



## ANALYTICAL REPORT

AH-7921

### Acknowledgement

Analytically evaluated sample was kindly provided by the Forensic Science Institute (FSI) Zurich, Switzerland. NMR analyses were performed in ETH Zürich Institute of Pharmaceutical Sciences by Dr. Bernhard Pfeiffer and are enclosed in this report by the permission of Dr. Michael Bovens.

MS and FTIR measurements shown in this report were done in NFL.

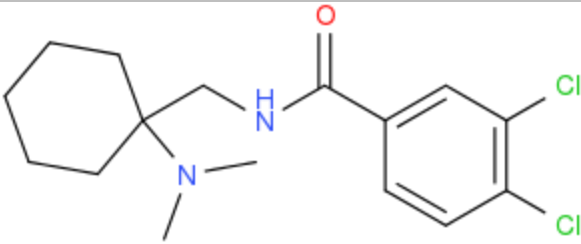
# ANALYTICAL REPORT

AH-7921 (C<sub>16</sub>H<sub>22</sub>Cl<sub>2</sub>N<sub>2</sub>O)

3,4-dichloro-N-[[1-(dimethylamino)cyclohexyl]methyl]benzamide

Remark – other active cpd. detected: **none**

|                         |                                                                                             |
|-------------------------|---------------------------------------------------------------------------------------------|
| Sample ID:              | 1434-16                                                                                     |
| Sample description:     | powder - white                                                                              |
| Sample type:            | collected/Kindly provided by Foresic Science Institute Zurich, Switzerland (NMR confirmed); |
| Comments <sup>1</sup> : |                                                                                             |
| Date of entry:          | 1/15/2016                                                                                   |

|                                                         |                                                                                    |
|---------------------------------------------------------|------------------------------------------------------------------------------------|
| Substance identified-structure <sup>2</sup> (base form) |  |
| Systematic name:                                        | 3,4-dichloro-N-[[1-(dimethylamino)cyclohexyl]methyl]benzamide                      |
| Other names:                                            |                                                                                    |
| Formula (per base form)                                 | C <sub>16</sub> H <sub>22</sub> Cl <sub>2</sub> N <sub>2</sub> O                   |
| M <sub>w</sub> (g/mol)                                  | 329,27                                                                             |
| Salt form:                                              | HCl                                                                                |
| StdInChIKey                                             | JMZROFPPEXCTST-UHFFFAOYSA-N                                                        |
| Compound Class                                          | Opioids                                                                            |
| Other active cpd. detected                              | none                                                                               |
| Add.info (purity..)                                     | app. 98%                                                                           |

<sup>1</sup> This report has been produced with the financial support of the Prevention of and fight against crime Programme of the European Union (grant agreement number JUST/2013/ISEC/DRUGS/AG/6413). The contents of this report are the sole responsibility of the National Forensic Laboratory and can in no way be taken to reflect the views of the European Commission.

<sup>2</sup> Created by OPSIN free tool: <http://opsin.ch.cam.ac.uk/> DOI: 10.1021/ci100384d

## Report updates

| date | comments (explanation) |
|------|------------------------|
|      |                        |
|      |                        |
|      |                        |
|      |                        |

## Supporting information

| Analytical technique:   | applied | remarks                                                      |
|-------------------------|---------|--------------------------------------------------------------|
| GC-MS (EI ionization)   | +       | NFL GC-RT (min): 10,31<br>BP(1): 126; BP(2): 127,BP(3) :173, |
| FTIR-ATR                | +       | direct measurement                                           |
| GC-IR (condensed phase) | +       | consistent with the one from the FSI Zurich (QM>0.99)        |

### GC-MS (Agilent):

GC-method is RT locked to tetracosane (RT=9.53 min).

Injection volume 1 ml and split mode (1:50) .

Injector temperature: 280 °C.

Chromatographic separation

Column: HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickness 0.25 mm.

Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 °C for 1 min, followed by heating up to 293 °C at a rate of 18 °C/min, hold for 6.1 min, then heating at 50 °C/min up to 325 °C and finally 2.8 min isothermal.

MSD source EI = 70 eV. GC-MS transfer line T= 235°C, source and quadrupole temperatures 280°C and 180°C, respectively. Scan range m/z scan range: from 50 (40) to 550 amu.

**FTIR-ATR** (Perkin Elmer): scan range 4000-400 cm<sup>-1</sup>; resolution 4cm<sup>-1</sup>

**GC- (MS)-IR** condensed phase (GC-MS (Agilent) & IR (Spectra analyses-Danny) IR scan range 4000 to 700, resolution 4cm<sup>-1</sup>

GC-method:

Injection volume 1 ml and split mode (1:5) .

Injector temperature: 280 °C.

Chromatographic separation

Column: HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickness 0.25 mm.

Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 °C for 1 min, followed by heating up to 293 °C at a rate of 18 °C/min, hold for 6.1 min, then heating at 50 °C/min up to 325 °C and finally 2.8 min isothermal.

Split MS : IR : (1:9)

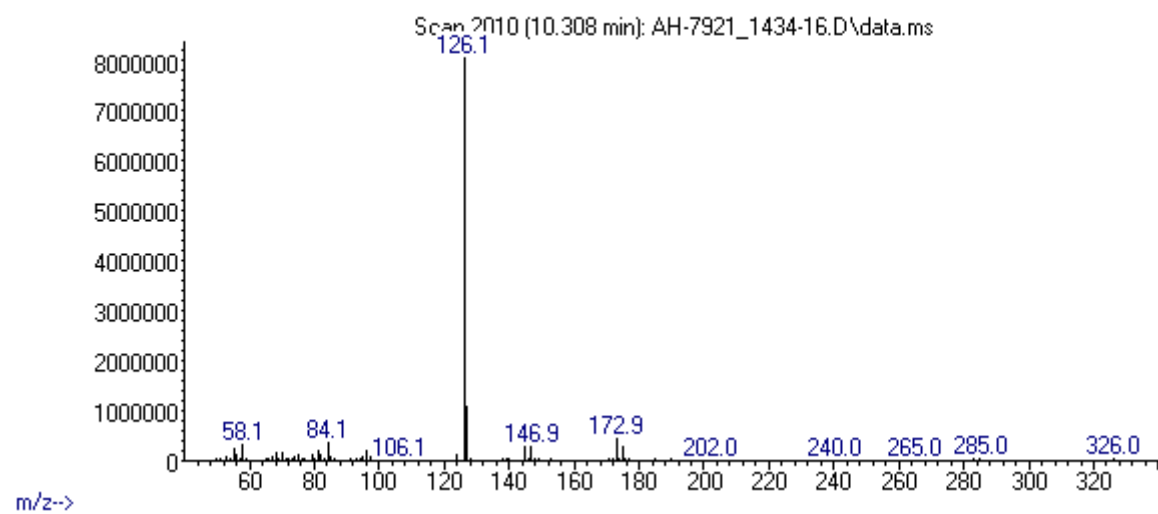
MSD source EI = 70 eV. GC-MS transfer line T= 235°C, source and quadrupole temperatures 280°C and 180°C, respectively. Scan range m/z scan range: from 50 (40) to 550 amu.

IR (condensed phase): IR scan range 4000 to 700, resolution 4cm<sup>-1</sup>

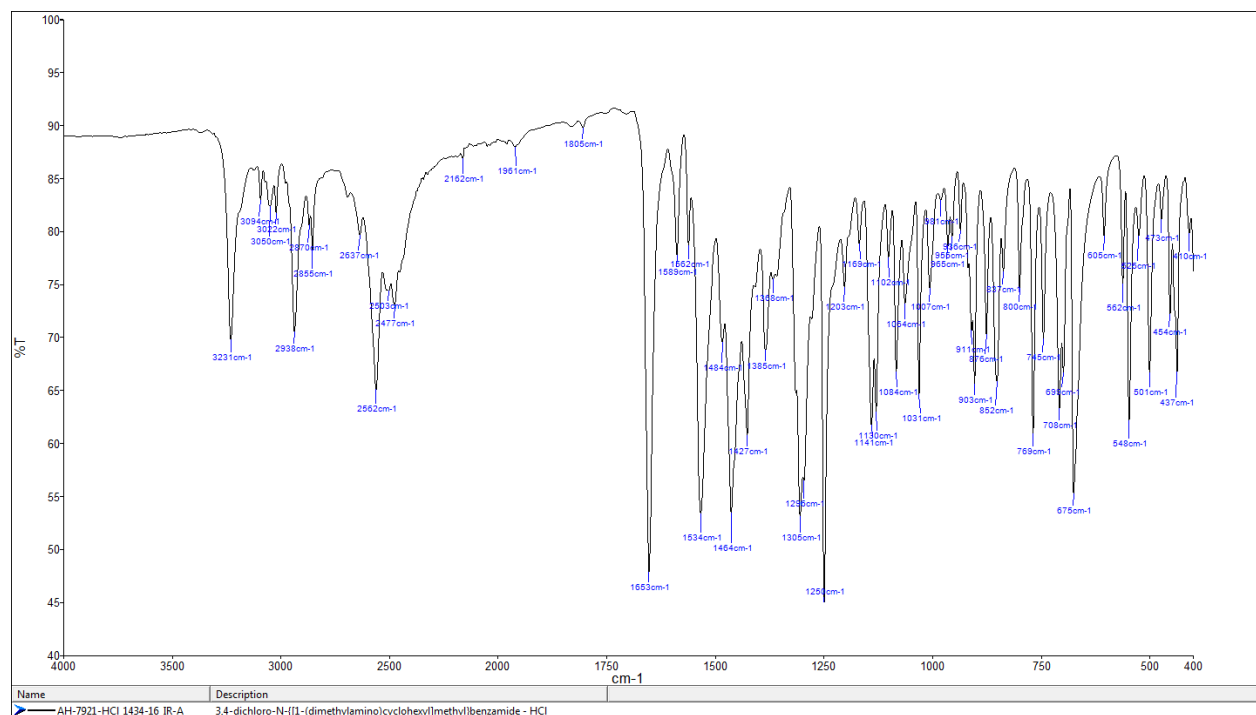
## FIGURES OF SPECTRA

MS (EI)

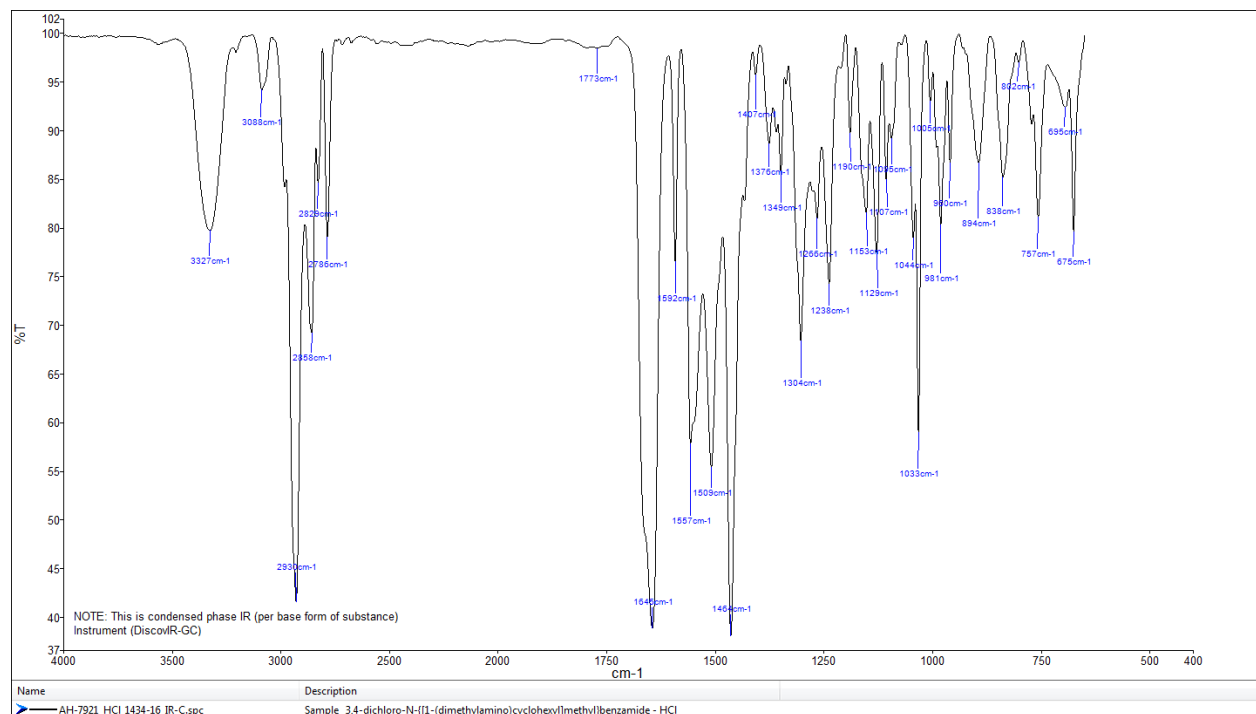
Abundance



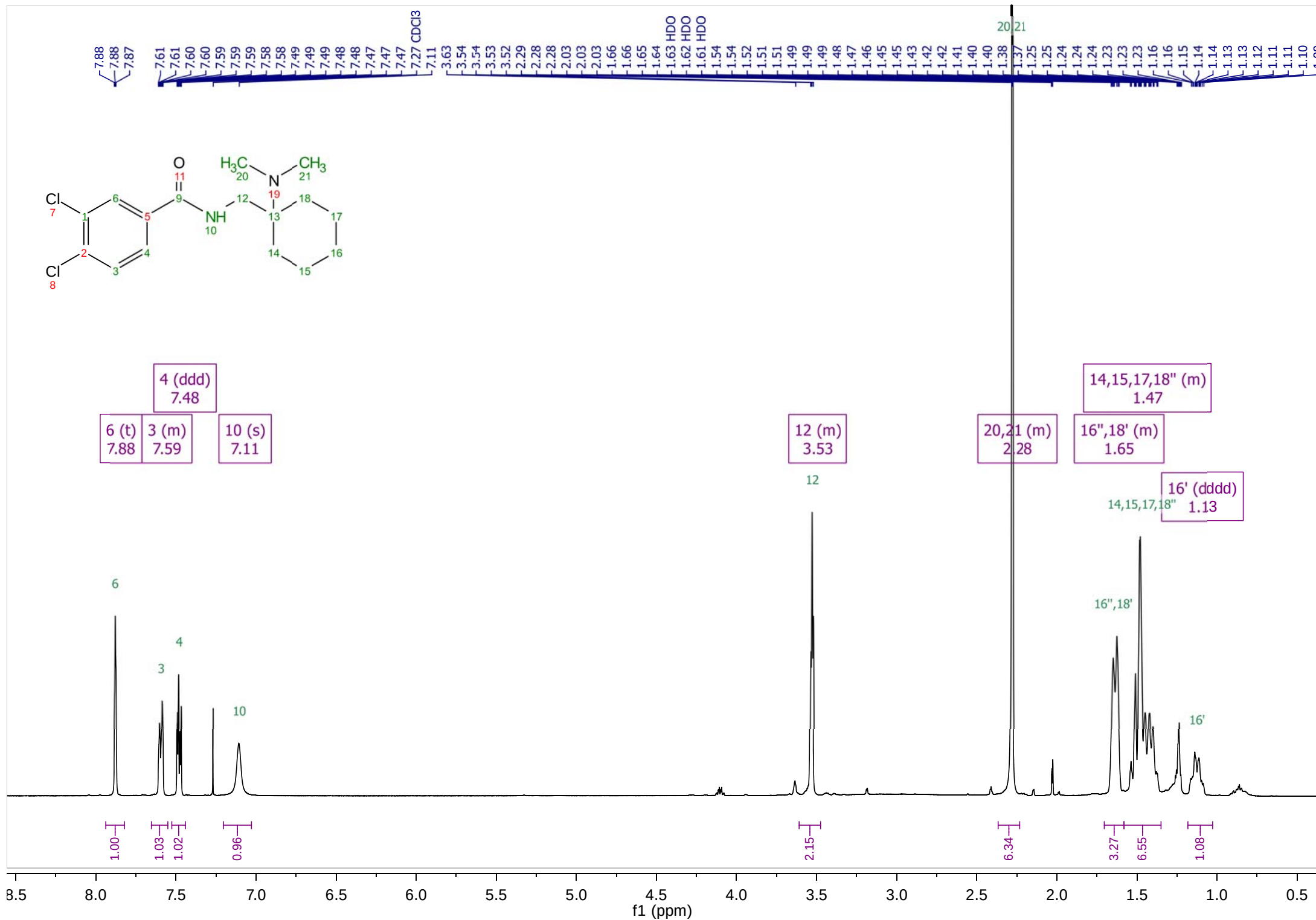
## FTIR-ATR

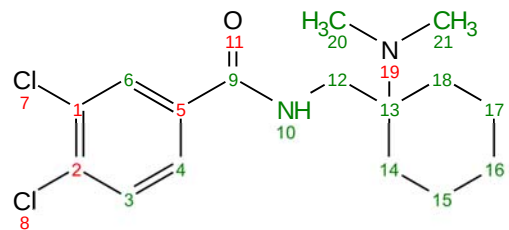


## IR-Condensed phase



END OF NFL data





165.22

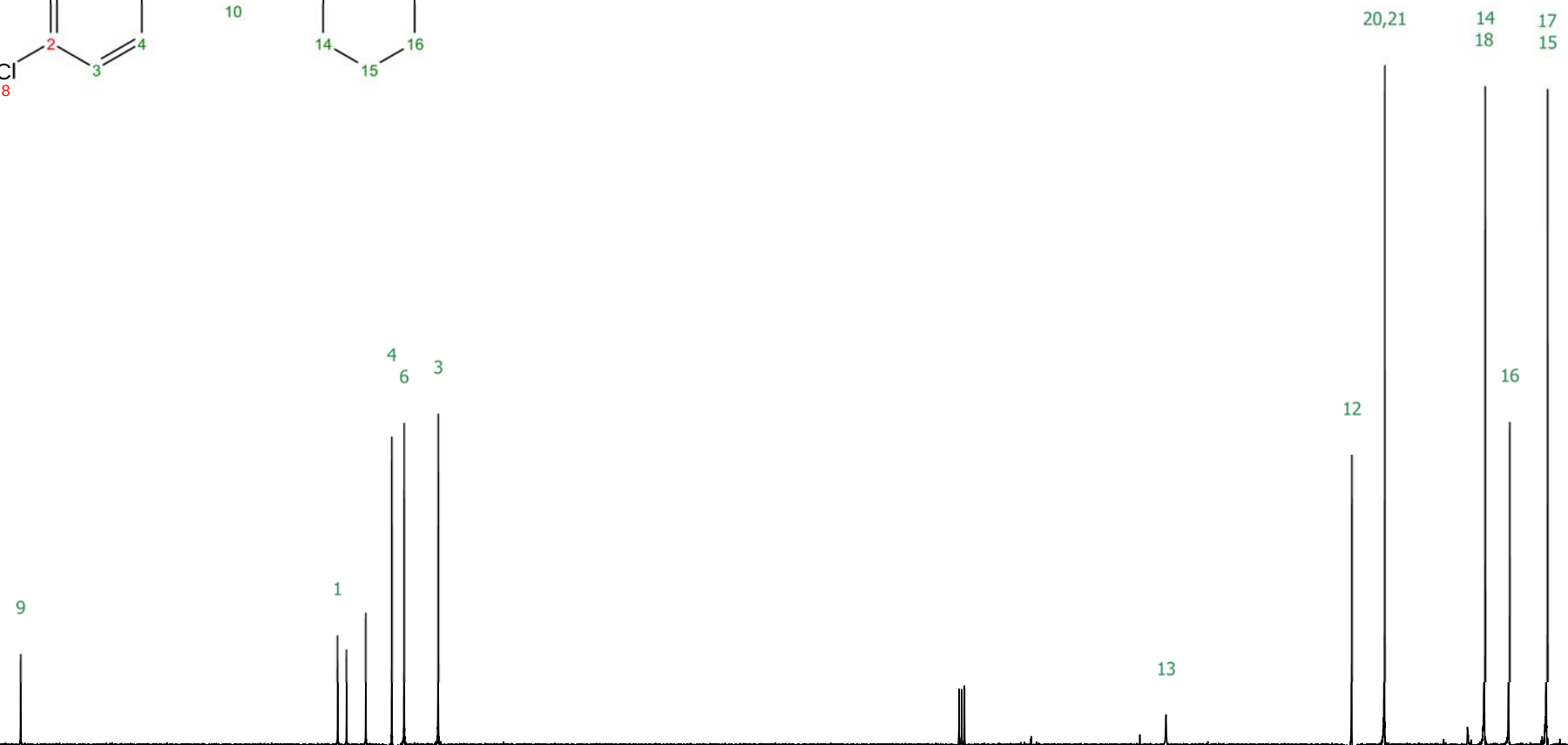
135.52  
134.69  
132.89  
130.45  
129.30  
126.11

77.31 CDCl<sub>3</sub>  
77.06 CDCl<sub>3</sub>  
76.80 CDCl<sub>3</sub>

57.93

40.54  
37.48

28.25  
28.12  
25.84  
22.36  
22.31



9

1

4  
6  
3

12

20,21

14  
18

16

17  
15

13

180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10

f1 (ppm)

