

## Supporting Information

*Research Article*

# Novel ring systems: Spiro[cycloalkane] derivatives of Triazolo- and Tetrazolo-pyridazines

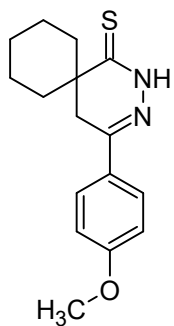
Csilla Sepsey Für<sup>1</sup>, Gergő Riszter<sup>1</sup>, Áron Szigetvári<sup>2</sup>, Miklós Dékány<sup>2</sup>, György Keglevich<sup>1</sup>, László Hazai<sup>1</sup> and Hedvig Bölcskei<sup>1,\*</sup>

<sup>1</sup> Department of Organic Chemistry and Technology, Budapest University of Technology and Economics, 1111 Budapest, Hungary; sepsey.fur.csilla@vbk.bme.hu (Cs.S.F.), riszter93@gmail.com (G.R.), keglevich.gyorgy@vbk.bme.hu (G.K), hazai.laszlo@vbk.bme.hu (L.H.), bolcskei.hedvig@vbk.bme.hu (H.B.)

<sup>2</sup> Gedeon Richter Plc. Budapest X., Gyömrői út 19-21., Budapest 10. POB.27. H-1475, Hungary; szigetvaria@richter.hu (Á.Sz.), m.dekany@richter.hu (D.M.)

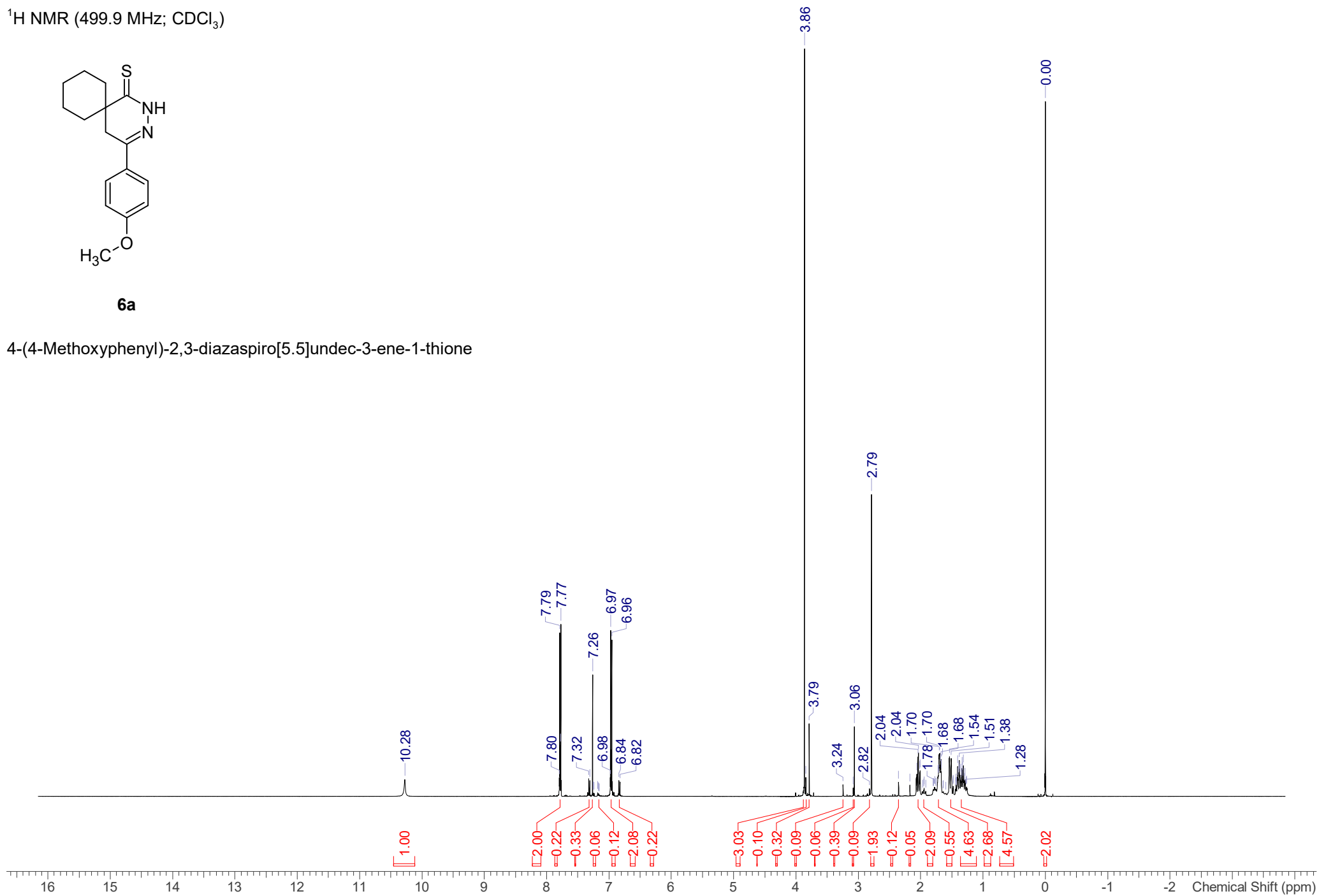
\* Correspondence: bolcskei.hedvig@vbk.bme.hu Tel.: Tel: +36-1-463-2229

<sup>1</sup>H NMR (499.9 MHz; CDCl<sub>3</sub>)

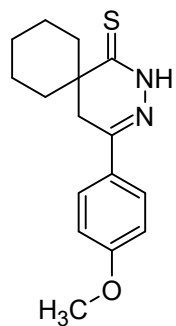


**6a**

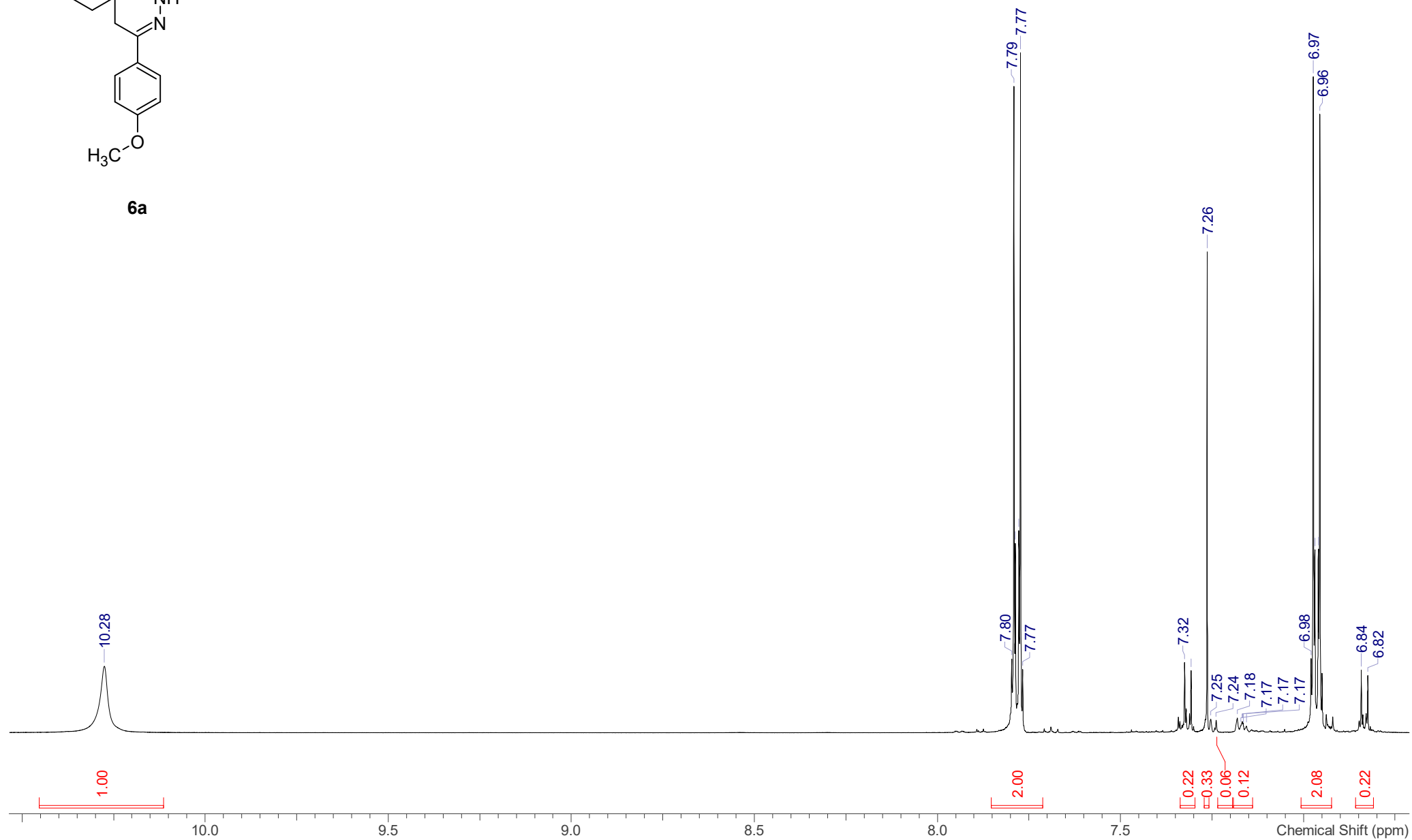
4-(4-Methoxyphenyl)-2,3-diazaspiro[5.5]undec-3-ene-1-thione



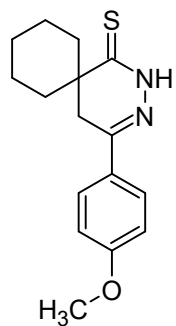
<sup>1</sup>H NMR (499.9 MHz; CDCl<sub>3</sub>)



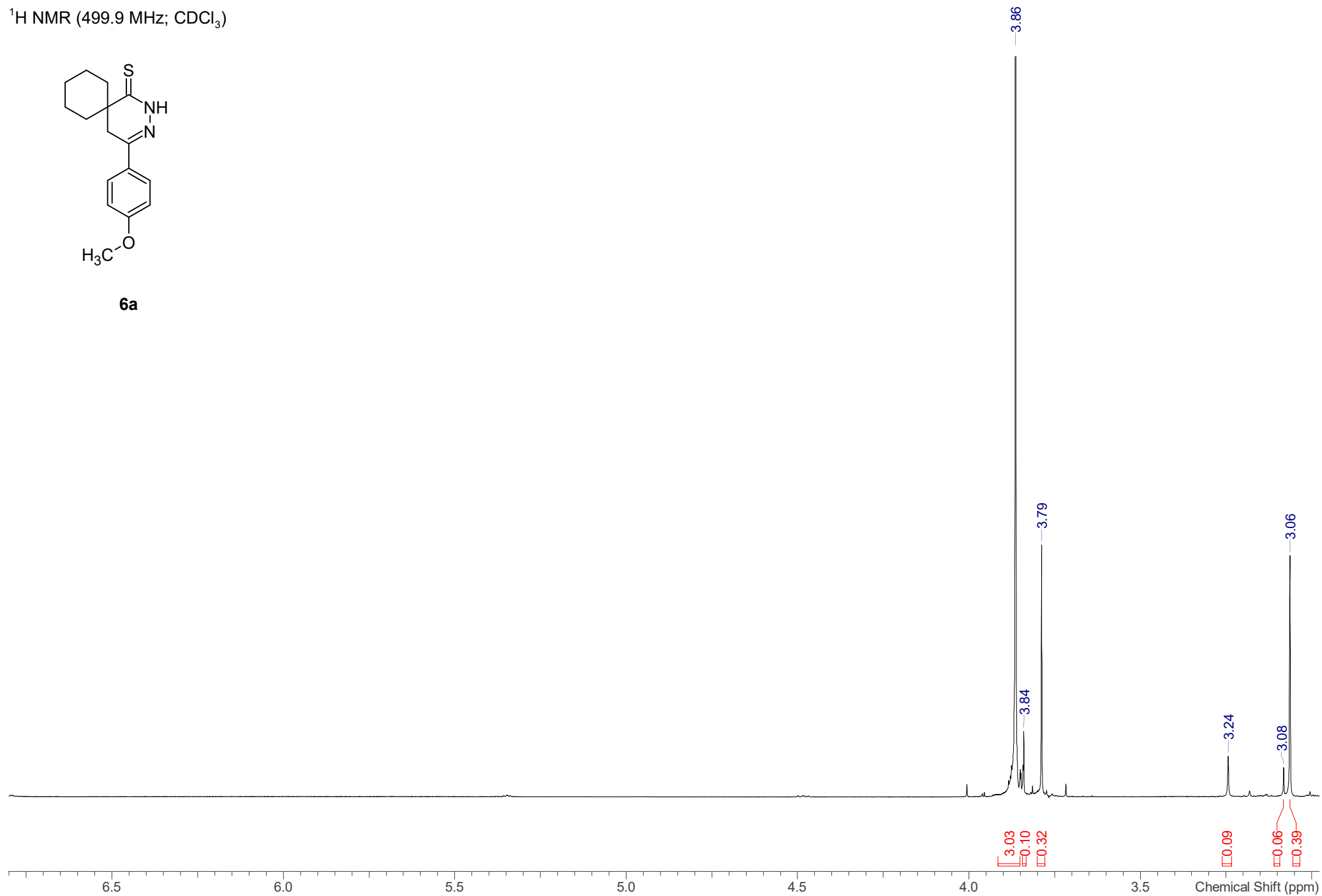
**6a**



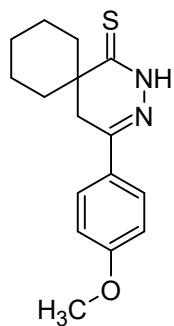
<sup>1</sup>H NMR (499.9 MHz; CDCl<sub>3</sub>)



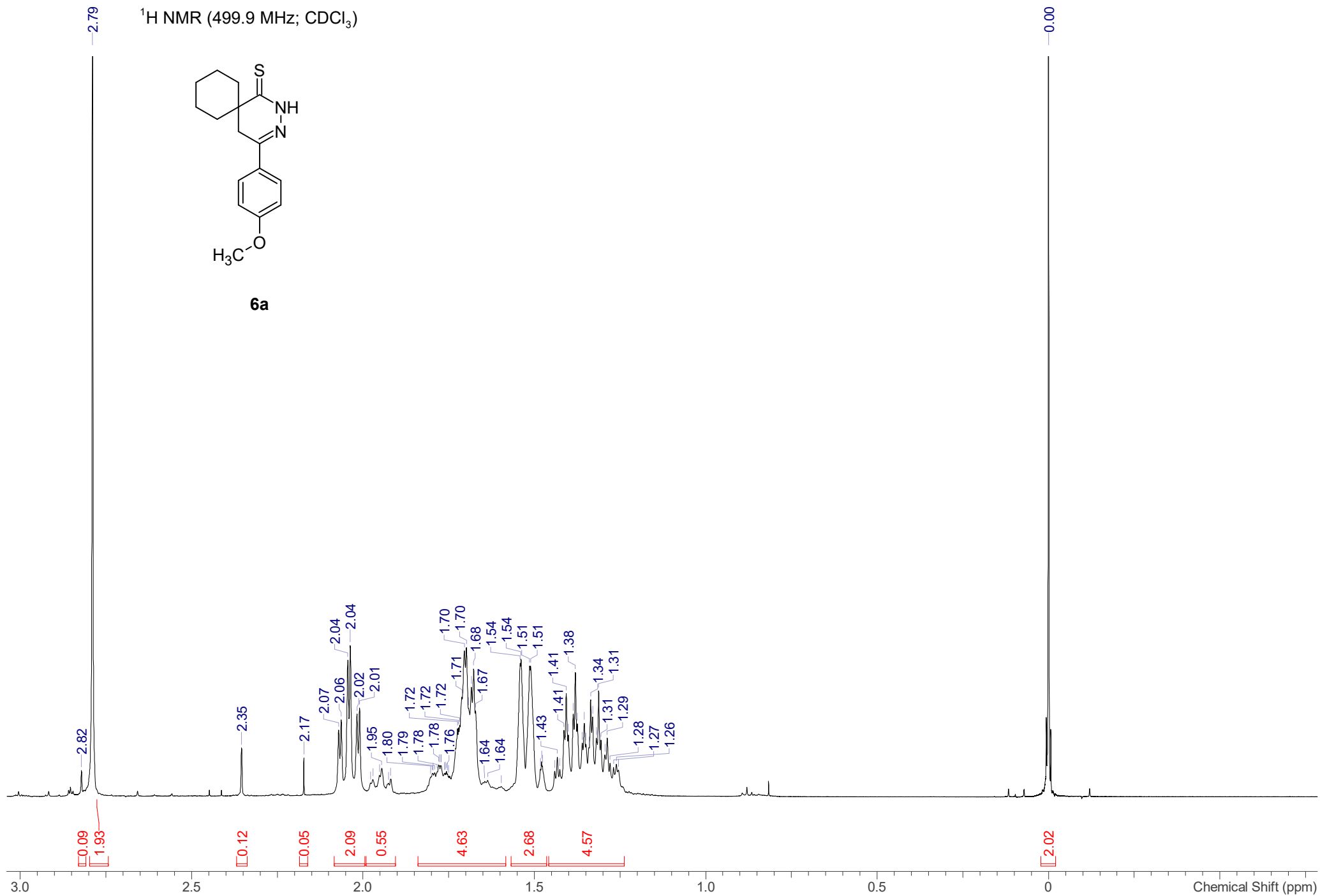
**6a**



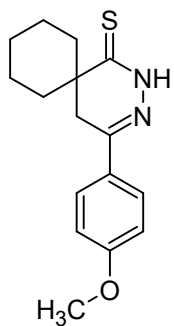
<sup>1</sup>H NMR (499.9 MHz; CDCl<sub>3</sub>)



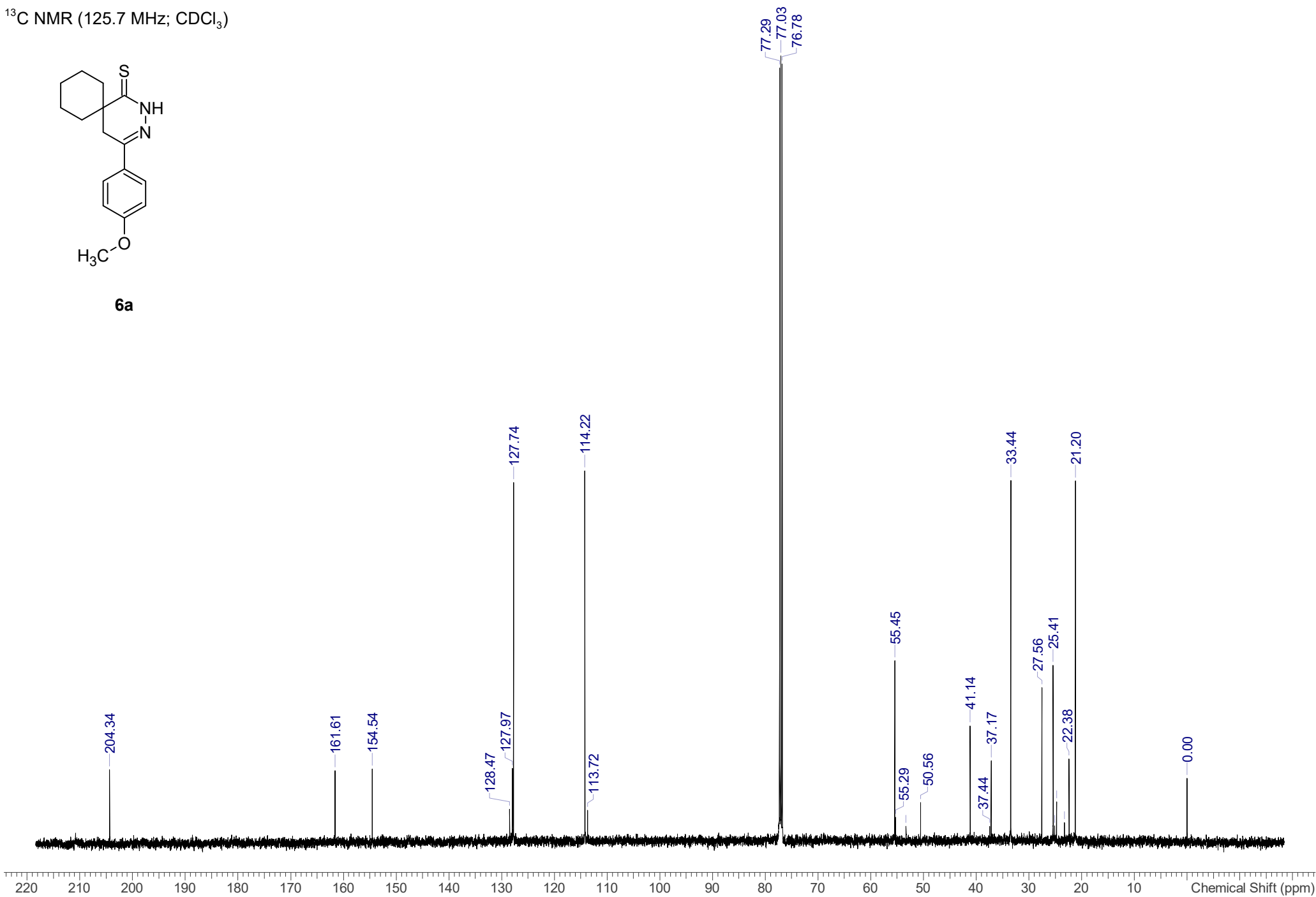
**6a**



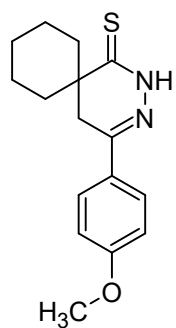
$^{13}\text{C}$  NMR (125.7 MHz;  $\text{CDCl}_3$ )



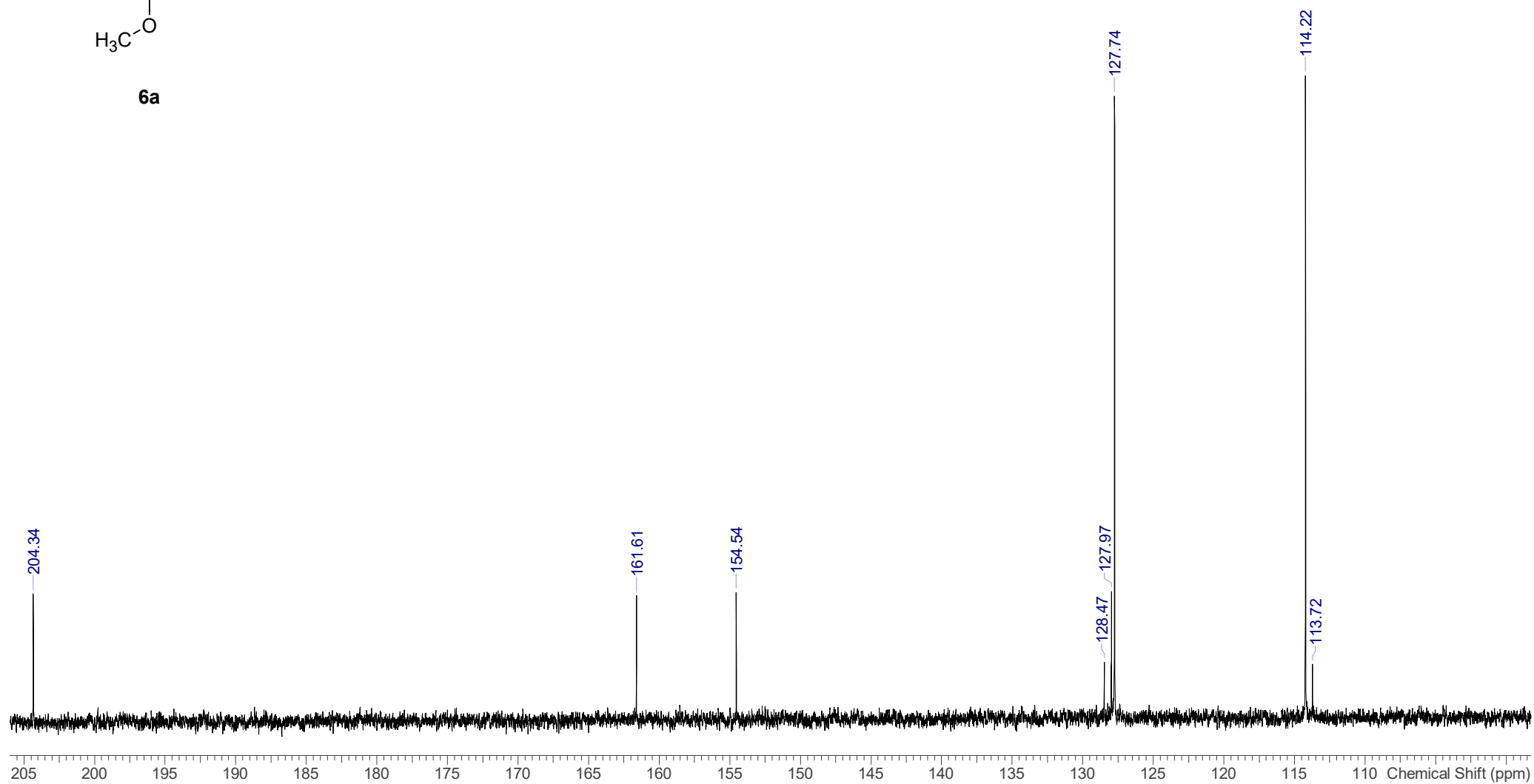
**6a**



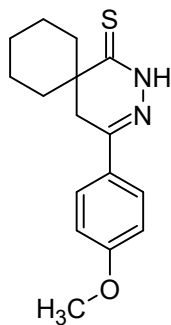
$^{13}\text{C}$  NMR (125.7 MHz;  $\text{CDCl}_3$ )



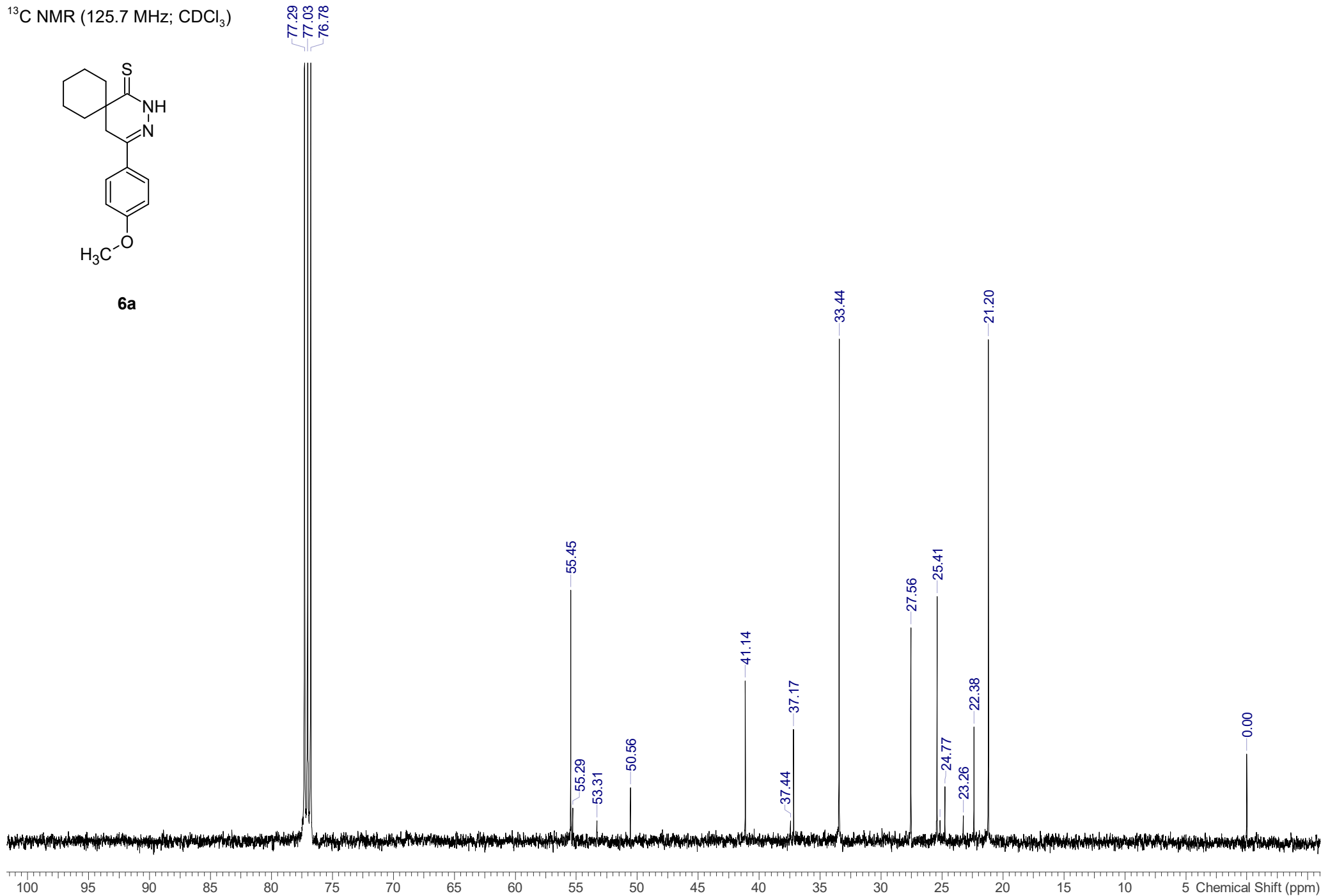
**6a**



<sup>13</sup>C NMR (125.7 MHz; CDCl<sub>3</sub>)



**6a**

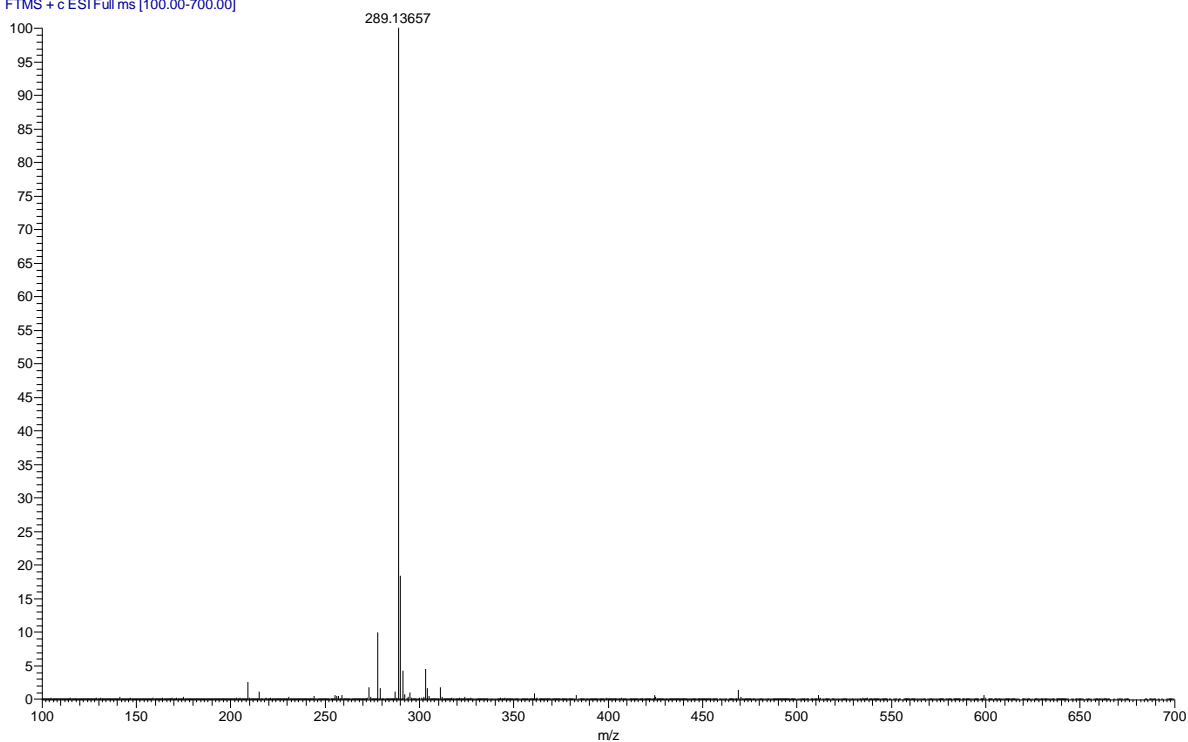




# Compound 6a

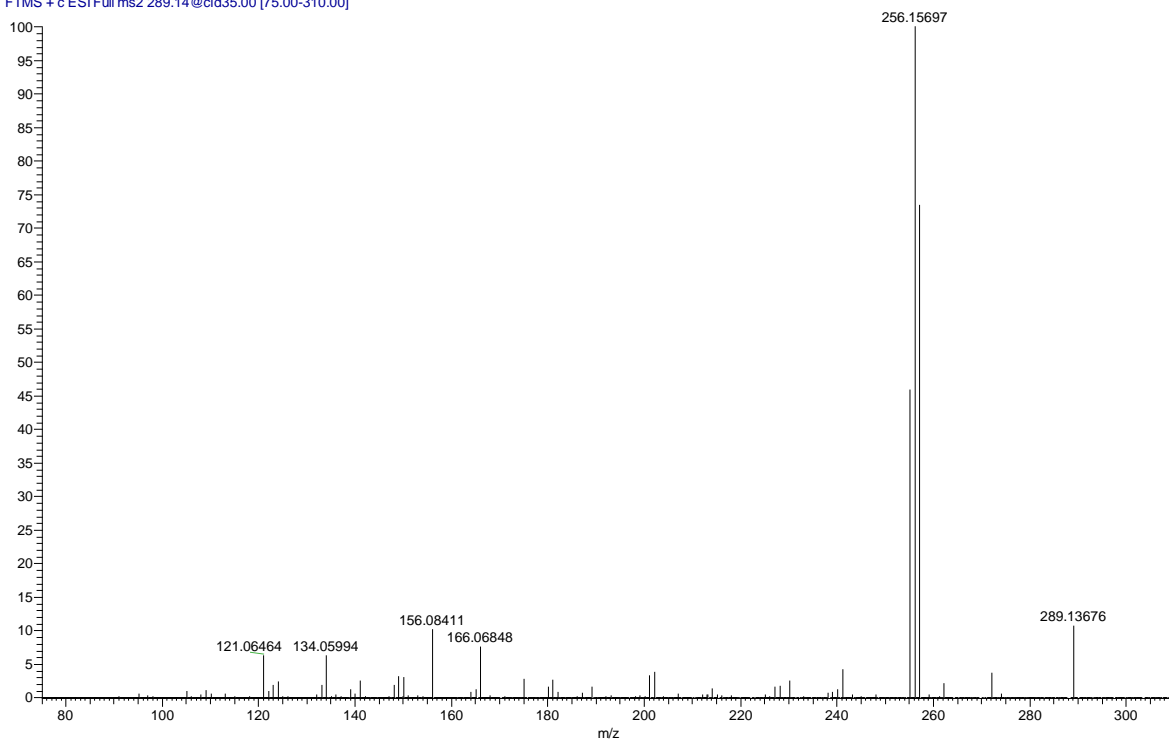
## HRMS spectrum (ESI)

ku67485\_sfc-122\_d\_ve1534 #1-43 RT: 0.00-0.20 AV: 43 NL: 2.12E7  
T: FTMS + c ESI Full ms [100.00-700.00]

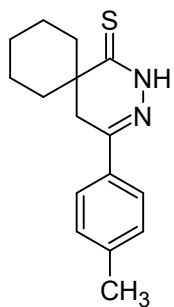


## HRMS spectrum (ESI daughter ion)

ku67485\_sfc-122\_d\_ve1535 #1-45 RT: 0.00-0.20 AV: 45 NL: 4.76E6  
T: FTMS + c ESI Full ms2 289.14@cid35.00 [75.00-310.00]

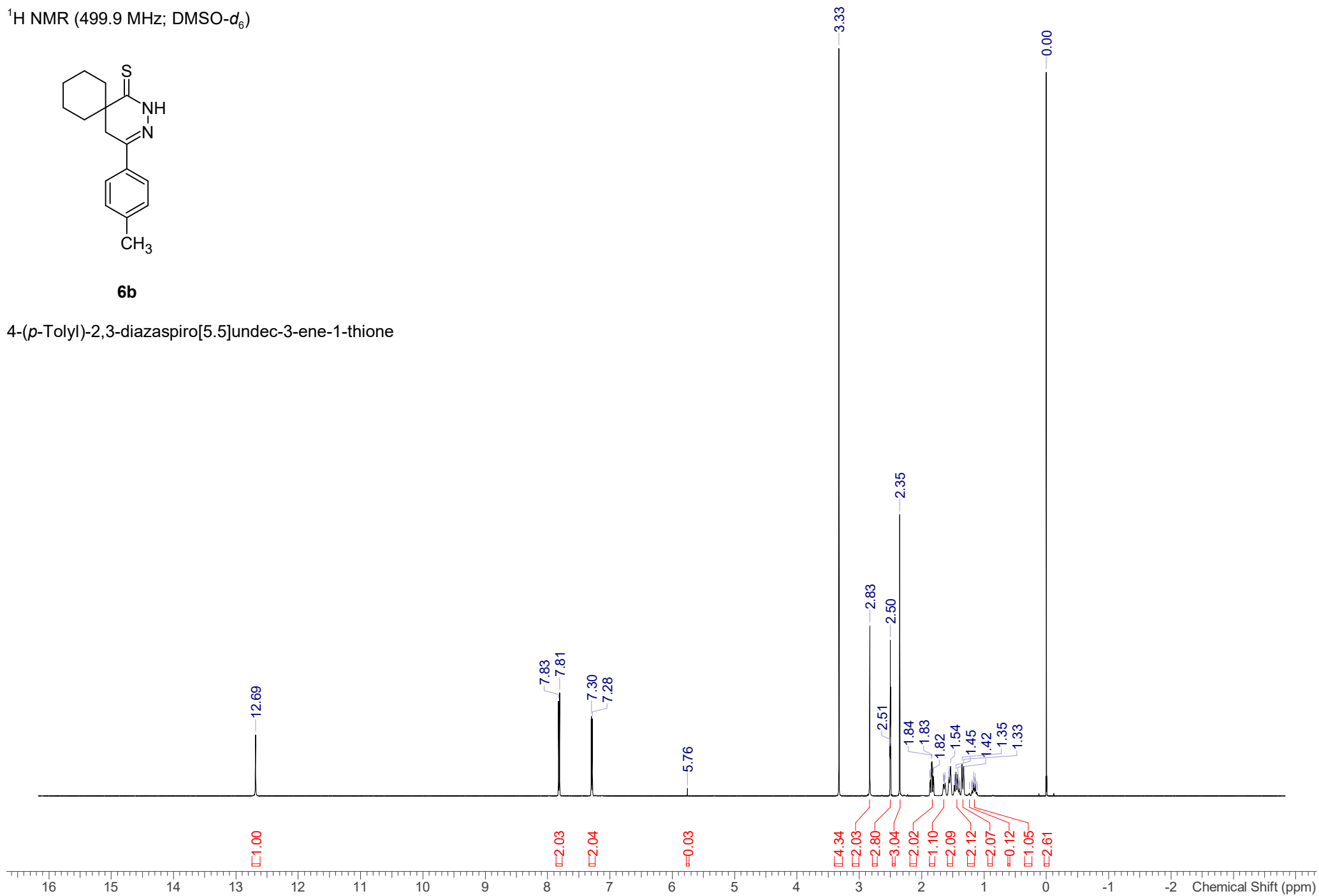


<sup>1</sup>H NMR (499.9 MHz; DMSO-d<sub>6</sub>)

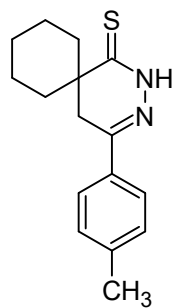


**6b**

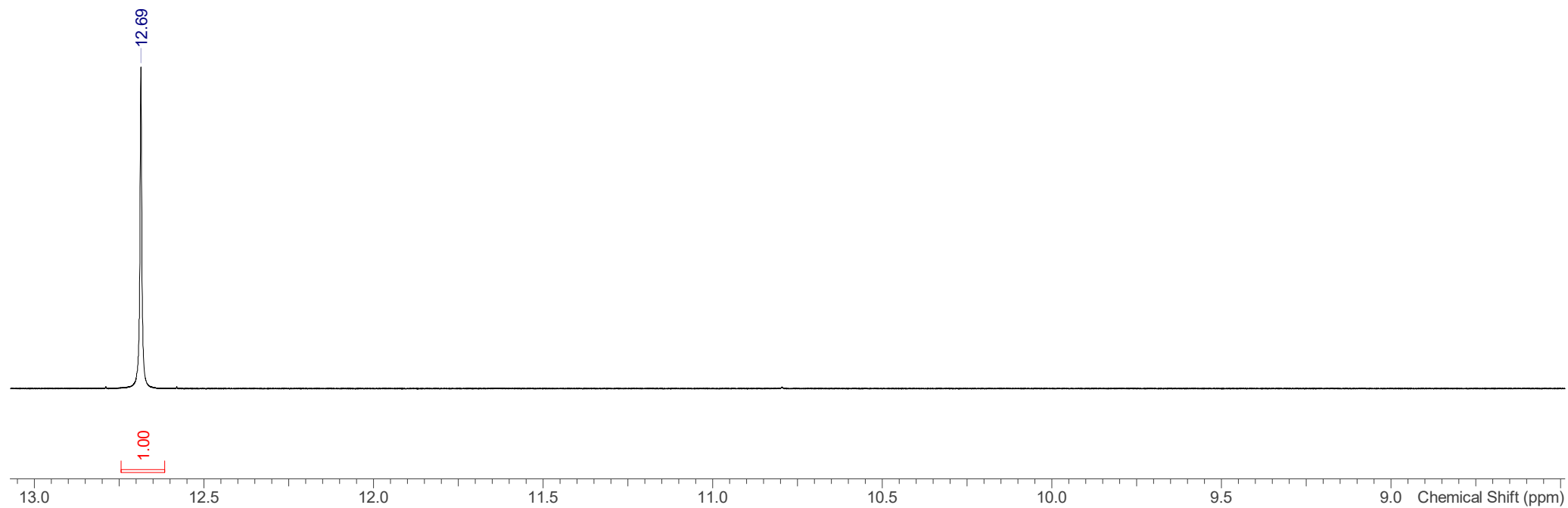
4-(*p*-Tolyl)-2,3-diazaspiro[5.5]undec-3-ene-1-thione



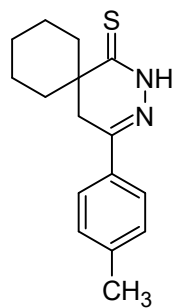
$^1\text{H}$  NMR (499.9 MHz;  $\text{DMSO-}d_6$ )



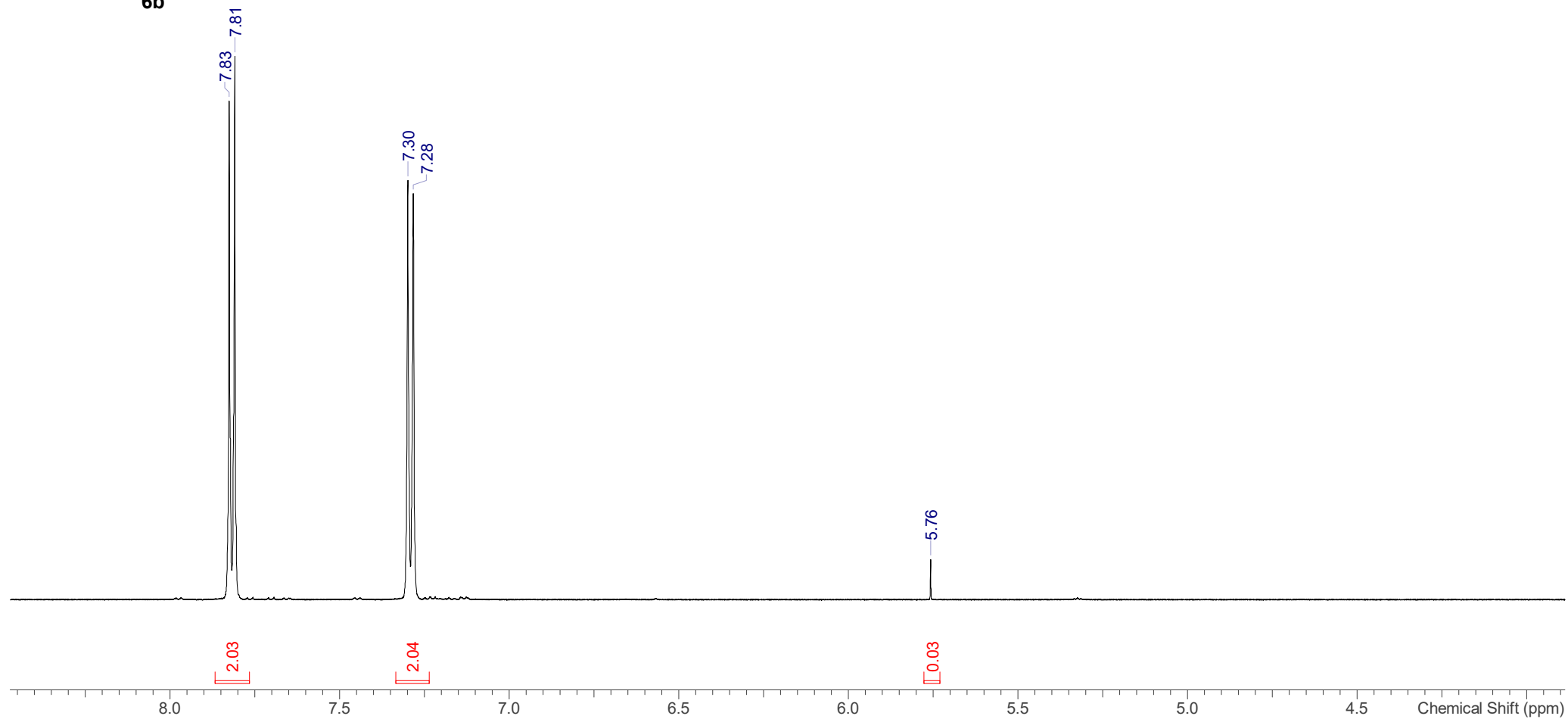
**6b**



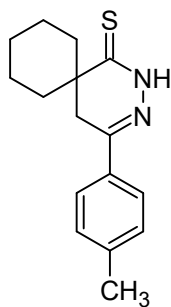
$^1\text{H}$  NMR (499.9 MHz;  $\text{DMSO}-d_6$ )



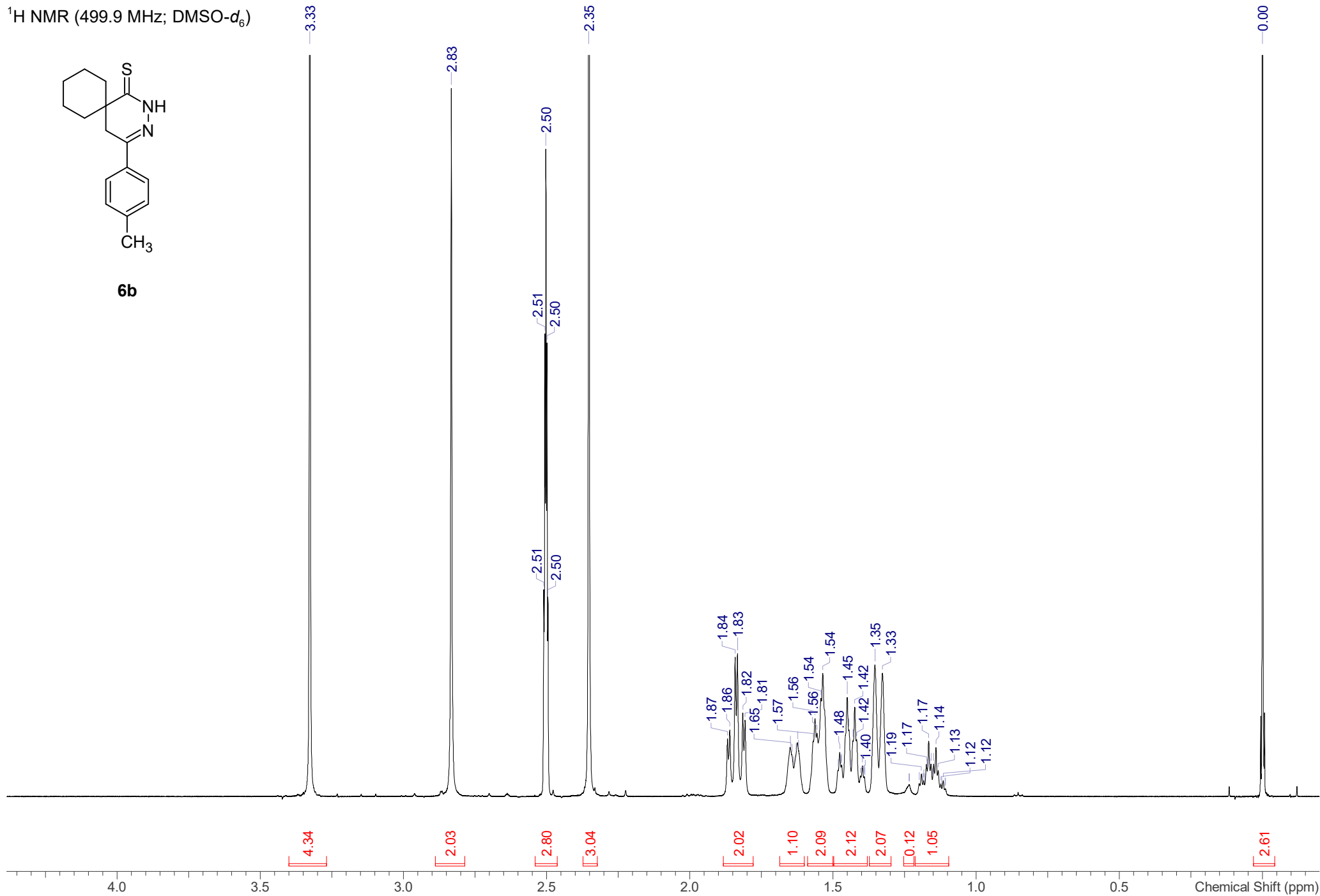
**6b**



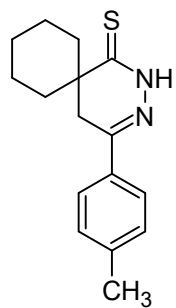
<sup>1</sup>H NMR (499.9 MHz; DMSO-d<sub>6</sub>)



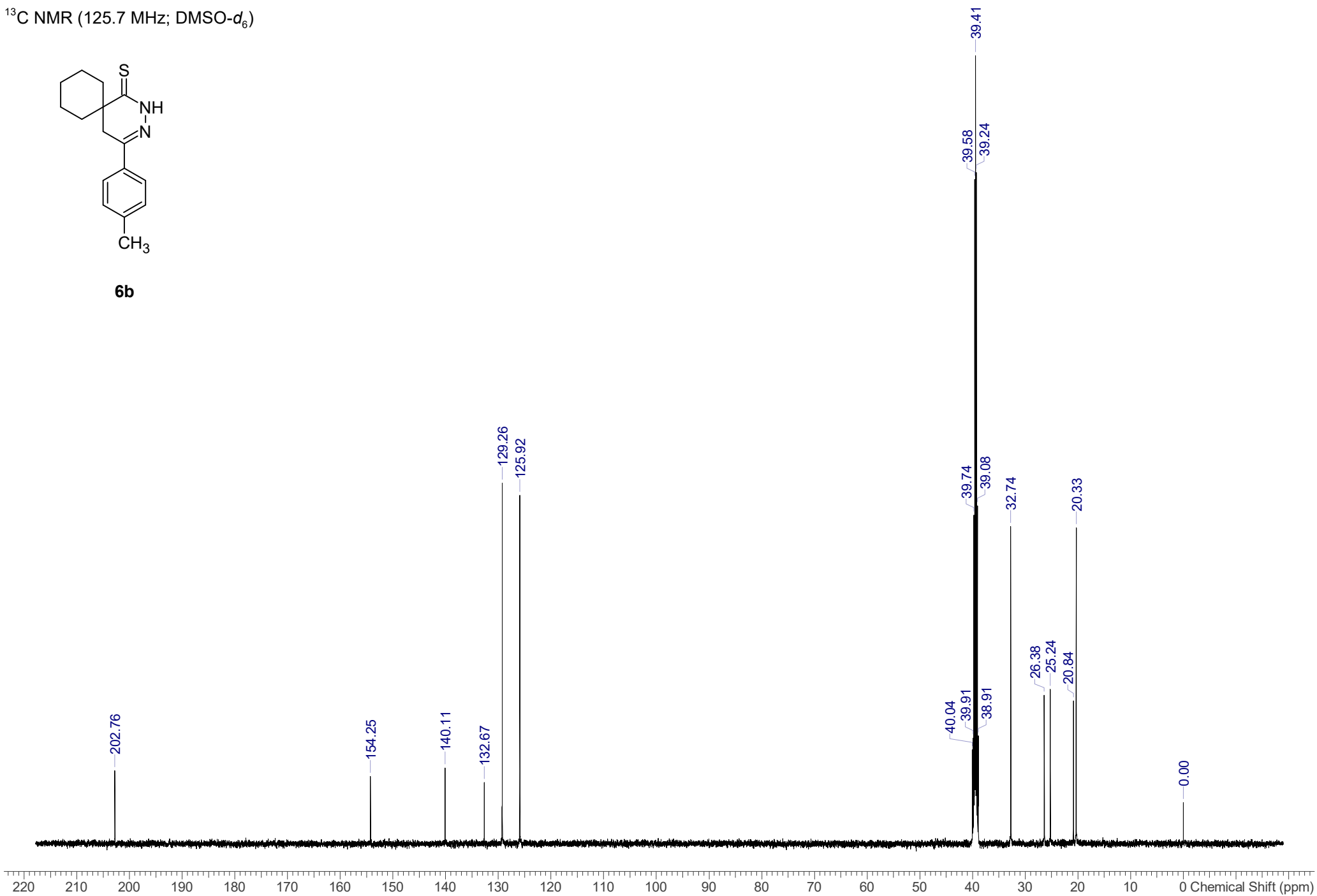
**6b**



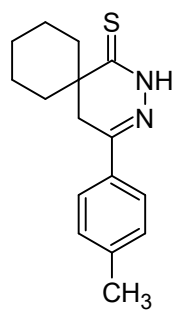
$^{13}\text{C}$  NMR (125.7 MHz;  $\text{DMSO-}d_6$ )



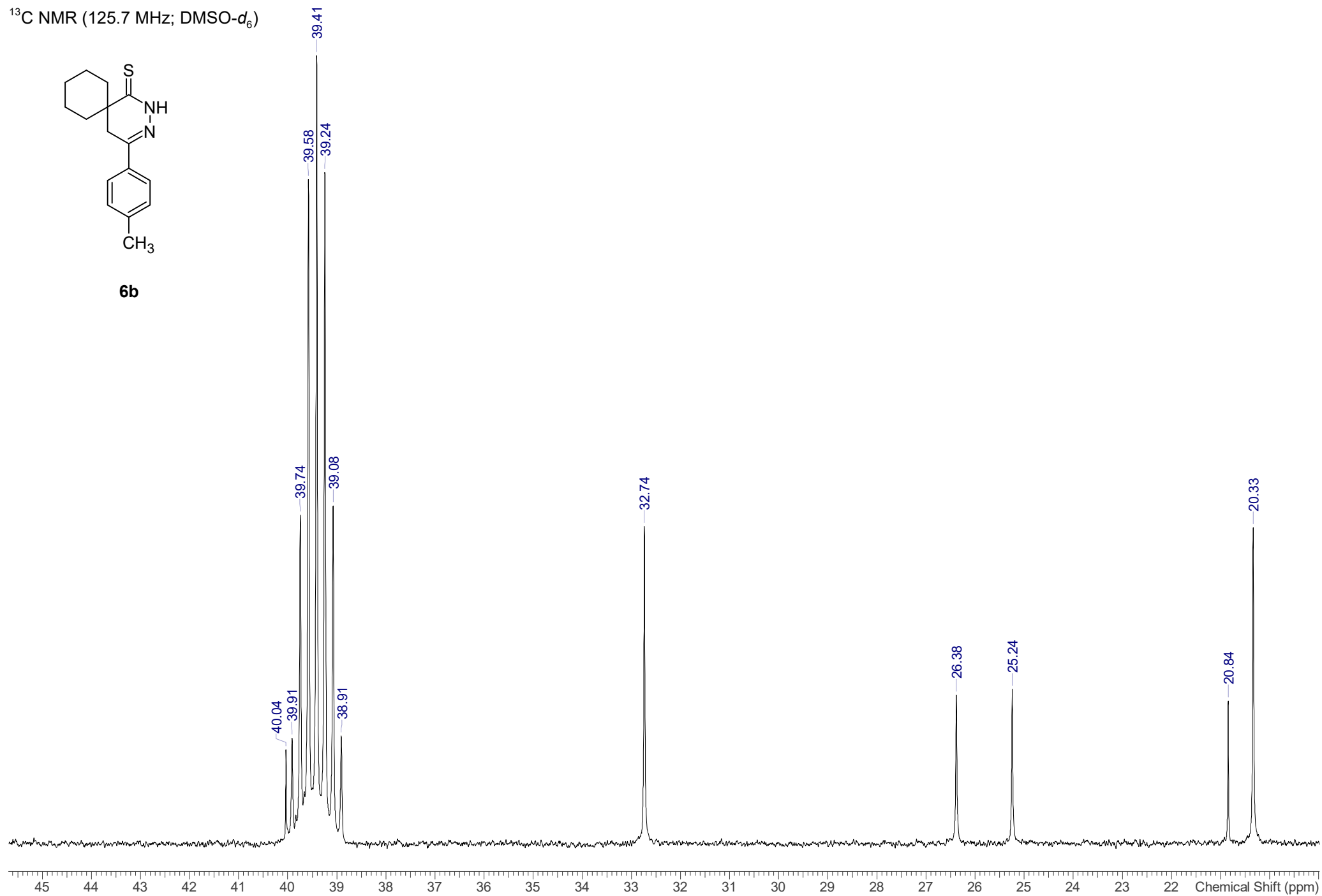
**6b**



$^{13}\text{C}$  NMR (125.7 MHz;  $\text{DMSO-}d_6$ )



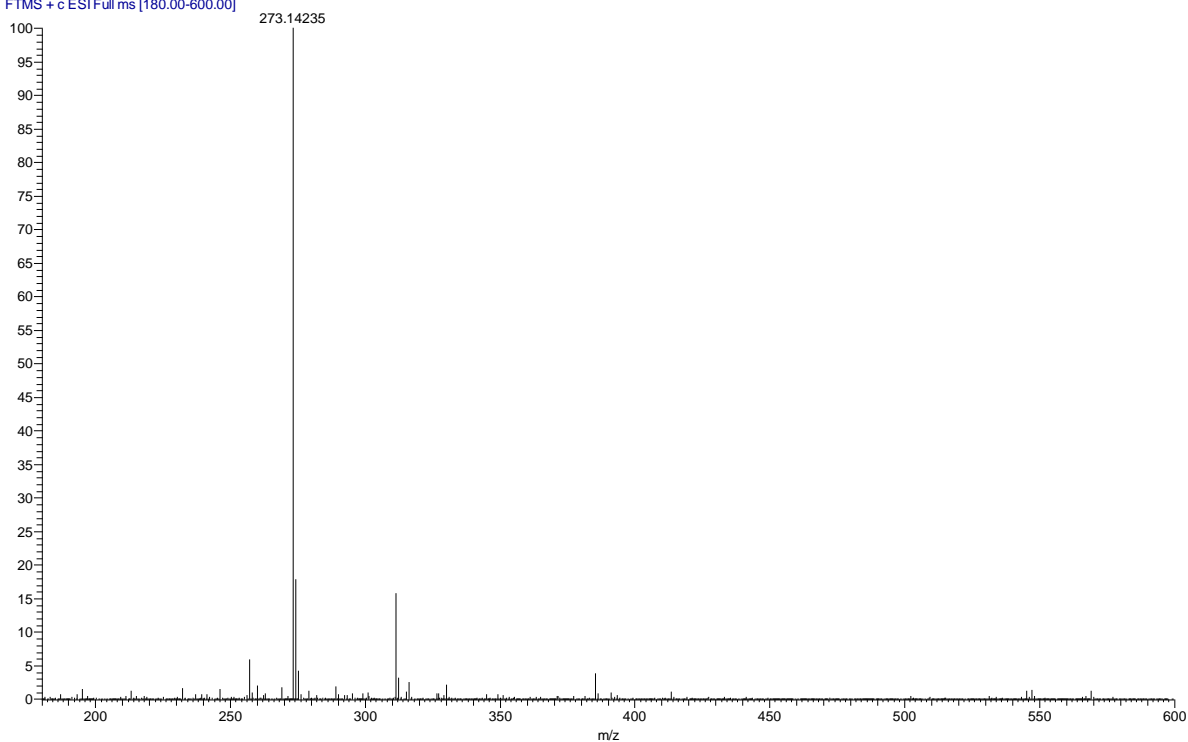
**6b**



# Compound **6b**

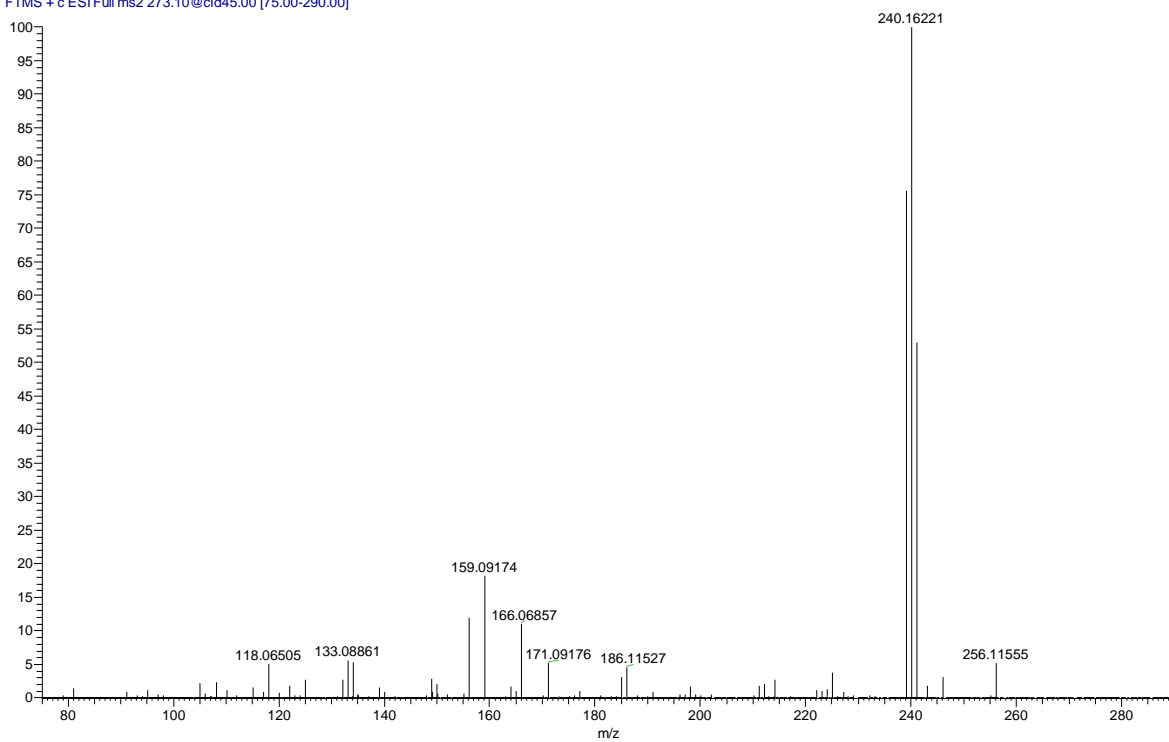
## HRMS spectrum (ESI)

ku71212\_sfc-179-1\_d\_ve4238 #1-23 RT: 0.00-0.19 AV: 23 NL: 1.36E7  
T: FTMS + c ESI Full ms [180.00-600.00]



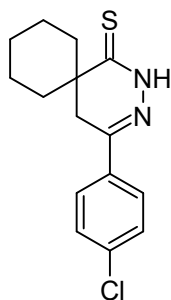
## HRMS spectrum (ESI daughter ion)

ku71212\_sfc-179-1\_d\_ve4239 #1-45 RT: 0.00-0.20 AV: 45 NL: 3.03E6  
T: FTMS + c ESI Full ms2 273.10@cid45.00 [75.00-290.00]



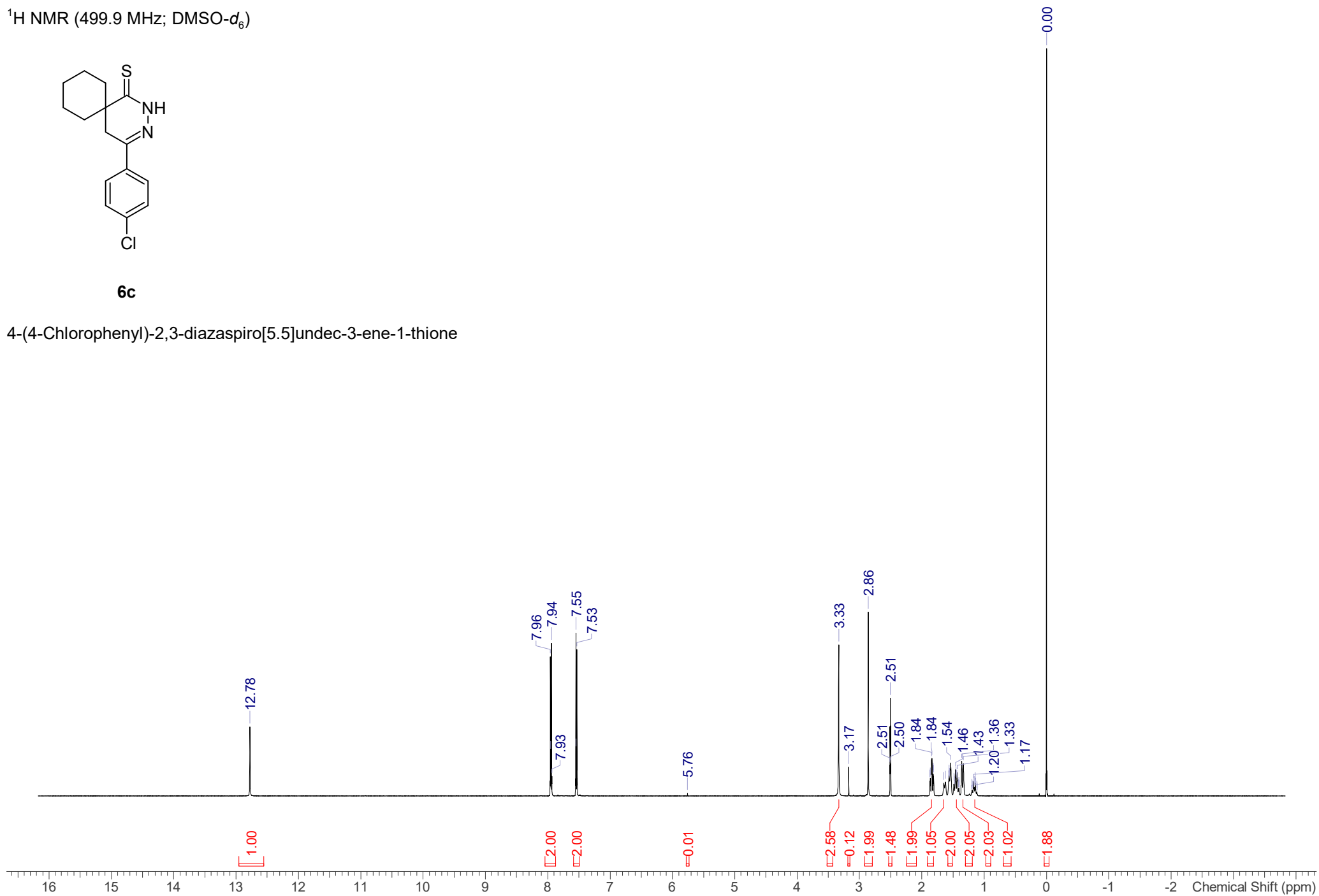


<sup>1</sup>H NMR (499.9 MHz; DMSO-d<sub>6</sub>)

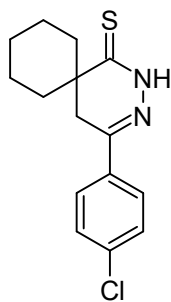


**6c**

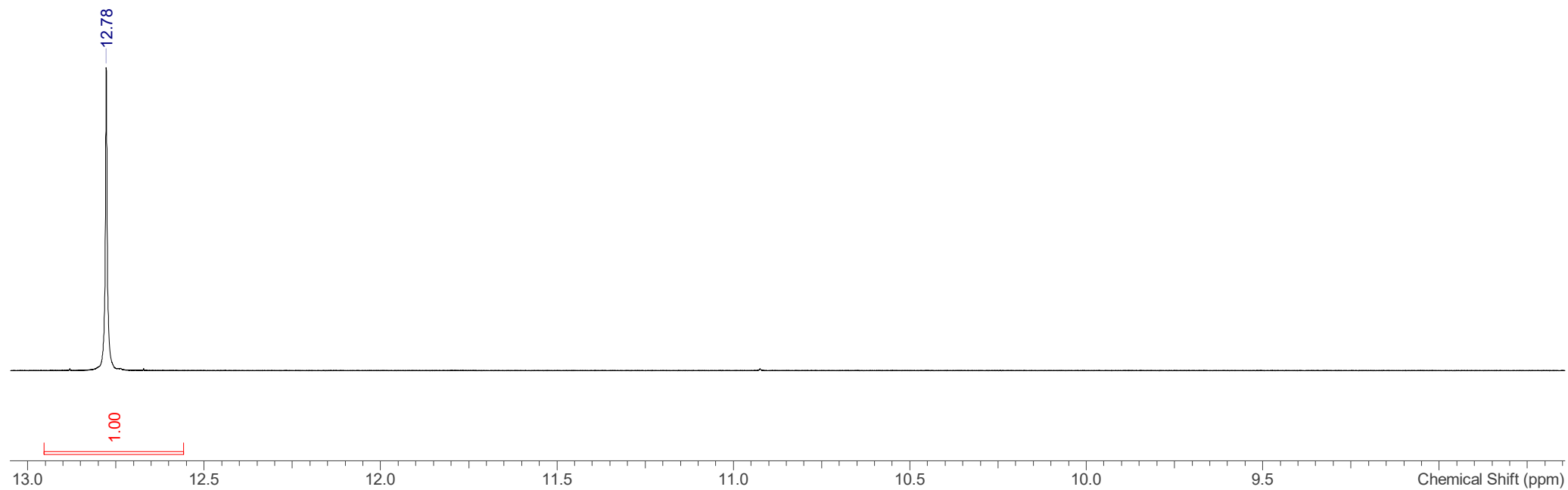
4-(4-Chlorophenyl)-2,3-diazaspiro[5.5]undec-3-ene-1-thione



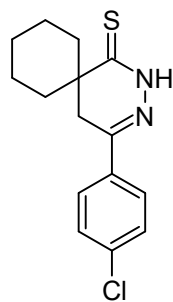
$^1\text{H}$  NMR (499.9 MHz;  $\text{DMSO-}d_6$ )



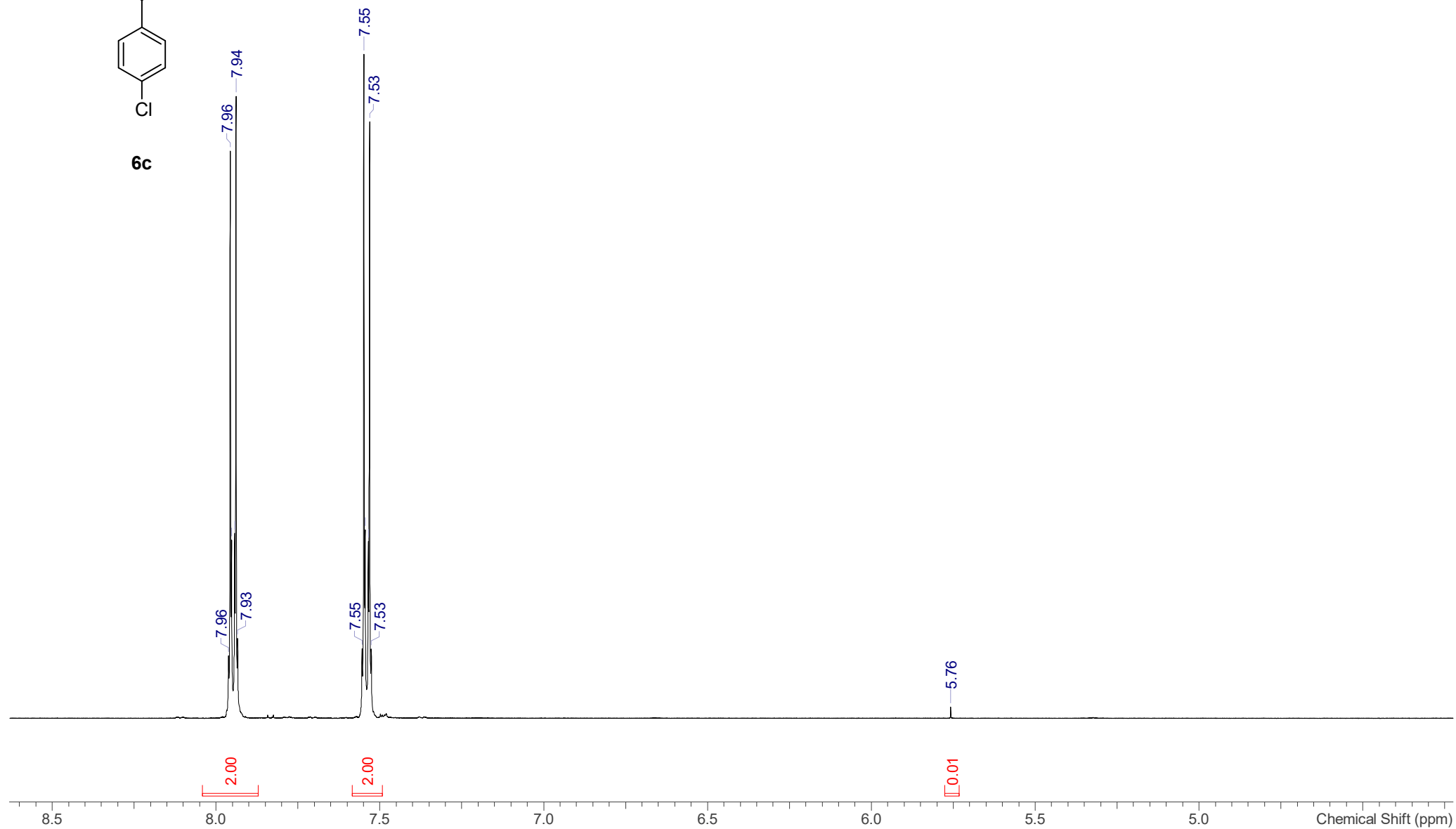
**6c**



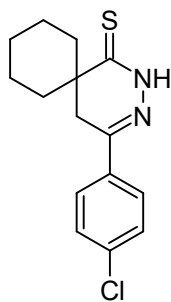
$^1\text{H}$  NMR (499.9 MHz;  $\text{DMSO-}d_6$ )



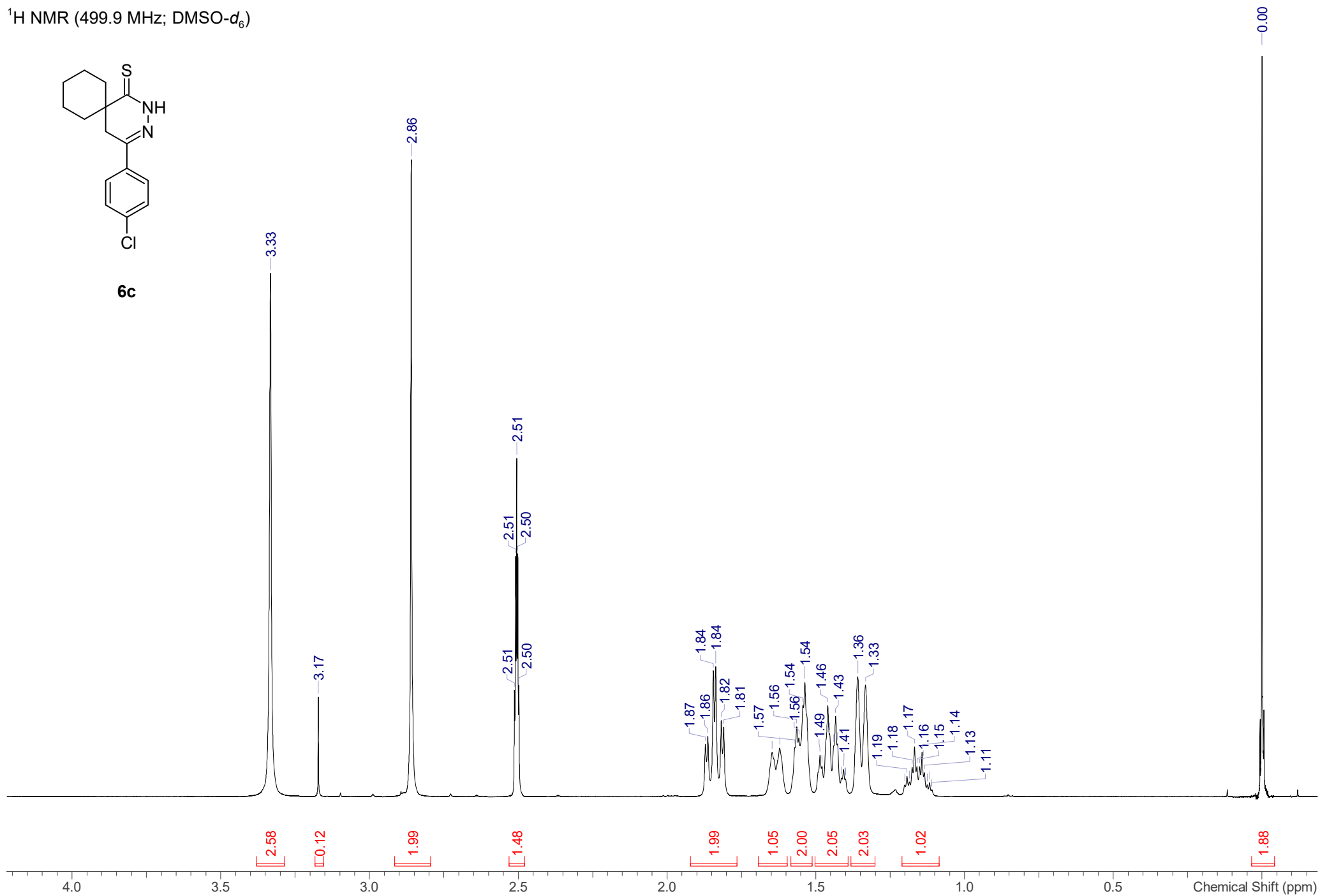
**6c**



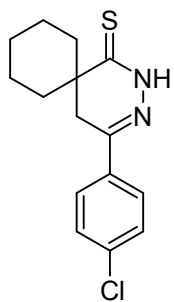
<sup>1</sup>H NMR (499.9 MHz; DMSO-d<sub>6</sub>)



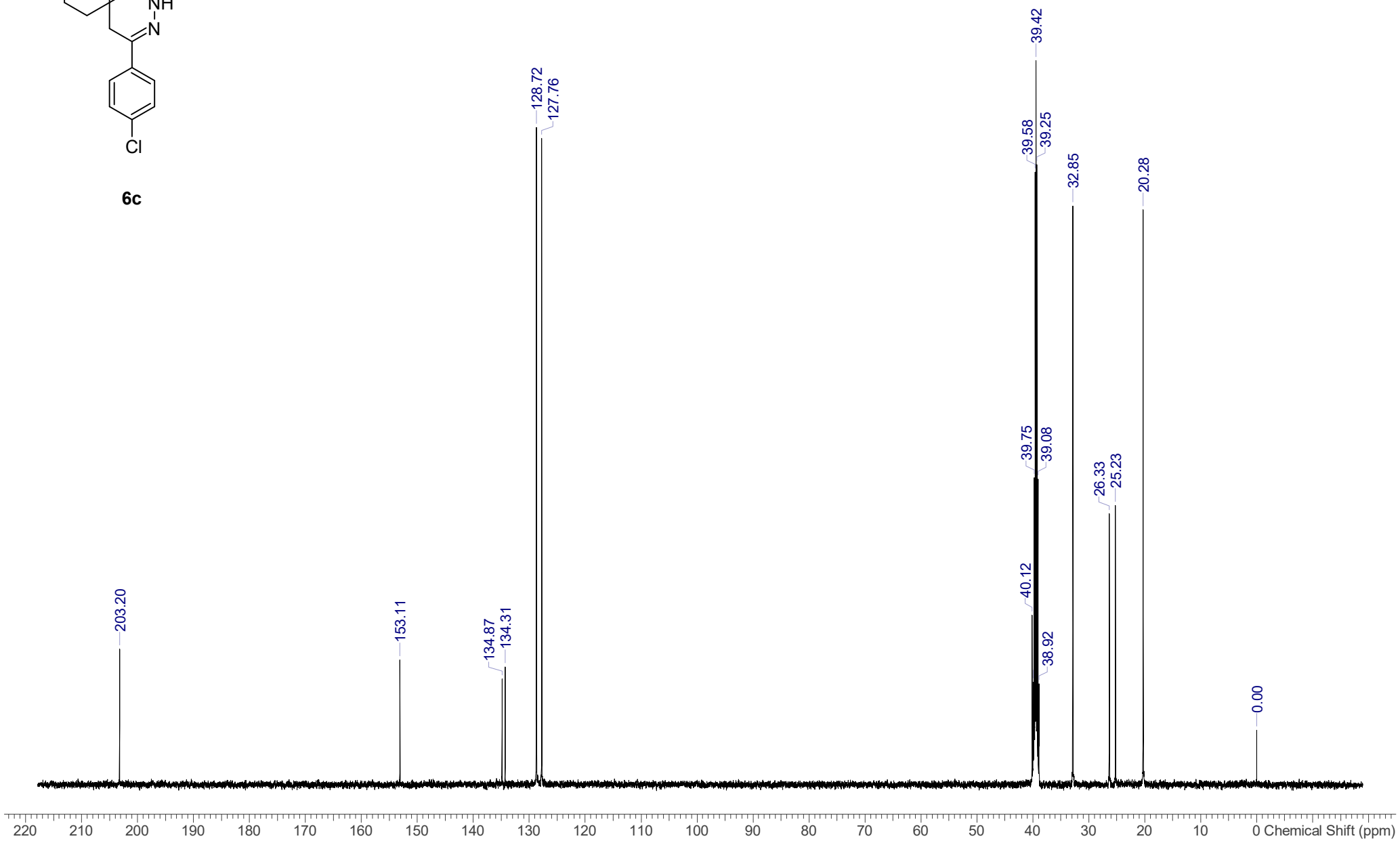
**6c**



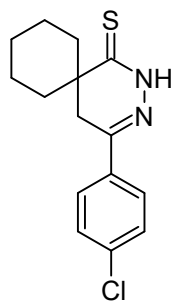
<sup>13</sup>C NMR (125.7 MHz; DMSO-d<sub>6</sub>)



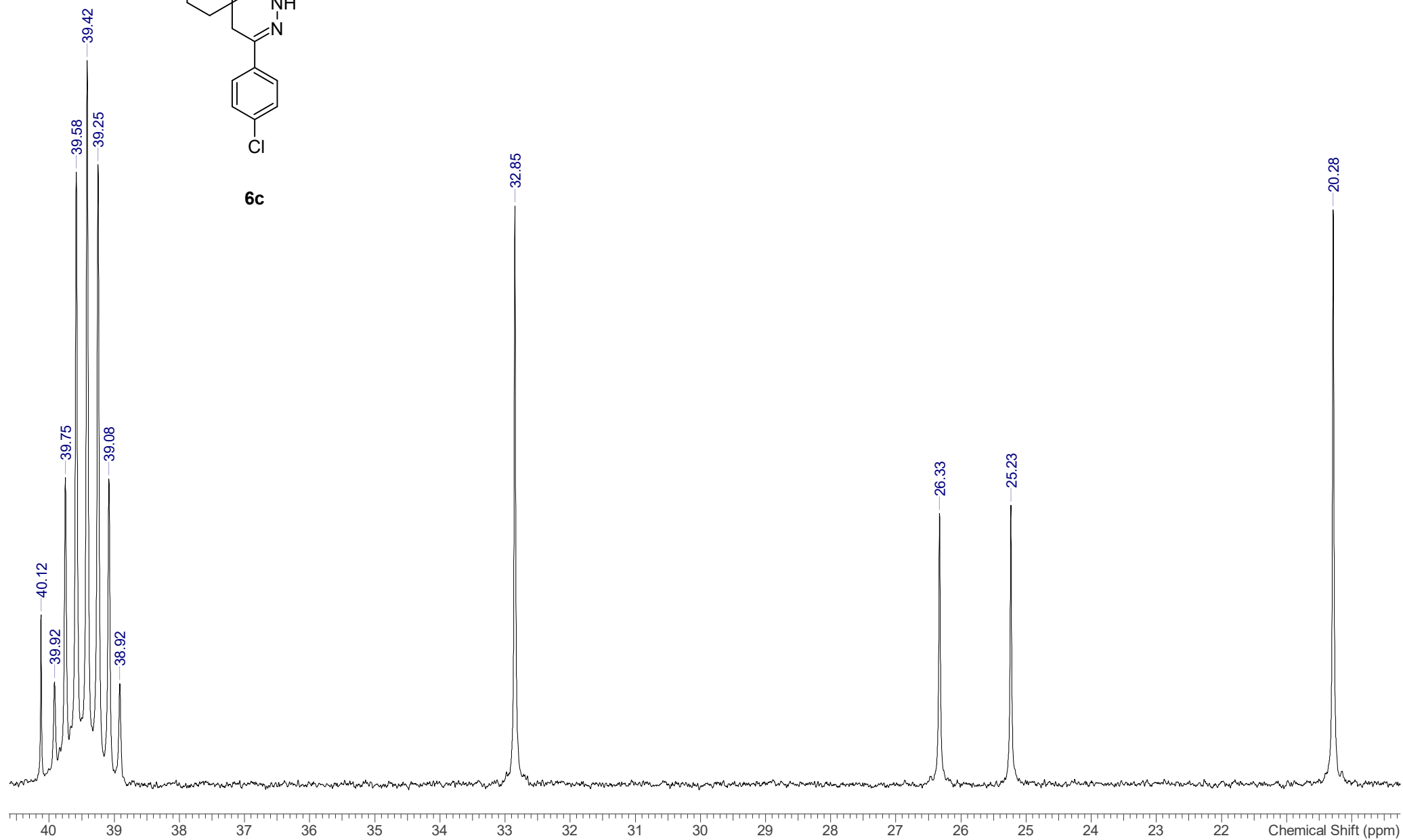
**6c**



$^{13}\text{C}$  NMR (125.7 MHz;  $\text{DMSO-}d_6$ )



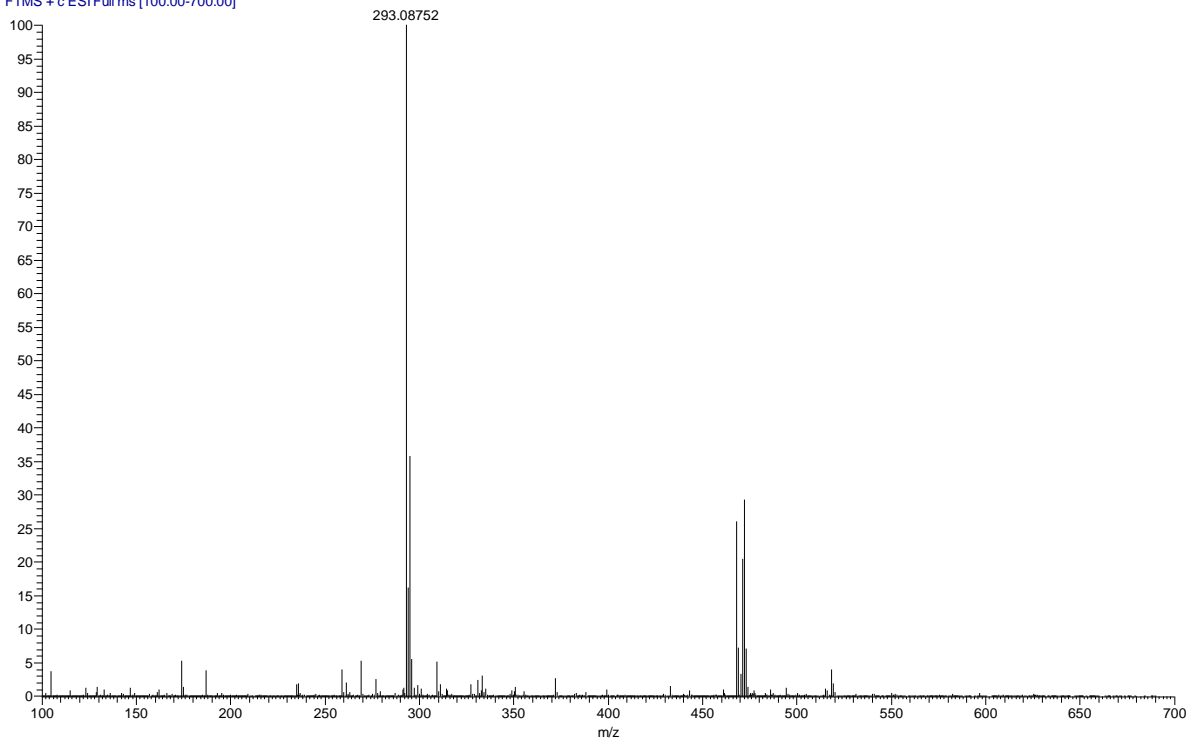
**6c**



# Compound 6c

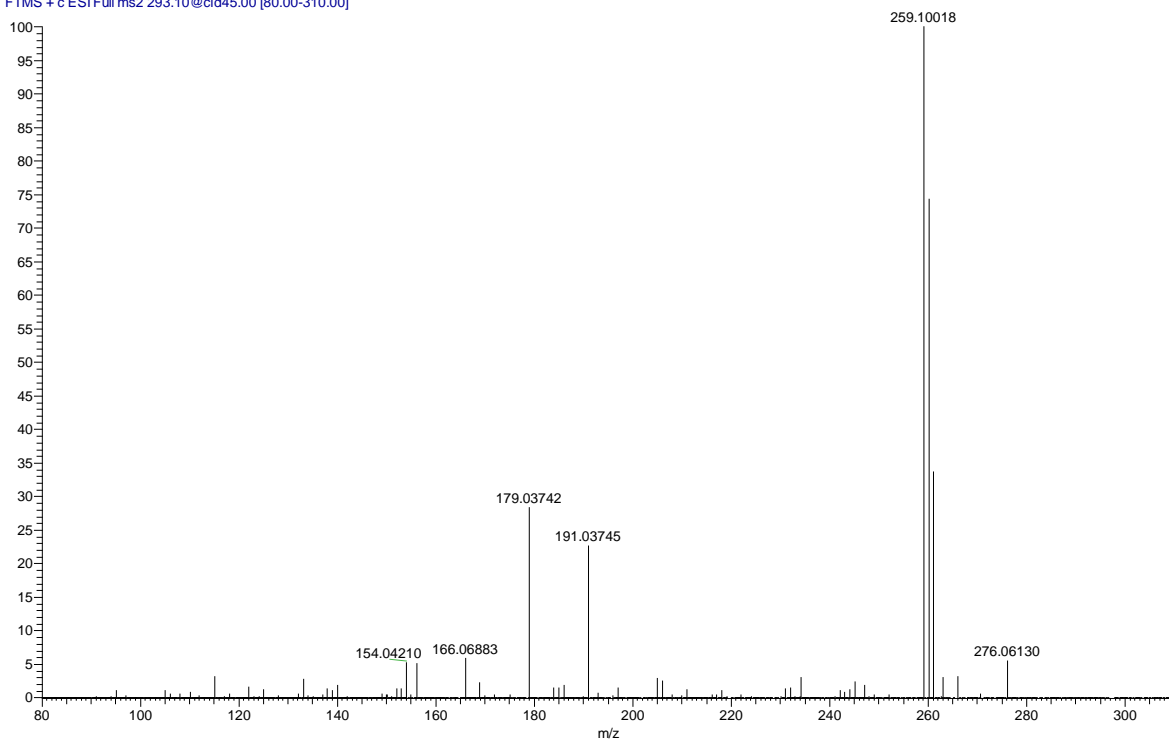
## HRMS spectrum (ESI)

ku70694\_sfc-167-1\_d\_ve3797 #1-23 RT: 0.00-0.20 AV: 23 NL: 5.48E6  
T: FTMS + c ESI Full ms [100.00-700.00]

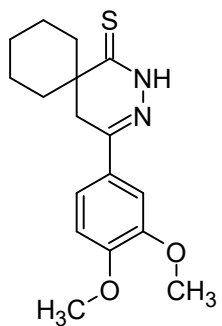


## HRMS spectrum (ESI daughter ion)

ku70694\_sfc-167-1\_d\_ve3798 #1-45 RT: 0.00-0.20 AV: 45 NL: 1.61E6  
T: FTMS + c ESI Full ms2 293.10@cid45.00 [80.00-310.00]

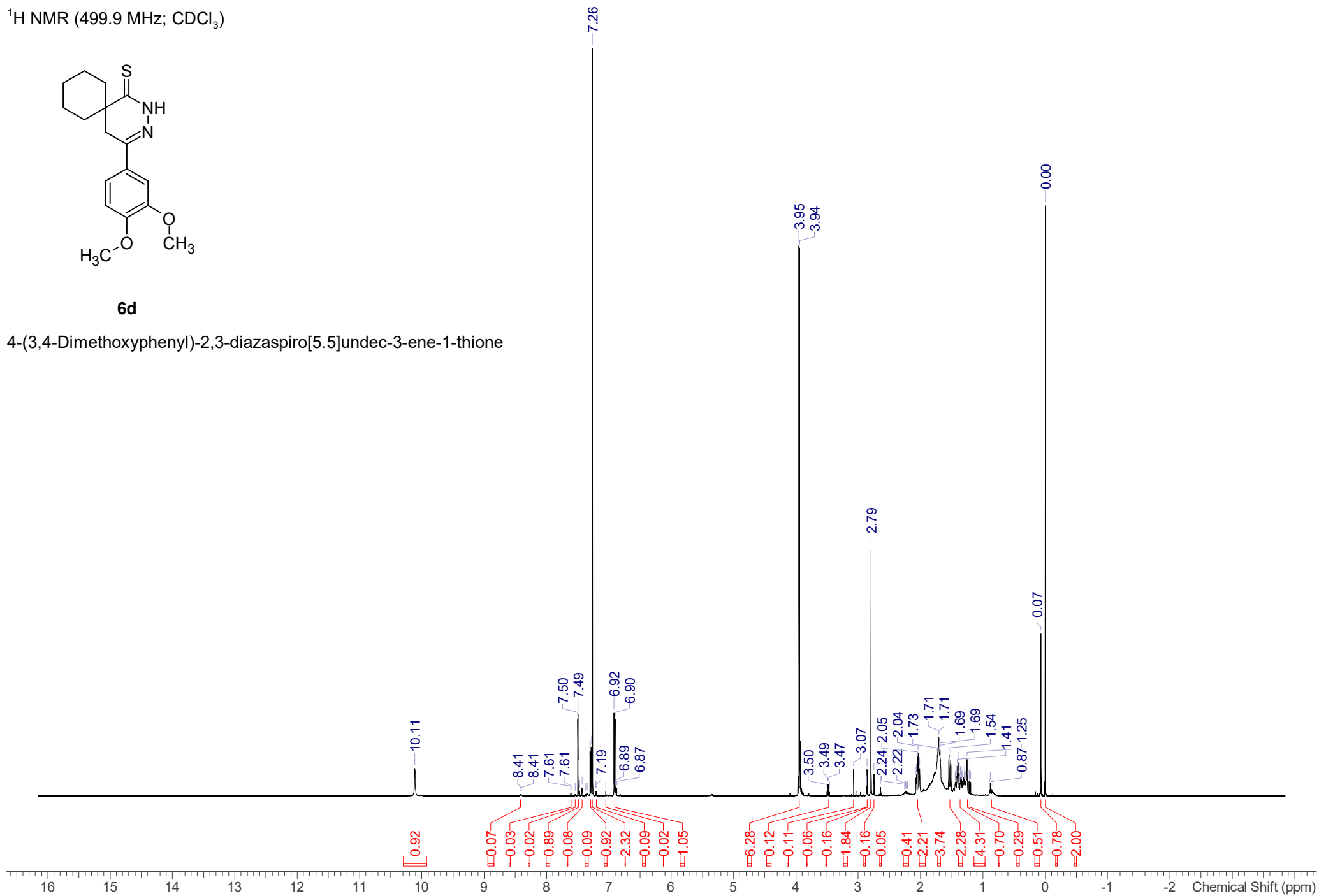


<sup>1</sup>H NMR (499.9 MHz; CDCl<sub>3</sub>)



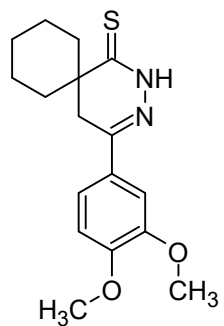
**6d**

4-(3,4-Dimethoxyphenyl)-2,3-diazaspiro[5.5]undec-3-ene-1-thione

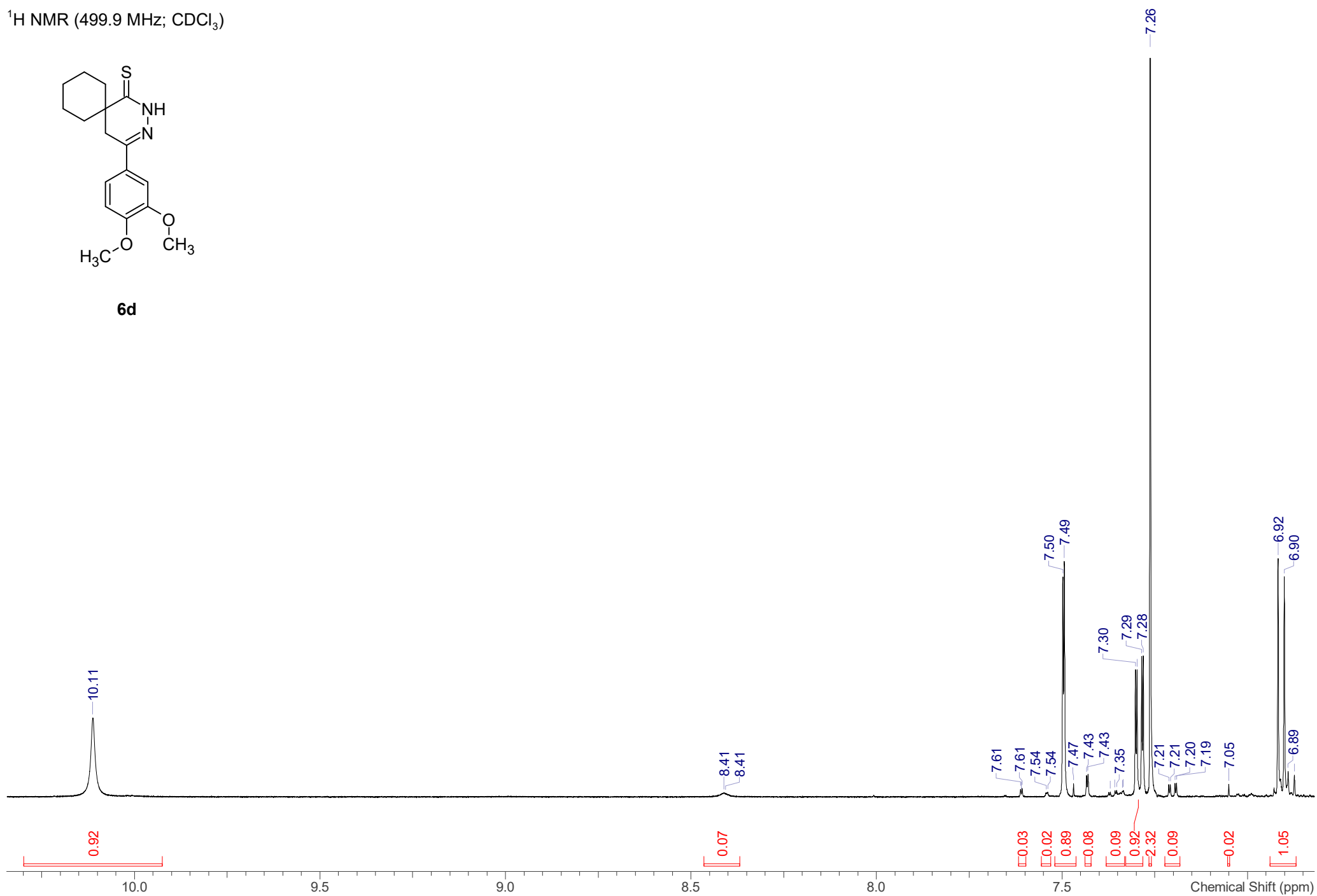




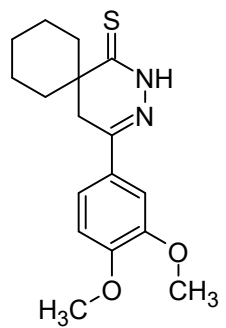
<sup>1</sup>H NMR (499.9 MHz; CDCl<sub>3</sub>)



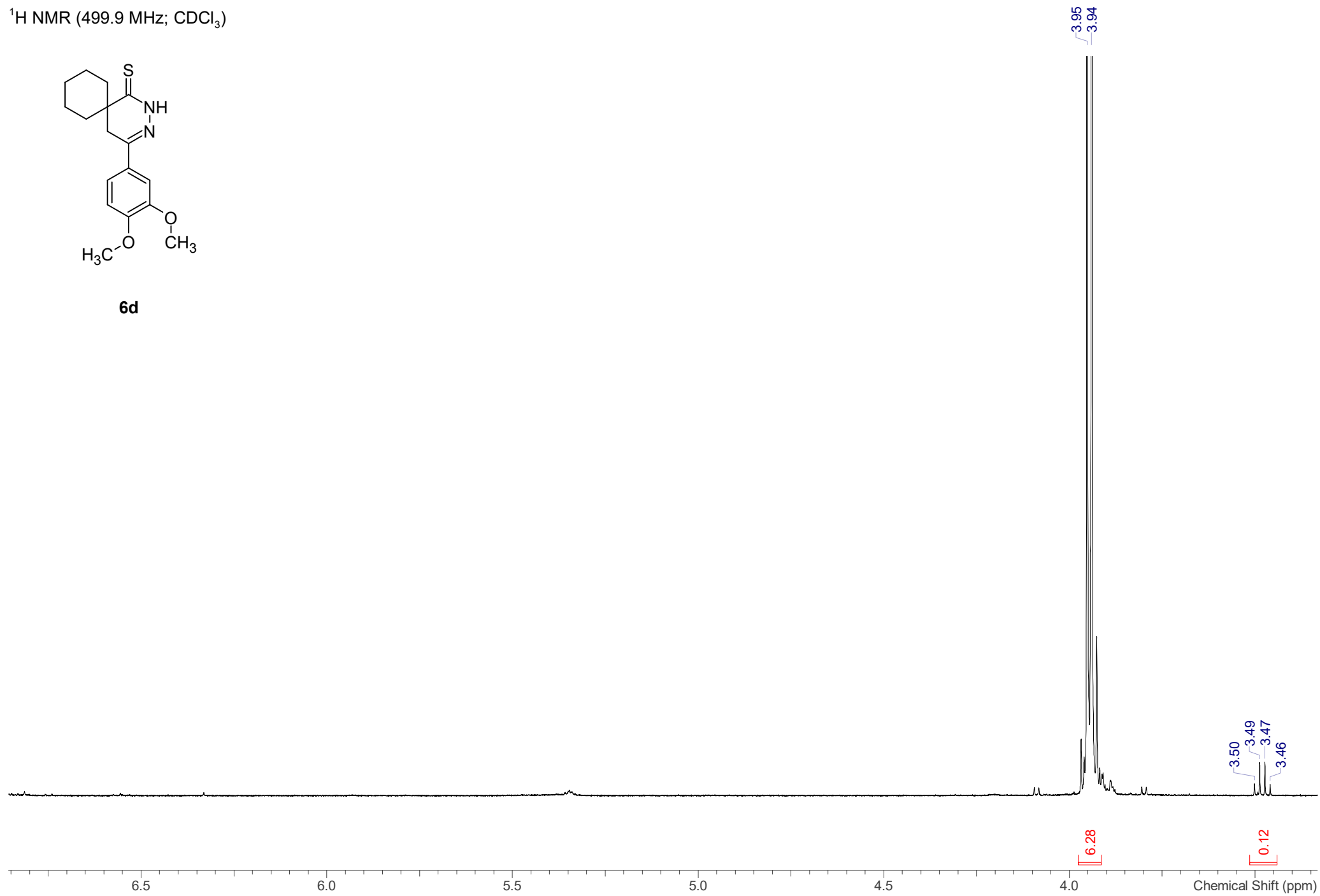
**6d**



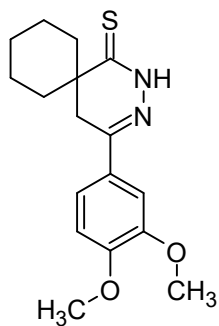
<sup>1</sup>H NMR (499.9 MHz; CDCl<sub>3</sub>)



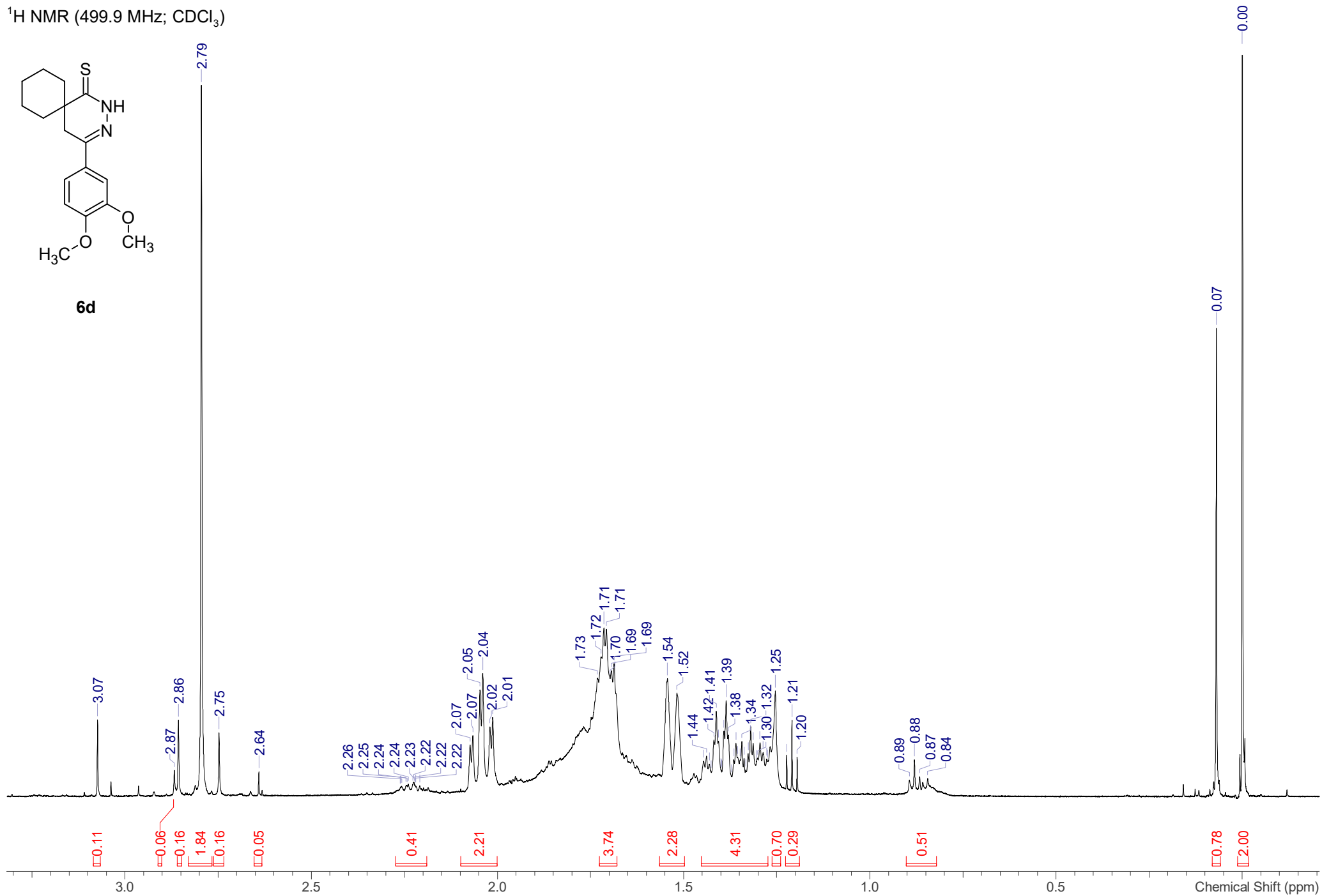
**6d**



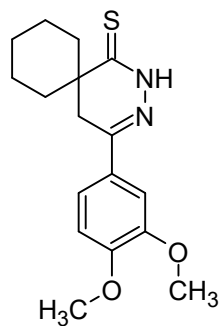
<sup>1</sup>H NMR (499.9 MHz; CDCl<sub>3</sub>)



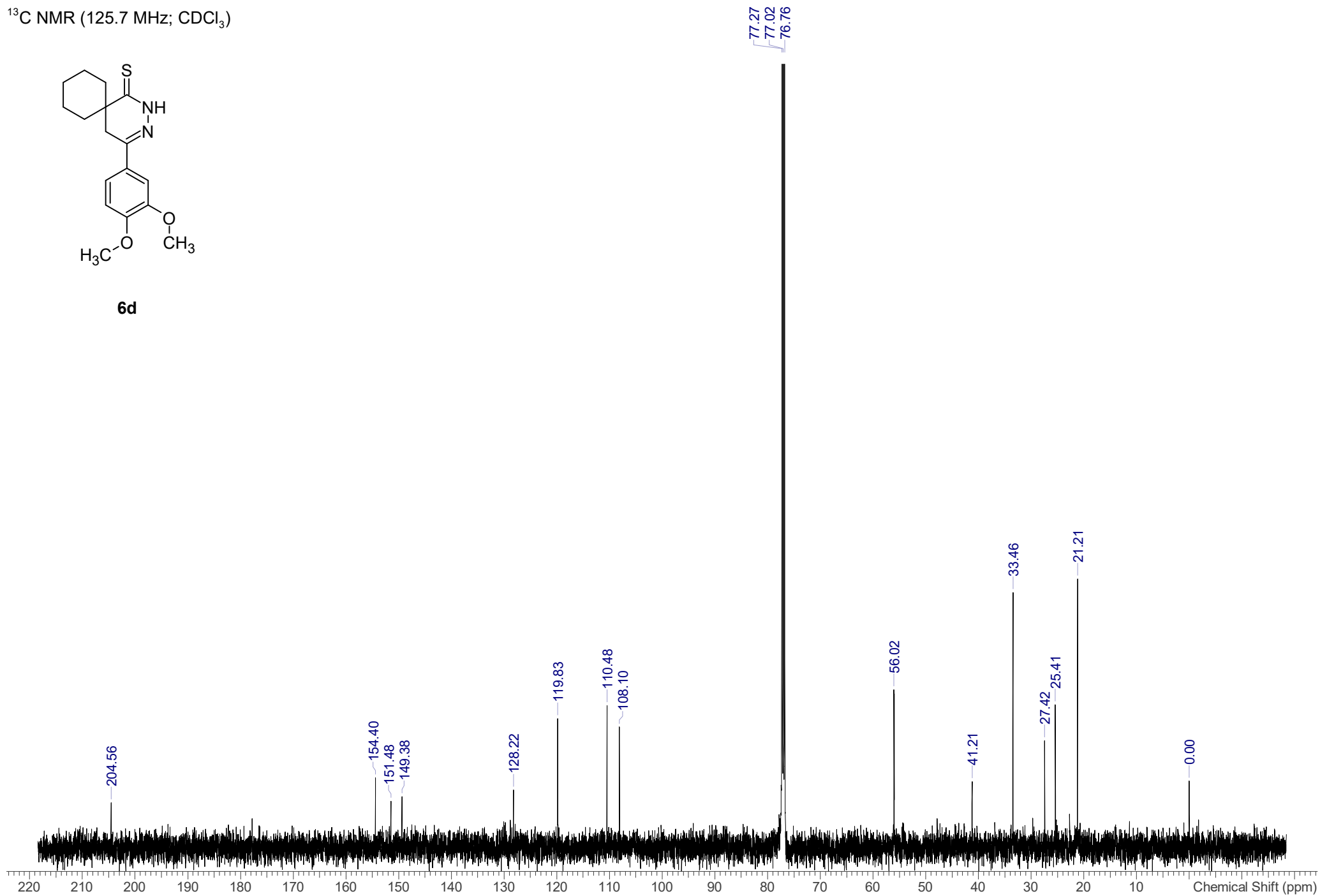
**6d**



$^{13}\text{C}$  NMR (125.7 MHz;  $\text{CDCl}_3$ )



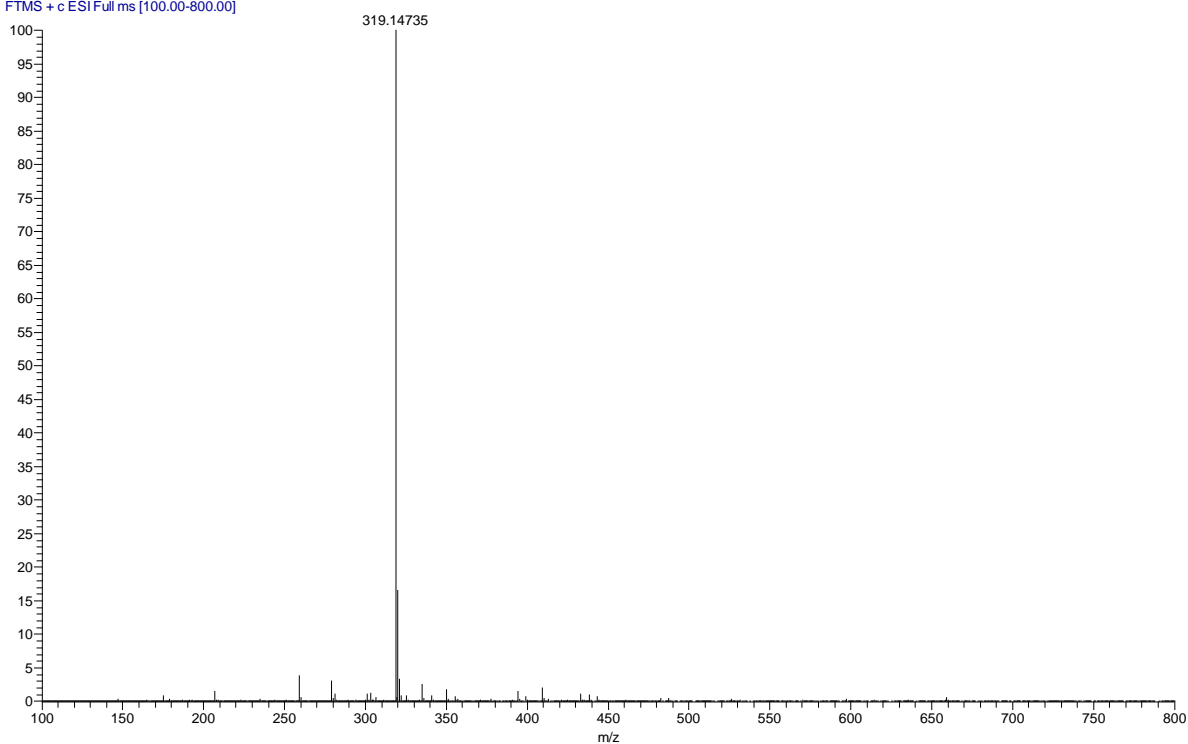
6d



# Compound 6d

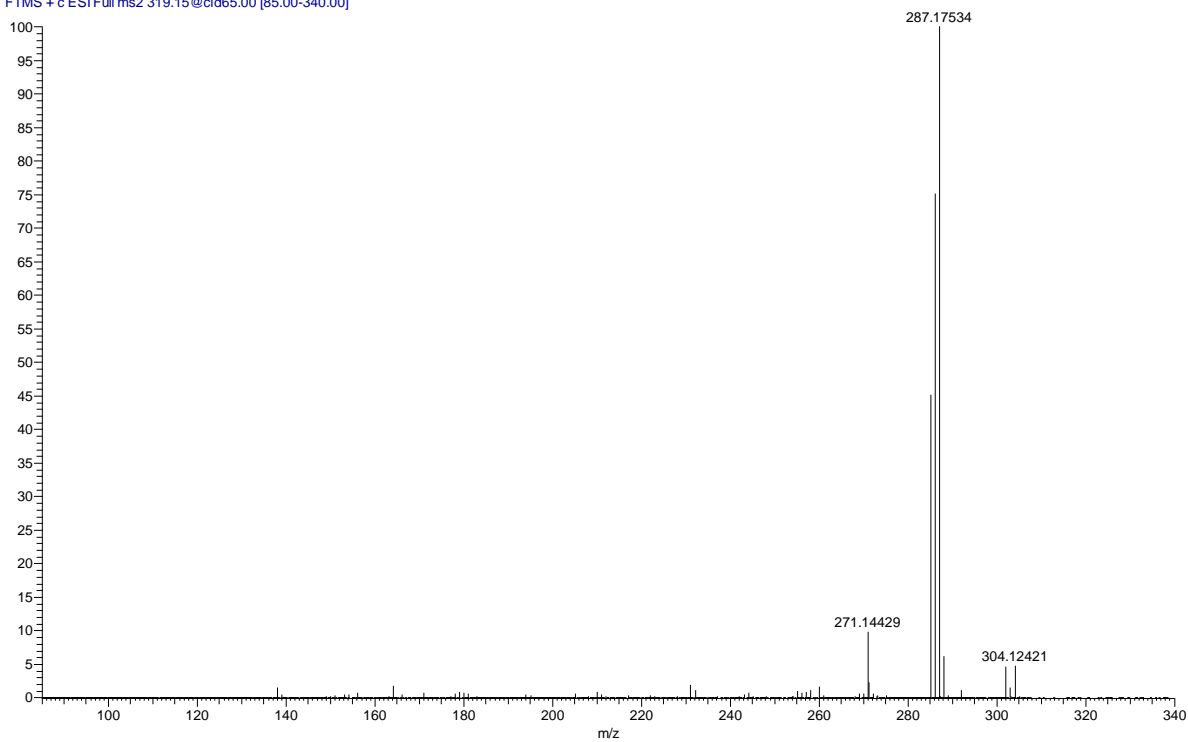
## HRMS spectrum (ESI)

ku66055\_rg-56\_ft24616 #1-30 RT: 0.00-0.27 AV: 30 NL: 5.99E6  
T: FTMS + c ESI Full ms [100.00-800.00]

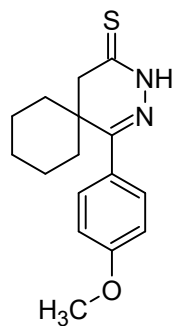


## HRMS spectrum (ESI daughter ion)

ku66055\_rg-56\_ft24617 #1-30 RT: 0.00-0.32 AV: 30 NL: 2.52E6  
T: FTMS + c ESI Full ms2 319.15@cid65.00 [85.00-340.00]

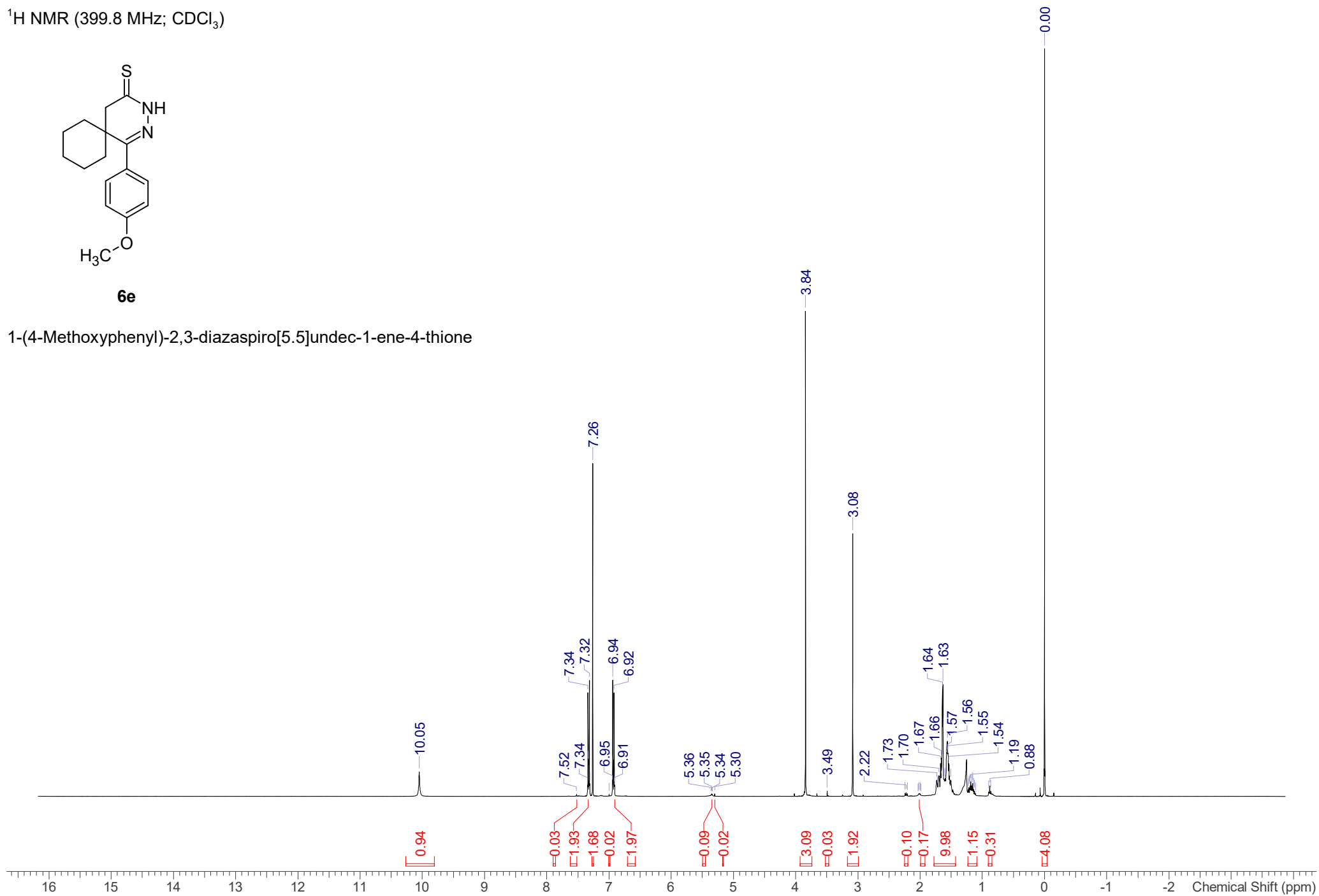


<sup>1</sup>H NMR (399.8 MHz; CDCl<sub>3</sub>)

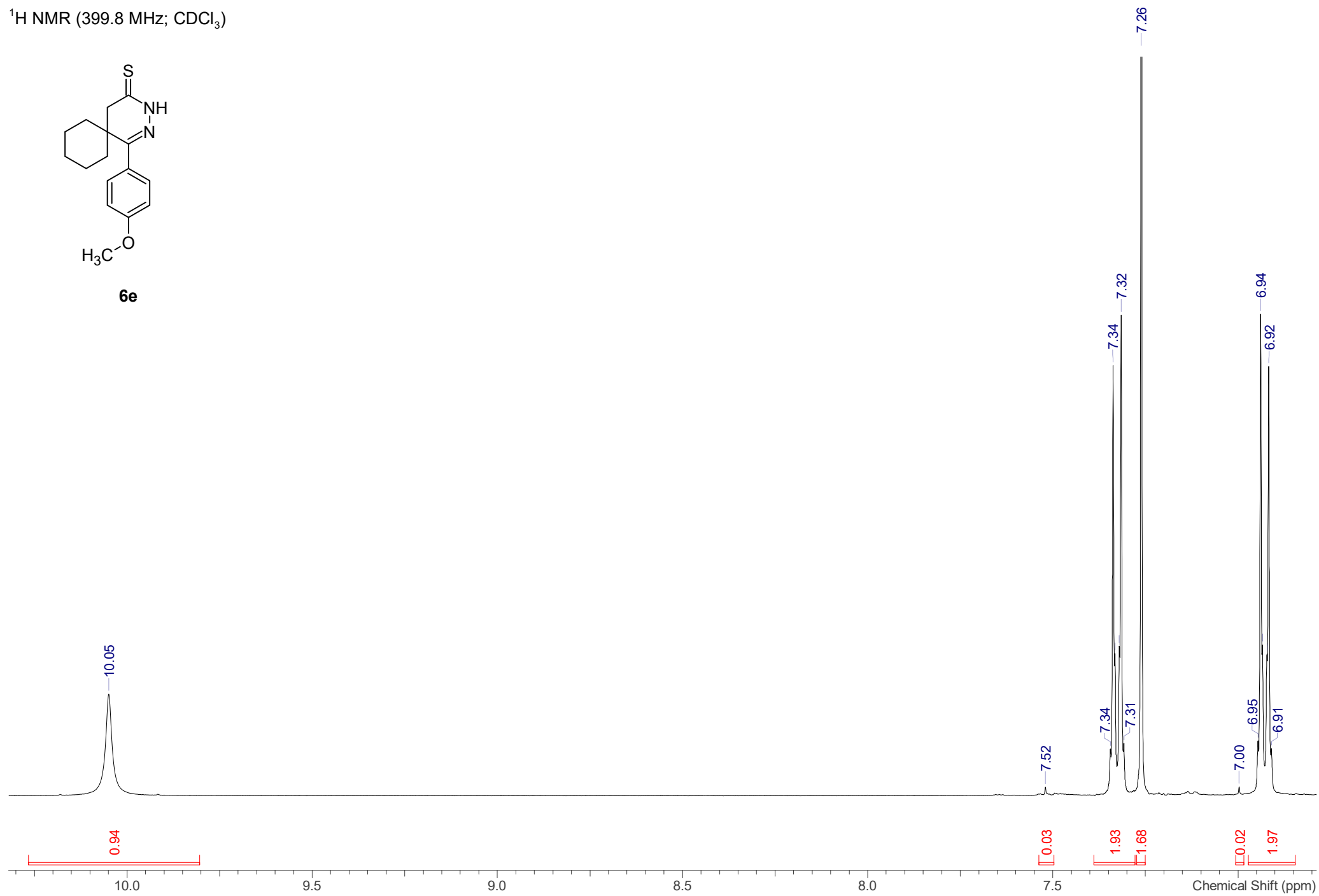
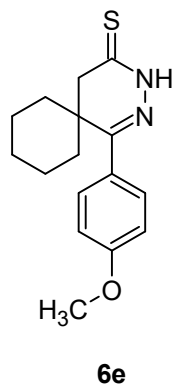


**6e**

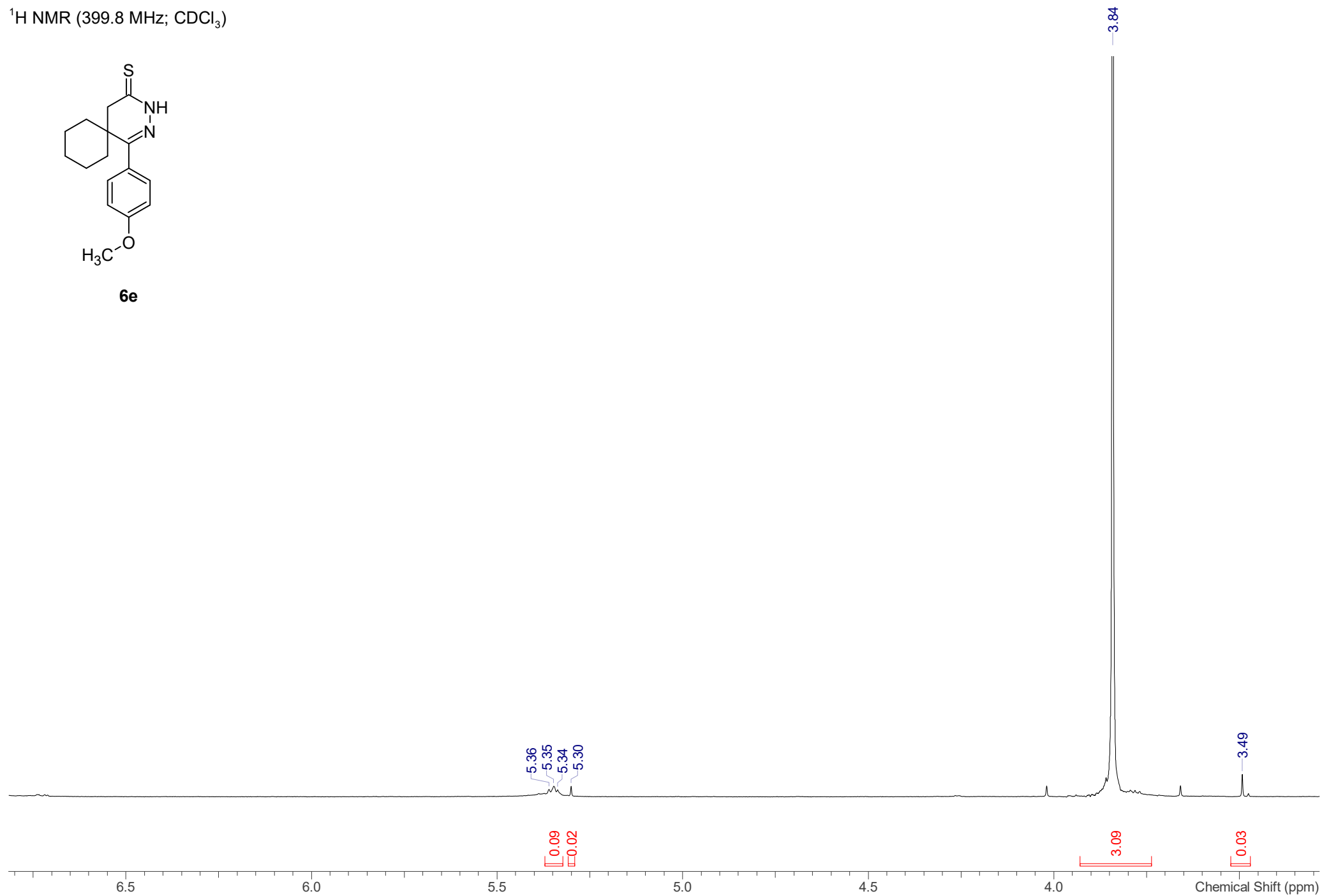
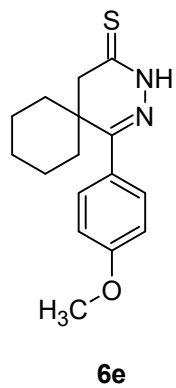
1-(4-Methoxyphenyl)-2,3-diazaspiro[5.5]undec-1-ene-4-thione



<sup>1</sup>H NMR (399.8 MHz; CDCl<sub>3</sub>)

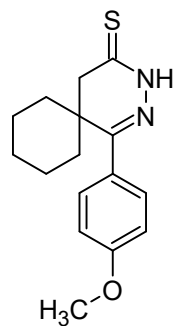


<sup>1</sup>H NMR (399.8 MHz; CDCl<sub>3</sub>)

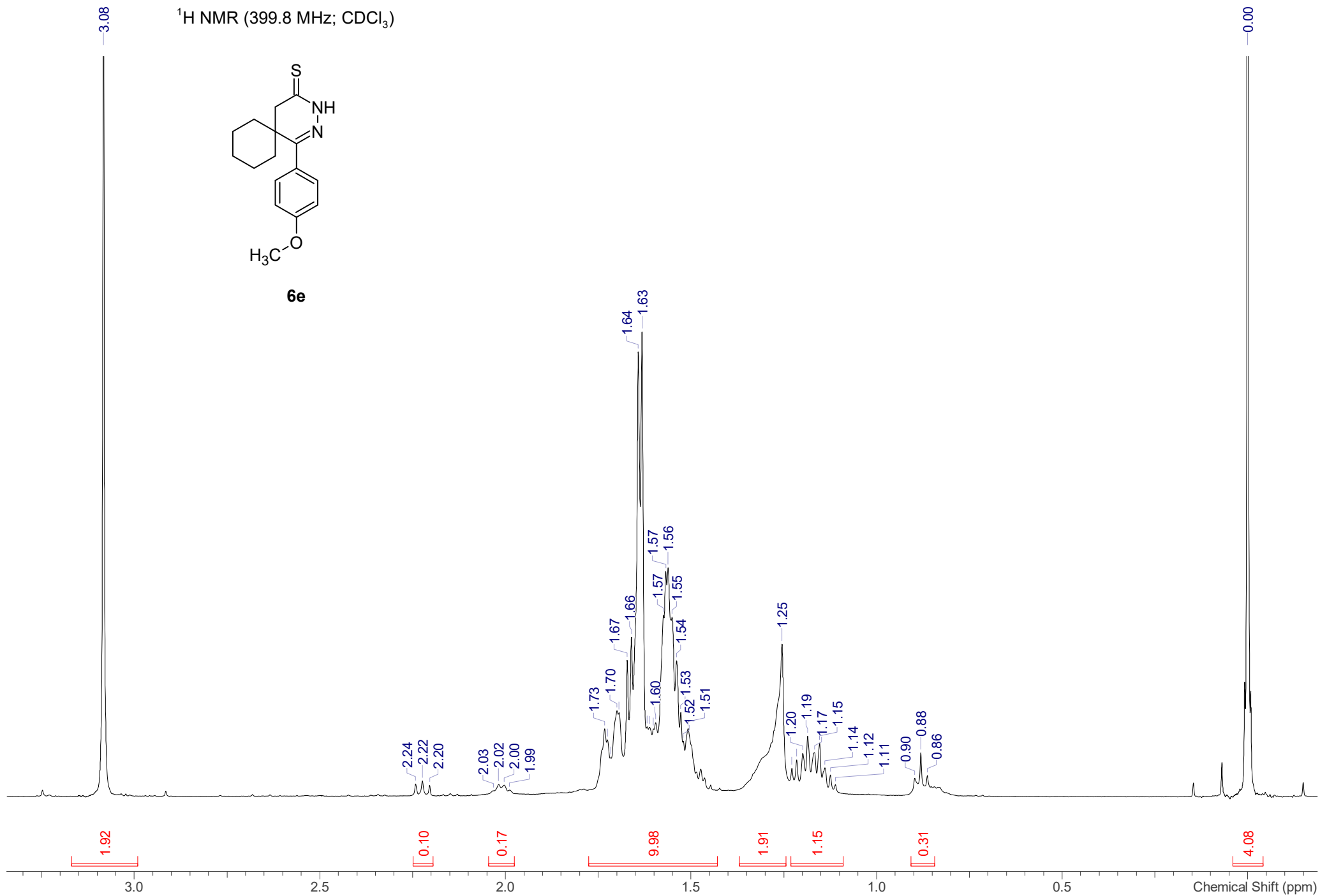




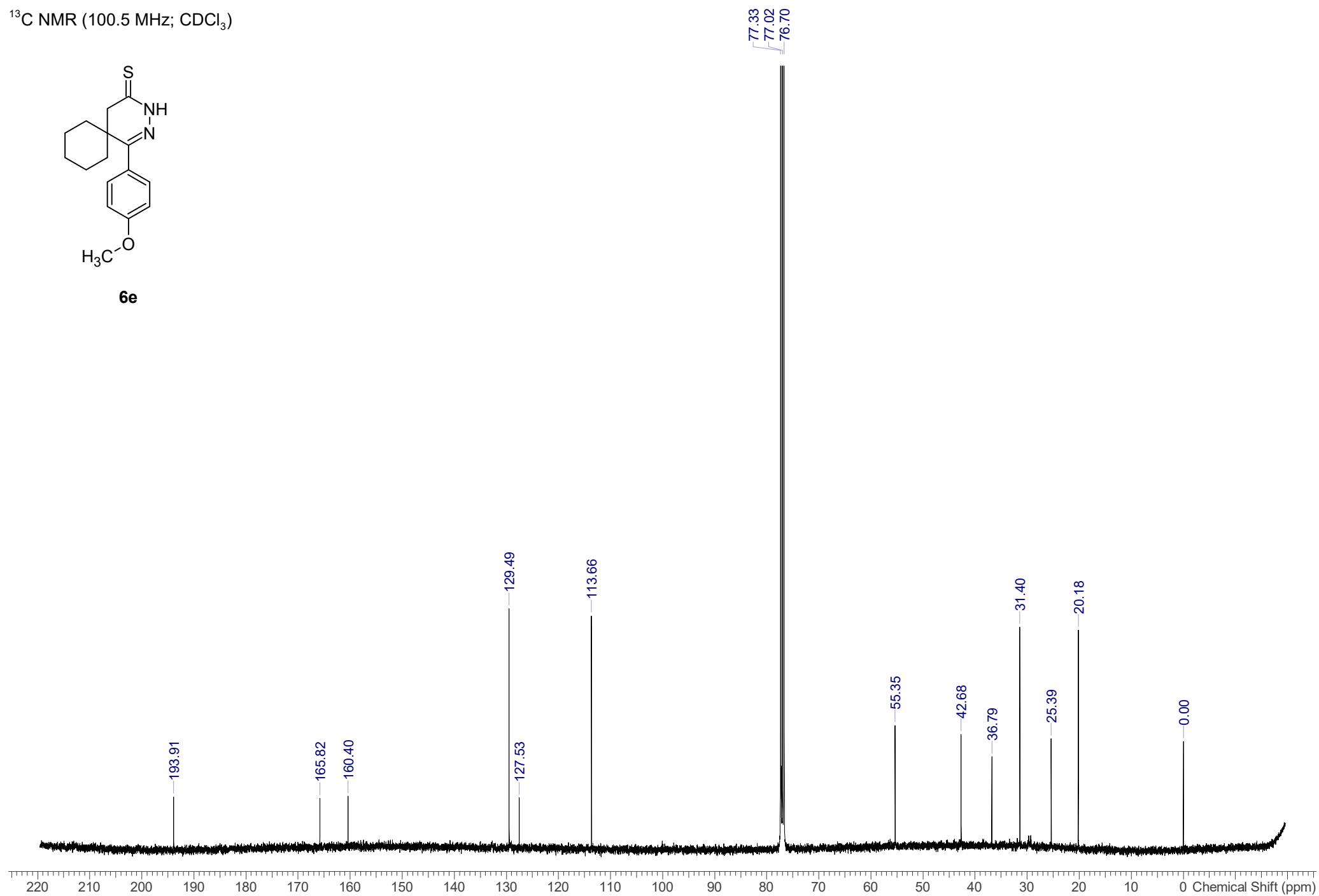
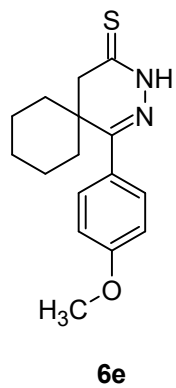
<sup>1</sup>H NMR (399.8 MHz; CDCl<sub>3</sub>)



6e



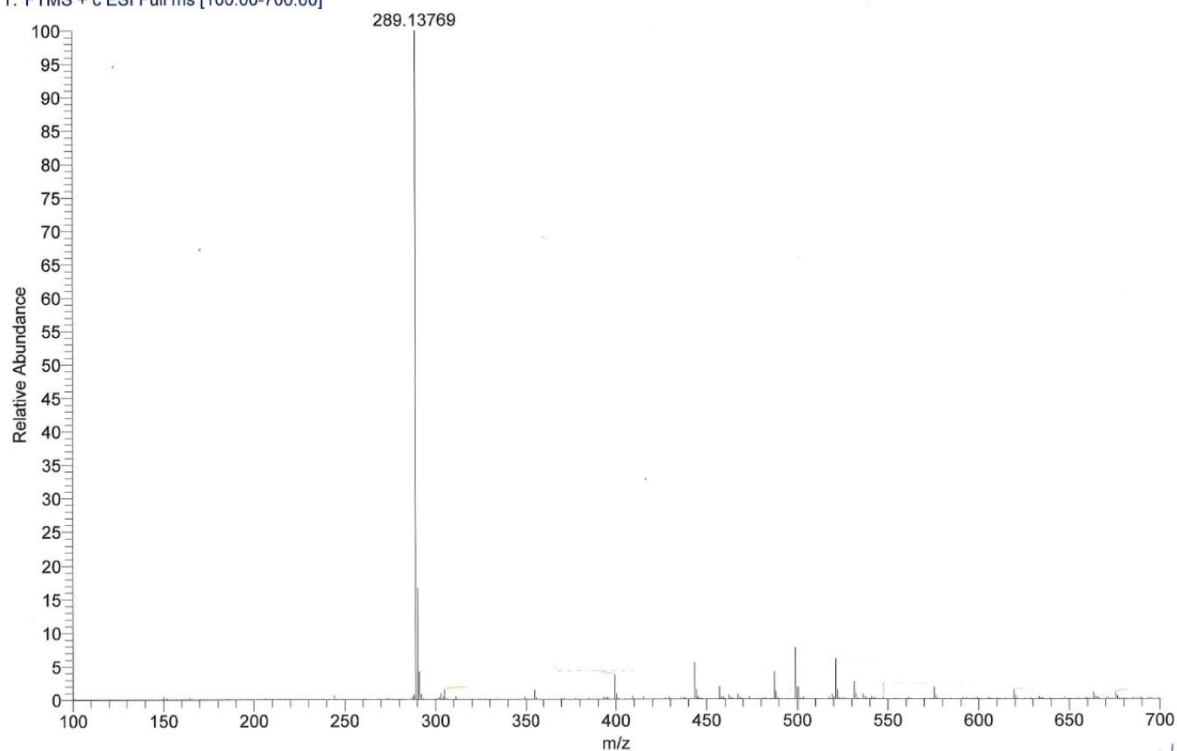
$^{13}\text{C}$  NMR (100.5 MHz;  $\text{CDCl}_3$ )



# Compound 6e

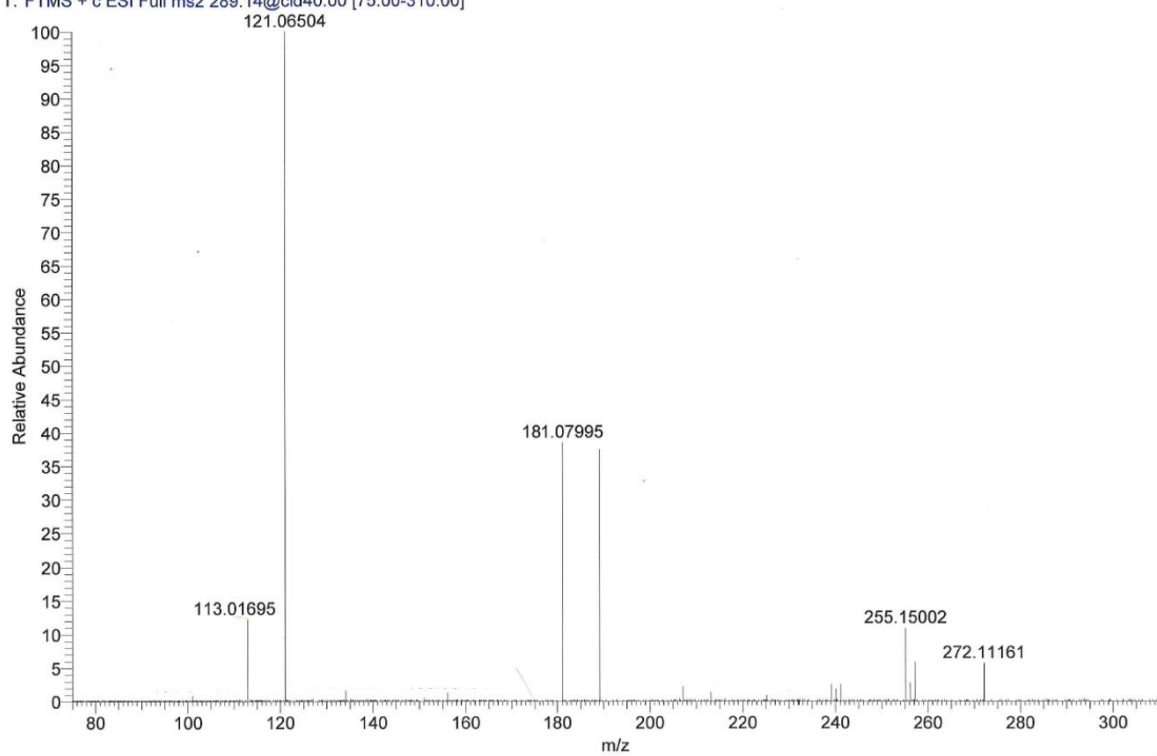
## HRMS spectrum (ESI)

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T: FTMS + c ESI Full ms [100.00-700.00]

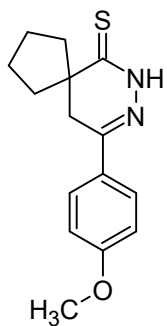


## HRMS spectrum (ESI daughter ion)

ku66333\_rg68\_ve106 #1-16 RT: 0.00-0.19 AV: 16 NL: 1.10E3  
T: FTMS + c ESI Full ms2 289.14@cid40.00 [75.00-310.00]

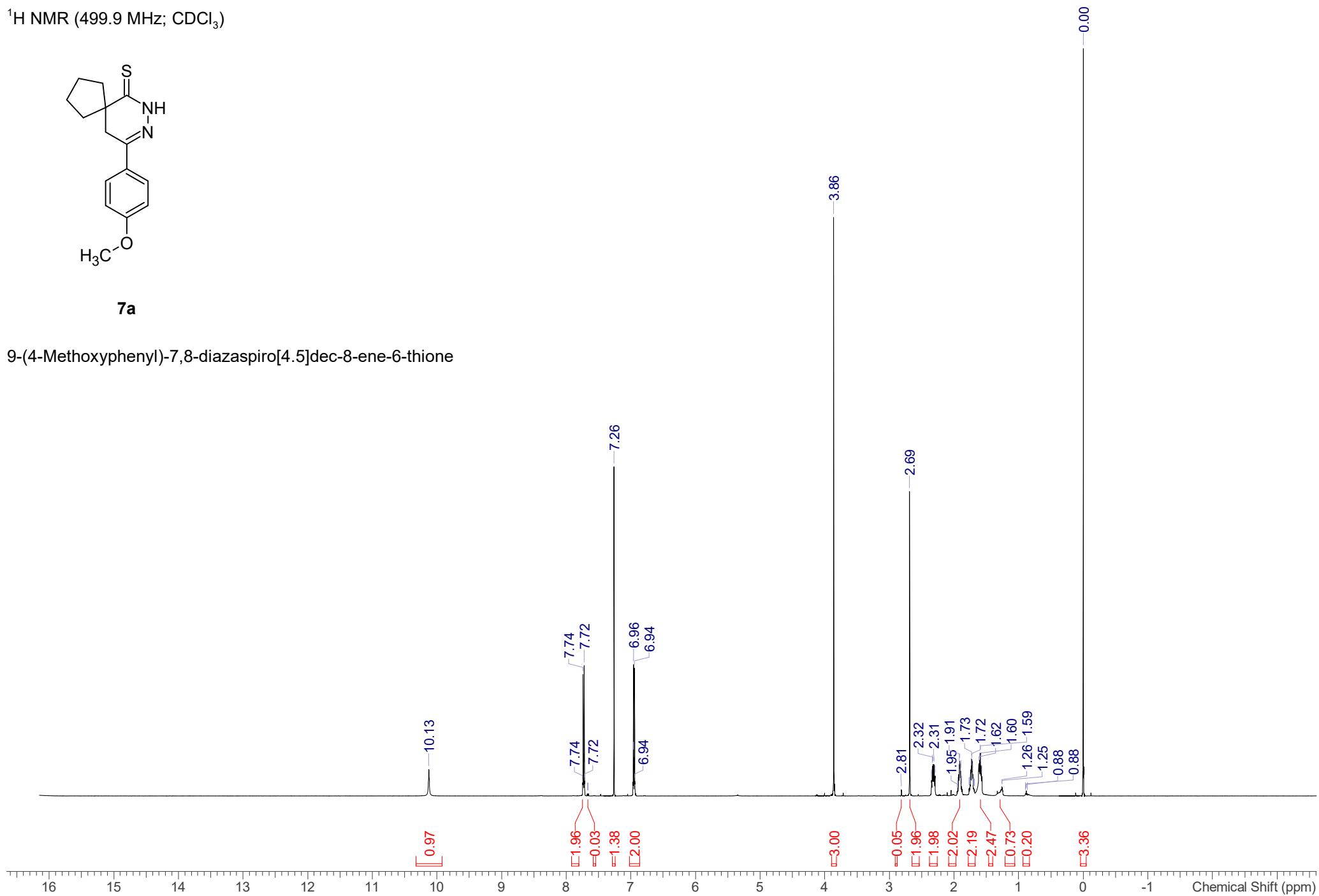


<sup>1</sup>H NMR (499.9 MHz; CDCl<sub>3</sub>)

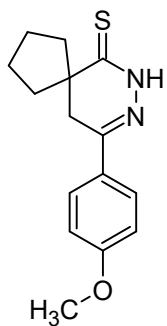


**7a**

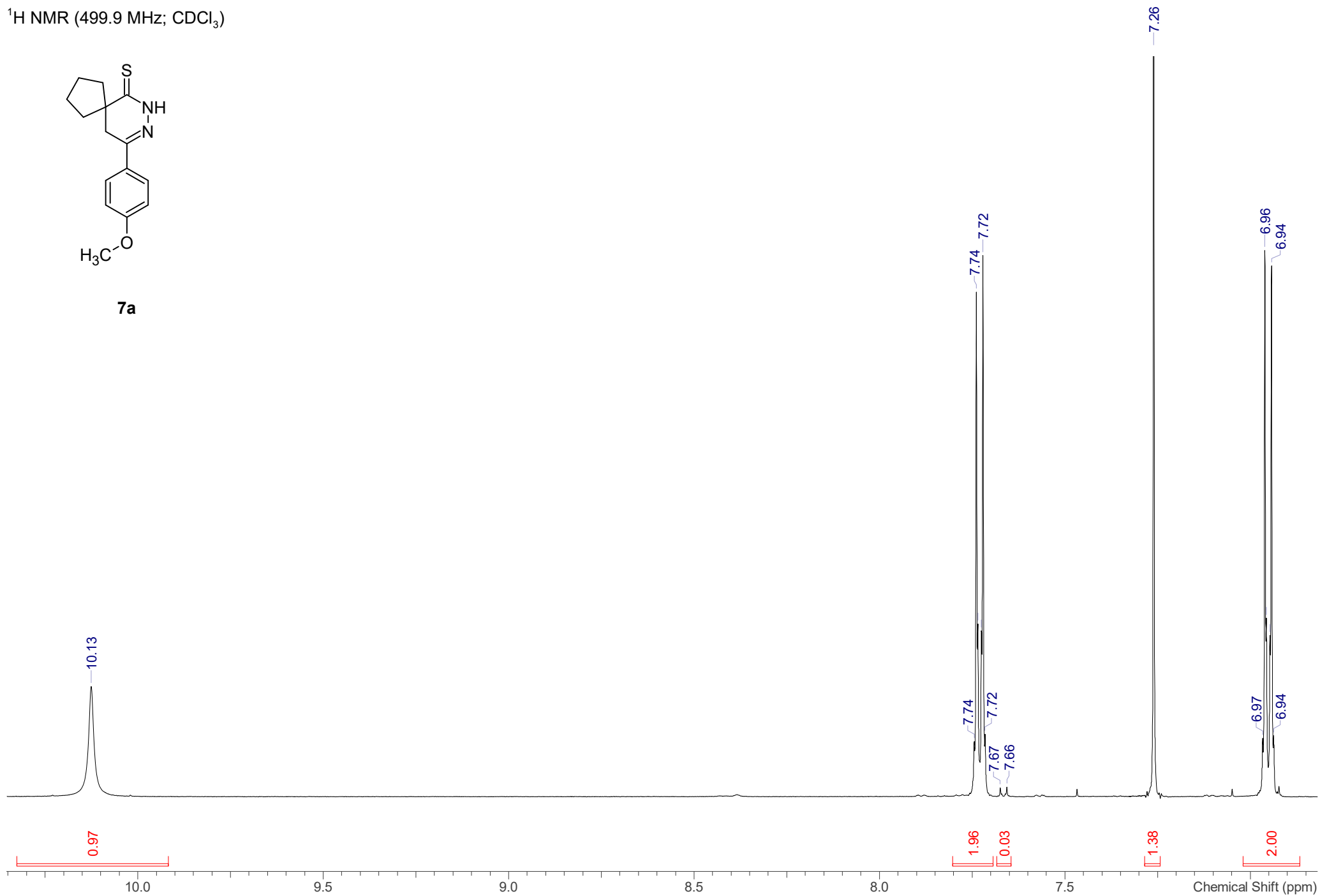
9-(4-Methoxyphenyl)-7,8-diazaspiro[4.5]dec-8-ene-6-thione



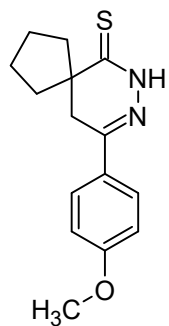
<sup>1</sup>H NMR (499.9 MHz; CDCl<sub>3</sub>)



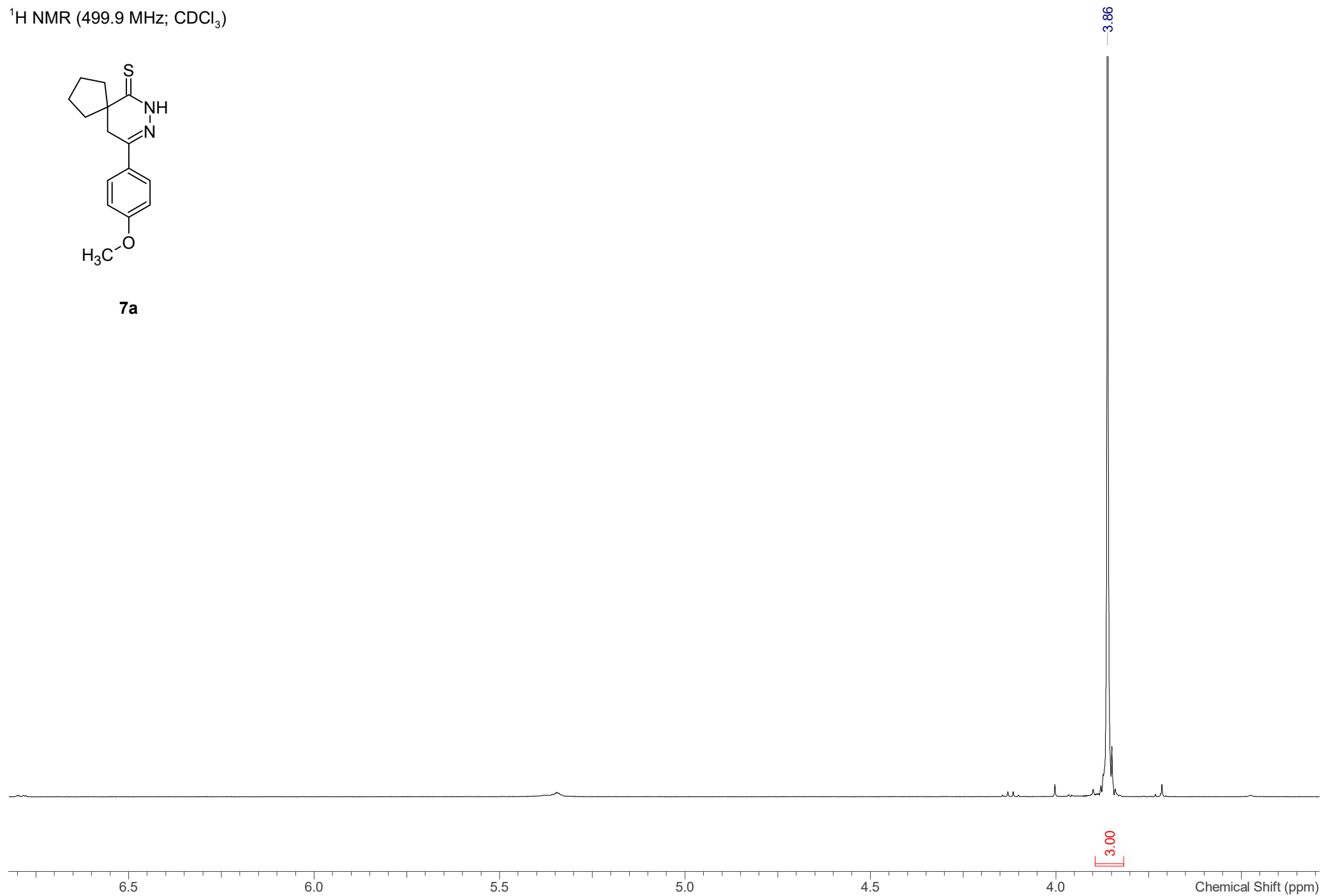
**7a**



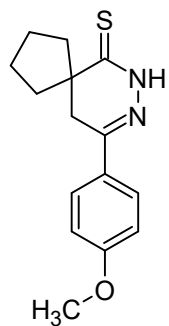
<sup>1</sup>H NMR (499.9 MHz; CDCl<sub>3</sub>)



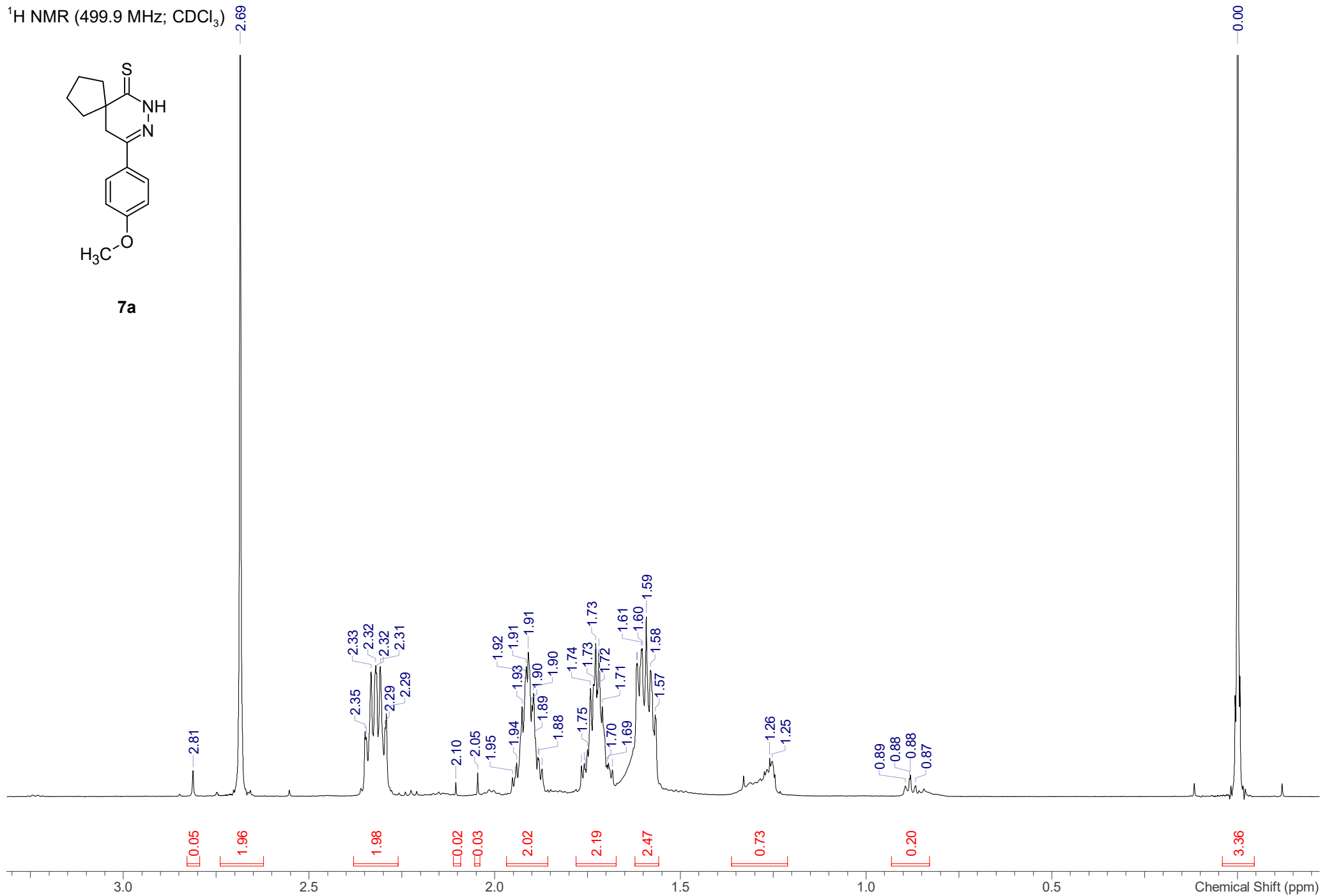
**7a**



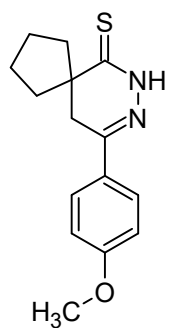
<sup>1</sup>H NMR (499.9 MHz; CDCl<sub>3</sub>)



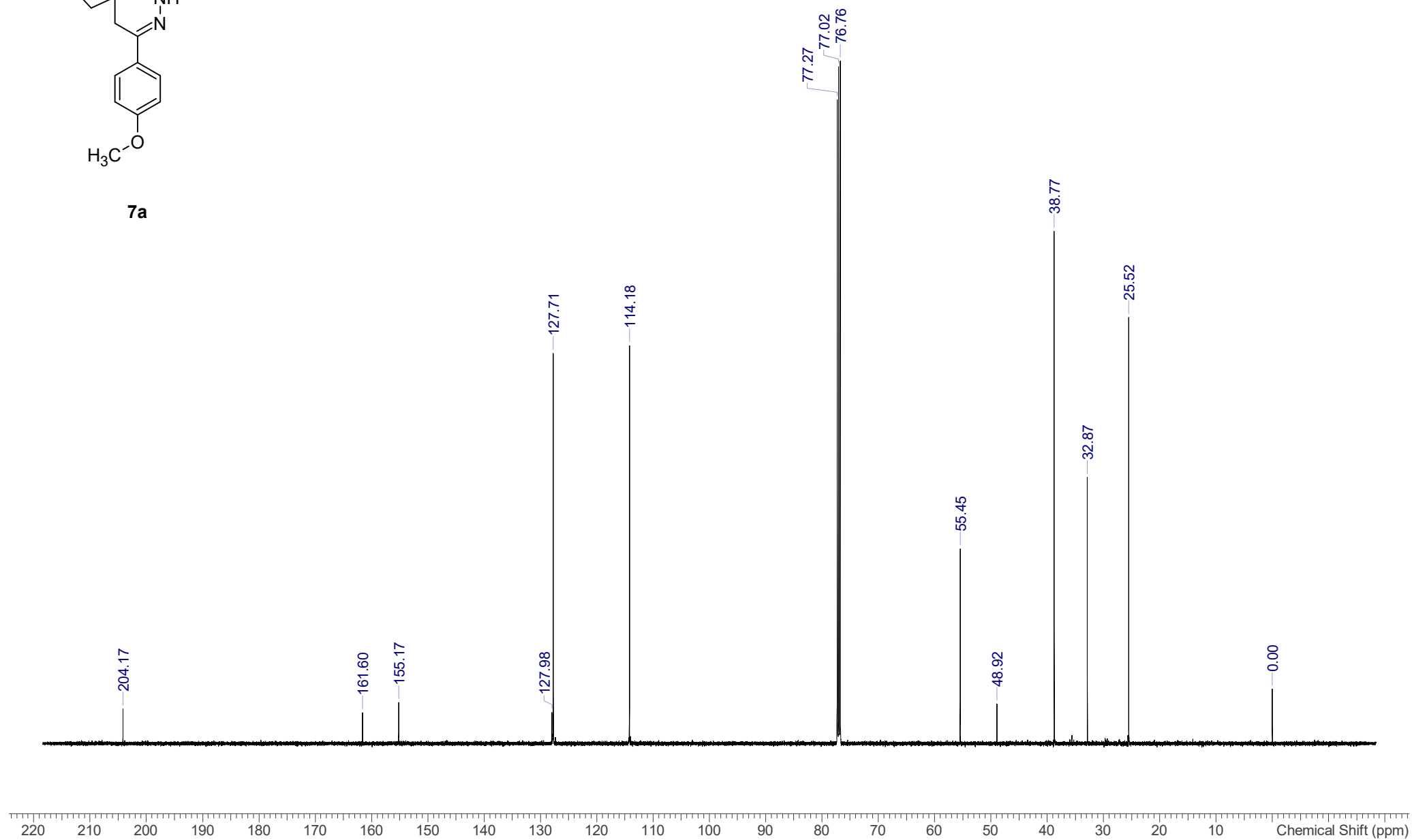
**7a**



$^{13}\text{C}$  NMR (125.7 MHz;  $\text{CDCl}_3$ )



**7a**

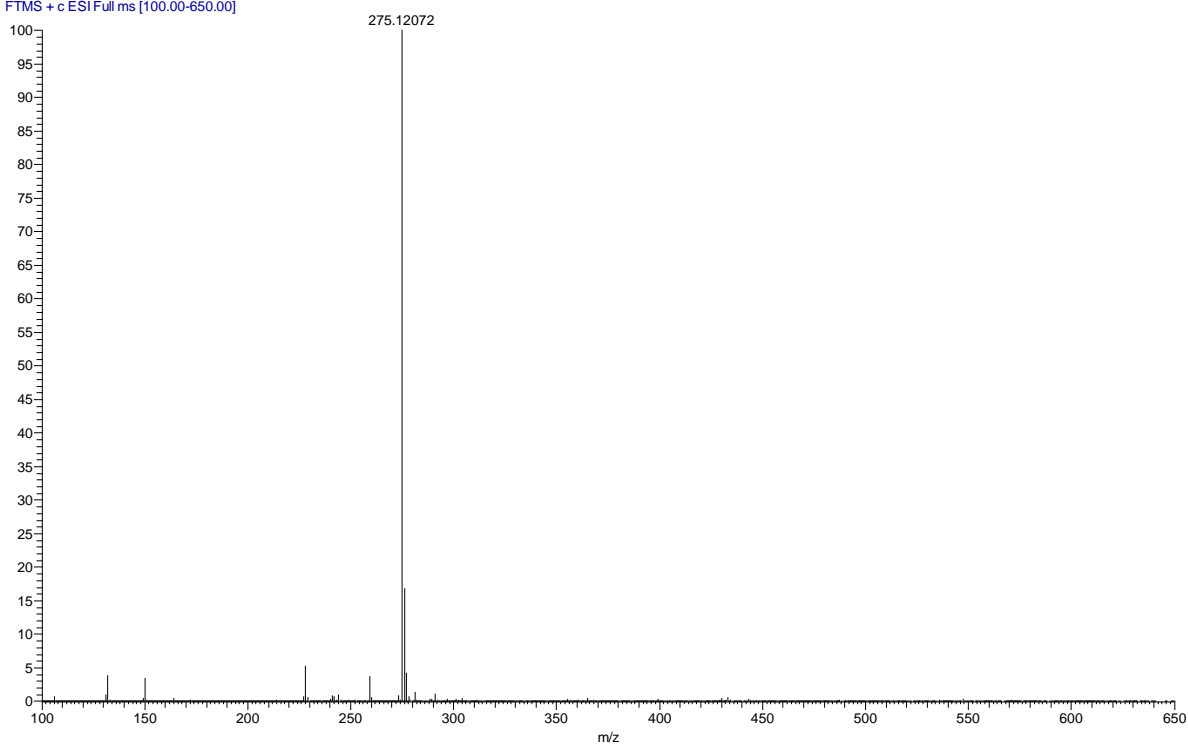




# Compound 7a

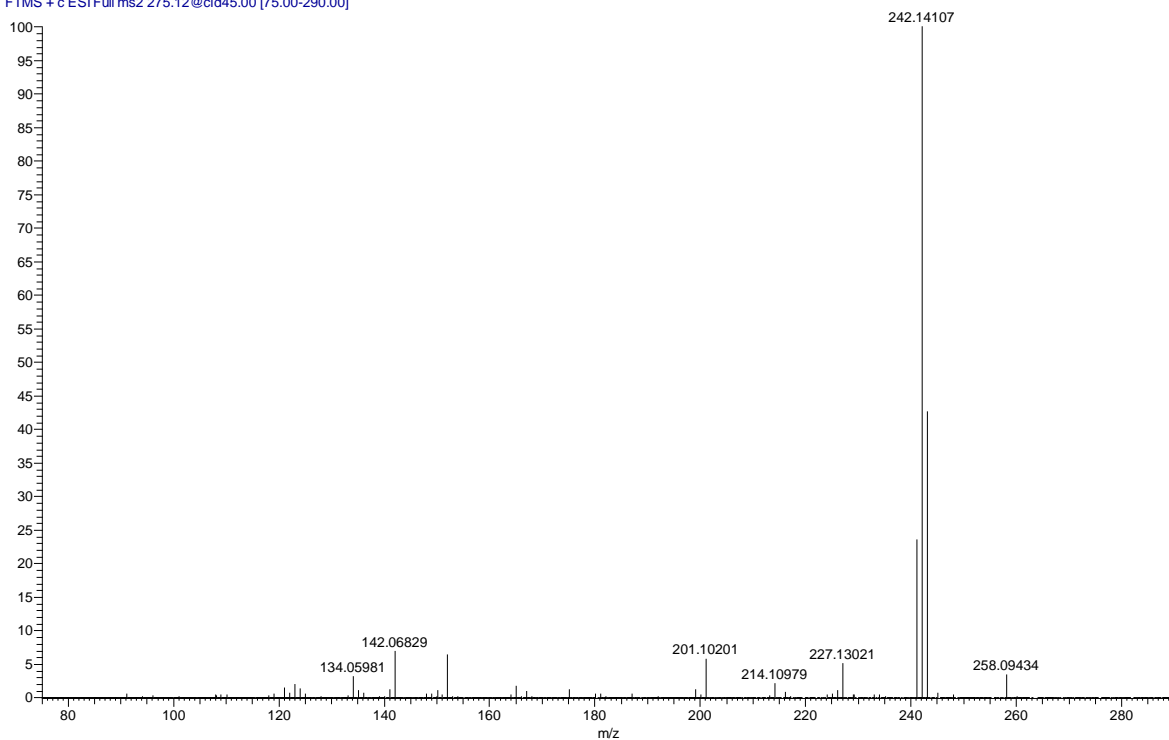
## HRMS spectrum (ESI)

ku66566\_rg-69\_d\_ve324 #1-45 RT: 0.00-0.20 AV: 45 NL: 2.66E7  
T: FTMS + c ESI Full ms [100.00-650.00]

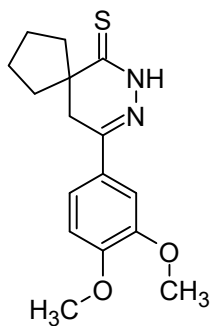


## HRMS spectrum (ESI daughter ion)

ku66566\_rg-69\_d\_ve325 #1-45 RT: 0.00-0.20 AV: 45 NL: 2.95E6  
T: FTMS + c ESI Full ms2 275.12@cid45.00 [75.00-290.00]

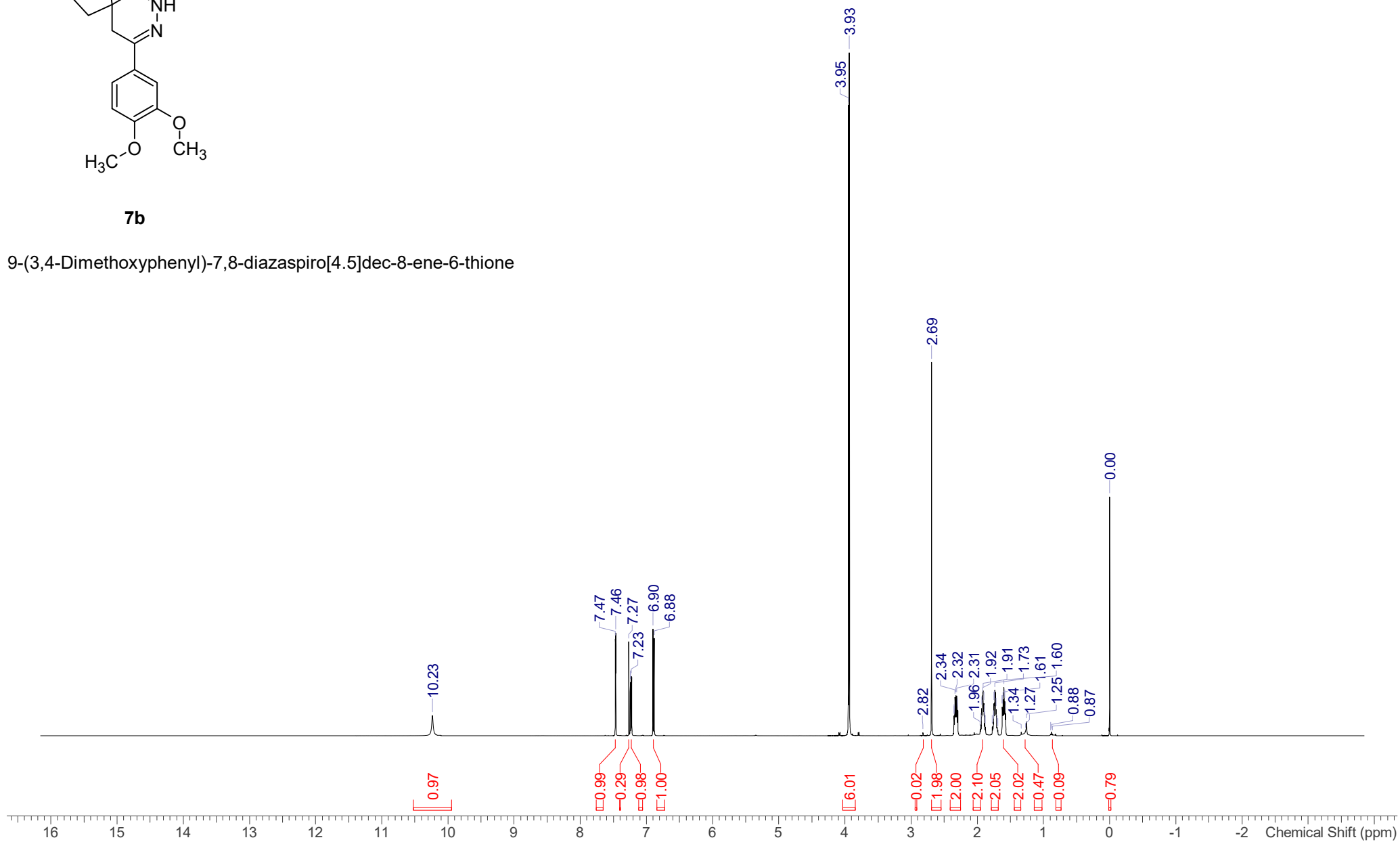


<sup>1</sup>H NMR (499.9 MHz; CDCl<sub>3</sub>)

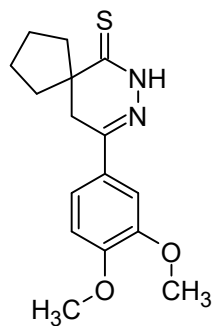


**7b**

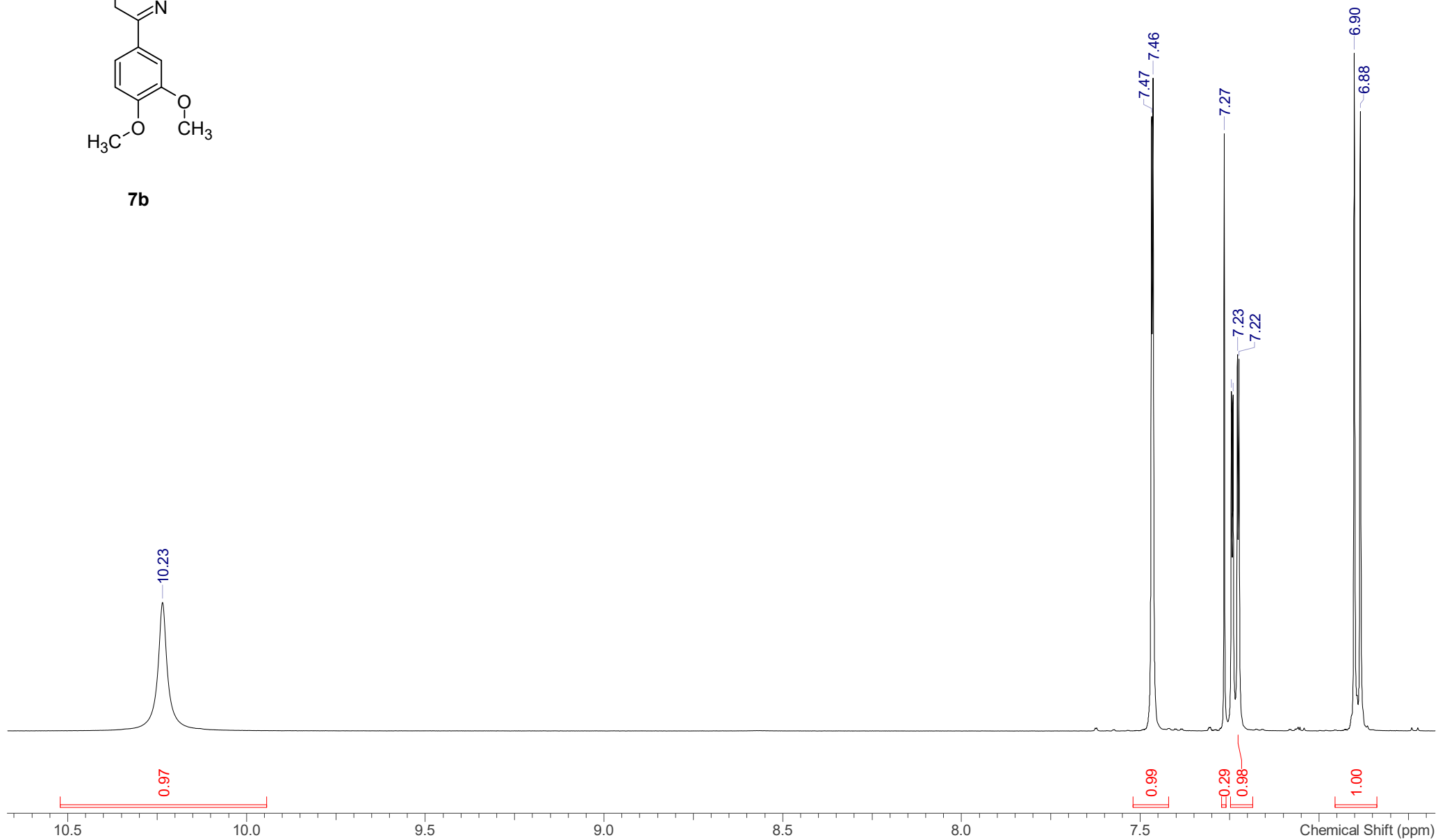
9-(3,4-Dimethoxyphenyl)-7,8-diazaspiro[4.5]dec-8-ene-6-thione



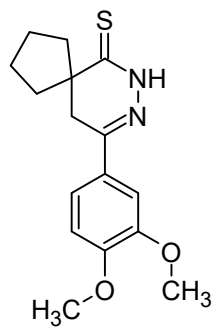
<sup>1</sup>H NMR (499.9 MHz; CDCl<sub>3</sub>)



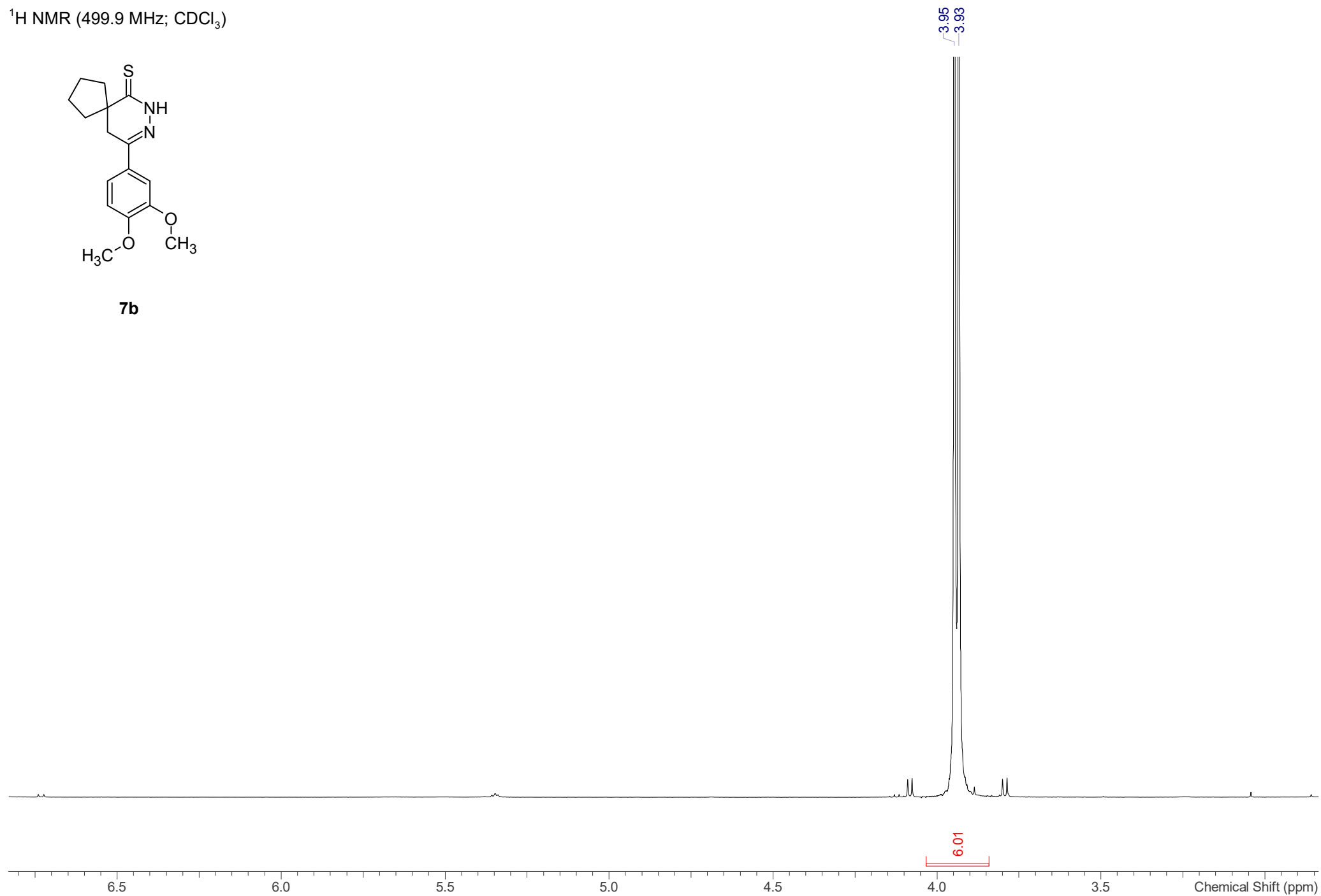
**7b**



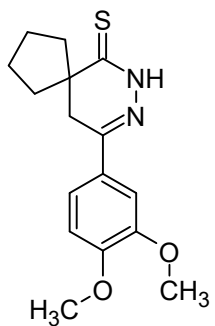
$^1\text{H}$  NMR (499.9 MHz;  $\text{CDCl}_3$ )



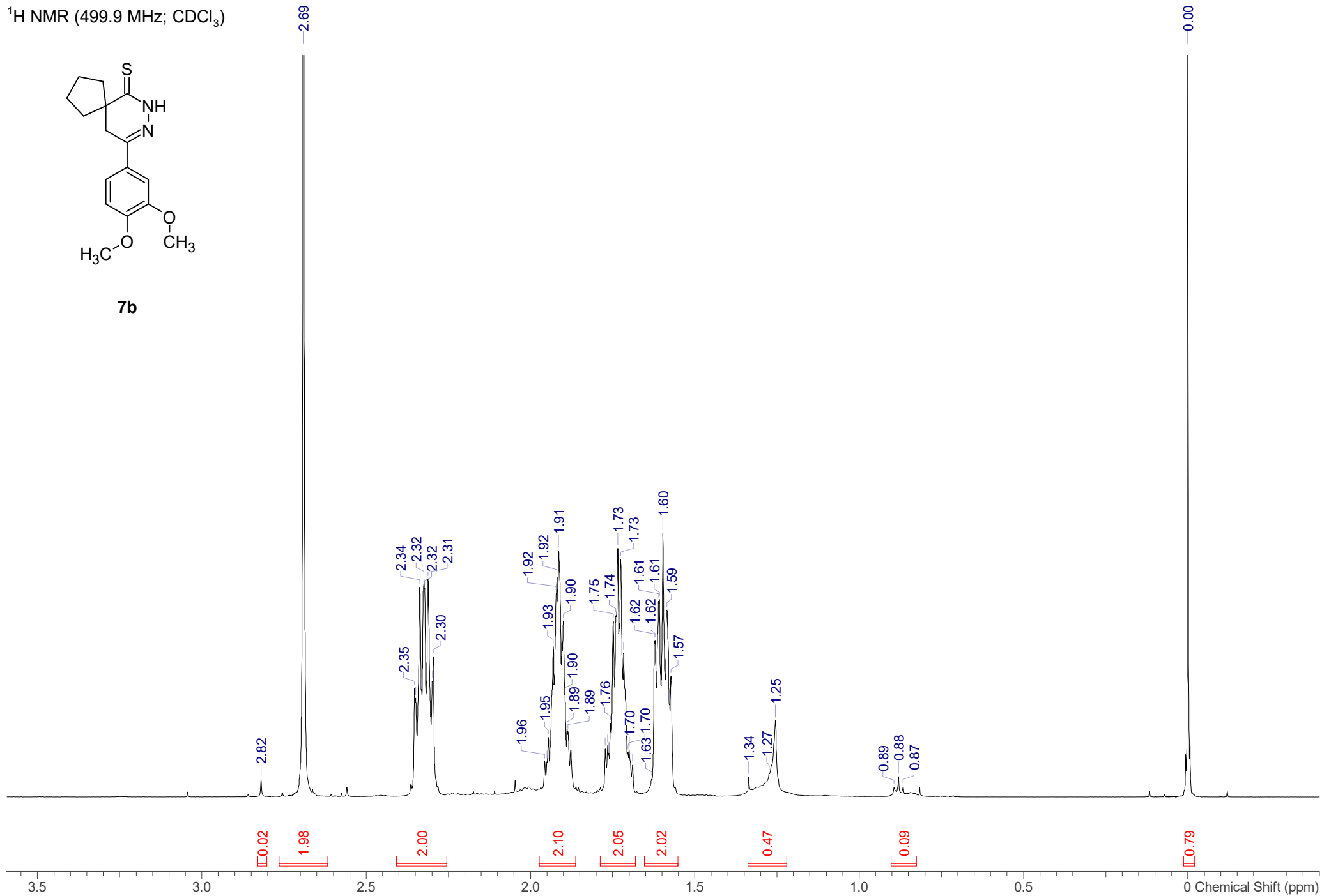
**7b**



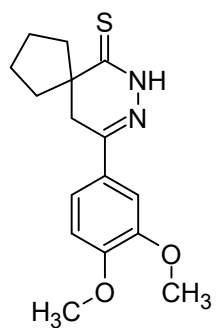
<sup>1</sup>H NMR (499.9 MHz; CDCl<sub>3</sub>)



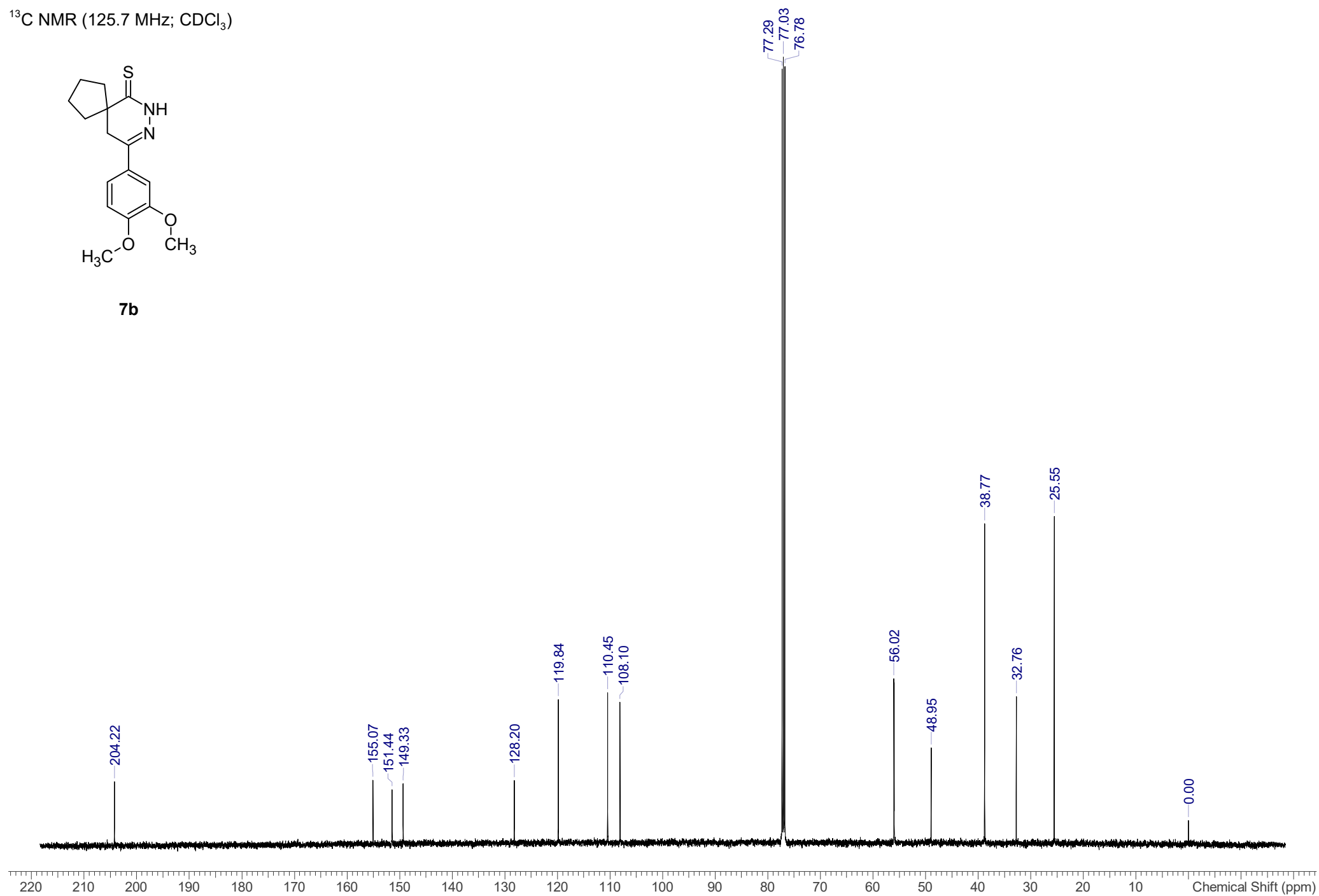
**7b**



$^{13}\text{C}$  NMR (125.7 MHz;  $\text{CDCl}_3$ )



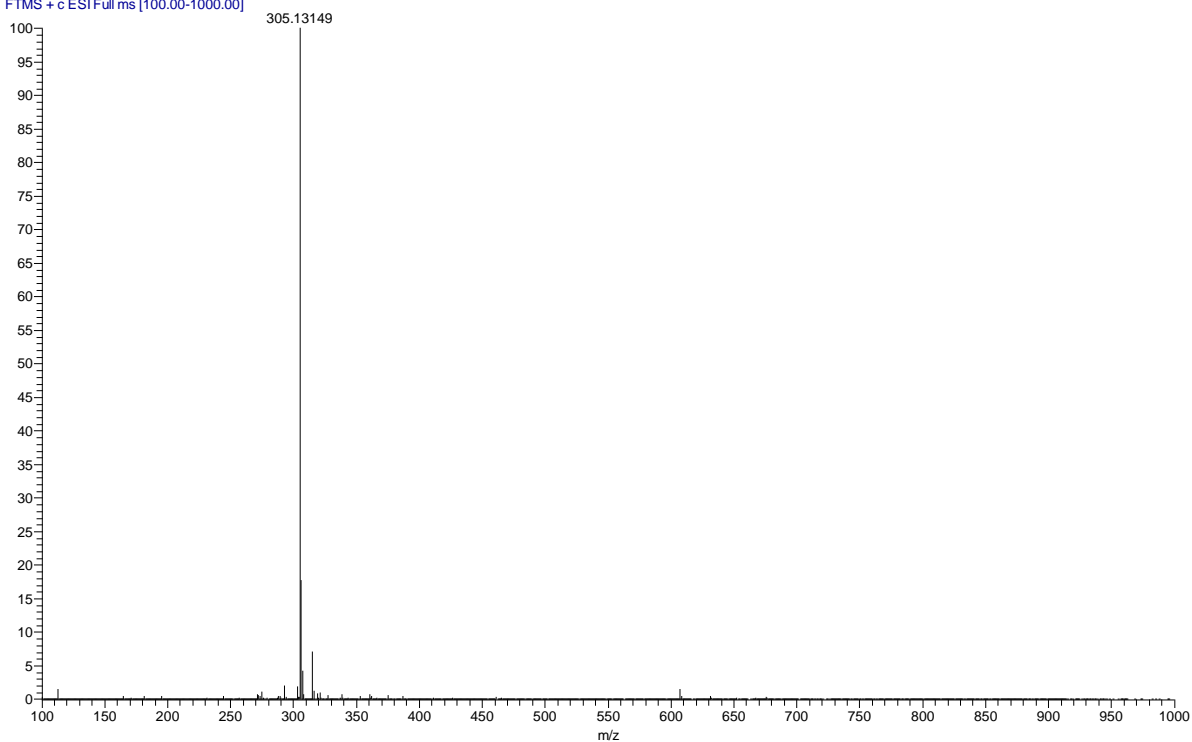
**7b**



# Compound 7b

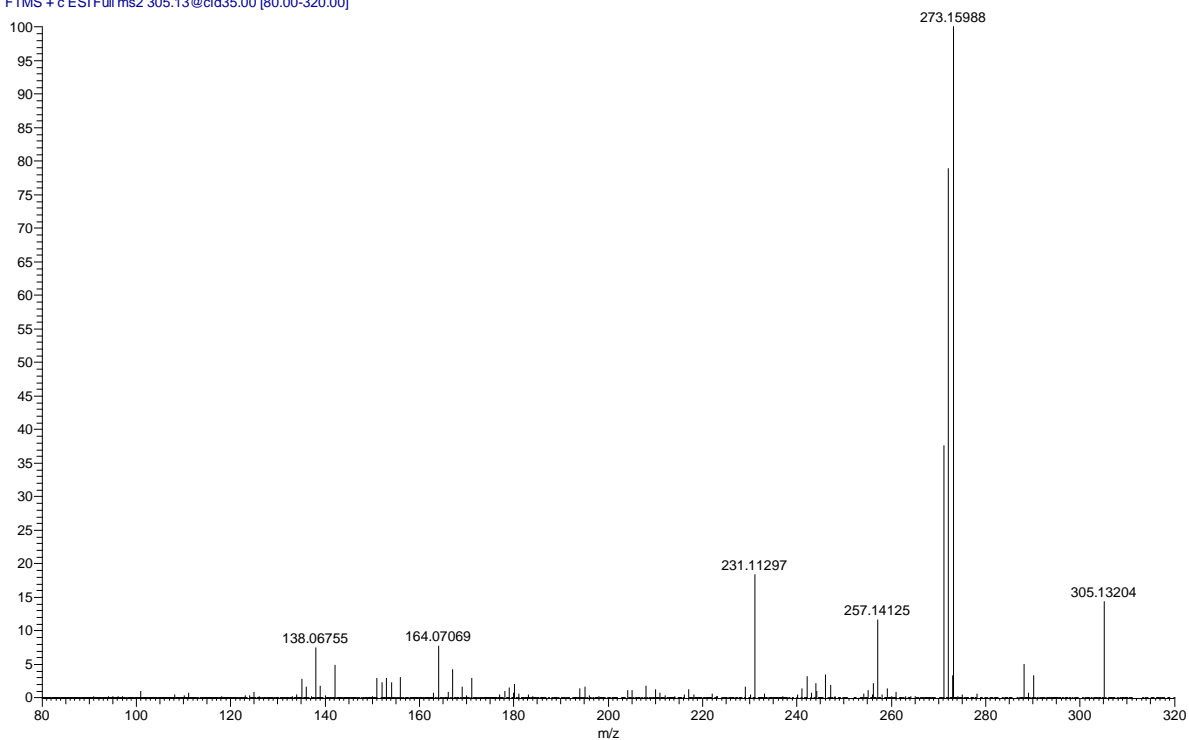
## HRMS spectrum (ESI)

ku66519\_rq-73\_d\_ve275 #1-28 RT: 0.00-0.19 AV: 28 NL: 4.95E6  
T: FTMS + c ESI Full ms [100.00-1000.00]

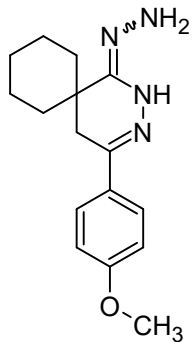


## HRMS spectrum (ESI daughter ion)

ku66519\_rq-73\_d\_ve276 #1-23 RT: 0.00-0.20 AV: 23 NL: 4.73E4  
T: FTMS + c ESI Full ms2 305.13@cid35.00 [80.00-320.00]

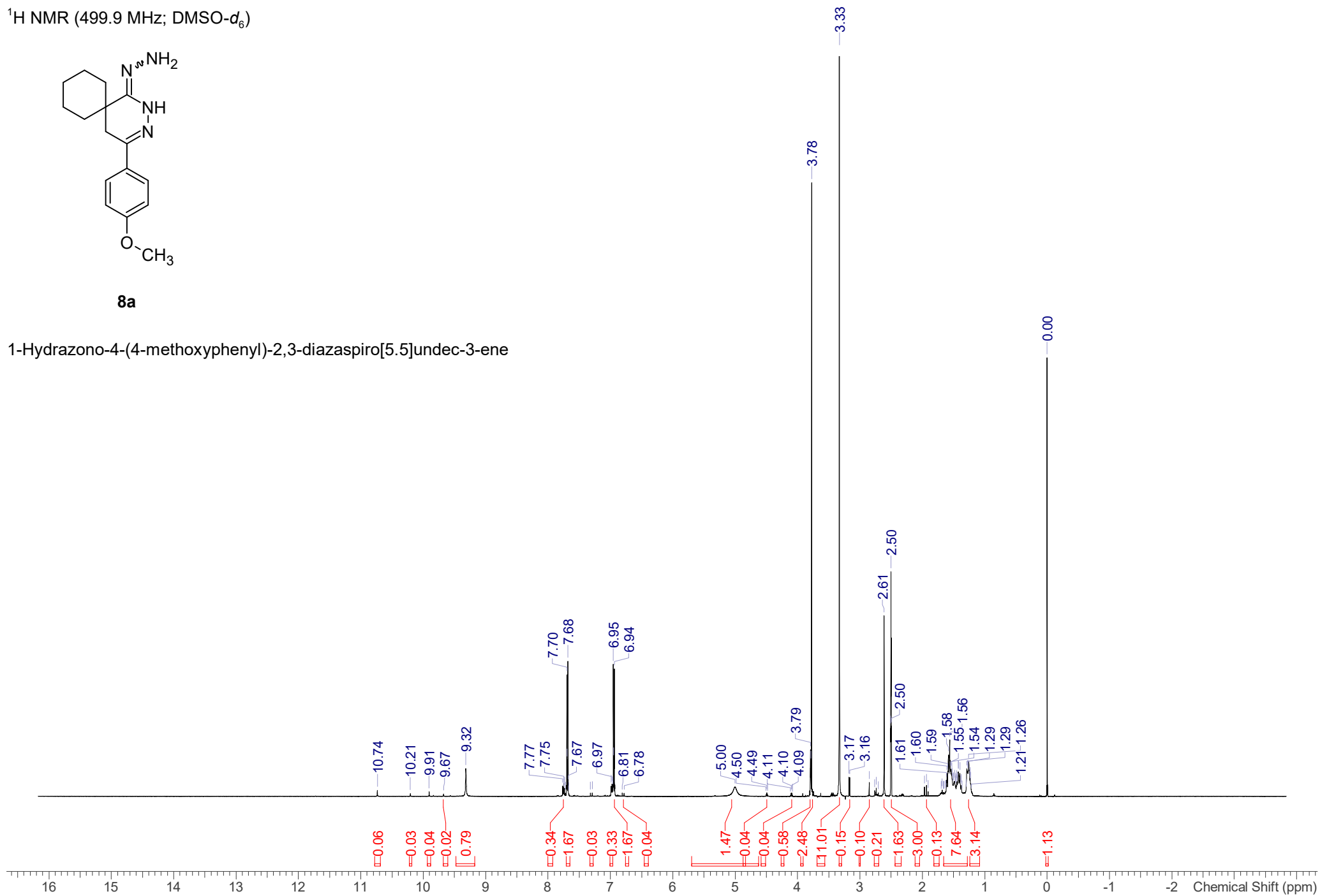


<sup>1</sup>H NMR (499.9 MHz; DMSO-d<sub>6</sub>)



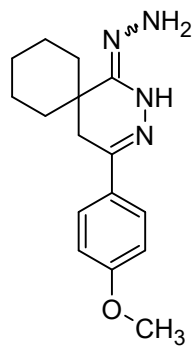
**8a**

1-Hydrazono-4-(4-methoxyphenyl)-2,3-diazaspiro[5.5]undec-3-ene

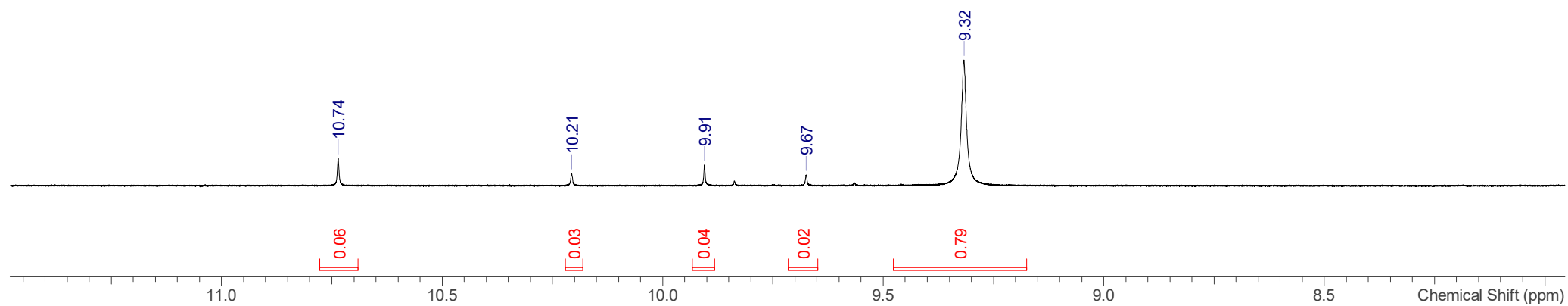




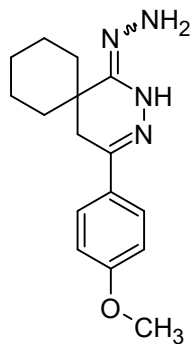
$^1\text{H}$  NMR (499.9 MHz;  $\text{DMSO-}d_6$ )



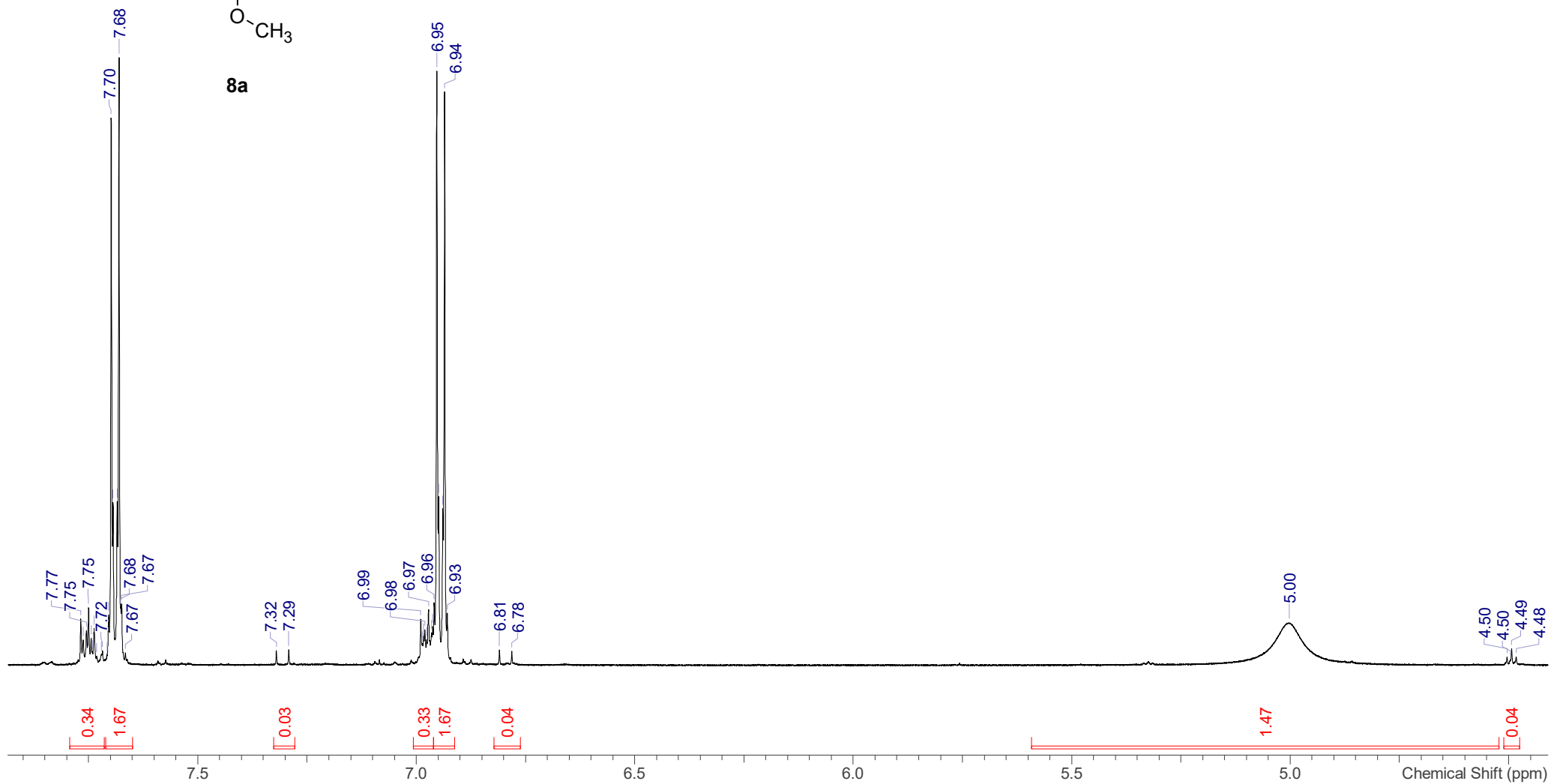
**8a**



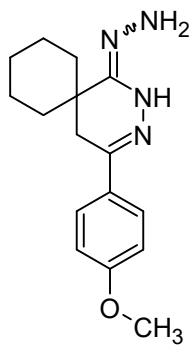
<sup>1</sup>H NMR (499.9 MHz; DMSO-d<sub>6</sub>)



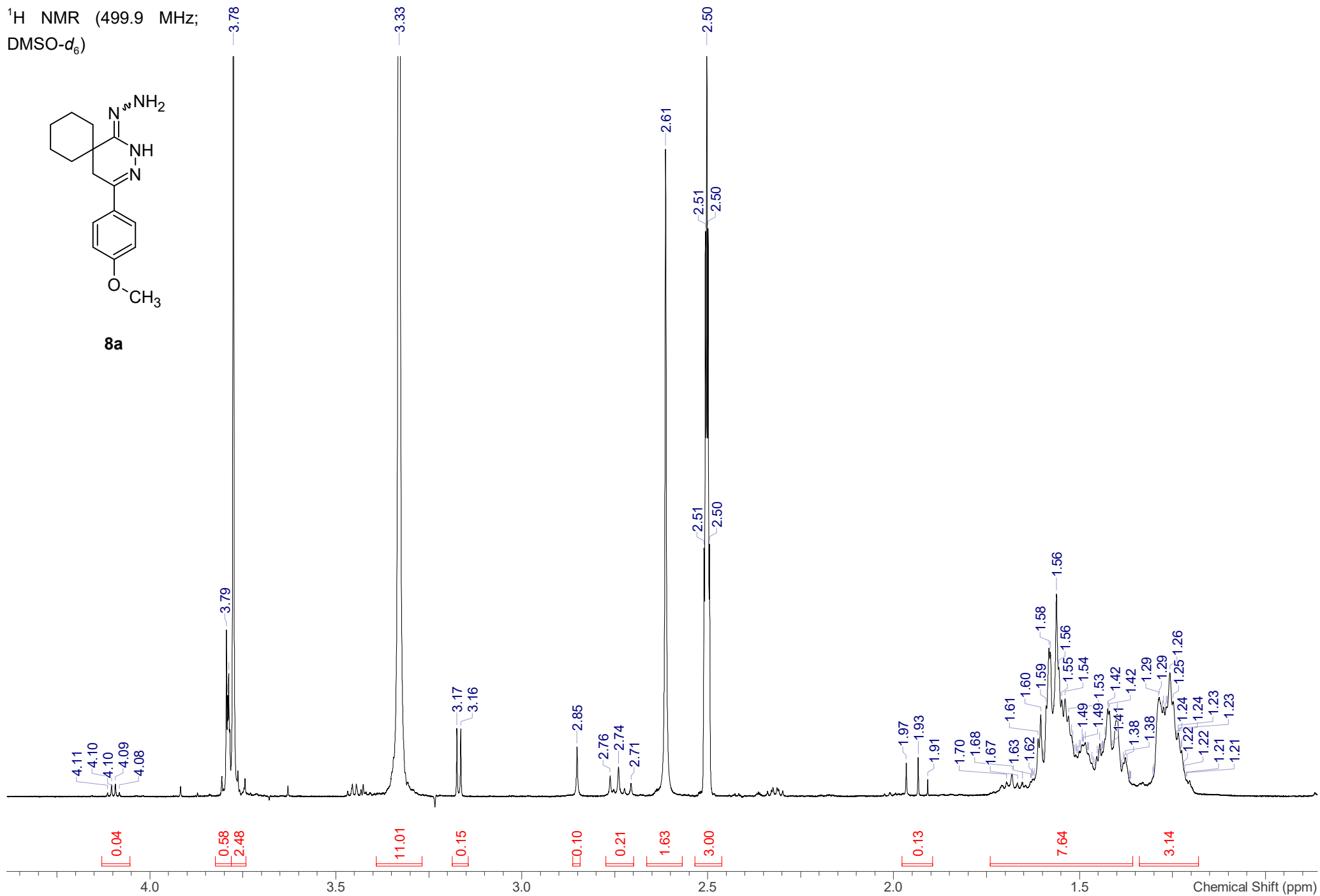
8a



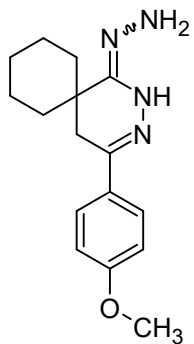
<sup>1</sup>H NMR (499.9 MHz;  
DMSO-d<sub>6</sub>)



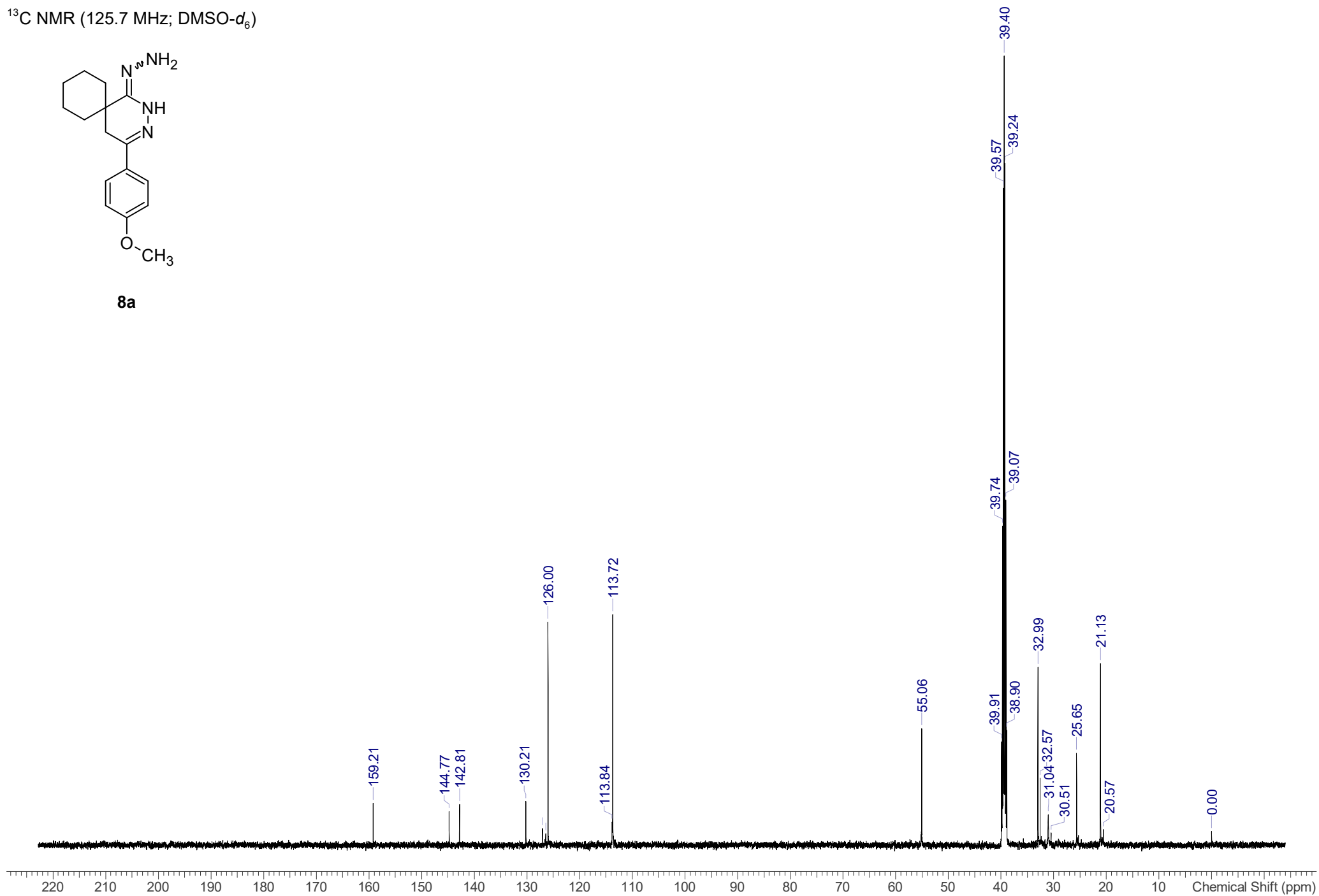
8a



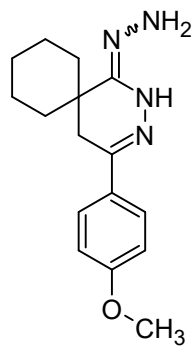
$^{13}\text{C}$  NMR (125.7 MHz;  $\text{DMSO-}d_6$ )



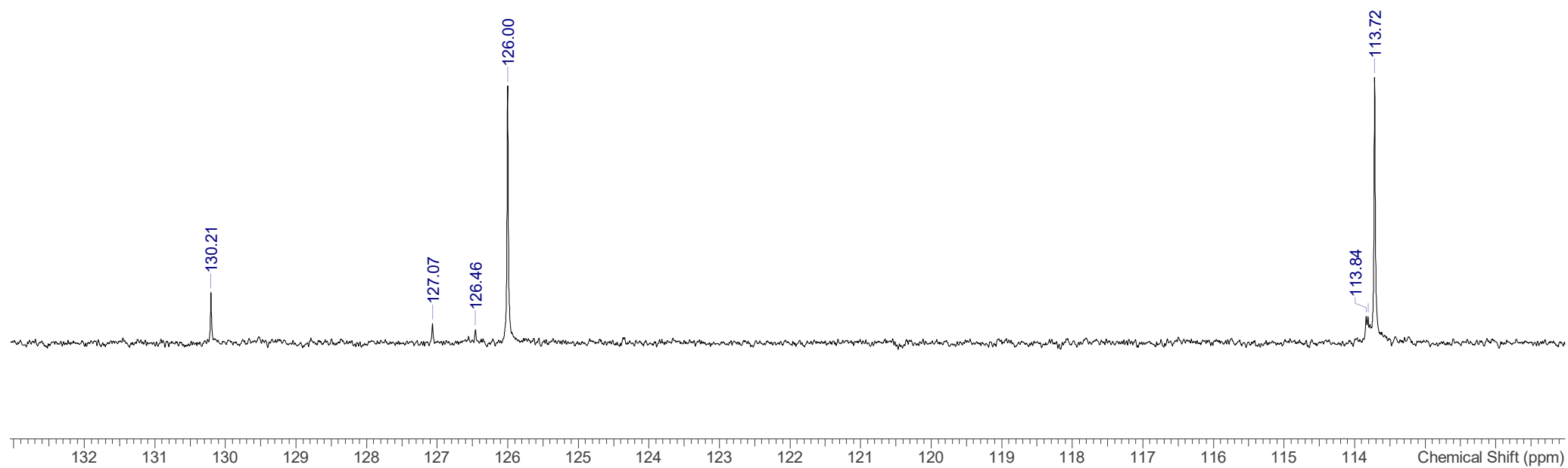
8a



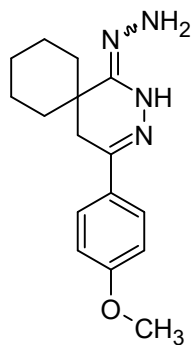
$^{13}\text{C}$  NMR (125.7 MHz;  $\text{DMSO-}d_6$ )



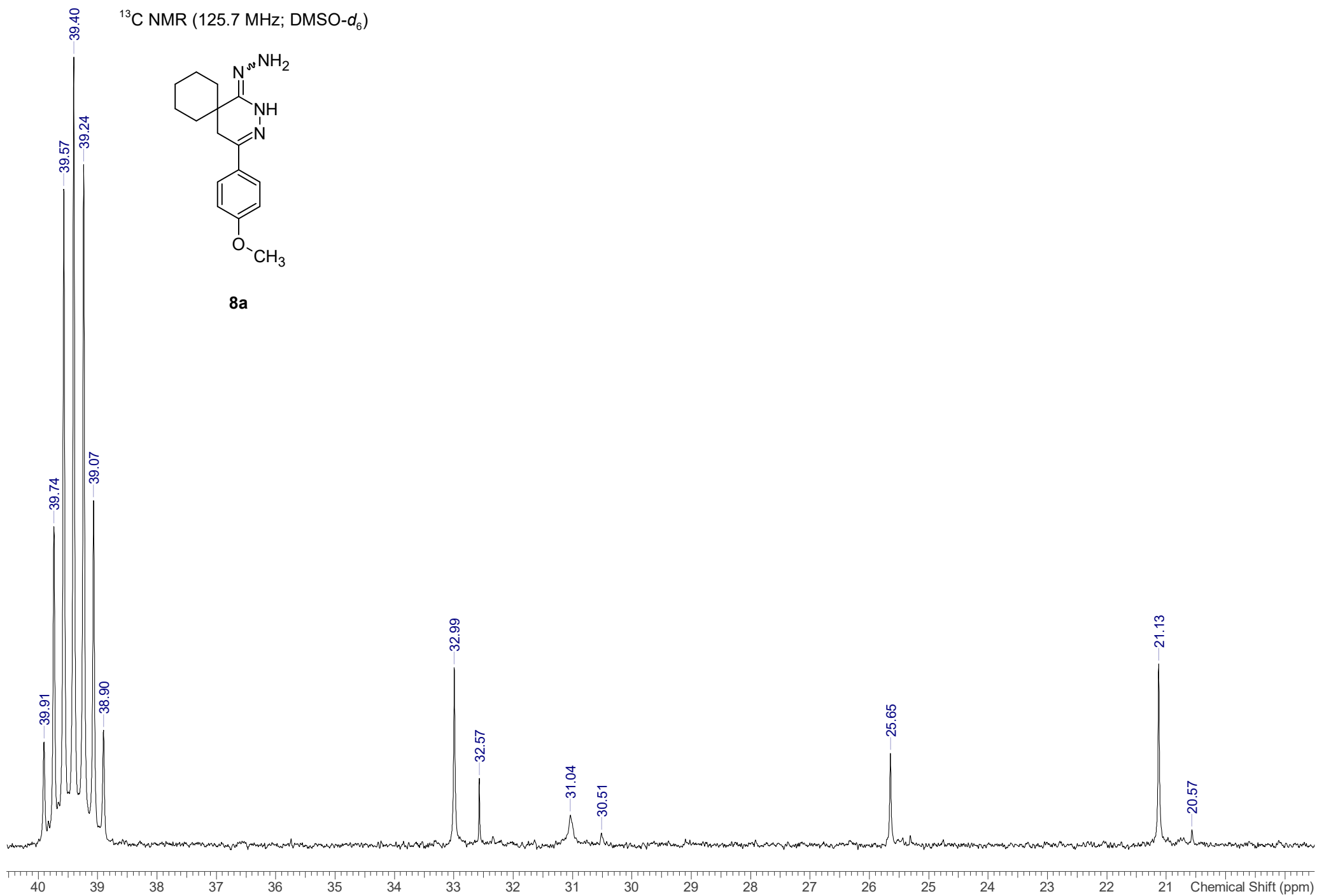
**8a**



$^{13}\text{C}$  NMR (125.7 MHz;  $\text{DMSO-}d_6$ )



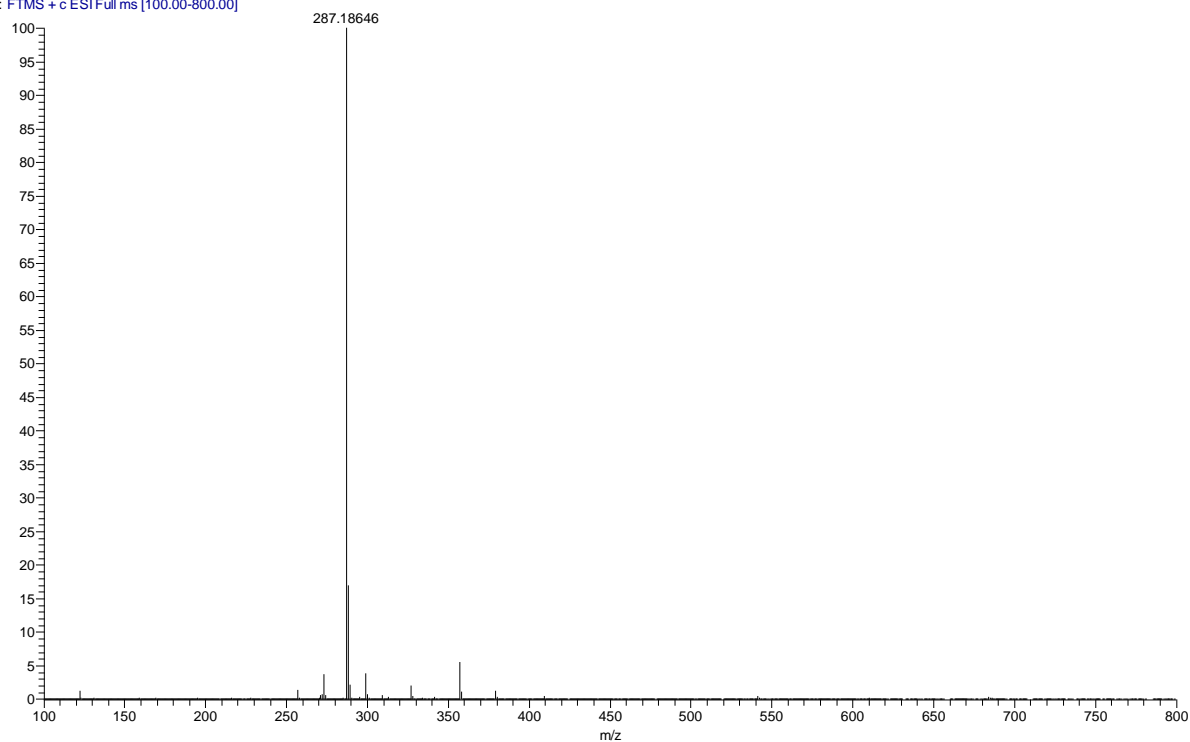
**8a**



# Compound 8a

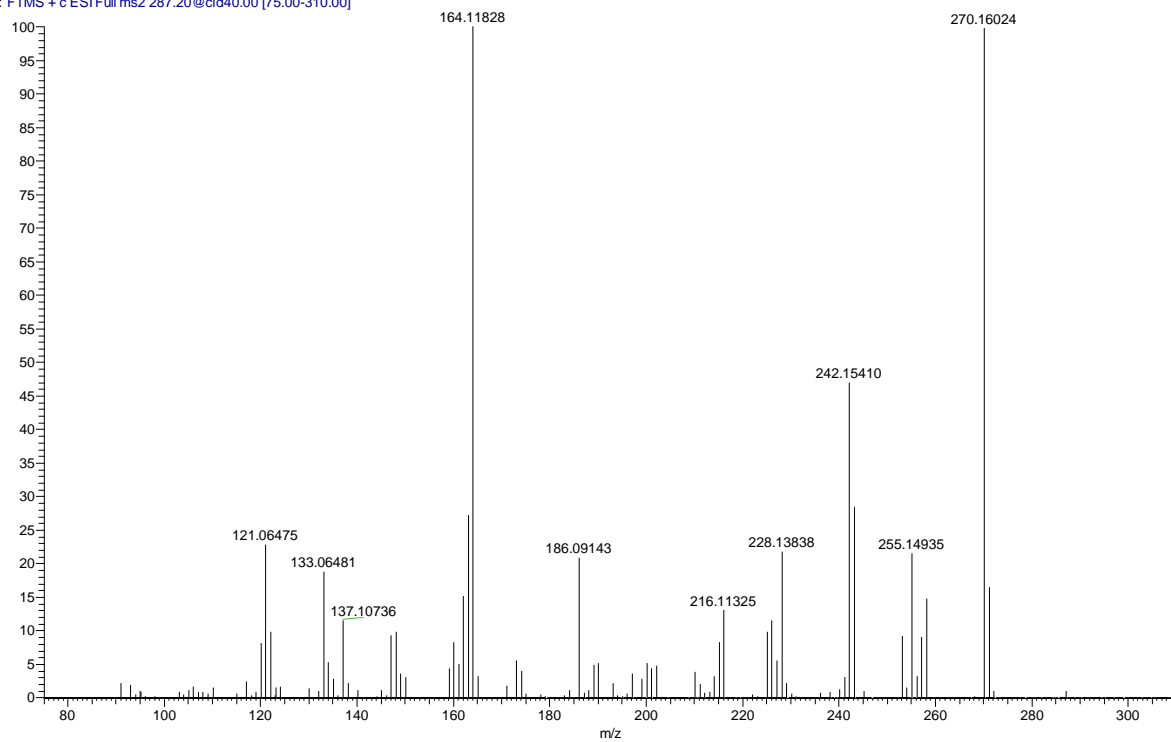
## HRMS spectrum (ESI)

ku74011\_sfc-222\_d\_ve6275 #1-49 RT: 0.00-0.20 AV: 49 NL: 4.96E7  
T: FTMS + c ESI Full ms [100.00-800.00]

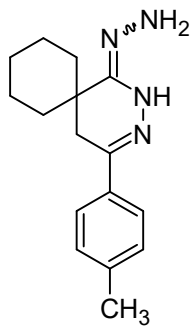


## HRMS spectrum (ESI daughter ion)

ku74011\_sfc-222\_d\_ve6276 #1-47 RT: 0.00-0.20 AV: 47 NL: 4.18E6  
T: FTMS + c ESI Full ms2 287.20@cid40.00 [75.00-310.00]

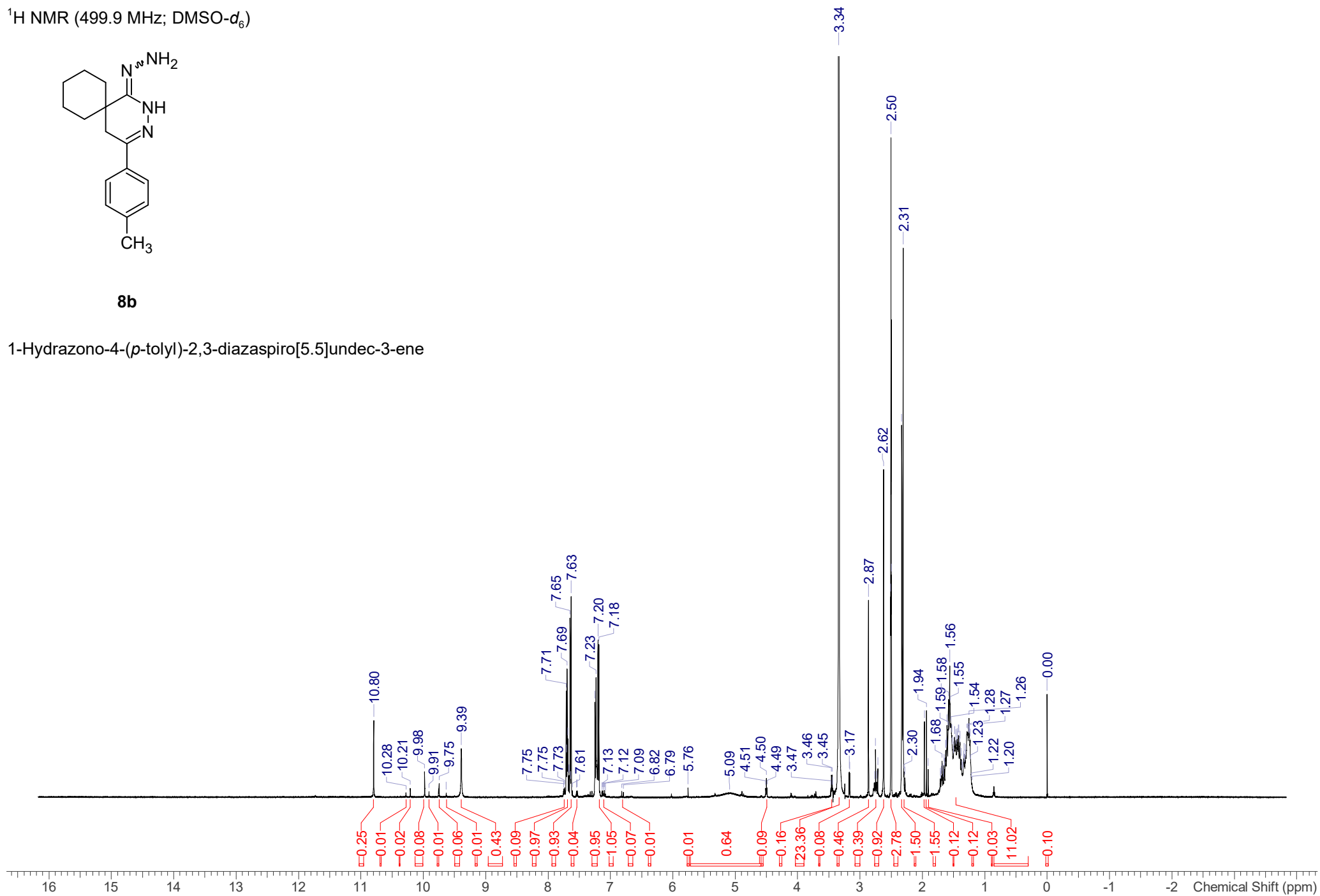


<sup>1</sup>H NMR (499.9 MHz; DMSO-d<sub>6</sub>)



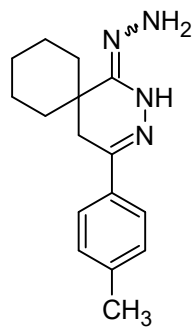
**8b**

1-Hydrazono-4-(*p*-tolyl)-2,3-diazaspiro[5.5]undec-3-ene

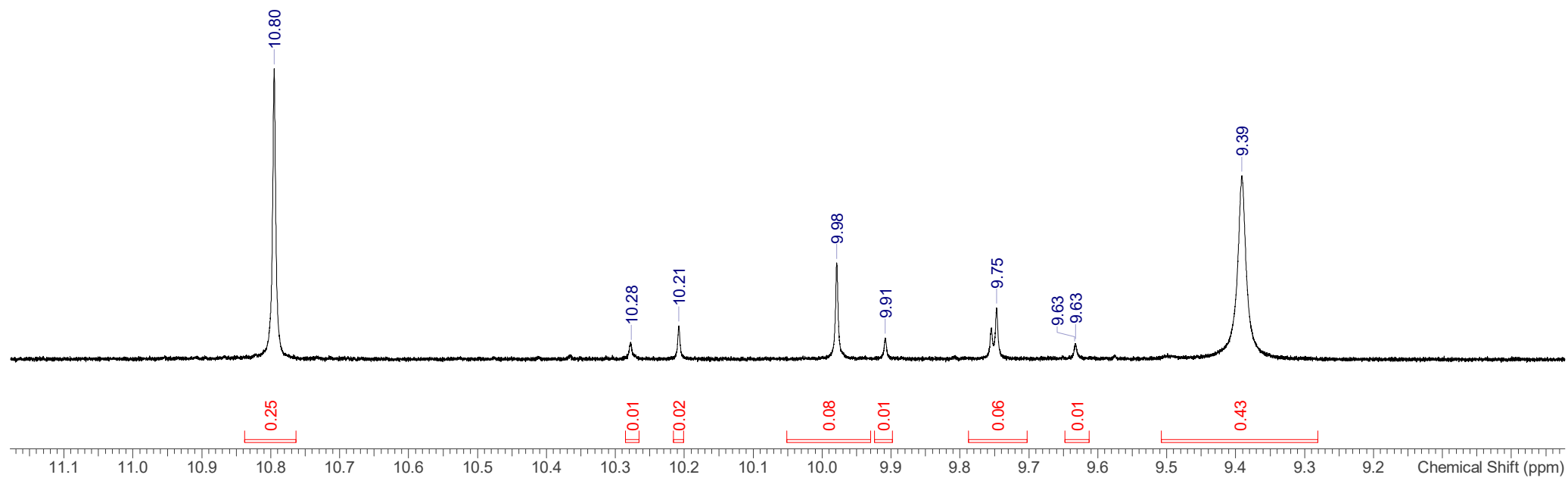




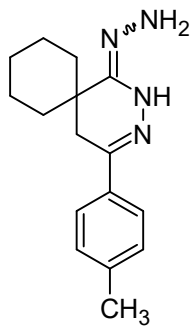
$^1\text{H}$  NMR (499.9 MHz;  $\text{DMSO-}d_6$ )



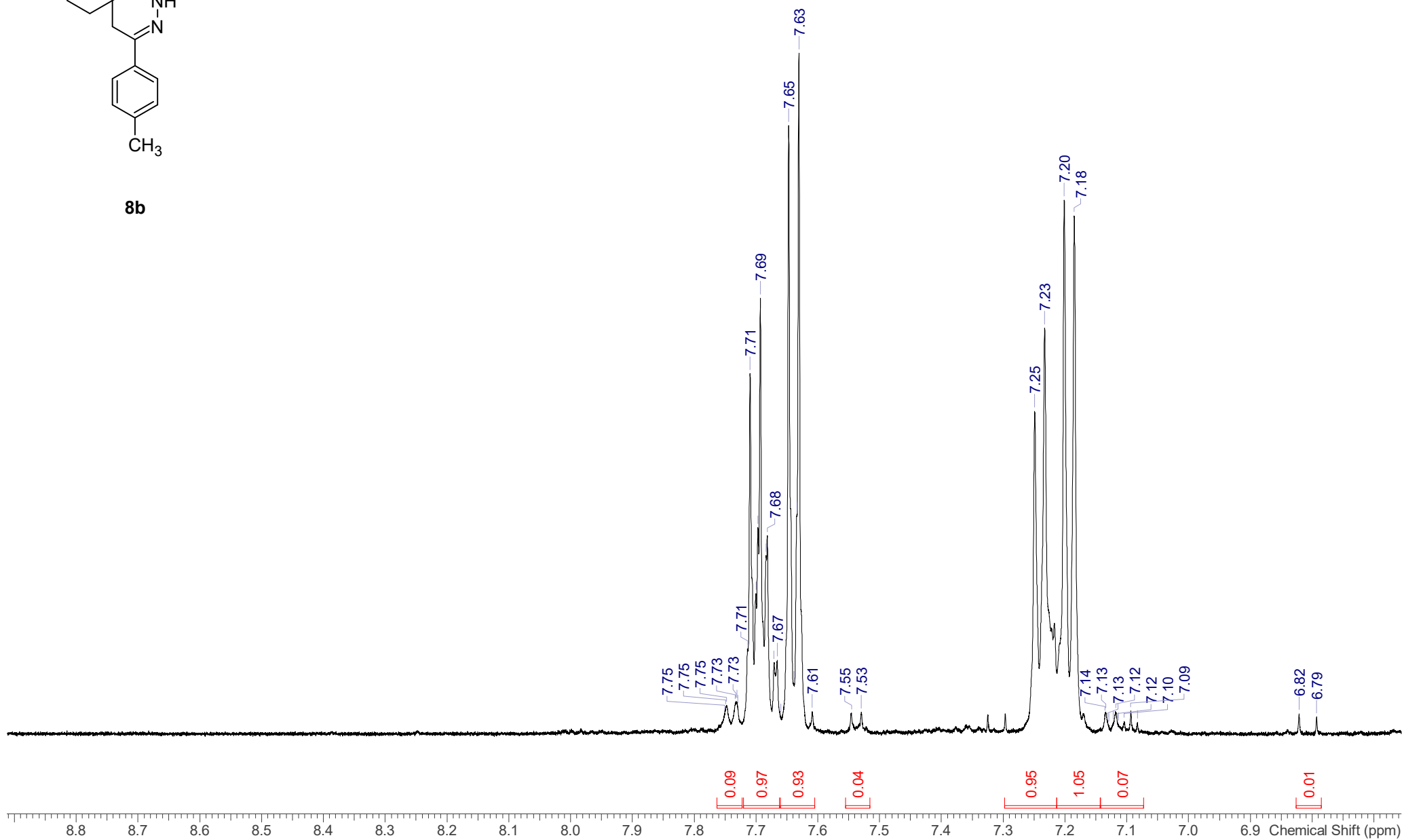
**8b**



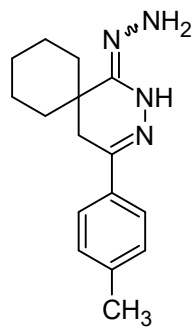
$^1\text{H}$  NMR (499.9 MHz;  $\text{DMSO-}d_6$ )



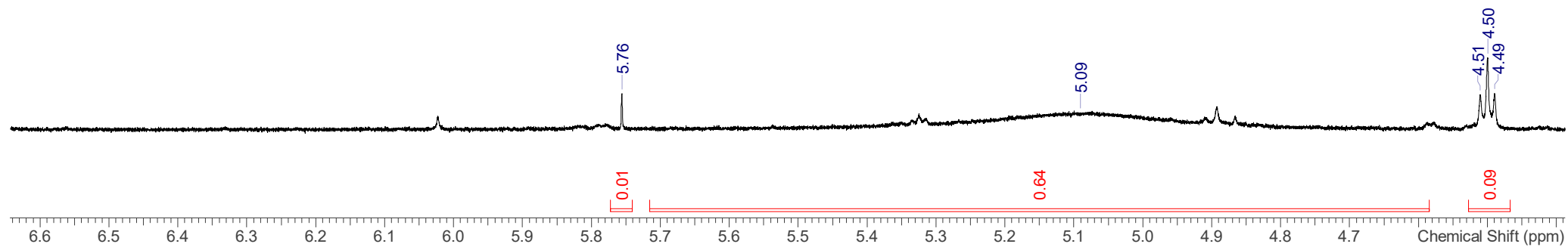
**8b**



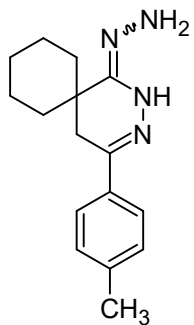
$^1\text{H}$  NMR (499.9 MHz;  $\text{DMSO}-d_6$ )



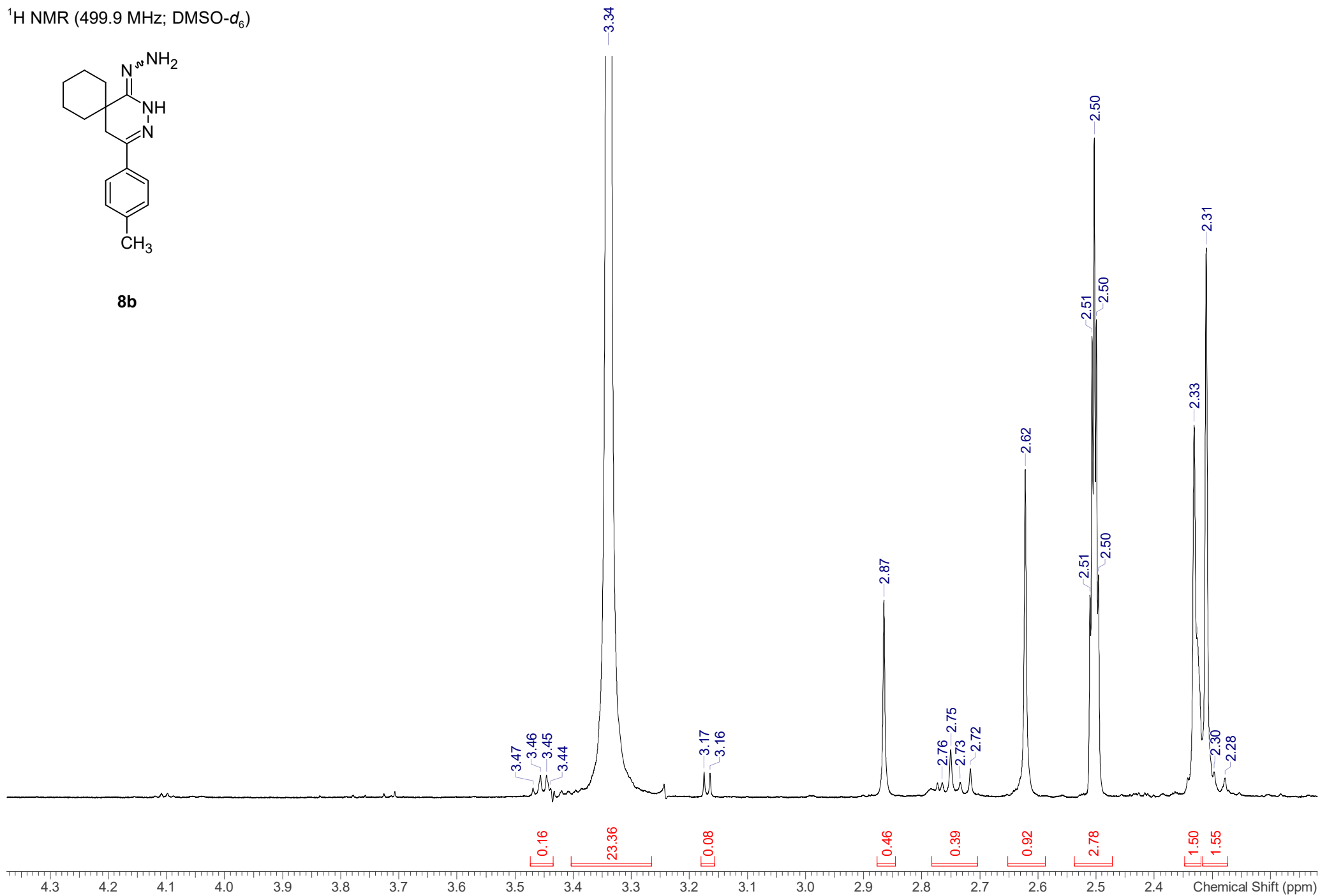
**8b**



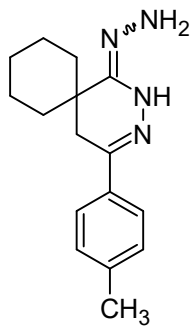
<sup>1</sup>H NMR (499.9 MHz; DMSO-d<sub>6</sub>)



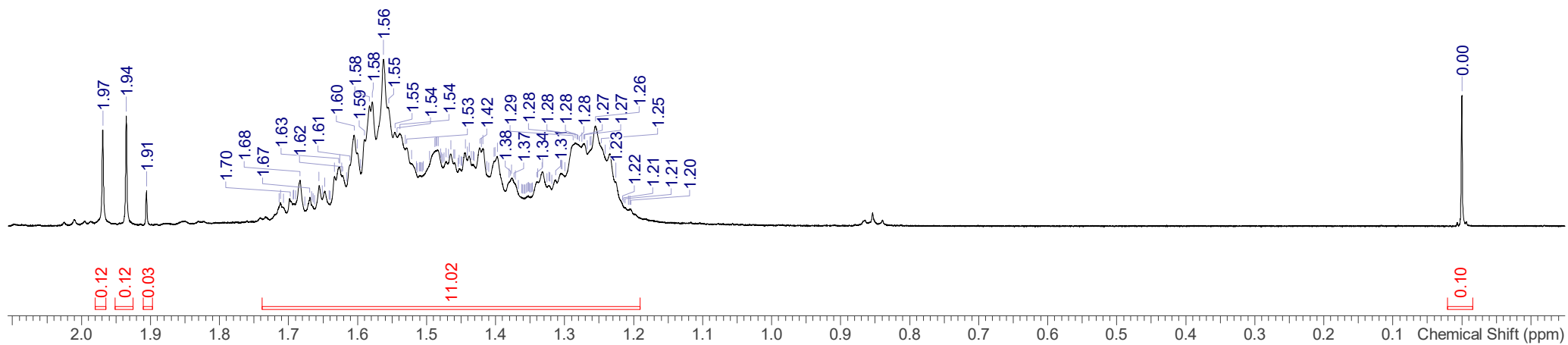
8b



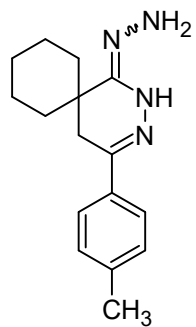
<sup>1</sup>H NMR (499.9 MHz; DMSO-d<sub>6</sub>)



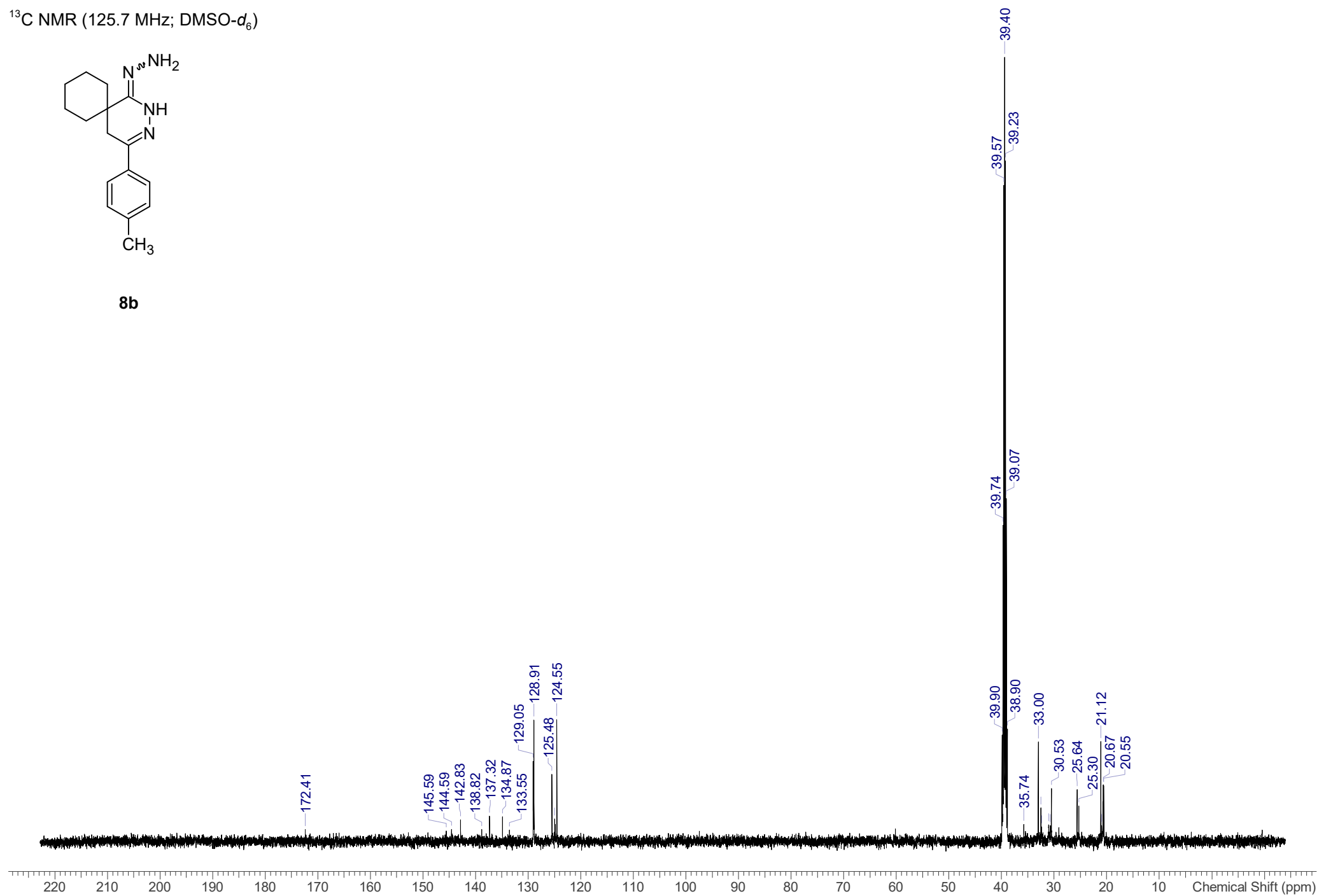
**8b**



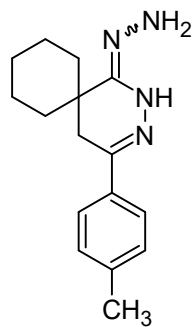
$^{13}\text{C}$  NMR (125.7 MHz;  $\text{DMSO-}d_6$ )



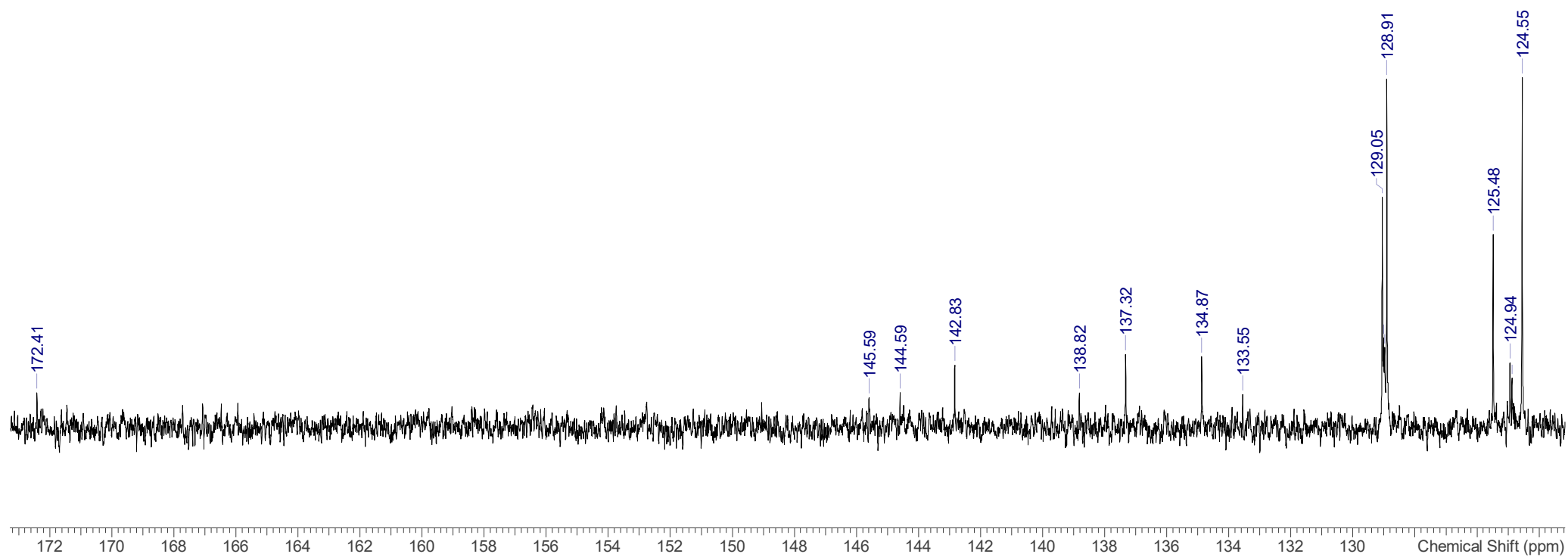
**8b**



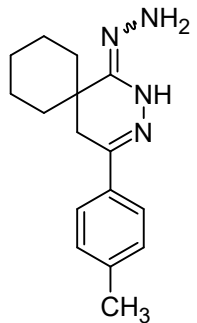
$^{13}\text{C}$  NMR (125.7 MHz;  $\text{DMSO-}d_6$ )



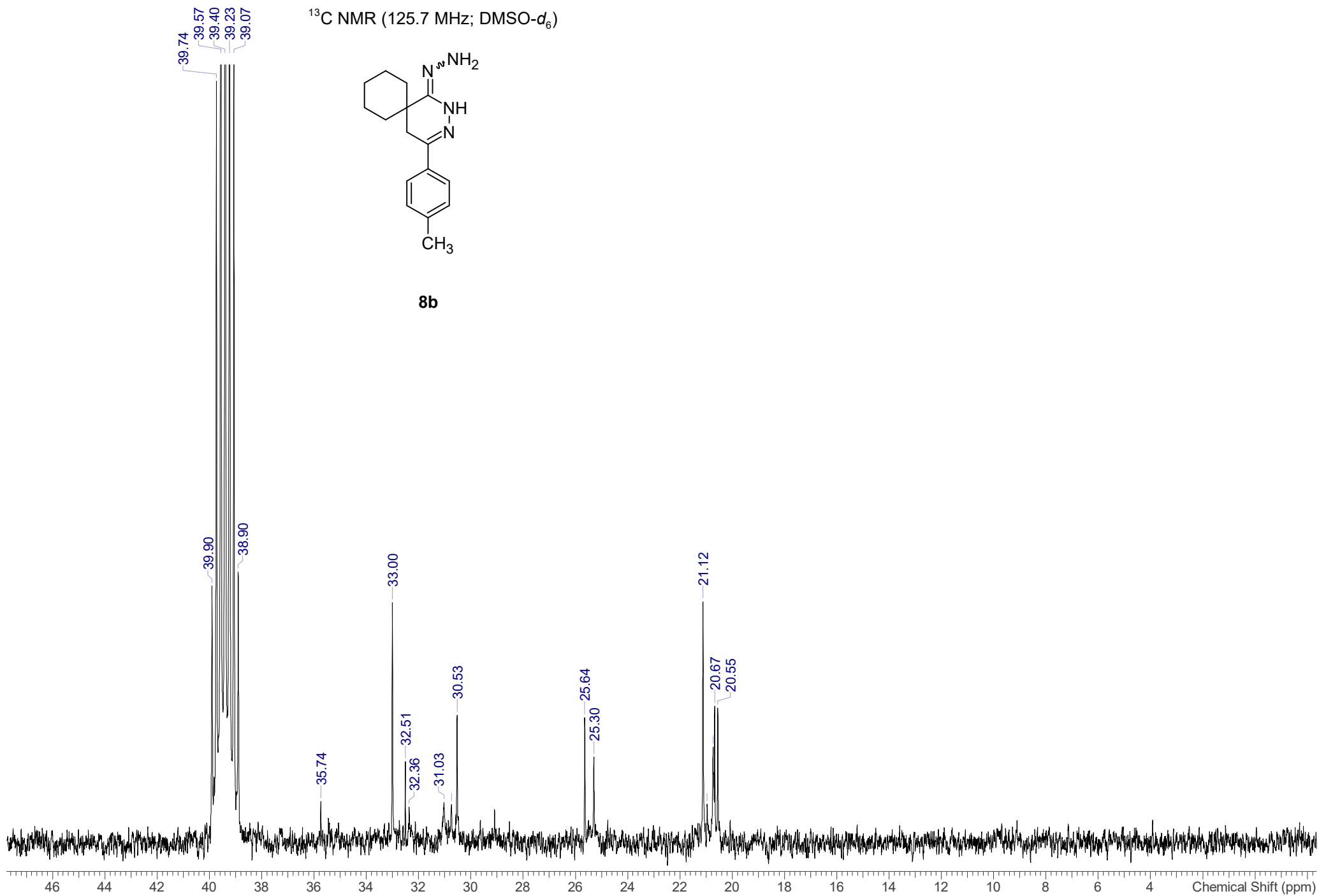
**8b**



$^{13}\text{C}$  NMR (125.7 MHz;  $\text{DMSO-}d_6$ )



**8b**

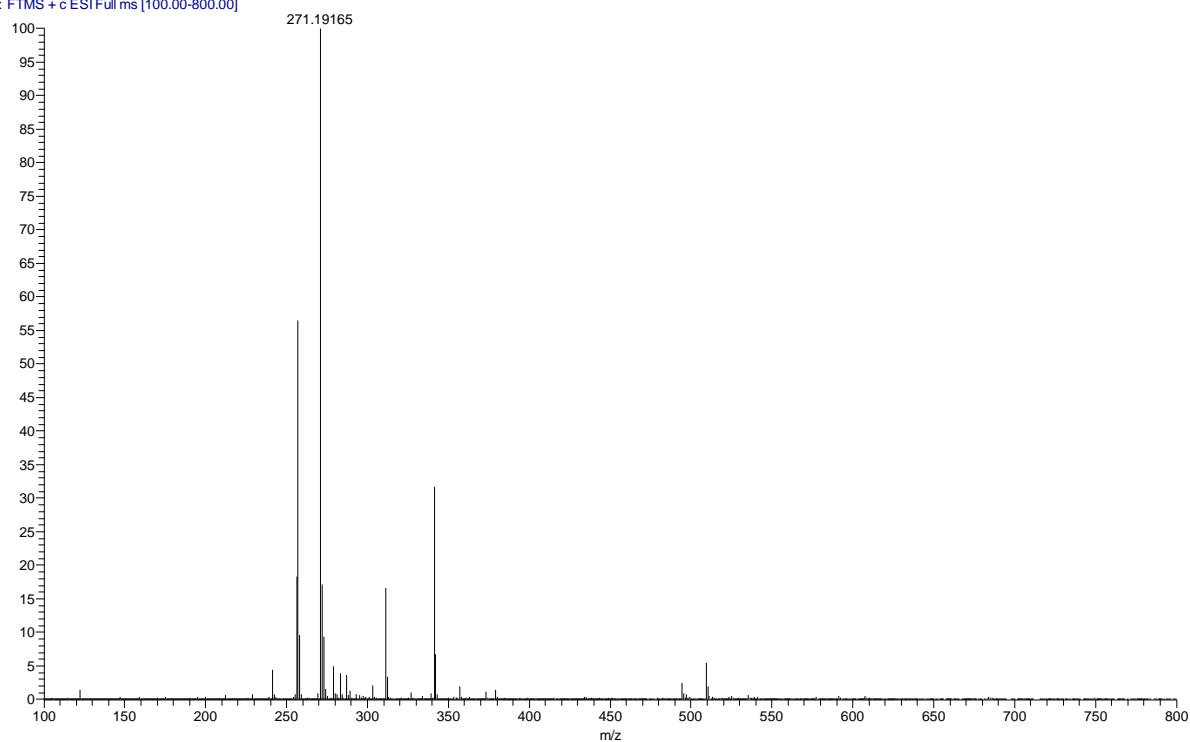




# Compound **8b**

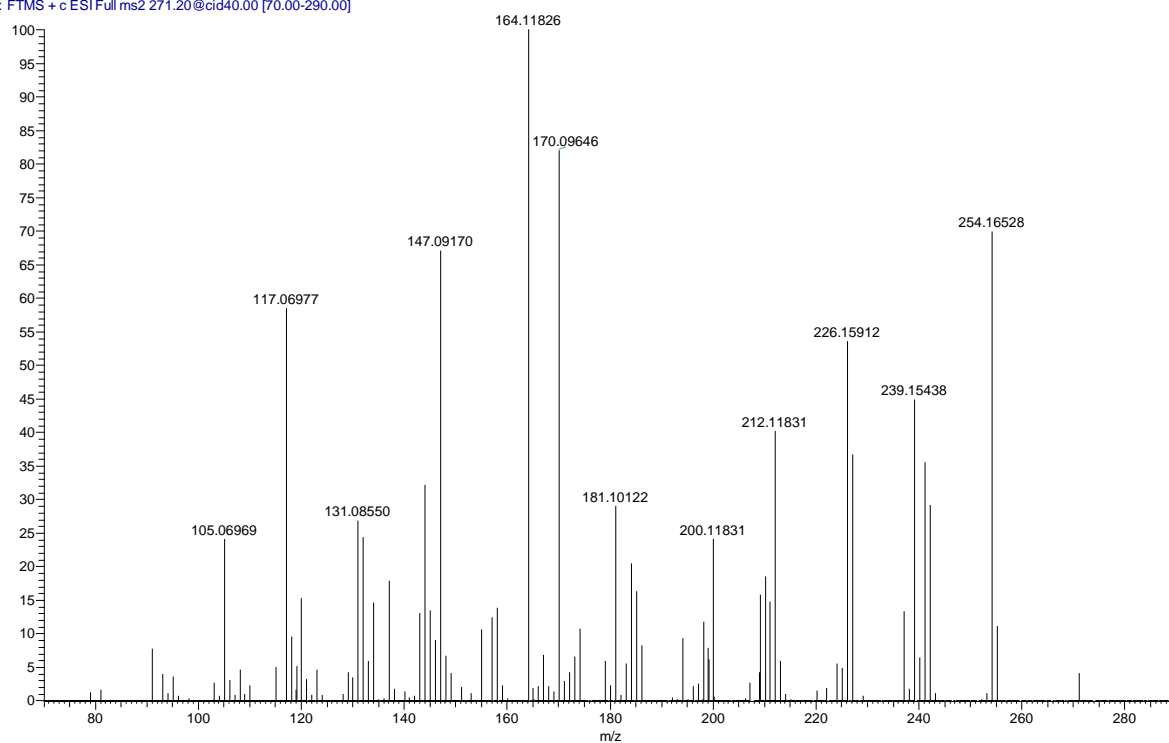
## HRMS spectrum (ESI)

ku74010\_sfc-217\_d\_ve6273 #1-50 RT: 0.00-0.20 AV: 50 NL: 3.18E7  
T: FTMS + c ESI Full ms [100.00-800.00]

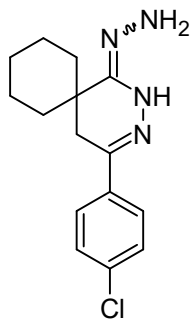


## HRMS spectrum (ESI daughter ion)

ku74010\_sfc-217\_d\_ve6274 #1-47 RT: 0.00-0.20 AV: 47 NL: 1.64E6  
T: FTMS + c ESI Full ms2 271.20@cid40.00 [70.00-290.00]

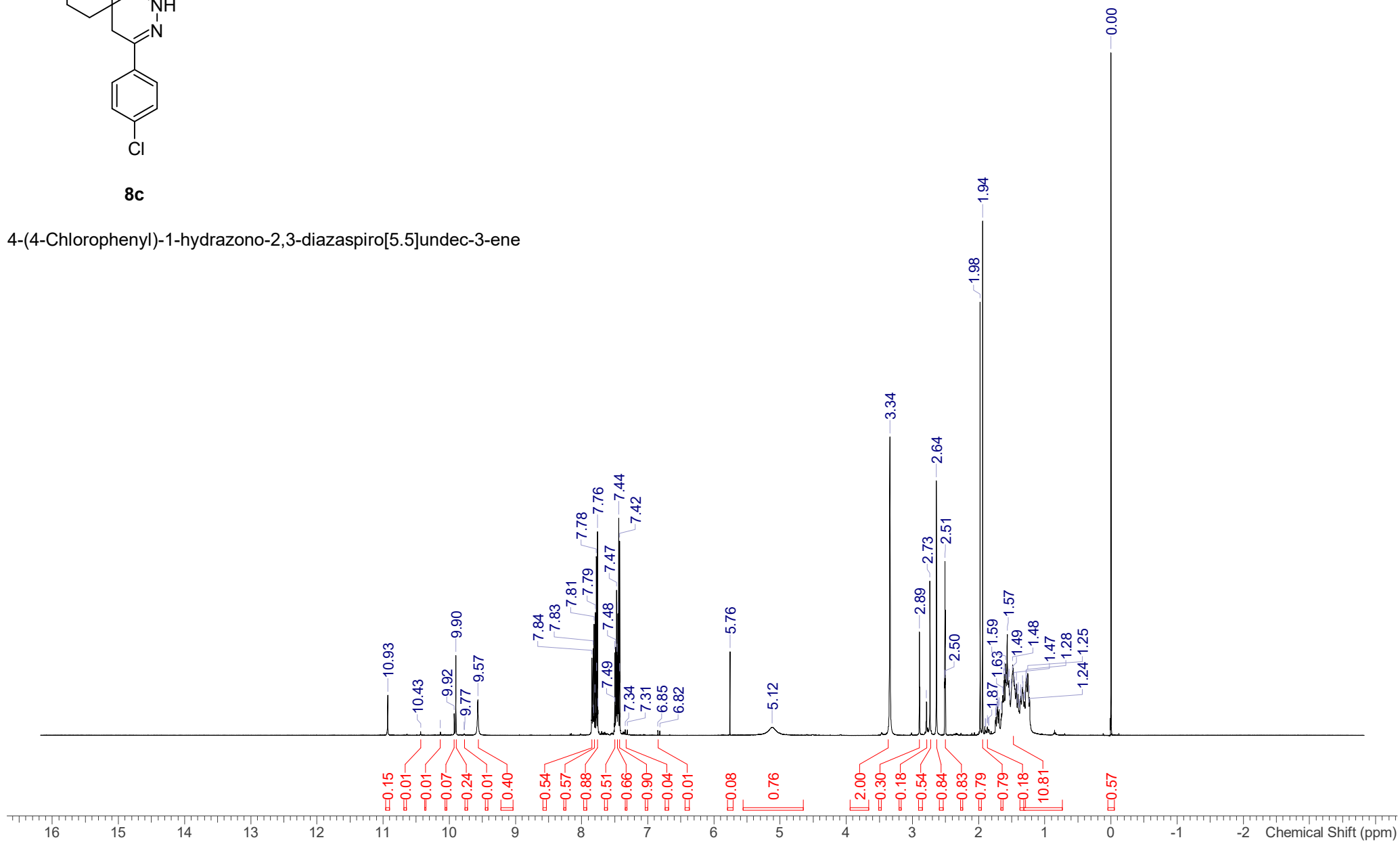


$^1\text{H}$  NMR (499.9 MHz;  $\text{DMSO}-d_6$ )

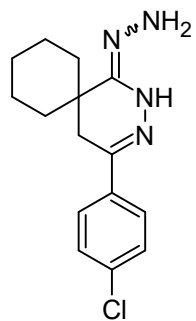


**8c**

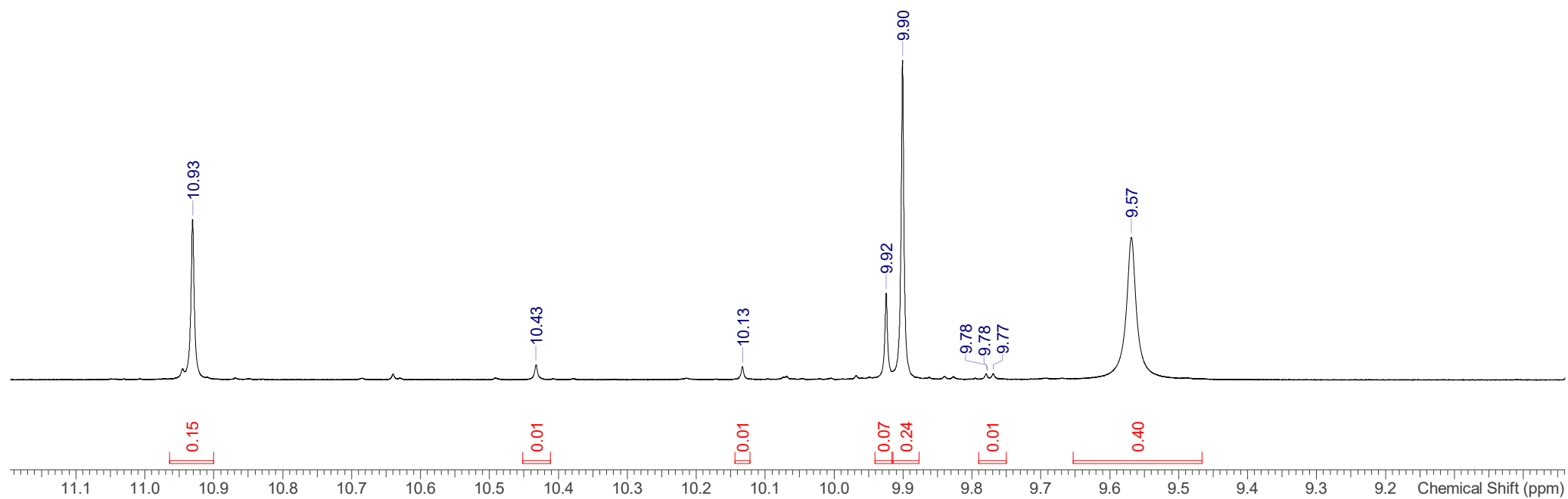
4-(4-Chlorophenyl)-1-hydrazono-2,3-diazaspiro[5.5]undec-3-ene



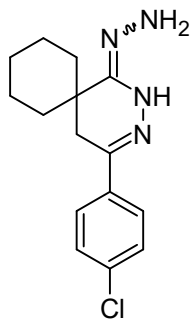
$^1\text{H}$  NMR (499.9 MHz;  $\text{DMSO-}d_6$ )



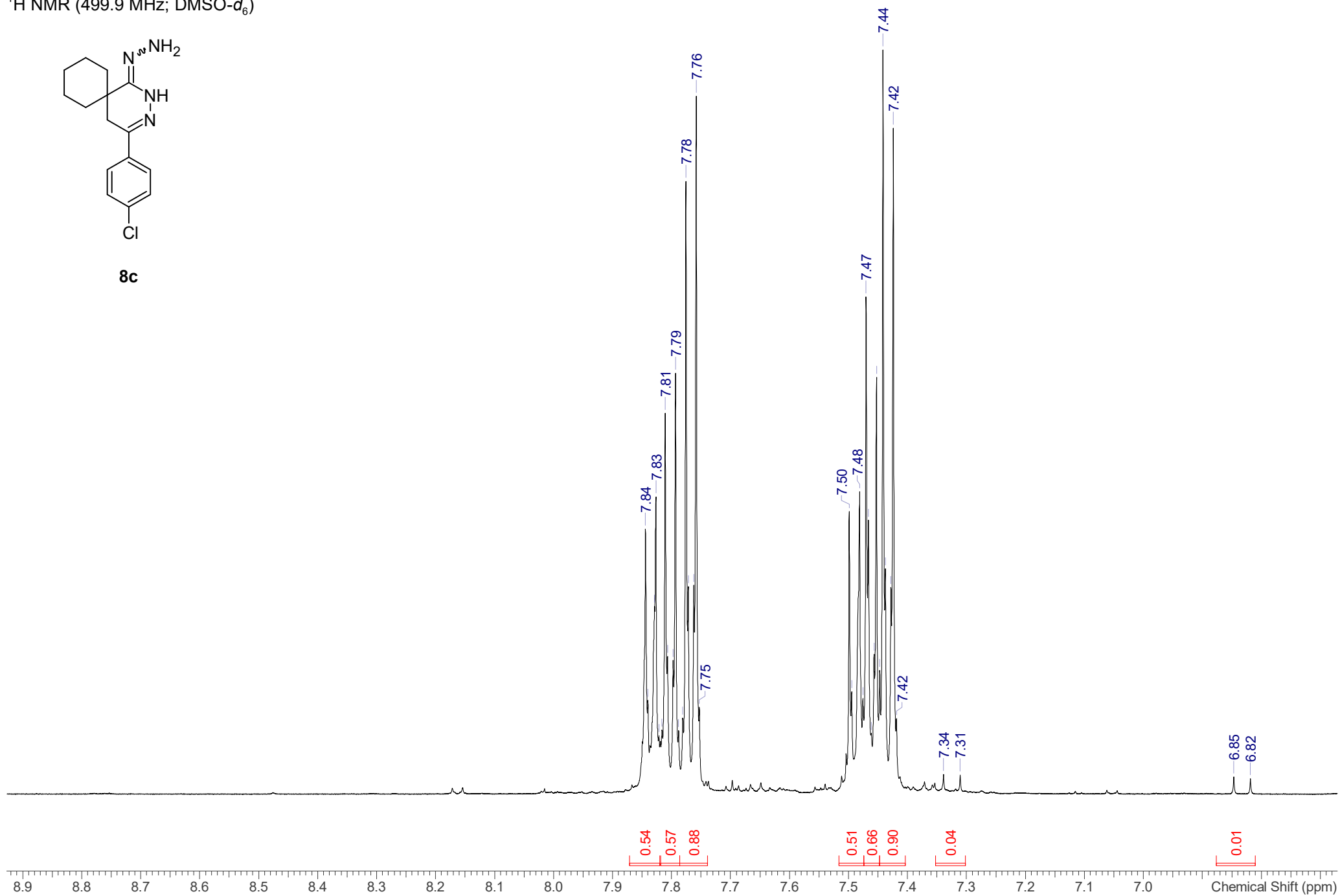
**8c**



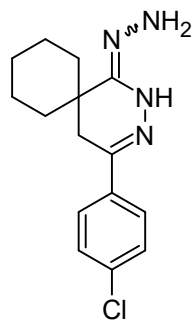
<sup>1</sup>H NMR (499.9 MHz; DMSO-d<sub>6</sub>)



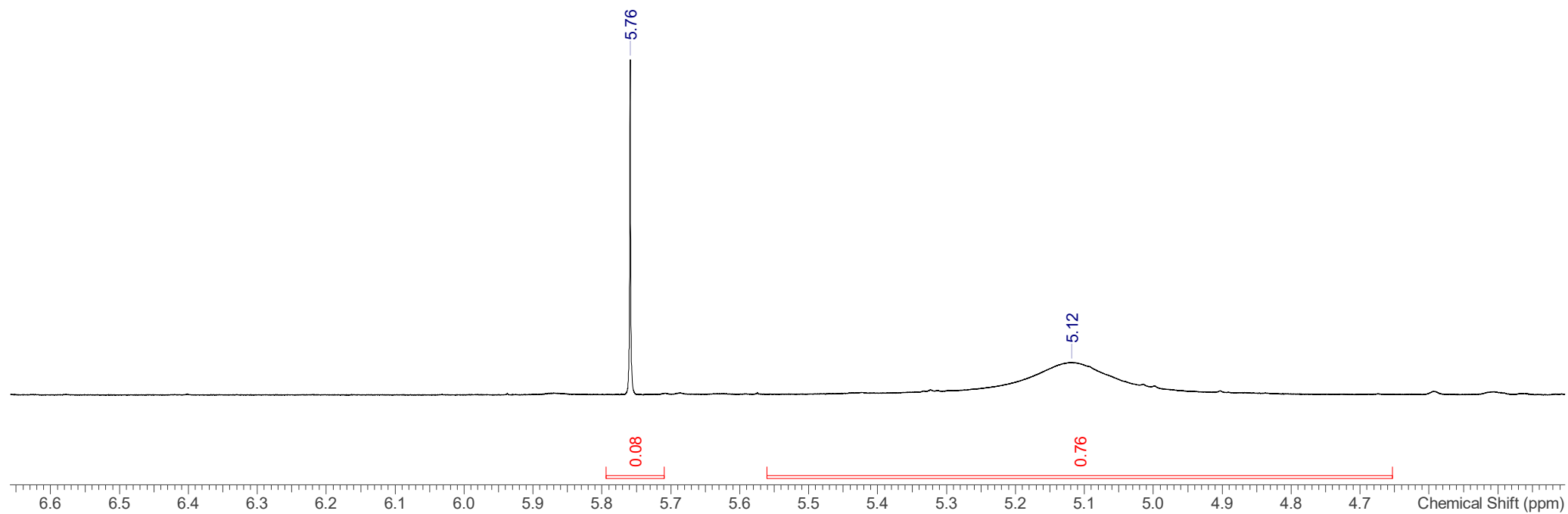
8c



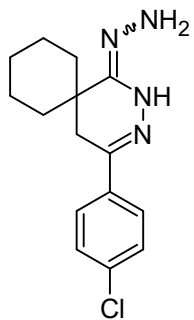
$^1\text{H}$  NMR (499.9 MHz;  $\text{DMSO-}d_6$ )



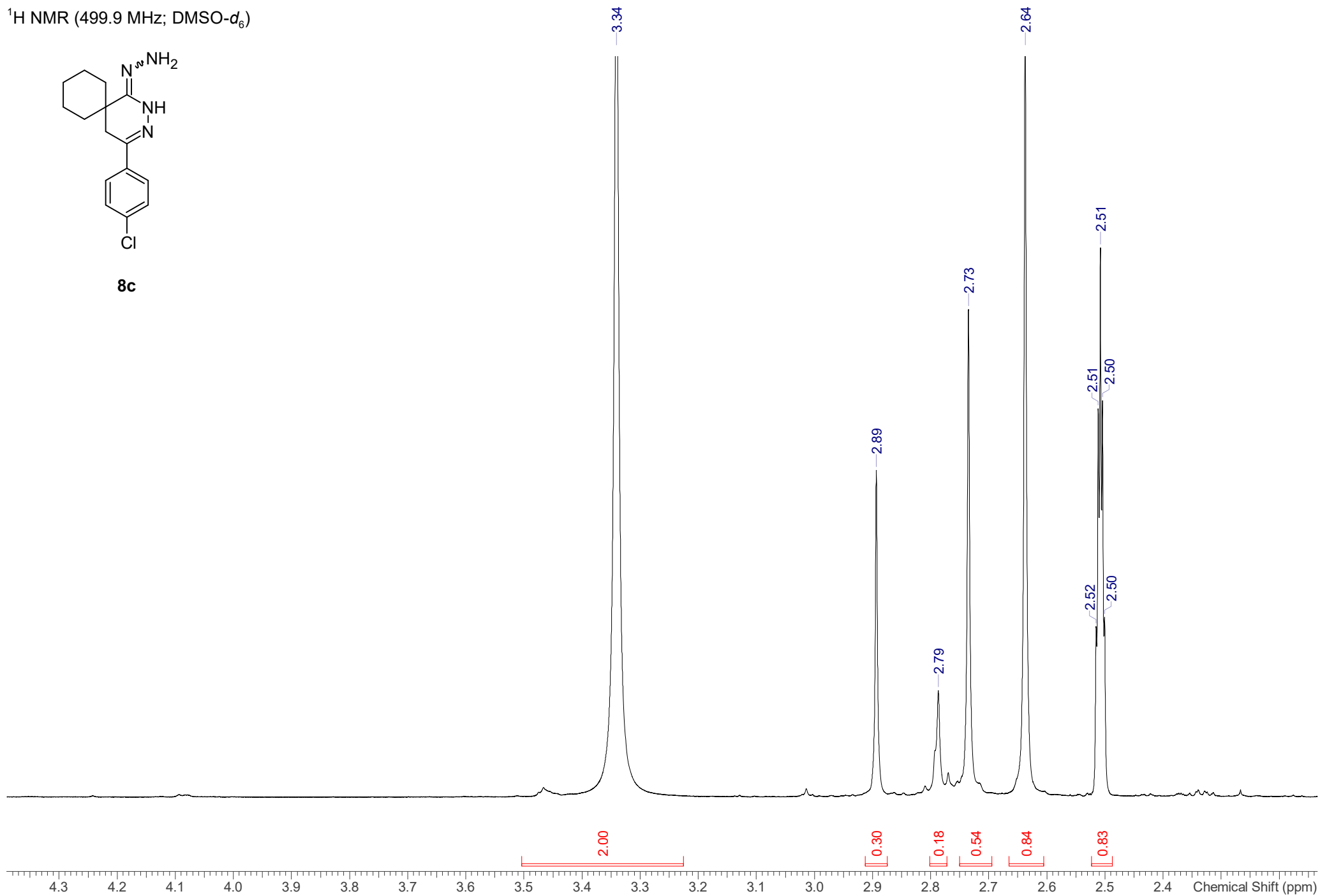
**8c**



$^1\text{H}$  NMR (499.9 MHz;  $\text{DMSO}-d_6$ )

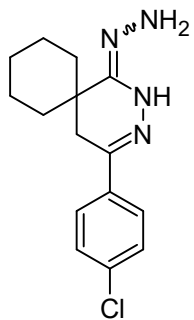


**8c**

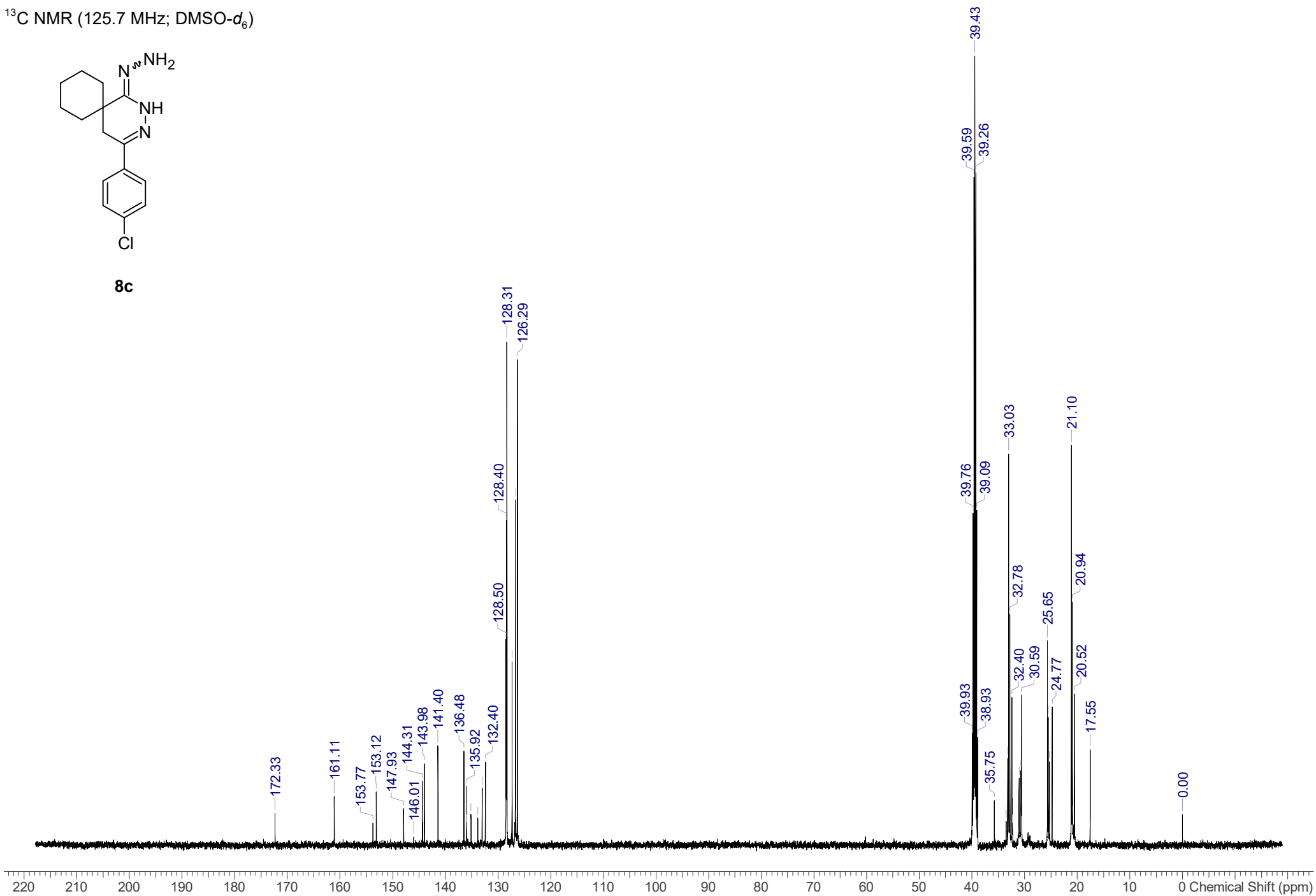




<sup>13</sup>C NMR (125.7 MHz; DMSO-d<sub>6</sub>)

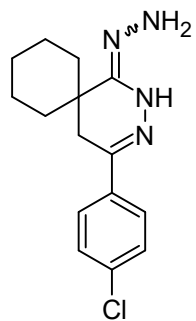


**8c**

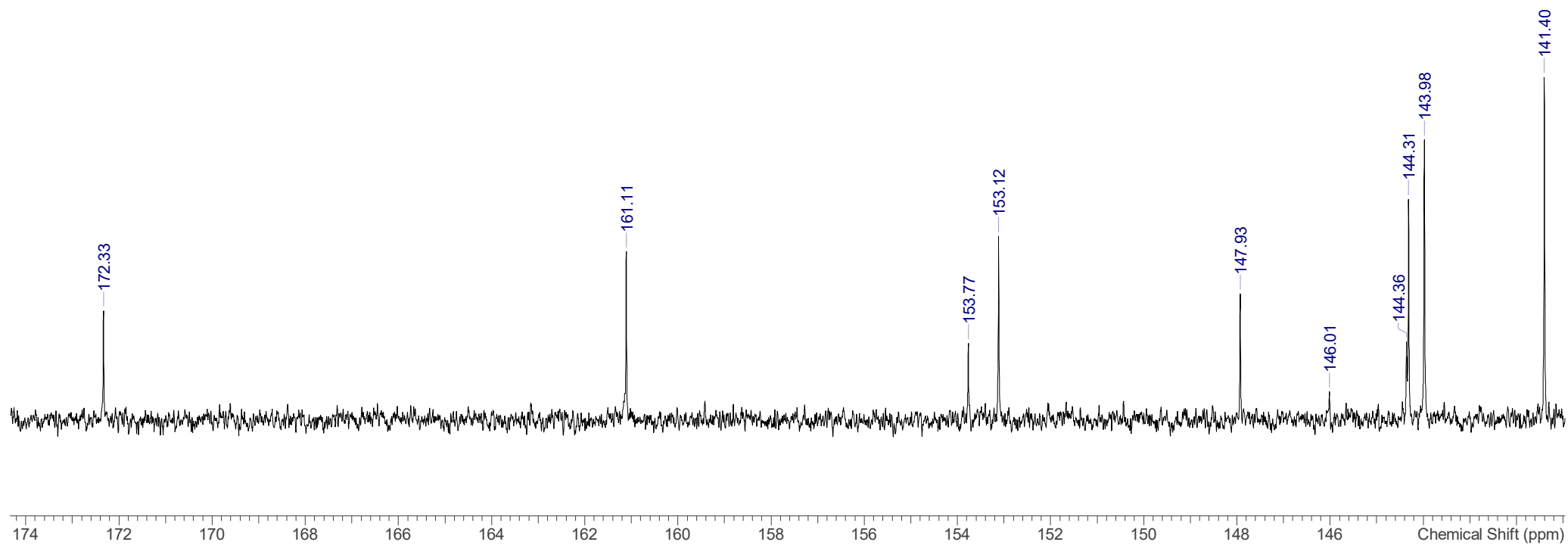




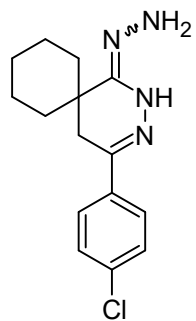
$^{13}\text{C}$  NMR (125.7 MHz;  $\text{DMSO-}d_6$ )



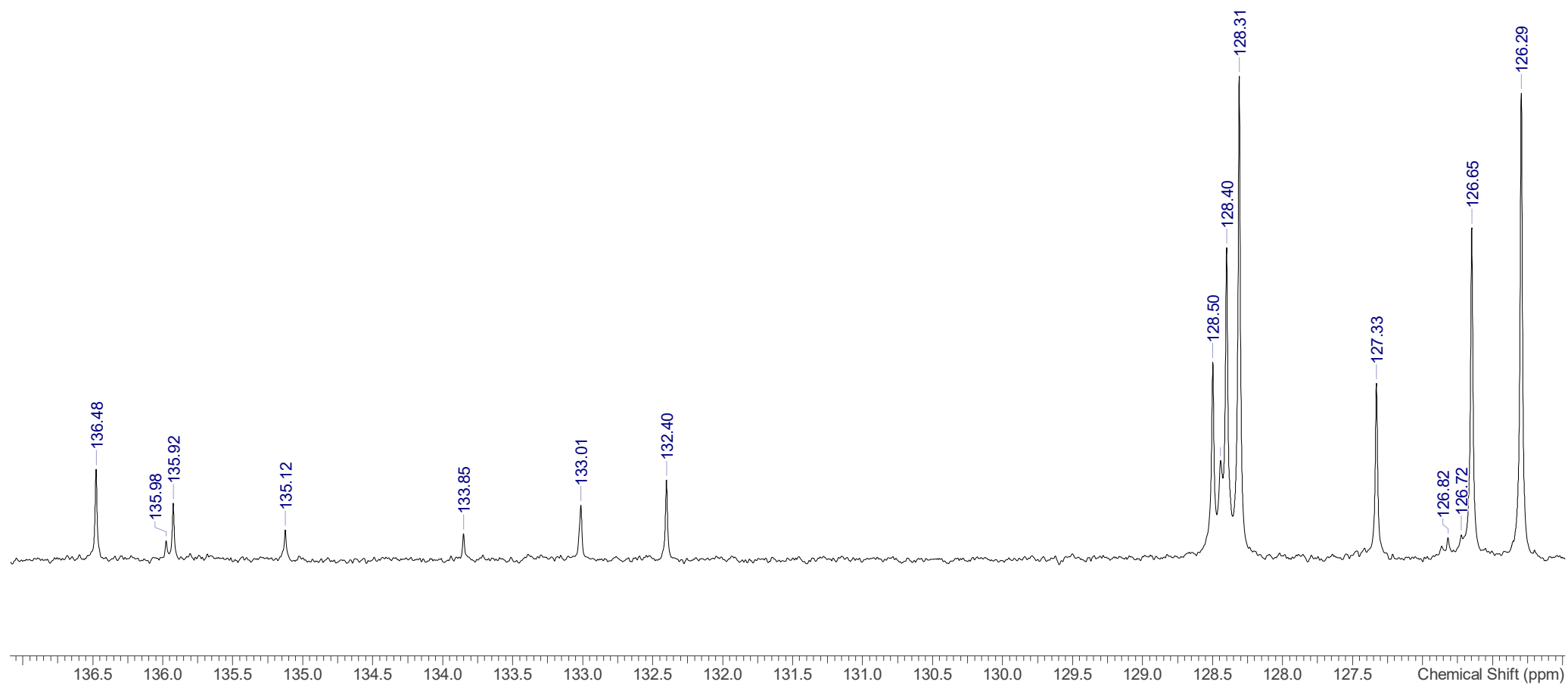
**8c**



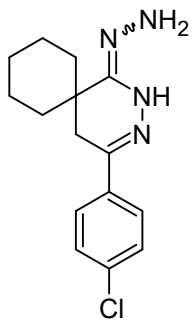
$^{13}\text{C}$  NMR (125.7 MHz;  $\text{DMSO-}d_6$ )



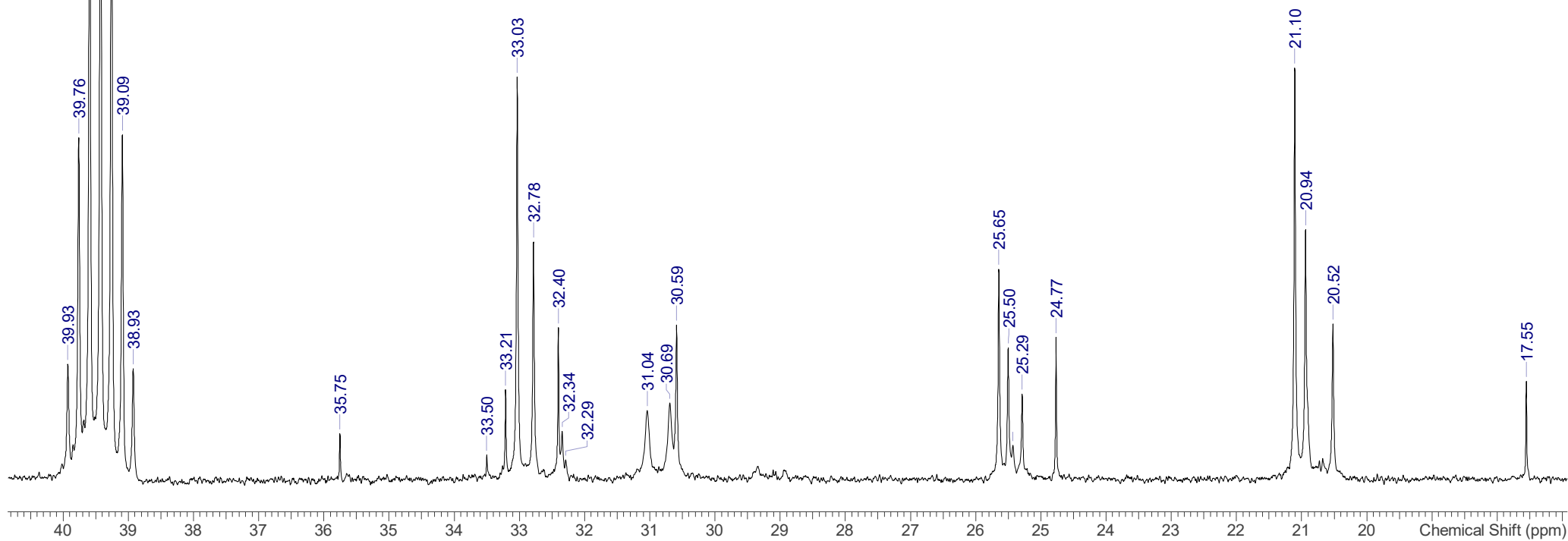
**8c**



$^{13}\text{C}$  NMR (125.7 MHz;  $\text{DMSO-}d_6$ )



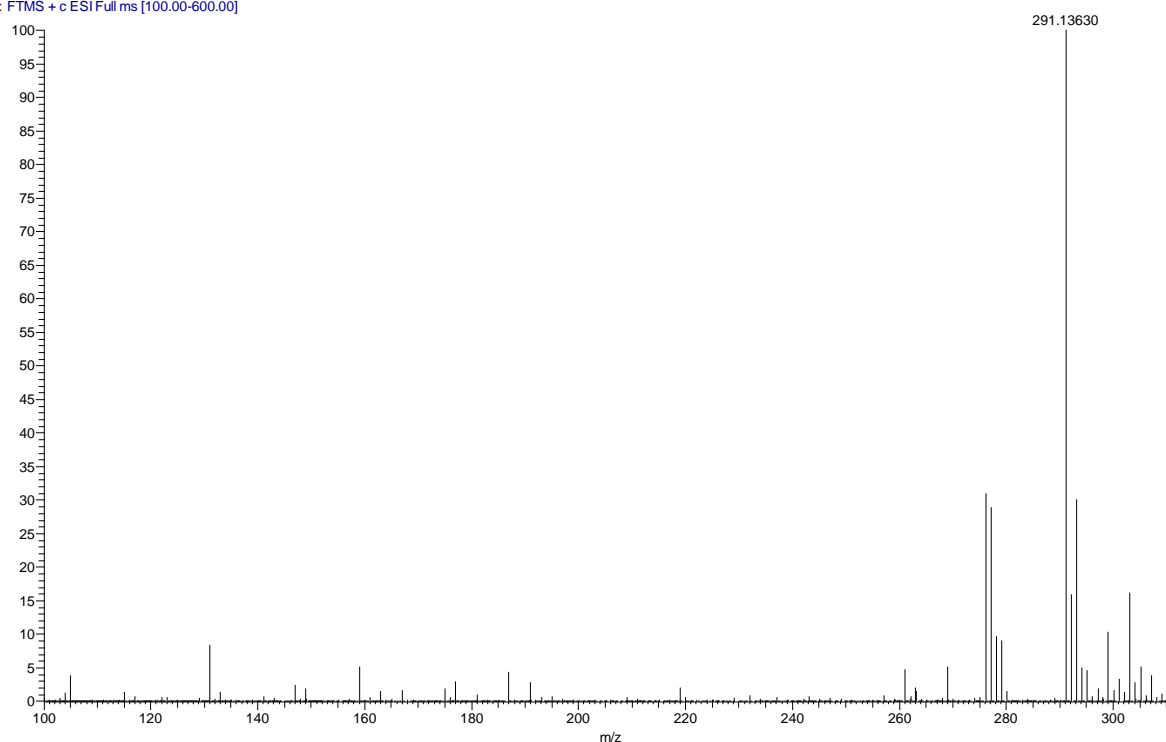
8c



# Compound 8c

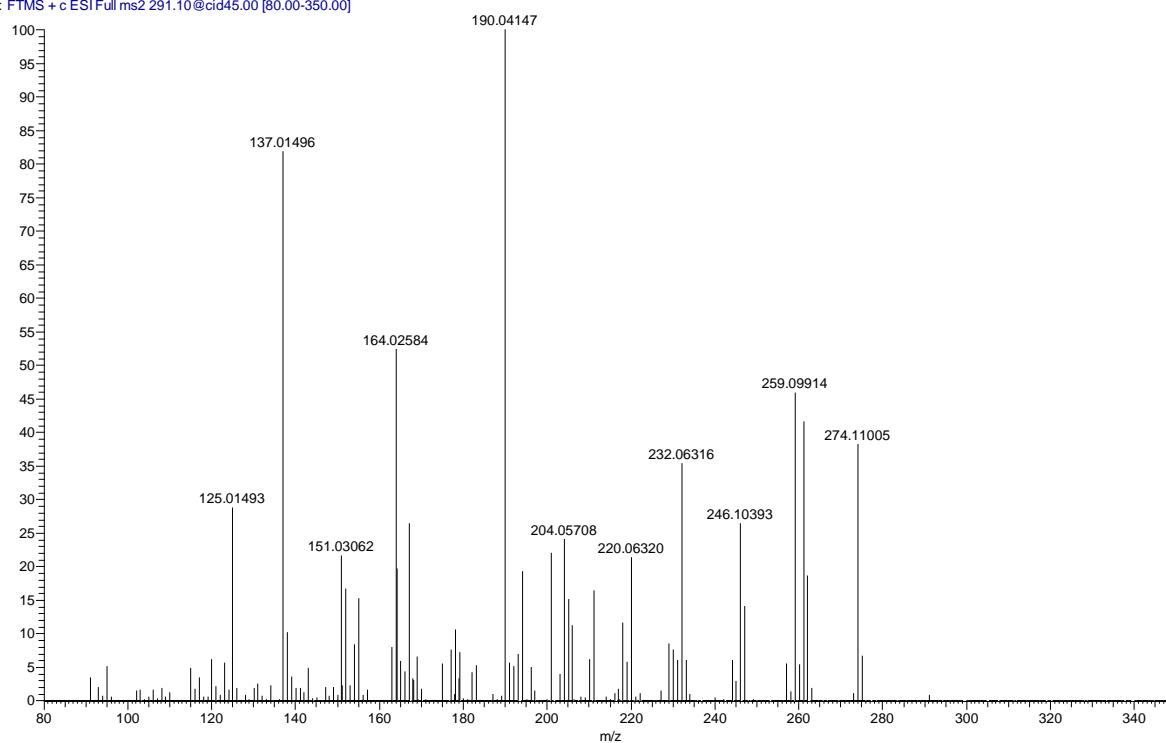
## HRMS spectrum (ESI)

ku70812\_sfc-170-2\_d\_ve3868 #1-25 RT: 0.00-0.20 AV: 25 NL: 1.13E7  
T: FTMS + c ESI Full ms [100.00-600.00]

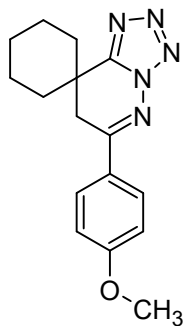


## HRMS spectrum (ESI daughter ion)

ku70812\_sfc-170-2\_d\_ve3869 #47-91 RT: 0.20-0.40 AV: 45 NL: 9.07E5  
T: FTMS + c ESI Full ms2 291.10@cid45.00 [80.00-350.00]

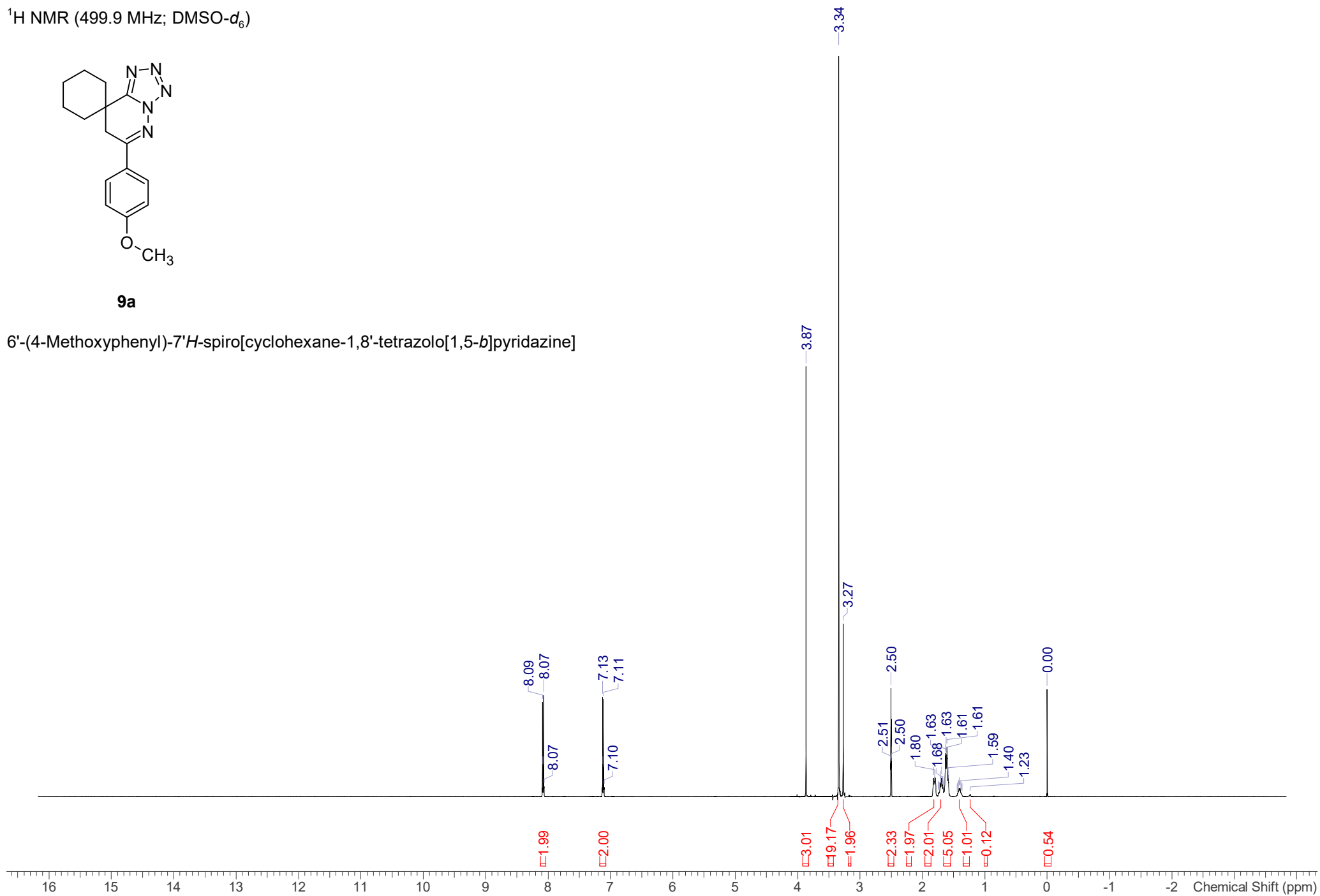


<sup>1</sup>H NMR (499.9 MHz; DMSO-*d*<sub>6</sub>)

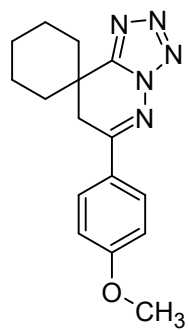


**9a**

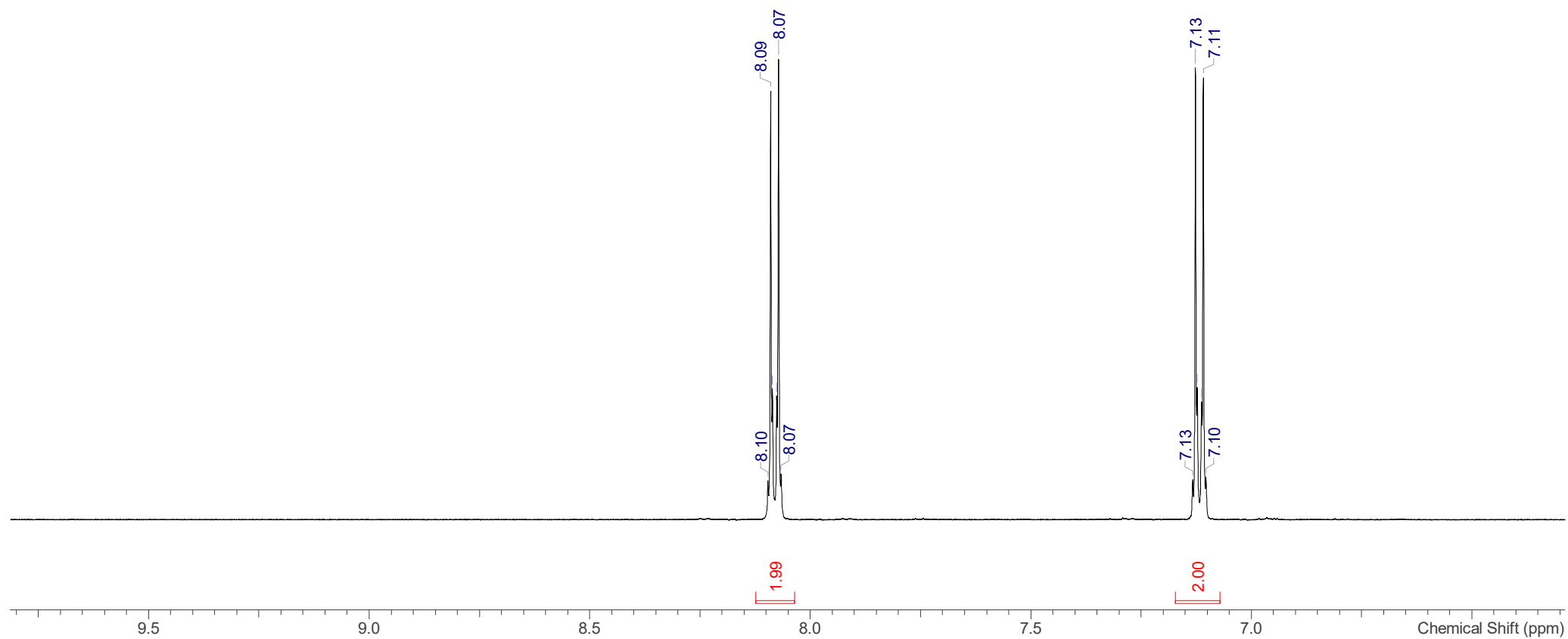
6'-(4-Methoxyphenyl)-7'*H*-spiro[cyclohexane-1,8'-tetrazolo[1,5-*b*]pyridazine]



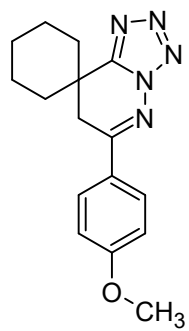
<sup>1</sup>H NMR (499.9 MHz; DMSO-d<sub>6</sub>)



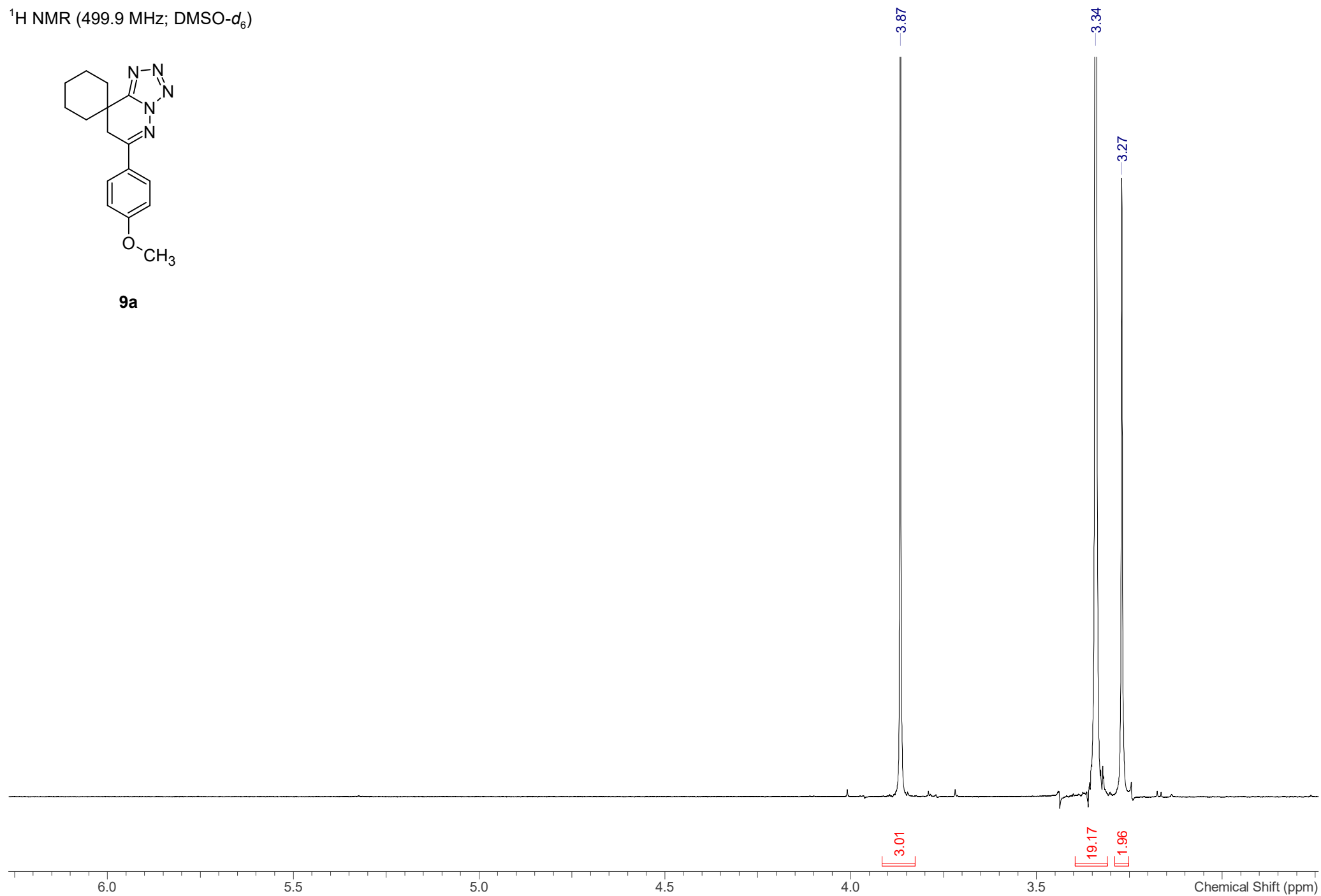
**9a**



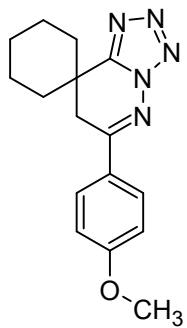
<sup>1</sup>H NMR (499.9 MHz; DMSO-*d*<sub>6</sub>)



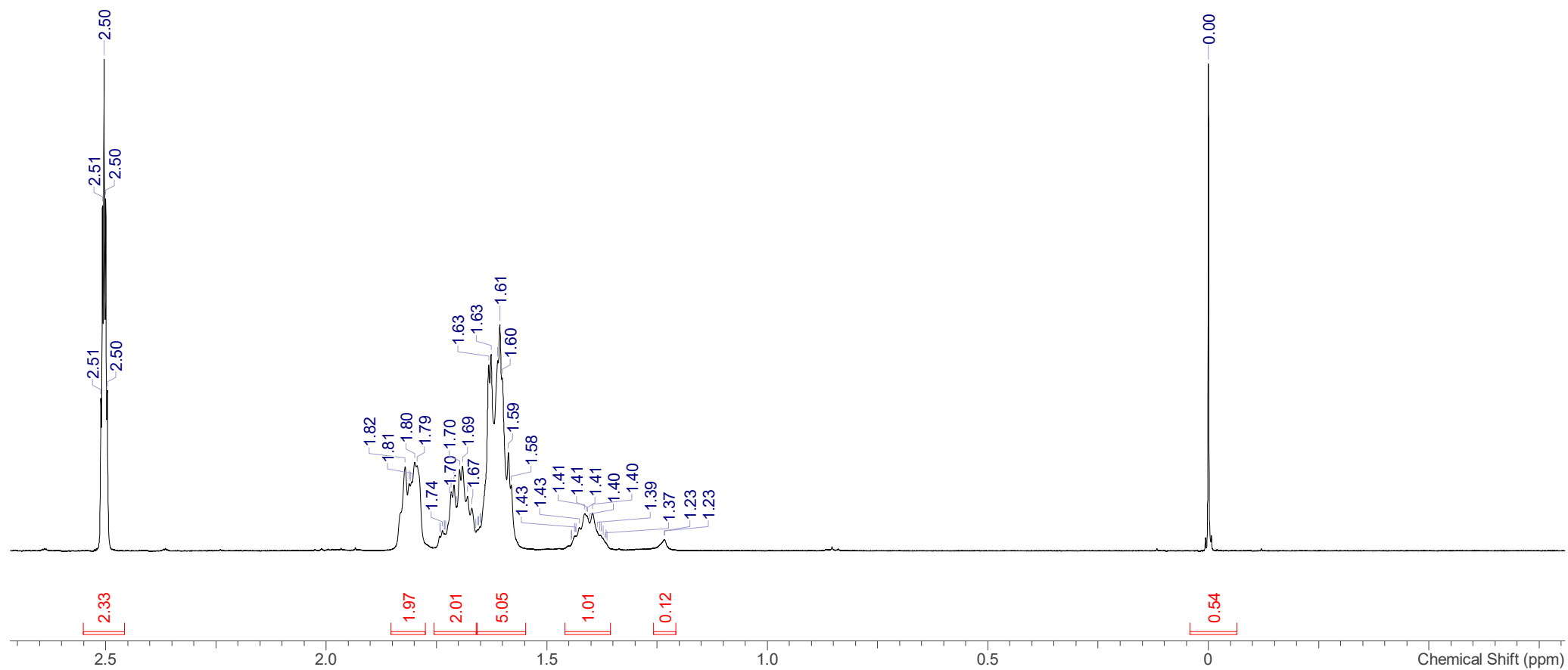
**9a**



$^1\text{H}$  NMR (499.9 MHz;  $\text{DMSO}-d_6$ )

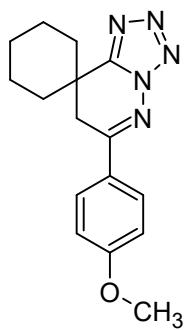


**9a**

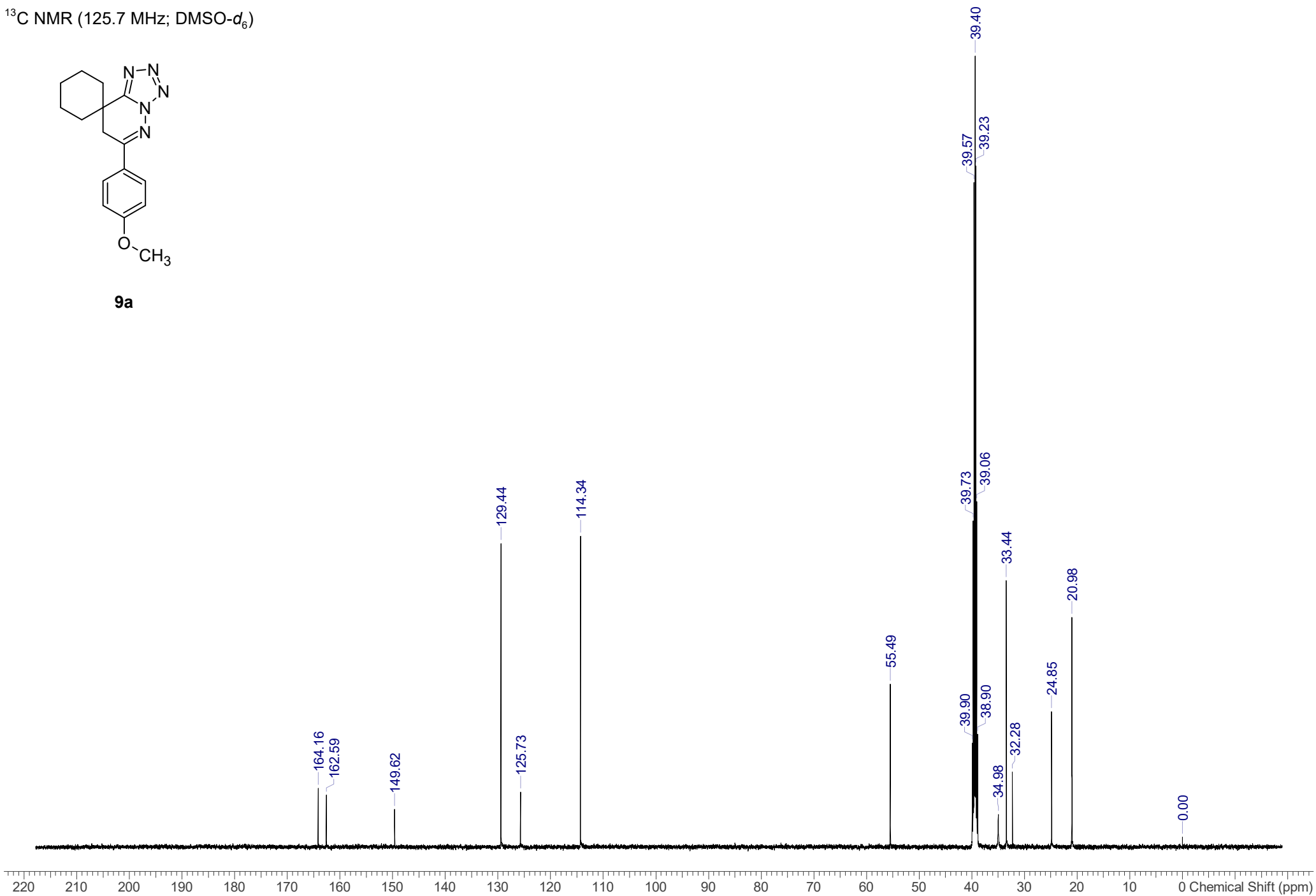




<sup>13</sup>C NMR (125.7 MHz; DMSO-d<sub>6</sub>)



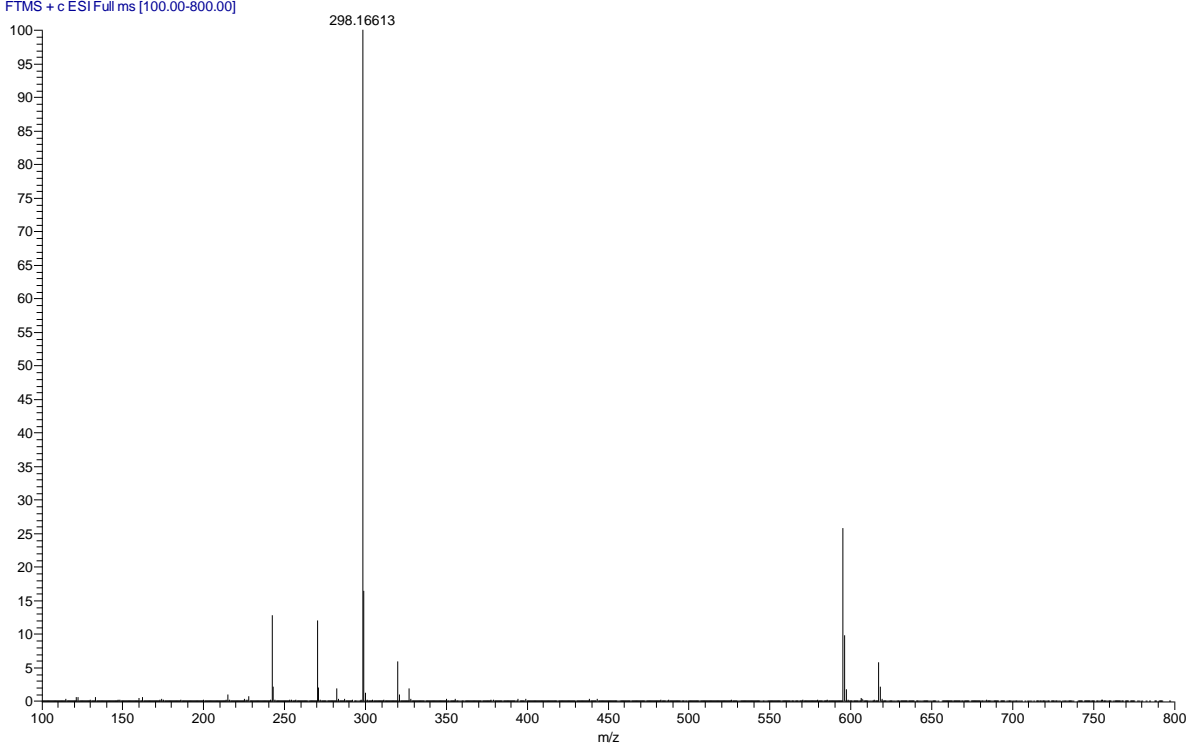
**9a**



# Compound 9a

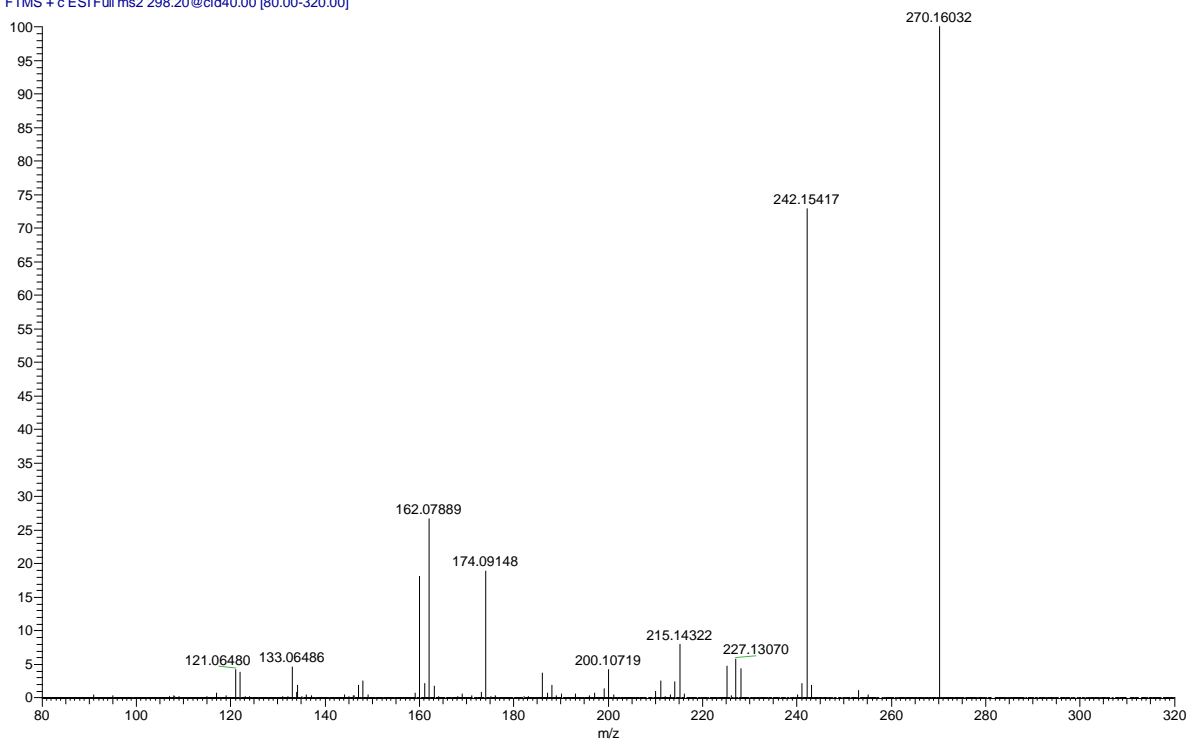
## HRMS spectrum (ESI)

ku74013\_sfc-224\_d\_ve6279 #1-50 RT: 0.00-0.20 AV: 50 NL: 7.99E7  
T: FTMS + c ESI Full ms [100.00-800.00]

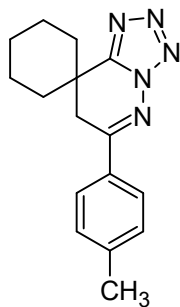


## HRMS spectrum (ESI daughter ion)

ku74013\_sfc-224\_d\_ve6280 #1-47 RT: 0.00-0.20 AV: 47 NL: 3.28E7  
T: FTMS + c ESI Full ms2 298.20@cid40.00 [80.00-320.00]

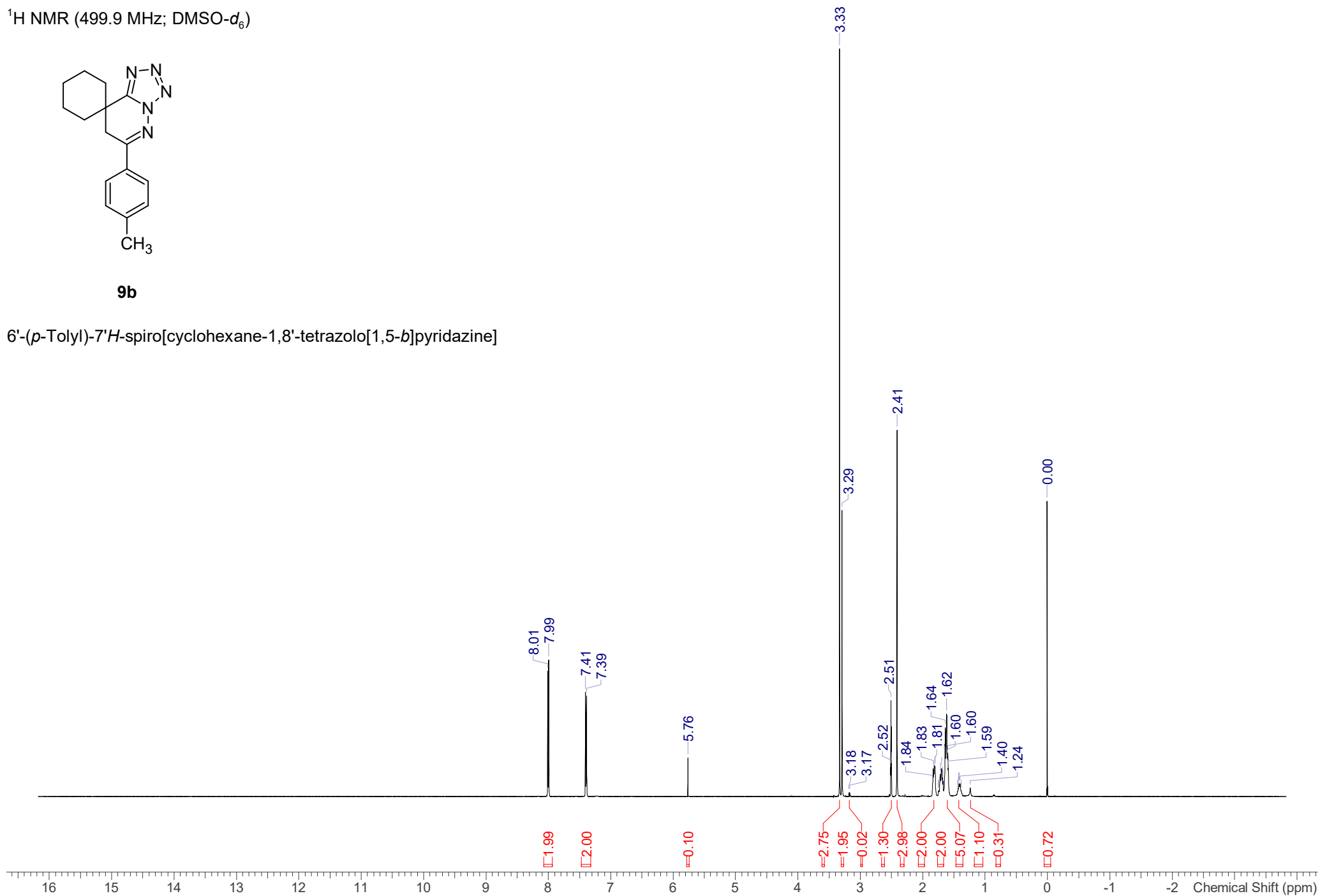


<sup>1</sup>H NMR (499.9 MHz; DMSO-d<sub>6</sub>)

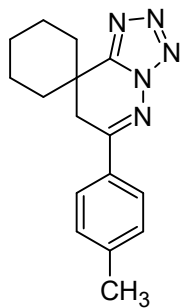


**9b**

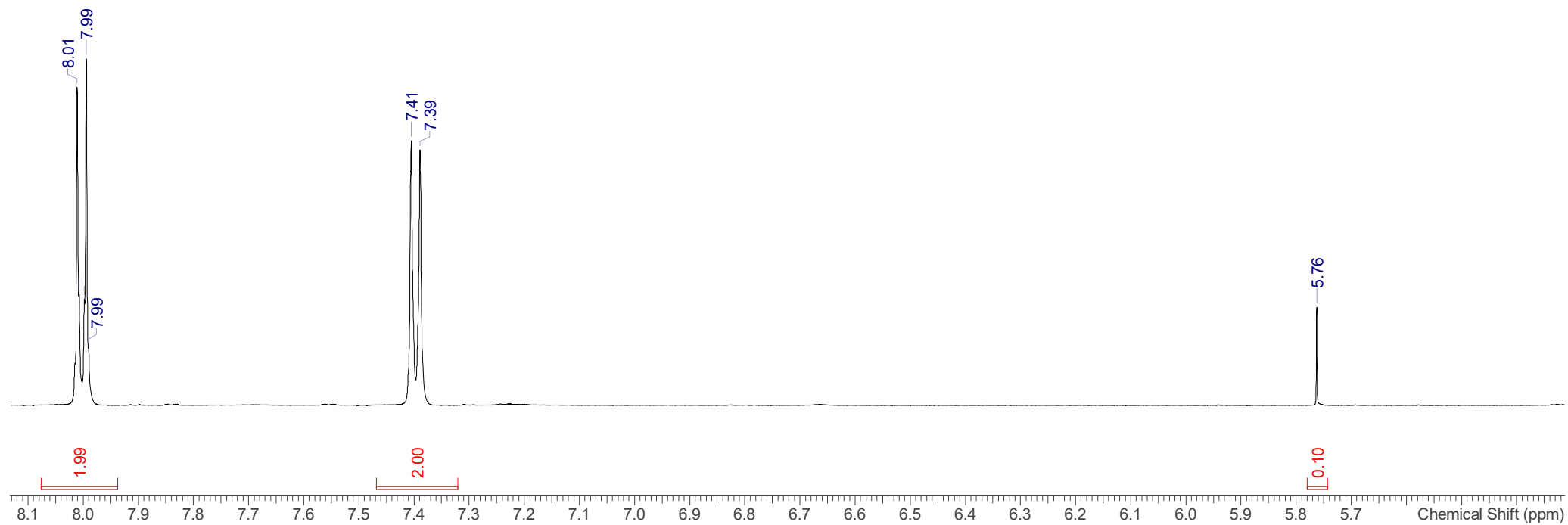
6'-(*p*-Tolyl)-7'*H*-spiro[cyclohexane-1,8'-tetrazolo[1,5-*b*]pyridazine]



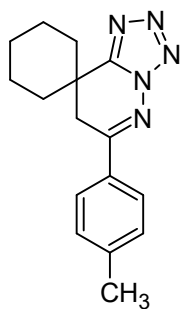
$^1\text{H}$  NMR (499.9 MHz;  $\text{DMSO-}d_6$ )



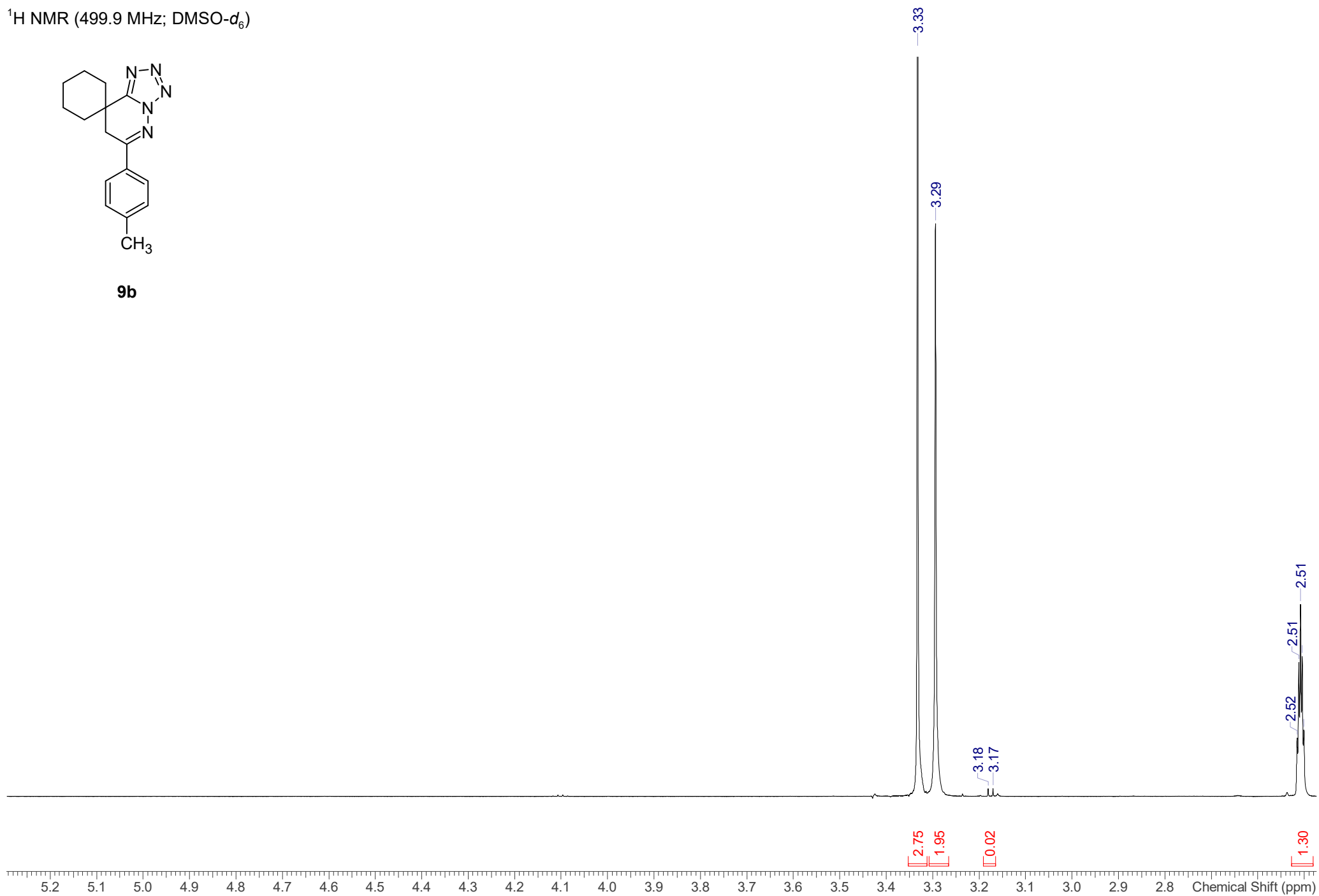
**9b**



<sup>1</sup>H NMR (499.9 MHz; DMSO-d<sub>6</sub>)

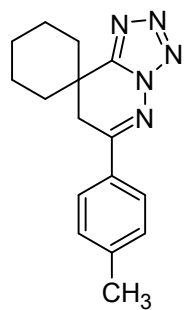


**9b**



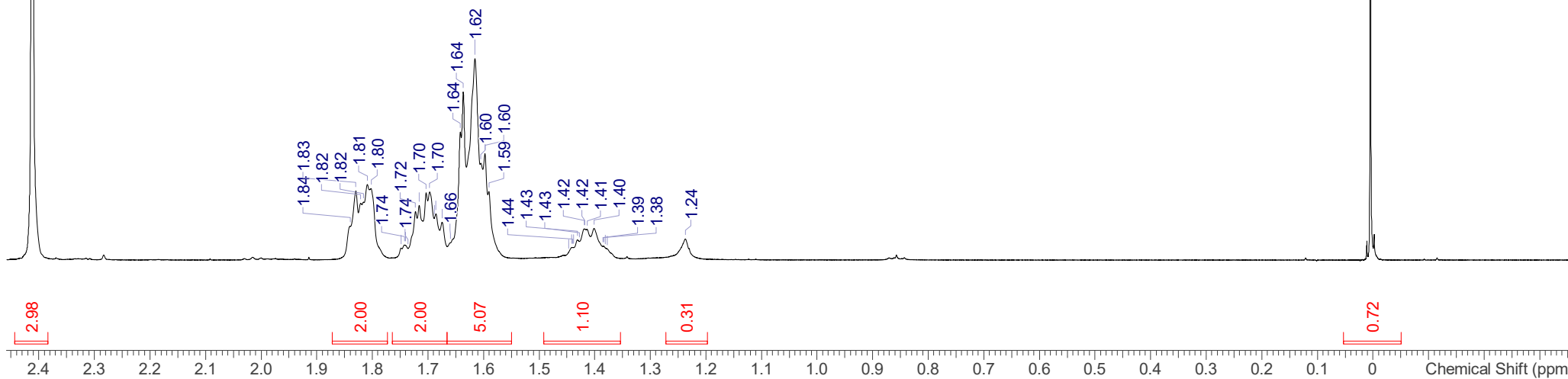
2.41

<sup>1</sup>H NMR (499.9 MHz; DMSO-d<sub>6</sub>)

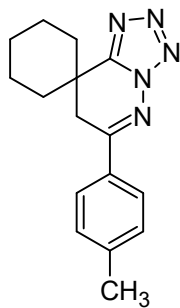


**9b**

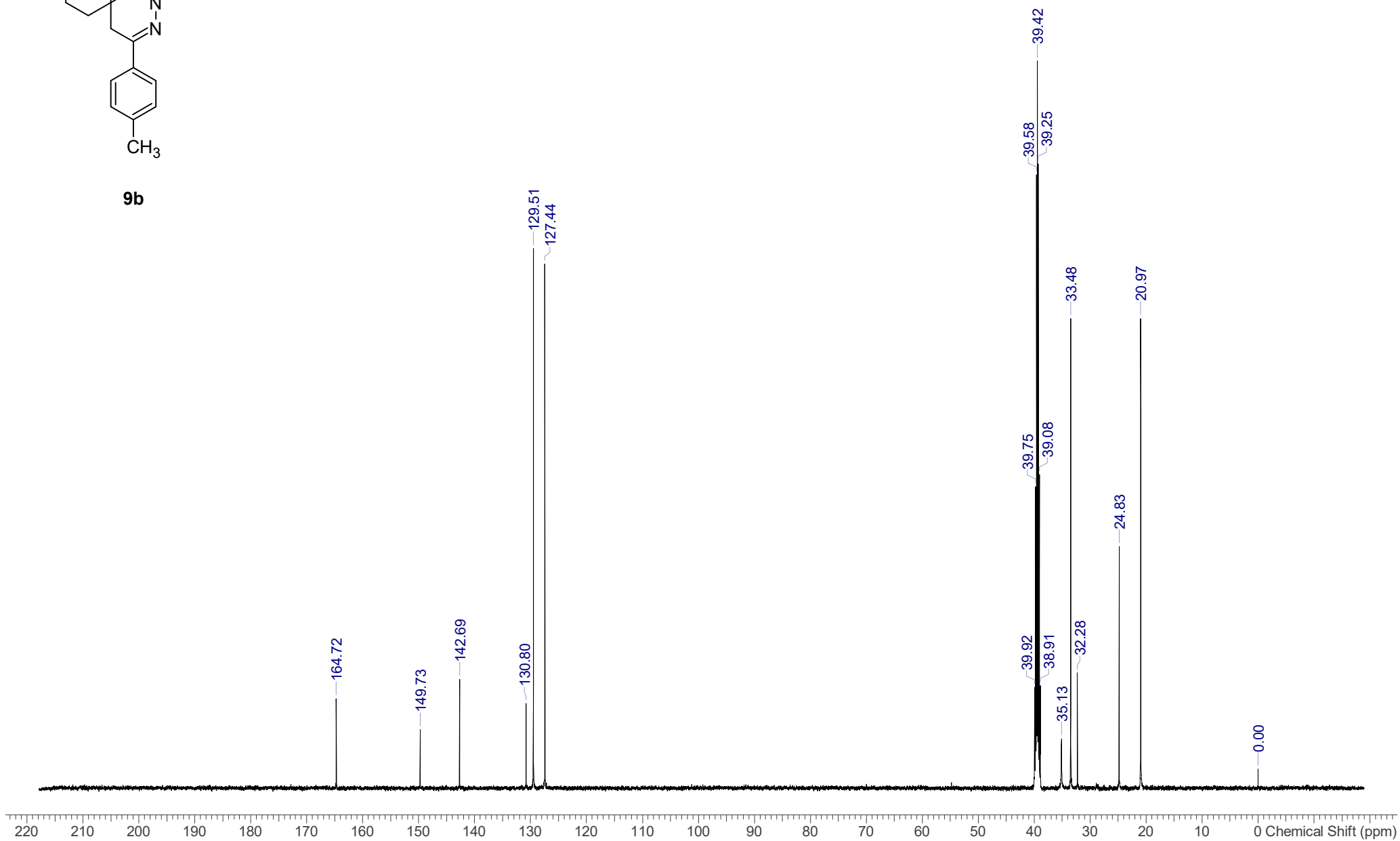
0.00



<sup>13</sup>C NMR (125.7 MHz; DMSO-d<sub>6</sub>)



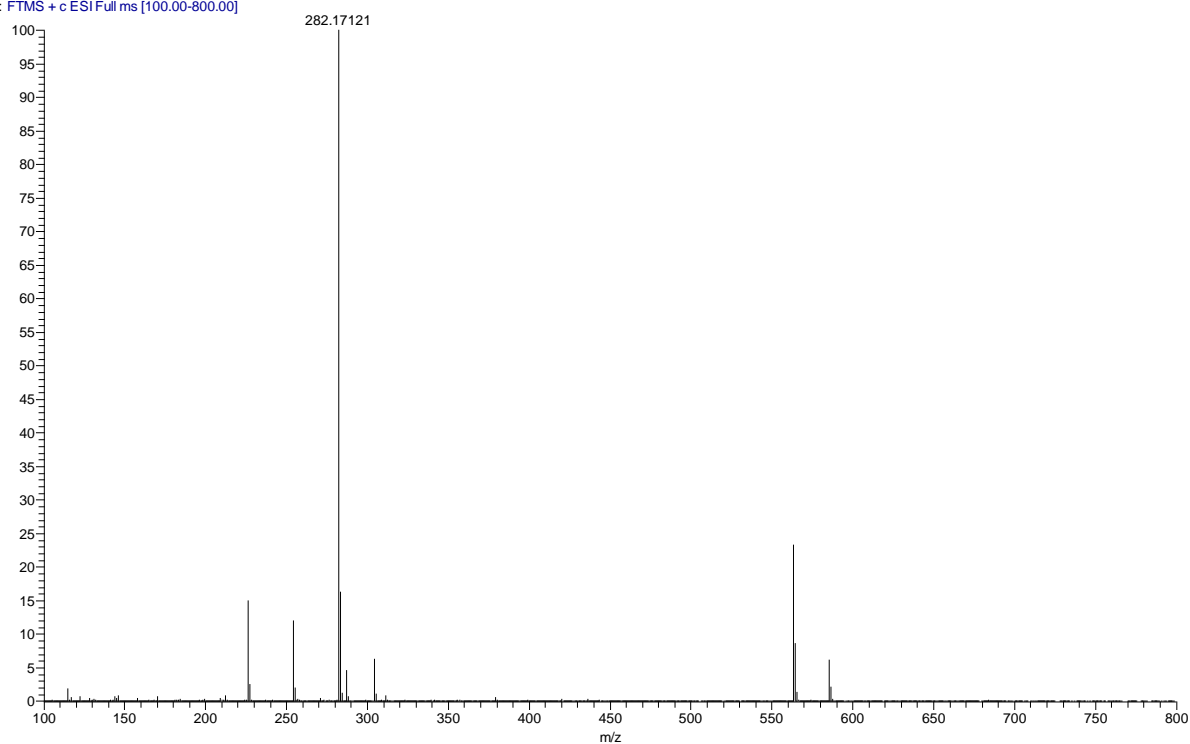
**9b**



# Compound 9b

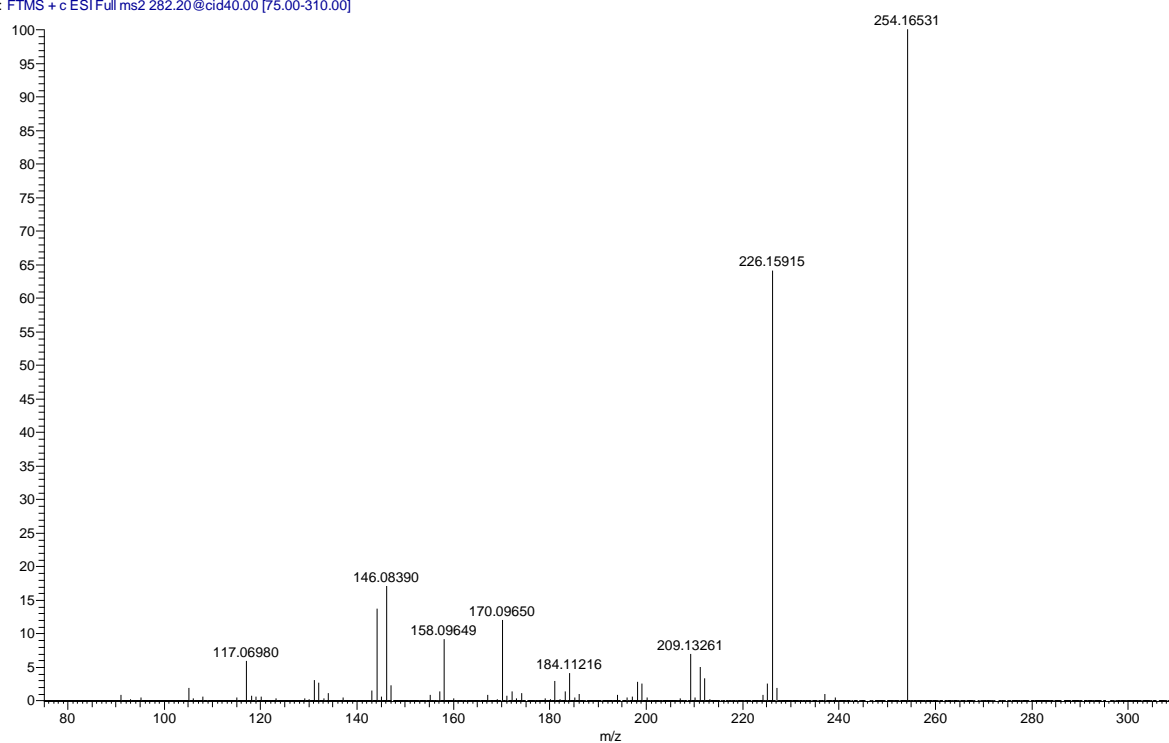
## HRMS spectrum (ESI)

ku74012\_sfc-223\_d\_ve6277 #1-50 RT: 0.00-0.20 AV: 50 NL: 7.65E7  
T: FTMS + c ESI Full ms [100.00-800.00]



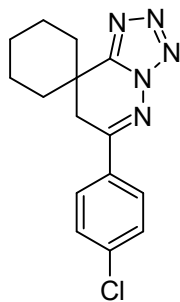
## HRMS spectrum (ESI daughter ion)

ku74012\_sfc-223\_d\_ve6278 #1-47 RT: 0.00-0.20 AV: 47 NL: 3.94E7  
T: FTMS + c ESI Full ms2 282.20@cid40.00 [75.00-310.00]



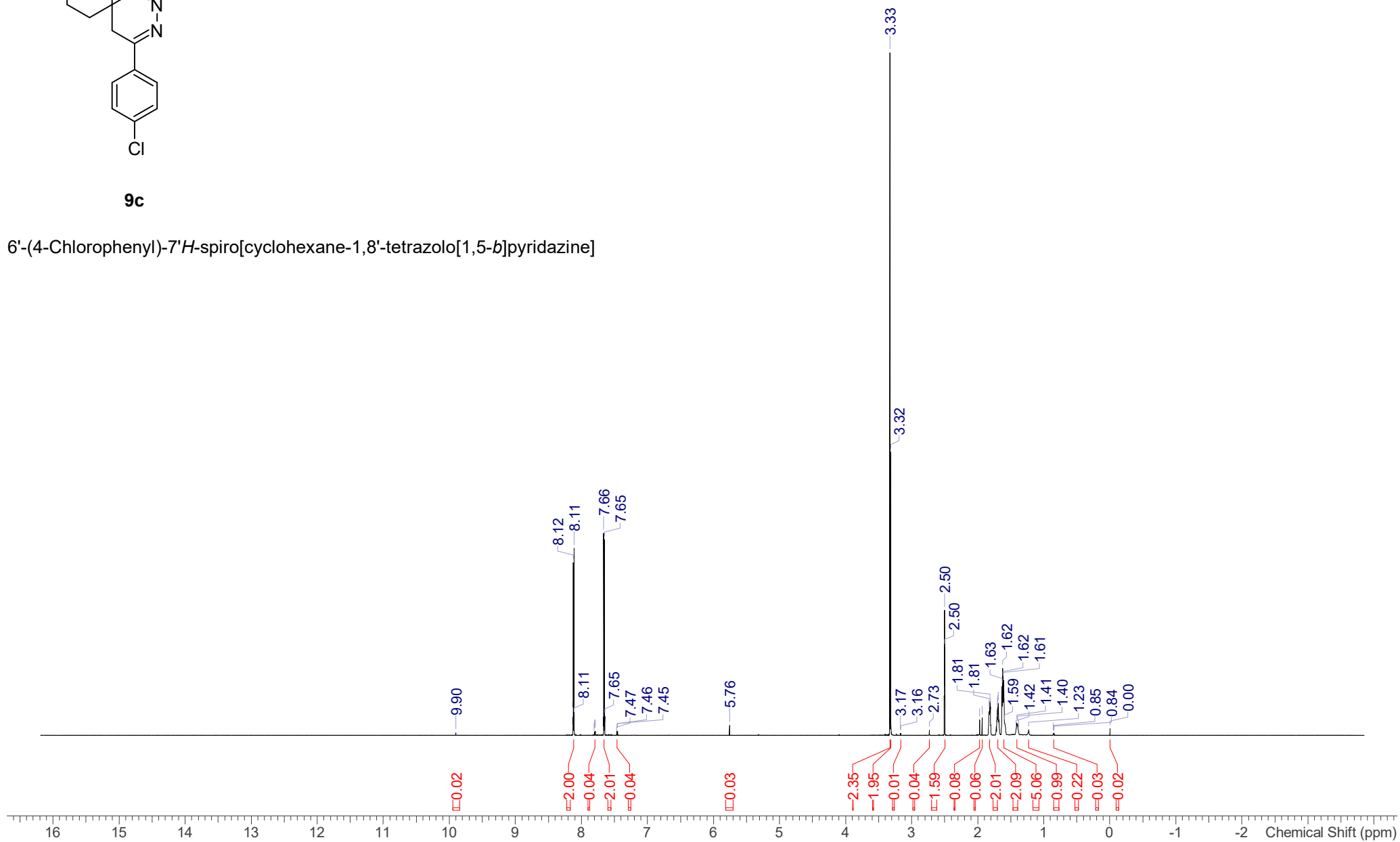


<sup>1</sup>H NMR (499.9 MHz; DMSO-d<sub>6</sub>)

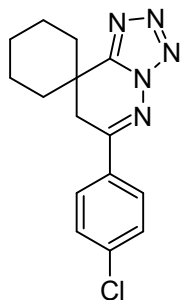


**9c**

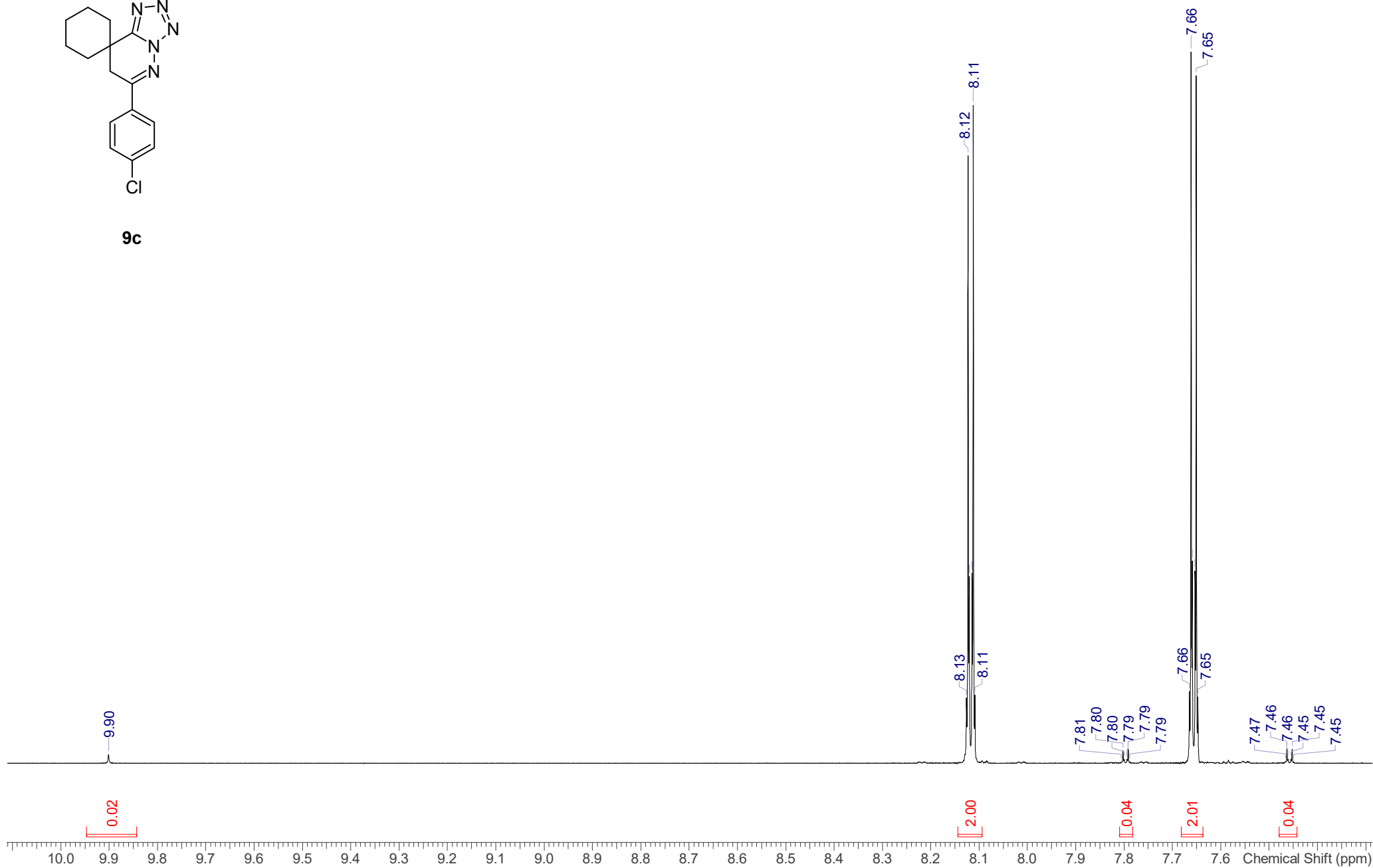
6'-(4-Chlorophenyl)-7'*H*-spiro[cyclohexane-1,8'-tetrazolo[1,5-*b*]pyridazine]



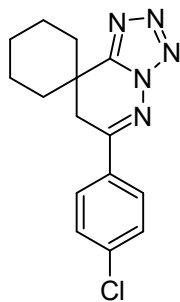
<sup>1</sup>H NMR (499.9 MHz; DMSO-d<sub>6</sub>)



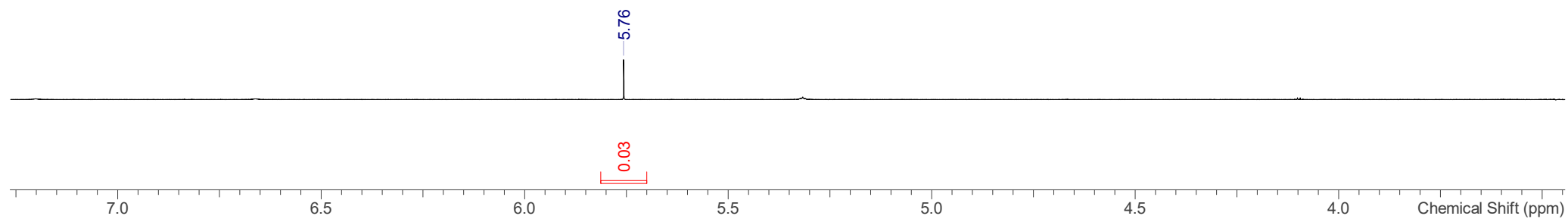
**9c**



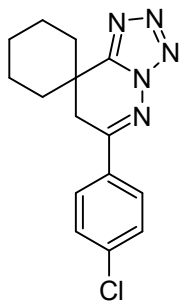
$^1\text{H}$  NMR (499.9 MHz;  $\text{DMSO}-d_6$ )



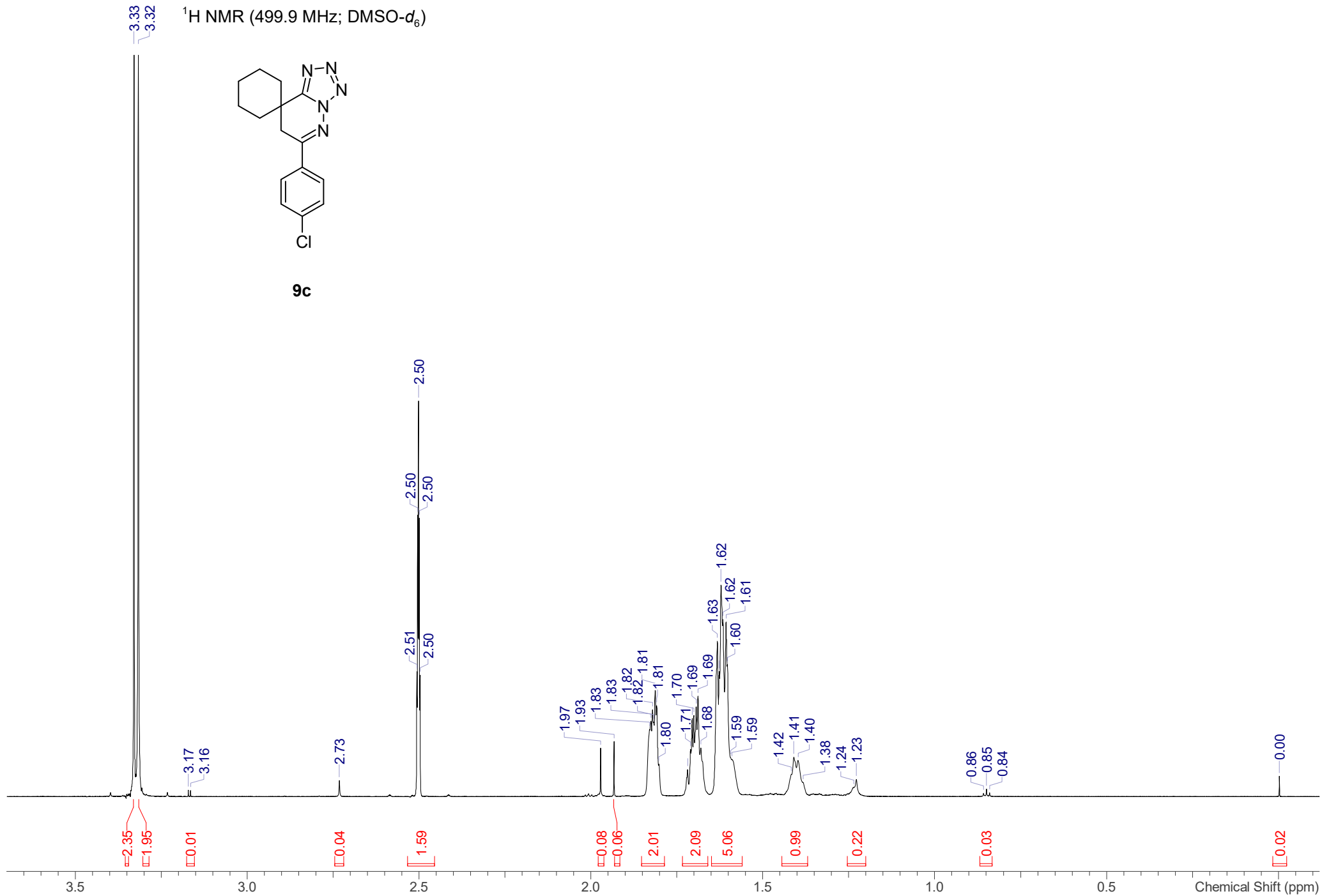
**9c**



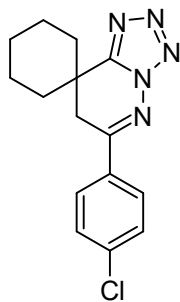
<sup>1</sup>H NMR (499.9 MHz; DMSO-d<sub>6</sub>)



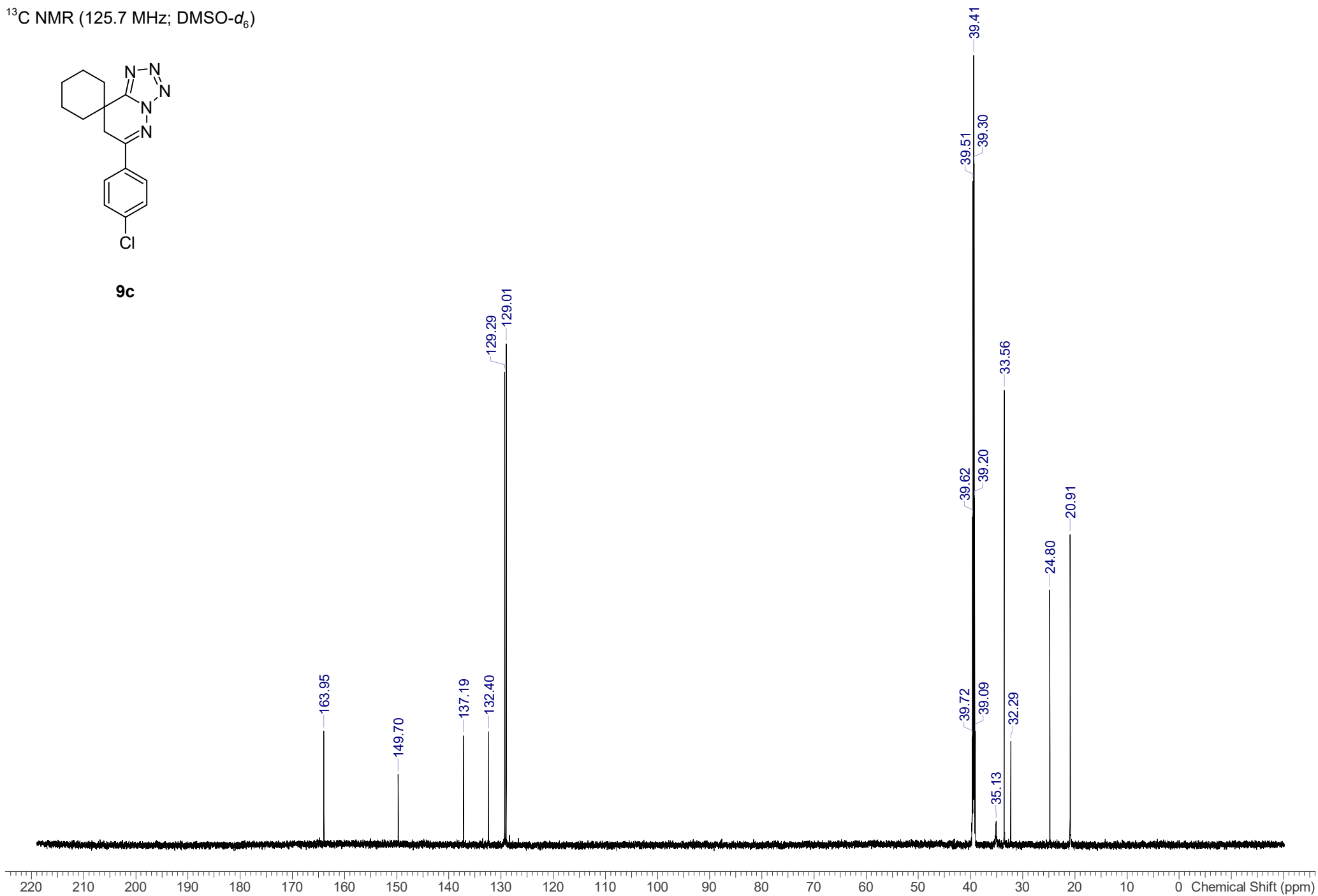
**9c**



$^{13}\text{C}$  NMR (125.7 MHz;  $\text{DMSO-}d_6$ )



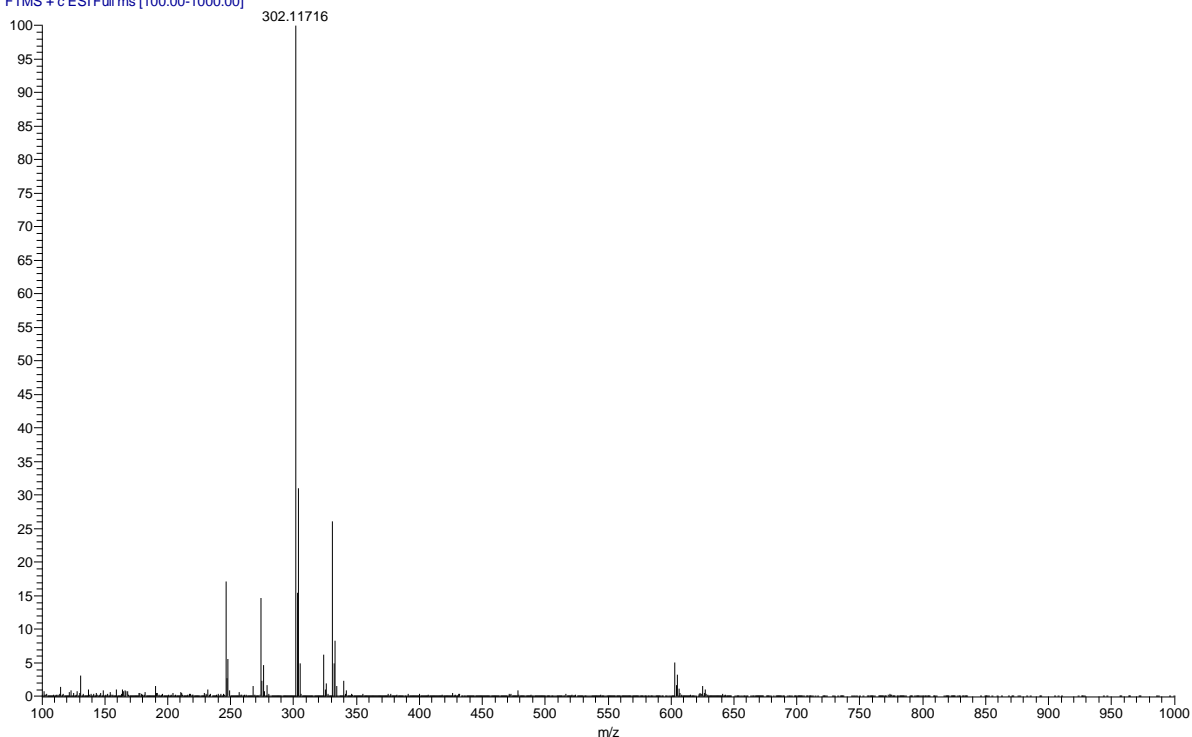
**9c**



# Compound 9c

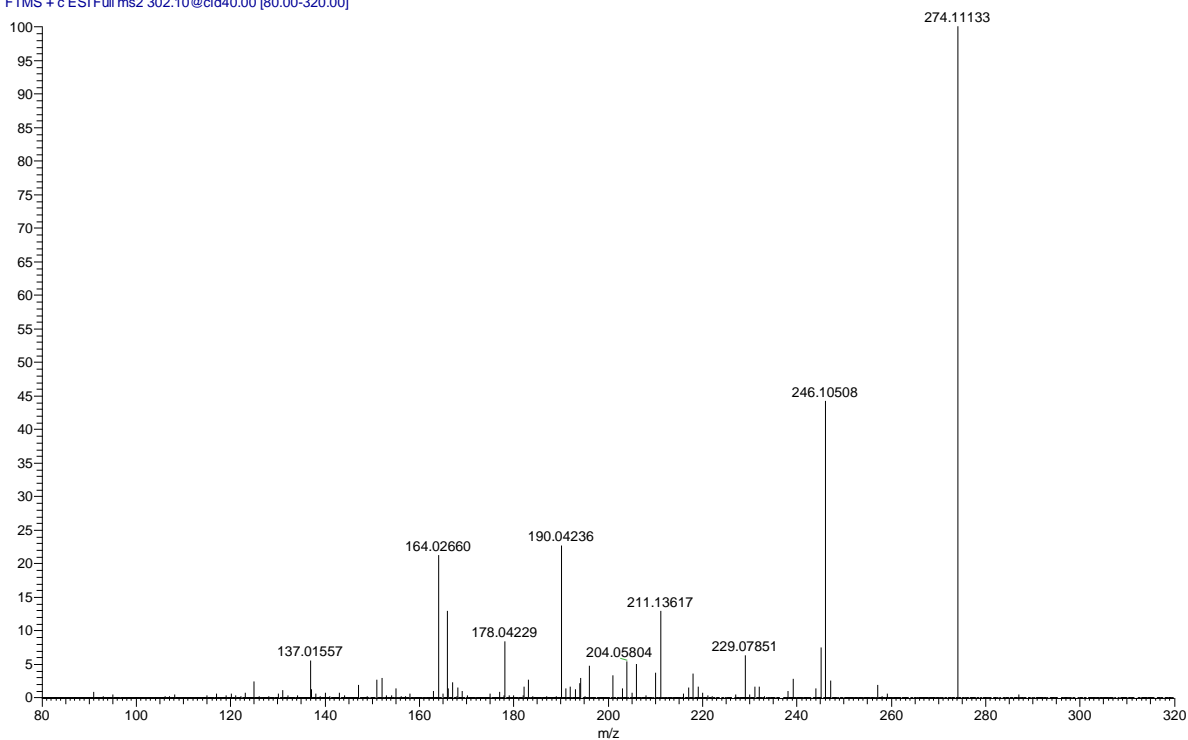
## HRMS spectrum (ESI)

ku71598\_sfc-185\_d\_ve4465 #1-25 RT: 0.00-0.20 AV: 25 NL: 3.12E7  
T: FTMS + c ESI Full ms [100.00-1000.00]

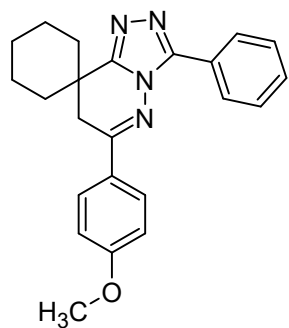


## HRMS spectrum (ESI daughter ion)

ku71598\_sfc-185\_d\_ve4466 #1-46 RT: 0.00-0.20 AV: 46 NL: 1.72E7  
T: FTMS + c ESI Full ms2 302.10@cid40.00 [80.00-320.00]

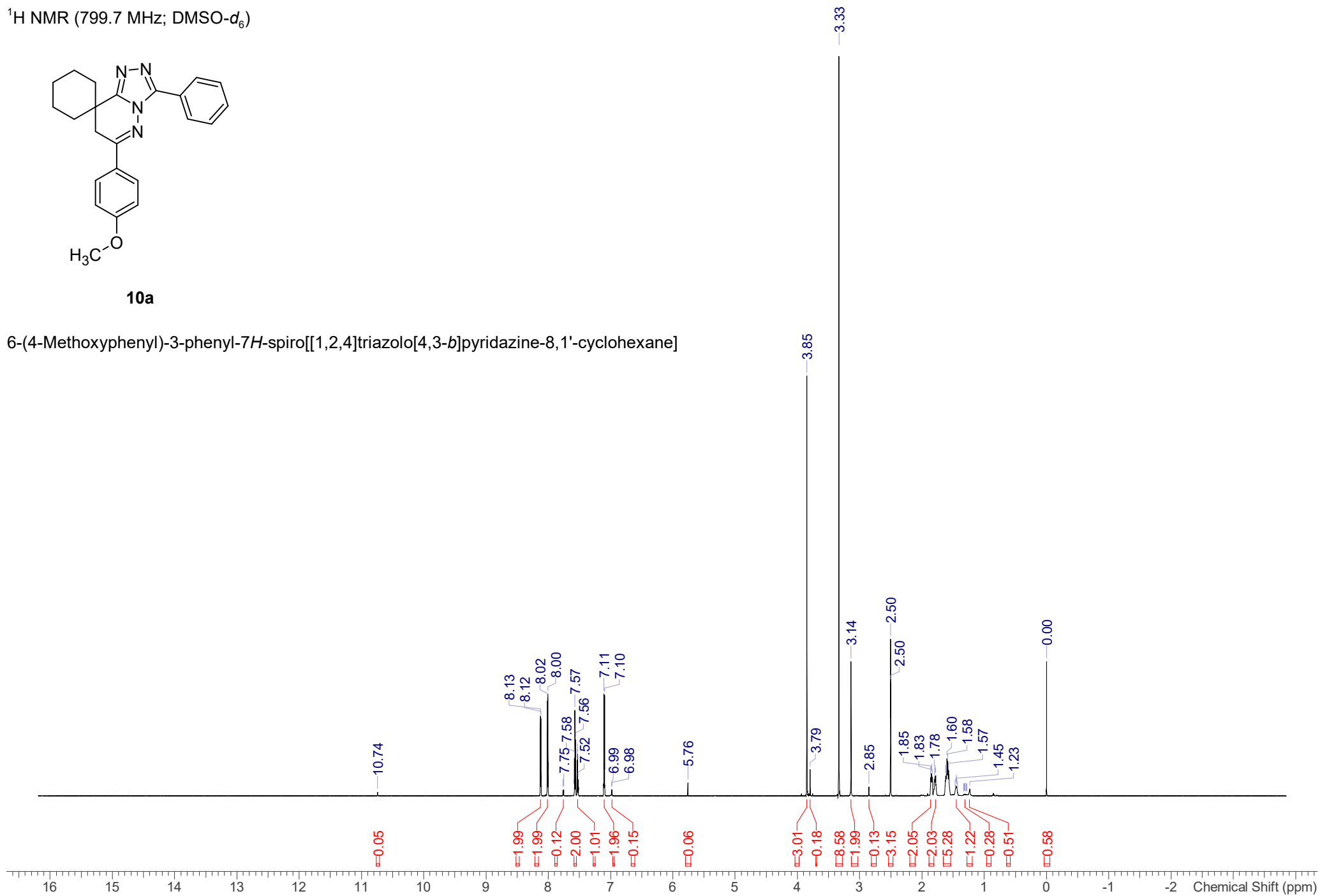


<sup>1</sup>H NMR (799.7 MHz; DMSO-d<sub>6</sub>)

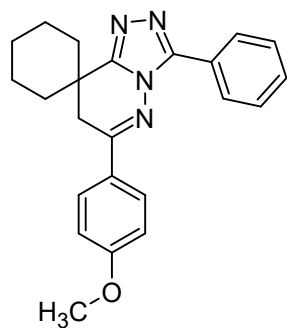


**10a**

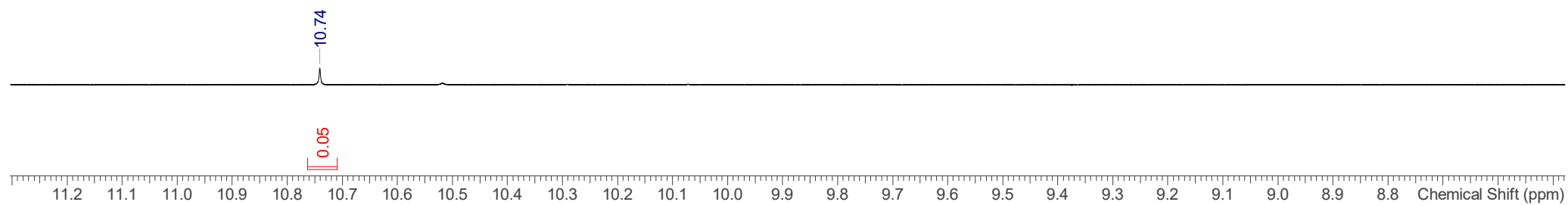
6-(4-Methoxyphenyl)-3-phenyl-7H-spiro[[1,2,4]triazolo[4,3-b]pyridazine-8,1'-cyclohexane]



<sup>1</sup>H NMR (799.7 MHz; DMSO-*d*<sub>6</sub>)

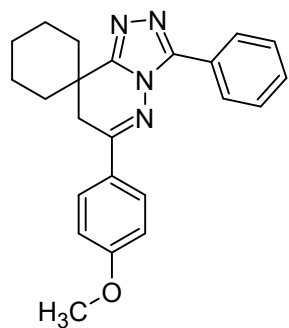


**10a**

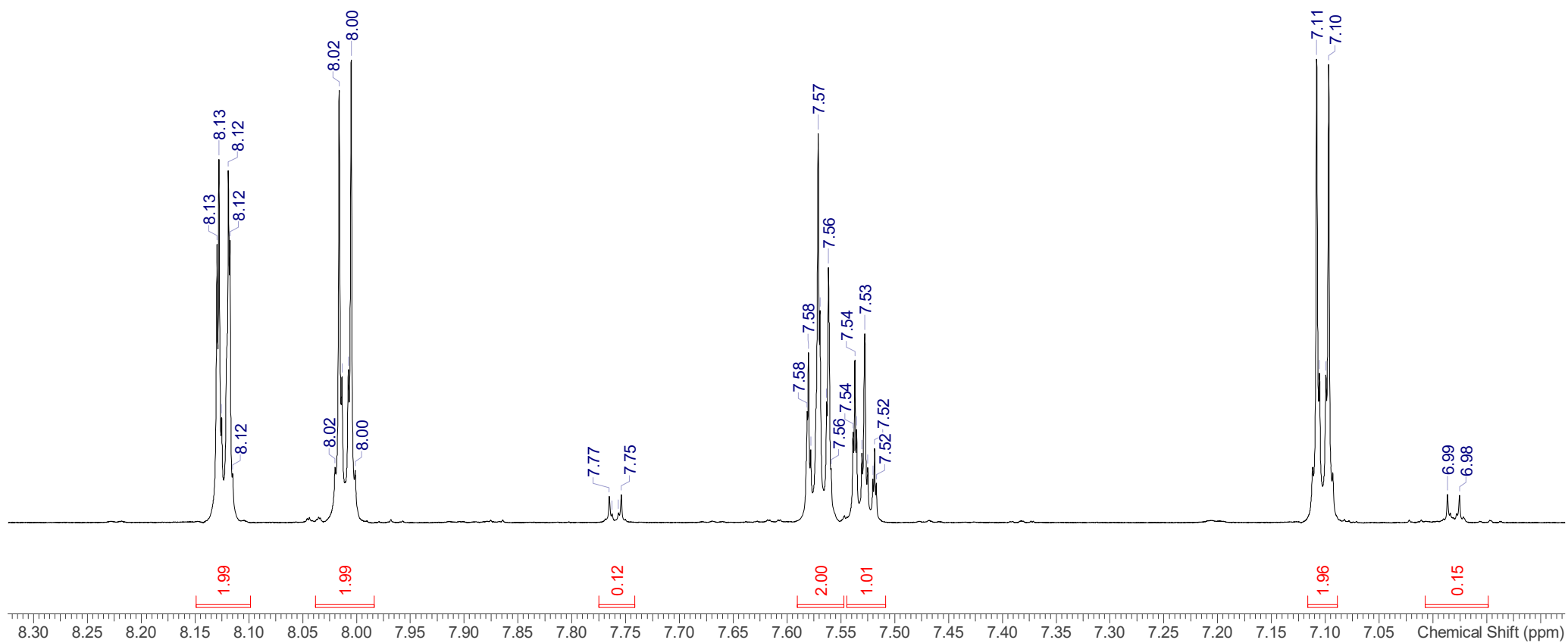




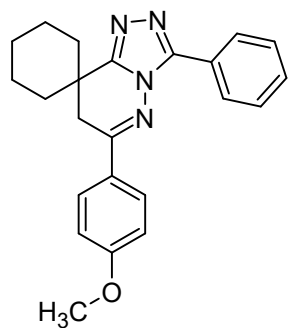
<sup>1</sup>H NMR (799.7 MHz; DMSO-d<sub>6</sub>)



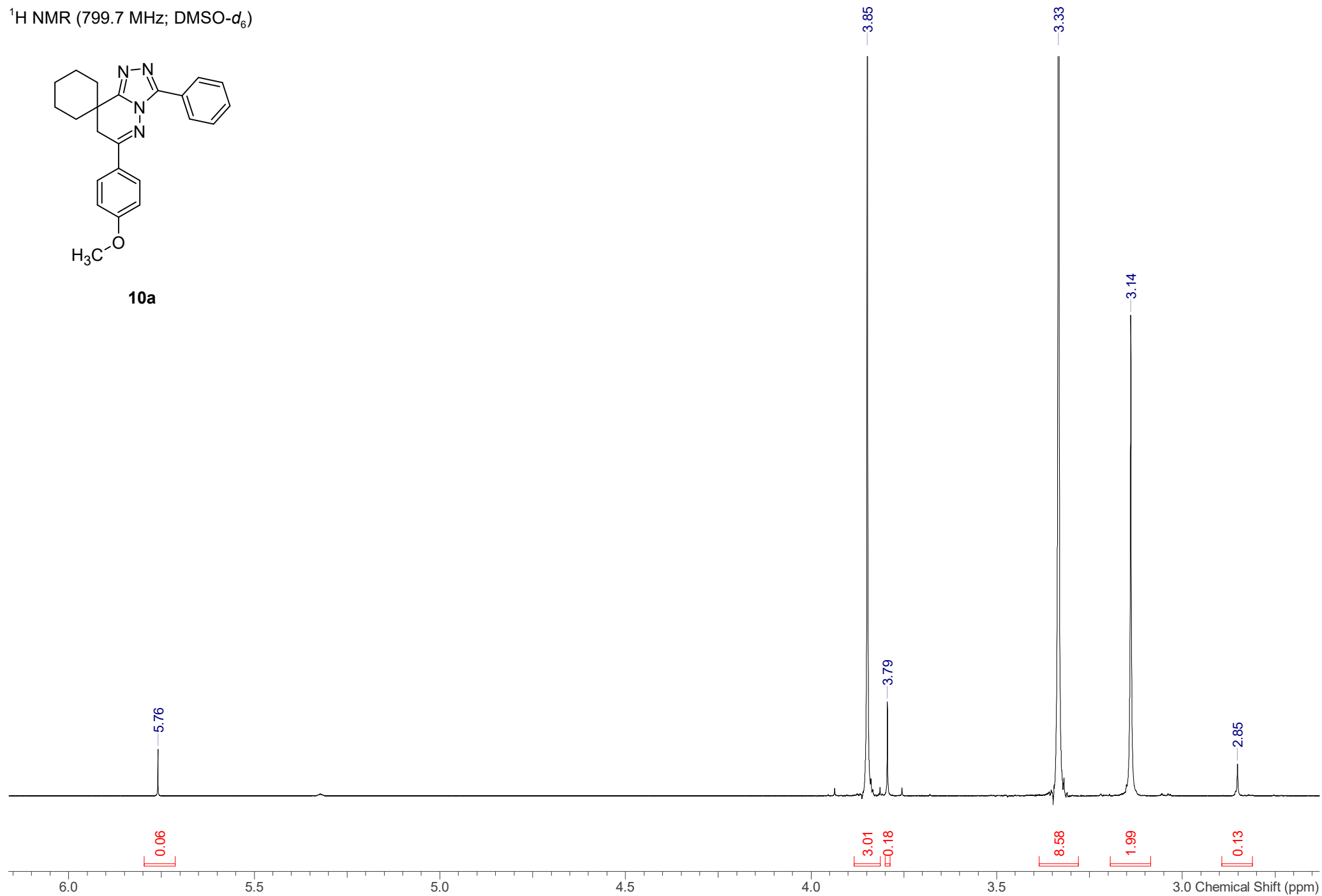
**10a**



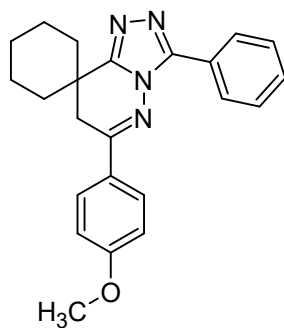
<sup>1</sup>H NMR (799.7 MHz; DMSO-d<sub>6</sub>)



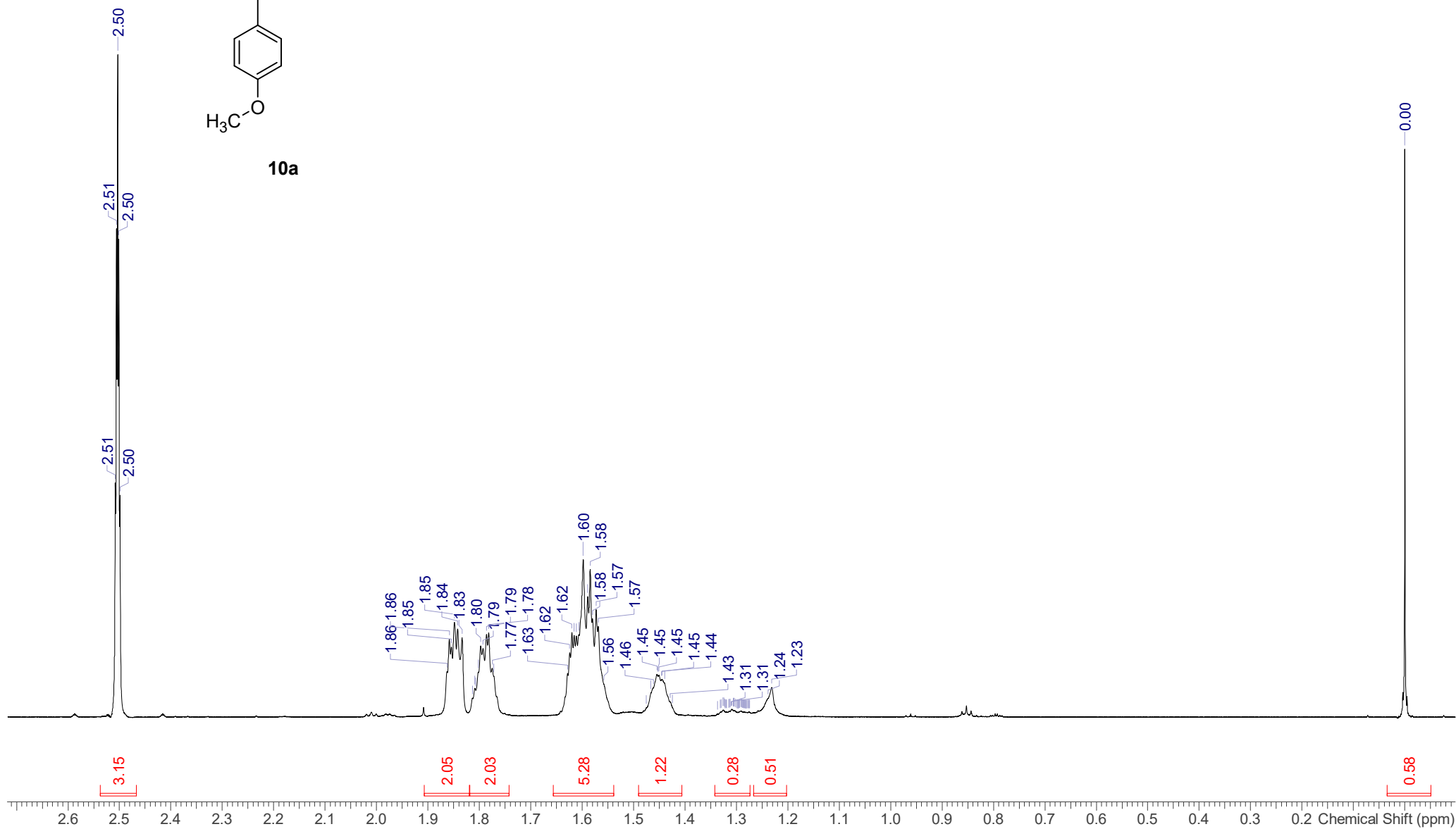
10a



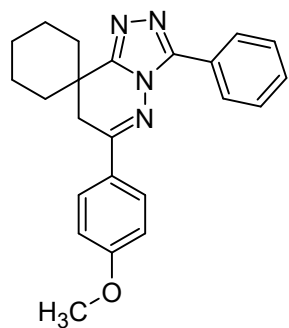
<sup>1</sup>H NMR (799.7 MHz; DMSO-d<sub>6</sub>)



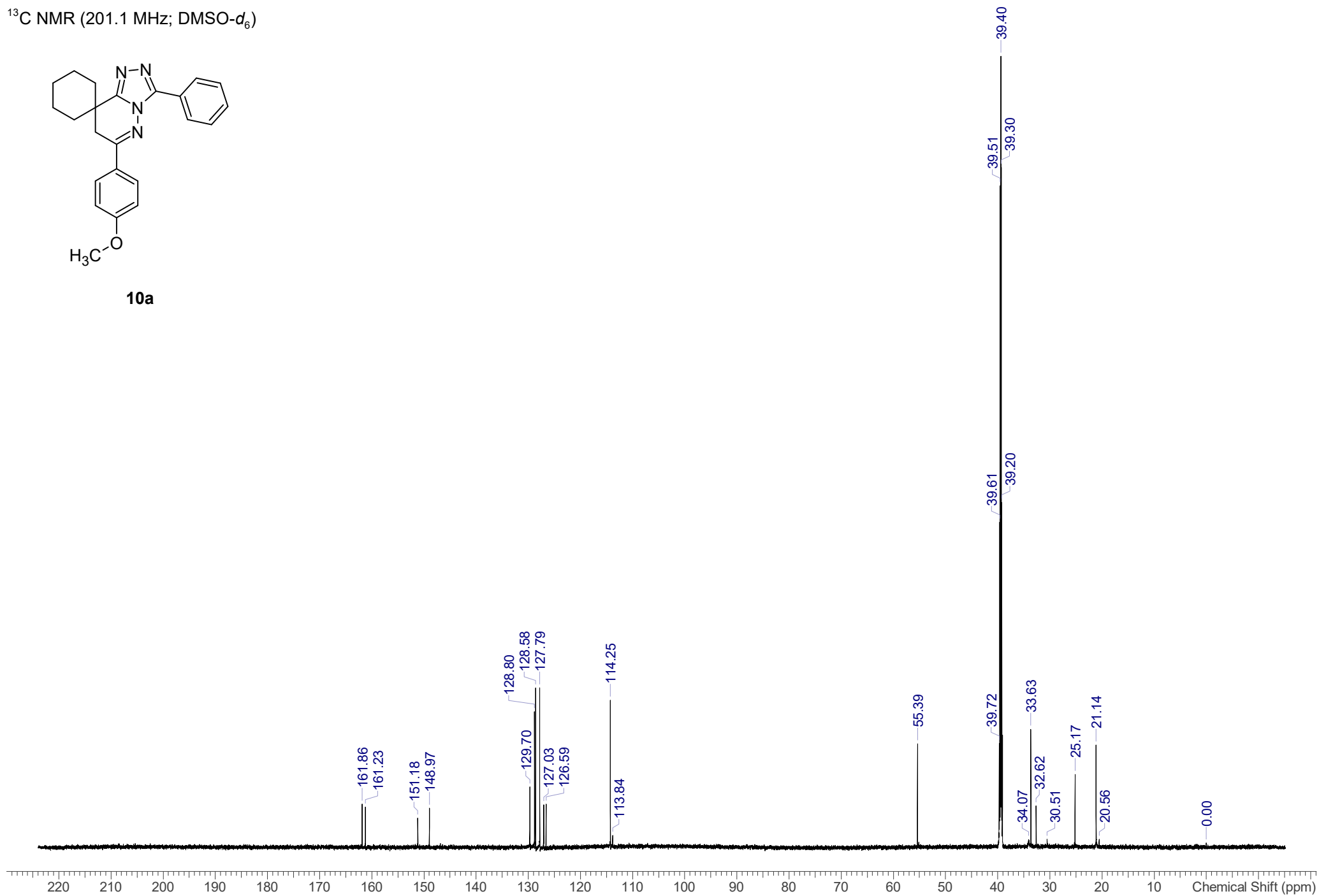
10a



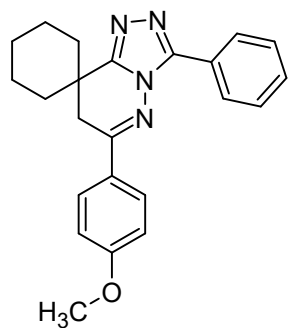
$^{13}\text{C}$  NMR (201.1 MHz;  $\text{DMSO-}d_6$ )



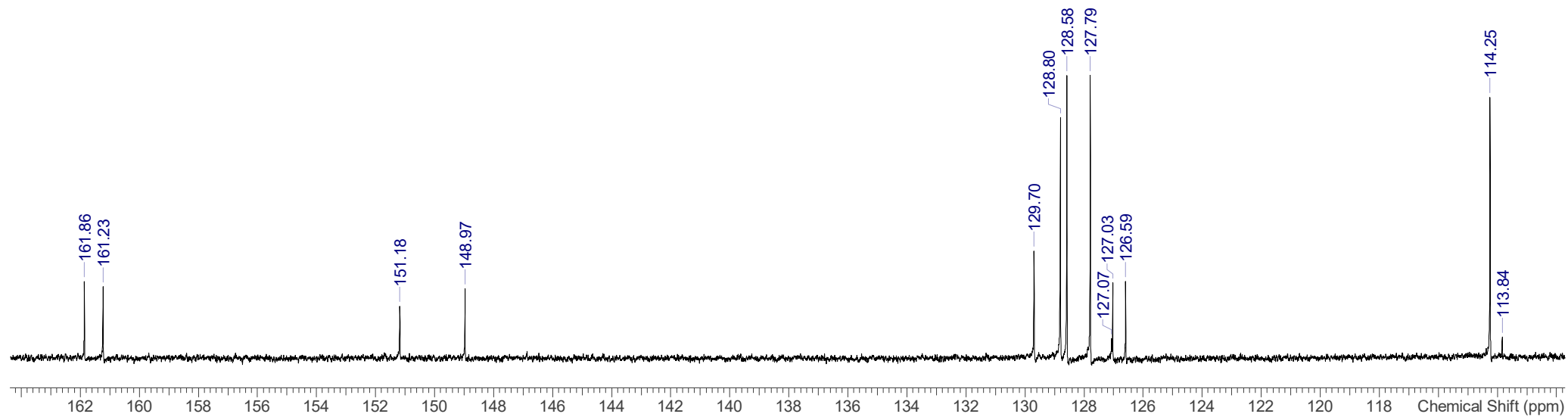
**10a**



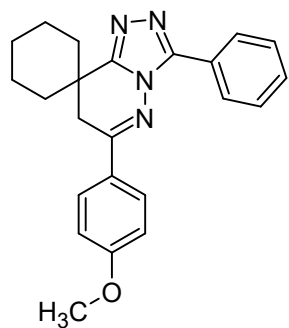
<sup>13</sup>C NMR (201.1 MHz; DMSO-*d*<sub>6</sub>)



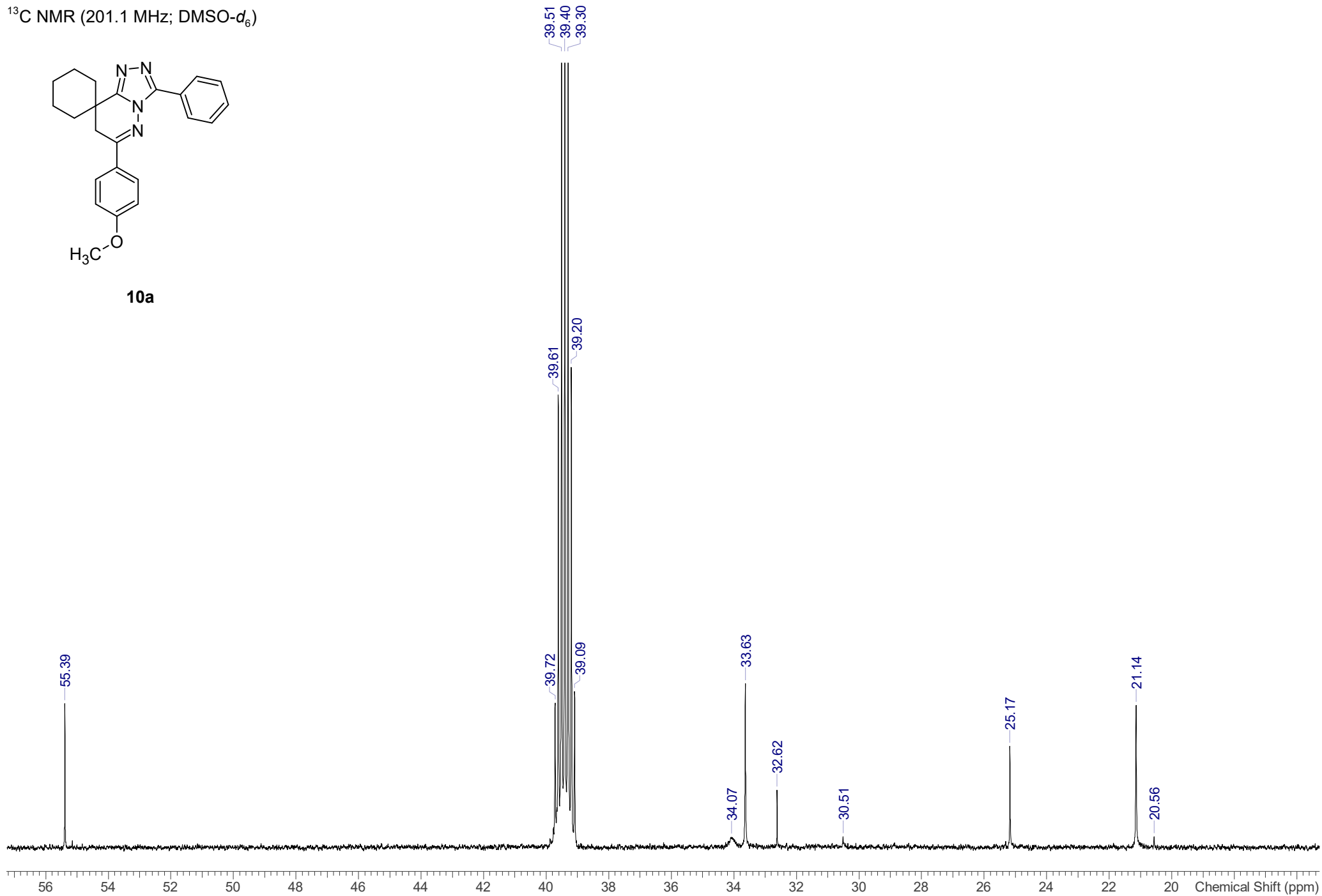
**10a**



$^{13}\text{C}$  NMR (201.1 MHz;  $\text{DMSO-}d_6$ )



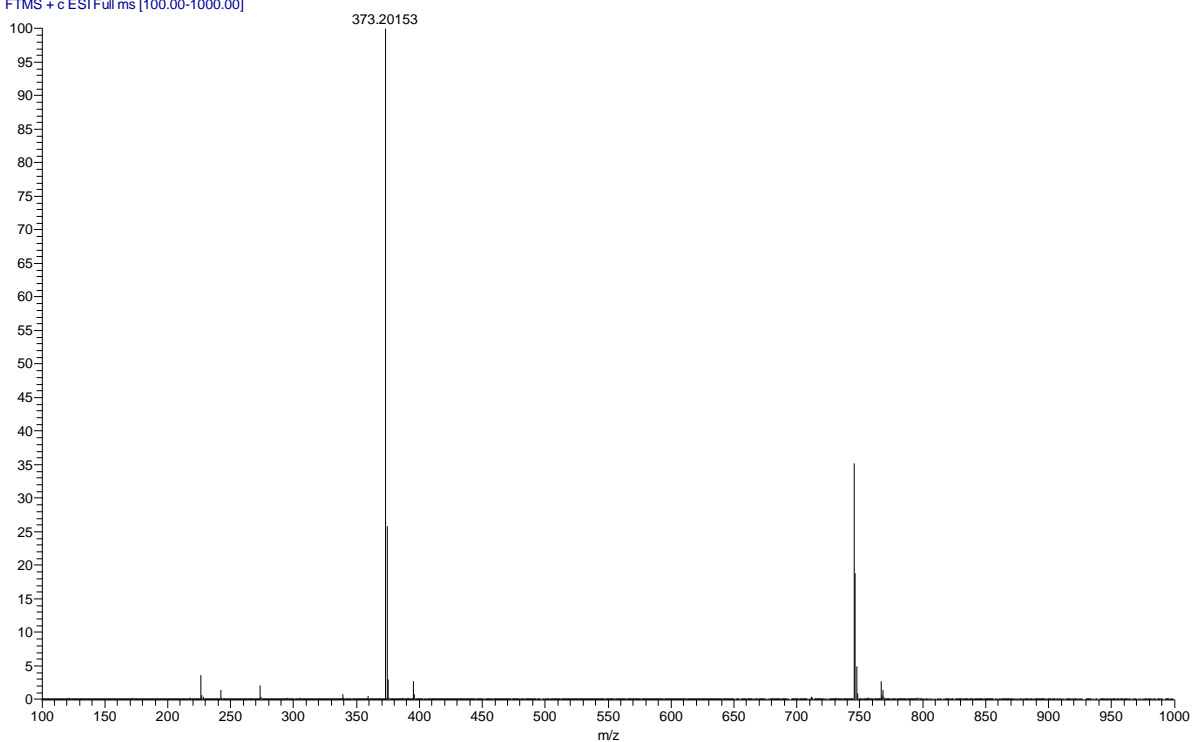
**10a**



# Compound 10a

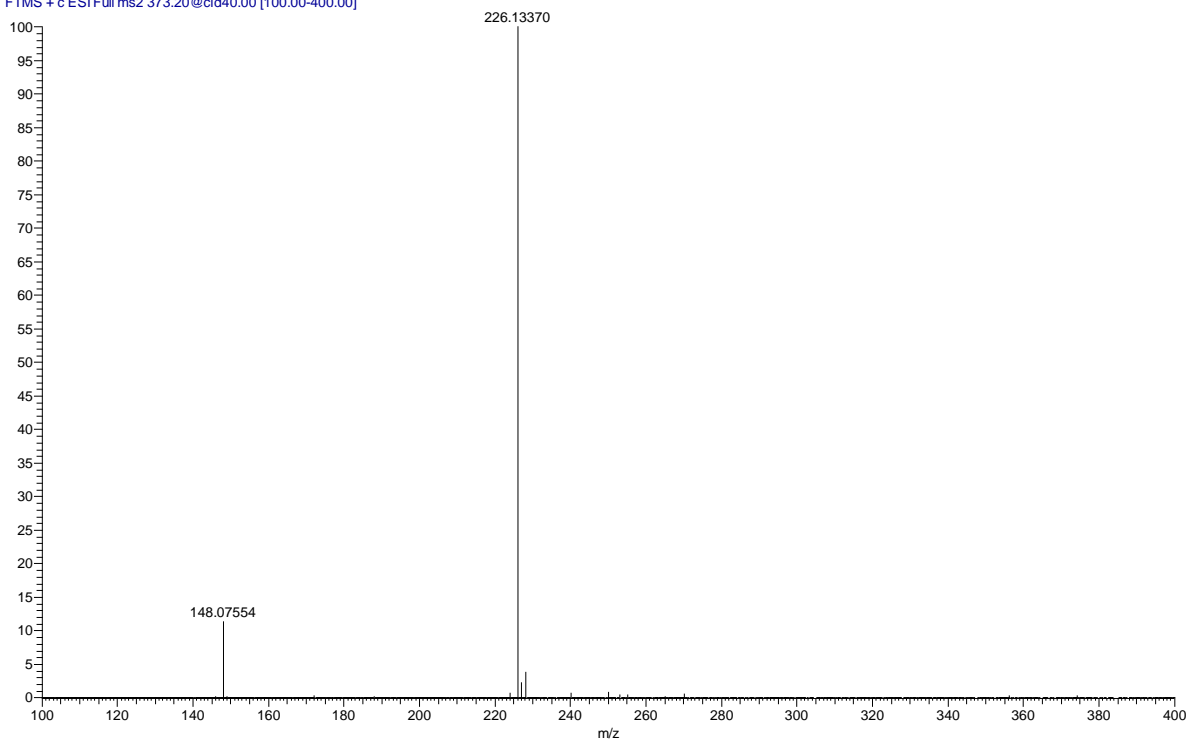
## HRMS spectrum (ESI)

ku73635\_sfc-209-2\_d\_ve5902 #1-51 RT: 0.00-0.20 AV: 51 NL: 1.62E8  
T: FTMS + c ESI Full ms [100.00-1000.00]

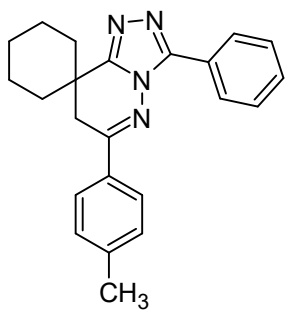


## HRMS spectrum (ESI daughter ion)

ku73635\_sfc-209-2\_d\_ve5903 #1-47 RT: 0.00-0.20 AV: 47 NL: 9.24E7  
T: FTMS + c ESI Full ms2 373.20@cid40.00 [100.00-400.00]

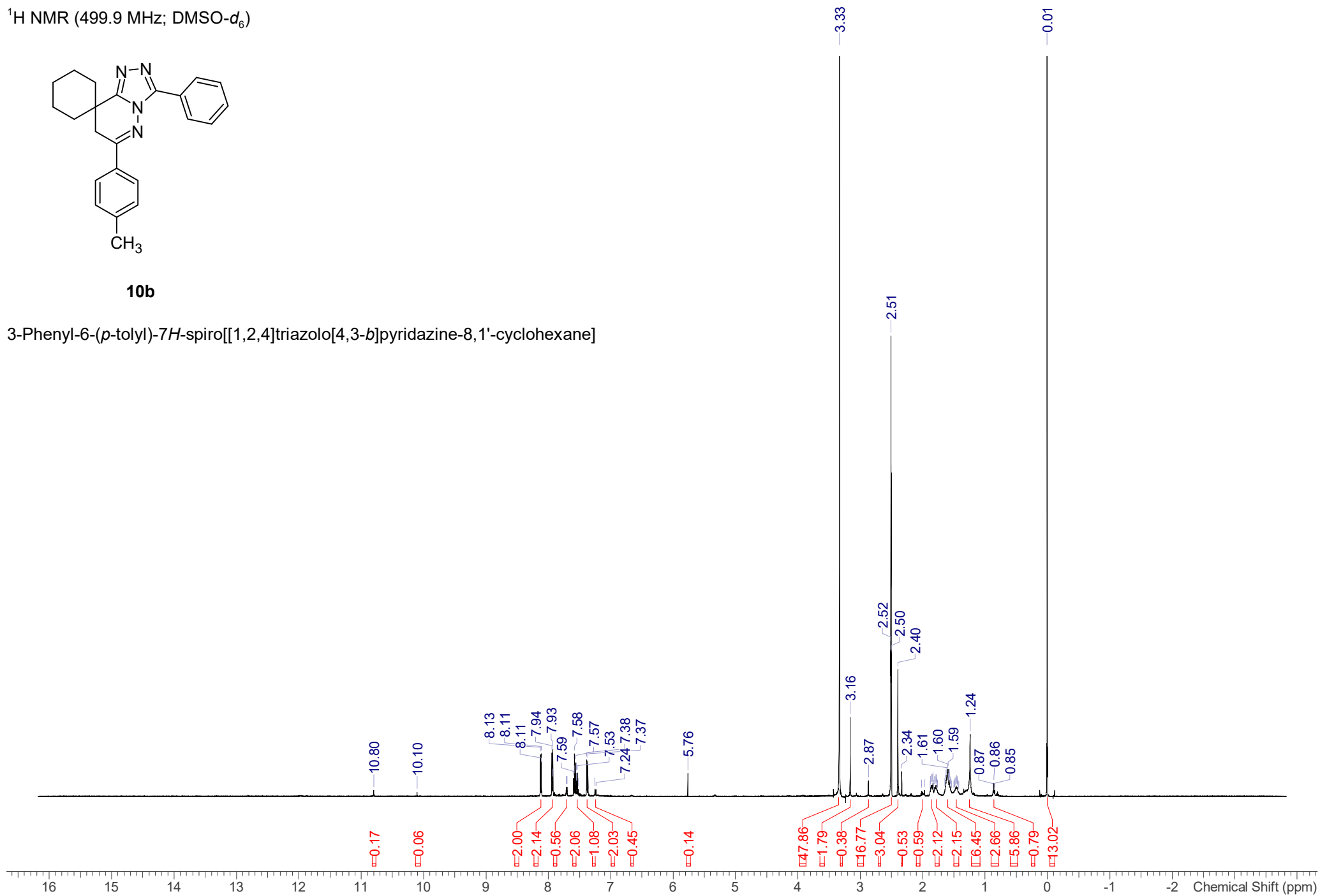


<sup>1</sup>H NMR (499.9 MHz; DMSO-d<sub>6</sub>)



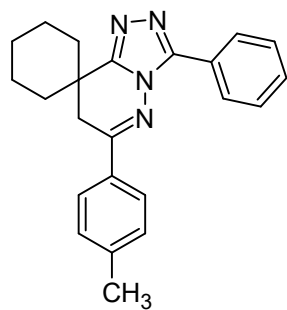
**10b**

3-Phenyl-6-(*p*-tolyl)-7*H*-spiro[[1,2,4]triazolo[4,3-*b*]pyridazine-8,1'-cyclohexane]

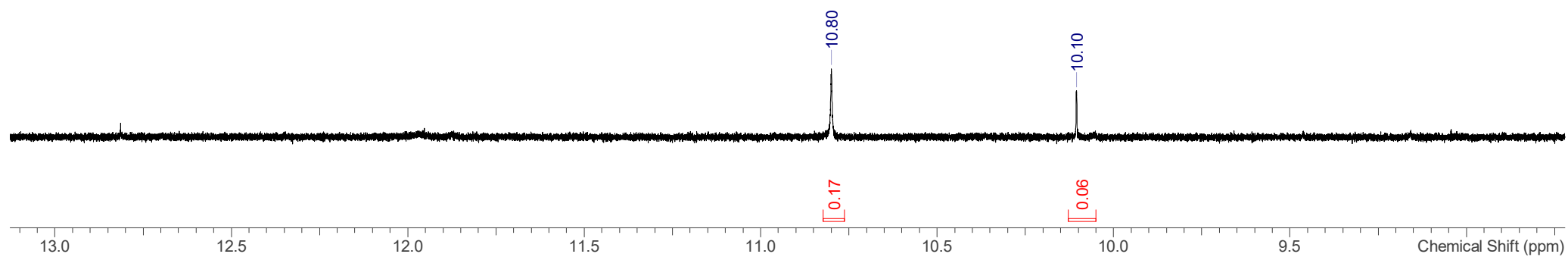




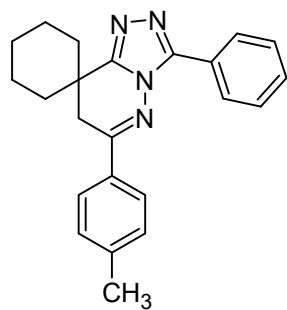
<sup>1</sup>H NMR (499.9 MHz; DMSO-d<sub>6</sub>)



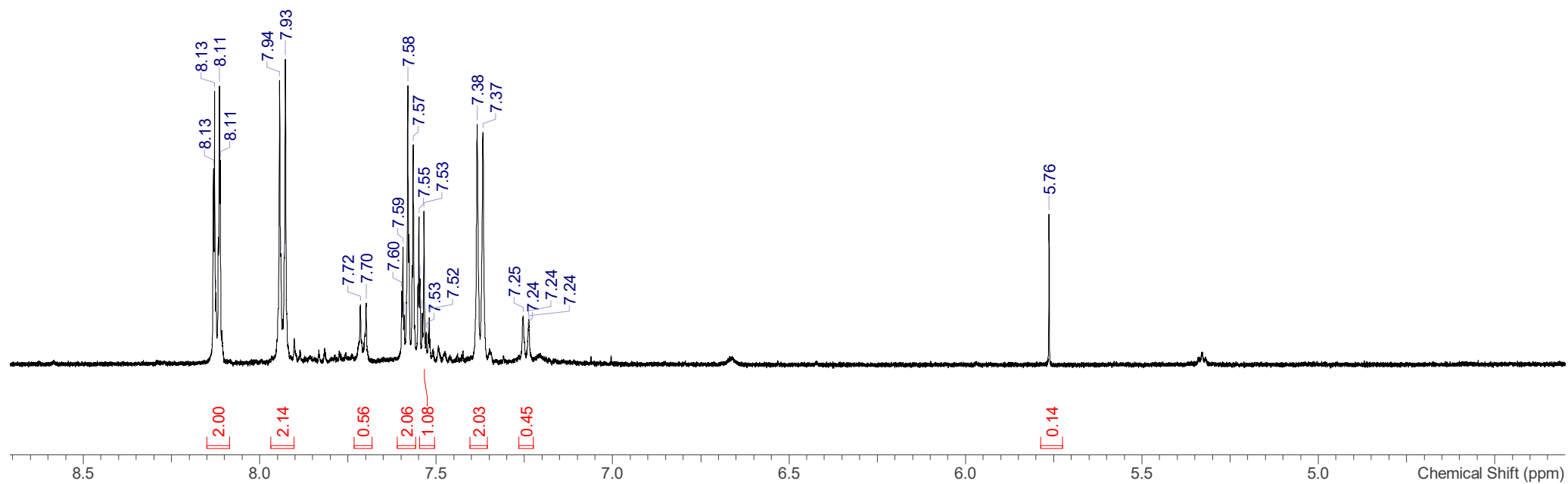
**10b**



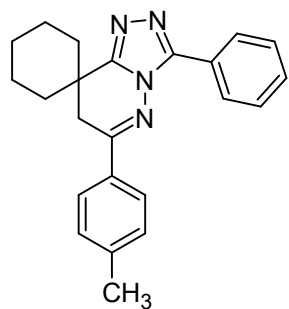
<sup>1</sup>H NMR (499.9 MHz; DMSO-d<sub>6</sub>)



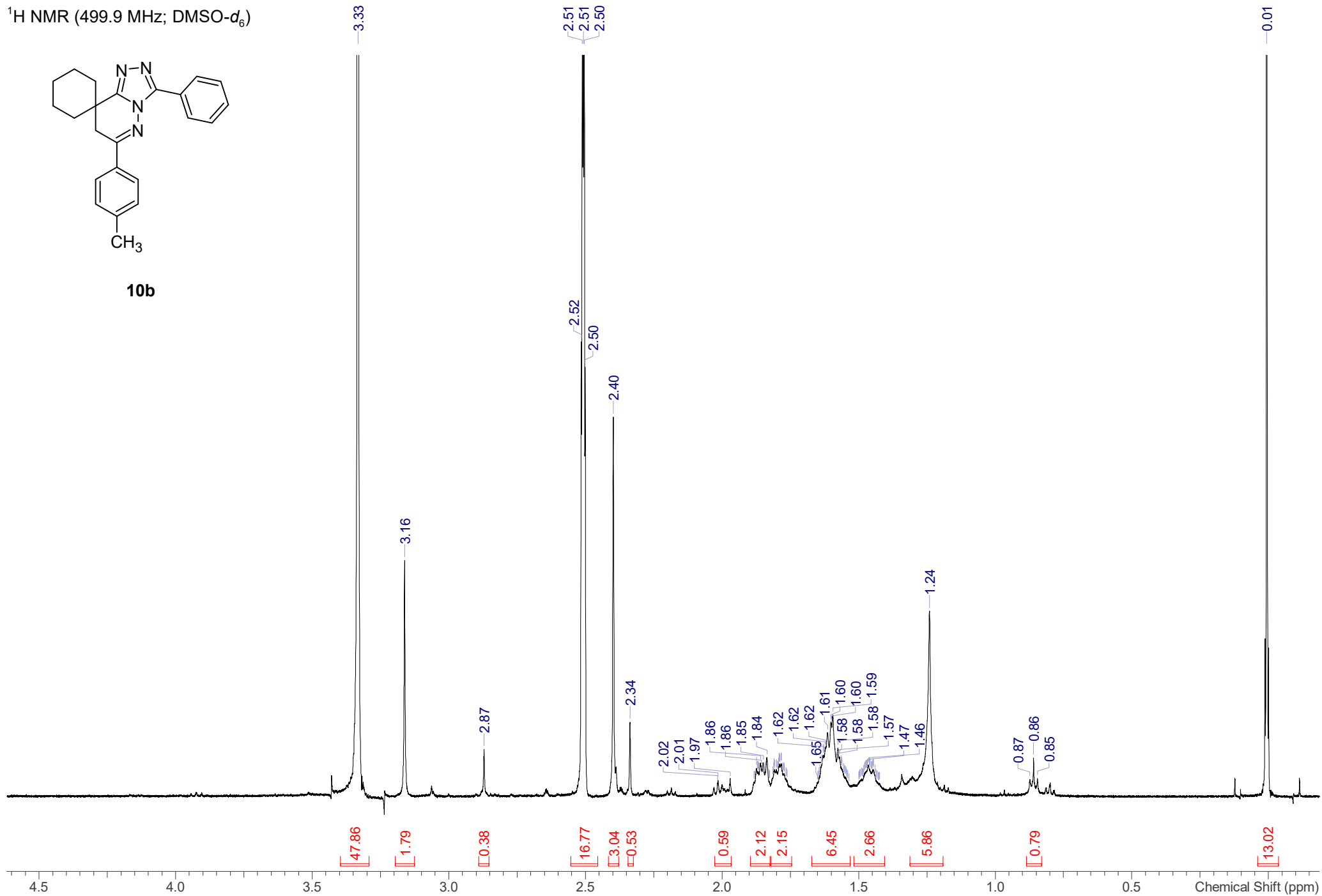
**10b**



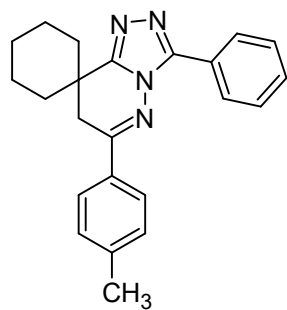
<sup>1</sup>H NMR (499.9 MHz; DMSO-d<sub>6</sub>)



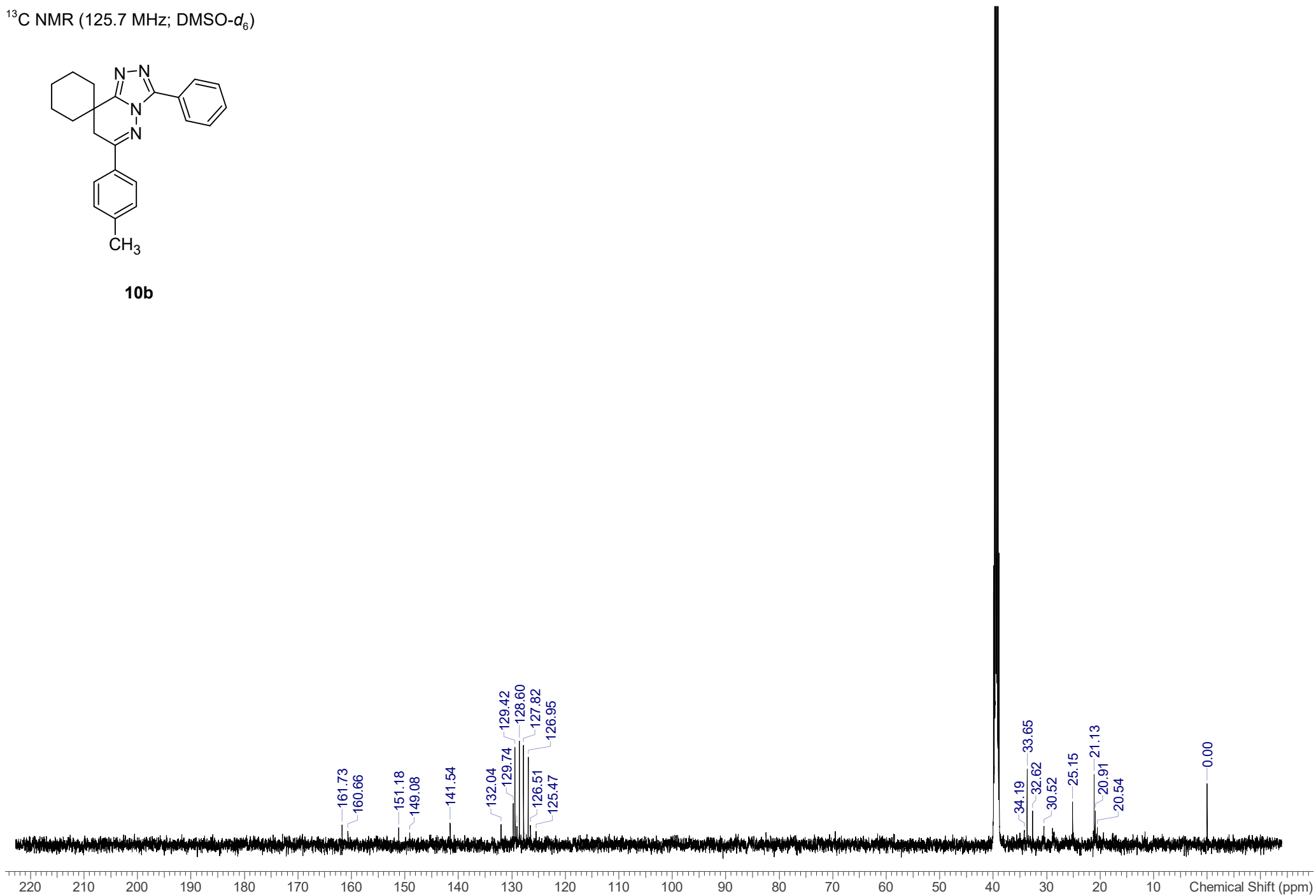
**10b**



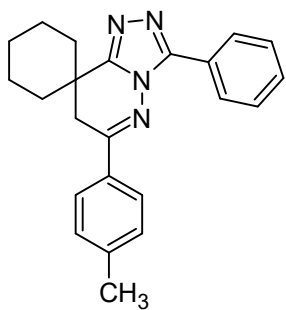
<sup>13</sup>C NMR (125.7 MHz; DMSO-*d*<sub>6</sub>)



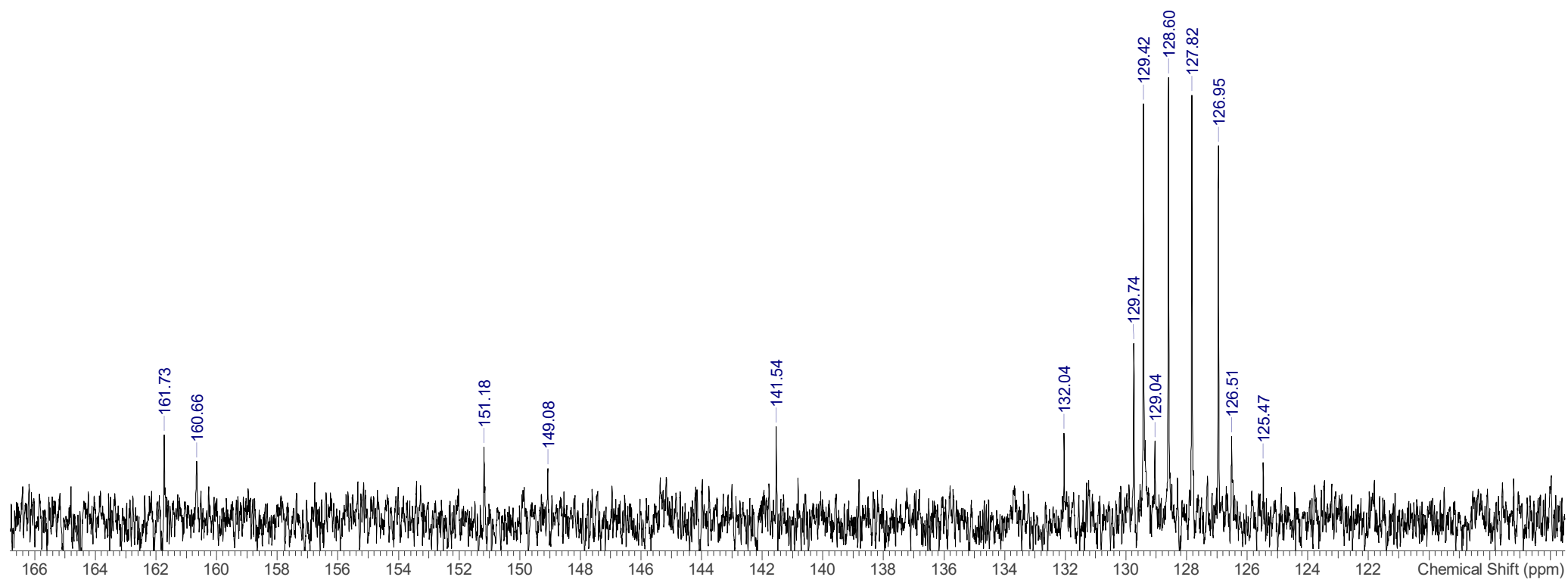
**10b**



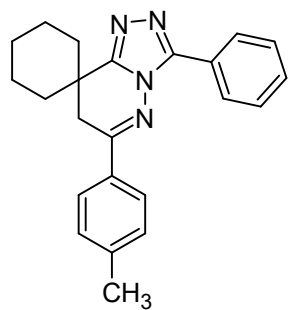
$^{13}\text{C}$  NMR (125.7 MHz;  $\text{DMSO-}d_6$ )



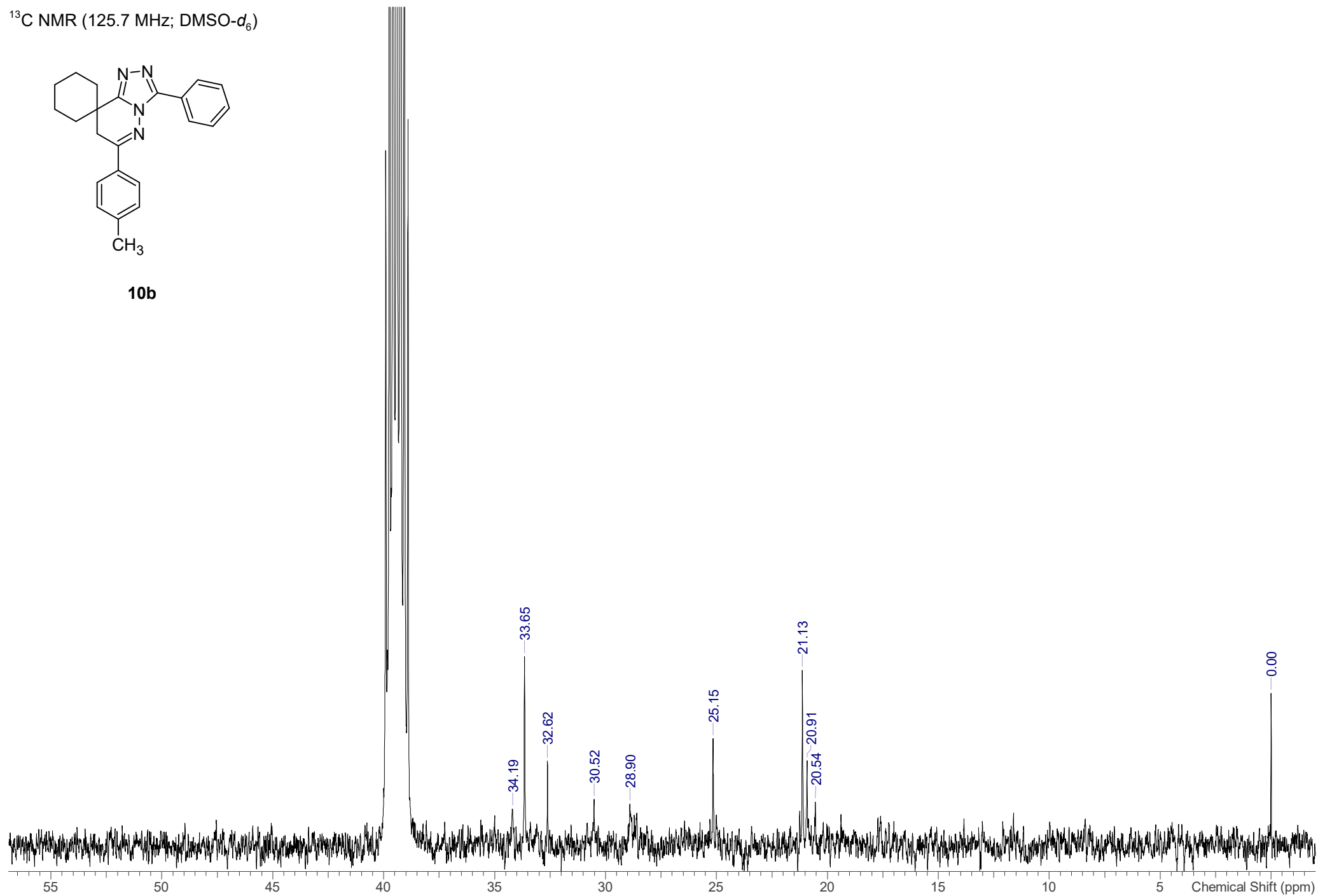
**10b**



$^{13}\text{C}$  NMR (125.7 MHz;  $\text{DMSO-}d_6$ )



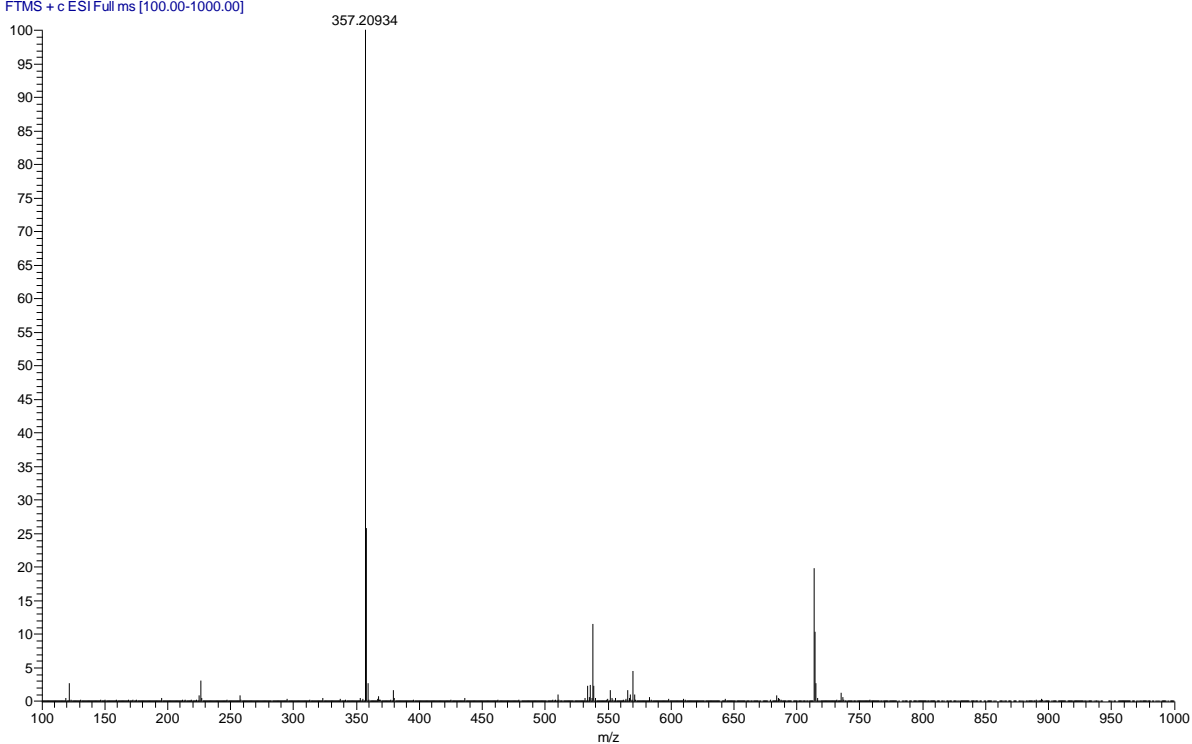
**10b**



# Compound 10b

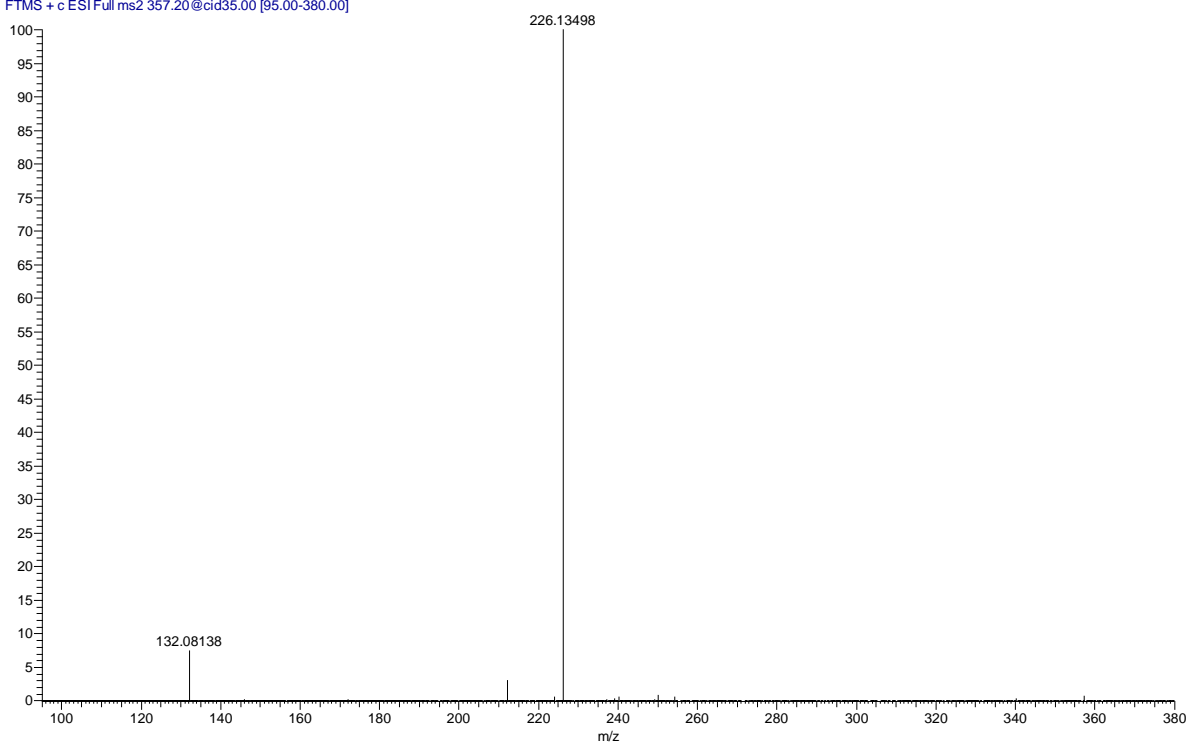
## HRMS spectrum (ESI)

ku73537\_sfc-207\_d\_ve5791 #1-50 RT: 0.00-0.20 AV: 50 NL: 4.03E7  
T: FTMS + c ESI Full ms [100.00-1000.00]

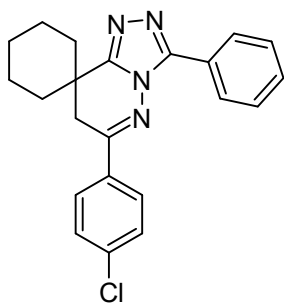


## HRMS spectrum (ESI daughter ion)

ku73537\_sfc-207\_d\_ve5792 #1-47 RT: 0.00-0.20 AV: 47 NL: 3.35E7  
T: FTMS + c ESI Full ms2 357.20@cid35.00 [95.00-380.00]

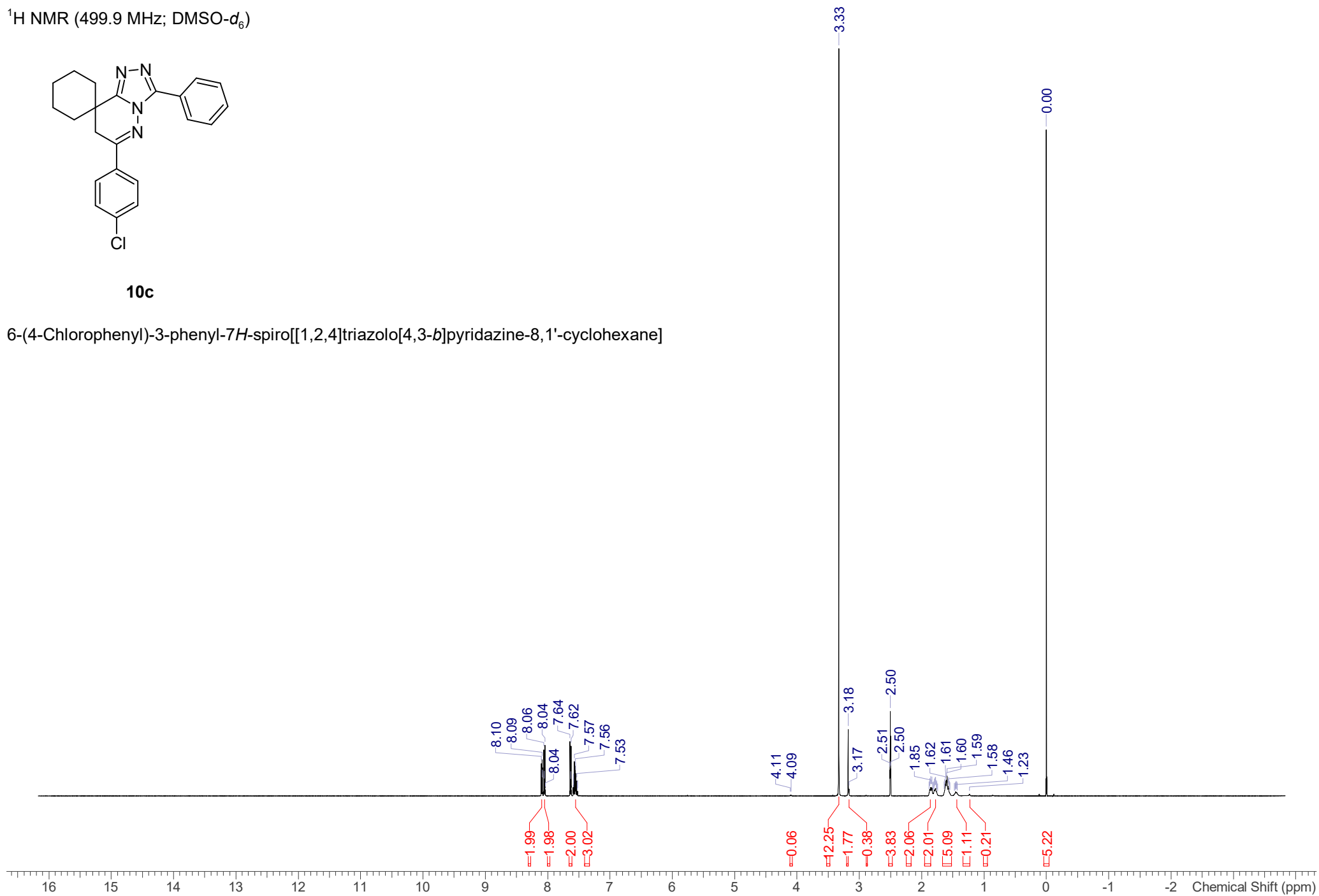


<sup>1</sup>H NMR (499.9 MHz; DMSO-d<sub>6</sub>)



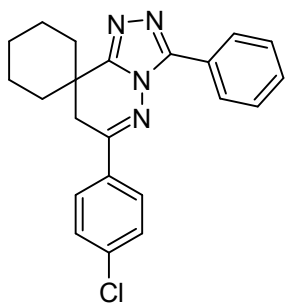
**10c**

6-(4-Chlorophenyl)-3-phenyl-7*H*-spiro[[1,2,4]triazolo[4,3-*b*]pyridazine-8,1'-cyclohexane]

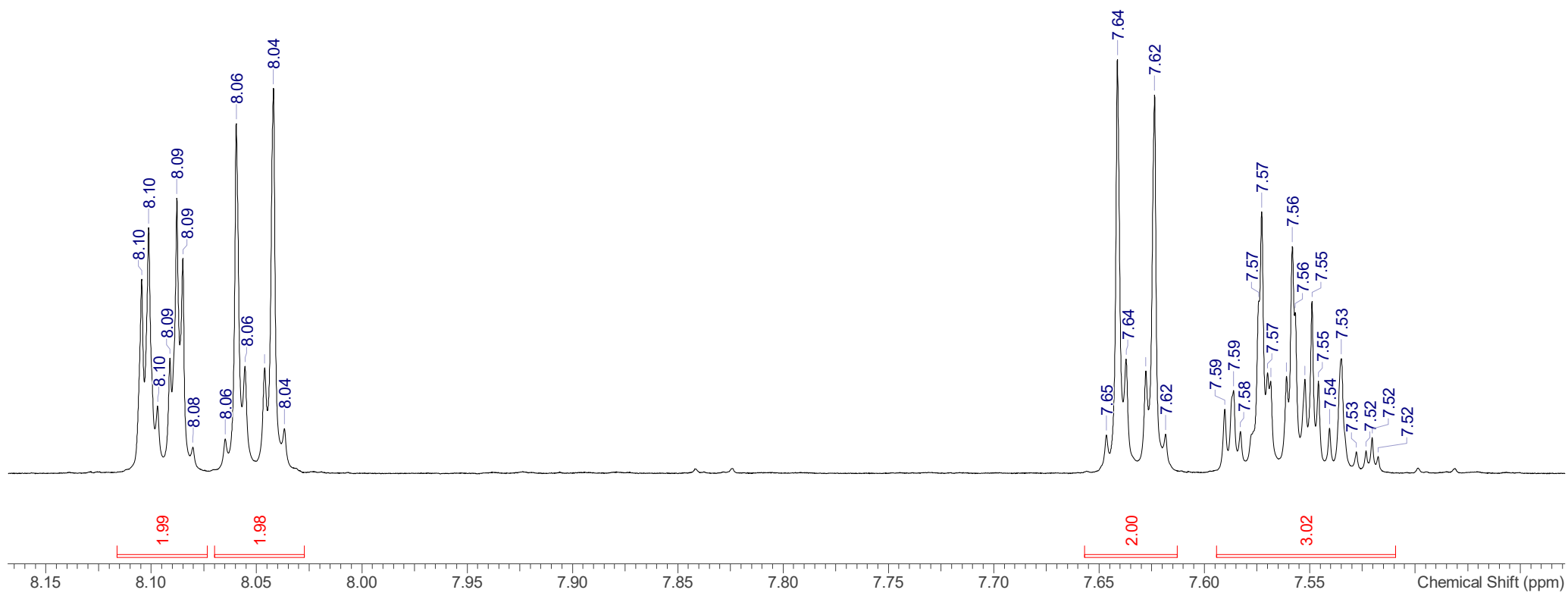




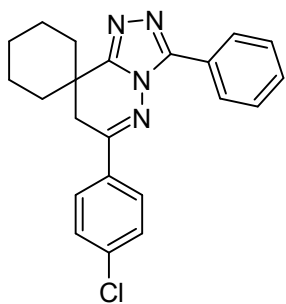
<sup>1</sup>H NMR (499.9 MHz; DMSO-d<sub>6</sub>)



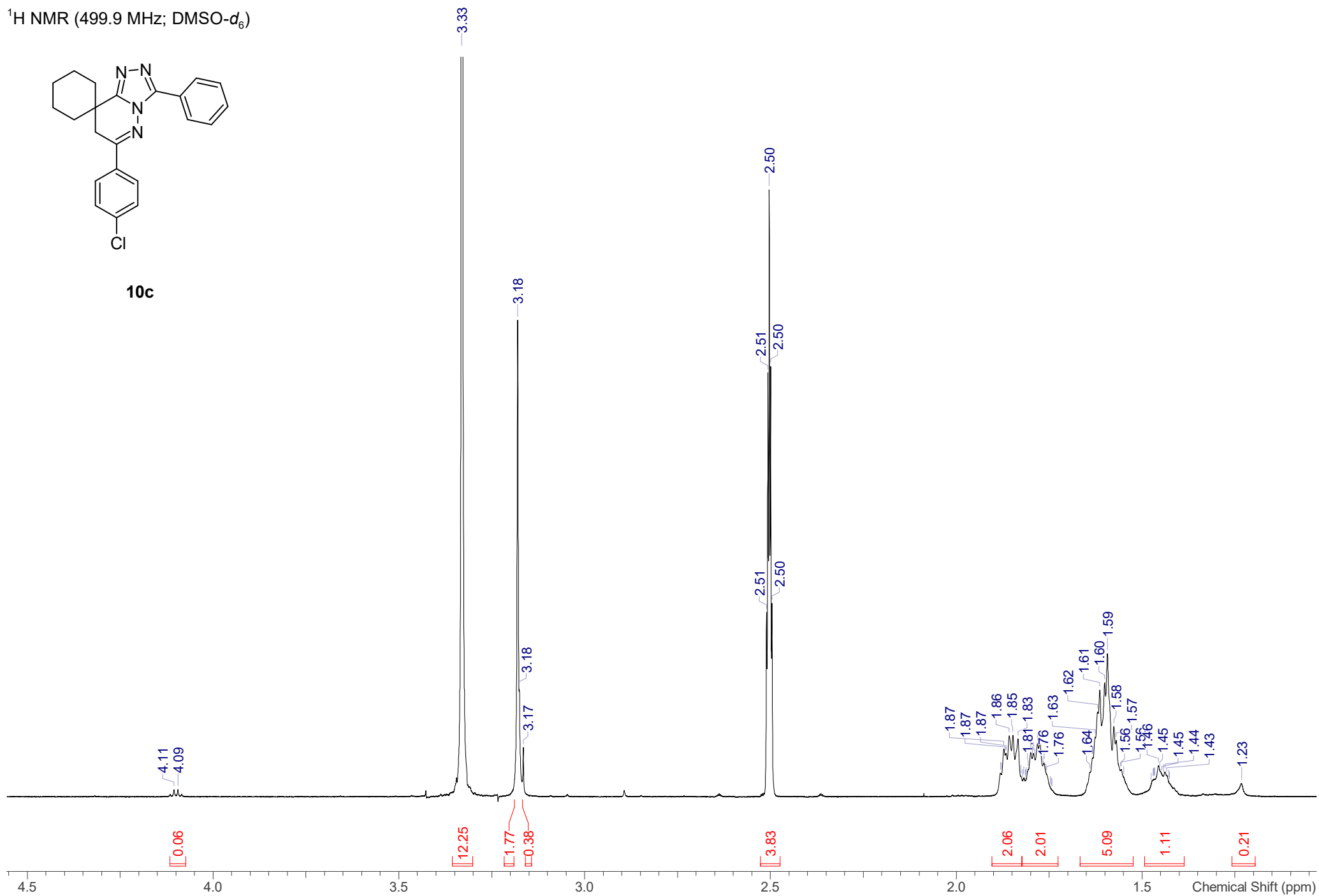
**10c**



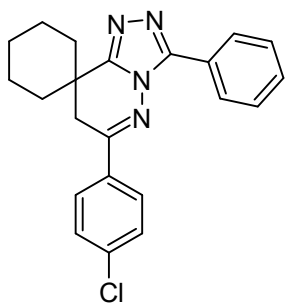
<sup>1</sup>H NMR (499.9 MHz; DMSO-d<sub>6</sub>)



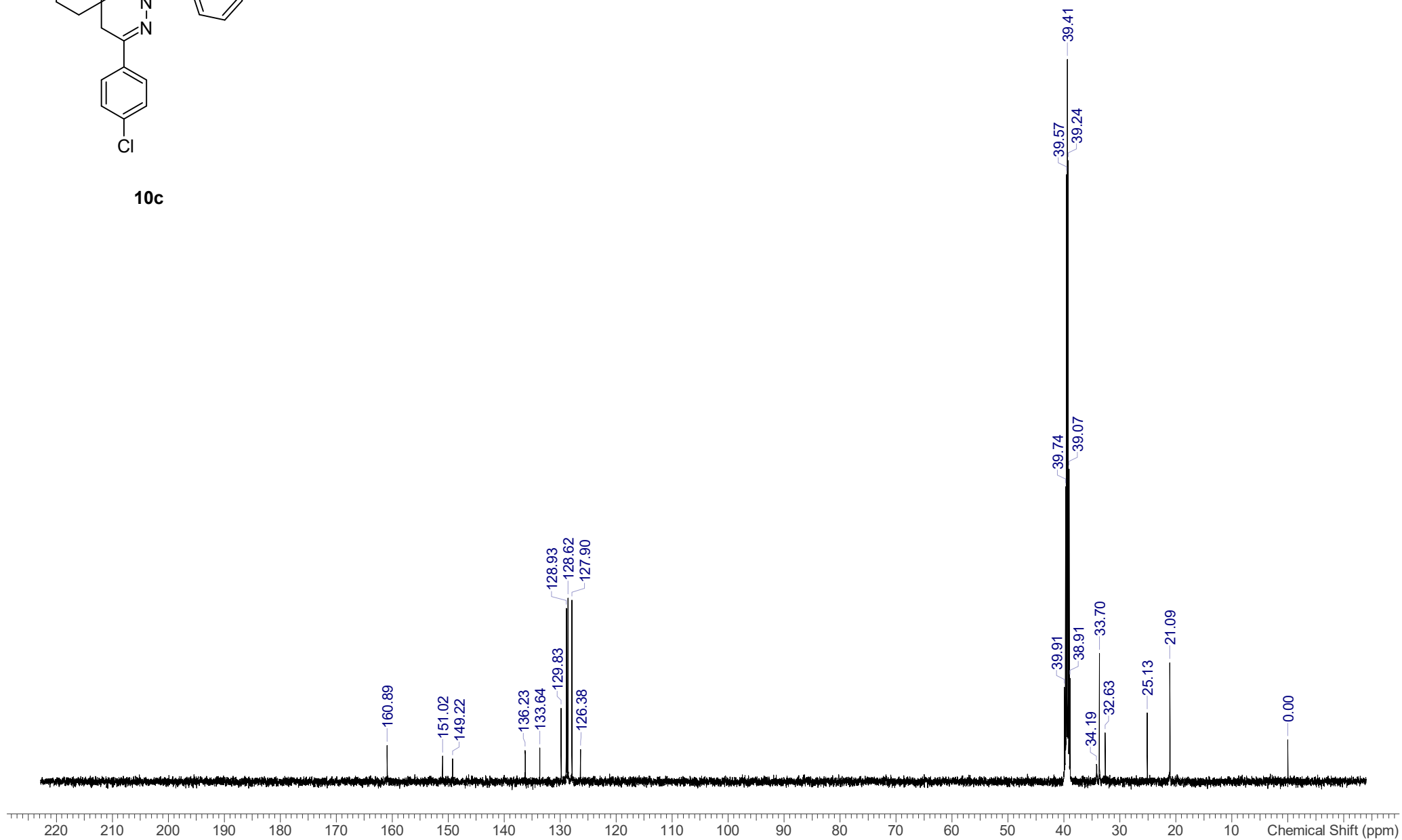
**10c**



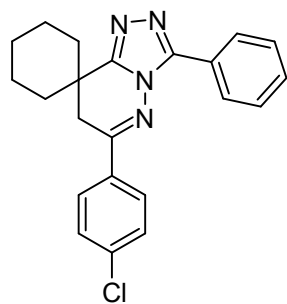
$^{13}\text{C}$  NMR (125.7 MHz;  $\text{DMSO-}d_6$ )



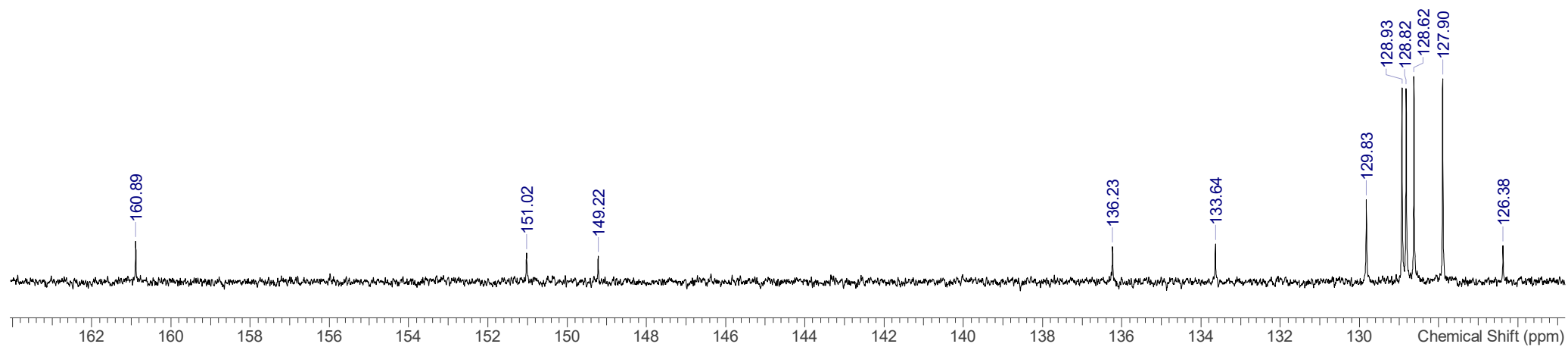
**10c**



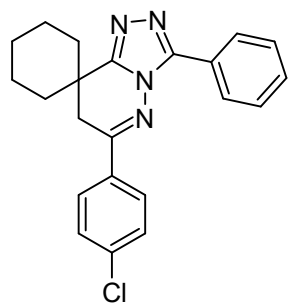
$^{13}\text{C}$  NMR (125.7 MHz;  $\text{DMSO-}d_6$ )



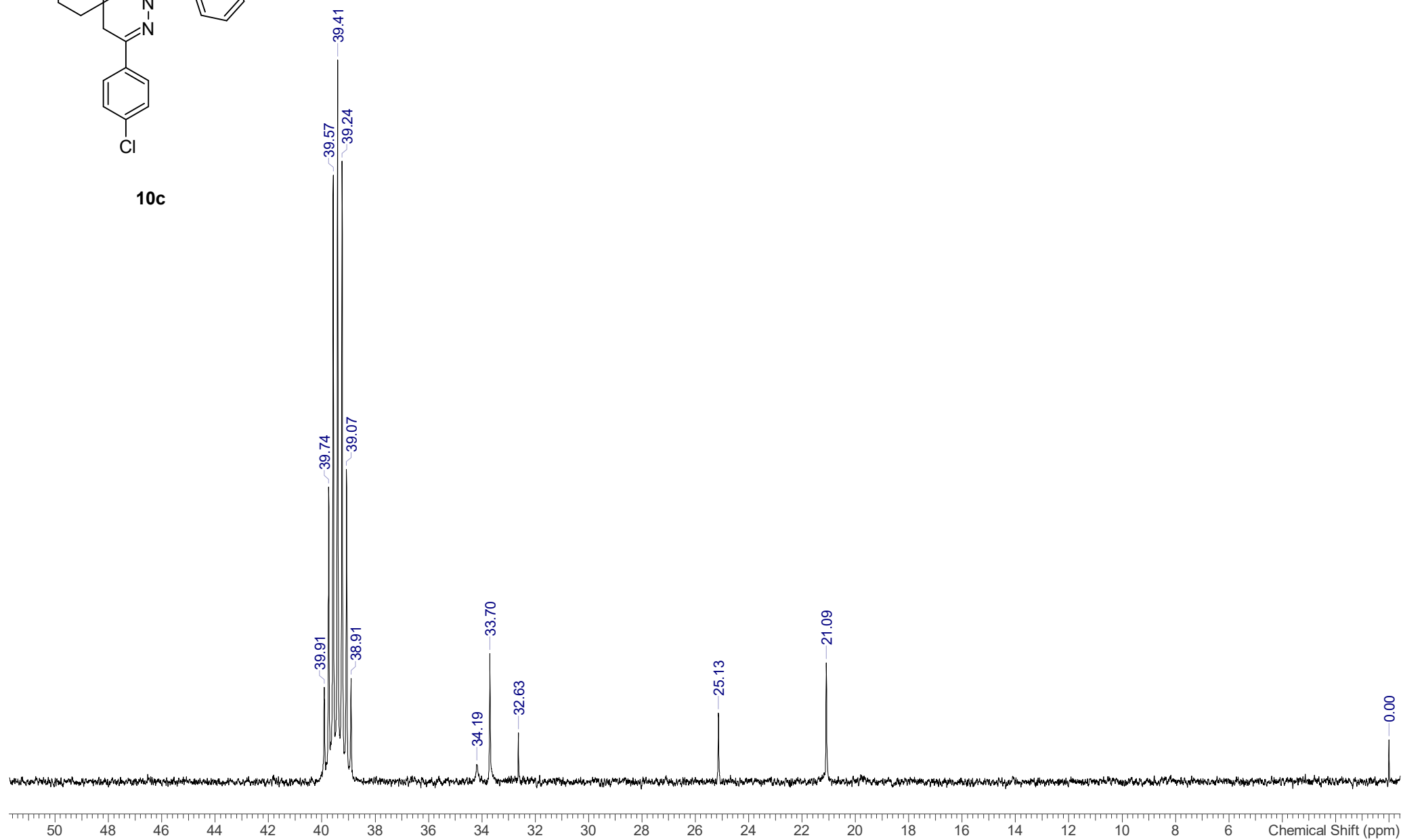
**10c**



$^{13}\text{C}$  NMR (125.7 MHz;  $\text{DMSO-}d_6$ )



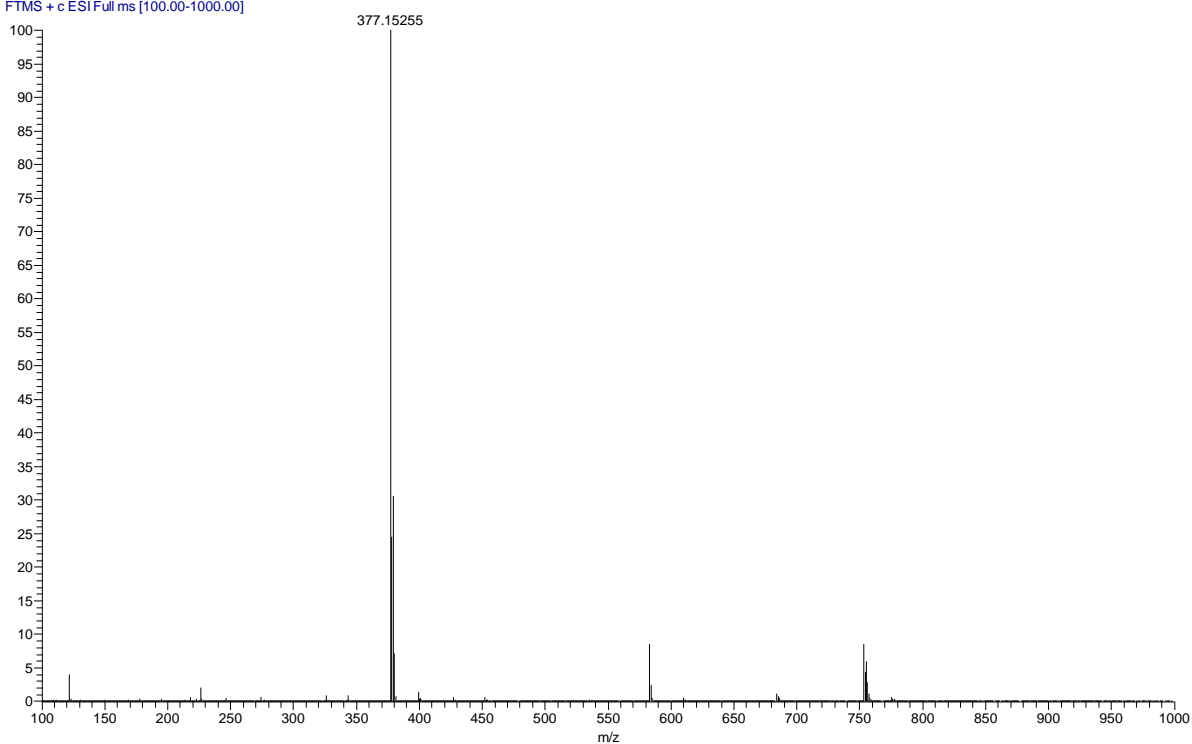
**10c**



# Compound 10c

## HRMS spectrum (ESI)

ku73296\_sfc-206\_d\_ve5779 #1-48 RT: 0.00-0.20 AV: 48 NL: 1.67E7  
T: FTMS + c ESI Full ms [100.00-1000.00]



## HRMS spectrum (ESI daughter ion)

ku73296\_sfc-206\_d\_ve5780 #1-46 RT: 0.00-0.20 AV: 46 NL: 1.48E7  
T: FTMS + c ESI Full ms2 377.20@cid35.00 [100.00-400.00]

