

Supplementary materials

Antioxidants as molecular probes: Structurally novel dihydro-*m*-terphenyls as turn-on fluorescence chemodosimeters for biologically relevant oxidants

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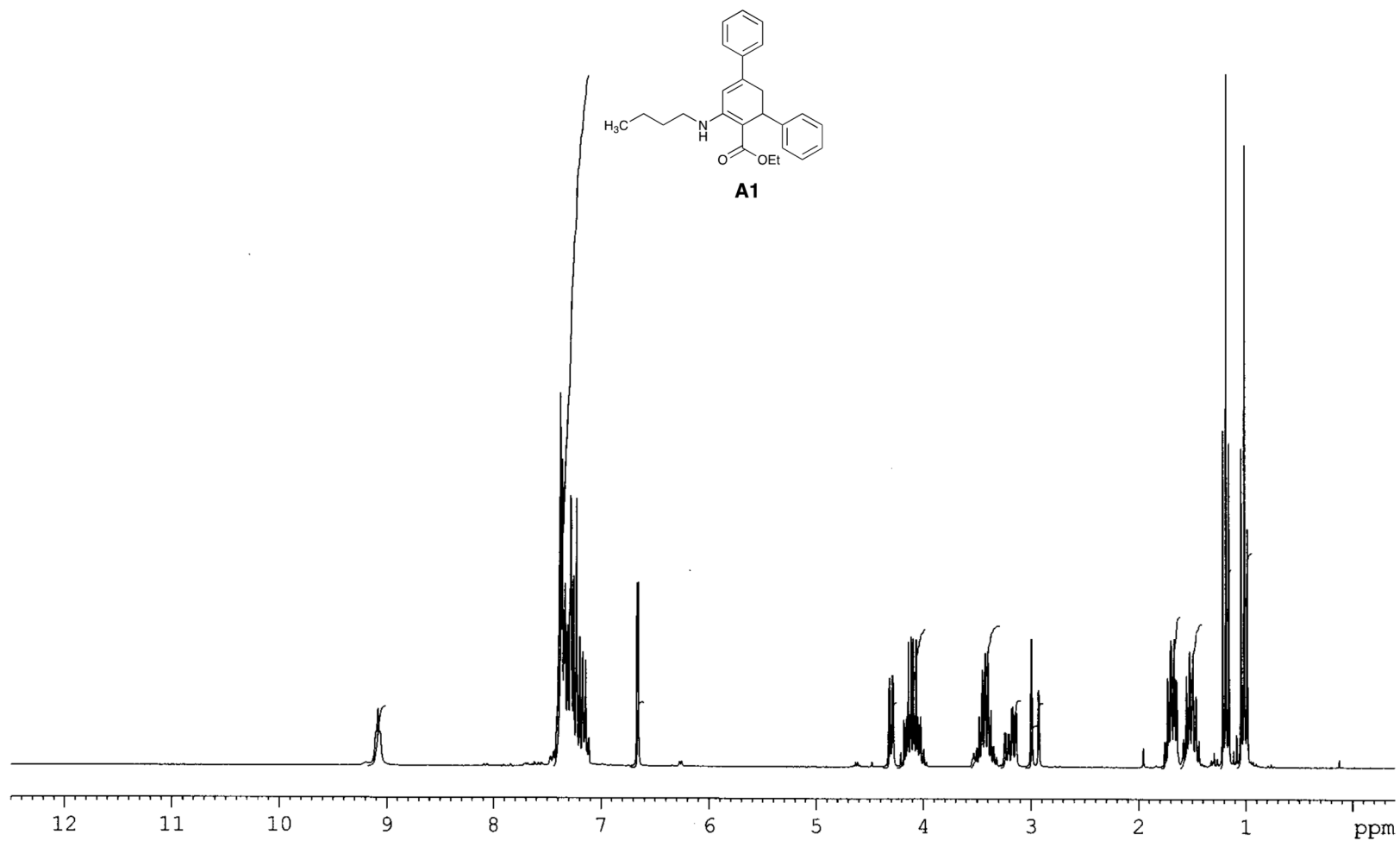
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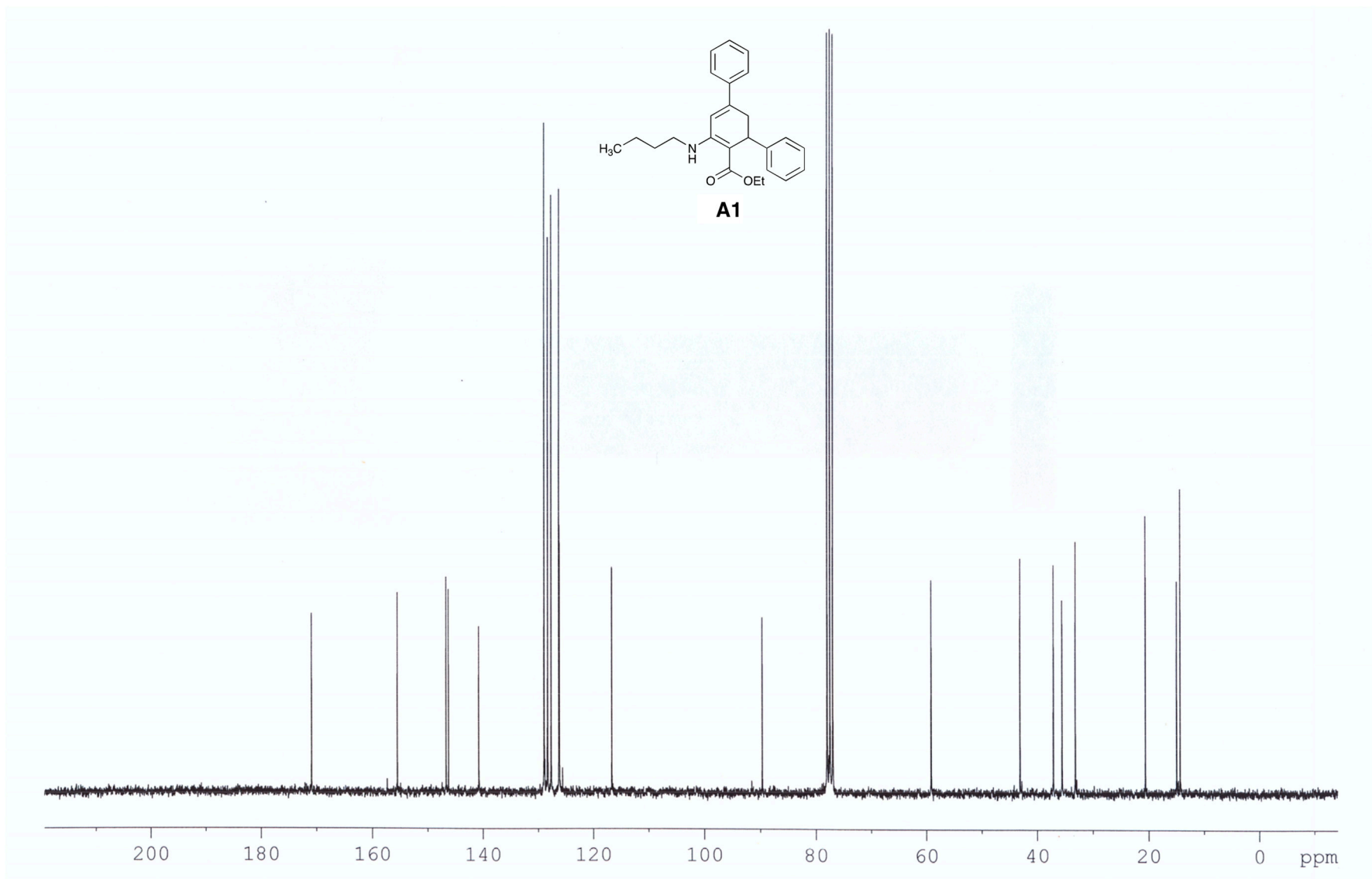
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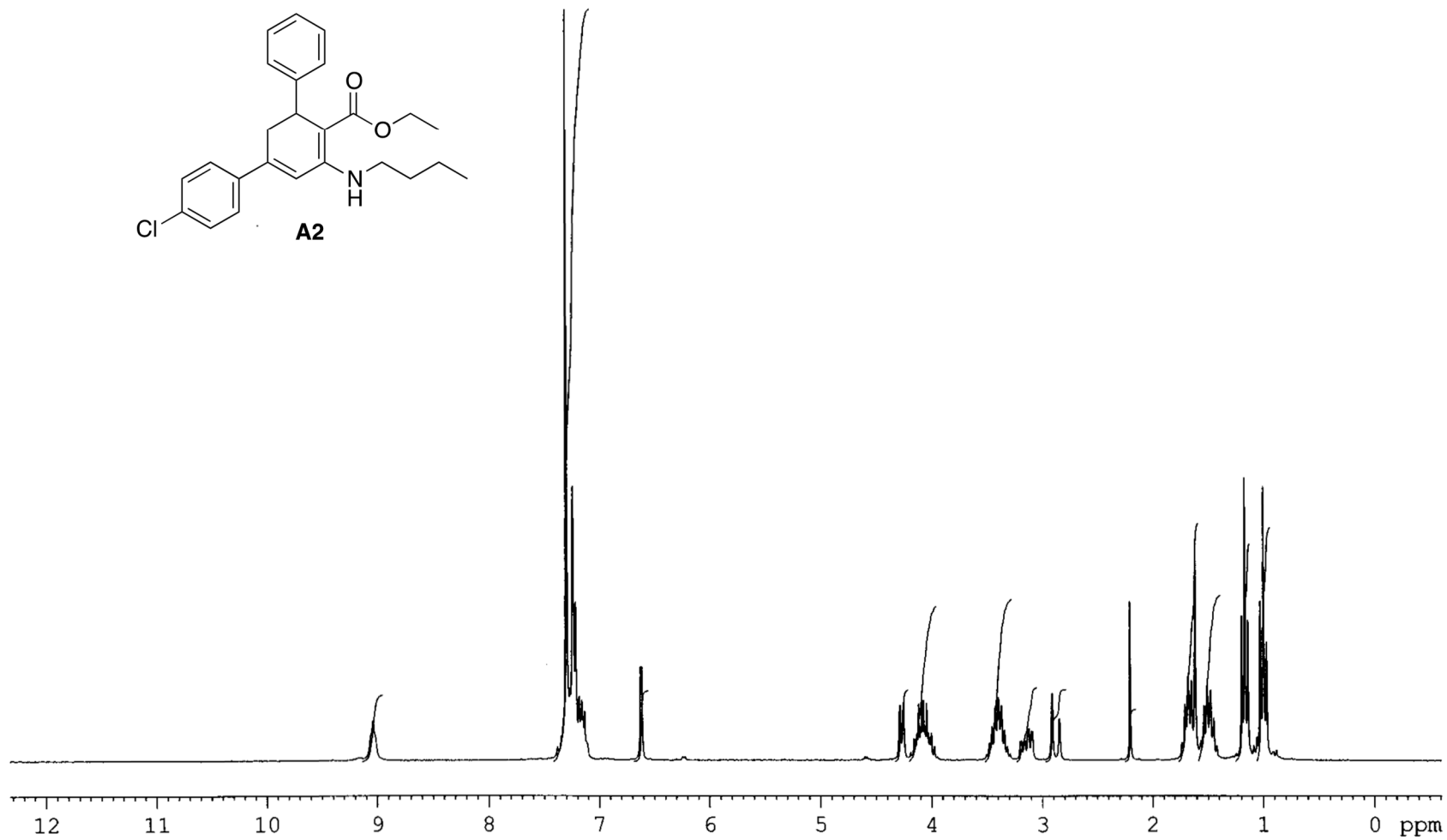
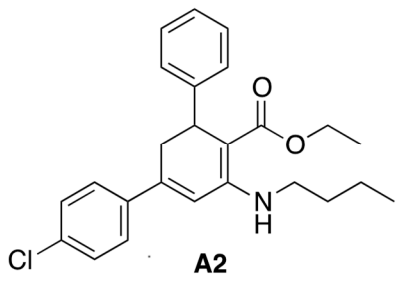
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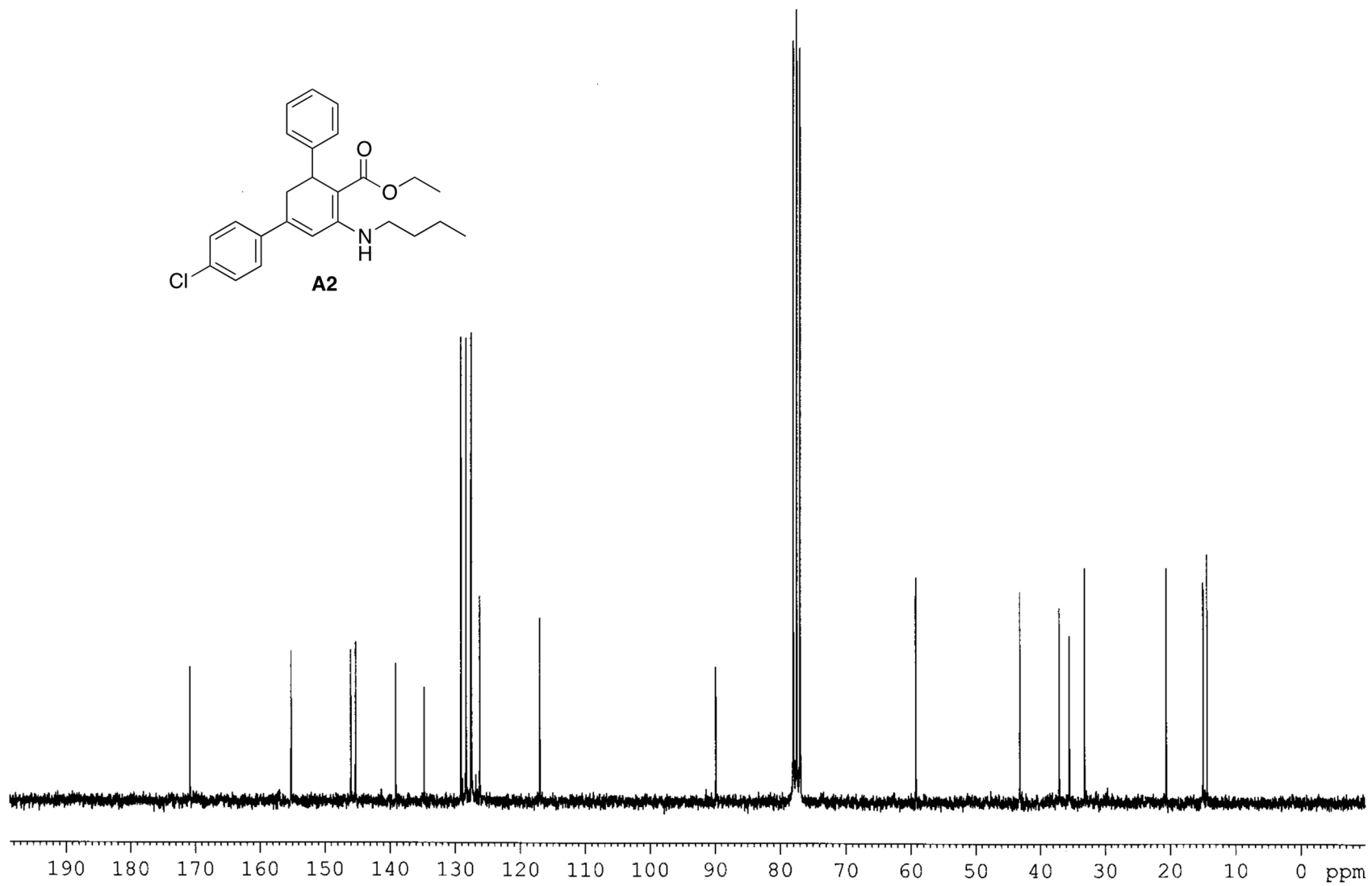
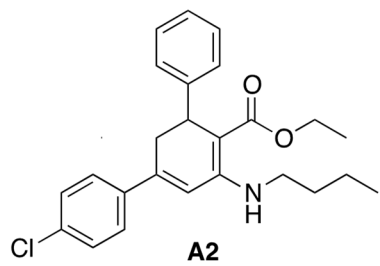
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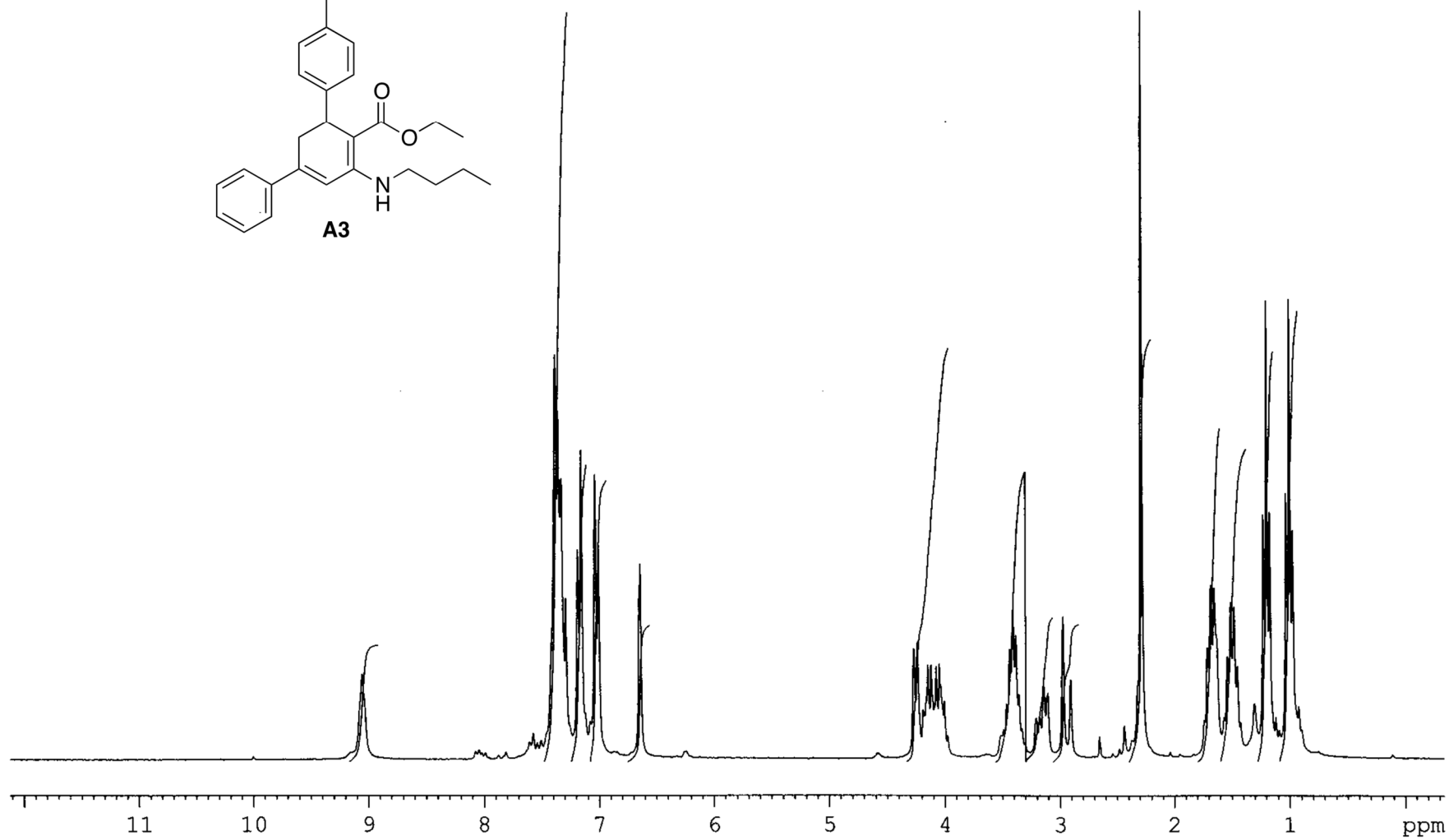
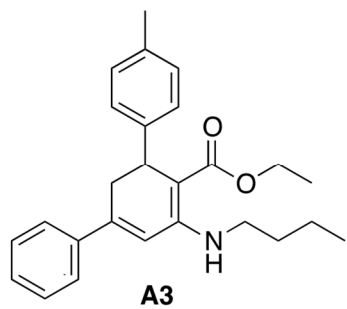
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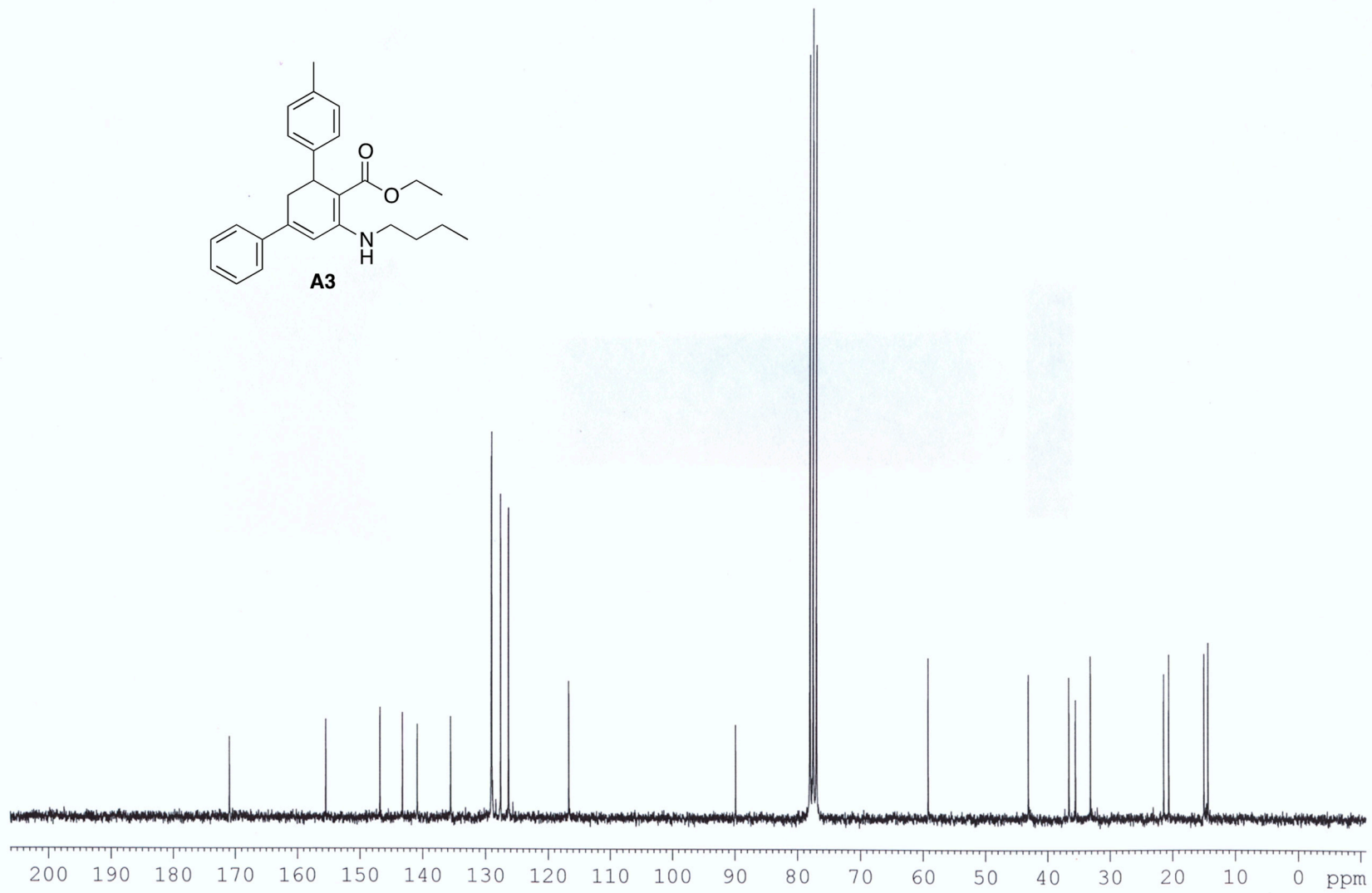
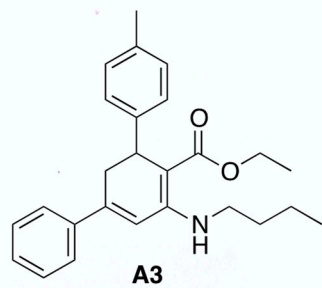


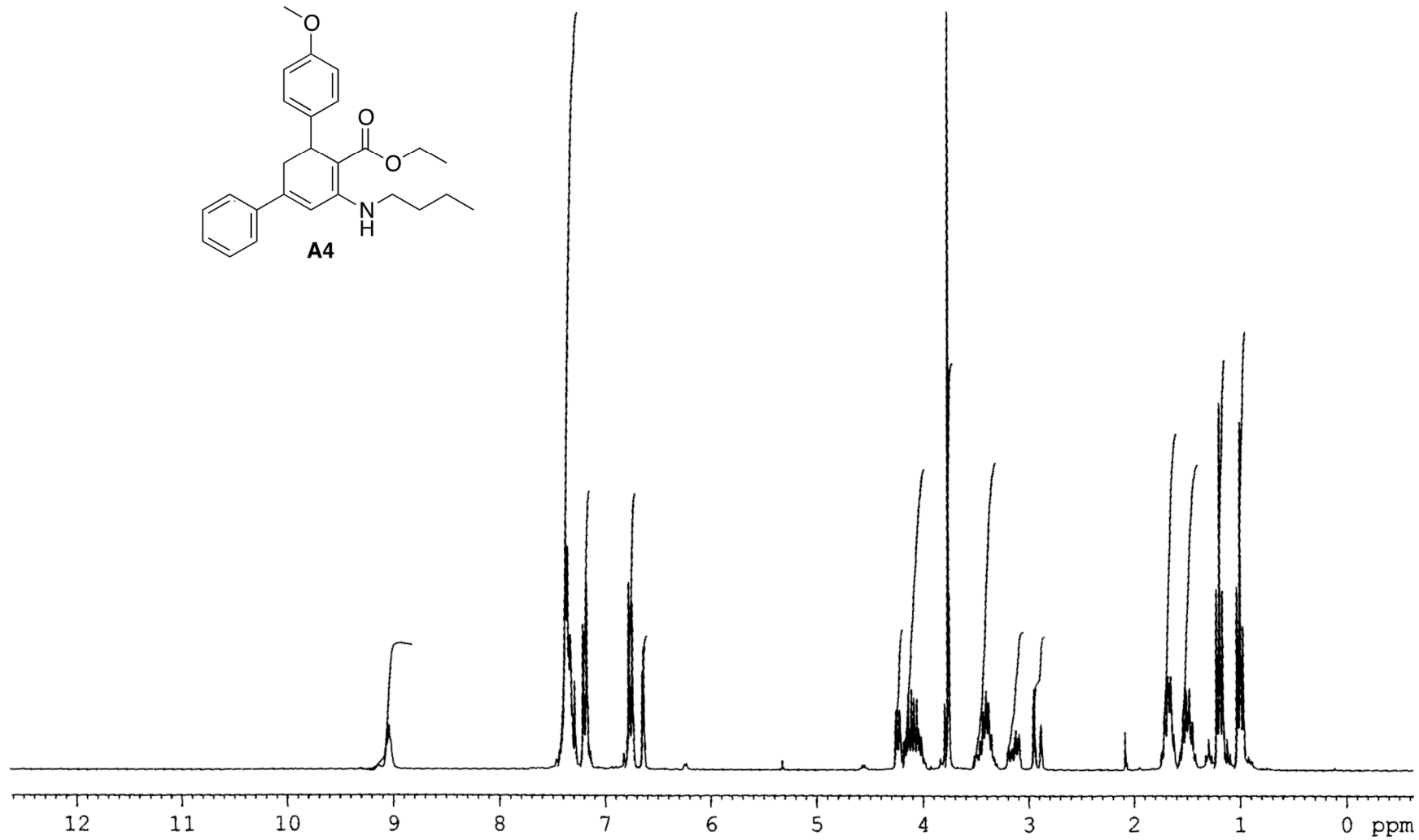
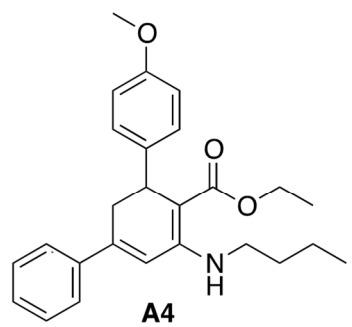


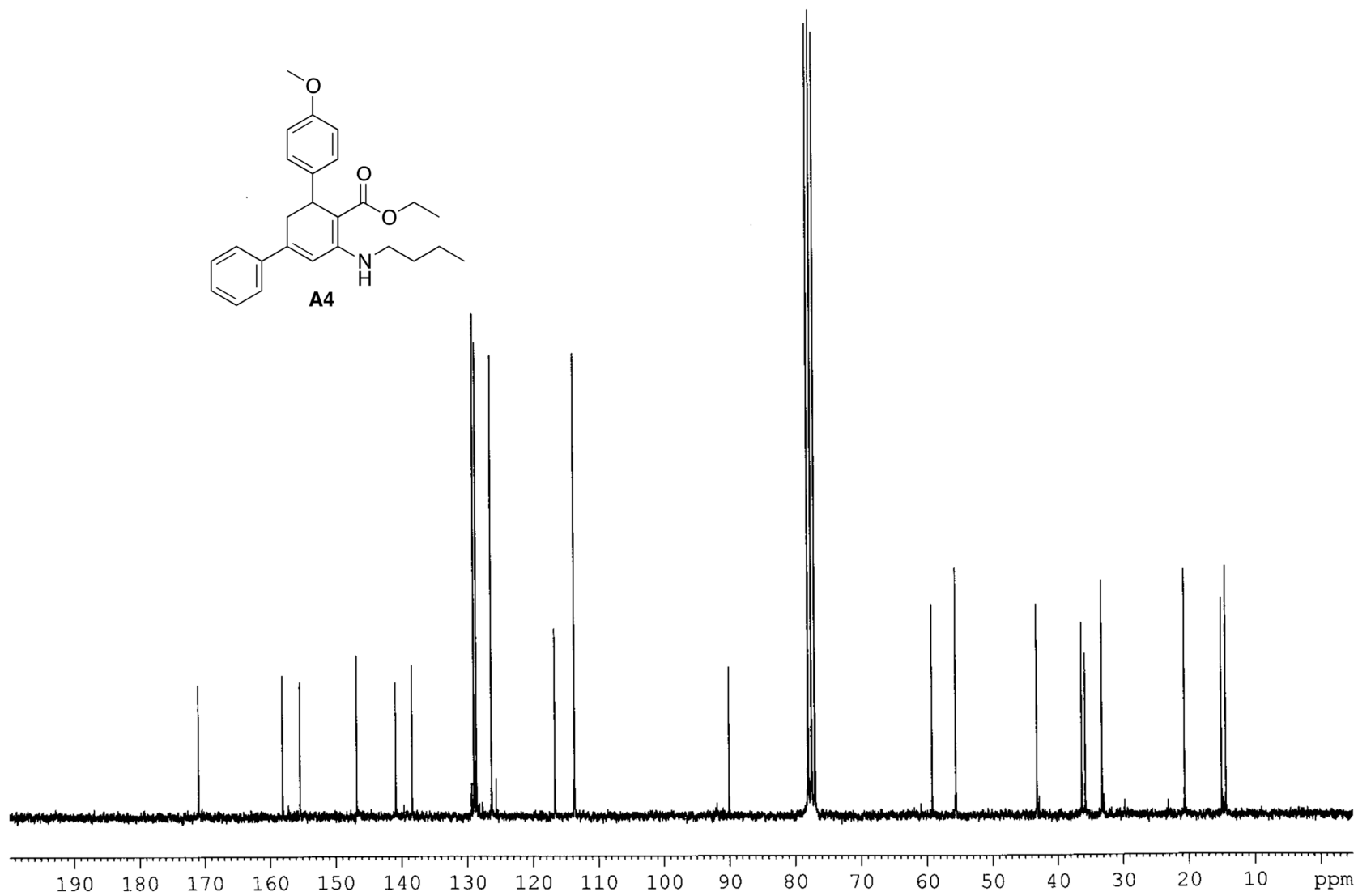
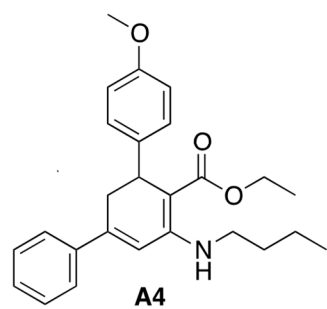


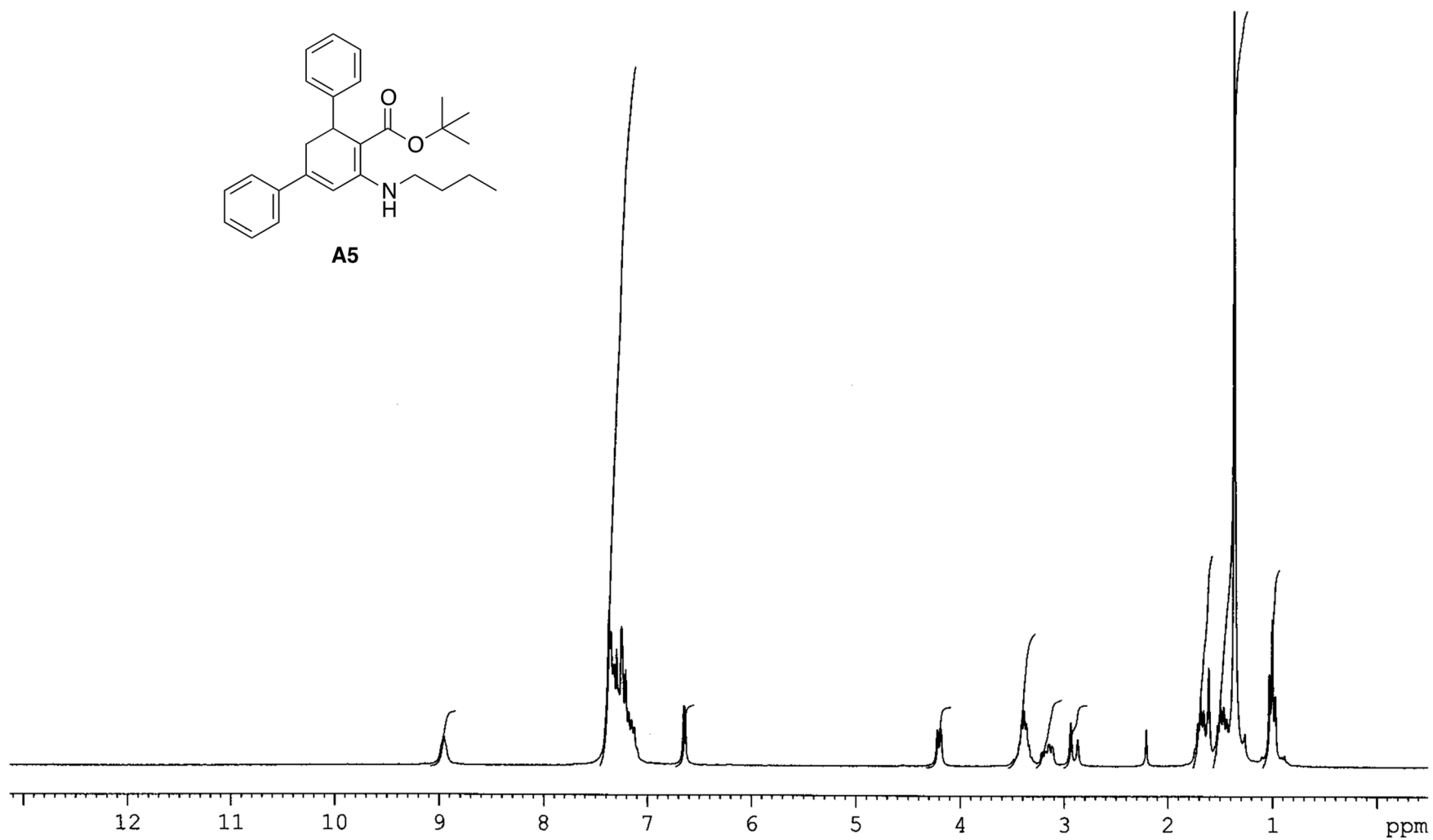
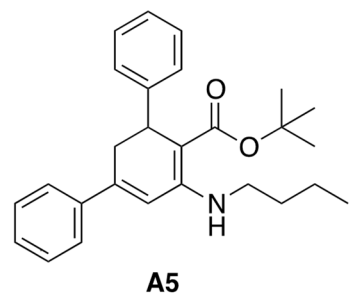


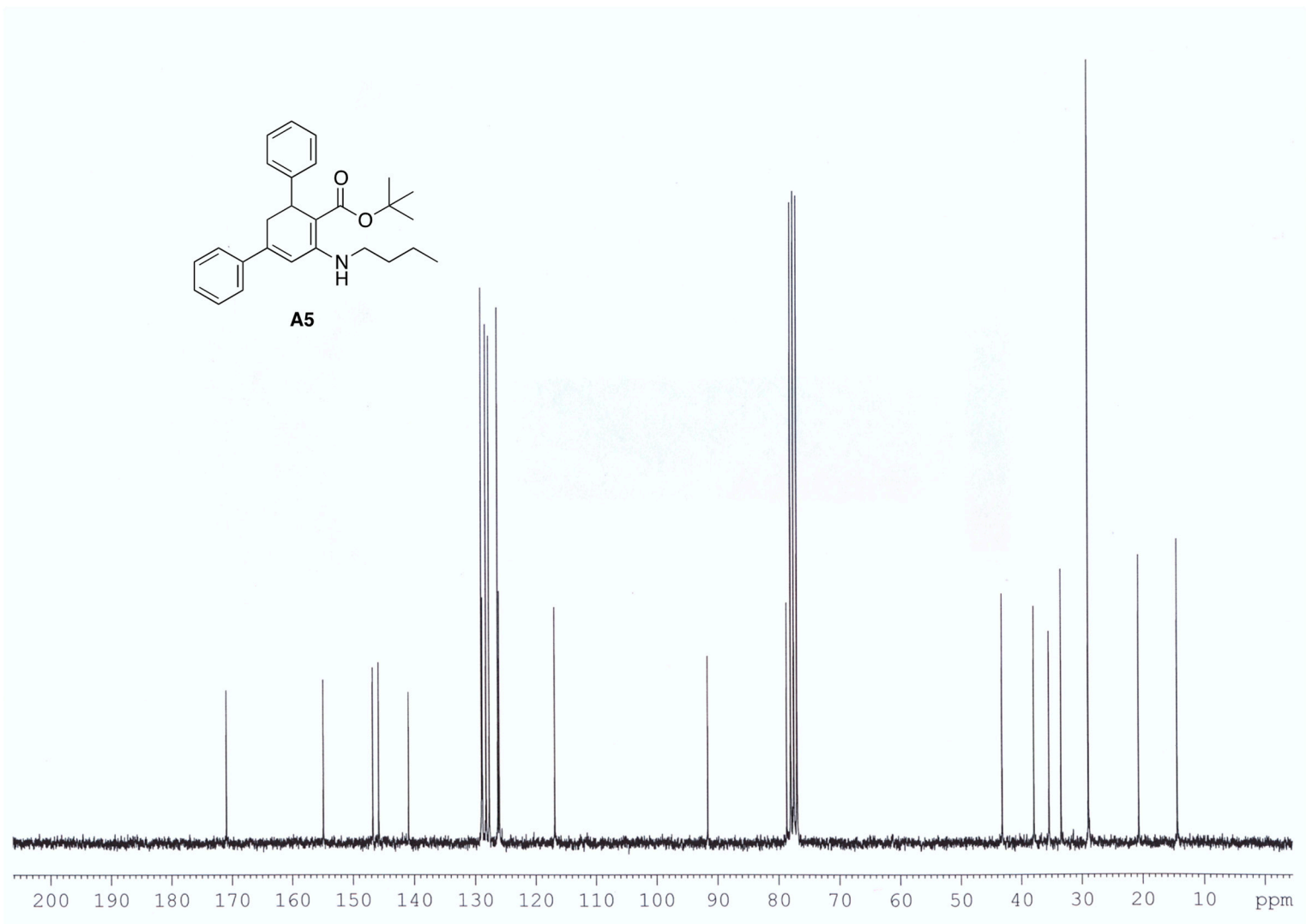
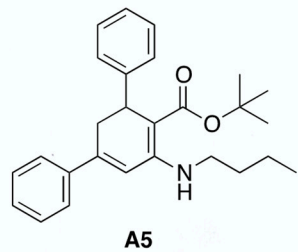


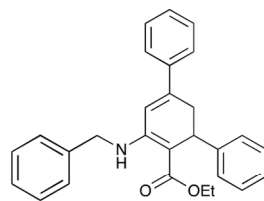




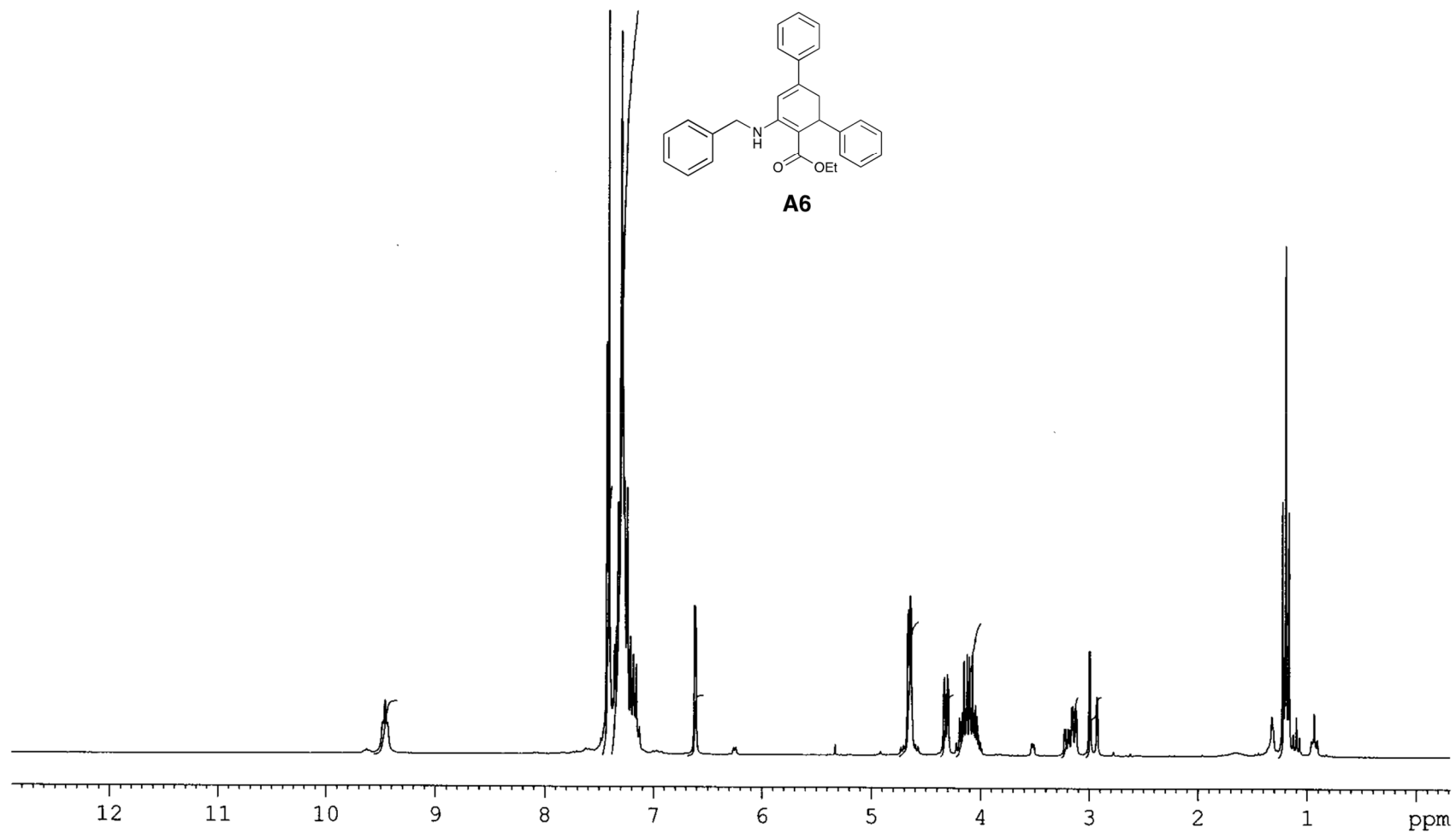


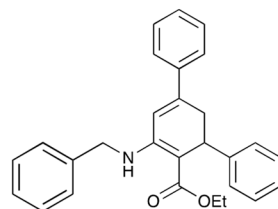




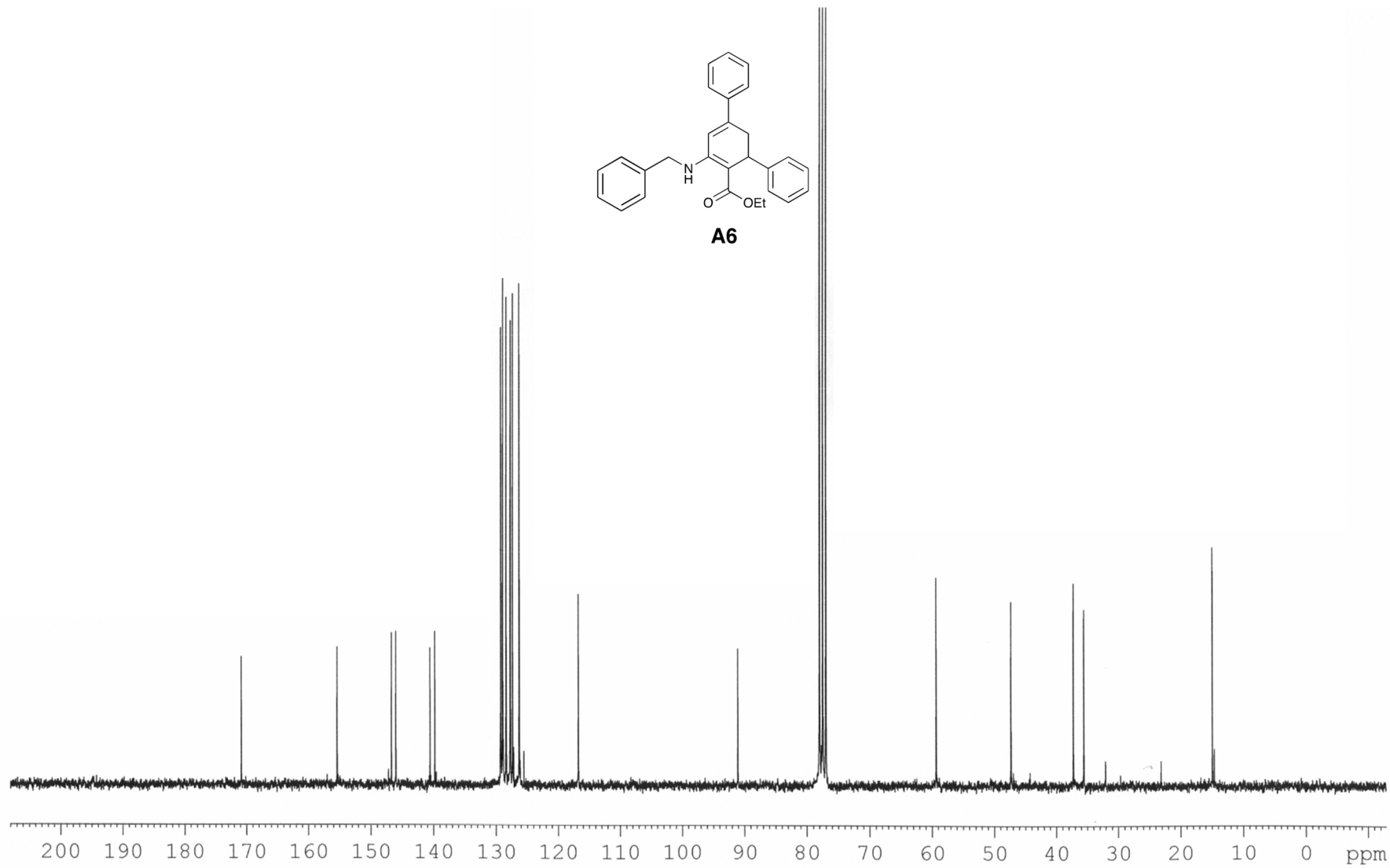


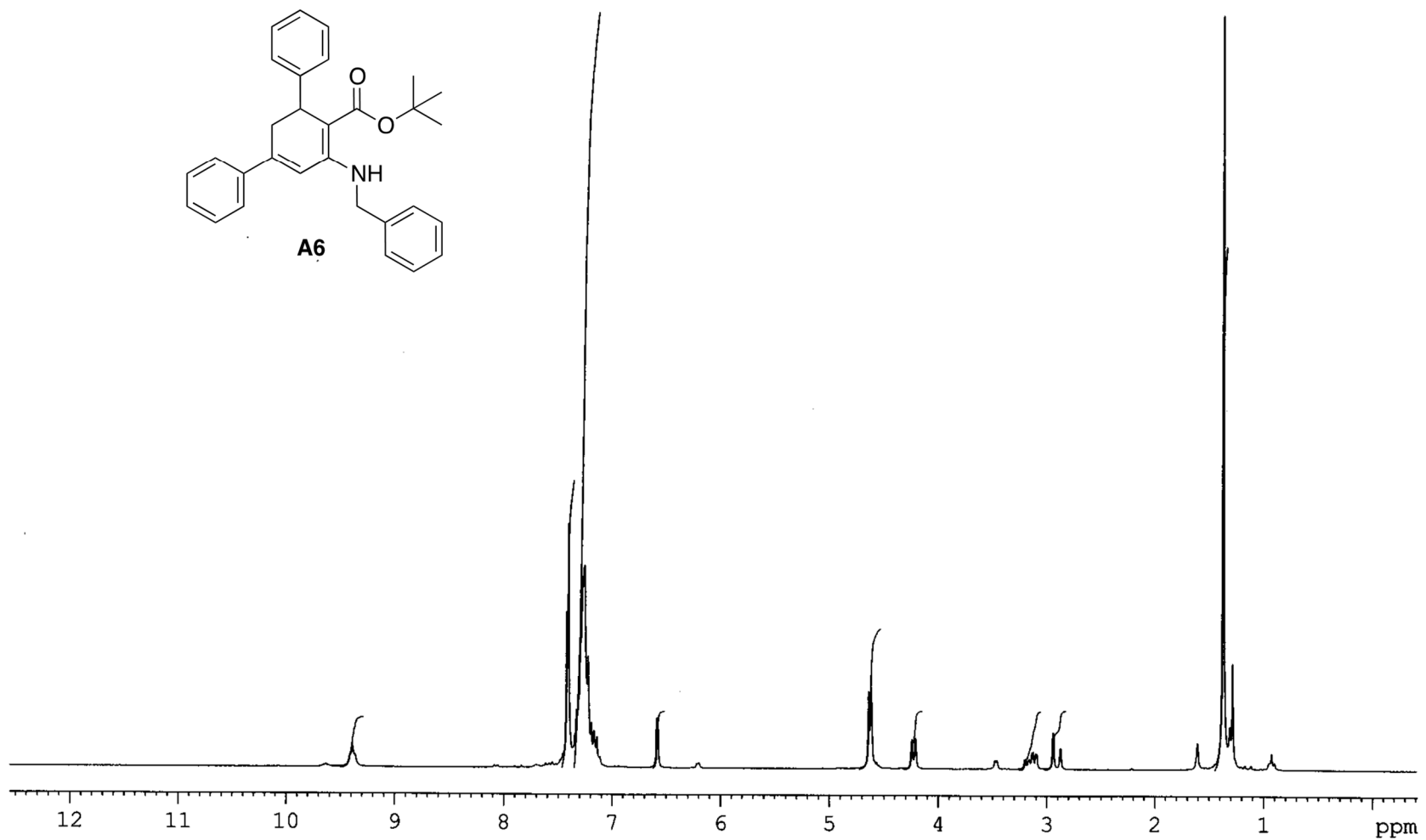
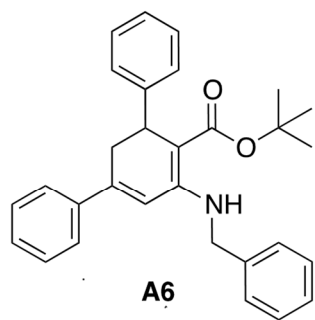
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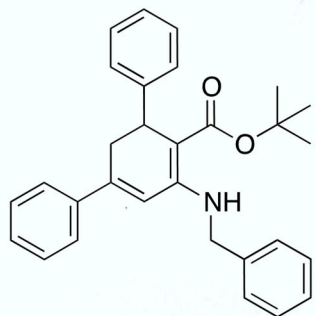




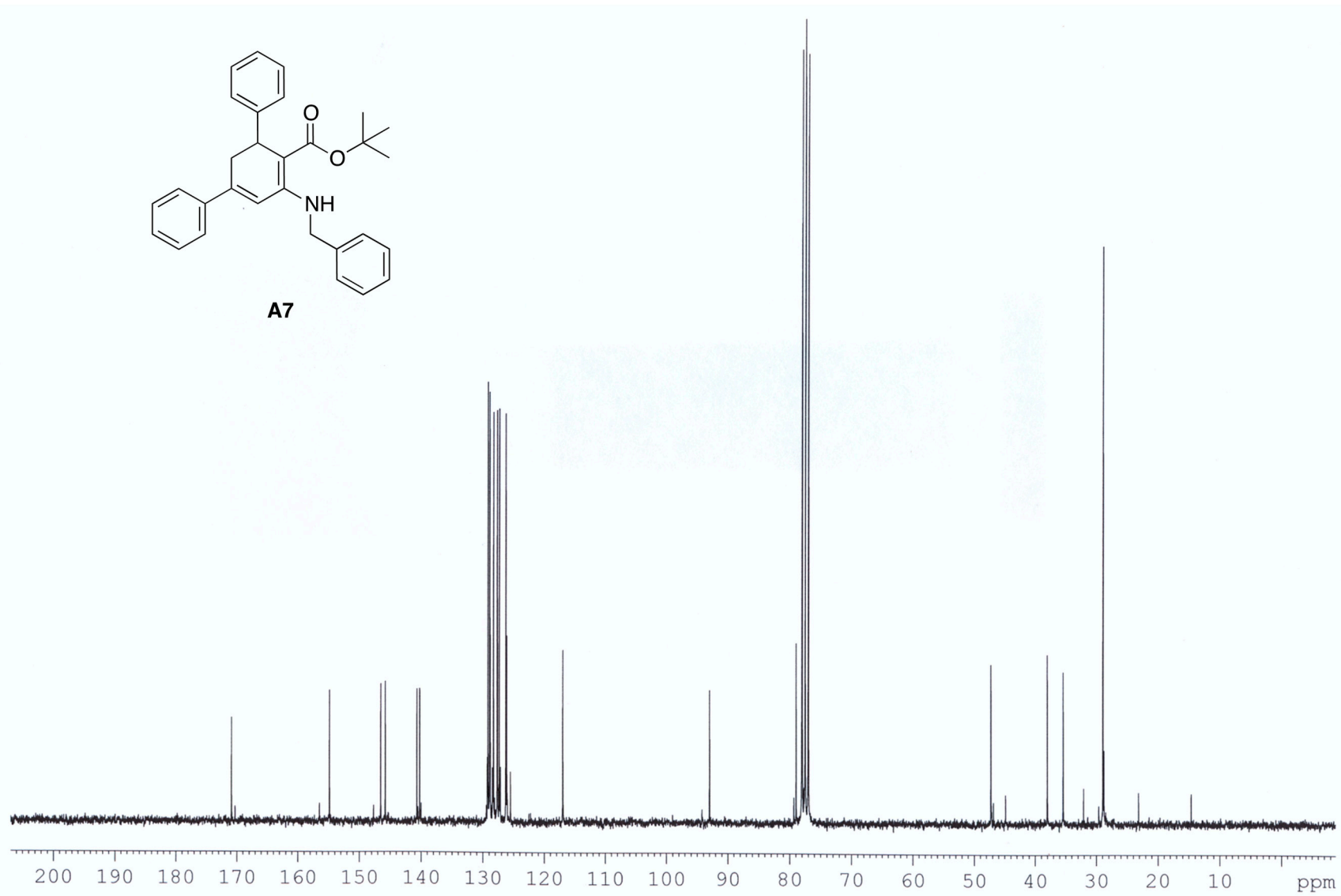
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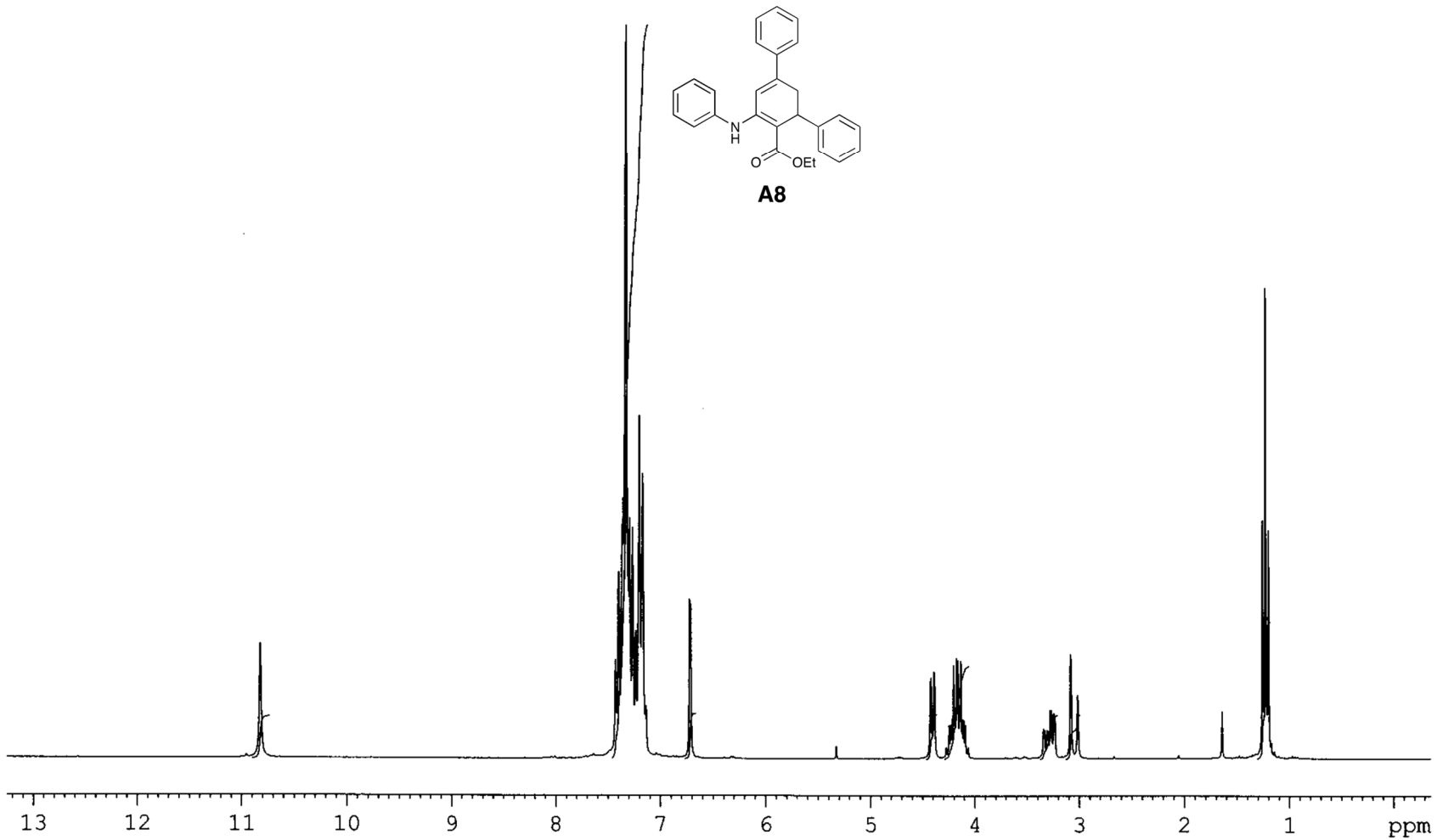
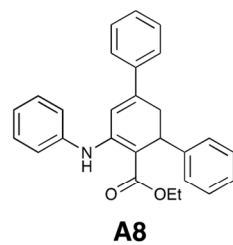


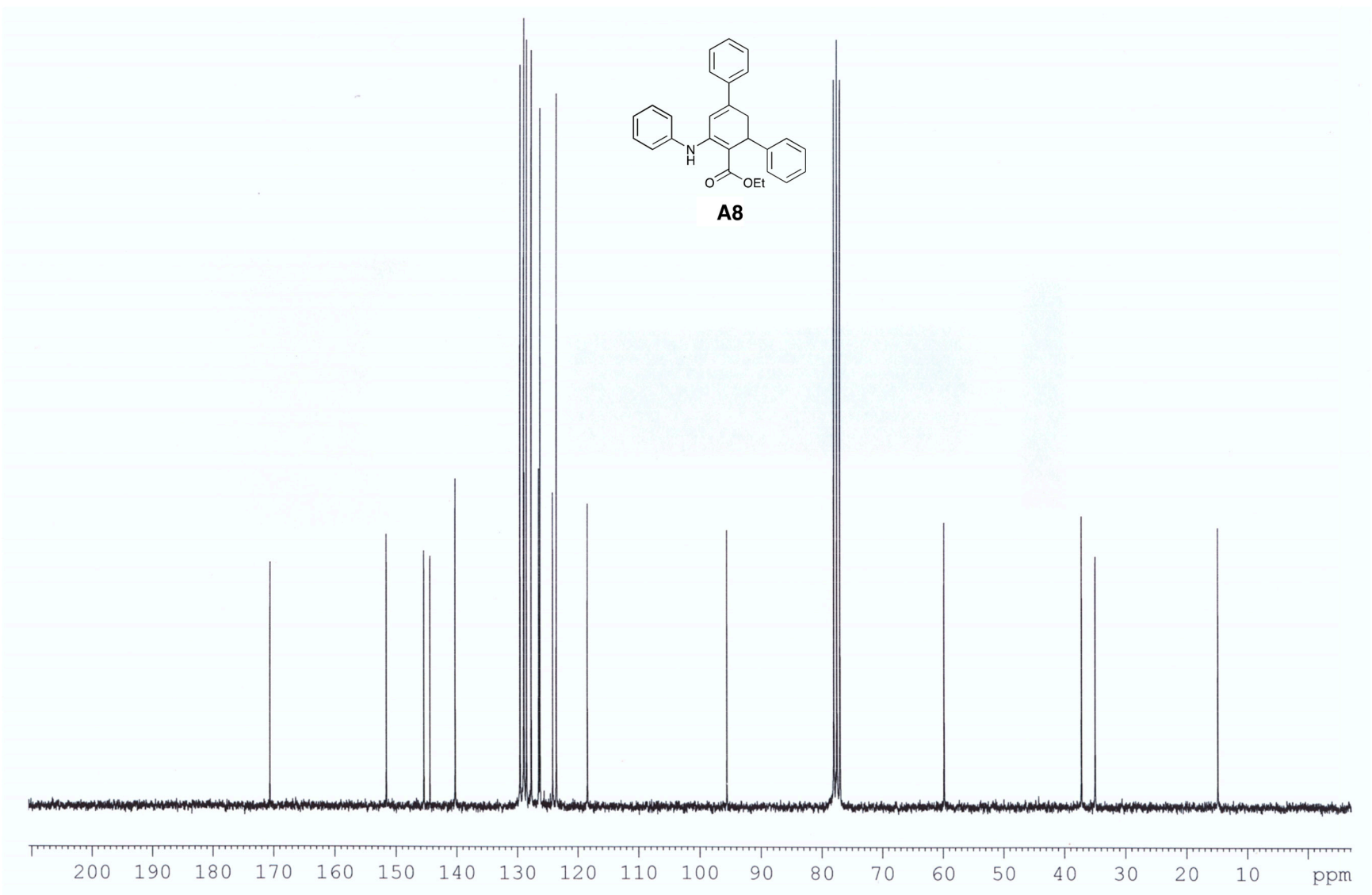
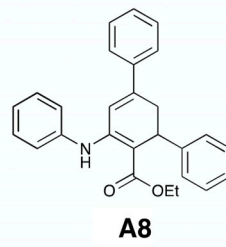


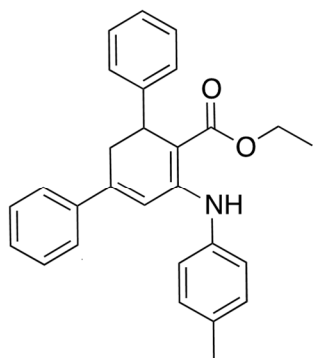


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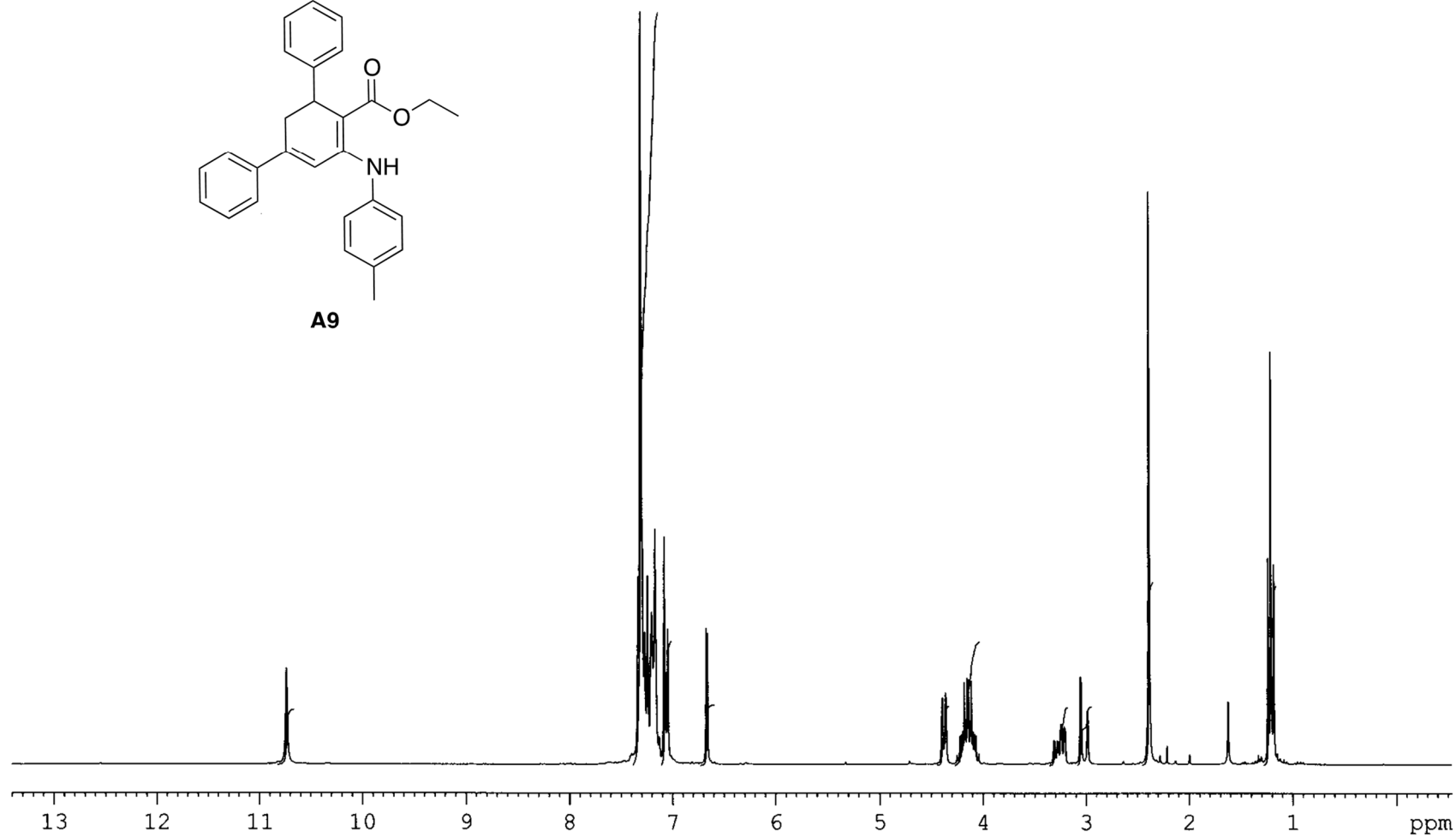


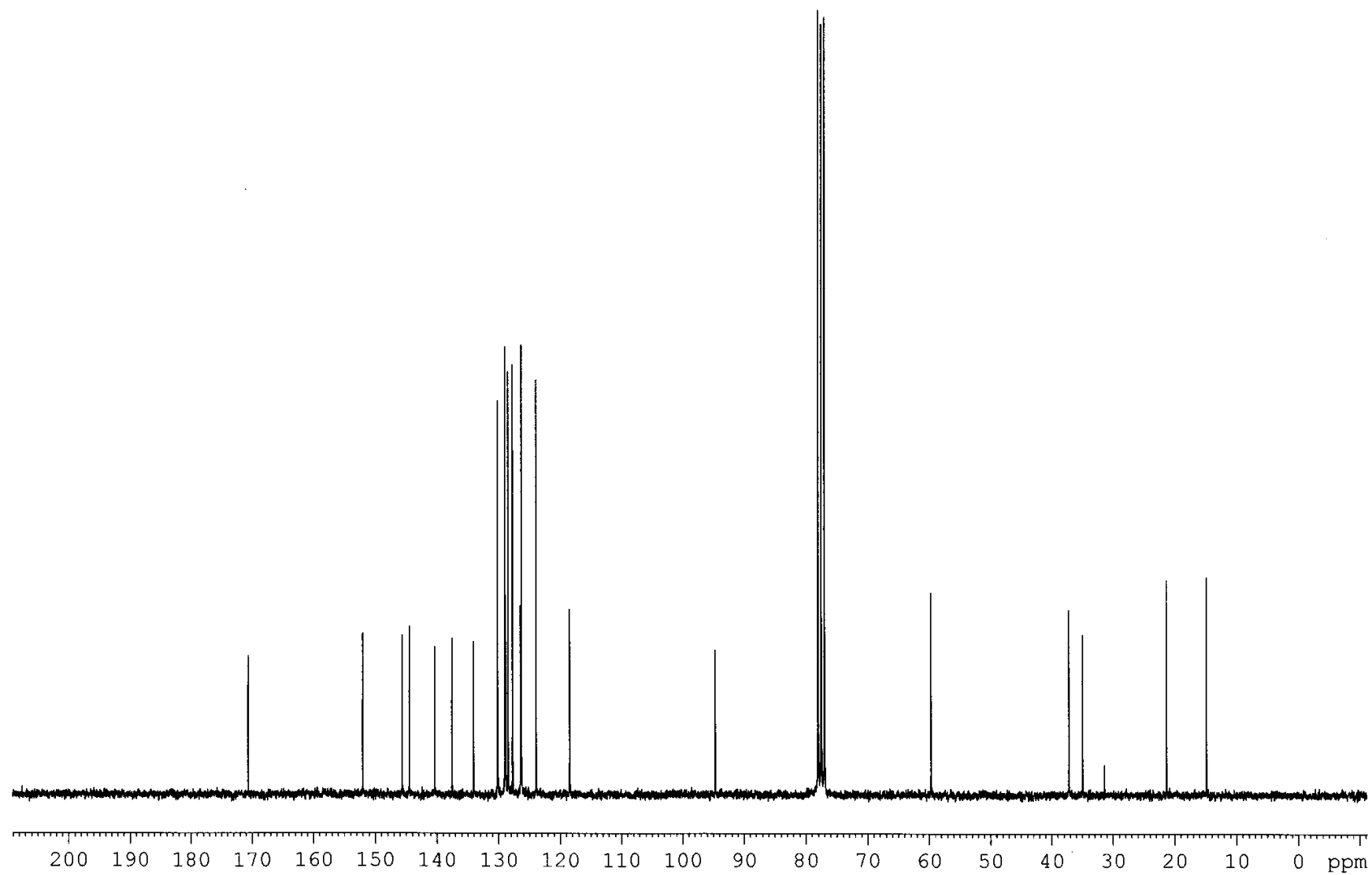


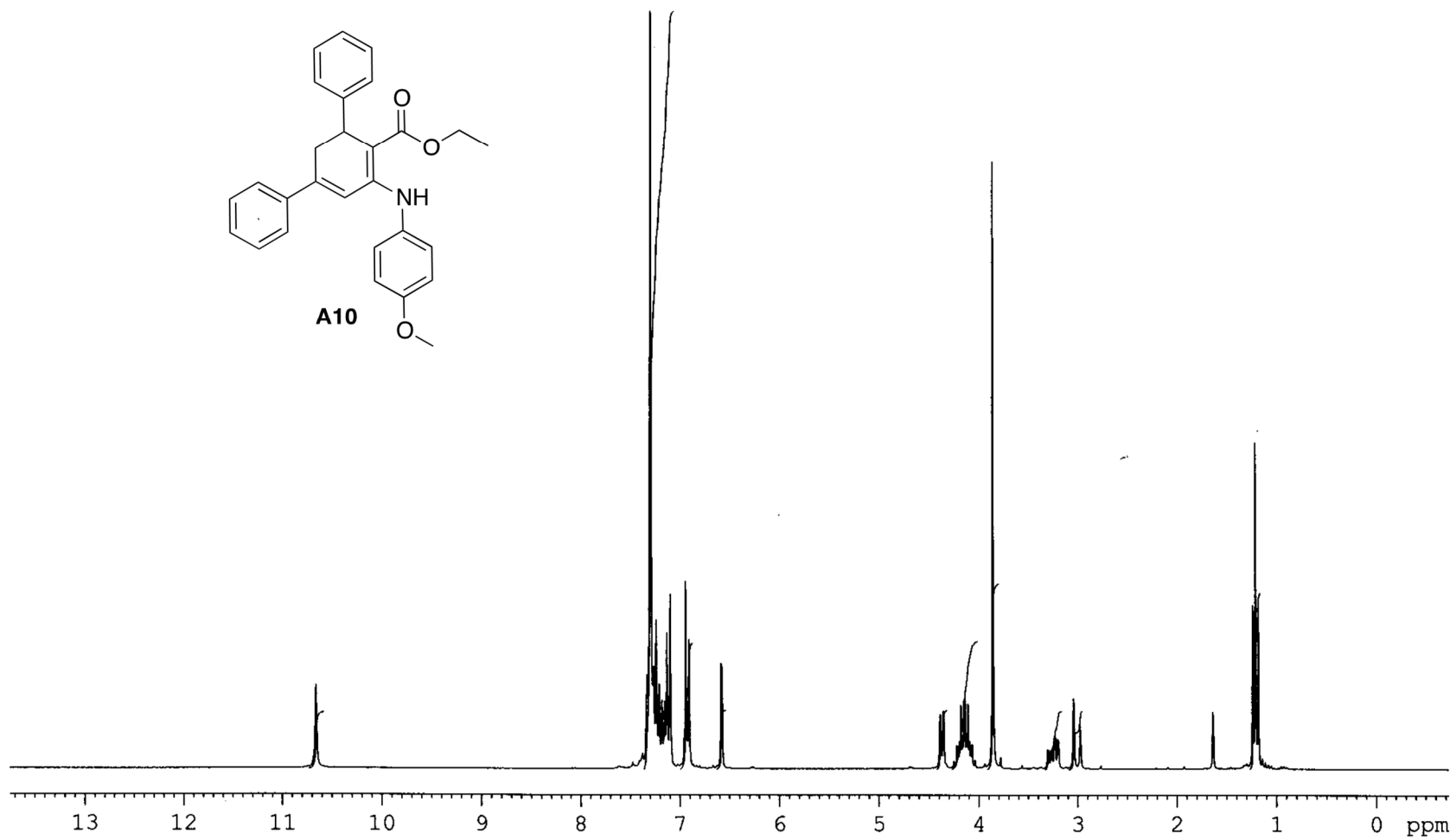
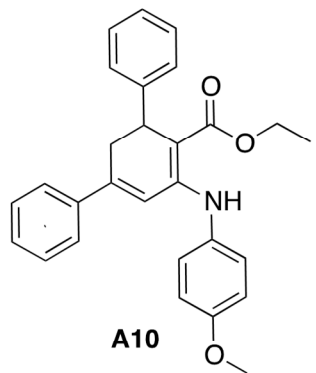


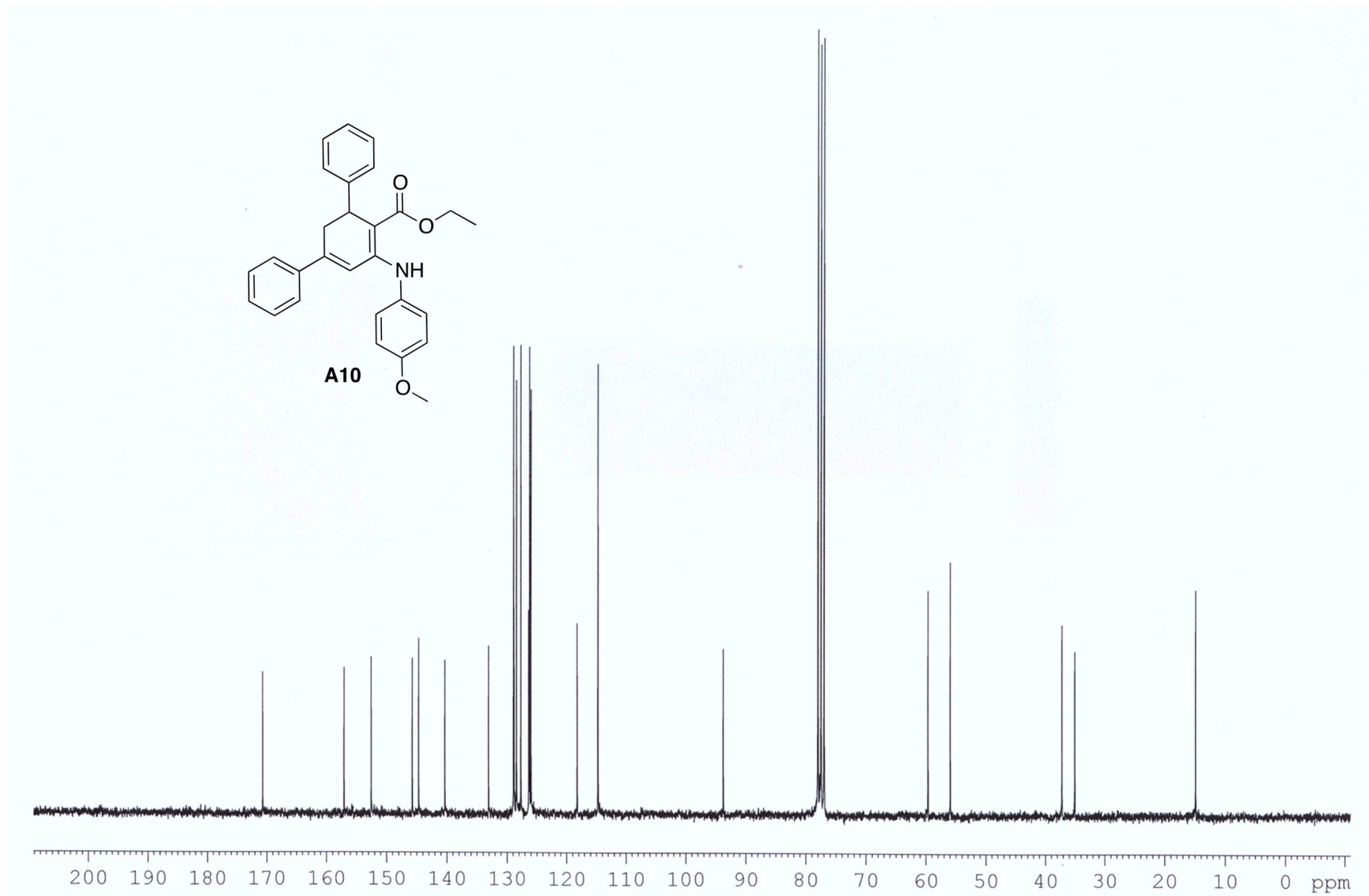


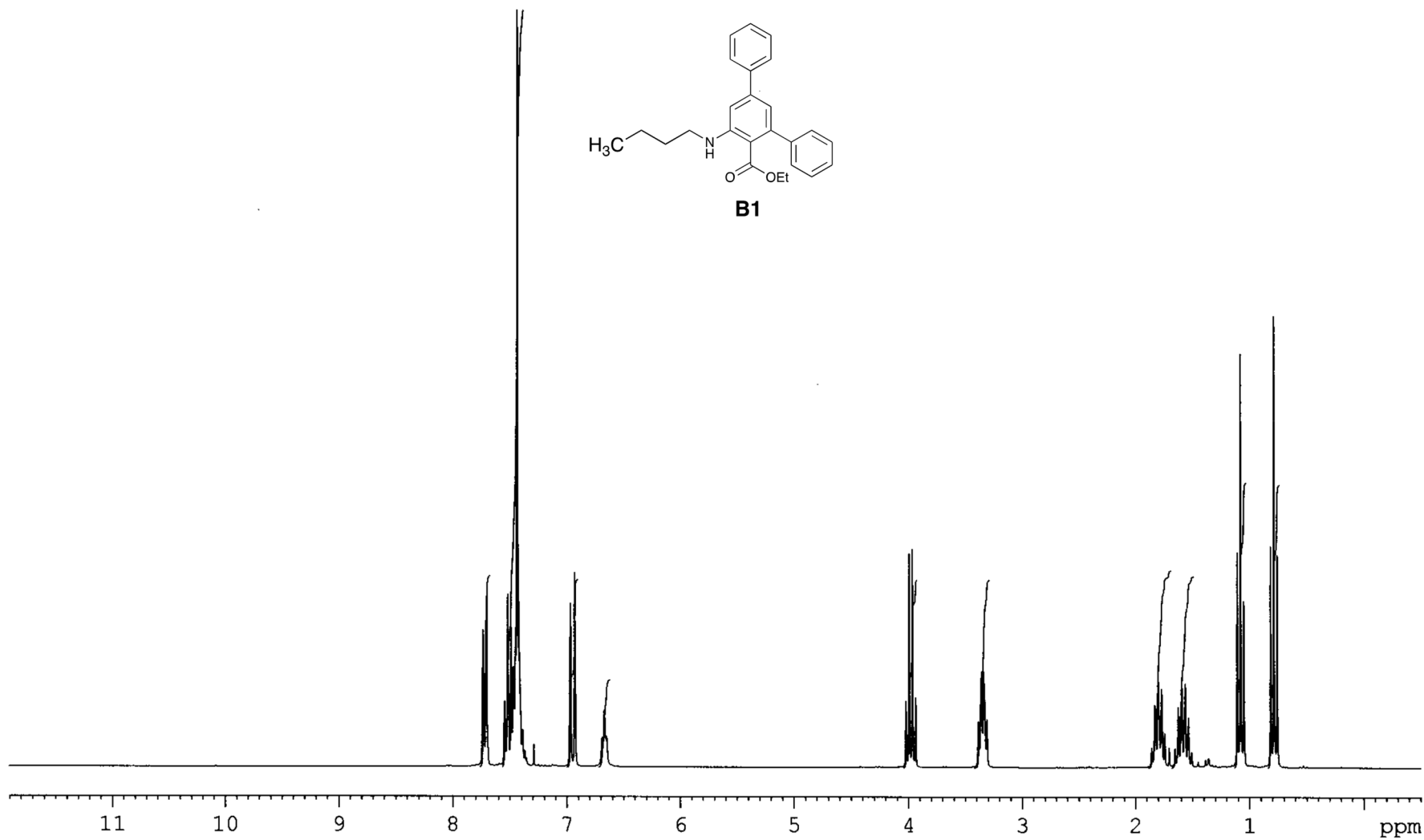
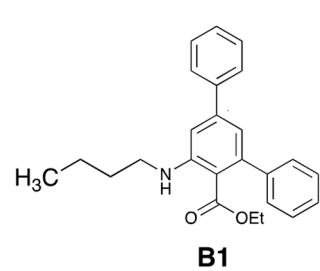
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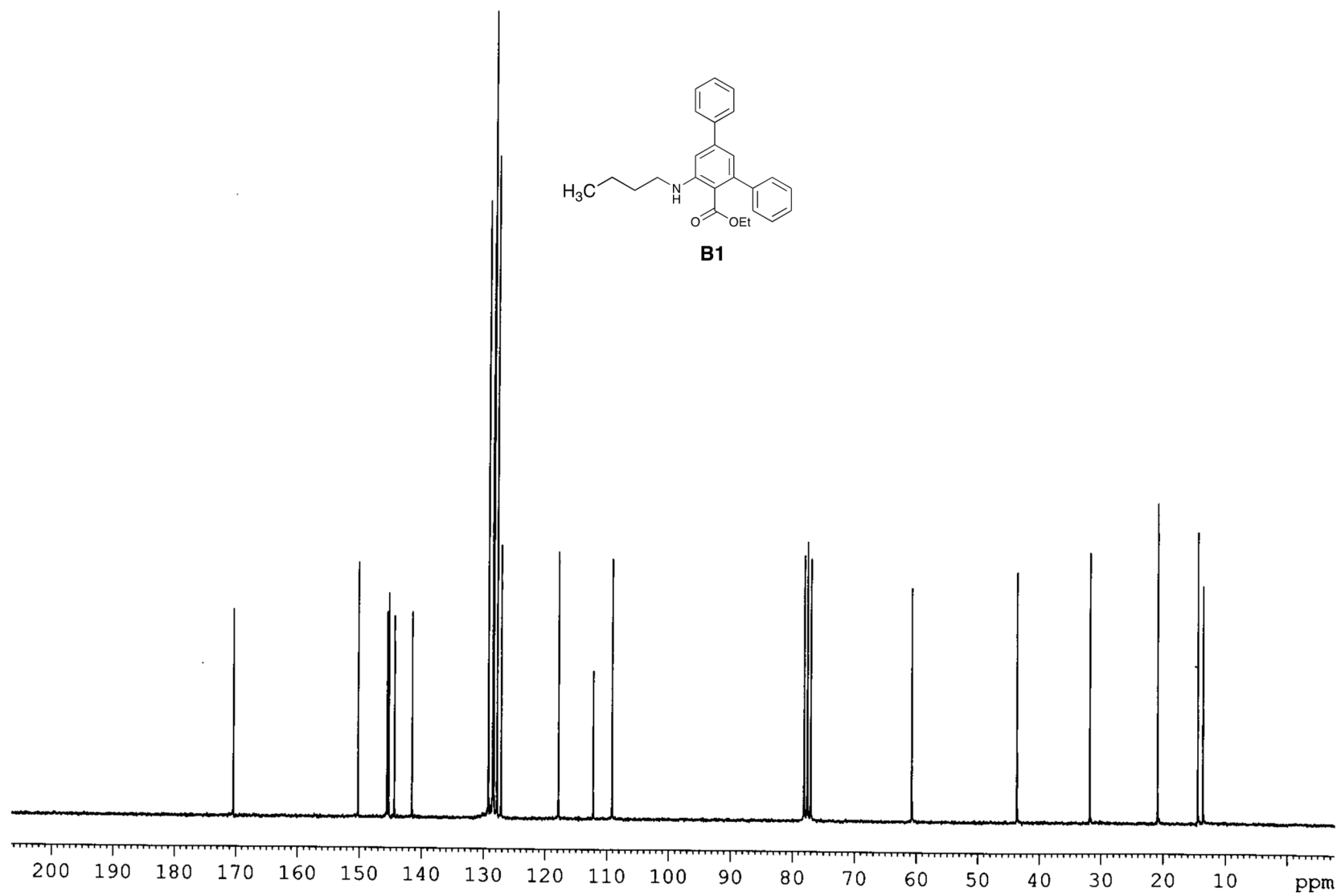
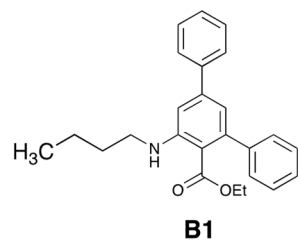


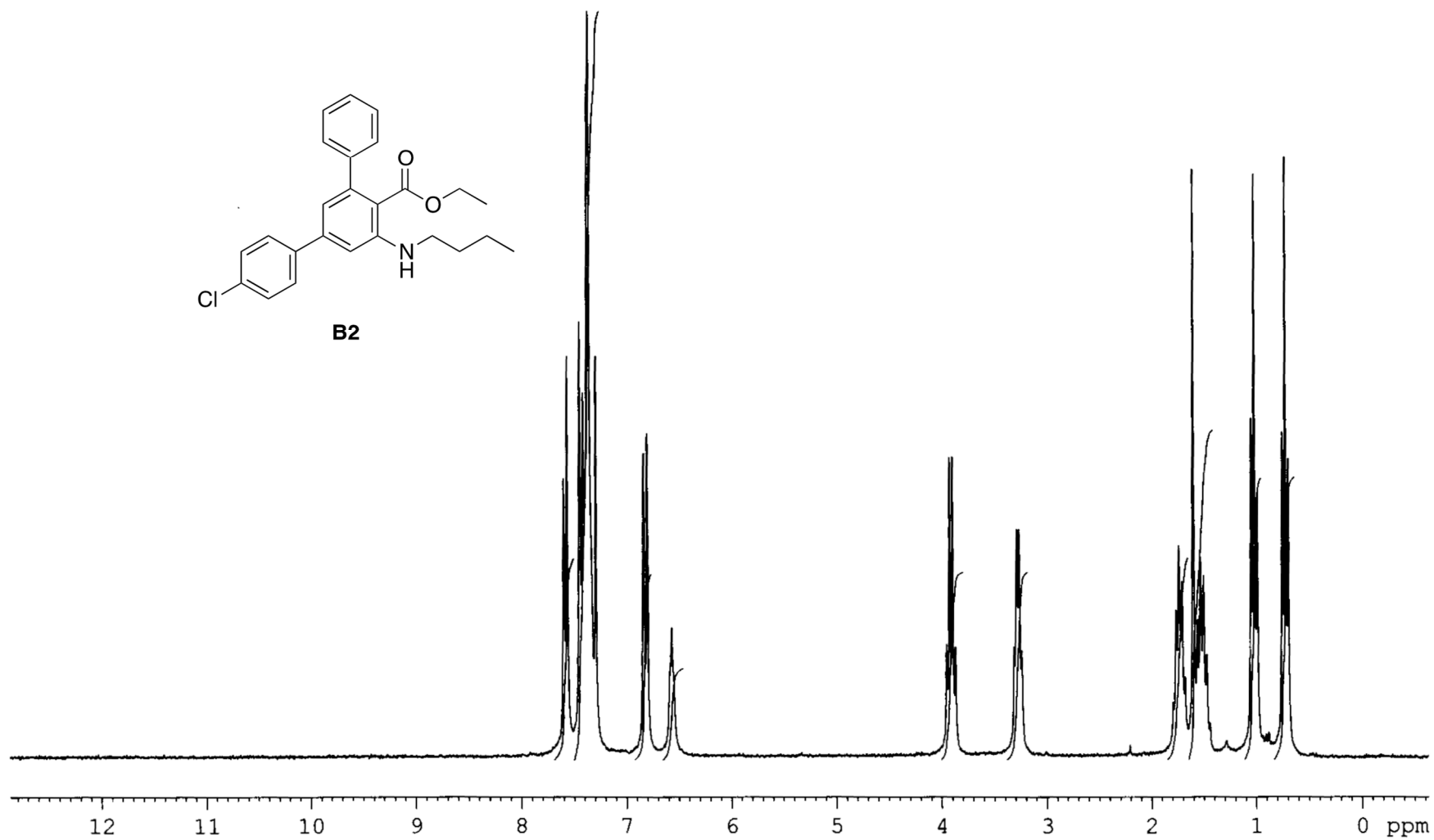
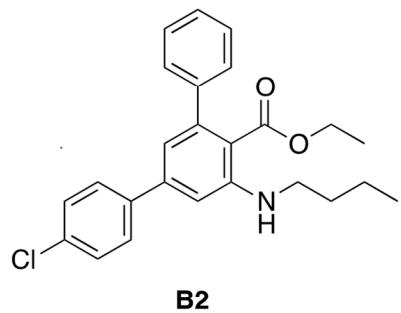


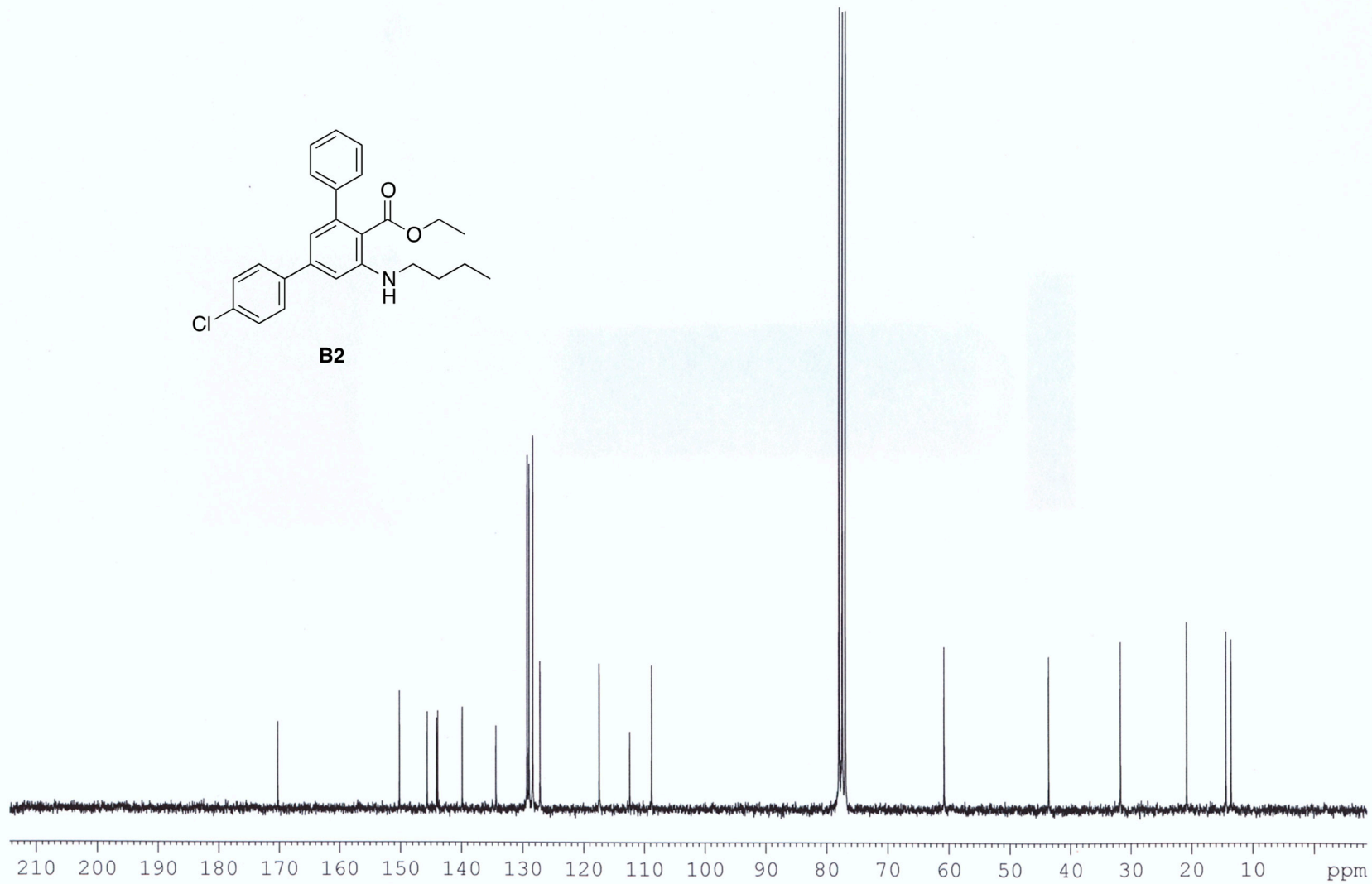
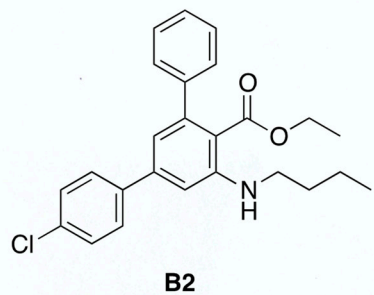


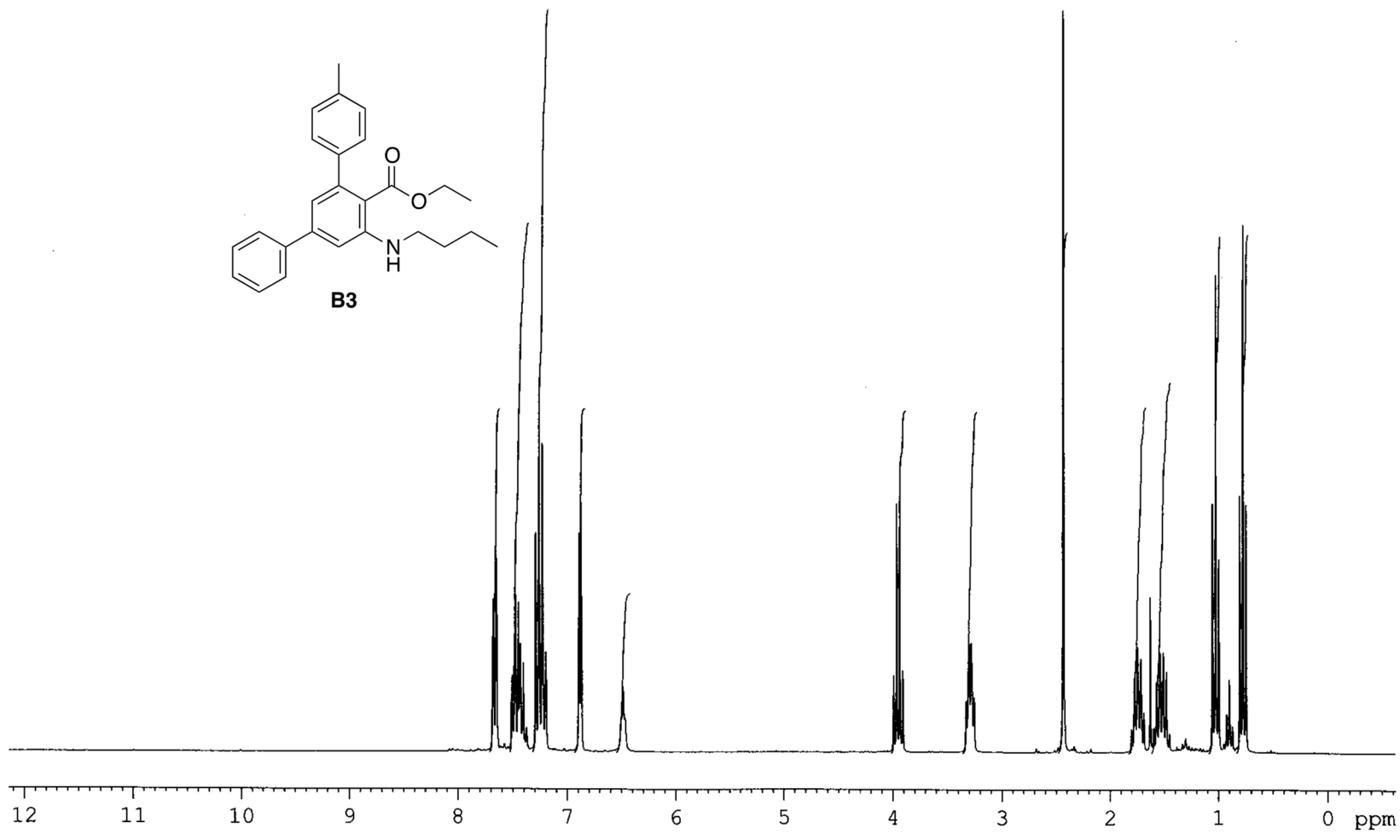
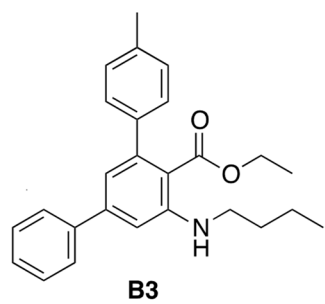


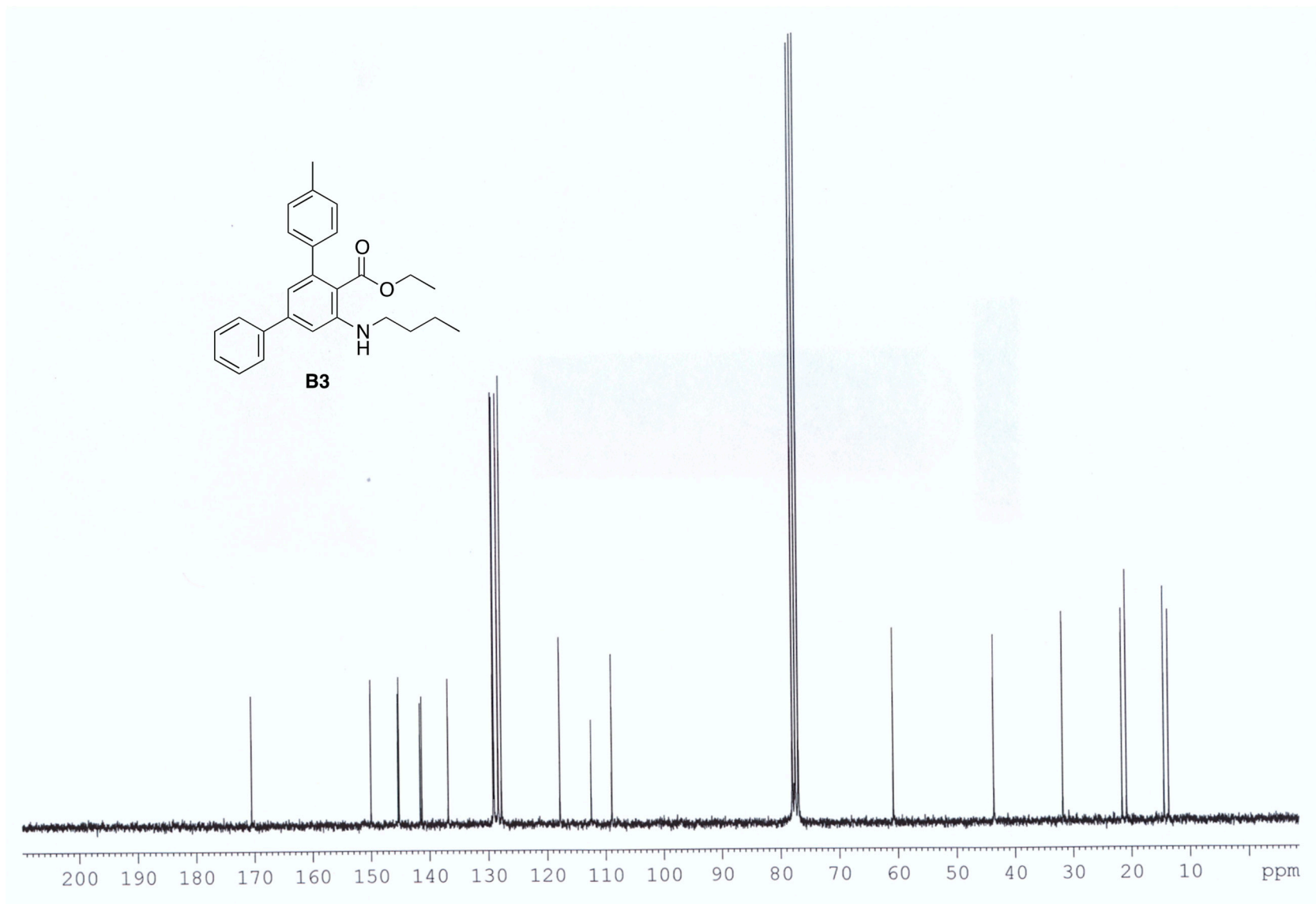


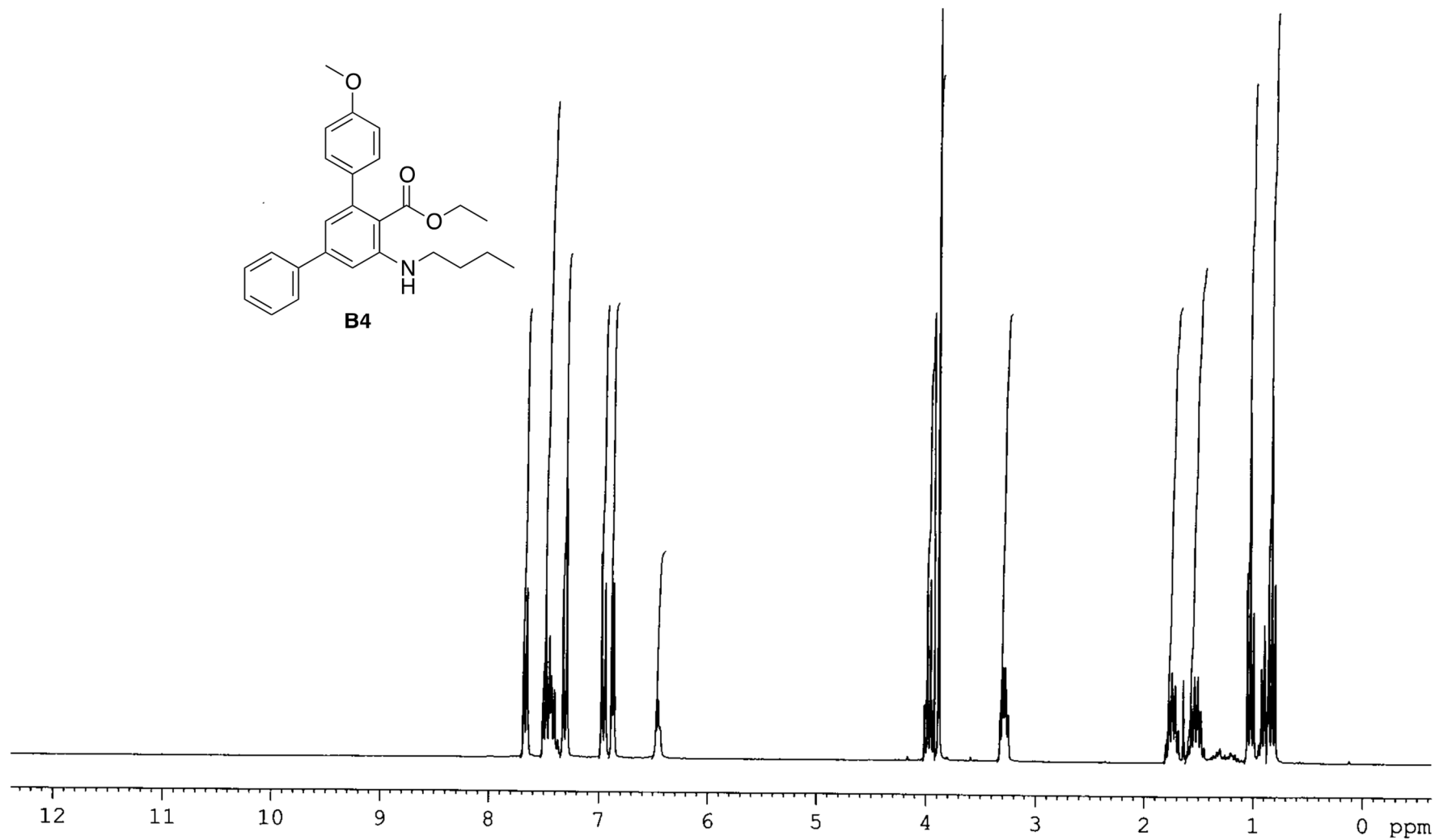
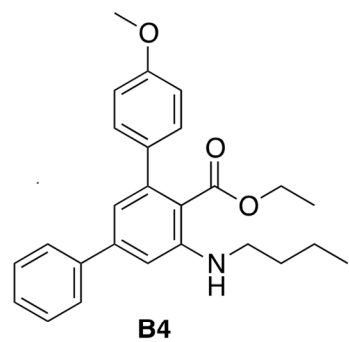


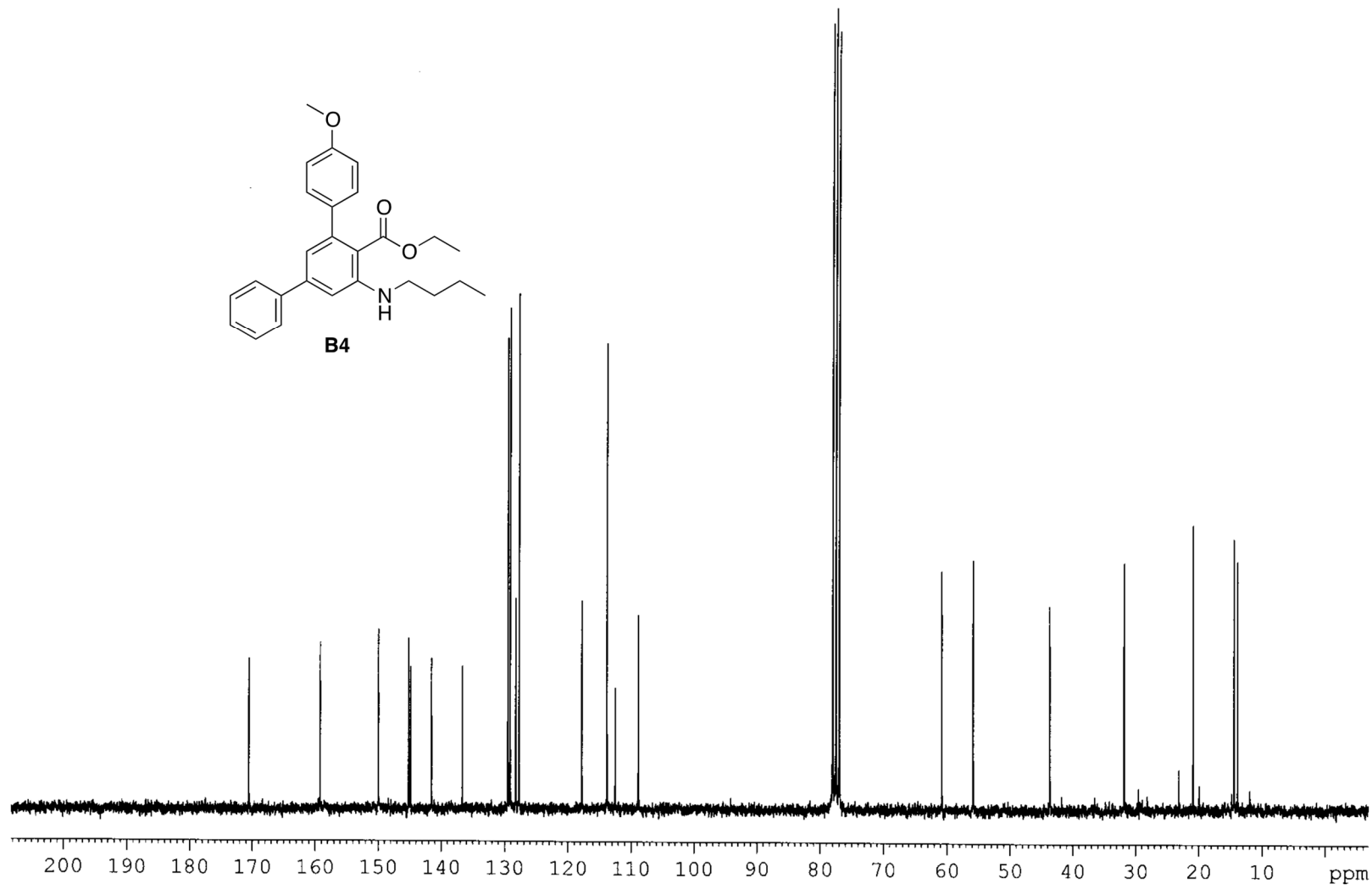
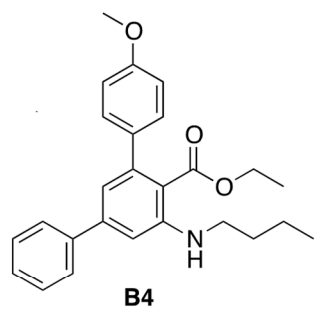


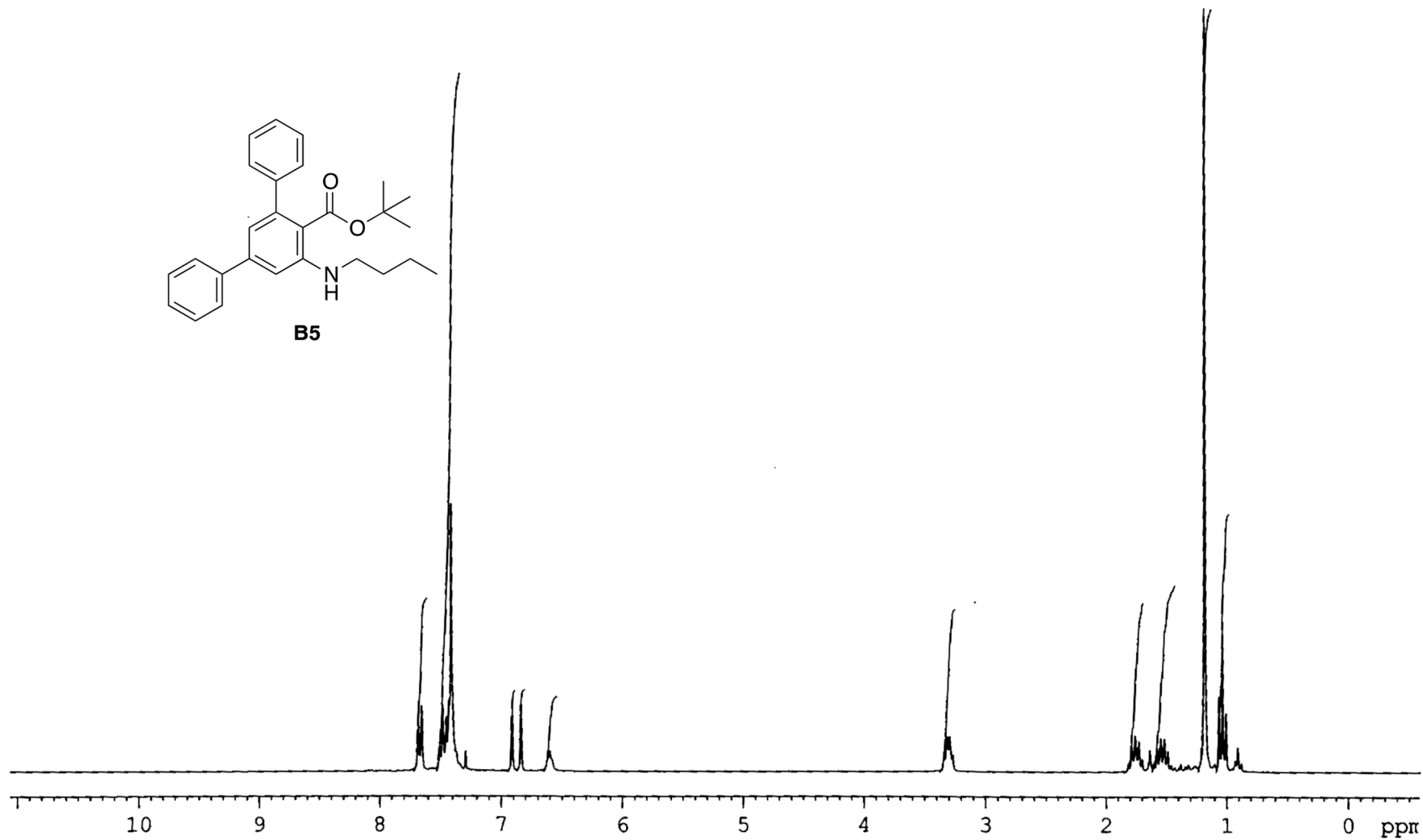
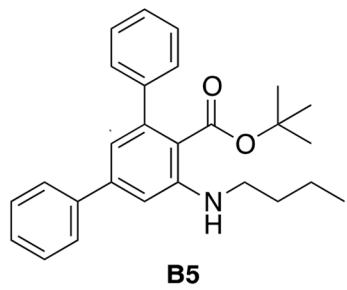


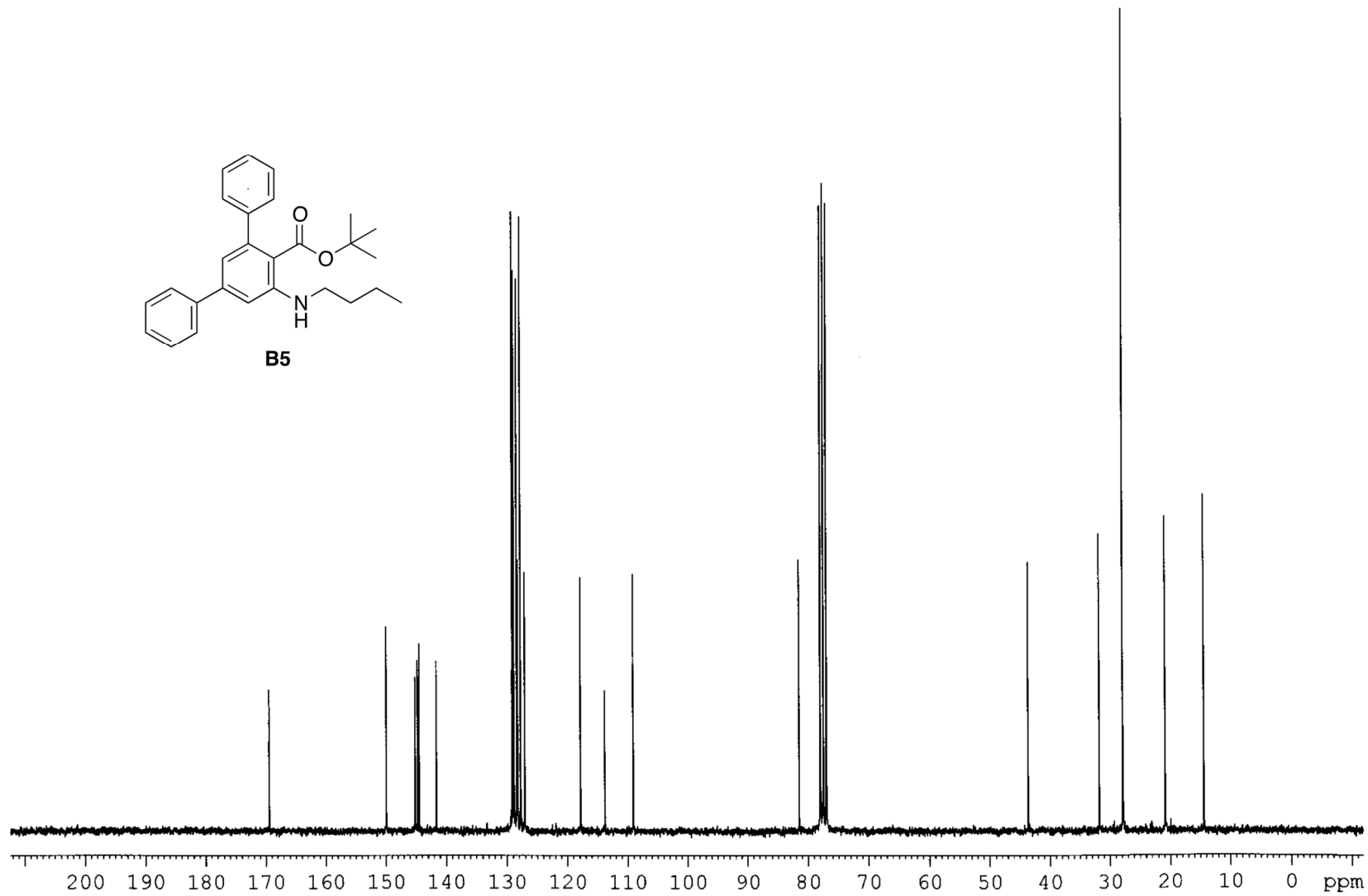
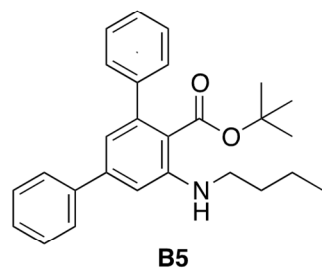


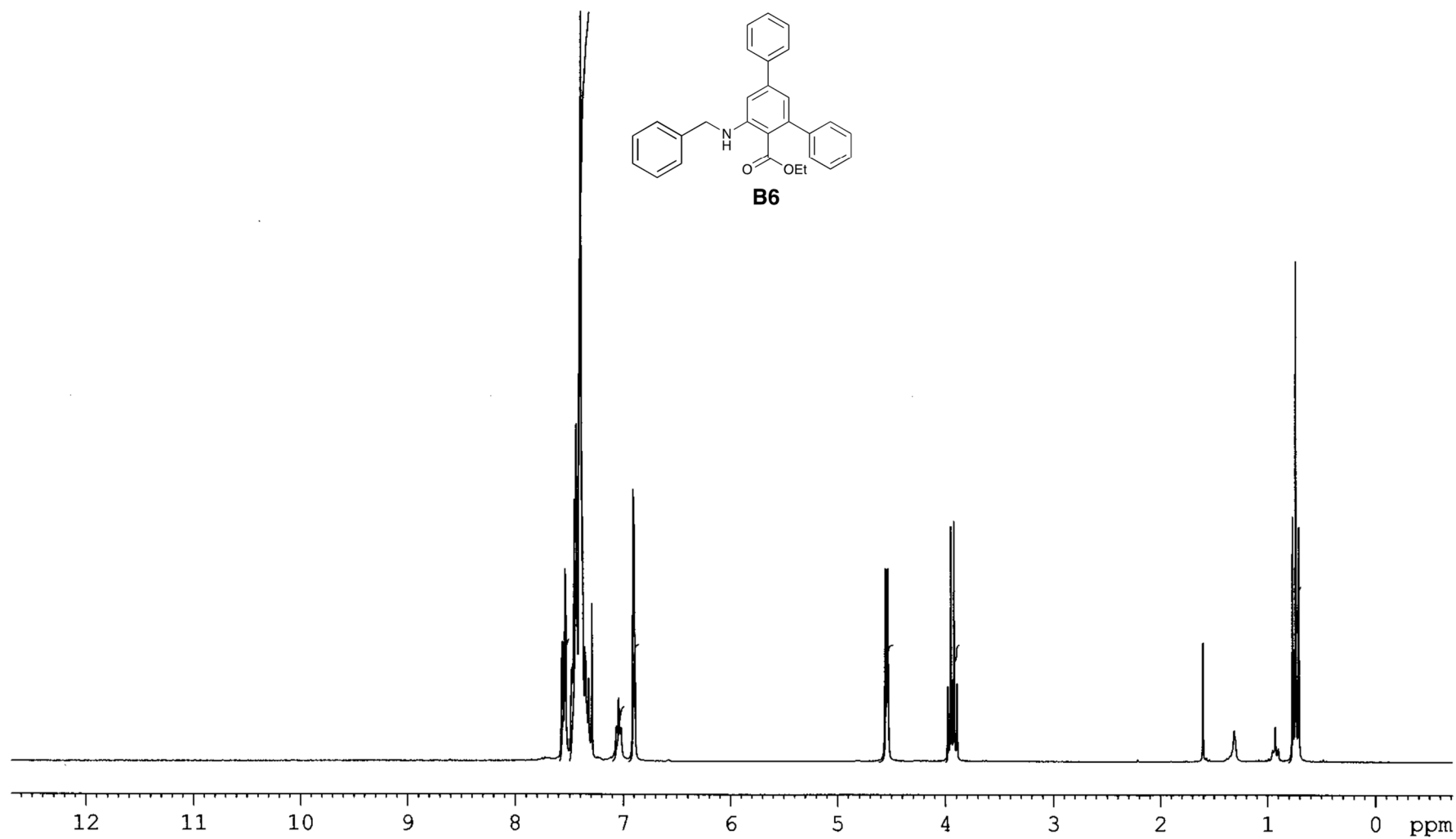
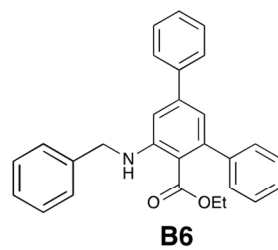


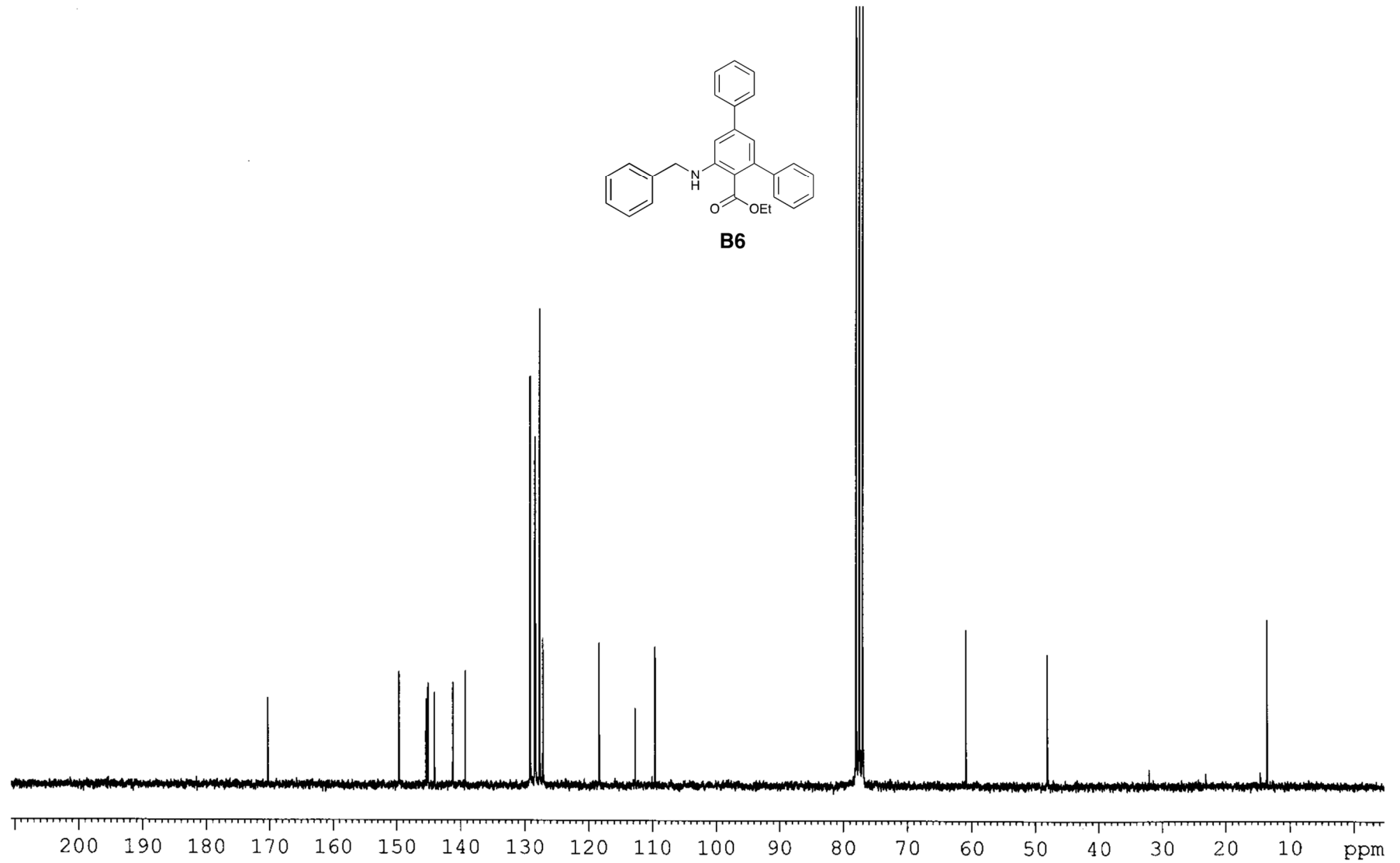
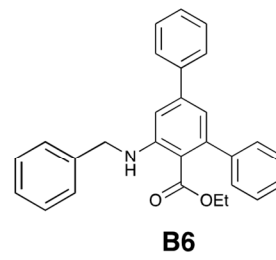


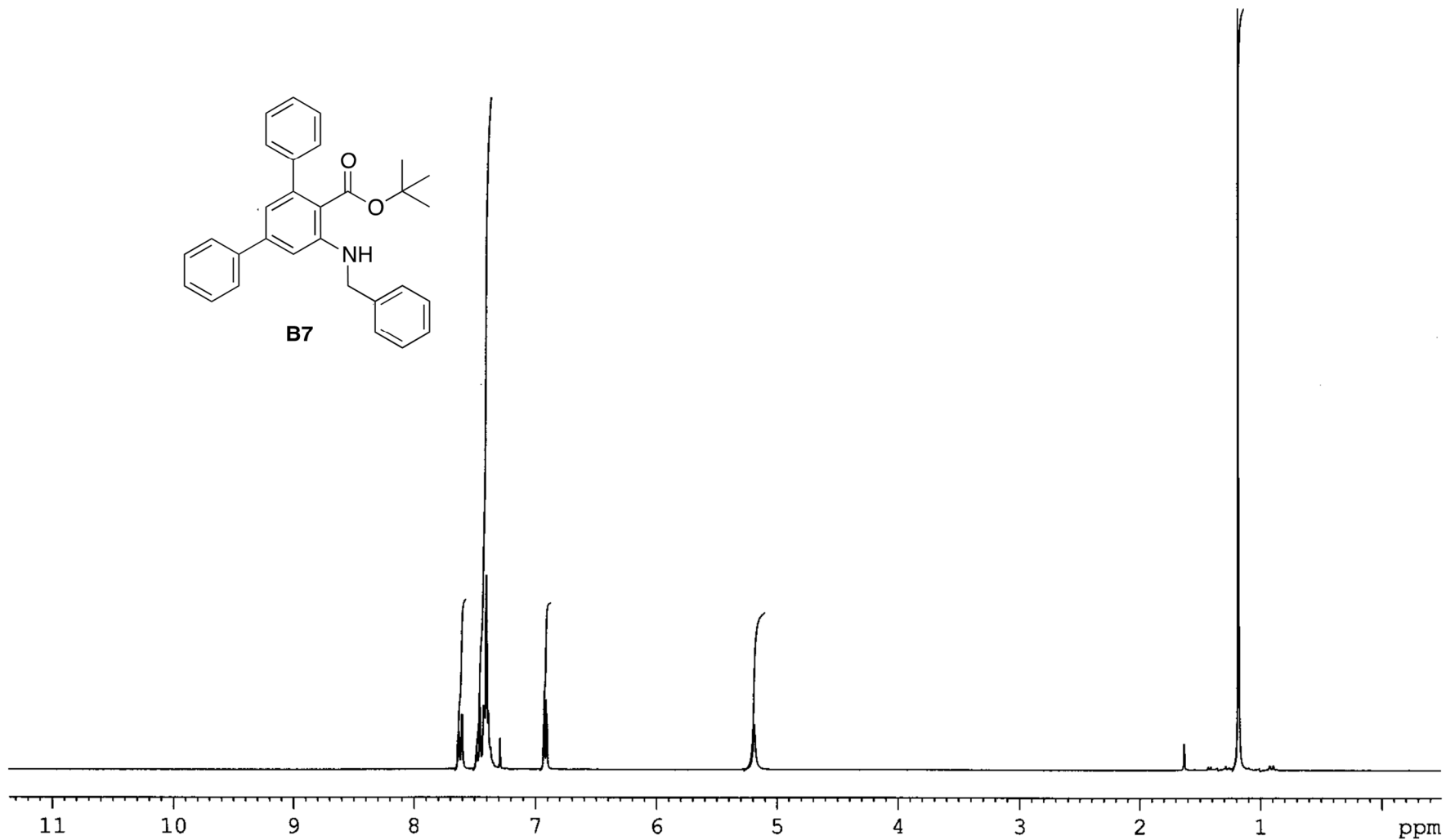
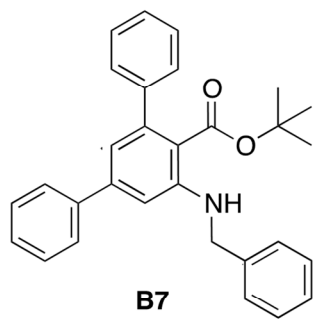


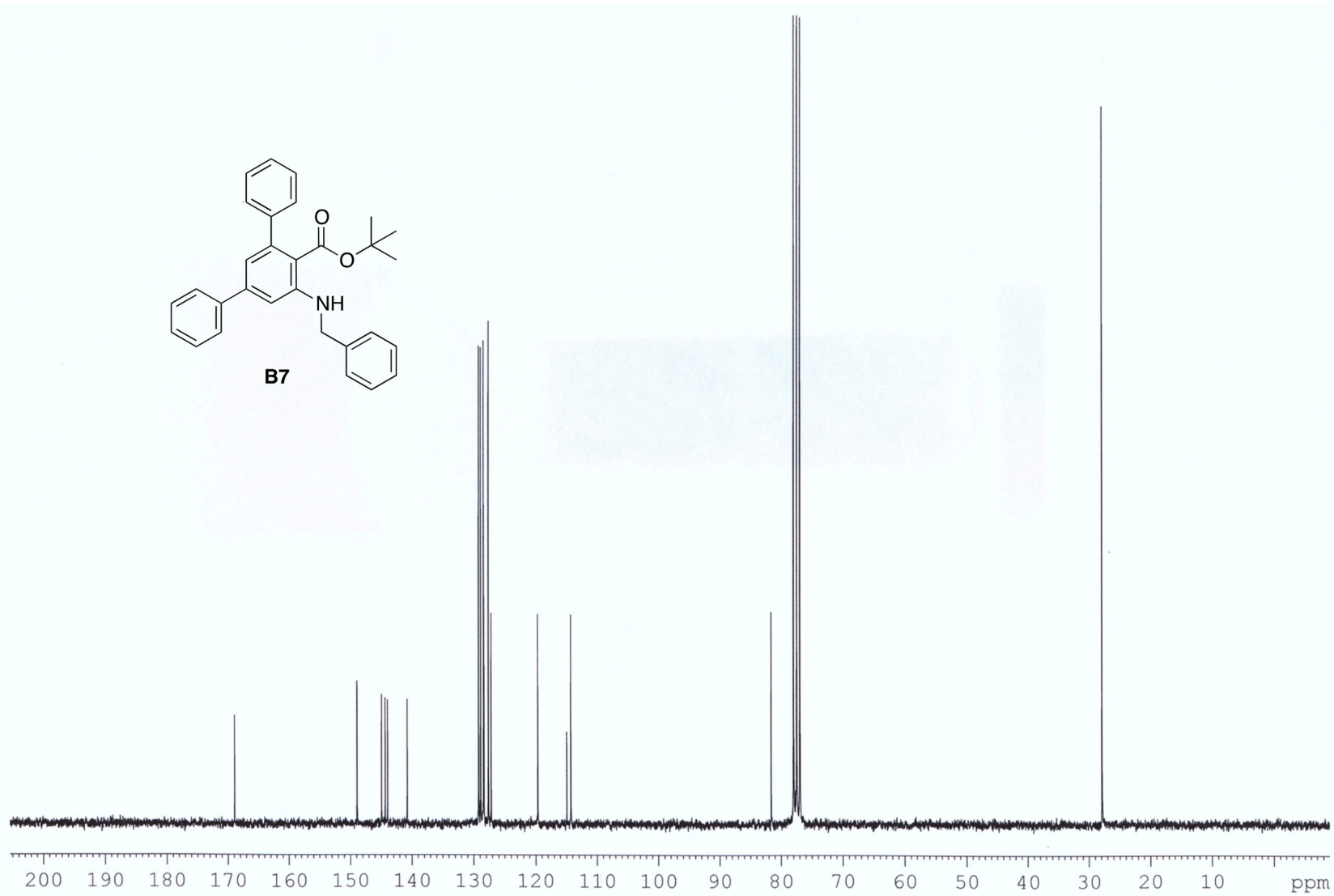
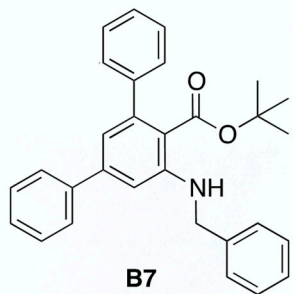


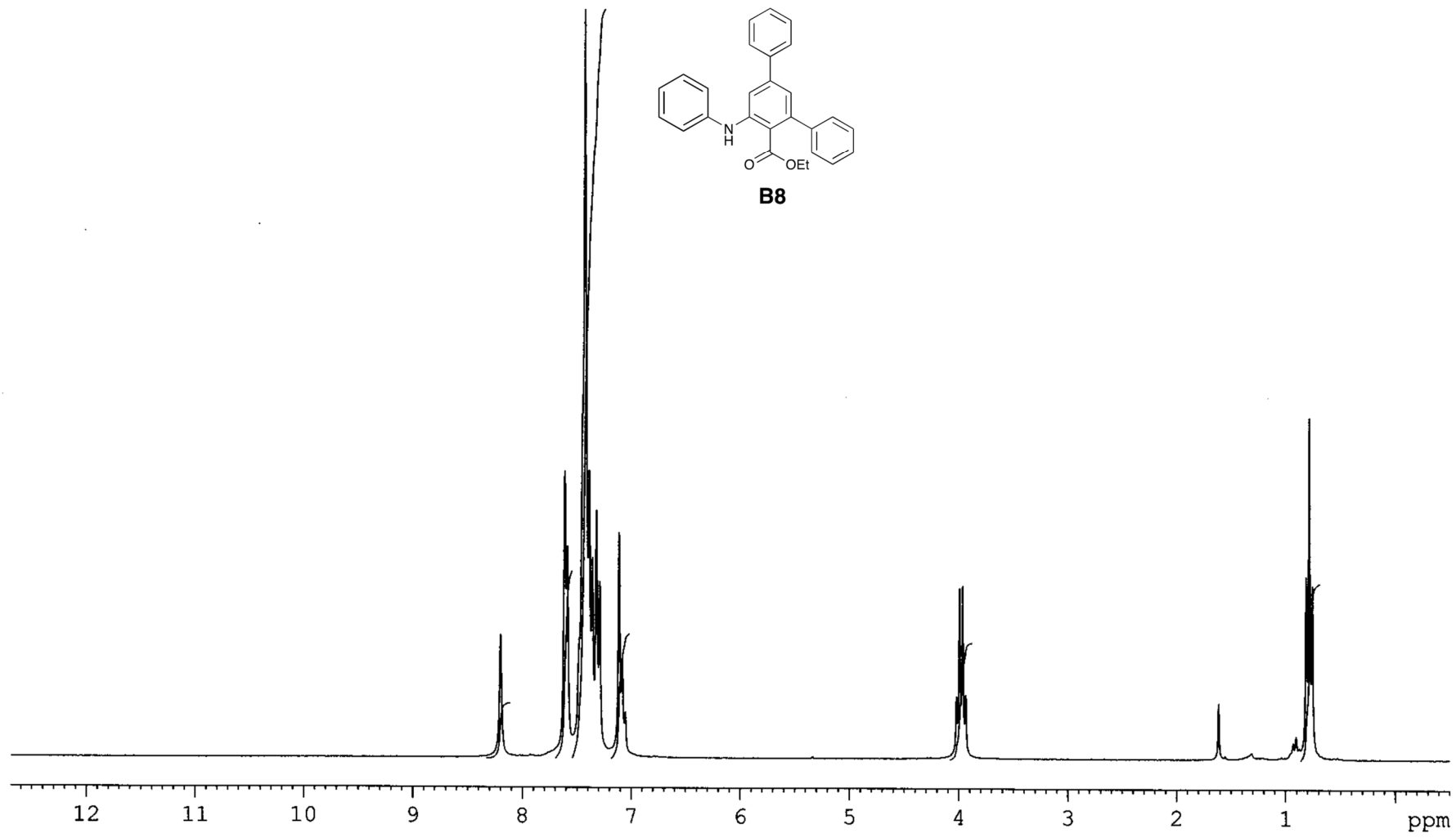
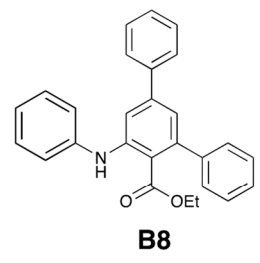


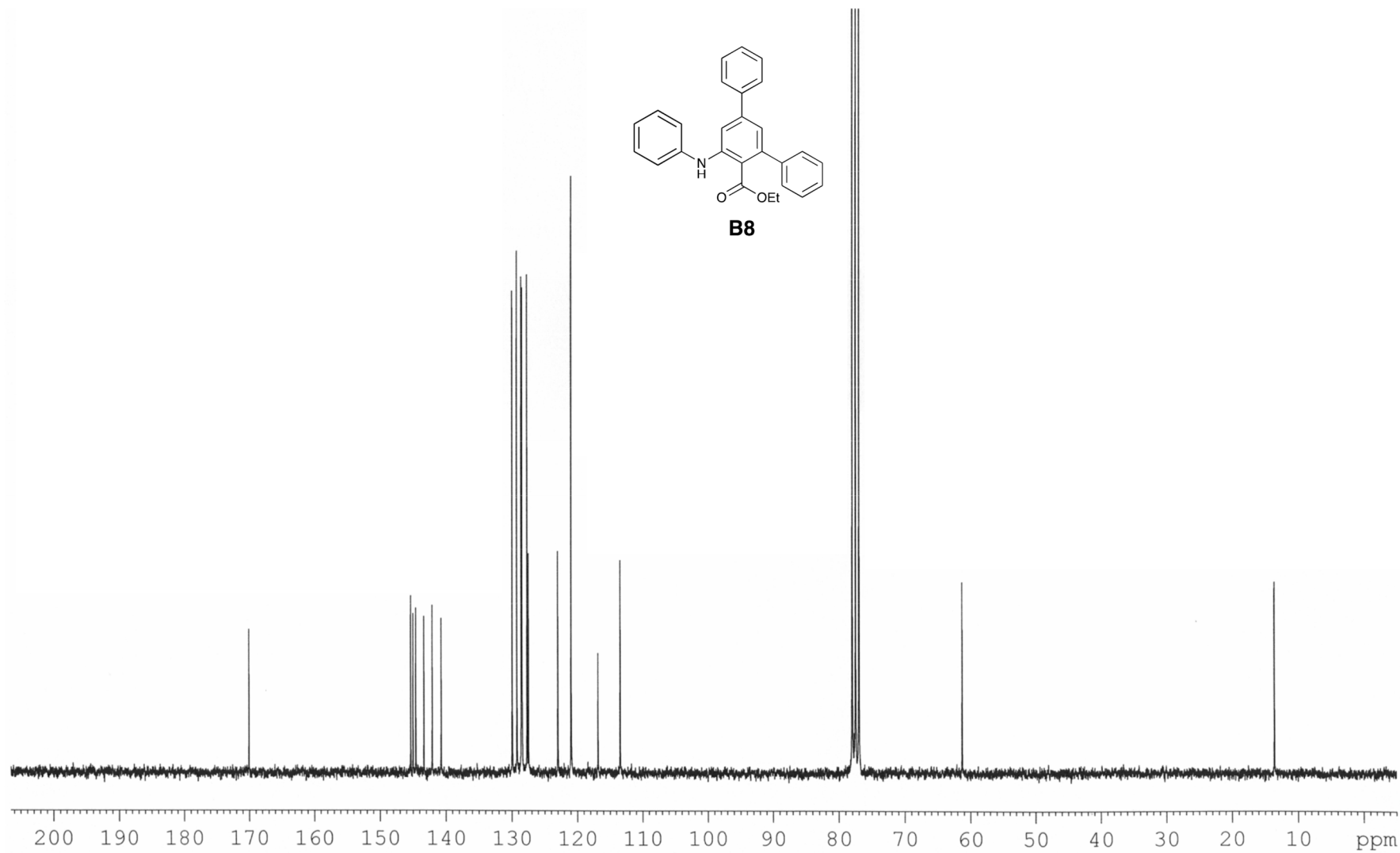
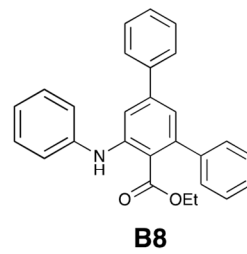


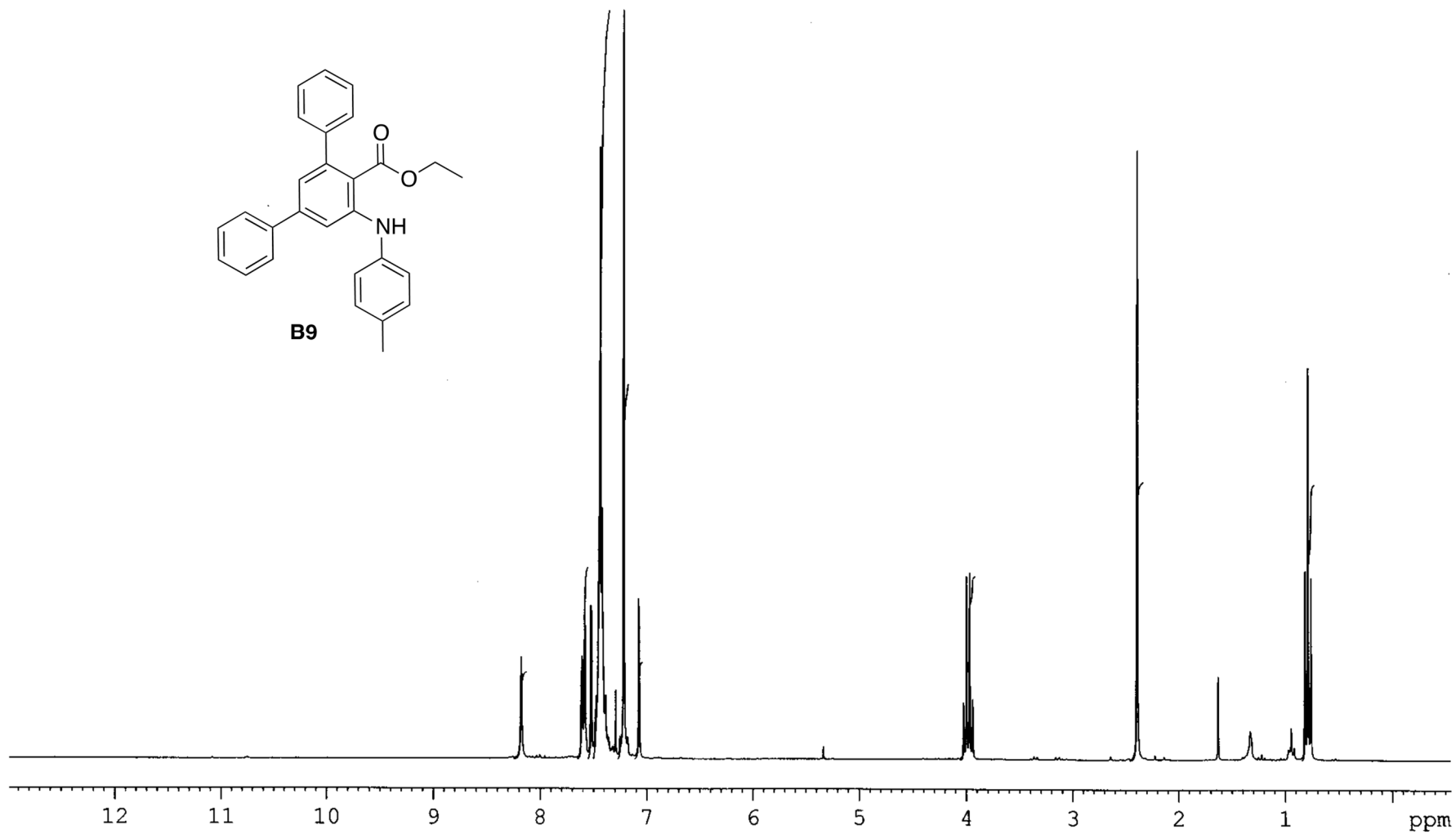
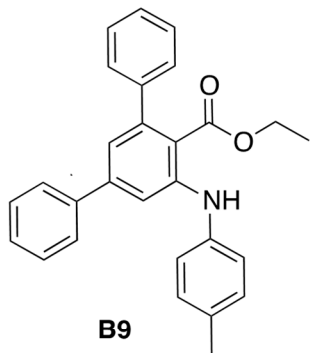


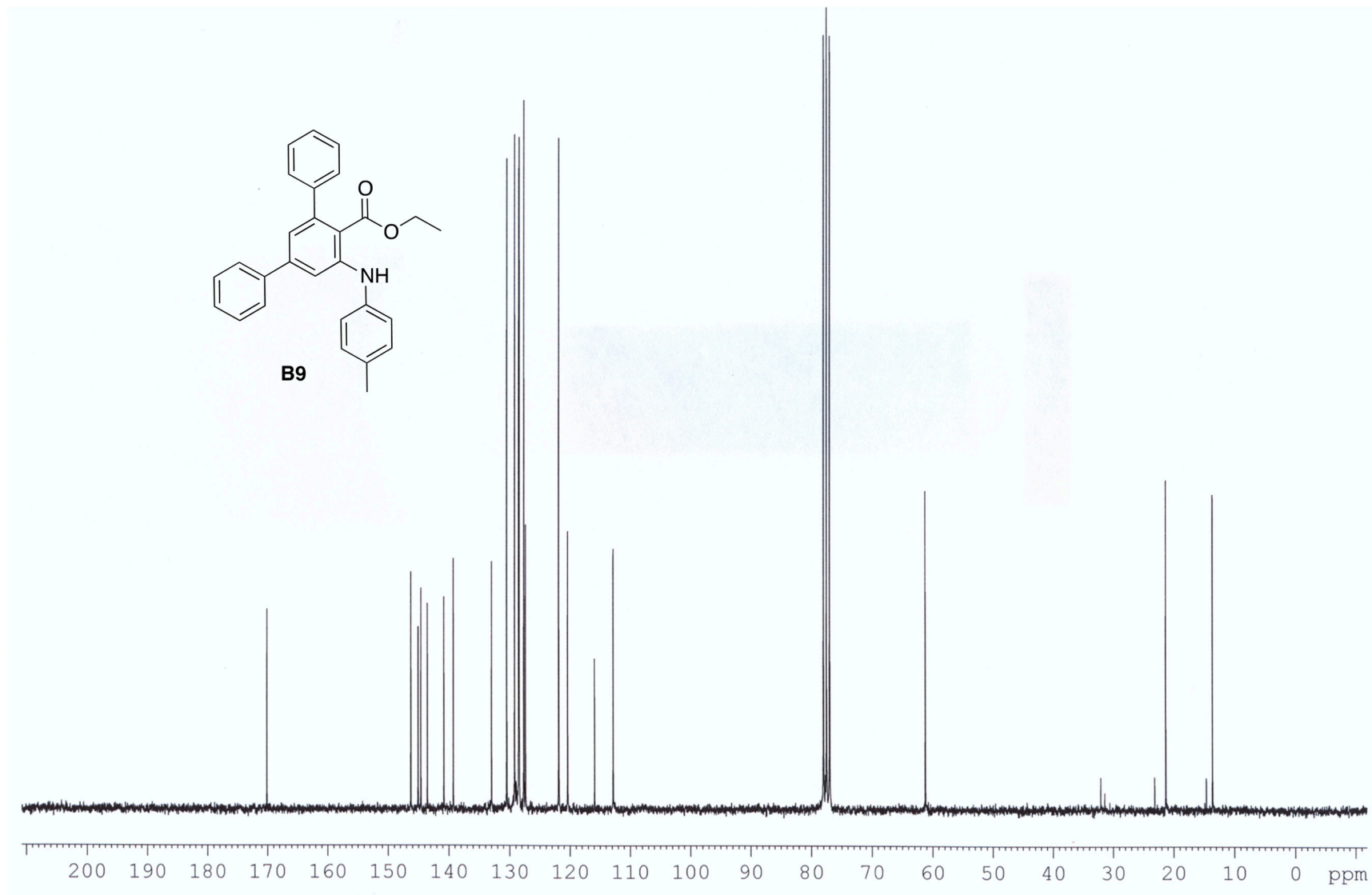


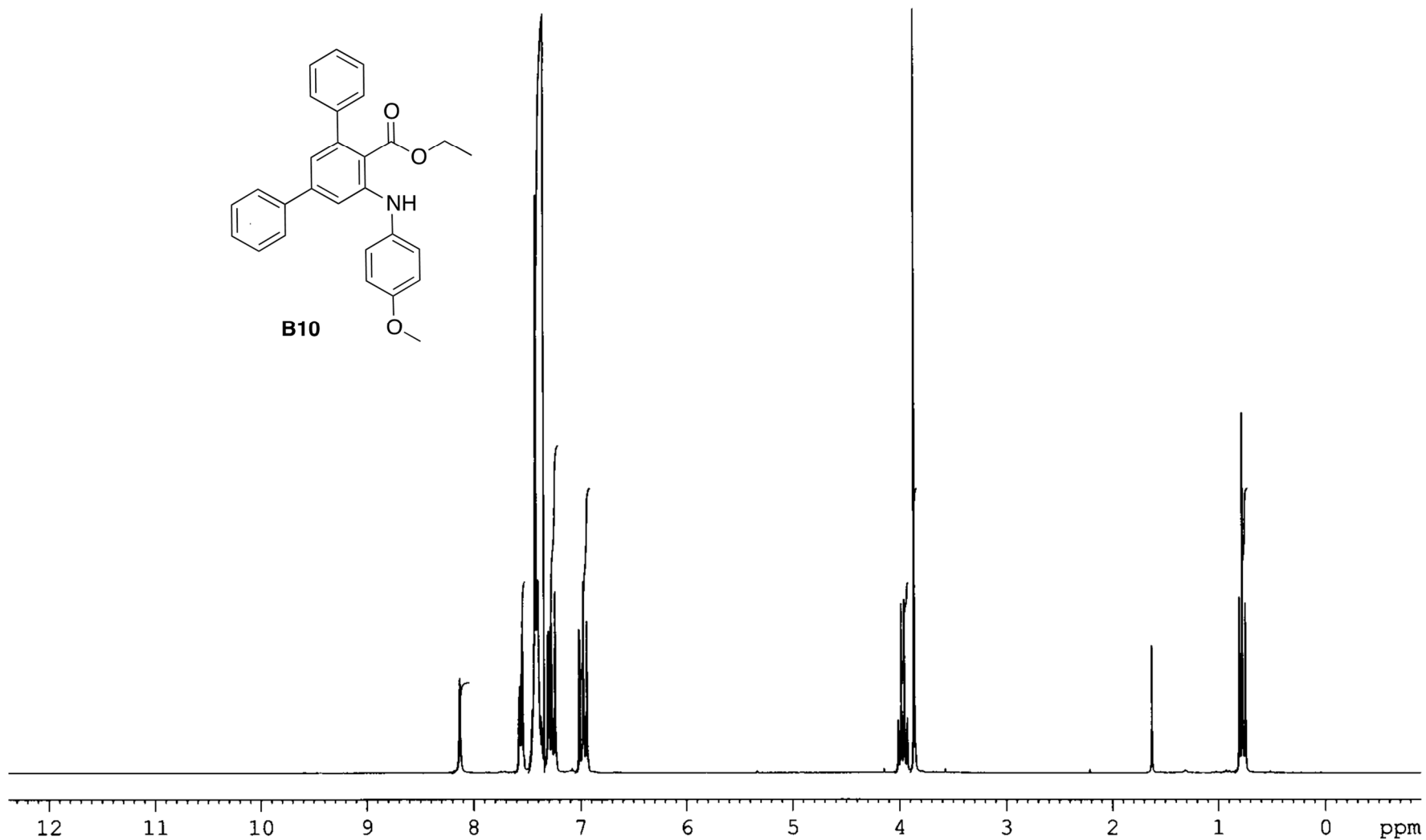
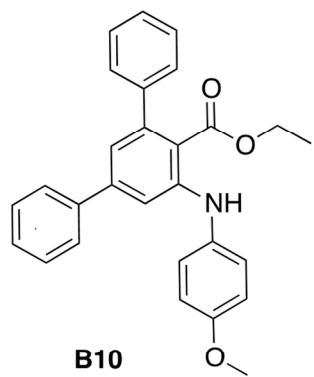


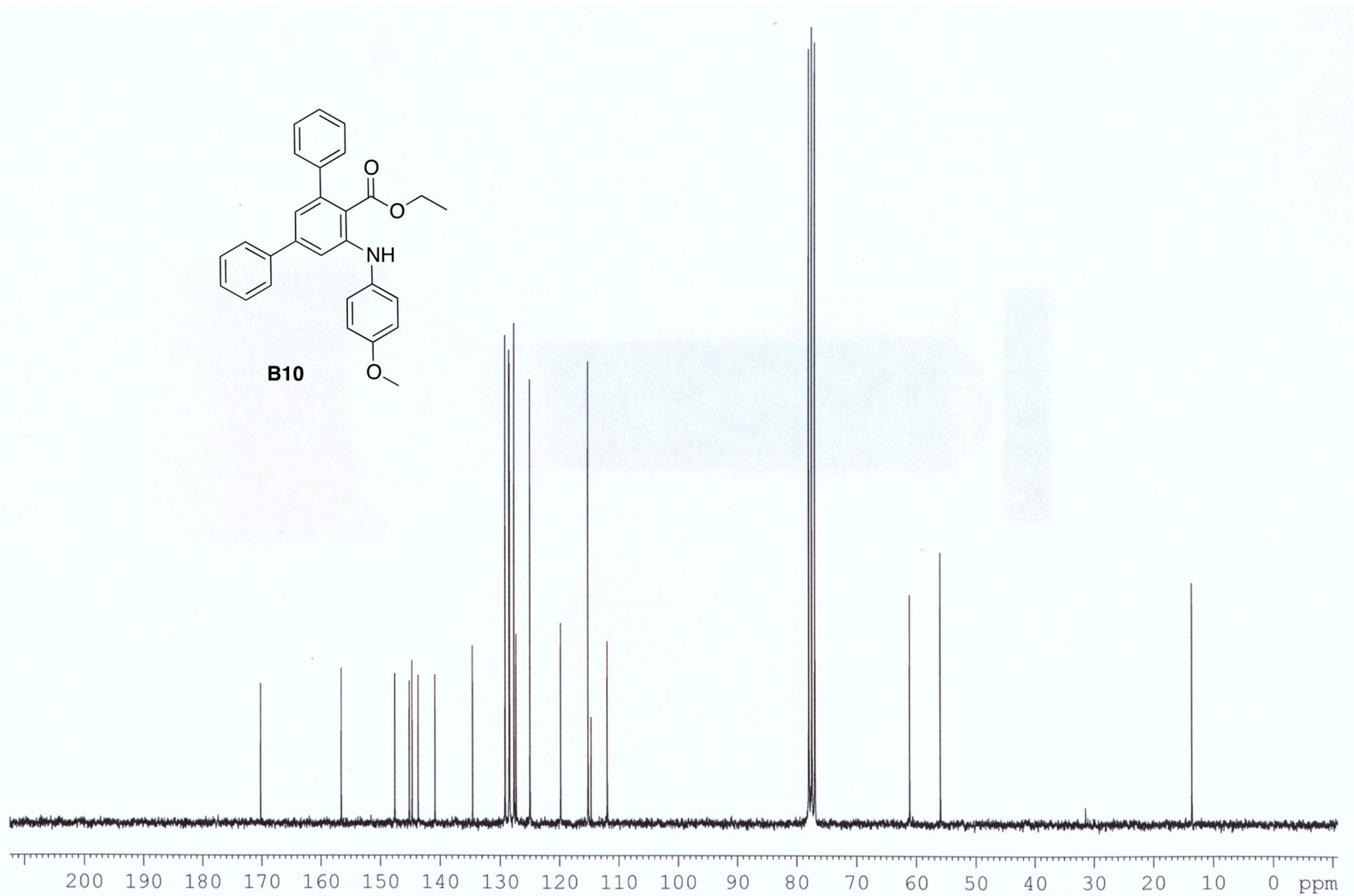
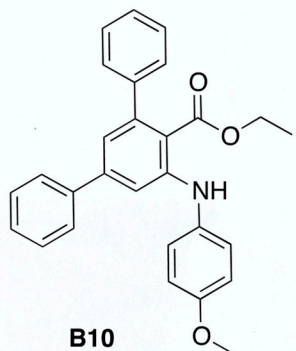












2. Spectroscopic study of compounds B

Table 1. UV-Visible absorption properties of compounds B^a

Comp.	<i>Cyclohexane</i>		<i>Ethanol</i>		<i>Acetonitrile</i>	
	λ_{\max} , nm	ϵ , M ⁻¹ cm ⁻¹ (log ϵ)	λ_{\max} , nm	ϵ , M ⁻¹ cm ⁻¹ (log ϵ)	λ_{\max} , nm	ϵ , M ⁻¹ cm ⁻¹ (log ϵ)
B1	244	36100 (4.56)	244	40100 (4.60)	244	38400 (4.58)
	367	4100 (3.61)	364	4900 (3.69)	364	3700 (3.57)
B2	253	44000 (4.64)	256	57000 (4.76)	253	47900 (4.68)
	368	4800 (3.68)	371	6000 (3.78)	367	5800 (3.76)
B3	248	32700 (4.51)	250	46100 (4.66)	249	38600 (4.59)
	261	4100 (3.61)	364	4100 (3.61)	361	4000 (3.60)
B4	255	46000 (4.66)	252	43400 (4.64)	254	47800 (4.68)
	363	4800 (3.68)	362	4300 (3.63)	364	4500 (3.65)
B5	250	35000 (4.54)	247	46000 (4.66)	247	42000 (4.62)
	369	2800 (3.45)	364	4500 (3.65)	364	4100 (3.61)
B6	245	47000 (4.67)	245	45000 (4.65)	245	54000 (4.73)
	362	3100 (3.49)	359	3700 (3.57)	359	4000 (3.60)
B7	242	41200 (4.61)	245	48000 (4.68)	245	38000 (4.58)
	362	3600 (3.56)	359	3500 (3.54)	359	3900 (3.59)
	244	13400 (4.13)	244	42500 (4.63)	244	19200 (4.28)
B8	271	11800 (4.07)	271	34500 (4.54)	274	15400 (4.19)
	364	3300 (3.52)	361	4300 (3.63)	358	3100 (3.49)
	246	34200 (4.53)	246	53900 (4.73)	247	36800 (4.57)
B9	273	27100 (4.43)	274	47400 (4.68)	271	28700 (4.46)
	364	5100 (3.71)	364	4300 (3.63)	362	4700 (3.67)
	246	58900 (4.77)	246	54100 (4.73)	247	49900 (4.70)
B10	273	47100 (4.67)	270	33000 (4.52)	270	37000 (4.57)
	364	4100 (3.61)	366	3700 (3.57)	362	3800 (3.58)

^a λ_{\max} : maximum absorption wavelength; ϵ : molar absorptivity (M⁻¹ cm⁻¹) at the maximum absorption wavelength

Table 2. Fluorescence properties of compounds **B**

Comp.	<i>Cyclohexane</i>			<i>Ethanol</i>			<i>Acetonitrile</i>		
	λ_{ex} , nm	λ_{em} , nm	Φ_{F}	λ_{ex} , nm	λ_{em} , nm	Φ_{F}	λ_{ex} , nm	λ_{em} , nm	Φ_{F}
B1	259, 366*	457	0.13	257, 364*	453	0.29	247, 364*	459	0.24
B2	265, 366*	443	0.24	260, 368*	455	0.10	259, 367*	457	0.10
B3	260, 365*	444	0.25	260, 365*	454	0.29	258, 365*	455	0.27
B4	260, 364*	444	0.21	256, 364*	454	0.28	258, 364*	455	0.23
B5	257, 366*	442	0.15	256, 364*	450	0.29	256, 364*	453	0.11
B6	259, 362*	437	0.22	261, 362*	449	0.42	257, 360*	450	0.25
B7	260, 362*	437	0.24	261, 359*	446	0.38	256, 360*	448	0.21
B8	260, 365*	442	0.019	262, 362*	472	0.005	262, 361*	468	0.004
B9	272, 357*	462	0.002	278, 364*	494	0.002	274, 364*	494	0.001
B10	273, 362*	483	0.0025	275, 368*	511	0.001	275, 362*	532	0.0007

^a λ_{ex} : maximum fluorescence excitation wavelength; λ_{em} : maximum fluorescence emission wavelength; Φ_{F} : fluorescence quantum yield; * fluorescence excitation wavelength employed for obtaining the emission spectra.

3. Analytical reactions with compounds A6 and A8

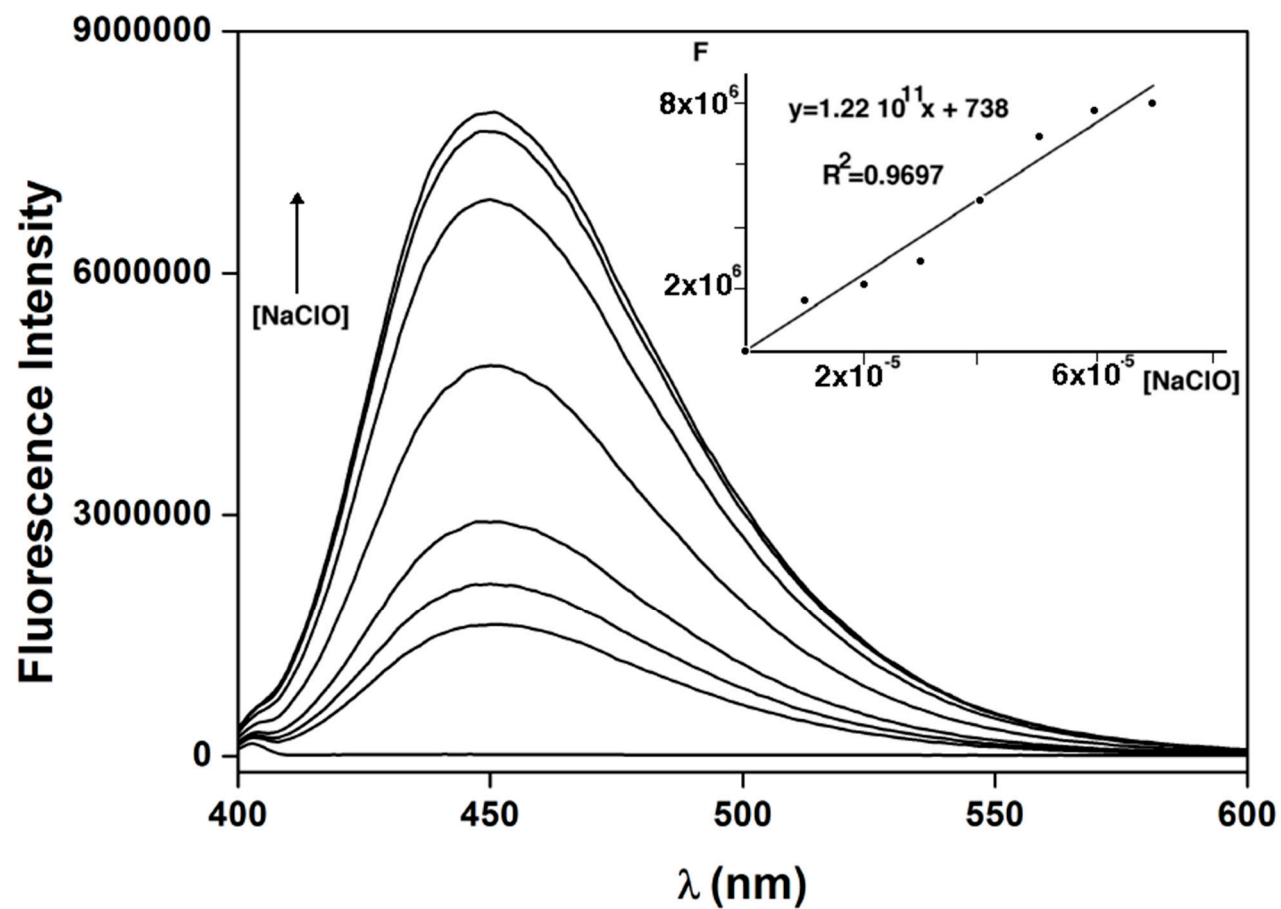


Figure S.1 Fluorescence emission spectra (λ_{ex} 360 nm) of the product obtained from the reaction of A6 with increasing amounts of sodium hypochlorite.

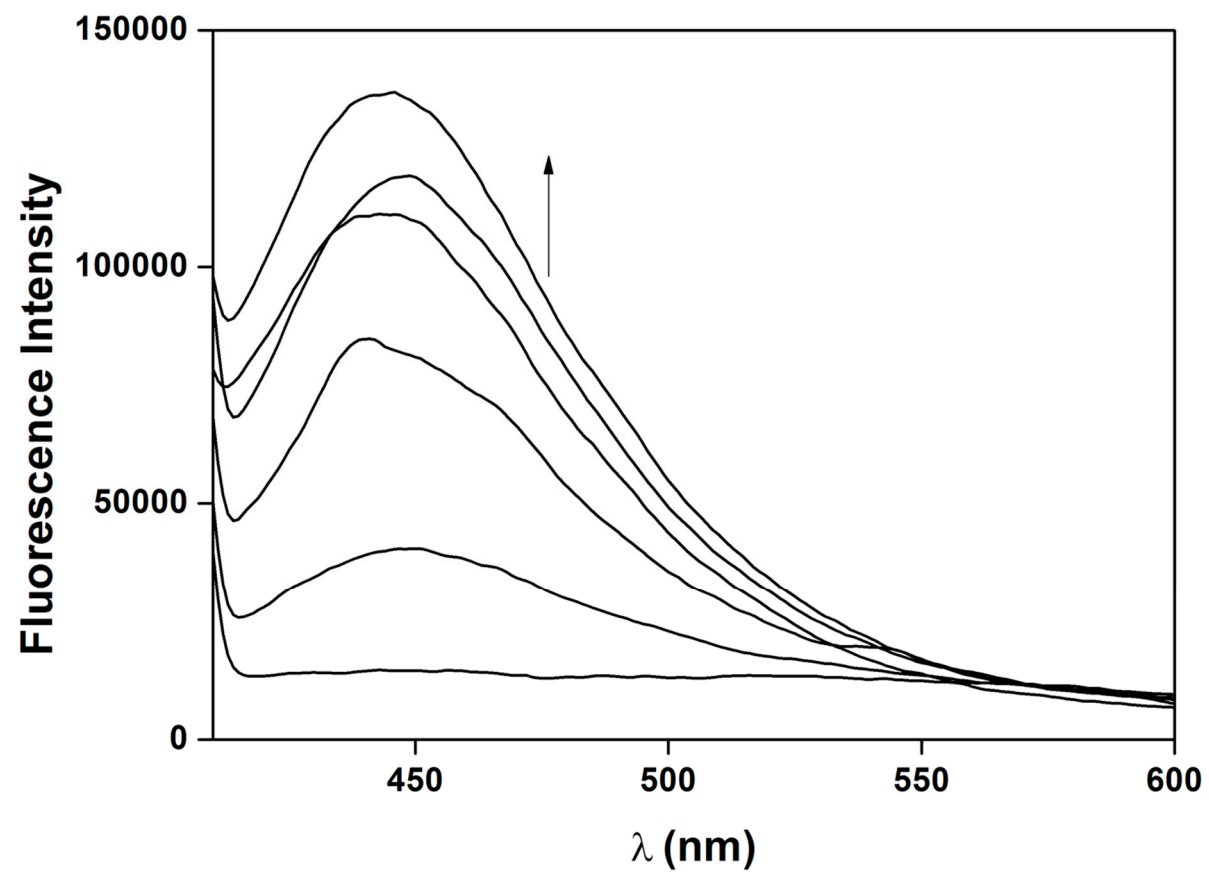


Figure S.2 Fluorescence emission spectra (λ_{ex} 360 nm) of the product obtained from the reaction of **A6** with increasing amounts of hydrogen peroxide.

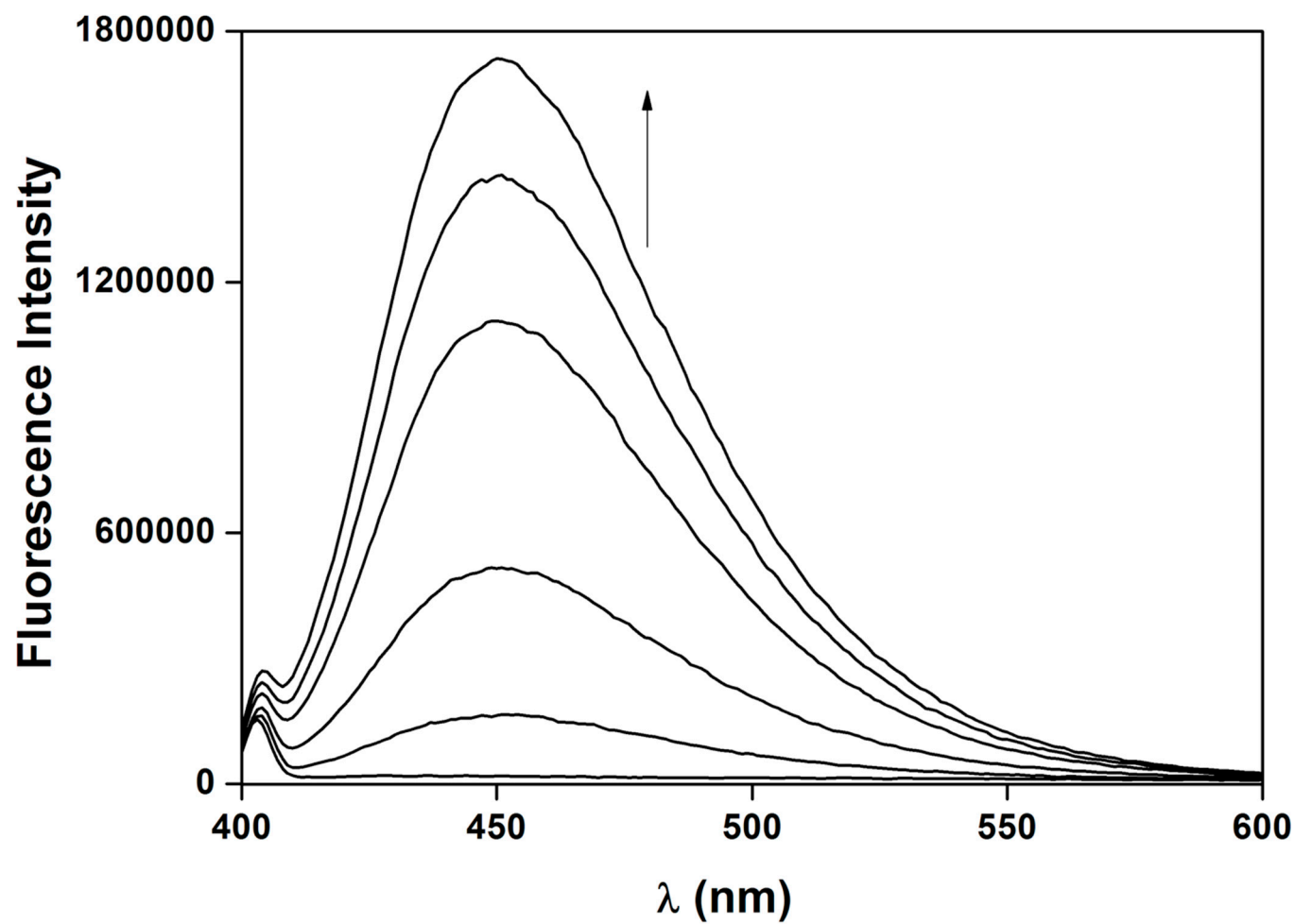


Figure S.3 Fluorescence emission spectra (λ_{ex} 360 nm) of the product obtained from the reaction of **A6** with increasing amounts of *tert*-butyl hydroperoxide

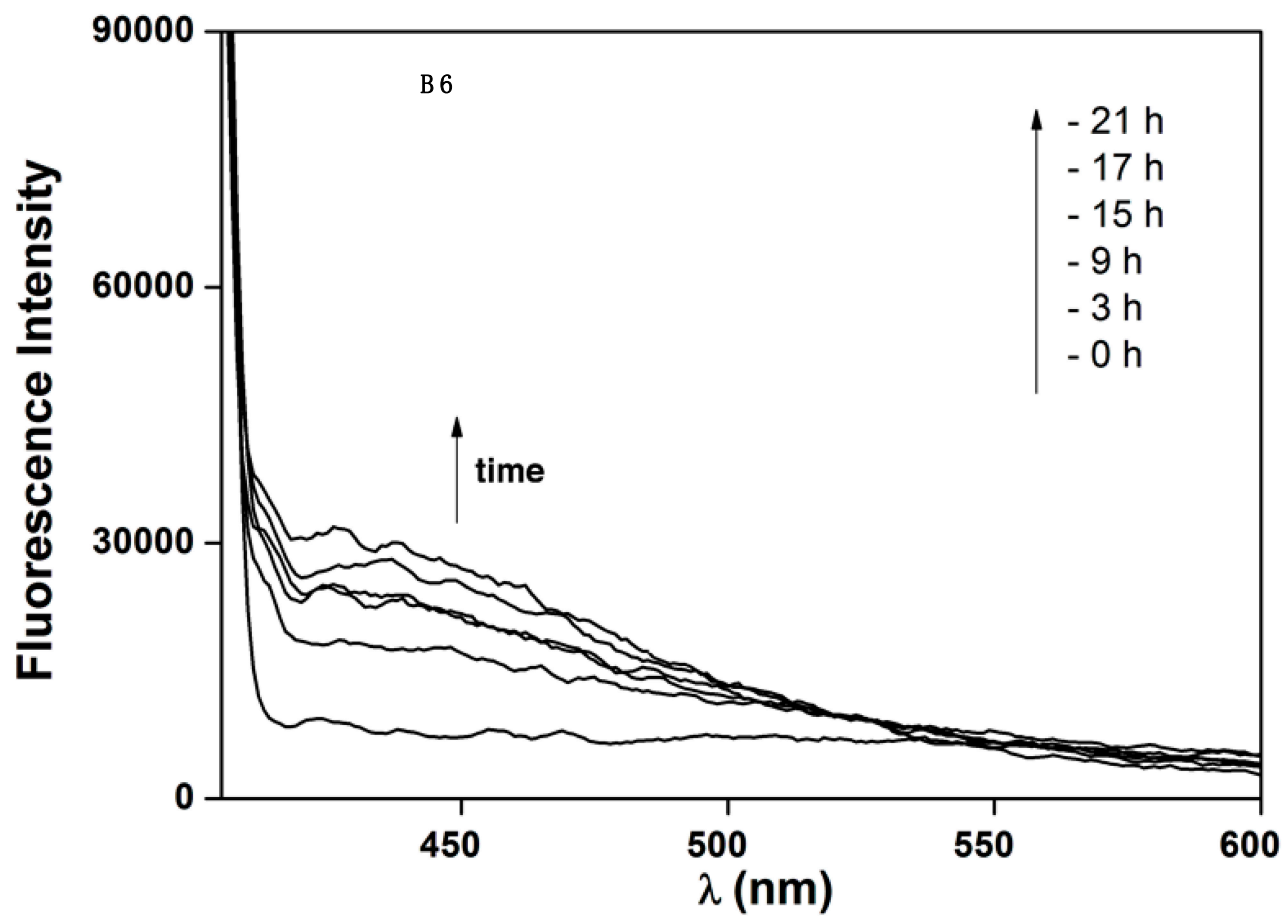


Figure S.4 Fluorescence emission spectra (λ_{ex} 361 nm) of the product obtained from the reaction of compound **A8** with the maximum amount of sodium hypochlorite employed for all other cases, after increasing the reaction time up to 21 h.