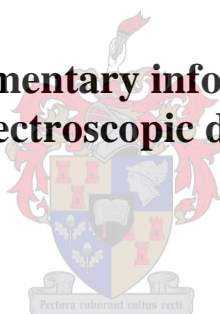


The Rational Design and Synthesis of Novel HIV Non-nucleoside Reverse Transcriptase Inhibitors

by
Ronel Müller

**Supplementary information
(Spectroscopic data)**



Supervisor: Dr Stephen C. Pelly
Co-supervisor: Prof Willem A. L. van Otterlo

December 2013

Ethyl 5-chloro-3-(1-phenylcyclopropyl)-1 <i>H</i> -indole-2-carboxylate – 2 (Crude compound).....	1
¹ H NMR Spectrum	1
Ethyl 3-benzoyl-5-chloro-1 <i>H</i> -indole-2-carboxylate - 3	1
¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1
gHSQC NMR Spectrum	1
Mass Spectrum.....	1
Infrared Spectrum	1
1- <i>Tert</i> -butyl 2-ethyl 3-benzoyl-5-chloro-1 <i>H</i> -indole-1,2-dicarboxylate - 4	1
¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1
gHSQC NMR Spectrum	1
Mass Spectrum.....	1
Infrared Spectrum	1
Ethyl 5-chloro-3-(1-phenylvinyl)-1 <i>H</i> -indole-2-carboxylate - 5	1
¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1
gHSQC NMR Spectrum	1
Mass Spectrum.....	1
Infrared Spectrum	1
1- <i>Tert</i> -butyl 2-ethyl 5-chloro-3-(1-phenylvinyl)-1 <i>H</i> -indole-1,2-dicarboxylate - 6	1
¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1
gHSQC NMR Spectrum	1
Mass Spectrum.....	1
Infrared Spectrum	1
Ethyl 3-benzoyl-5-chloro-1-tosyl-1 <i>H</i> -indole-2-carboxylate - 7	1
¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1

gHSQC NMR Spectrum	1
Mass Spectrum.....	1
Infrared Spectrum	1
Ethyl 5-chloro-3-(1-phenylvinyl)-1-tosyl-1 <i>H</i> -indole-2-carboxylate - 8.....	1
¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1
gHSQC NMR Spectrum	1
Mass Spectrum.....	1
Infrared Spectrum	1
(1-Chlorocyclopropyl)benzene – 10 (Crude compound)	1
¹ H NMR Spectrum	1
<i>Tert</i> -butyldimethyl(1-phenylvinyl)oxy)silane - 13.....	1
¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1
gHSQC NMR Spectrum	1
Mass Spectrum.....	1
Infrared Spectrum	1
<i>Tert</i> -butyldimethyl(1-phenylcyclopropoxy)silane - 14.....	1
¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1
gHSQC NMR Spectrum	1
Mass Spectrum.....	1
Infrared Spectrum	1
5-Chloro-3-(1-phenylpropyl)-1 <i>H</i> -indole – 15	1
¹ H NMR Spectrum	1
Ethyl 3-benzyl-5-chloro-1 <i>H</i> -indole-2-carboxylate -16	1
¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1
gHSQC NMR Spectrum	1
Mass Spectrum.....	1

Infrared Spectrum	1
Infrared Spectrum	1
(2-Chloropropan-2-yl)benzene – 18.....	1
Ethyl 5-chloro-3-(cyanomethyl)-1 <i>H</i> -indole-2-carboxylate – 23	1
¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1
gHSQC NMR Spectrum	1
Mass Spectrum.....	1
Infrared Spectrum	1
2-(5-chloro-1 <i>H</i> -indol-3-yl)acetonitrile – 32.....	1
¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1
gHSQC NMR Spectrum	1
Mass Spectrum.....	1
Infrared Spectrum	1
<i>Tert</i> -butyl 5-chloro-3-(cyanomethyl)-1 <i>H</i> -indole-1-carboxylate – 33	1
¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1
gHSQC NMR Spectrum	1
Mass Spectrum.....	1
Infrared Spectrum	1
2-(5-Chloro-1-tosyl-1 <i>H</i> -indol-3-yl)acetonitrile - 35.....	1
¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1
gHSQC NMR Spectrum	1
Mass Spectrum.....	1
Infrared Spectrum	1
2-(5-Chloro-1-tosyl-1 <i>H</i> -indol-3-yl)-2-methylpropanenitrile – 36.....	1
¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1

COSY NMR Spectrum	1
gHSQC NMR Spectrum	1
Mass Spectrum.....	1
Infrared Spectrum	1
2-(5-Chloro-1 <i>H</i> -indol-3-yl)-2-methylpropanenitrile – 37	1
¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1
gHSQC NMR Spectrum	1
Mass Spectrum.....	1
Infrared Spectrum	1
1-(5-Chloro-1-tosyl-1 <i>H</i> -indol-3-yl)cyclopropanecarbonitrile – 38	1
¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1
gHSQC NMR Spectrum	1
Mass Spectrum.....	1
Infrared Spectrum	1
1-(5-Chloro-1 <i>H</i> -indol-3-yl)cyclopropanecarbonitrile - 39	1
¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1
gHSQC NMR Spectrum	1
Mass Spectrum.....	1
Infrared Spectrum	1
3-Benzyl-5-chloro-2-(1 <i>H</i> -tetrazol-5-yl)-1 <i>H</i> -indole - 46	1
¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1
gHSQC NMR Spectrum	1
Mass Spectrum.....	1
Infrared Spectrum	1
5-Chloro-1 <i>H</i> -indole-2-carboxylic acid – 47	1
¹ H NMR Spectrum	1

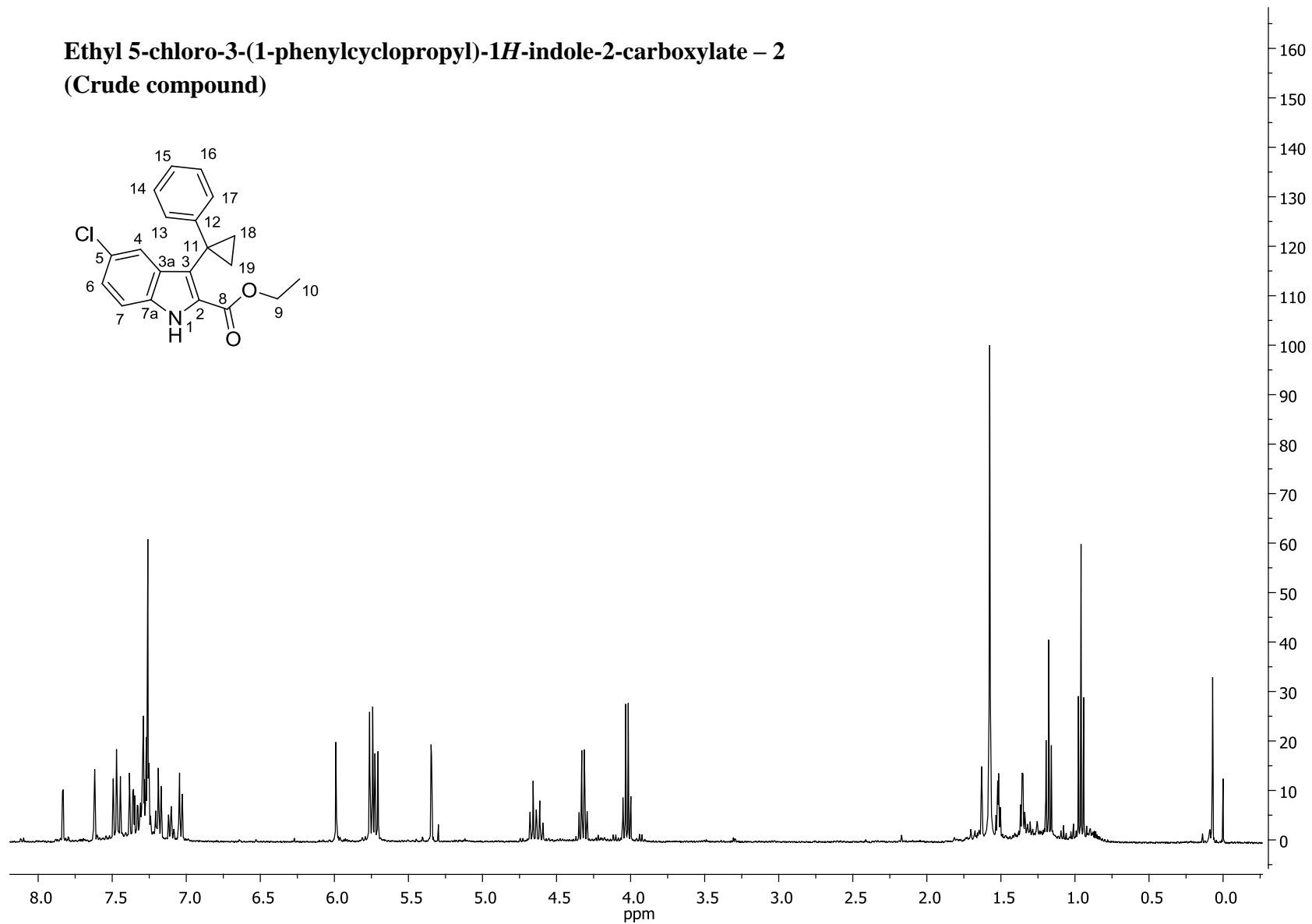
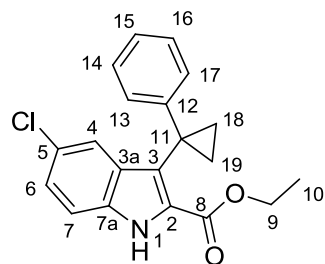
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1
gHSQC NMR Spectrum	1
Mass Spectrum.....	1
Infrared Spectrum	1
5-Chloro-1 <i>H</i> -indole-2-carboxamide – 49	1
¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1
gHSQC NMR Spectrum	1
Mass Spectrum.....	1
Infrared Spectrum	1
3-Benzyl-5-chloro-1 <i>H</i> -indole-2-carboxylic acid – 50.....	1
¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1
gHSQC NMR Spectrum	1
Mass Spectrum.....	1
Infrared Spectrum	1
3-Benzyl-5-chloro-1 <i>H</i> -indole-2-carboxamide – 52.....	1
¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1
gHSQC NMR Spectrum	1
Mass Spectrum.....	1
Infrared Spectrum	1
3-Benzyl-5-chloro-1 <i>H</i> -indole-2-carbonitrile – 53.....	1
¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1
gHSQC NMR Spectrum	1
Mass Spectrum.....	1
Infrared Spectrum	1
3-Benzyl-5-chloro-1-tosyl-1 <i>H</i> -indole-2-carbonitrile – 54.....	1

¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1
gHSQC NMR Spectrum	1
Mass Spectrum.....	1
Infrared Spectrum.....	1
<i>R/S</i> -ethyl 5-chloro-3-(methoxy(phenyl)methyl)-1 <i>H</i> -indole-2-carboxylate – 59- <i>R/S</i>	1
¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1
gHSQC NMR Spectrum	1
Mass Spectrum.....	1
Infrared Spectrum.....	1
<i>R/S</i> -ethyl 5-chloro-3-(hydroxy(phenyl)methyl)-1-tosyl-1 <i>H</i> -indole-2-carboxylate – 61- <i>R/S</i>	1
¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1
gHSQC NMR Spectrum	1
Mass Spectrum.....	1
Infrared Spectrum.....	1
<i>R/S</i> -ethyl 5-chloro-3-(methoxy(phenyl)methyl)-1-tosyl-1 <i>H</i> -indole-2-carboxylate - 62- <i>R/S</i>	1
¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1
gHSQC NMR Spectrum	1
Mass Spectrum.....	1
Infrared Spectrum.....	1
<i>R/S</i> -ethyl 5-chloro-3-(ethoxy(phenyl)methyl)-1-tosyl-1 <i>H</i> -indole-2-carboxylate -70- <i>R/S</i>	1
¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1
gHSQC NMR Spectrum	1
Mass Spectrum.....	1
Infrared Spectrum.....	1

<i>R/S</i> -ethyl 5-chloro-3-(ethoxy(phenyl)methyl)-1 <i>H</i> -indole-2-carboxylate -71- <i>R/S</i>	1
¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1
gHSQC NMR Spectrum	1
Mass Spectrum.....	1
Infrared Spectrum	1
<i>R/S</i> -ethyl 5-chloro-3-(hydroxy(phenyl)methyl)-1 <i>H</i> -indole-2-carboxylate – 72- <i>R/S</i>	1
¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1
gHSQC NMR Spectrum	1
Mass Spectrum.....	1
Infrared Spectrum	1
(5-Chloro-1 <i>H</i> -indol-3-yl)(phenyl)methanone - 73.....	1
¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1
gHSQC NMR Spectrum	1
Mass Spectrum.....	1
Infrared Spectrum	1
<i>R/S</i> -(5-chloro-1 <i>H</i> -indol-3-yl)(phenyl)methanol – 74- <i>R/S</i>	1
¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1
gHSQC NMR Spectrum	1
Mass Spectrum.....	1
Infrared Spectrum	1
Ethyl 5-chloro-3-(((7,7-dimethyl-2-oxobicyclo[2.2.1]heptan-1-yl)methylsulfonyloxy)(phenyl)methyl)- 1 <i>H</i> -indole-2-carboxylate -78	1
¹ H NMR Spectrum	1
¹³ C NMR Spectrum	1
COSY NMR Spectrum	1
gHSQC NMR Spectrum	1

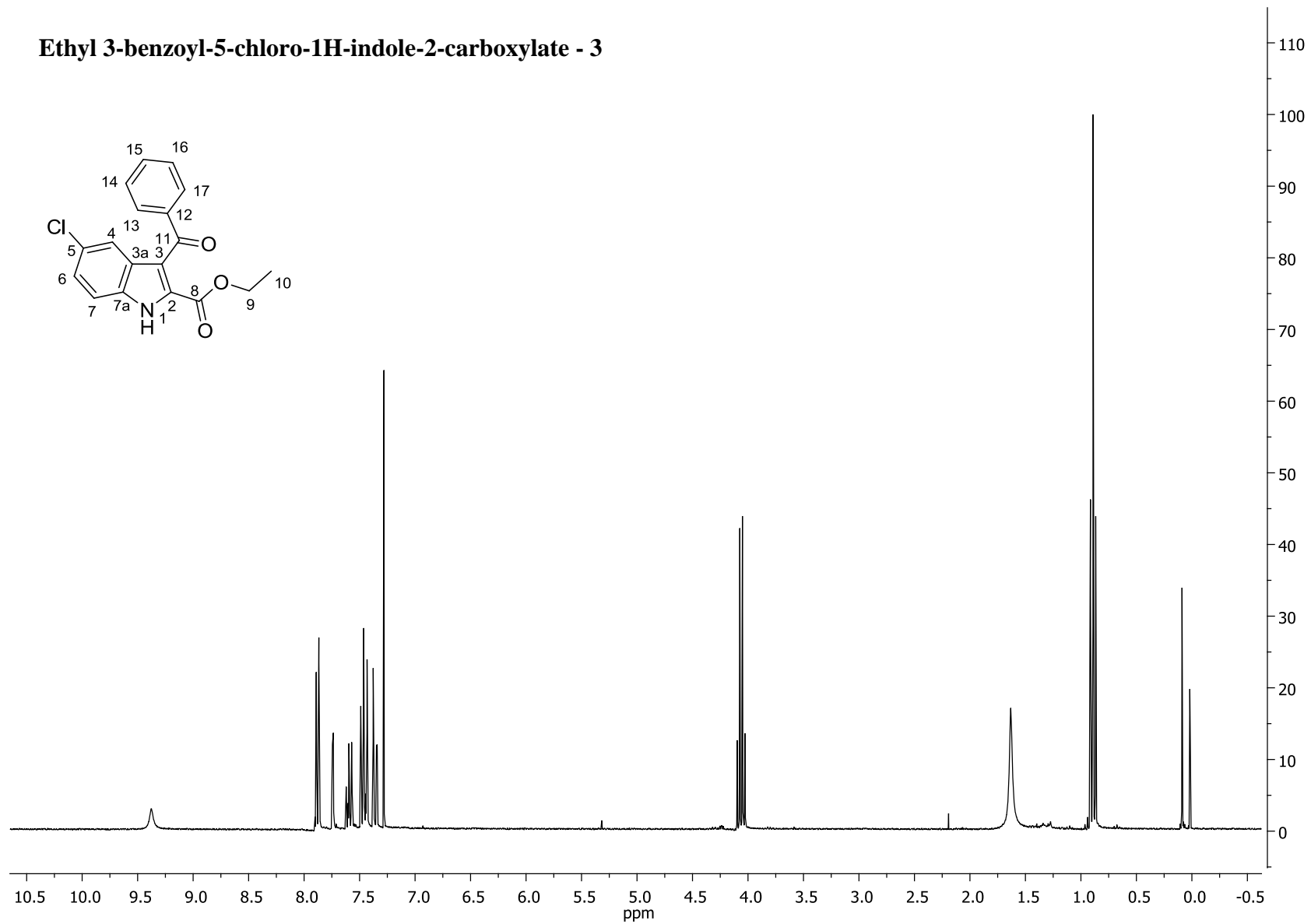
Mass Spectrum.....	1
Infrared Spectrum	1

Ethyl 5-chloro-3-(1-phenylcyclopropyl)-1H-indole-2-carboxylate – 2
(Crude compound)

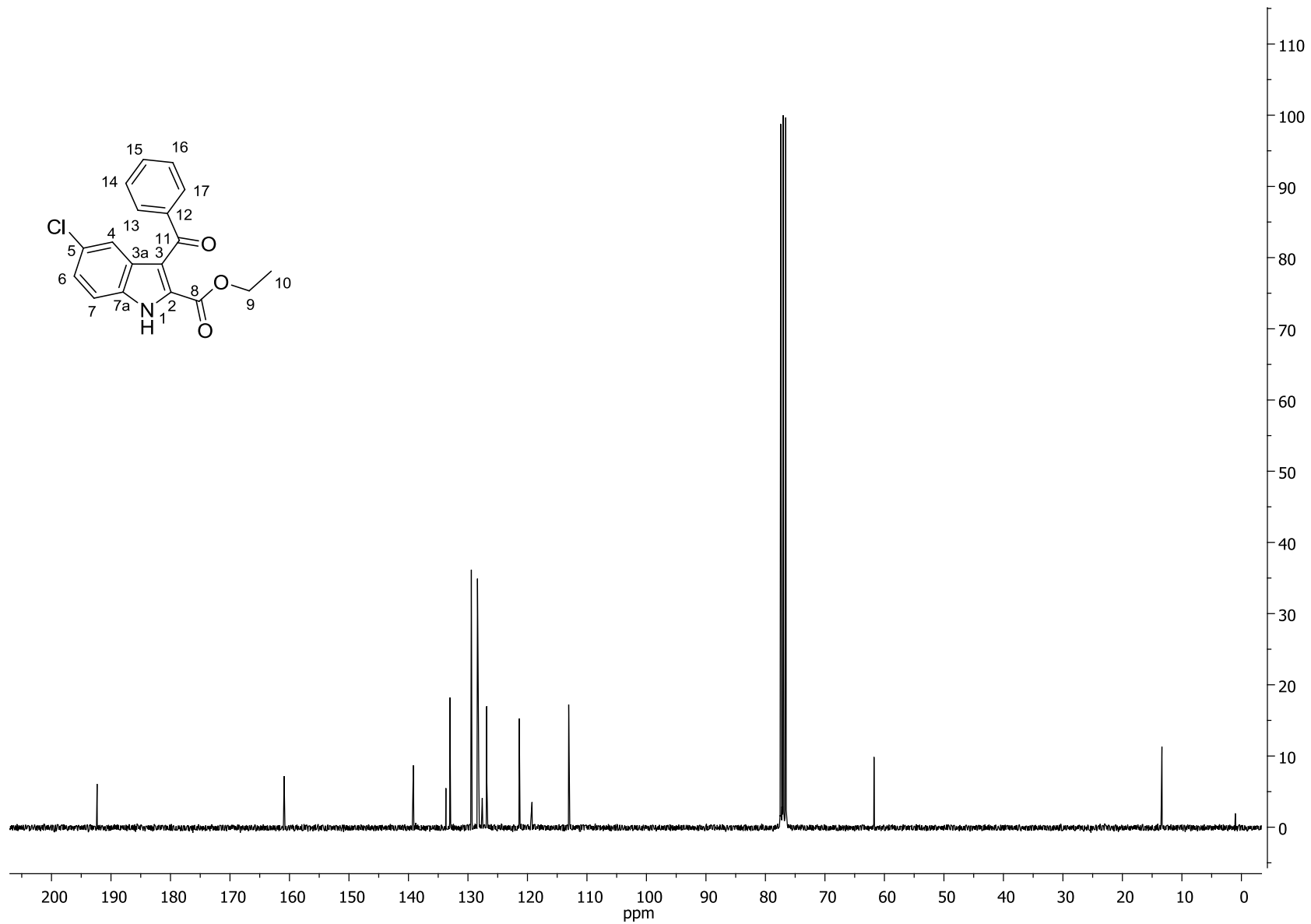


¹H NMR Spectrum
400 MHz Varian Unity Inova

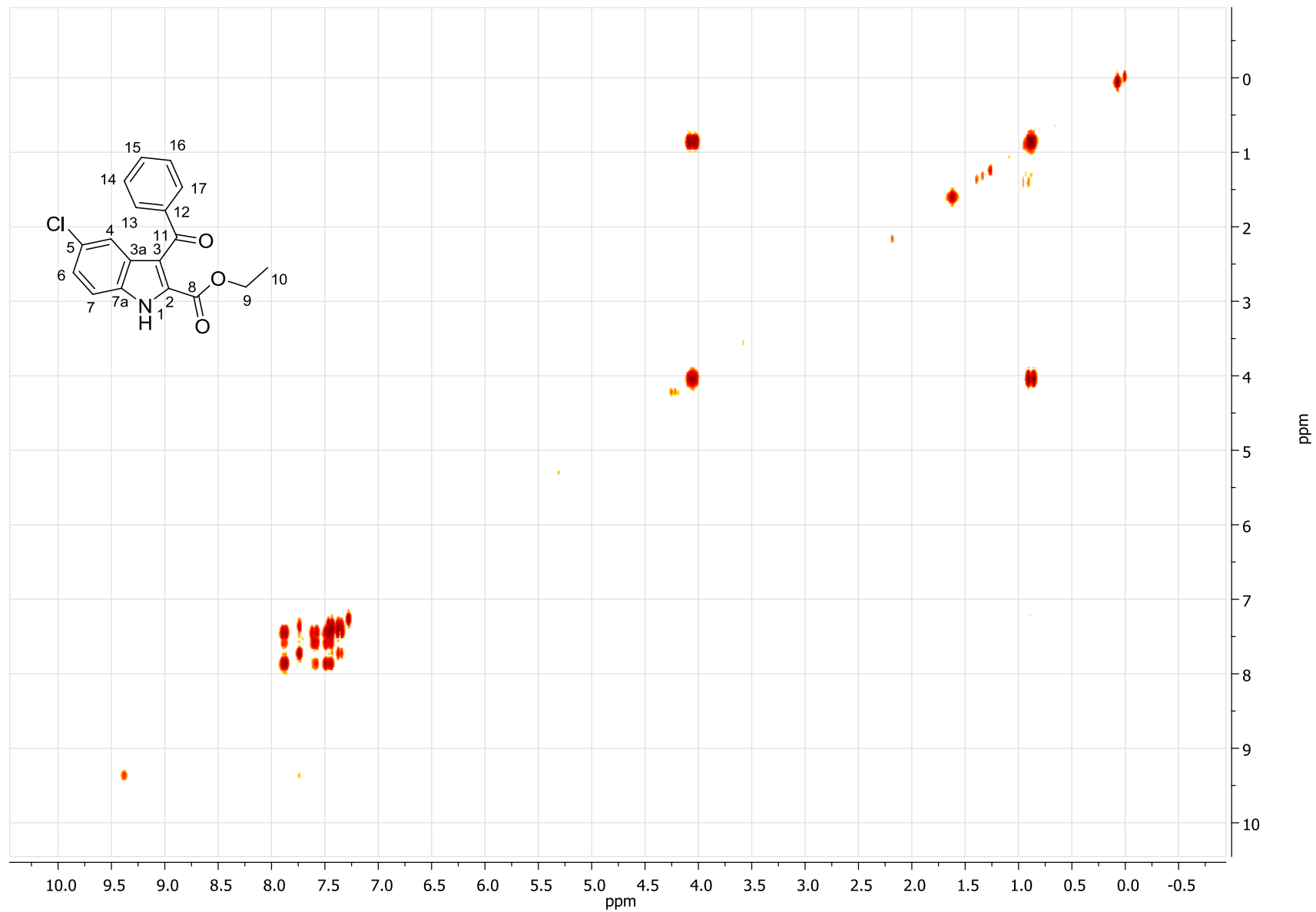
Ethyl 3-benzoyl-5-chloro-1H-indole-2-carboxylate - 3



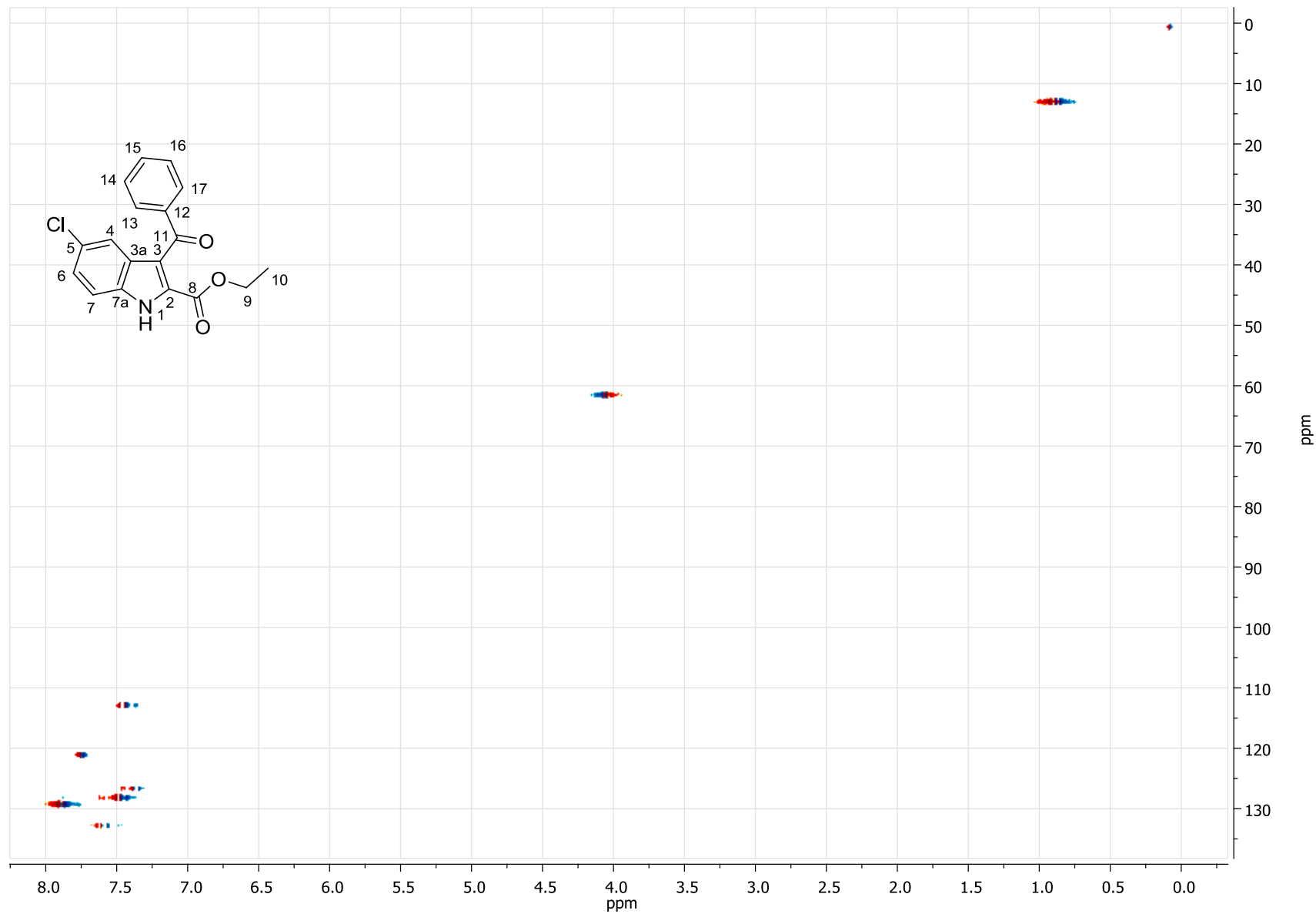
¹H NMR Spectrum
300 MHz Varian VNMRS



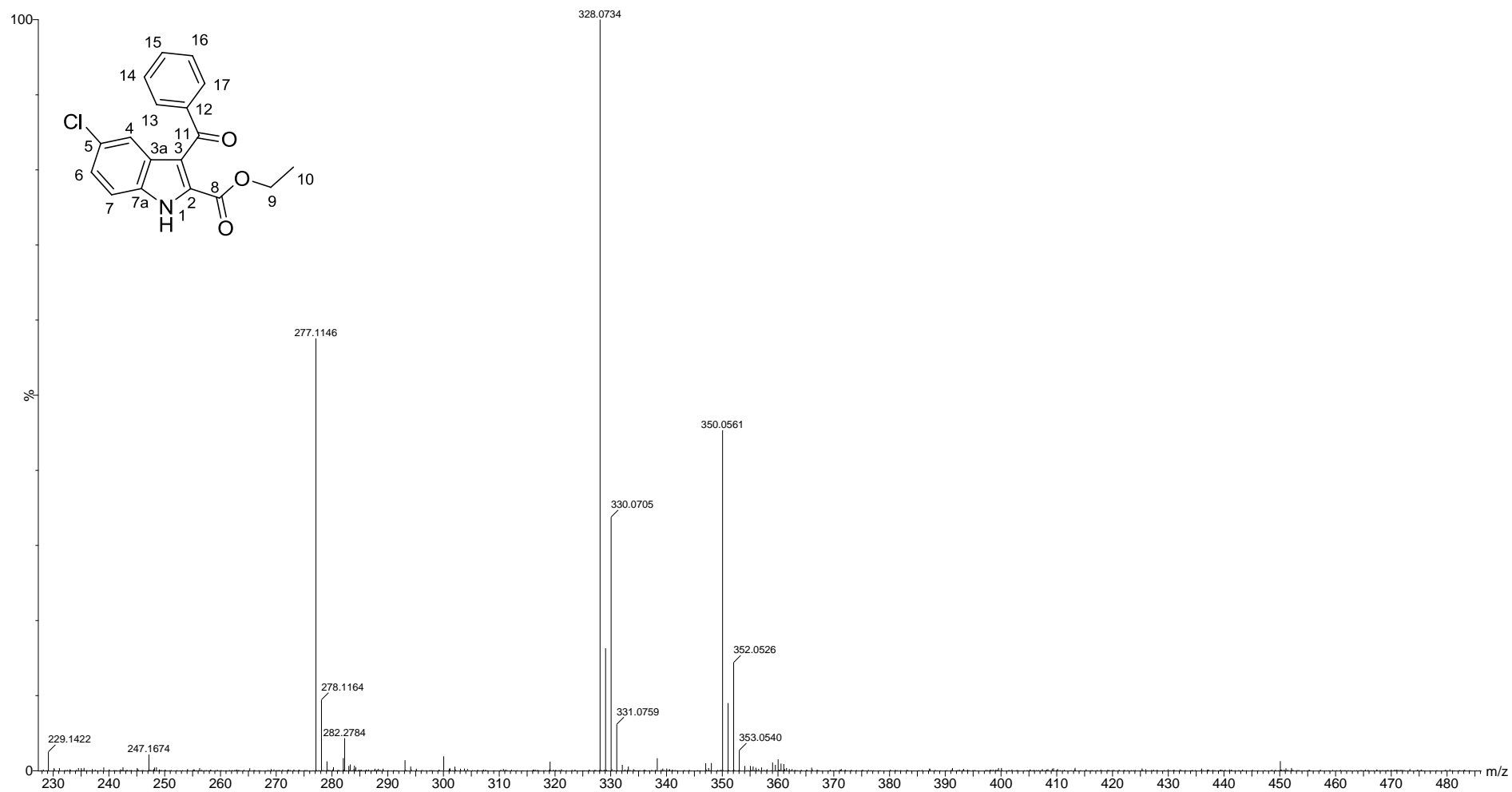
^{13}C NMR Spectrum
75 MHz Varian VNMRS



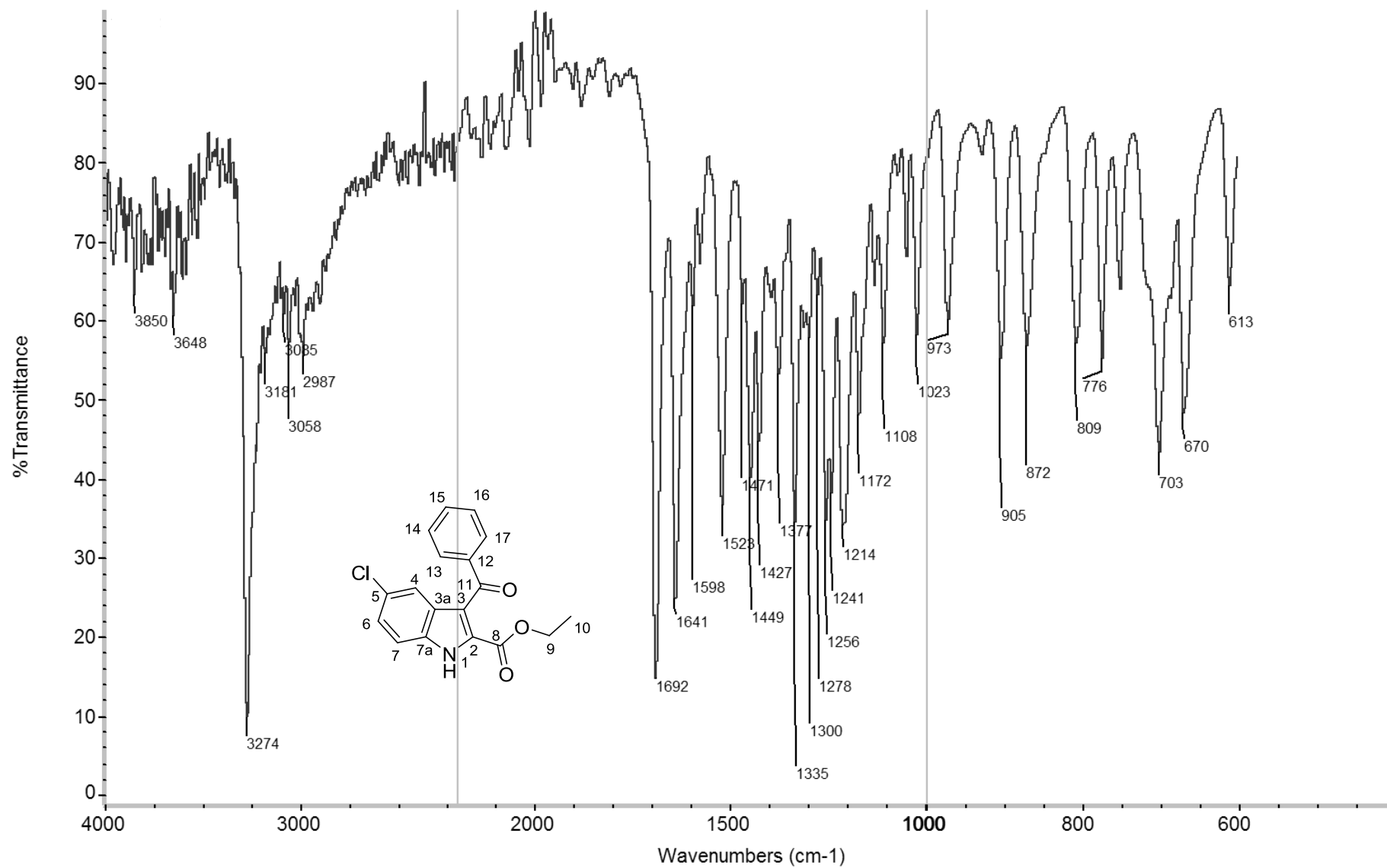
COSY NMR Spectrum
300 MHz Varian VNMRS



gHSQC NMR Spectrum
300 MHz Varian VNMRS

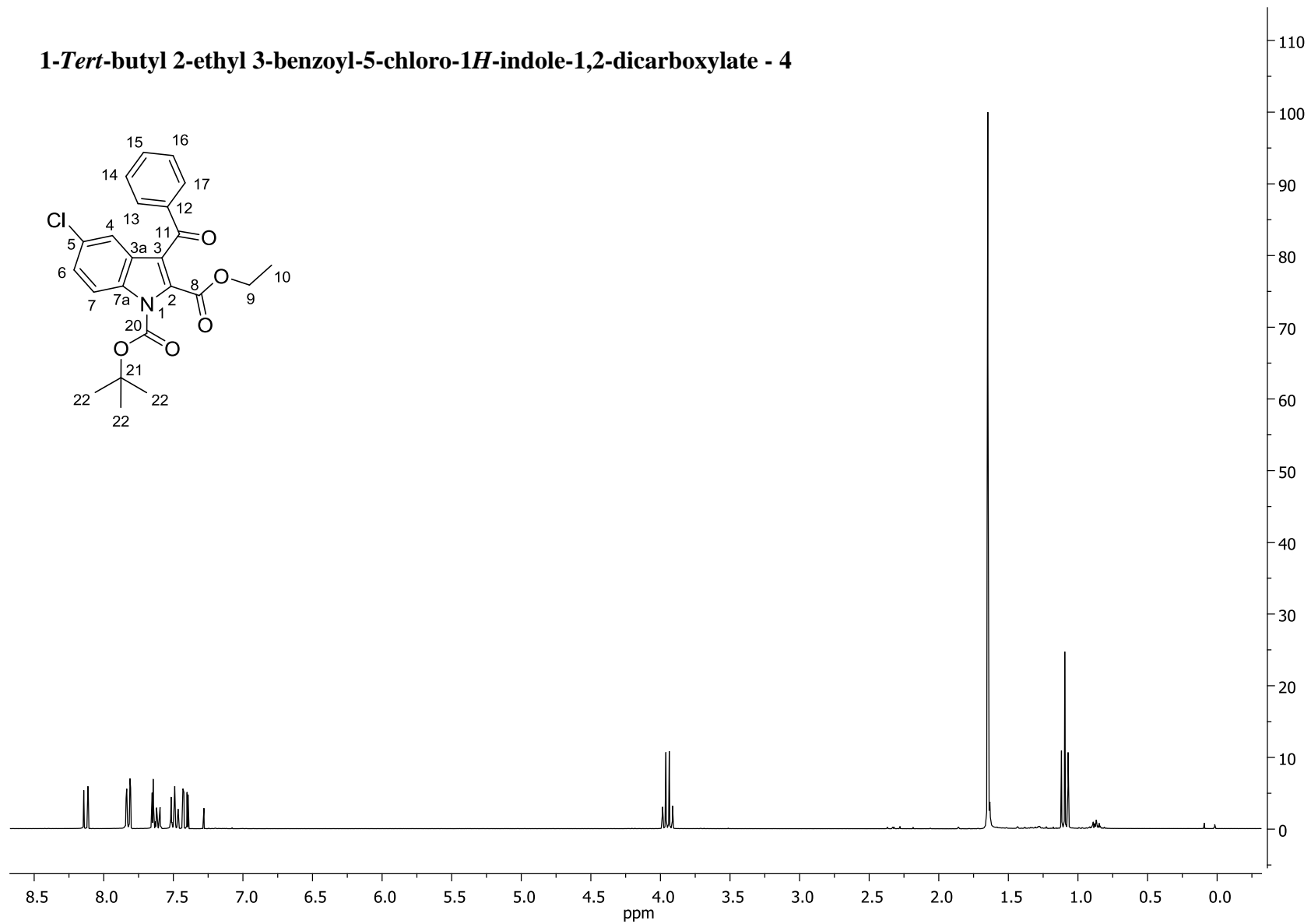


Mass Spectrum
Waters SYNAPT G2

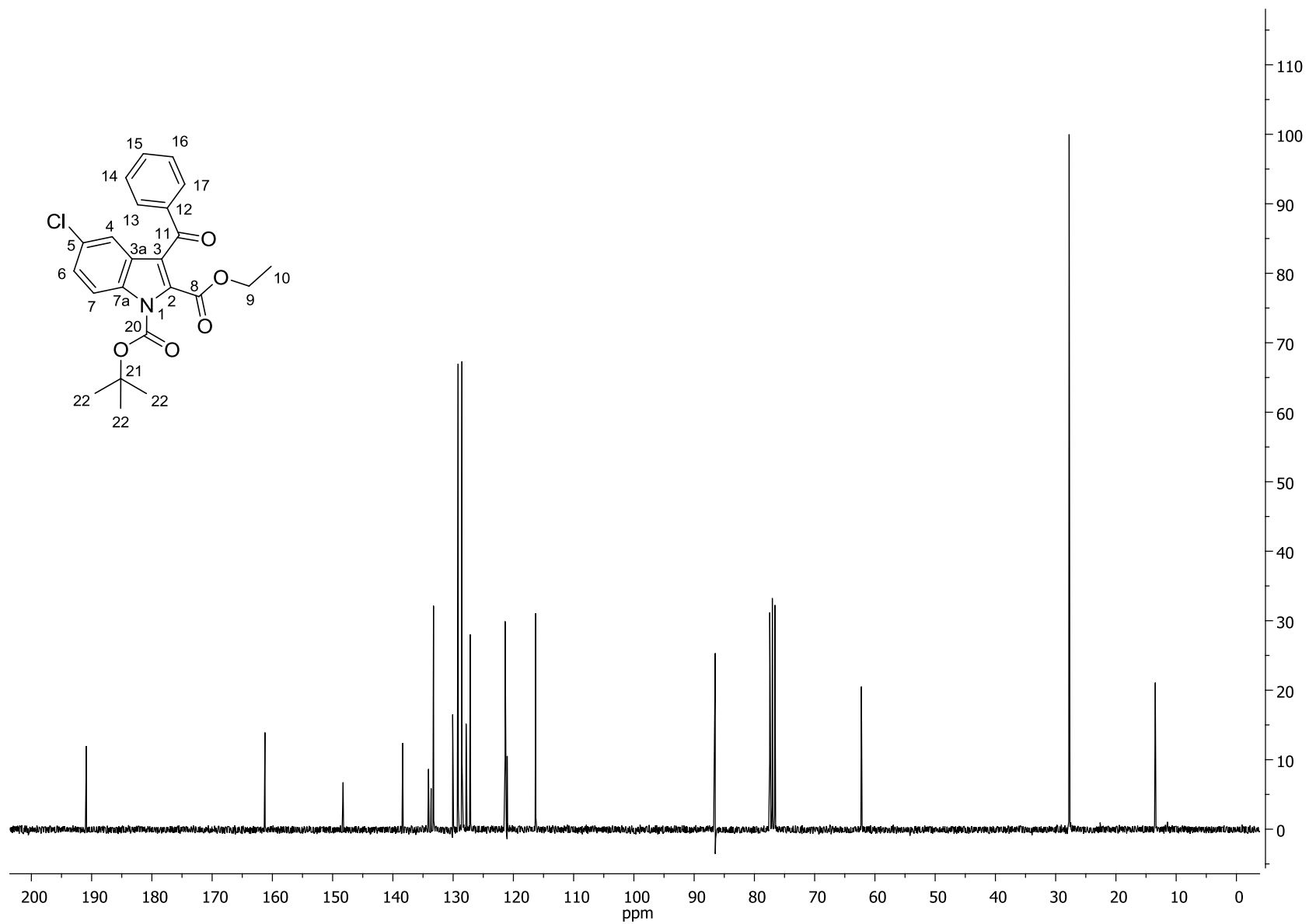


Infrared Spectrum
Thermo Nicolet Nexus 470

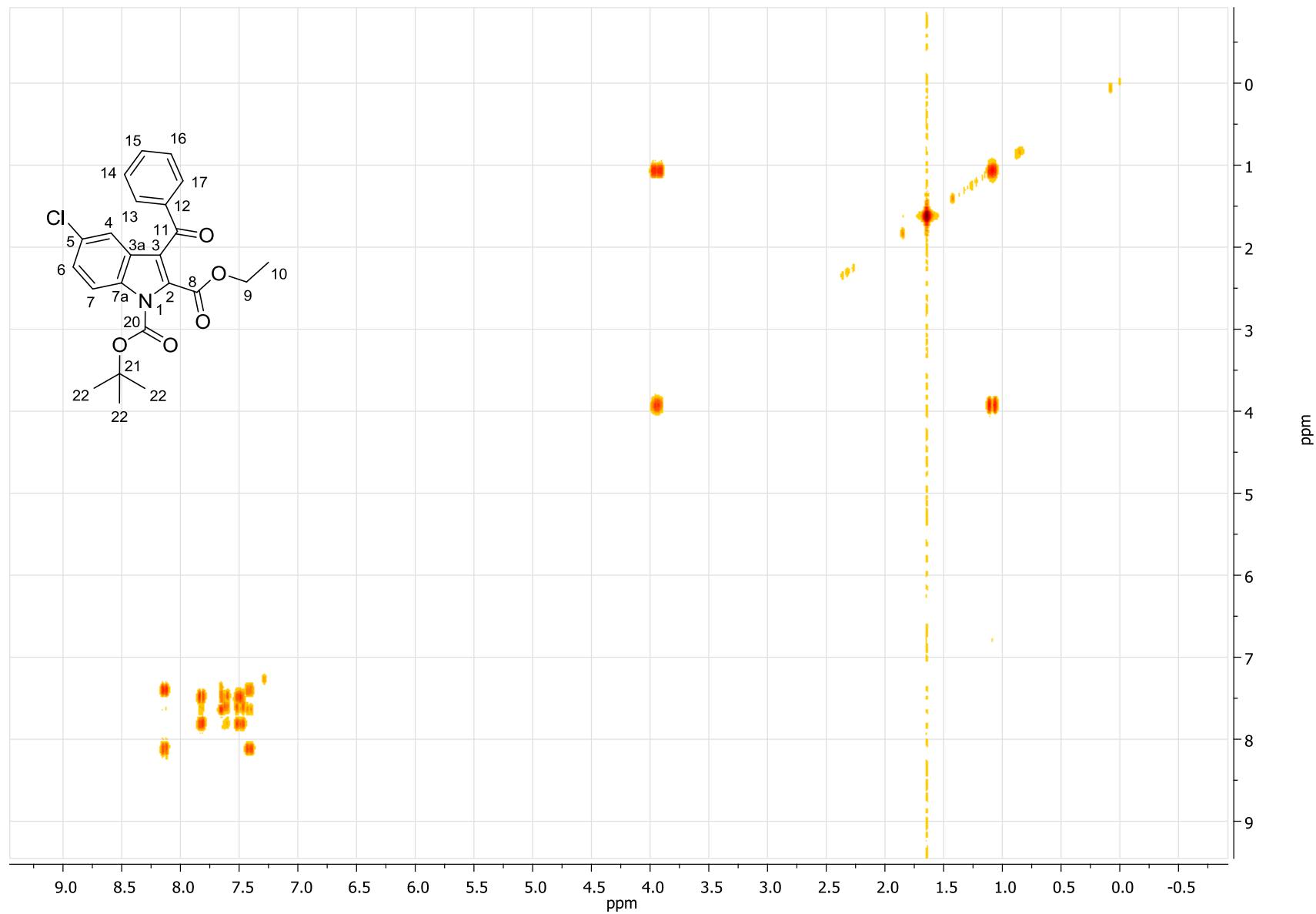
1-*Tert*-butyl 2-ethyl 3-benzoyl-5-chloro-1*H*-indole-1,2-dicarboxylate - 4



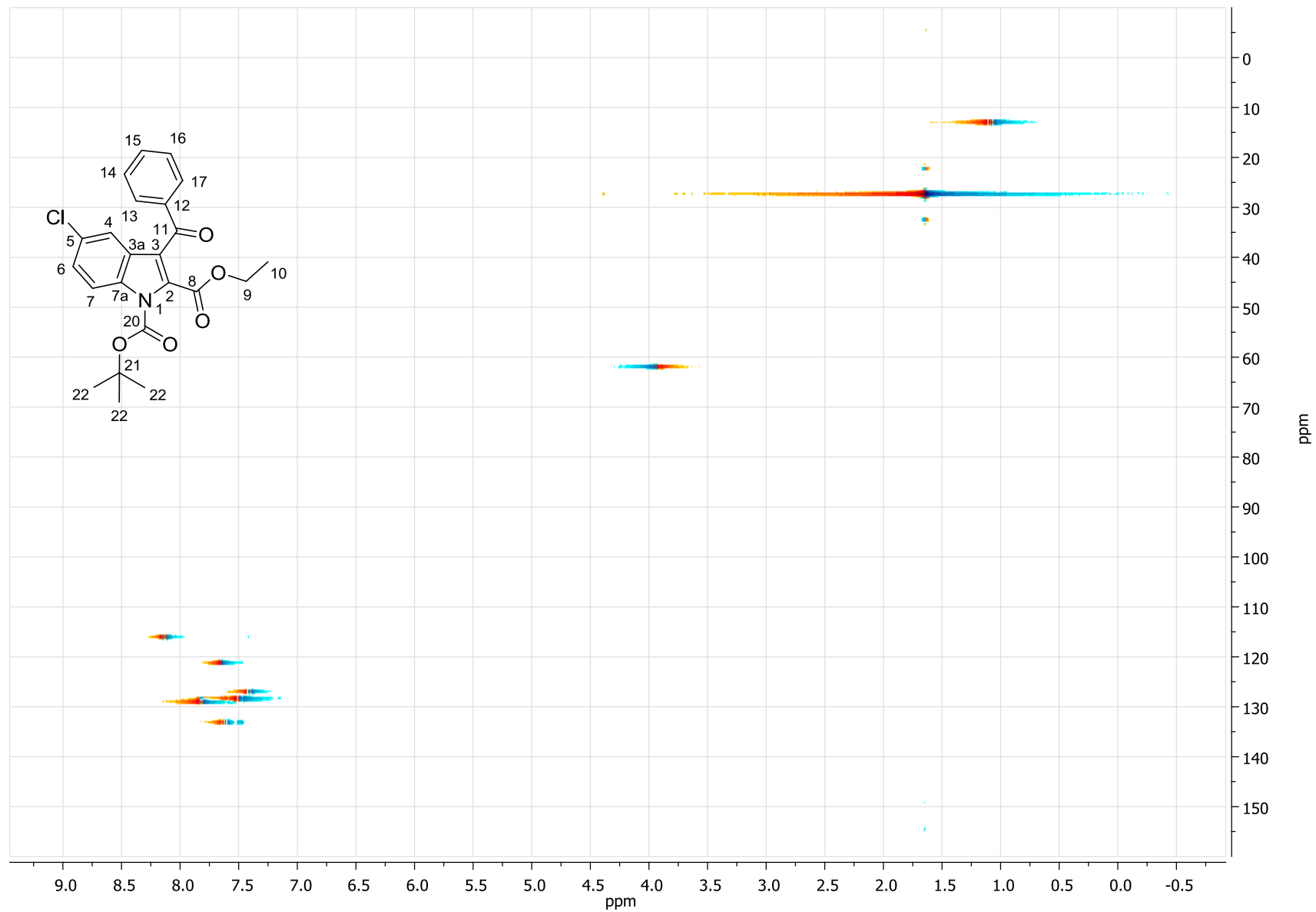
¹H NMR Spectrum
300 MHz Varian VNMRS



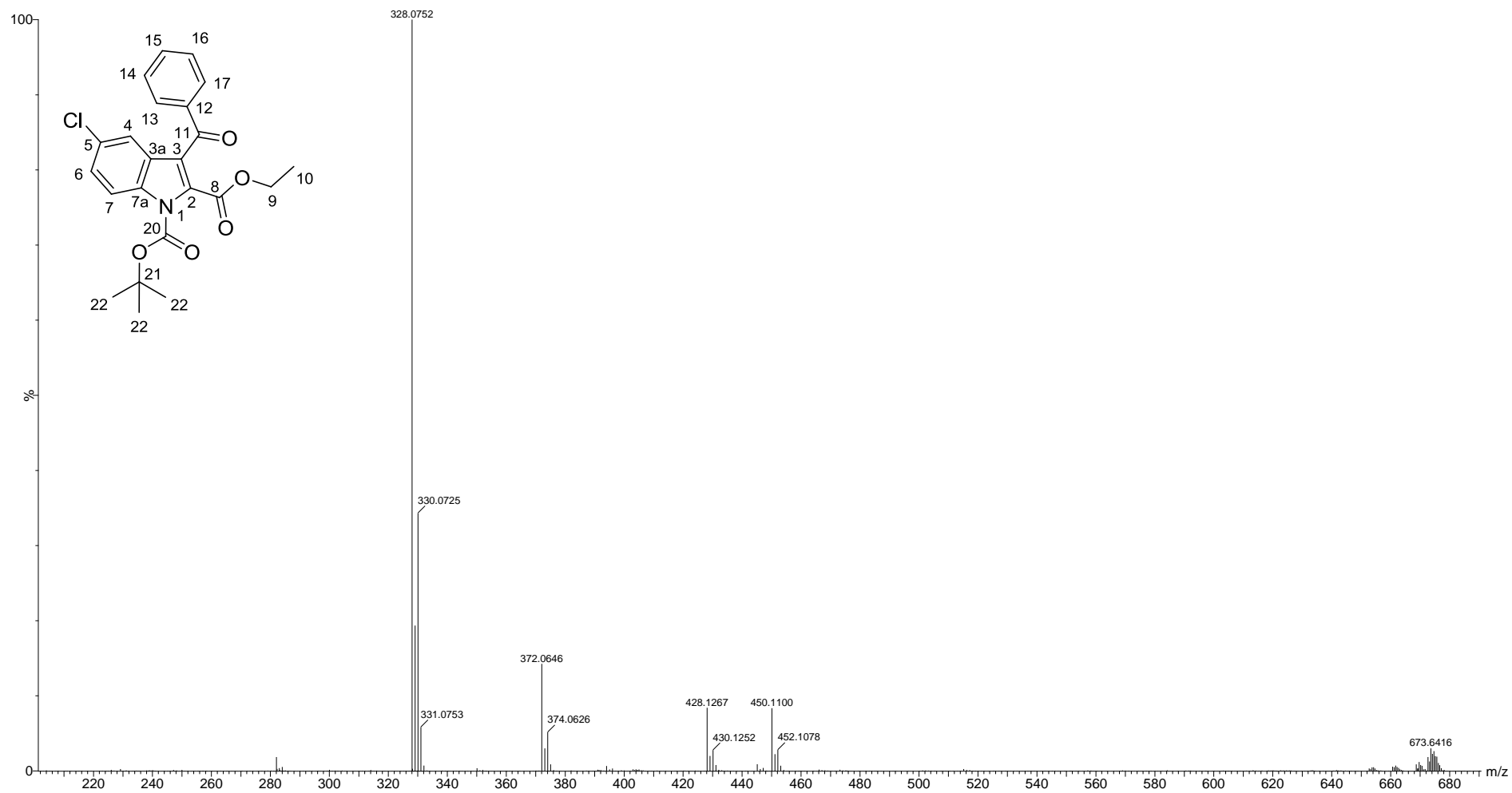
¹³C NMR Spectrum
75 MHz Varian VNMRS



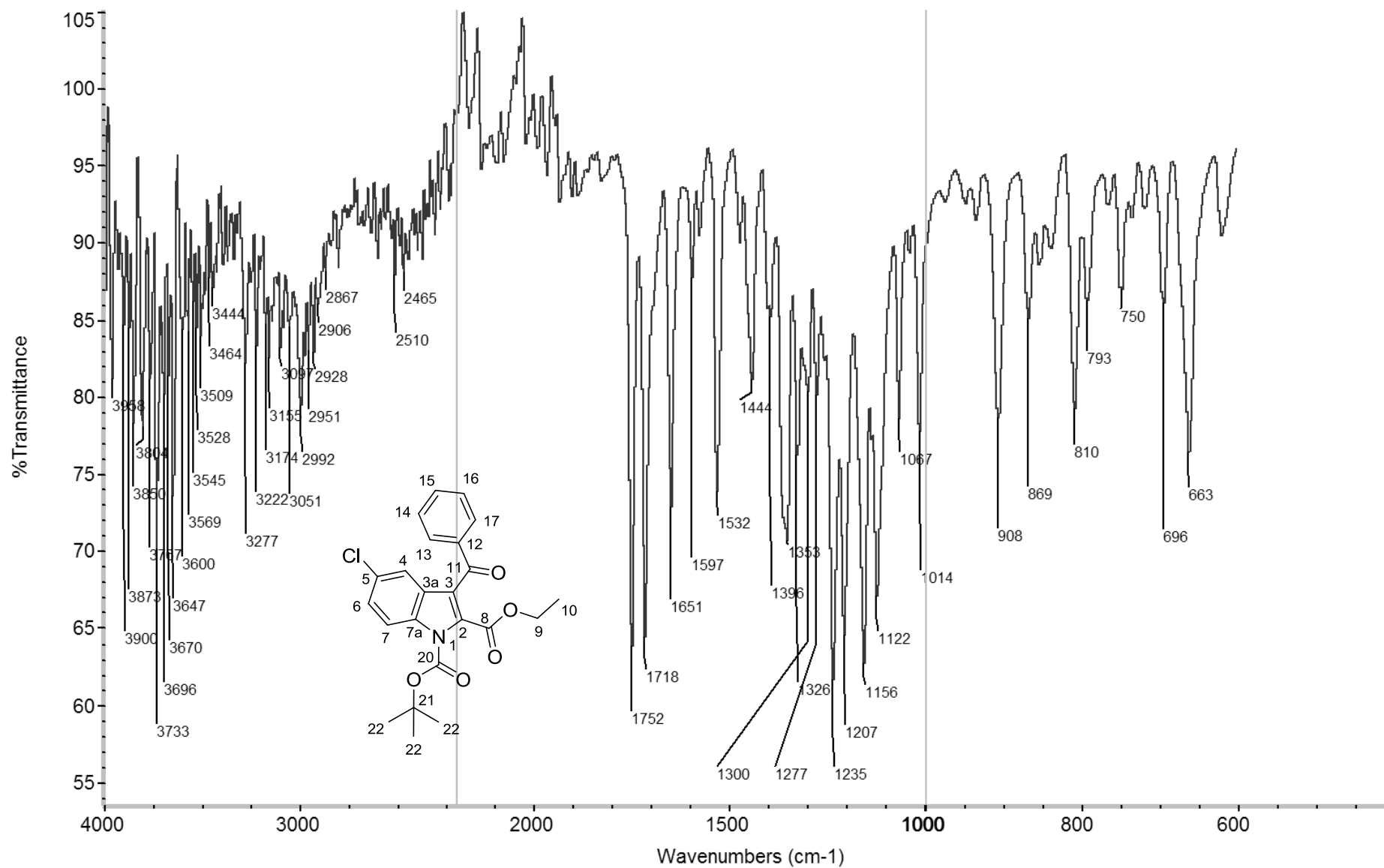
COSY NMR Spectrum
300 MHz Varian VNMRS



gHSQC NMR Spectrum
300 MHz Varian VNMRS

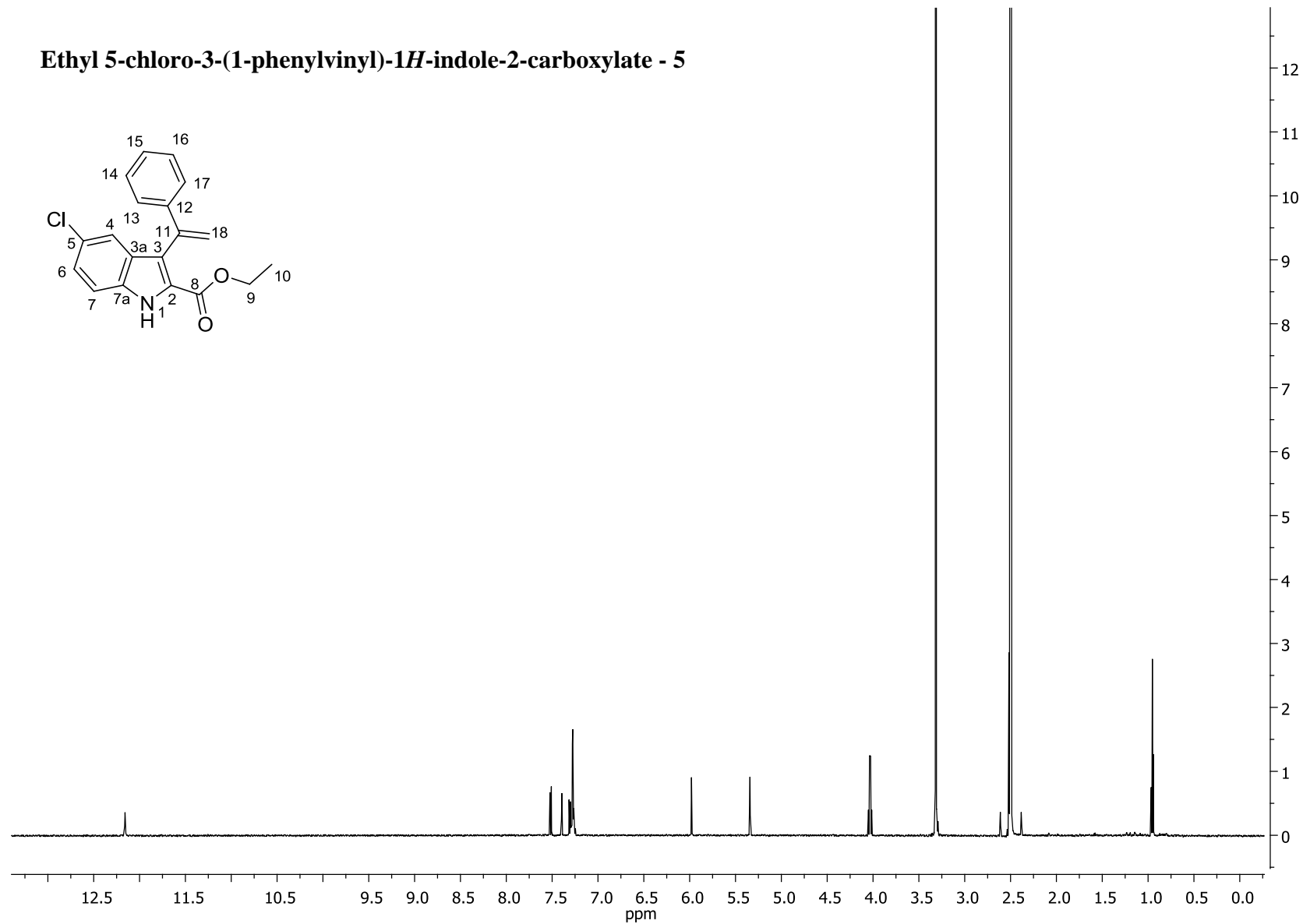
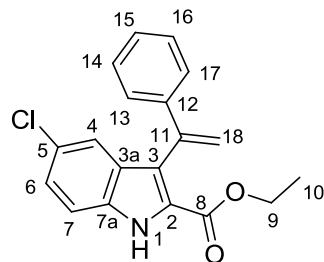


Mass Spectrum
Waters SYNAPT G2

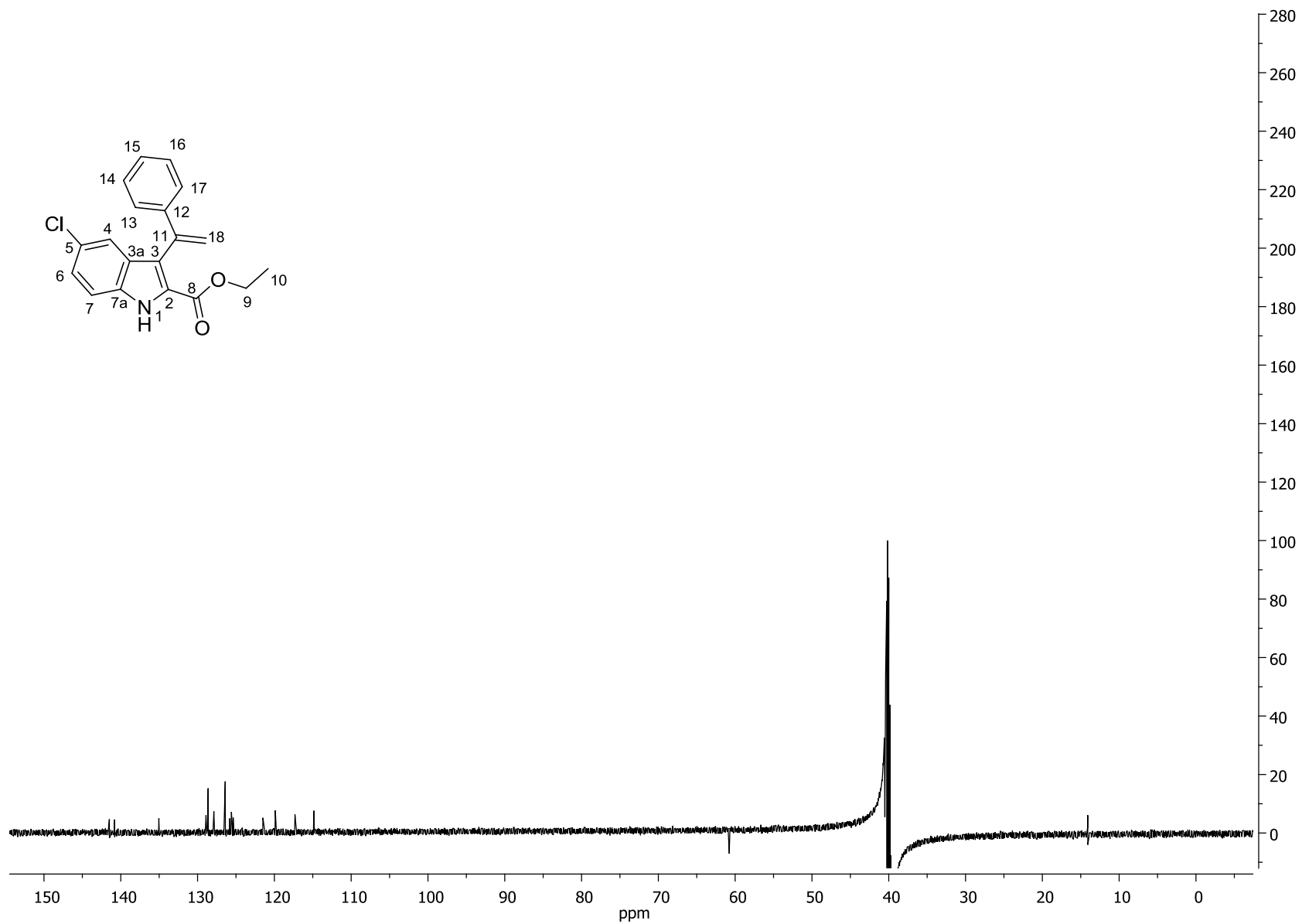


Infrared Spectrum
Thermo Nicolet Nexus 470

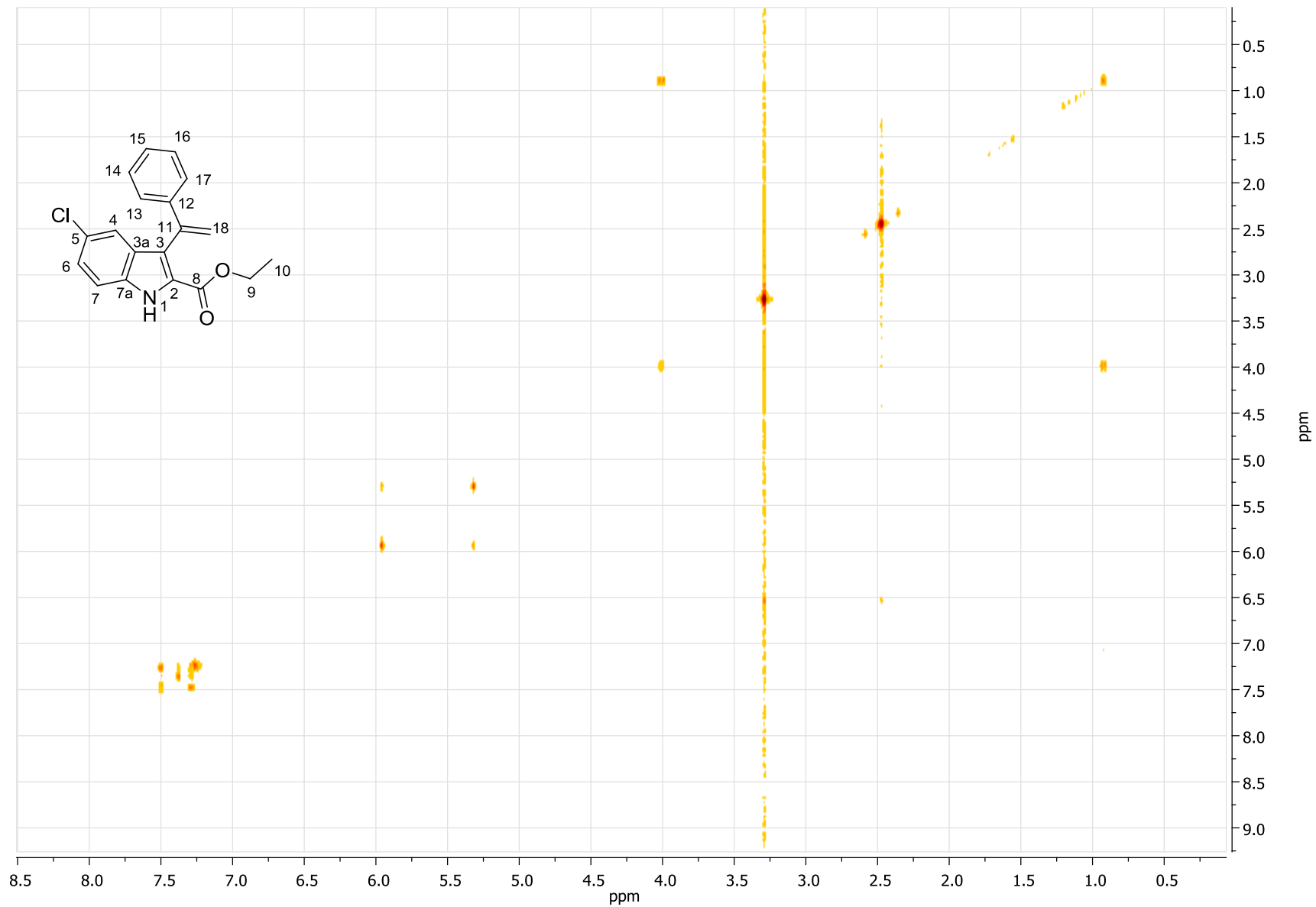
Ethyl 5-chloro-3-(1-phenylvinyl)-1H-indole-2-carboxylate - 5

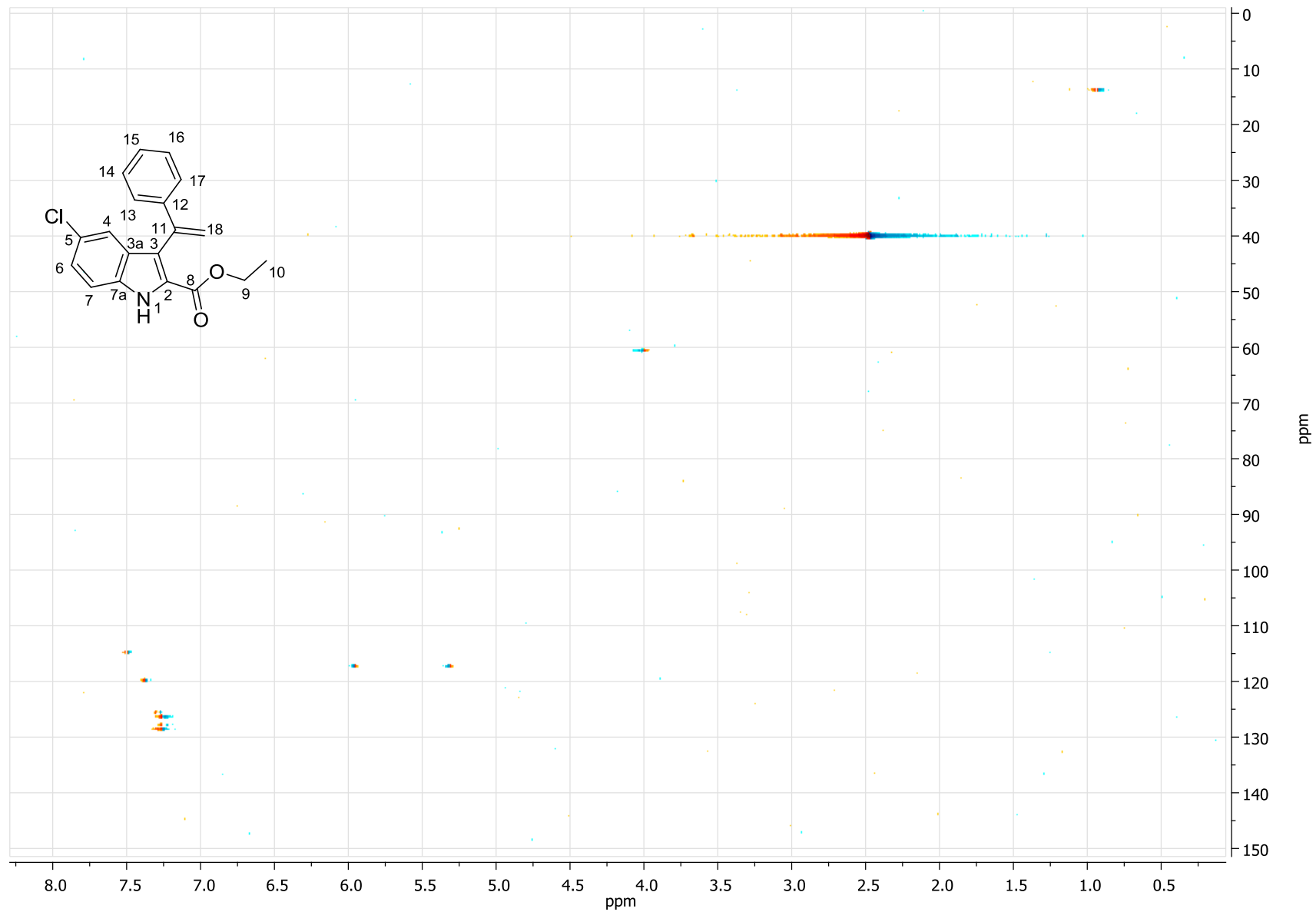


¹H NMR Spectrum
600 MHz Varian Unity Inova

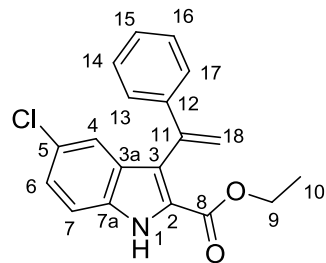
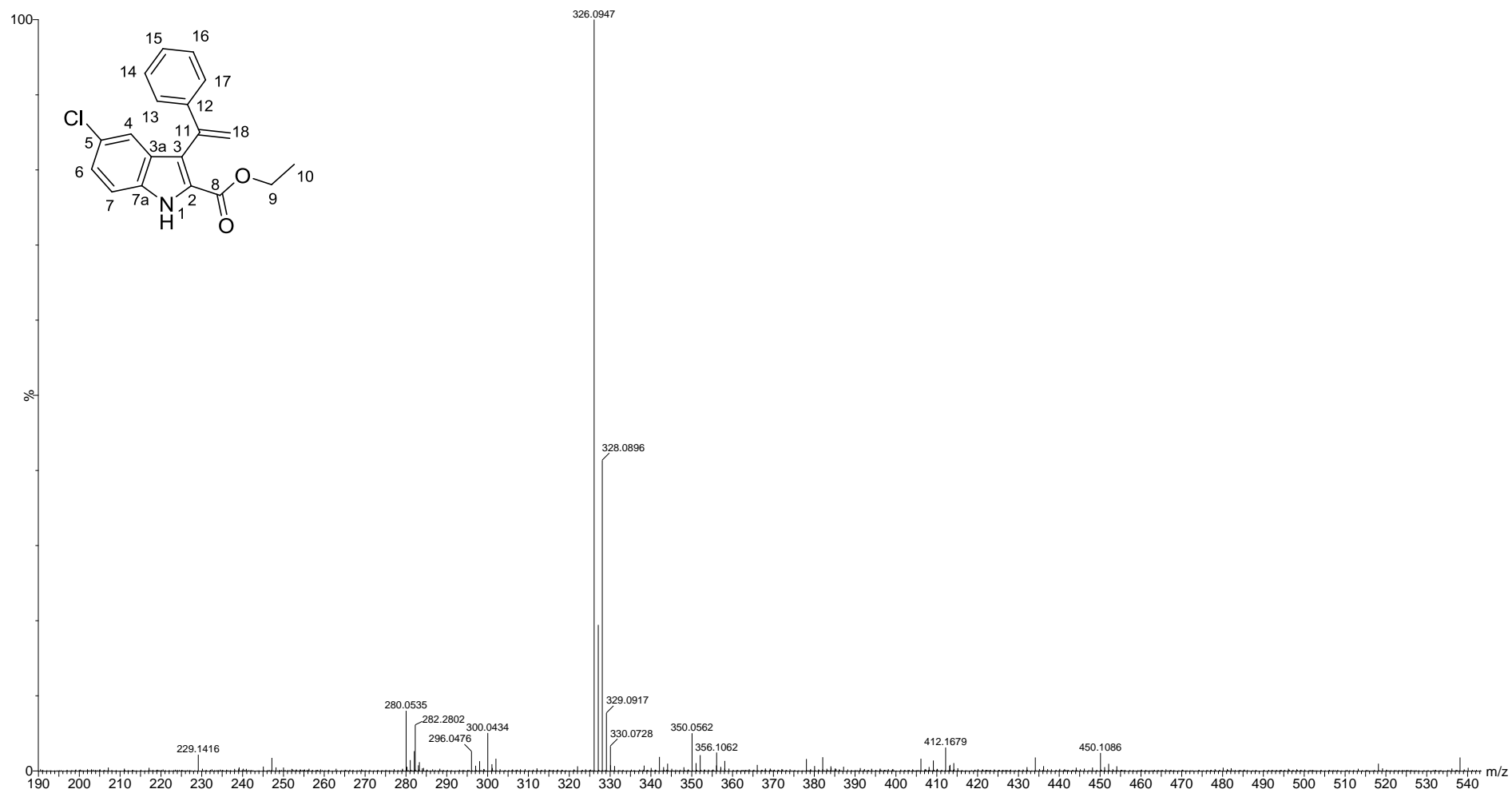


^{13}C NMR Spectrum
150 MHz Varian Unity Inova

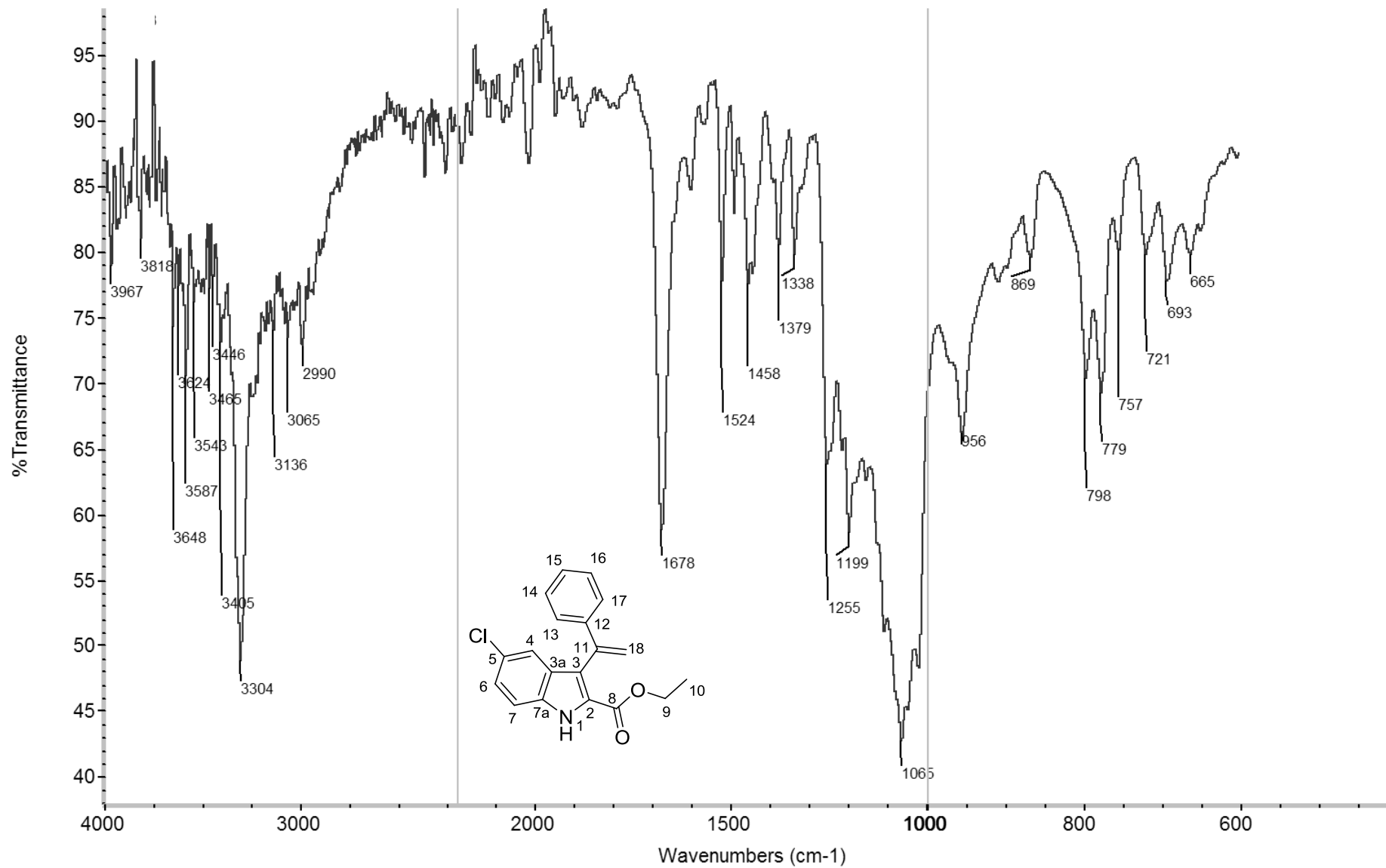




gHSQC NMR Spectrum
600 MHz Varian Unity Inova

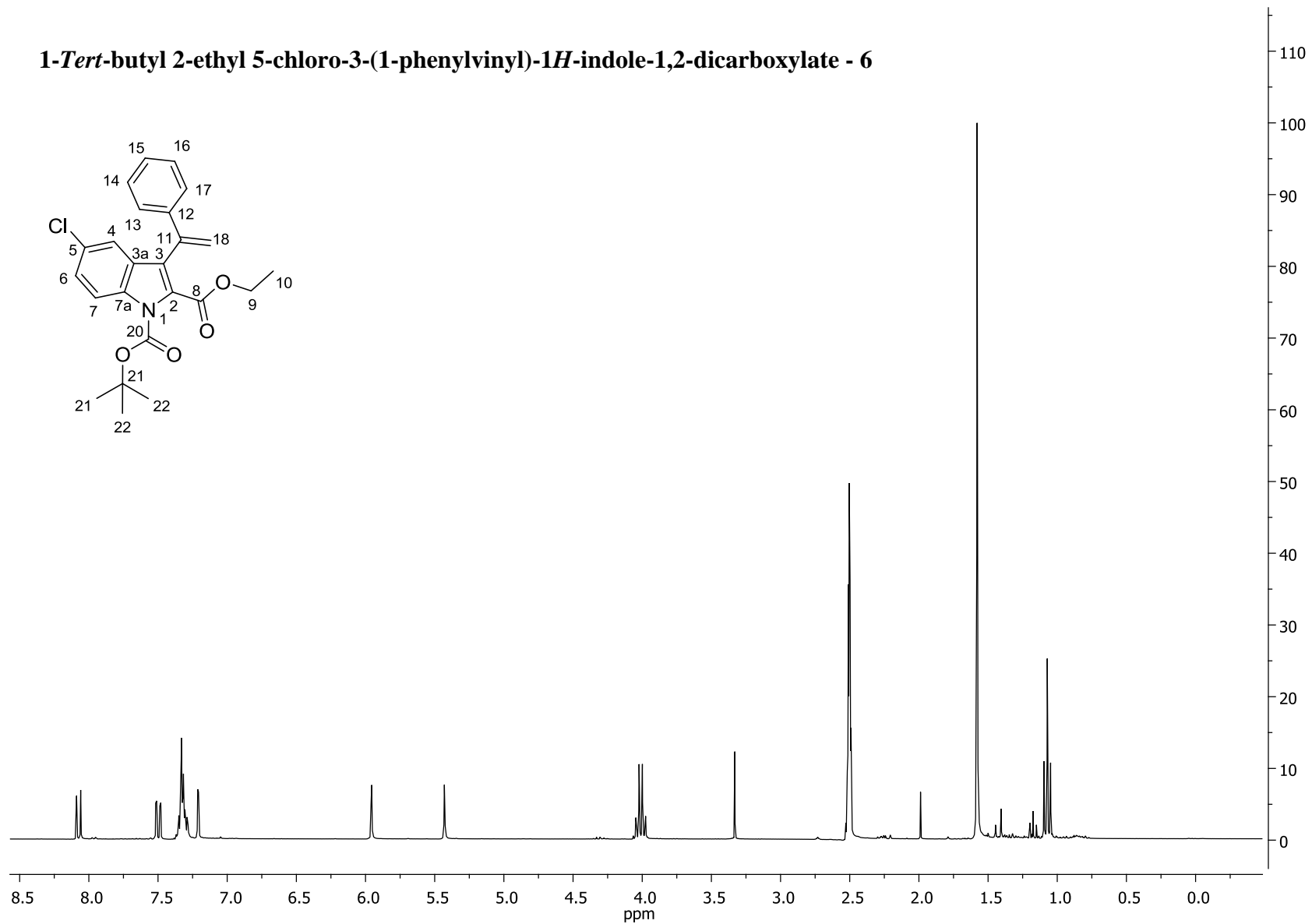
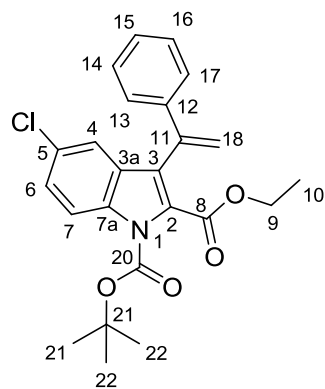


Mass Spectrum
Waters SYNAPT G2

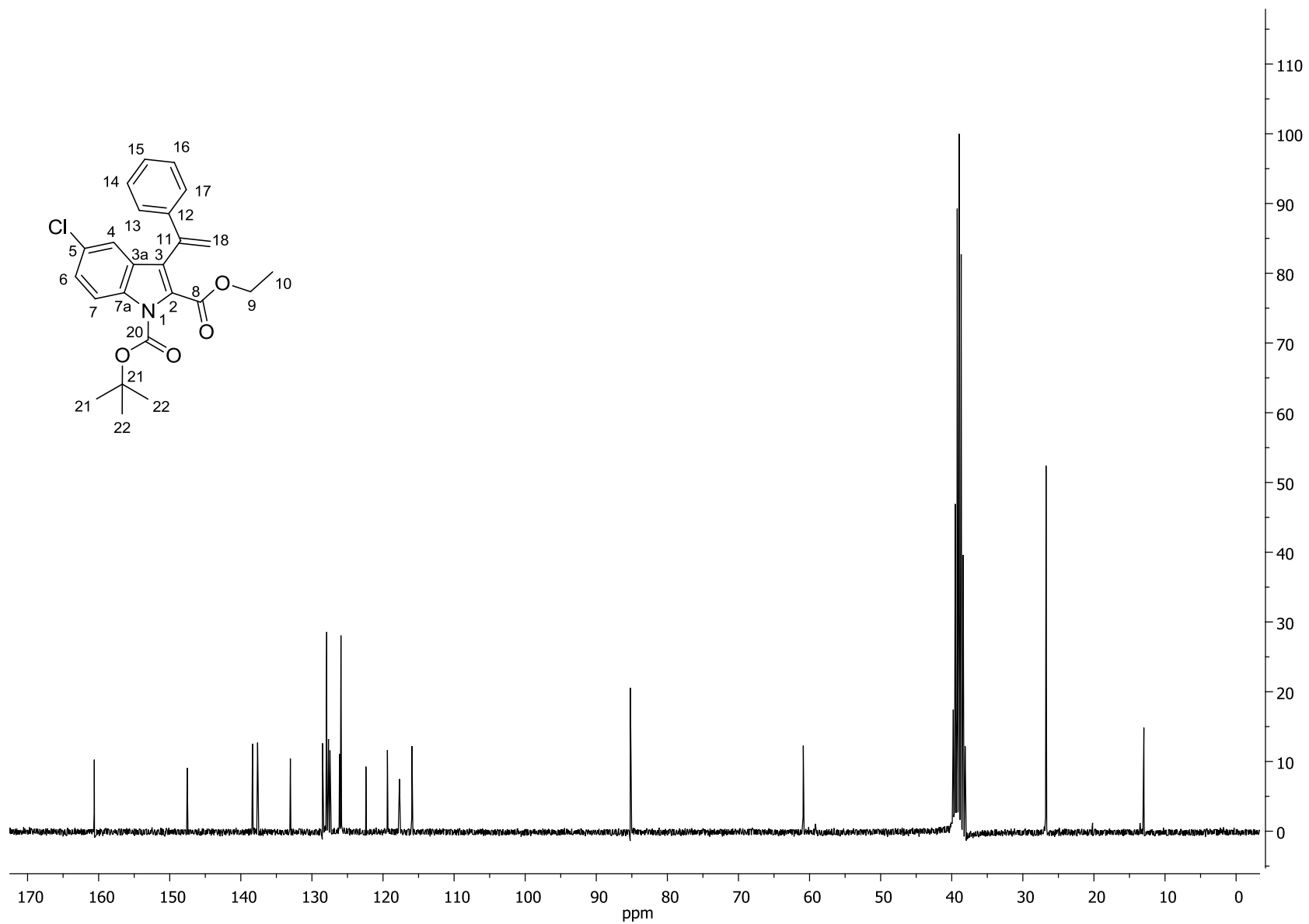


Infrared Spectrum
Thermo Nicolet Nexus 470

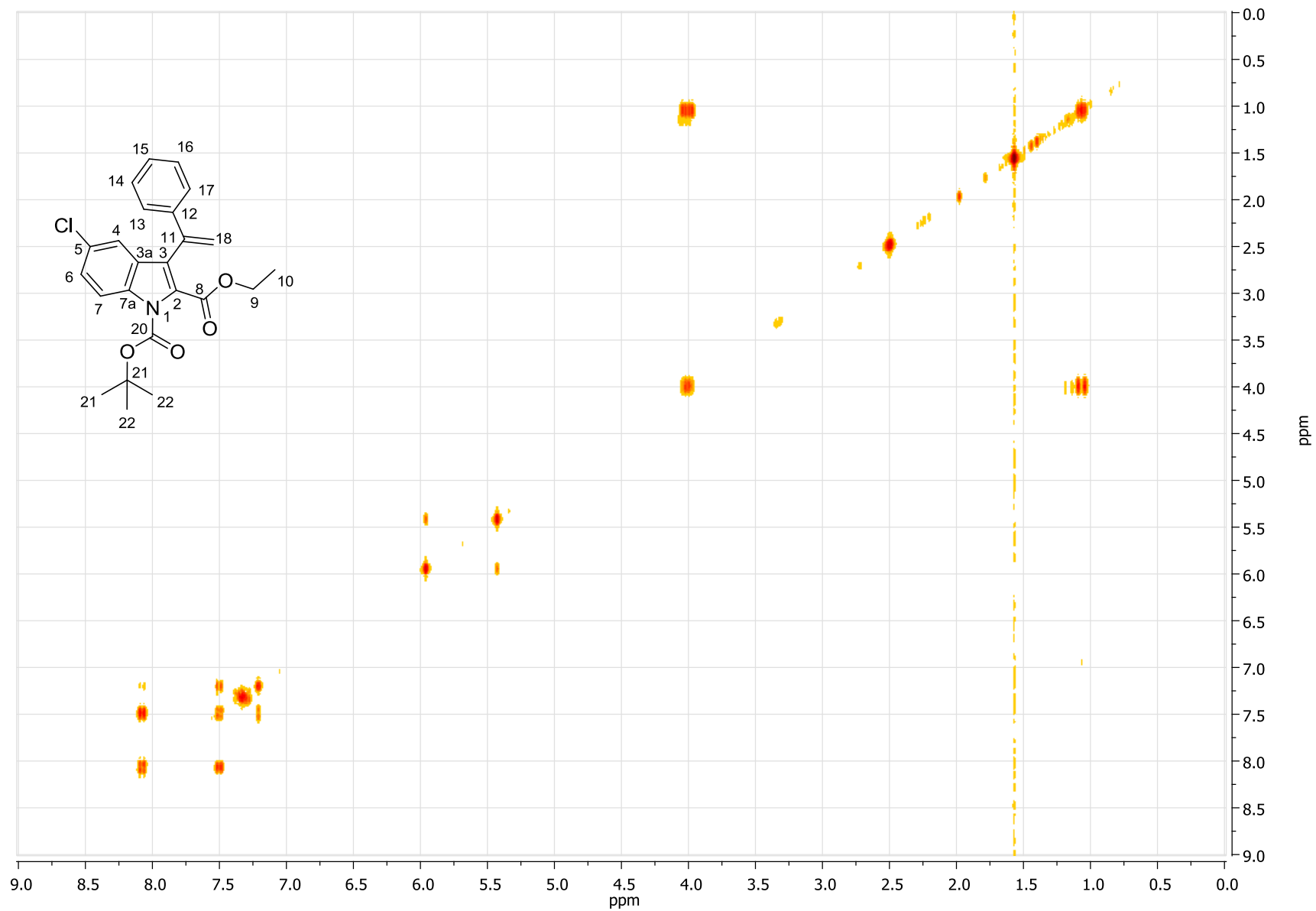
1-Tert-butyl 2-ethyl 5-chloro-3-(1-phenylvinyl)-1H-indole-1,2-dicarboxylate - 6



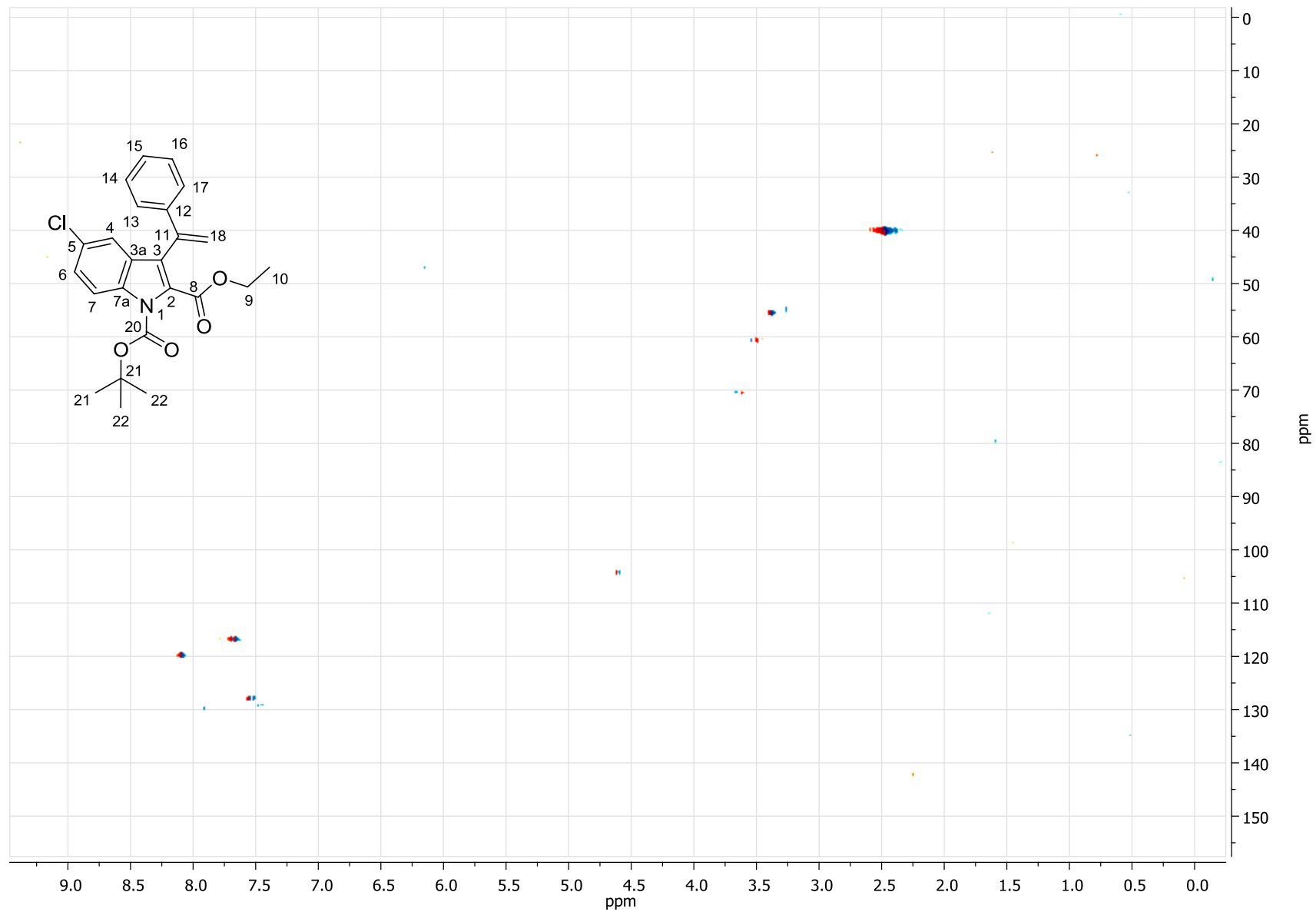
¹H NMR Spectrum
300 MHz Varian VNMRS



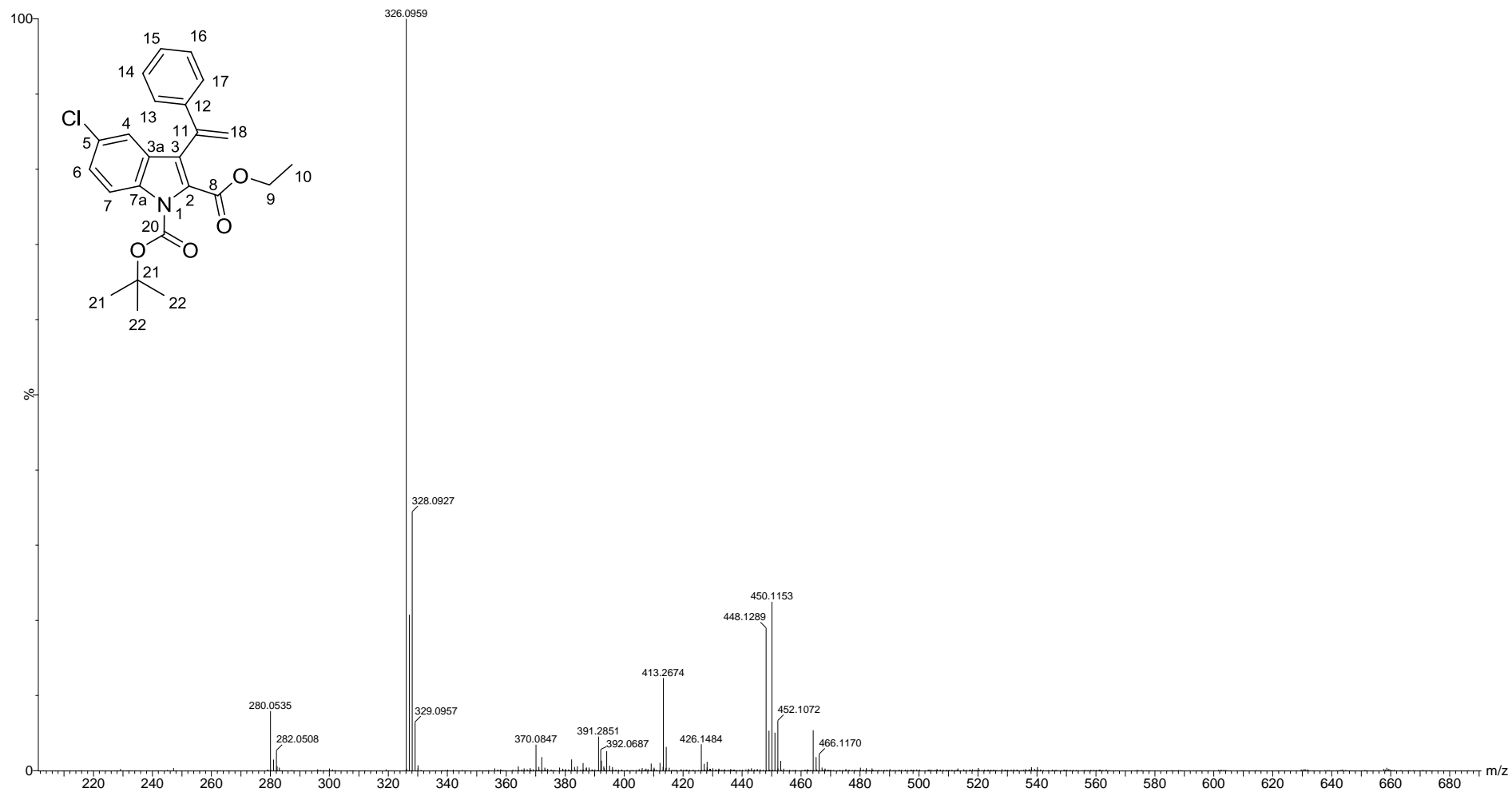
¹³C NMR Spectrum
75 MHz Varian VNMRS



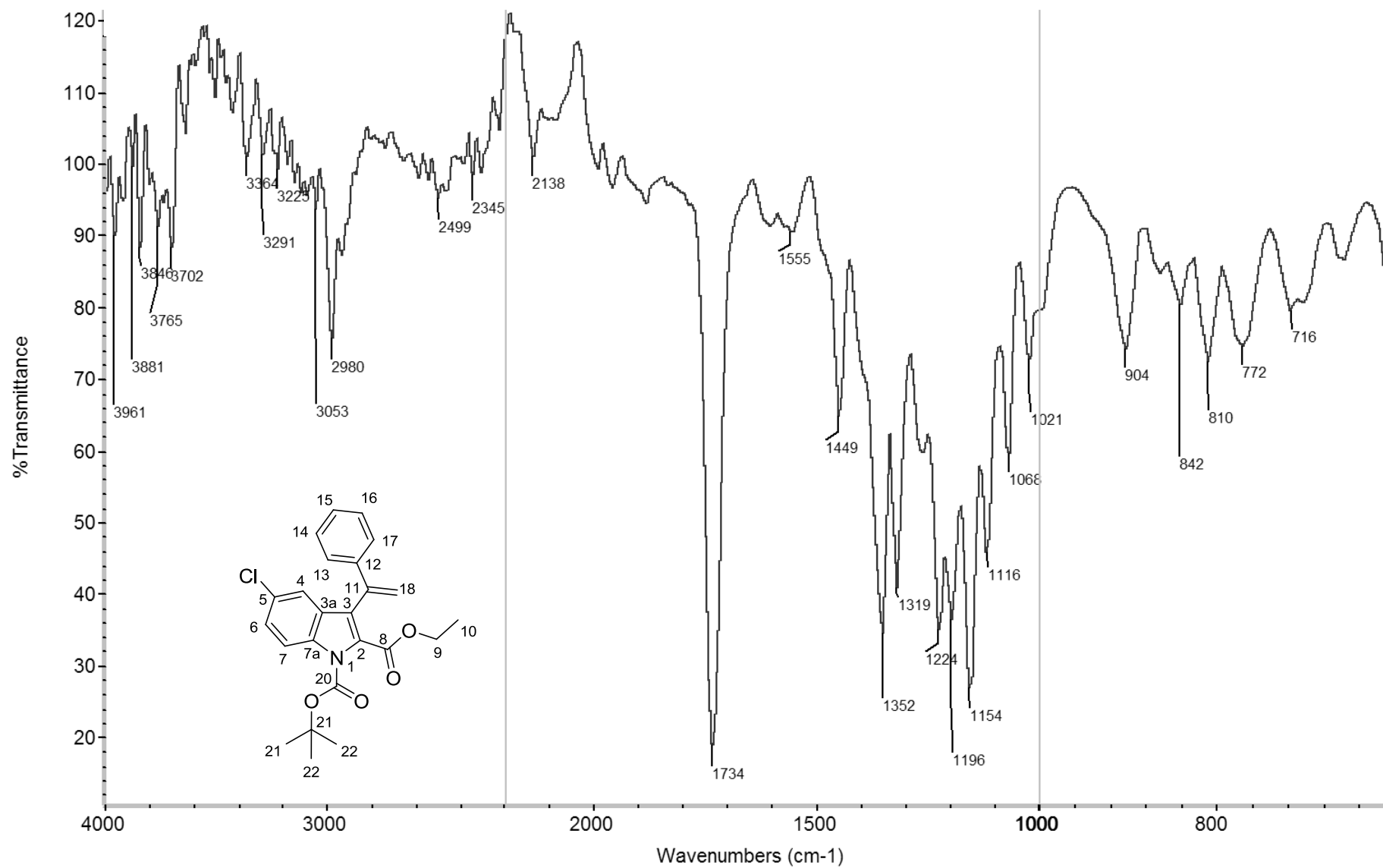
COSY NMR Spectrum
300 MHz Varian VNMRS



gHSQC NMR Spectrum
300 MHz Varian VNMRS

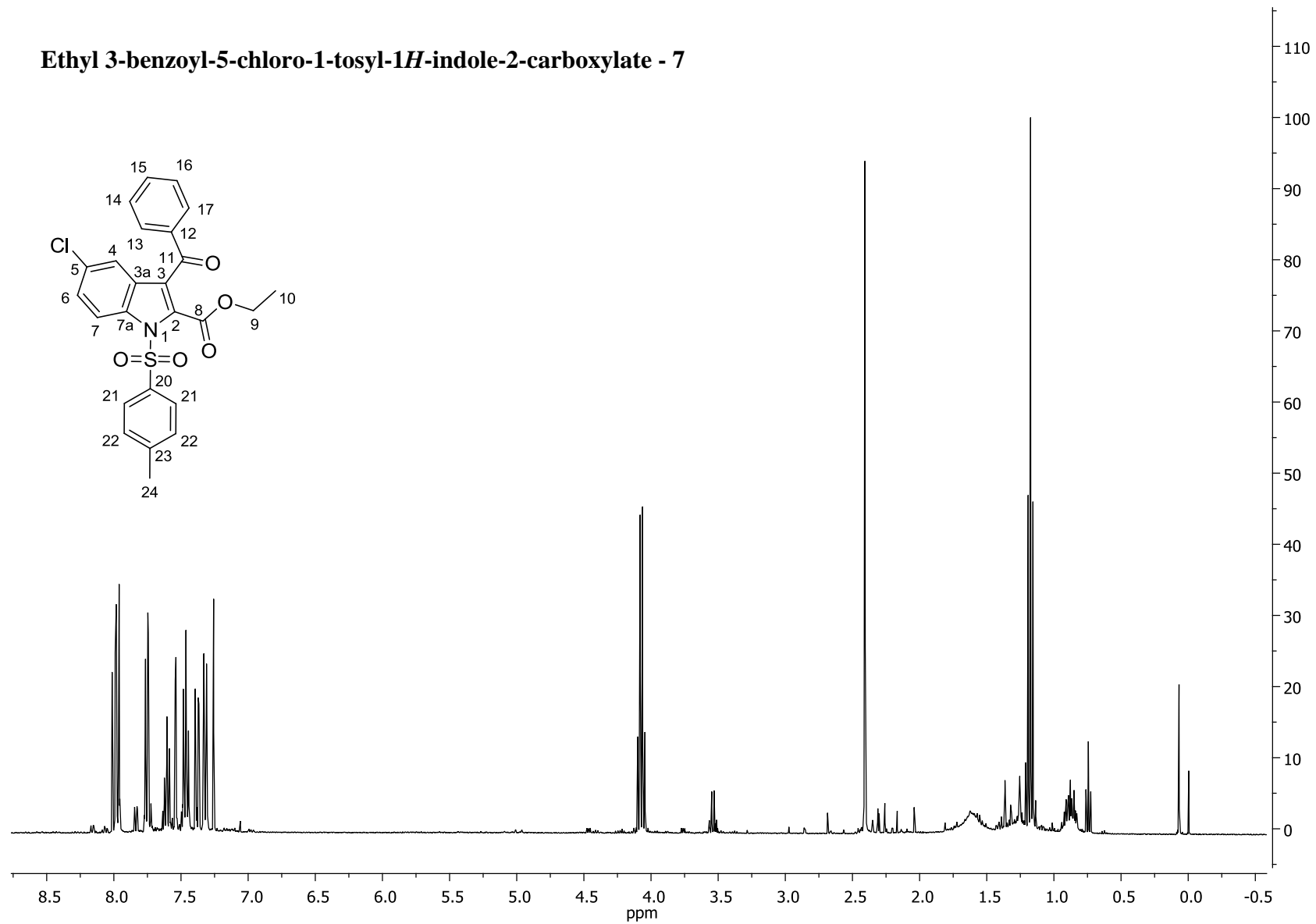


Mass Spectrum
Waters SYNAPT G2

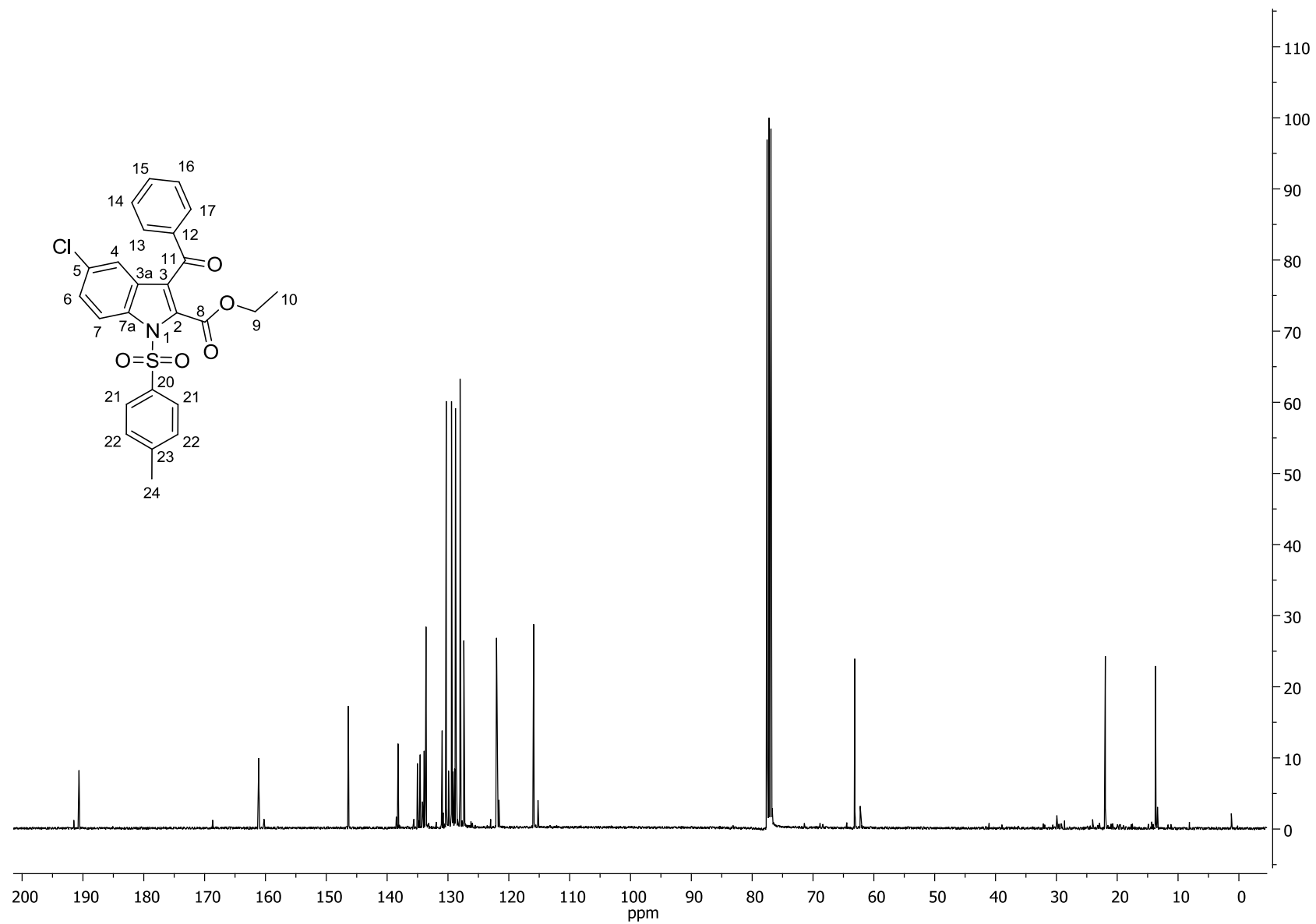


Infrared Spectrum
Thermo Nicolet Nexus 470

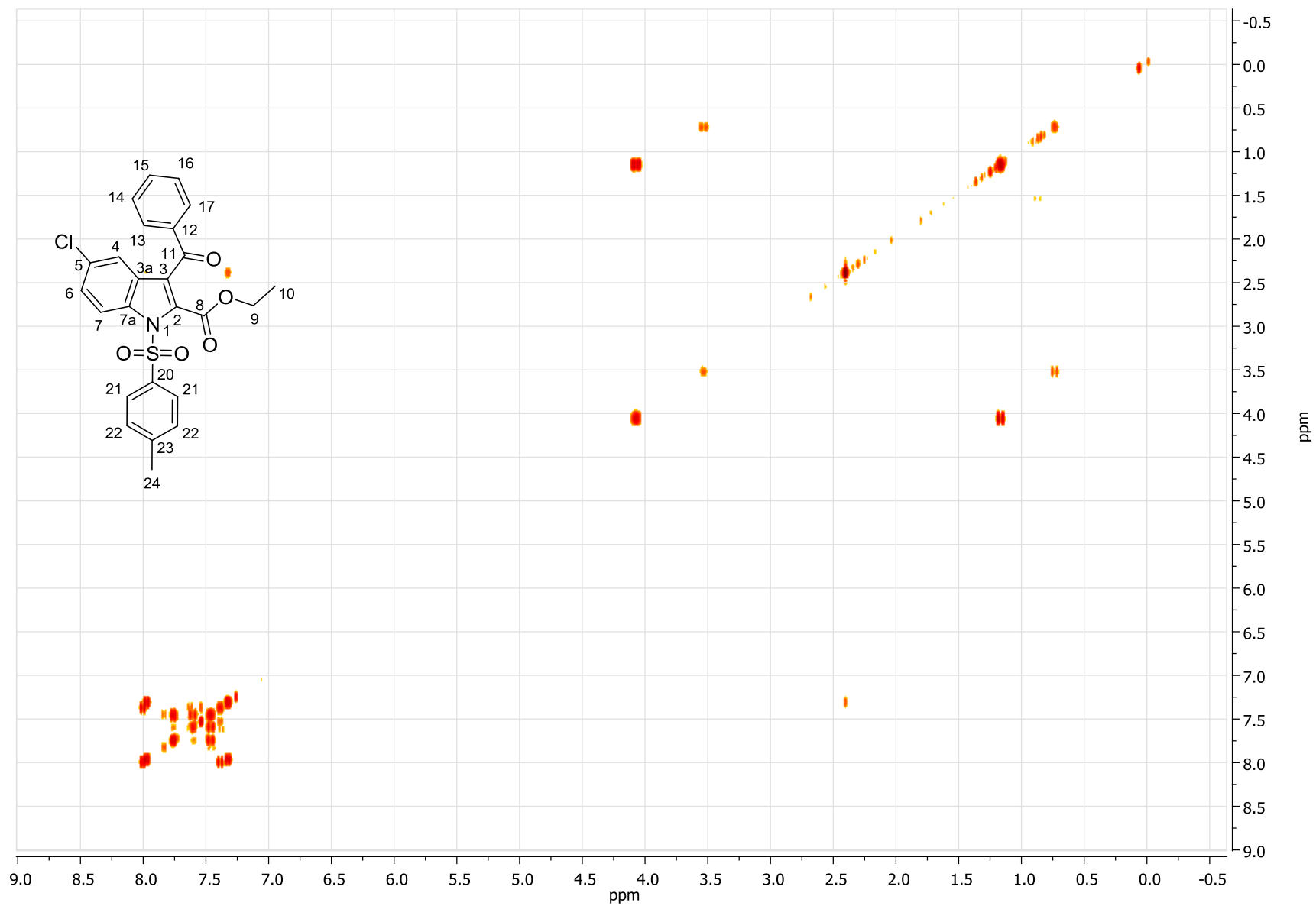
Ethyl 3-benzoyl-5-chloro-1-tosyl-1H-indole-2-carboxylate - 7



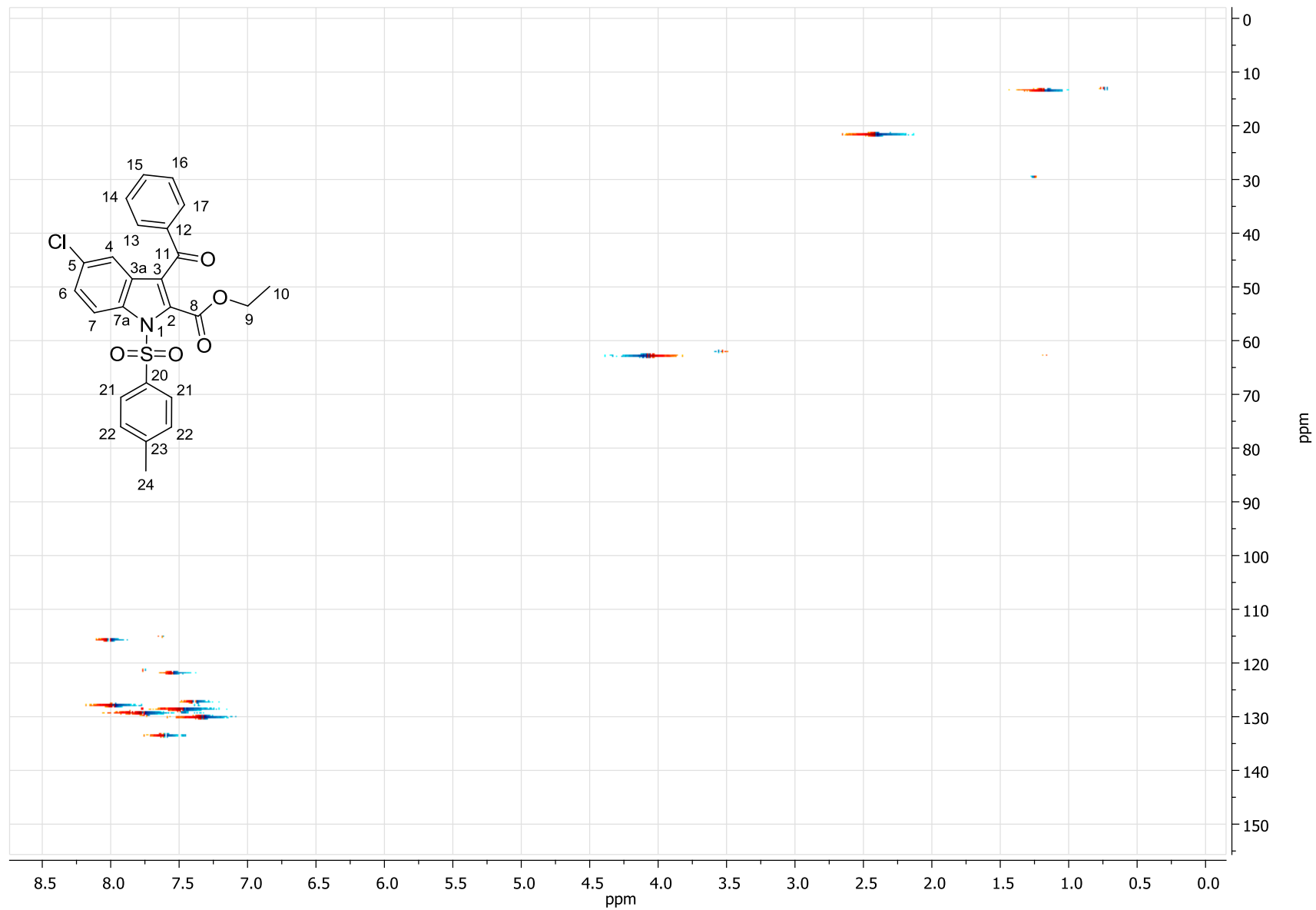
¹H NMR Spectrum
300 MHz Varian VNMRS



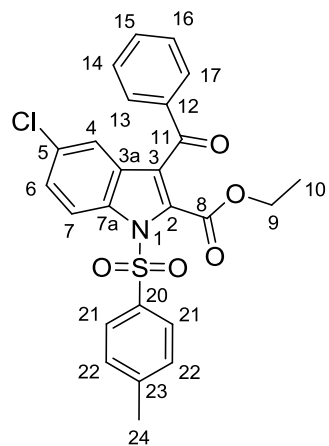
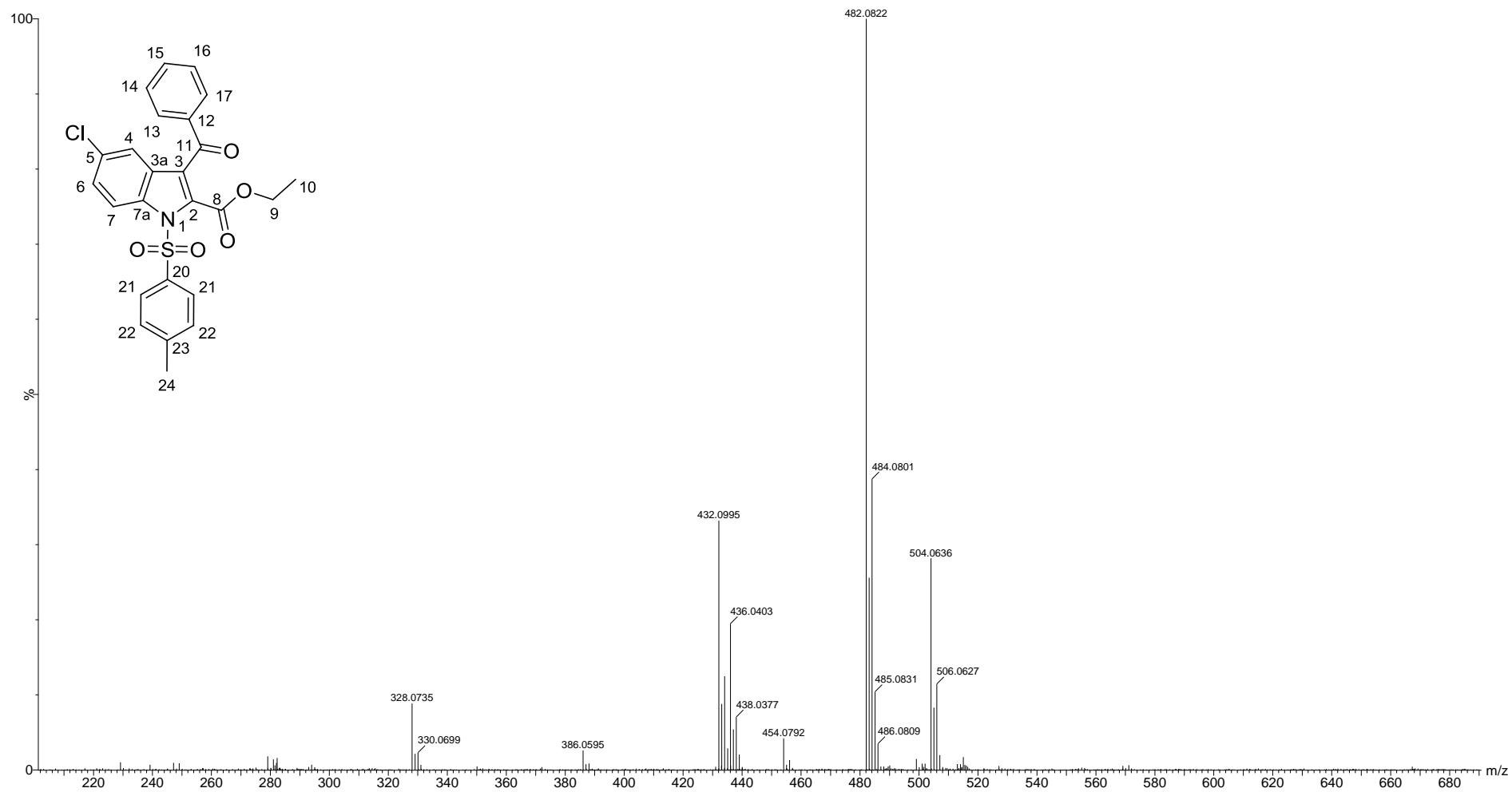
¹³C NMR Spectrum
75 MHz Varian VNMRS



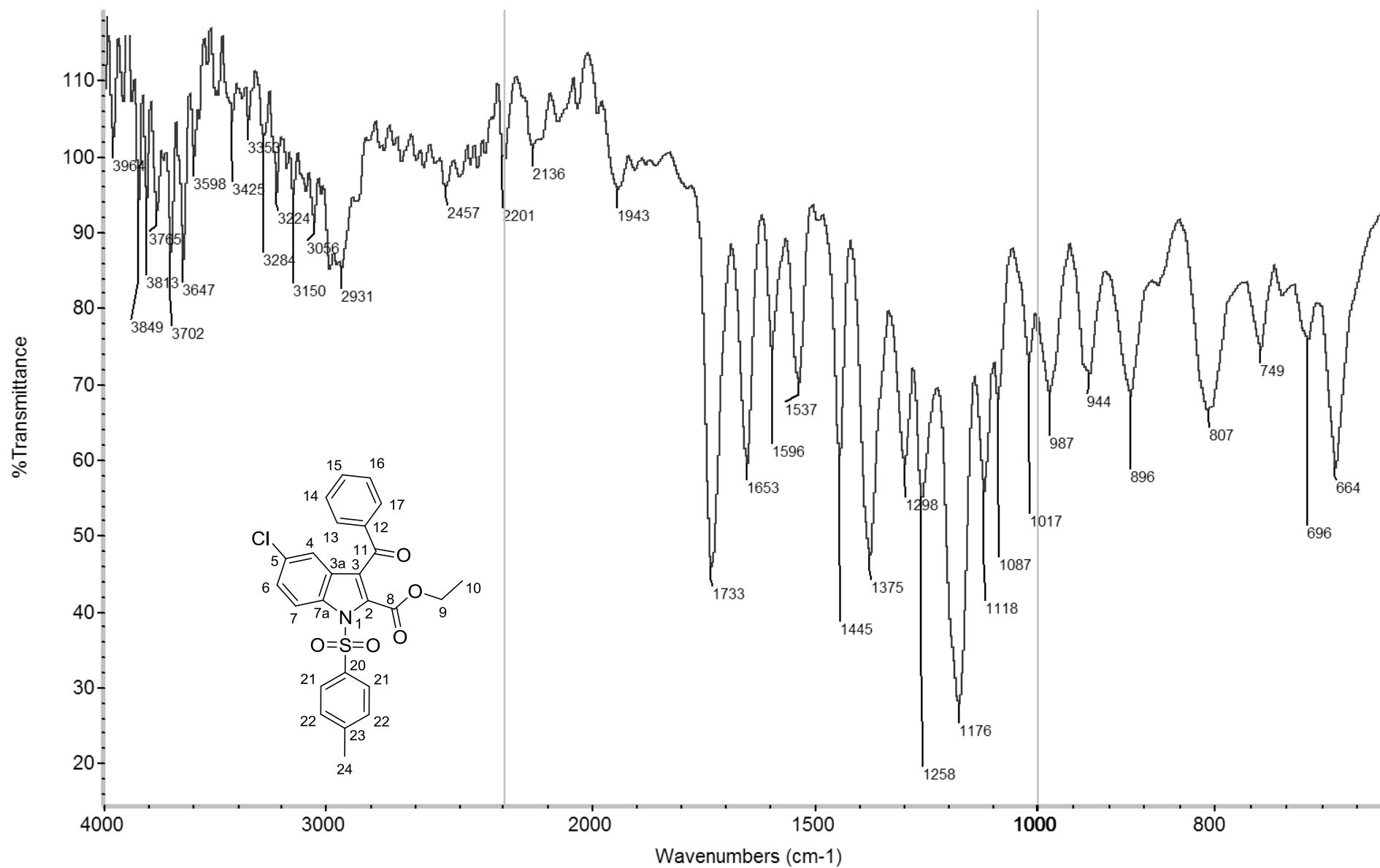
COSY NMR Spectrum
300 MHz Varian VNMRS



gHSQC NMR Spectrum
300 MHz Varian VNMRS

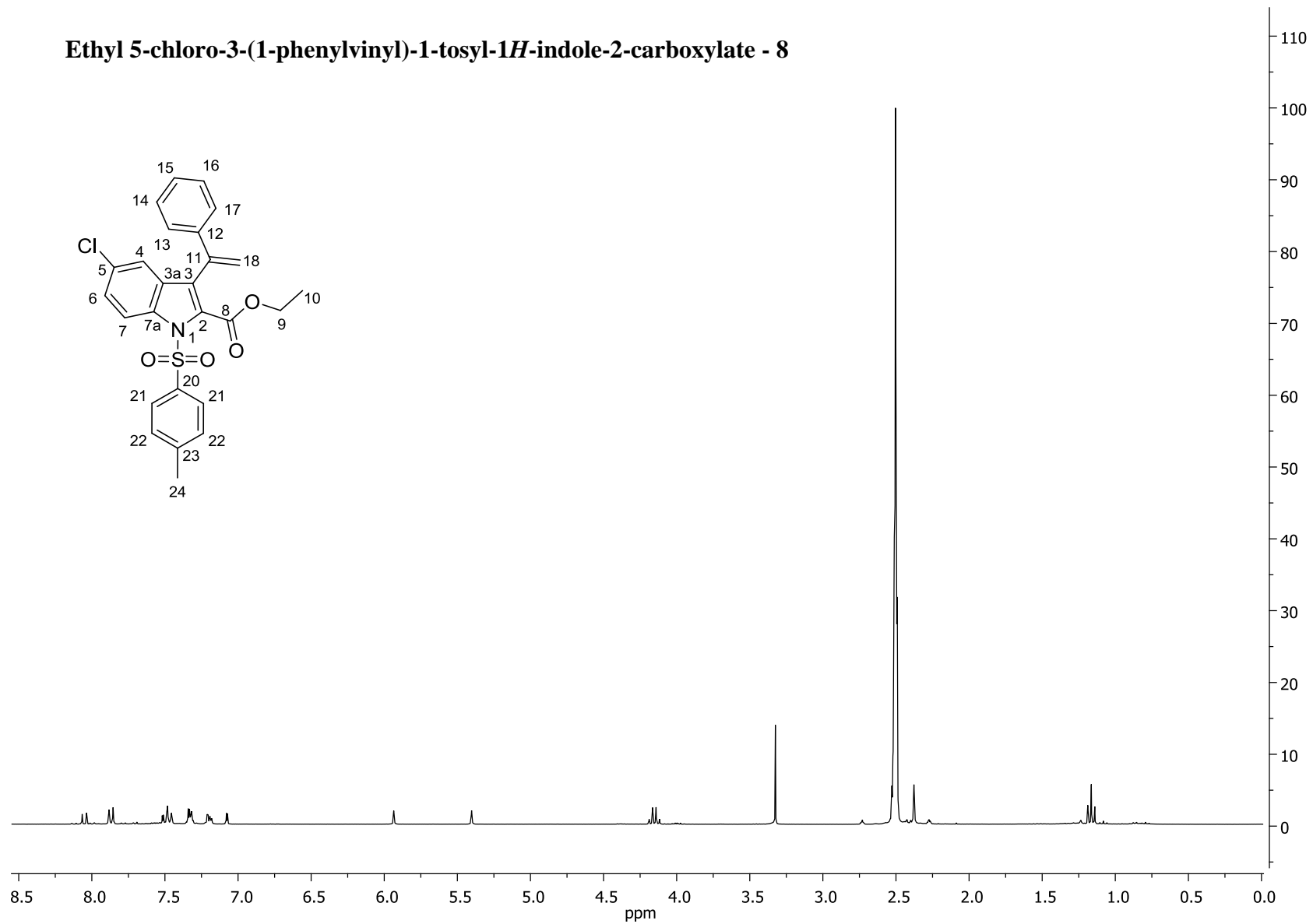


Mass Spectrum
Waters SYNAPT G2

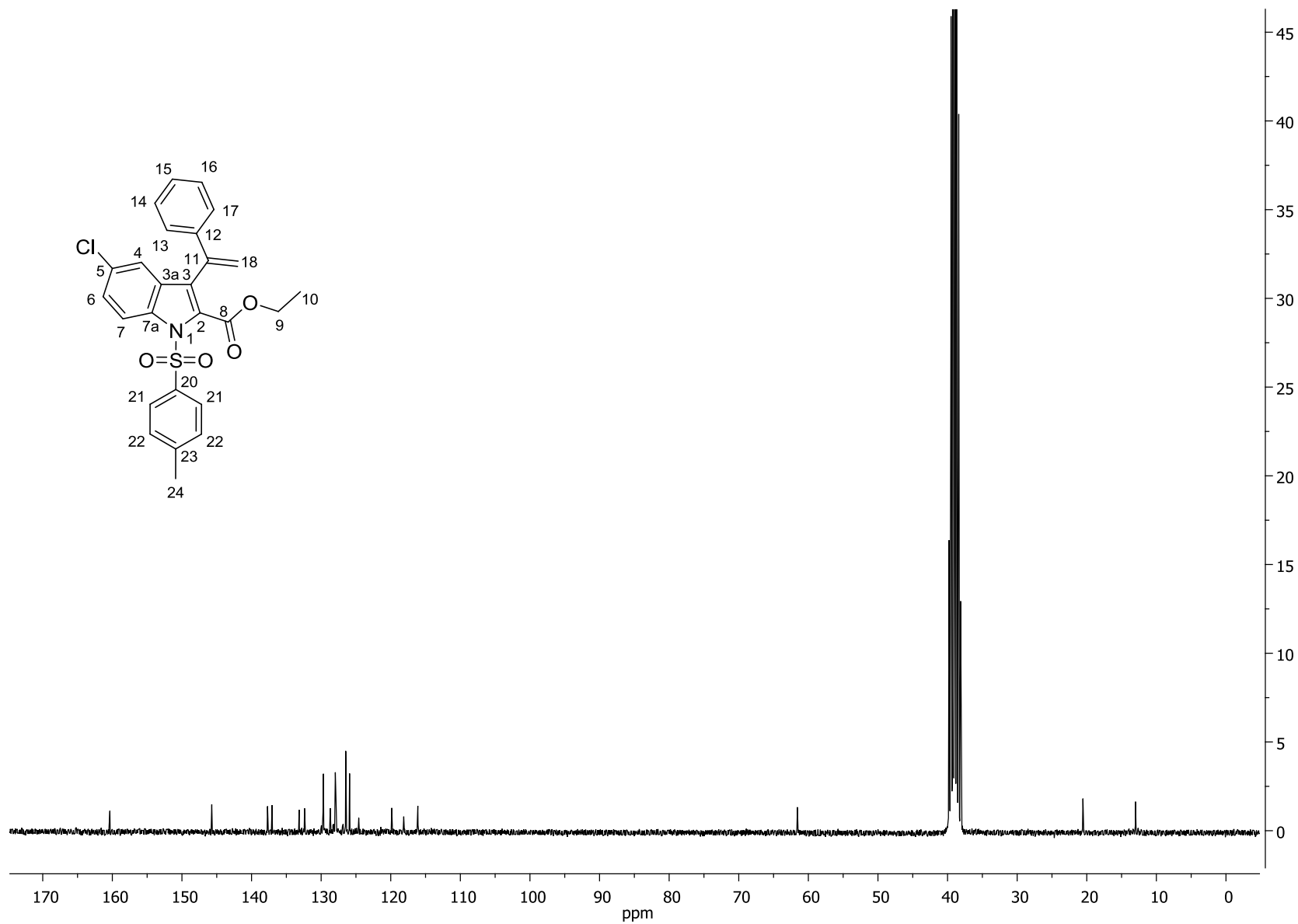


Infrared Spectrum
Thermo Nicolet Nexus 470

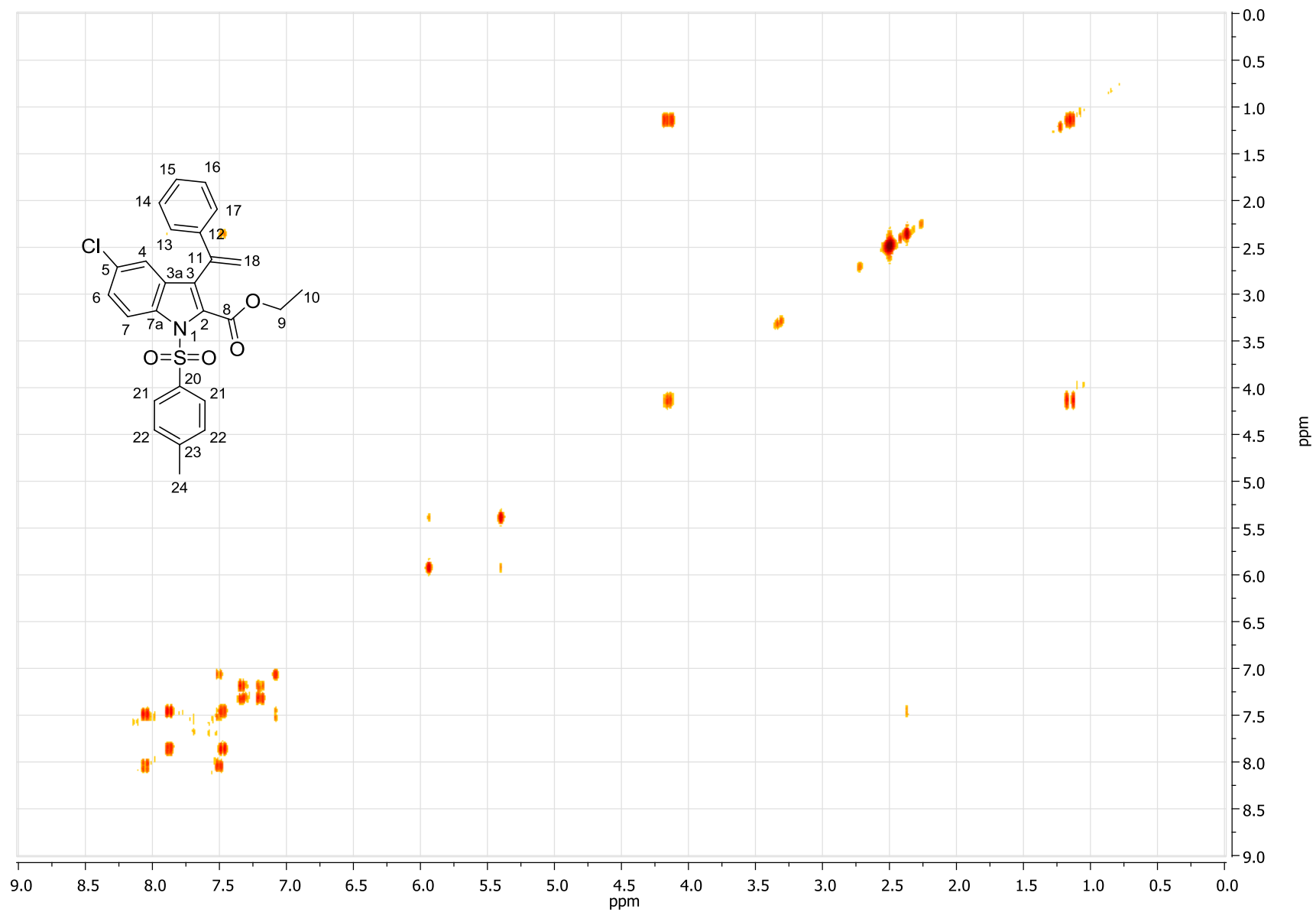
Ethyl 5-chloro-3-(1-phenylvinyl)-1-tosyl-1H-indole-2-carboxylate - 8



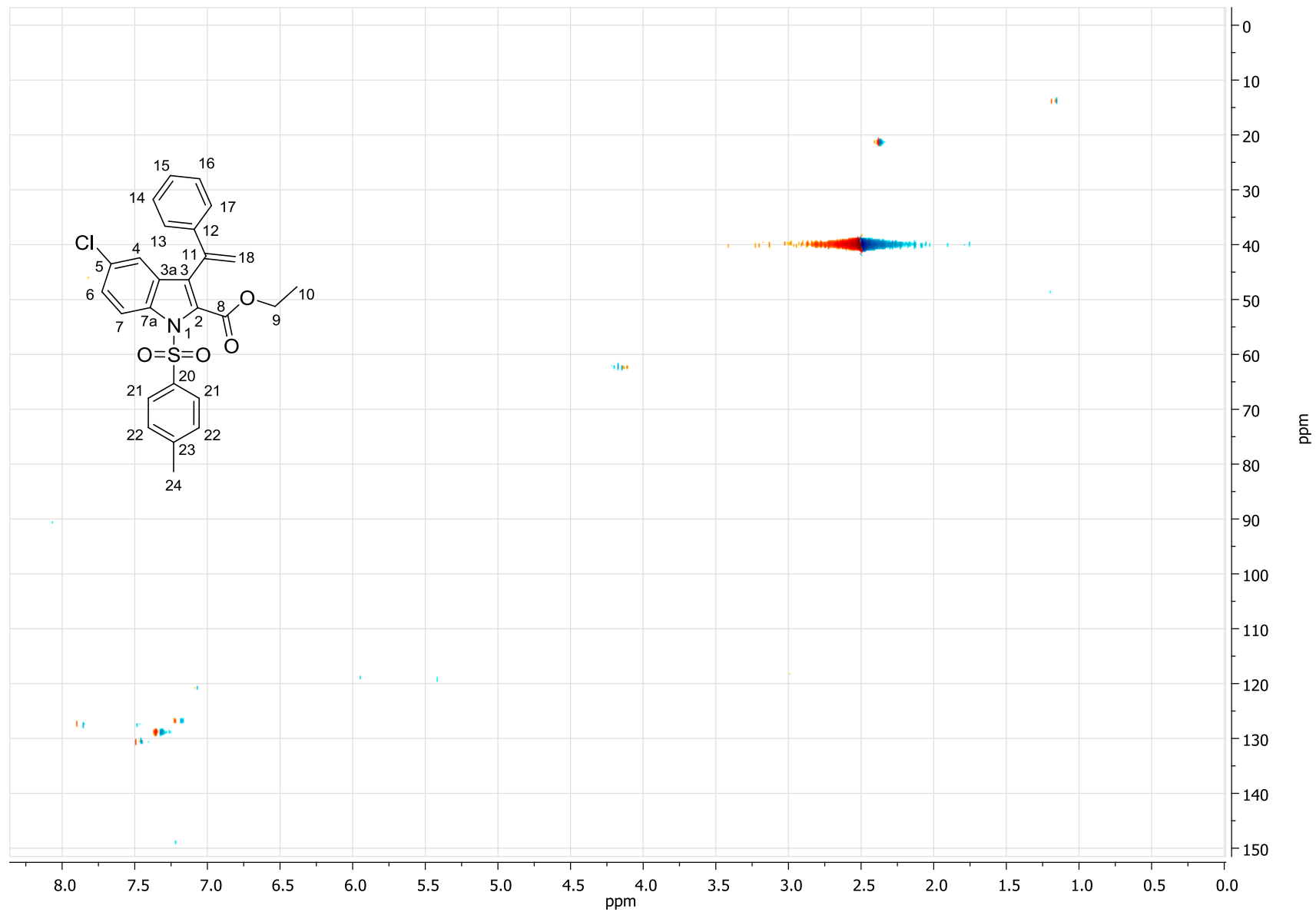
^1H NMR Spectrum
300 MHz Varian VNMRS

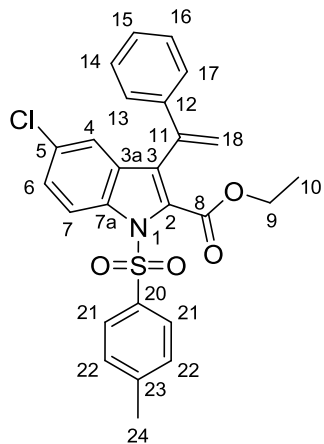
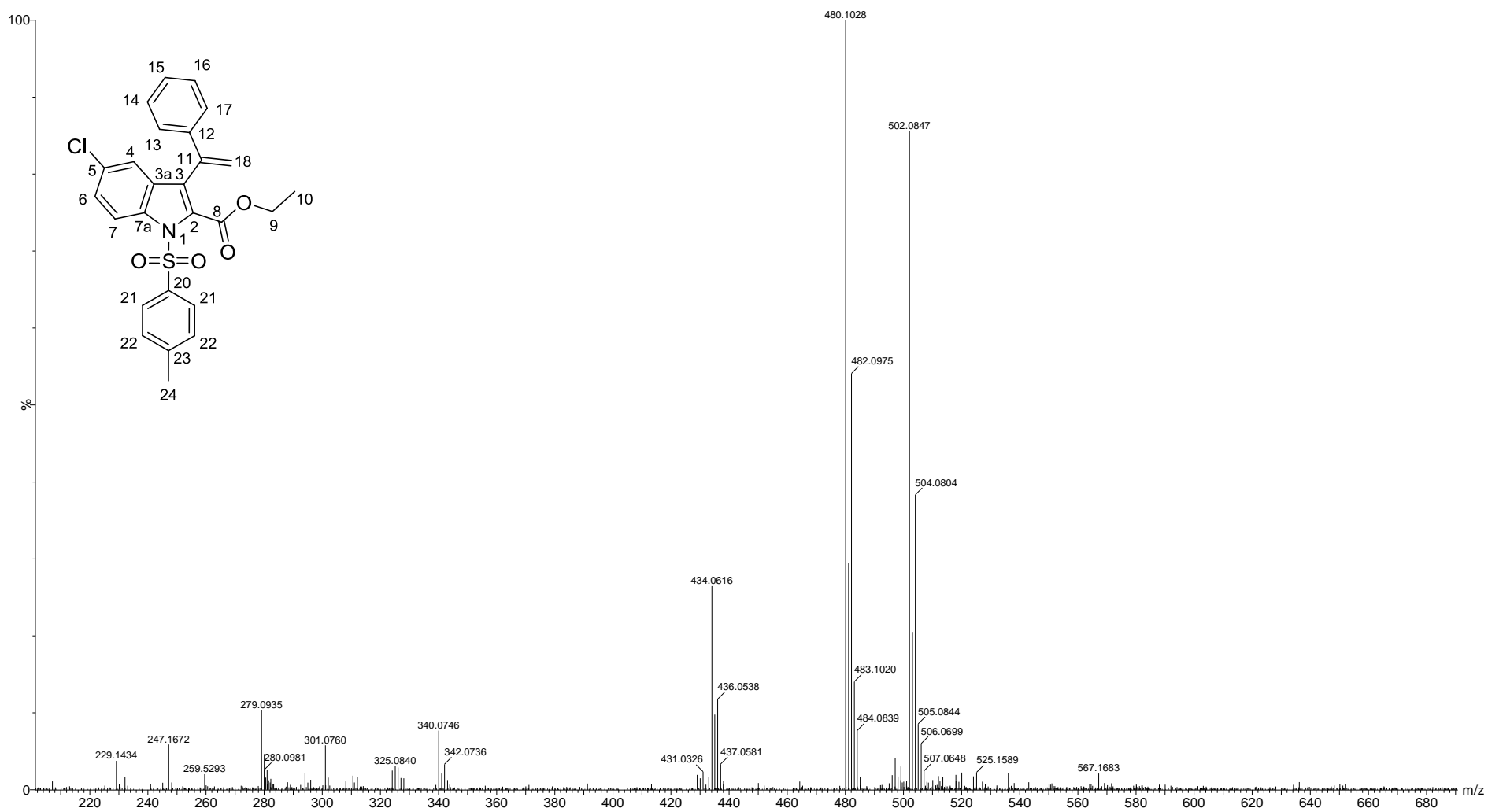


^{13}C NMR Spectrum
75 MHz Varian VNMRS

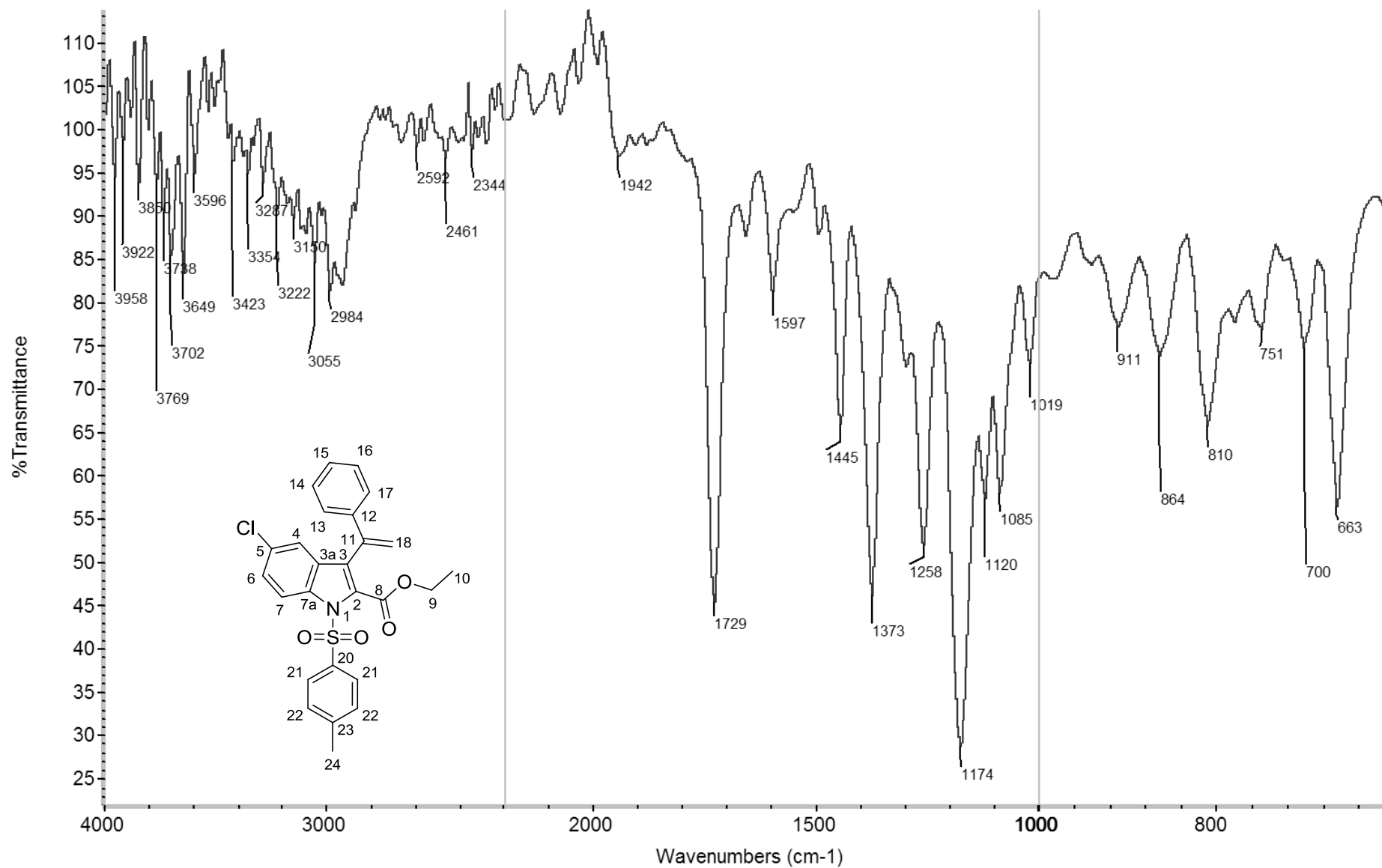


COSY NMR Spectrum
300 MHz Varian VNMRS



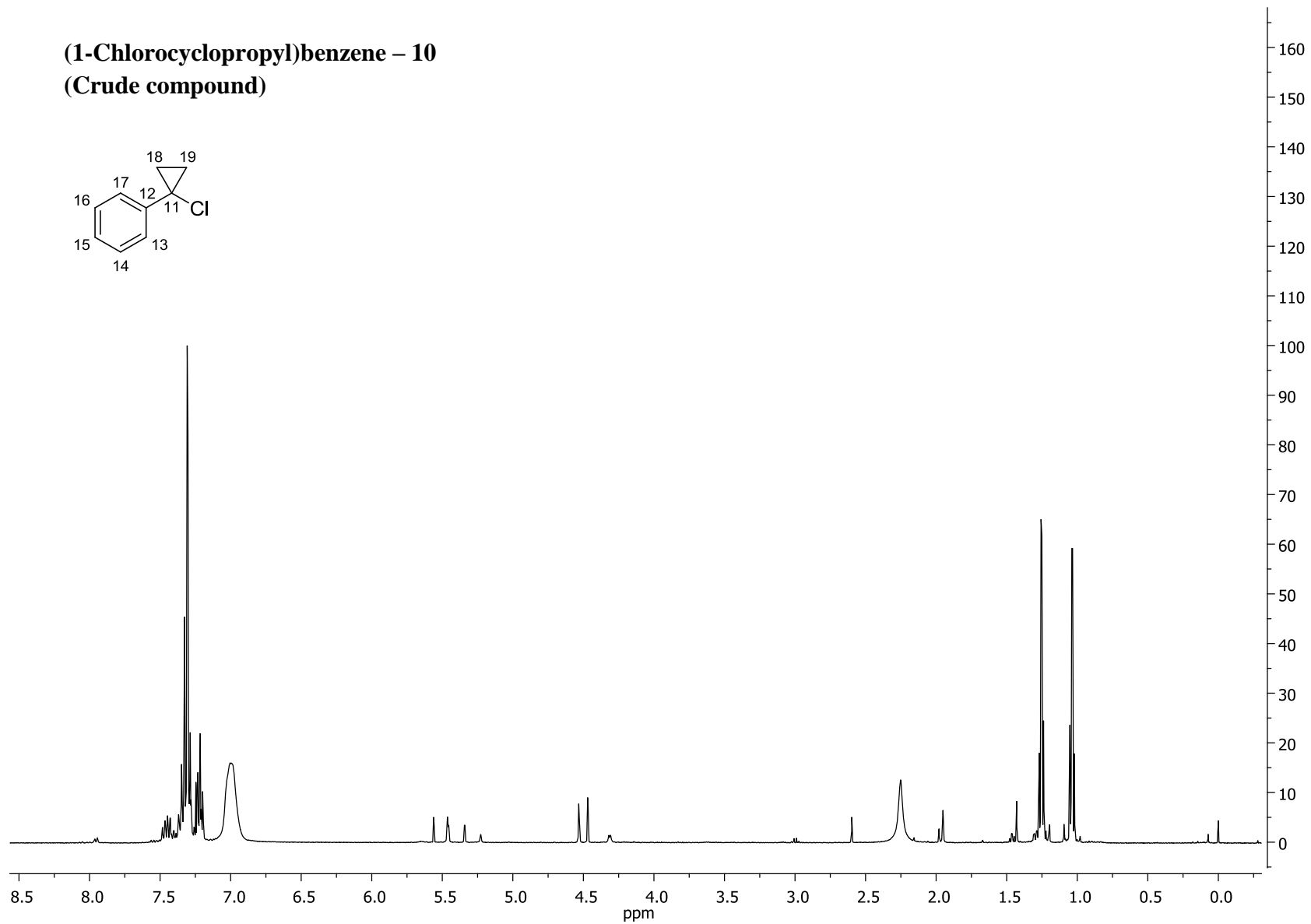
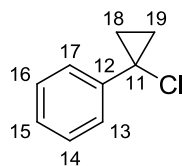


Mass Spectrum
Waters SYNAPT G2



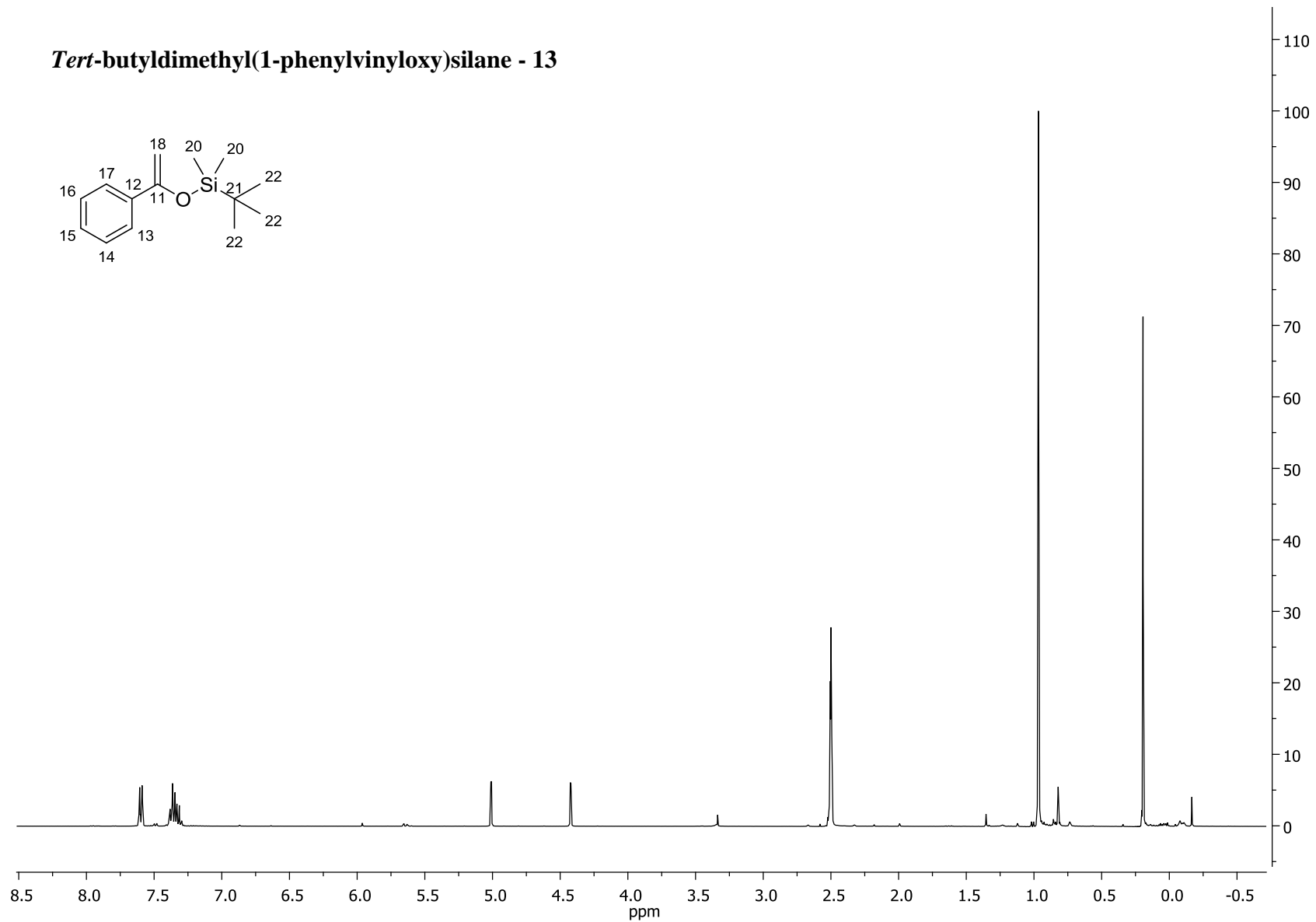
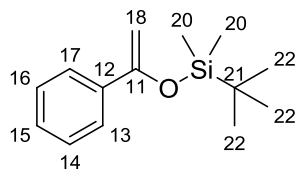
Infrared Spectrum
Thermo Nicolet Nexus 470

(1-Chlorocyclopropyl)benzene – 10
(Crude compound)

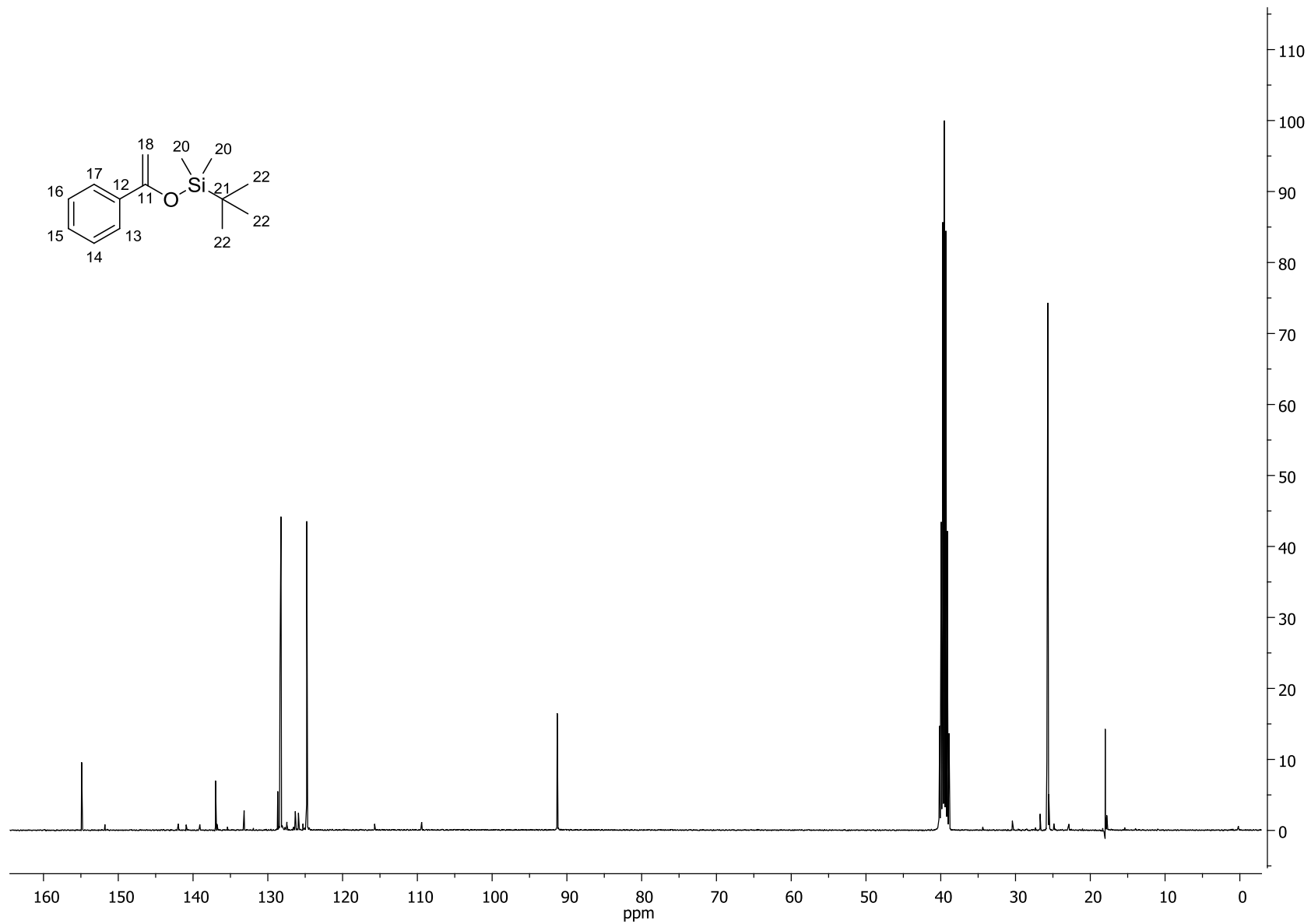


¹H NMR Spectrum
400 MHz Varian Unity Inova

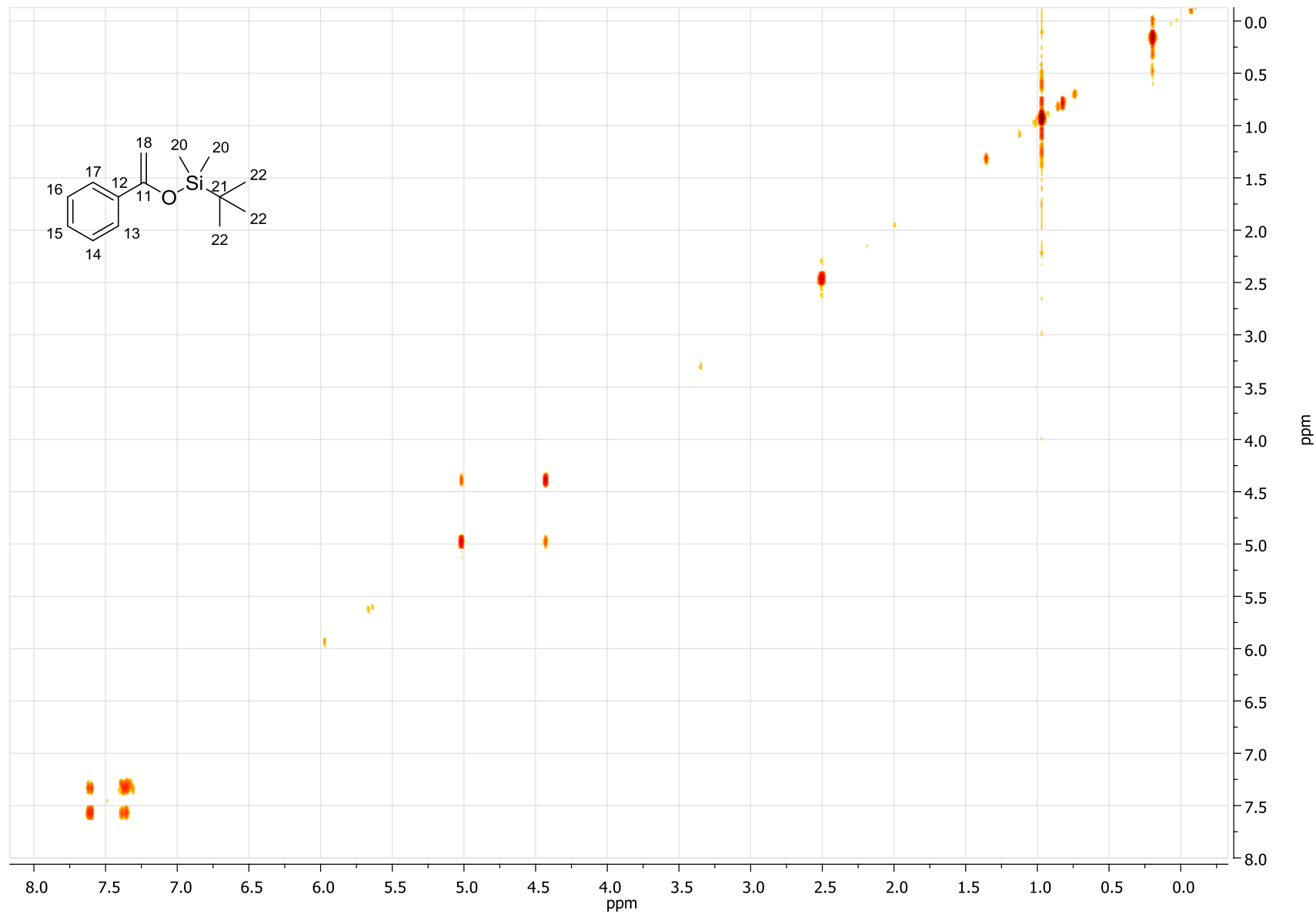
***Tert*-butyldimethyl(1-phenylvinyl)oxy)silane - 13**



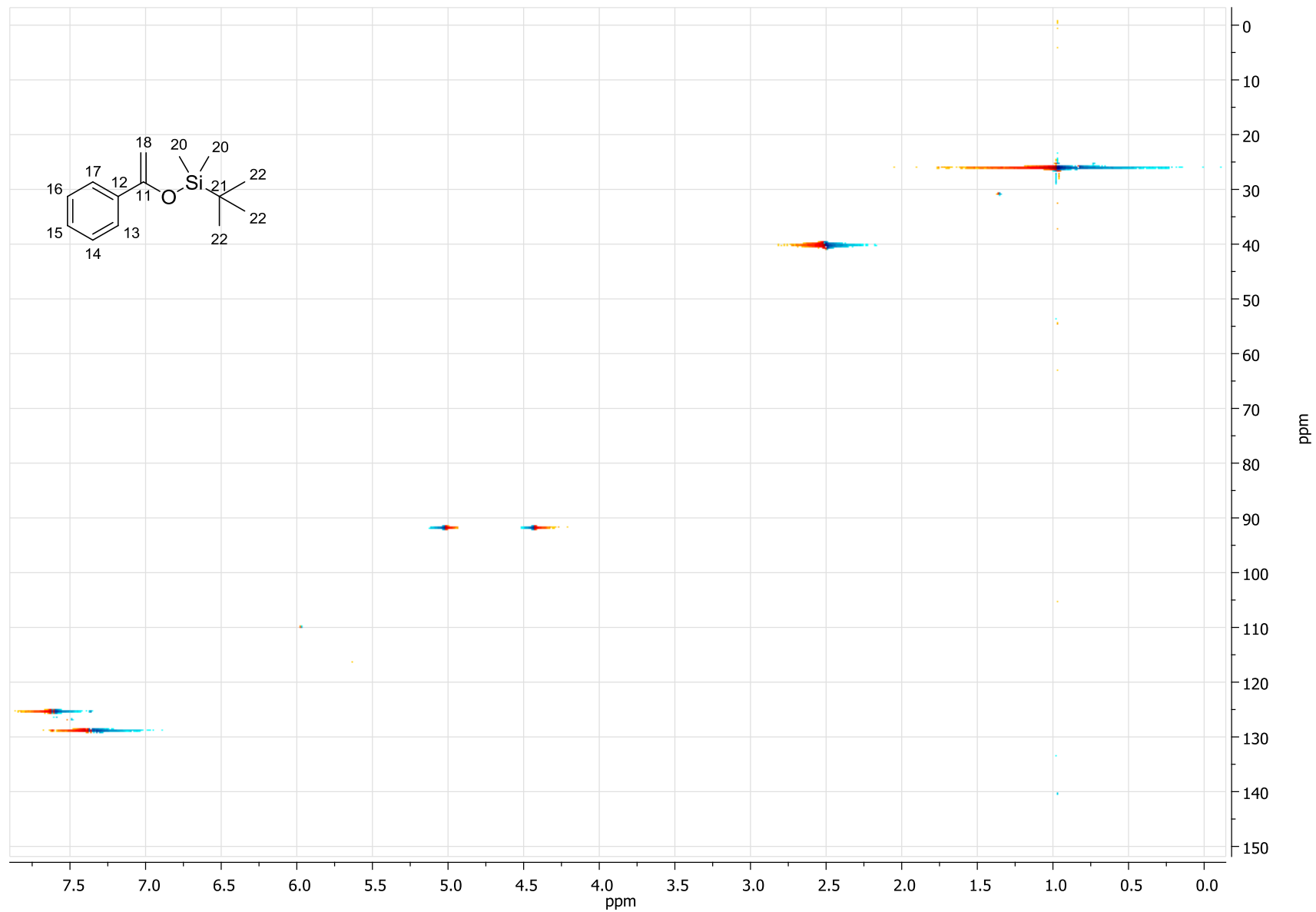
¹H NMR Spectrum
400 MHz Varian Unity Inova



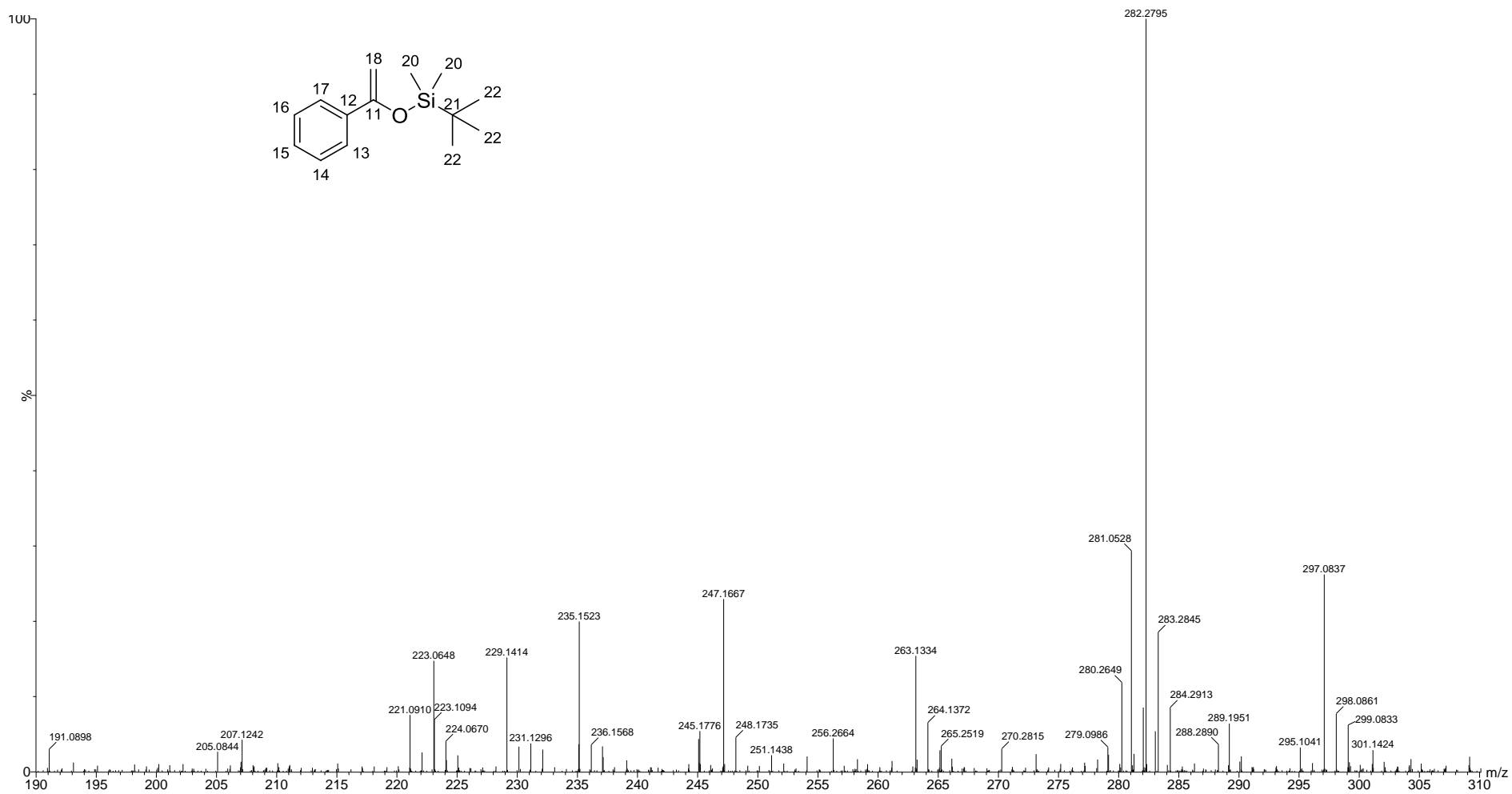
¹³C NMR Spectrum
101 MHz Varian Unity Inova



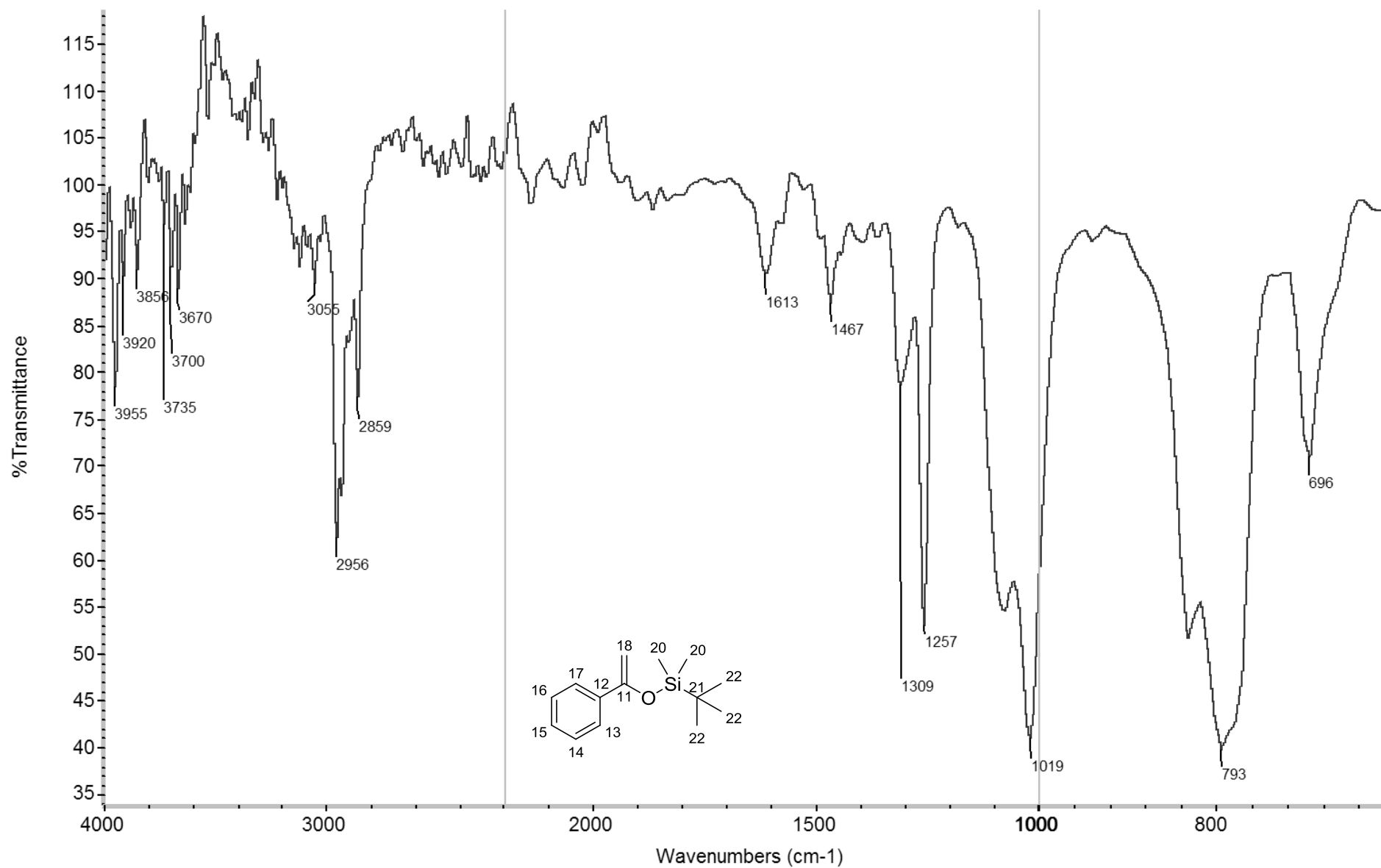
COSY NMR Spectrum
400 MHz Varian Unity Inova



gHSQC NMR Spectrum
400 MHz Varian Unity Inova

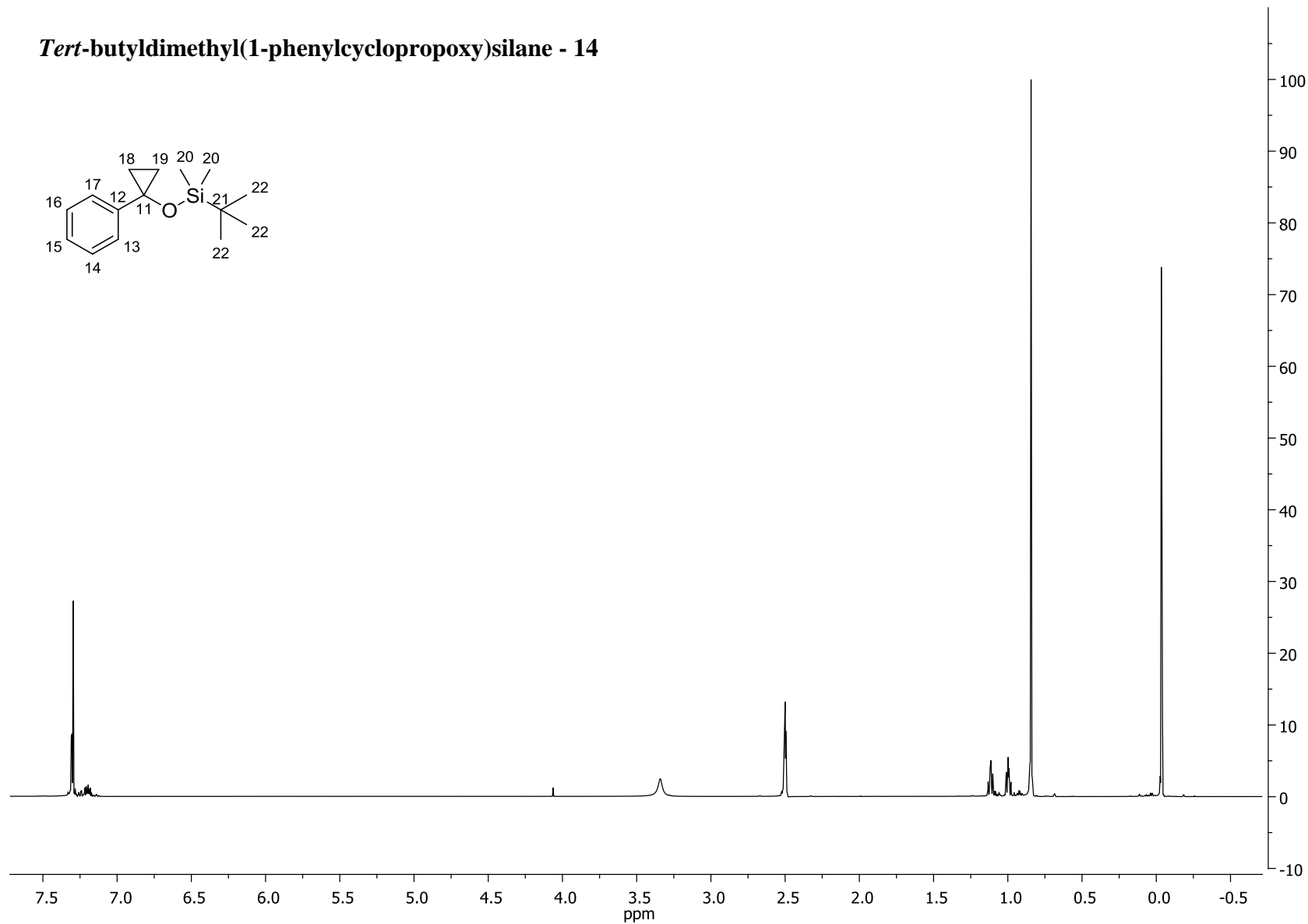


Mass Spectrum
Waters SYNAPT G2

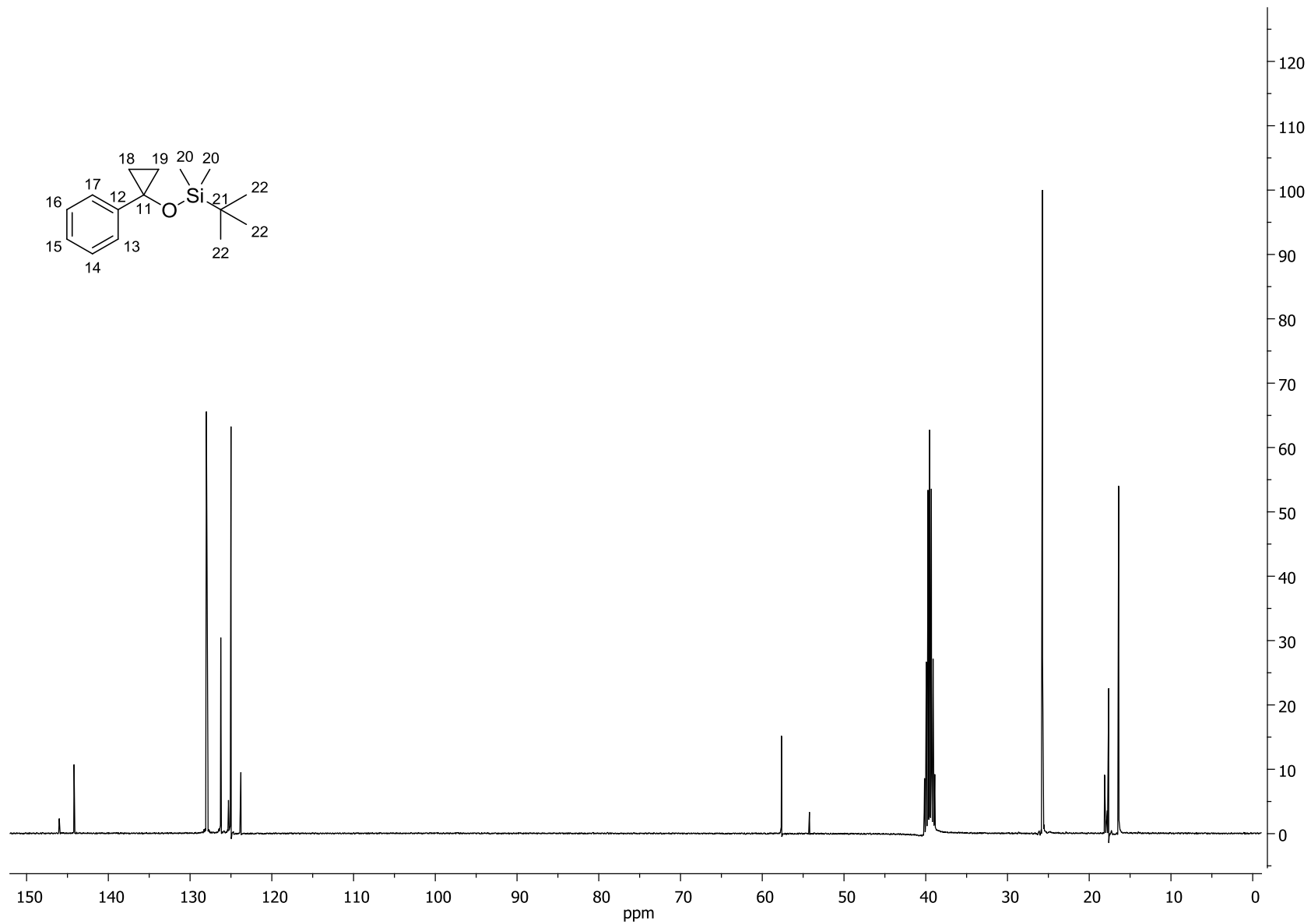


Infrared Spectrum
Thermo Nicolet Nexus 470

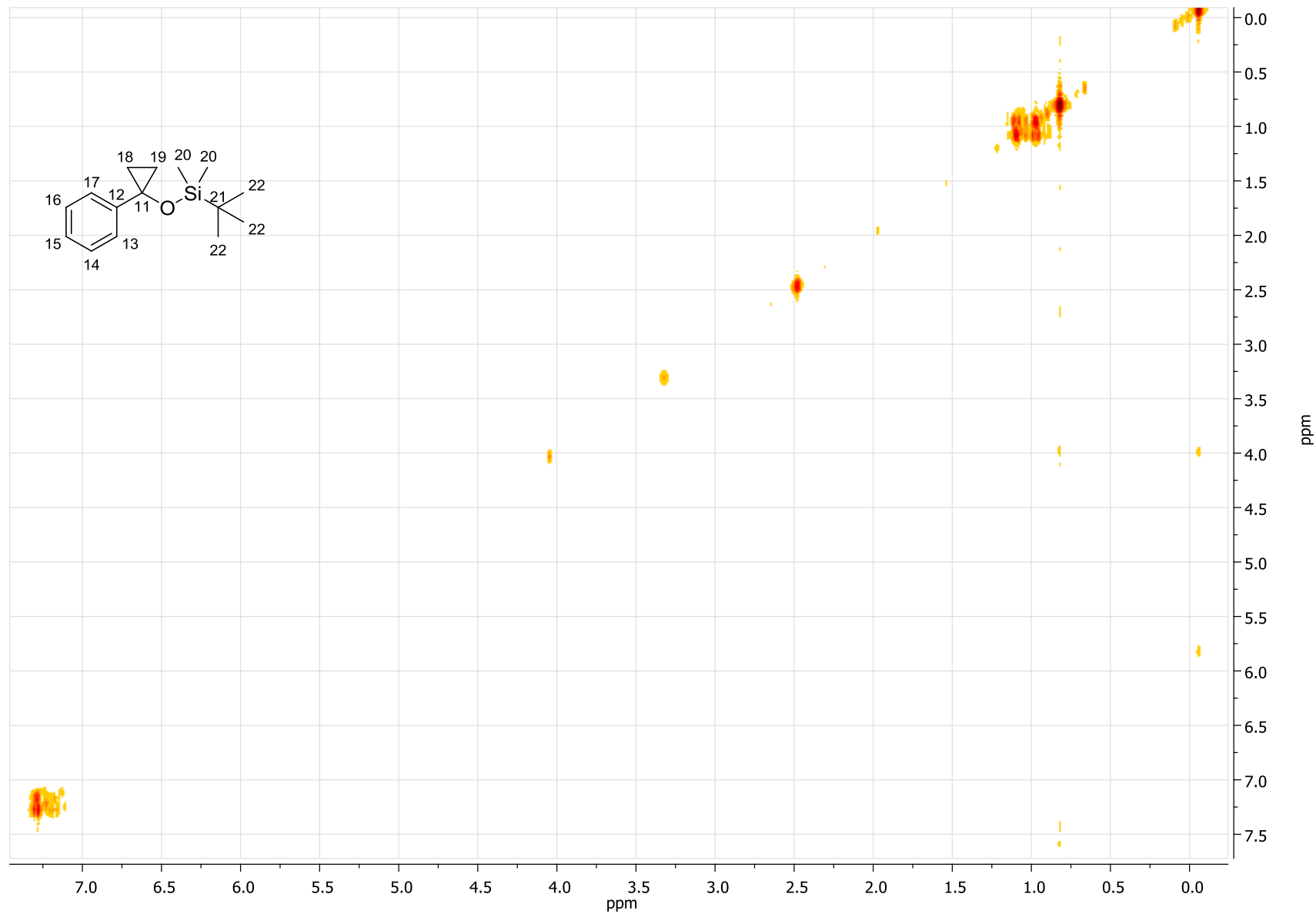
***Tert*-butyldimethyl(1-phenylcyclopropoxy)silane - 14**



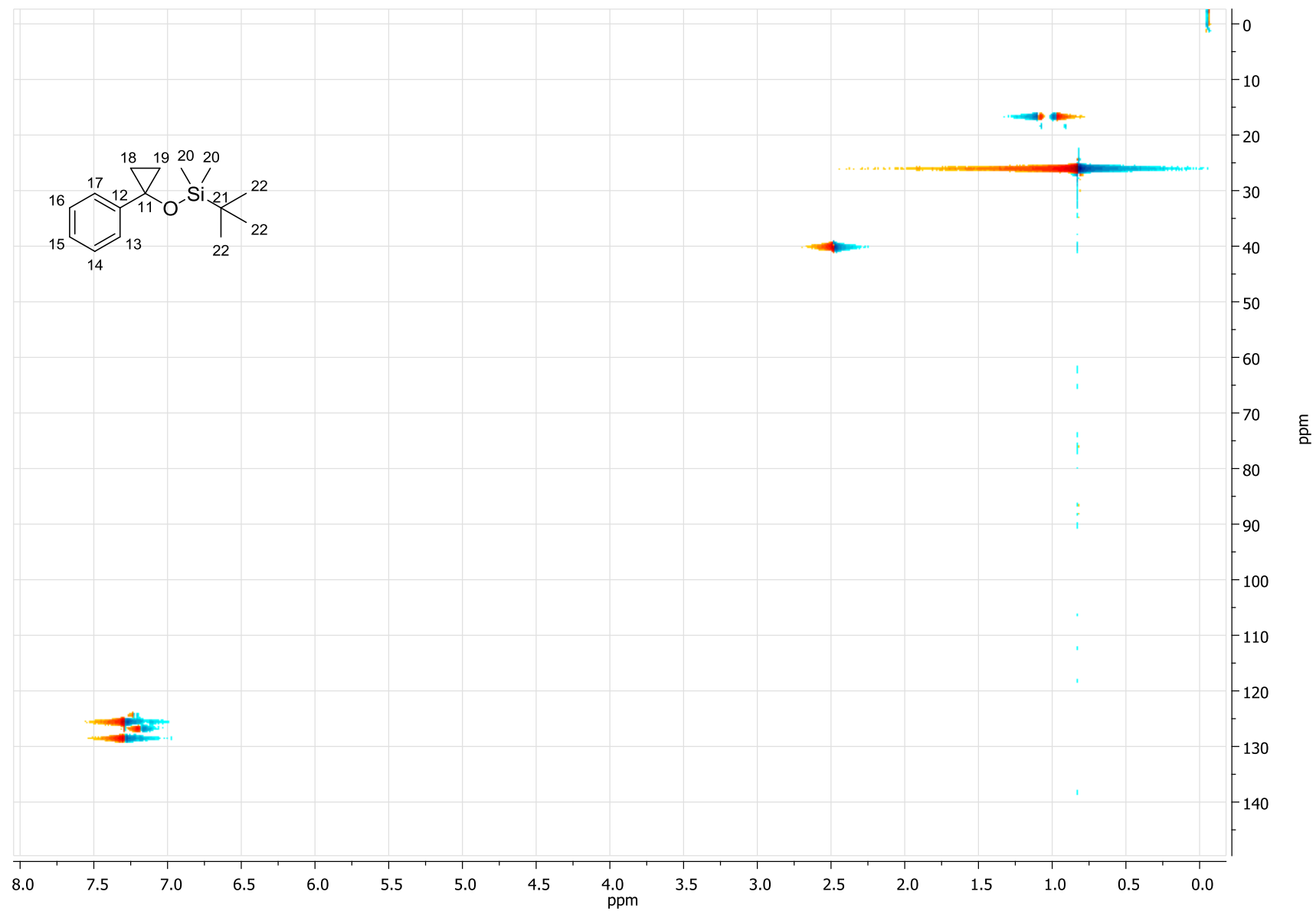
¹H NMR Spectrum
400 MHz Varian Unity Inova



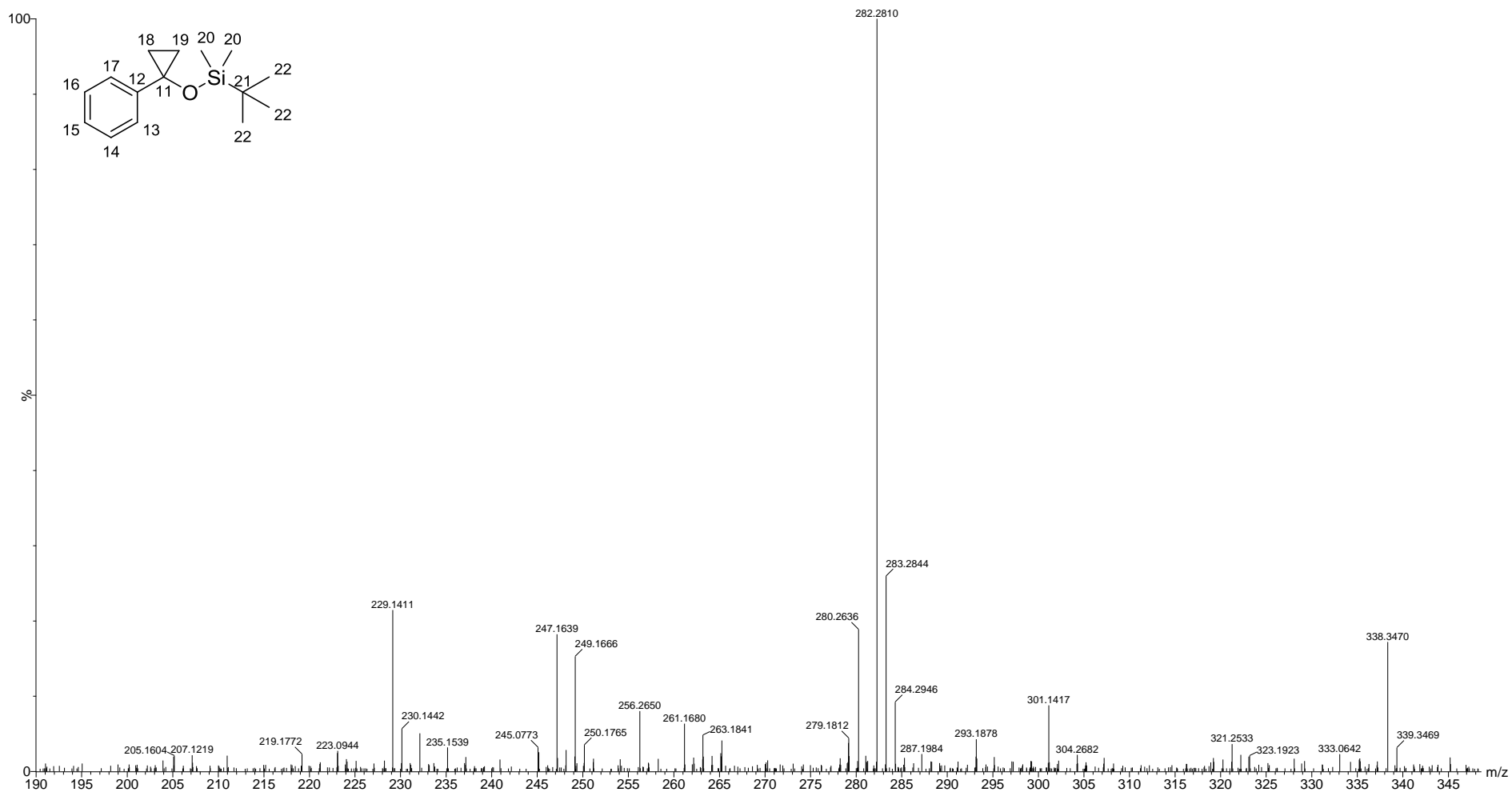
^{13}C NMR Spectrum
101 MHz Varian Unity Inova



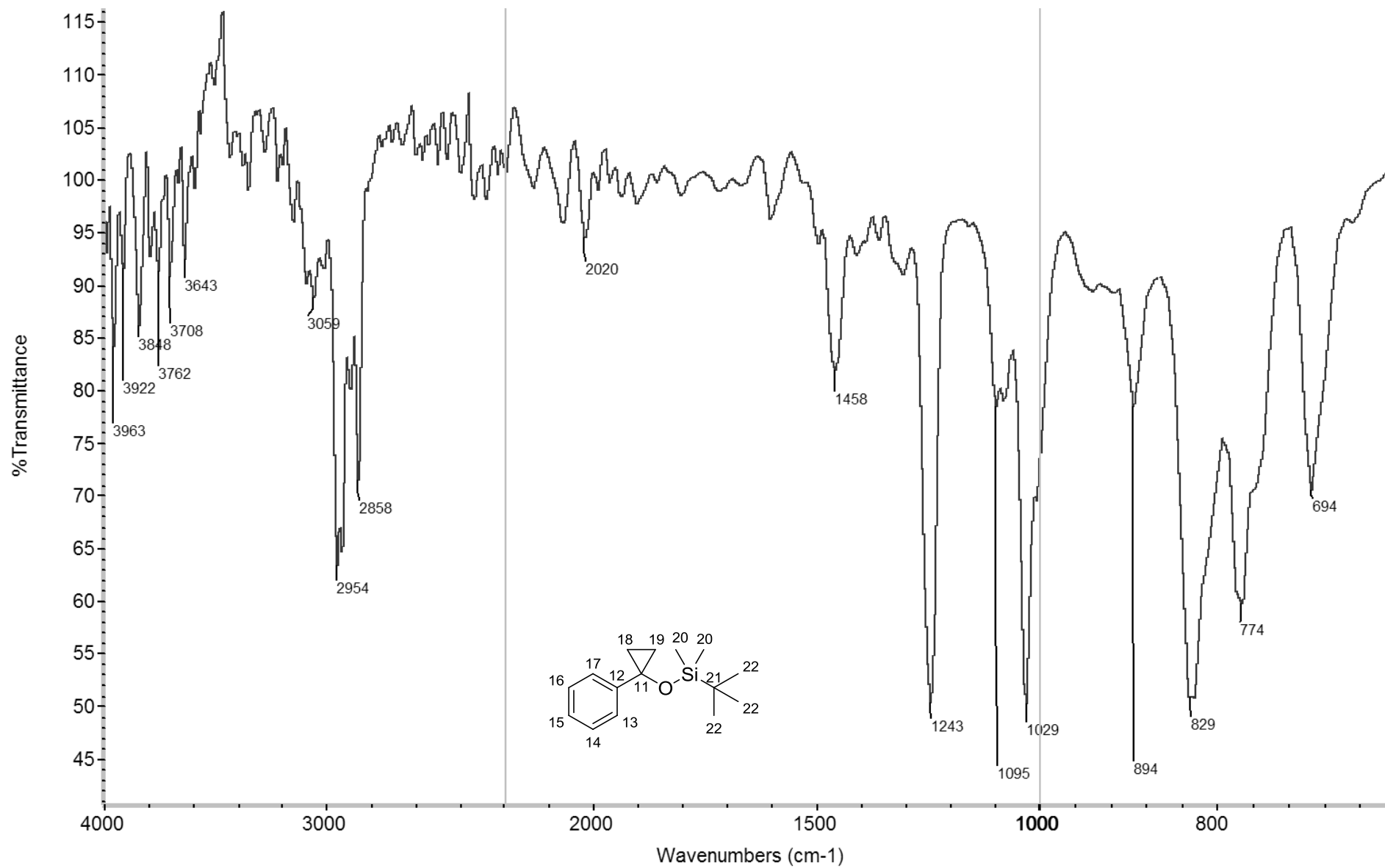
COSY NMR Spectrum
400 MHz Varian Unity Inova



gHSQC NMR Spectrum
400 MHz Varian Unity Inova

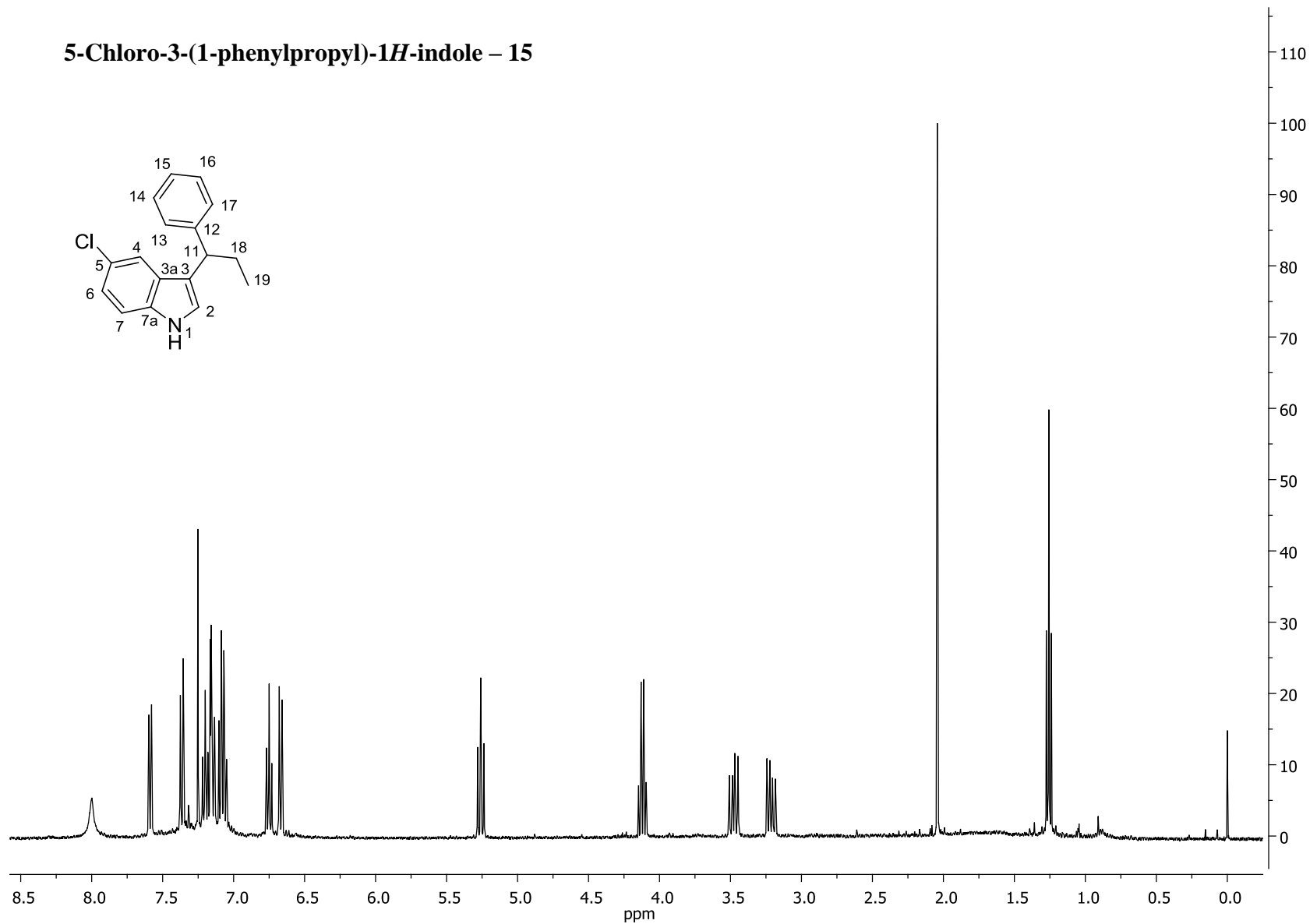
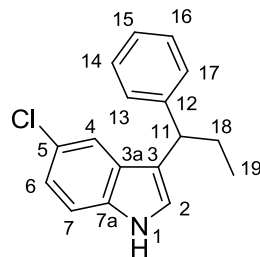


Mass Spectrum
Waters SYNAPT G2



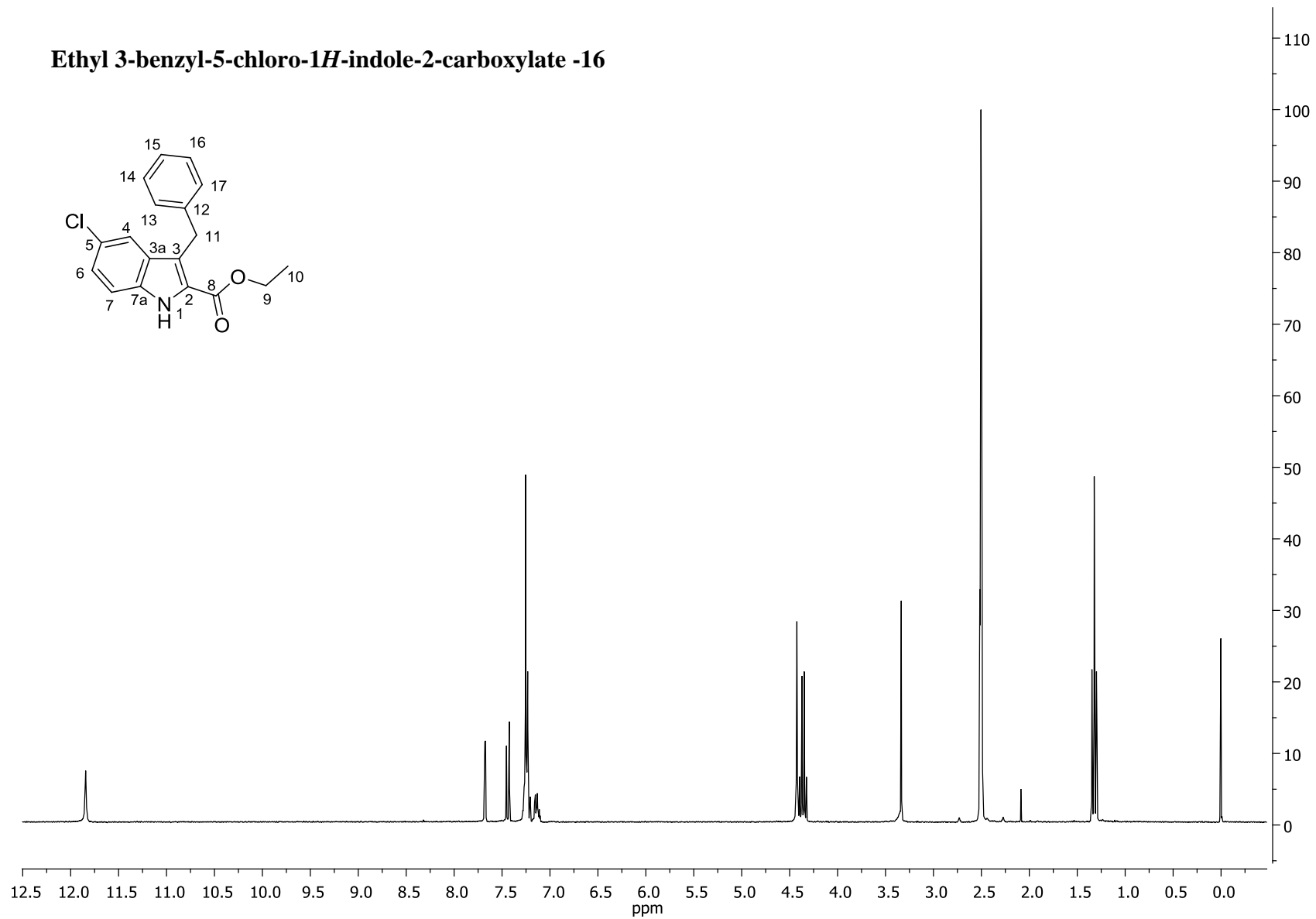
Infrared Spectrum
Thermo Nicolet Nexus 470

5-Chloro-3-(1-phenylpropyl)-1H-indole – 15

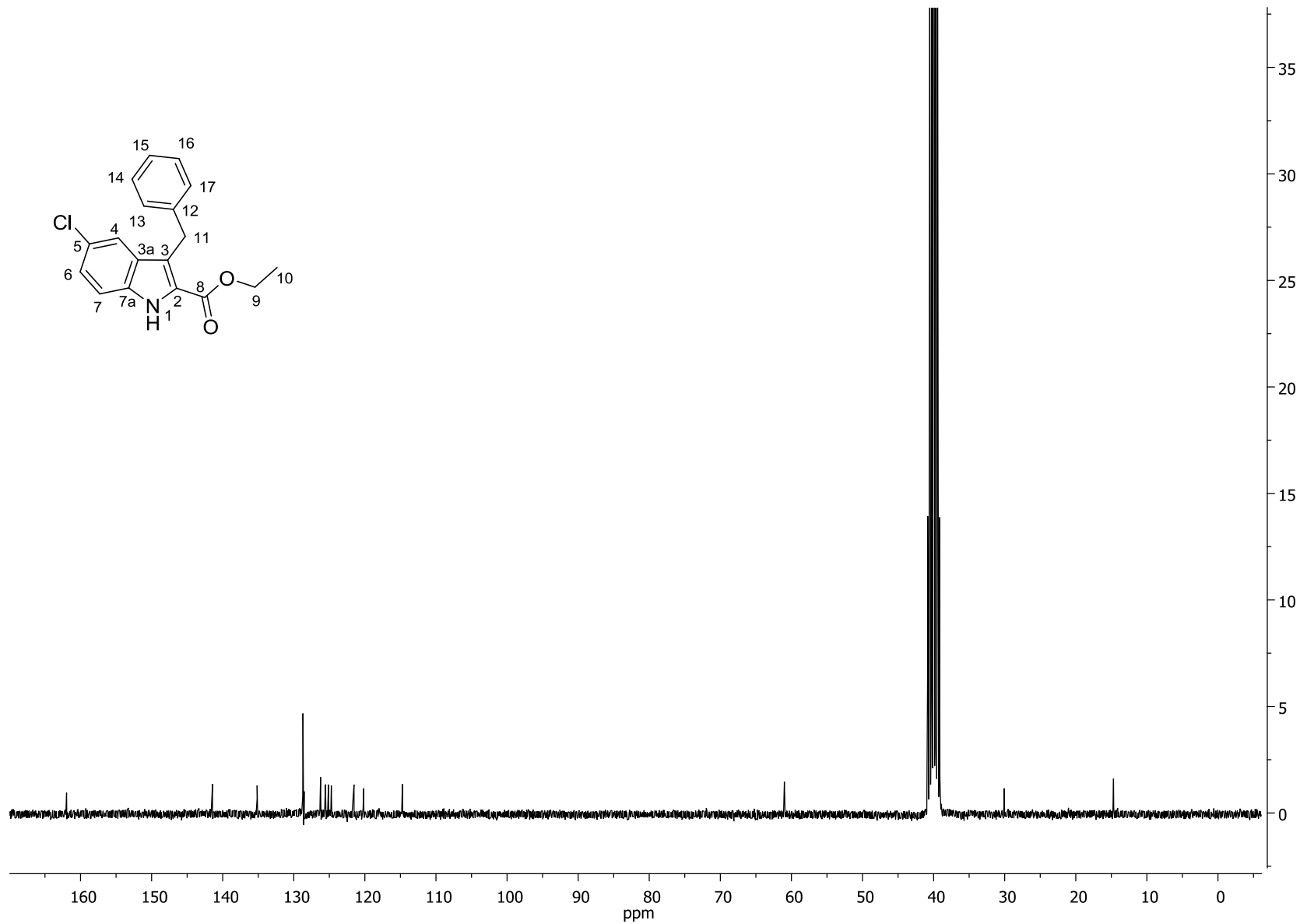


¹H NMR Spectrum
400 MHz Varian Unity Inova

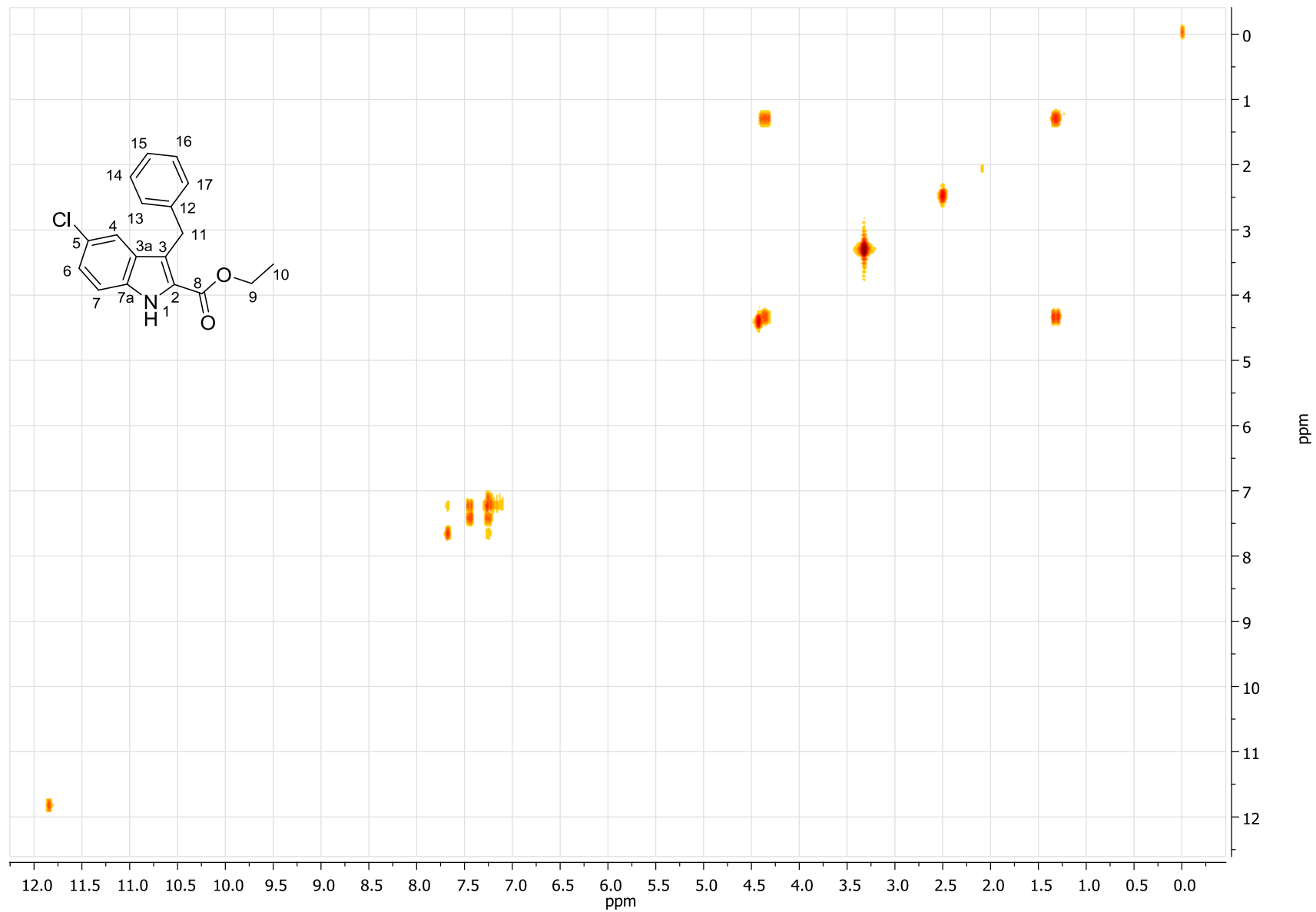
Ethyl 3-benzyl-5-chloro-1H-indole-2-carboxylate -16



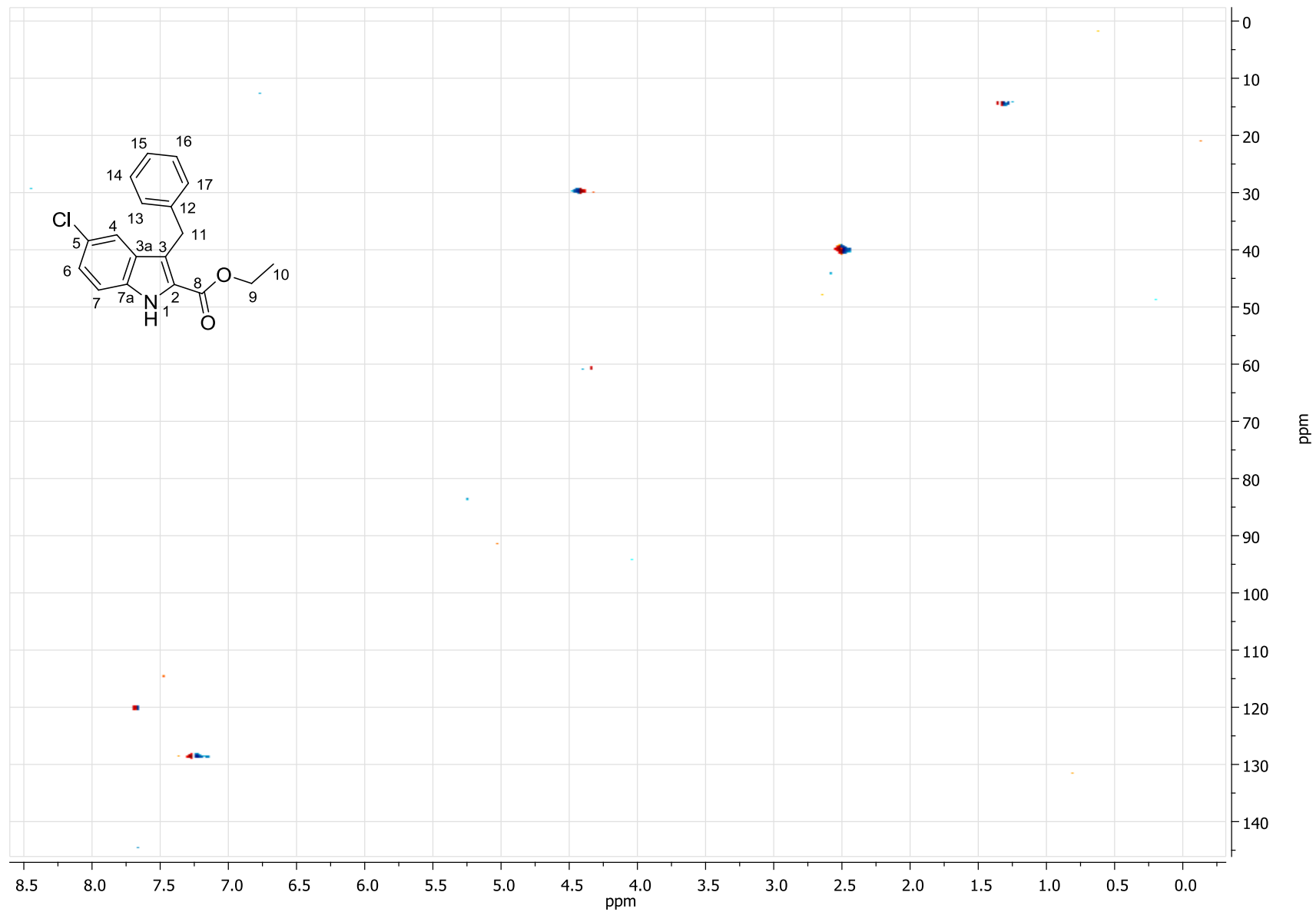
^1H NMR Spectrum
300 MHz Varian VNMRS



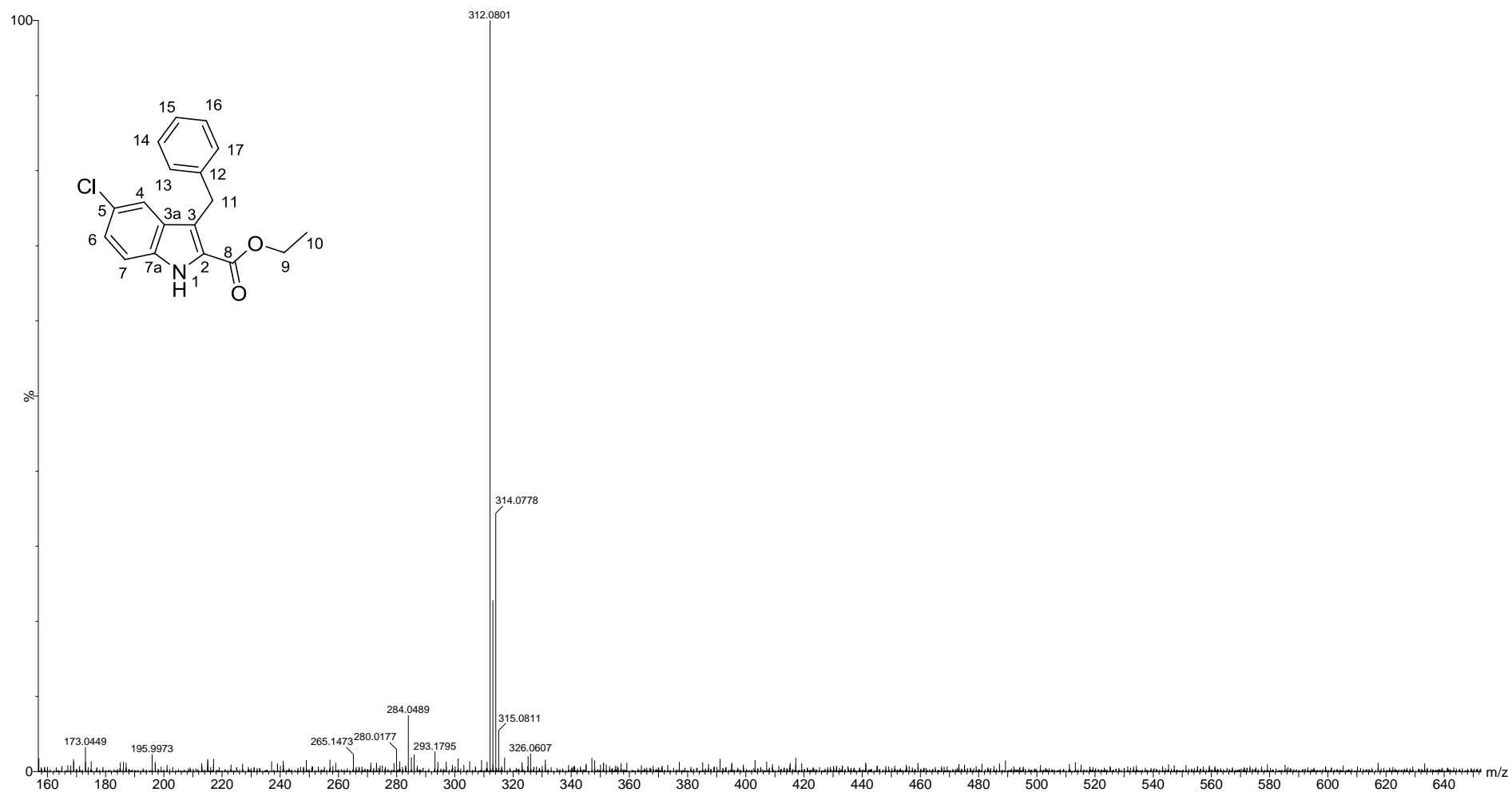
^{13}C NMR Spectrum
75 MHz Varian VNMRS



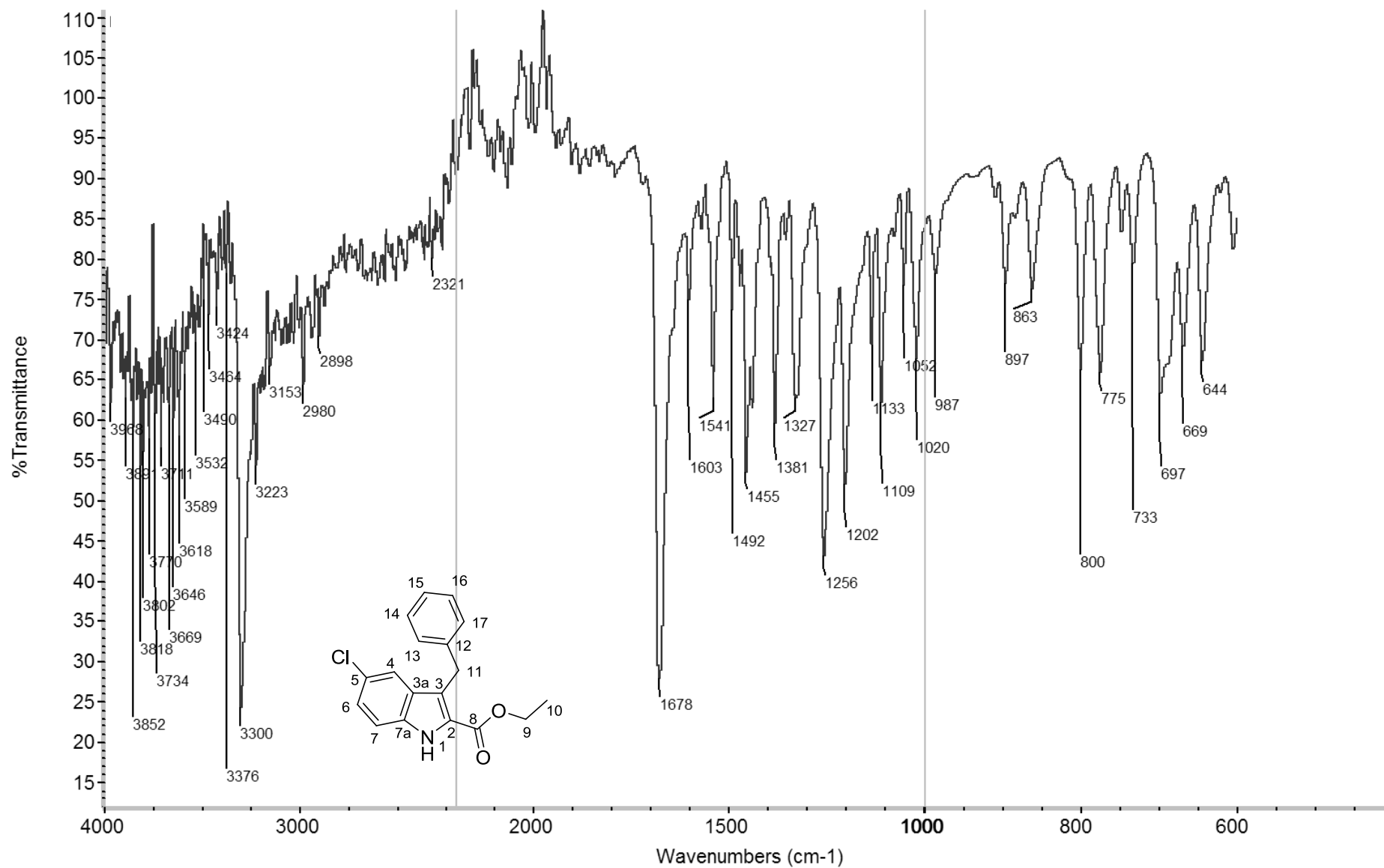
COSY NMR Spectrum
300 MHz Varian VNMRS



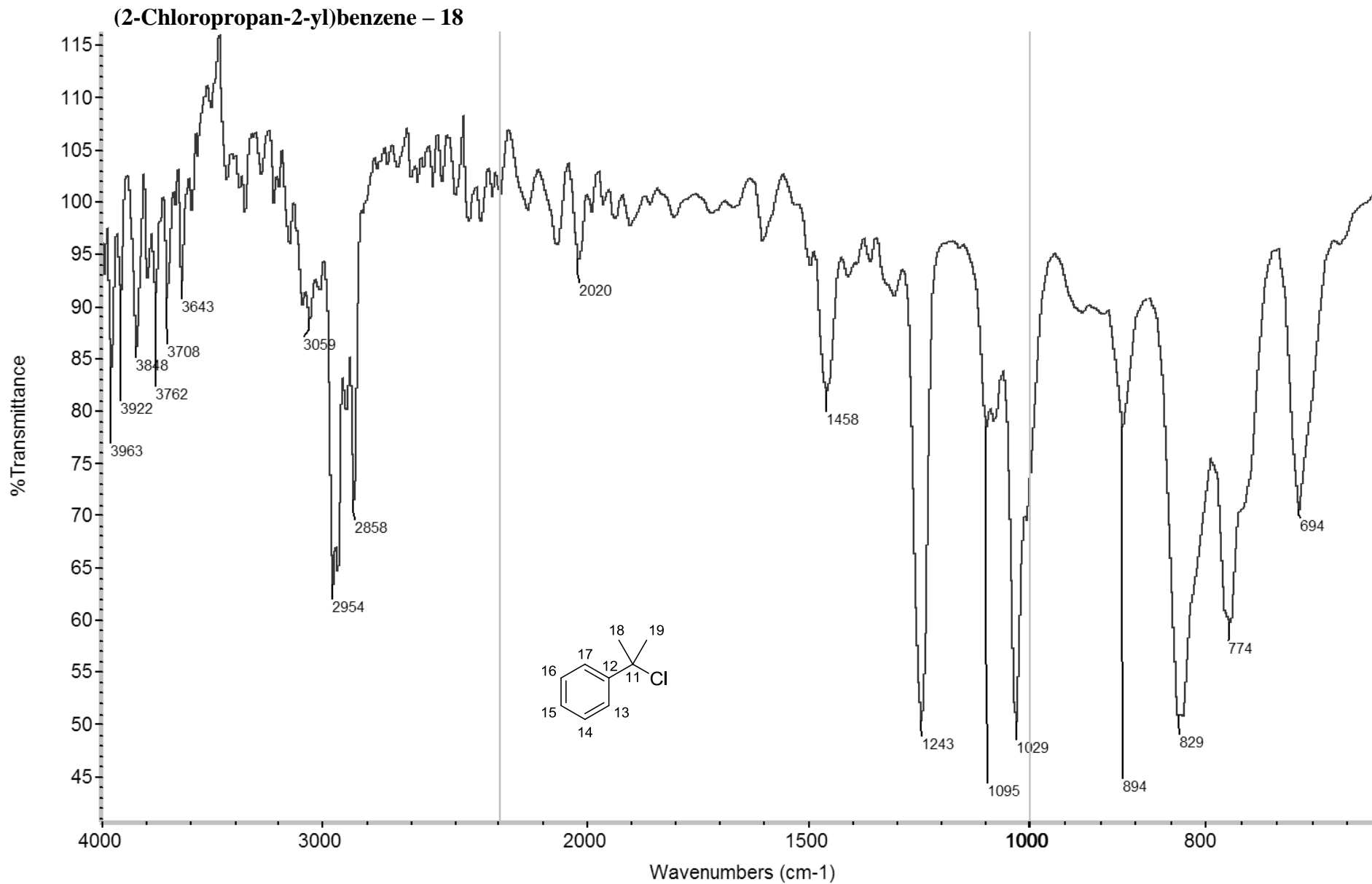
gHSQC NMR Spectrum
300 MHz Varian VNMRS



Mass Spectrum
Waters SYNAPT G2

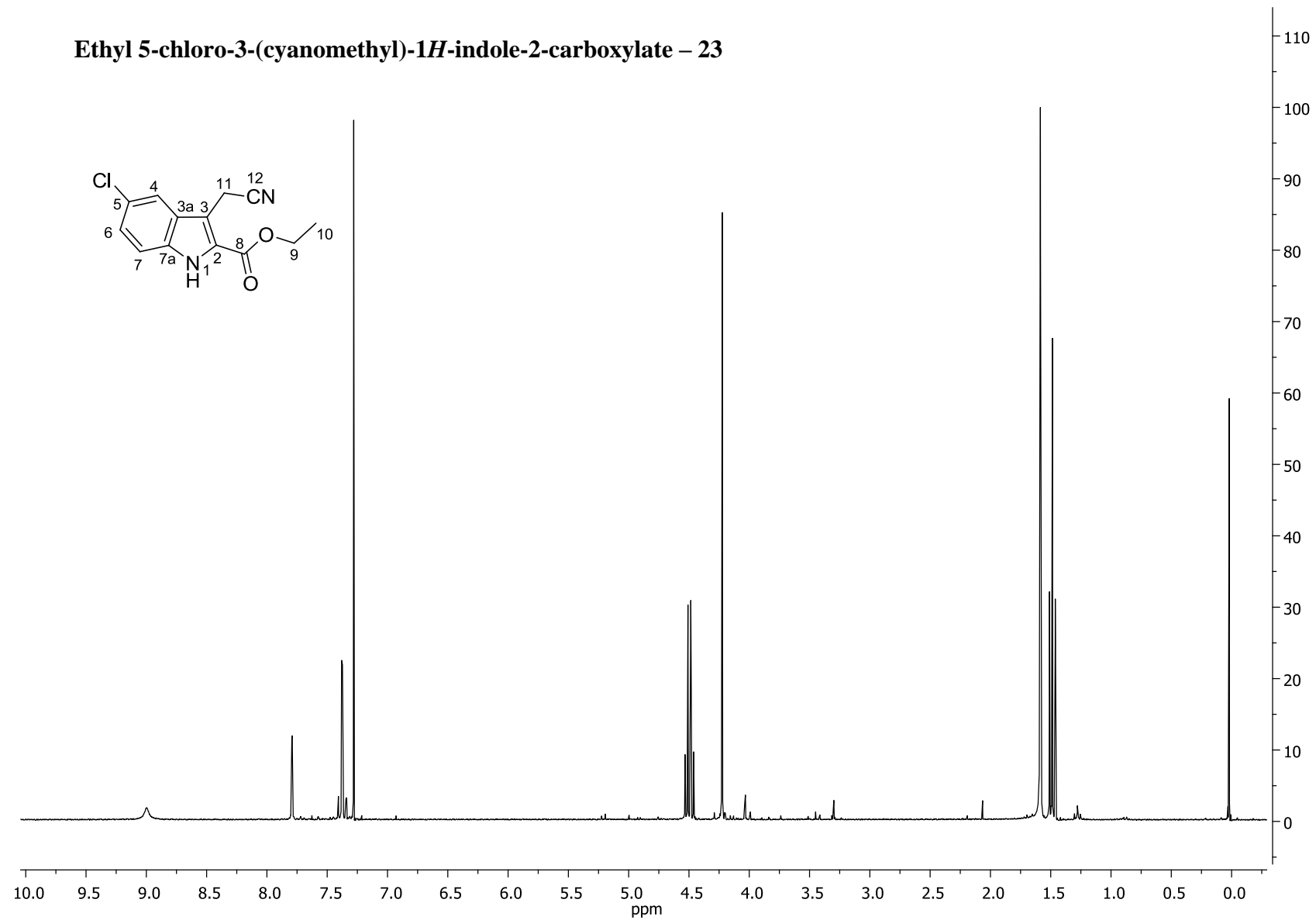


Infrared Spectrum
Thermo Nicolet Nexus 470

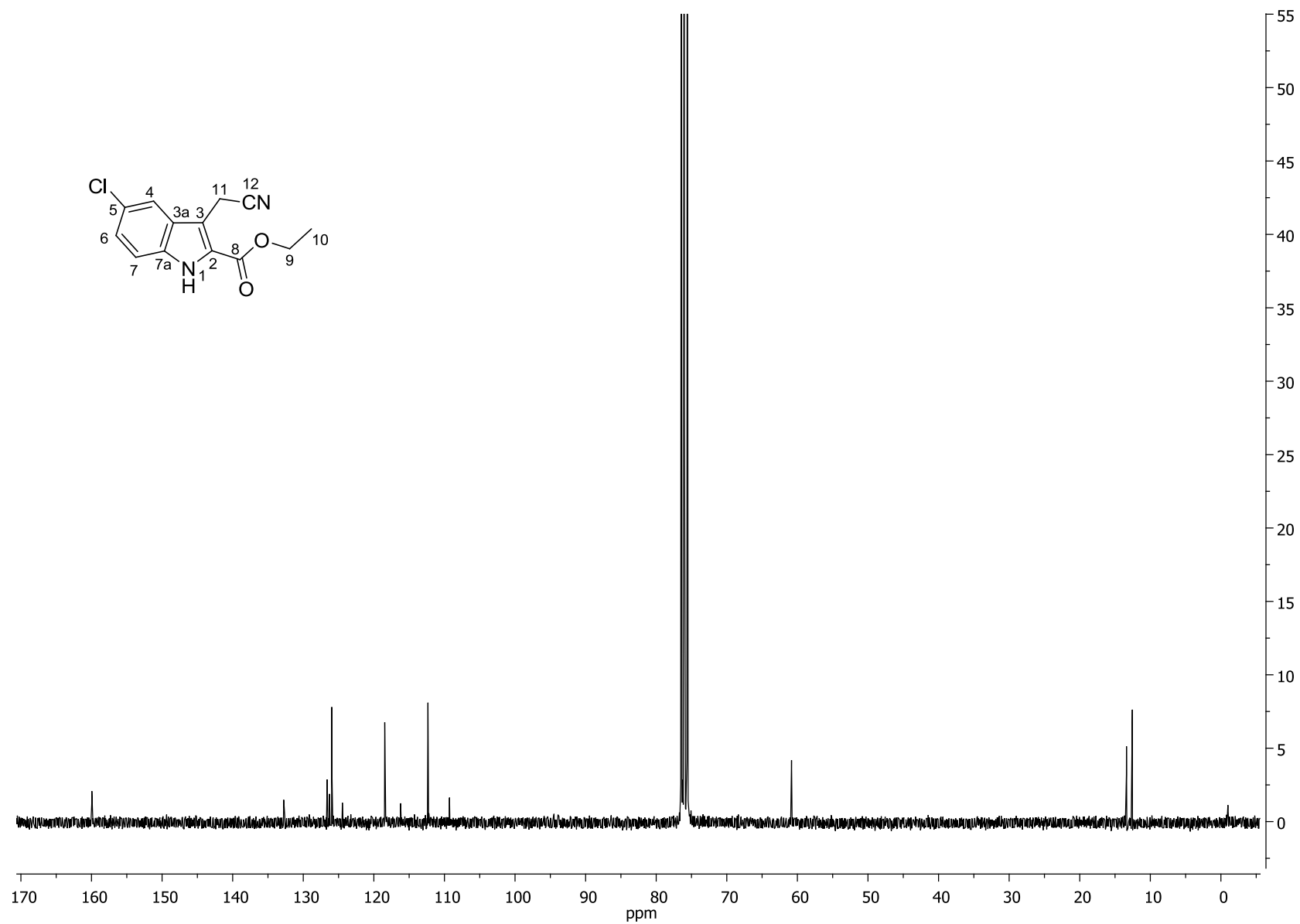


Infrared Spectrum
Thermo Nicolet Nexus 470

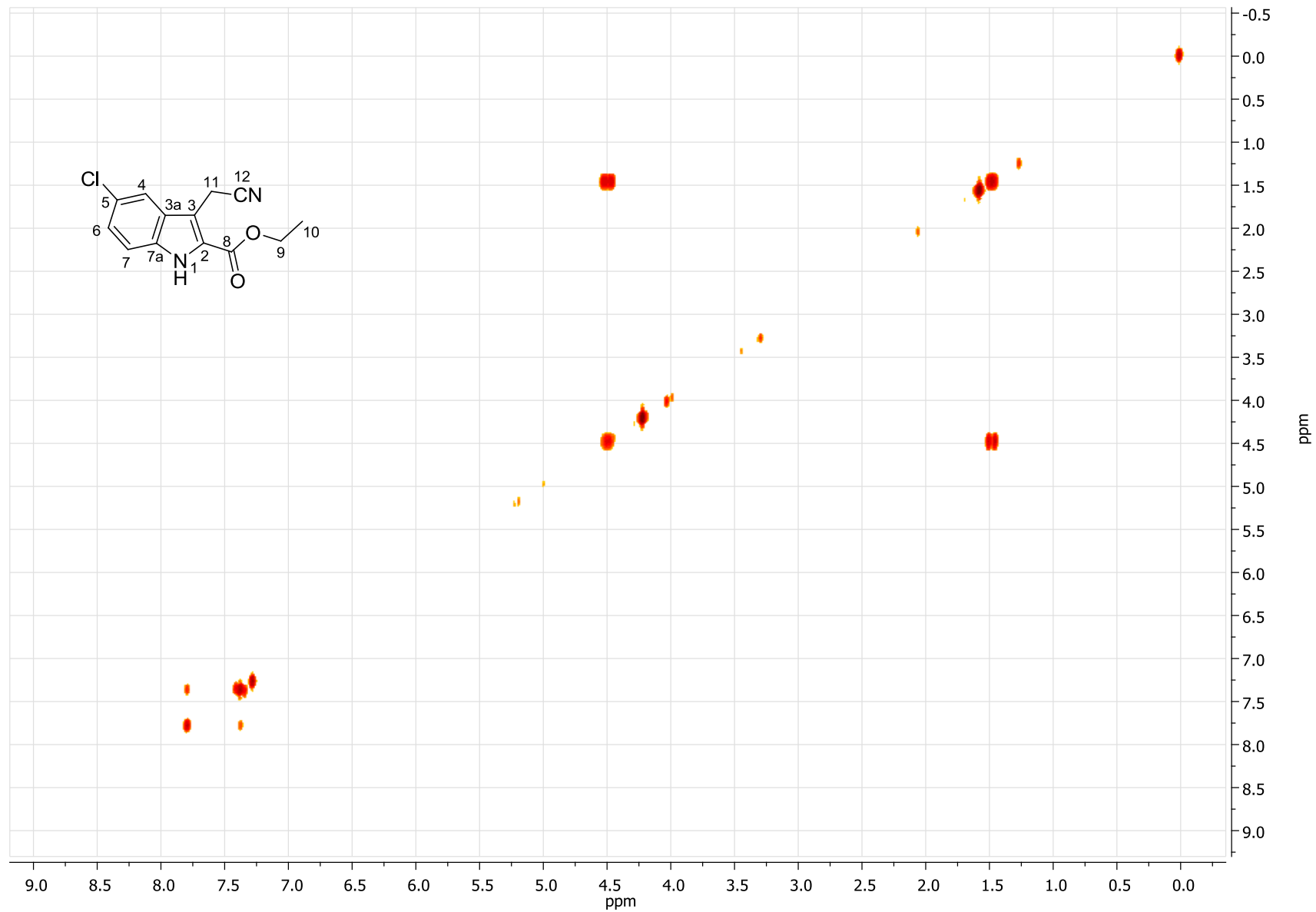
Ethyl 5-chloro-3-(cyanomethyl)-1H-indole-2-carboxylate – 23



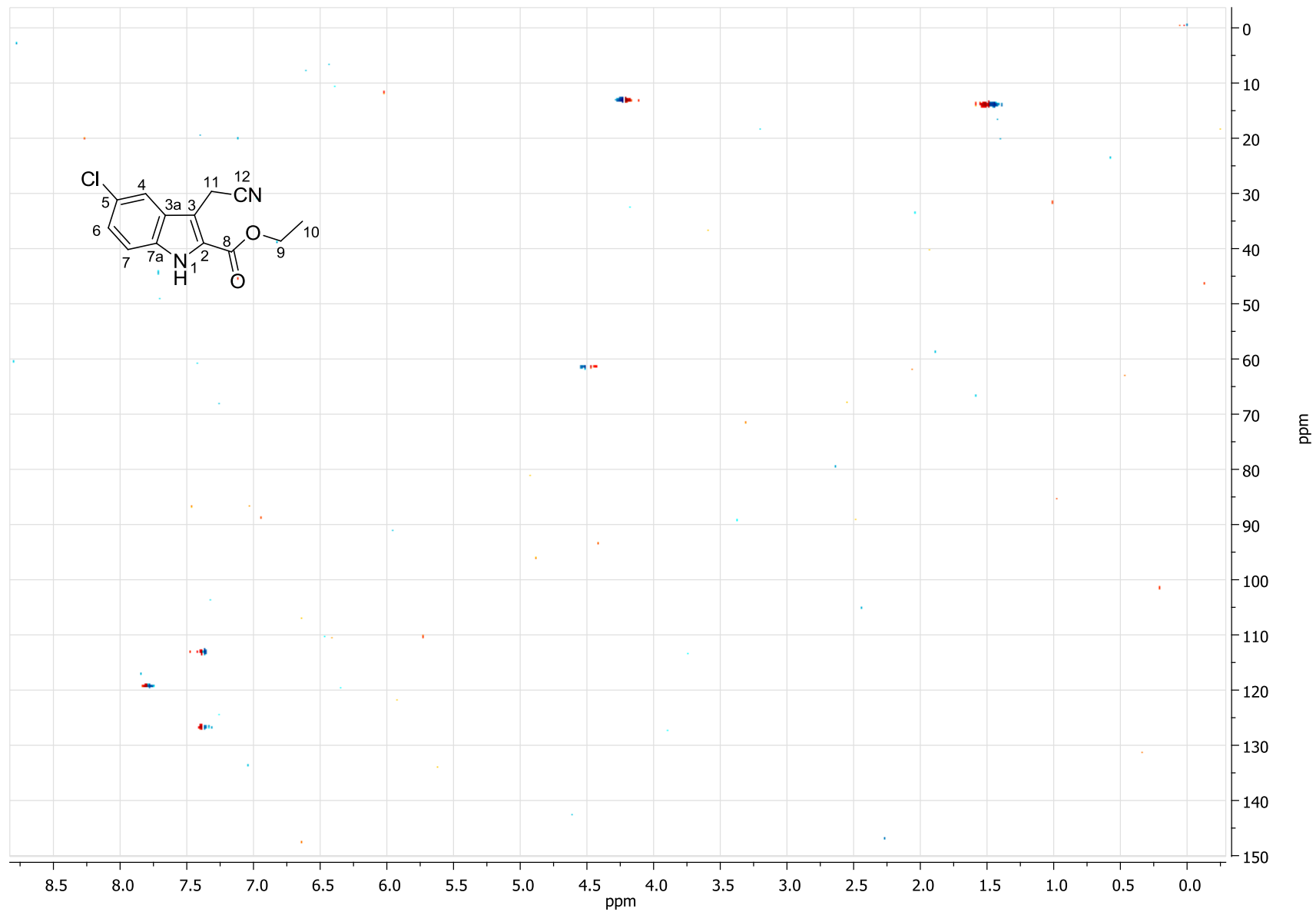
¹H NMR Spectrum
300 MHz Varian VNMRS



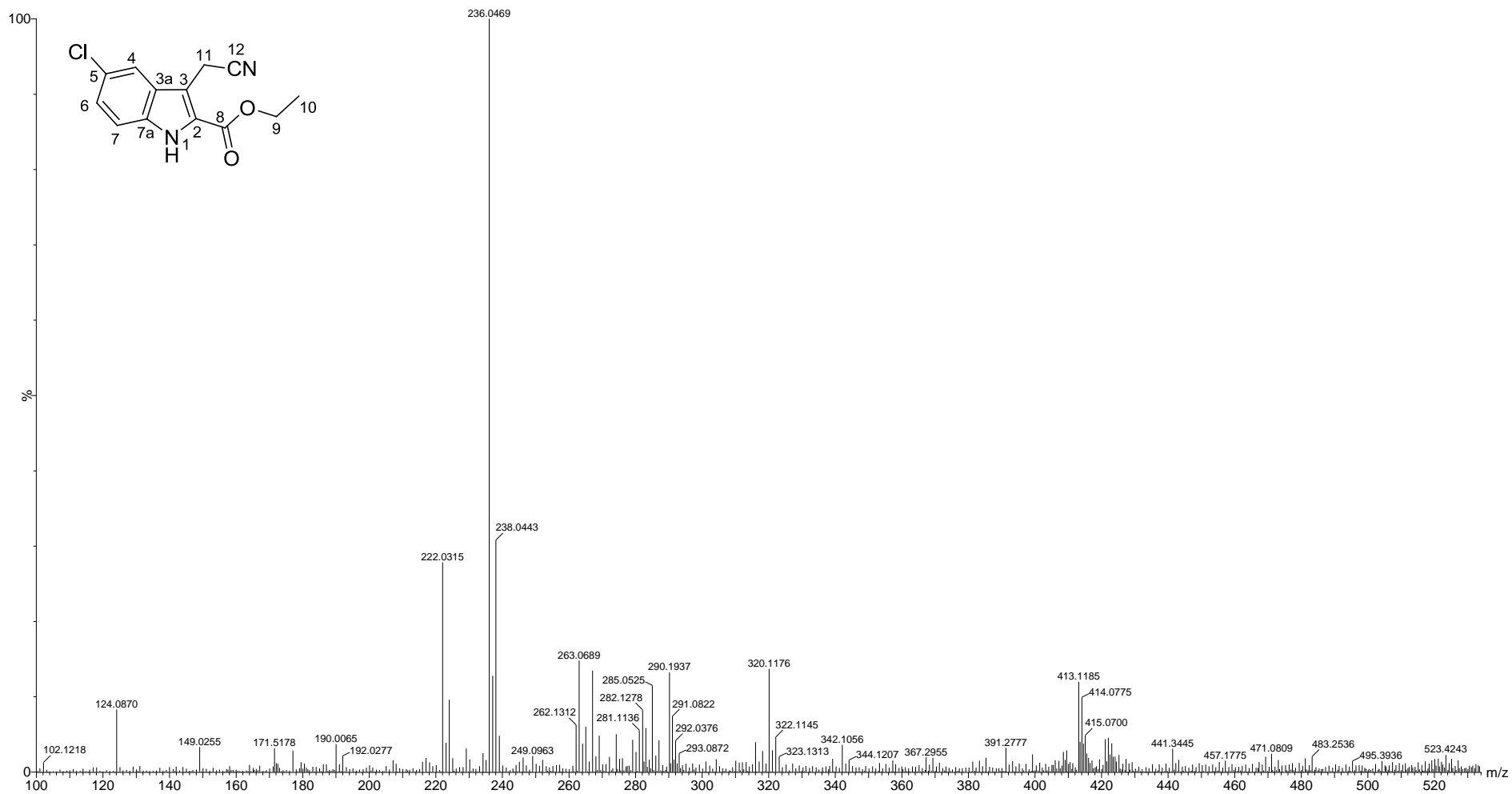
^{13}C NMR Spectrum
75 MHz Varian VNMRS



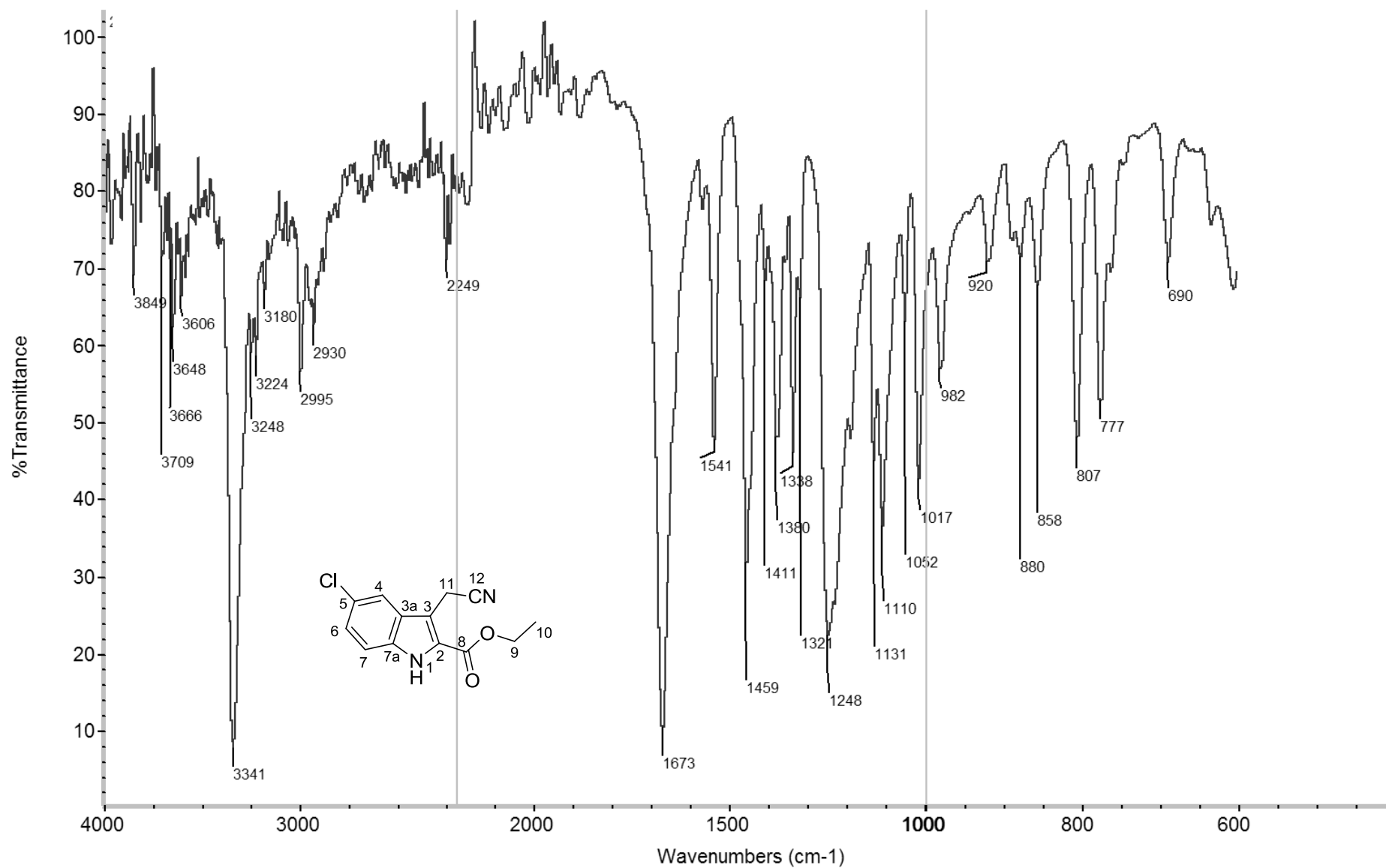
COSY NMR Spectrum
300 MHz Varian VNMRS



gHSQC NMR Spectrum
300 MHz Varian VNMRS

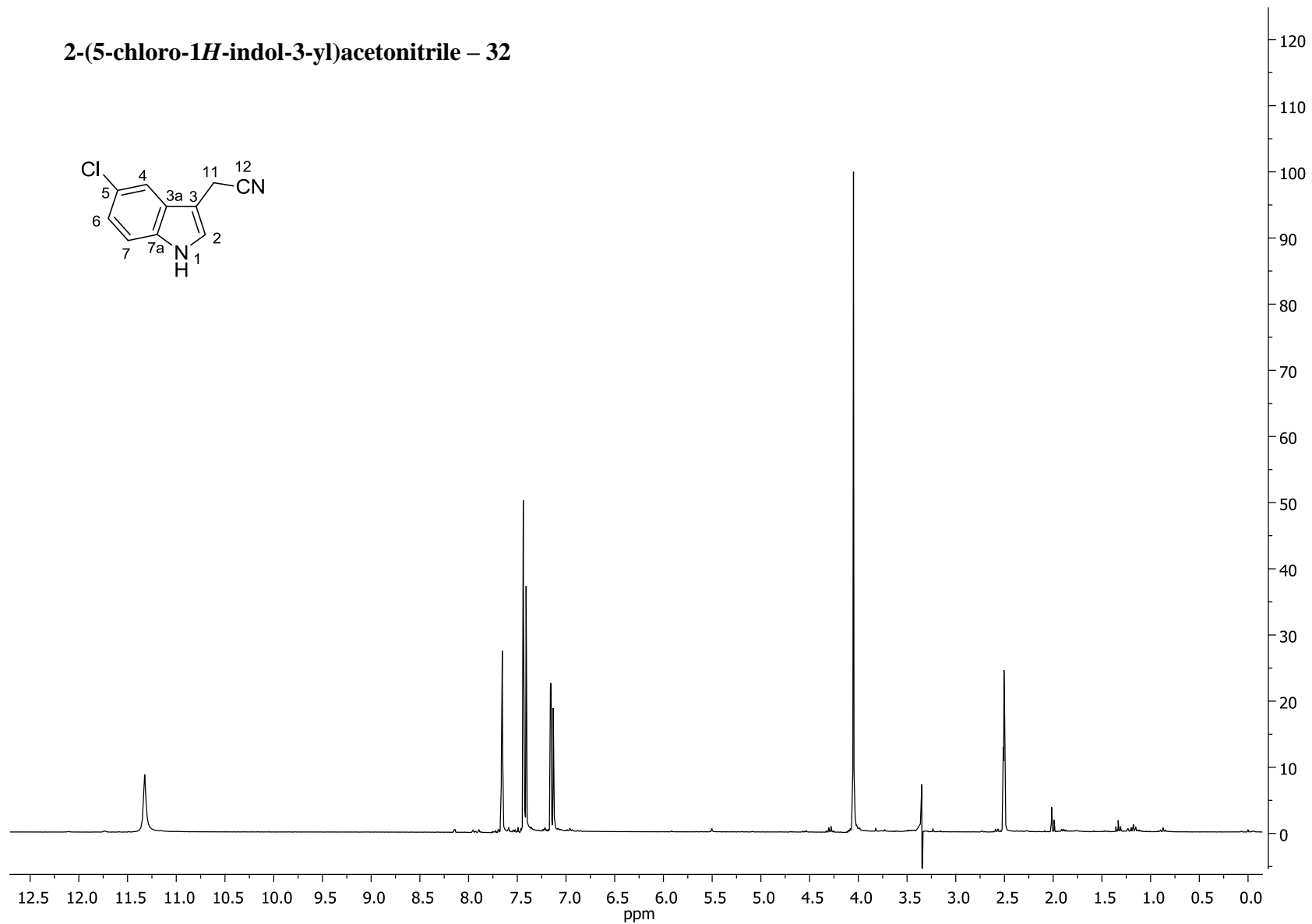


Mass Spectrum
Waters SYNAPT G2

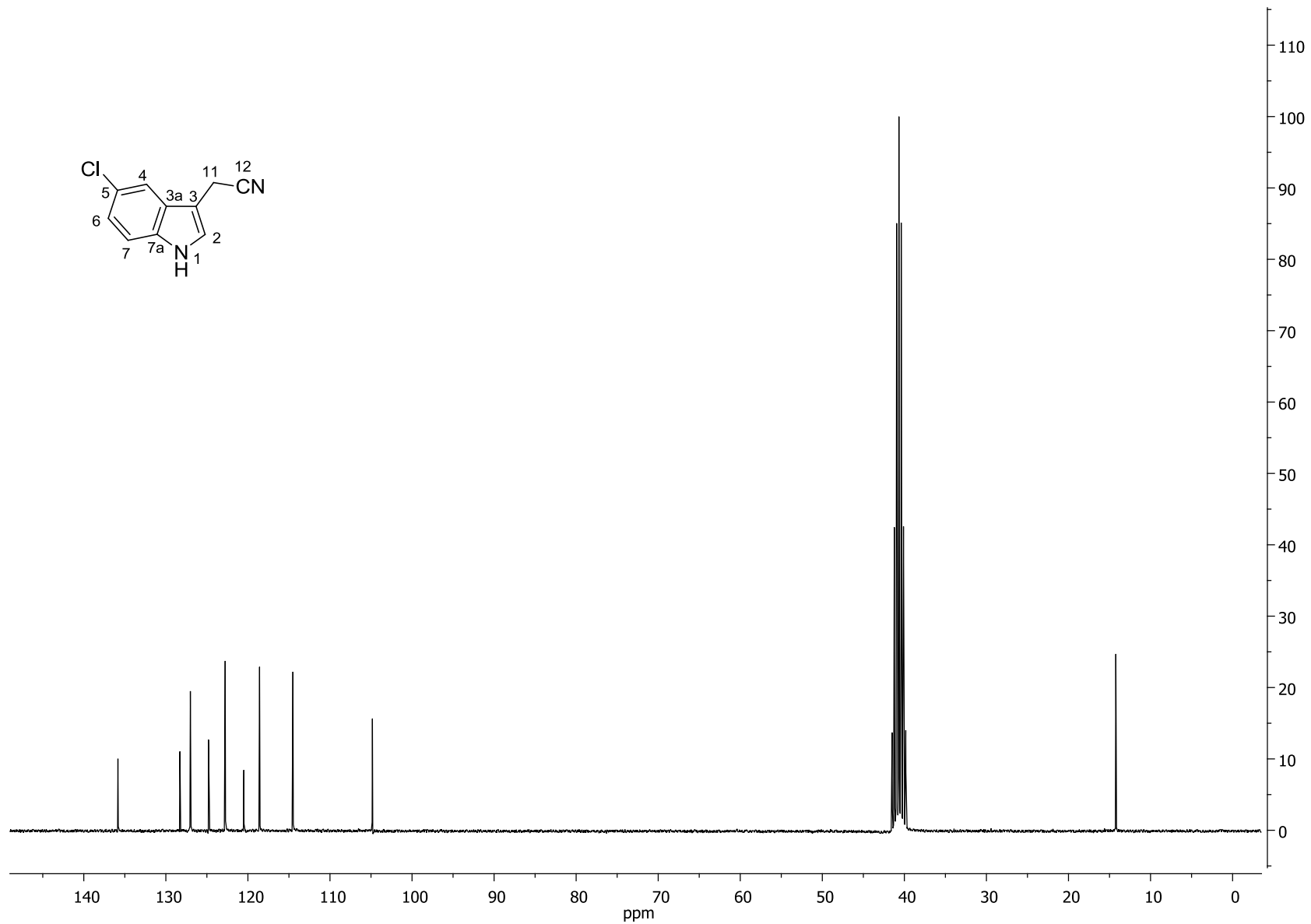


Infrared Spectrum
Thermo Nicolet Nexus 470

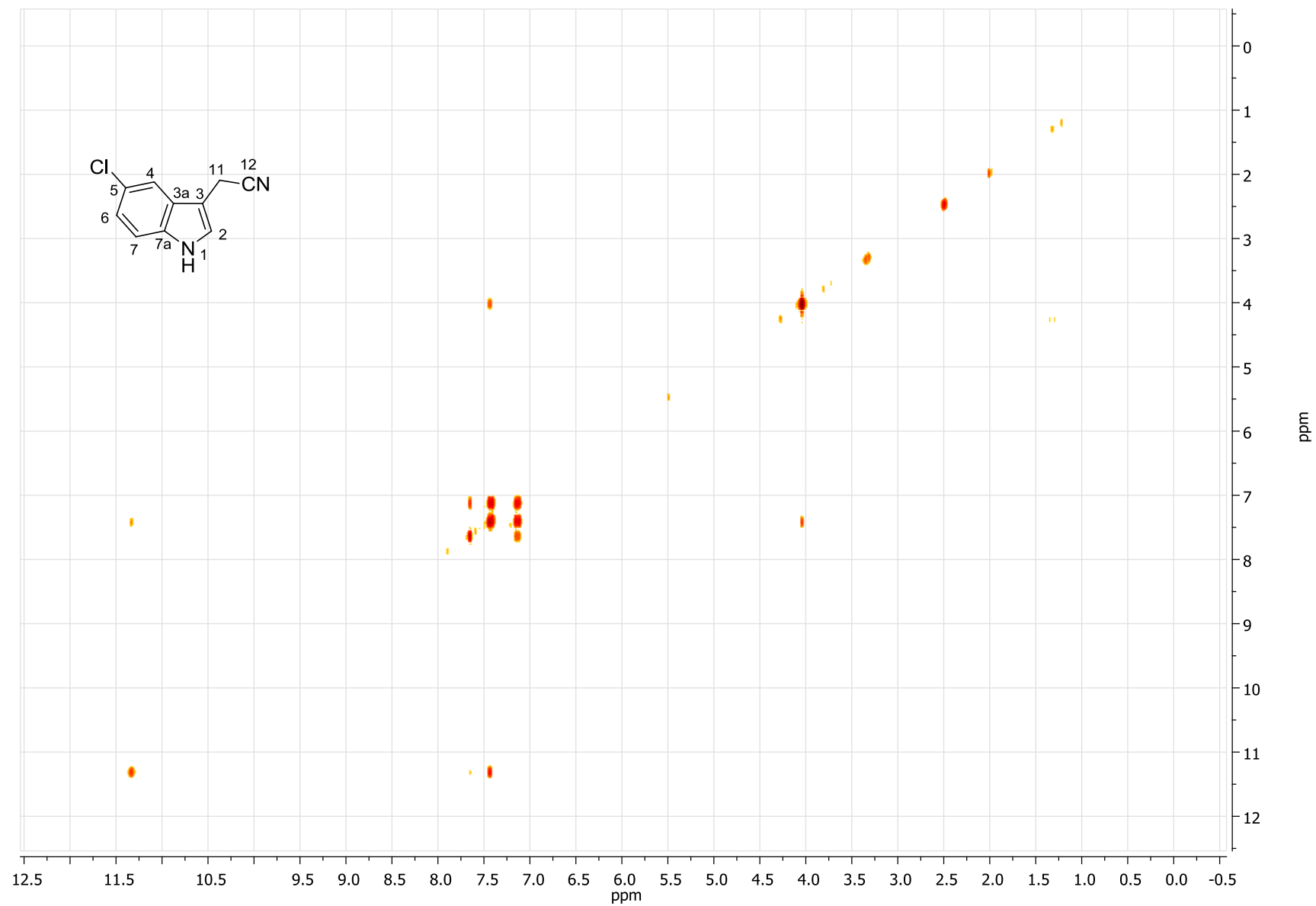
2-(5-chloro-1H-indol-3-yl)acetonitrile – 32



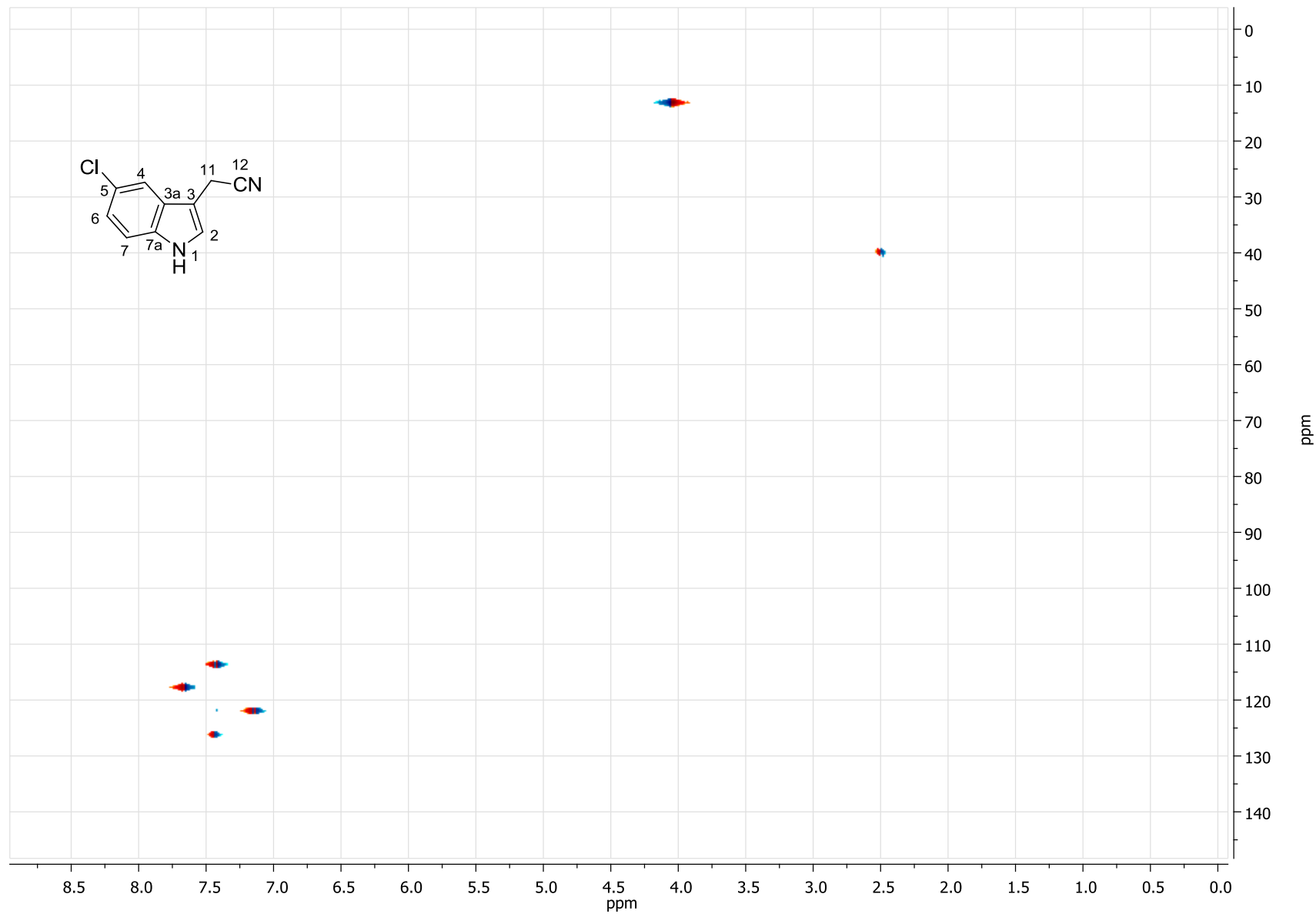
¹H NMR Spectrum
300 MHz Varian VNMRS



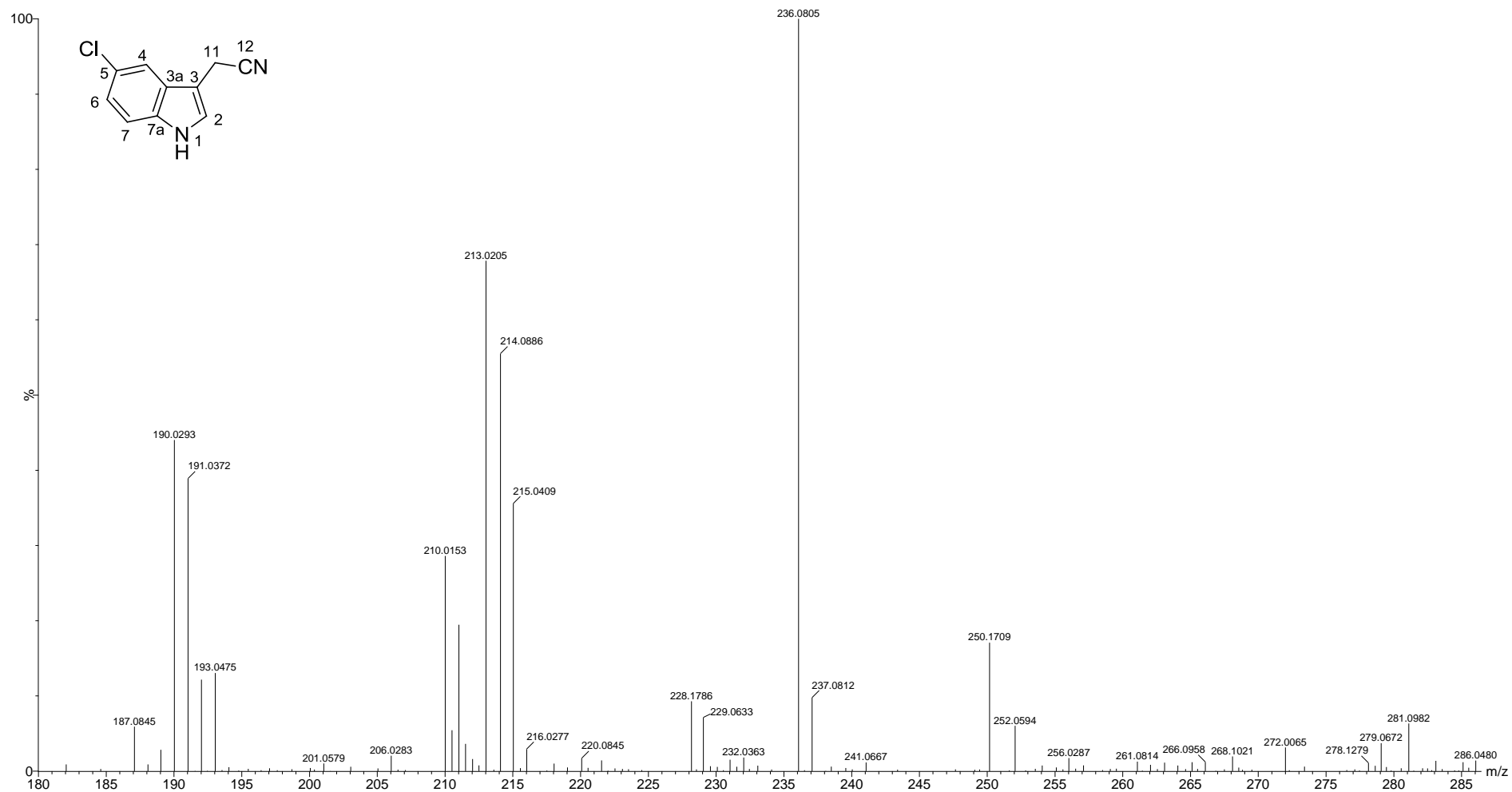
^{13}C NMR Spectrum
75 MHz Varian VNMRS



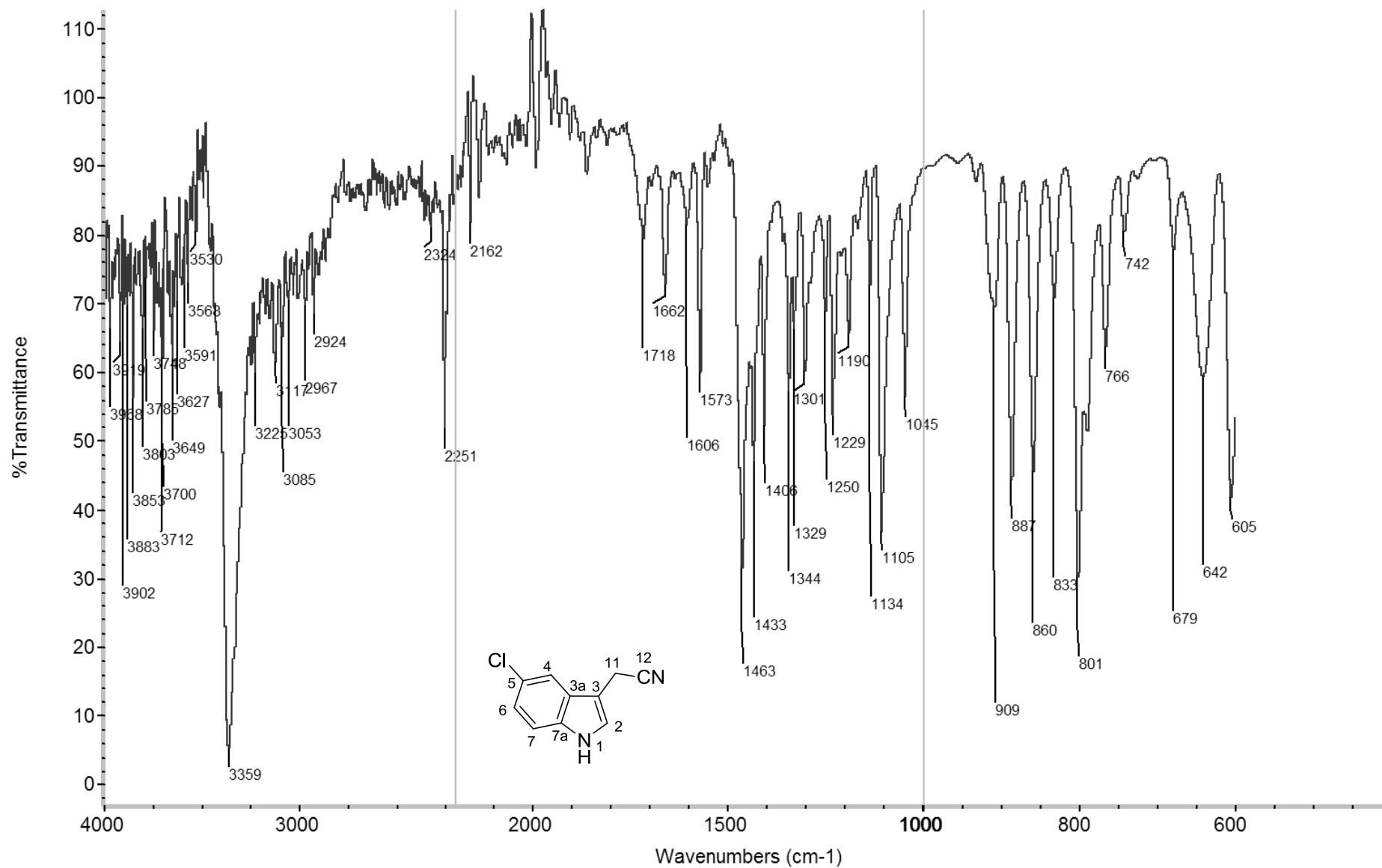
COSY NMR Spectrum
300 MHz Varian VNMRS



gHSQC NMR Spectrum
300 MHz Varian VNMRS

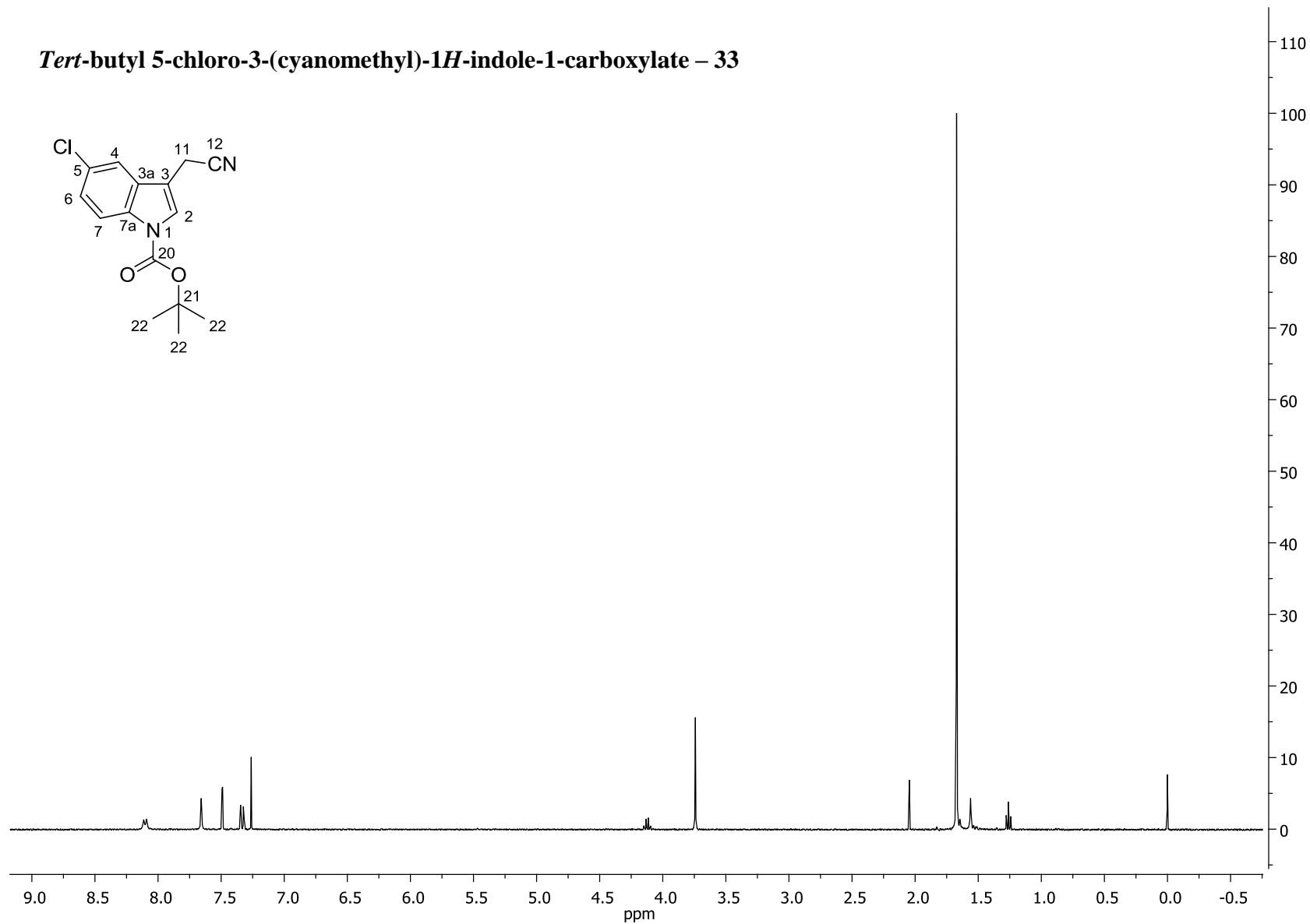
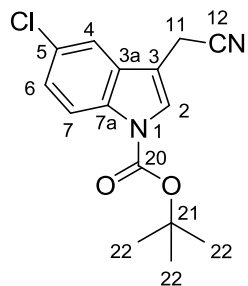


Mass Spectrum
Waters SYNAPT G2

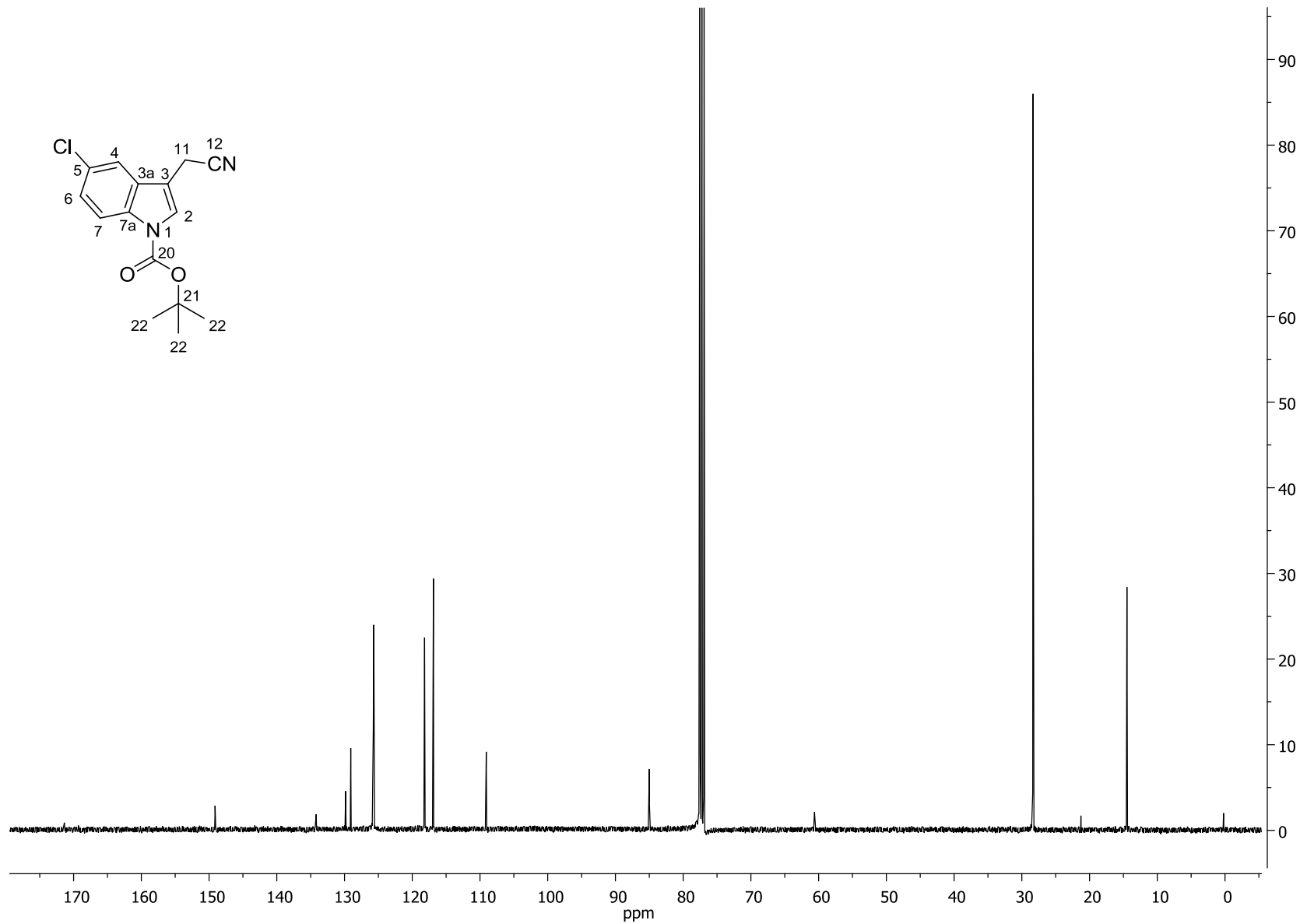


Infrared Spectrum
Thermo Nicolet Nexus 470

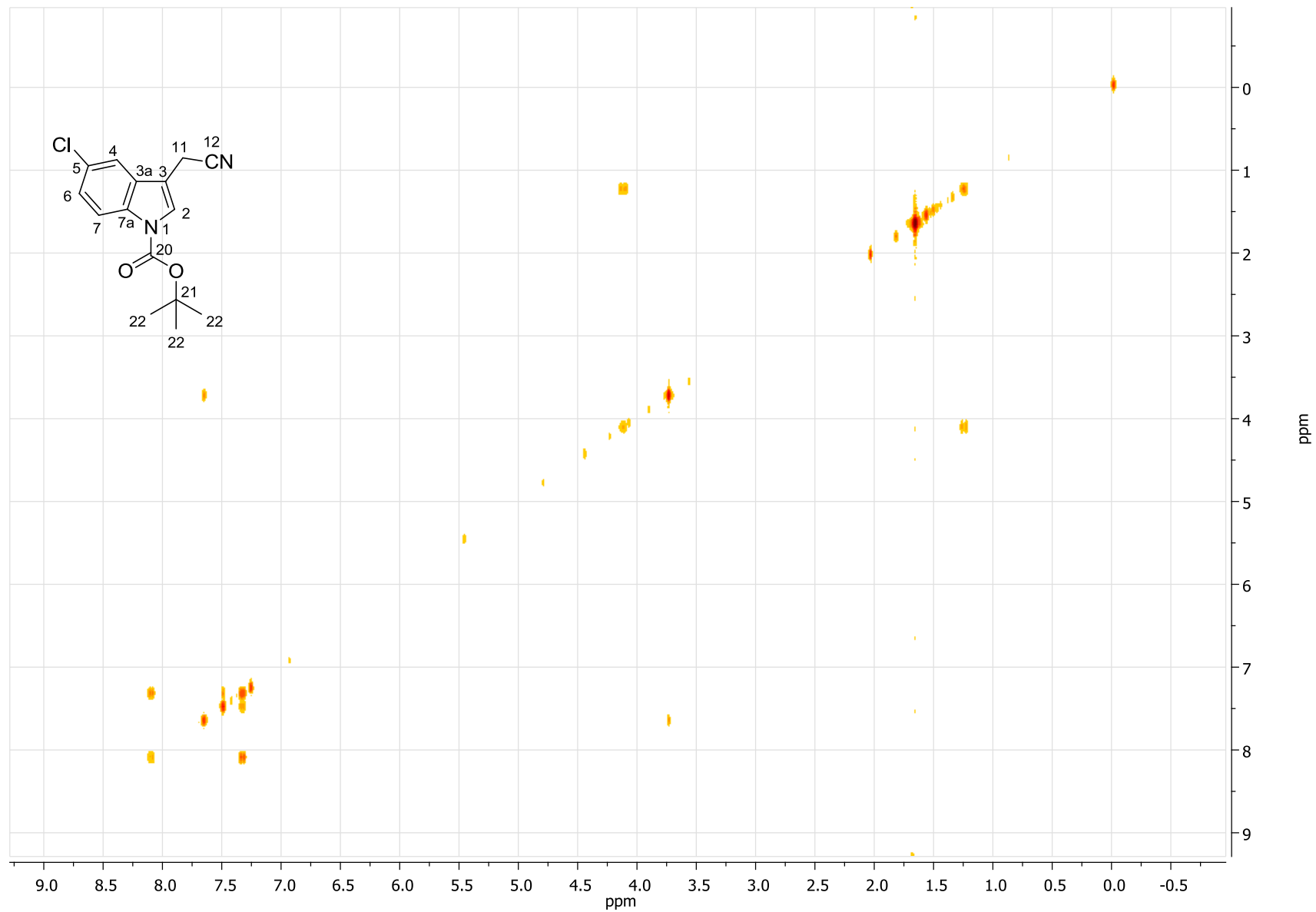
***Tert*-butyl 5-chloro-3-(cyanomethyl)-1*H*-indole-1-carboxylate – 33**



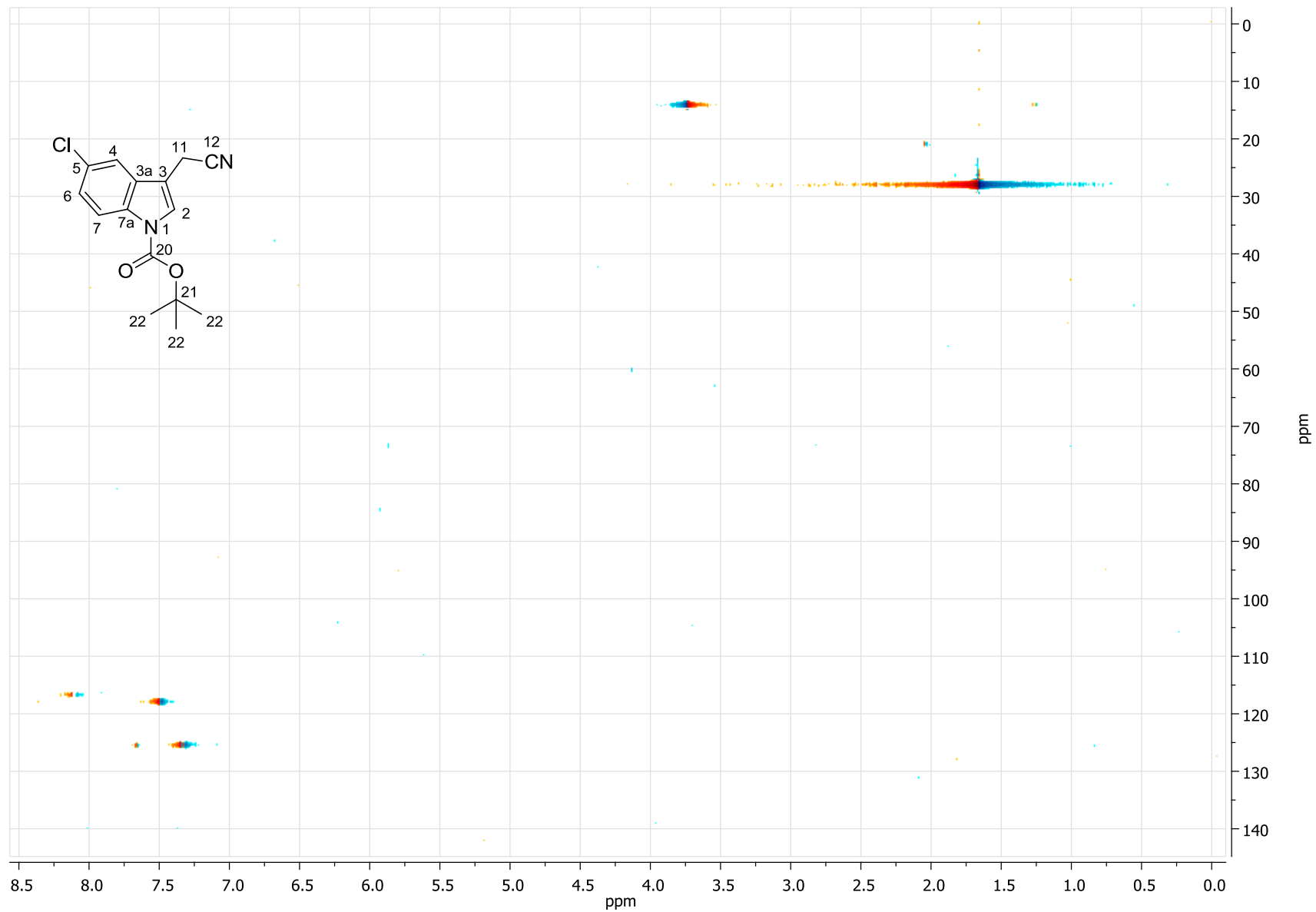
¹H NMR Spectrum
400 MHz Varian Unity Inova



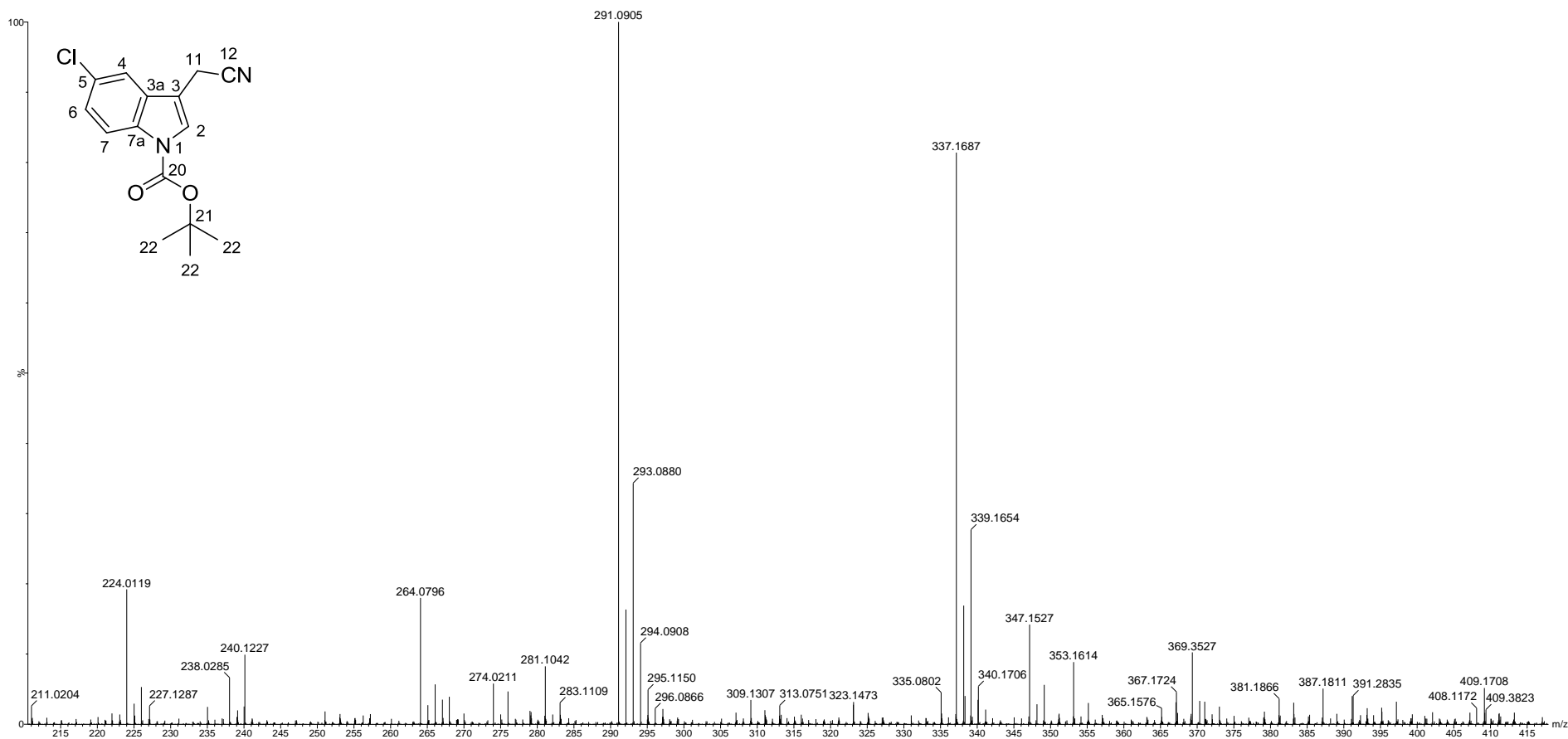
^{13}C NMR Spectrum
101 MHz Varian Unity Inova



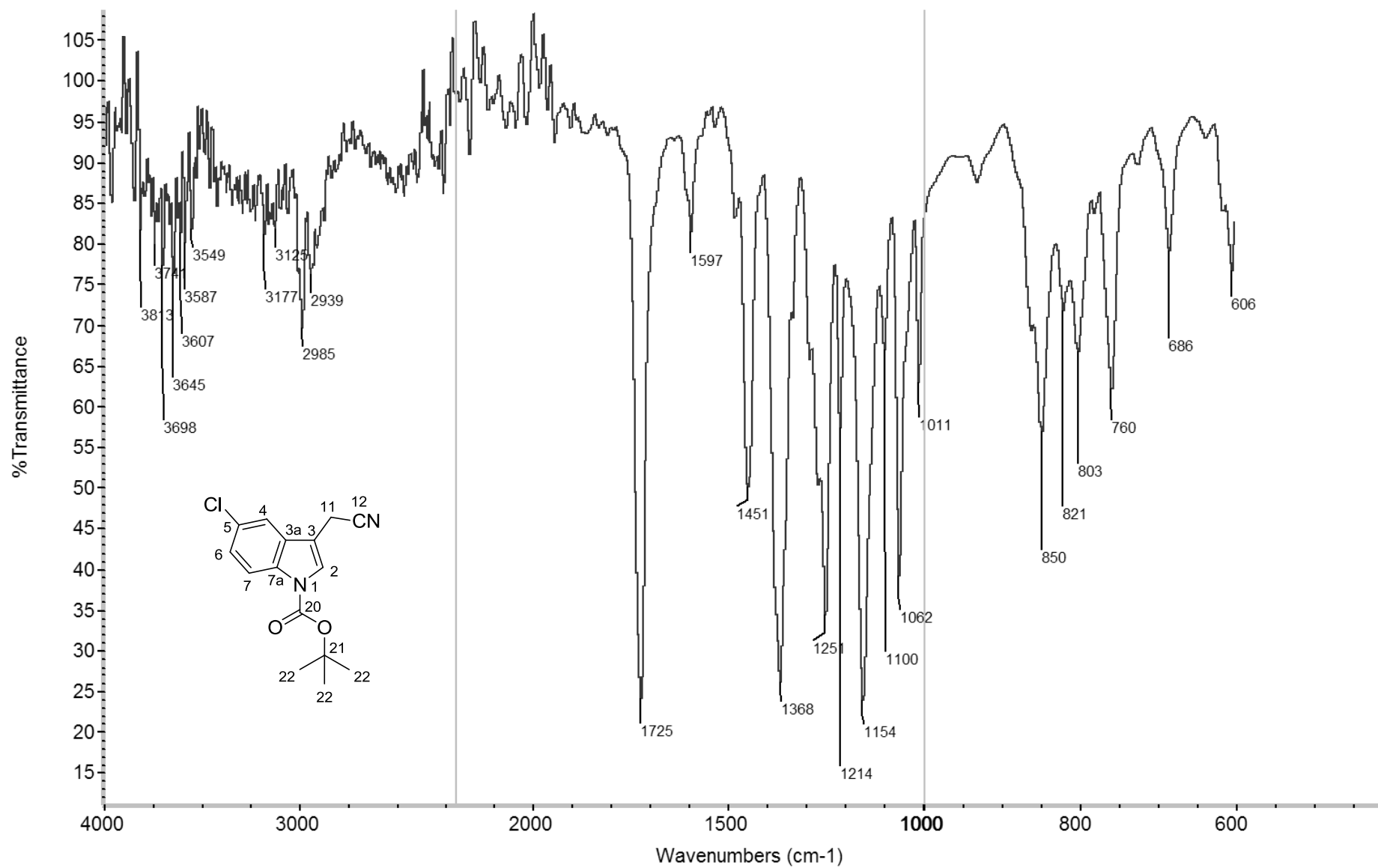
COSY NMR Spectrum
400 MHz Varian Unity Inova



gHSQC NMR Spectrum
400 MHz Varian Unity Inova

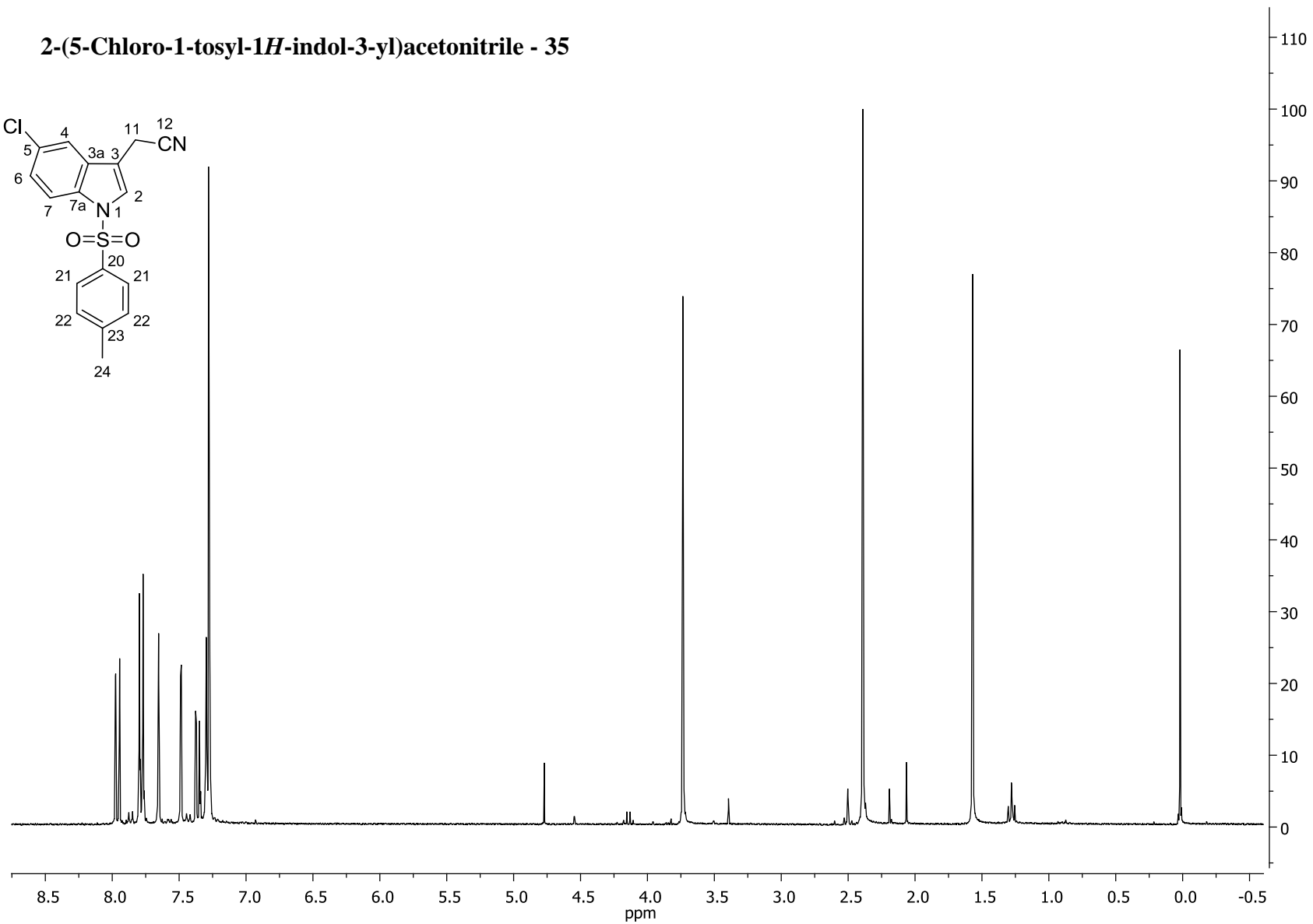
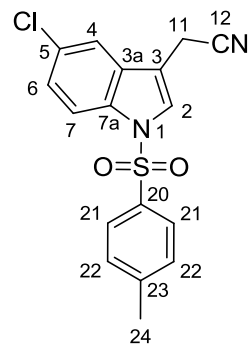


Mass Spectrum
Waters SYNAPT G2

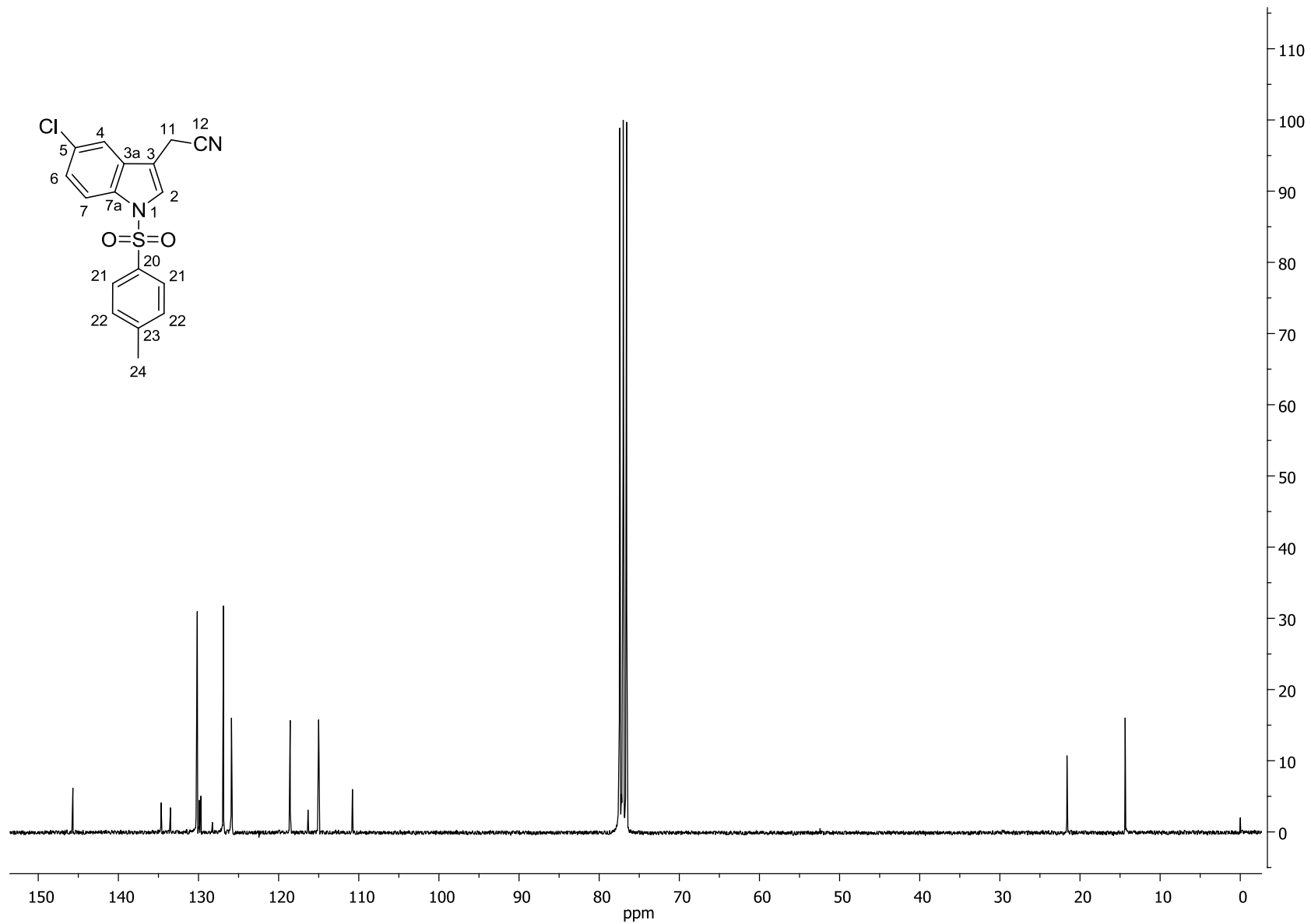


Infrared Spectrum
Thermo Nicolet Nexus 470

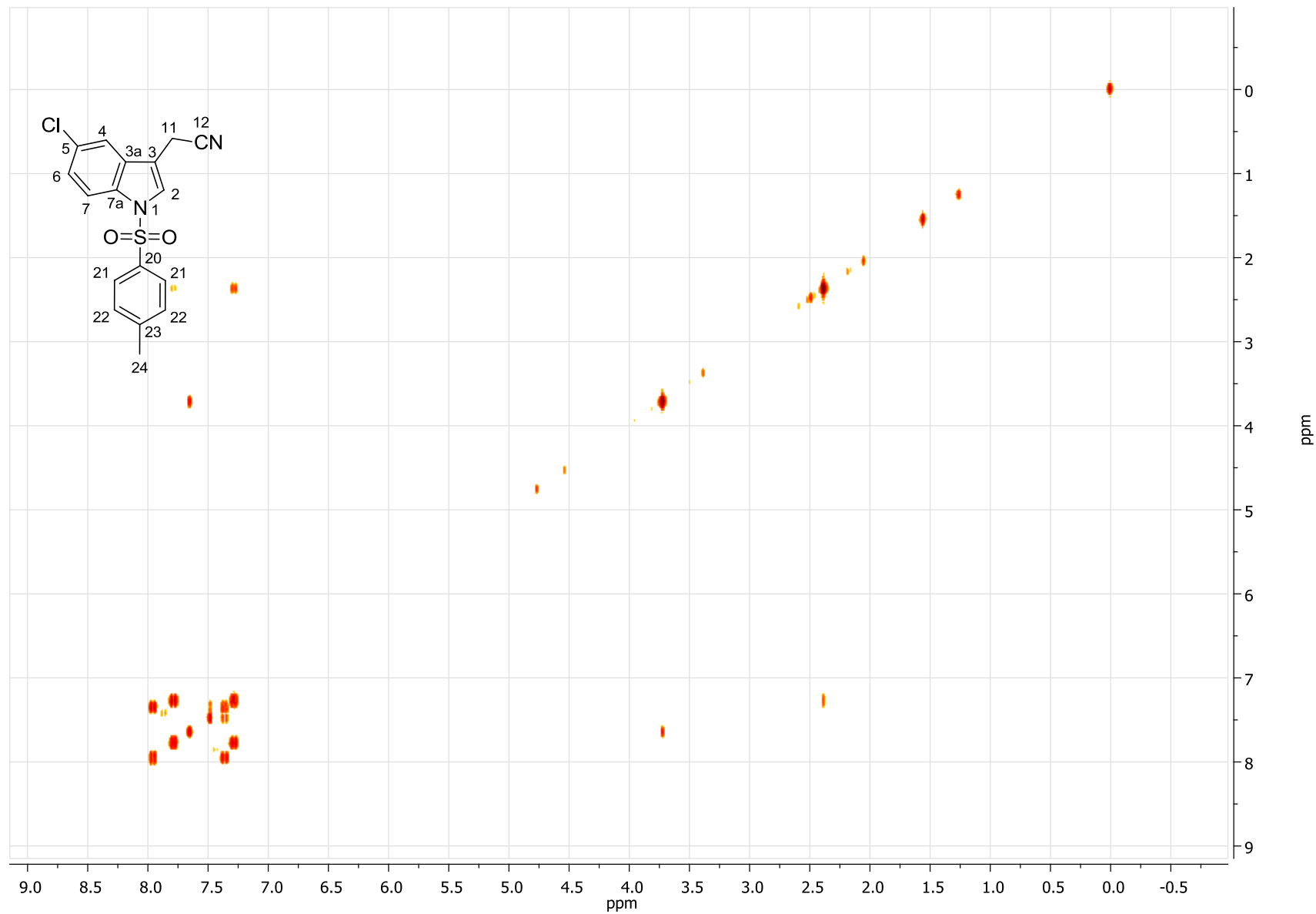
2-(5-Chloro-1-tosyl-1H-indol-3-yl)acetonitrile - 35



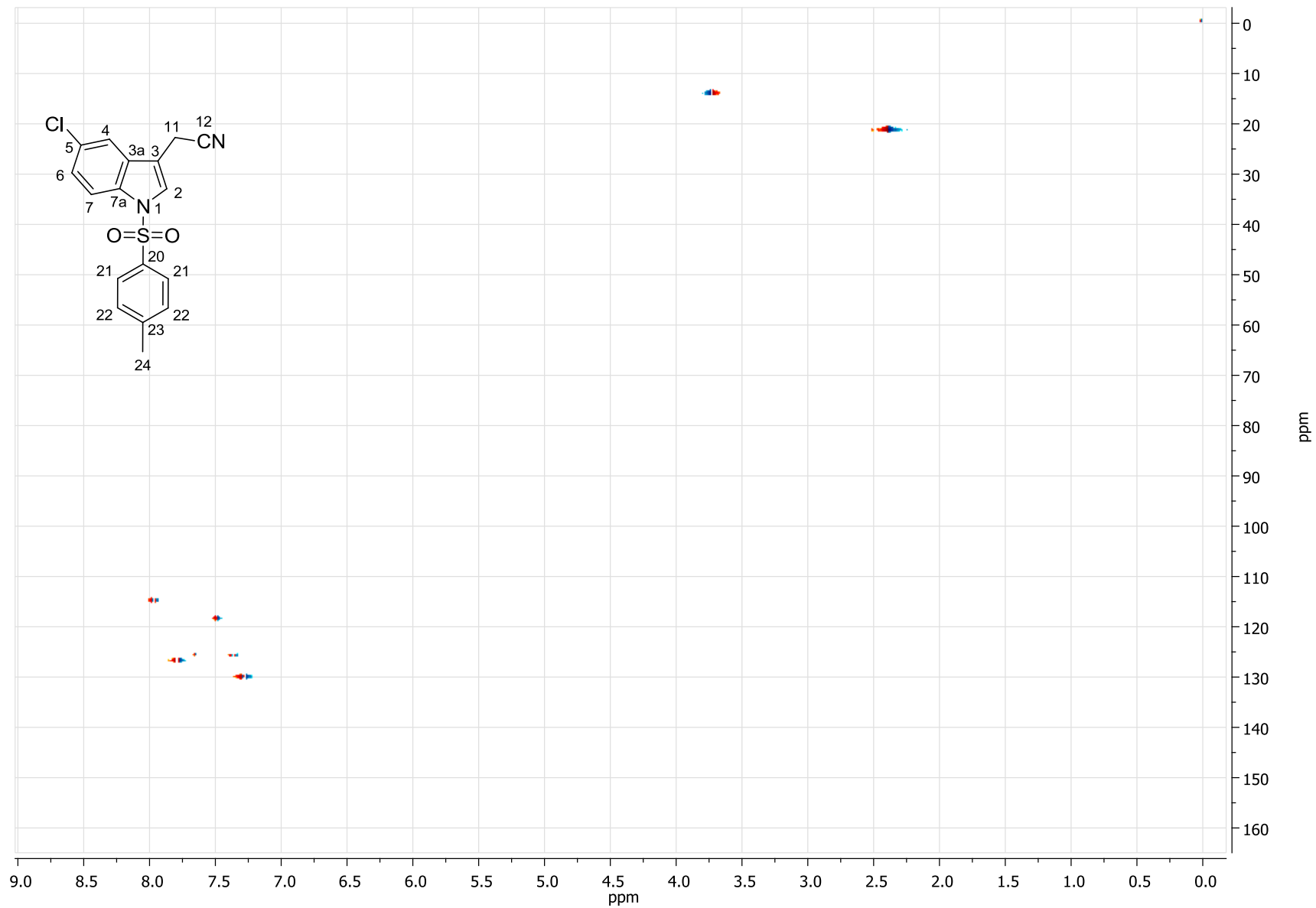
¹H NMR Spectrum
300 MHz Varian VNMRS



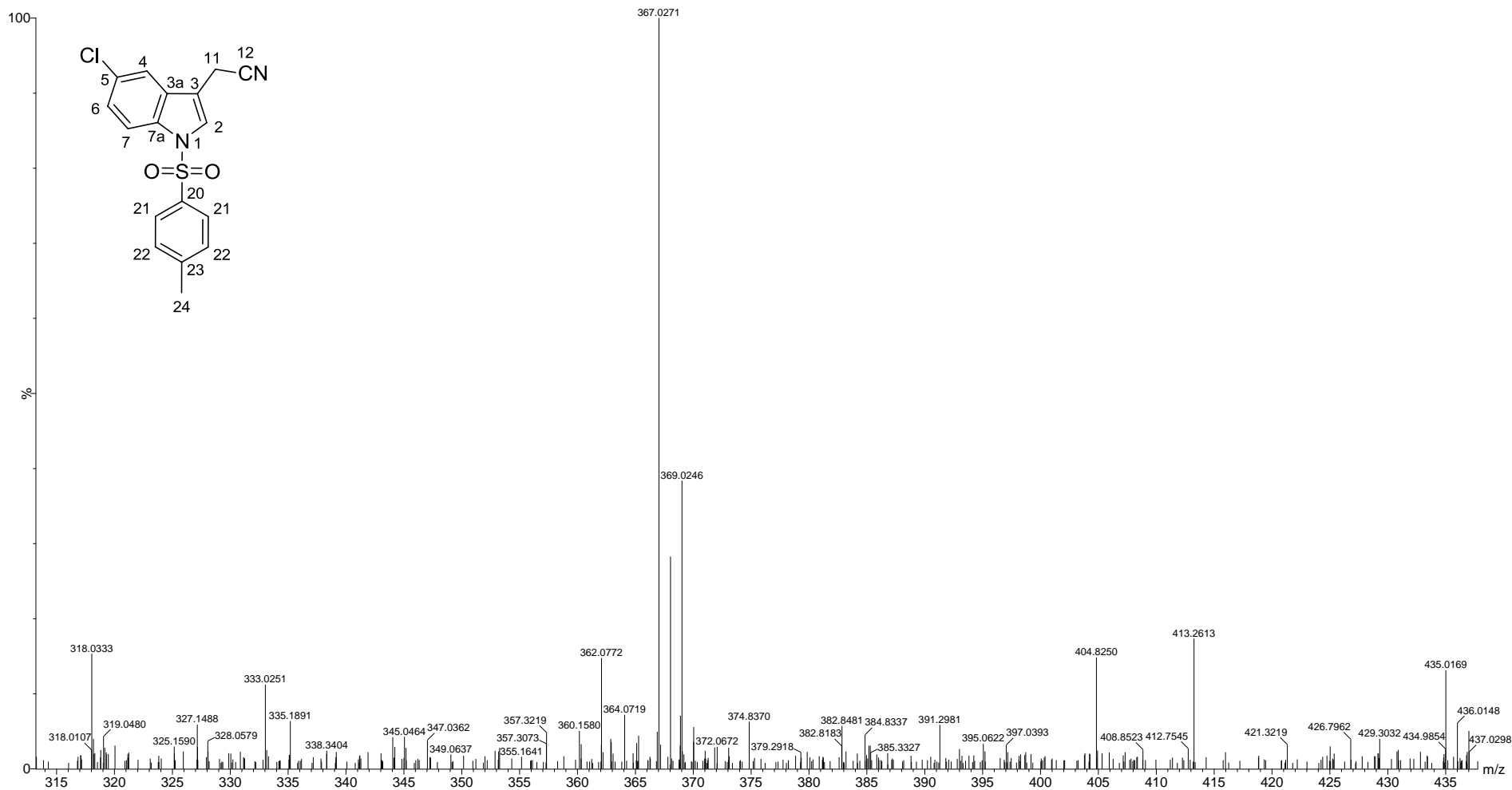
^{13}C NMR Spectrum
75 MHz Varian VNMRS



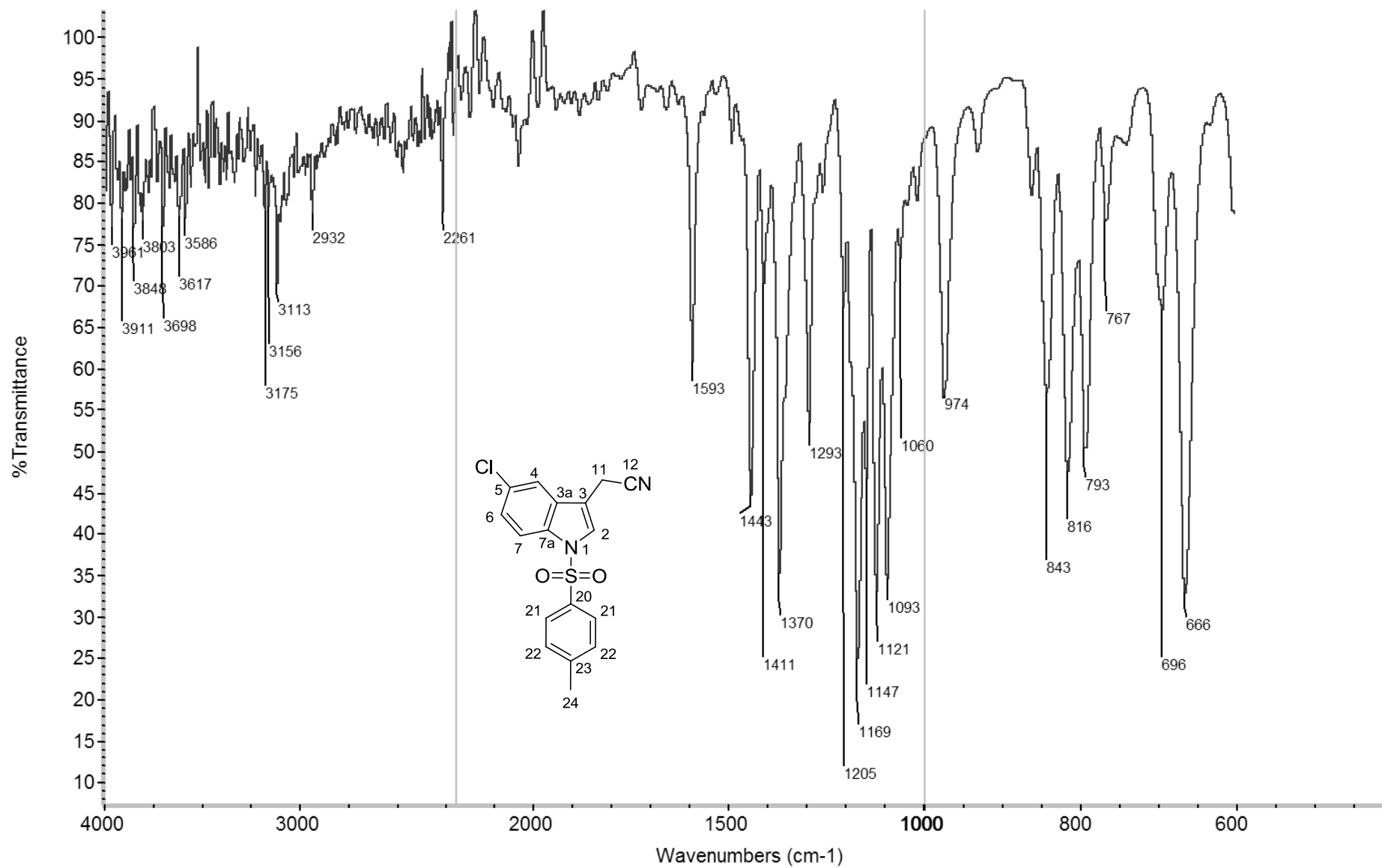
COSY NMR Spectrum
300 MHz Varian VNMRS



gHSQC NMR Spectrum
300 MHz Varian VNMRS

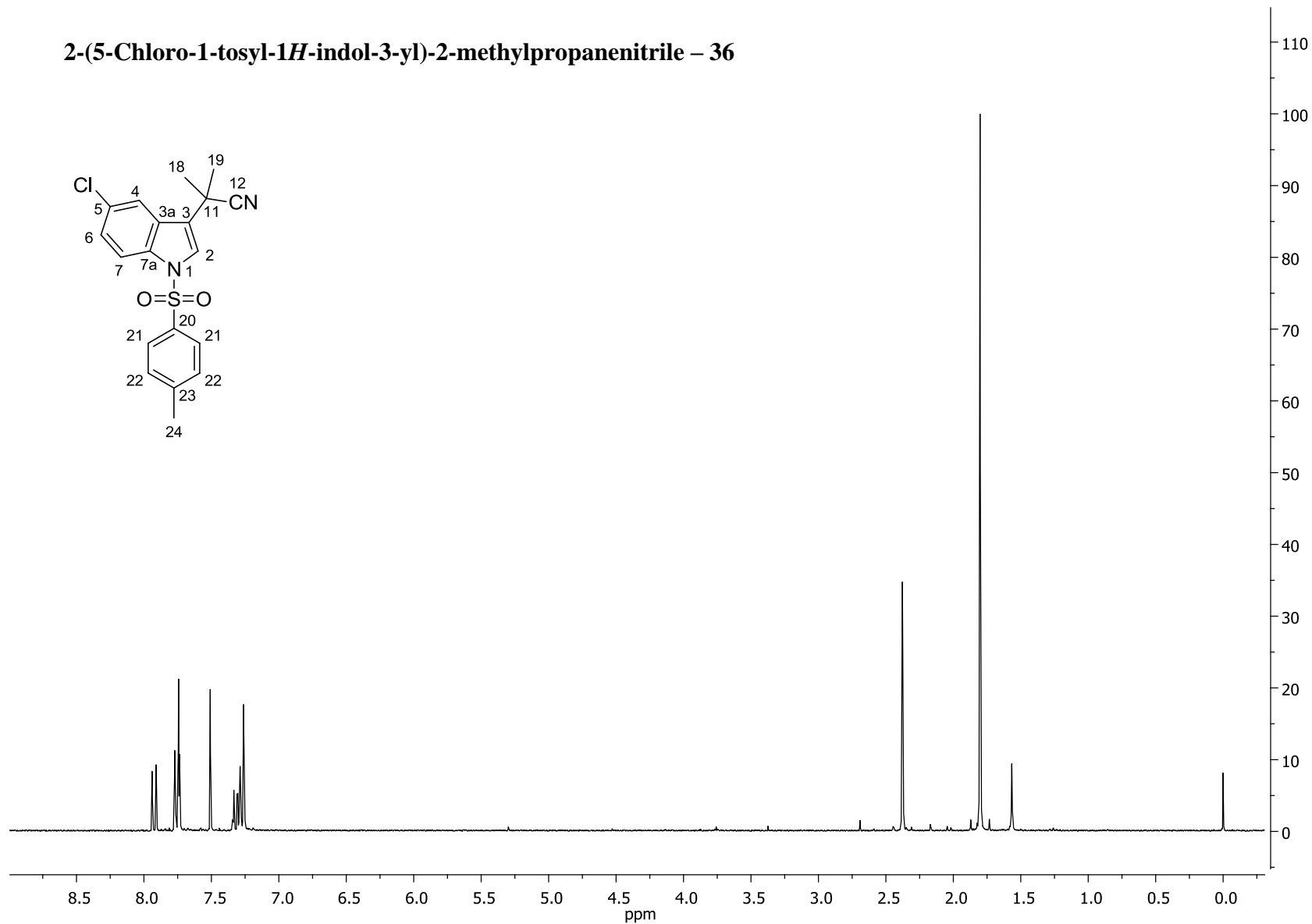


Mass Spectrum
Waters SYNAPT G2

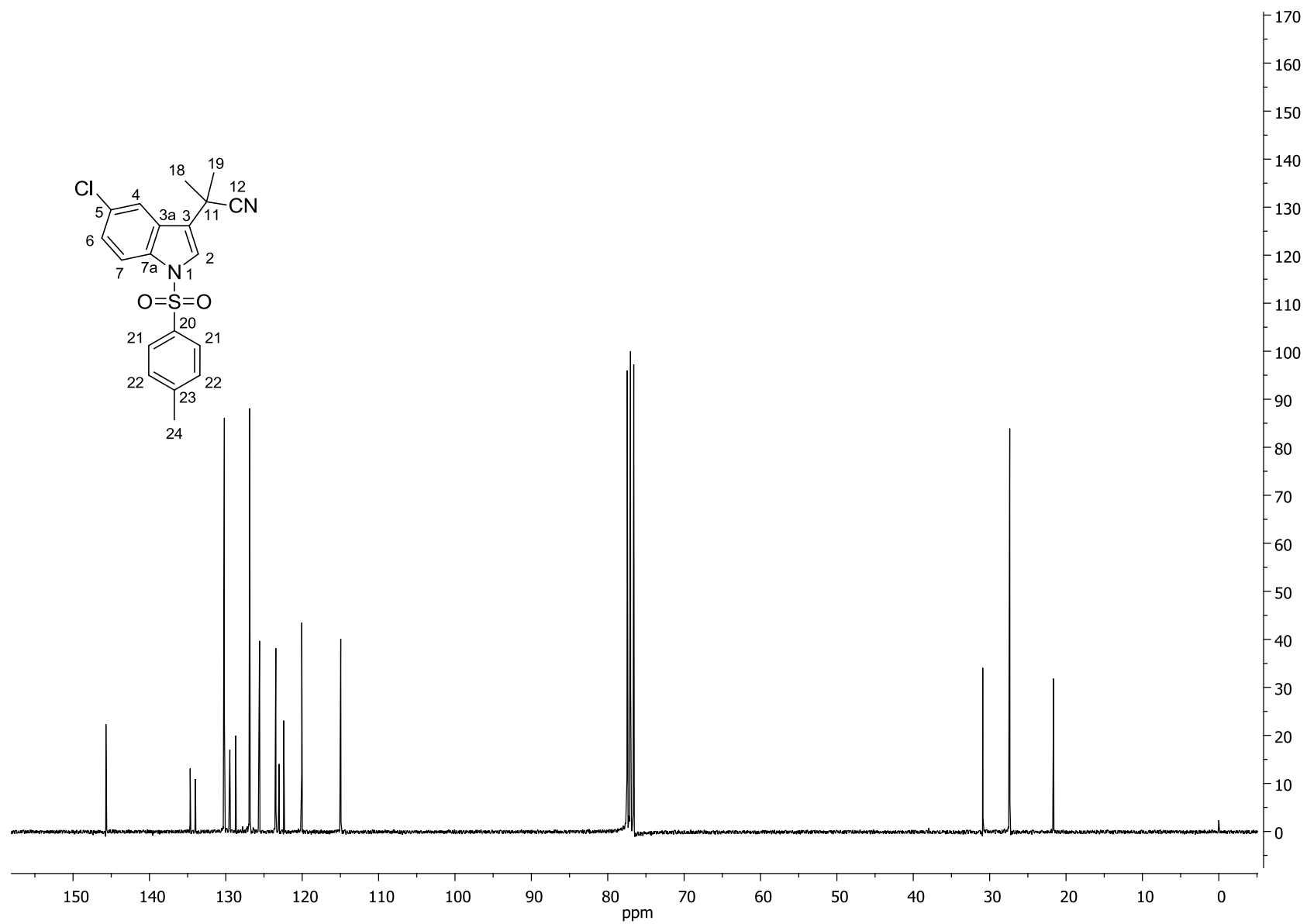


Infrared Spectrum
Thermo Nicolet Nexus 470

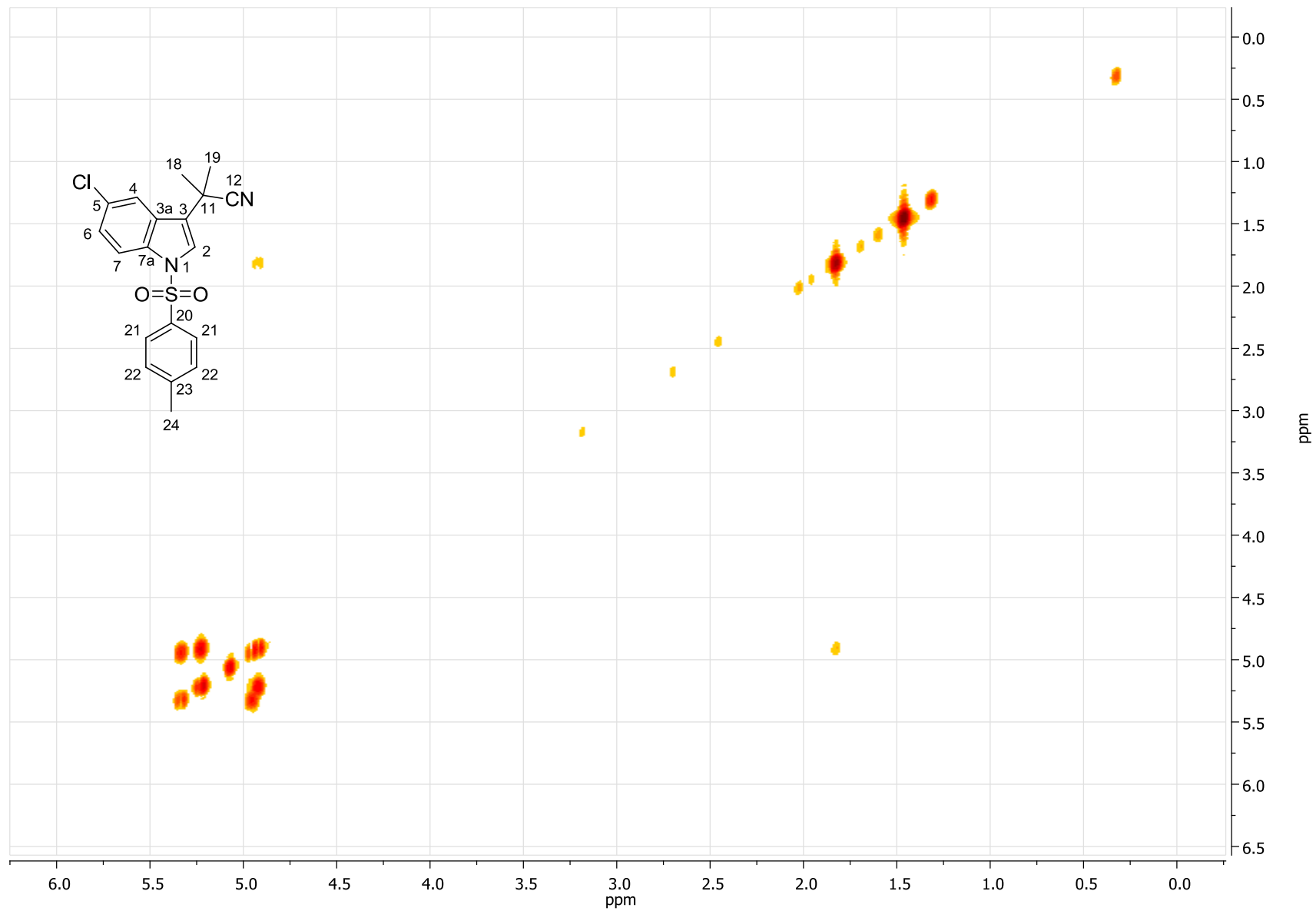
2-(5-Chloro-1-tosyl-1H-indol-3-yl)-2-methylpropanenitrile – 36



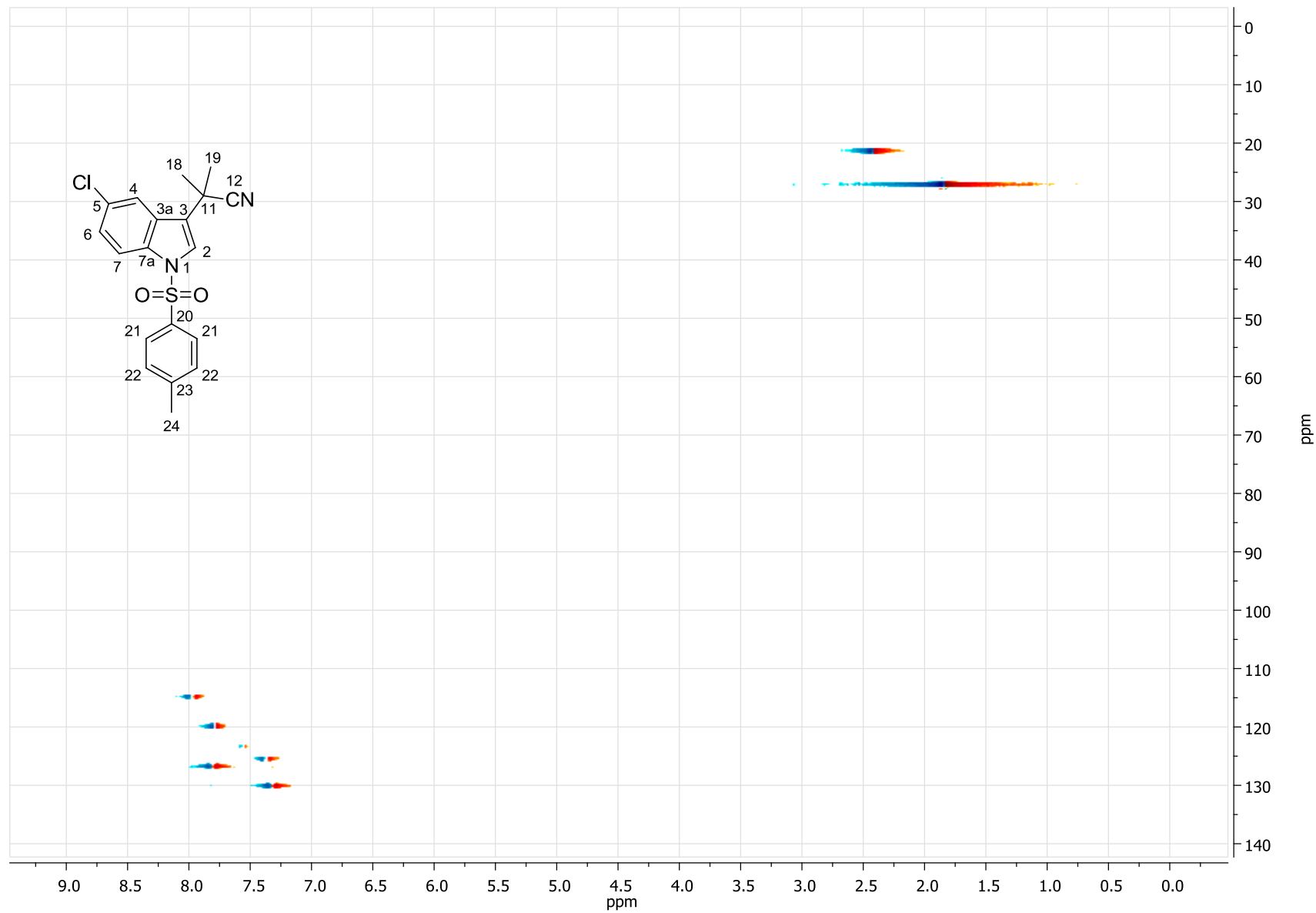
¹H NMR Spectrum
300 MHz Varian VNMRS



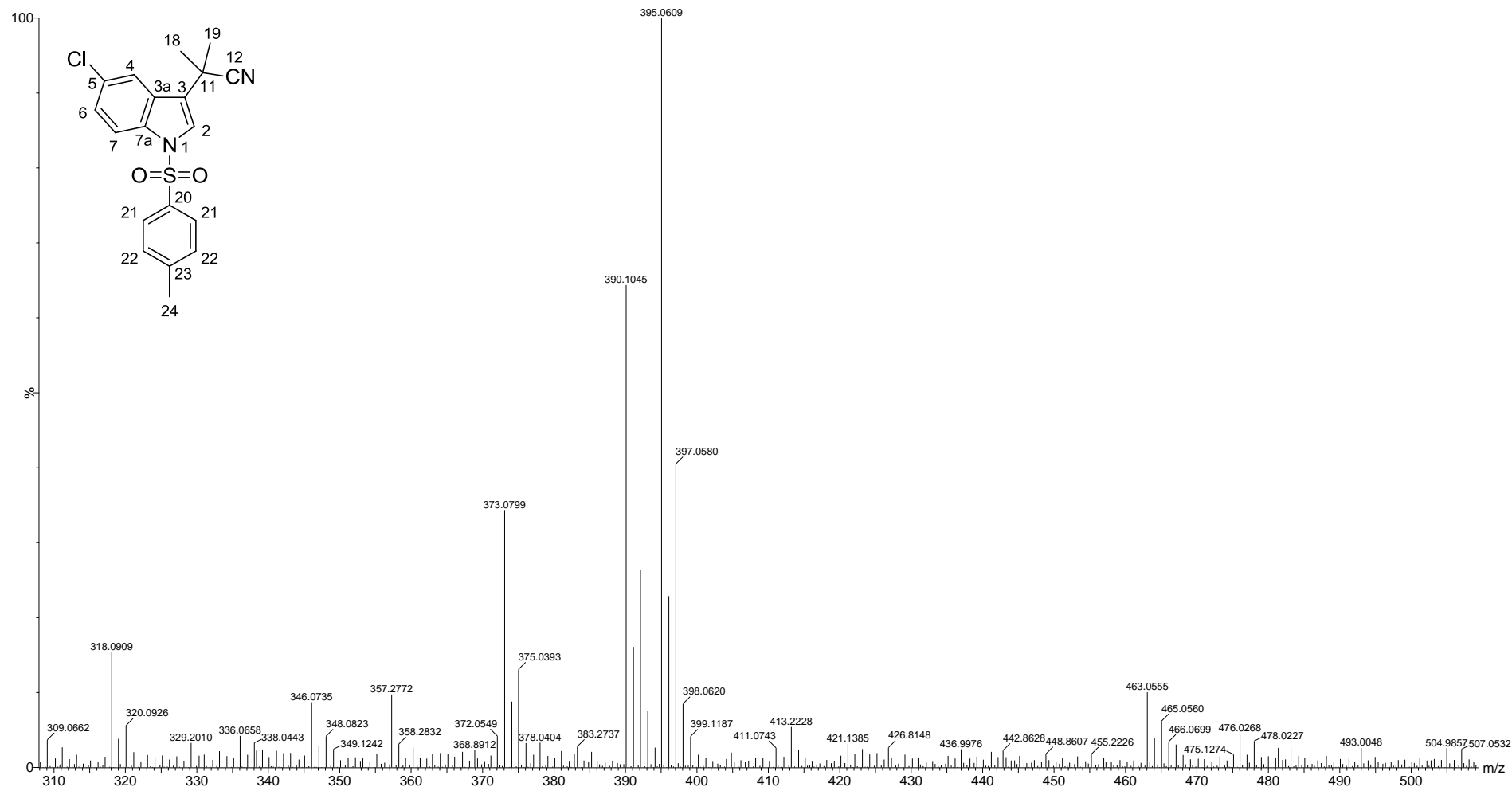
^{13}C NMR Spectrum
75 MHz Varian VNMRS



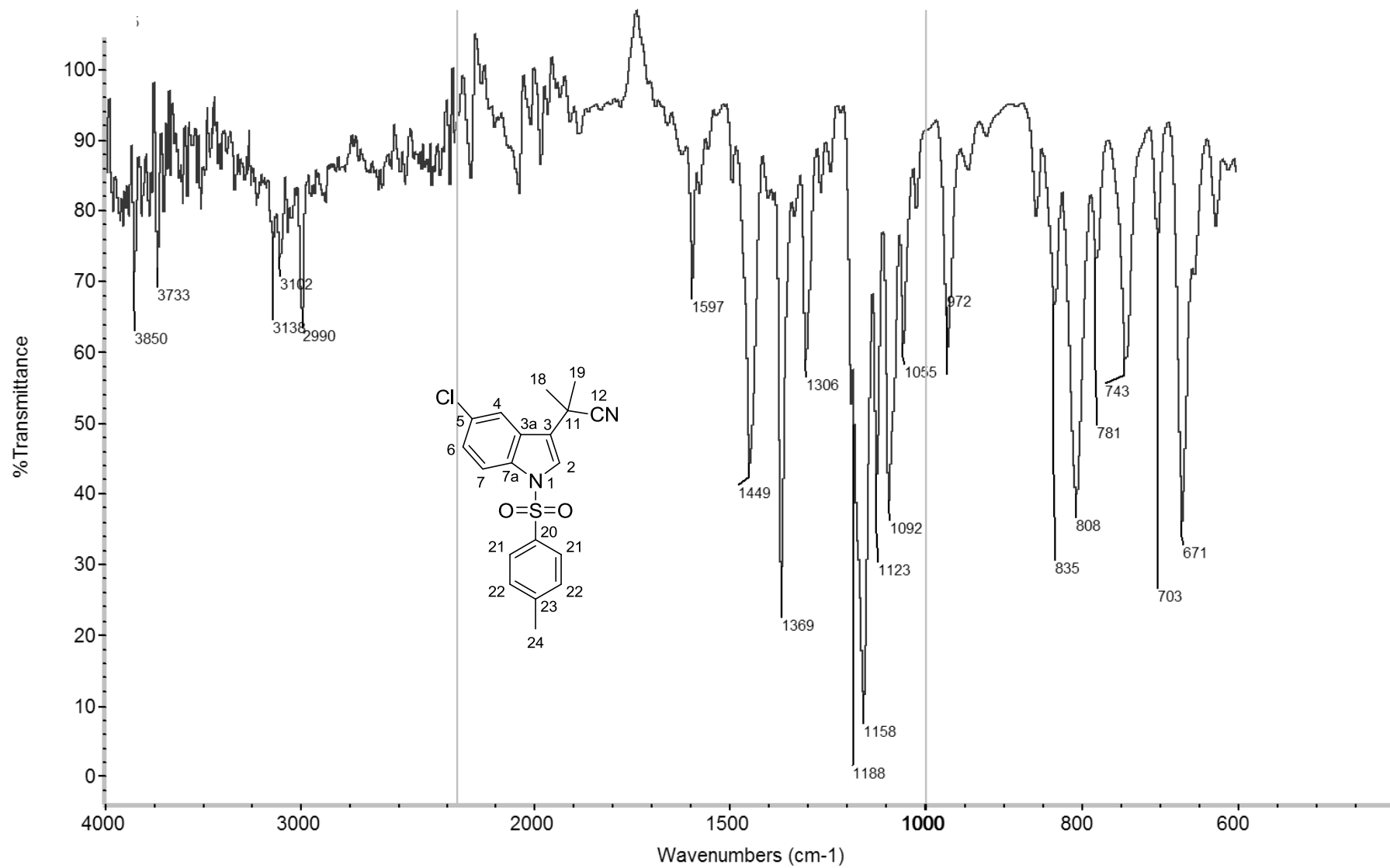
COSY NMR Spectrum
300 MHz Varian VNMRS



gHSQC NMR Spectrum
300 MHz Varian VNMRS

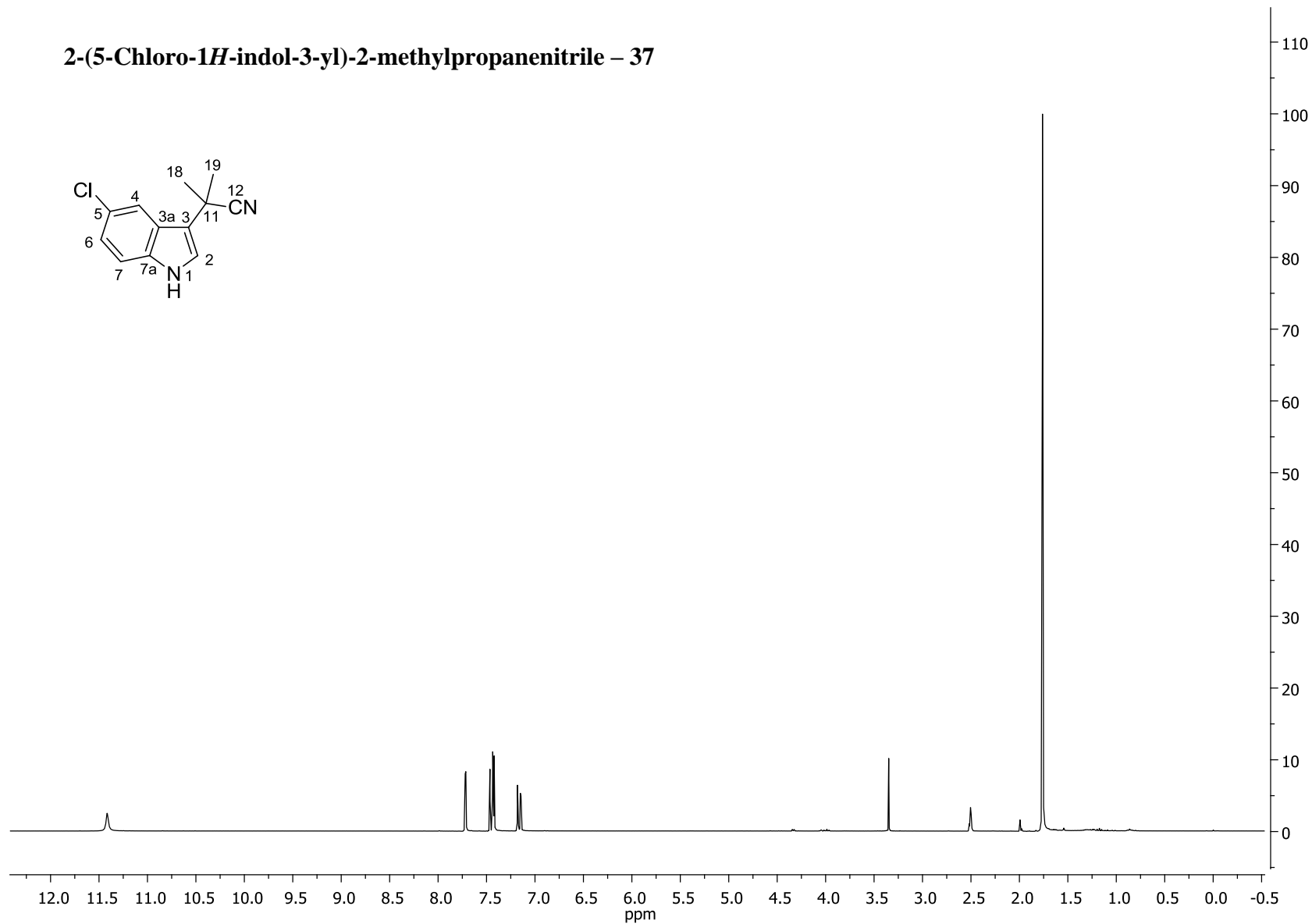
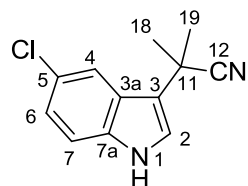


Mass Spectrum
Waters SYNAPT G2

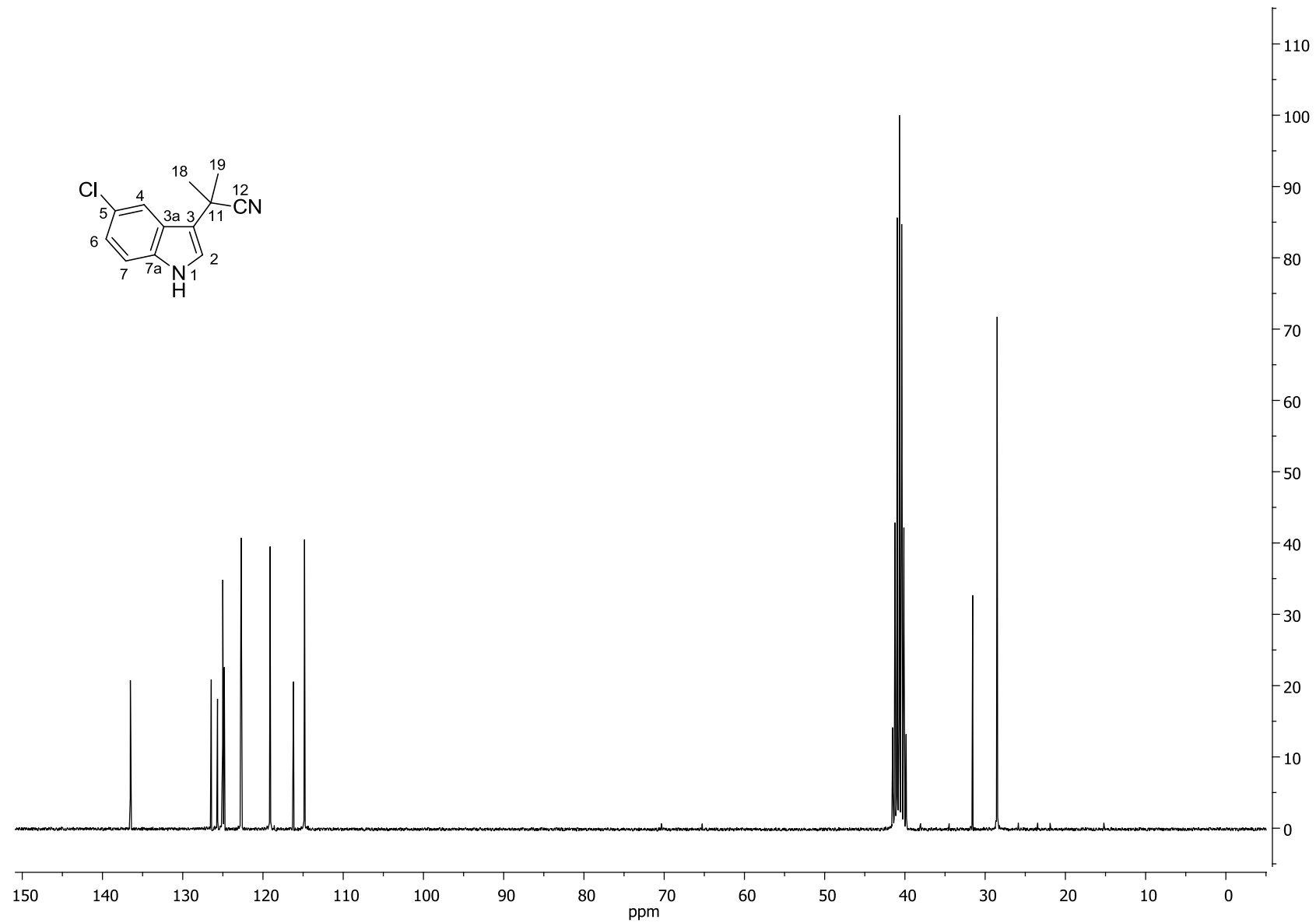


Infrared Spectrum
Thermo Nicolet Nexus 470

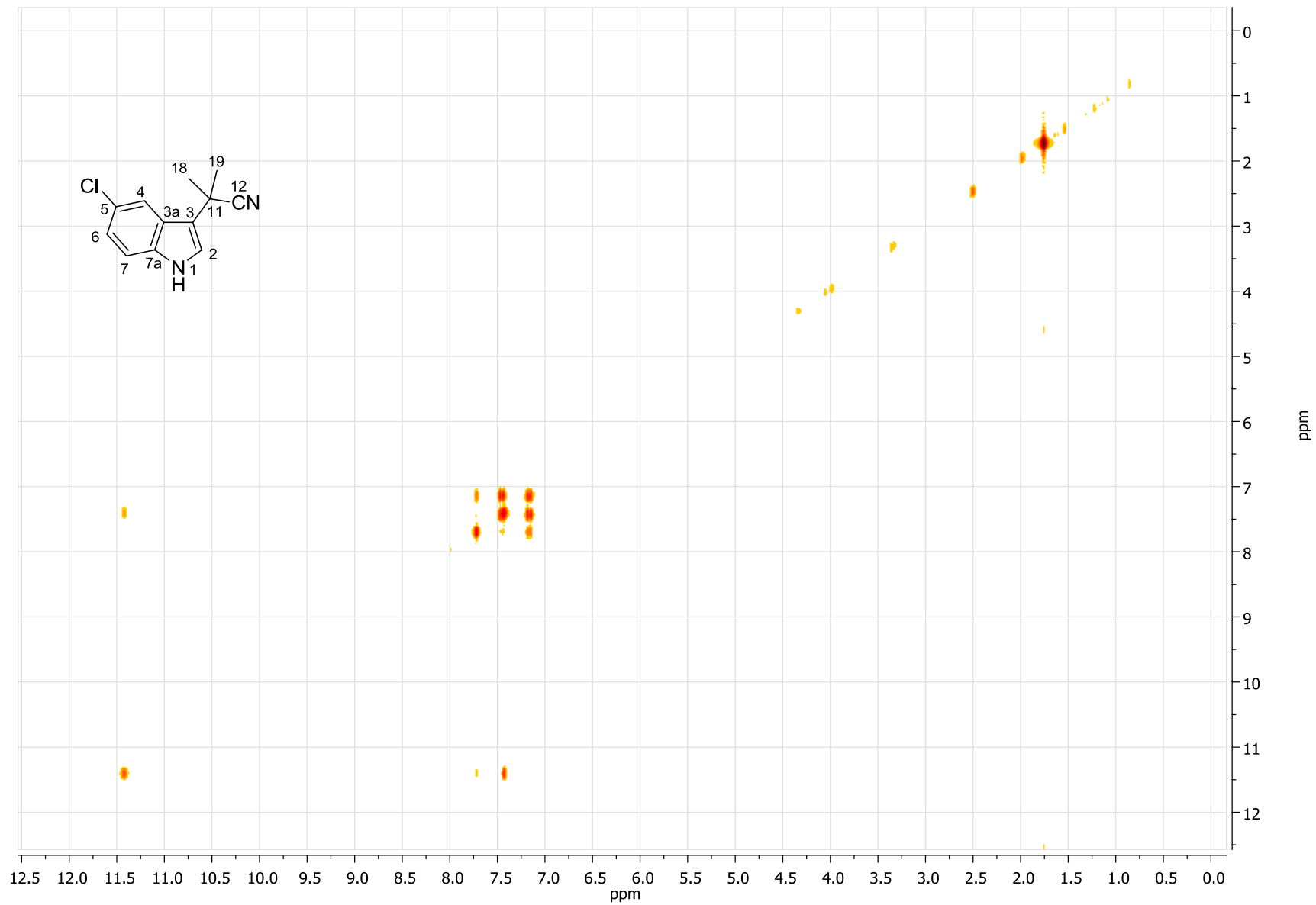
2-(5-Chloro-1*H*-indol-3-yl)-2-methylpropanenitrile – 37



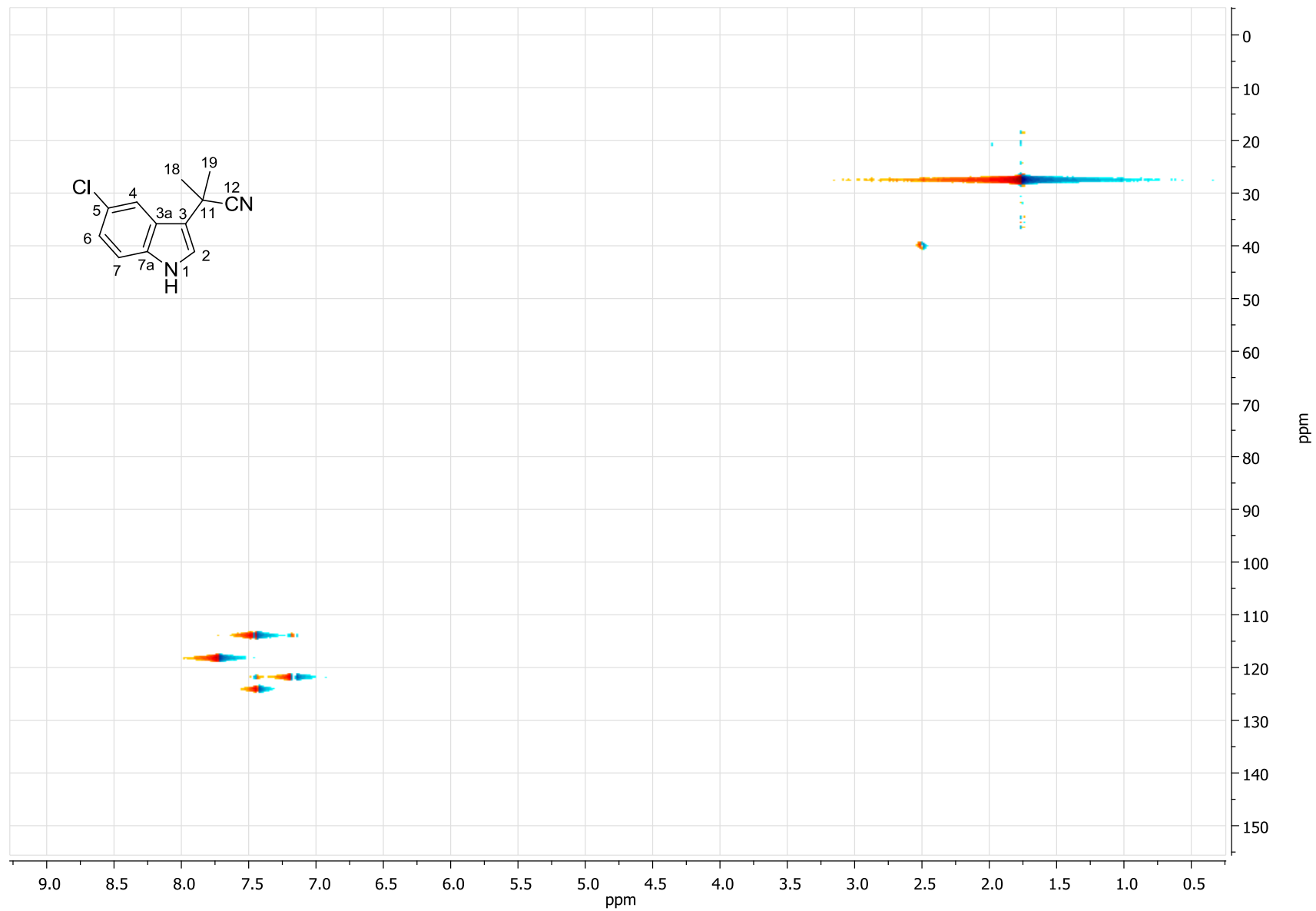
¹H NMR Spectrum
300 MHz Varian VNMRS



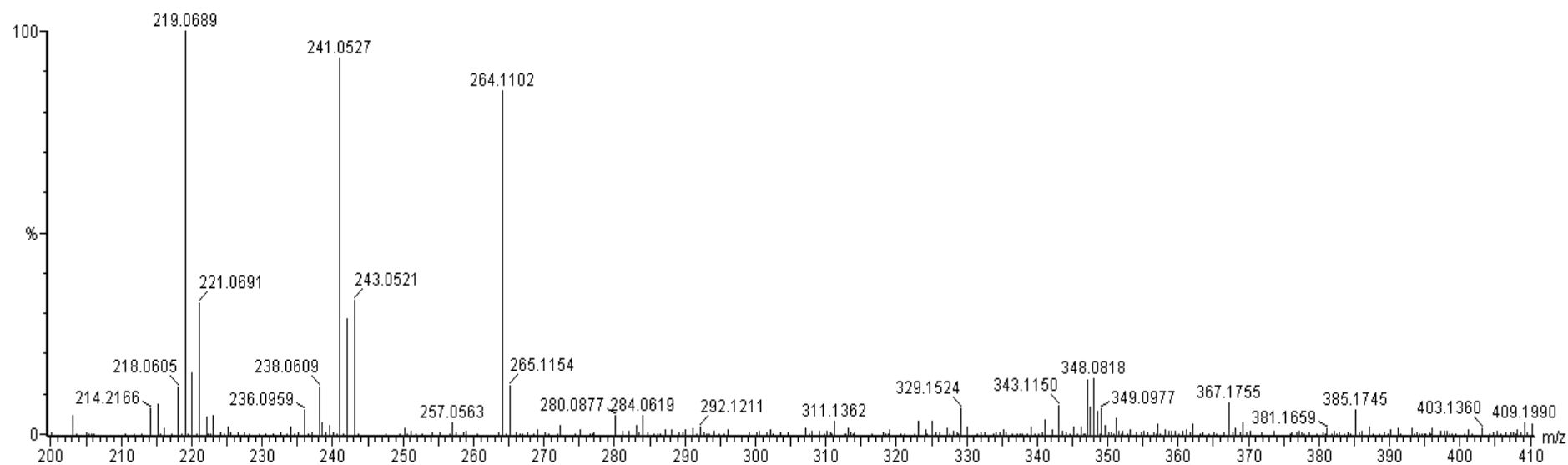
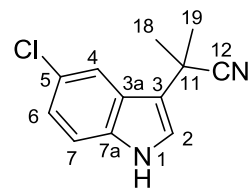
^{13}C NMR Spectrum
75 MHz Varian VNMRS



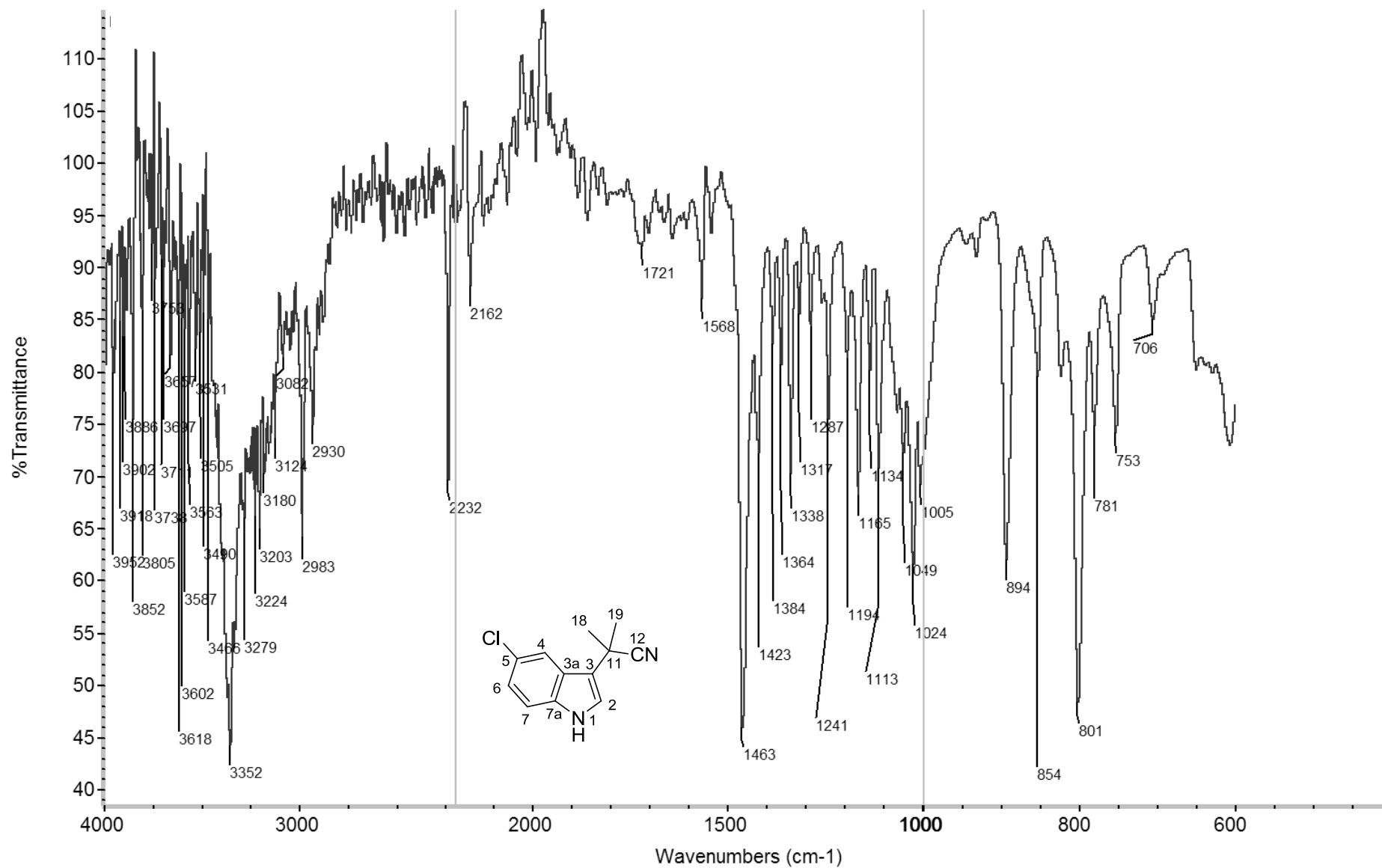
COSY NMR Spectrum
300 MHz Varian VNMRS



gHSQC NMR Spectrum
300 MHz Varian VNMRS

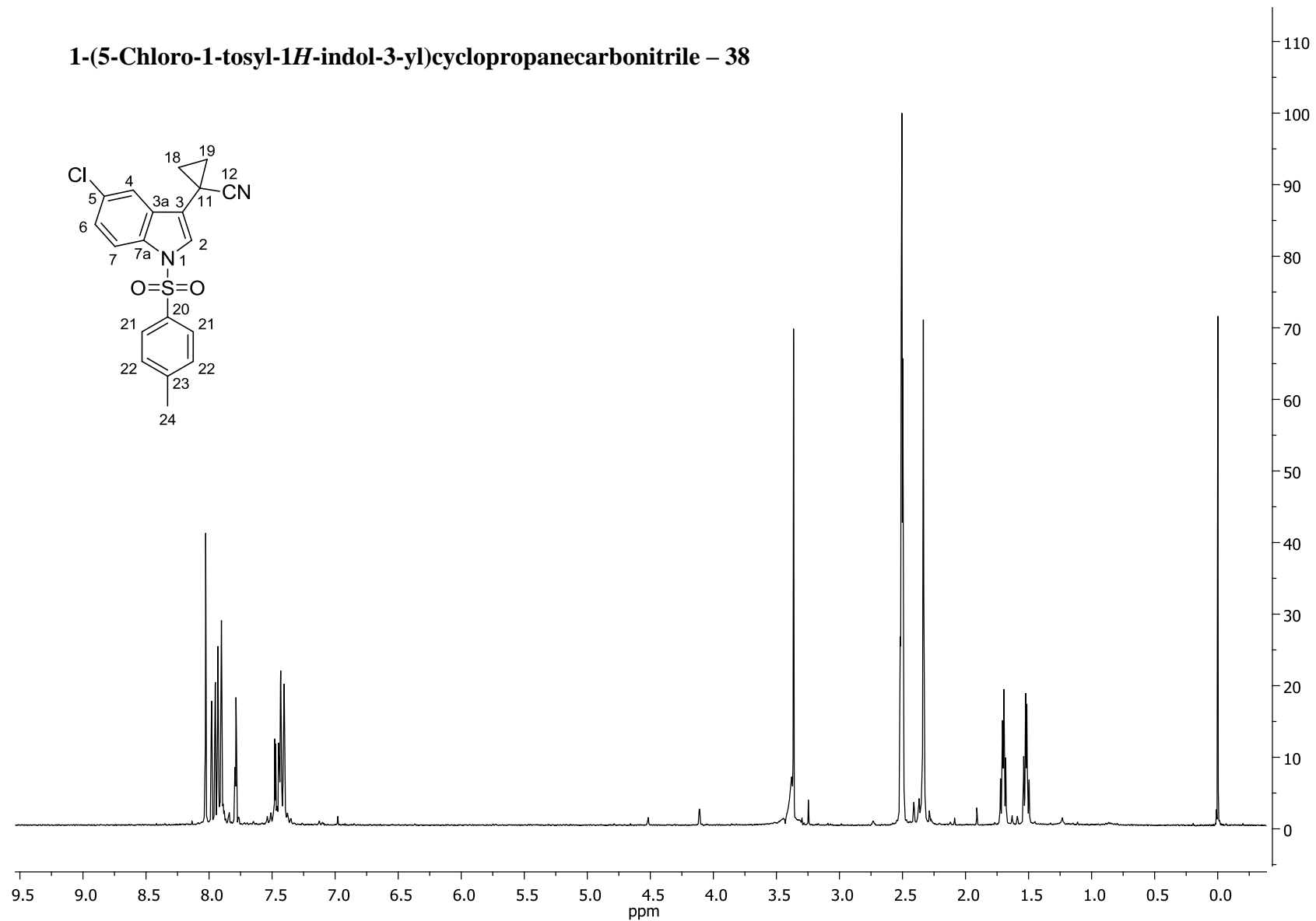


Mass Spectrum
Waters SYNAPT G2

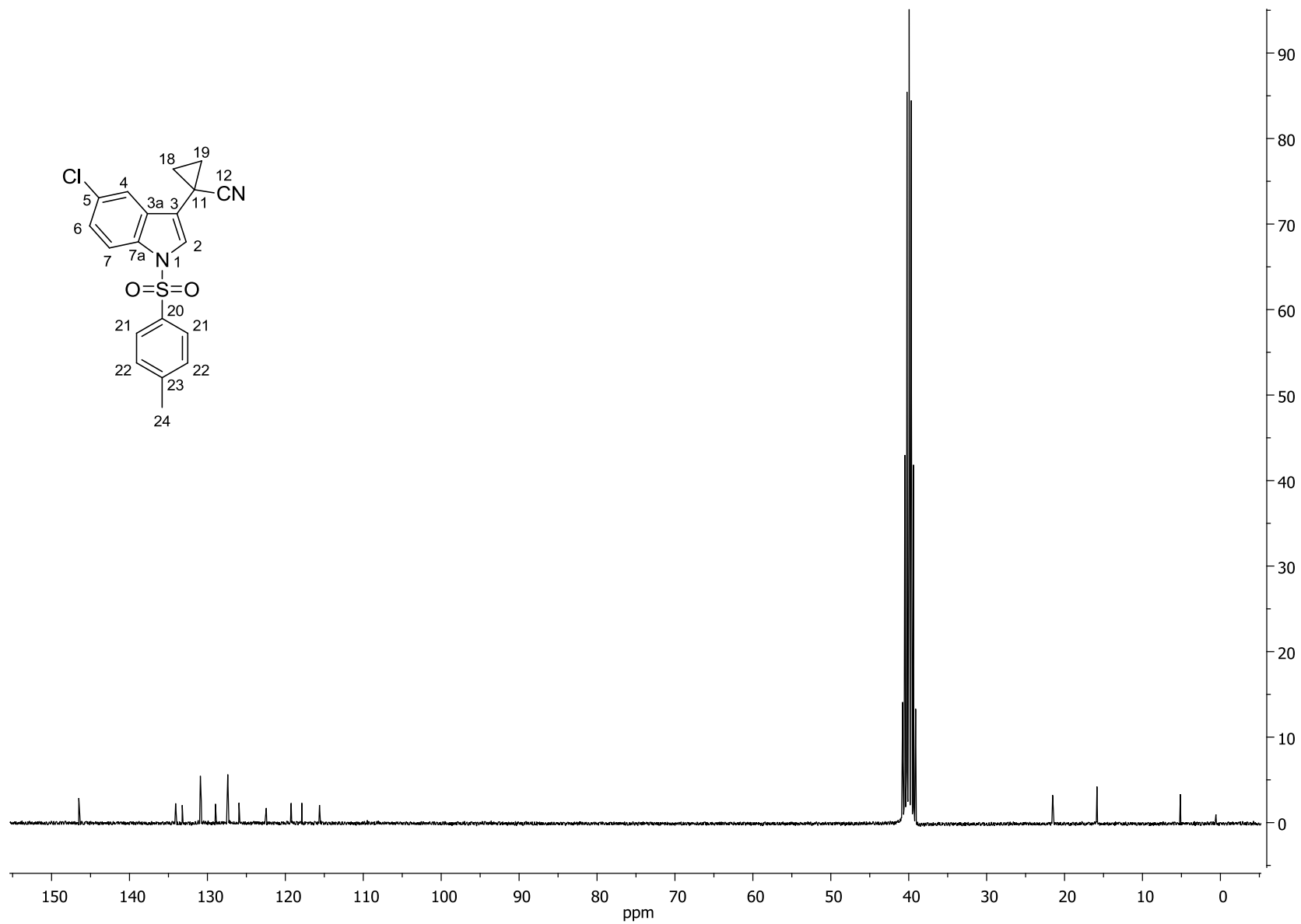


Infrared Spectrum
Thermo Nicolet Nexus 470

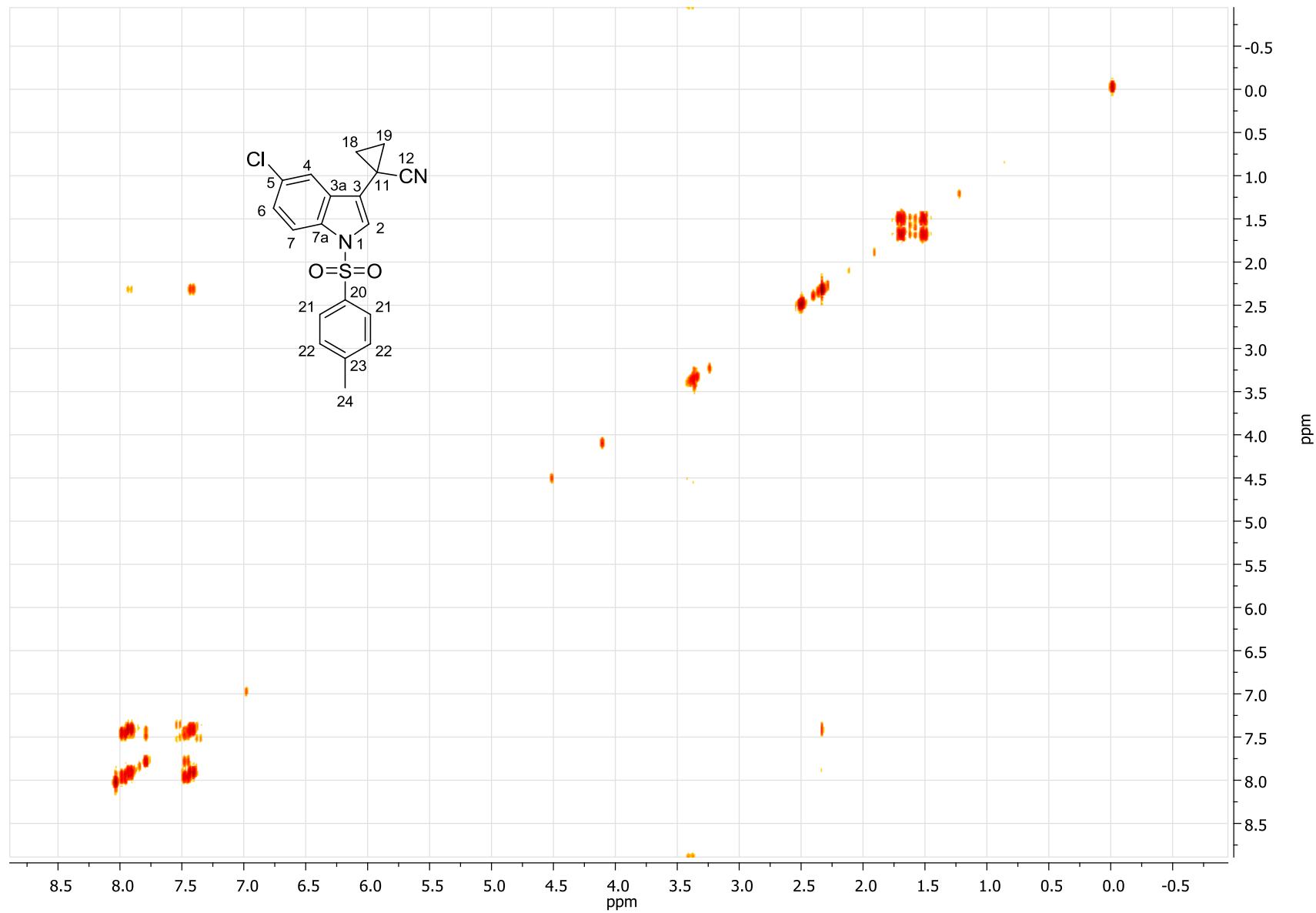
1-(5-Chloro-1-tosyl-1H-indol-3-yl)cyclopropanecarbonitrile – 38



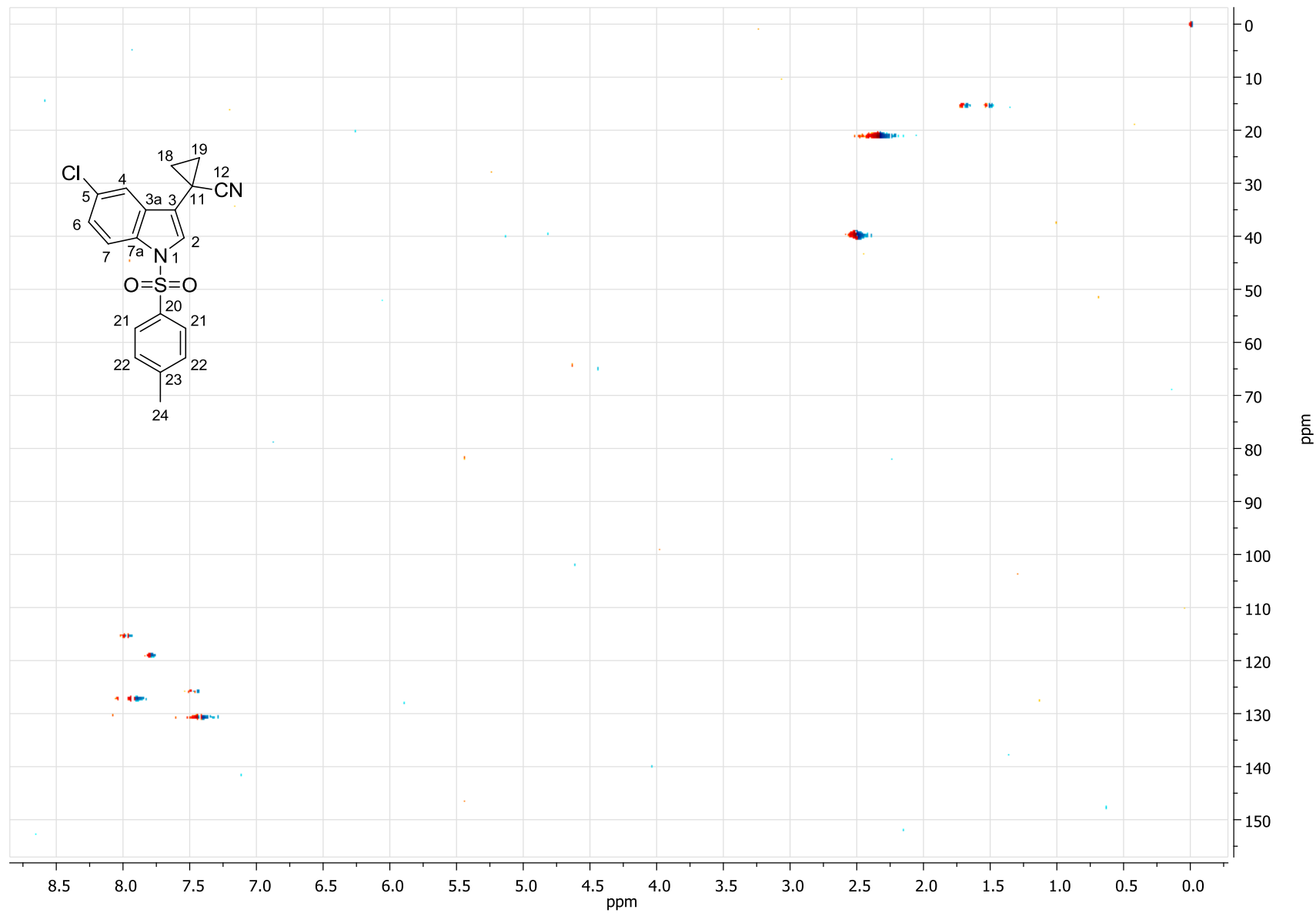
¹H NMR Spectrum
300 MHz Varian VNMRS



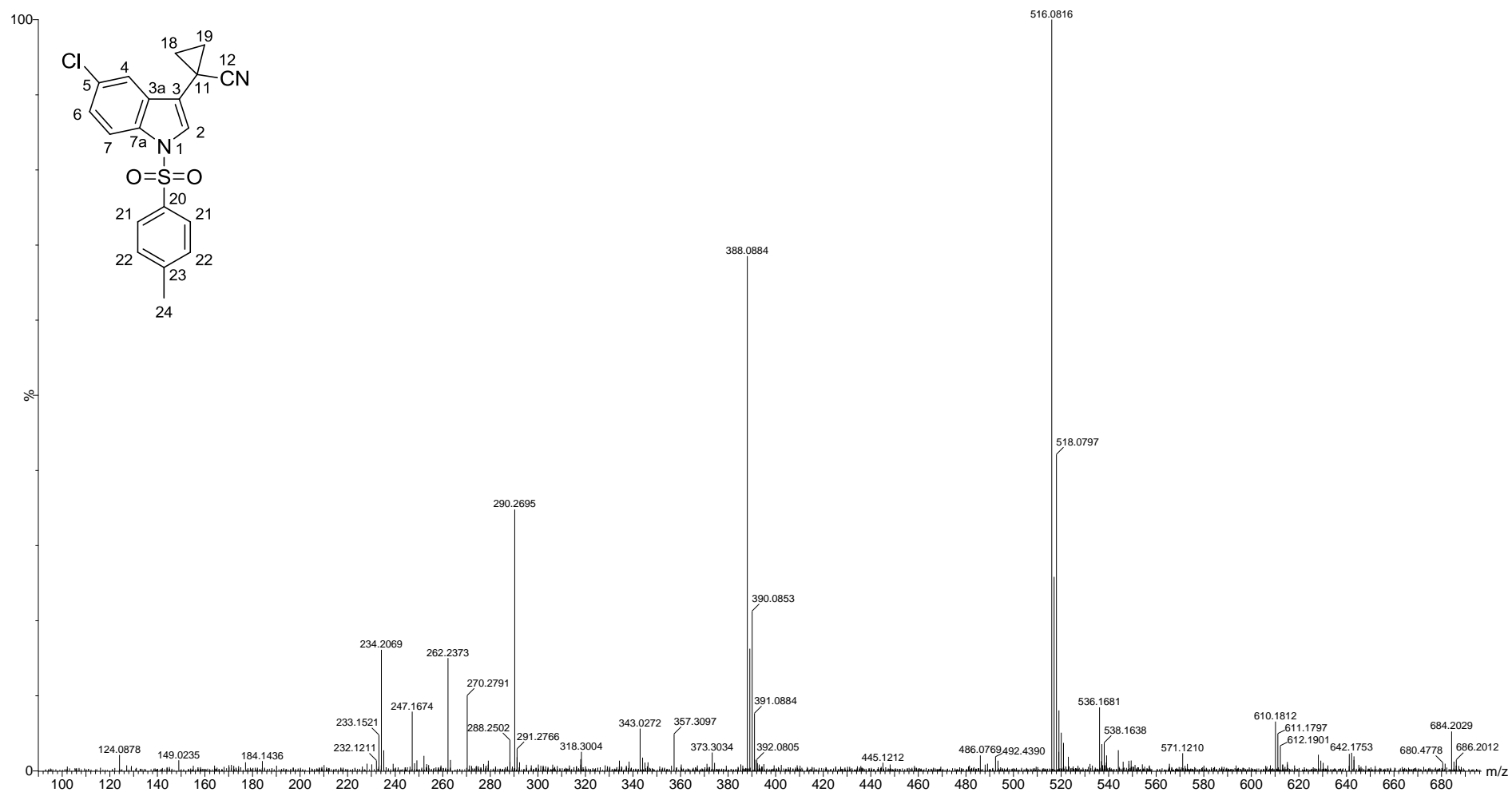
^{13}C NMR Spectrum
75 MHz Varian VNMRS



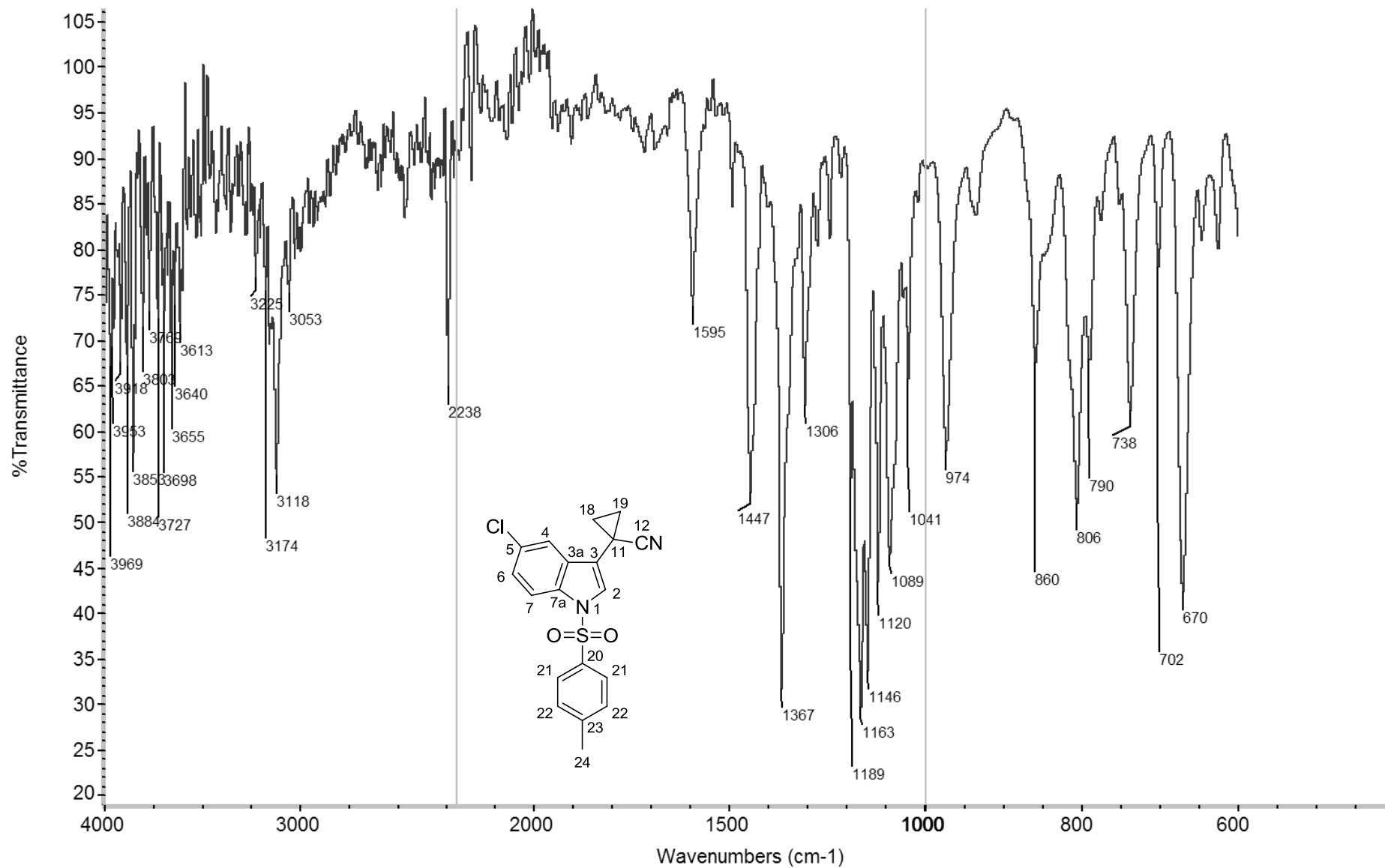
COSY NMR Spectrum
300 MHz Varian VNMRS



gHSQC NMR Spectrum
300 MHz Varian VNMRS

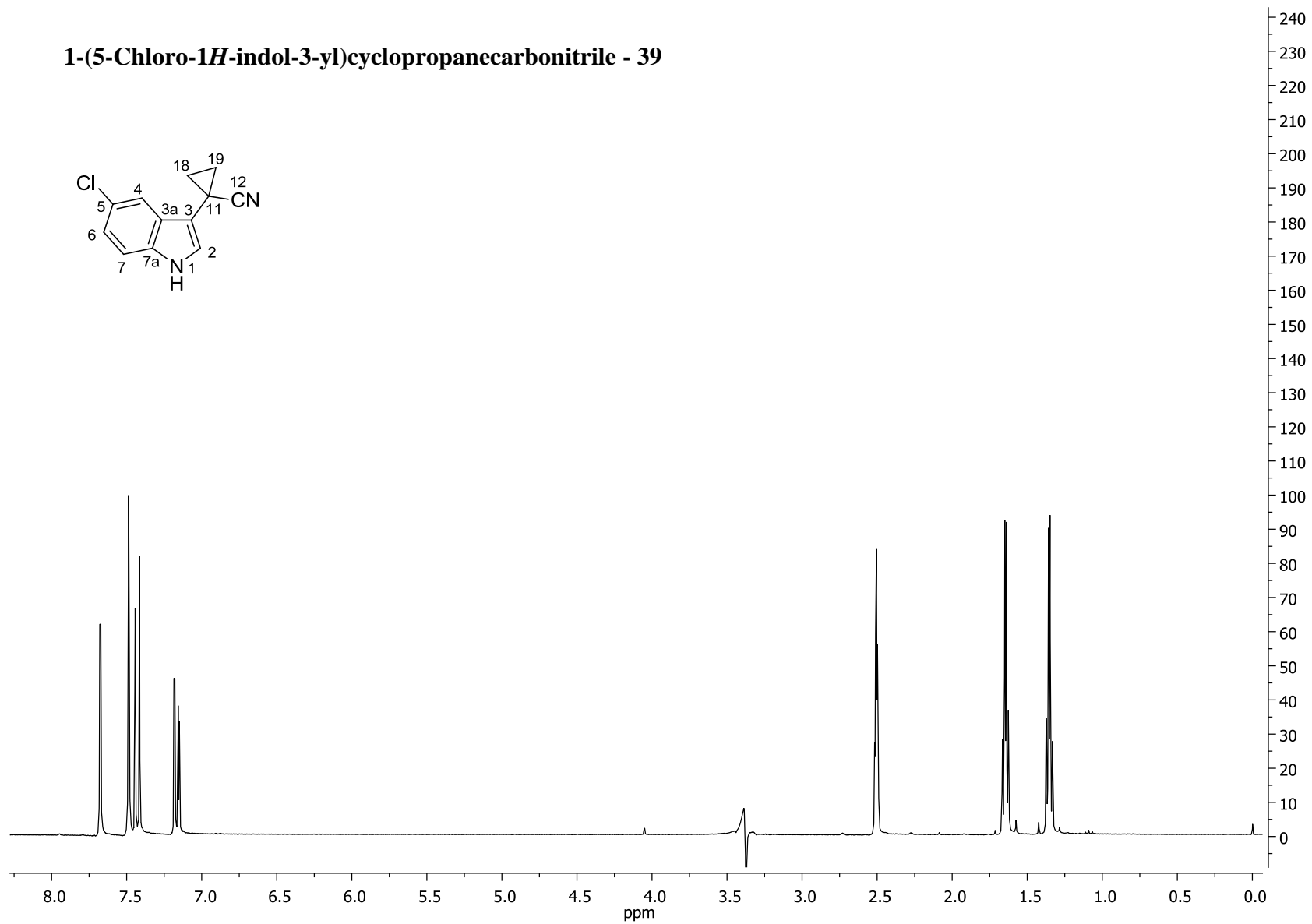
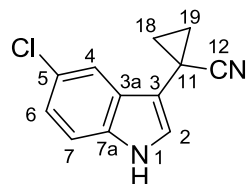


Mass Spectrum
Waters SYNAPT G2

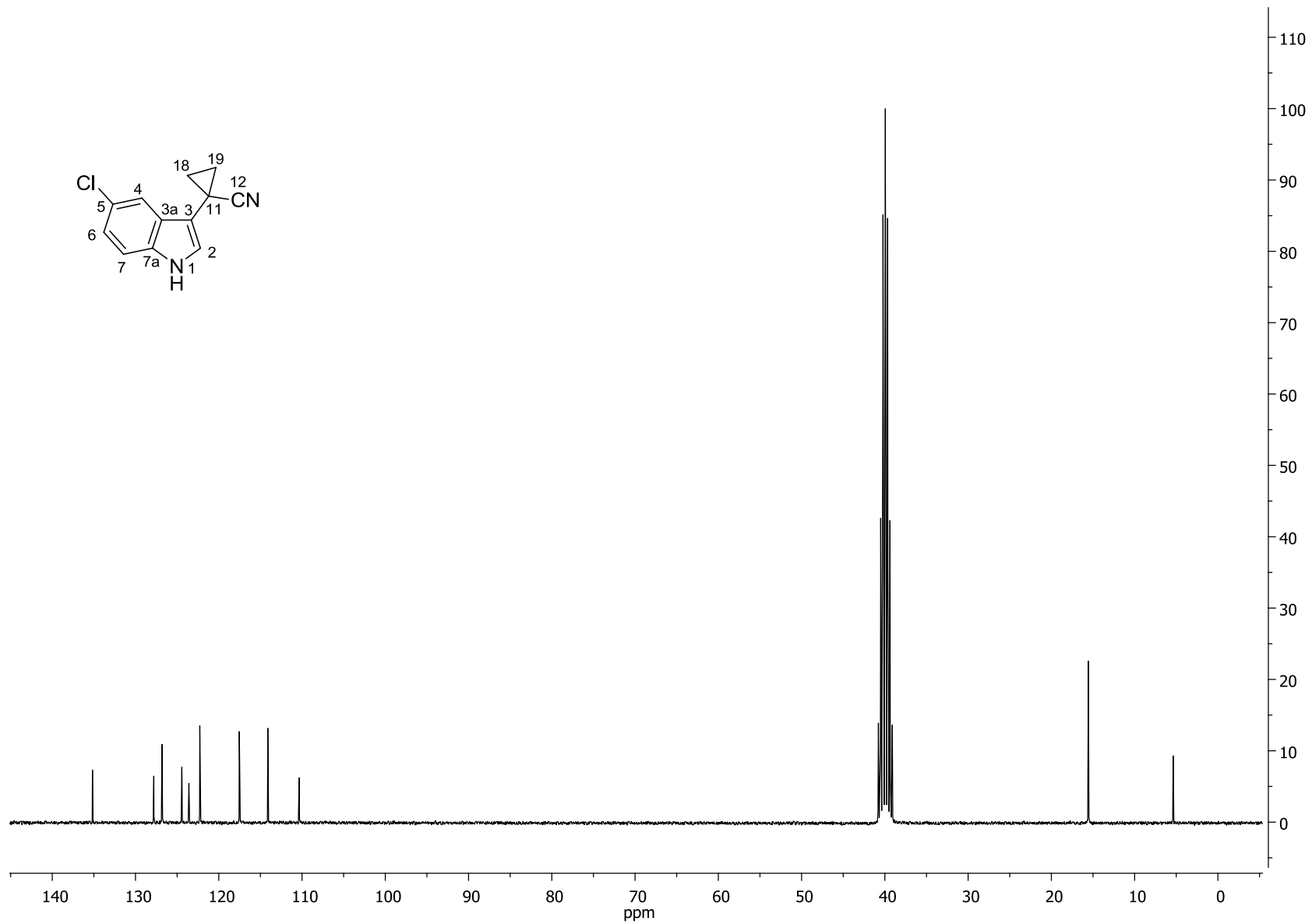


Infrared Spectrum
Thermo Nicolet Nexus 470

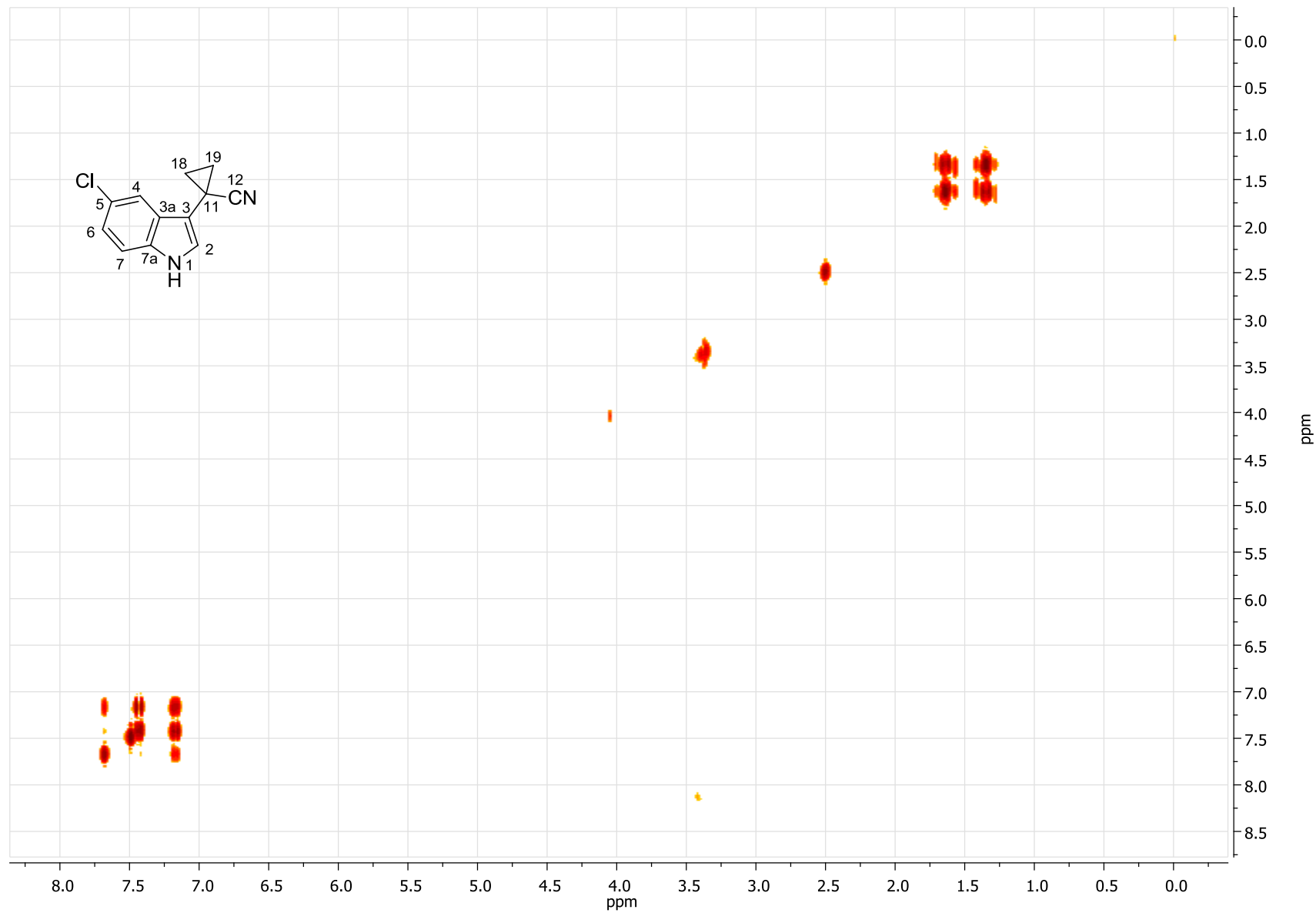
1-(5-Chloro-1*H*-indol-3-yl)cyclopropanecarbonitrile - 39



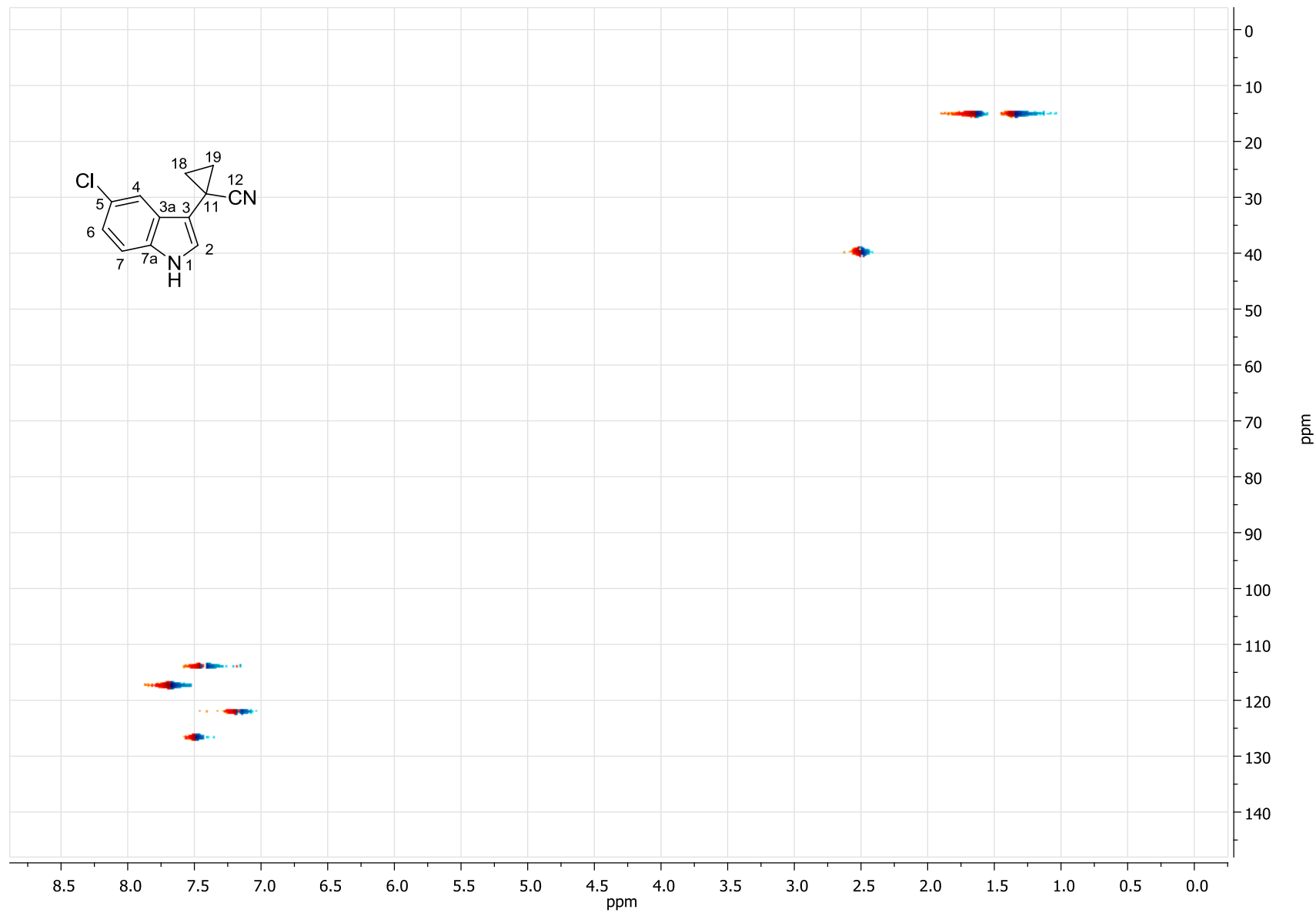
¹H NMR Spectrum
300 MHz Varian VNMRS



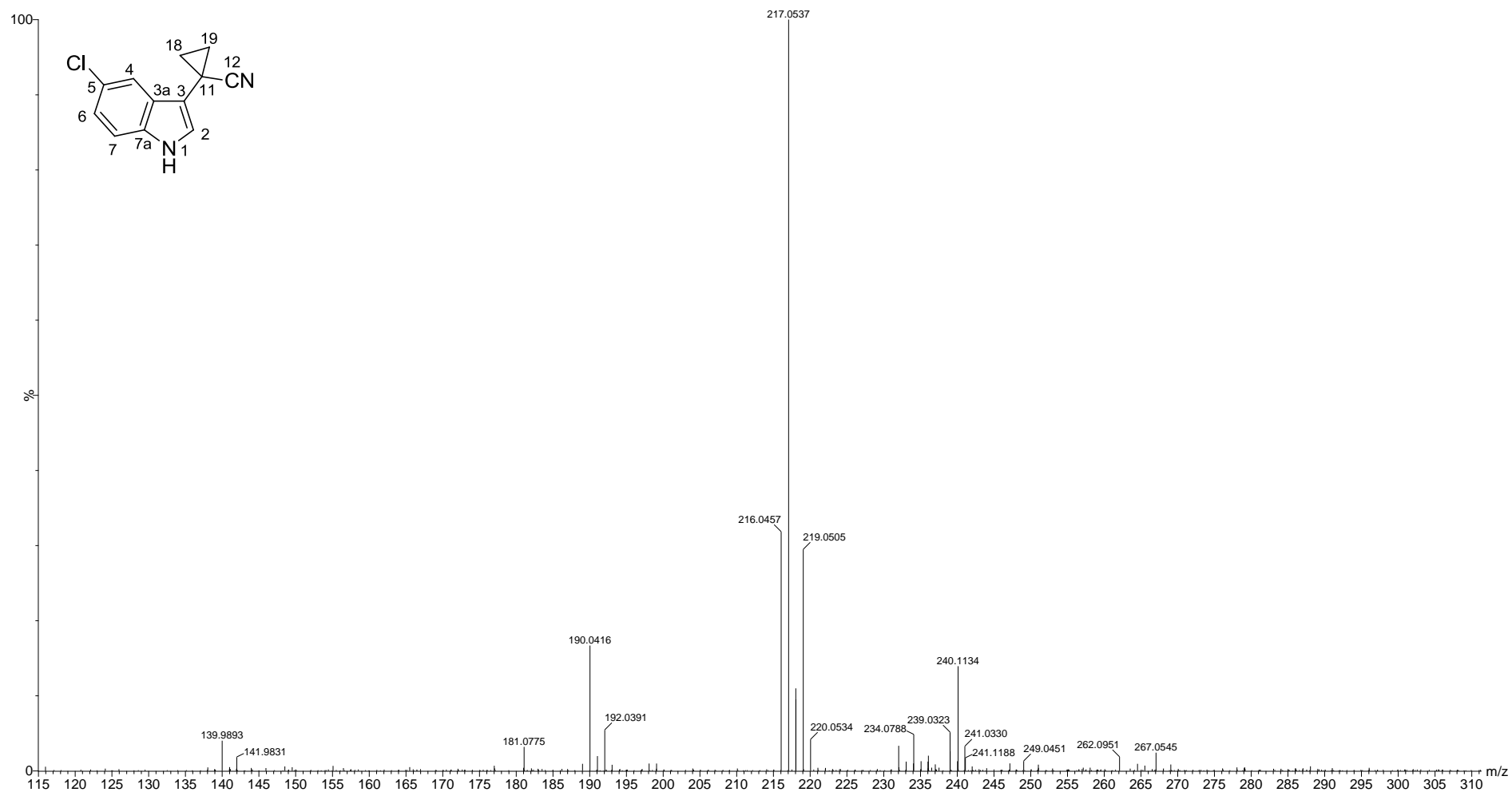
^{13}C NMR Spectrum
75 MHz Varian VNMRS



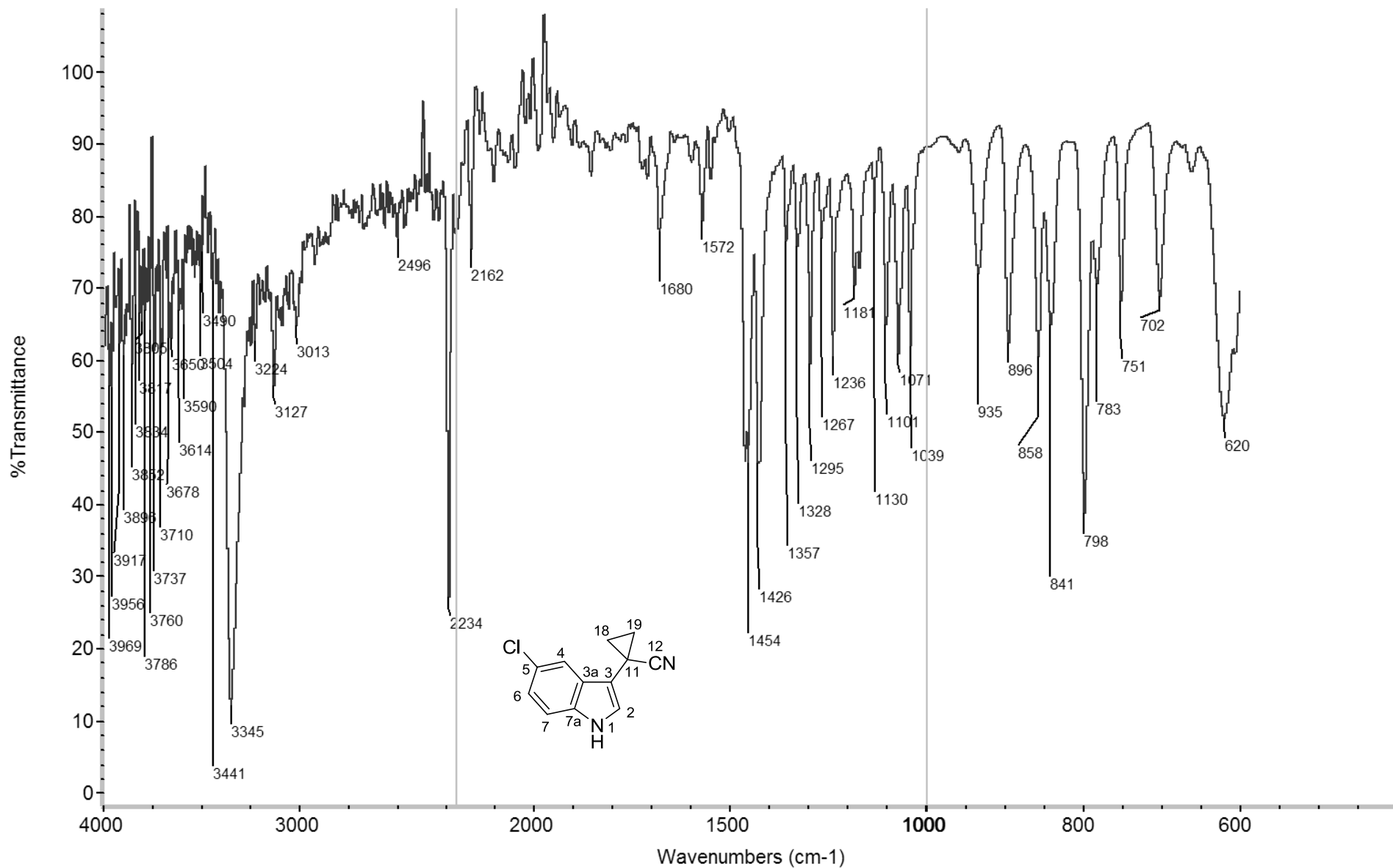
COSY NMR Spectrum
300 MHz Varian VNMRS



gHSQC NMR Spectrum
300 MHz Varian VNMRS

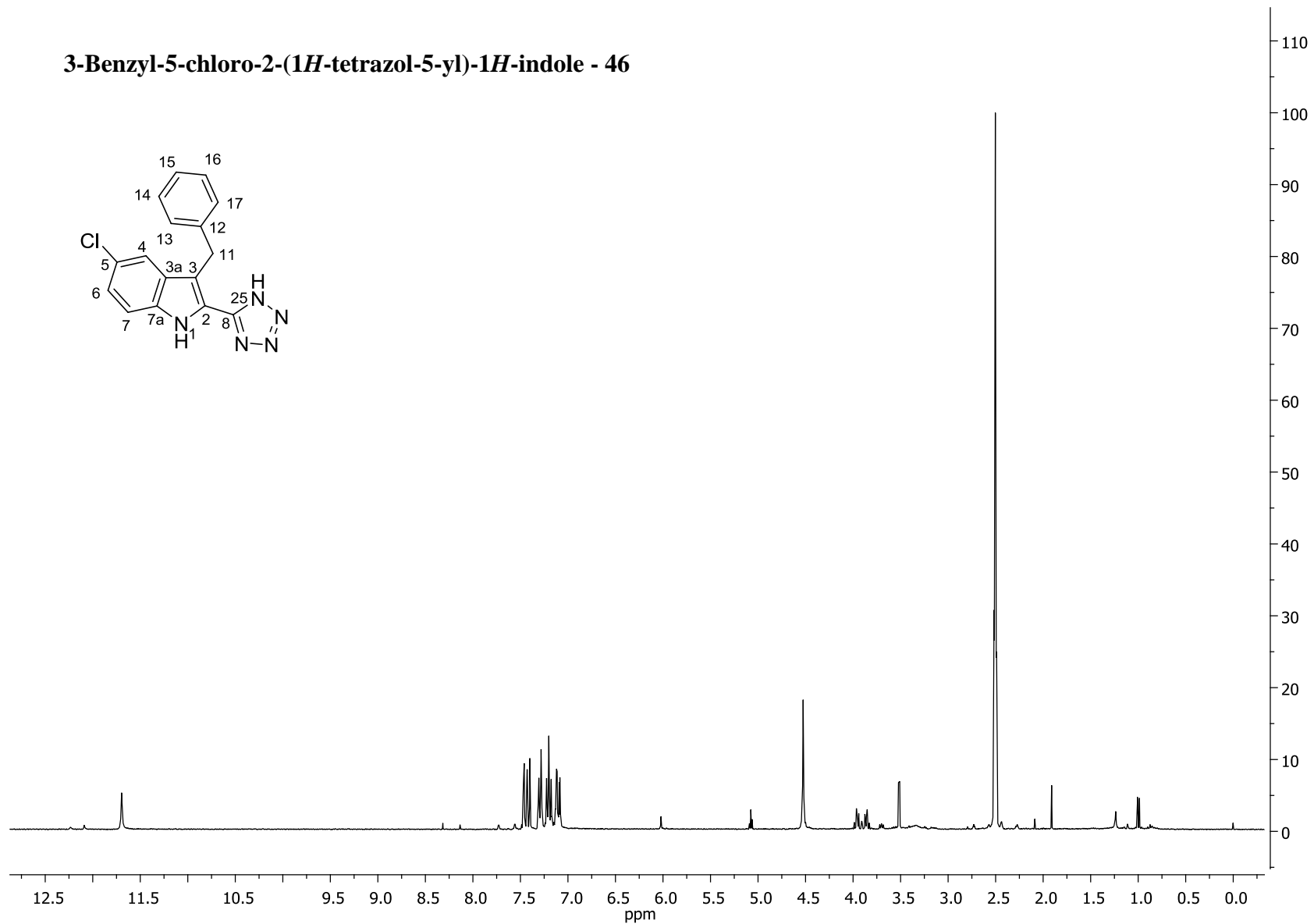


Mass Spectrum
Waters SYNAPT G2

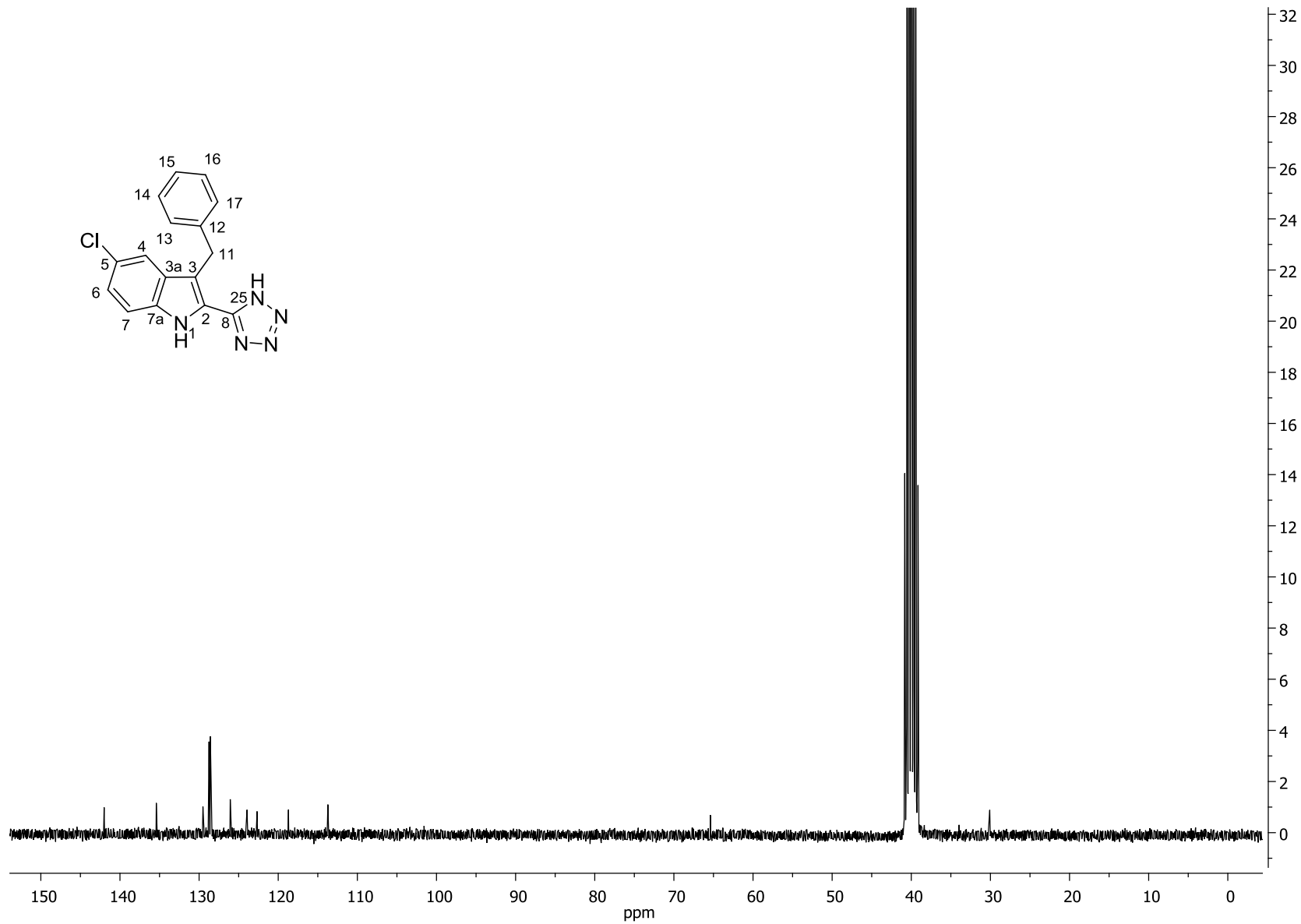


Infrared Spectrum
Thermo Nicolet Nexus 470

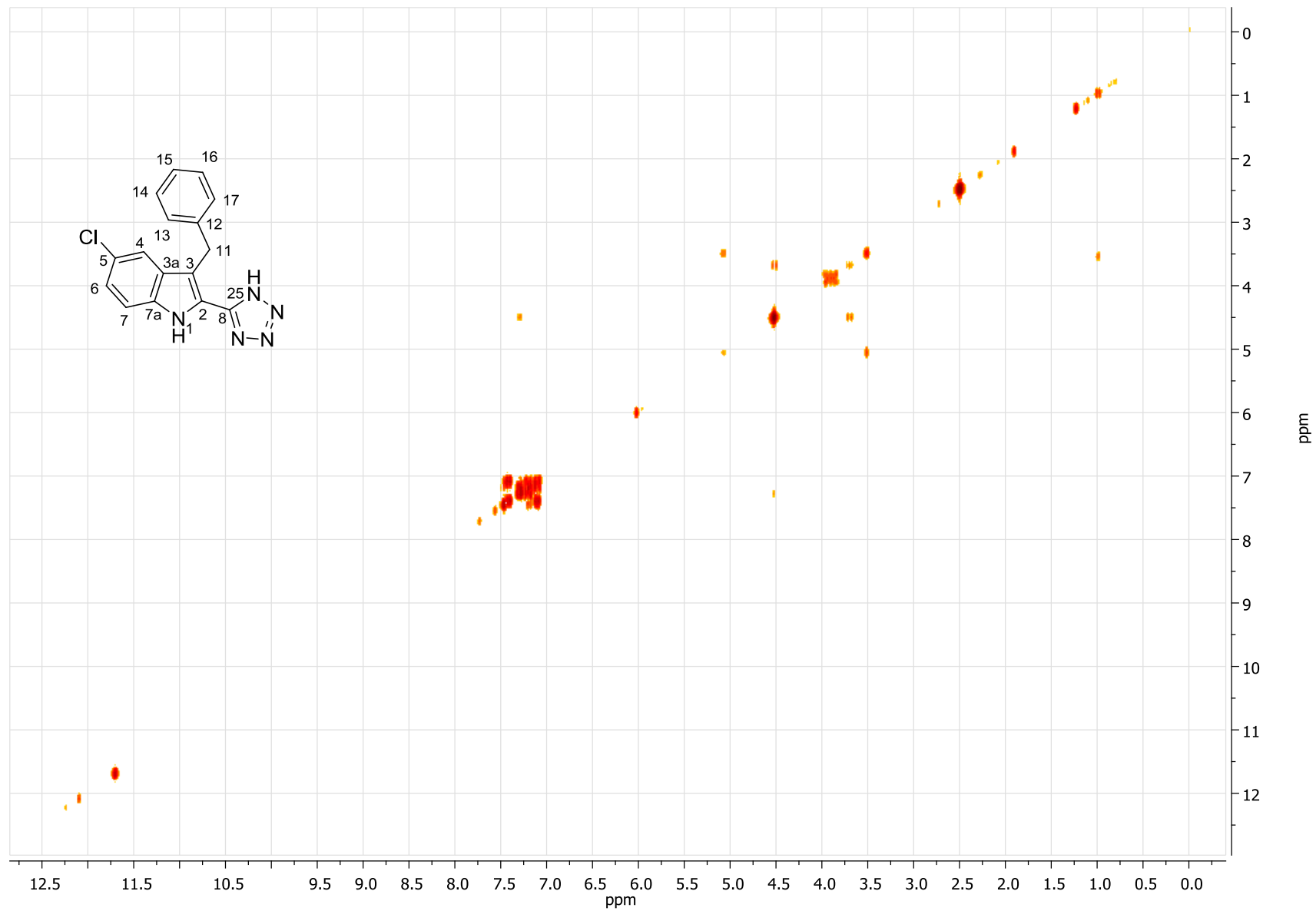
3-Benzyl-5-chloro-2-(1H-tetrazol-5-yl)-1H-indole - 46



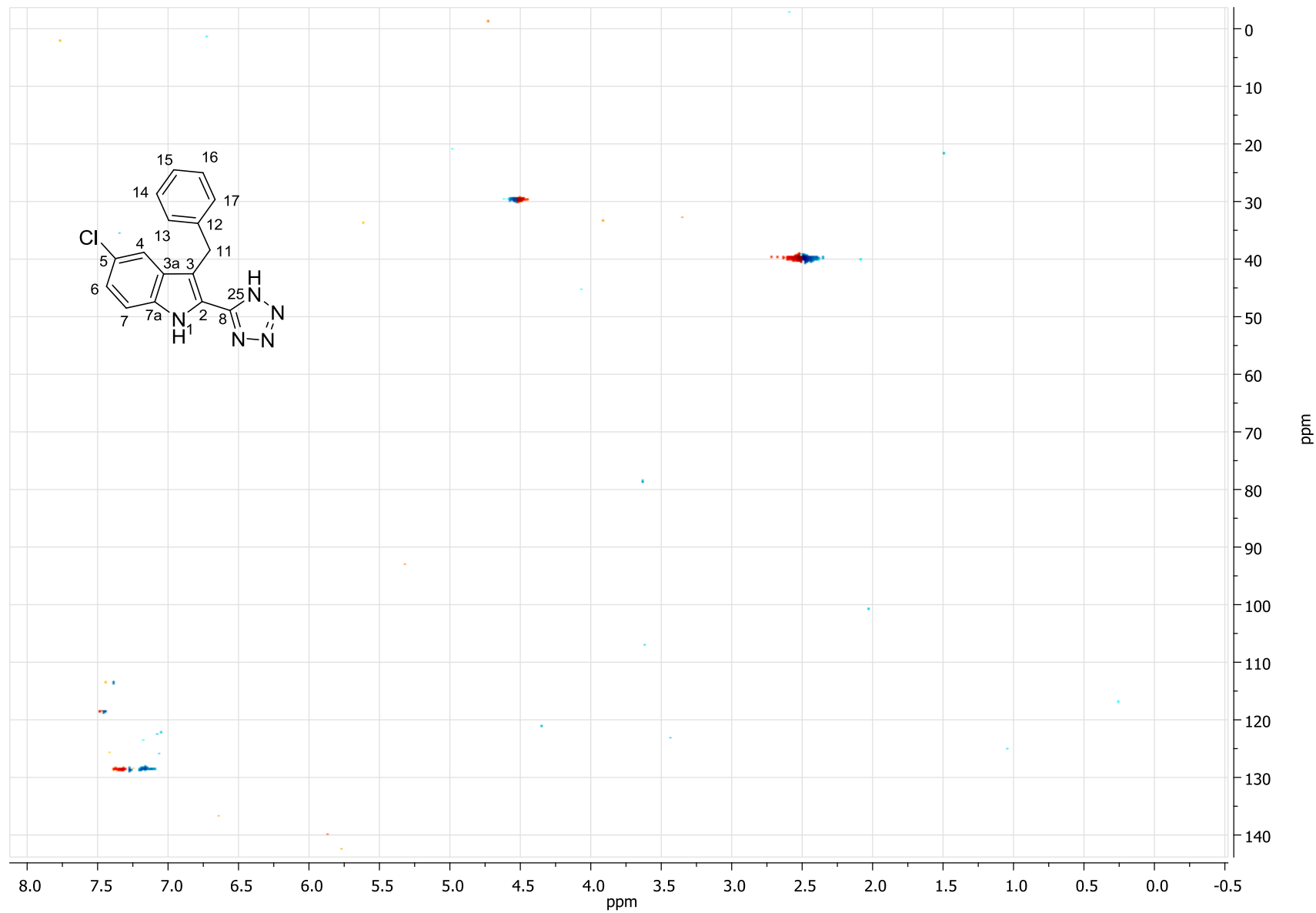
¹H NMR Spectrum
300 MHz Varian VNMRS



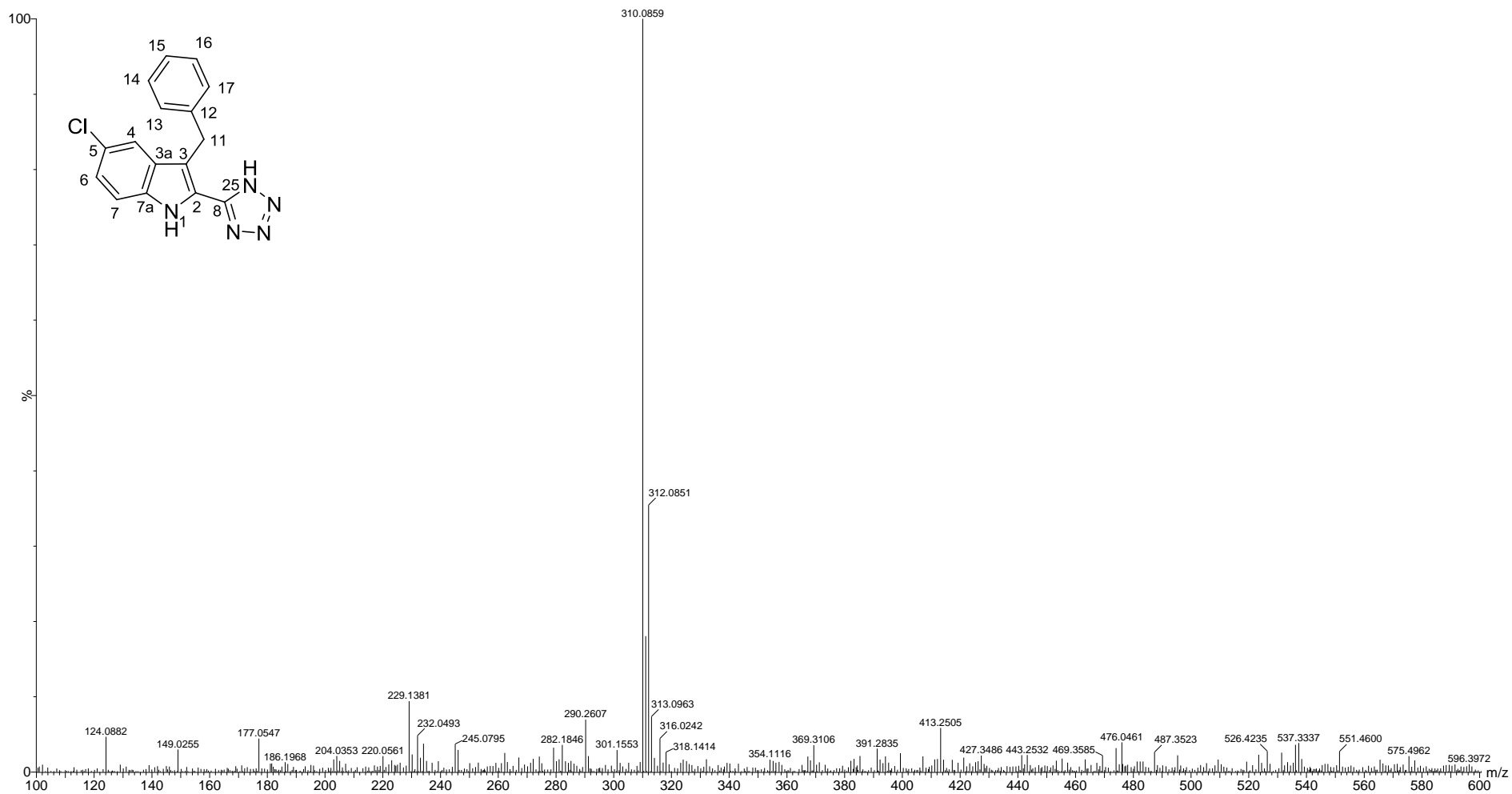
^{13}C NMR Spectrum
75 MHz Varian VNMRS



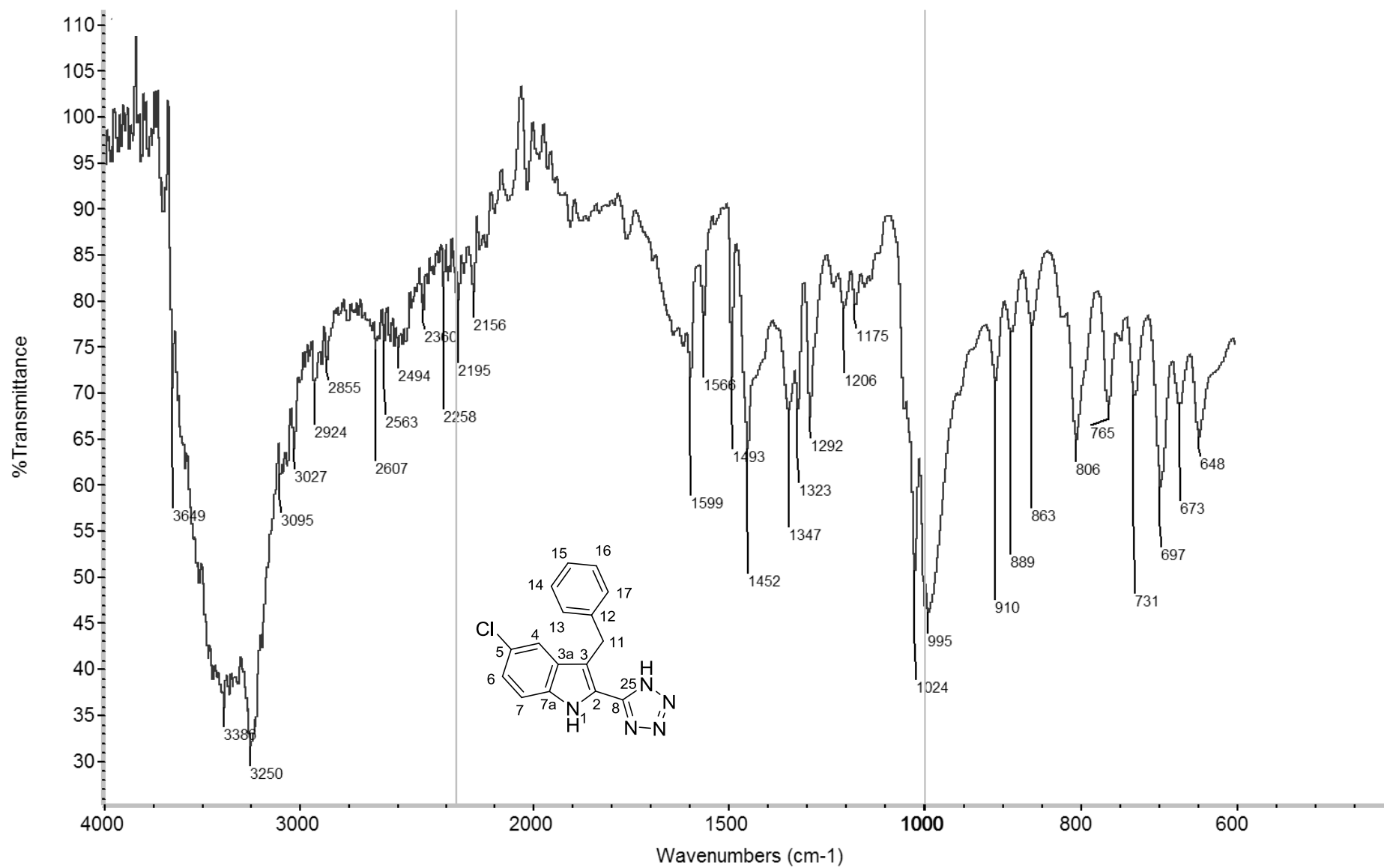
COSY NMR Spectrum
300 MHz Varian VNMRS



gHSQC NMR Spectrum
300 MHz Varian VNMRS

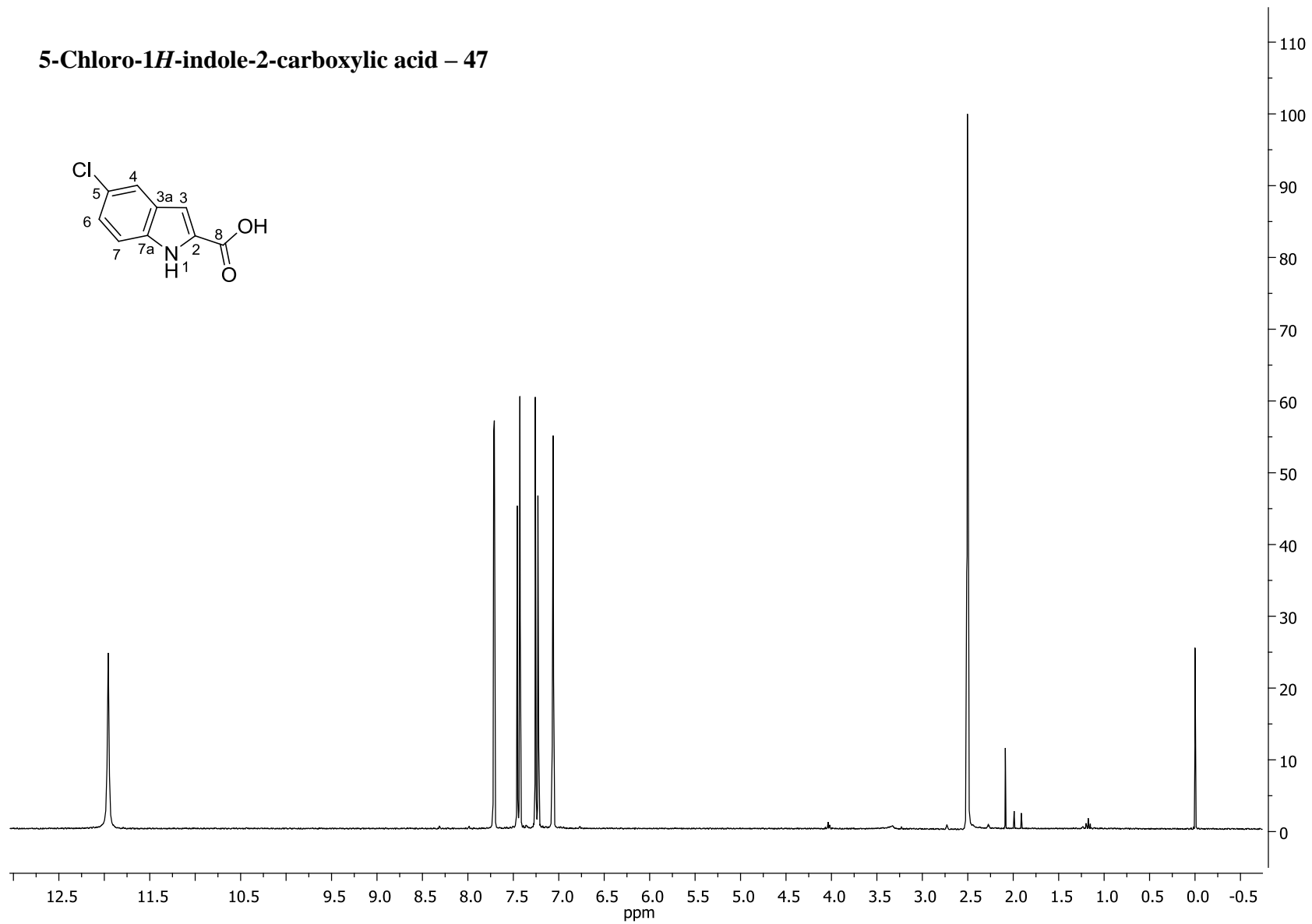
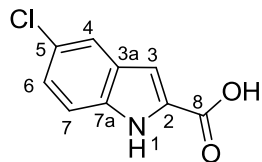


Mass Spectrum
Waters SYNAPT G2

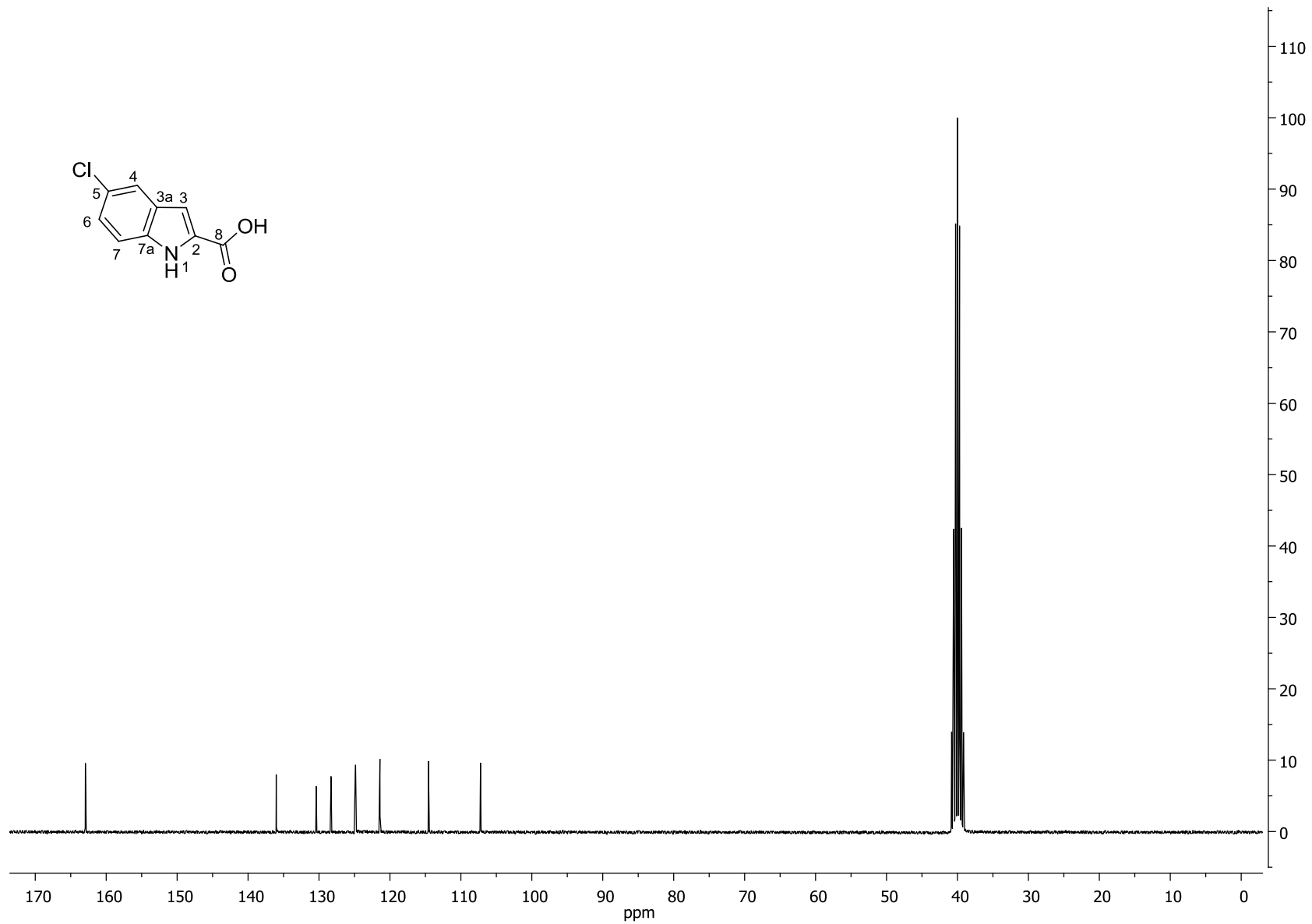


Infrared Spectrum
Thermo Nicolet Nexus 470

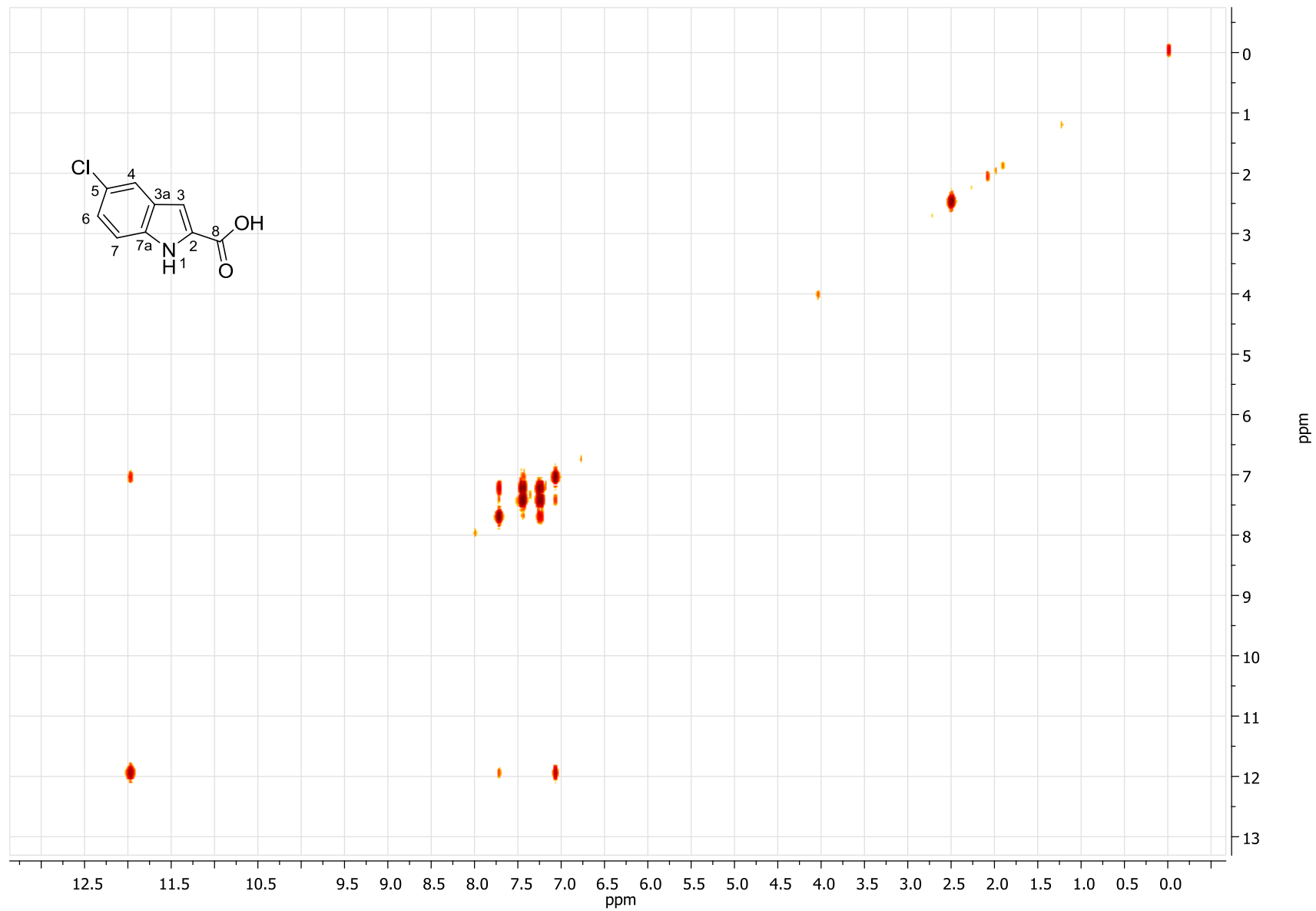
5-Chloro-1H-indole-2-carboxylic acid – 47



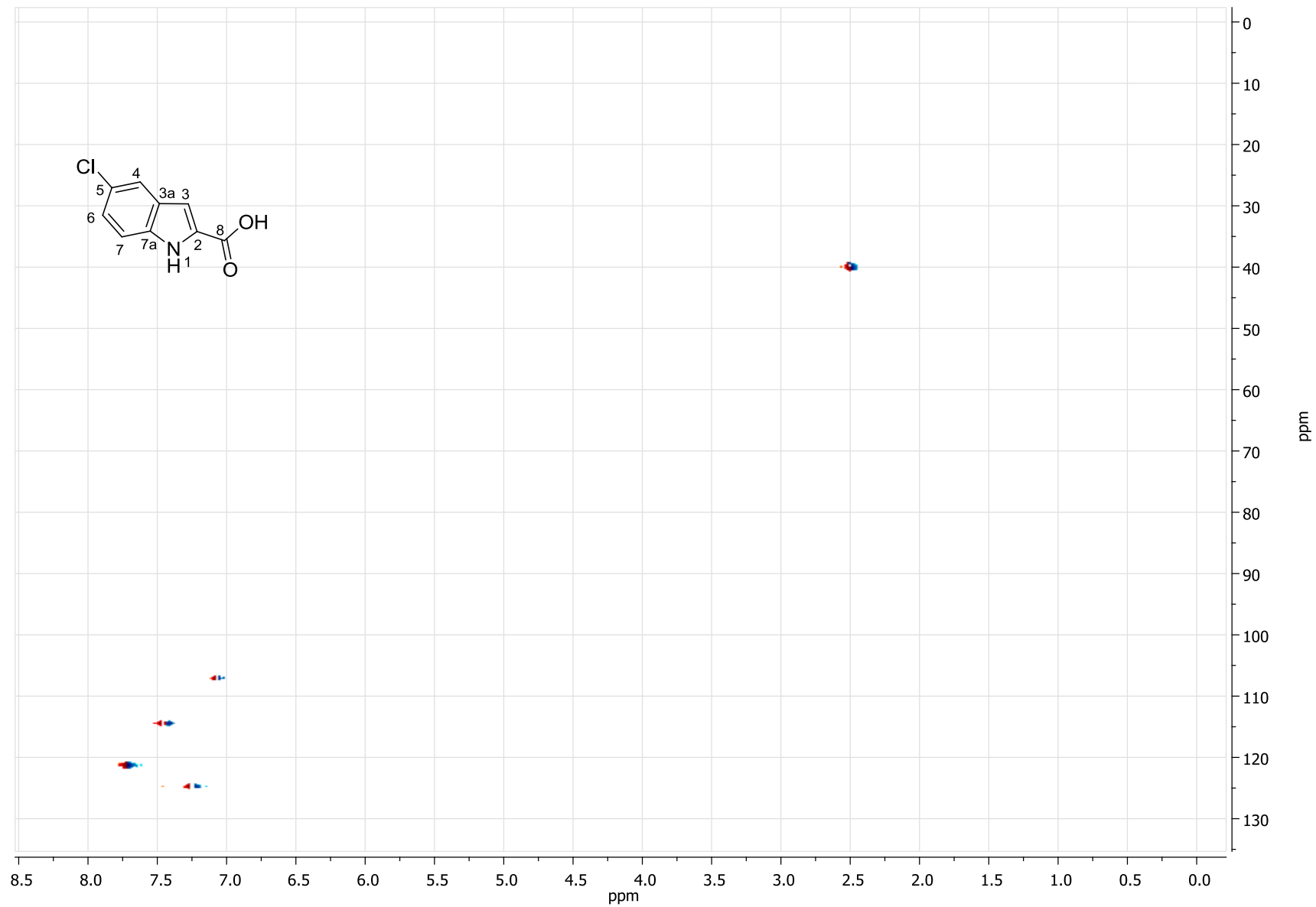
¹H NMR Spectrum
300 MHz Varian VNMRS



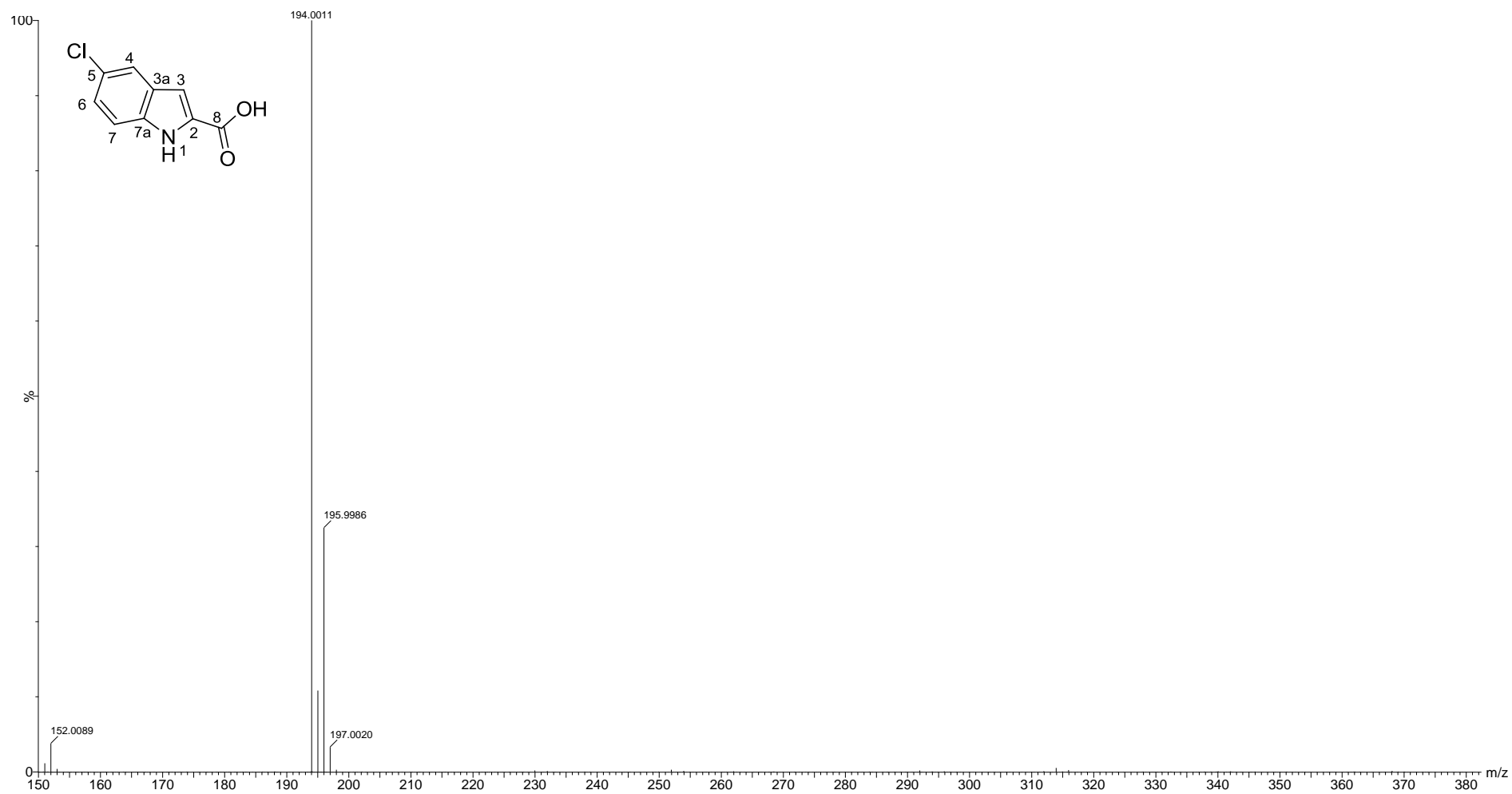
^{13}C NMR Spectrum
75 MHz Varian VNMRS



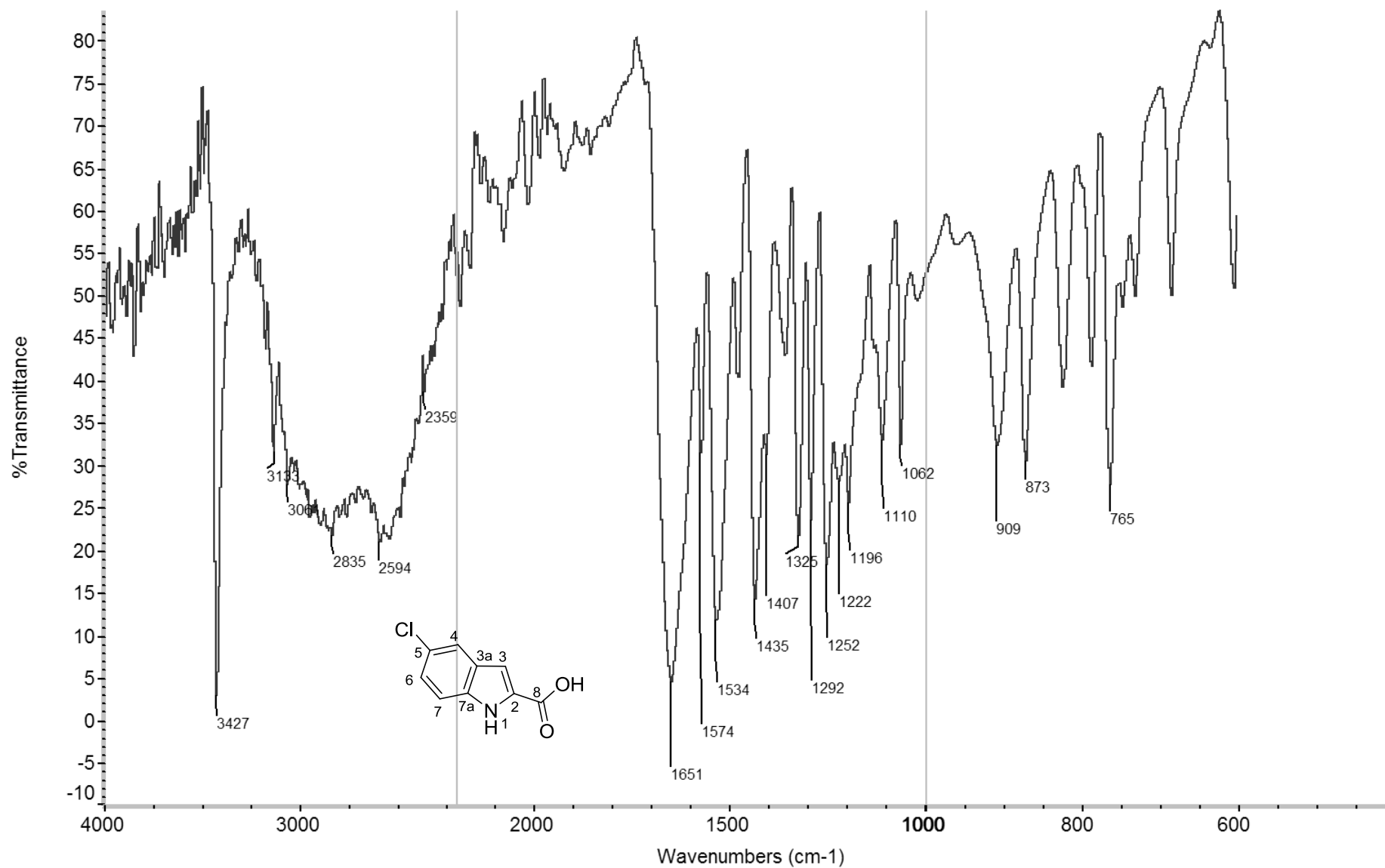
COSY NMR Spectrum
300 MHz Varian VNMRS



gHSQC NMR Spectrum
300 MHz Varian VNMRS

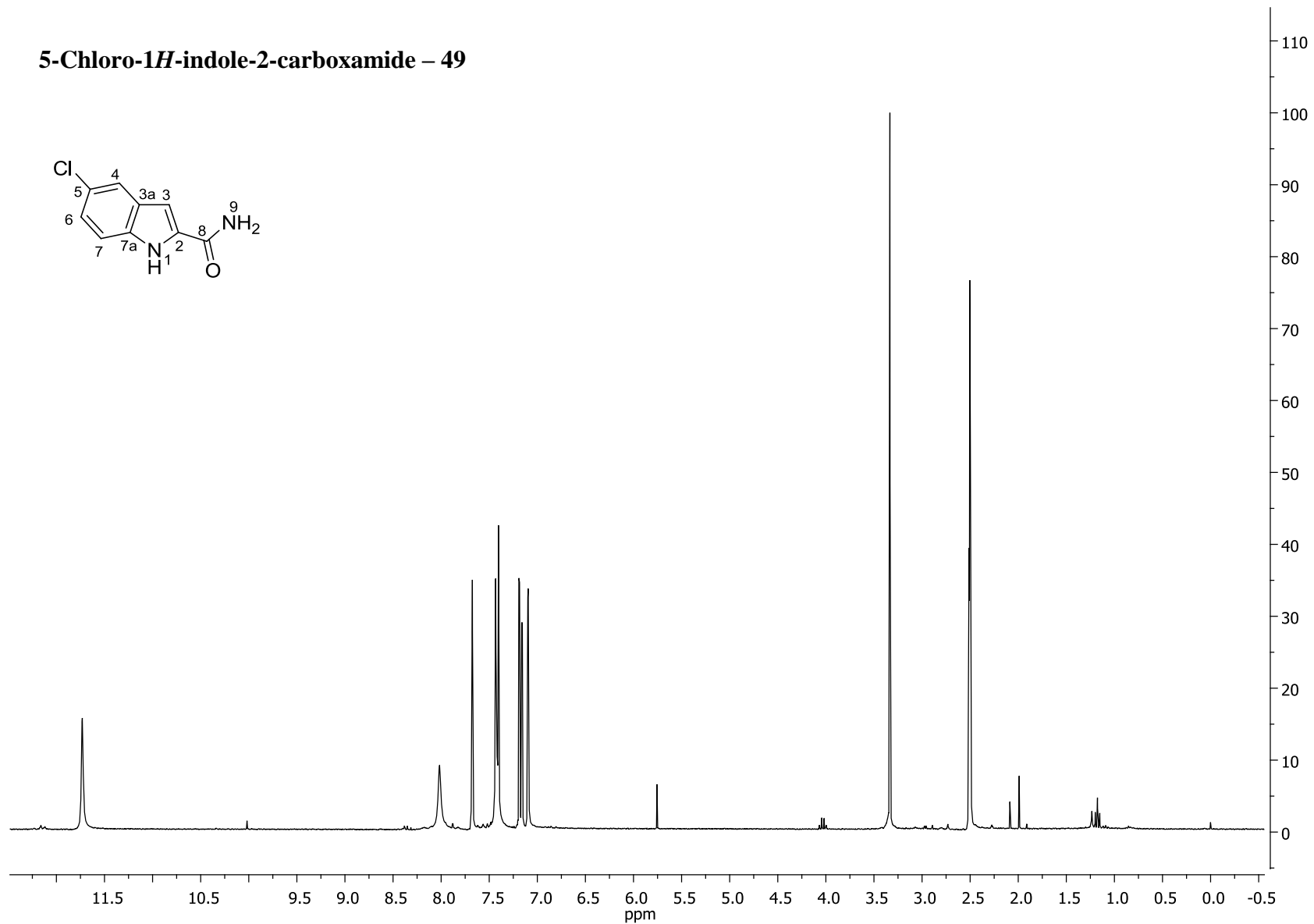
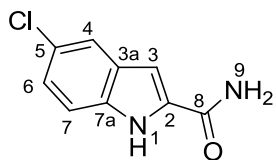


Mass Spectrum
Waters SYNAPT G2

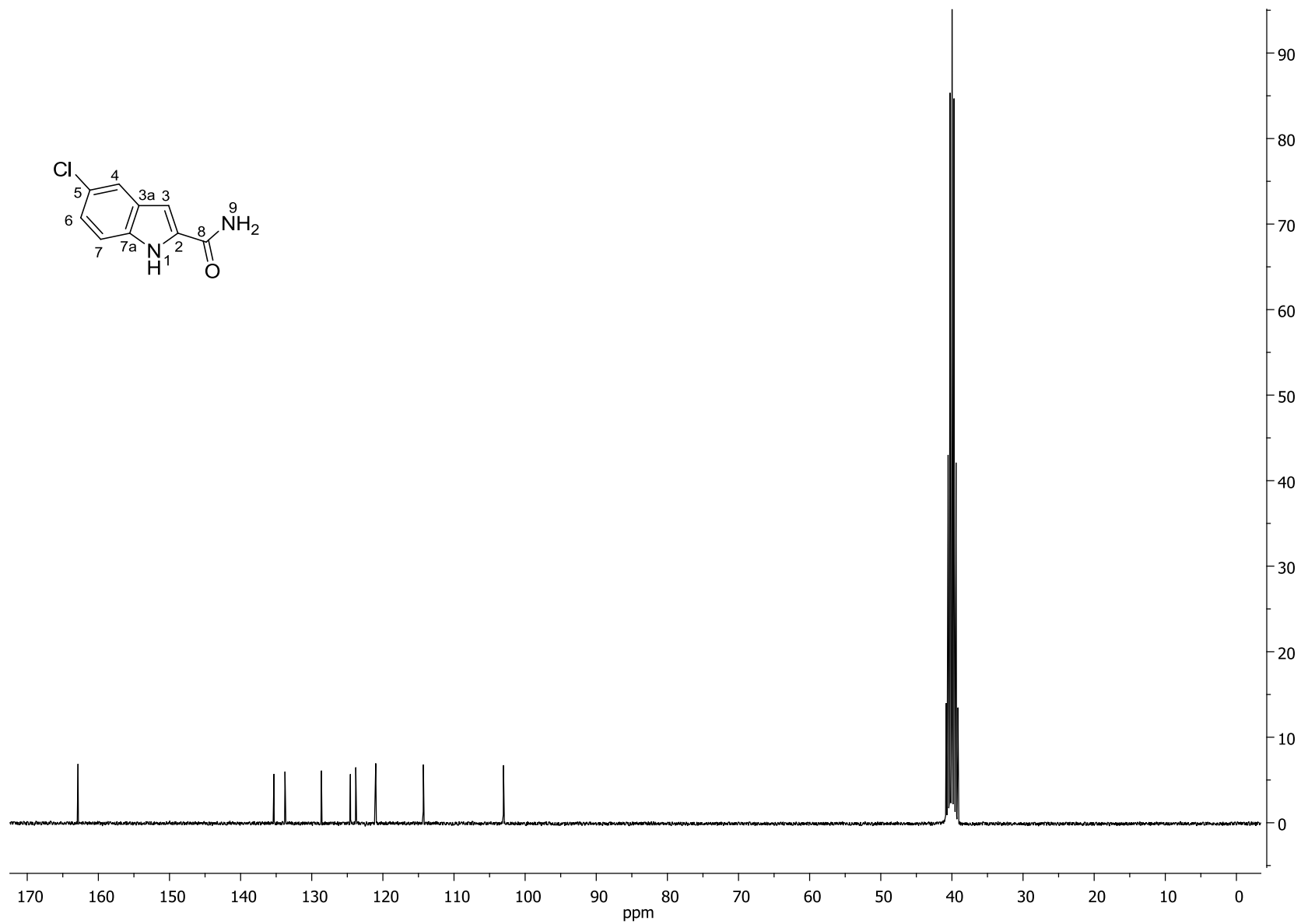


Infrared Spectrum
Thermo Nicolet Nexus 470

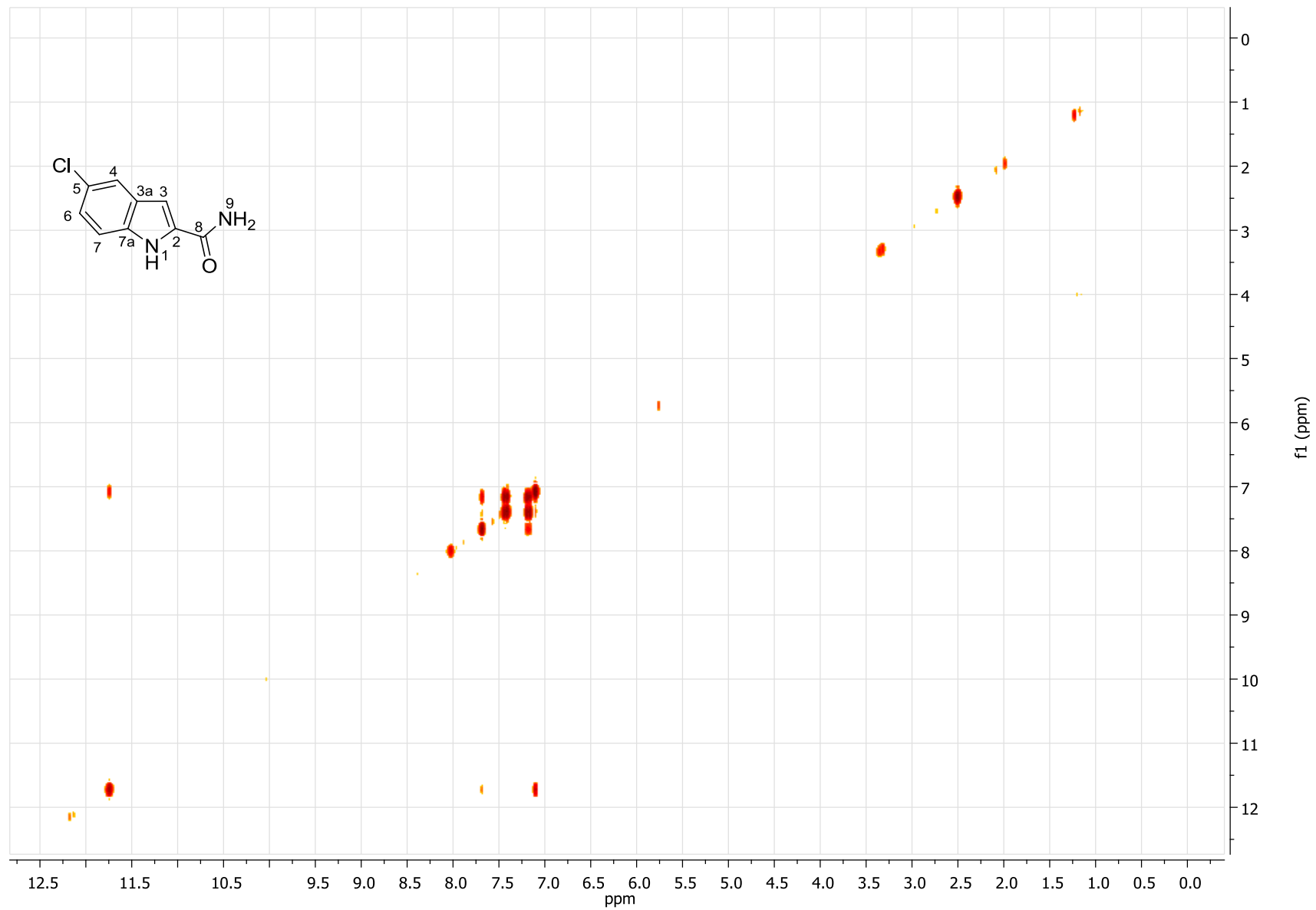
5-Chloro-1H-indole-2-carboxamide – 49



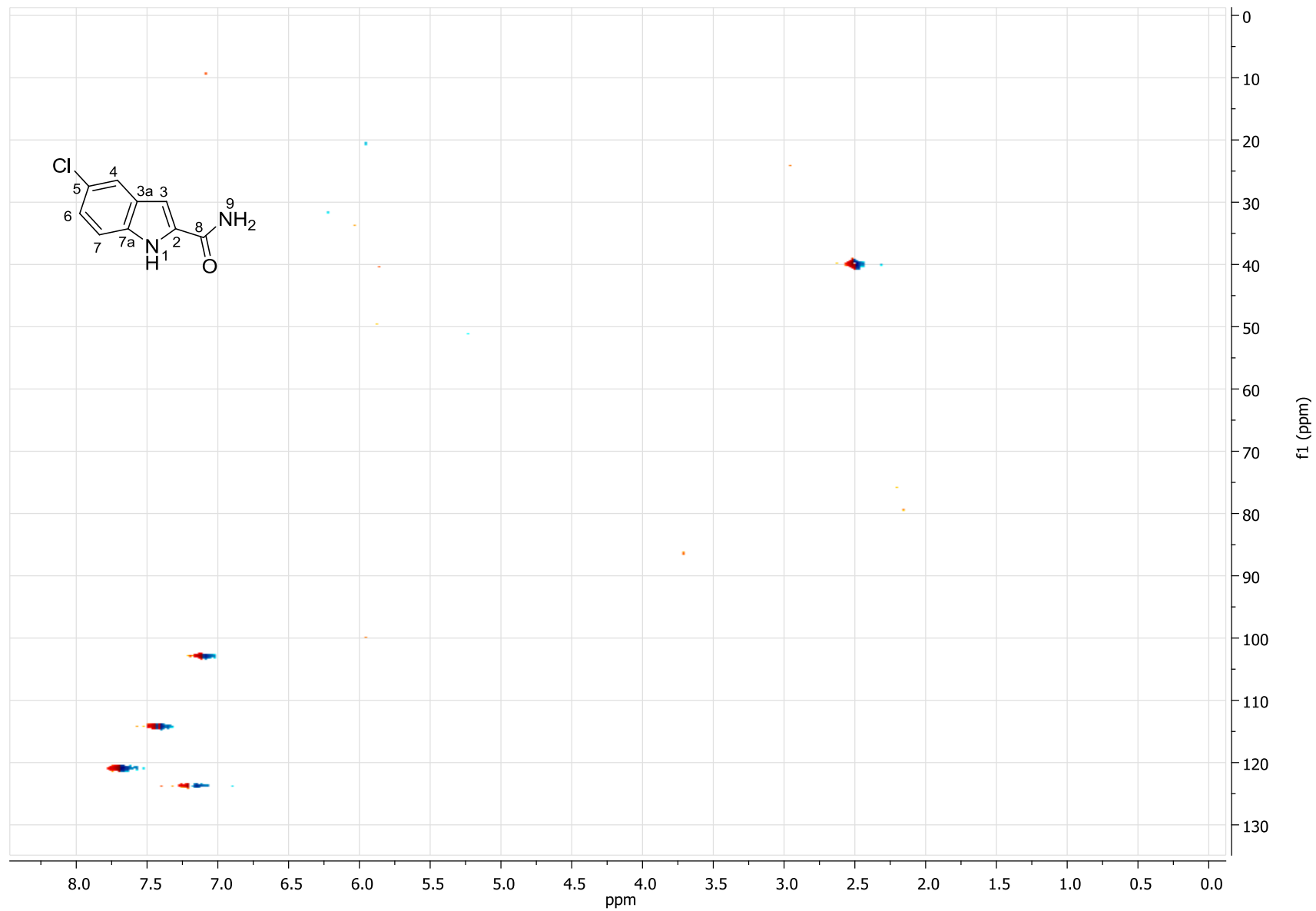
¹H NMR Spectrum
300 MHz Varian VNMRS



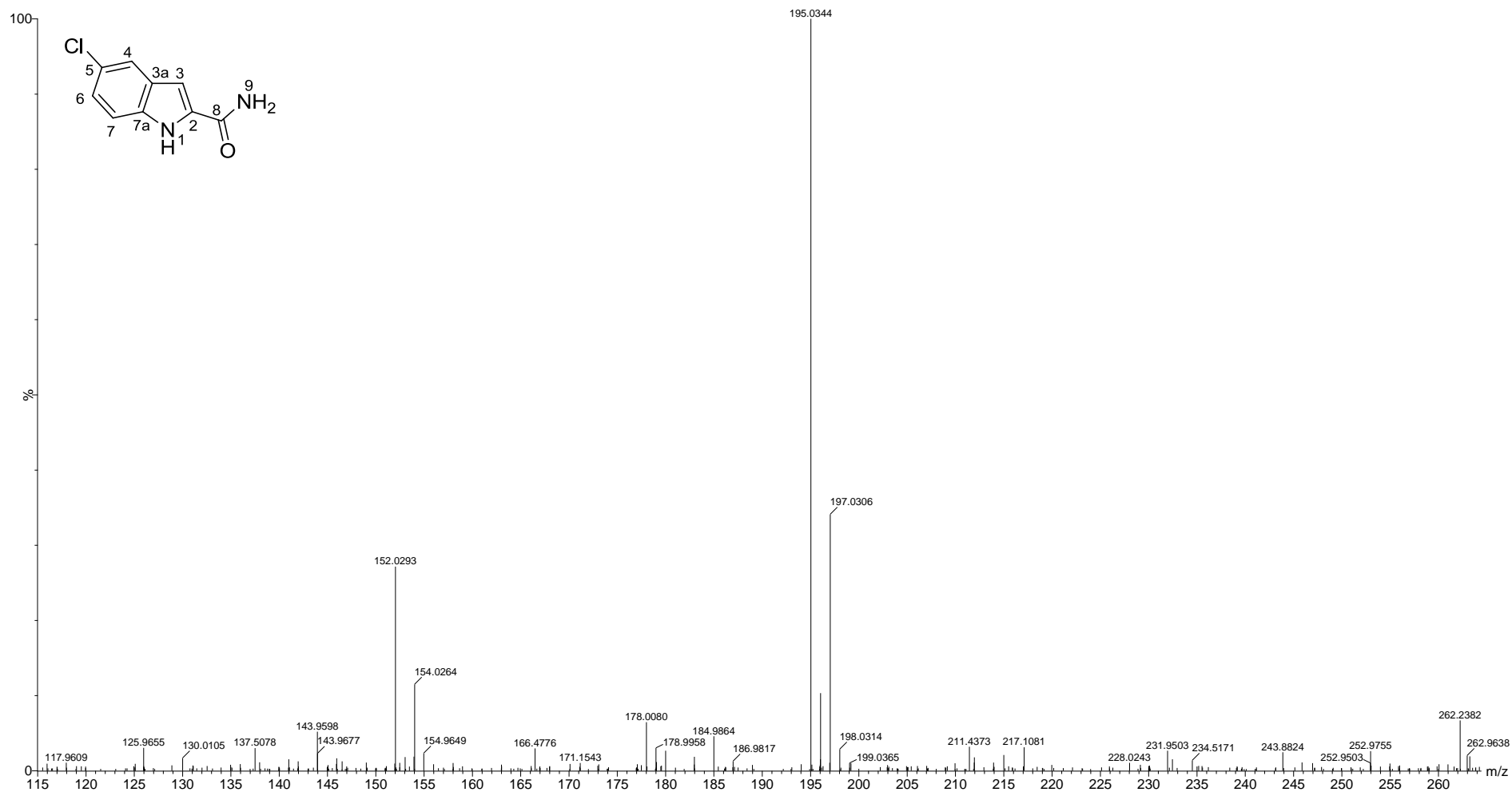
^{13}C NMR Spectrum
75 MHz Varian VNMRS



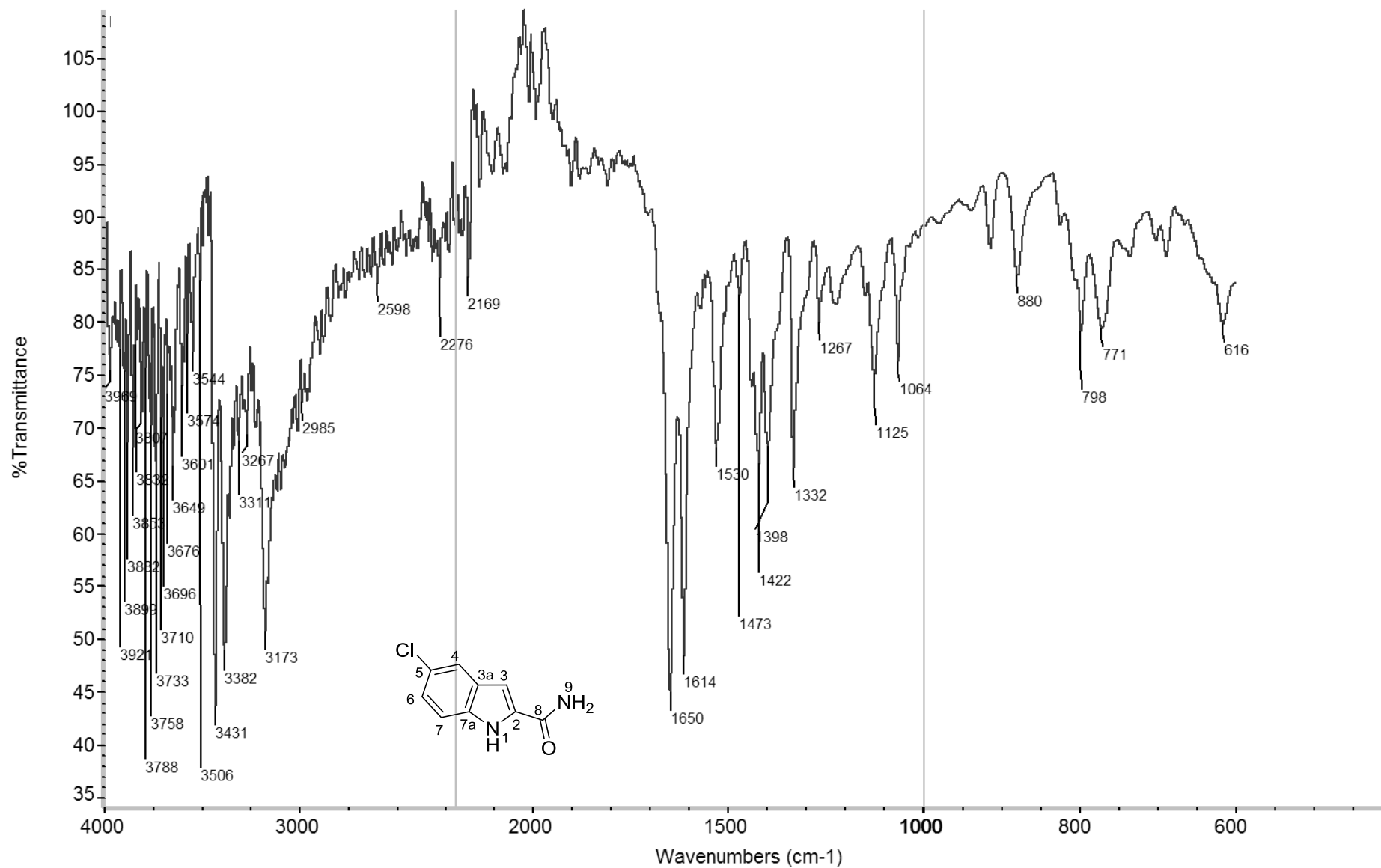
COSY NMR Spectrum
300 MHz Varian VNMRS



gHSQC NMR Spectrum
300 MHz Varian VNMRS

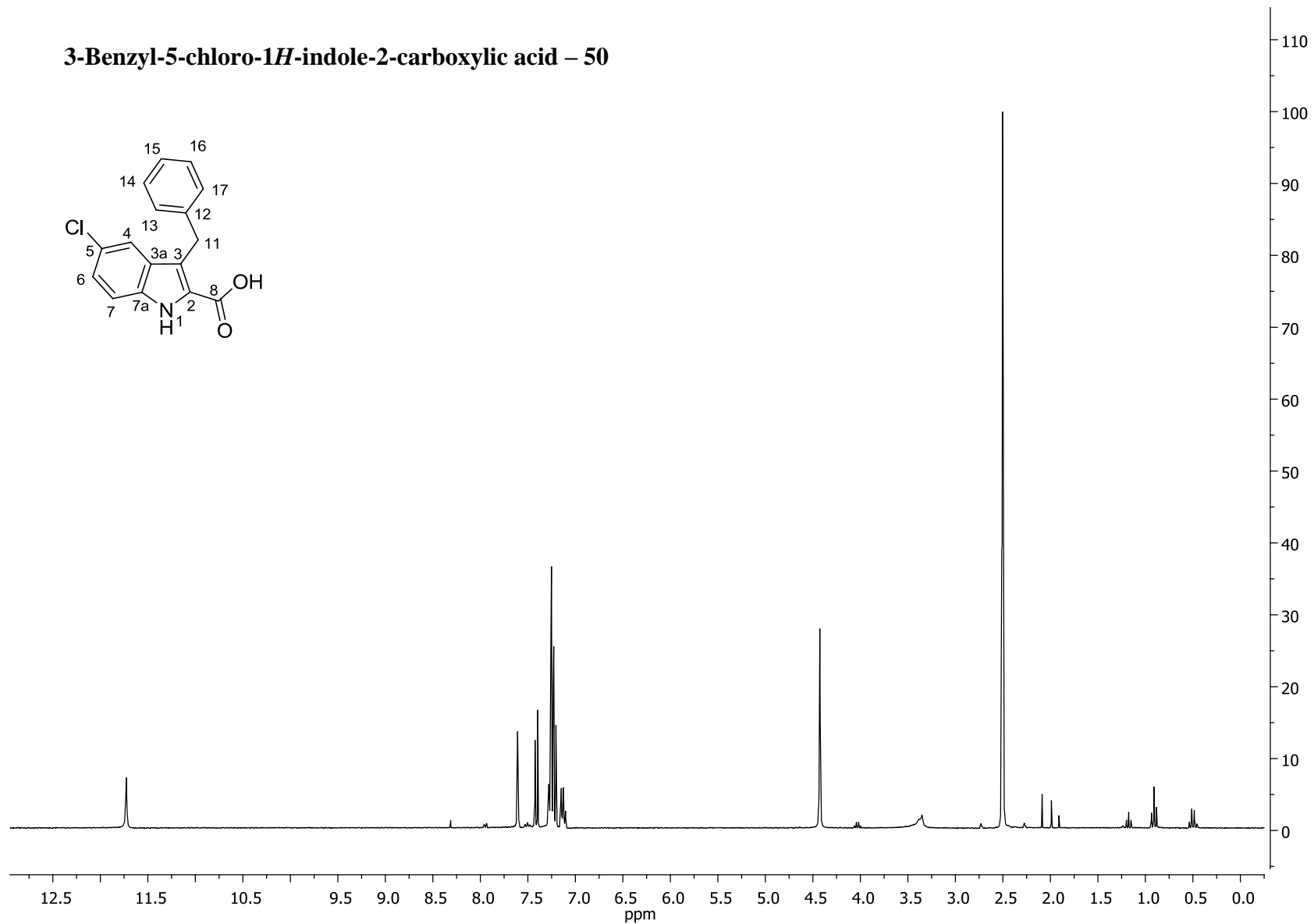


Mass Spectrum
Waters SYNAPT G2

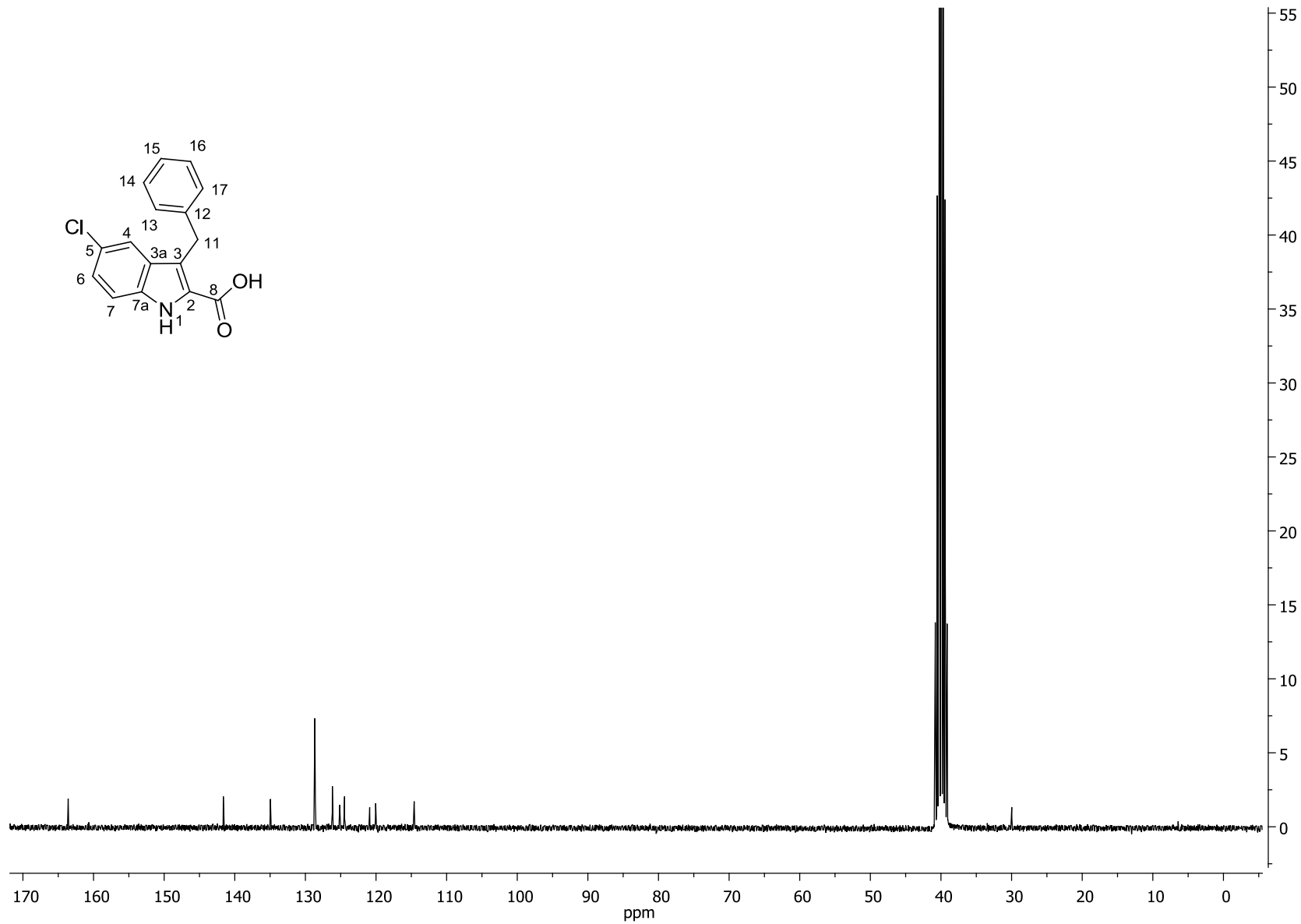


Infrared Spectrum
Thermo Nicolet Nexus 470

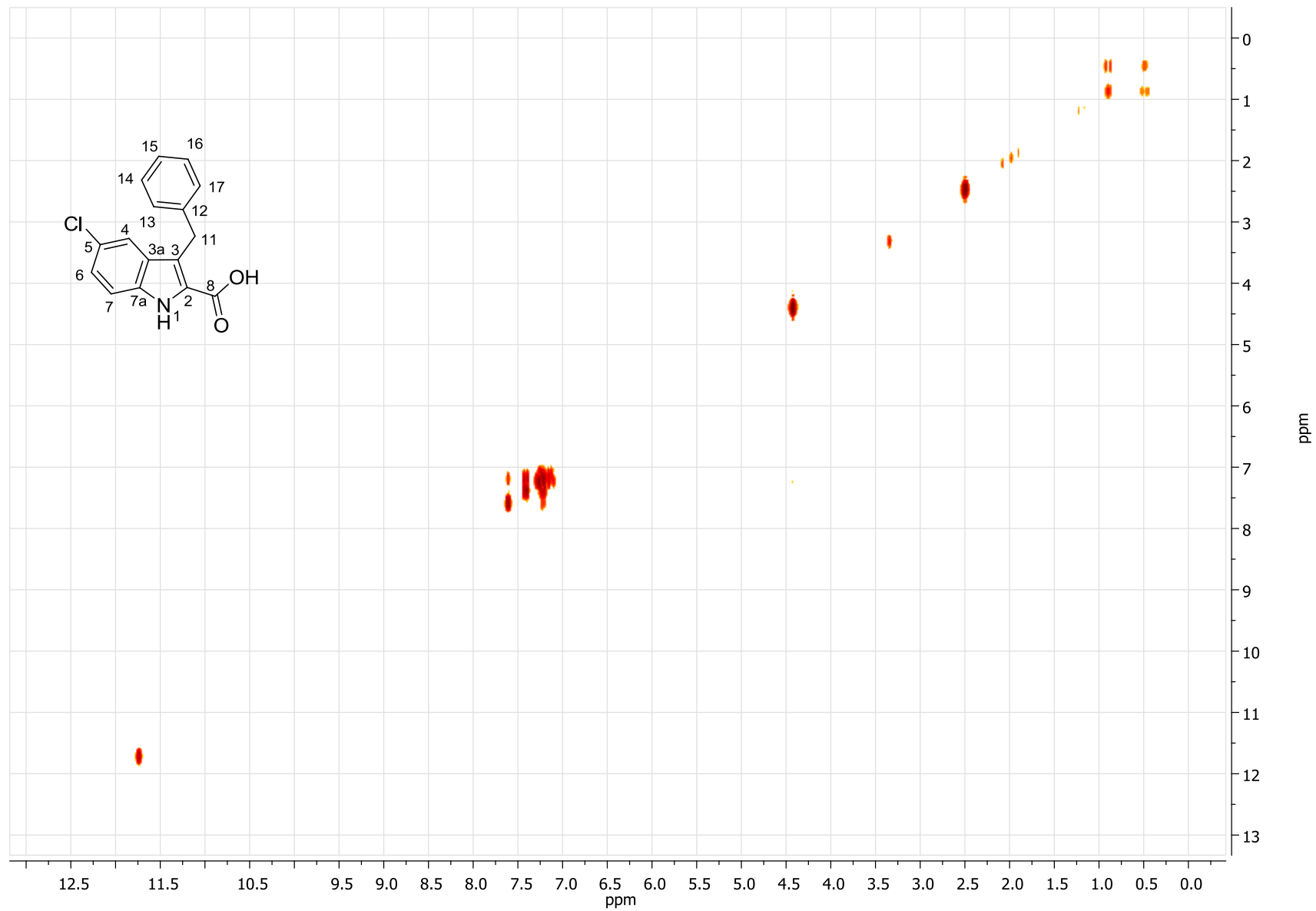
3-Benzyl-5-chloro-1H-indole-2-carboxylic acid – 50

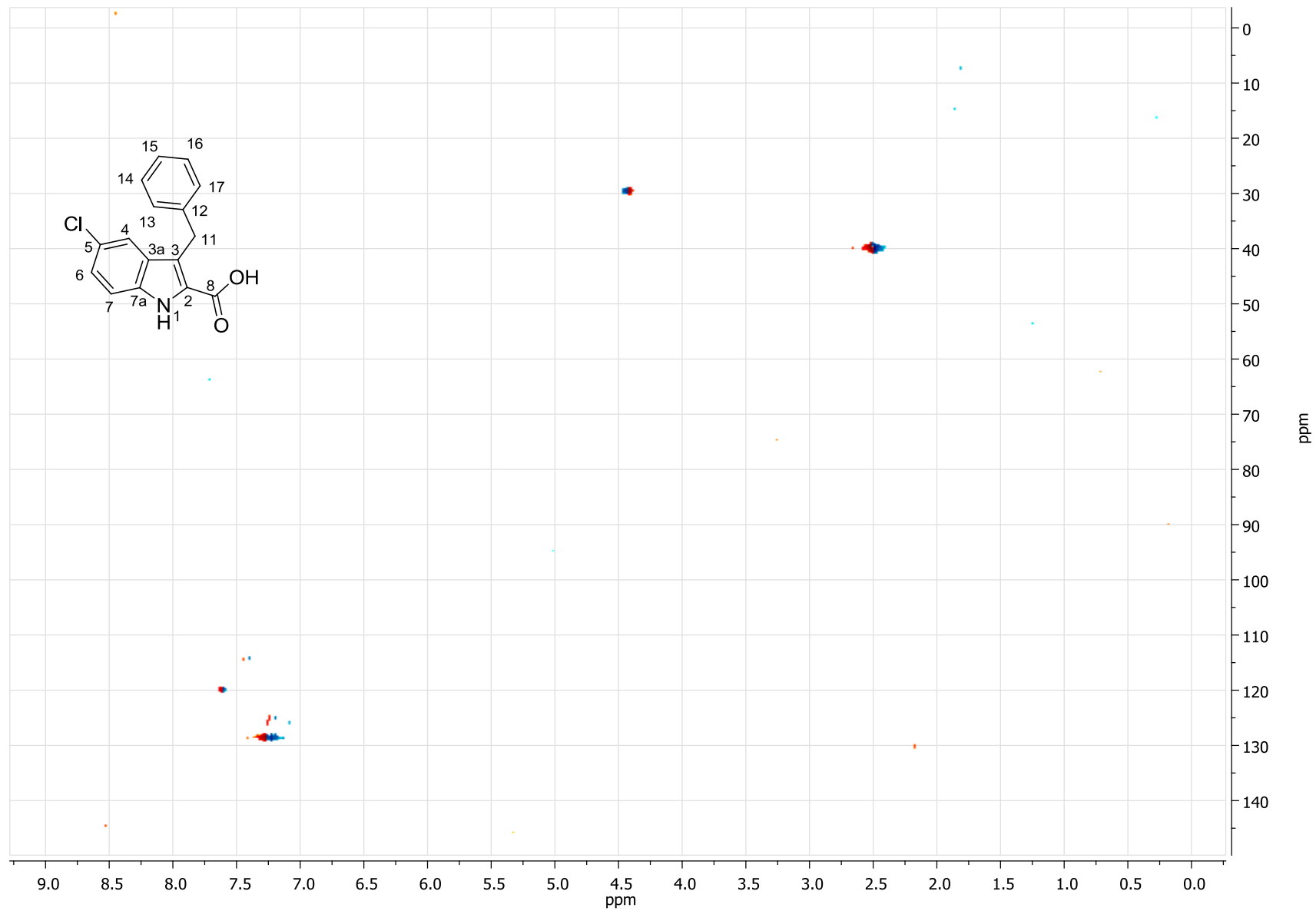


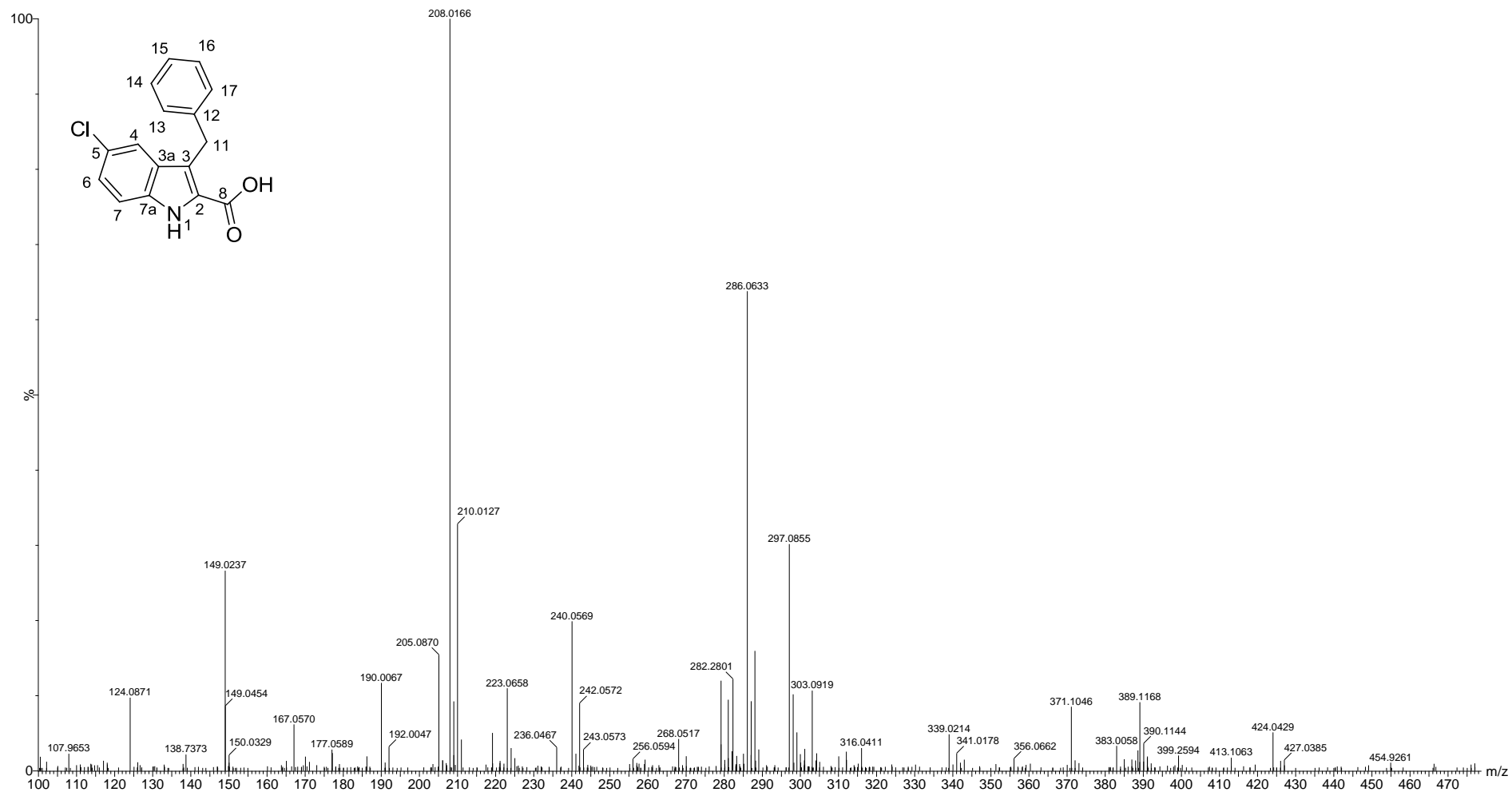
¹H NMR Spectrum
300 MHz Varian VNMRS



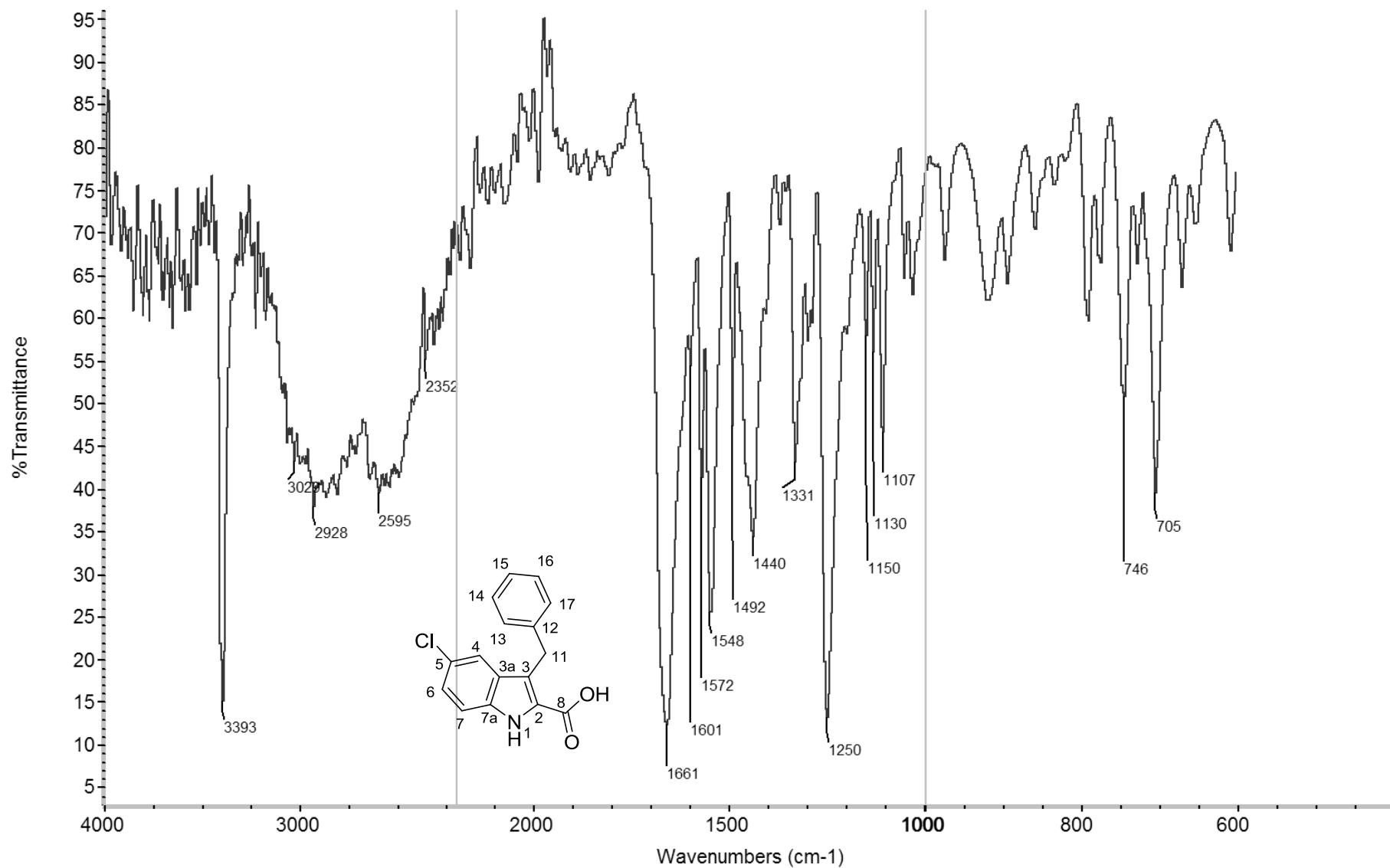
^{13}C NMR Spectrum
75 MHz Varian VNMRS





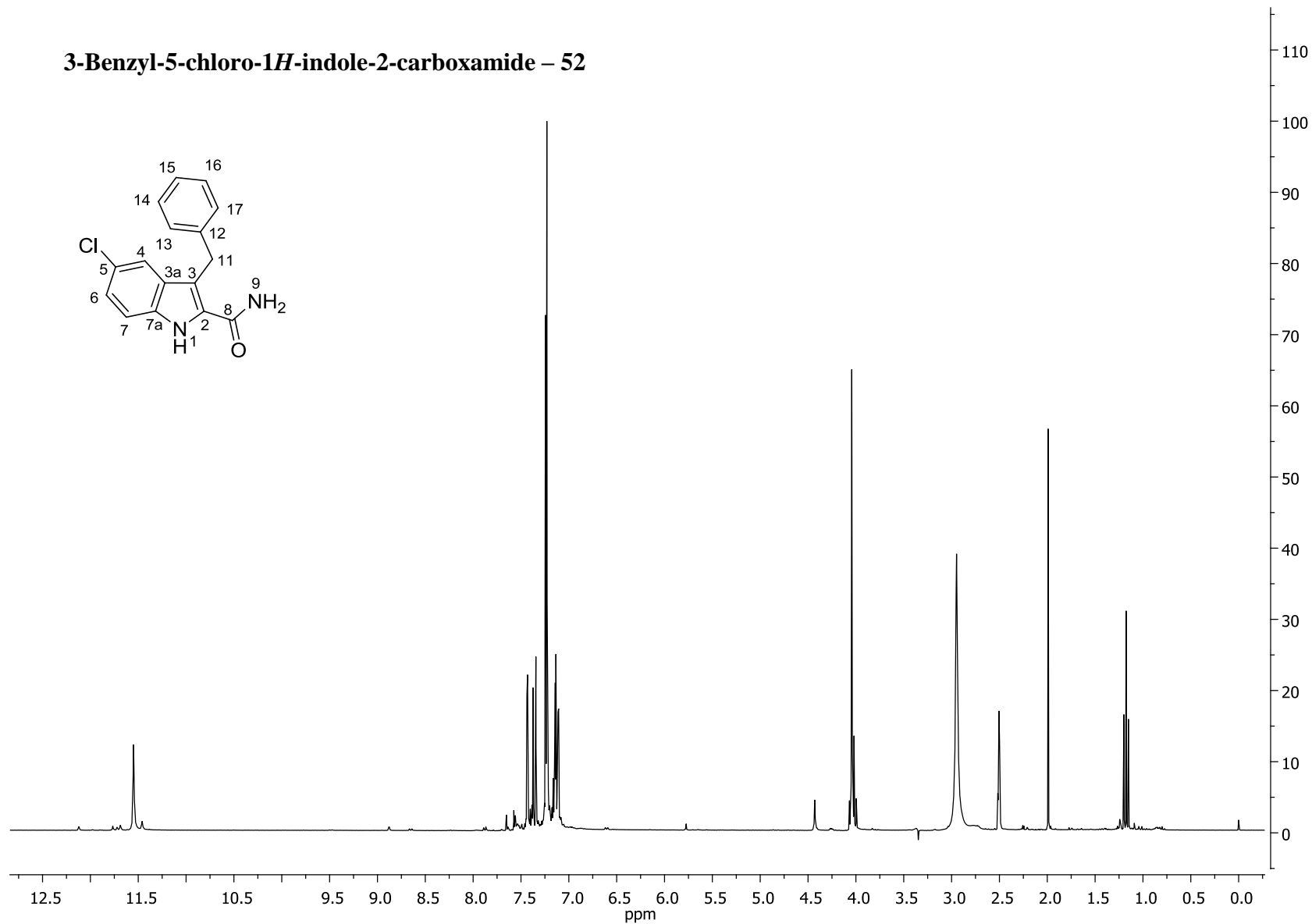
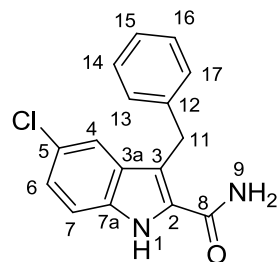


Mass Spectrum
Waters SYNAPT G2

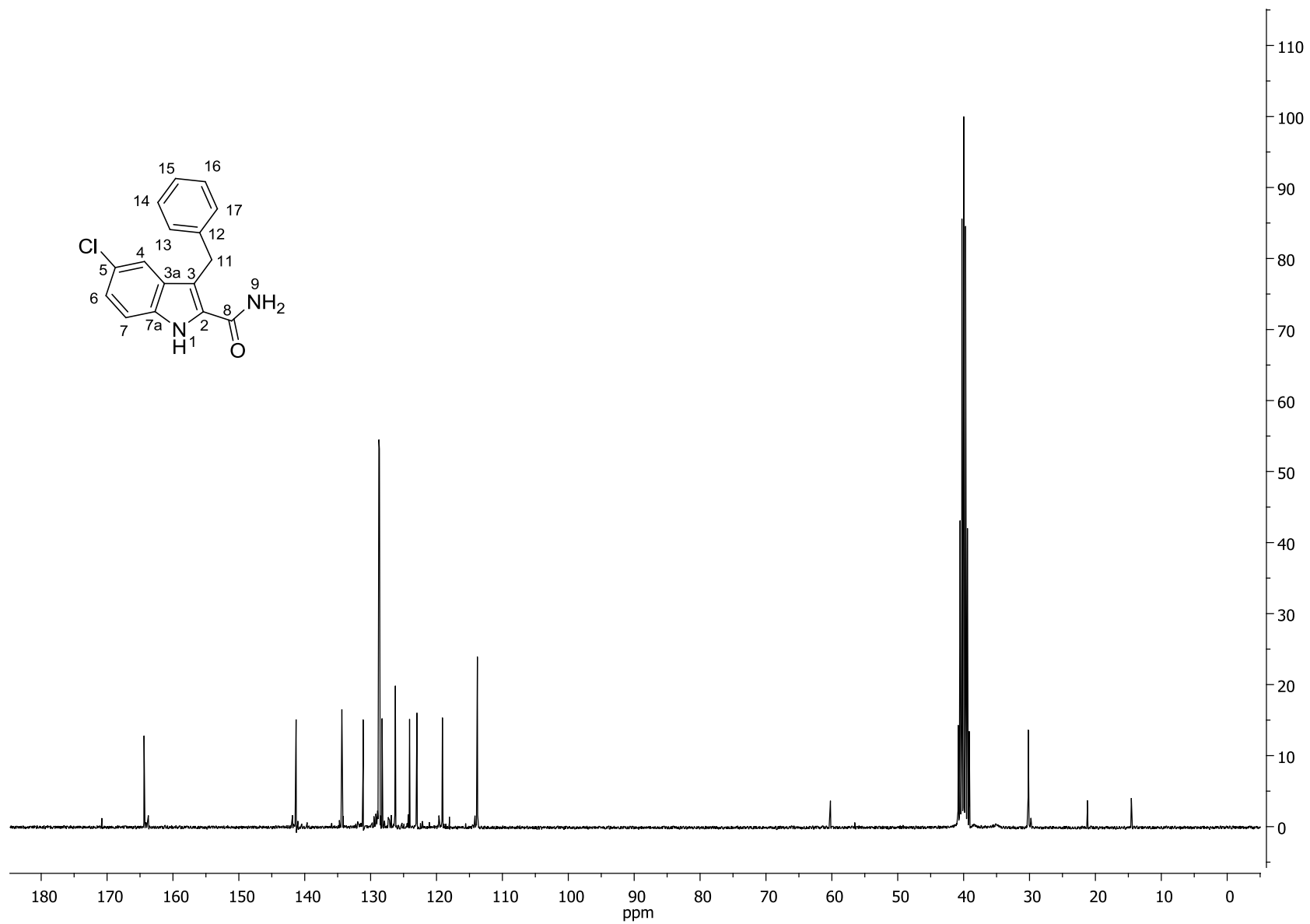


Infrared Spectrum
Thermo Nicolet Nexus 470

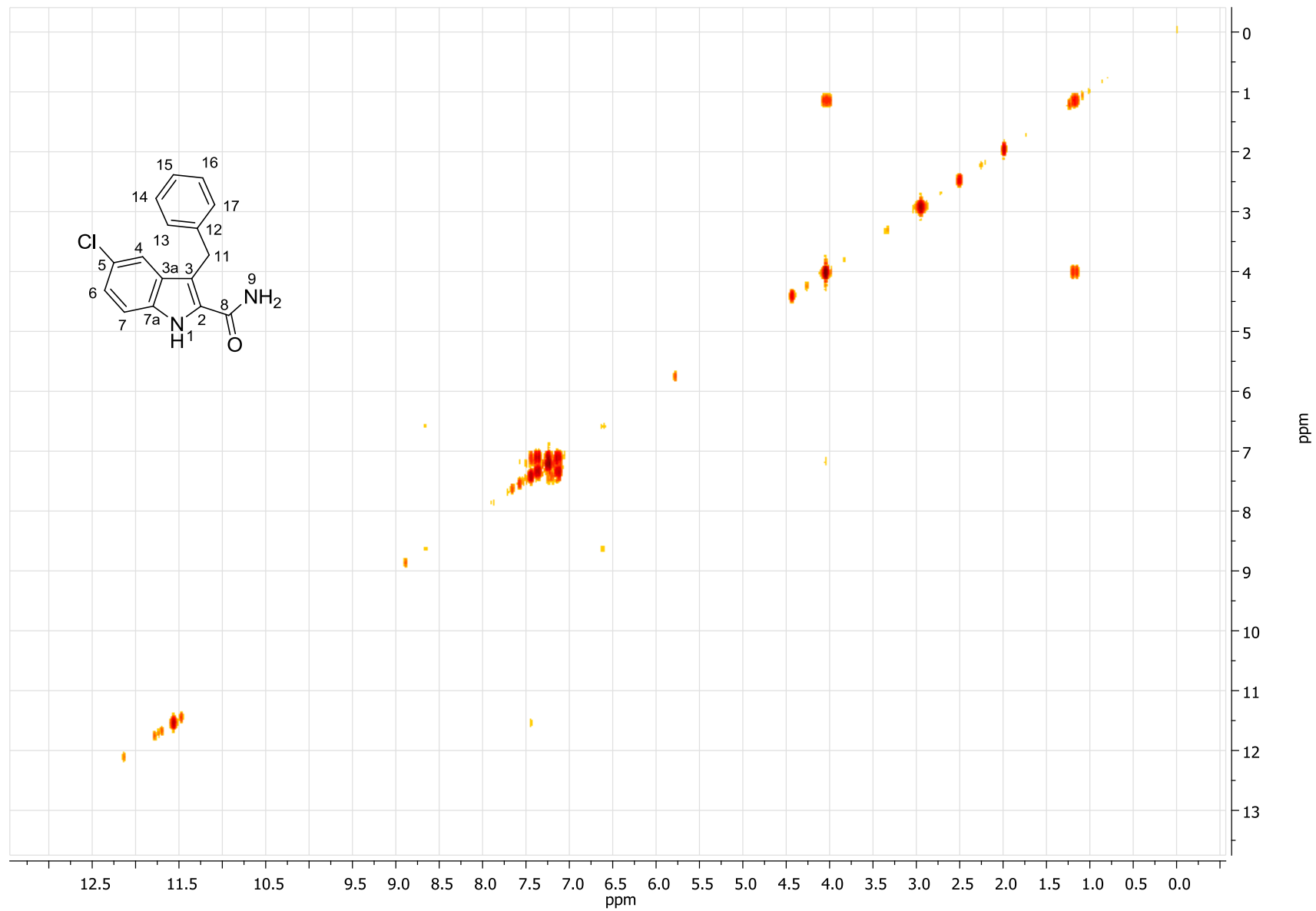
3-Benzyl-5-chloro-1*H*-indole-2-carboxamide – 52



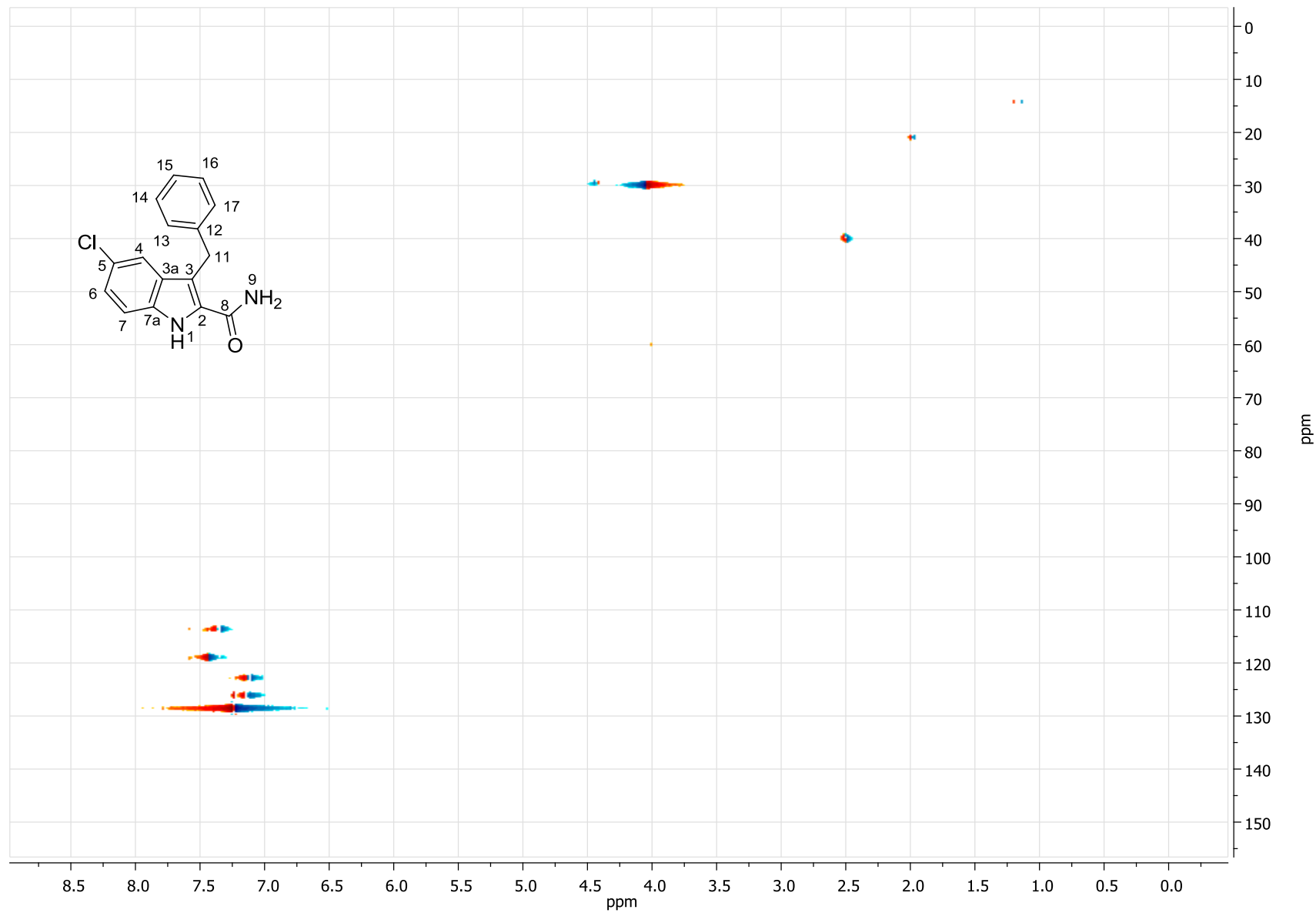
¹H NMR Spectrum
300 MHz Varian VNMRS



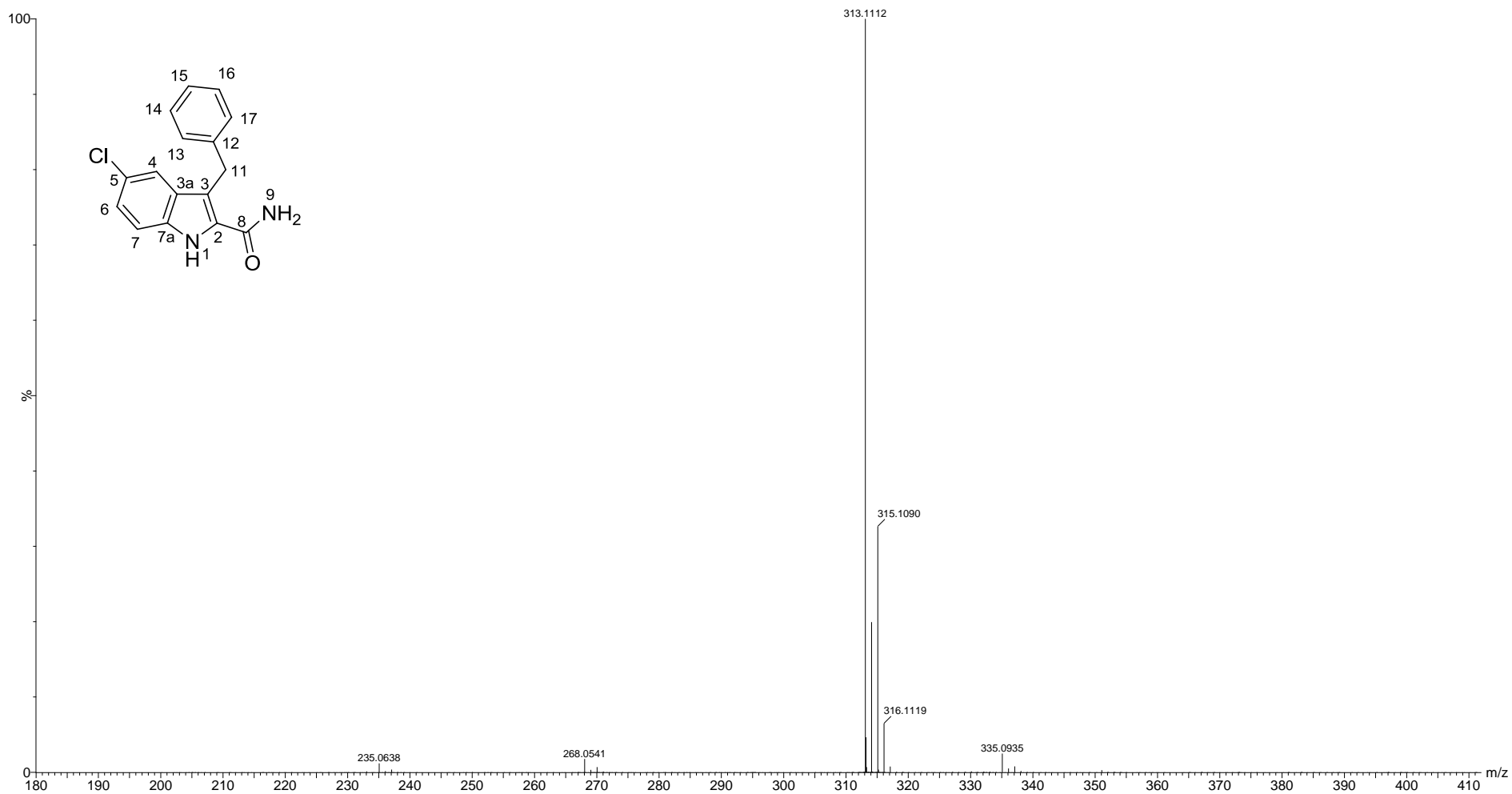
^{13}C NMR Spectrum
75 MHz Varian VNMRS



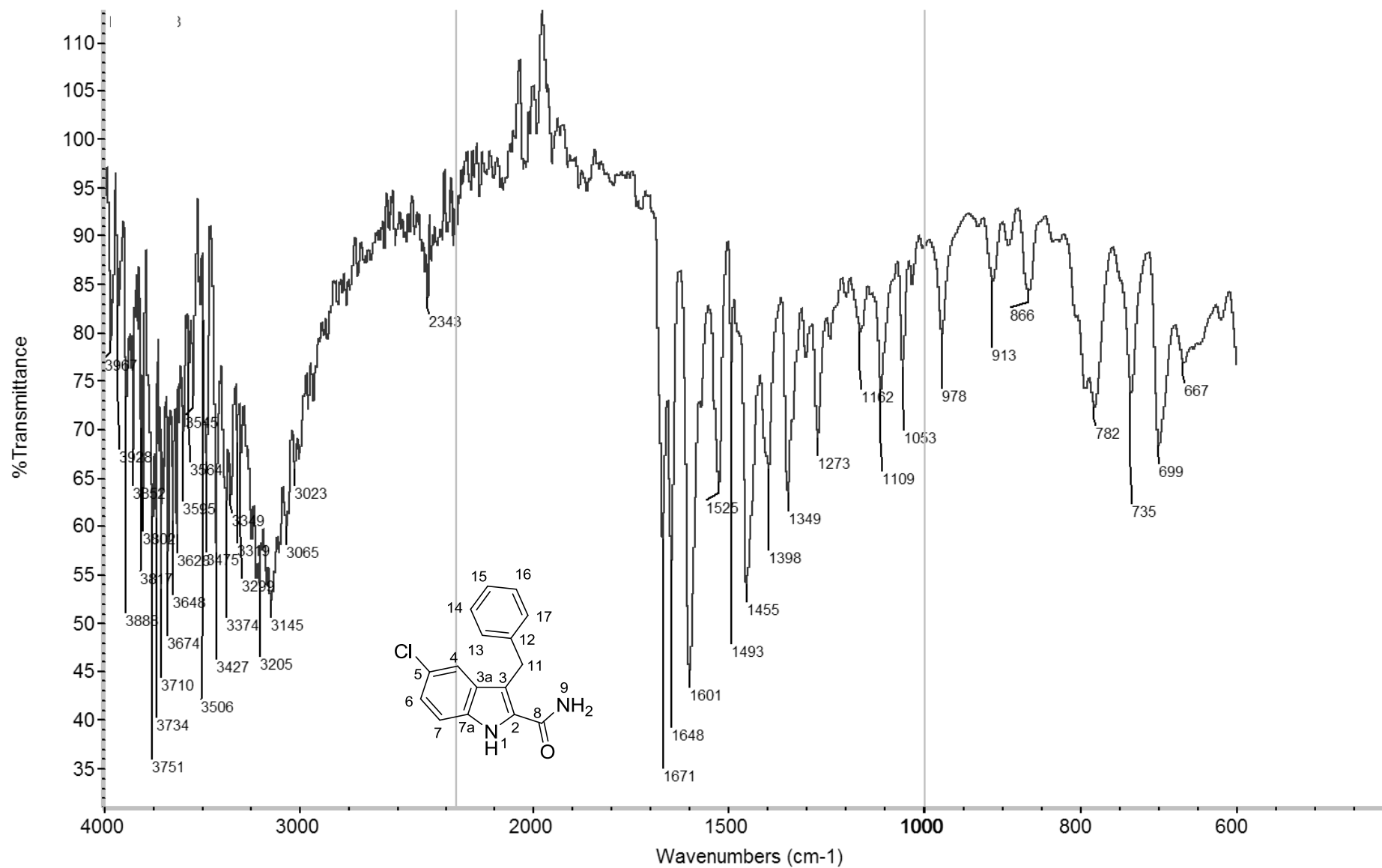
COSY NMR Spectrum
300 MHz Varian VNMRS



gHSQC NMR Spectrum
300 MHz Varian VNMRS

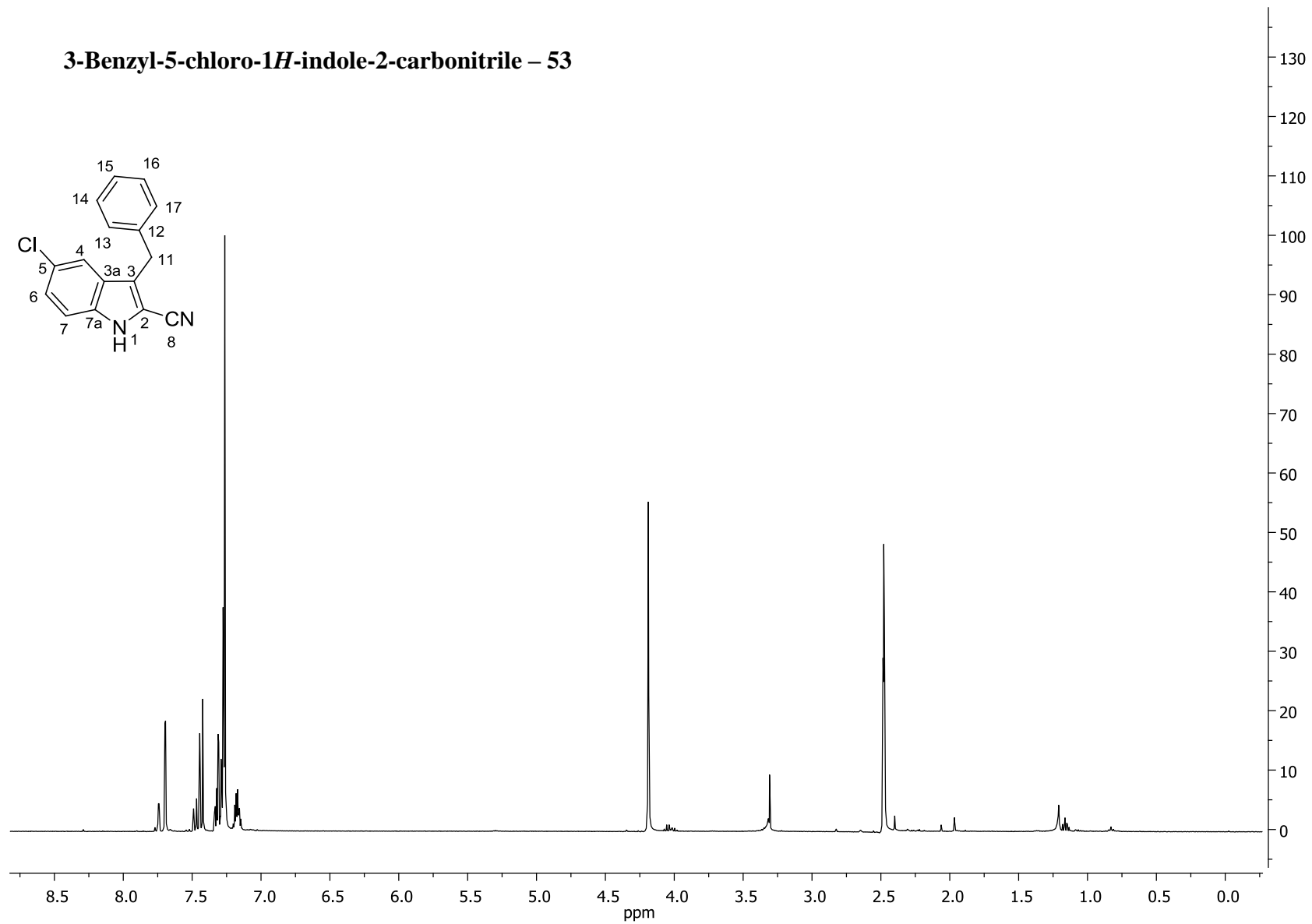
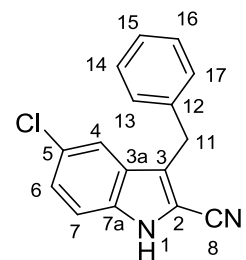


Mass Spectrum
Waters SYNAPT G2

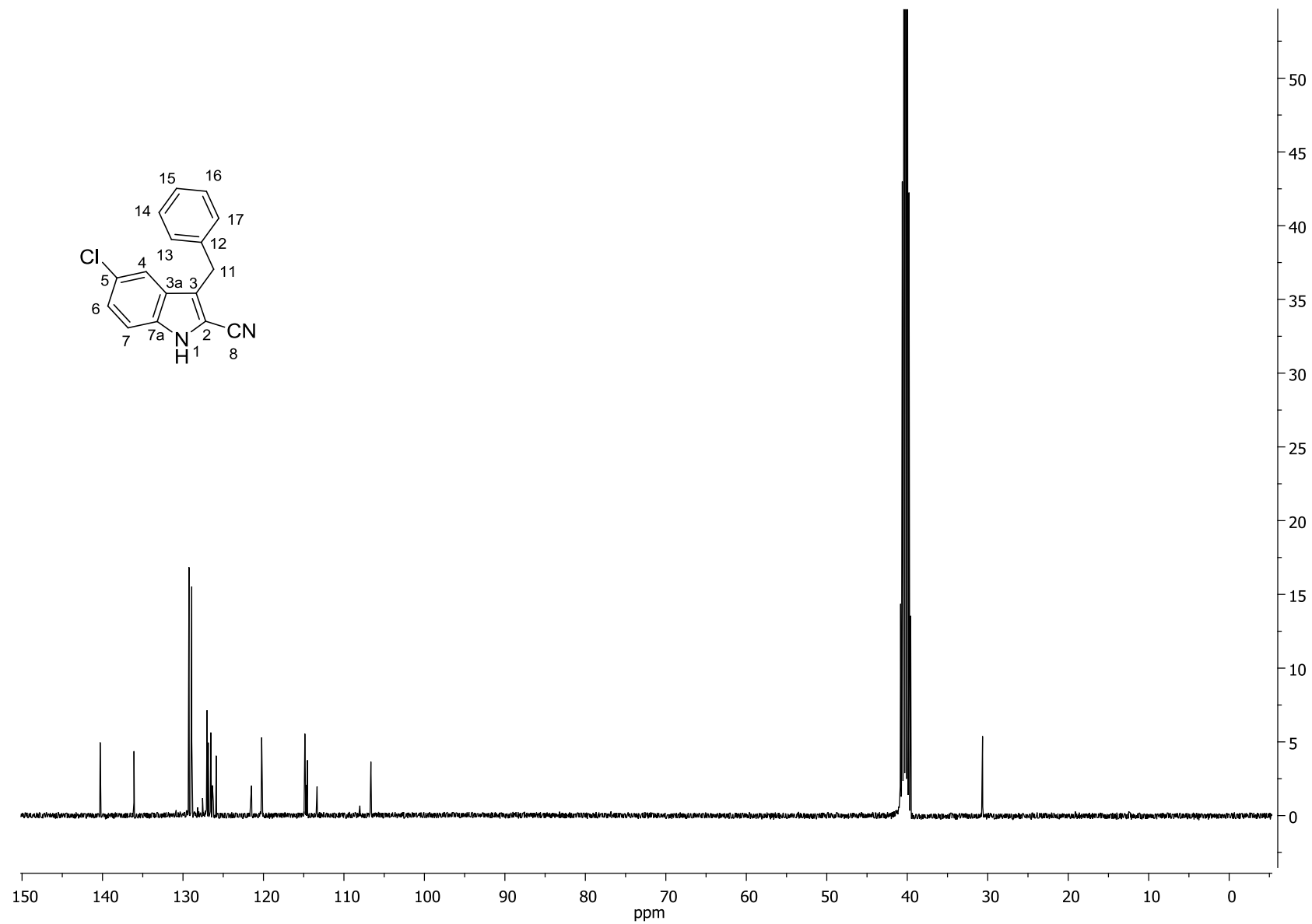


Infrared Spectrum
Thermo Nicolet Nexus 470

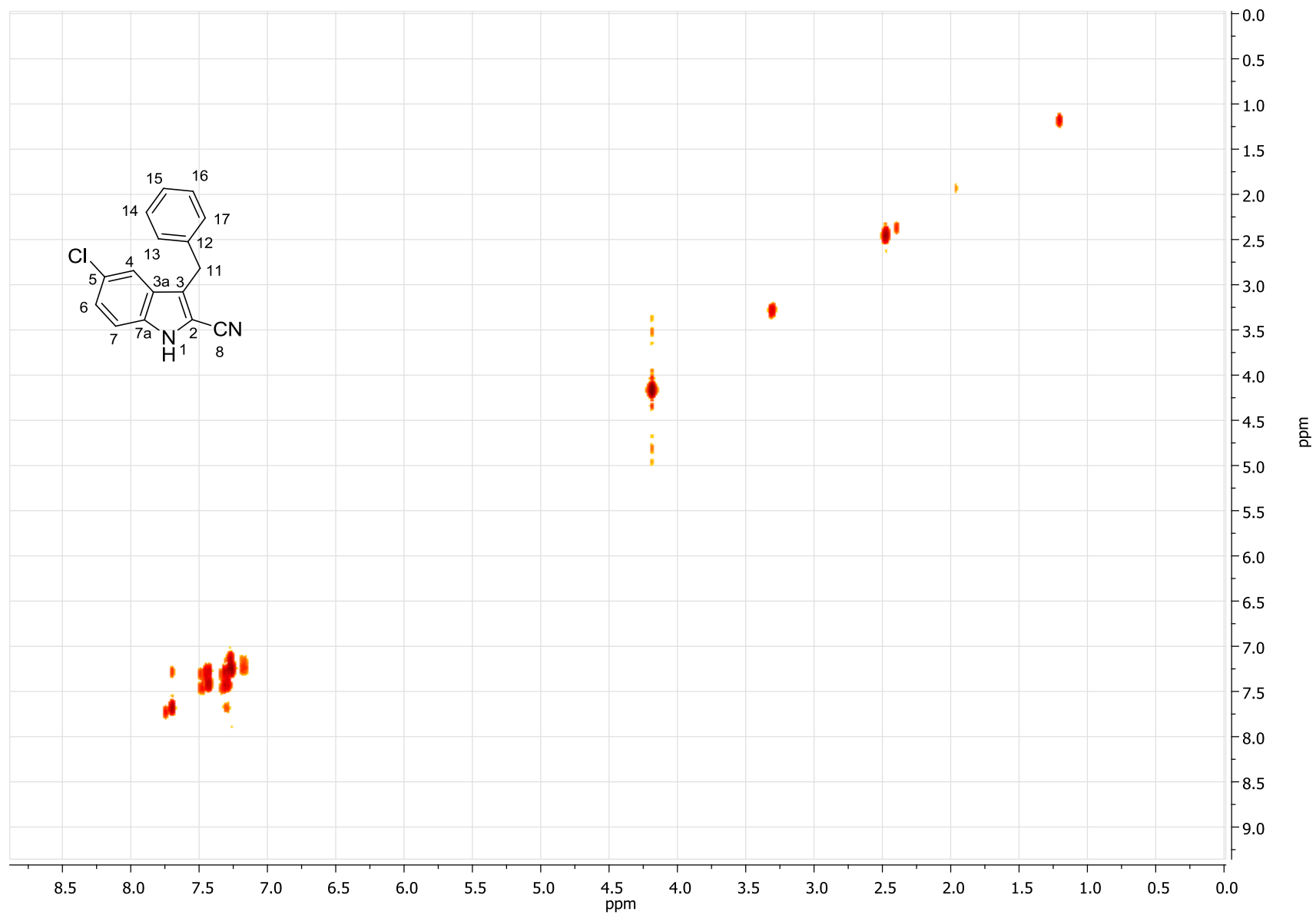
3-Benzyl-5-chloro-1H-indole-2-carbonitrile – 53



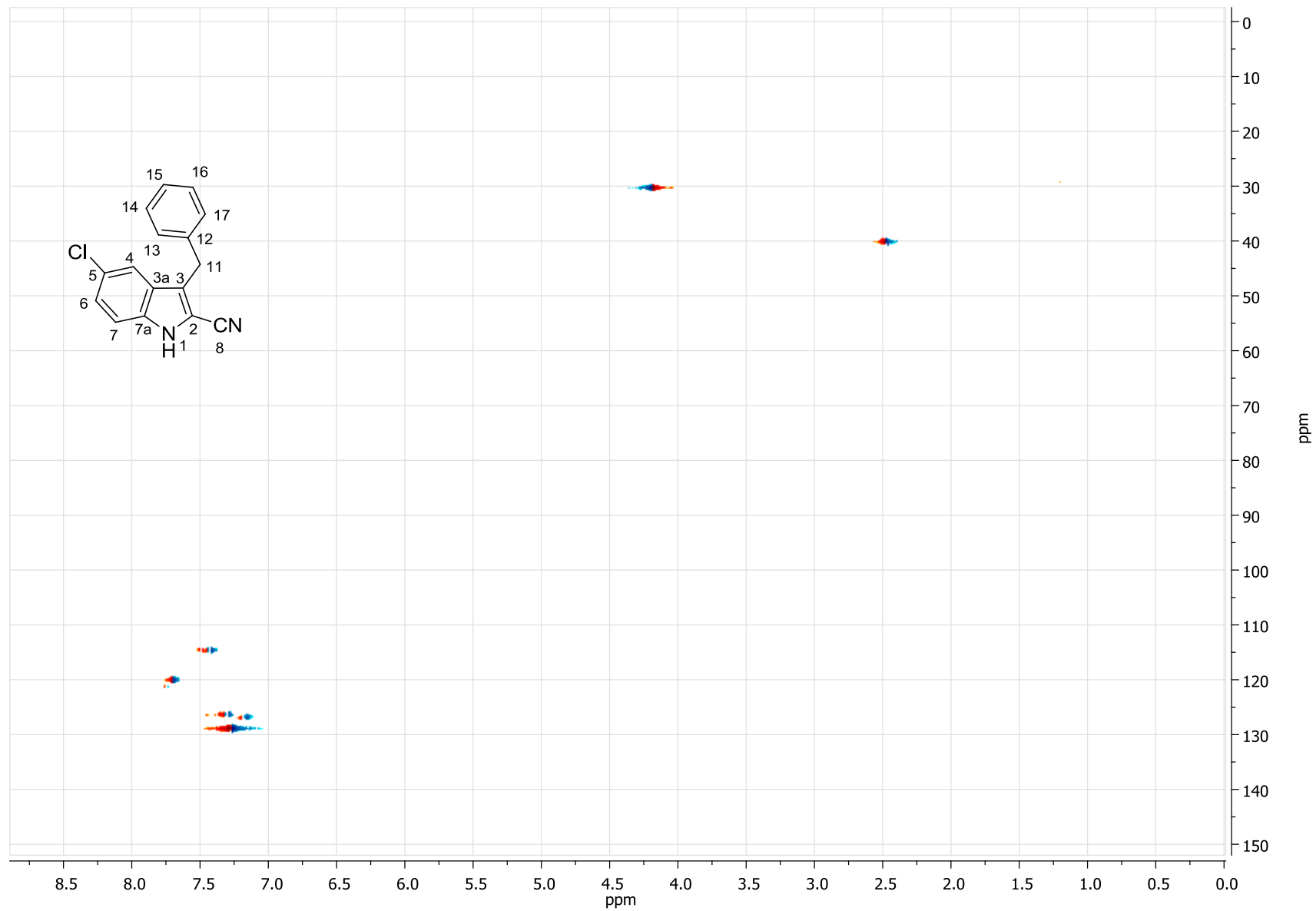
¹H NMR Spectrum
400 MHz Varian Unity Inova



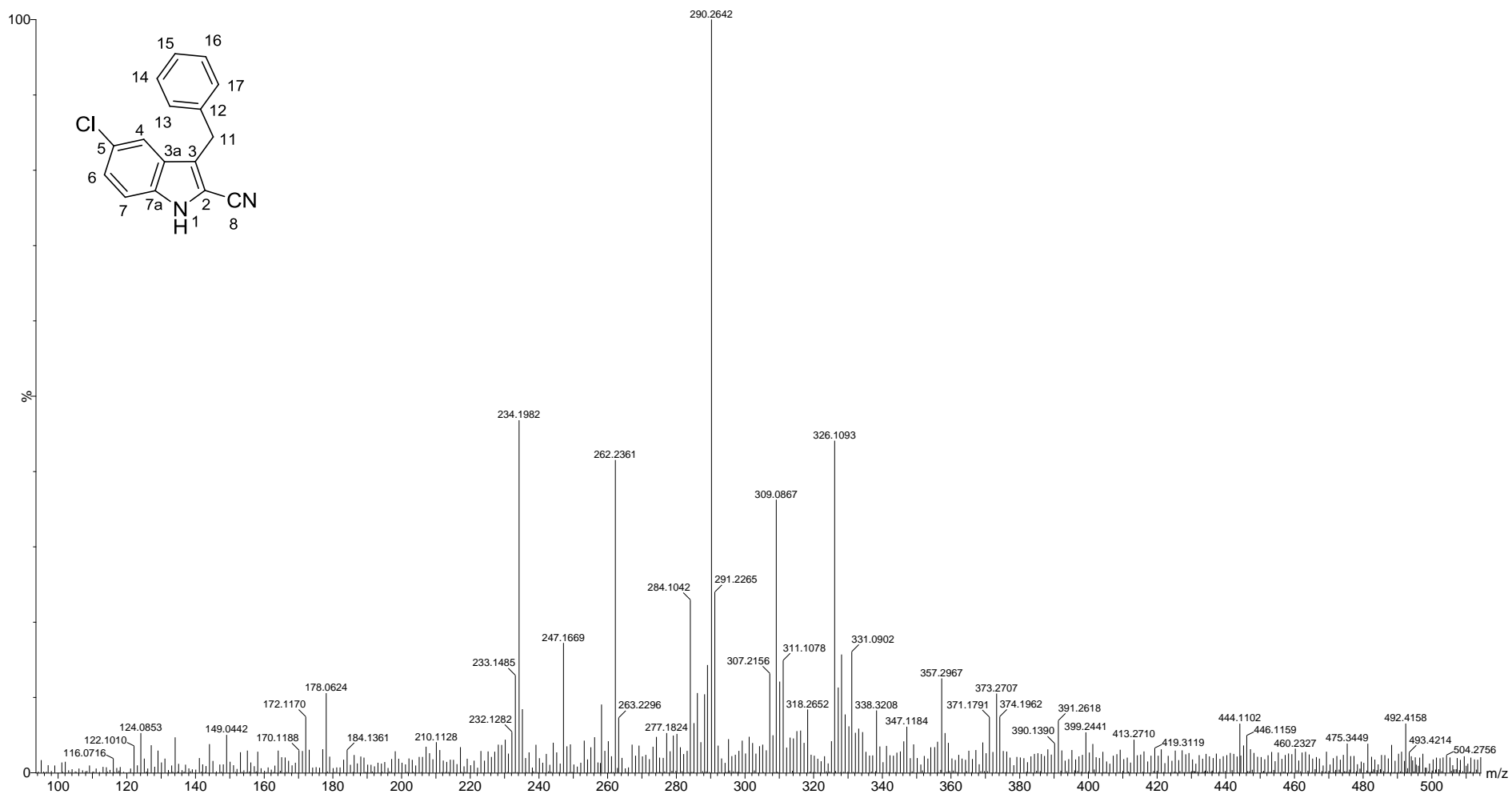
^{13}C NMR Spectrum
101 MHz Varian Unity Inova



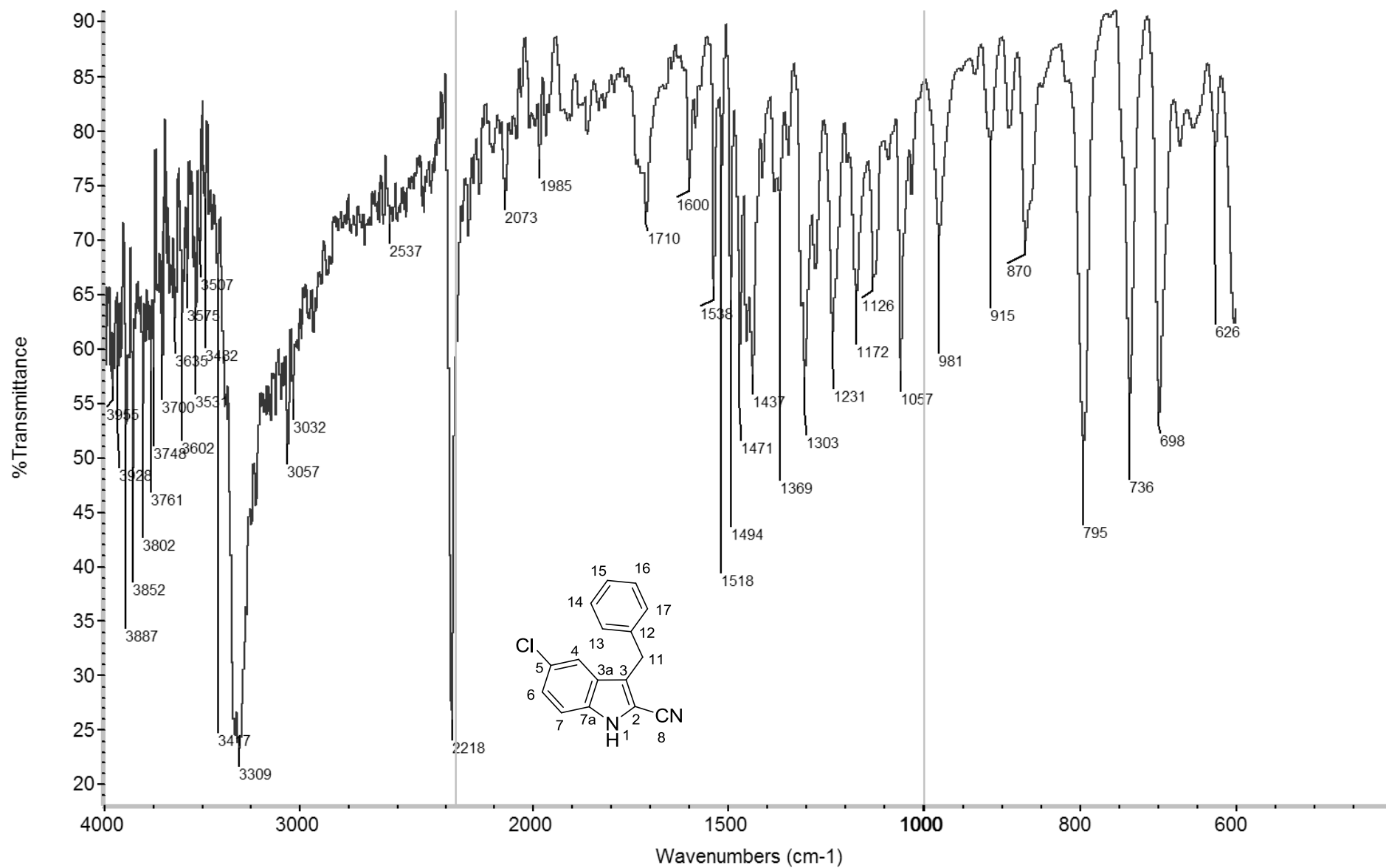
COSY NMR Spectrum
400 MHz Varian Unity Inova



gHSQC NMR Spectrum
400 MHz Varian Unity Inova

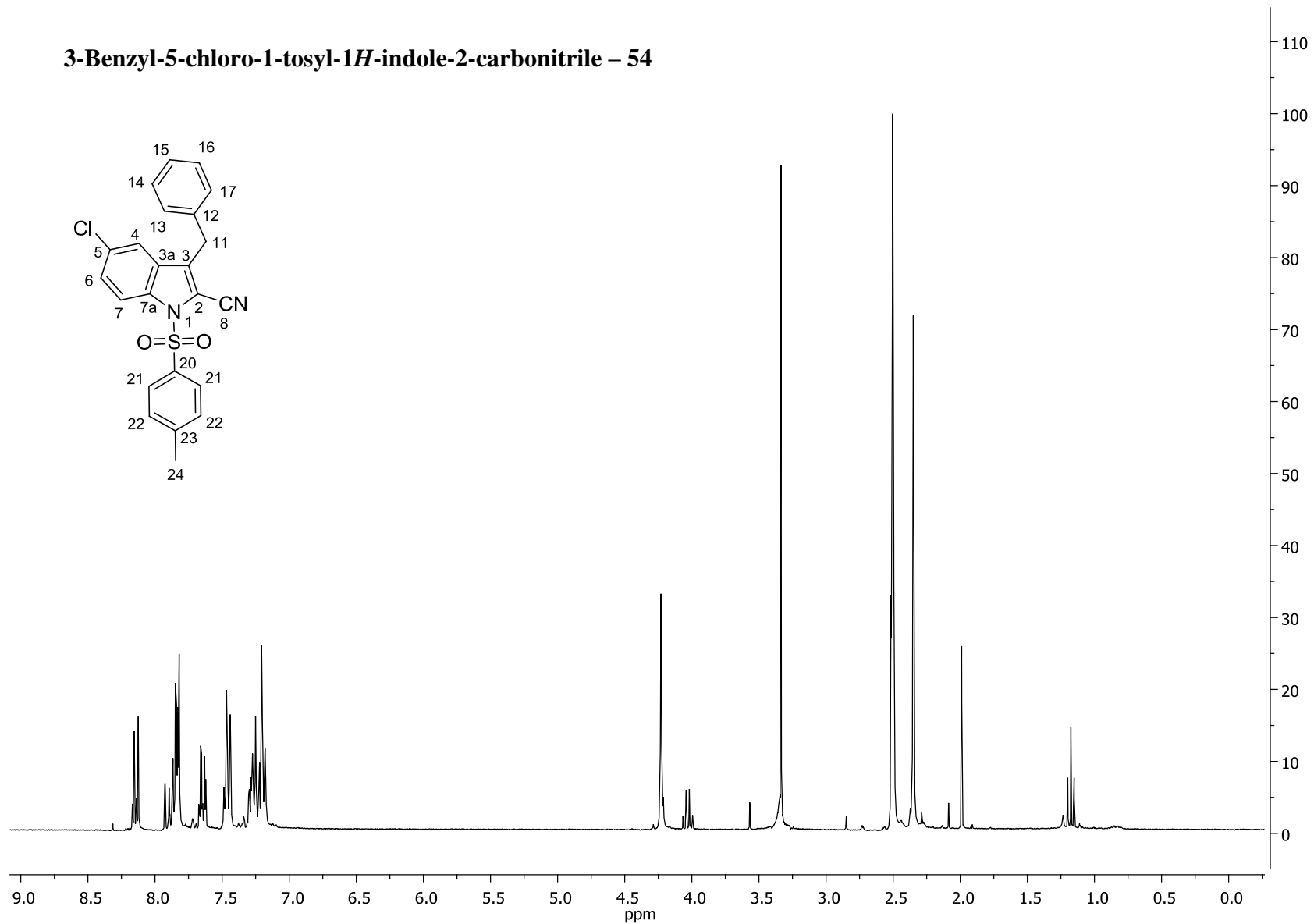


Mass Spectrum
Waters SYNAPT G2

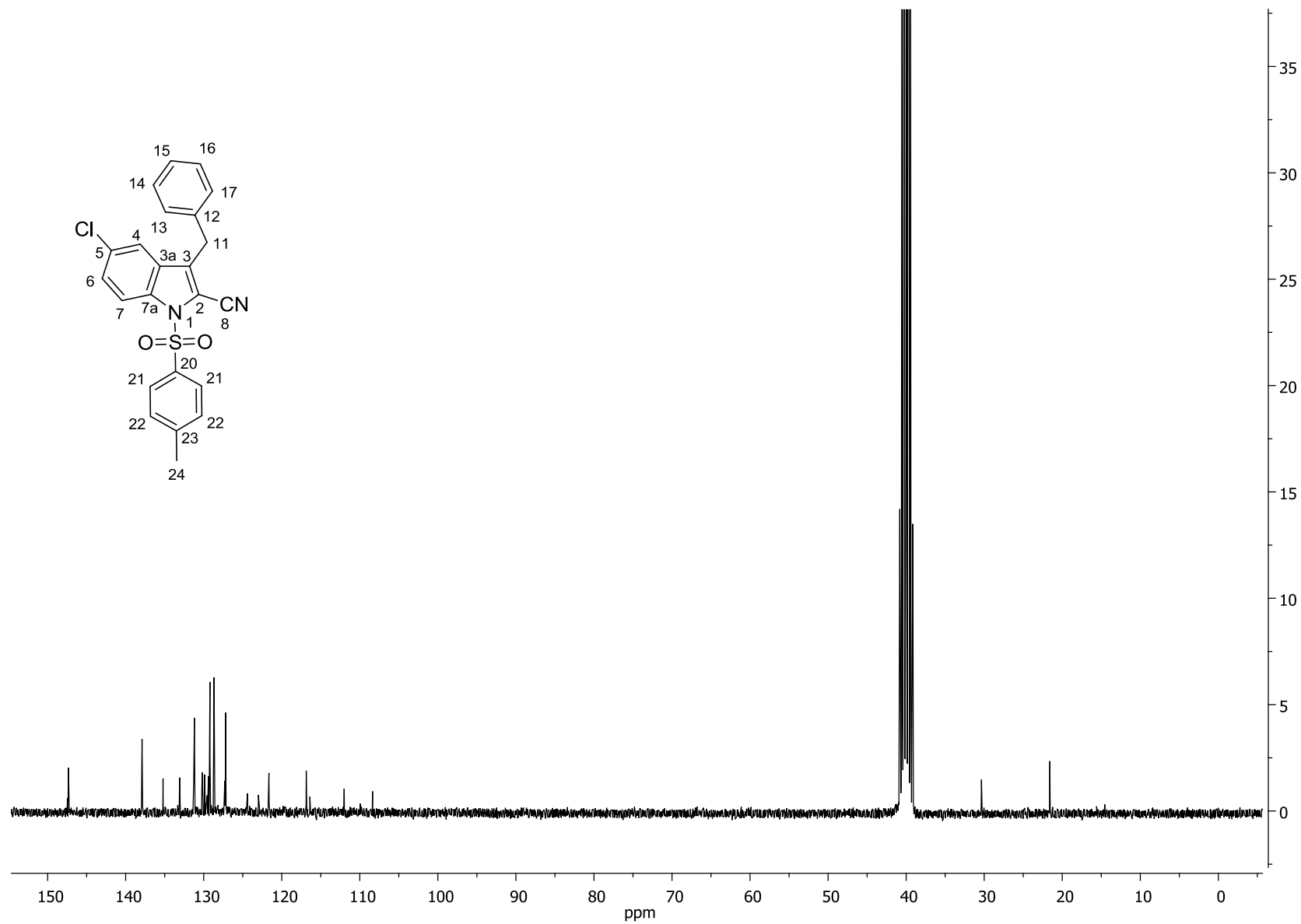


Infrared Spectrum
Thermo Nicolet Nexus 470

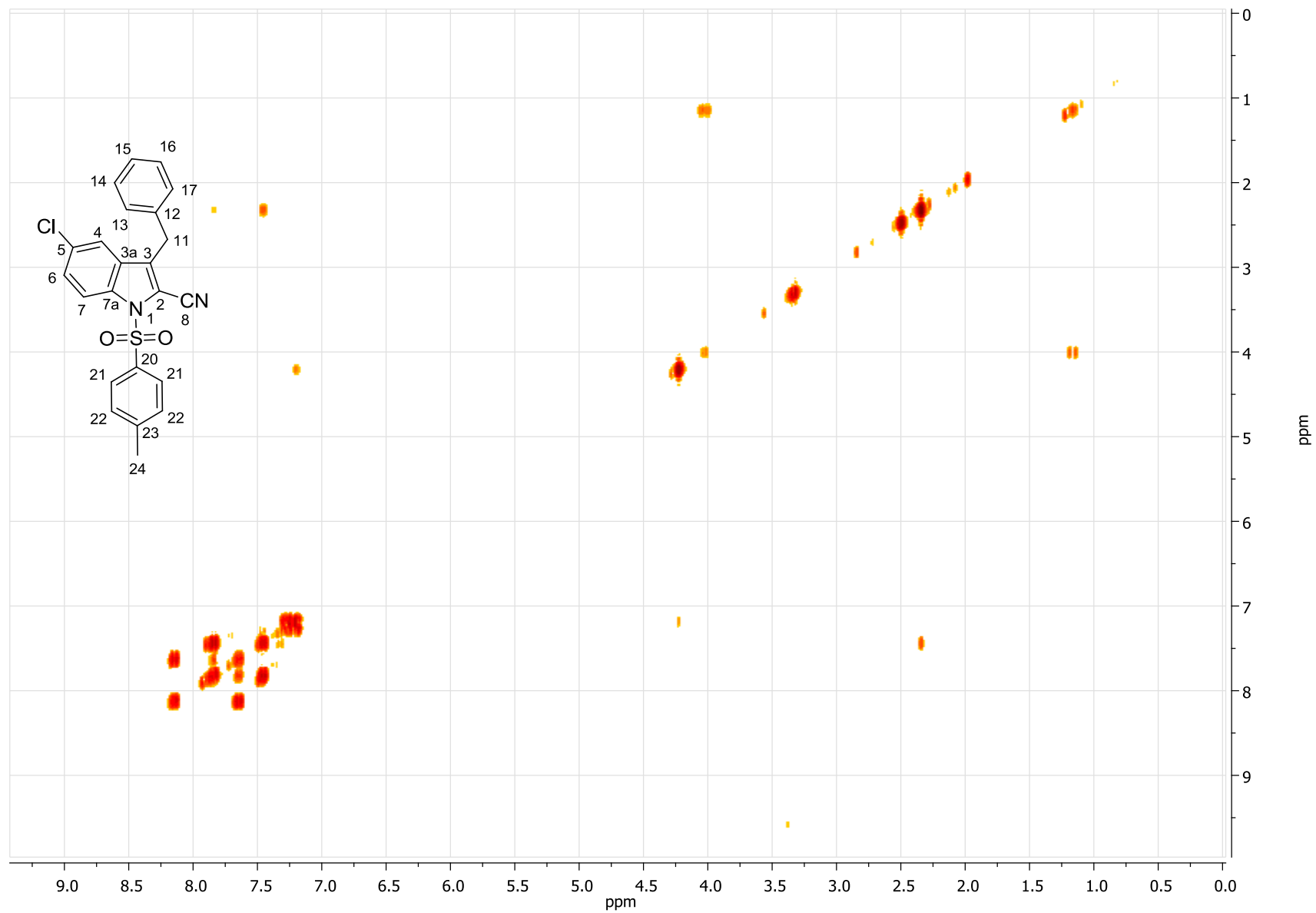
3-Benzyl-5-chloro-1-tosyl-1H-indole-2-carbonitrile – 54



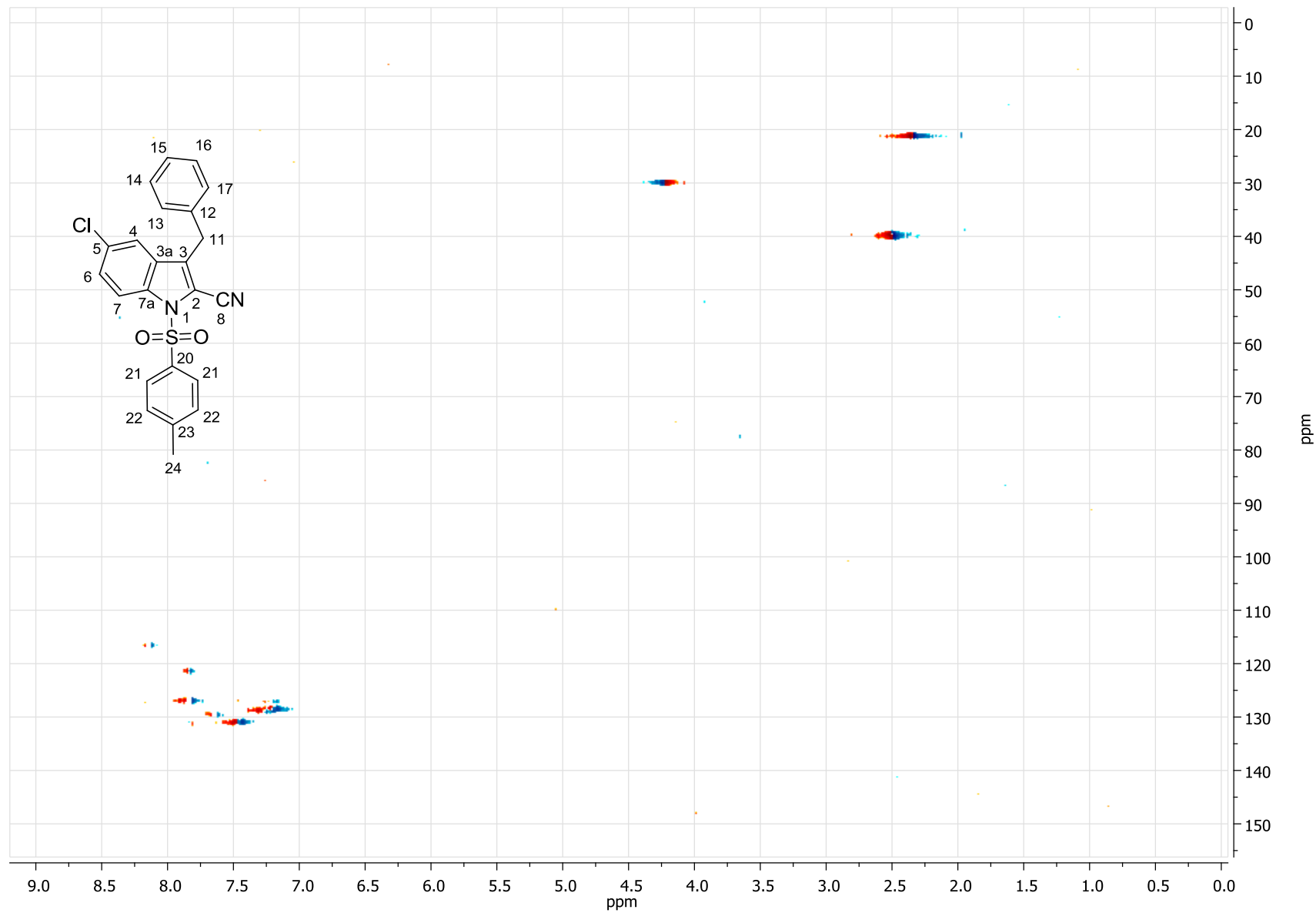
¹H NMR Spectrum
300 MHz Varian VNMRS



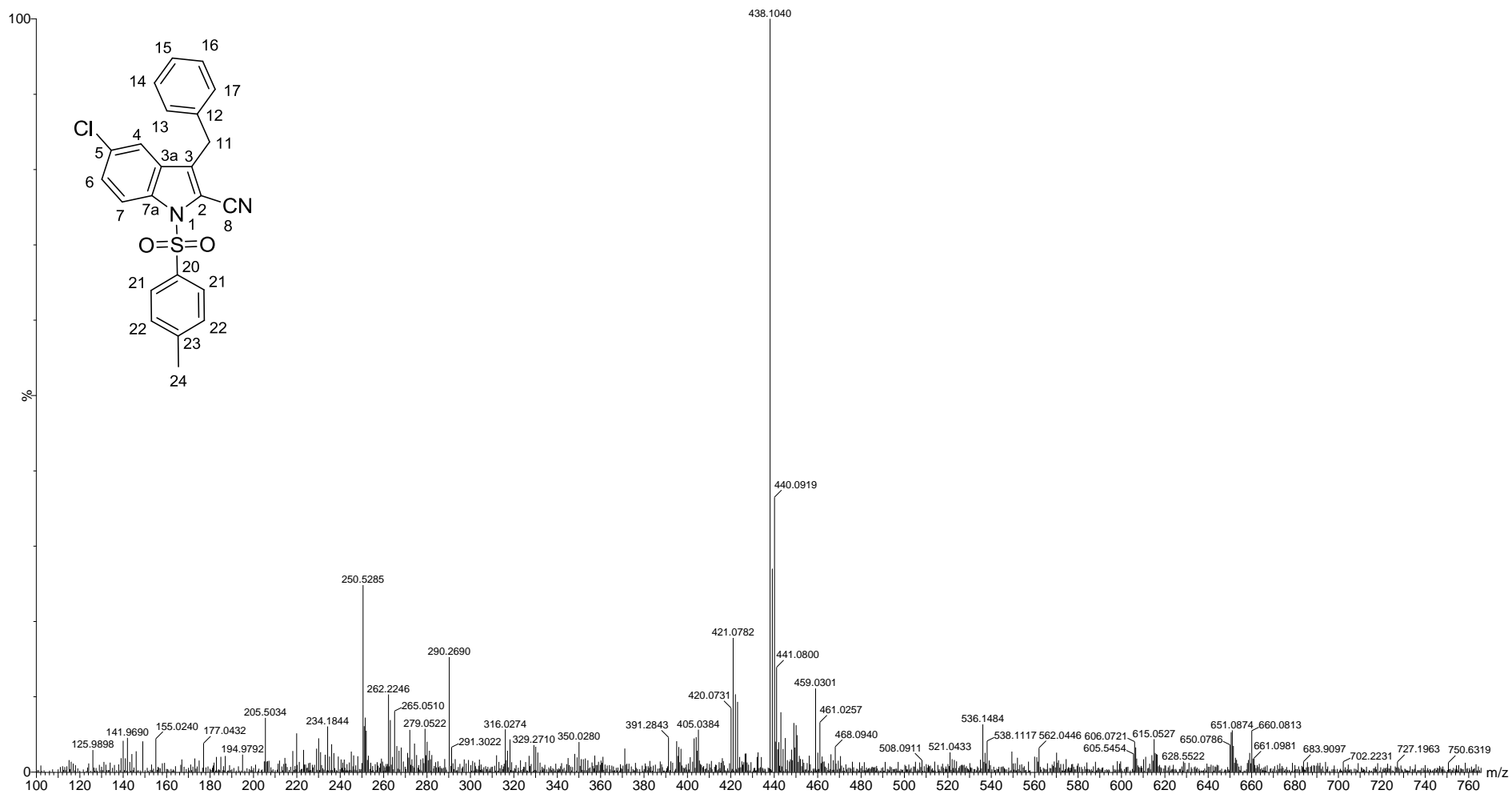
^{13}C NMR Spectrum
75 MHz Varian VNMRS



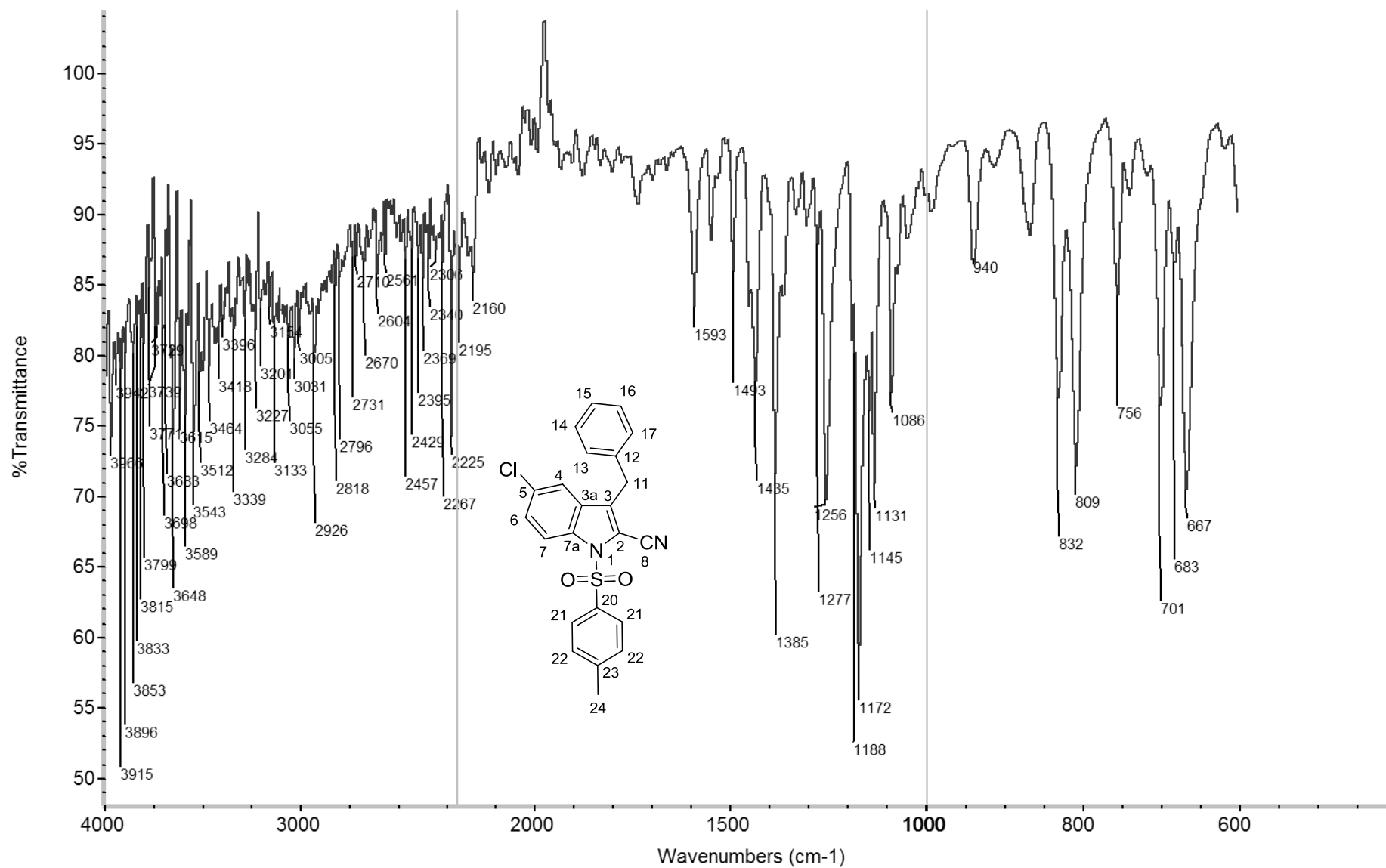
COSY NMR Spectrum
300 MHz Varian VNMRS



gHSQC NMR Spectrum
300 MHz Varian VNMRS

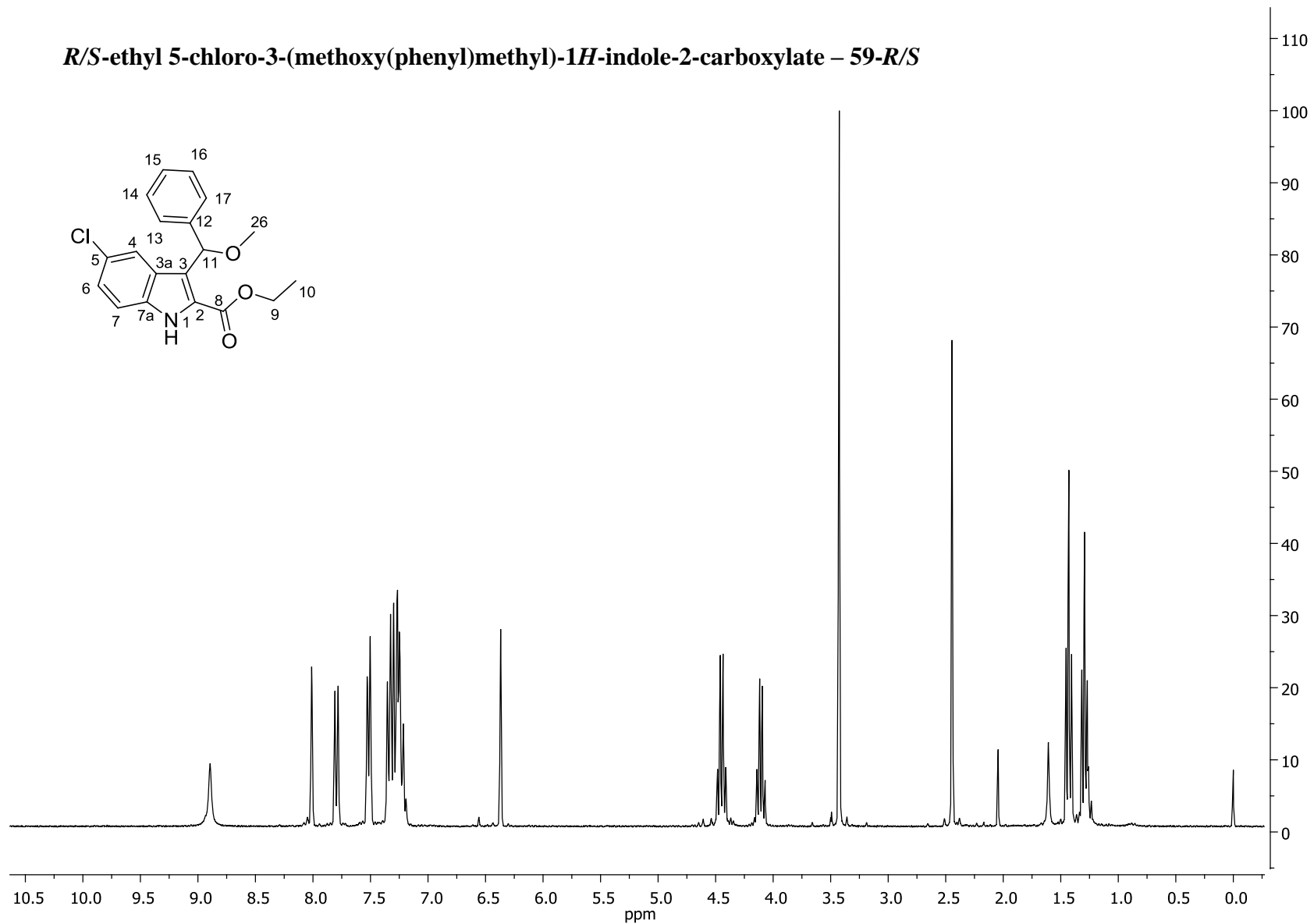


Mass Spectrum
Waters SYNAPT G2

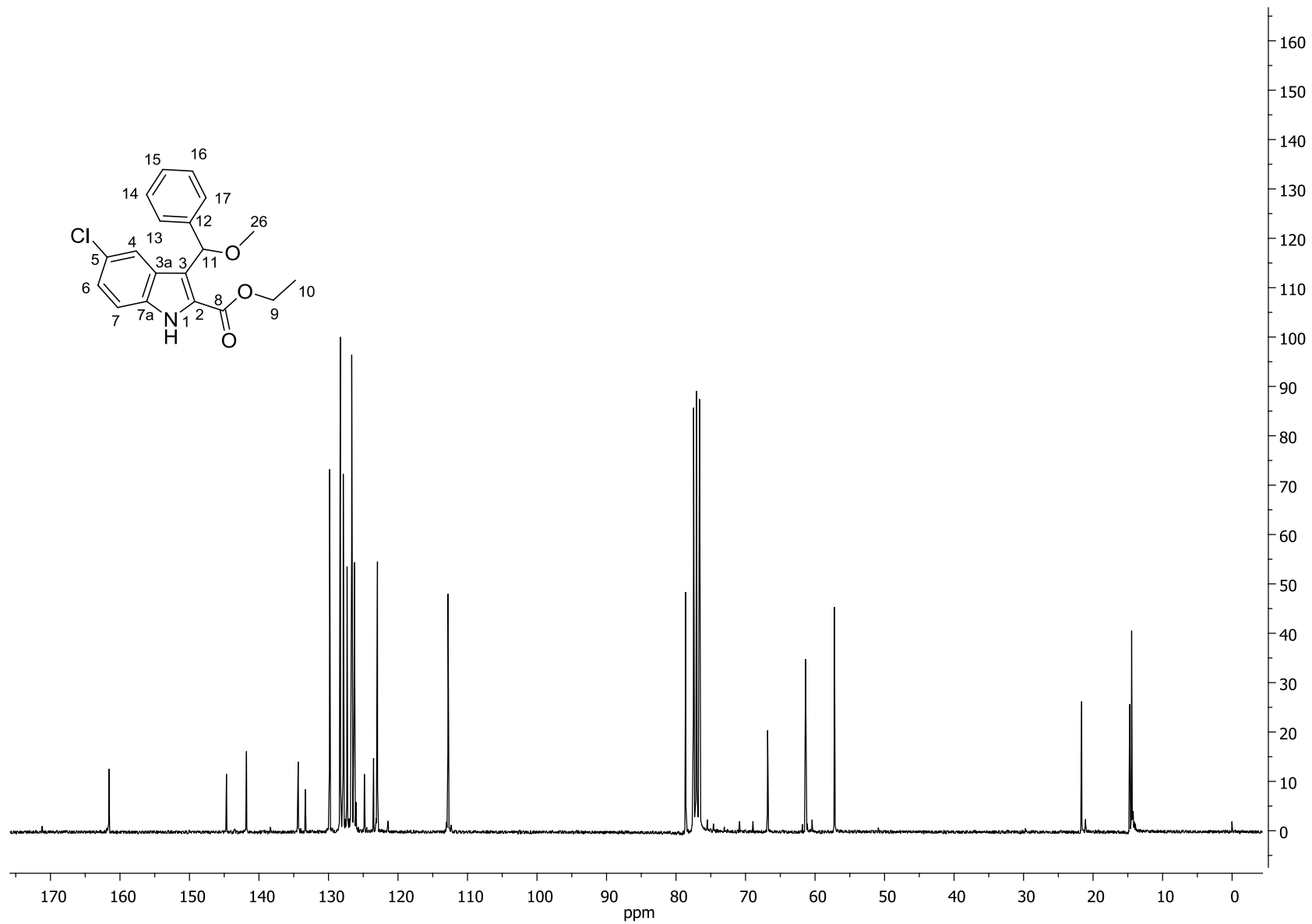


Infrared Spectrum
Thermo Nicolet Nexus 470

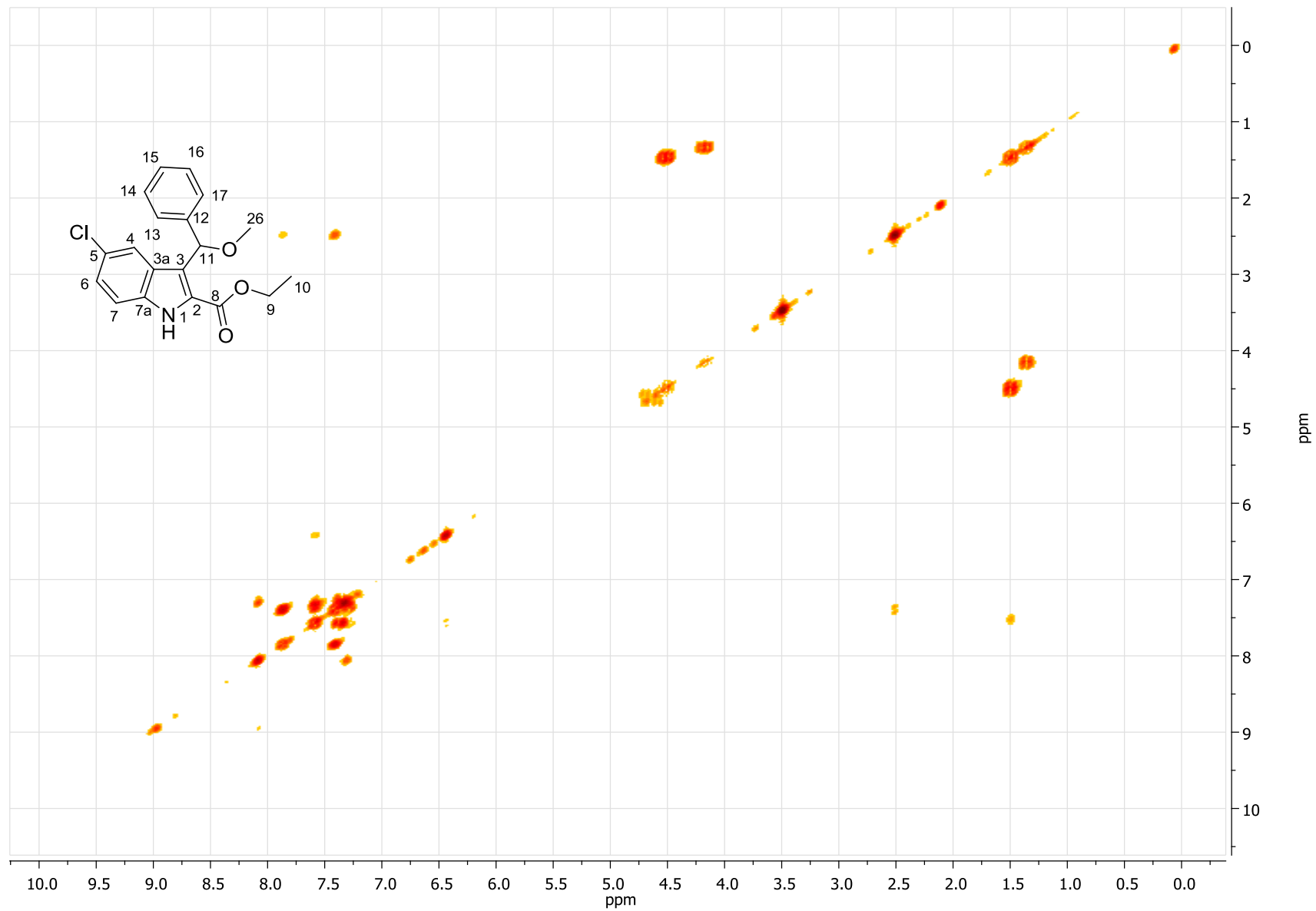
R/S*-ethyl 5-chloro-3-(methoxy(phenyl)methyl)-1*H*-indole-2-carboxylate – 59-*R/S



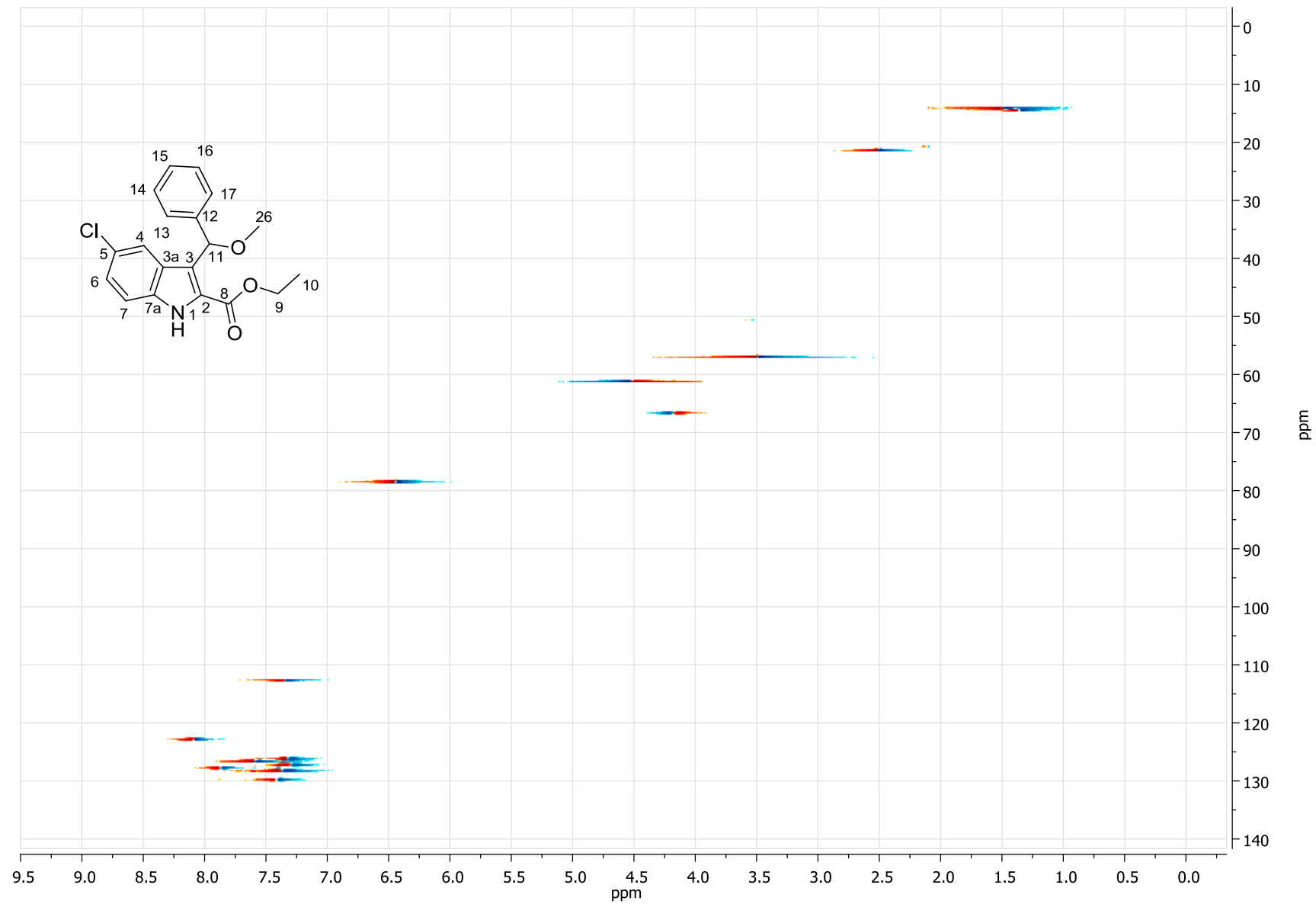
¹H NMR Spectrum
300 MHz Varian VNMRS



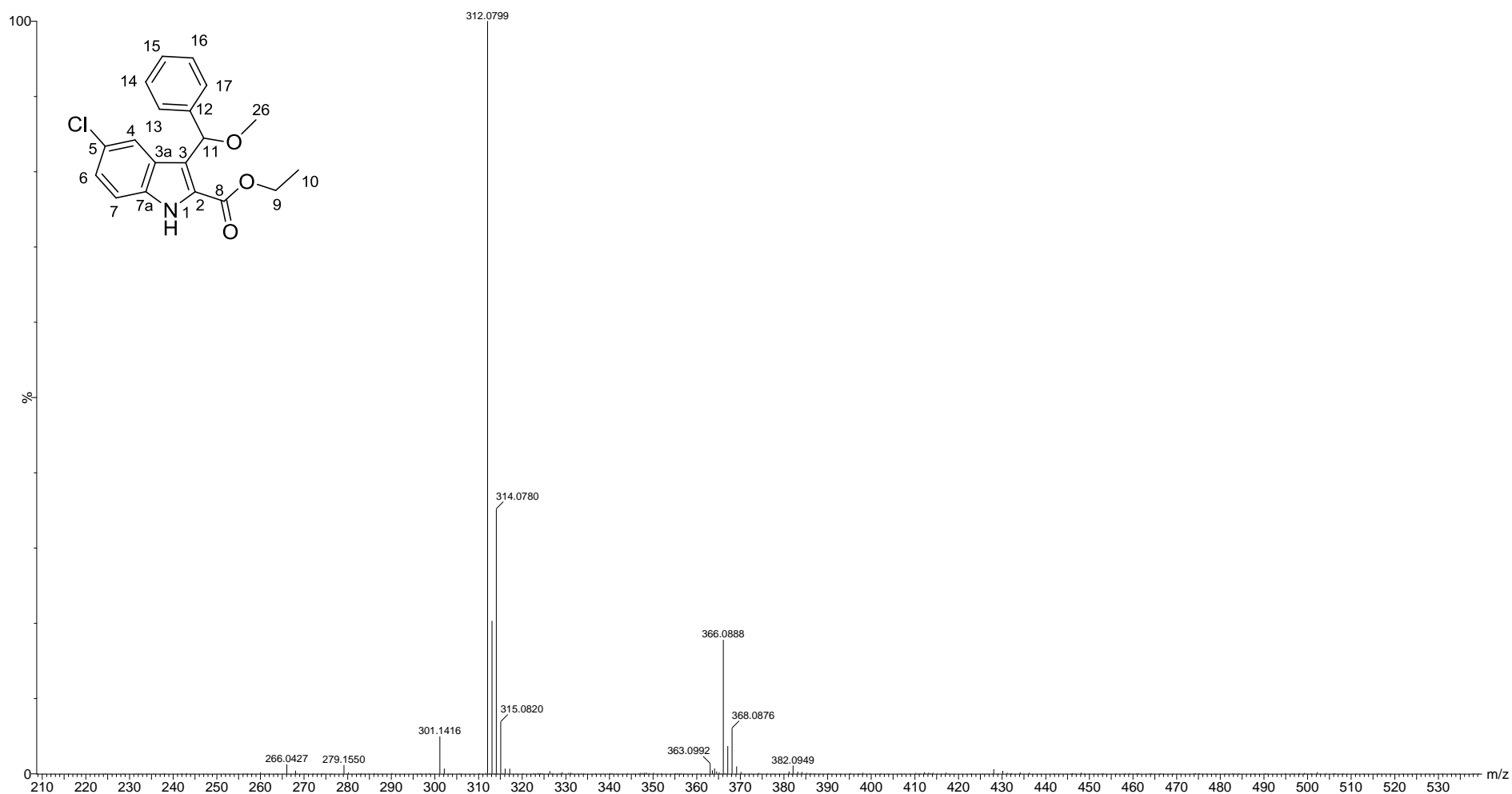
^{13}C NMR Spectrum
75 MHz Varian VNMRS



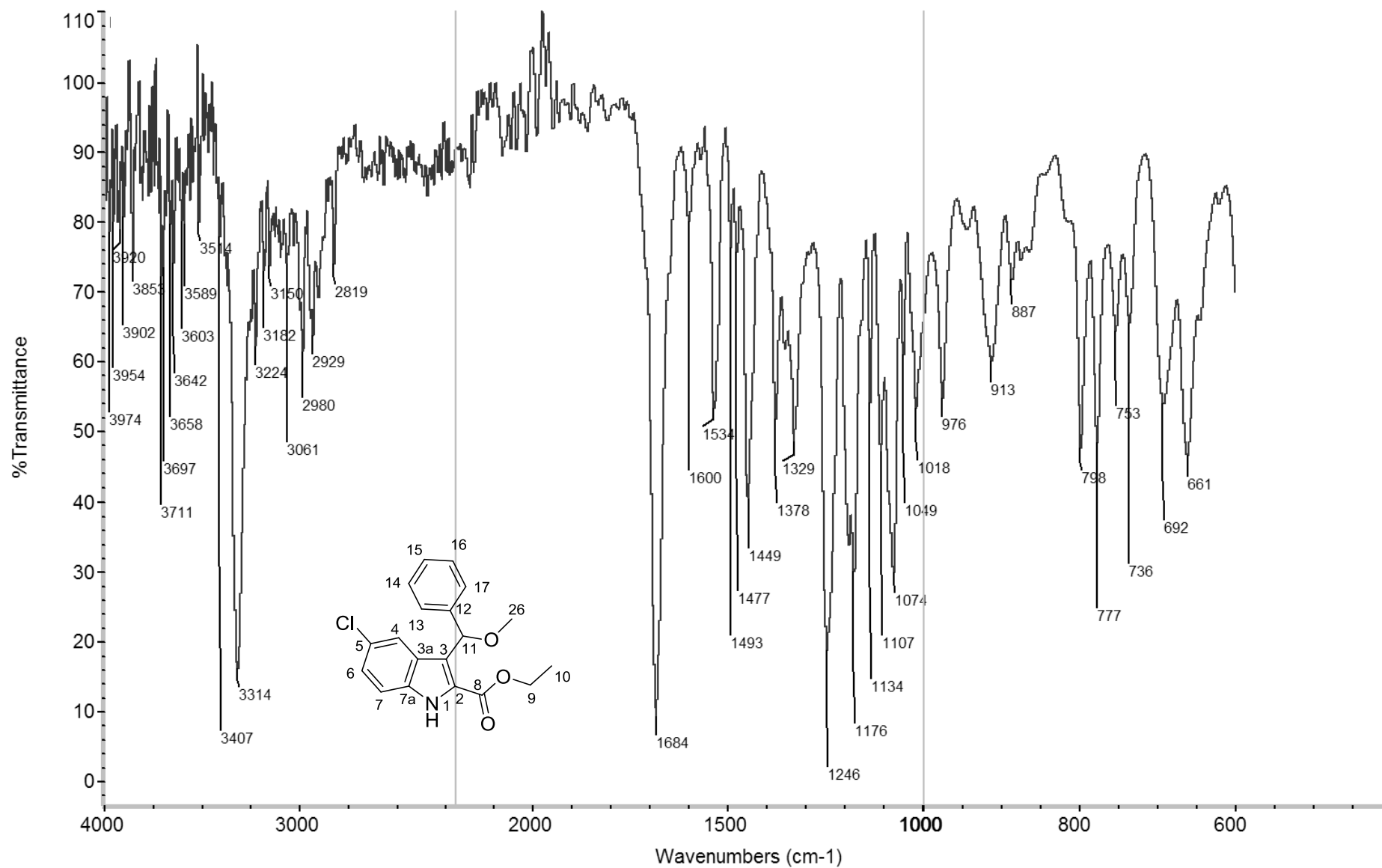
COSY NMR Spectrum
300 MHz Varian VNMRS



gHSQC NMR Spectrum
300 MHz Varian VNMRS

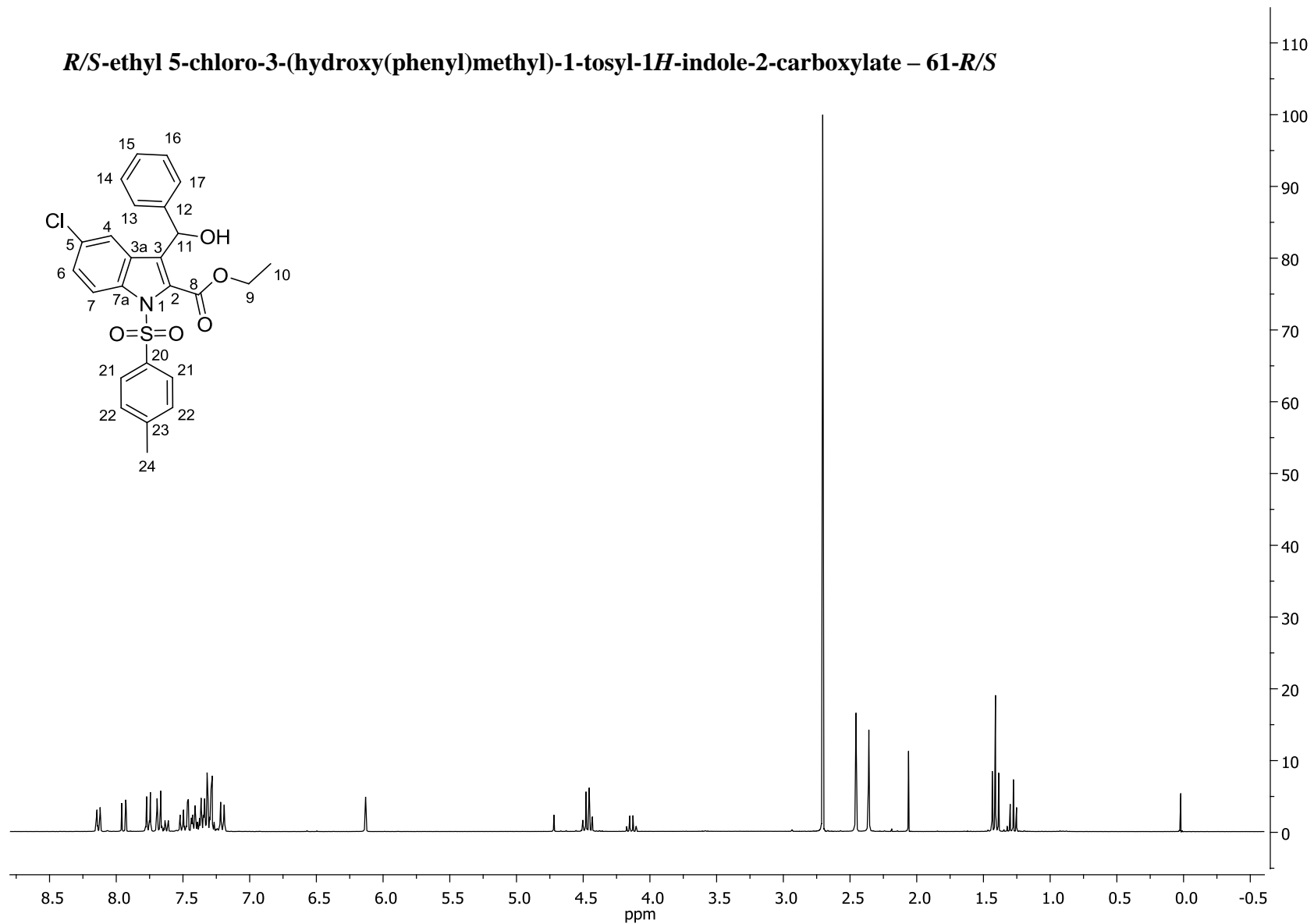


Mass Spectrum
Waters SYNAPT G2

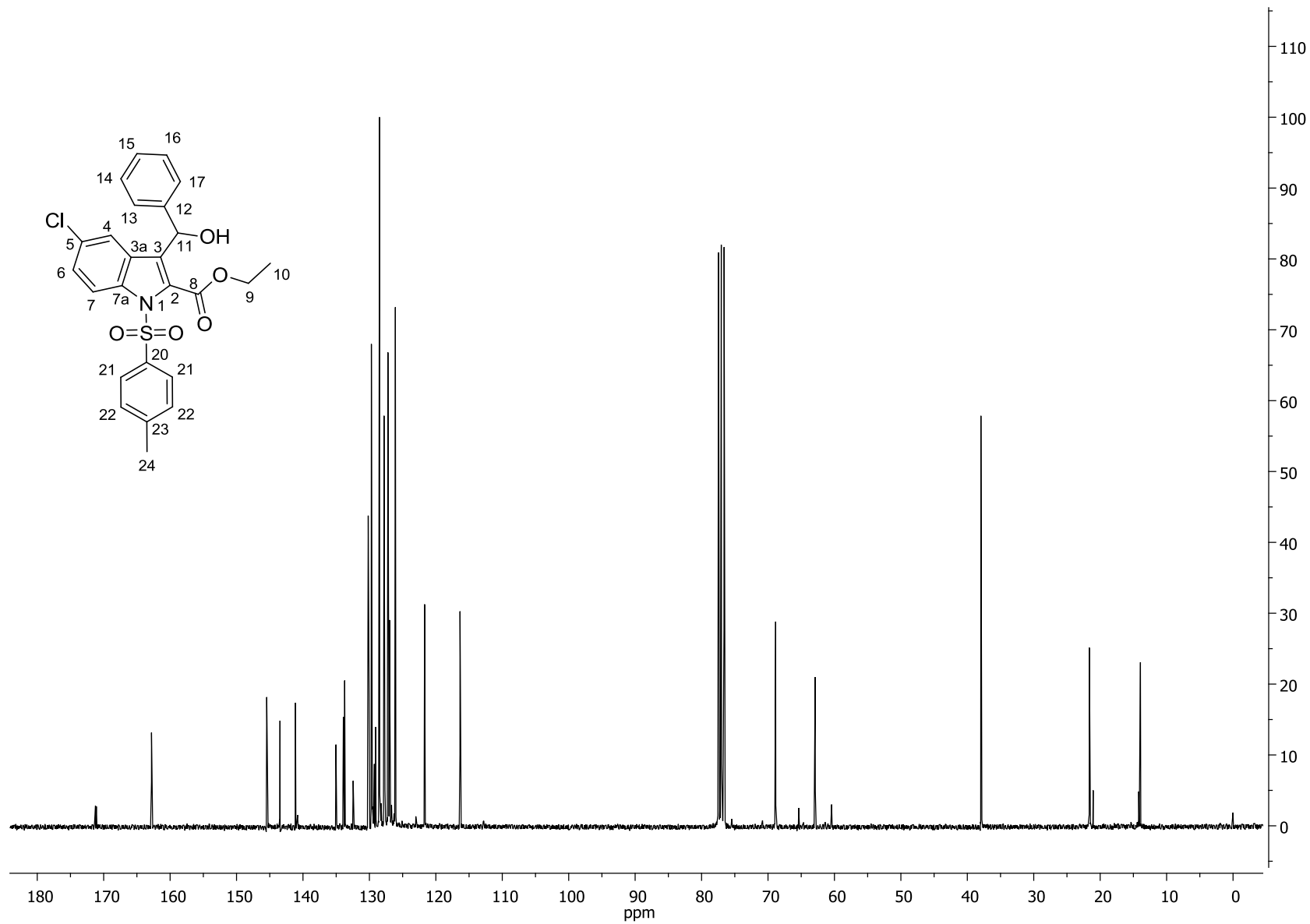


Infrared Spectrum
Thermo Nicolet Nexus 470

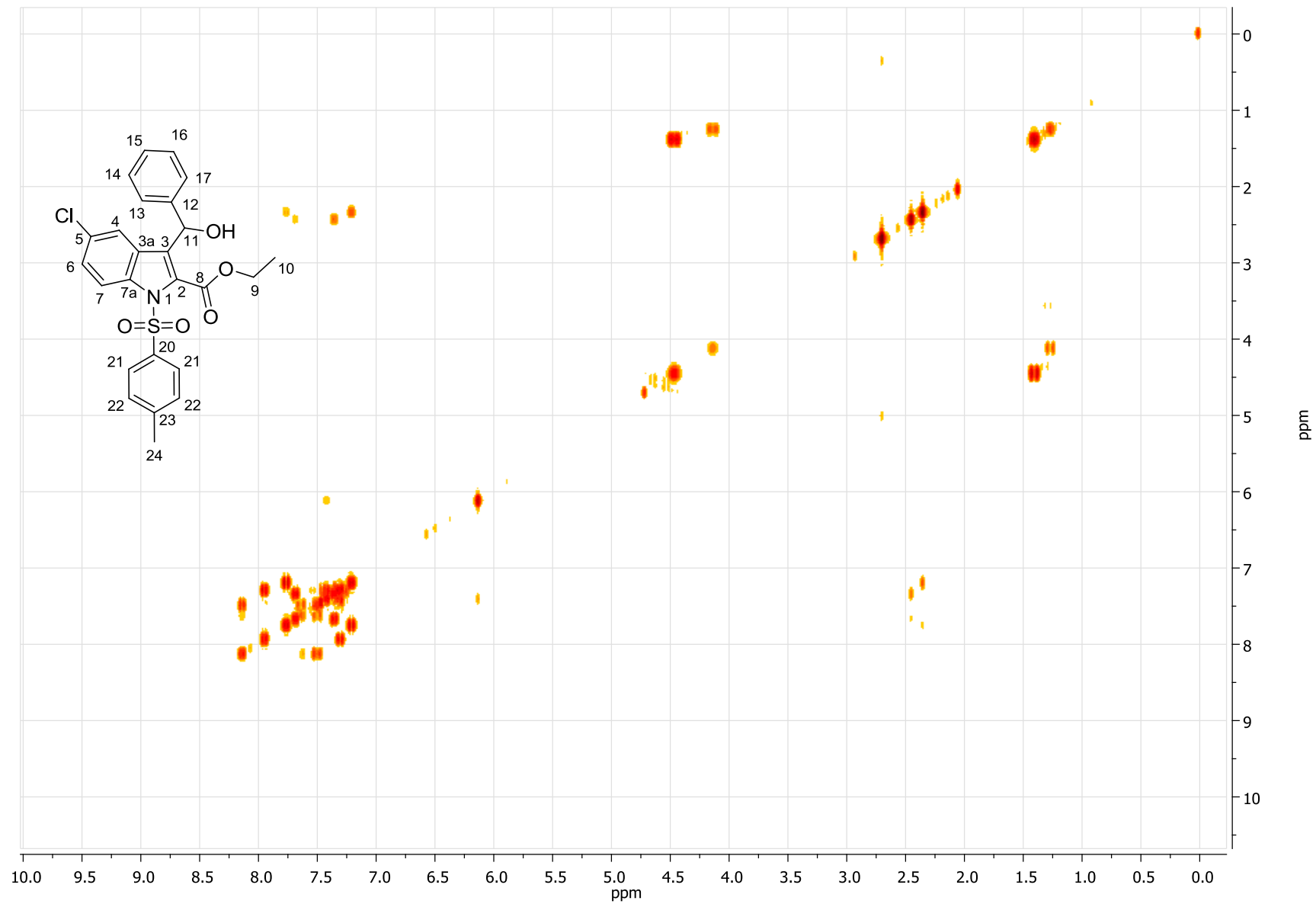
R/S*-ethyl 5-chloro-3-(hydroxy(phenyl)methyl)-1-tosyl-1*H*-indole-2-carboxylate – 61-*R/S



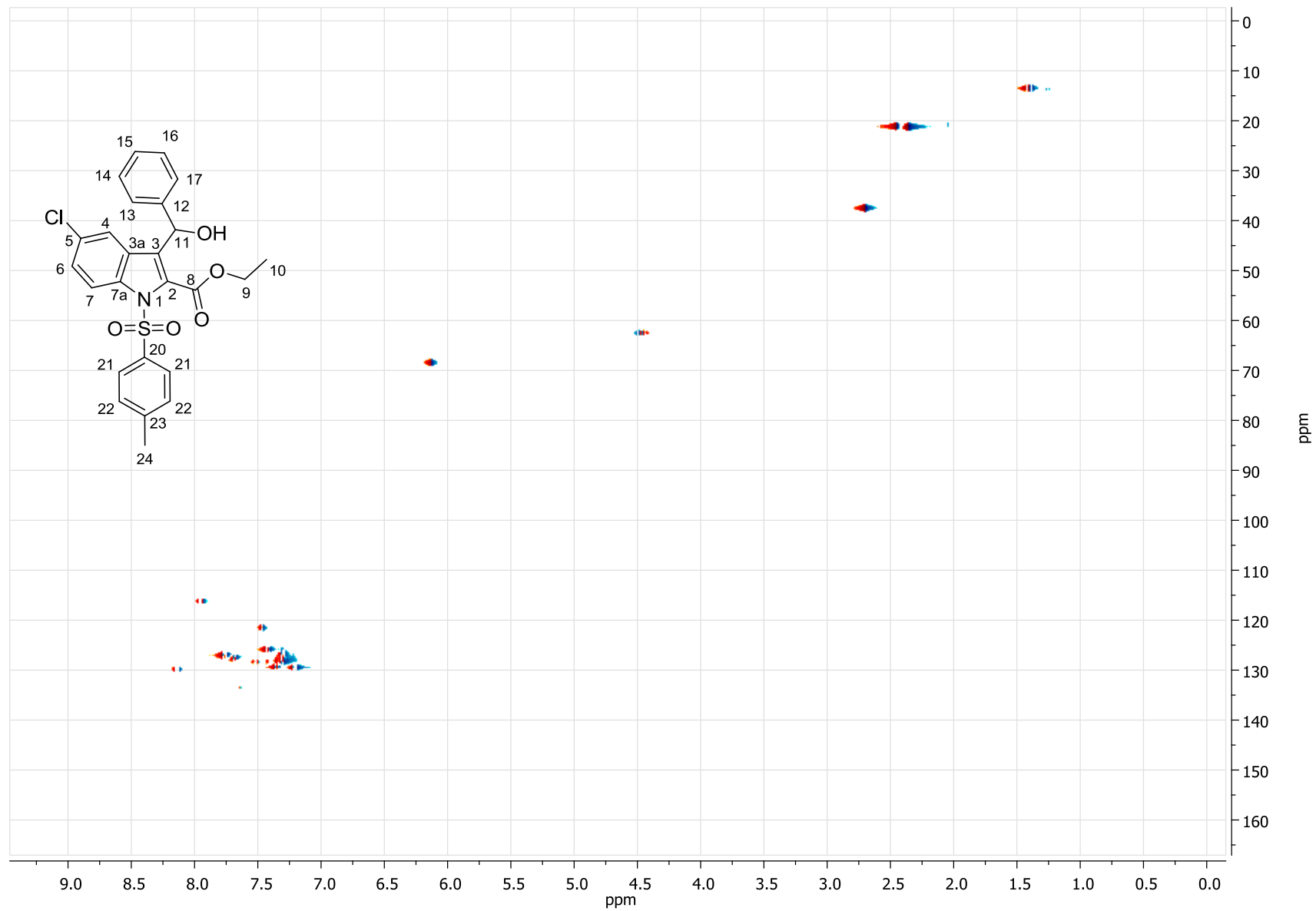
¹H NMR Spectrum
300 MHz Varian VNMRS



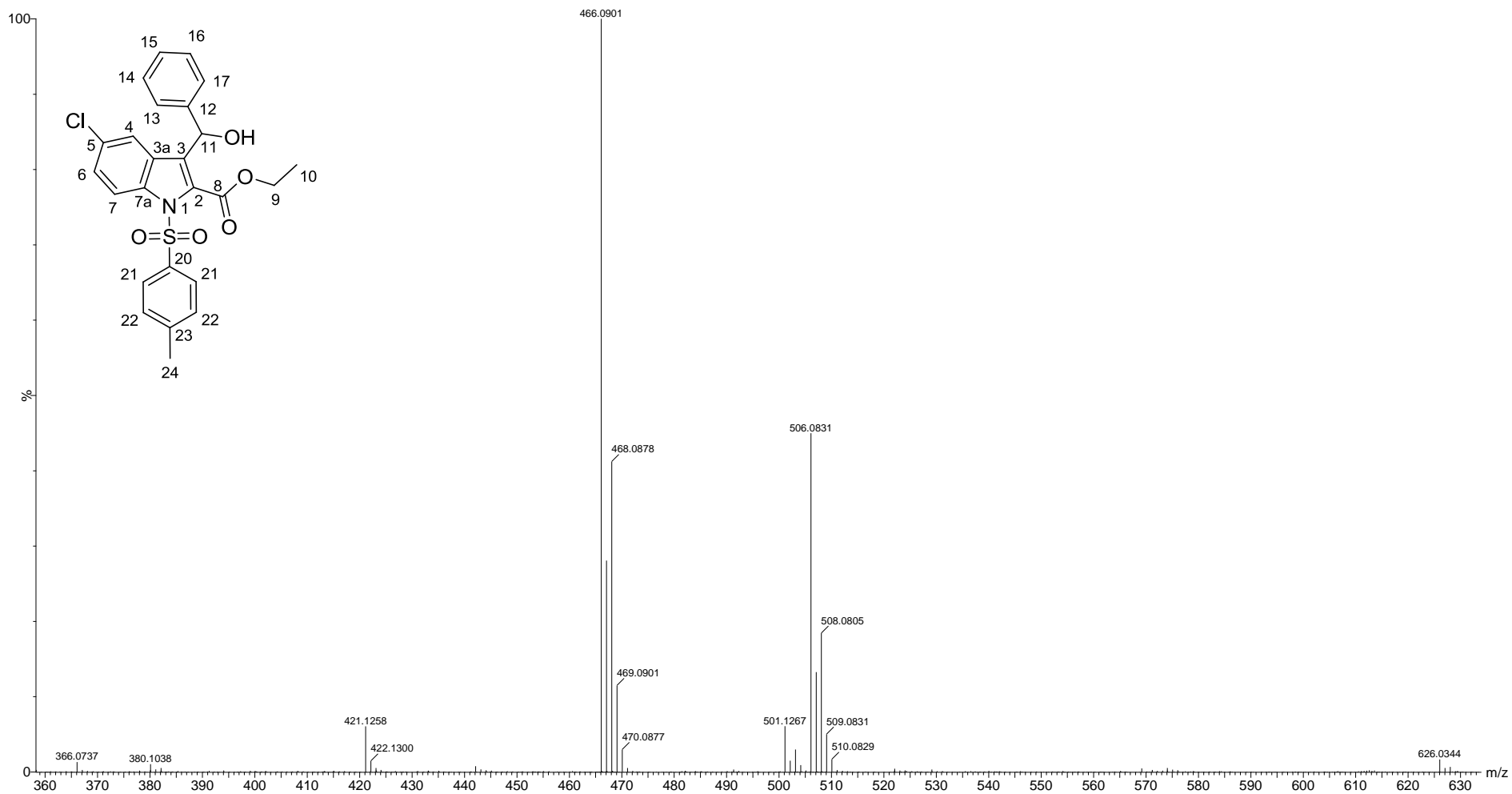
¹³C NMR Spectrum
75 MHz Varian VNMRS



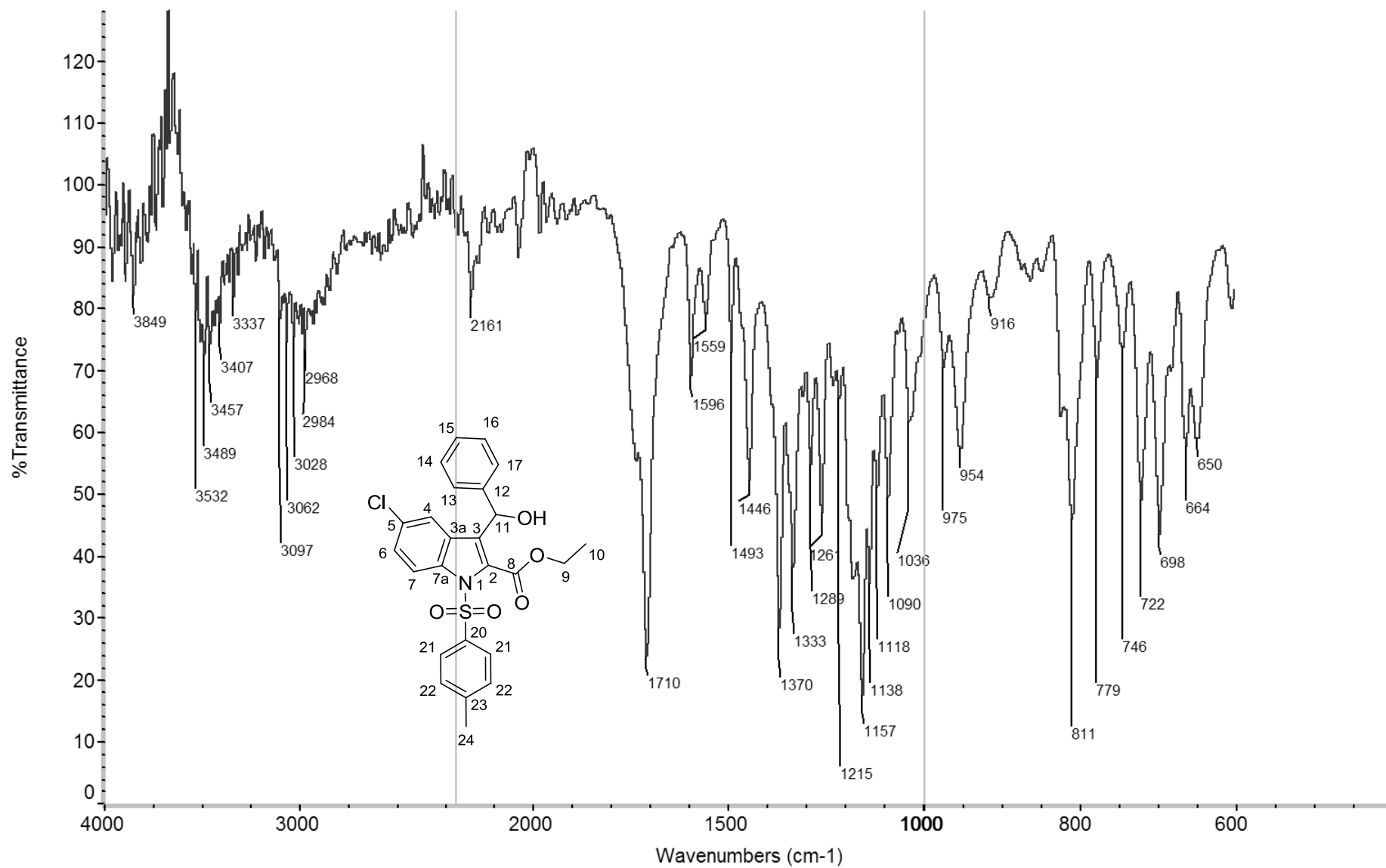
COSY NMR Spectrum
300 MHz Varian VNMRS



gHSQC NMR Spectrum
300 MHz Varian VNMRS

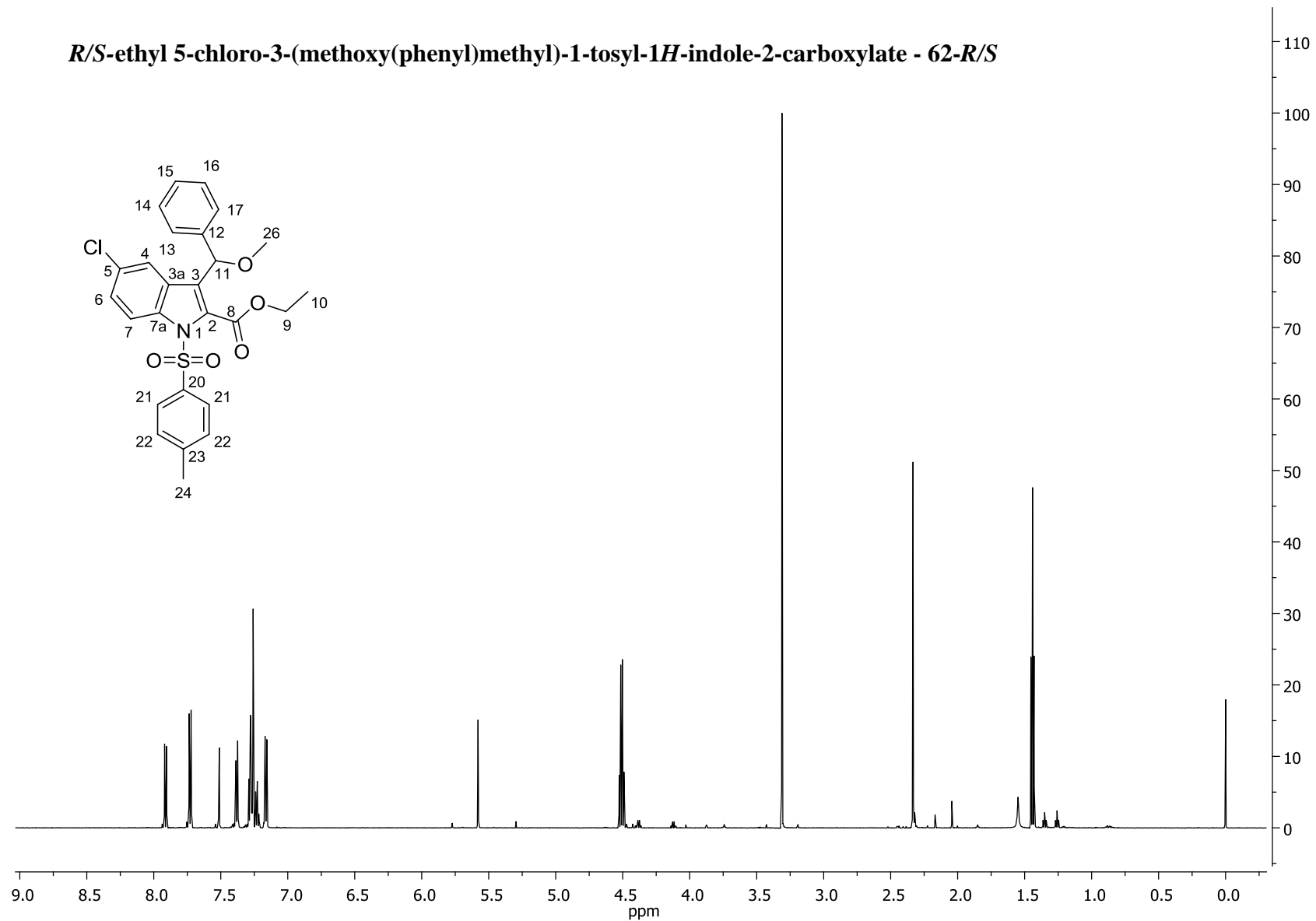


Mass Spectrum
Waters SYNAPT G2

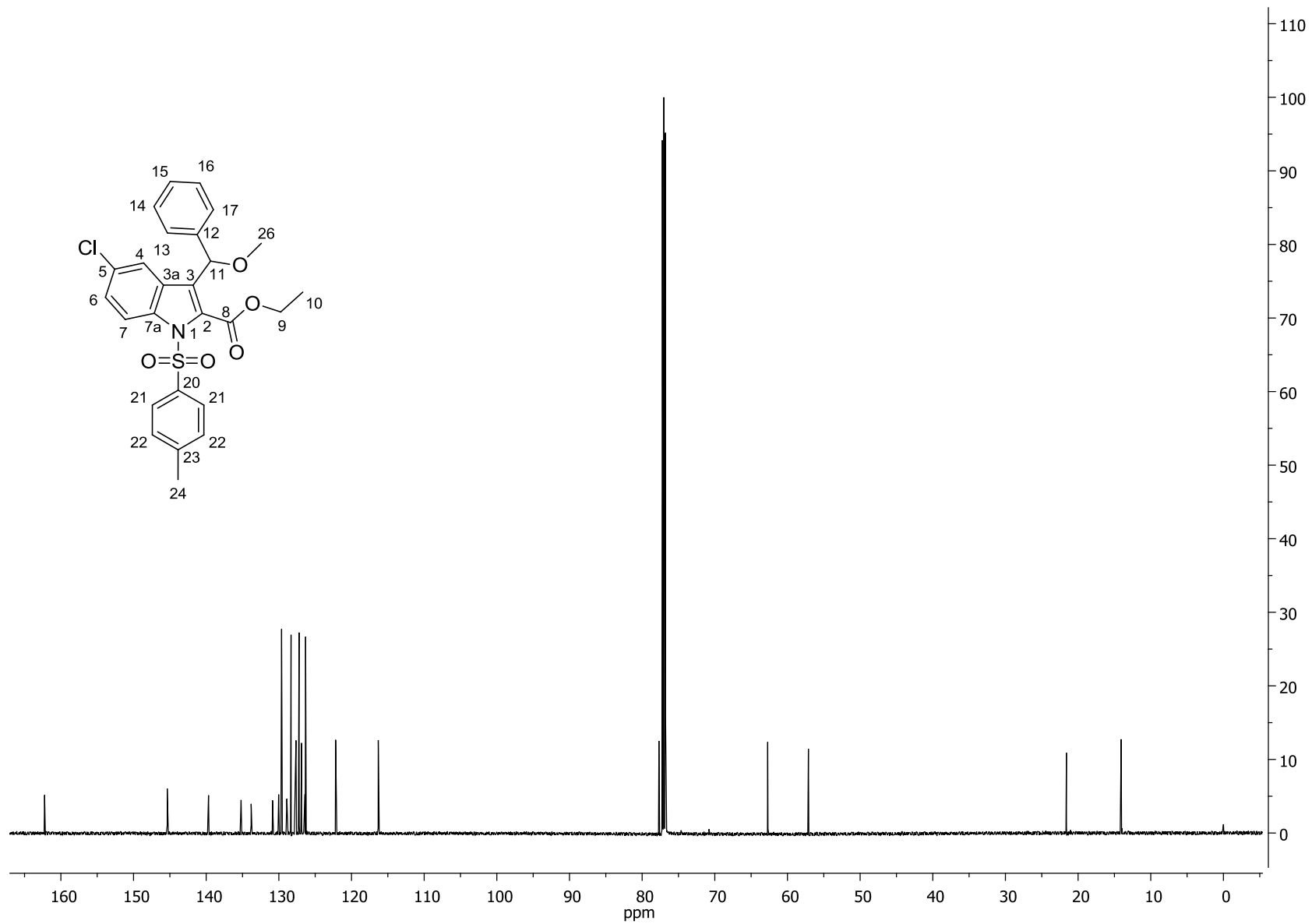


Infrared Spectrum
Thermo Nicolet Nexus 470

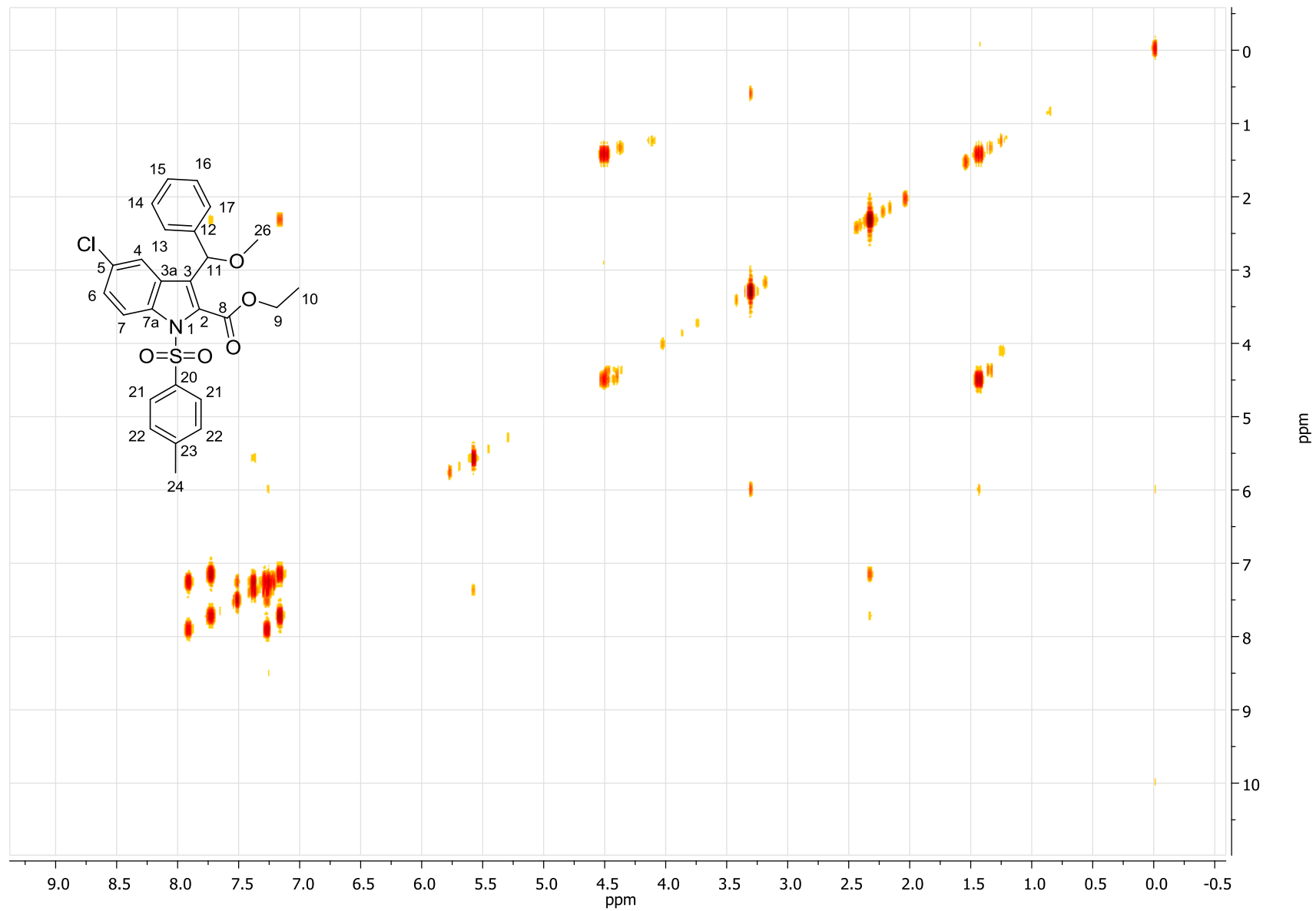
R/S*-ethyl 5-chloro-3-(methoxy(phenyl)methyl)-1-tosyl-1*H*-indole-2-carboxylate - 62-*R/S



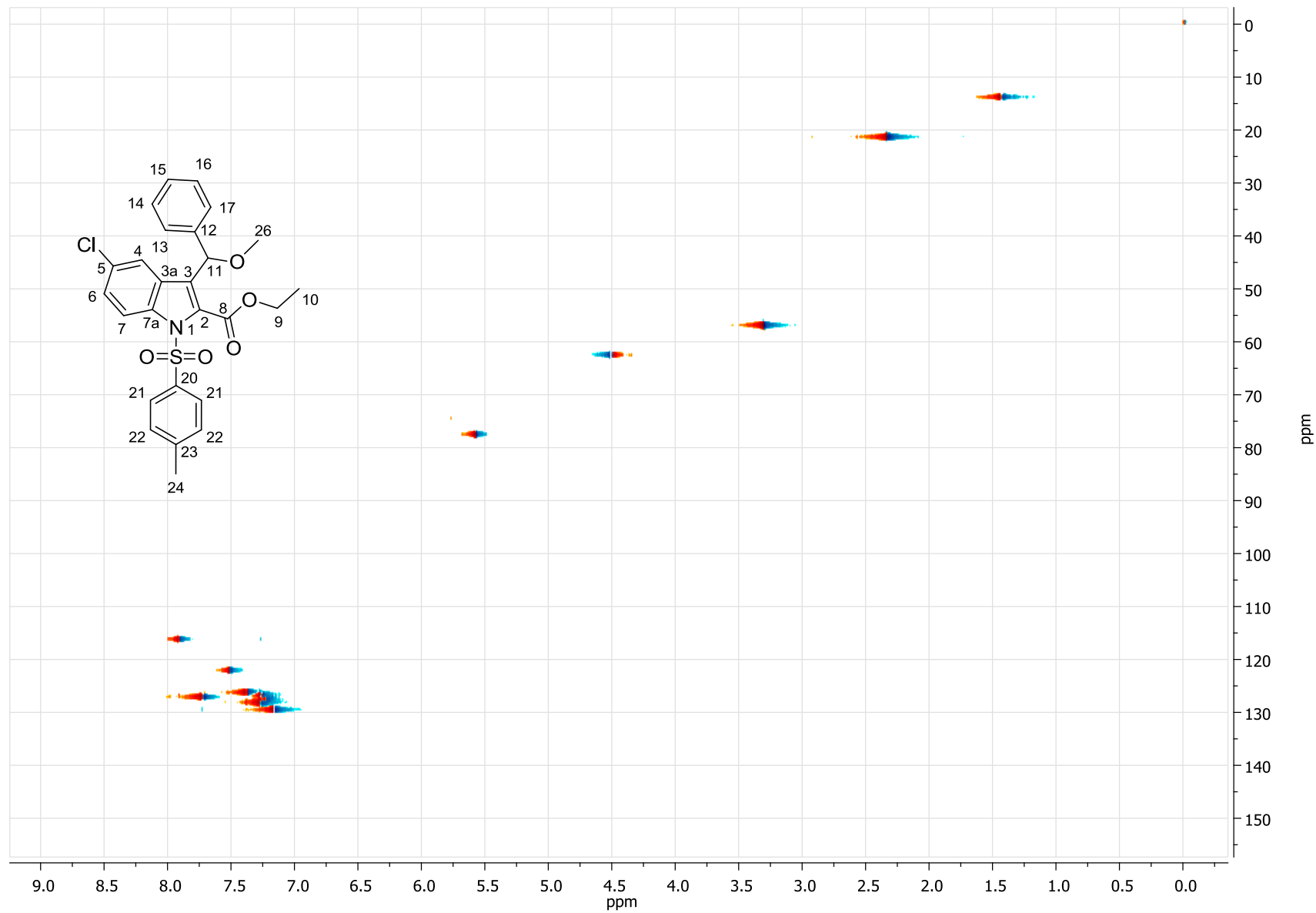
¹H NMR Spectrum
600 MHz Varian Unity Inova



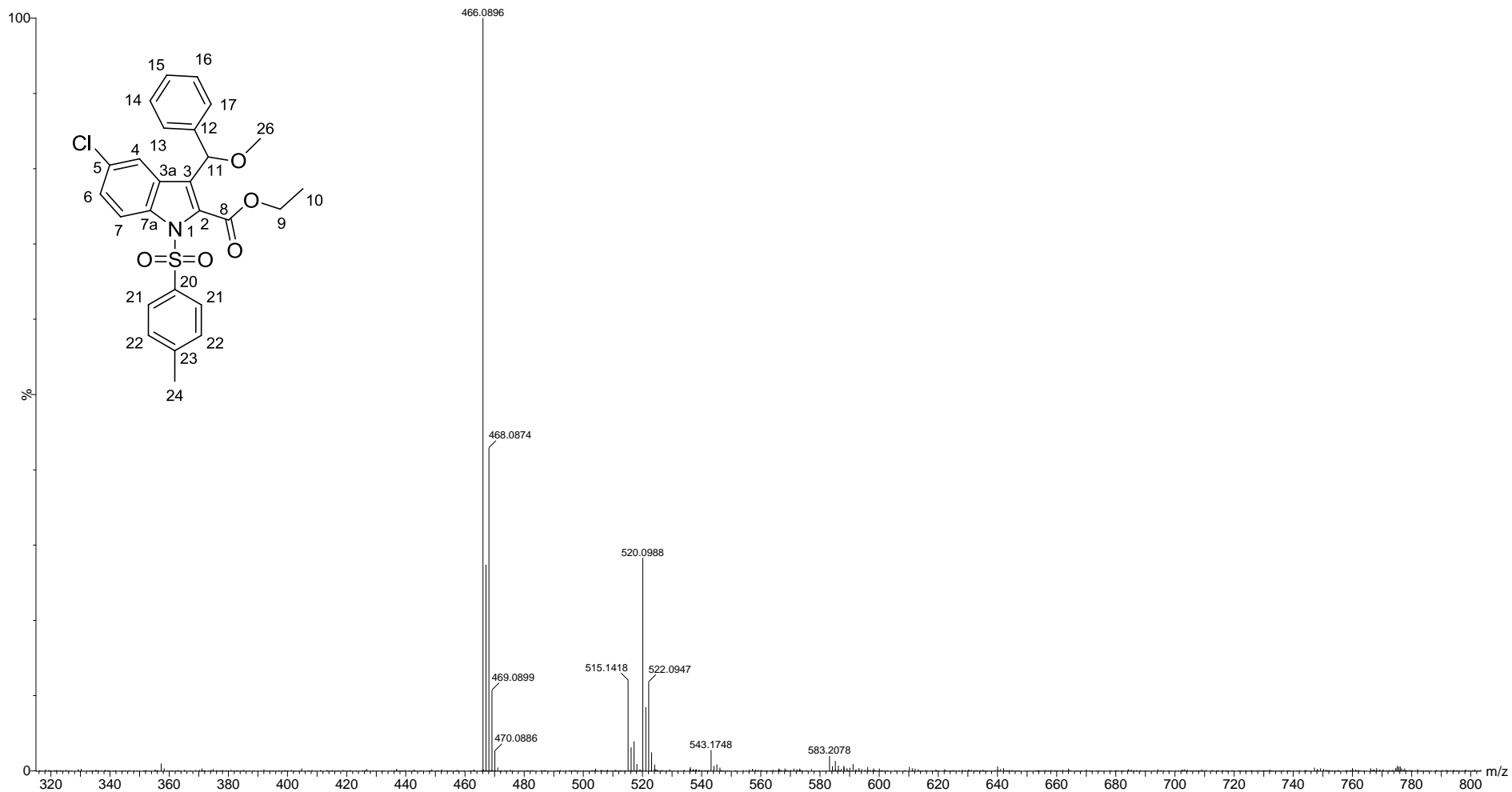
^{13}C NMR Spectrum
150 MHz Varian Unity Inova



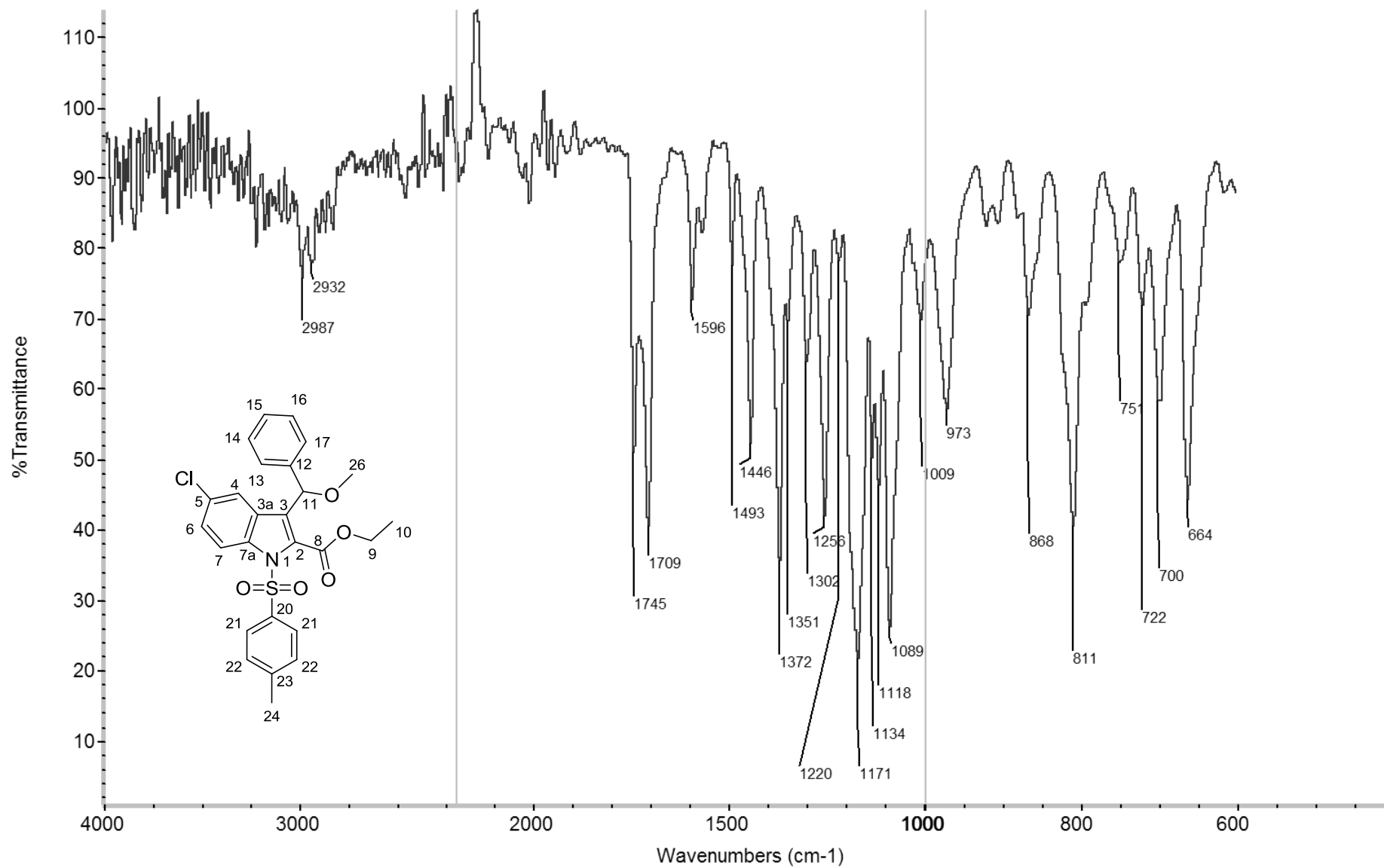
COSY NMR Spectrum
600 MHz Varian Unity Inova



gHSQC NMR Spectrum
600 MHz Varian Unity Inova

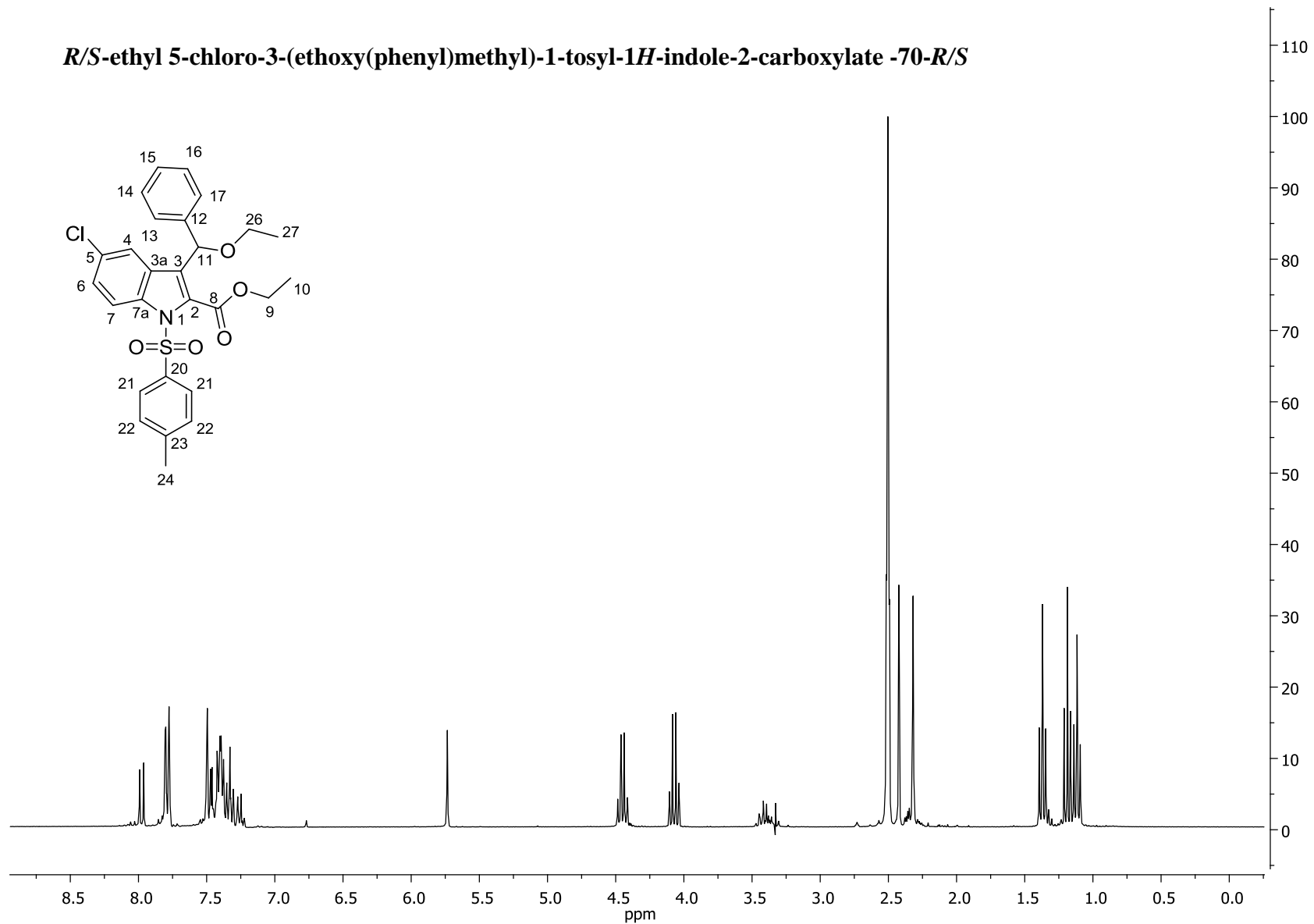


Mass Spectrum
Waters SYNAPT G2

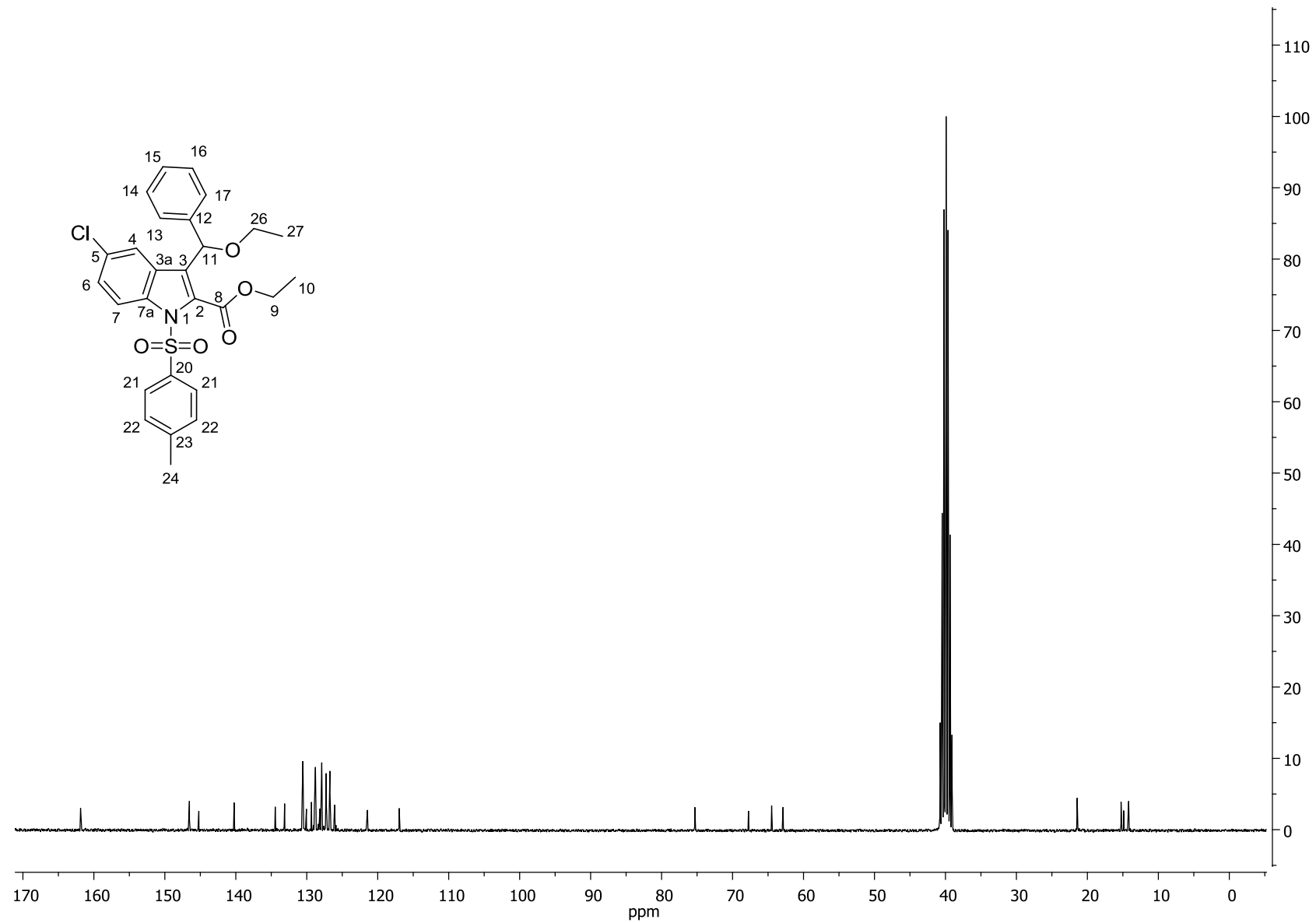


Infrared Spectrum
Thermo Nicolet Nexus 470

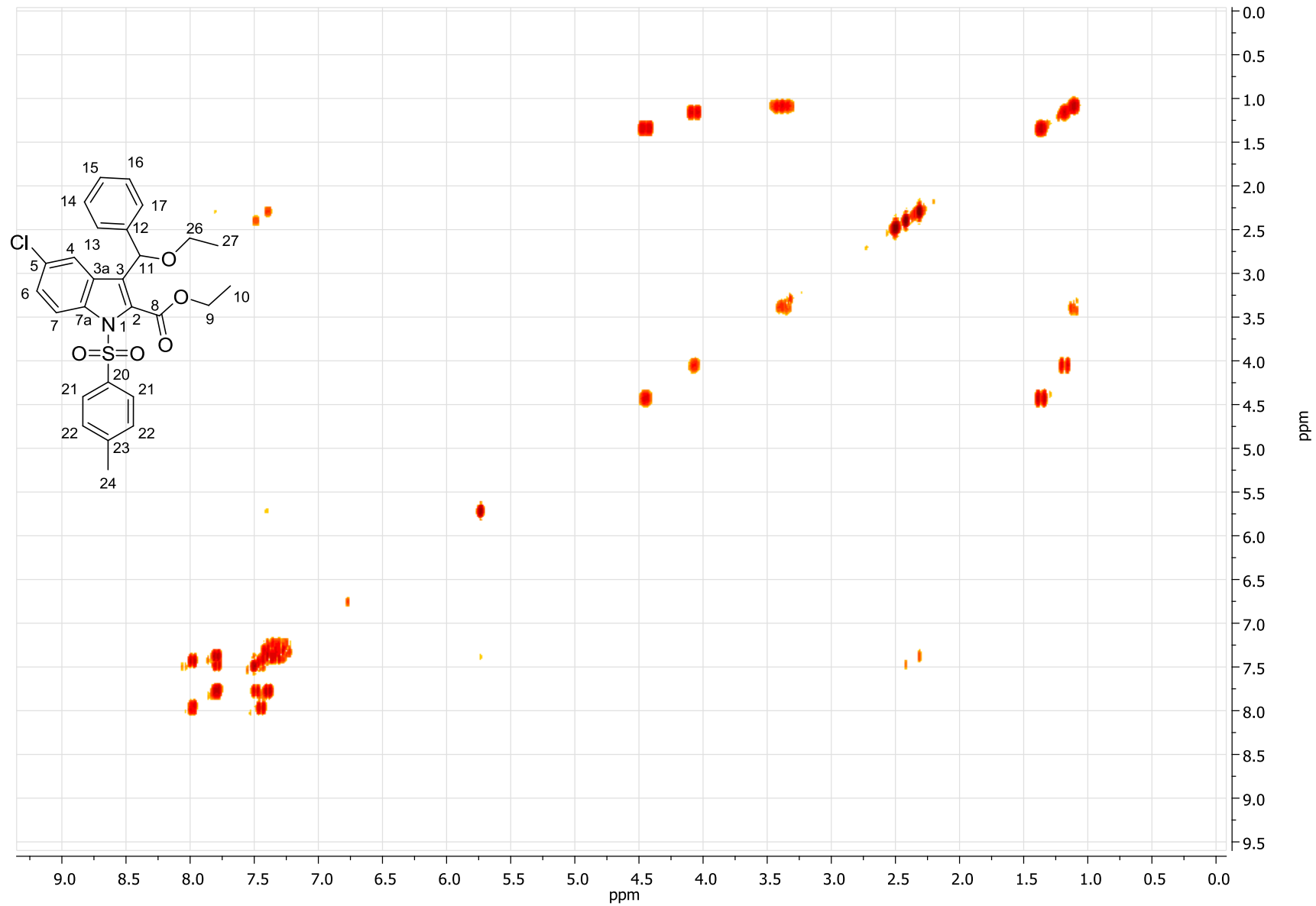
R/S*-ethyl 5-chloro-3-(ethoxy(phenyl)methyl)-1-tosyl-1*H*-indole-2-carboxylate -70-*R/S



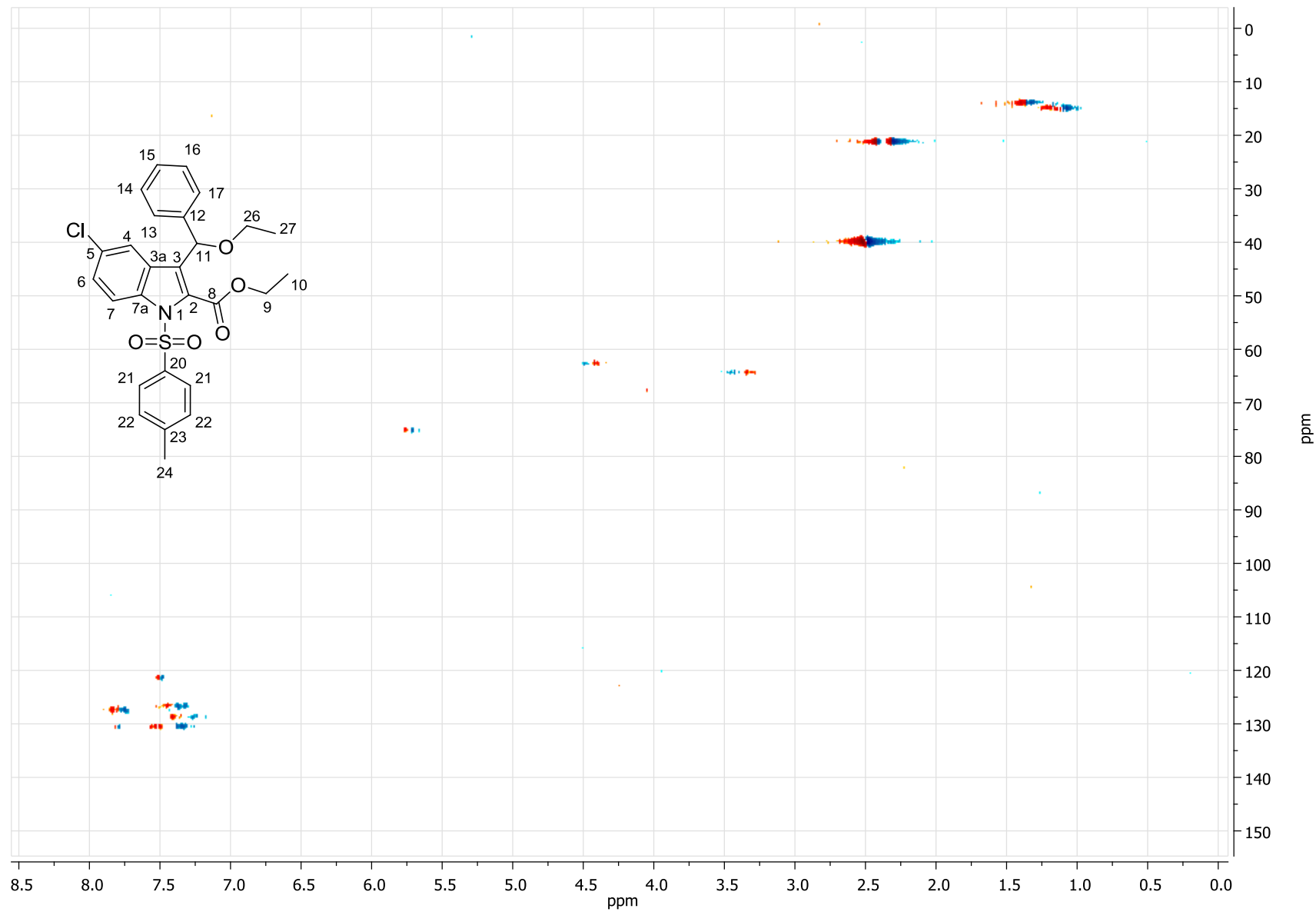
¹H NMR Spectrum
300 MHz Varian VNMRS



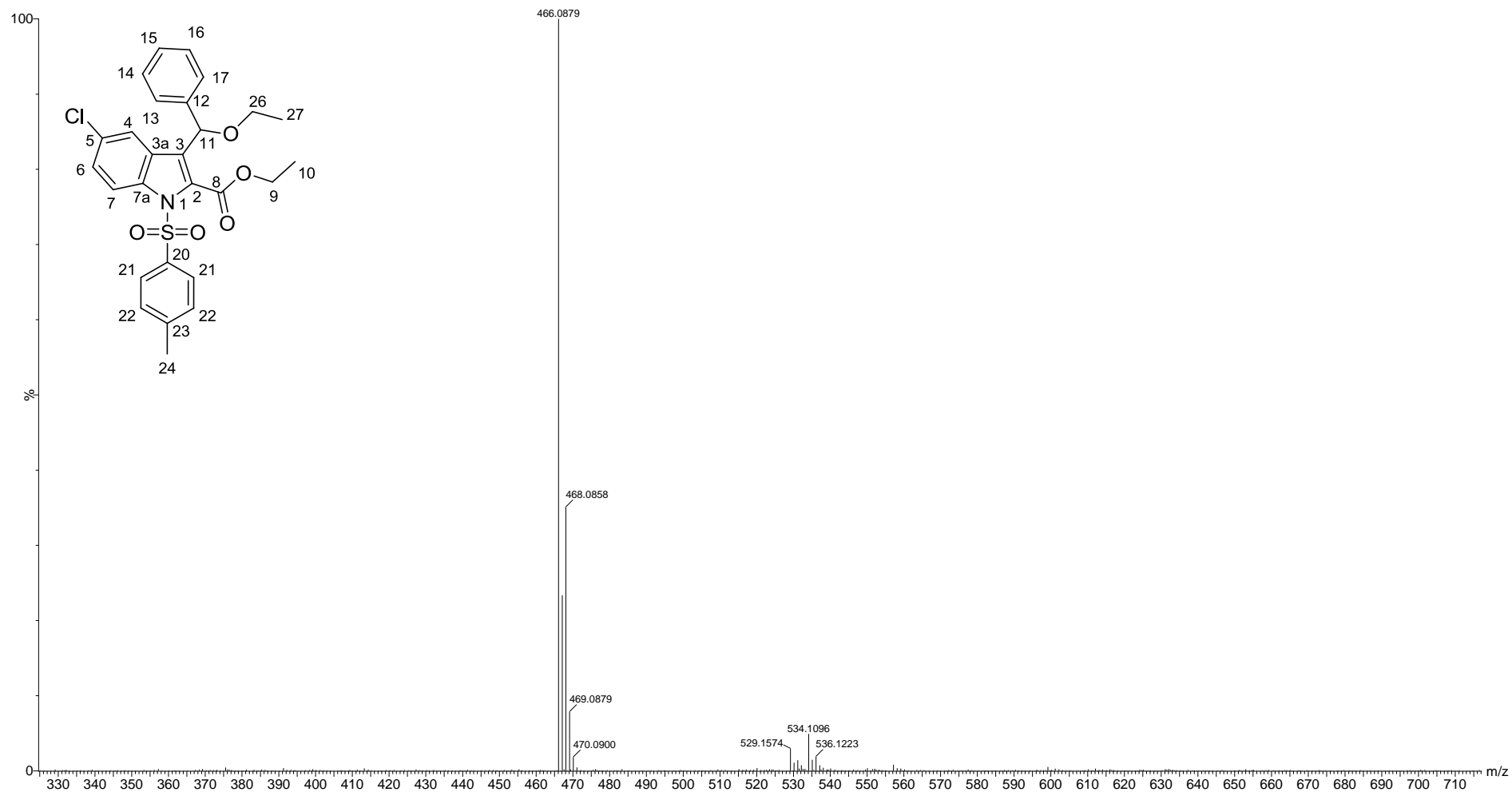
^{13}C NMR Spectrum
75 MHz Varian VNMRS



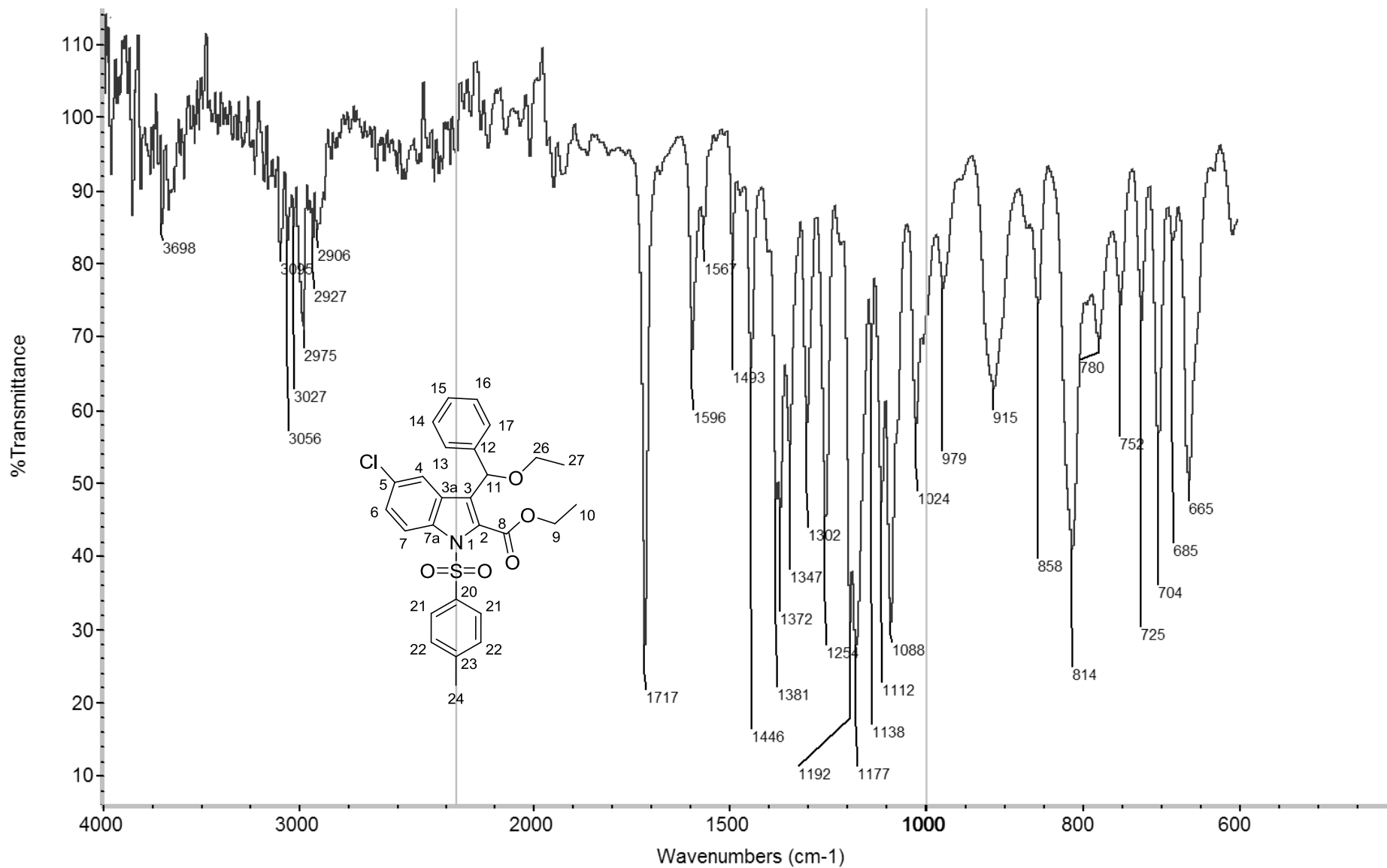
COSY NMR Spectrum
300 MHz Varian VNMRS



gHSQC NMR Spectrum
300 MHz Varian VNMRS

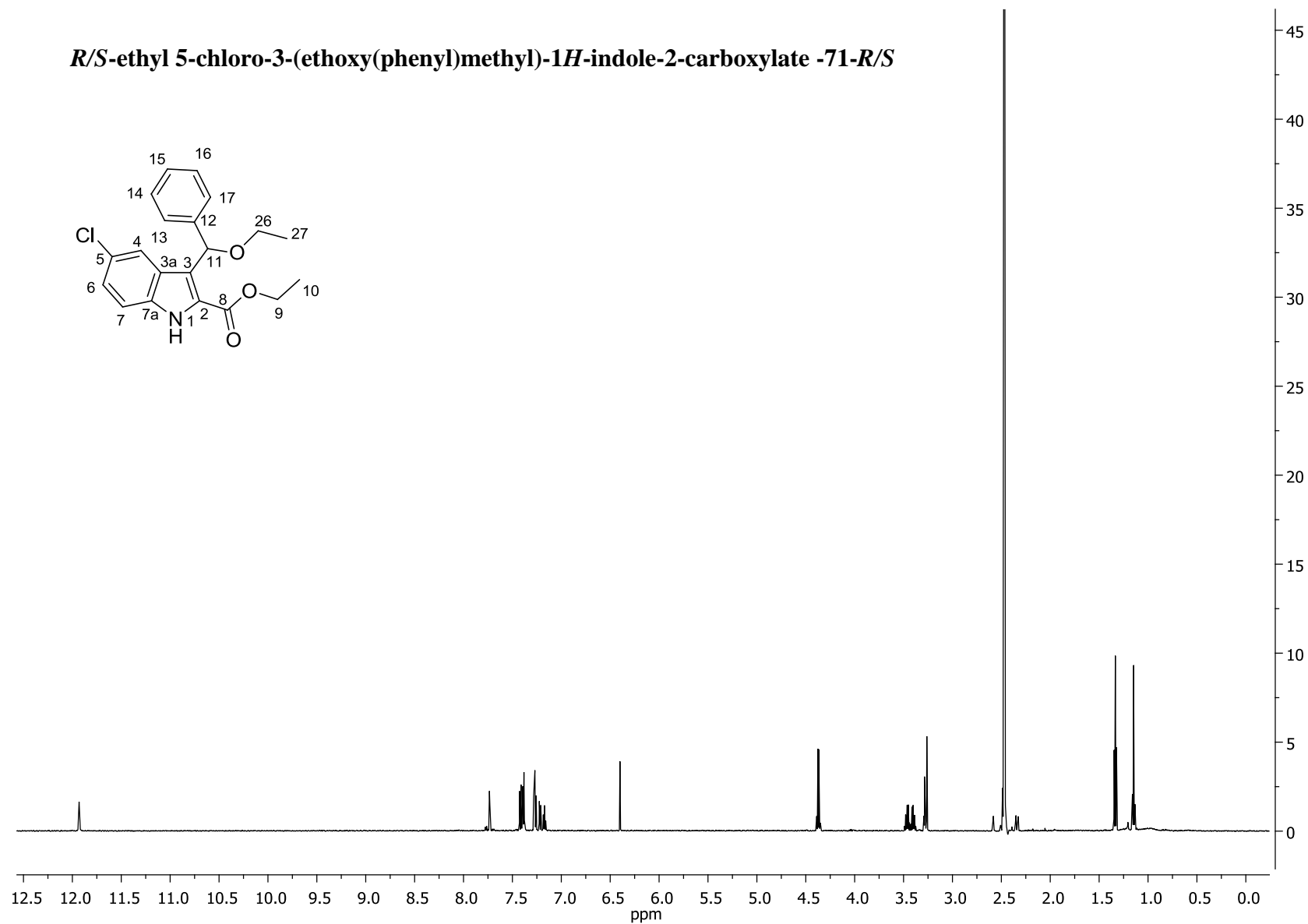


Mass Spectrum
Waters SYNAPT G2

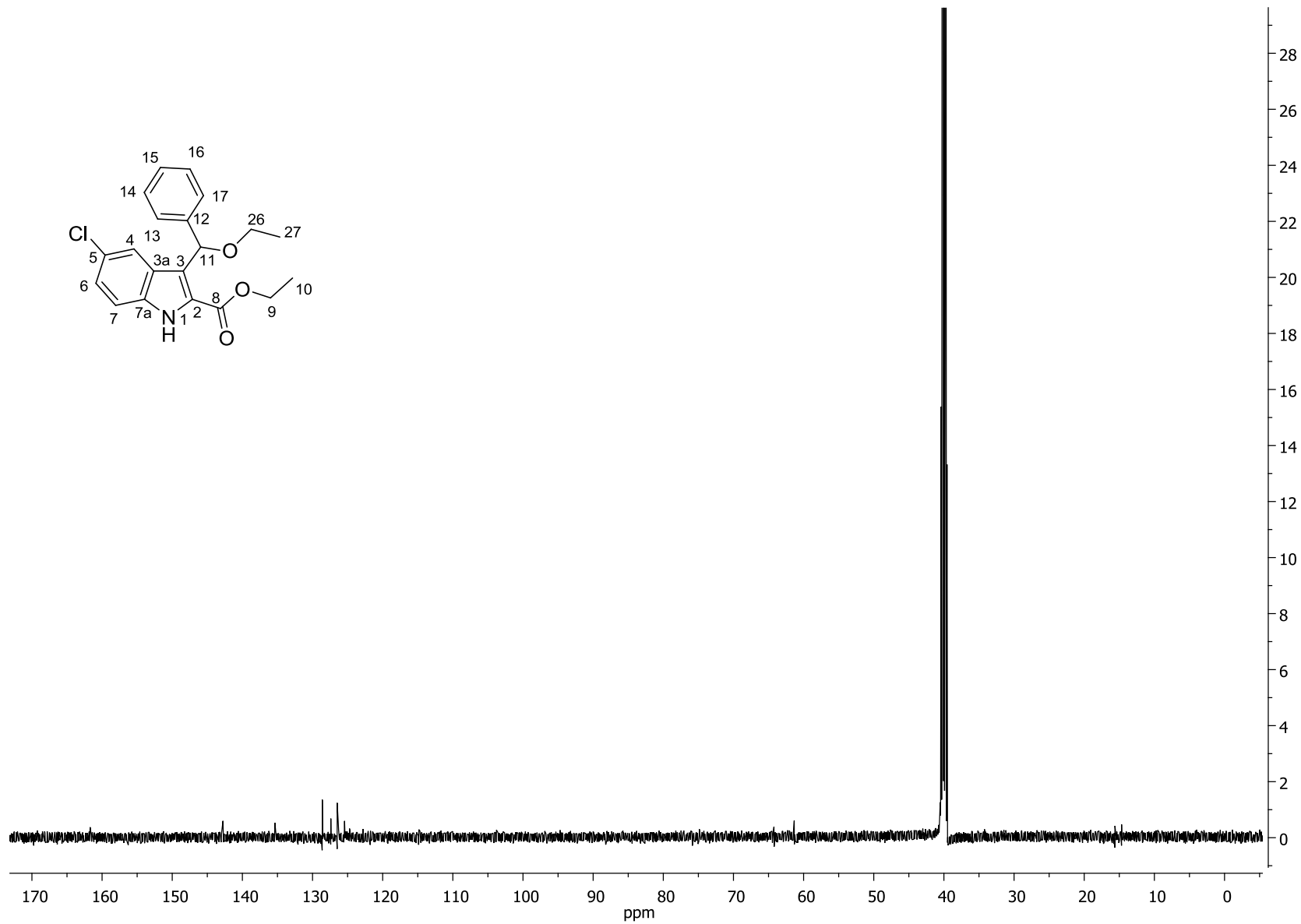


Infrared Spectrum
Thermo Nicolet Nexus 470

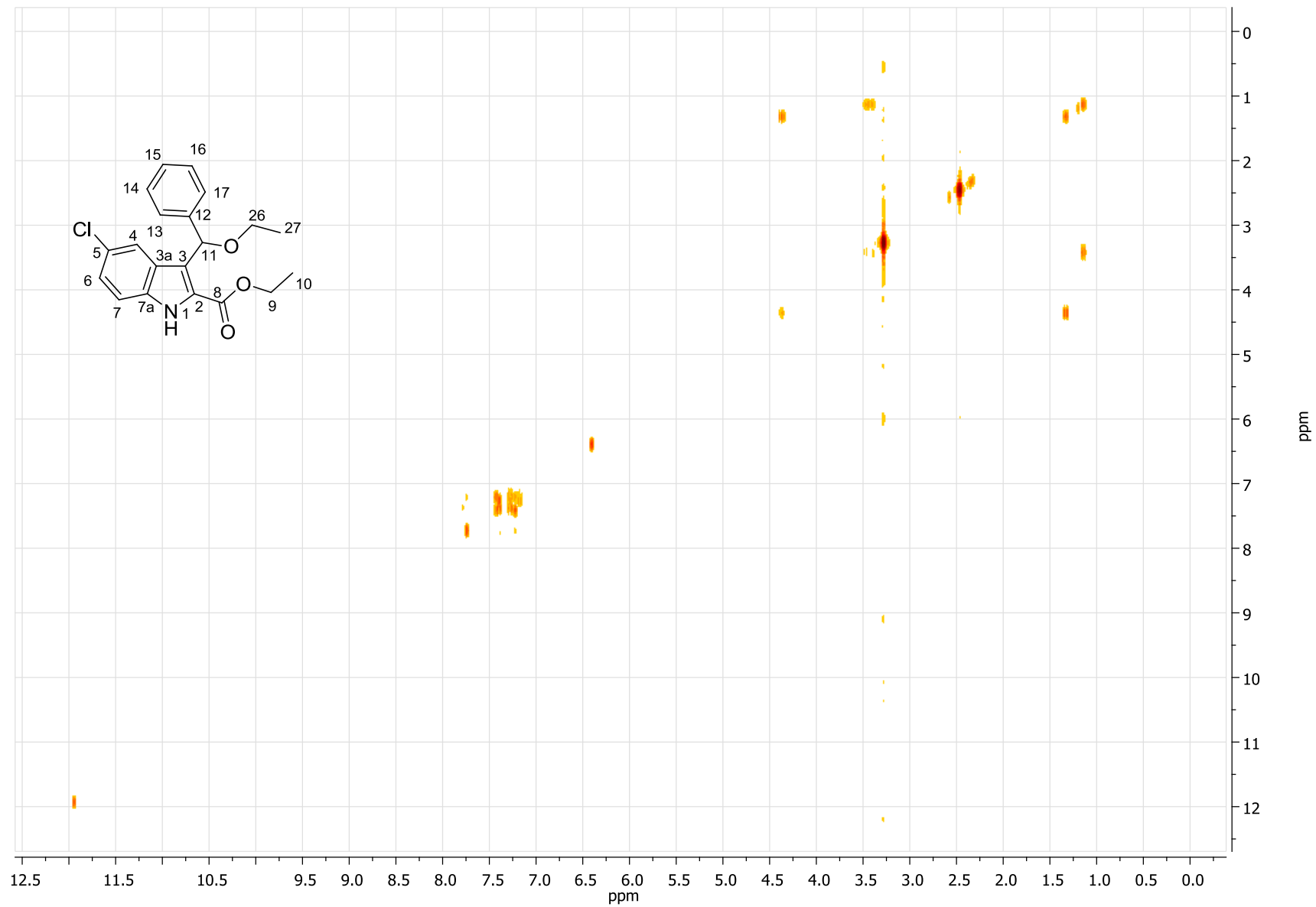
R/S*-ethyl 5-chloro-3-(ethoxy(phenyl)methyl)-1*H*-indole-2-carboxylate -71-*R/S



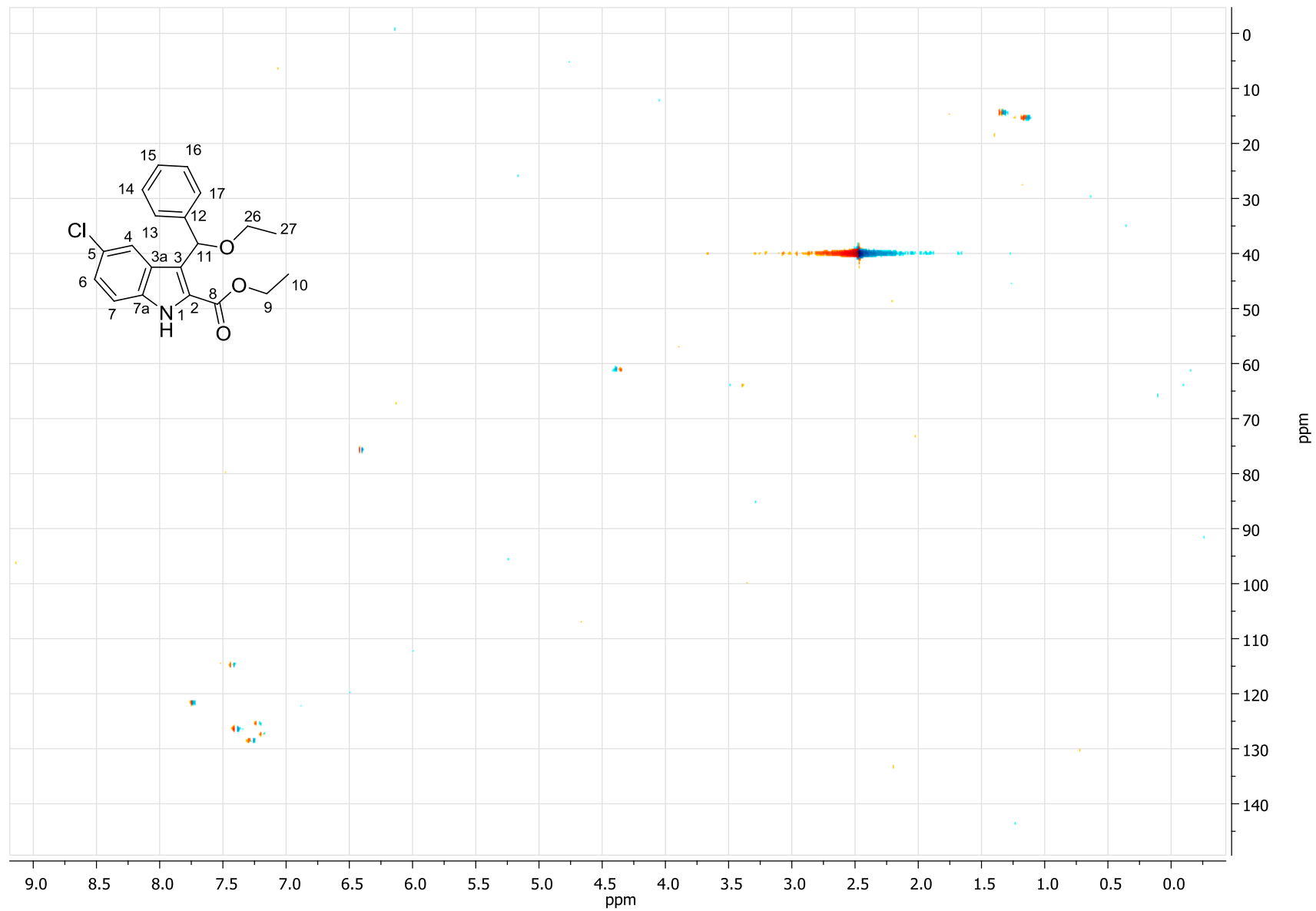
¹H NMR Spectrum
300 MHz Varian VNMRS



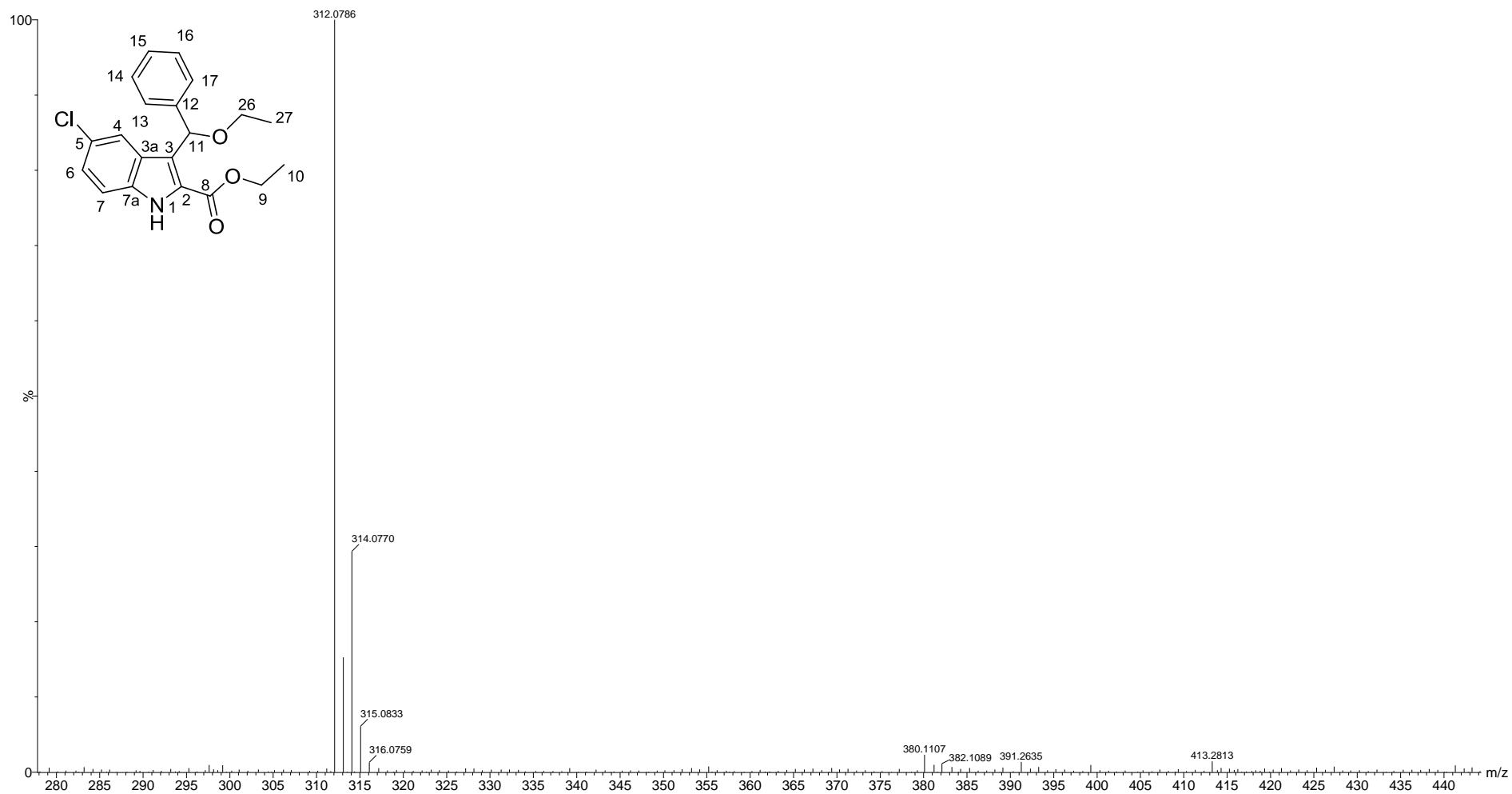
^{13}C NMR Spectrum
75 MHz Varian VNMRS



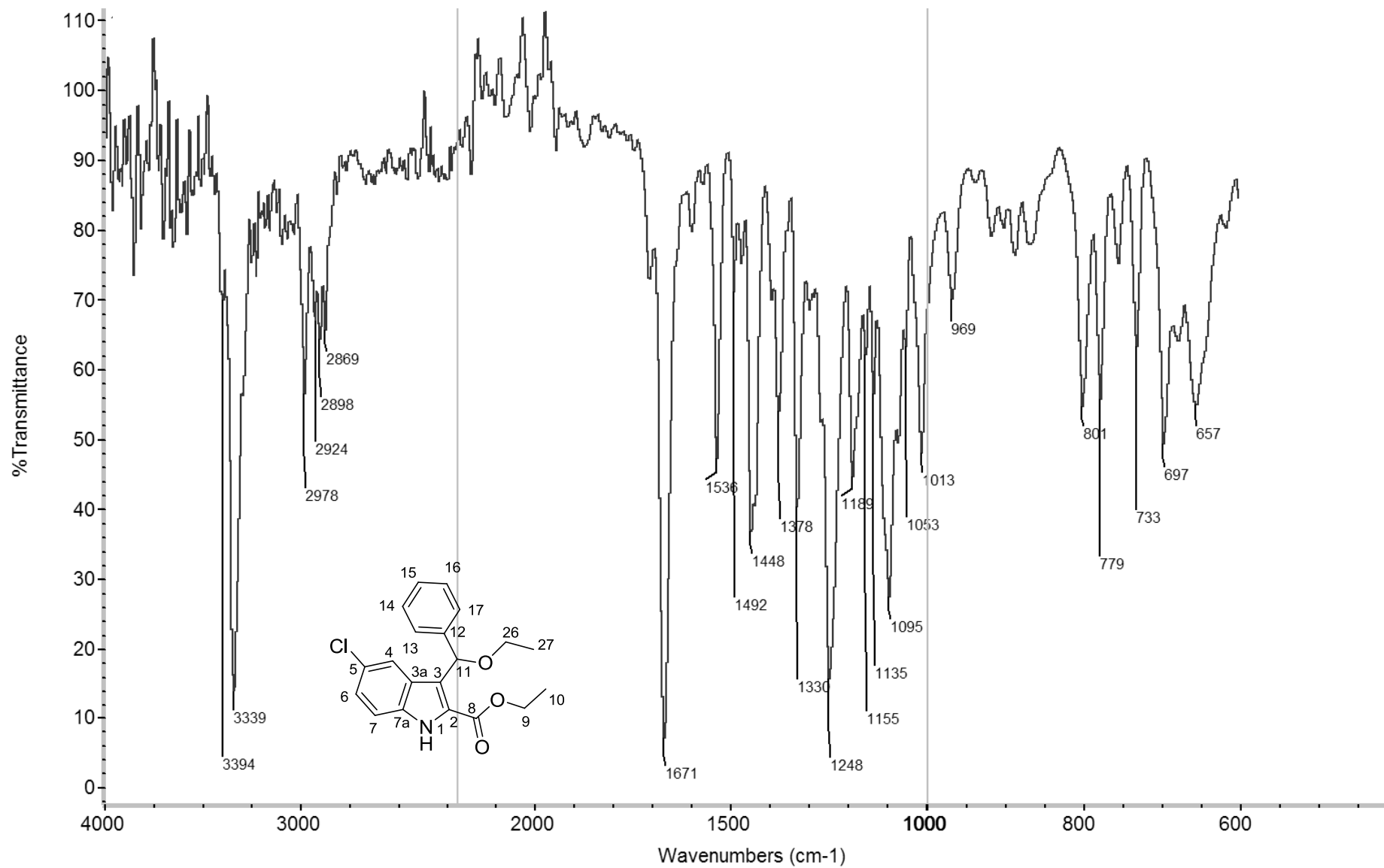
COSY NMR Spectrum
300 MHz Varian VNMRS



gHSQC NMR Spectrum
300 MHz Varian VNMRS

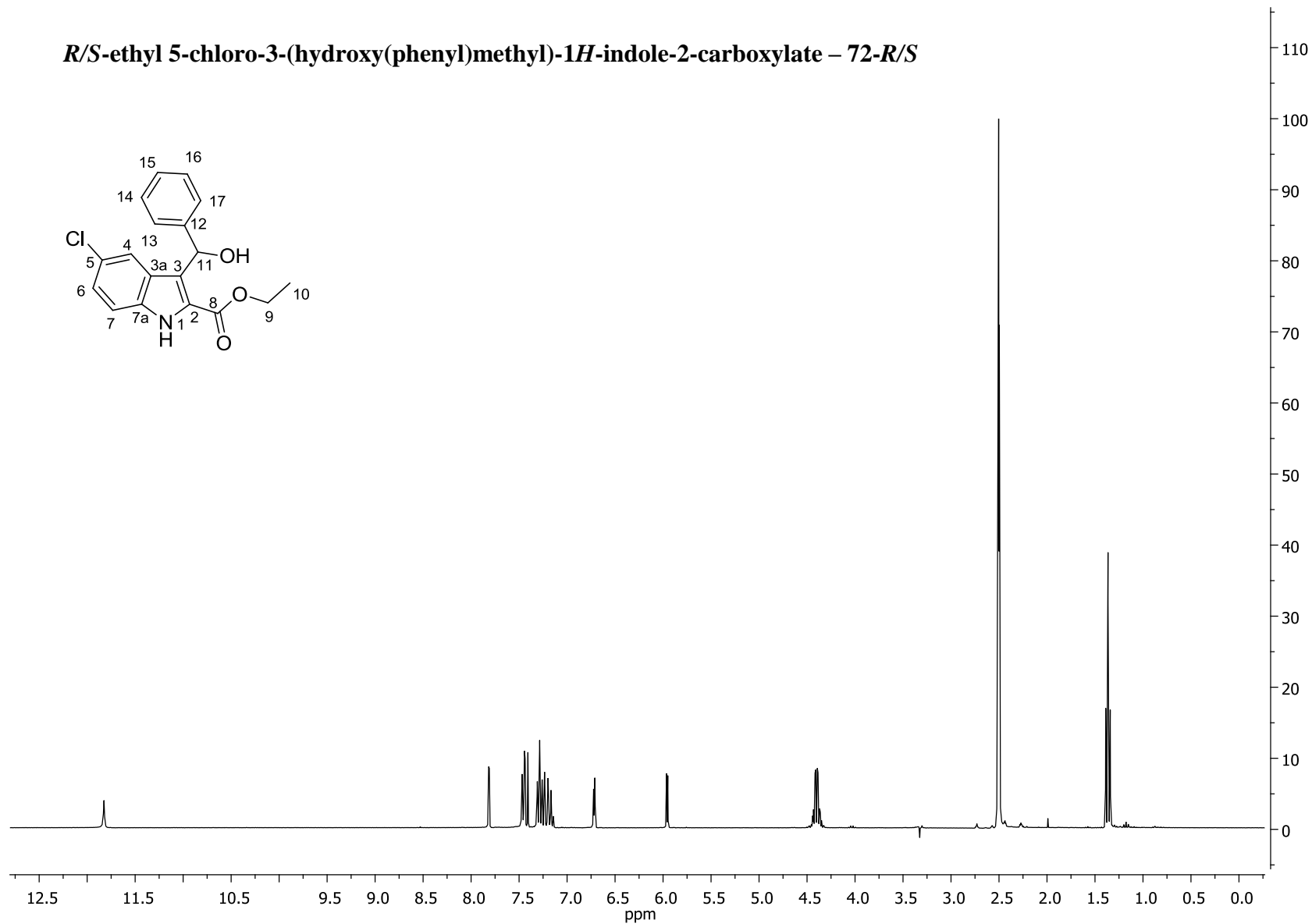


Mass Spectrum
Waters SYNAPT G2

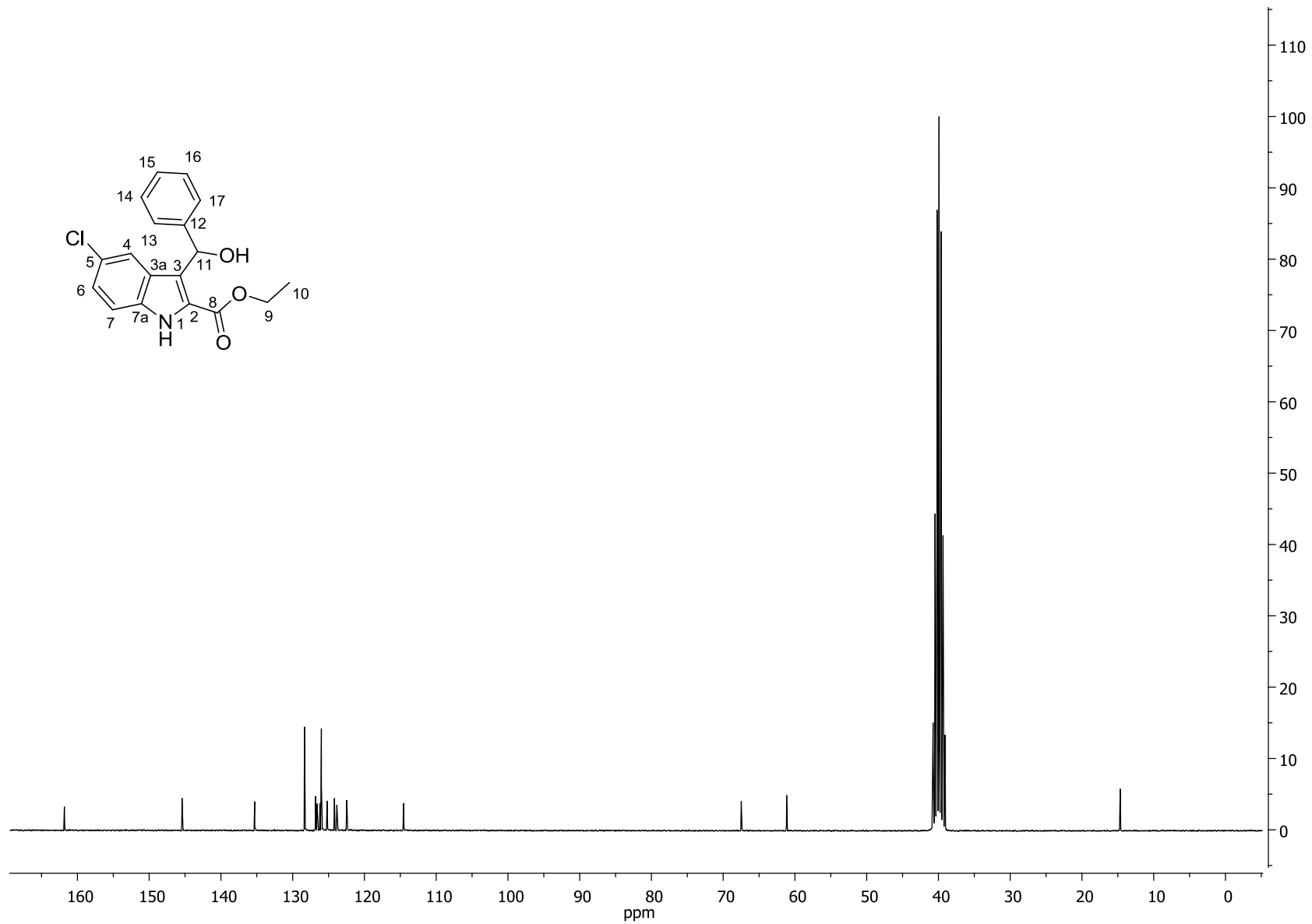


Infrared Spectrum
Thermo Nicolet Nexus 470

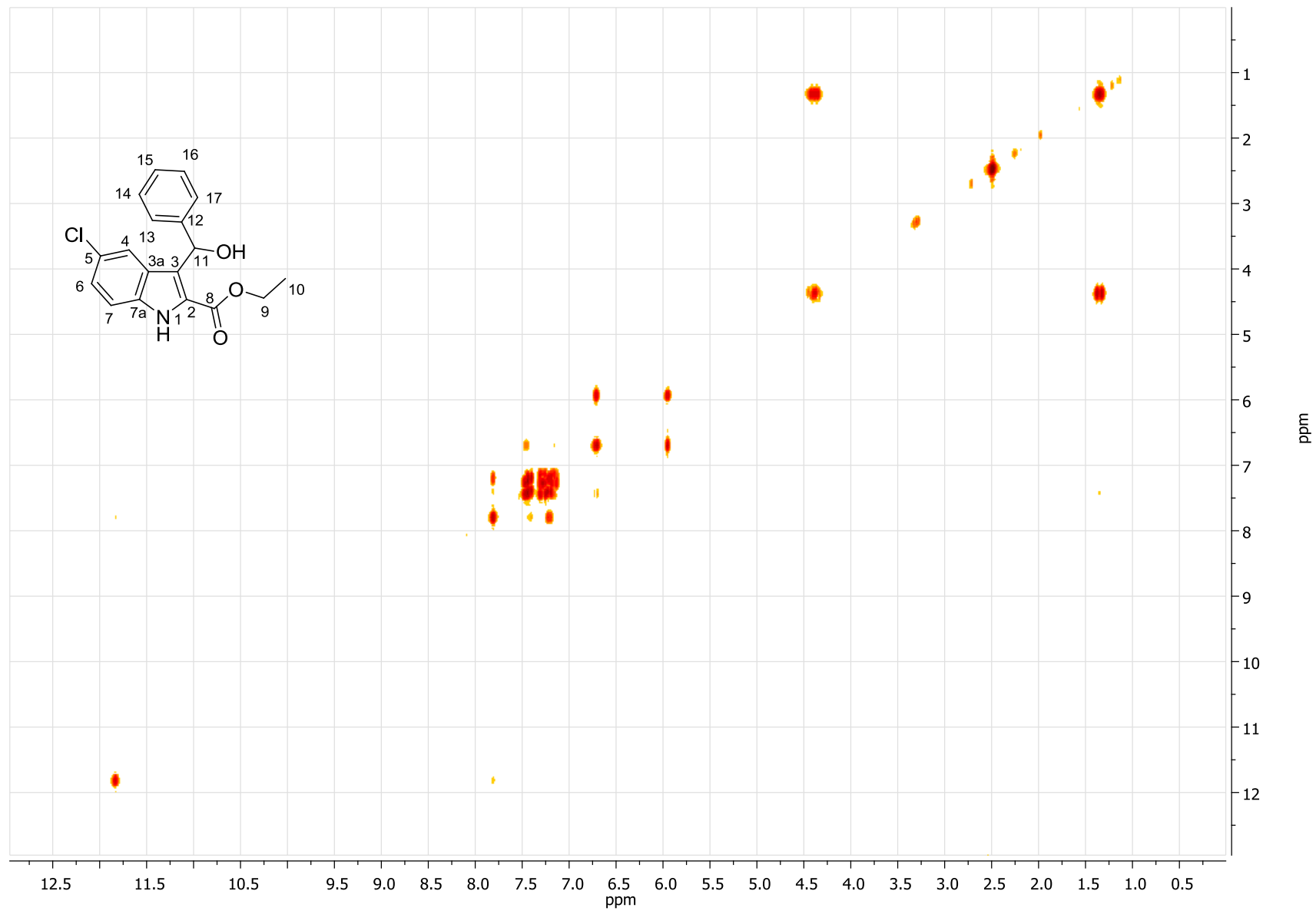
R/S*-ethyl 5-chloro-3-(hydroxy(phenyl)methyl)-1*H*-indole-2-carboxylate – 72-*R/S



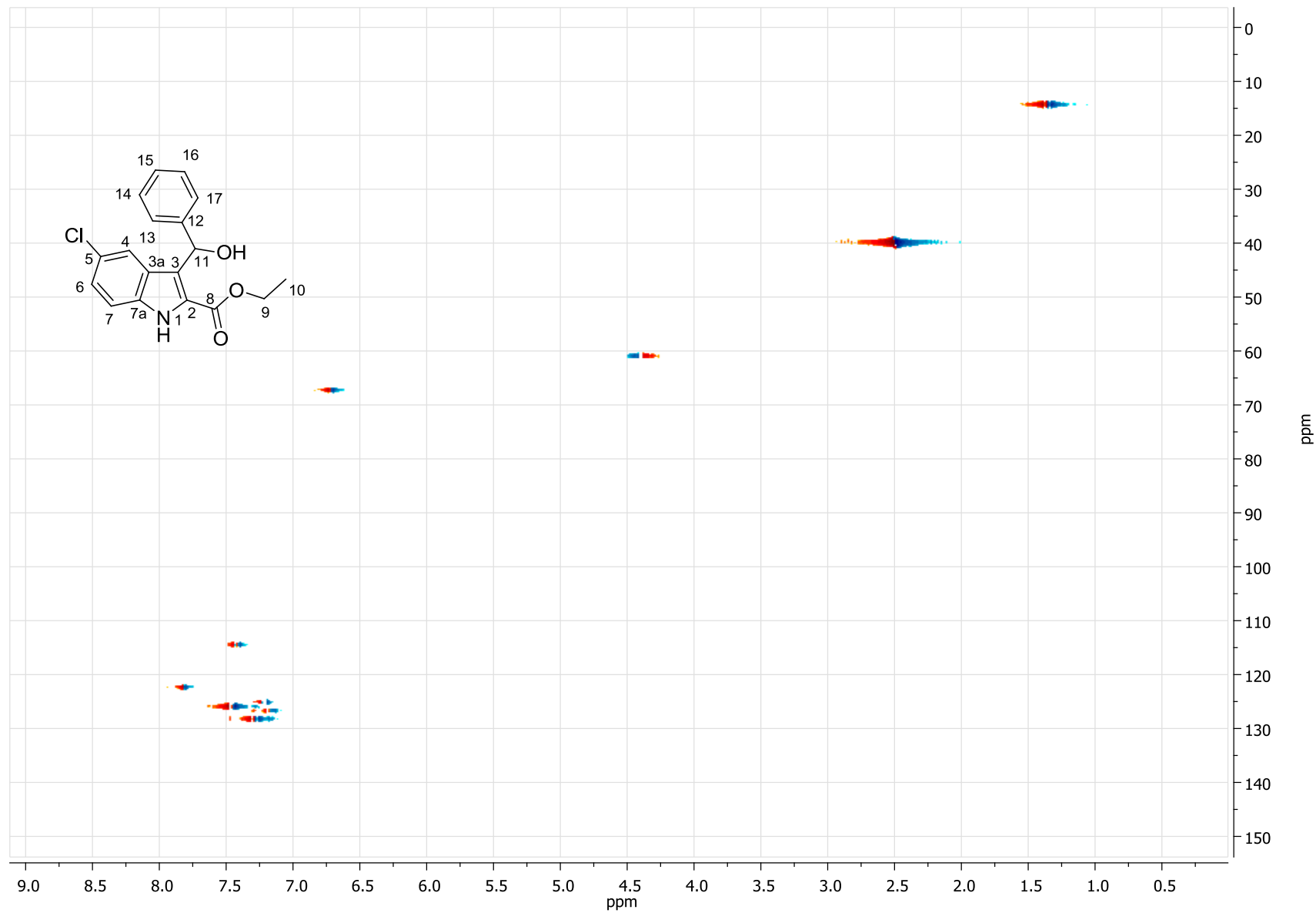
¹H NMR Spectrum
300 MHz Varian VNMRS



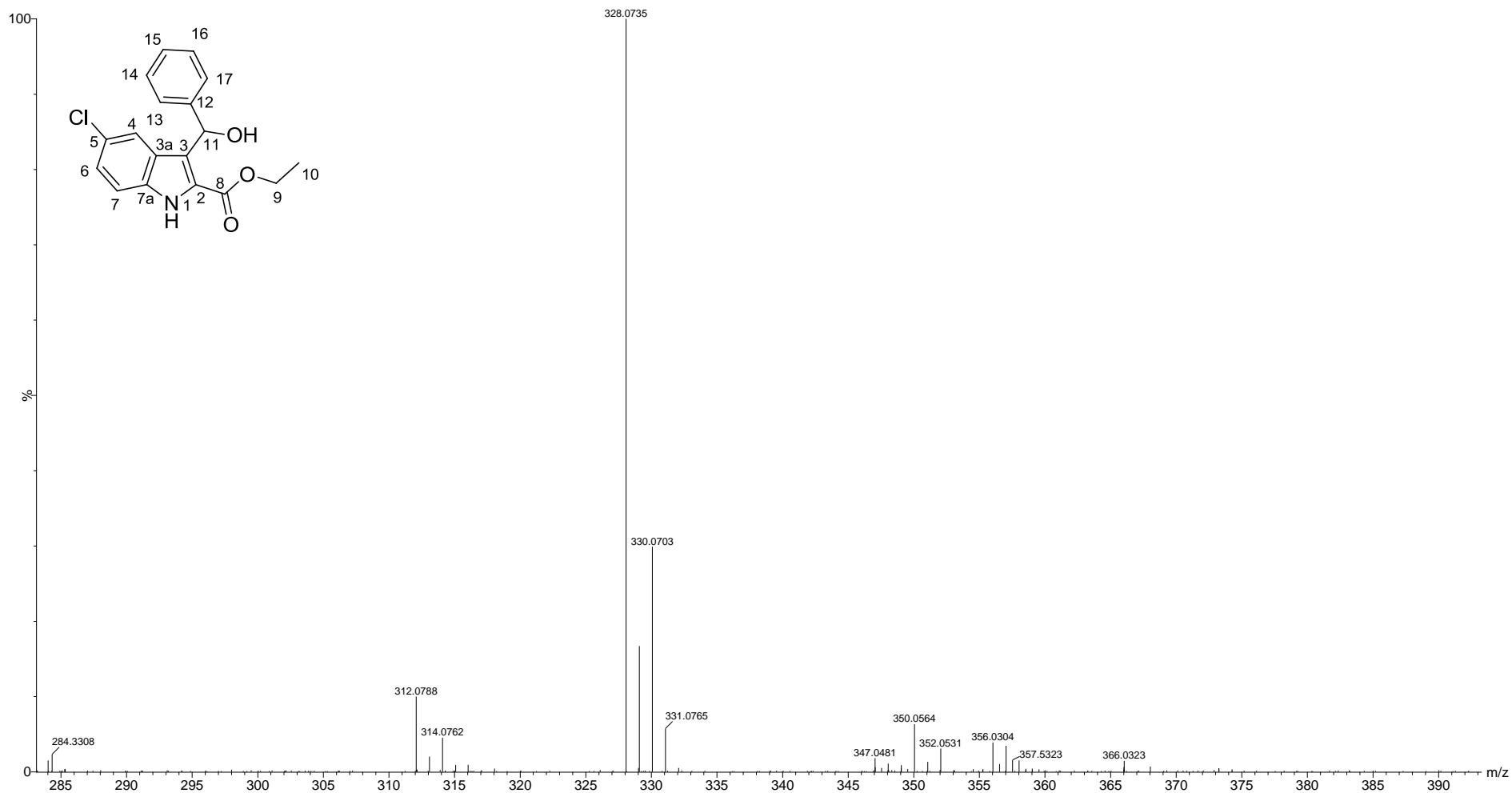
^{13}C NMR Spectrum
75 MHz Varian VNMRS



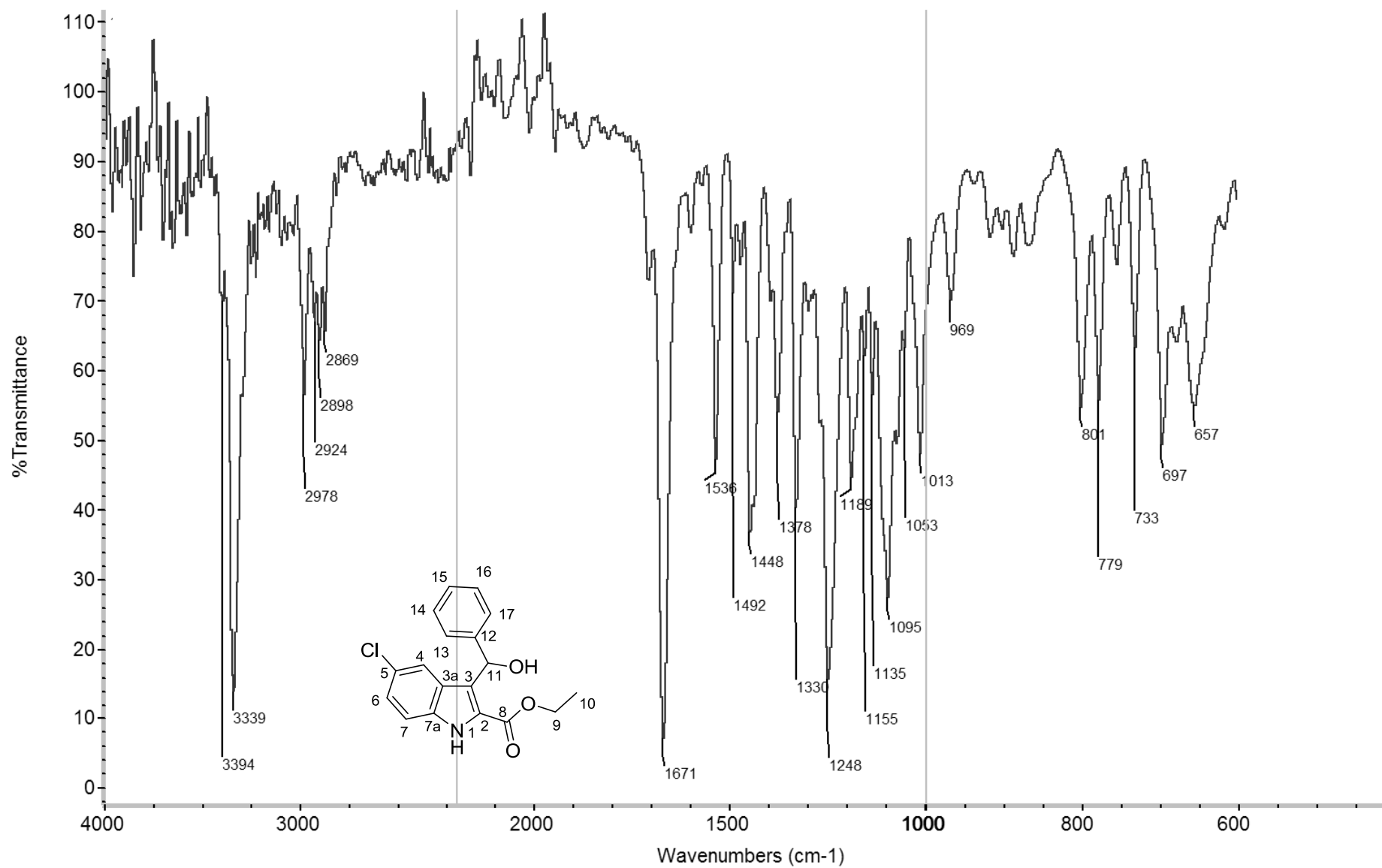
COSY NMR Spectrum
300 MHz Varian VNMRS



gHSQC NMR Spectrum
300 MHz Varian VNMRS

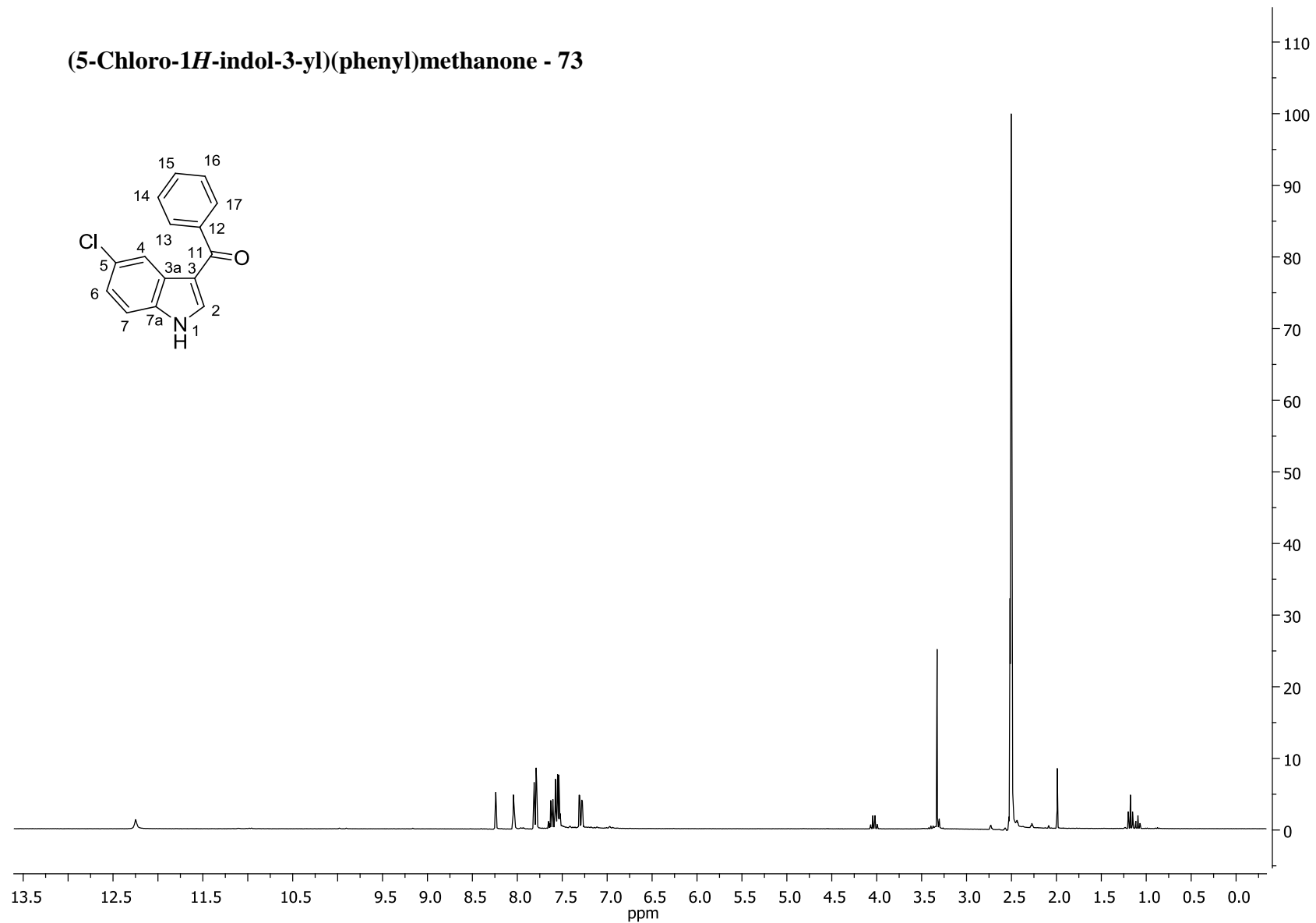
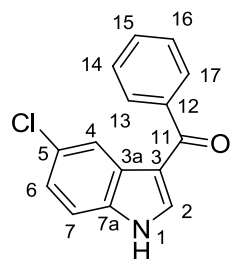


Mass Spectrum
Waters SYNAPT G2

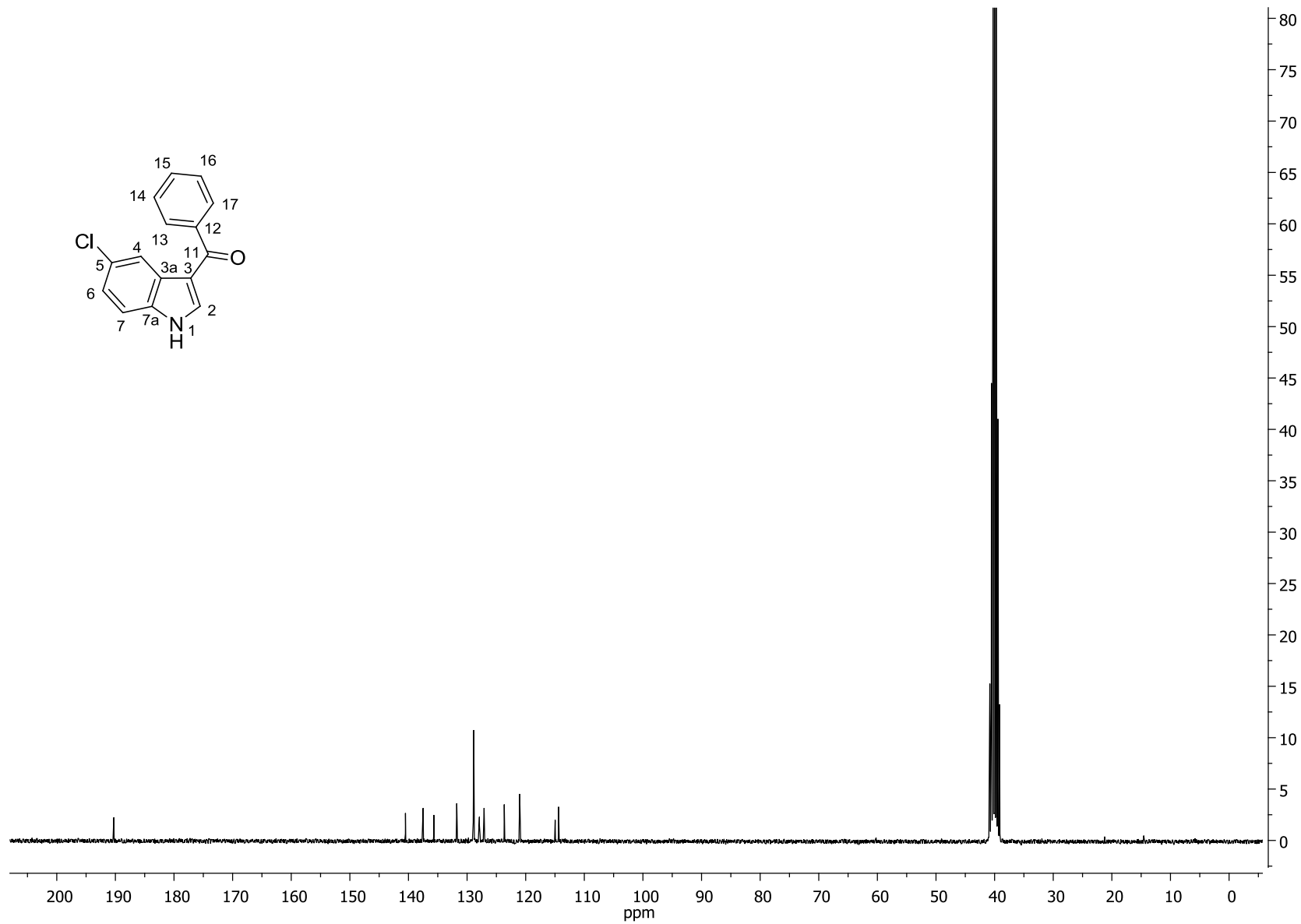


Infrared Spectrum
Thermo Nicolet Nexus 470

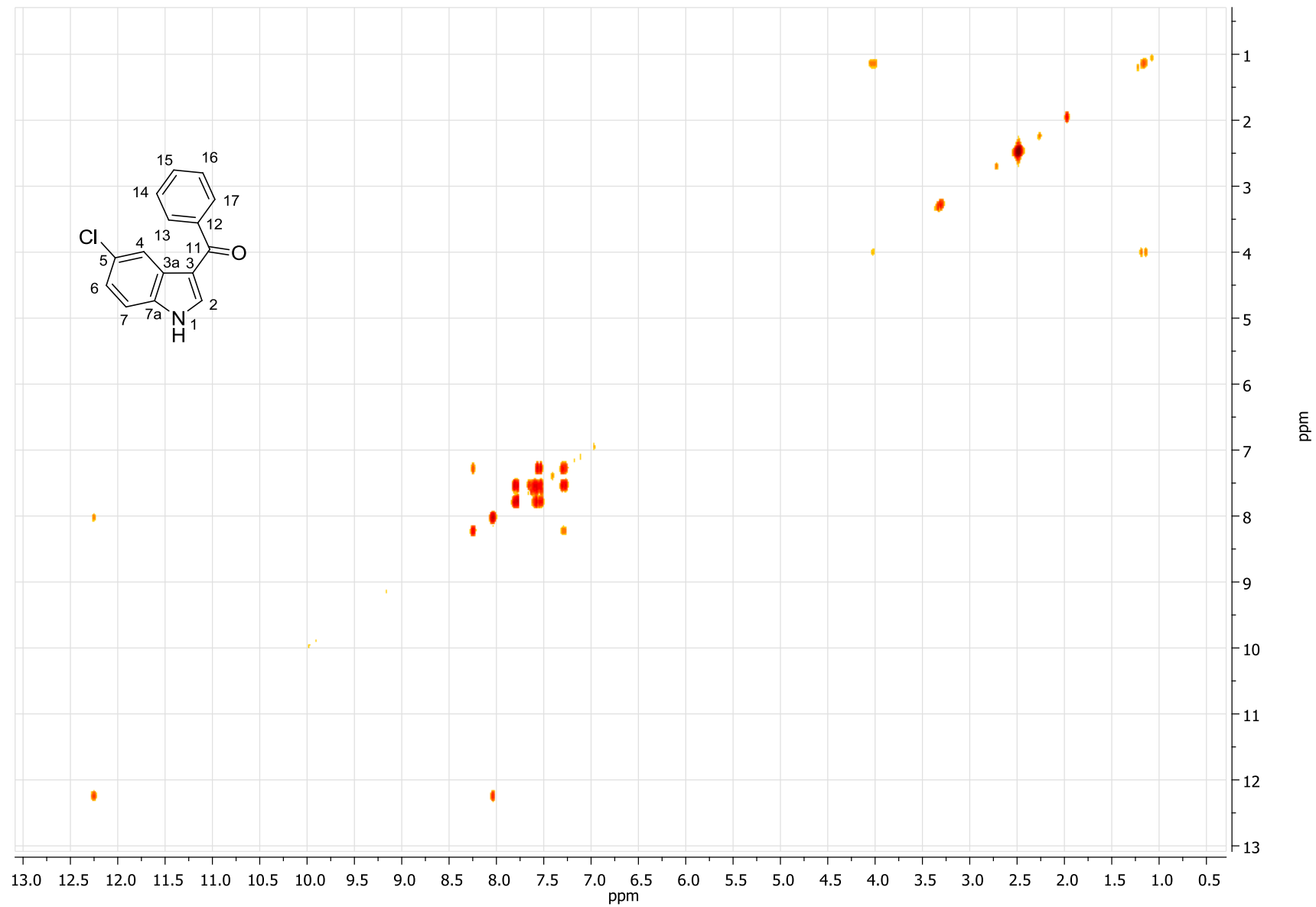
(5-Chloro-1*H*-indol-3-yl)(phenyl)methanone - 73



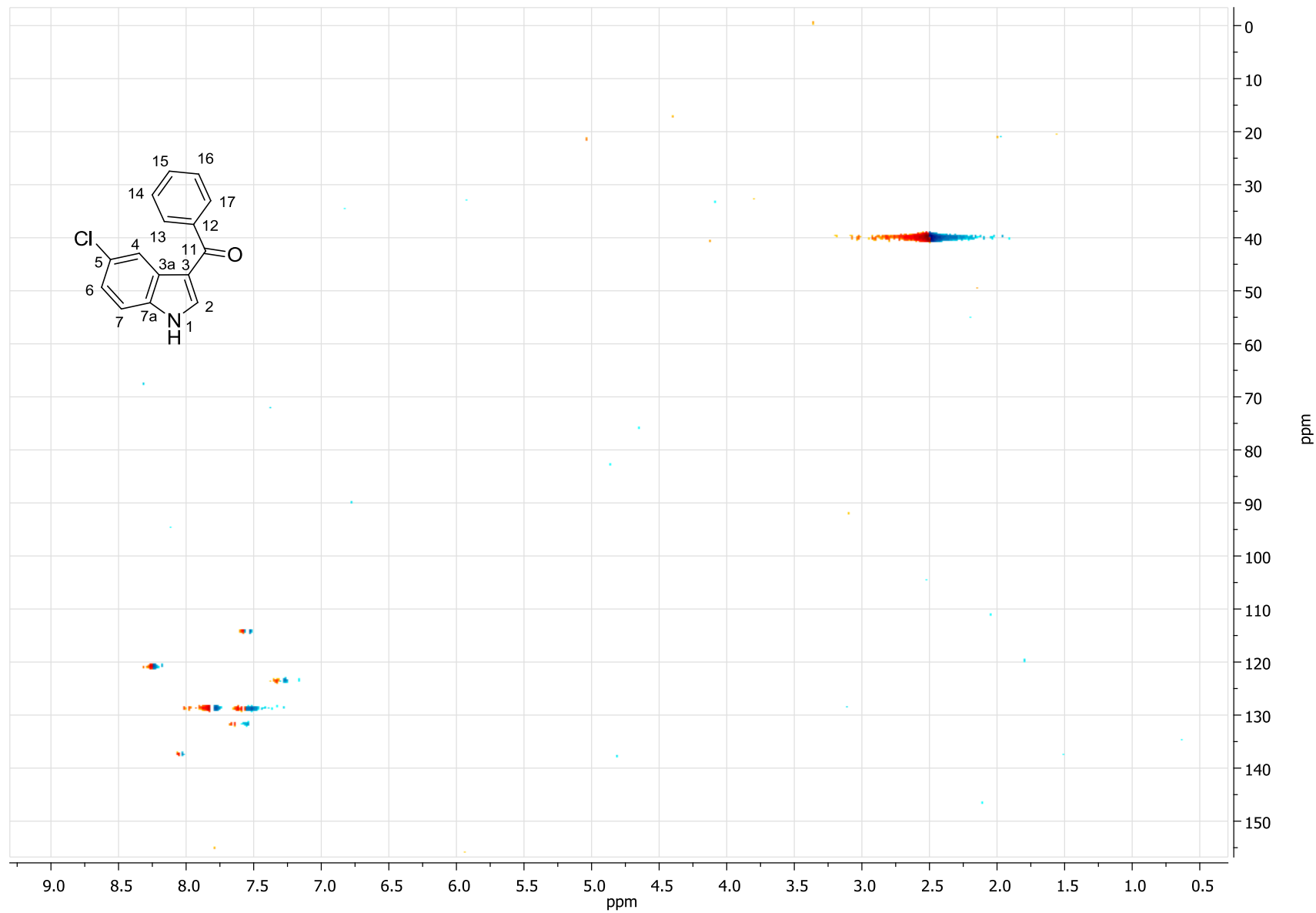
¹H NMR Spectrum
300 MHz Varian VNMRS



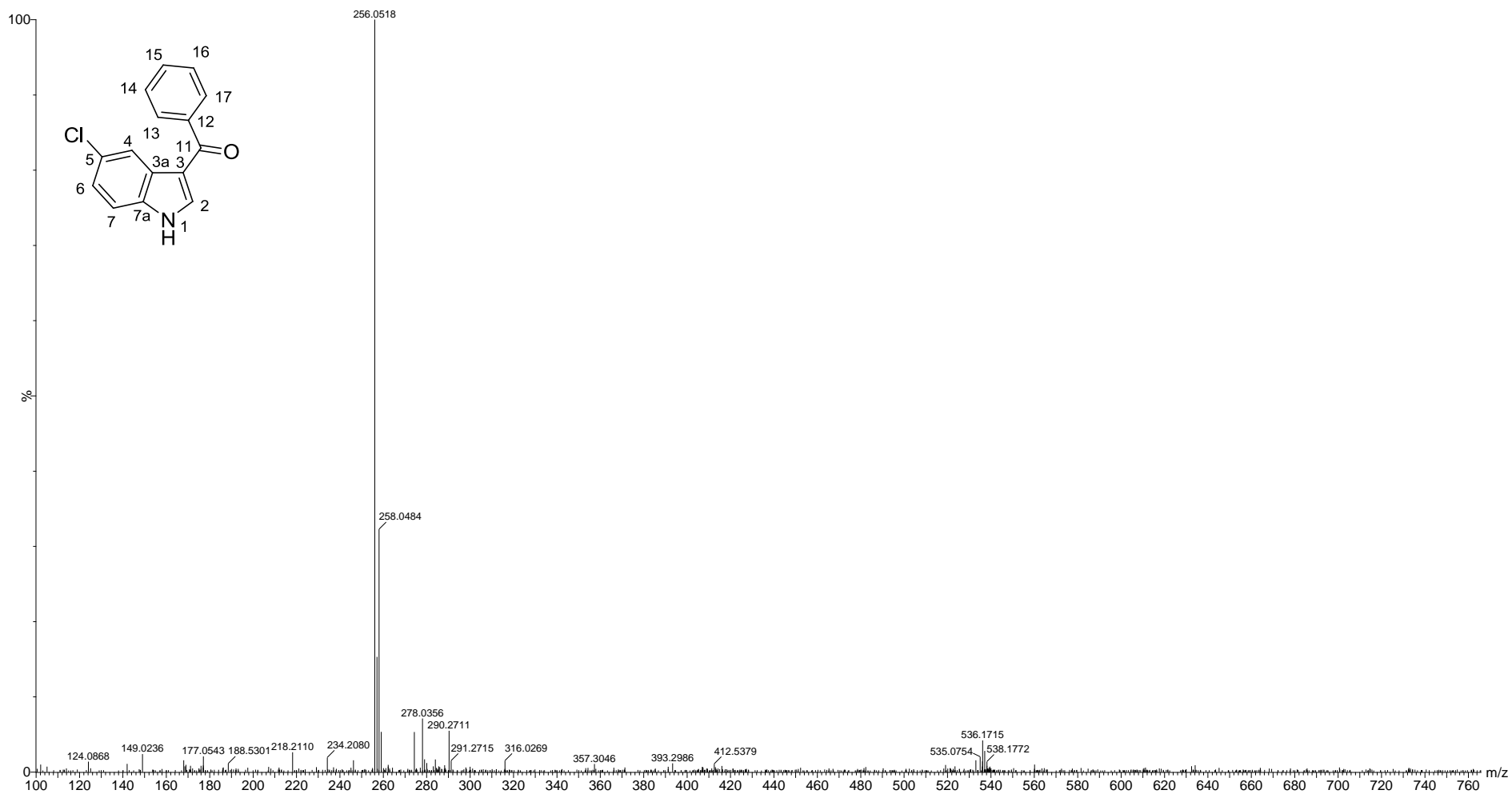
^{13}C NMR Spectrum
75 MHz Varian VNMRS



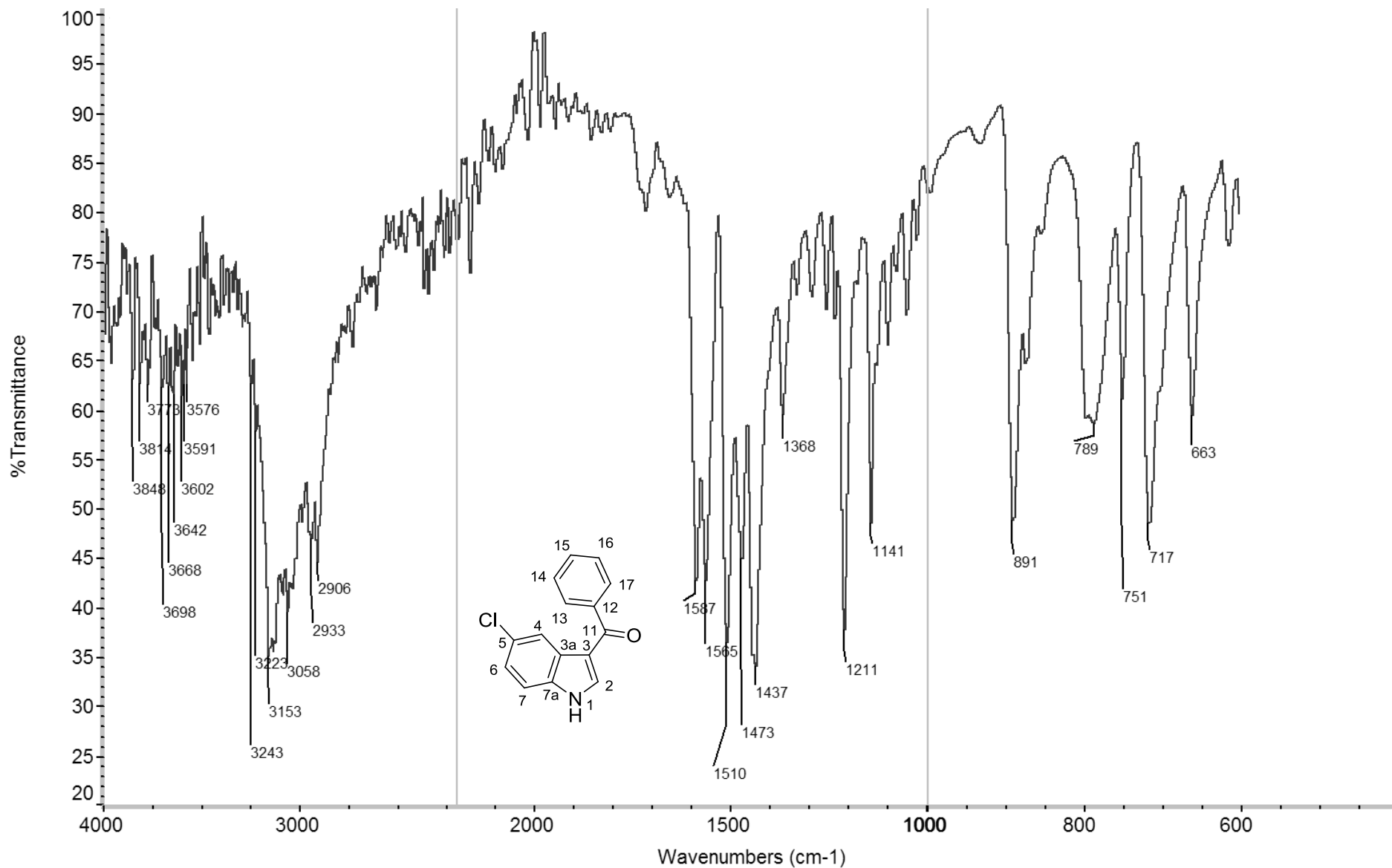
COSY NMR Spectrum
300 MHz Varian VNMRS



gHSQC NMR Spectrum
300 MHz Varian VNMRS

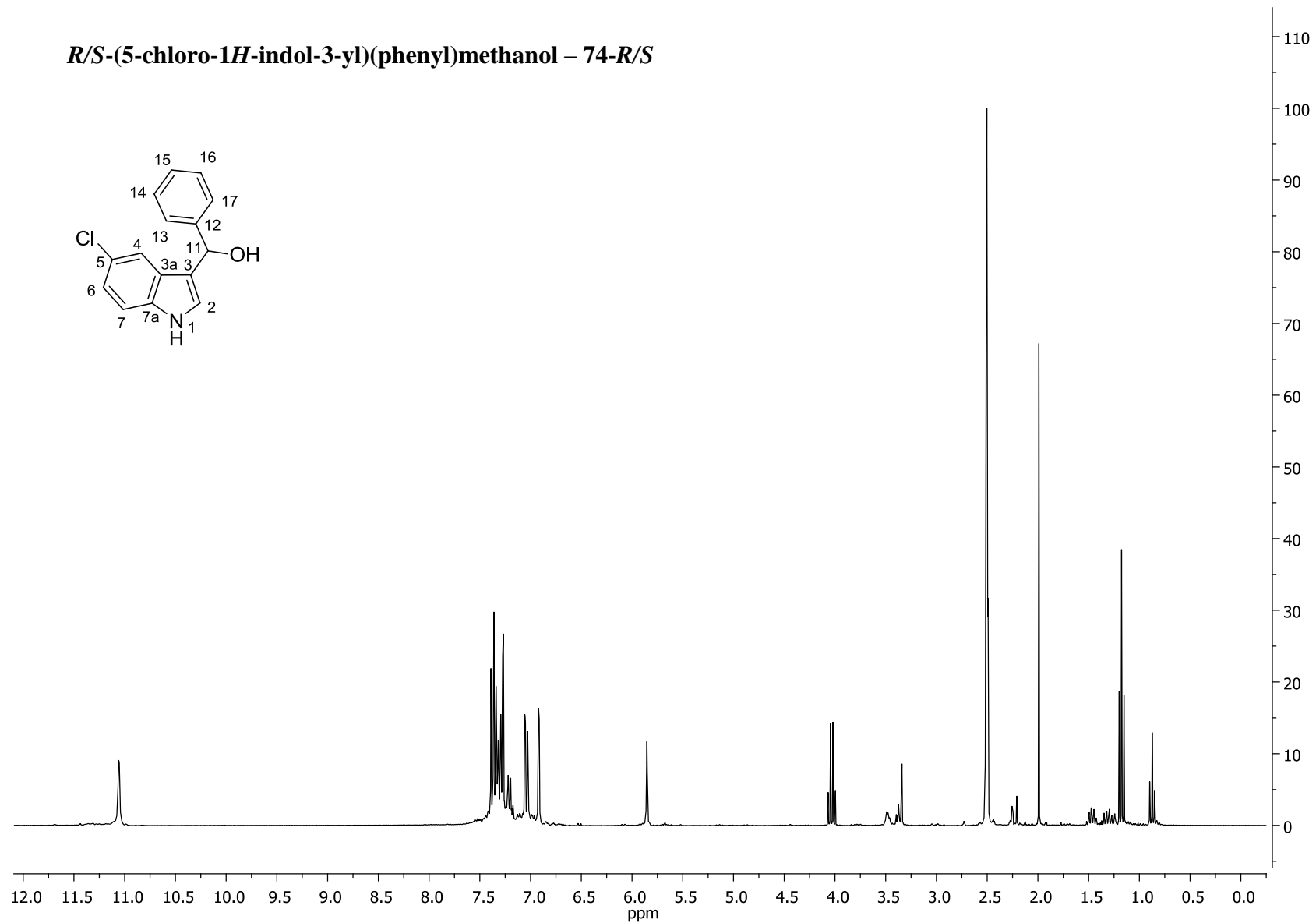


Mass Spectrum
Waters SYNAPT G2

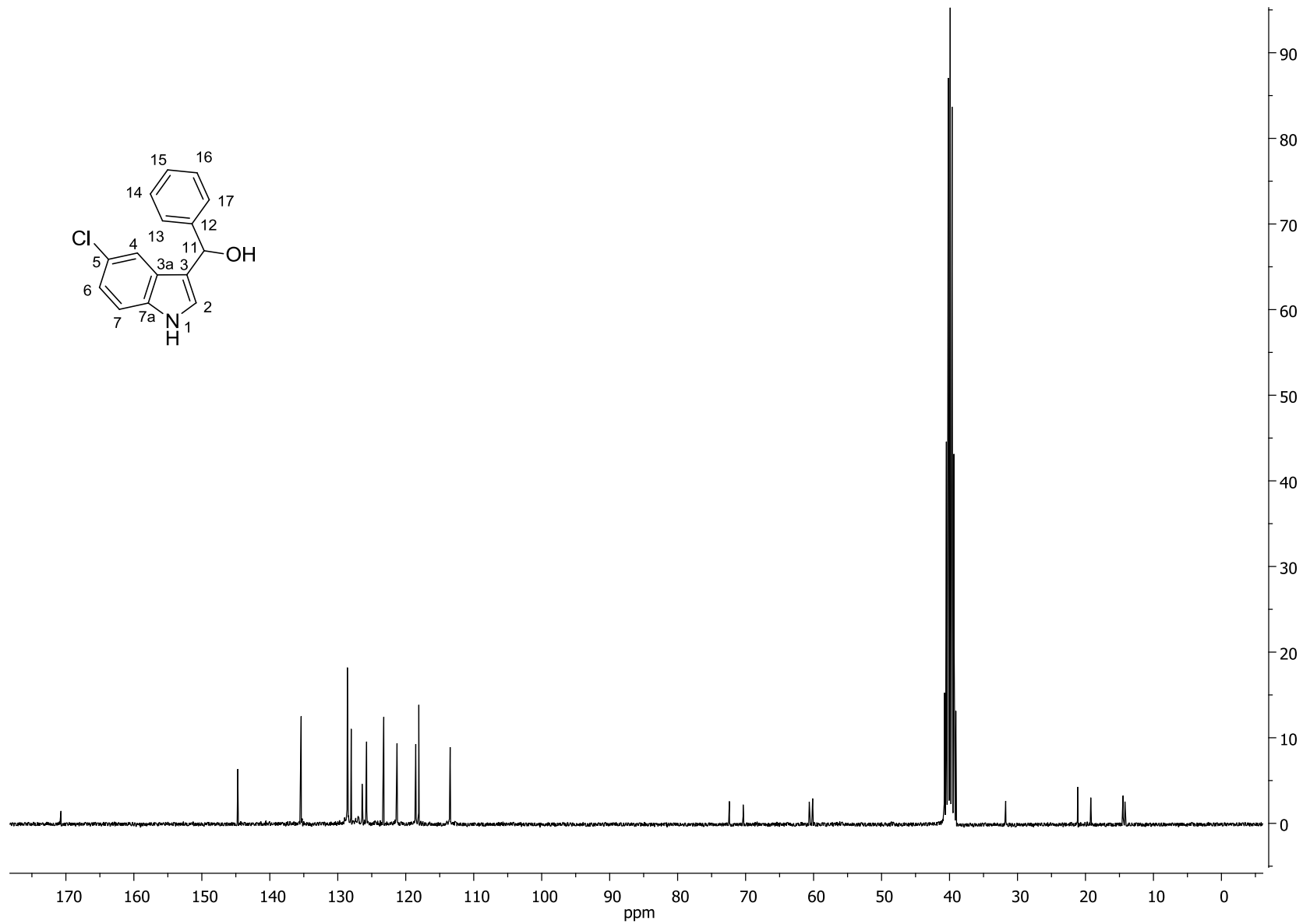


Infrared Spectrum
Thermo Nicolet Nexus 470

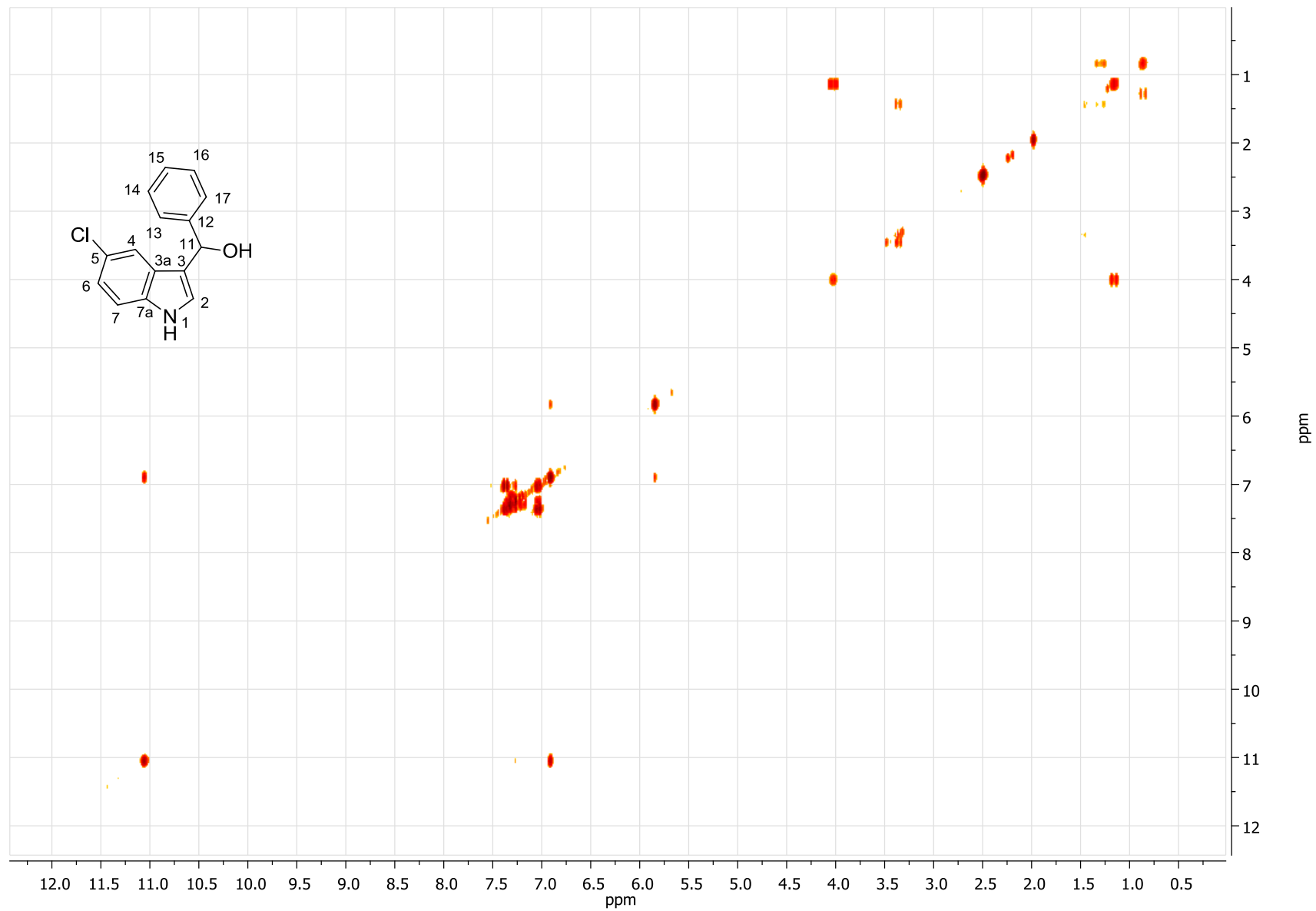
R/S*-(5-chloro-1*H*-indol-3-yl)(phenyl)methanol – 74-*R/S



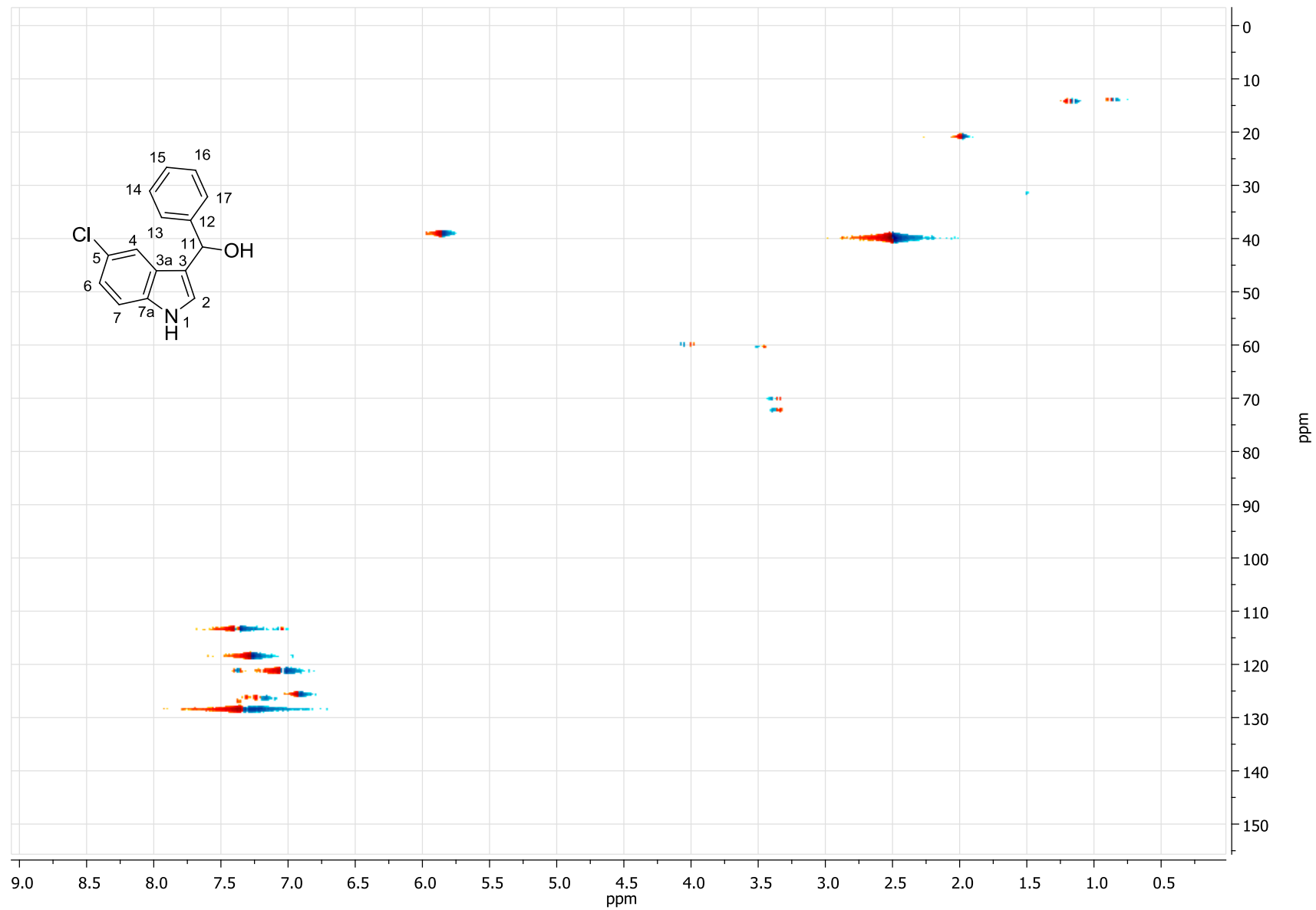
^1H NMR Spectrum
300 MHz Varian VNMRS



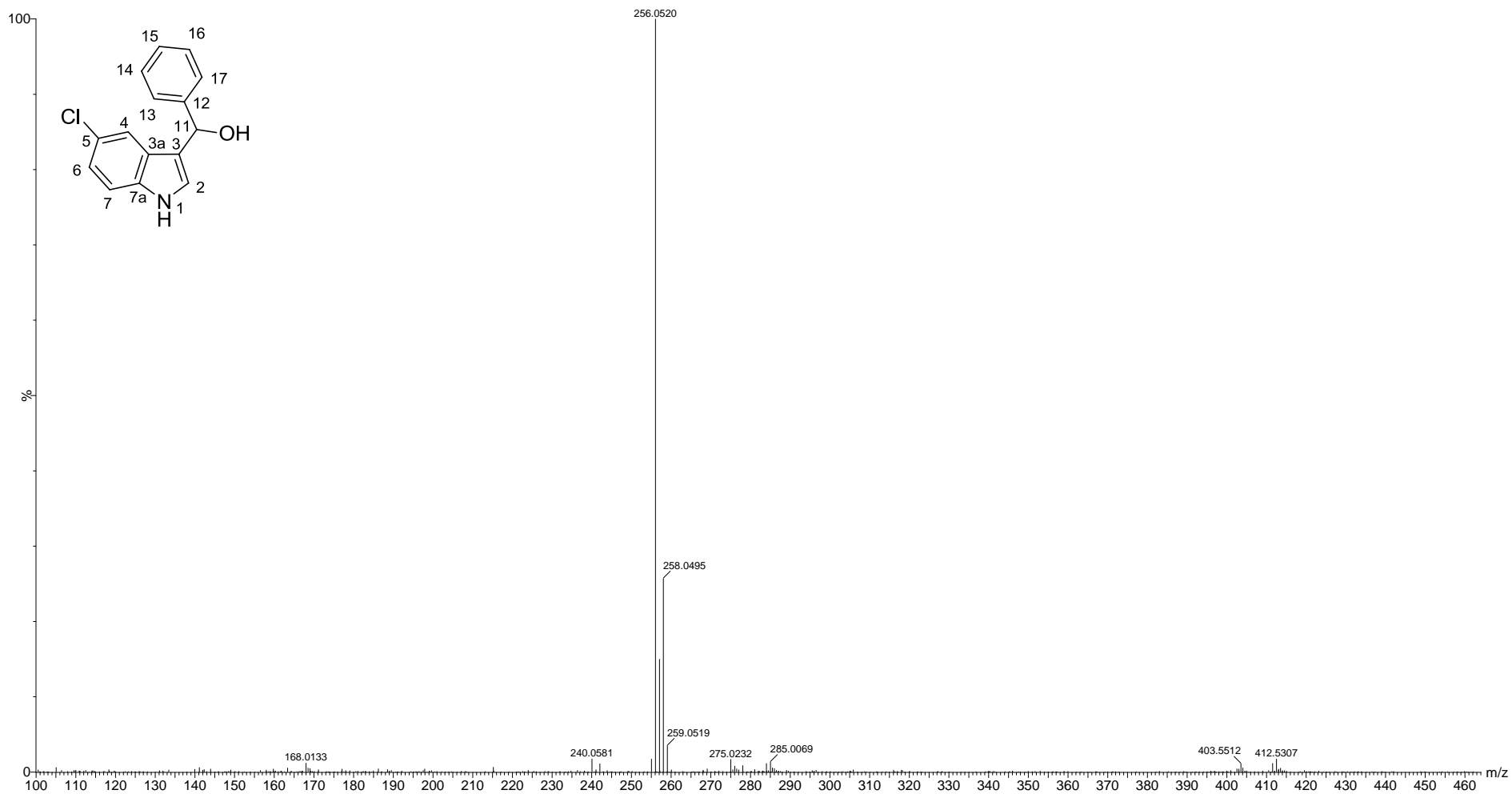
^{13}C NMR Spectrum
75 MHz Varian VNMRS



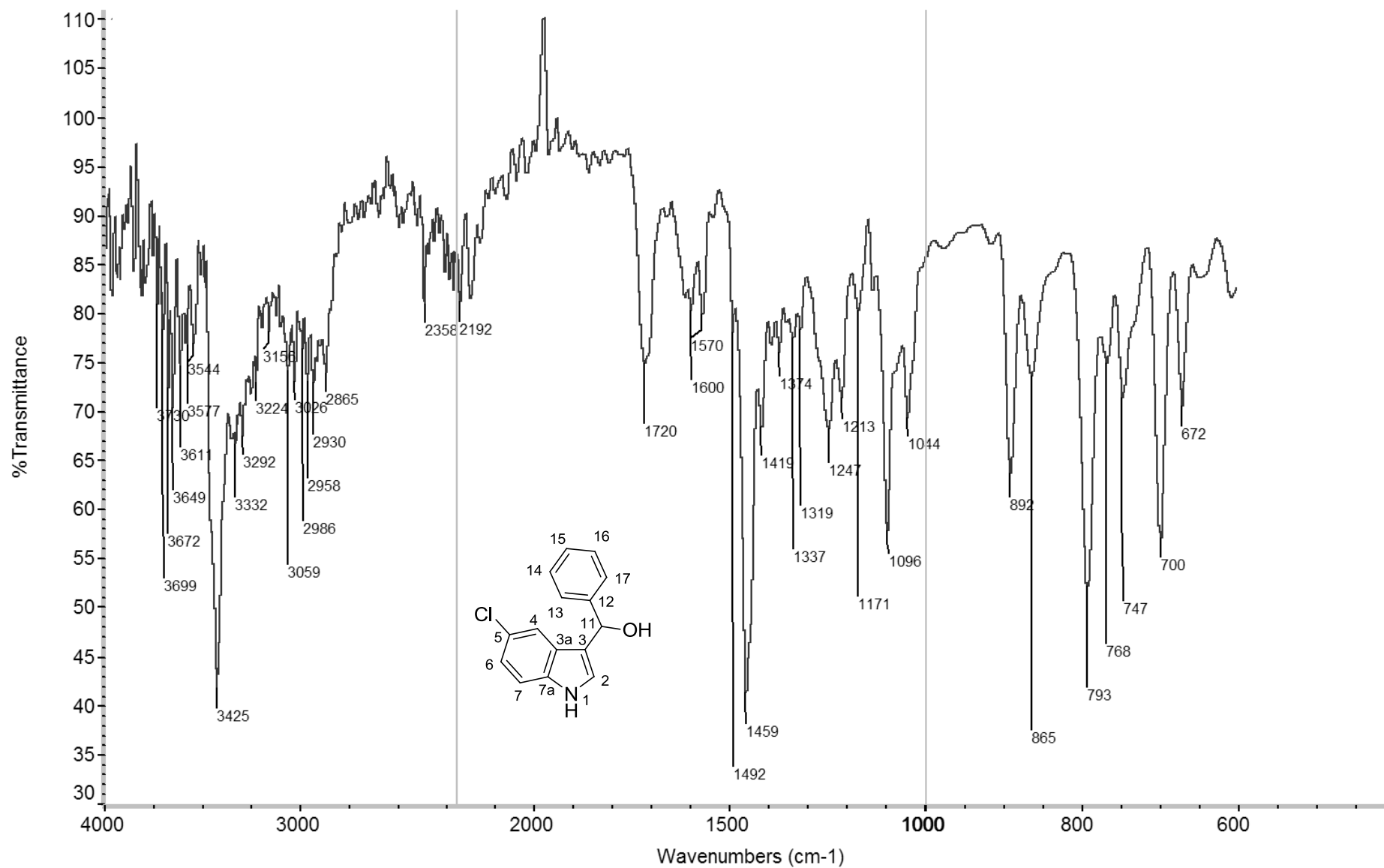
COSY NMR Spectrum
300 MHz Varian VNMRS



gHSQC NMR Spectrum
300 MHz Varian VNMRS

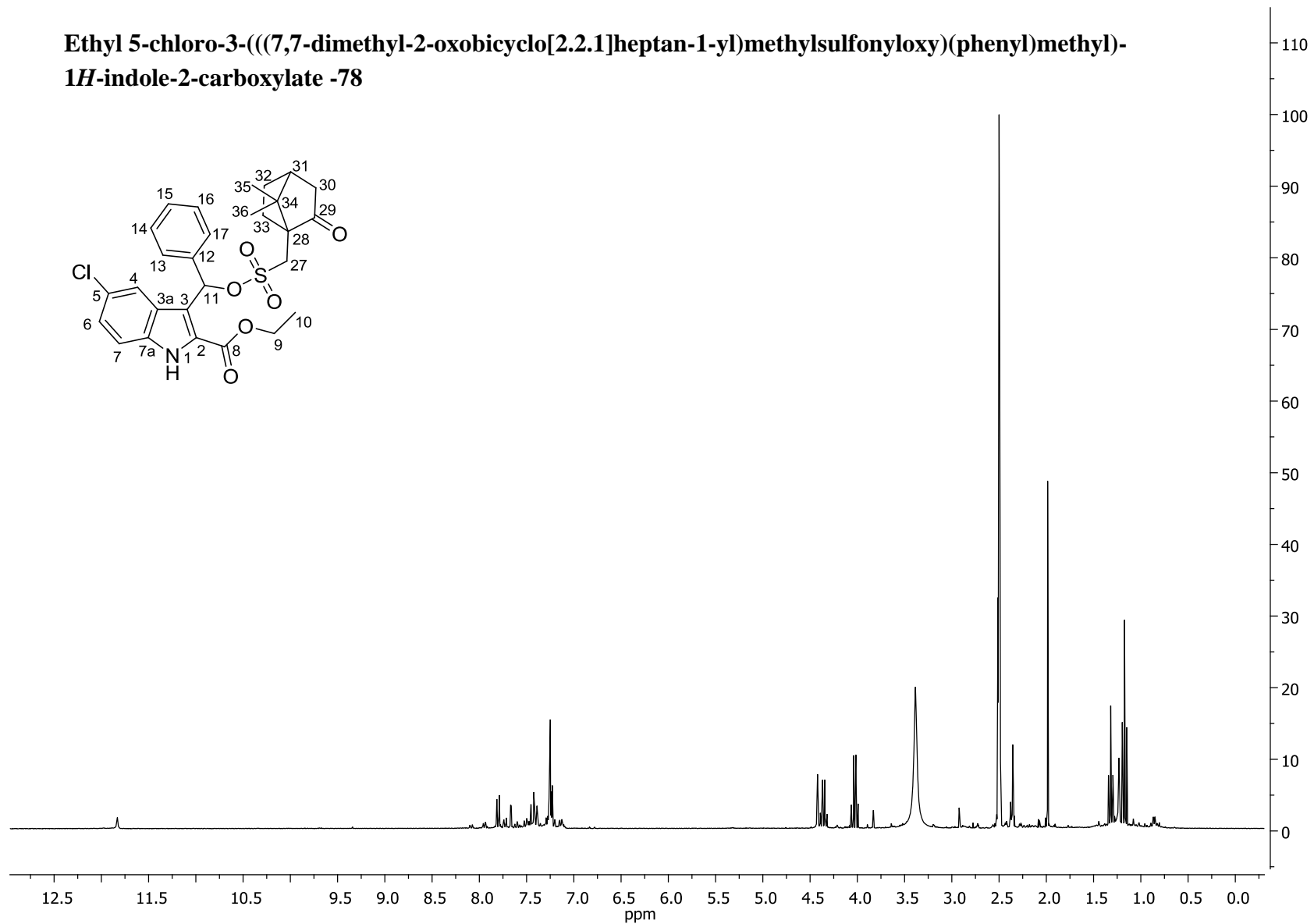


Mass Spectrum
Waters SYNAPT G2

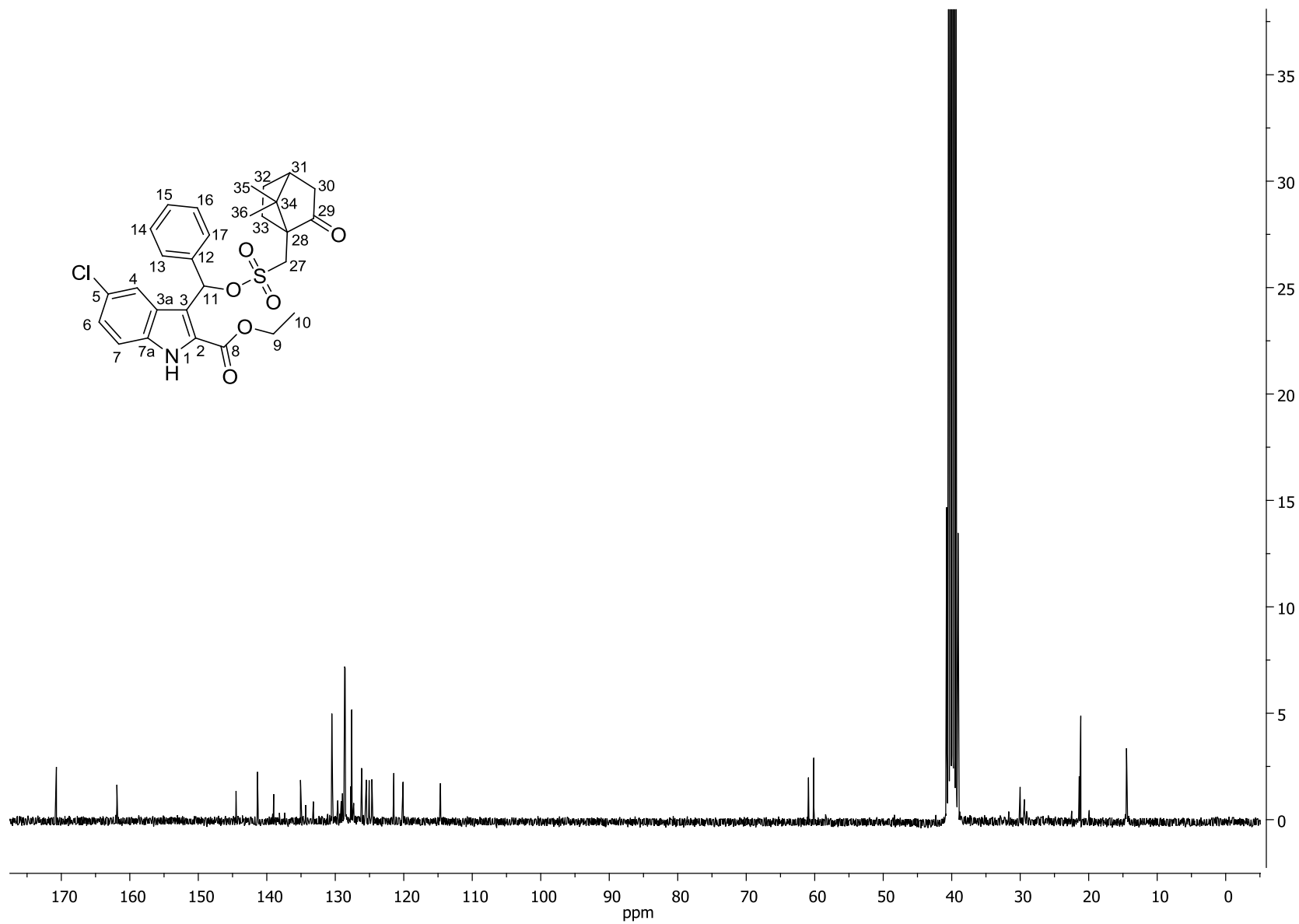


Infrared Spectrum
Thermo Nicolet Nexus 470

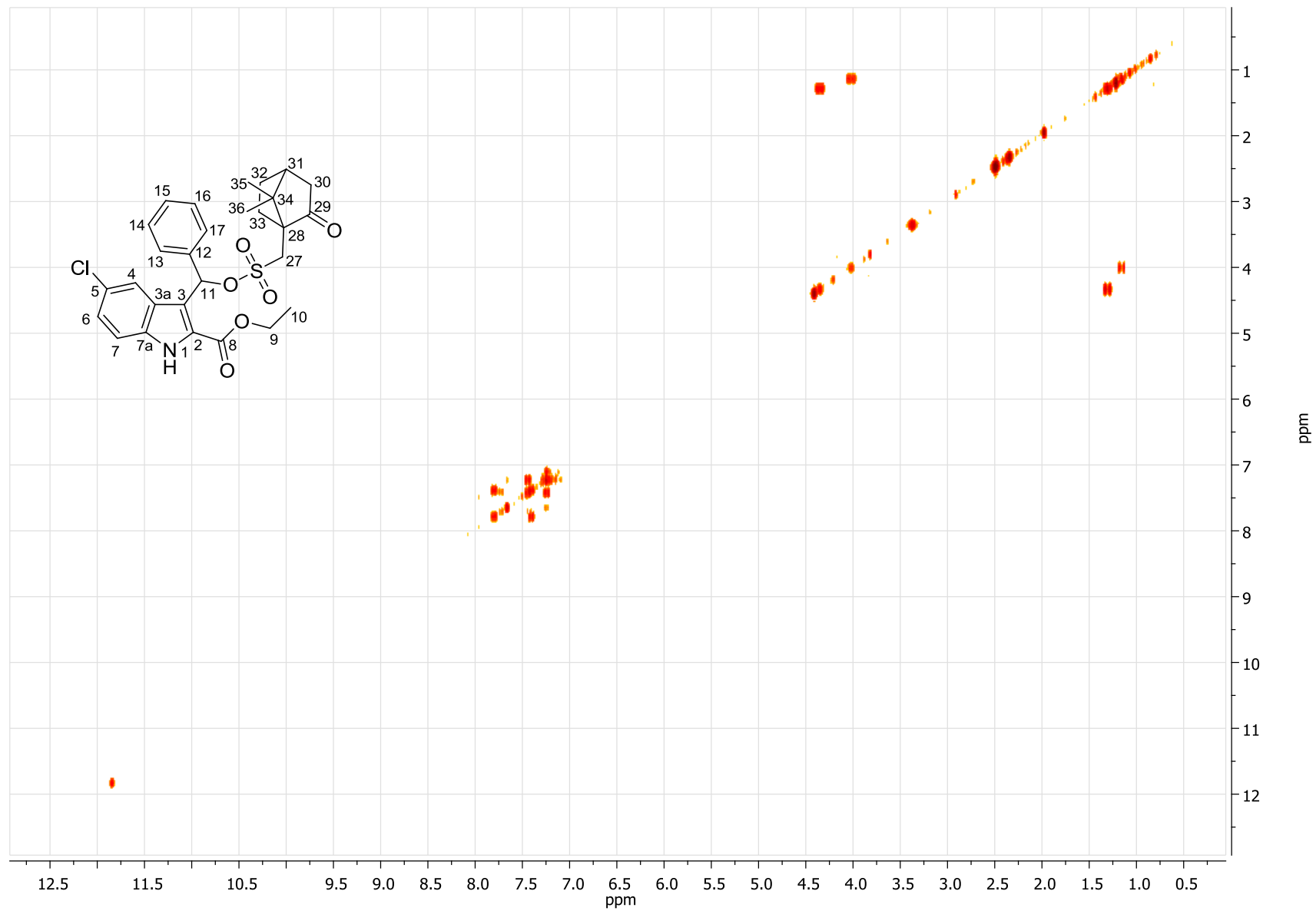
Ethyl 5-chloro-3-(((7,7-dimethyl-2-oxobicyclo[2.2.1]heptan-1-yl)methylsulfonyloxy)(phenyl)methyl)-1H-indole-2-carboxylate -78



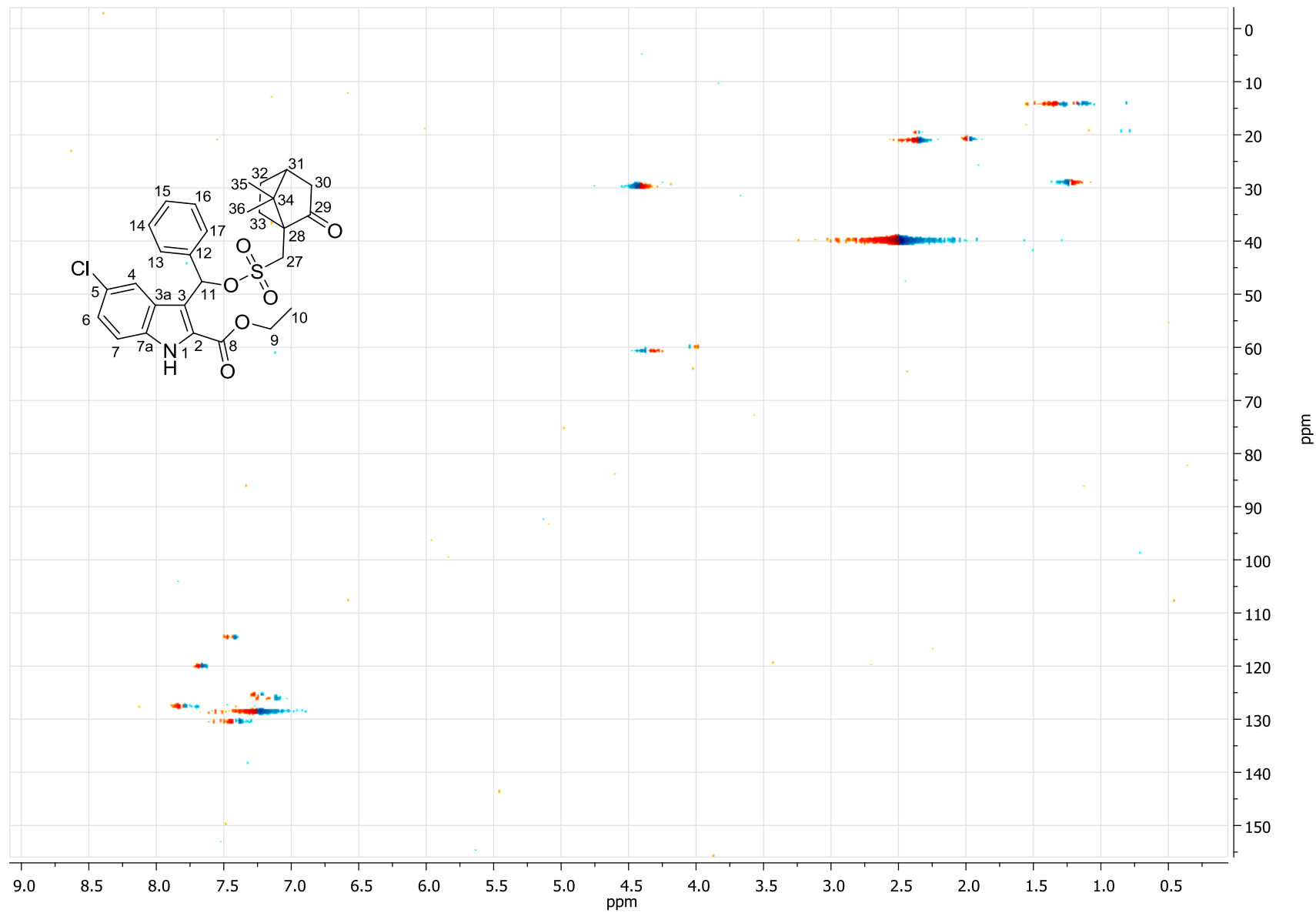
¹H NMR Spectrum
300 MHz Varian VNMRS



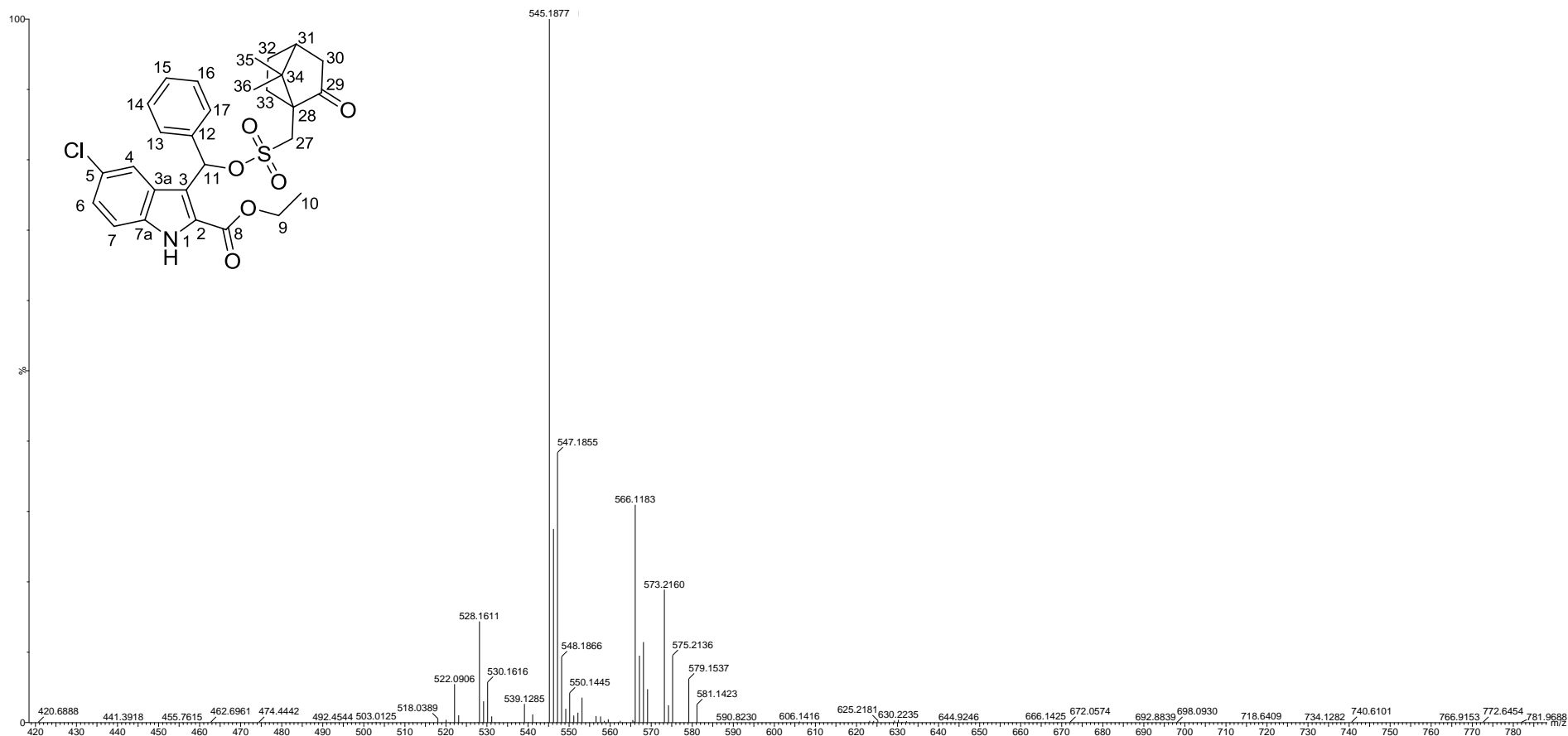
^{13}C NMR Spectrum
75 MHz Varian VNMRS

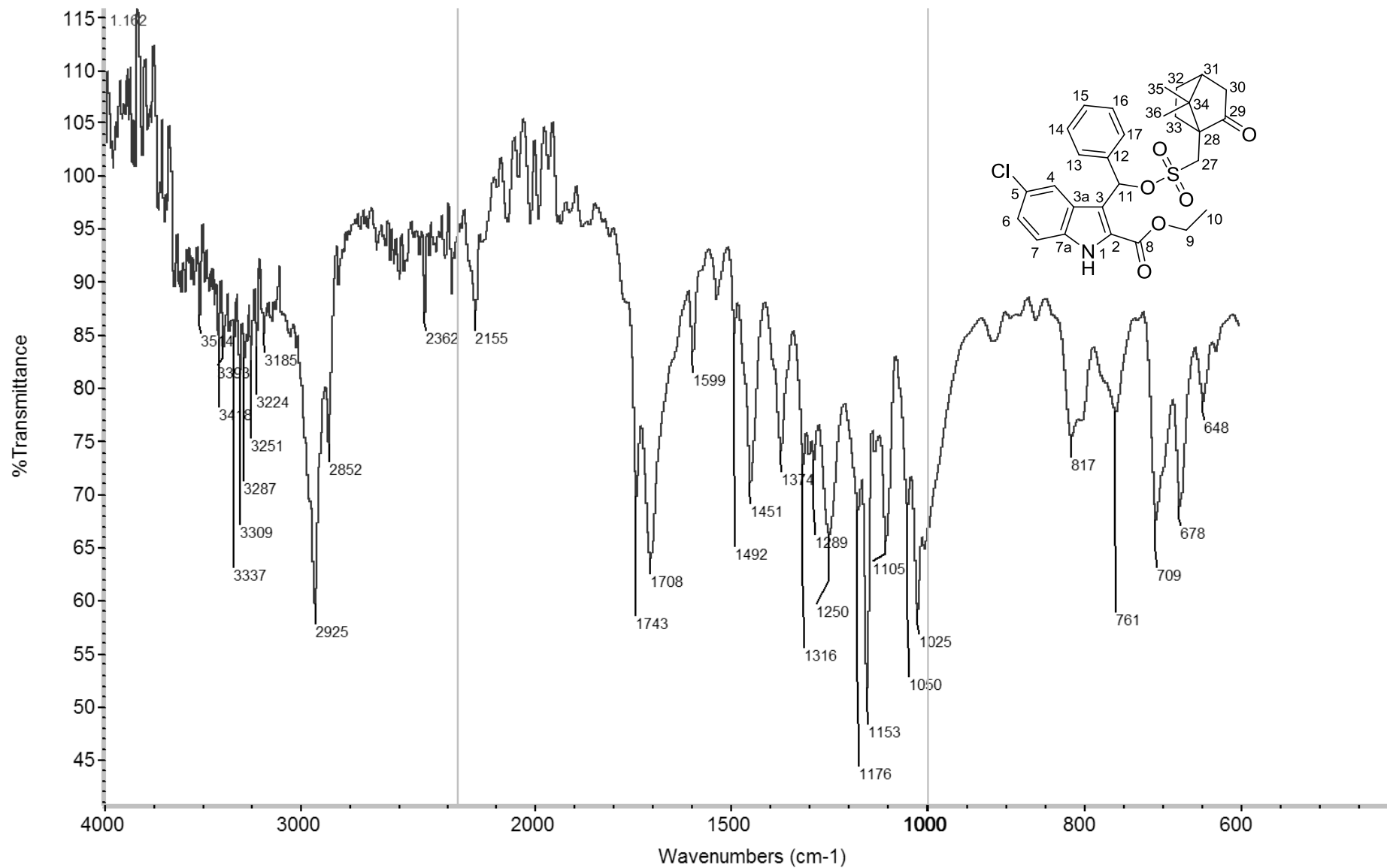


COSY NMR Spectrum
300 MHz Varian VNMRS



gHSQC NMR Spectrum
300 MHz Varian VNMRS





Infrared Spectrum
Thermo Nicolet Nexus 470