

Supplementary Material

Palladium catalyzed hydroesterification of substituted alkenes under microwave conditions

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Table S1. Quantities of reagents for the methoxycarbonylation of 1-octene (**3**), styrene (**4**), allylbenzenes (**9** - **11**) and β -methylstyrene (**12**) under microwave conditions at 95 °C (150 watt) with 12 bar CO pressure in MeOH (4 ml)

Alkene	1-Octene (3)	Styrene (4)	β -methylstyrene (12)
	0.238 g, 2.12 mmol	0.221 g, 2.12 mmol	0.251 g, 2.12 mmol
Pd(OAc) ₂	0.0251 g, 0.112 mmol	0.0246 g, 0.110 mmol	0.0239 g, 0.106 mmol
Al(OTf) ₃	0.102 g, 0.215 mmol	0.102 g, 0.215 mmol	0.102 g, 0.215 mmol
PPh ₃	0.114 g, 0.435 mmol	0.114 g, 0.435 mmol	0.112 g, 0.427 mmol
Xylene	0.260 g, 2.45 mmol	0.254 g, 2.39 mmol	0.253 g, 2.38 mmol
Products	5 and 6	7 and 8	13, 14 and 15
Alkene	Allylbenzene (9)	1-allyl-4-methoxybenzene (10)	1-allyl-2-methoxybenzene (11)
	0.252 g, 2.13 mmol	0.316 g, 2.13 mmol	0.312 g, 2.11 mmol
Pd(OAc) ₂	0.0254 g, 0.131 mmol	0.0251 g, 0.112 mmol	0.0235 g, 0.105 mmol
Al(OTf) ₃	0.101 g, 0.213 mmol	0.102 g, 0.215 mmol	0.102 g, 0.215 mmol
PPh ₃	0.114 g, 0.435 mmol	0.111 g, 0.422 mmol	0.112 g, 0.427 mmol
Xylene	0.253 g, 2.38 mmol	0.253 g, 2.38 mmol	0.253 g, 2.38 mmol
Products	13, 14 and 15	16, 17 and 18	19, 20 and 21

Table S2. Quantities of reagents for the methoxycarbonylation of 1-octene (**3**), styrene (**4**), allylbenzenes (**9** - **11**) and β -methylstyrene (**12**) under autoclave conditions at 95°C under 12 bar CO pressure in MeOH (8 ml)

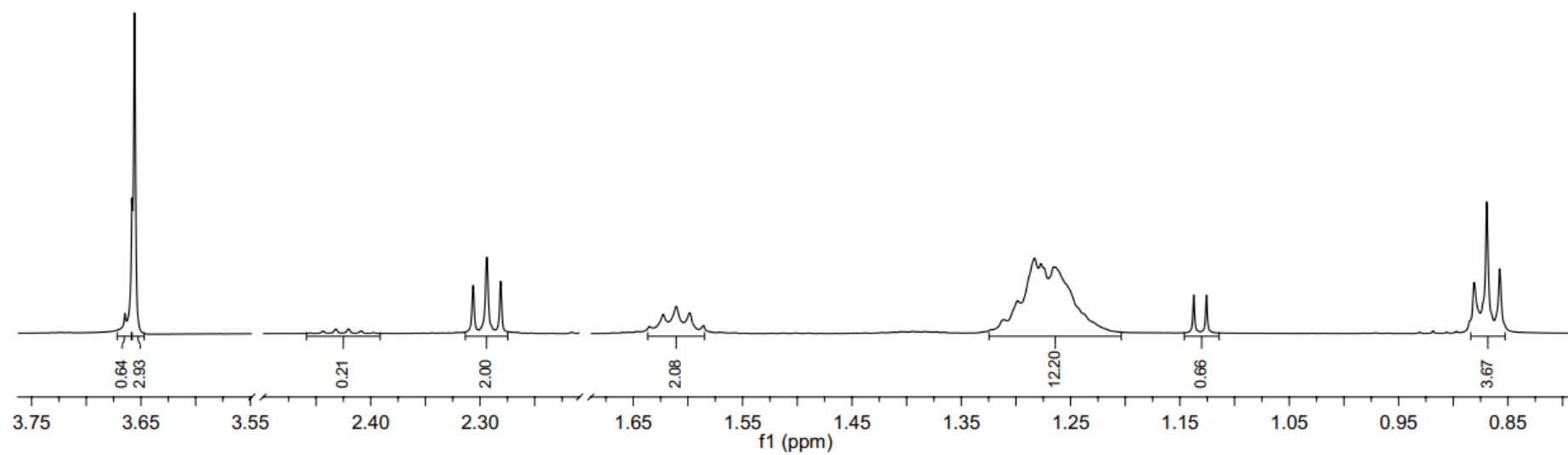
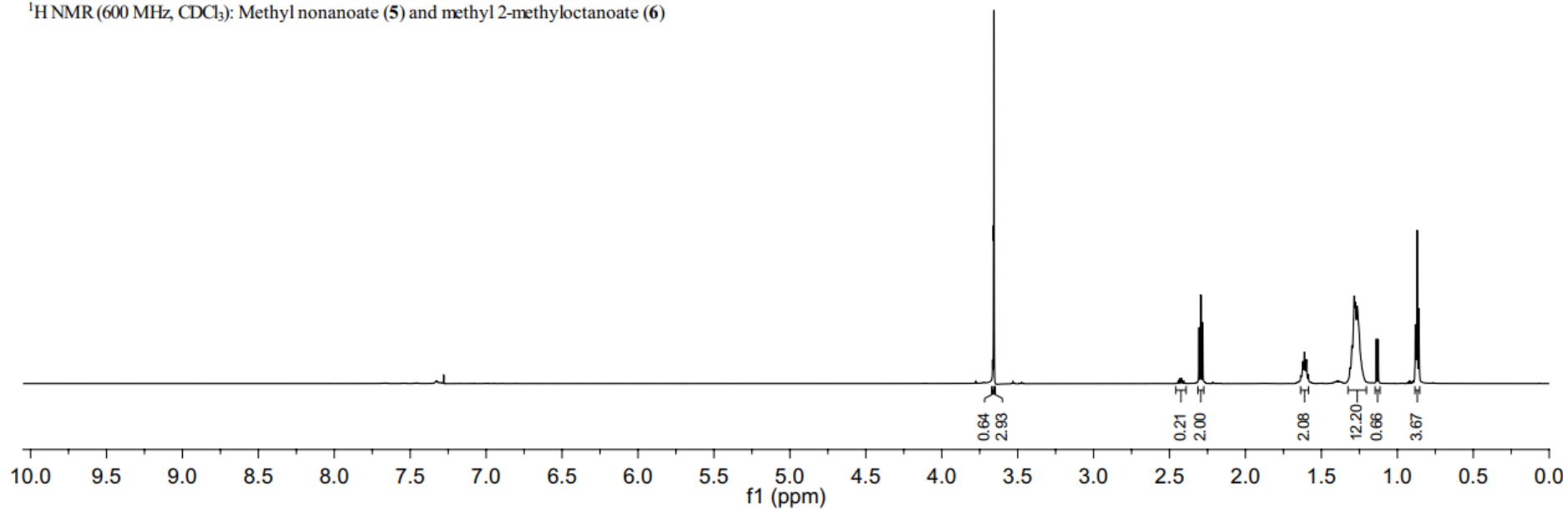
Alkene	1-Octene (3)	Styrene (4)	β -methylstyrene (12)
	0.477 g, 4.25 mmol	0.441 g, 4.23 mmol	0.501 g, 4.24 mmol
Pd(OAc) ₂	0.0475 g, 0.212 mmol	0.0473 g, 0.211 mmol	0.0487 g, 0.217 mmol
Al(OTf) ₃	0.201 g, 0.424 mmol	0.201 g, 0.424 mmol	0.202 g, 0.426 mmol
PPh ₃	0.224 g, 0.854 mmol	0.222 g, 0.846 mmol	0.227 g, 0.865 mmol
Xylene	0.499 g, 4.70 mmol	0.499 g, 4.70 mmol	0.500 g, 4.71 mmol
Products	5 and 6	7 and 8	13, 14 and 15
Alkene	Allylbenzene (9)	1-allyl-4-methoxybenzene (10)	1-allyl-2-methoxybenzene (11)
	0.500 g, 4.23 mmol	0.629 g, 4.24 mmol	0.625 g, 4.22 mmol
Pd(OAc) ₂	0.0464 g, 0.207 mmol	0.0474 g, 0.211 mmol	0.0473 g, 0.211 mmol
Al(OTf) ₃	0.202 g, 0.426 mmol	0.201 g, 0.424 mmol	0.201 g, 0.424 mmol
PPh ₃	0.222 g, 0.846 mmol	0.224 g, 0.854 mmol	0.221 g, 0.843 mmol
Xylene	0.508 g, 4.79 mmol	0.509 g, 4.79 mmol	0.505 g, 4.77 mmol
Products	13, 14 and 15	16, 17 and 18	19, 20 and 21

Table S3. Quantities of reagents for the methoxycarbonylation of 1-octene (**3**), styrene (**4**), allylbenzenes (**9** - **11**) and β -methylstyrene (**12**) under autoclave conditions at 95°C under 35 bar CO pressure in MeOH (8 ml)

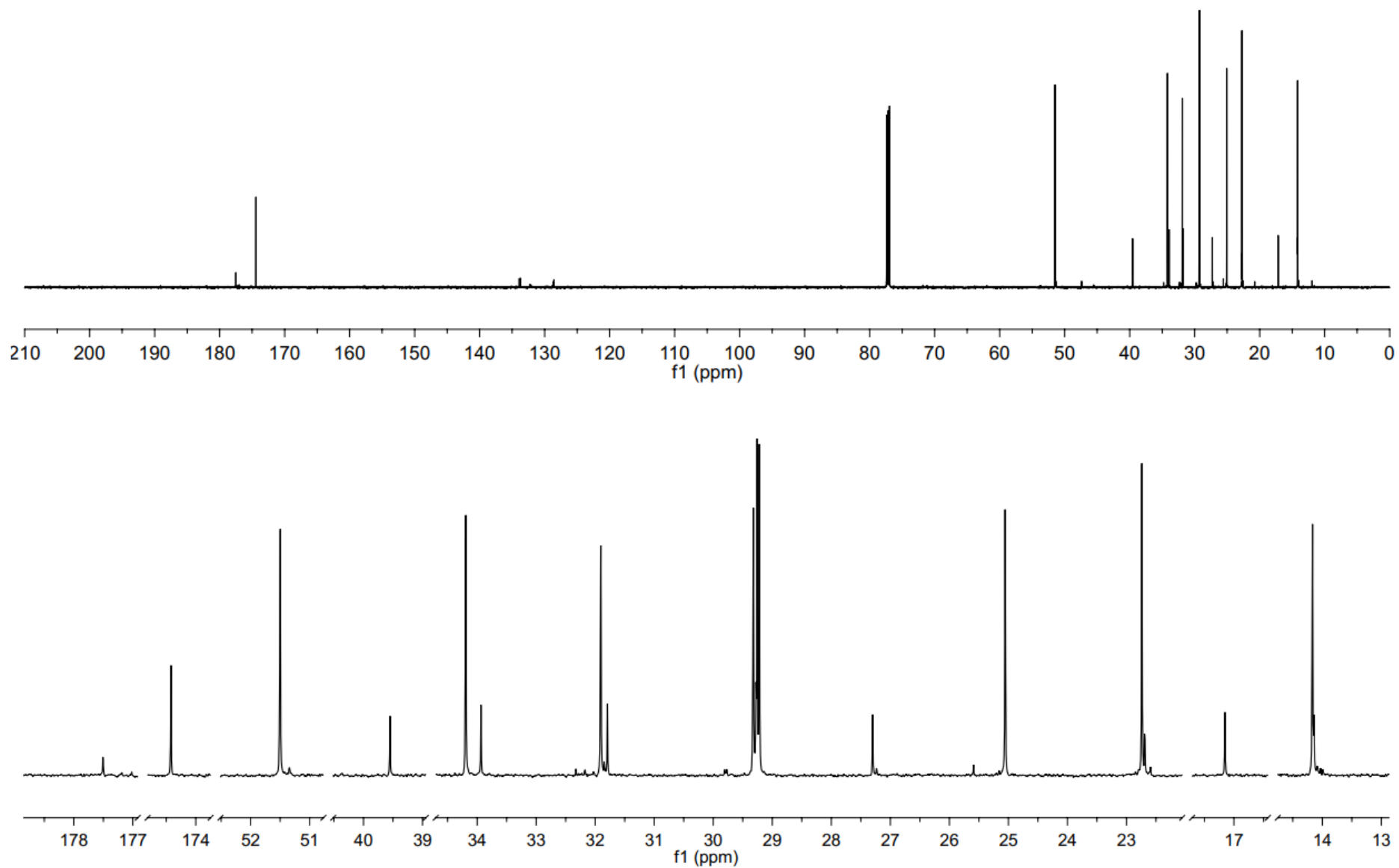
Alkene	1-Octene (3)	Styrene (4)	β -methylstyrene (12)
	0.474 g, 4.23 mmol	0.442 g, 4.25 mmol	0.501 g, 4.24 mmol
Pd(OAc) ₂	0.0476 g, 0.212 mmol	0.0476 g, 0.212 mmol	0.0481 g, 0.214 mmol
Al(OTf) ₃	0.201 g, 0.424 mmol	0.201 g, 0.424 mmol	0.202 g, 0.426 mmol
PPh ₃	0.223 g, 0.850 mmol	0.224 g, 0.854 mmol	0.226 g, 0.862 mmol
Xylene	0.504 g, 4.75 mmol	0.499 g, 4.70 mmol	0.501 g, 4.72 mmol
Products	5 and 6	7 and 8	13, 14 and 15
Alkene	Allylbenzene (9)	1-allyl-4-methoxybenzene (10)	1-allyl-2-methoxybenzene (11)
	0.502 g, 4.25 mmol	0.629 g, 4.24 mmol	0.627 g, 4.23 mmol
Pd(OAc) ₂	0.0496 g, 0.221 mmol	0.0478 g, 0.213 mmol	0.0477 g, 0.212 mmol
Al(OTf) ₃	0.202 g, 0.426 mmol	0.201 g, 0.424 mmol	0.202 g, 0.426 mmol
PPh ₃	0.225 g, 0.858 mmol	0.223 g, 0.850 mmol	0.224 g, 0.854 mmol
Xylene	0.502 g, 4.73 mmol	0.500 g, 4.71 mmol	0.501 g, 4.72 mmol
Products	13, 14 and 15	16, 17 and 18	19, 20 and 21

All ¹H NMR and ¹³C NMR spectra were recorded on a Bruker AVANCE II AM 600 FT-spectrometer at 293 K, with deuteriochloroform (CDCl₃) as solvent. Chemical shifts are reported in parts per million (ppm) with the solvent residual resonance at 7.26 ppm for proton spectra and 77.2 ppm for carbon spectra as reference signal.

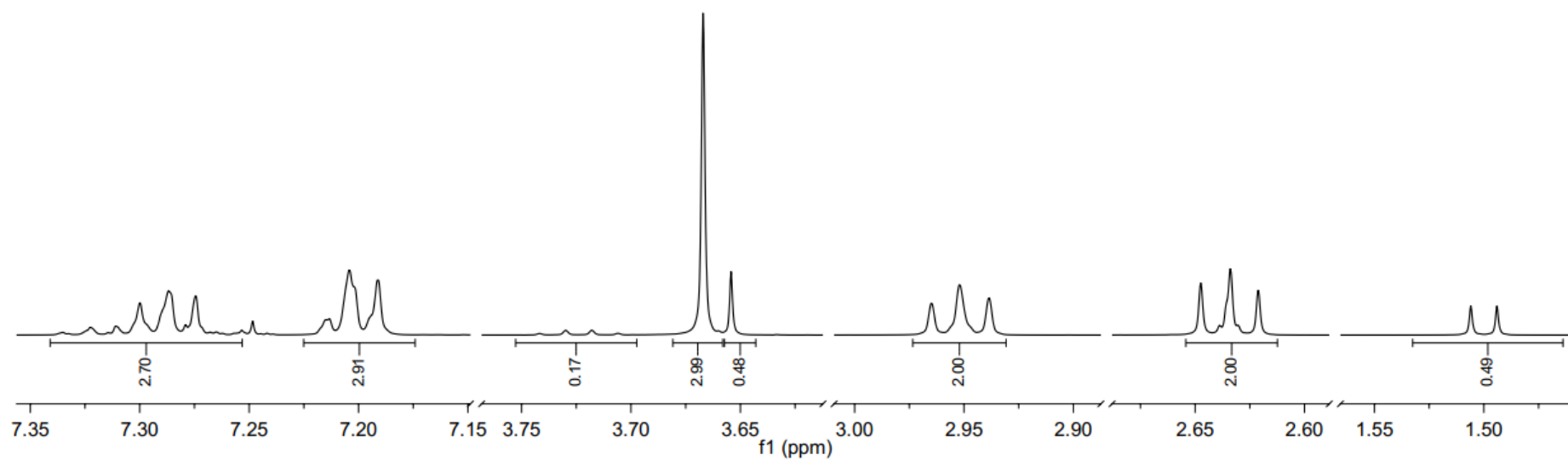
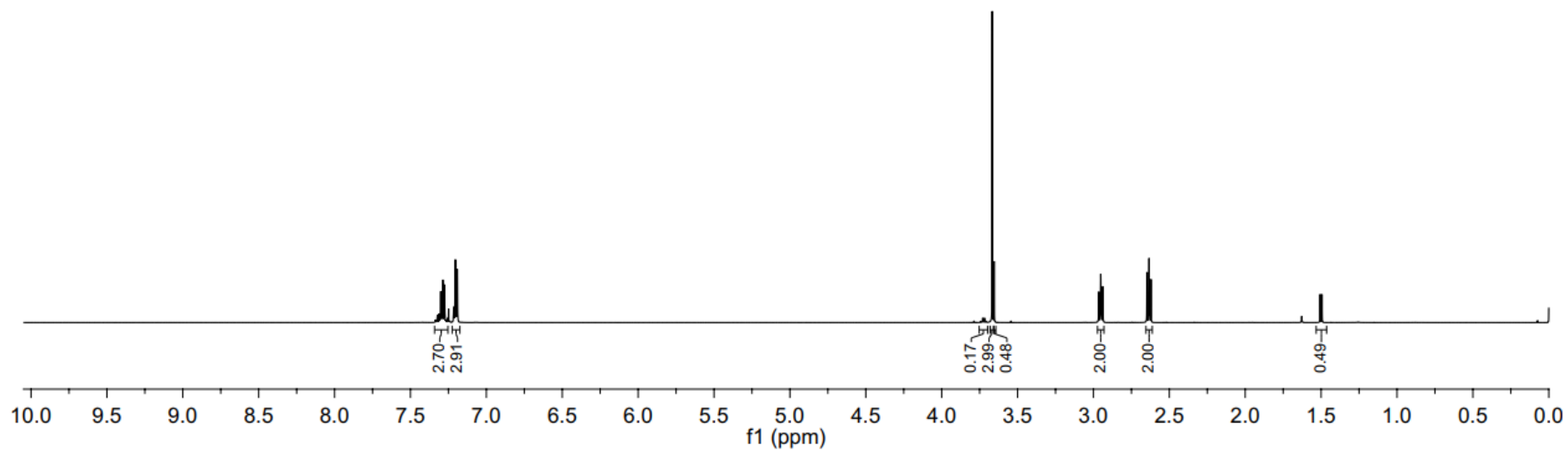
¹H NMR (600 MHz, CDCl₃): Methyl nonanoate (**5**) and methyl 2-methyloctanoate (**6**)



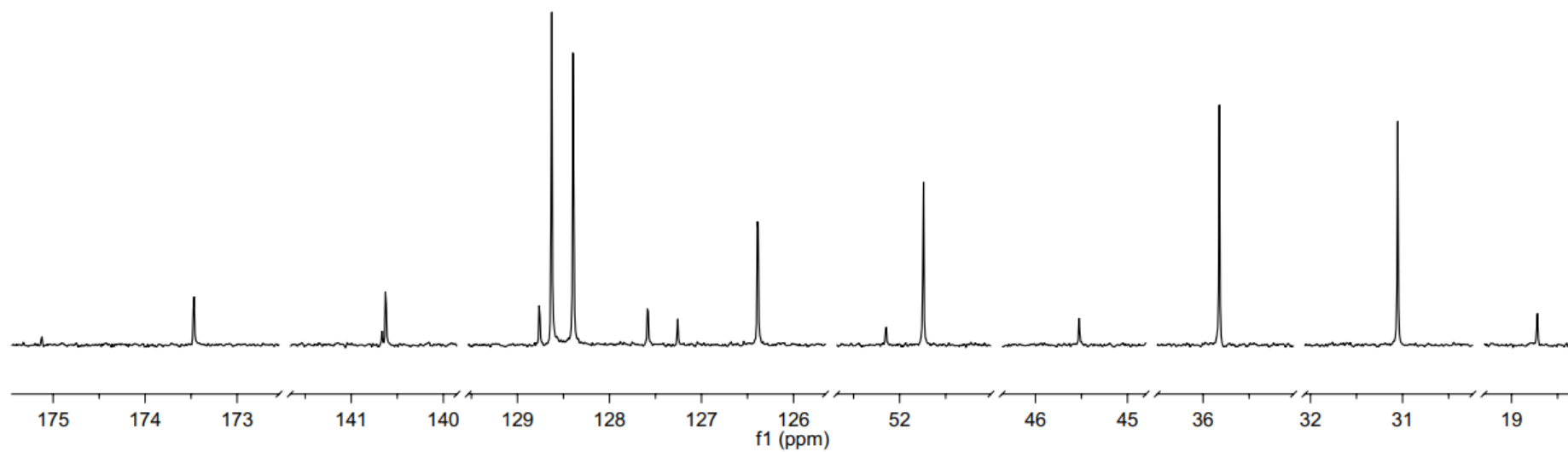
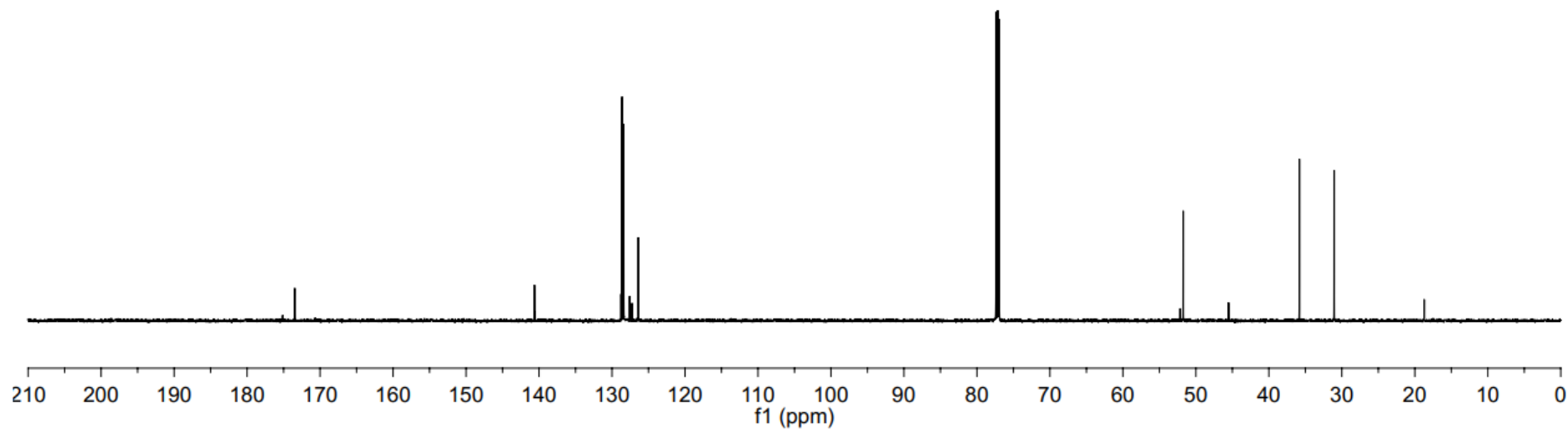
^{13}C NMR (151 MHz, CDCl_3): Methyl nonanoate (**5**) and methyl 2-methyloctanoate (**6**)



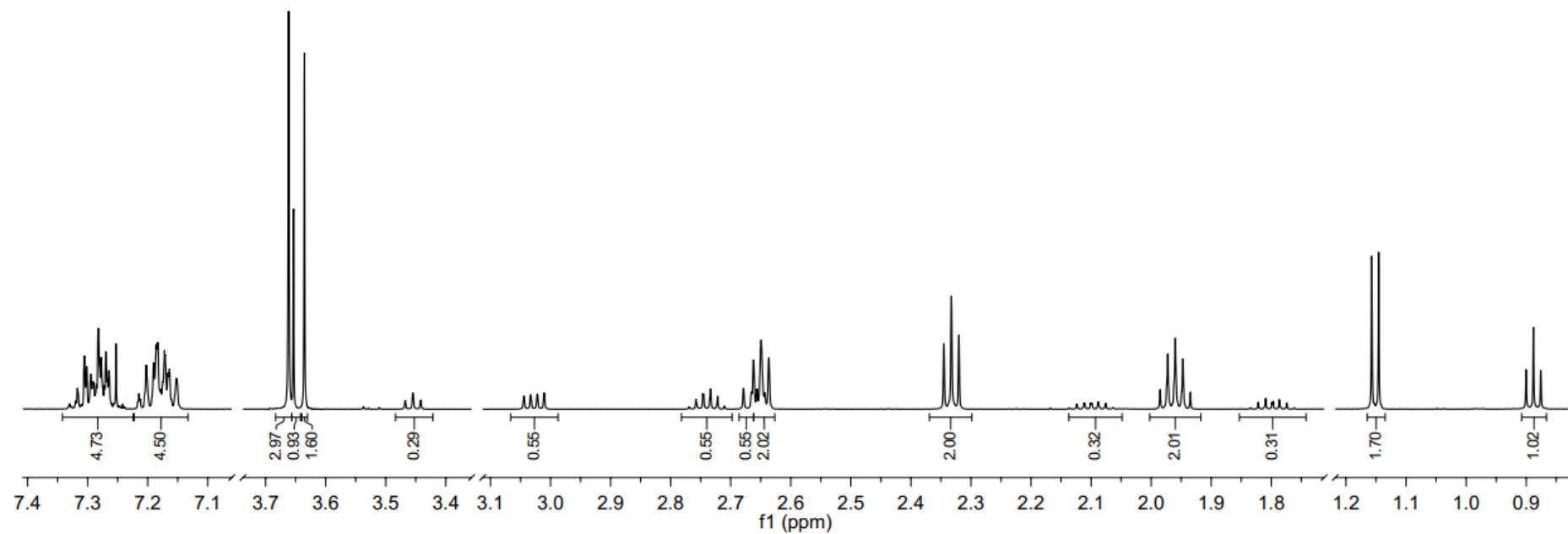
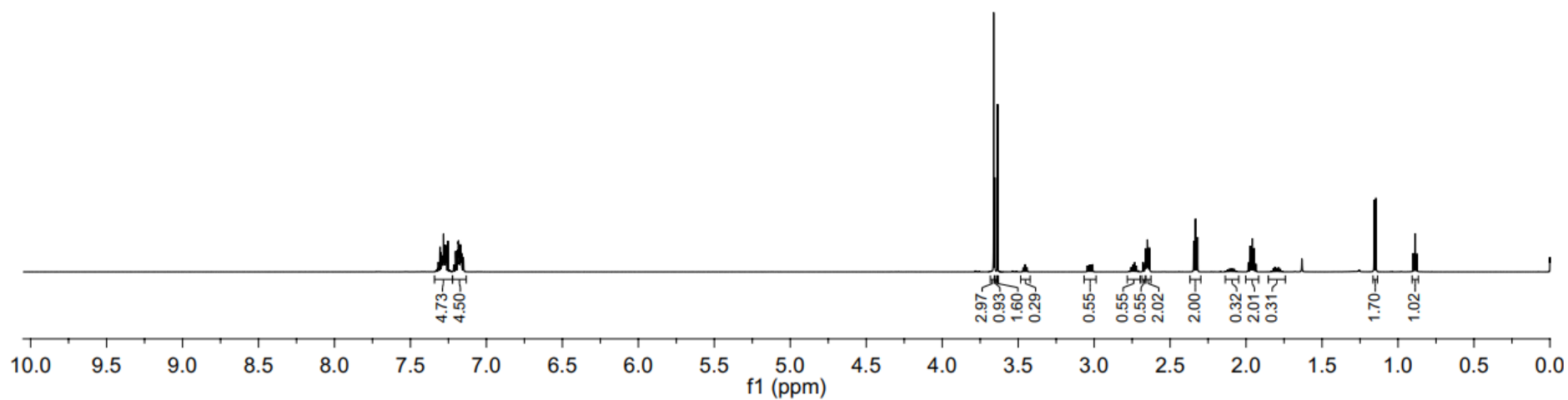
¹H NMR (600 MHz, CDCl₃): Methyl 3-phenylpropanoate (7) and methyl 2-phenylpropanoate (8)



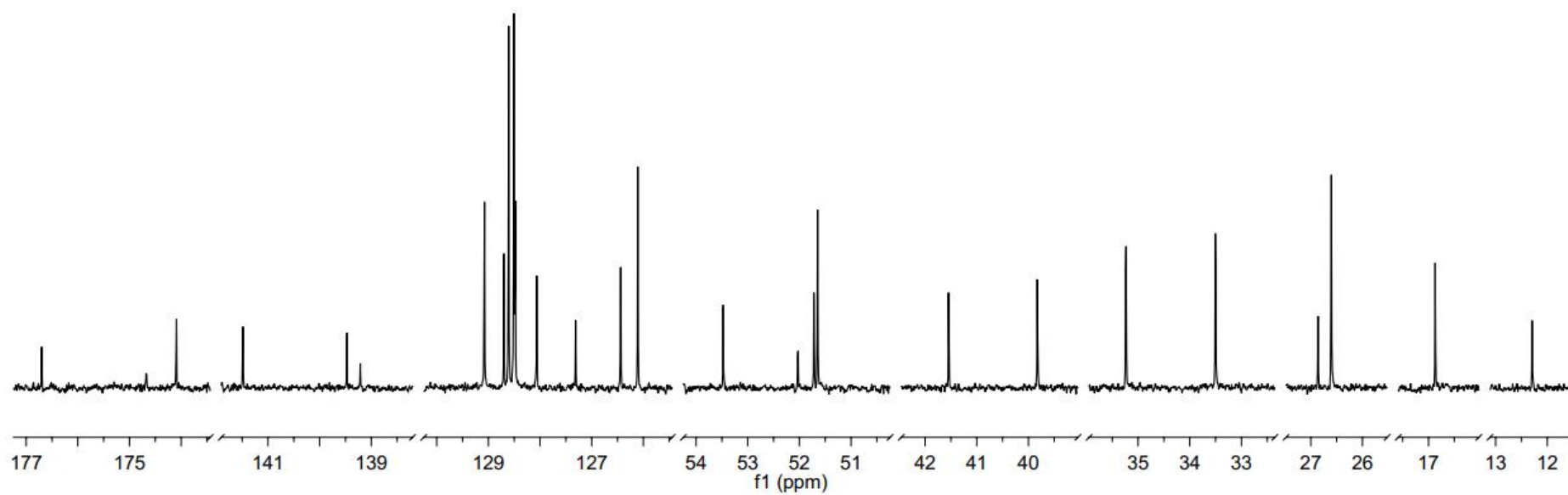
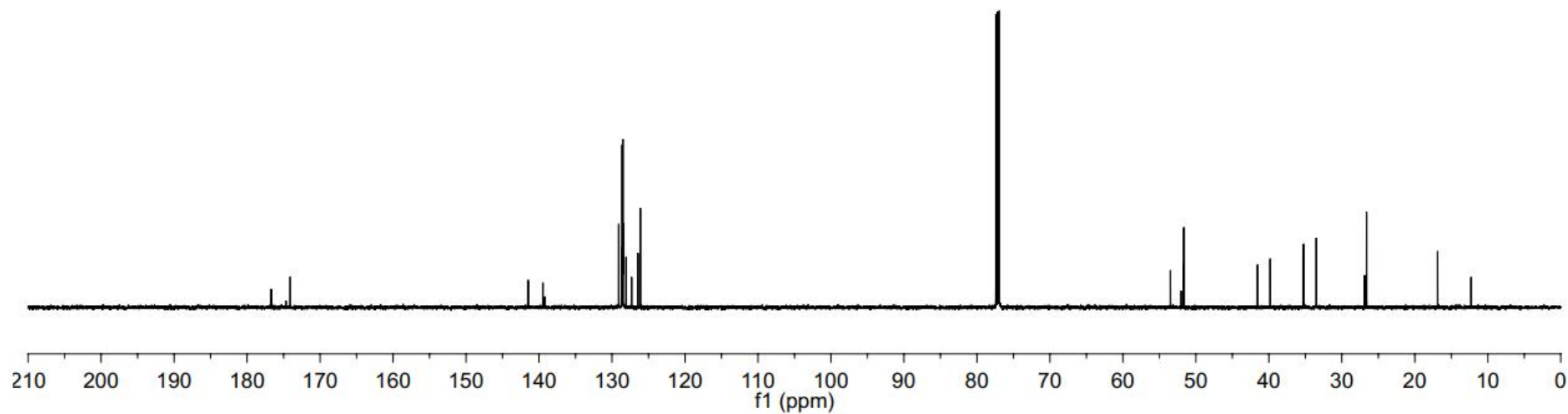
^{13}C NMR (151 MHz, CDCl_3): Methyl 3-phenylpropanoate (**7**) and methyl 2-phenylpropanoate (**8**)



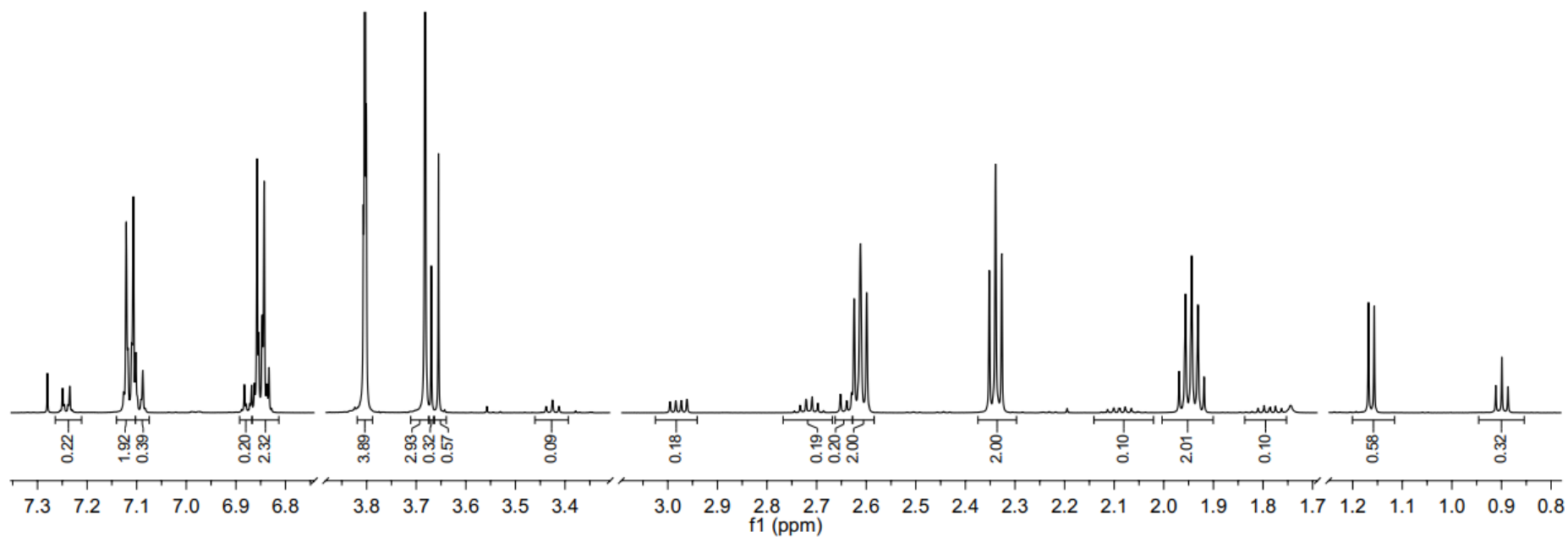
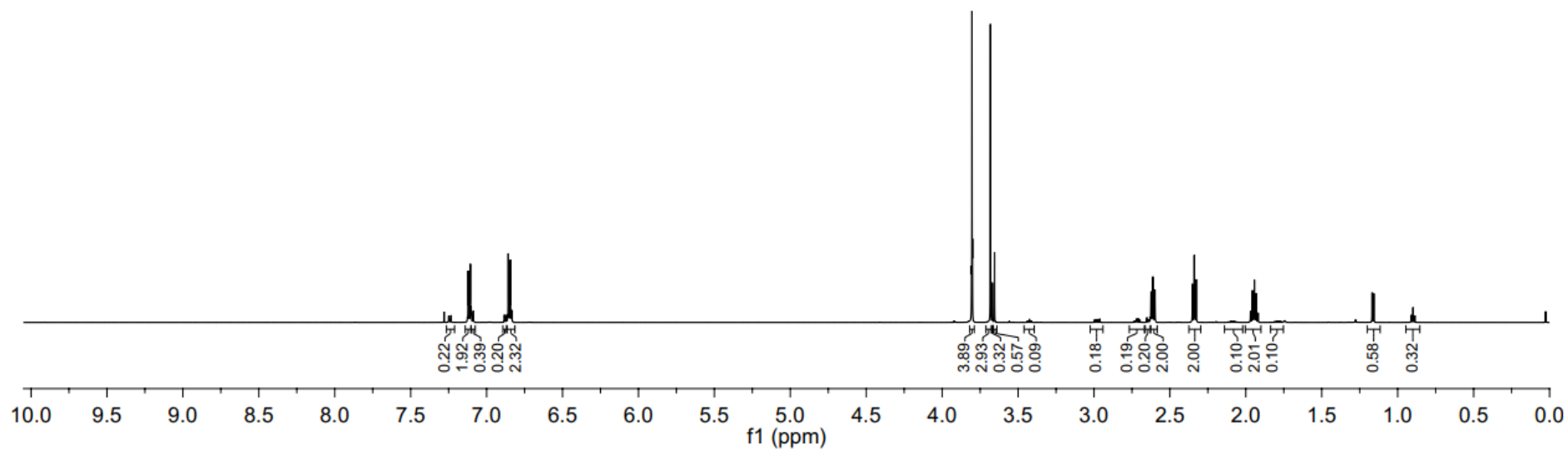
¹H NMR (600 MHz, CDCl₃): Methyl 4-phenylbutanoate (**13**), methyl 2-methyl-3-phenylpropanoate (**14**) and methyl 2-phenylbutanoate (**15**)



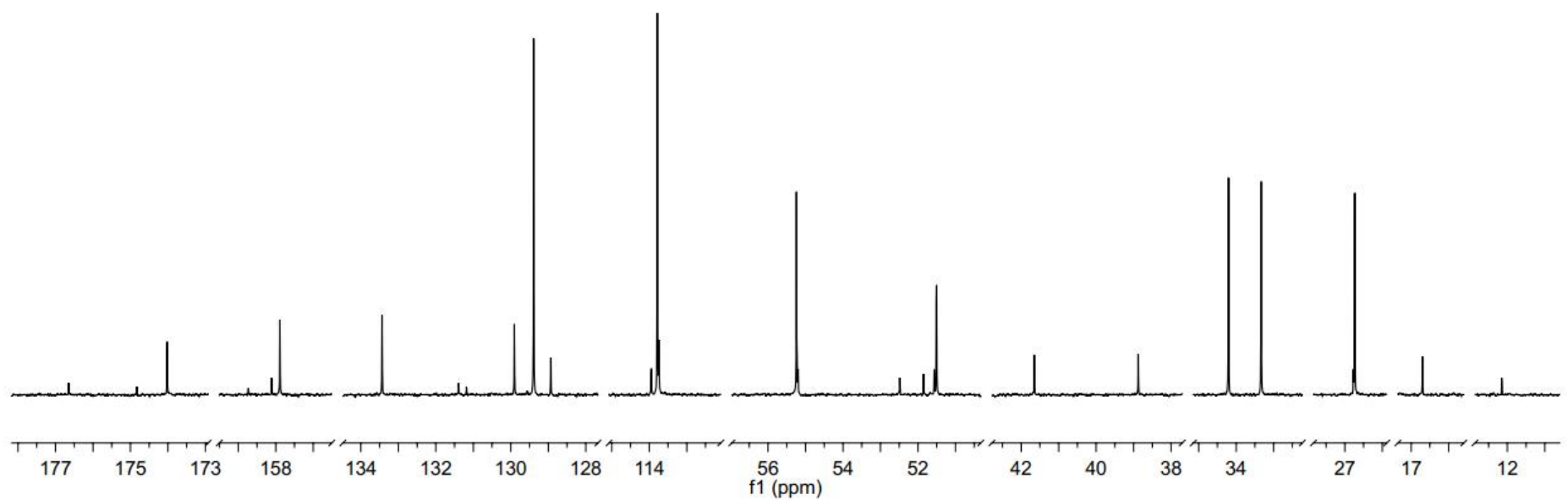
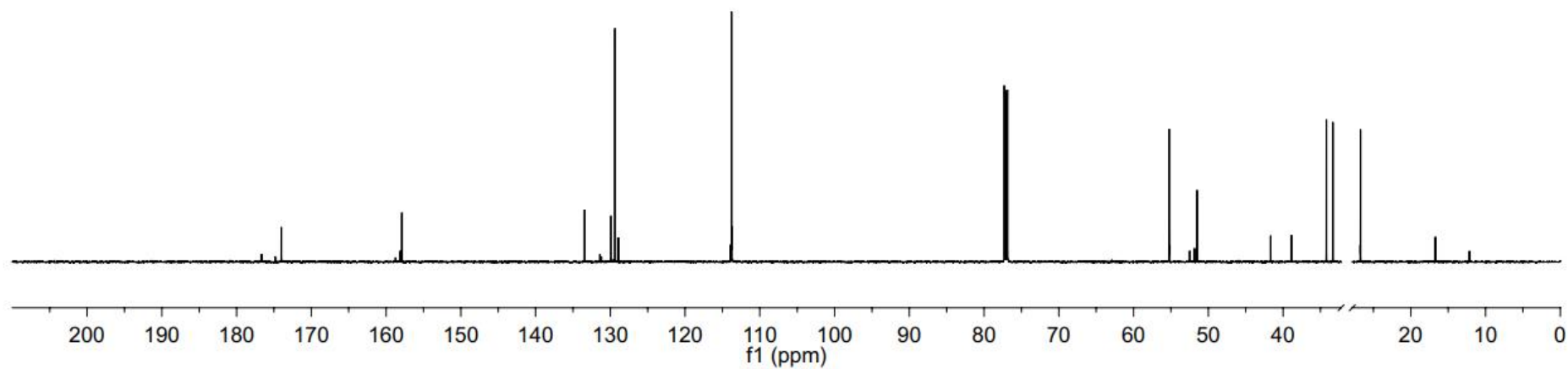
^{13}C NMR (151 MHz, CDCl_3): Methyl 4-phenylbutanoate (**13**), methyl 2-methyl-3-phenylpropanoate (**14**) and methyl 2-phenylbutanoate (**15**)



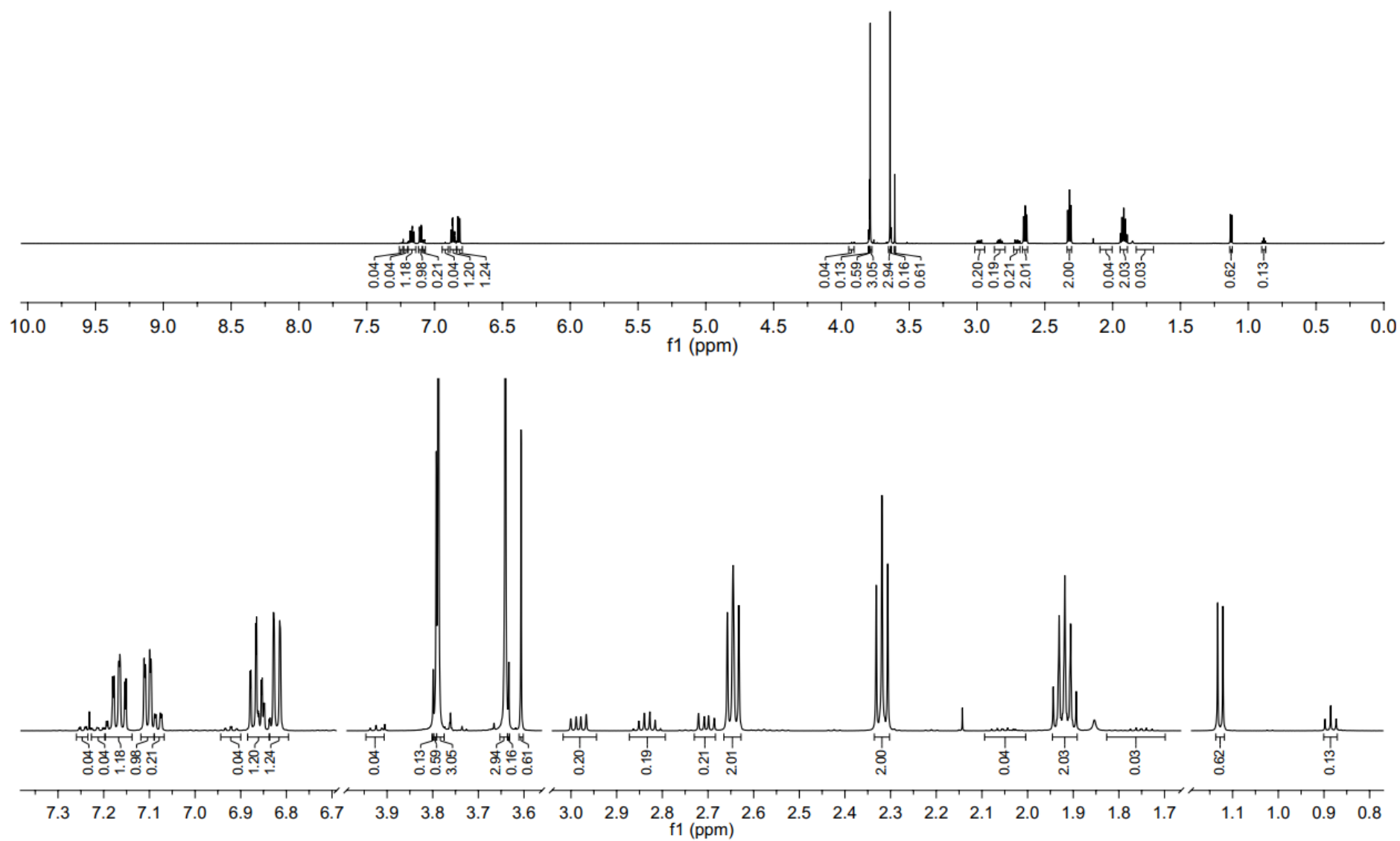
¹H NMR (600 MHz, CDCl₃): Methyl 4-(4'-methoxyphenyl)butanoate (**16**), methyl 3-(4'-methoxyphenyl)-2-methylpropanoate (**17**) and methyl 2-(4'-methoxyphenyl)butanoate (**18**)



^{13}C NMR (151 MHz, CDCl_3): Methyl 4-(4'-methoxyphenyl)butanoate (**16**), methyl 3-(4'-methoxyphenyl)-2-methylpropanoate (**17**) and methyl 2-(4'-methoxyphenyl)butanoate (**18**)



¹H NMR (600 MHz, CDCl₃): Methyl 4-(2'-methoxyphenyl)butanoate (**19**), methyl 3-(2'-methoxyphenyl)-2-methylpropanoate (**20**) and methyl 2-(2'-methoxyphenyl)butanoate (**21**)



^{13}C NMR (151 MHz, CDCl_3): Methyl 4-(2'-methoxyphenyl)butanoate (**19**), methyl 3-(2'-methoxyphenyl)-2-methylpropanoate (**20**) and methyl 2-(2'-methoxyphenyl)butanoate (**21**)

