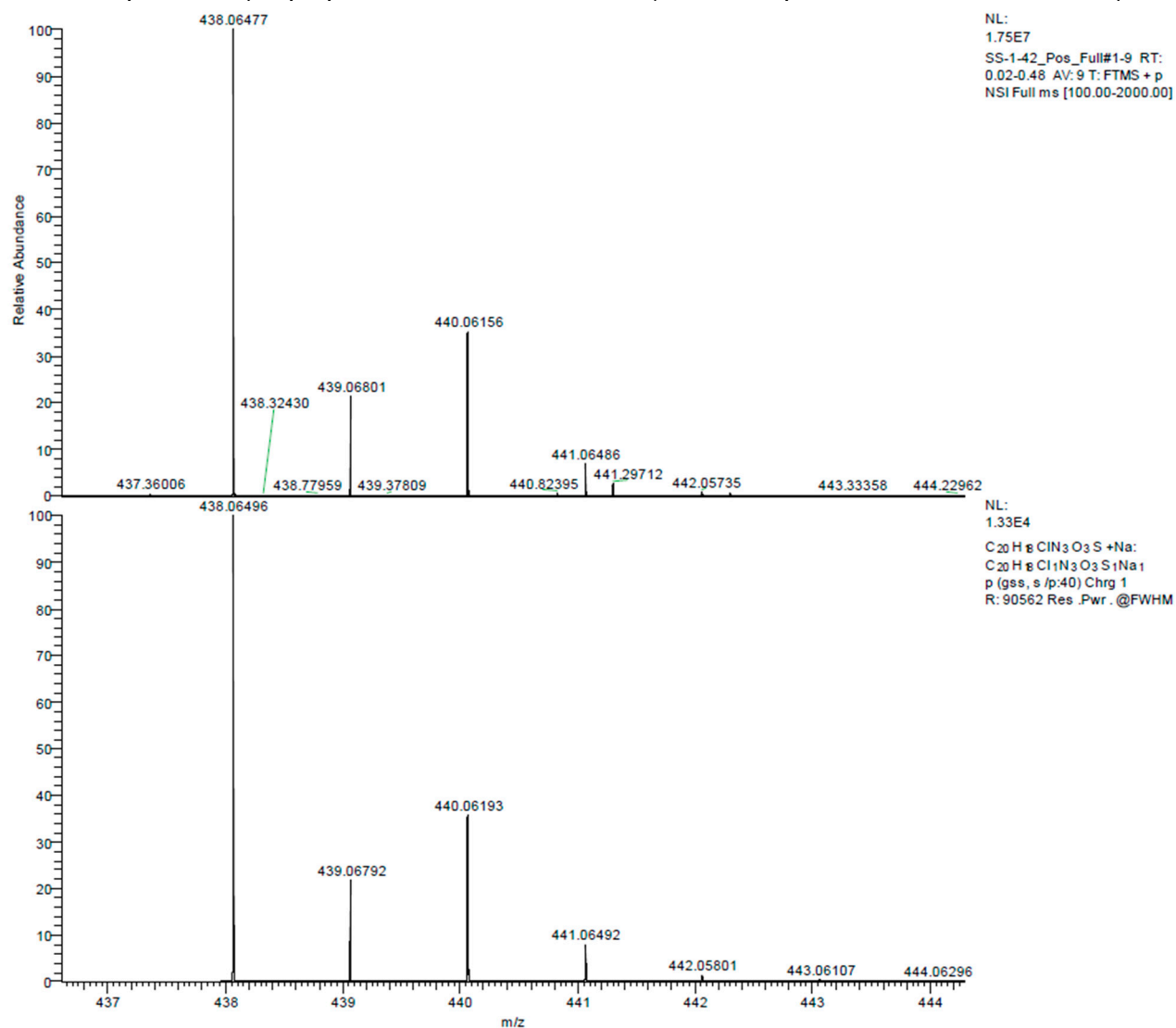
2-((6-Chloro-3-cyclopropyl-4-oxo-3,4-dihydroquinazolin-2-yl)thio)-N-(4-methoxyphenyl)acetamide (**5k**)

Full spectrum

SS-1-42_Pos_Full #1-9 RT: 0.02-0.48 AV: 9 NL: 1.75E7
T: FTMS + p NSI Full ms [100.00-2000.00]



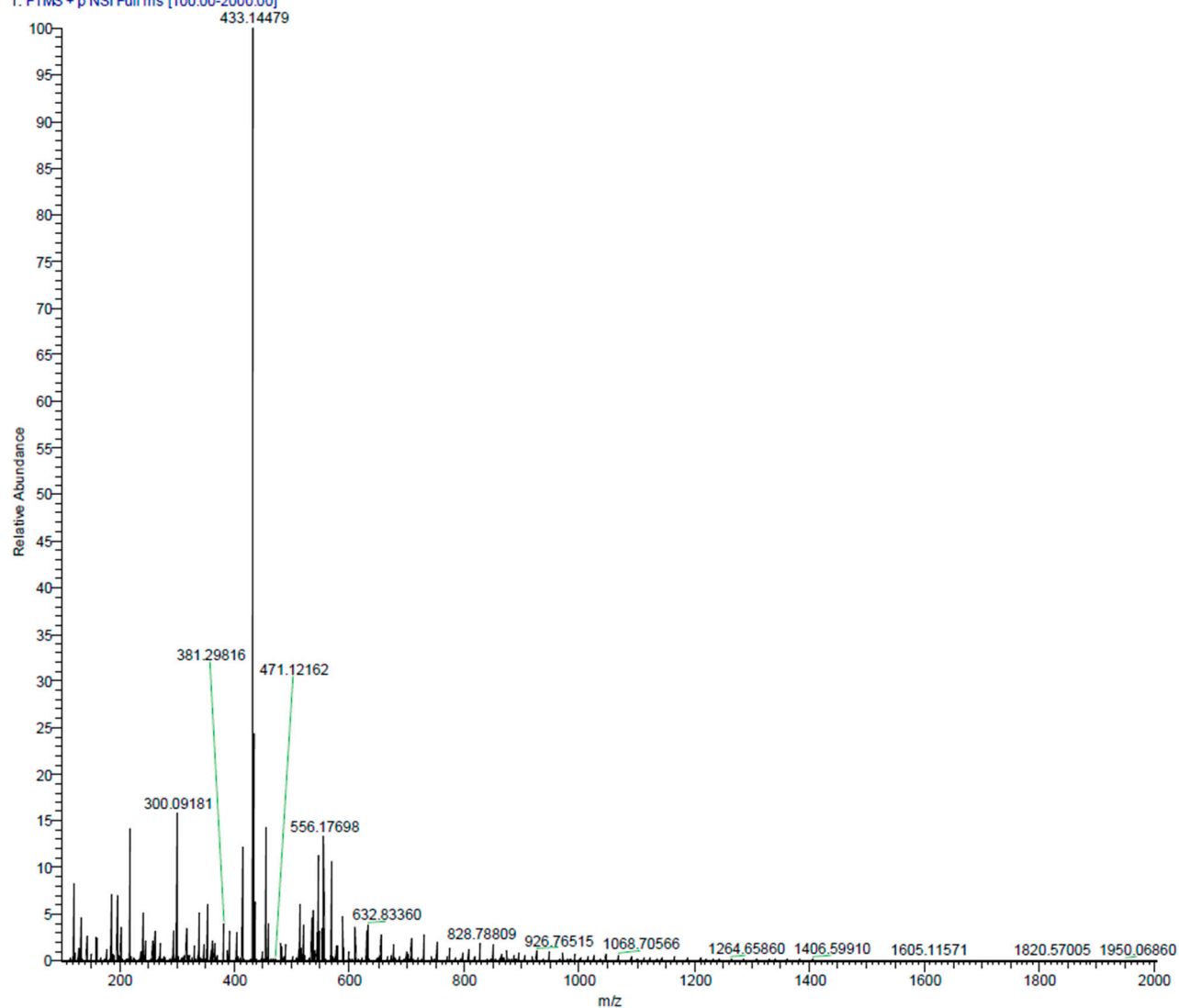
Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)



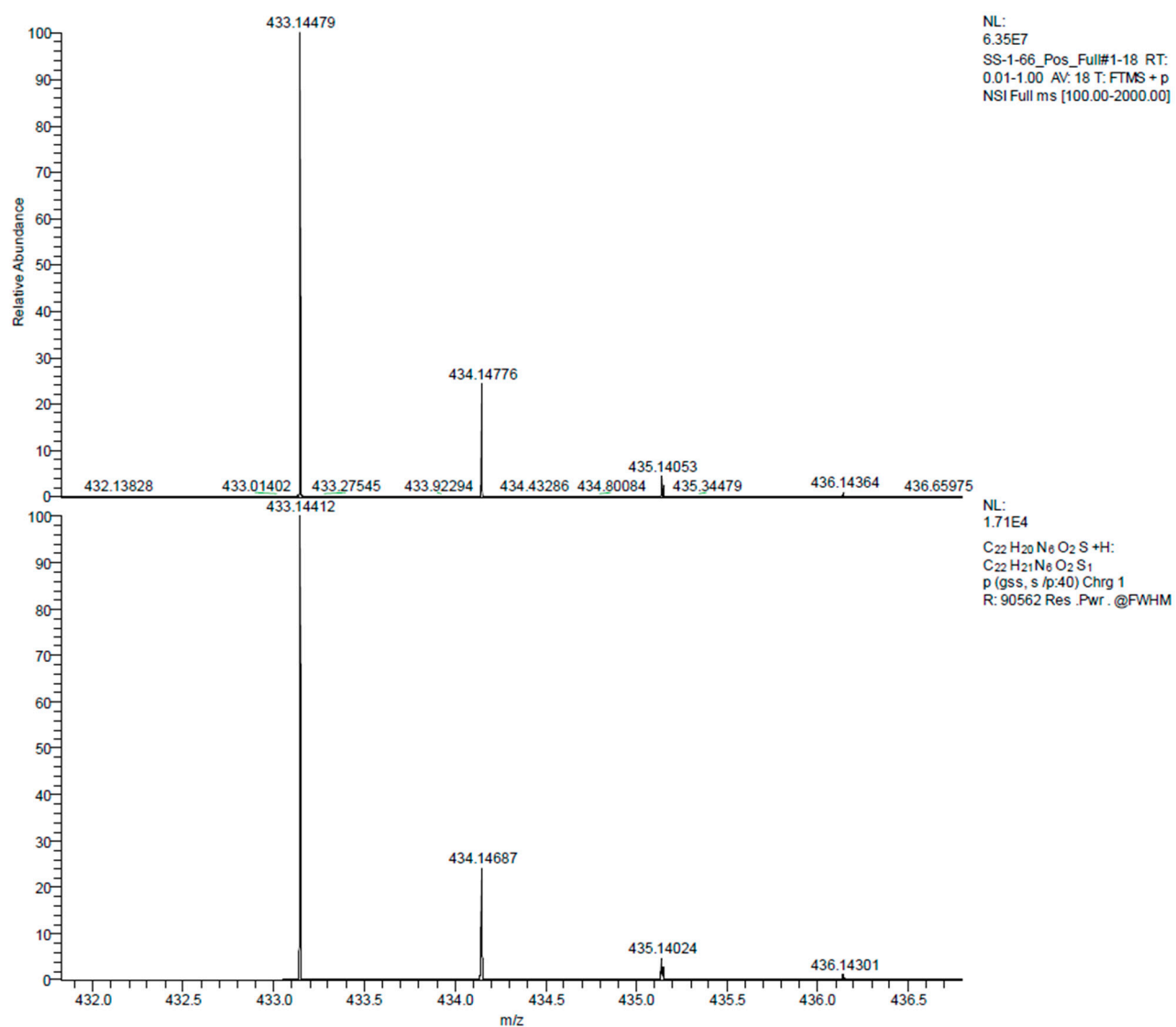
2-(4-(((3-Cyclopropyl-4-oxo-3,4-dihydroquinazolin-2-yl)thio)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-phenylacetamide (**6a**)

Full spectrum

SS-1-66_Pos_Full #1-18 RT: 0.01-1.00 AV: 18 NL: 6.35E7
T: FTMS + p NSI Full ms [100.00-2000.00]



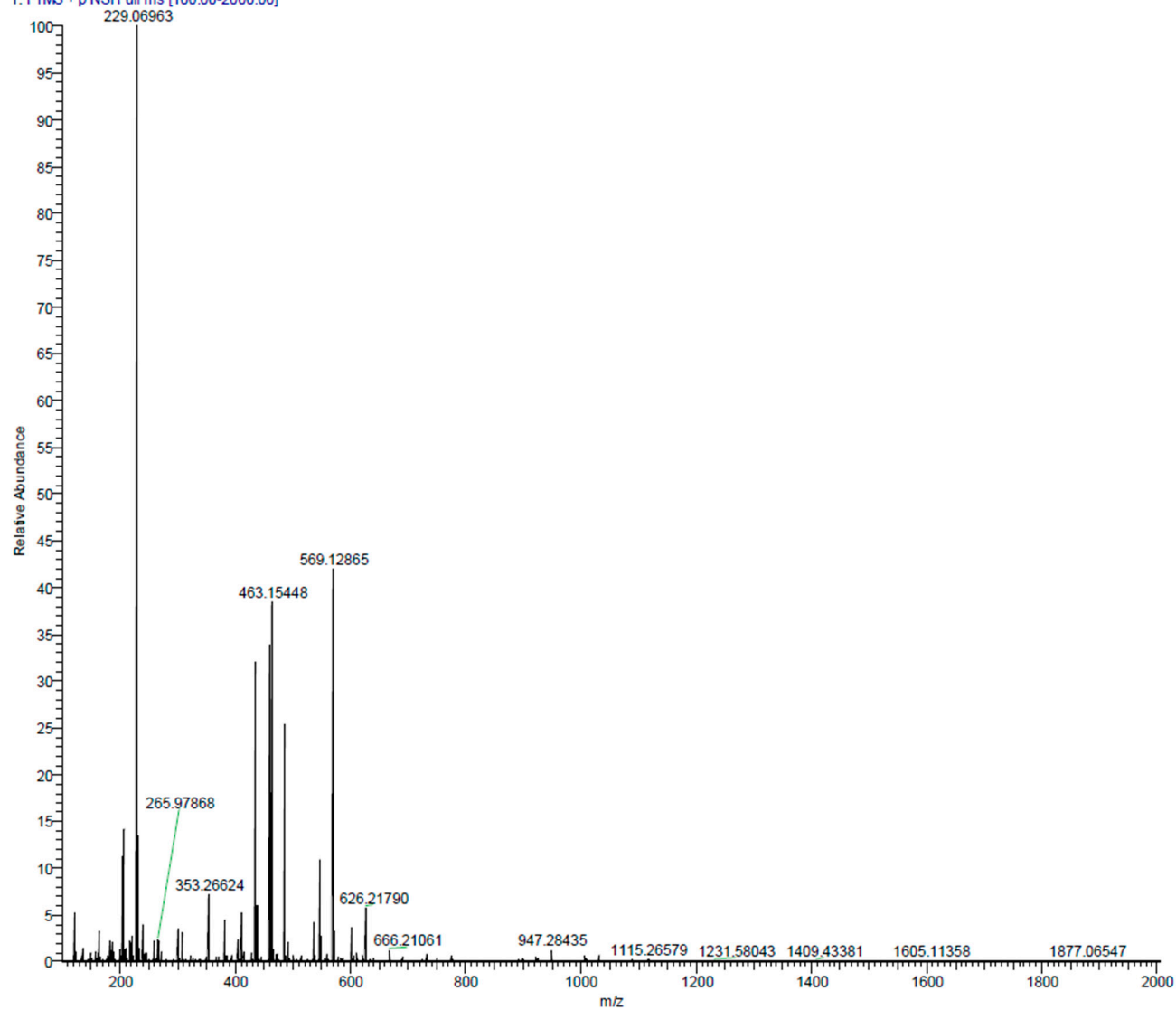
Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)



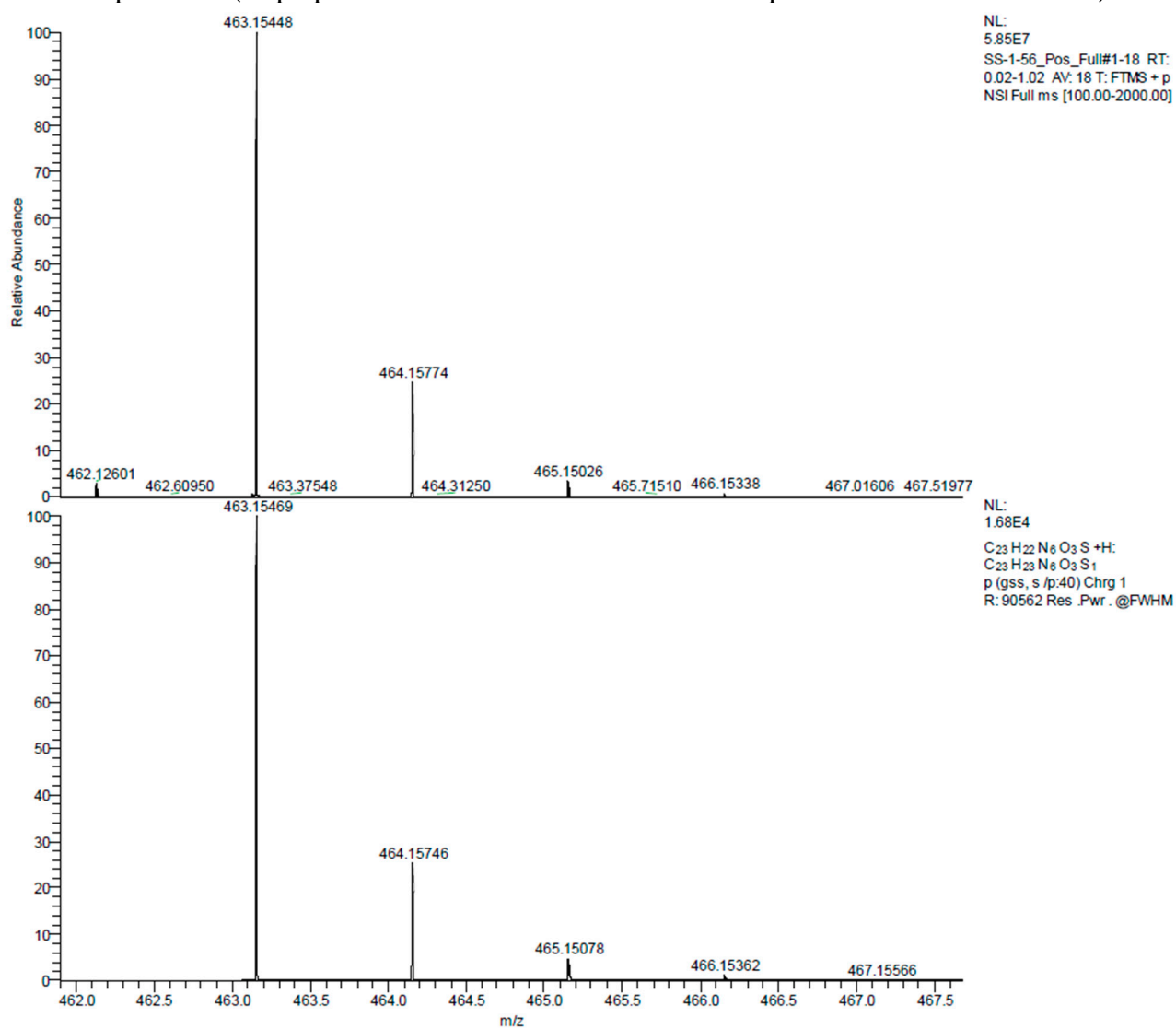
2-(4-(((3-Cyclopropyl-4-oxo-3,4-dihydroquinazolin-2-yl)thio)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-(4-methoxyphenyl)acetamide (**6b**)

Full spectrum

SS-1-56_Pos_Full #1-18 RT: 0.02-1.02 AV: 18 NL: 1.52E8
T: FTMS + p NSI Full ms [100.00-2000.00]



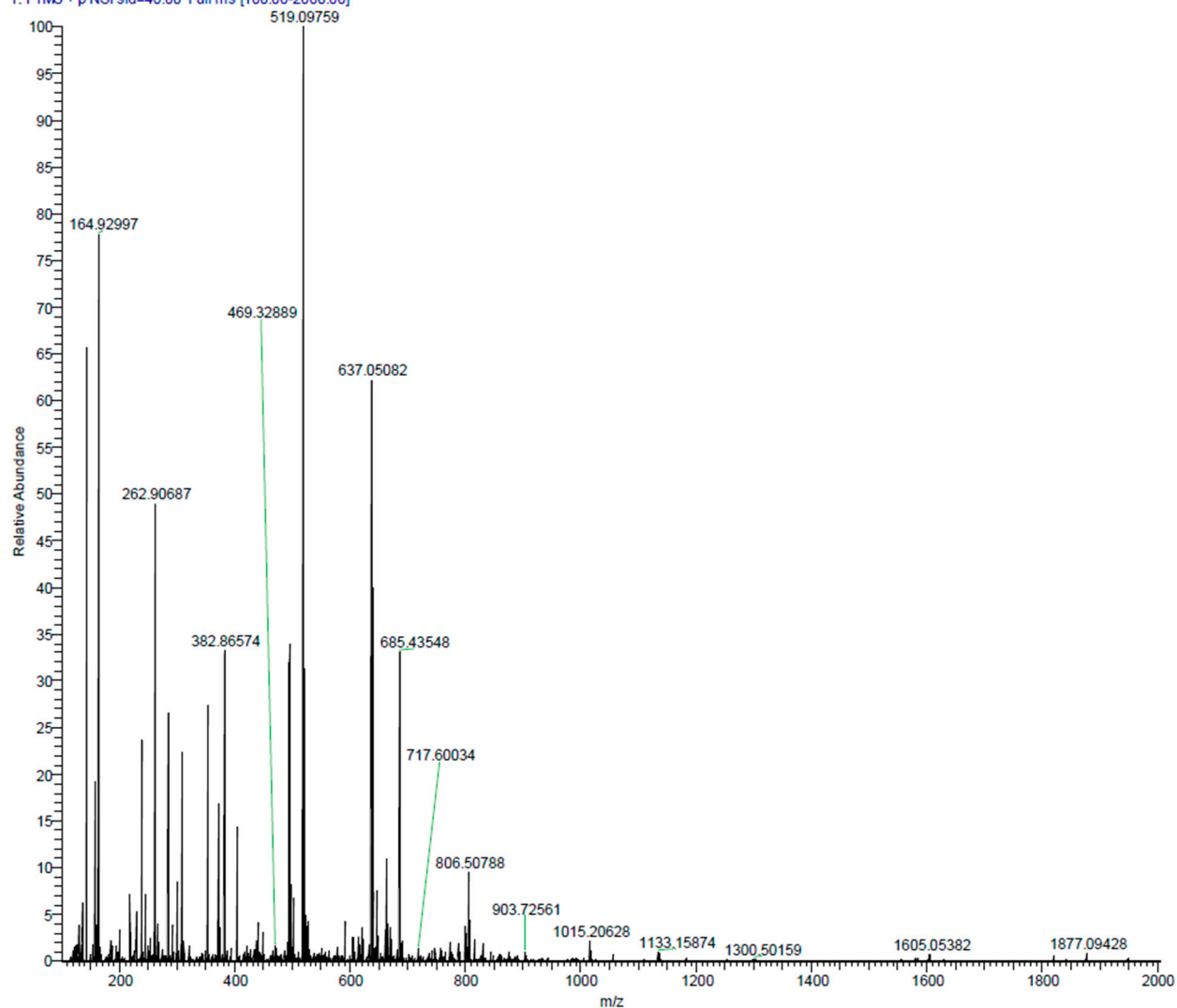
Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)



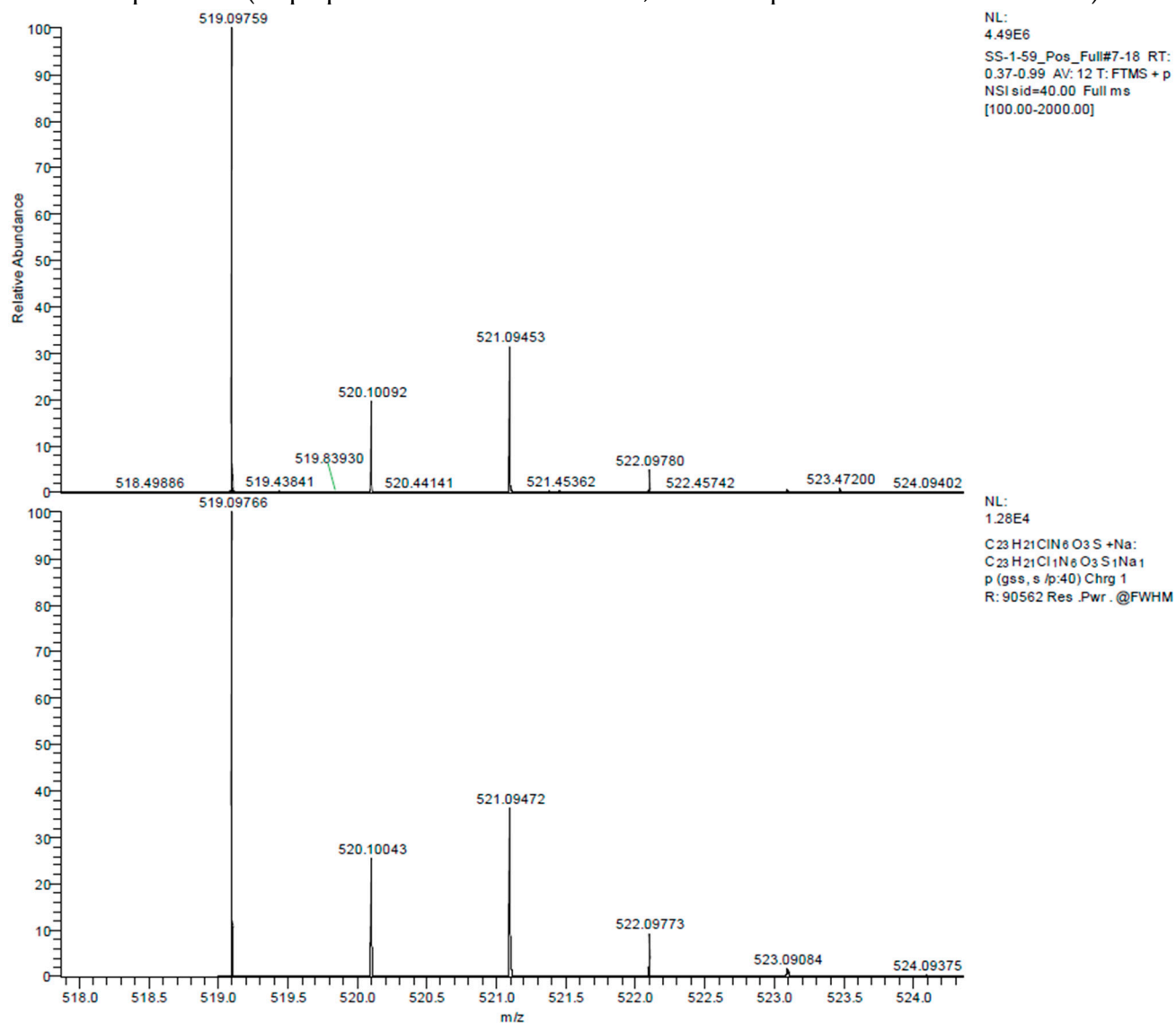
2-(4-(((6-Chloro-3-cyclopropyl-4-oxo-3,4-dihydroquinazolin-2-yl)thio)methyl)-1H-1,2,3-triazol-1-yl)-N-(4-methoxyphenyl)acetamide (**6c**)

Full spectrum

SS-1-59_Pos_Full #7-18 RT: 0.37-0.99 AV: 12 NL: 4.49E6
T: FTMS + p NSI sid=40.00 Full ms [100.00-2000.00]



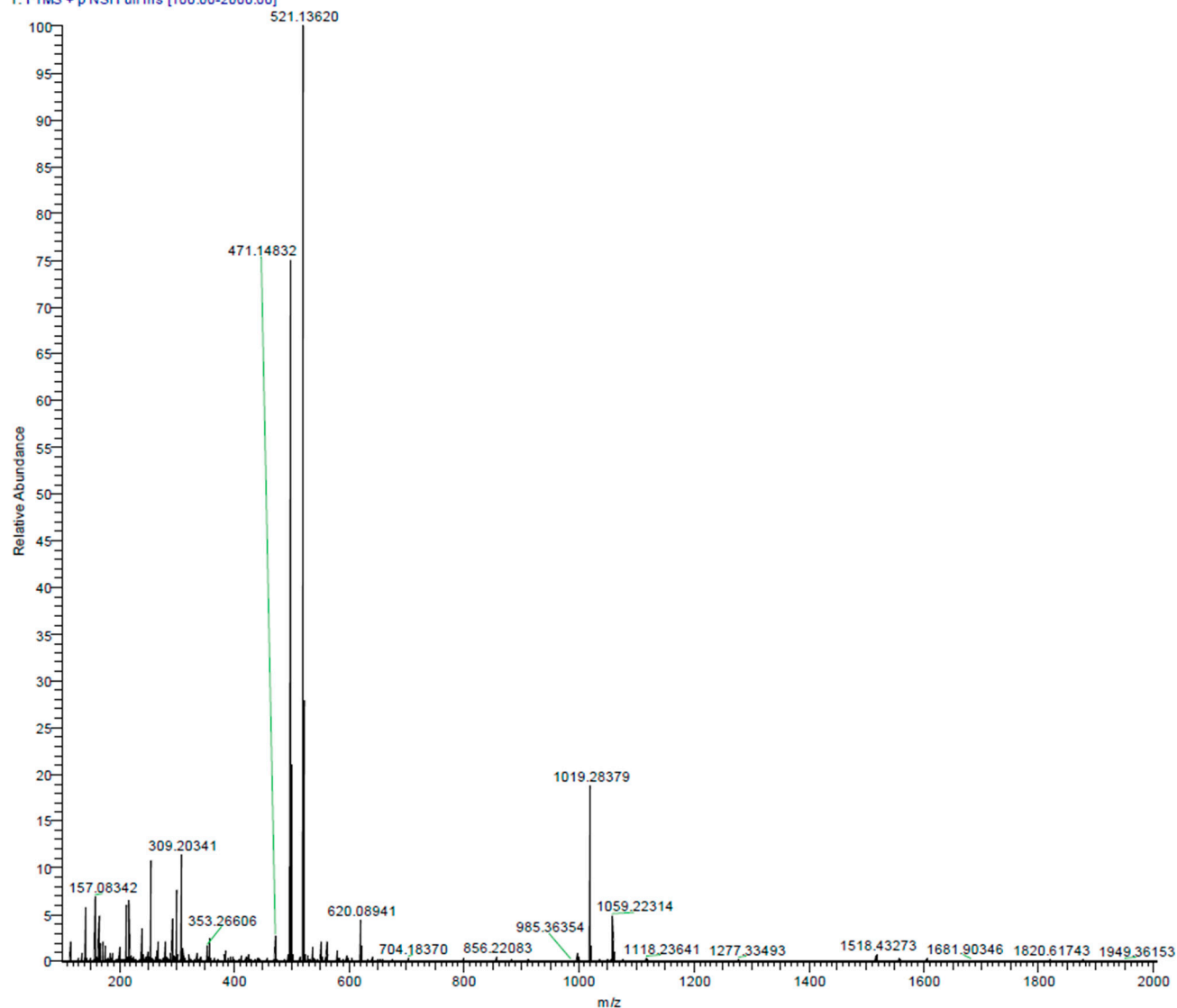
Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)



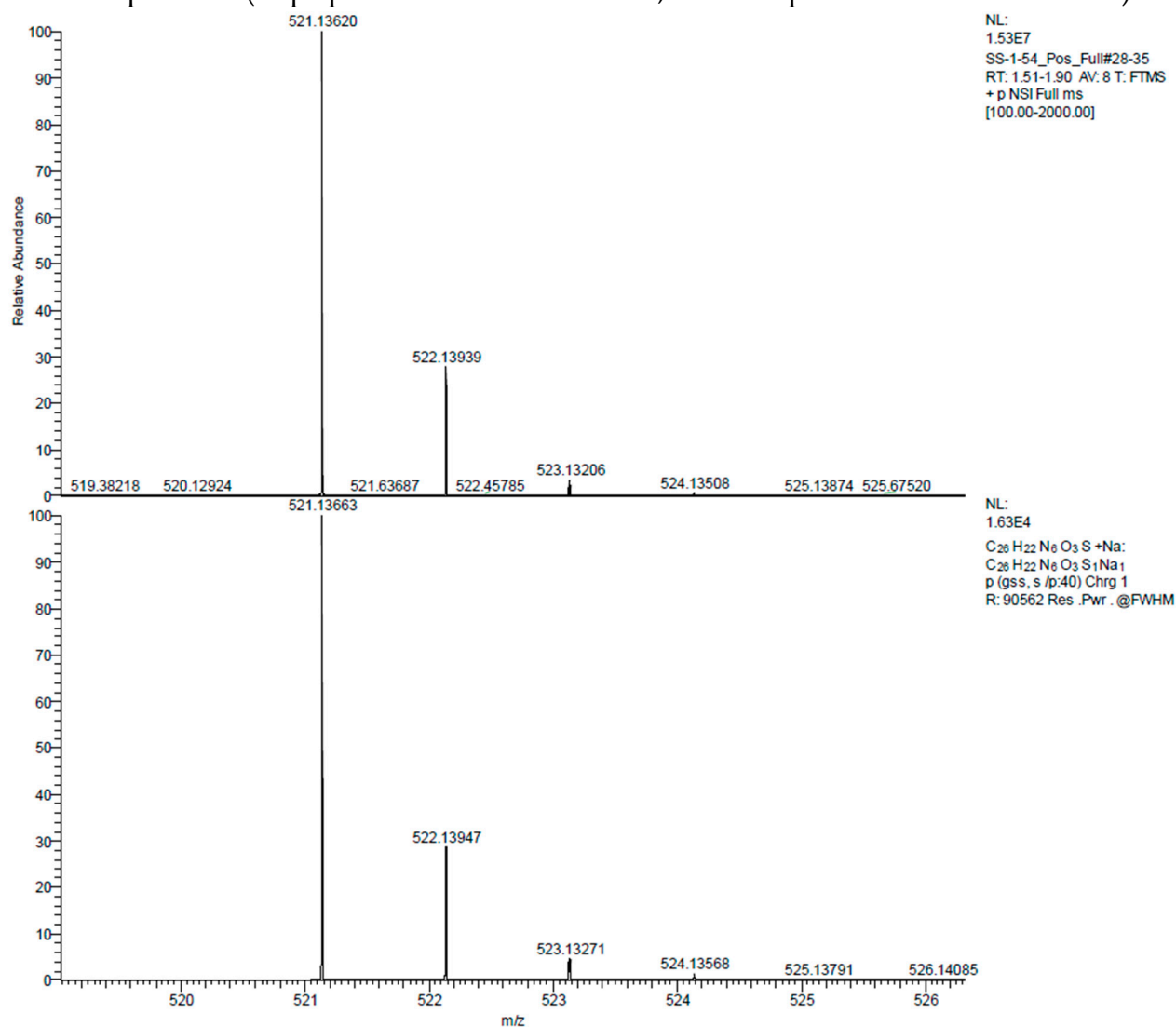
N-(4-Methoxyphenyl)-2-(4-(((4-oxo-3-phenyl-3,4-dihydroquinazolin-2-yl)thio)methyl)-1*H*-1,2,3-triazol-1-yl)acetamide (**6d**)

Full spectrum

SS-1-54_Pos_Full #28-35 RT: 1.51-1.90 AV: 8 NL: 1.53E7
T: FTMS + p NSI Full ms [100.00-2000.00]



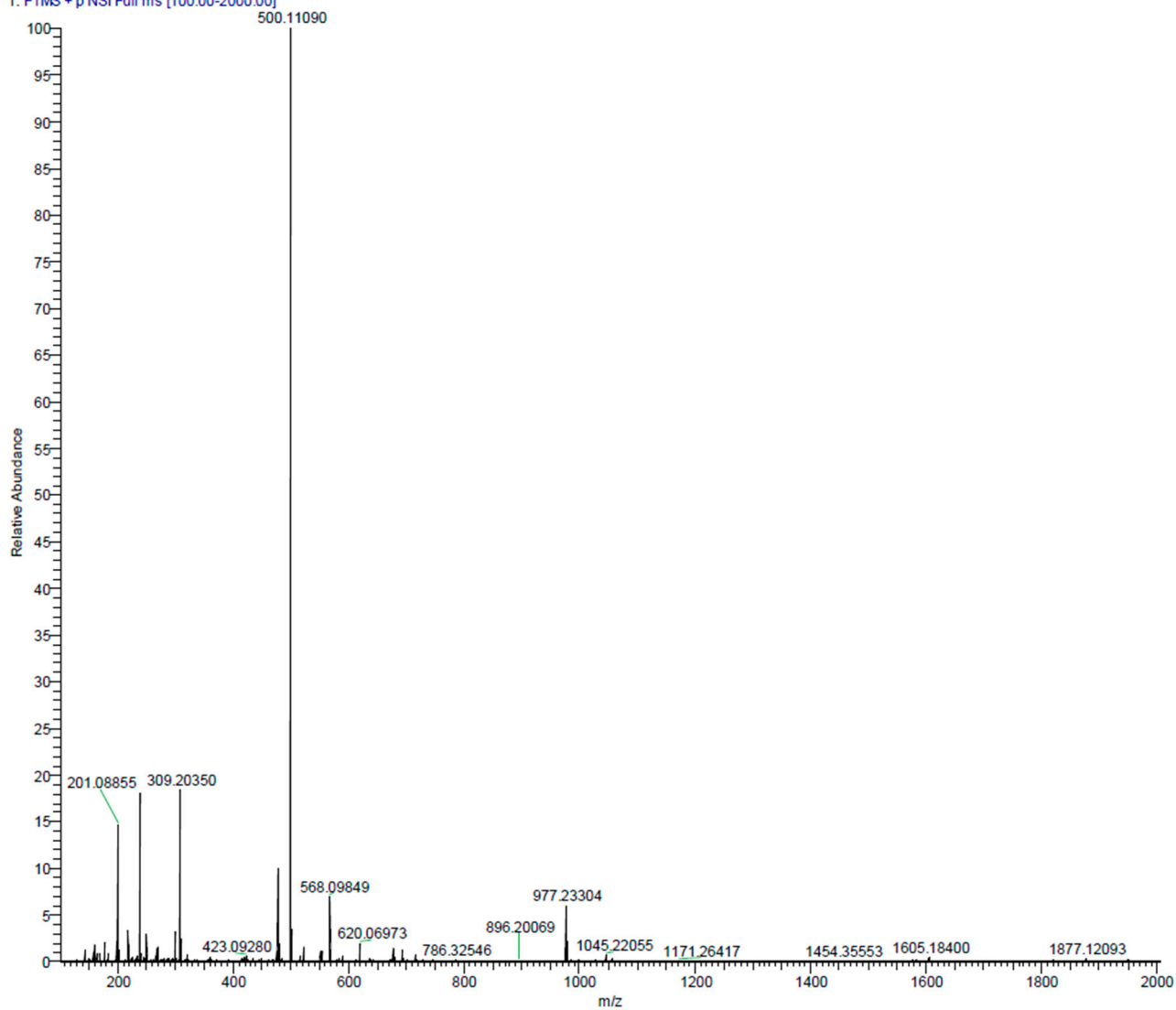
Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)



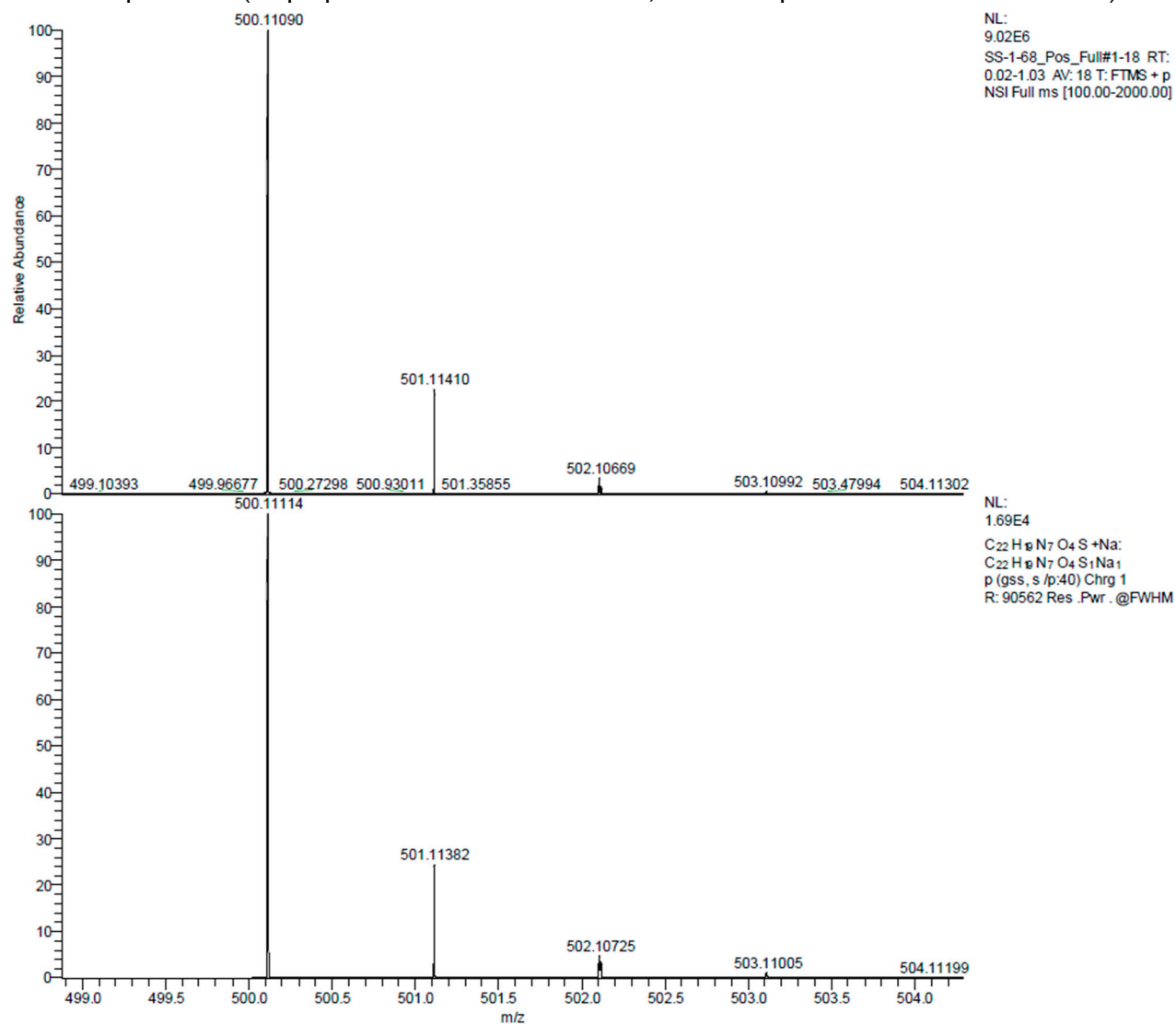
2-(4-(((3-Cyclopropyl-4-oxo-3,4-dihydroquinazolin-2-yl)thio)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-(4-nitrophenyl)acetamide (**6e**)

Full spectrum

SS-1-68_Pos_Full #1-18 RT: 0.02-1.03 AV: 18 NL: 9.02E6
T: FTMS + p NSI Full ms [100.00-2000.00]



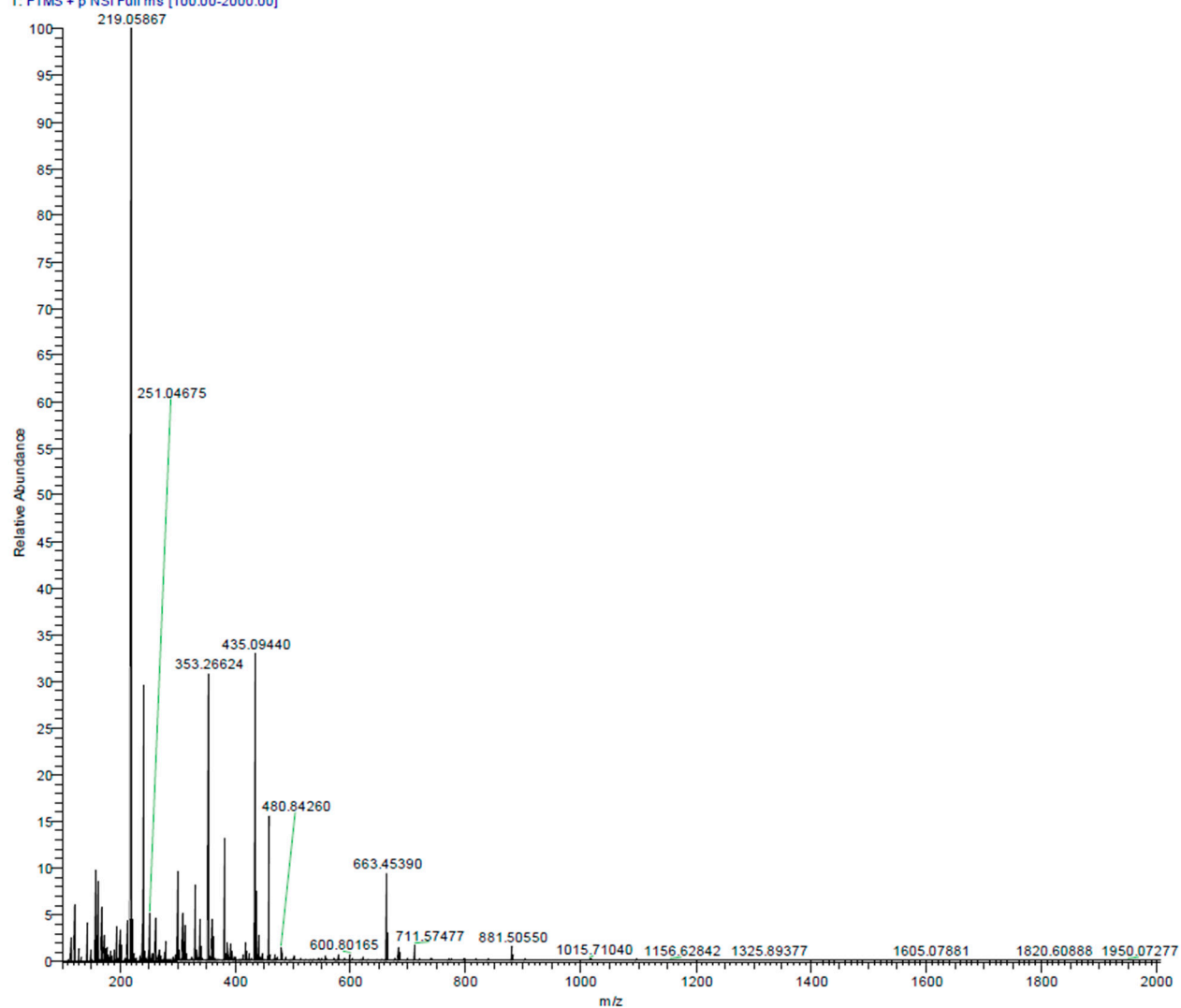
Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)



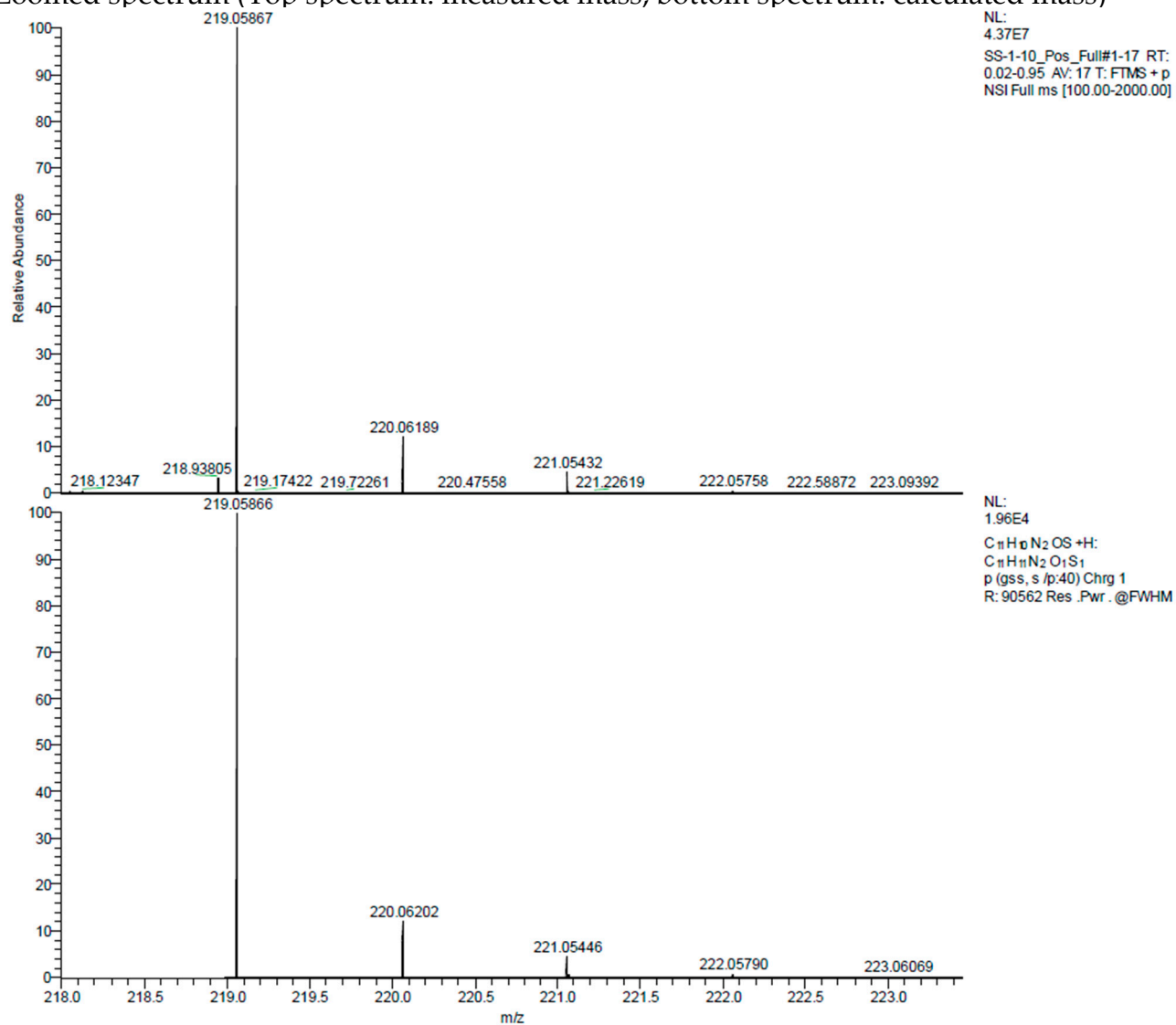
3-Cyclopropyl-2-mercaptoquinazolin-4(3H)-one (8a)

Full spectrum

SS-1-10_Pos_Full #1-17 RT: 0.02-0.95 AV: 17 NL: 4.37E7
T: FTMS + p NSI Full ms [100.00-2000.00]



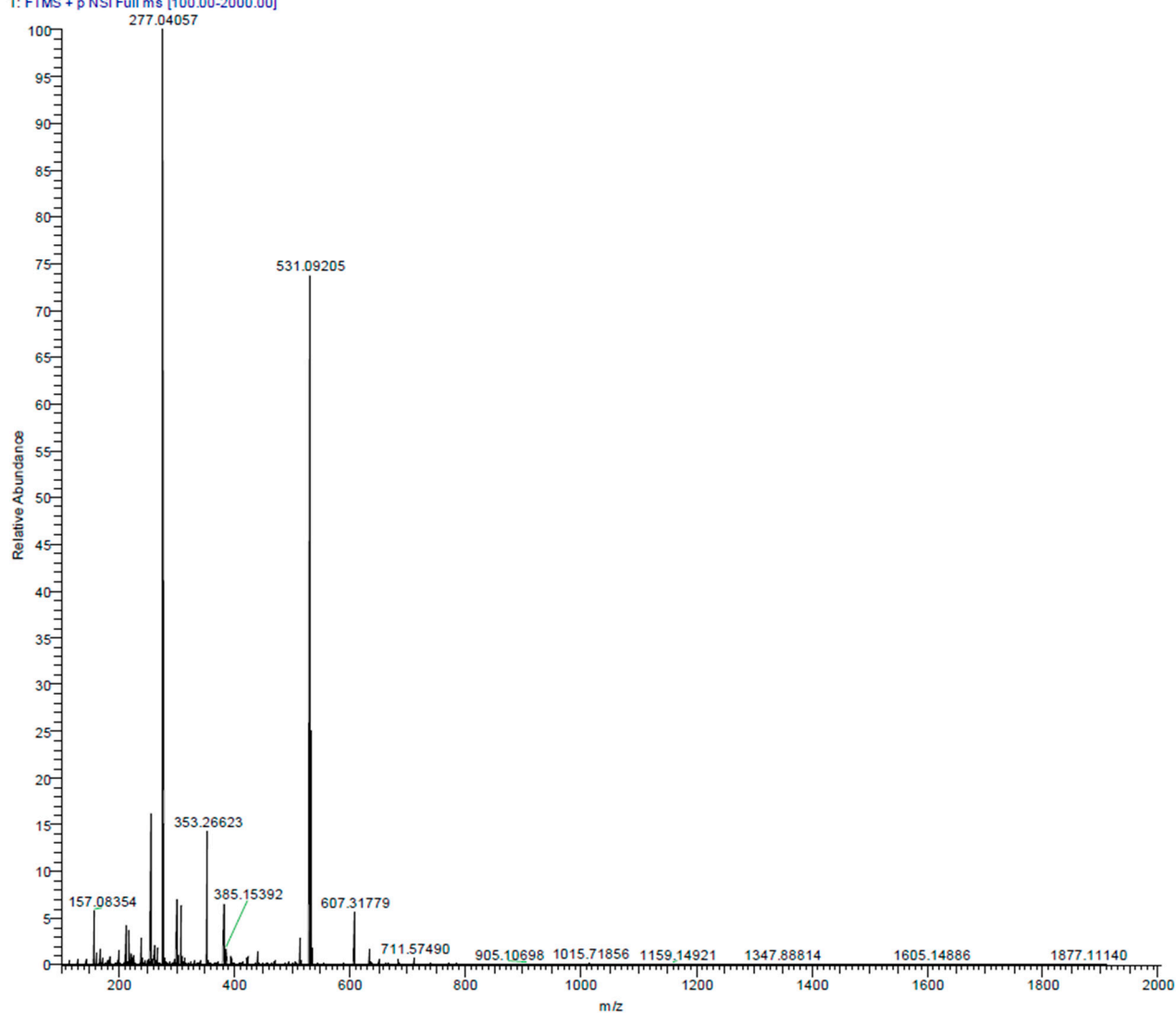
Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)



2-Mercapto-3-phenylquinazolin-4(3H)-one (8b)

Full spectrum

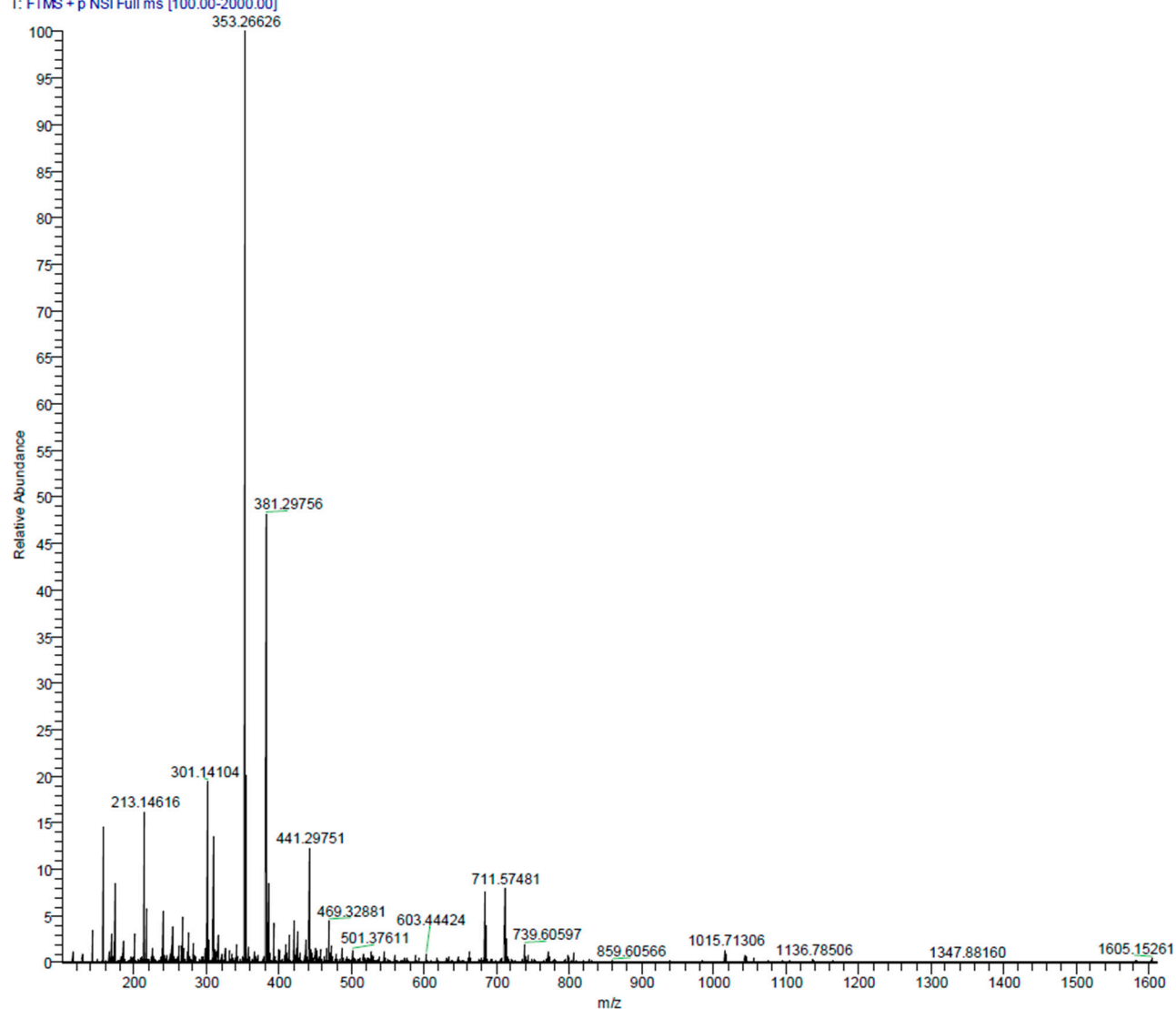
SS-1-14_Pos_Full #2-30 RT: 0.08-1.68 AV: 29 NL: 1.36E8
T: FTMS + p NSI Full ms [100.00-2000.00]



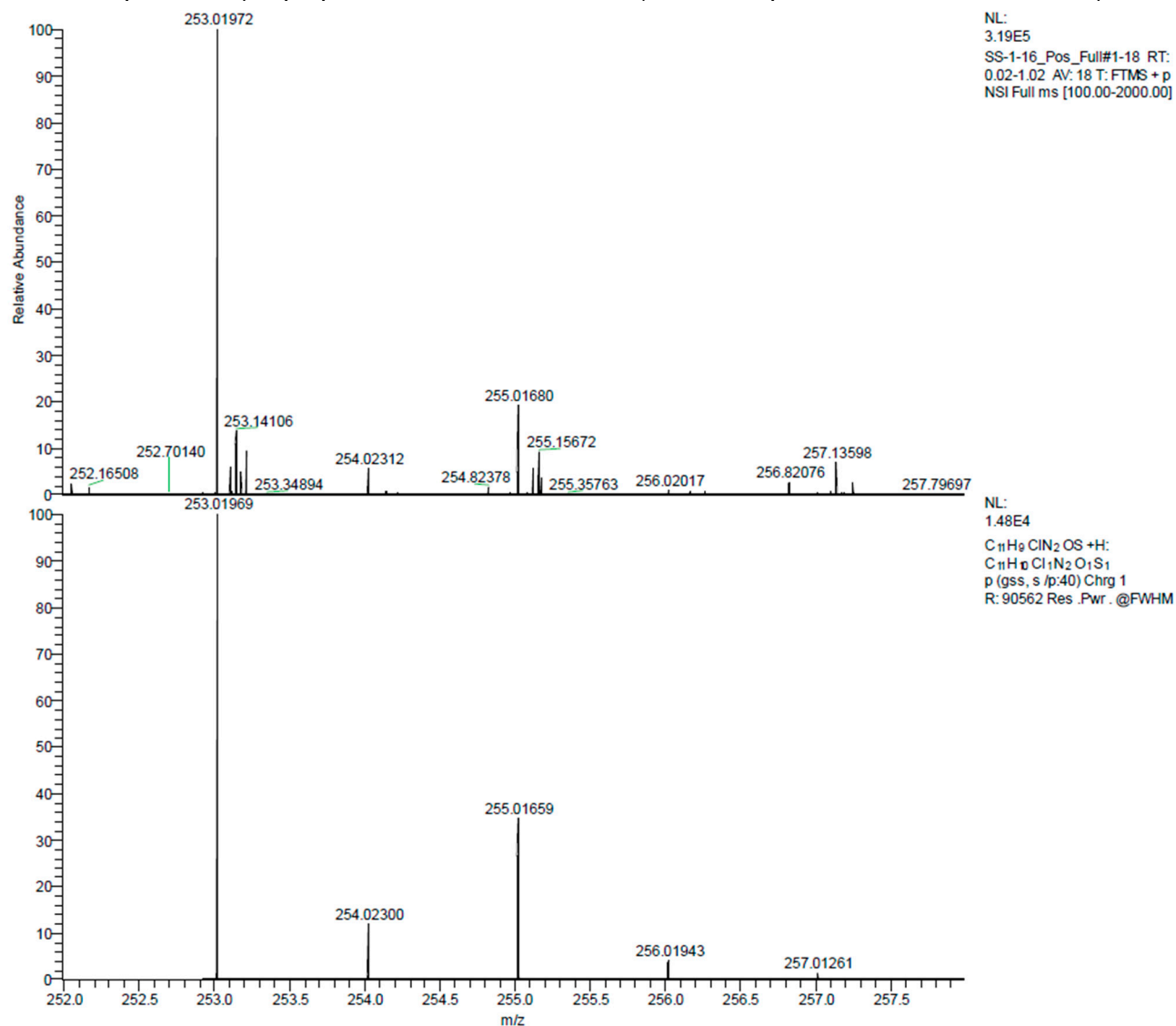
6-Chloro-3-cyclopropyl-2-mercaptoquinazolin-4(3H)-one (8c)

Full spectrum

SS-1-16_Pos_Full #1-18 RT: 0.02-1.02 AV: 18 NL: 8.41E6
T: FTMS + p NSI Full ms [100.00-2000.00]



Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)

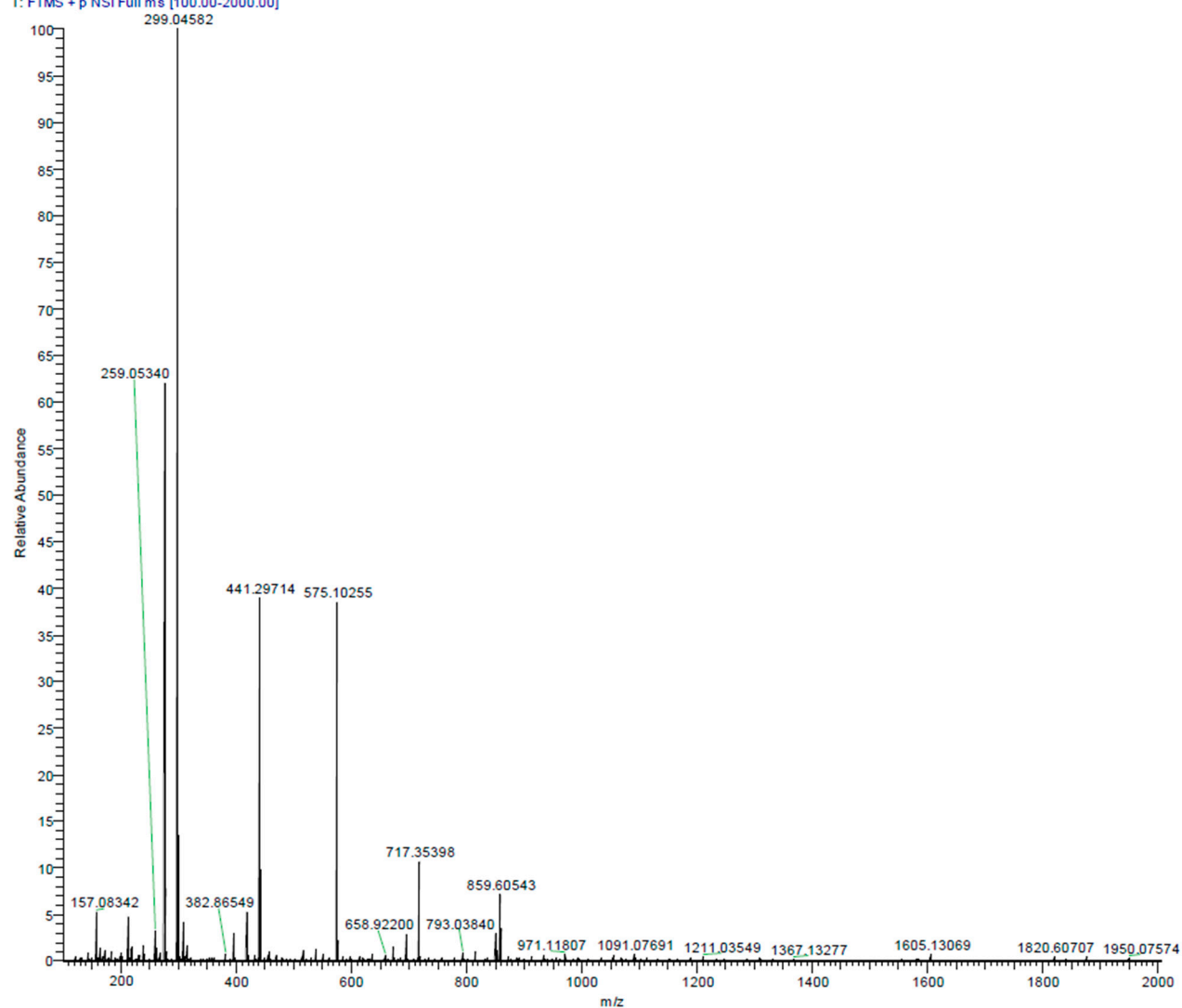


2-((3-Cyclopropyl-4-oxo-3,4-dihydroquinazolin-2-yl)thio)acetic acid (**9a**)

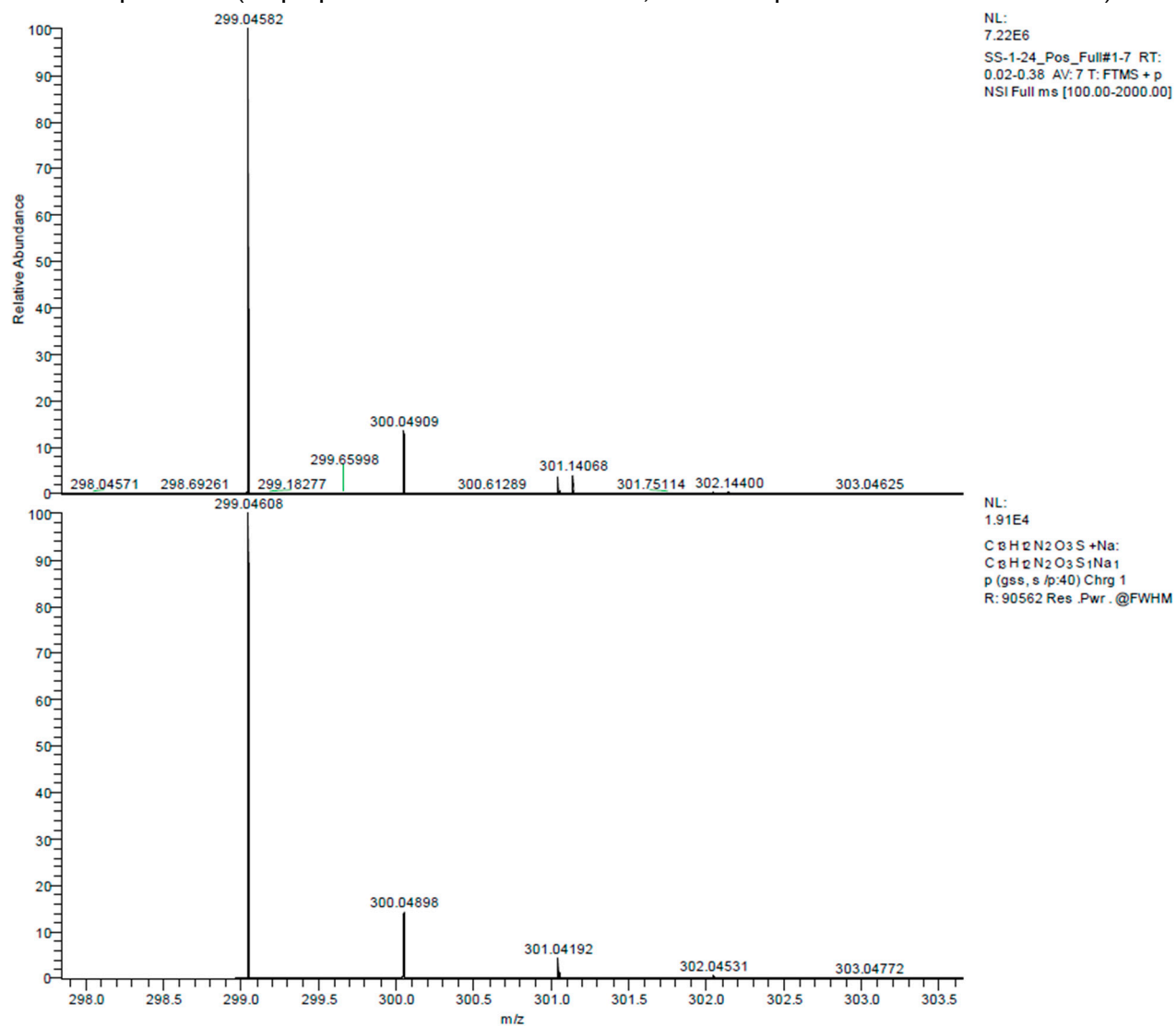
Full spectrum

SS-1-24_Pos_Full #1-7 RT: 0.02-0.38 AV: 7 NL: 7.22E6

T: FTMS + p NSI Full ms [100.00-2000.00]



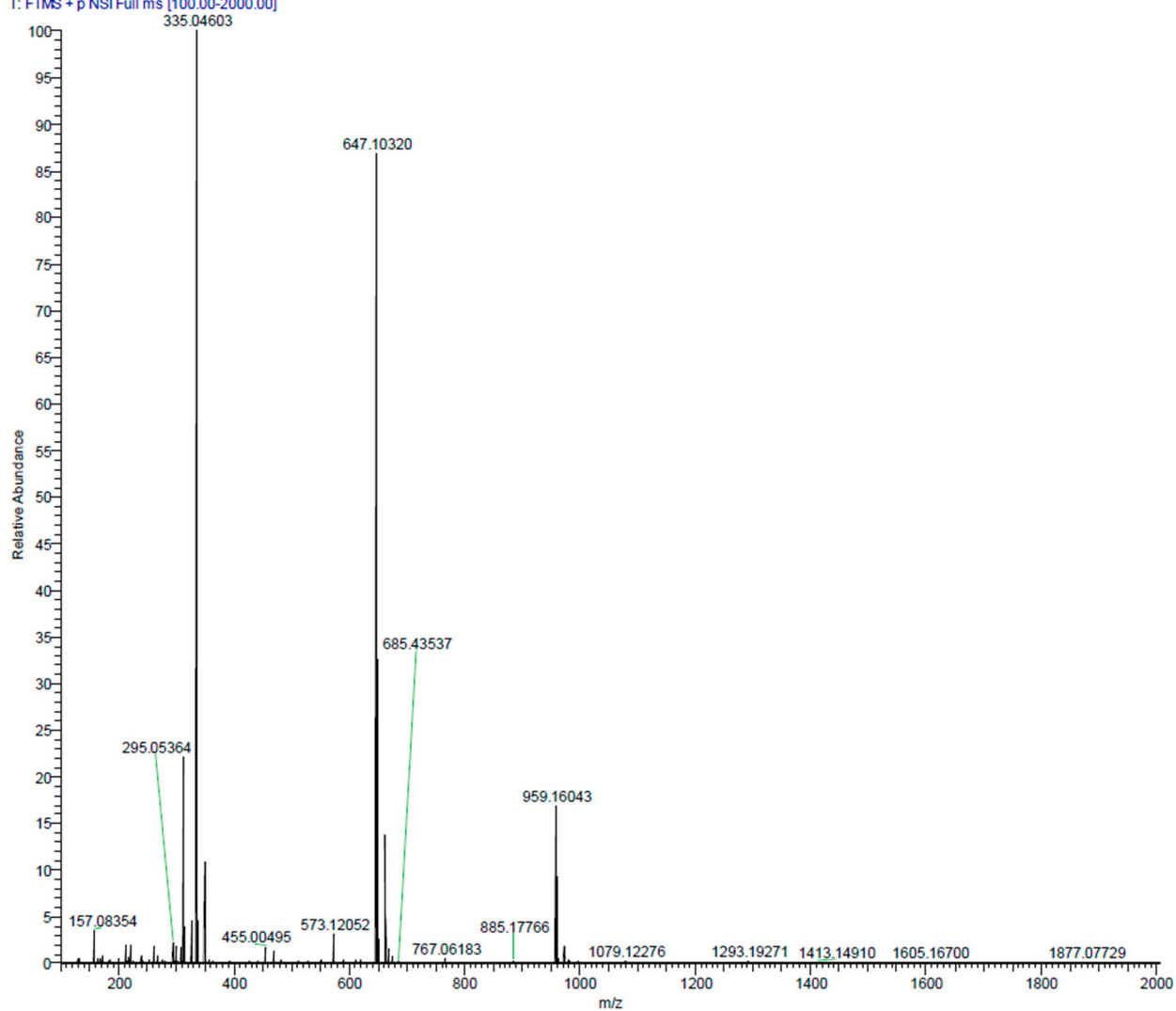
Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)



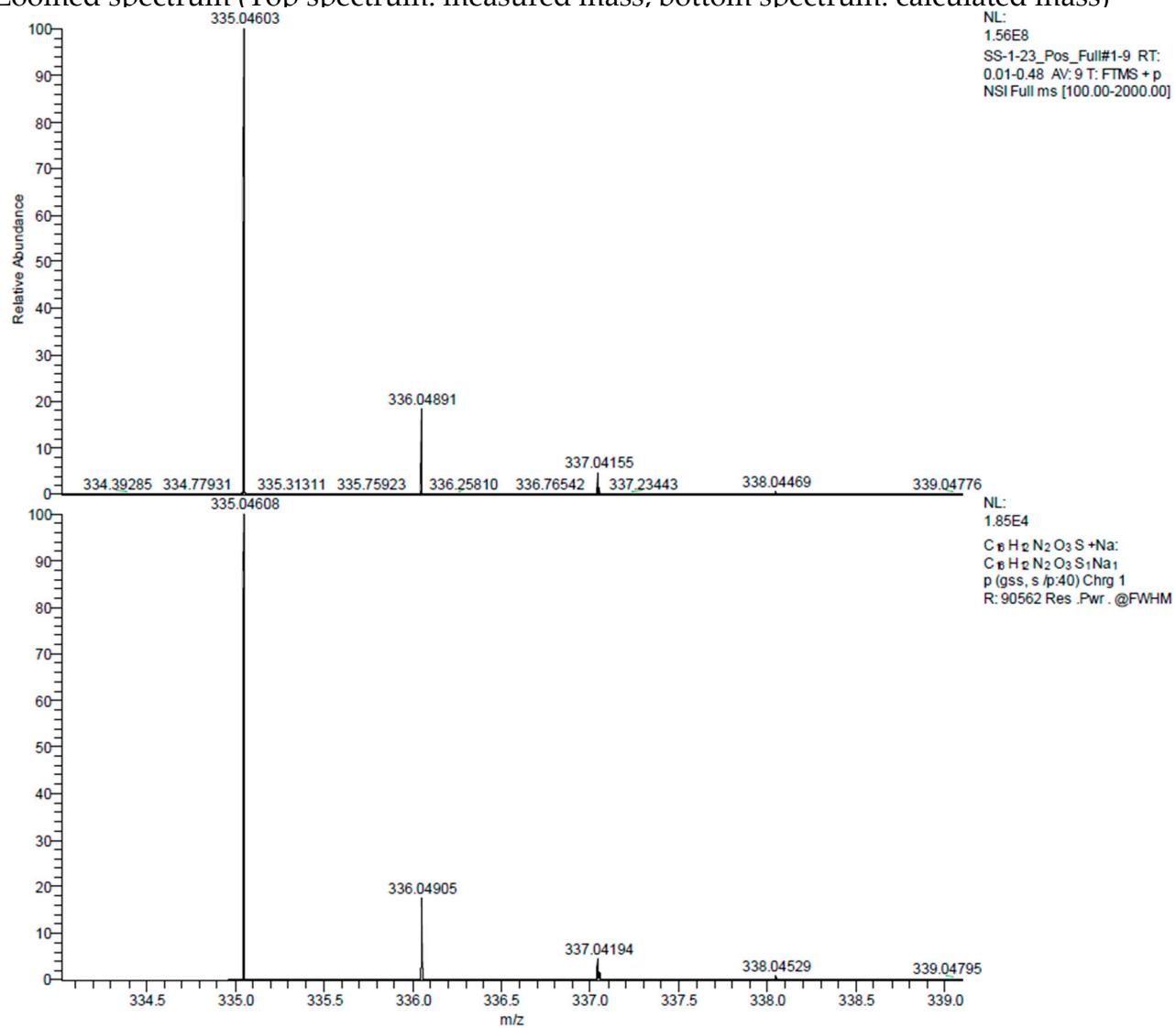
2-((4-Oxo-3-phenyl-3,4-dihydroquinazolin-2-yl)thio)acetic acid (**9b**)

Full spectrum

SS-1-23_Pos_Full #1-9 RT: 0.01-0.48 AV: 9 NL: 1.56E8
T: FTMS + p NSI Full ms [100.00-2000.00]



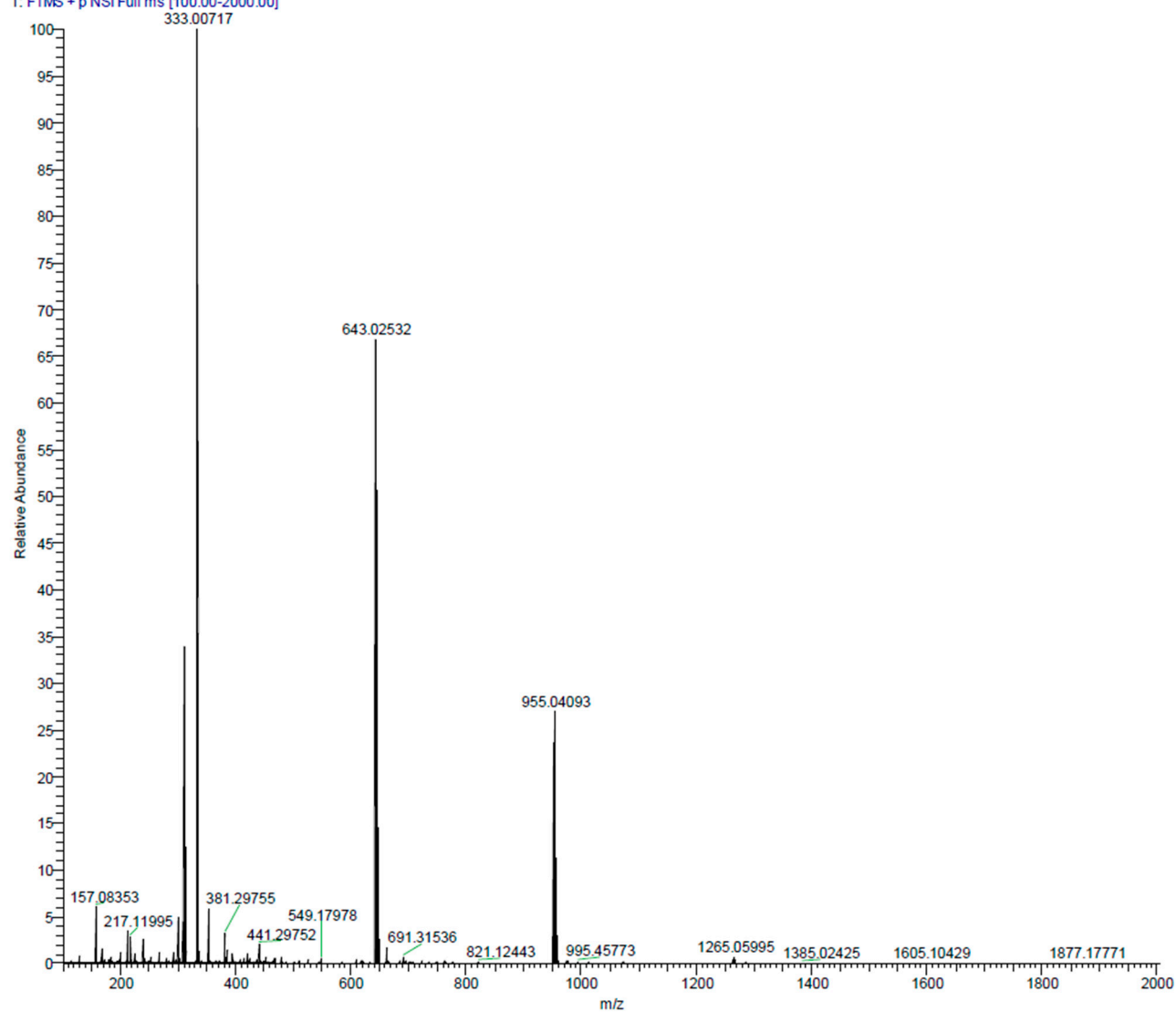
Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)



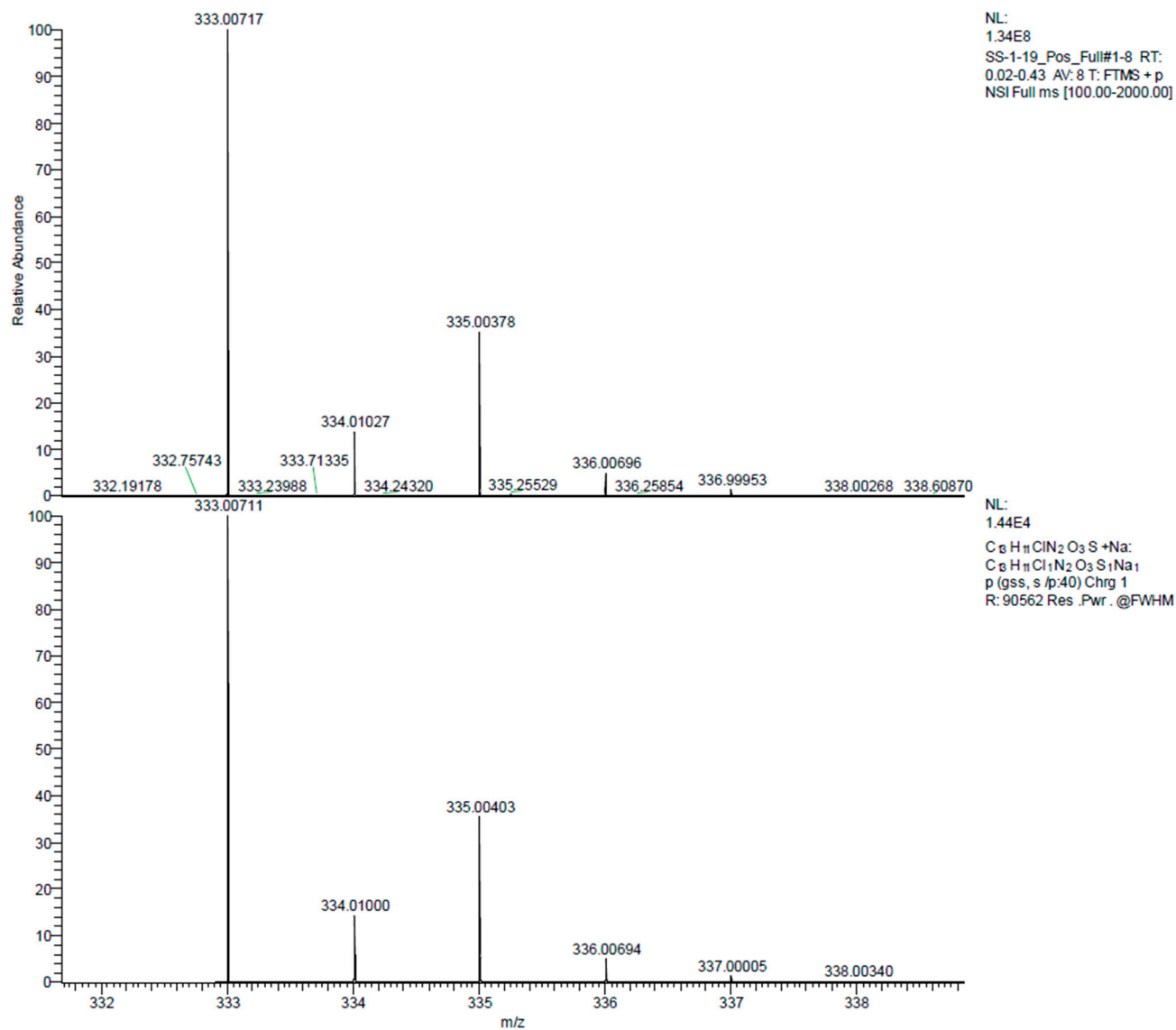
2-((6-Chloro-3-cyclopropyl-4-oxo-3,4-dihydroquinazolin-2-yl)thio)acetic acid (9c)

Full spectrum

SS-1-19_Pos_Full #1-8 RT: 0.02-0.43 AV: 8 NL: 1.34E8
T: FTMS + p NSI Full ms [100.00-2000.00]



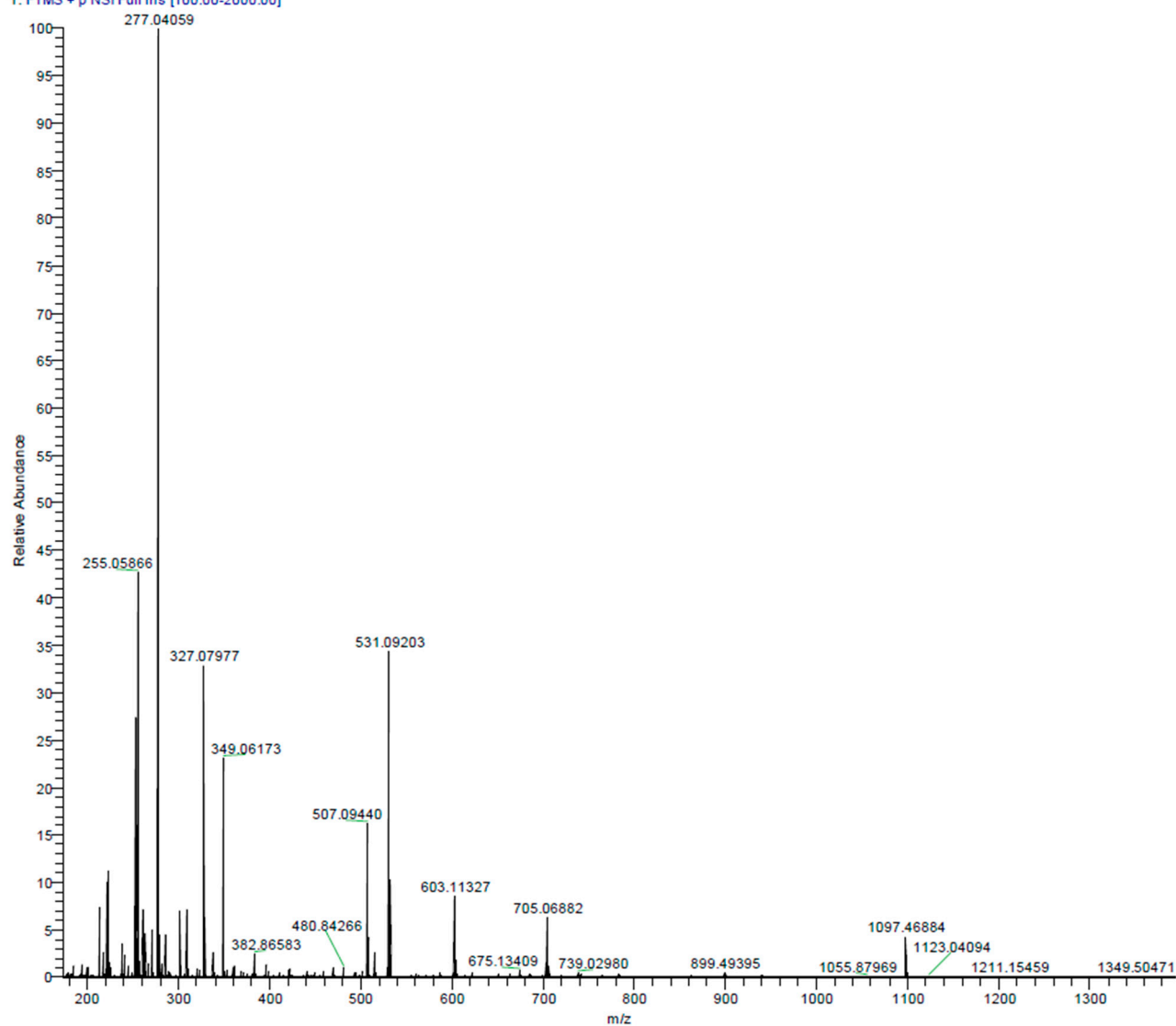
Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)



3-((4-Oxo-3-phenyl-3,4-dihydroquinazolin-2-yl)thio)propanoic acid (**9d**)

Full spectrum

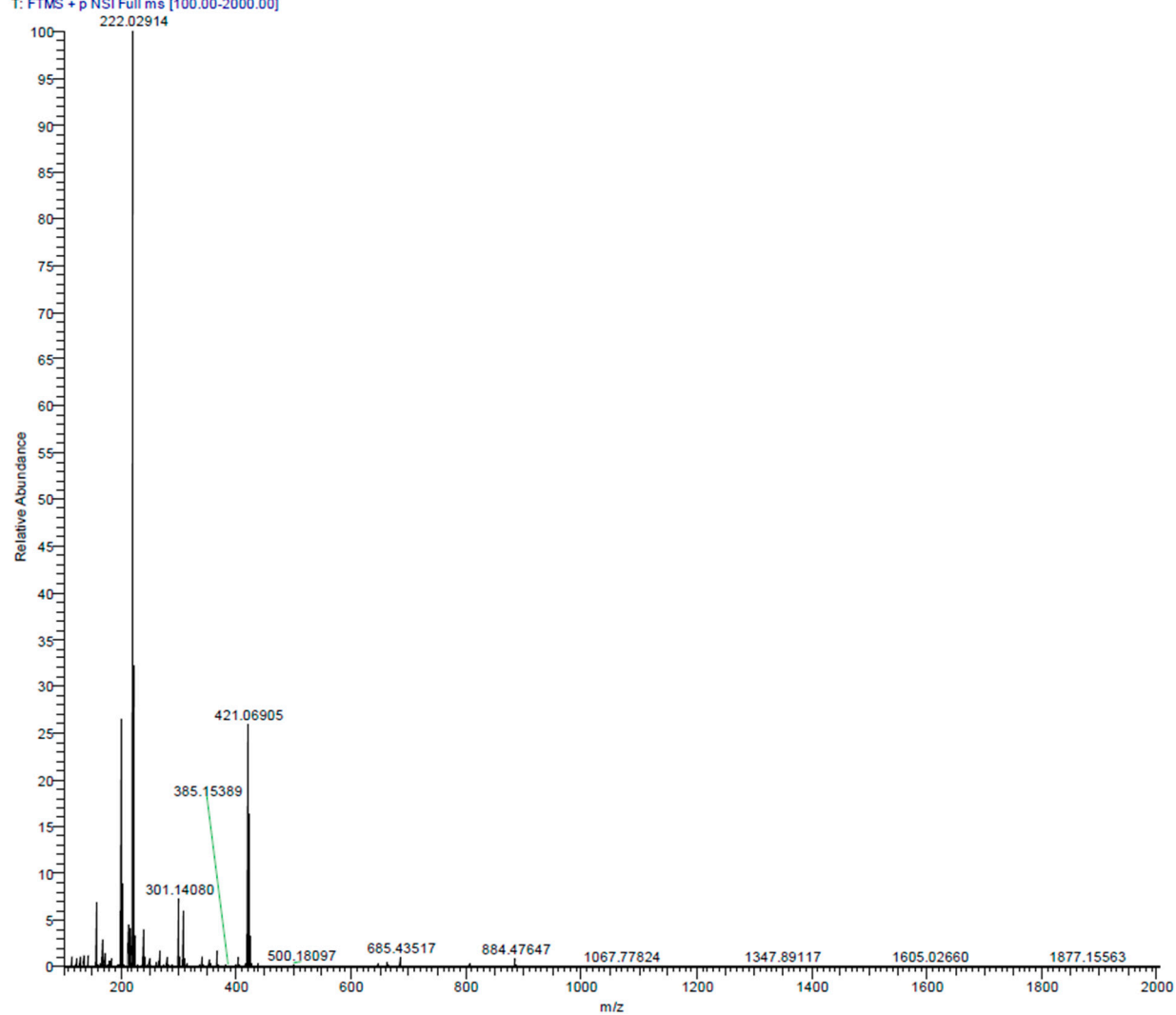
SS-1-31_Pos_Full#1-18 RT: 0.02-1.02 AV: 18 NL: 2.52E7
T: FTMS + p NSI Full ms [100.00-2000.00]



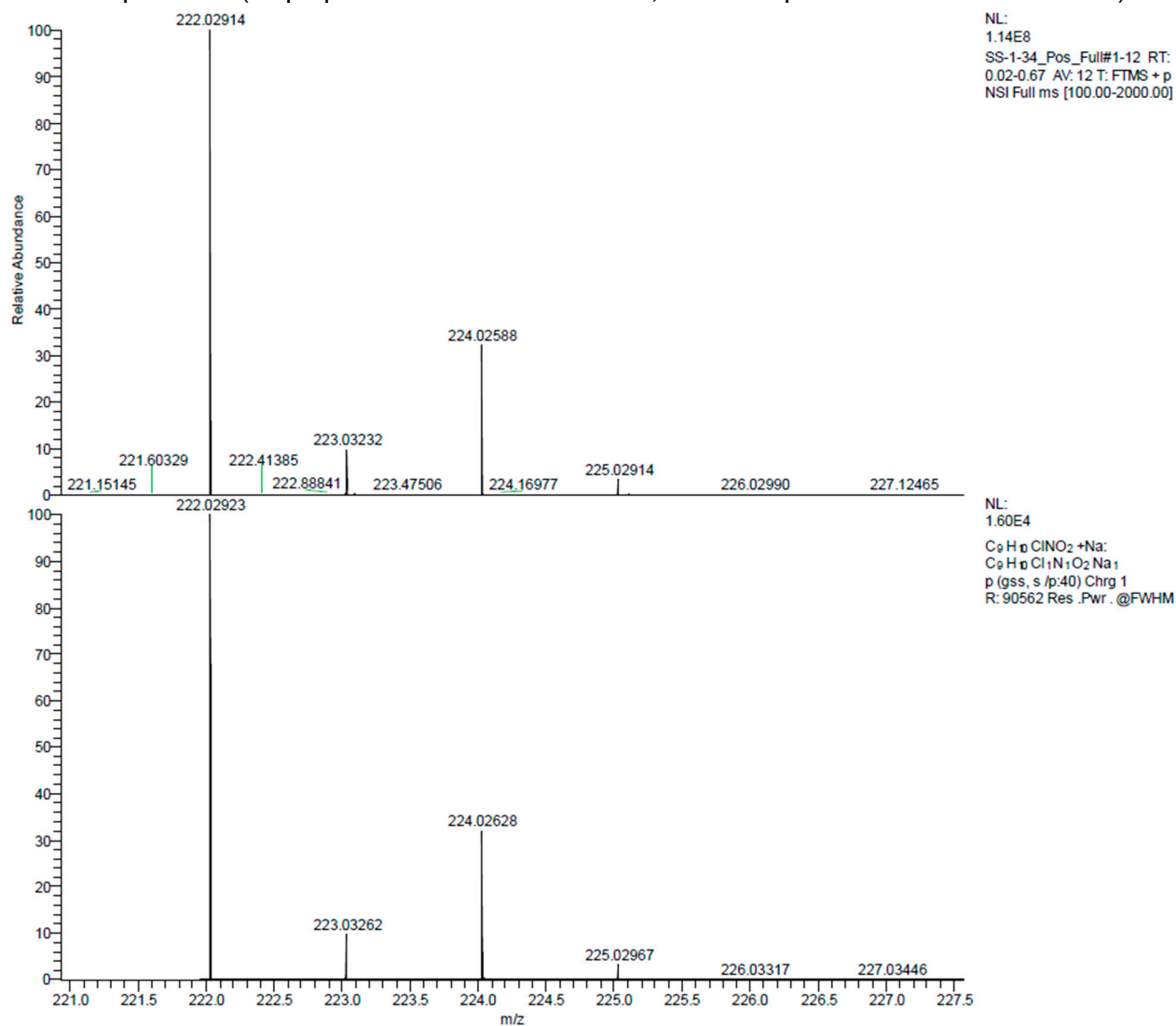
2-Chloro-*N*-(4-methoxyphenyl)acetamide (**12**)

Full spectrum

SS-1-34_Pos_Full #1-12 RT: 0.02-0.67 AV: 12 NL: 1.14E8
T: FTMS + p NSI Full ms [100.00-2000.00]



Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)

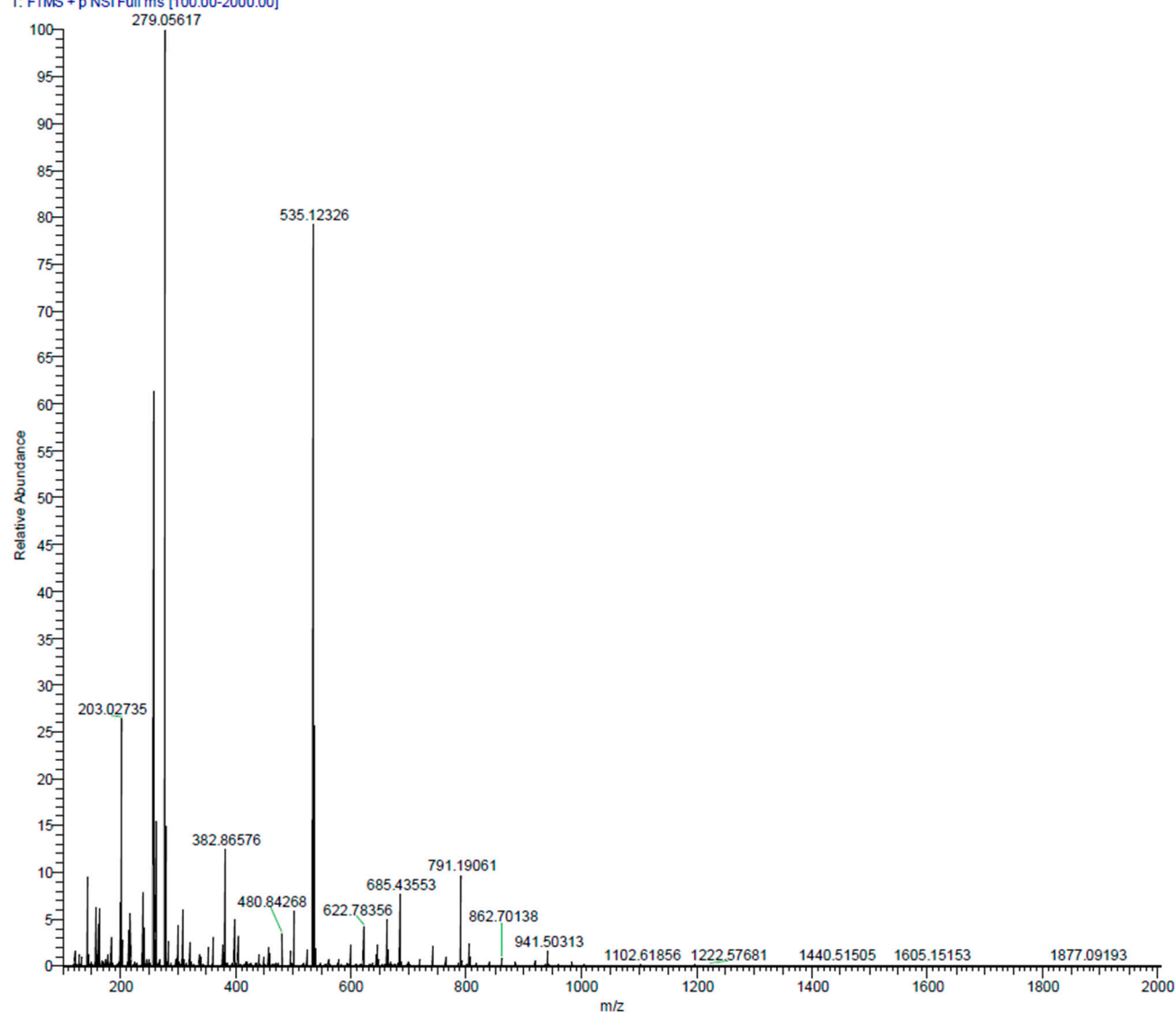


3-Cyclopropyl-2-(prop-2-yn-1-ylthio)quinazolin-4(3*H*)-one (**13a**)

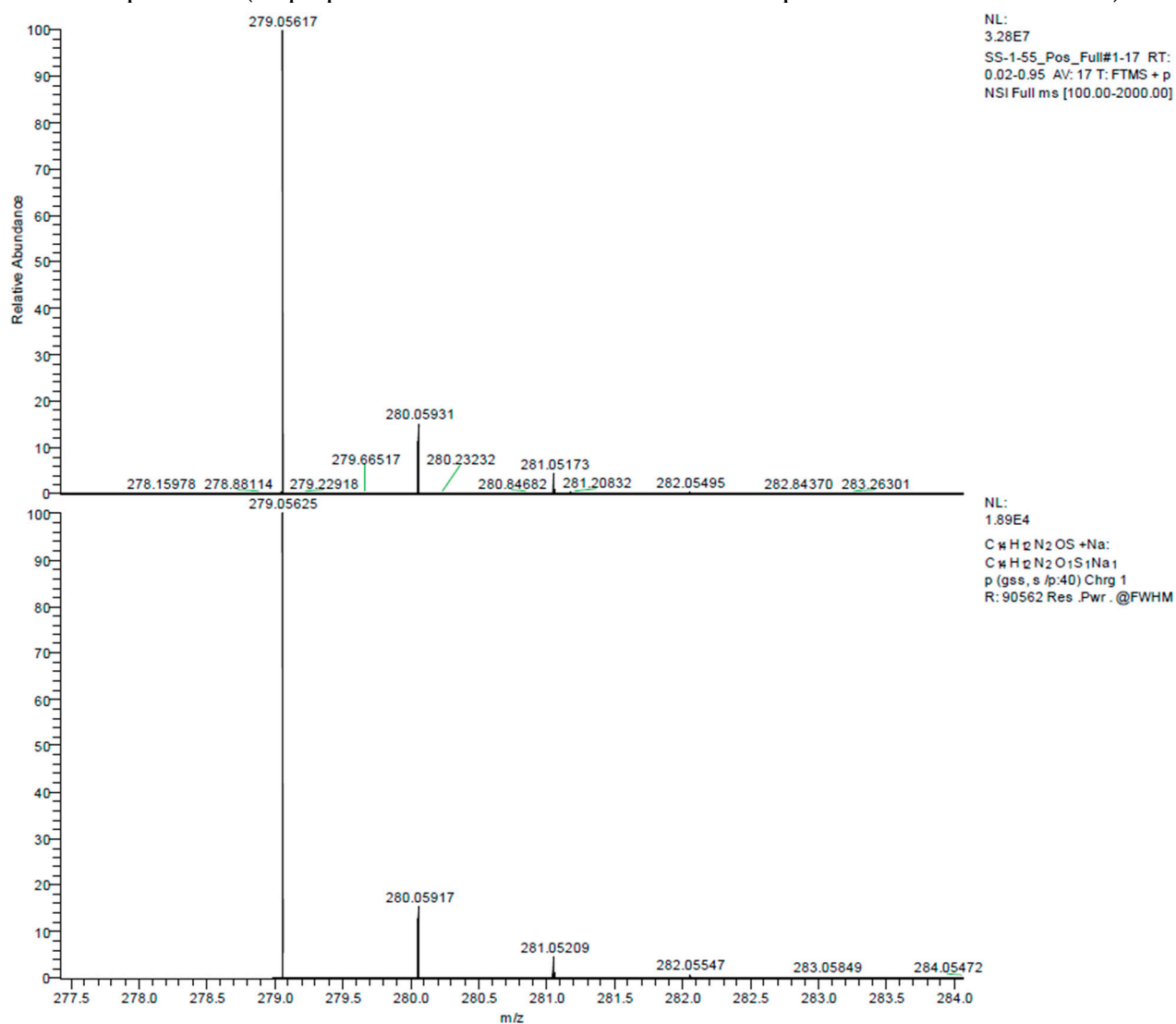
Full spectrum

SS-1-55_Pos_Full #1-17 RT: 0.02-0.95 AV: 17 NL: 3.28E7

T: FTMS + p NSI Full ms [100.00-2000.00]



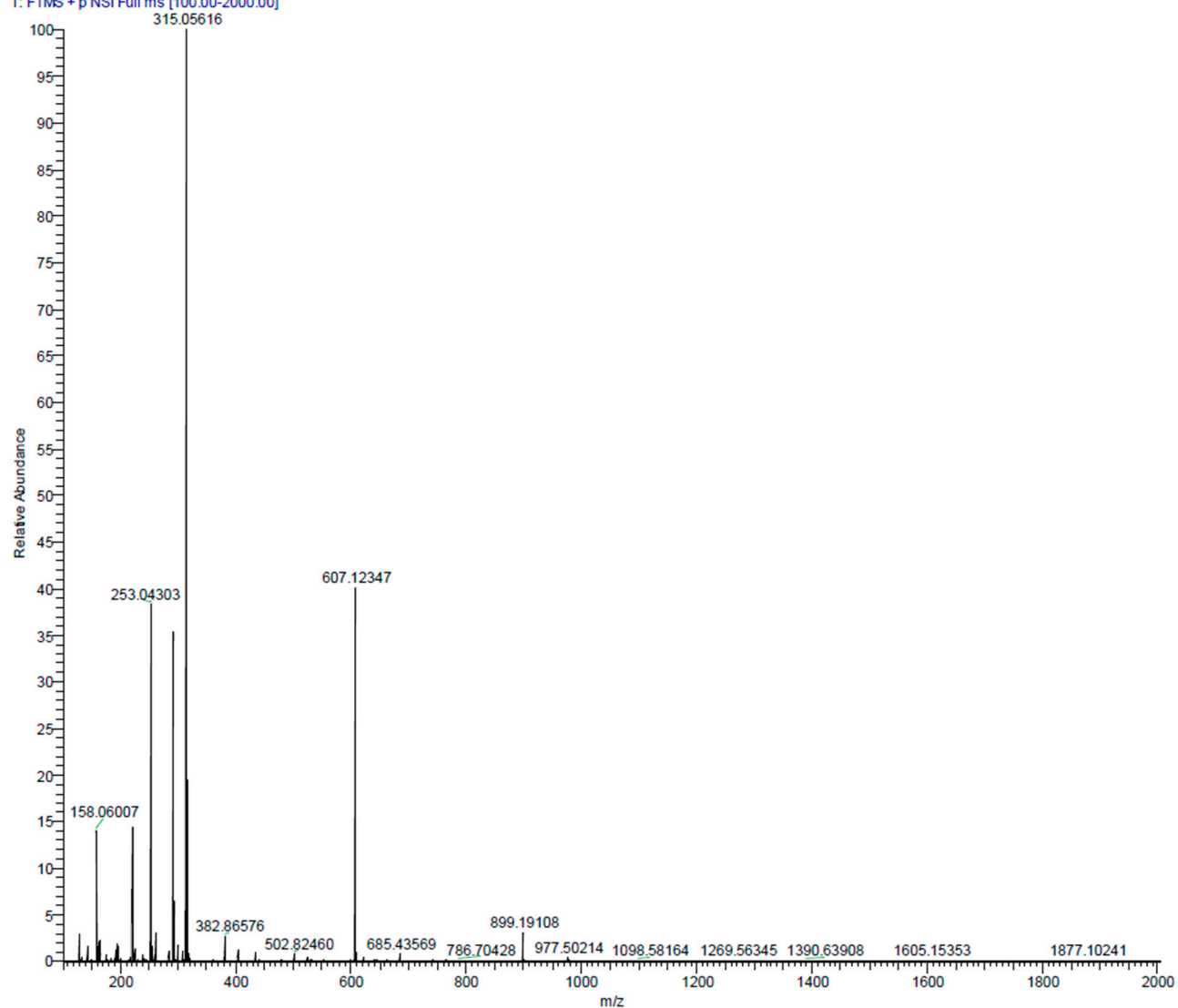
Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)



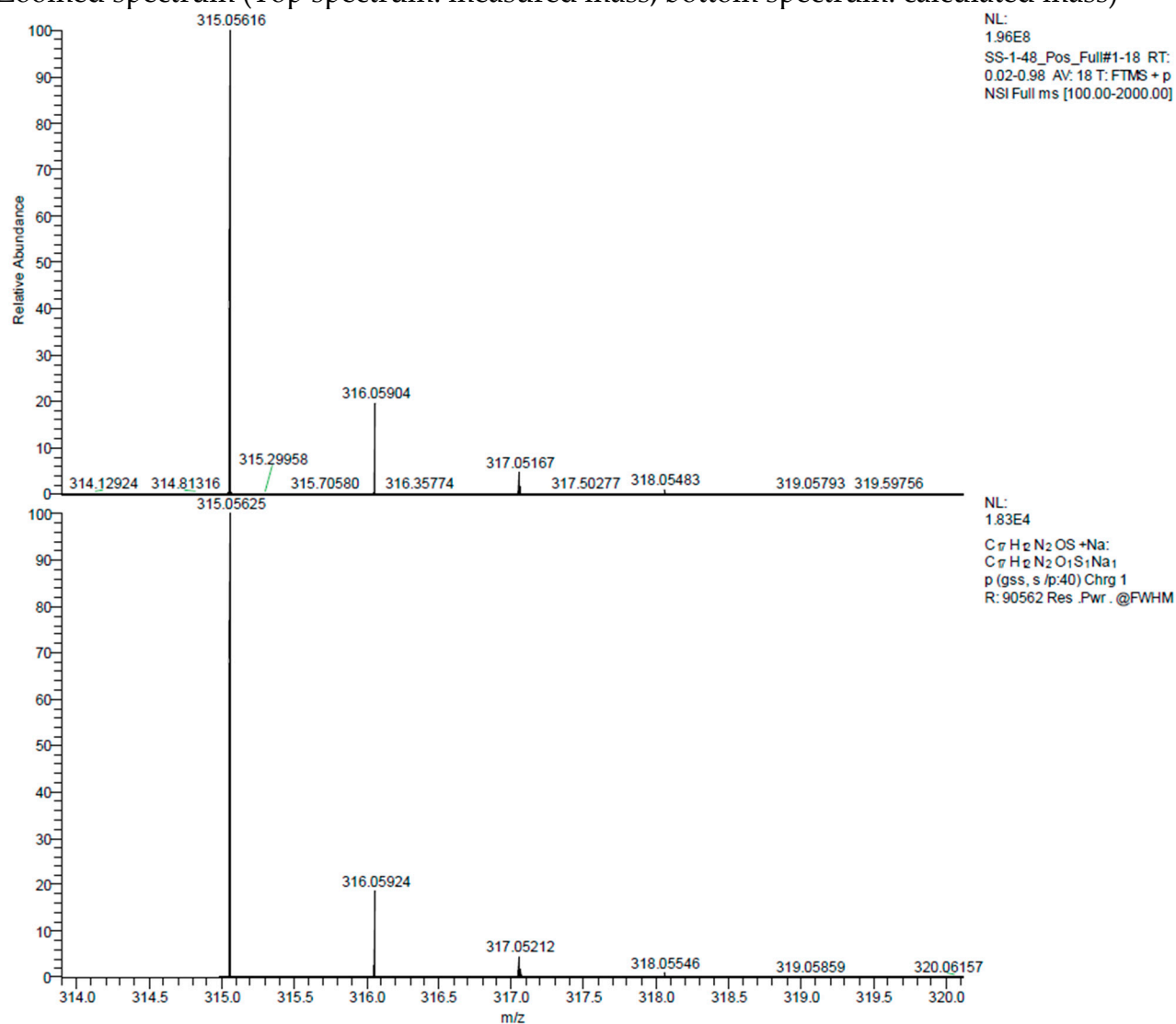
3-Phenyl-2-(prop-2-yn-1-ylthio)quinazolin-4(3H)-one (**13b**)

Full spectrum

SS-1-48_Pos_Full #1-18 RT: 0.02-0.98 AV: 18 NL: 1.96E8
T: FTMS + p NSI Full ms [100.00-2000.00]



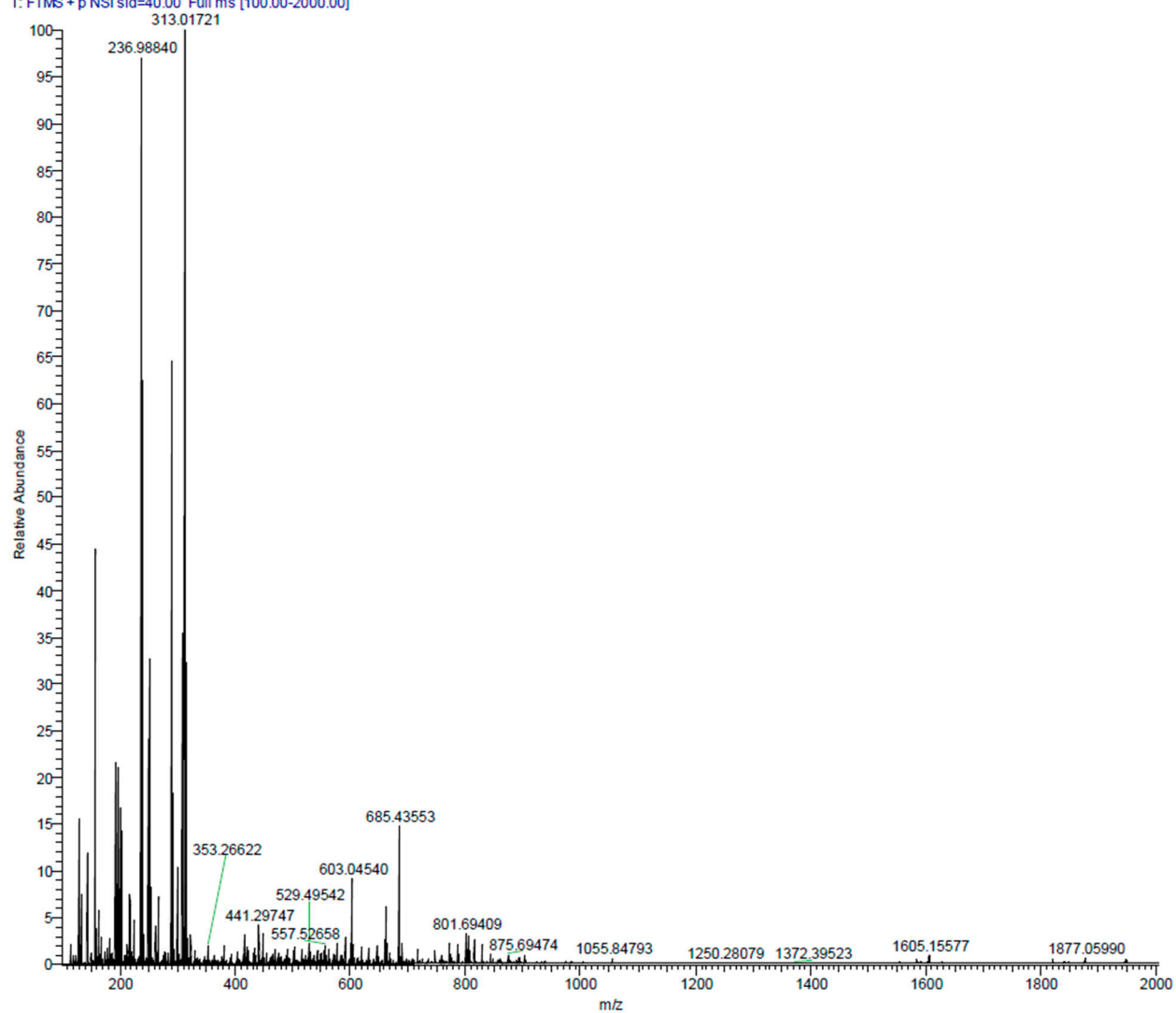
Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)



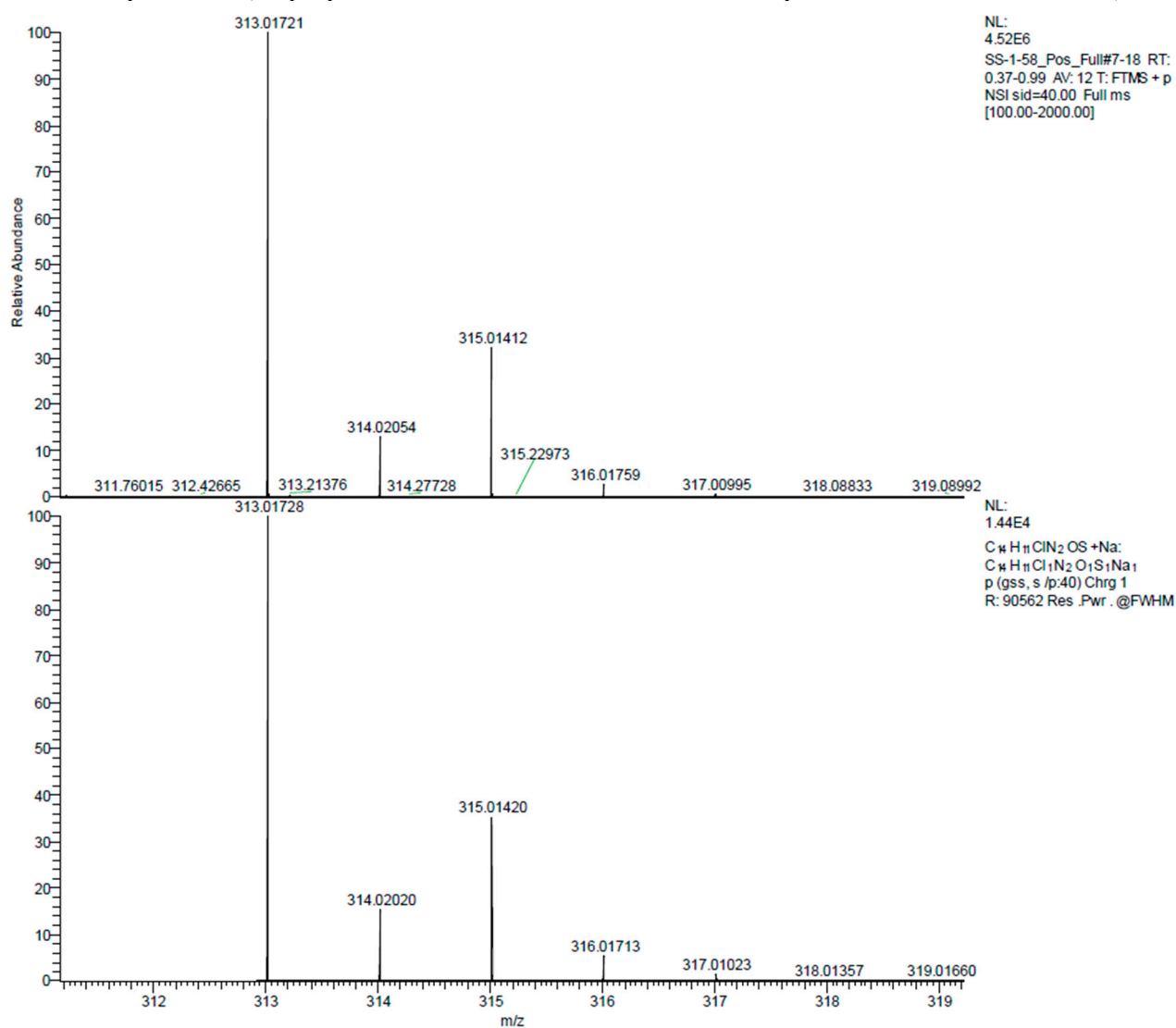
6-Chloro-3-cyclopropyl-2-(prop-2-yn-1-ylthio)quinazolin-4(3*H*)-one (**13c**)

Full spectrum

SS-1-58_Pos_Full #7-18 RT: 0.37-0.99 AV: 12 NL: 4.52E6
T: FTMS + p NSI sid=40.00 Full ms [100.00-2000.00]



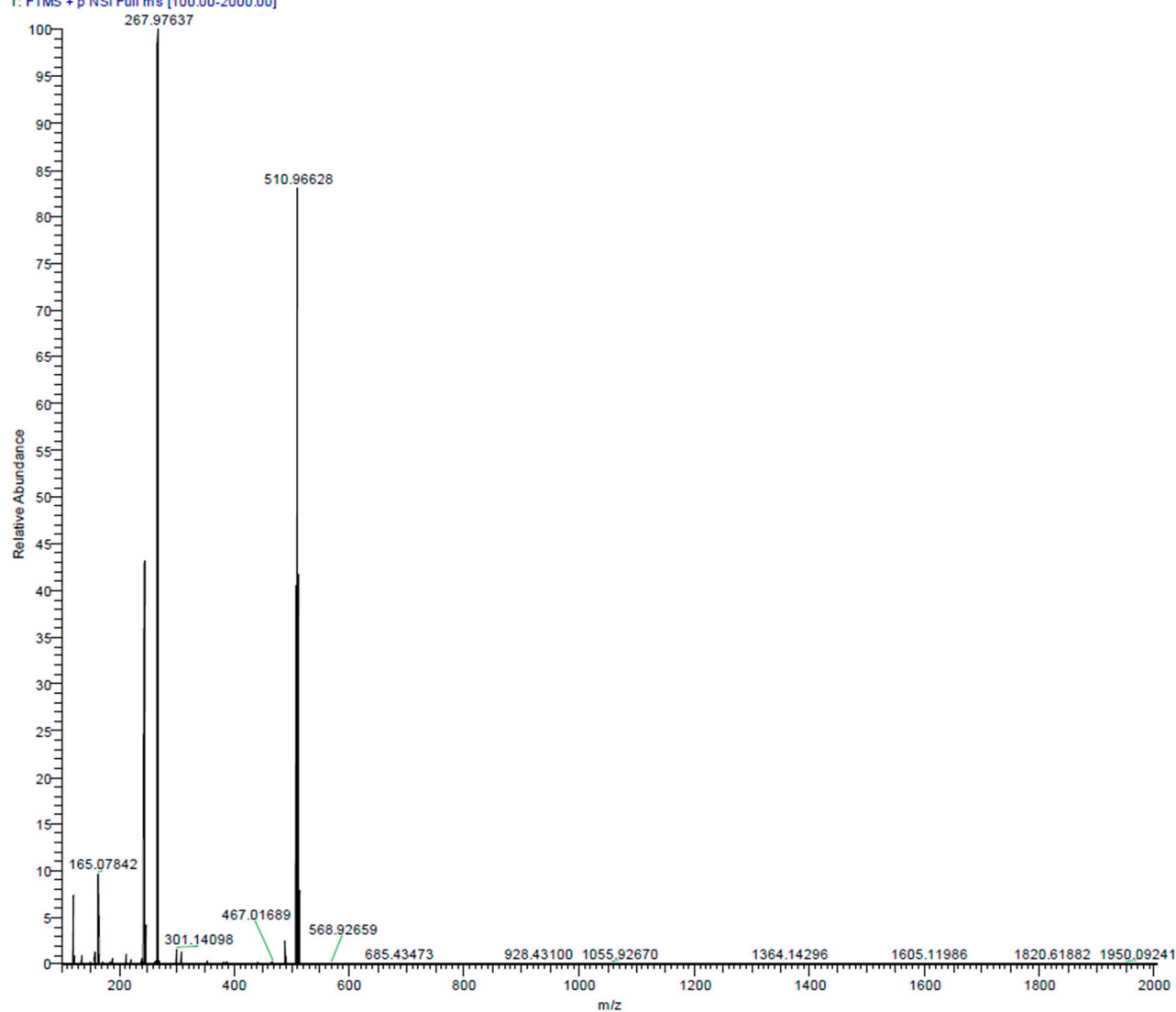
Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)



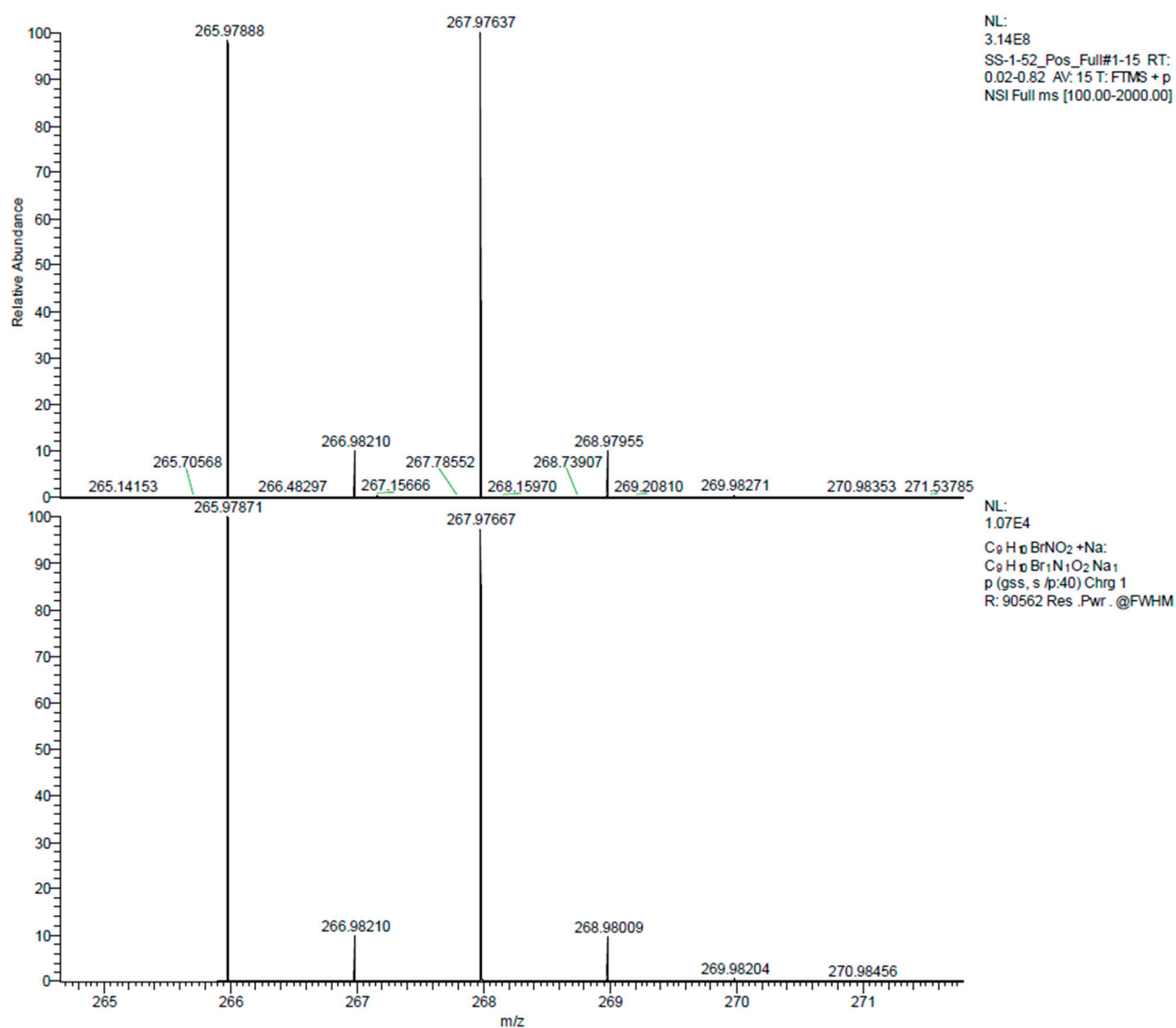
2-Bromo-*N*-(4-methoxyphenyl)acetamide (**15a**)

Full spectrum

SS-1-52_Pos_Full #1-15 RT: 0.02-0.82 AV: 15 NL: 3.14E8
T: FTMS + p NSI Full ms [100.00-2000.00]



Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)

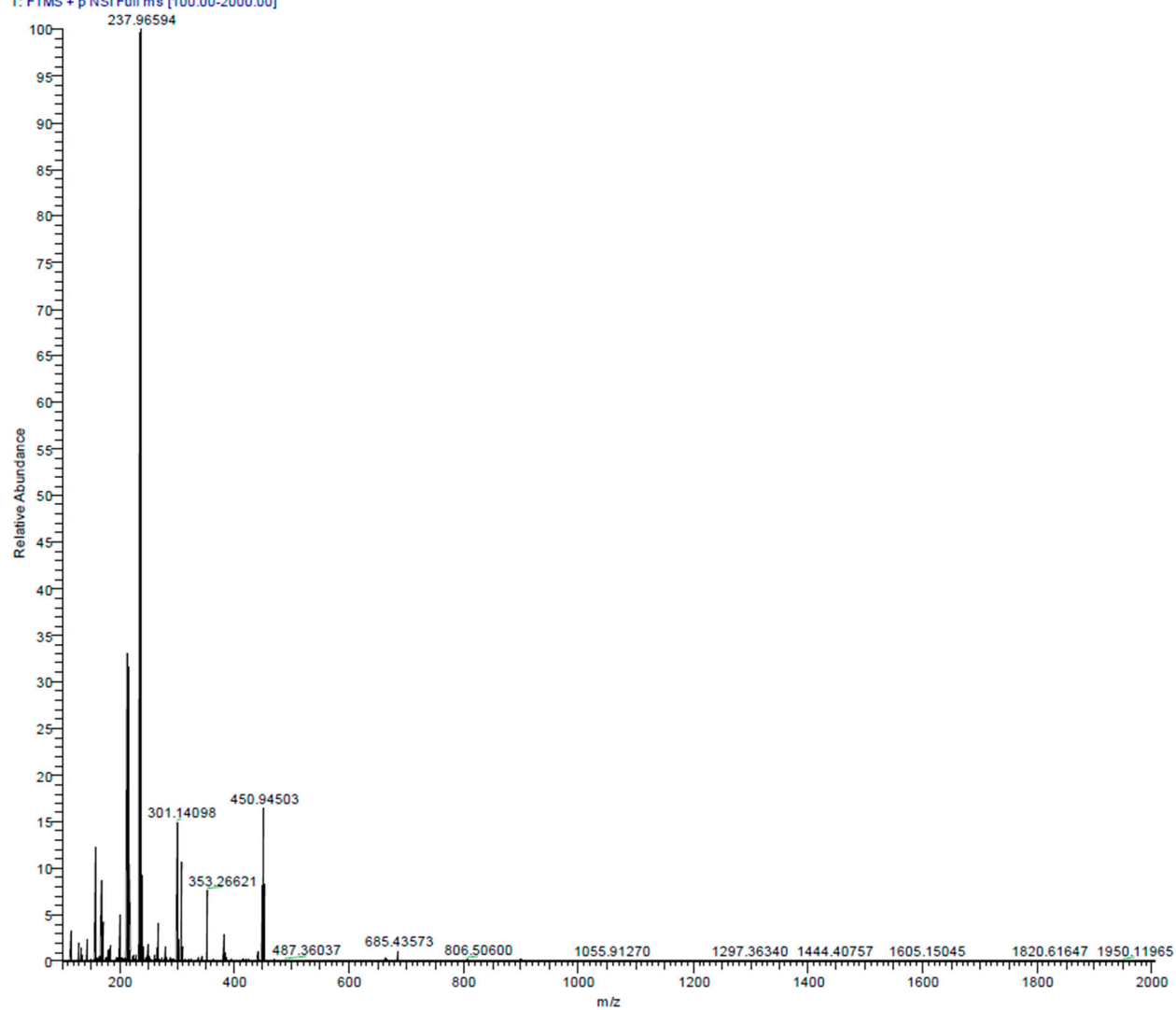


2-Bromo-*N*-phenylacetamide (**15b**)

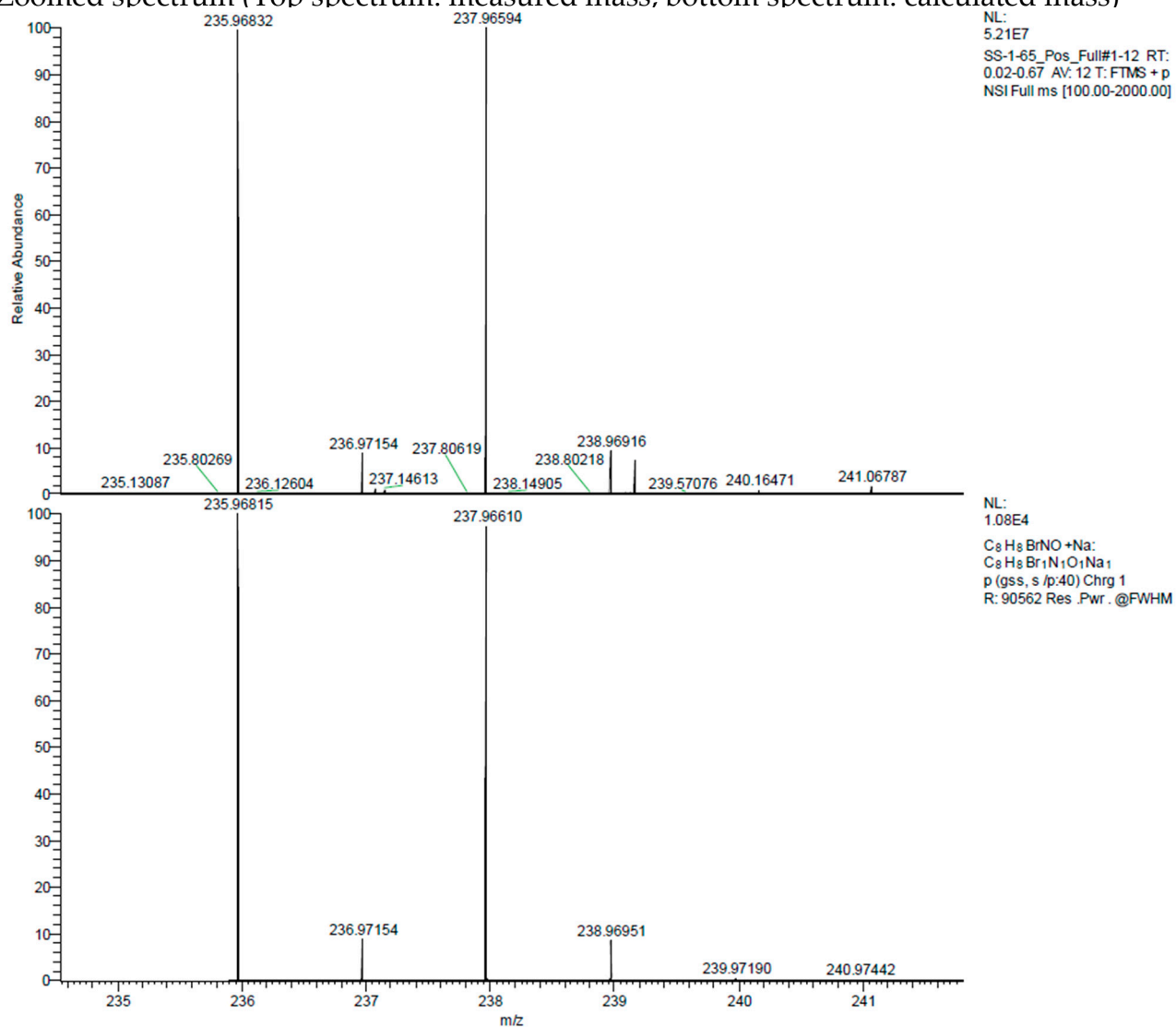
Full spectrum

SS-1-65_Pos_Full #1-12 RT: 0.02-0.67 AV: 12 NL: 5.21E7

T: FTMS + p NSI Full ms [100.00-2000.00]



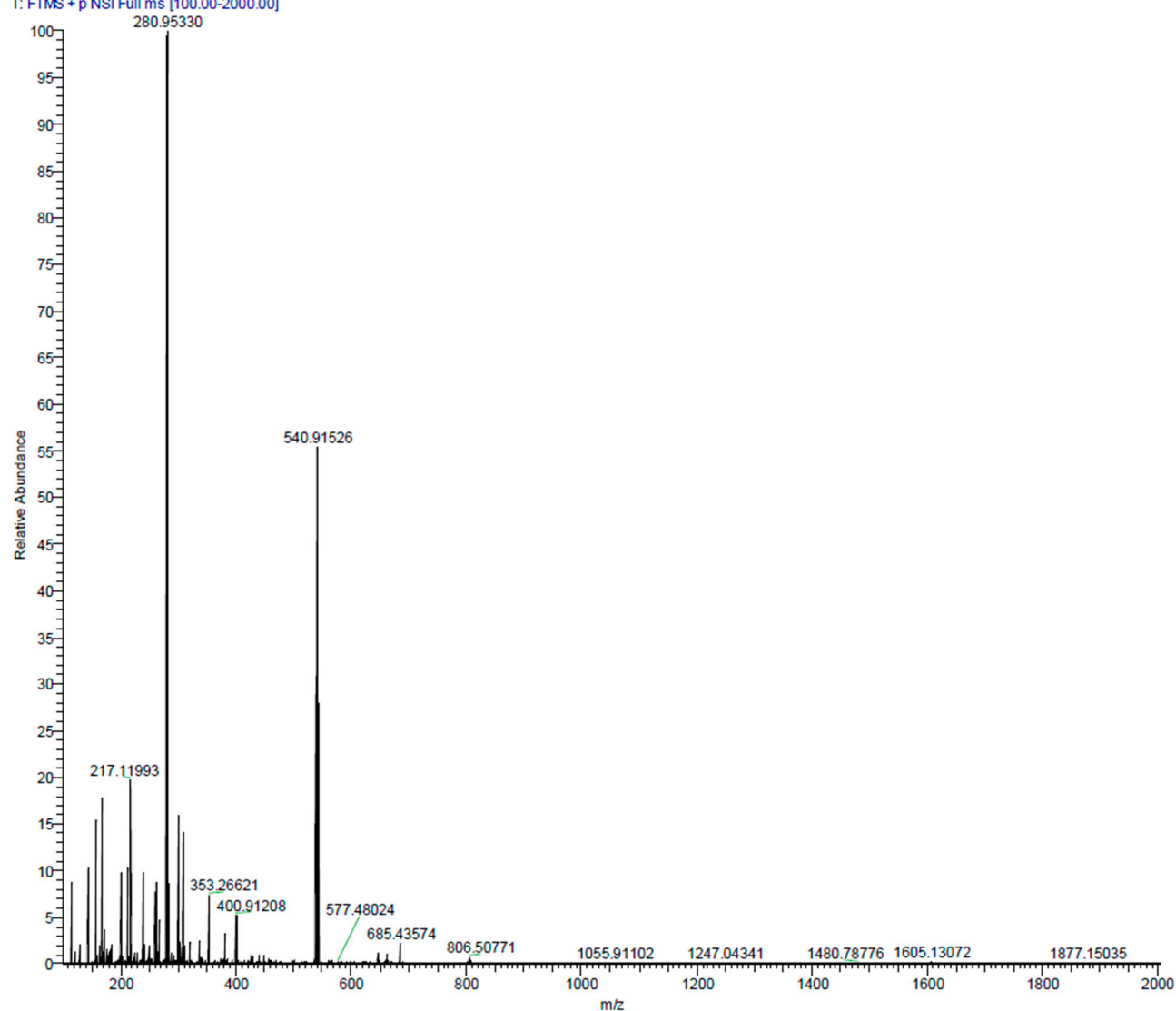
Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)



2-Bromo-N-(4-nitrophenyl)acetamide (**15c**)

Full spectrum

SS-1-67_Pos_Full #1-11 RT: 0.02-0.61 AV: 11 NL: 2.75E7
T: FTMS + p NSI Full ms [100.00-2000.00]



Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)

