

# REARRANGEMENT OF 2-(2,5-DIOXOPYRROLIDIN-1-YL)GUANIDINE: AN EFFICIENT SYNTHESIS AND STRUCTURE OF 3-(5-AMINO-1H-1,2,4-TRIAZOL-3-YL)PROPANOIC ACID AND DERIVATIVES

*Victor M. Chernyshev,<sup>a\*</sup> Anna V. Chernysheva<sup>a</sup> and Zoya A. Starikova<sup>b</sup>*

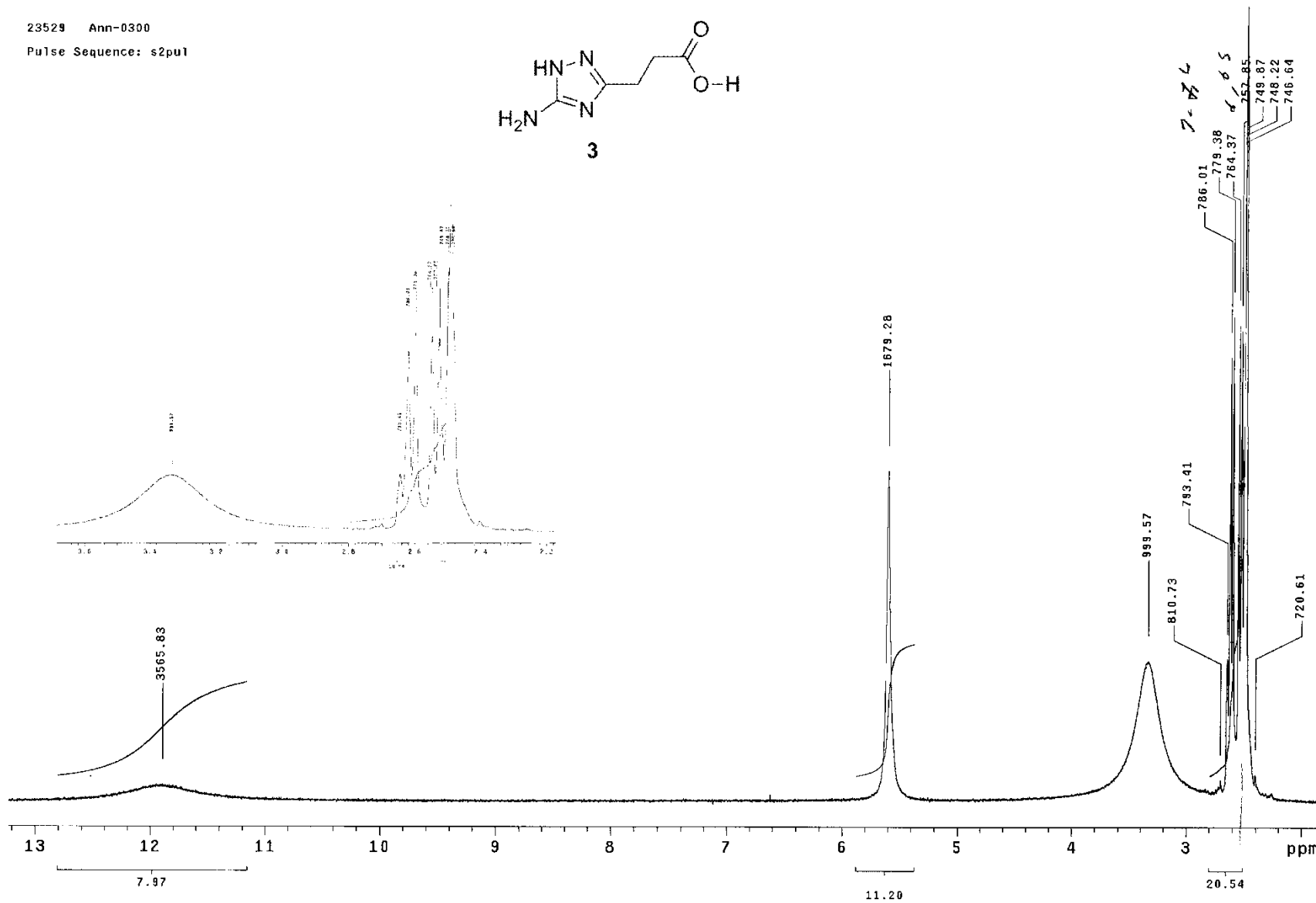
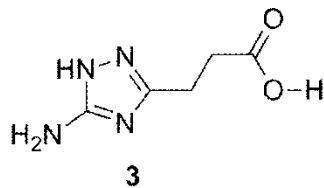
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*[chem13@yandex.ru](mailto:chem13@yandex.ru).*

*<sup>b</sup>A. N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, 119991 Moscow, Russian Federation*

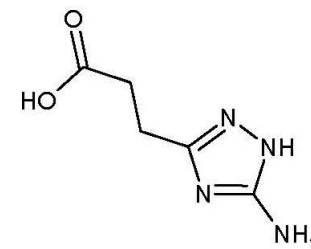
## **Supplementary Material** **Selected Spectra of Synthesized Compounds**

23529 Ann-0300  
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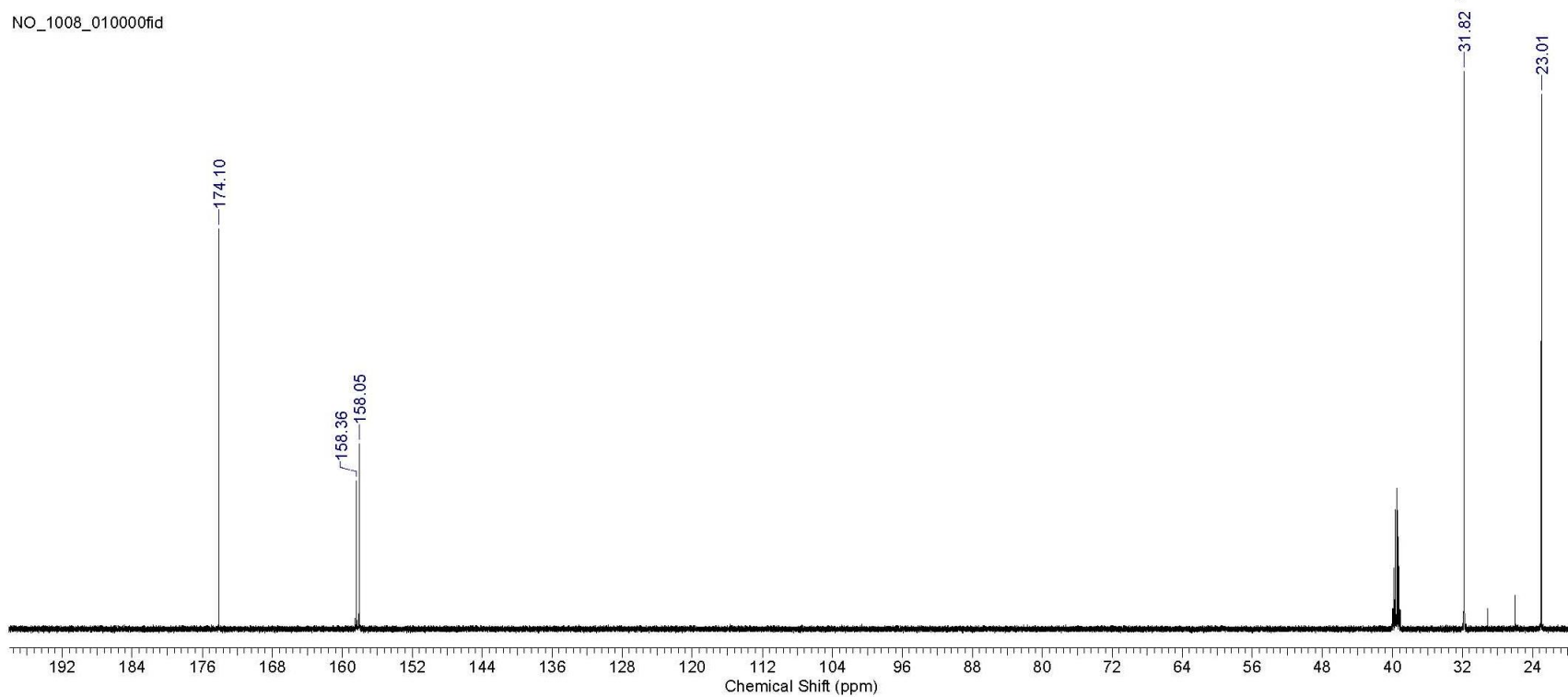


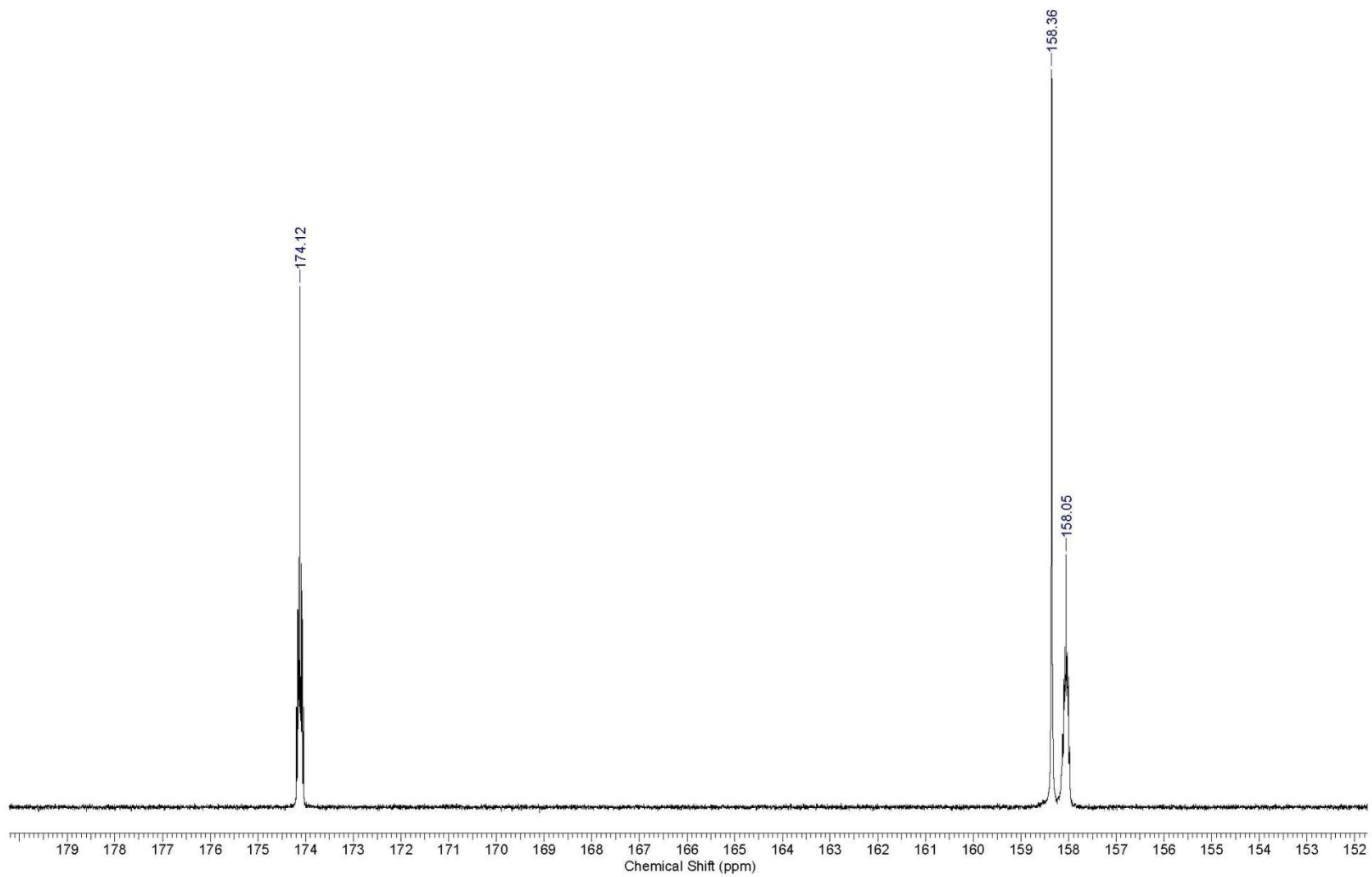
<sup>1</sup>H NMR spectrum (300 MHz) of compound **3**

Acquisition Time (sec)	3.6351	Comment	NO_1008 Chern-151 13C		Date	28 Jan 2010 14:04:48			
Date Stamp	28 Jan 2010 14:04:48	File Name	E:\SpectraAll\NOVOCH\NO_1008\NO_1008_010000fid		Frequency (MHz)	150.96			
Nucleus	13C	Number of Transients	256	Origin	spect	Original Points Count	131072	Owner	nmr
Points Count	131072	Pulse Sequence	zgpg	Receiver Gain	203.00	SW(cyclical) (Hz)	36057.70	Solvent	DMSO-d6
Spectrum Offset (Hz)	15048.0215	Sweep Width (Hz)	36057.42	Temperature (degree C)	31.000				

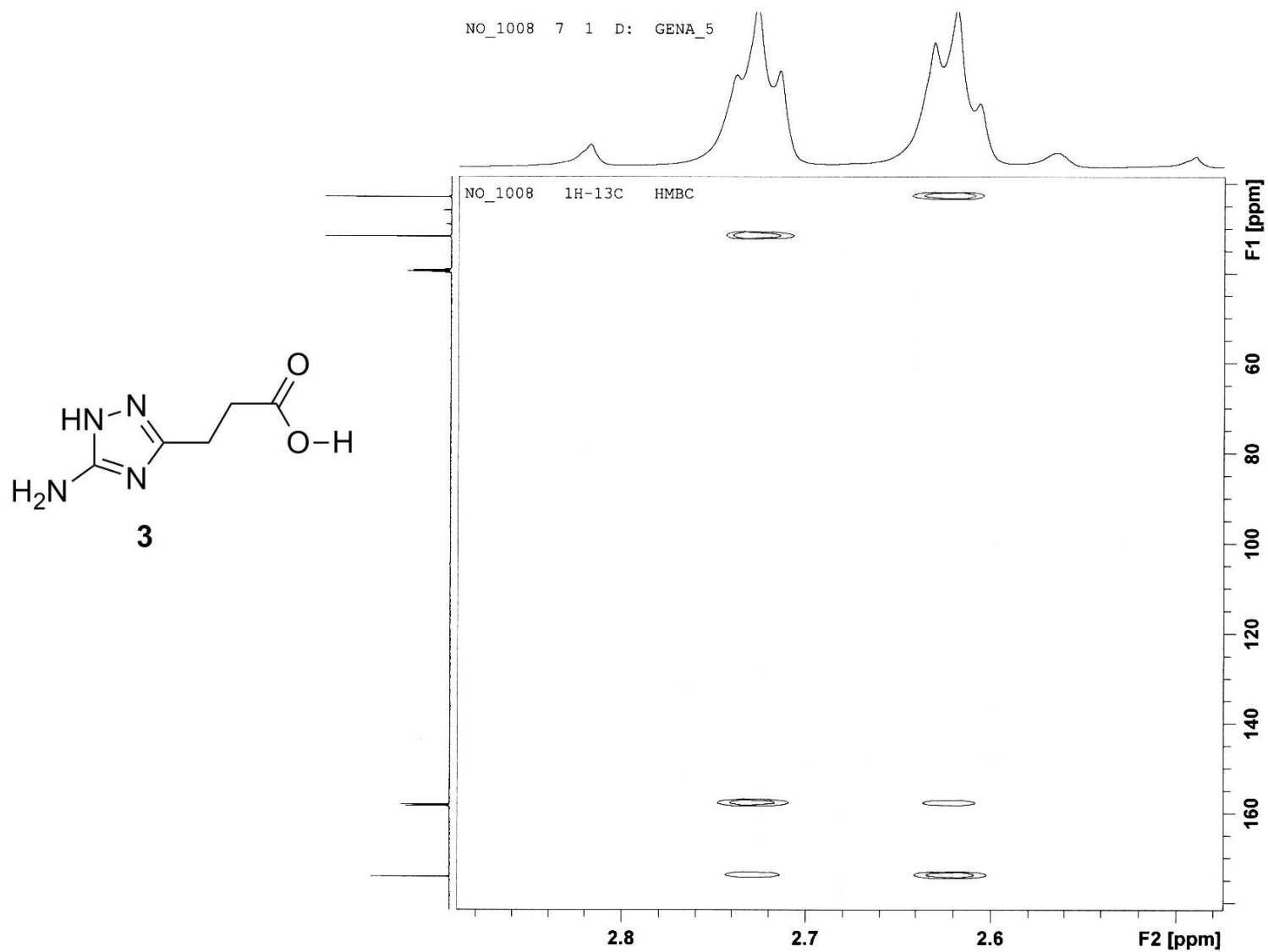


NO\_1008\_010000fid

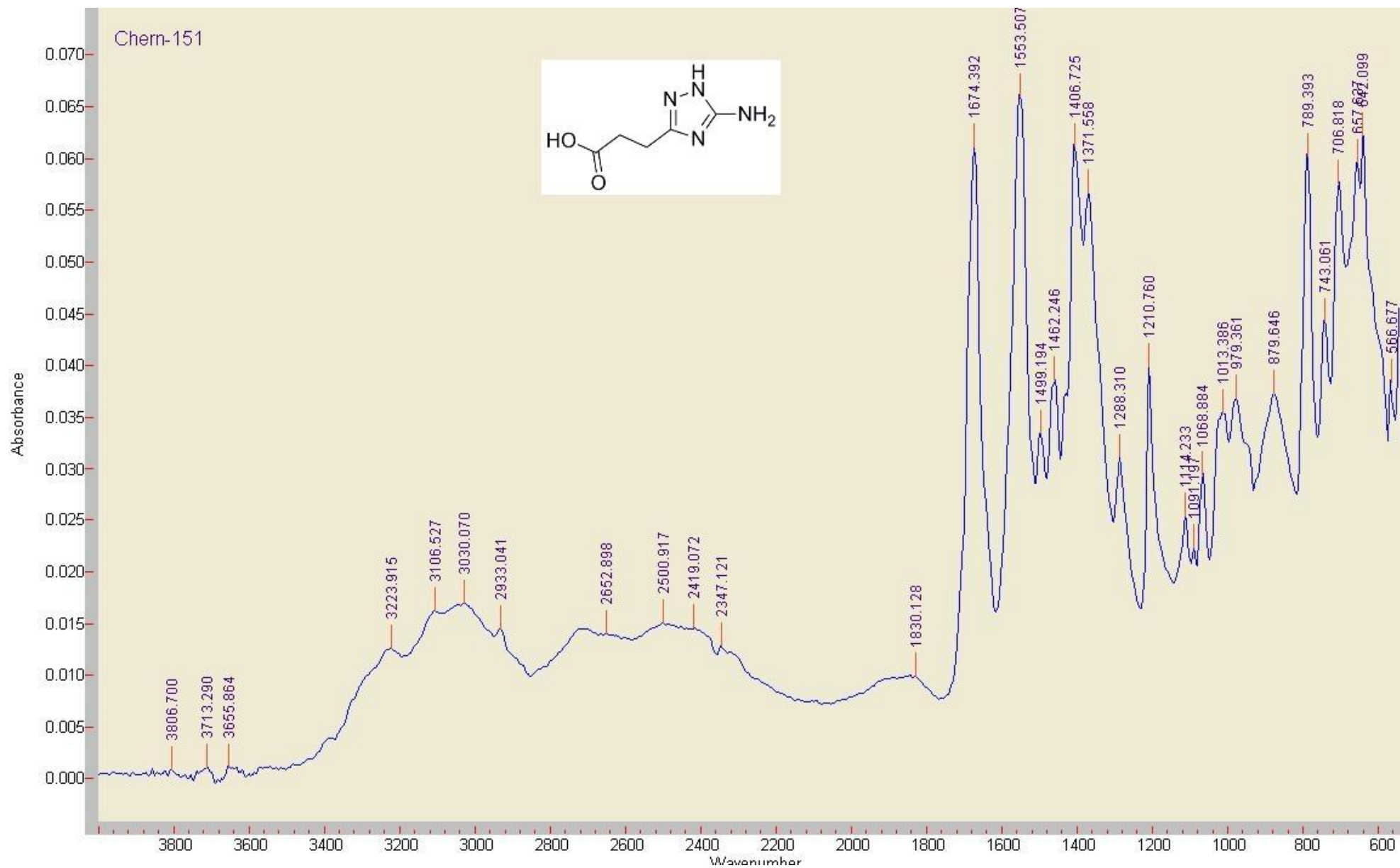
 $^{13}\text{C}$  NMR spectrum (150 MHz) of compound **3**



Fragment of proton coupled <sup>13</sup>C NMR spectrum (150 MHz) of compound **3**

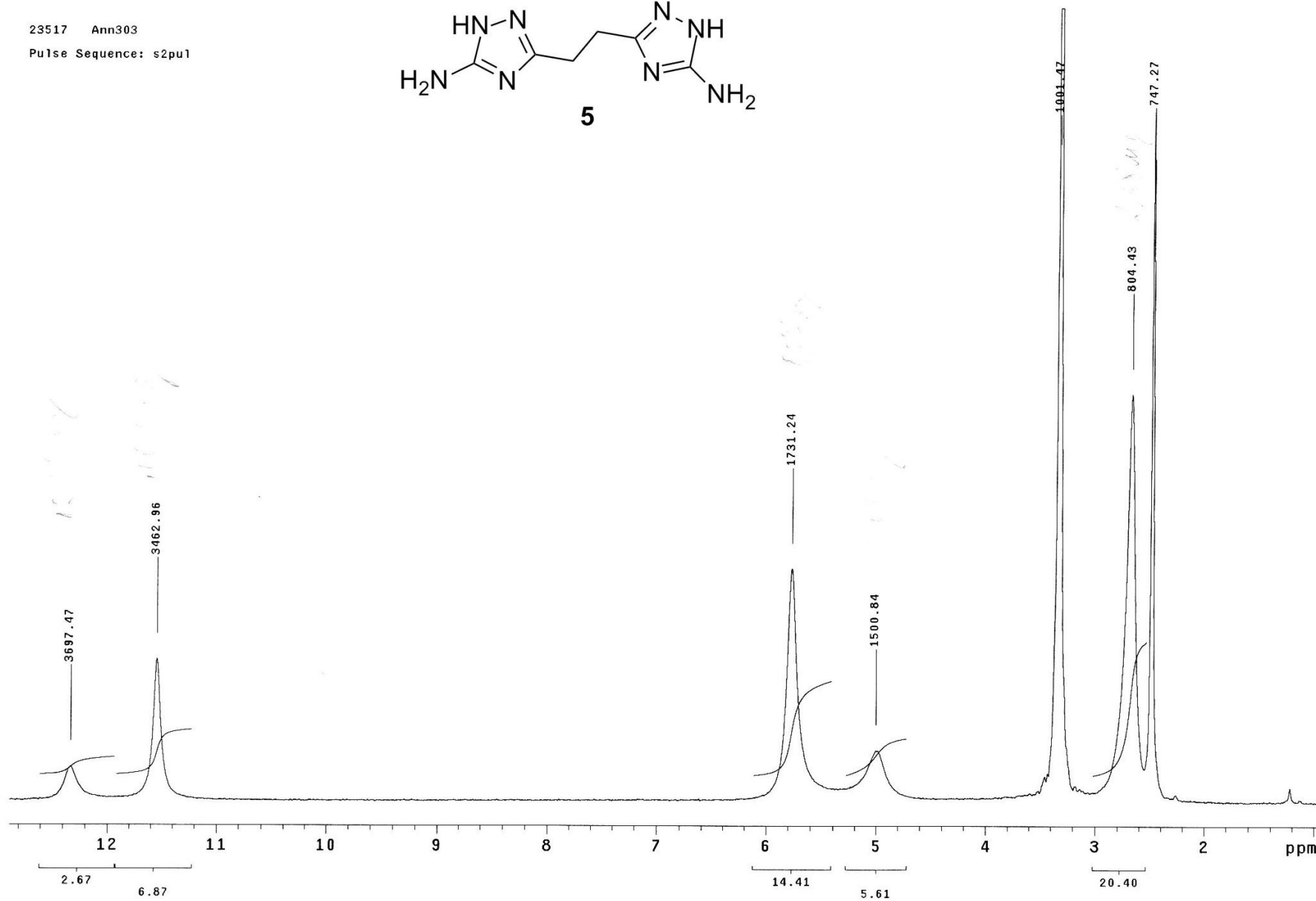
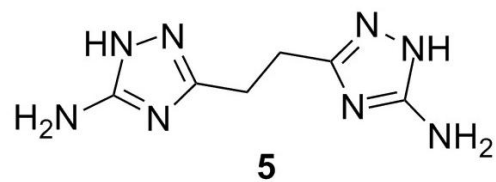


$^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **3**



FTIR spectrum of compound 3

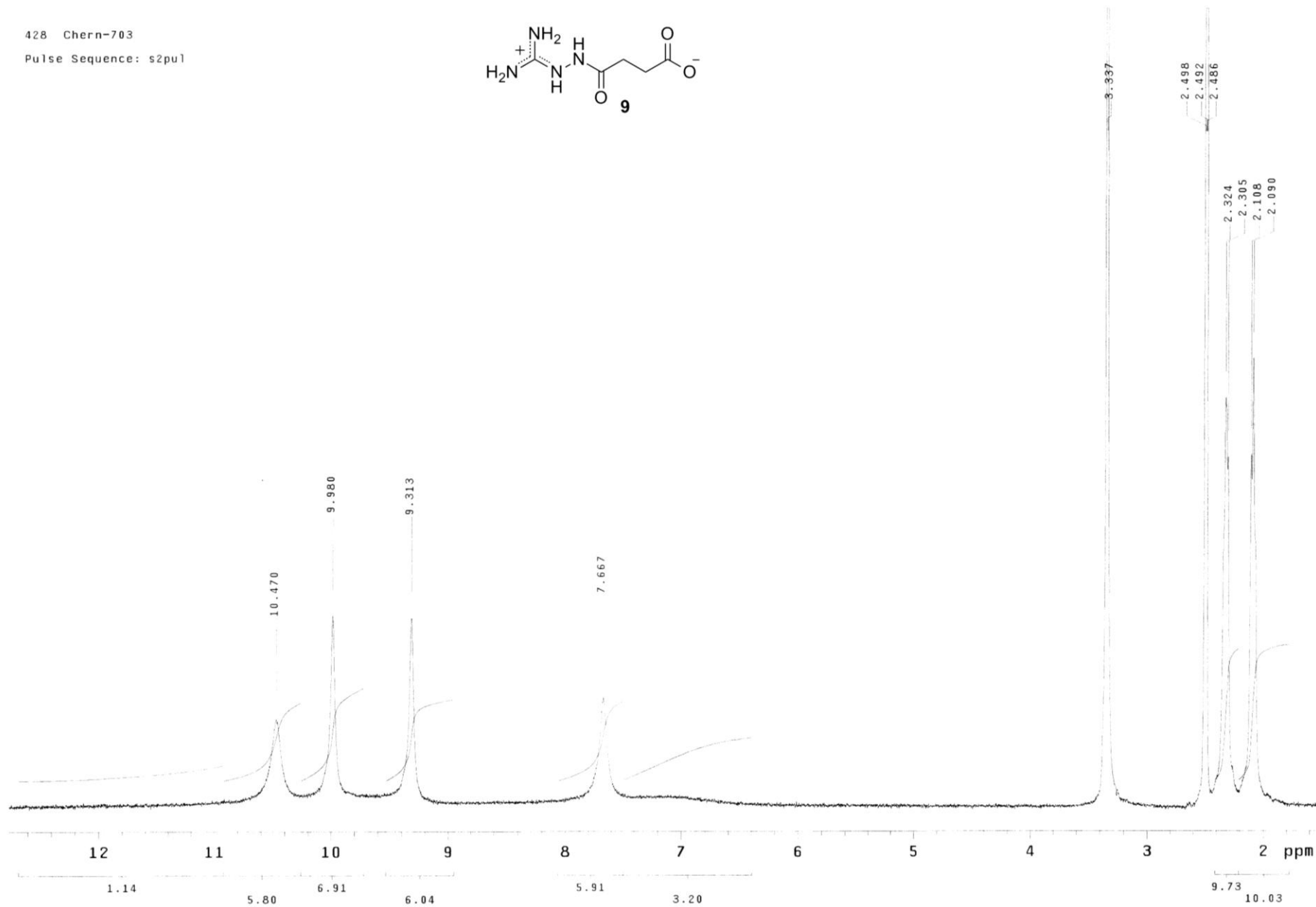
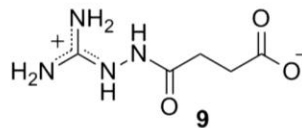
23517 Ann303  
Pulse Sequence: s2pu1



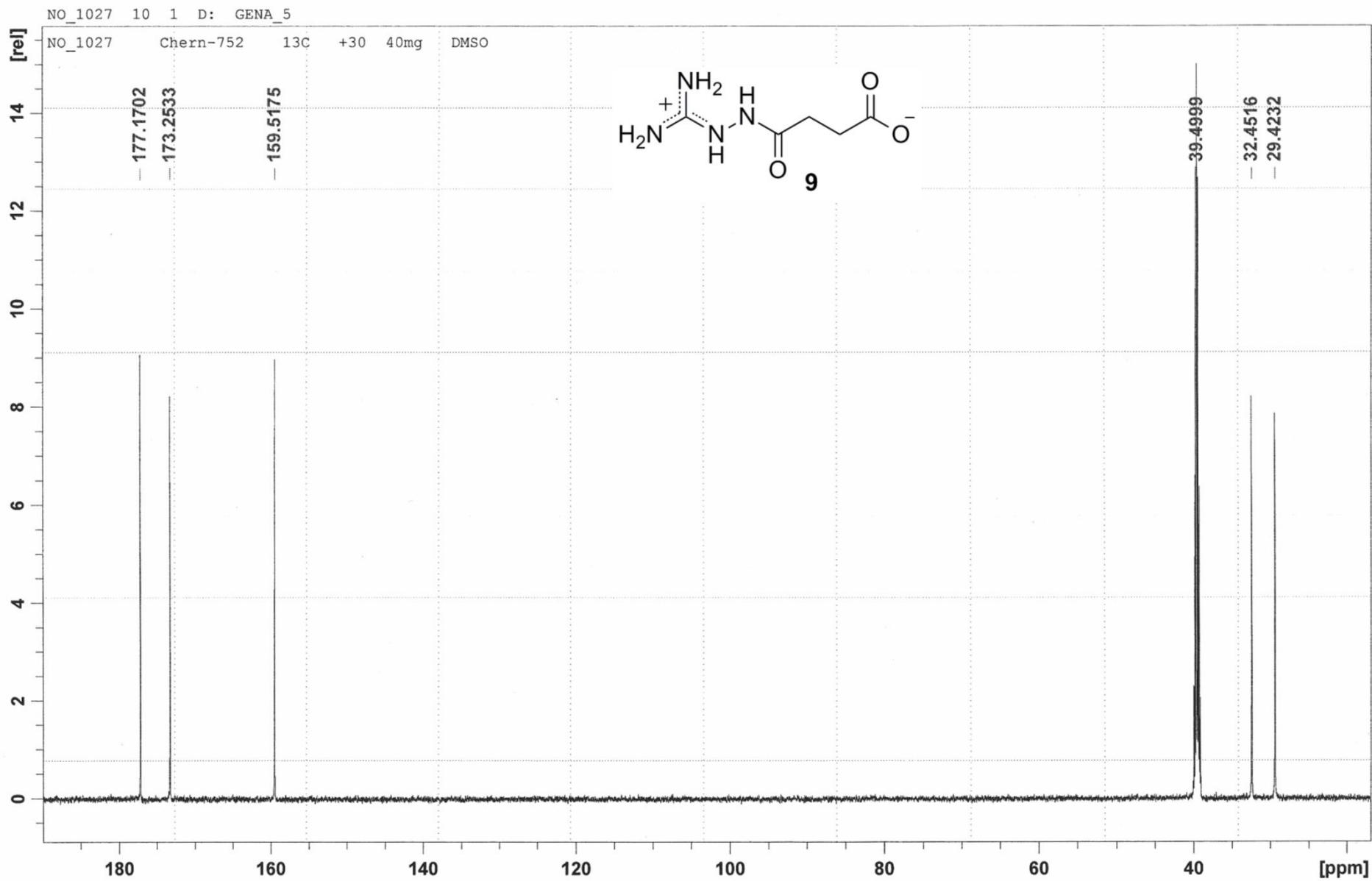
<sup>1</sup>H NMR spectrum (300 MHz) of compound **5** (two tautomers are observed)

428 Chern-703

Pulse Sequence: s2pu1

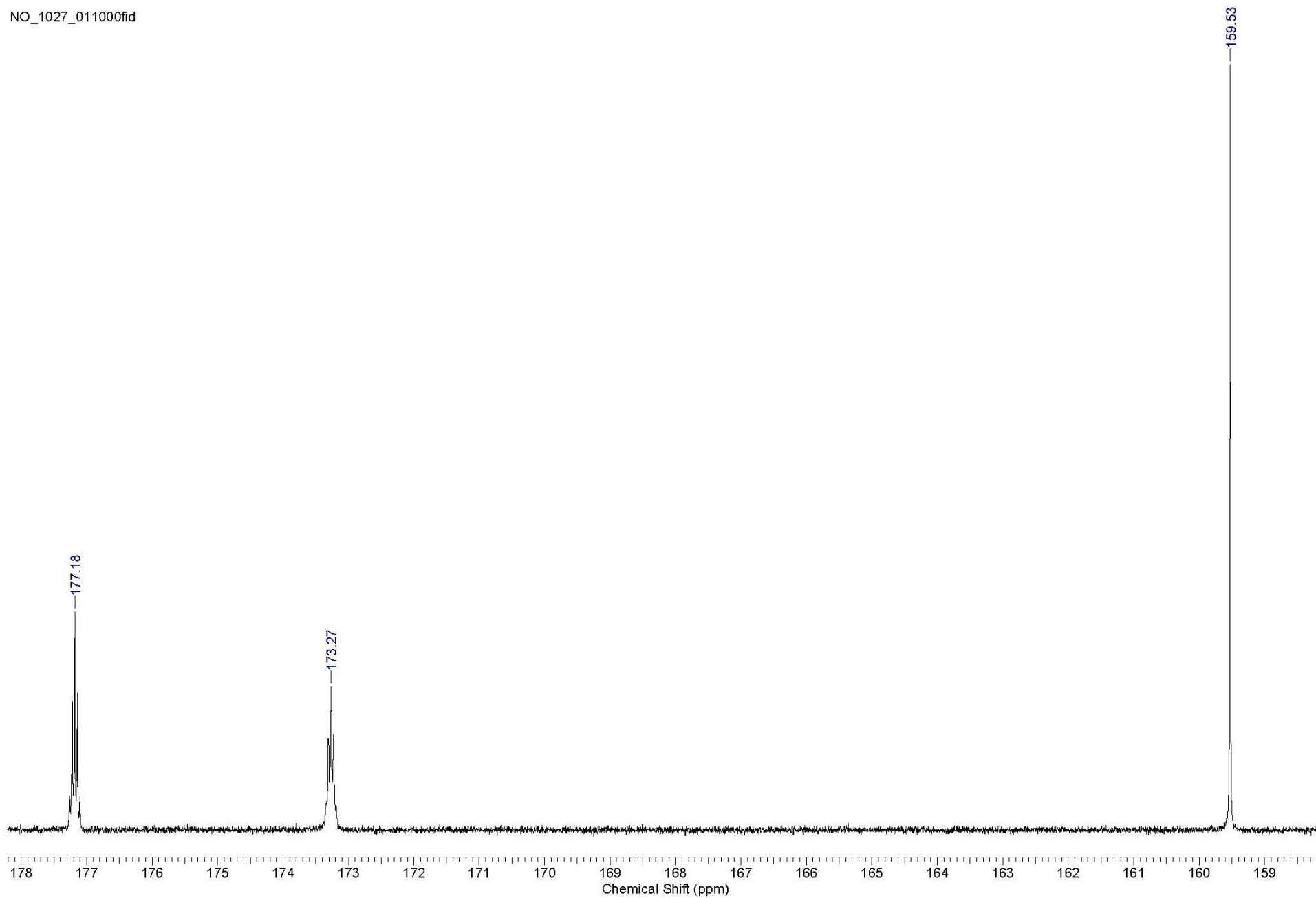


<sup>1</sup>H NMR spectrum (300 MHz) of compound **9** (apparently, two tautomers are observed)



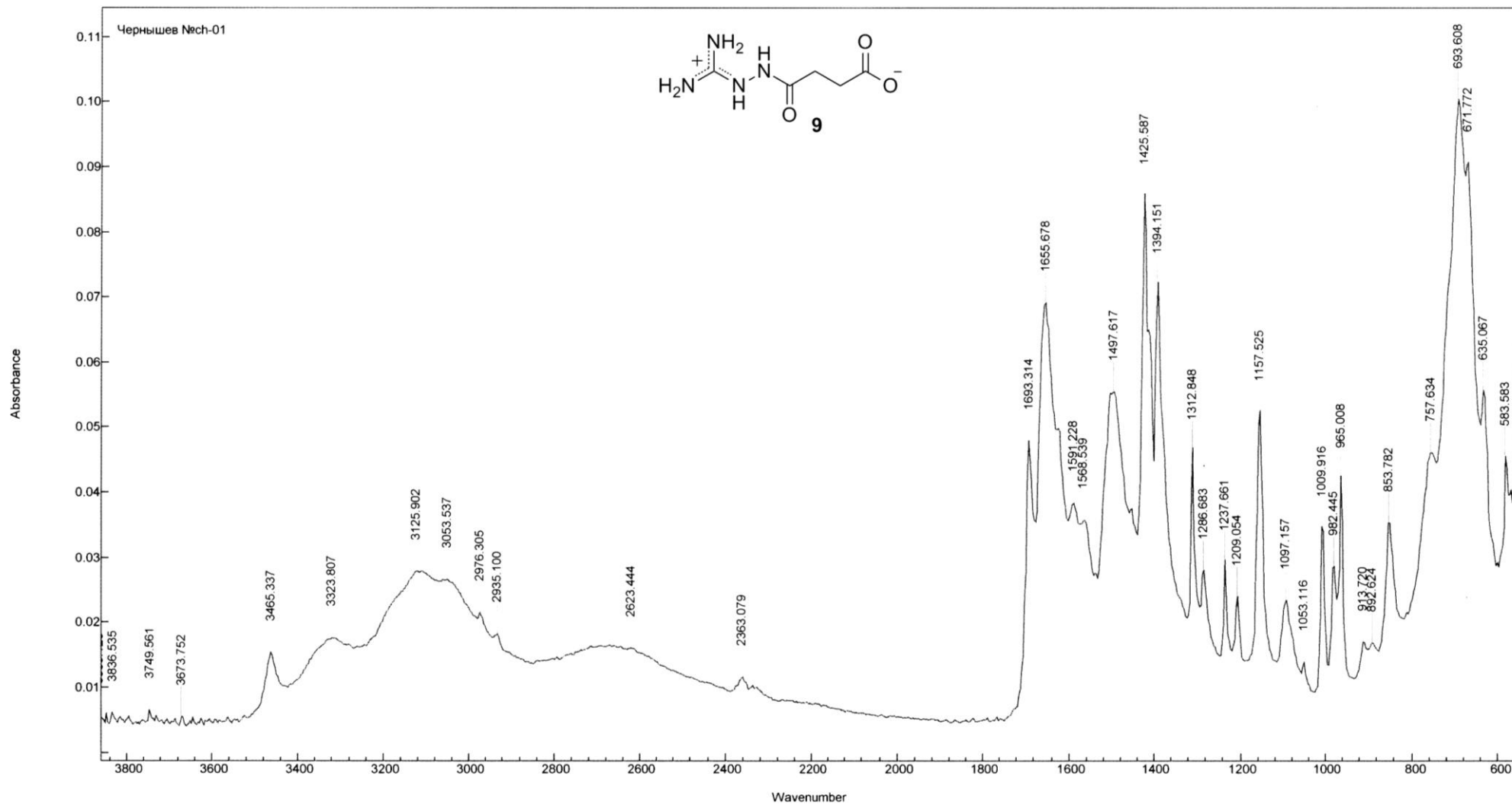
$^{13}\text{C}$  NMR spectrum (150 MHz) of compound **9**

NO\_1027\_011000fid



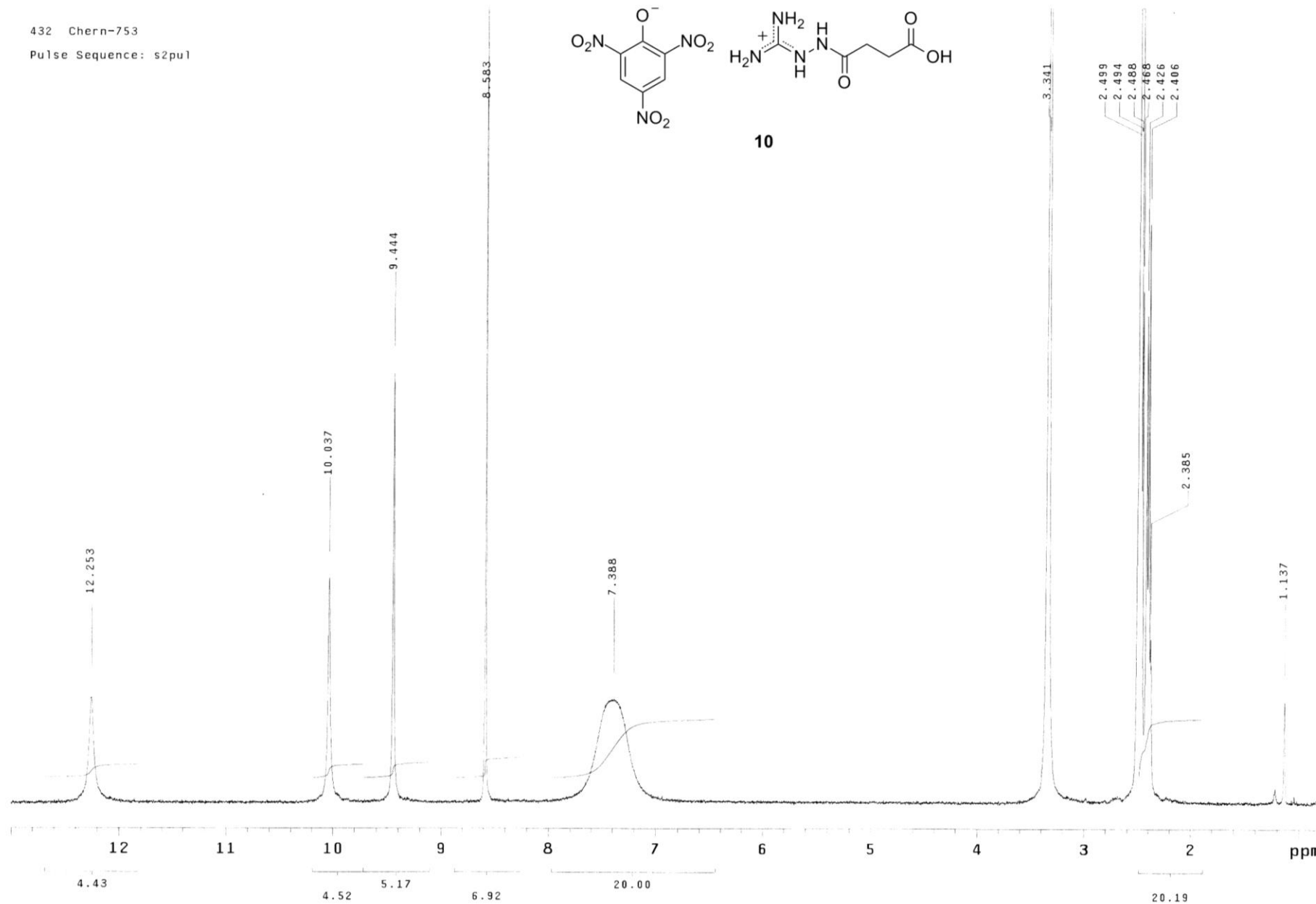
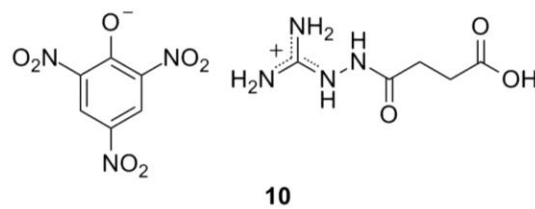
Fragment of the proton coupled  $^{13}\text{C}$  NMR spectrum (150 MHz) of compound **9**

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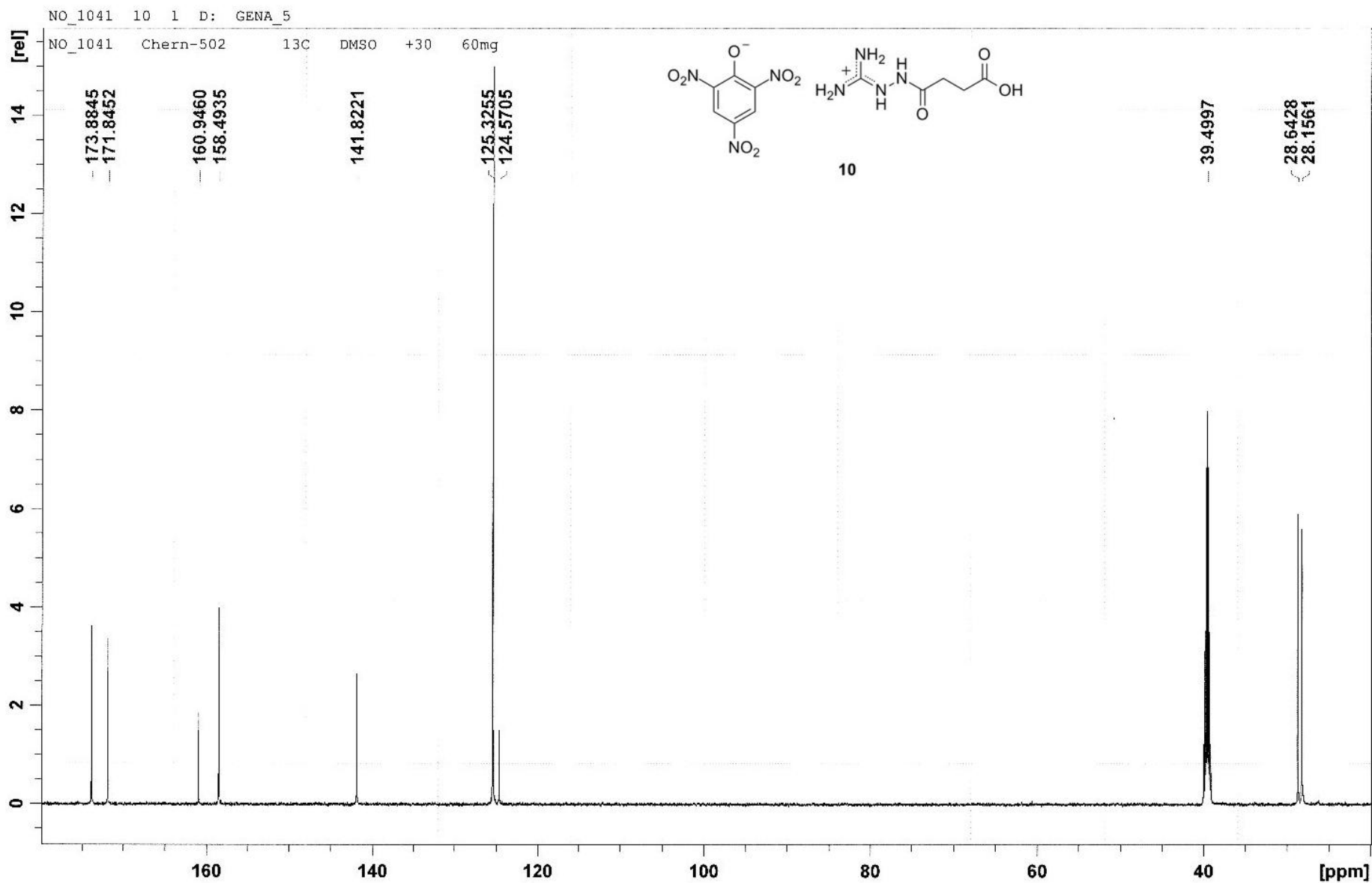


FTIR spectrum of compound 9

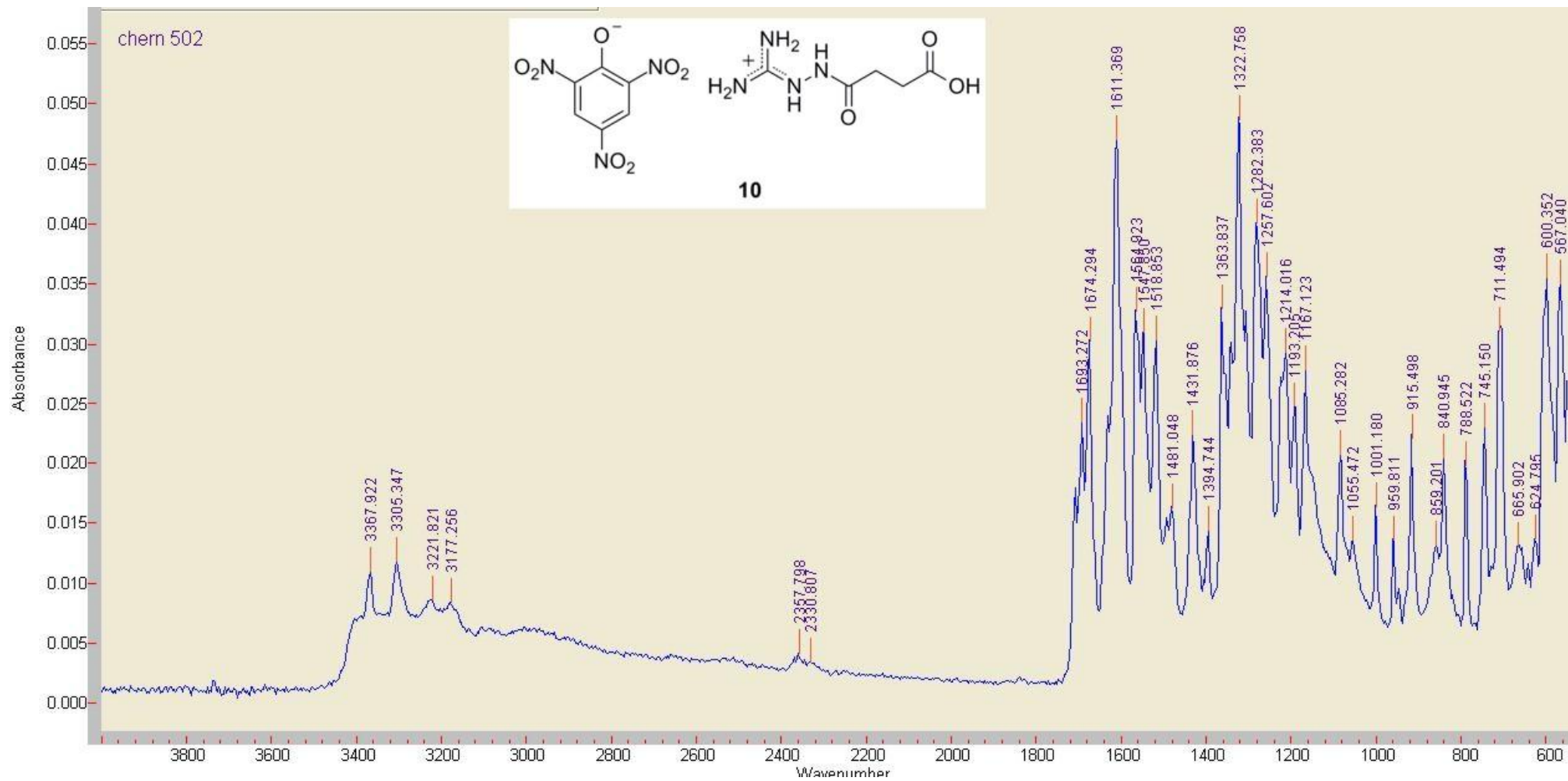
432 Chern-753  
Pulse Sequence: s2pu1



<sup>1</sup>H NMR spectrum (300 MHz) of compound 10



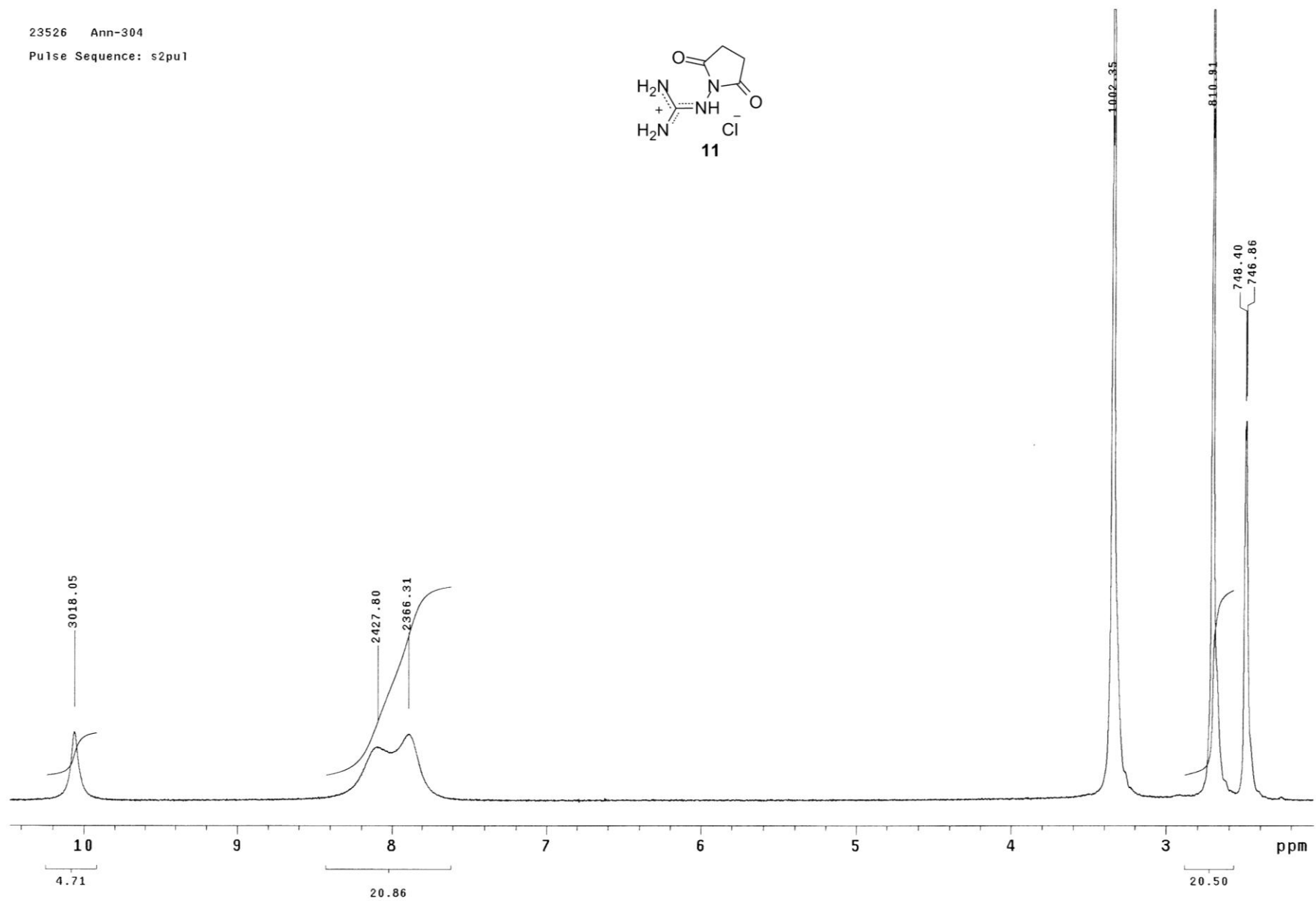
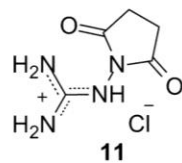
$^{13}\text{C}$  NMR spectrum (150 MHz) of compound **10**



FTIR spectrum of compound **10**

23526 Ann-304

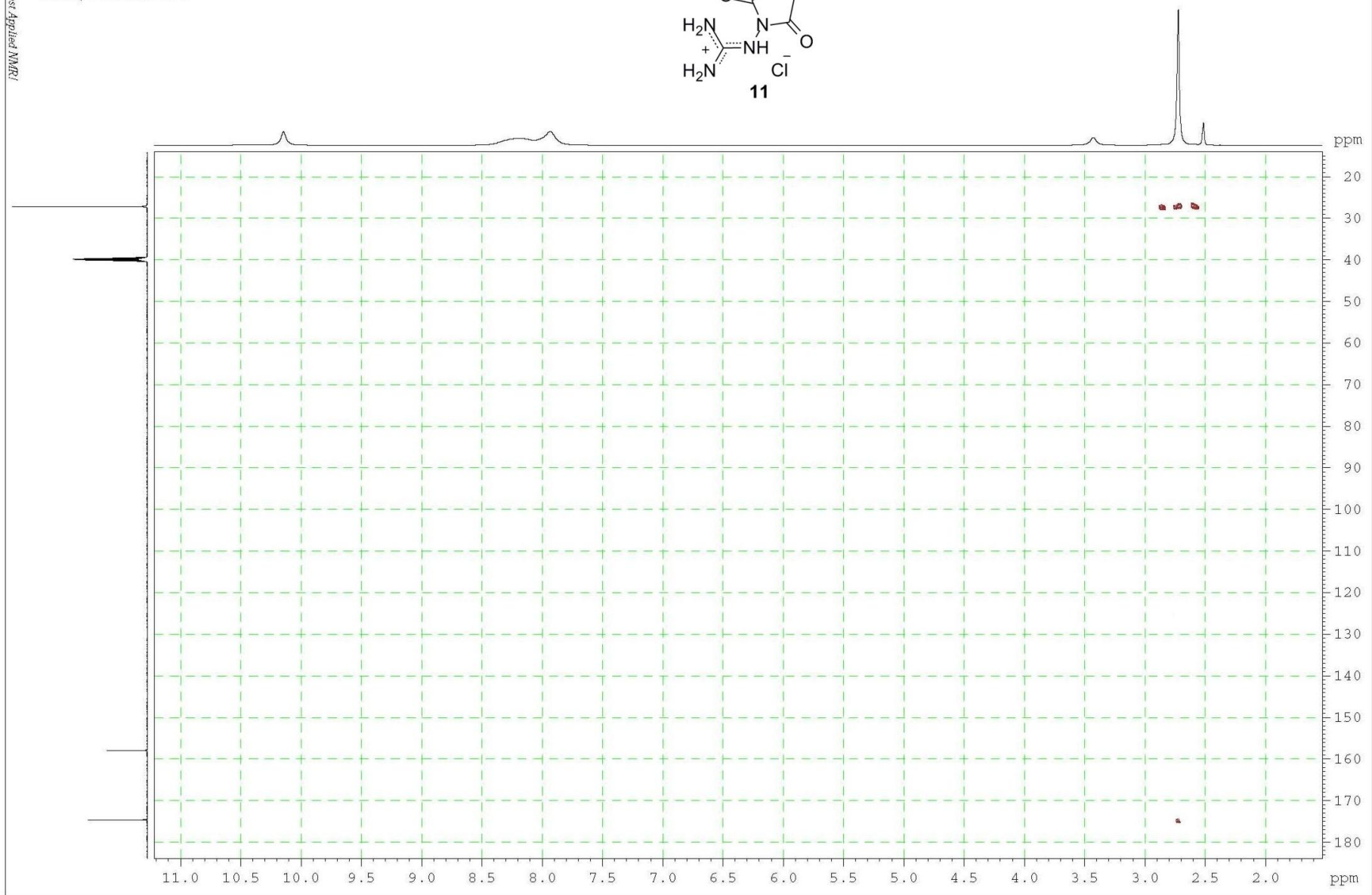
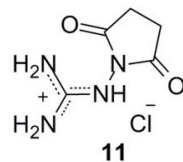
Pulse Sequence: s2pu1



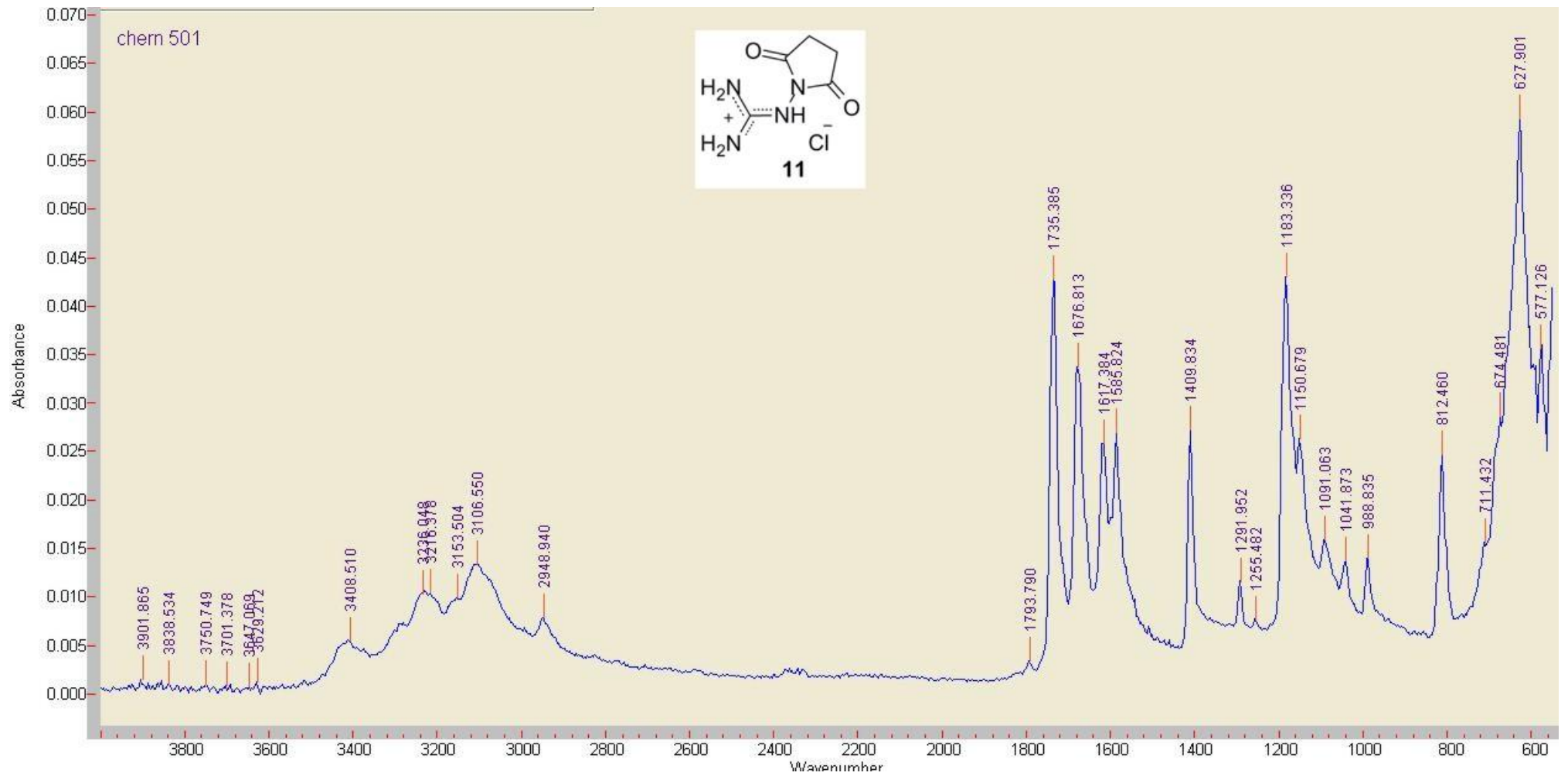
<sup>1</sup>H NMR spectrum (300 MHz) of compound **11**



NMR/18247297

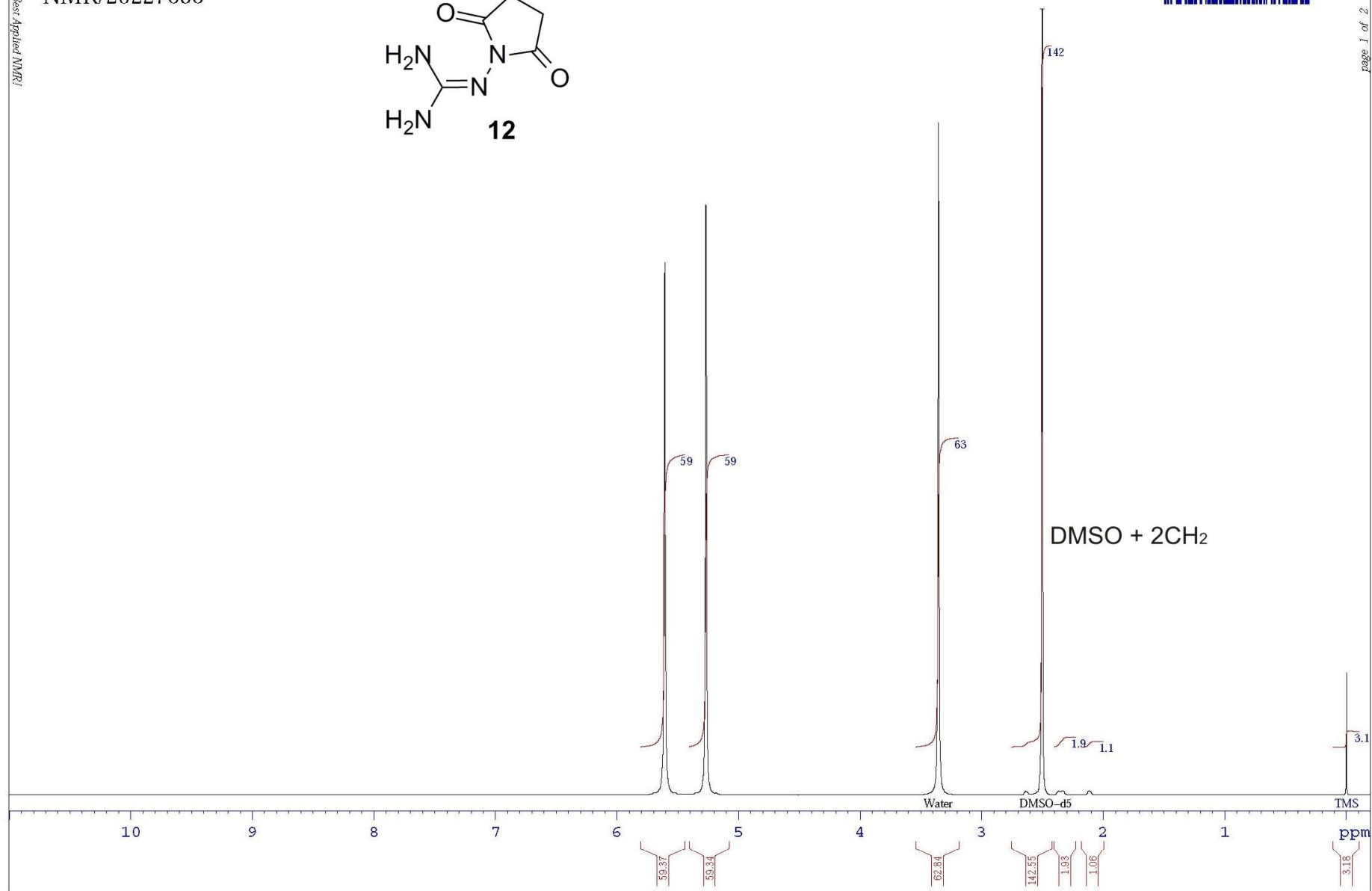
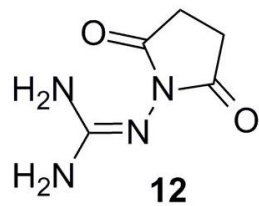


$^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **11**



FTIR spectrum of compound **11**

NMR/20227636

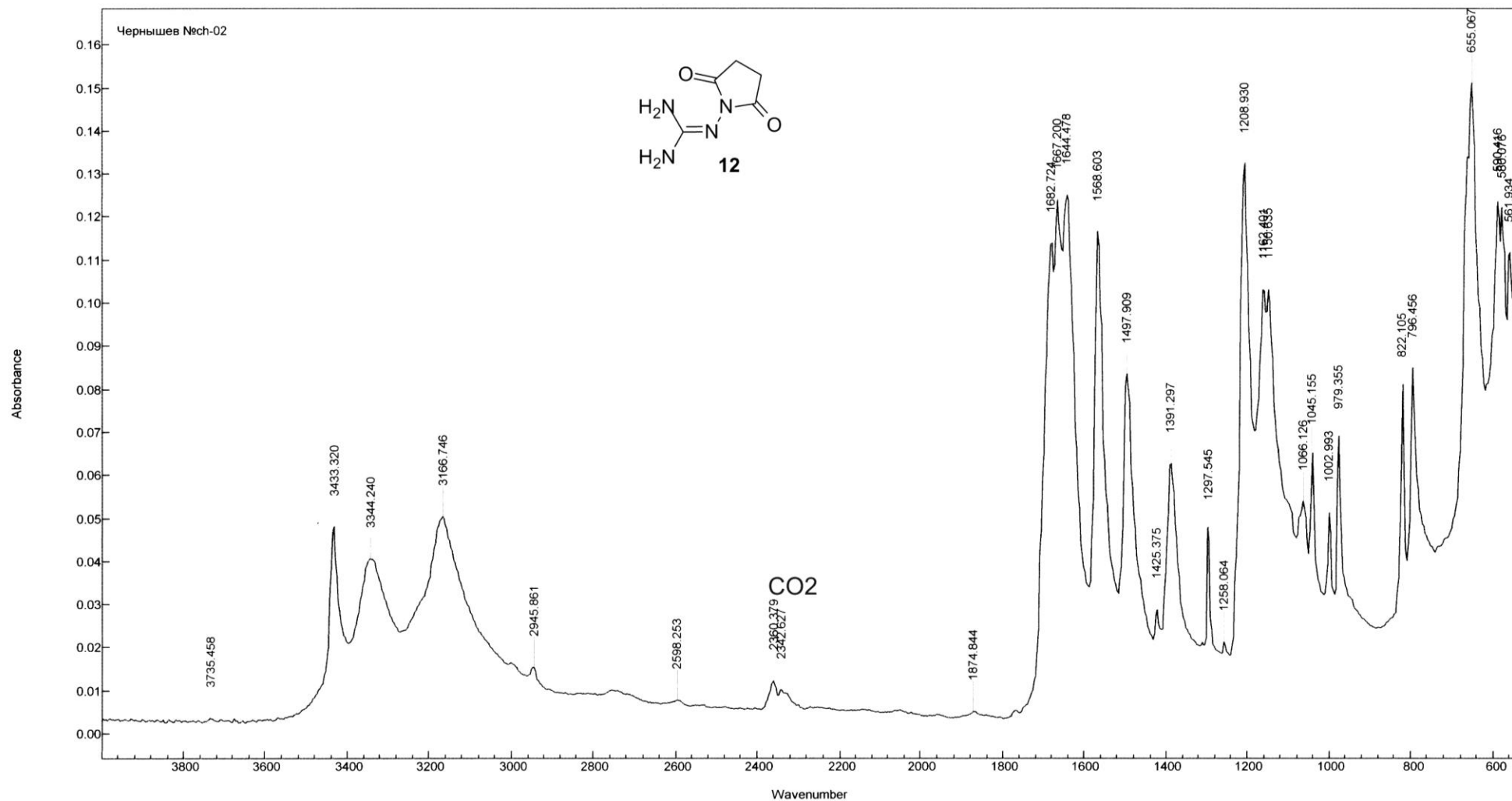


<sup>1</sup>H NMR spectrum (500 MHz) of compound **12**

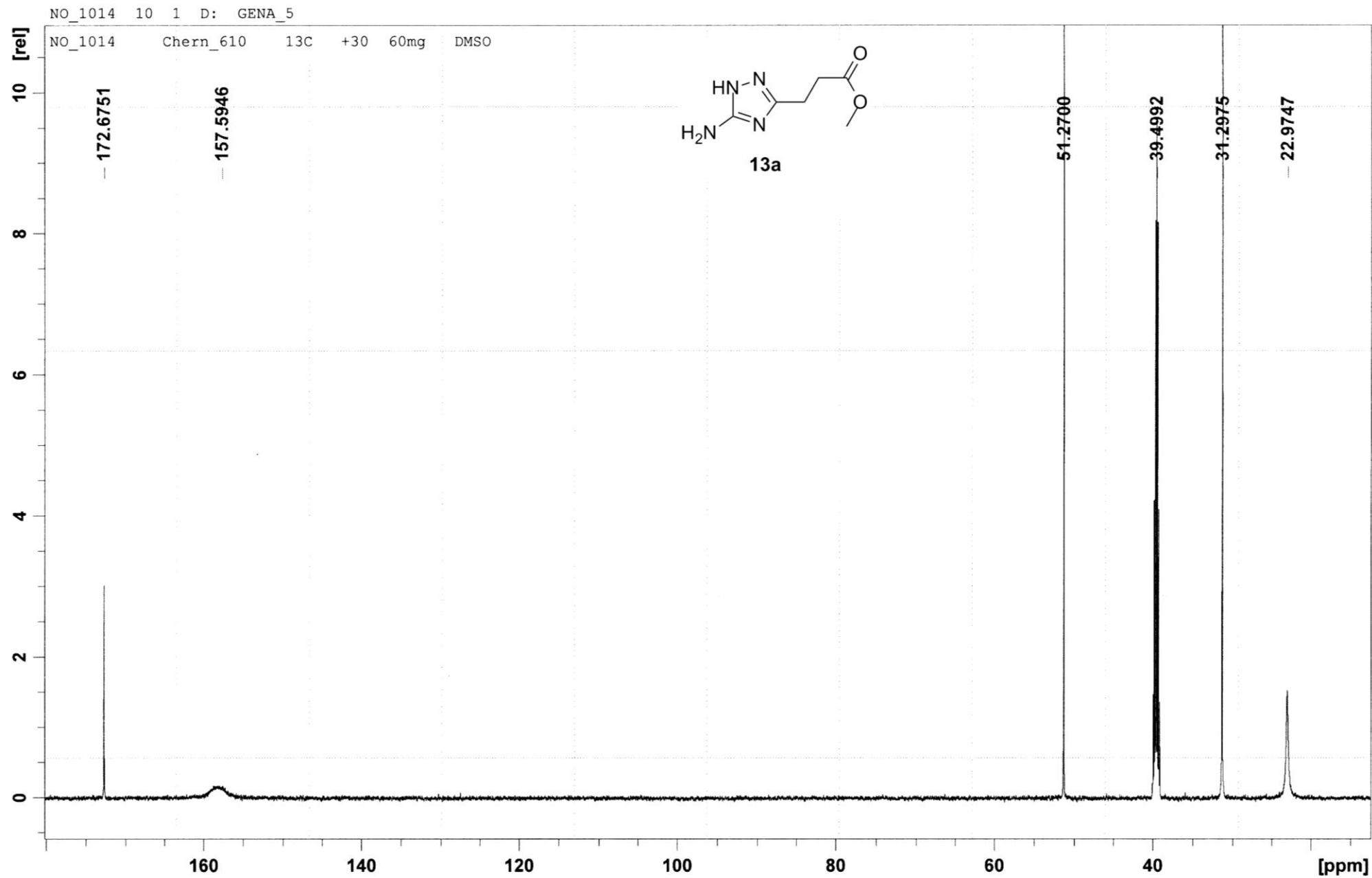


<sup>13</sup>C NMR spectrum (125 MHz) of compound **12**

# Varian Excalibur 3100 FT-IR

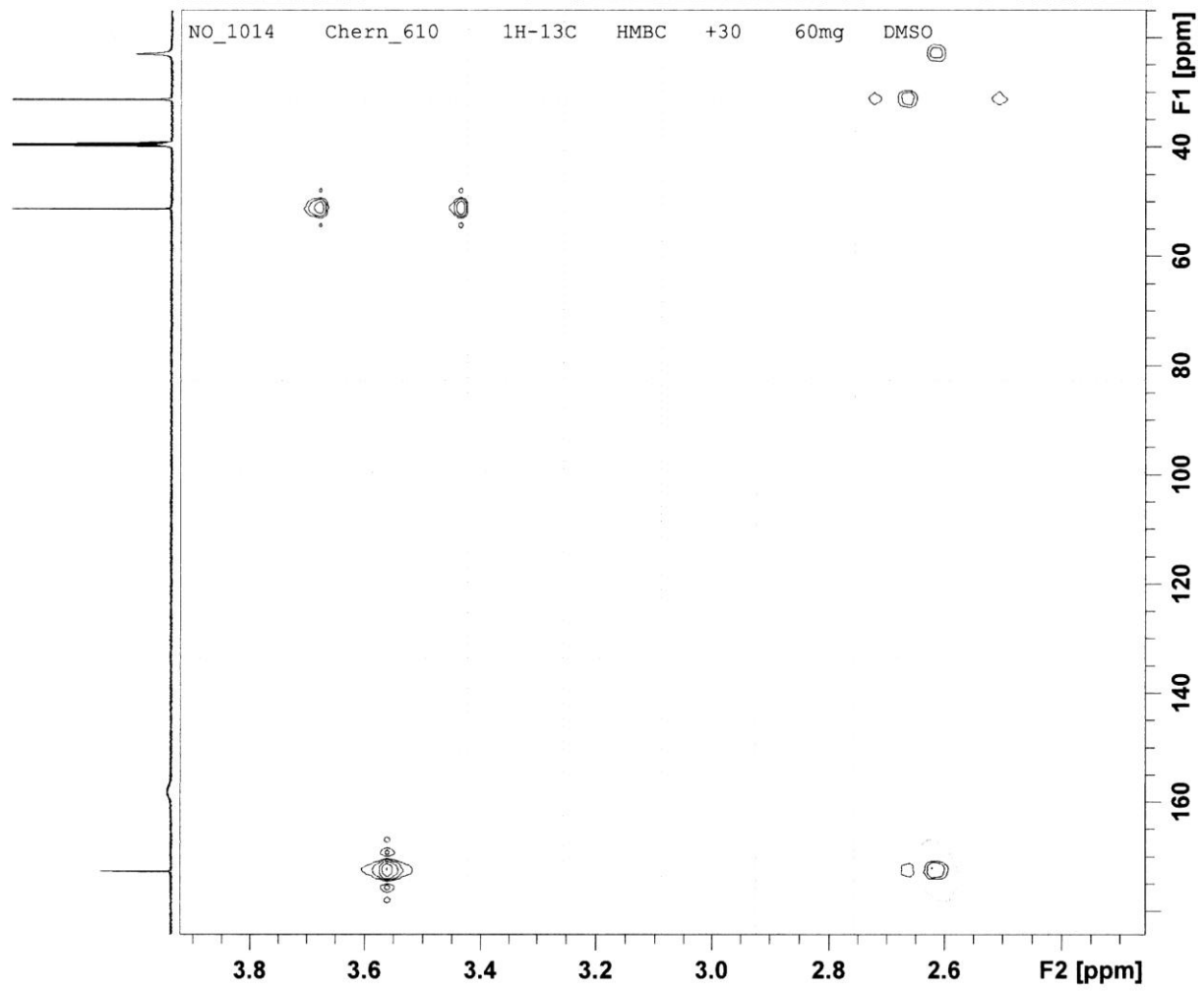
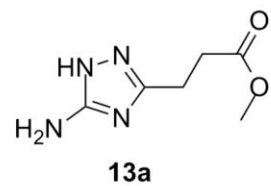


FTIR spectrum of compound 12



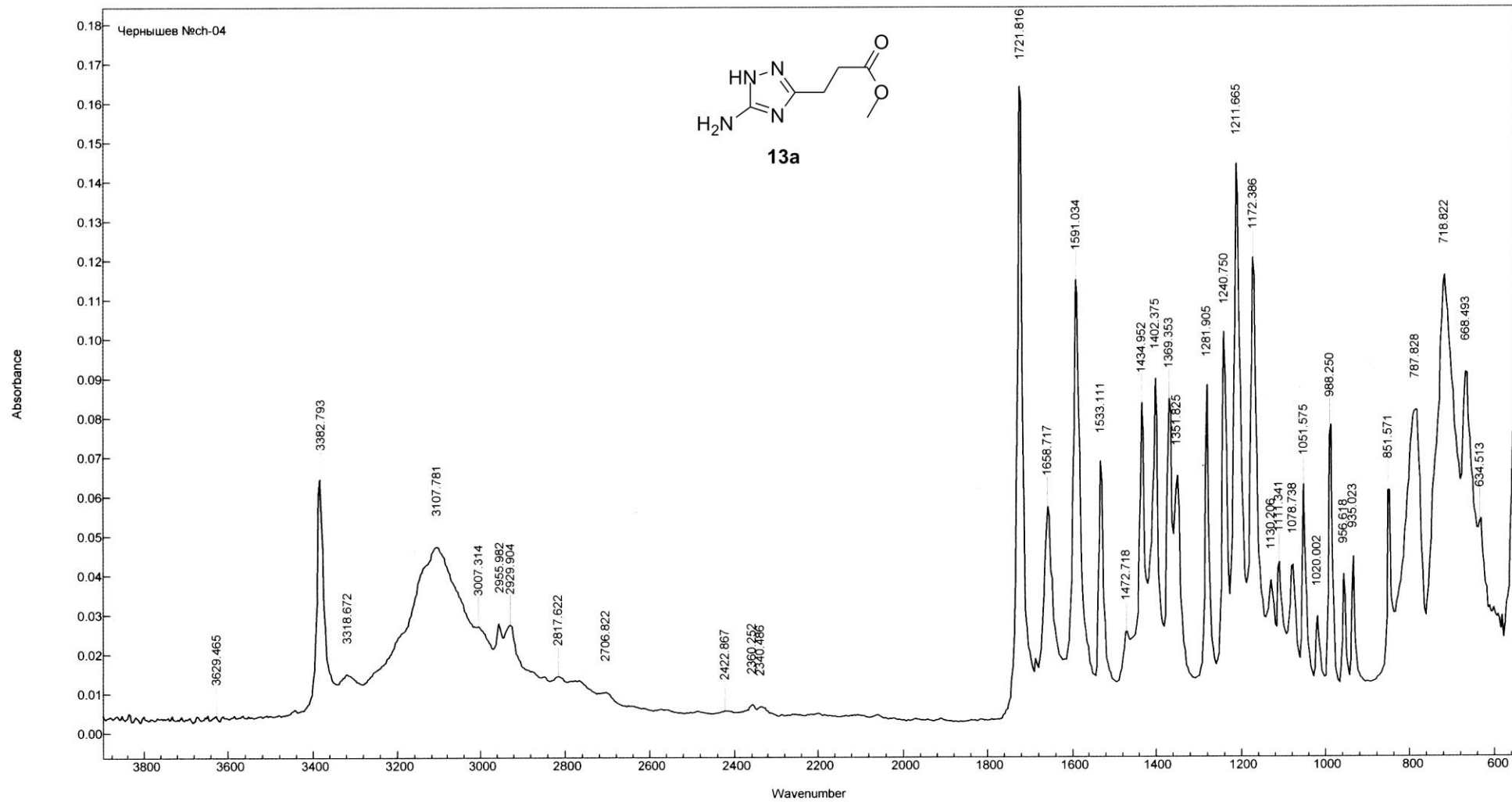
<sup>13</sup>C NMR spectrum (150 MHz) of compound **13a**

NO\_1014 7 2 D: GENA\_5



$^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **13a**

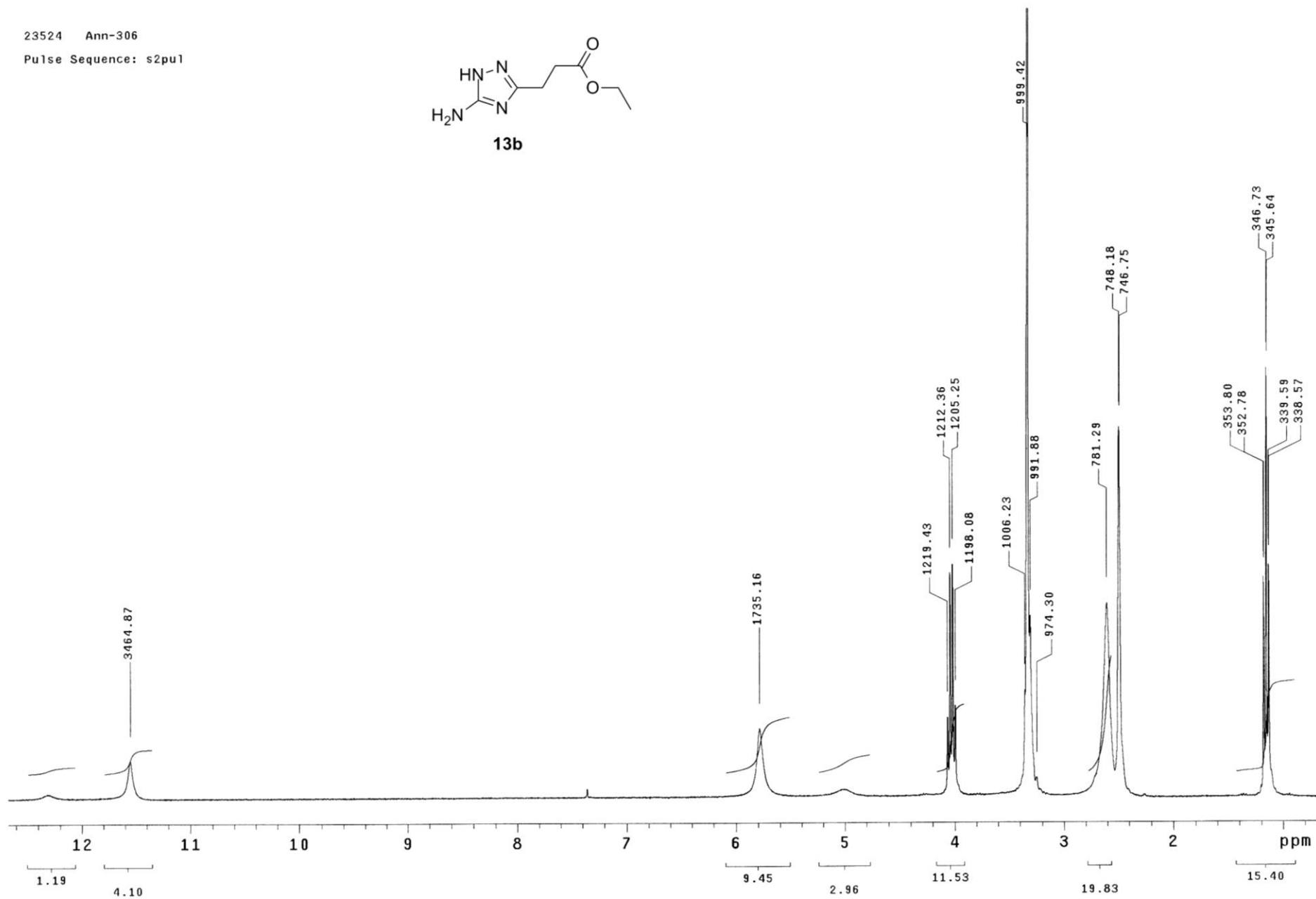
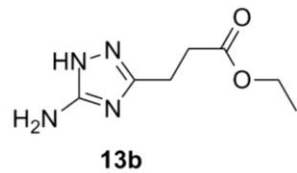
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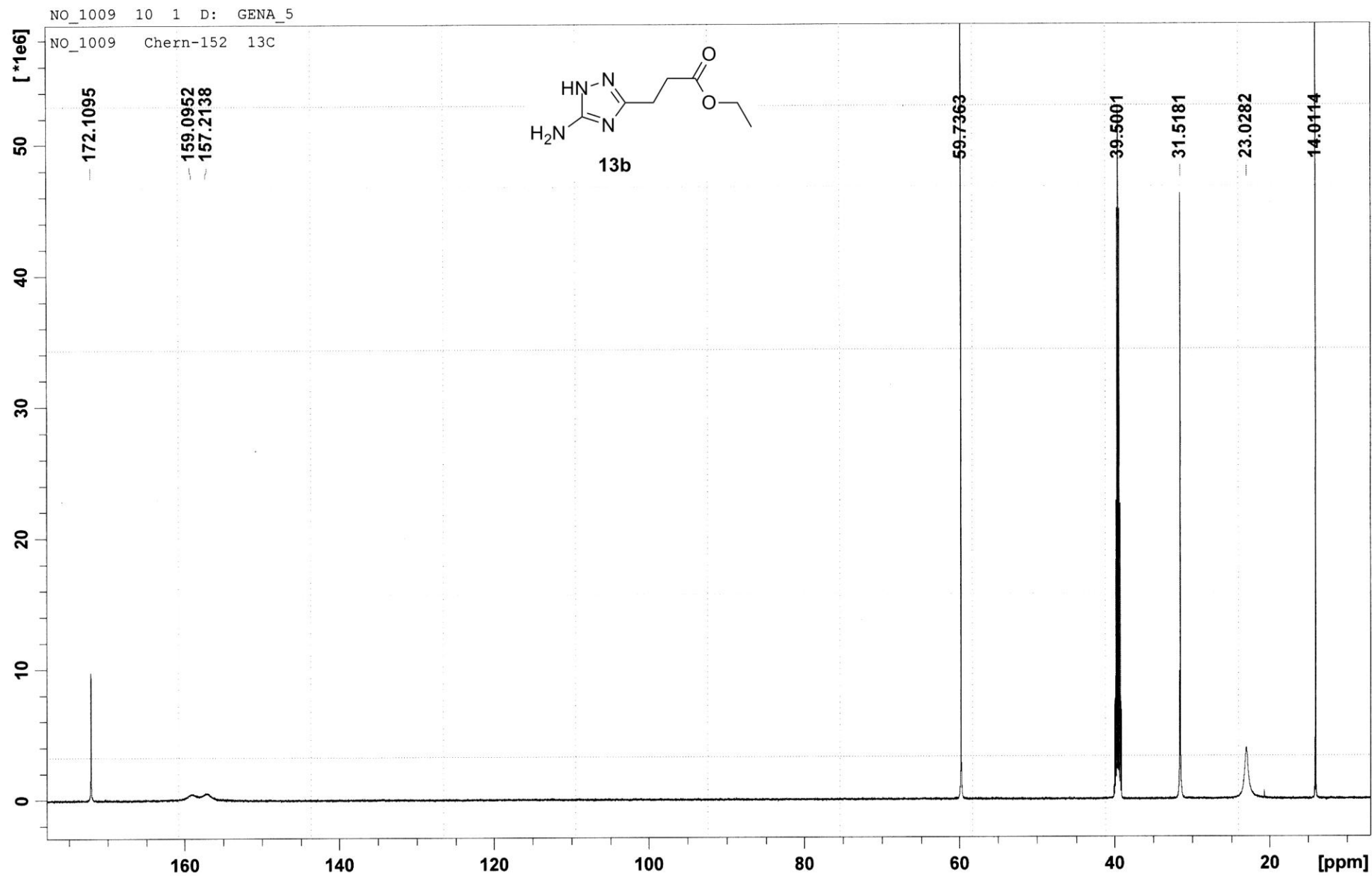
FTIR spectrum of compound 13a

23524 Ann-306

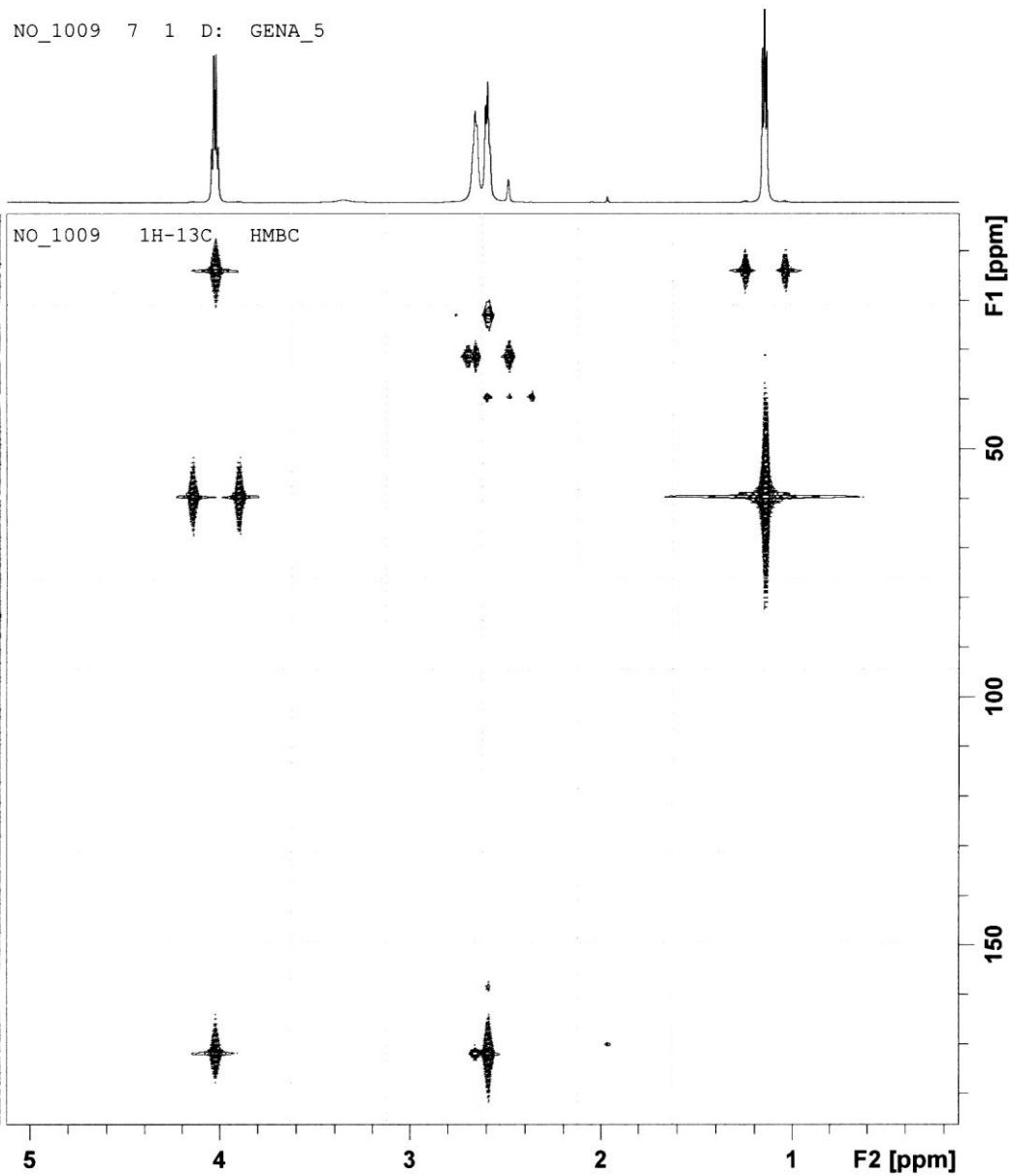
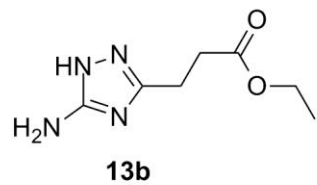
Pulse Sequence: s2pu1



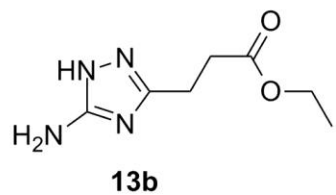
<sup>1</sup>H NMR spectrum (300 MHz) of compound **13b**



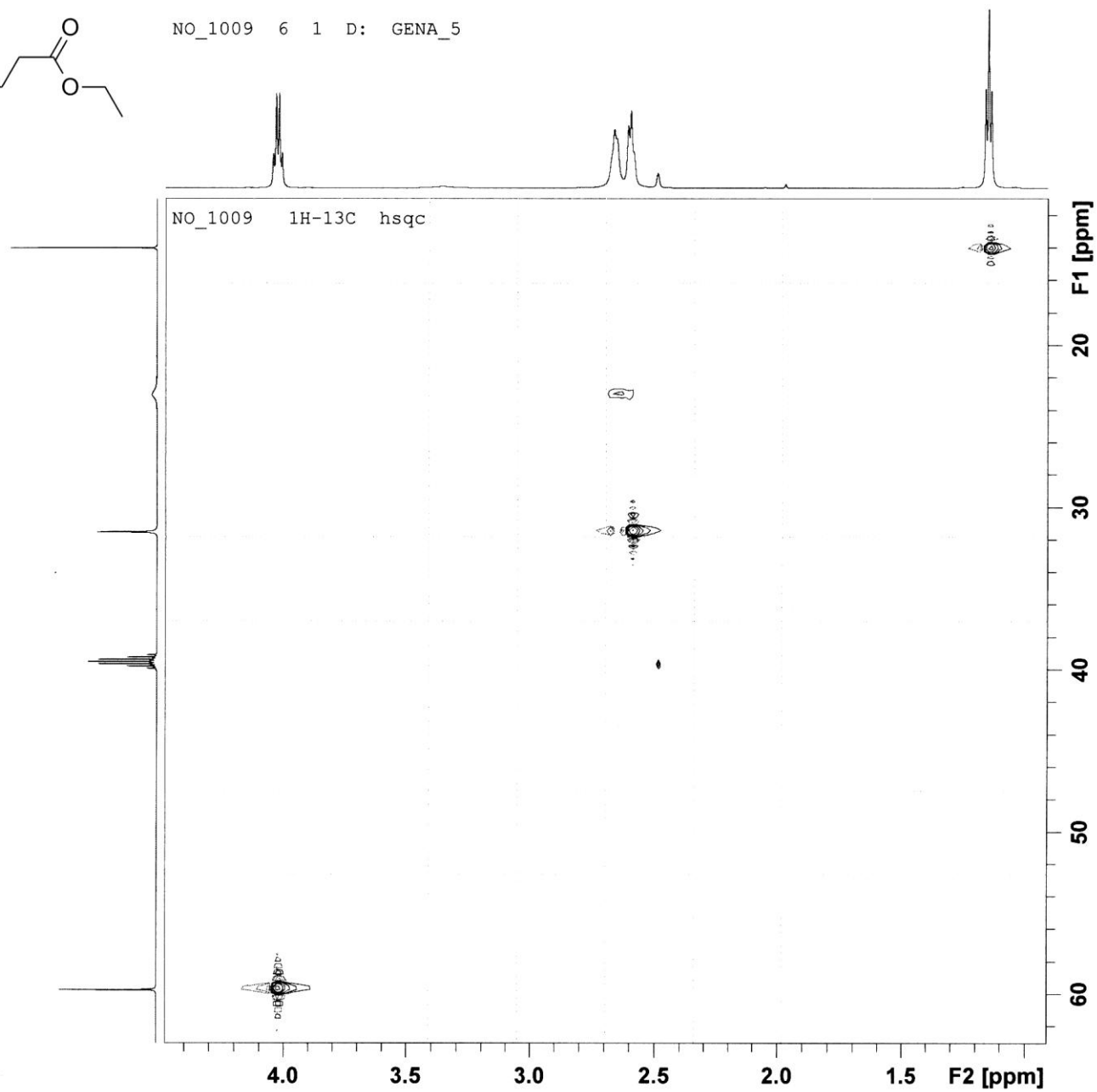
$^{13}\text{C}$  NMR spectrum (150 MHz) of compound **13b**



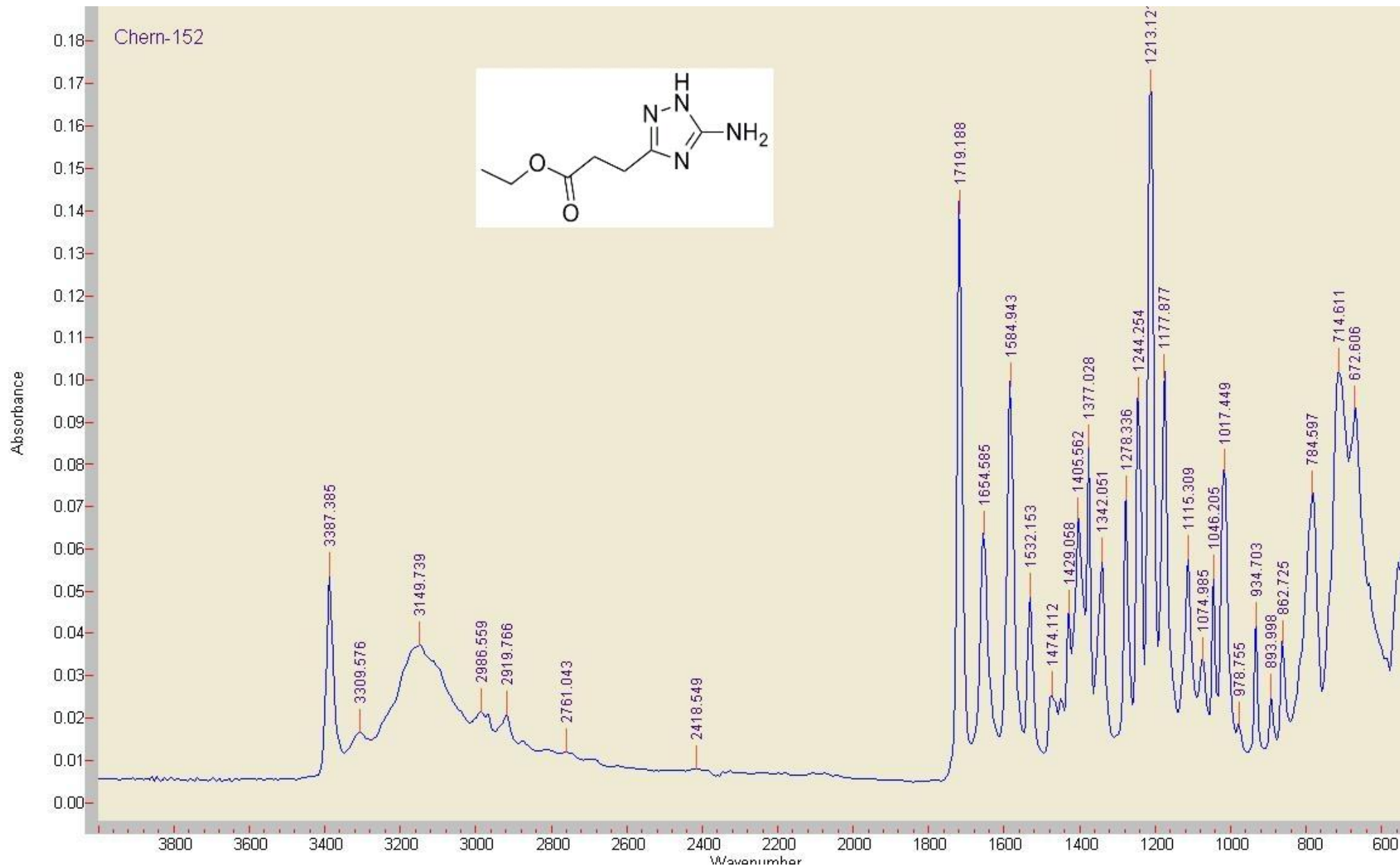
$^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **13b**



NO\_1009 6 1 D: GENA\_5



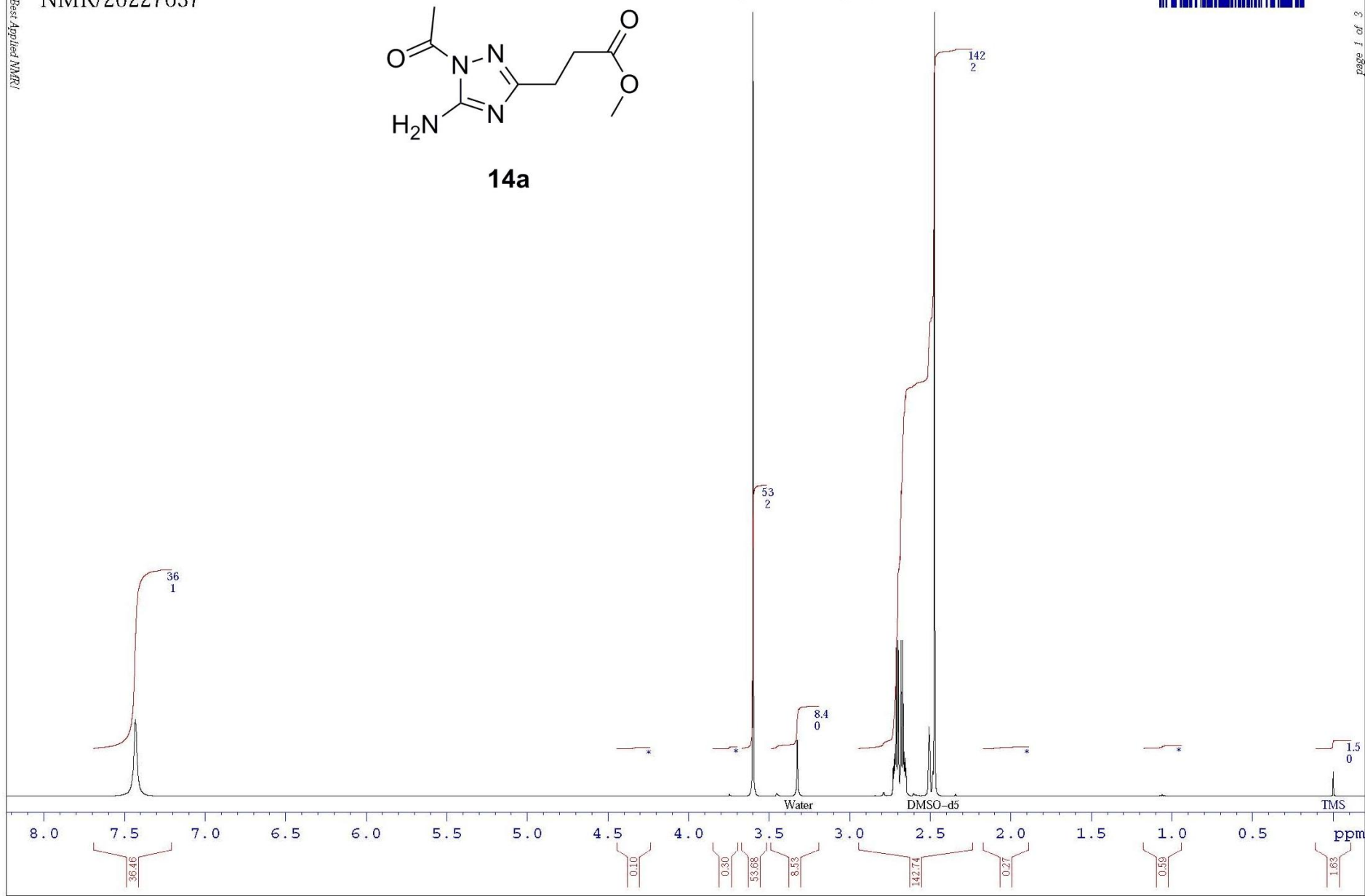
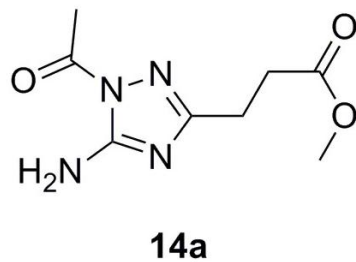
$^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of compound **13b**



FTIR spectrum of compound **13b**

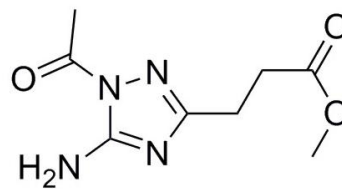
NMR/20227637

Found protons = 5 impurity\* = 0.4 %

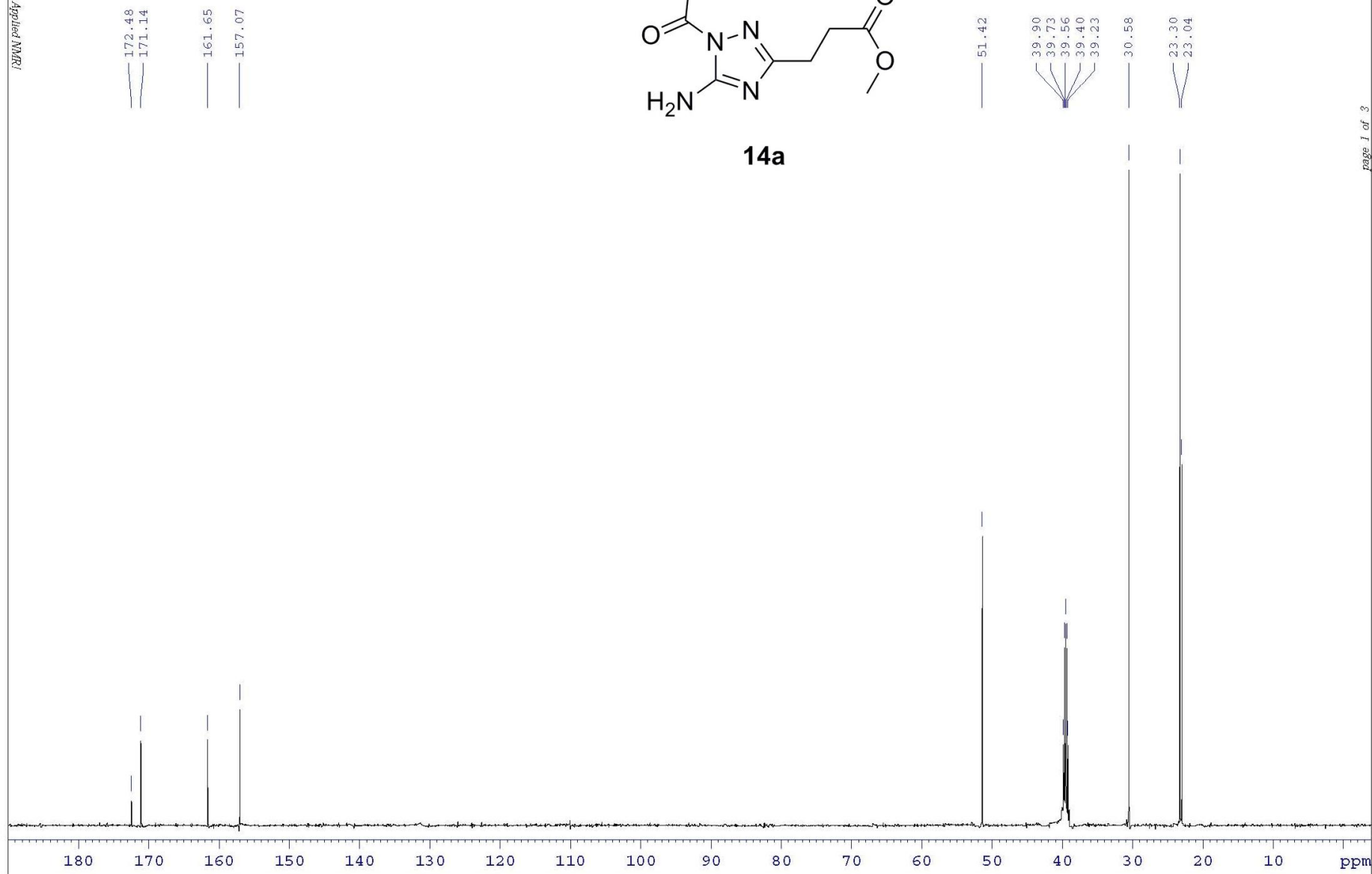


<sup>1</sup>H NMR spectrum (500 MHz) of compound **14a**

NMR/20227637

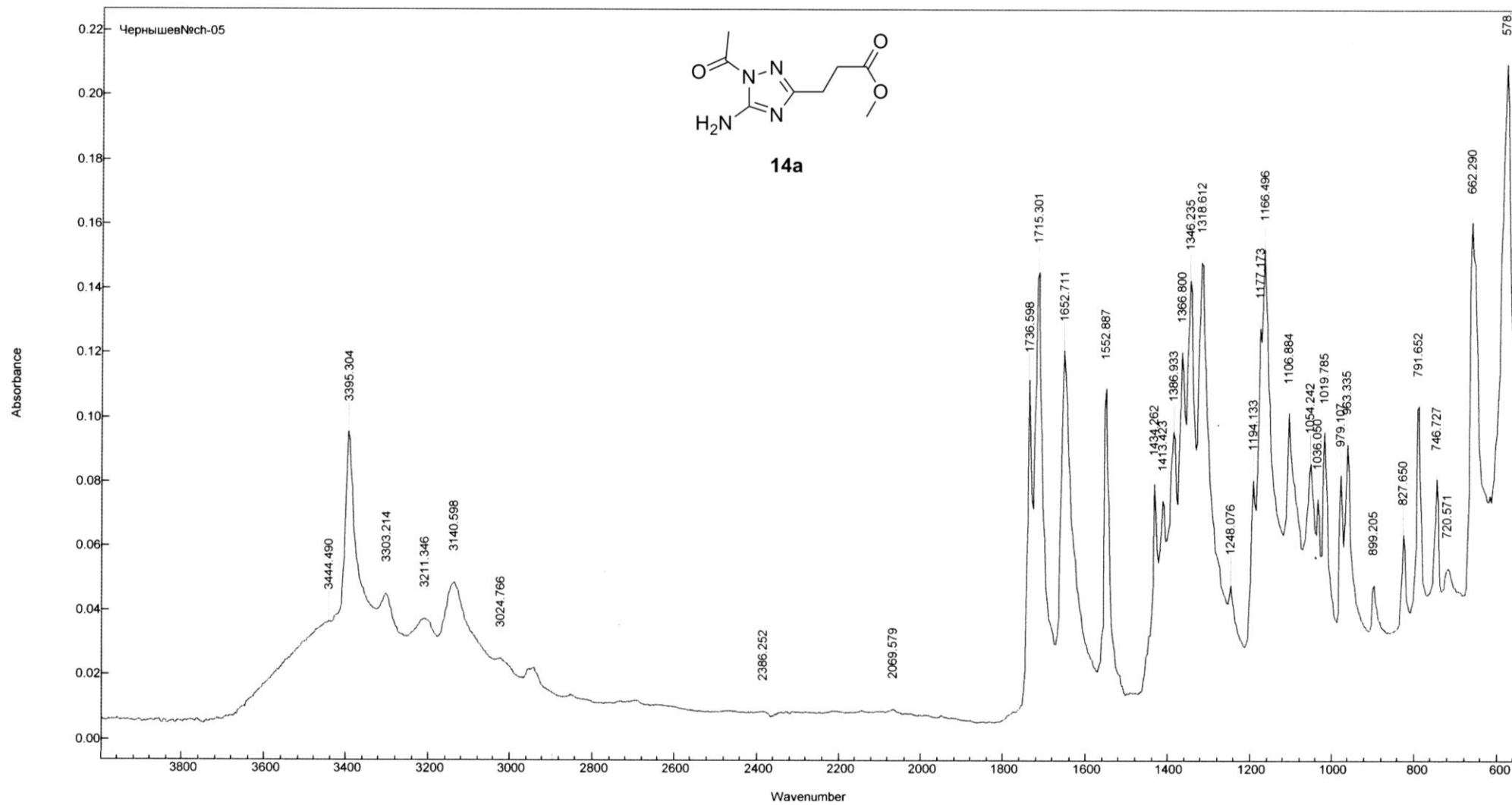


14a



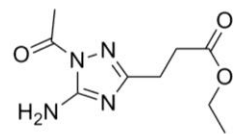
<sup>13</sup>C NMR spectrum (125 MHz) of compound 14a

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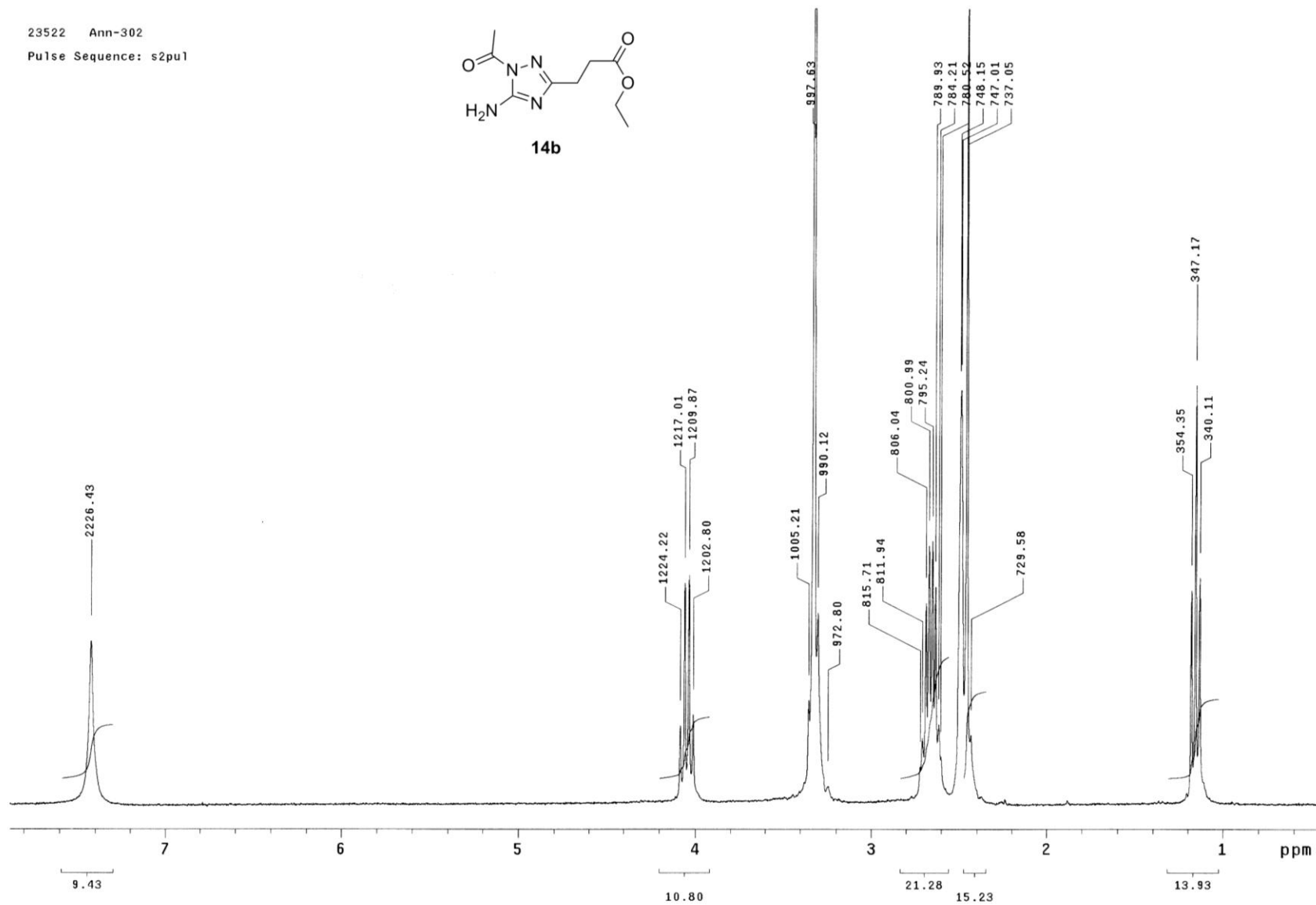


FTIR spectrum of compound 14a

23522 Ann-302  
Pulse Sequence: s2pu1

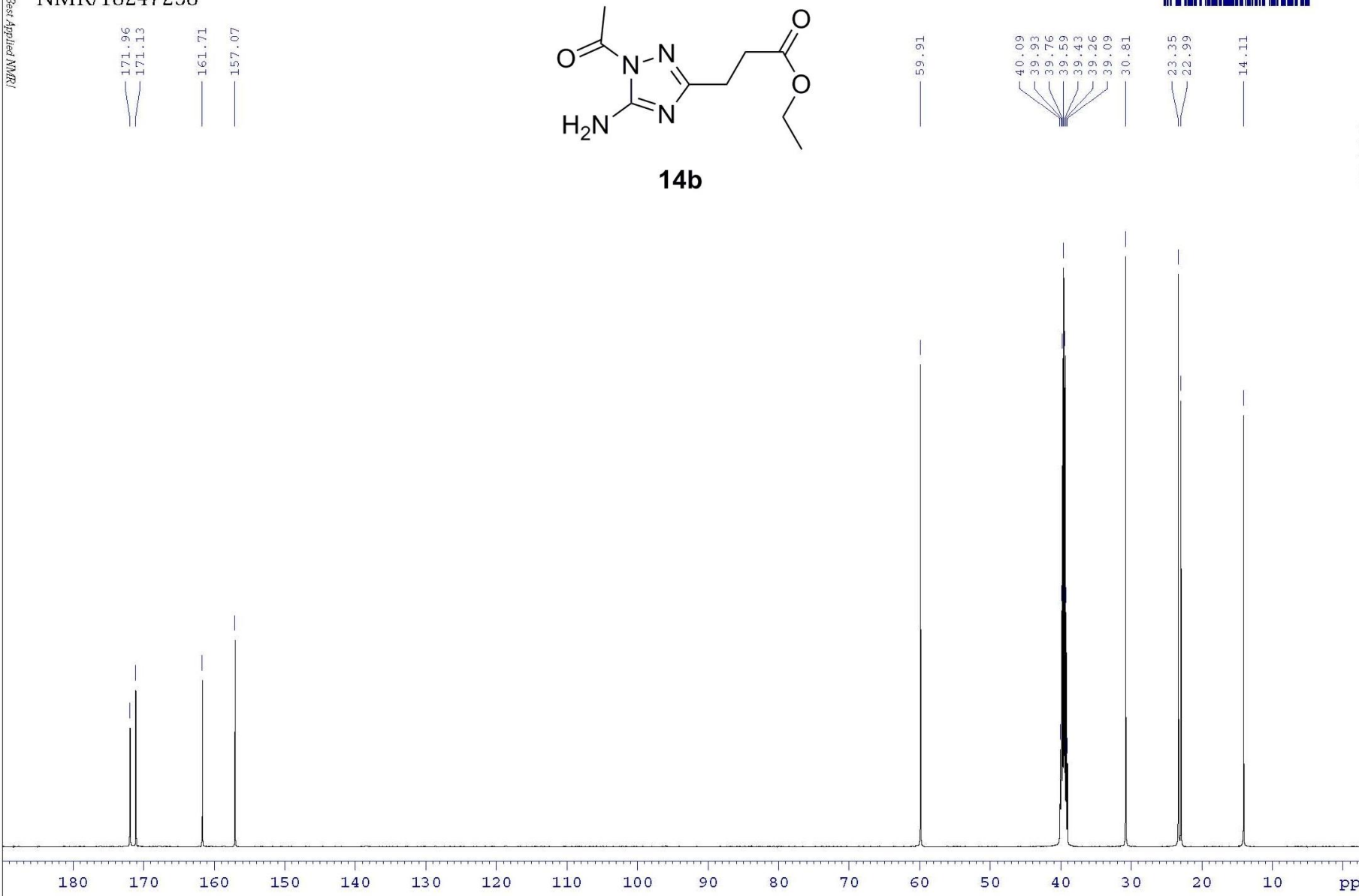


**14b**

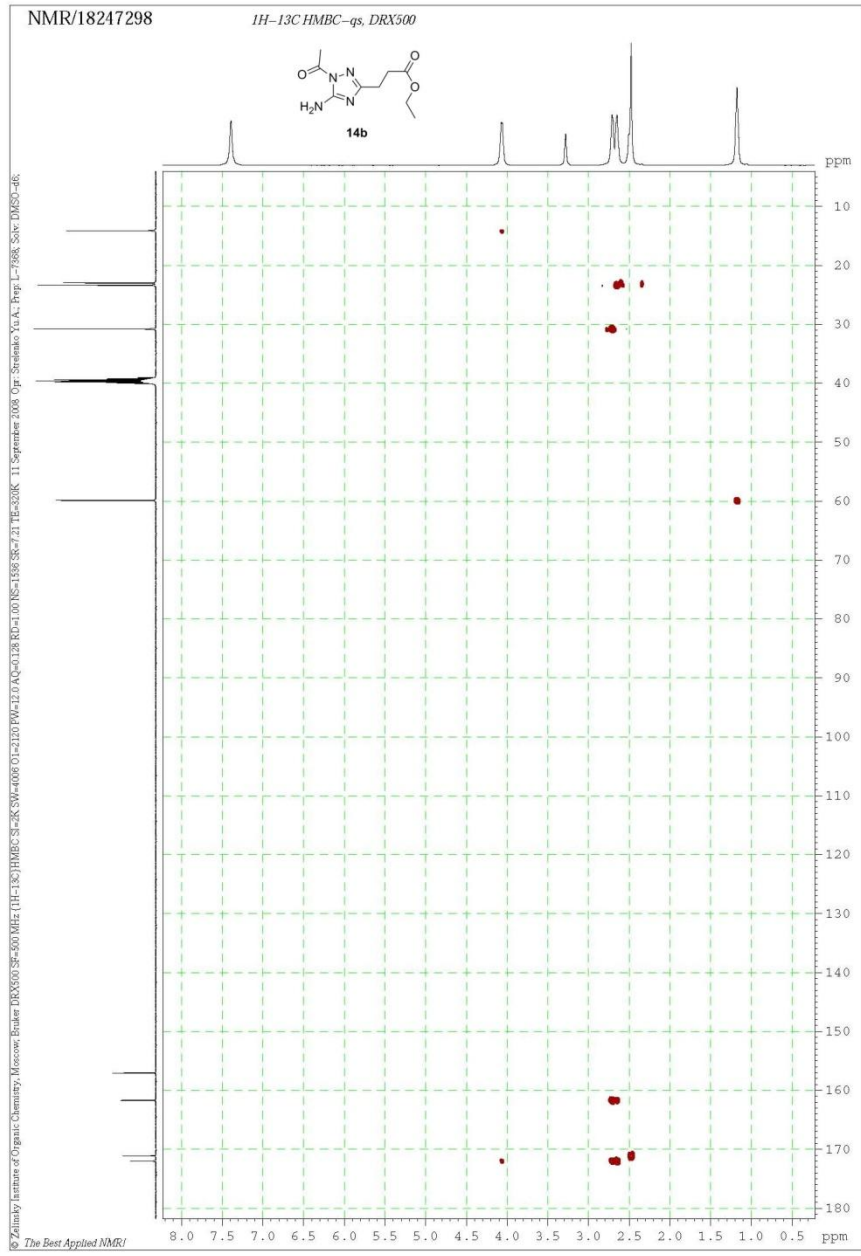


<sup>1</sup>H NMR spectrum (300 MHz) of compound **14b**

NMR/18247298

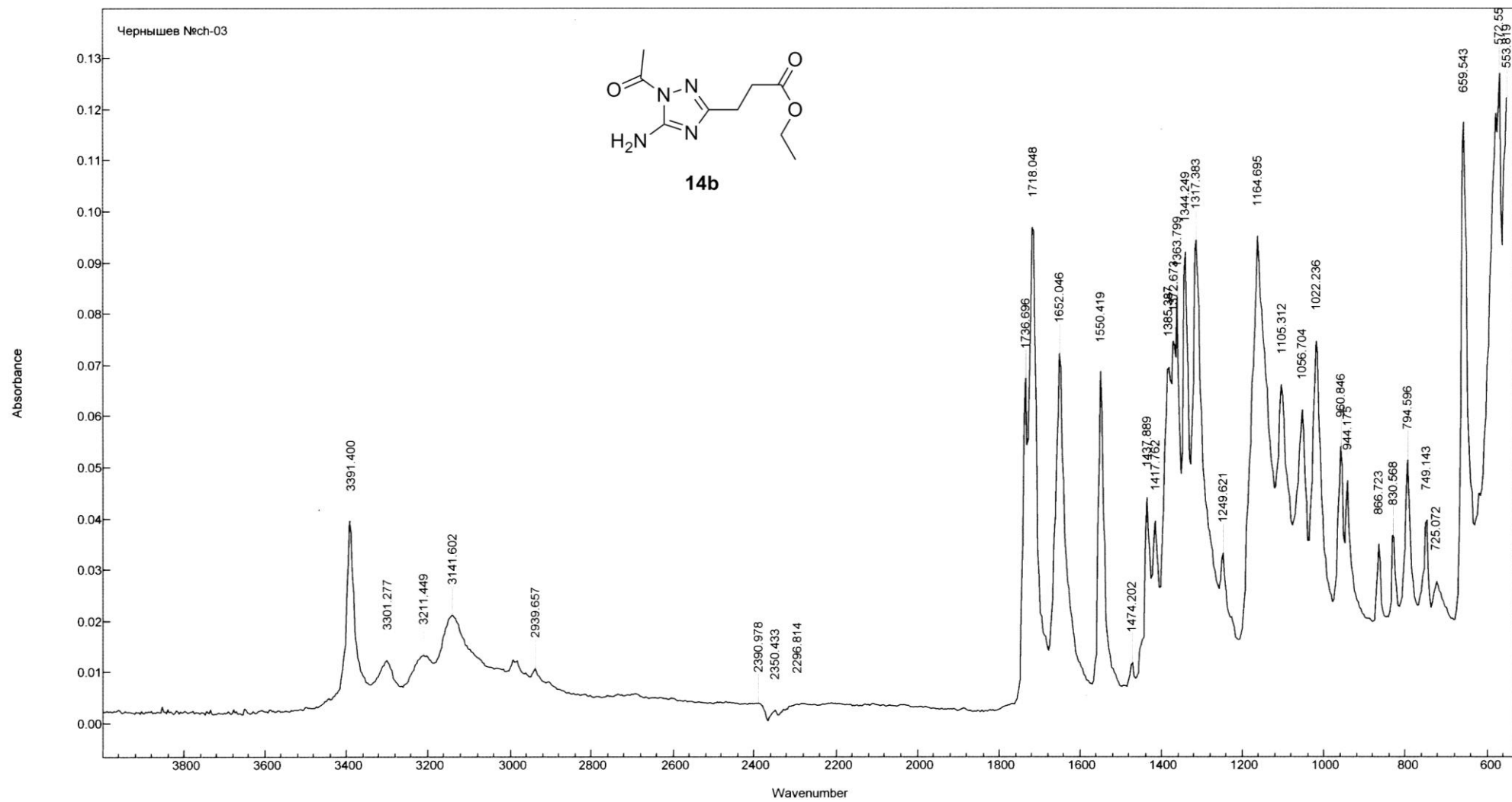


<sup>13</sup>C NMR spectrum (125 MHz) of compound **14b**



$^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **14b**

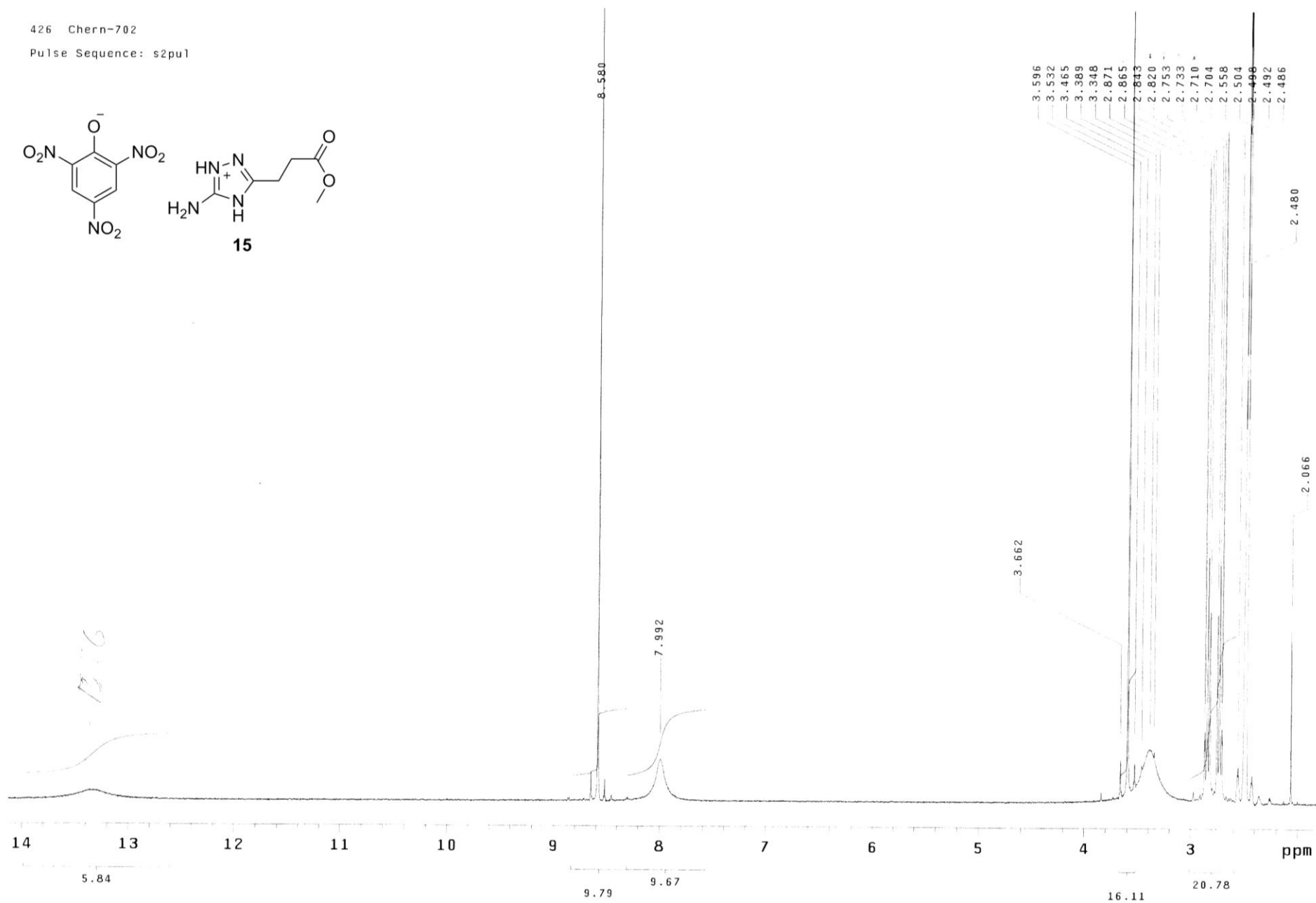
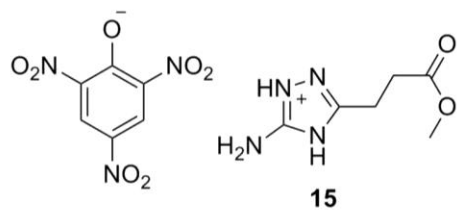
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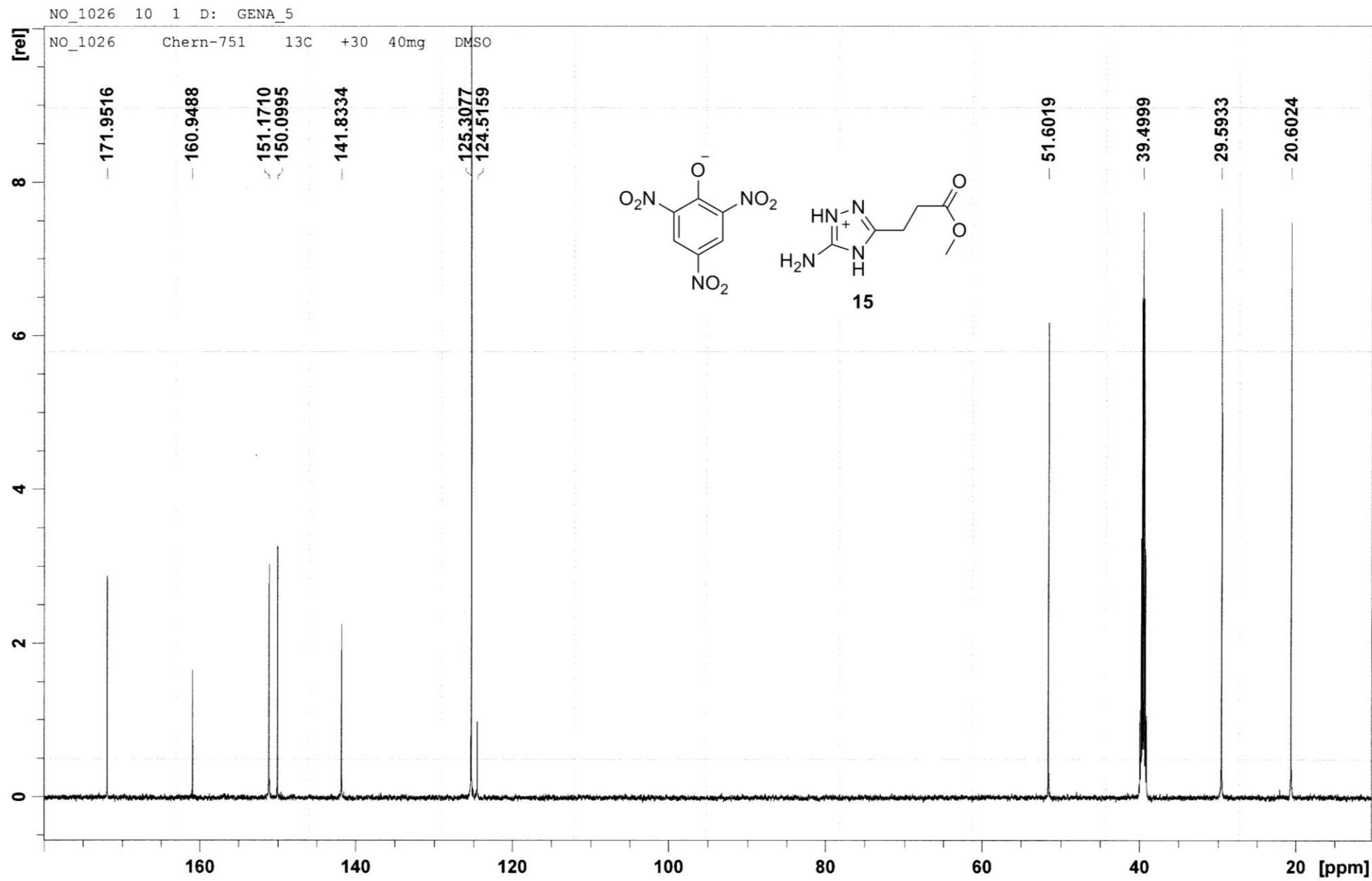
FTIR spectrum of compound **14b**

426 Chern-702

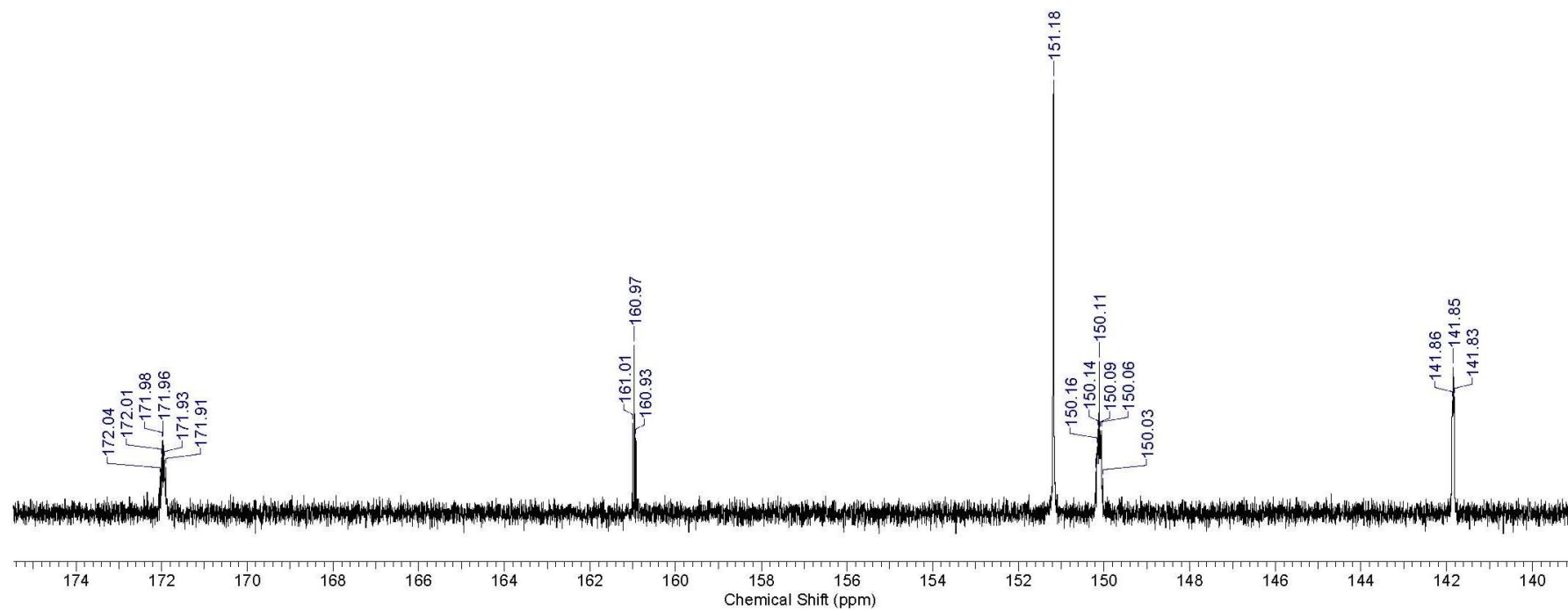
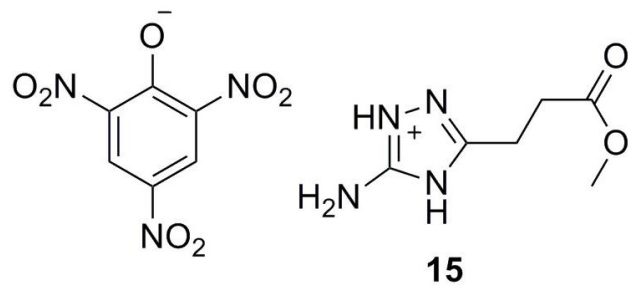
Pulse Sequence: s2pu1



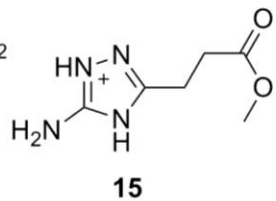
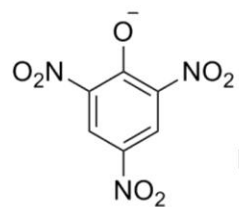
<sup>1</sup>H NMR spectrum (300 MHz) of compound **15**



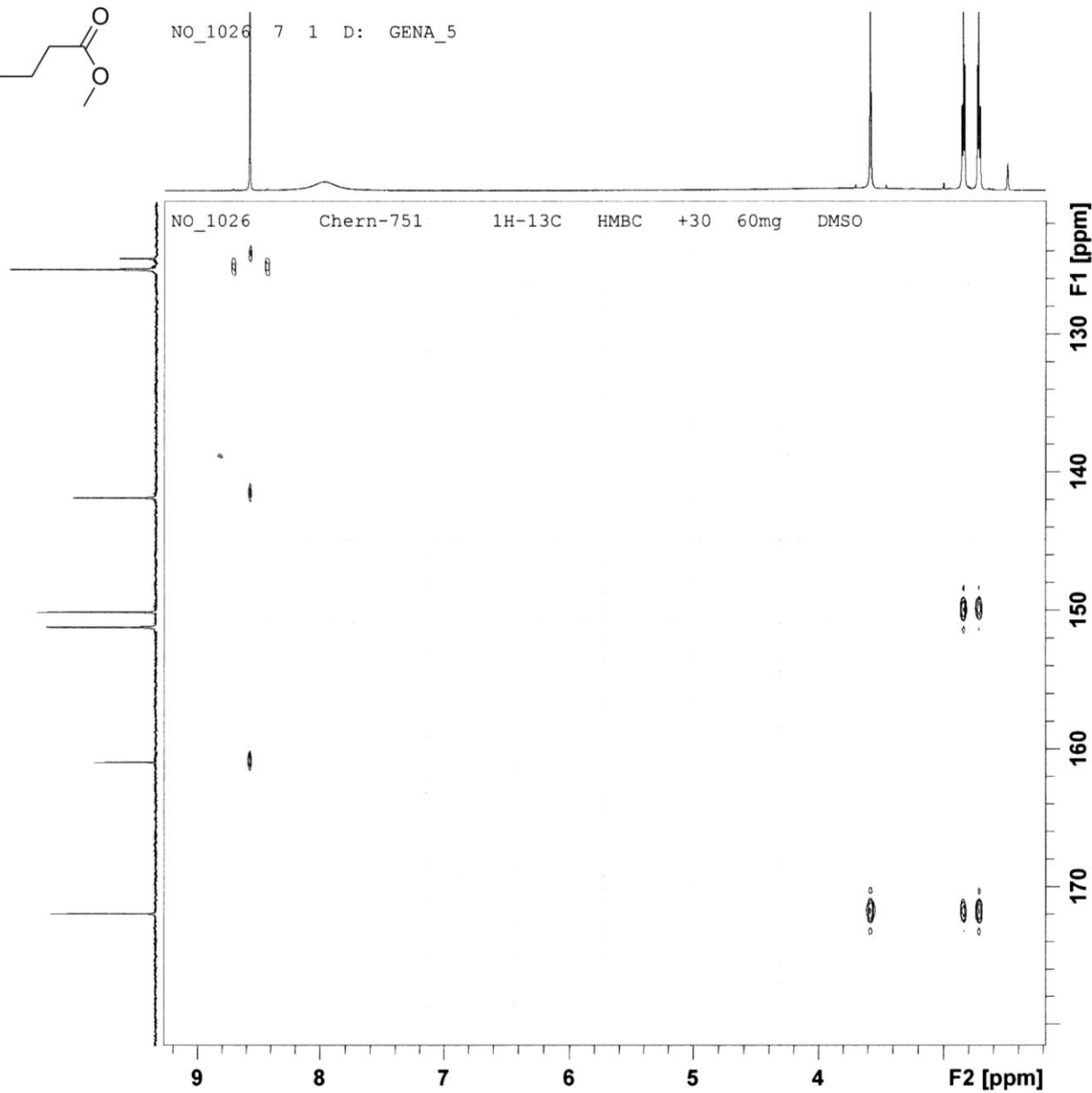
$^{13}\text{C}$  NMR spectrum (150 MHz) of compound 15



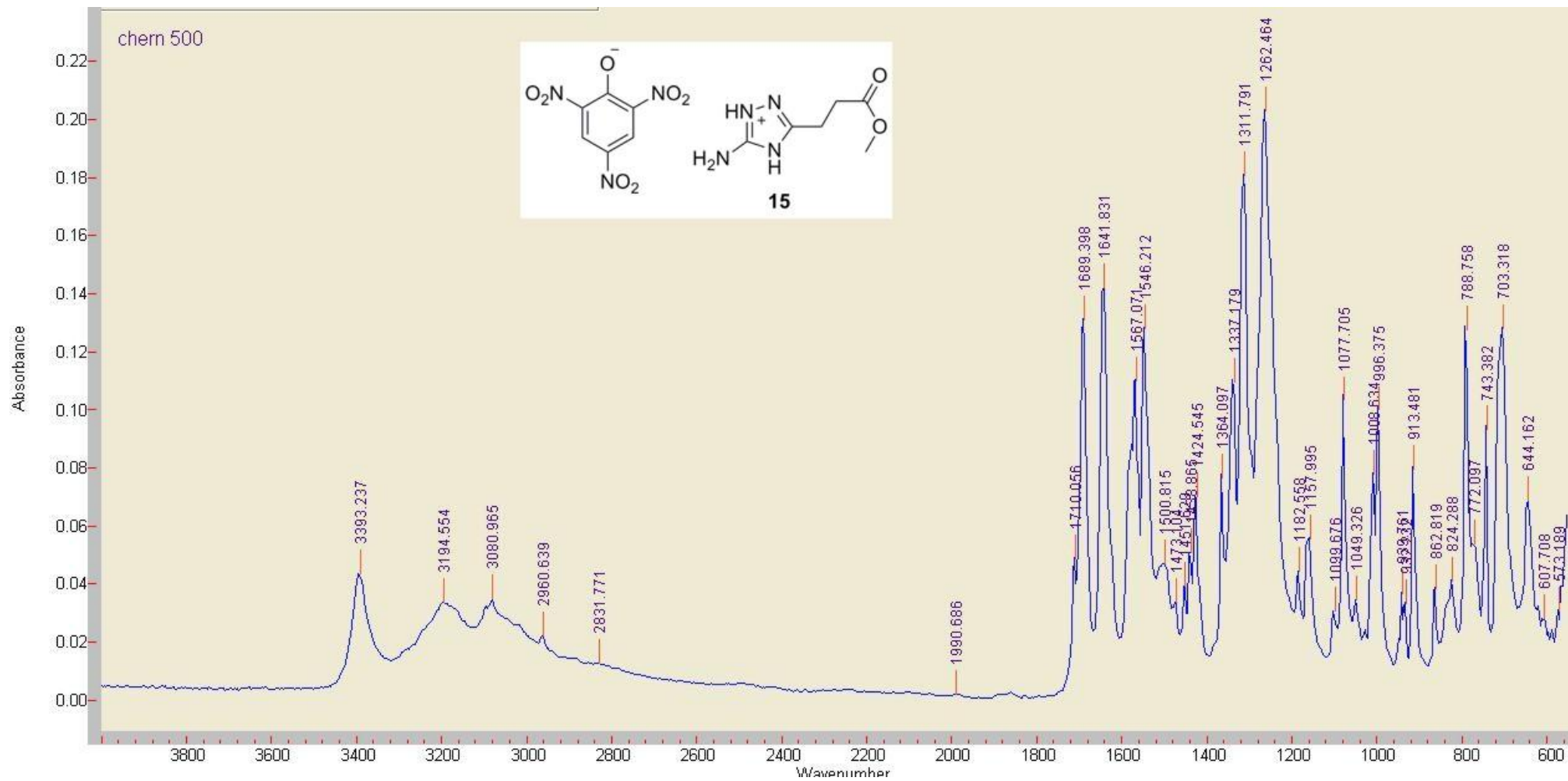
Fragment of proton coupled  $^{13}\text{C}$  NMR spectrum (150 MHz) of compound **15**



NO\_1026 7 1 D: GENA\_5



$^1\text{H}$ - $^{13}\text{C}$  HMBC spectrum of compound **15**



FTIR spectrum of compound **15**