

Supporting Information

Enantioselective Synthesis of (+)-Coerulescine by Phase-transfer Catalytic Allylation of Diphenylmethyl tert-butyl α -(2-nitrophenyl)malonate

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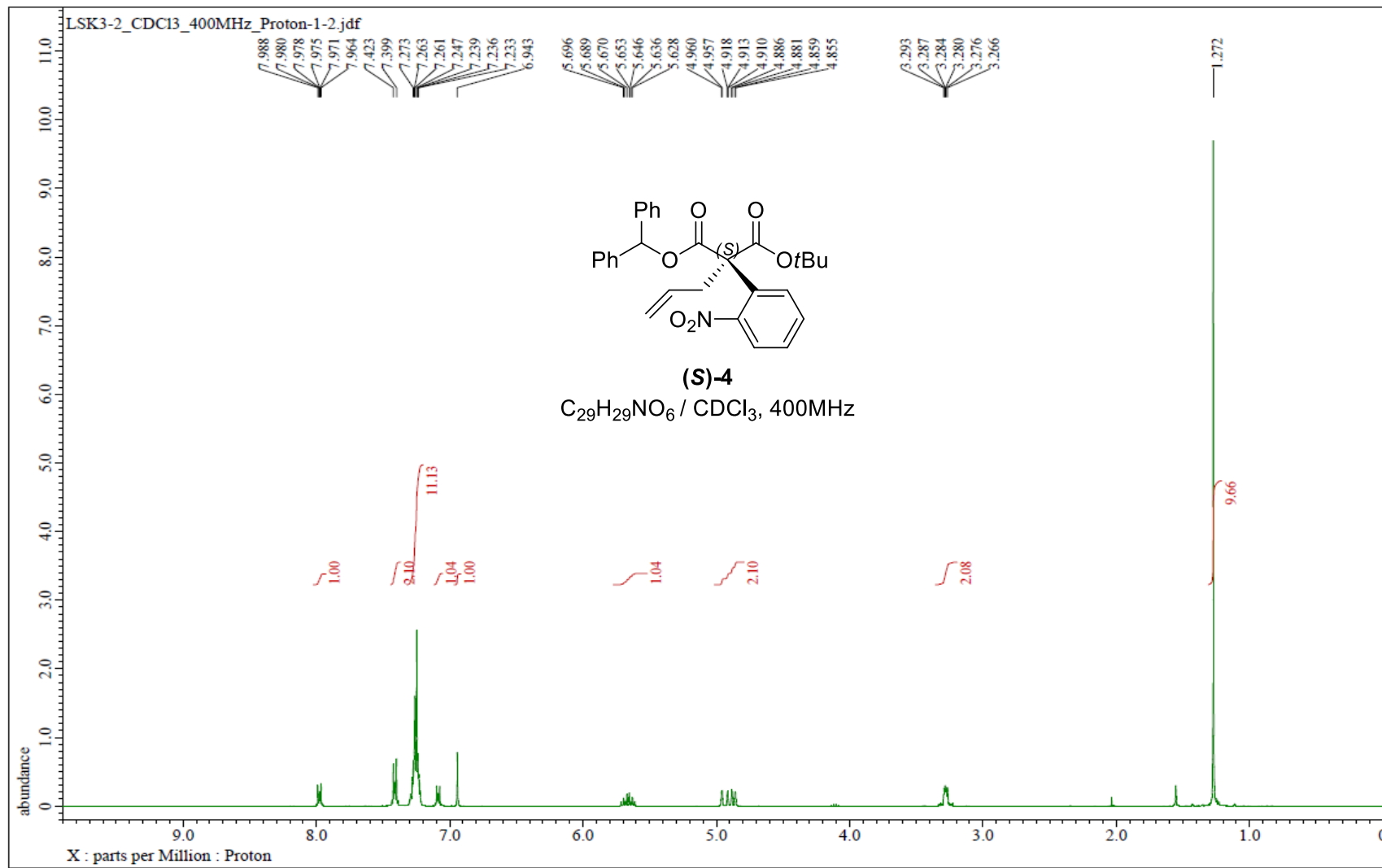
hgpk@snu.ac.kr

List of Contents

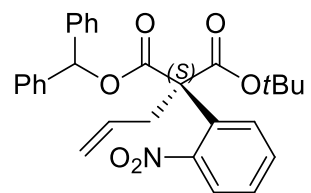
(1) ¹ H & ¹³ C NMR Spectra -----	S2
(2) Chiral HPLC Chromatogram -----	S16

(1) ^1H & ^{13}C NMR Spectra

^1H -NMR of compound (4)

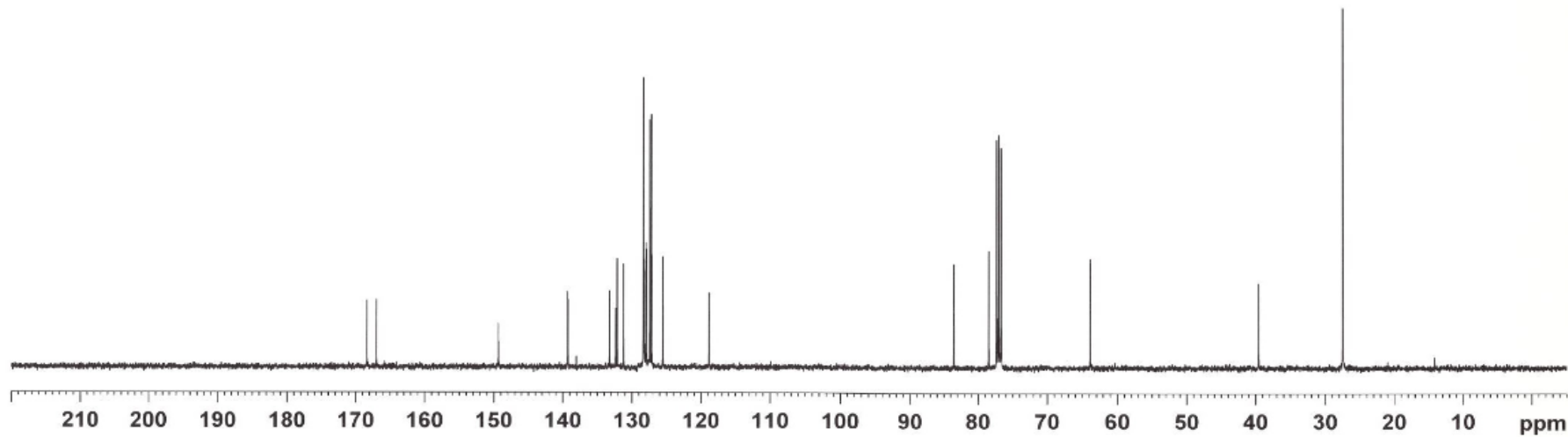


¹³C-NMR of compound (4)

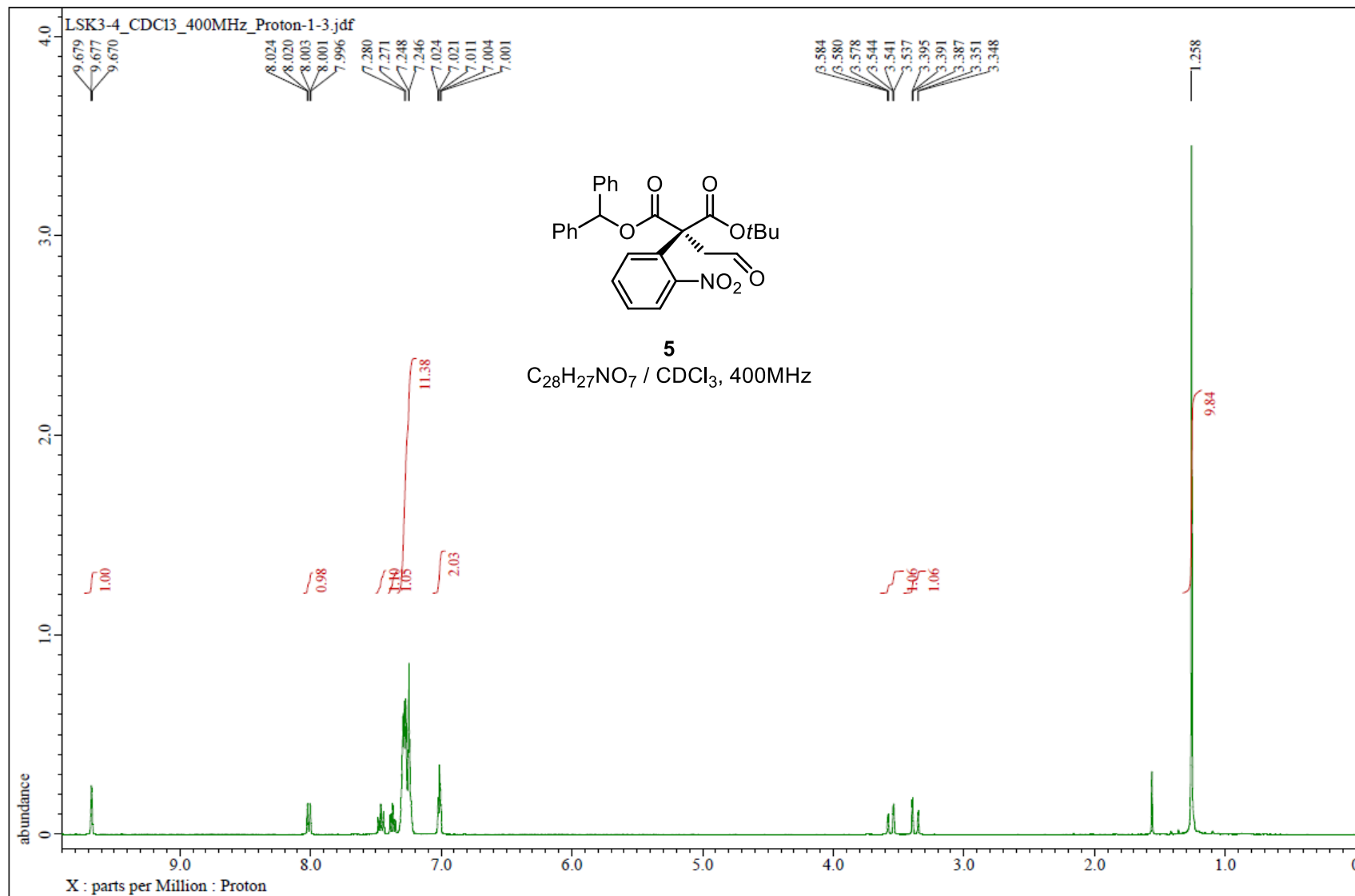


(S)-4

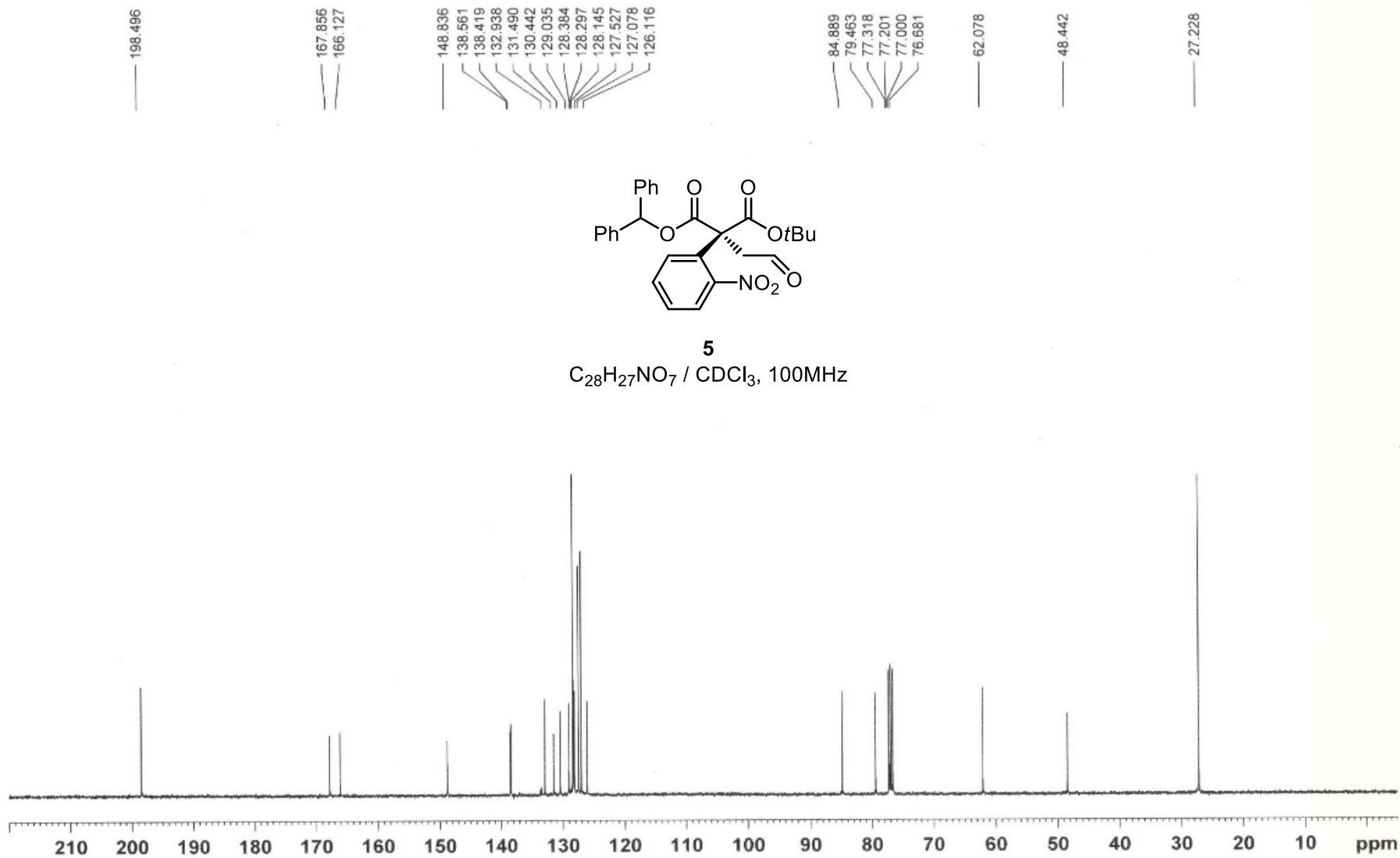
C₂₉H₂₉NO₆ / CDCl₃, 100MHz



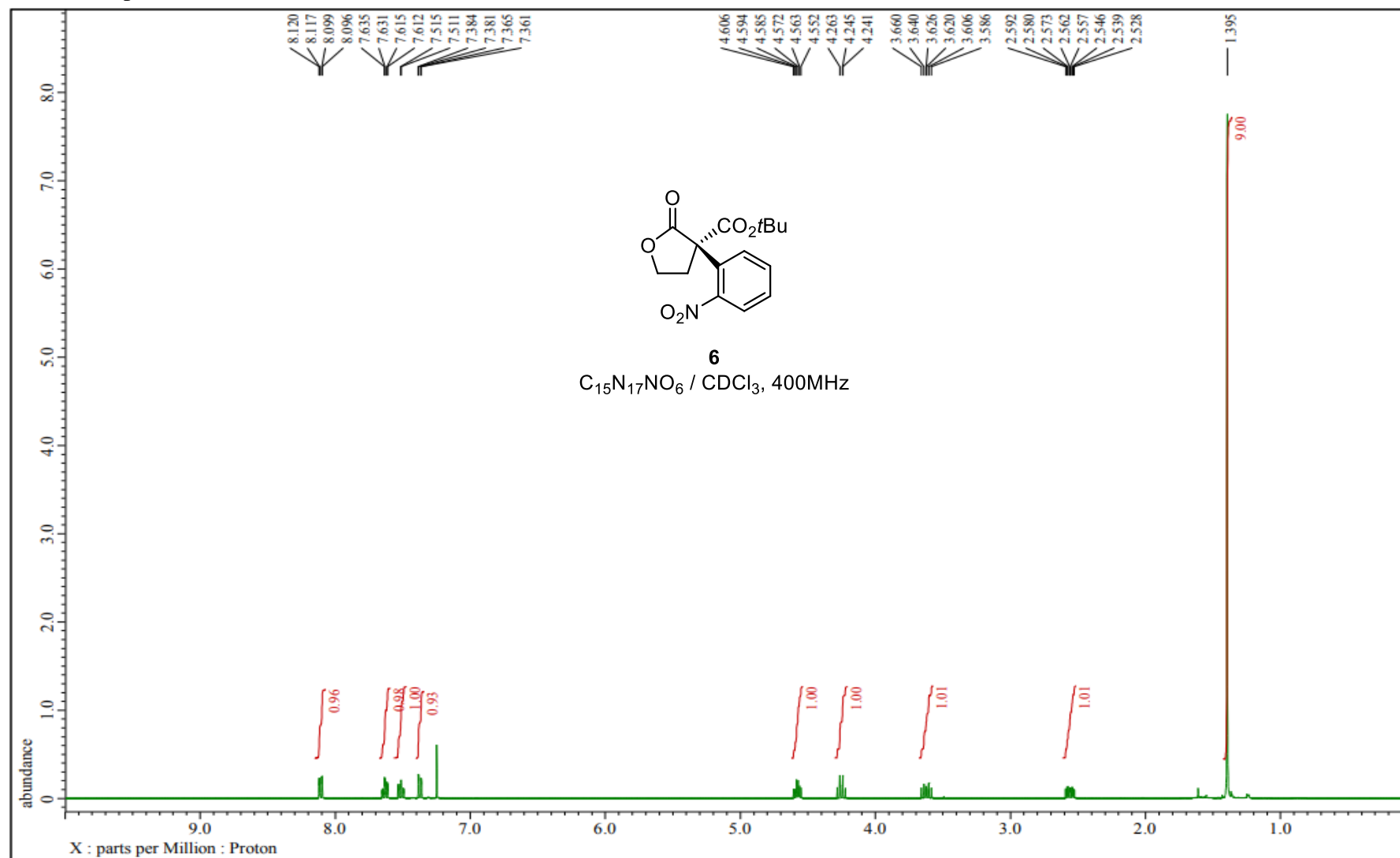
¹H-NMR of compound (5)



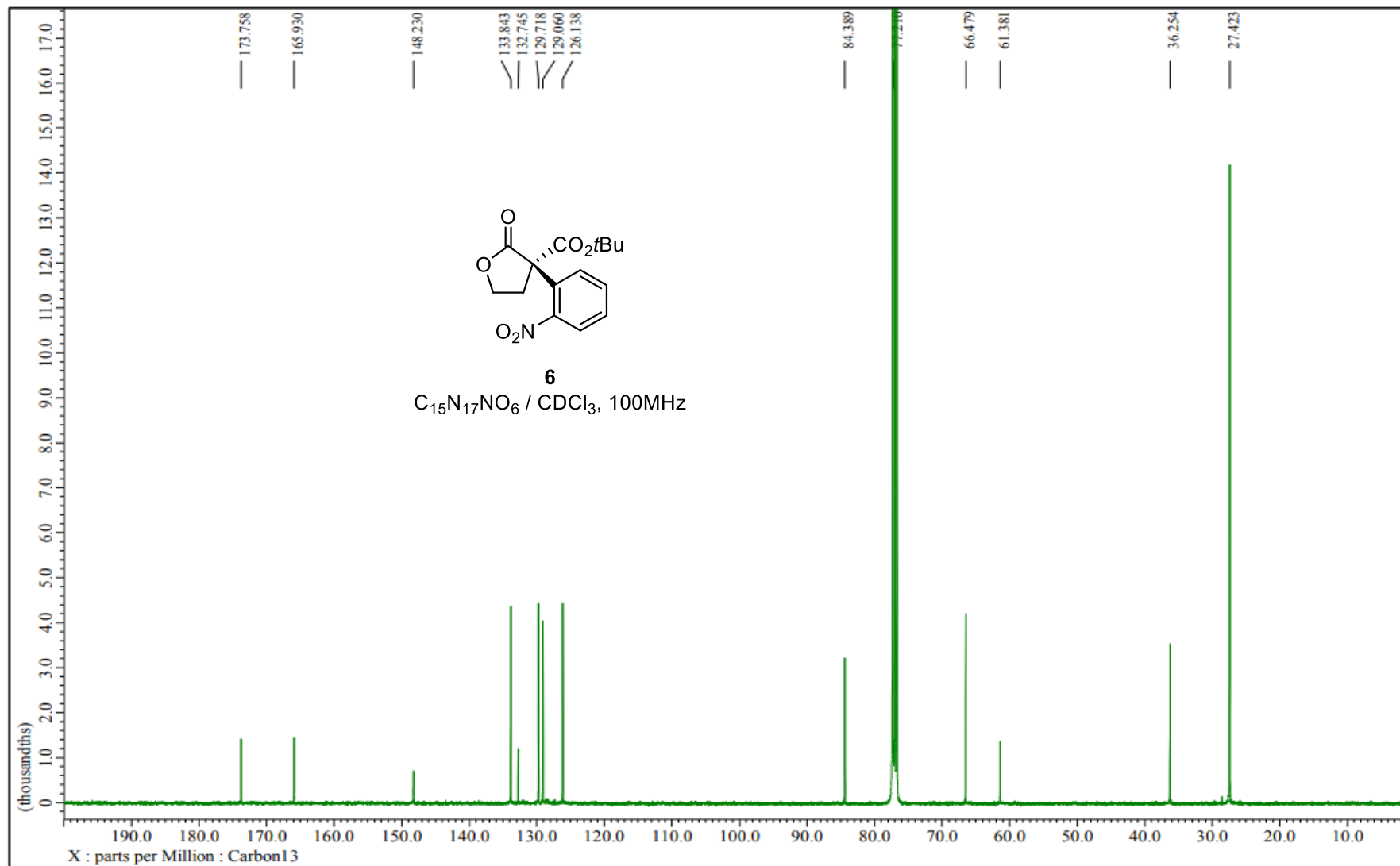
¹³C-NMR of compound (5)



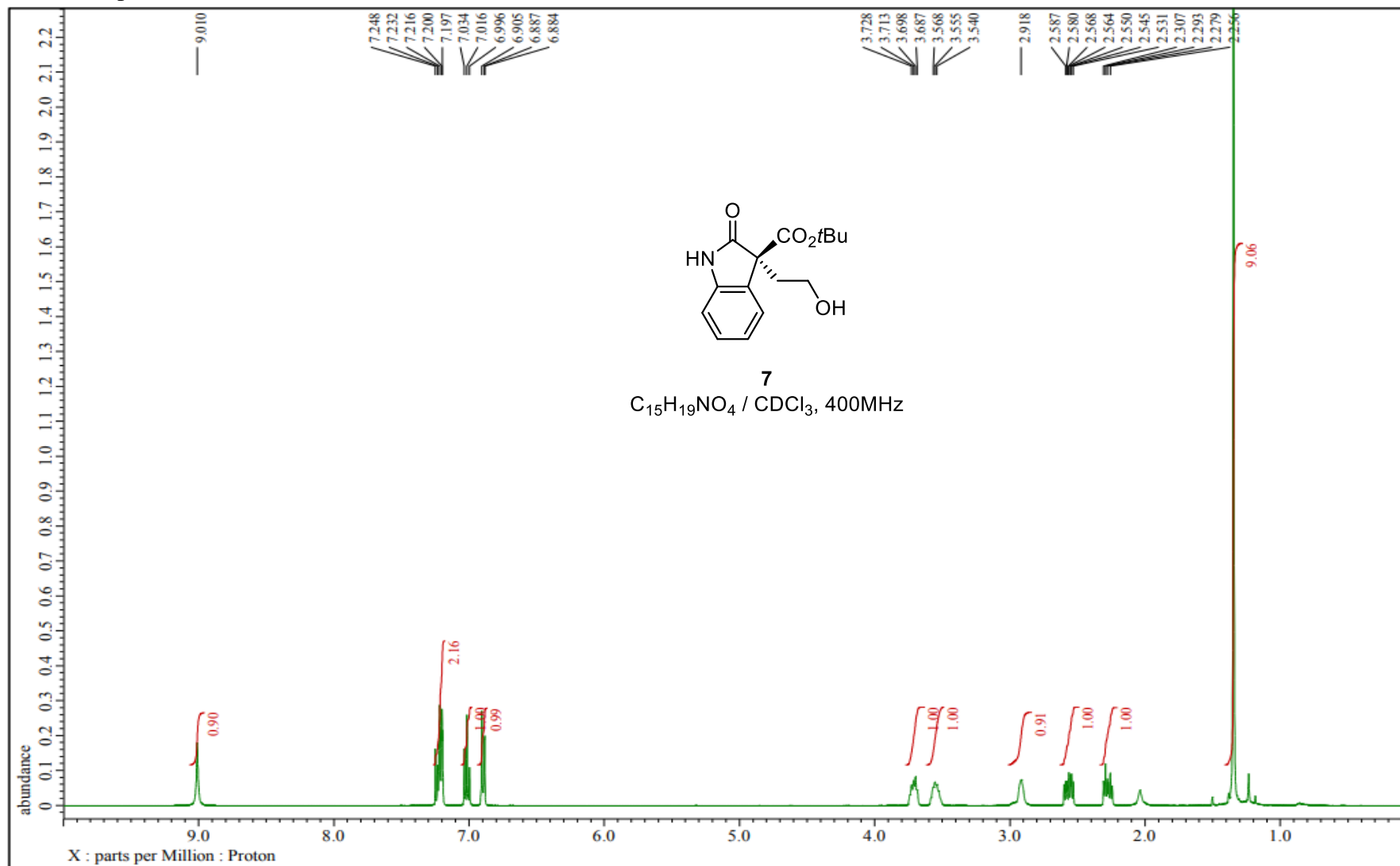
¹H-NMR of compound (6)



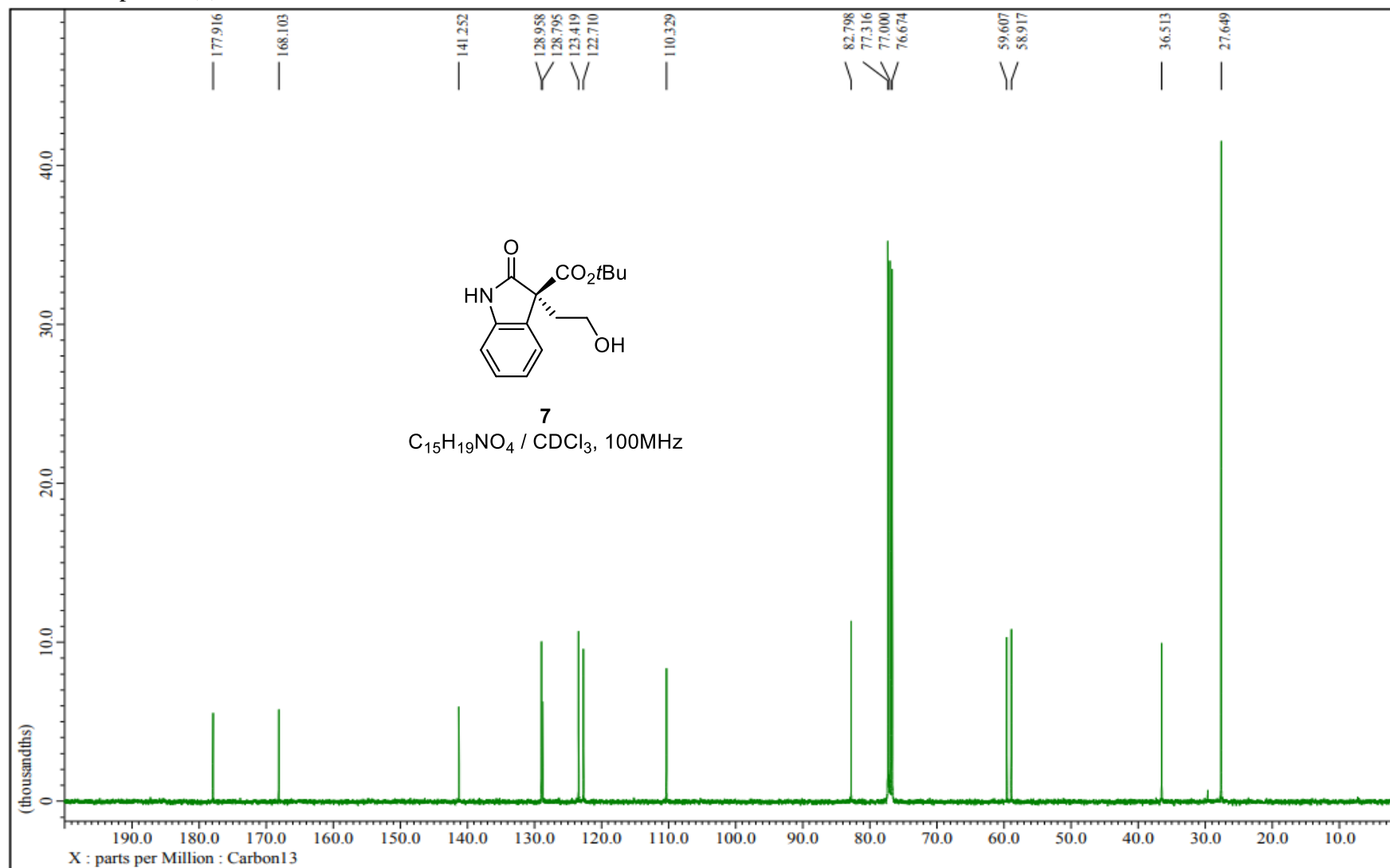
¹³C-NMR of compound (6)



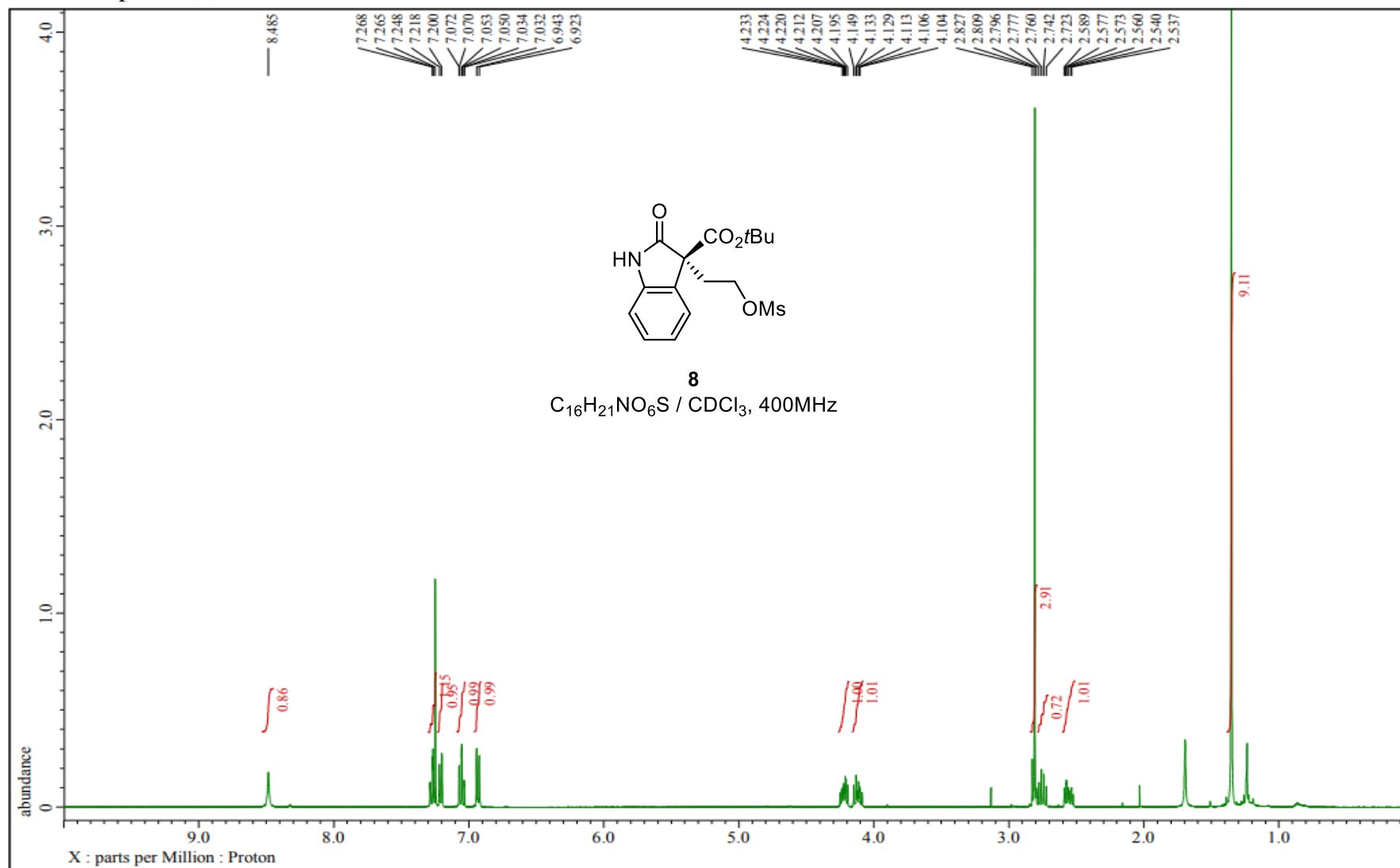
¹H-NMR of compound (7)



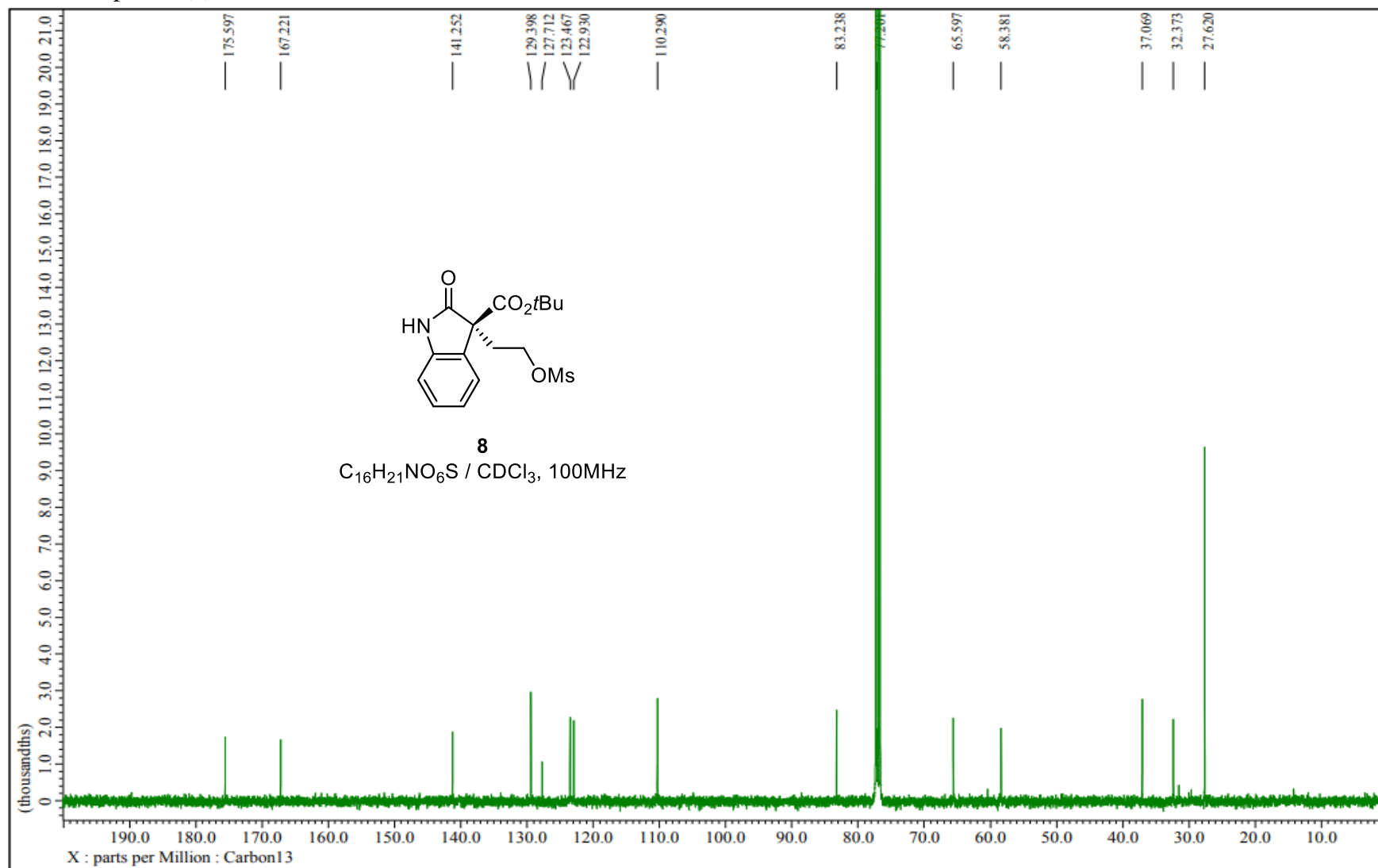
¹³C-NMR of compound (7)



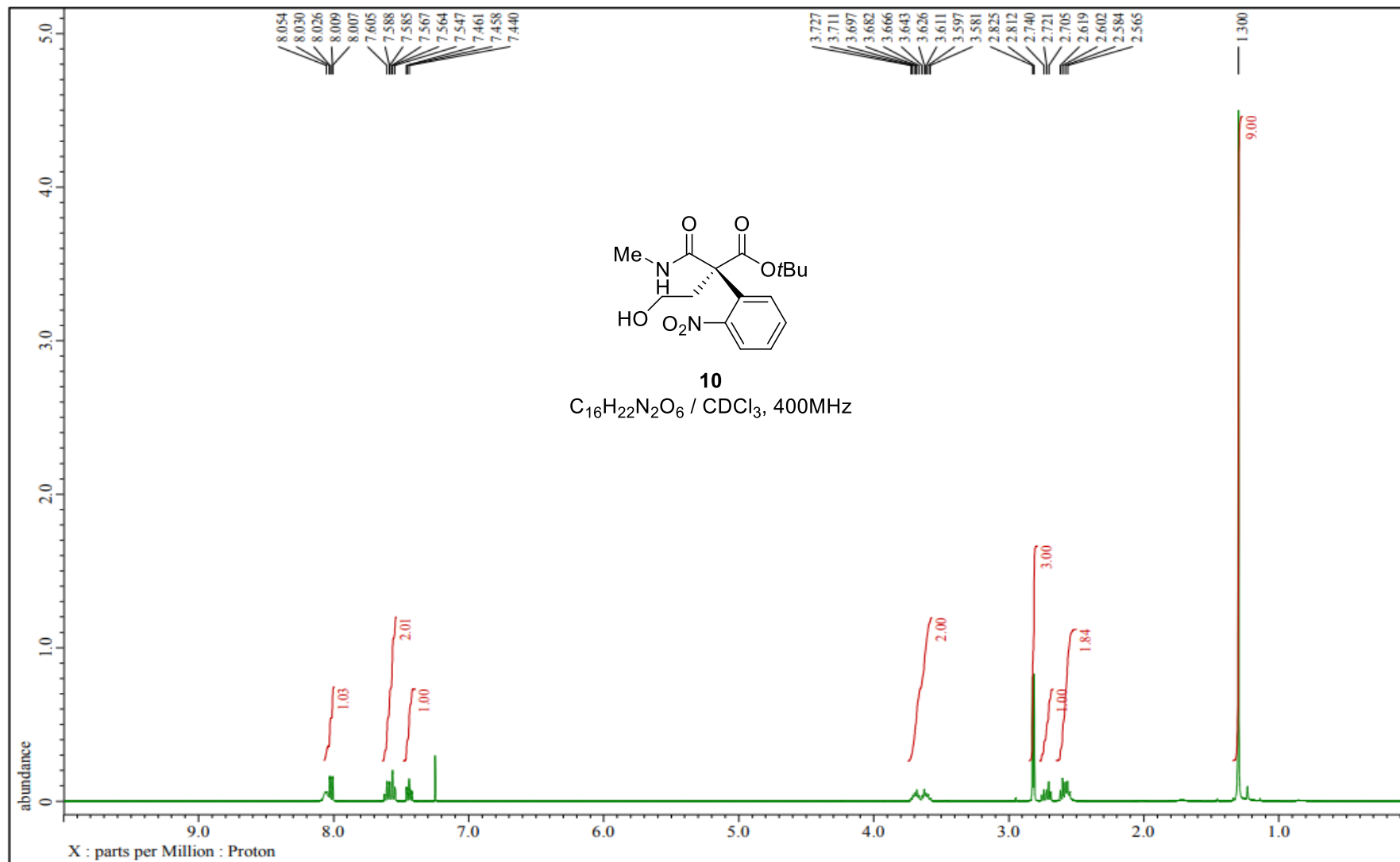
¹H-NMR of compound (8)



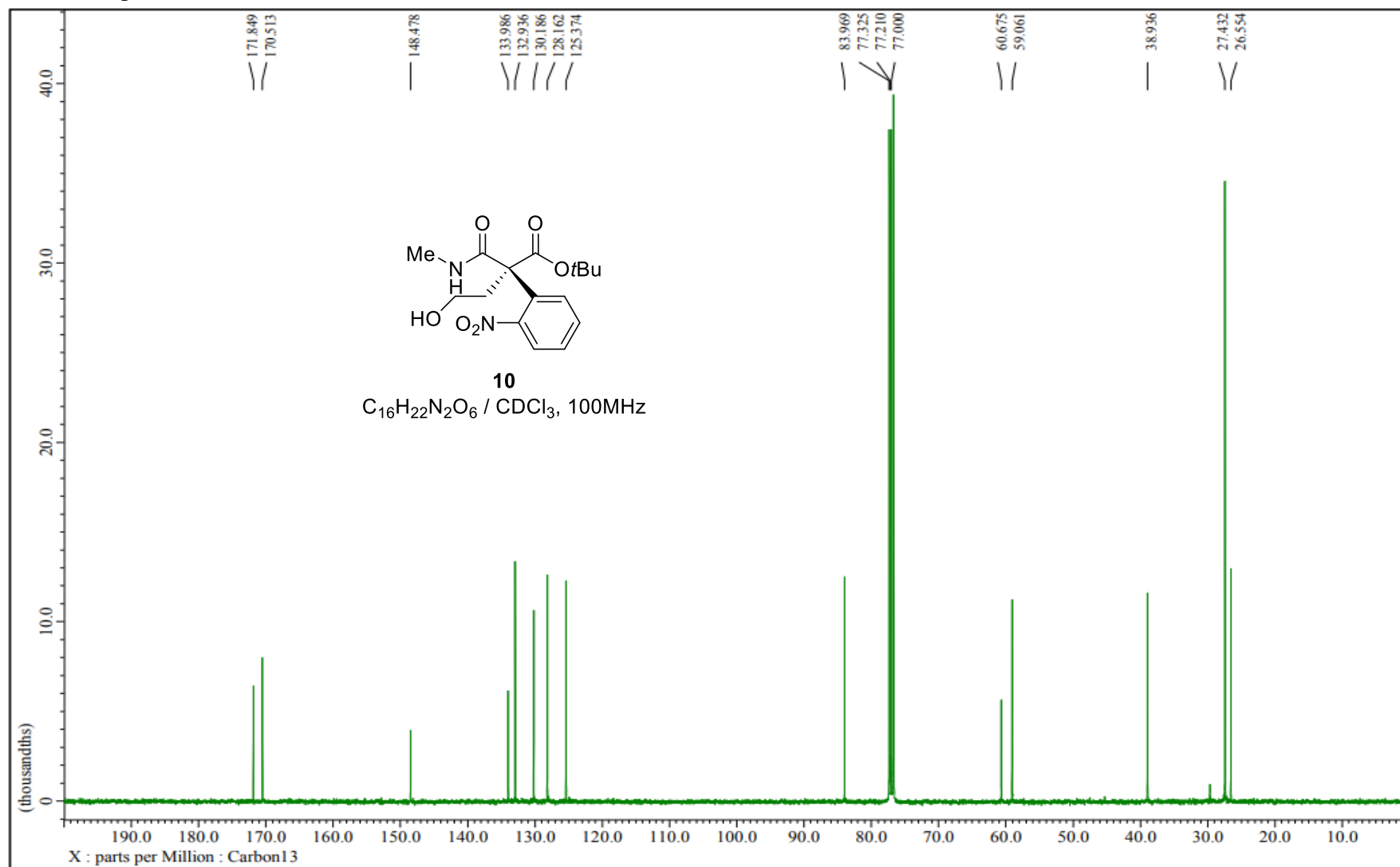
¹³C-NMR of compound (8)



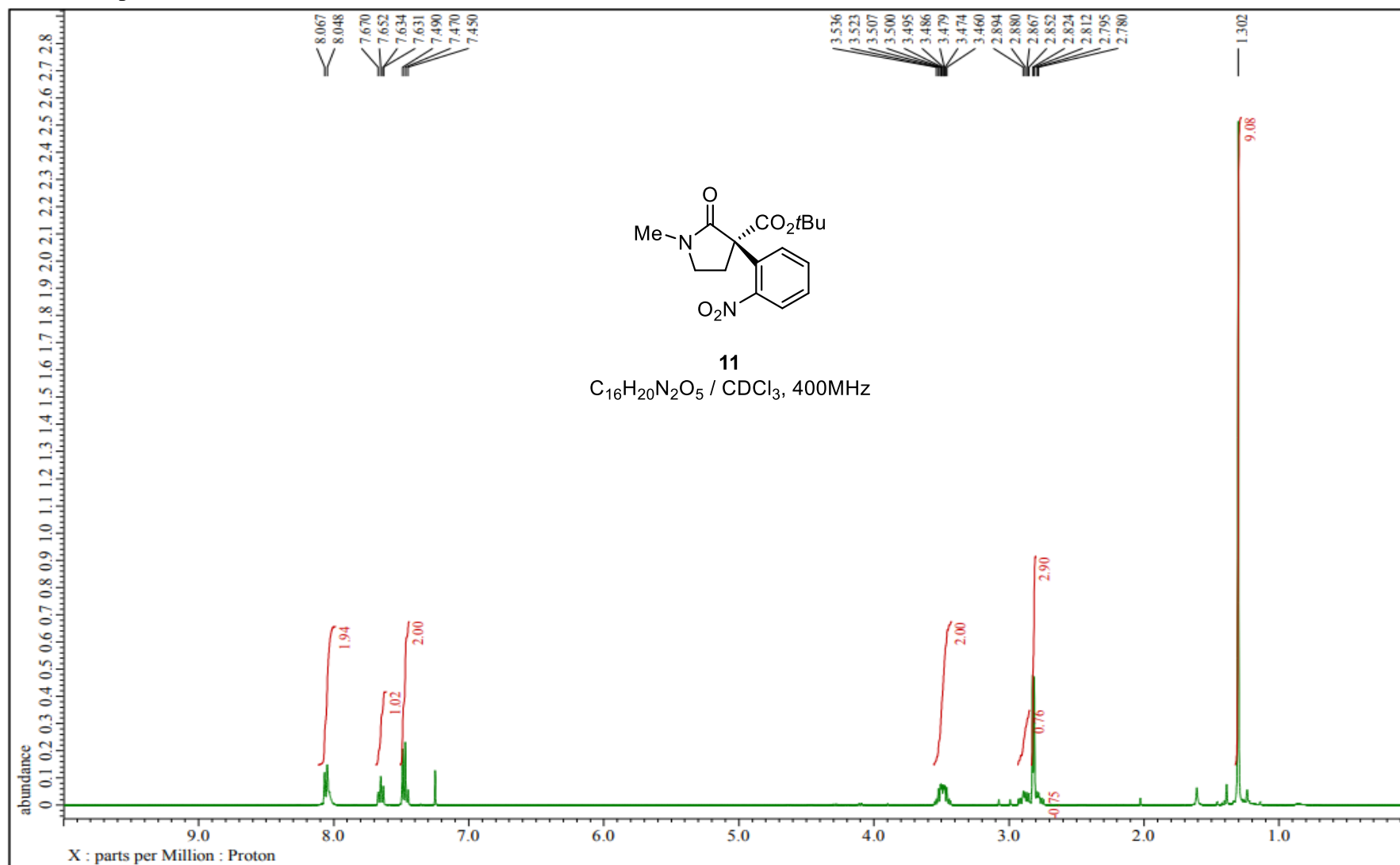
¹H-NMR of compound (10)



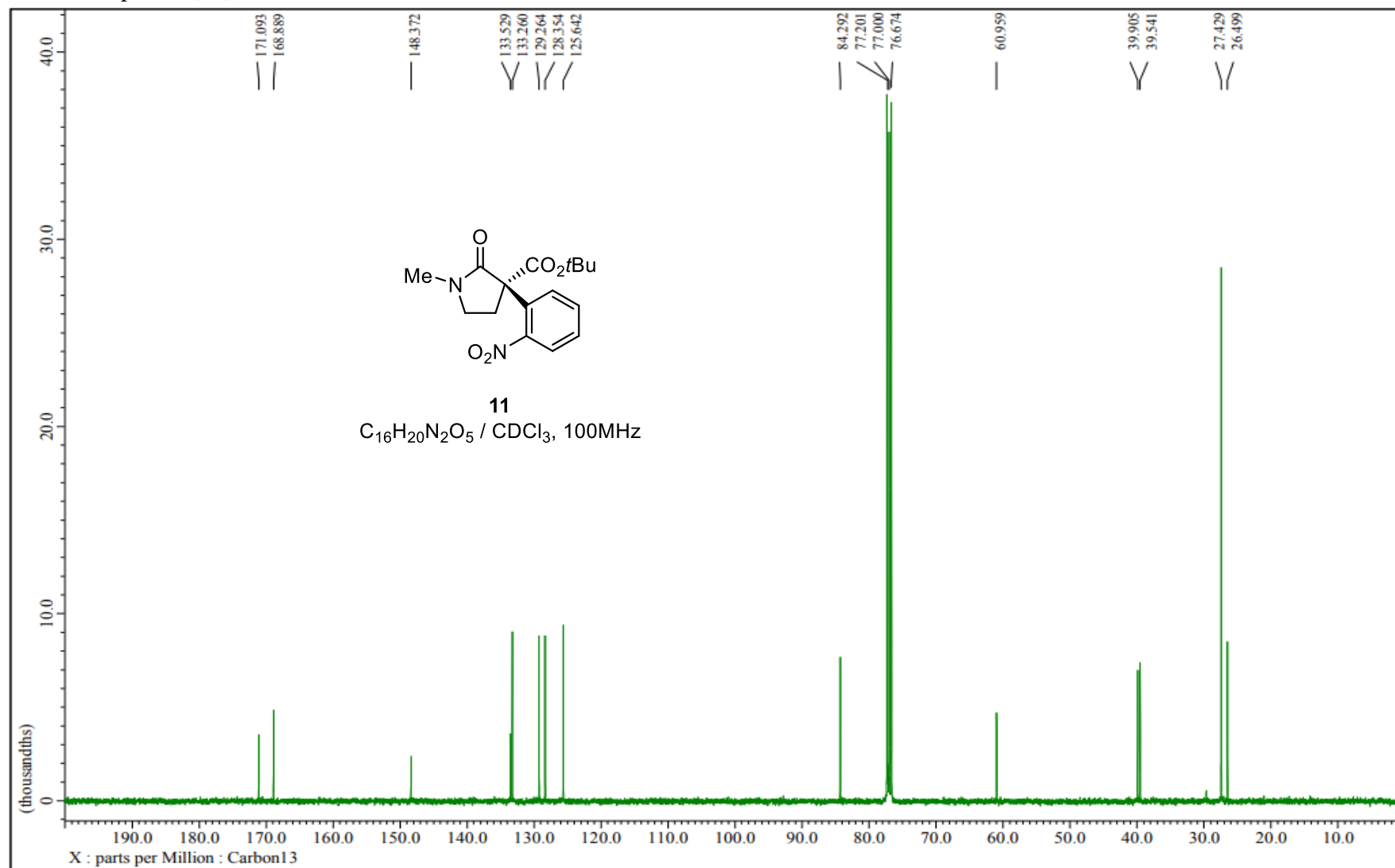
¹³C-NMR of compound (10)



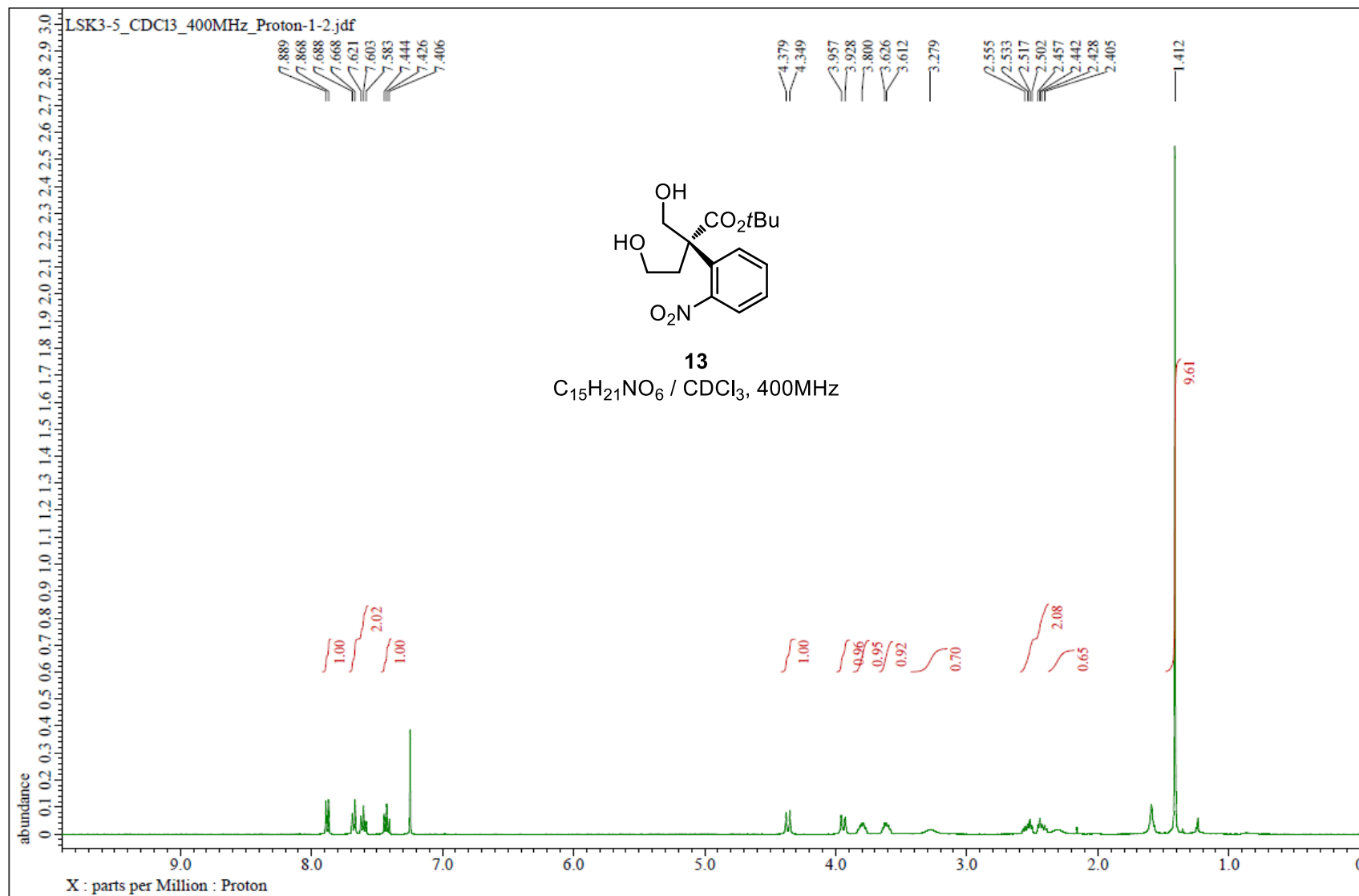
¹H-NMR of compound (11)



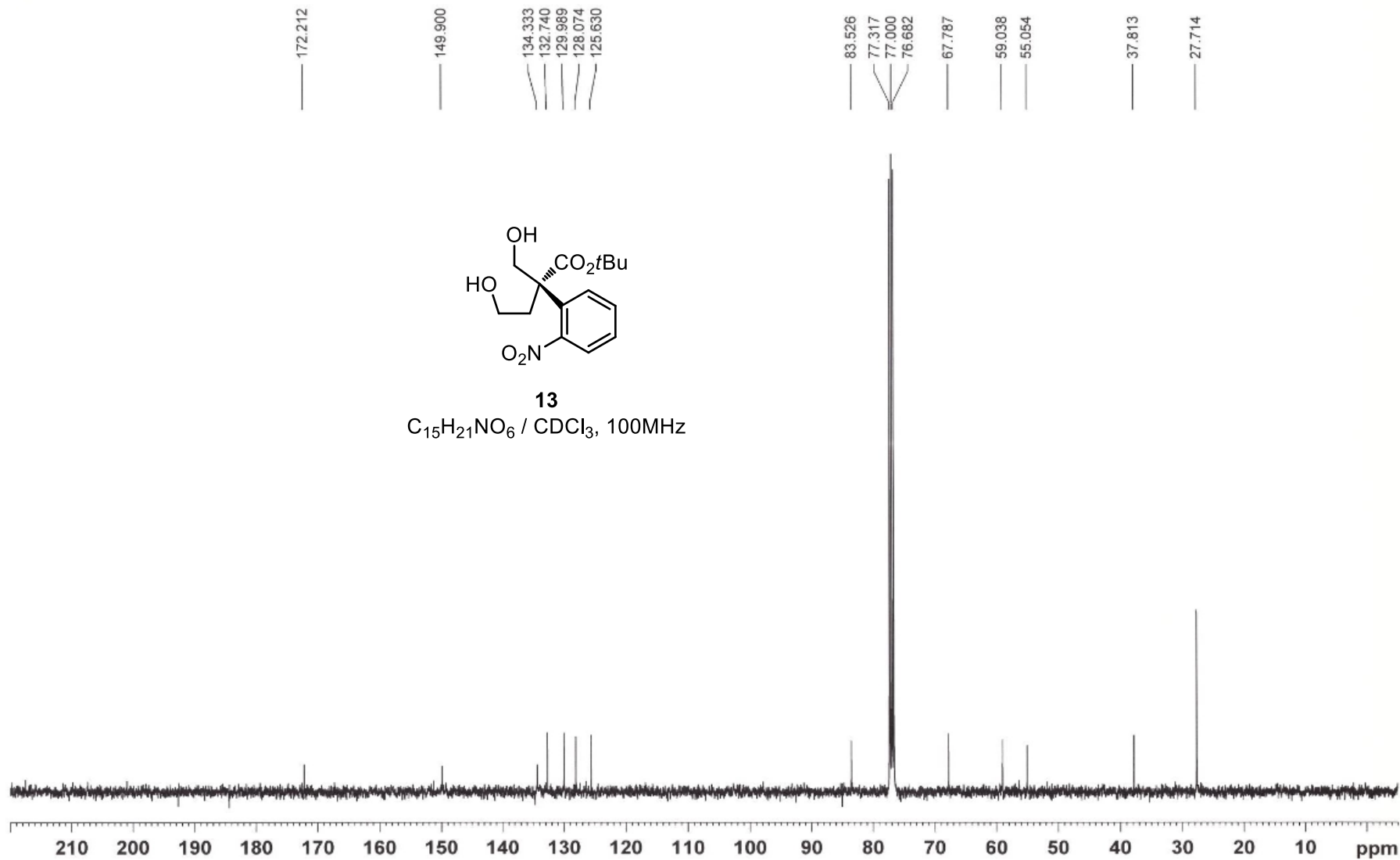
¹³C-NMR of compound (11)



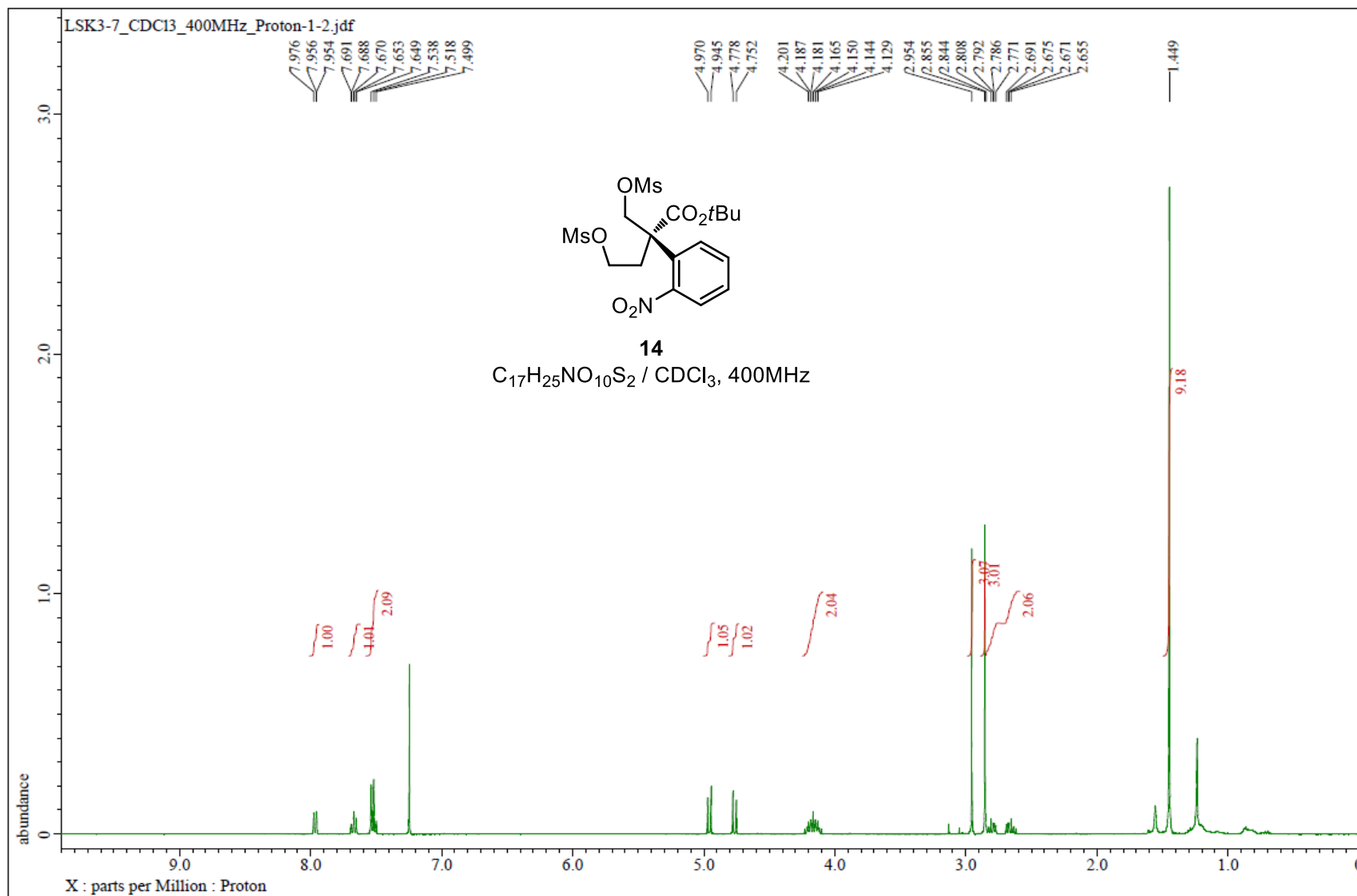
¹H-NMR of compound (13)



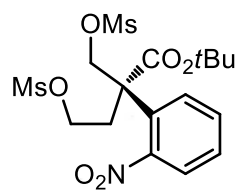
¹³C-NMR of compound (13)



¹H-NMR of compound (14)

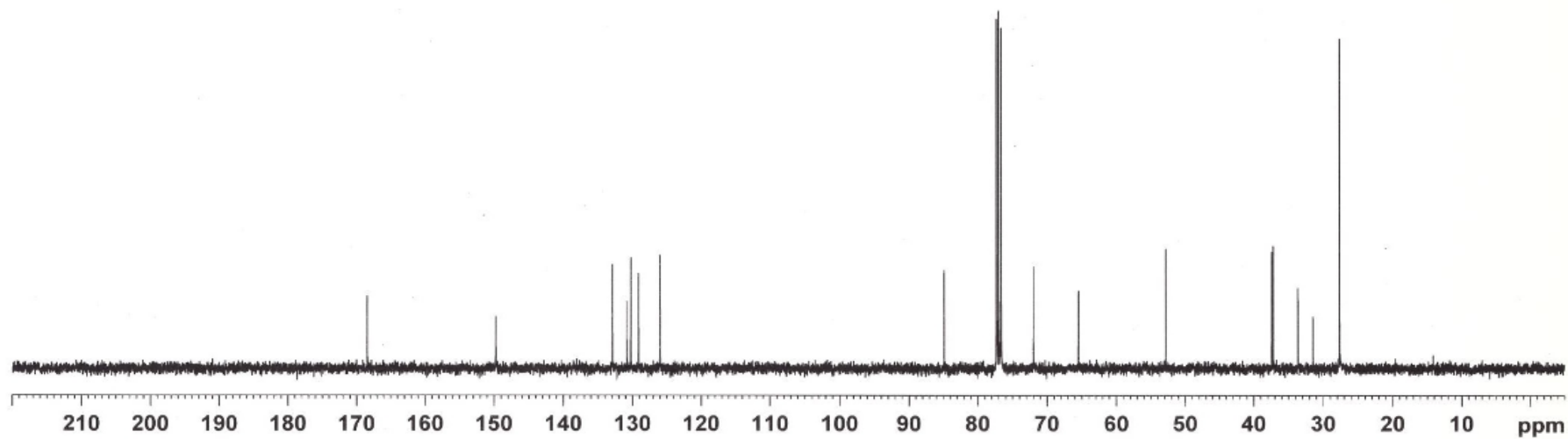


^{13}C -NMR of compound (**14**)

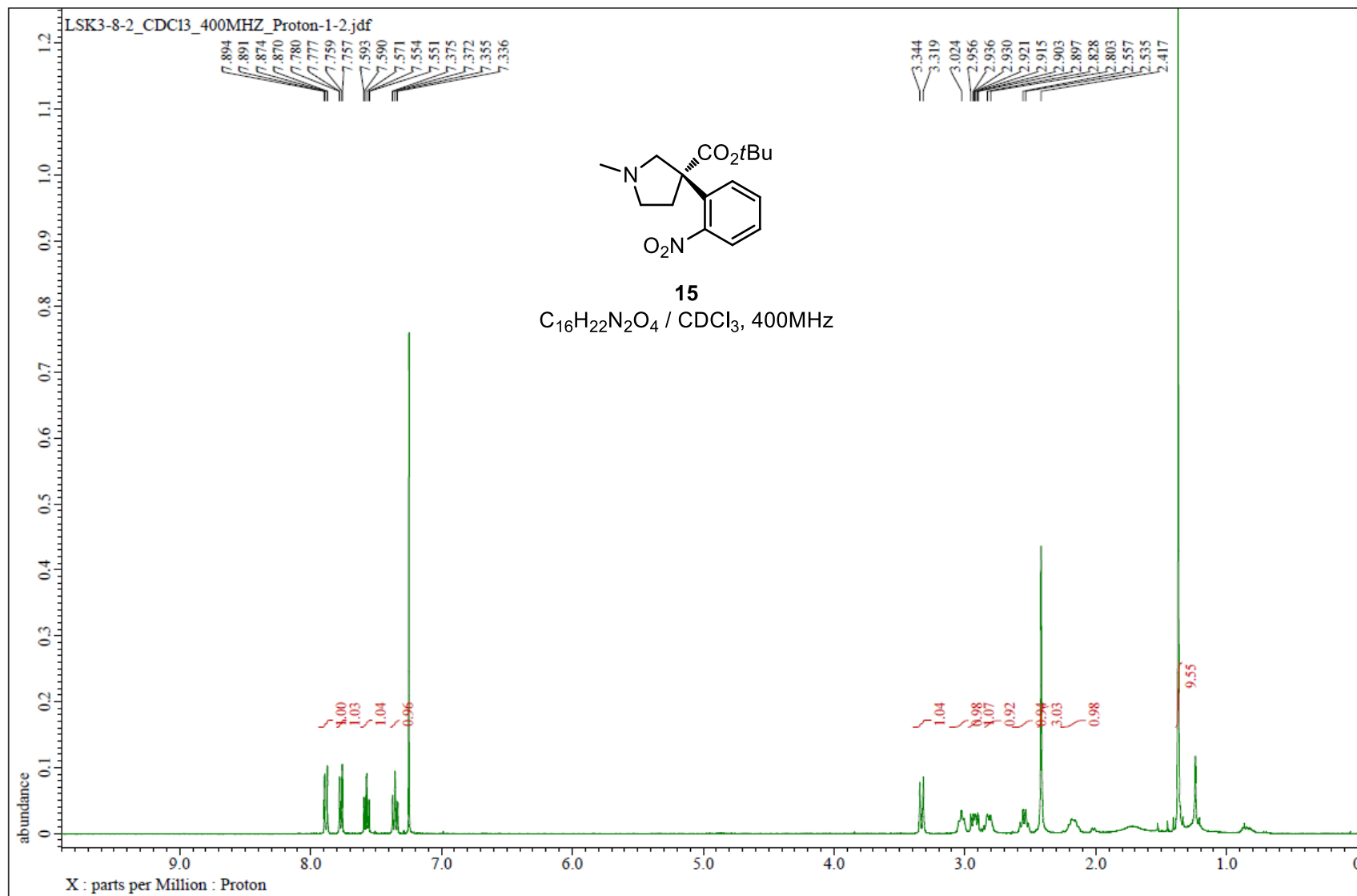


14

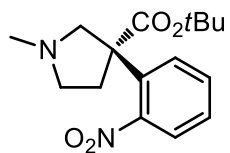
C₁₇H₂₅NO₁₀S₂ / CDCl₃, 100MHz



¹H-NMR of compound (15)

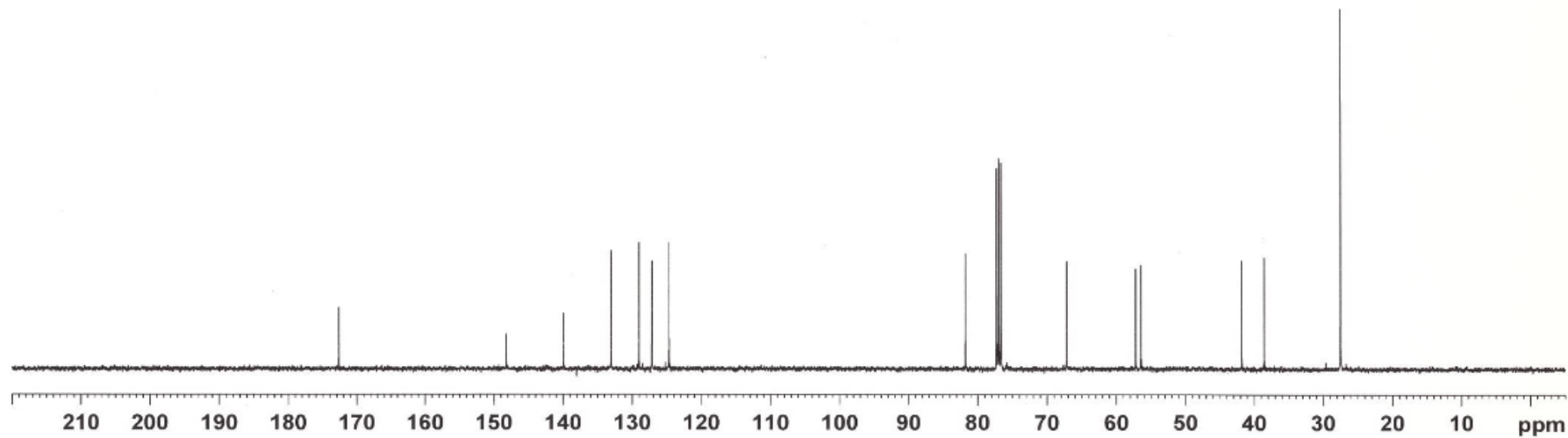


¹³C-NMR of compound (15)

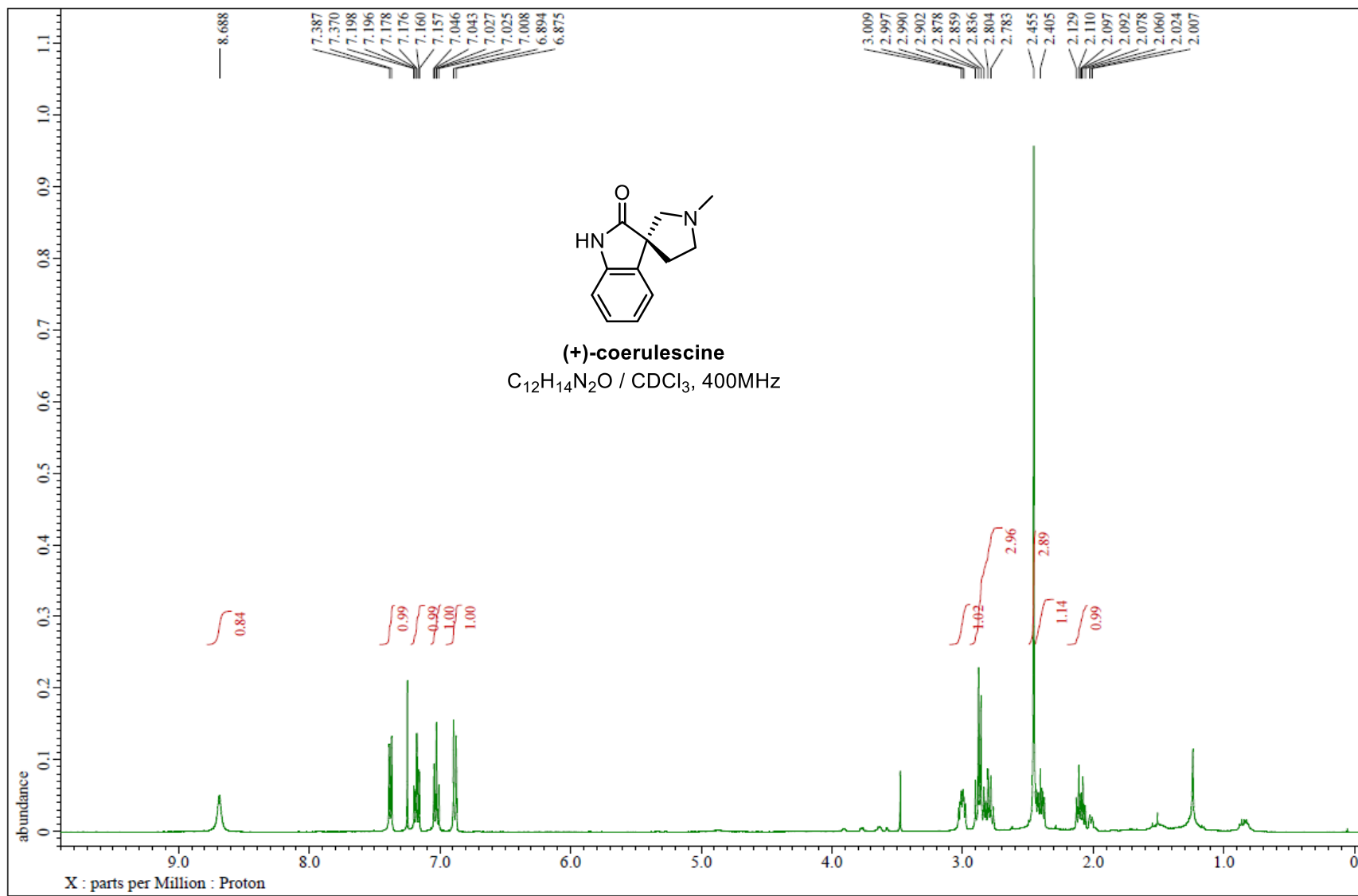


15

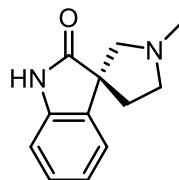
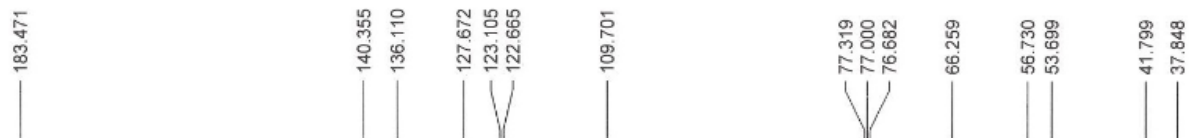
C₁₆H₂₂N₂O₄ / CDCl₃, 100MHz



¹H-NMR of compound (+)-coerulescine

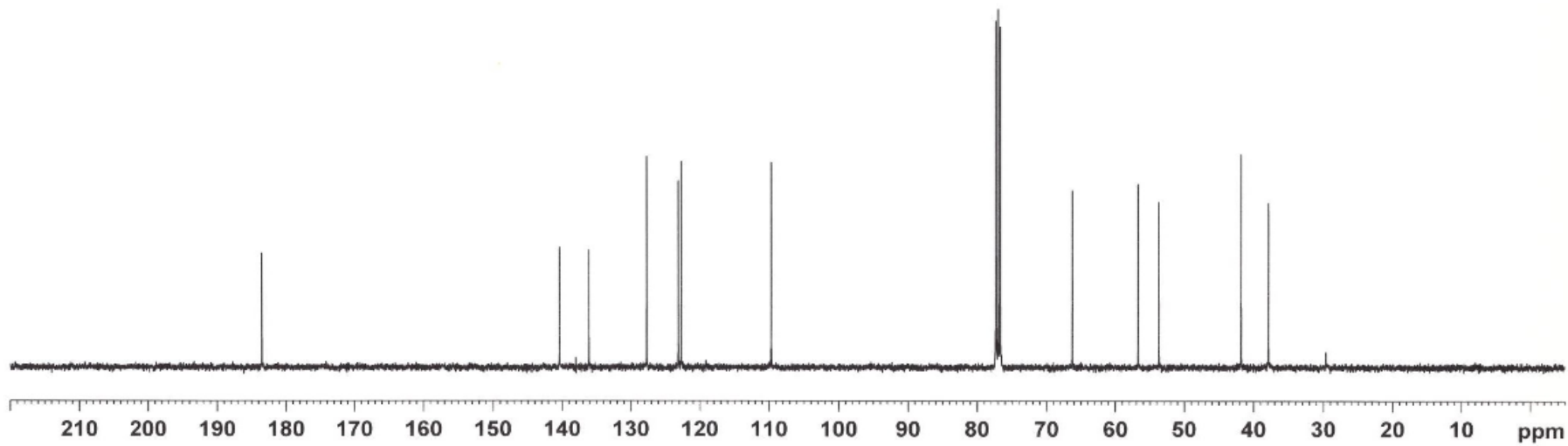


¹³C-NMR of compound (+)-coerulescine



(+)-coerulescine

C₁₂H₁₄N₂O / CDCl₃, 100MHz



(2) Chiral HPLC spectra

Area Percent Report

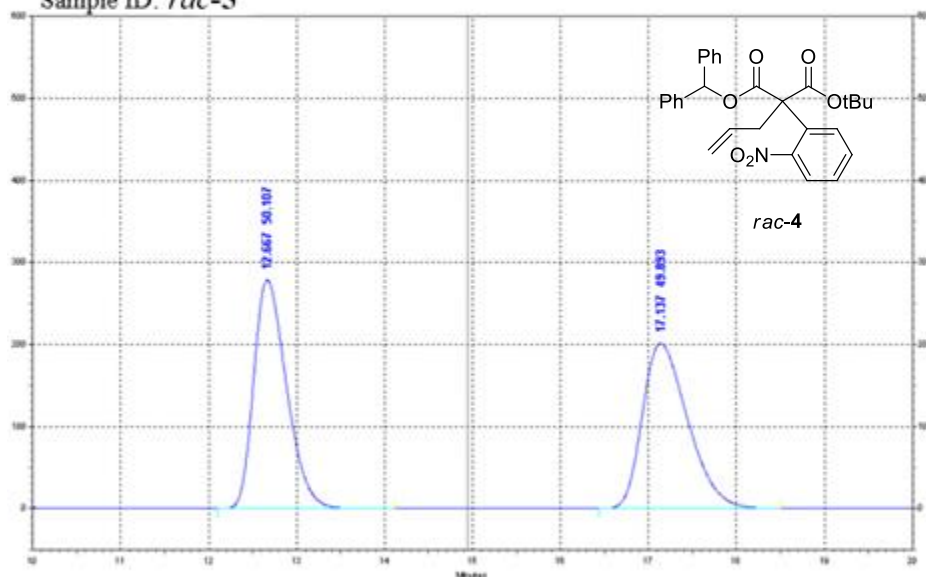
Instrument Name : L-2000

Software Version : Version LaChrom 8908800-07

Acquisition Method : Daicel Chiralpak AD-H, Hexane : 2-Propanol = 95:5, λ = 254 nm,

flow rate = 1.0 mL/min

Sample ID: *rac-5*



UV Results

Name	Retention Time	Area	Area Percent	Integration Codes
	12.667	28889196	50.107	BI
	17.137	28766122	49.893	BB

Totals		57655318	100.000	
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Area Percent Report

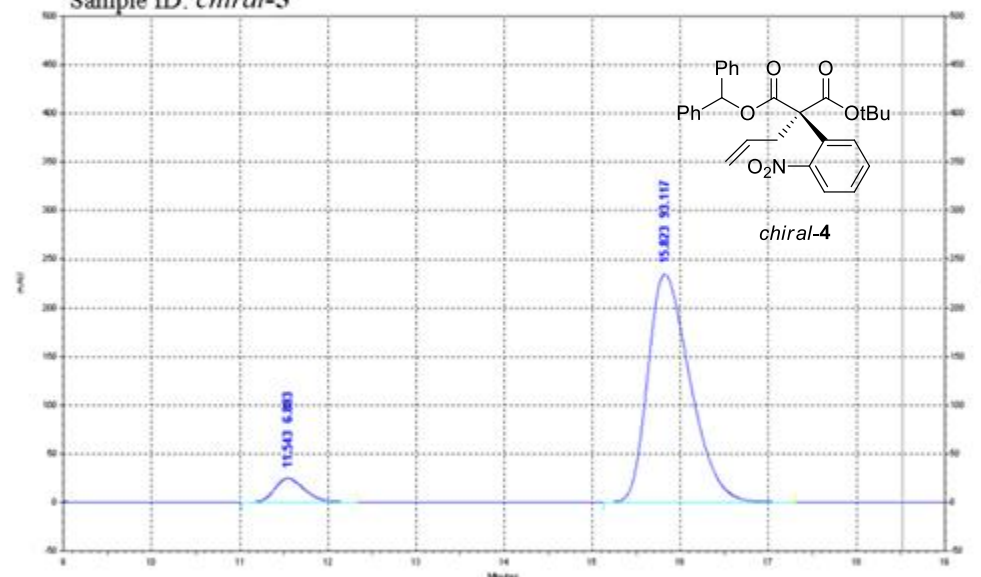
Instrument Name : L-2000

Software Version : Version LaChrom 8908800-07

Acquisition Method : Daicel Chiralpak AD-H, Hexane : 2-Propanol = 95:5, λ = 254 nm,

flow rate = 1.0 mL/min

Sample ID: *chiral-5*



UV Results

Name	Retention Time	Area	Area Percent	Integration Codes
	11.543	2310121	6.883	MM
	15.823	31251904	93.117	MM

Totals		33562025	100.000	
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Area Percent Report

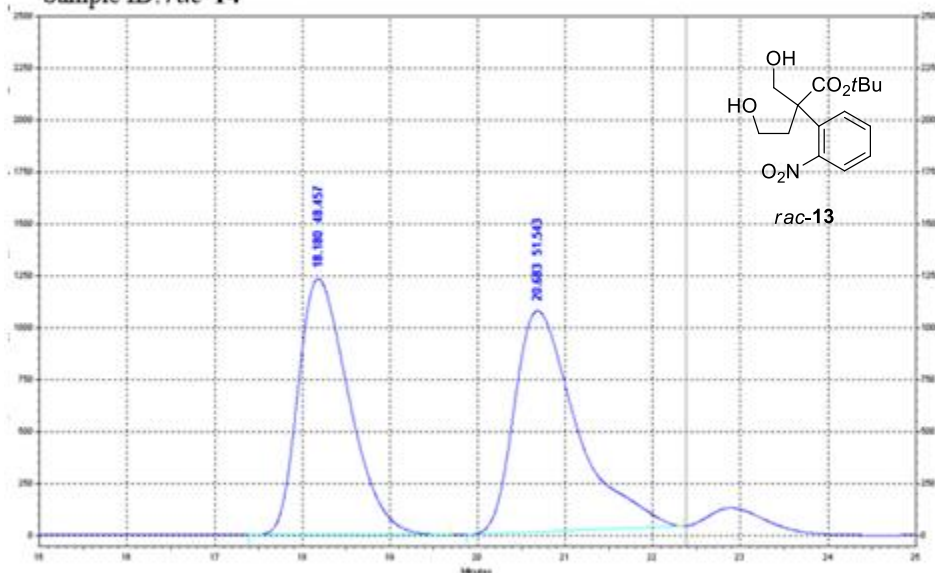
Instrument Name : L-2000

Software Version : Version LaChrom 8908800-07

Acquisition Method : Daicel Chiralpak AD-H, Hexane : 2-Propanol = 90:10, λ = 254 nm,

flow rate = 1.0 mL/min

Sample ID: *rac-14*



UV Results

Name	Retention Time	Area	Area Percent	Integration Codes
	18.180	198513832	48.457	MM
	20.683	211155480	51.543	MM

Totals		409669312	100.000	
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Area Percent Report

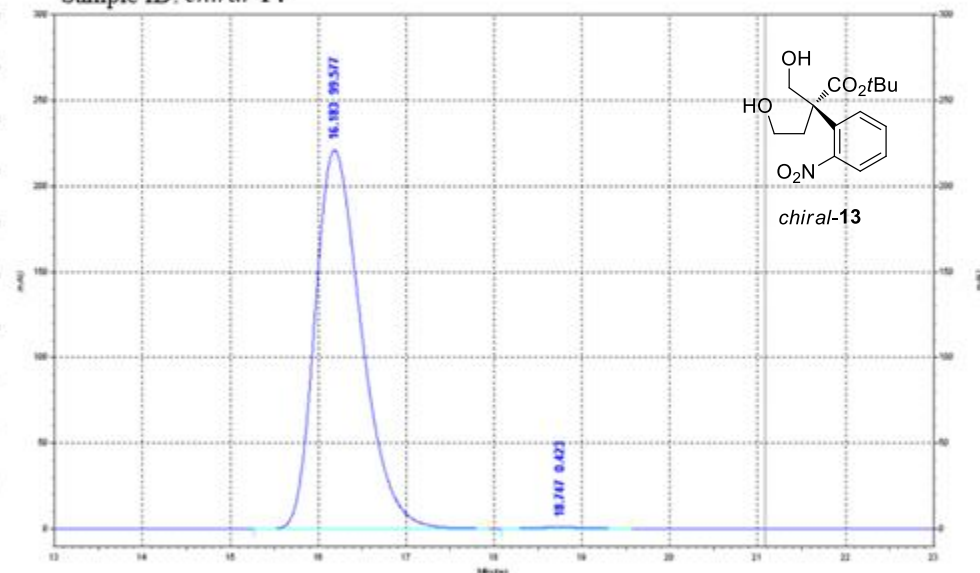
Instrument Name : L-2000

Software Version : Version LaChrom 8908800-07

Acquisition Method : Daicel Chiralpak AD-H, Hexane : 2-Propanol = 90:10, λ = 254 nm,

flow rate = 1.0 mL/min

Sample ID: *chiral-14*



UV Results

Name	Retention Time	Area	Area Percent	Integration Codes
	16.183	32374002	99.577	MM
	18.747	137537	0.423	MM

Totals		32511539	100.000	
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Area Percent Report

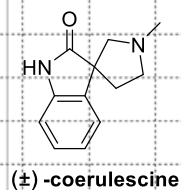
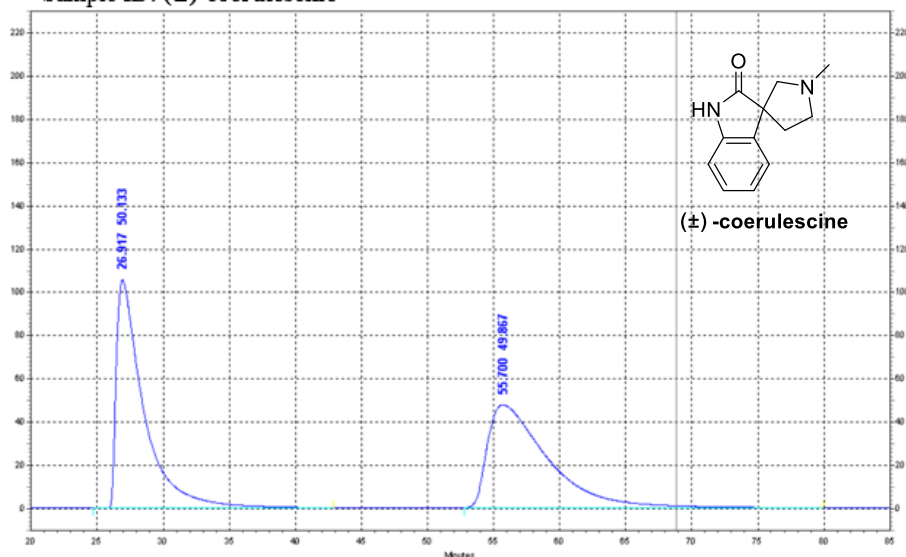
Instrument Name : L-2000

Software Version : Version LaChrom 8908800-07

Acquisition Method : Daicel Chiralpak AS-H, Hexane : 2-Propanol = 90:10, λ = 254 nm,

flow rate = 1.0 mL/min

Sample ID: (\pm)-coerulescine



UV Results

Name	Retention Time	Area	Area Percent	Integration Codes
	26.917	60791357	50.133	MM
	55.700	60468972	49.867	MM

Totals		121260329	100.000	
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Area Percent Report

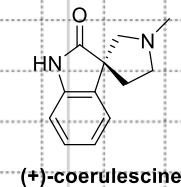
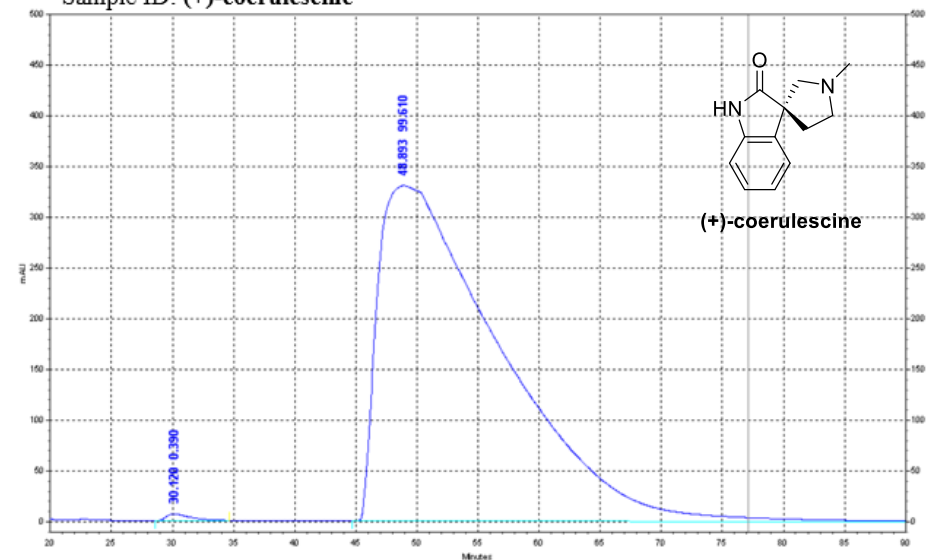
Instrument Name : L-2000

Software Version : Version LaChrom 8908800-07

Acquisition Method : Daicel Chiralpak AS-H, Hexane : 2-Propanol = 90:10, λ = 254 nm,

flow rate = 1.0 mL/min

Sample ID: (+)-coerulescine



UV Results

Name	Retention Time	Area	Area Percent	Integration Codes
	30.120	3610356	0.390	MM
	48.893	921745041	99.610	MM

Totals		925355397	100.000	
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