

## **APPENDIX 6**

*Spectra Related to Chapter 4:*

*Enantio-, Diastereo- and Regioselective Iridium-Catalyzed*

*Asymmetric Allylic Alkylation of Acyclic  $\beta$ -Ketoesters*

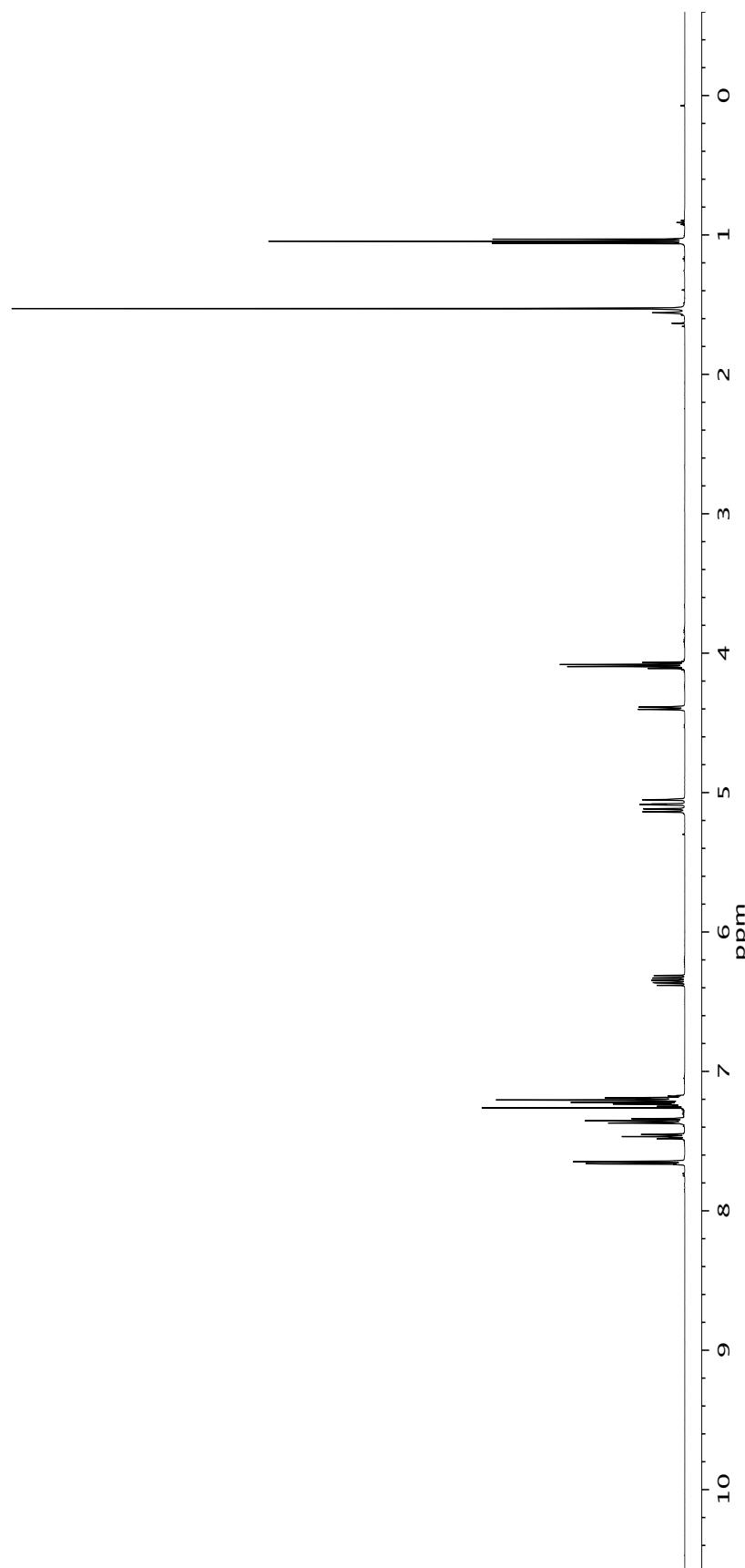
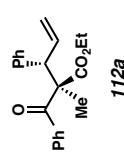


Figure A6.1  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of compound 112a.

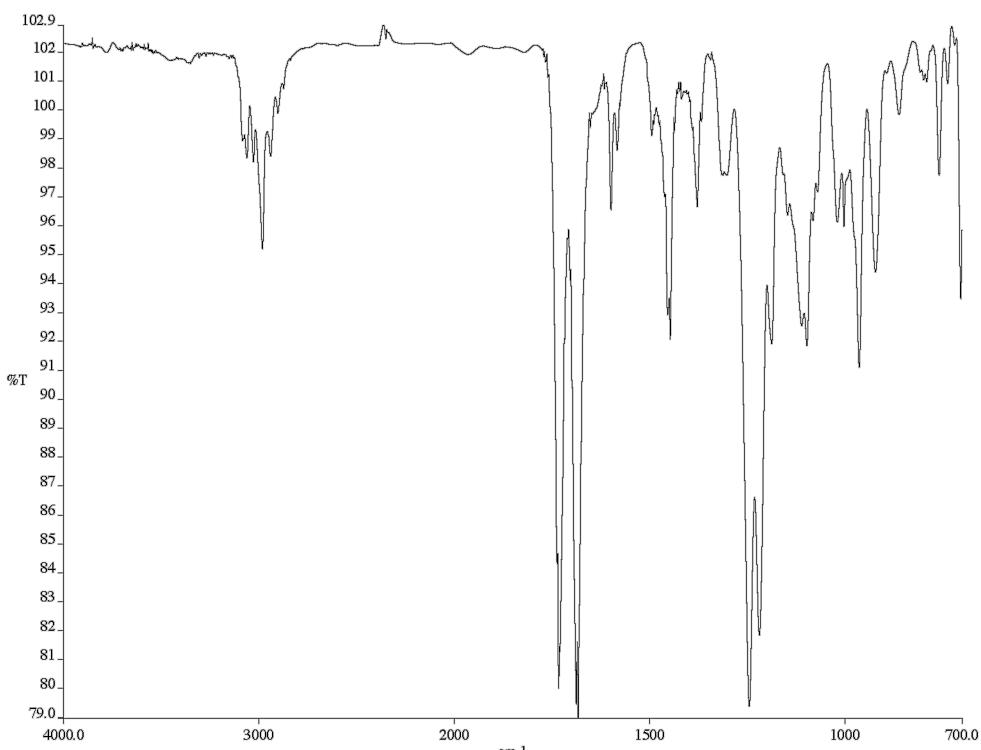


Figure A6.2 Infrared spectrum (thin film/NaCl) of compound 112a.

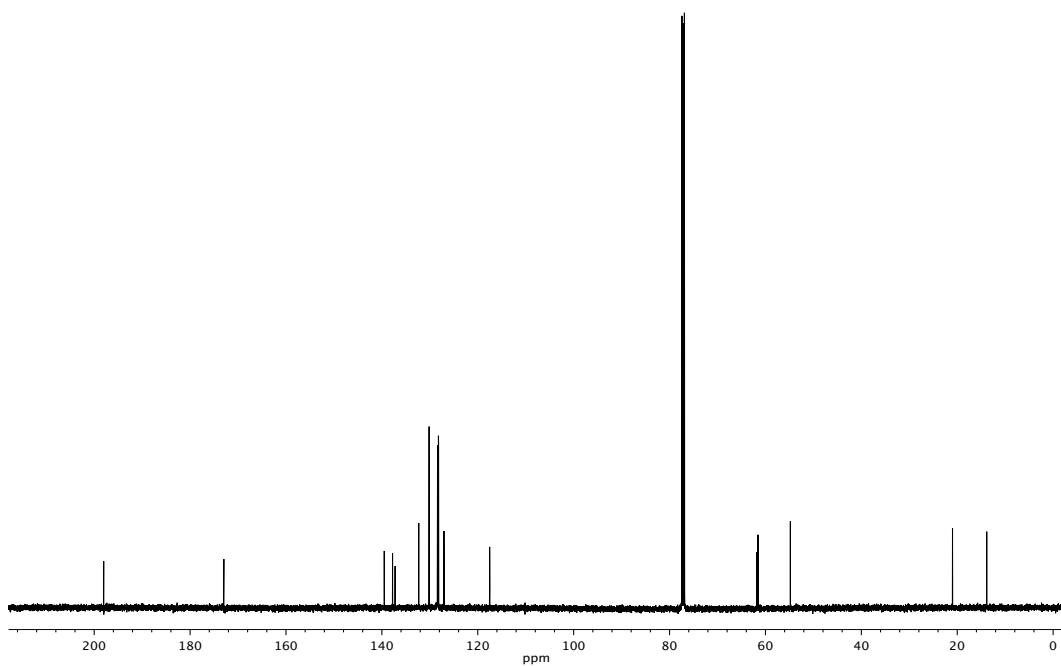


Figure A6.3  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) of compound 112a.

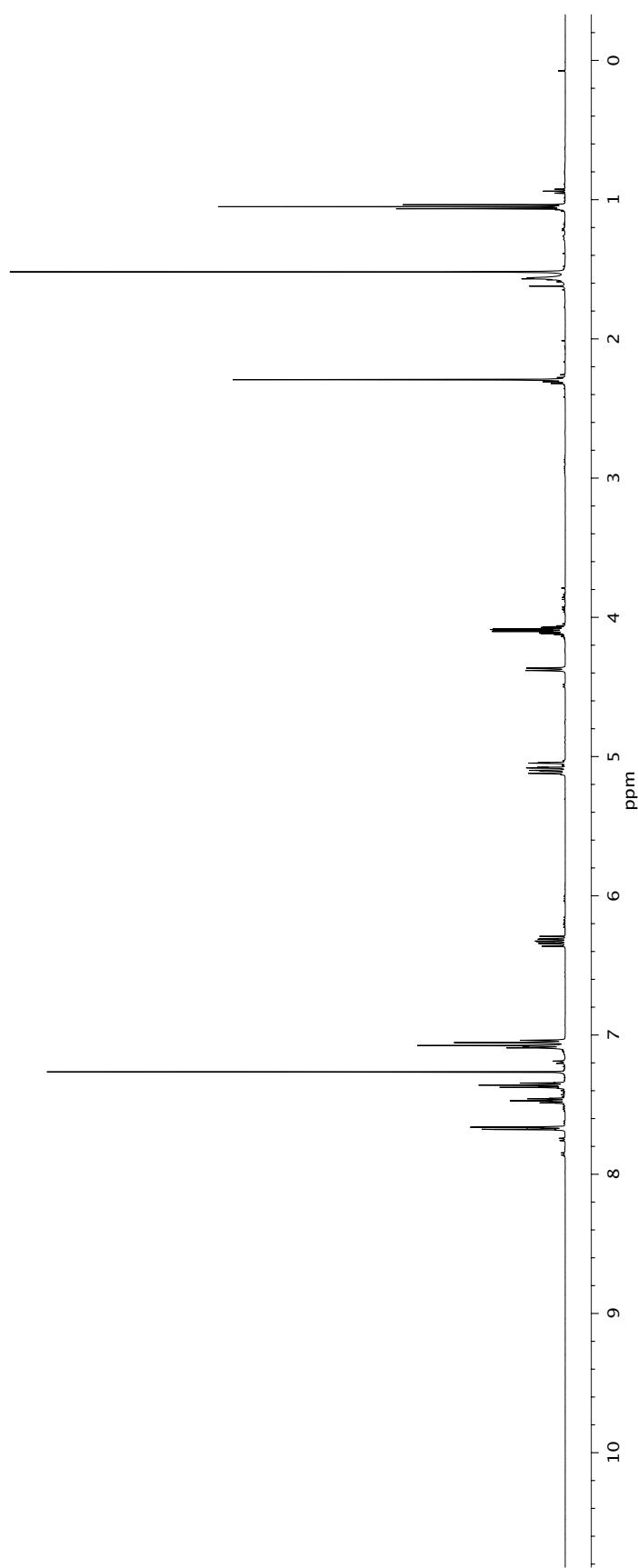
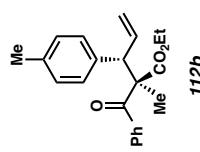


Figure A6.4  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of compound 112b.

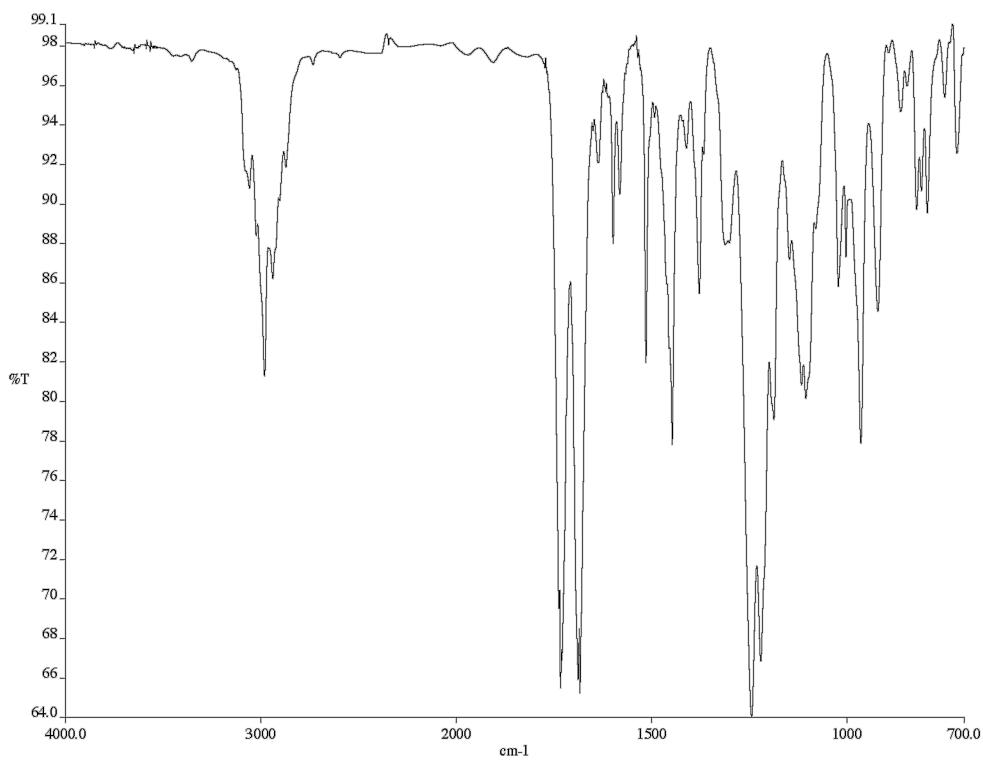


Figure A6.5 Infrared spectrum (thin film/NaCl) of compound **112b**.

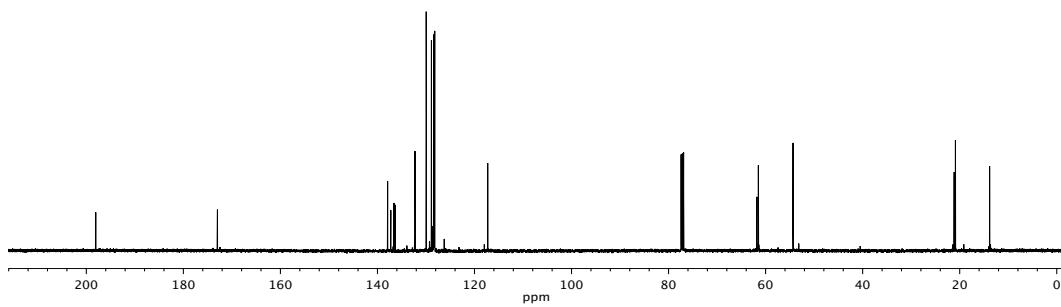


Figure A6.6  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) of compound **112b**.

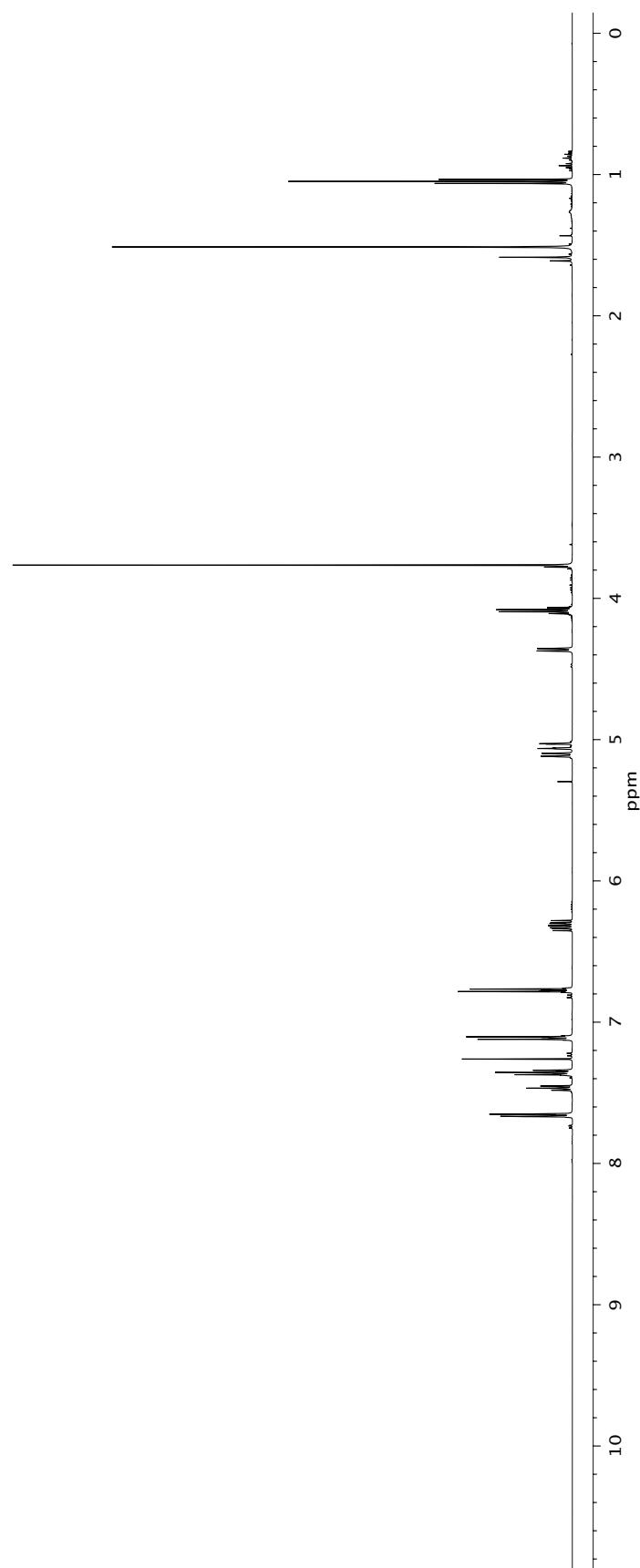
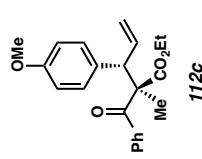


Figure A6.7 <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) of compound 112c.

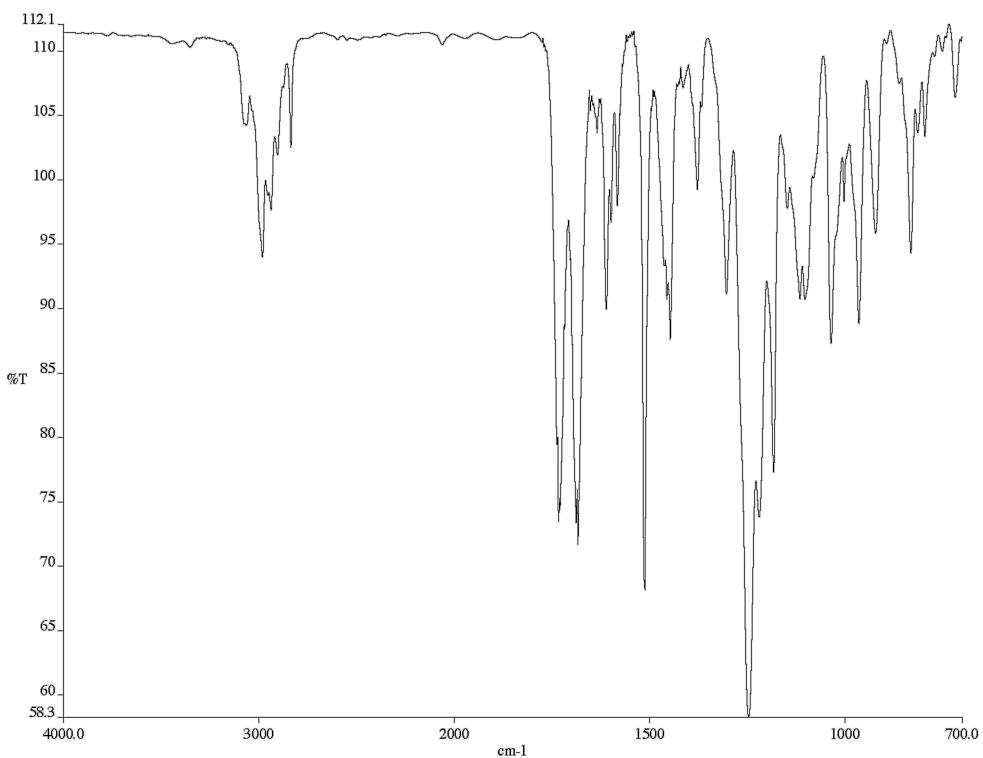


Figure A6.8 Infrared spectrum (thin film/NaCl) of compound **112c**.

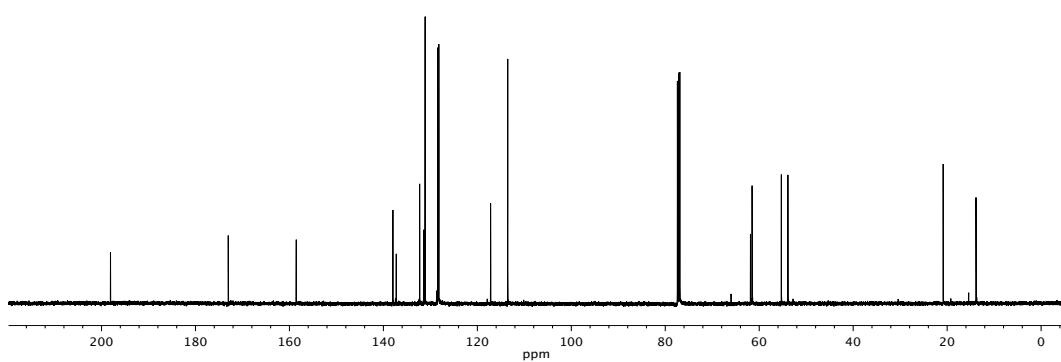


Figure A6.9 <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound **112c**.

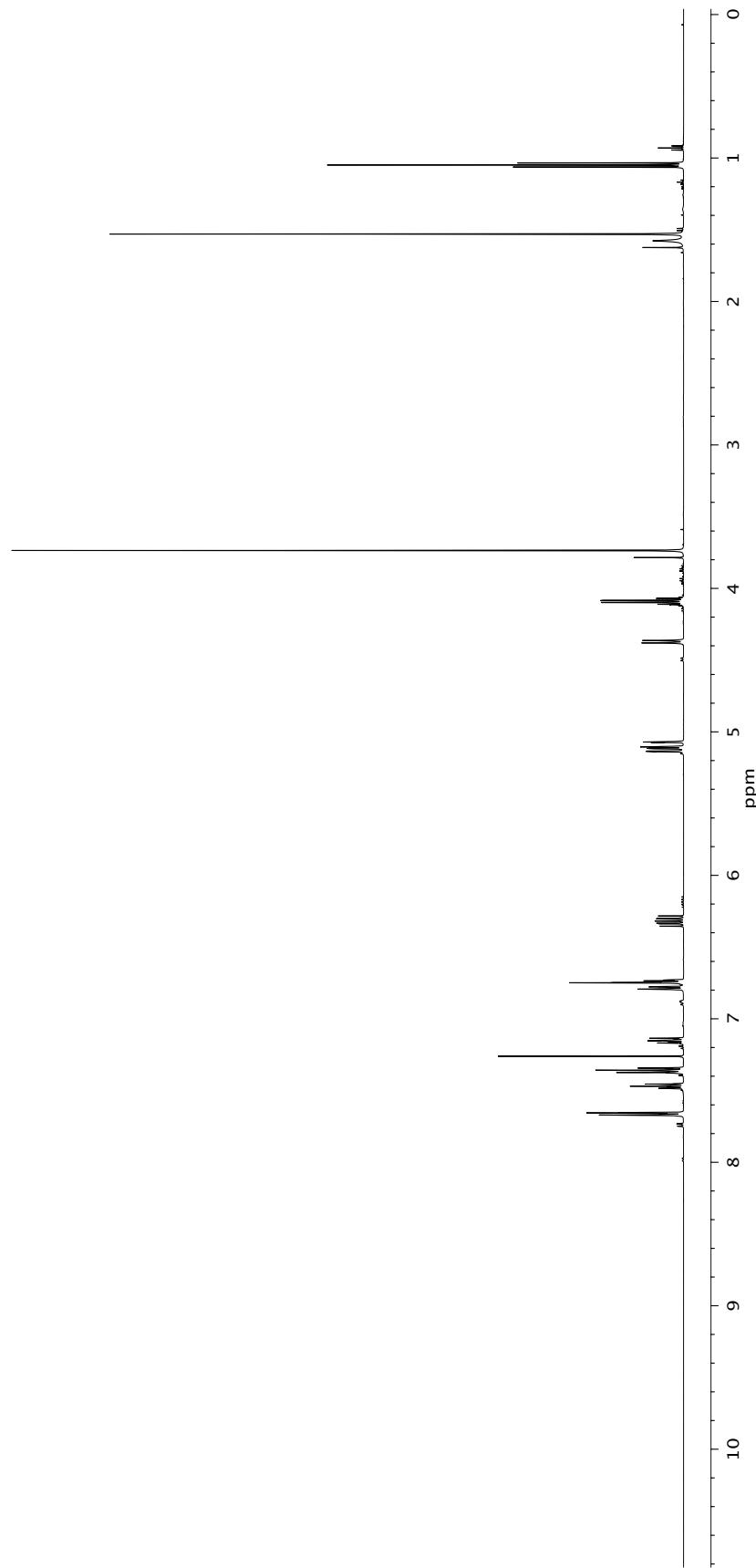
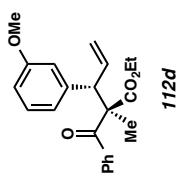


Figure A6.10 <sup>1</sup>H NMR (500 MHz,  $\text{CDCl}_3$ ) of compound 112d.

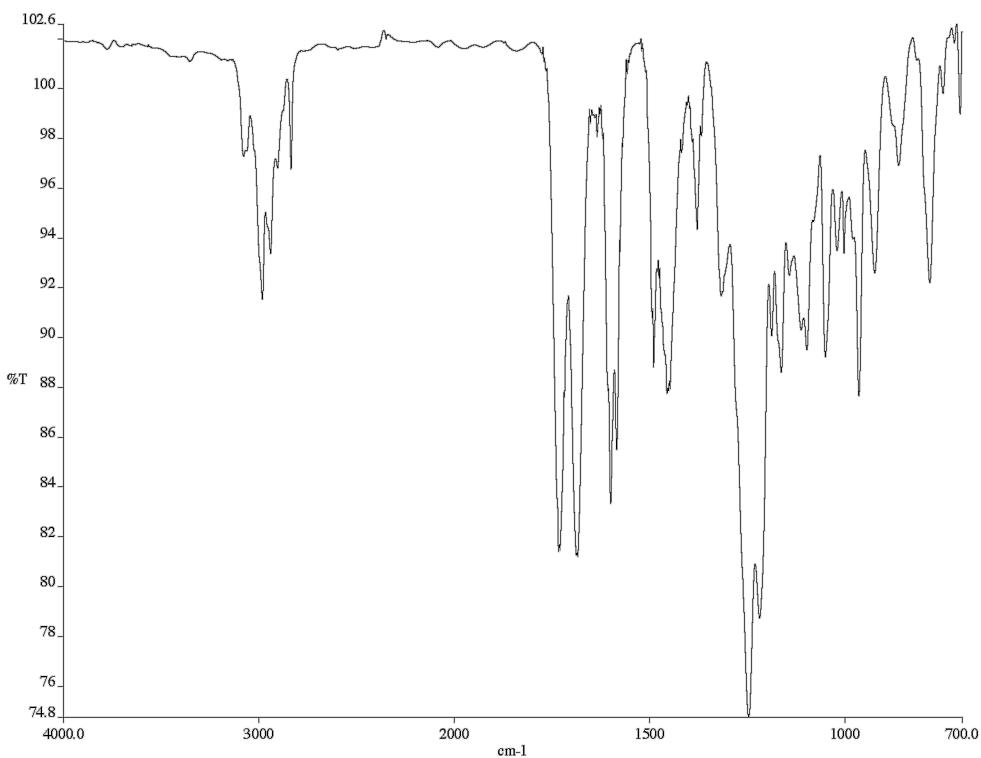


Figure A6.11 Infrared spectrum (thin film/NaCl) of compound **112d**.

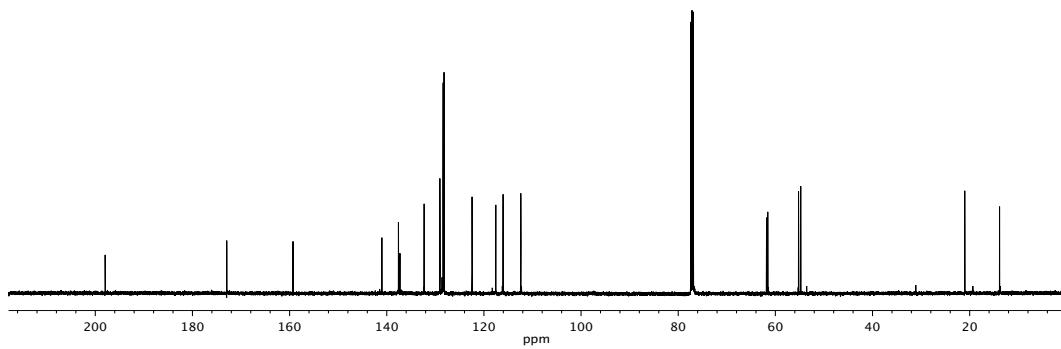


Figure A6.12  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) of compound **112d**.

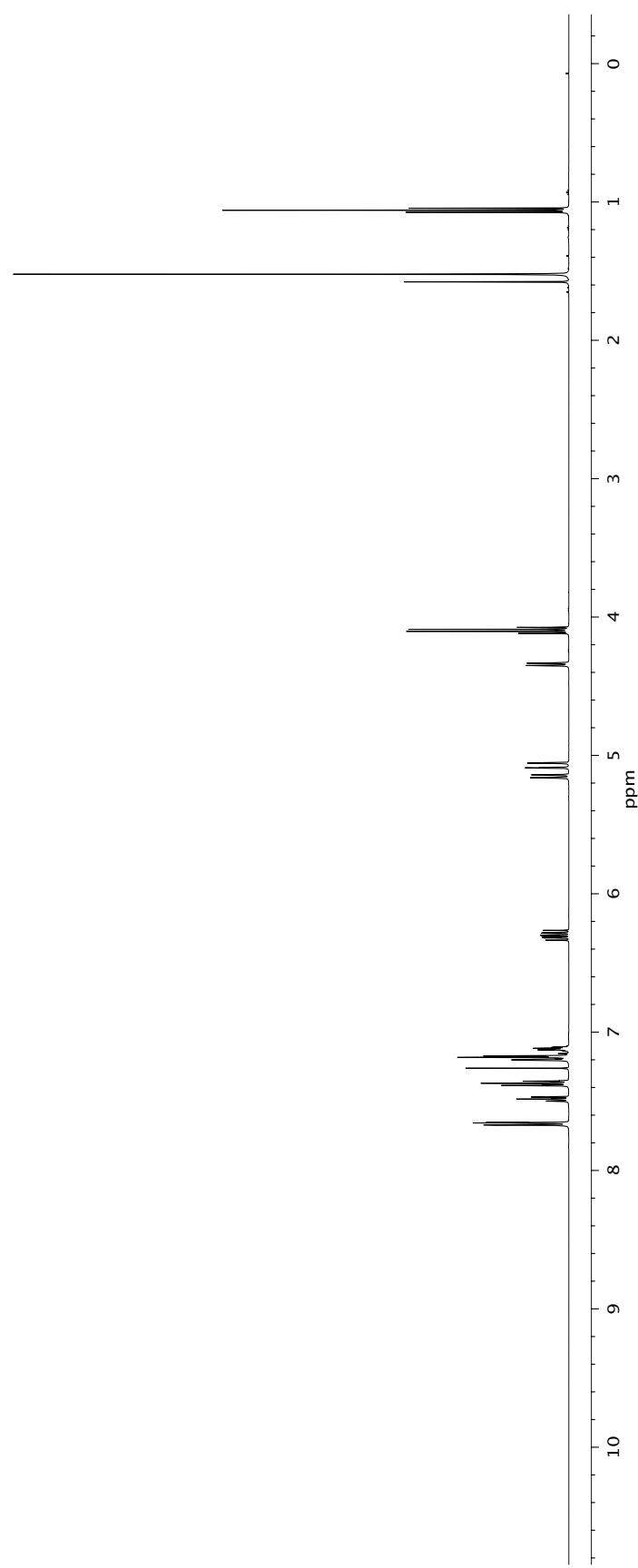
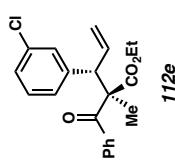


Figure A6.13 <sup>1</sup>H NMR (500 MHz,  $\text{CDCl}_3$ ) of compound 112e.

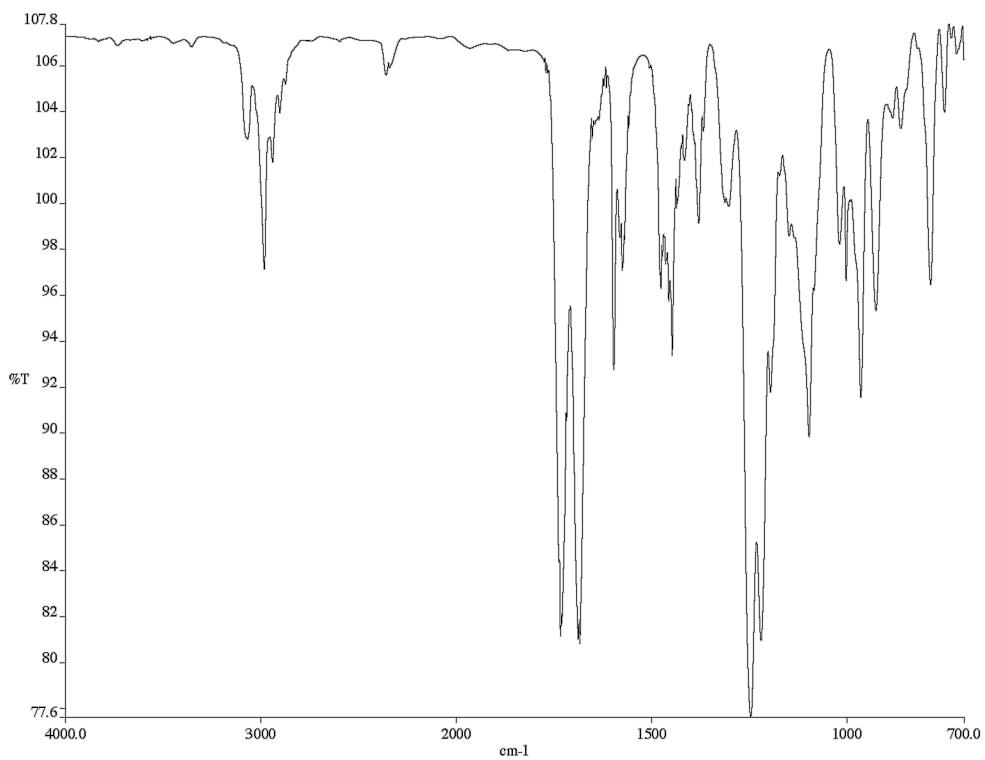


Figure A6.14 Infrared spectrum (thin film/NaCl) of compound **112e**.

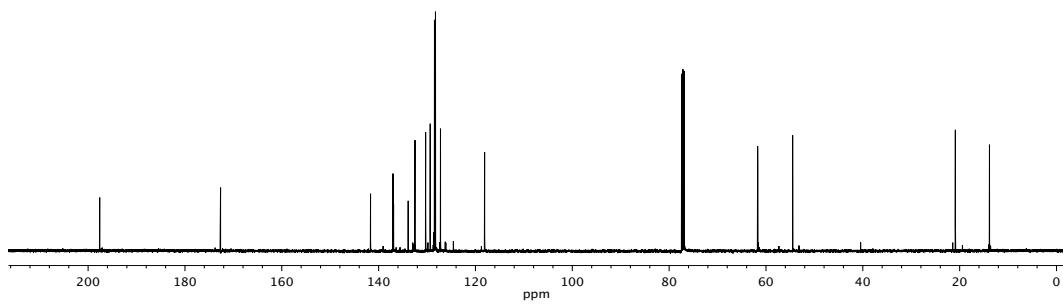


Figure A6.15 <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound **112e**.

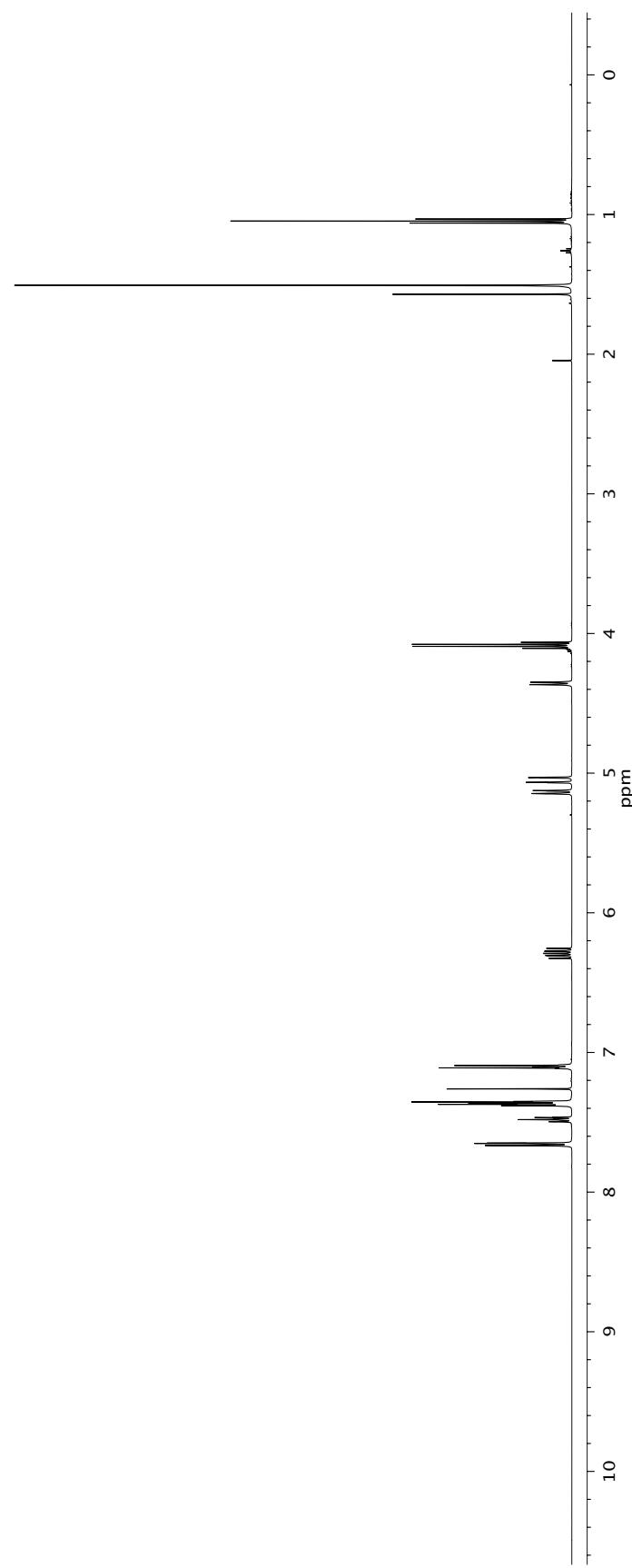
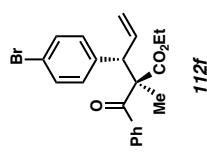


Figure A6.16  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of compound 112f.

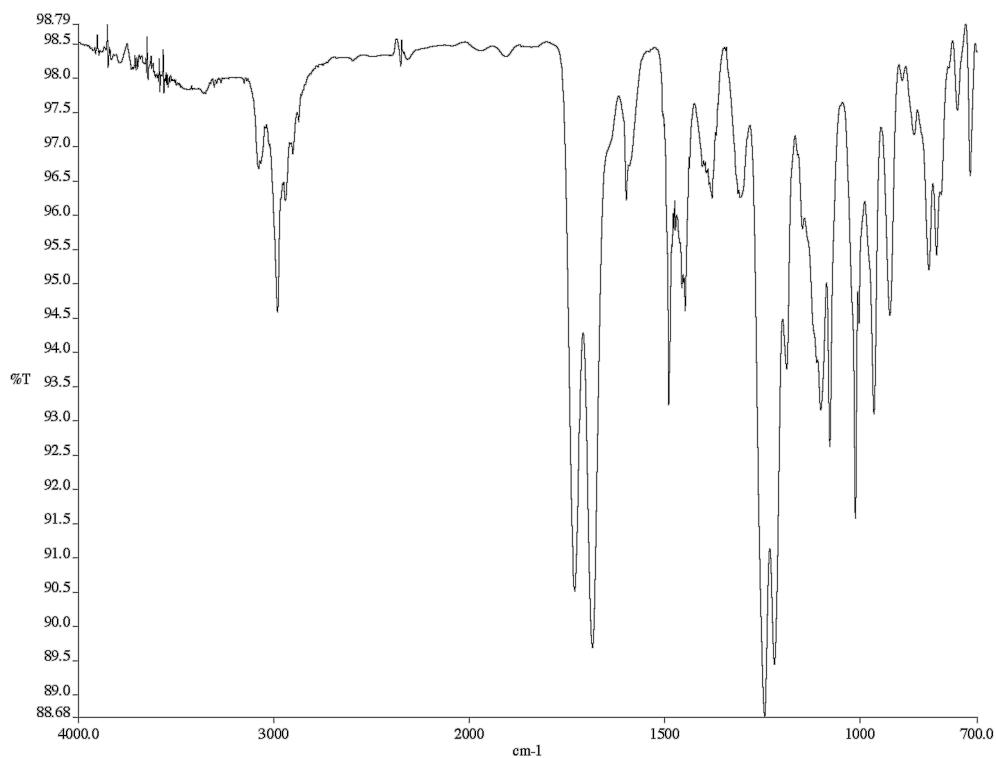


Figure A6.17 Infrared spectrum (thin film/NaCl) of compound **112f**.

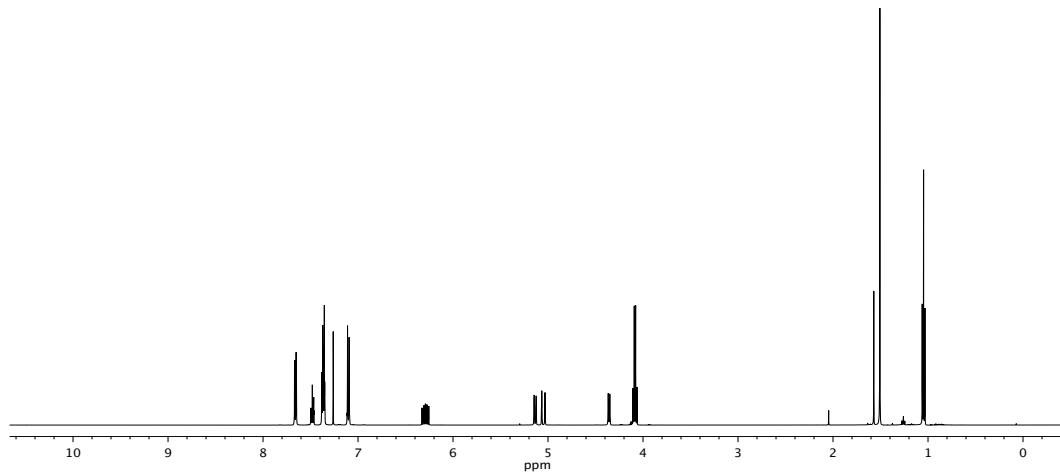


Figure A6.18  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) of compound **112f**.

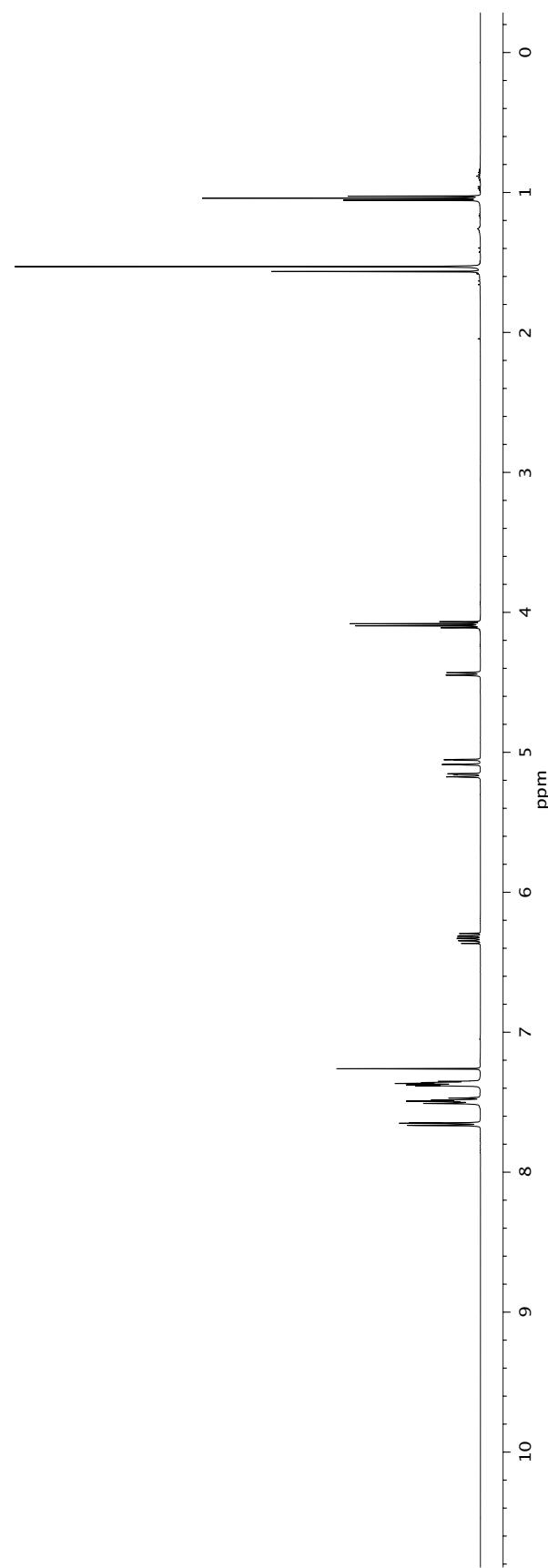
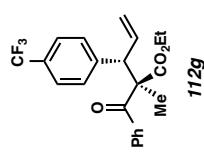


Figure A6.19  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of compound 112g.

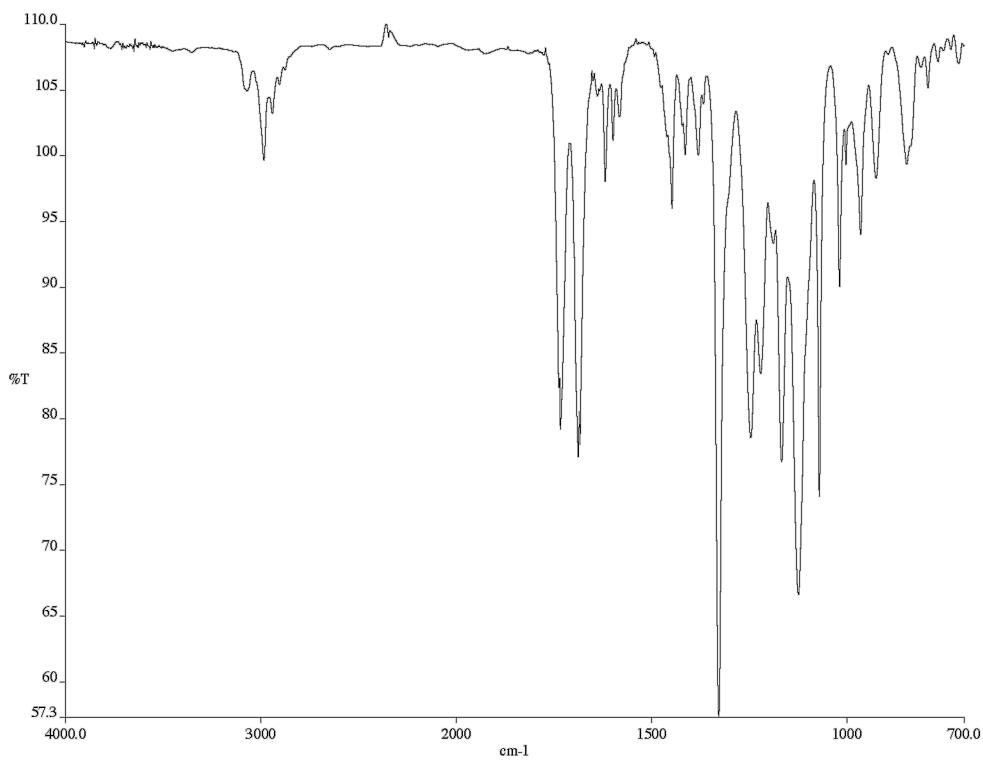


Figure A6.20 Infrared spectrum (thin film/NaCl) of compound **112g**.

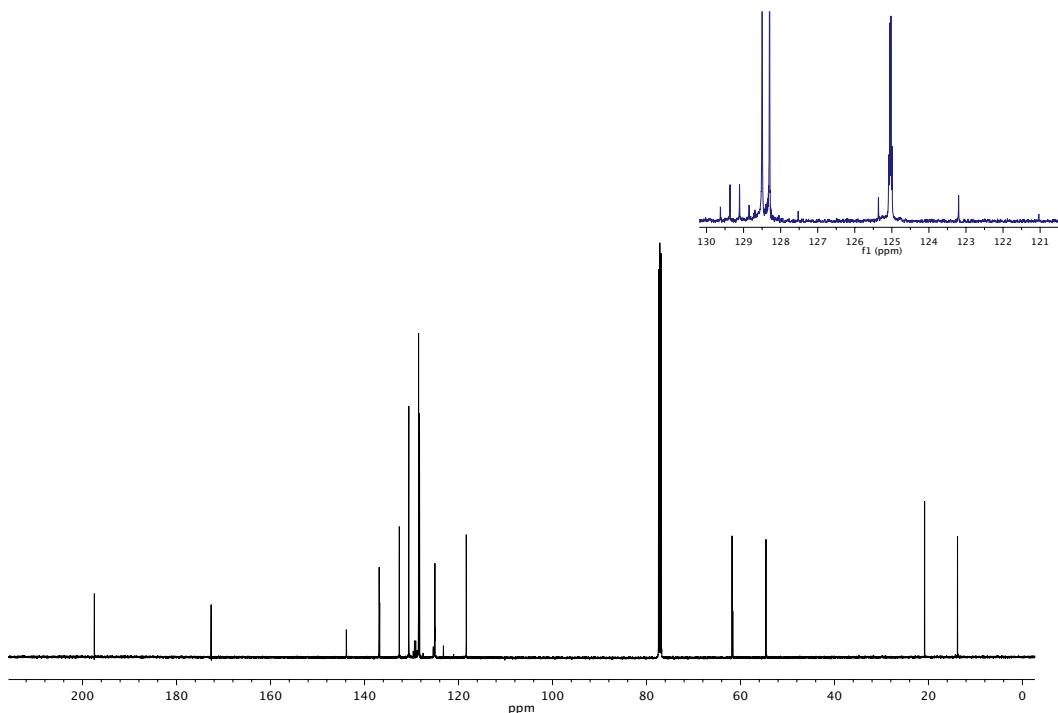


Figure A6.21  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) of compound **112g**.

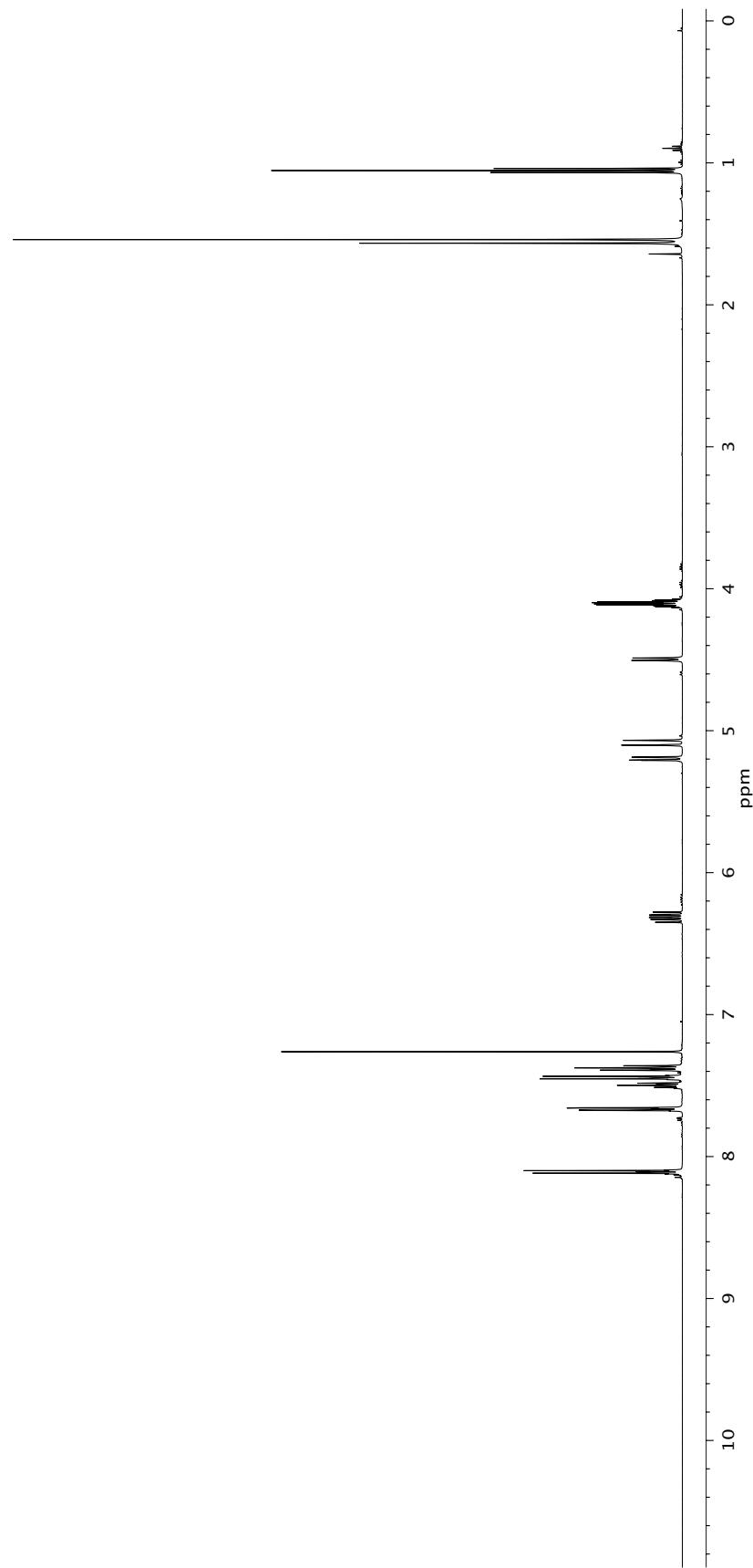
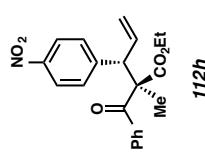


Figure A6.22  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of compound 112h.

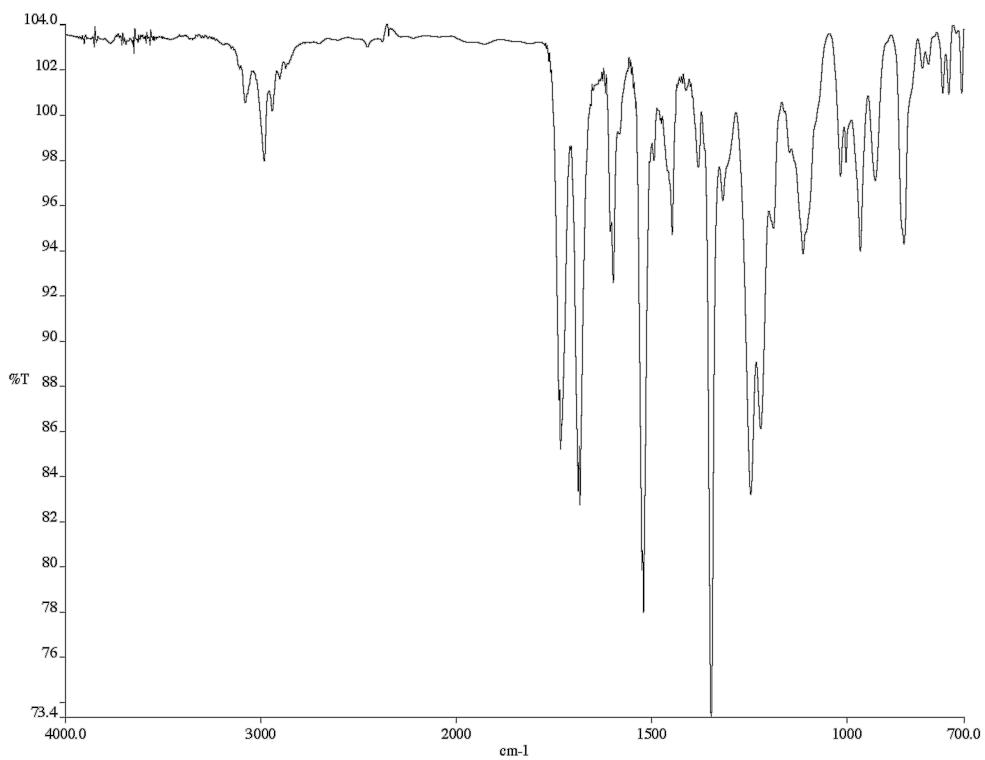


Figure A6.23 Infrared spectrum (thin film/NaCl) of compound **112h**.

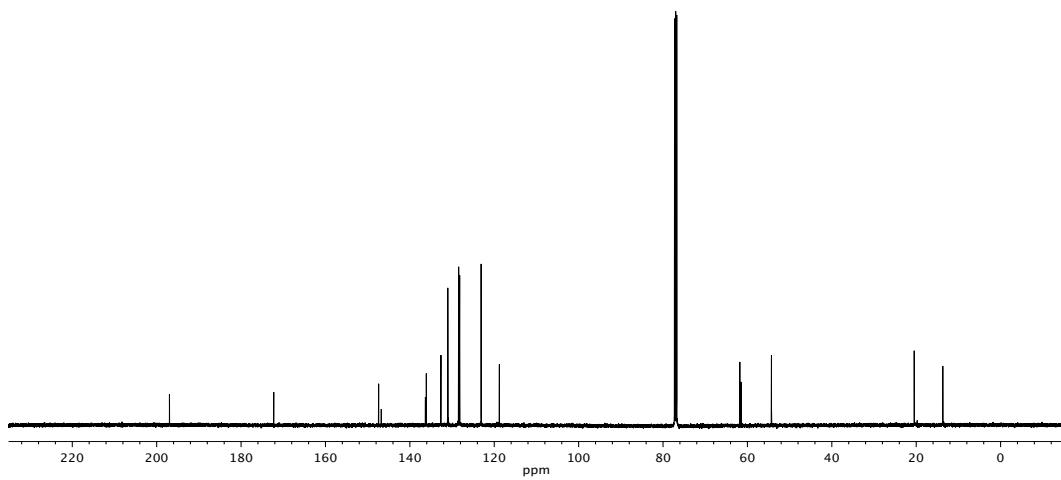


Figure A6.24 <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound **112h**.

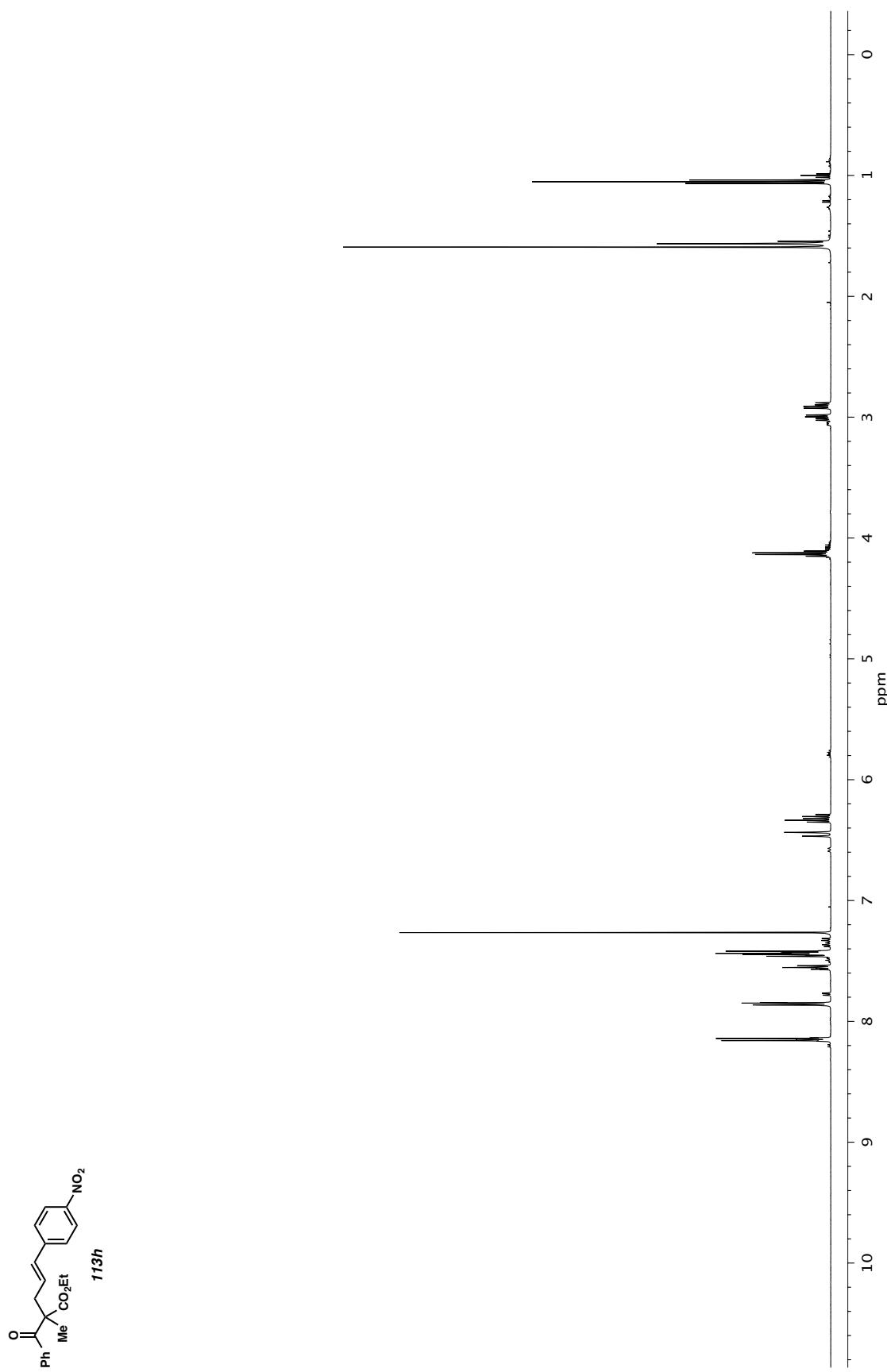


Figure A6.25 <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) of compound **113h**.

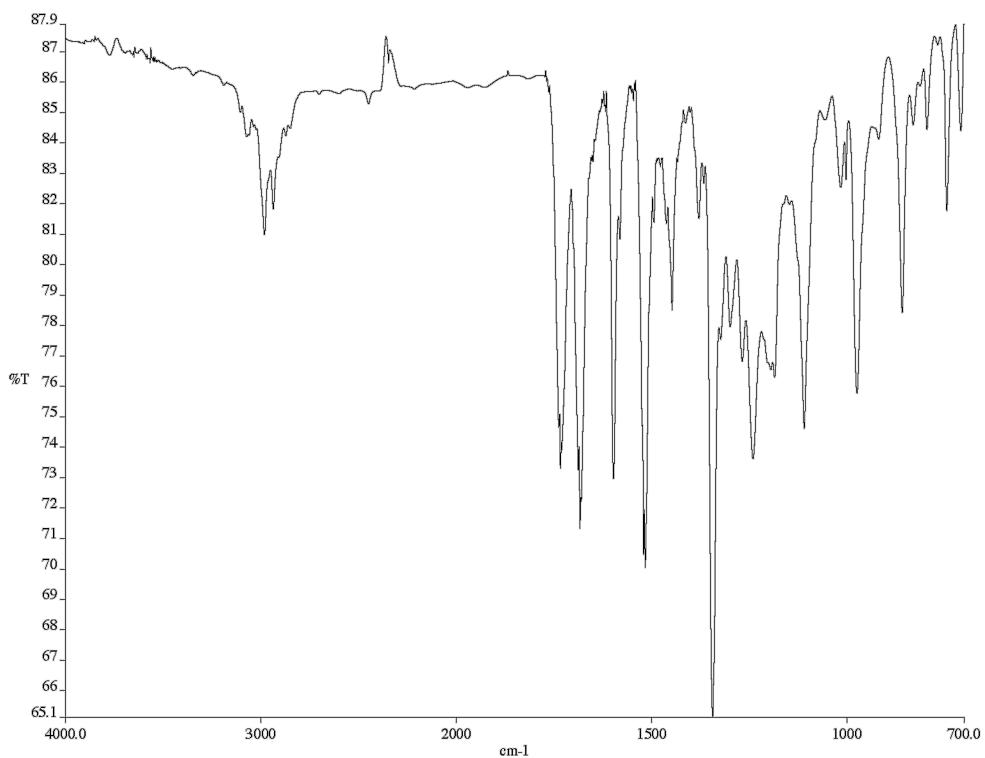


Figure A6.26 Infrared spectrum (thin film/NaCl) of compound **113h**.

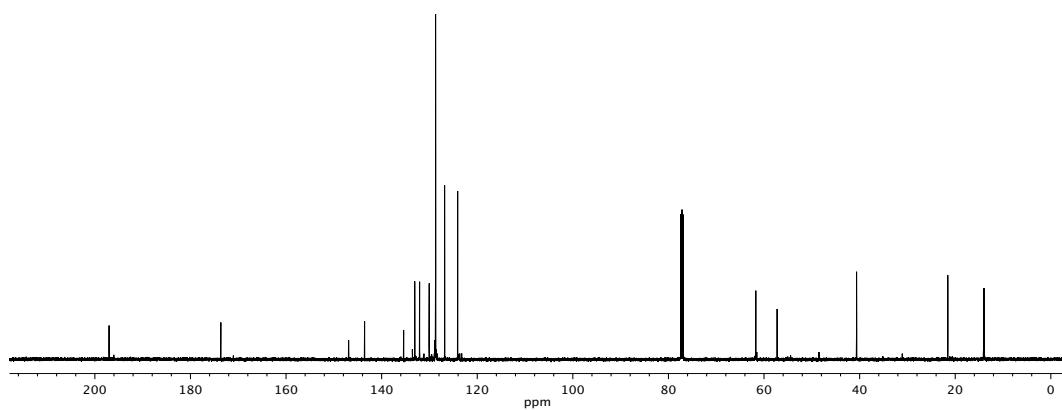


Figure A6.27 <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound **113h**.

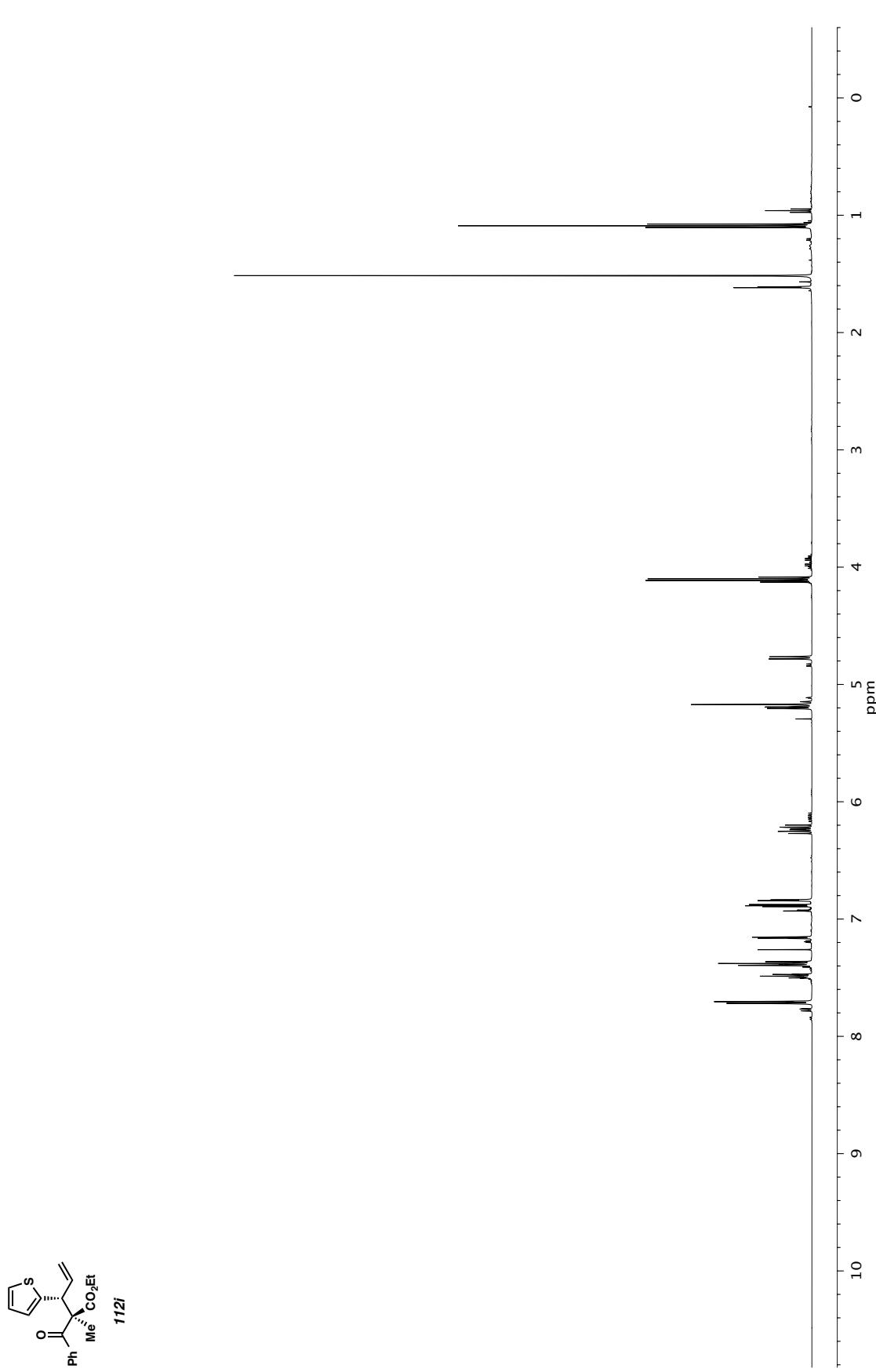


Figure A6.28  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of compound 112i.

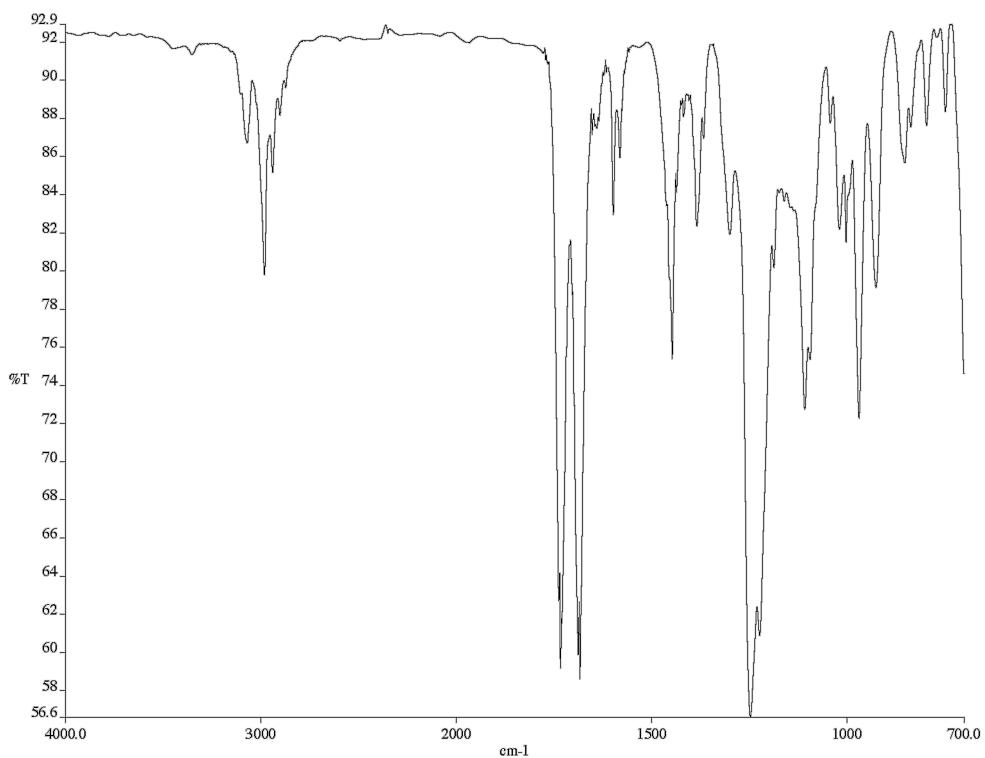


Figure A6.29 Infrared spectrum (thin film/NaCl) of compound **112i**.

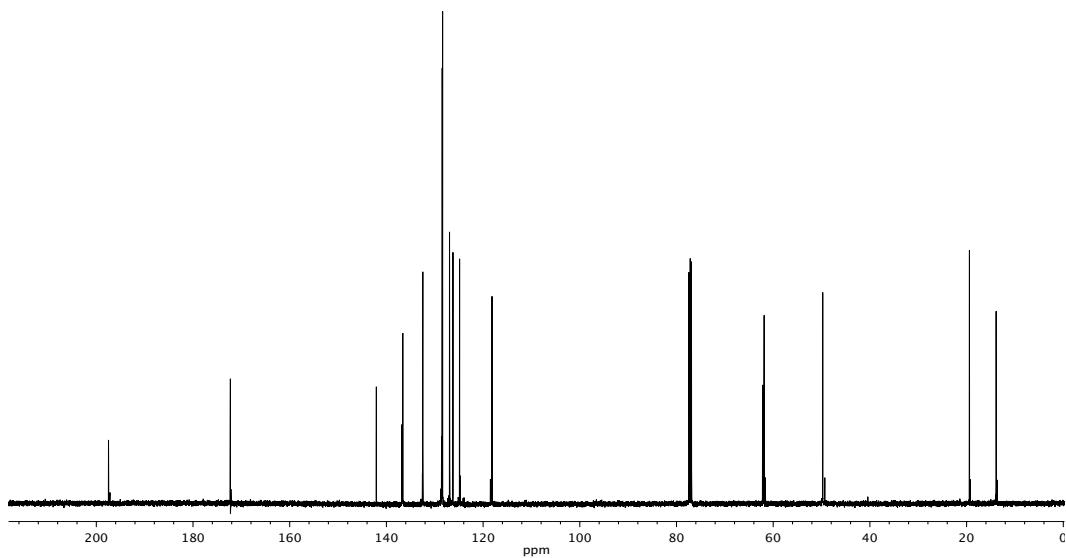


Figure A6.30  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) of compound **112i**.

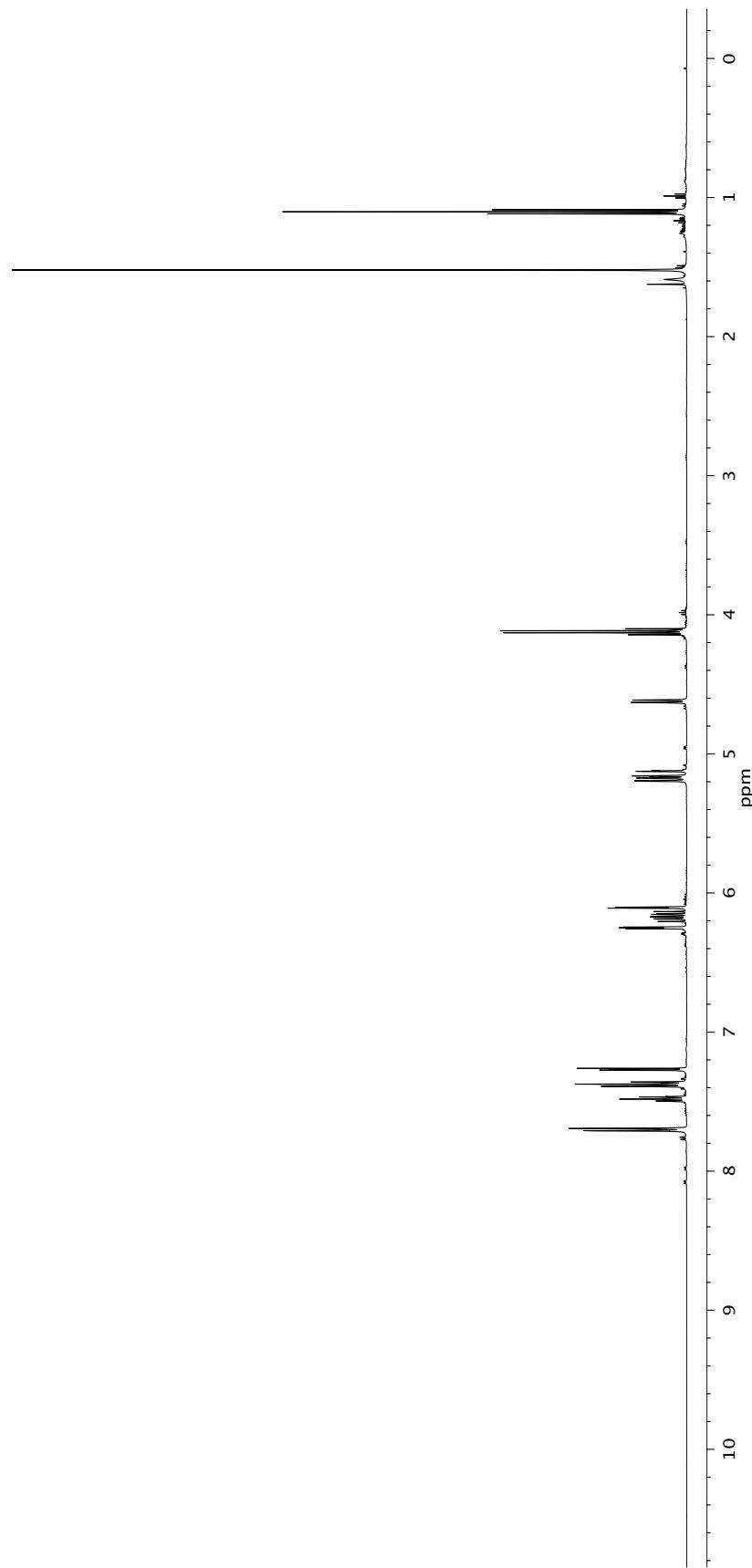
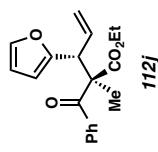


Figure A6.31 <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) of compound 112j.

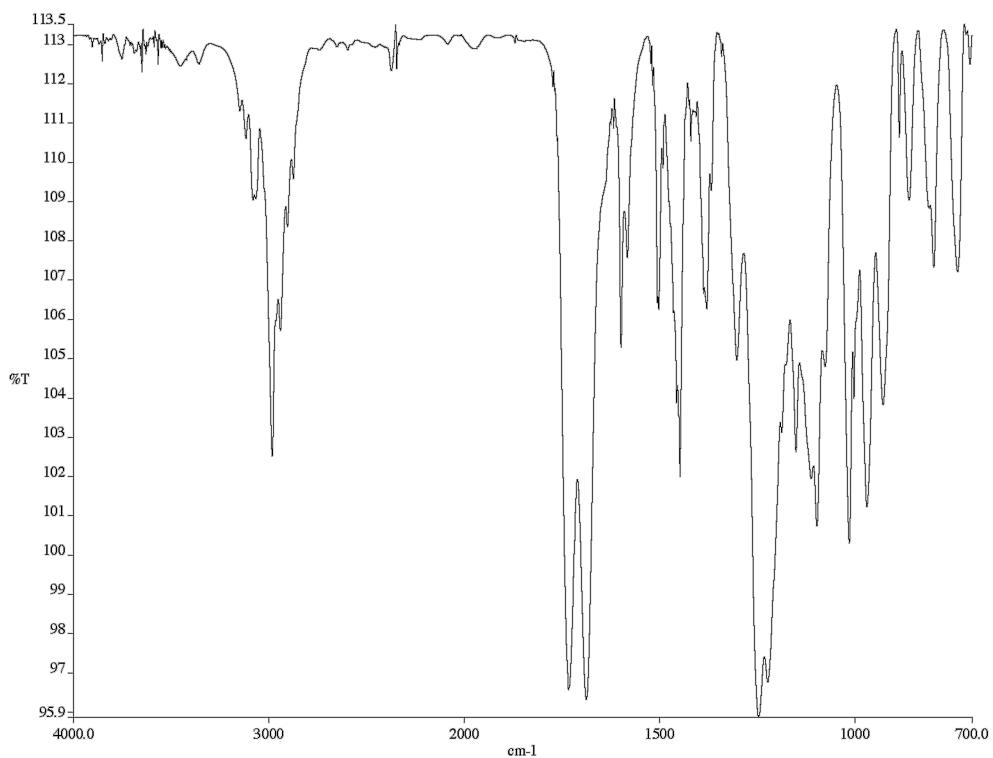


Figure A6.32 Infrared spectrum (thin film/NaCl) of compound **112j**.

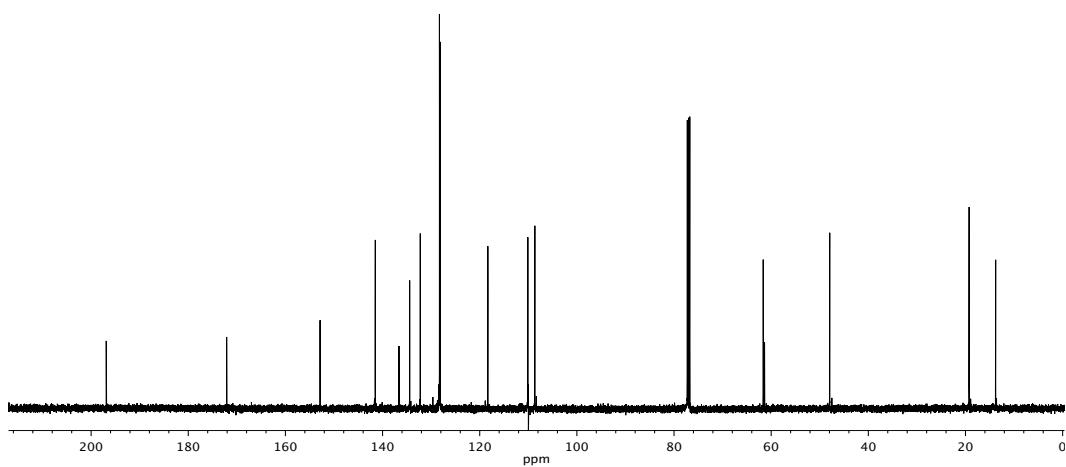


Figure A6.33  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) of compound **112j**.

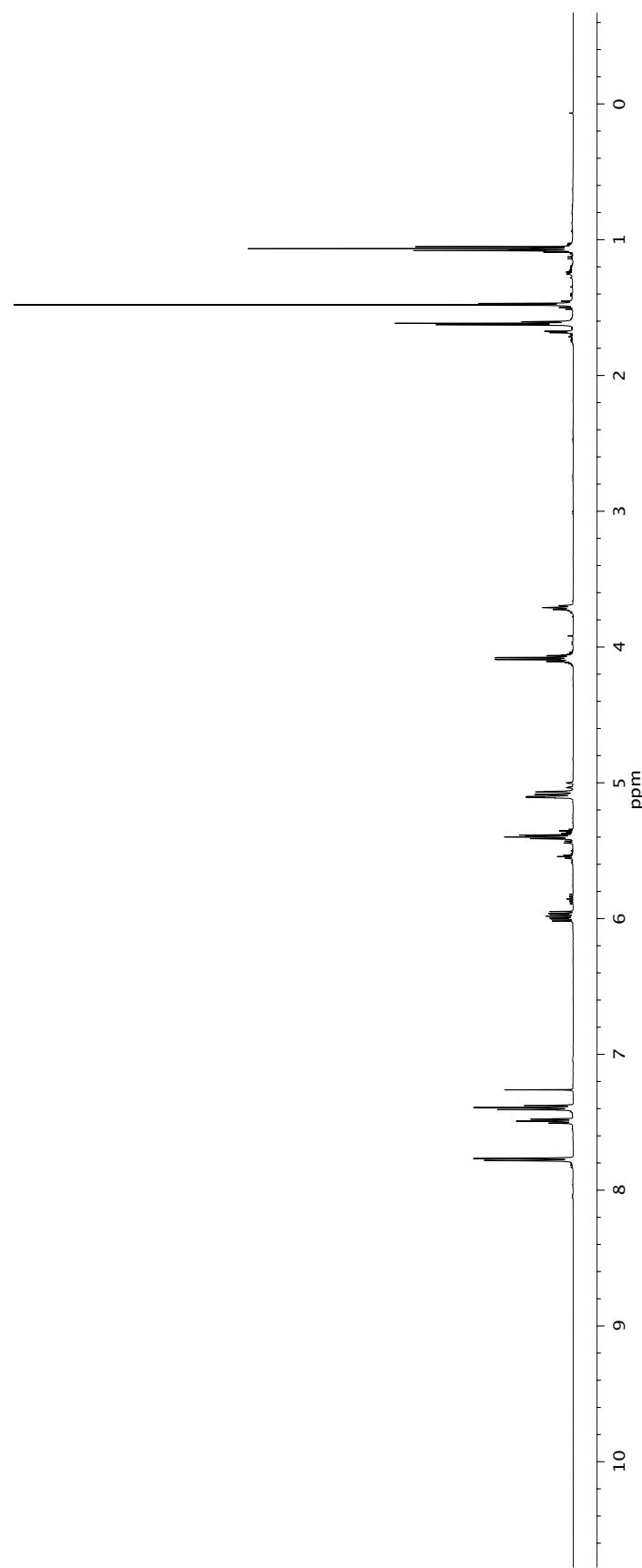
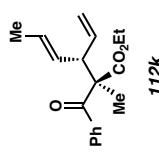


Figure A6.34  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of compound 112k.

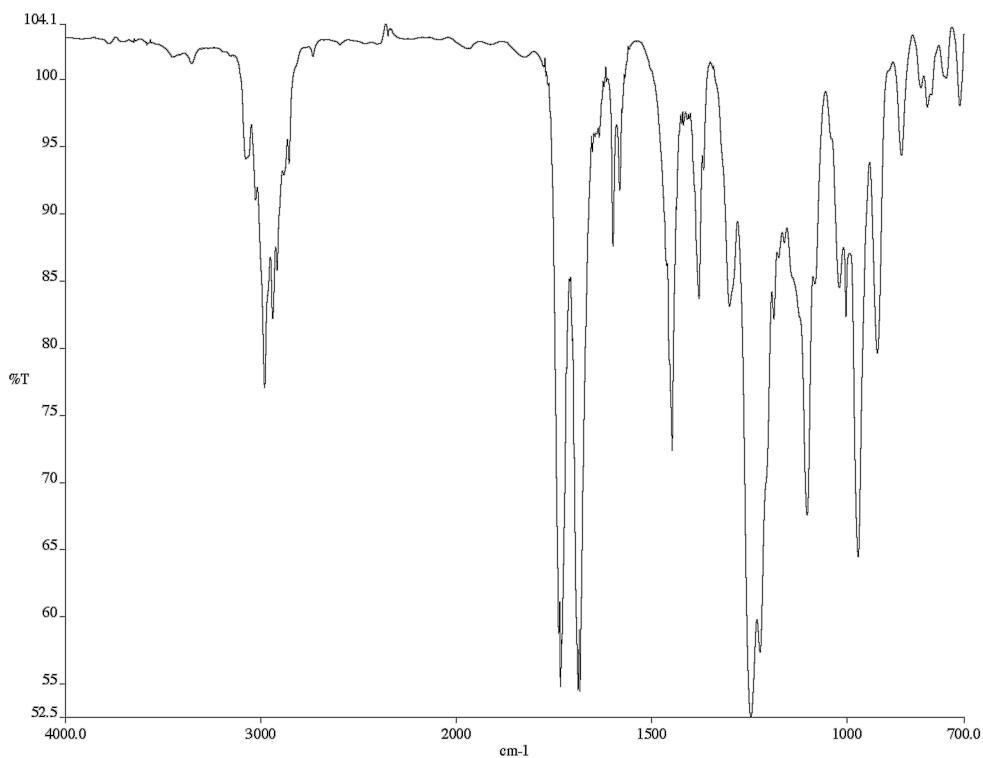


Figure A6.35 Infrared spectrum (thin film/NaCl) of compound **112k**.

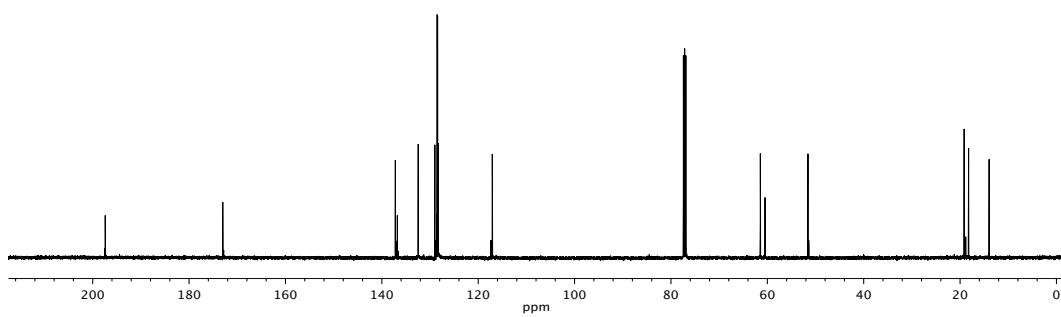


Figure A6.36 <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound **112k**.

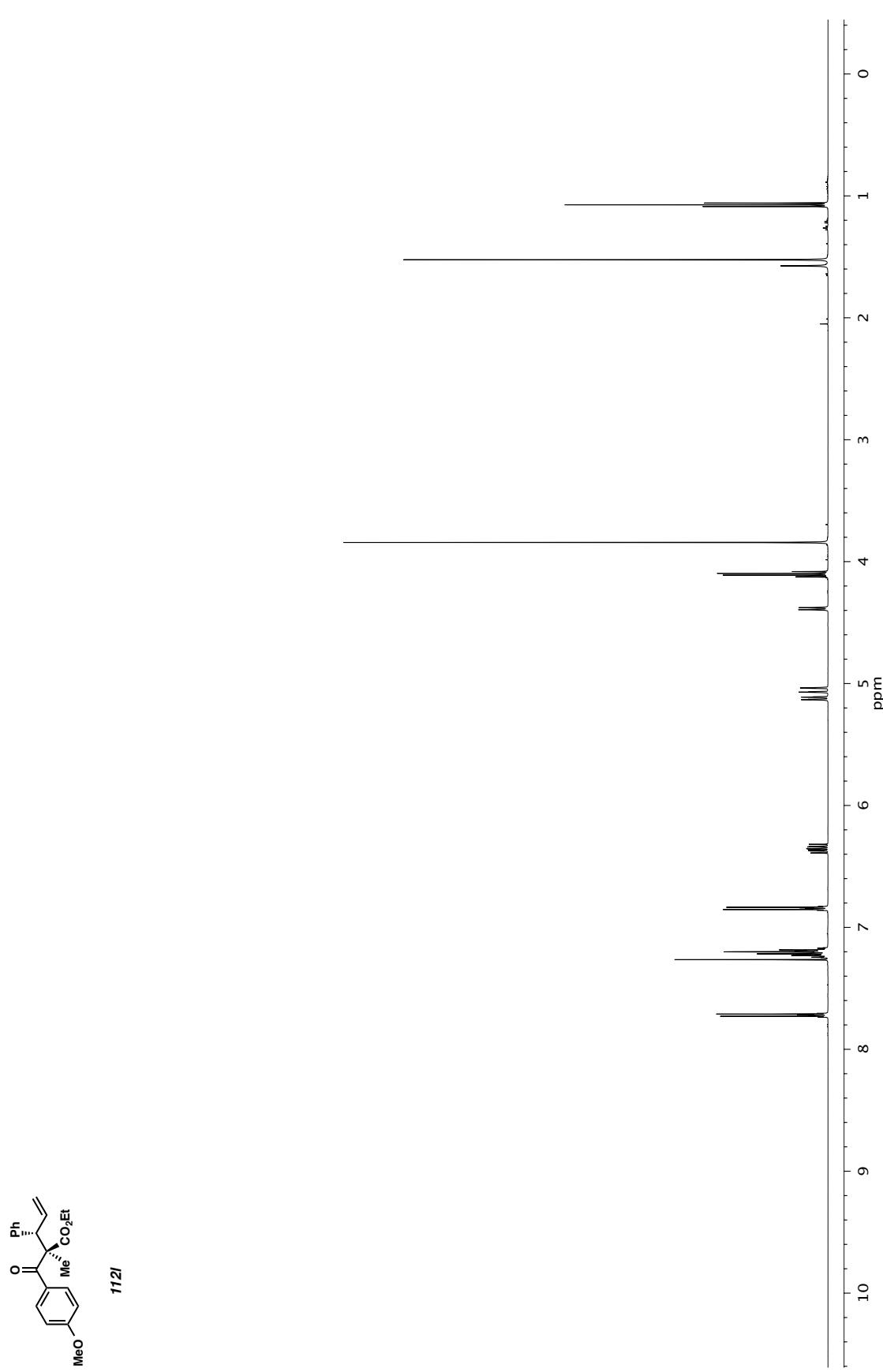


Figure A6.37  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of compound 112l.

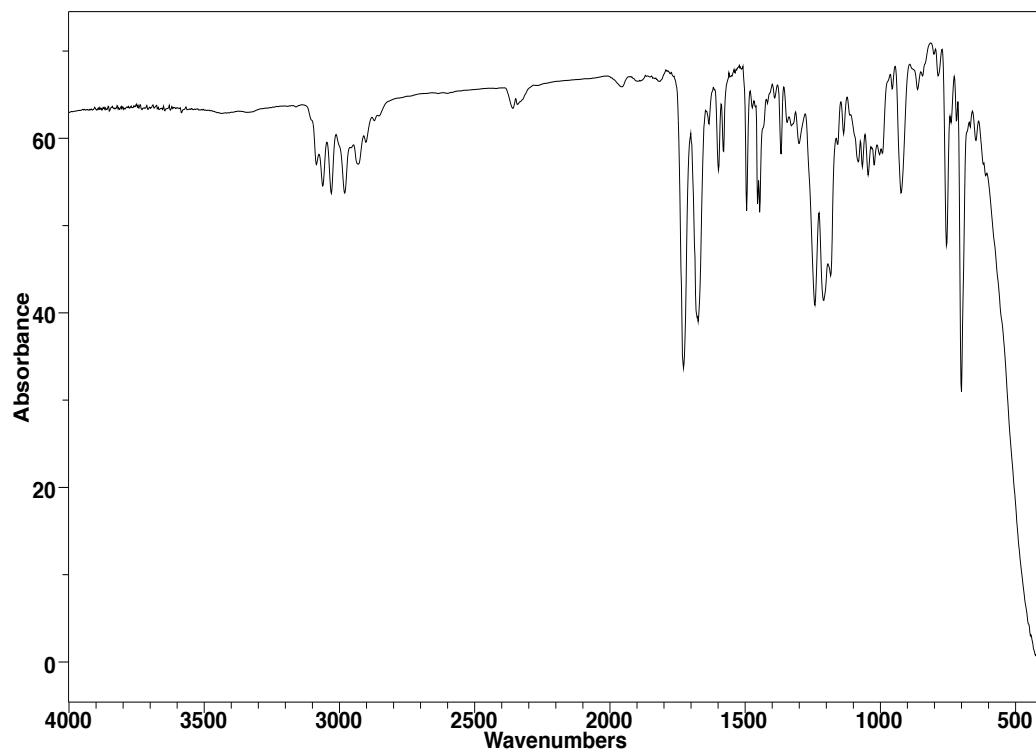


Figure A6.38 Infrared spectrum (thin film/NaCl) of compound **112l**.

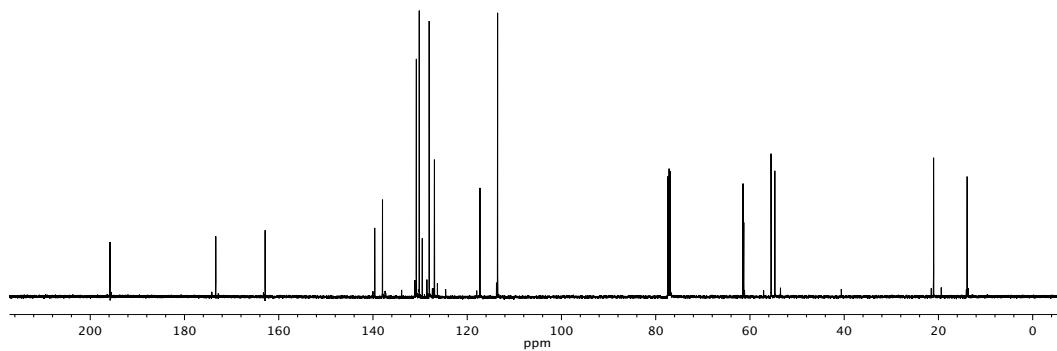


Figure A6.39 <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound **112l**.

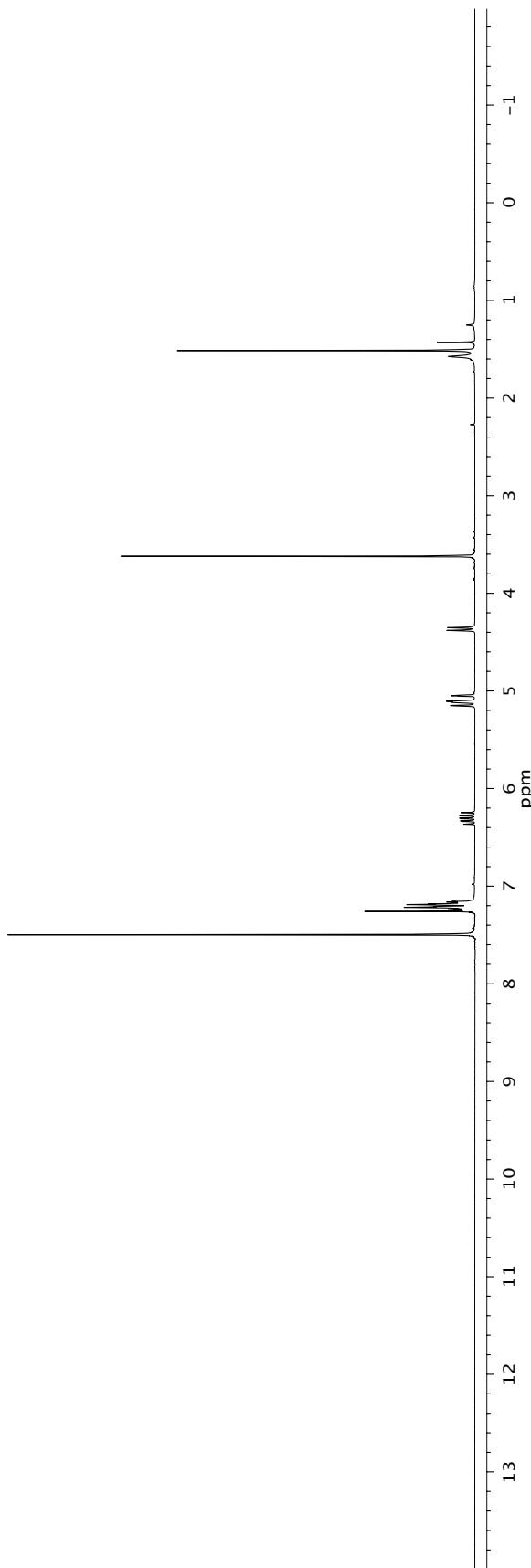
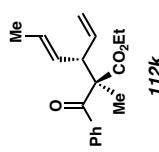


Figure A6.40  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of compound 112m.

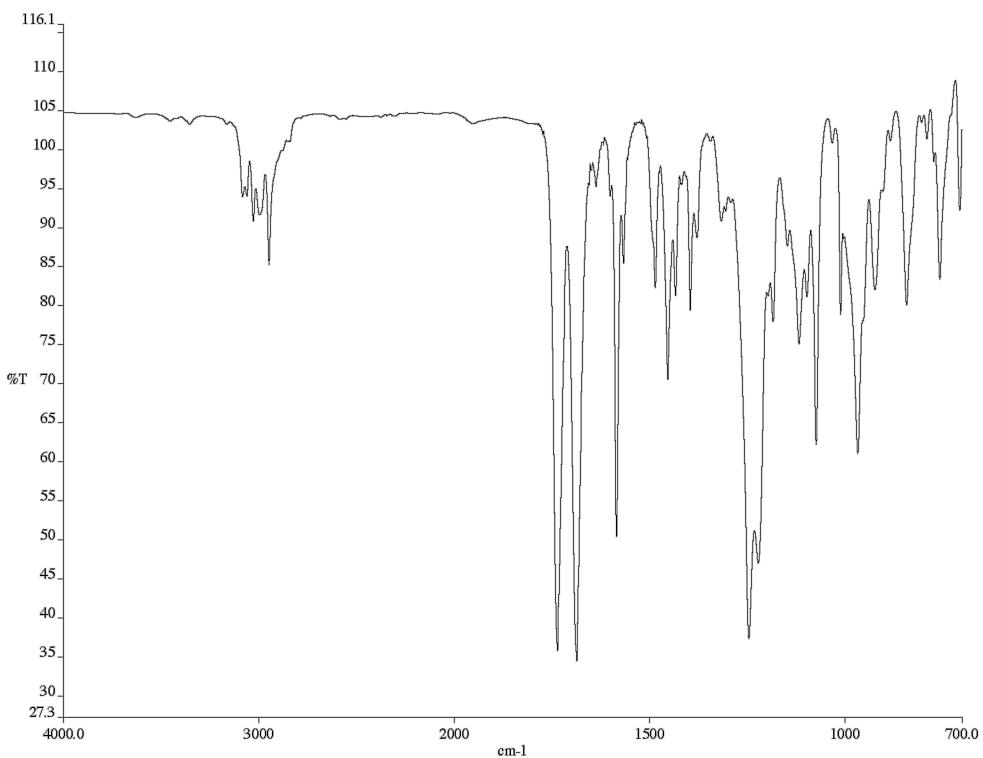


Figure A6.41 Infrared spectrum (thin film/NaCl) of compound **112m**.

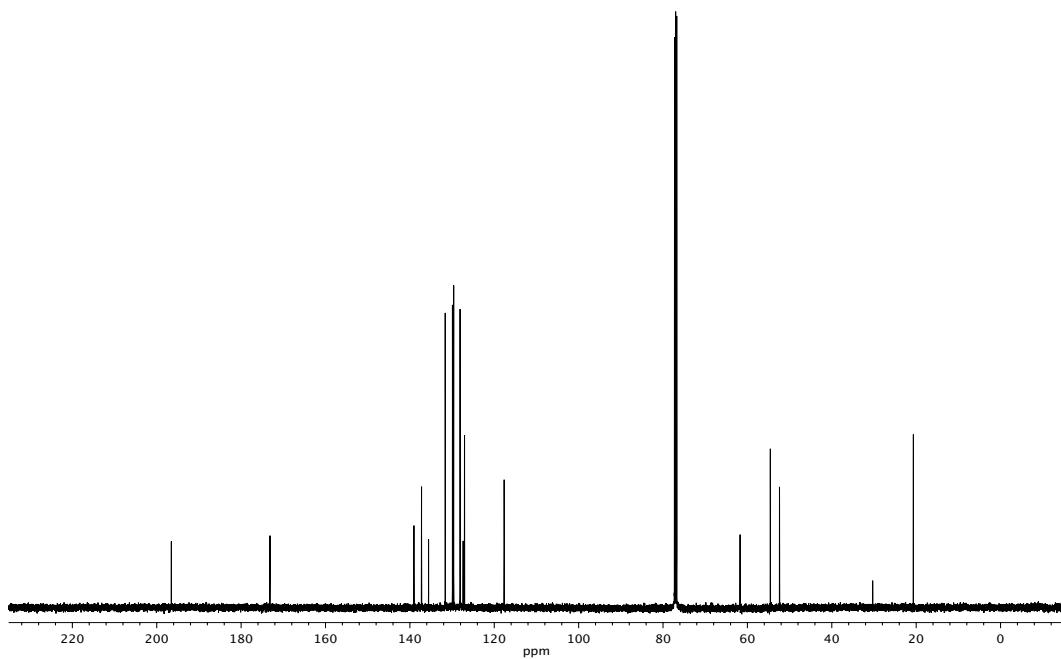


Figure A6.42 <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound **112m**.

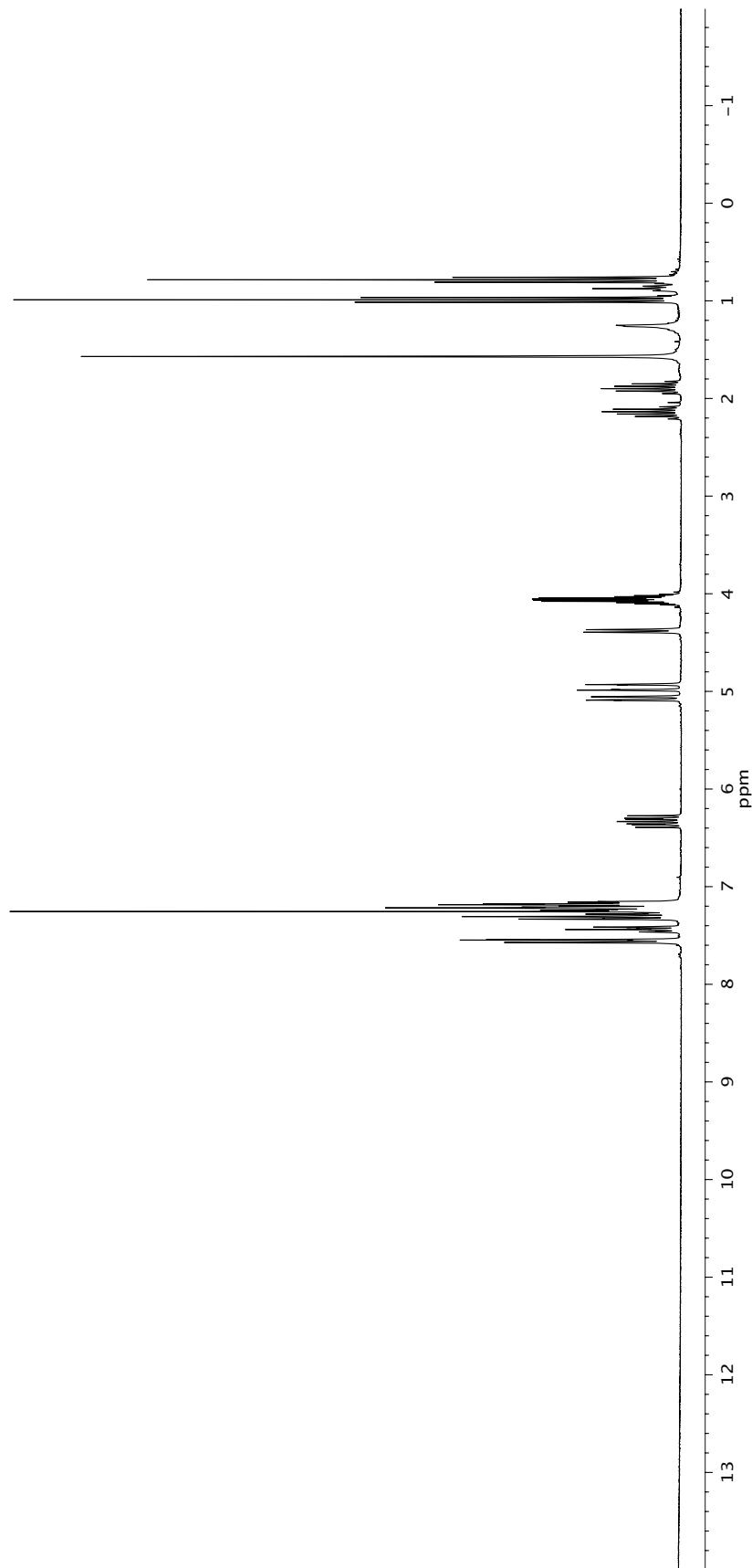
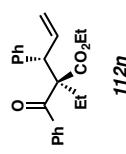


Figure A6.43  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of compound 112n.

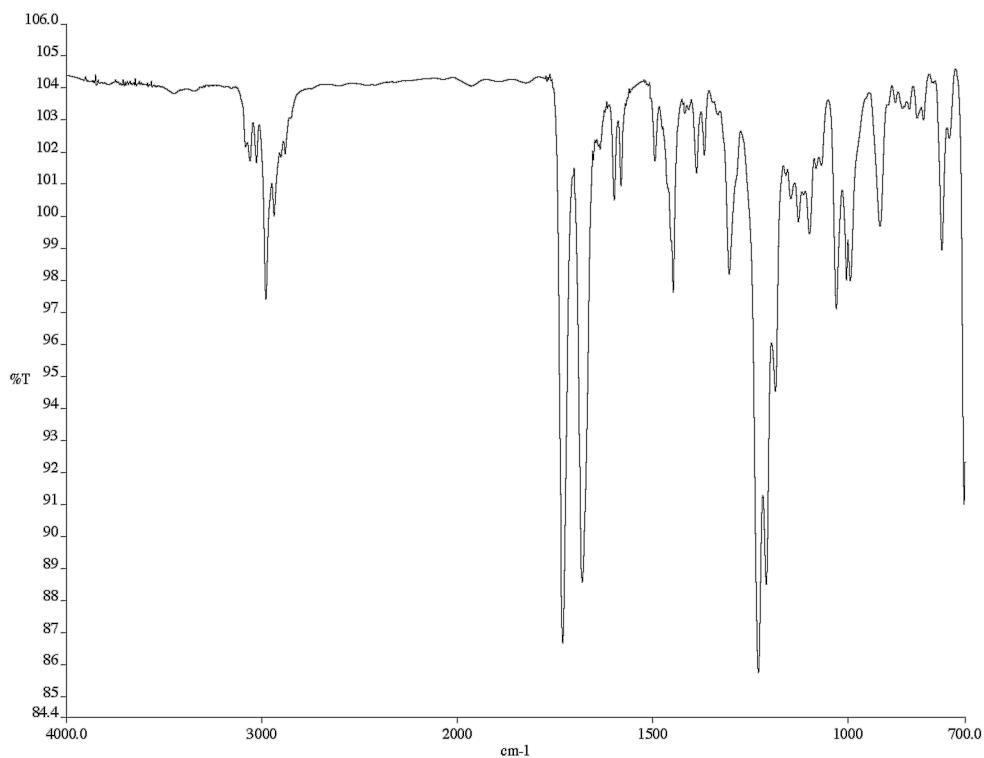


Figure A6.44 Infrared spectrum (thin film/NaCl) of compound **112n**.

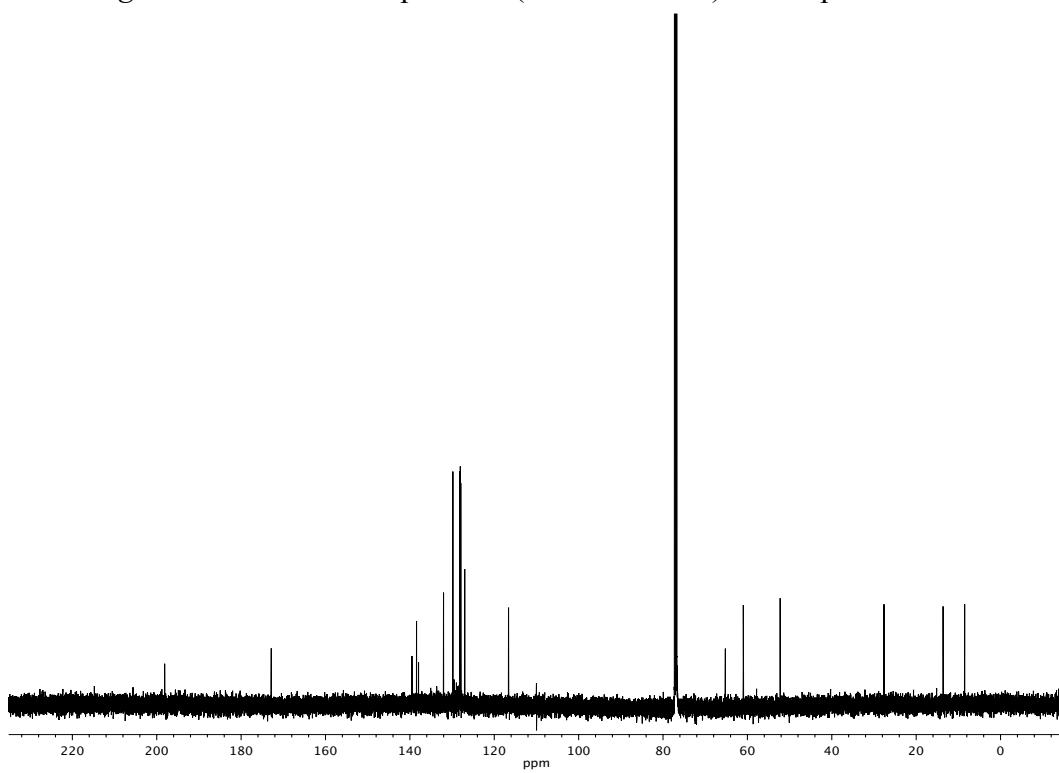


Figure A6.45 <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound **112n**.

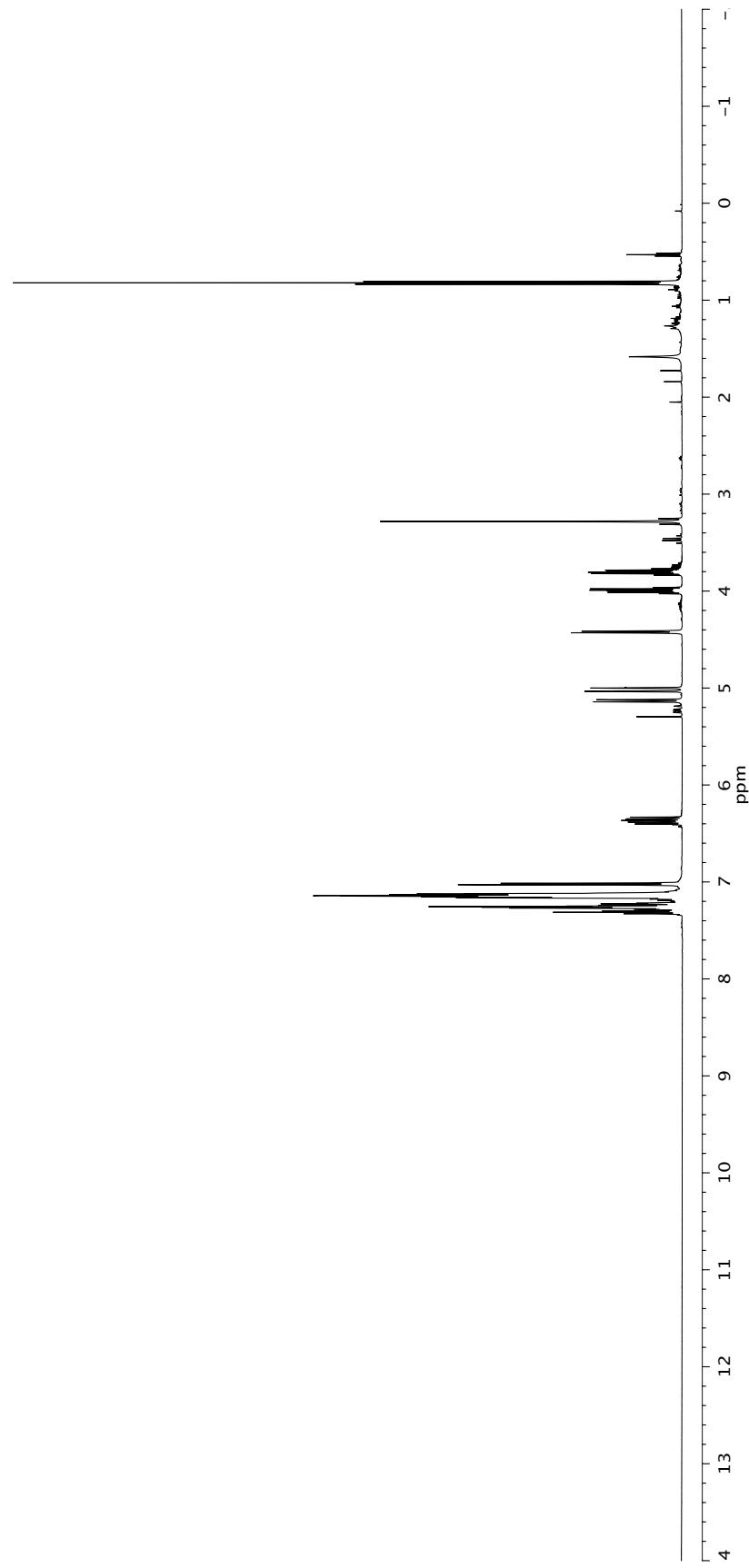
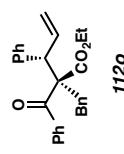


Figure A6.46  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of compound 112o.

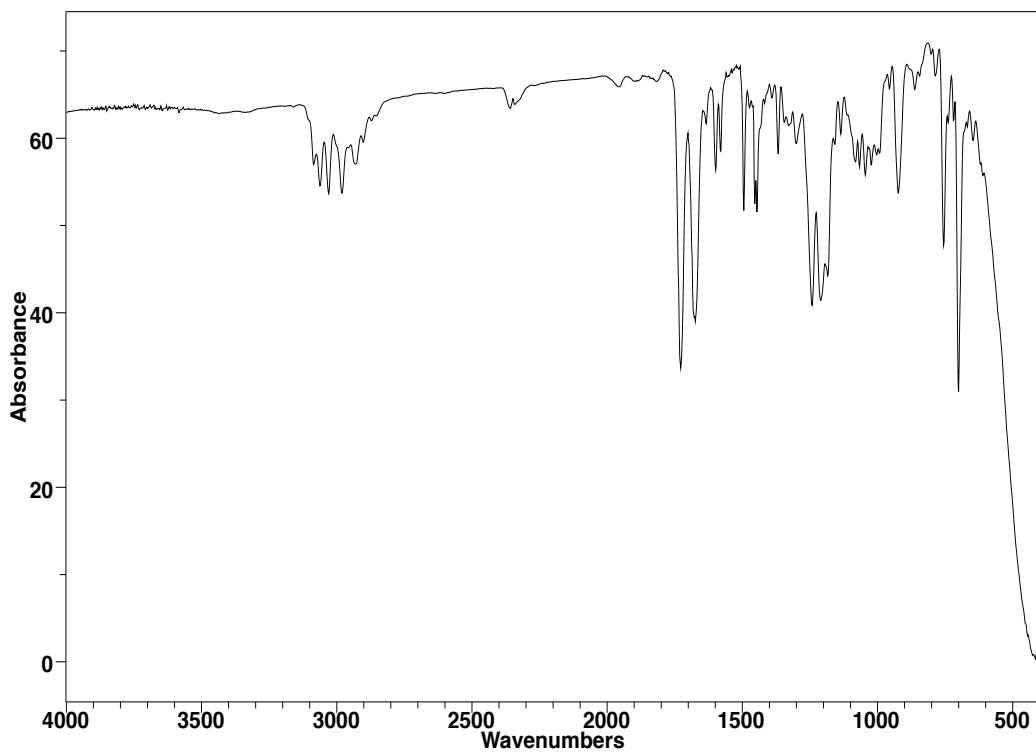


Figure A6.47 Infrared spectrum (thin film/NaCl) of compound **112o**.

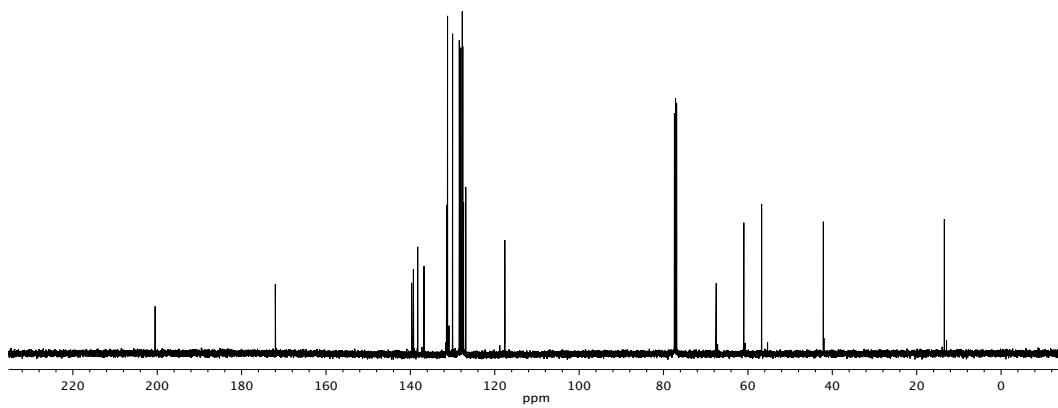


Figure A6.48 <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound **112o**.

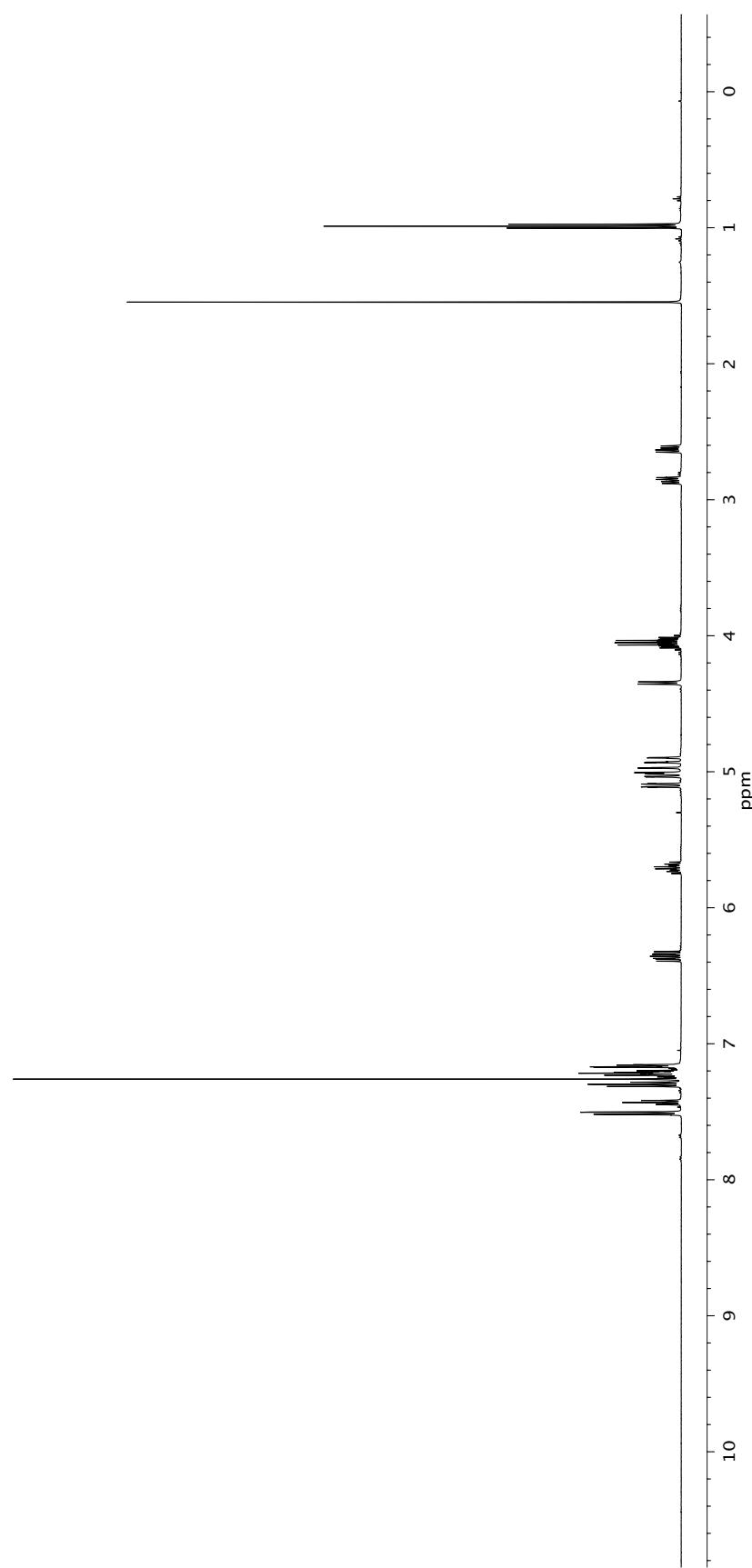
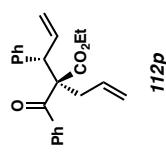


Figure A6.49 <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) of compound 112p.

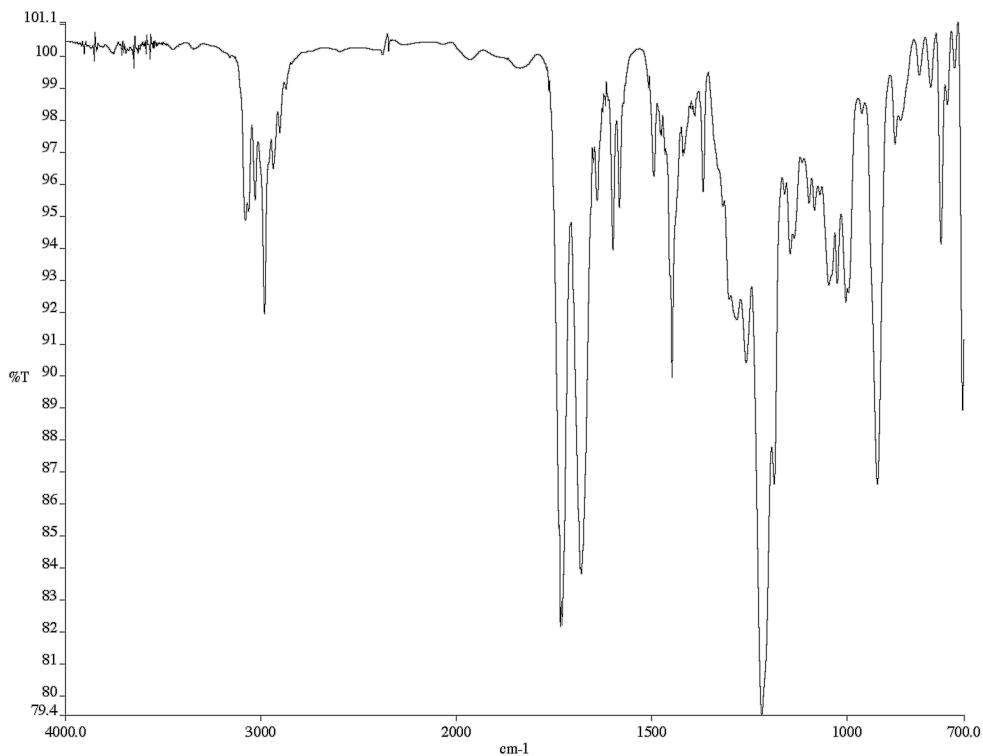


Figure A6.50 Infrared spectrum (thin film/NaCl) of compound **112p**.

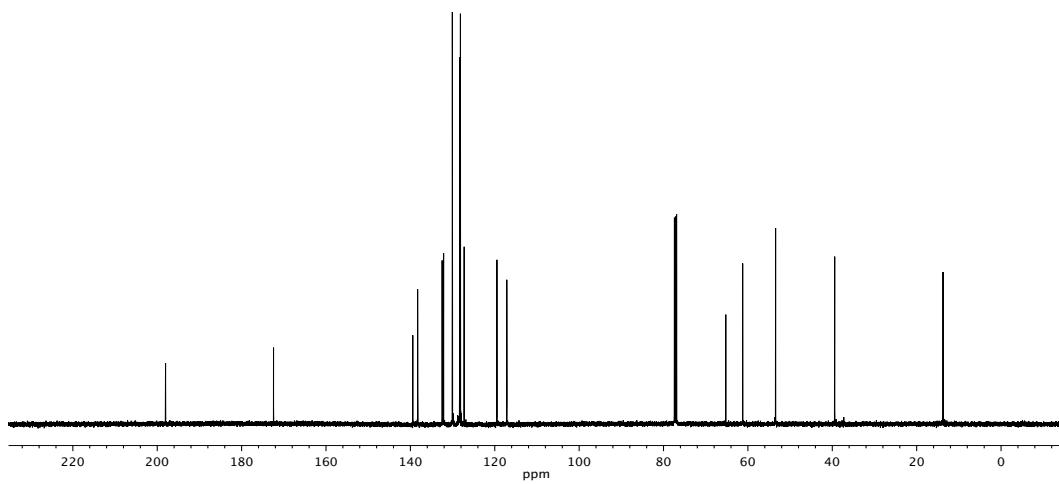


Figure A6.51  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) of compound **112p**.

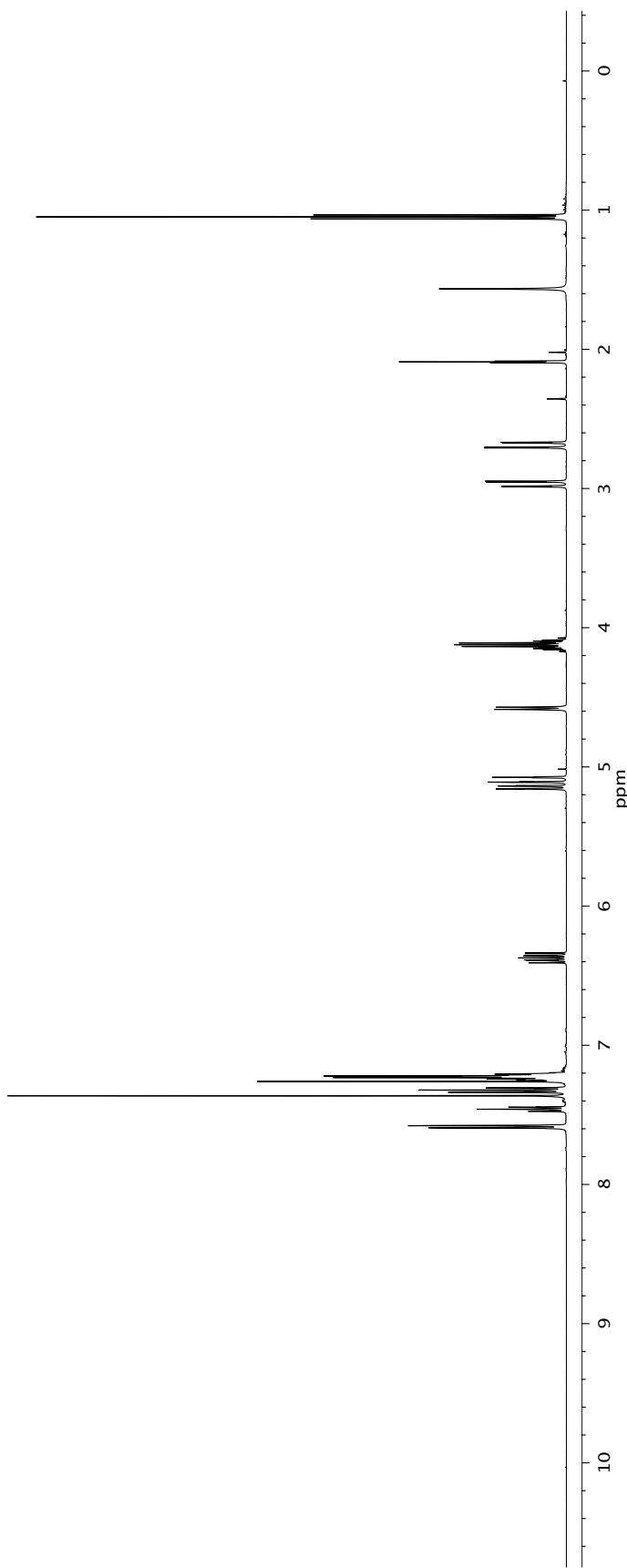
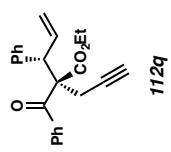


Figure A6.52 <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) of compound 112q.

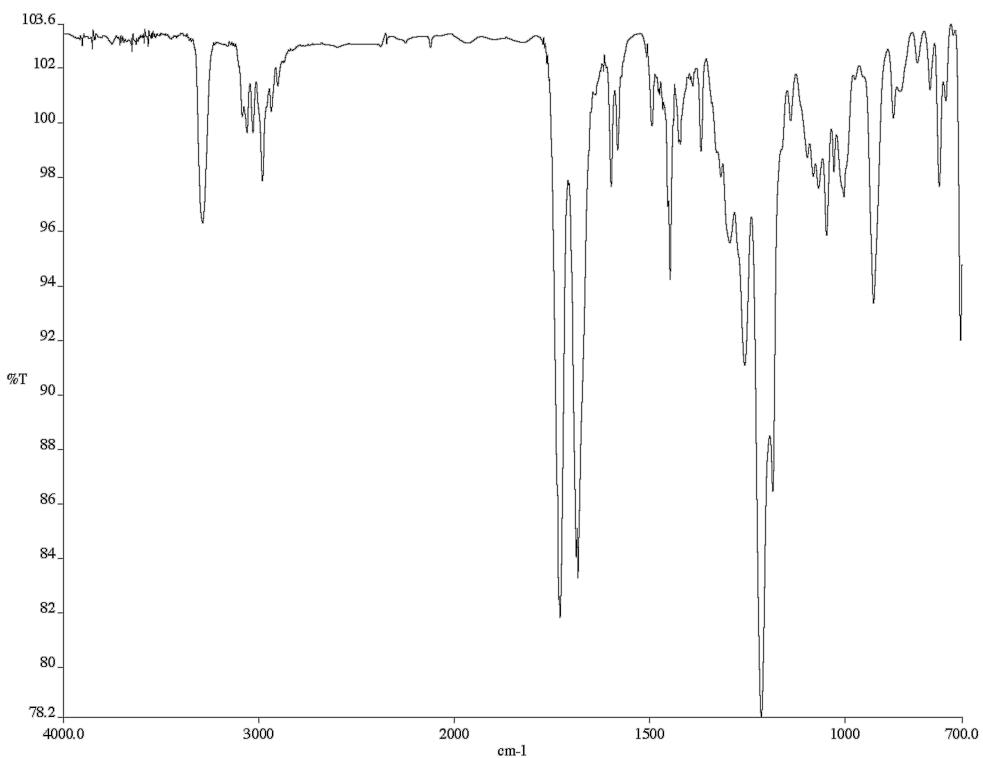


Figure A6.53 Infrared spectrum (thin film/NaCl) of compound **112q**.

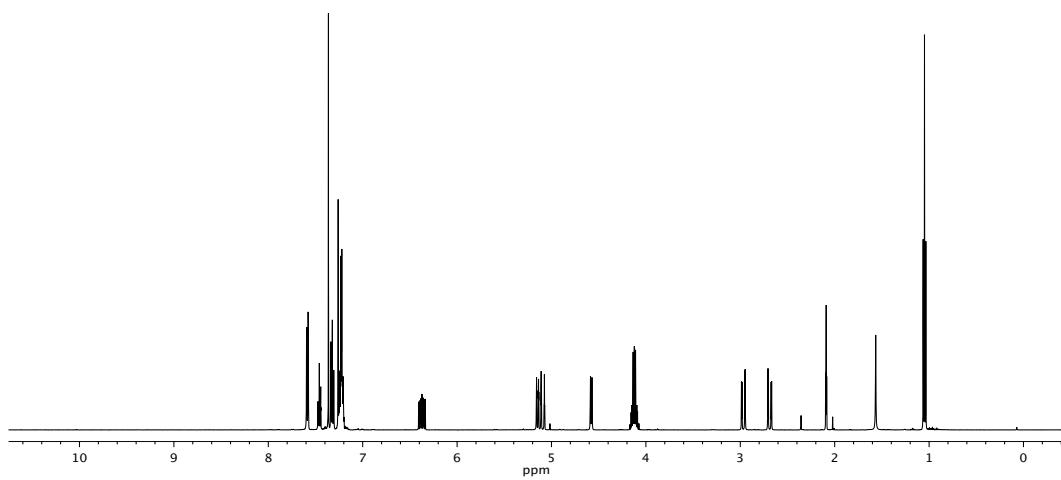


Figure A6.54 <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound **112q**.

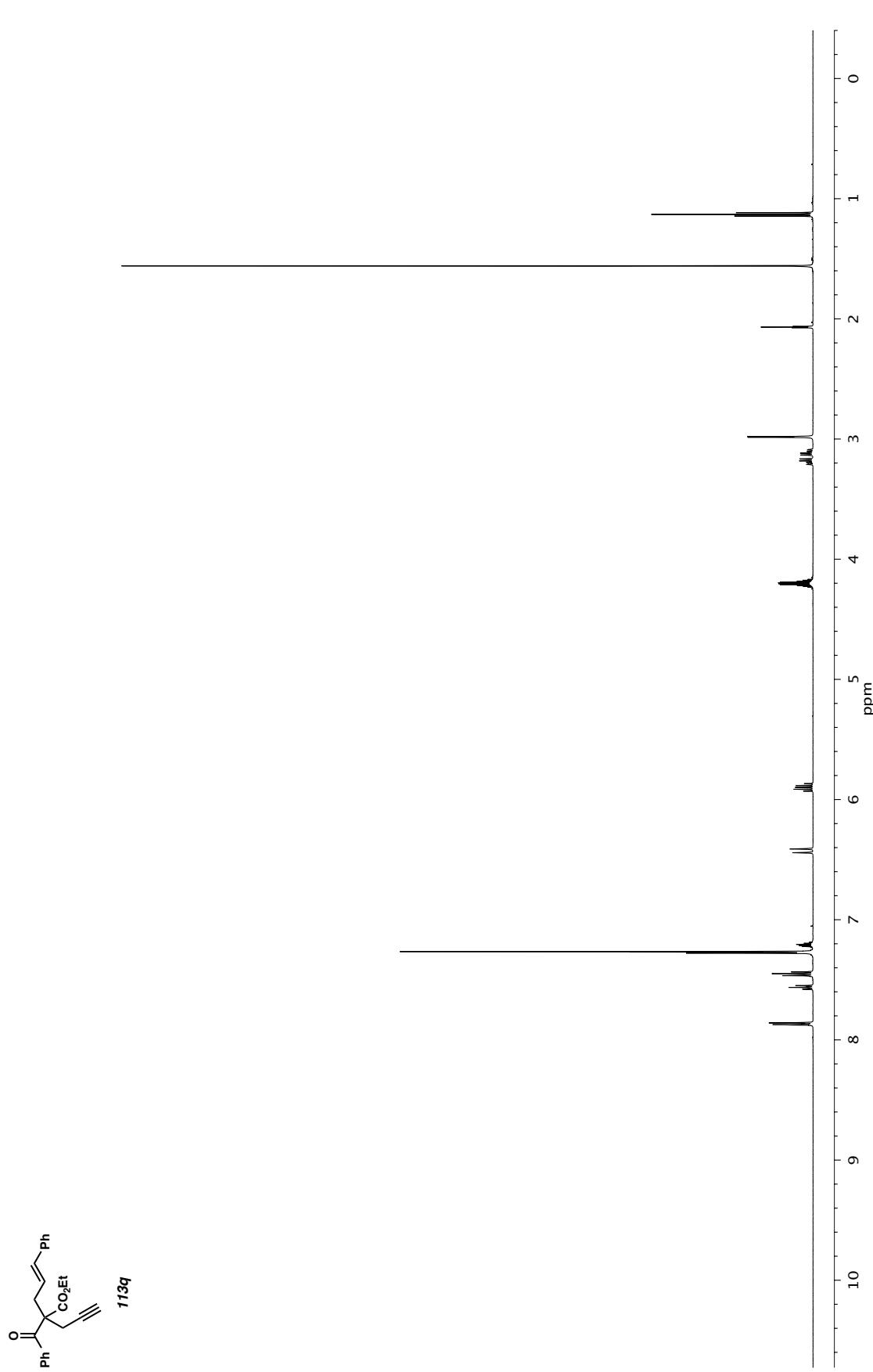


Figure A6.55  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of compound 113q.

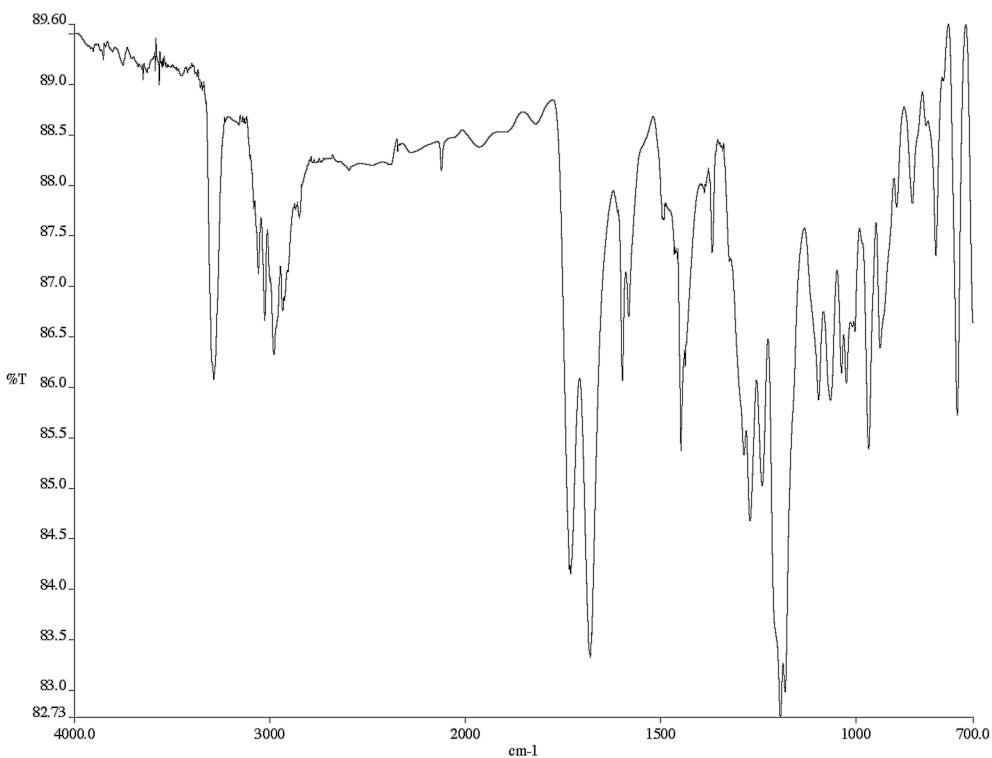


Figure A6.56 Infrared spectrum (thin film/NaCl) of compound **113q**.

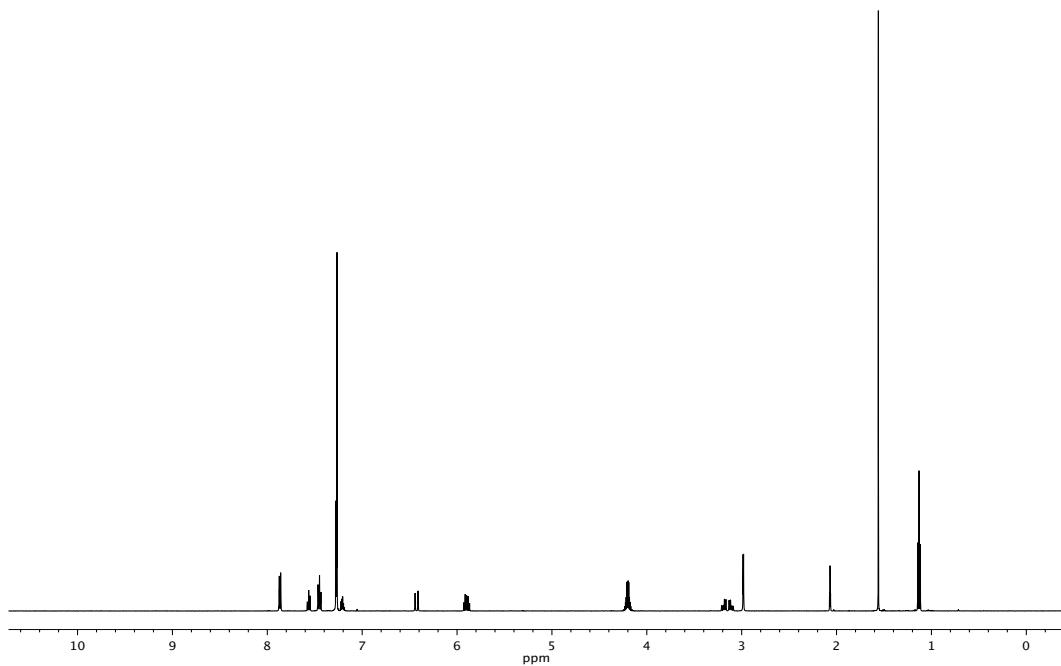


Figure A6.57 <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound **113q**.

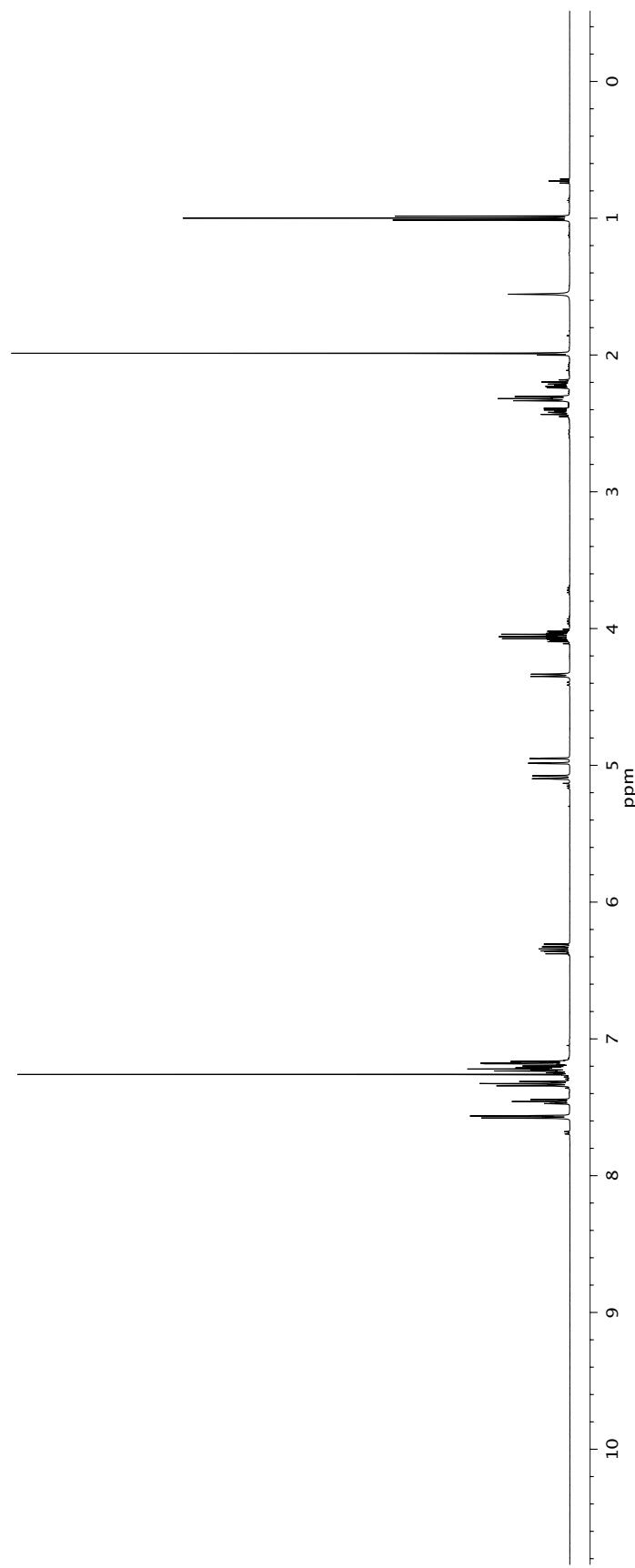
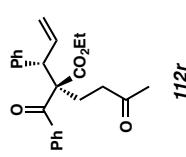


Figure A6.58 <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) of compound 112r.

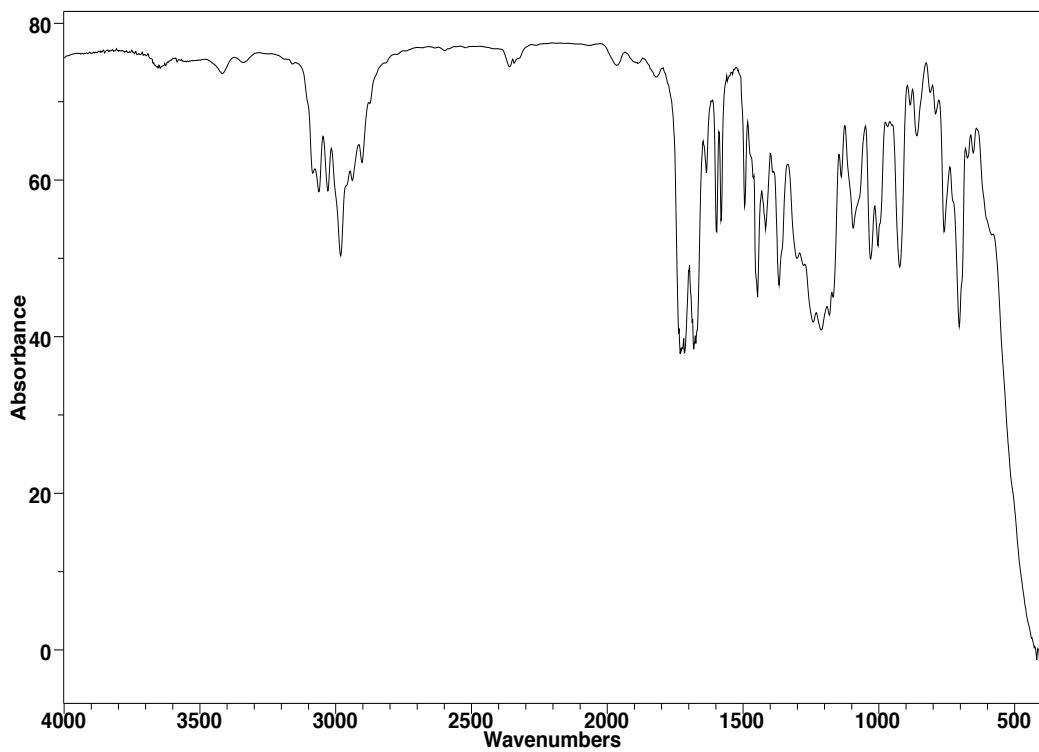


Figure A6.59 Infrared spectrum (thin film/NaCl) of compound **112r**.

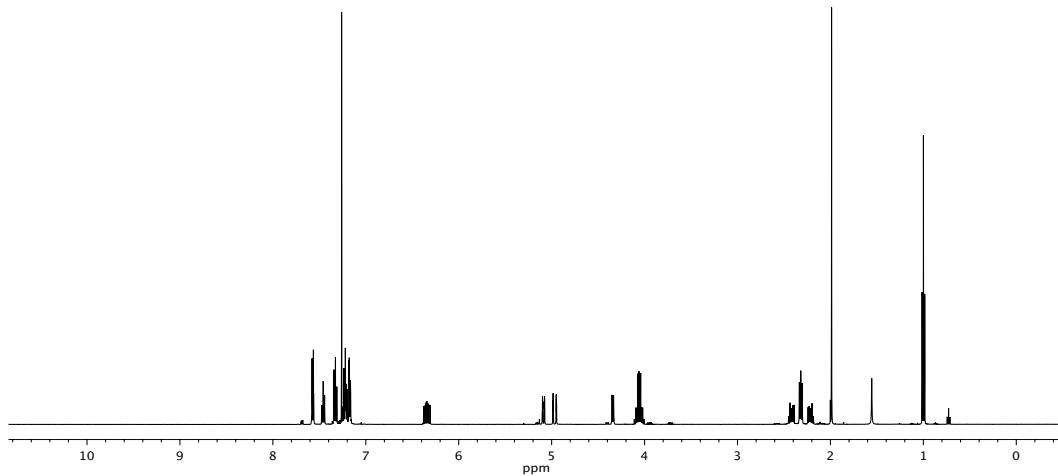


Figure A6.60 <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound **112r**.

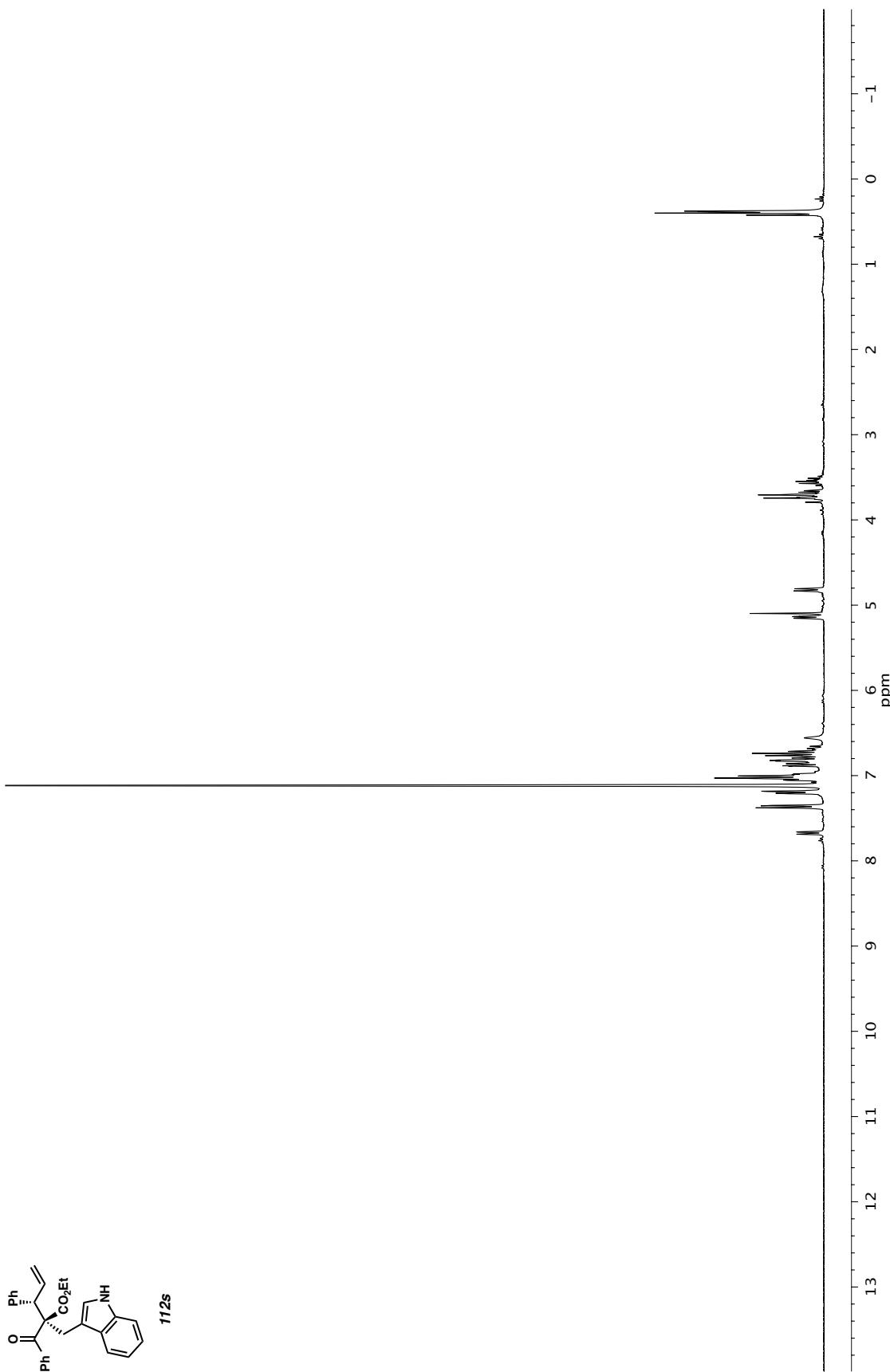


Figure A6.61  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of compound 112s.

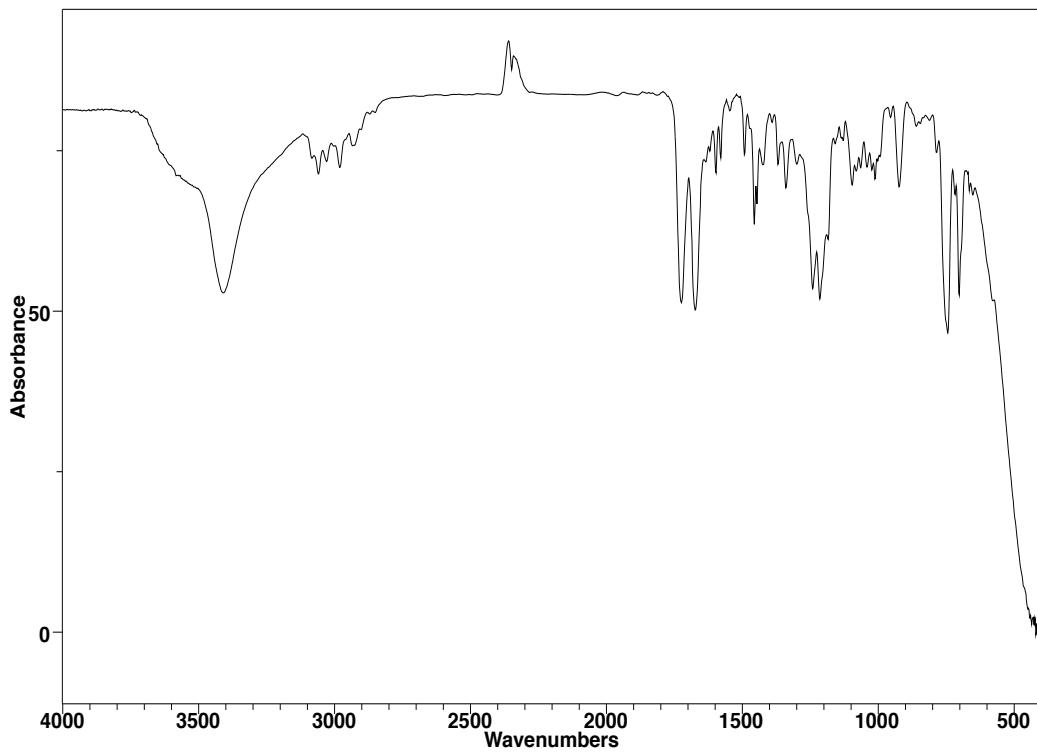


Figure A6.62 Infrared spectrum (thin film/NaCl) of compound **112s**.

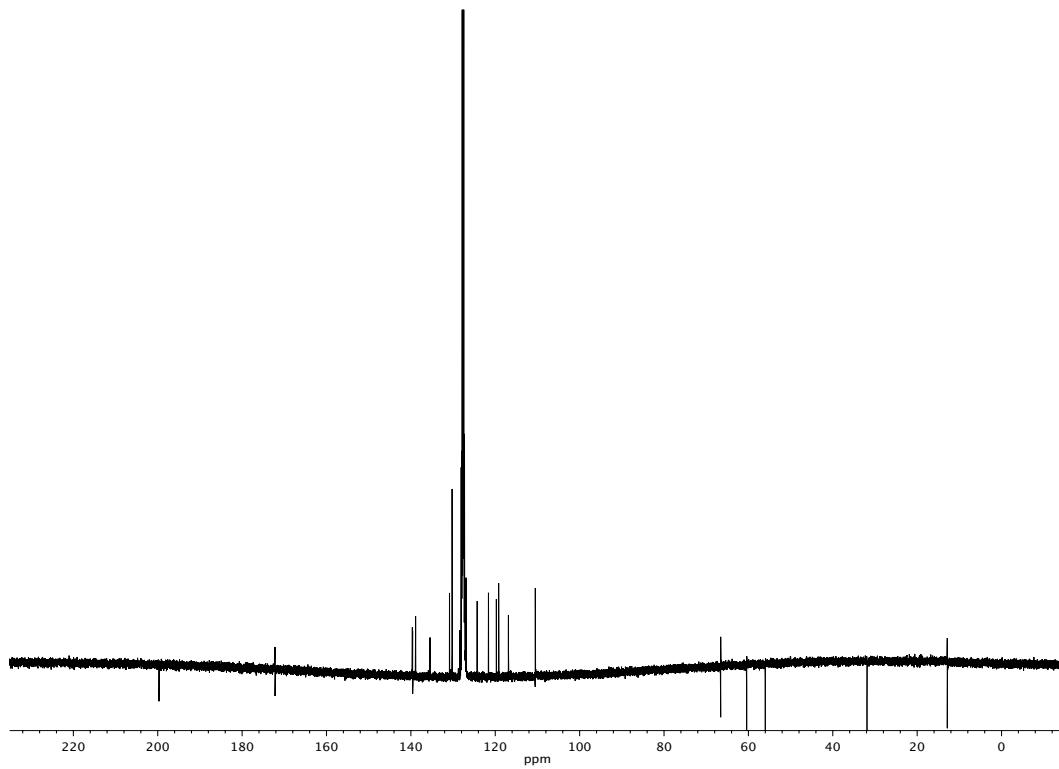


Figure A6.63 <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound **112s**.

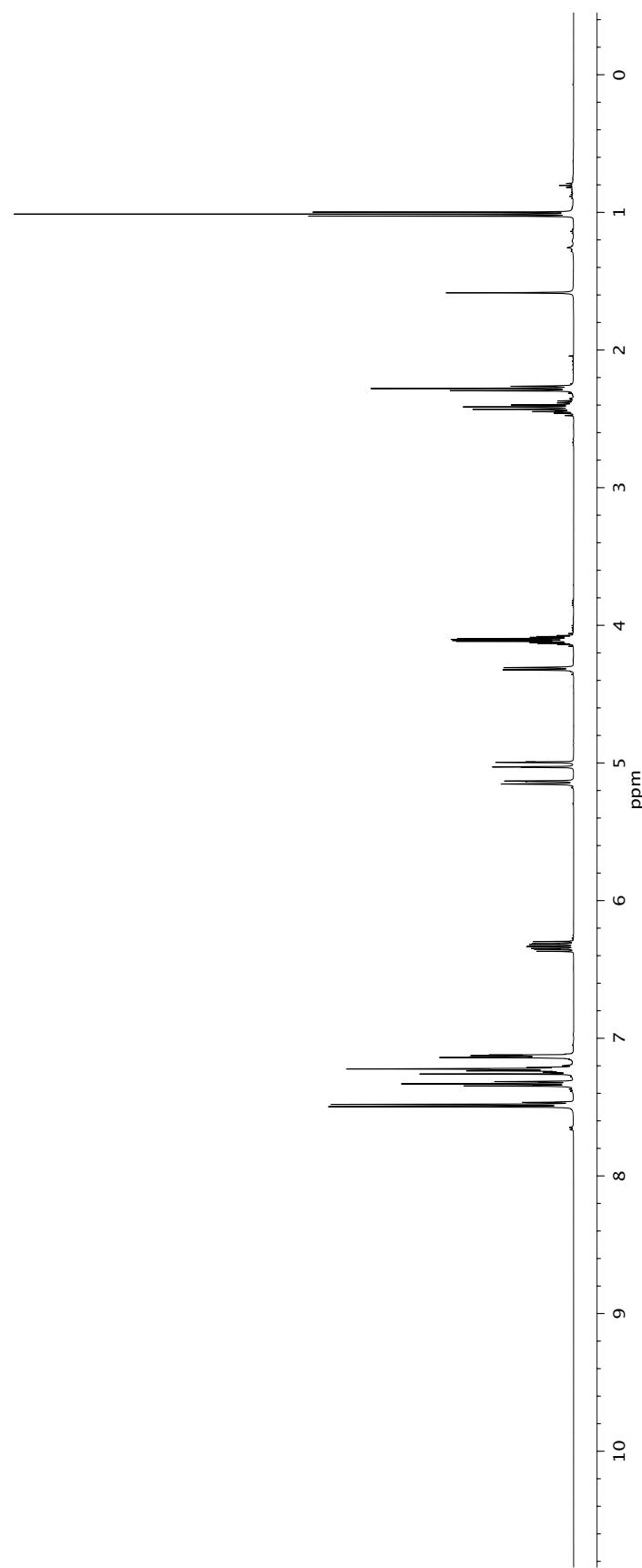
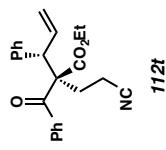


Figure A6.64  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of compound 112t.

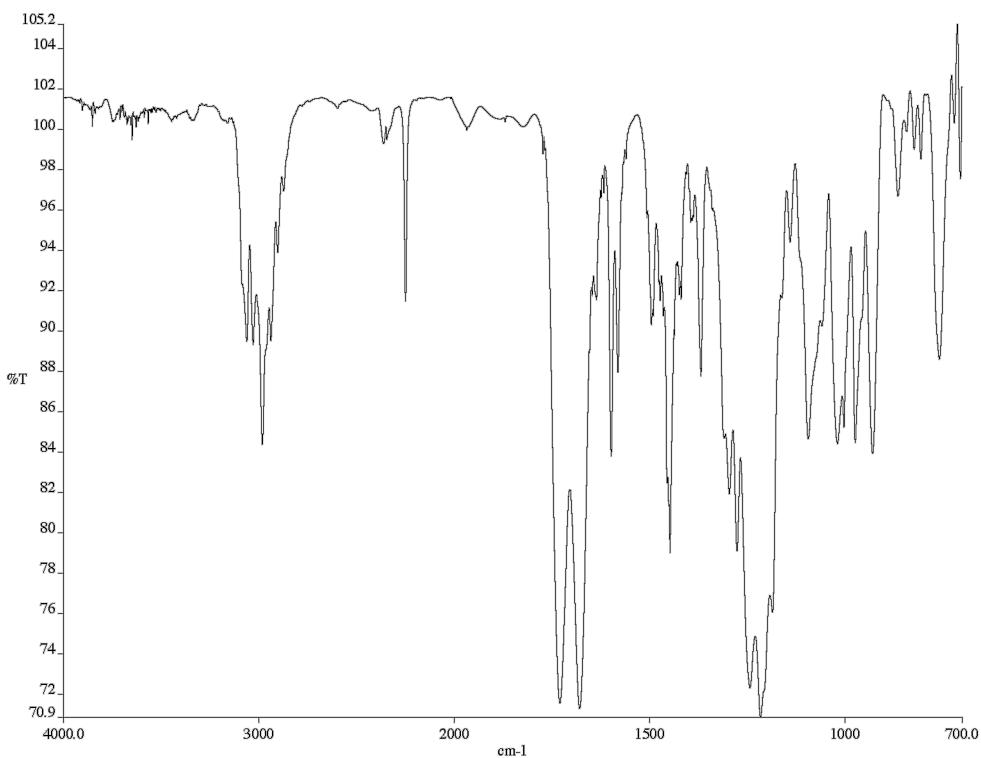


Figure A6.65 Infrared spectrum (thin film/NaCl) of compound **112t**.

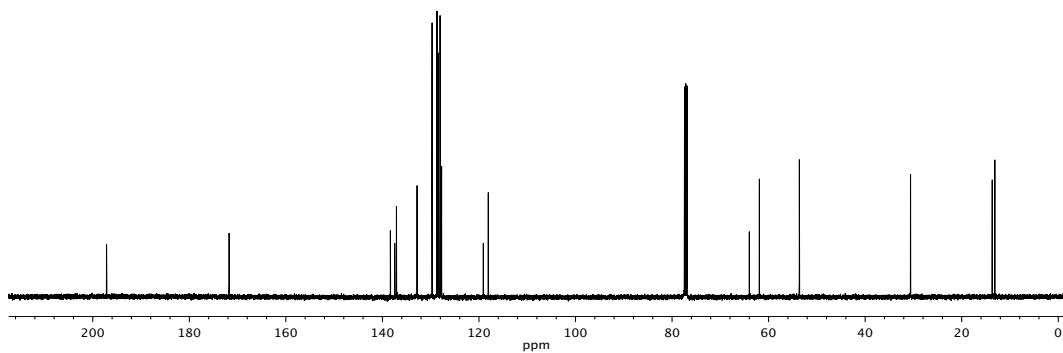


Figure A6.66  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) of compound **112t**.

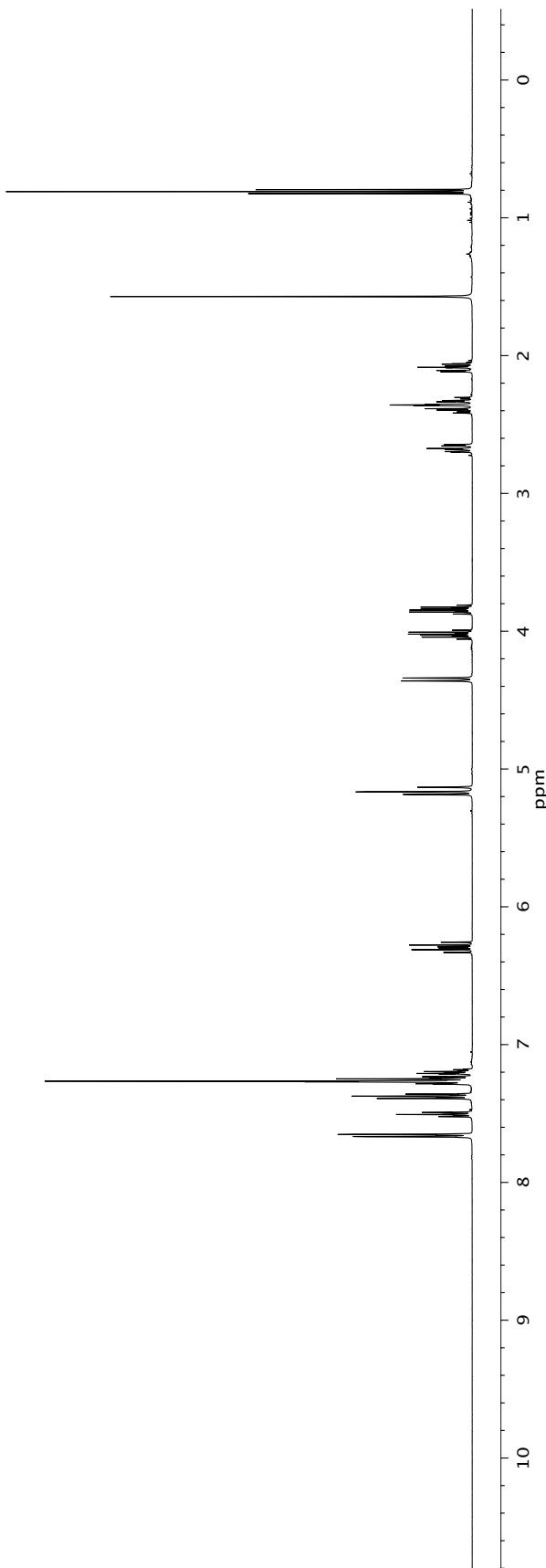
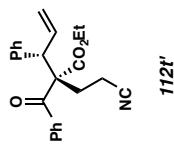


Figure A6.67  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of compound 112t'.

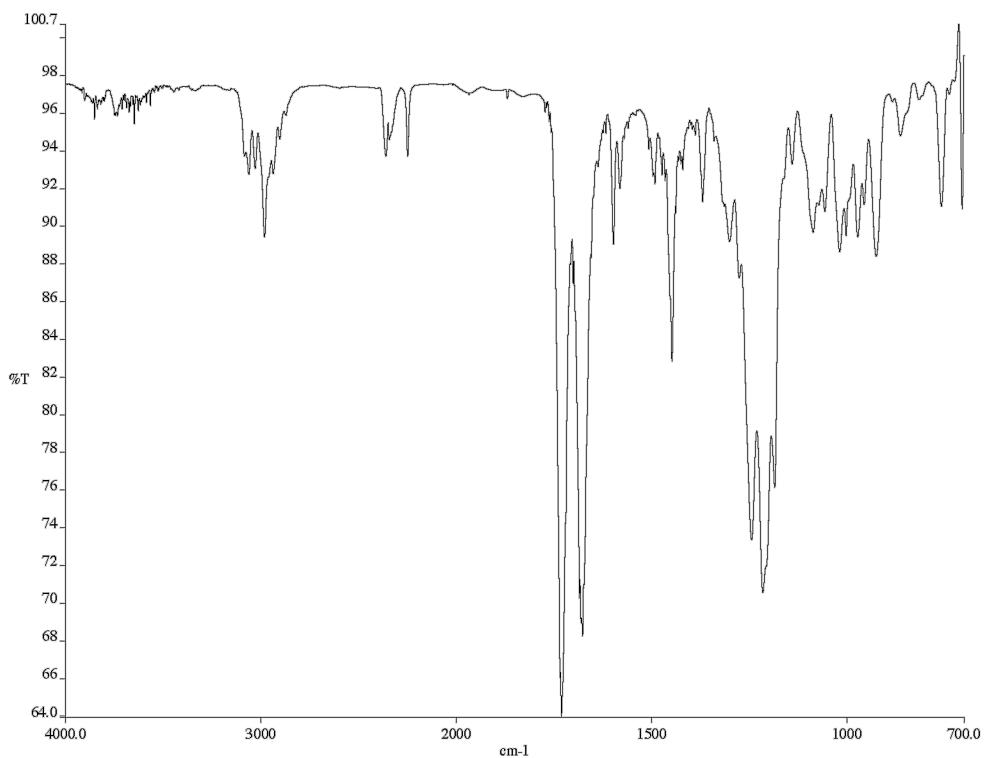


Figure A6.68 Infrared spectrum (thin film/NaCl) of compound **112t'**.

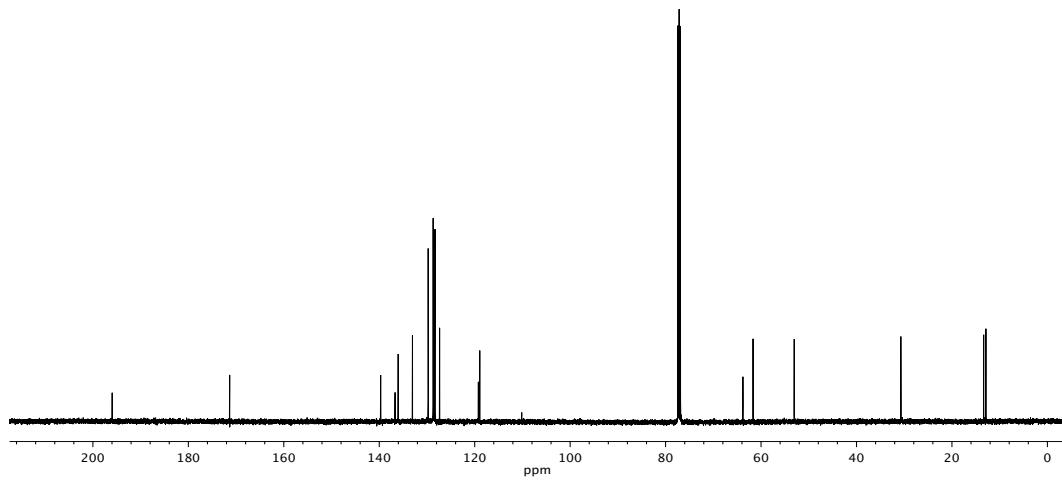


Figure A6.69 <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound **112t'**.

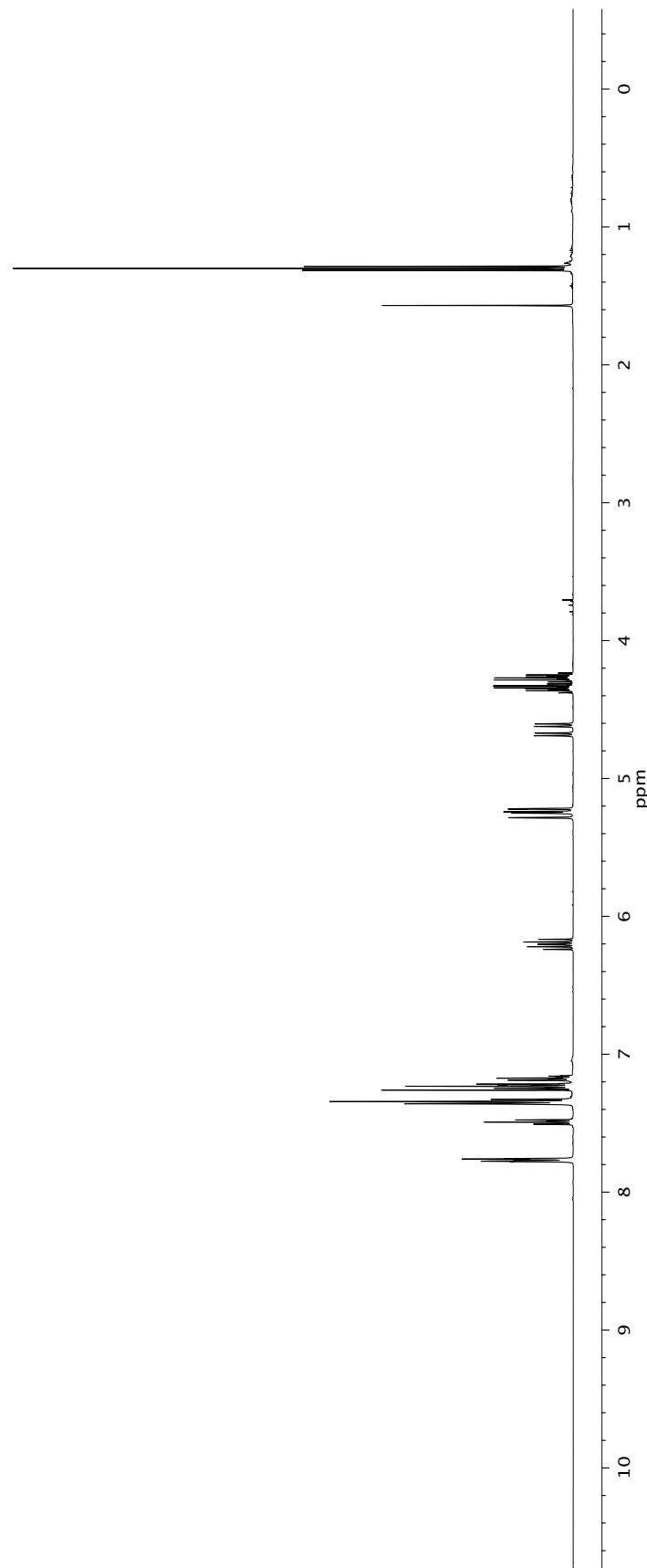
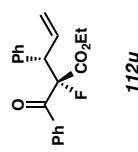


Figure A6.70  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of compound 112u.

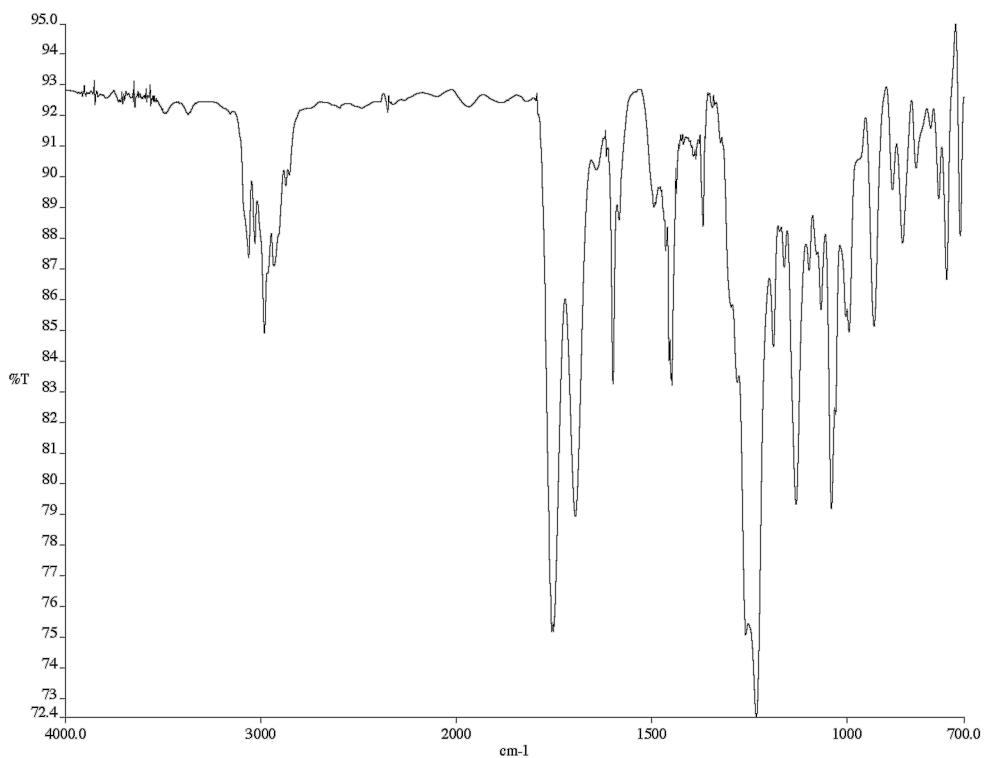


Figure A6.71 Infrared spectrum (thin film/NaCl) of compound **112u**.

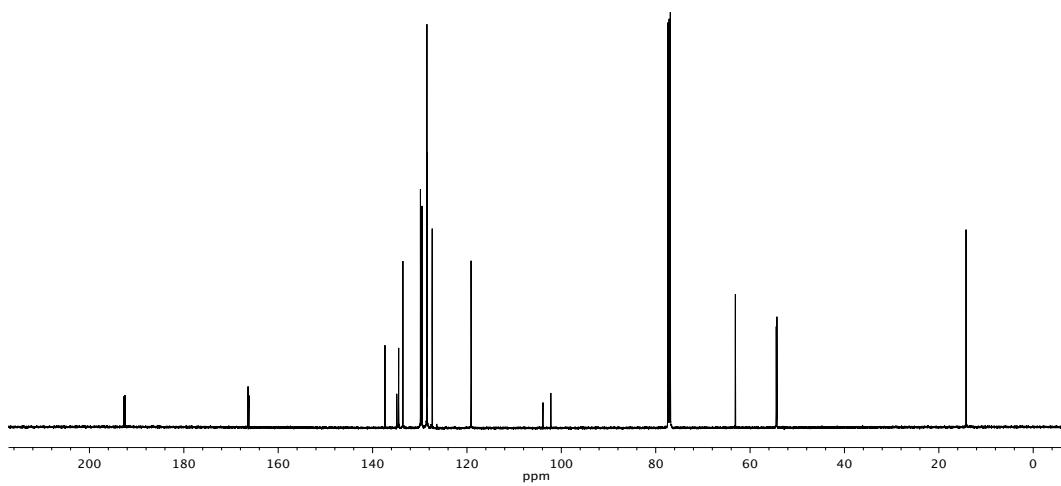


Figure A6.72  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) of compound **112u**.

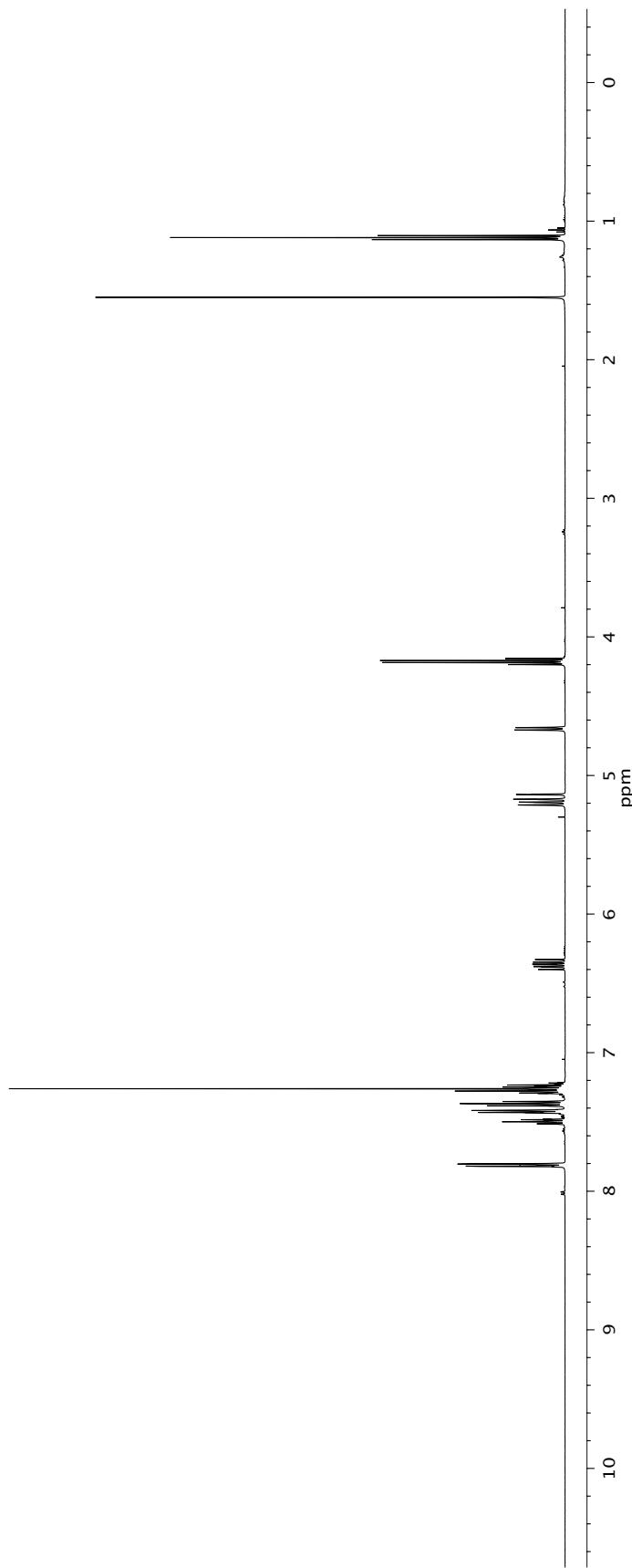
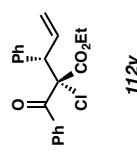


Figure A6.73  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of compound 112v.

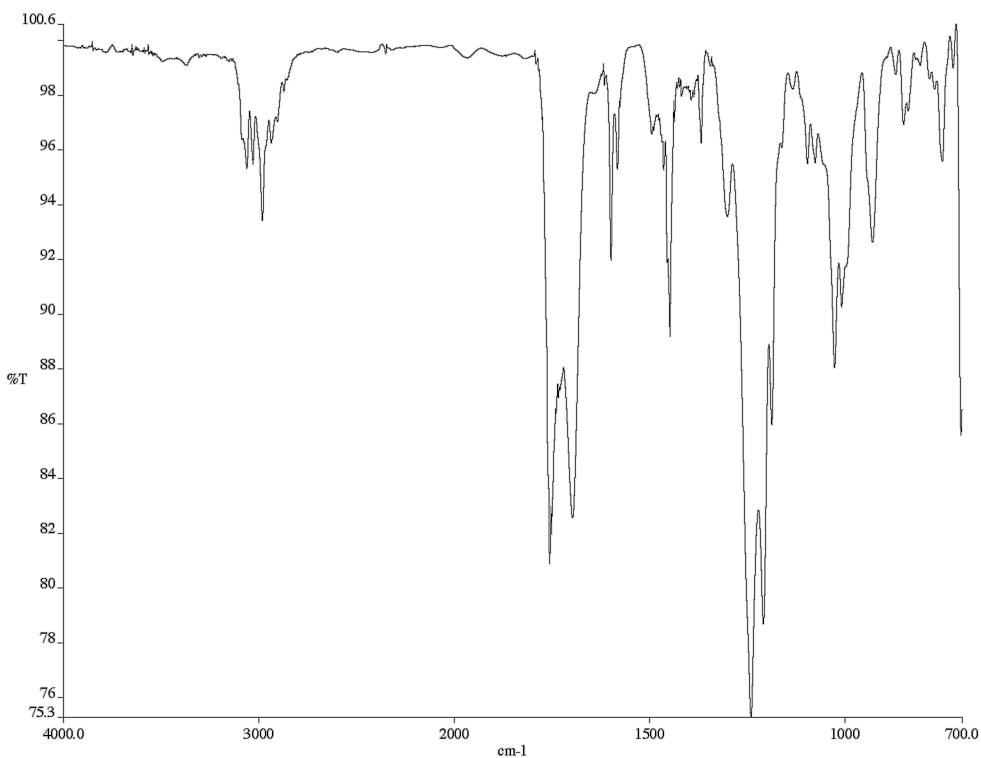


Figure A6.74 Infrared spectrum (thin film/NaCl) of compound **112v**.

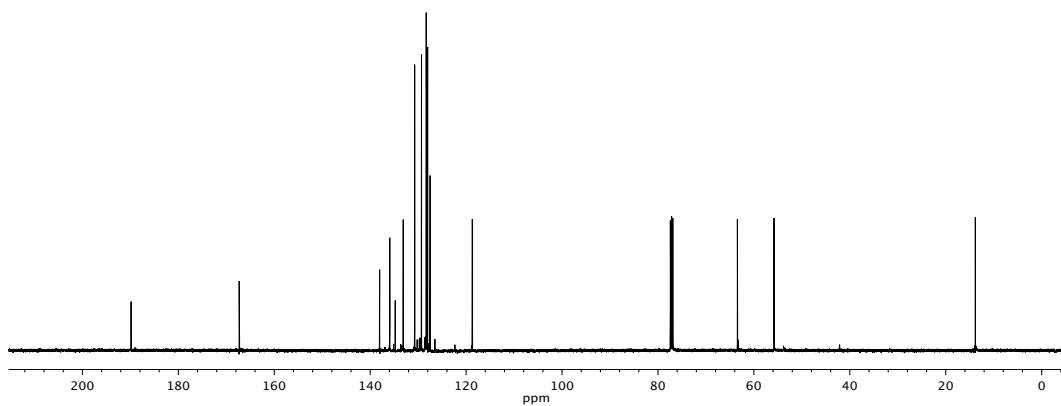


Figure A6.75  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) of compound **112v**.

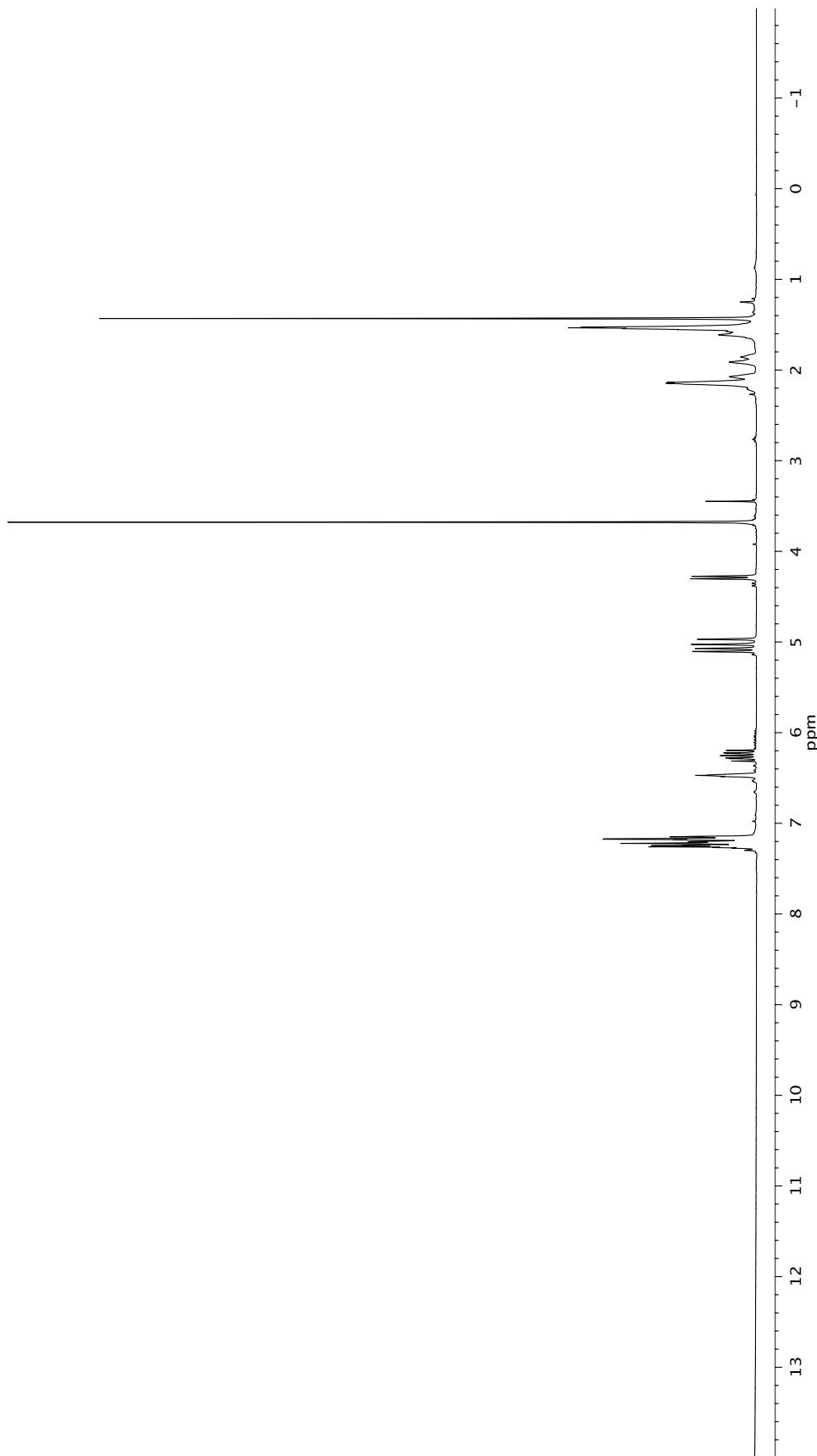
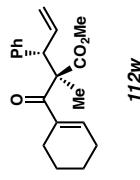


Figure A6.76  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of compound 112w.

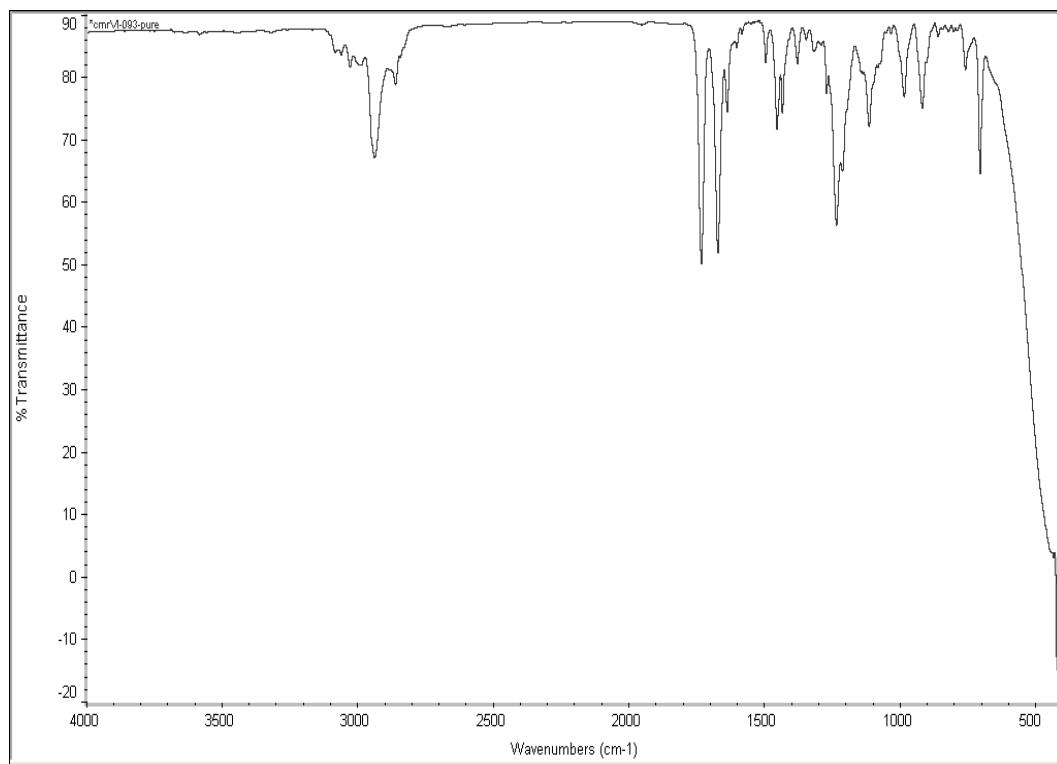


Figure A6.77 Infrared spectrum (thin film/NaCl) of compound **112w**.

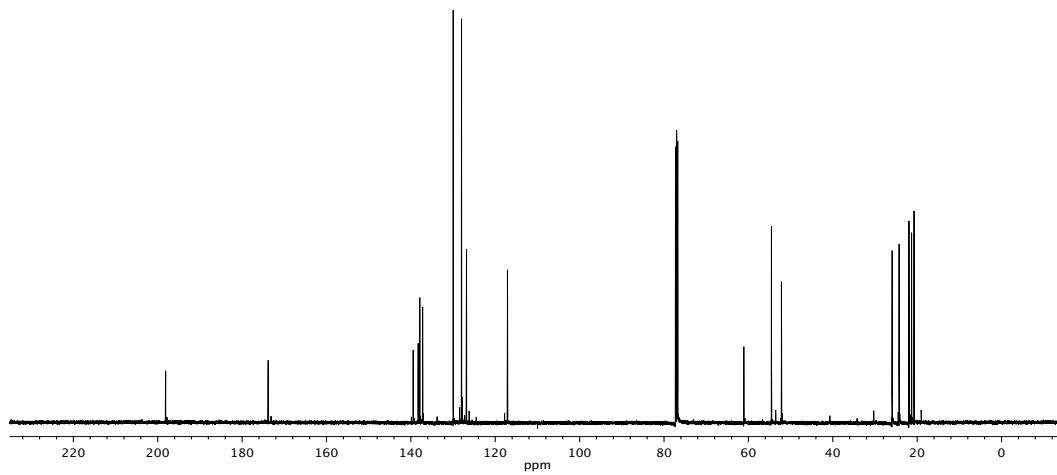


Figure A6.78 <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound **112w**.

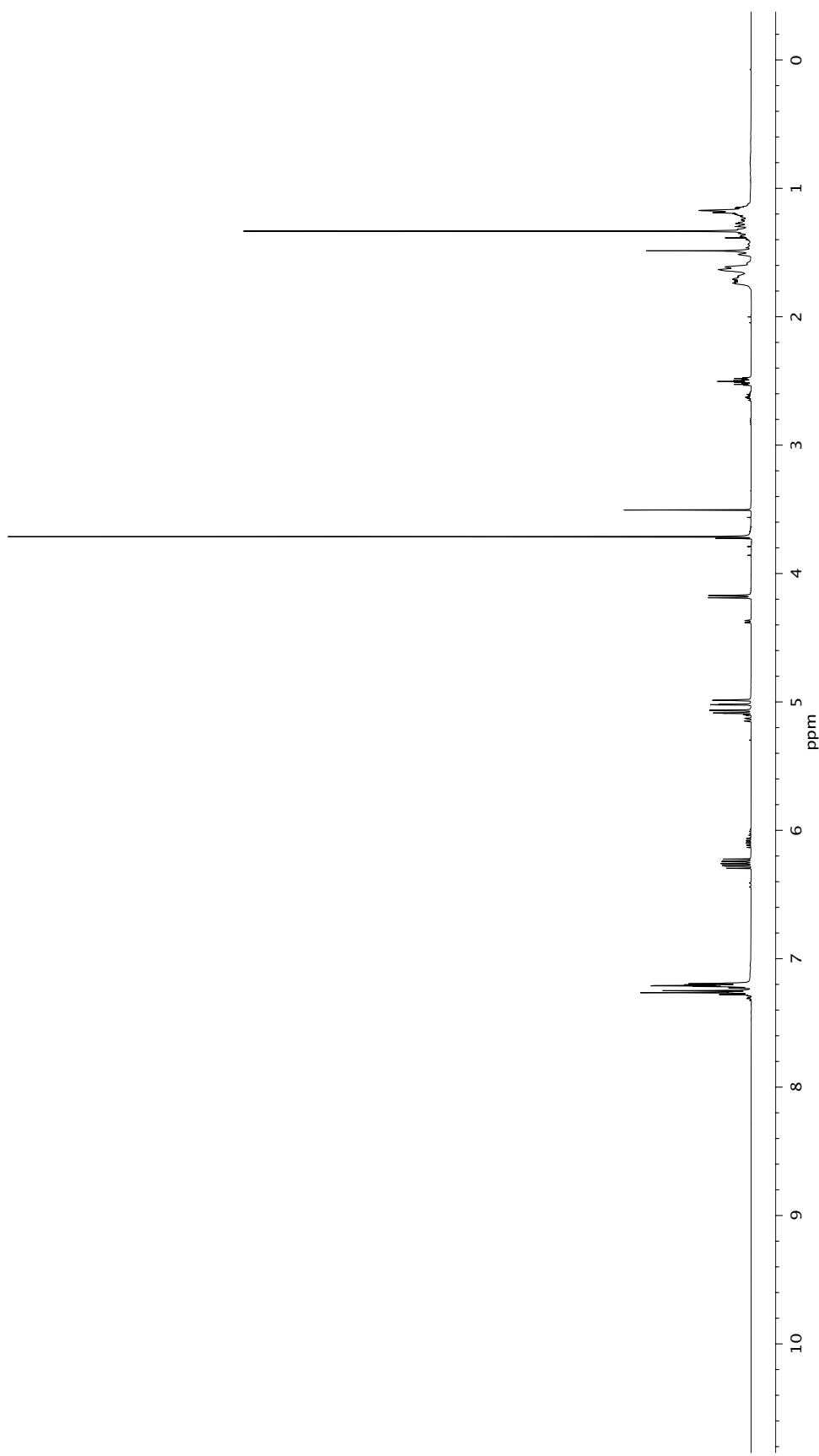
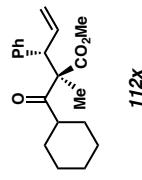


Figure A6.79  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of compound 112x.

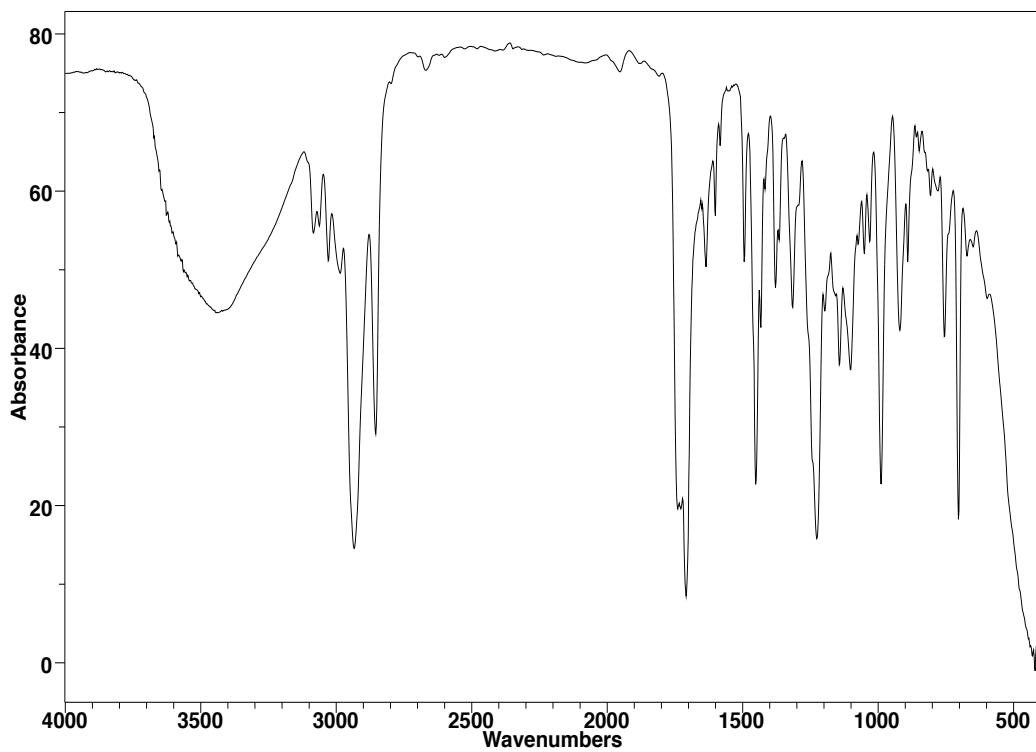


Figure A6.80 Infrared spectrum (thin film/NaCl) of compound **112x**.

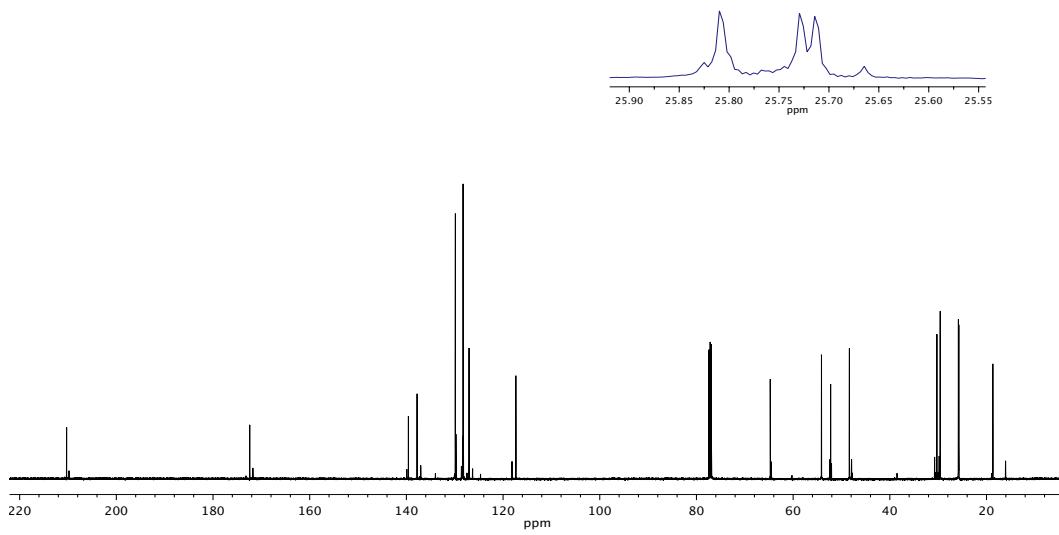


Figure A6.81 <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound **112x**.

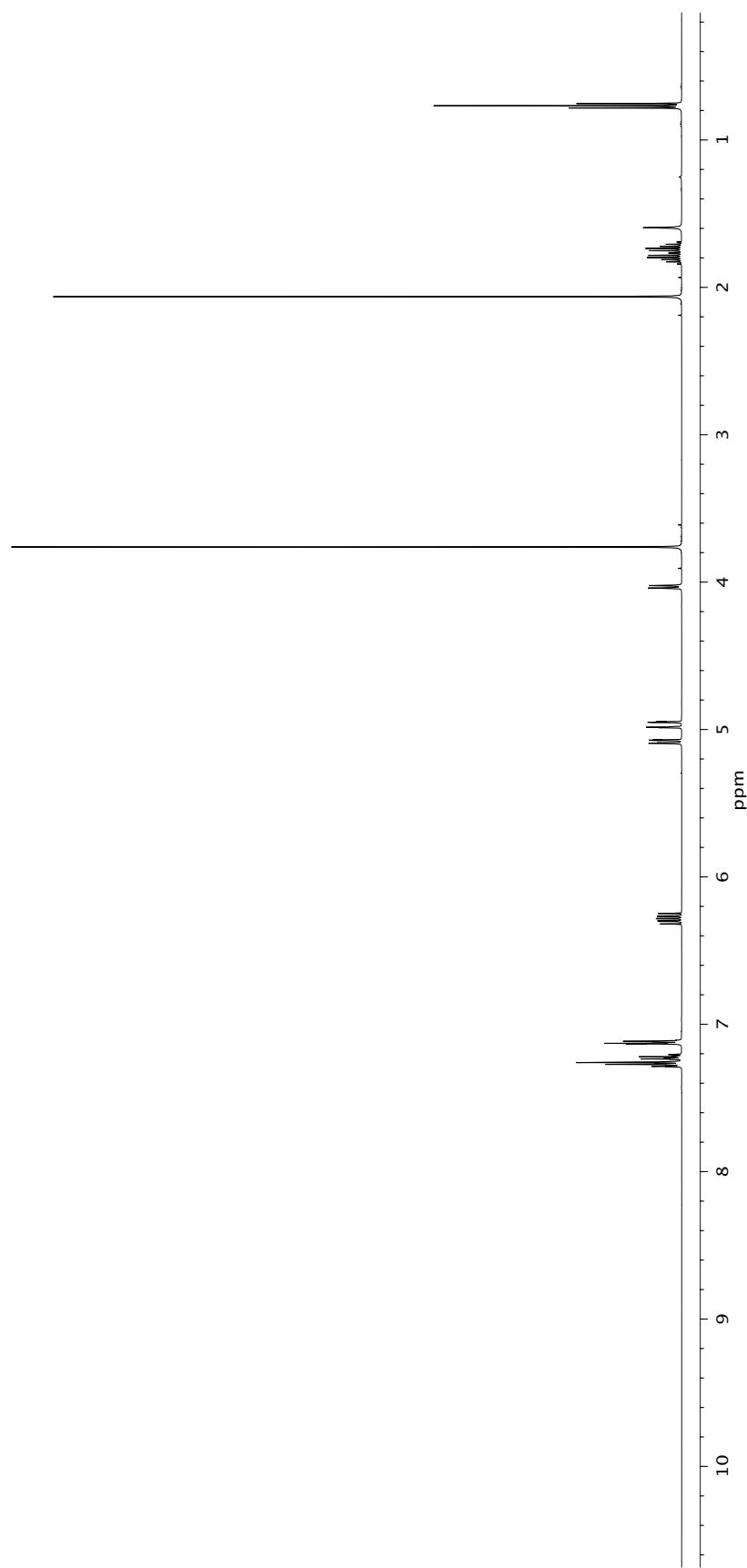
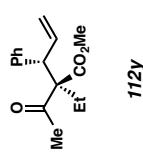


Figure A6.82  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of compound 112y.

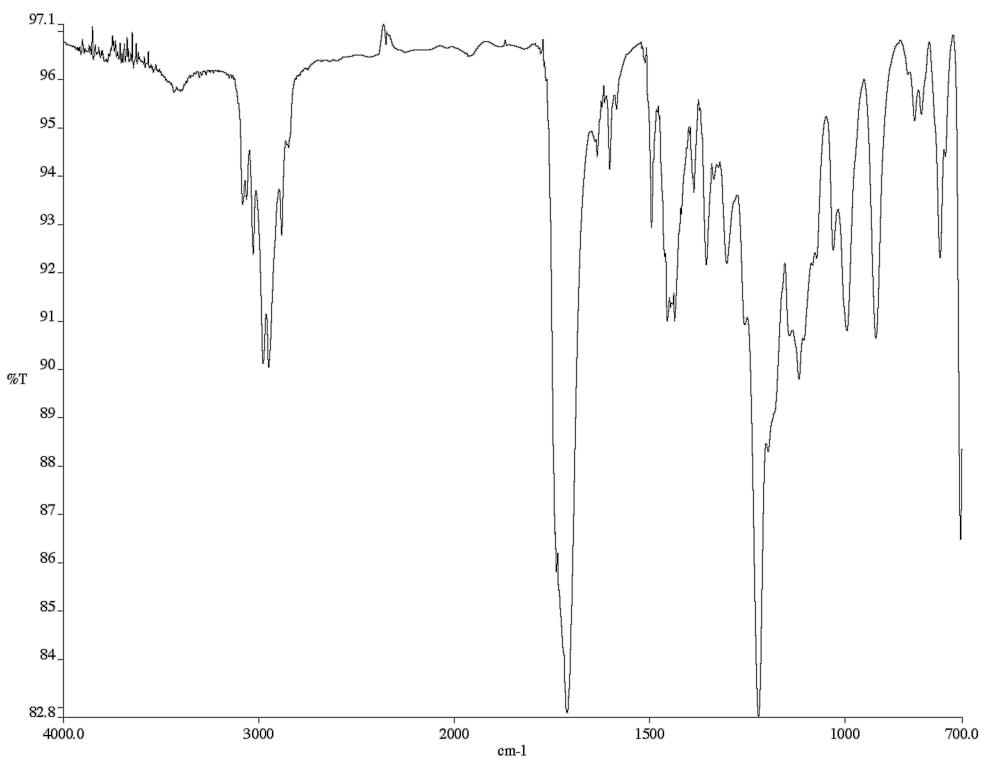


Figure A6.83 Infrared spectrum (thin film/NaCl) of compound **112y**.

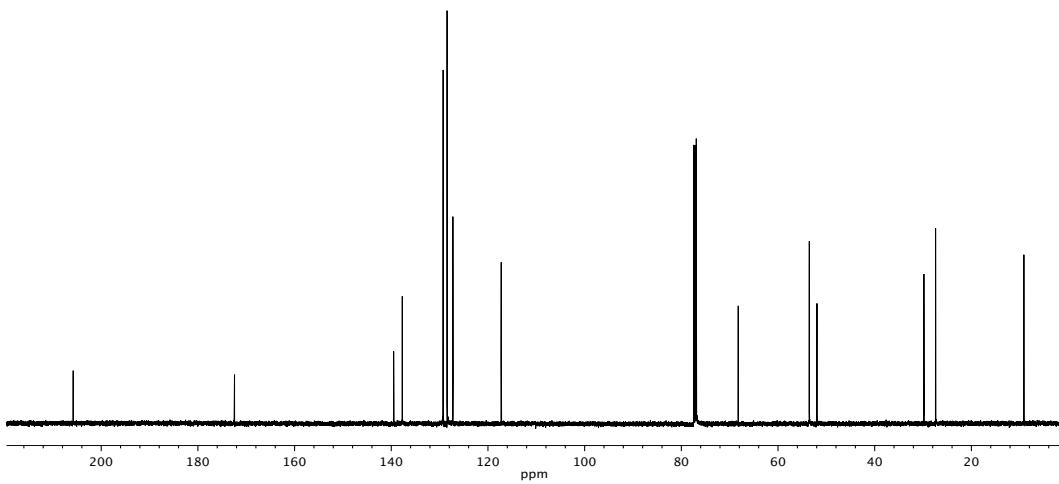


Figure A6.84  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) of compound **112y**.

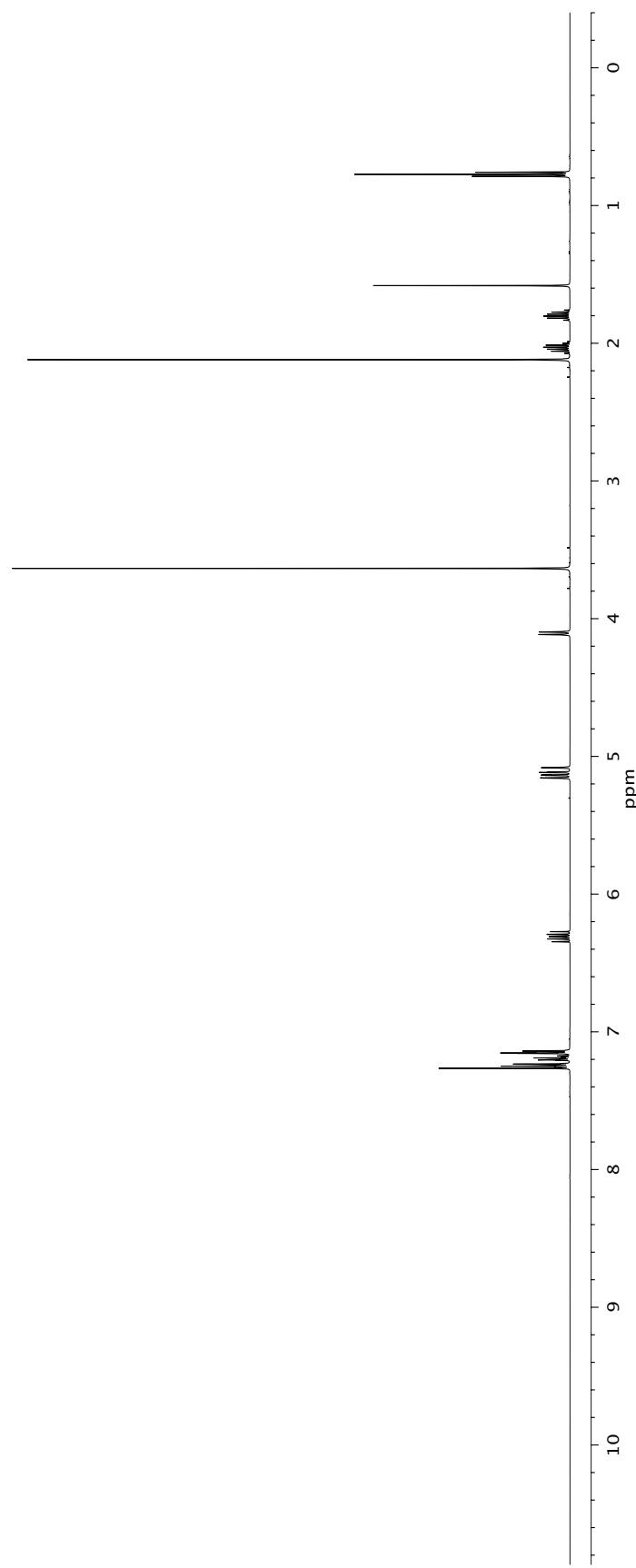
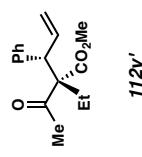


Figure A6.85  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of compound 112y'.

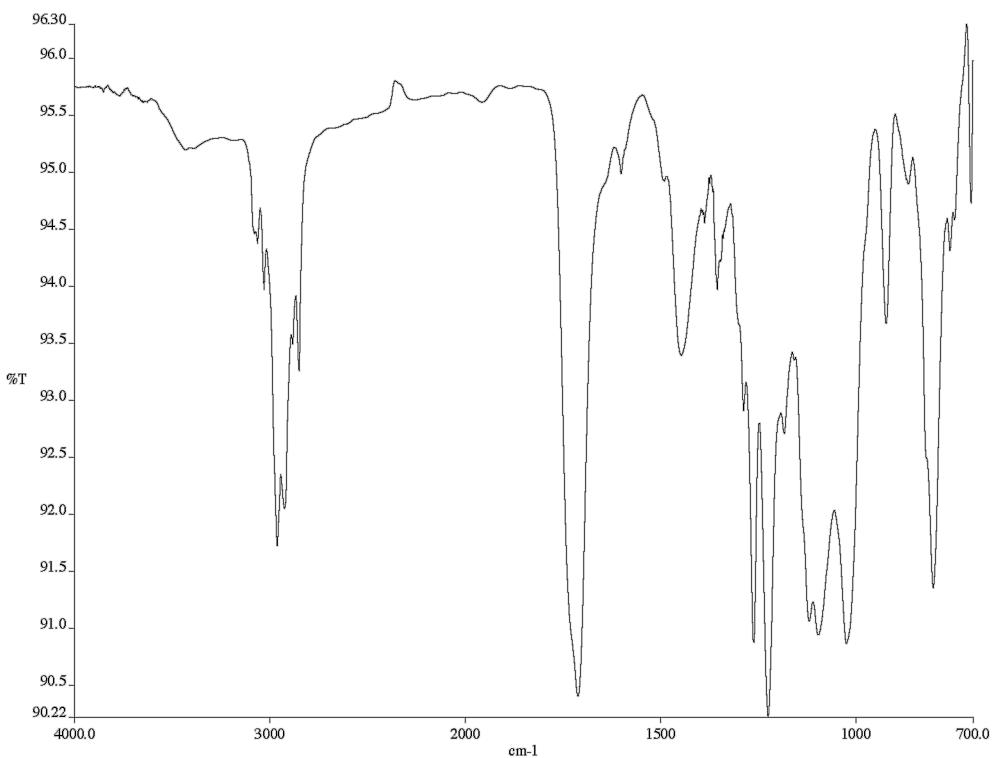


Figure A6.86 Infrared spectrum (thin film/NaCl) of compound **112y'**.

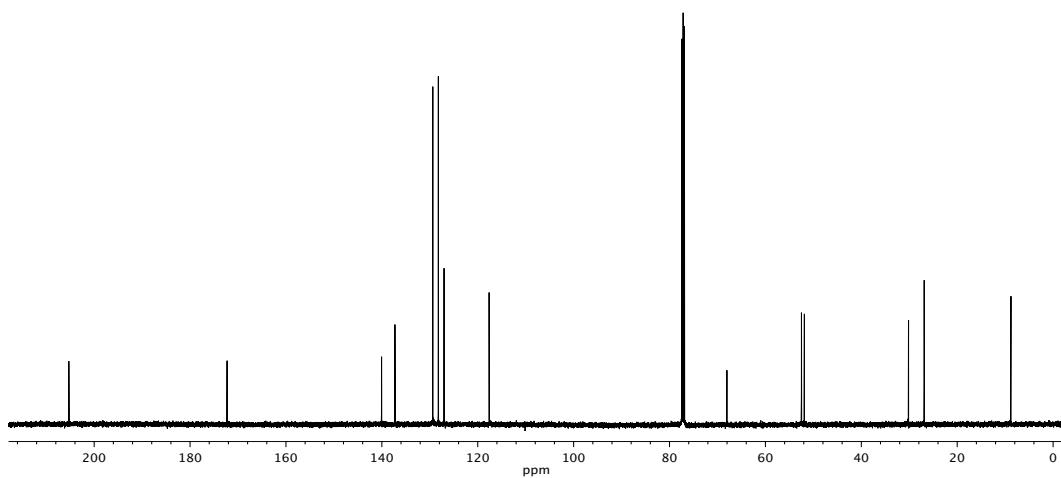


Figure A6.87 <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound **112y'**.

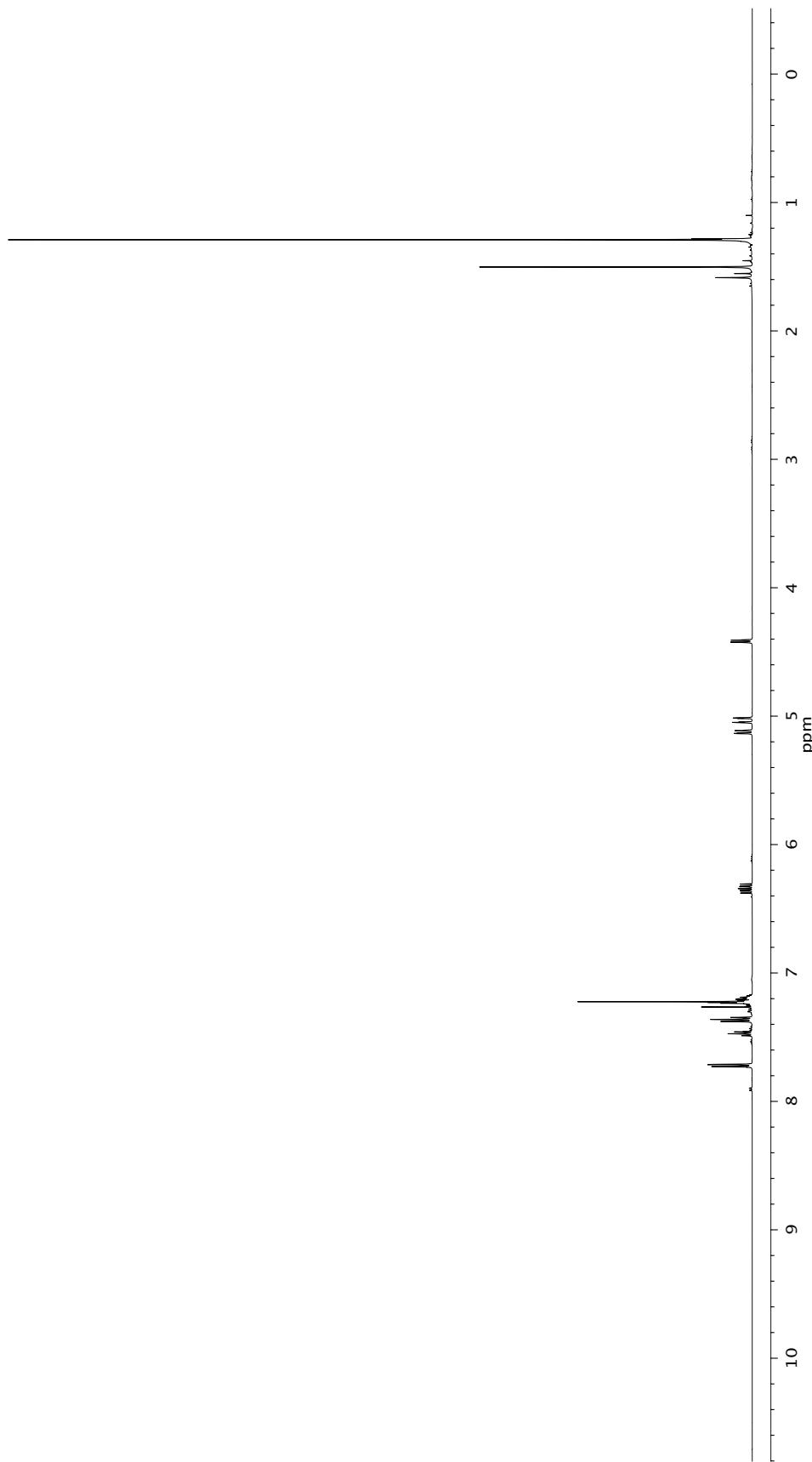
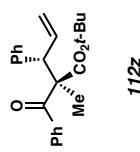


Figure A6.88  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of compound 112z.

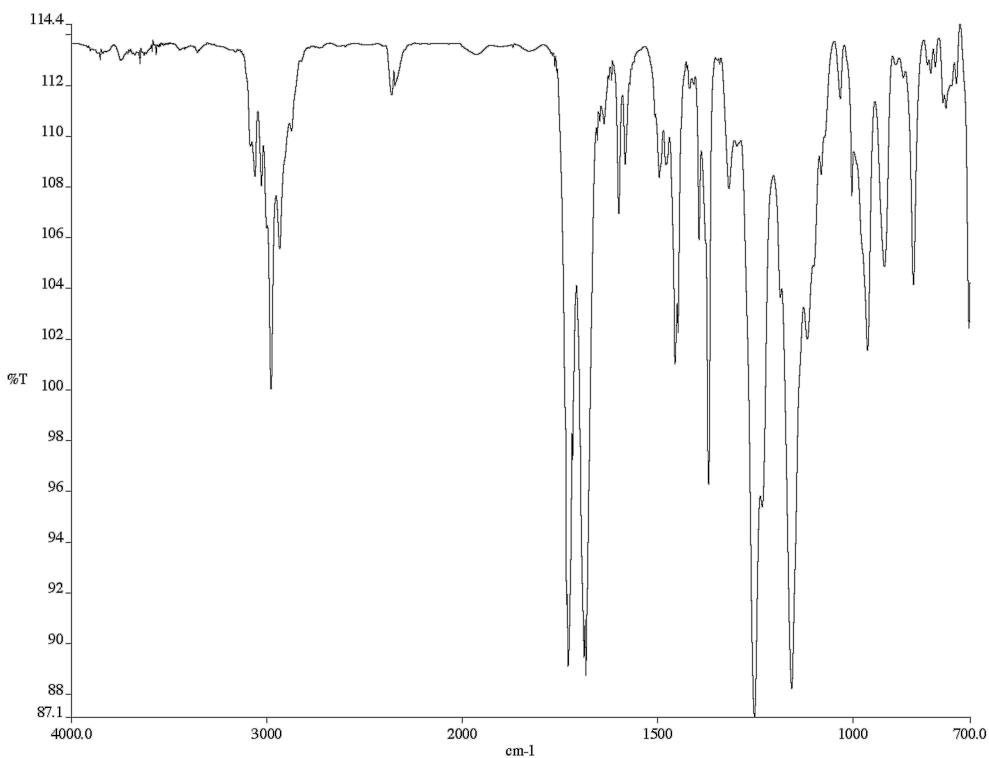


Figure A6.89 Infrared spectrum (thin film/NaCl) of compound **112z**.

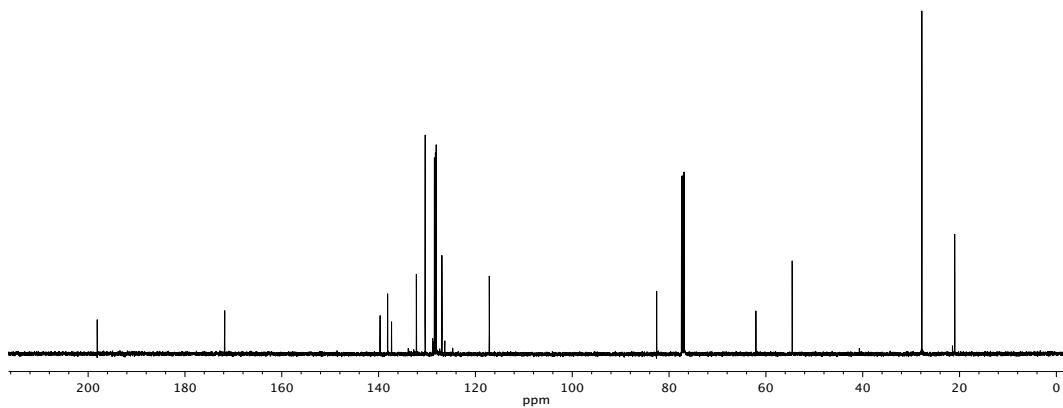


Figure A6.90  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) of compound **112z**.

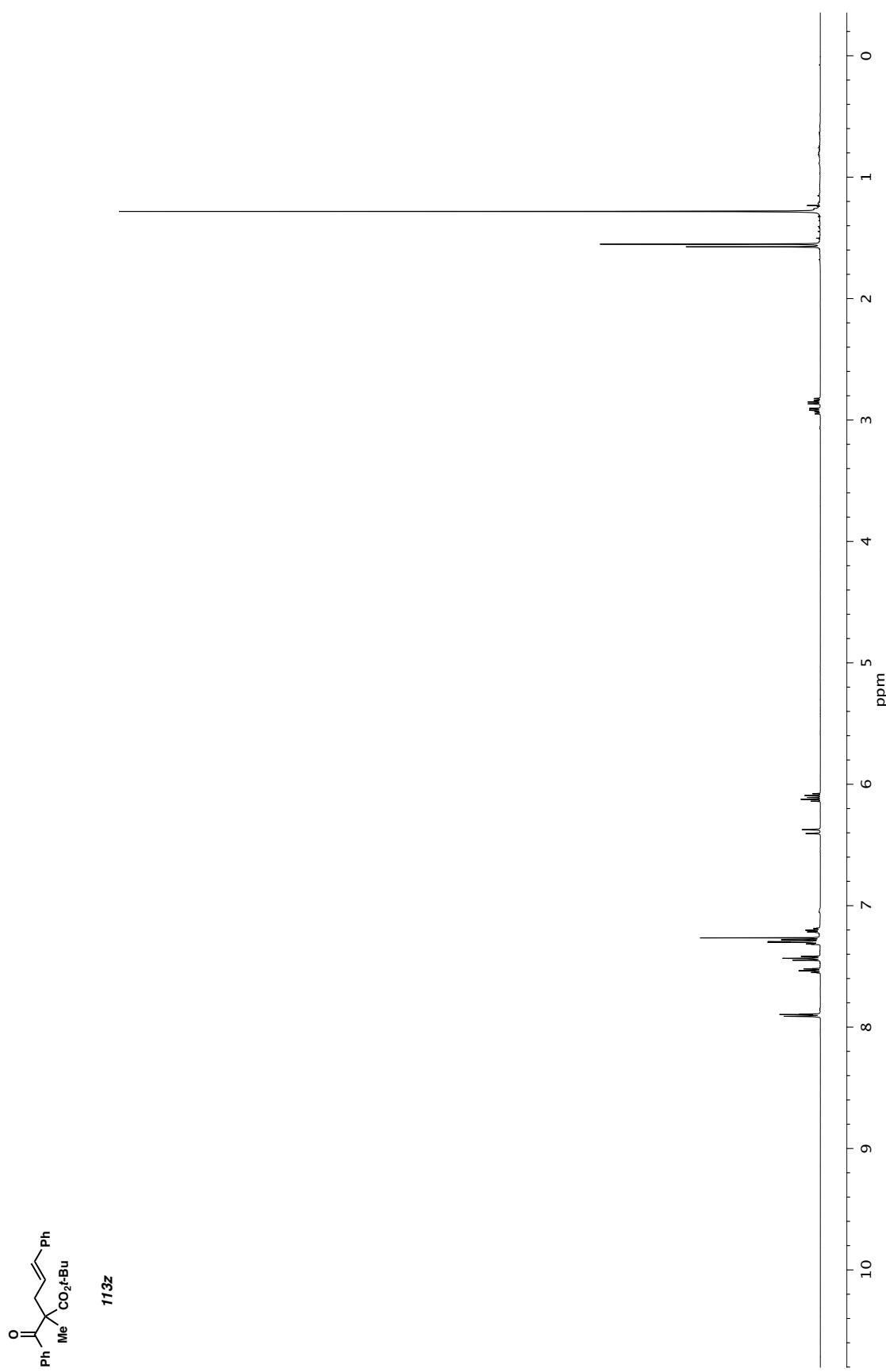


Figure A6.91  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of compound 113z.

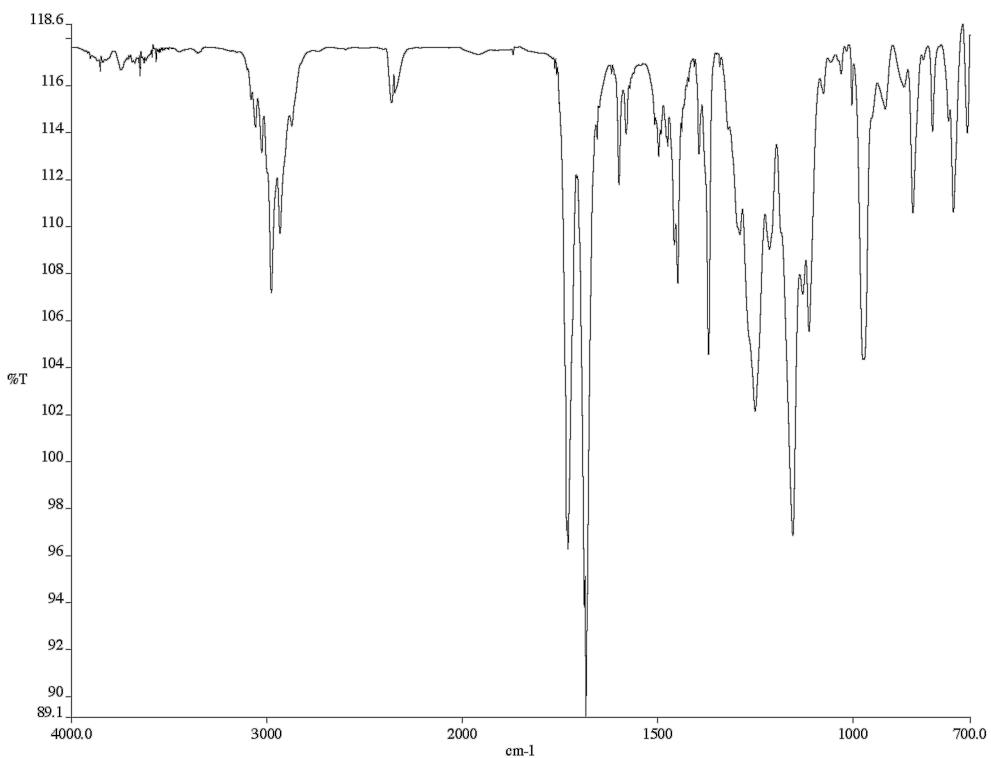


Figure A6.92 Infrared spectrum (thin film/NaCl) of compound **113z**.

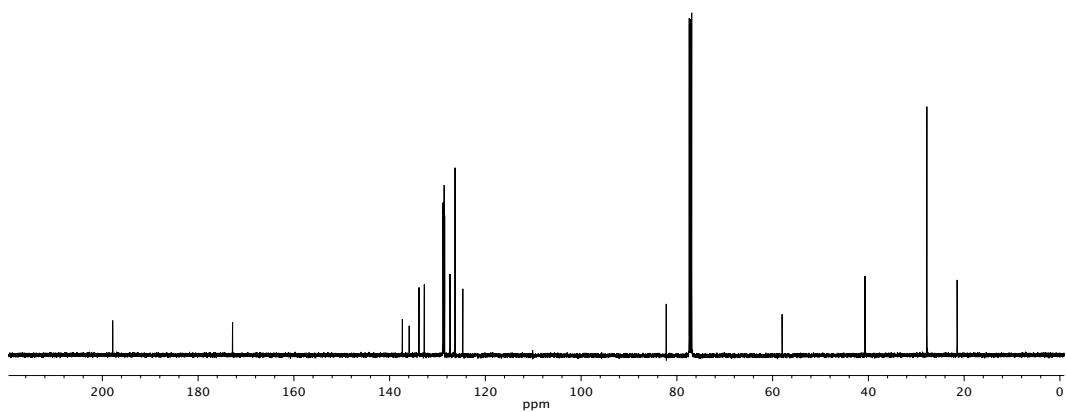


Figure A6.93  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) of compound **113z**.

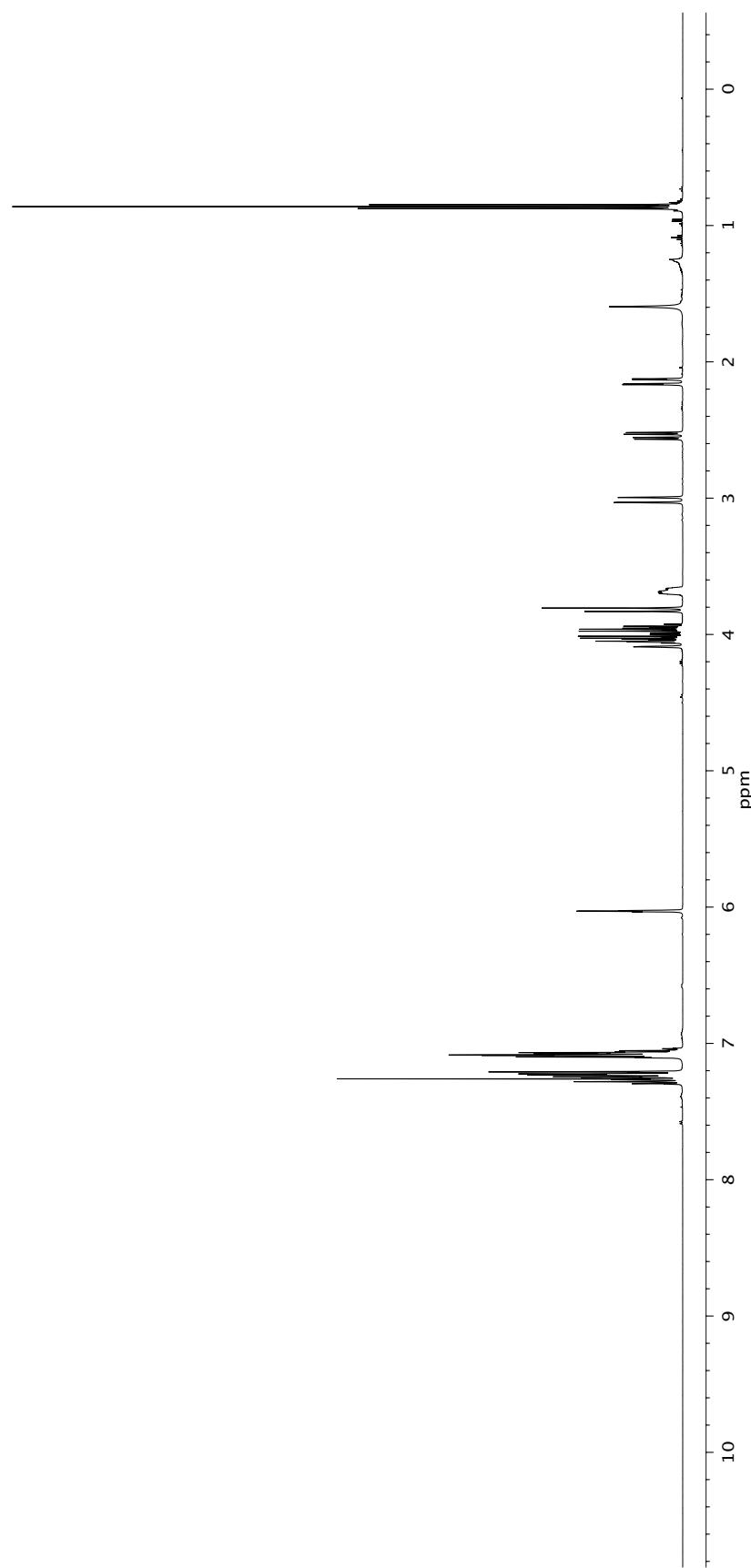
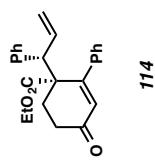


Figure A6.94  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of compound 114.

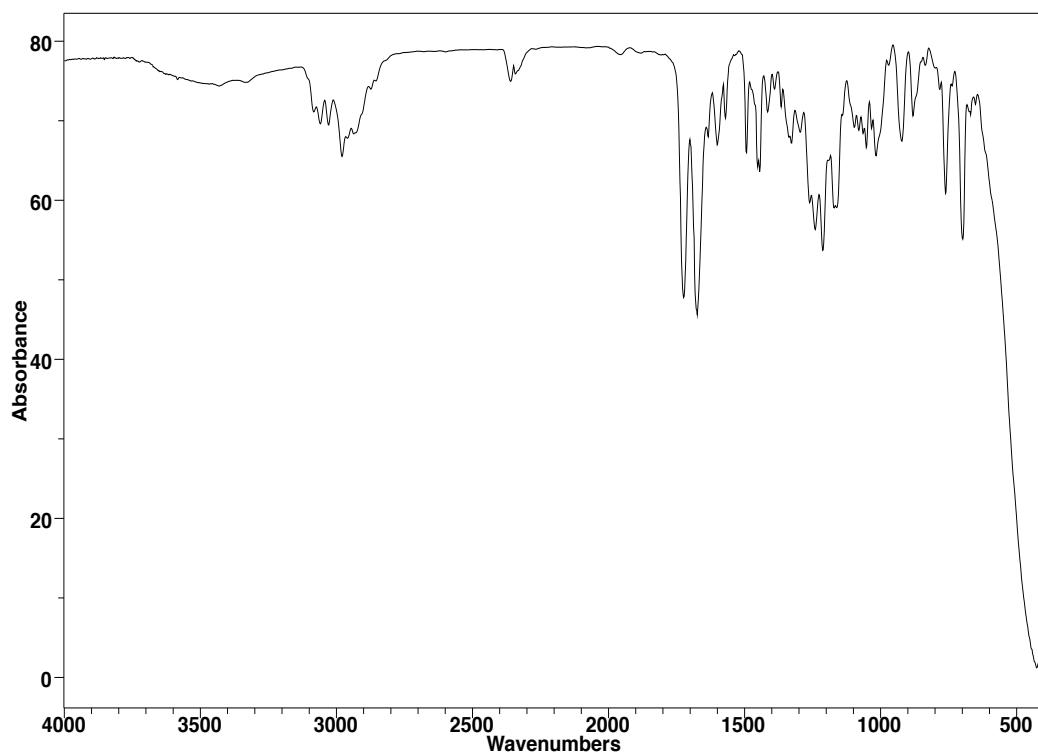


Figure A6.95 Infrared spectrum (thin film/NaCl) of compound **114**.

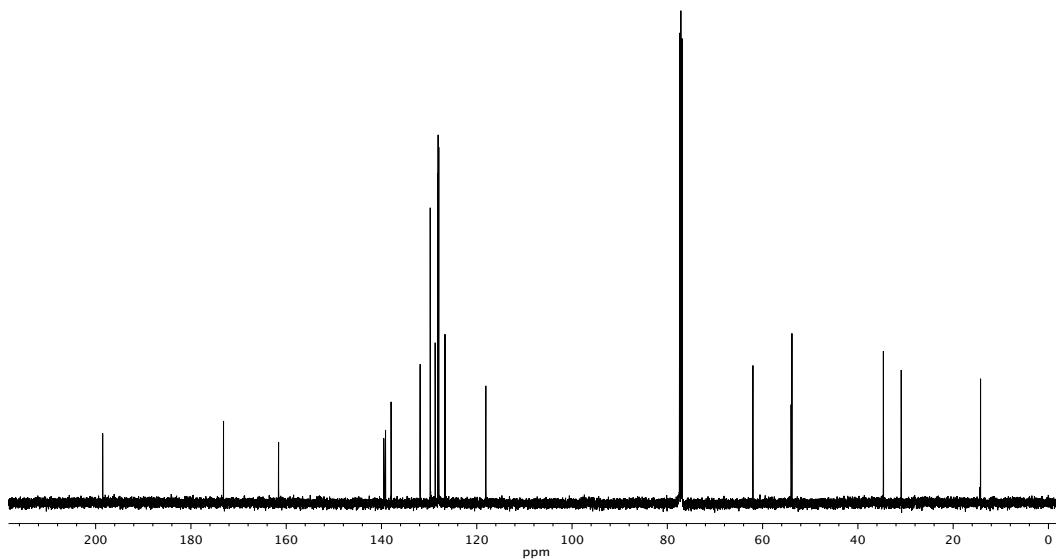


Figure A6.96  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) of compound **114**.

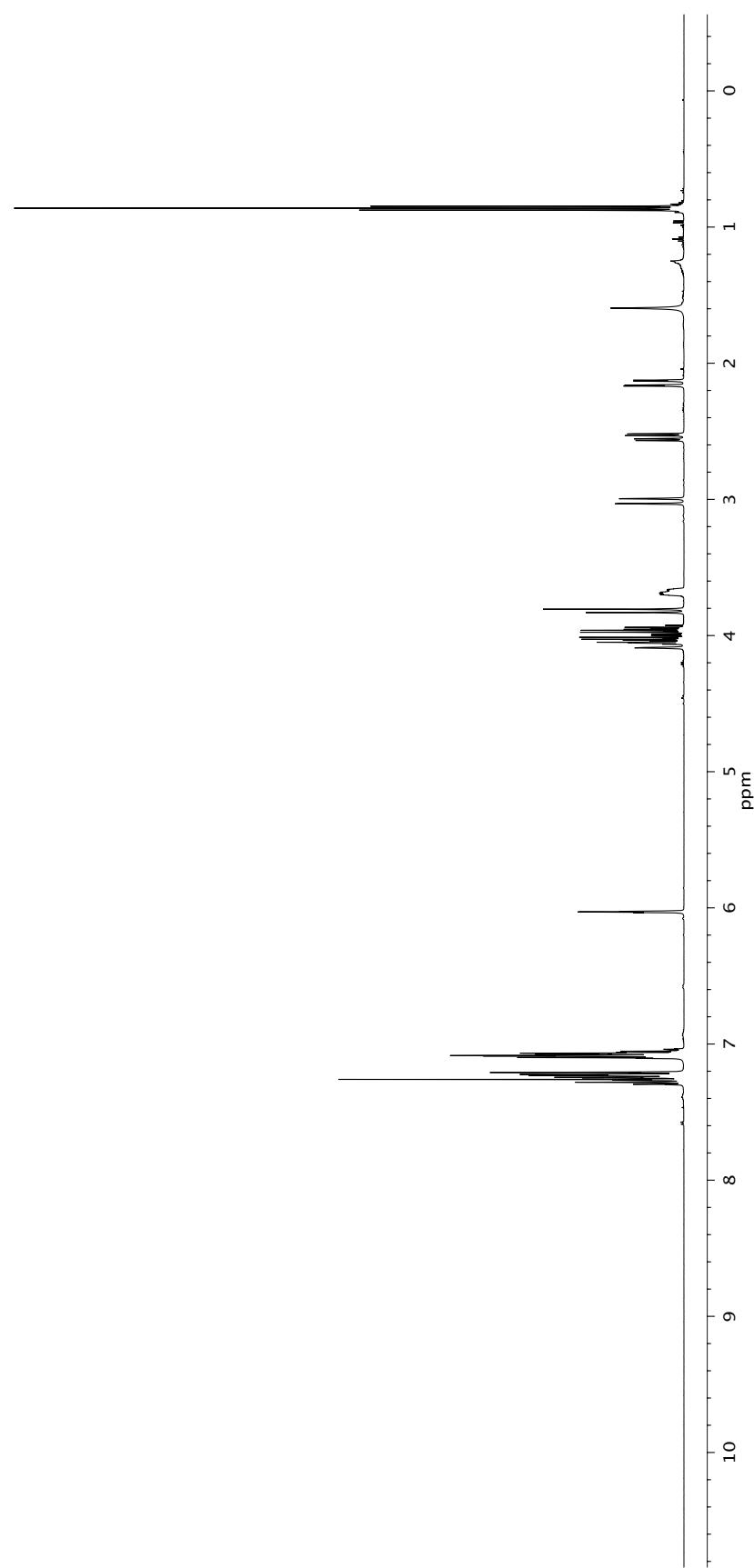
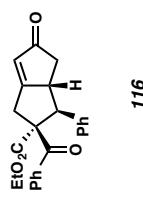


Figure A6.97 <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) of compound 116.

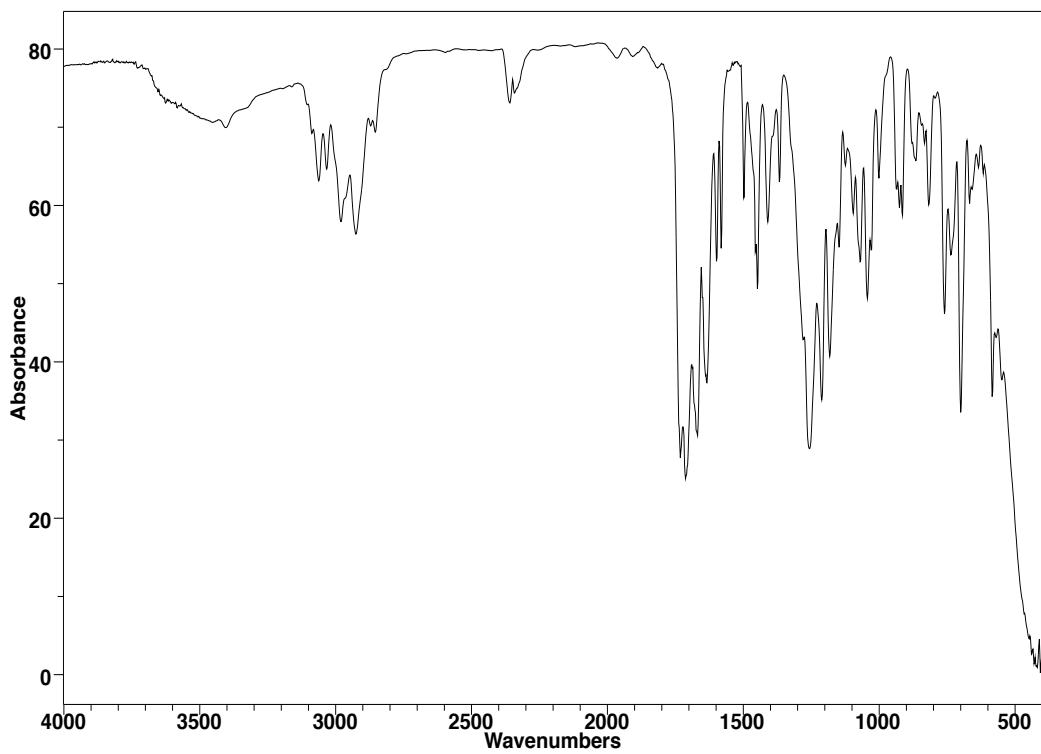


Figure A6.98 Infrared spectrum (thin film/NaCl) of compound **116**.

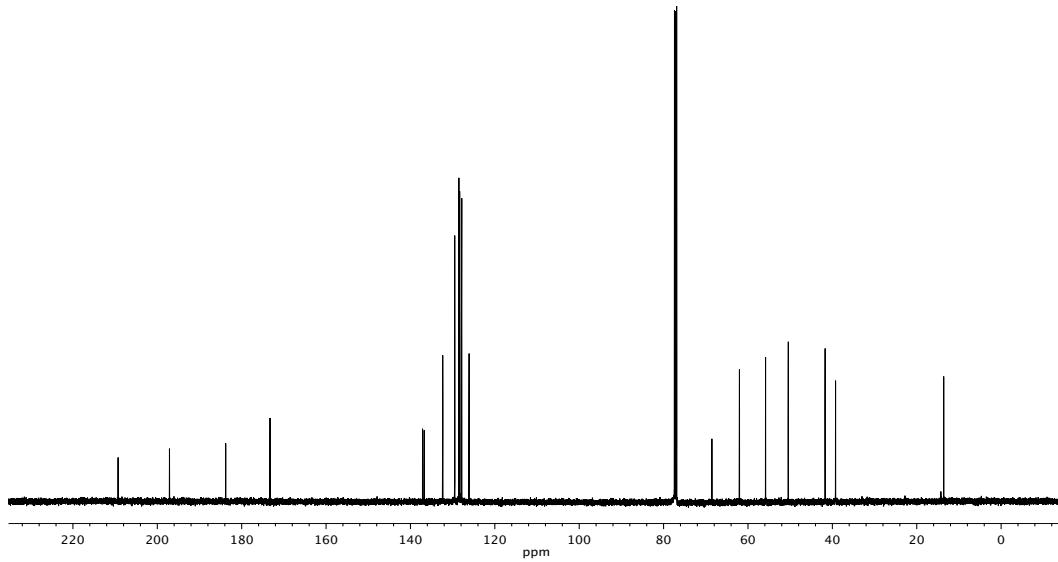


Figure A6.99 <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound **116**.

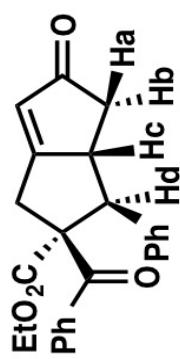
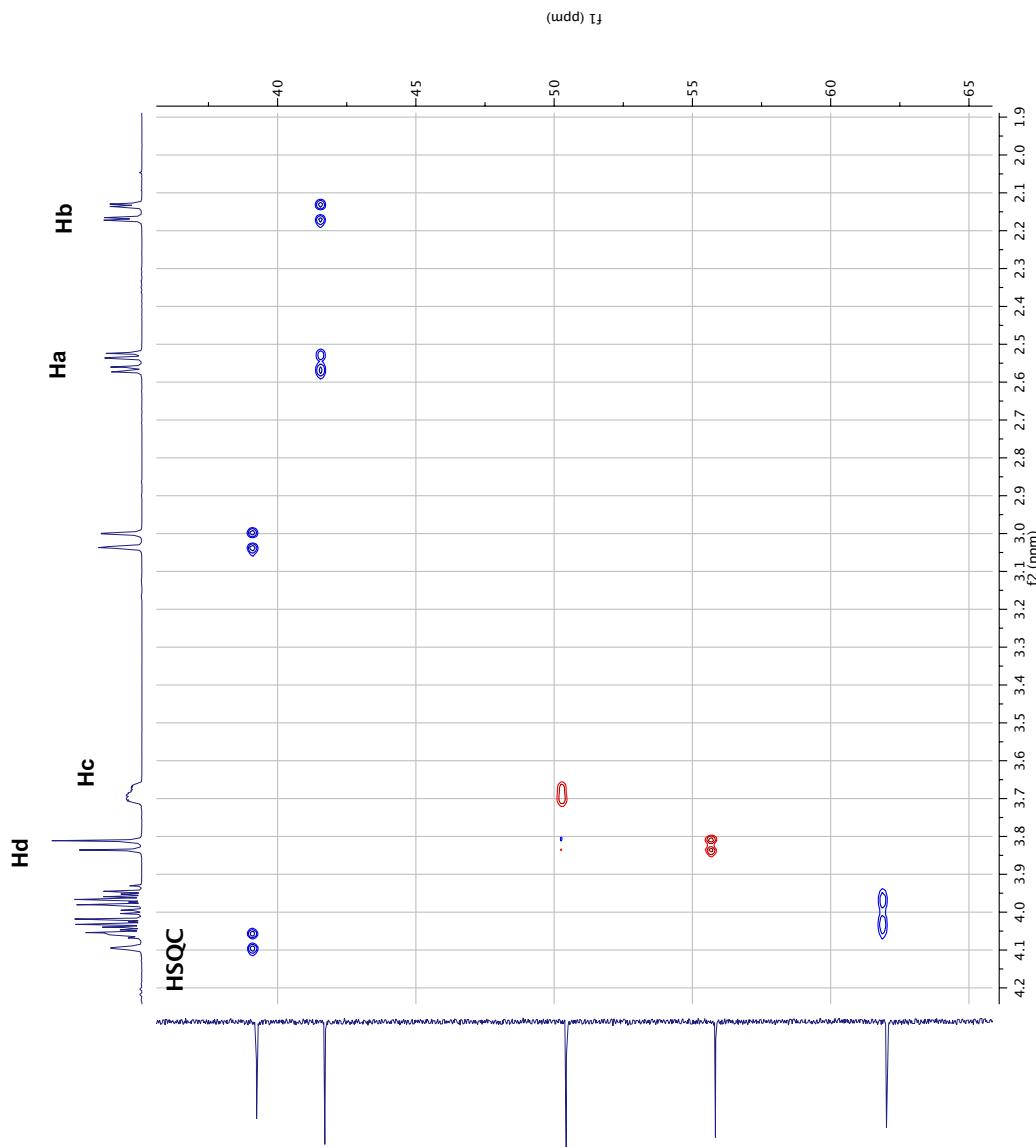
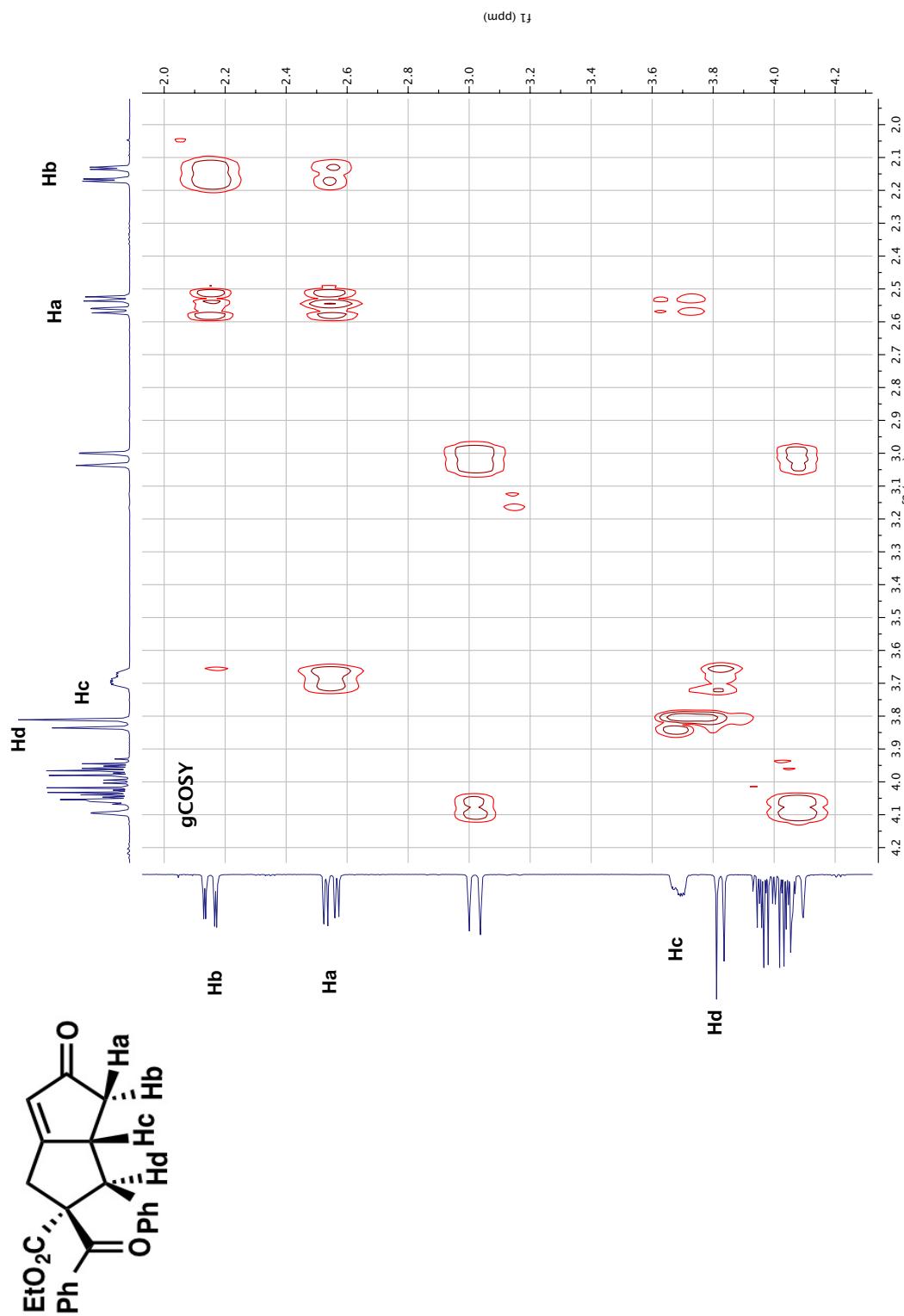


Figure A6.100 HSQC NMR (500 MHz,  $\text{CDCl}_3$ ) of compound 116.

Figure A6.101 gCOSY NMR (500 MHz,  $\text{CDCl}_3$ ) of compound 116.

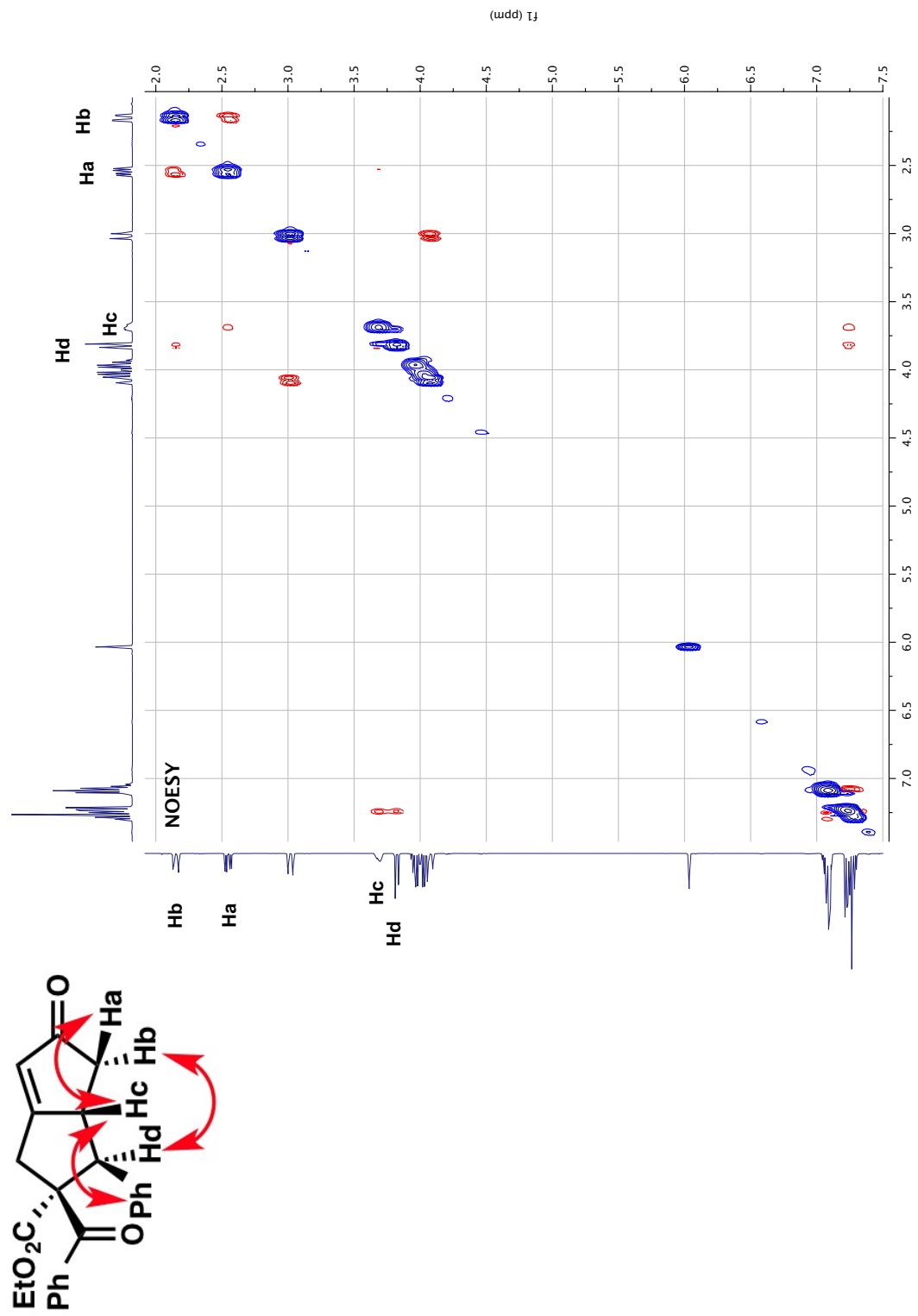


Figure A6.102 NOESY NMR (500 MHz,  $\text{CDCl}_3$ ) of compound 116.

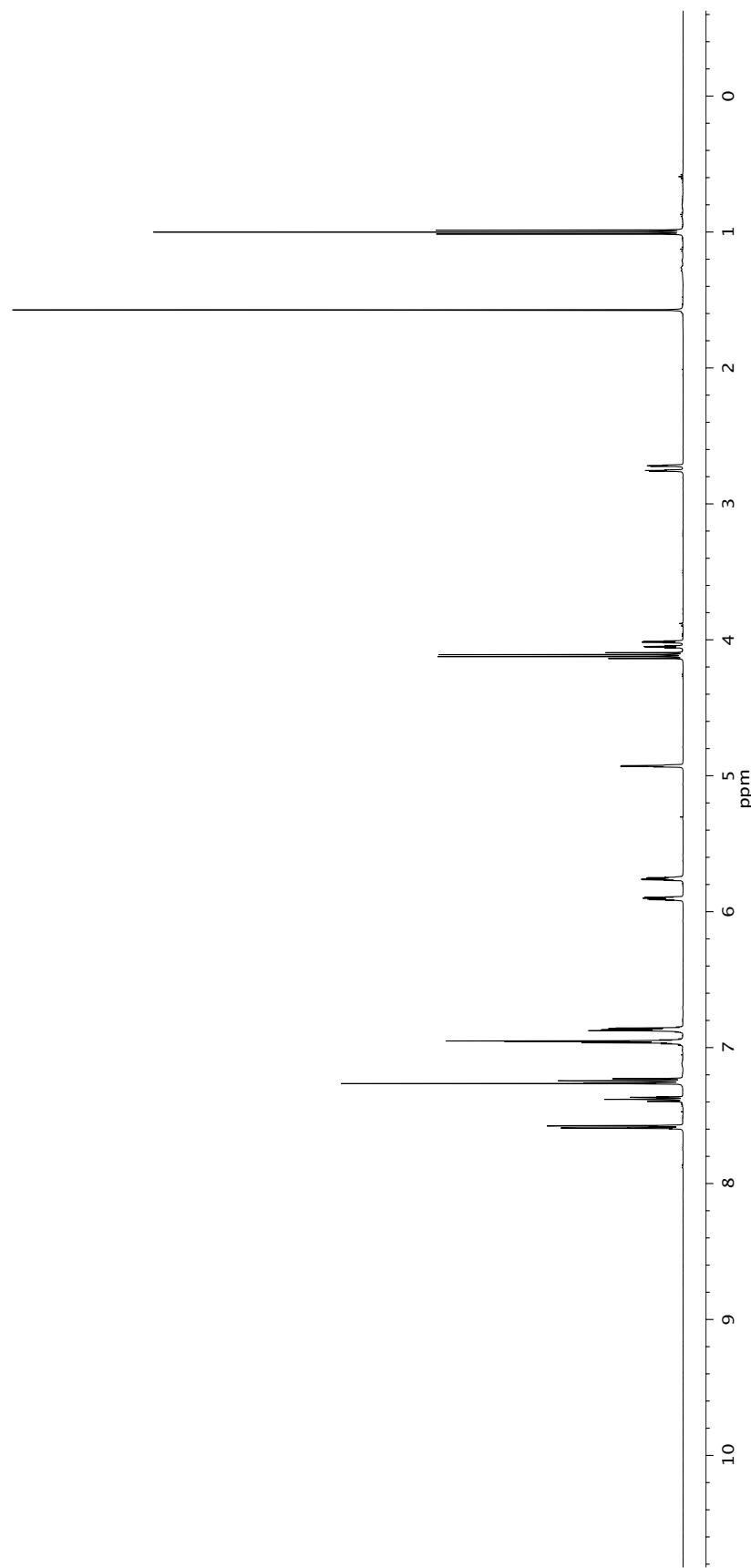
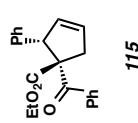


Figure A6.103  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ ) of compound 115.

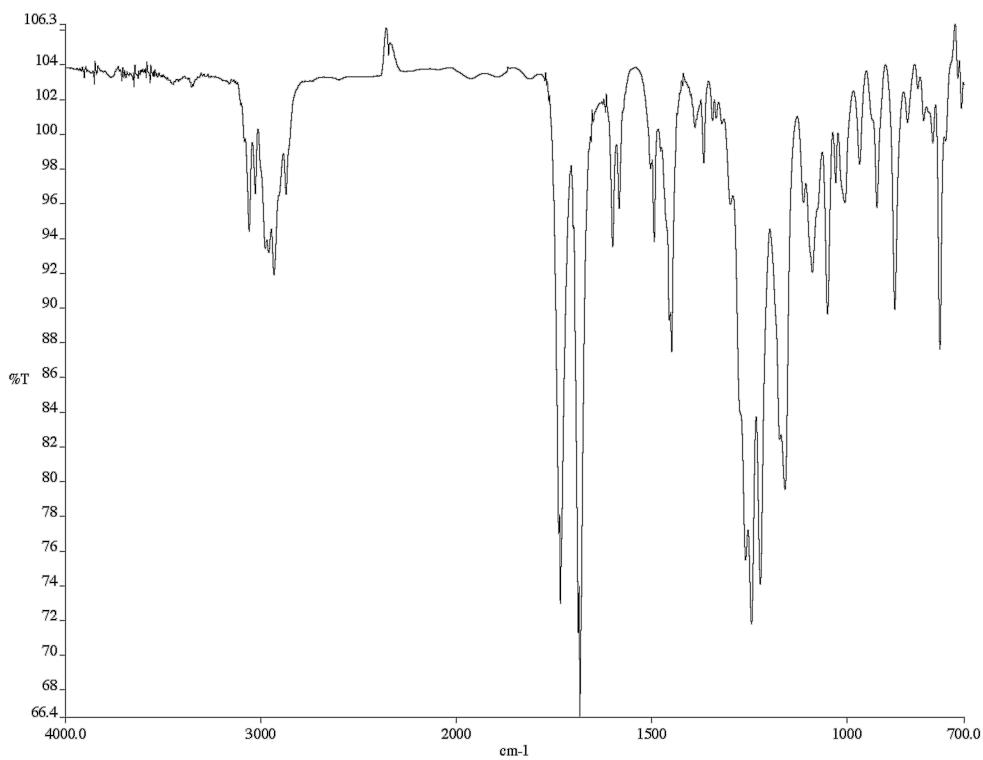


Figure A6.104 Infrared spectrum (thin film/NaCl) of compound 115.

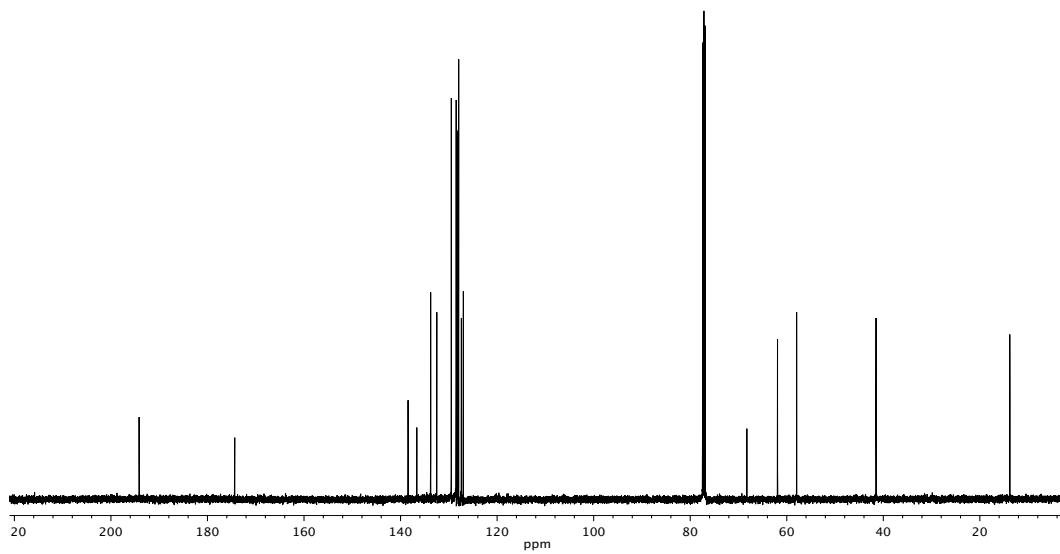


Figure A6.105 <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound 115.



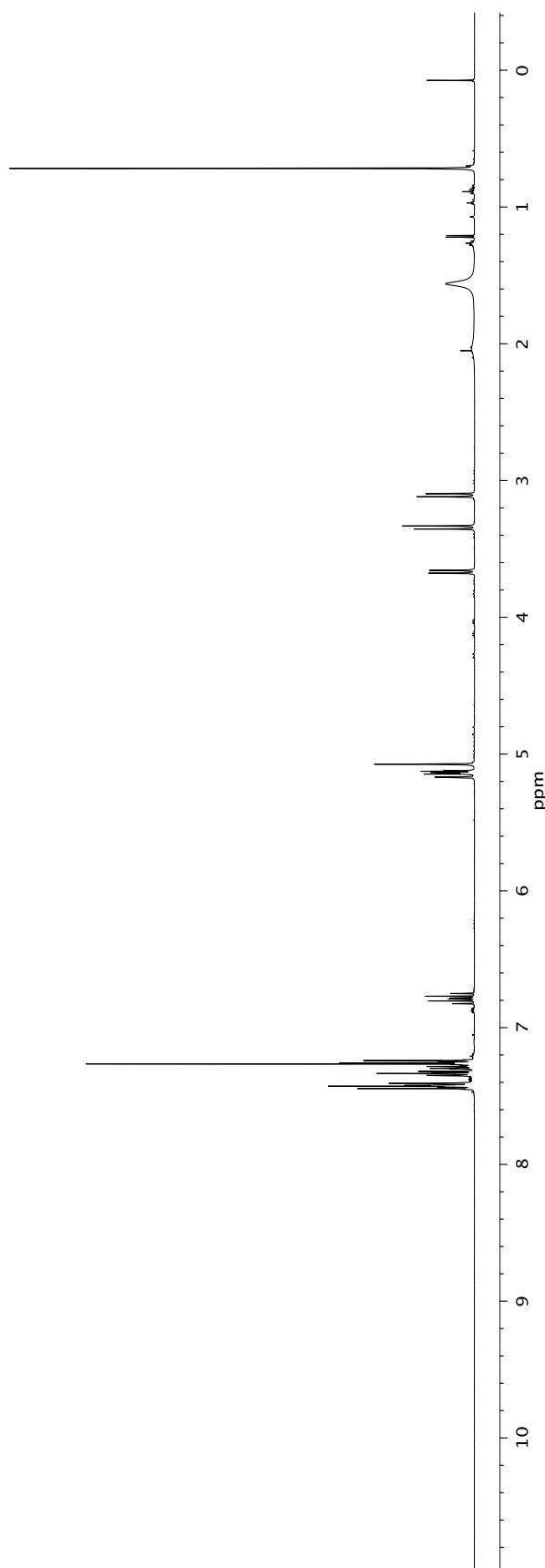
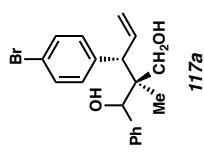


Figure A6.106 <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) of compound 117a.

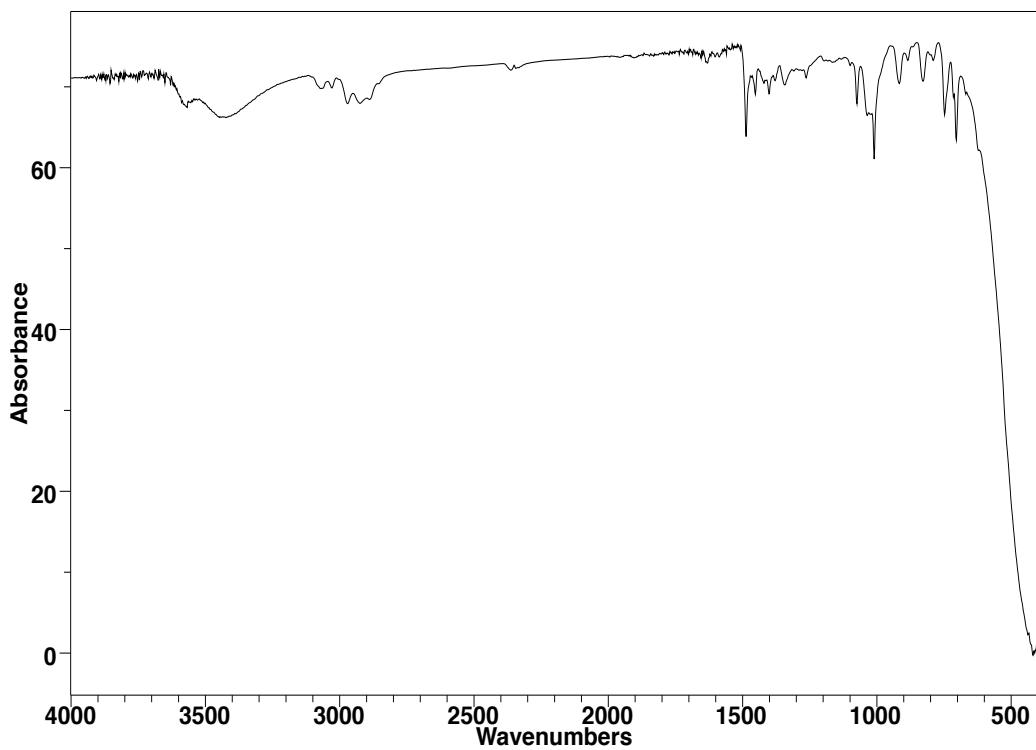


Figure A6.107 Infrared spectrum (thin film/NaCl) of compound **117a**.

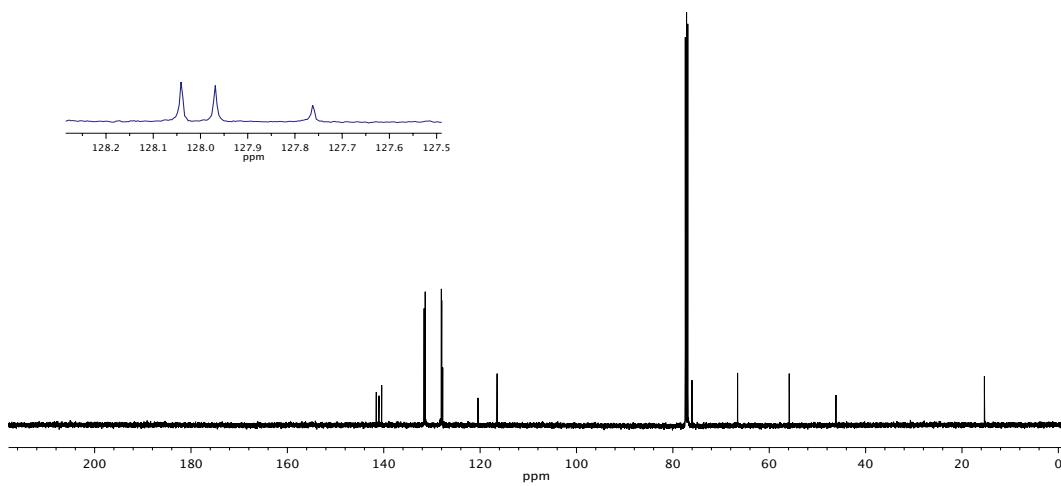


Figure A6.108  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) of compound **117a**.

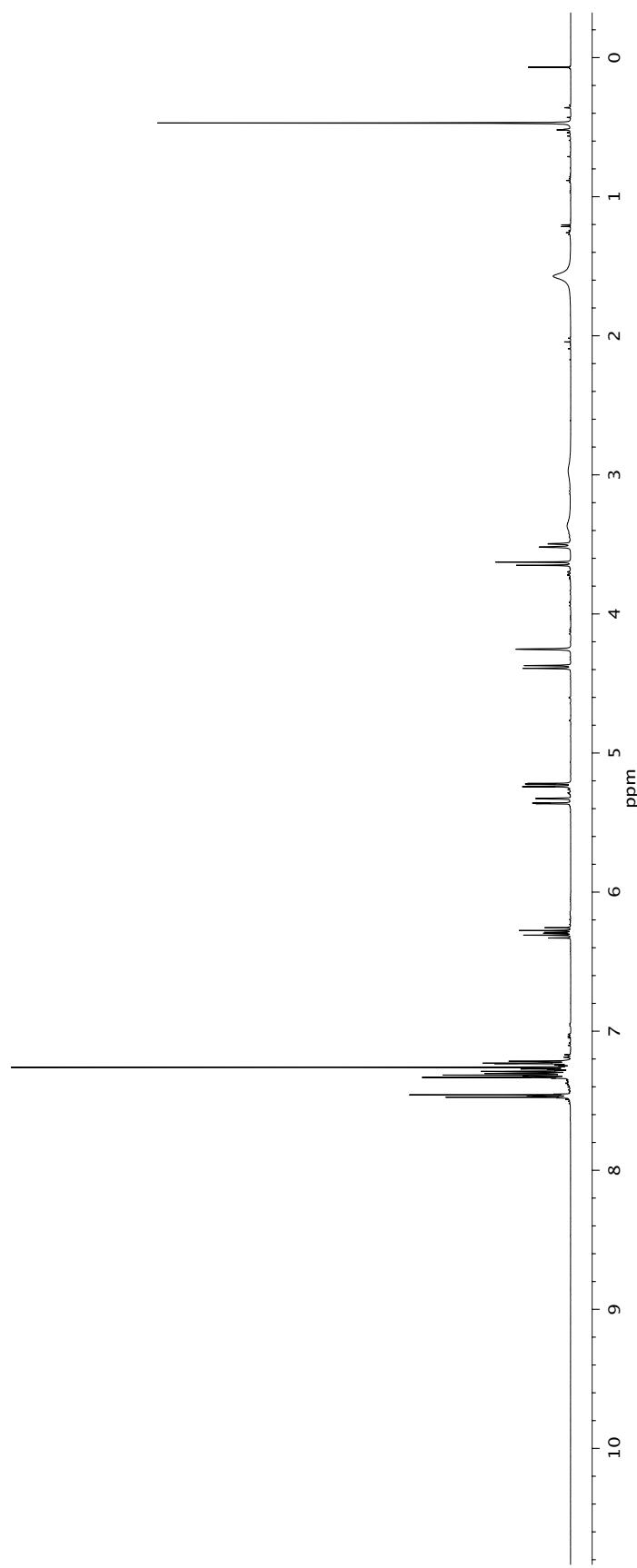
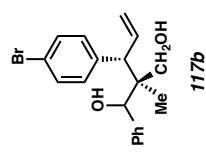


Figure A6.109 <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) of compound 117b.

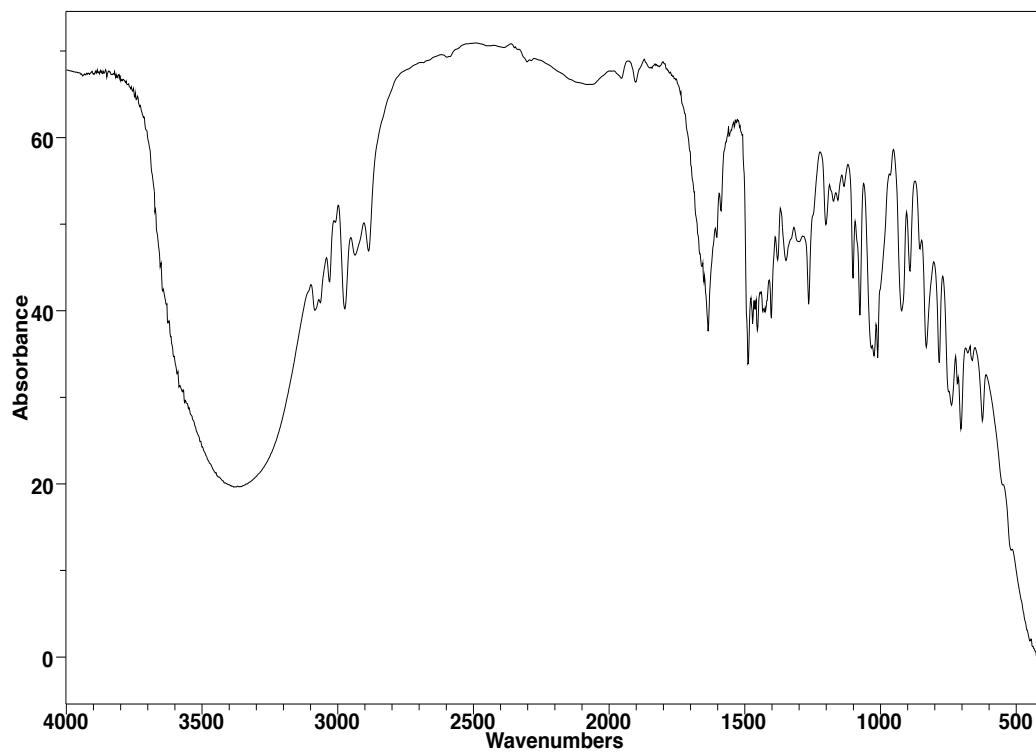


Figure A6.110 Infrared spectrum (thin film/NaCl) of compound **117b**.

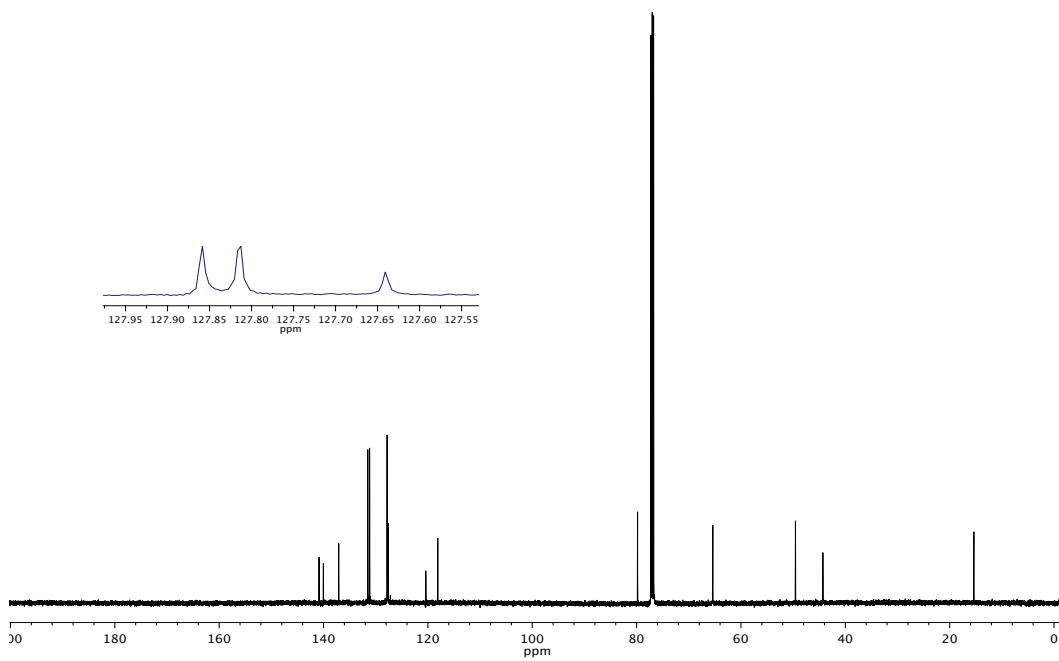


Figure A6.111  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ ) of compound **117b**.