

Supporting Information

Dual activity of Grubbs-type catalyst in the transvinylation of carboxylic acids and ring closing-metathesis reactions.

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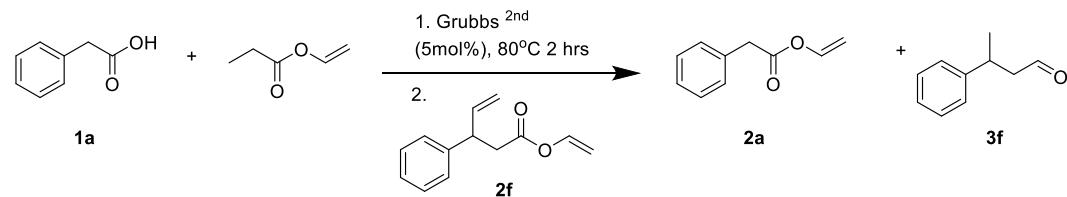
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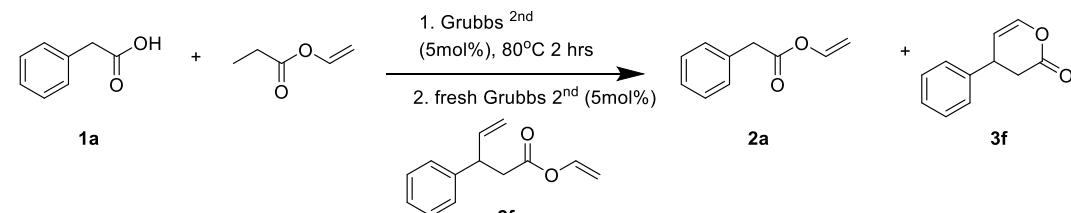
1. The studies on catalyst activity – conversion, reaction rate and TON calculation.

Scheme S1. The studies on catalyst activity

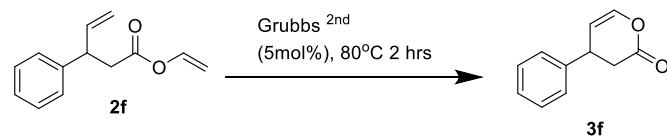
Reaction A:



Reaction B:



Reaction C:



For RCM reactions of **2f**(A, B, C presented in Table 4 in main text) the conversions was calculated by HPLC (Kromasil SI 60/5 um column); hexane/isopropanol (98:), $\lambda = 216$ nm; 0.5 mL/min, retention time (in min): $t_{2a} = 4.8$, $t_{2f} = 5.1$, $t_{3f} = 11.3$ using standard curve methodology. For compounds **2f** and **3f** standard curves was determined. These curves were constructed with five different concentrations for each compound. Samples of the reaction mixtures (A, B, C) were analysed by HPLC.

Fig S1. The standard curve for compound **2f**.

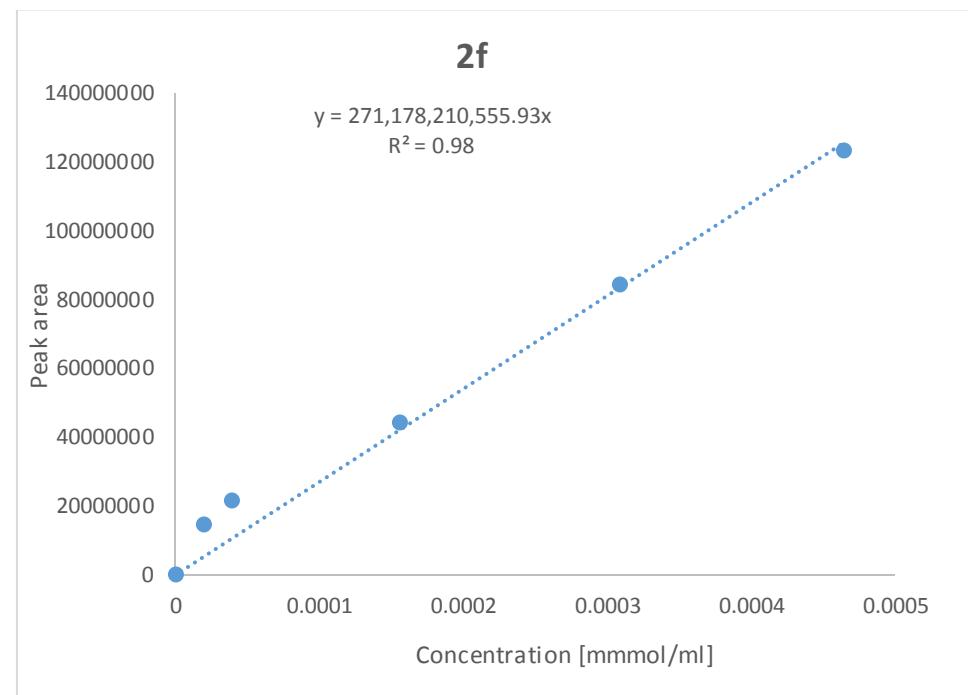


Fig S2. The standard curve for compound **3f**.

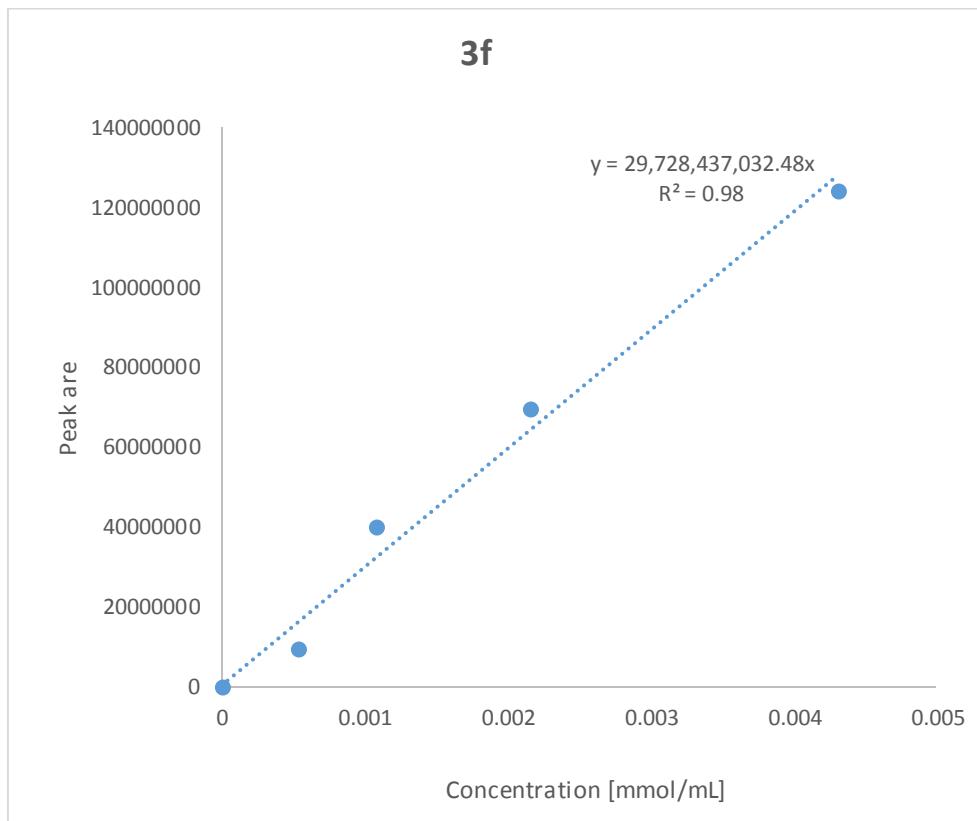
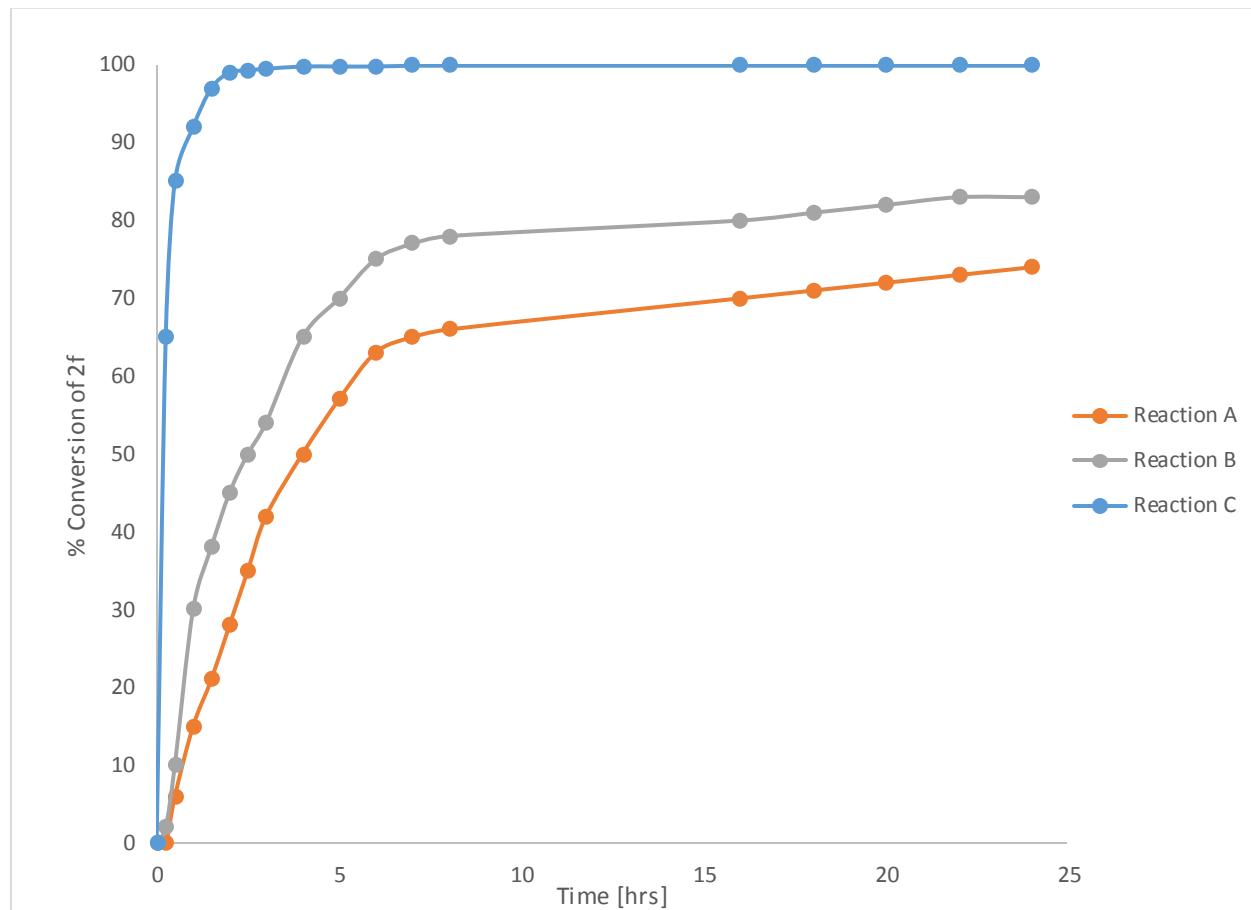


Fig S3. The progress of reactions A, B and C.



The calculation of initial rates of RCM reactions:

The initial reaction rates were determined by graphical procedure. The initial reaction rate of mentioned RCM reactions at any time t is given by the slope of a straight line that is tangent to the curve at that time. Thus the initial rates of presented reactions were calculated from the slope.

The calculated initial rates:

Reaction A: $V_{RCM} = 3.9 \times 10^{-7} [\text{mol/L}\cdot\text{s}]$

Reaction B: $V_{RCM} = 7.2 \times 10^{-7} [\text{mol/L}\cdot\text{s}]$

Reaction C: $V_{RCM} = 5.2 \times 10^{-6} [\text{mol/L}\cdot\text{s}]$

The calculation of TON:

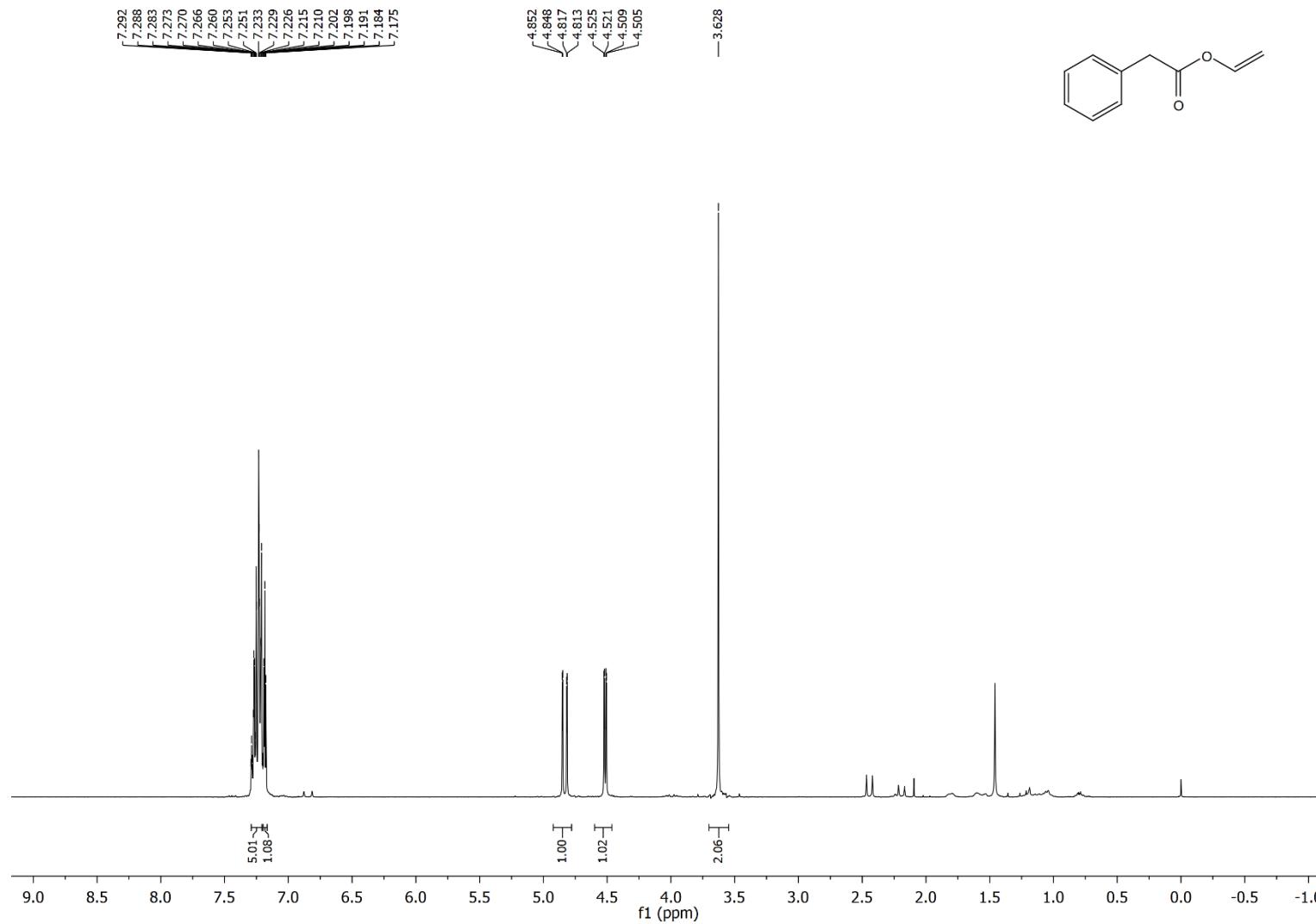
TON was calculated from equation:

$$TON = \frac{yield \times no}{100}, \text{ where } no = \text{initial moles of 2f; } ncat = \text{moles of catalyst used}$$

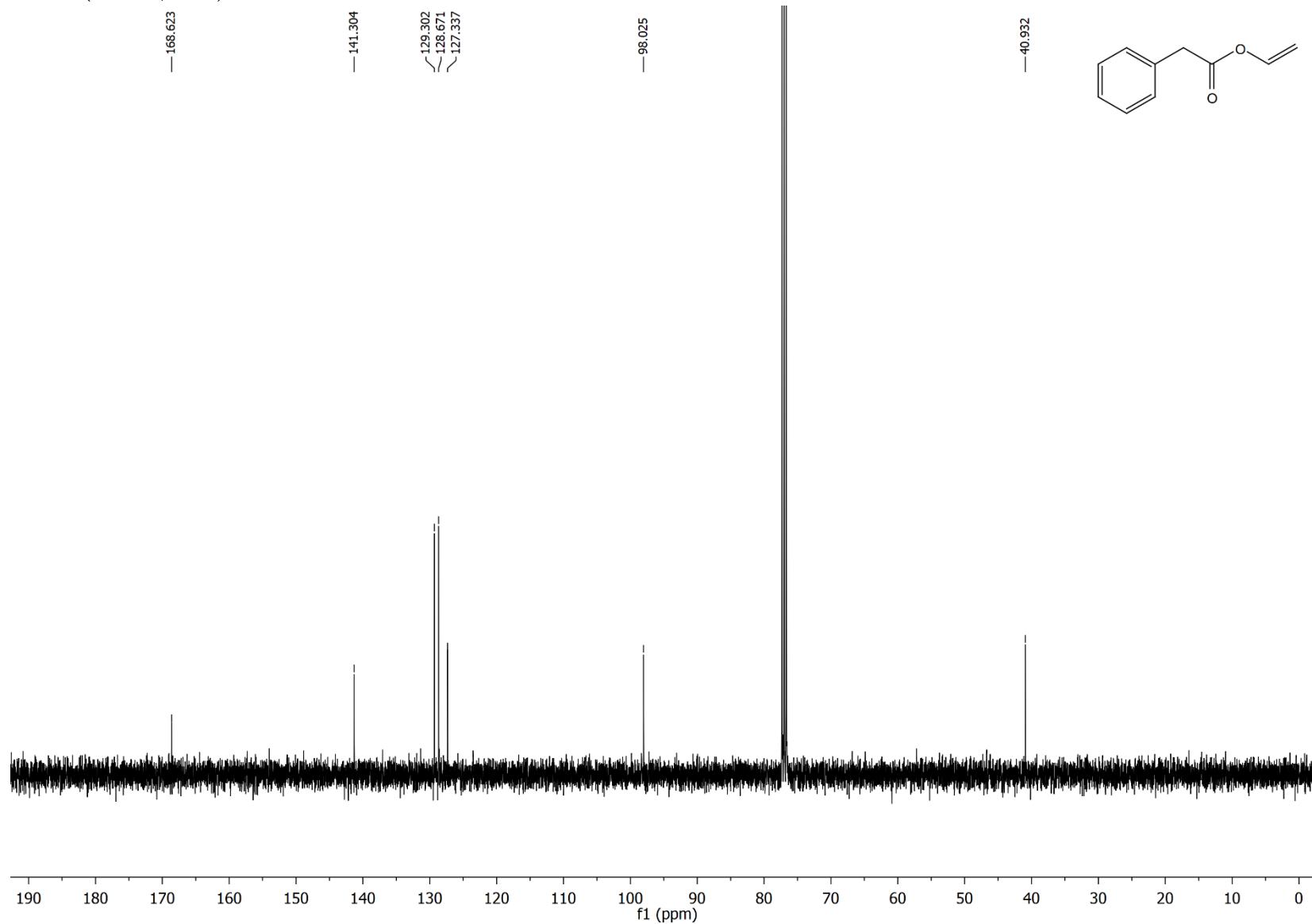
2. ^1H NMR and ^{13}C NMR spectra

Vinyl phenylacetate (**2a**)

^1H NMR (400 MHz, CDCl_3)

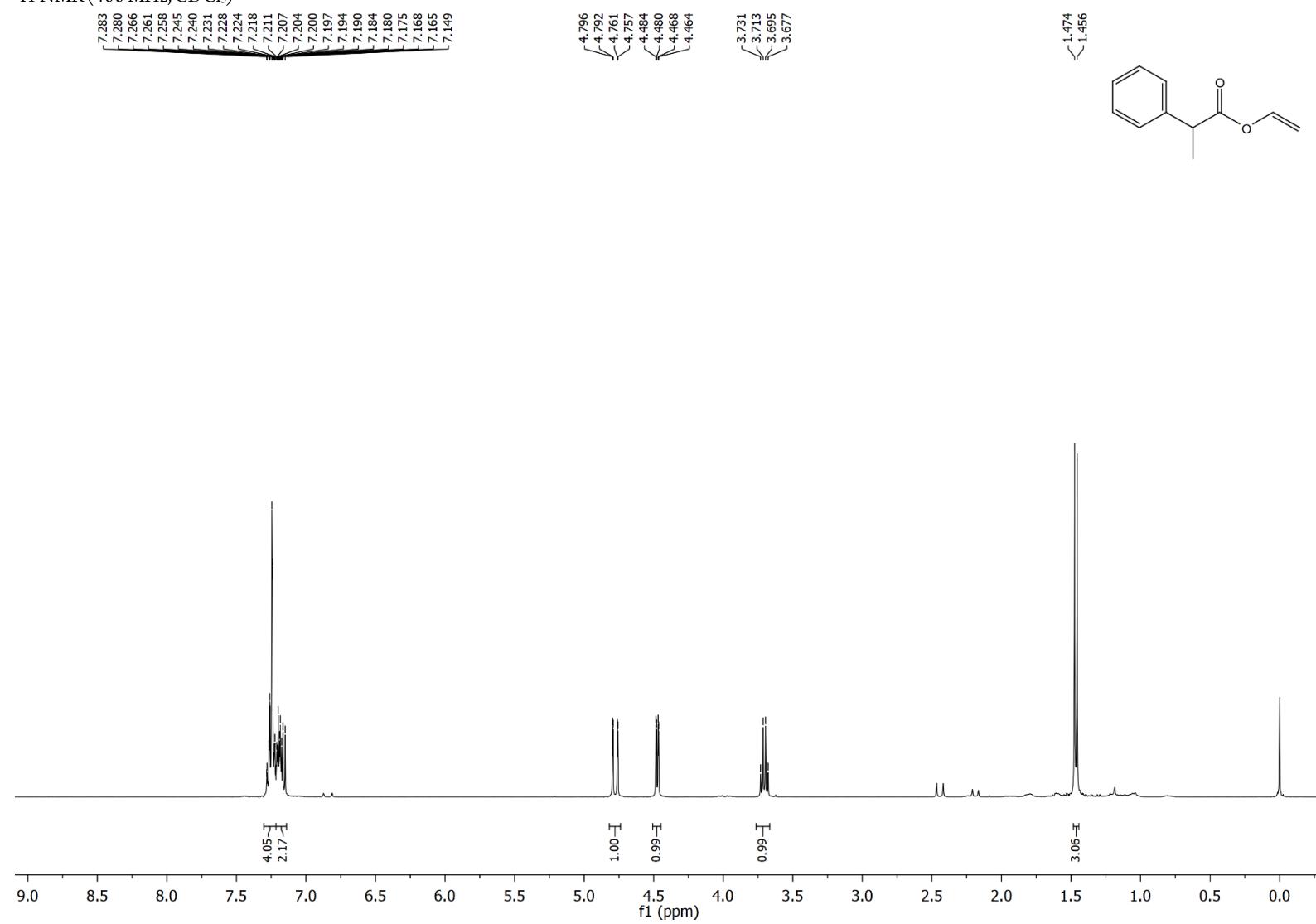


^{13}C NMR ($100\text{ MHz}, \text{CDCl}_3$)

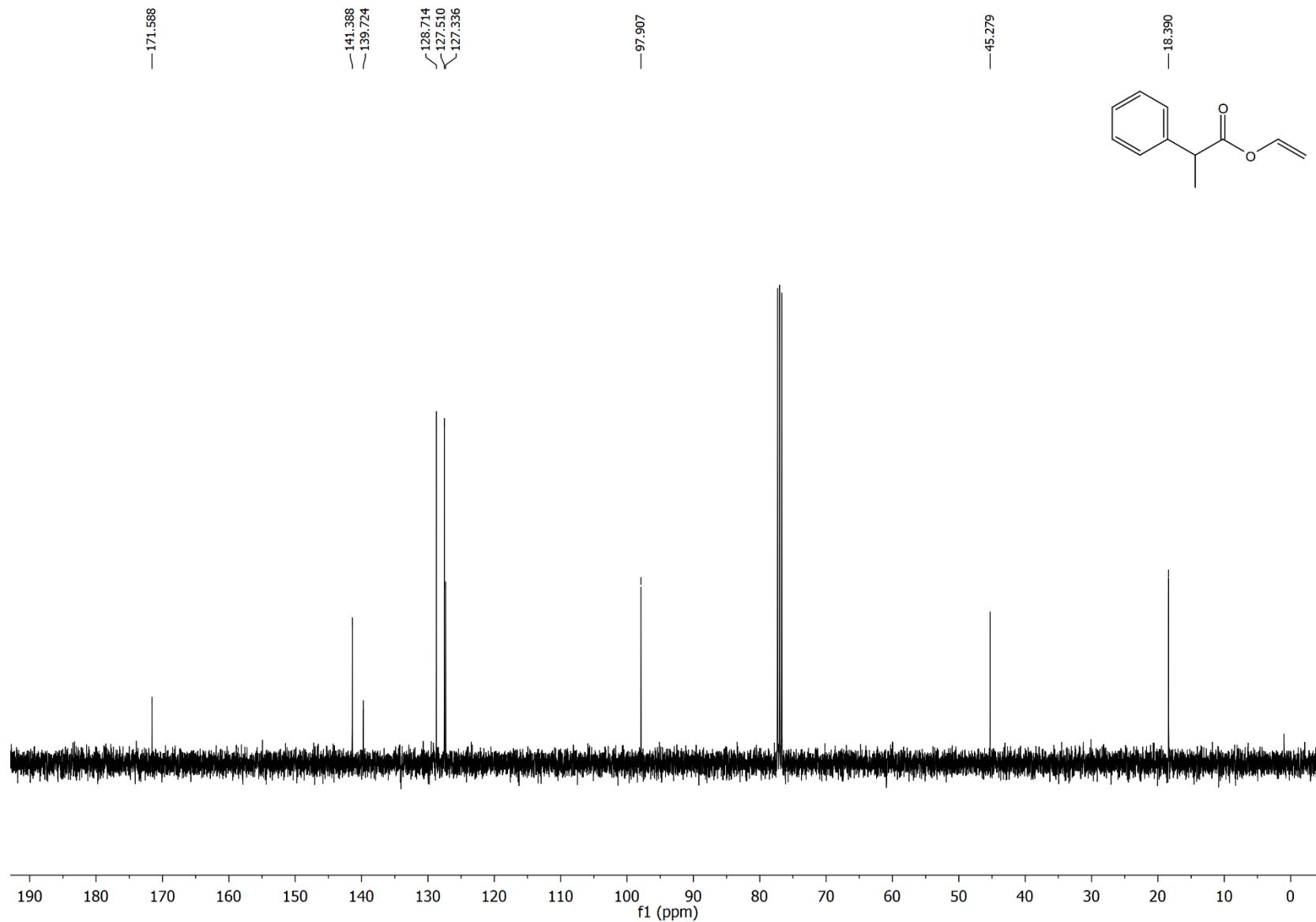


Vinyl 2-phenylpropionate (2b)

¹H NMR (400 MHz, CDCl₃)

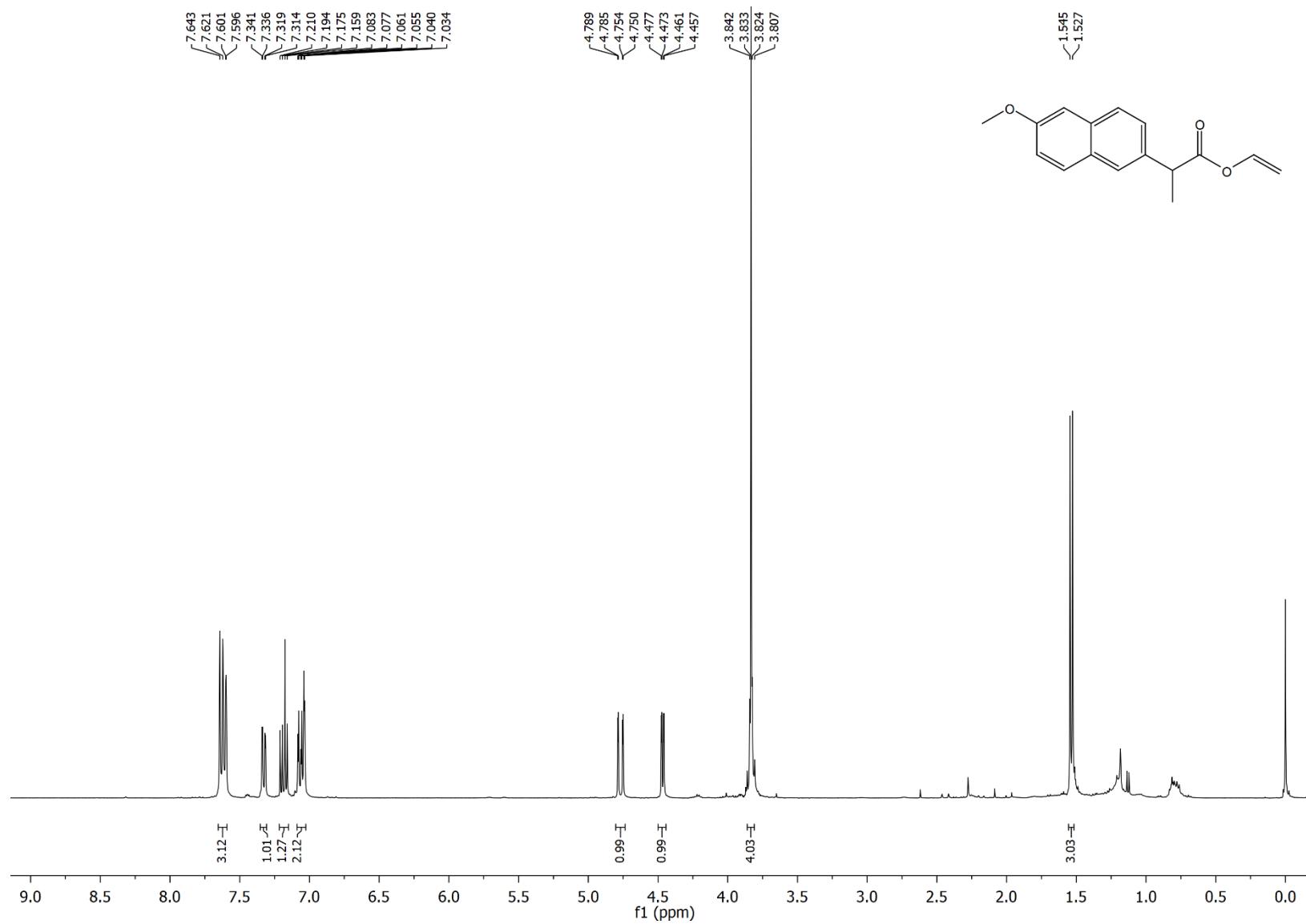


¹³C NMR (100 MHz, CDCl₃)

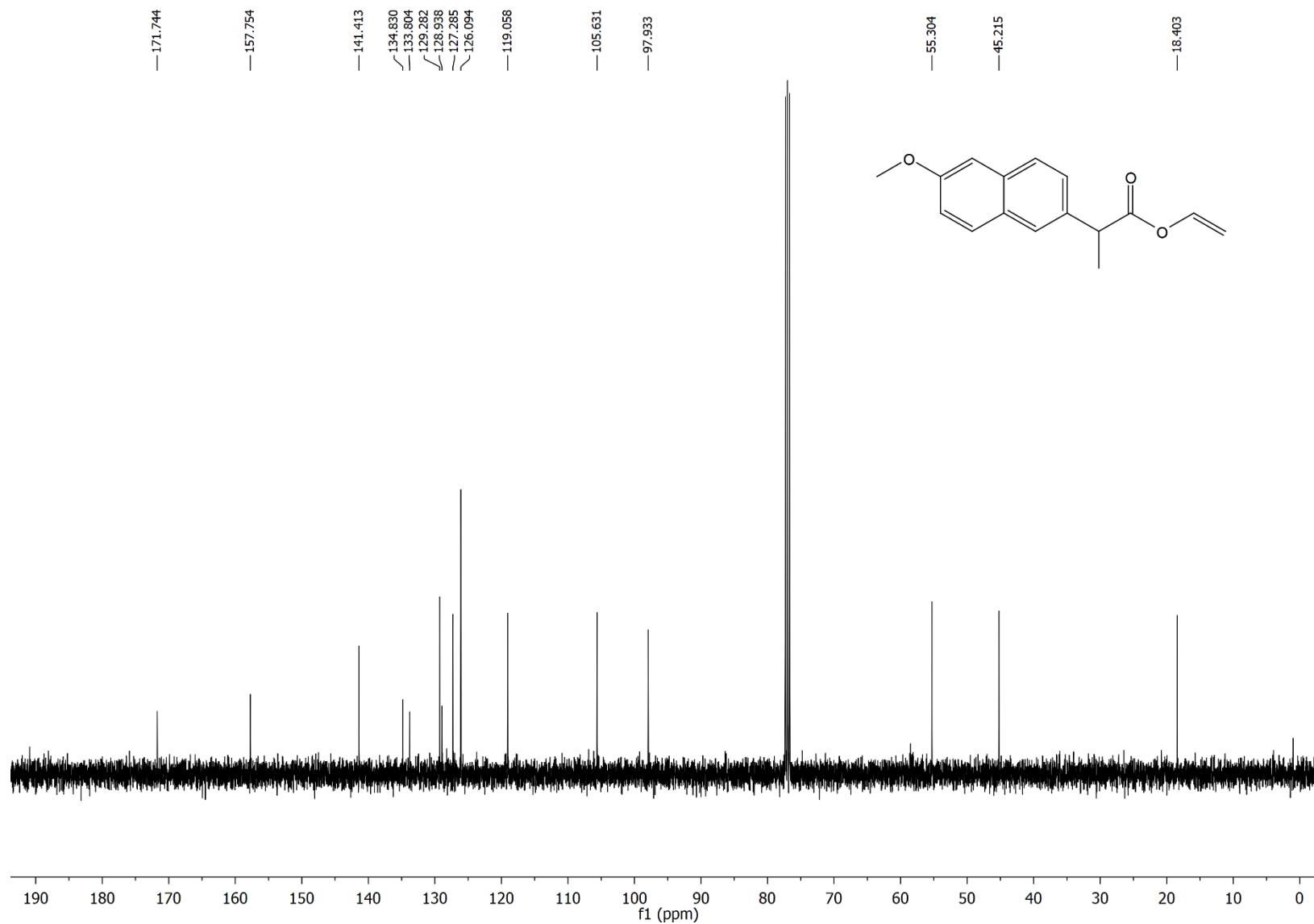


Vinyl 2-(6-Methoxy-2-naphthyl)propionate (2c)

¹H NMR (400 MHz, CDCl₃)

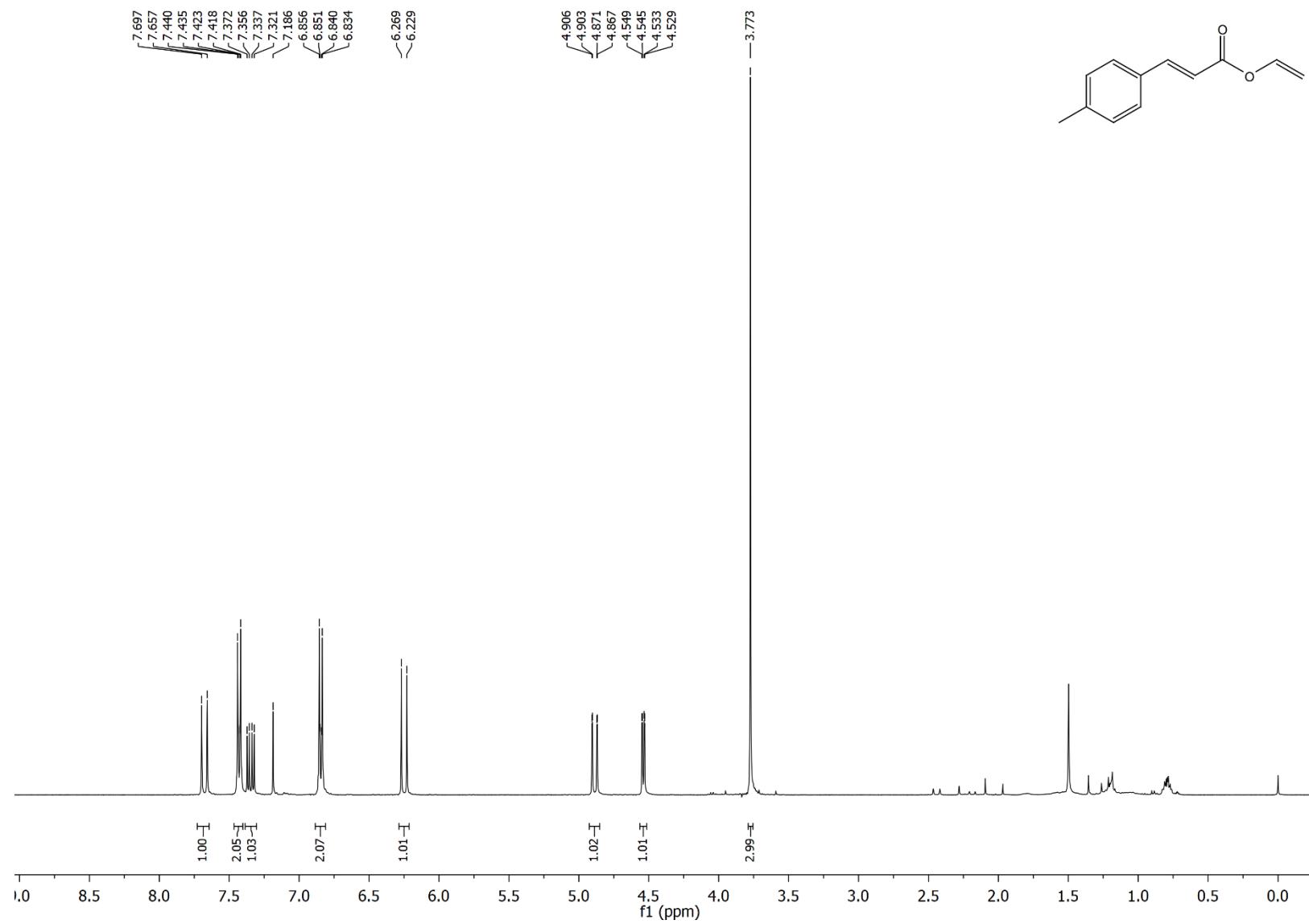


¹³C NMR (100 MHz, CDCl₃)

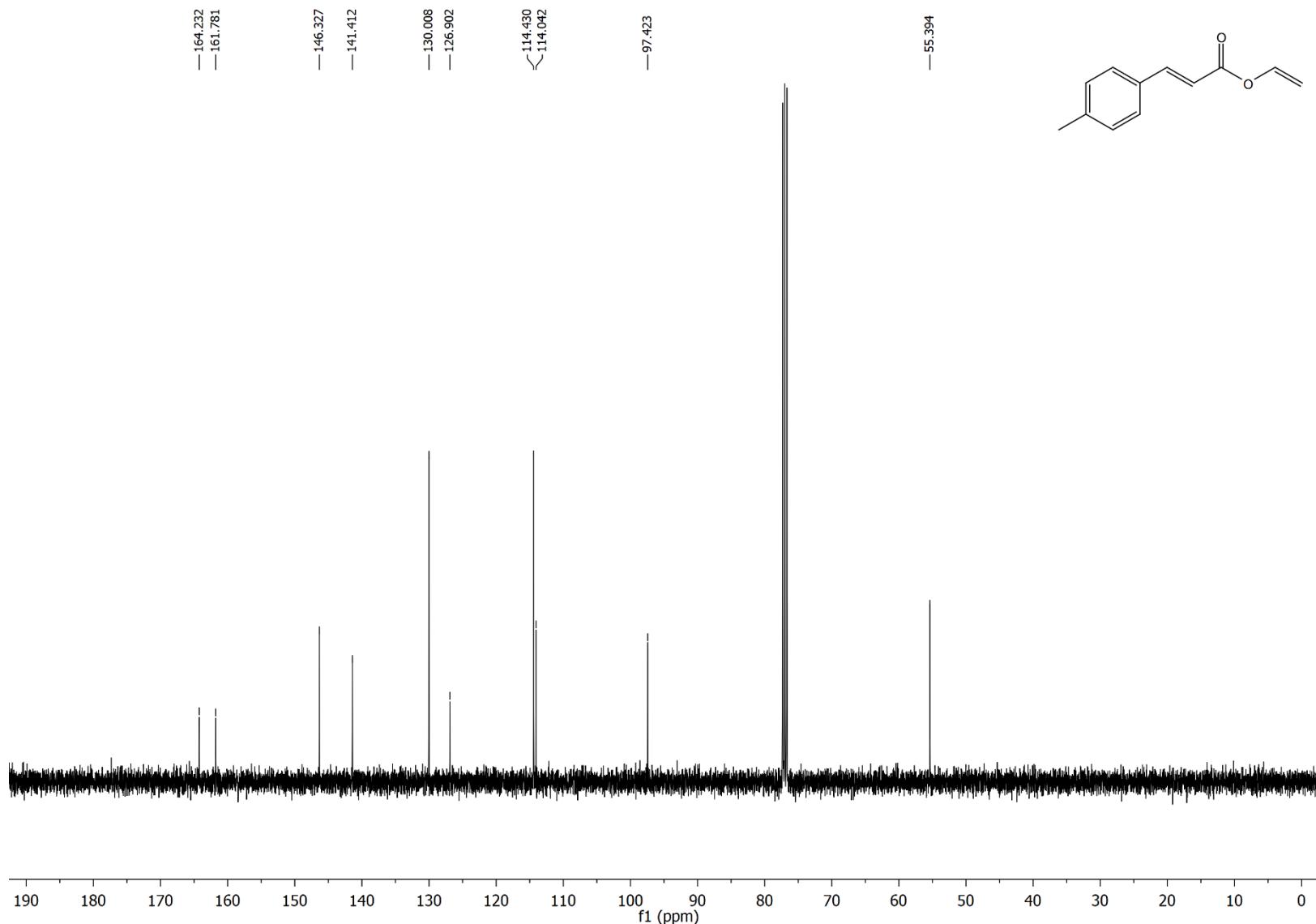


Vinyl 4-methylcinnamate (2d)

¹H NMR (400 MHz, CDCl₃)

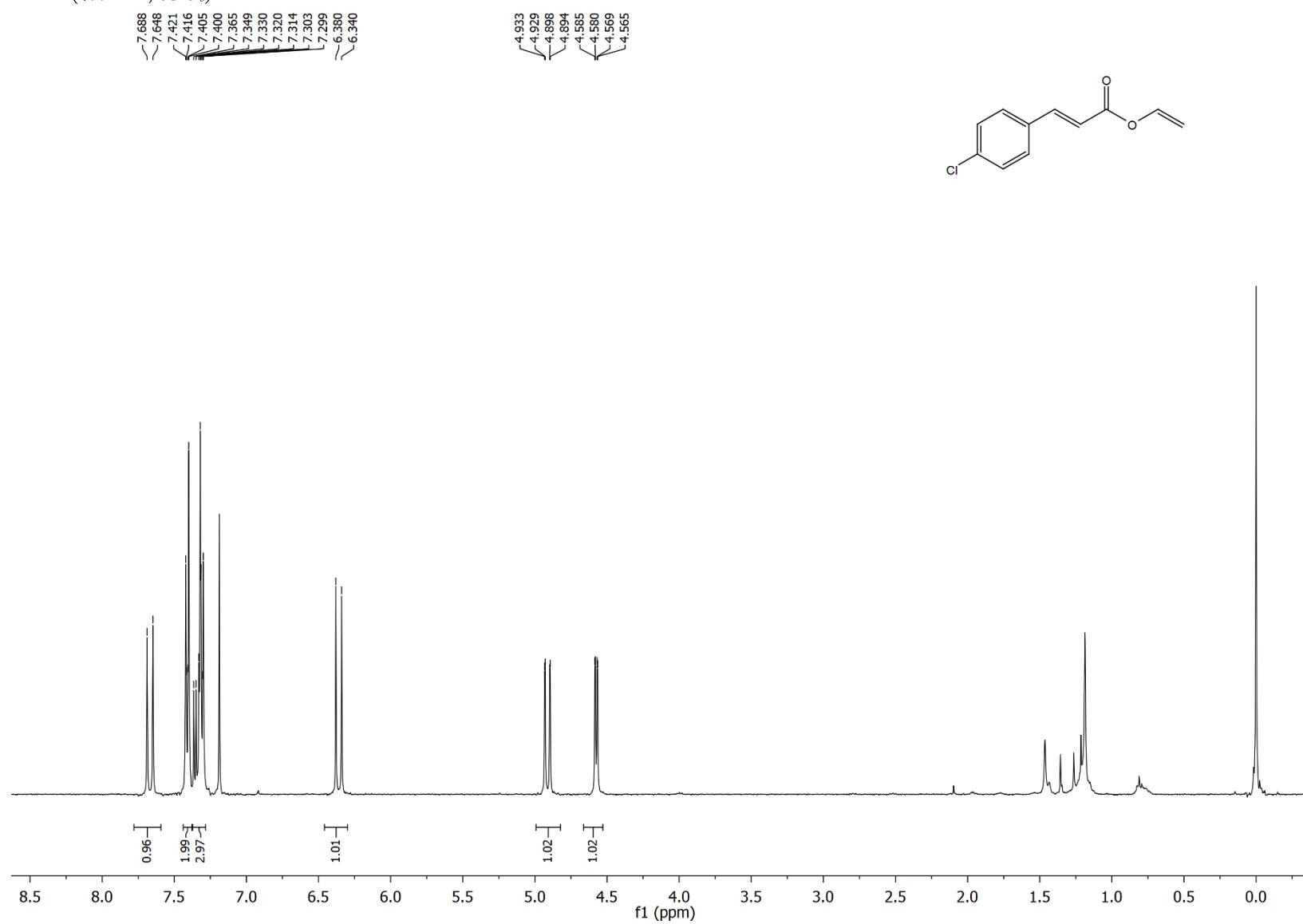


¹³C NMR (100 MHz, CDCl₃)

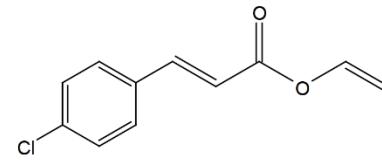
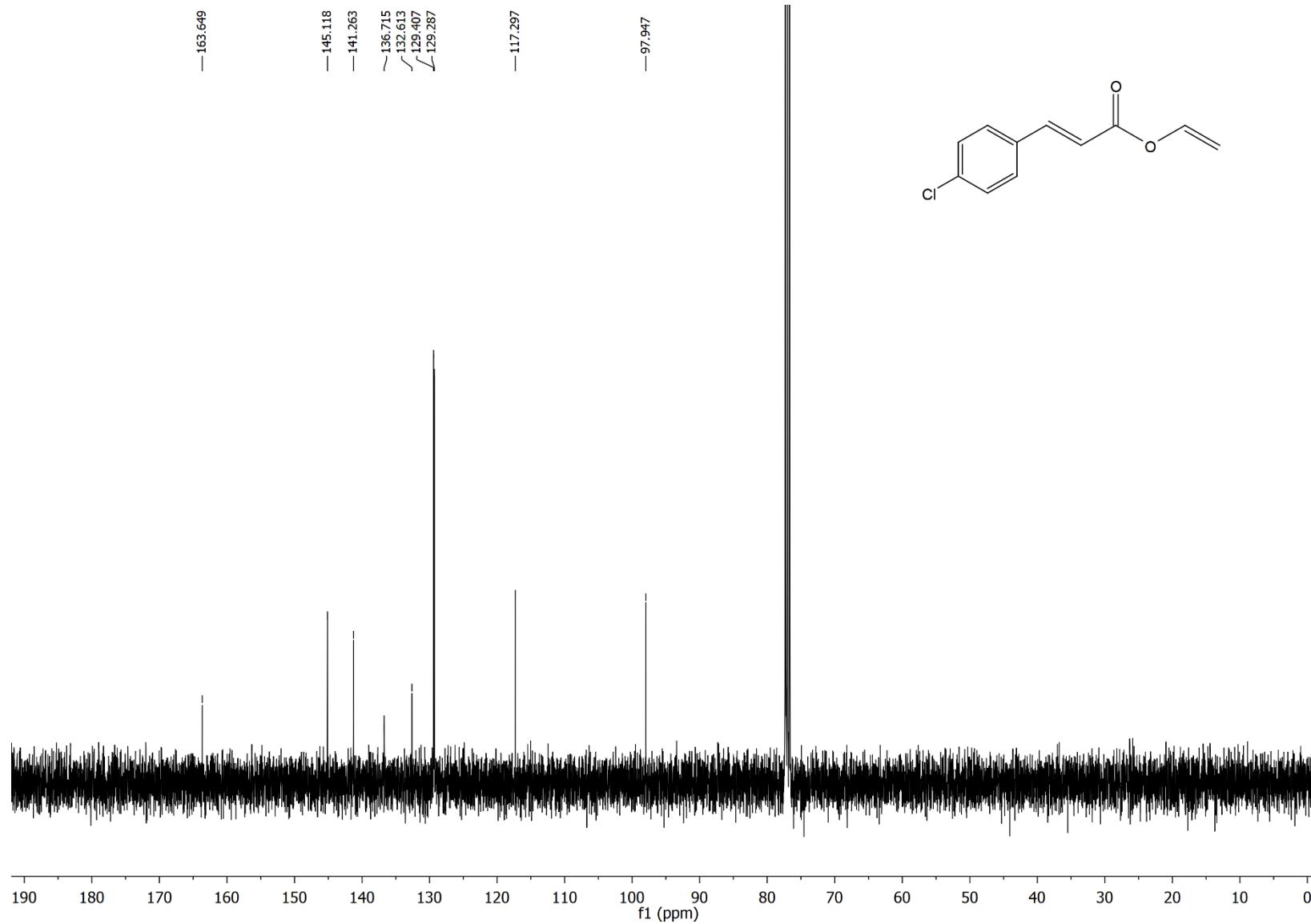


Vinyl 4-chlorocinnamate (2e)

¹H NMR (400 MHz, CDCl₃)

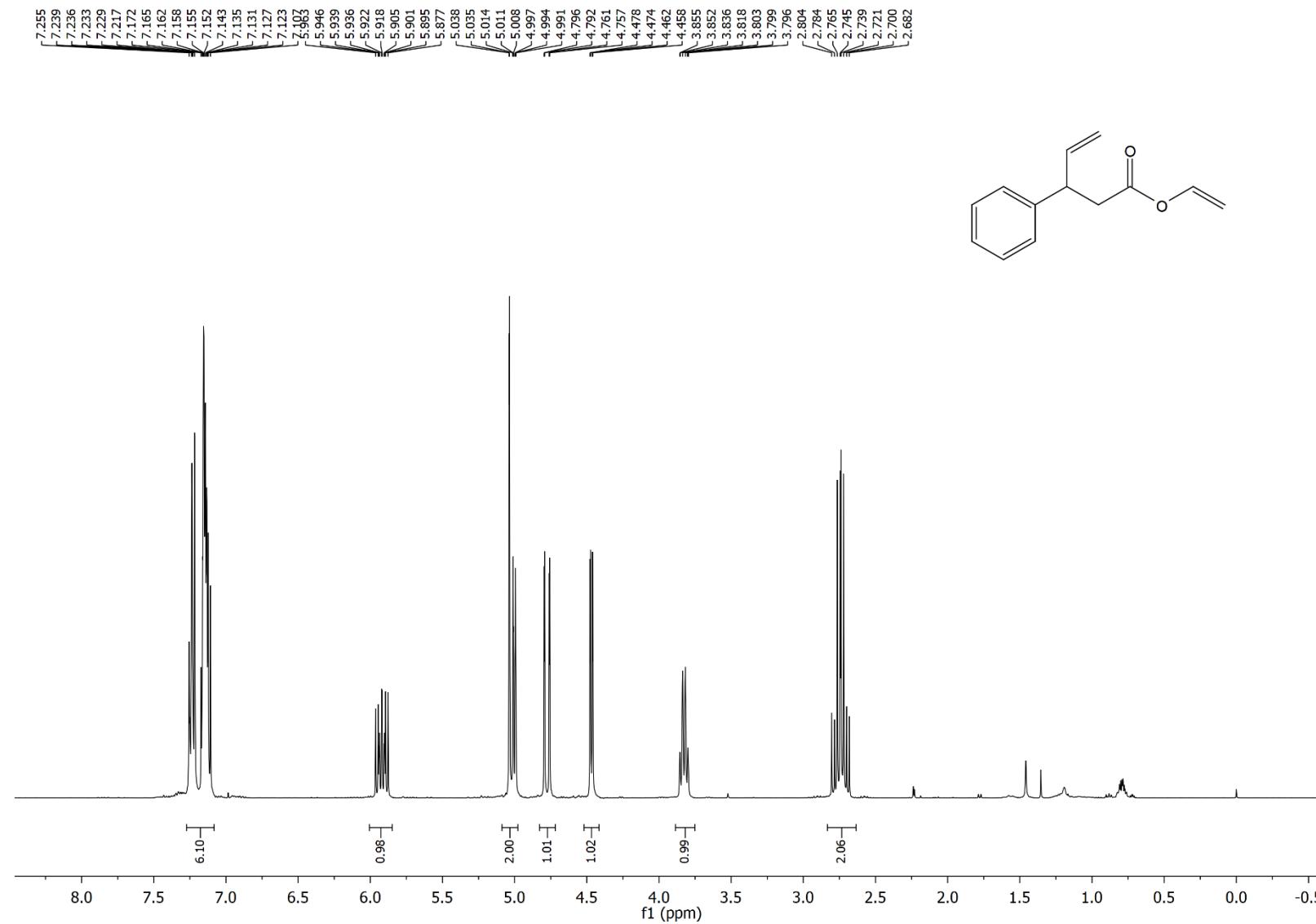


¹³C NMR (100 MHz, CDCl₃)

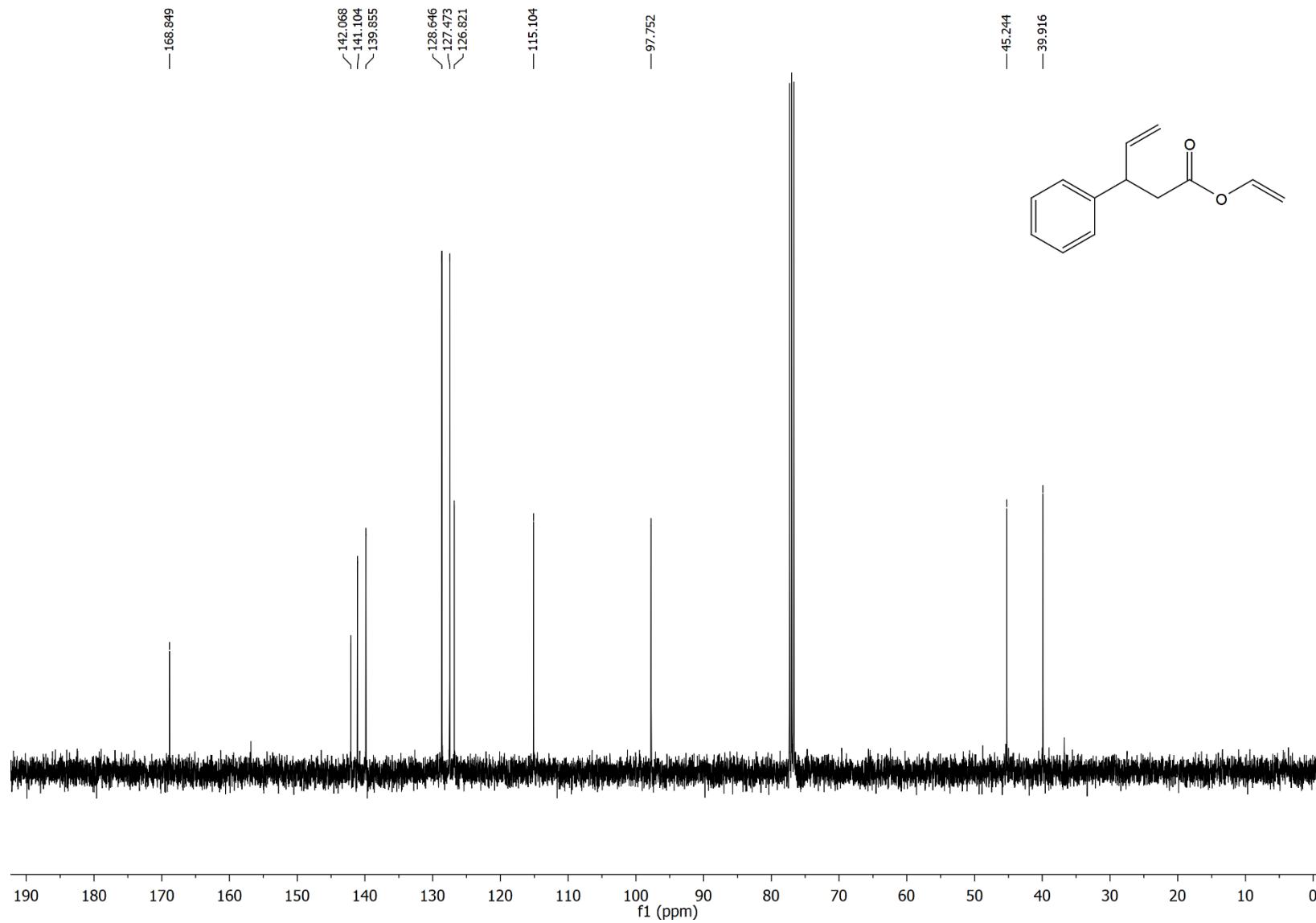


Vinyl 3-phenyl-4-pentenoate (2f)

^1H NMR (400 MHz, CDCl_3)

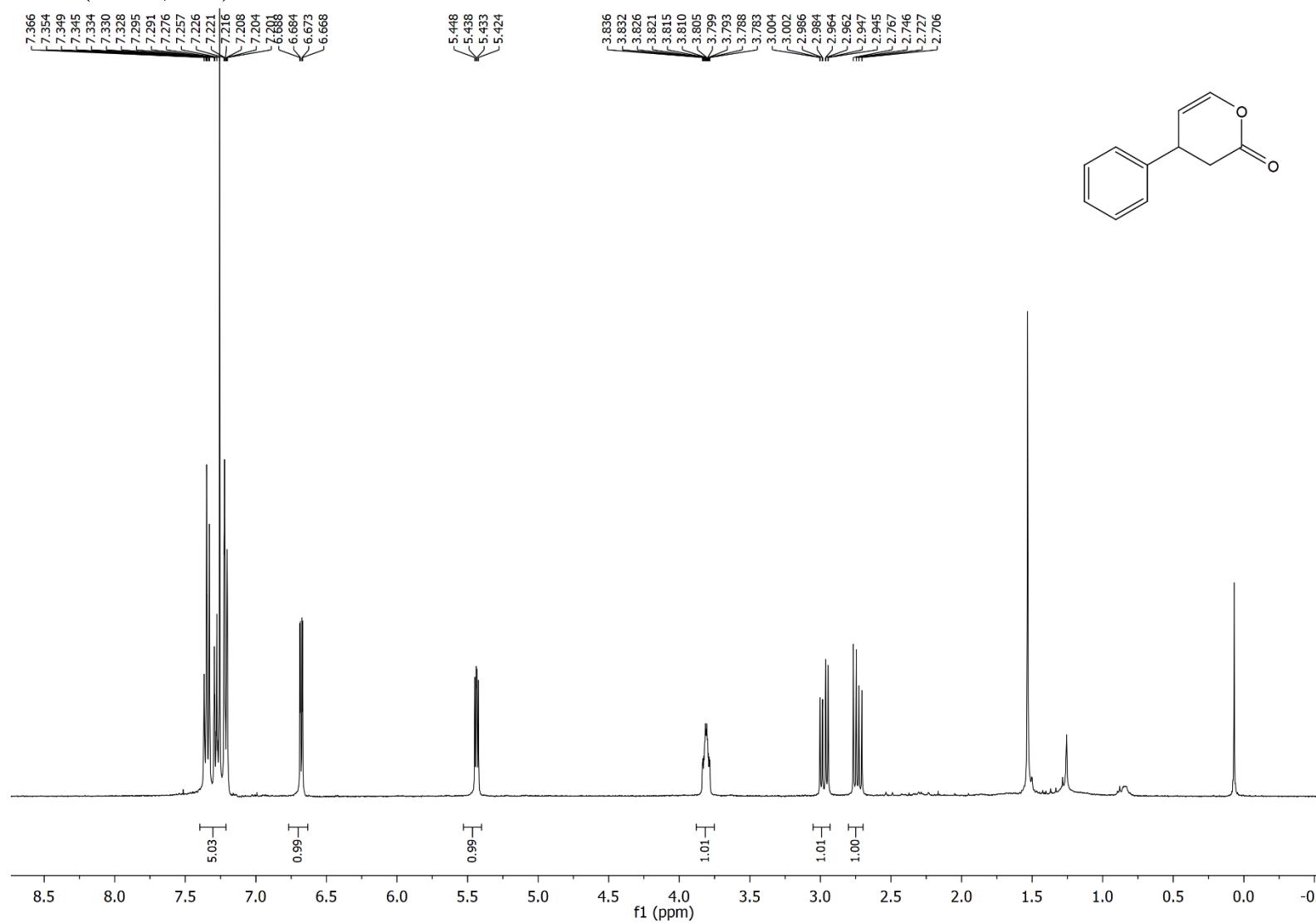


¹³C NMR (100 MHz, CDCl₃)

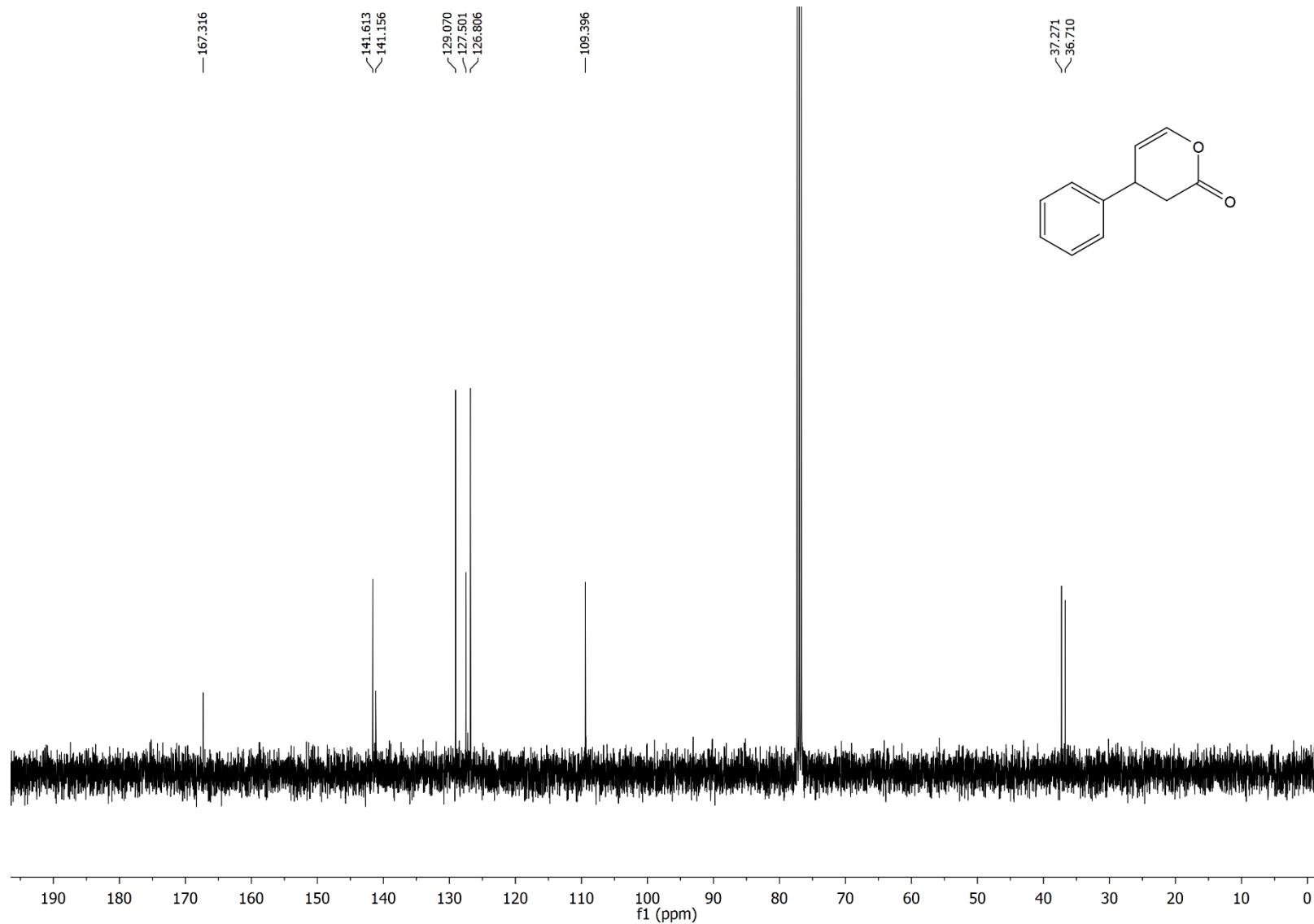


4-Phenyl-3,4-dihydro-2H-pyran-2-one (3f)

^1H NMR (400 MHz, CDCl_3)

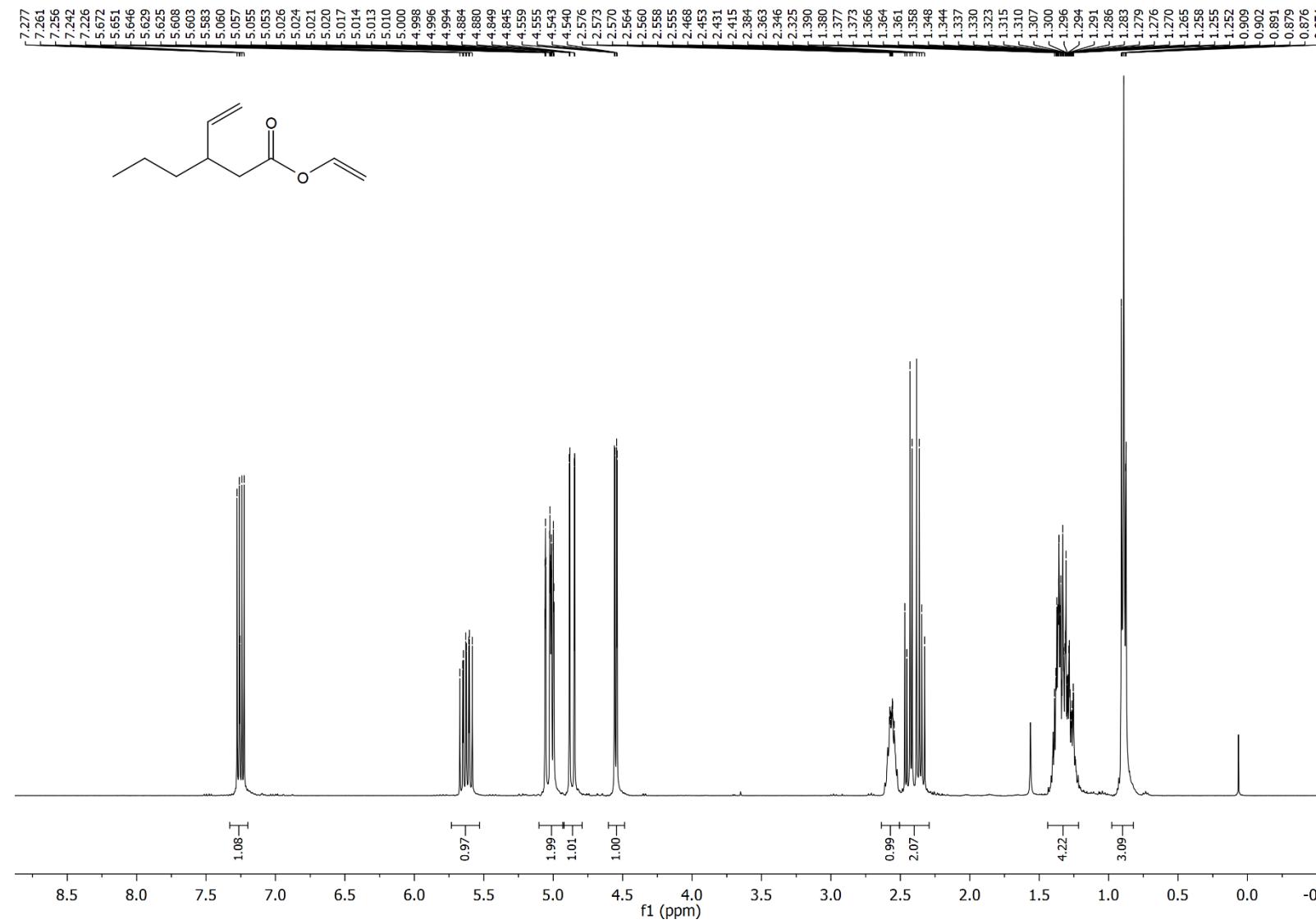


¹³C NMR (100 MHz, CDCl₃)

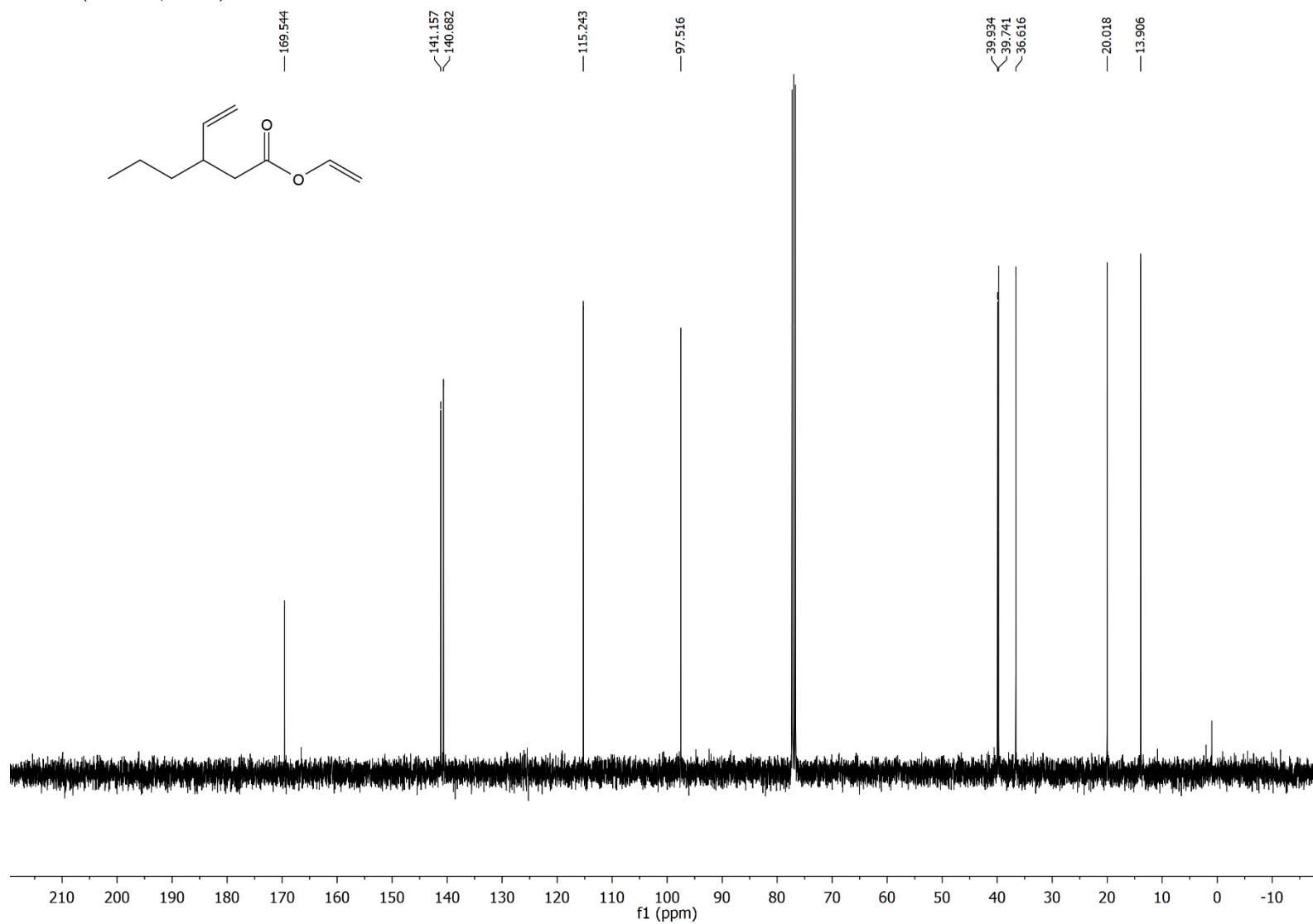


Vinyl 3-propyl-4-pentenoate (2g)

¹H NMR (400 MHz, CDCl₃)

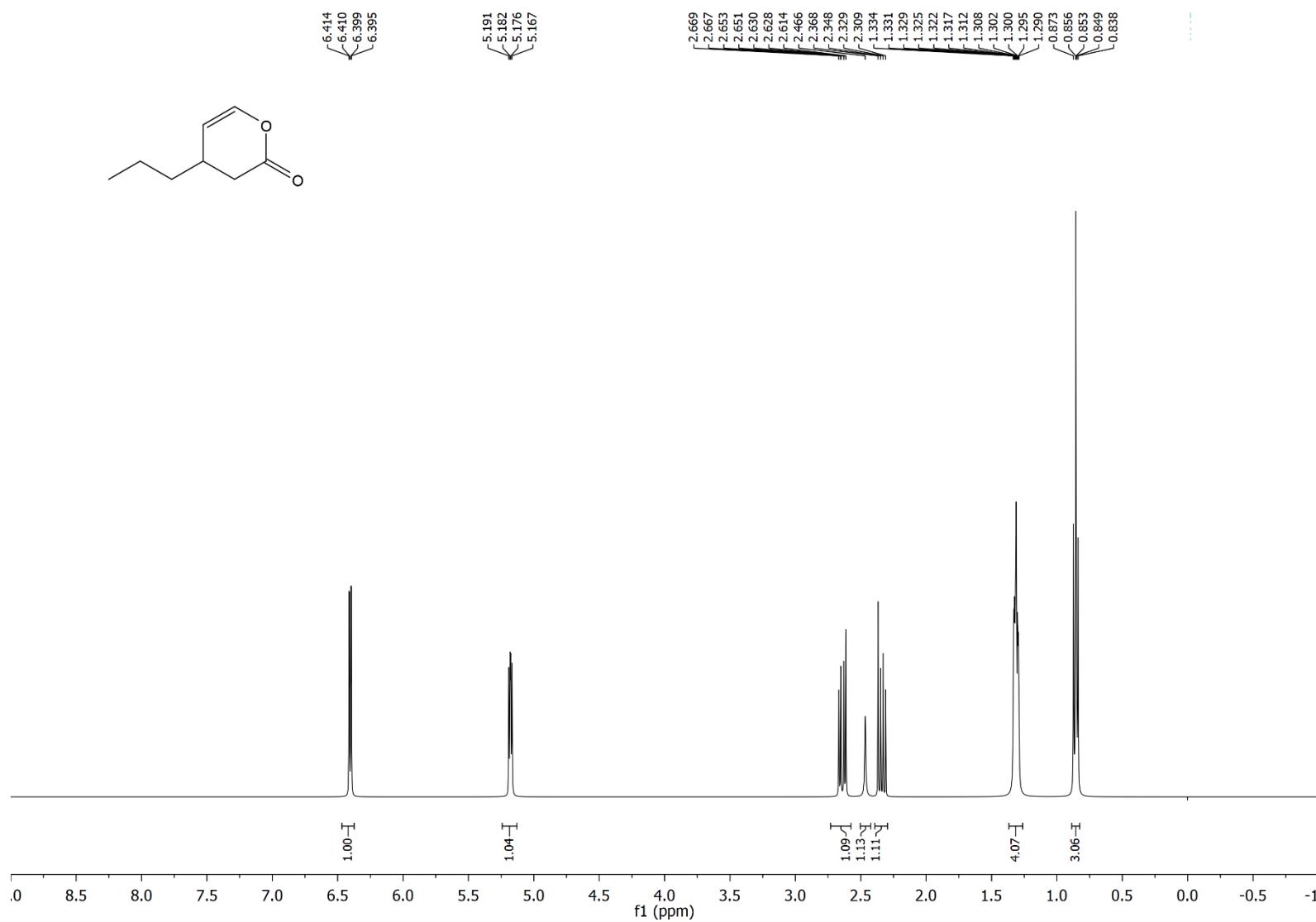


¹³C NMR (100 MHz, CDCl₃)

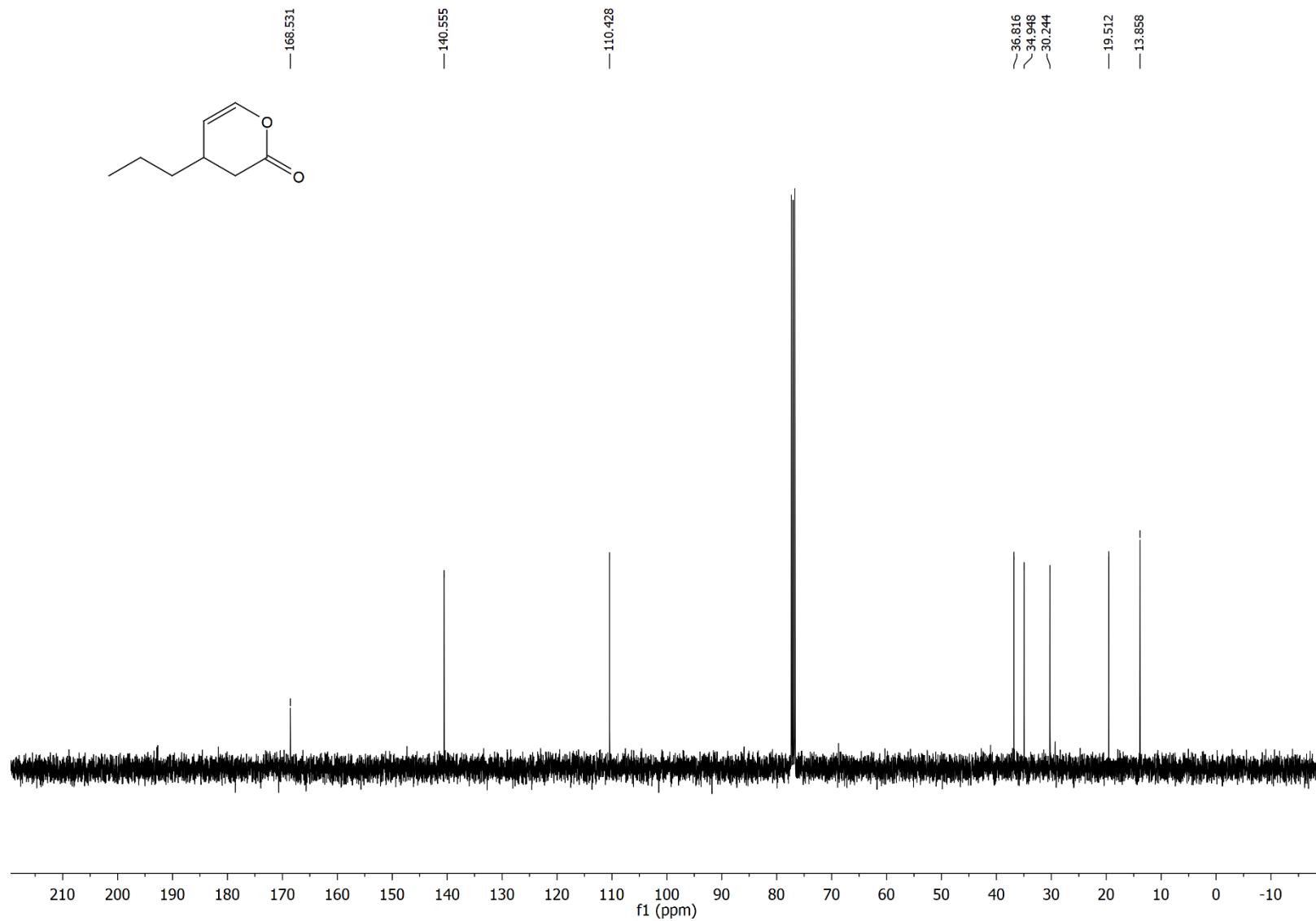


4-Propyl-3,4-dihydro-2H-pyran-2-one (3g)

¹H NMR (400 MHz, CDCl₃)

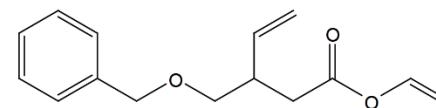
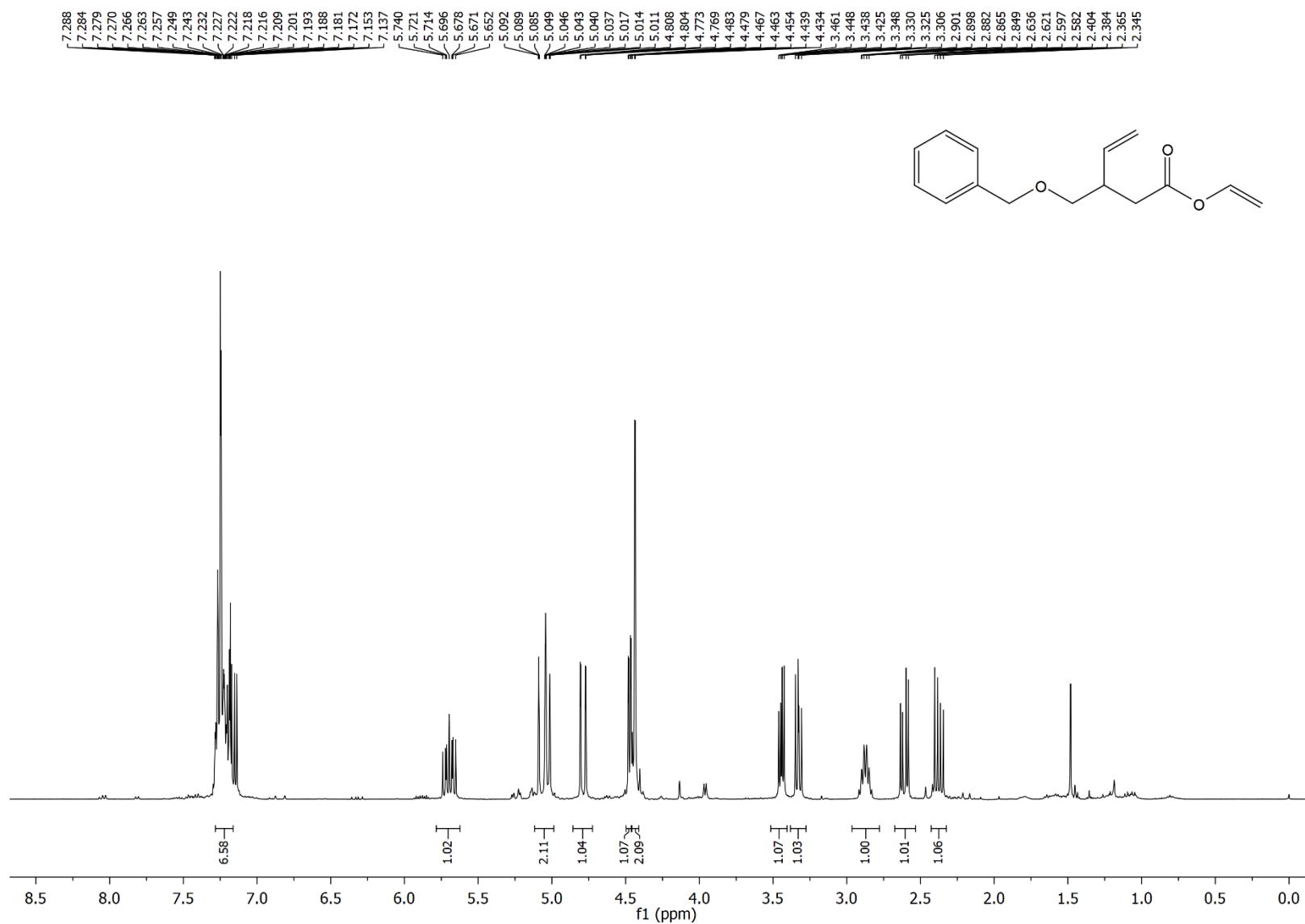


¹³C NMR (100 MHz, CDCl₃)

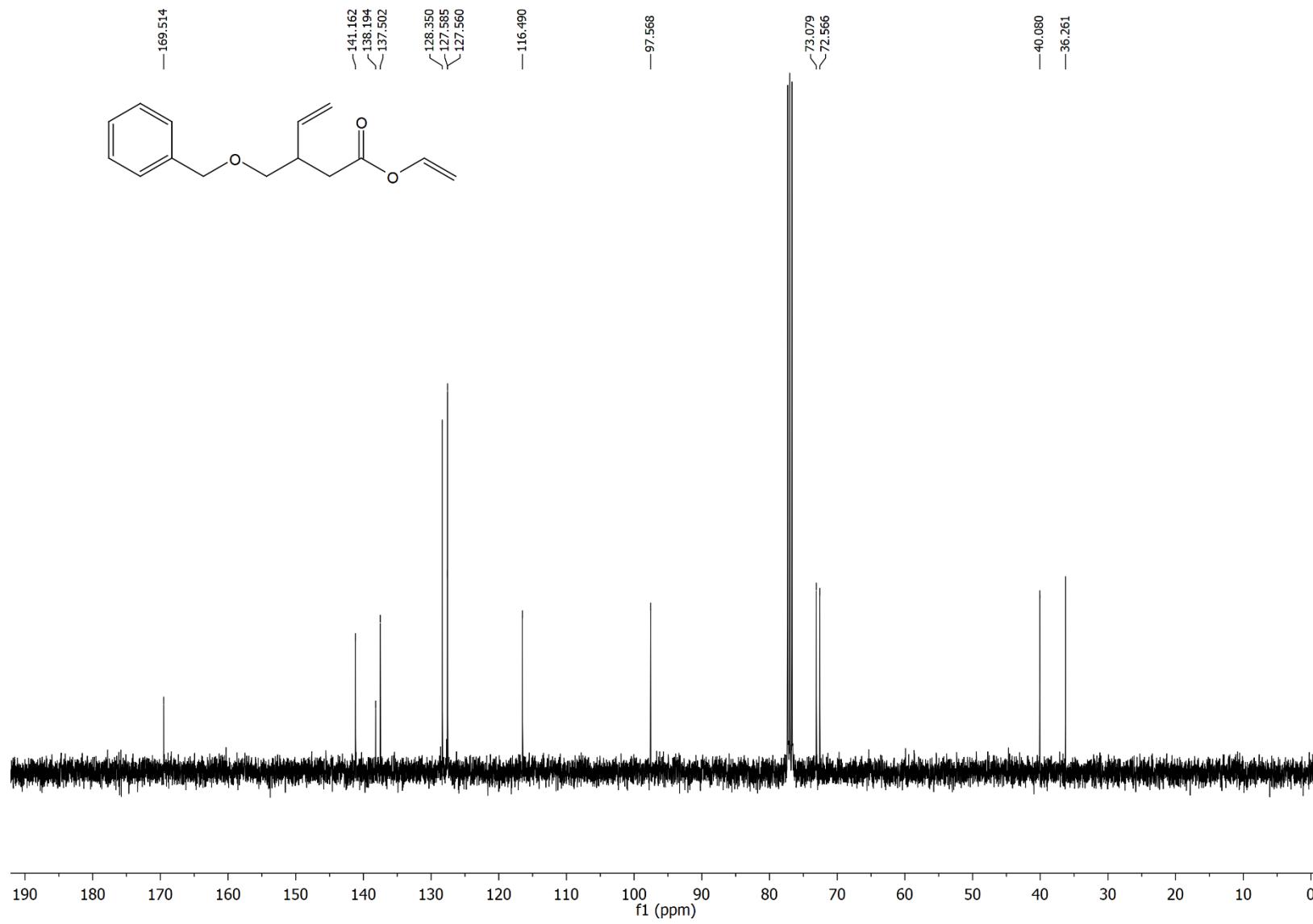


Vinyl 3-(benzyloxymethyl)-4-pentenoate (2h)

¹H NMR (400 MHz, CDCl₃)

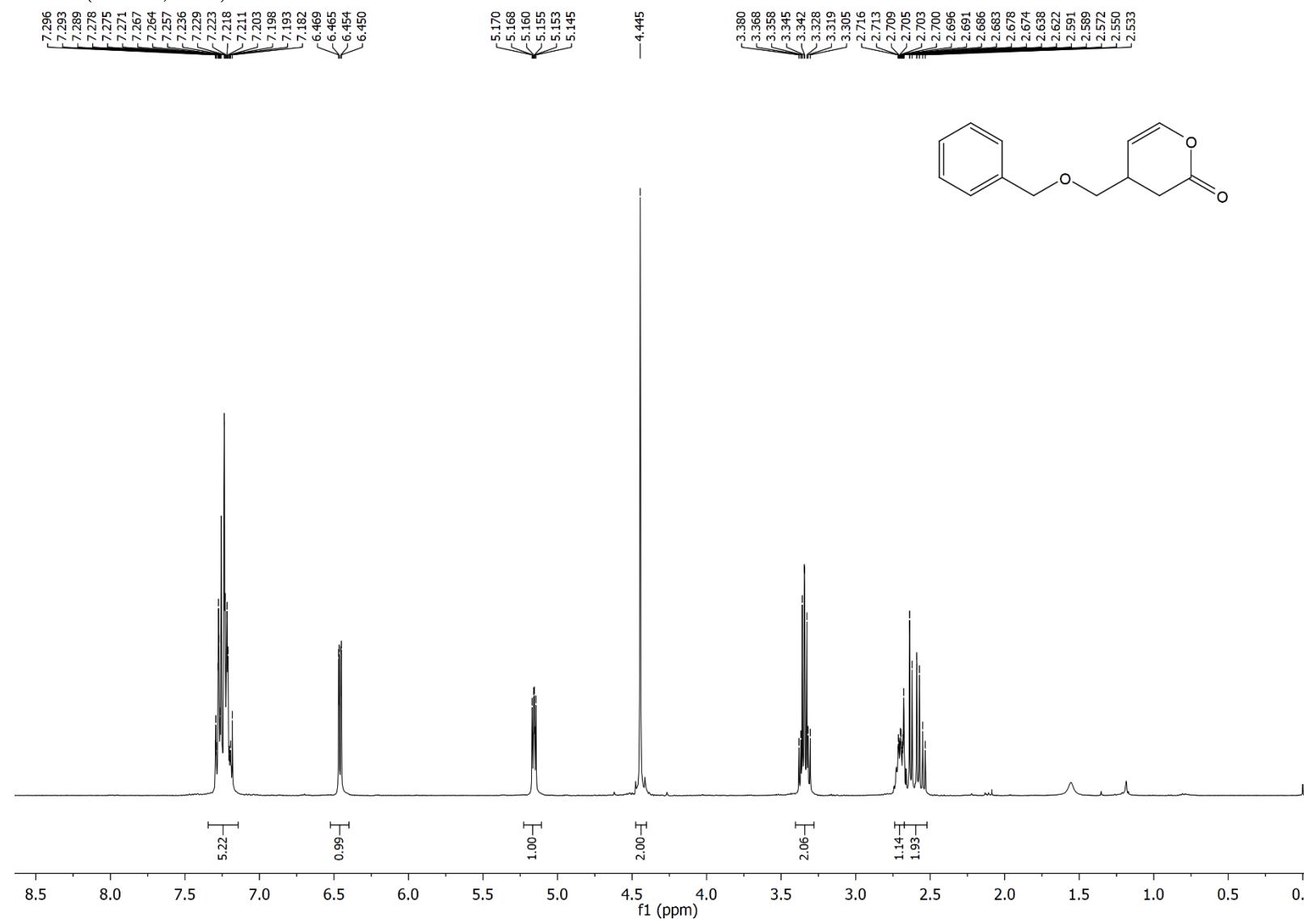


¹³C NMR (100 MHz, CDCl₃)

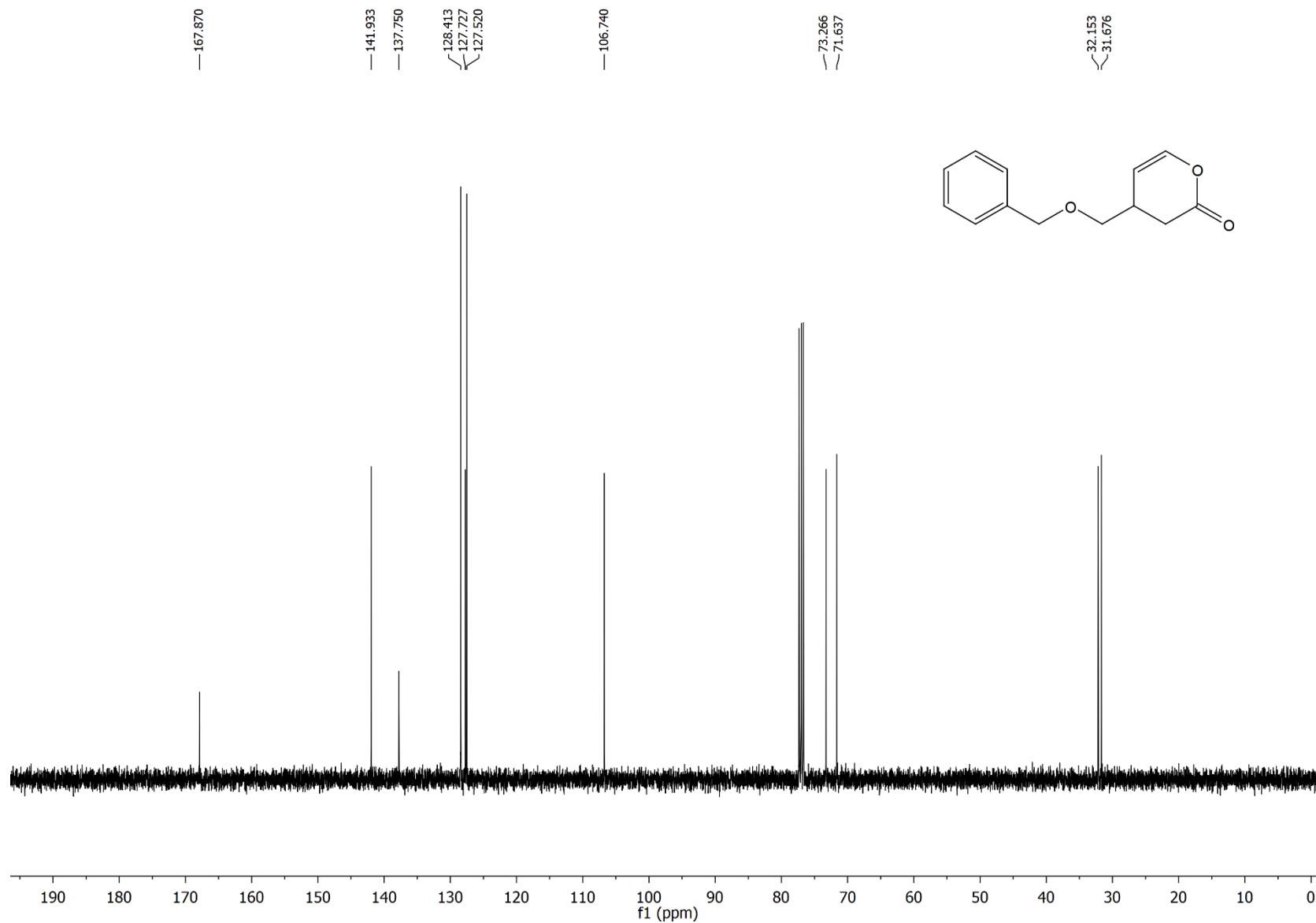


4-(Benzylloxymethyl) -3,4-dihydro-2H-pyran-2-one (3h)

¹H NMR (400 MHz, CDCl₃)

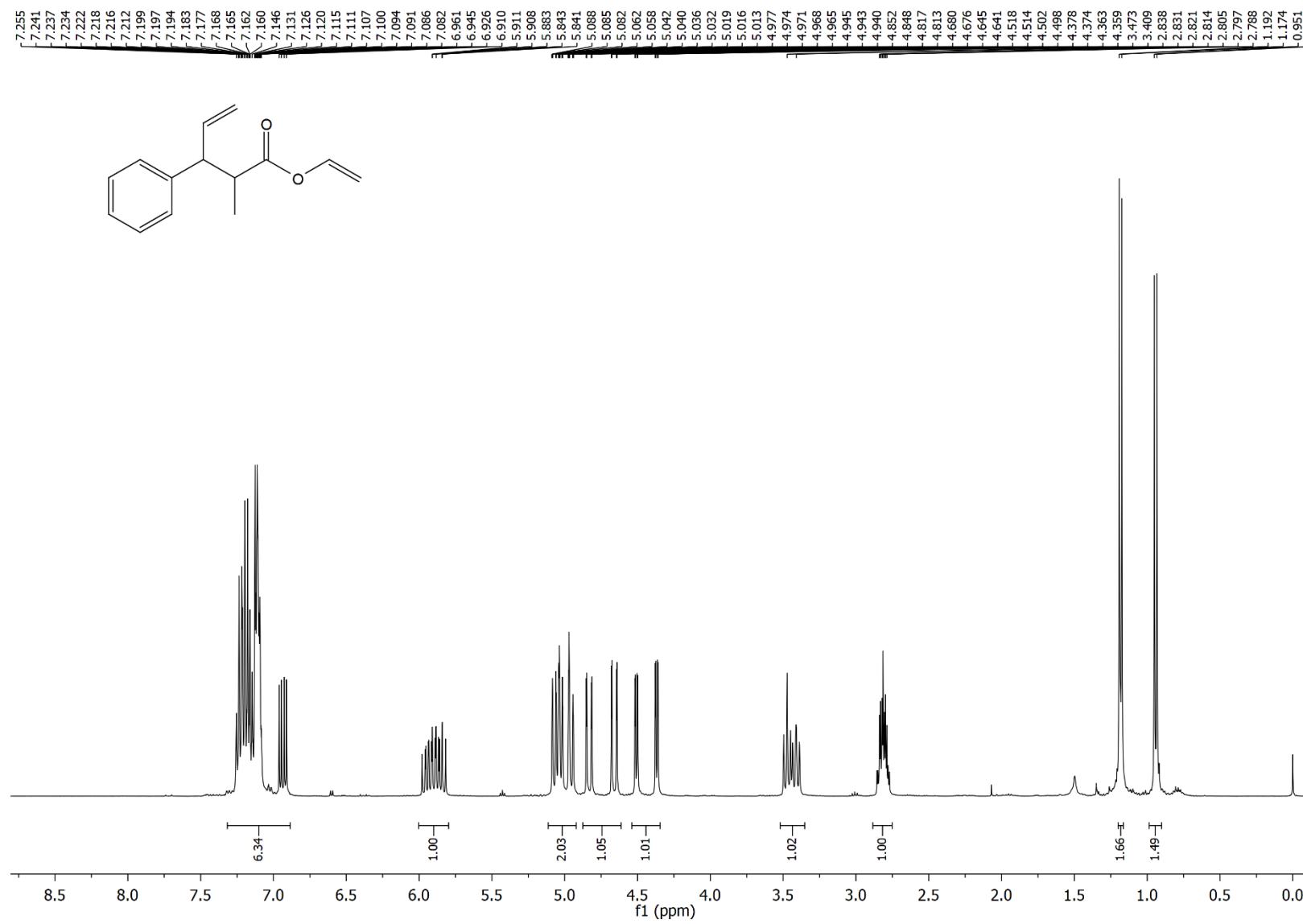


¹³C NMR (100 MHz, CDCl₃)

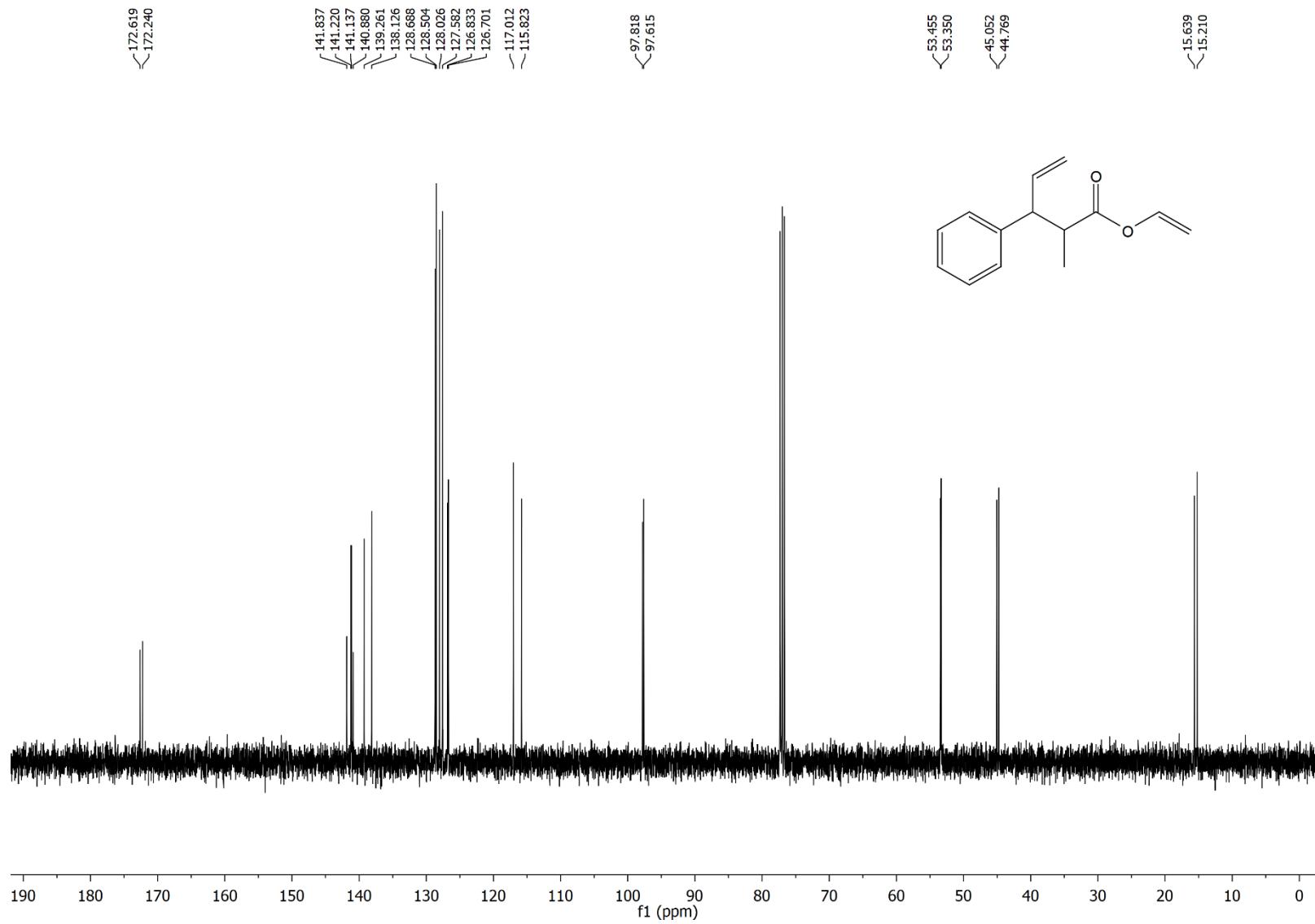


Vinyl 2-methyl-3-phenyl-4-pentenoate (2i)

¹H NMR (400 MHz, CDCl₃)



¹³C NMR (100 MHz, CDCl₃)

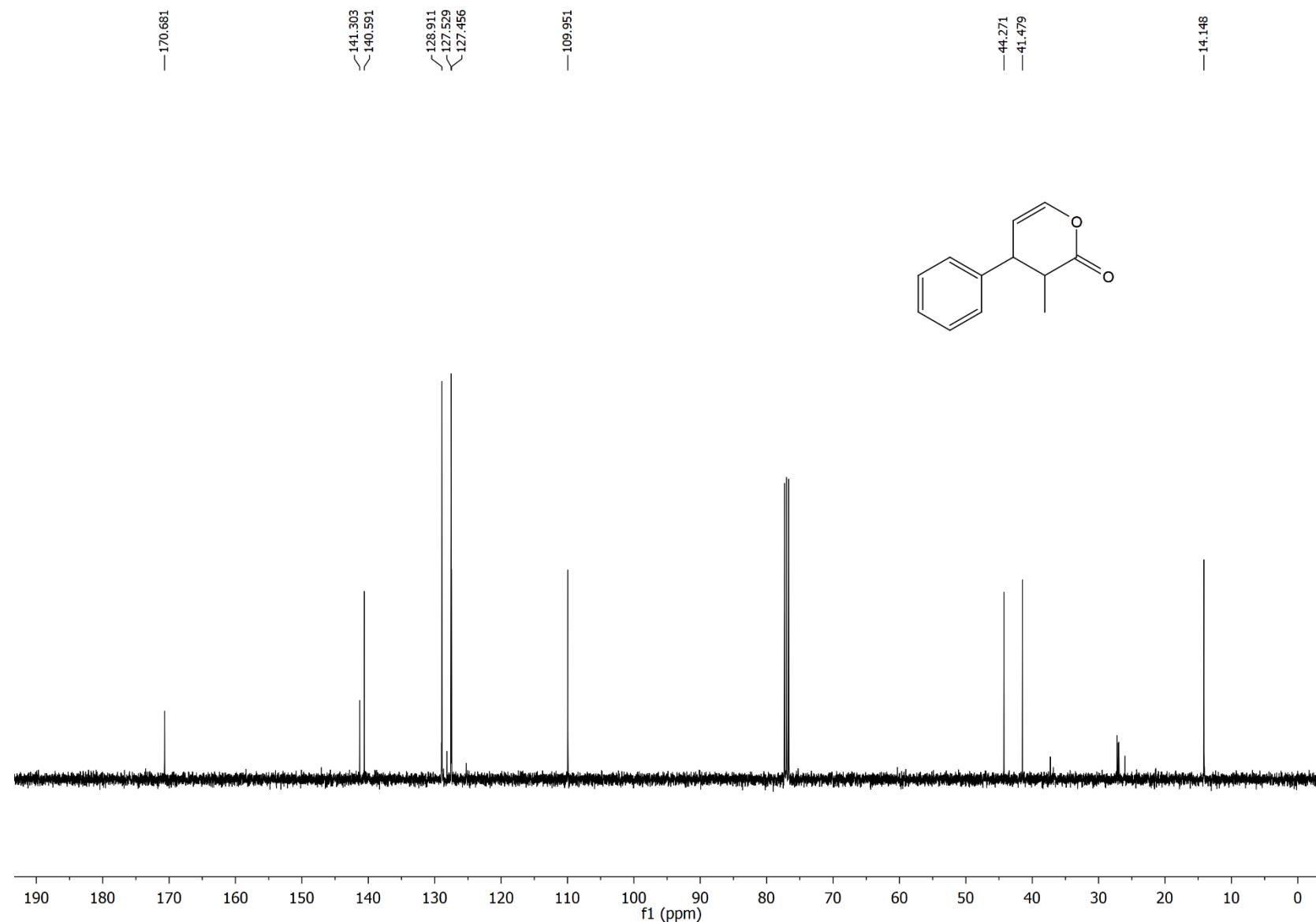


Trans-4-phenyl-5-methyl-3,4-dihydro-2H-pyran-2-one (3i)

^1H NMR (400 MHz, CDCl_3)

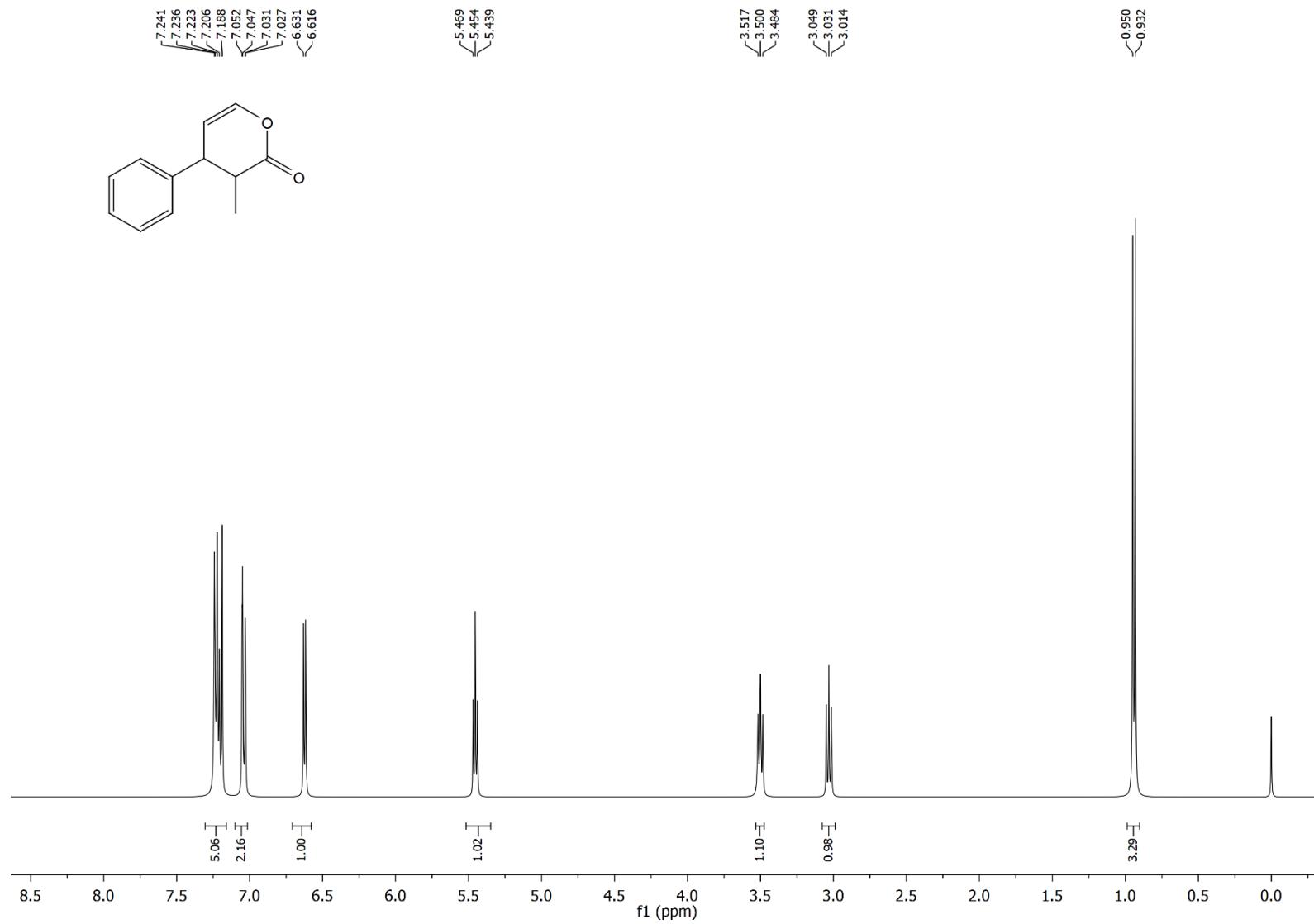
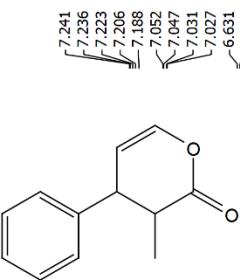


¹³C NMR (100 MHz, CDCl₃)

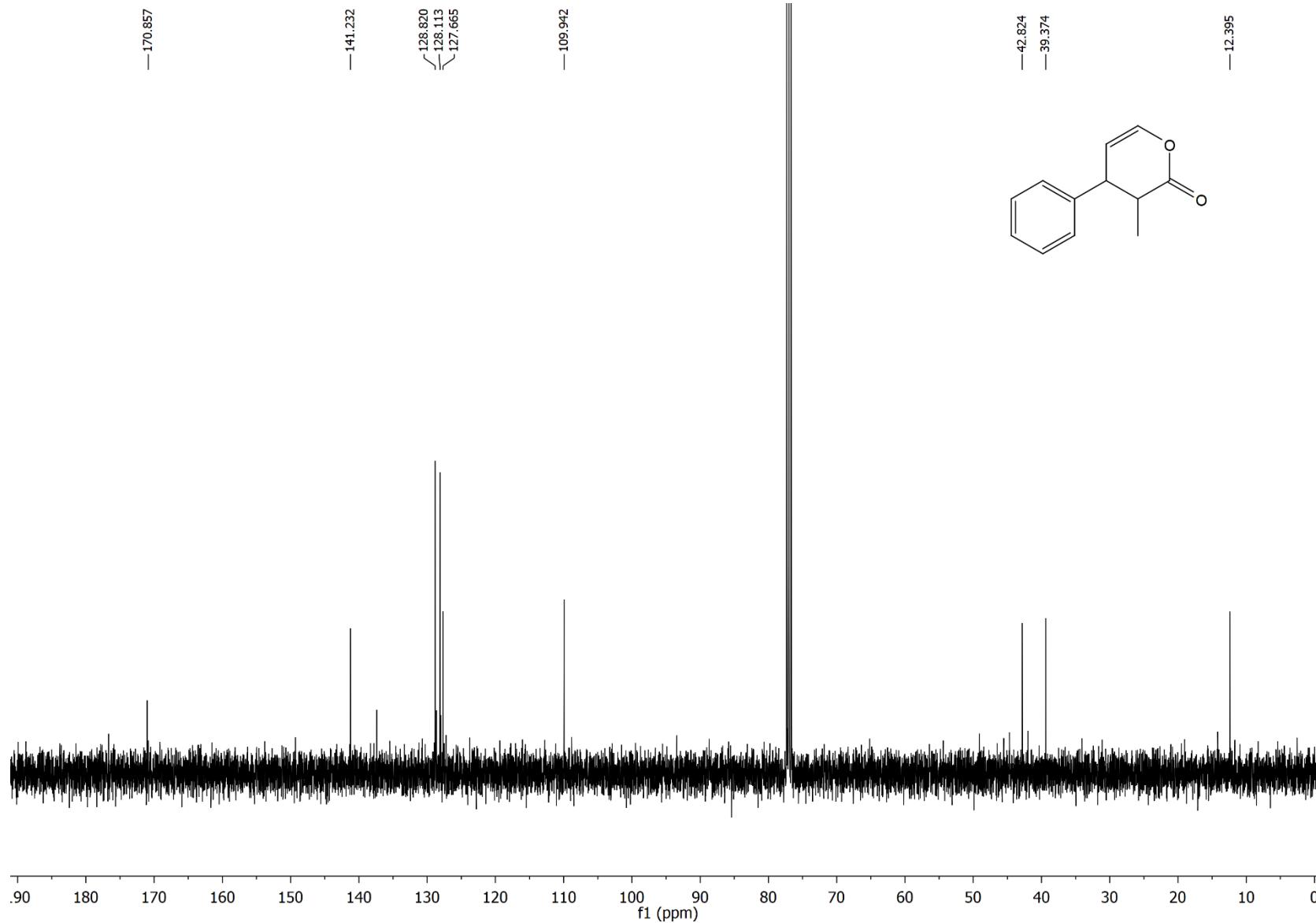


Cis-4-phenyl-5-methyl-3,4-dihydro-2H-pyran-2-one (3i)

¹H NMR (400 MHz, CDCl₃)

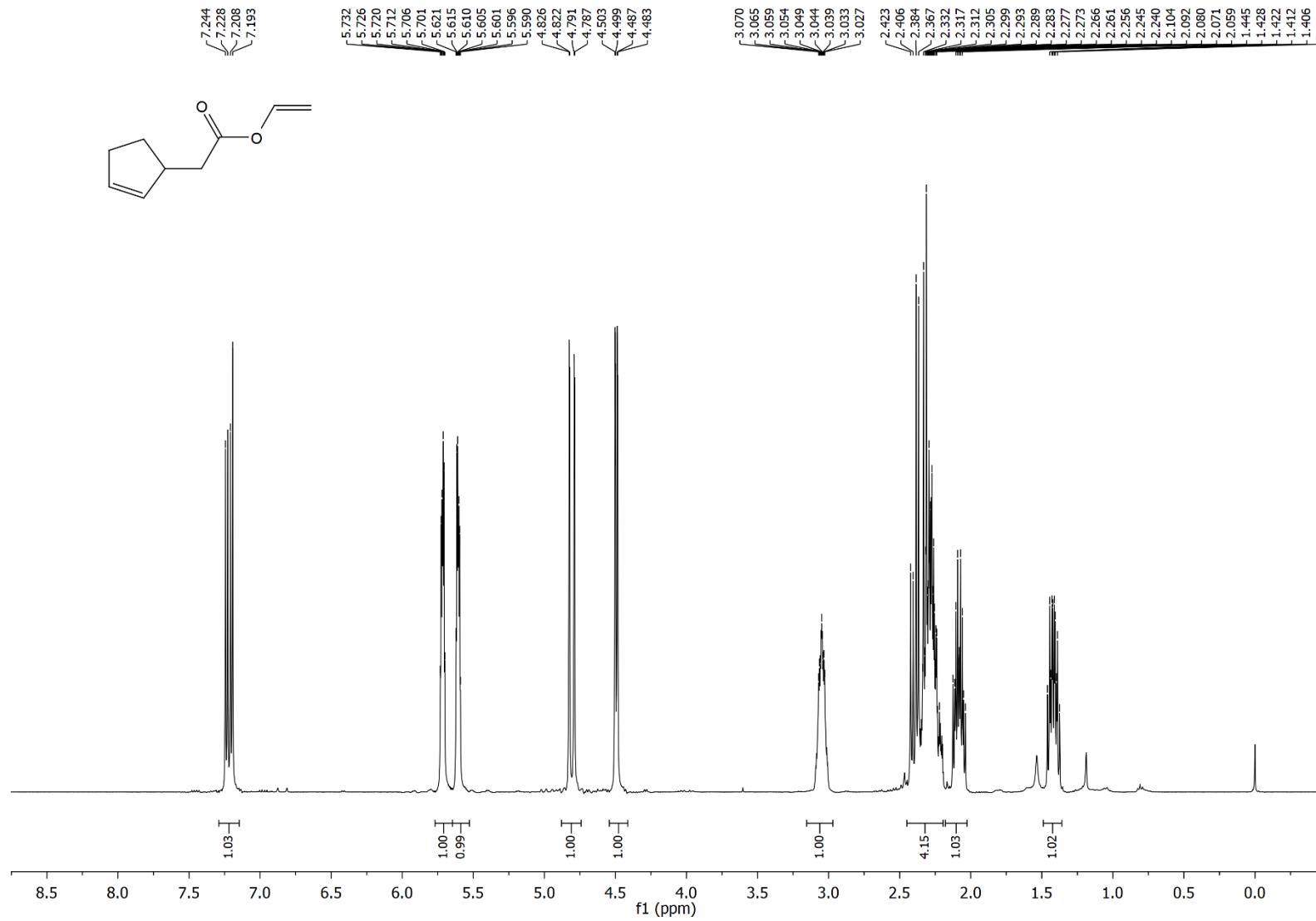


¹³C NMR (100 MHz, CDCl₃)

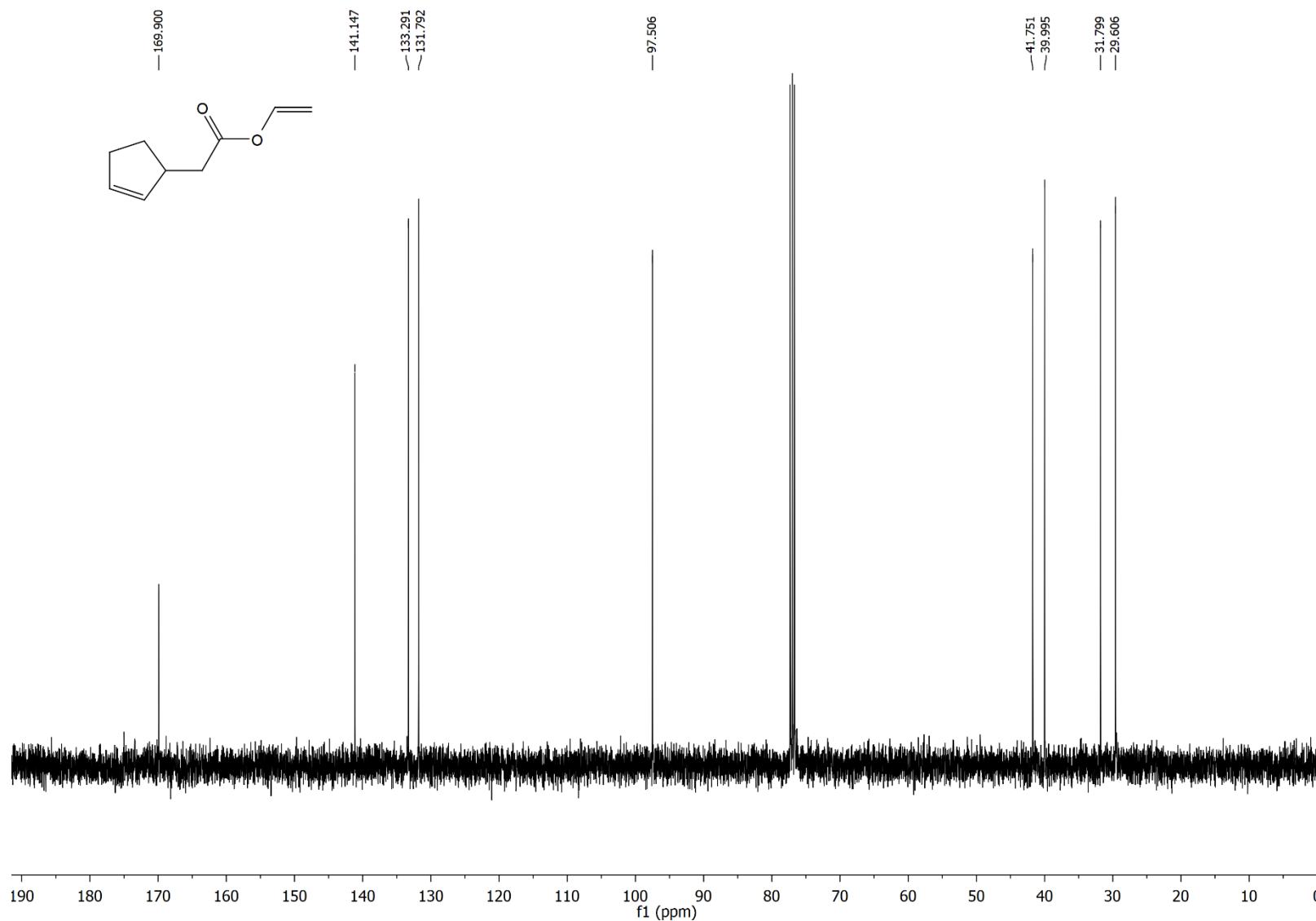


Vinyl 2-cyclopent-1-acetate (2j)

¹H NMR (400 MHz, CDCl₃)

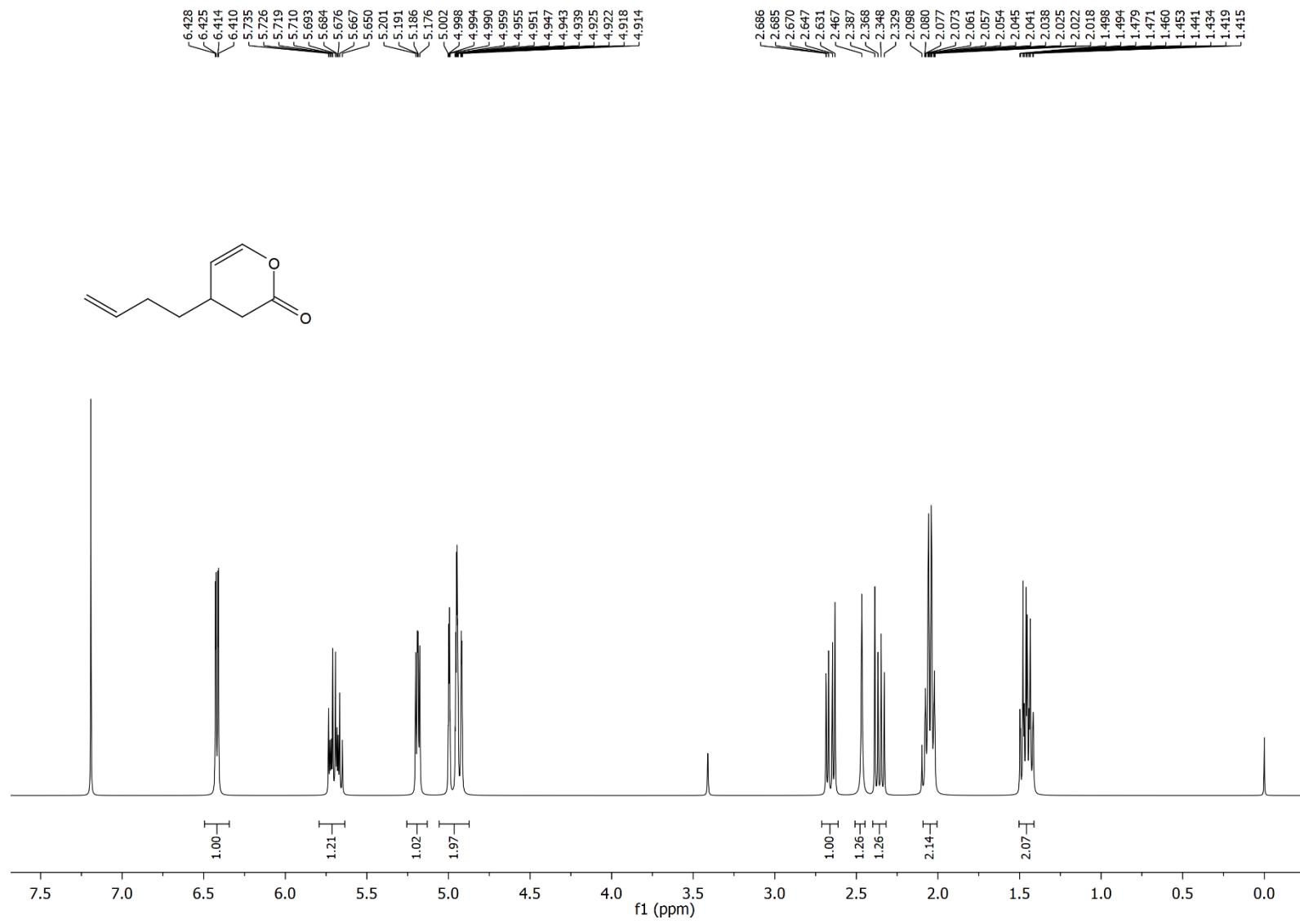


¹³C NMR (100 MHz, CDCl₃)

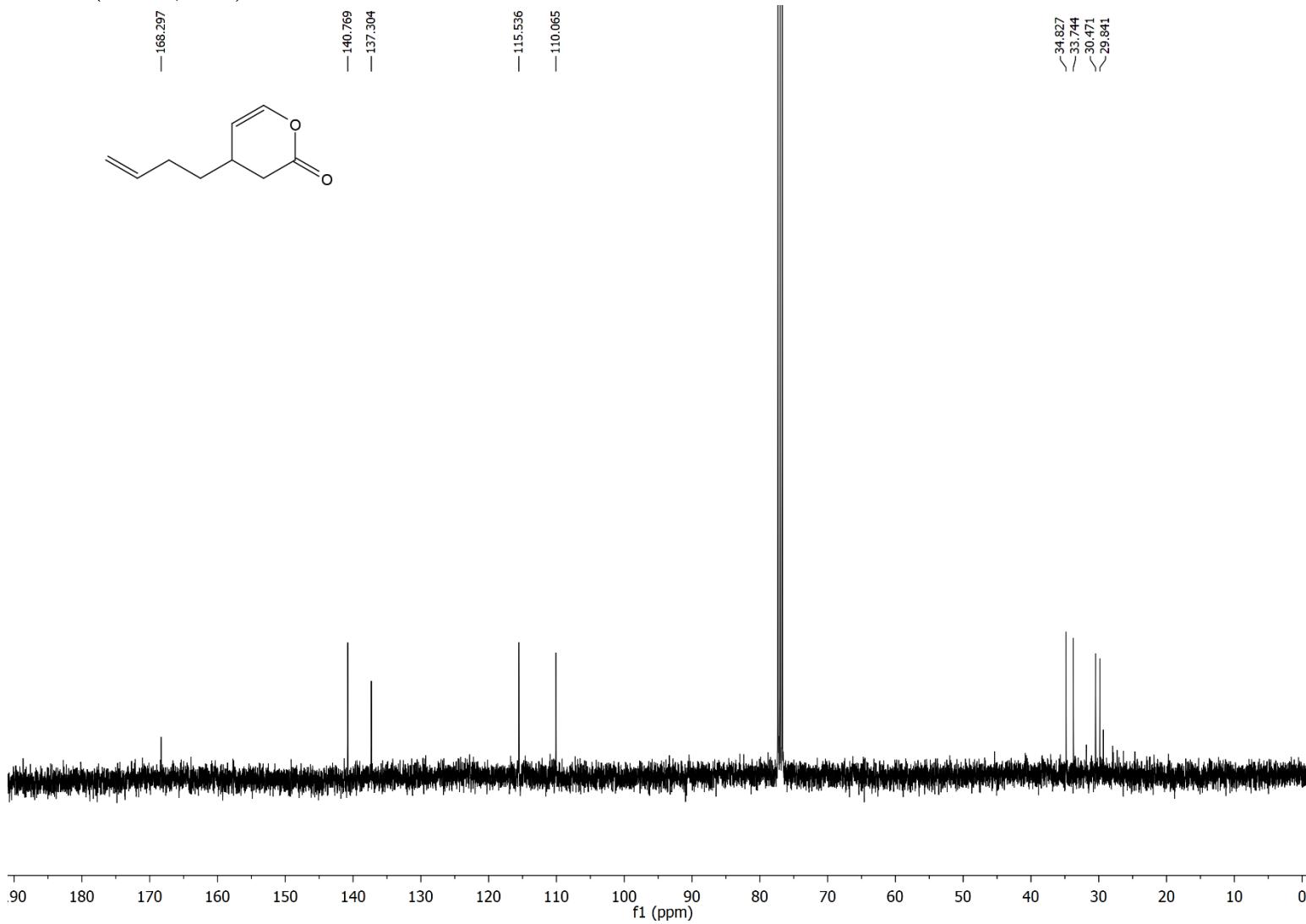


4-(But-3-en-1-yl) -3,4-dihydro-2H-pyran-2-one (3j)

¹H NMR (400 MHz, CDCl₃)

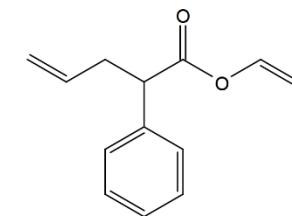
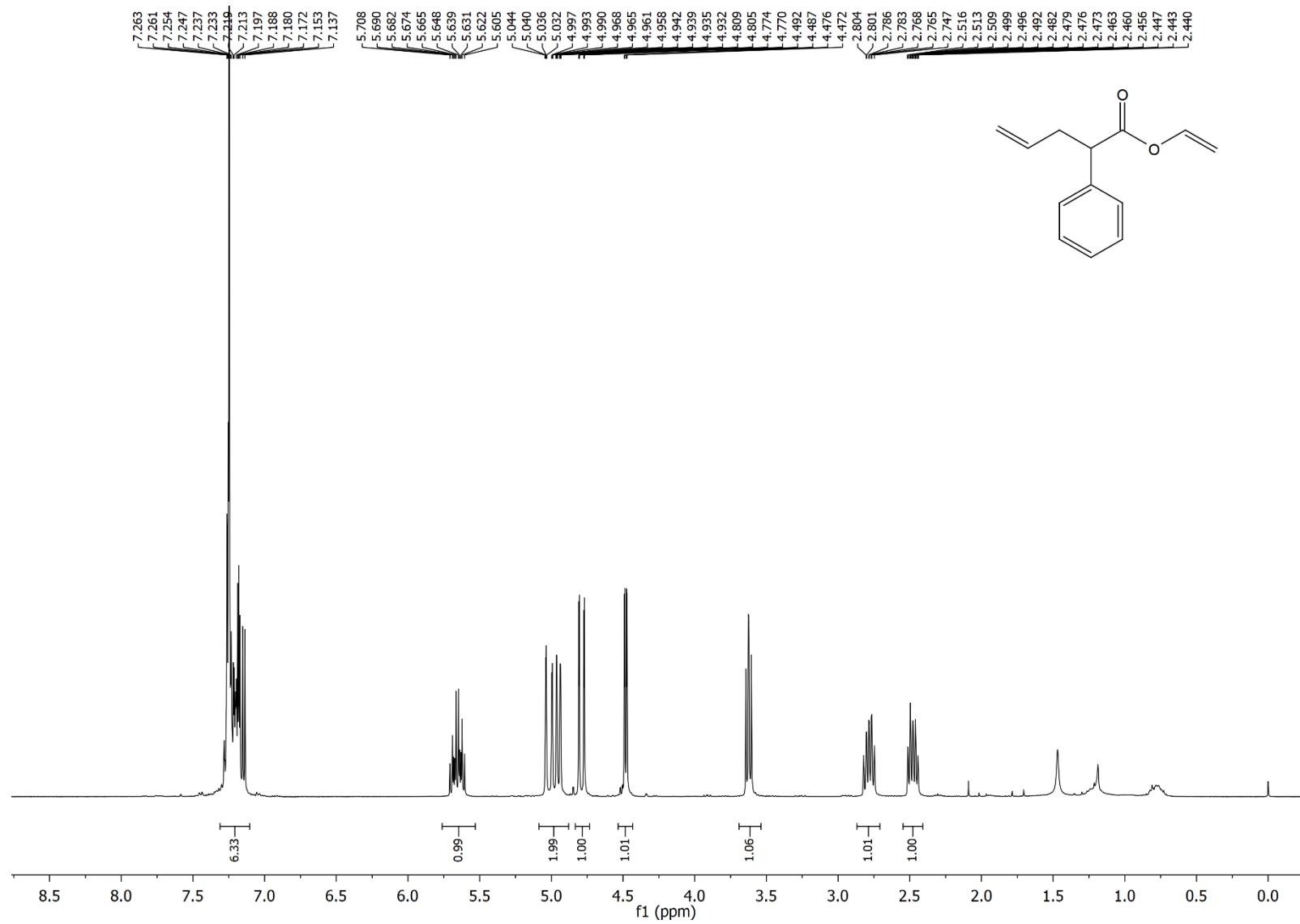


¹³C NMR (100 MHz, CDCl₃)

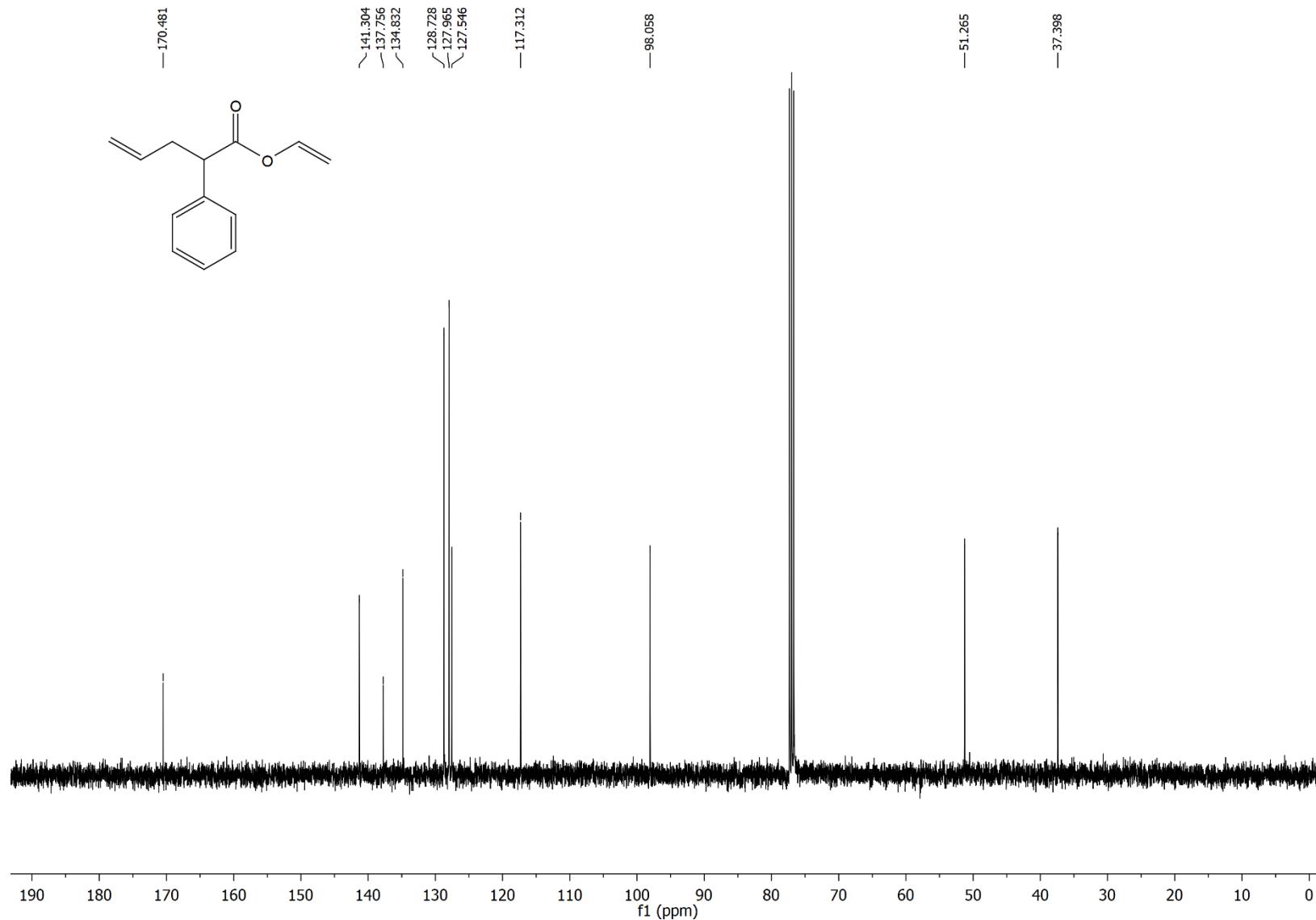


Vinyl 2-phenyl-4-pentenoate (2k)

¹H NMR (400 MHz, CDCl₃)

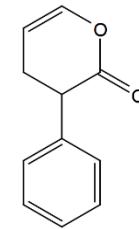
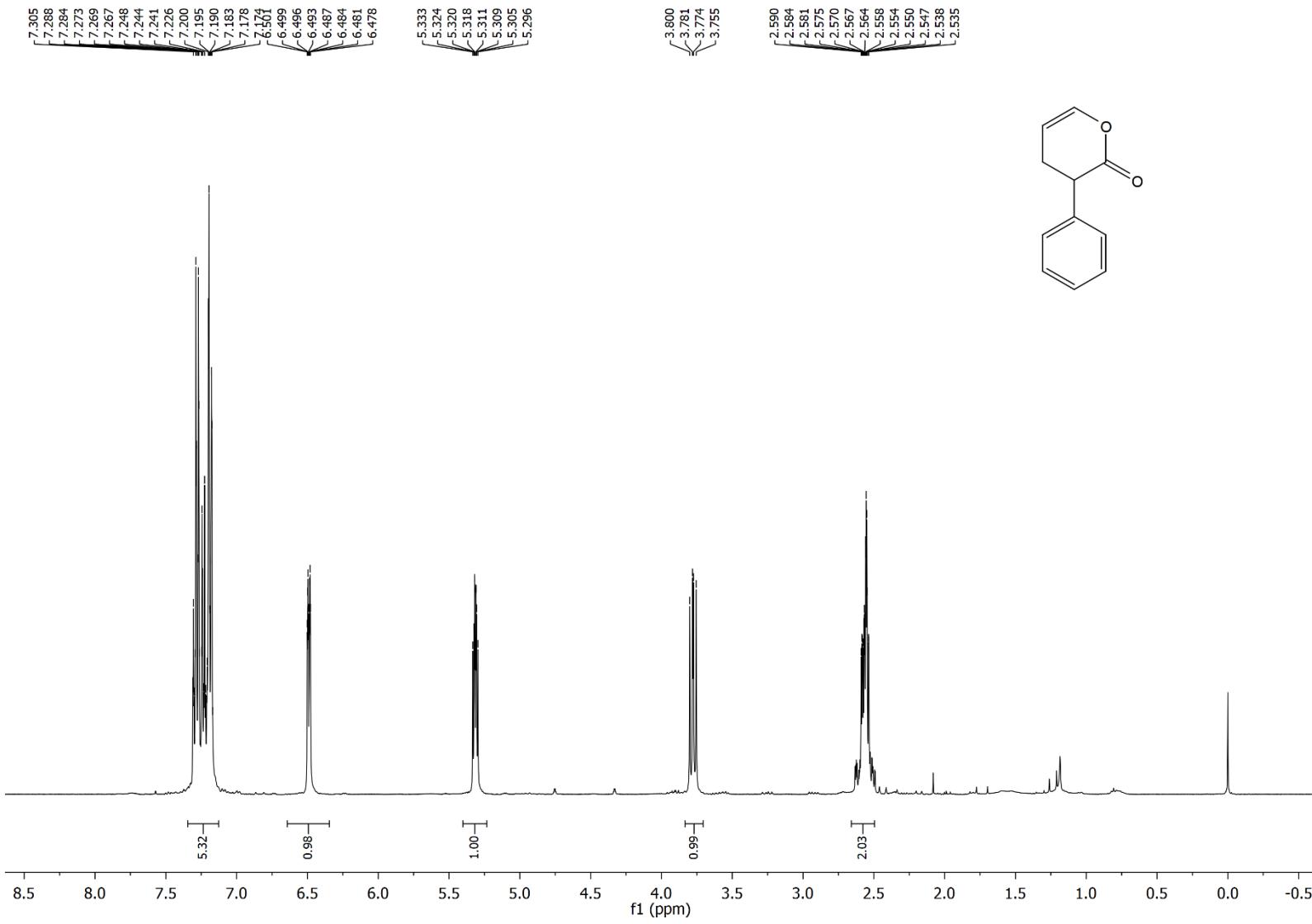


^{13}C NMR (100 MHz , CDCl_3)

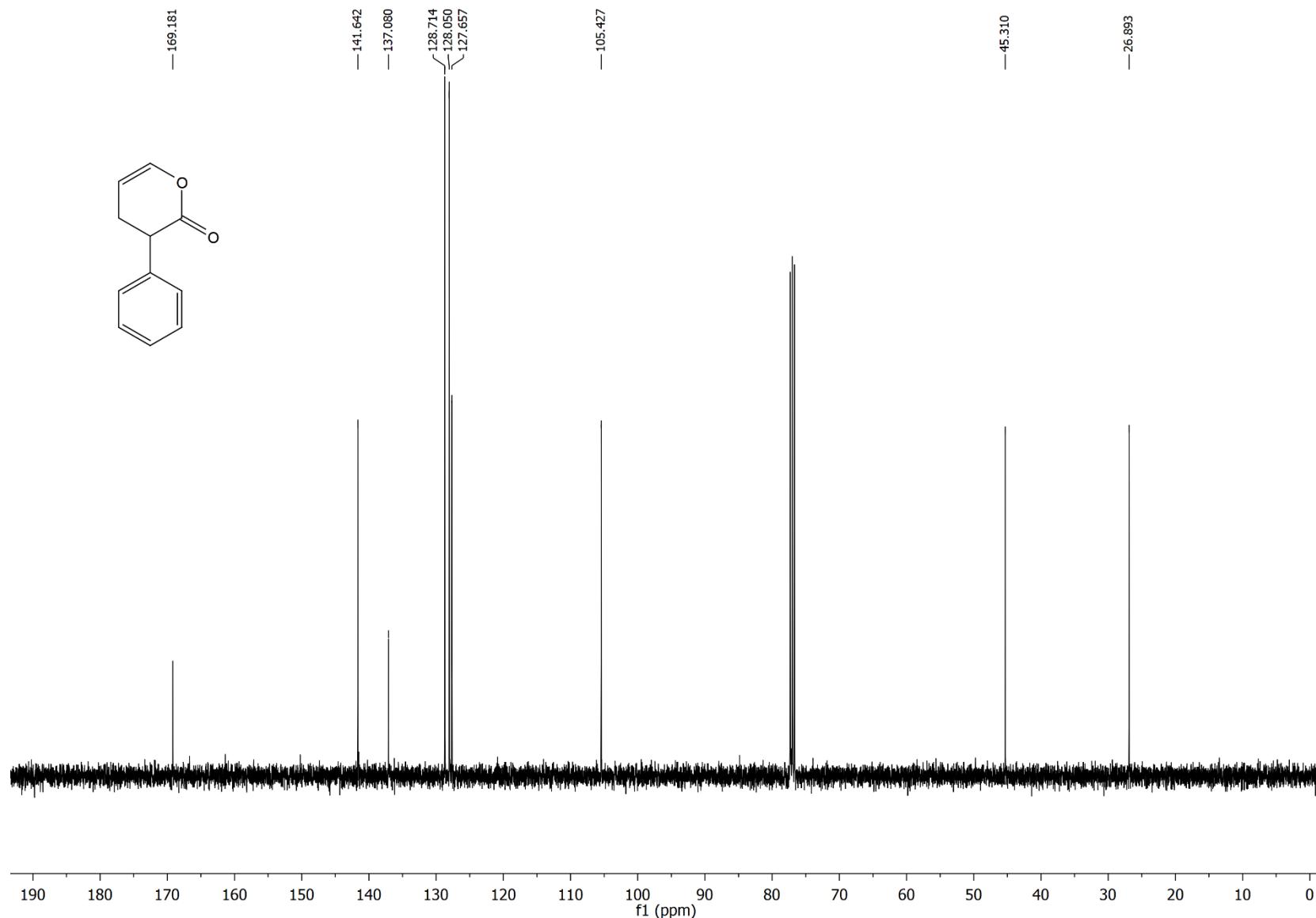


5-Phenyl-3,4-dihydro-2H-pyran-2-one (3k)

¹H NMR (400 MHz, CDCl₃)

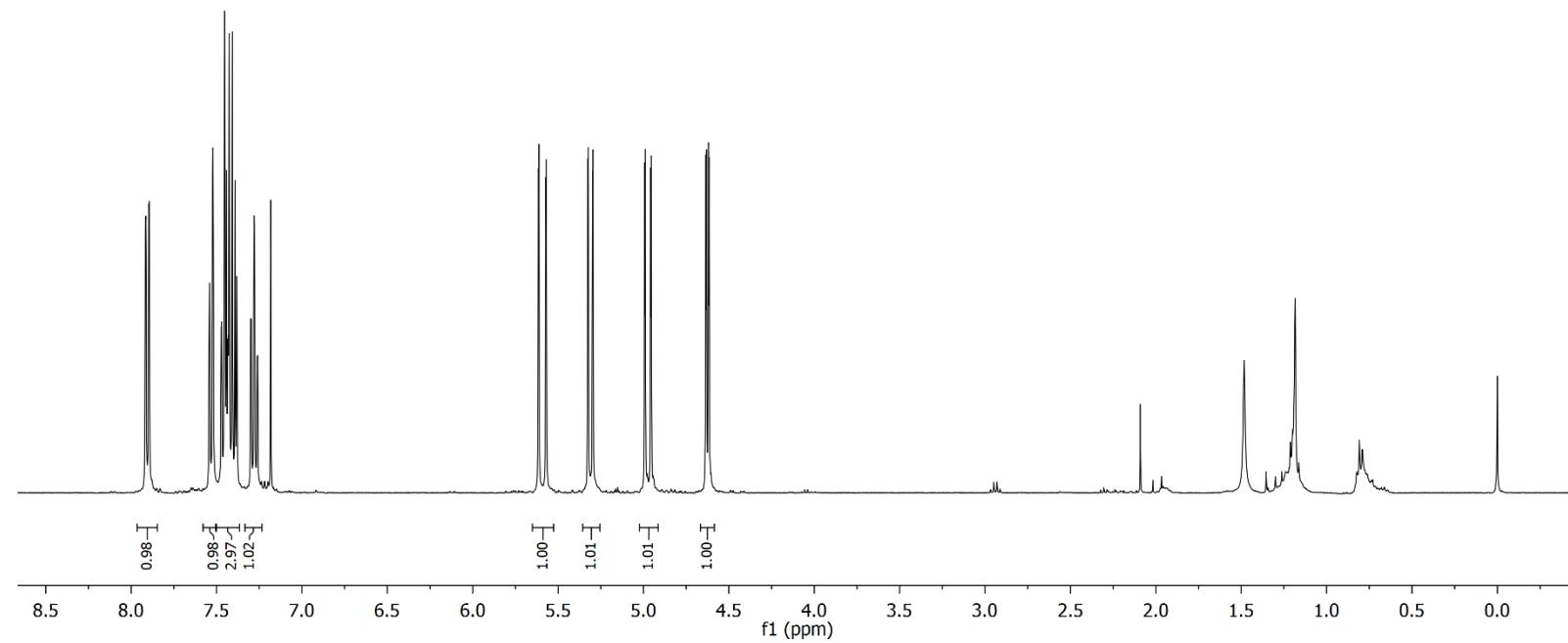
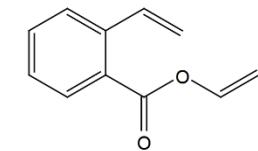
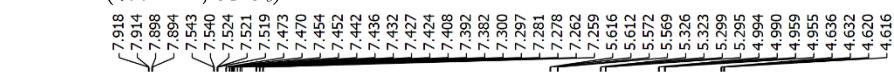


^{13}C NMR ($100\text{ MHz}, \text{CDCl}_3$)

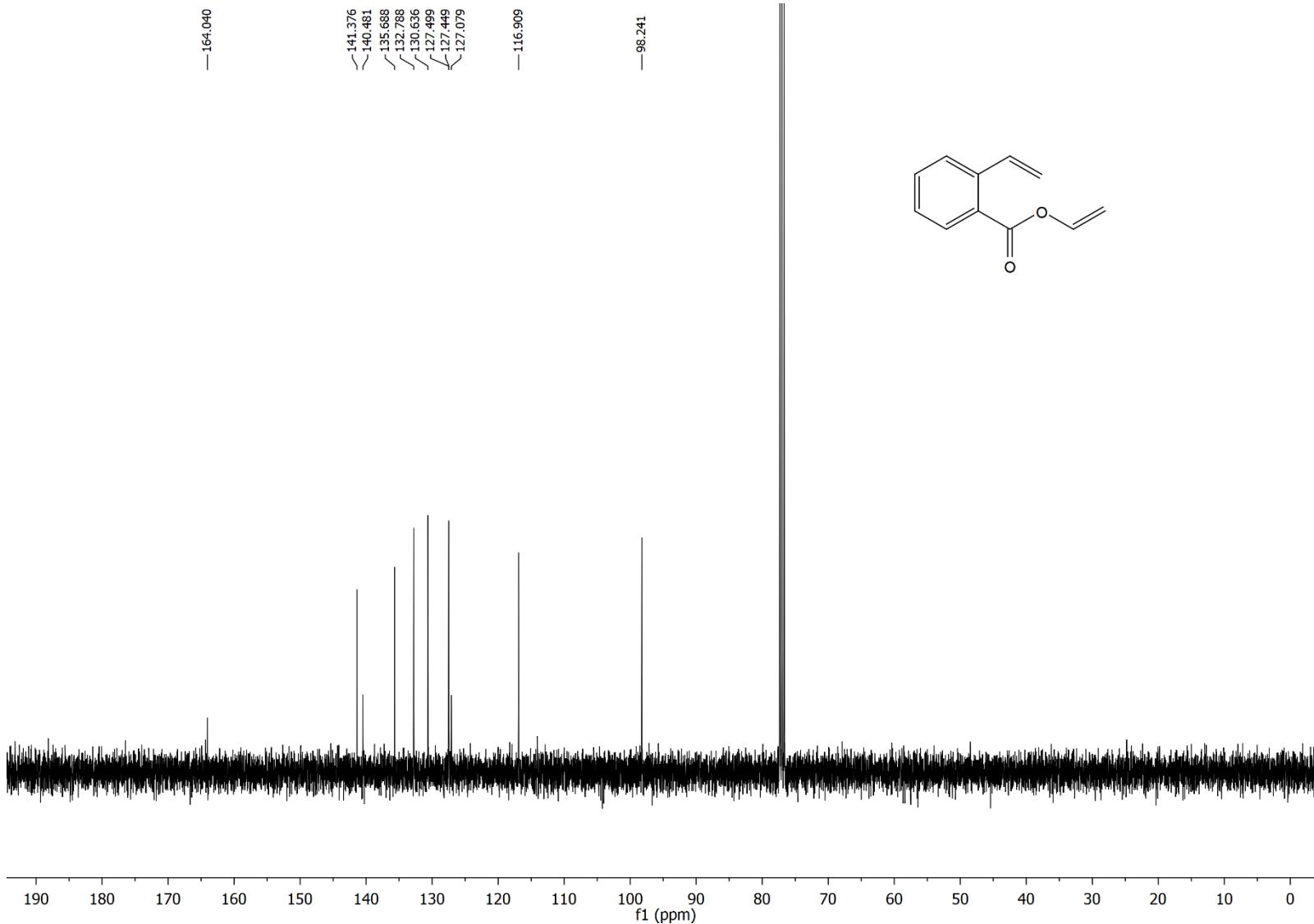


Vinyl 2-vinylbenzoate (2l)

¹H NMR (400 MHz, CDCl₃)



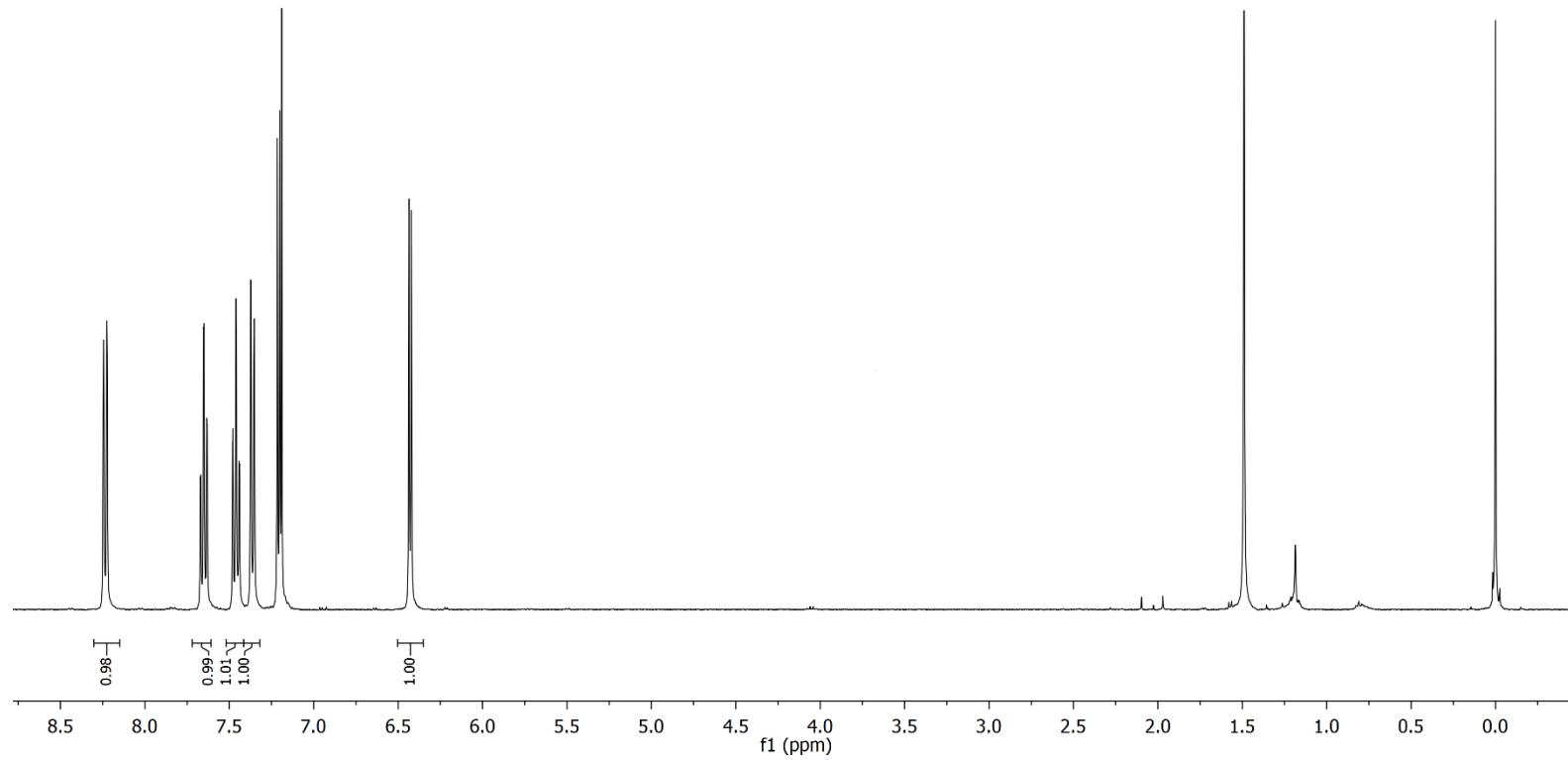
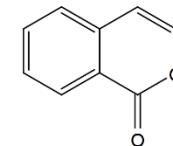
¹³C NMR (100 MHz, CDCl₃)

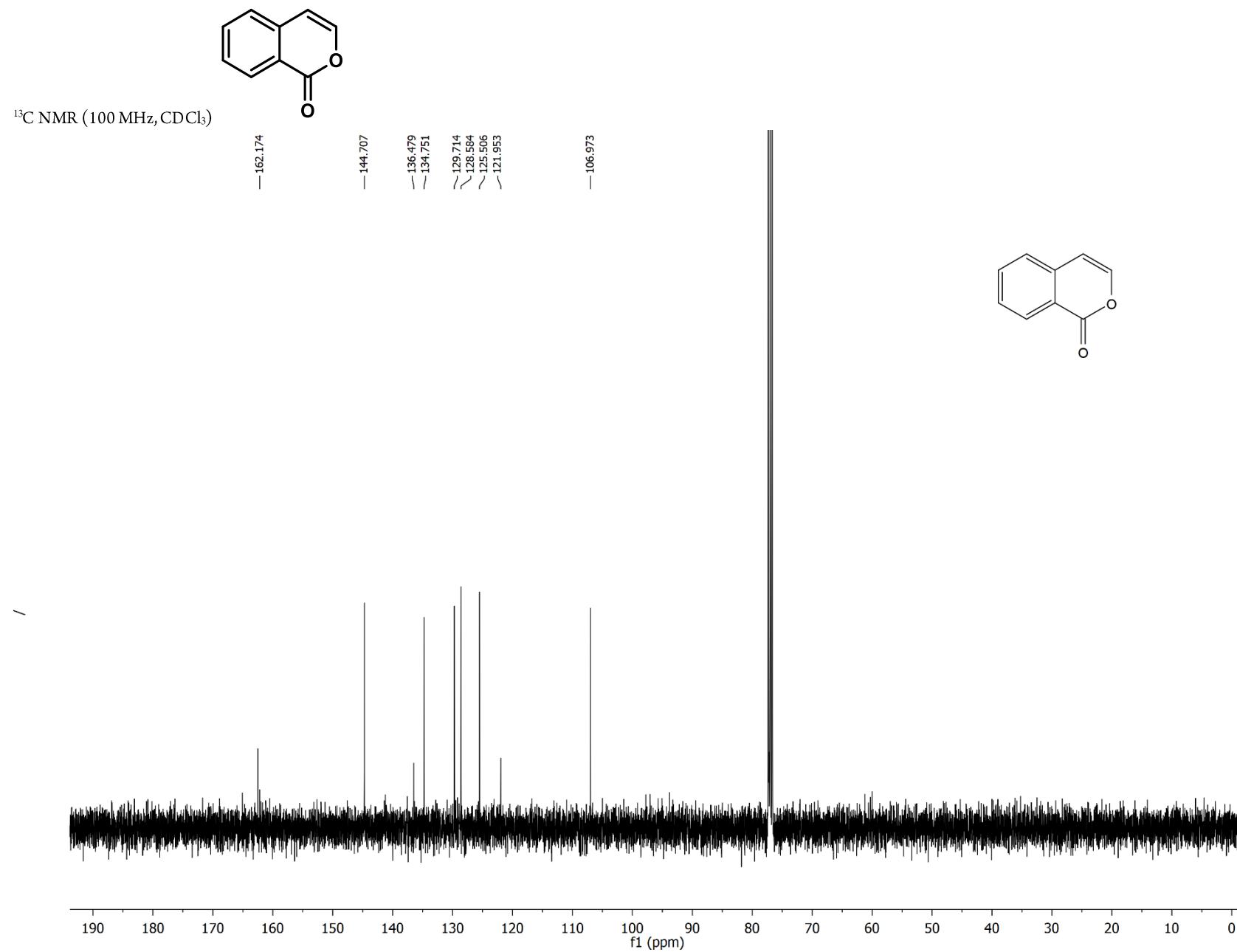


Isocumarin (3l)

^1H NMR (400 MHz, CDCl_3)

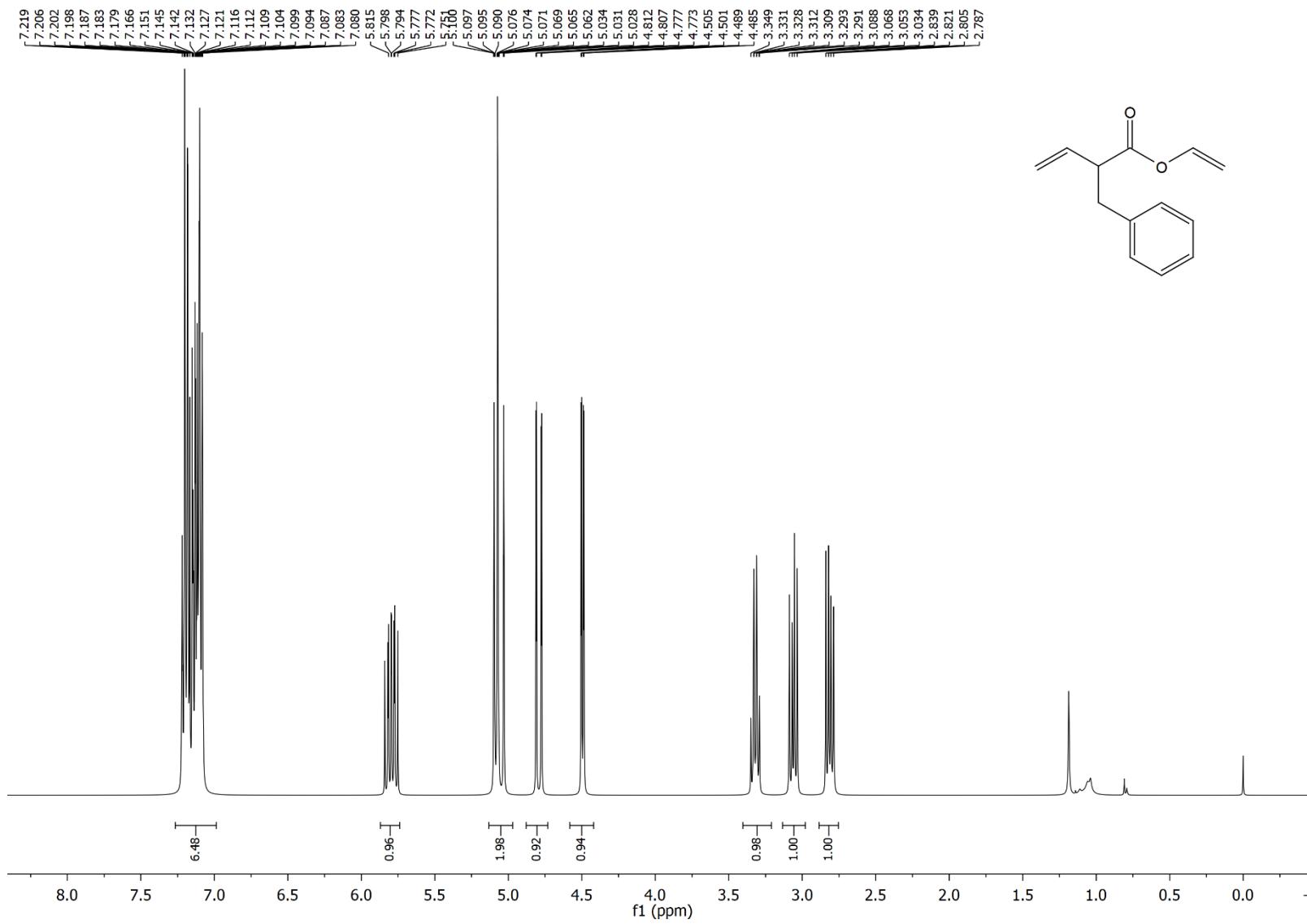
8.247
8.243
8.226
8.223
7.672
7.668
7.653
7.649
7.634
7.630
7.481
7.478
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7.372
7.353
7.215
7.201
7.190
6.436
6.422



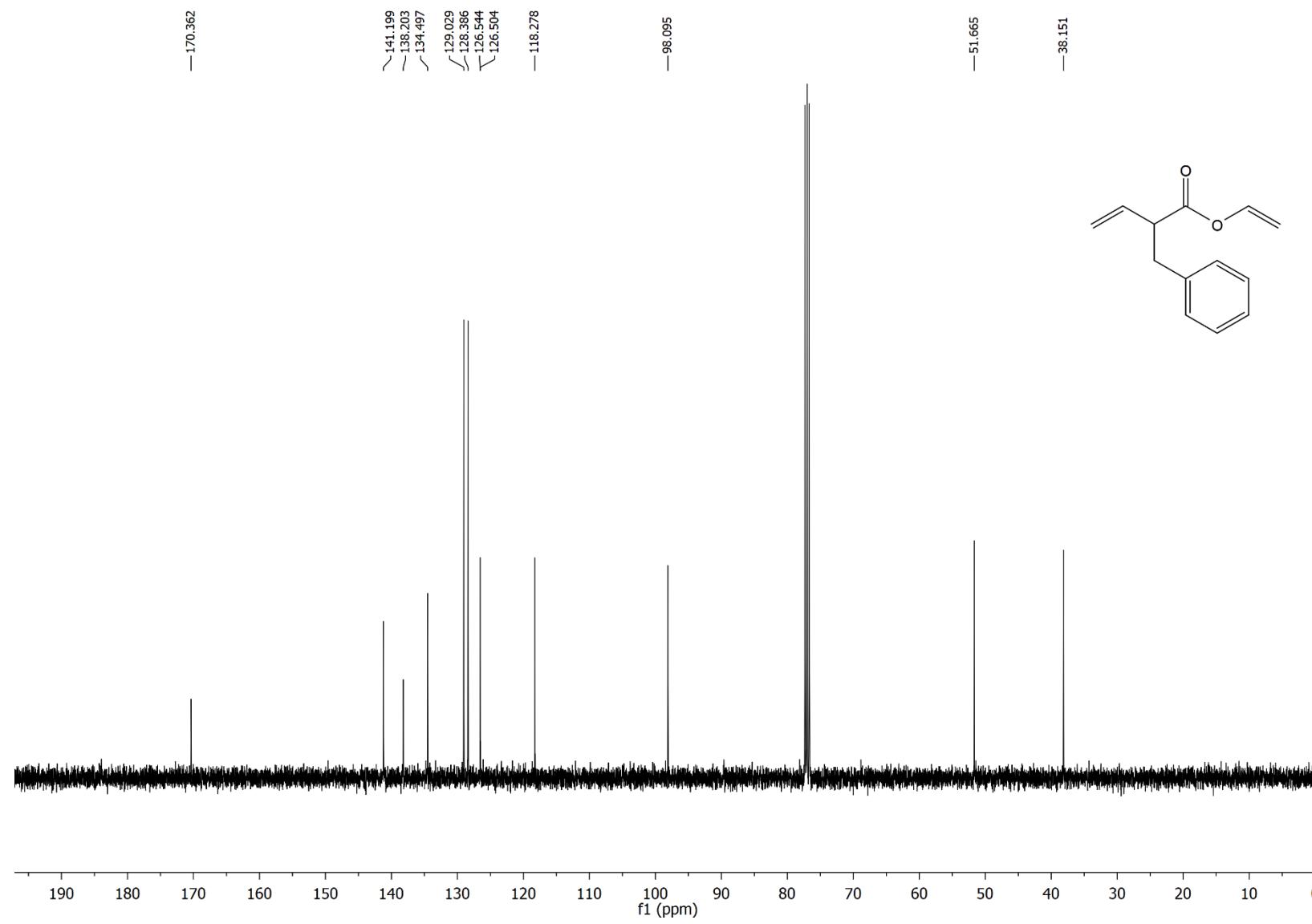


Vinyl 2-benzyl-3-butenoate (2m)

¹H NMR (400 MHz, CDCl₃)

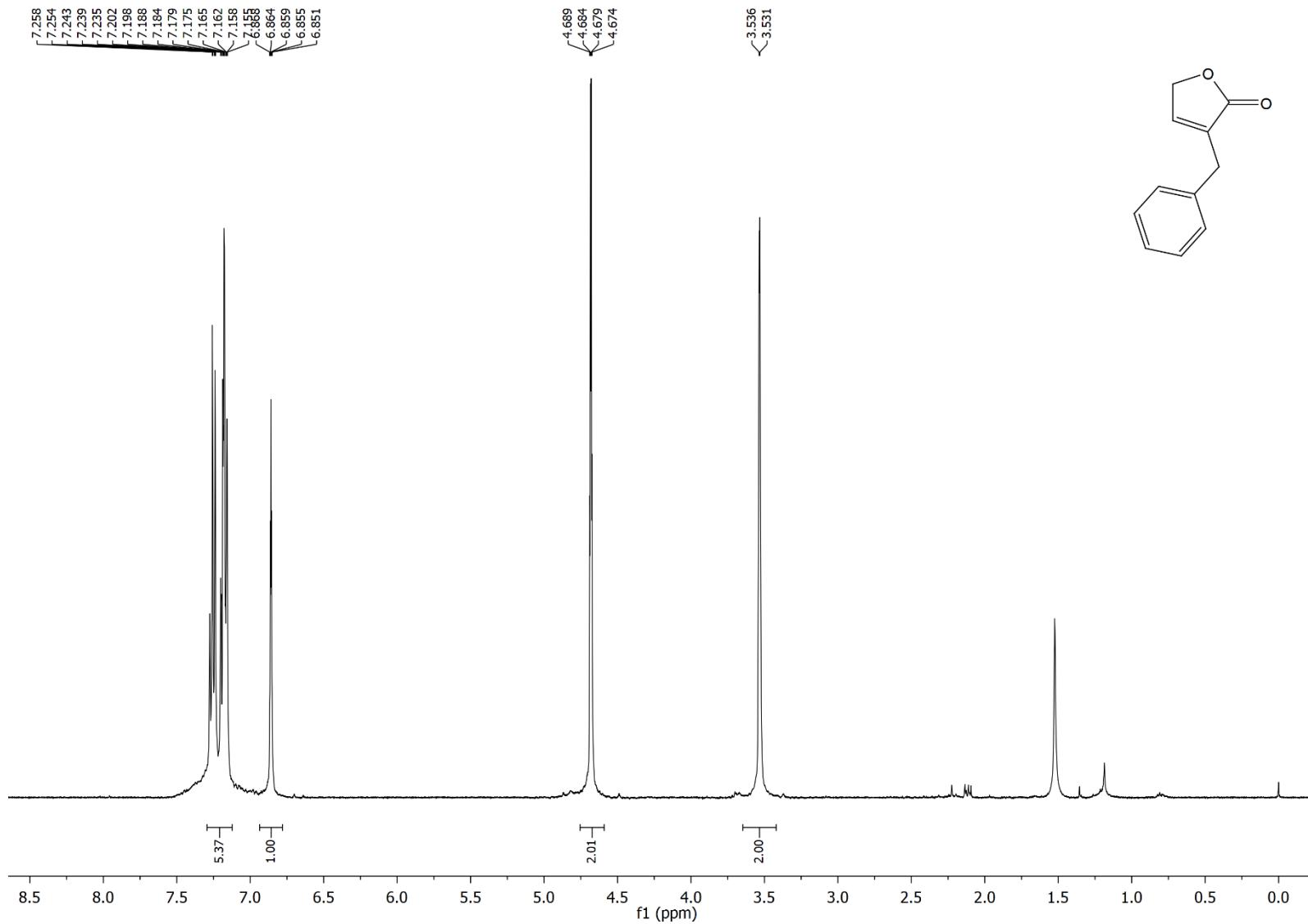


^{13}C NMR (100 MHz, CDCl_3)

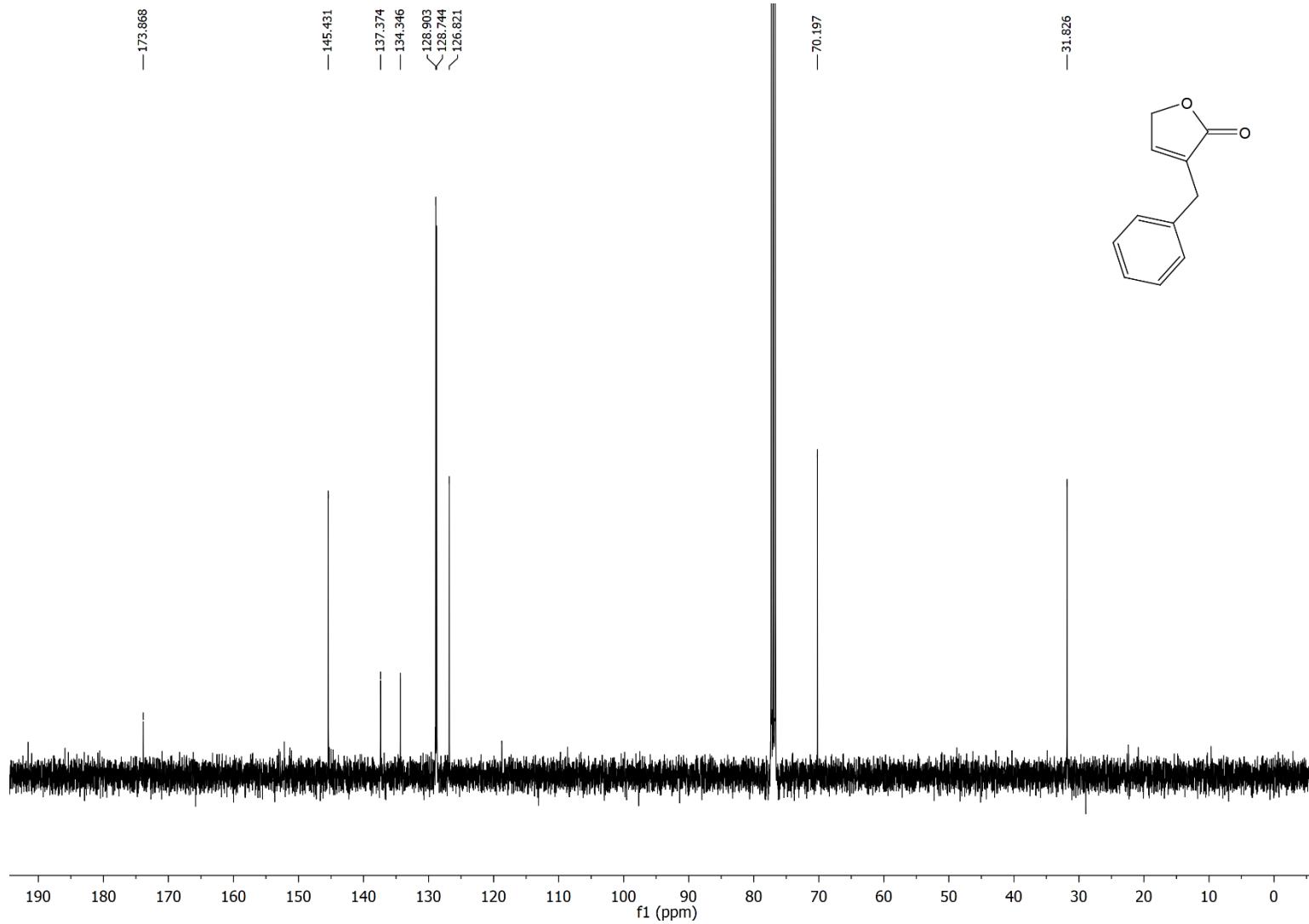


3-(Phenylmethyl)-2(5H)-furanone (3m)

¹H NMR (400 MHz, CDCl₃)

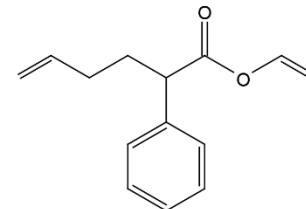
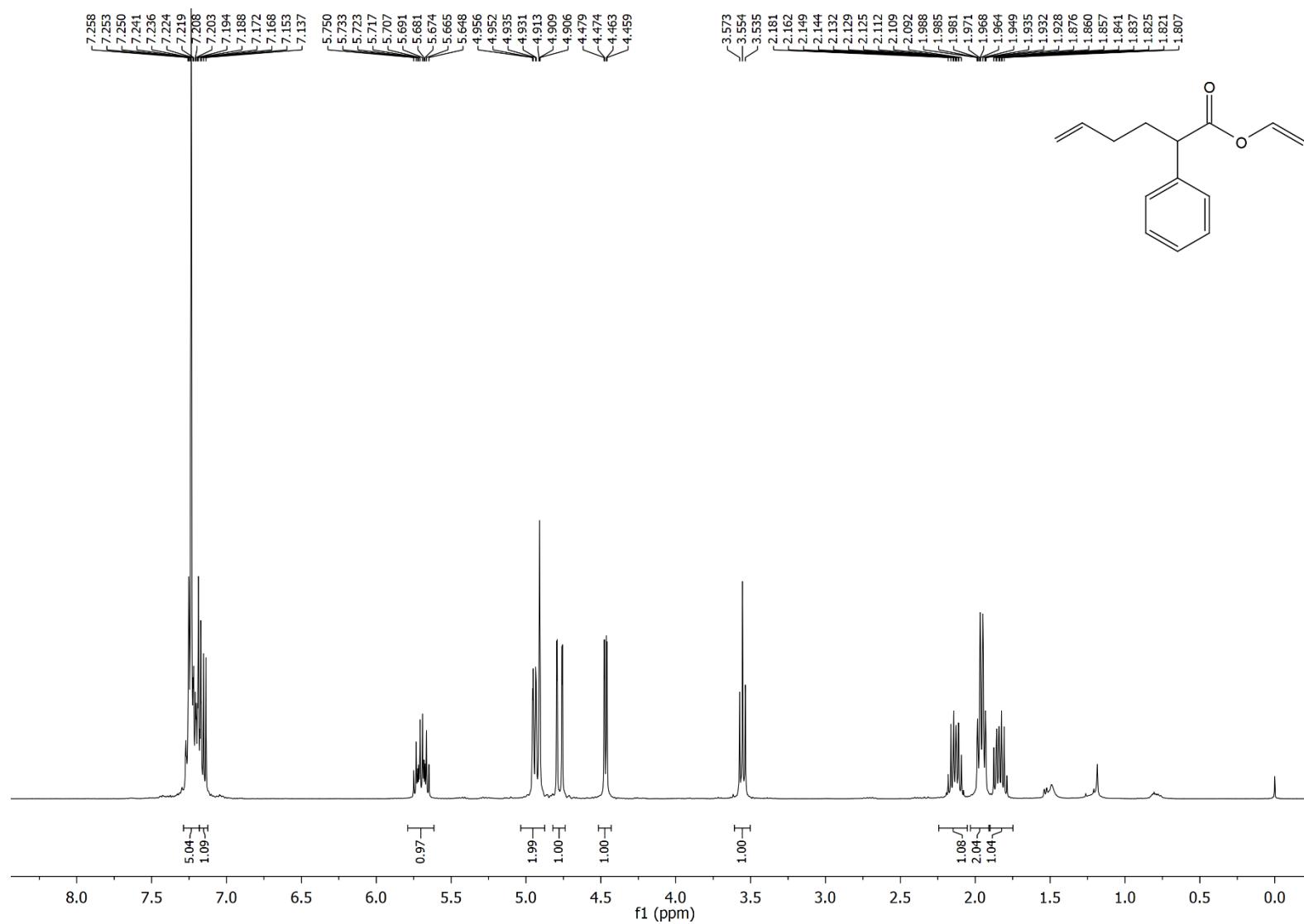


¹³C NMR (100 MHz, CDCl₃)

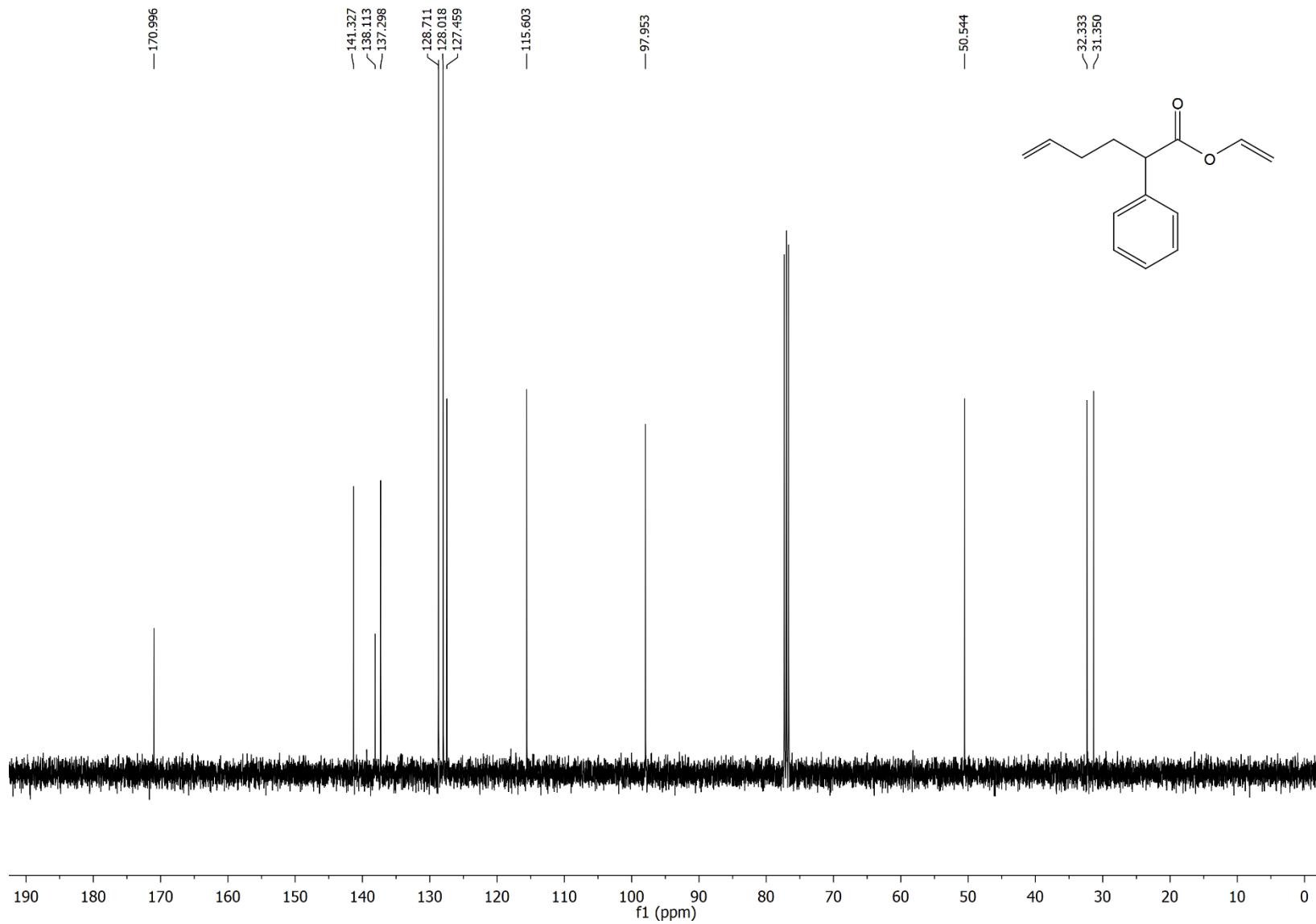


Vinyl 2-phenyl-5-hexenoate (2n)

¹H NMR (400 MHz, CDCl₃)

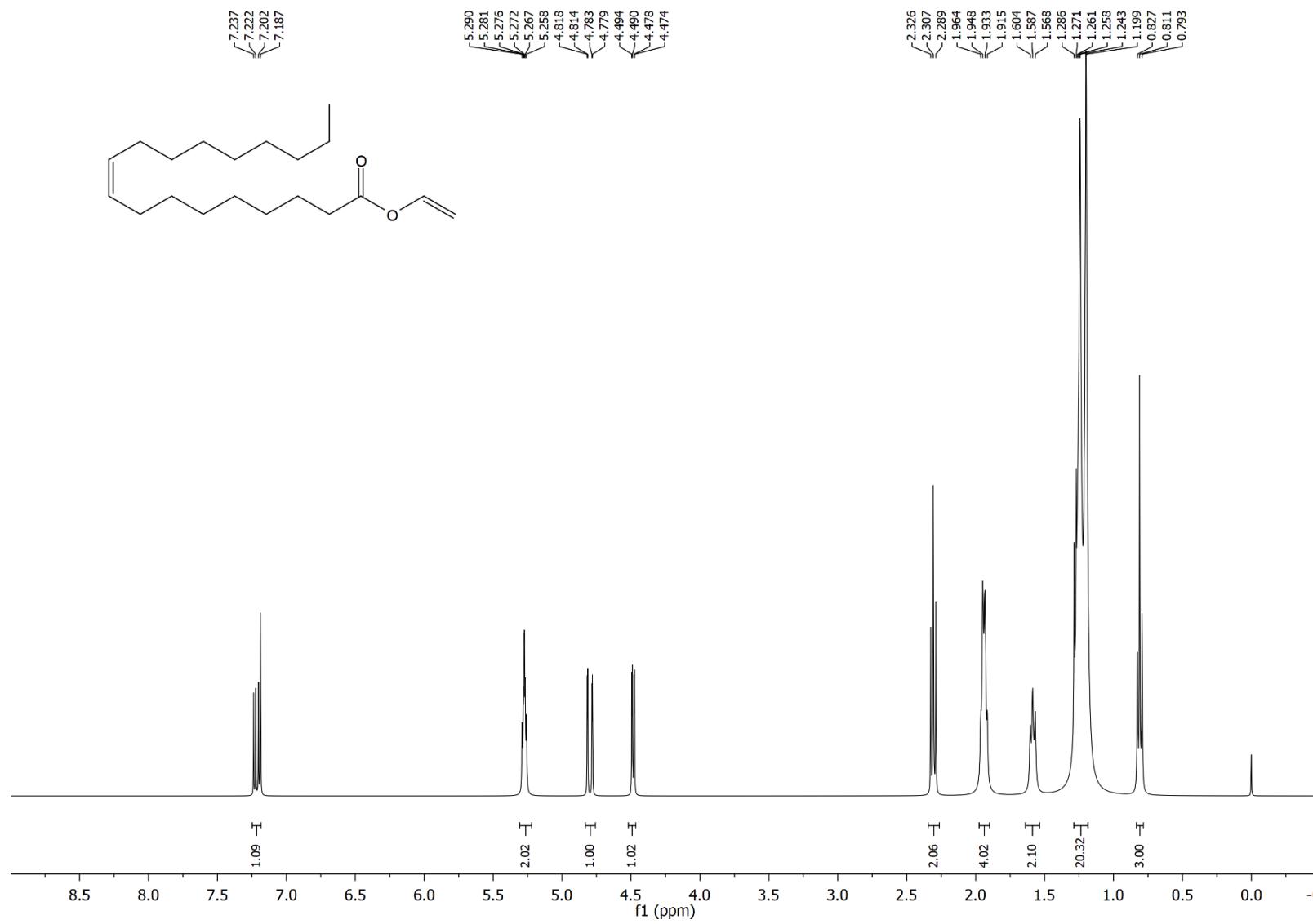


¹³C NMR (100 MHz, CDCl₃)

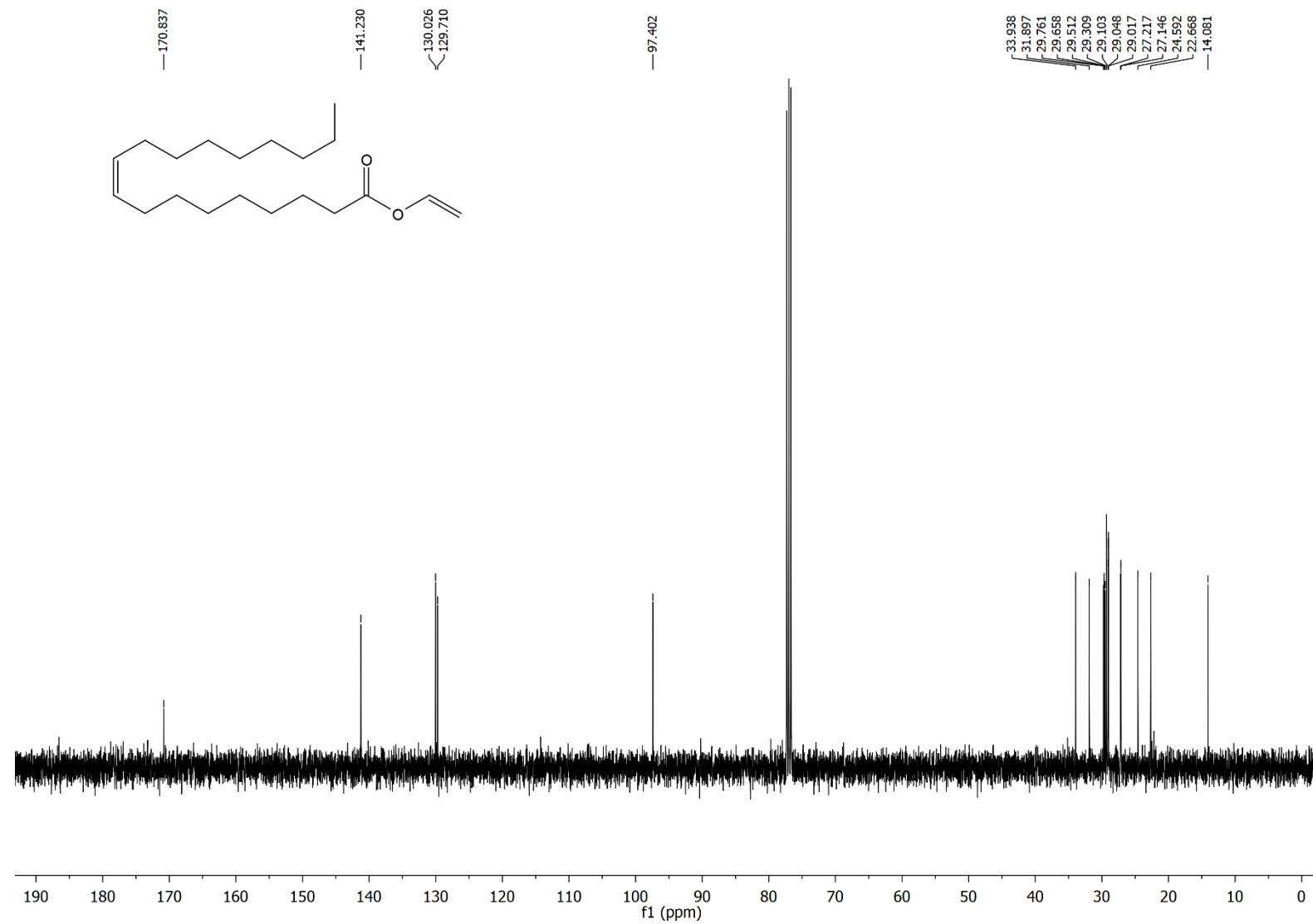


Vinyl oleate (2o**)**

¹H NMR (400 MHz, CDCl₃)

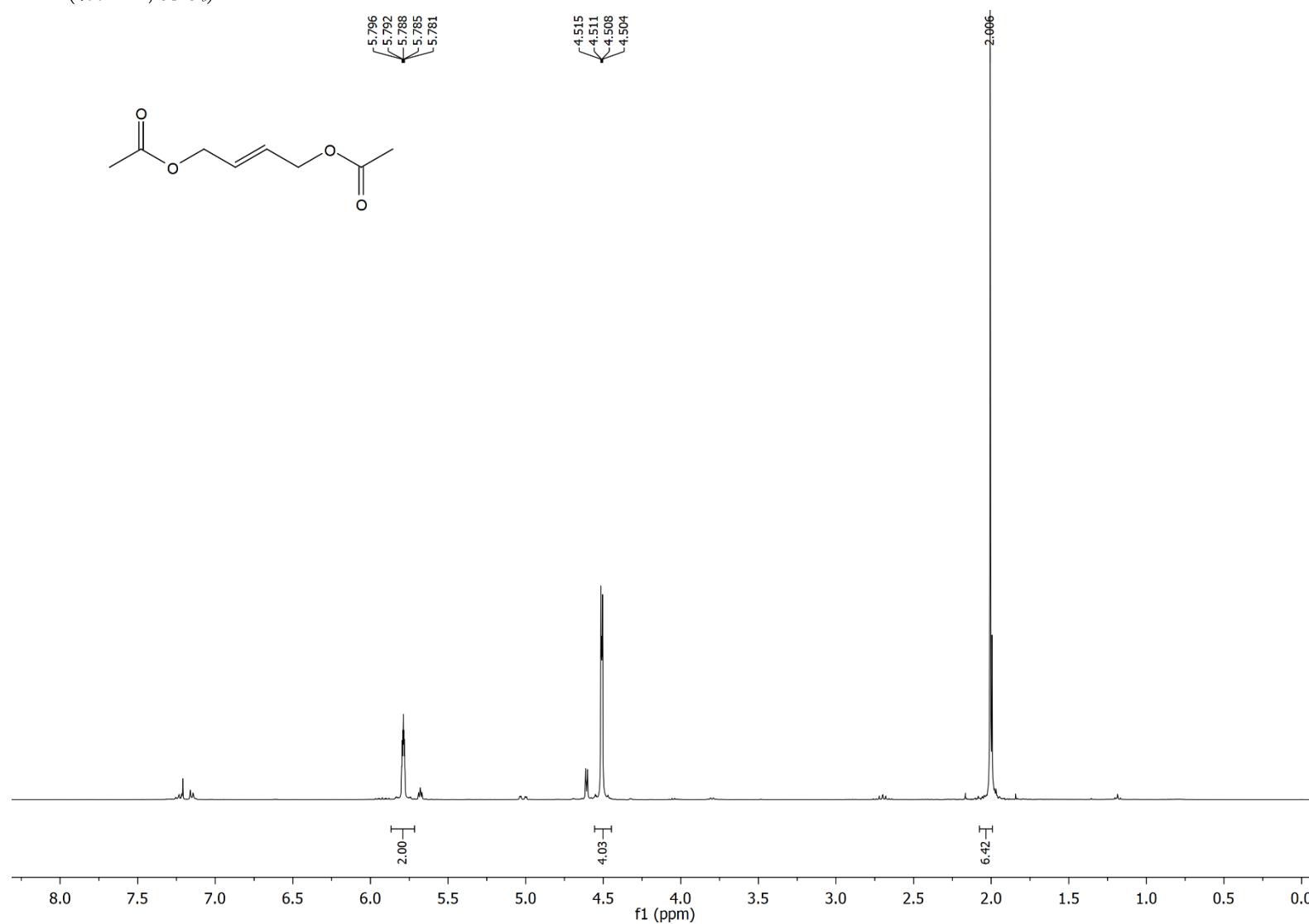


¹³C NMR (100 MHz, CDCl₃)

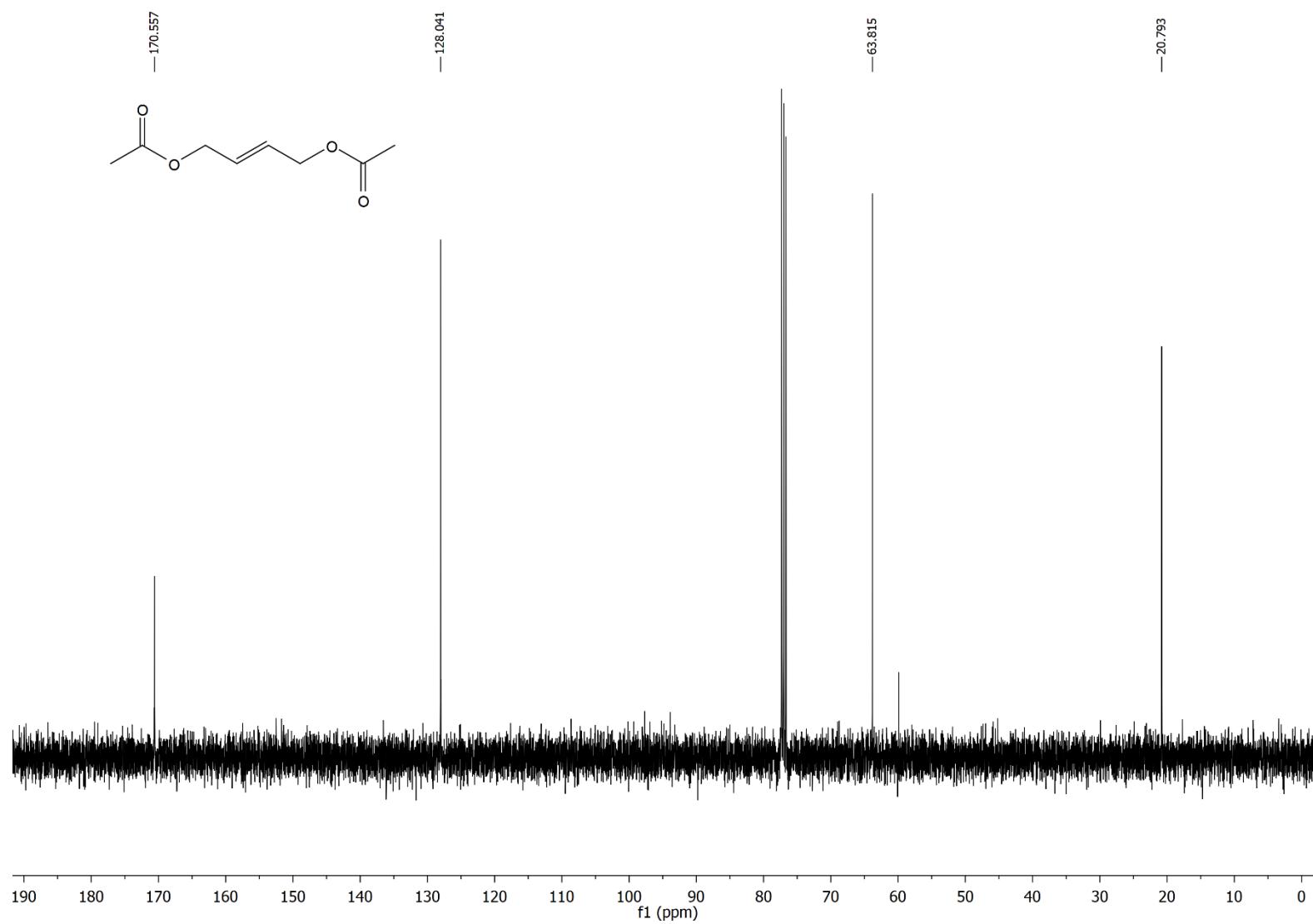


1,4-diacetoxybut-2-ene (6**)**

¹H NMR (400 MHz, CDCl₃)

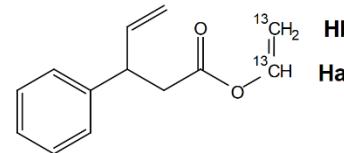
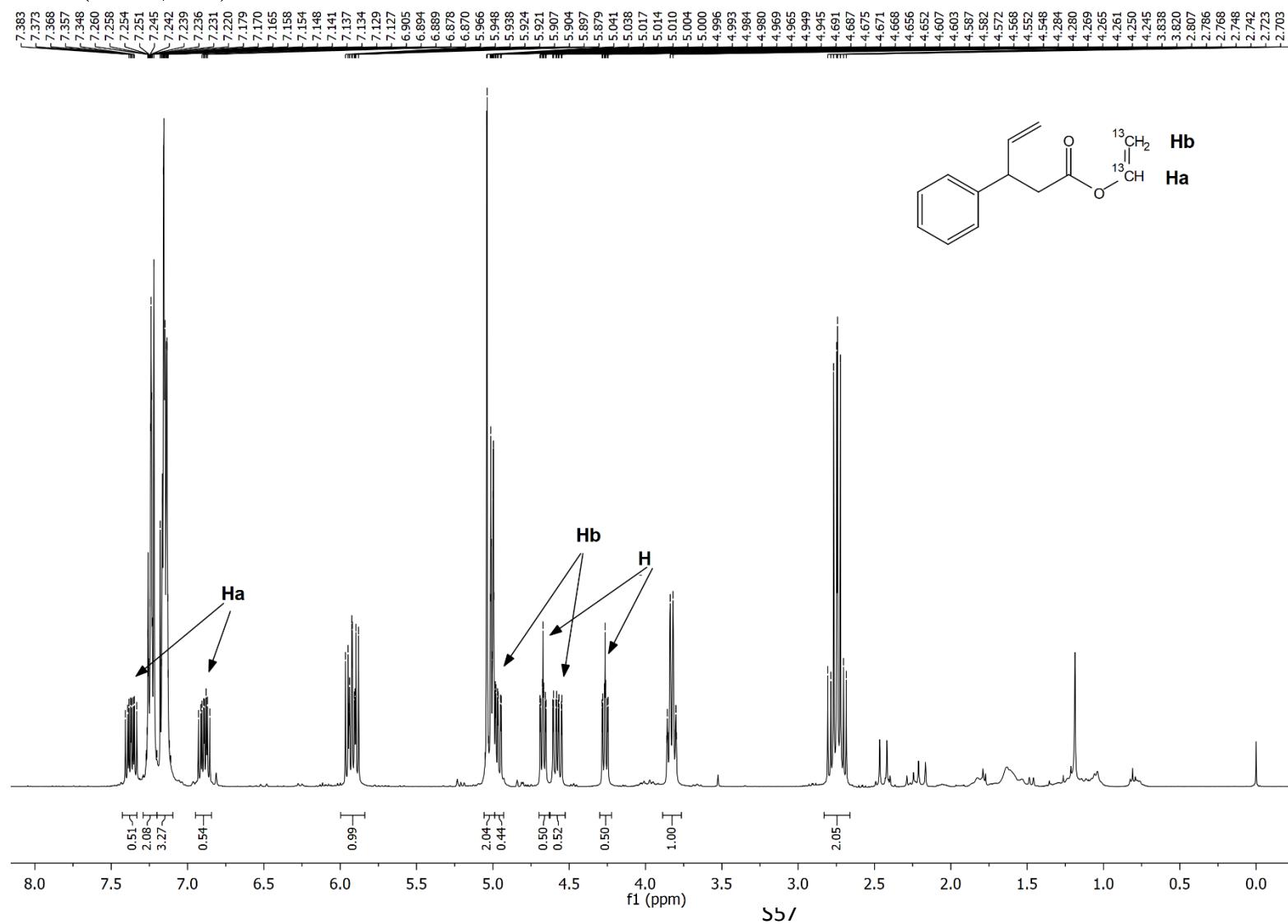


^{13}C NMR (100 MHz, CDCl_3)

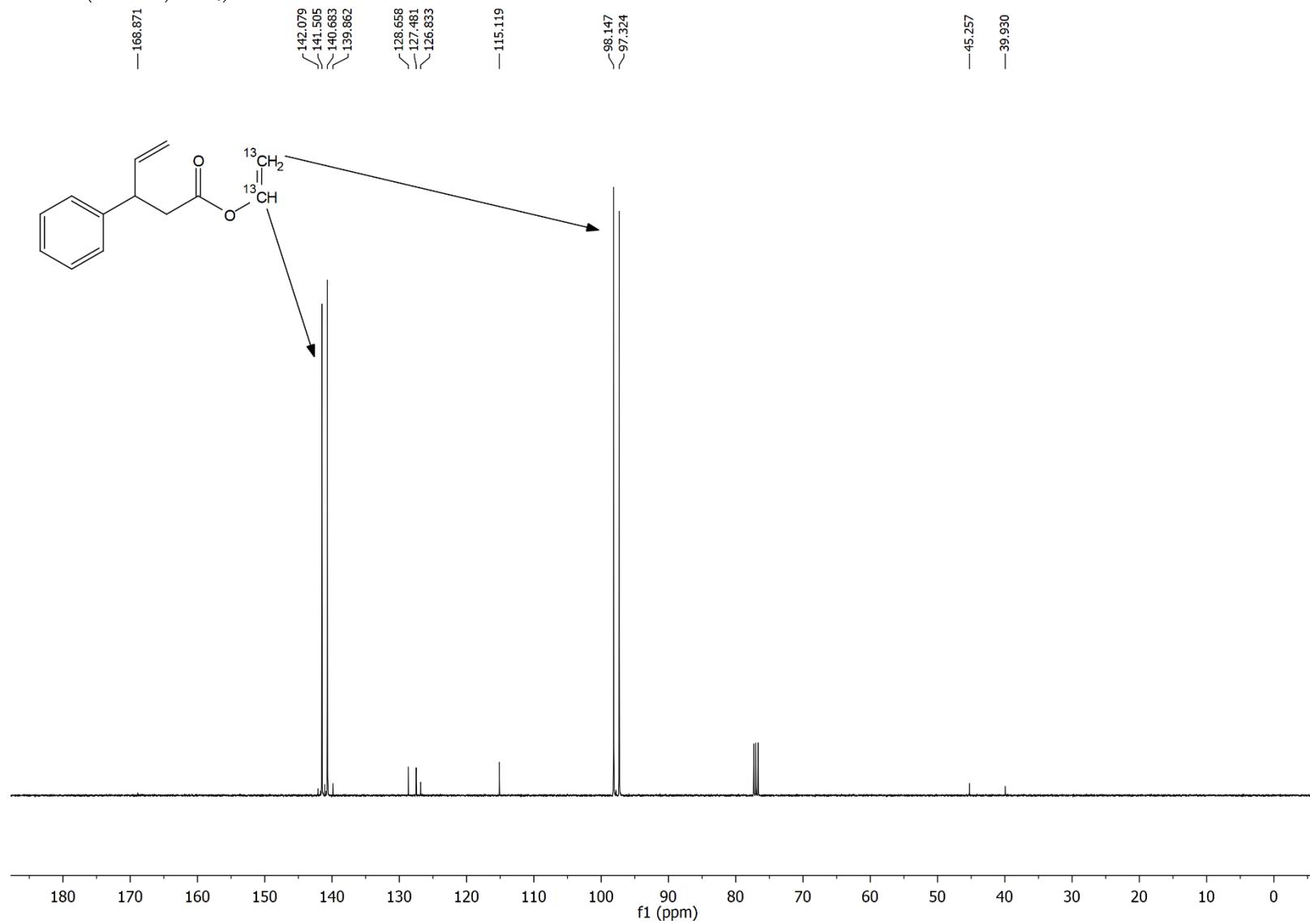


Vinyl-¹³C₂ 3-phenyl-4-pentenoate

¹H NMR (400 MHz, CDCl₃)

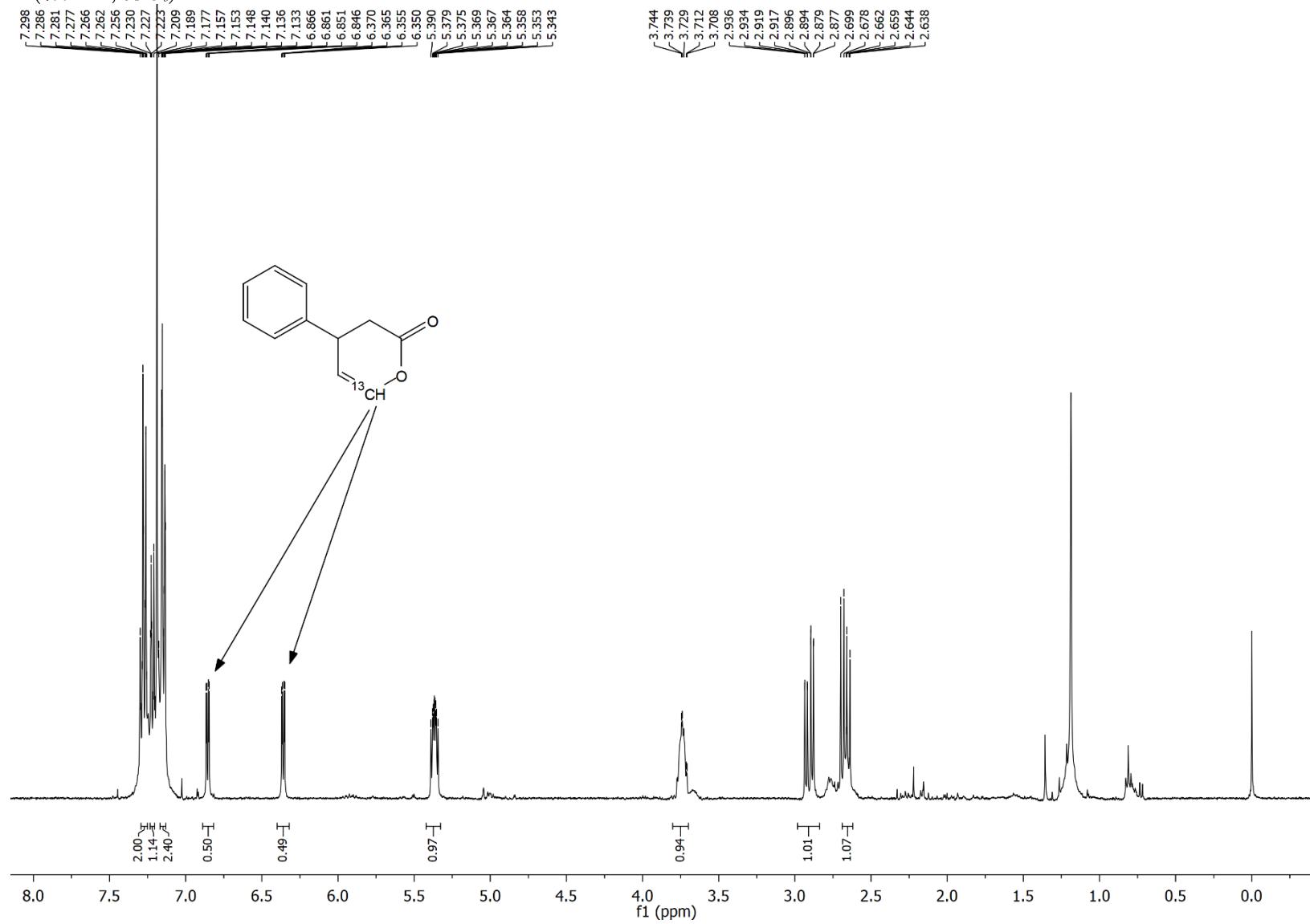


¹³C NMR (100 MHz, CDCl₃)



4-Phenyl(6-¹³C)-3,4-dihydro-2H-pyran-2-one

¹H NMR (400 MHz, CDCl₃)



¹³C NMR (100 MHz, CDCl₃)\

