

## SUPPORTING INFORMATION

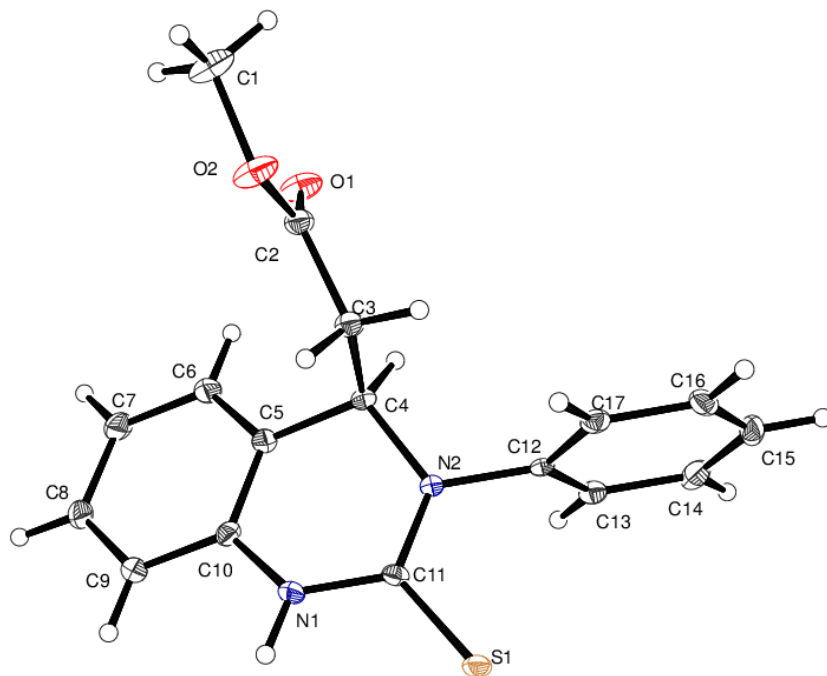
### **Pd-catalyzed Heck-conjoined amidation and concomitant chemoselective Michael-addition: An efficient tandem approach to highly functionalized tetrahydroquinazolines from *o*-haloanilines**

Rakesh K. Saunthwal<sup>†</sup>, Monika Patel<sup>†</sup>, Abhinandan K. Danodia,<sup>†</sup> and Akhilesh K. Verma<sup>†\*</sup>

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S.No	Table of contents	Page
1	X-ray crystallographic studies	2-3
2	References	4-4
3	Copies of <sup>1</sup> H, <sup>13</sup> C NMR, HRMS and chiral HPLC spectra	5-96

# X-Ray Crystallographic Studies



**Figure I.** ORTEP structure of compound **4a**

The intensity data for **4a** was collected on an Oxford Xcalibur CCD diffractometer equipped with graphite monochromatic Mo-K $\alpha$  radiation ( $\lambda = 0.71073 \text{ \AA}$ ) at 293(2) K<sup>2</sup>. A multi-scan correction was applied. The structure was solved by the direct methods using SIR-92 and refined by full-matrix least-squares refinement techniques on  $F^2$  using SHELXL97<sup>3</sup>. The hydrogen atoms were placed into the calculated positions and included in the last cycles of the refinement. All calculations were done using Wingx software package<sup>4</sup>.

**Table I.** Crystallographic data and structure refinement for compounds **4a**.

Empirical formula	C <sub>17</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub> S
Formula weight	312.38
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	<i>P</i> 2 <sub>1</sub> / <i>n</i>
<i>A</i>	9.751(5) Å
<i>B</i>	18.905(5) Å
<i>C</i>	16.646(5) Å
∠	90°
∠	92.408°
∠	90°
Volume	3066(2) Å <sup>3</sup>
<i>Z</i>	8
Density (calculated)	1.354 Mg/m <sup>3</sup>
Absorption coefficient	0.220 mm <sup>-1</sup>
<i>F</i> (000)	1312
Crystal size	0.25 x 0.23 x 0.20 mm <sup>3</sup>
Theta range for data collection	2.15 to 24.99°
Index ranges	-11 ≤ <i>h</i> ≤ 11, -17 ≤ <i>k</i> ≤ 22, -19 ≤ <i>l</i> ≤ 19
Reflections collected	20532
Independent reflections	5414 [ <i>R</i> (int) = 0.0456]
Data completeness	100 %
Absorption correction	Multi-scan
Max. and min. transmission	0.9574 and 0.9471
Refinement method	Full-matrix least-squares on <i>F</i> <sup>2</sup>
Data / restraints / parameters	5414 / 0 / 413
Goodness-of-fit on <i>F</i> <sup>2</sup>	1.033
Final <i>R</i> indices [ <i>I</i> > 2σ( <i>I</i> )] <sup>a, b</sup>	<i>R</i> <sub>1</sub> = 0.0418, <i>wR</i> <sub>2</sub> = 0.0958
<i>R</i> indices (all data)	<i>R</i> <sub>1</sub> = 0.0602, <i>wR</i> <sub>2</sub> = 0.1018
Largest diff. peak and hole	0.376 and -0.266 e.Å <sup>-3</sup>

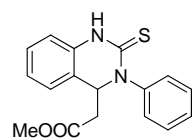
$$^a R = \sum(|F_o| - |F_c|) / \sum |F_o|; ^b R_w = \{\sum[w(F_o^2 - F_c^2)^2] / \sum[w(F_o^2)^2]\}^{1/2}$$

## References:

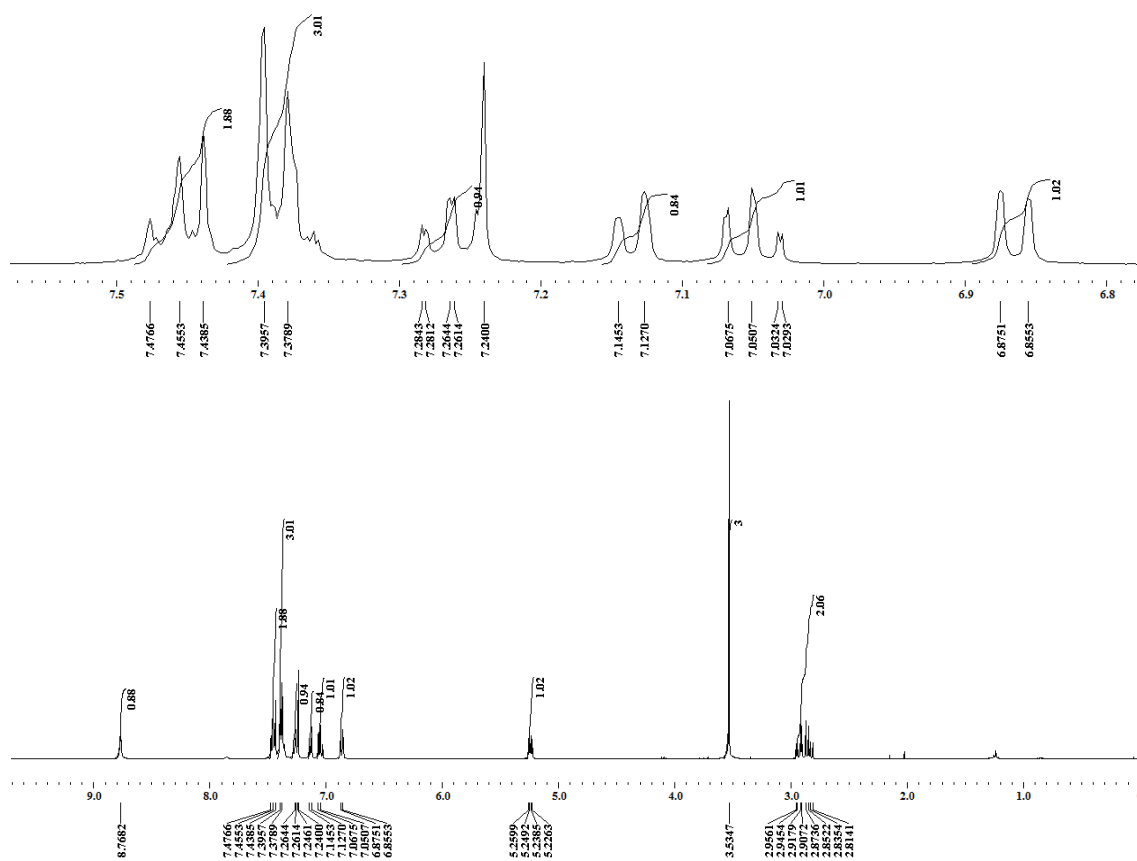
1. (a) Kantam, M. L.; Srinivas, P.; Yadav, J.; Likhar, P. R.; Bhargava, S.; *J. Org. Chem.*, **2009**, *74*, 4882; (b) Karimi, B.; Enders, D.; *Org. Lett.*, **2006**, *8*, 1237; (c) Cui, X.; Li, J.; Zhang, Z. P.; Fu, Y.; Liu, L.; Guo, Q.X. *J. Org. Chem.*, **2007**, *72*, 9342.
2. CrysAlisPro, *Agilent Technologies*, Version 1.171.34.49 (2011).
3. Sheldrick, G. M. *Acta Cryst.* **2008**, *A64*, 112.
4. Farrugia, L. J. WinGX Version 1.80.05, *An integrated system of Windows Programs for the Solution, Refinement and Analysis of Single Crystal X-Ray Diffraction Data*; Department of Chemistry, University of Glasgow (1997-2009).

# ***SPECTRA***

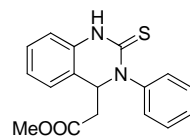
# <sup>1</sup>H NMR



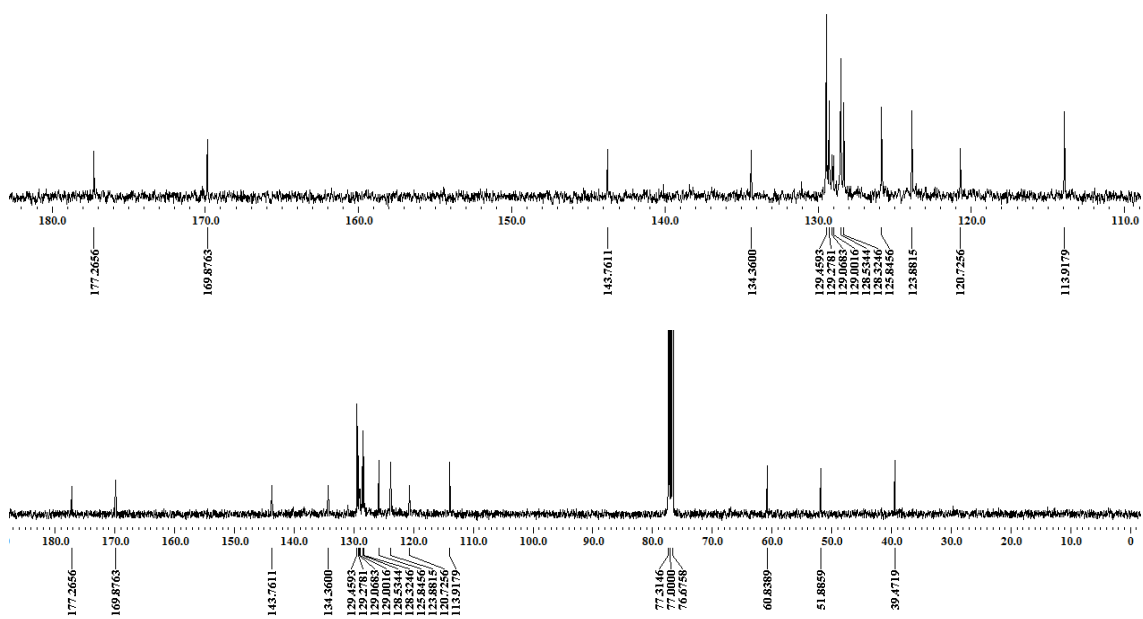
Methyl 2-(3-phenyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4a)



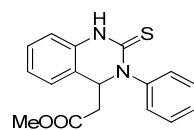
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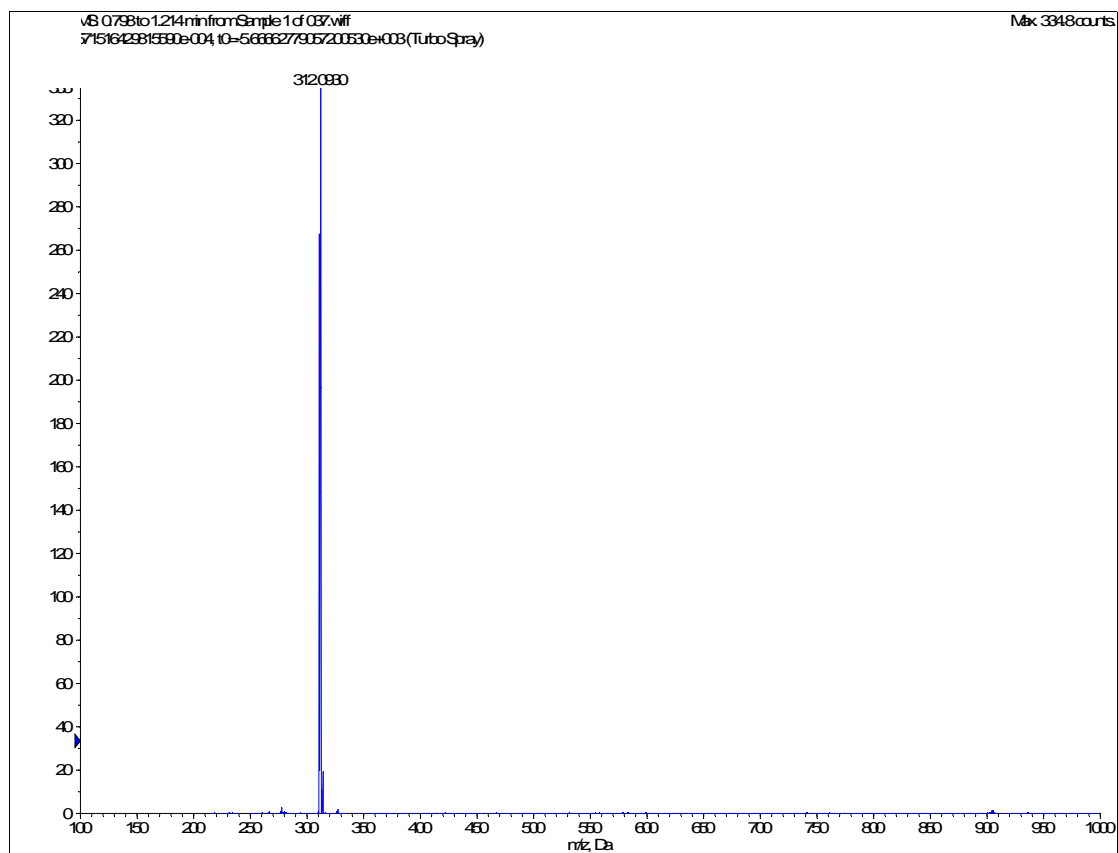
Methyl 2-(3-phenyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4a)



# HRMS

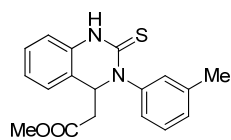


## Methyl 2-(3-phenyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4a)

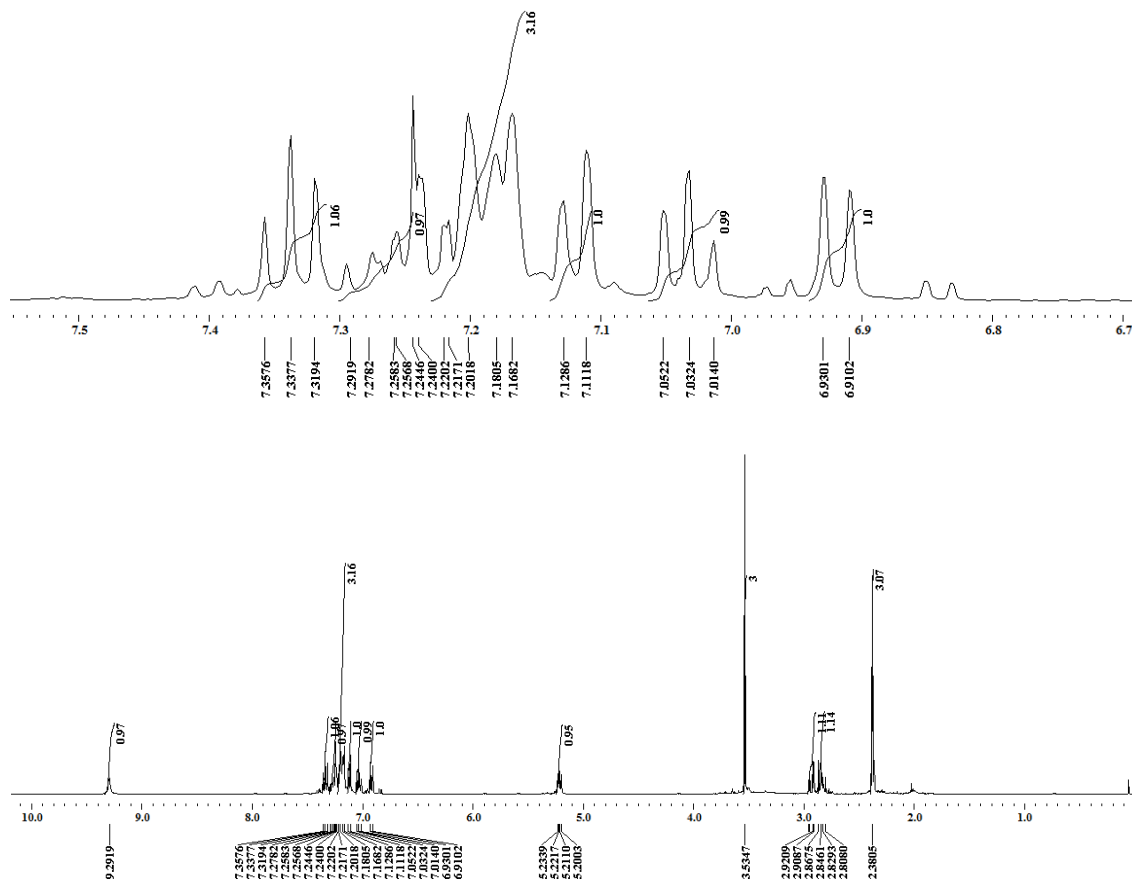




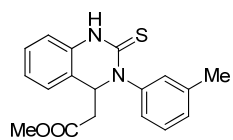
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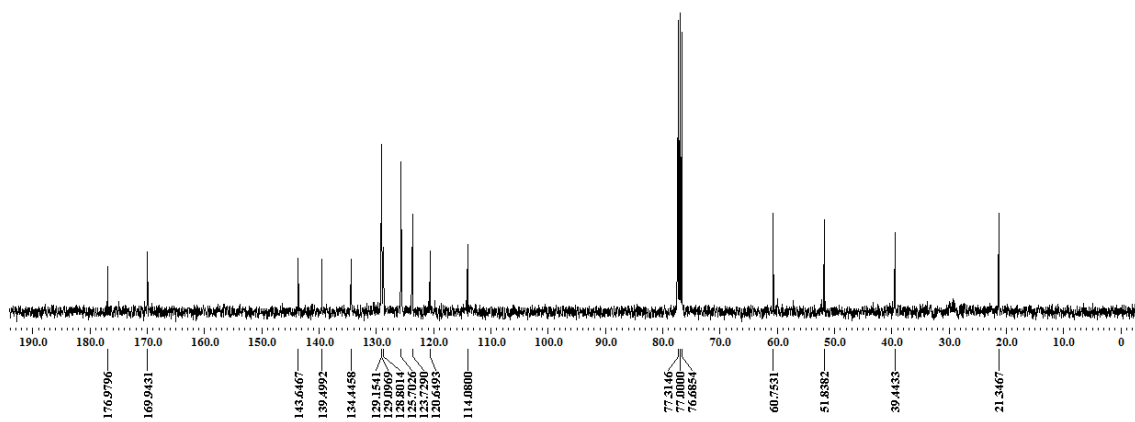
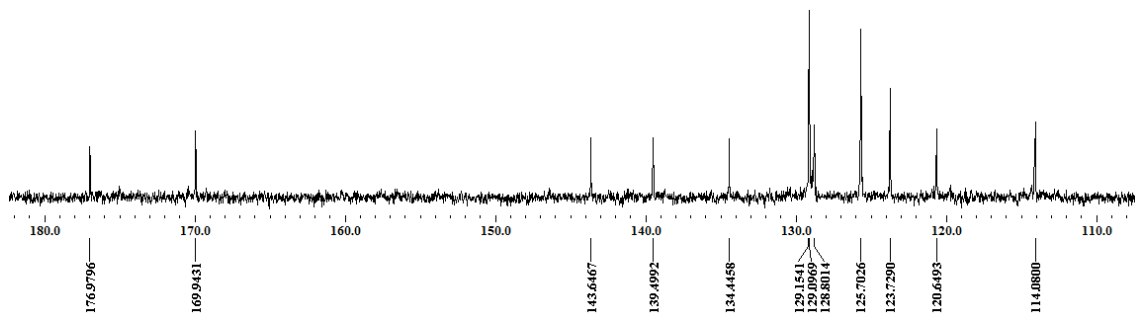
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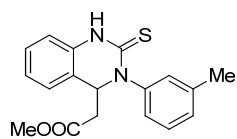
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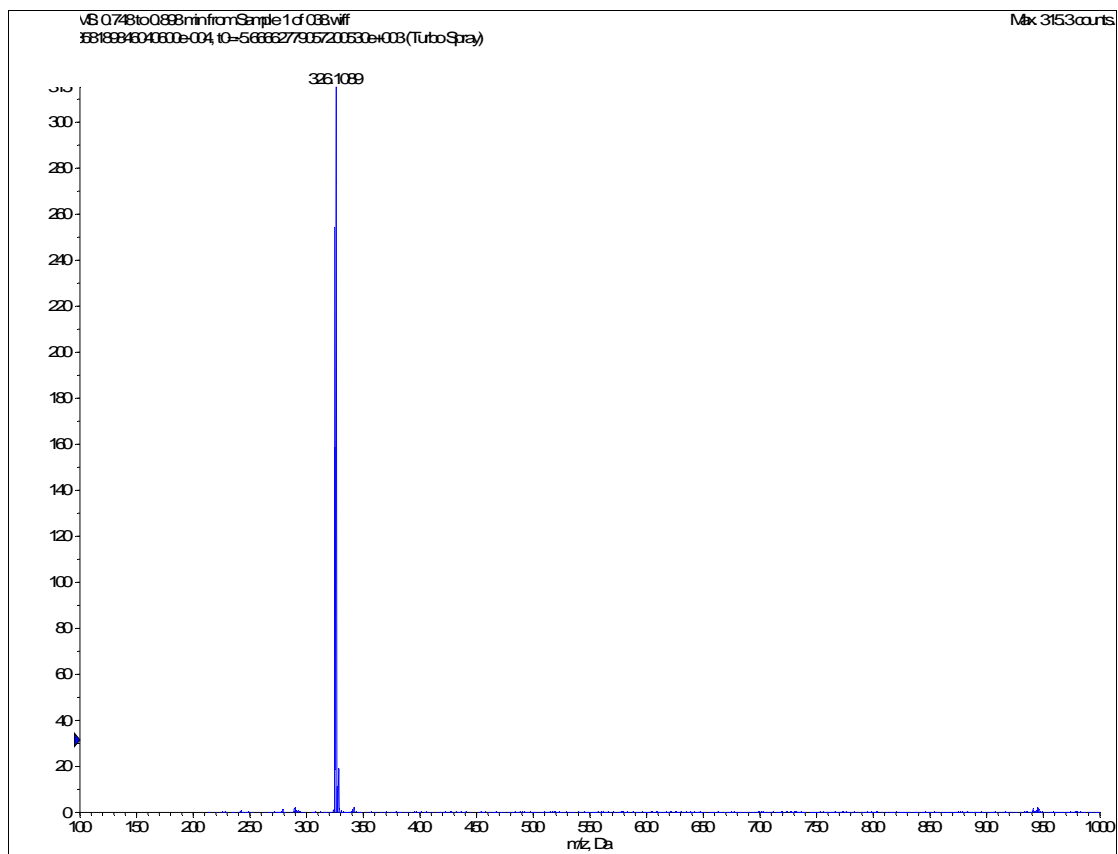
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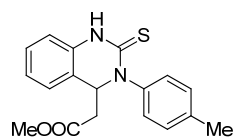
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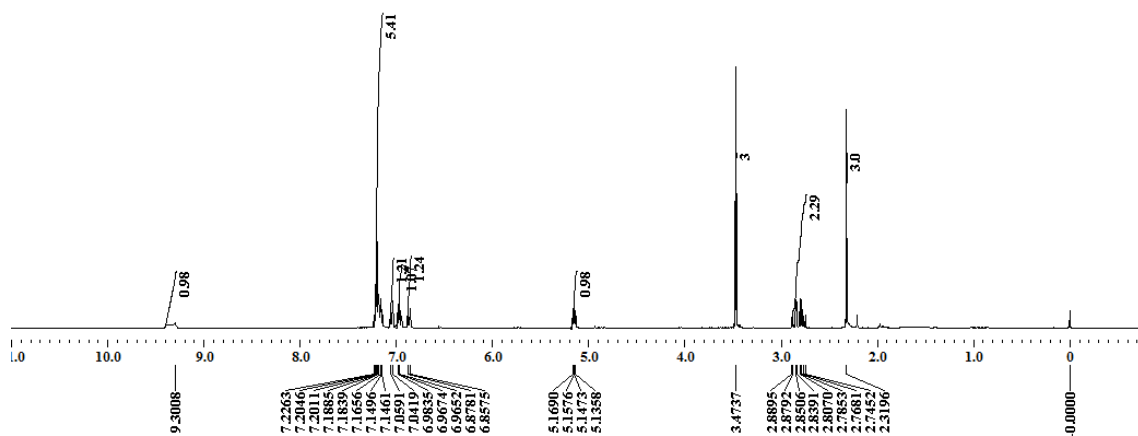
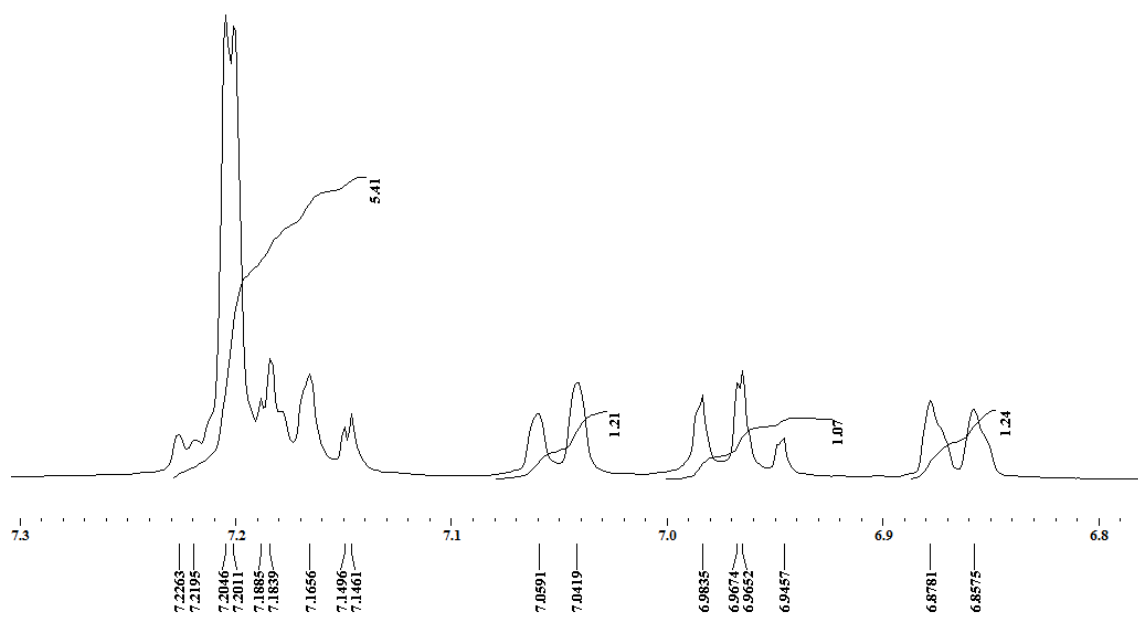
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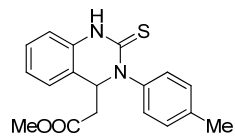
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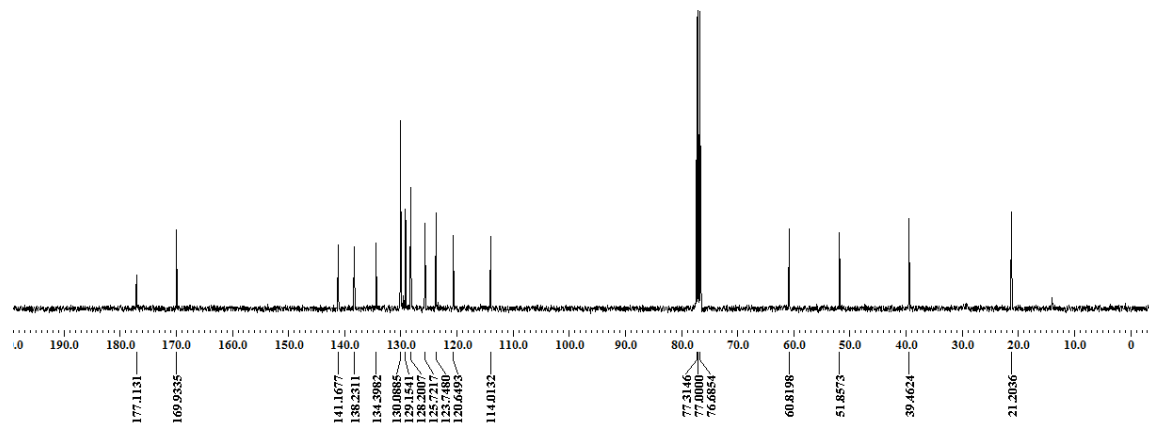
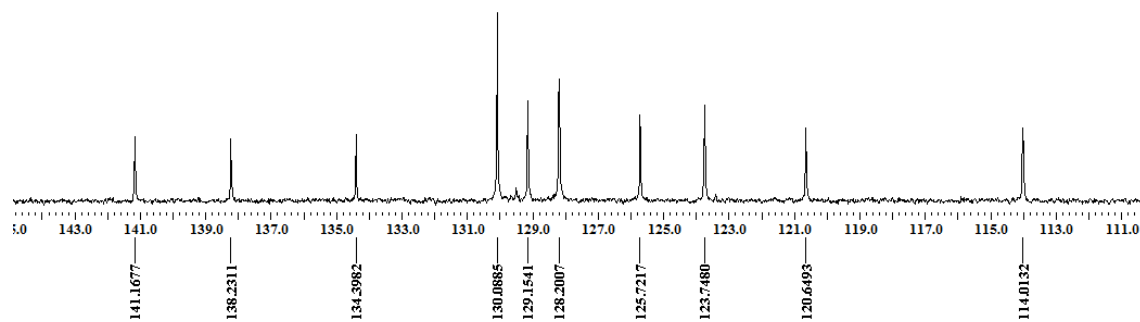
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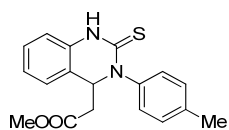
<sup>13</sup>C NMR



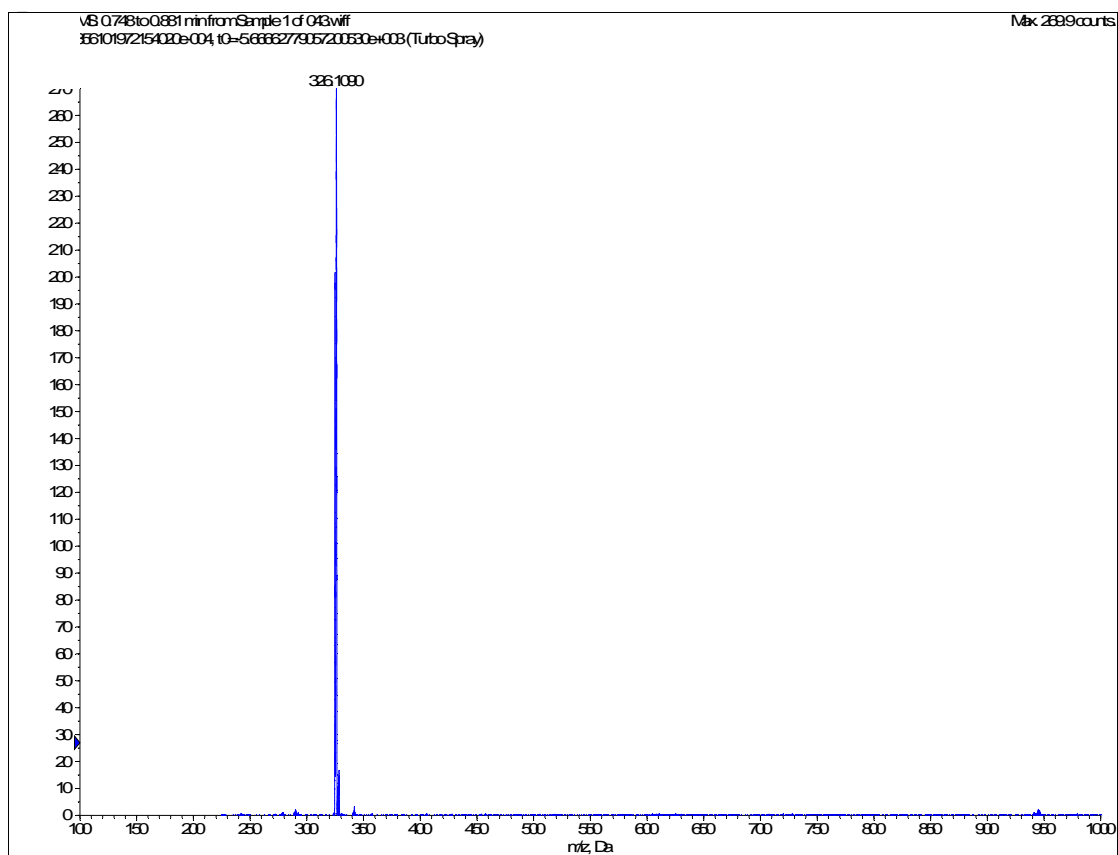
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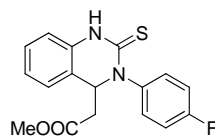
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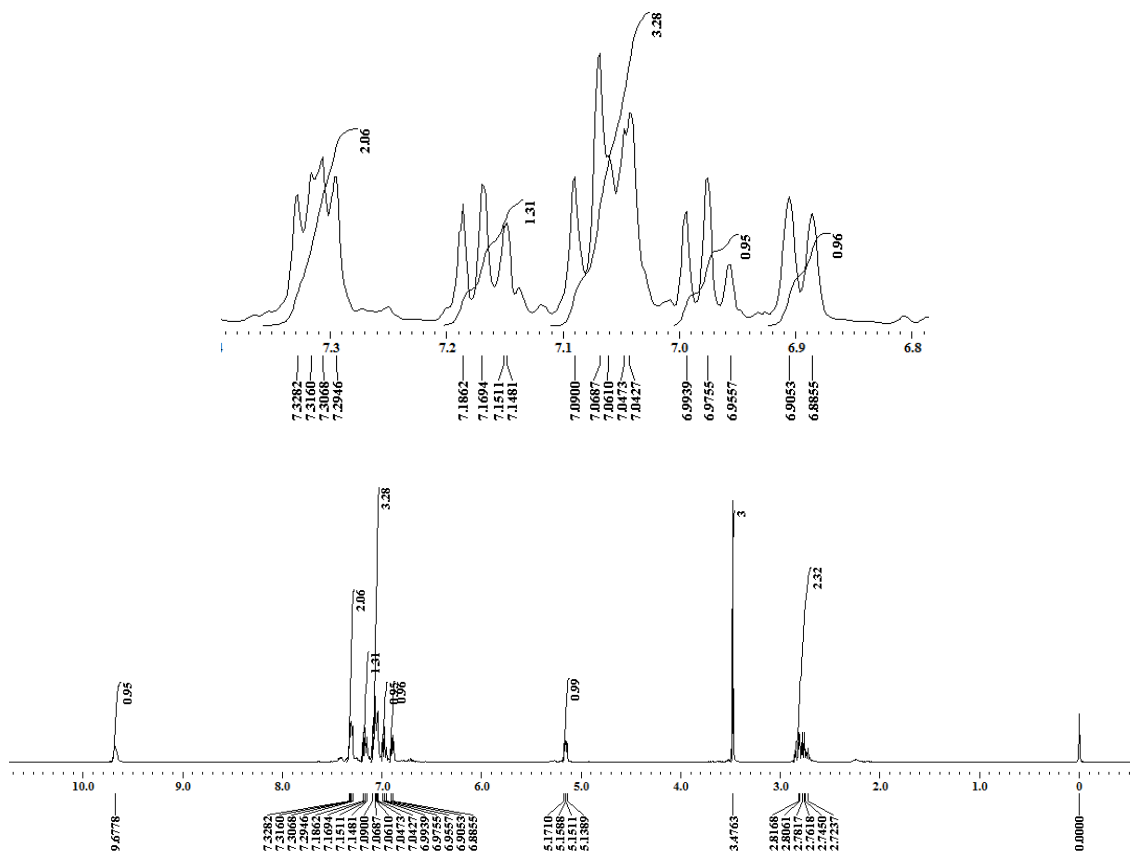
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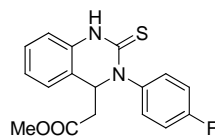
# <sup>1</sup>H NMR



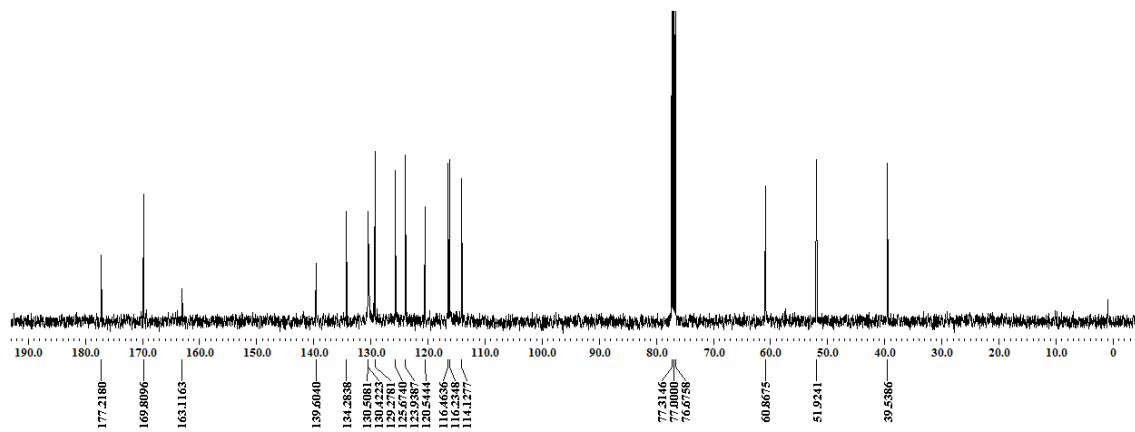
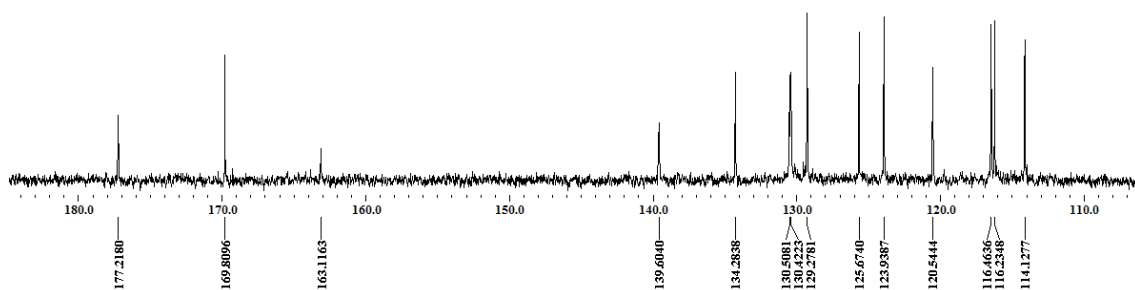
Methyl 2-(3-(4-fluorophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4d)



<sup>13</sup>C NMR

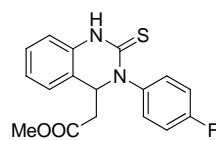


Methyl 2-(3-(4-fluorophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4d)

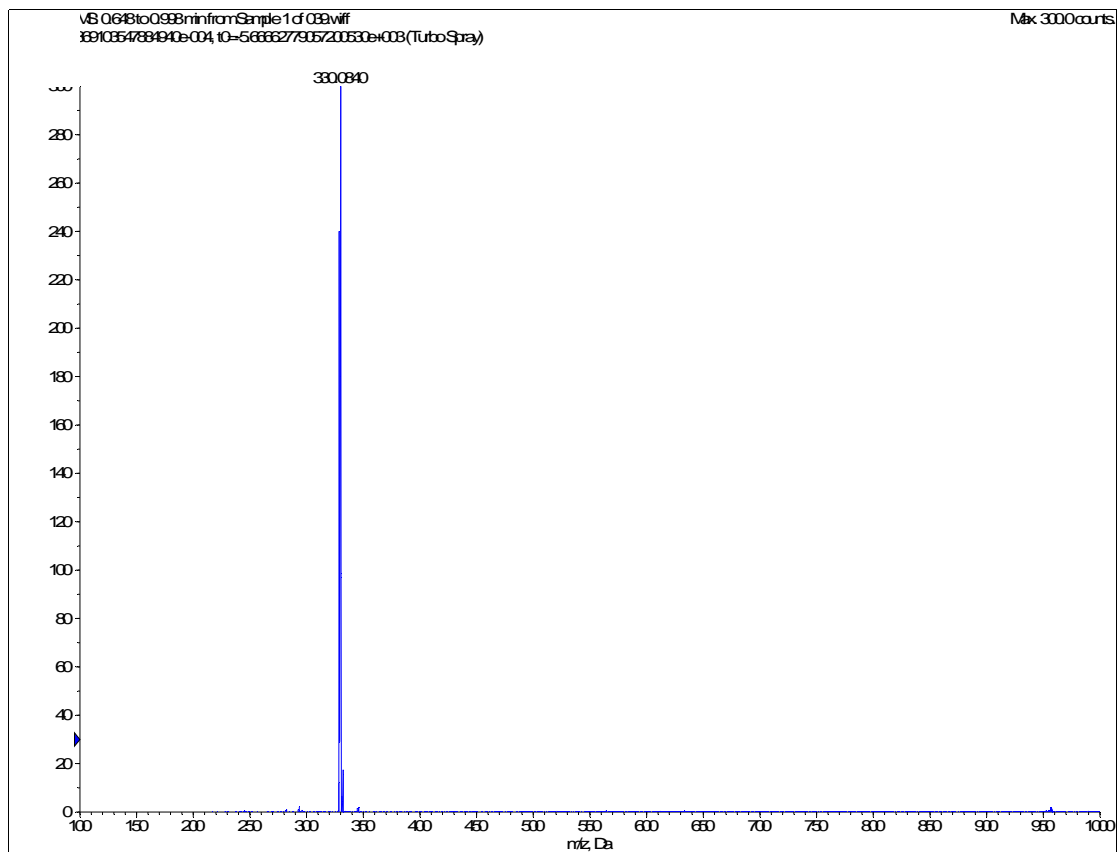




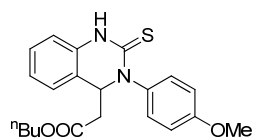
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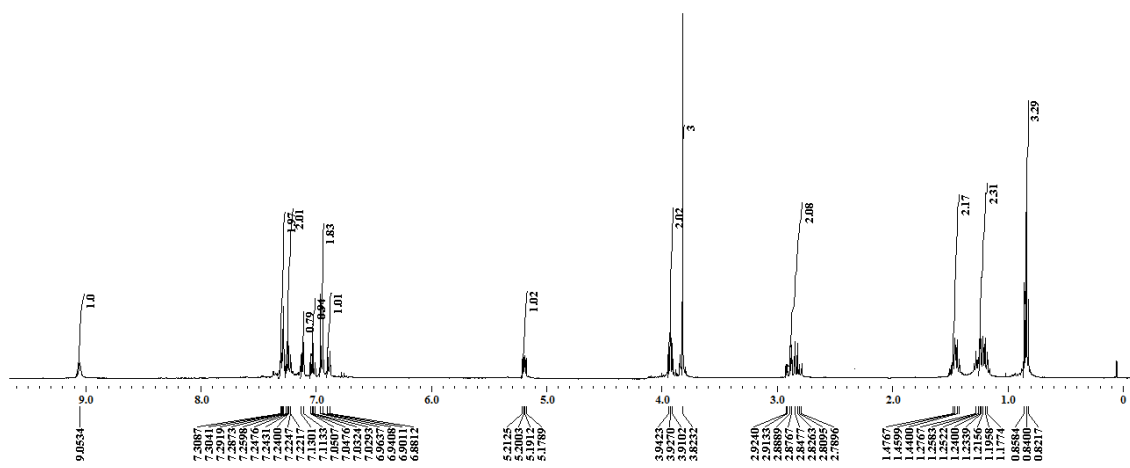
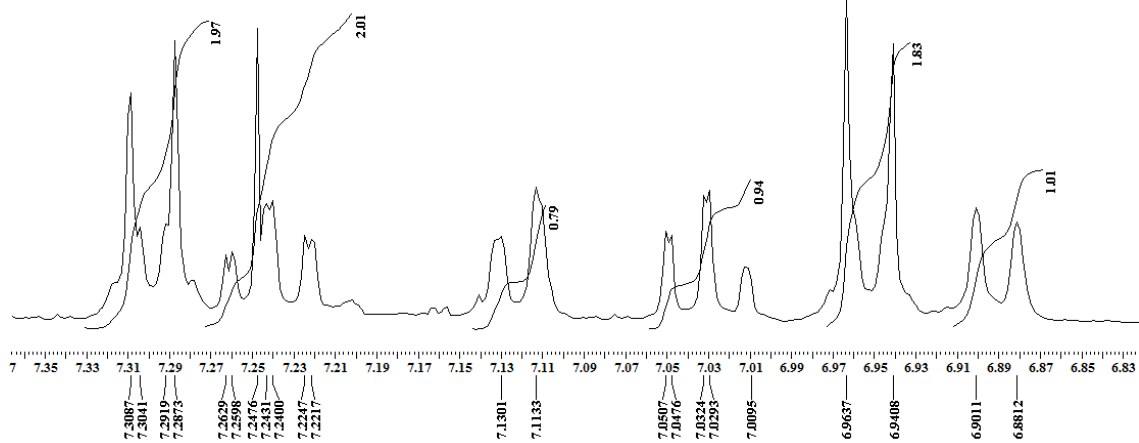
## Methyl 2-(3-(4-fluorophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4d)



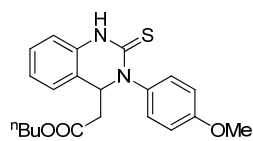
# <sup>1</sup>H NMR



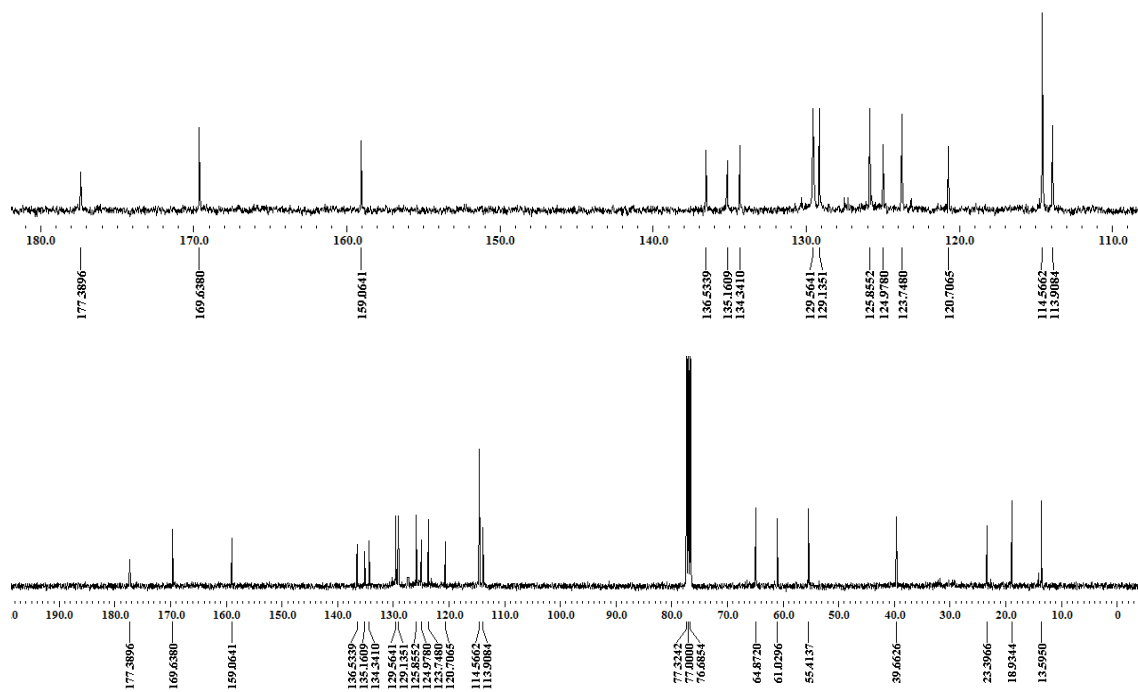
Butyl 2-(3-(4-methoxyphenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4e)



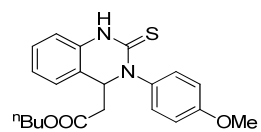
# <sup>13</sup>C NMR



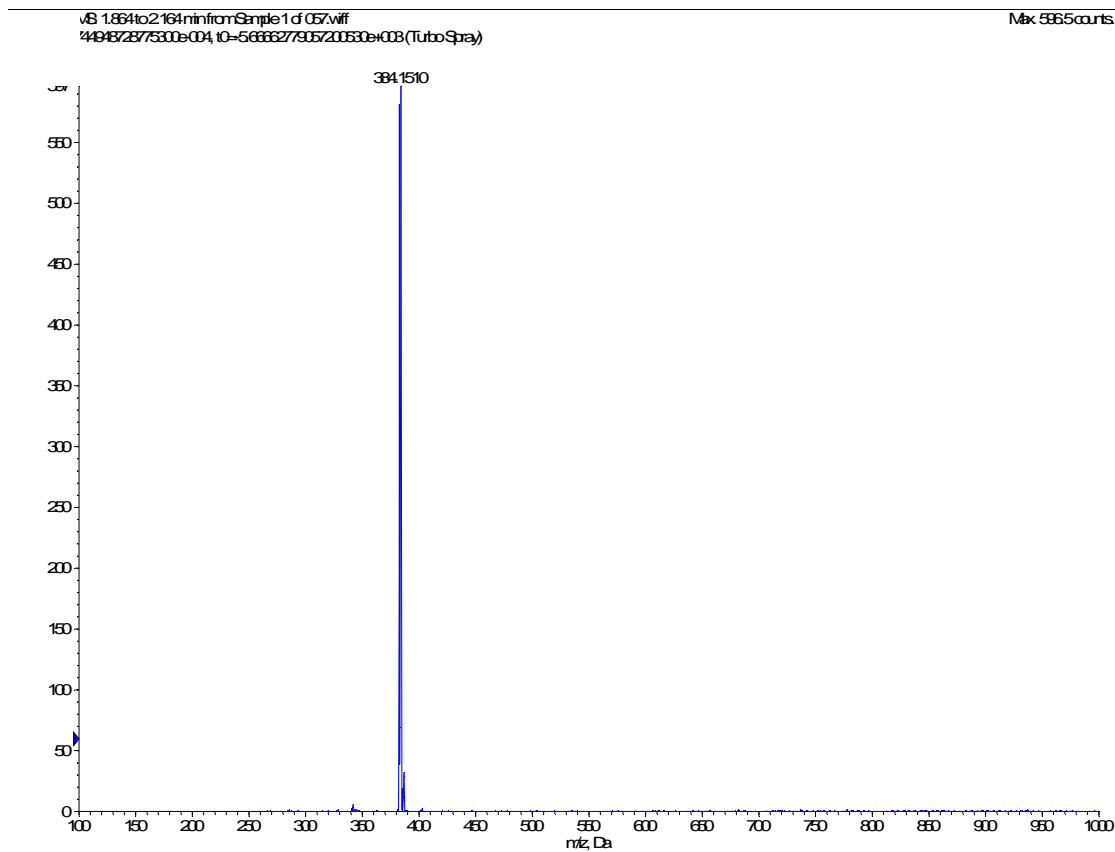
**Butyl 2-(3-(4-methoxyphenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4e)**



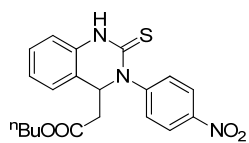
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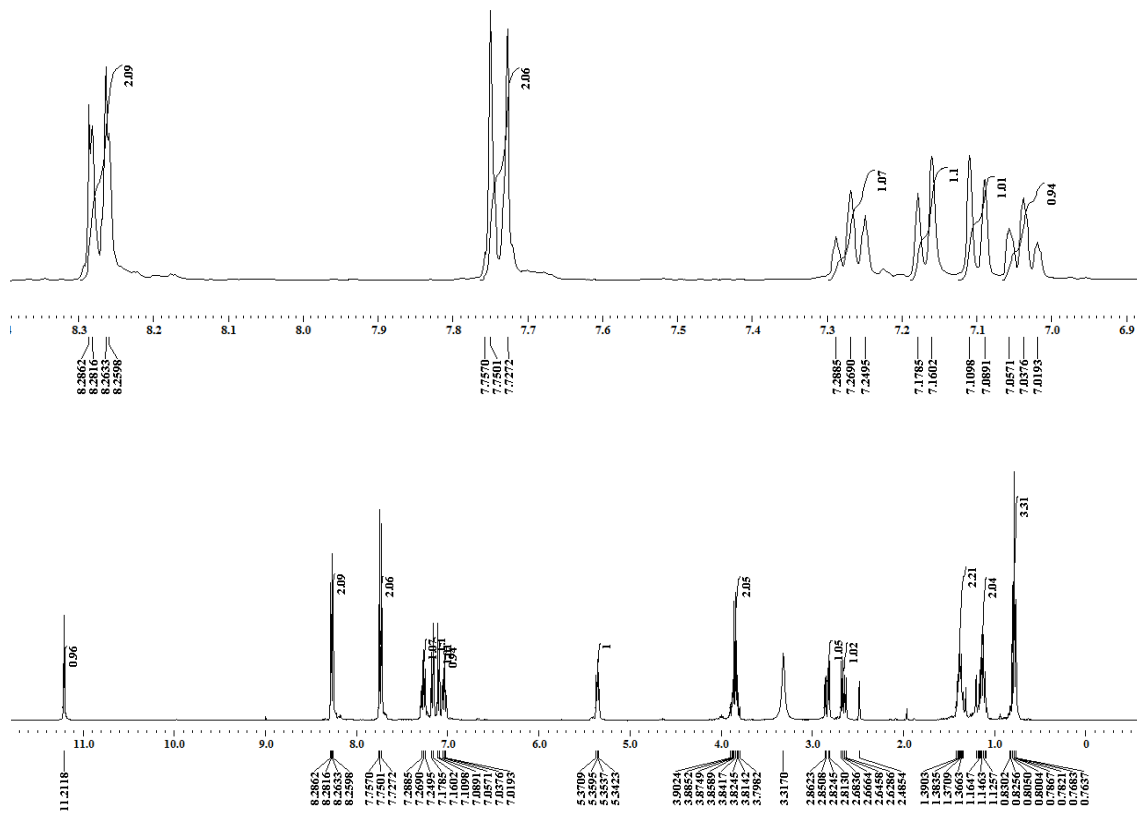
### Butyl 2-(3-(4-methoxyphenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4e)



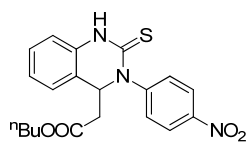
# <sup>1</sup>H NMR



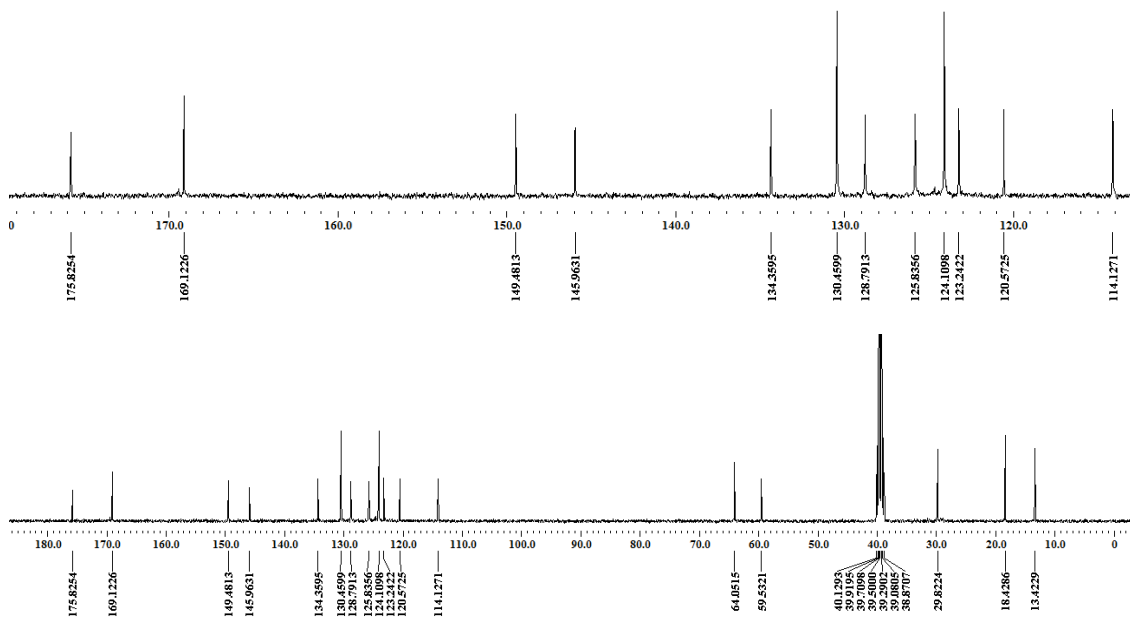
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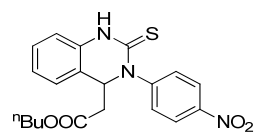
# <sup>13</sup>C NMR



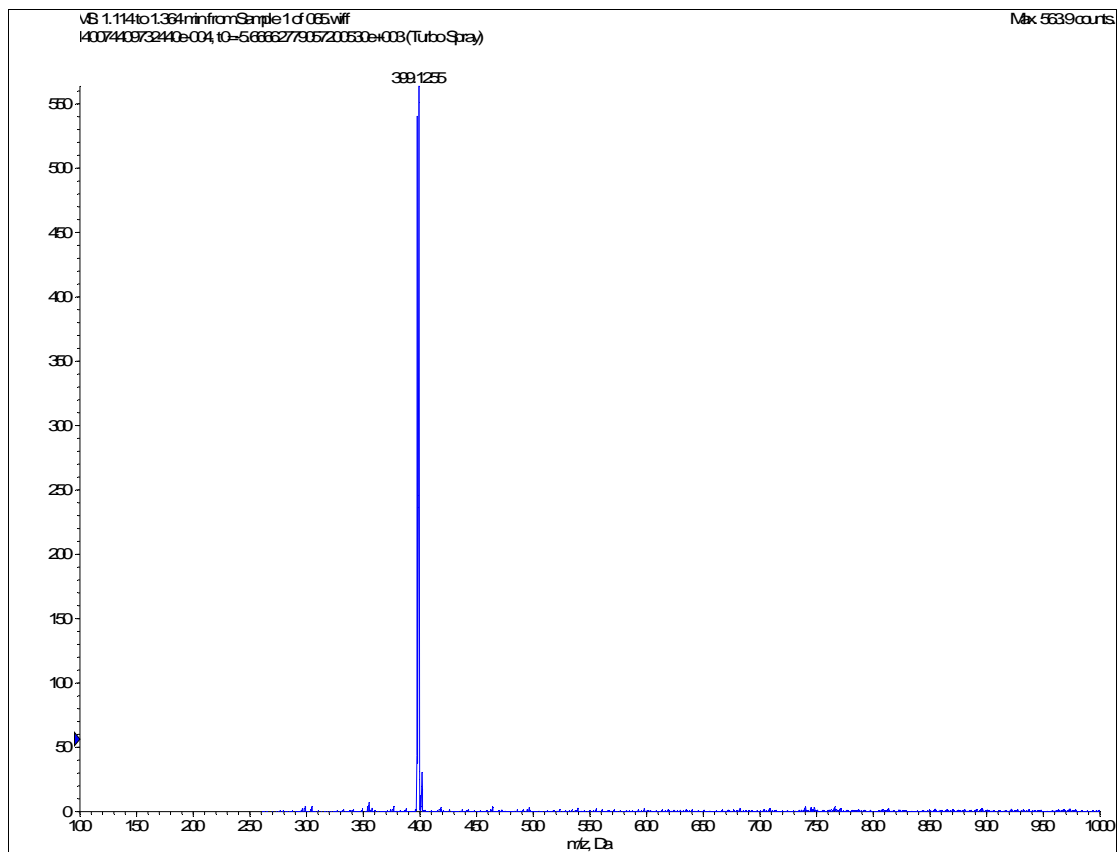
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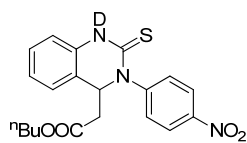
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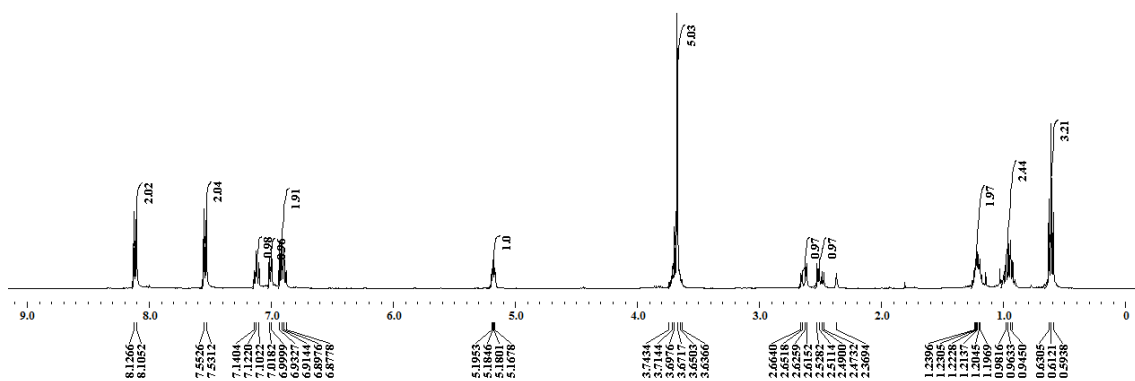
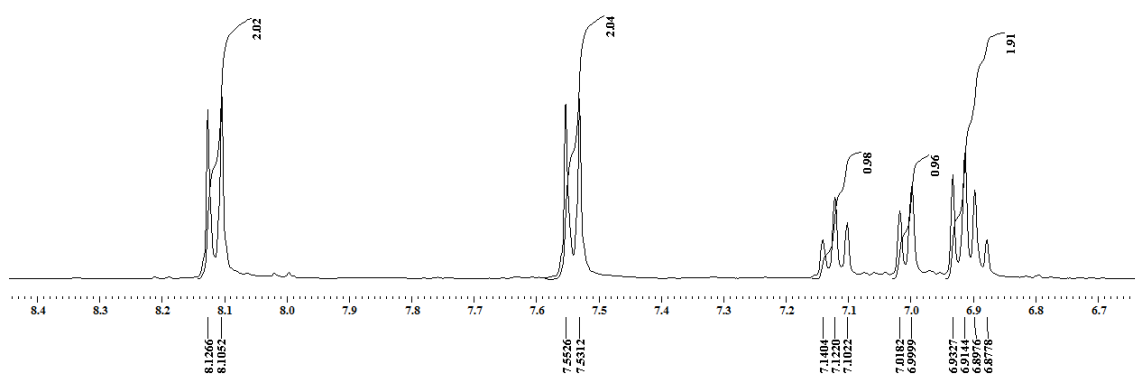
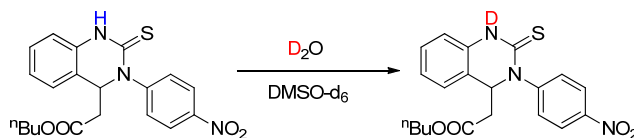
### Butyl 2-(3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4f)



# <sup>1</sup>H NMR

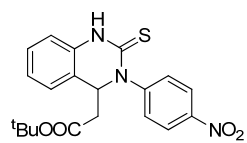


Butyl 2-(3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-D-4-yl)acetate (4f')

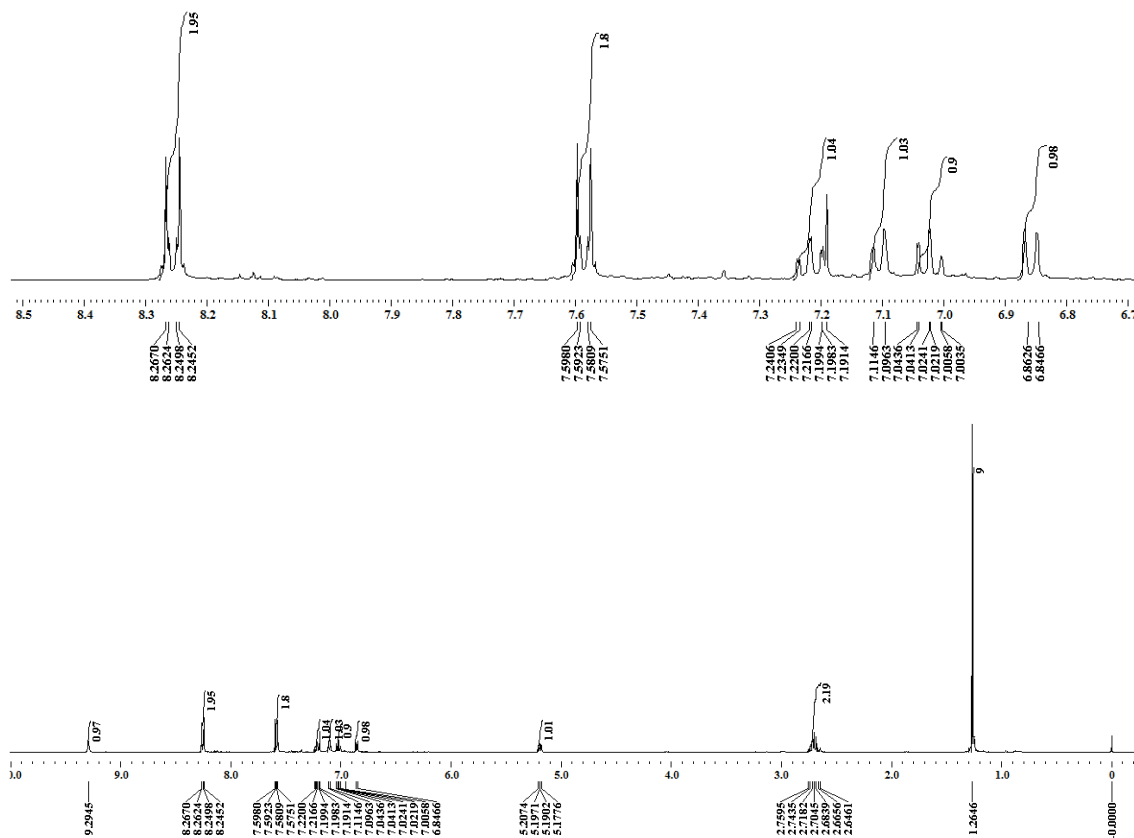




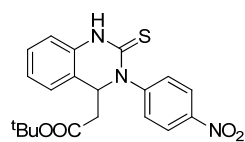
# <sup>1</sup>H NMR



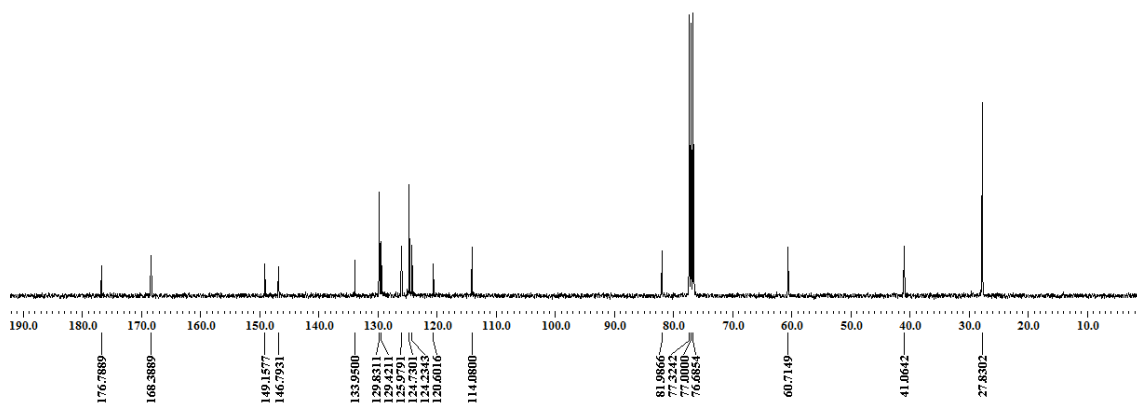
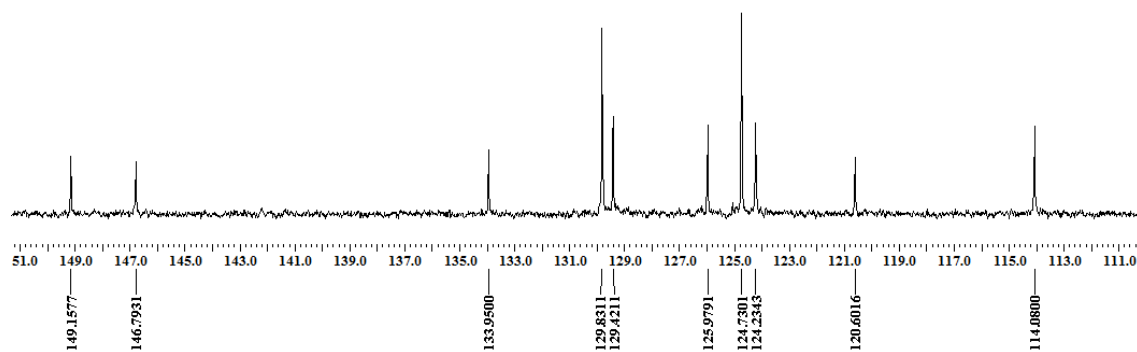
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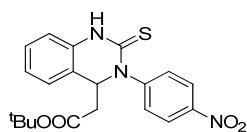
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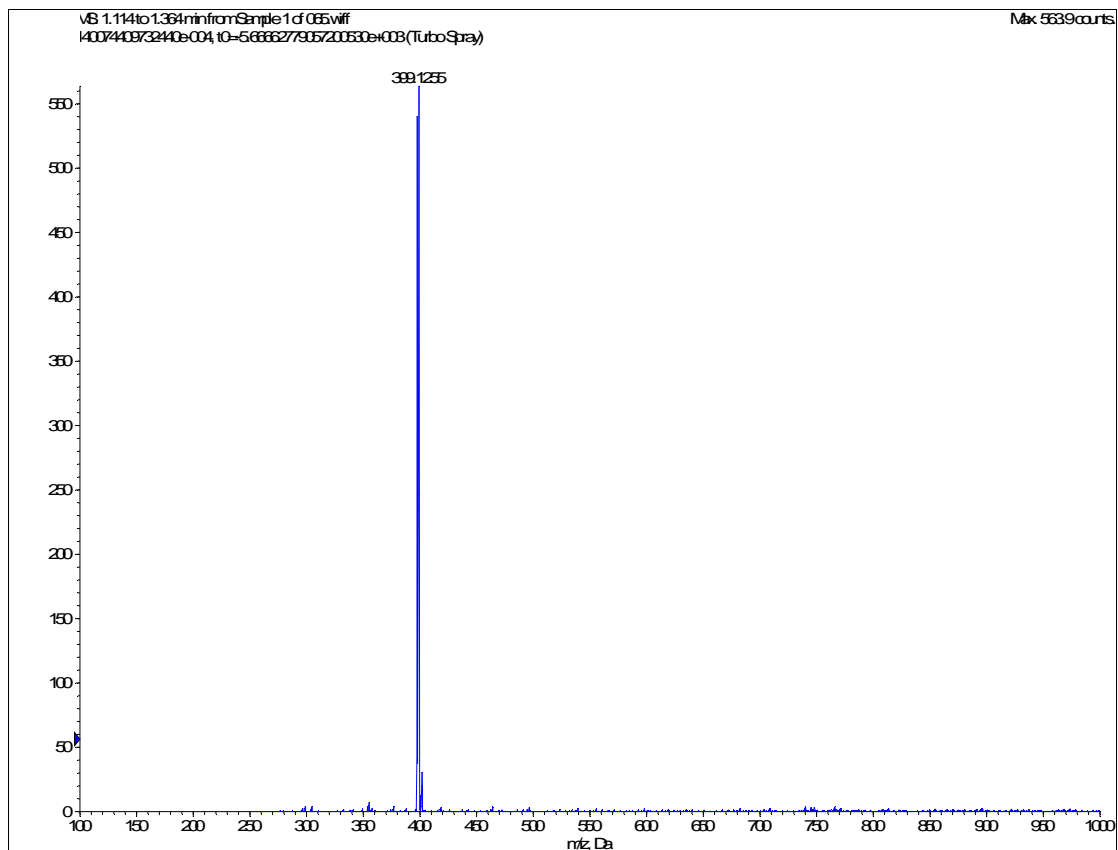
*tert*-Butyl 2-(3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4g)



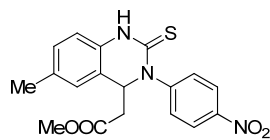
### HRMS



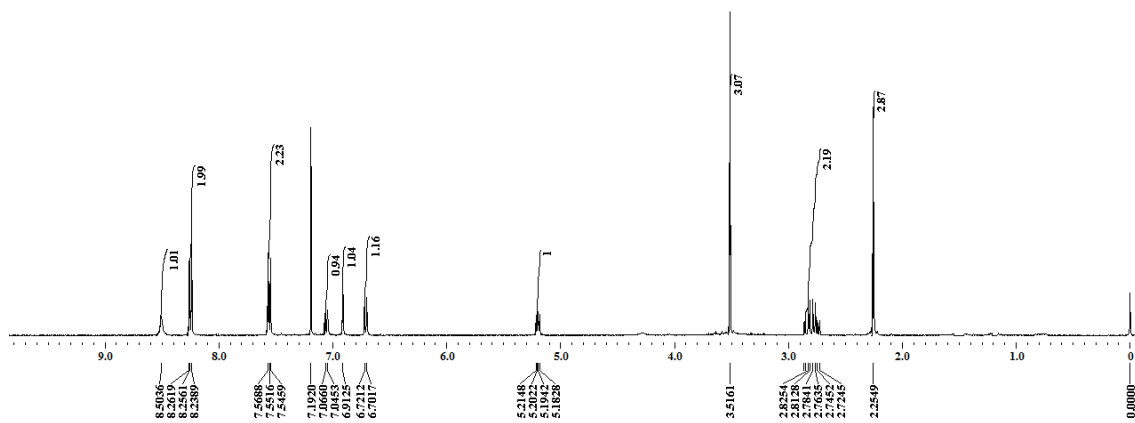
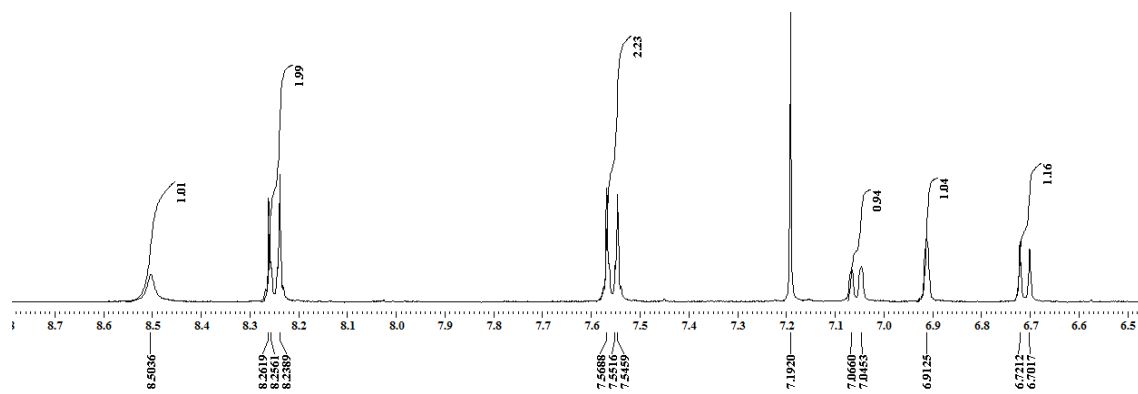
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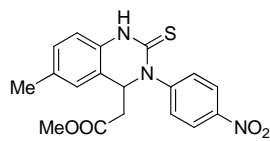
# <sup>1</sup>H NMR



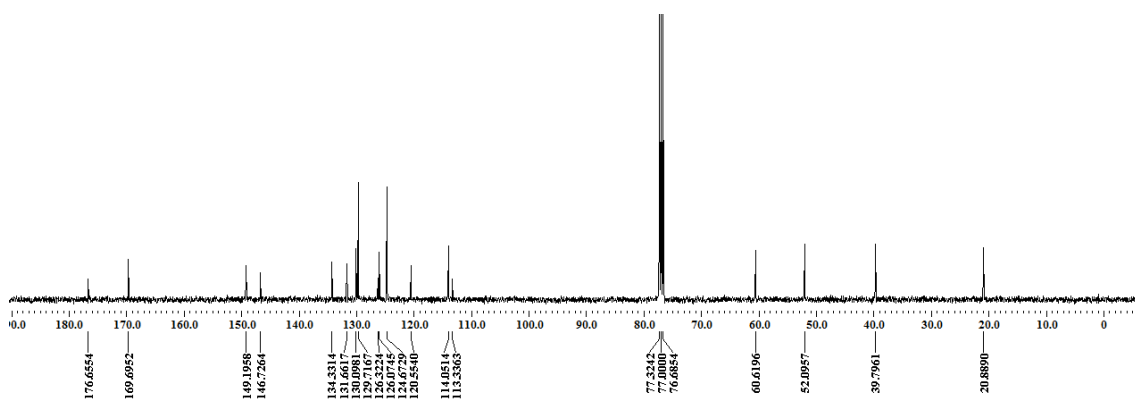
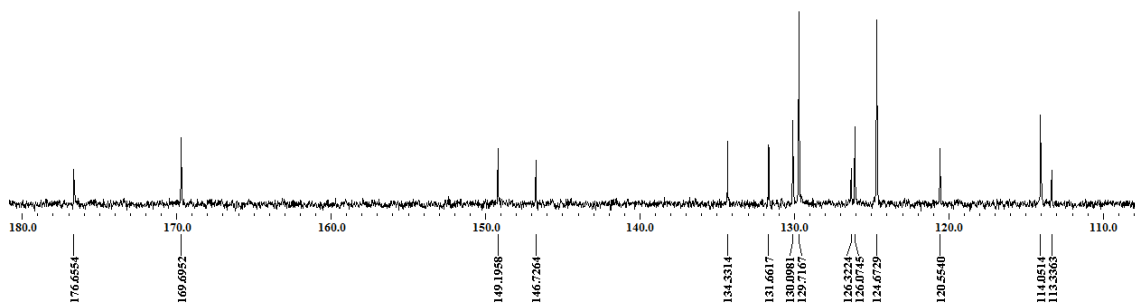
**Methyl 2-(6-methyl-3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4h)**



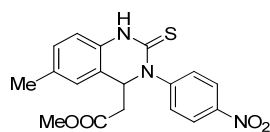
# <sup>13</sup>C NMR



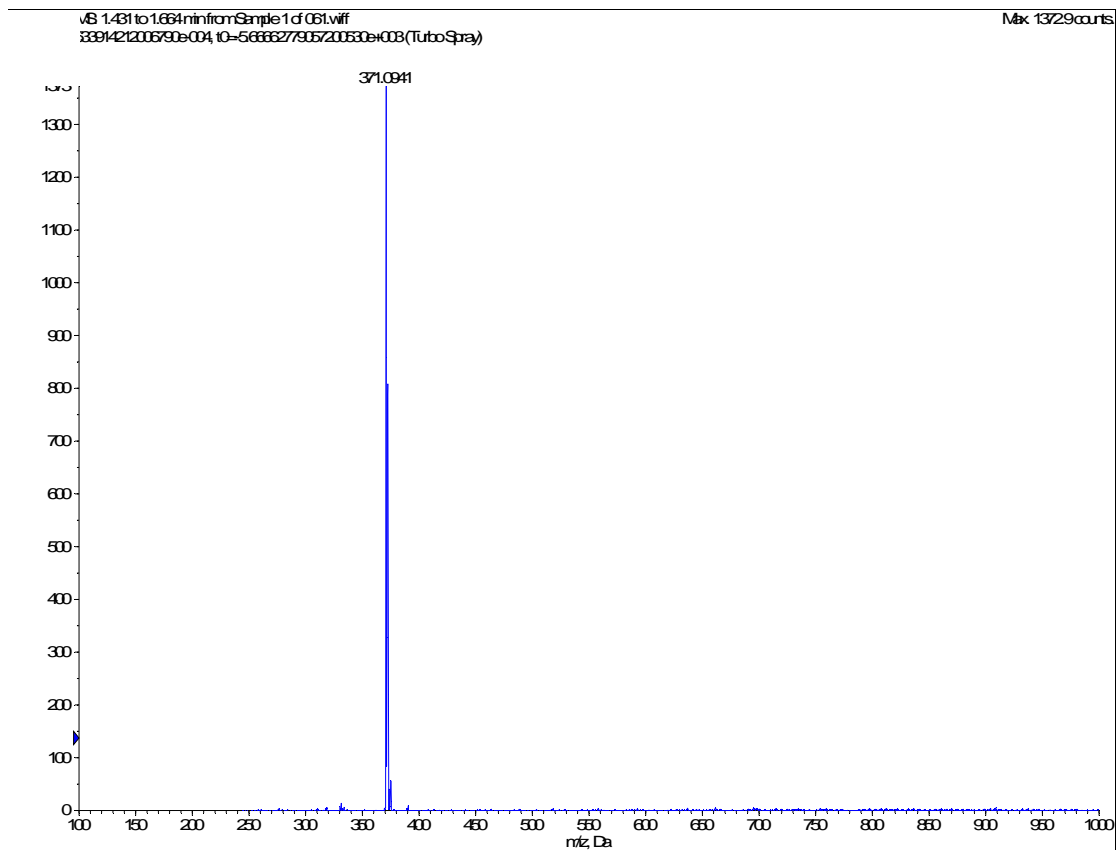
**Methyl 2-(6-methyl-3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4h)**



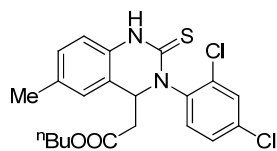
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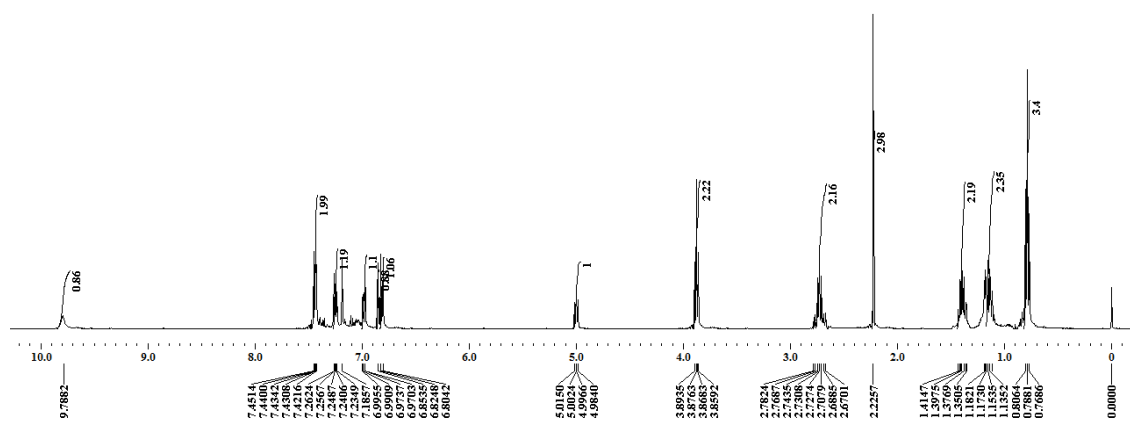
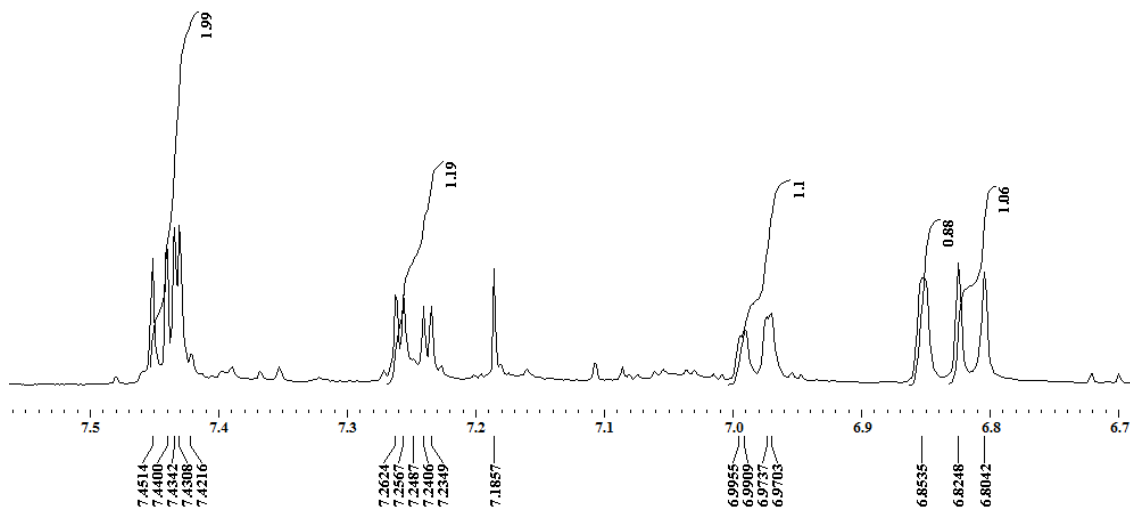
### Methyl 2-(6-methyl-3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4h)



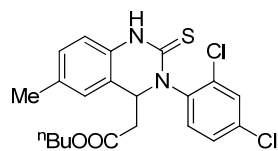
# <sup>1</sup>H NMR



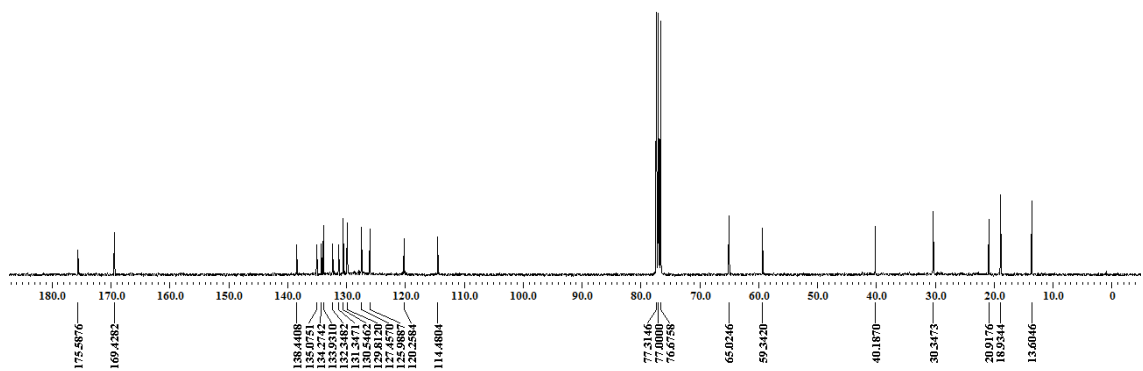
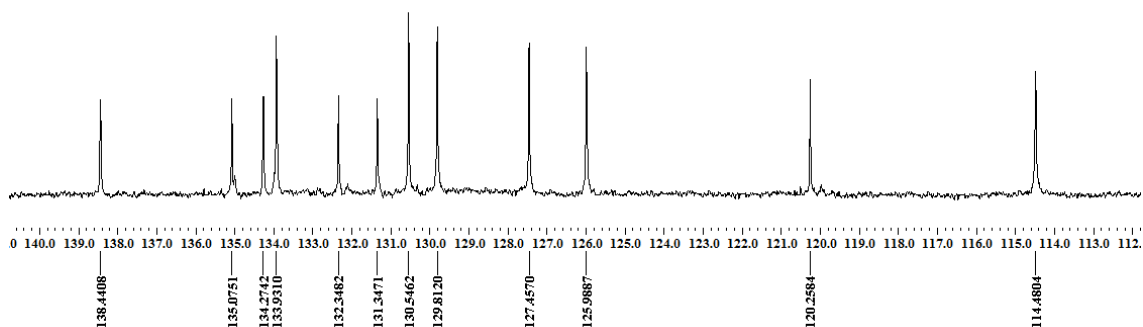
Butyl 2-(3-(2,4-dichlorophenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4i)



<sup>13</sup>C NMR

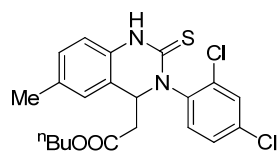


Butyl 2-(3-(2,4-dichlorophenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4i)

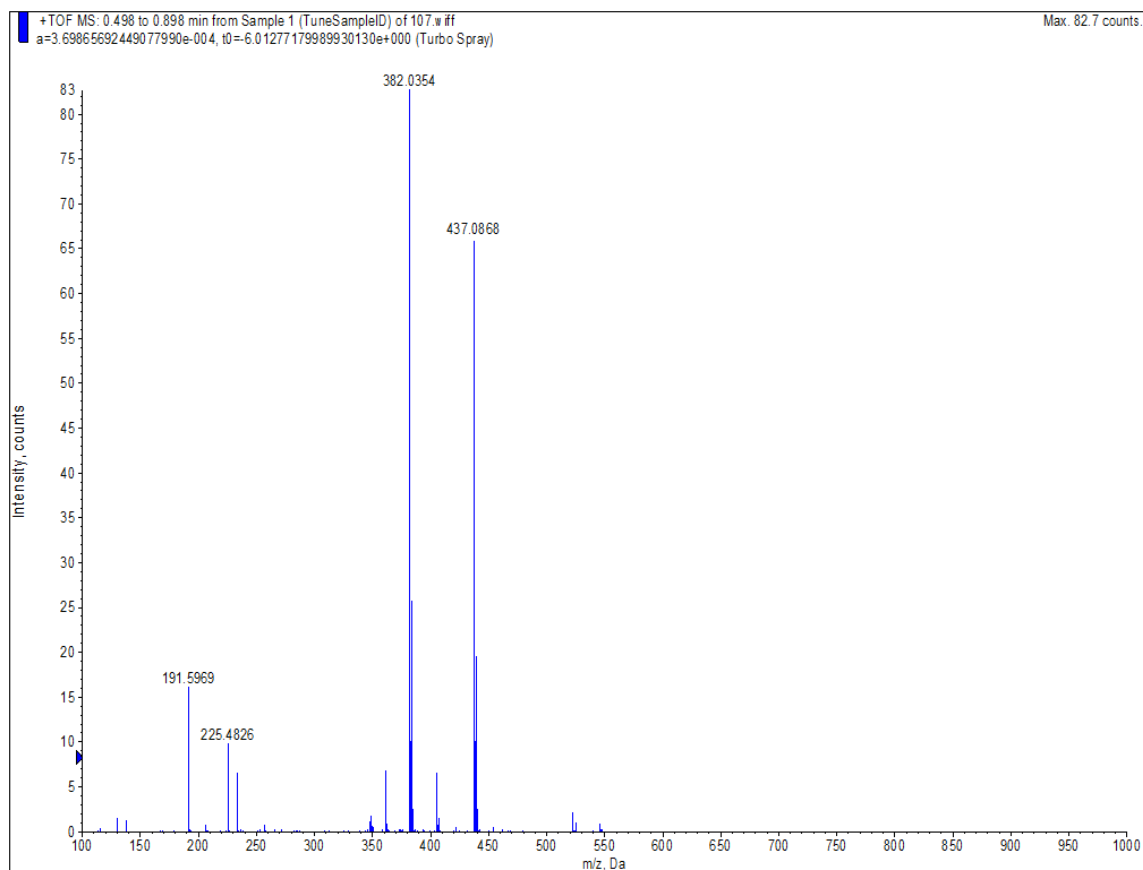




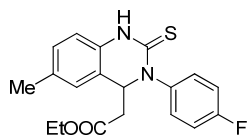
## HRMS



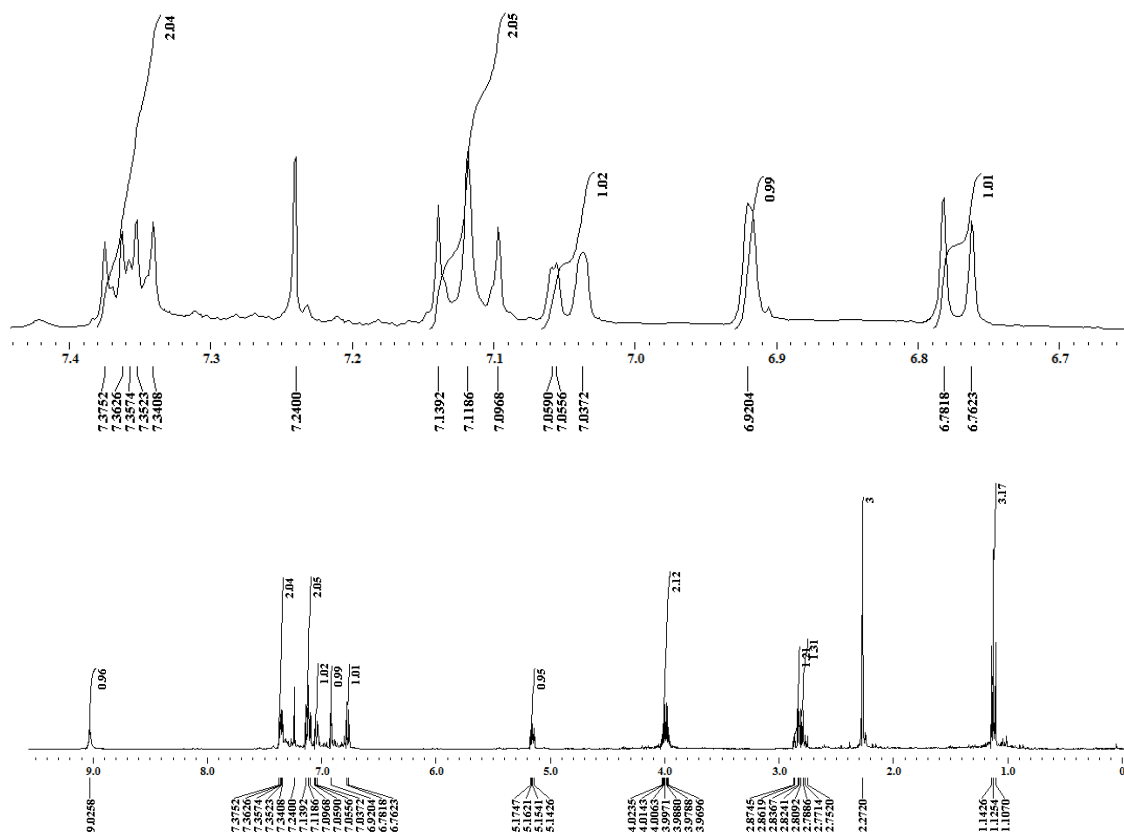
**Butyl 2-(3-(2,4-dichlorophenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4i)**



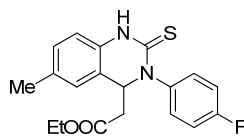
# <sup>1</sup>H NMR



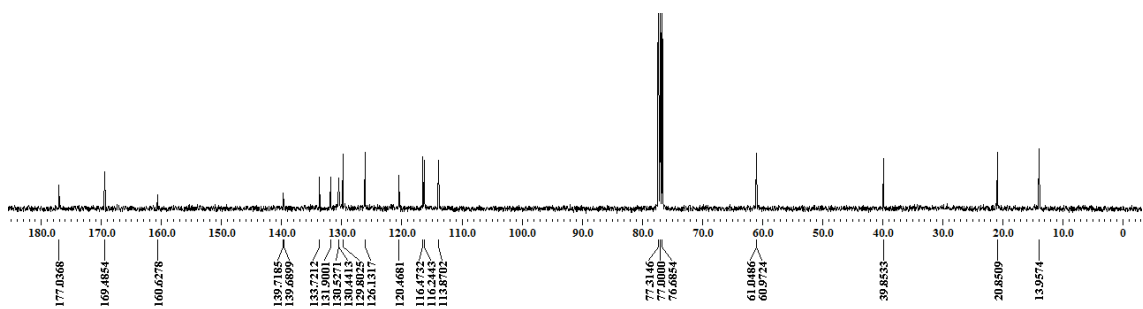
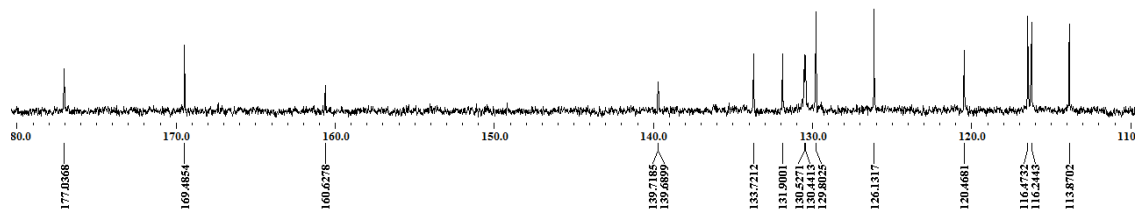
**Ethyl 2-(3-(4-fluorophenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4j)**



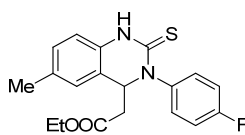
# <sup>13</sup>C NMR



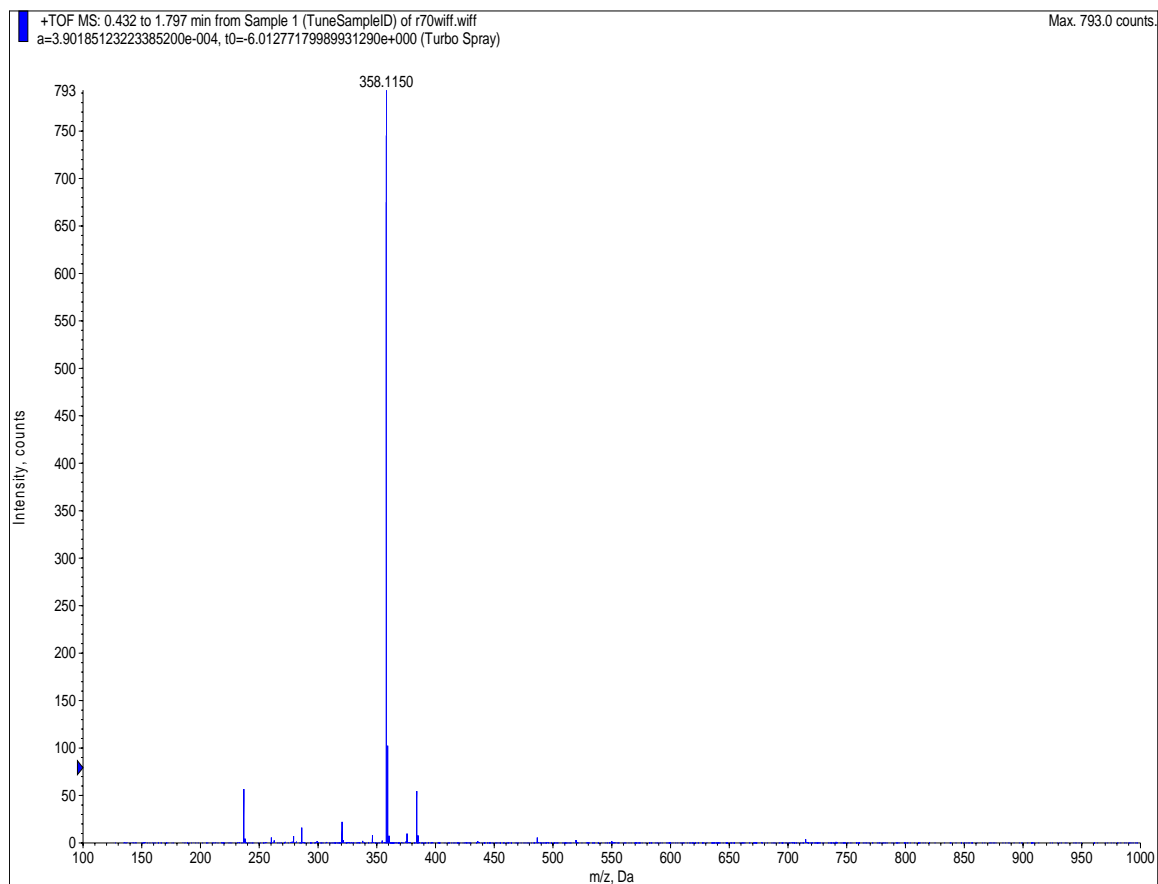
**Ethyl 2-(3-(4-fluorophenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate  
(4j)**



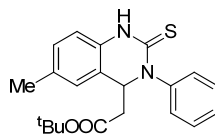
## HRMS



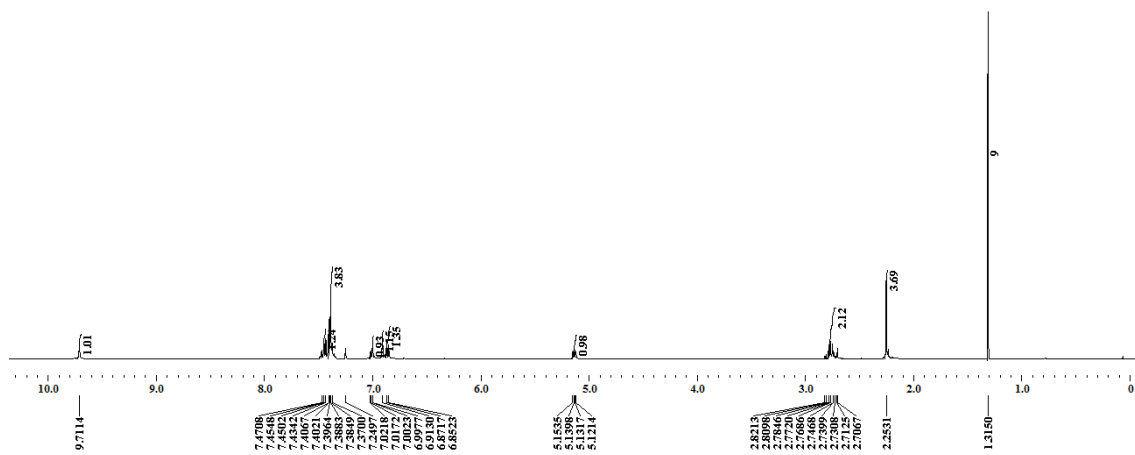
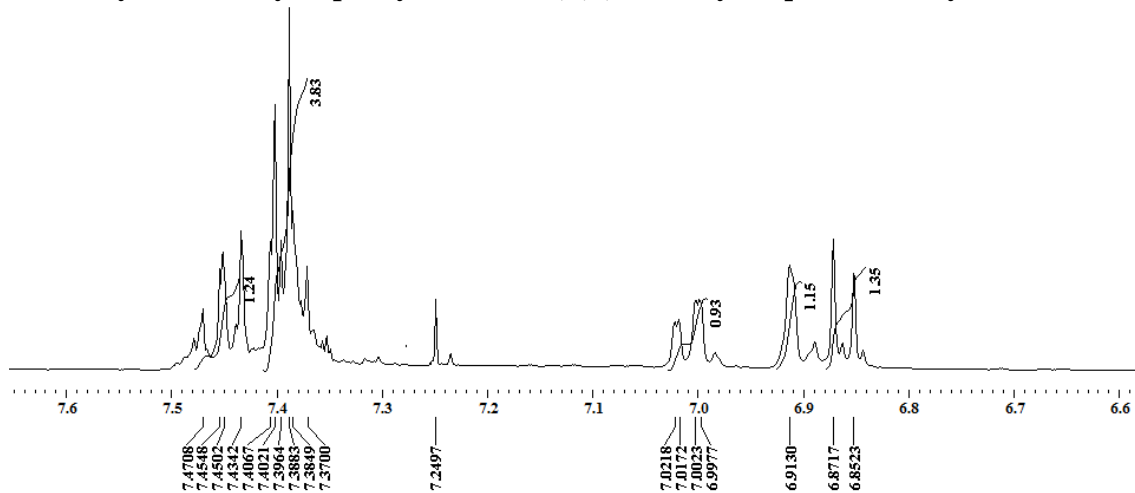
### Ethyl 2-(3-(4-fluorophenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4j)



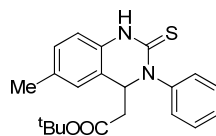
# <sup>1</sup>H NMR



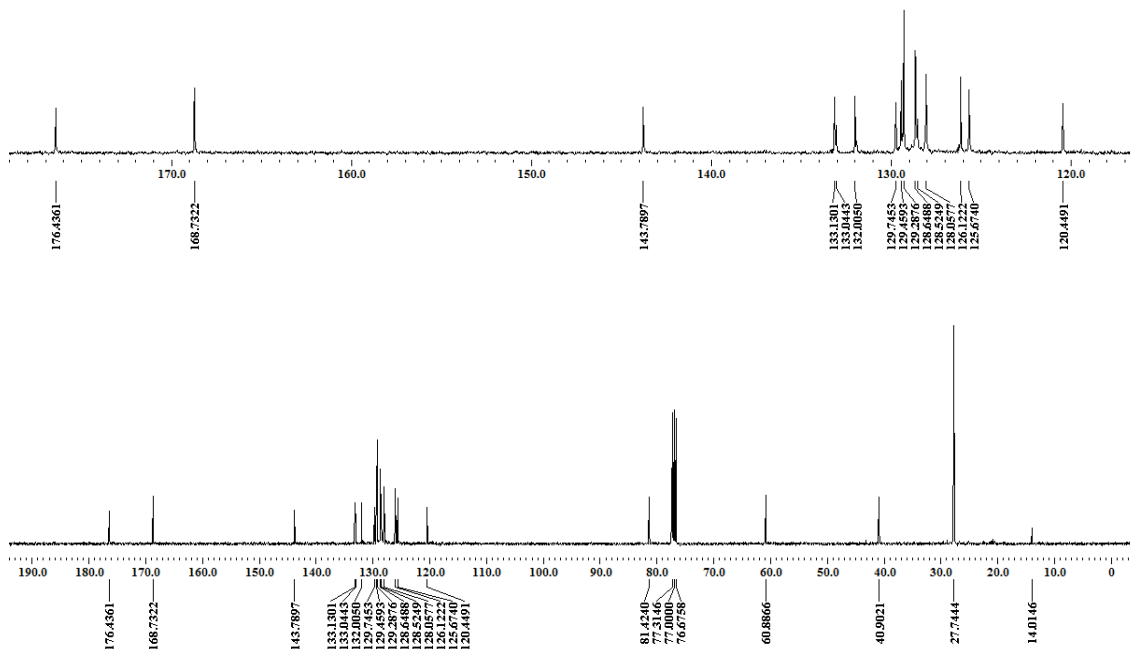
*tert*-Butyl 2-(6-methyl-3-phenyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4k)



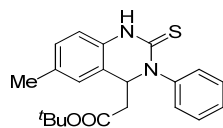
<sup>13</sup>CNMR



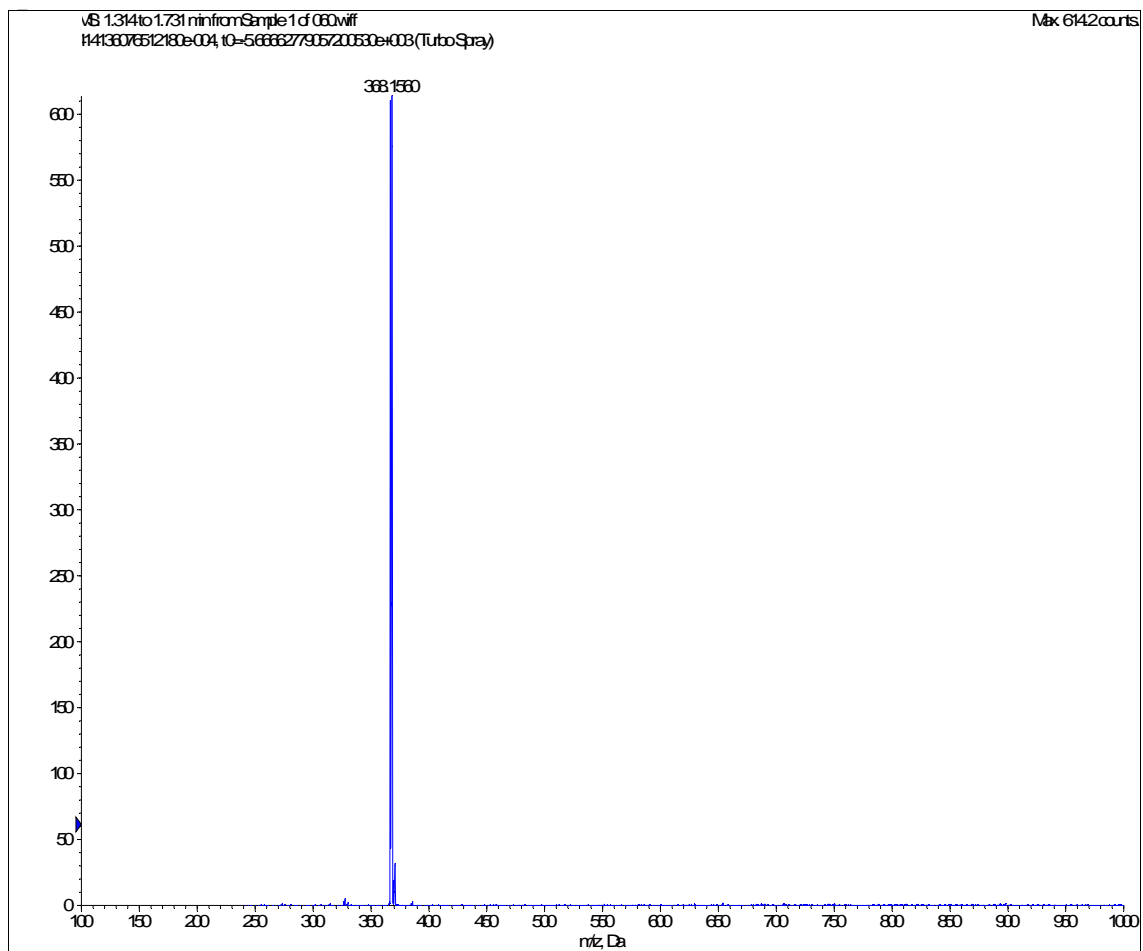
*tert*-Butyl 2-(6-methyl-3-phenyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4k)



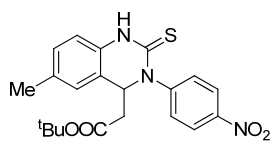
## HRMS



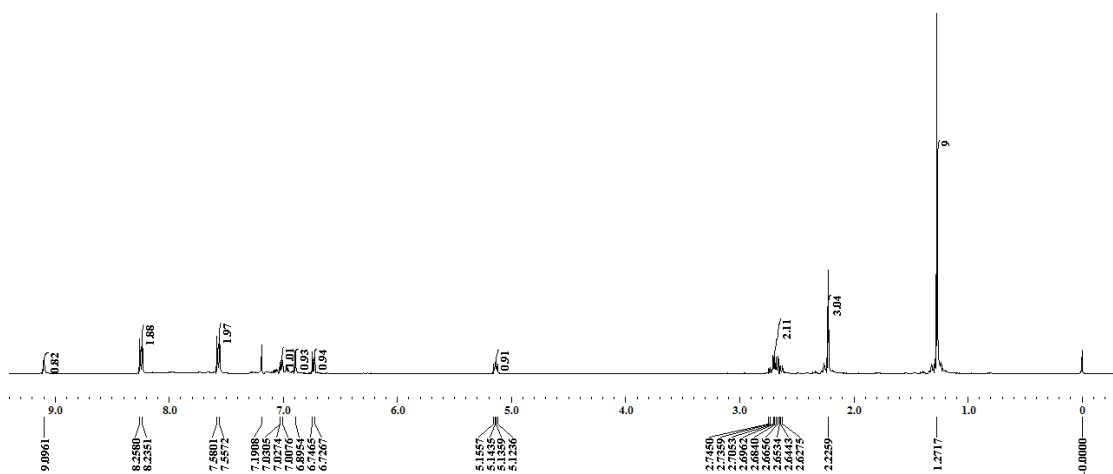
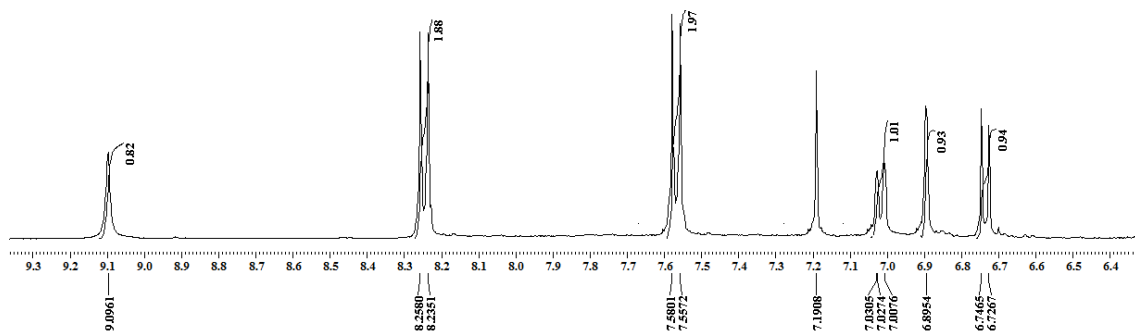
*tert*-butyl 2-(6-methyl-3-phenyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4k)



# <sup>1</sup>H NMR

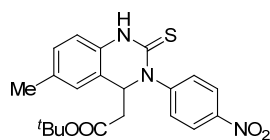


*tert*-Butyl 2-(6-methyl-3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4l)

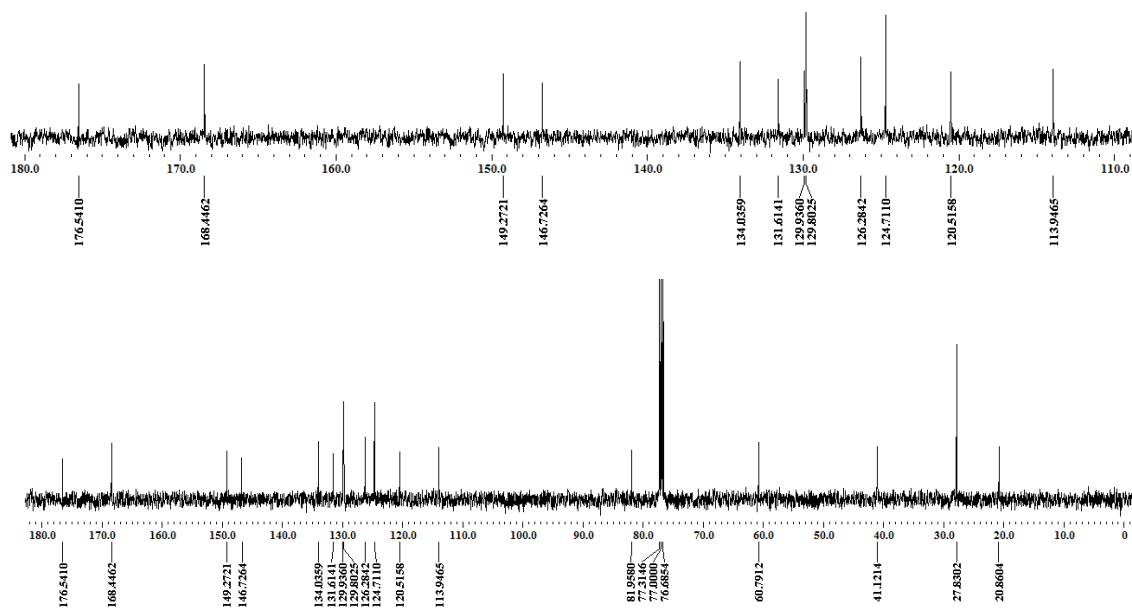




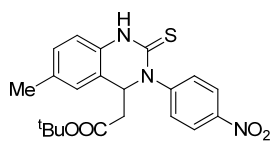
# <sup>13</sup>C NMR



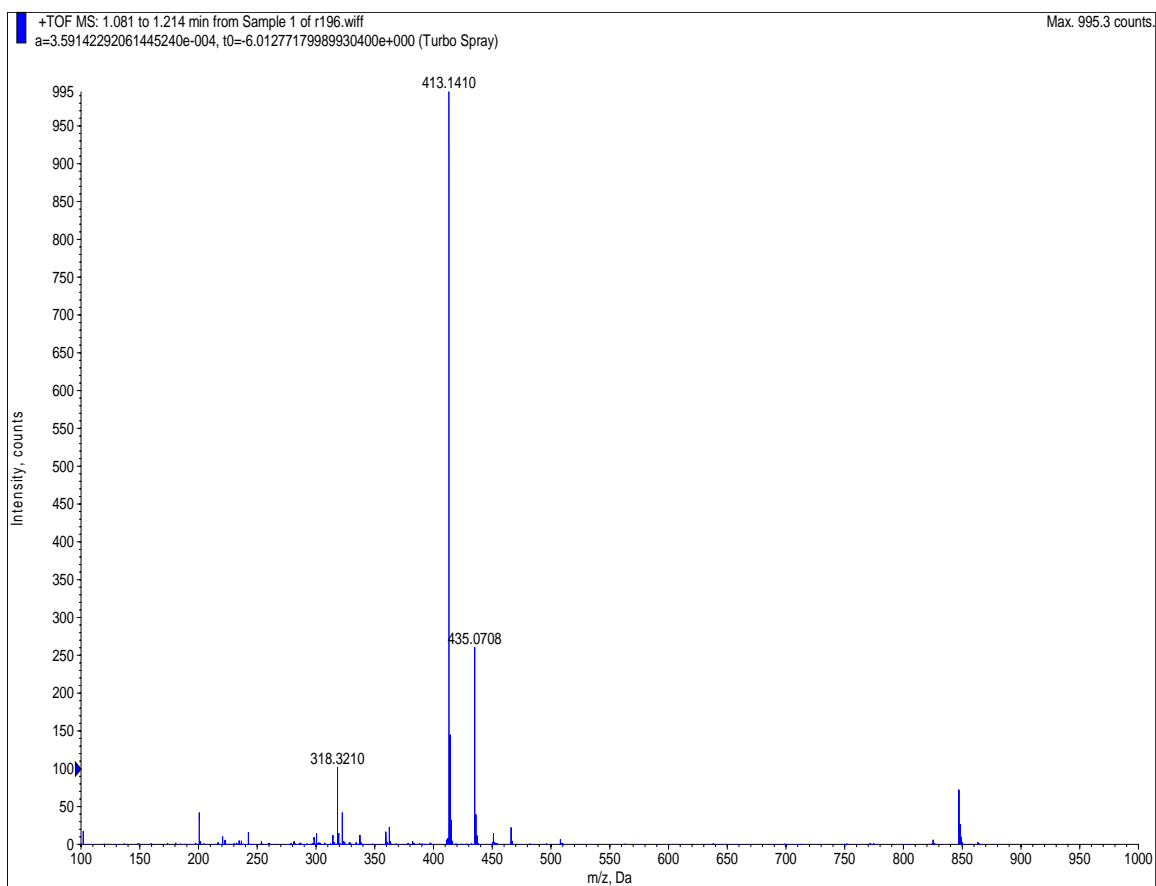
*tert*-Butyl 2-(6-methyl-3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4l)



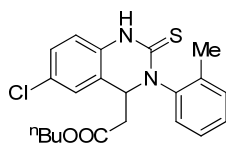
## HRMS



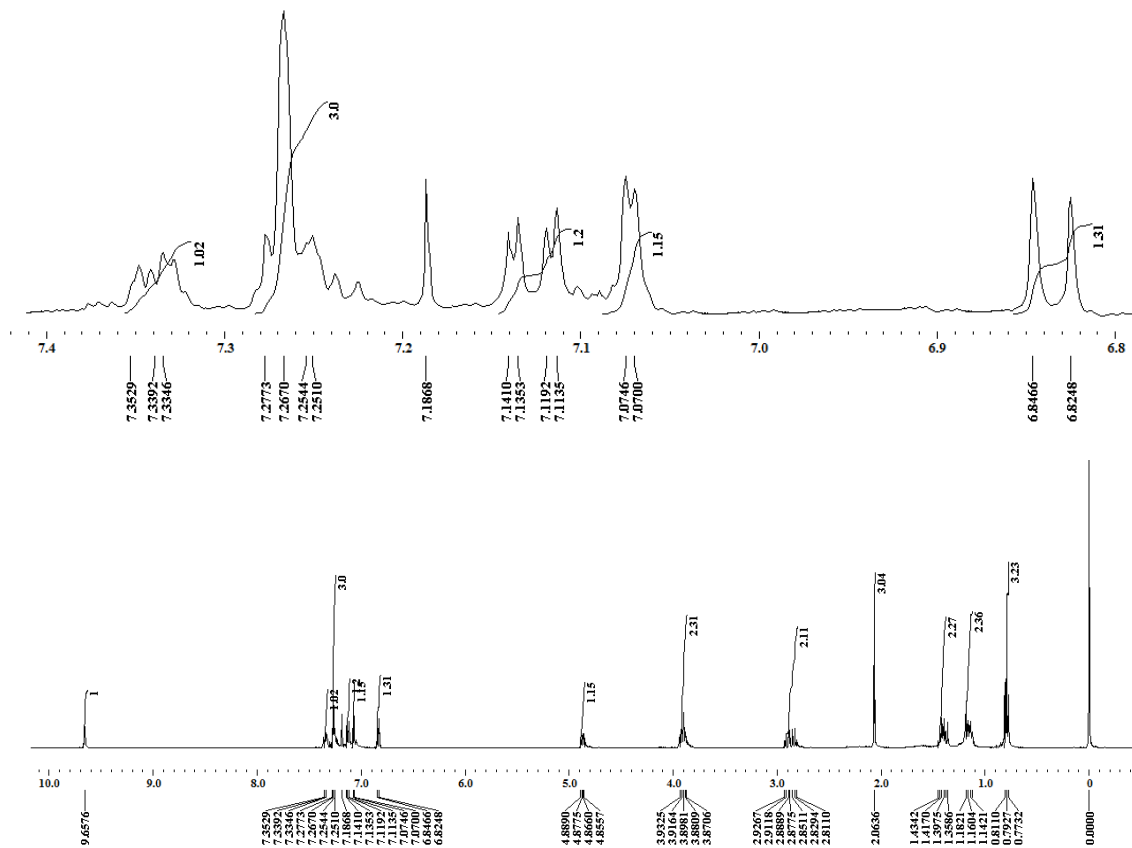
### *tert*-Butyl 2-(6-methyl-3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4I)



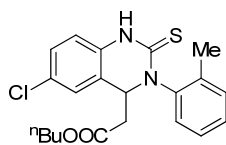
# <sup>1</sup>H NMR



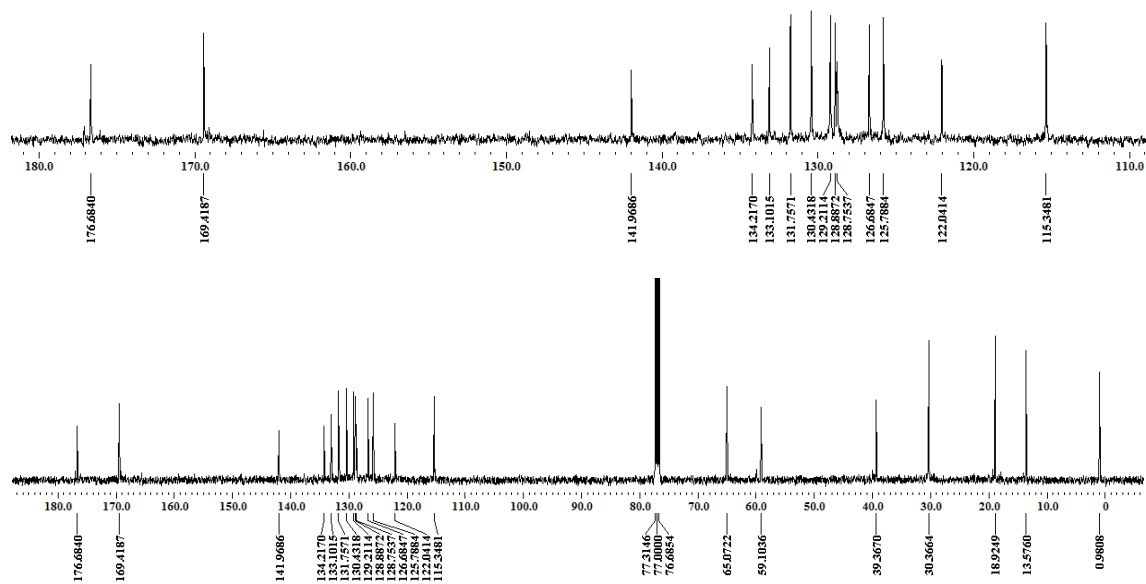
Butyl 2-(6-chloro-2-thioxo-3-(*o*-tolyl)-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4m)



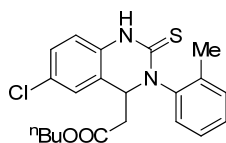
# <sup>13</sup>C NMR



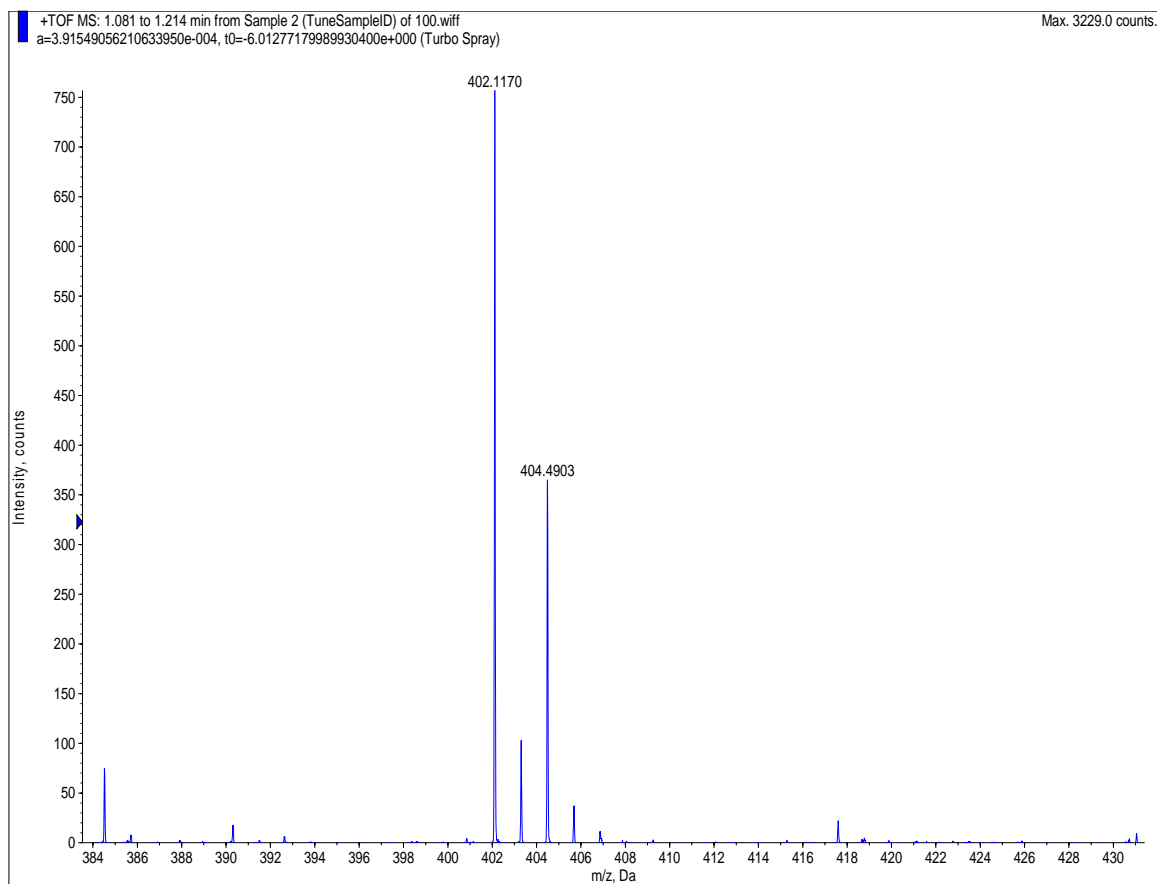
Butyl 2-(6-chloro-2-thioxo-3-(*o*-tolyl)-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4m)



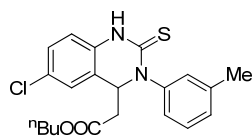
## HRMS



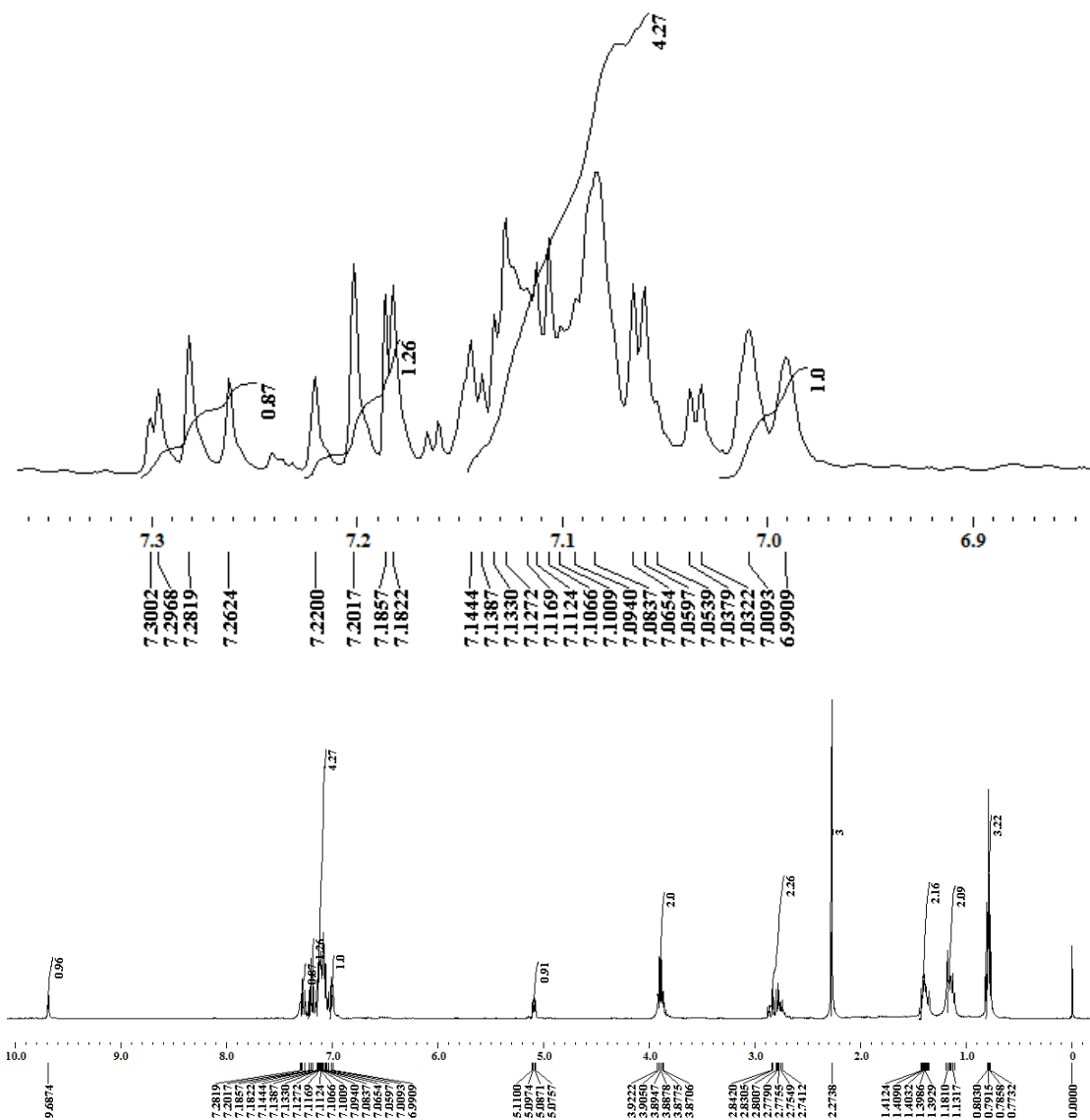
### Butyl 2-(6-chloro-2-thioxo-3-(*o*-tolyl)-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4m)



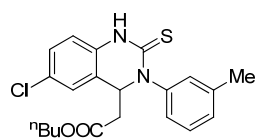
# <sup>1</sup>H NMR



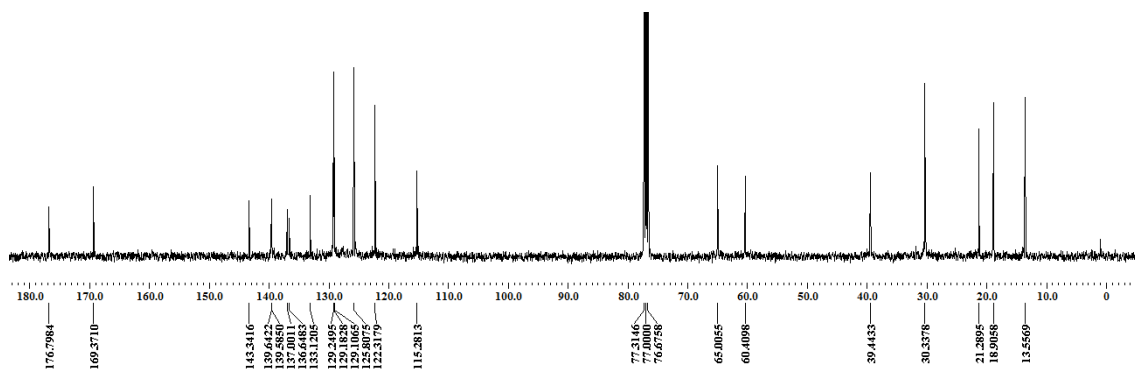
Butyl 2-(6-chloro-2-thioxo-3-(*m*-tolyl)-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4n)



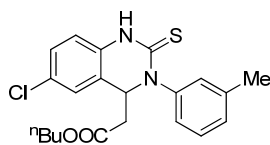
<sup>13</sup>C NMR



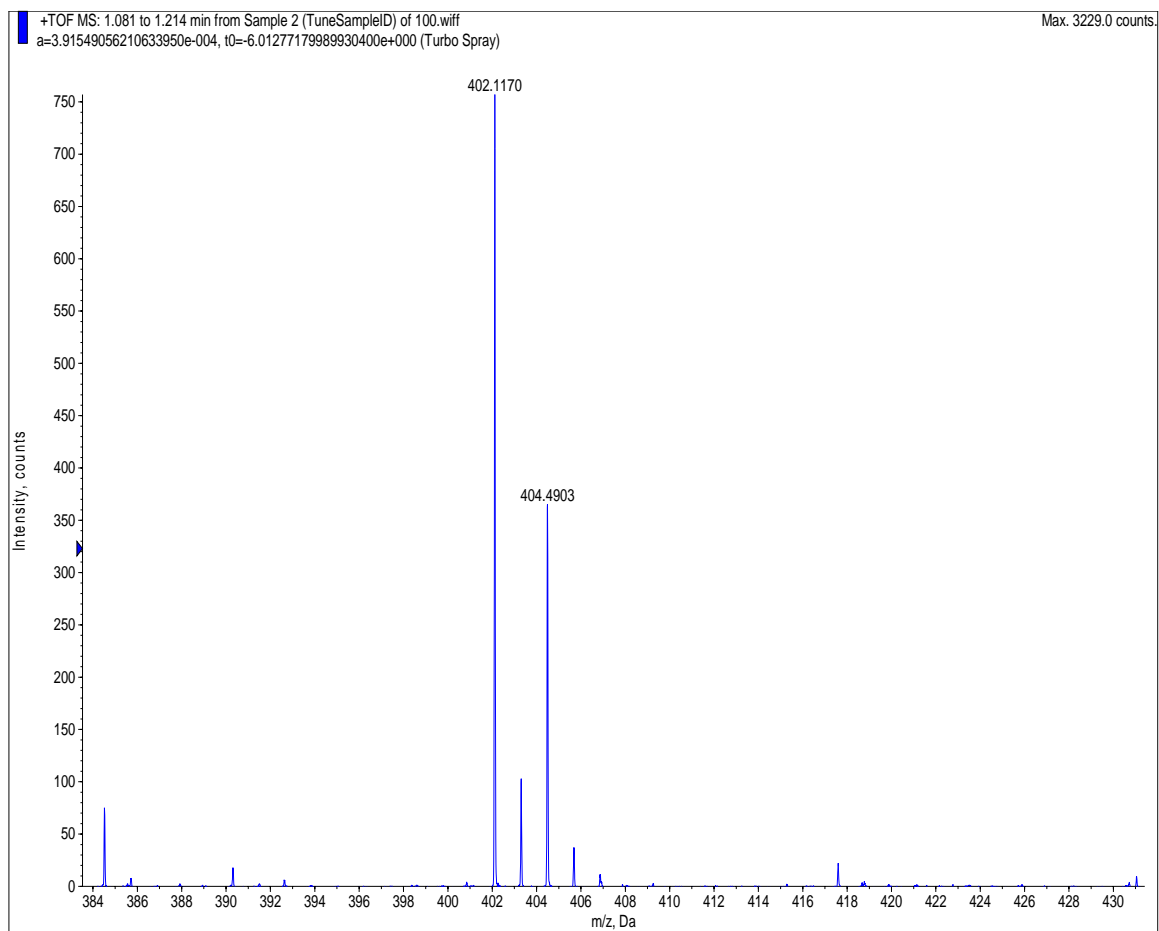
Butyl 2-(6-chloro-2-thioxo-3-(*m*-tolyl)-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4n)



## HRMS

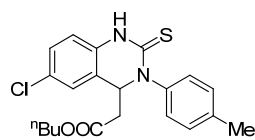


### Butyl 2-(6-chloro-2-thioxo-3-(*m*-tolyl)-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4n)

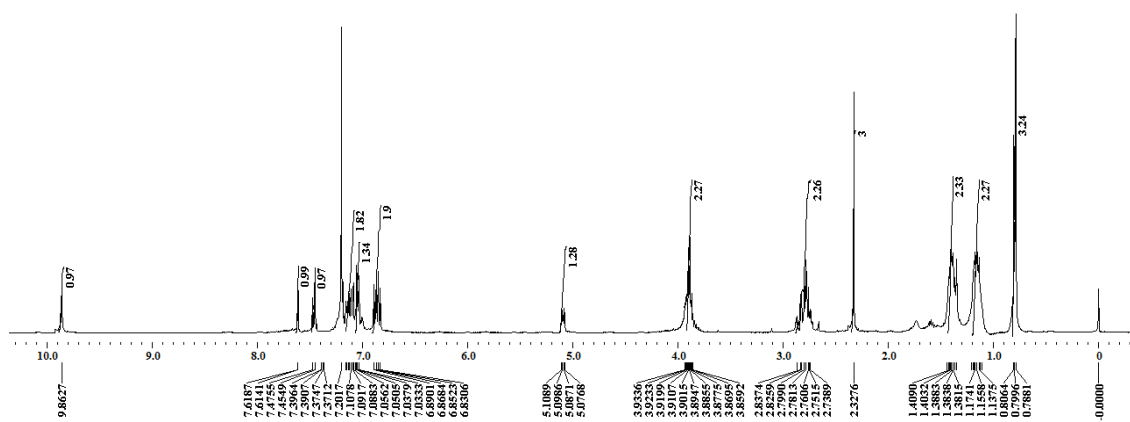
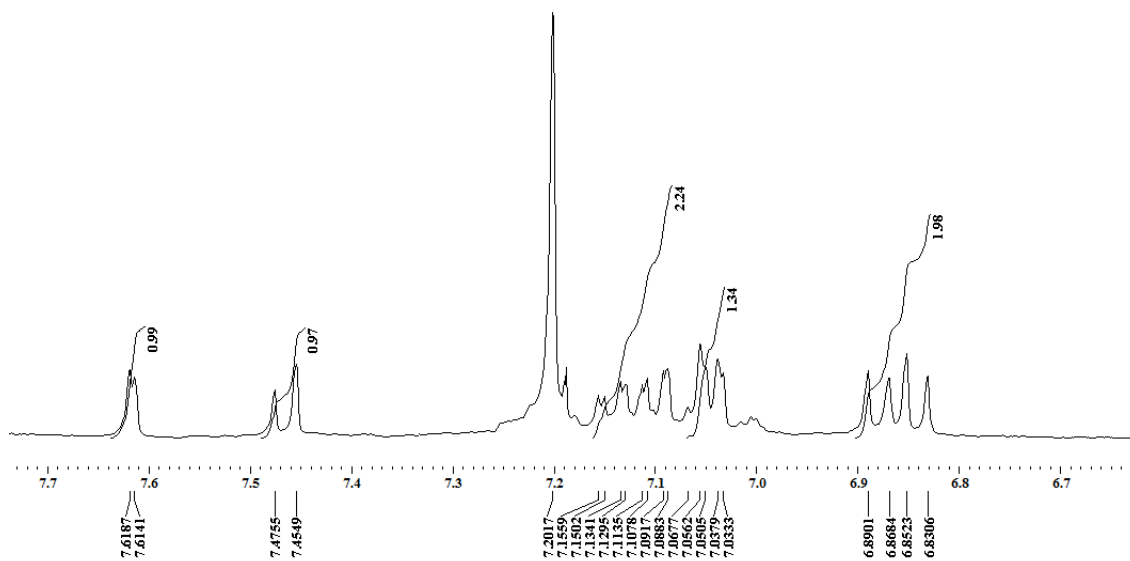




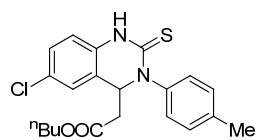
# <sup>1</sup>H NMR



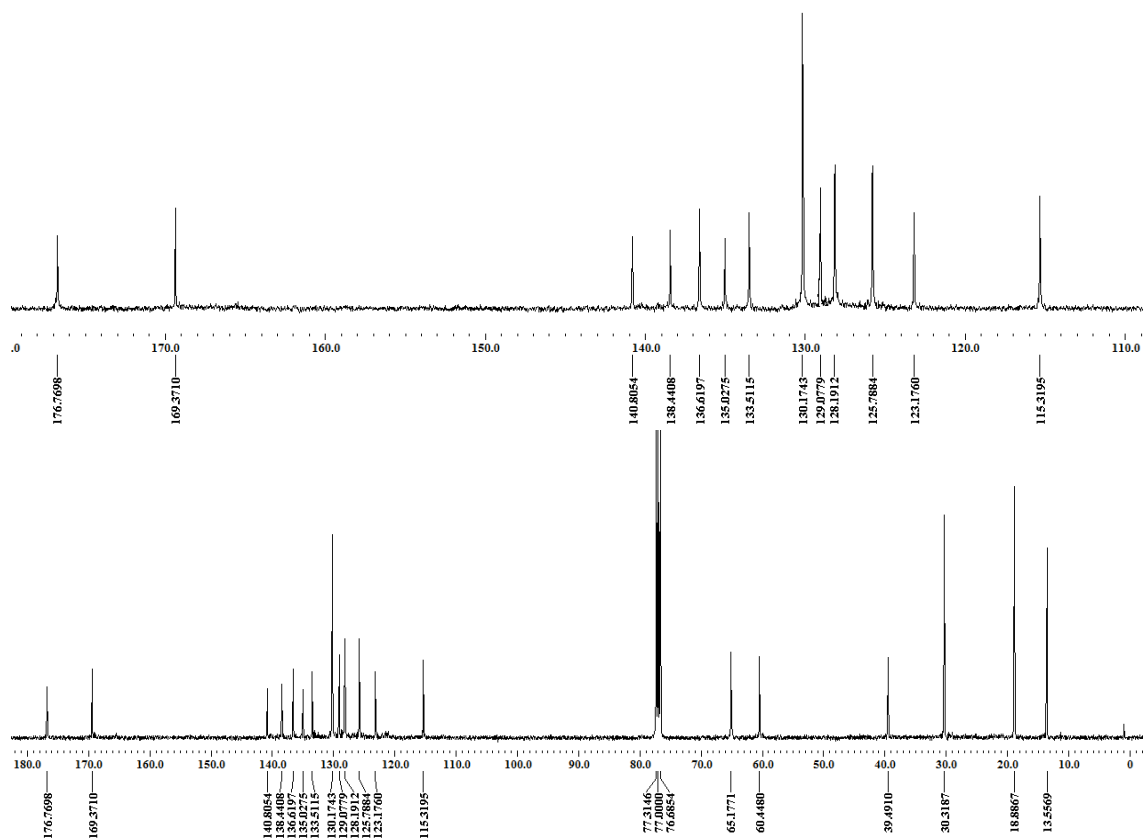
Butyl 2-(6-chloro-2-thioxo-3-(*p*-tolyl)-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4o)



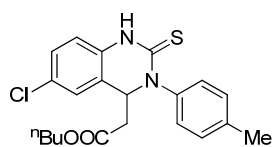
<sup>13</sup>C NMR



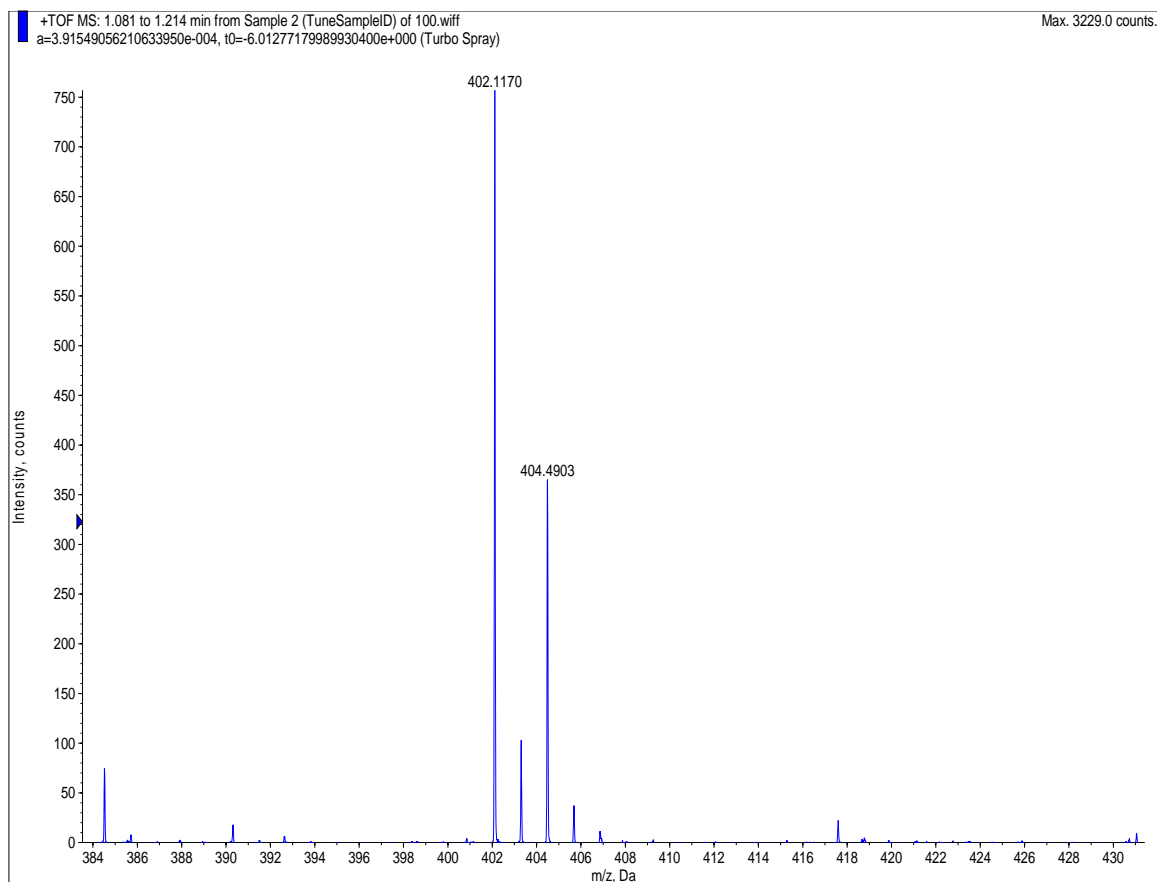
Butyl 2-(6-chloro-2-thioxo-3-(p-tolyl)-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4o)



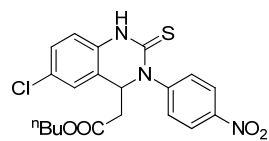
## HRMS



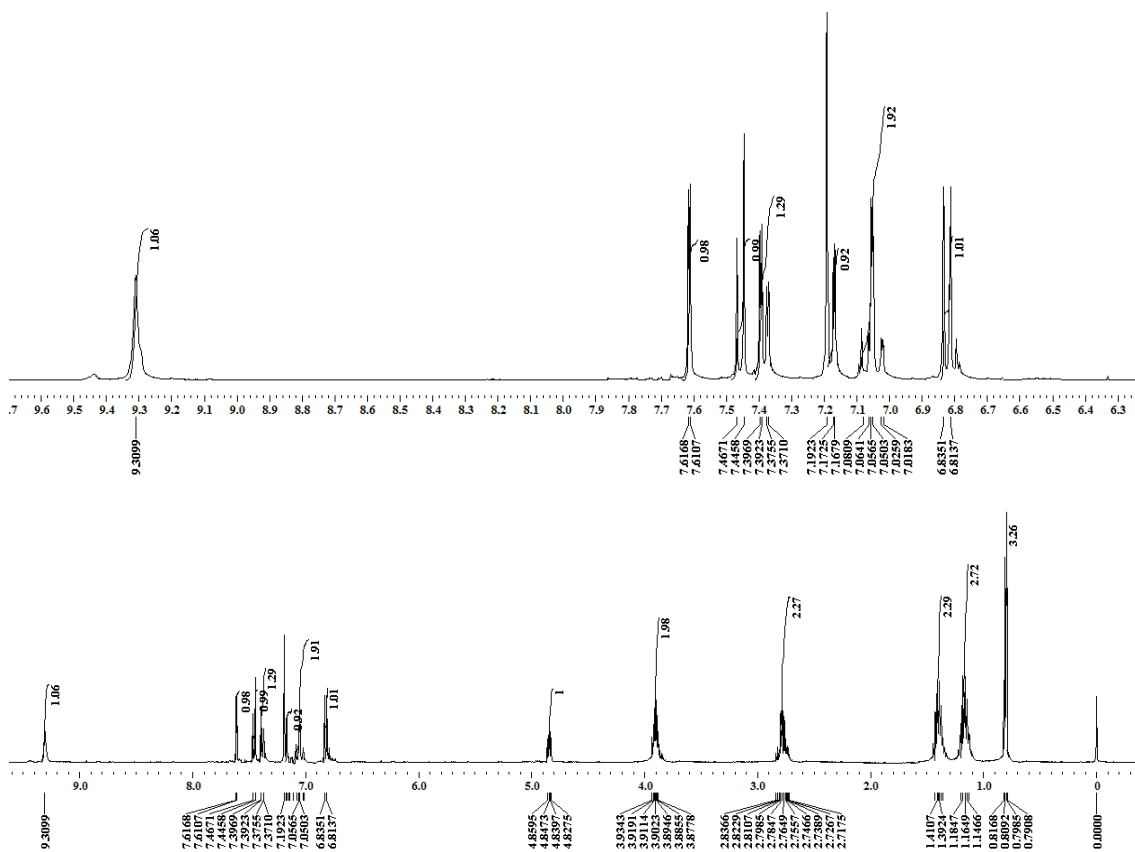
### Butyl 2-(6-chloro-2-thioxo-3-(*p*-tolyl)-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (**4o**)



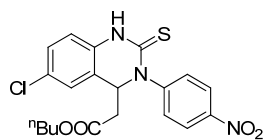
# <sup>1</sup>H NMR



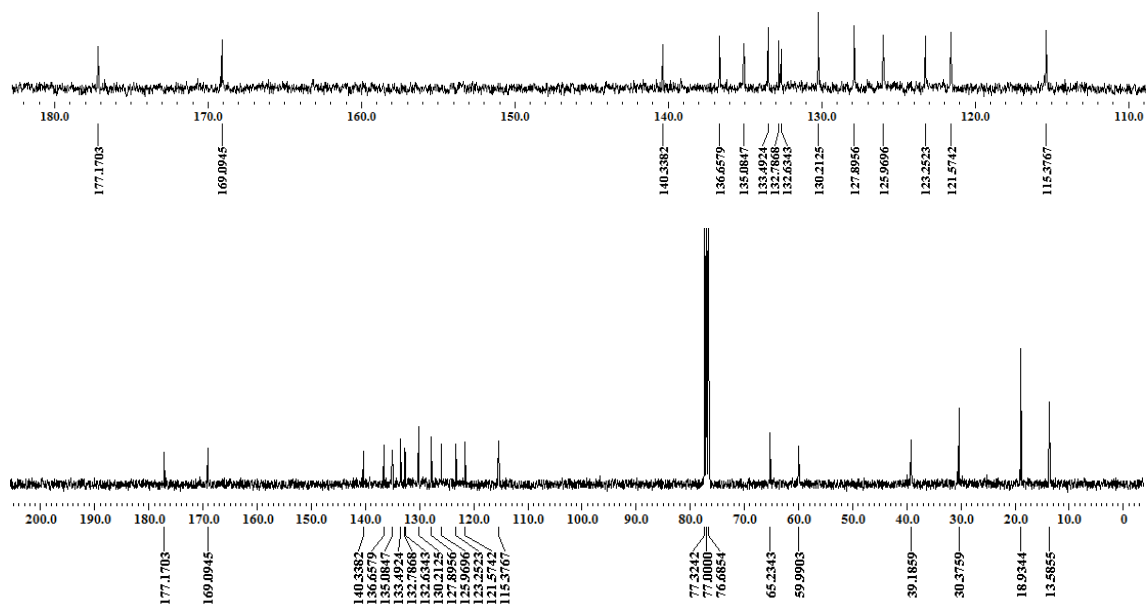
**Butyl 2-(6-chloro-3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4p)**



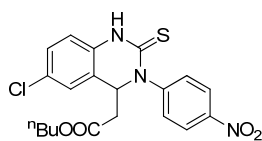
<sup>13</sup>C NMR



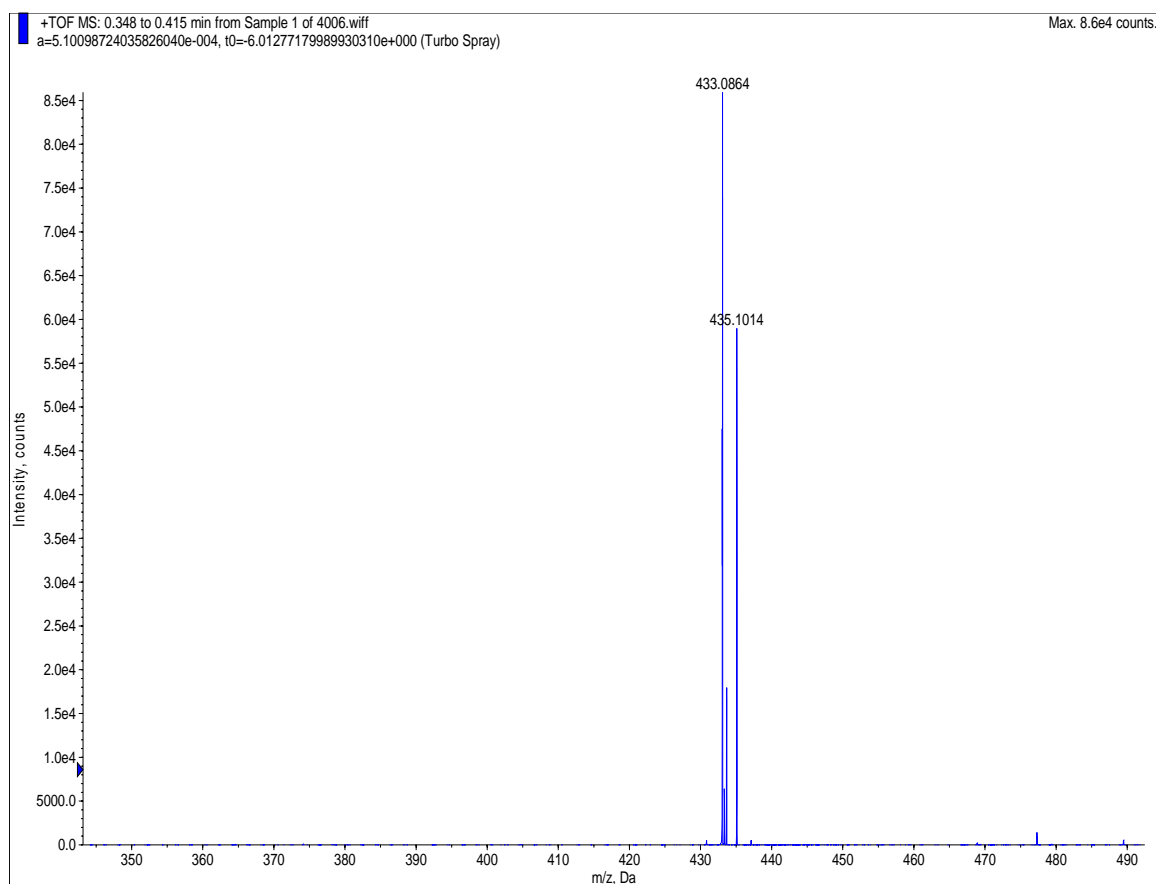
Butyl 2-(6-chloro-3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate  
(4p)



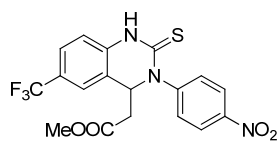
## HRMS



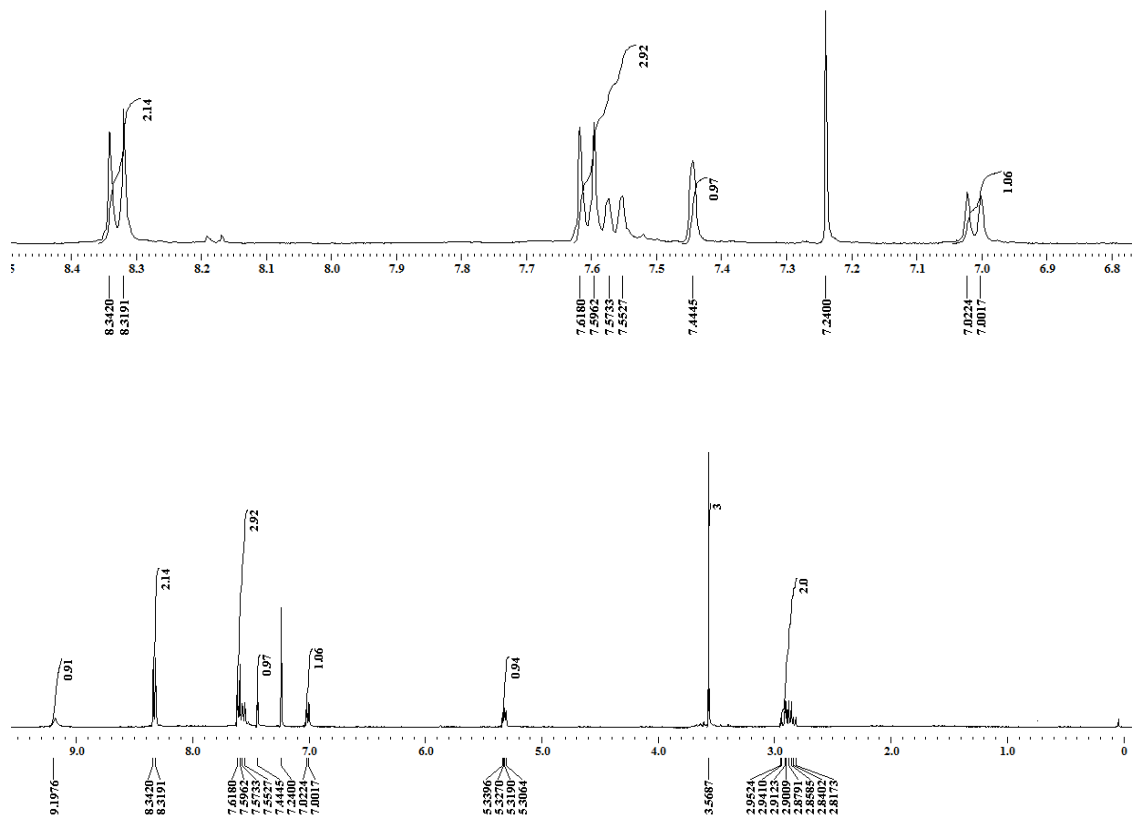
**Butyl 2-(6-chloro-3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate**  
**(4p)**



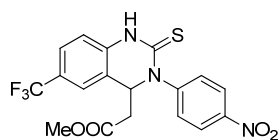
# <sup>1</sup>H NMR



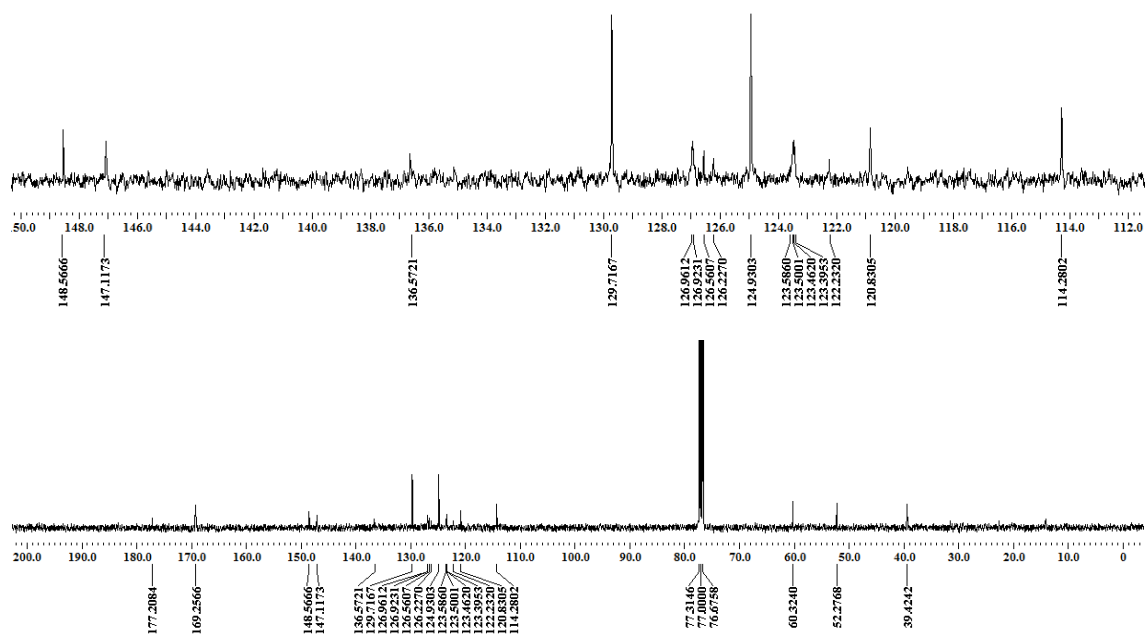
**Methyl 2-(3-(4-nitrophenyl)-2-thioxo-6-(trifluoromethyl)-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4q)**



# <sup>13</sup>C NMR

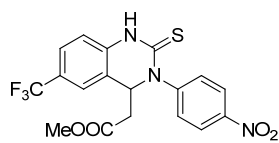


**Methyl 2-(3-(4-nitrophenyl)-2-thioxo-6-(trifluoromethyl)-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4q)**

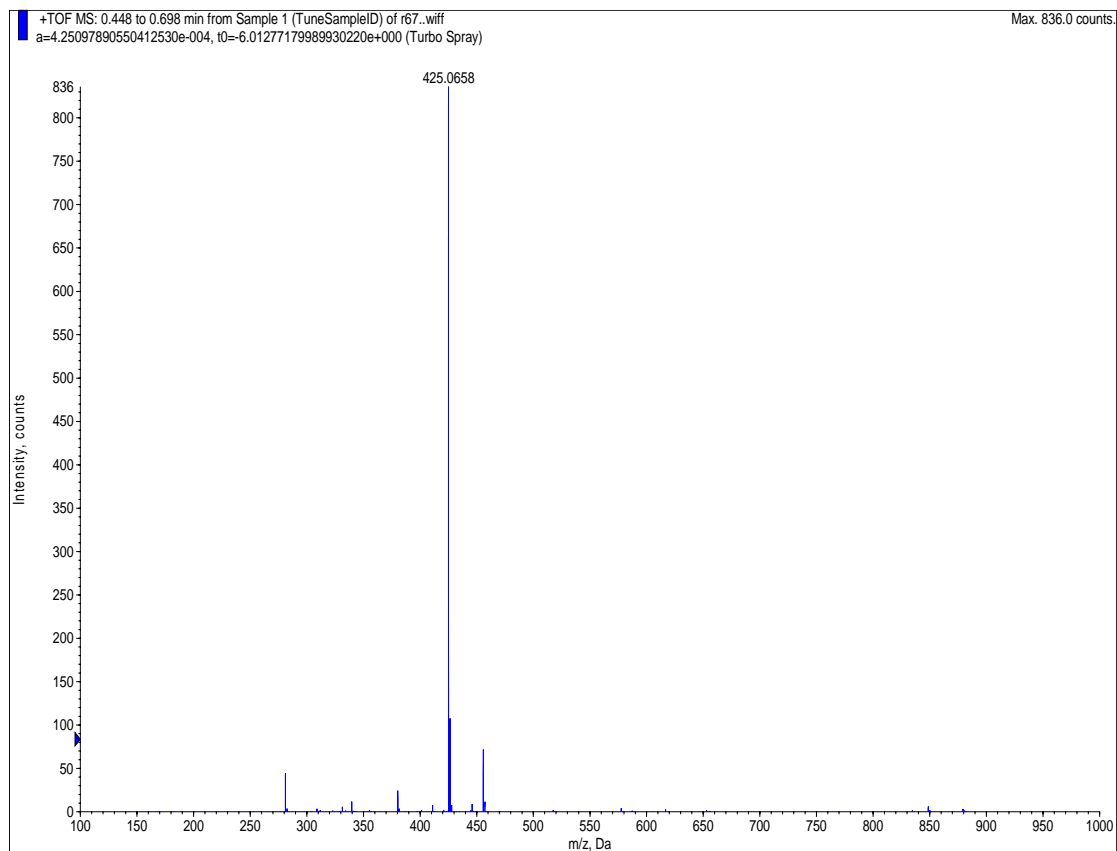




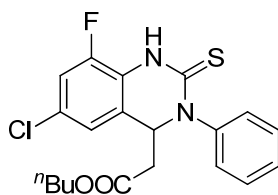
## HRMS



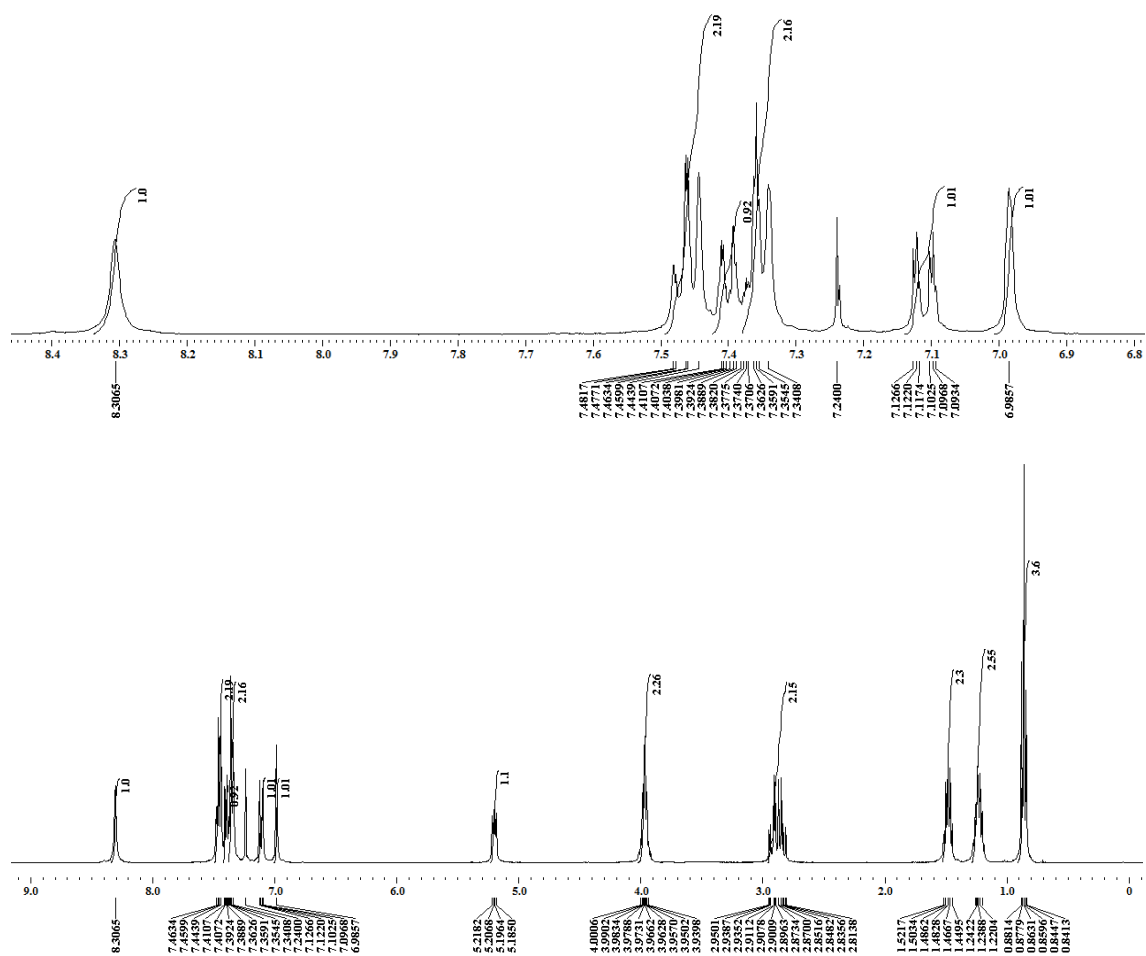
### Methyl 2-(3-(4-nitrophenyl)-2-thioxo-6-(trifluoromethyl)-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4q)



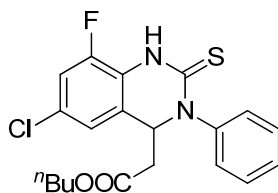
# <sup>1</sup>H NMR



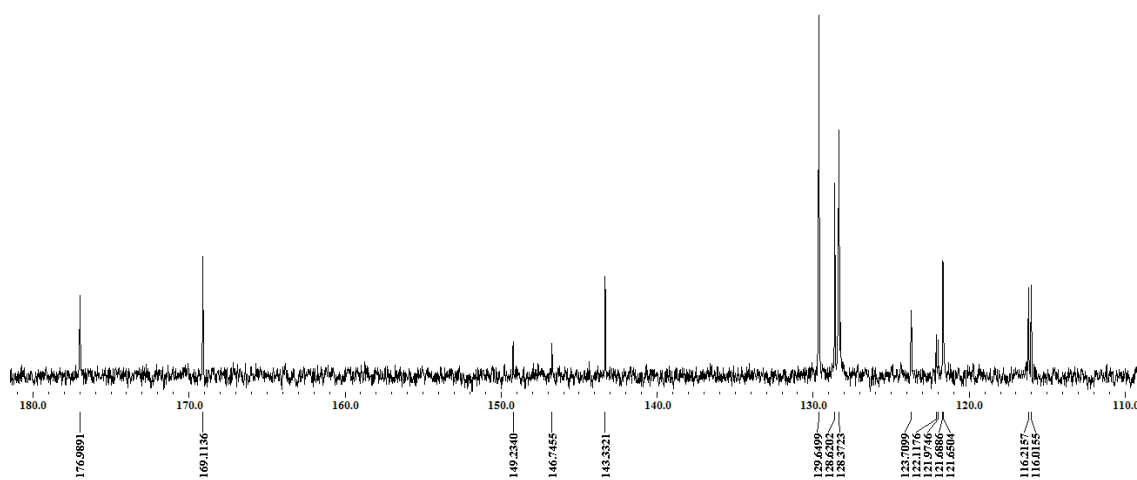
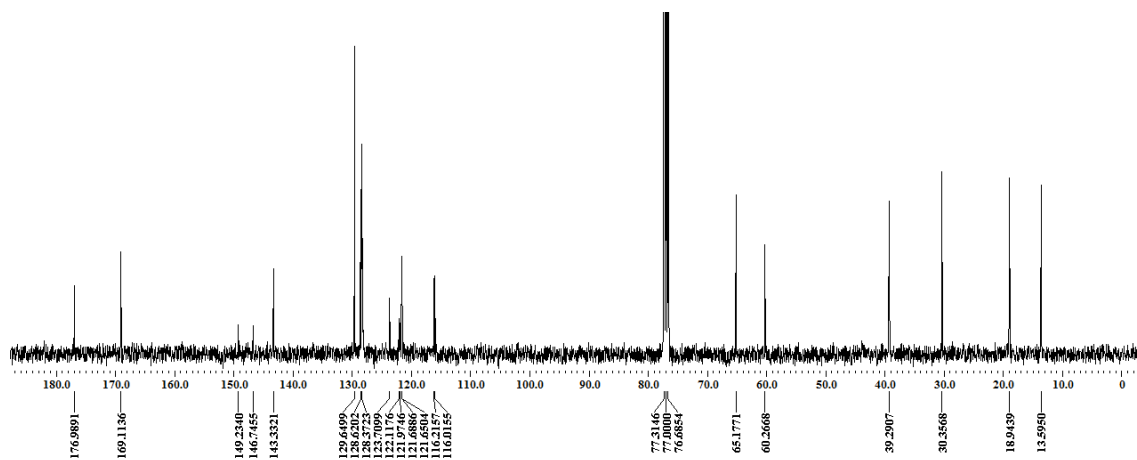
Butyl 2-(6-chloro-8-fluoro-3-phenyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate  
(4r)



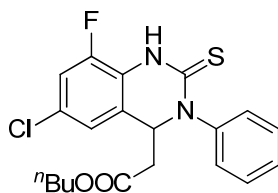
<sup>13</sup>C NMR



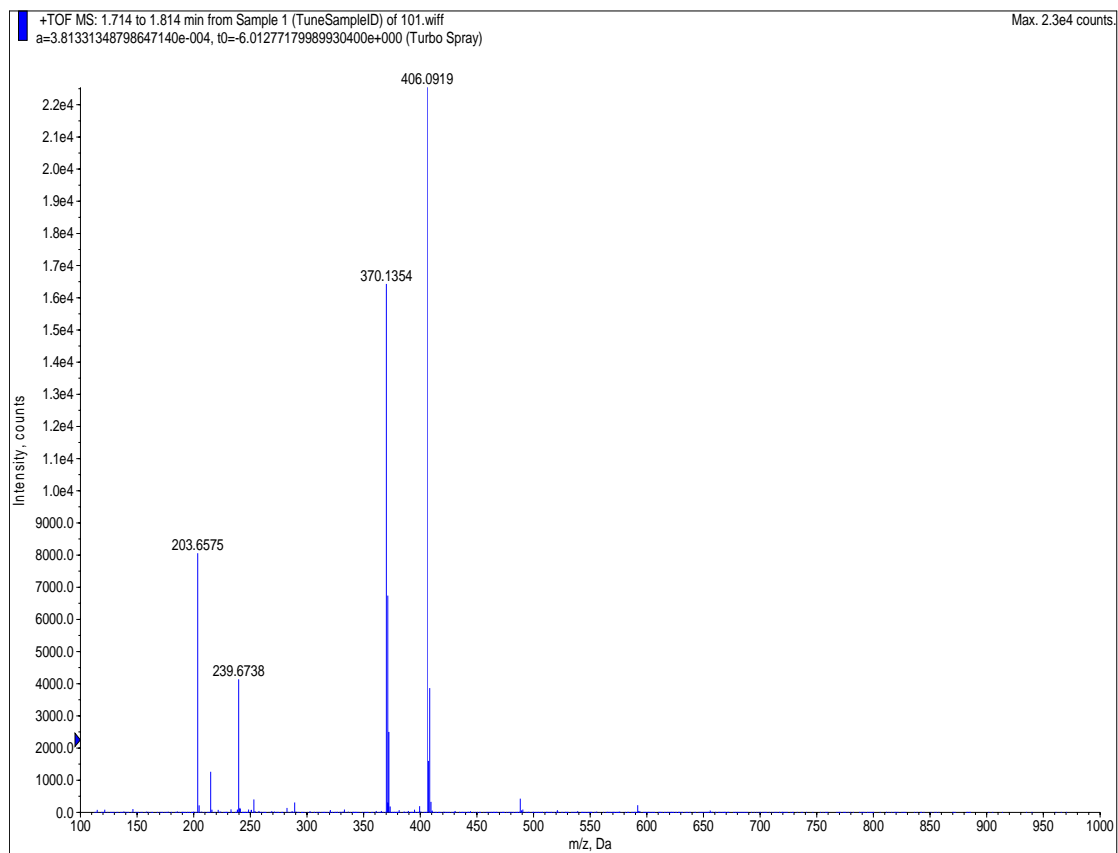
Butyl 2-(6-chloro-8-fluoro-3-phenyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate  
(4r)



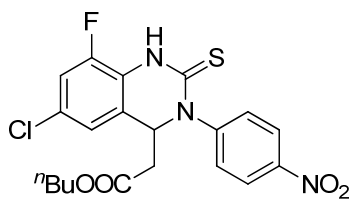
## HRMS



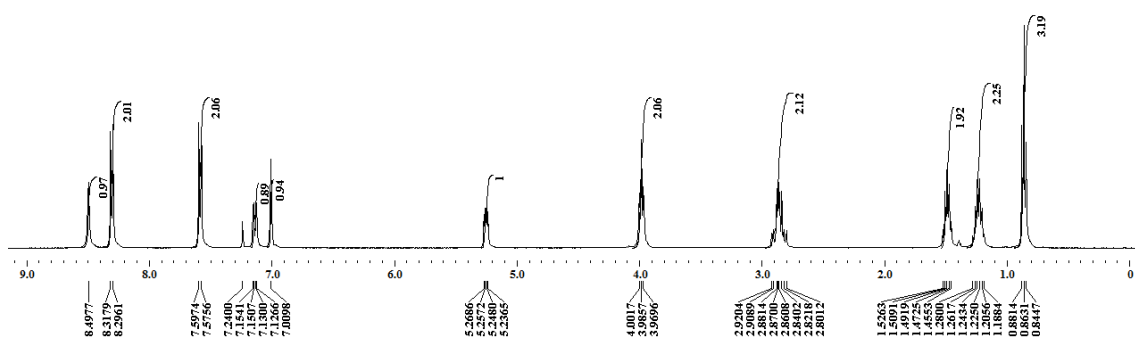
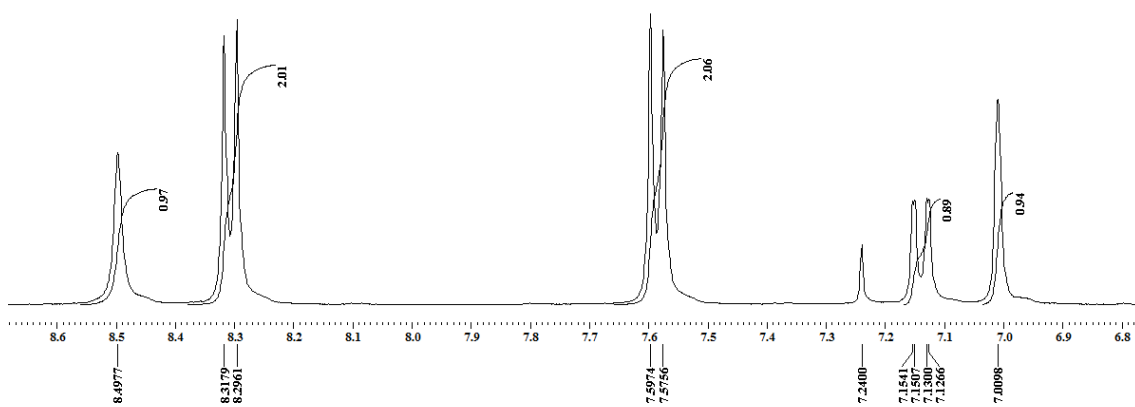
**Butyl 2-(6-chloro-8-fluoro-3-phenyl-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate  
(4r)**



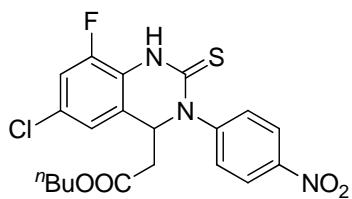
# <sup>1</sup>H NMR



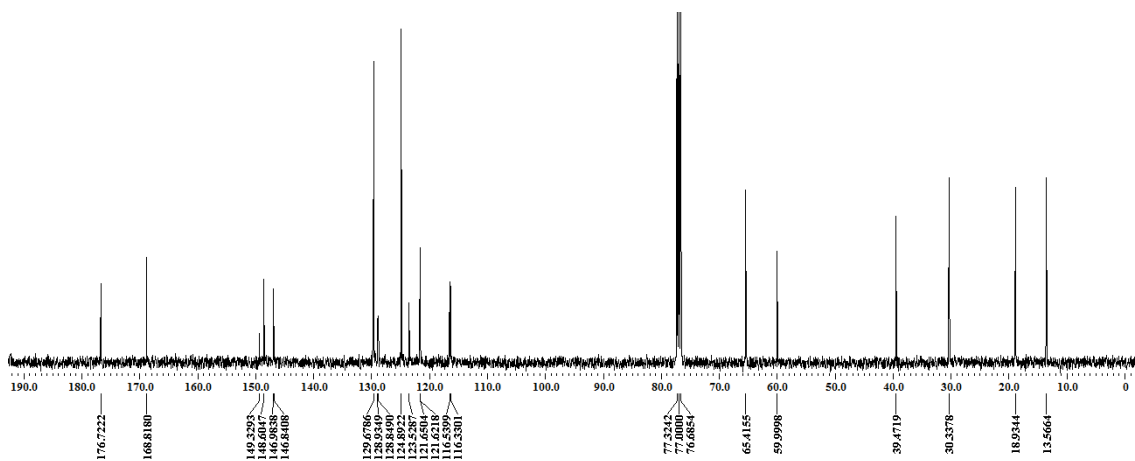
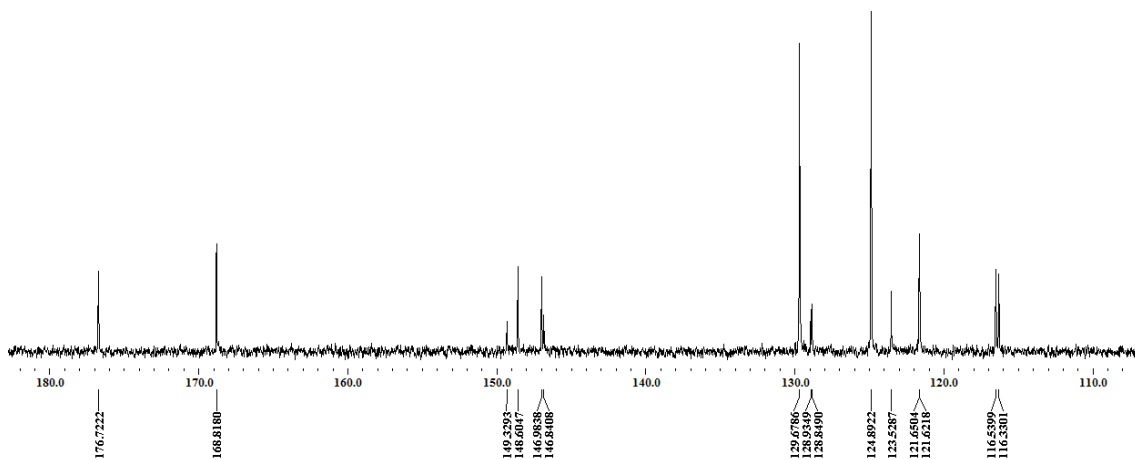
**Butyl 2-(6-chloro-8-fluoro-3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4s)**



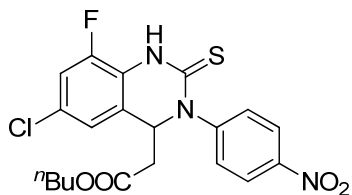
# <sup>13</sup>C NMR



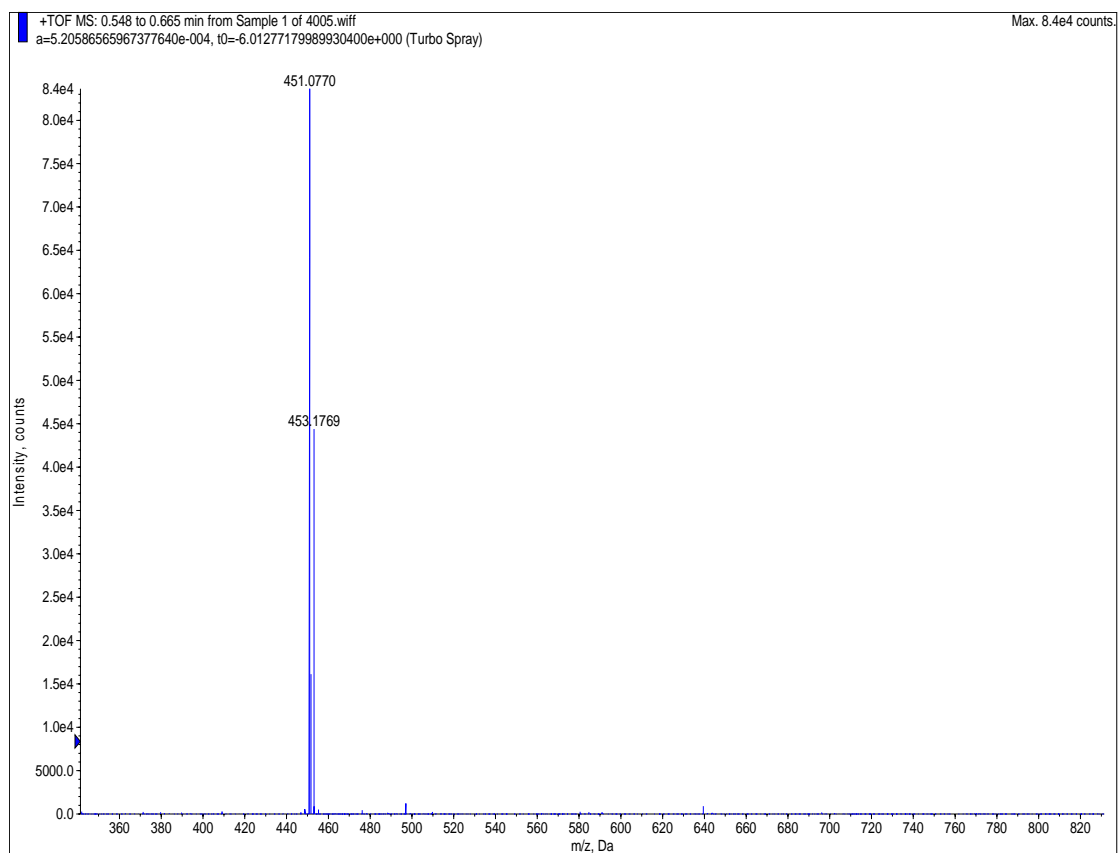
**Butyl 2-(6-chloro-8-fluoro-3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4s)**



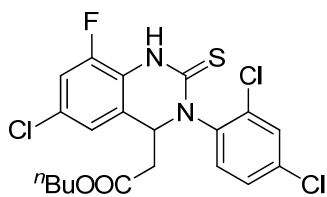
## HRMS



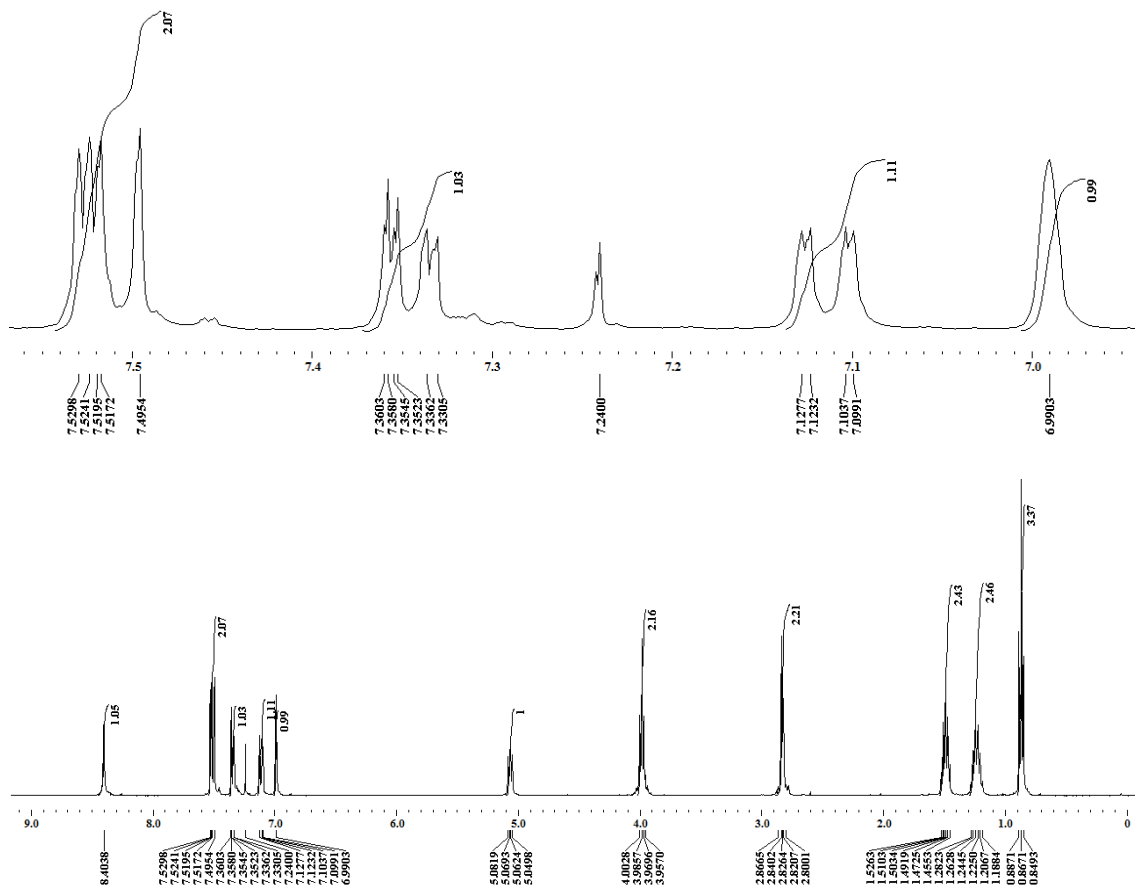
### Butyl 2-(6-chloro-8-fluoro-3-(4-nitrophenyl)-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4s)



# <sup>1</sup>H NMR

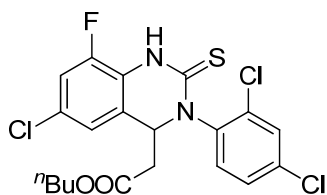


Butyl 2-(6-chloro-3-(2,4-dichlorophenyl)-8-fluoro-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4t)

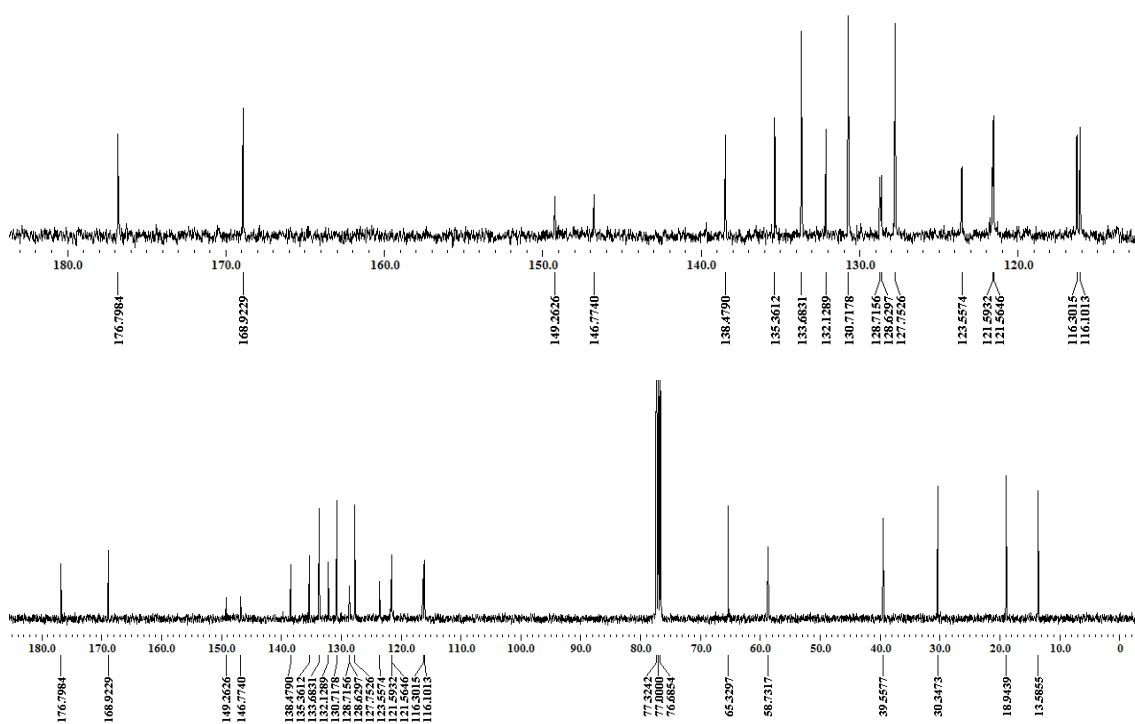




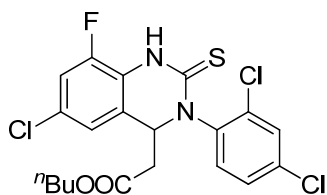
<sup>13</sup>C NMR



Butyl 2-(6-chloro-3-(2,4-dichlorophenyl)-8-fluoro-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4t)

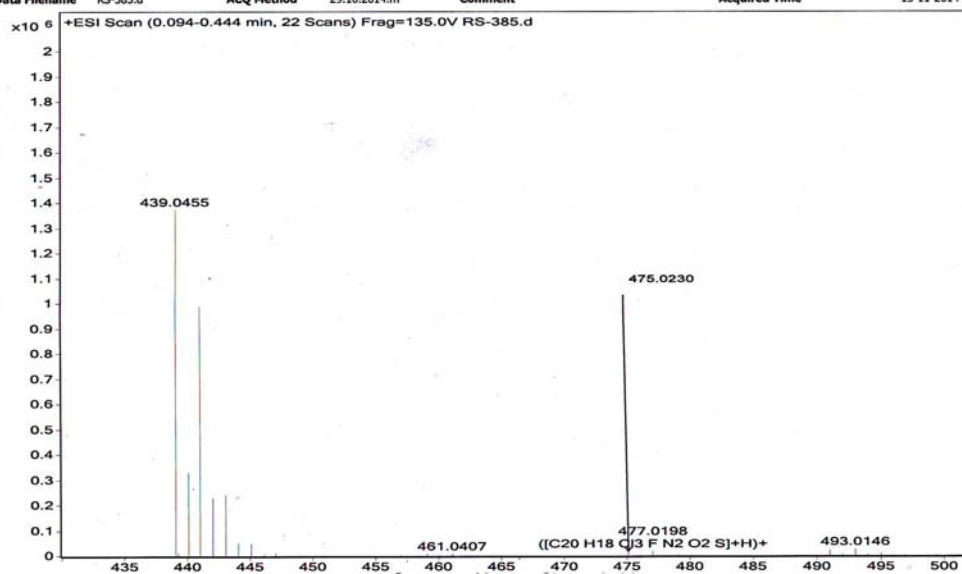


## HRMS

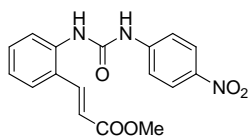


**Butyl 2-(6-chloro-3-(2,4-dichlorophenyl)-8-fluoro-2-thioxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (4t)**

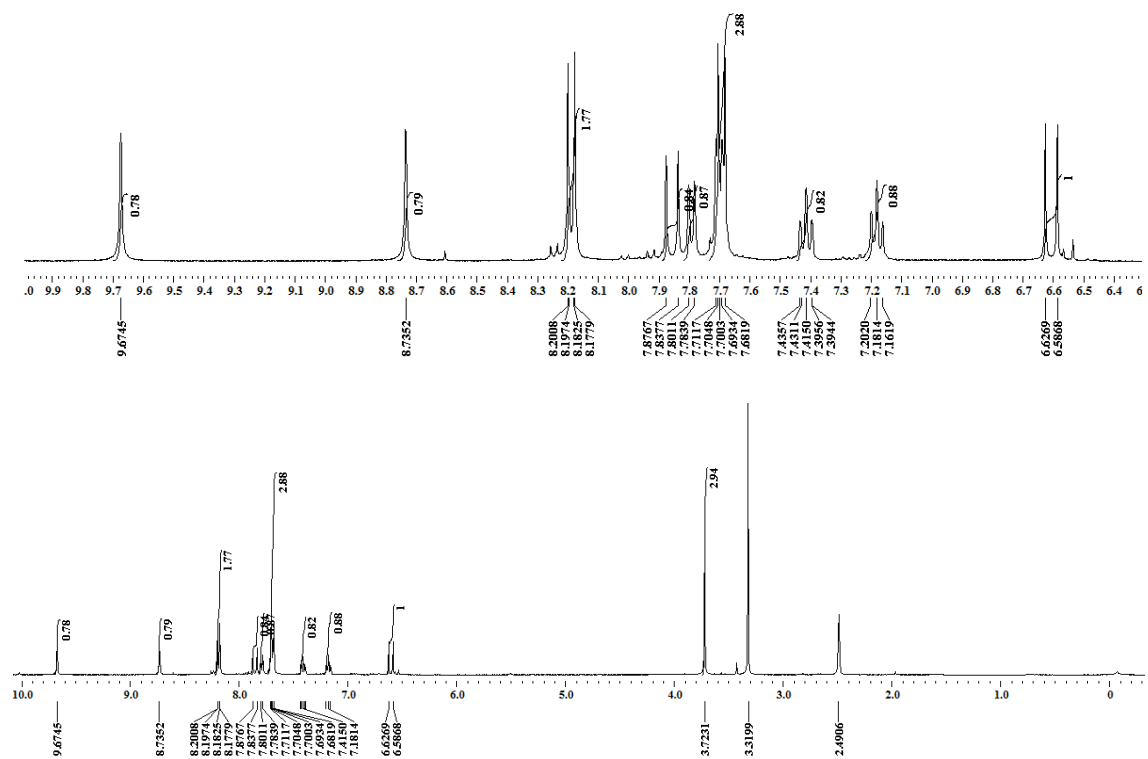
Sample Name	RS-385	Position	P1F4	Instrument Name	6530 QTOF LCMS	User Name	lcmsdu-PC\admin
Inj Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	RS-385.d	ACQ Method	29.10.2014.m	Comment		Acquired Time	13-11-2014 16:08:29



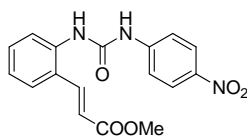
# <sup>1</sup>H NMR



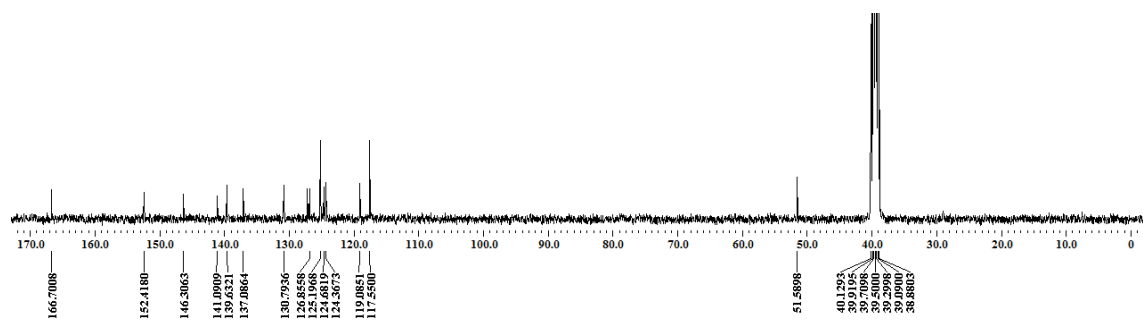
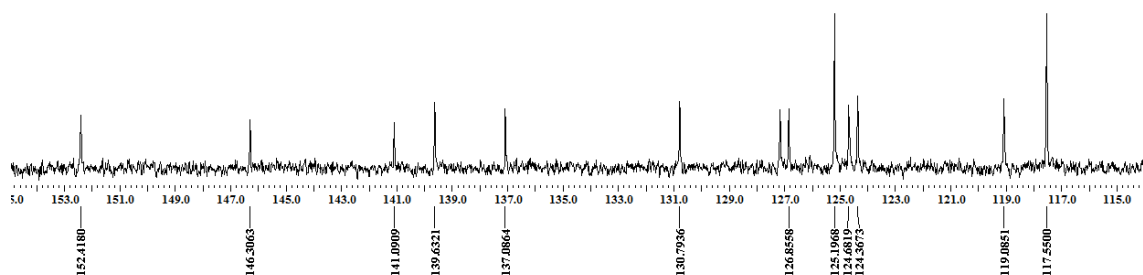
(*E*)-Methyl 3-(2-(3-(4-nitrophenyl)ureido)phenyl)acrylate  
(5a')



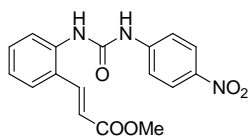
<sup>13</sup>C NMR



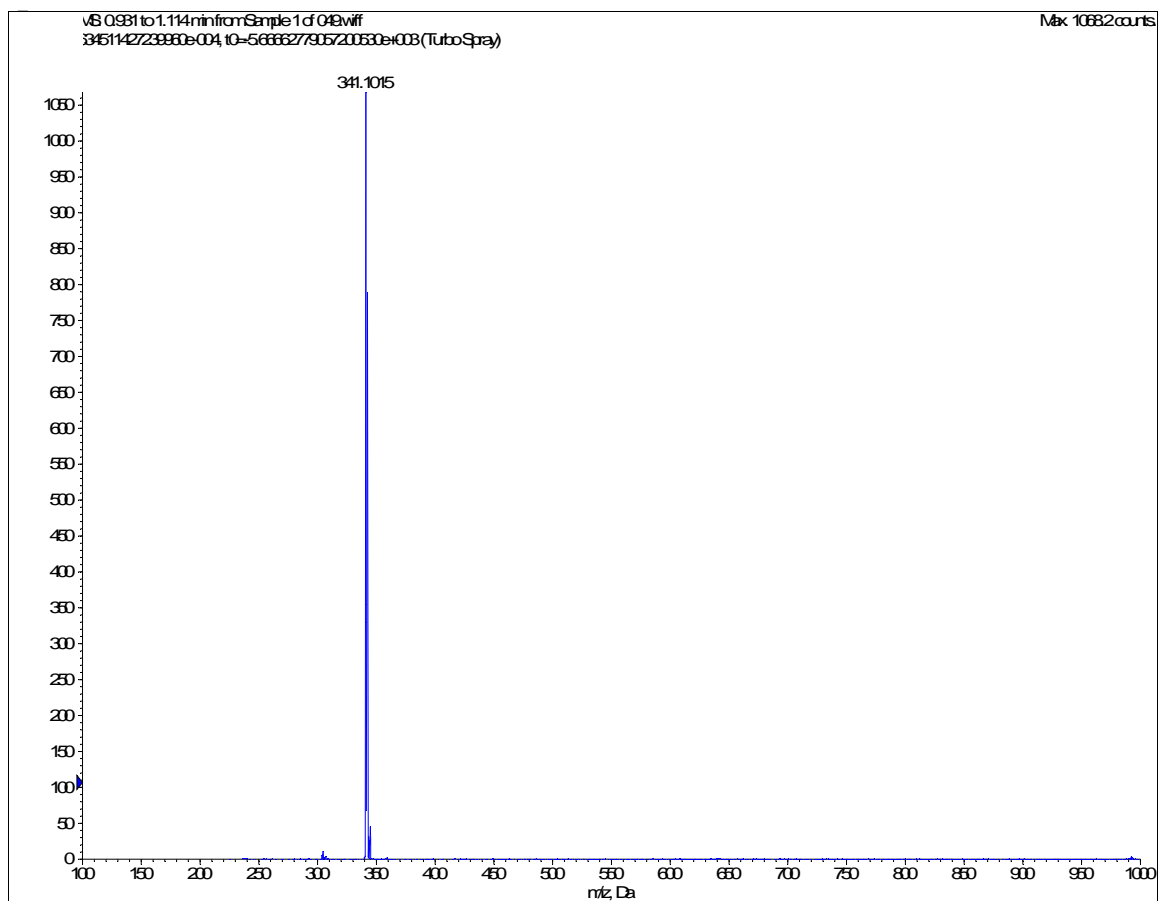
**(E)-Methyl 3-(2-(3-(4-nitrophenyl)ureido)phenyl)acrylate**  
**(5a')**



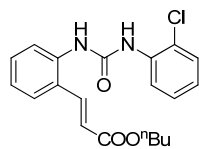
### HRMS



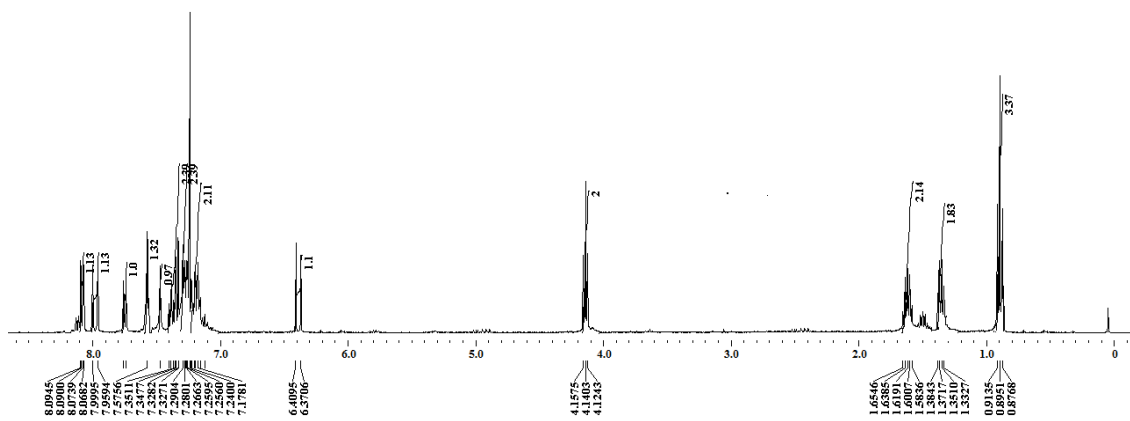
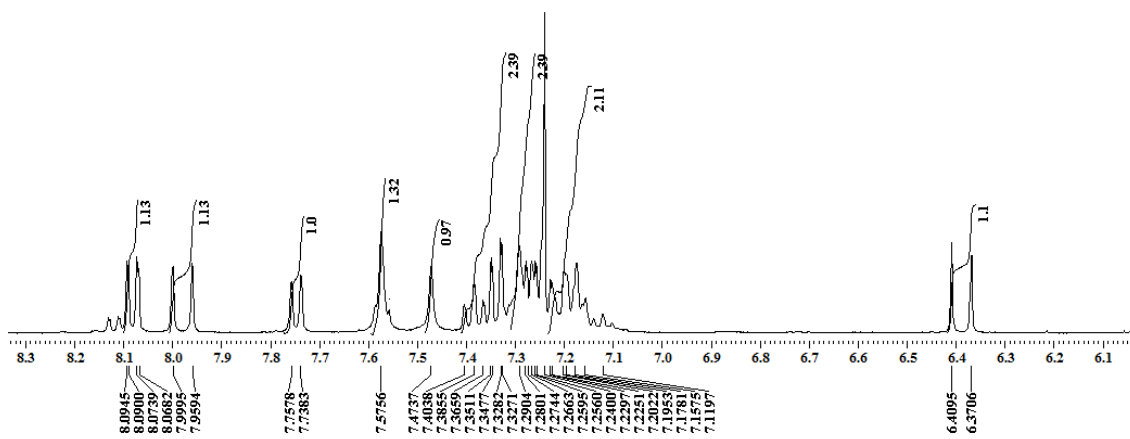
**(E)-Methyl 3-(2-(3-(4-nitrophenyl)ureido)phenyl)acrylate**  
**(5a')**



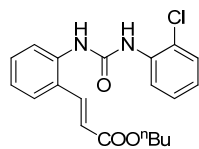
# <sup>1</sup>H NMR



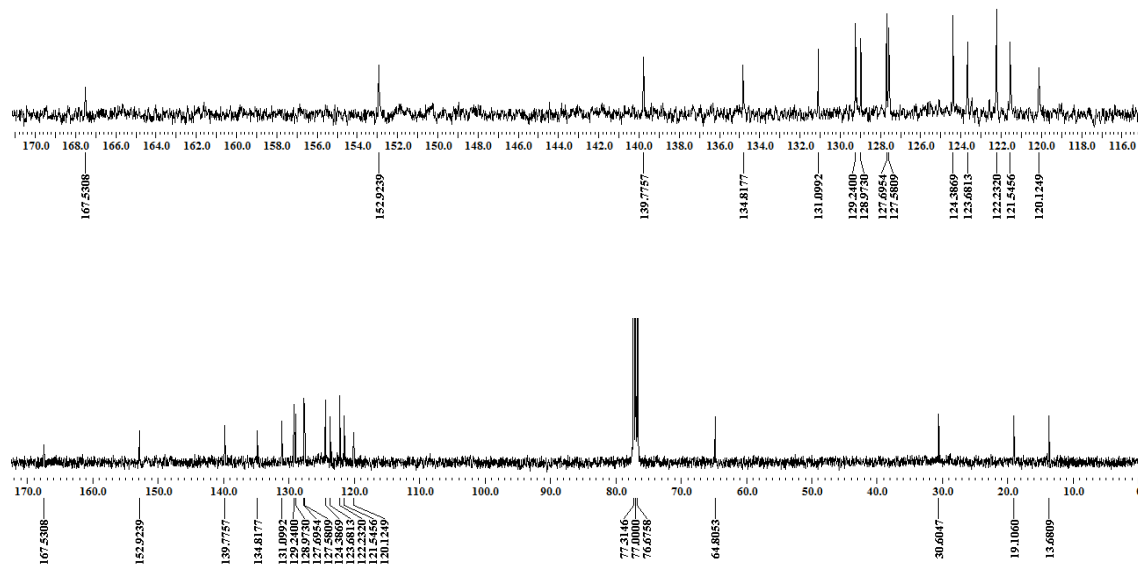
(*E*)-Butyl 3-(2-(3-(2-chlorophenyl)ureido)phenyl)acrylate (5b')



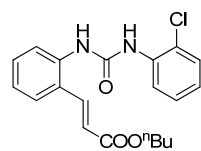
# <sup>13</sup>C NMR



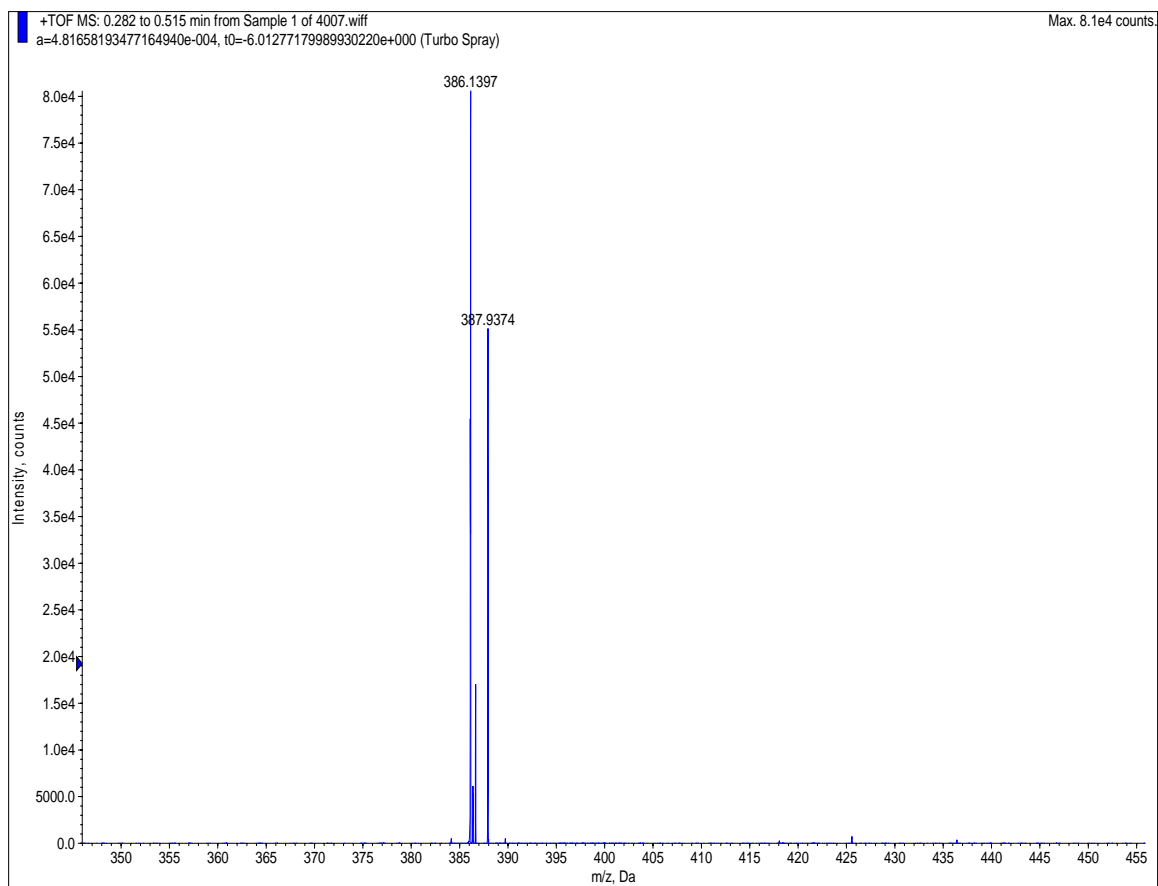
**(E)-Butyl 3-(2-(3-(2-chlorophenyl)ureido)phenyl)acrylate (5b')**



# HRMS

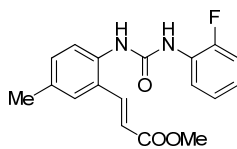


**(E)-Butyl 3-(2-(3-(2-chlorophenyl)ureido)phenyl)acrylate (5b')**



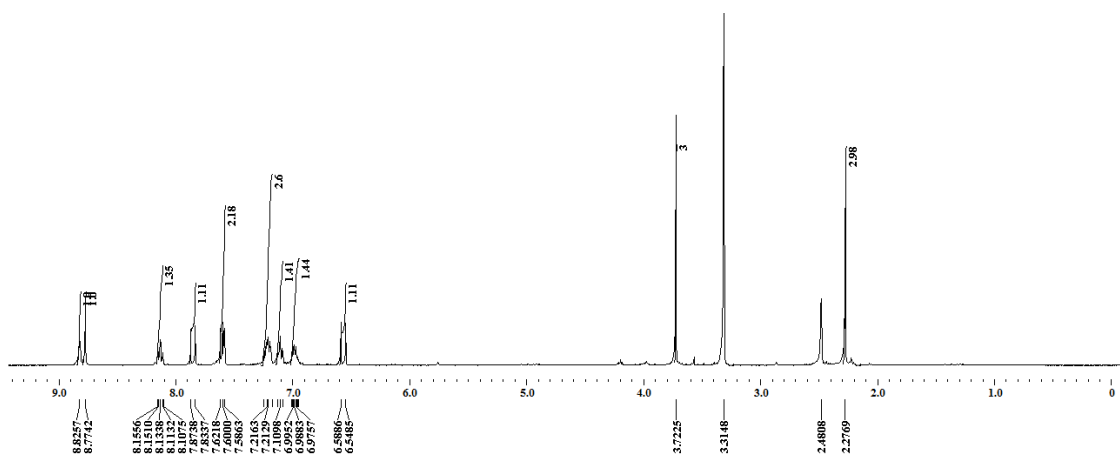
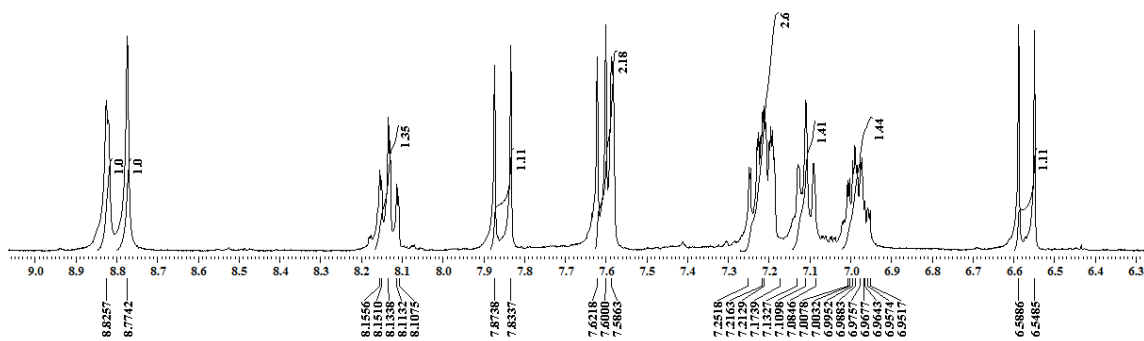


# <sup>1</sup>H NMR

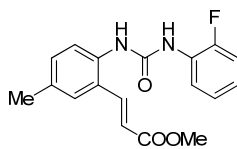


(*E*)-Methyl 3-(2-(3-(2-fluorophenyl)ureido)-5-methylphenyl)acrylate

(5c')

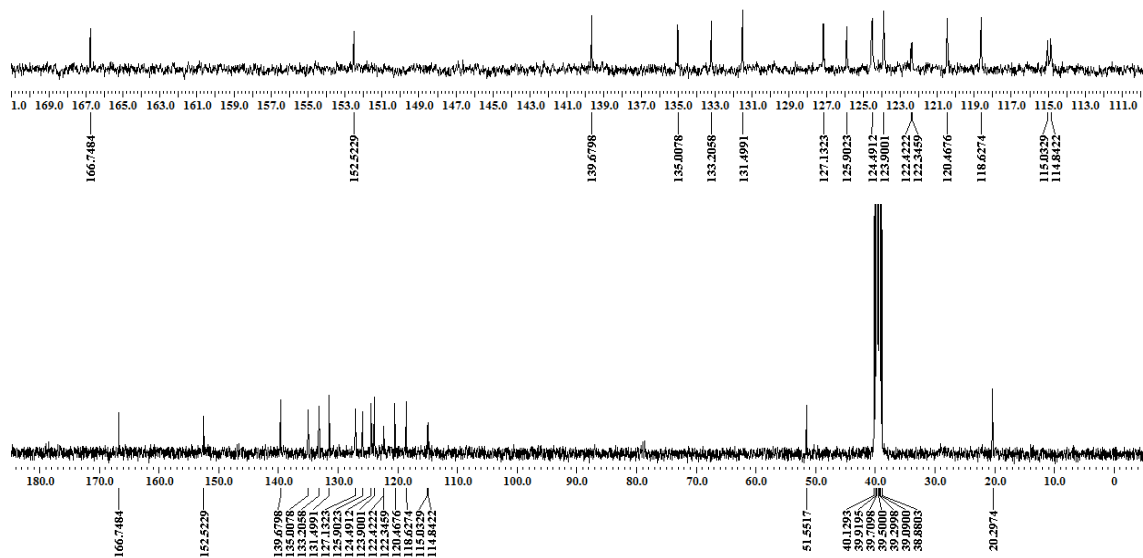


# <sup>13</sup>C NMR

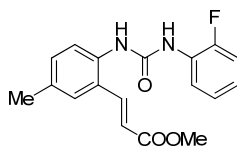


**(E)-Methyl 3-(2-(3-(2-fluorophenyl)ureido)-5-methylphenyl)acrylate**

**(5c')**

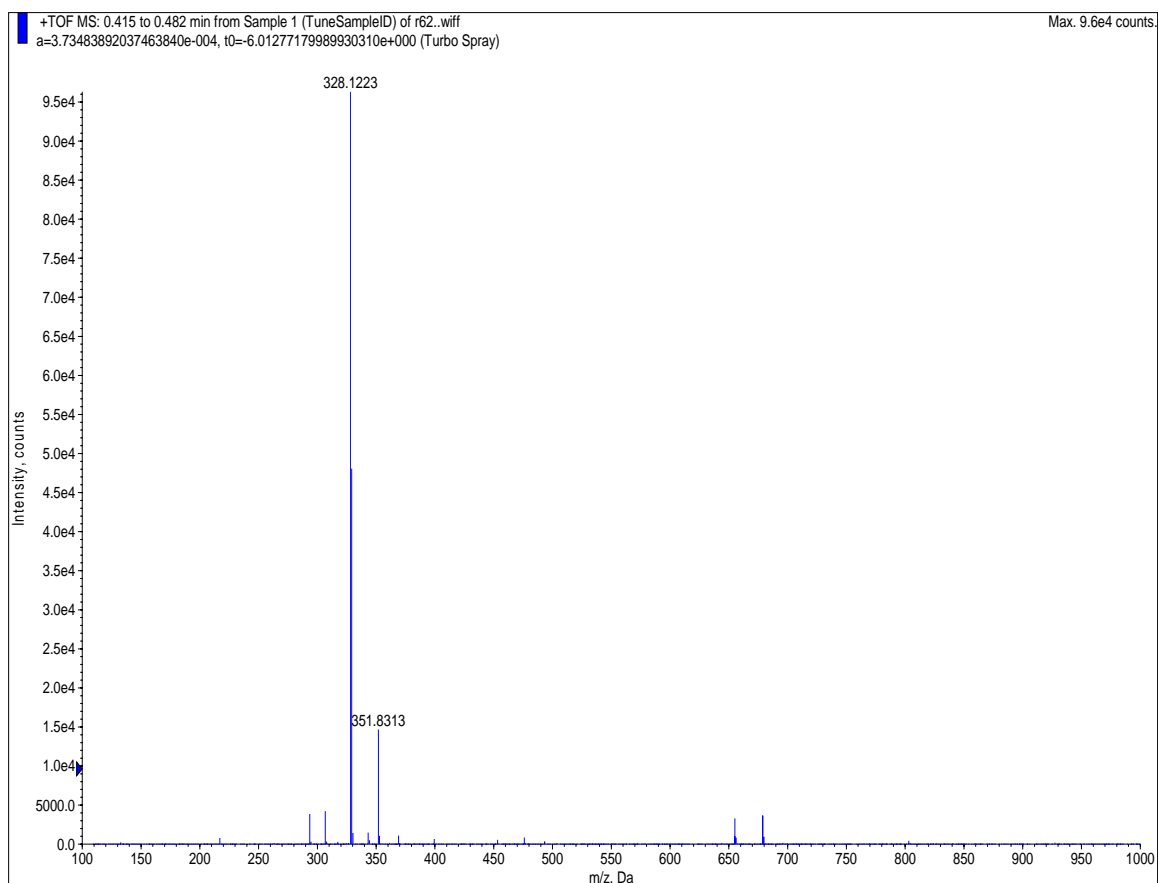


# HRMS

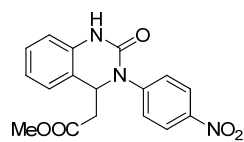


**(E)-Methyl 3-(2-(3-(2-fluorophenyl)ureido)-5-methylphenyl)acrylate**

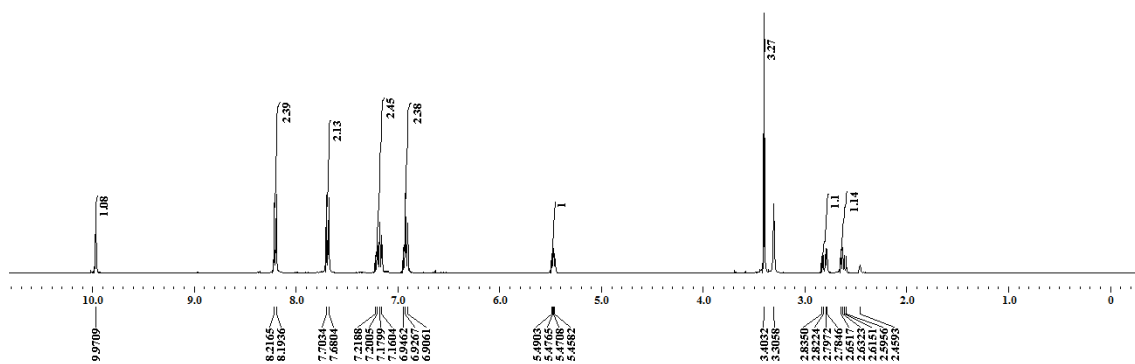
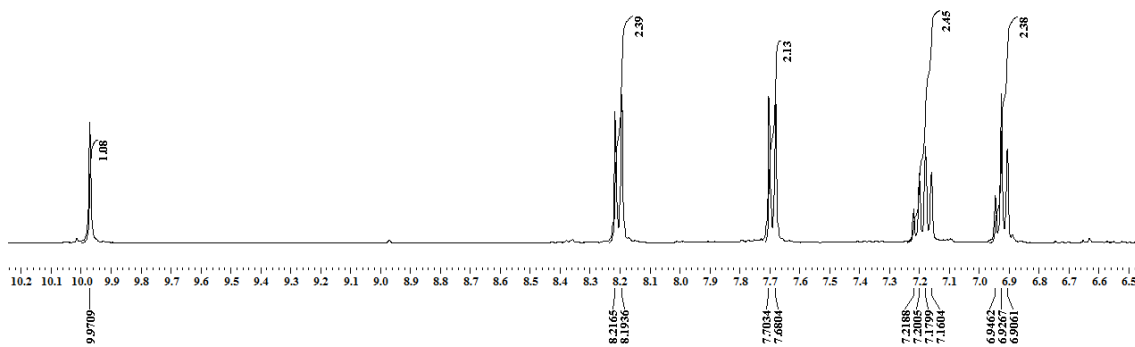
**(5c')**



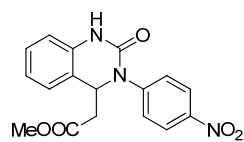
# <sup>1</sup>H NMR



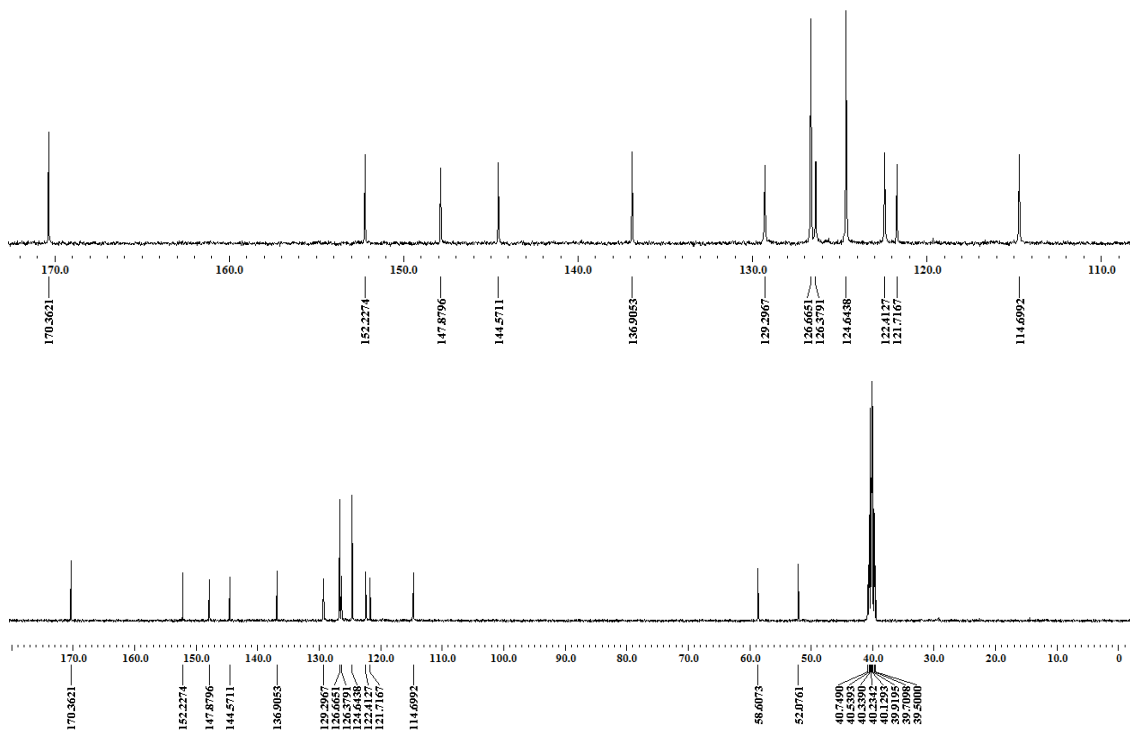
Methyl 2-(3-(4-nitrophenyl)-2-oxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (5a)



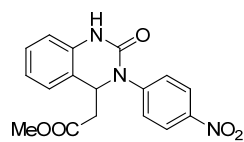
<sup>13</sup>C NMR



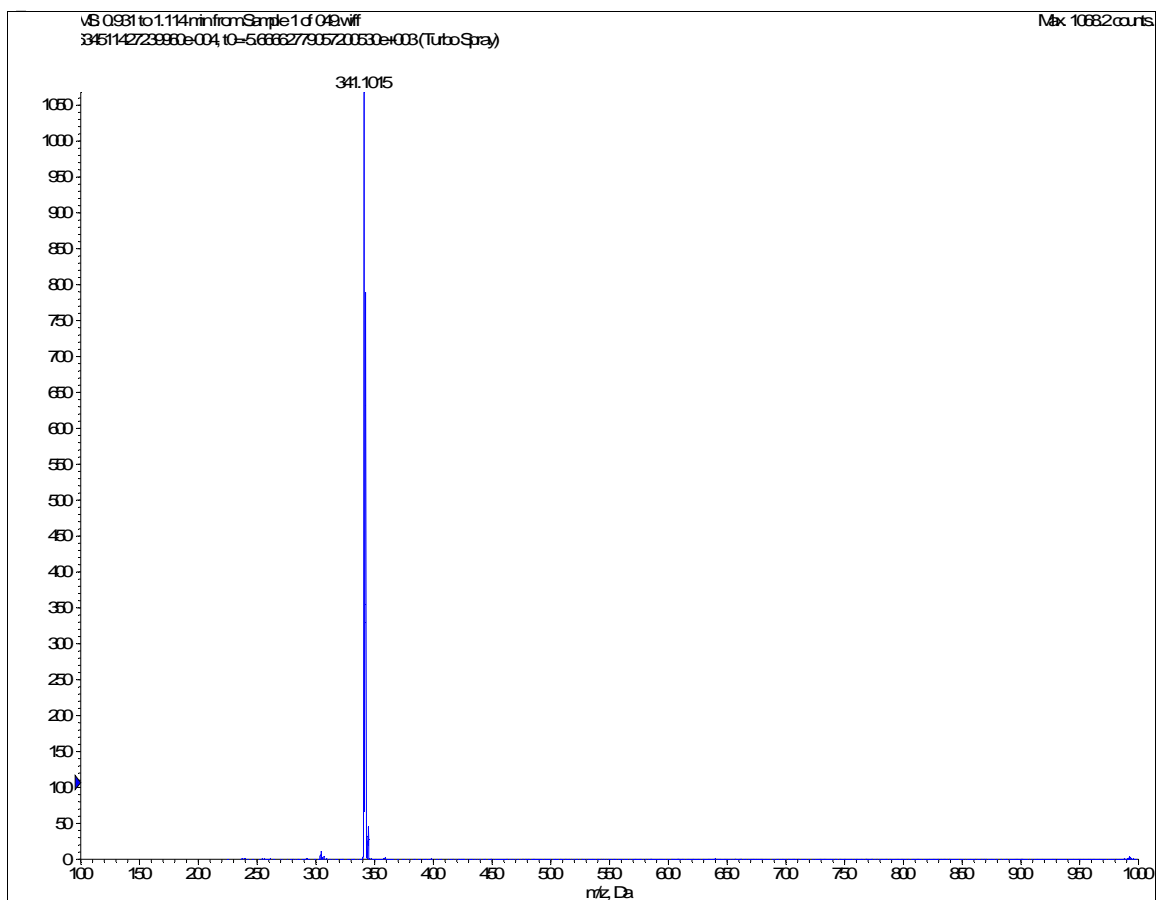
Methyl 2-(3-(4-nitrophenyl)-2-oxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (5a)



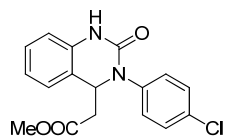
## HRMS



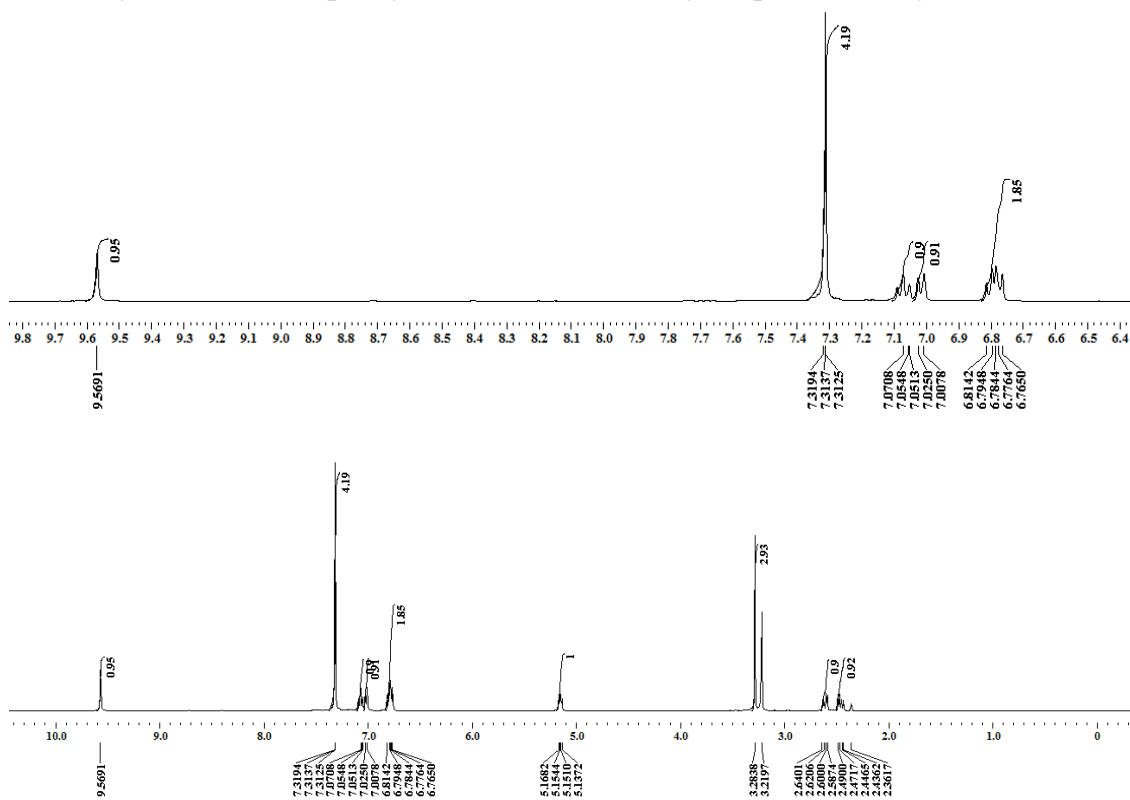
**Methyl 2-(3-(4-nitrophenyl)-2-oxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (5a)**



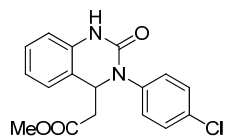
# <sup>1</sup>H NMR



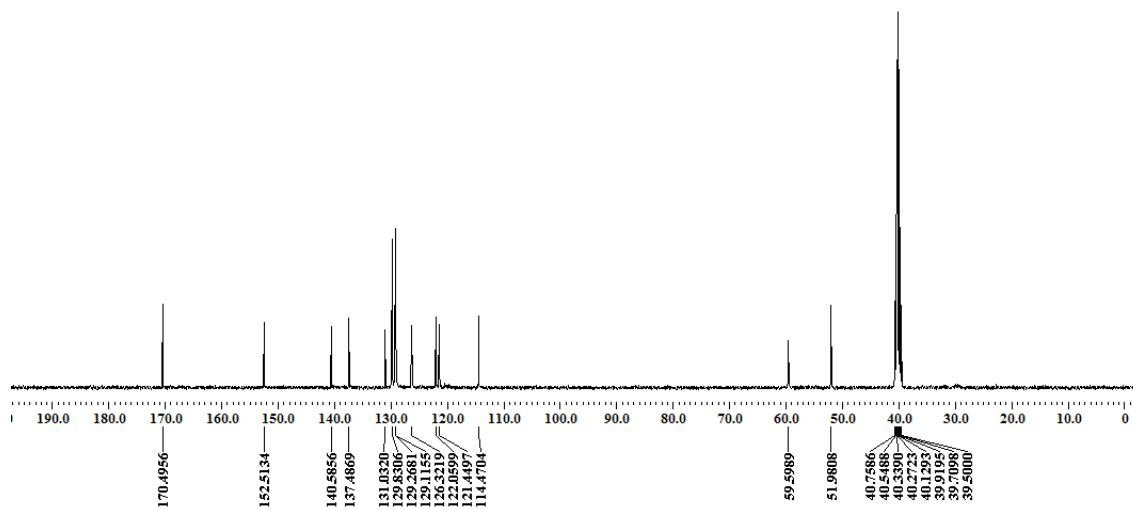
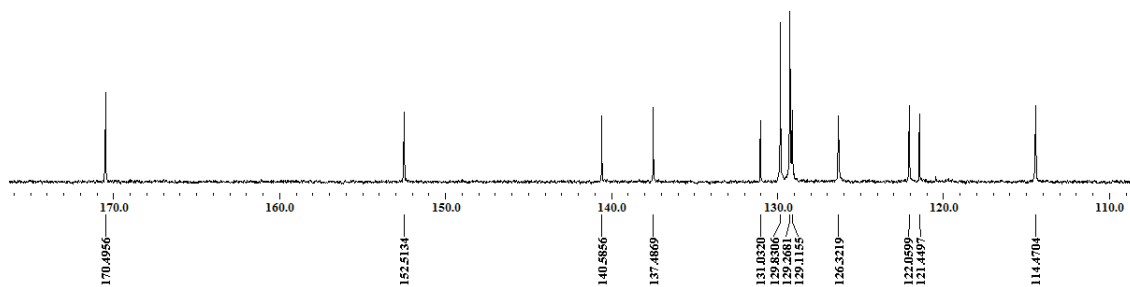
Methyl 2-(3-(4-chlorophenyl)-2-oxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (5b)



<sup>13</sup>C NMR

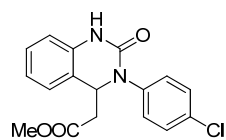


Methyl 2-(3-(4-chlorophenyl)-2-oxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (5b)

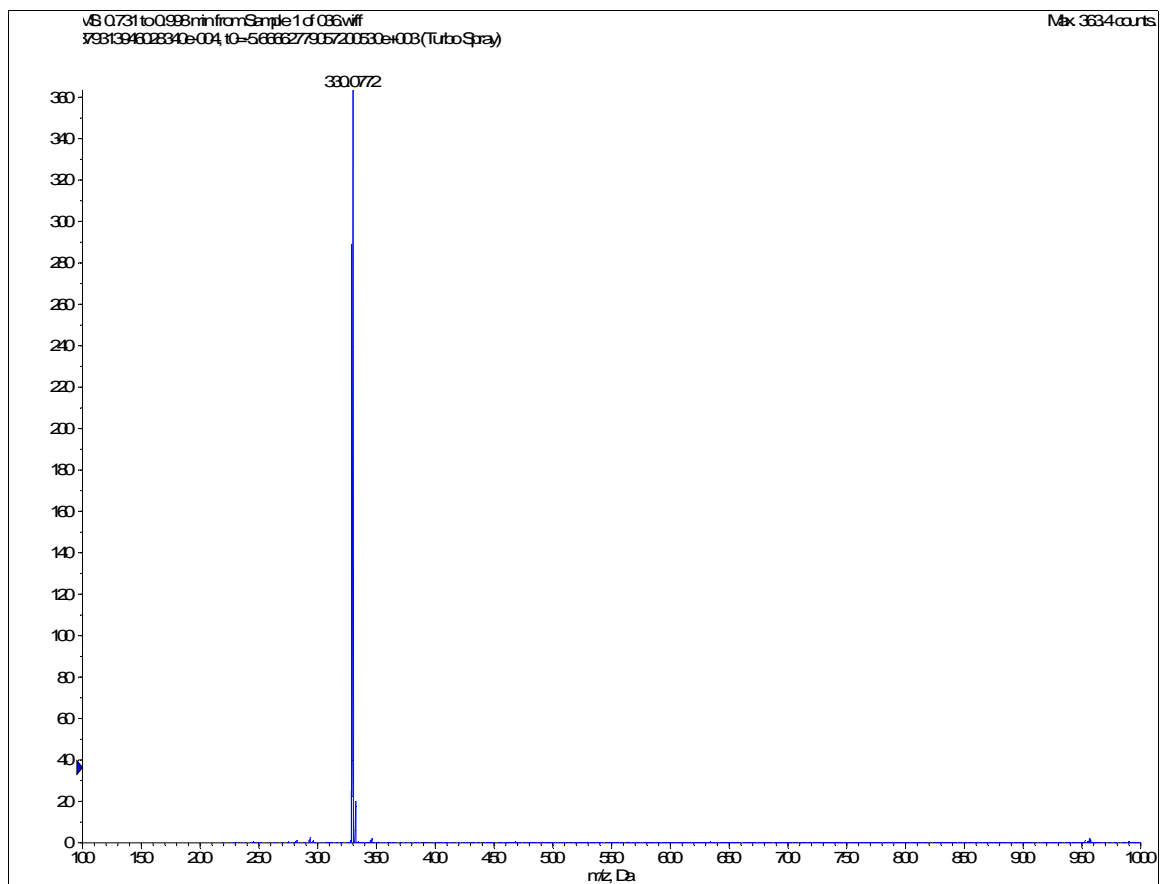




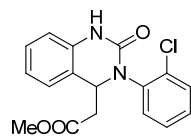
## HRMS



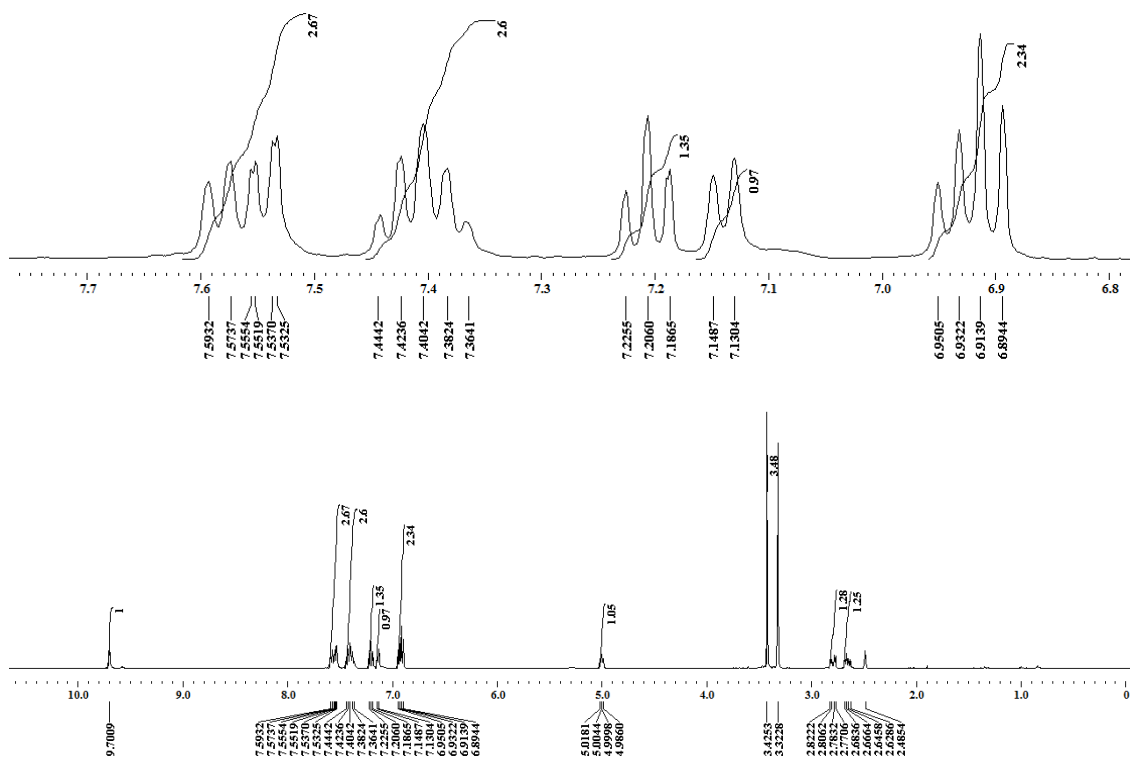
### Methyl 2-(3-(4-chlorophenyl)-2-oxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (5b)



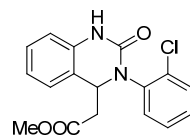
# <sup>1</sup>H NMR



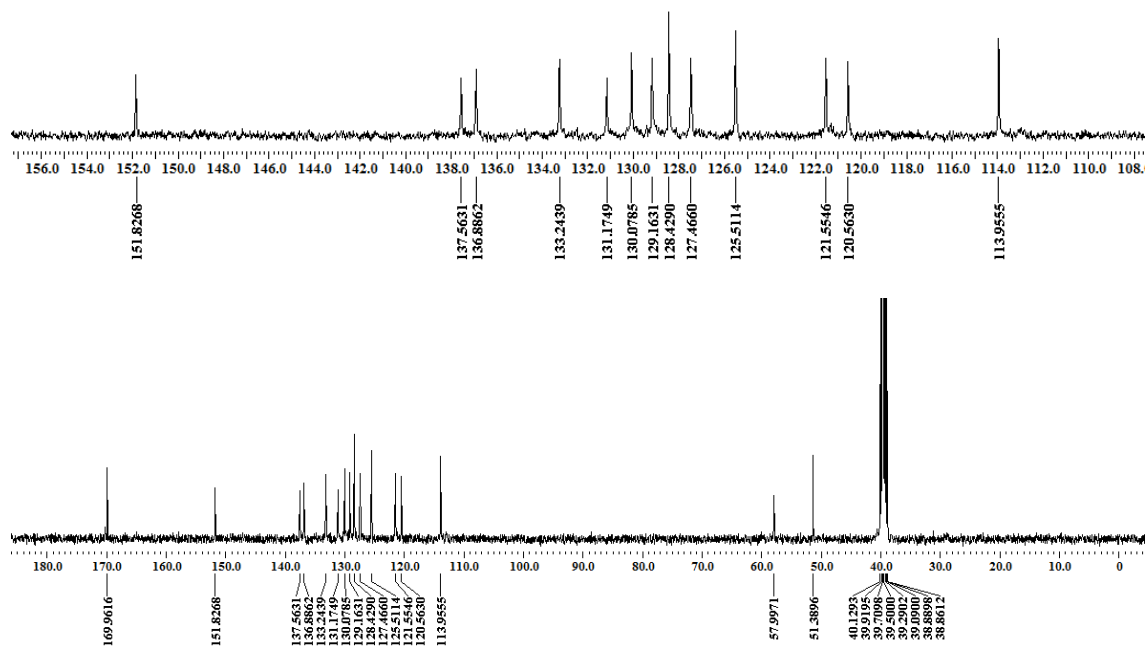
Methyl 2-(3-(2-chlorophenyl)-2-oxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (5c)



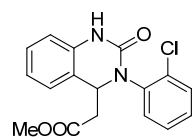
<sup>13</sup>C NMR



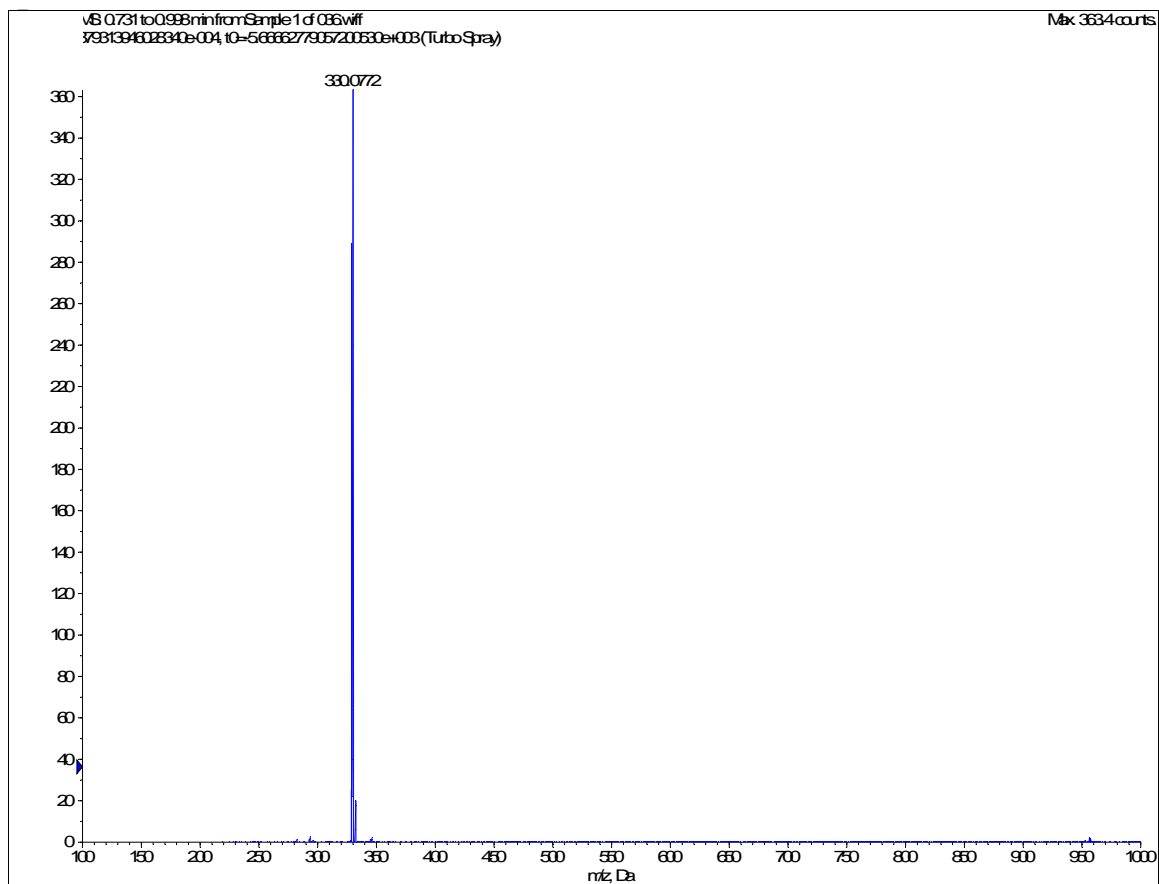
Methyl 2-(3-(2-chlorophenyl)-2-oxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (5c)



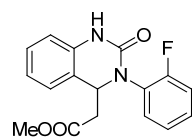
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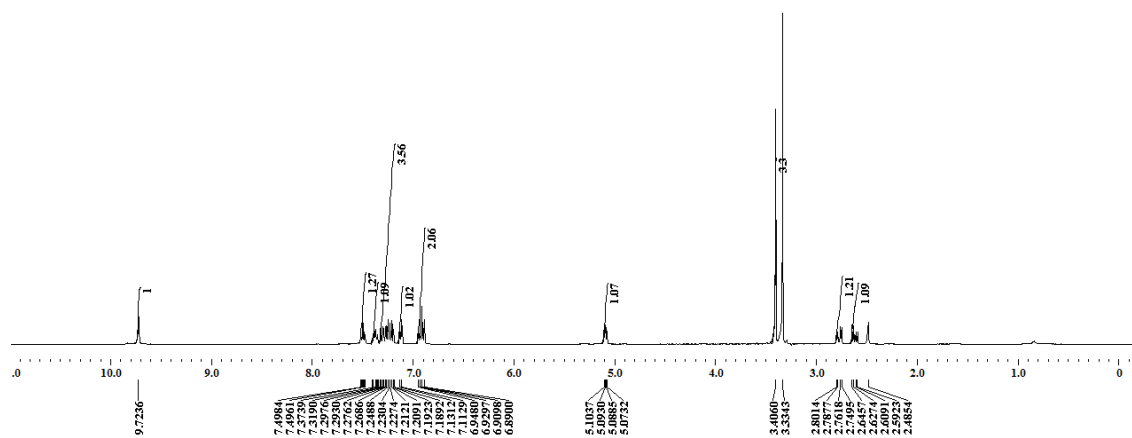
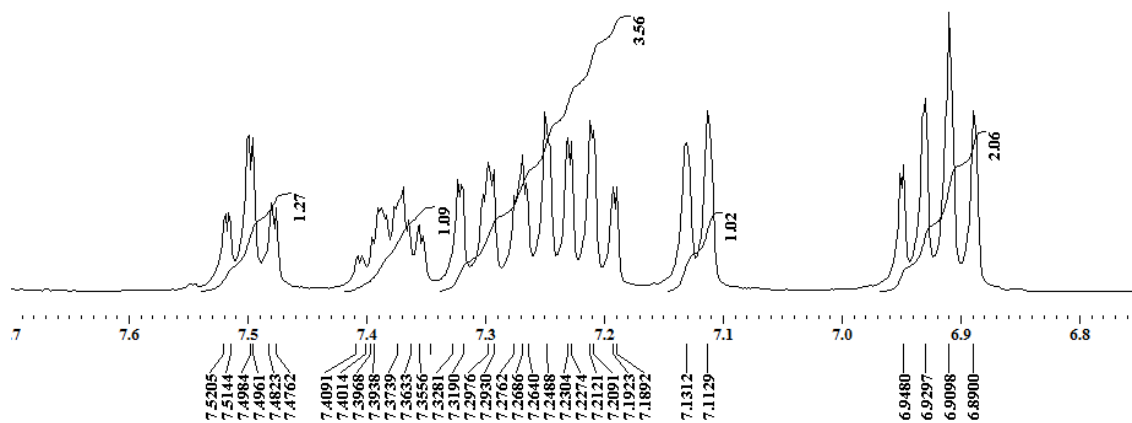
## Methyl 2-(3-(2-chlorophenyl)-2-oxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (5c)



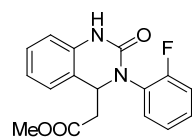
# <sup>1</sup>H NMR



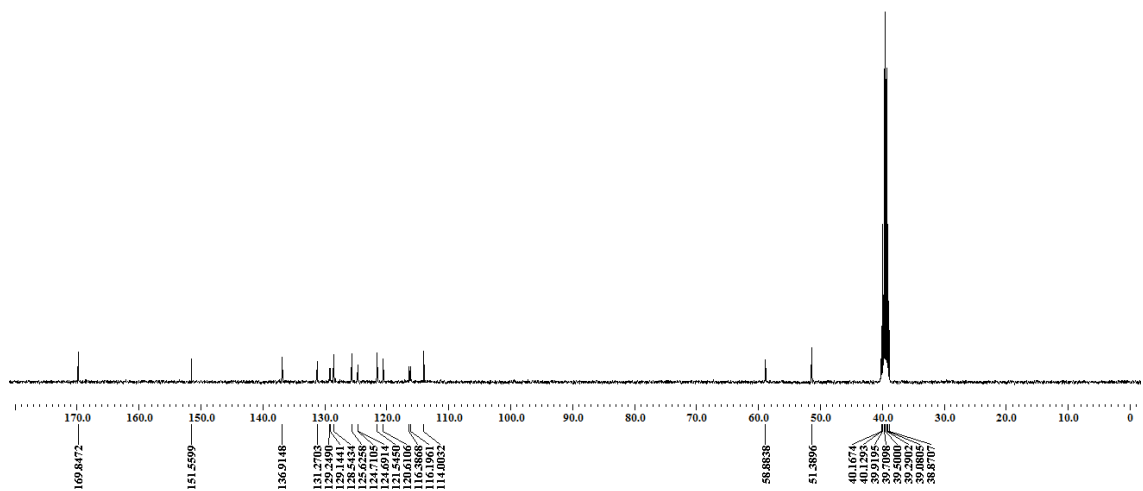
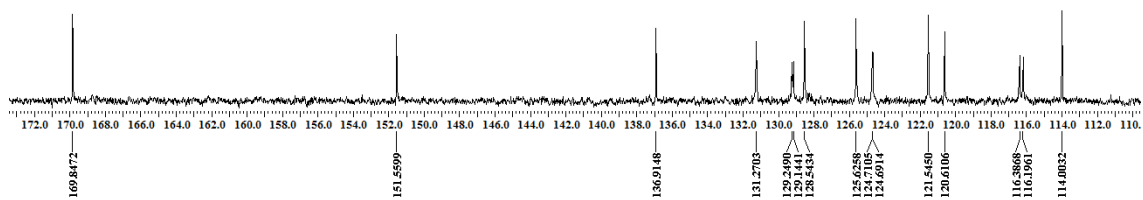
Methyl 2-(3-(2-fluorophenyl)-2-oxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (5d)



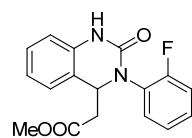
<sup>13</sup>C NMR



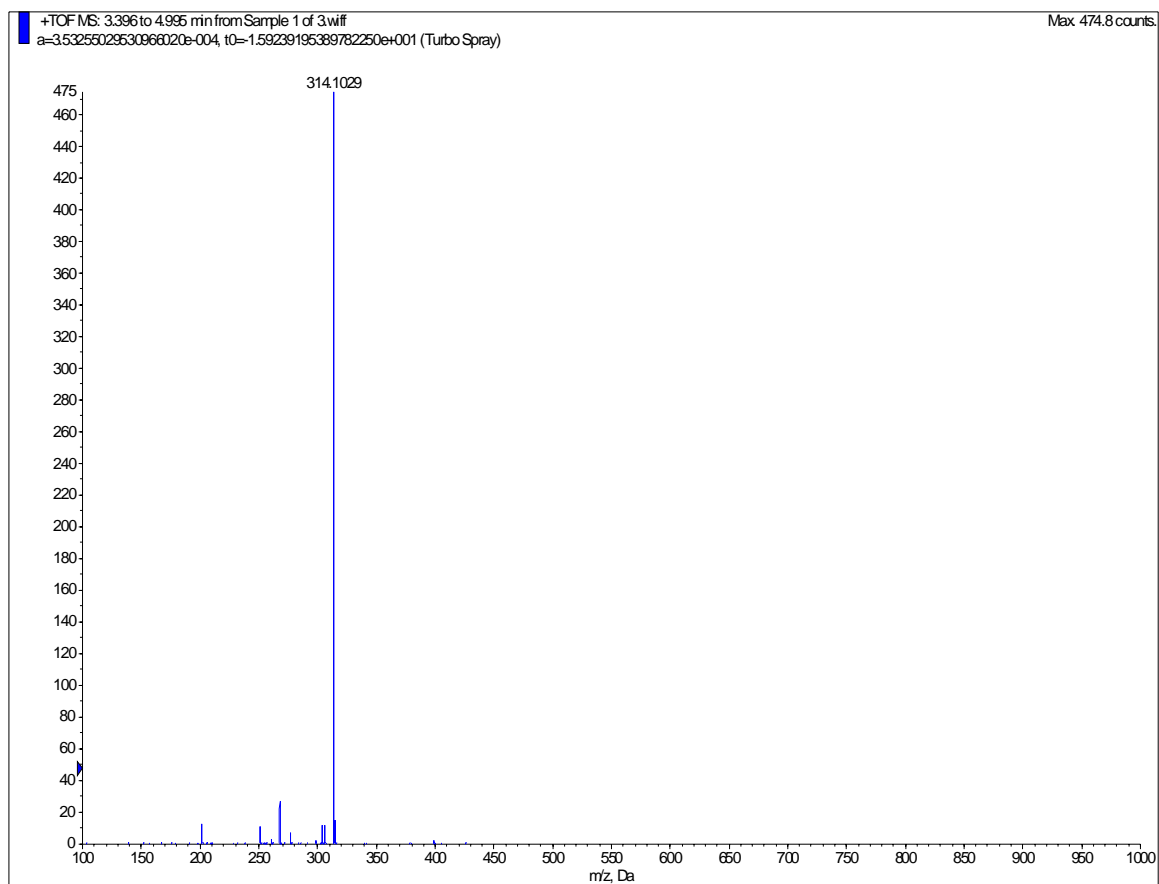
Methyl 2-(3-(2-fluorophenyl)-2-oxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (5d)



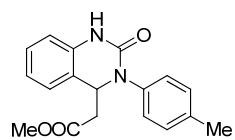
## HRMS



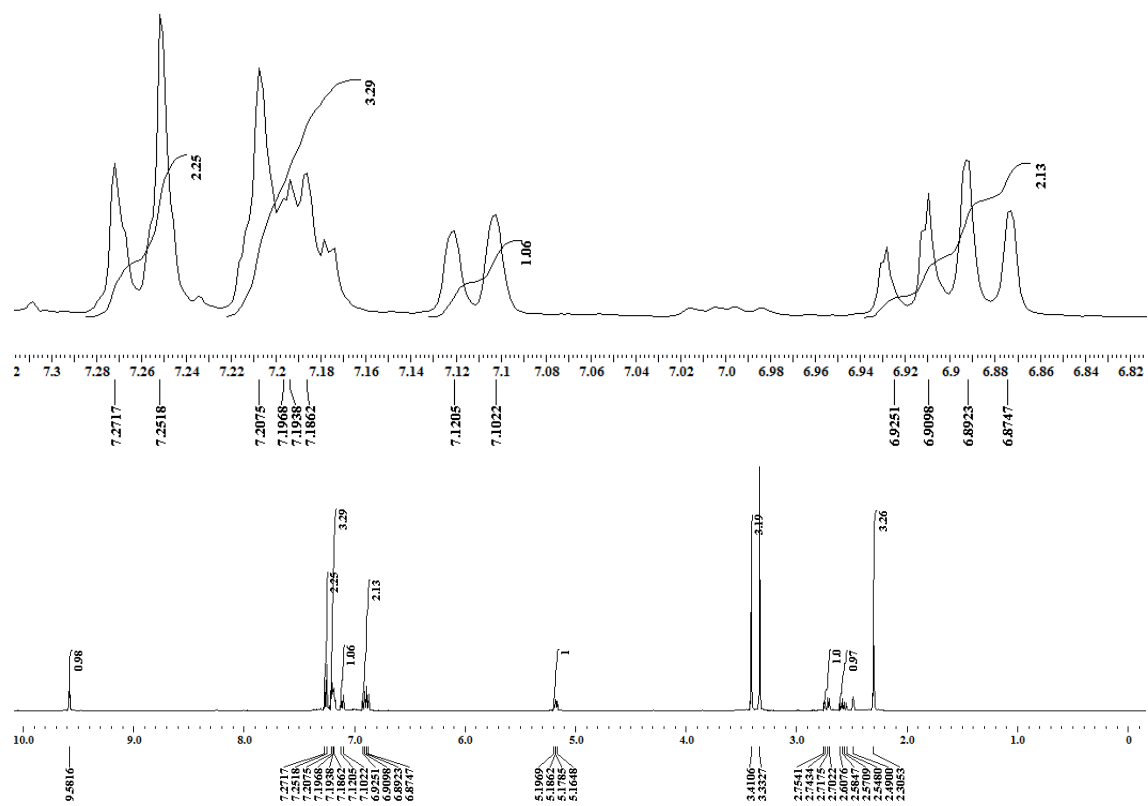
### Methyl 2-(3-(2-fluorophenyl)-2-oxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (5d)



# <sup>1</sup>H NMR

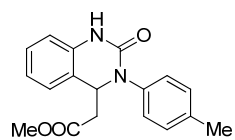


Methyl 2-(2-oxo-3-(p-tolyl)-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (5e)

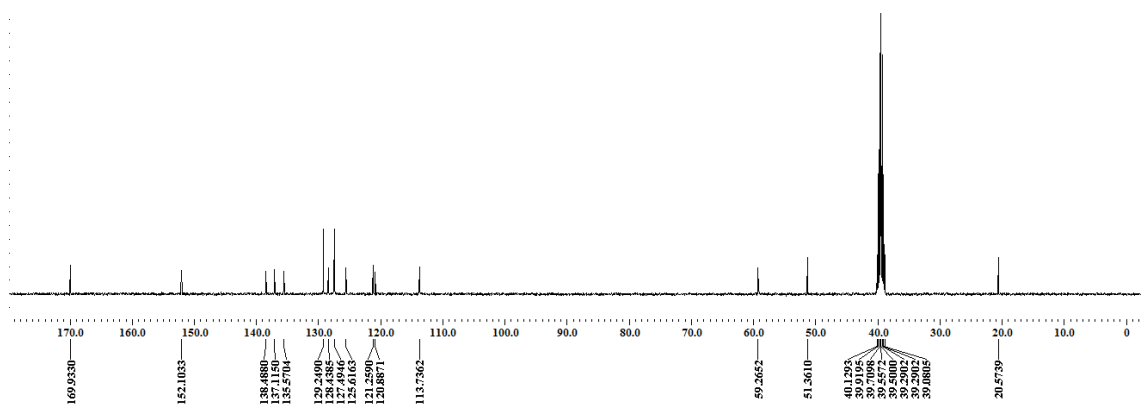
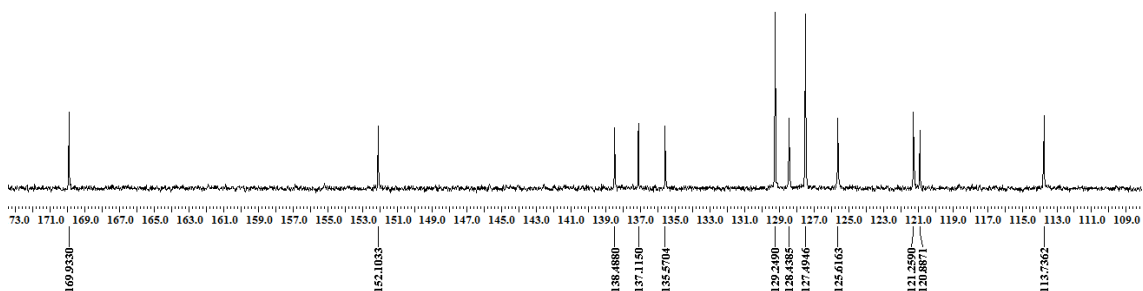




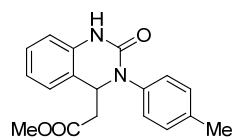
# <sup>13</sup>C NMR



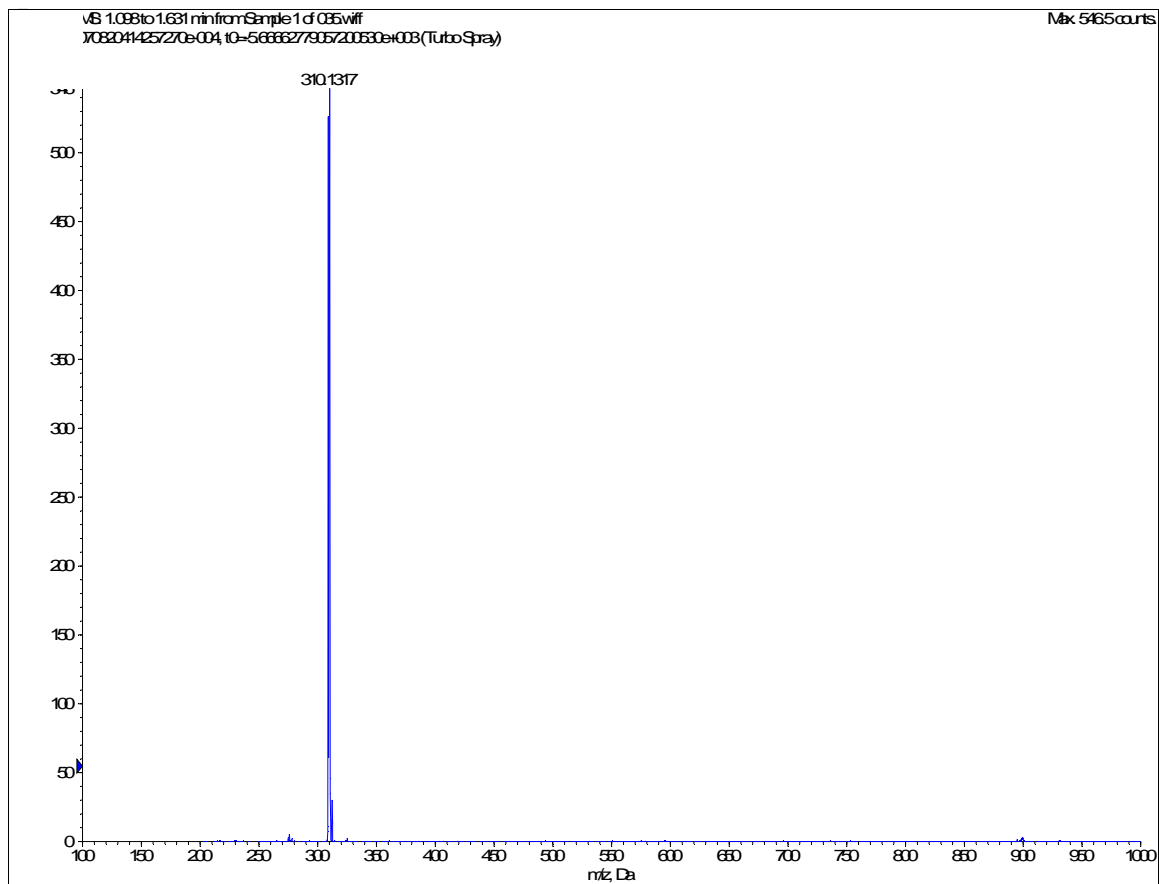
Methyl 2-(2-oxo-3-(p-tolyl)-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (5e)



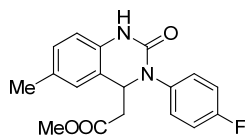
## HRMS



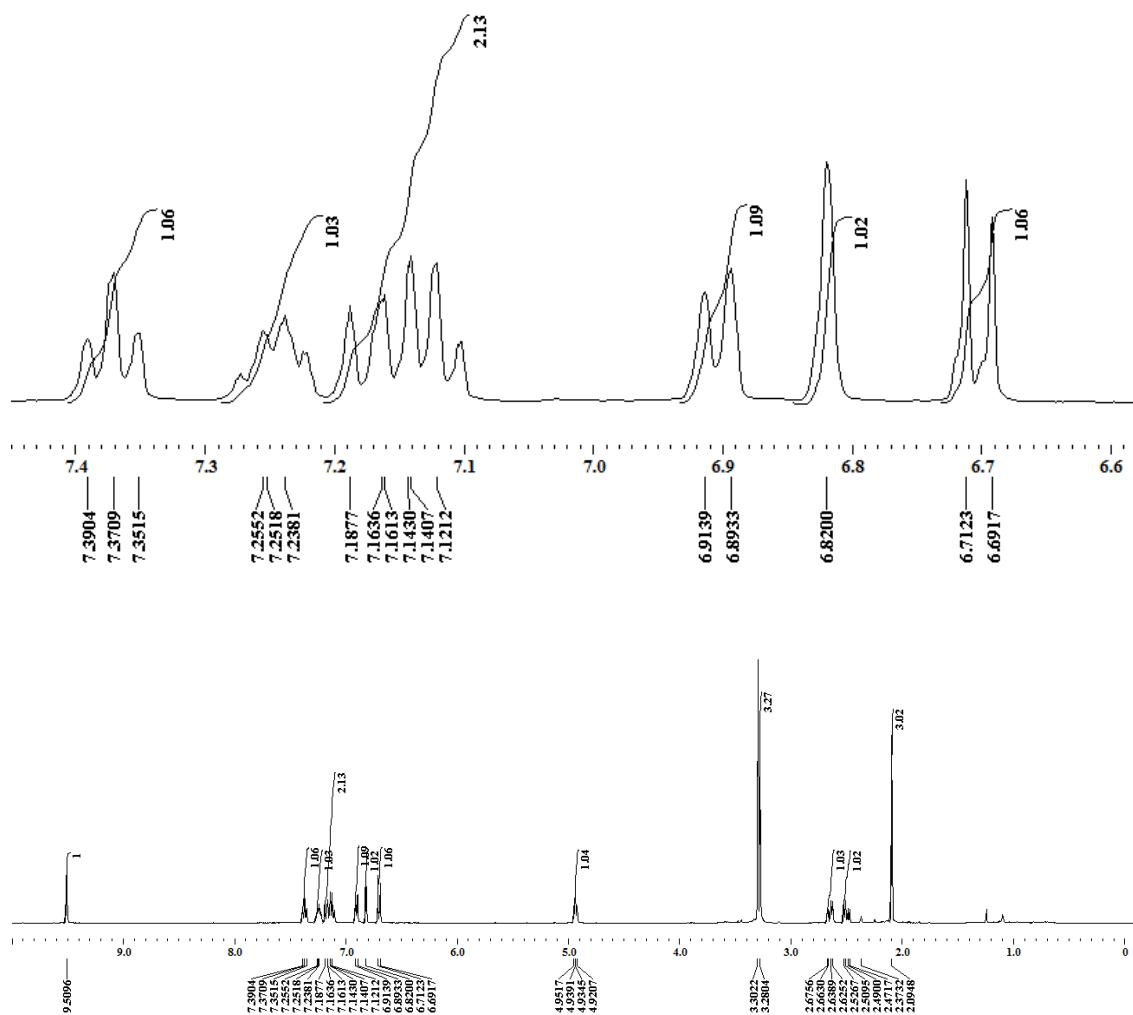
### Methyl 2-(2-oxo-3-(*p*-tolyl)-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (5e)



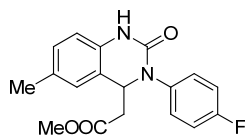
# <sup>1</sup>H NMR



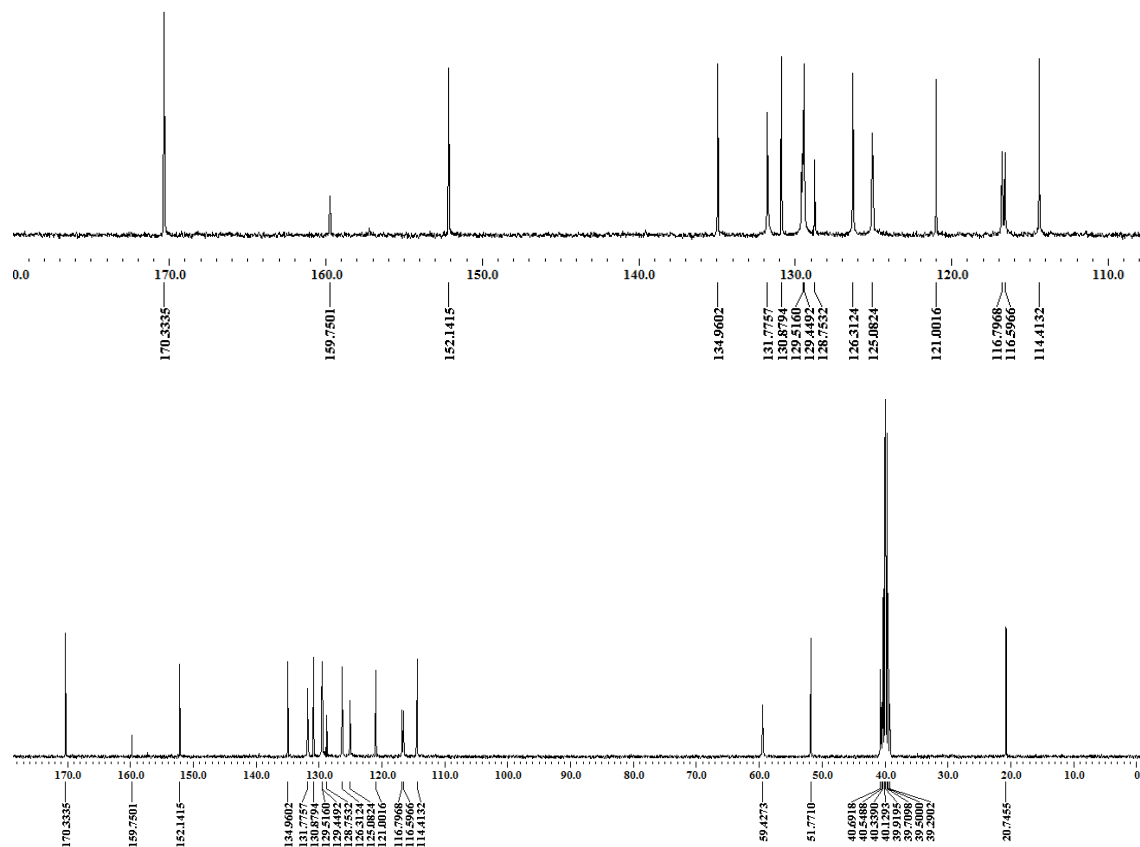
Methyl 2-(3-(4-fluorophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate  
(5f)



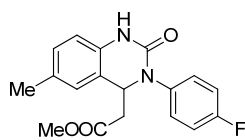
<sup>13</sup>C NMR



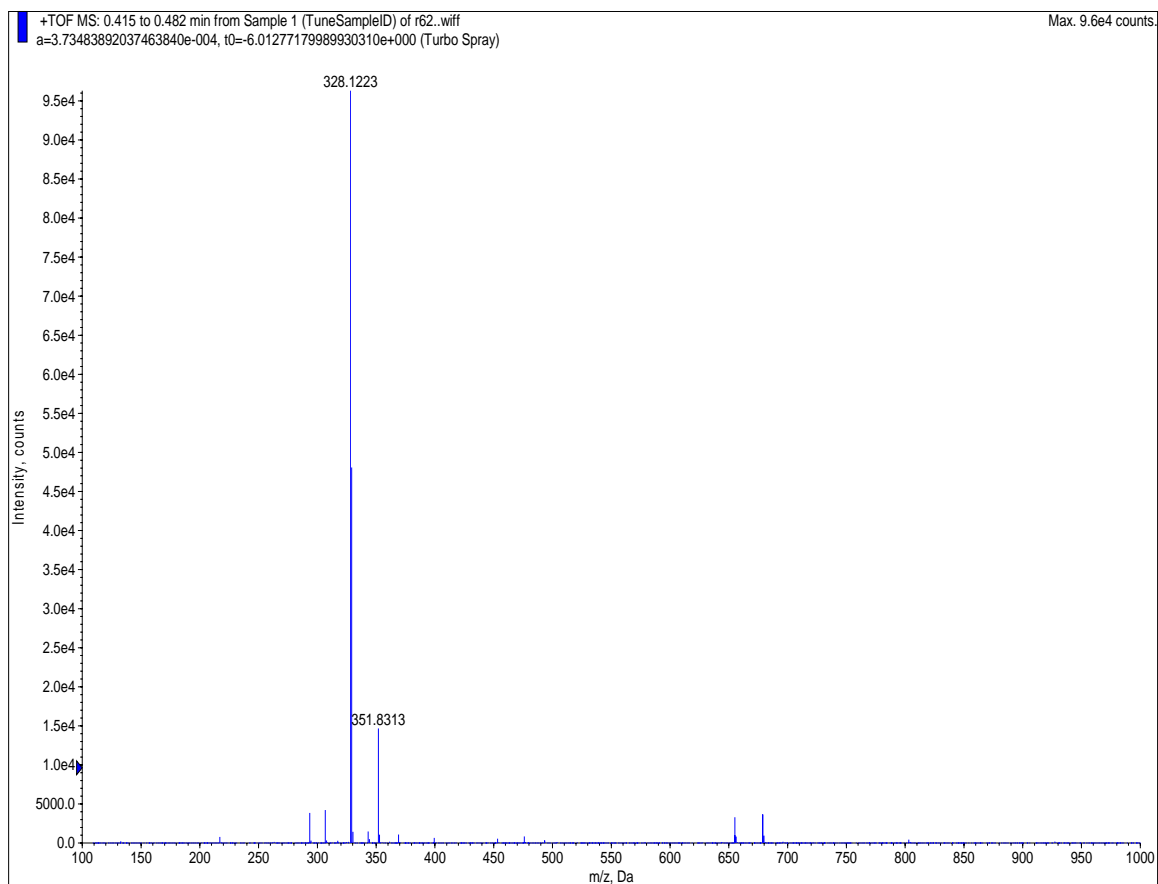
Methyl 2-(3-(4-fluorophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate  
(5f)



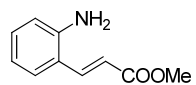
## HRMS



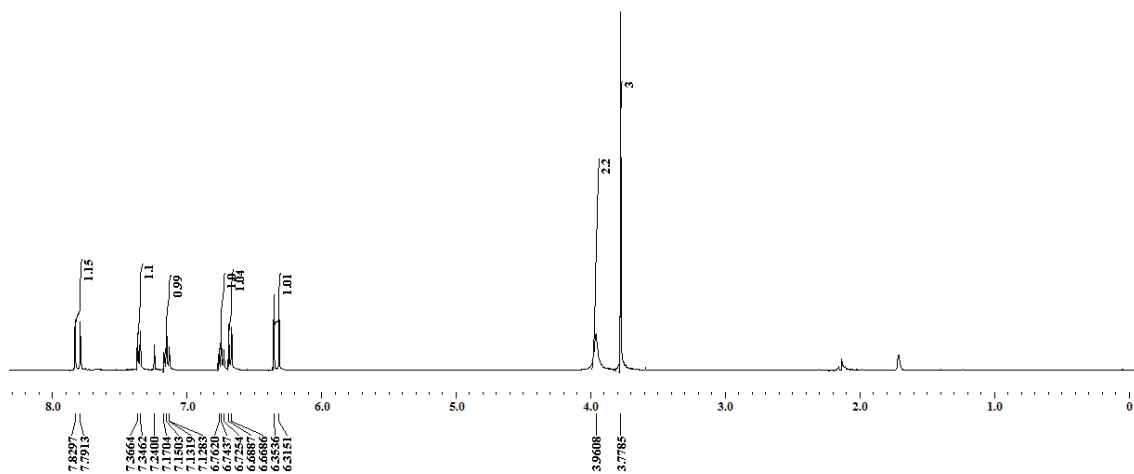
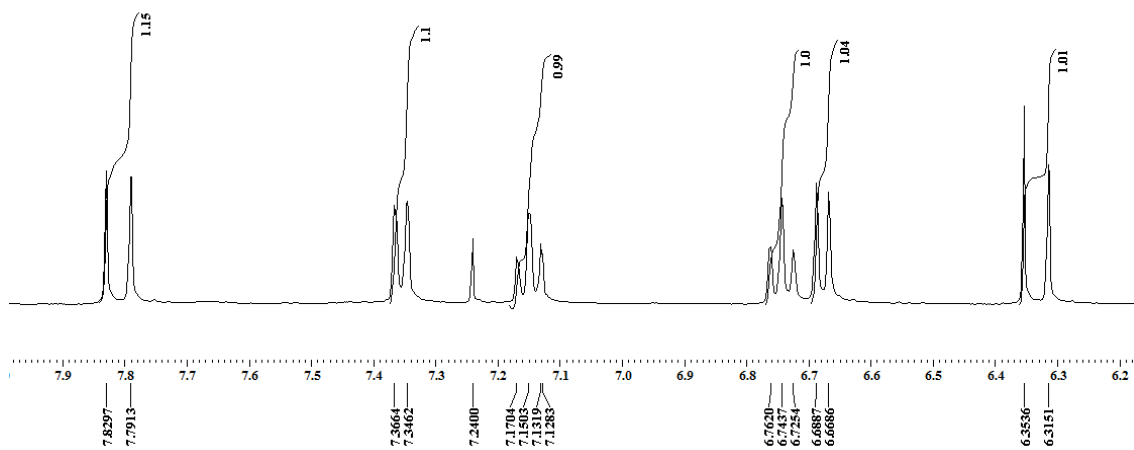
### Methyl 2-(3-(4-fluorophenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydroquinazolin-4-yl)acetate (5f)



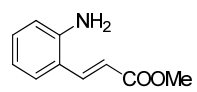
# <sup>1</sup>H NMR



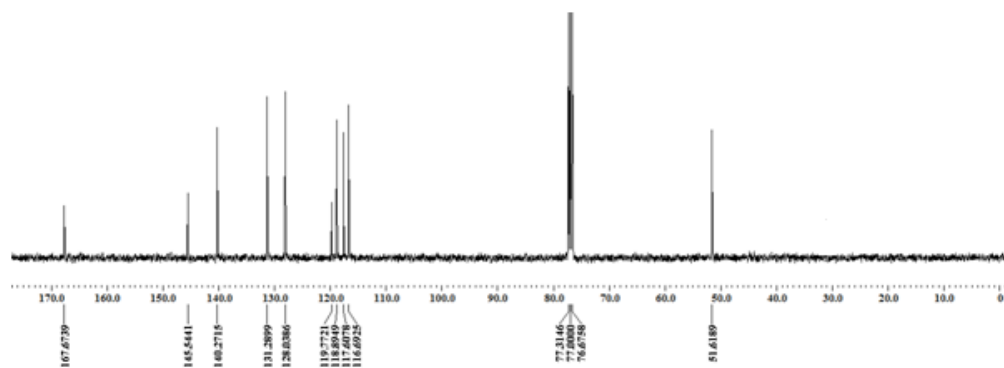
(*E*)-Methyl 3-(2-aminophenyl)acrylate (6)



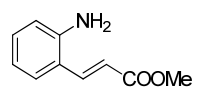
<sup>13</sup>C NMR



(E)-Methyl 3-(2-aminophenyl)acrylate (6)



# HRMS



**(E)-Methyl 3-(2-aminophenyl)acrylate (6)**

