

Comparison of Substituting Ability of Nitronate versus Enolate for Direct Substitution of a Nitro Group

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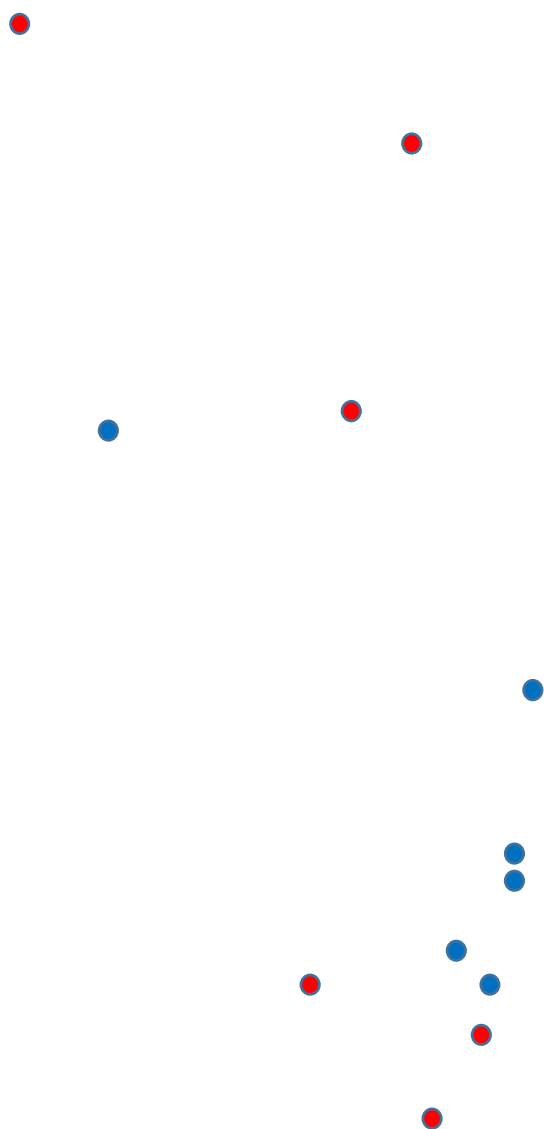
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Supporting Information

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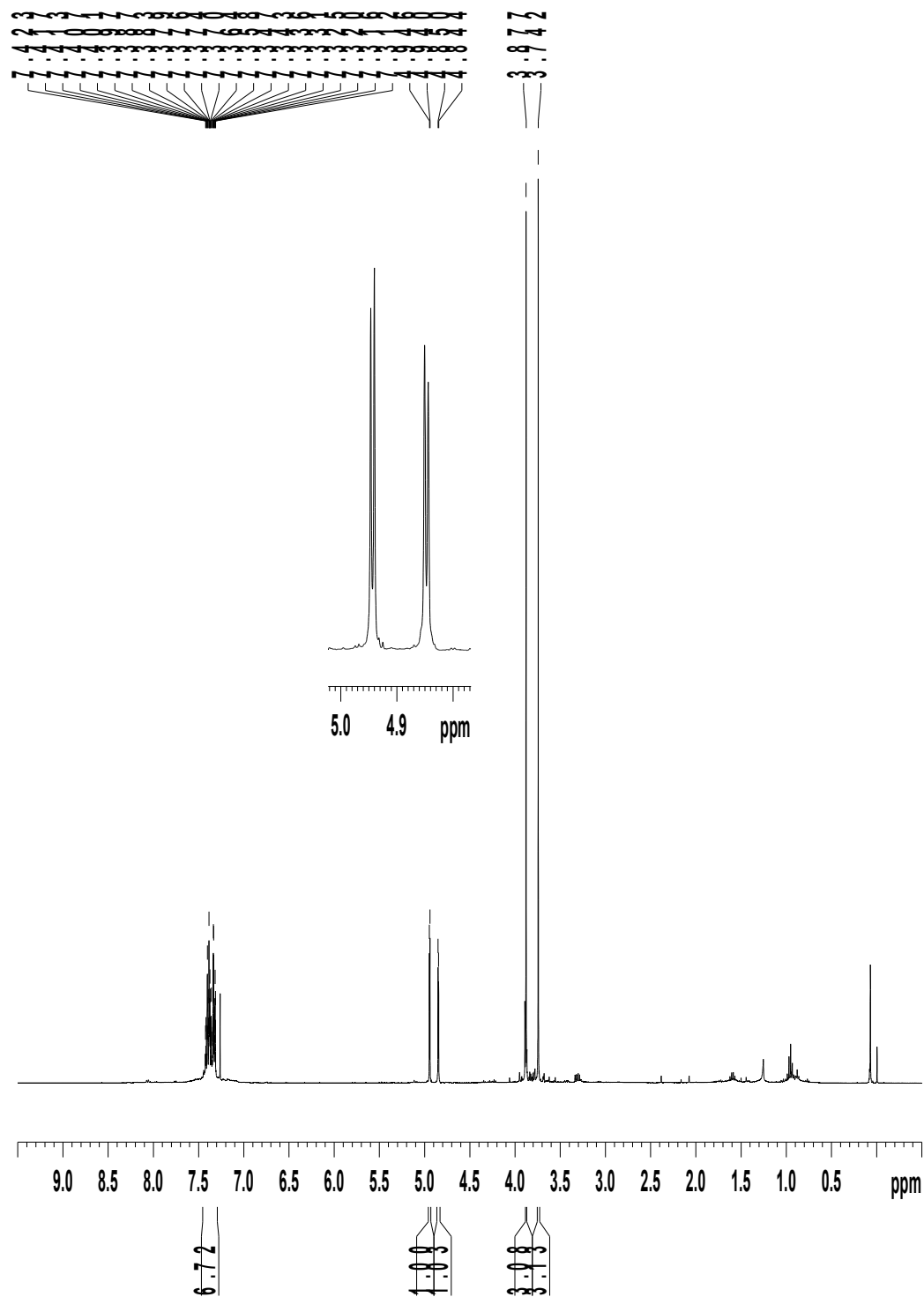
Compound	Spectra	Page
Reaction mixture including adduct 2a and <i>N</i> -propylimine 3	¹ H NMR	S2
3,5-Bis(methoxycarbonyl)-4-phenyl-2-isoxazoline 2-oxide (4a)	¹ H and ¹³ C NMR	S3–S4
3,5-Bis(ethoxycarbonyl)-4-phenyl-2-isoxazoline 2-oxide (4b)	¹ H and ¹³ C NMR	S5–S6
2,4-Bis(ethoxycarbonyl)-2,3-dihydro-5-methyl-3-phenylfuran (6a)	¹ H and ¹³ C NMR	S7–S8
2,4-Bis(ethoxycarbonyl)-5-trifluoromethyl-2,3-dihydro-3-phenylfuran (6b)	¹ H and ¹³ C NMR	S9–S10
2,4-Bis(ethoxycarbonyl)-2,3-dihydro-1,3-diphenylfuran (6c)	¹ H and ¹³ C NMR	S11–S12
4-Ethanoyl-2-ethoxycarbonyl-2,3-dihydro-5-methyl-3-phenylfuran (6d)	¹ H and ¹³ C NMR	S13–S14
5,6-Cyclohexa-2-ethoxycarbonyl-2,3-dihydro-3-phenylfuran-4-one (6e)	¹ H and ¹³ C NMR	S15–S16
3-Ethoxycarbonyl-4,5-dihydro-5-(4-methylbenzoyl)-4-phenylisoxazoline 2-oxide (13)	¹ H, ¹³ C and ¹ H- ¹ H COSY 2D NMR	S17–S19

^1H NMR (400 MHz, CDCl_3) of the reaction mixture including adduct **2a** (blue mark) and *N*-propylimine **3** (red mark)

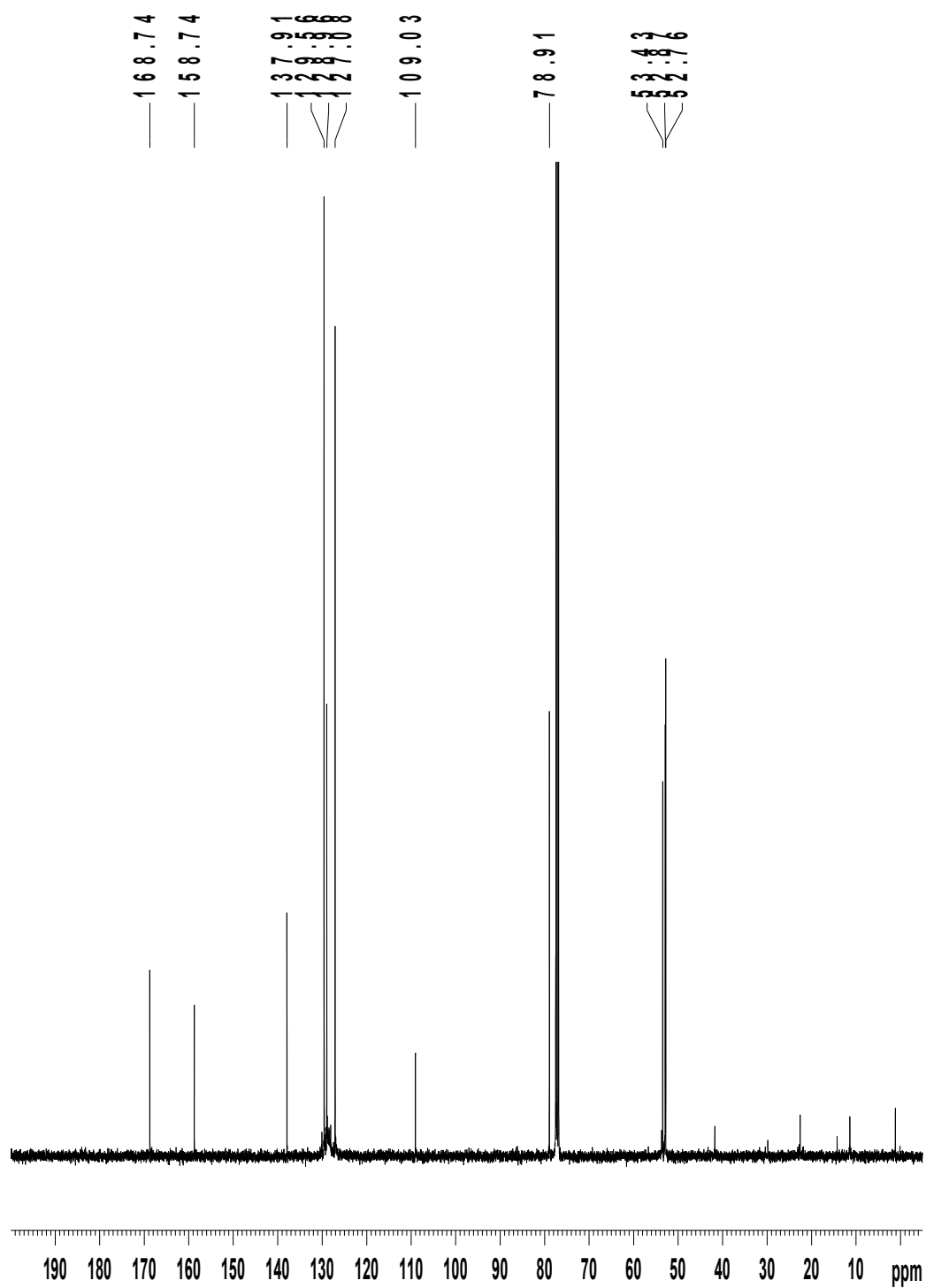


3,5-Bis(methoxycarbonyl)-4-phenyl-2-isoxazoline 2-oxide (**4a**)

^1H NMR (400 MHz, CDCl_3)

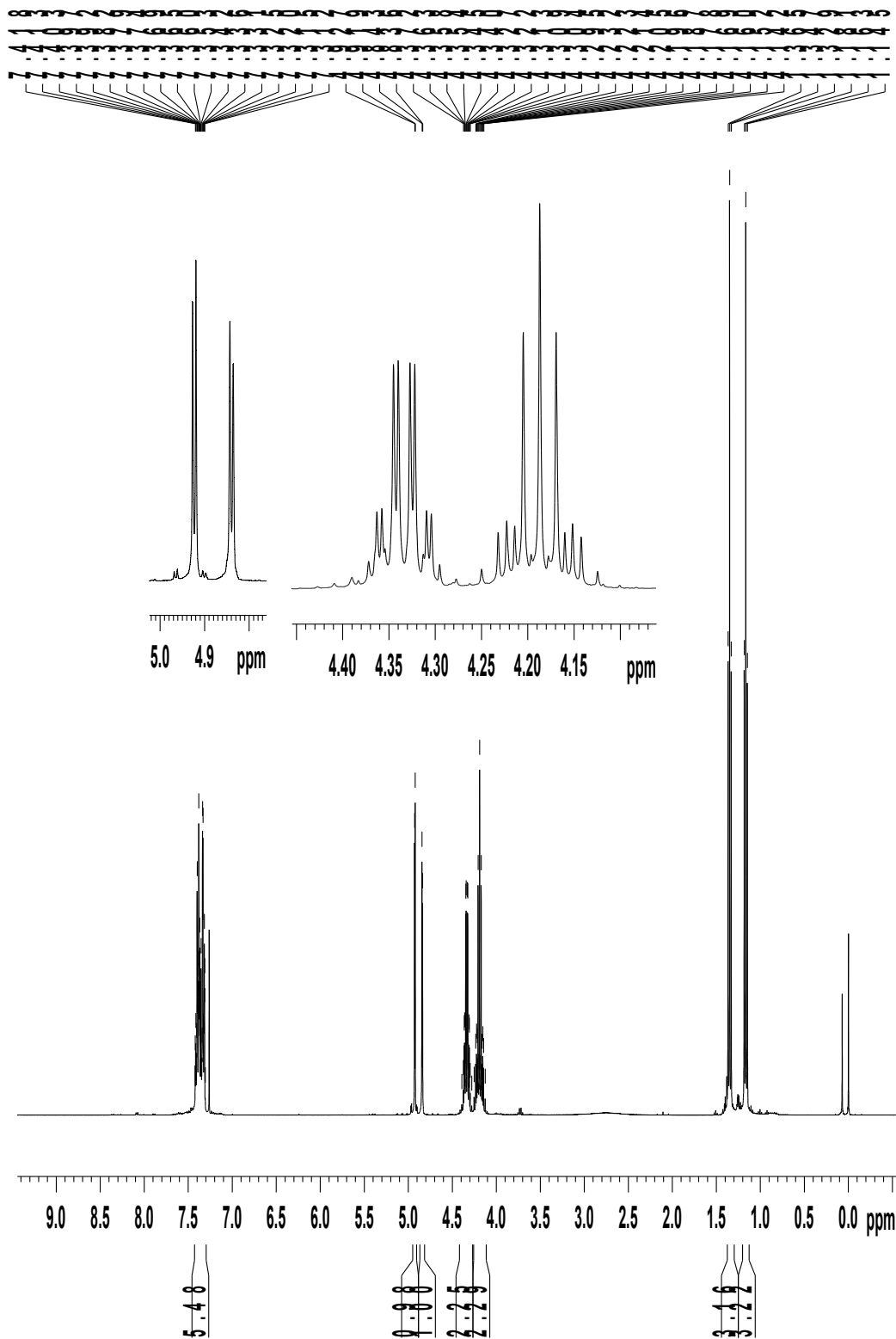


^{13}C NMR (100 MHz, CDCl_3)

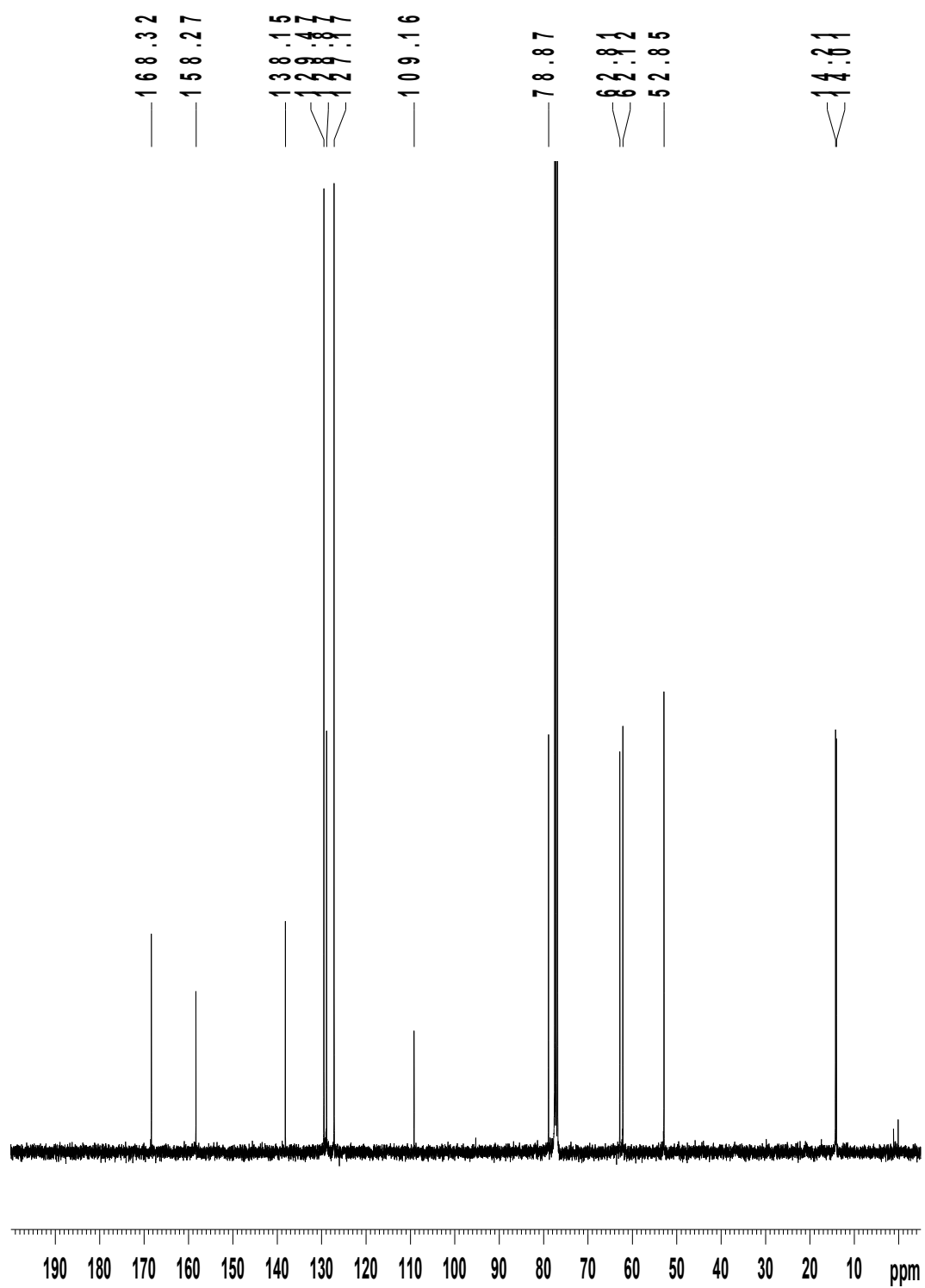


3,5-Bis(ethoxycarbonyl)-4-phenyl-2-isoxazoline 2-oxide (**4b**)

^1H NMR (400 MHz, CDCl_3)

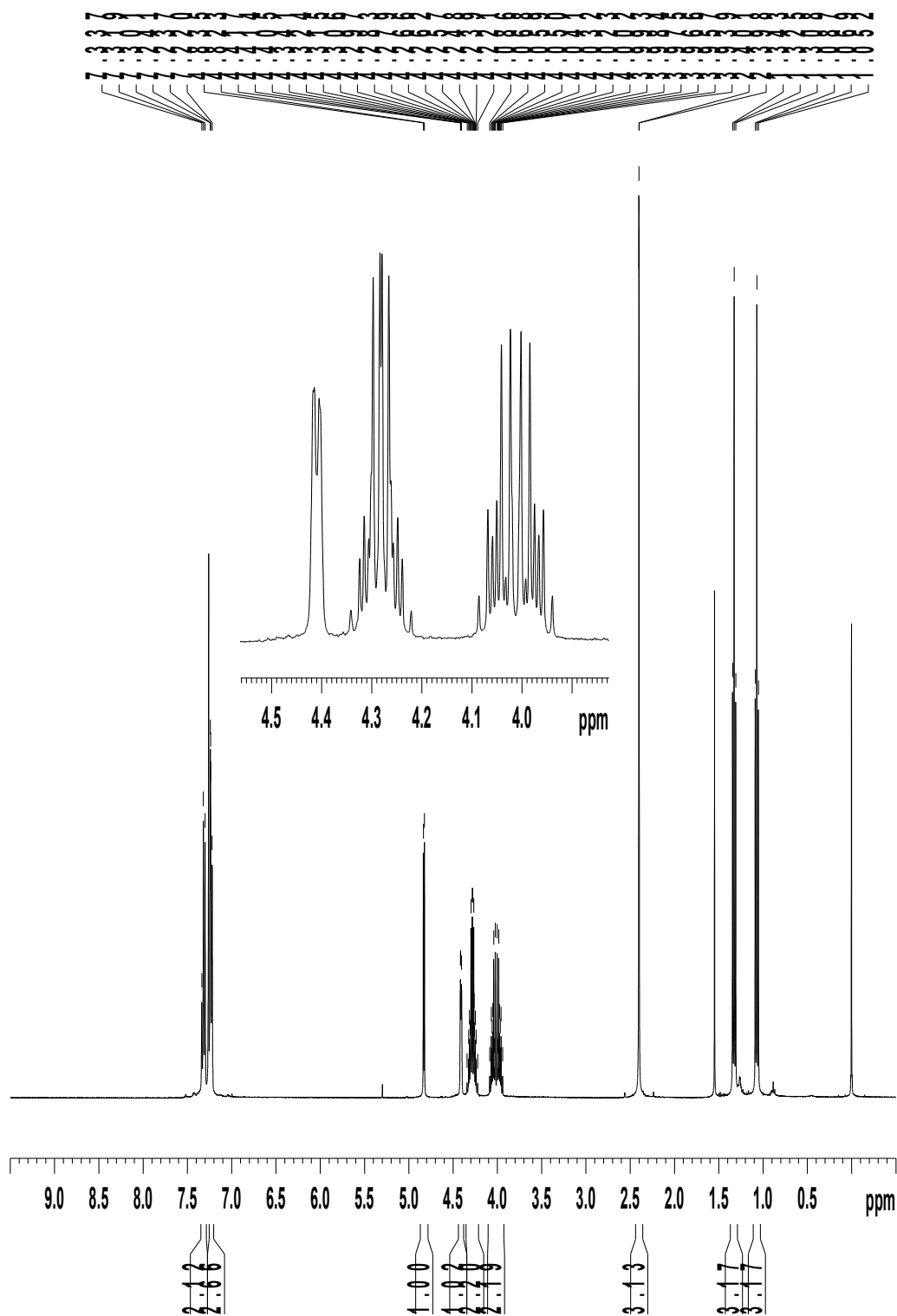


^{13}C NMR (100 MHz, CDCl_3)

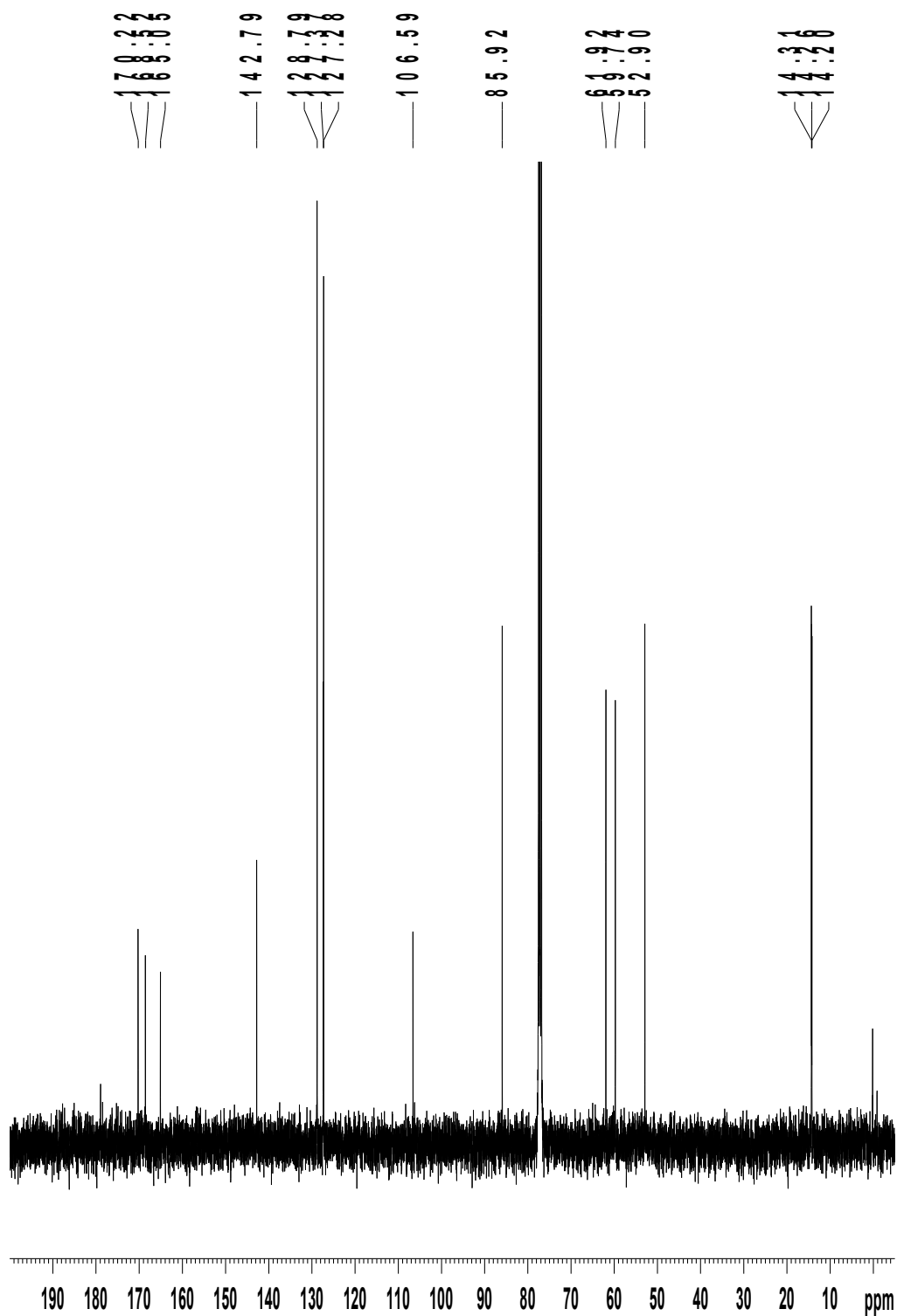


2,4-Bis(ethoxycarbonyl)-2,3-dihydro-5-methyl-3-phenylfuran (**6a**)

^1H NMR (400 MHz, CDCl_3)

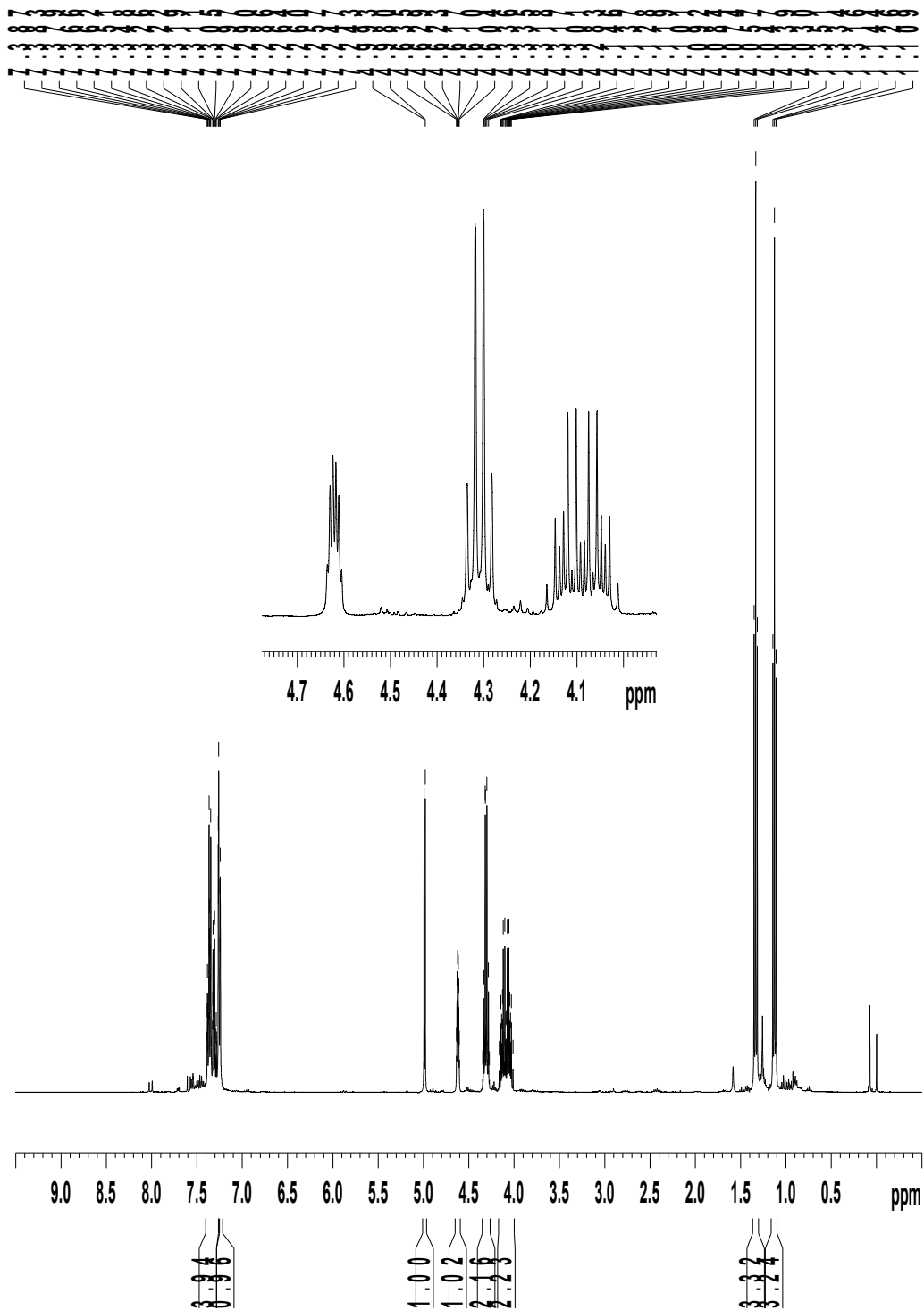


^{13}C NMR (100 MHz, CDCl_3)

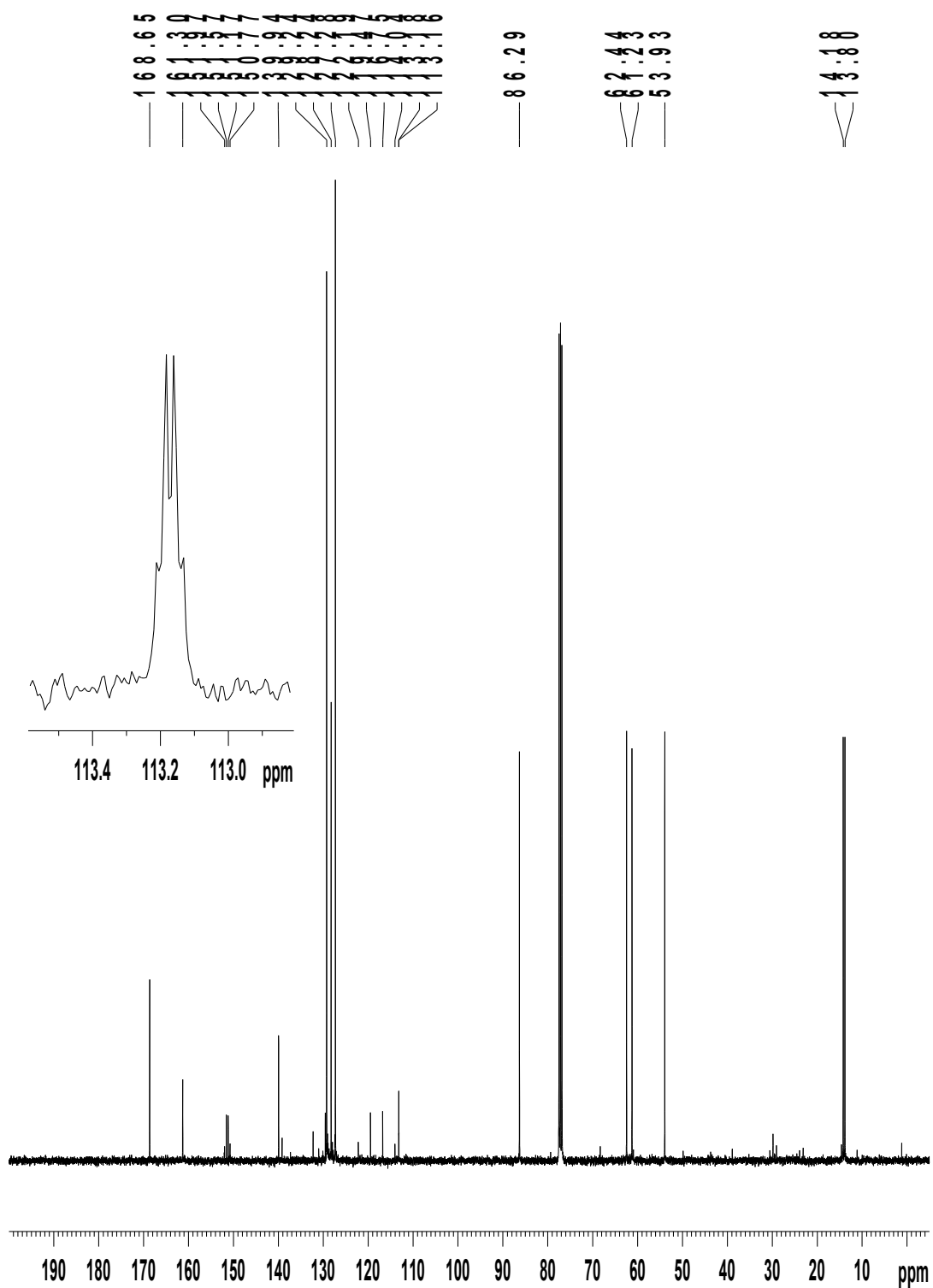


2,4-Bis(ethoxycarbonyl)-5-trifluoromethyl-2,3-dihydro-3-phenylfuran (**6b**)

^1H NMR (400 MHz, CDCl_3)

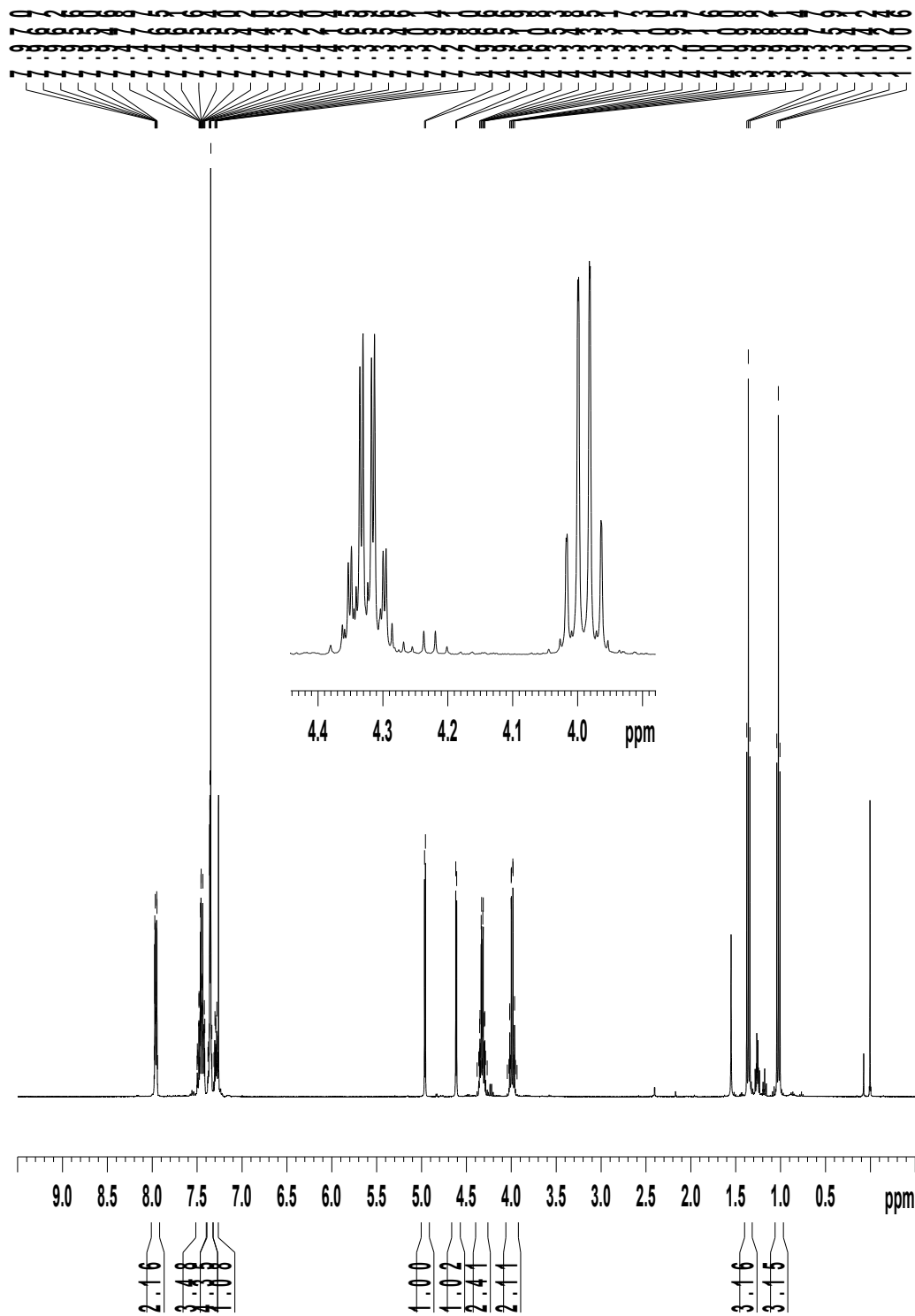


^{13}C NMR (100 MHz, CDCl_3)

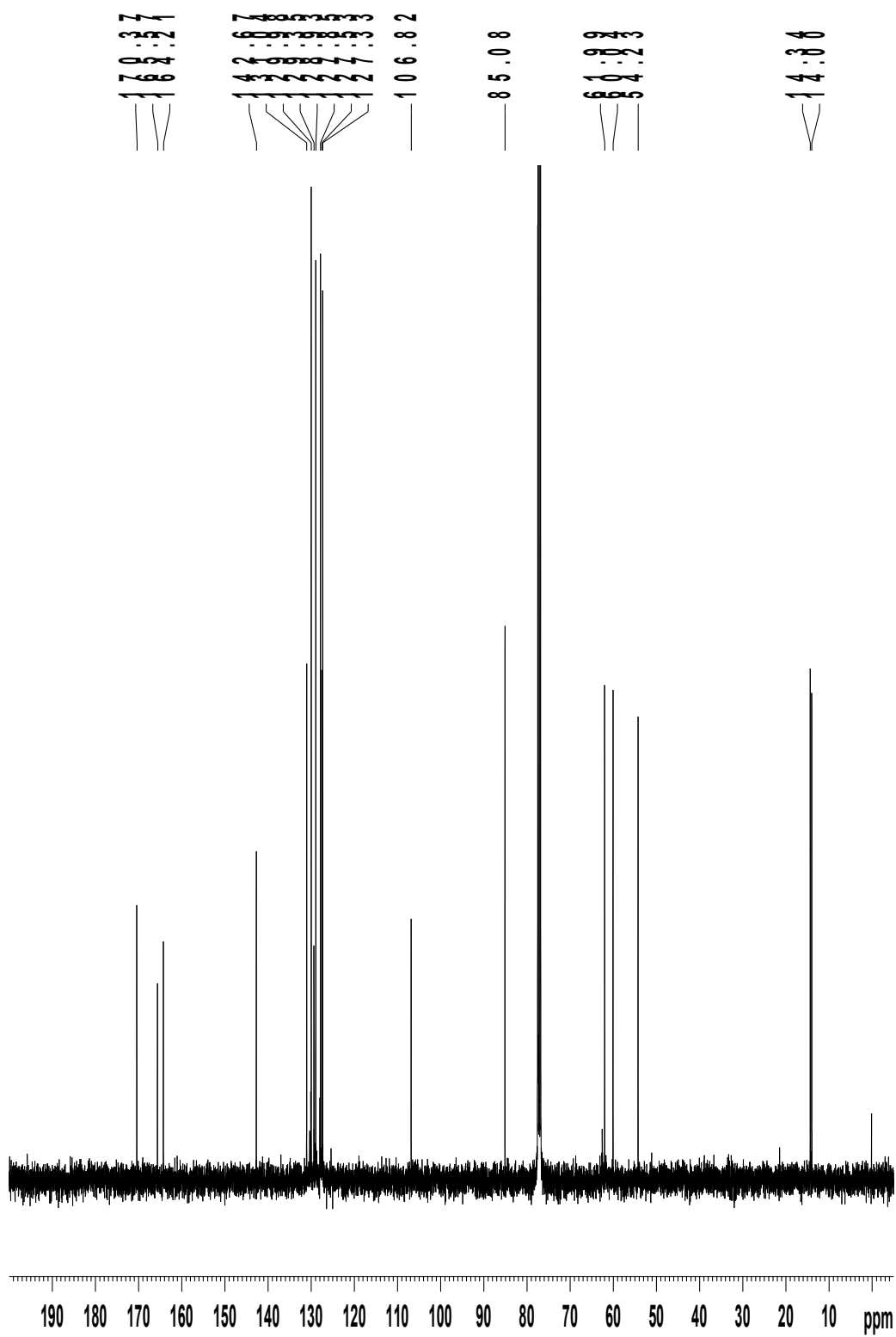


2,4-Bis(ethoxycarbonyl)-2,3-dihydro-1,3-diphenylfuran (**6c**)

^1H NMR (400 MHz, CDCl_3)

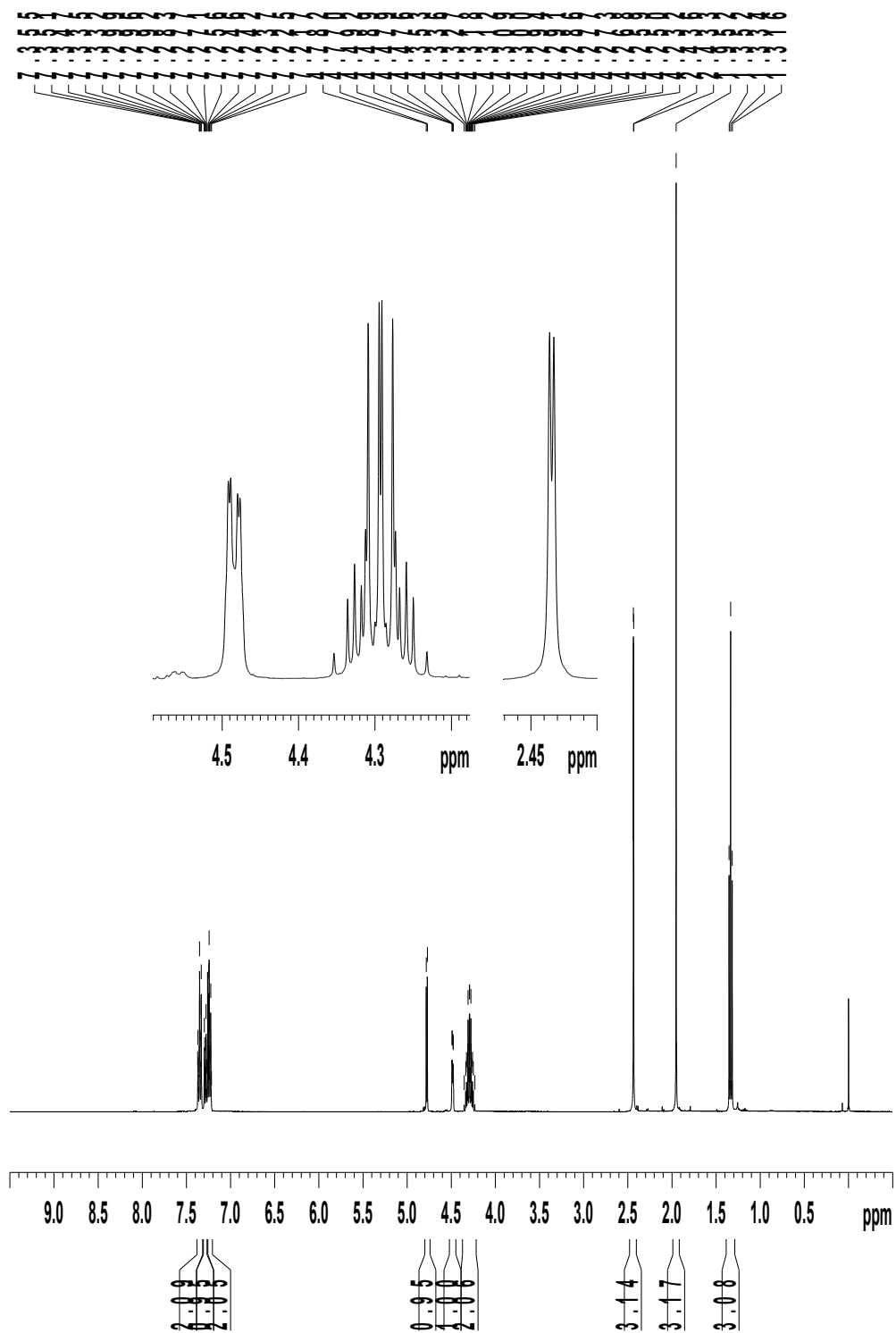


^{13}C NMR (100 MHz, CDCl_3)

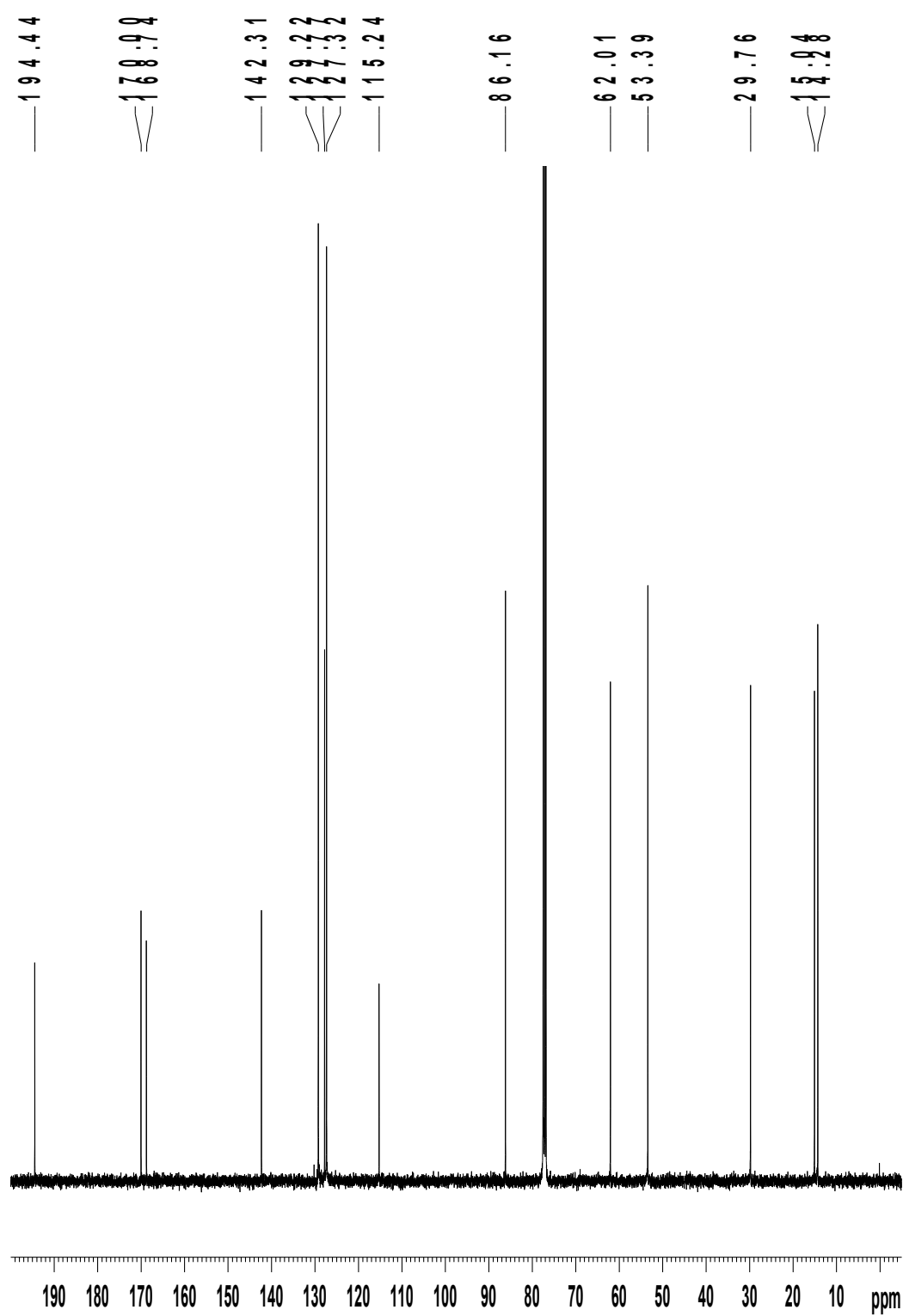


4-Ethanoyl-2-ethoxycarbonyl-2,3-dihydro-5-methyl-3-phenylfuran (**6d**)

^1H NMR (400 MHz, CDCl_3)

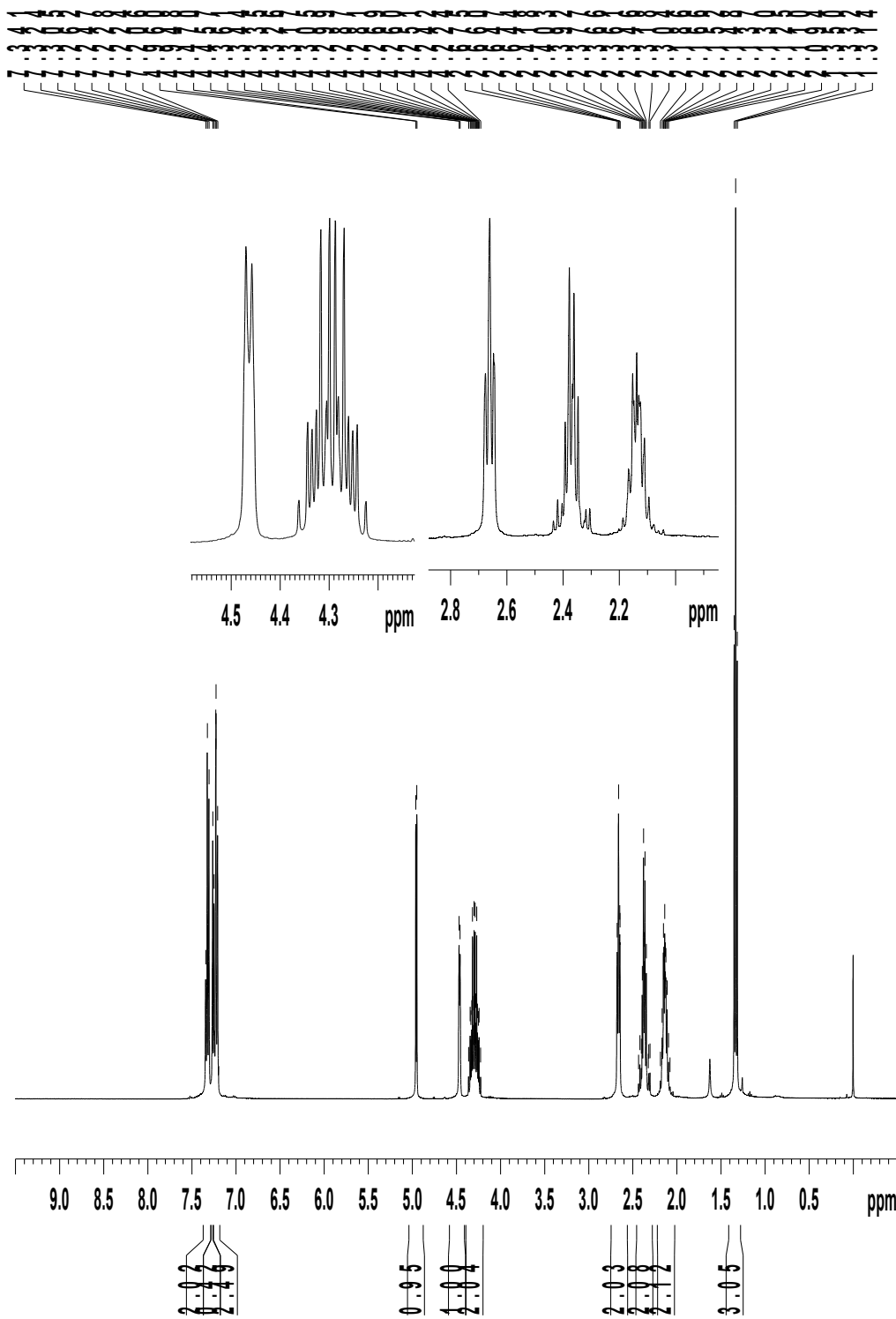


^{13}C NMR (100 MHz, CDCl_3)

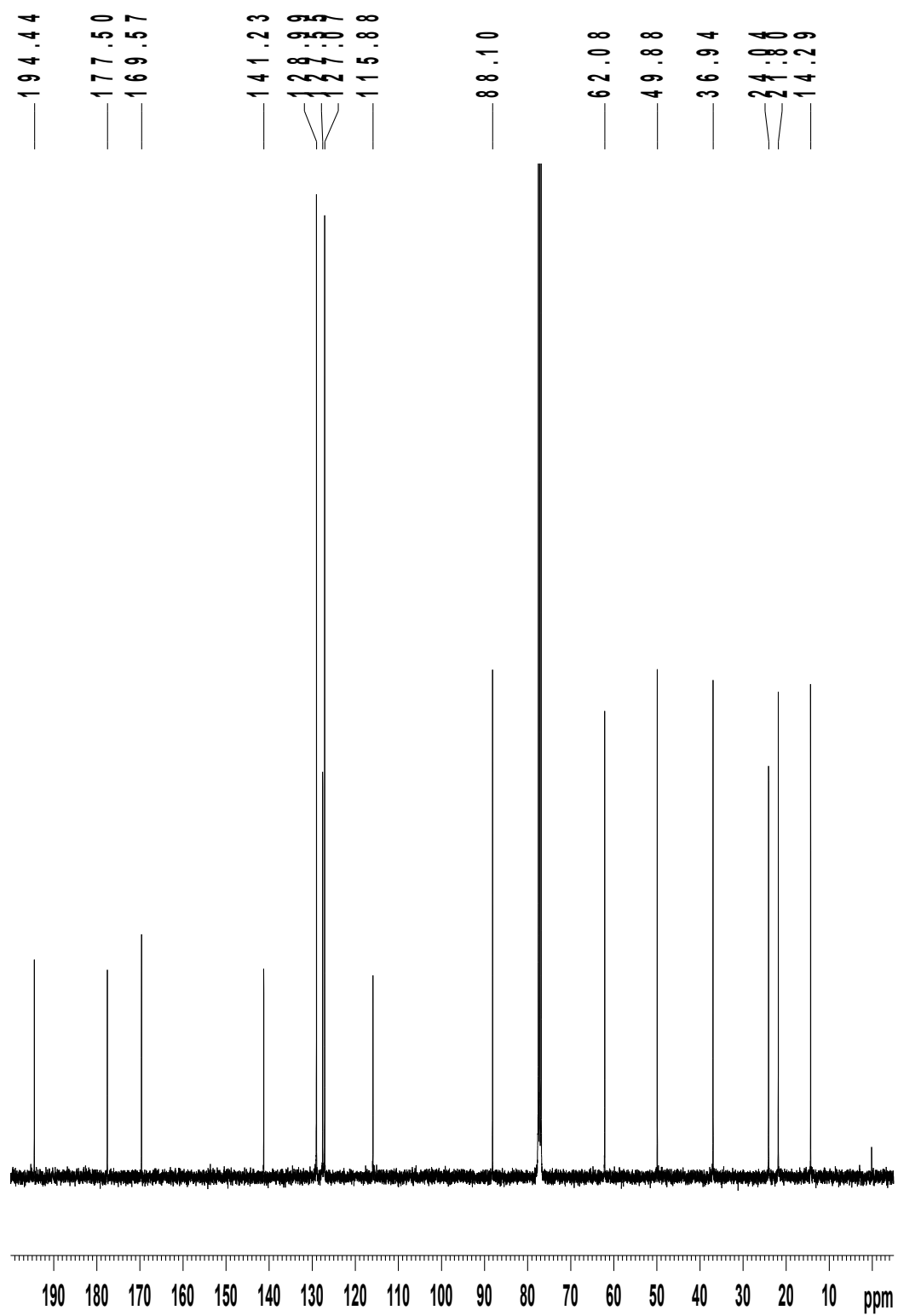


5,6-Cyclohexa-2-ethoxycarbonyl-2,3-dihydro-3-phenylfuran-4-one (**6e**)

^1H NMR (400 MHz, CDCl_3)

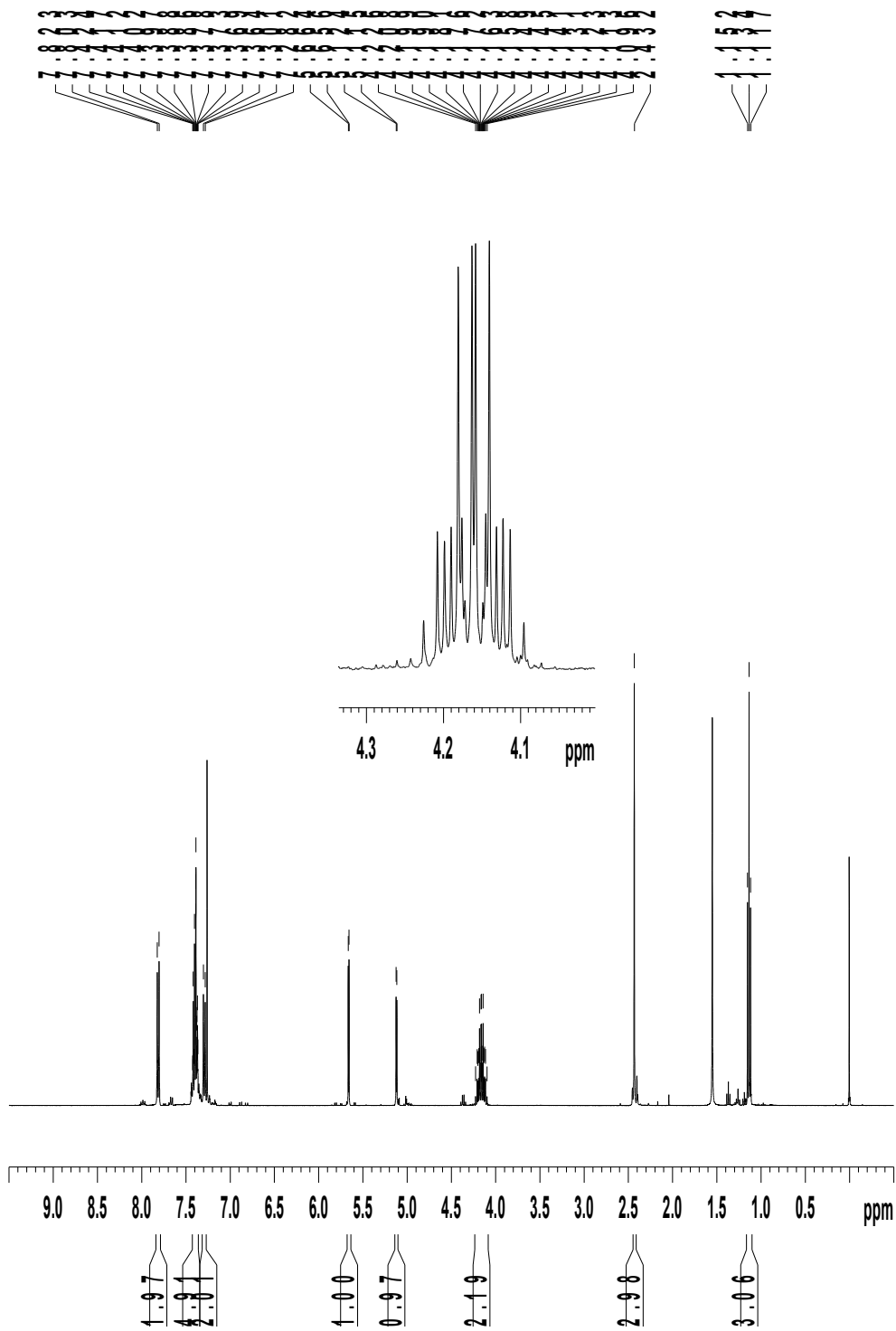


^{13}C NMR (100 MHz, CDCl_3)

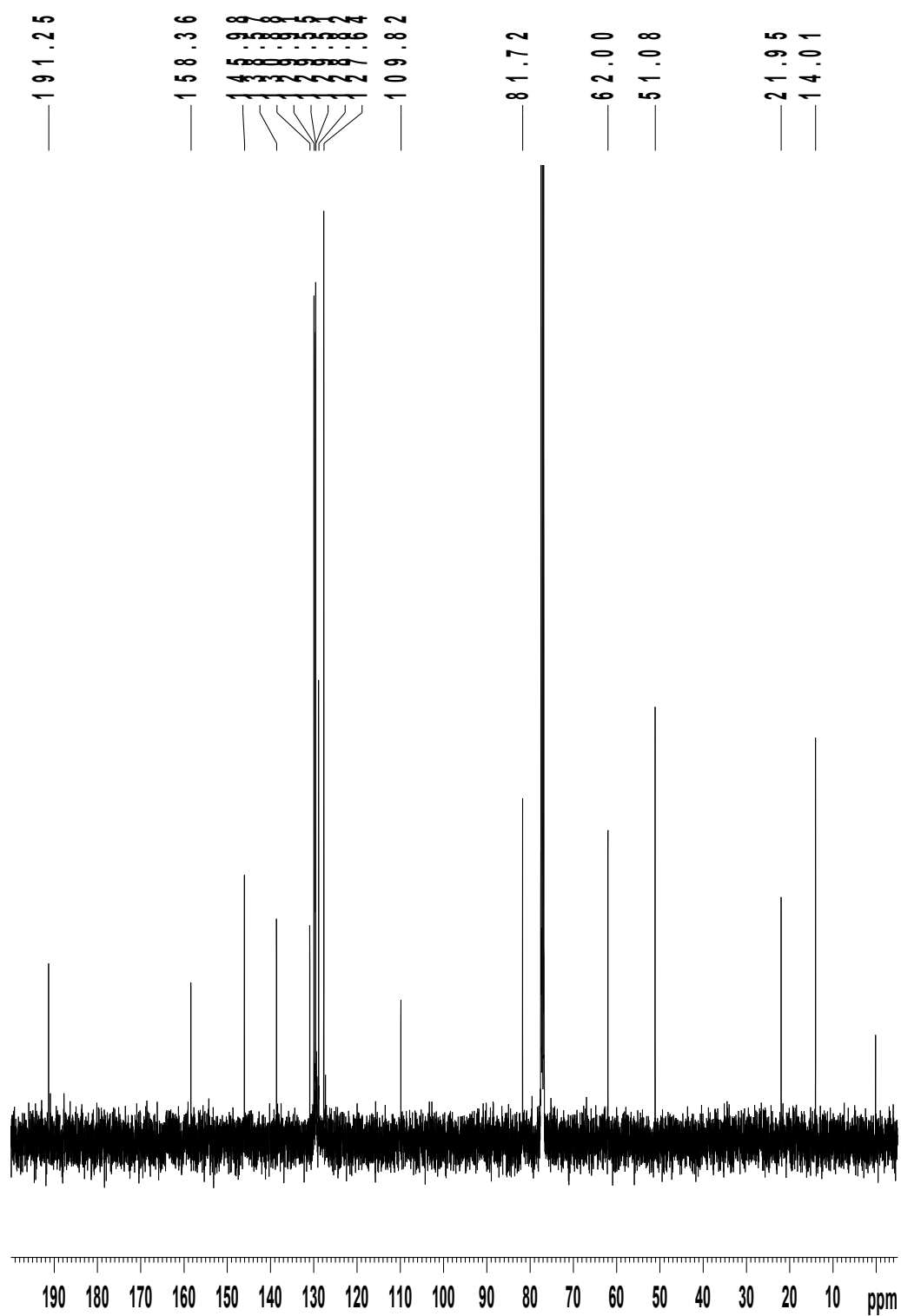


3-Ethoxycarbonyl-4,5-dihydro-5-(4-methylbenzoyl)-4-phenylisoxazoline 2-oxide (**13**)

^1H NMR (400 MHz, CDCl_3)



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



^1H - ^1H 2D NMR

