Supporting Information

TMSOTf-Catalyzed Synthesis of Substituted Quinazolines Using Hexamethyldisilazane as Nitrogen Source under Neat and Microwave Irradiation

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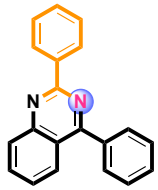	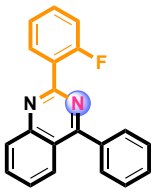	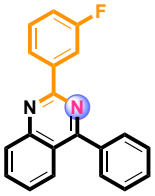	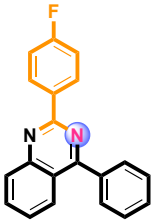	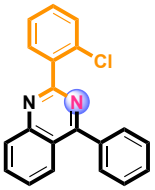	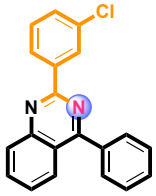
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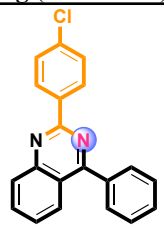	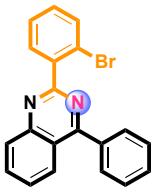	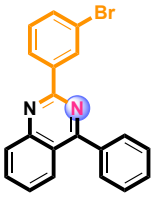	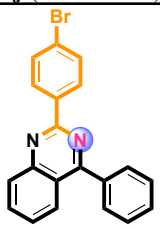	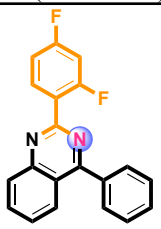	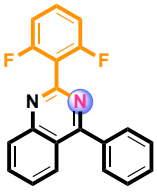
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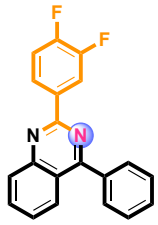	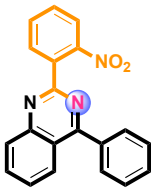	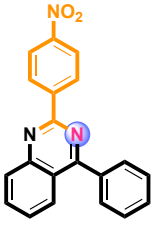	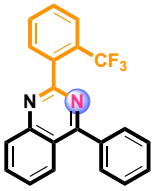	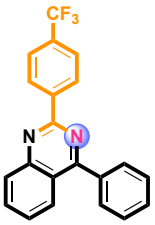	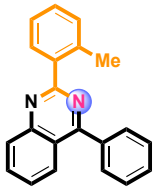
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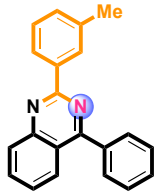	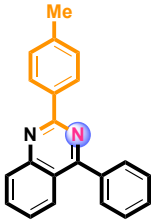	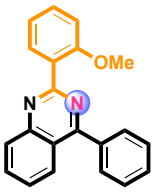	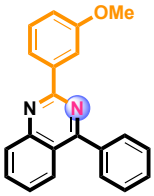	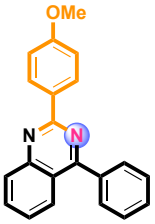	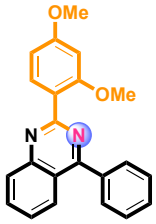
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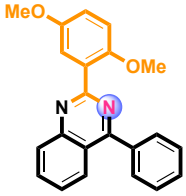	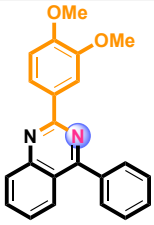	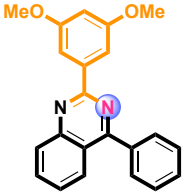	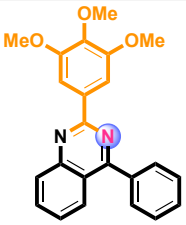	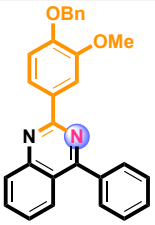	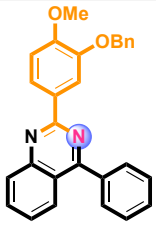
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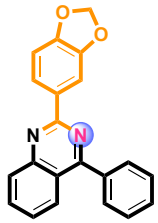	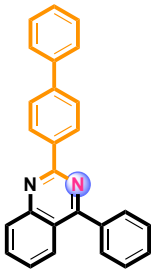	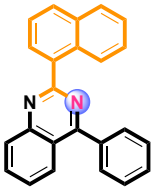	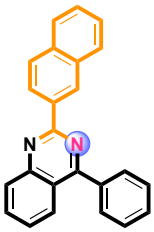	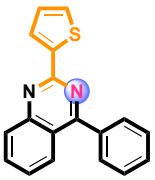	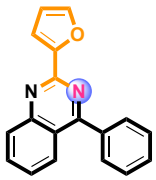
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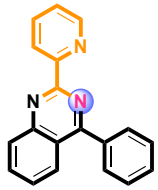	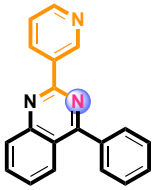	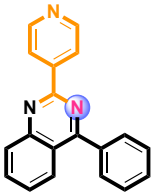	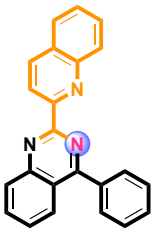	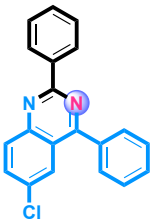	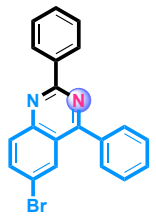

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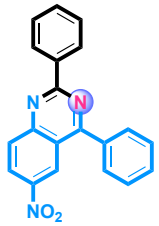	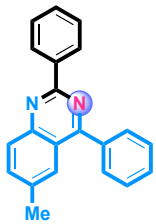	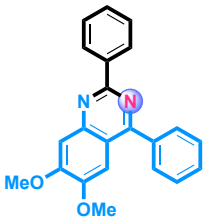	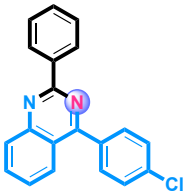	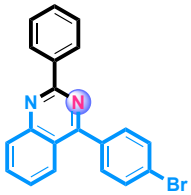	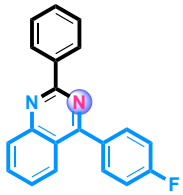

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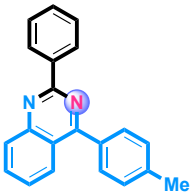
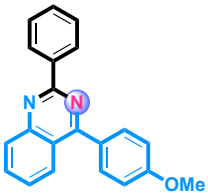
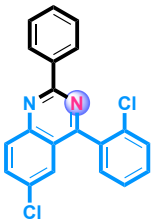
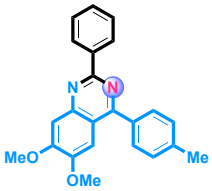
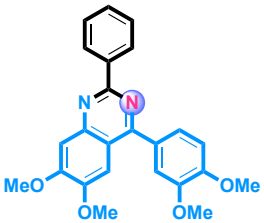
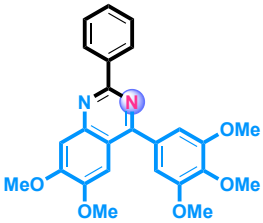
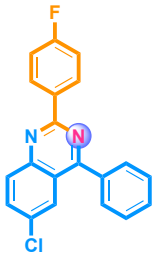
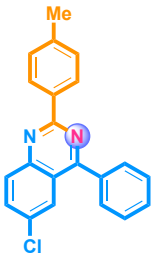
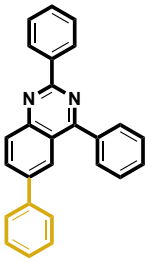
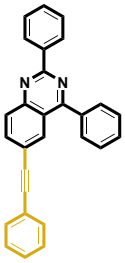
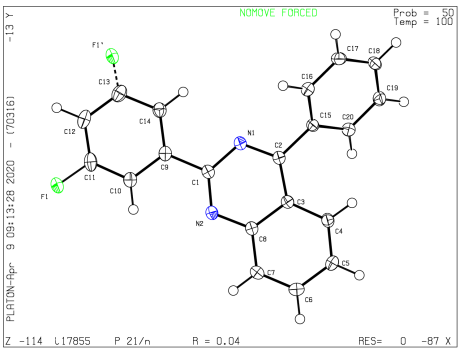
				

4n (S-222~S-225)	**5a** (S-226~S-229)	**5b** (S-230~S-233)	**6** (S-234~S-237)	**7** (S-238~S-241)
				

Crystal data and structure refinement for compound **3c**

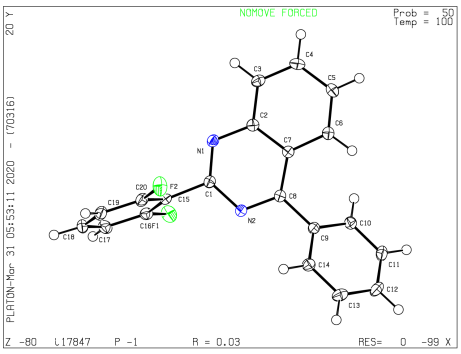
(the thermal ellipsoid was drawn at the 50% probability level)



Identification code	i17855	
Empirical formula	C20 H12 F N2	
Formula weight	299.32	
Temperature	100.0(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 10.3439(4) Å	a= 90°.
	b = 6.8286(2) Å	b= 97.8600(10)°.
	c = 20.1913(7) Å	g = 90°.
Volume	1412.80(8) $Å^3$	
Z, Density (calculated)	4, 1.407 Mg/m^3	
Absorption coefficient	0.093 mm^{-1}	
F(000)	620	
Crystal size	0.327 x 0.256 x 0.168 mm^3	
Theta range for data collection	3.152 to 27.101°.	
Index ranges	-13<=h<=13, -8<=k<=8, -25<=l<=25	
Reflections collected	44058	
Independent reflections	3120 [R(int) = 0.0448]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Numerical	
Max. and min. transmission	1 and 0.9713	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3120 / 0 / 212	
Goodness-of-fit on F^2	1.056	
Final R indices [I>2sigma(I)]	R1 = 0.0413, wR2 = 0.1090	
R indices (all data)	R1 = 0.0481, wR2 = 0.1140	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.299 and -0.223 e.$Å^{-3}$	

Crystal data and structure refinement for compound **3l**

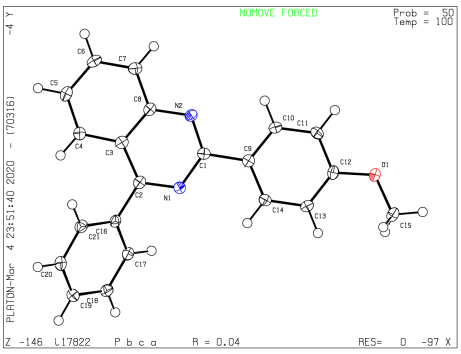
(the thermal ellipsoid was drawn at the 50% probability level)



Identification code	i17847	
Empirical formula	C20 H12 F2 N2	
Formula weight	318.32	
Temperature	100.0(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 7.8602(2) Å	a= 94.7750(10)°.
	b = 8.9830(2) Å	b= 108.4430(10)°.
	c = 11.3189(3) Å	g = 100.7540(10)°.
Volume	736.11(3) $Å^3$	
Z, Density (calculated)	2, 1.436 Mg/m^3	
Absorption coefficient	0.103 mm^{-1}	
F(000)	328	
Crystal size	0.240 x 0.227 x 0.207 mm^3	
Theta range for data collection	1.919 to 27.100°.	
Index ranges	-10<=h<=10, -11<=k<=11, -14<=l<=14	
Reflections collected	31661	
Independent reflections	3247 [R(int) = 0.0347]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Numerical	
Max. and min. transmission	1 and 0.9803	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3247 / 0 / 217	
Goodness-of-fit on F^2	1.057	
Final R indices [I>2sigma(I)]	R1 = 0.0346, wR2 = 0.0839	
R indices (all data)	R1 = 0.0391, wR2 = 0.0874	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.270 and -0.245 e.$Å^{-3}$	

Crystal data and structure refinement for compound **3w**

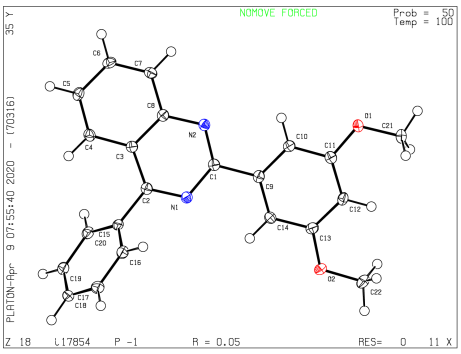
(the thermal ellipsoid was drawn at the 50% probability level)



Identification code	i17822	
Empirical formula	C21 H16 N2 O	
Formula weight	312.36	
Temperature	100.0(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P b c a	
Unit cell dimensions	a = 14.6384(3) Å	a= 90°.
	b = 6.90900(10) Å	b= 90°.
	c = 30.7229(7) Å	g = 90°.
Volume	3107.21(11) $Å^3$	
Z, Density (calculated)	8, 1.335 Mg/m^3	
Absorption coefficient	0.656 mm^{-1}	
F(000)	1312	
Crystal size	0.288 x 0.184 x 0.164 mm^3	
Theta range for data collection	2.877 to 65.073°.	
Index ranges	-17<=h<=17, -8<=k<=8, -36<=l<=36	
Reflections collected	60225	
Independent reflections	2641 [R(int) = 0.0450]	
Completeness to theta = 65.073°	100.0 %	
Absorption correction	Numerical	
Max. and min. transmission	1 and 0.8284	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2641 / 0 / 218	
Goodness-of-fit on F^2	1.119	
Final R indices [I>2sigma(I)]	R1 = 0.0375, wR2 = 0.0963	
R indices (all data)	R1 = 0.0433, wR2 = 0.0997	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.175 and -0.202 e.$Å^{-3}$	

Crystal data and structure refinement for compound **3aa**

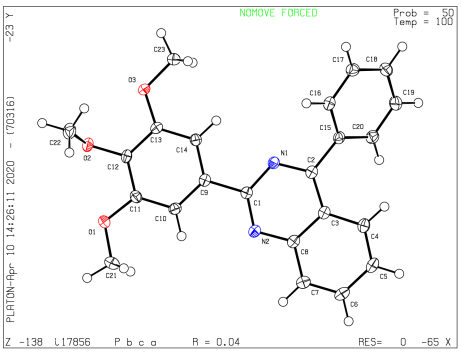
(the thermal ellipsoid was drawn at the 50% probability level)



Identification code	i17854	
Empirical formula	C22 H18 N2 O2	
Formula weight	342.38	
Temperature	100.0(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 5.9542(2) Å	a= 83.162(2)°.
	b = 10.6468(4) Å	b= 86.529(2)°.
	c = 13.6281(5) Å	g = 76.8570(10)°.
Volume	834.81(5) $Å^3$	
Z, Density (calculated)	2, 1.362 Mg/m^3	
Absorption coefficient	0.088 mm^{-1}	
F(000)	360	
Crystal size	0.323 x 0.313 x 0.160 mm^3	
Theta range for data collection	1.976 to 27.103°.	
Index ranges	-7<=h<=7, -13<=k<=13, -17<=l<=17	
Reflections collected	36007	
Independent reflections	3684 [R(int) = 0.0818]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Numerical	
Max. and min. transmission	1 and 0.8094	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3684 / 0 / 237	
Goodness-of-fit on F^2	1.064	
Final R indices [I>2sigma(I)]	R1 = 0.0494, wR2 = 0.1179	
R indices (all data)	R1 = 0.0552, wR2 = 0.1237	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.736 and -0.388 e.$Å^{-3}$	

Crystal data and structure refinement for compound **3ab**

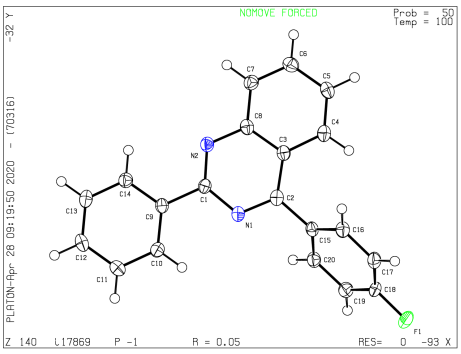
(the thermal ellipsoid was drawn at the 50% probability level)



Identification code	i17856	
Empirical formula	C23 H20 N2 O3	
Formula weight	372.41	
Temperature	100.0(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P b c a	
Unit cell dimensions	a = 14.2321(7) Å	a= 90°.
	b = 13.7476(6) Å	b= 90°.
	c = 19.4973(9) Å	g = 90°.
Volume	3814.8(3) $Å^3$	
Z, Density (calculated)	8, 1.297 Mg/m^3	
Absorption coefficient	0.087 mm^{-1}	
F(000)	1568	
Crystal size	0.307 x 0.238 x 0.120 mm^3	
Theta range for data collection	2.309 to 27.103°.	
Index ranges	-17<=h<=18, -17<=k<=17, -24<=l<=24	
Reflections collected	103031	
Independent reflections	4210 [R(int) = 0.1218]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Numerical	
Max. and min. transmission	1 and 0.7376	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4210 / 0 / 257	
Goodness-of-fit on F^2	1.076	
Final R indices [I>2sigma(I)]	R1 = 0.0389, wR2 = 0.0879	
R indices (all data)	R1 = 0.0608, wR2 = 0.1031	
Extinction coefficient	0.0078(7)	
Largest diff. peak and hole	0.297 and -0.216 e.$Å^{-3}$	

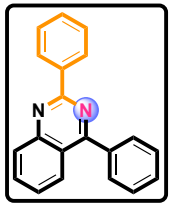
Crystal data and structure refinement for compound **4h**

(the thermal ellipsoid was drawn at the 50% probability level)



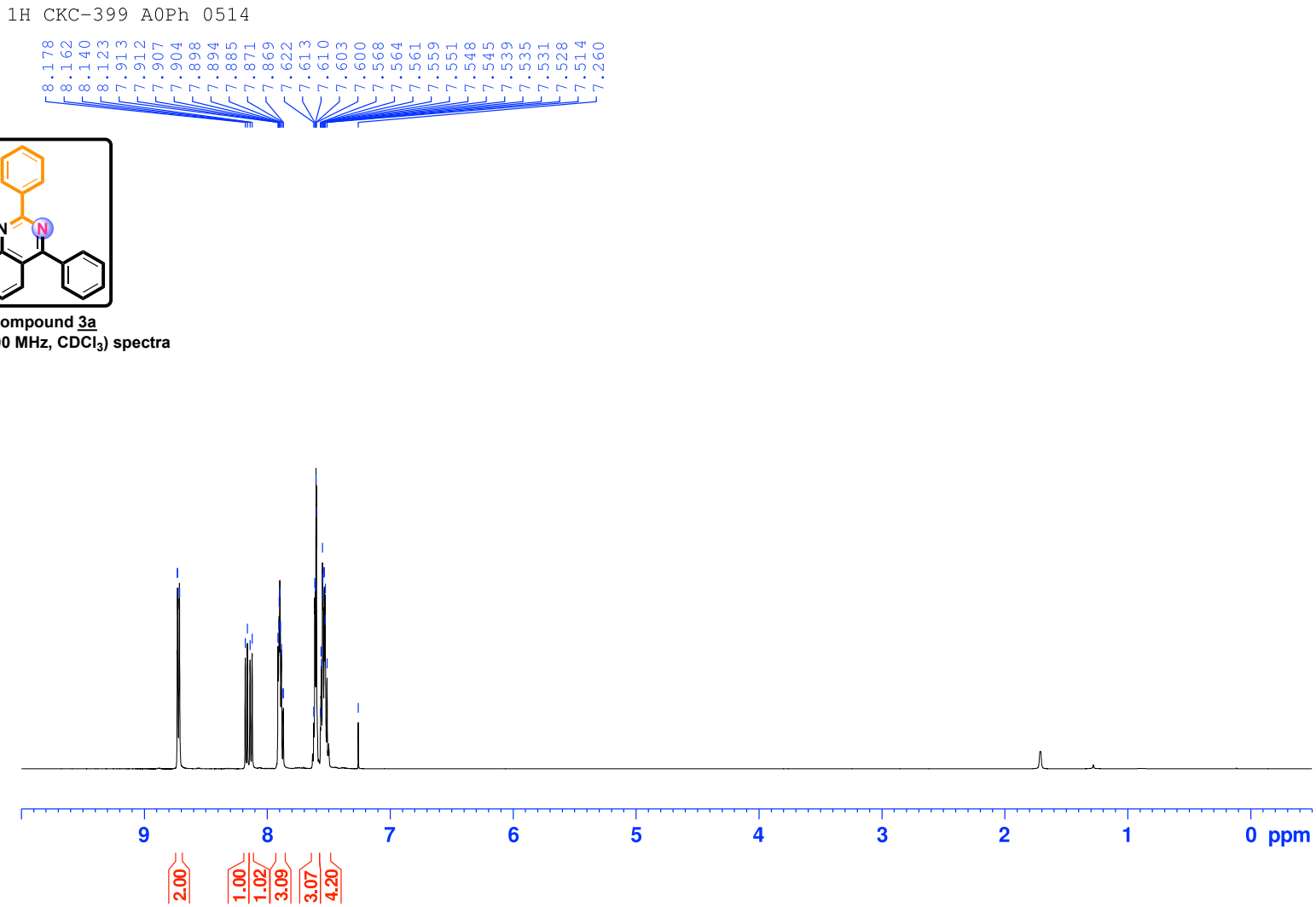
Identification code	i17869	
Empirical formula	C20 H13 F N2	
Formula weight	300.32	
Temperature	100.0(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 6.0455(5) Å	a= 112.103(4)°.
	b = 11.0023(10) Å	b= 96.044(4)°.
	c = 11.7294(10) Å	g = 93.256(4)°.
Volume	714.87(11) $Å^3$	
Z, Density (calculated)	2, 1.395 Mg/m^3	
Absorption coefficient	0.092 mm^{-1}	
F(000)	312	
Crystal size	0.248 x 0.208 x 0.166 mm^3	
Theta range for data collection	2.009 to 27.096°.	
Index ranges	-7<=h<=7, -14<=k<=14, -15<=l<=15	
Reflections collected	29678	
Independent reflections	3149 [R(int) = 0.0942]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Numerical	
Max. and min. transmission	1 and 0.8496	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3149 / 0 / 208	
Goodness-of-fit on F^2	1.052	
Final R indices [I>2sigma(I)]	R1 = 0.0472, wR2 = 0.1189	
R indices (all data)	R1 = 0.0783, wR2 = 0.1408	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.280 and -0.240 e.$Å^{-3}$	

Compound 3a

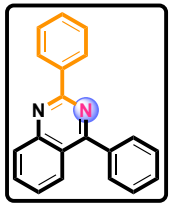


Compound 3a

^{1}H NMR (500 MHz, $CDCl_3$) spectra

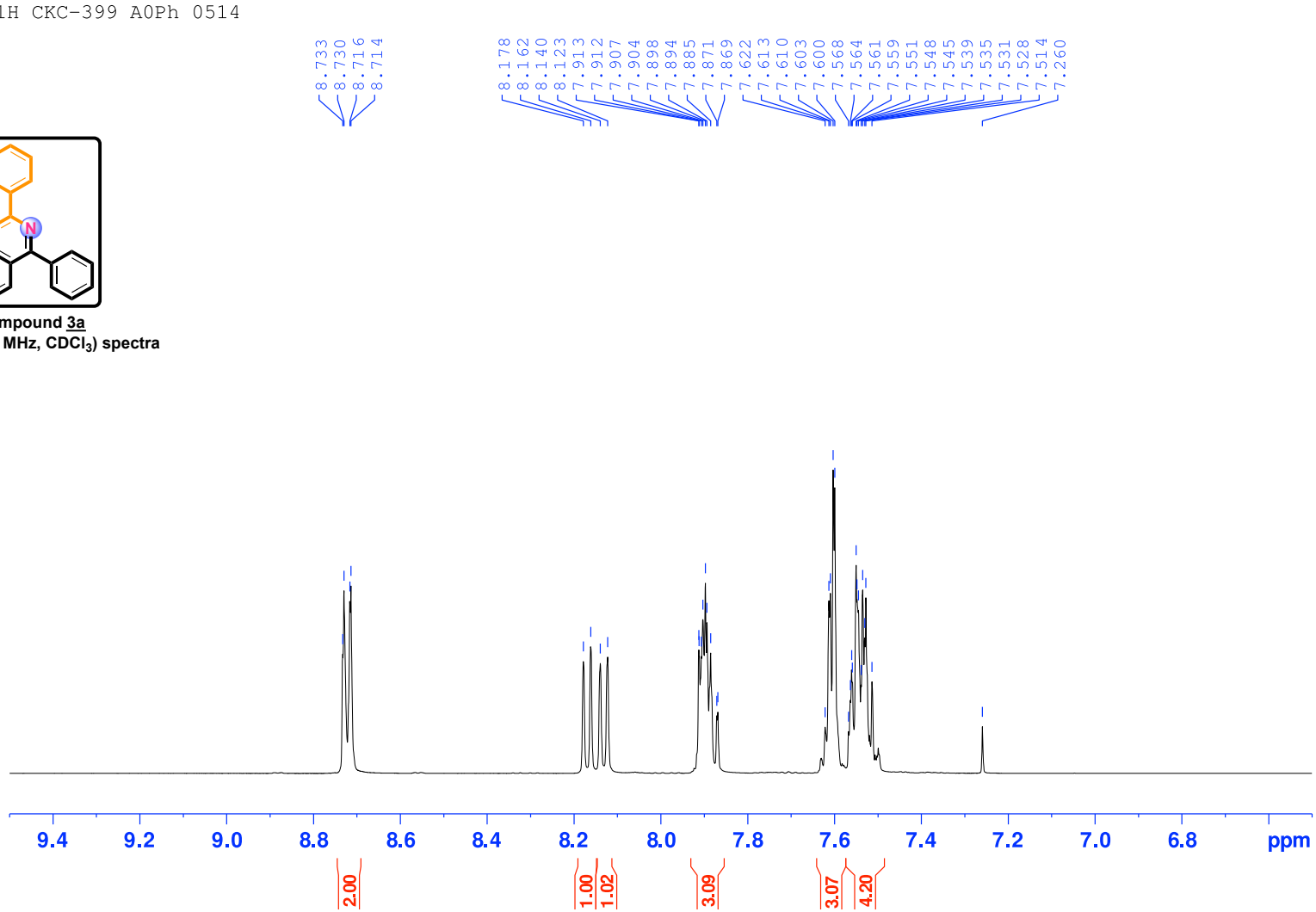


Compound 3a

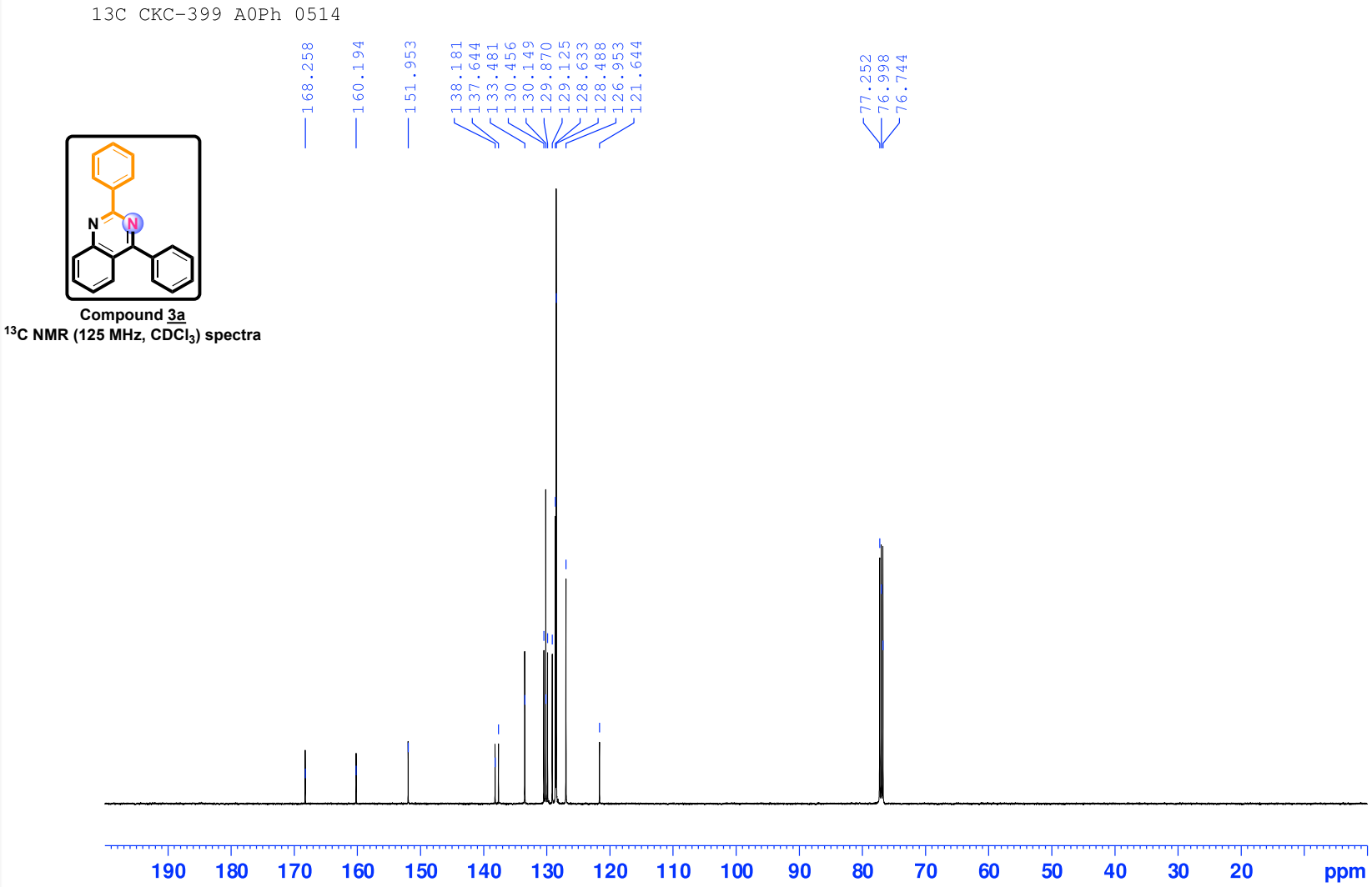


Compound 3a

^{1}H NMR (500 MHz, $CDCl_3$) spectra

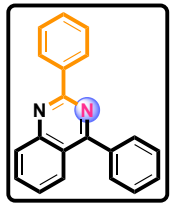


Compound 3a



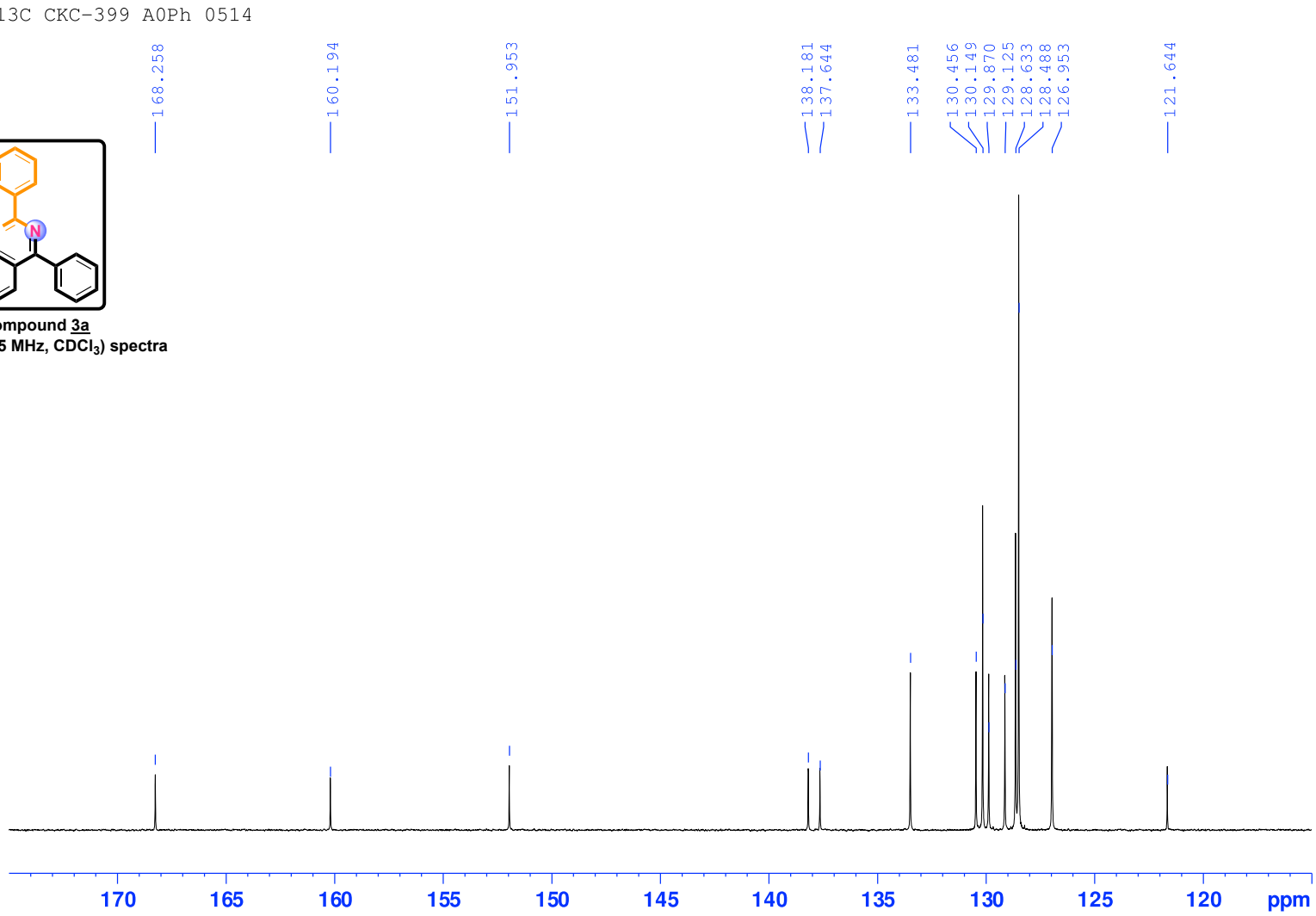
Compound 3a
^{13}C NMR (125 MHz, $CDCl_3$) spectra

Compound 3a

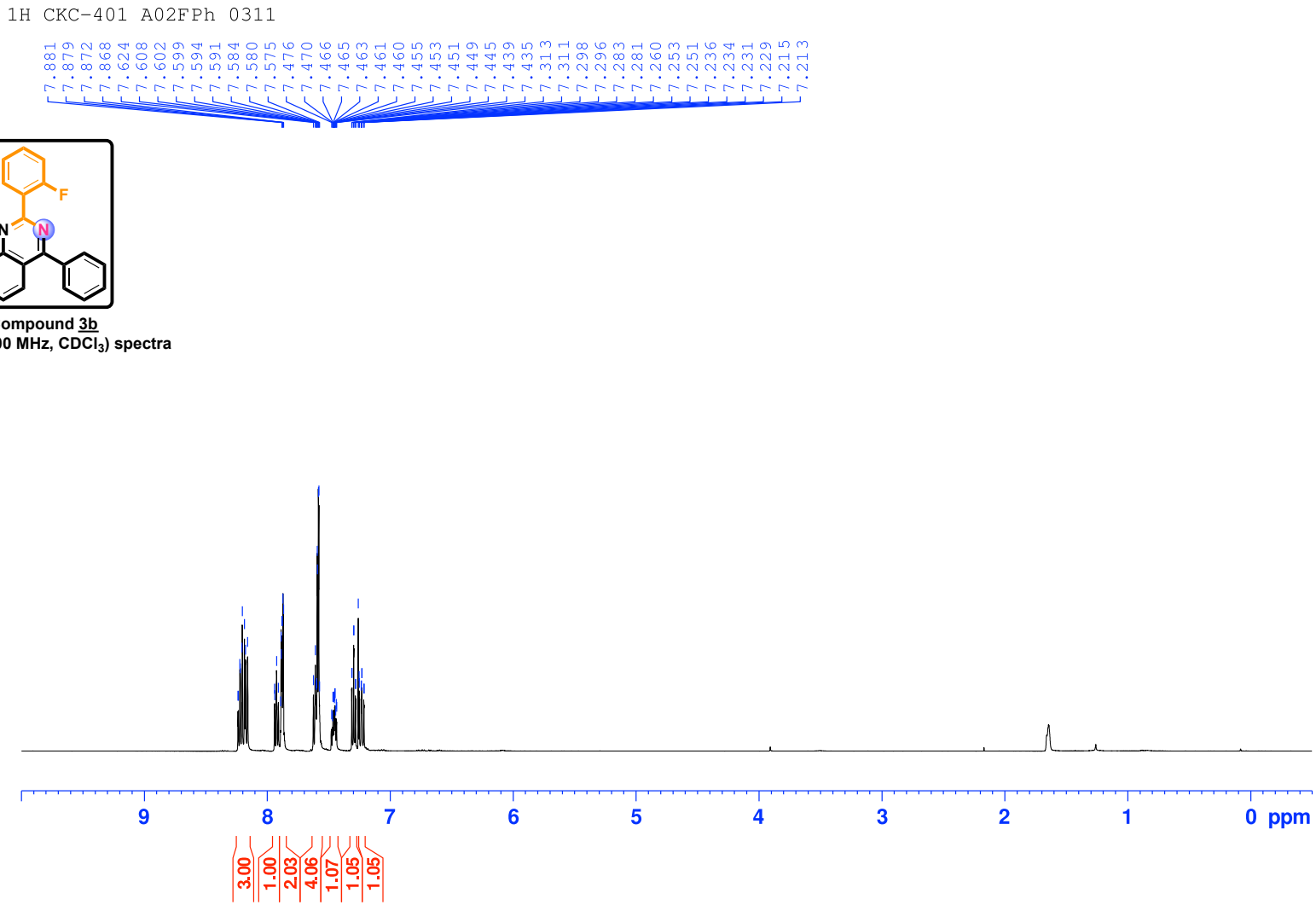


Compound 3a

^{13}C NMR (125 MHz, $CDCl_3$) spectra

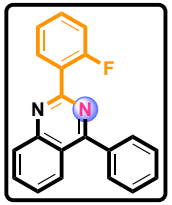


Compound 3b

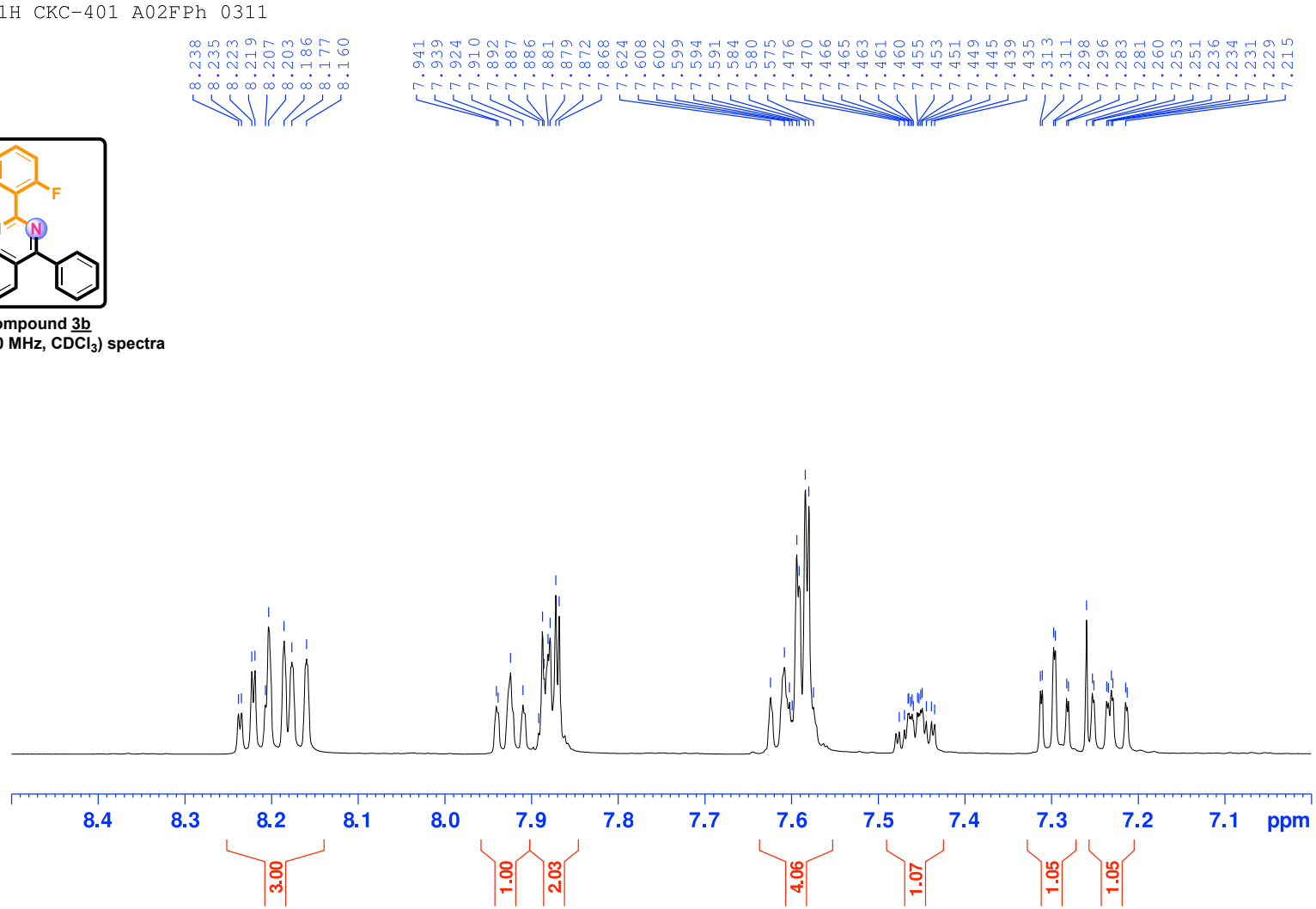


Compound 3b
^{1}H NMR (500 MHz, $CDCl_3$) spectra

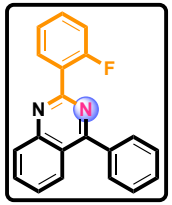
Compound 3b



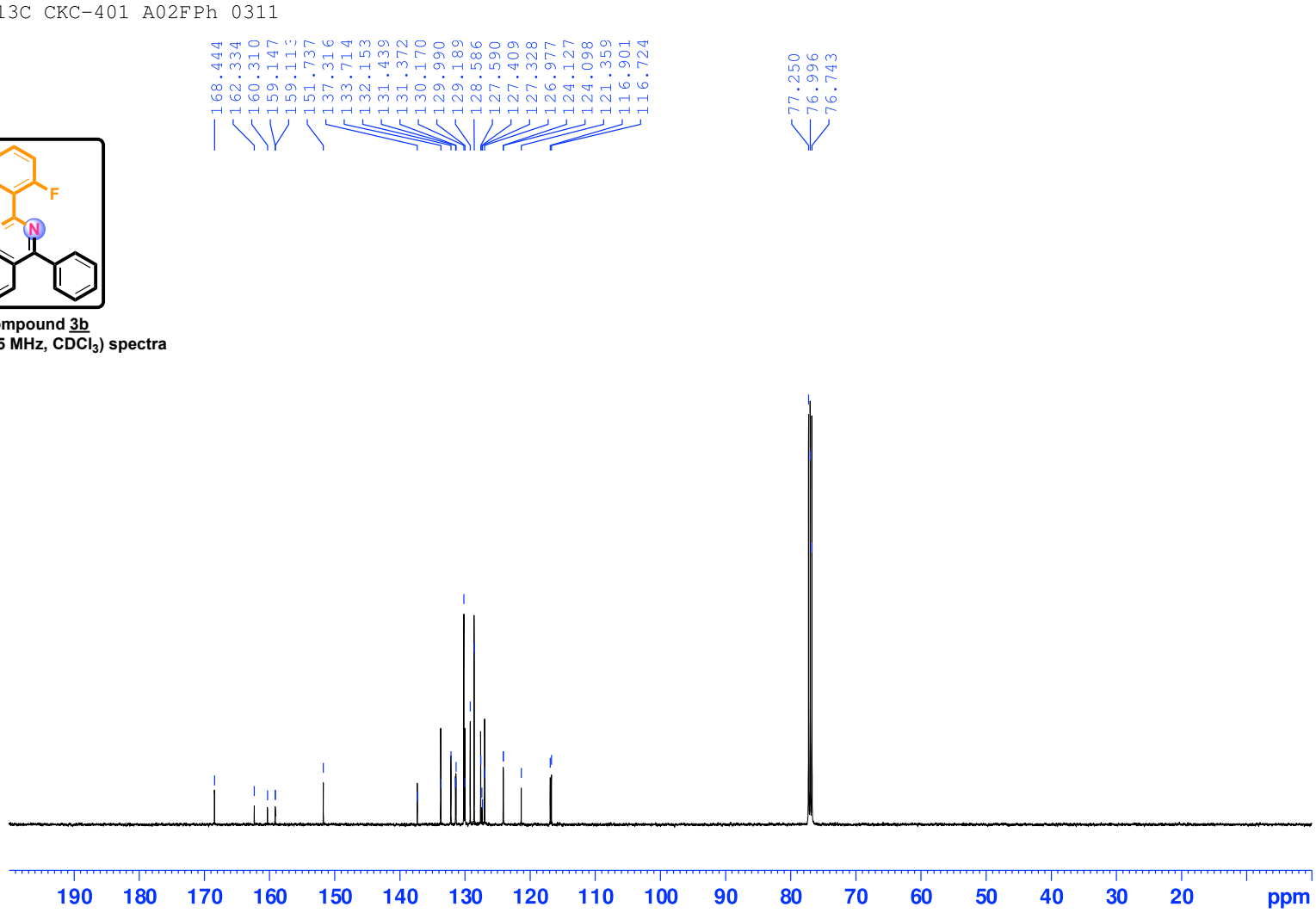
Compound 3b
^{1}H NMR (500 MHz, $CDCl_3$) spectra



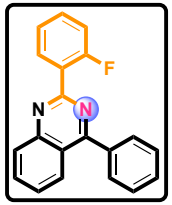
Compound 3b



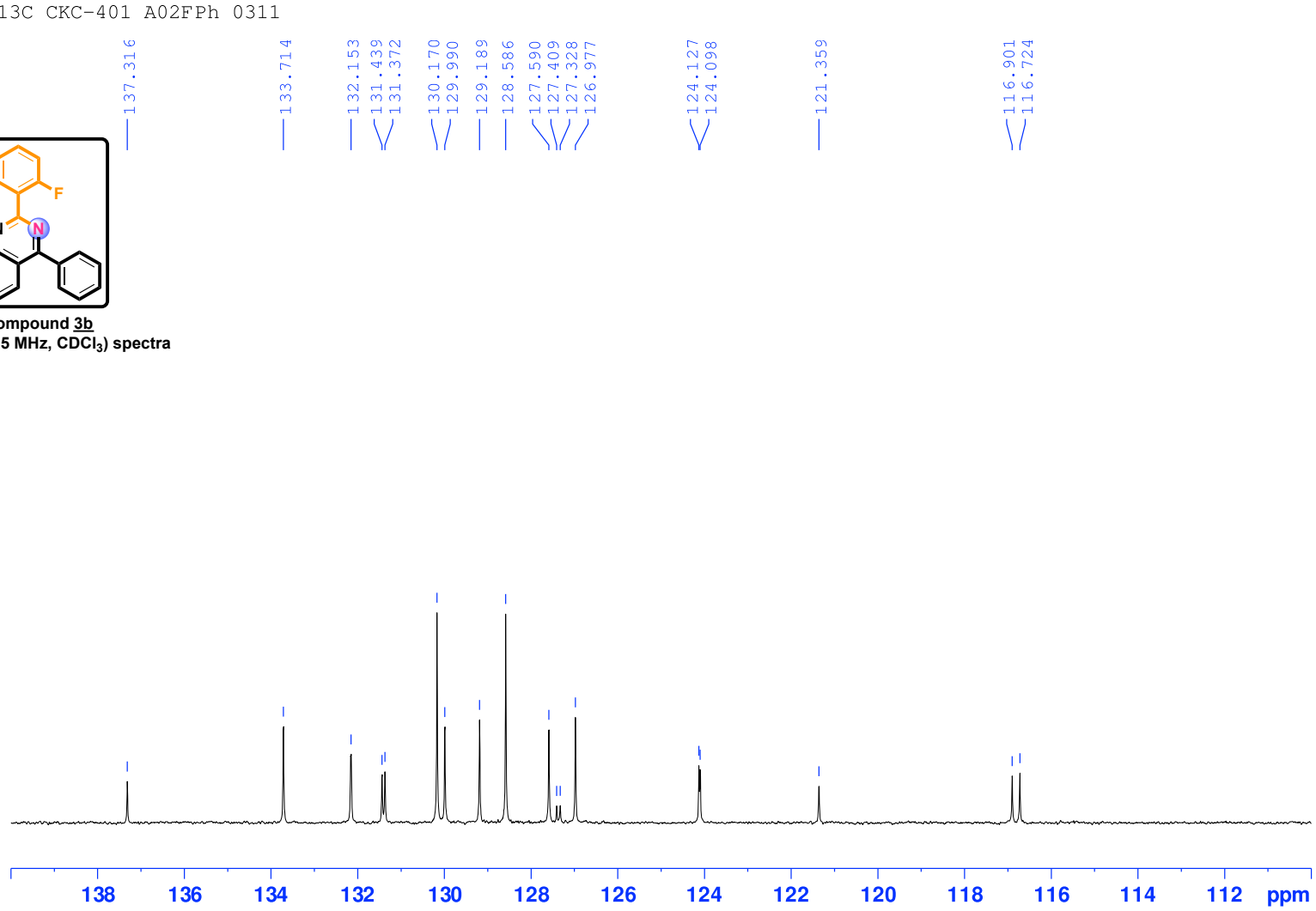
Compound 3b
^{13}C NMR (125 MHz, $CDCl_3$) spectra



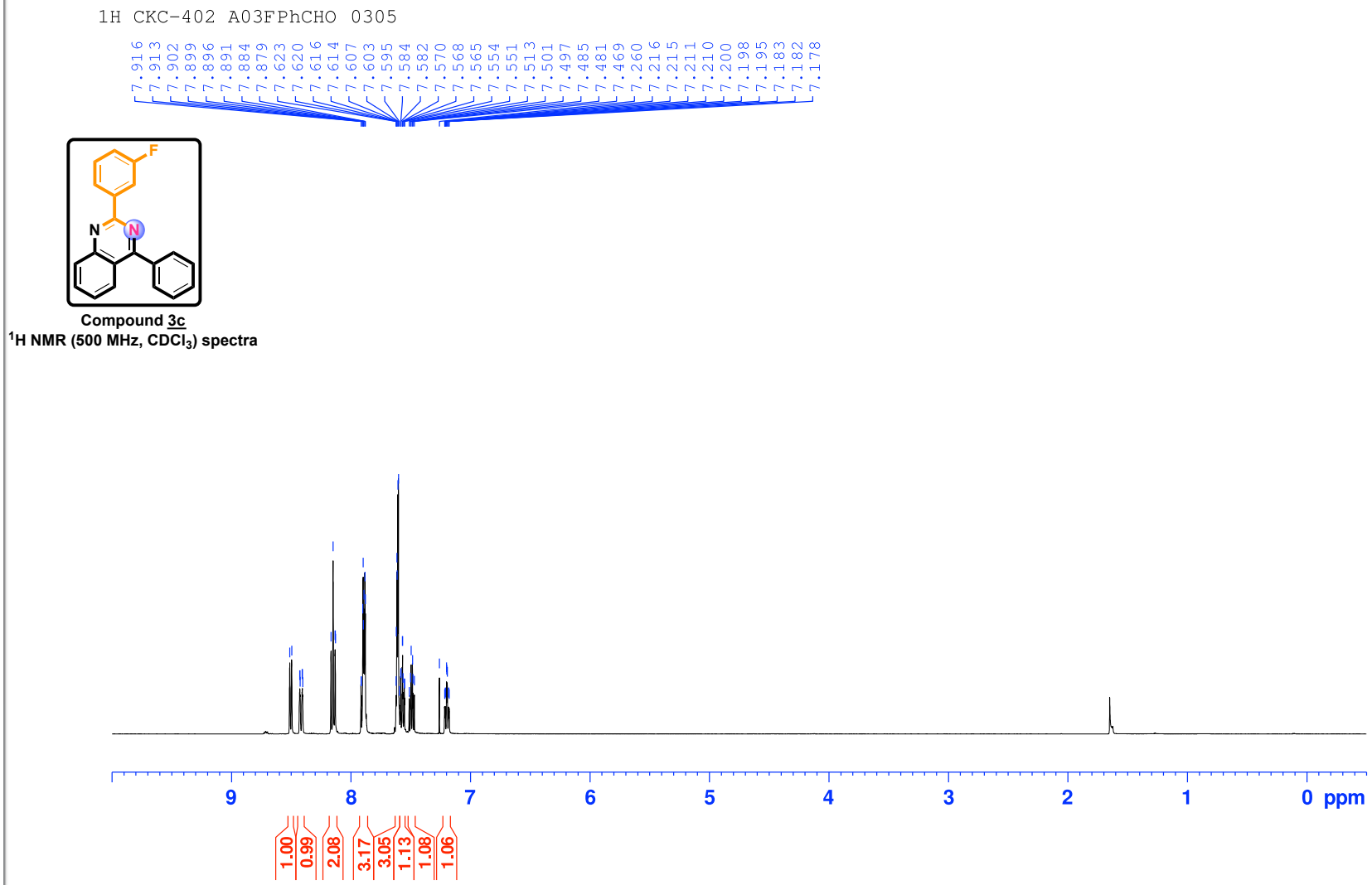
Compound 3b



Compound 3b
^{13}C NMR (125 MHz, $CDCl_3$) spectra

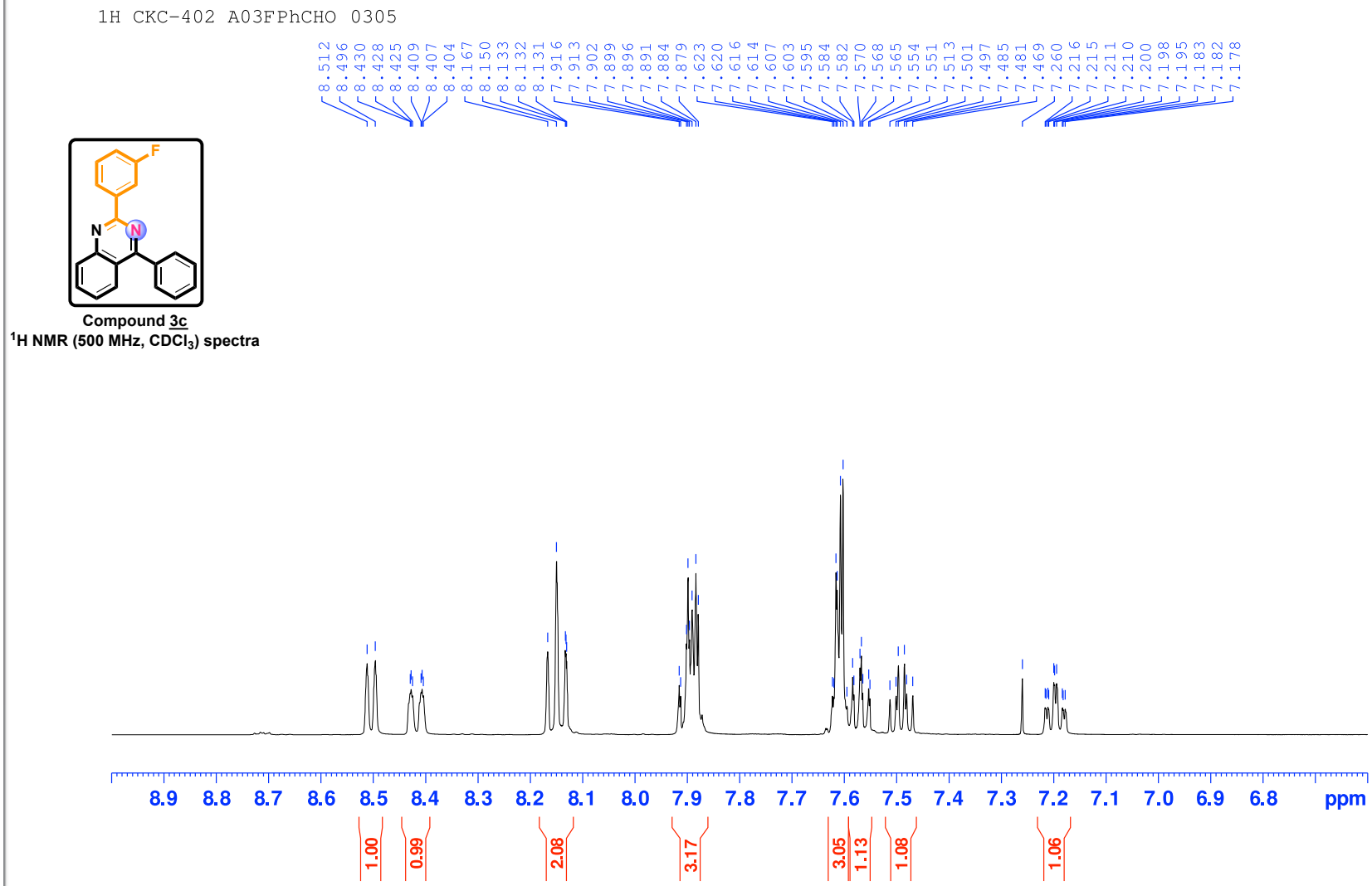


Compound 3c



Compound 3c
^{1}H NMR (500 MHz, $CDCl_3$) spectra

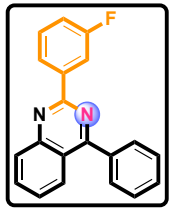
Compound 3c



Compound 3c

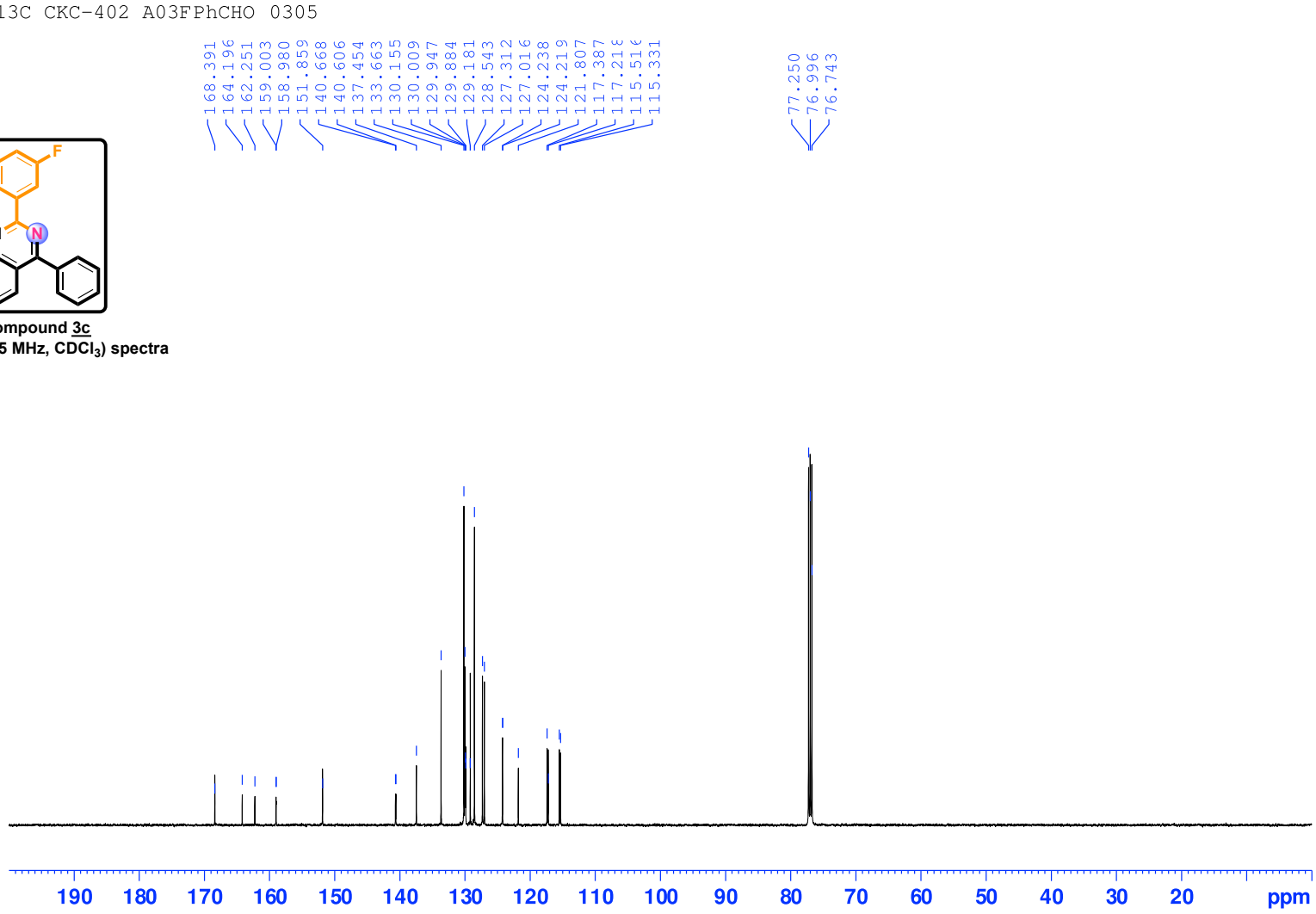
^{1}H NMR (500 MHz, $CDCl_3$) spectra

Compound 3c

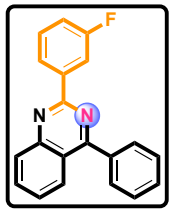


Compound 3c

^{13}C NMR (125 MHz, $CDCl_3$) spectra

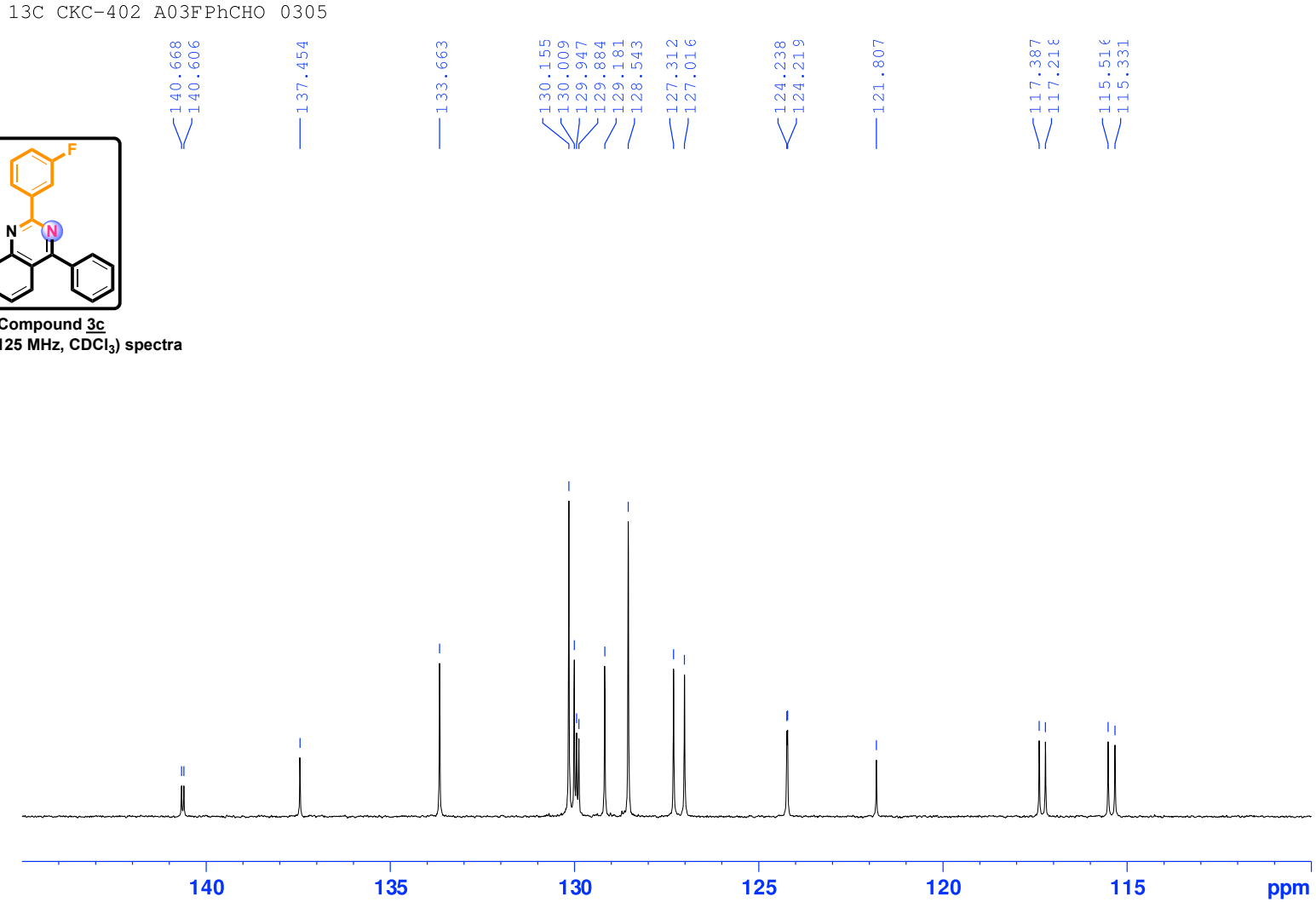


Compound 3c

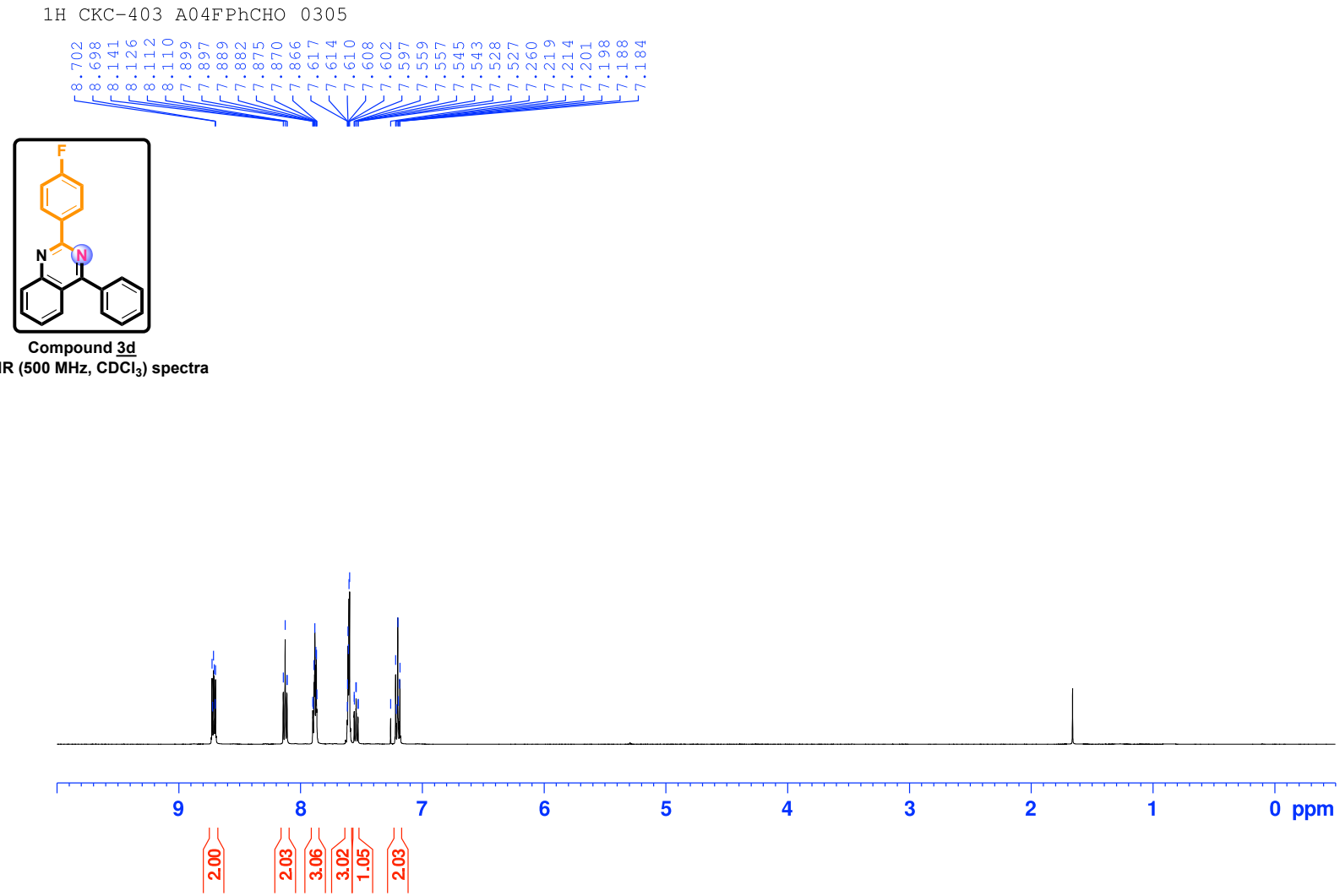


Compound 3c

^{13}C NMR (125 MHz, $CDCl_3$) spectra



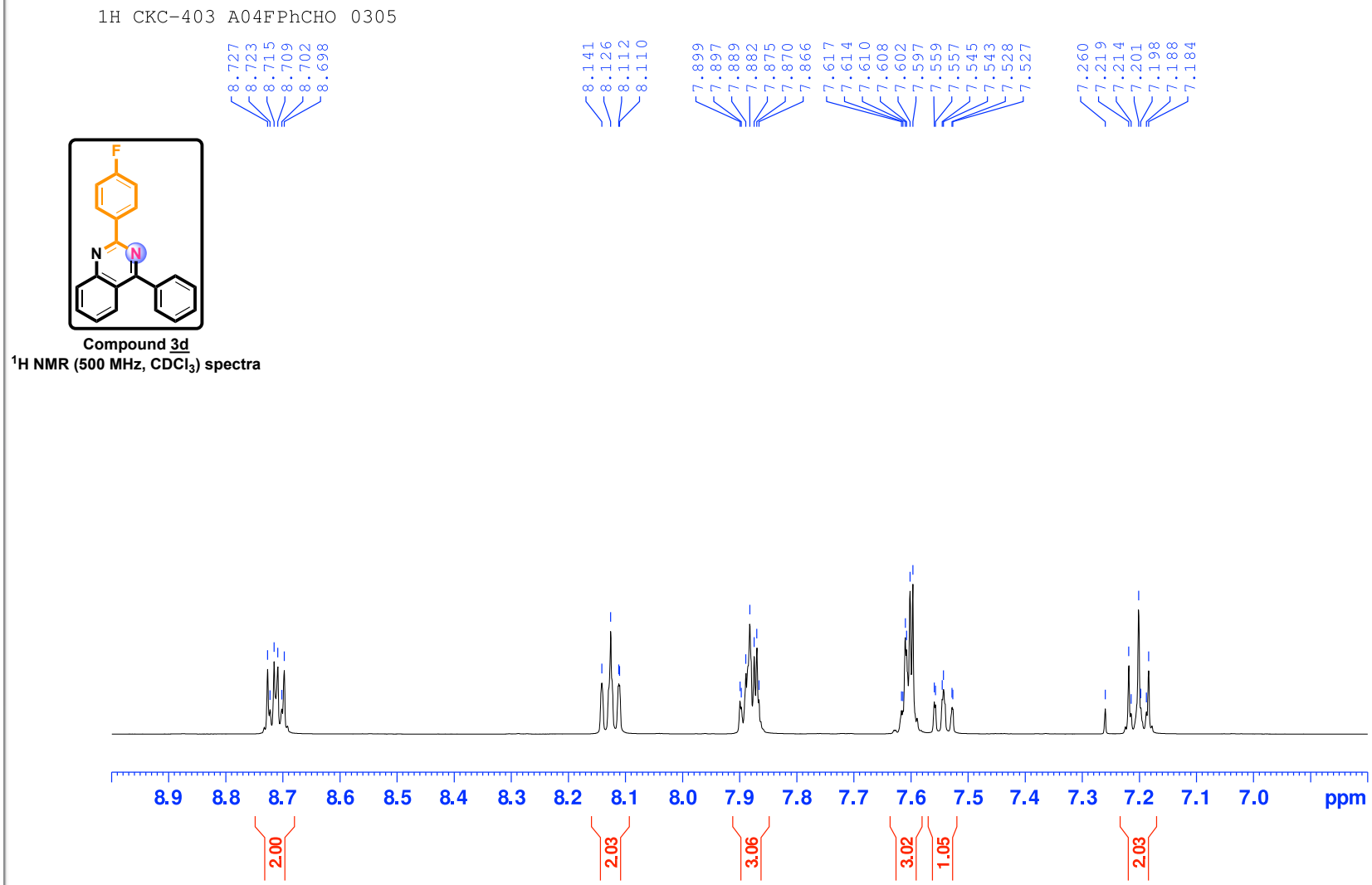
Compound 3d



Compound 3d

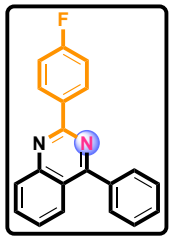
^{1}H NMR (500 MHz, $CDCl_3$) spectra

Compound 3d



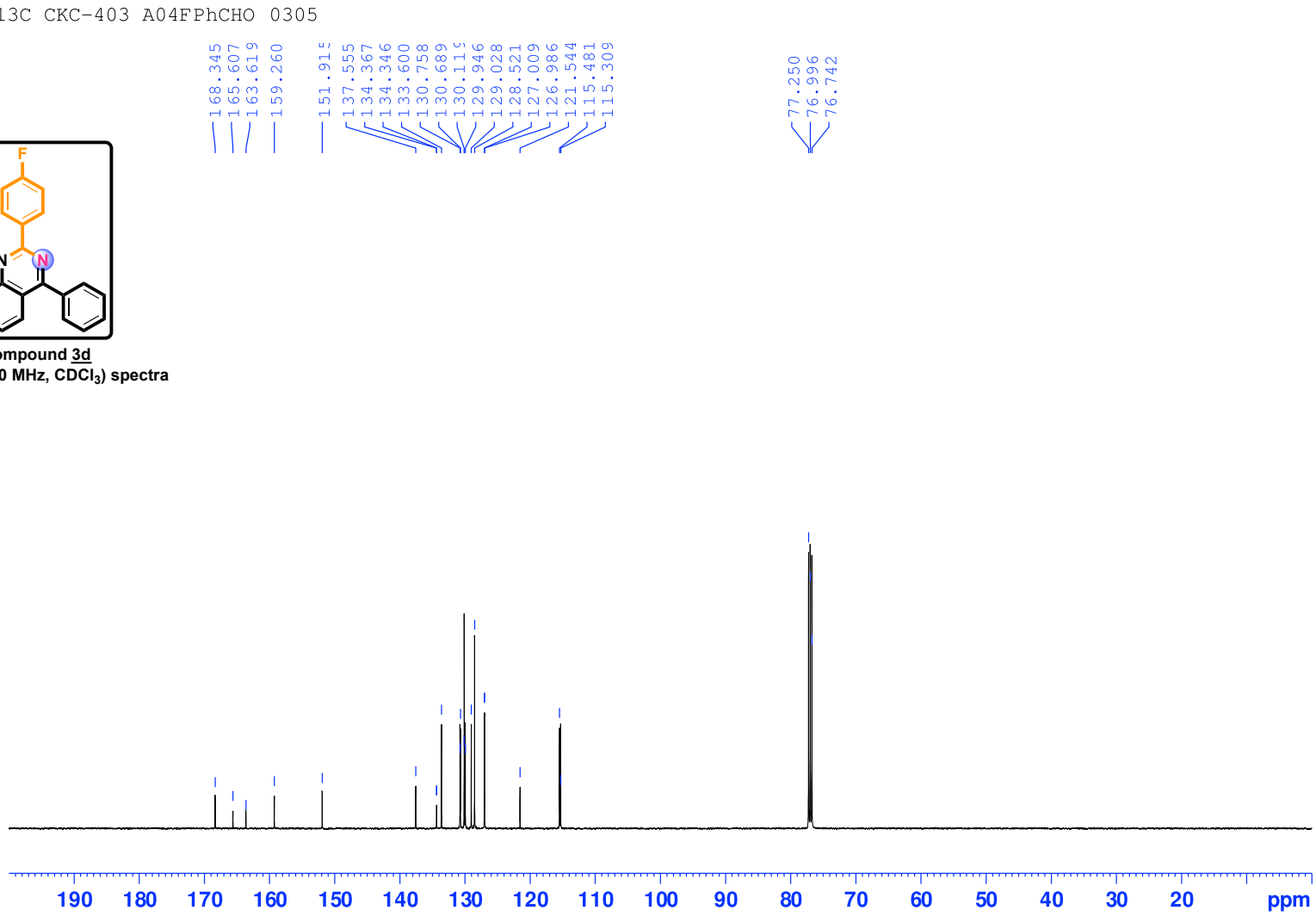
Compound 3d
^{1}H NMR (500 MHz, $CDCl_3$) spectra

Compound 3d

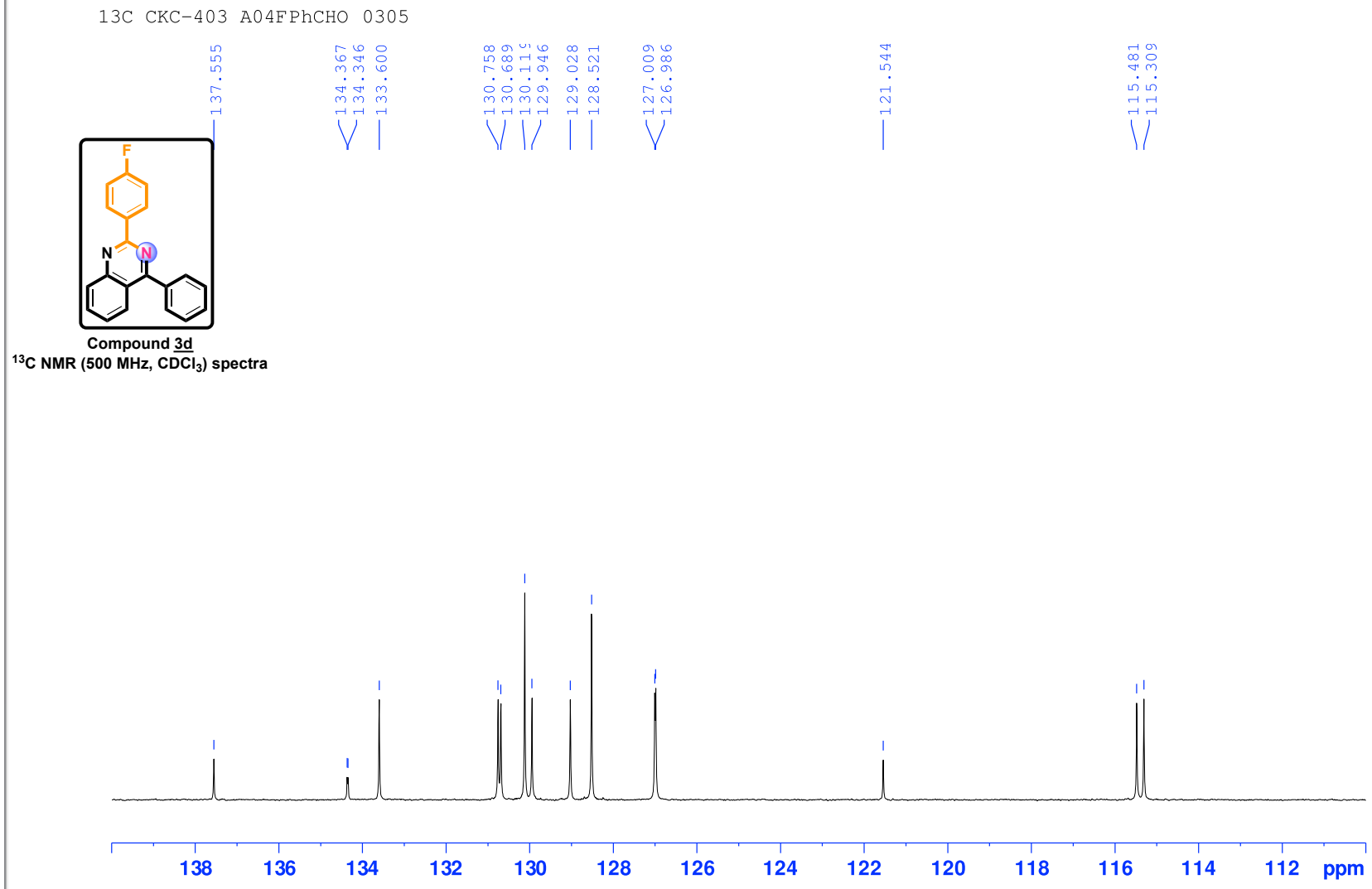


Compound 3d

^{13}C NMR (500 MHz, $CDCl_3$) spectra



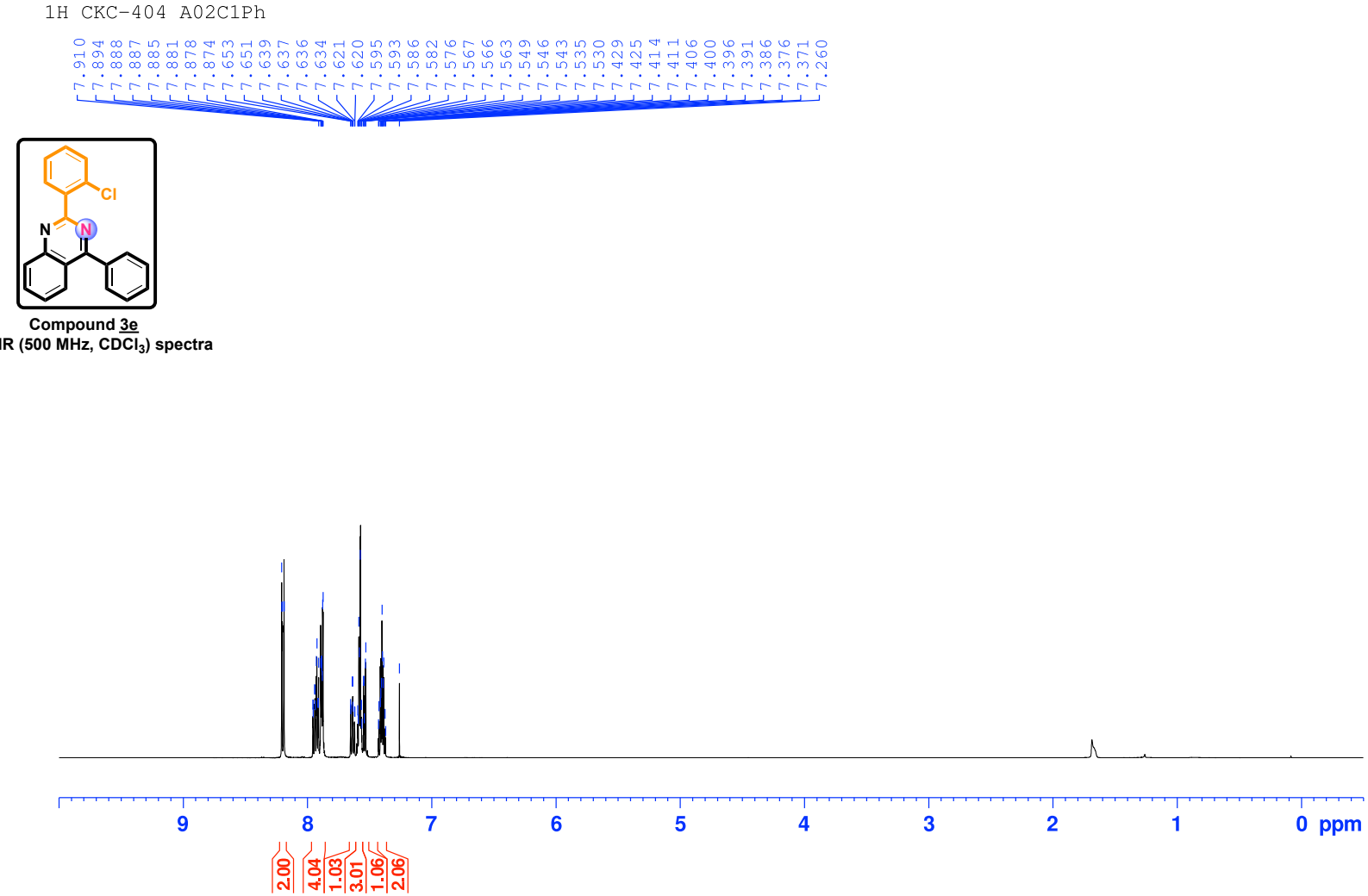
Compound 3d



Compound 3d

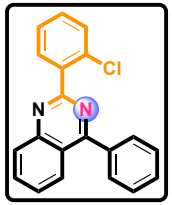
^{13}C NMR (500 MHz, $CDCl_3$) spectra

Compound 3e

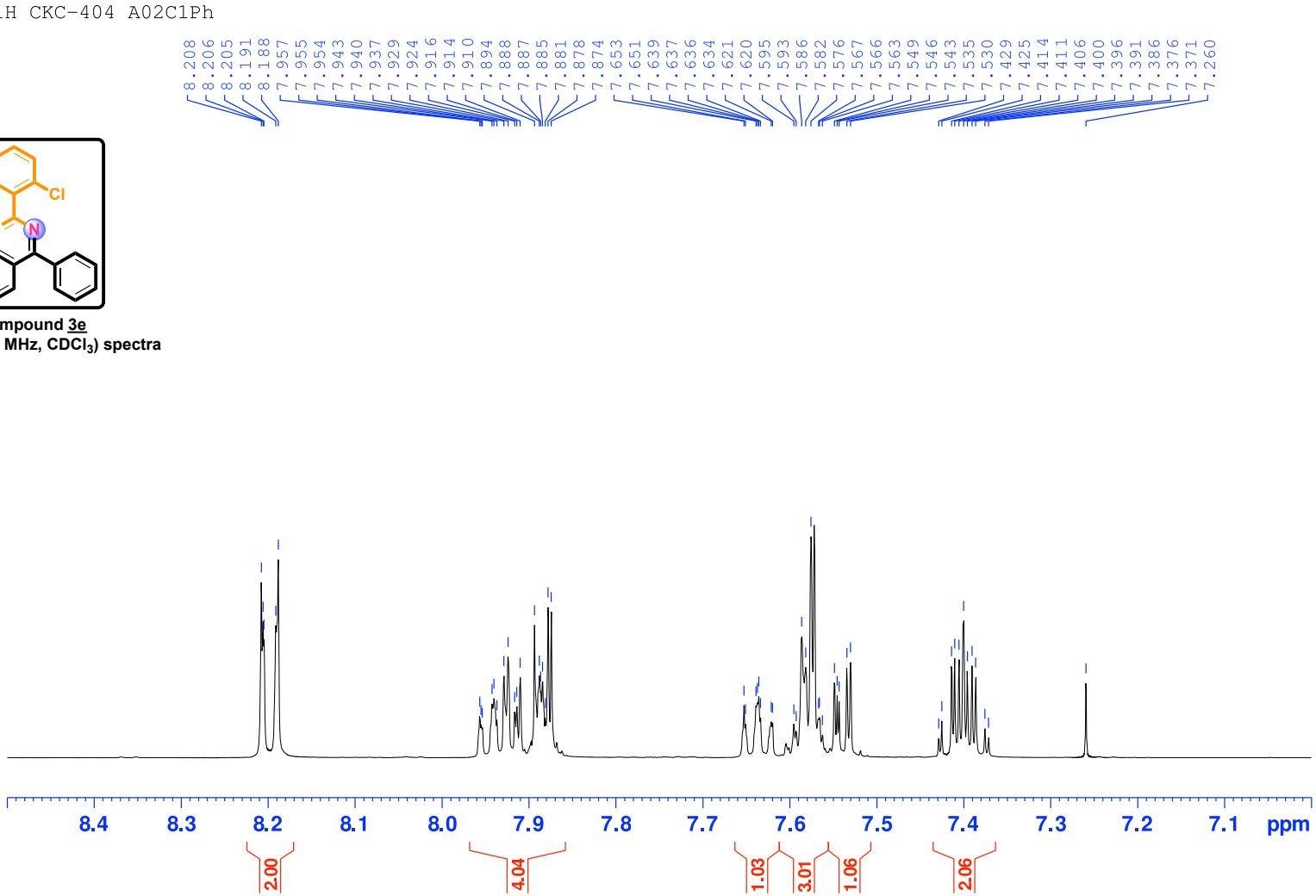


Compound 3e
^{1}H NMR (500 MHz, $CDCl_3$) spectra

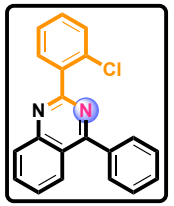
Compound 3e



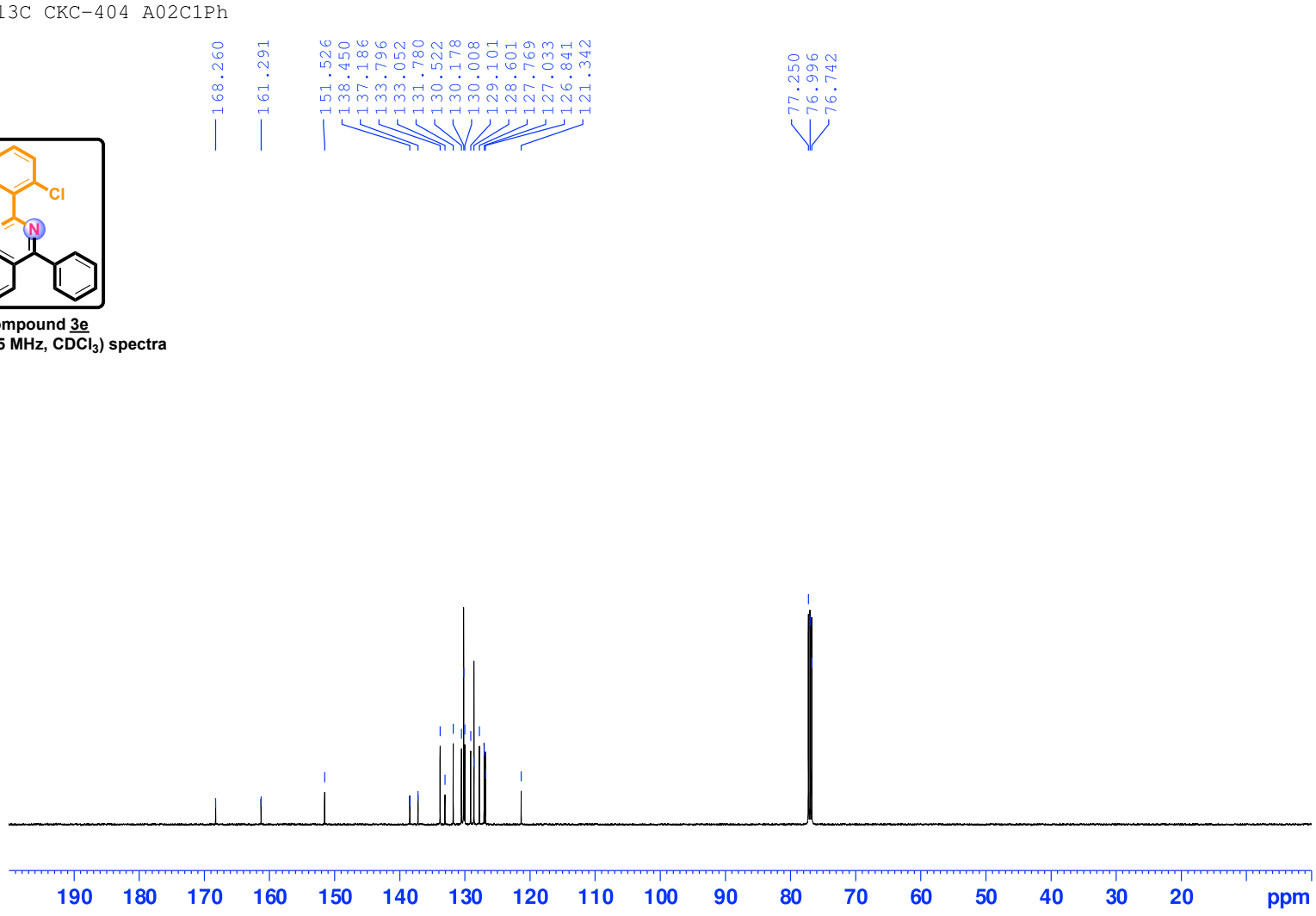
Compound 3e
^{1}H NMR (500 MHz, $CDCl_3$) spectra



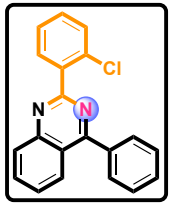
Compound 3e



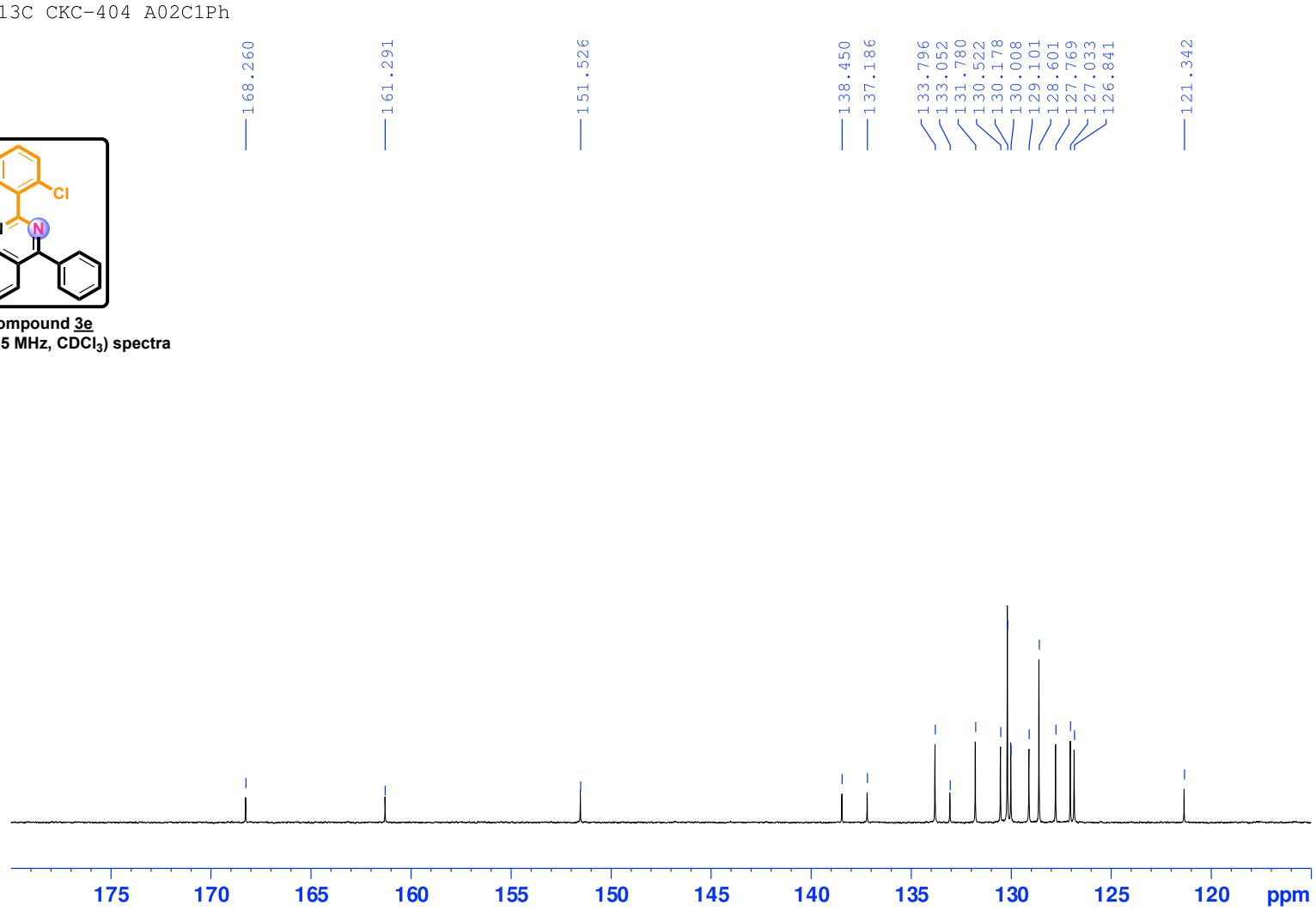
Compound 3e
^{13}C NMR (125 MHz, $CDCl_3$) spectra



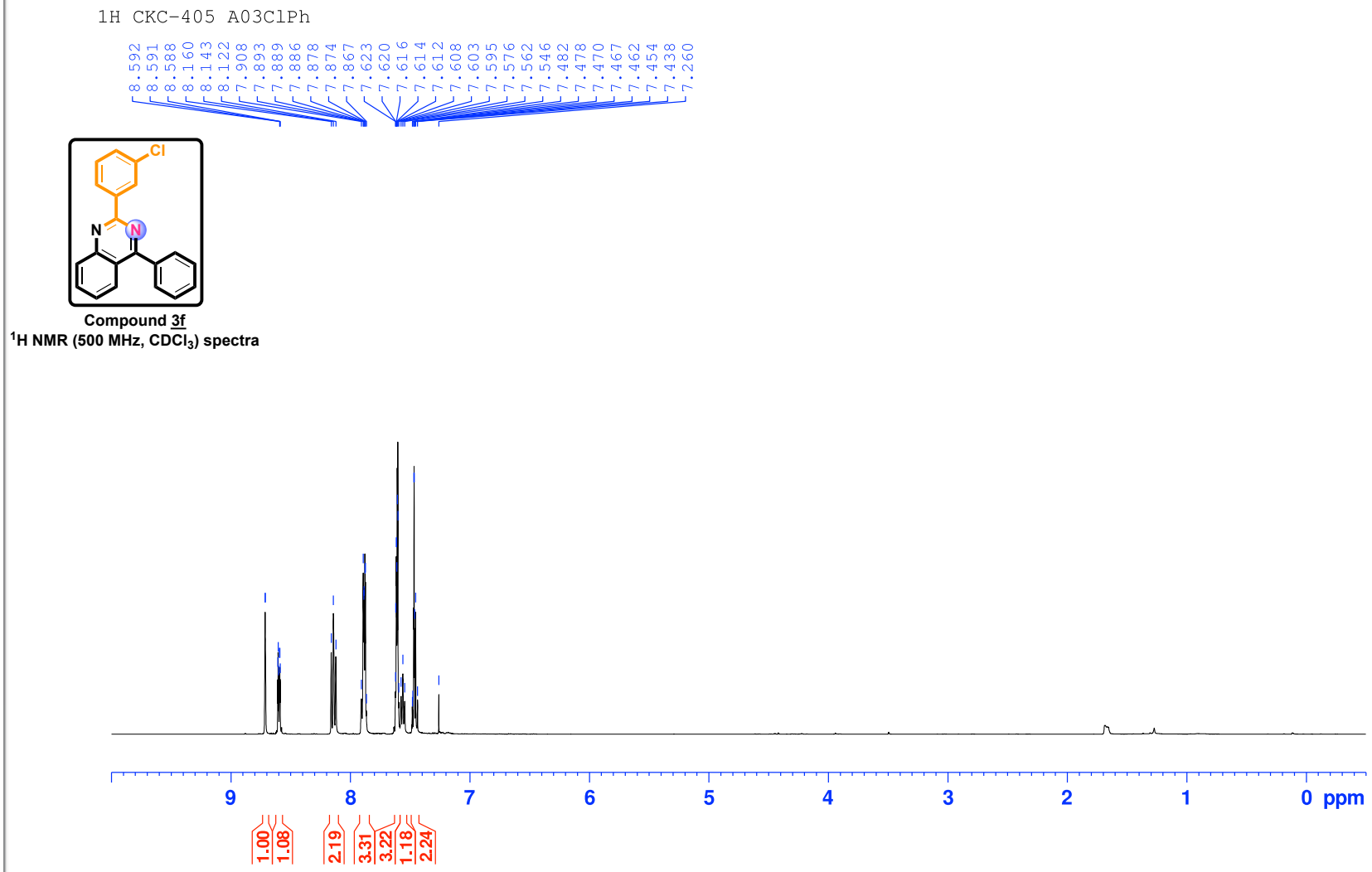
Compound 3e



Compound 3e
^{13}C NMR (125 MHz, $CDCl_3$) spectra



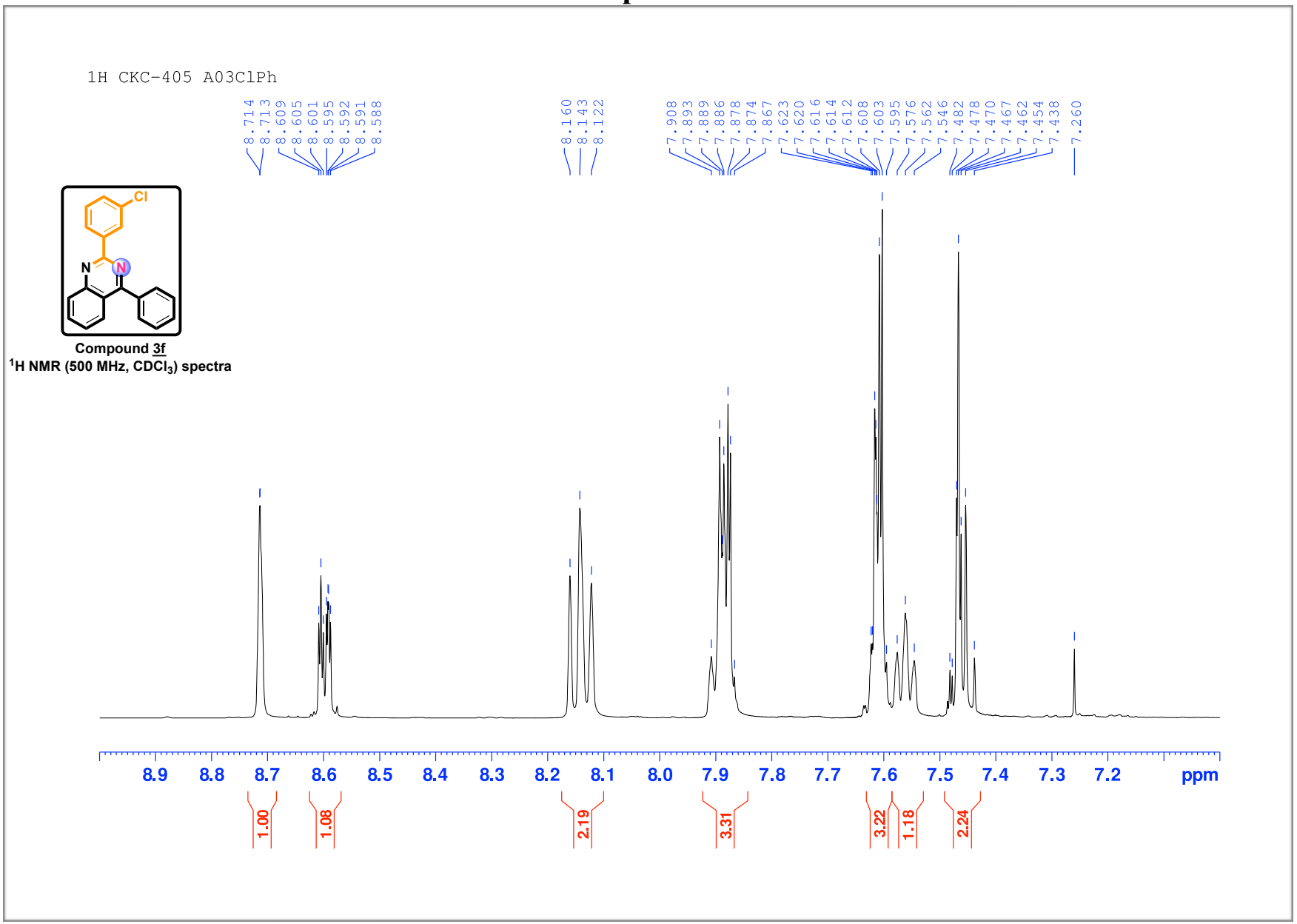
Compound 3f



Compound 3f

^{1}H NMR (500 MHz, $CDCl_3$) spectra

Compound 3f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7.612
7.608
7.603
7.595
7.576
7.562
7.546
7.482
7.478
7.470
7.467
7.462
7.454
7.438
7.260
Cl
N
N
Compound 3f
1H NMR (500 MHz, CDCl3) spectra
8.9
8.8
8.7
8.6
8.5
8.4
8.3
8.2
8.1
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7.7
7.6
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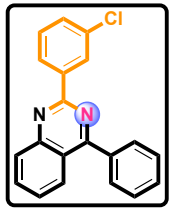
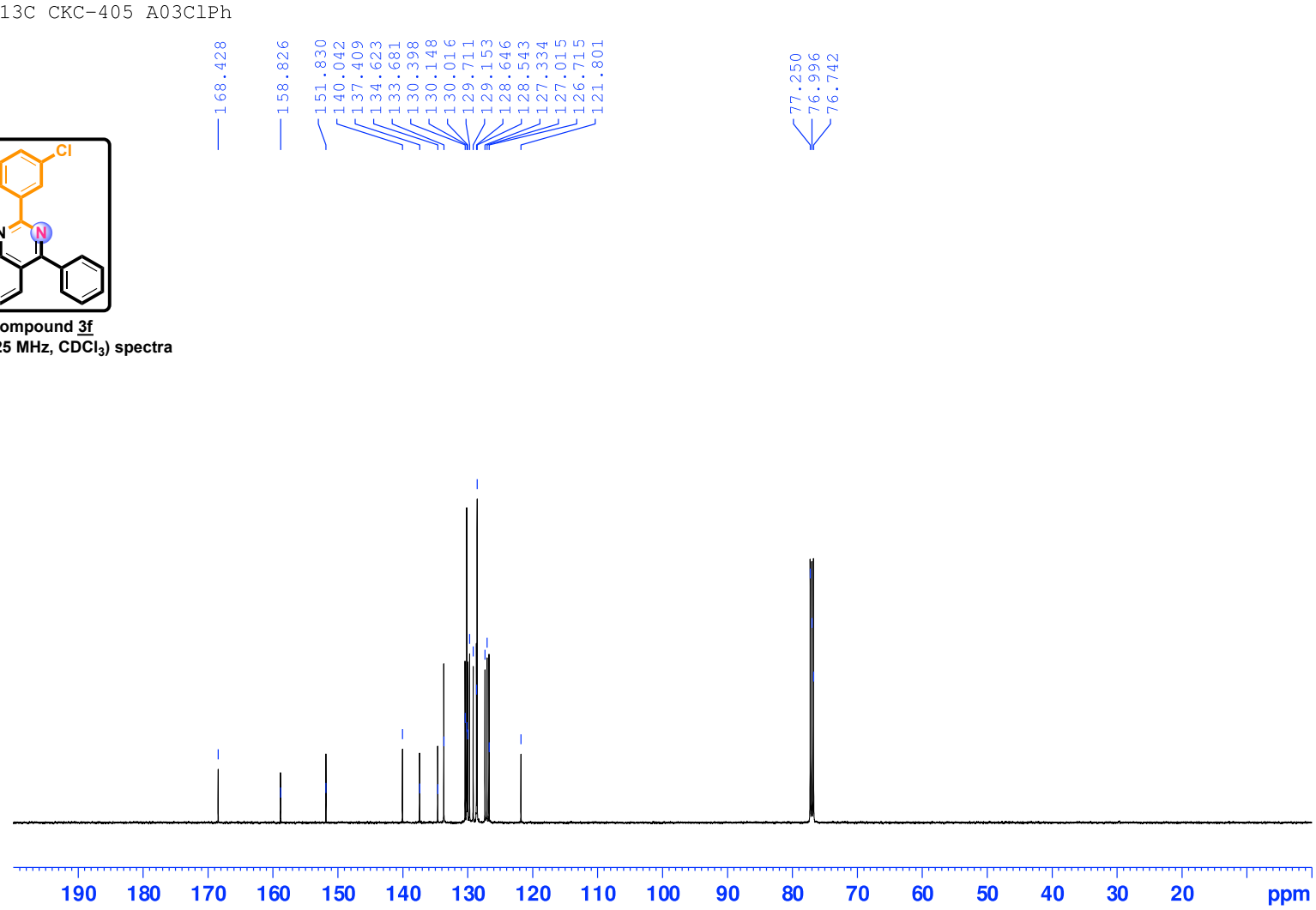
Compound 3f

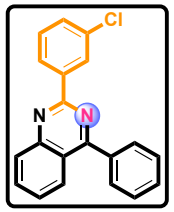


Compound 3f

^{13}C NMR (125 MHz, $CDCl_3$) spectra

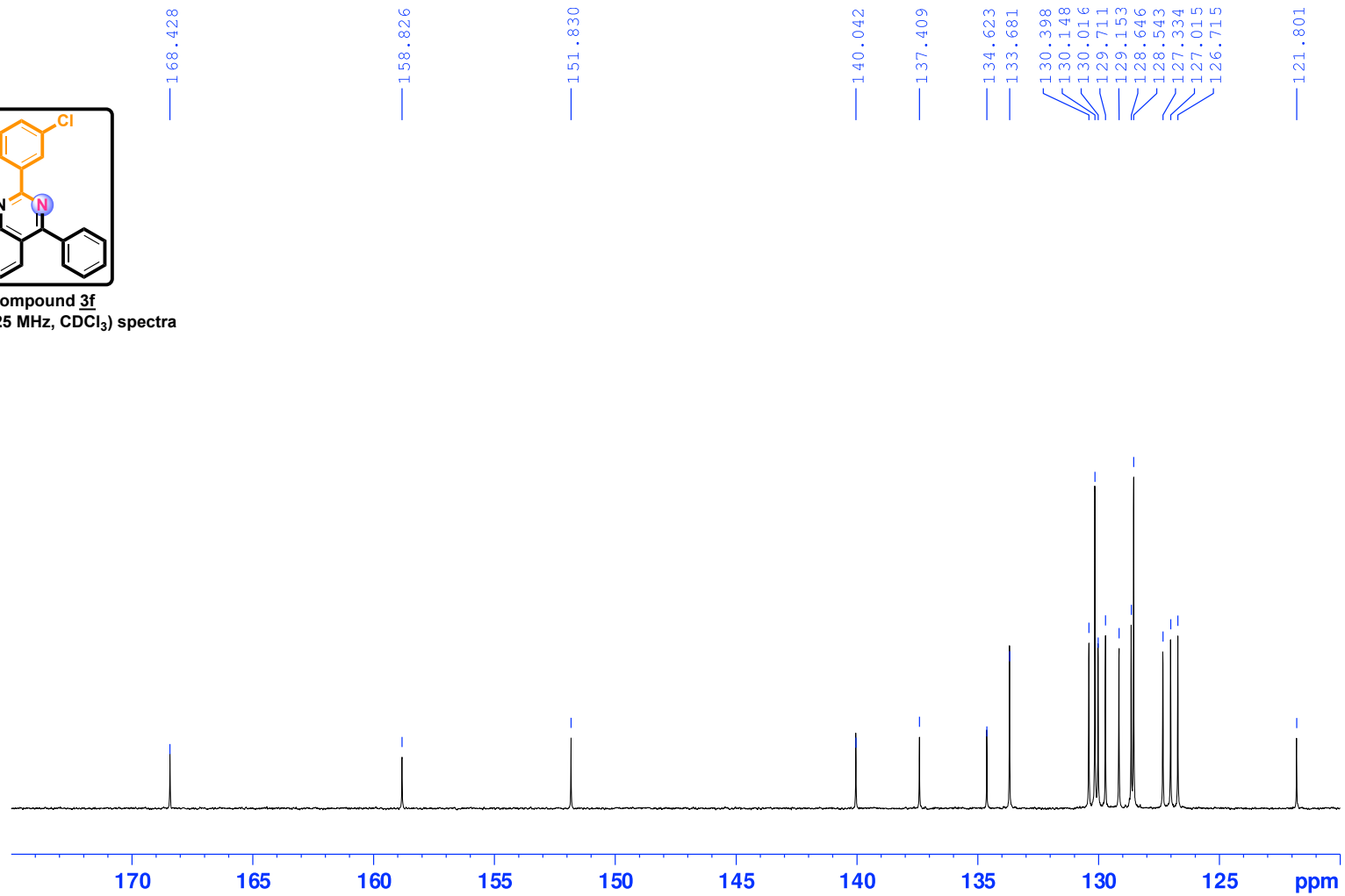


Compound 3f

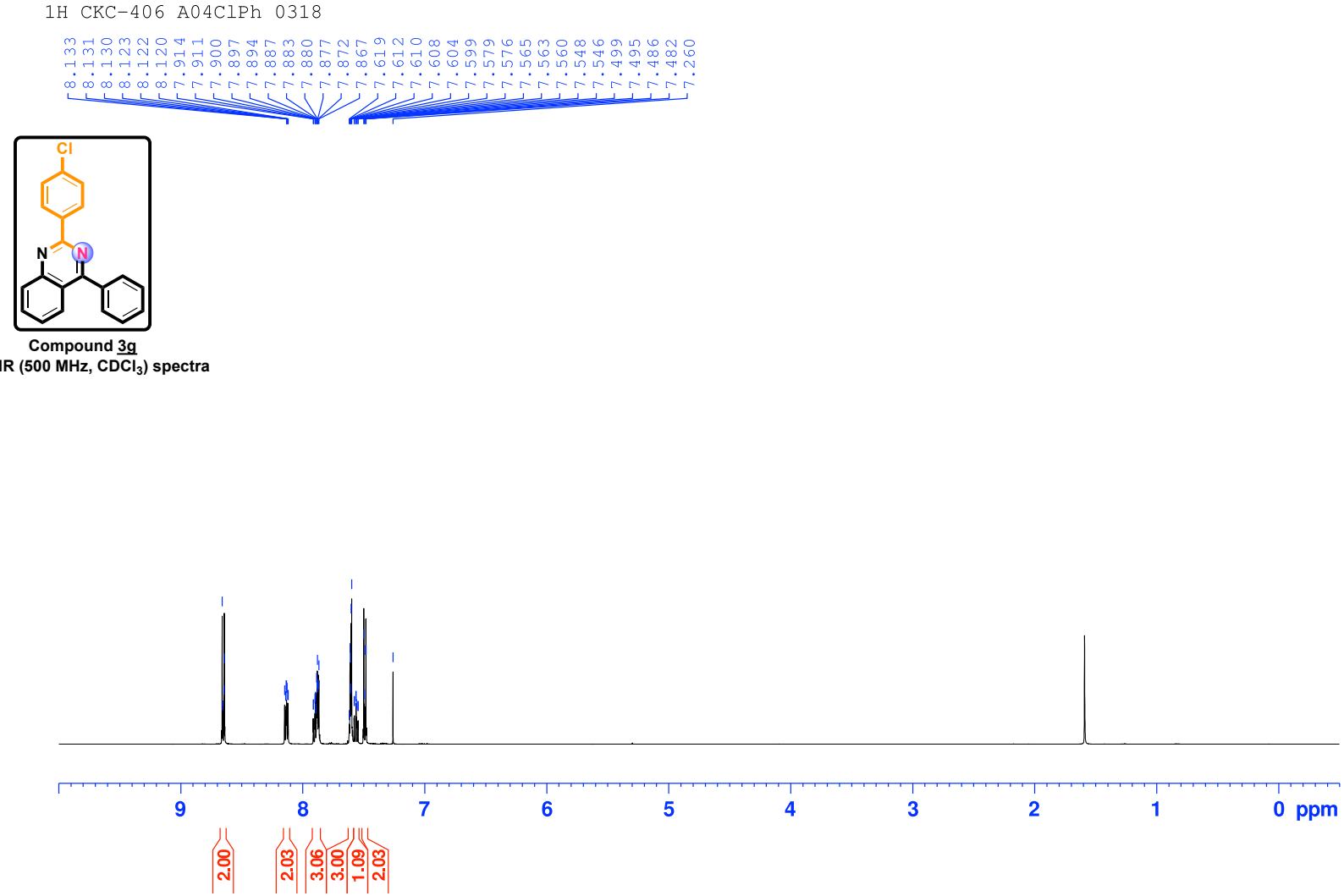


Compound 3f

^{13}C NMR (125 MHz, $CDCl_3$) spectra

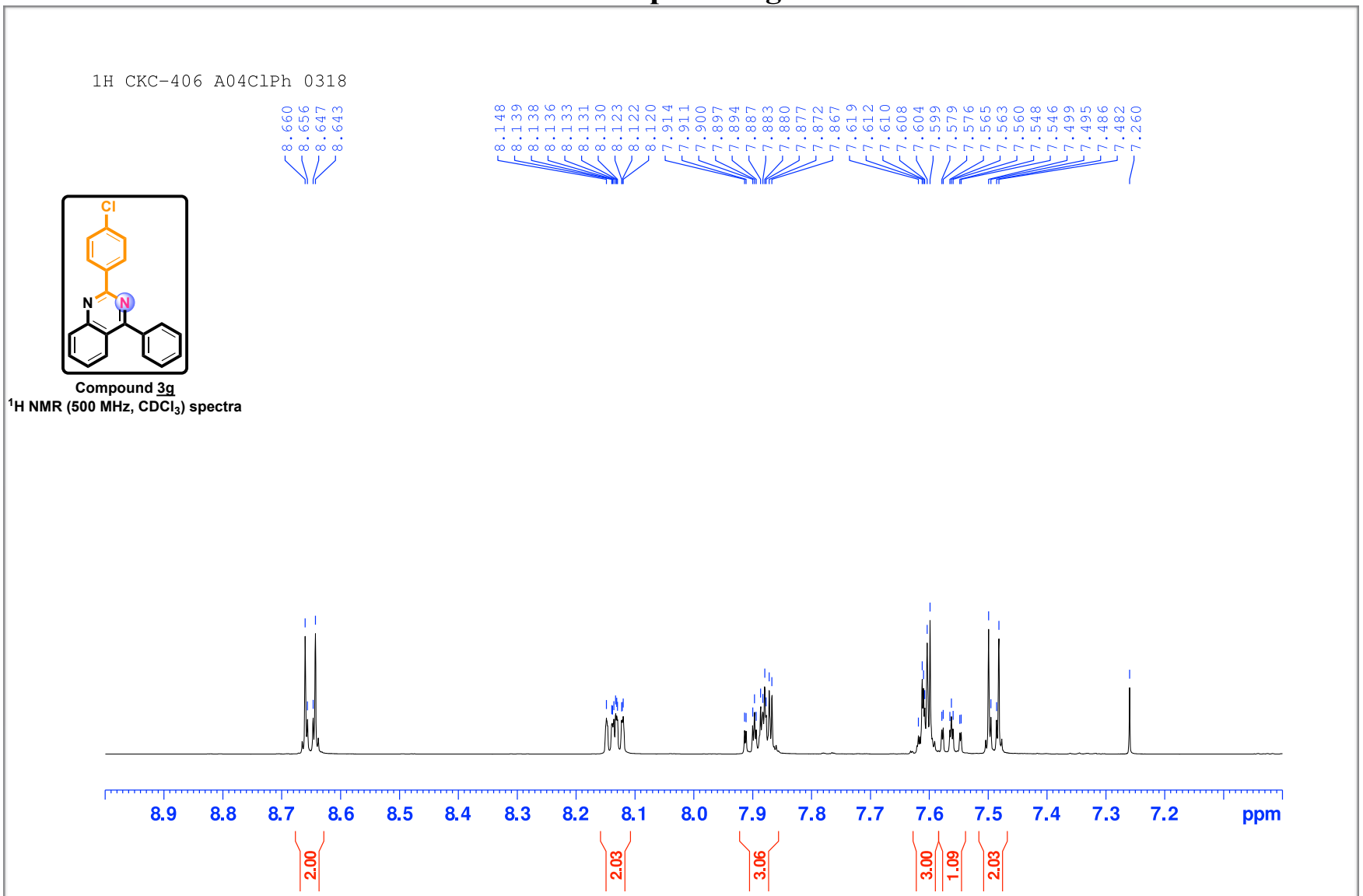


Compound 3g



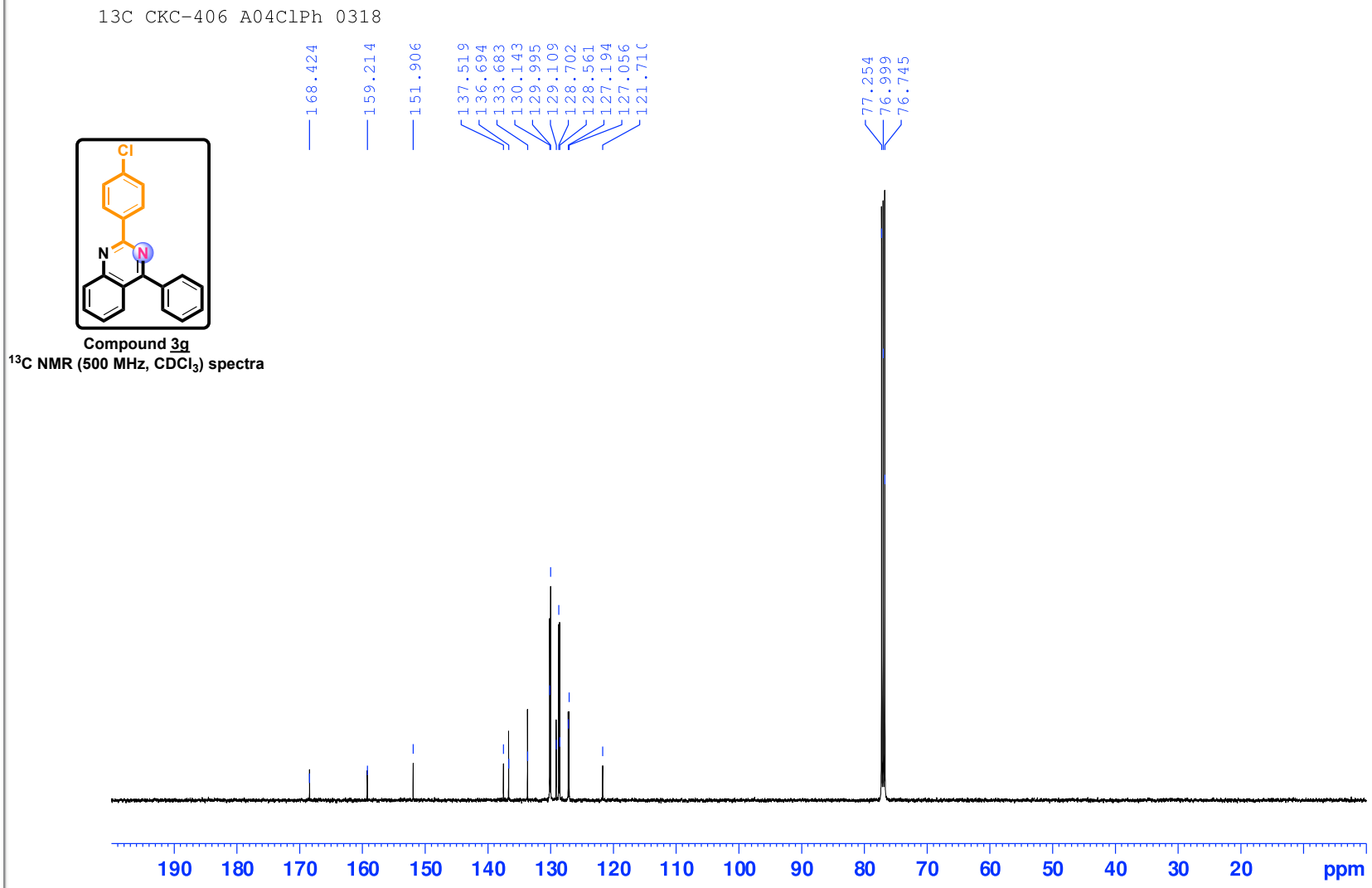
Compound 3g
^{1}H NMR (500 MHz, $CDCl_3$) spectra

Compound 3g



Compound 3g
^{1}H NMR (500 MHz, $CDCl_3$) spectra

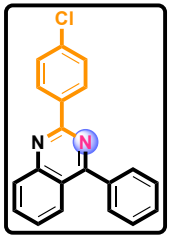
Compound 3g



Compound 3g

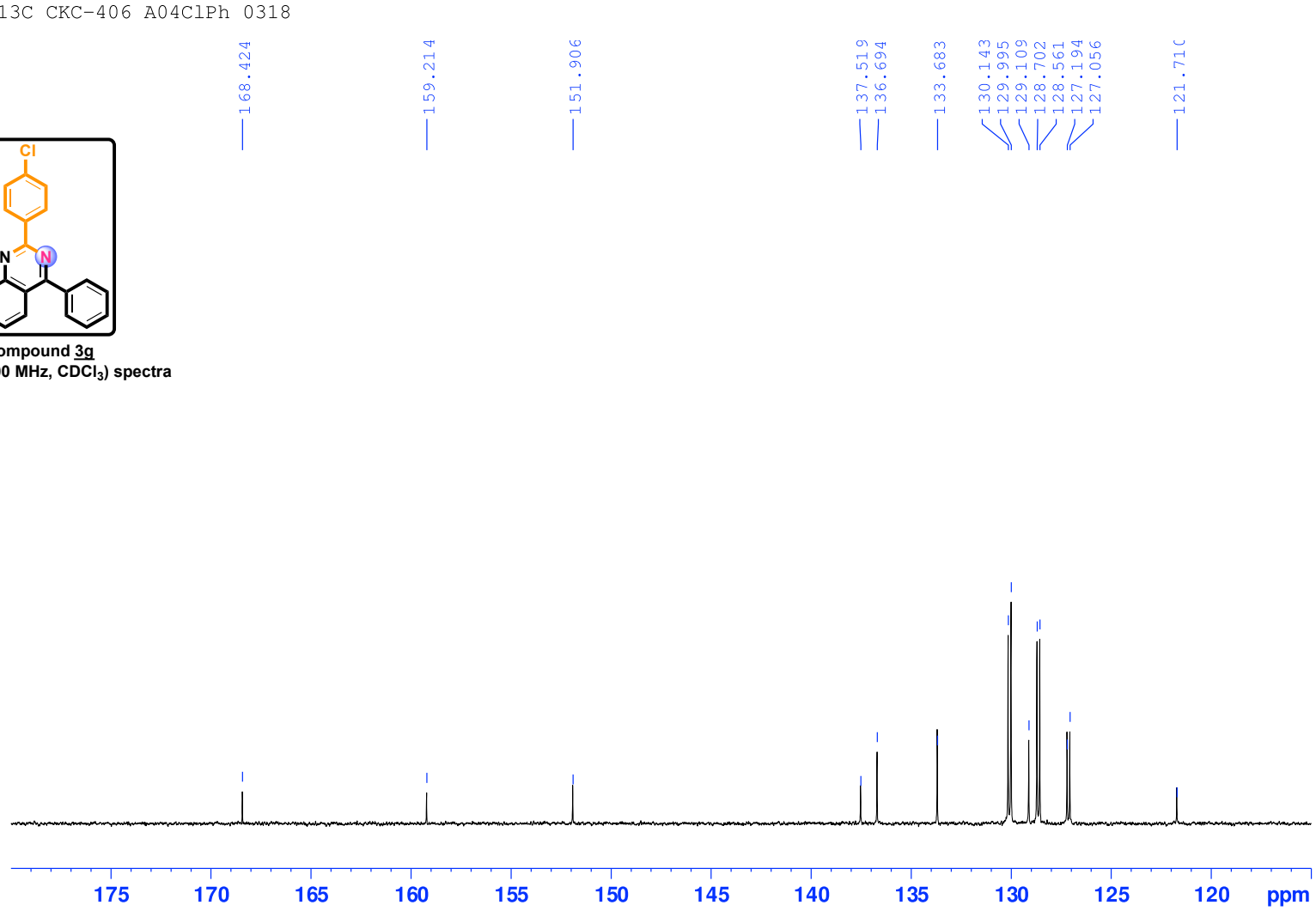
^{13}C NMR (500 MHz, $CDCl_3$) spectra

Compound 3g

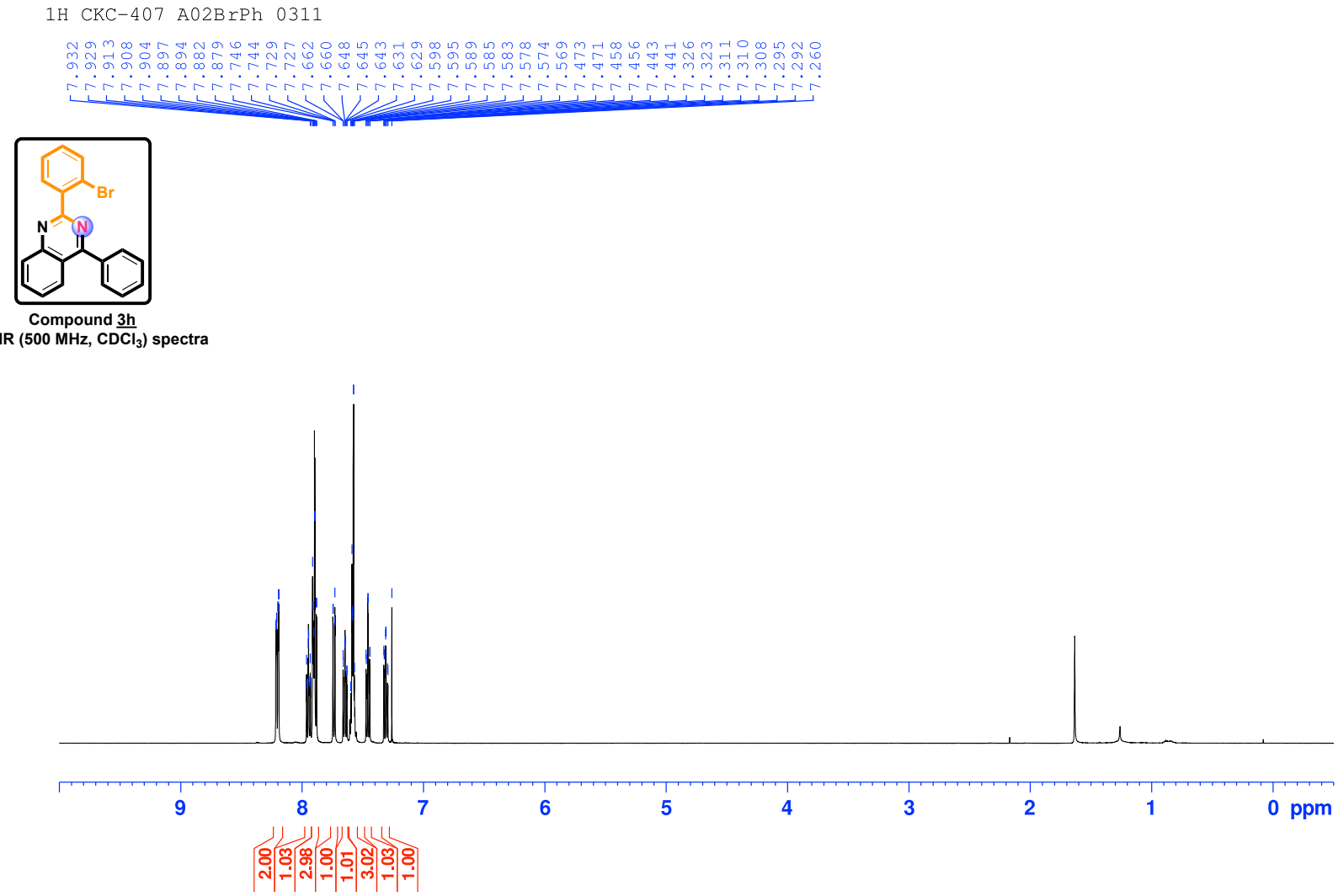


Compound 3g

^{13}C NMR (500 MHz, $CDCl_3$) spectra

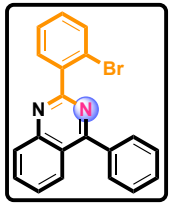


Compound 3h

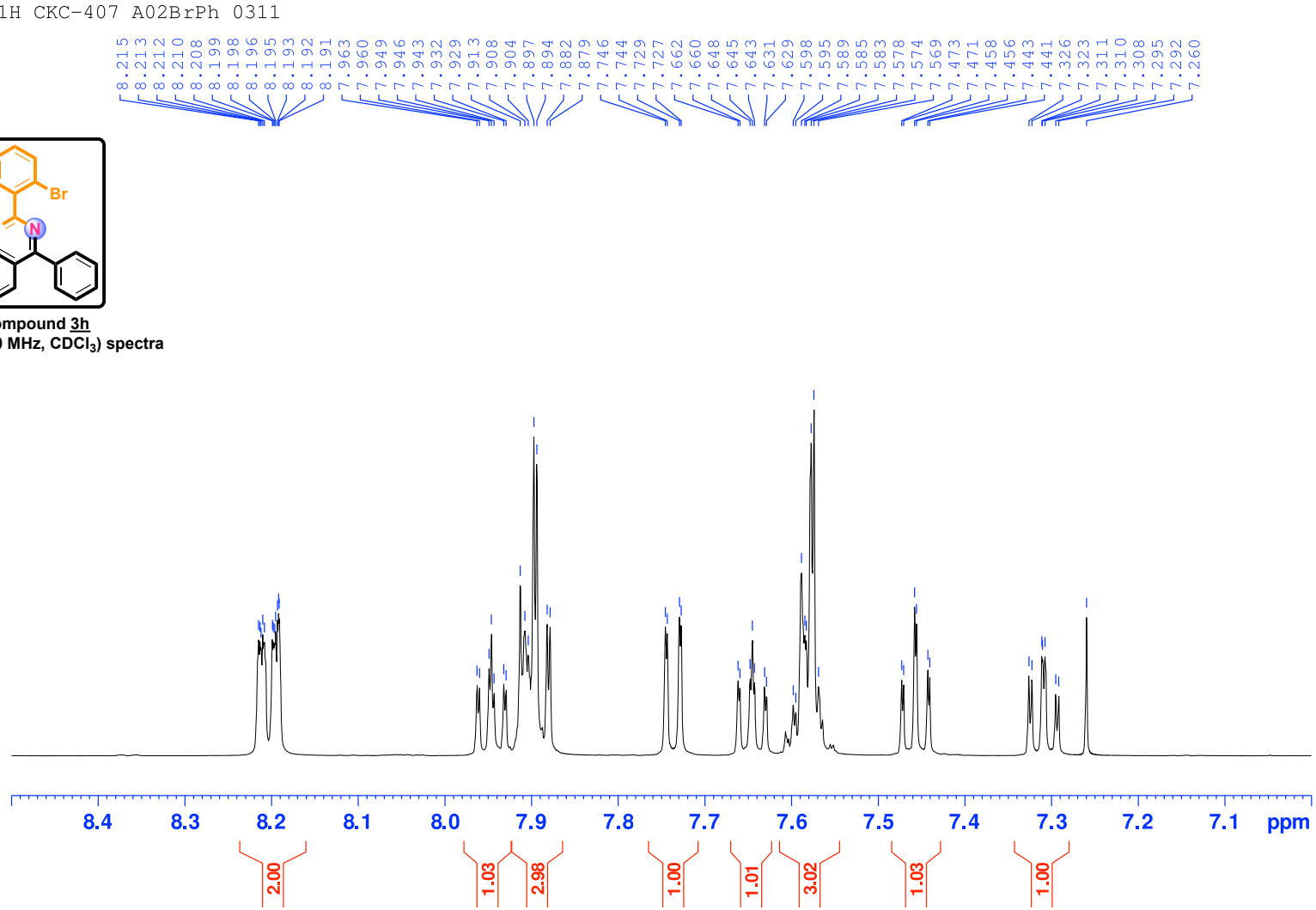


Compound 3h
^{1}H NMR (500 MHz, $CDCl_3$) spectra

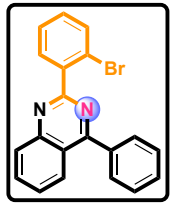
Compound 3h



Compound 3h
^{1}H NMR (500 MHz, $CDCl_3$) spectra

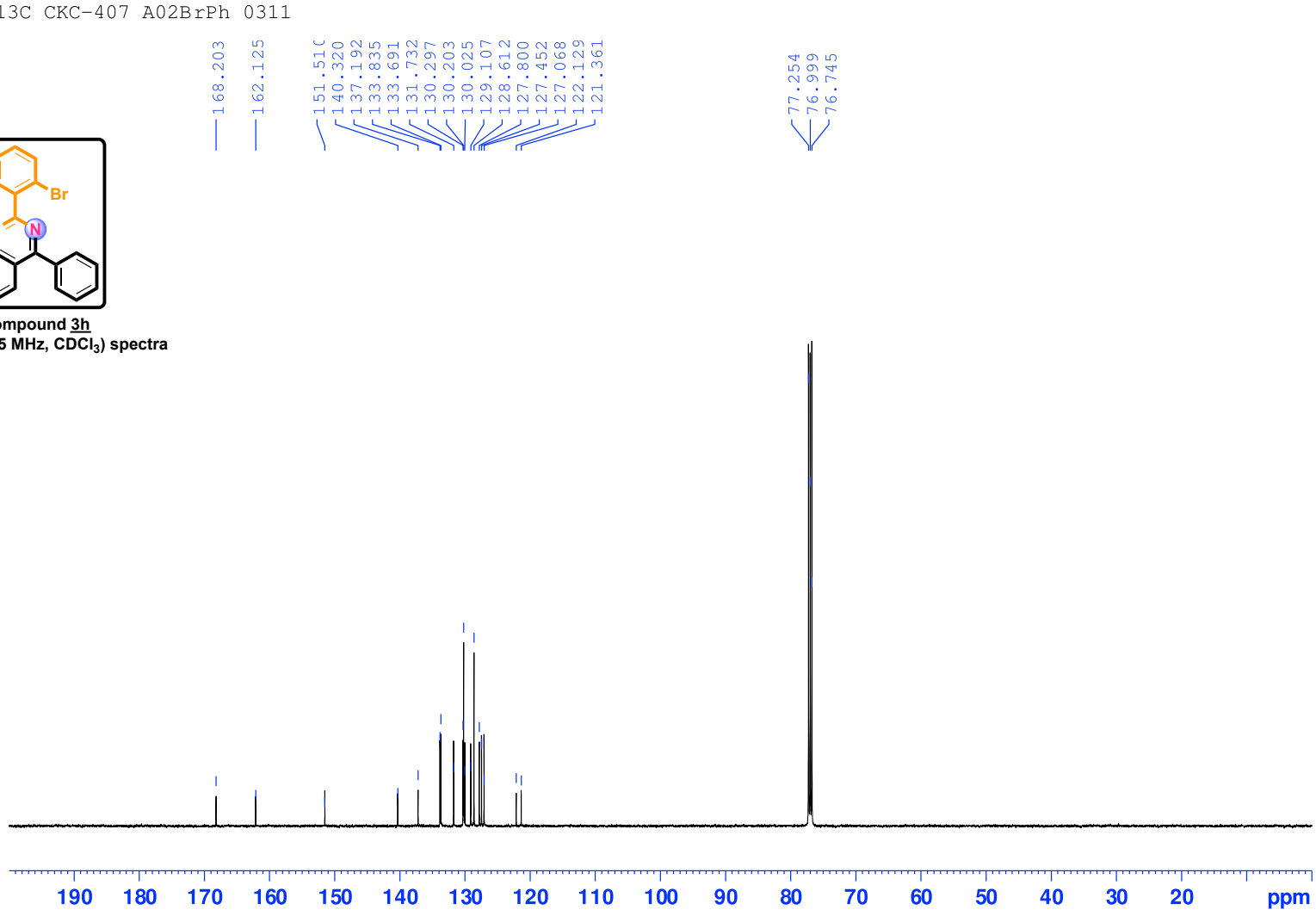


Compound 3h

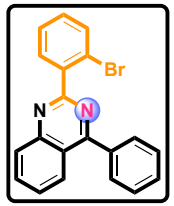


Compound 3h

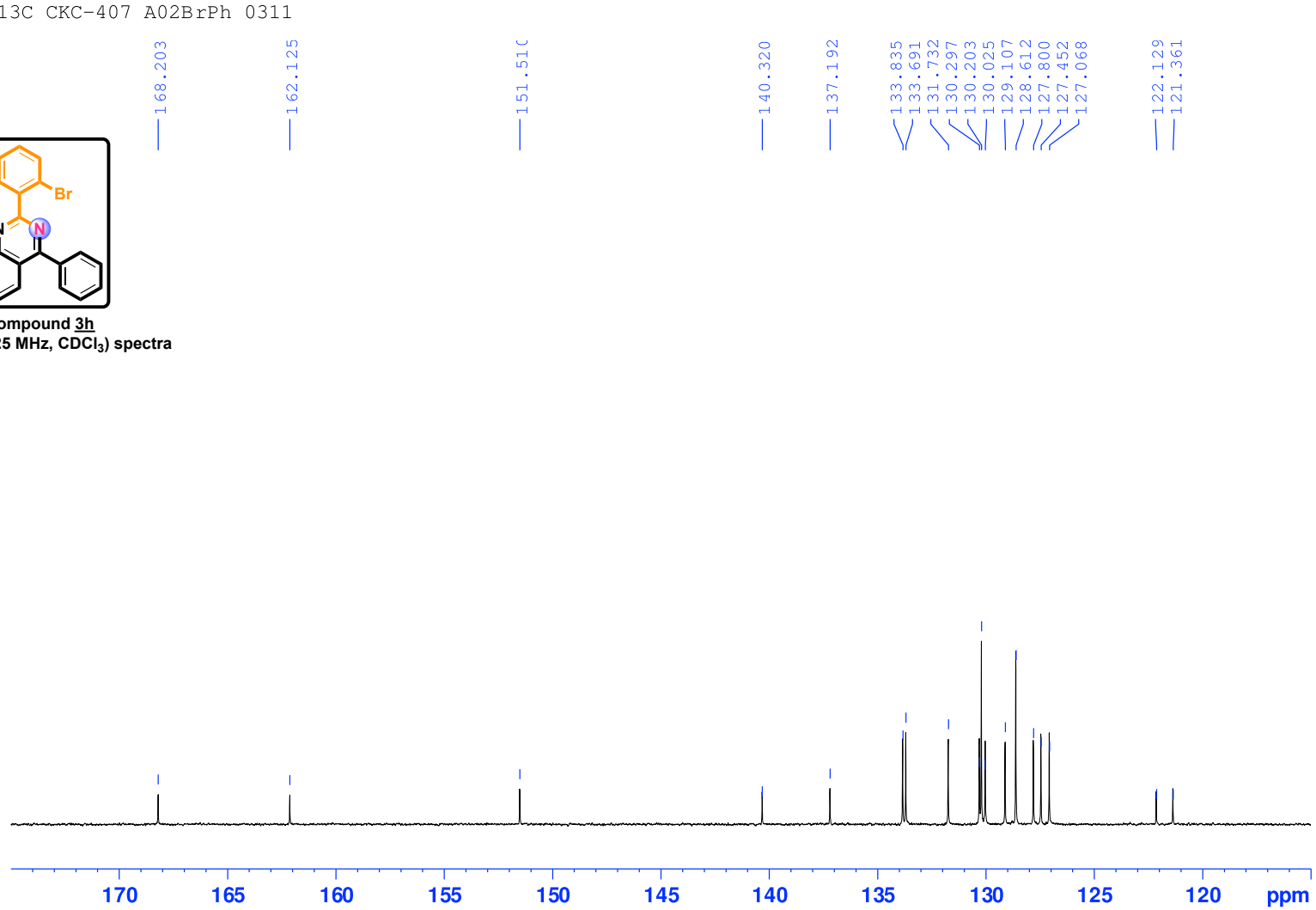
^{13}C NMR (125 MHz, $CDCl_3$) spectra



Compound 3h

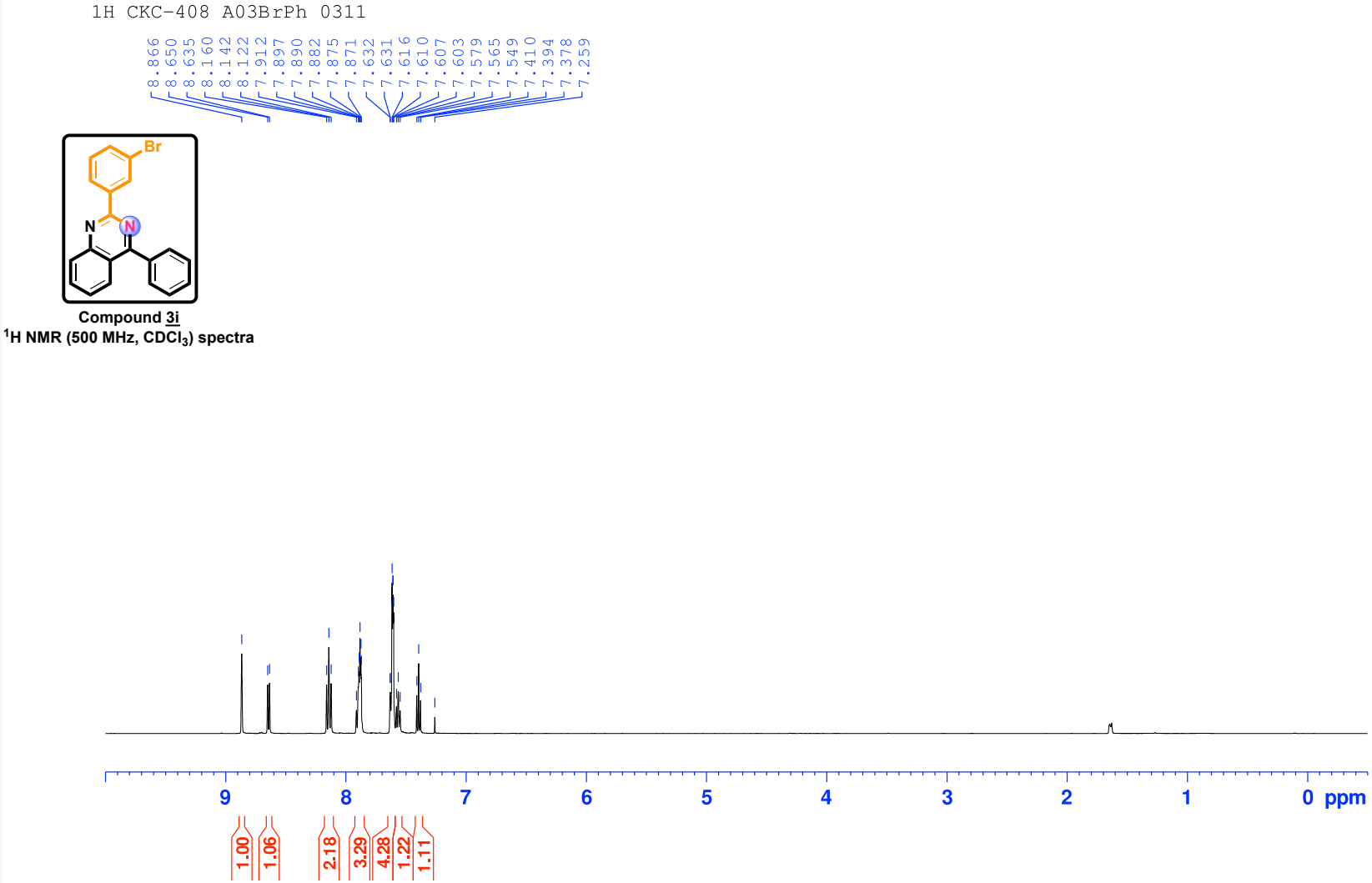


Compound 3h
^{13}C NMR (125 MHz, $CDCl_3$) spectra

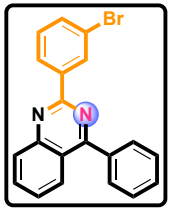


Compound 3i

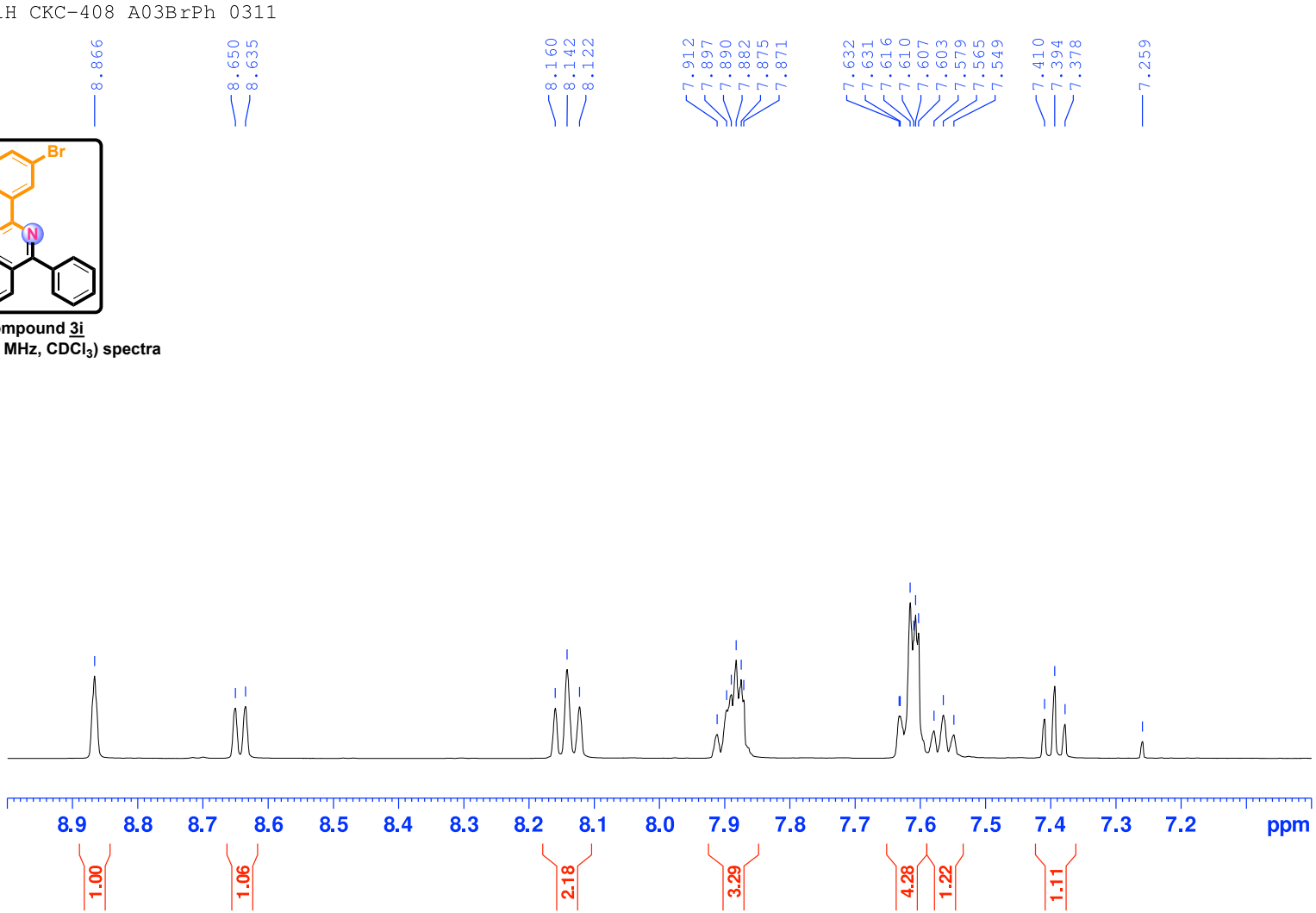
Compound 3i
^{1}H NMR (500 MHz, $CDCl_3$) spectra



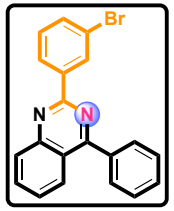
Compound 3i



Compound 3i
^{1}H NMR (500 MHz, $CDCl_3$) spectra

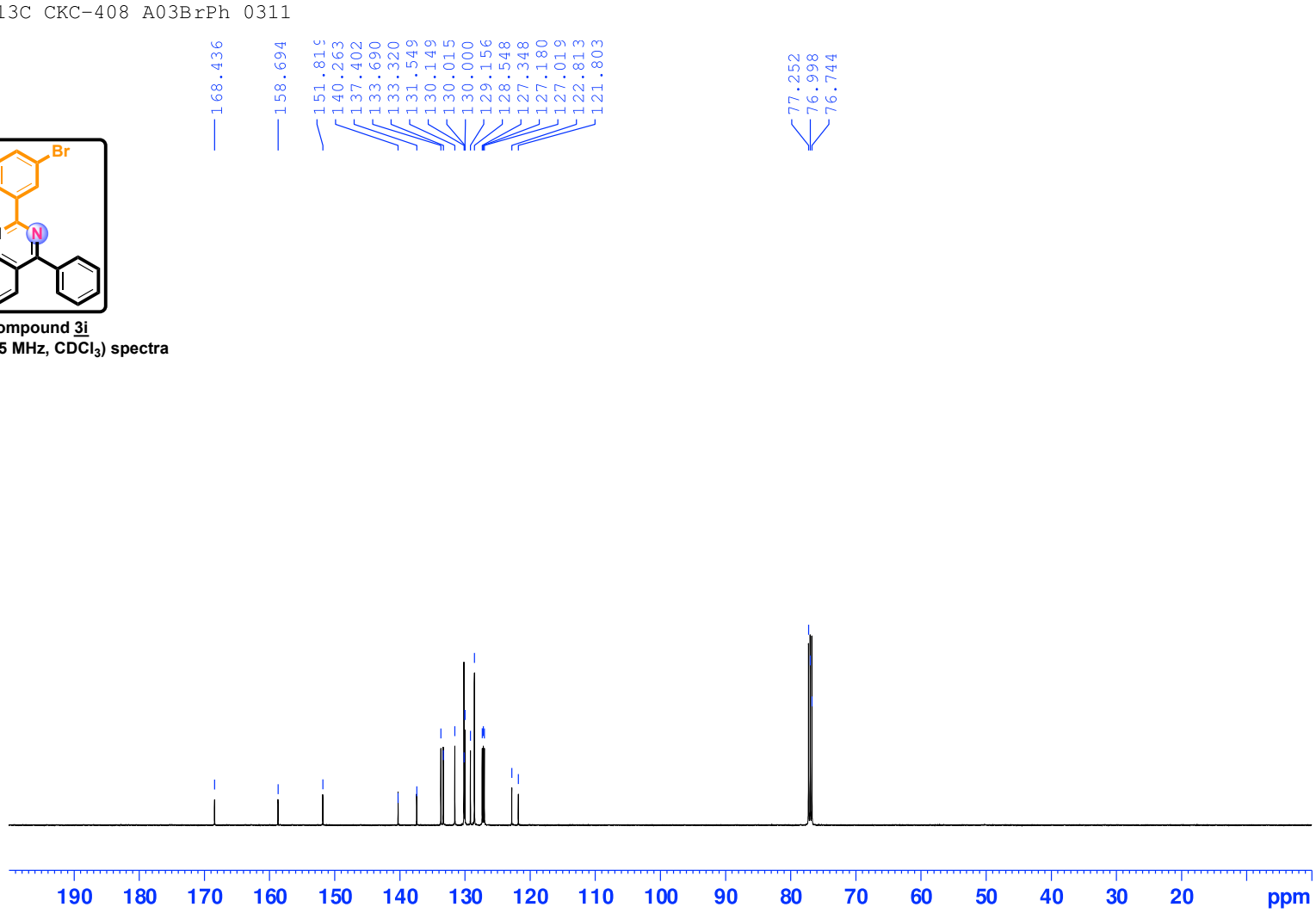


Compound 3i

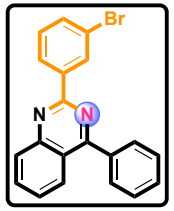


Compound 3i

^{13}C NMR (125 MHz, $CDCl_3$) spectra

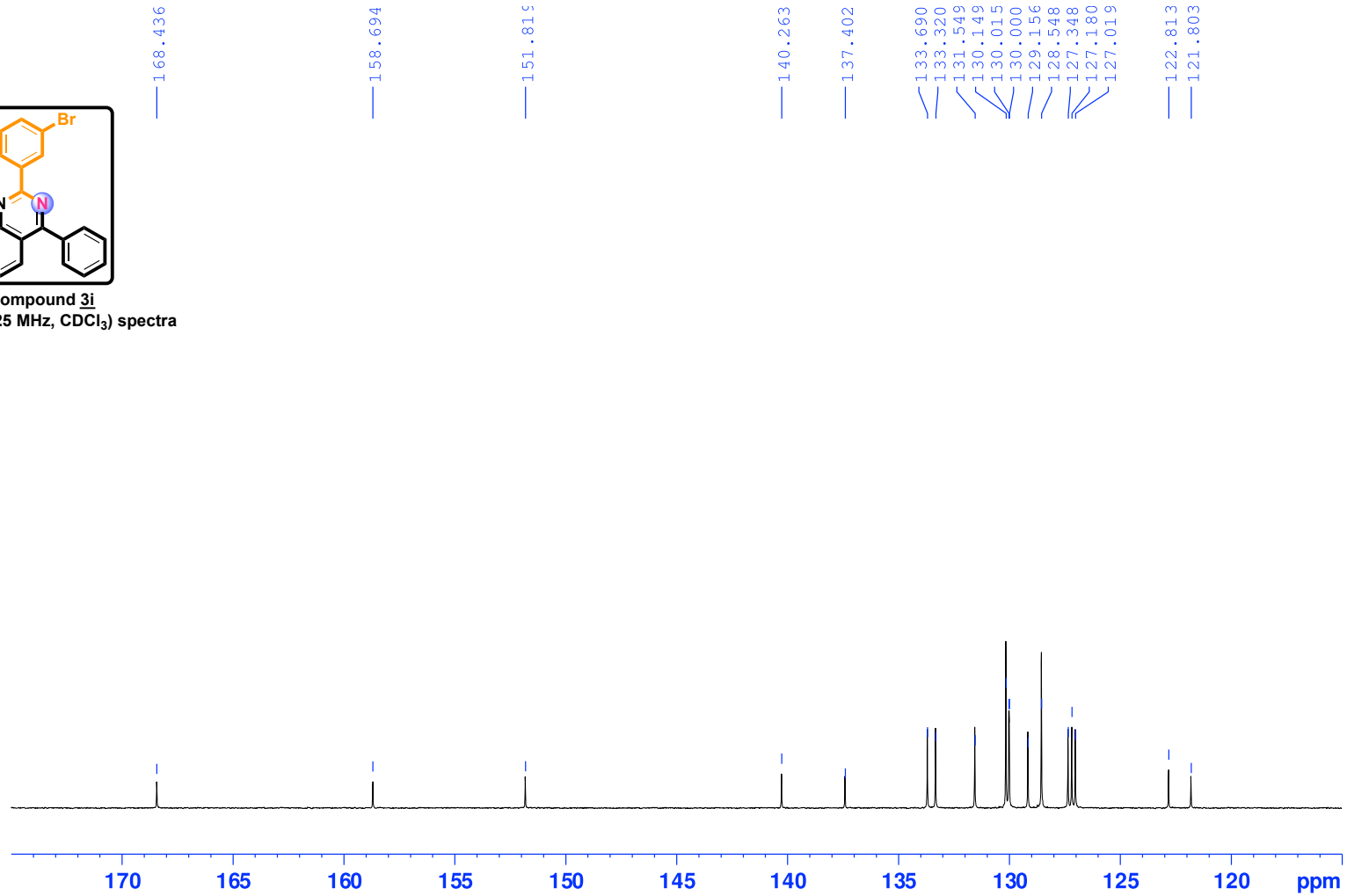


Compound 3i

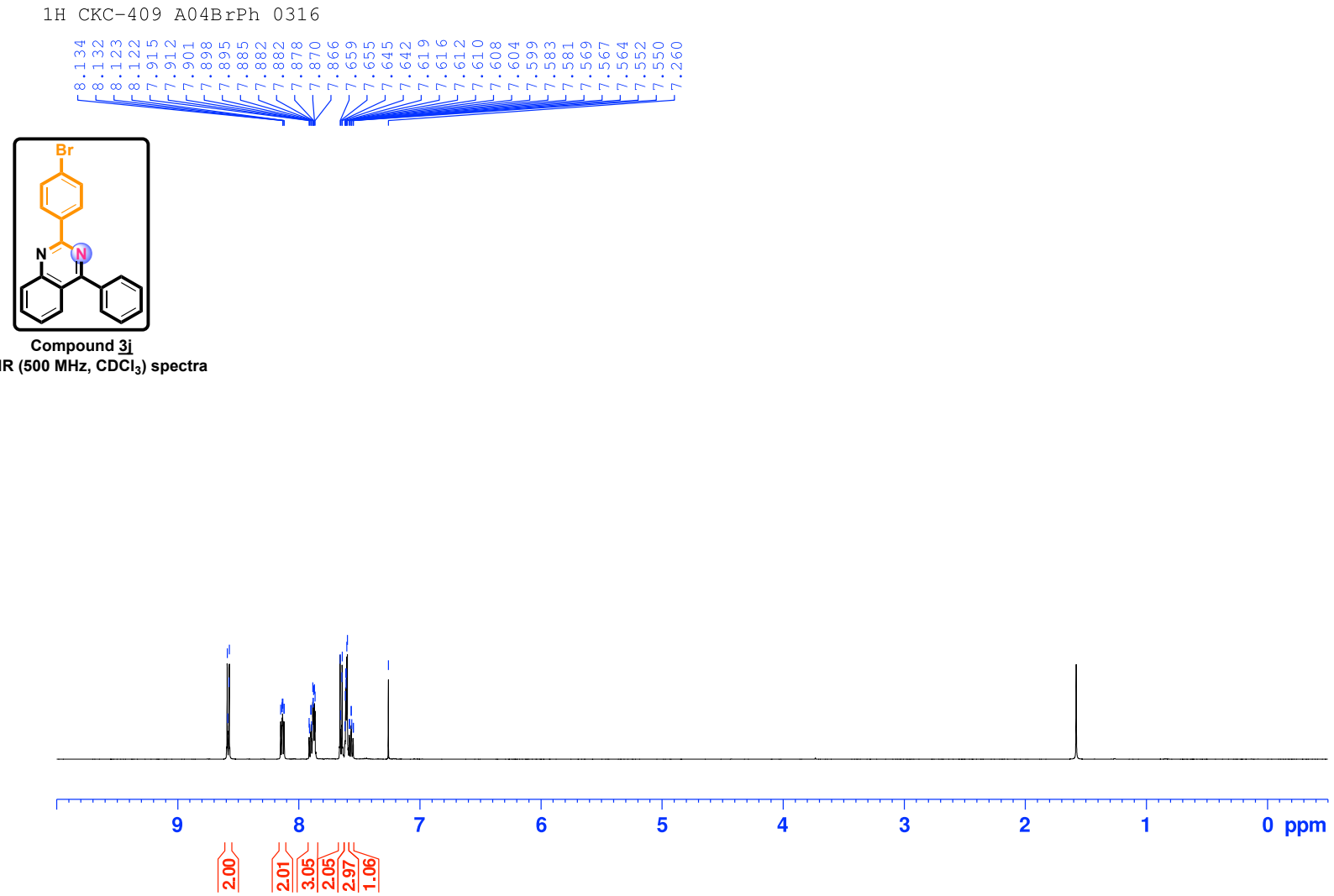


Compound 3i

^{13}C NMR (125 MHz, $CDCl_3$) spectra

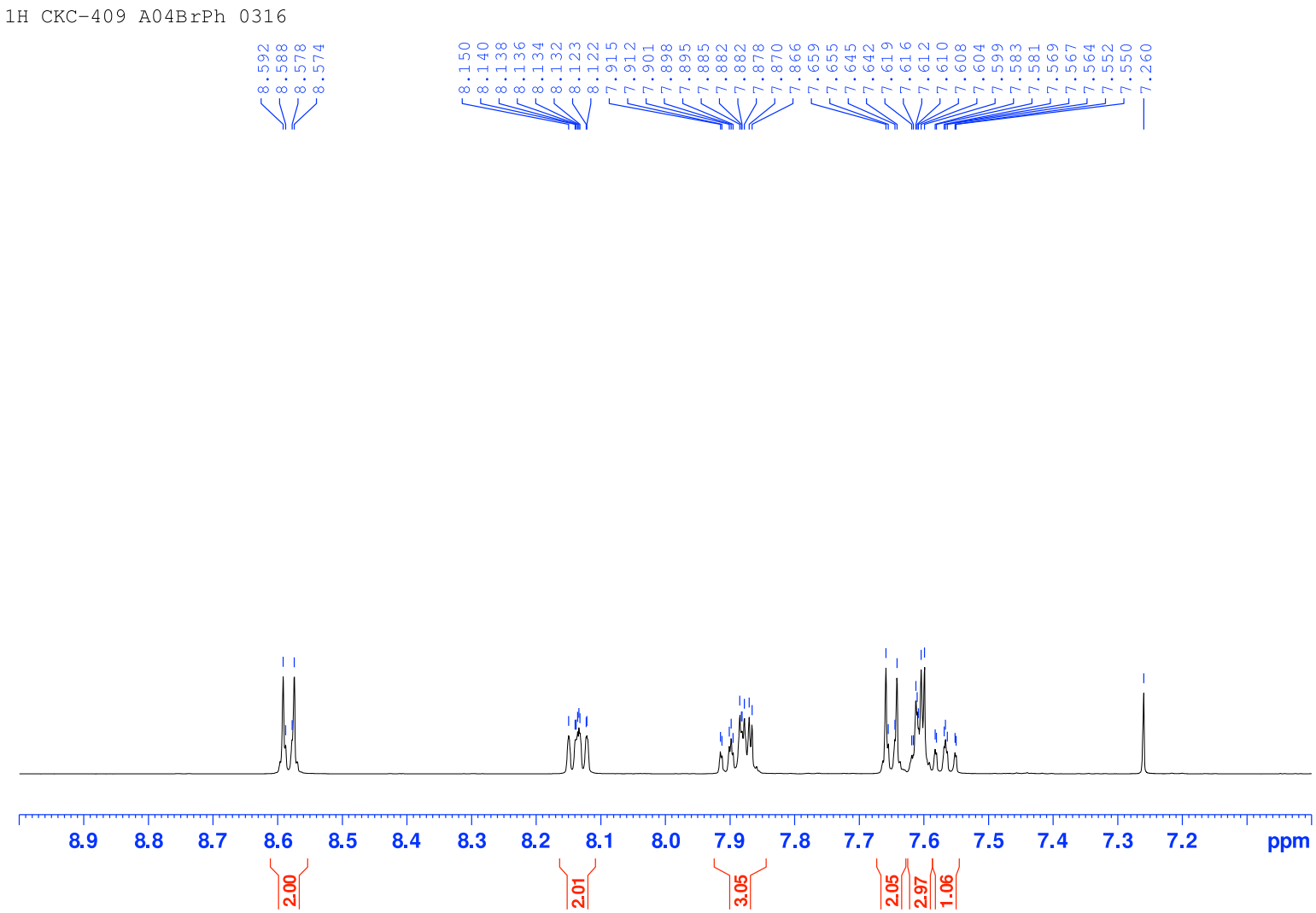


Compound 3j



Compound 3j
^{1}H NMR (500 MHz, $CDCl_3$) spectra

Compound 3j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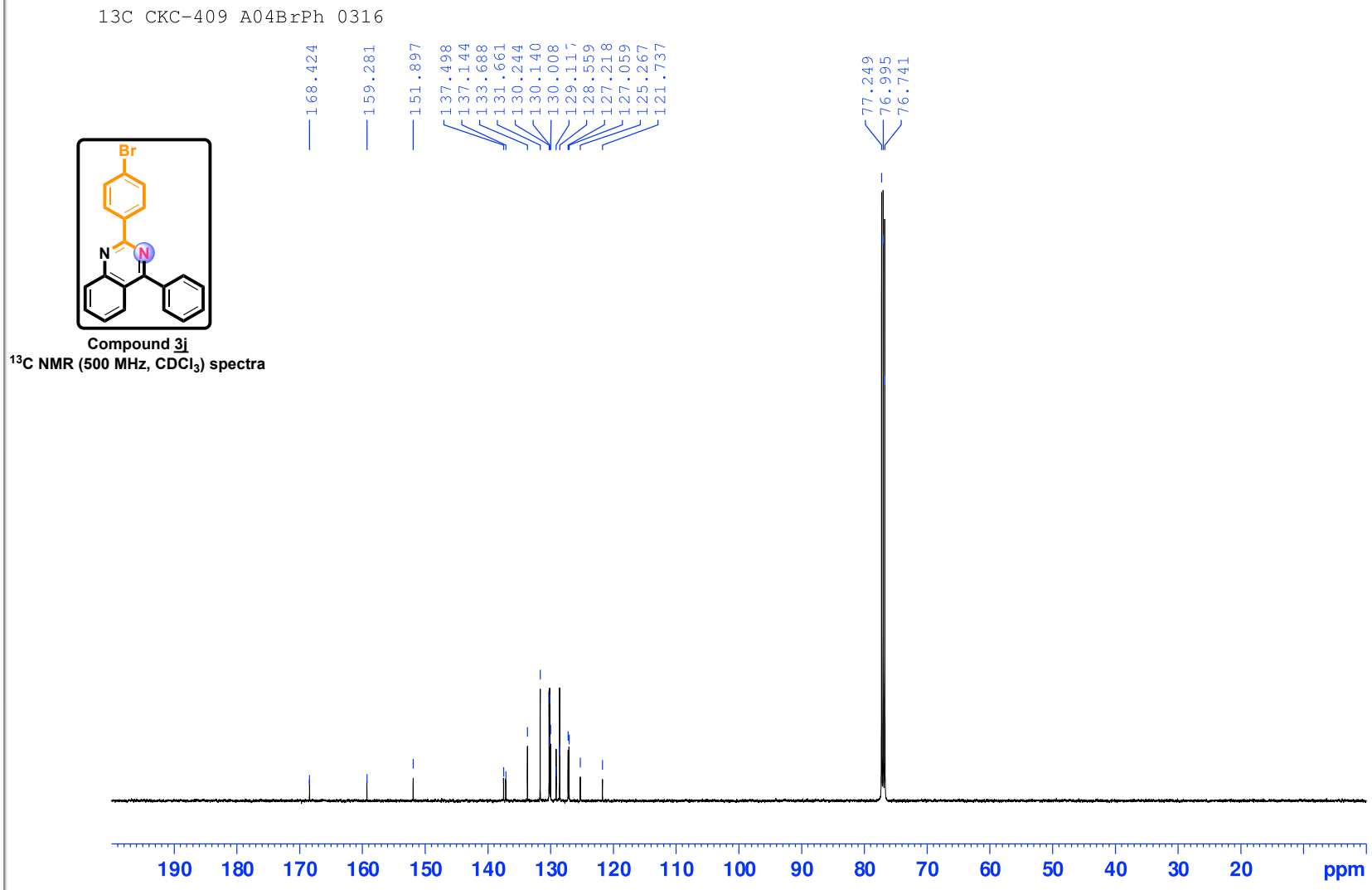
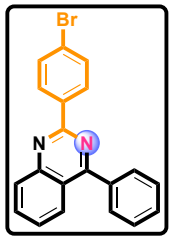
Compound 3j



Compound 3j

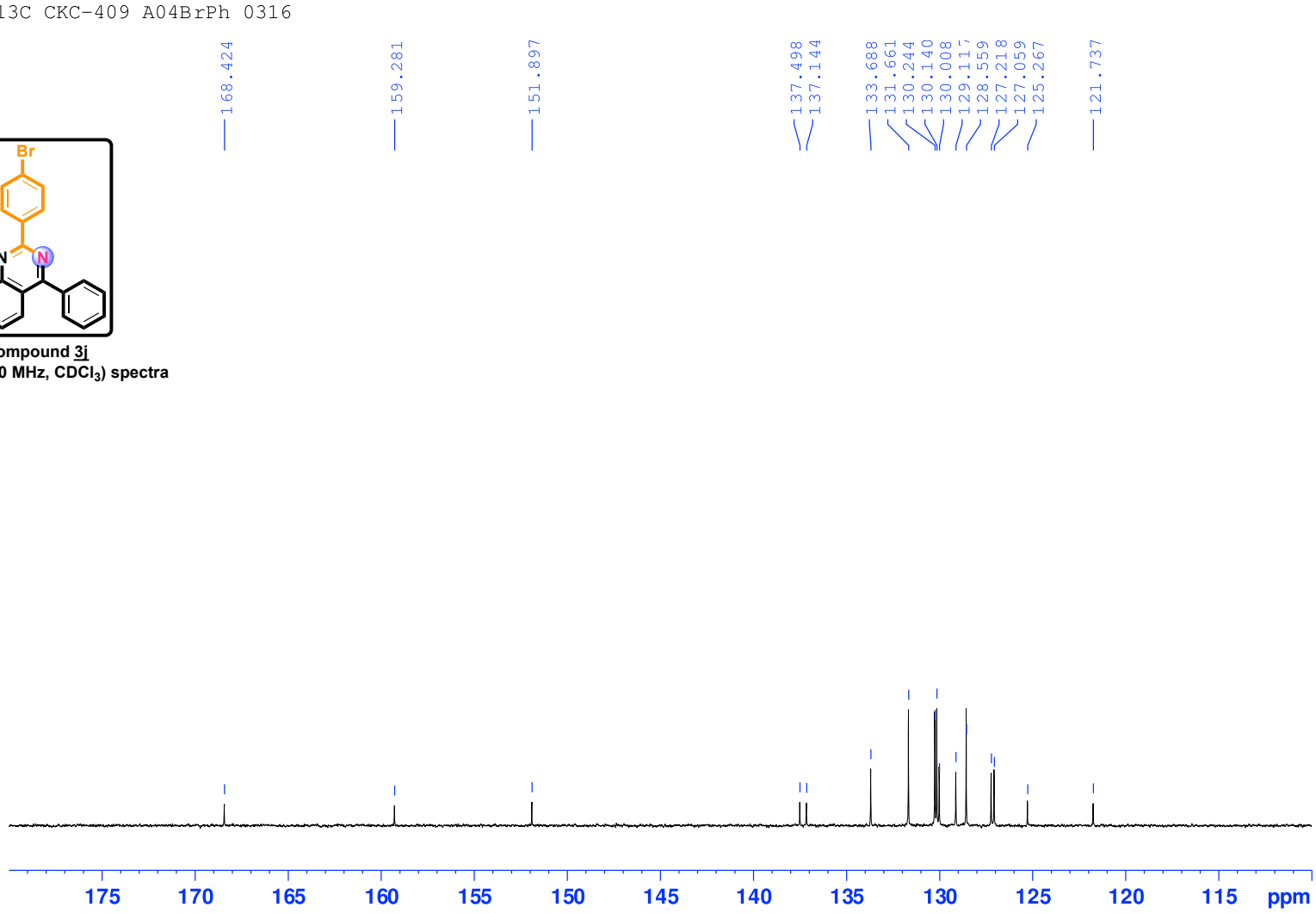
^{13}C NMR (500 MHz, $CDCl_3$) spectra

Compound 3j

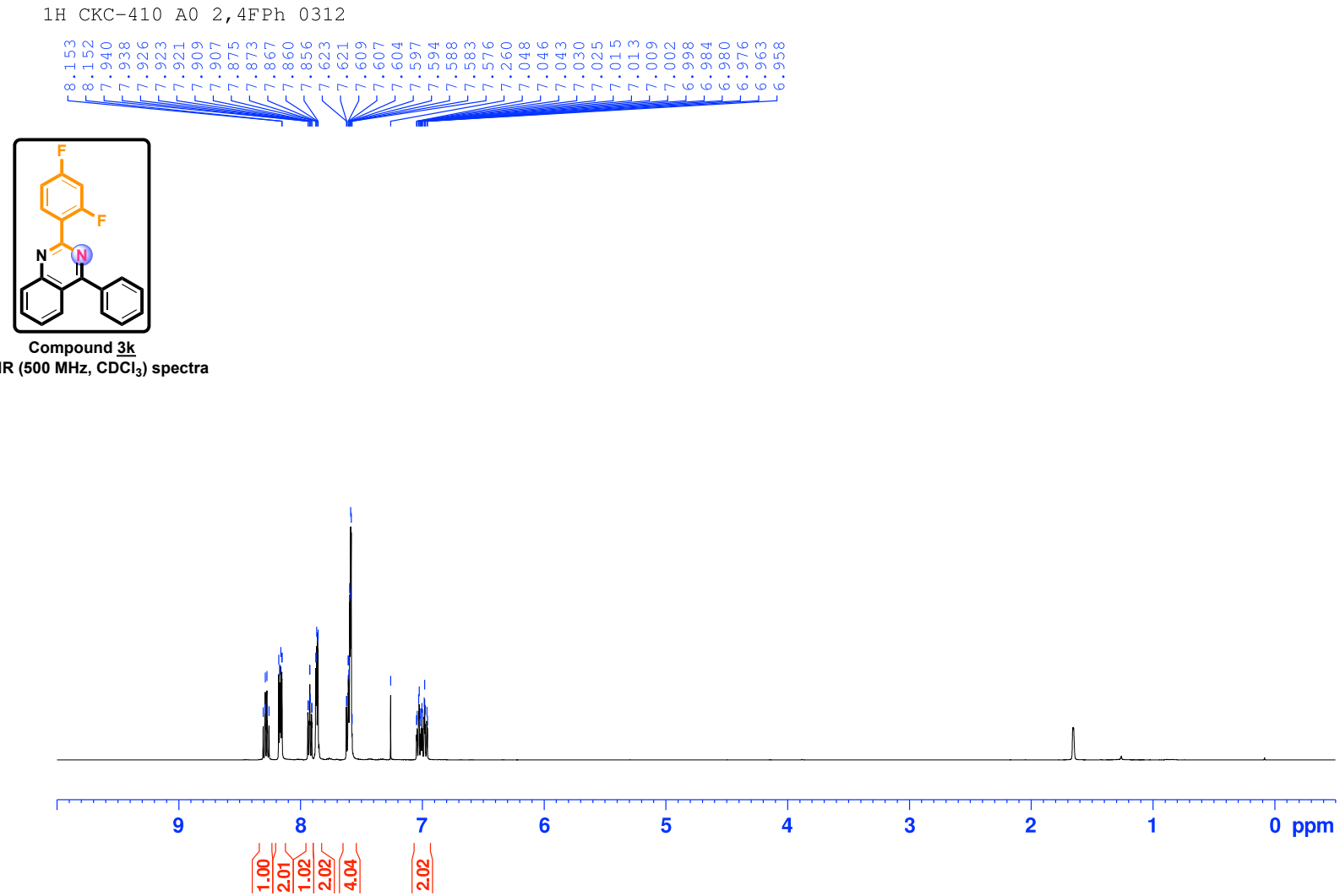


Compound 3j

^{13}C NMR (500 MHz, $CDCl_3$) spectra

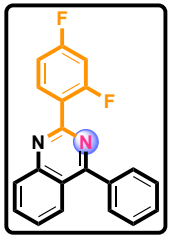


Compound 3k

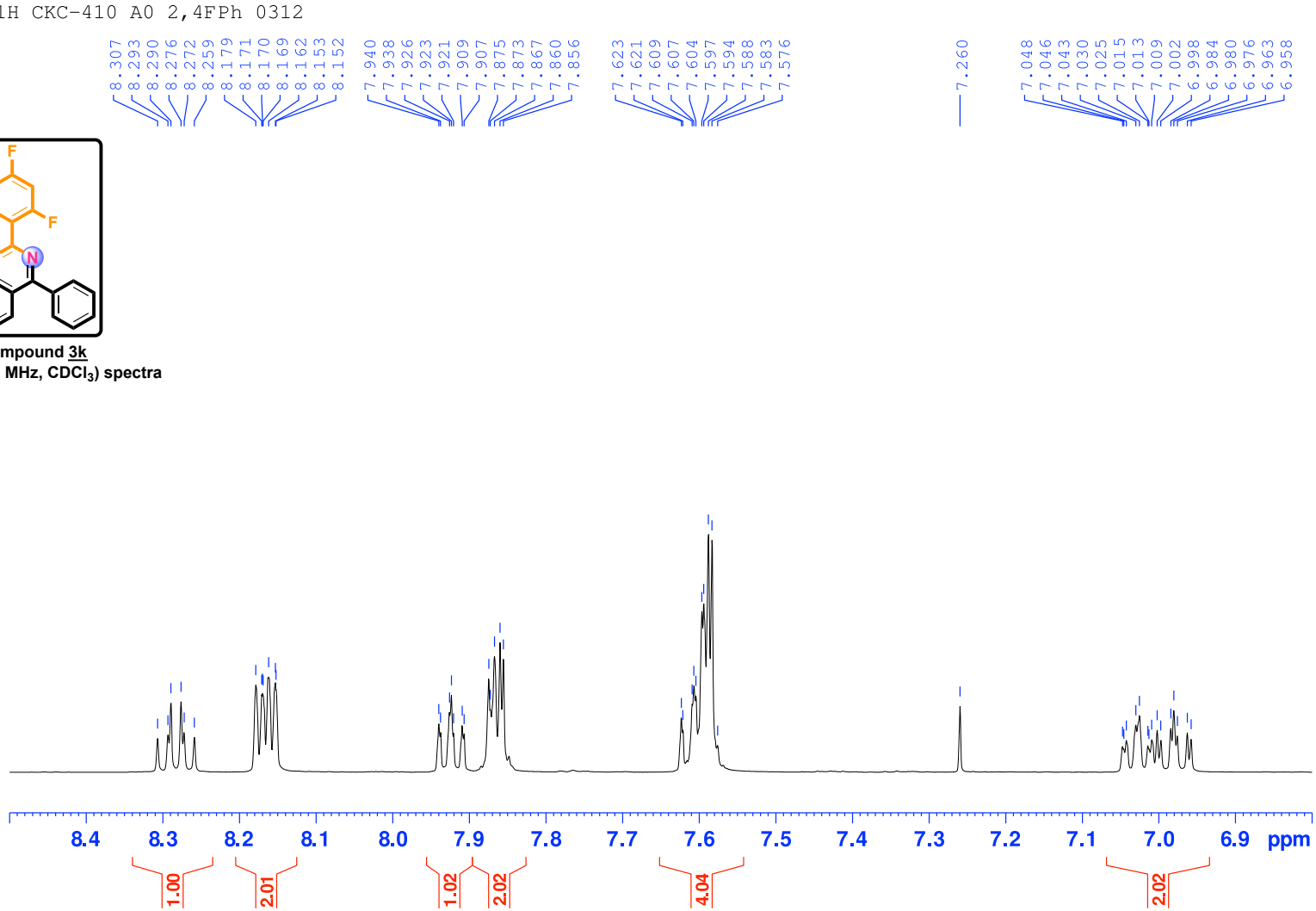


Compound 3k
^{1}H NMR (500 MHz, $CDCl_3$) spectra

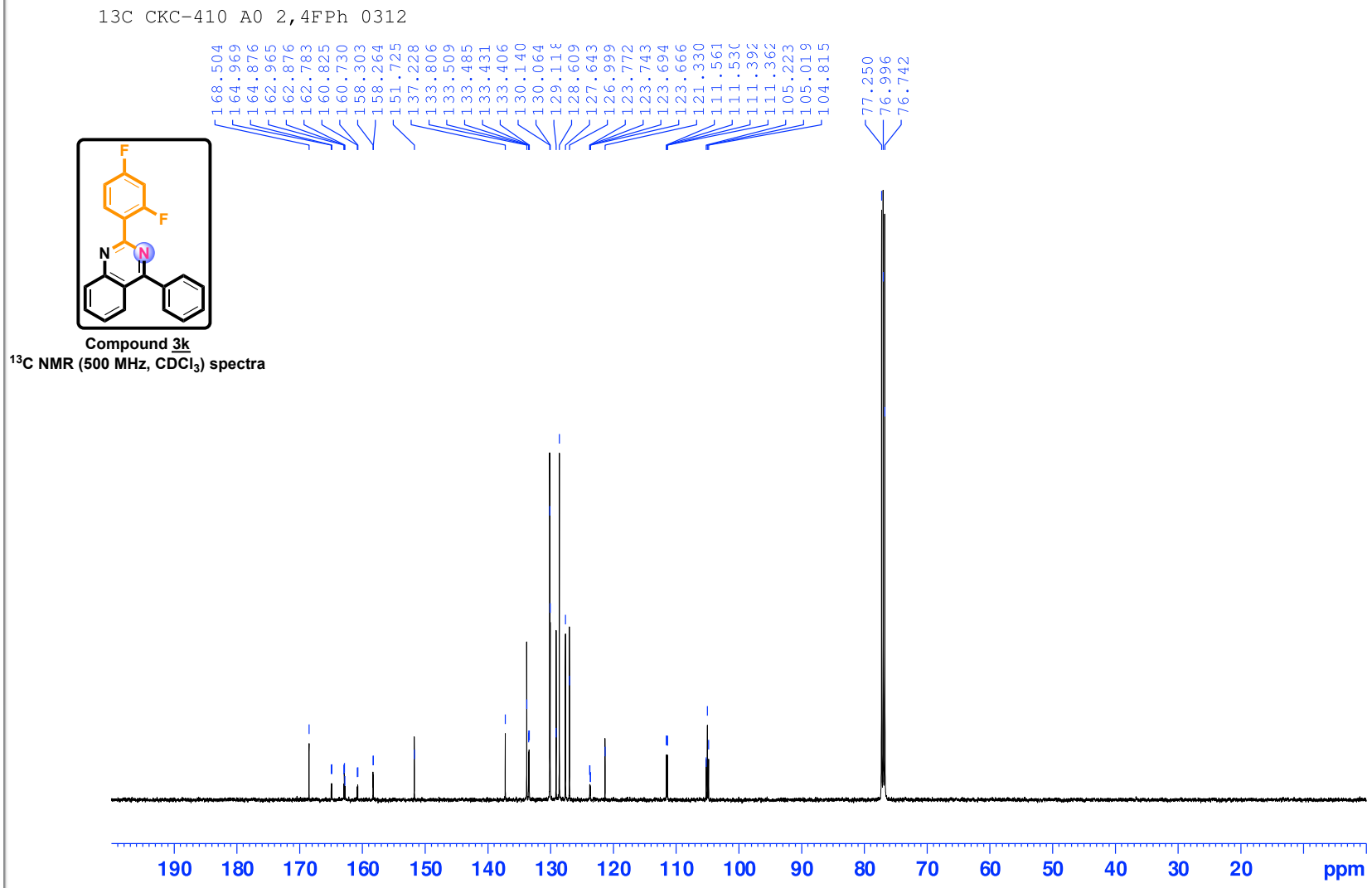
Compound 3k



Compound 3k
^{1}H NMR (500 MHz, $CDCl_3$) spectra



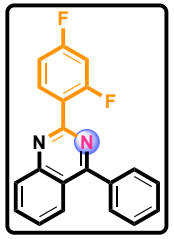
Compound 3k



Compound 3k

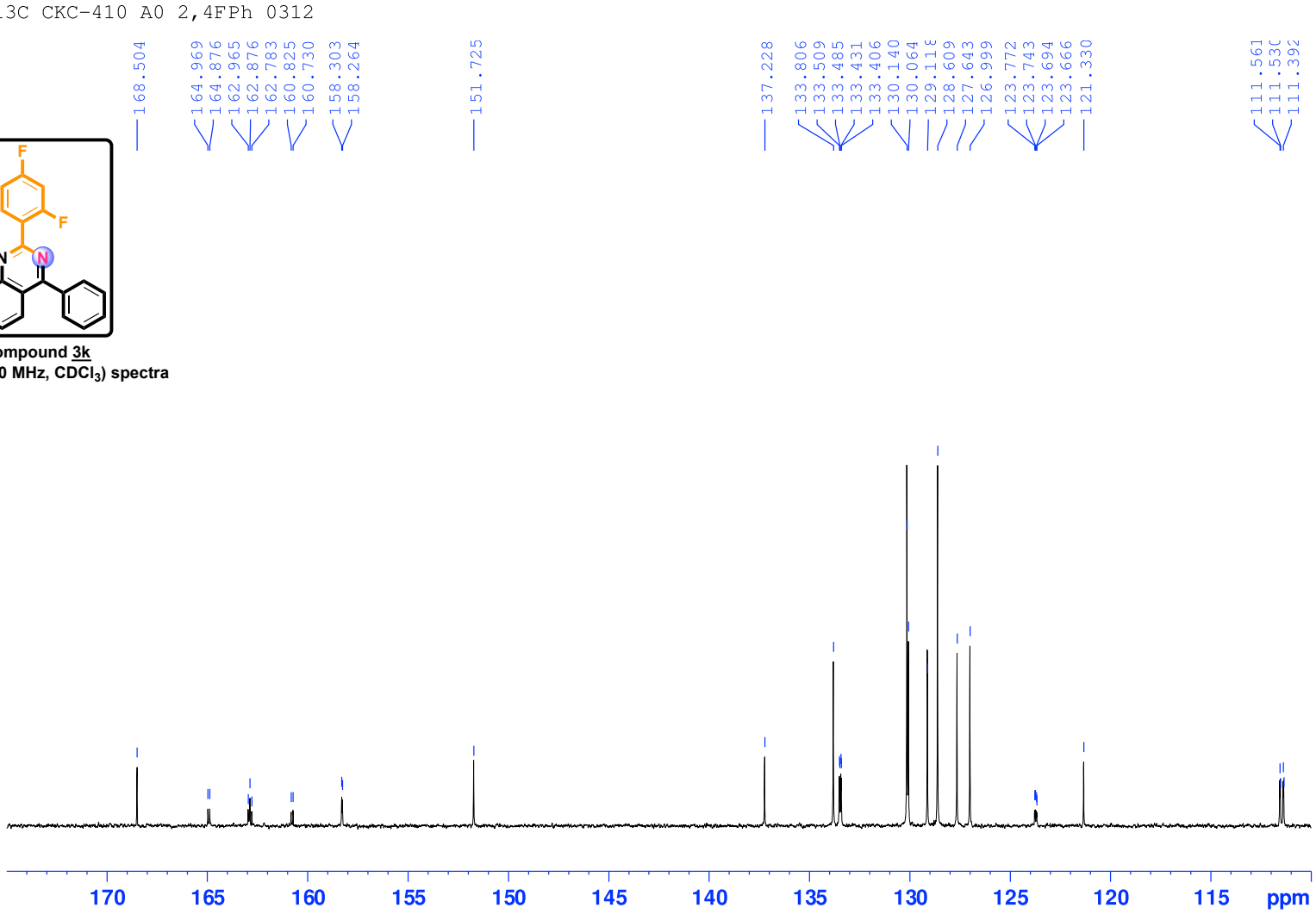
^{13}C NMR (500 MHz, $CDCl_3$) spectra

Compound 3k

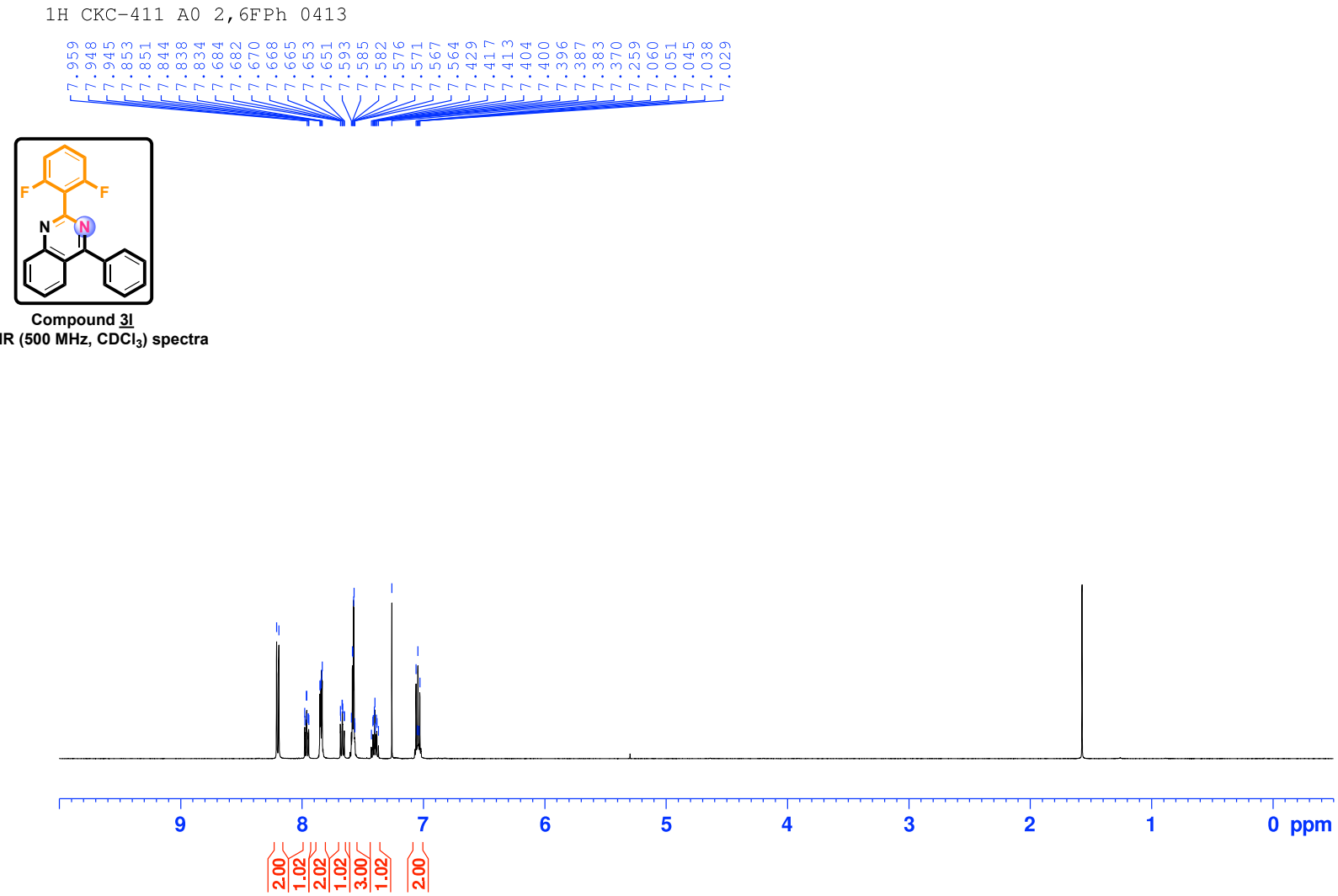


Compound 3k

^{13}C NMR (500 MHz, $CDCl_3$) spectra

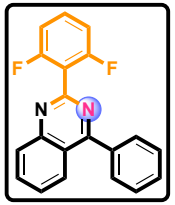


Compound 3l

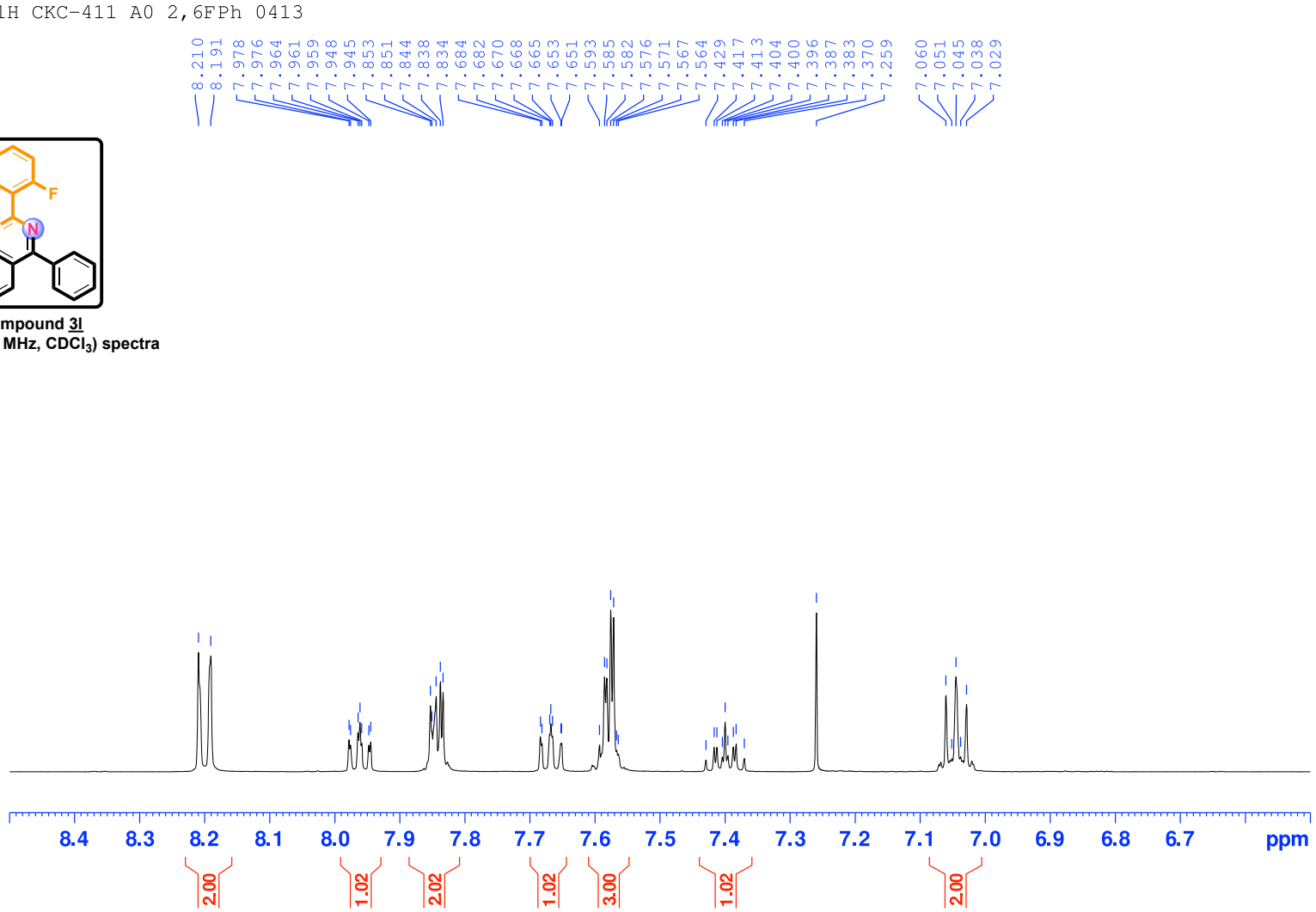


Compound 3l
^{1}H NMR (500 MHz, $CDCl_3$) spectra

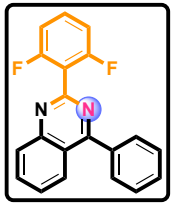
Compound 3l



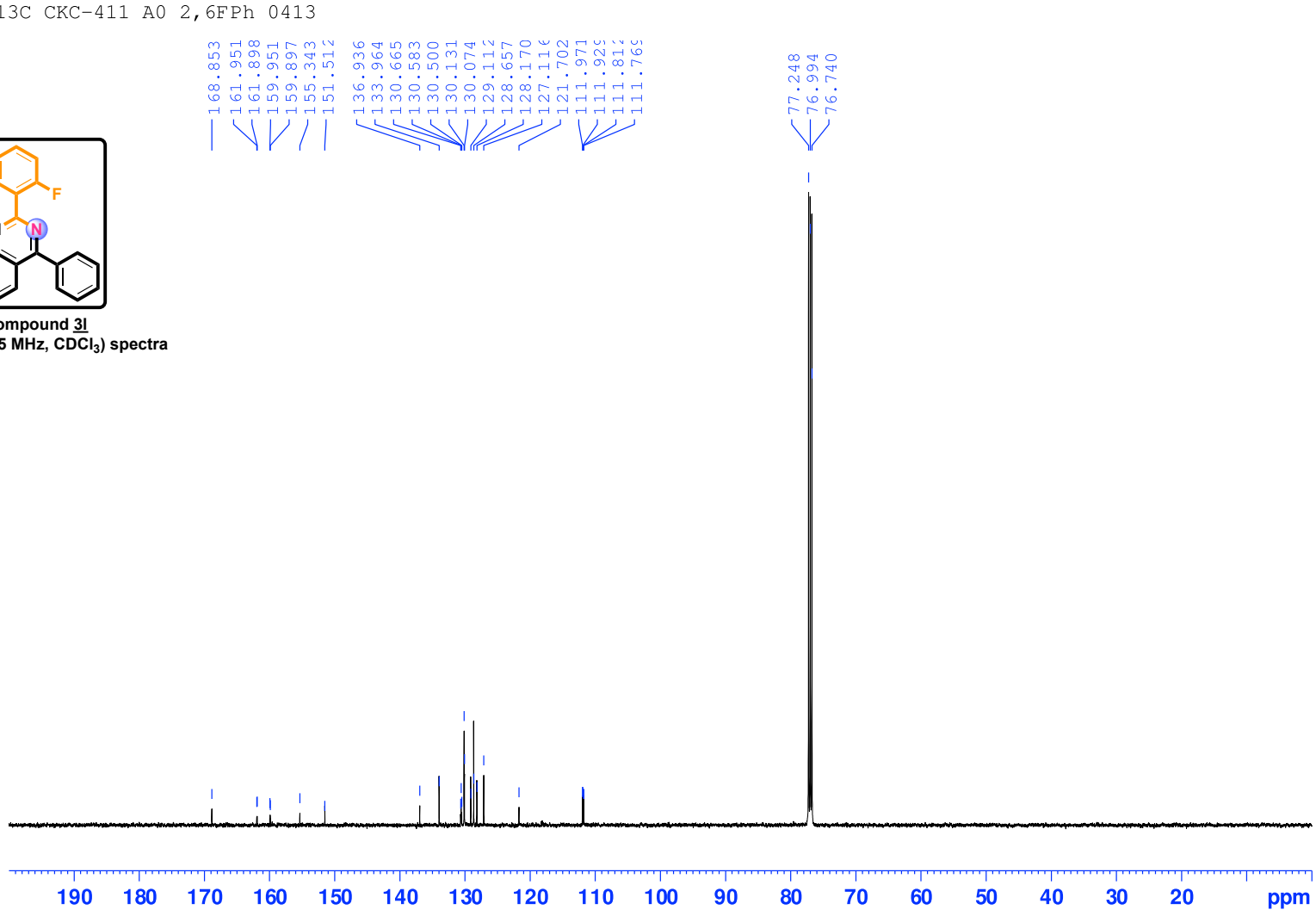
Compound 3l
^{1}H NMR (500 MHz, $CDCl_3$) spectra



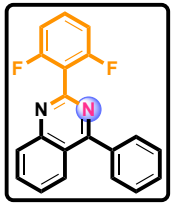
Compound 3l



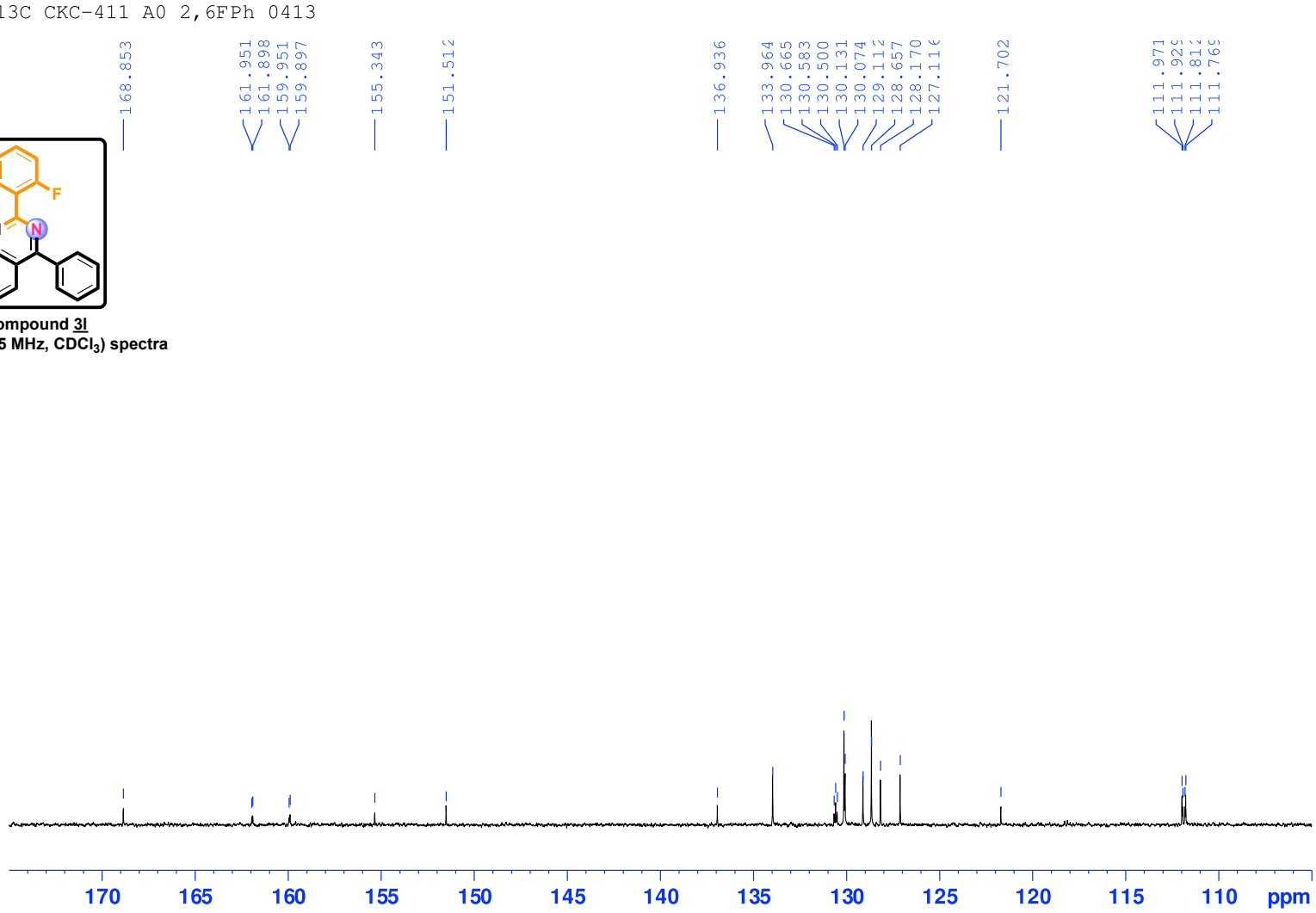
Compound 3l
^{13}C NMR (125 MHz, $CDCl_3$) spectra



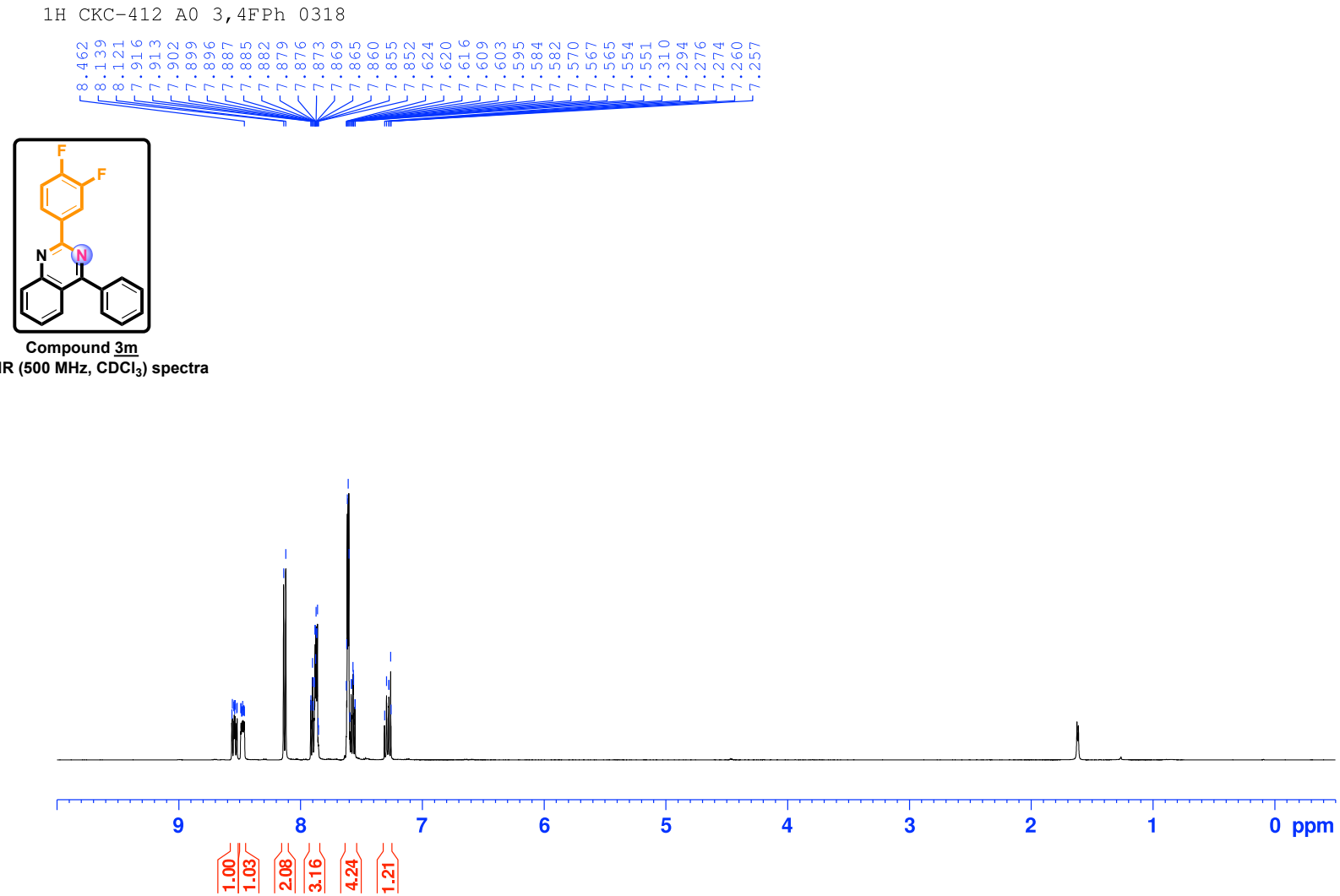
Compound 3l



Compound 3l
^{13}C NMR (125 MHz, $CDCl_3$) spectra



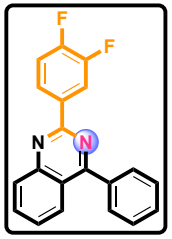
Compound 3m



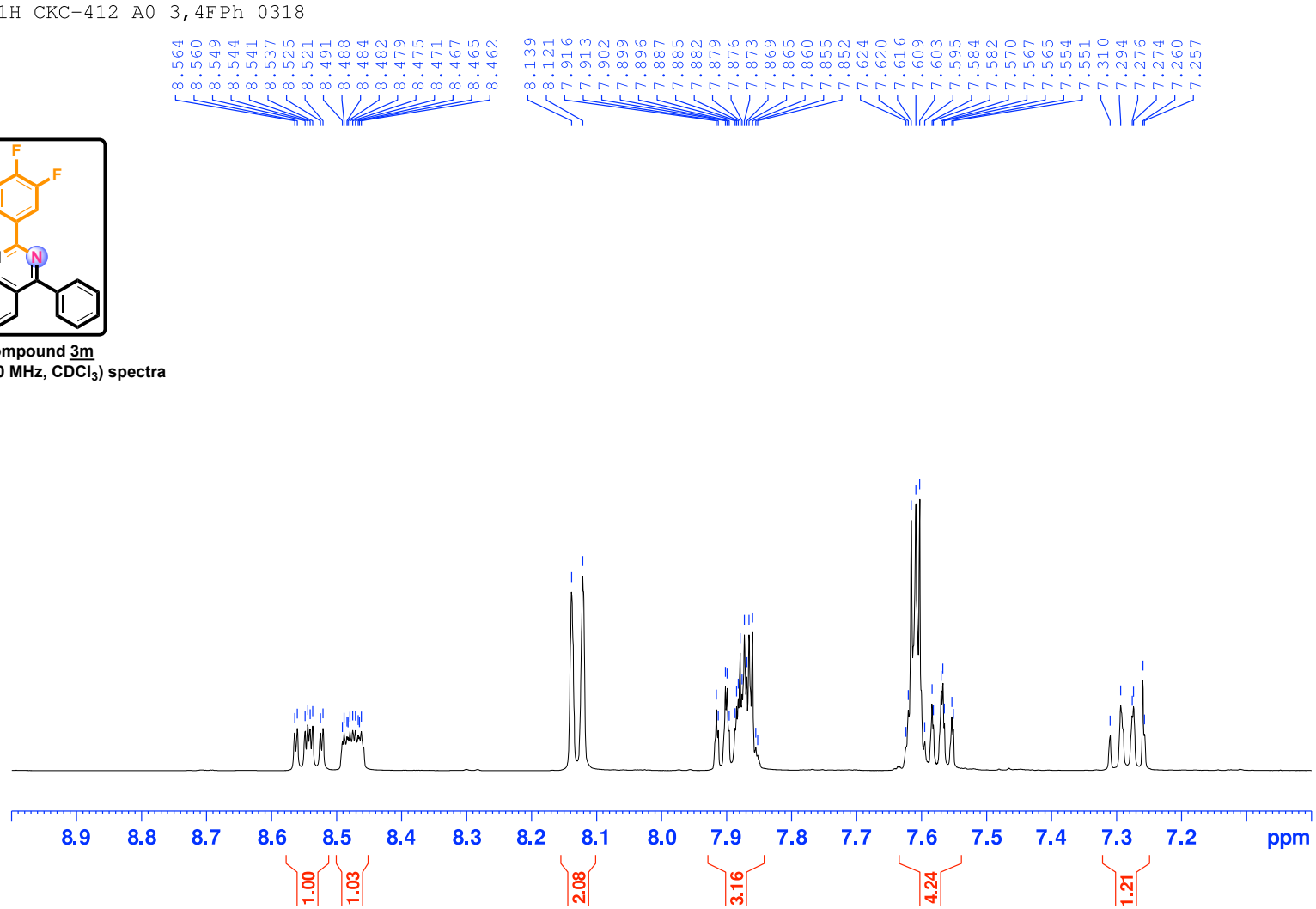
Compound 3m

^{1}H NMR (500 MHz, $CDCl_3$) spectra

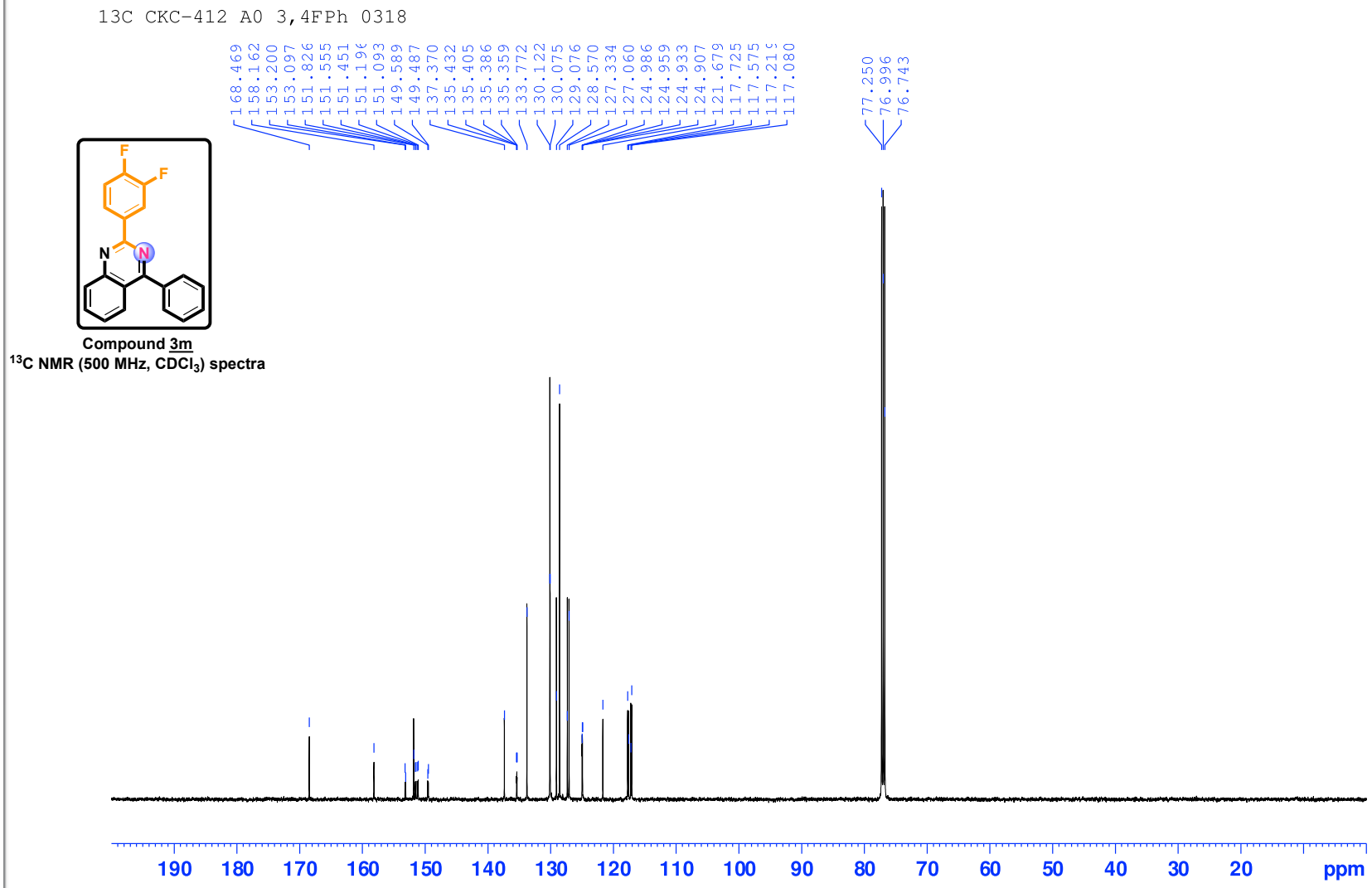
Compound 3m



Compound 3m
^{1}H NMR (500 MHz, $CDCl_3$) spectra



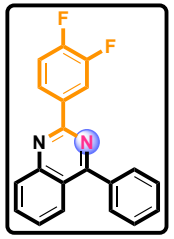
Compound 3m



Compound 3m

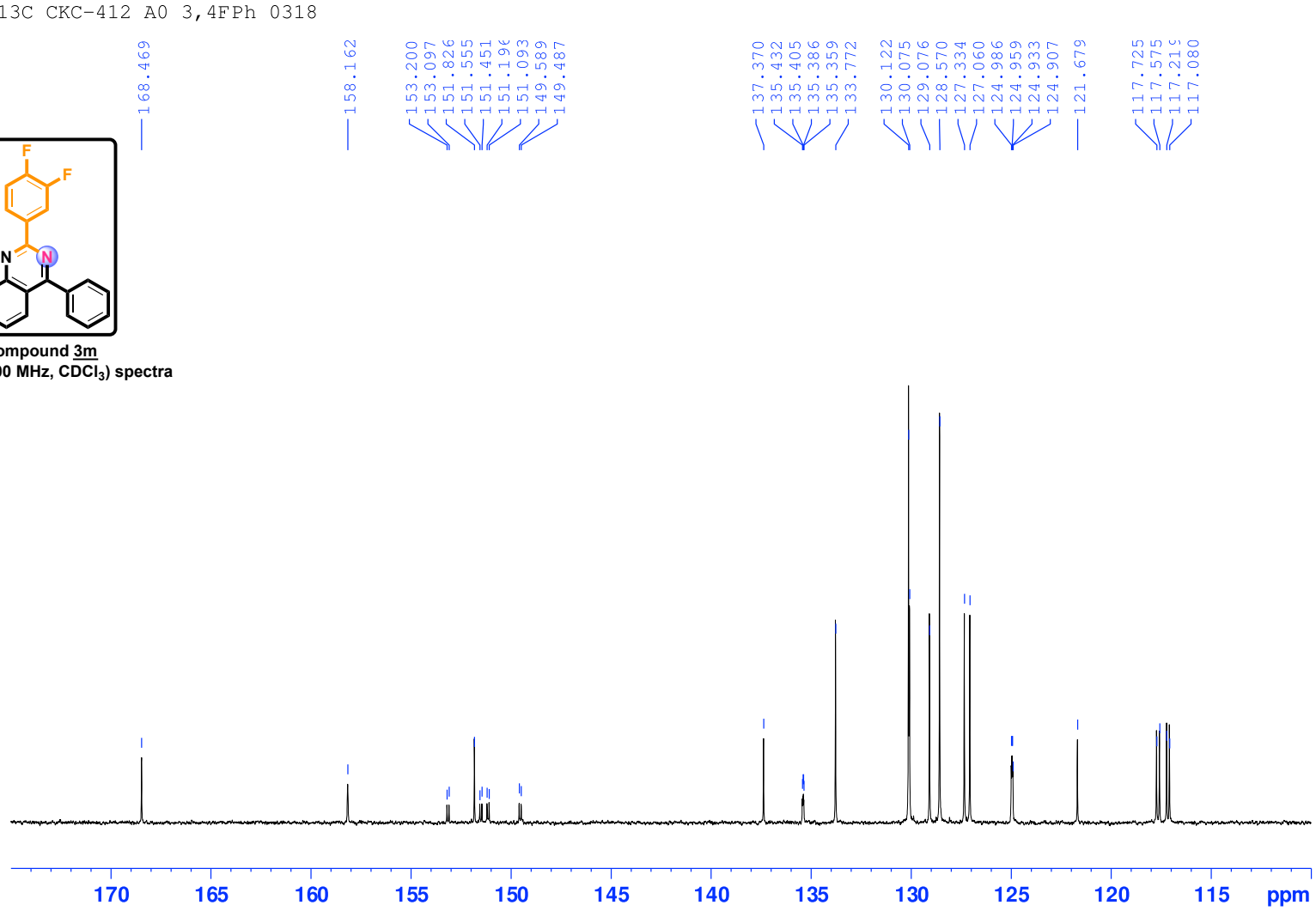
^{13}C NMR (500 MHz, $CDCl_3$) spectra

Compound 3m

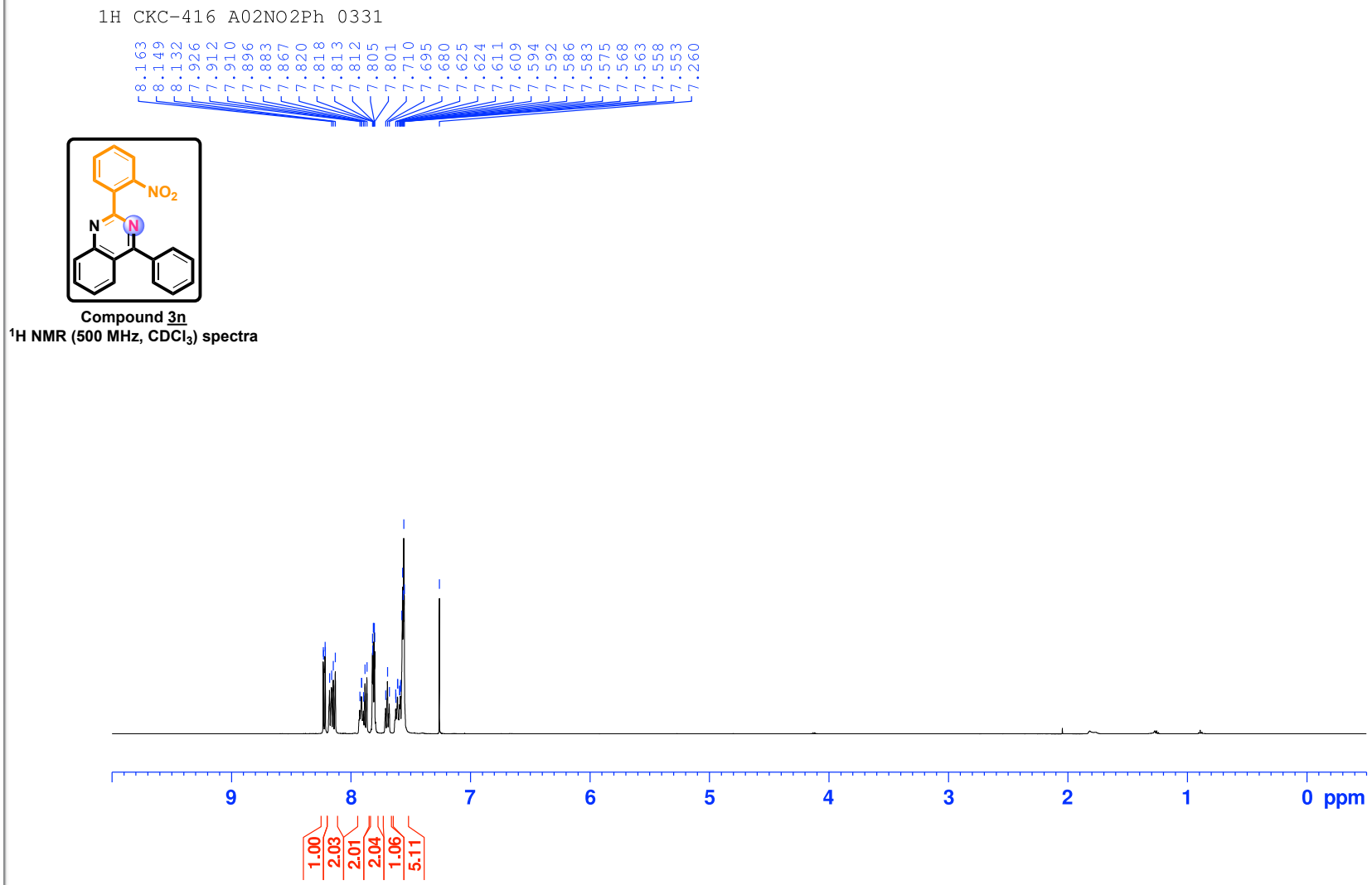


Compound 3m

^{13}C NMR (500 MHz, $CDCl_3$) spectra

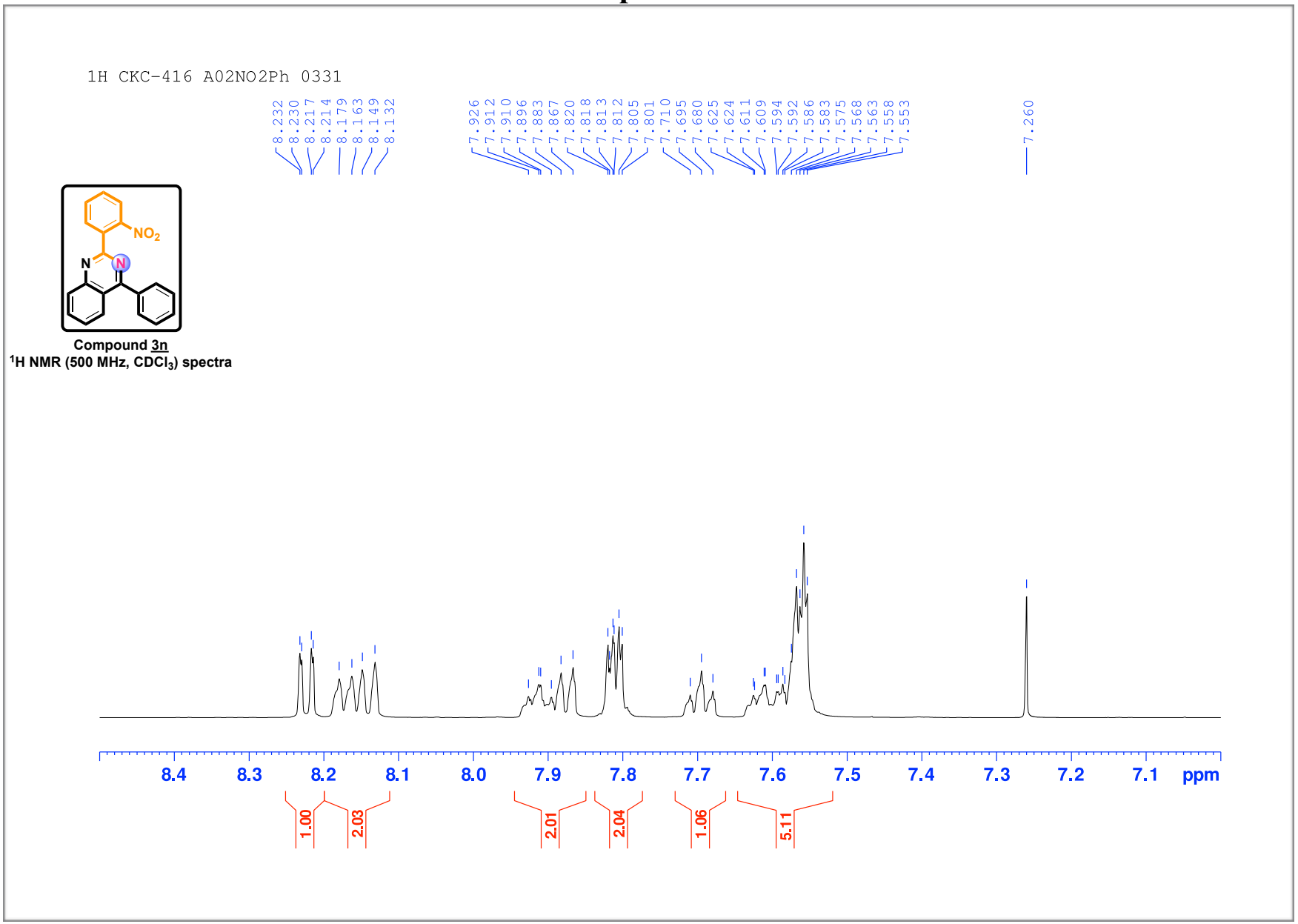


Compound 3n



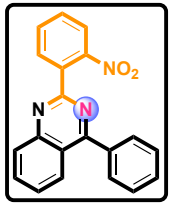
Compound 3n
^{1}H NMR (500 MHz, $CDCl_3$) spectra

Compound 3n

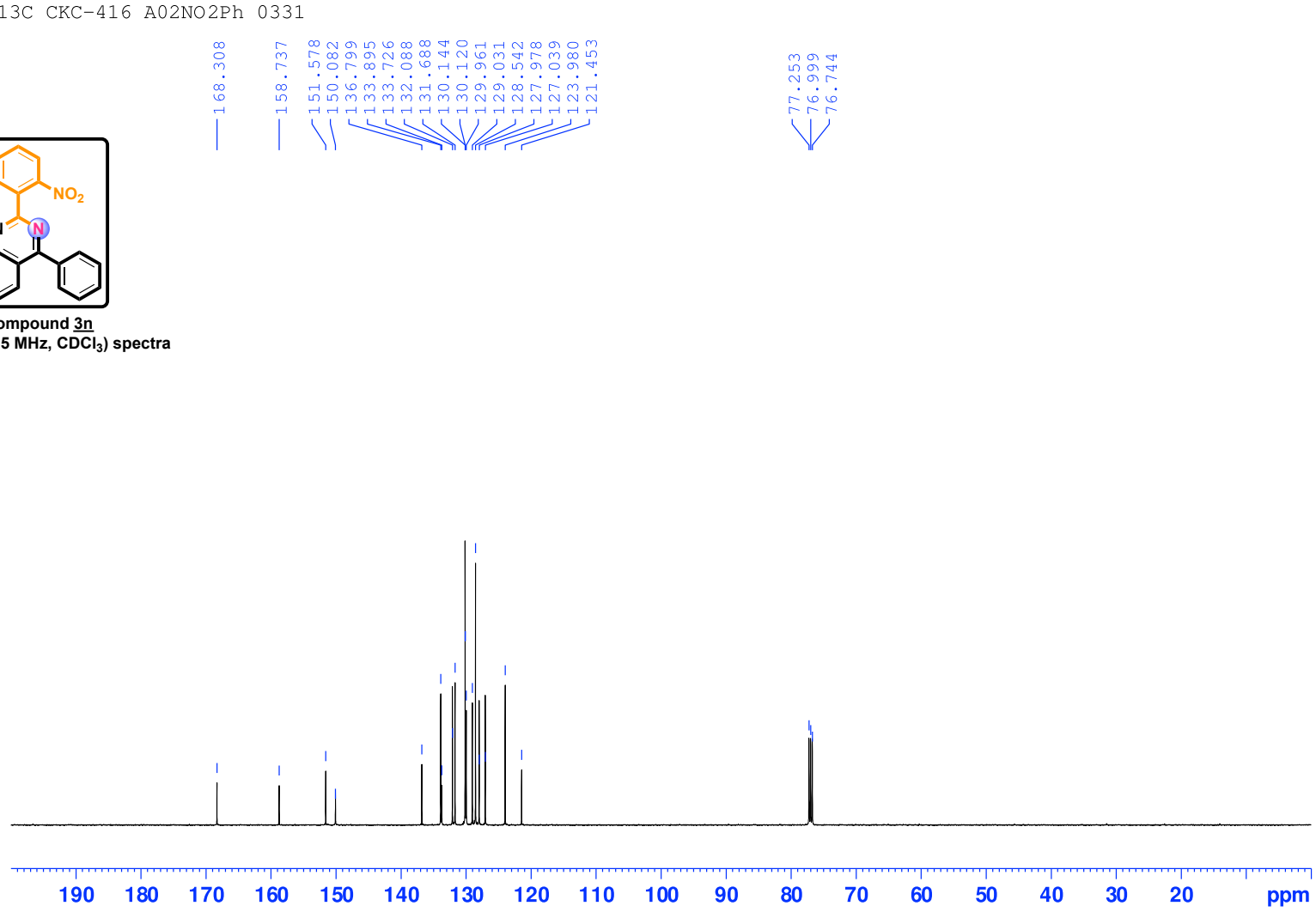


Compound 3n
^{1}H NMR (500 MHz, $CDCl_3$) spectra

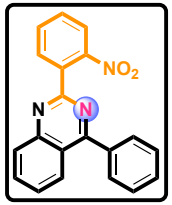
Compound 3n



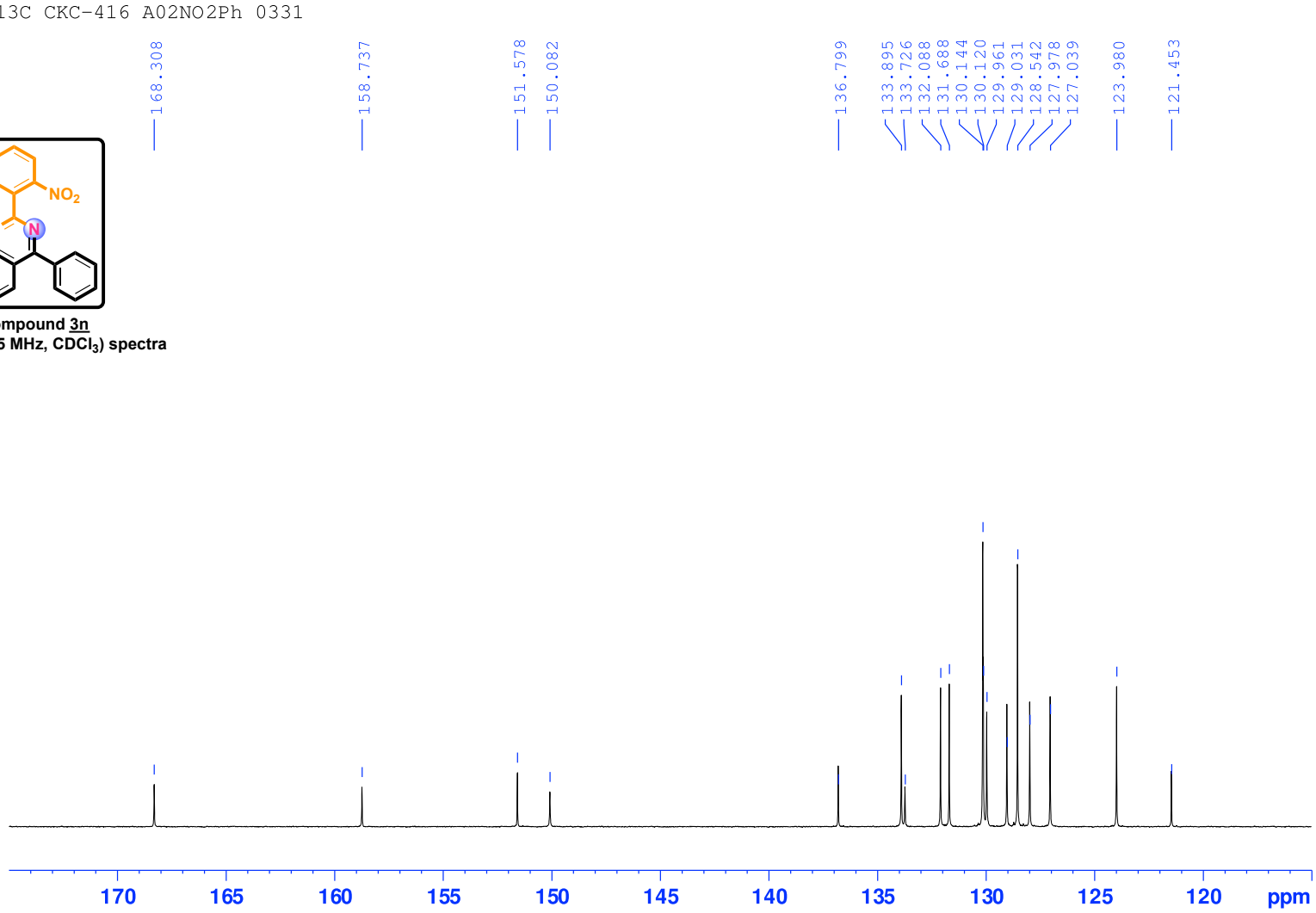
Compound 3n
^{13}C NMR (125 MHz, $CDCl_3$) spectra



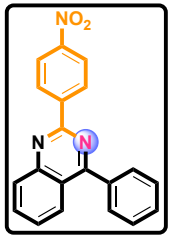
Compound 3n



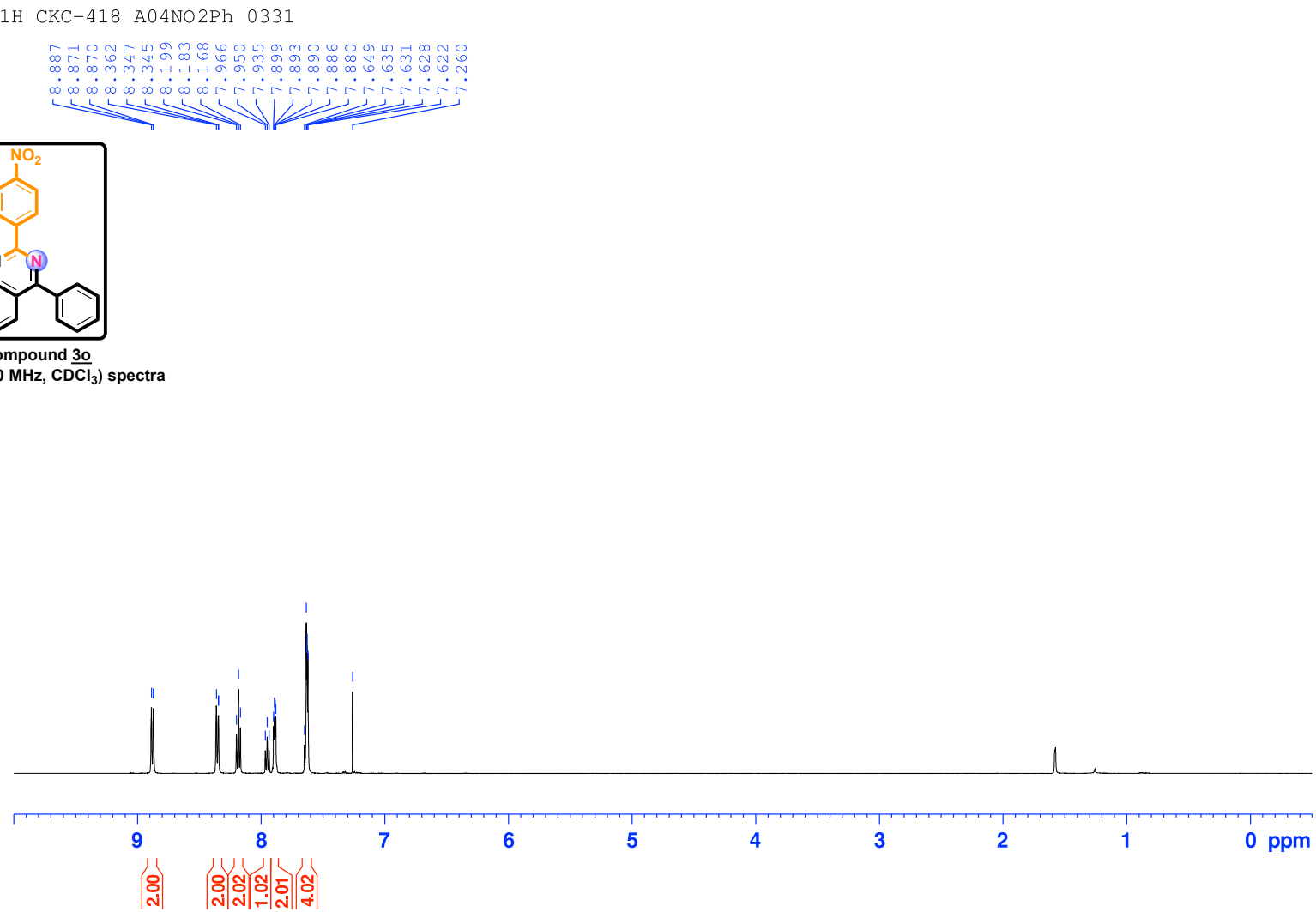
Compound 3n
^{13}C NMR (125 MHz, $CDCl_3$) spectra



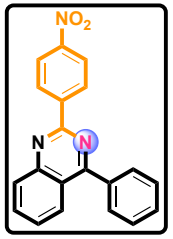
Compound 3o



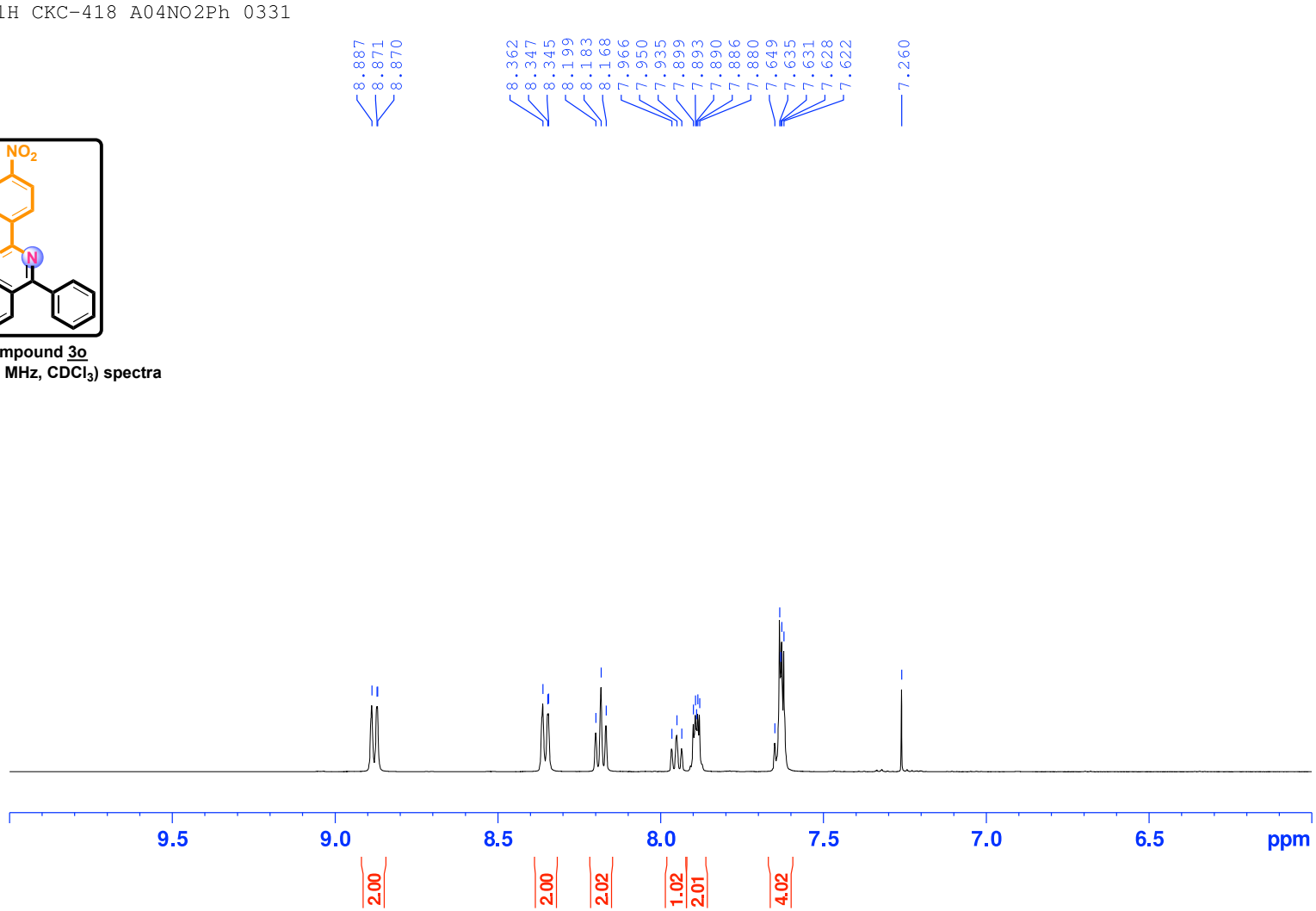
Compound 3o
^{1}H NMR (500 MHz, $CDCl_3$) spectra



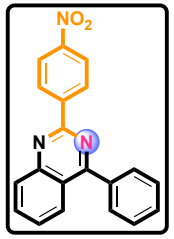
Compound 3o



Compound 3o
^{1}H NMR (500 MHz, $CDCl_3$) spectra

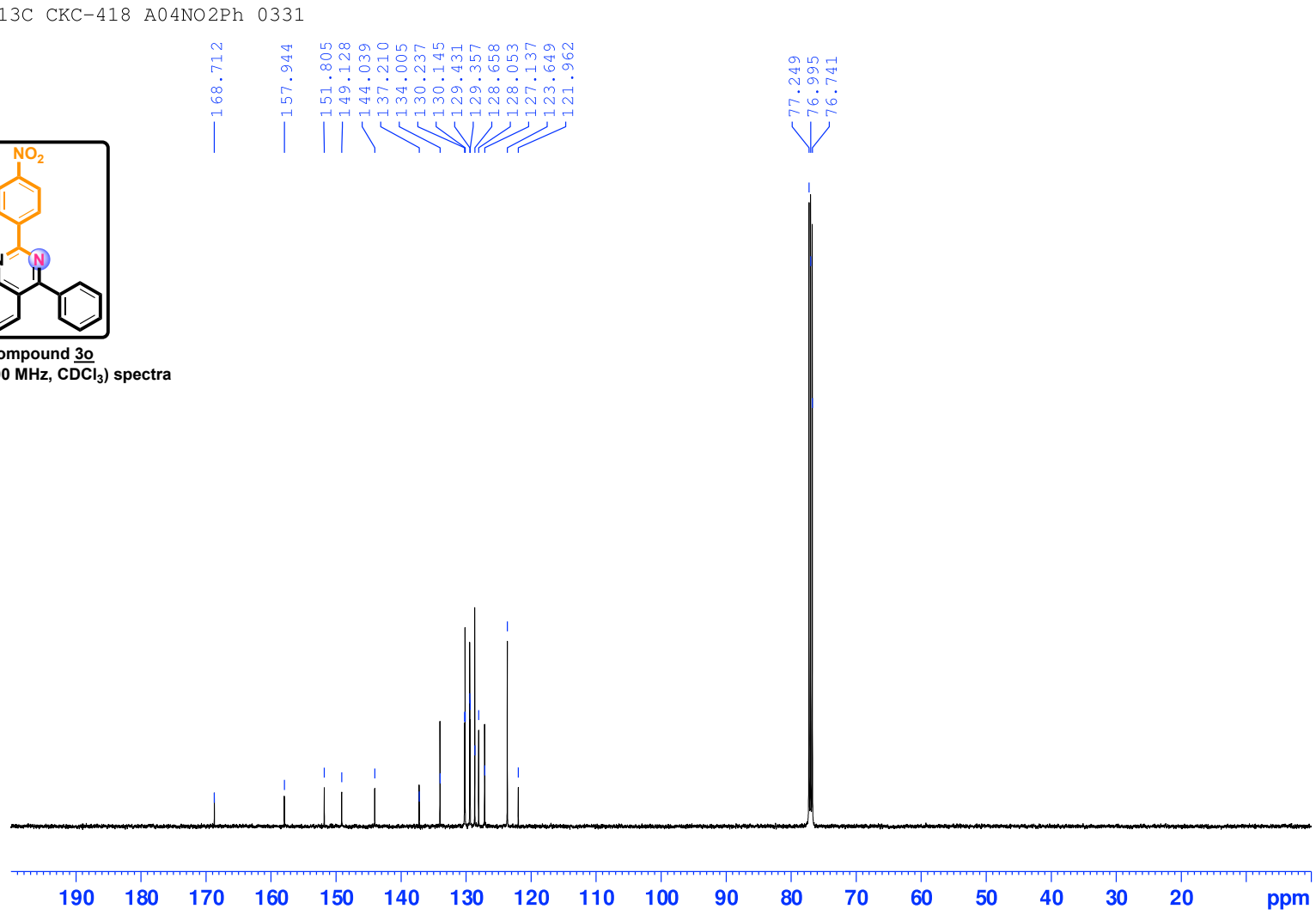


Compound 3o

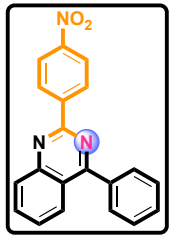


Compound 3o

^{13}C NMR (500 MHz, $CDCl_3$) spectra

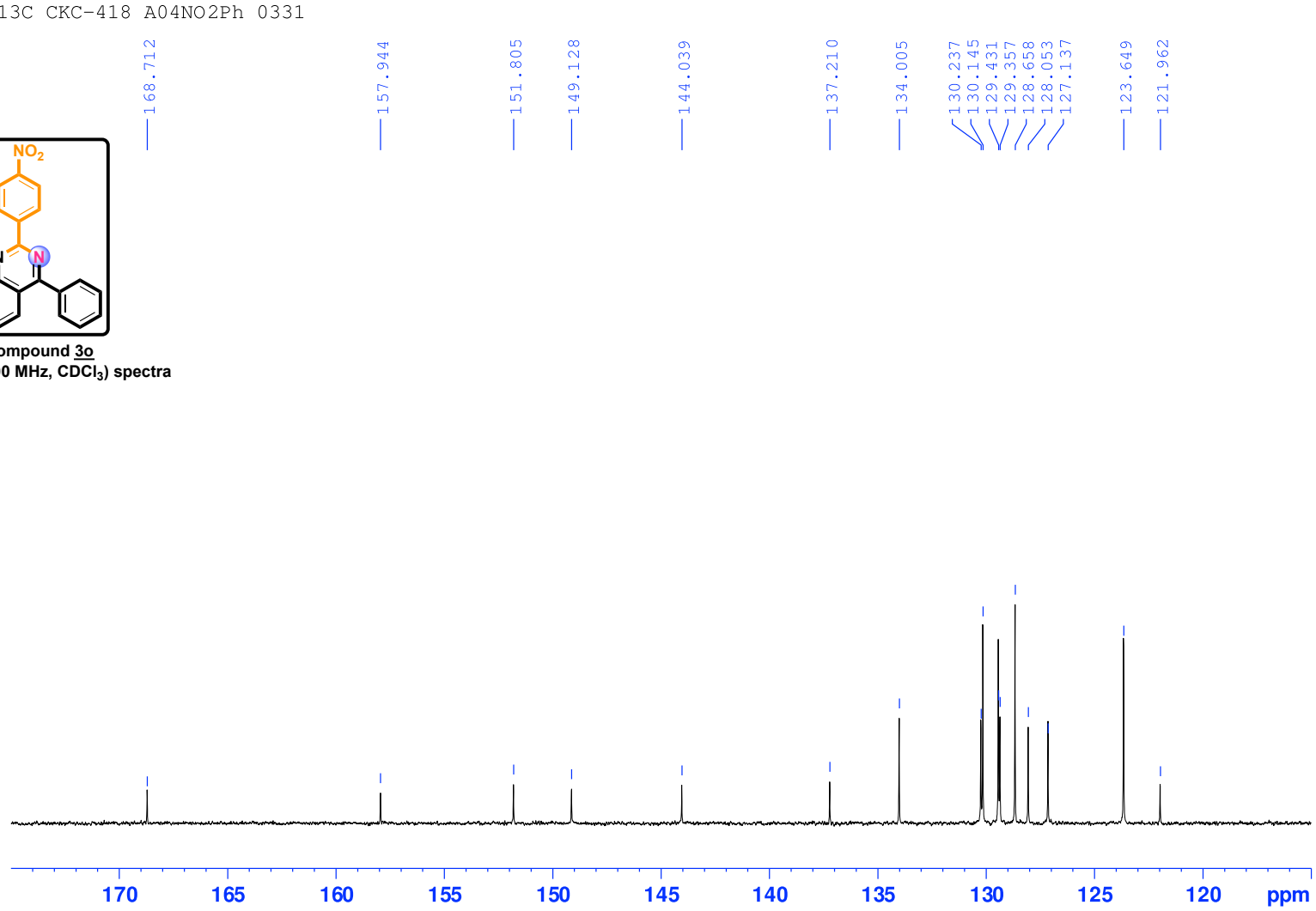


Compound 3o

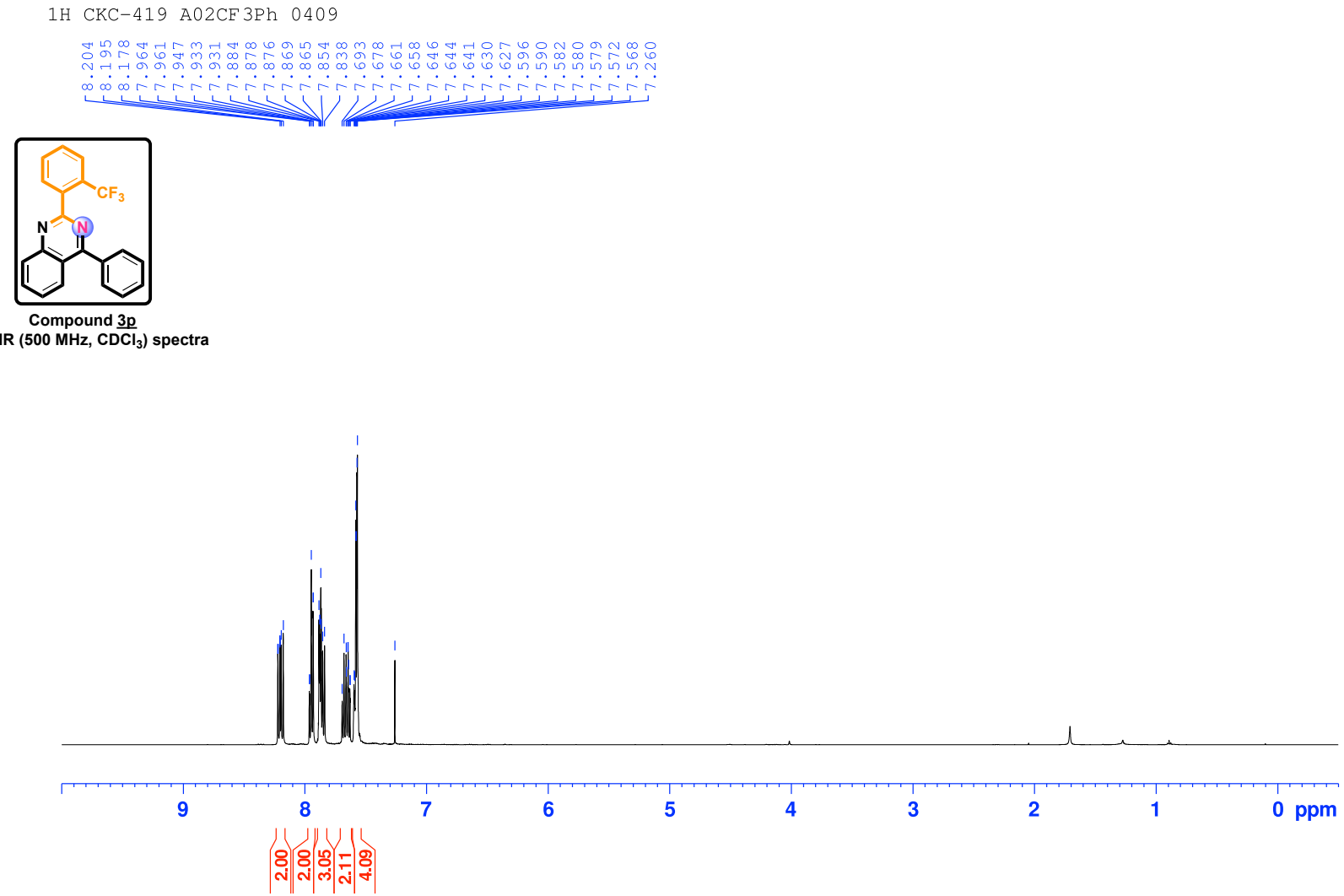


Compound 3o

^{13}C NMR (500 MHz, $CDCl_3$) spectra

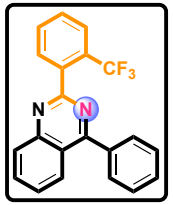


Compound 3p

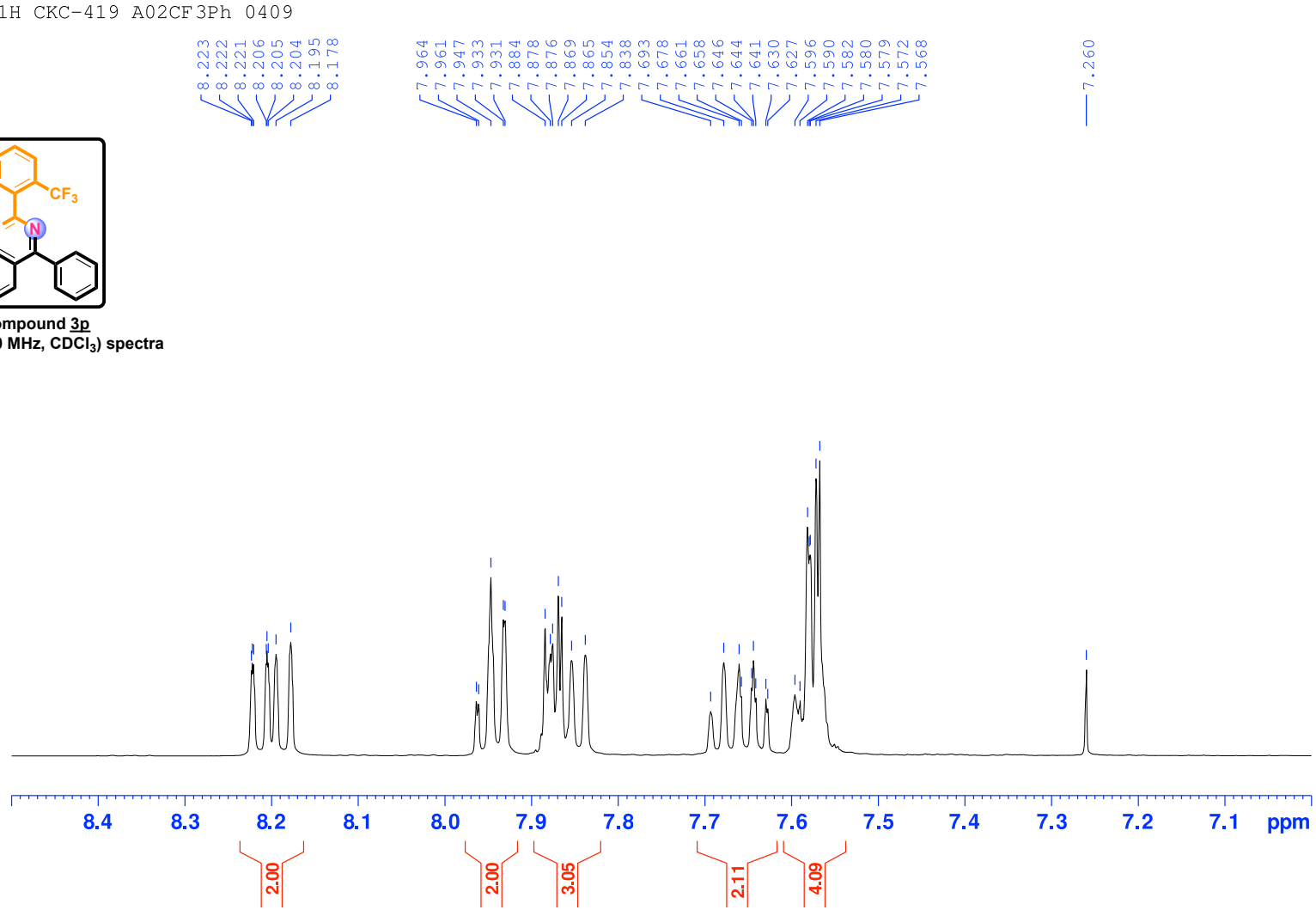


Compound 3p
^{1}H NMR (500 MHz, $CDCl_3$) spectra

Compound 3p



Compound 3p
^{1}H NMR (500 MHz, $CDCl_3$) spectra



Compound 3p

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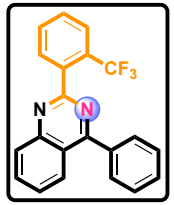
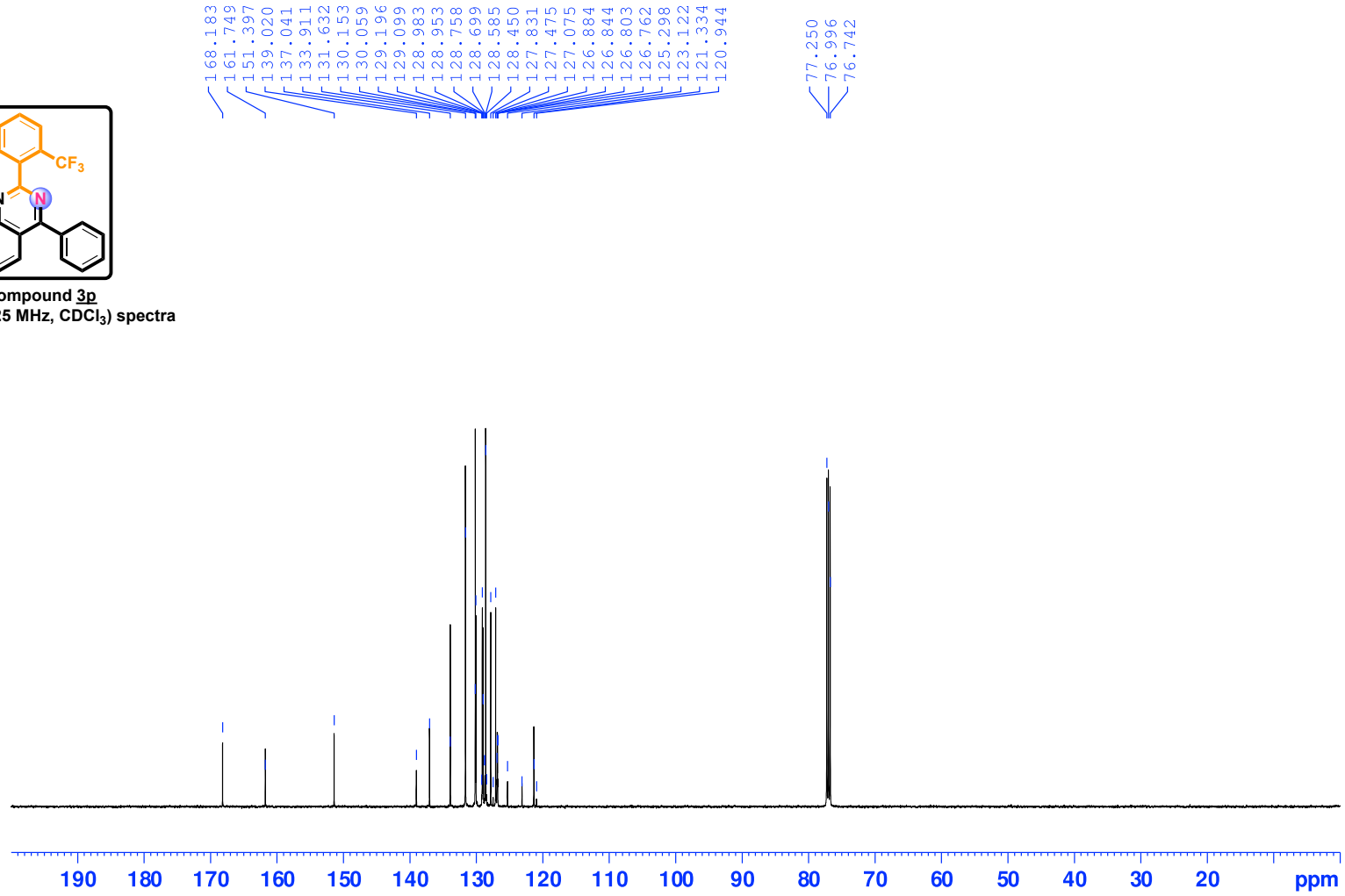
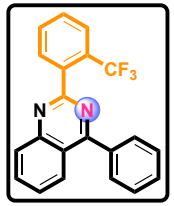


Compound 3p
^{13}C NMR (125 MHz, $CDCl_3$) spectra

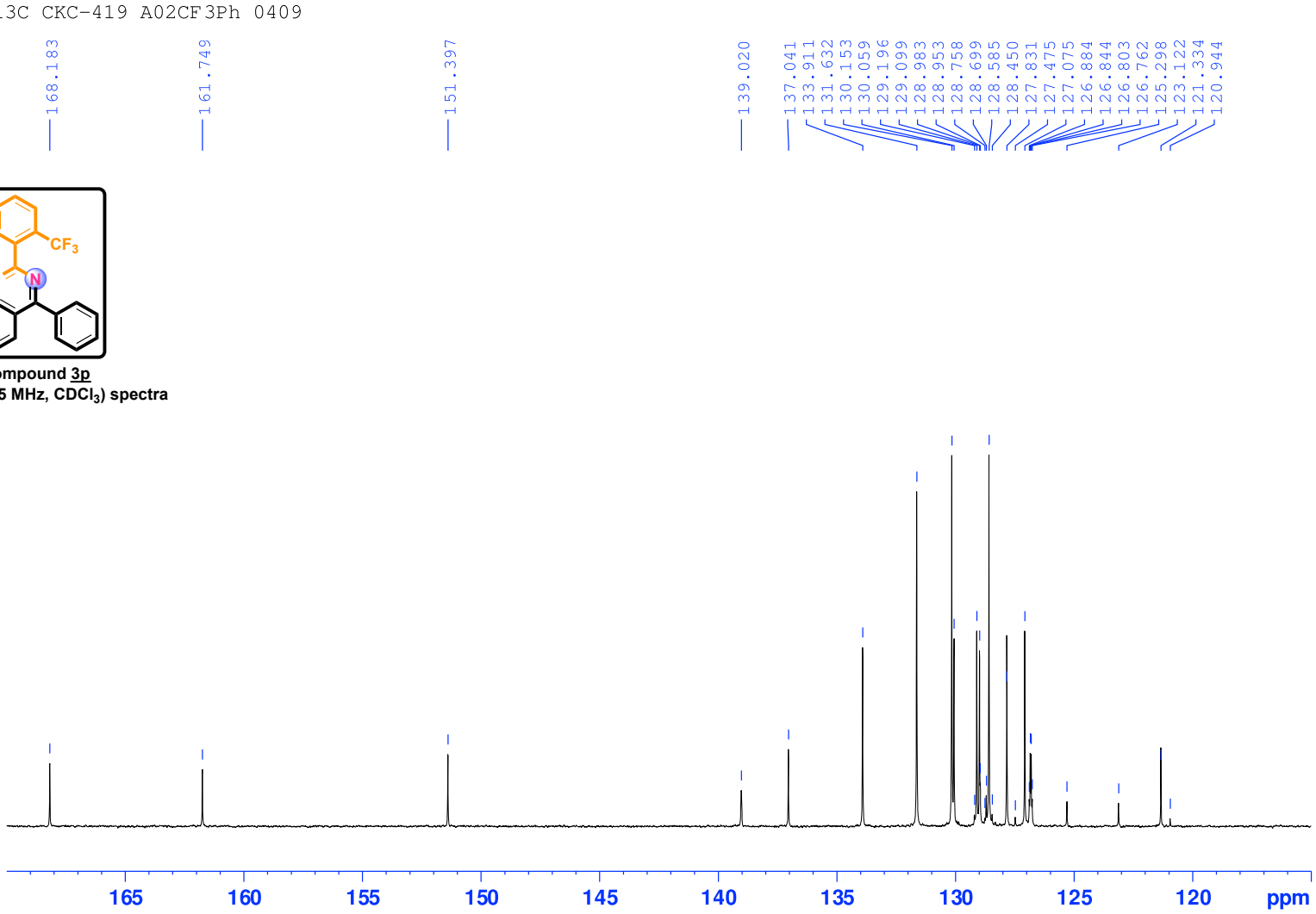


Compound 3p

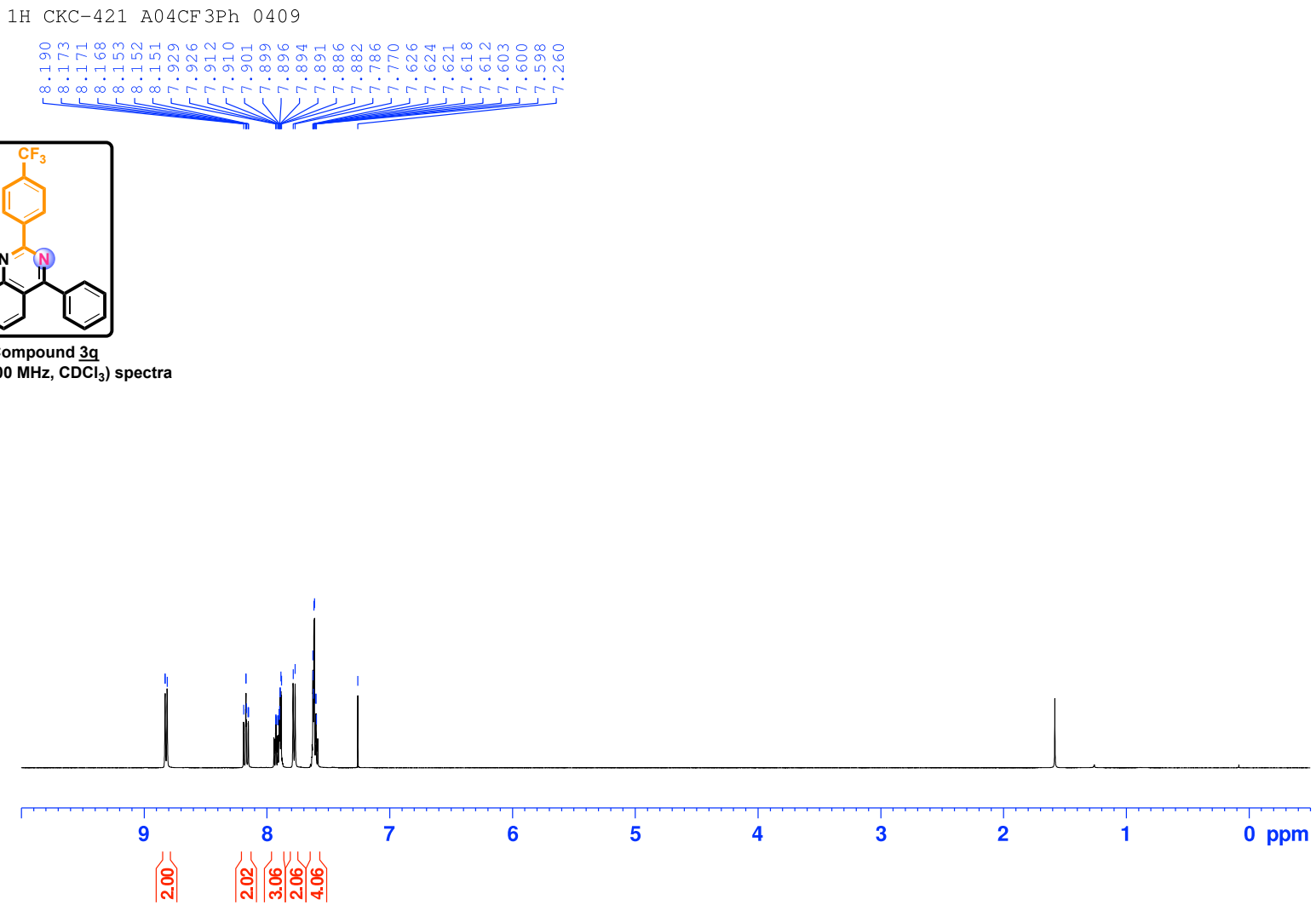


Compound 3p

^{13}C NMR (125 MHz, $CDCl_3$) spectra

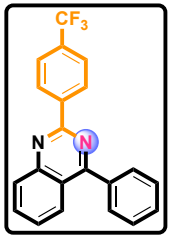


Compound 3q

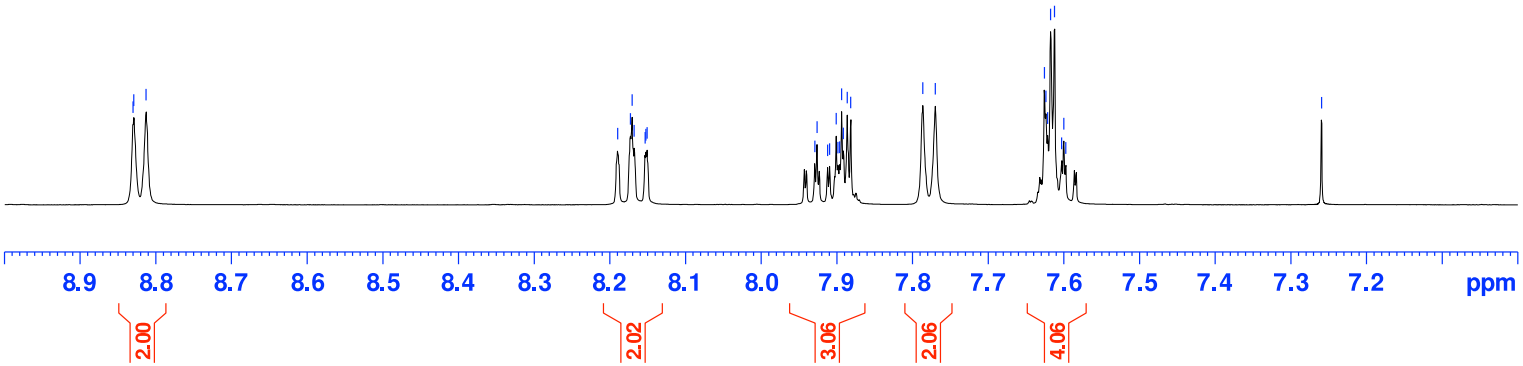


Compound 3q
^{1}H NMR (500 MHz, $CDCl_3$) spectra

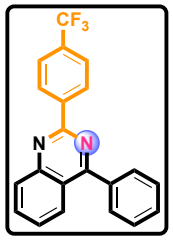
Compound 3q



Compound 3q
^{1}H NMR (500 MHz, $CDCl_3$) spectra

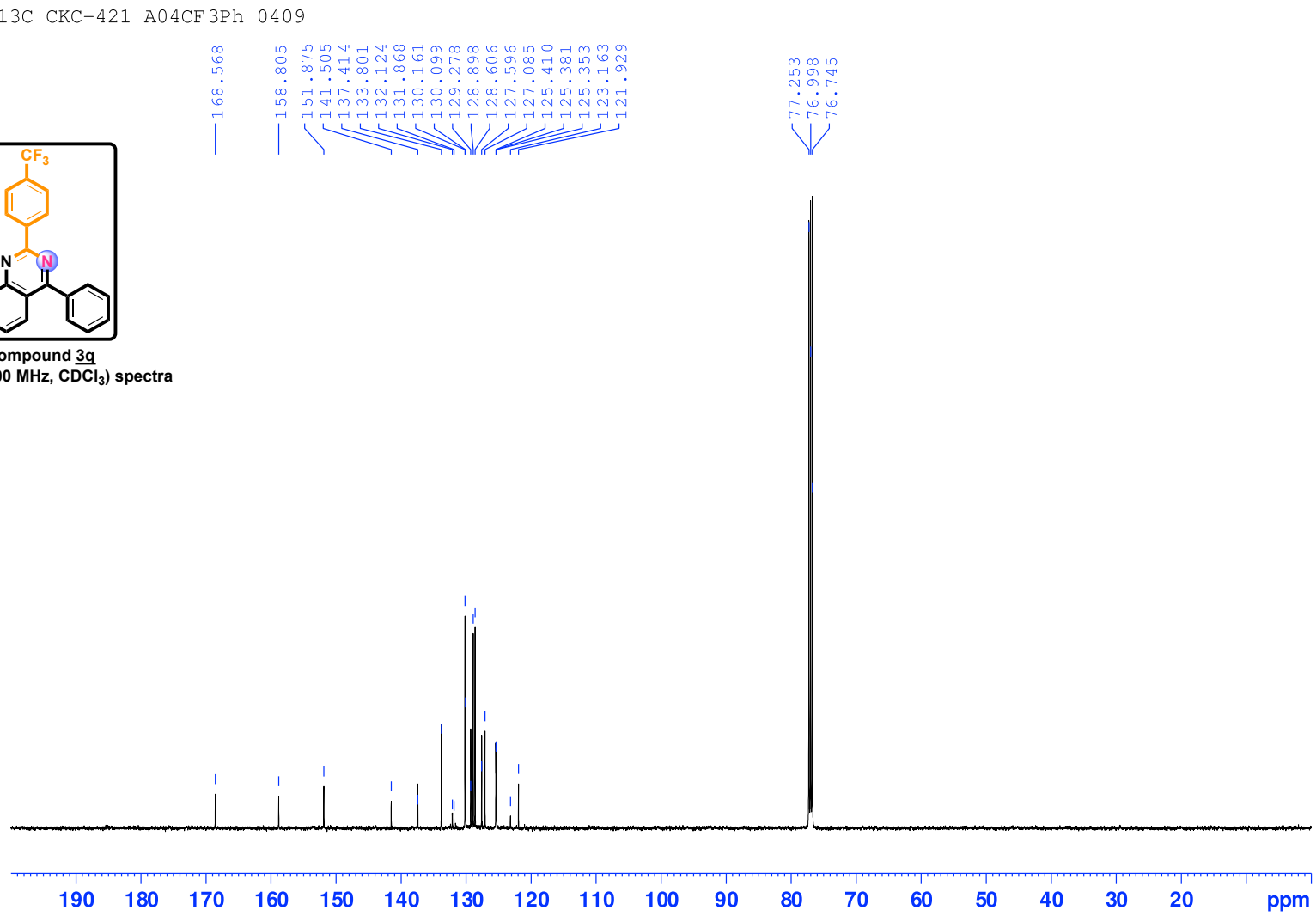


Compound 3q

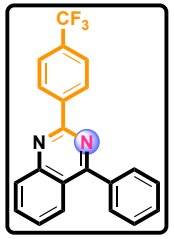


Compound 3q

^{13}C NMR (500 MHz, $CDCl_3$) spectra

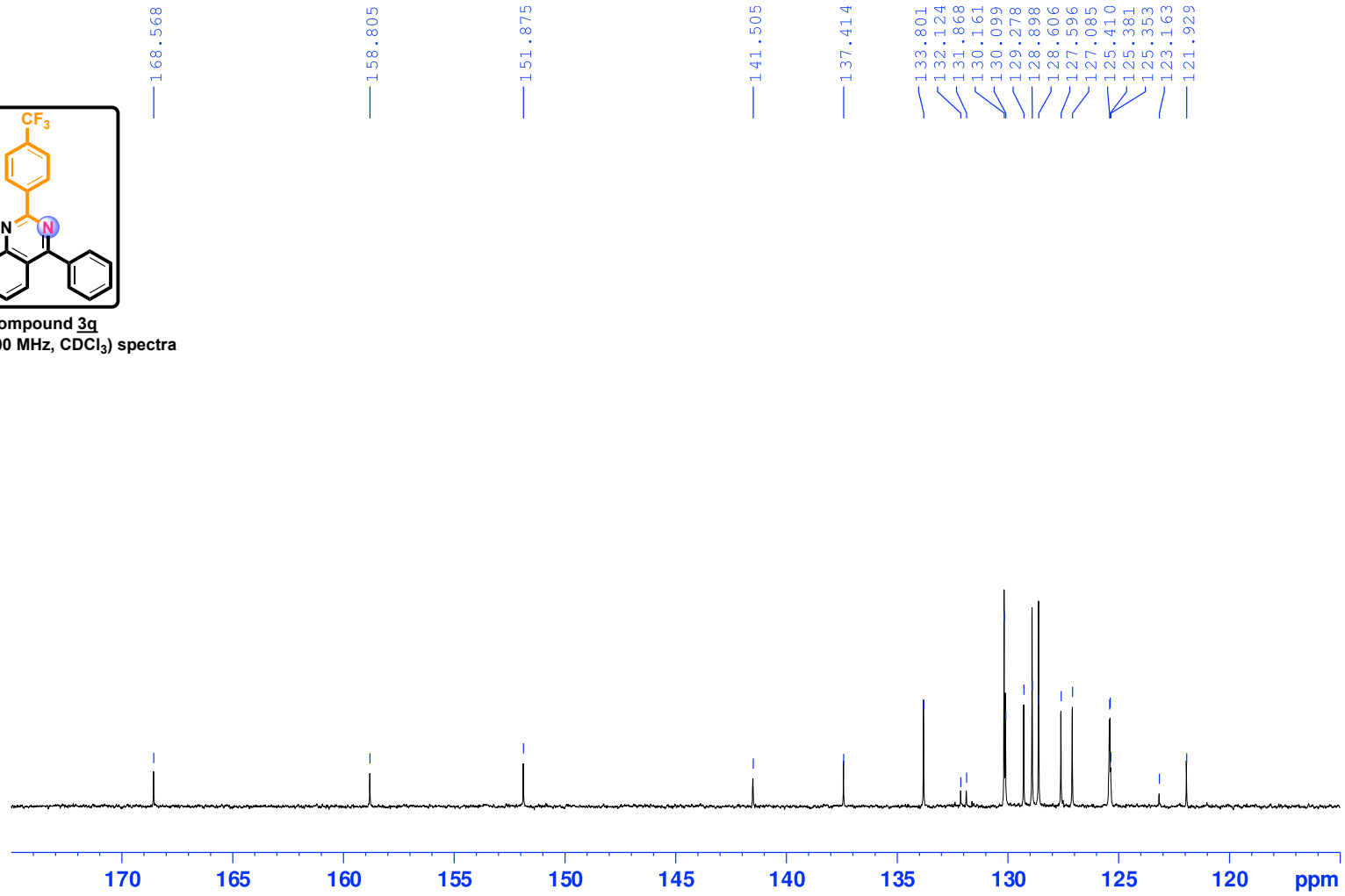


Compound 3q

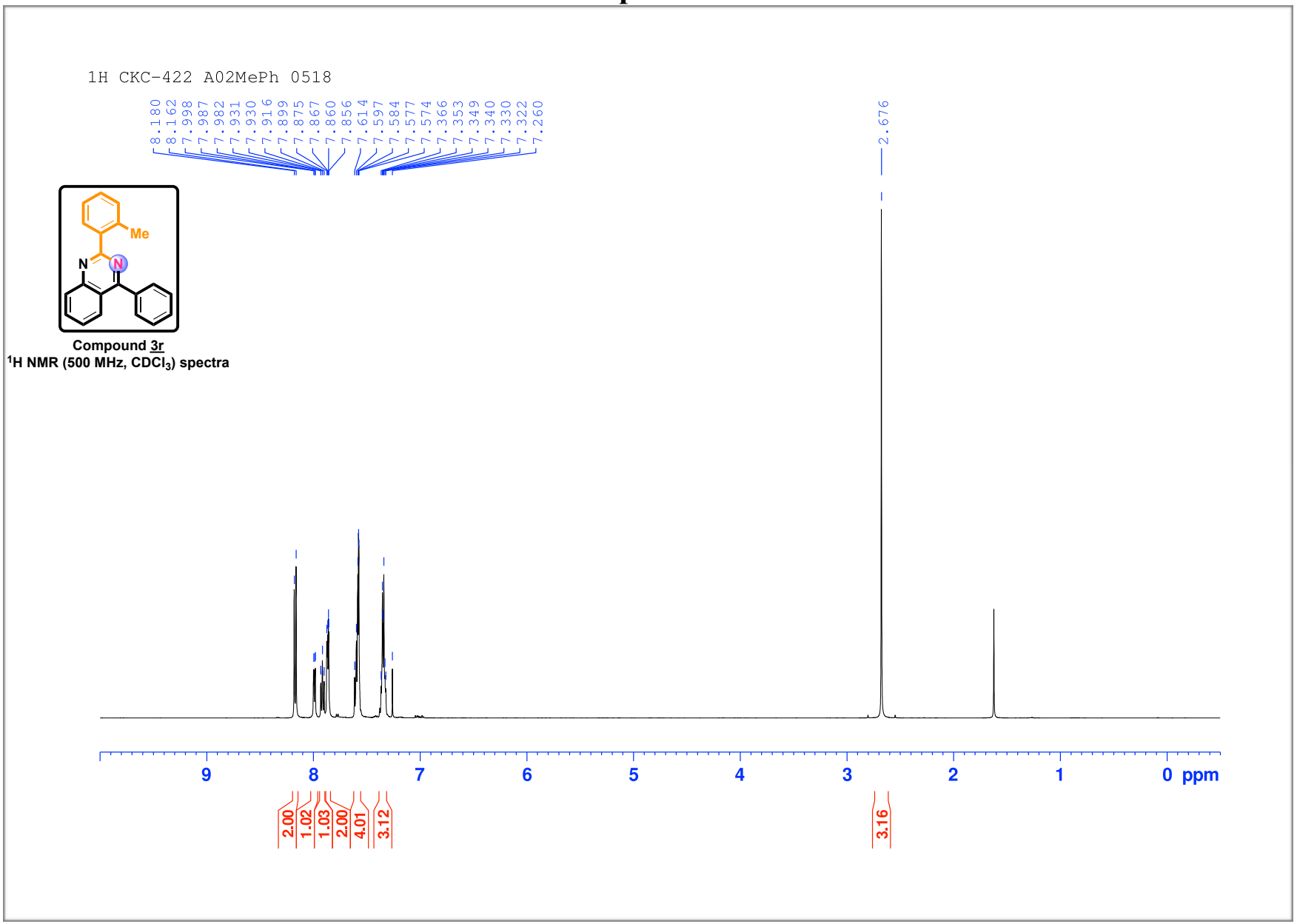


Compound 3q

^{13}C NMR (500 MHz, $CDCl_3$) spectra

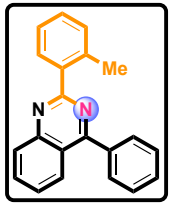


Compound 3r

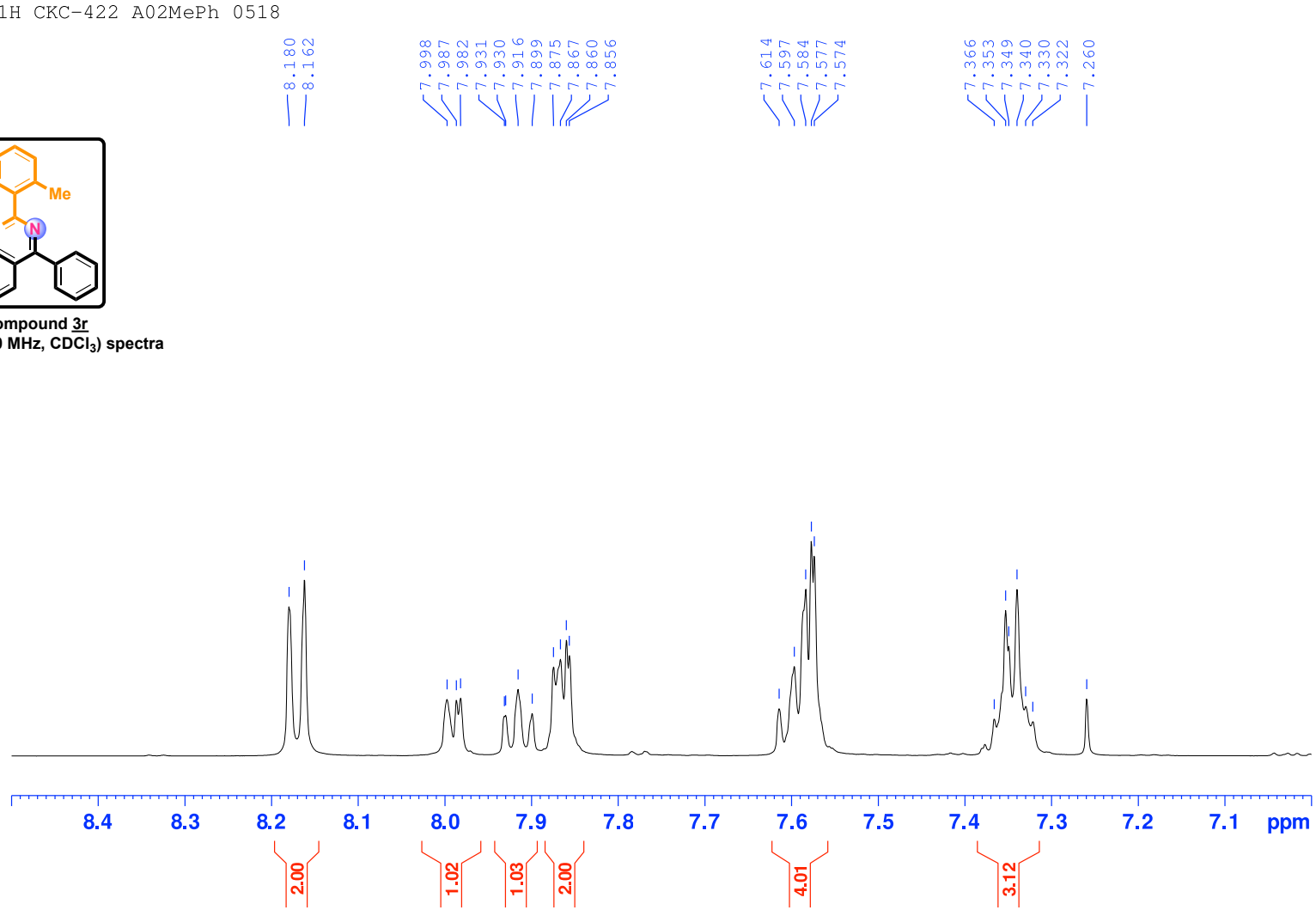


Compound 3r
^{1}H NMR (500 MHz, $CDCl_3$) spectra

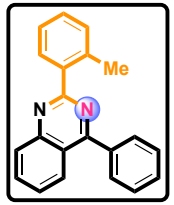
Compound 3r



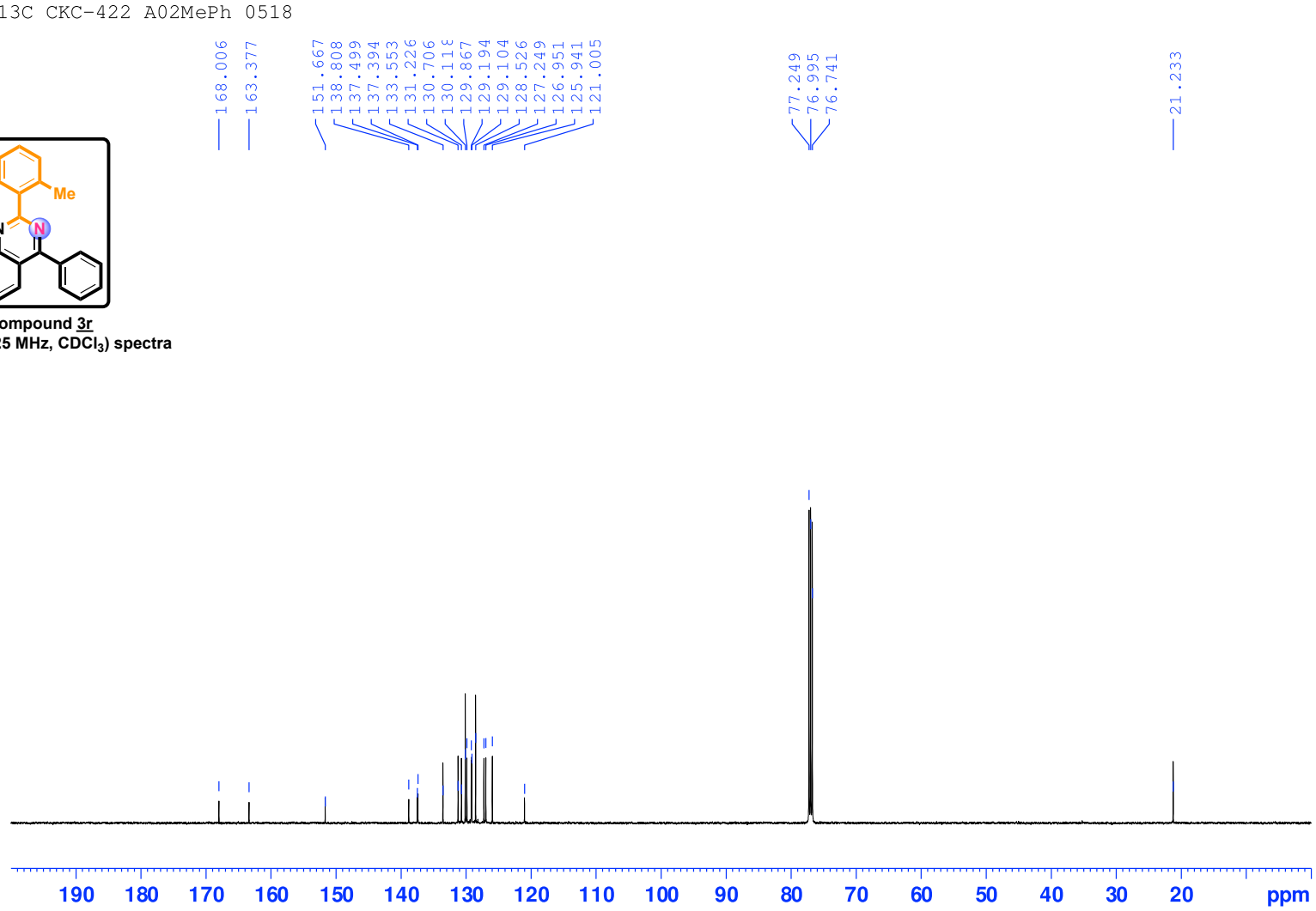
Compound 3r
^{1}H NMR (500 MHz, $CDCl_3$) spectra



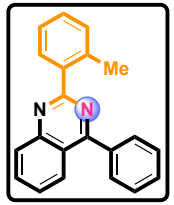
Compound 3r



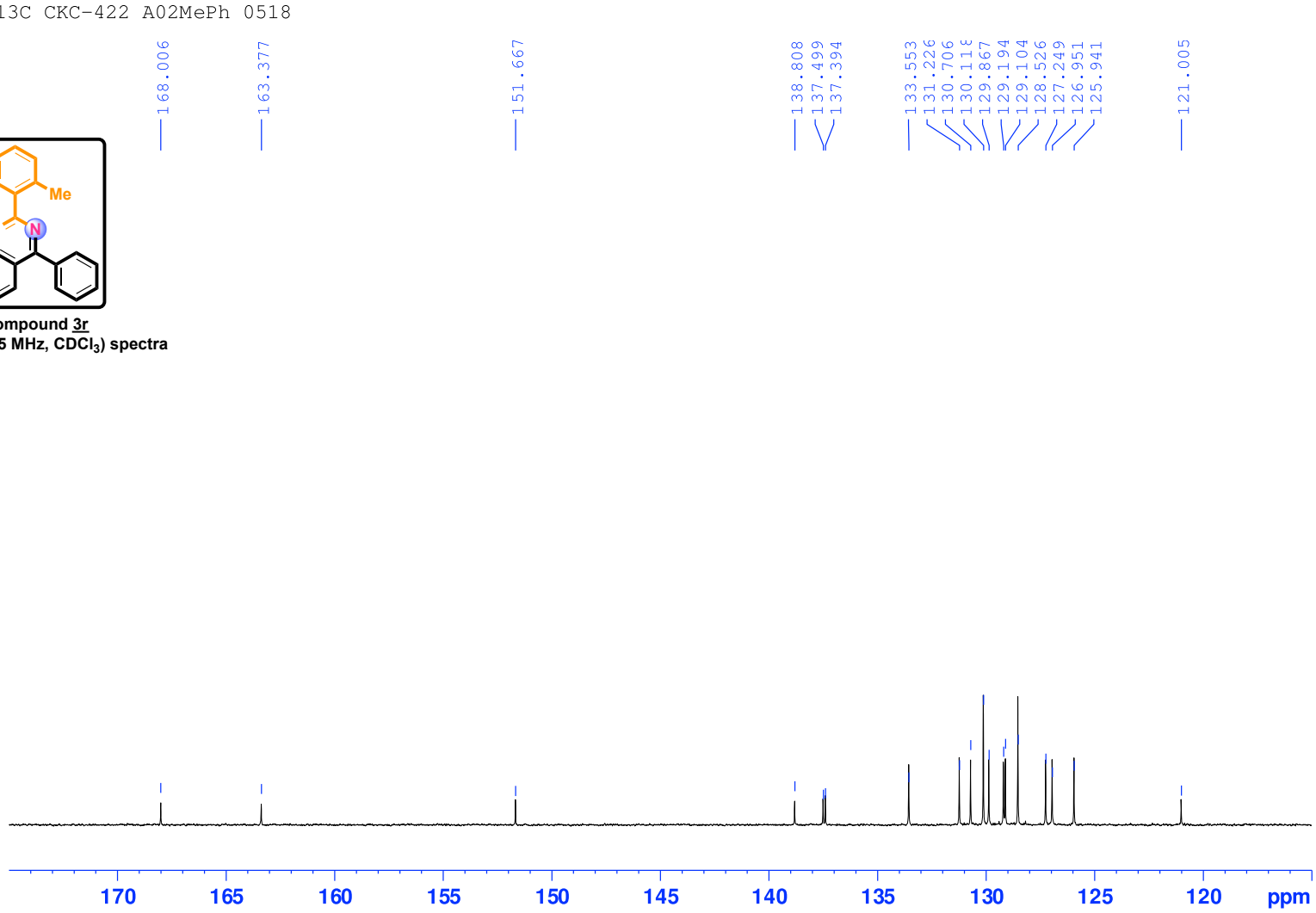
Compound 3r
^{13}C NMR (125 MHz, $CDCl_3$) spectra



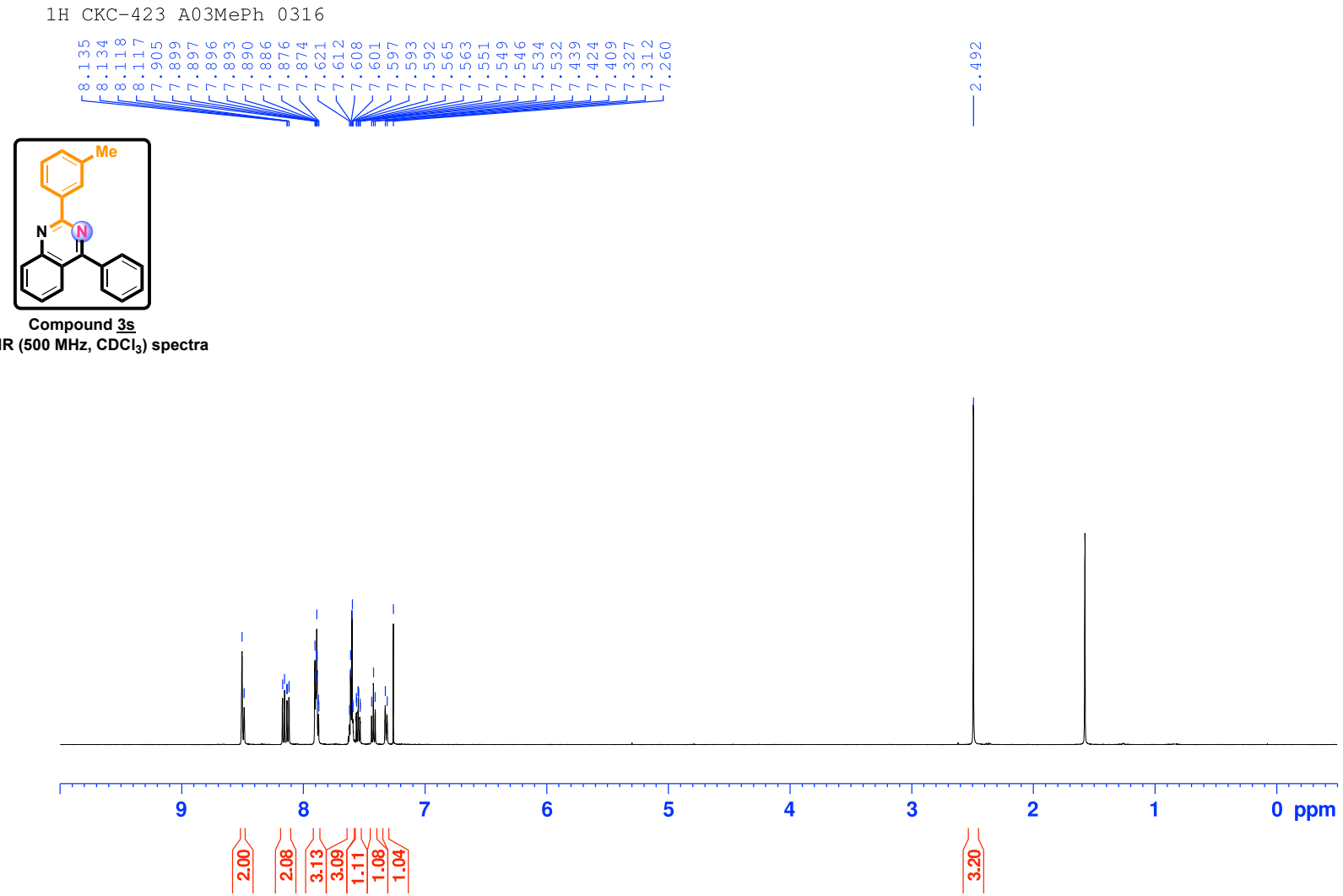
Compound 3r



Compound 3r
^{13}C NMR (125 MHz, $CDCl_3$) spectra

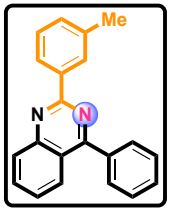


Compound 3s

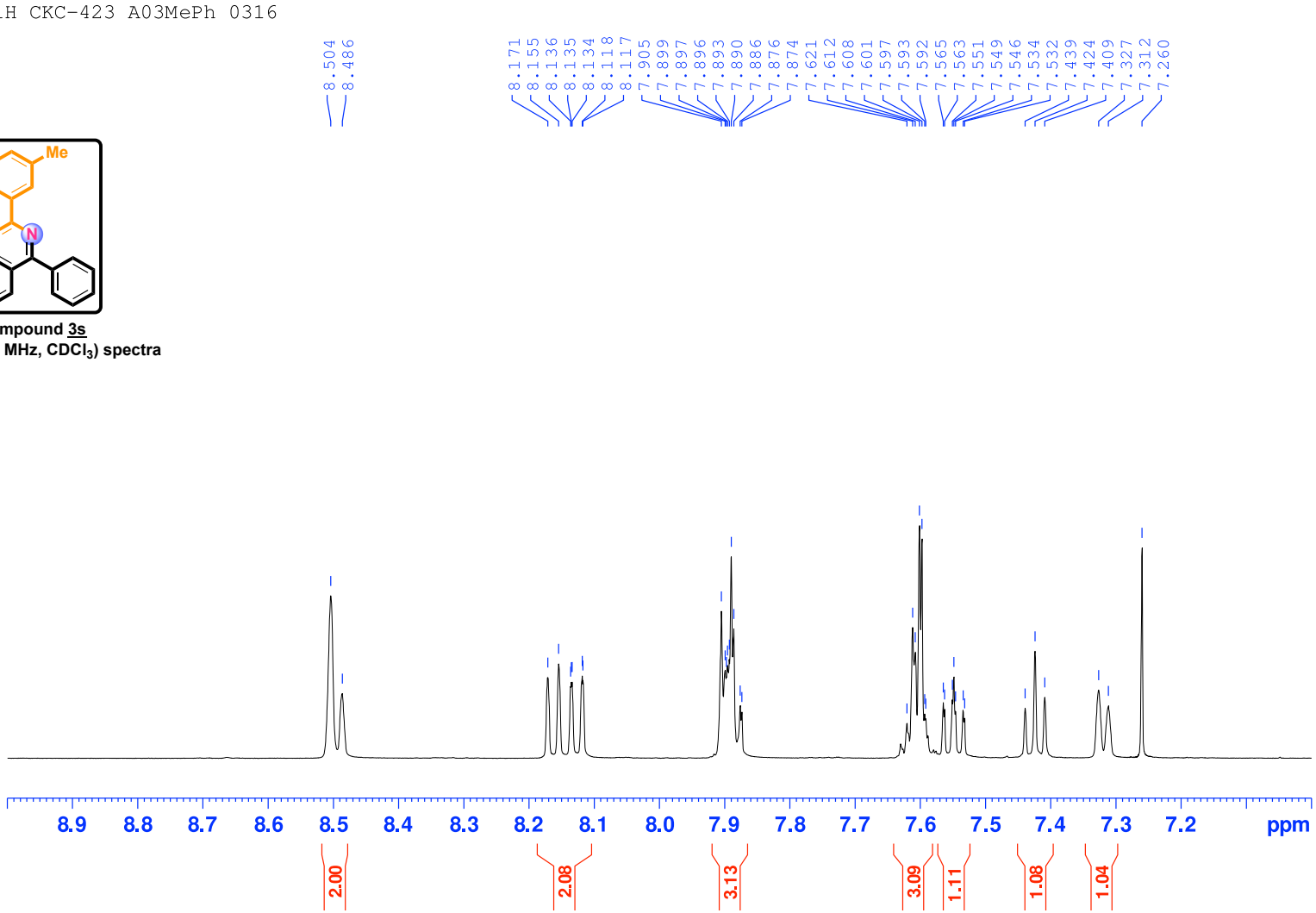


Compound 3s
^{1}H NMR (500 MHz, $CDCl_3$) spectra

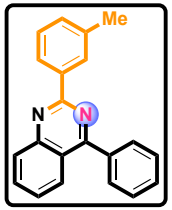
Compound 3s



Compound 3s
^{1}H NMR (500 MHz, $CDCl_3$) spectra

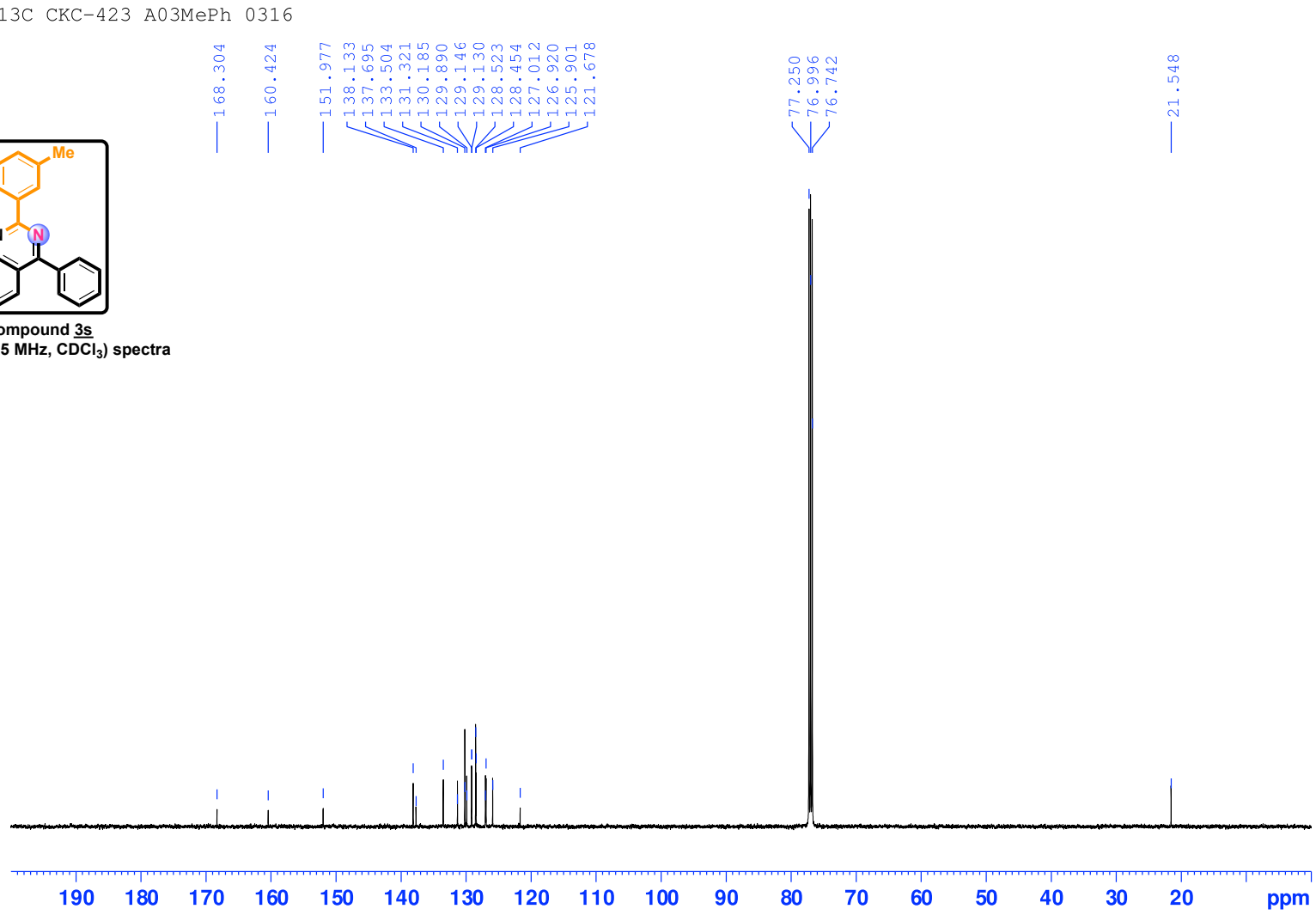


Compound 3s

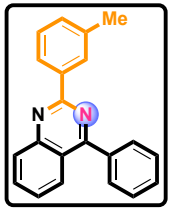


Compound 3s

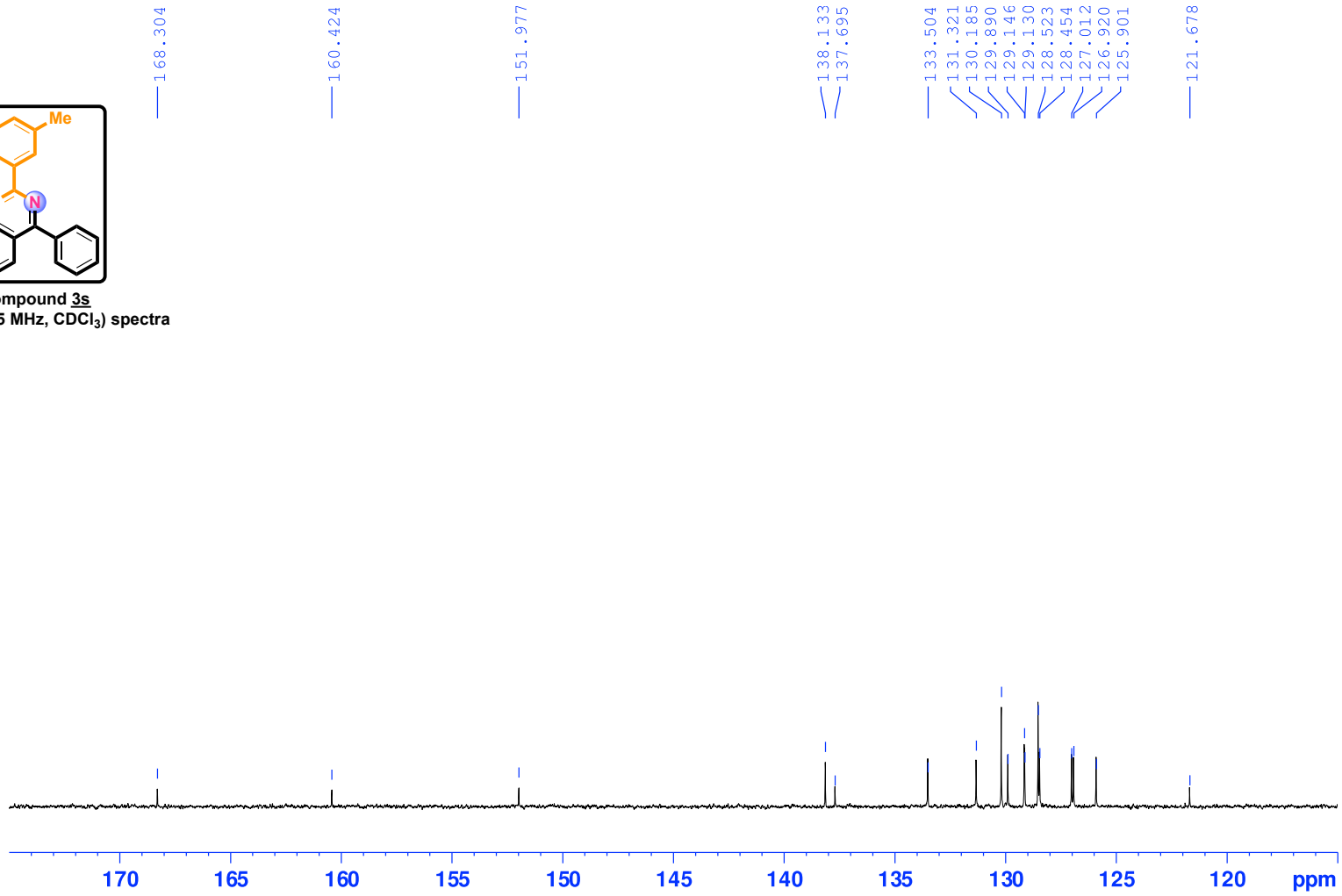
^{13}C NMR (125 MHz, $CDCl_3$) spectra



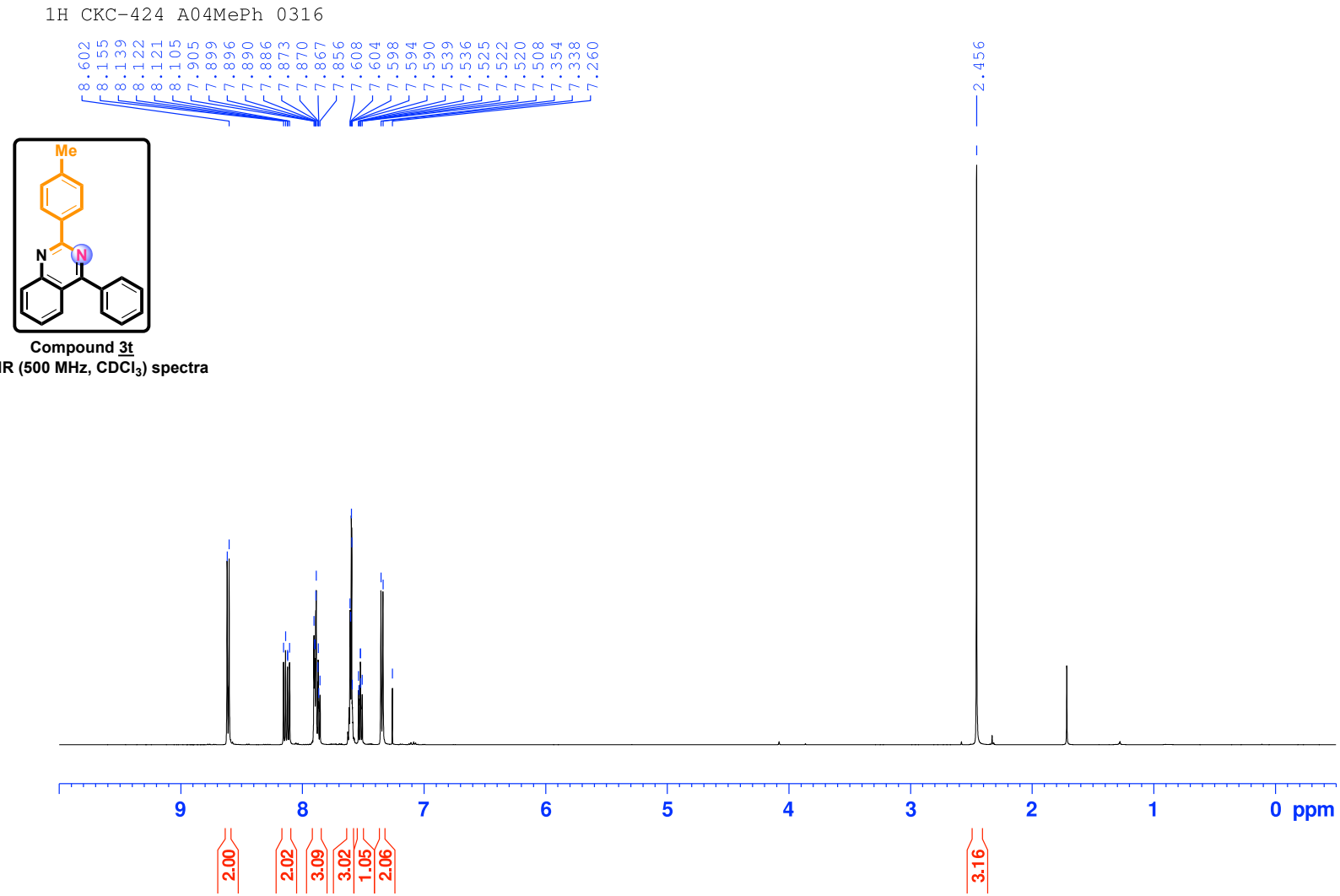
Compound 3s



Compound 3s
^{13}C NMR (125 MHz, $CDCl_3$) spectra

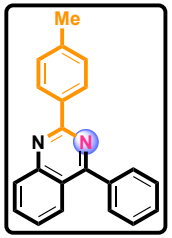


Compound 3t

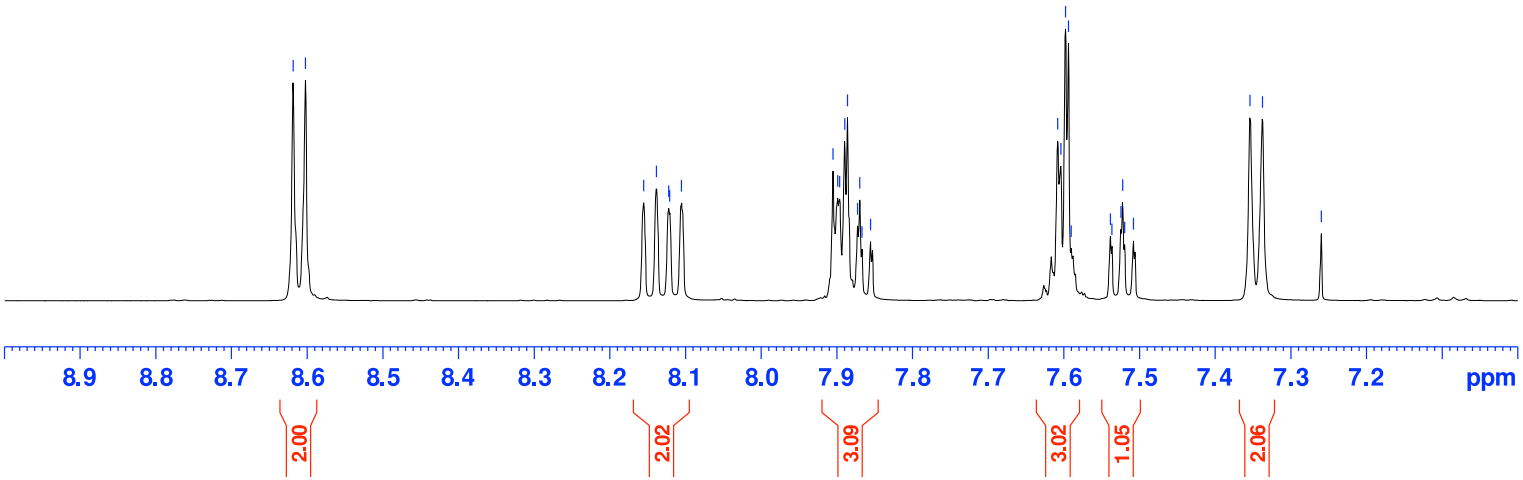


Compound 3t
^{1}H NMR (500 MHz, $CDCl_3$) spectra

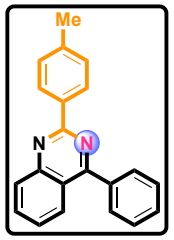
Compound 3t



Compound 3t
^{1}H NMR (500 MHz, $CDCl_3$) spectra

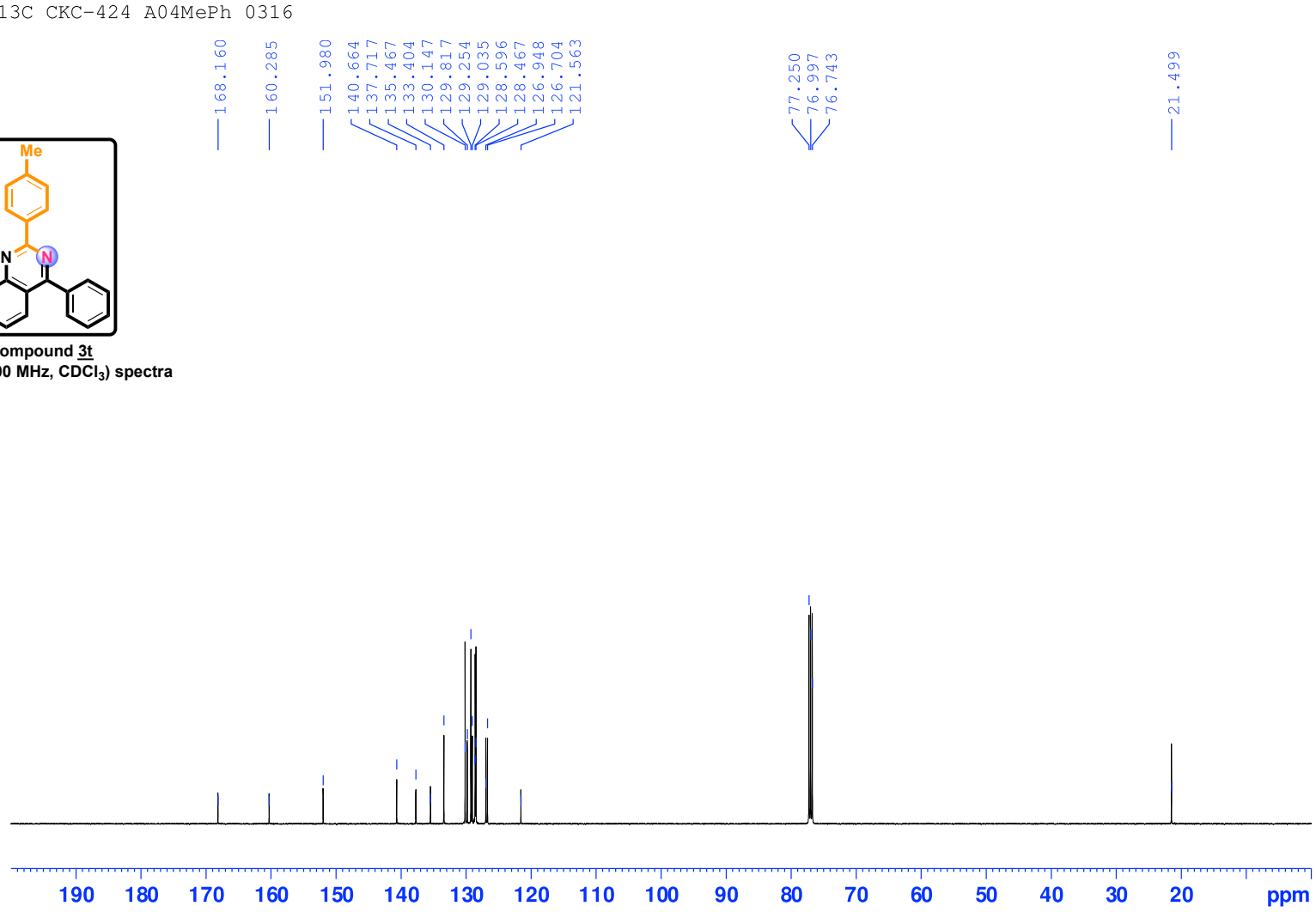


Compound 3t



Compound 3t

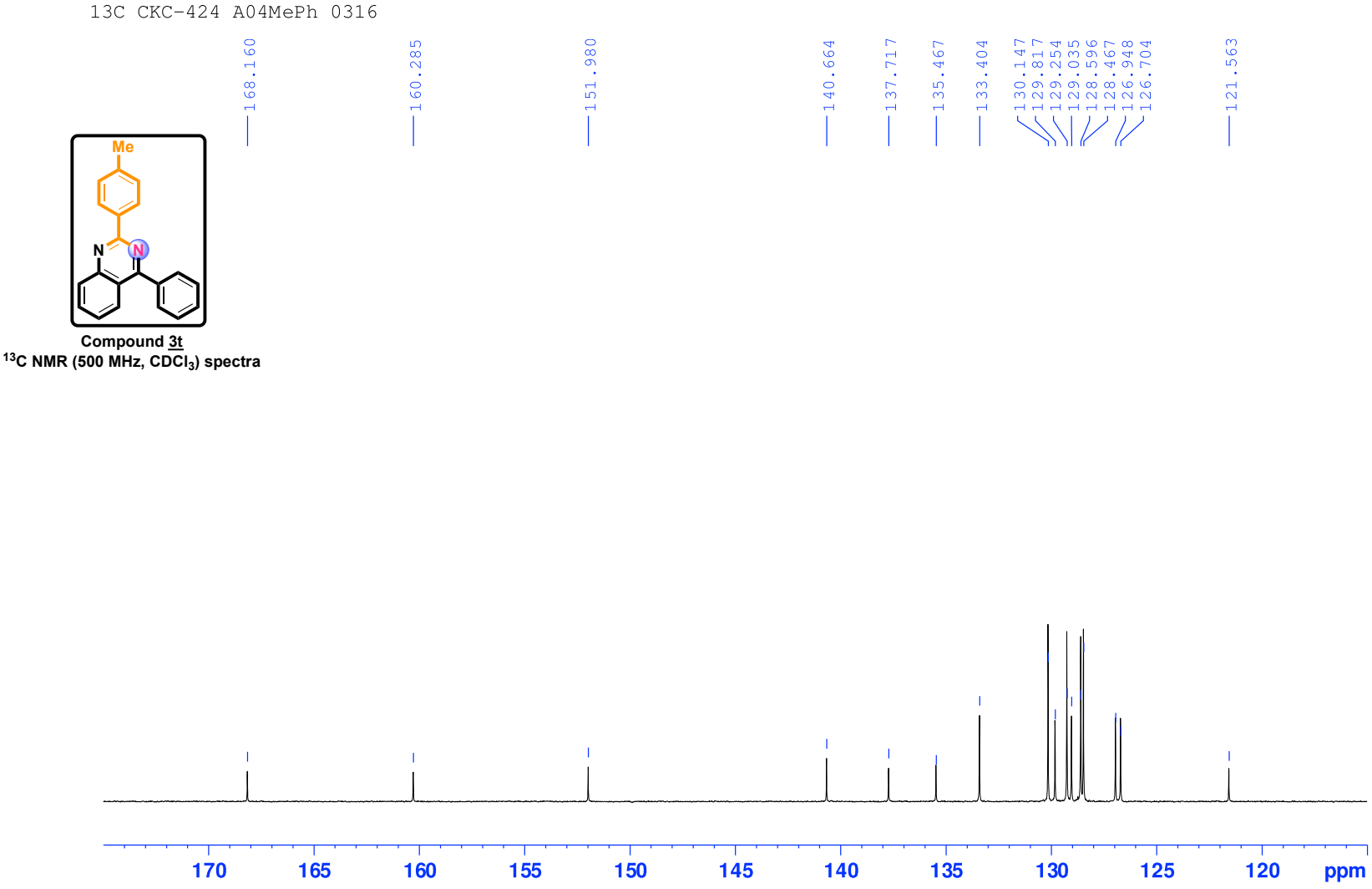
^{13}C NMR (500 MHz, $CDCl_3$) spectra



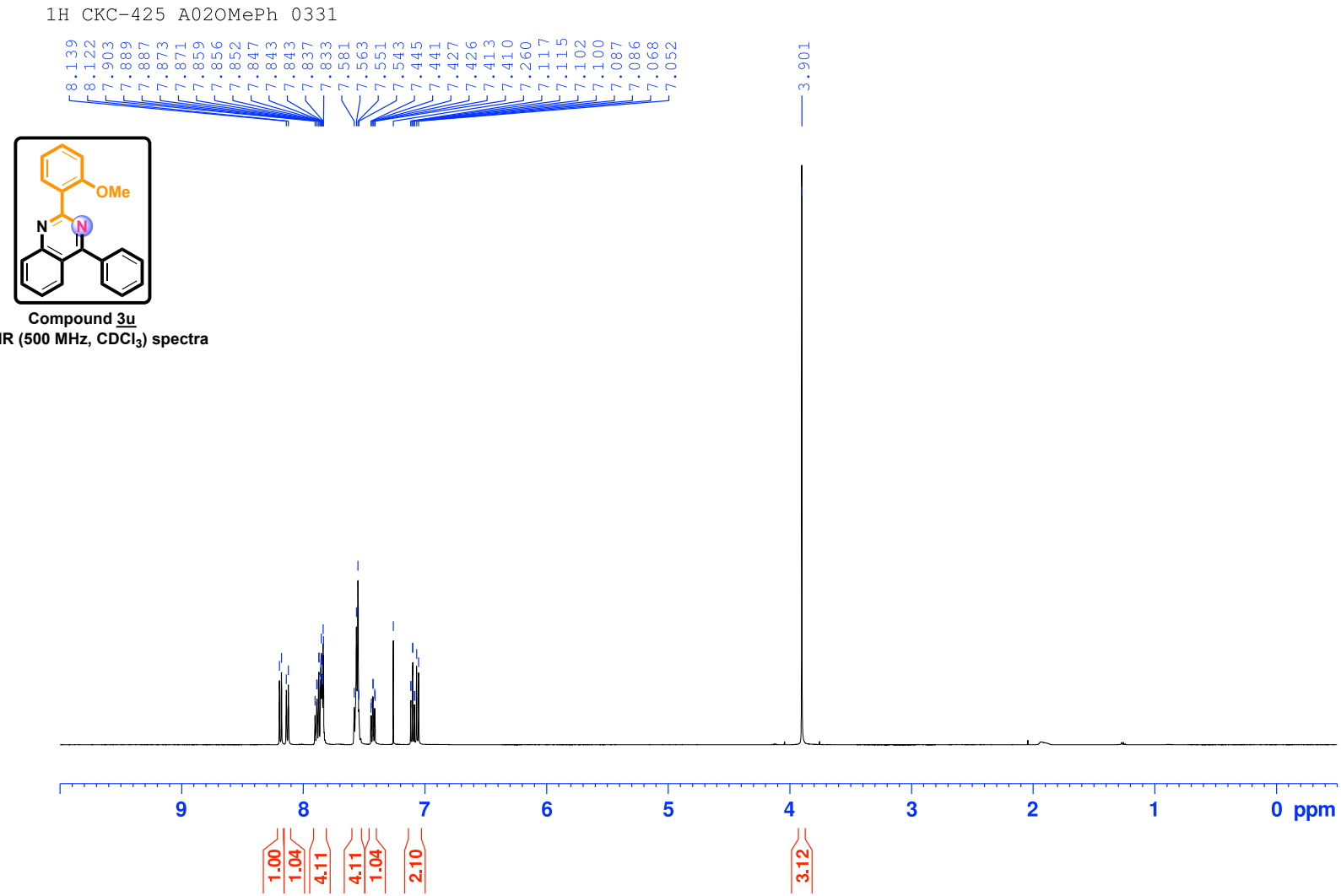
Compound 3t

Compound 3t

^{13}C NMR (500 MHz, $CDCl_3$) spectra

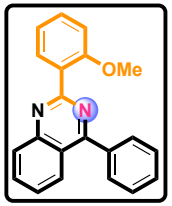


Compound 3u

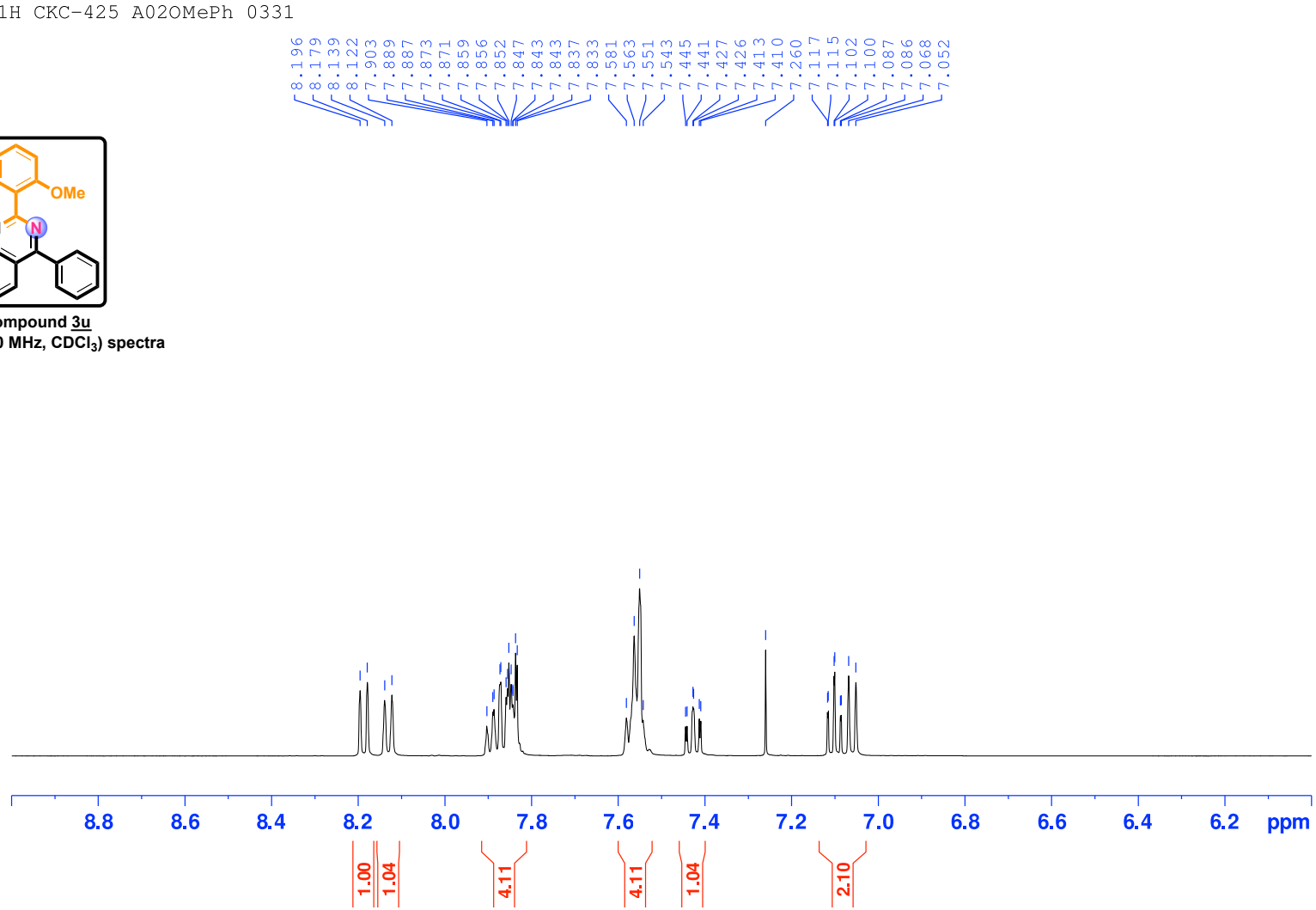


Compound 3u
^{1}H NMR (500 MHz, $CDCl_3$) spectra

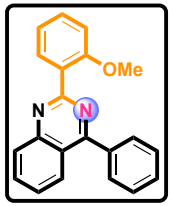
Compound 3u



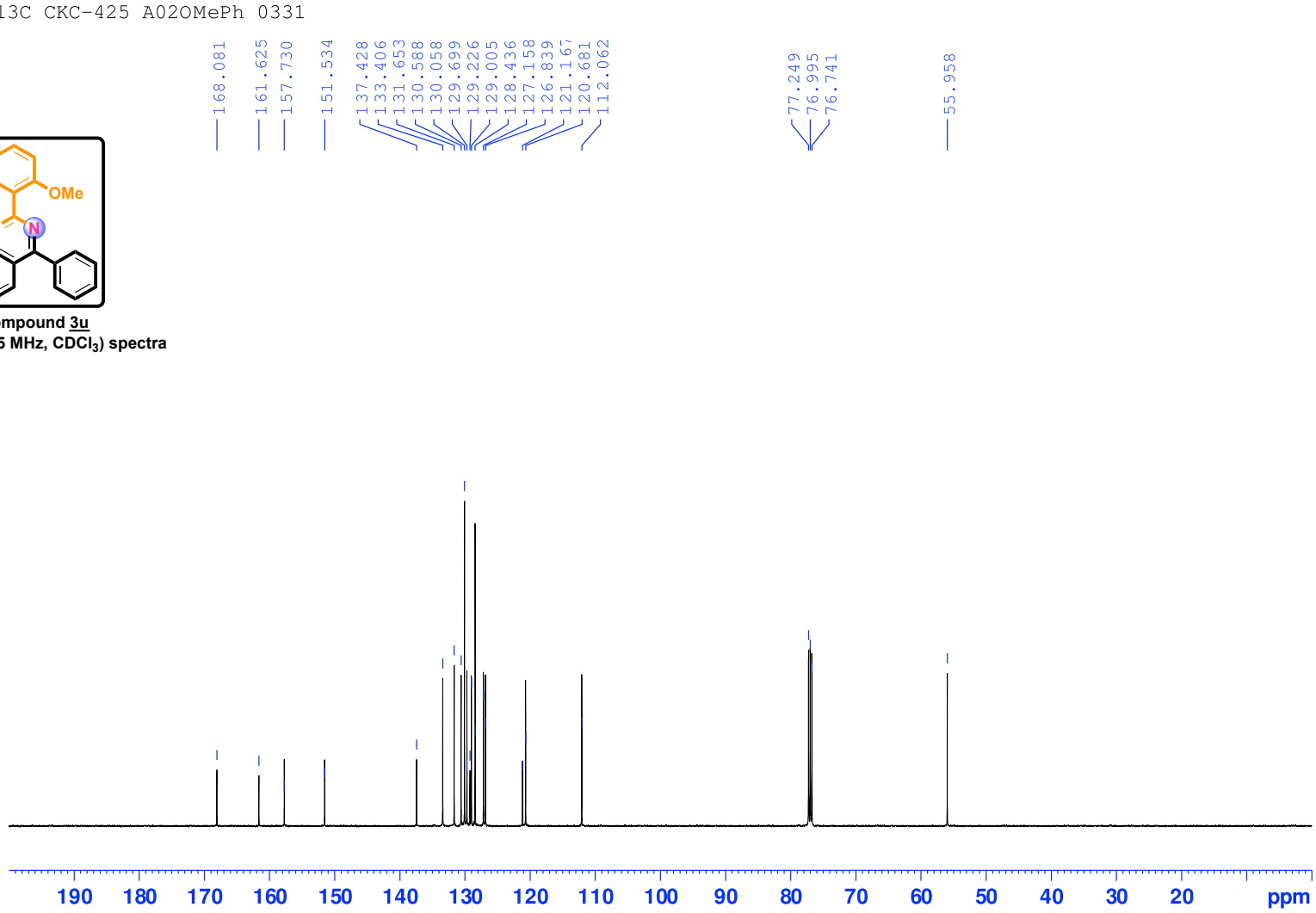
Compound 3u
^{1}H NMR (500 MHz, $CDCl_3$) spectra



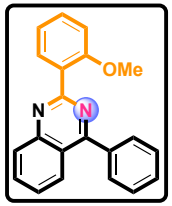
Compound 3u



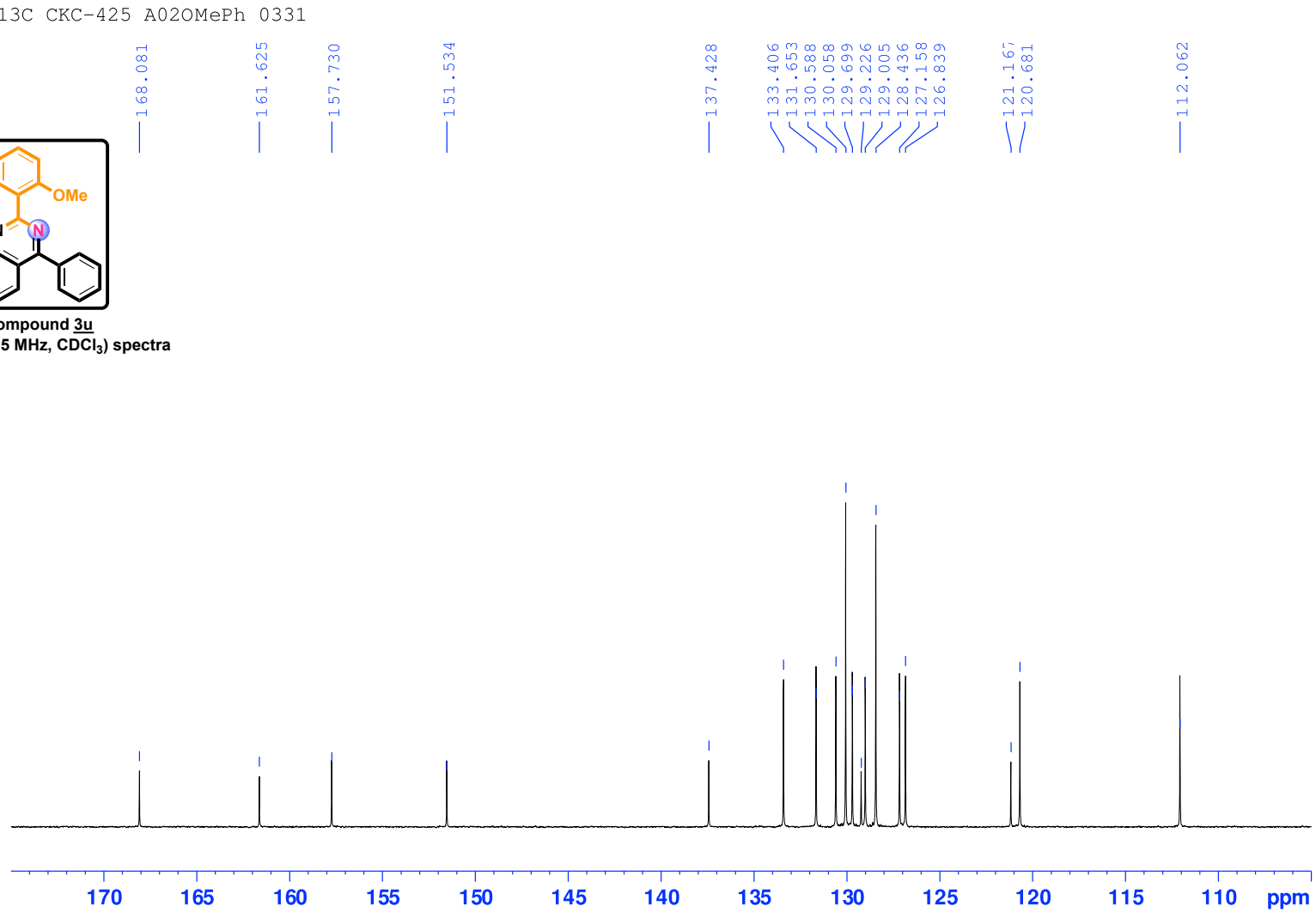
Compound 3u
^{13}C NMR (125 MHz, $CDCl_3$) spectra



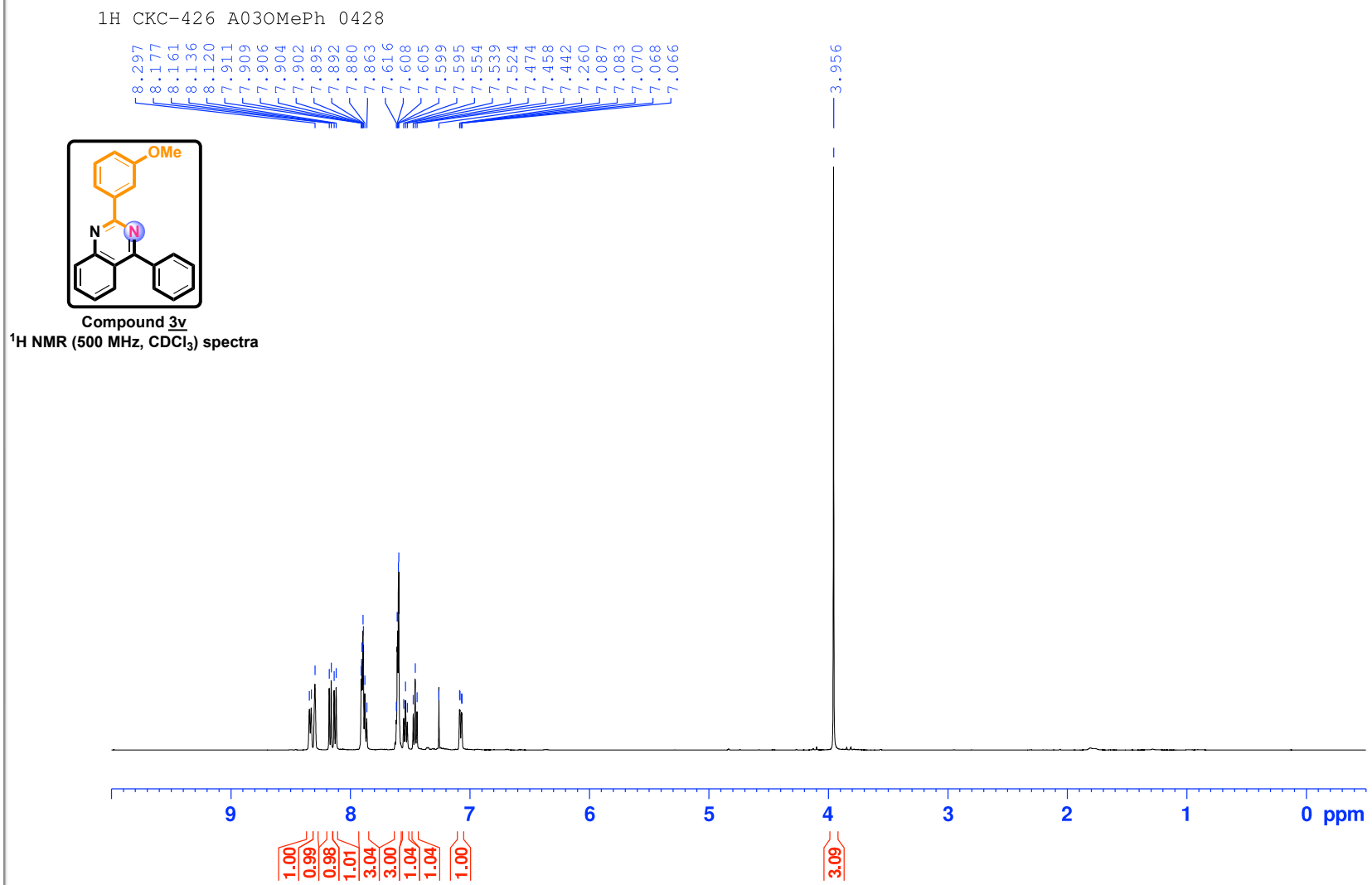
Compound 3u



Compound 3u
^{13}C NMR (125 MHz, $CDCl_3$) spectra

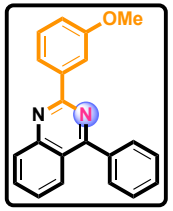


Compound 3v

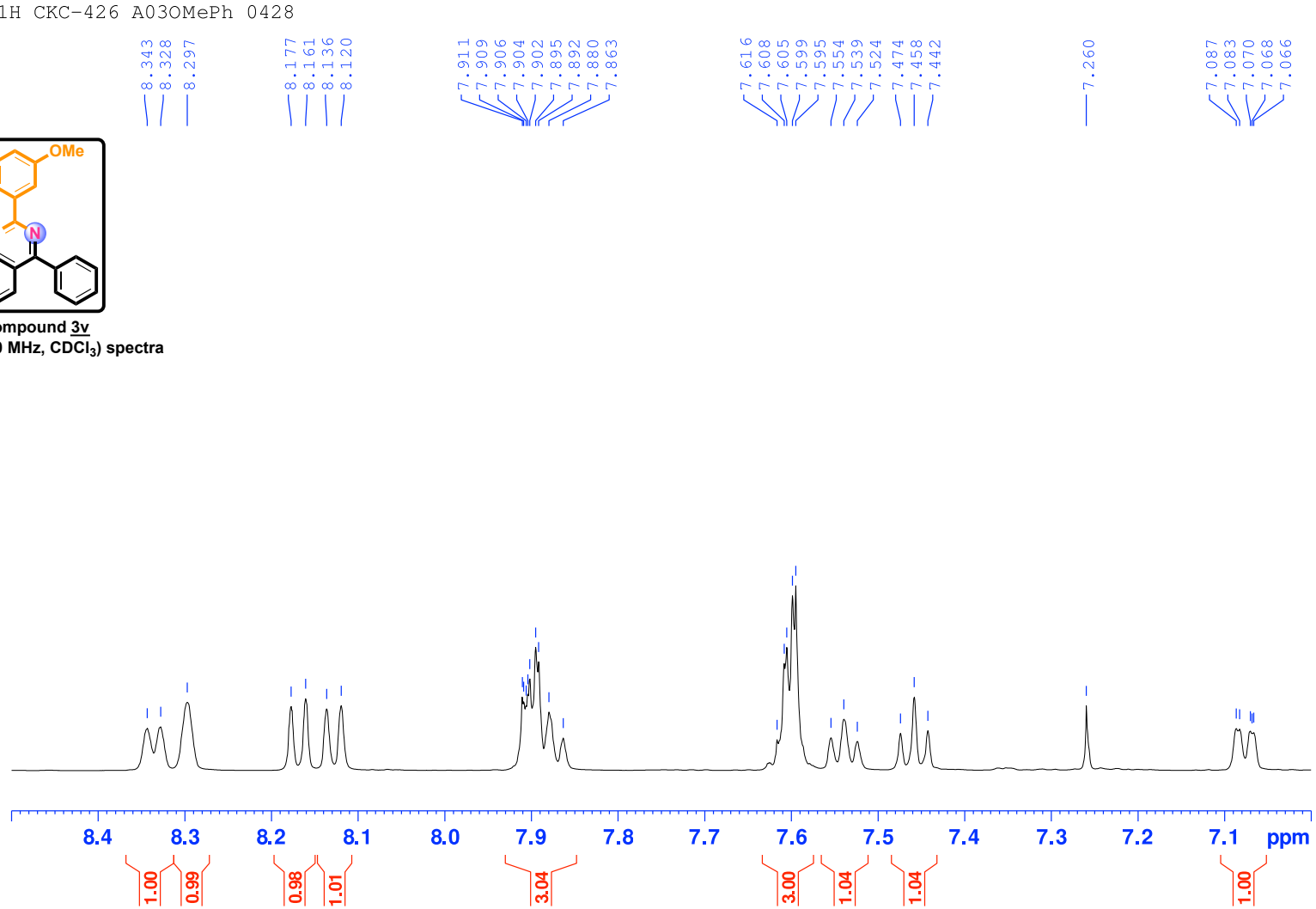


Compound 3v
^{1}H NMR (500 MHz, $CDCl_3$) spectra

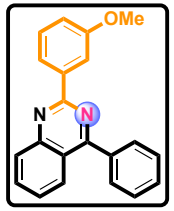
Compound 3v



Compound 3v
^{1}H NMR (500 MHz, $CDCl_3$) spectra

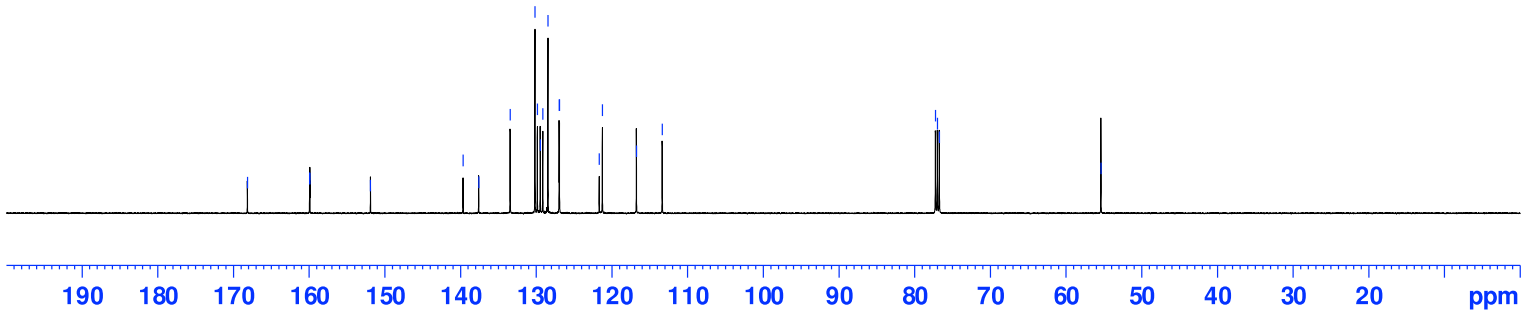


Compound 3v

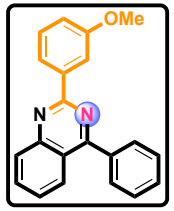


Compound 3v

^{13}C NMR (125 MHz, $CDCl_3$) spectra

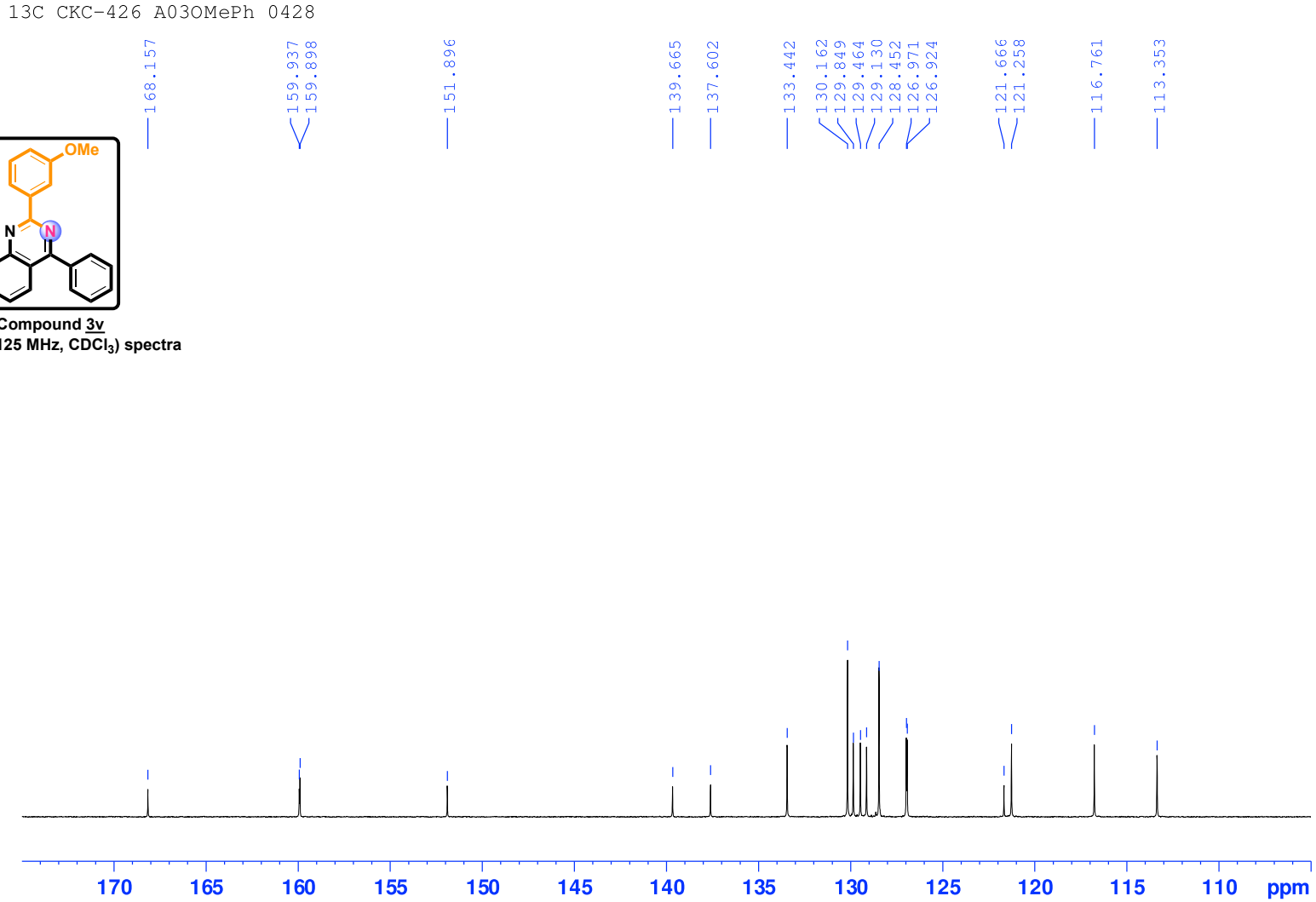


Compound 3v

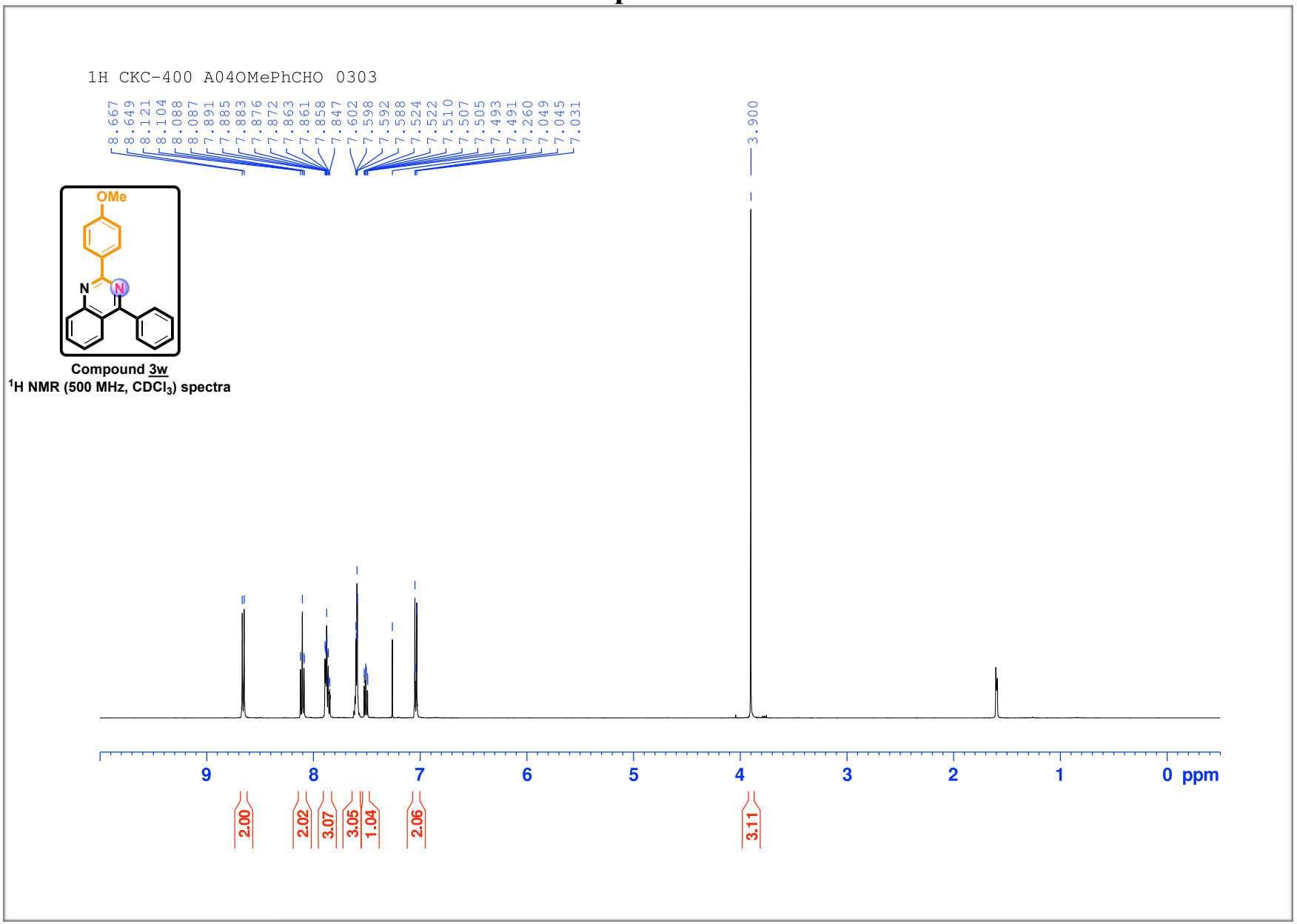


Compound 3v

^{13}C NMR (125 MHz, $CDCl_3$) spectra



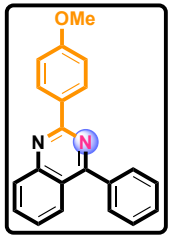
Compound 3w



Compound 3w

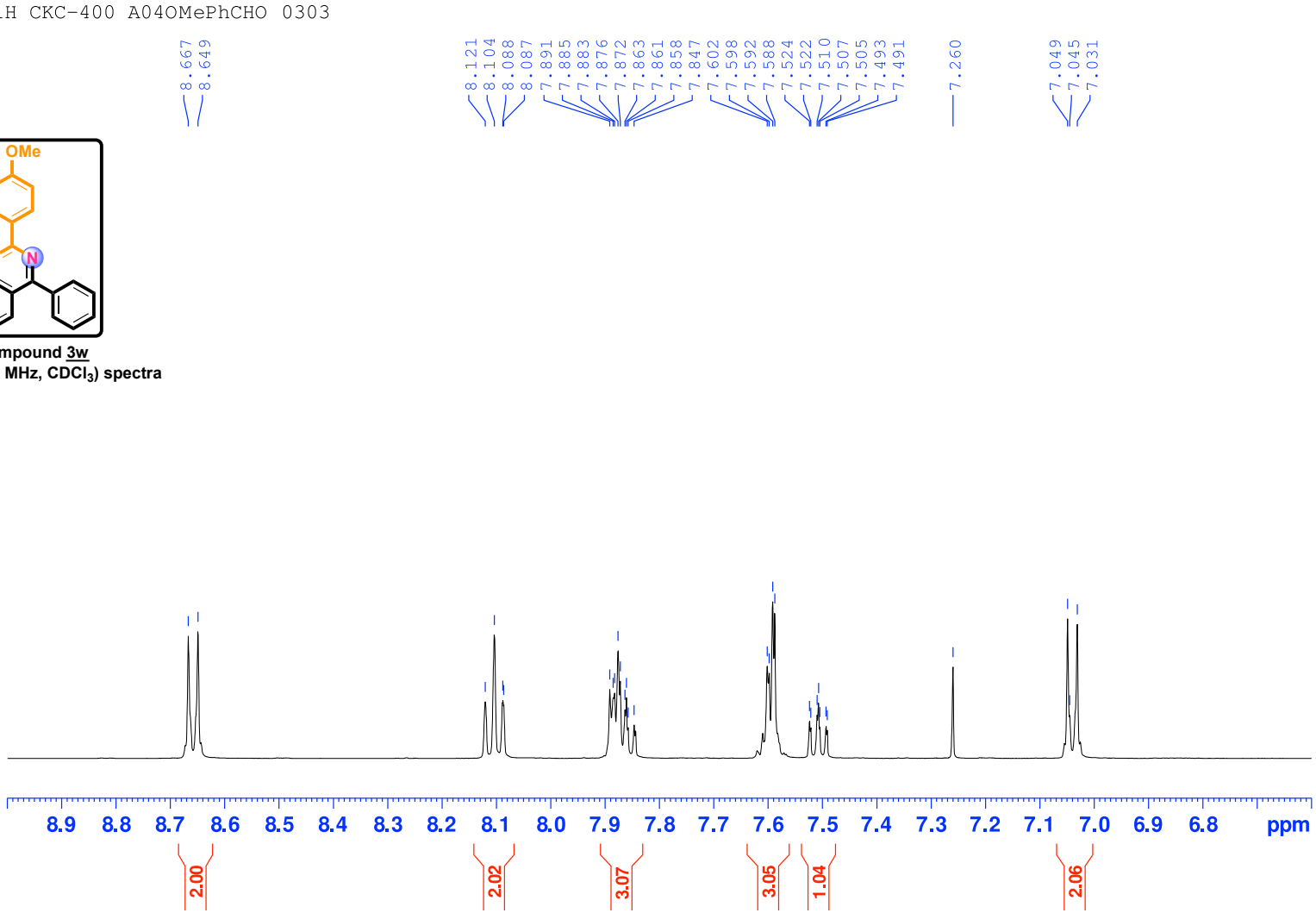
^{1}H NMR (500 MHz, $CDCl_3$) spectra

Compound 3w

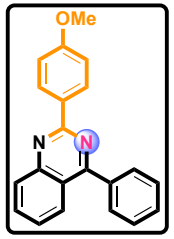


Compound 3w

^{1}H NMR (500 MHz, $CDCl_3$) spectra

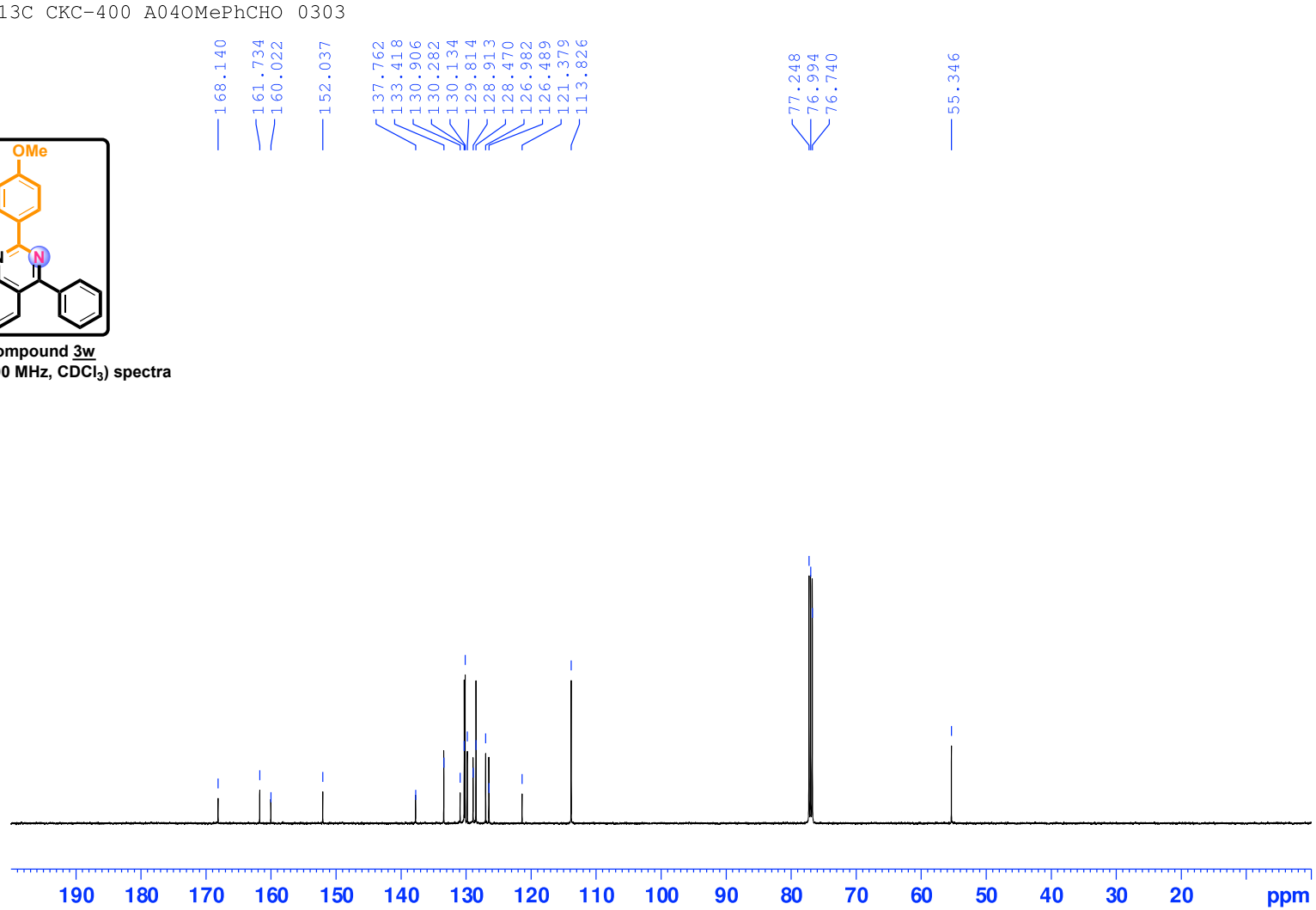


Compound 3w

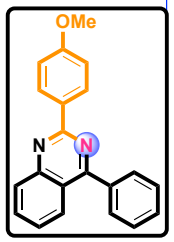


Compound 3w

^{13}C NMR (500 MHz, $CDCl_3$) spectra

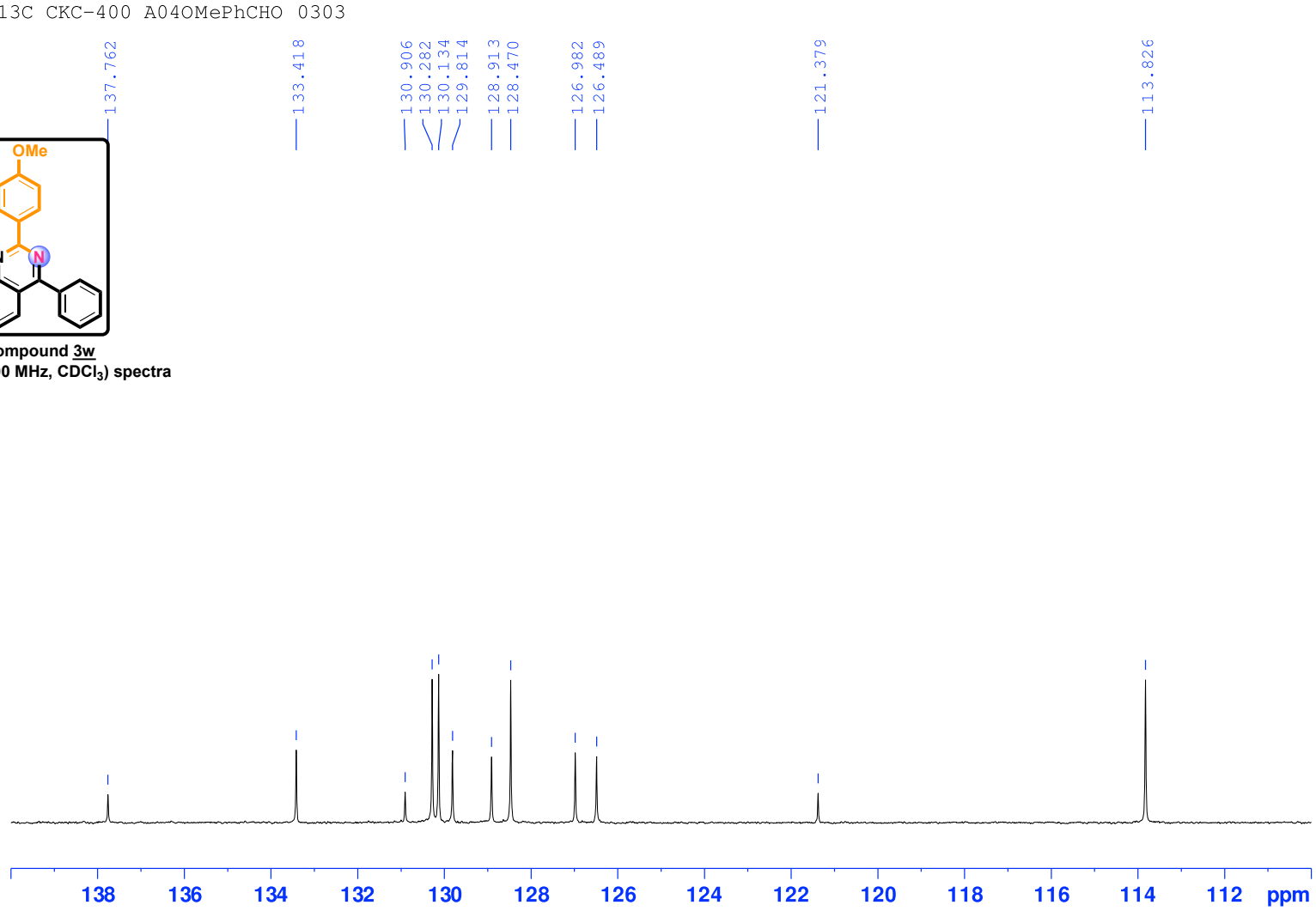


Compound 3w

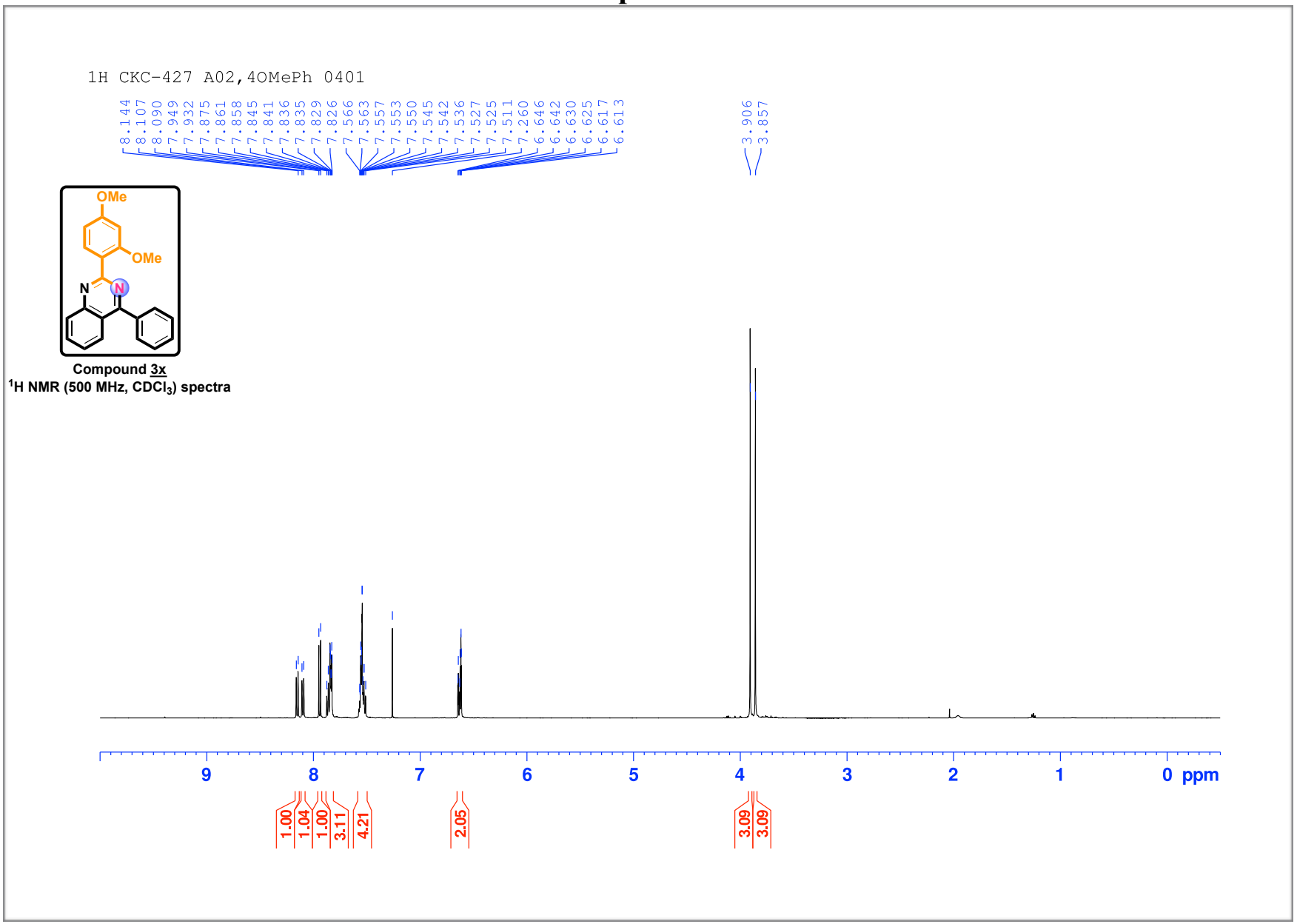


Compound 3w

^{13}C NMR (500 MHz, $CDCl_3$) spectra

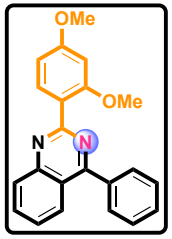


Compound 3x

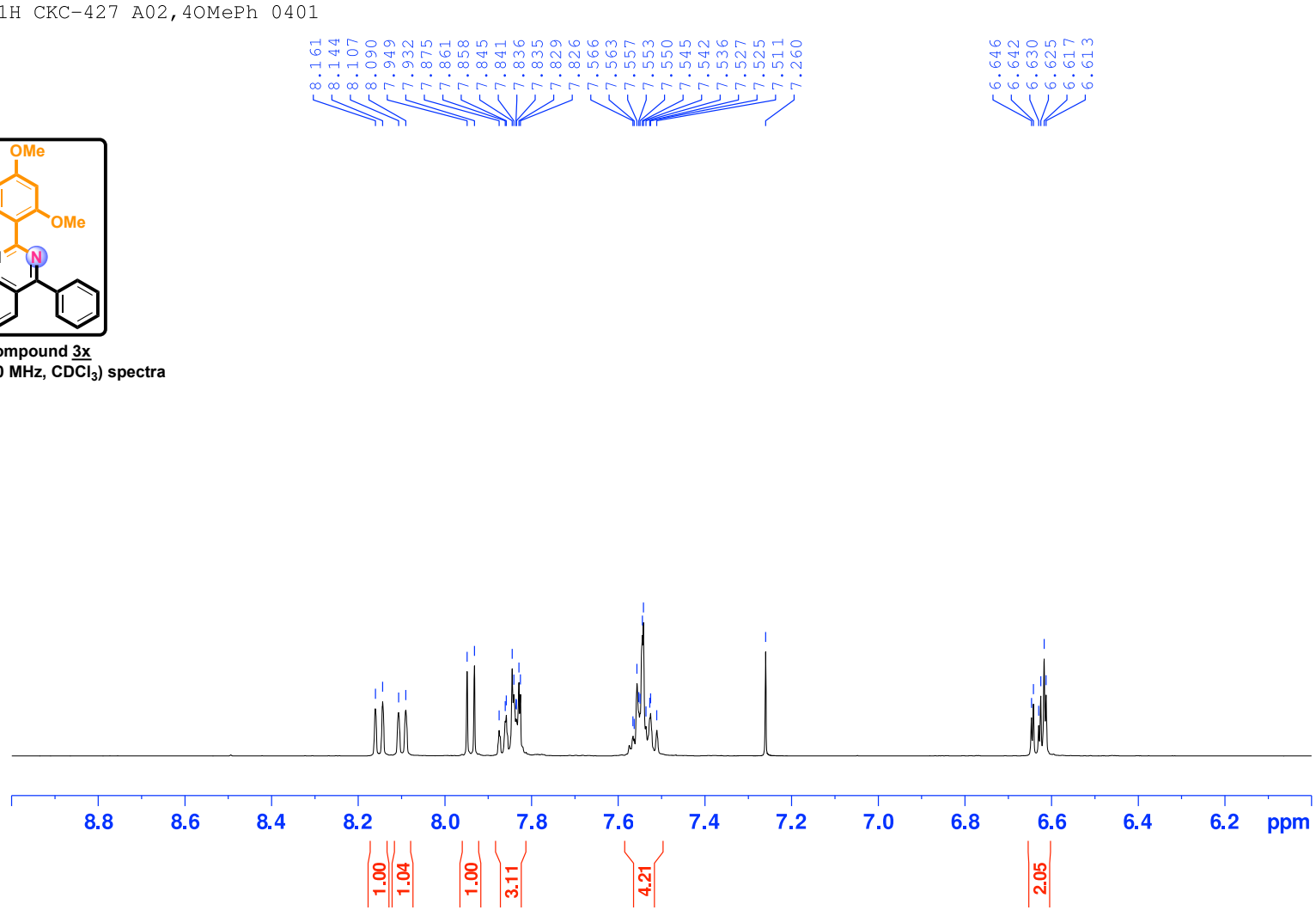


Compound 3x
^{1}H NMR (500 MHz, $CDCl_3$) spectra

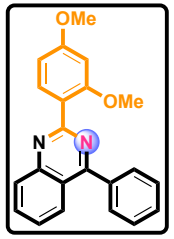
Compound 3x



Compound 3x
^{1}H NMR (500 MHz, $CDCl_3$) spectra

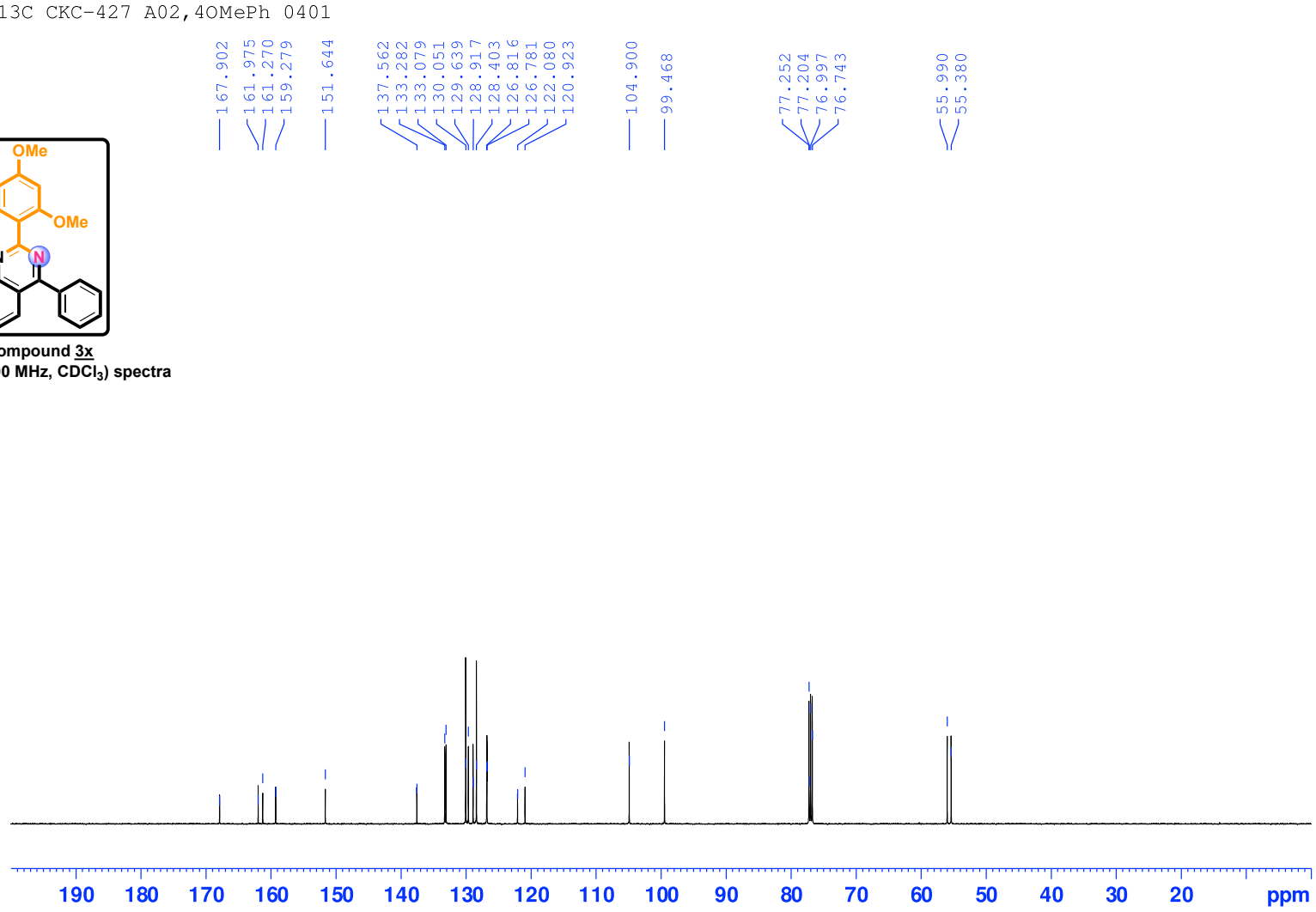


Compound 3x

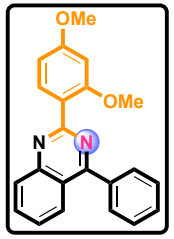


Compound 3x

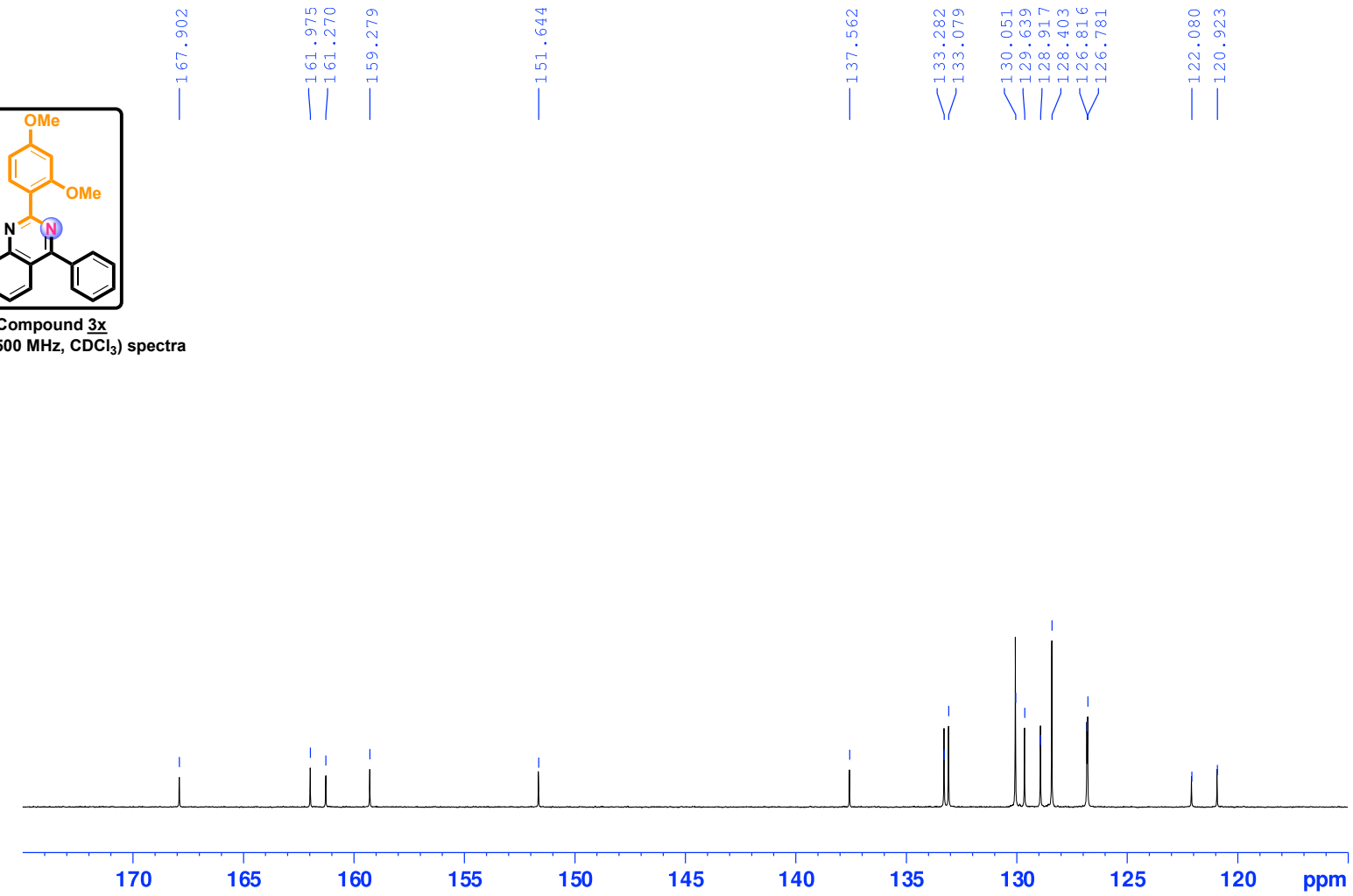
^{13}C NMR (500 MHz, $CDCl_3$) spectra



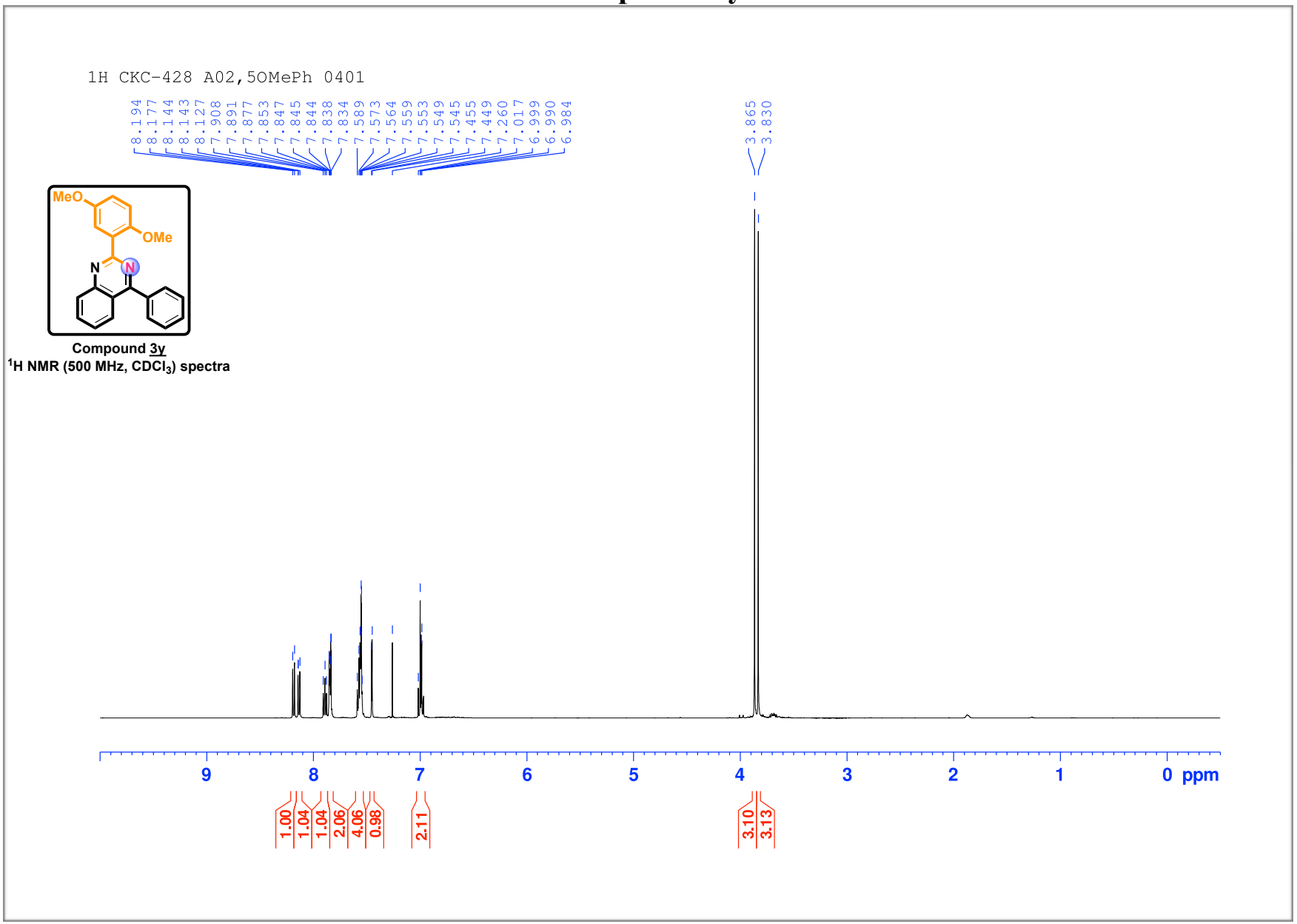
Compound 3x



Compound 3x
^{13}C NMR (500 MHz, $CDCl_3$) spectra

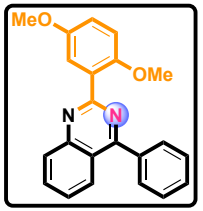


Compound 3y

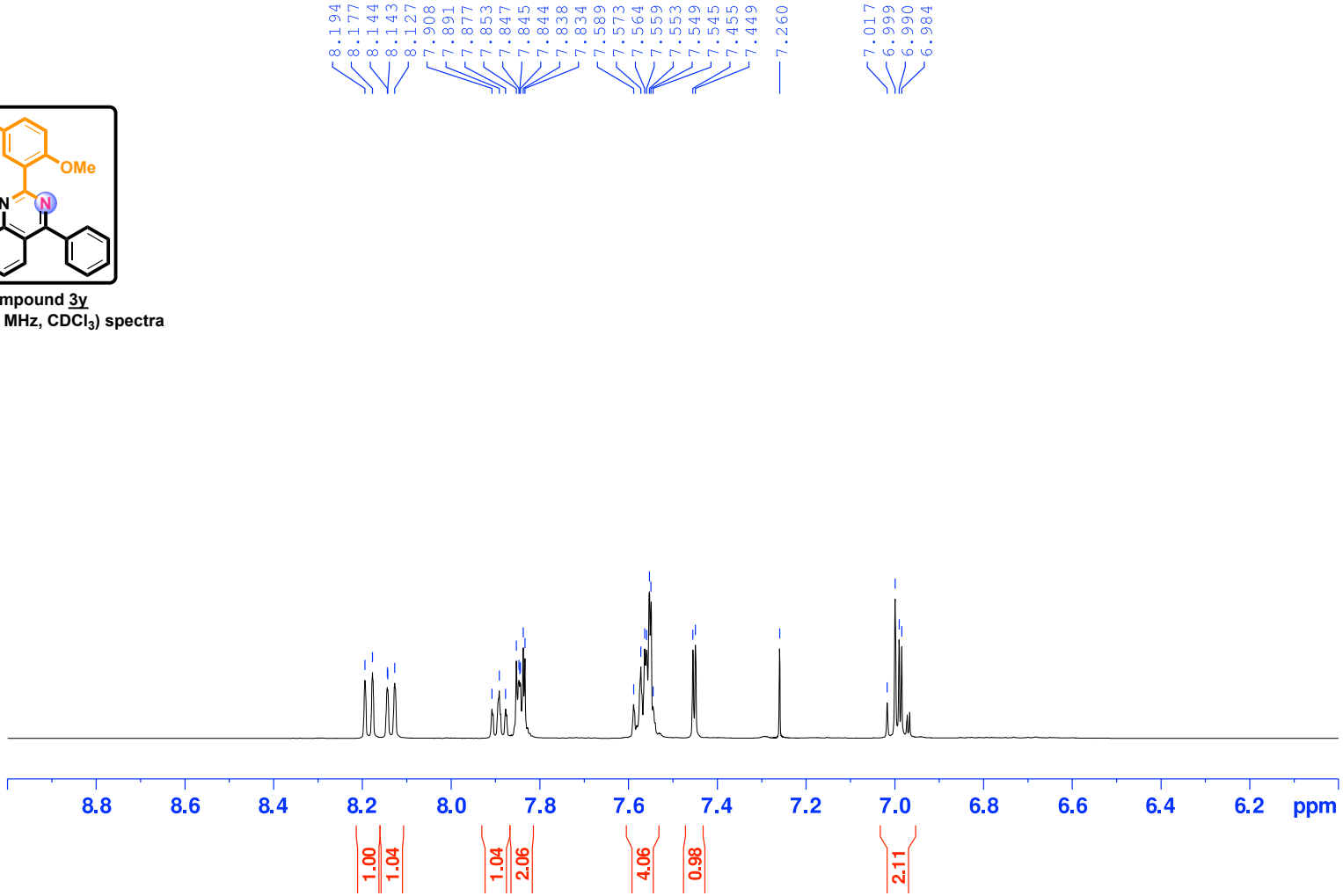


Compound 3y
^{1}H NMR (500 MHz, $CDCl_3$) spectra

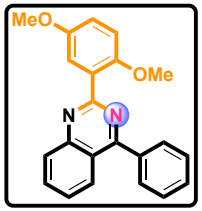
Compound 3y



Compound 3y
^{1}H NMR (500 MHz, $CDCl_3$) spectra

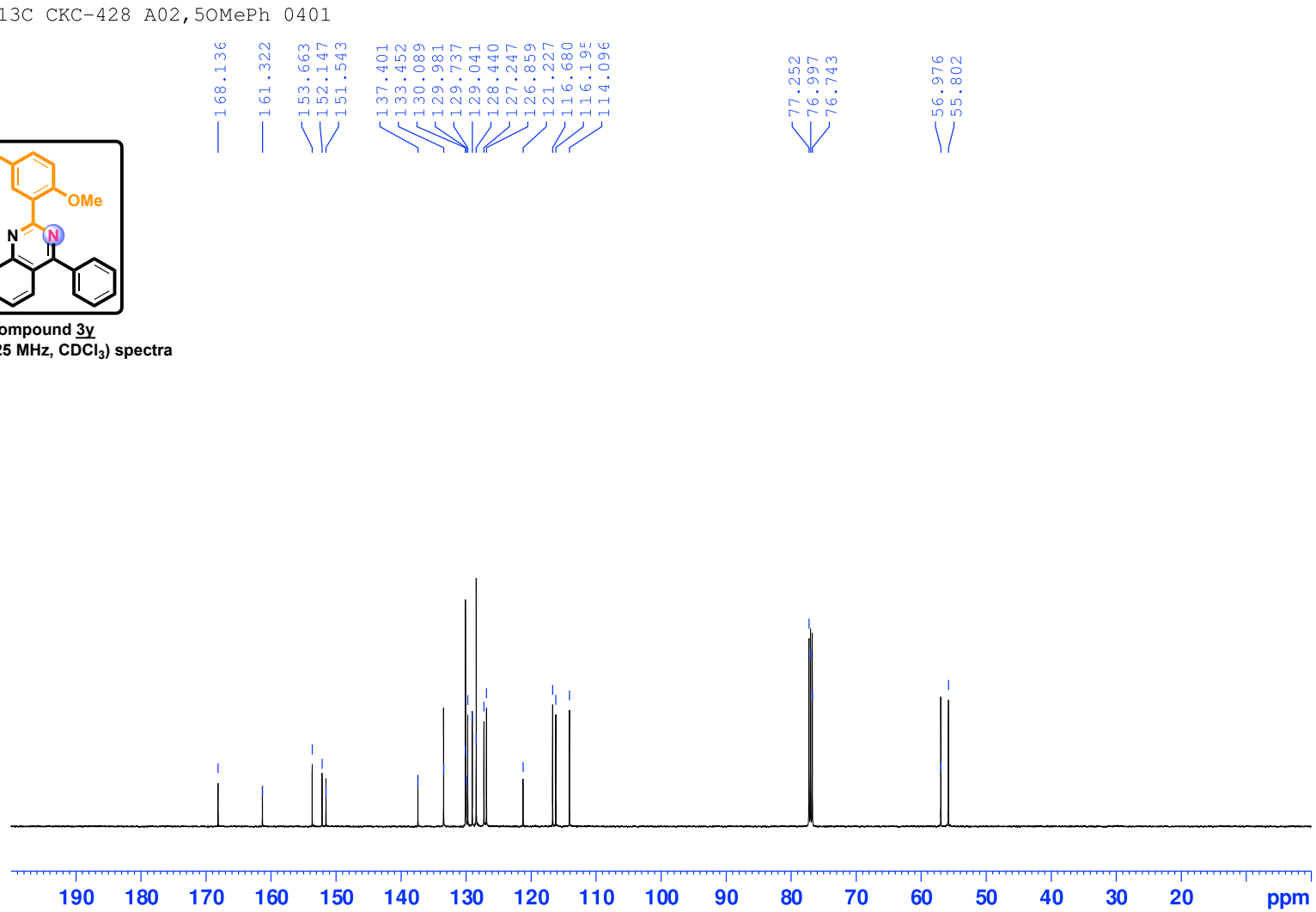


Compound 3y

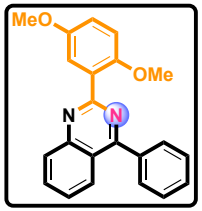


Compound 3y

^{13}C NMR (125 MHz, $CDCl_3$) spectra

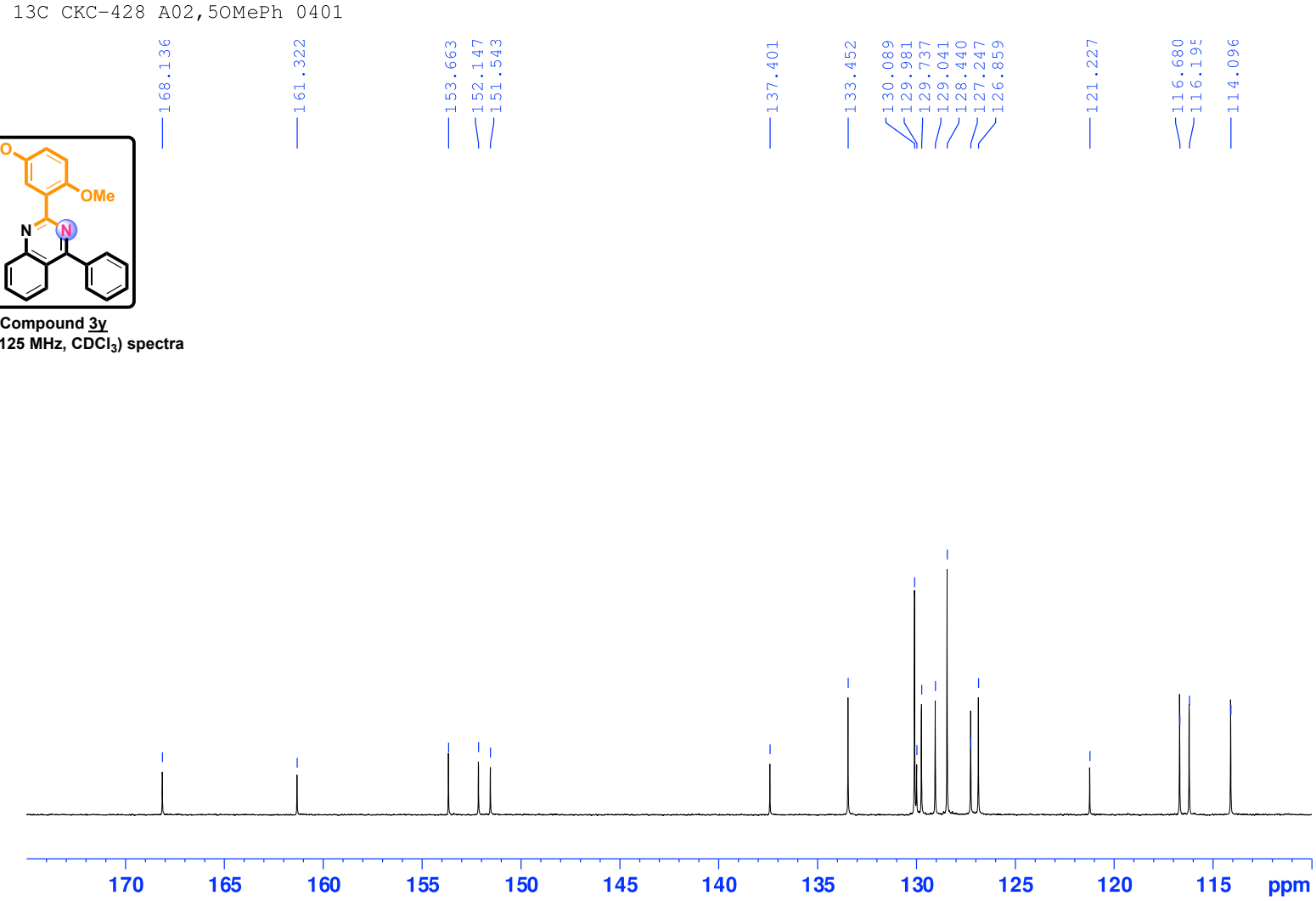


Compound 3y

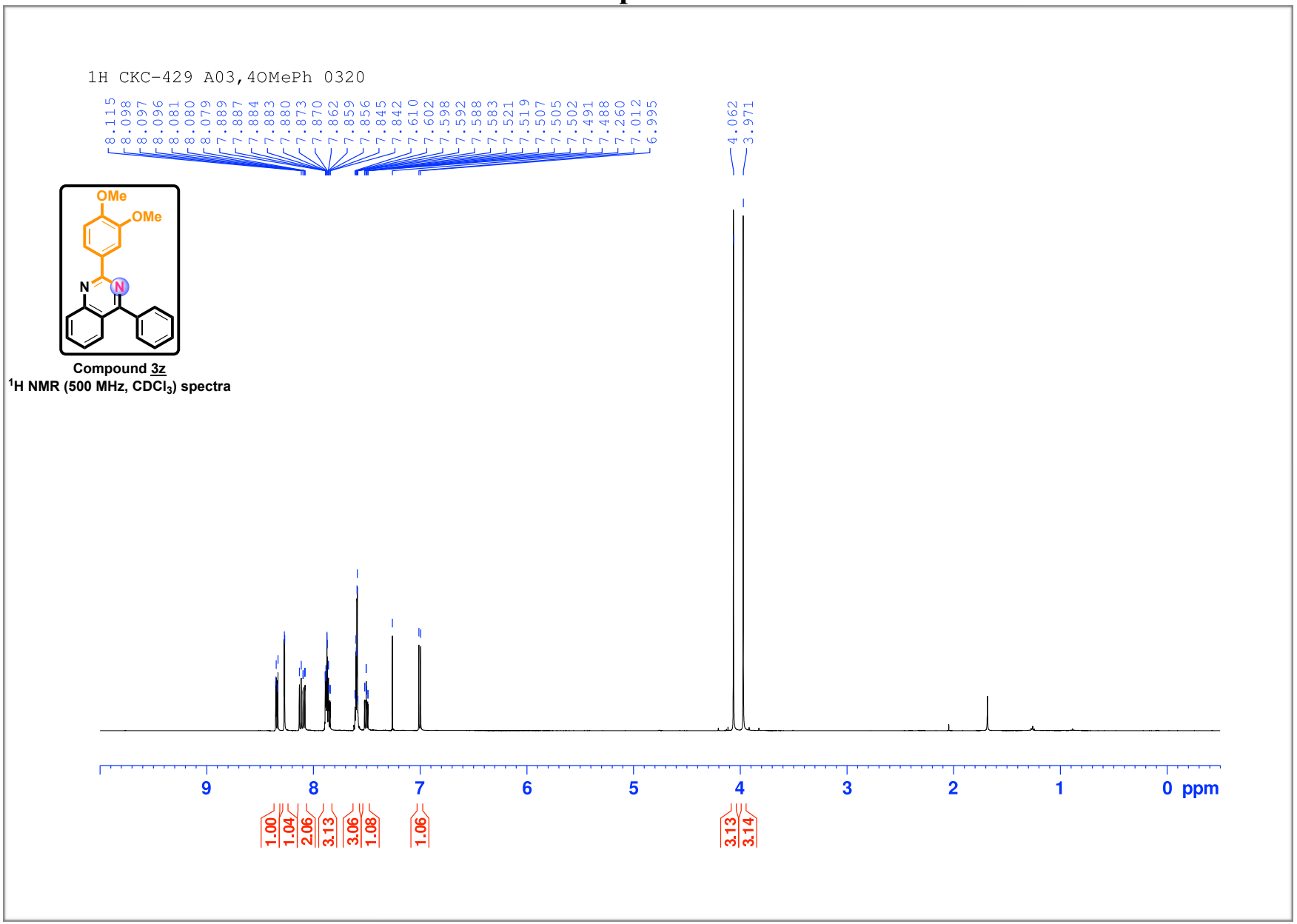


Compound 3y

^{13}C NMR (125 MHz, $CDCl_3$) spectra

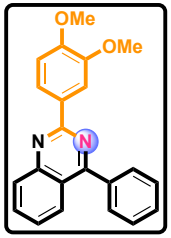


Compound 3z

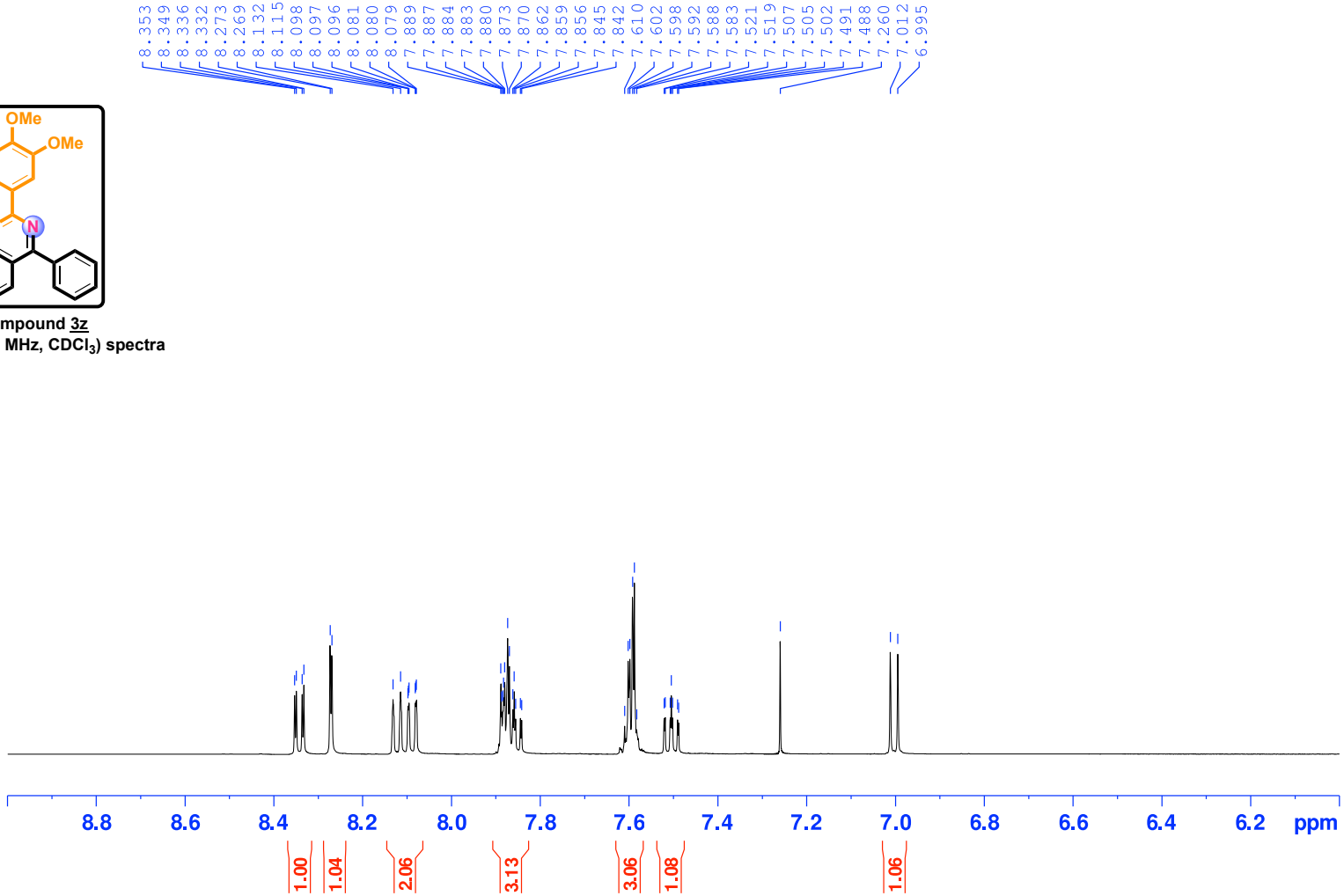


Compound 3z
^{1}H NMR (500 MHz, $CDCl_3$) spectra

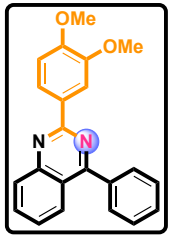
Compound 3z



Compound 3z
^{1}H NMR (500 MHz, $CDCl_3$) spectra

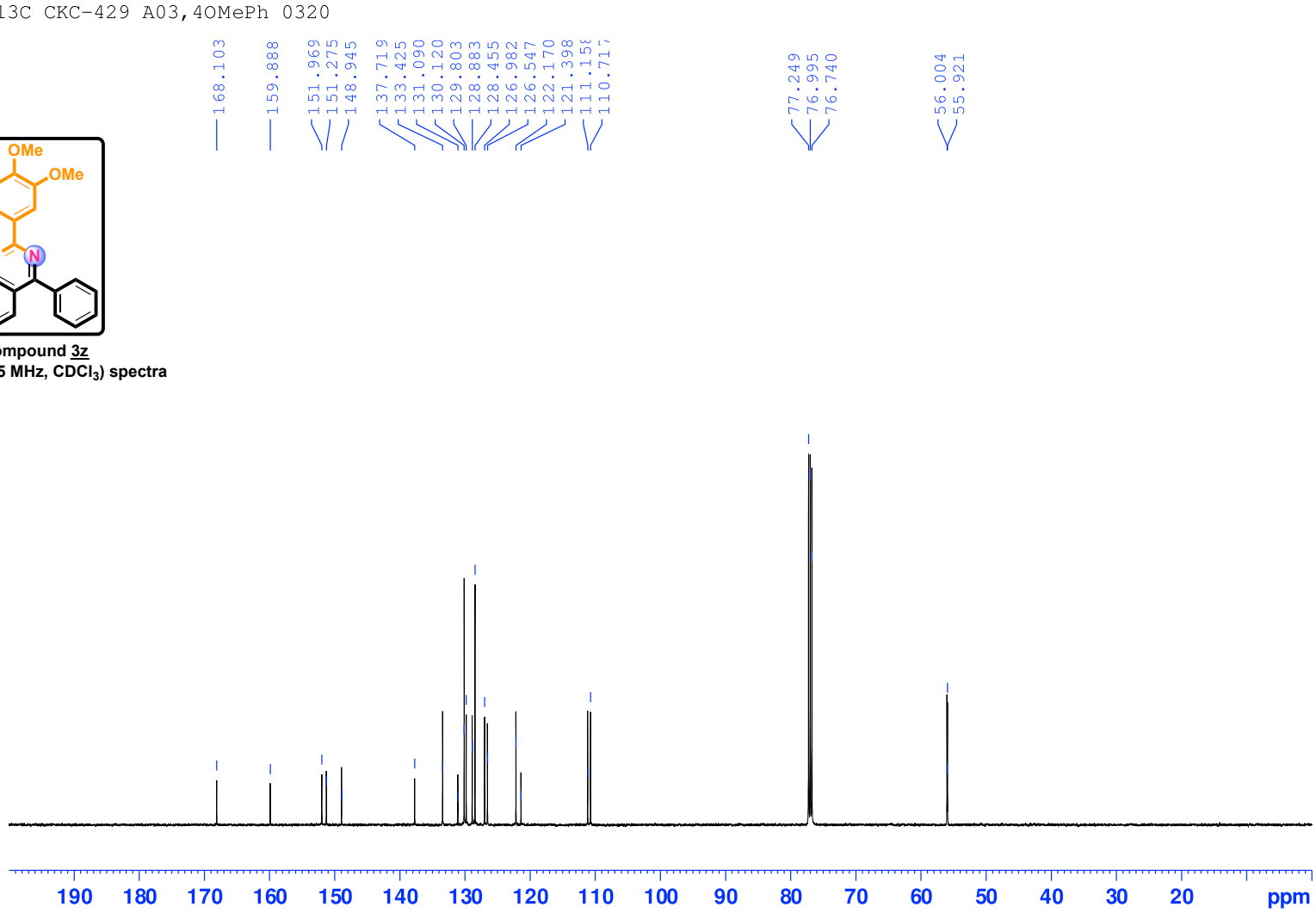


Compound 3z

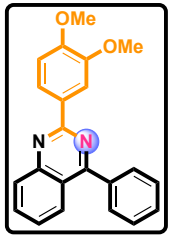


Compound 3z

^{13}C NMR (125 MHz, $CDCl_3$) spectra

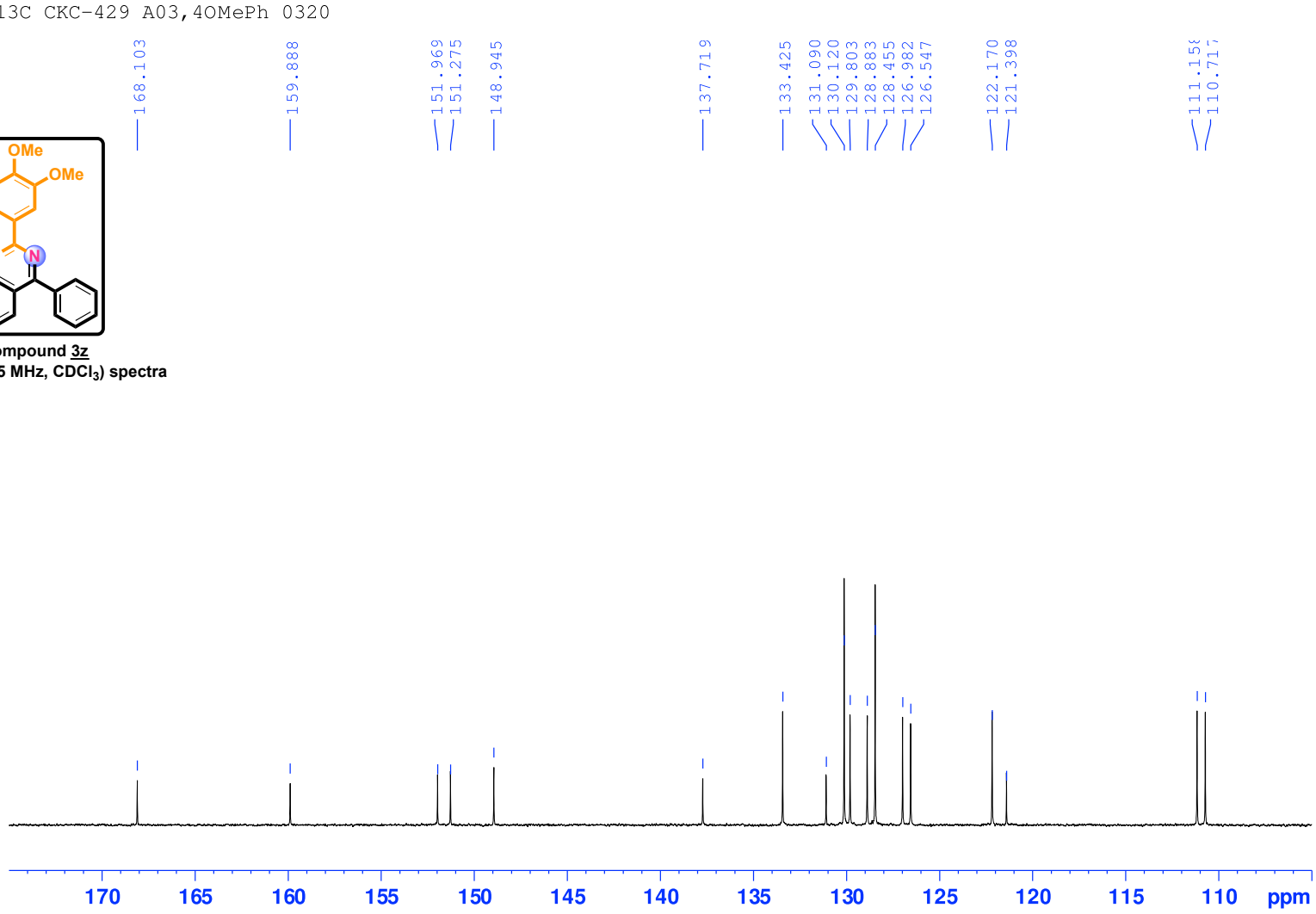


Compound 3z

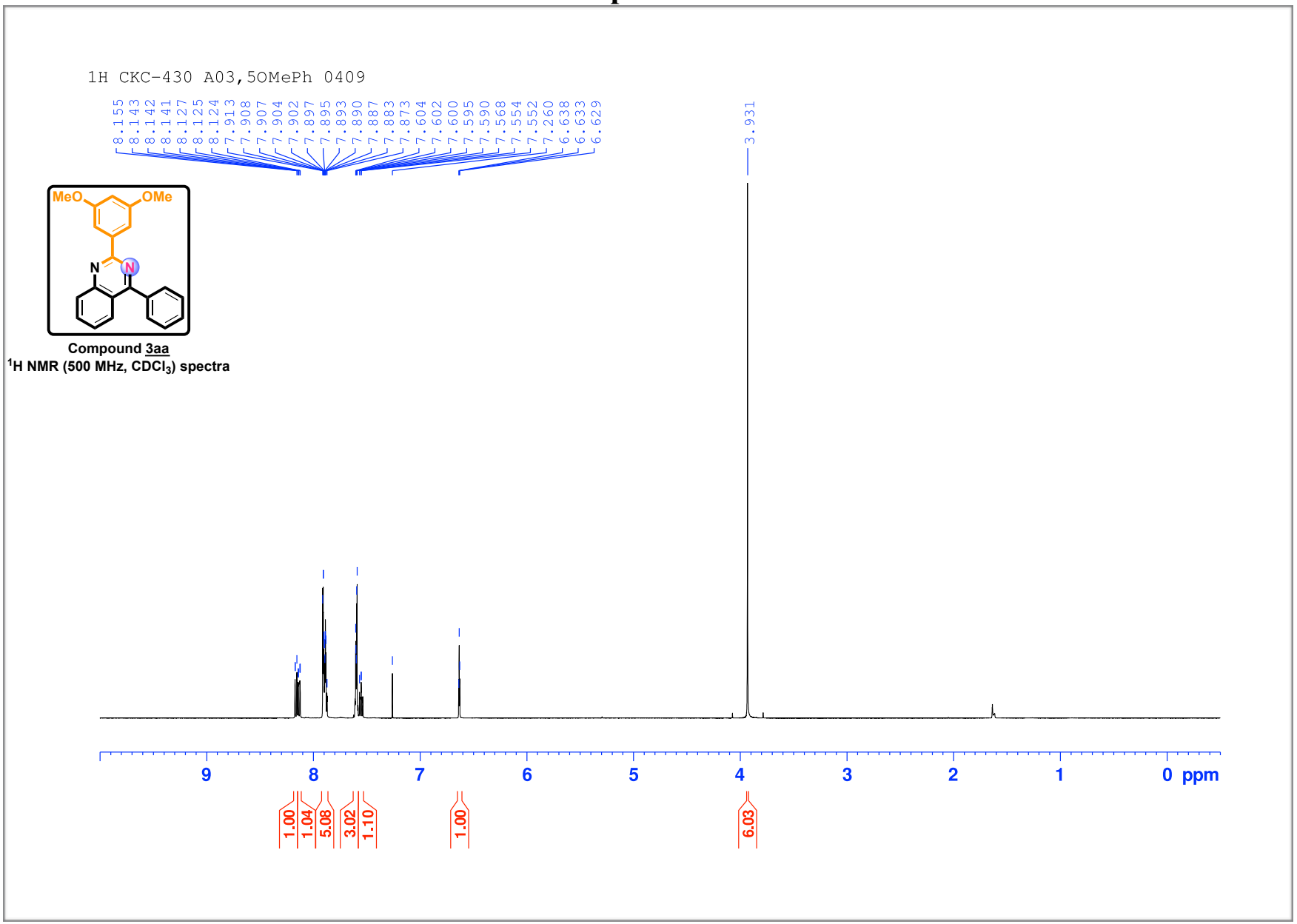


Compound 3z

^{13}C NMR (125 MHz, $CDCl_3$) spectra

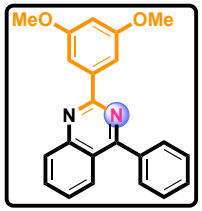


Compound 3aa

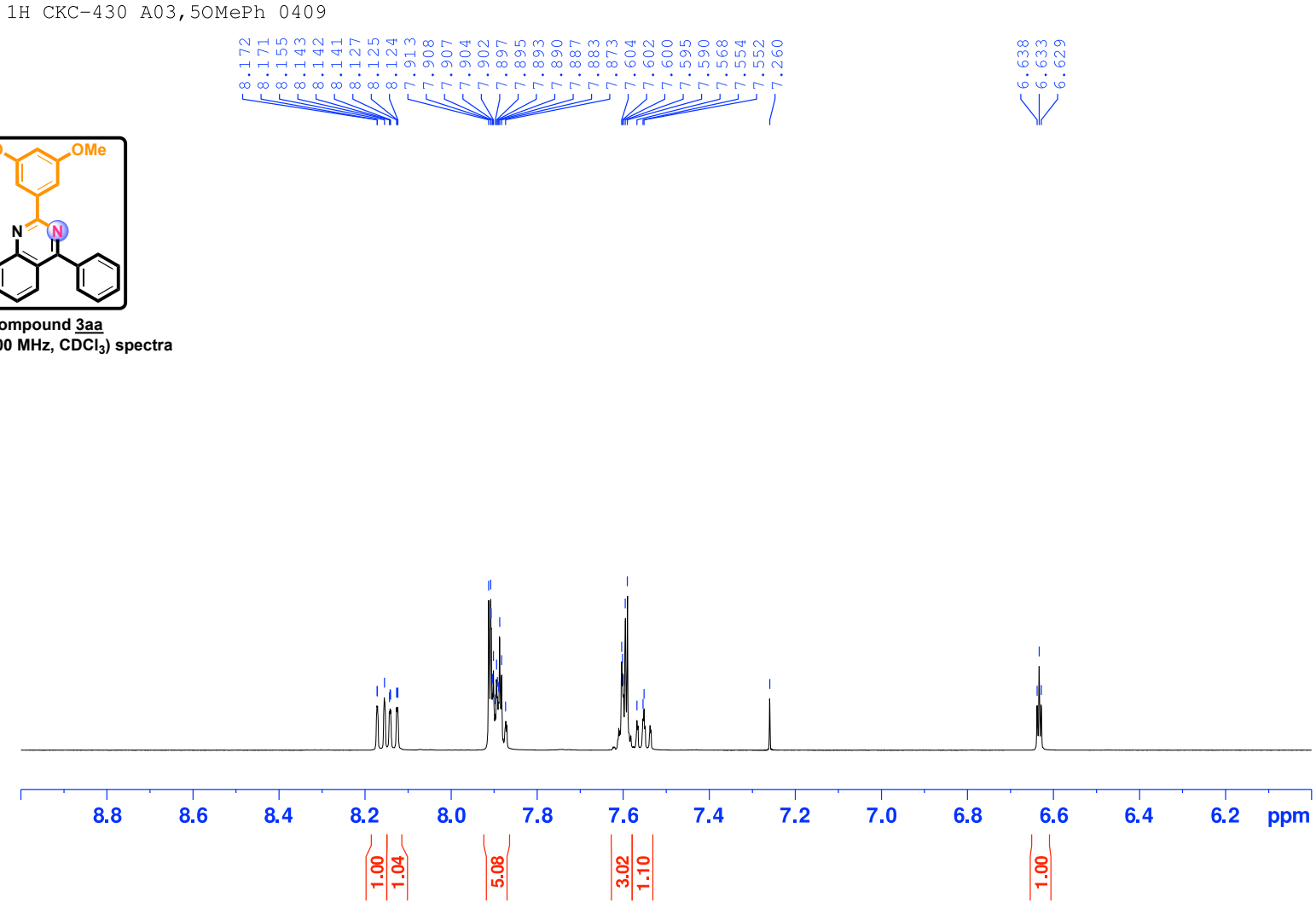


Compound 3aa
^{1}H NMR (500 MHz, $CDCl_3$) spectra

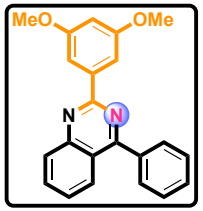
Compound 3aa



Compound 3aa
^{1}H NMR (500 MHz, $CDCl_3$) spectra

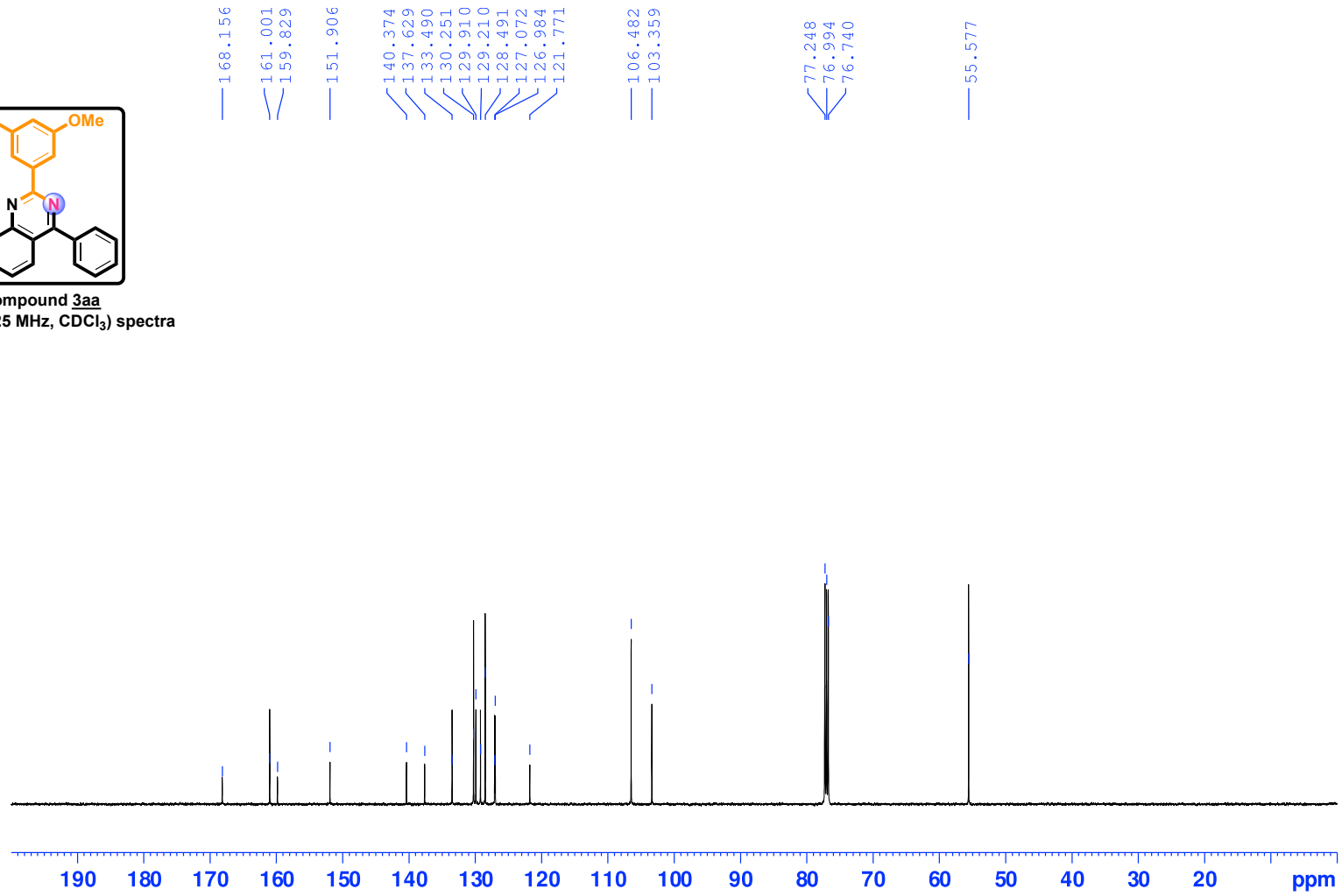


Compound 3aa

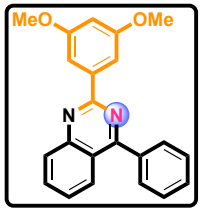


Compound 3aa

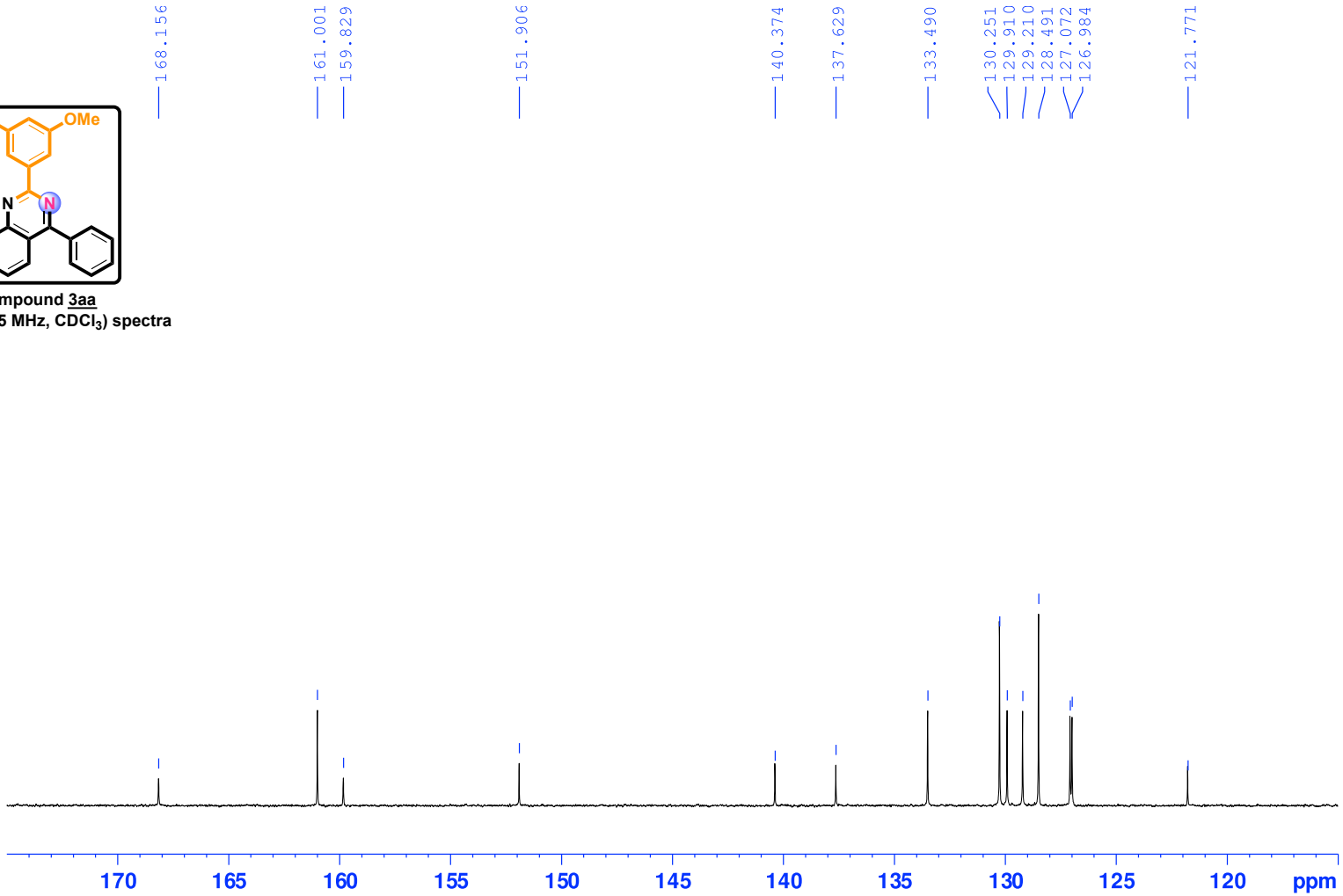
^{13}C NMR (125 MHz, $CDCl_3$) spectra



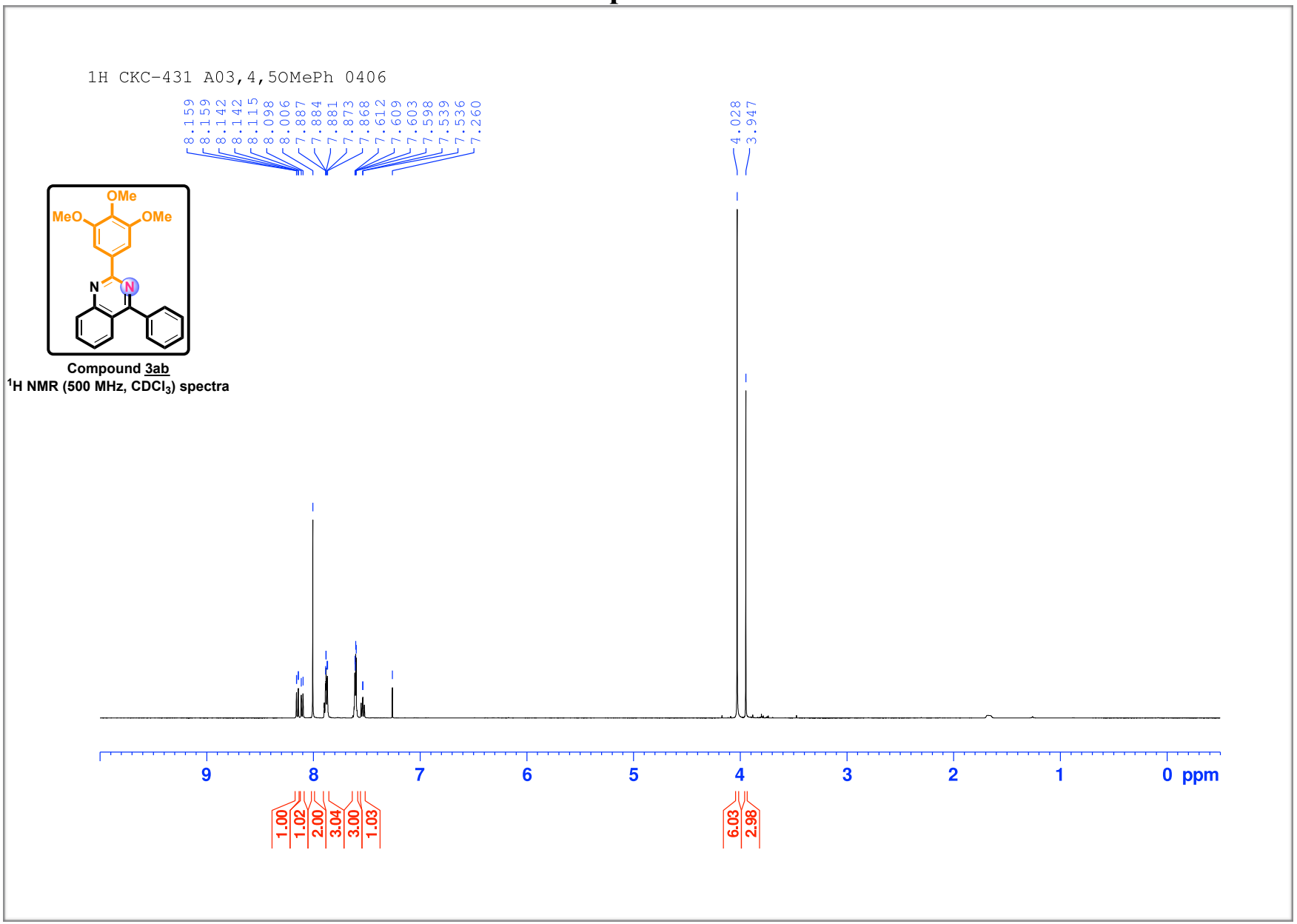
Compound 3aa



Compound 3aa
^{13}C NMR (125 MHz, $CDCl_3$) spectra

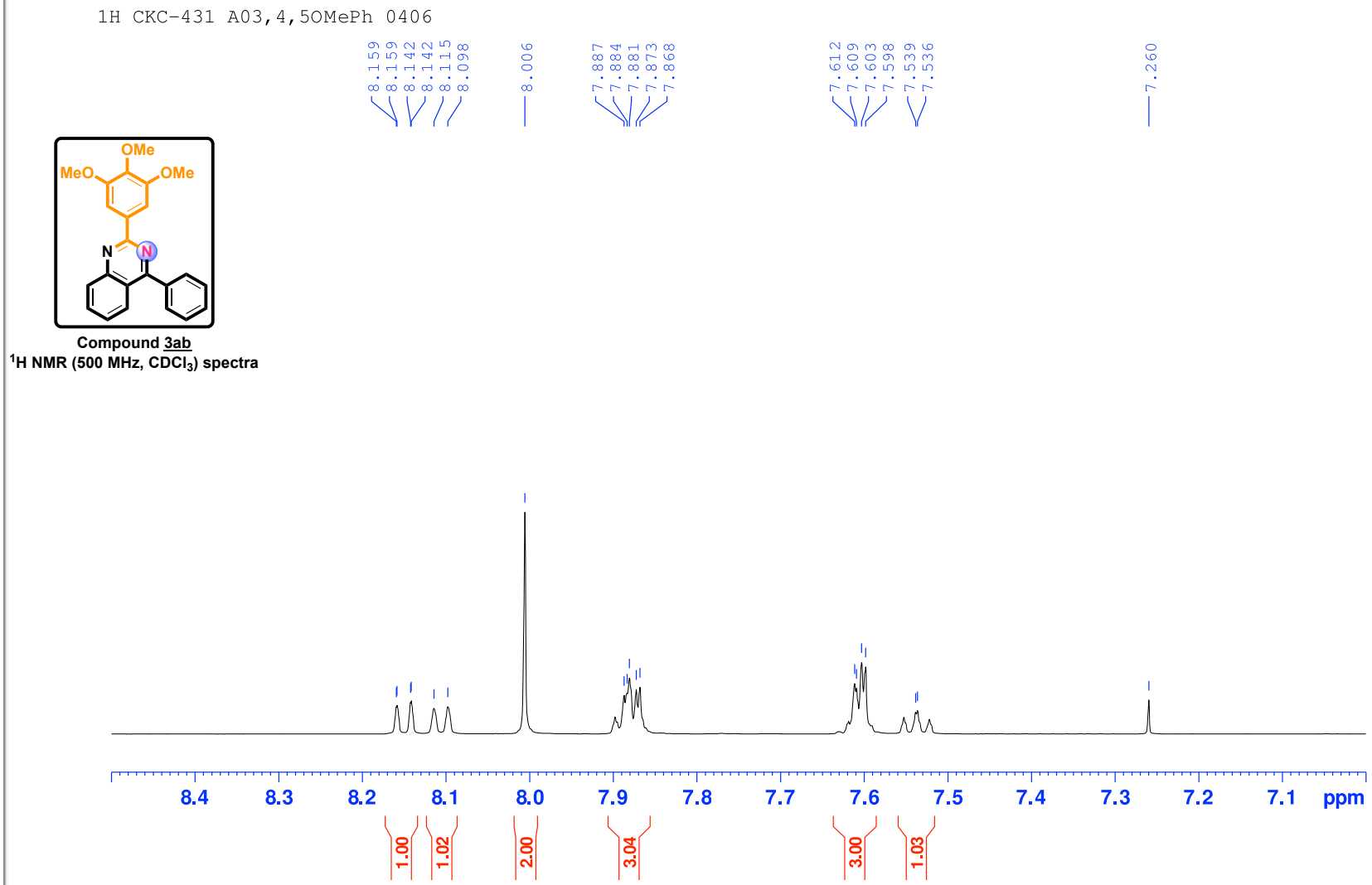


Compound 3ab



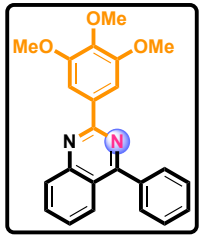
Compound 3ab
^{1}H NMR (500 MHz, $CDCl_3$) spectra

Compound 3ab



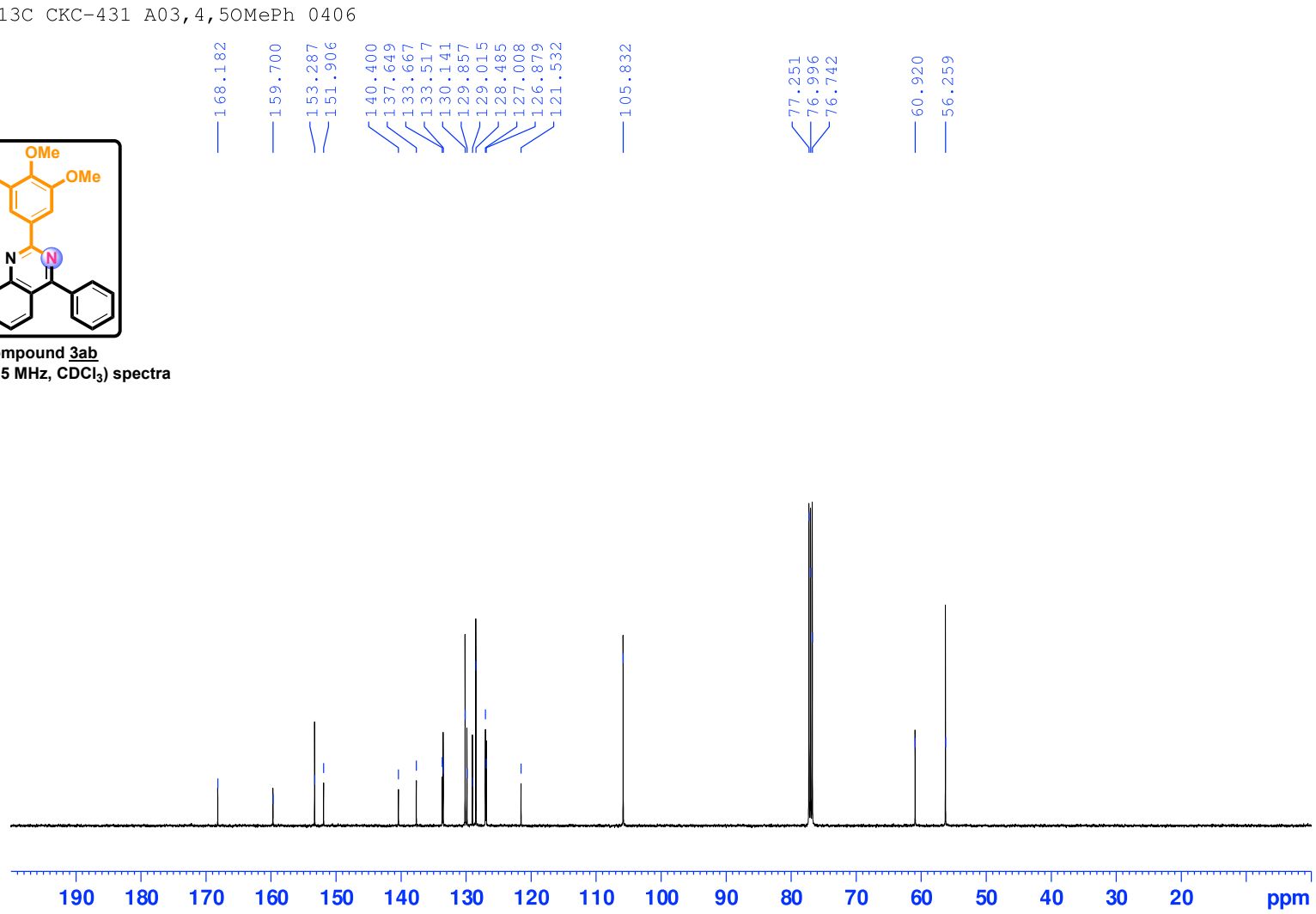
Compound 3ab
^{1}H NMR (500 MHz, $CDCl_3$) spectra

Compound 3ab

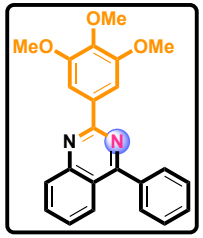


Compound 3ab

^{13}C NMR (125 MHz, $CDCl_3$) spectra

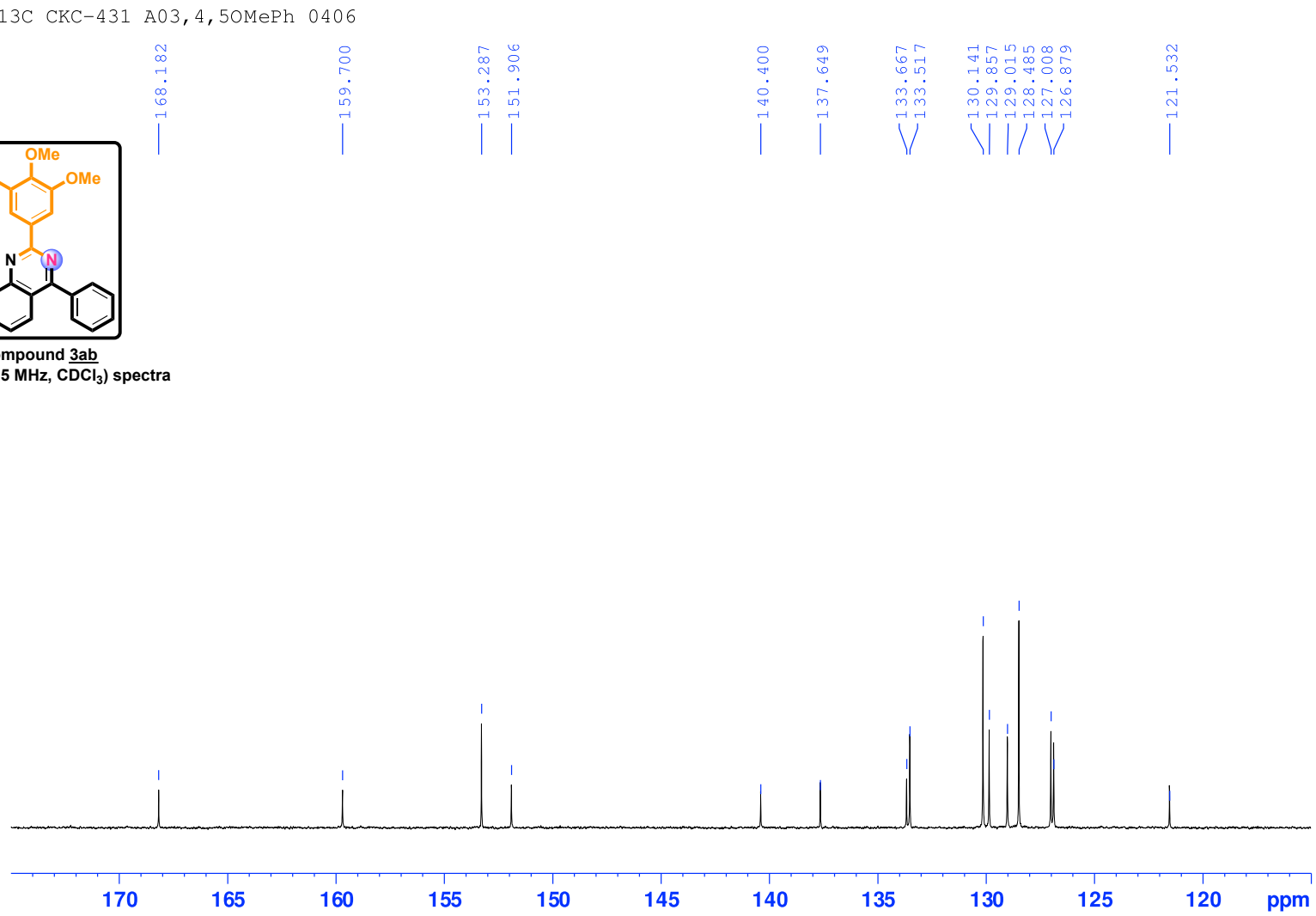


Compound 3ab

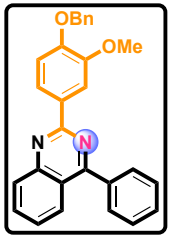


Compound 3ab

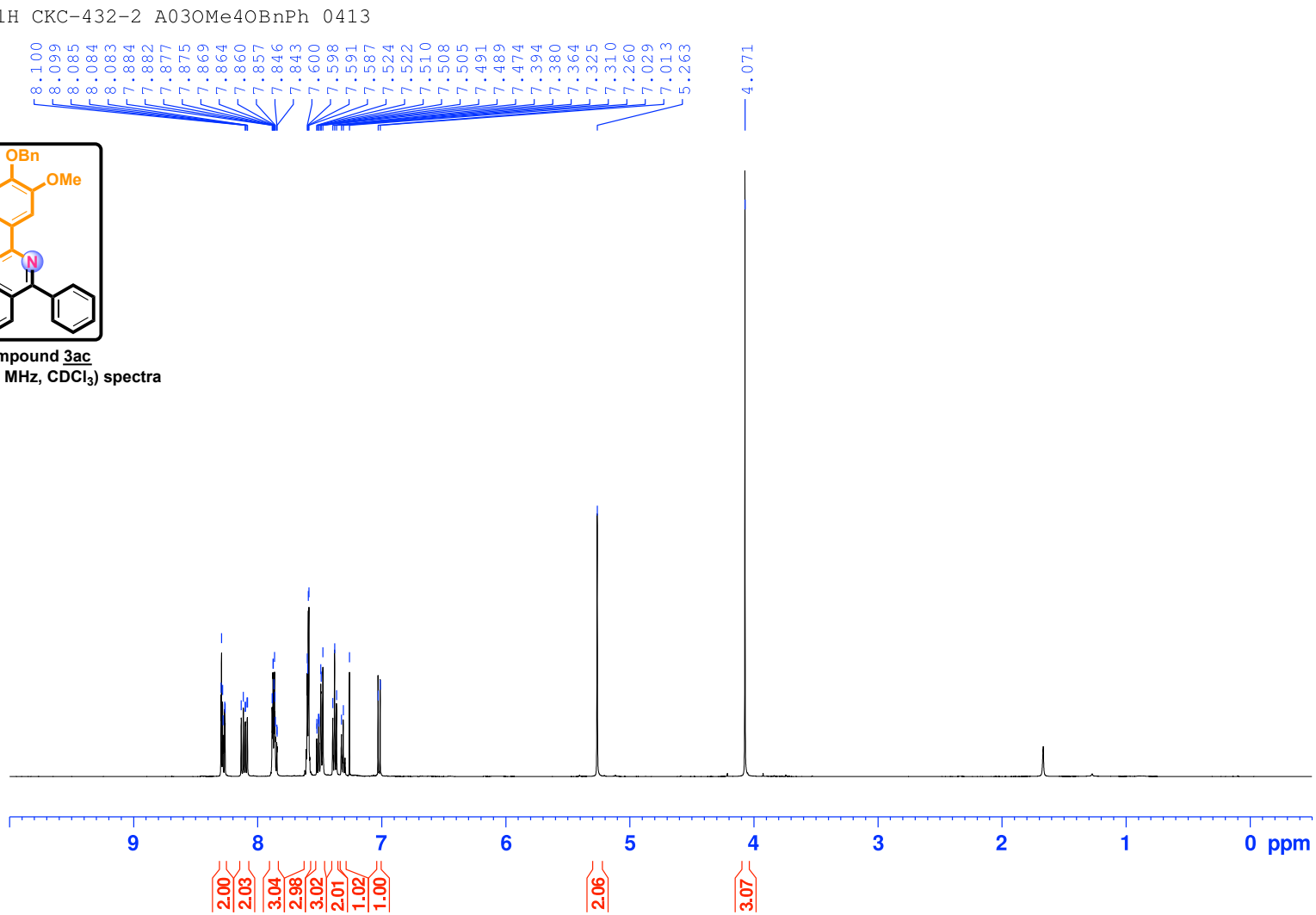
^{13}C NMR (125 MHz, $CDCl_3$) spectra



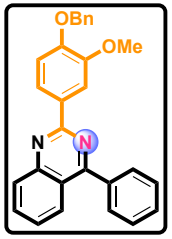
Compound 3ac



Compound 3ac
^{1}H NMR (500 MHz, $CDCl_3$) spectra

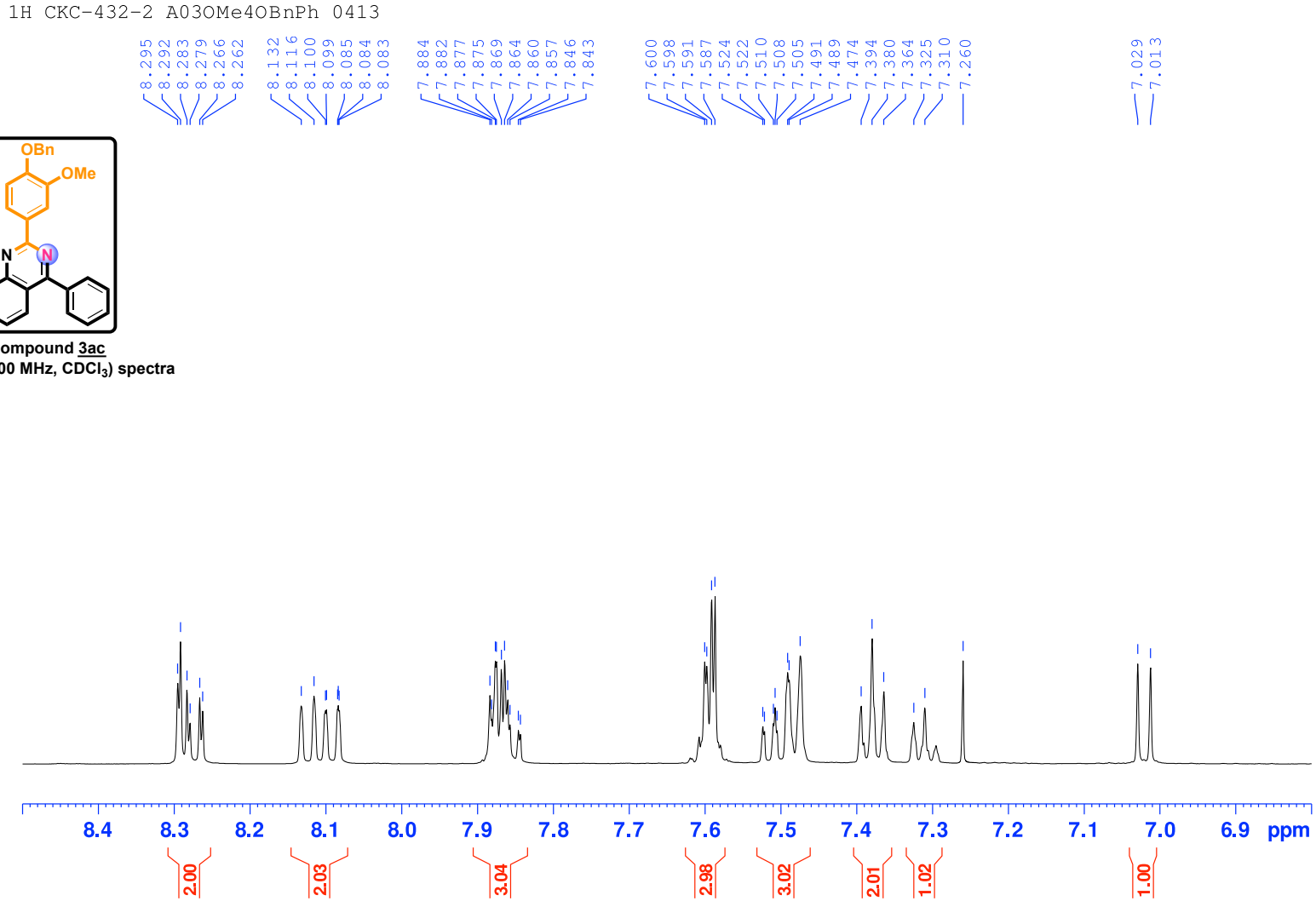


Compound 3ac

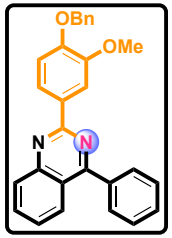


Compound 3ac

^{1}H NMR (500 MHz, $CDCl_3$) spectra

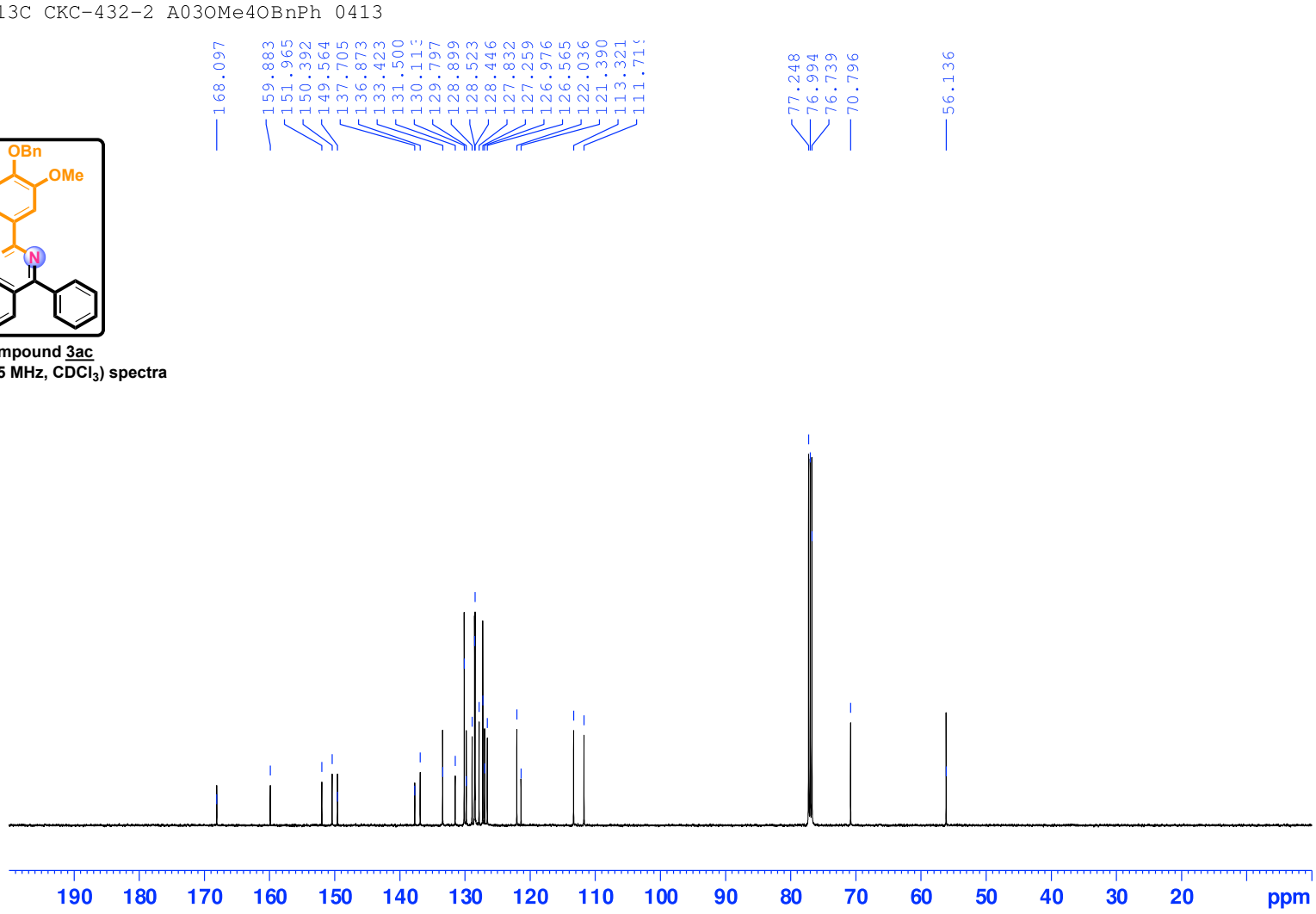


Compound 3ac

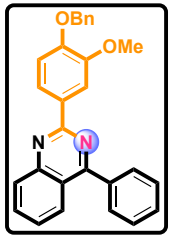


Compound 3ac

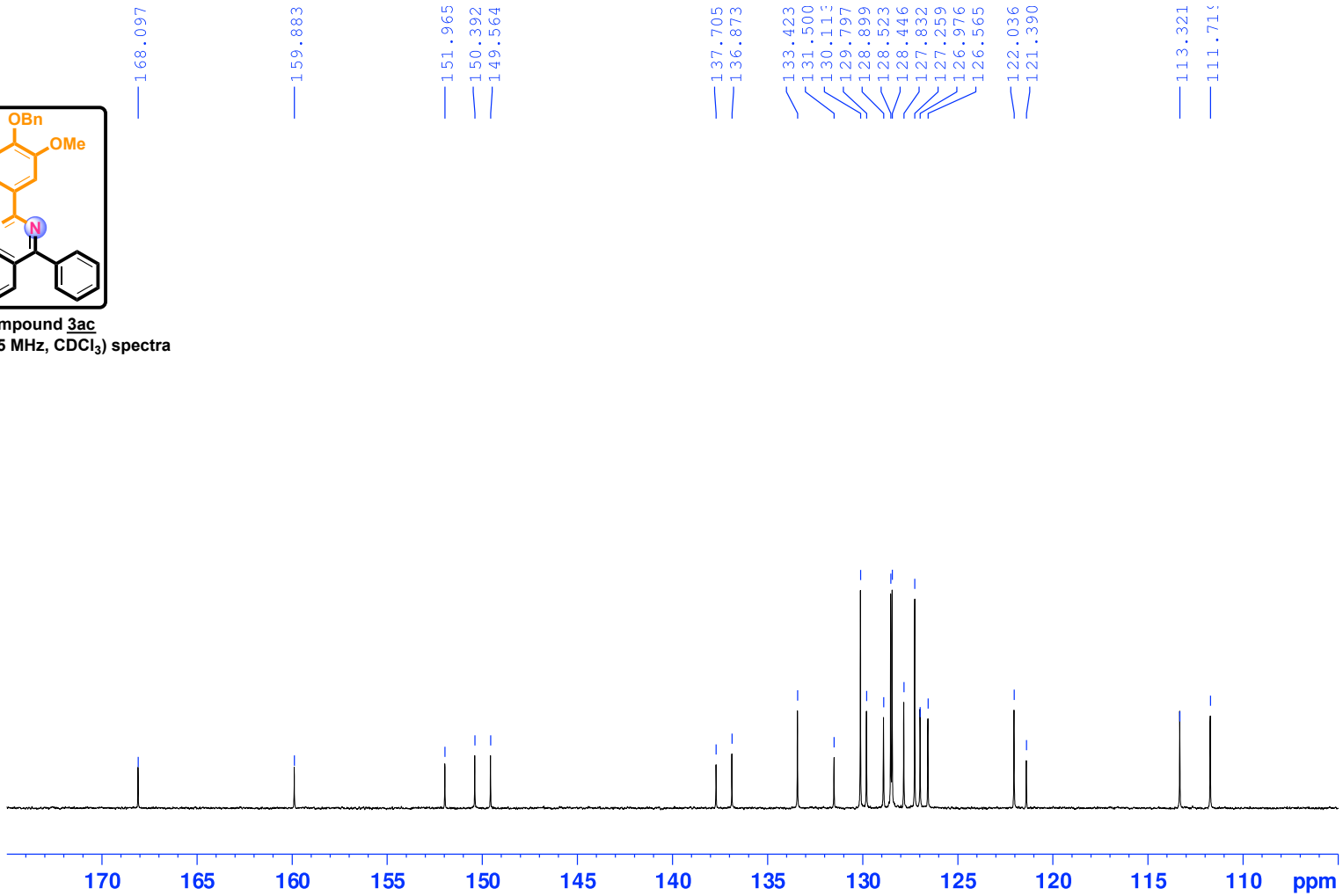
^{13}C NMR (125 MHz, $CDCl_3$) spectra



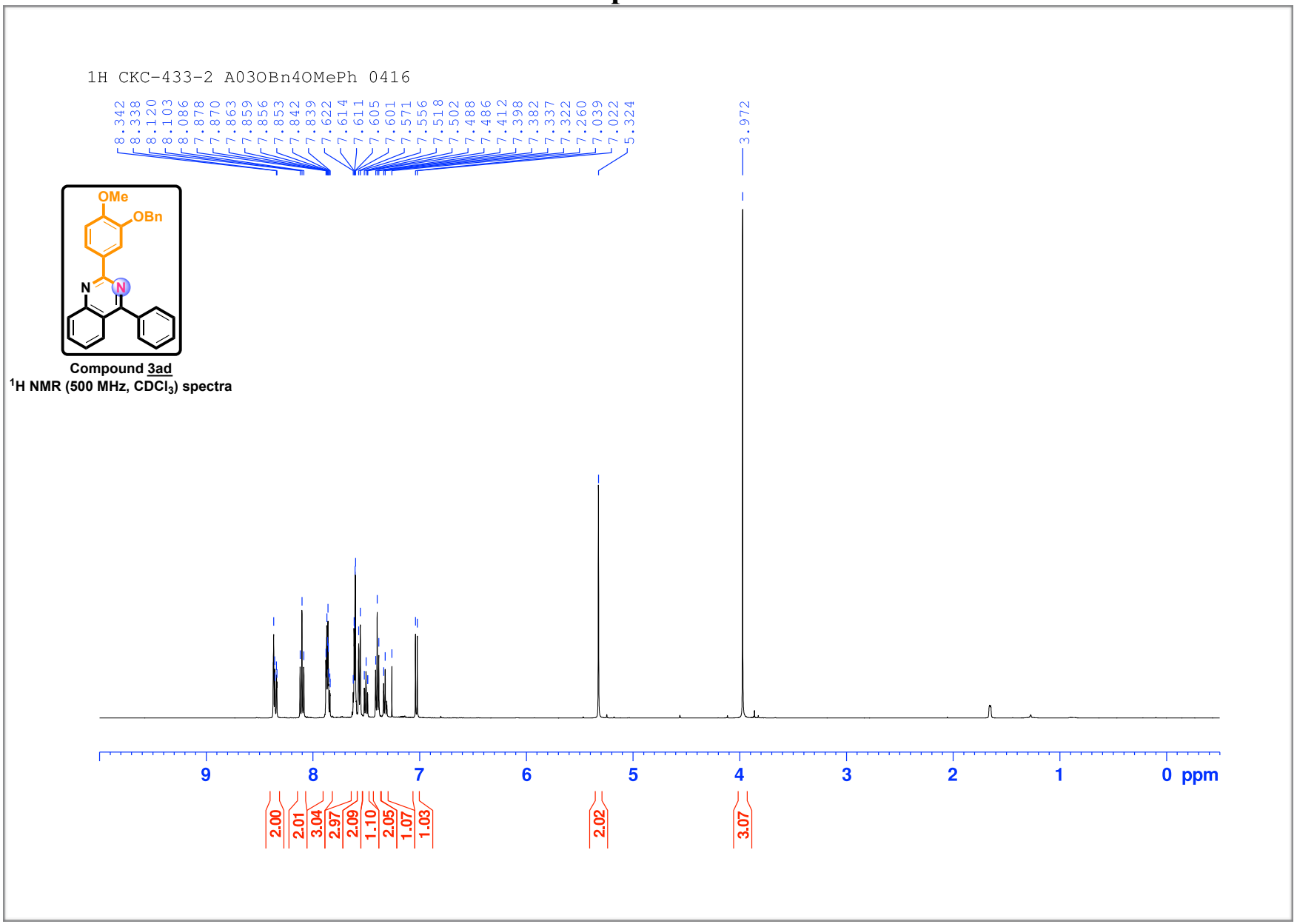
Compound 3ac



Compound 3ac
^{13}C NMR (125 MHz, $CDCl_3$) spectra



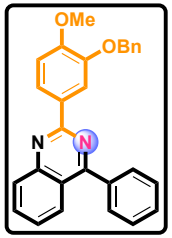
Compound 3ad



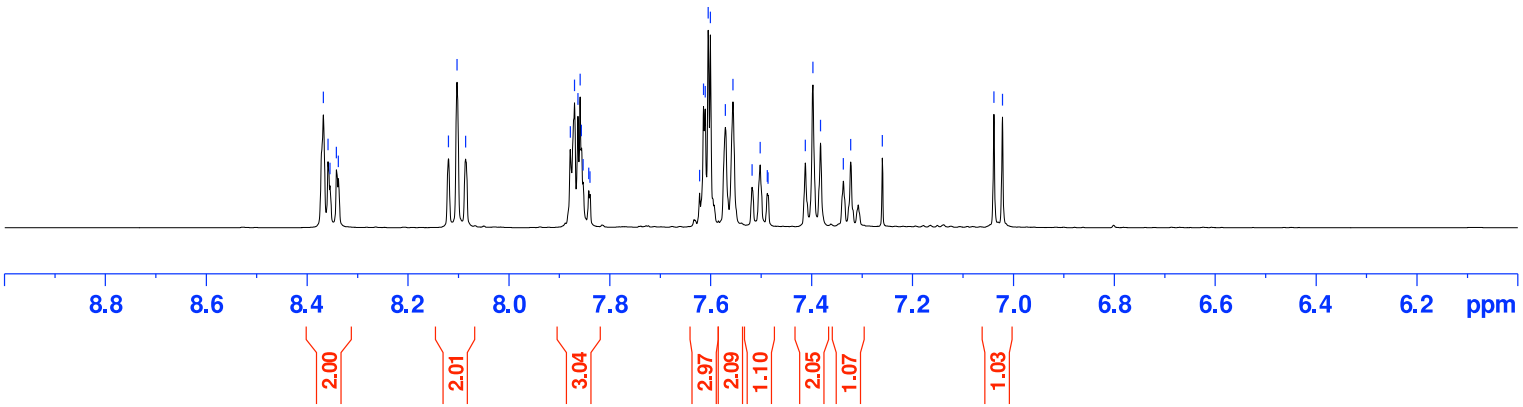
Compound 3ad

^{1}H NMR (500 MHz, $CDCl_3$) spectra

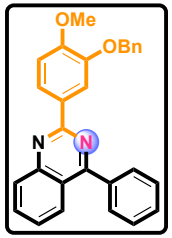
Compound 3ad



Compound 3ad
^{1}H NMR (500 MHz, $CDCl_3$) spectra

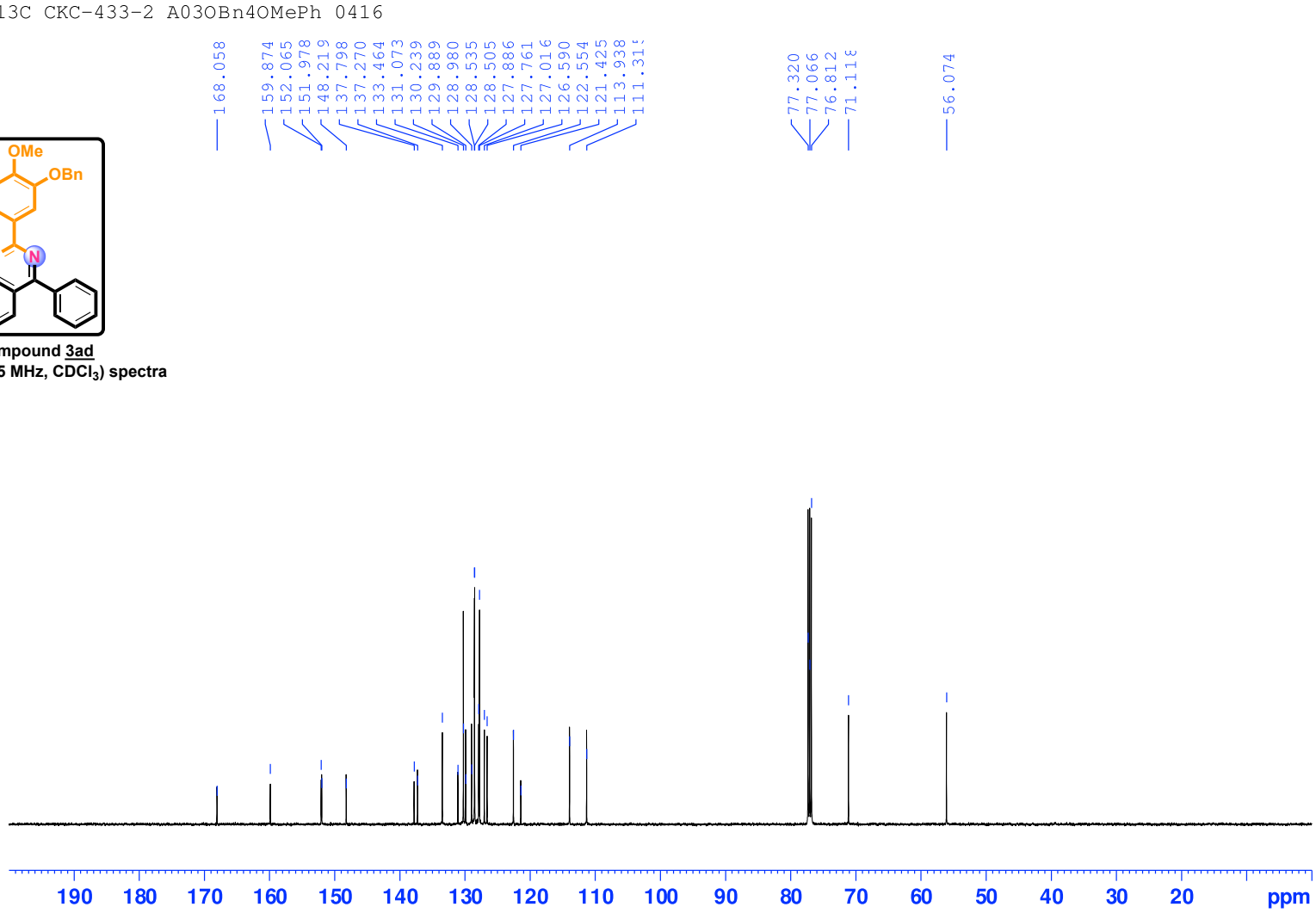


Compound 3ad

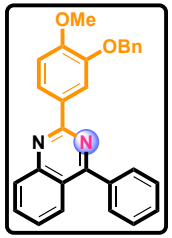


Compound 3ad

^{13}C NMR (125 MHz, $CDCl_3$) spectra

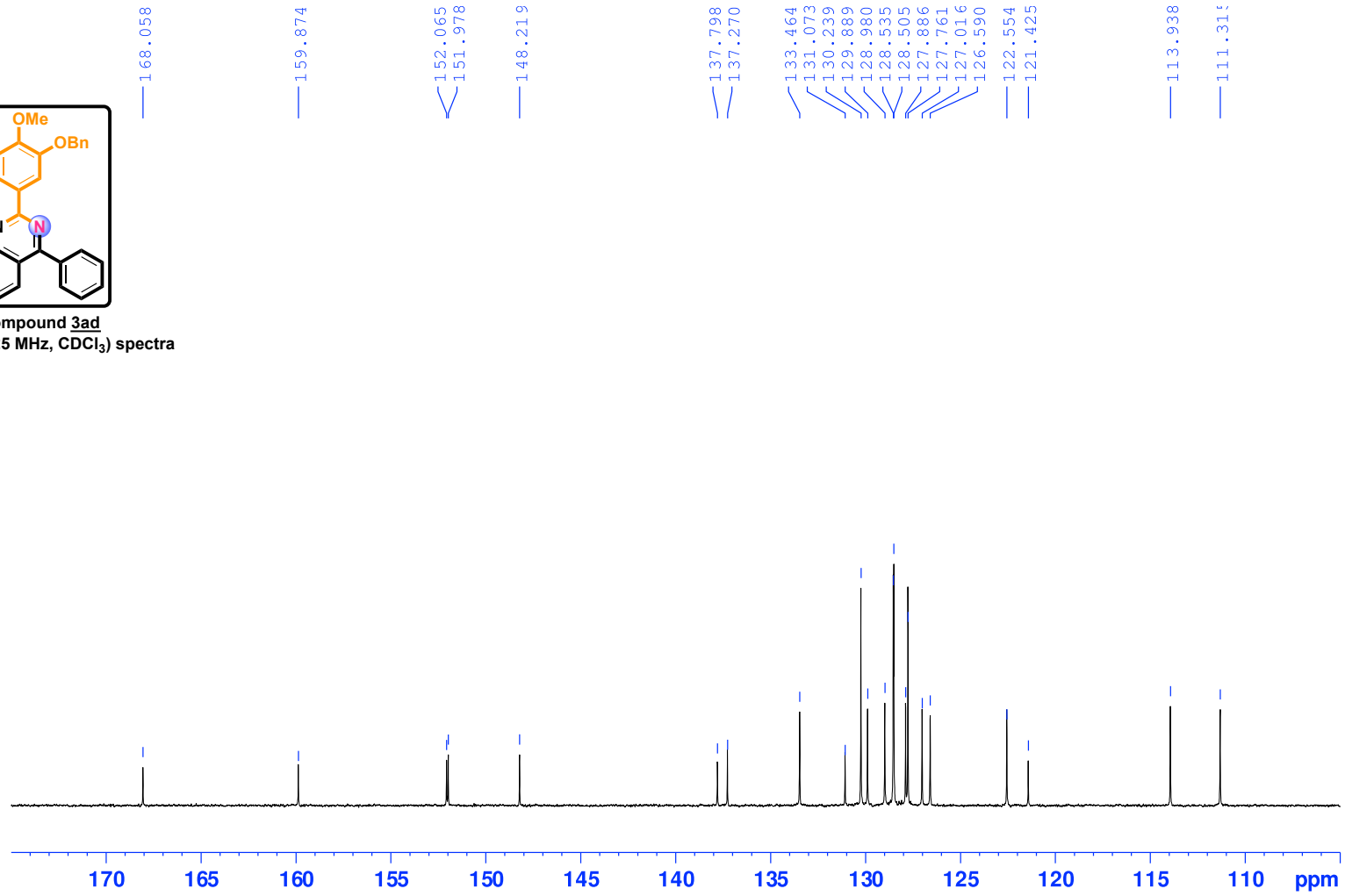


Compound 3ad

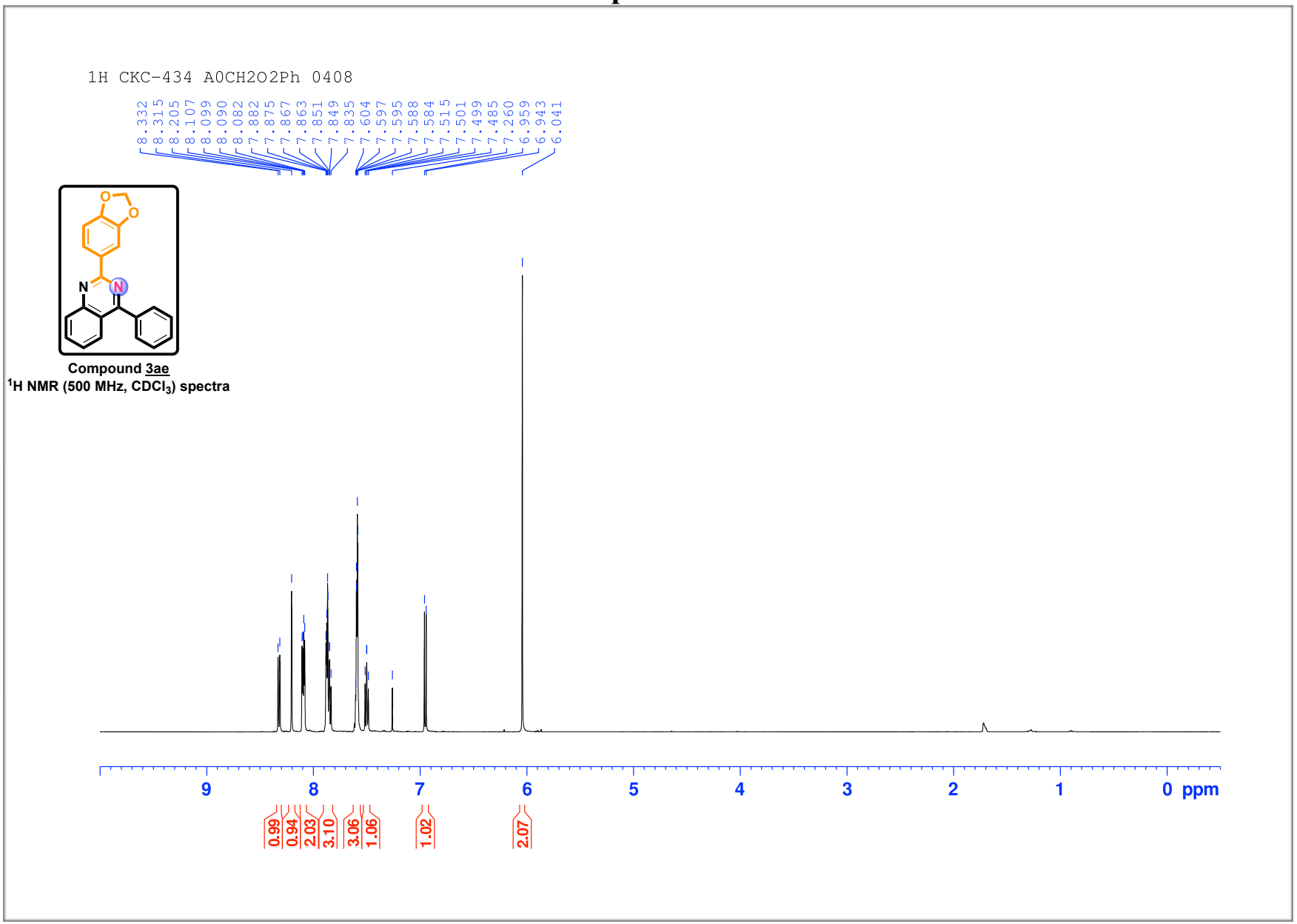


Compound 3ad

^{13}C NMR (125 MHz, $CDCl_3$) spectra

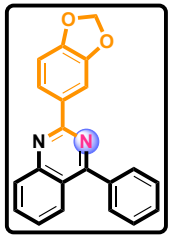


Compound 3ae

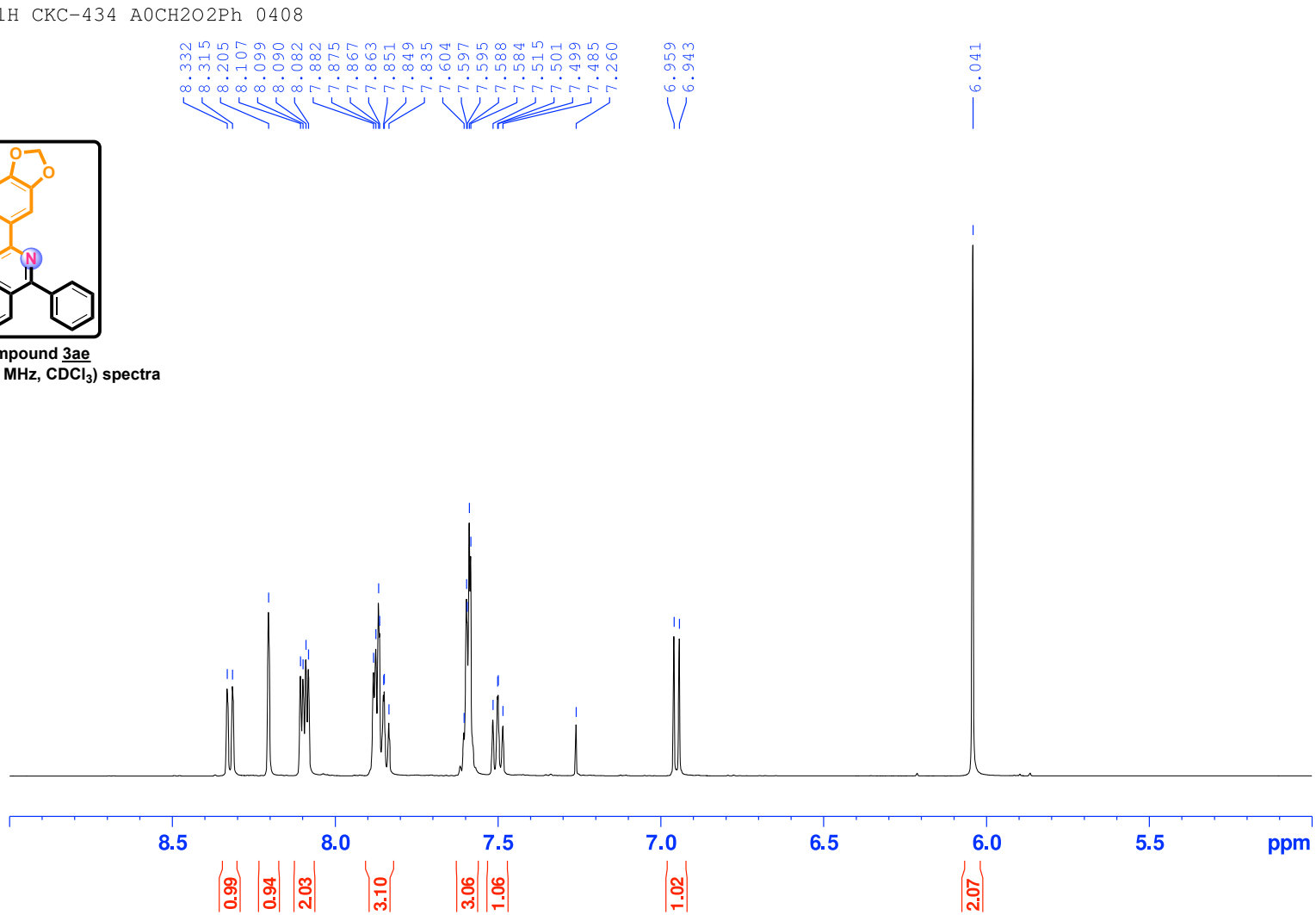


Compound 3ae
^{1}H NMR (500 MHz, $CDCl_3$) spectra

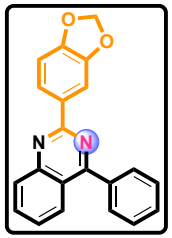
Compound 3ae



Compound 3ae
^{1}H NMR (500 MHz, $CDCl_3$) spectra

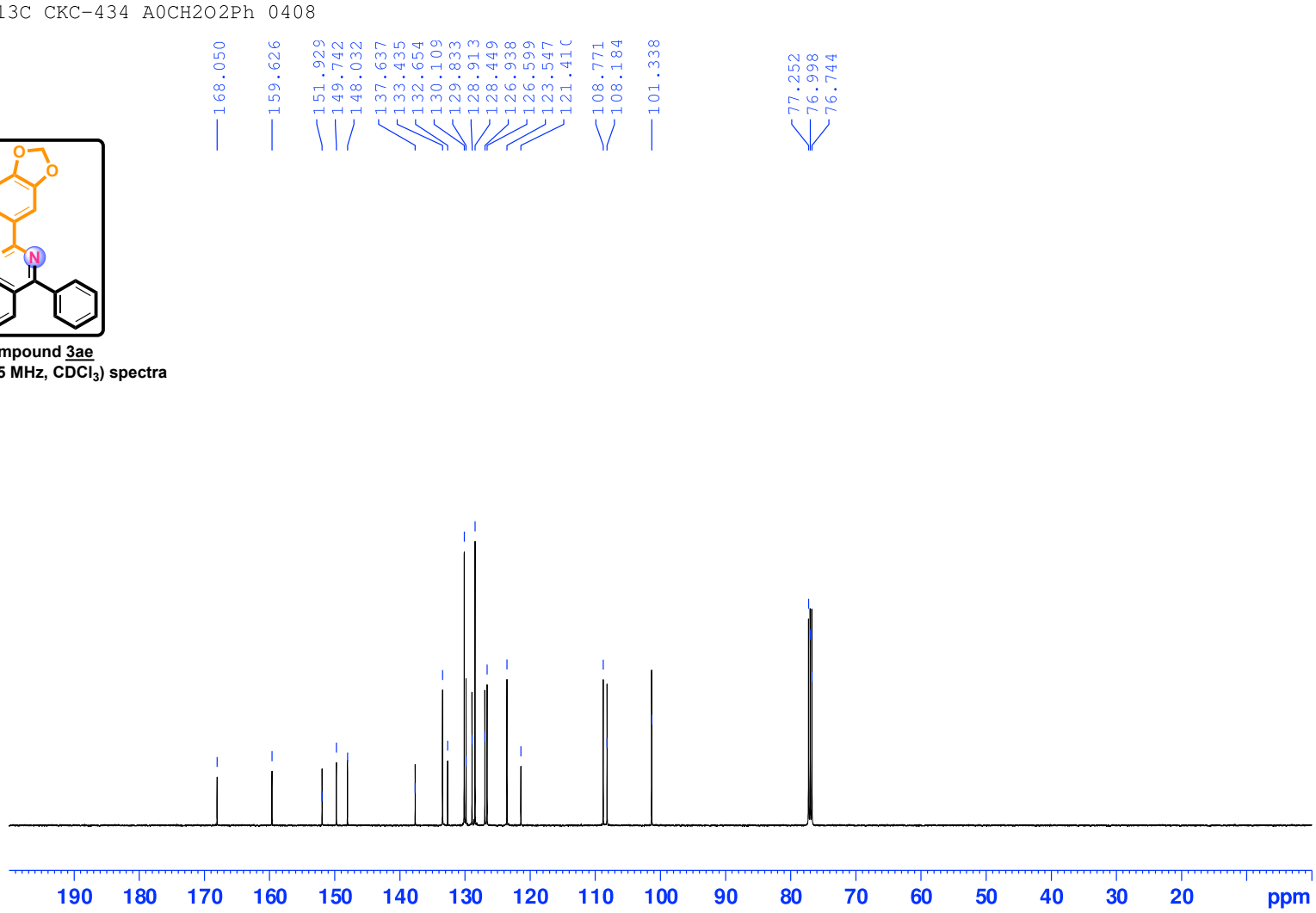


Compound 3ae



Compound 3ae

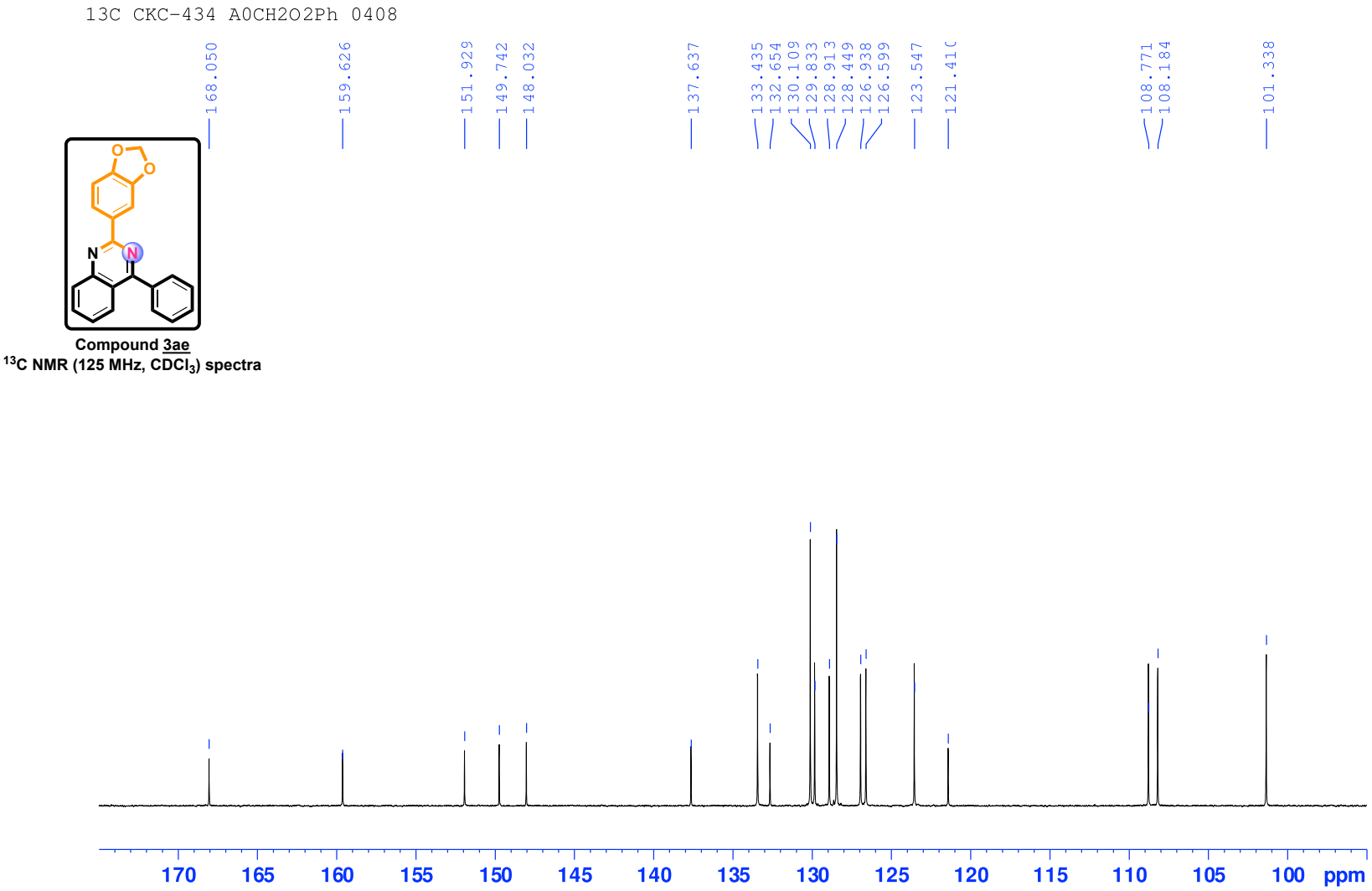
^{13}C NMR (125 MHz, $CDCl_3$) spectra



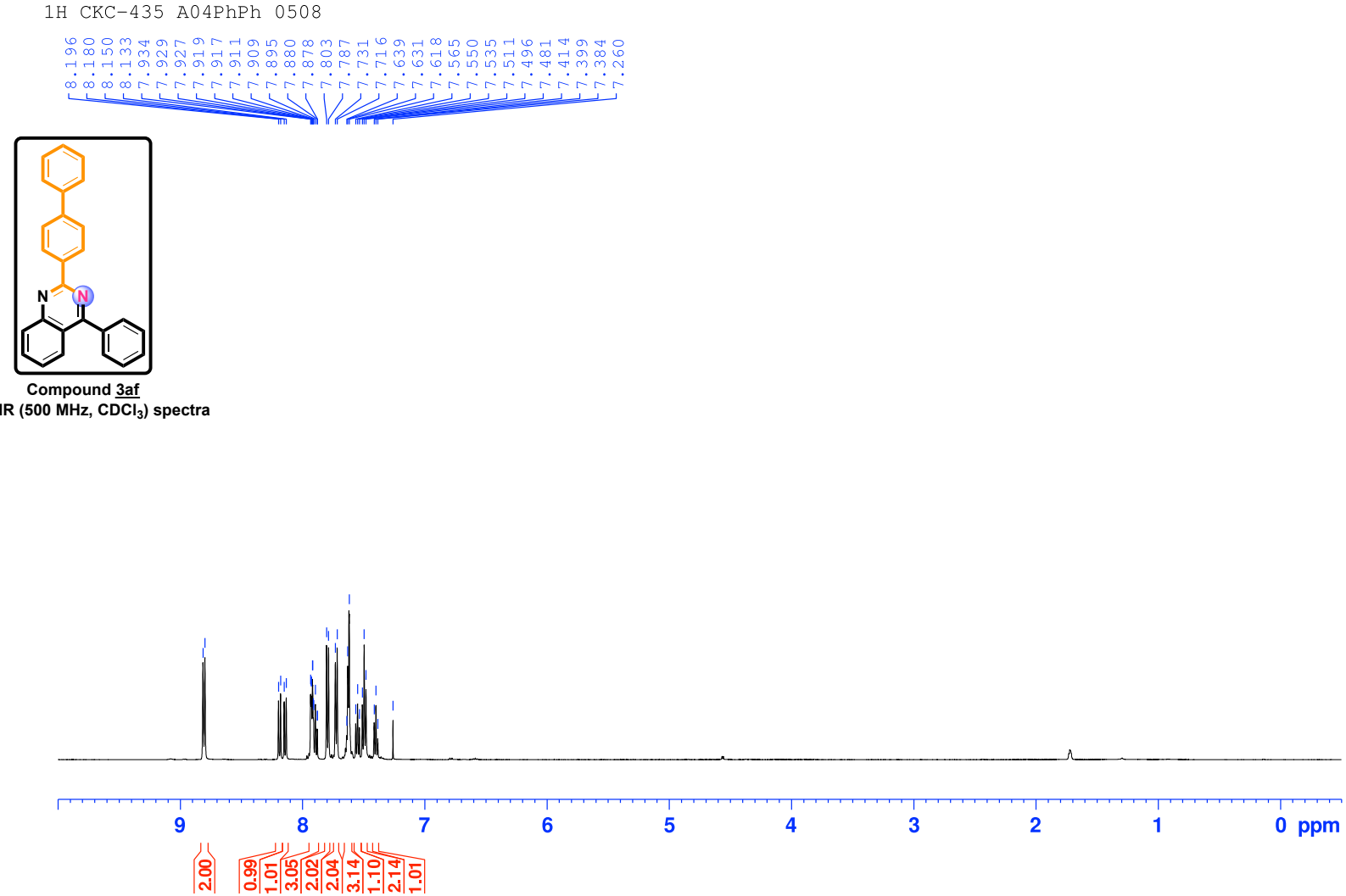
Compound 3ae

Compound 3ae

^{13}C NMR (125 MHz, $CDCl_3$) spectra

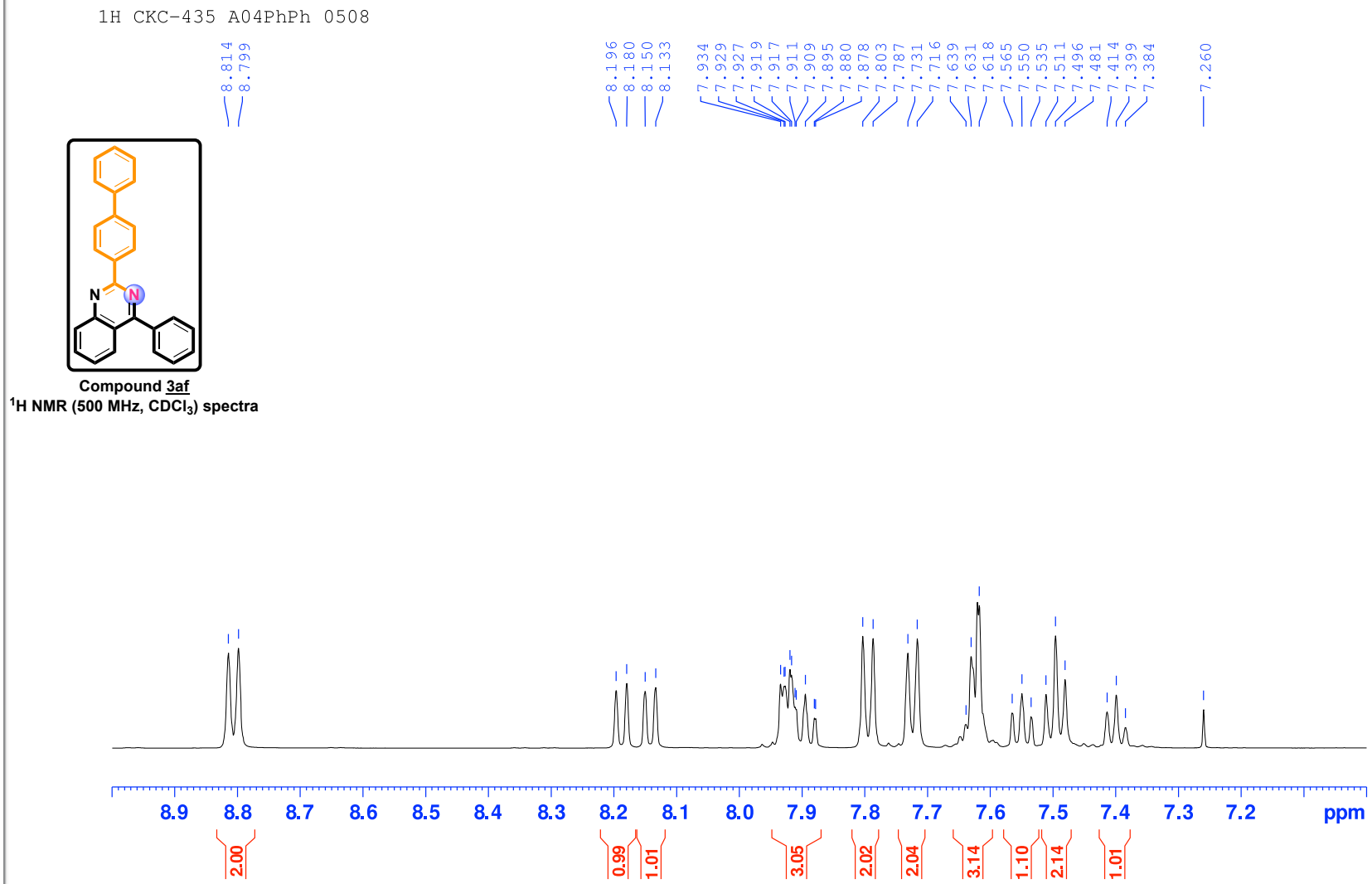


Compound 3af



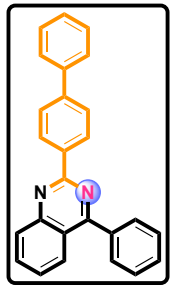
Compound 3af
^{1}H NMR (500 MHz, $CDCl_3$) spectra

Compound 3af

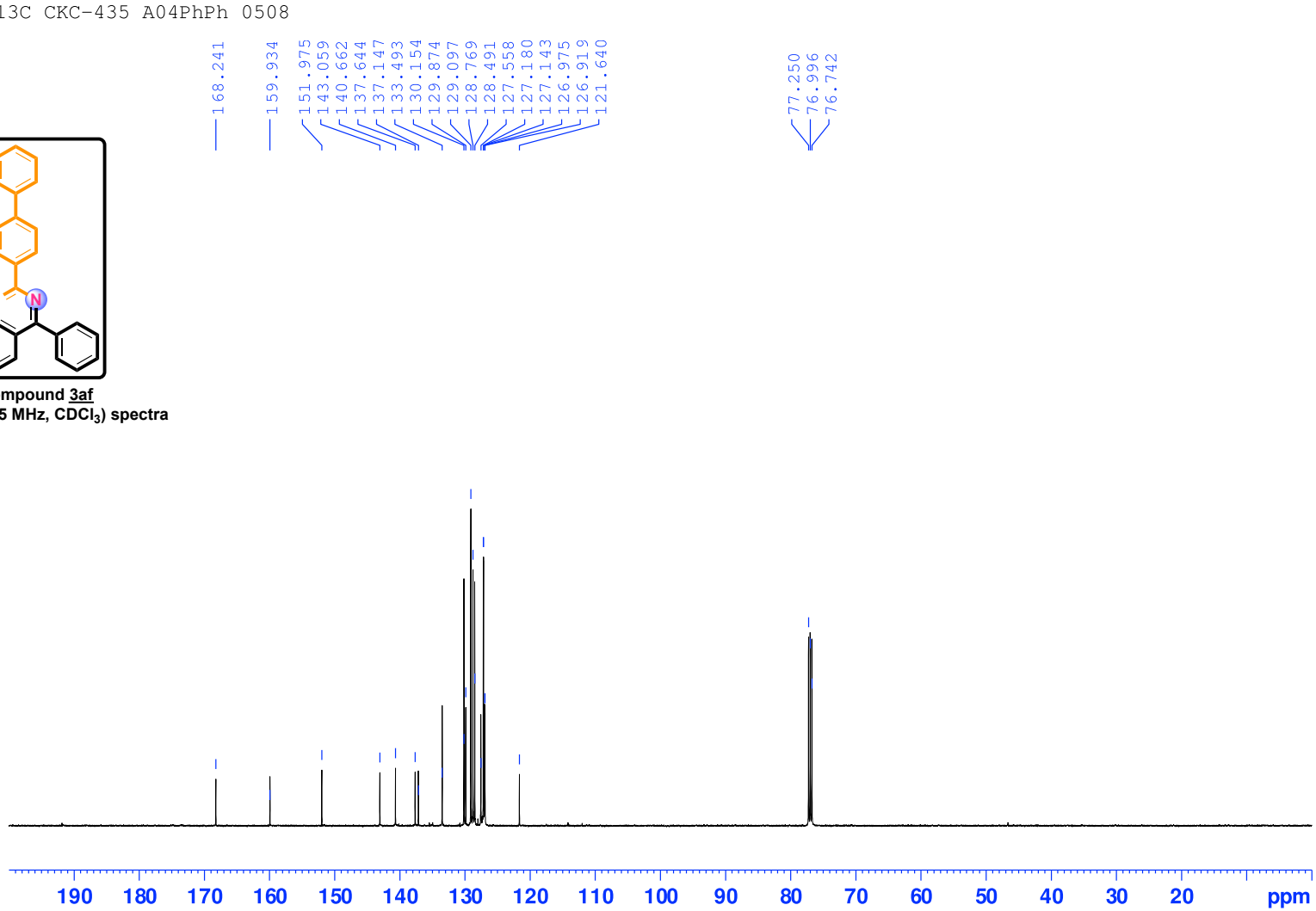


Compound 3af
^{1}H NMR (500 MHz, $CDCl_3$) spectra

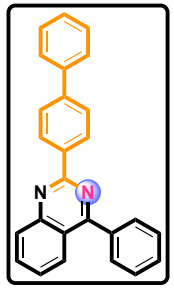
Compound 3af



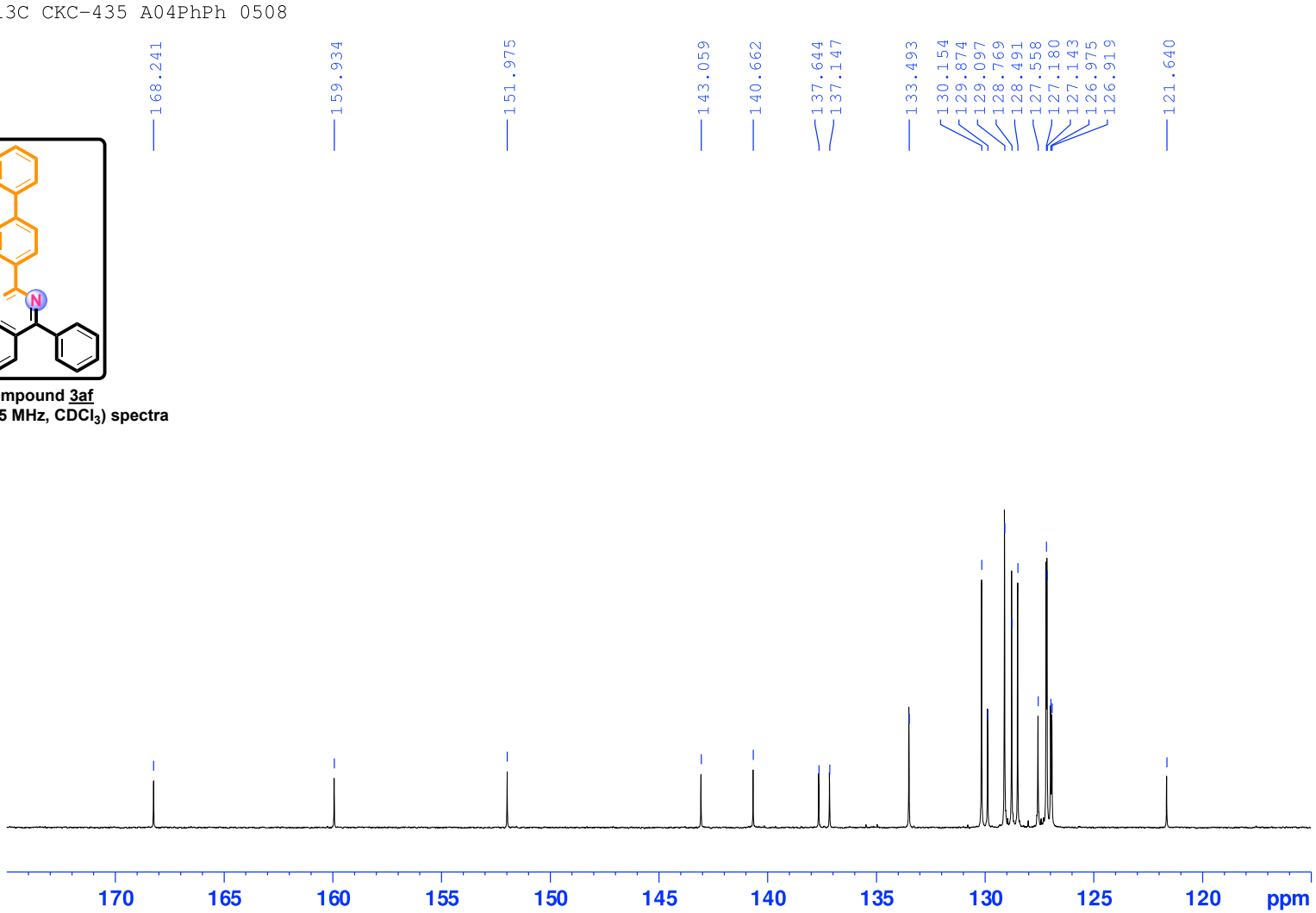
Compound 3af
^{13}C NMR (125 MHz, $CDCl_3$) spectra



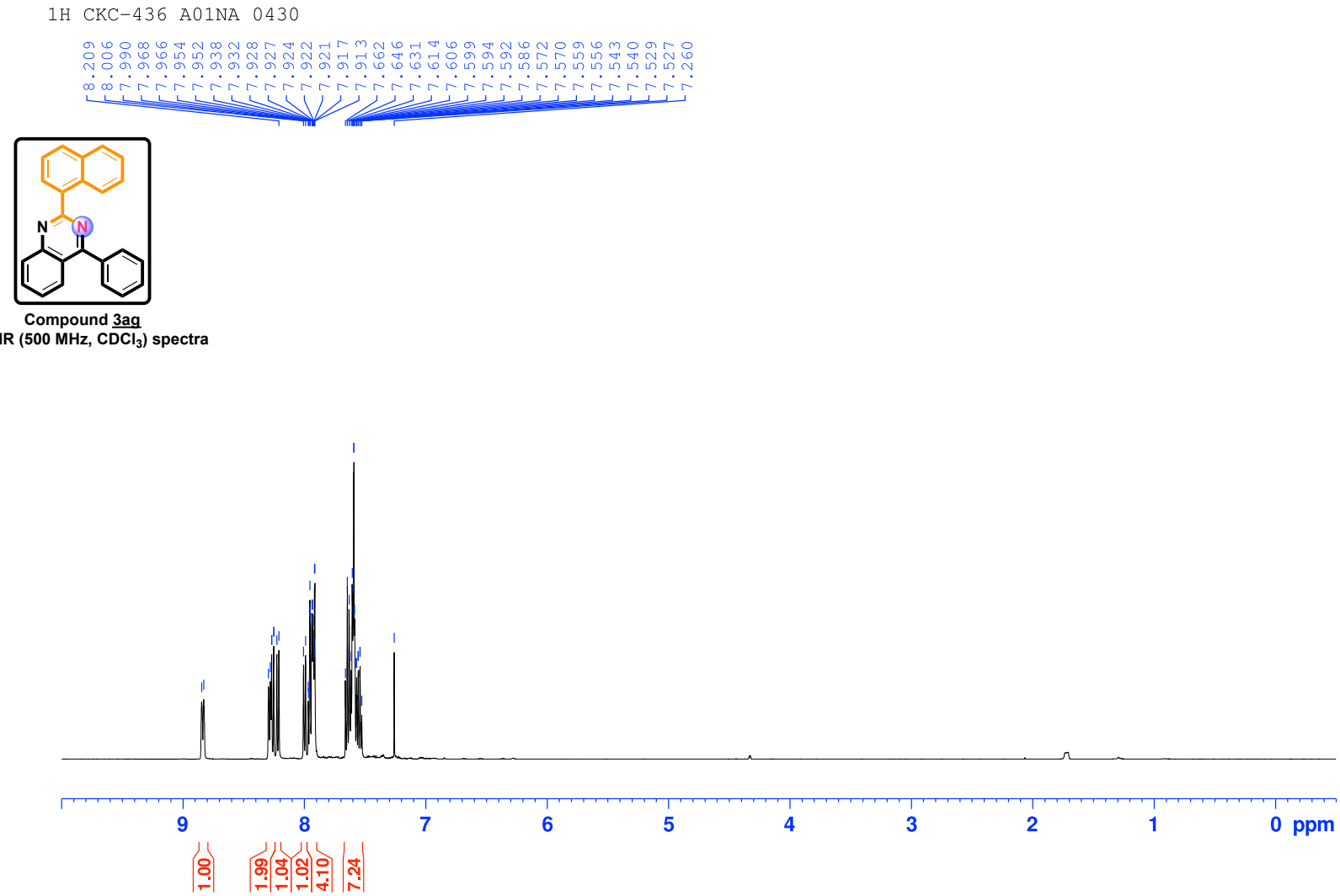
Compound 3af



Compound 3af
^{13}C NMR (125 MHz, $CDCl_3$) spectra

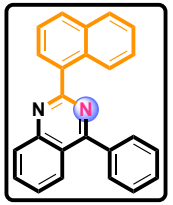


Compound 3ag

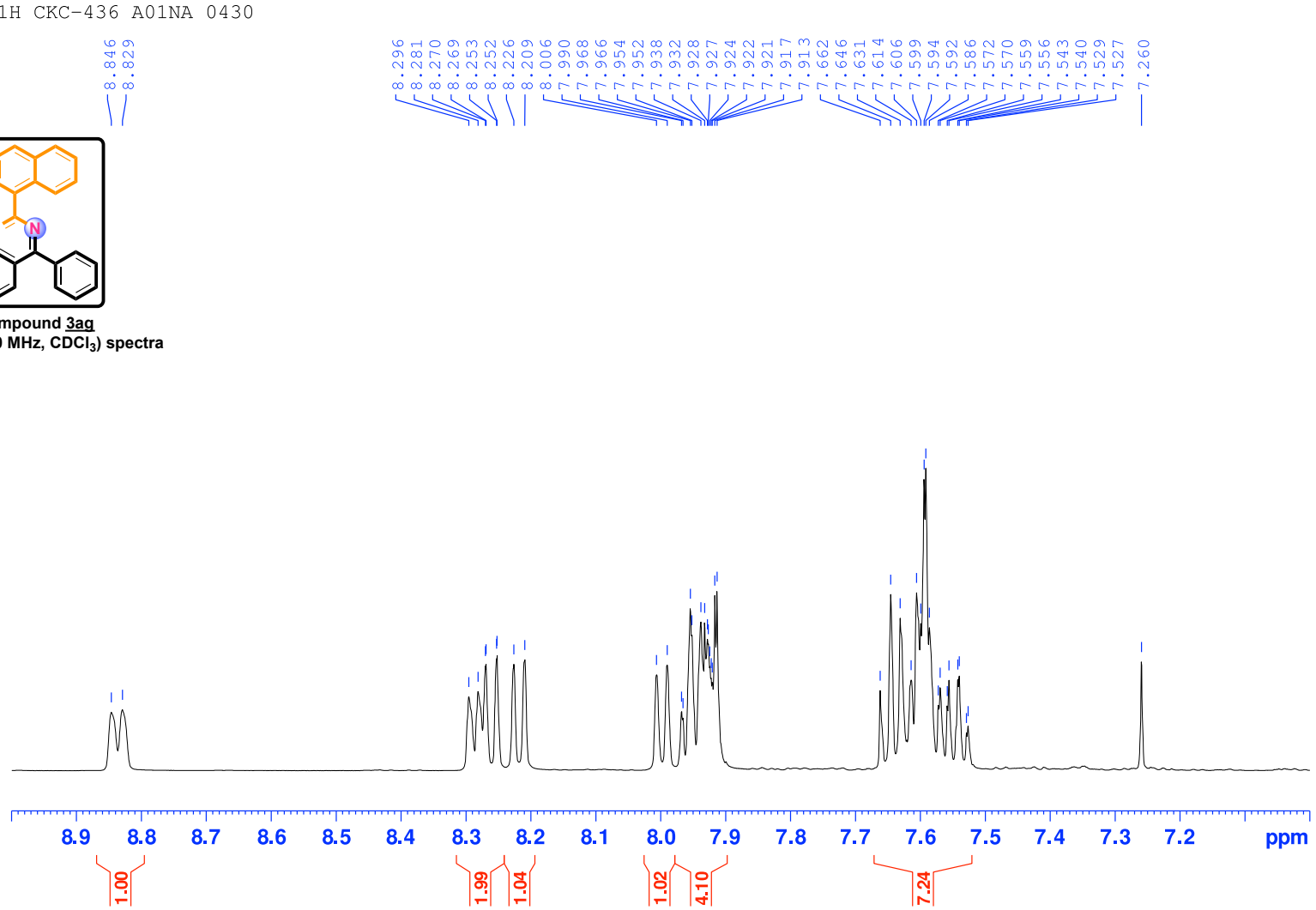


Compound 3ag
^{1}H NMR (500 MHz, $CDCl_3$) spectra

Compound 3ag

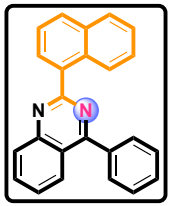


Compound 3ag
^{1}H NMR (500 MHz, $CDCl_3$) spectra

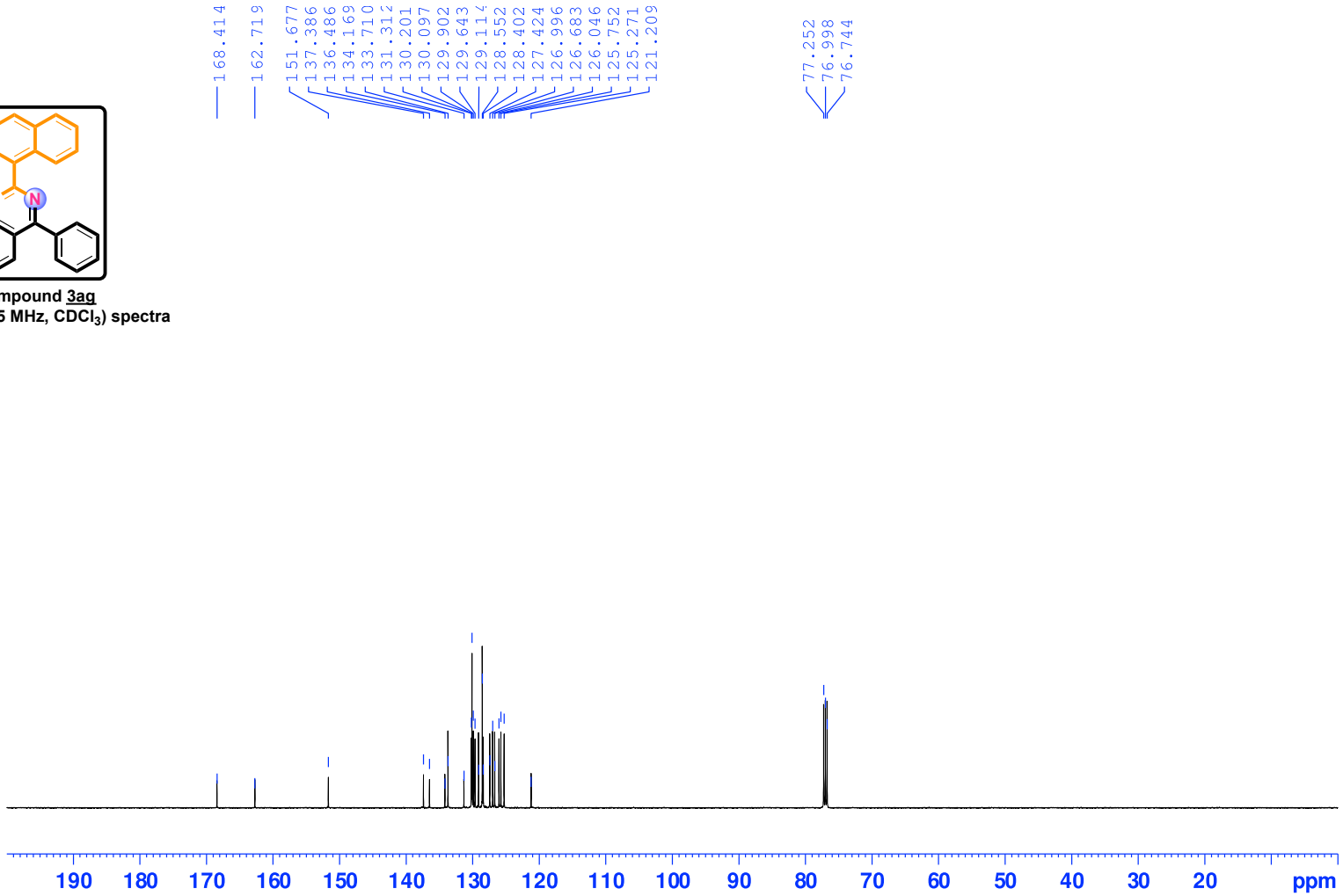


Compound 3ag

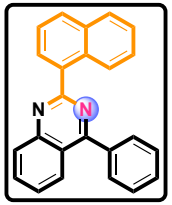
13C CKC-436 A01NA 0430



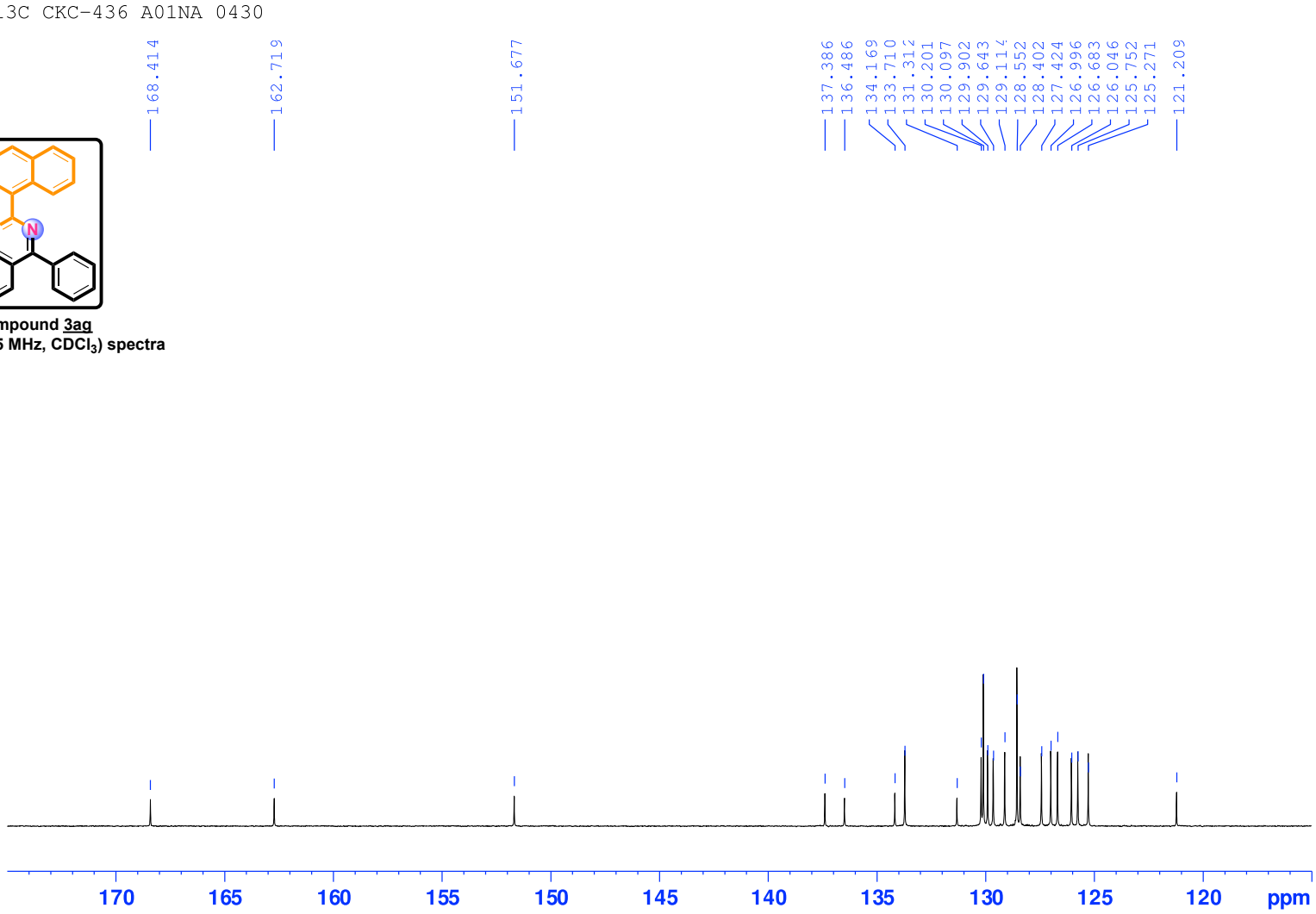
Compound 3ag
^{13}C NMR (125 MHz, $CDCl_3$) spectra



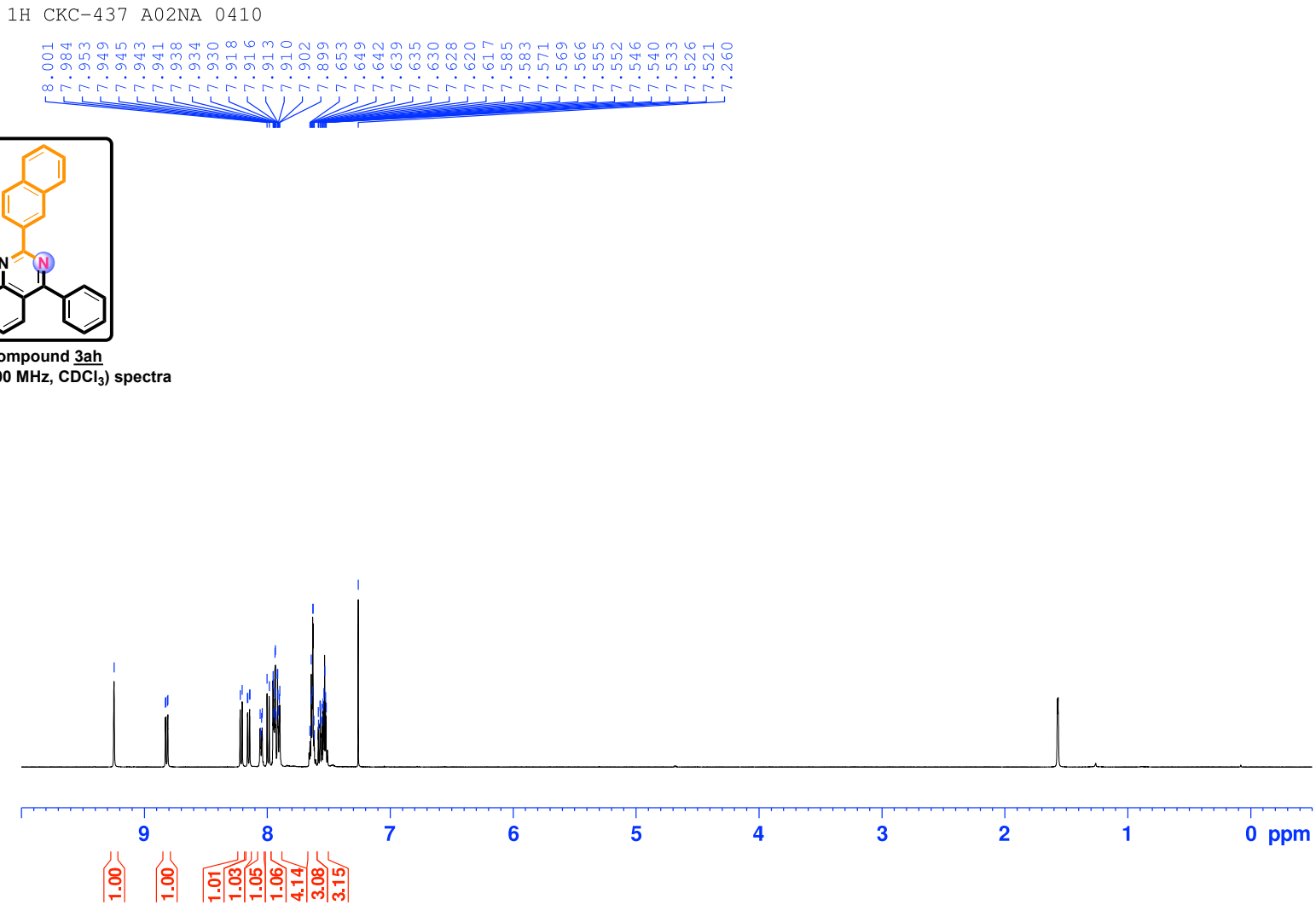
Compound 3ag



Compound 3ag
^{13}C NMR (125 MHz, $CDCl_3$) spectra

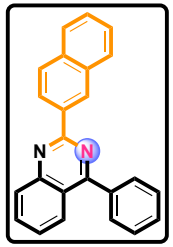


Compound 3ah

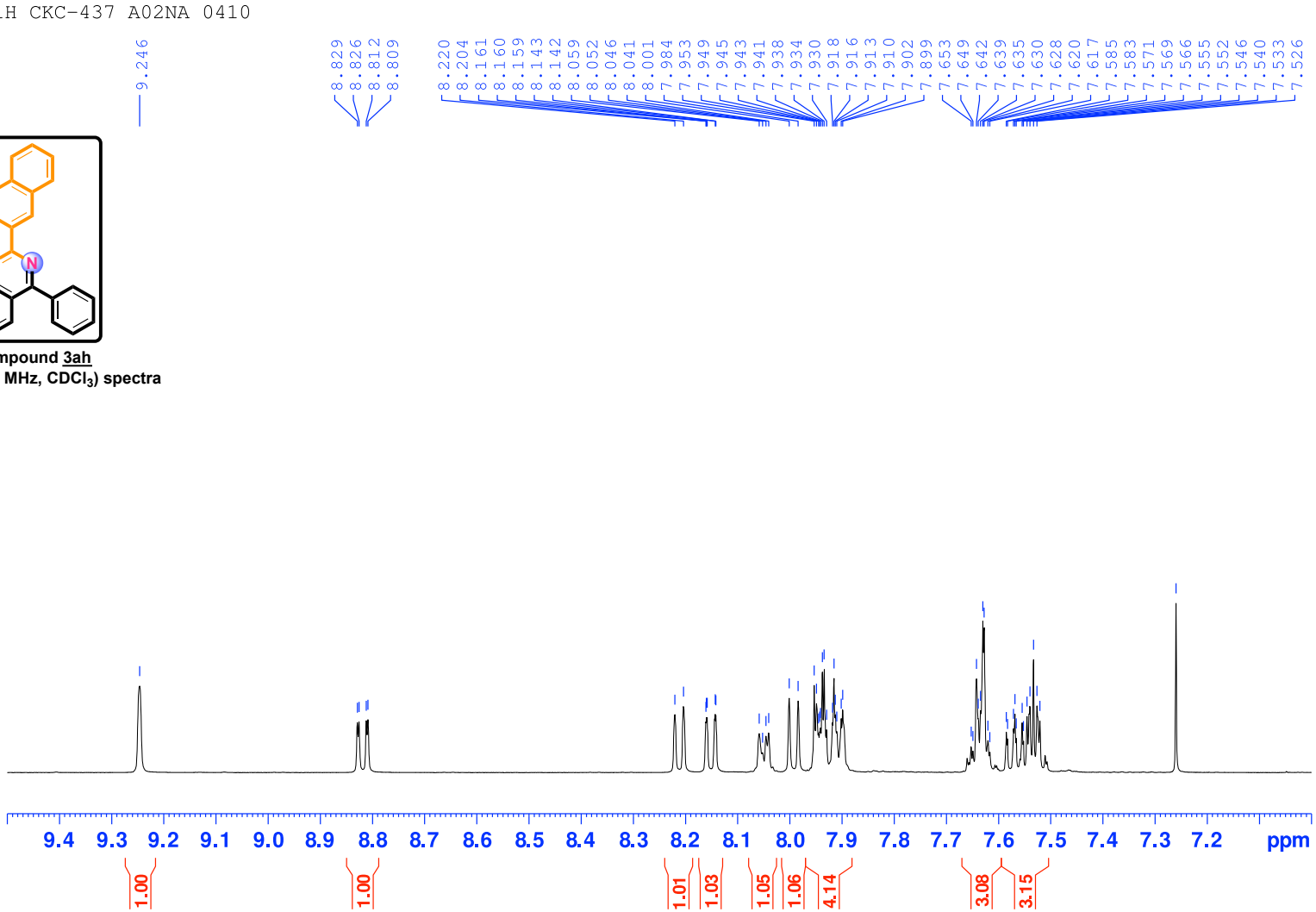


Compound 3ah
^{1}H NMR (500 MHz, $CDCl_3$) spectra

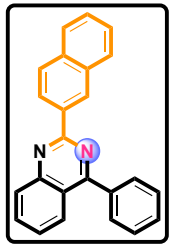
Compound 3ah



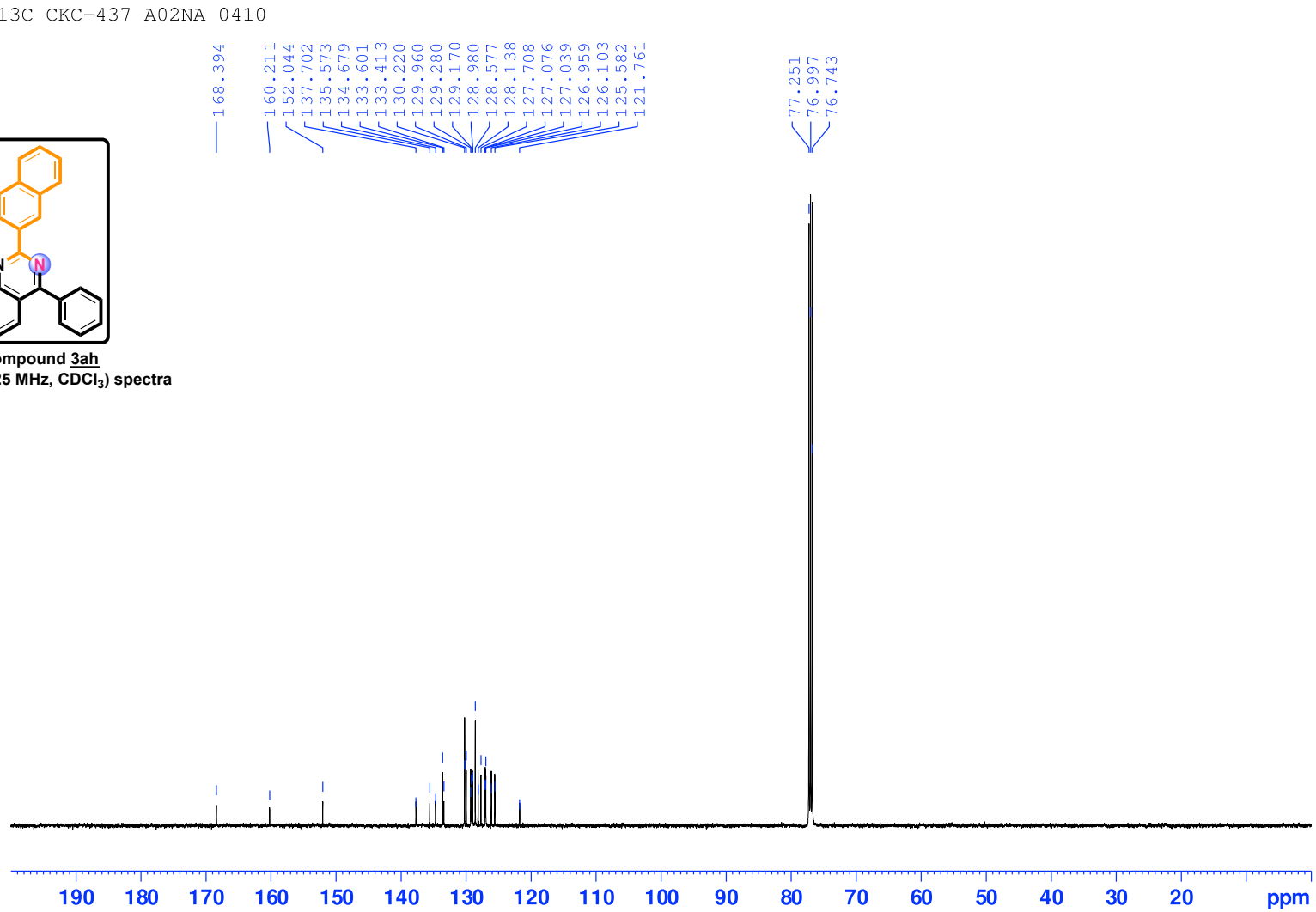
Compound 3ah
^{1}H NMR (500 MHz, $CDCl_3$) spectra



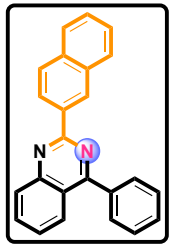
Compound 3ah



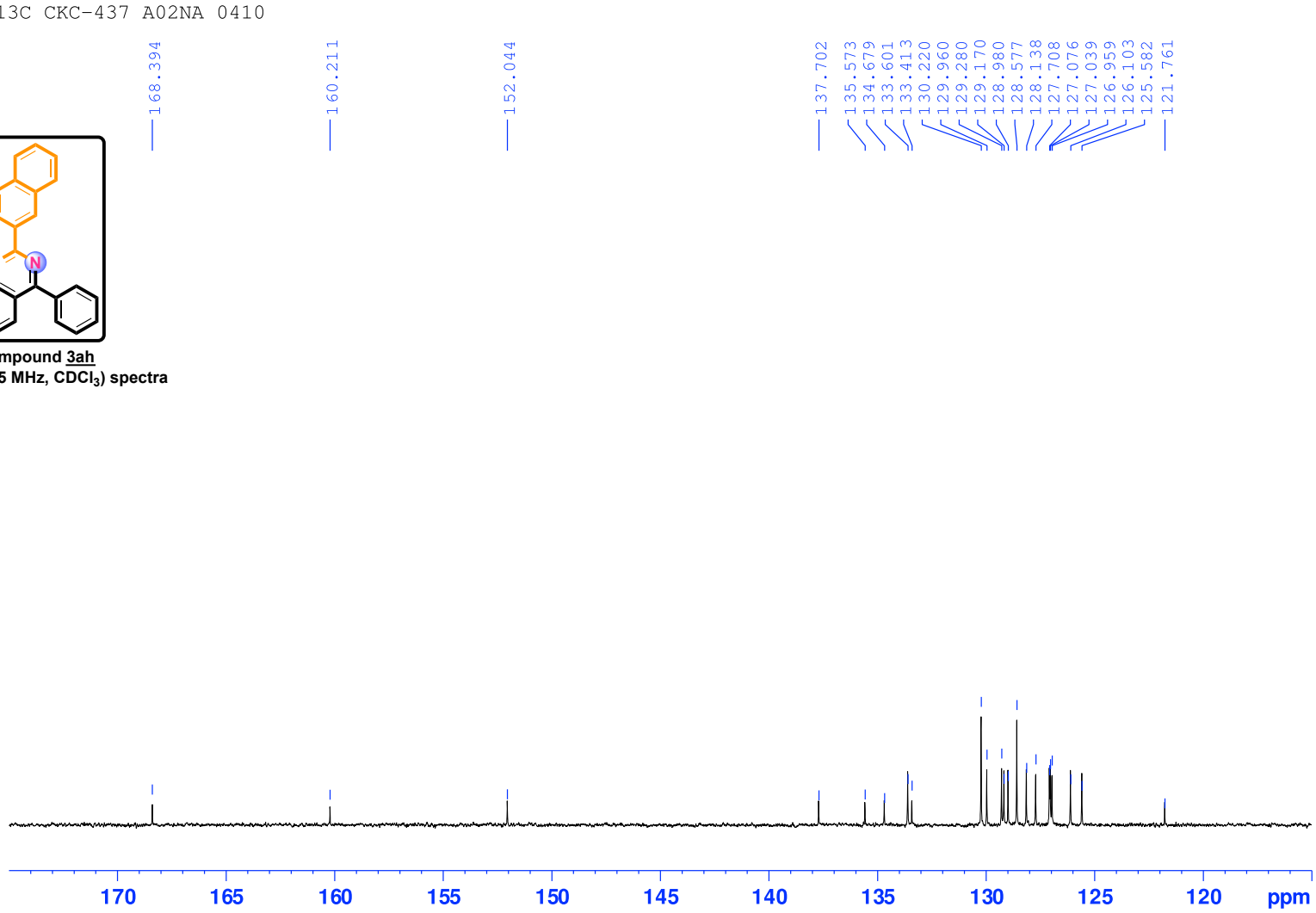
Compound 3ah
^{13}C NMR (125 MHz, $CDCl_3$) spectra



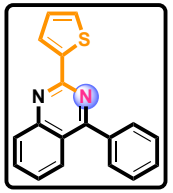
Compound 3ah



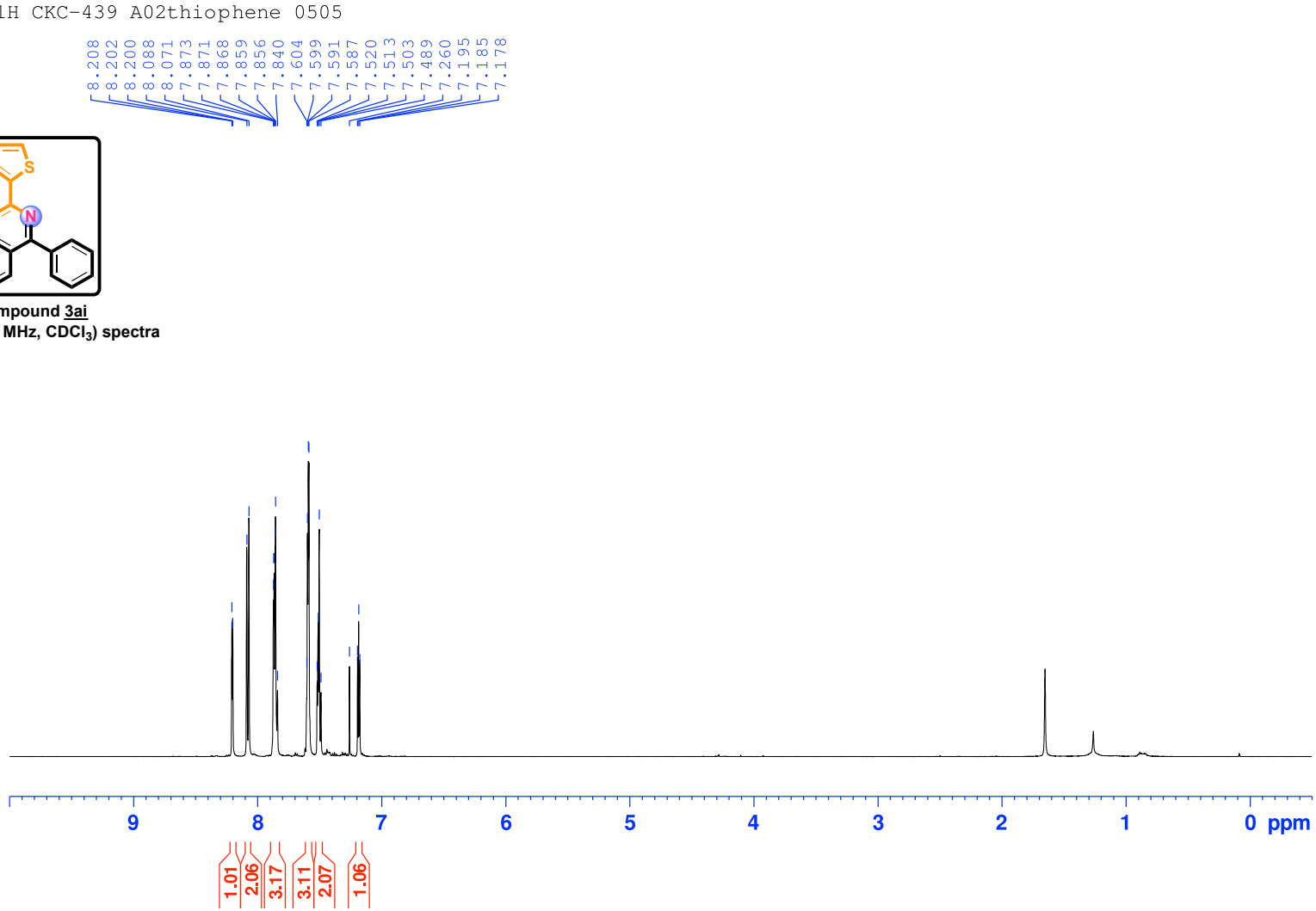
Compound 3ah
^{13}C NMR (125 MHz, $CDCl_3$) spectra



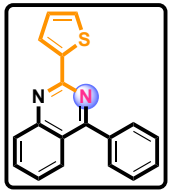
Compound 3ai



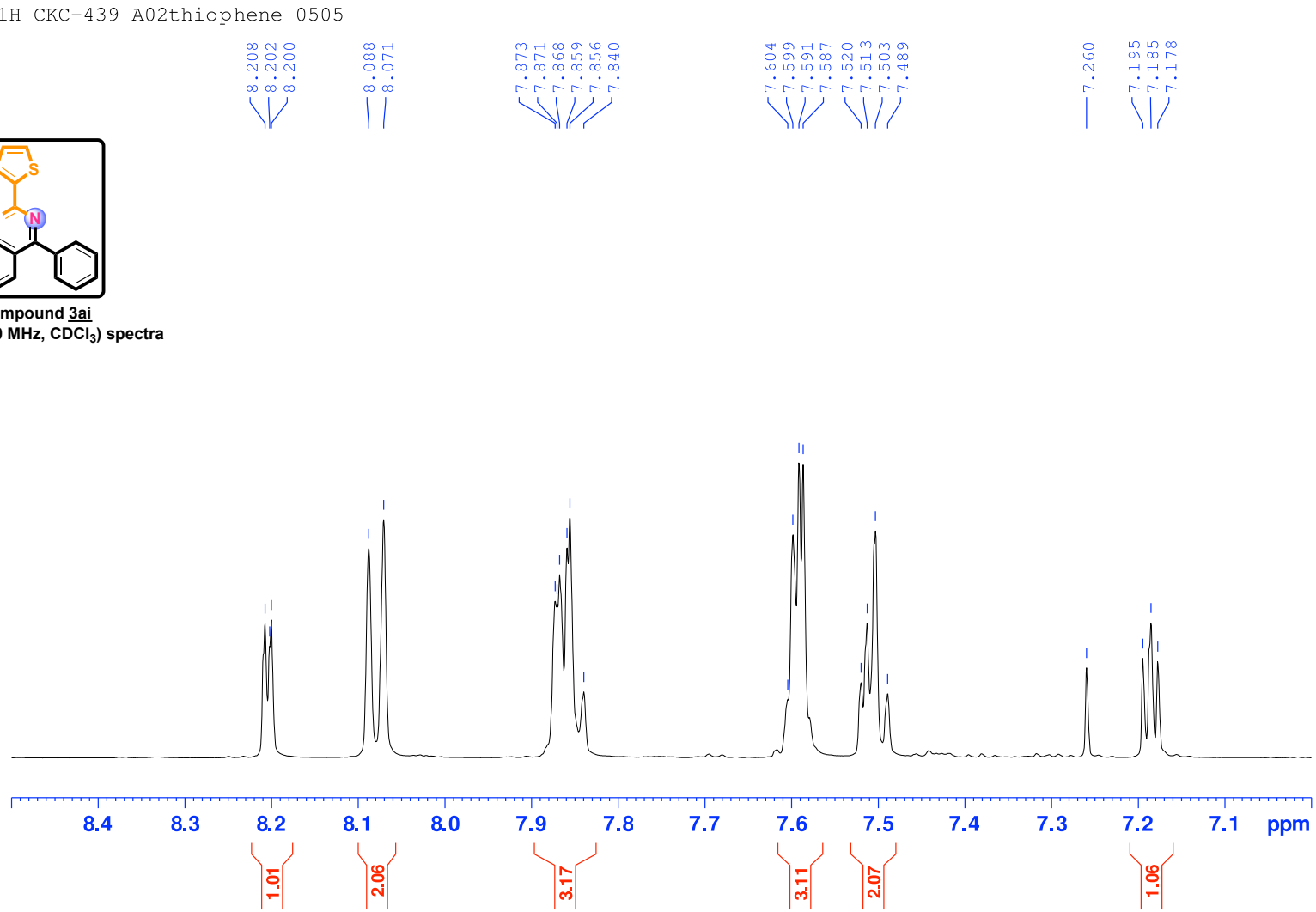
Compound 3ai
^{1}H NMR (500 MHz, $CDCl_3$) spectra



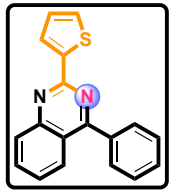
Compound 3ai



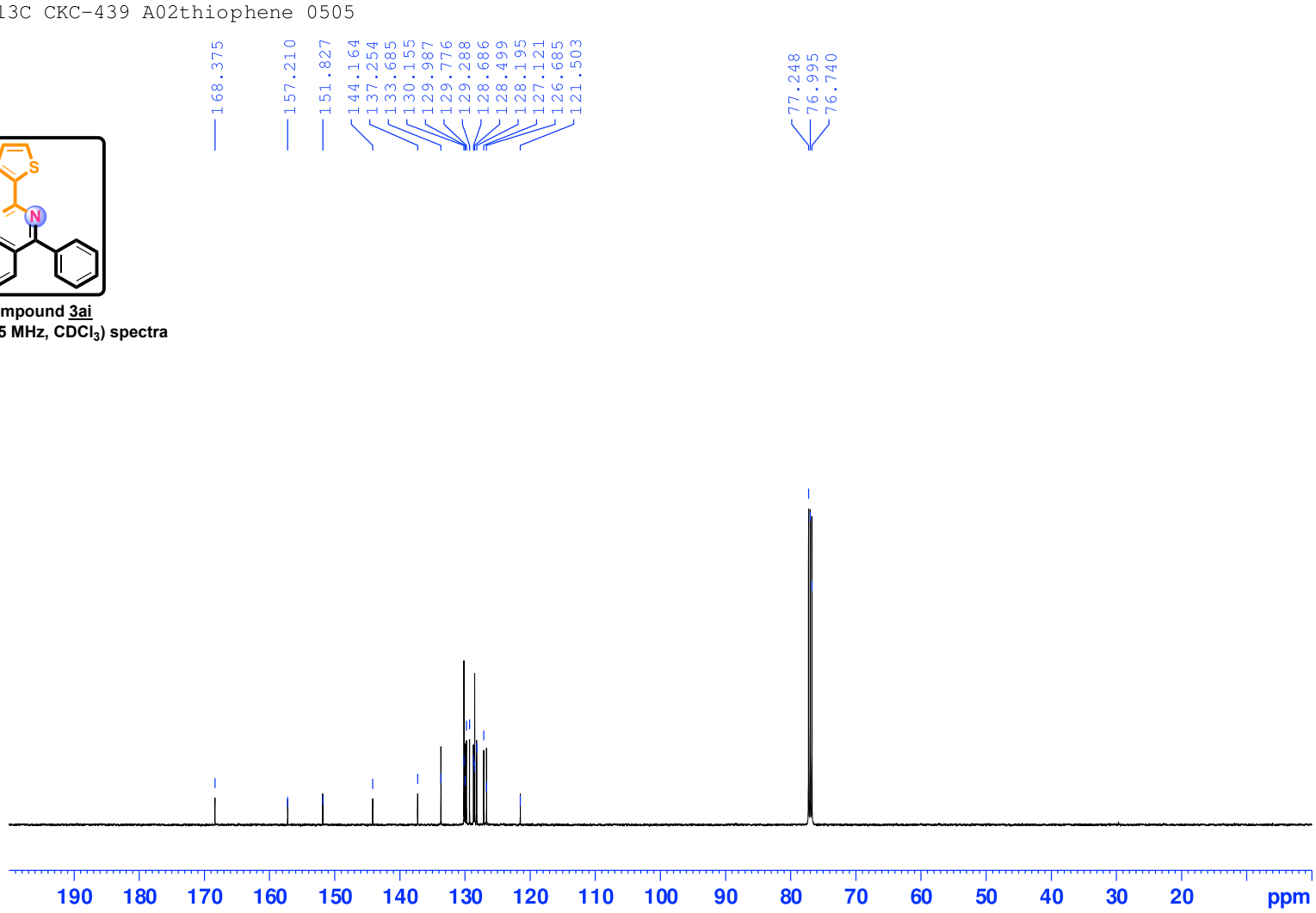
Compound 3ai
^{1}H NMR (500 MHz, $CDCl_3$) spectra



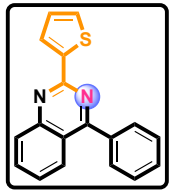
Compound 3ai



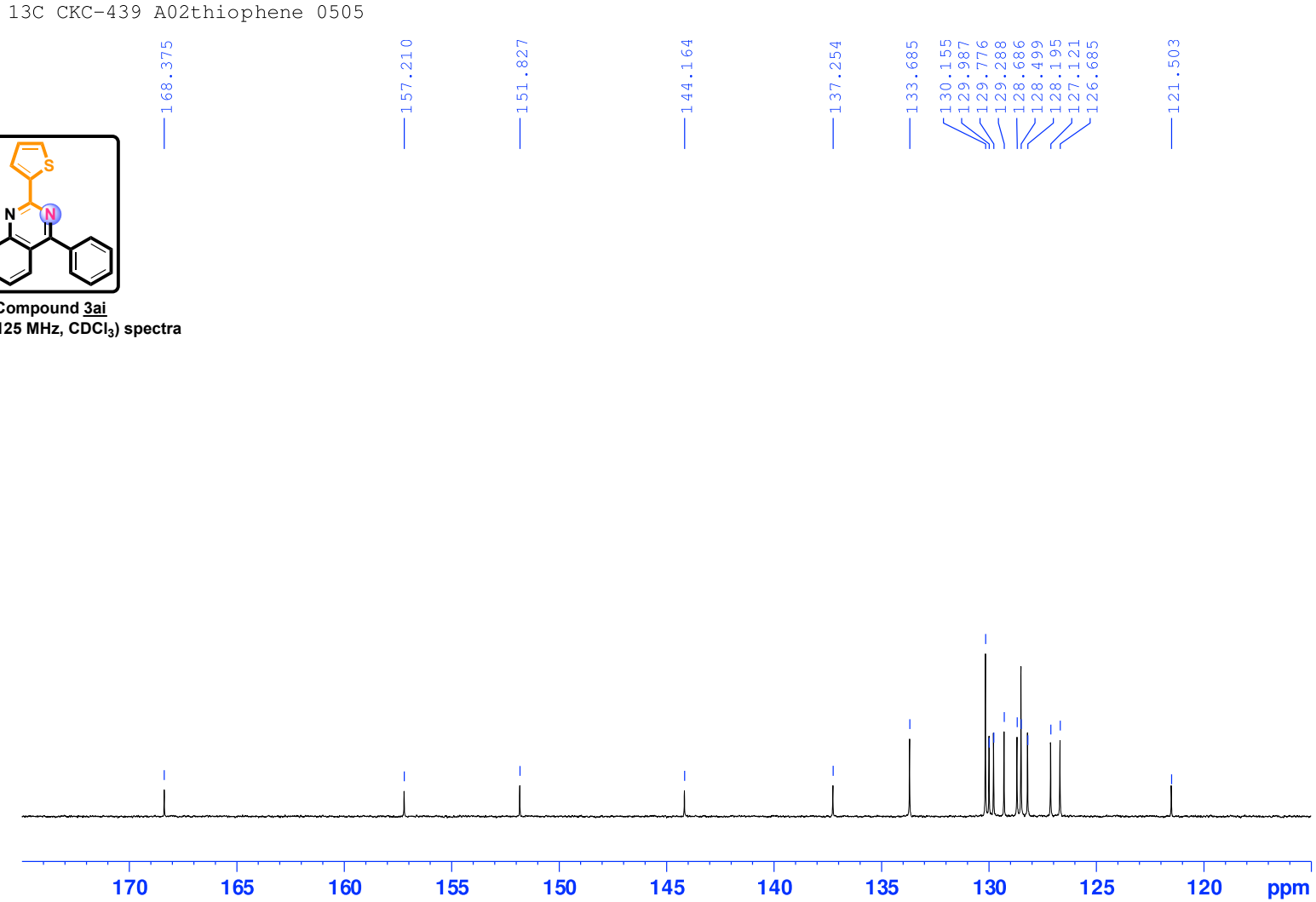
Compound 3ai
^{13}C NMR (125 MHz, $CDCl_3$) spectra



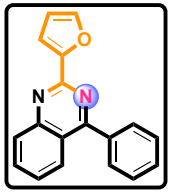
Compound 3ai



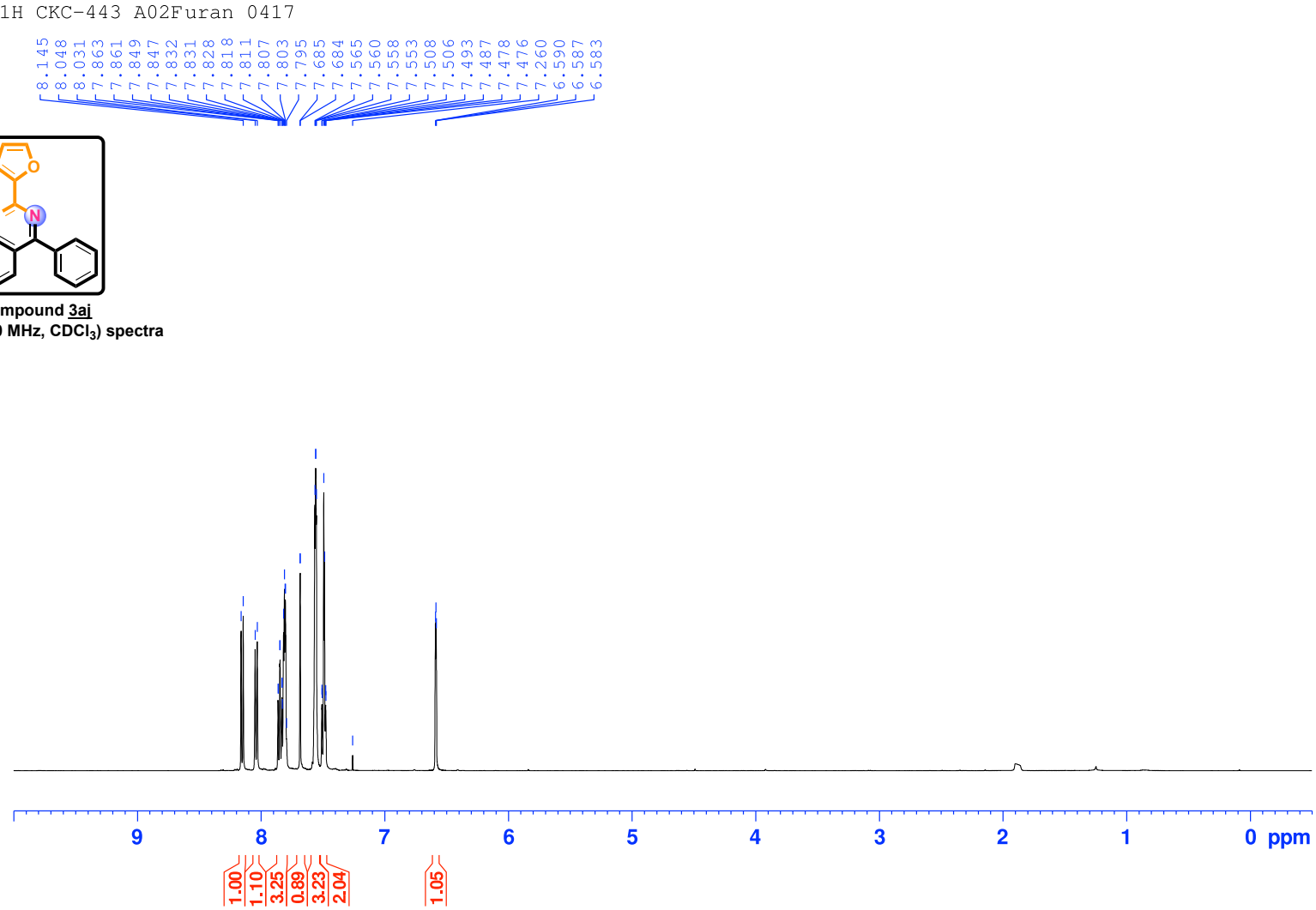
Compound 3ai
^{13}C NMR (125 MHz, $CDCl_3$) spectra



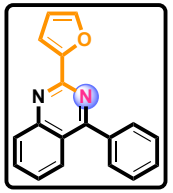
Compound 3aj



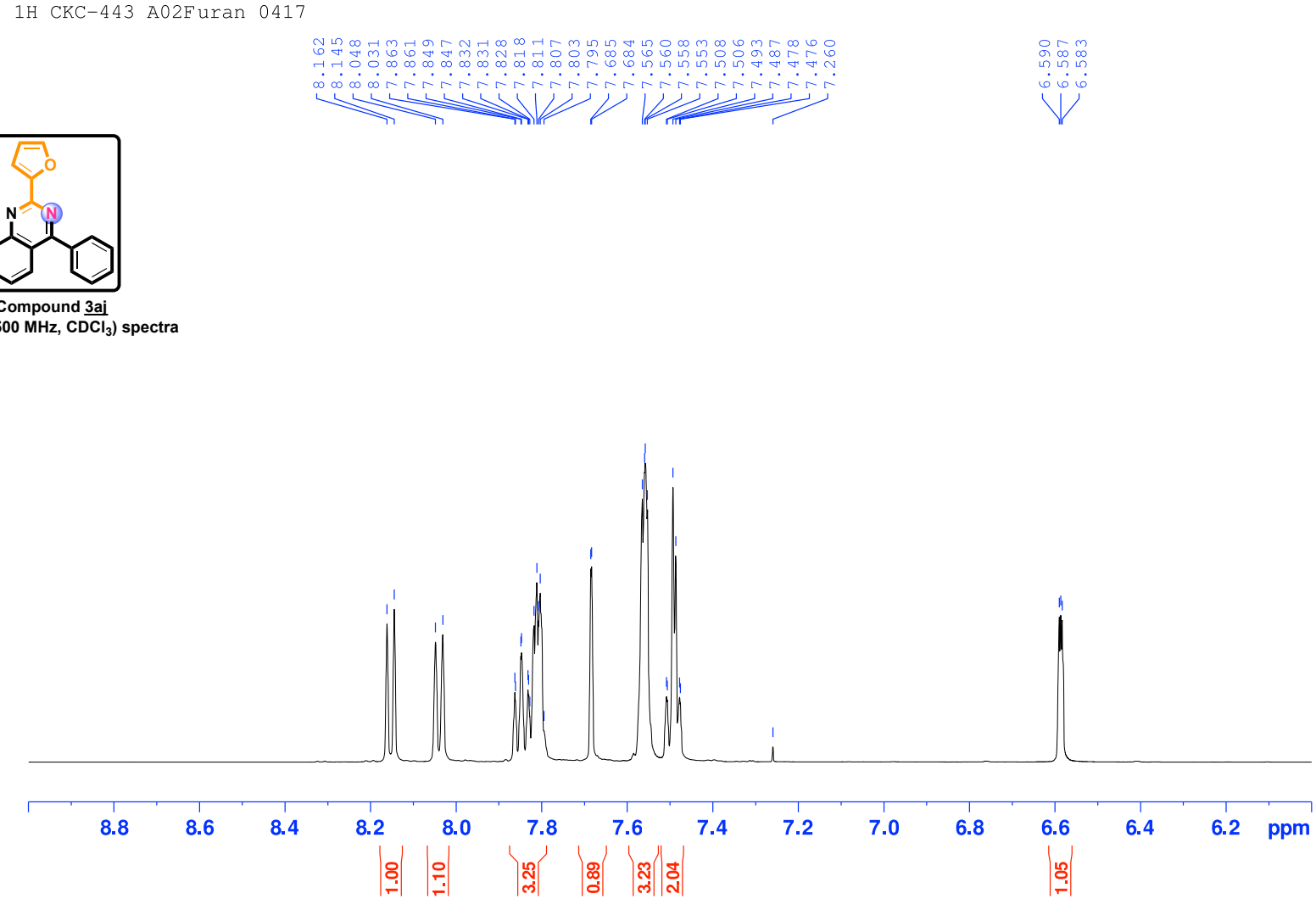
Compound 3aj
^{1}H NMR (500 MHz, $CDCl_3$) spectra



Compound 3aj

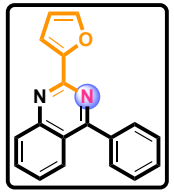


Compound 3aj
^{1}H NMR (500 MHz, $CDCl_3$) spectra

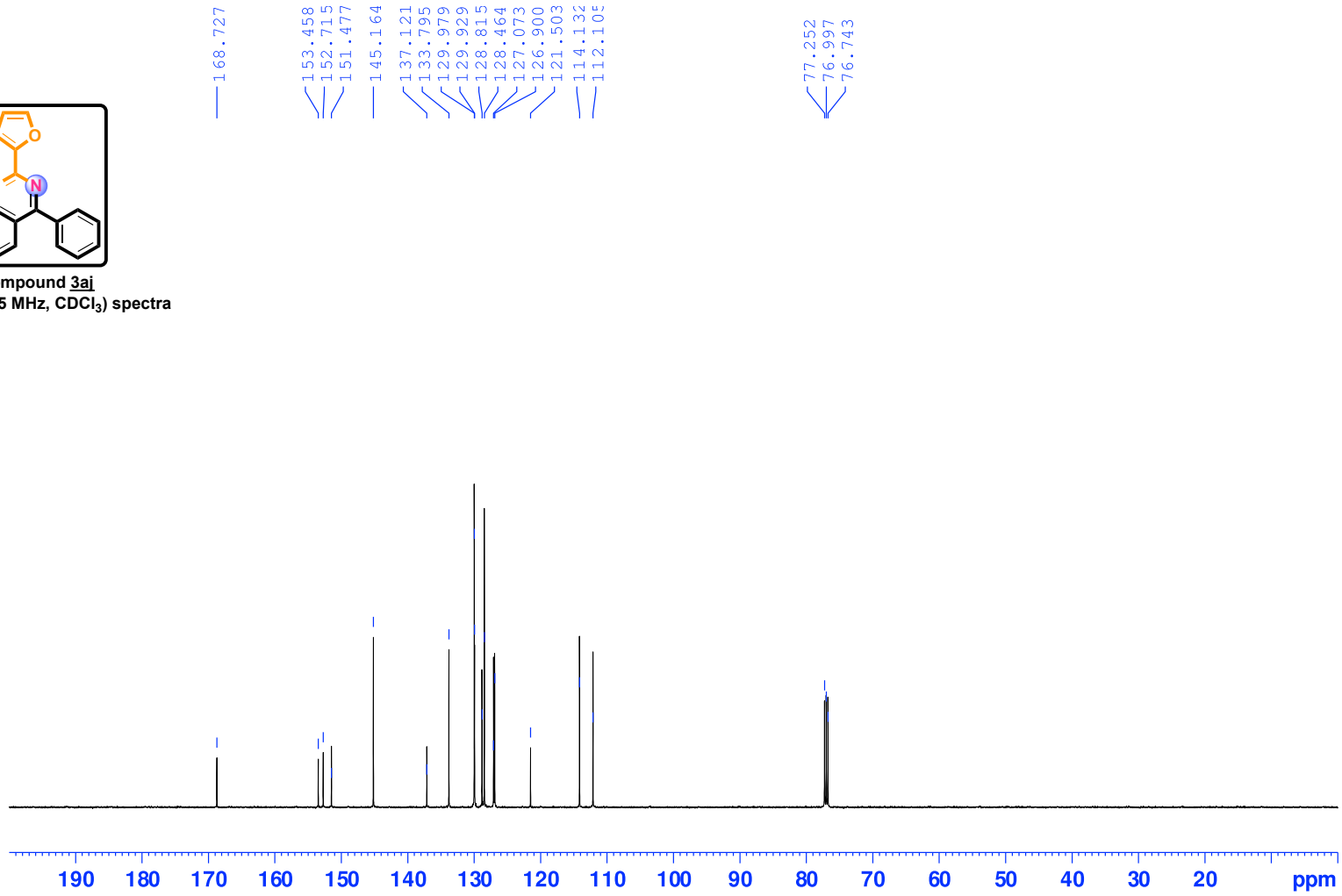


Compound 3aj

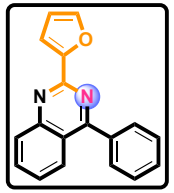
13C CKC-443 A02Furan 0417



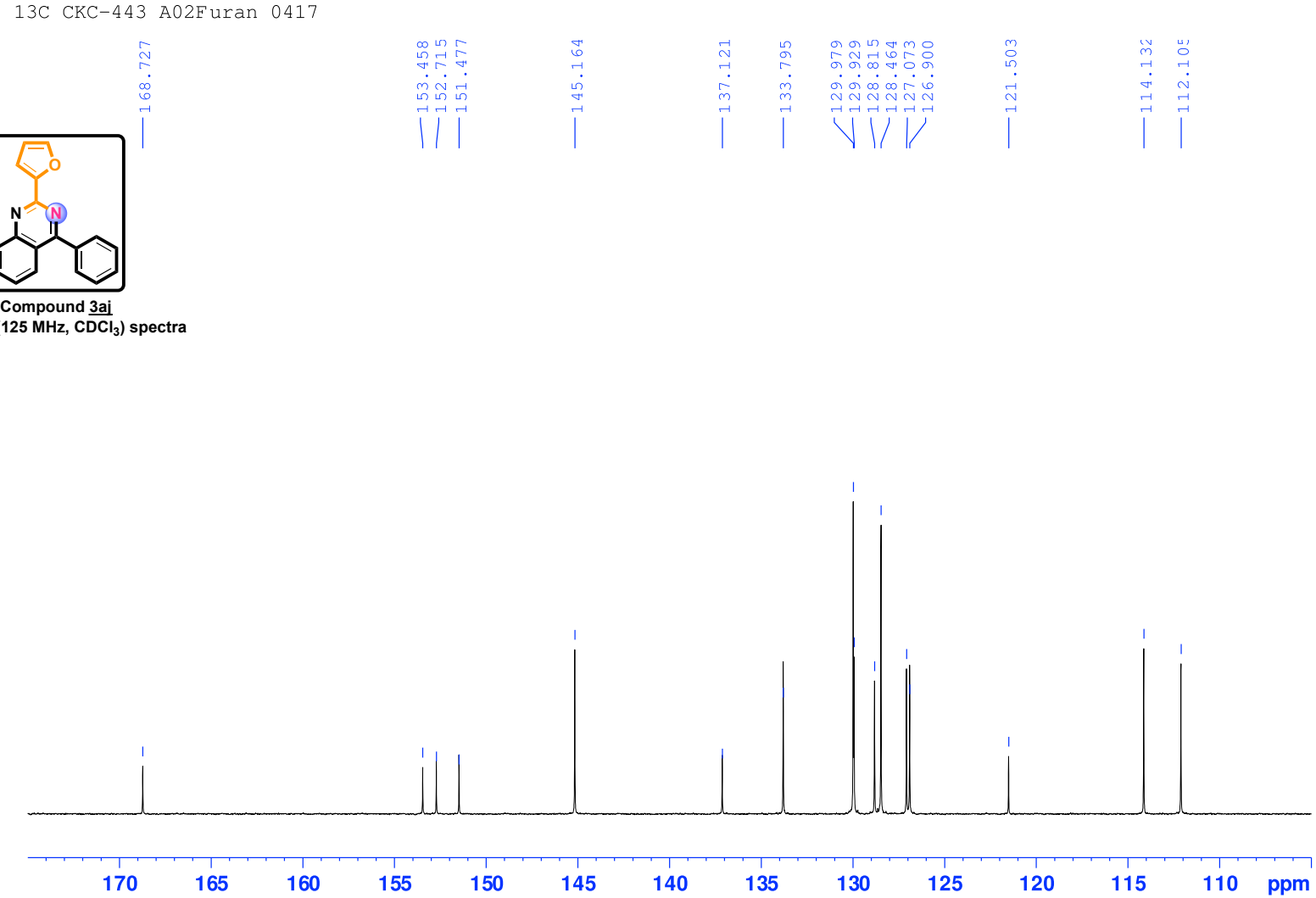
Compound 3aj
^{13}C NMR (125 MHz, $CDCl_3$) spectra



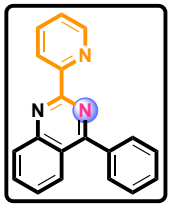
Compound 3aj



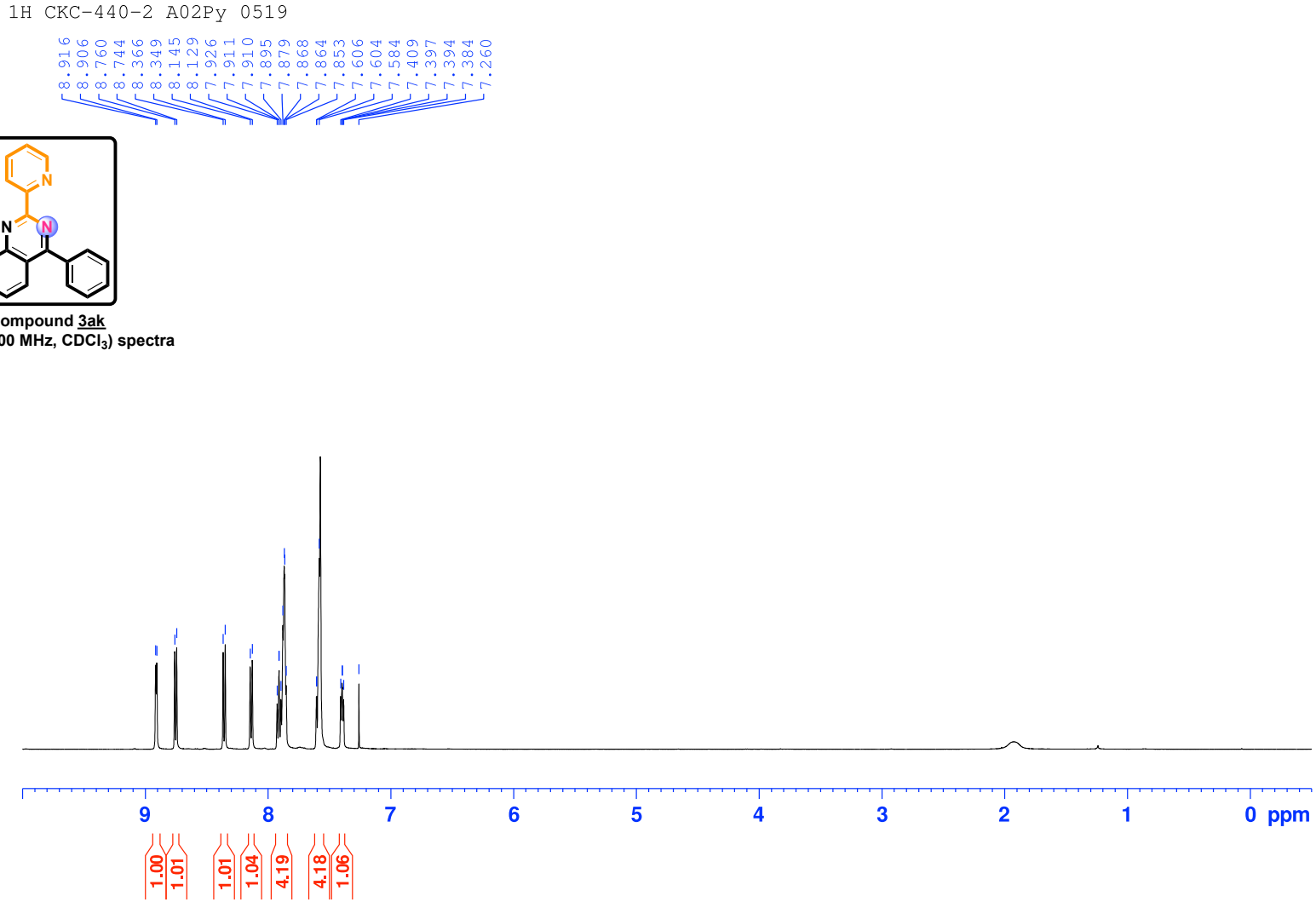
Compound 3aj
^{13}C NMR (125 MHz, $CDCl_3$) spectra



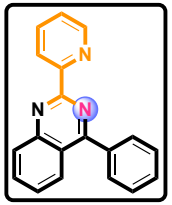
Compound 3ak



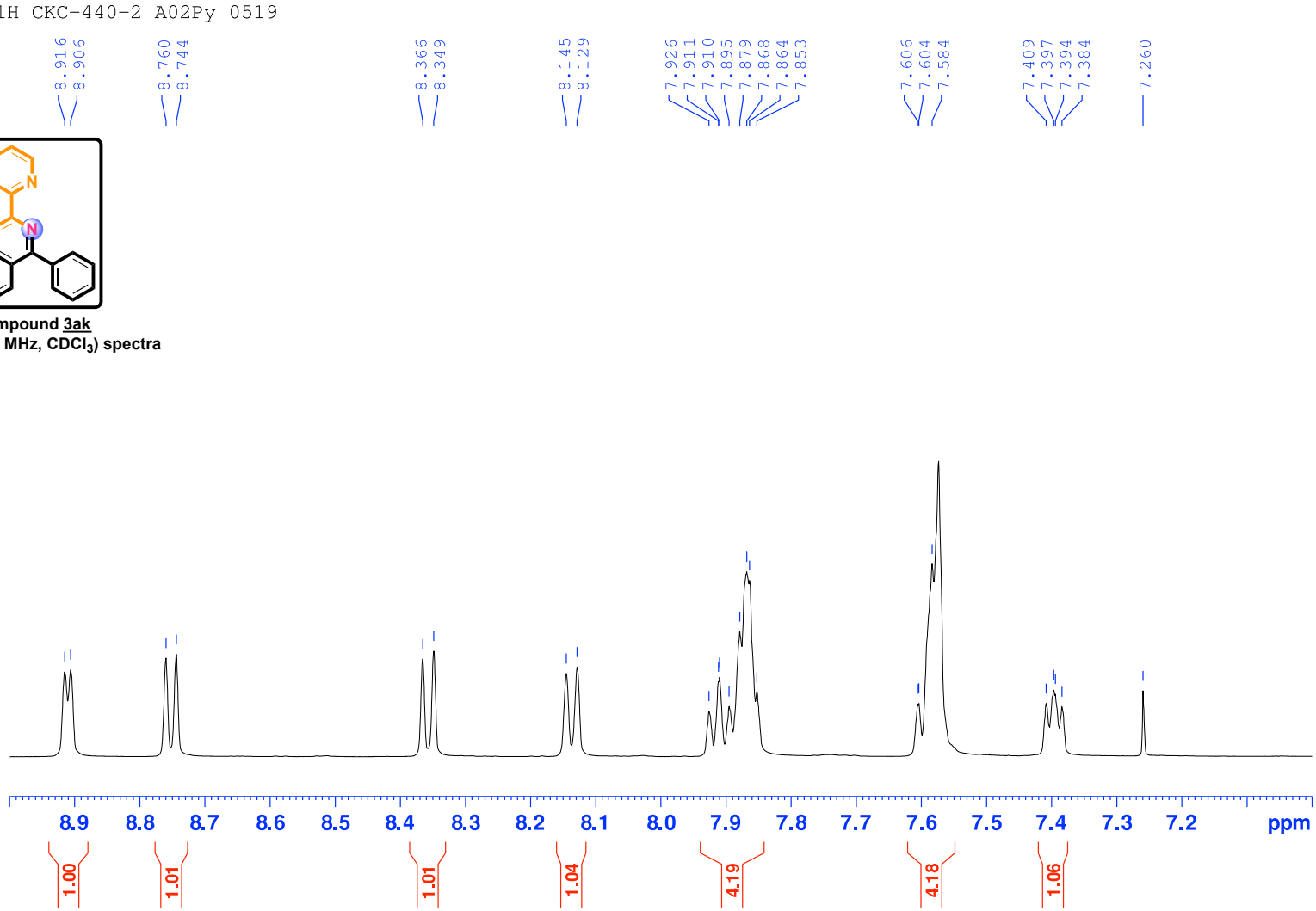
Compound 3ak
^{1}H NMR (500 MHz, $CDCl_3$) spectra



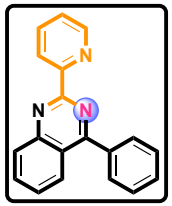
Compound 3ak



Compound 3ak
^{1}H NMR (500 MHz, $CDCl_3$) spectra



Compound 3ak



Compound 3ak
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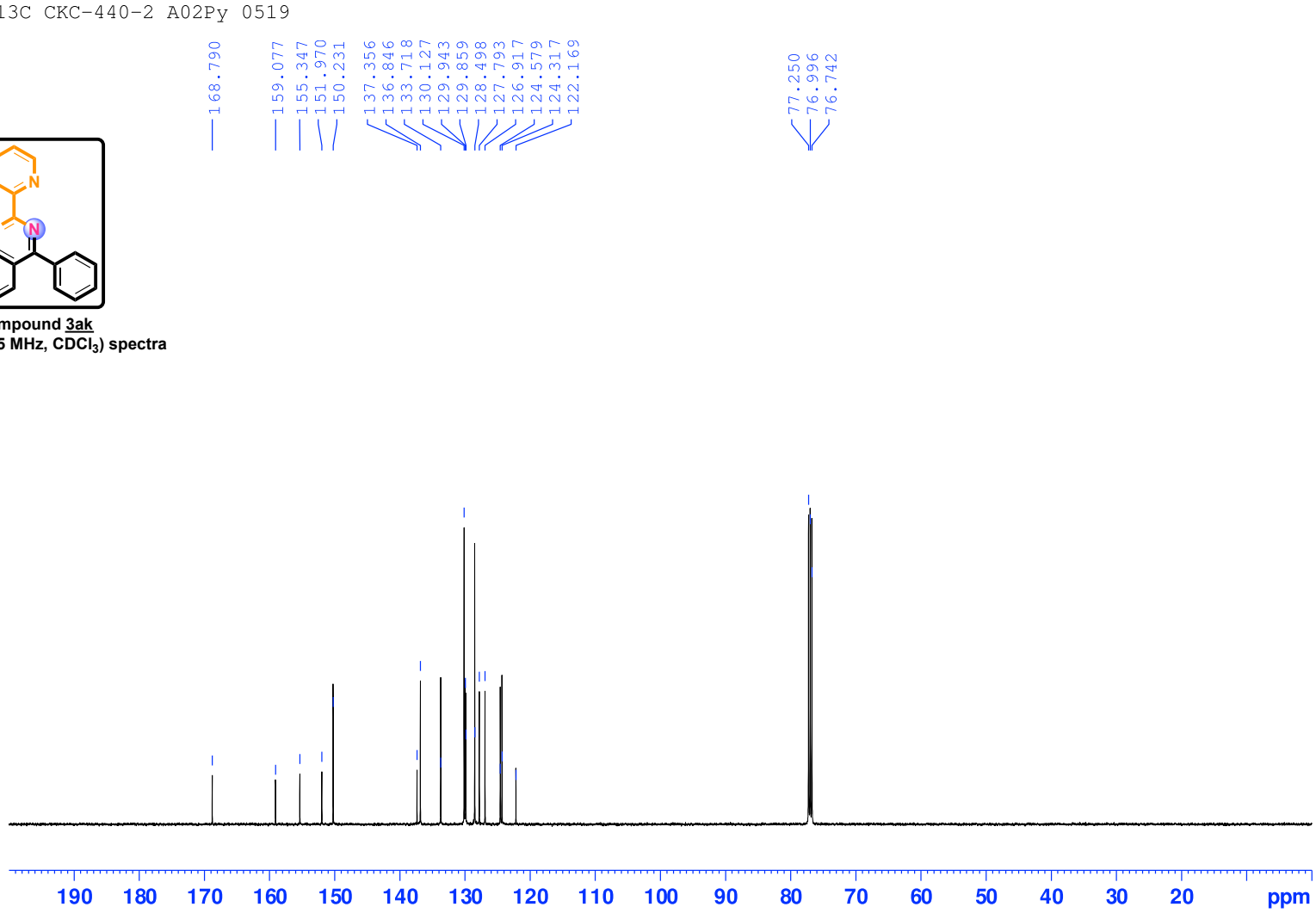

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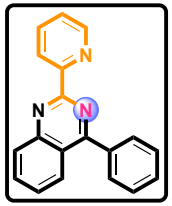
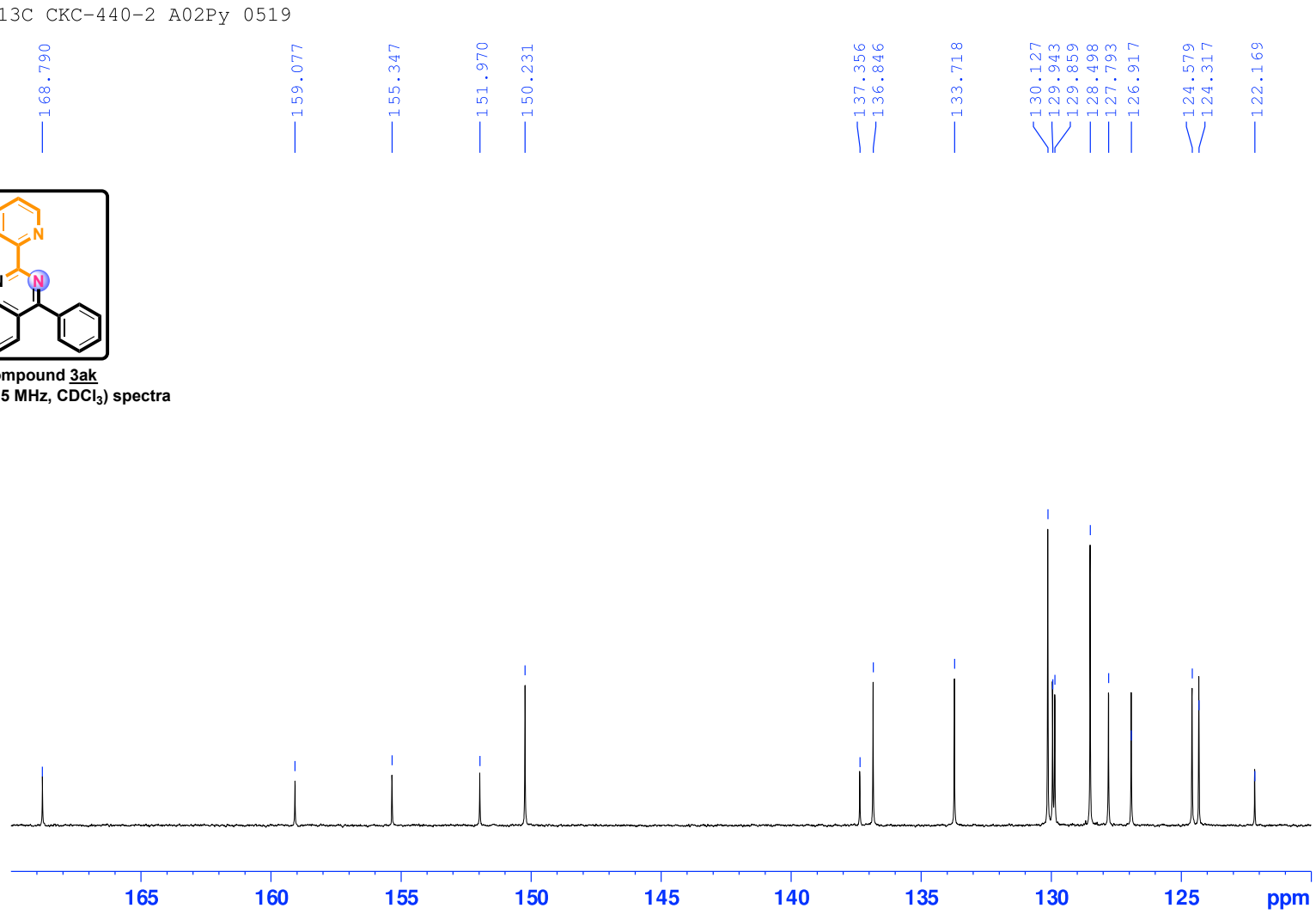
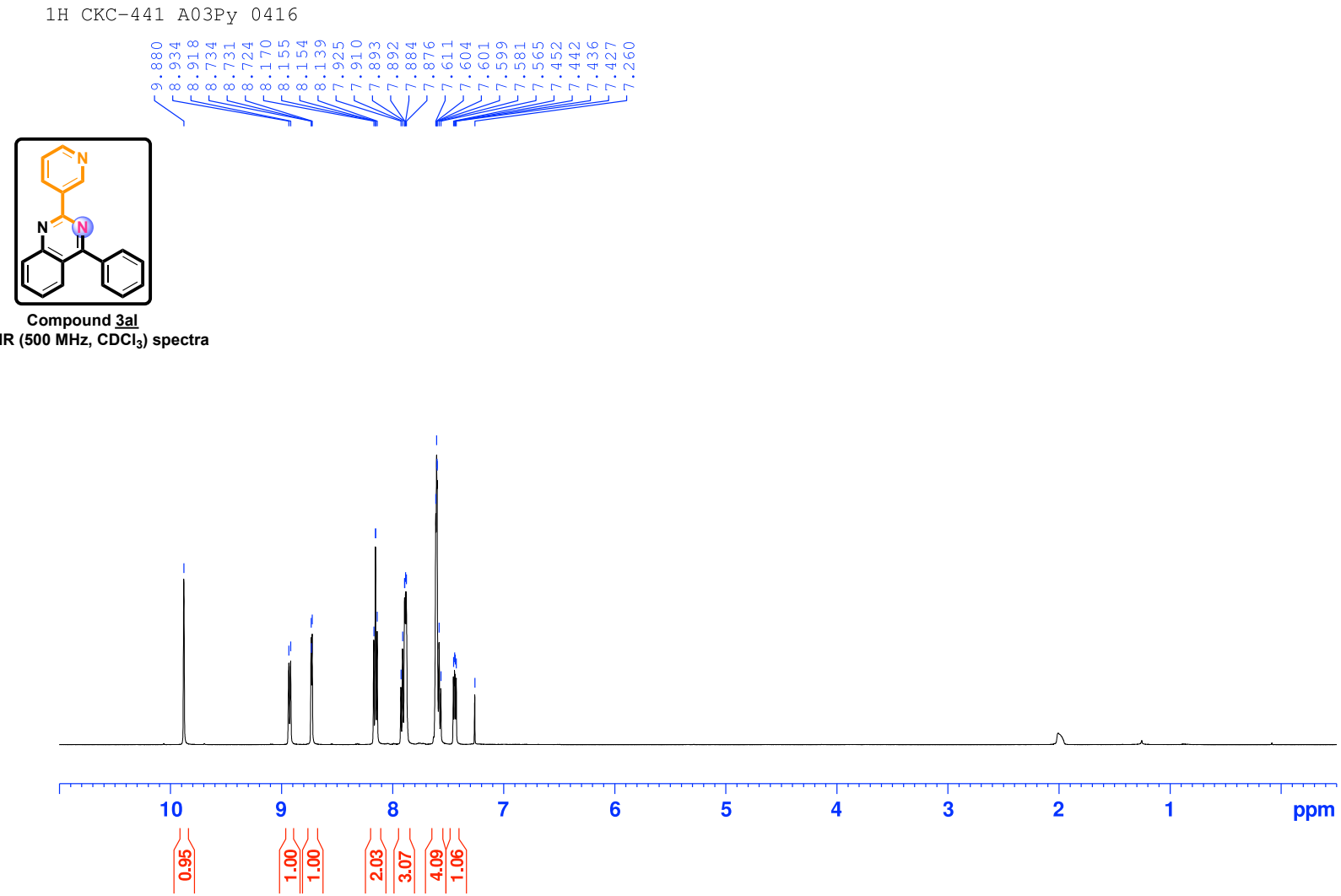


Compound 3ak

^{13}C NMR (125 MHz, $CDCl_3$) spectra

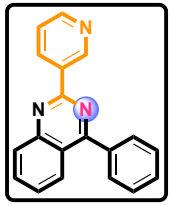


Compound 3al

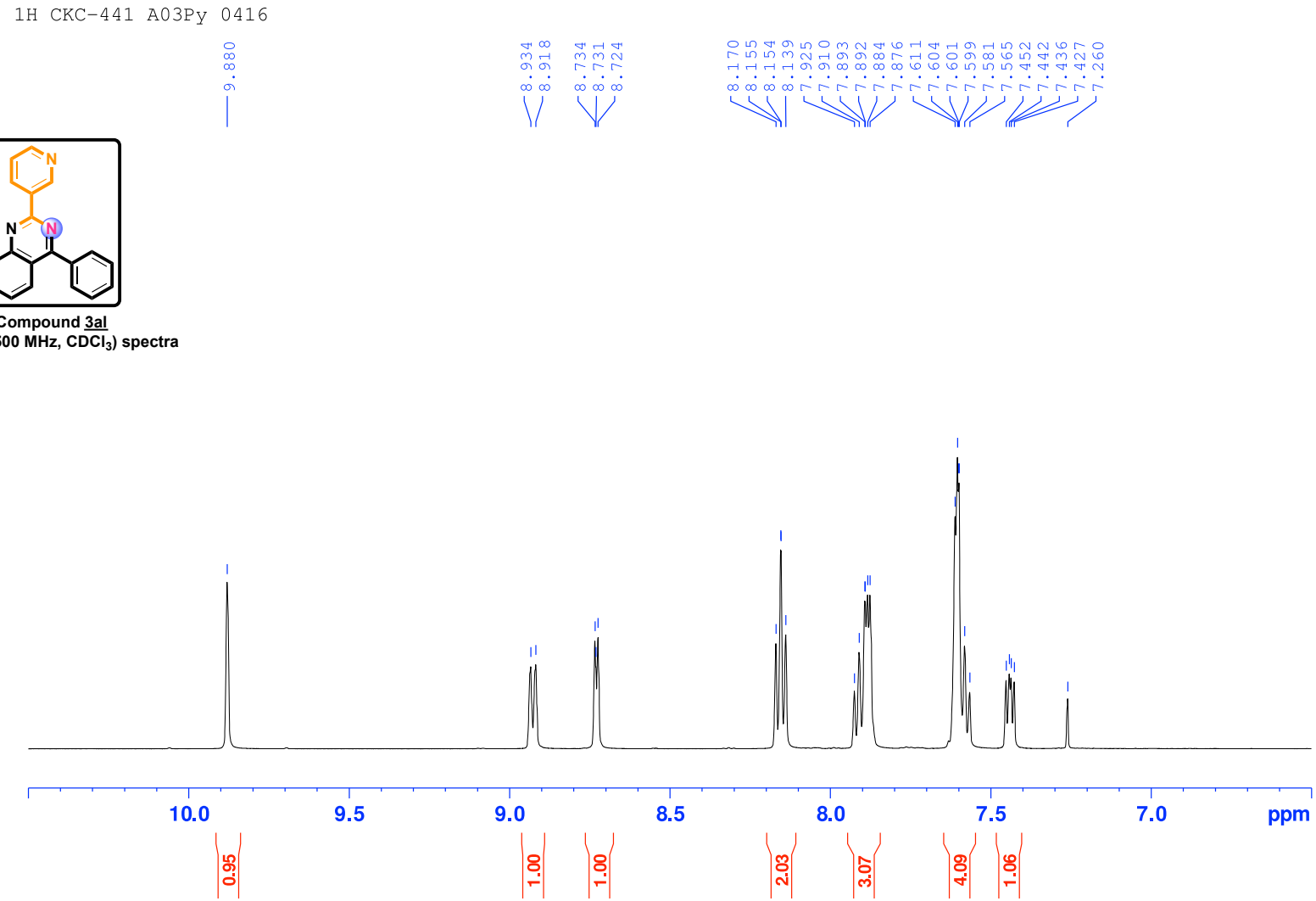


Compound 3al
^{1}H NMR (500 MHz, $CDCl_3$) spectra

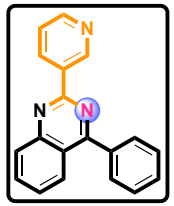
Compound 3al



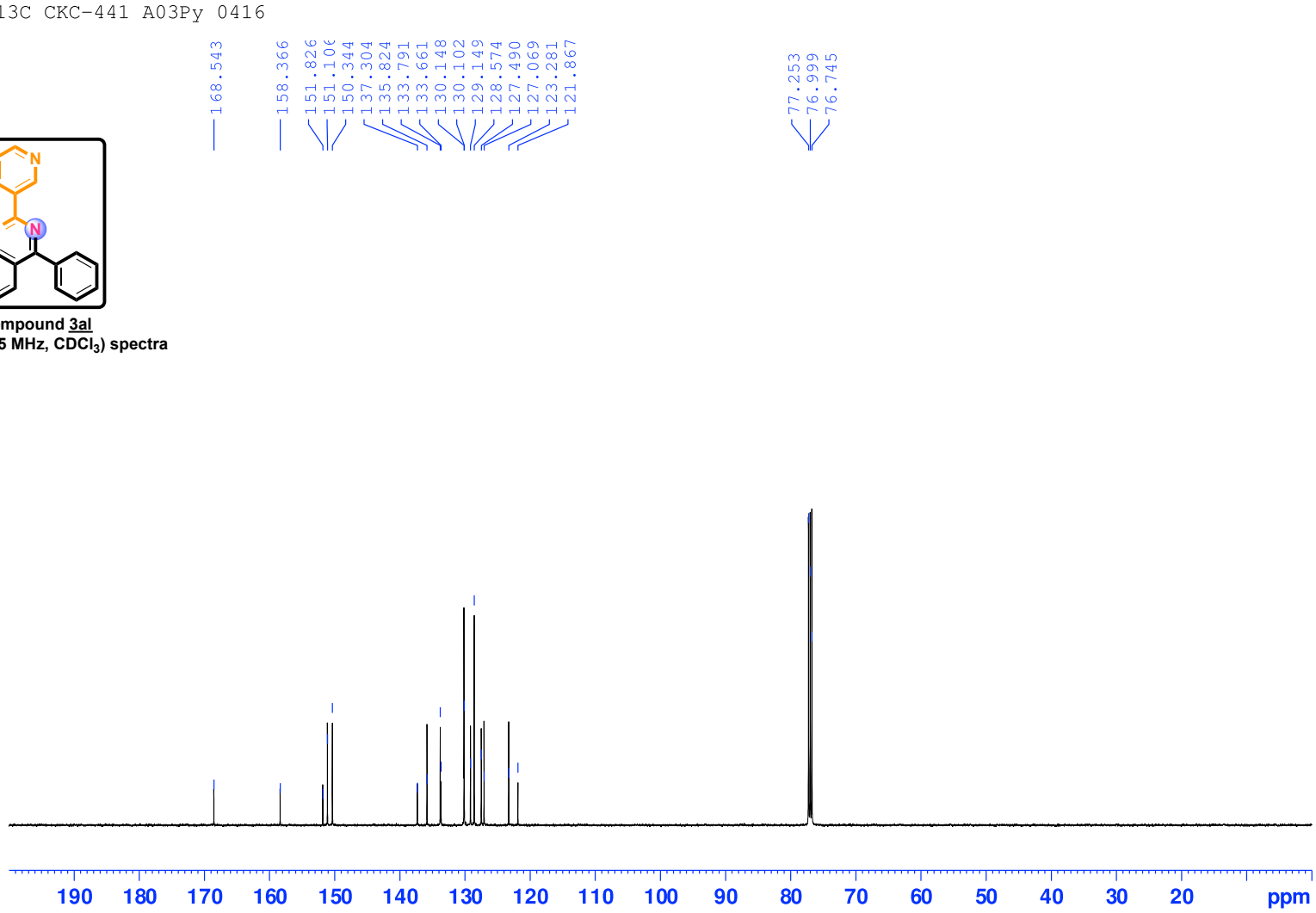
Compound 3al
^{1}H NMR (500 MHz, $CDCl_3$) spectra



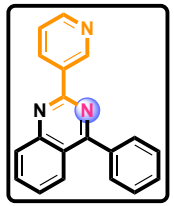
Compound 3al



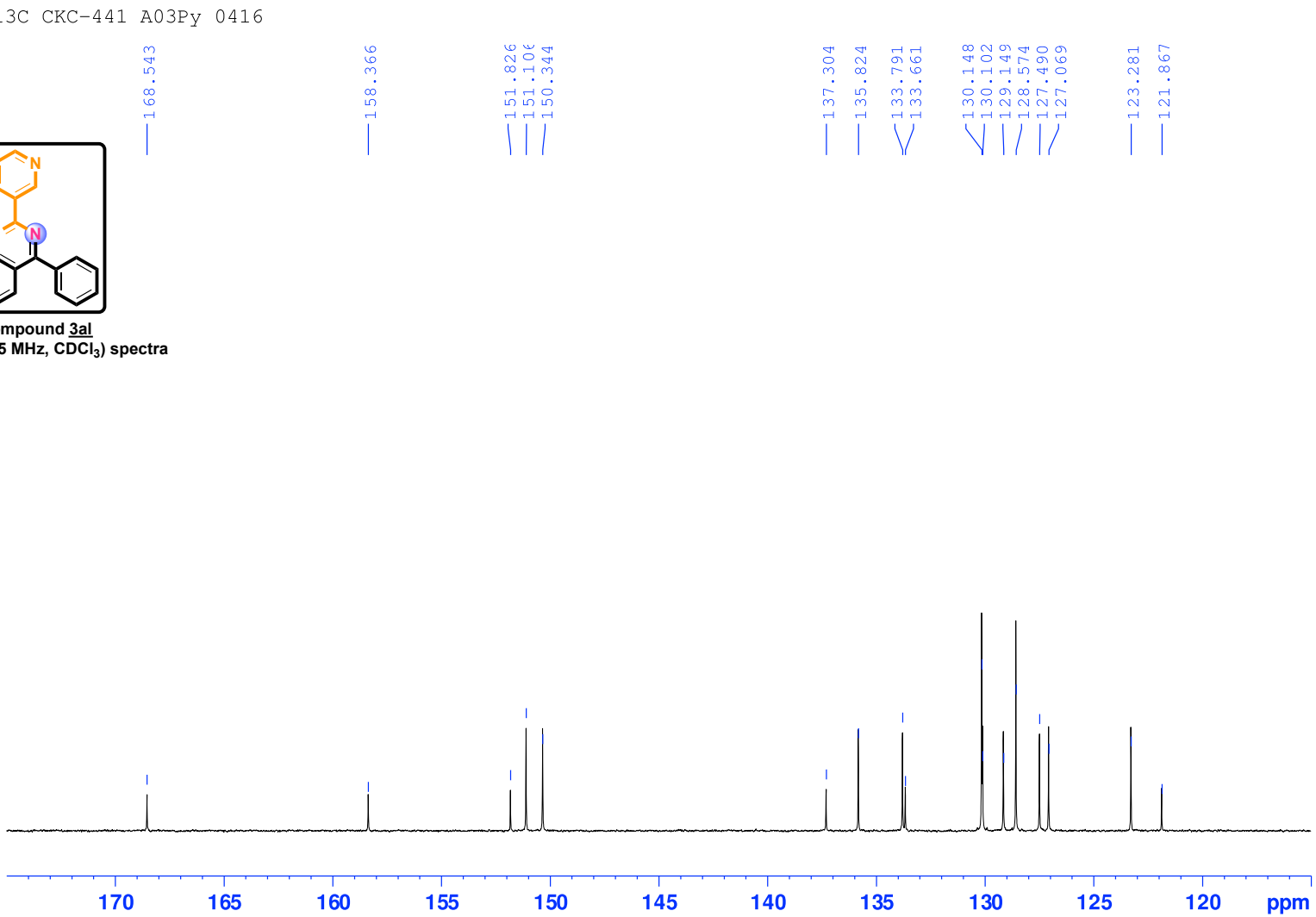
Compound 3al
^{13}C NMR (125 MHz, $CDCl_3$) spectra



Compound 3al



Compound 3al
^{13}C NMR (125 MHz, $CDCl_3$) spectra



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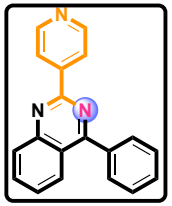

Compound 3am
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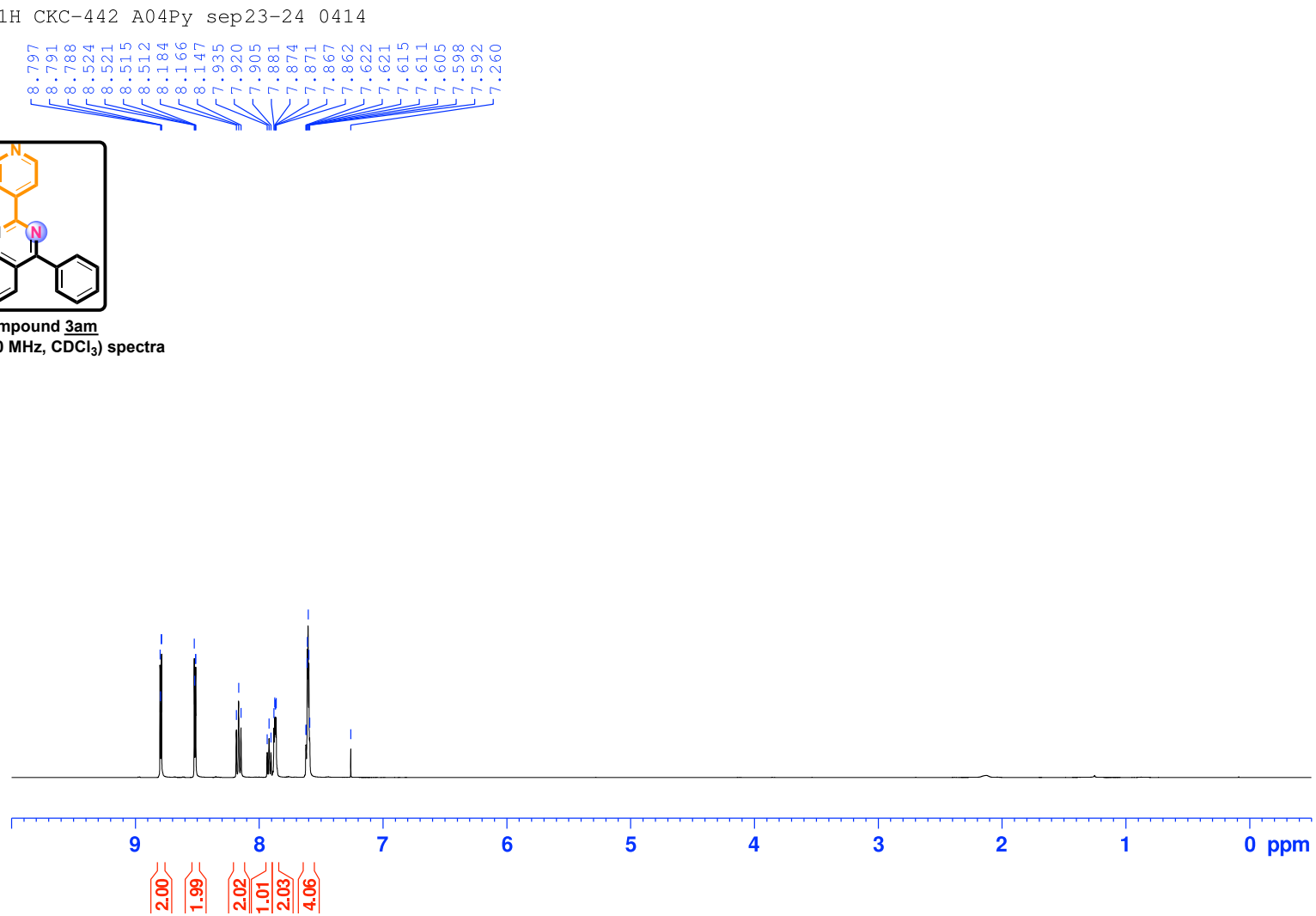

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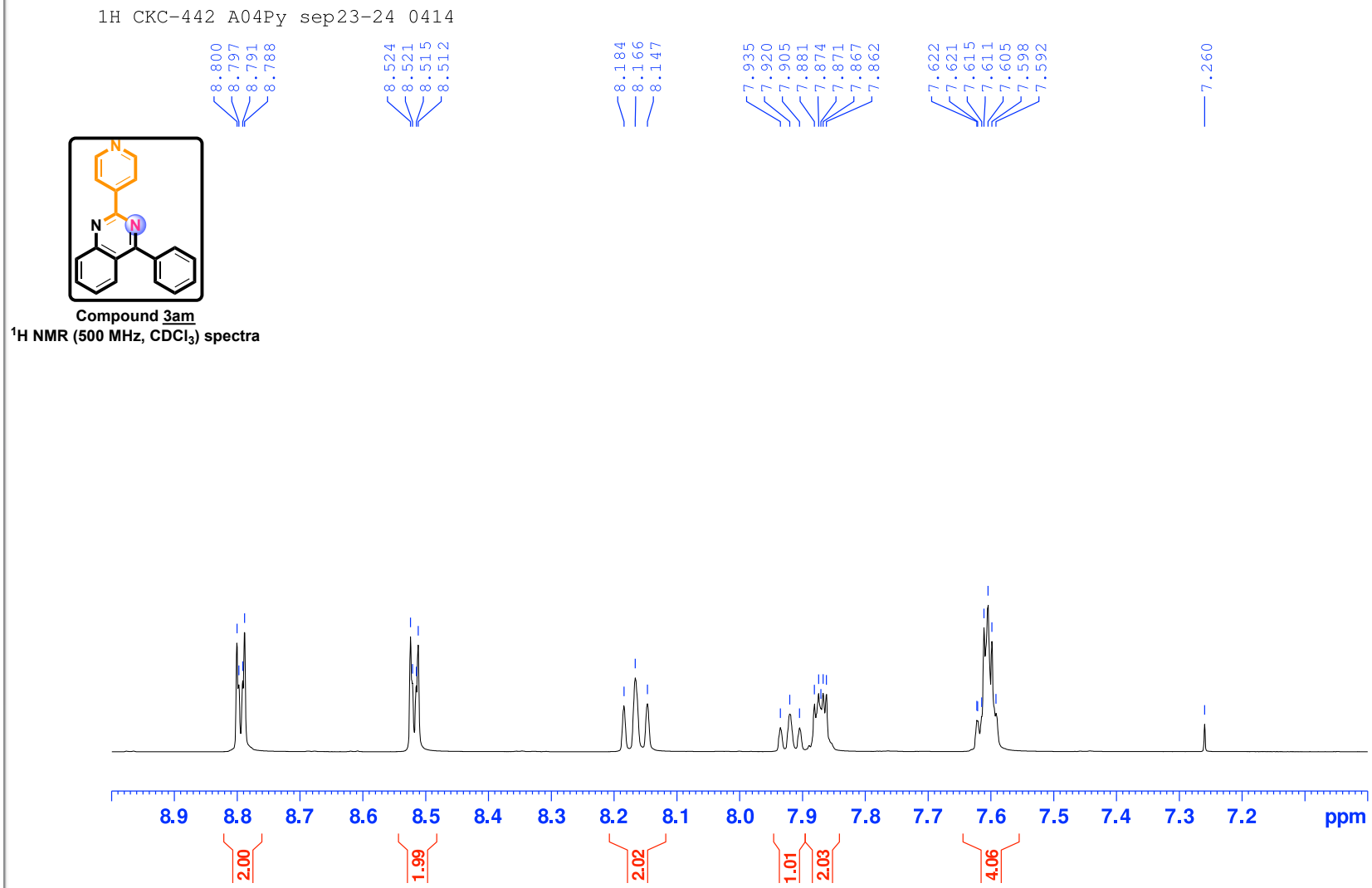
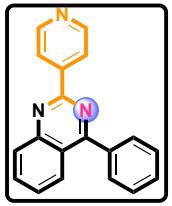
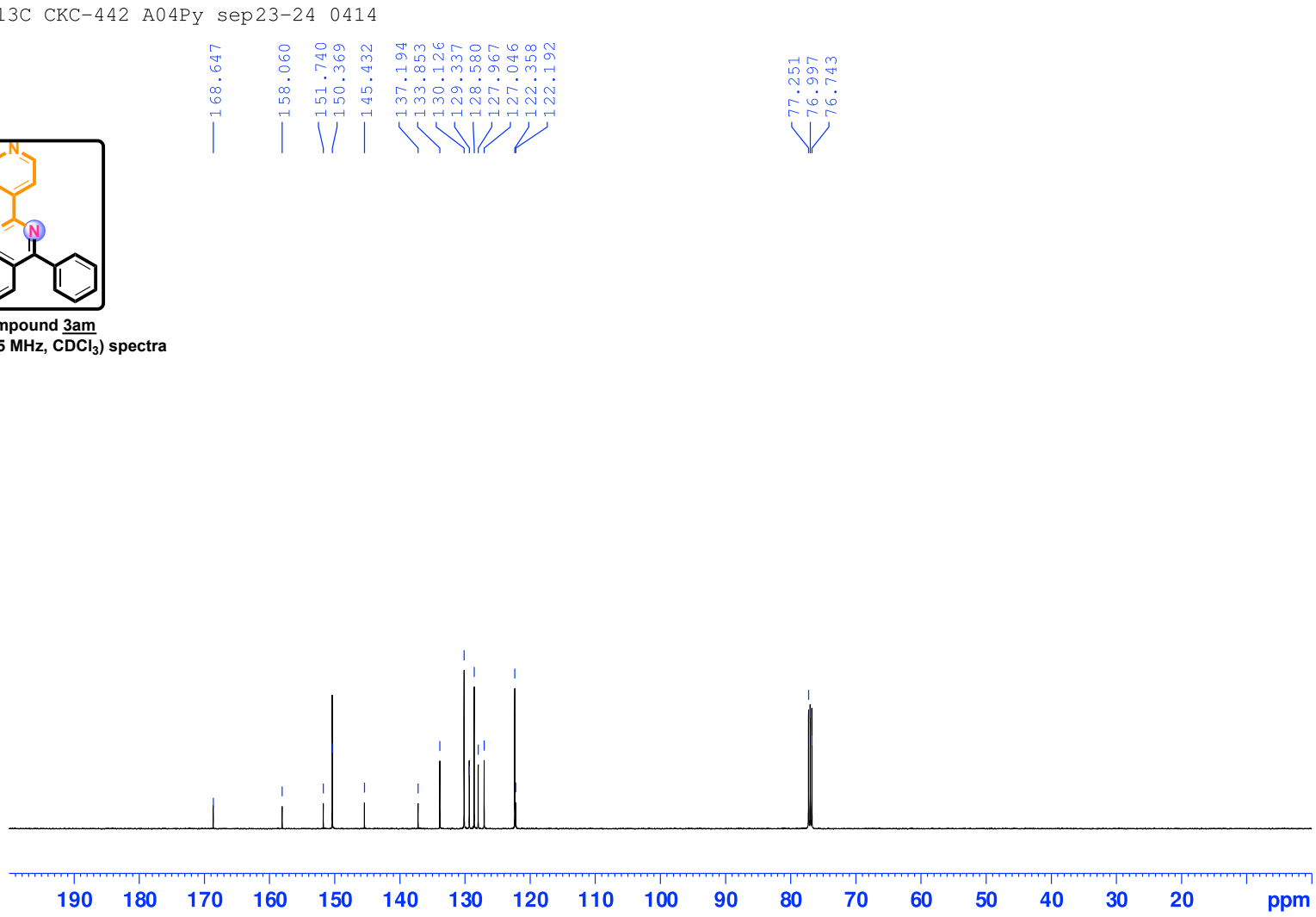


Compound 3am
^{1}H NMR (500 MHz, $CDCl_3$) spectra

Compound 3am

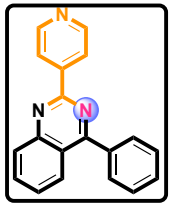


Compound 3am
^{13}C NMR (125 MHz, $CDCl_3$) spectra

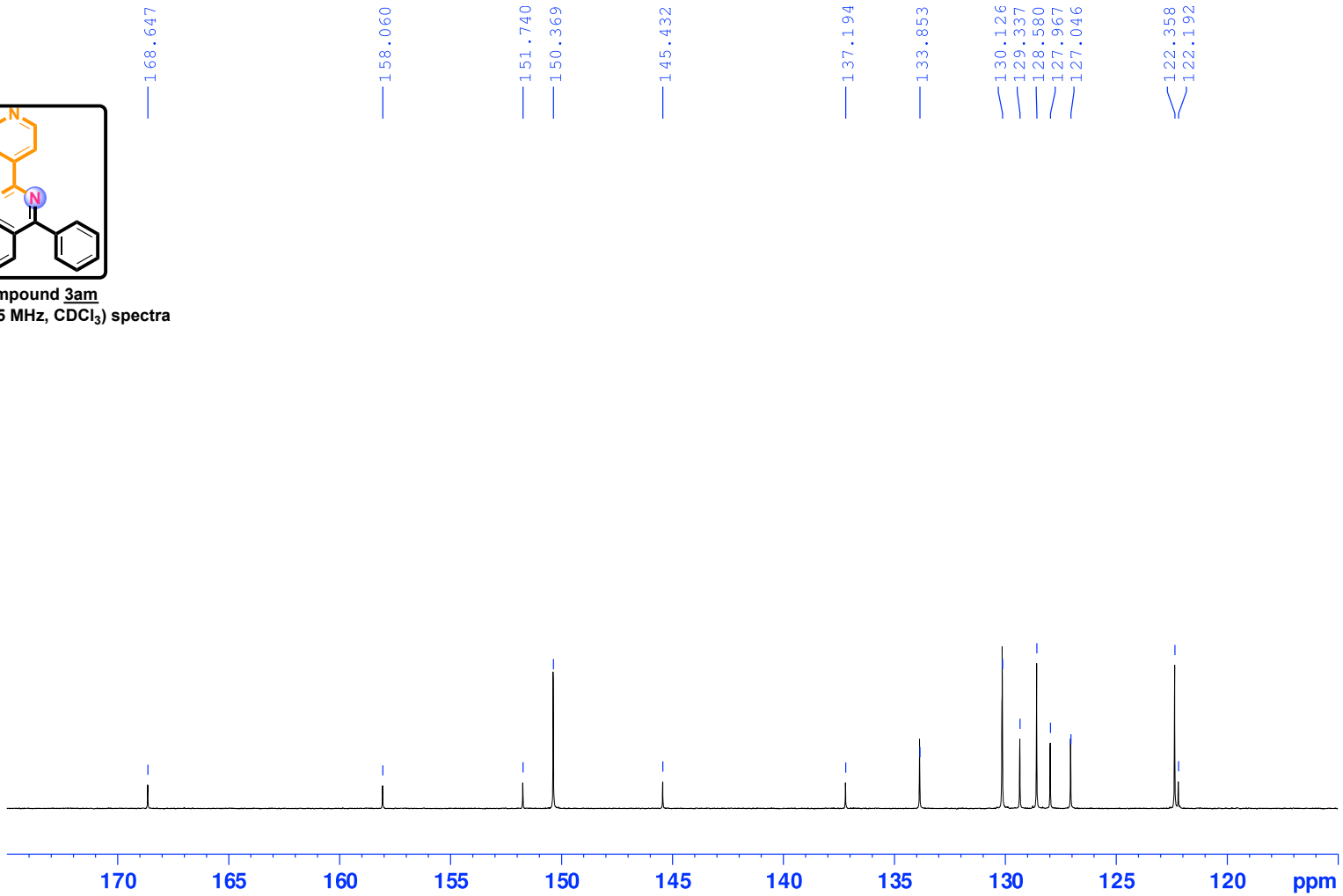


Compound 3am

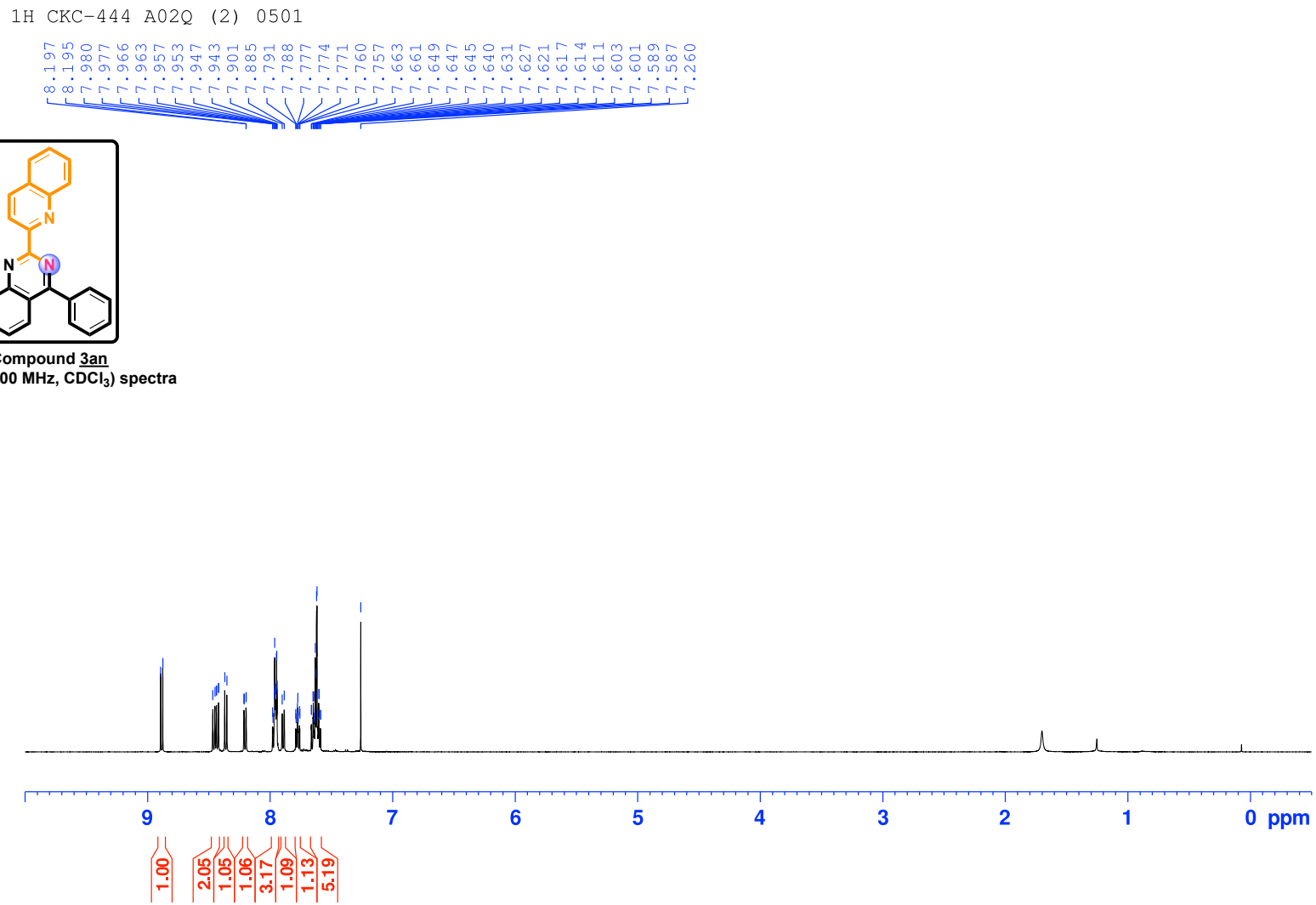
13C CKC-442 A04Py sep23-24 0414



Compound 3am
^{13}C NMR (125 MHz, $CDCl_3$) spectra

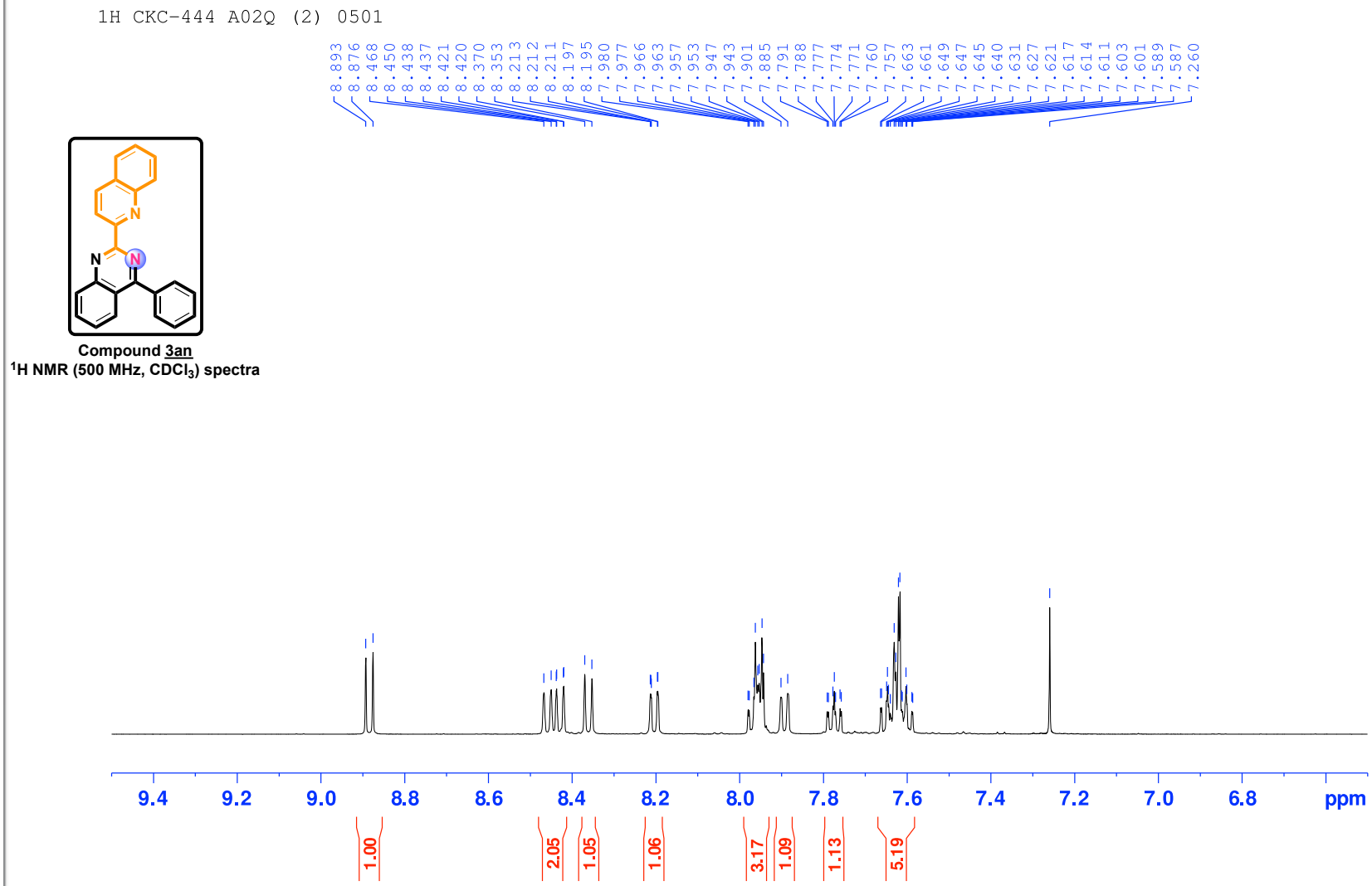


Compound 3an



Compound 3an
^{1}H NMR (500 MHz, $CDCl_3$) spectra

Compound 3an



Compound 3an
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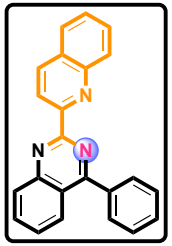
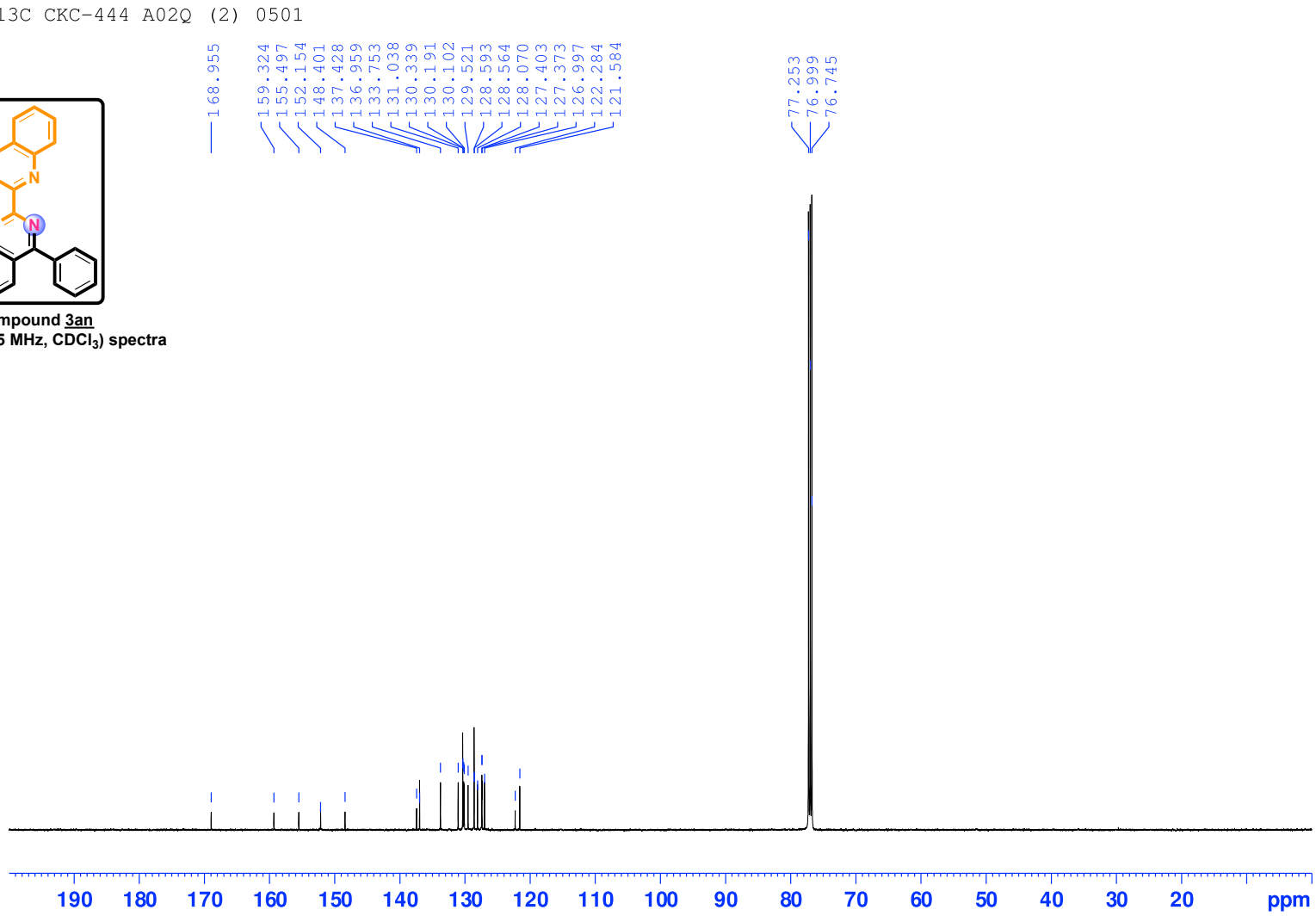
Compound 3an



Compound 3an
^{13}C NMR (125 MHz, $CDCl_3$) spectra



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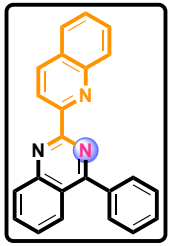

Compound 3an
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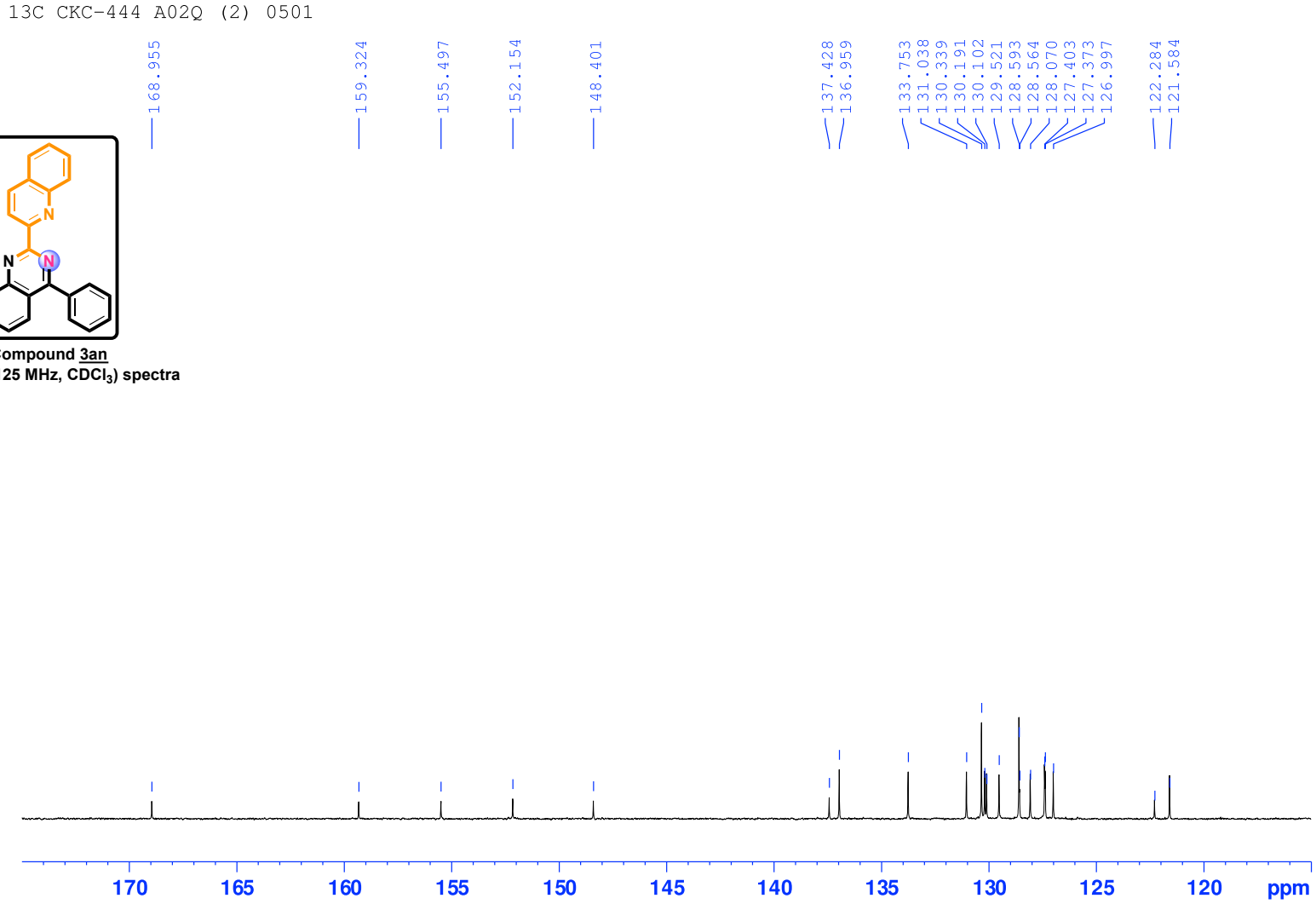
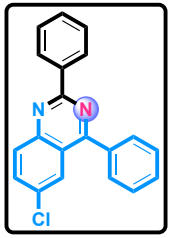


Compound 4a



Compound 4a
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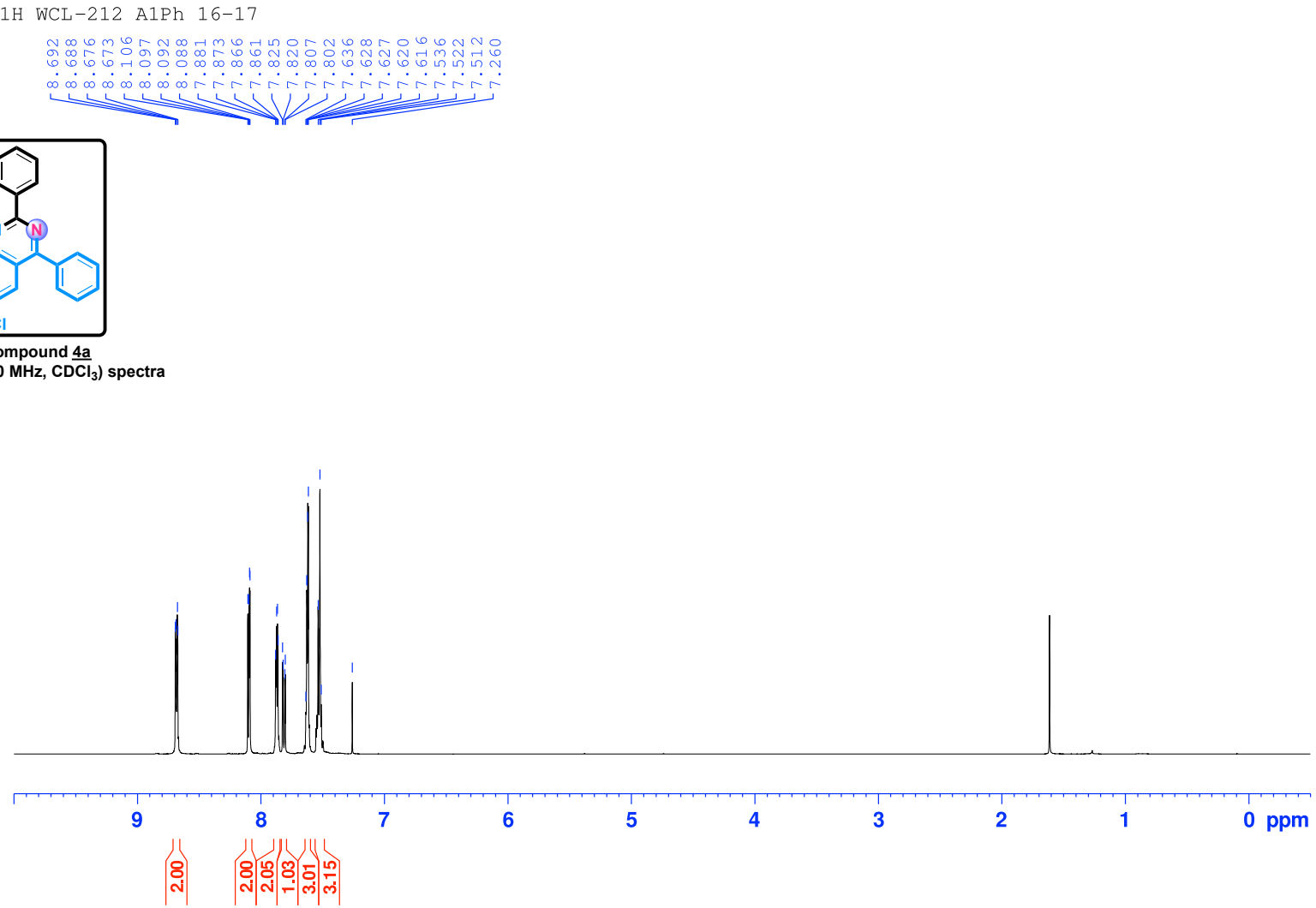

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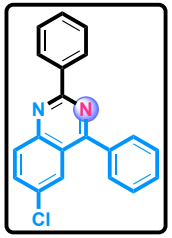

Compound 4a
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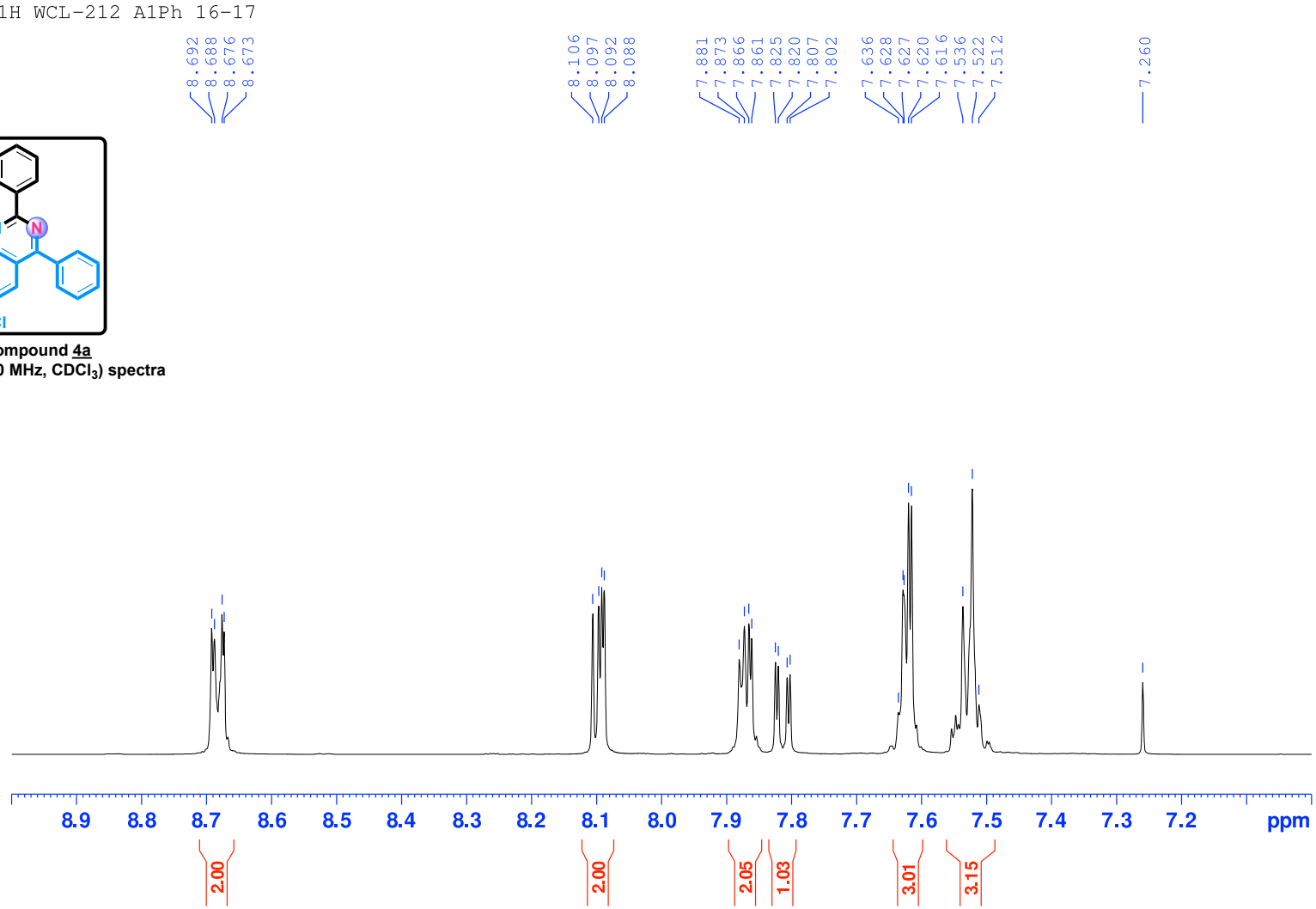

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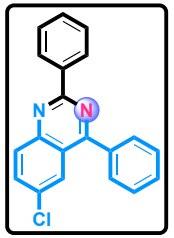
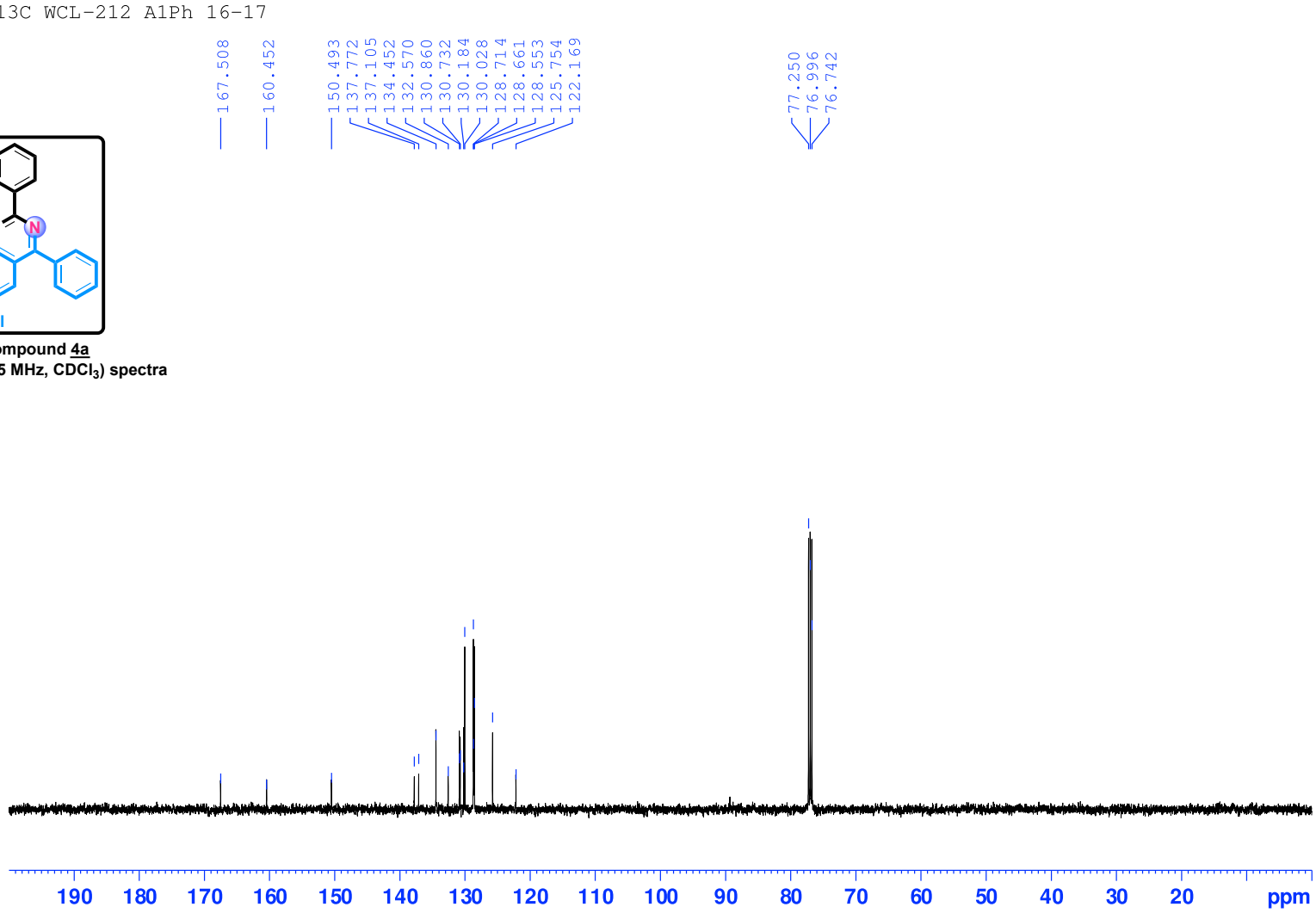


Compound 4a

^{13}C NMR (125 MHz, $CDCl_3$) spectra



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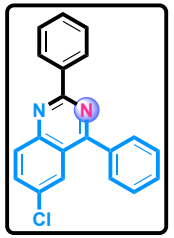
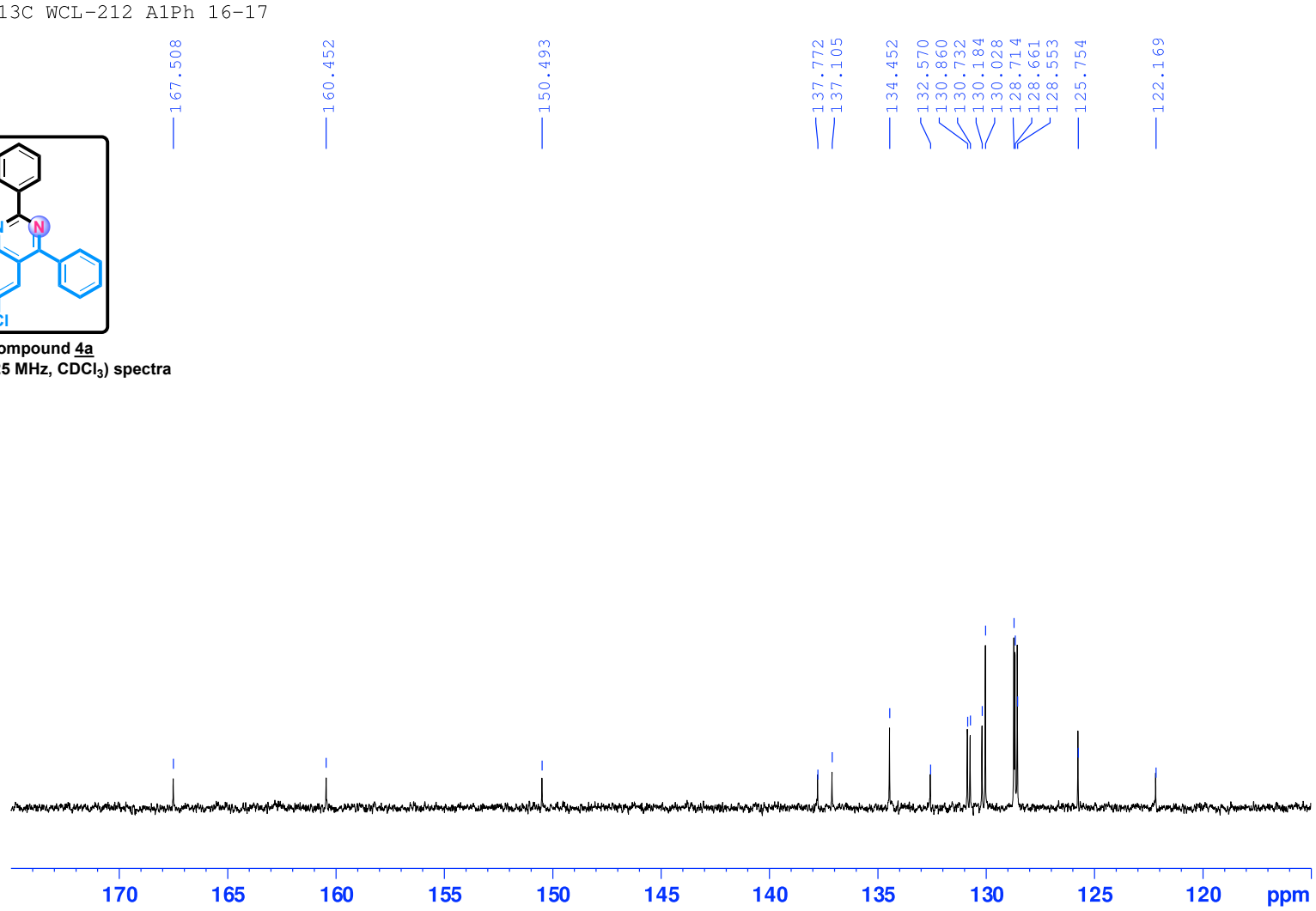


Compound 4a
^{13}C NMR (125 MHz, $CDCl_3$) spectra



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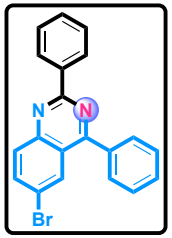
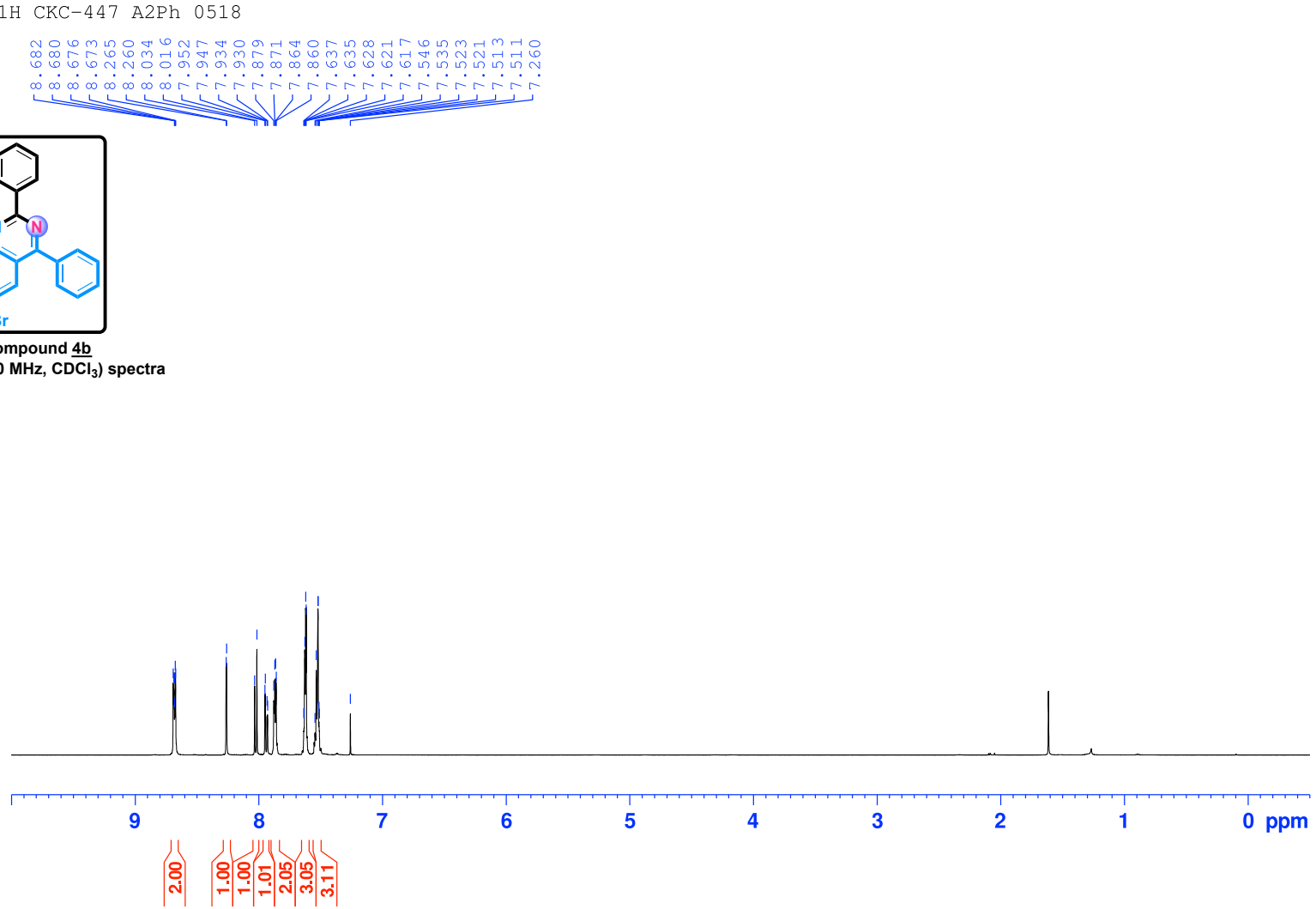
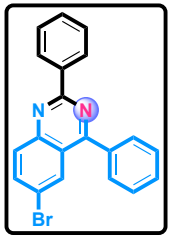


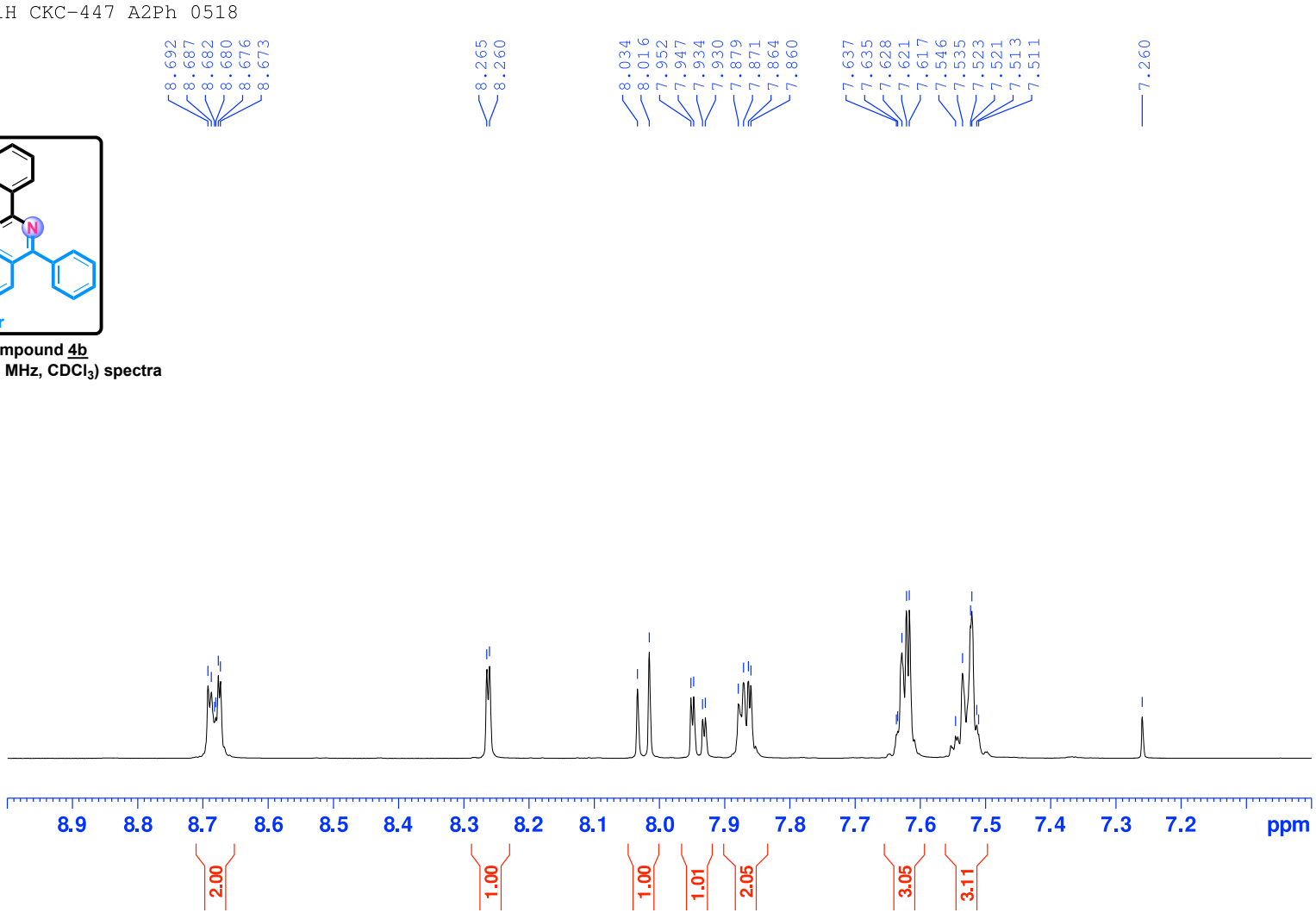
Compound 4b
^{1}H NMR (500 MHz, $CDCl_3$) spectra



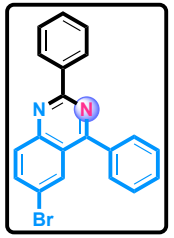
Compound 4b



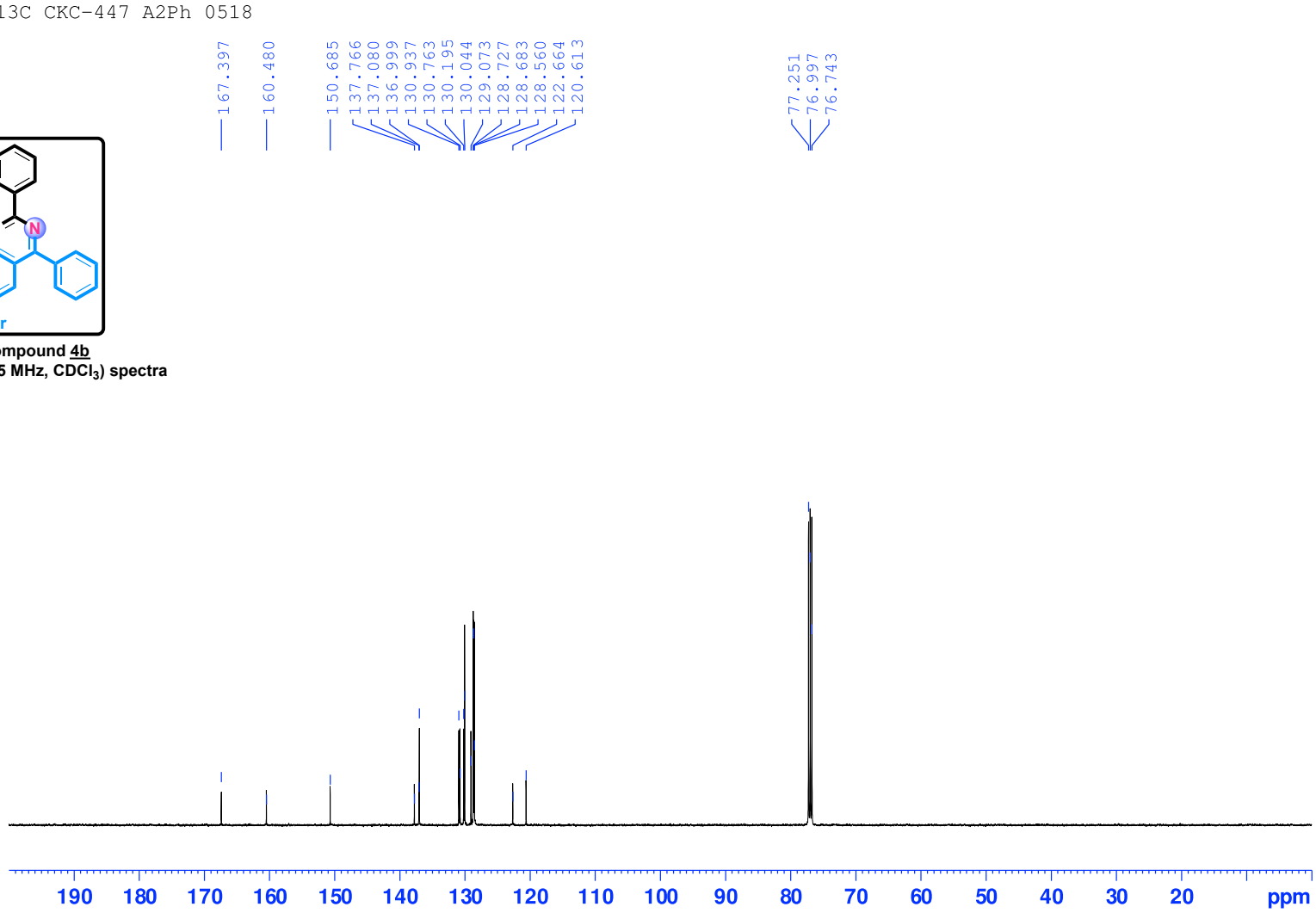
Compound 4b
^{1}H NMR (500 MHz, $CDCl_3$) spectra



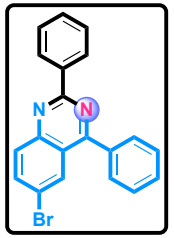
Compound 4b



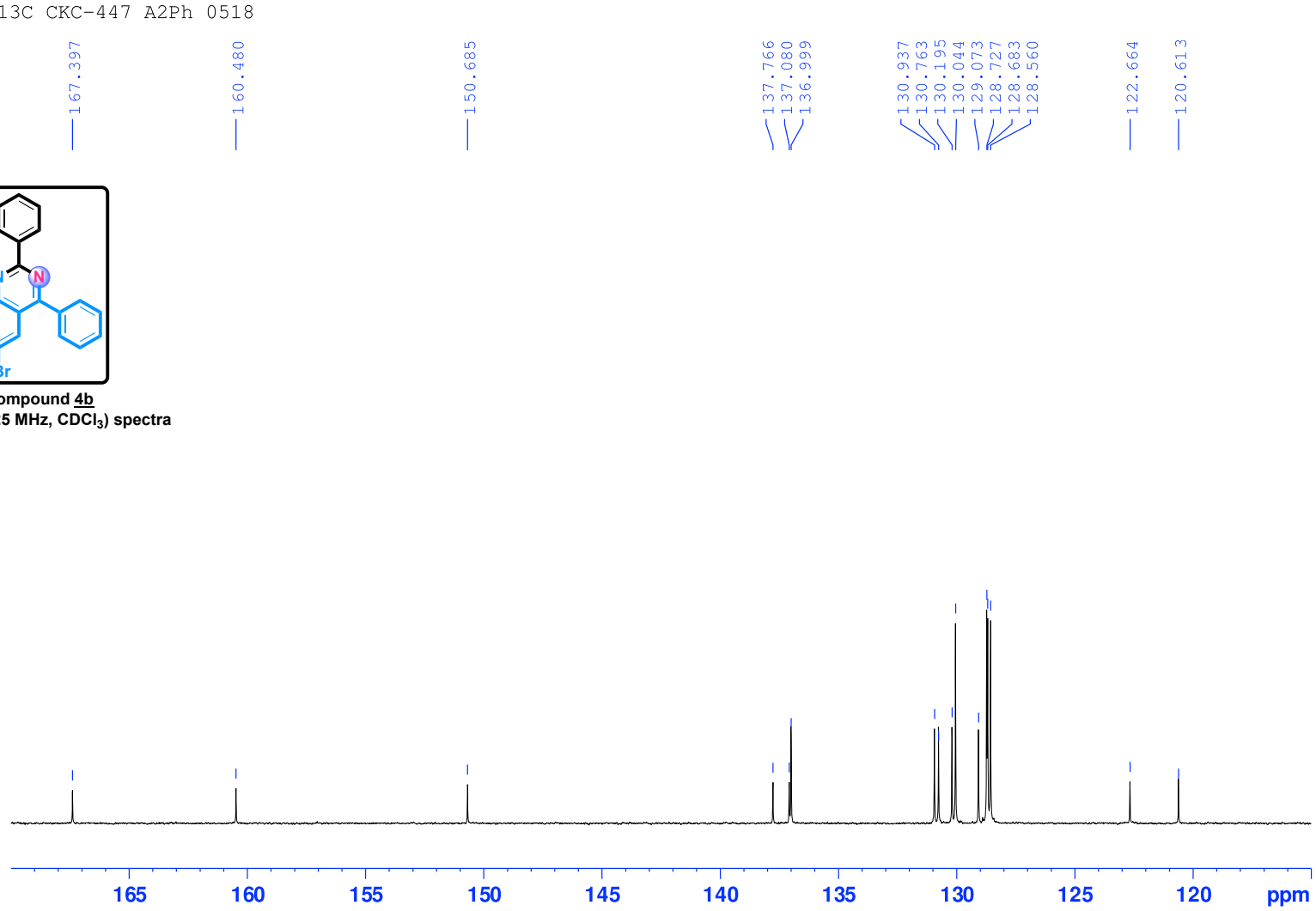
Compound 4b
^{13}C NMR (125 MHz, $CDCl_3$) spectra



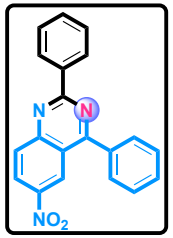
Compound 4b



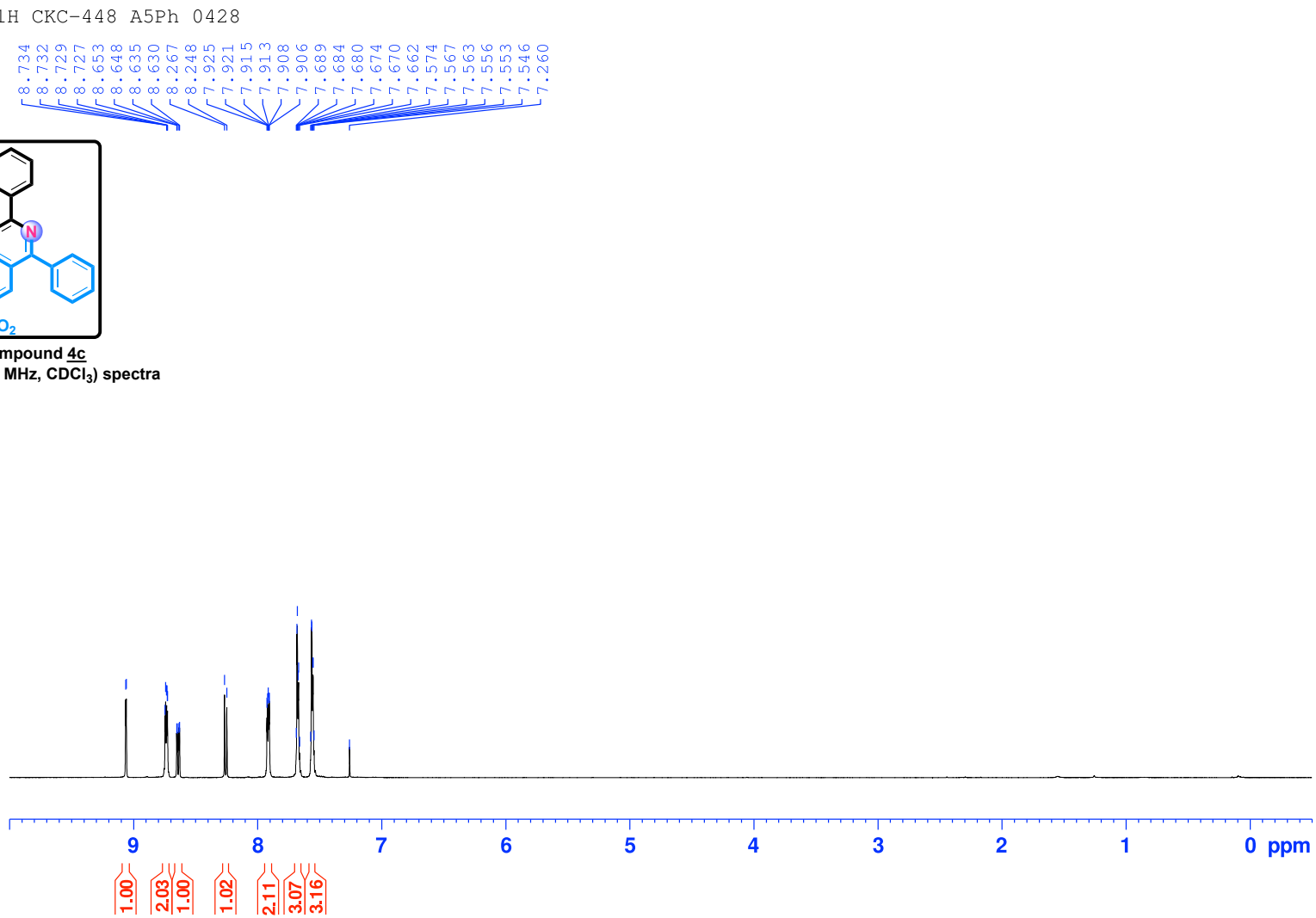
Compound 4b
^{13}C NMR (125 MHz, $CDCl_3$) spectra



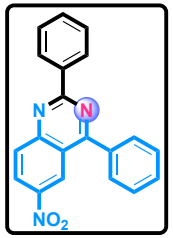
Compound 4c



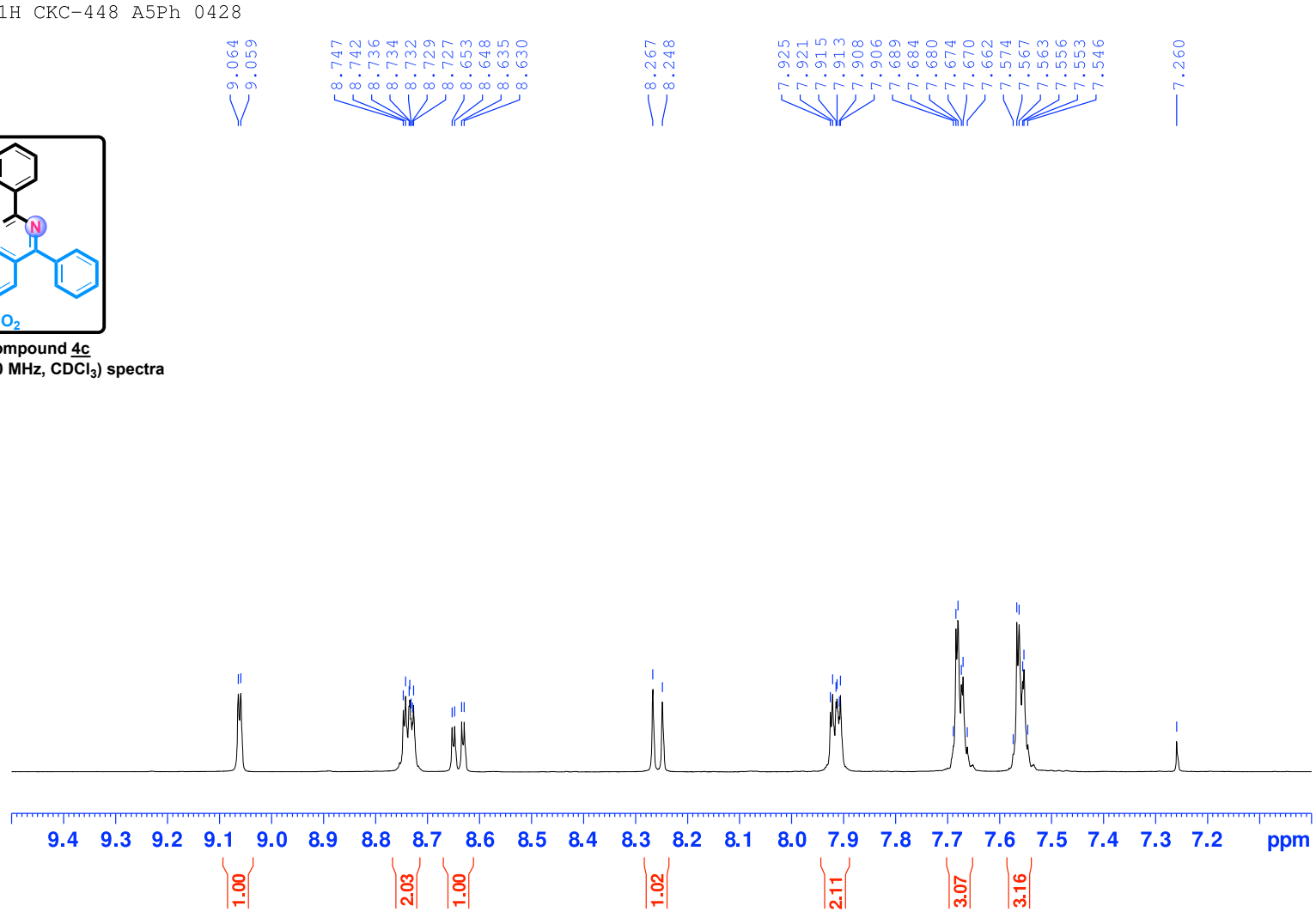
Compound 4c
^{1}H NMR (500 MHz, $CDCl_3$) spectra



Compound 4c



Compound 4c
^{1}H NMR (500 MHz, $CDCl_3$) spectra



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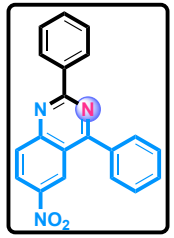
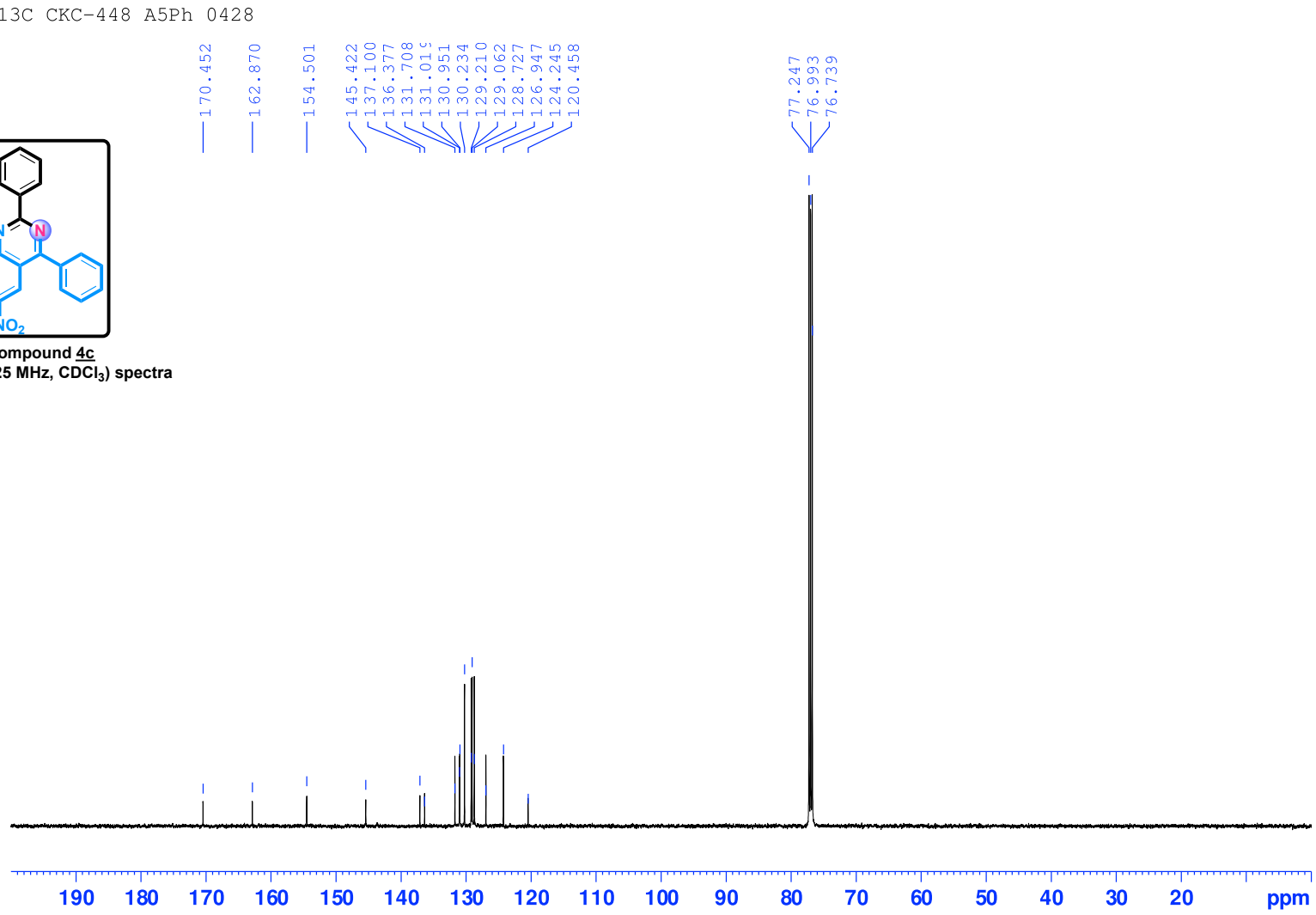
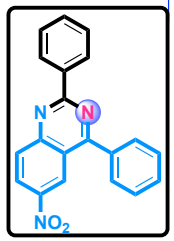


Compound 4c

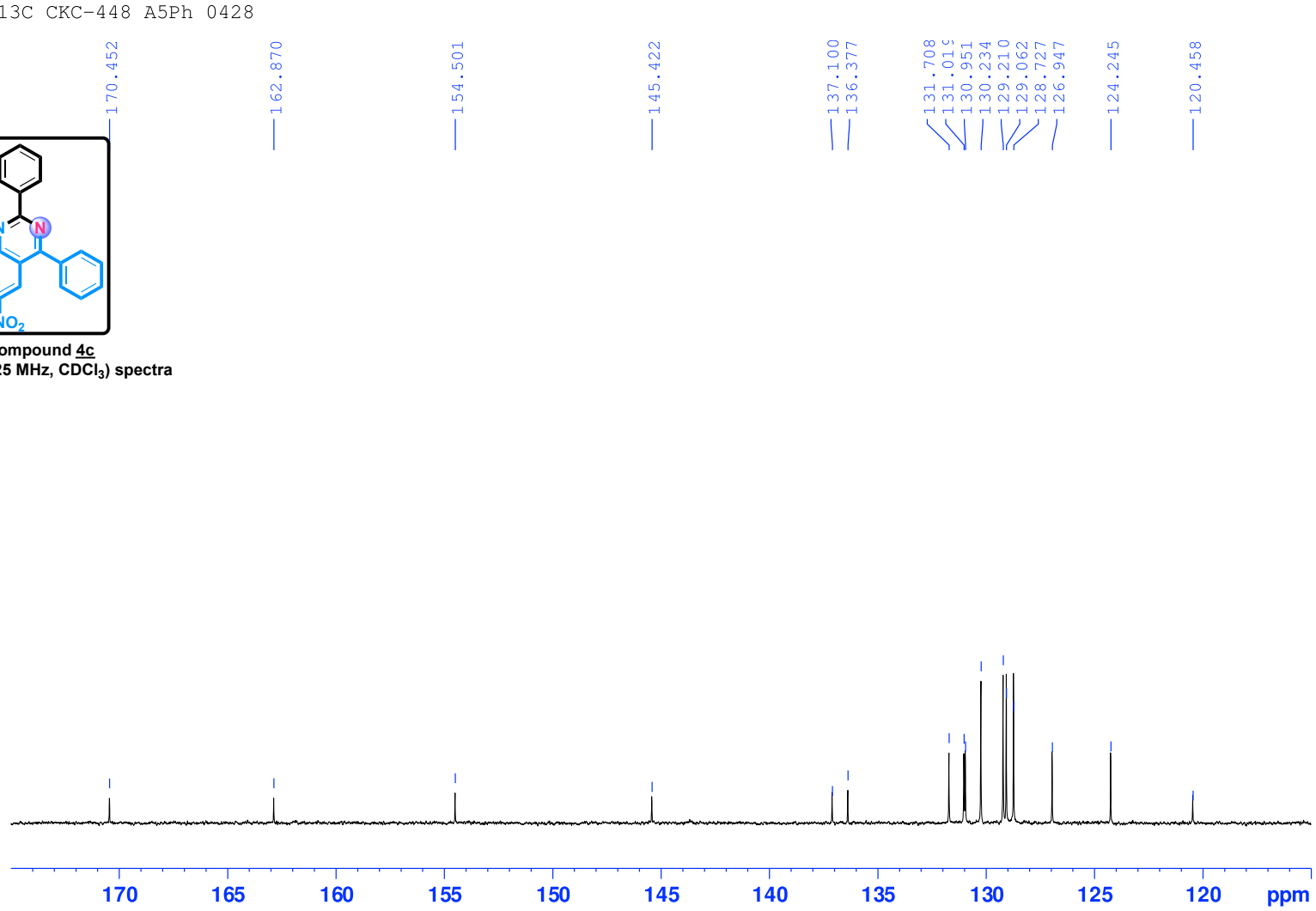
^{13}C NMR (125 MHz, $CDCl_3$) spectra



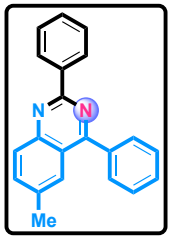
Compound 4c



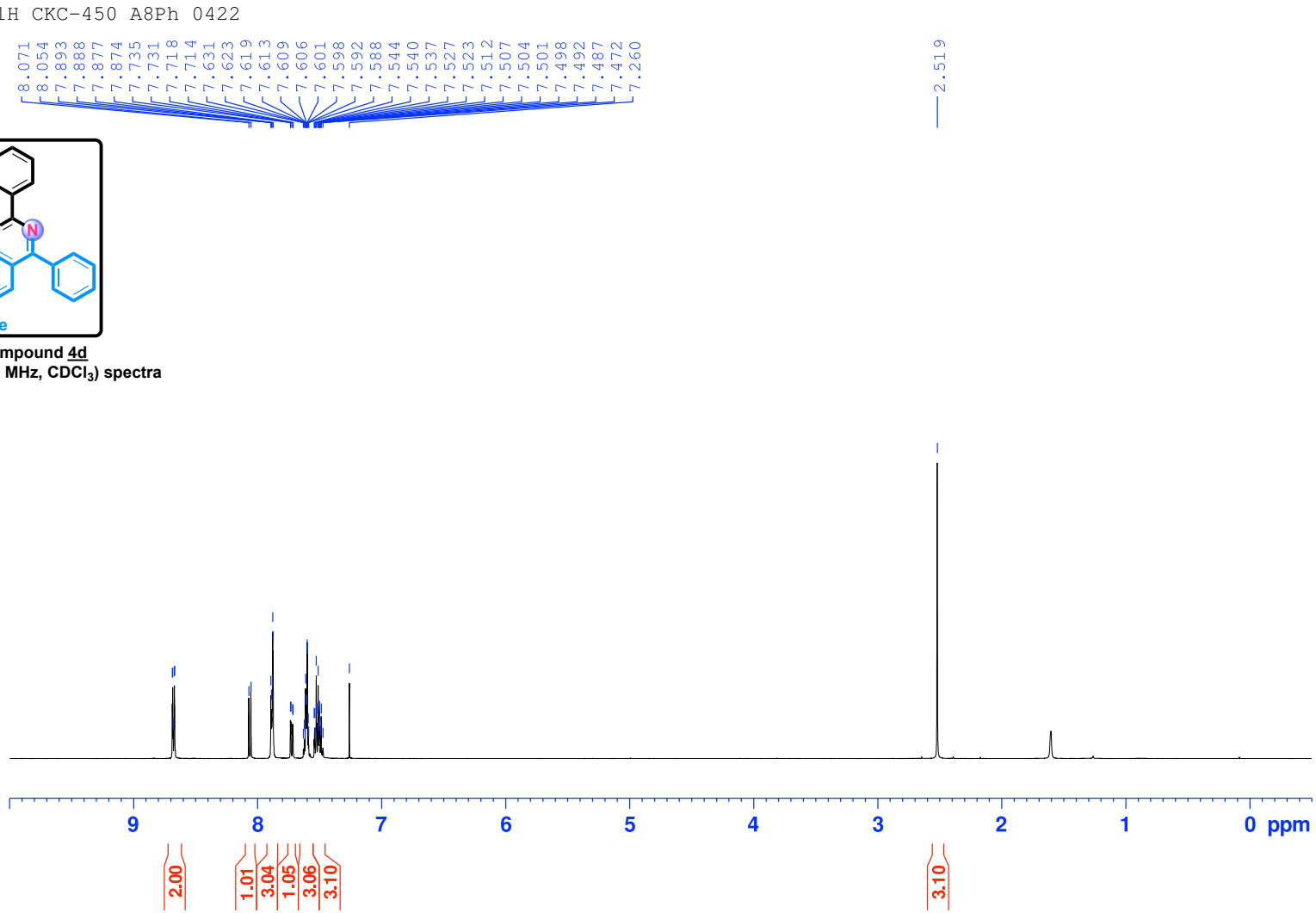
Compound 4c
^{13}C NMR (125 MHz, $CDCl_3$) spectra



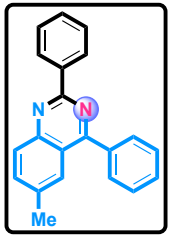
Compound 4d



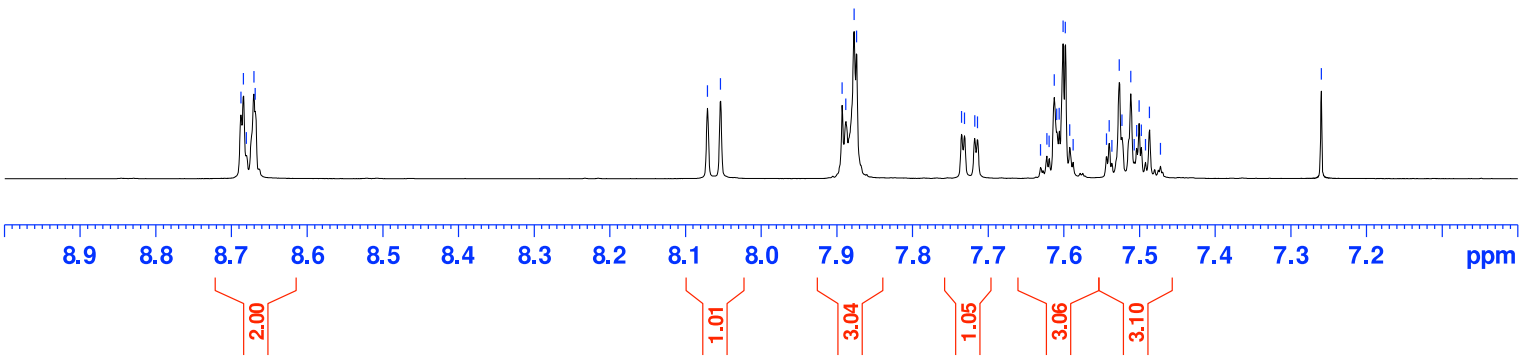
Compound 4d
^{1}H NMR (500 MHz, $CDCl_3$) spectra



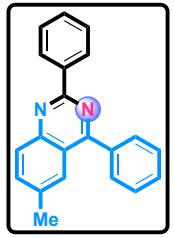
Compound 4d



Compound 4d
^{1}H NMR (500 MHz, $CDCl_3$) spectra

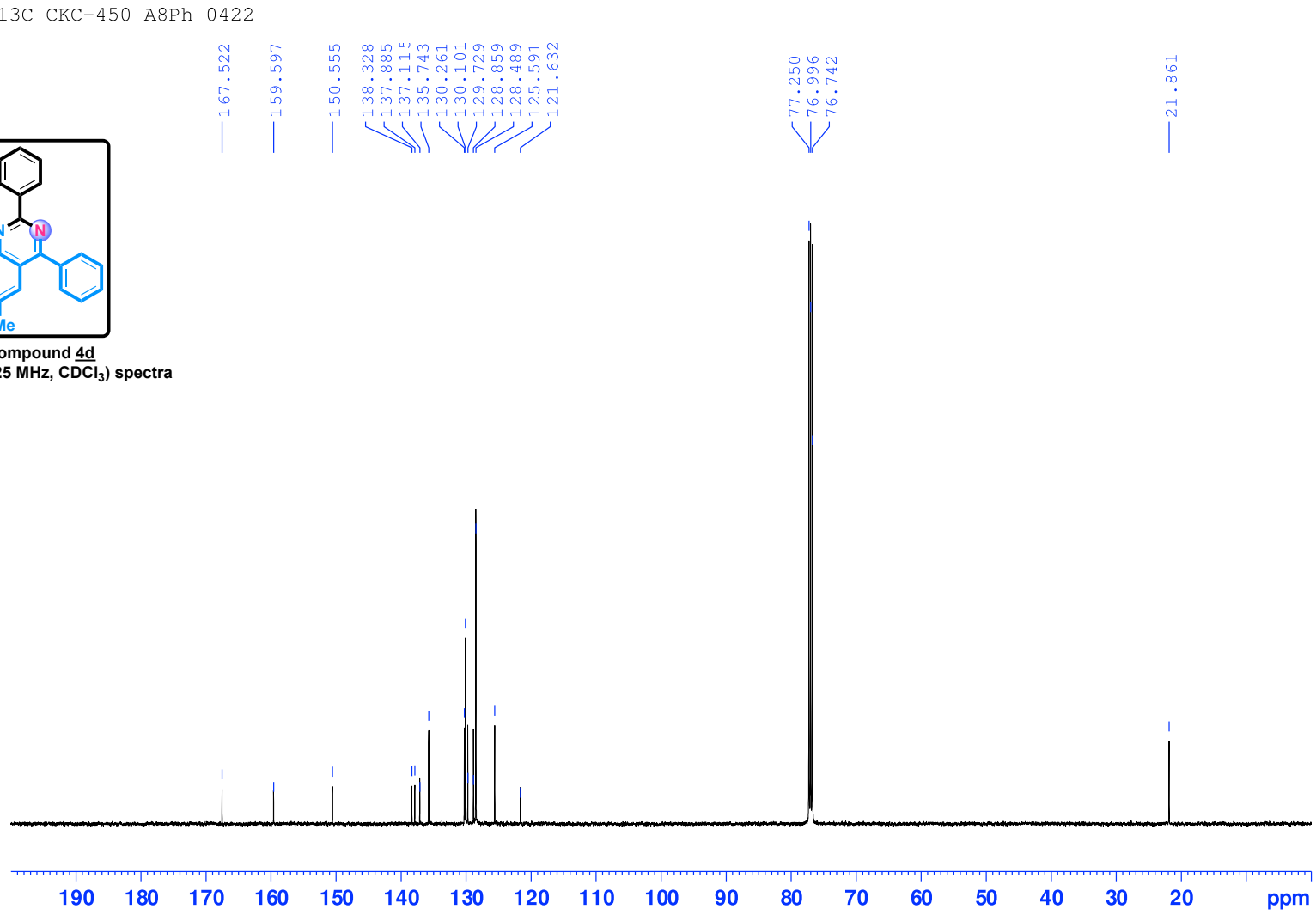


Compound 4d

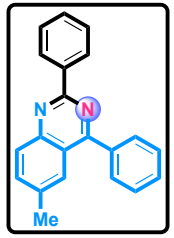


Compound 4d

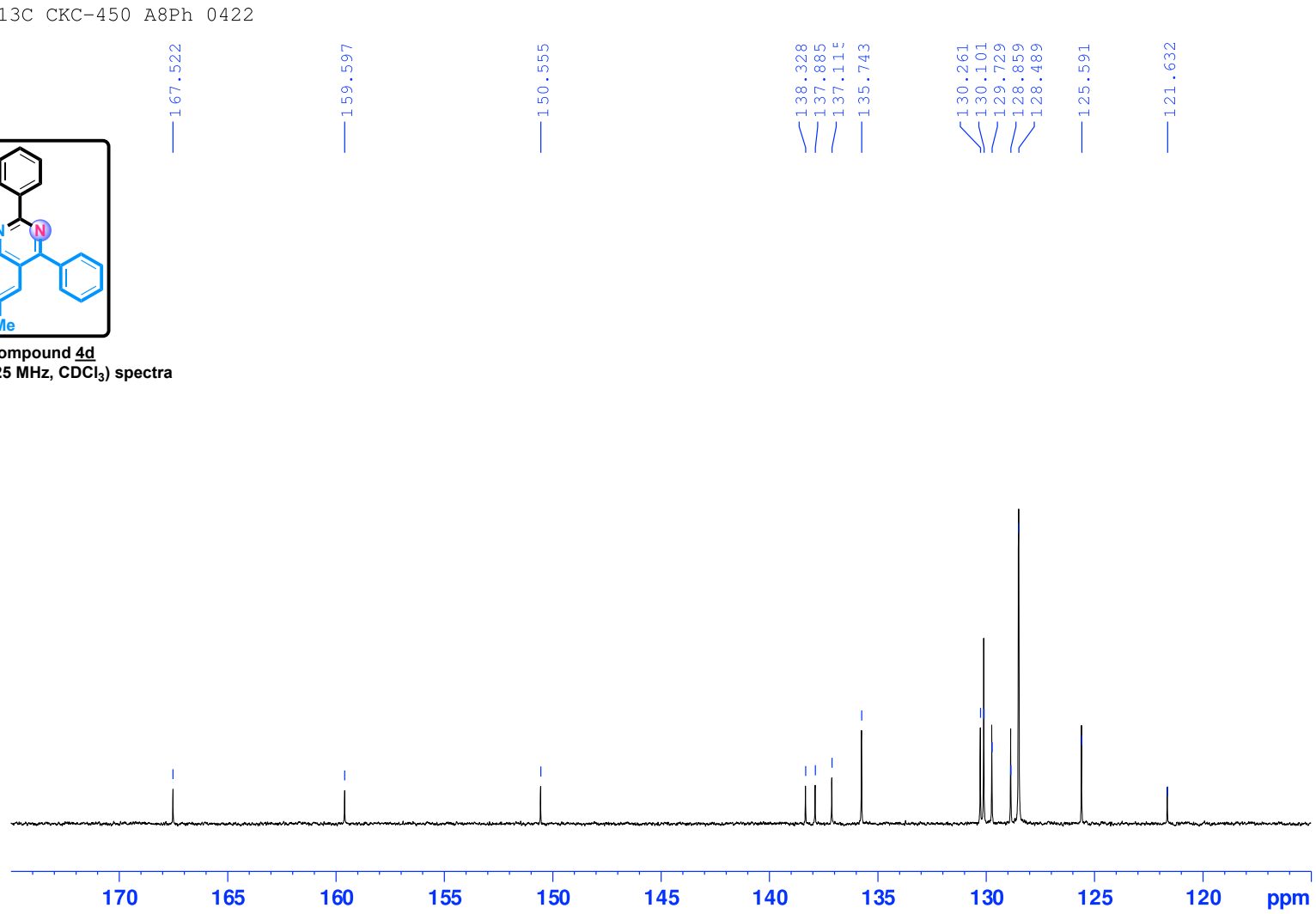
^{13}C NMR (125 MHz, $CDCl_3$) spectra



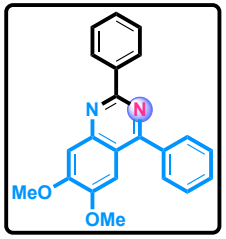
Compound 4d



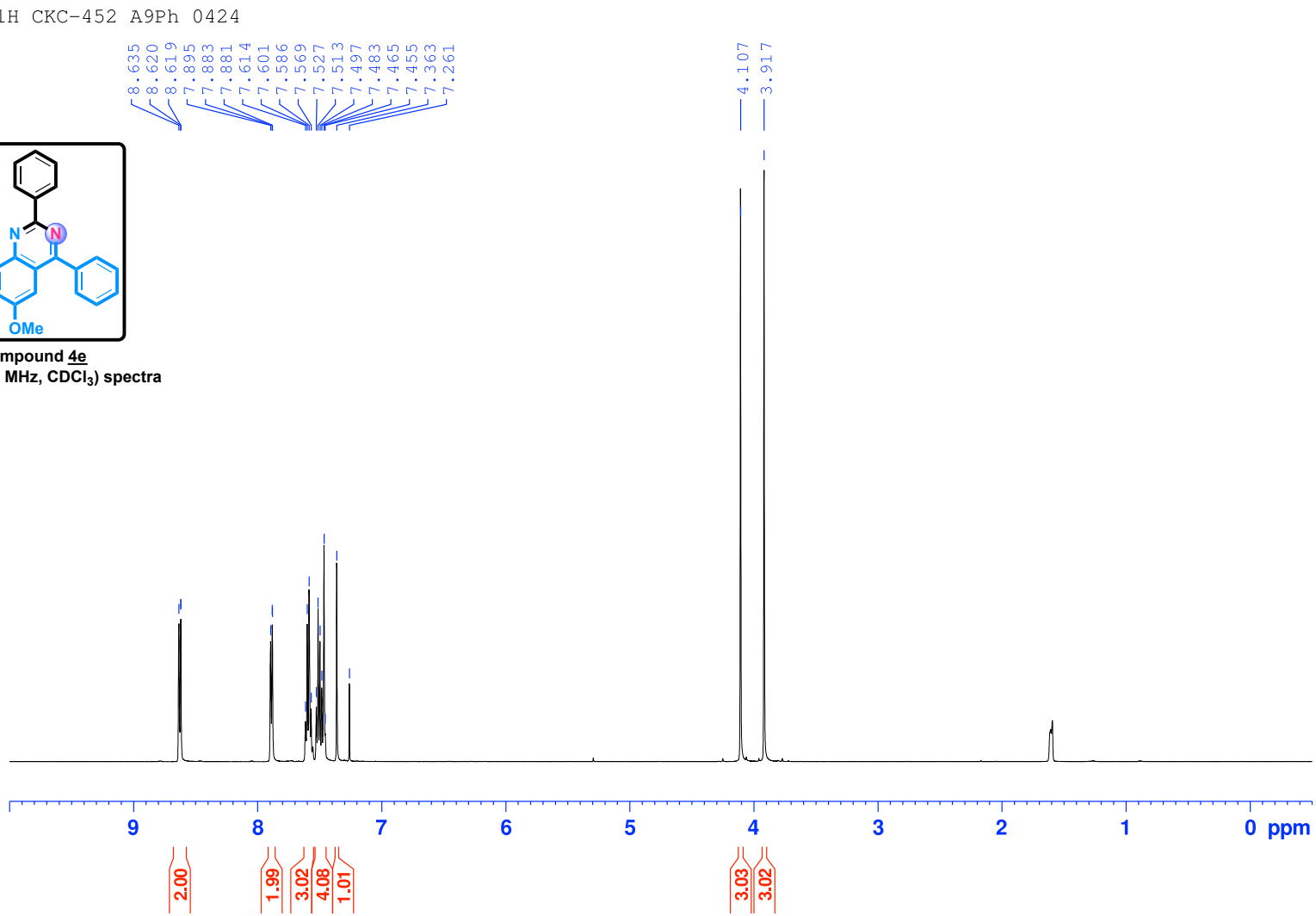
Compound 4d
^{13}C NMR (125 MHz, $CDCl_3$) spectra



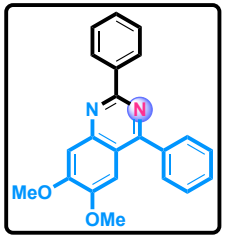
Compound 4e



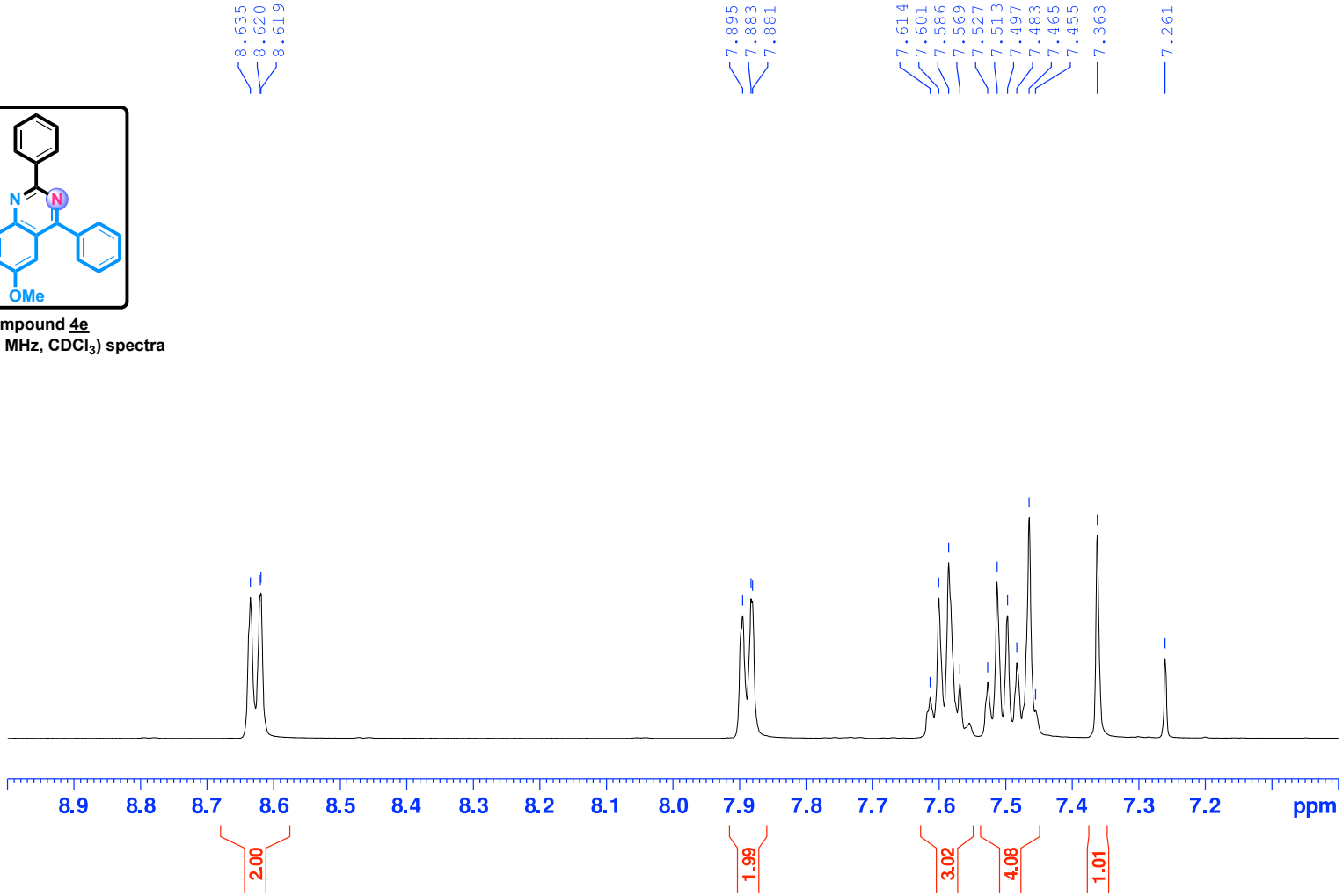
Compound 4e
^{1}H NMR (500 MHz, $CDCl_3$) spectra



Compound 4e



Compound 4e
^{1}H NMR (500 MHz, $CDCl_3$) spectra



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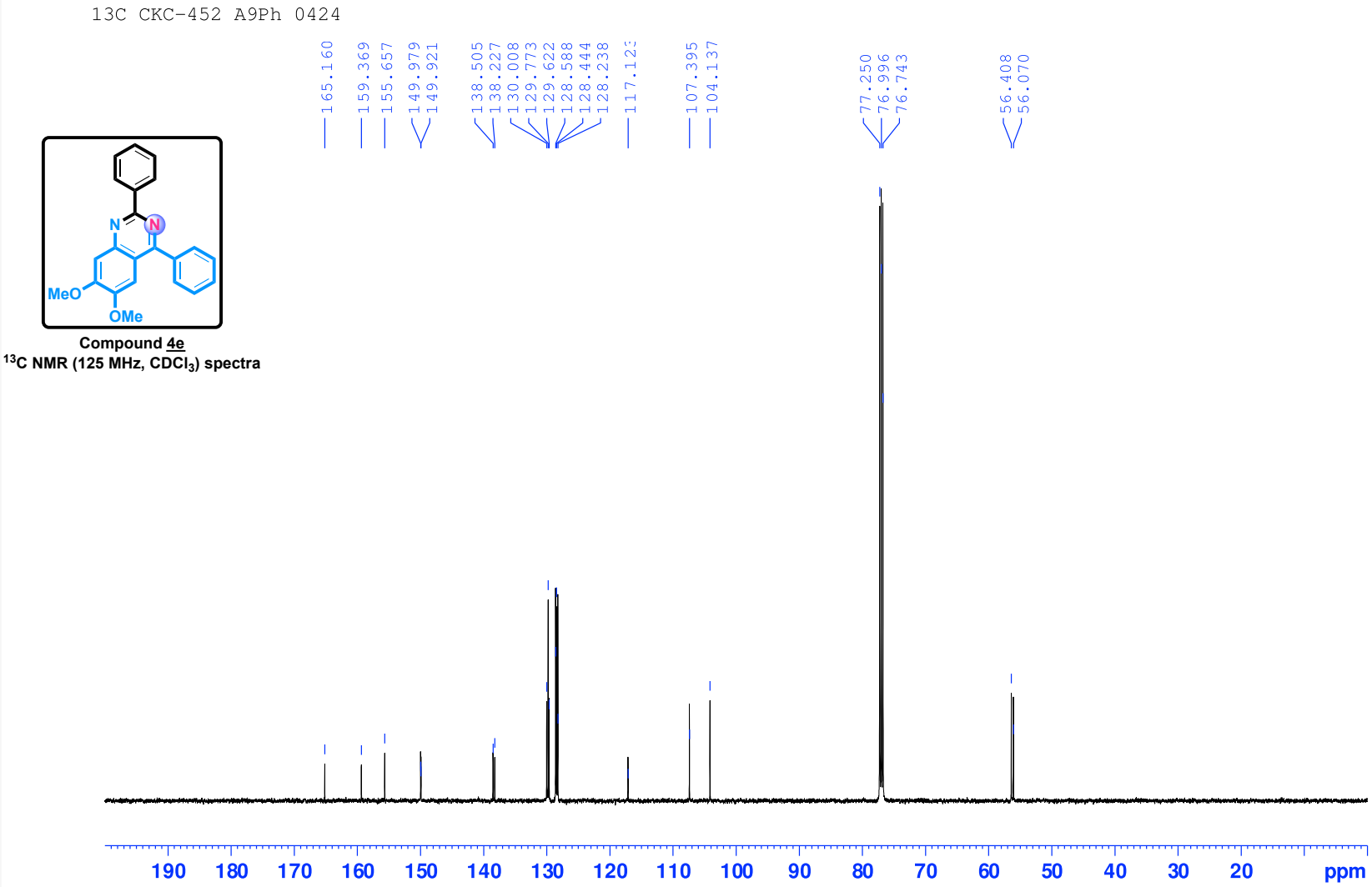
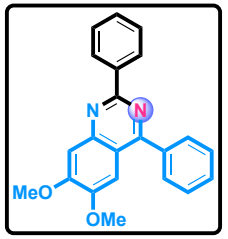


Compound 4e

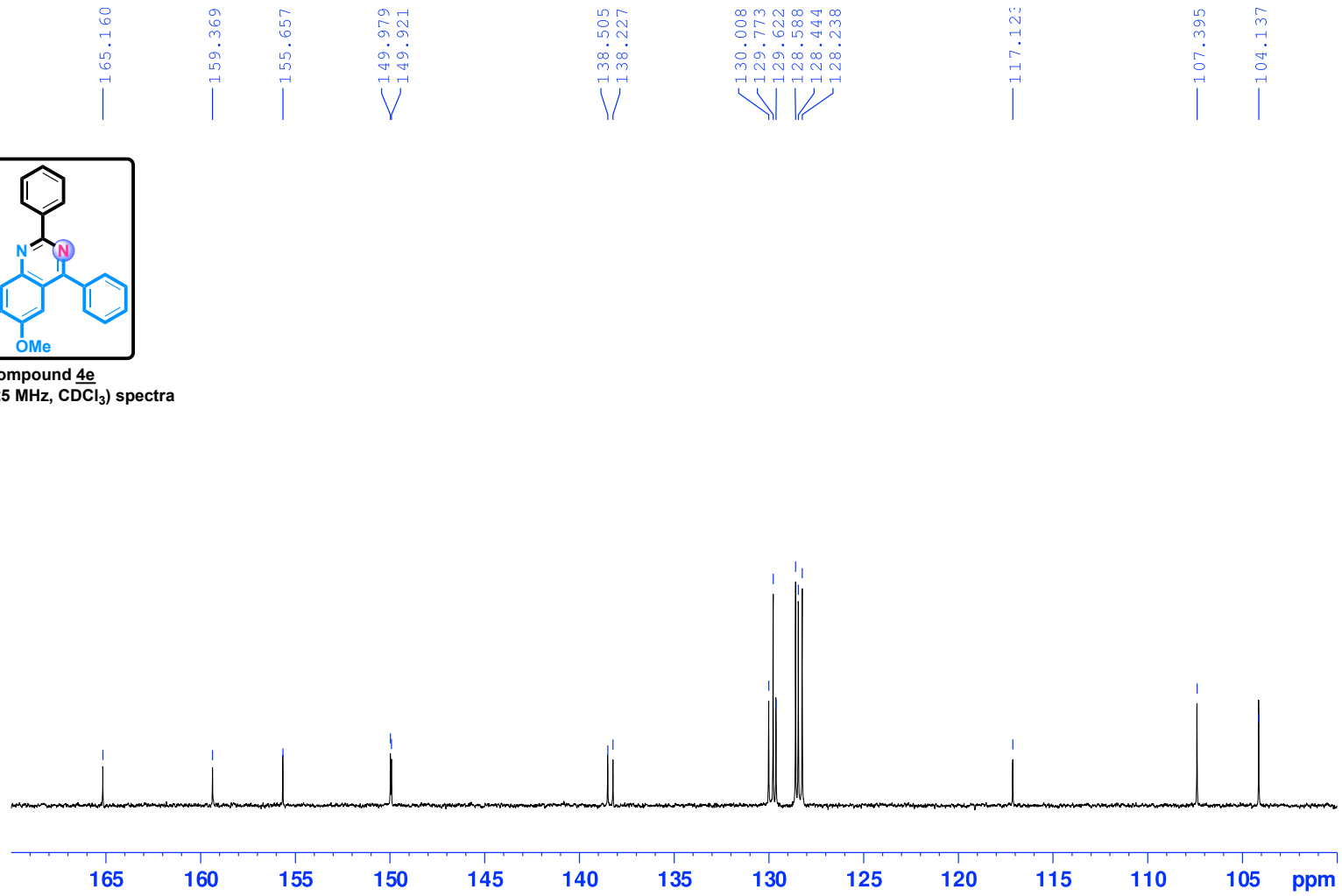
^{13}C NMR (125 MHz, $CDCl_3$) spectra

Compound 4e

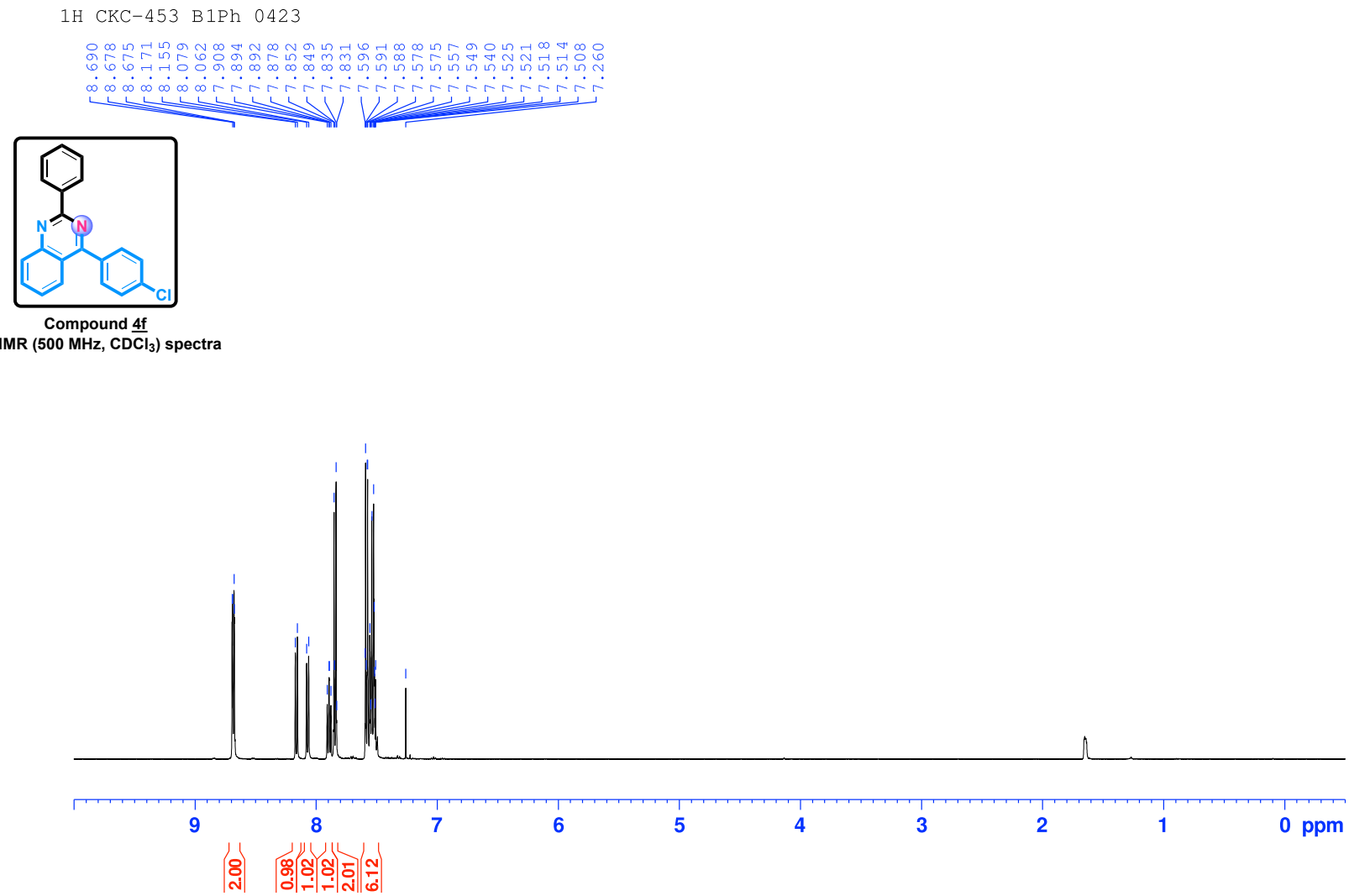


Compound 4e

^{13}C NMR (125 MHz, $CDCl_3$) spectra

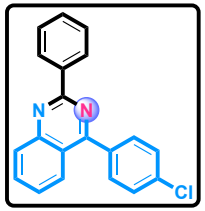


Compound 4f

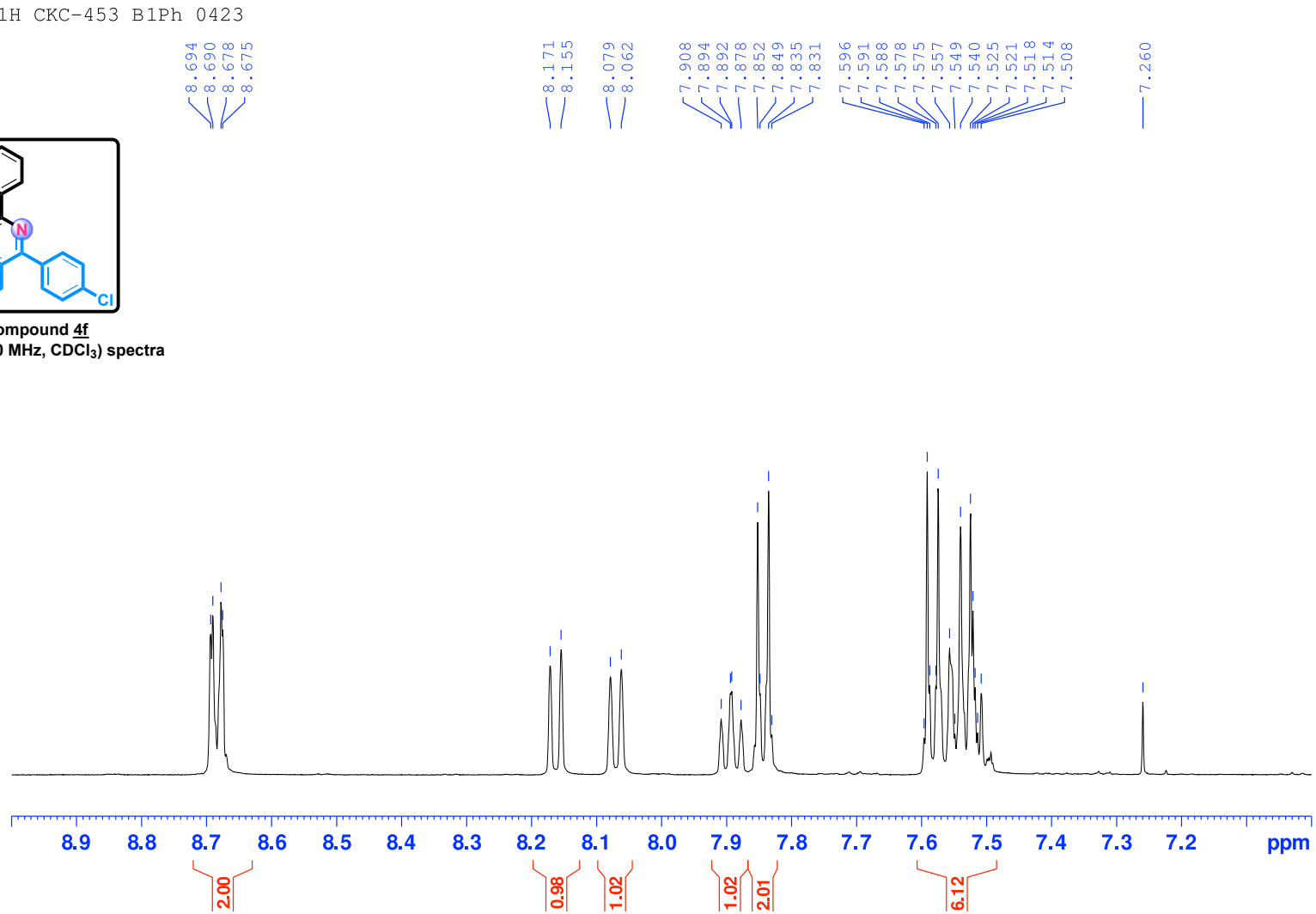


Compound 4f
^{1}H NMR (500 MHz, $CDCl_3$) spectra

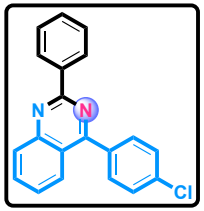
Compound 4f



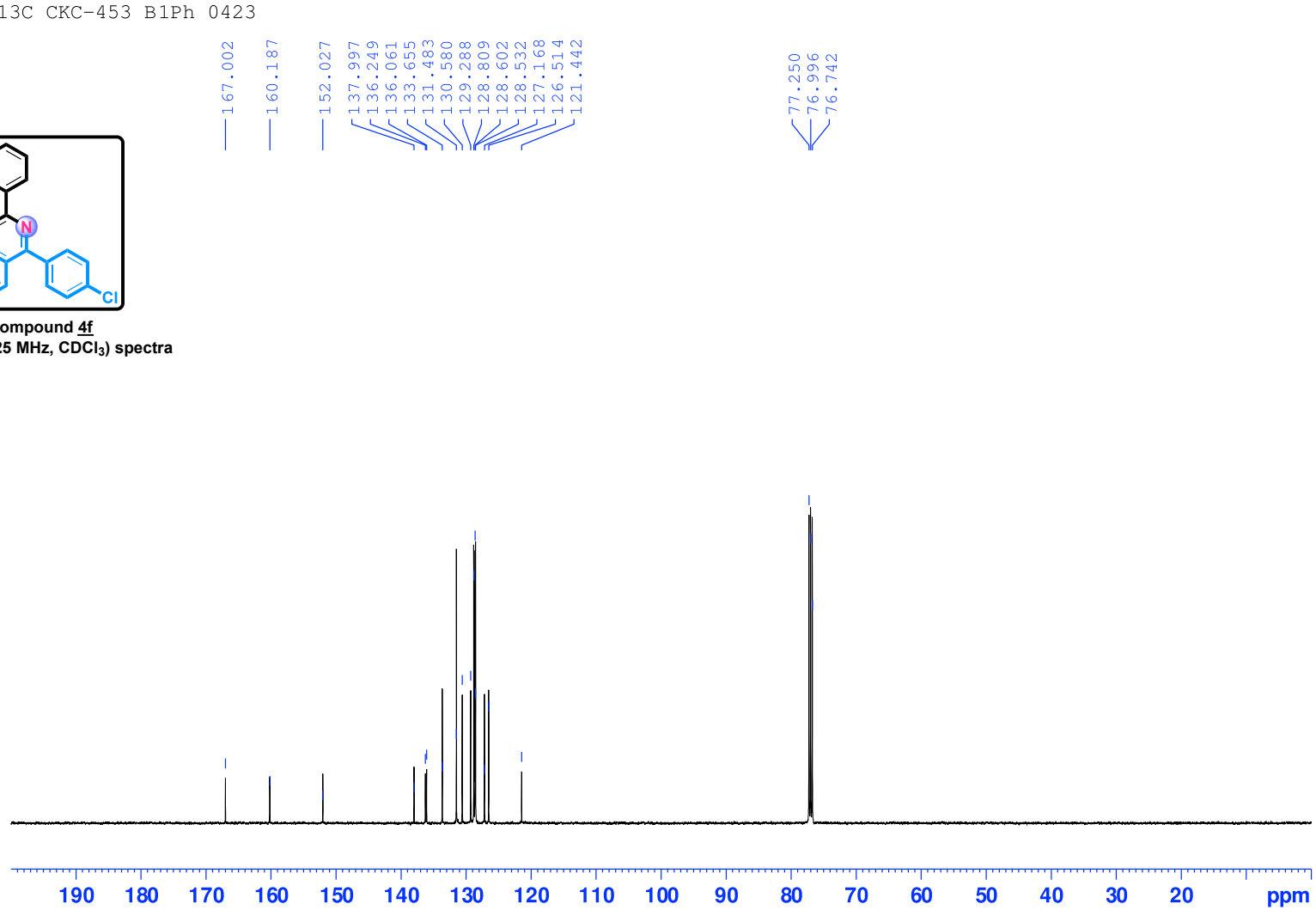
Compound 4f
^{1}H NMR (500 MHz, $CDCl_3$) spectra



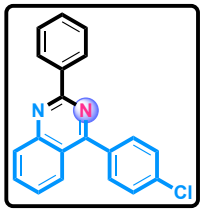
Compound 4f



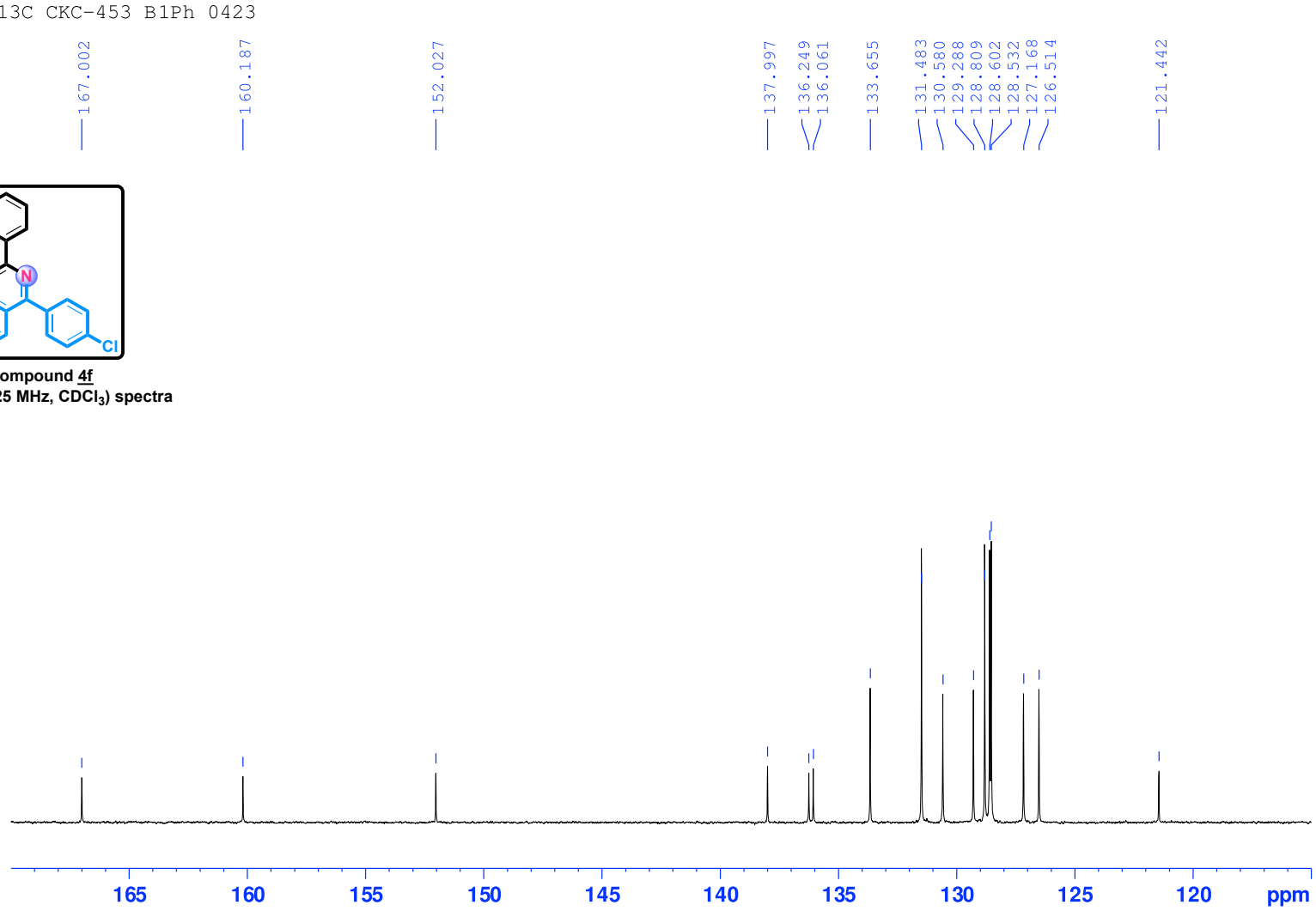
Compound 4f
^{13}C NMR (125 MHz, $CDCl_3$) spectra



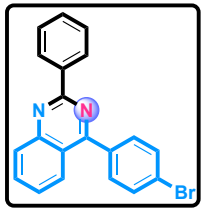
Compound 4f



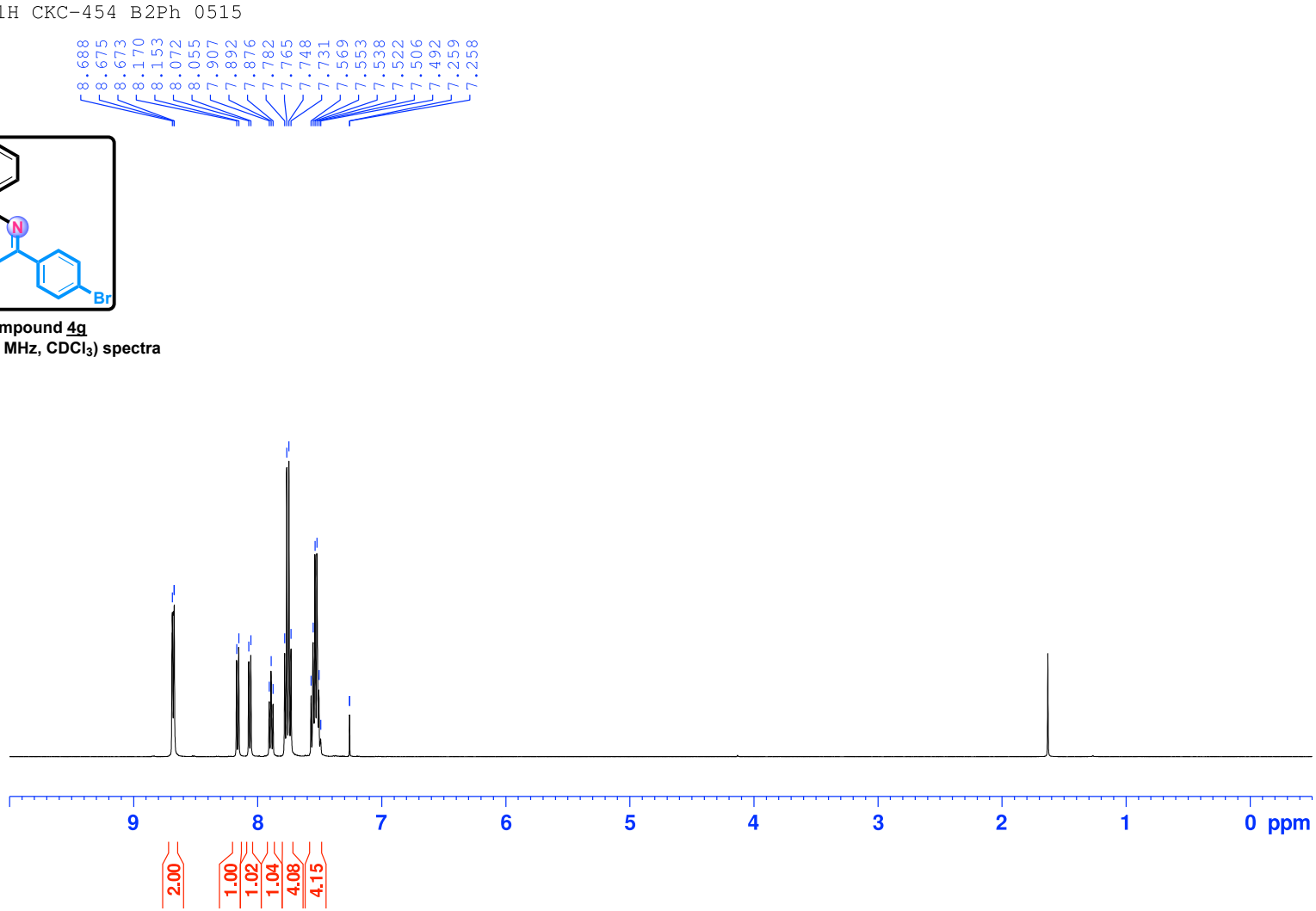
Compound 4f
^{13}C NMR (125 MHz, $CDCl_3$) spectra



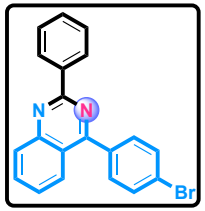
Compound 4g



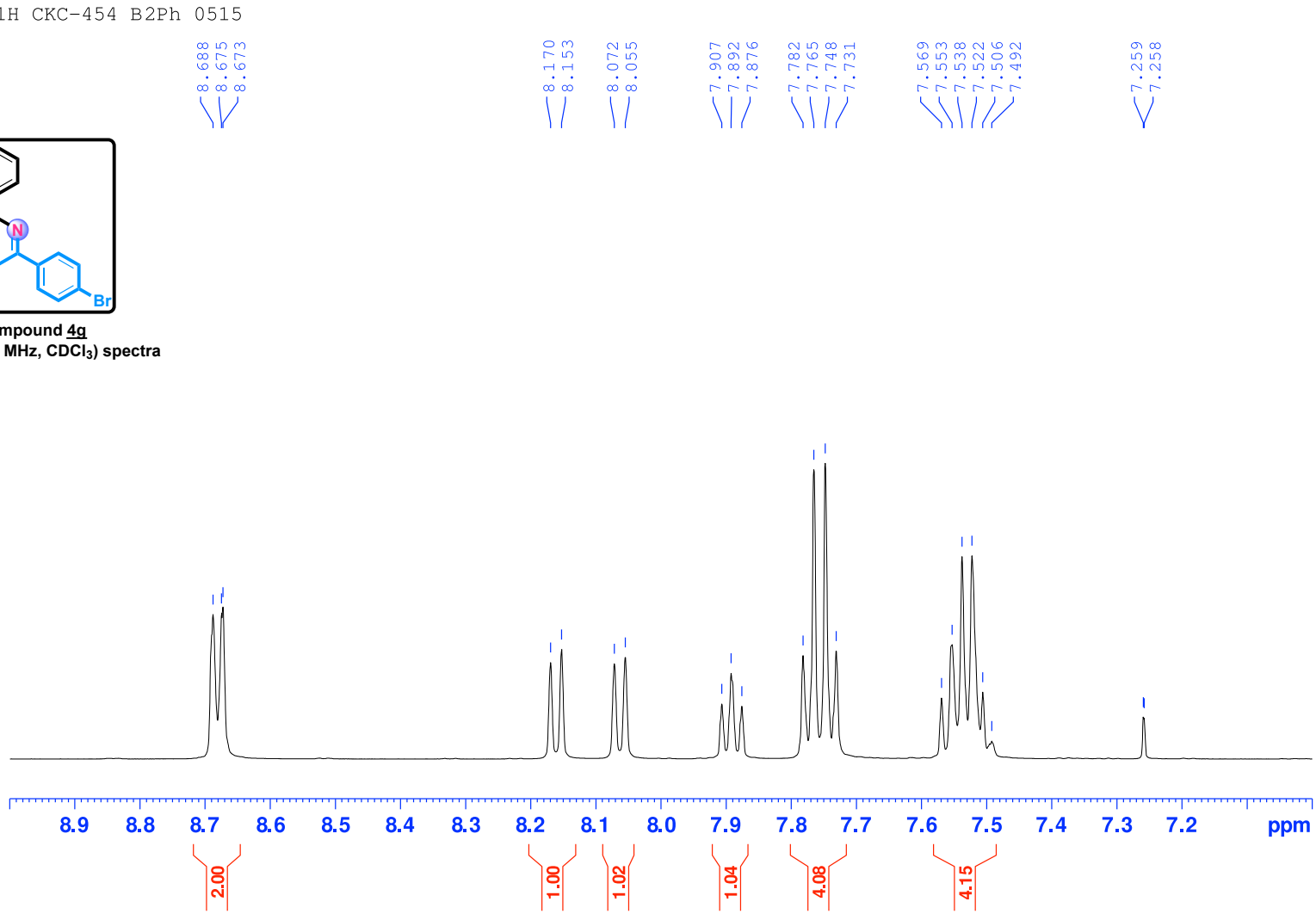
Compound 4g
^{1}H NMR (500 MHz, $CDCl_3$) spectra



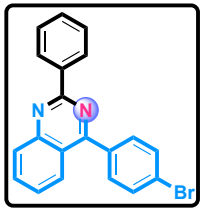
Compound 4g



Compound 4g
^{1}H NMR (500 MHz, $CDCl_3$) spectra

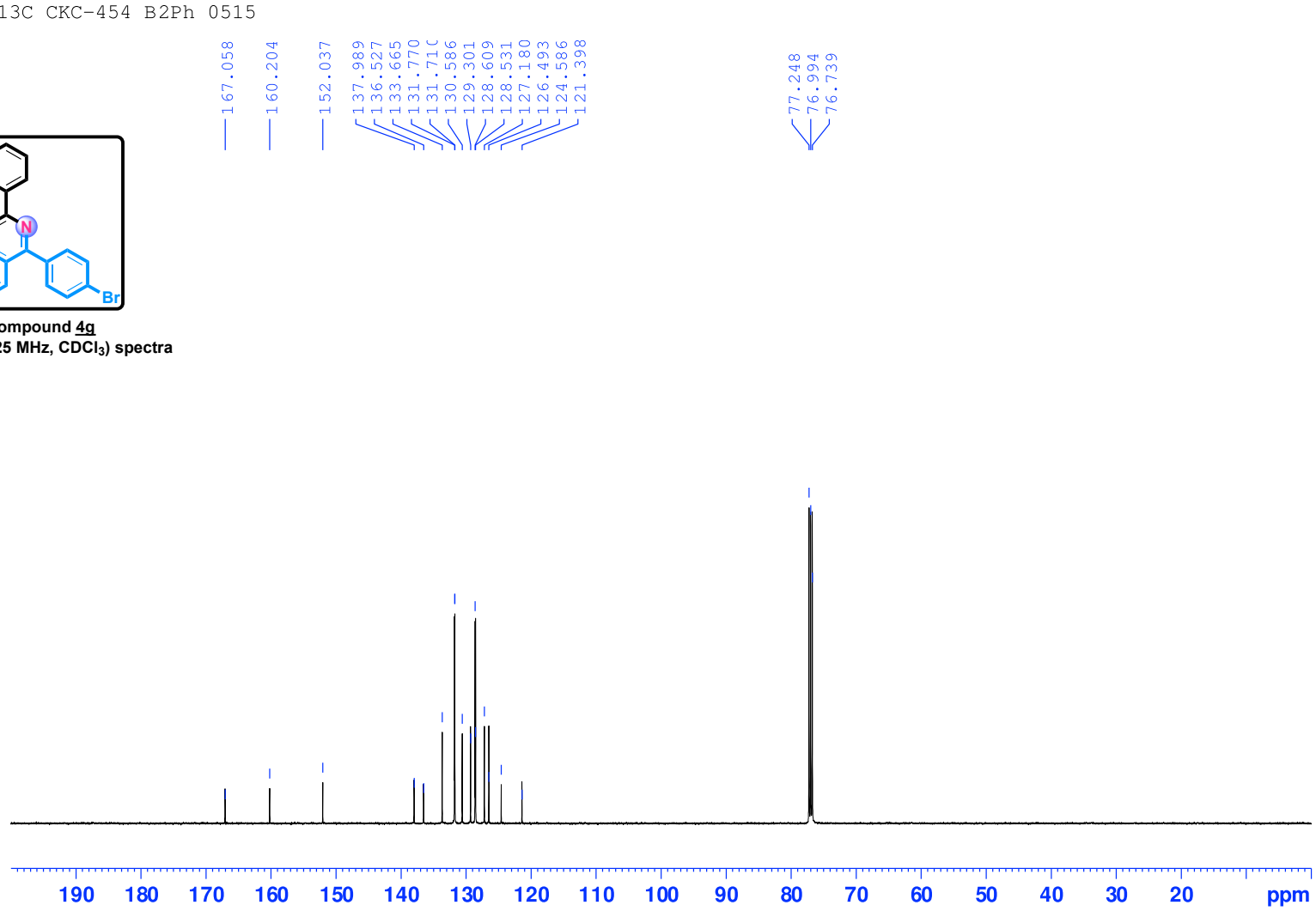


Compound 4g



Compound 4g

^{13}C NMR (125 MHz, $CDCl_3$) spectra



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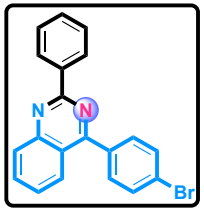
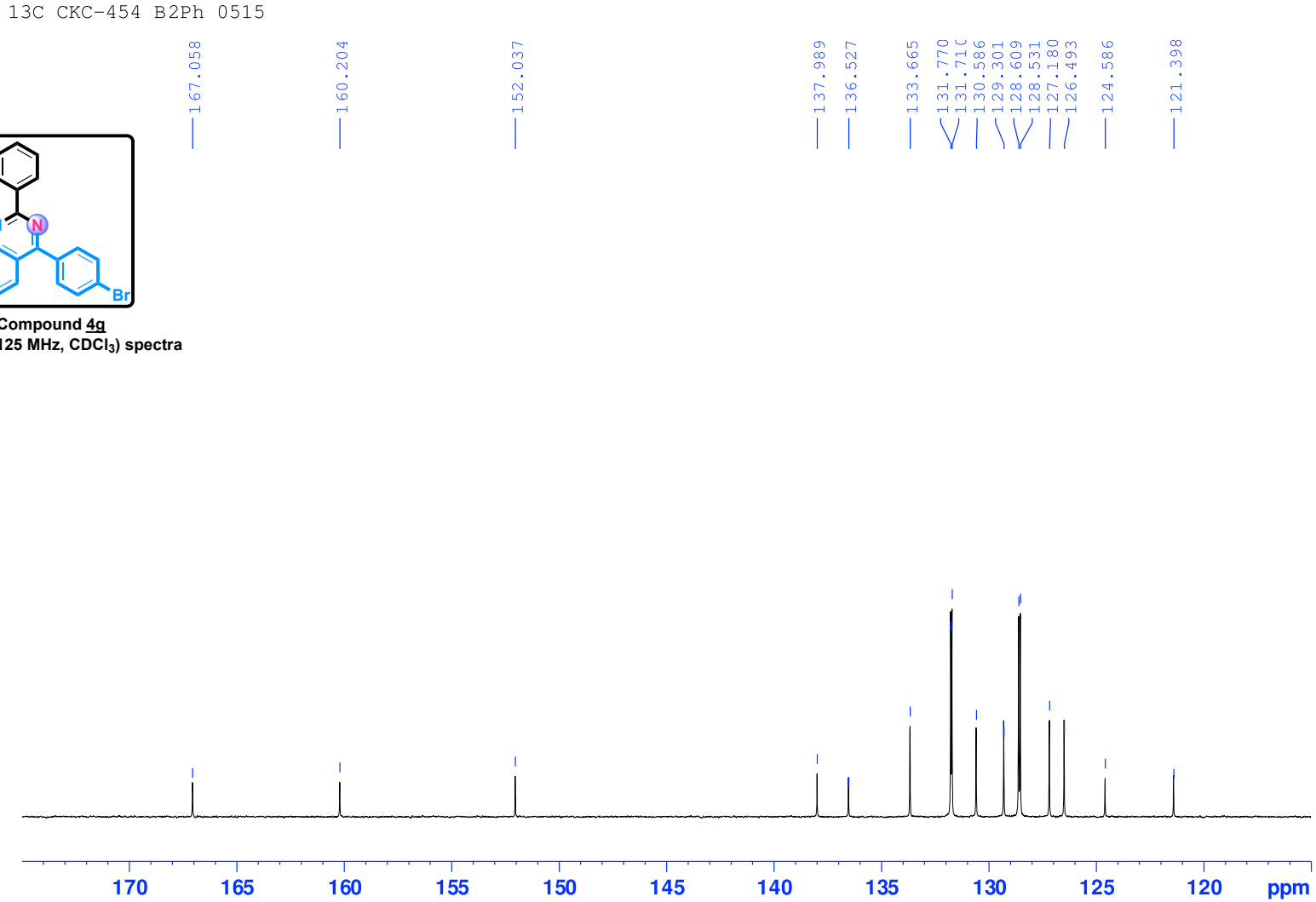
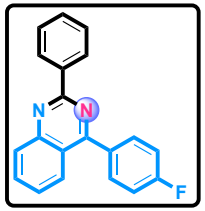


Compound 4g

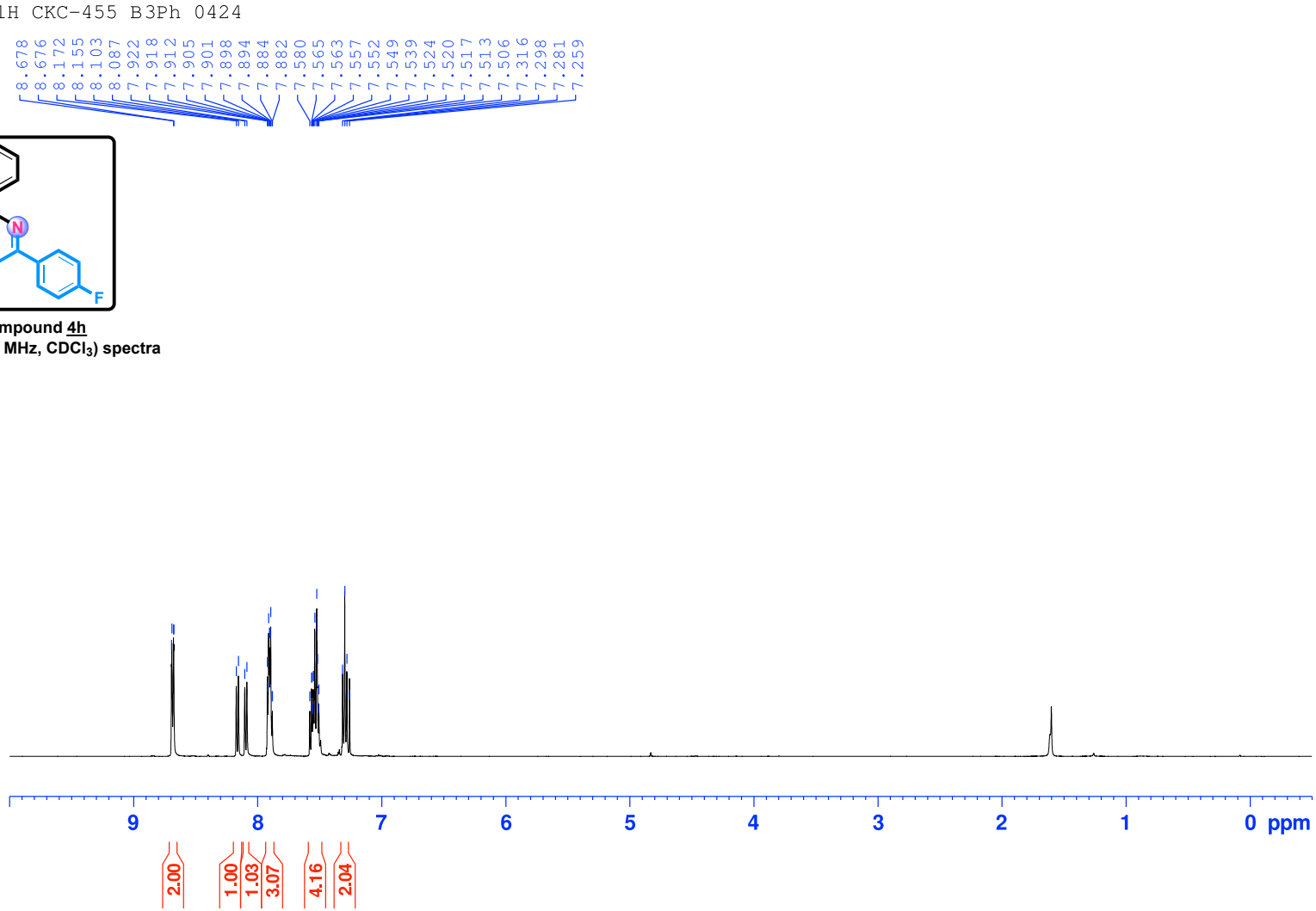
^{13}C NMR (125 MHz, $CDCl_3$) spectra



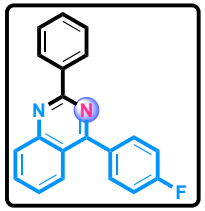
Compound 4h



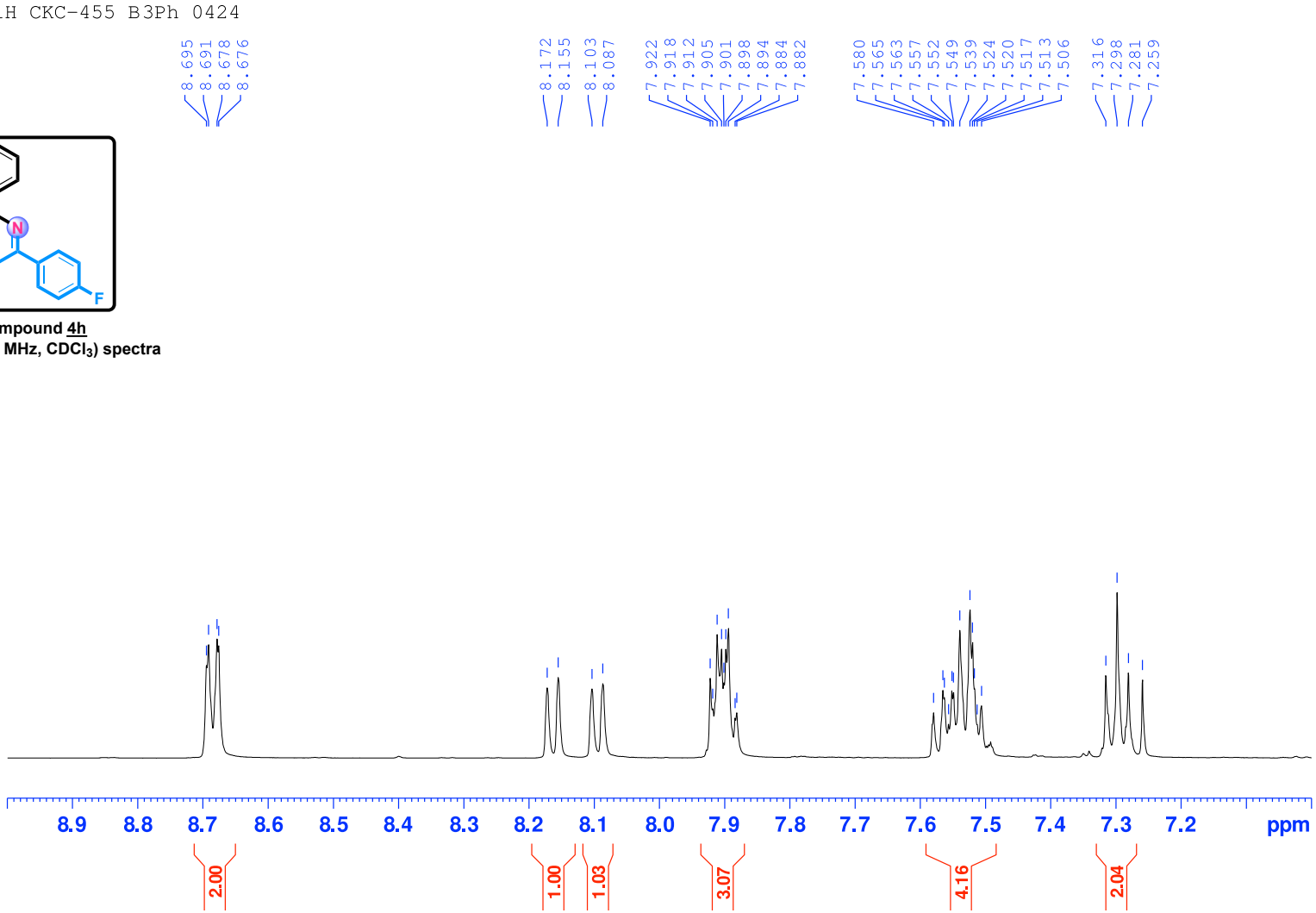
Compound 4h
^{1}H NMR (500 MHz, $CDCl_3$) spectra



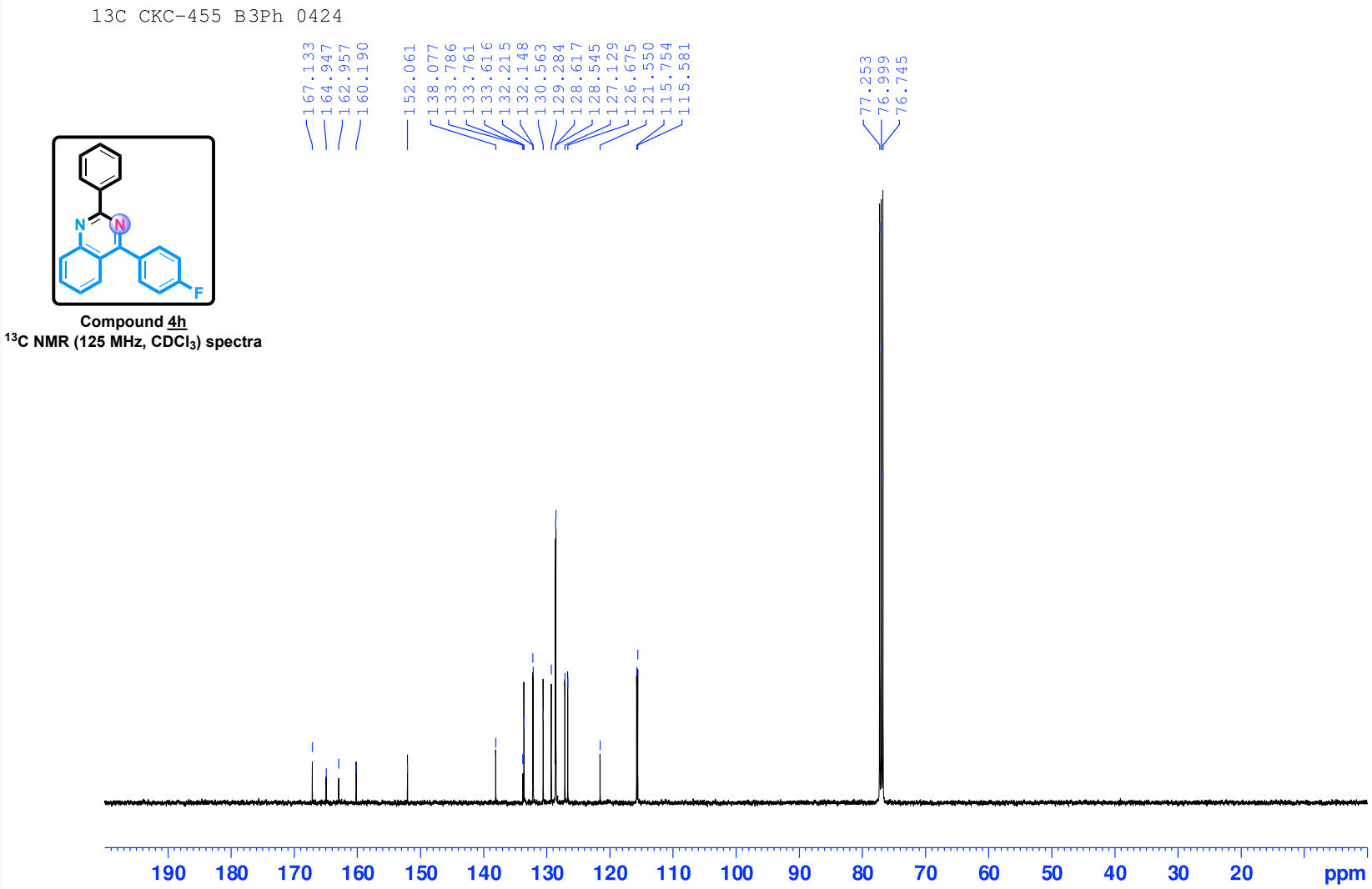
Compound 4h



Compound 4h
^{1}H NMR (500 MHz, $CDCl_3$) spectra

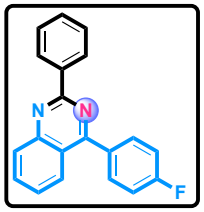


Compound 4h



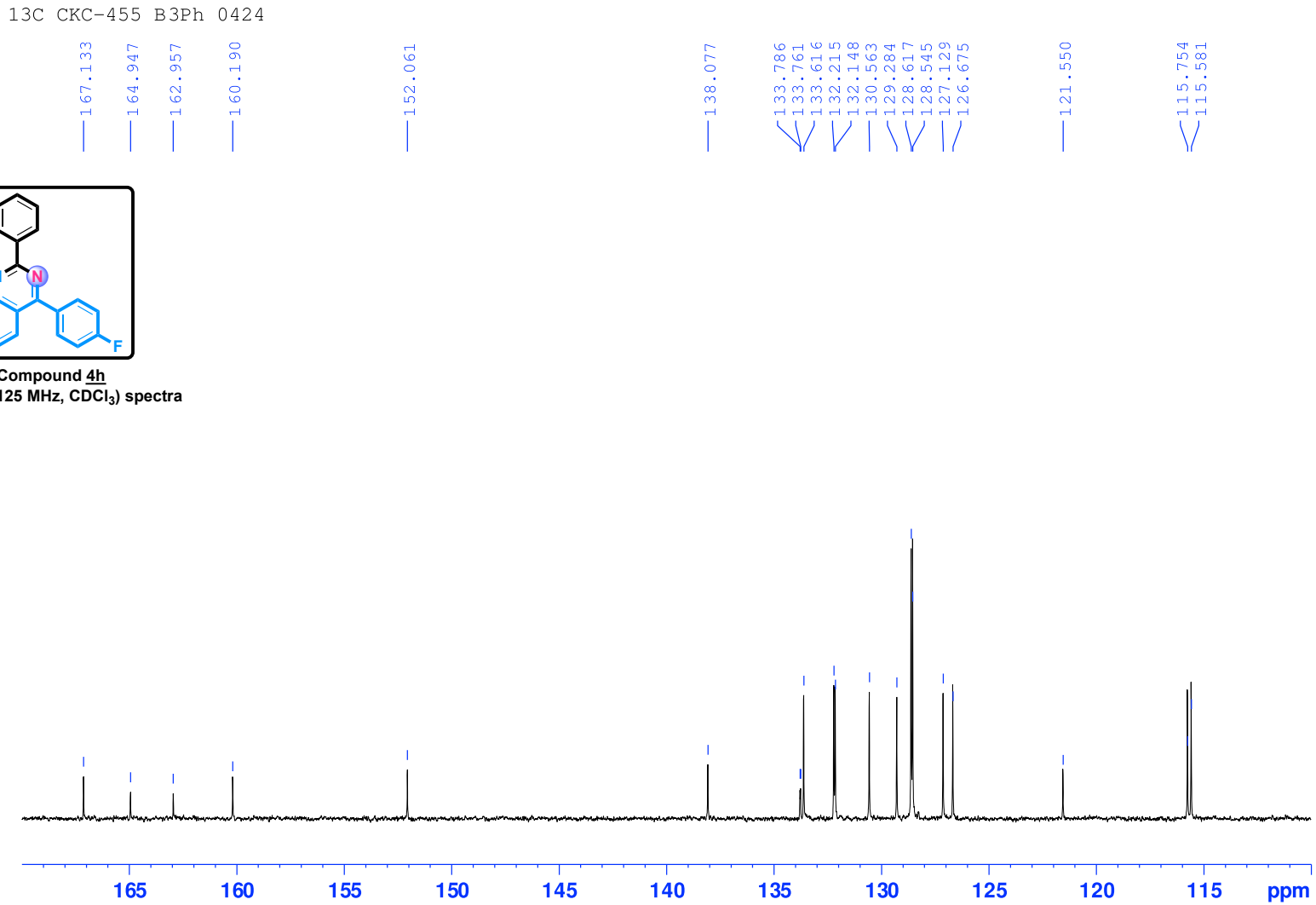
Compound 4h
^{13}C NMR (125 MHz, $CDCl_3$) spectra

Compound 4h

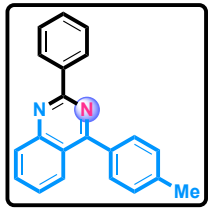


Compound 4h

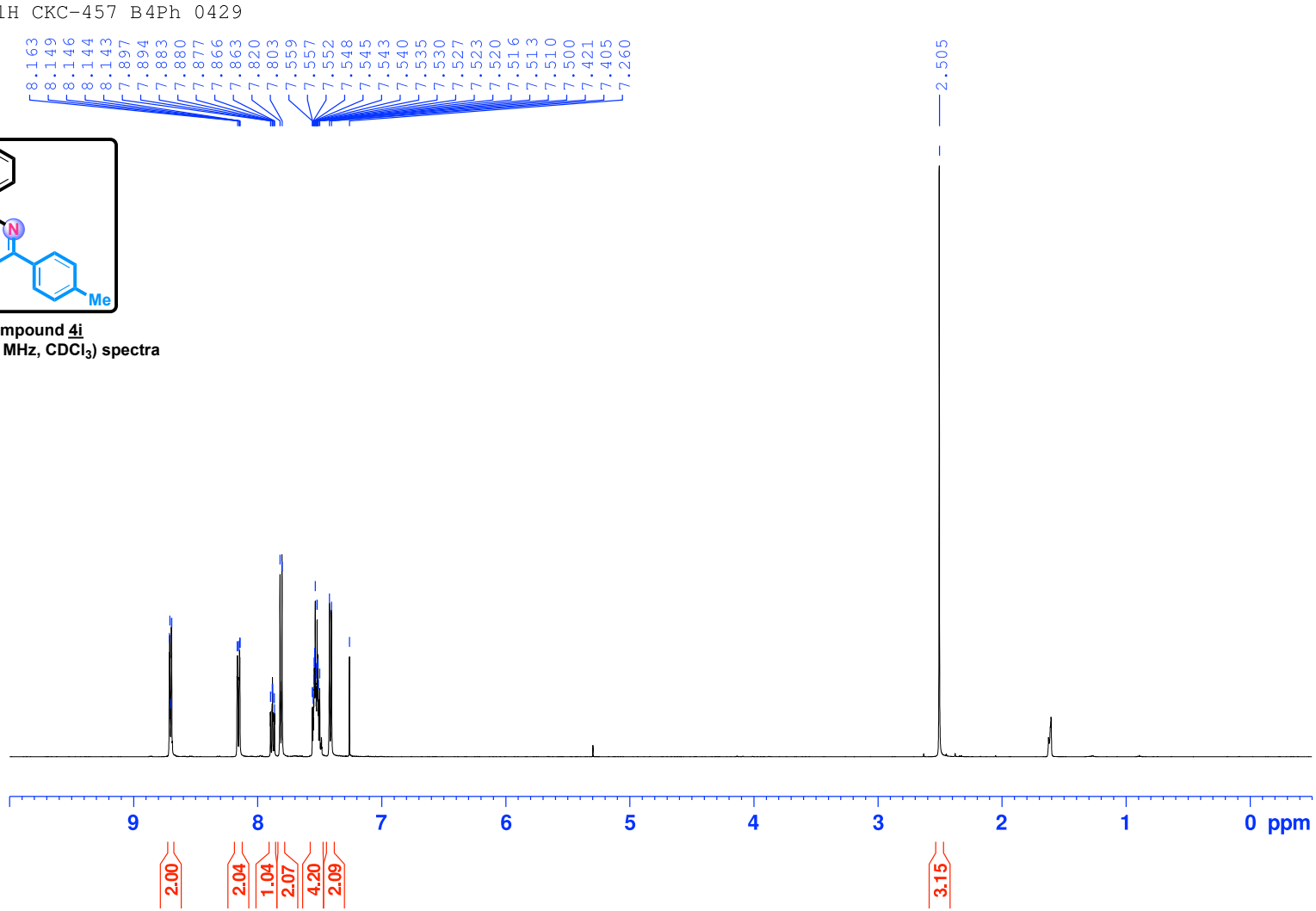
^{13}C NMR (125 MHz, $CDCl_3$) spectra



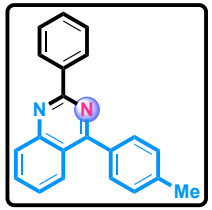
Compound 4i



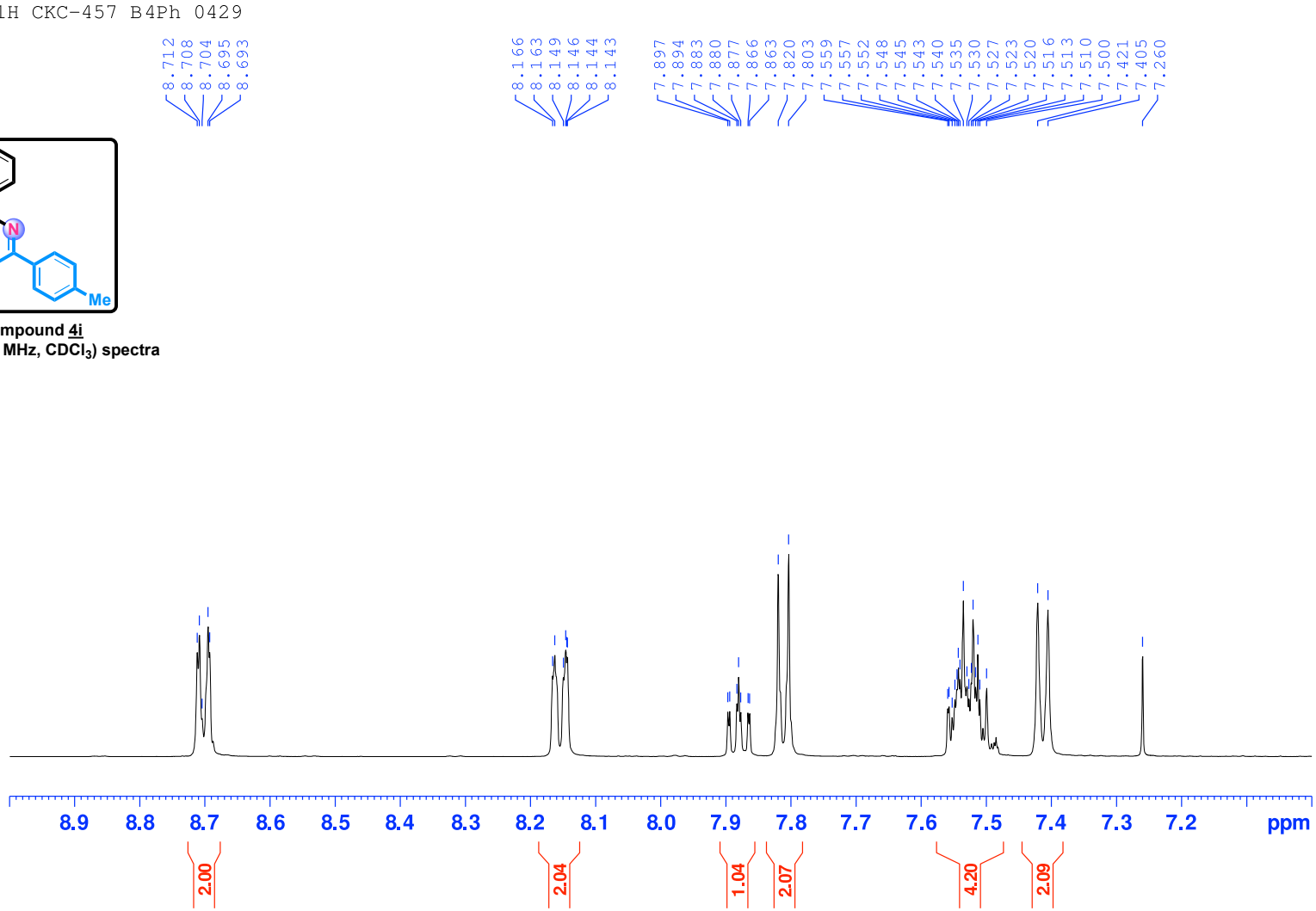
Compound 4i
^{1}H NMR (500 MHz, $CDCl_3$) spectra



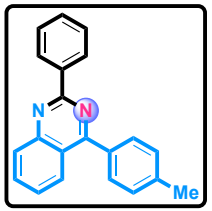
Compound 4i



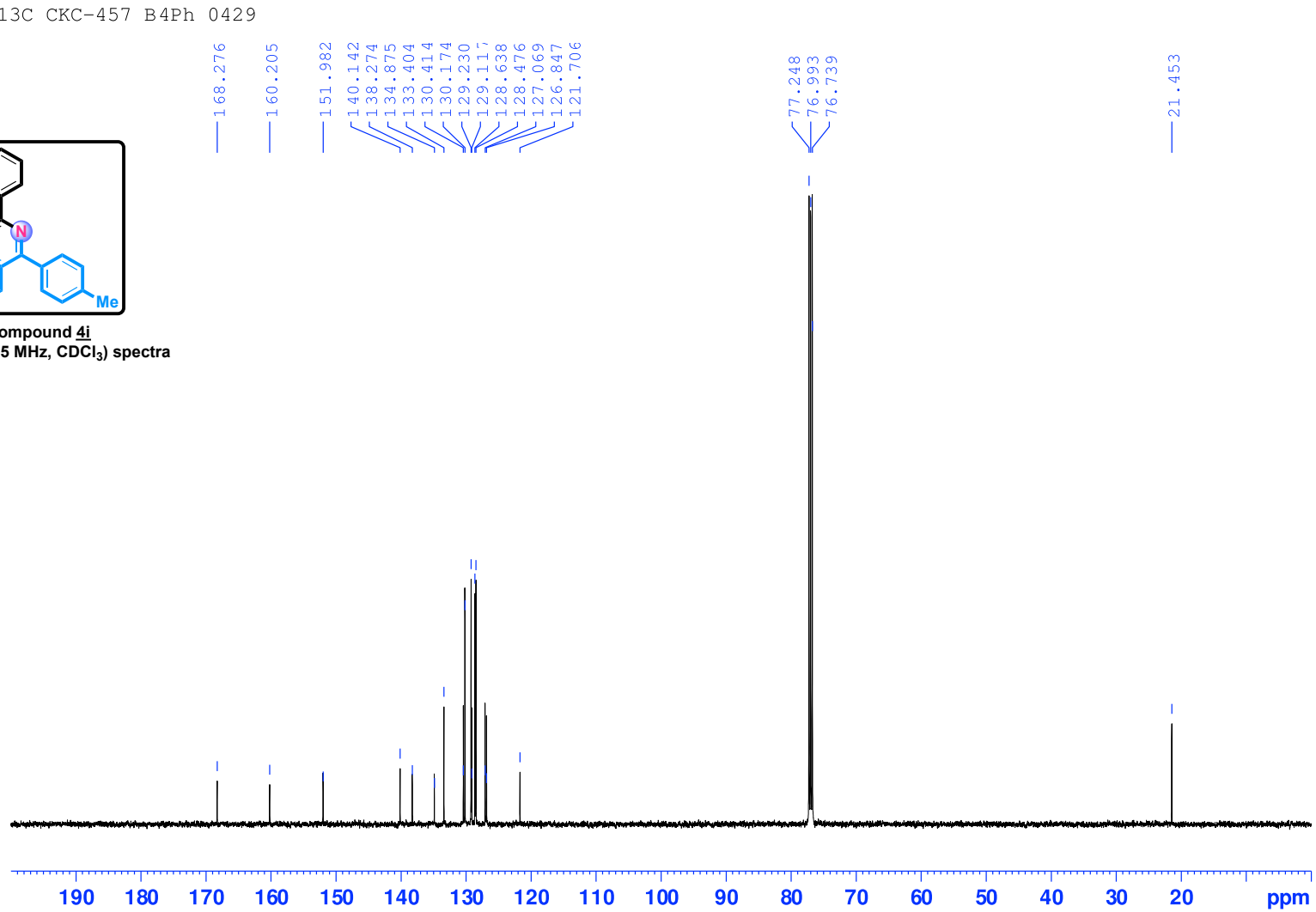
Compound 4i
^{1}H NMR (500 MHz, $CDCl_3$) spectra



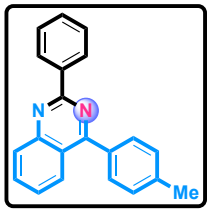
Compound 4i



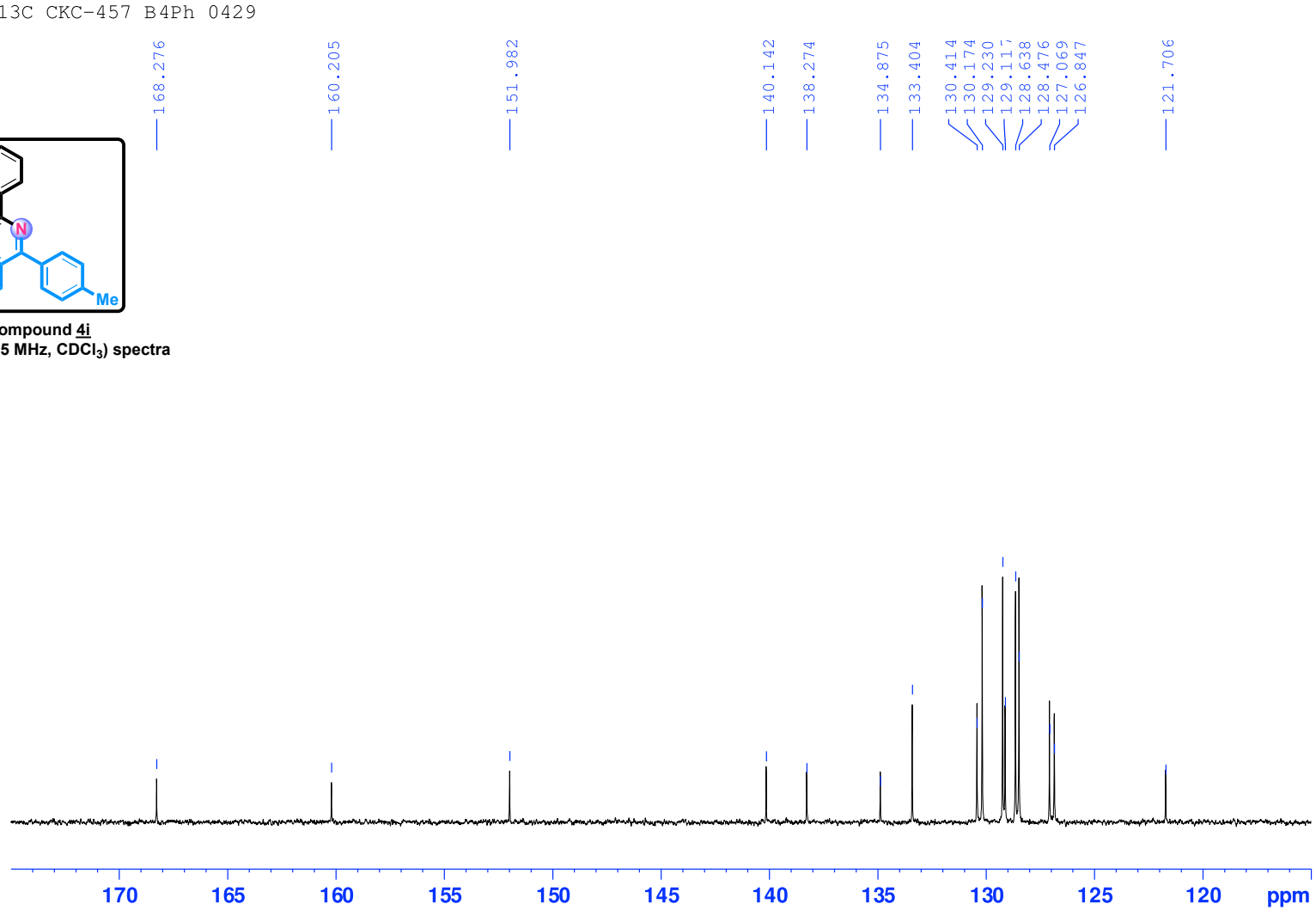
Compound 4i
^{13}C NMR (125 MHz, $CDCl_3$) spectra



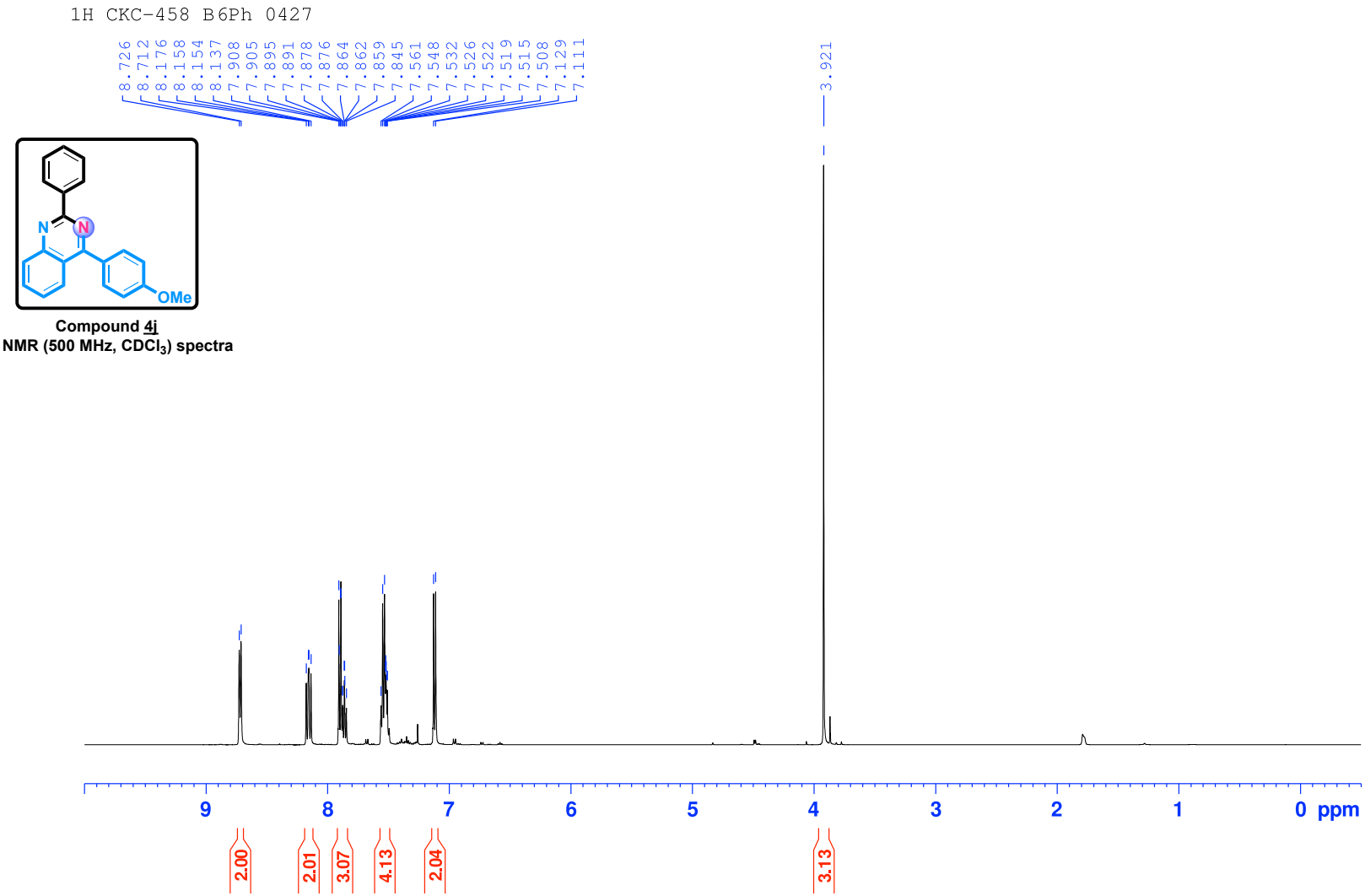
Compound 4i



Compound 4i
^{13}C NMR (125 MHz, $CDCl_3$) spectra

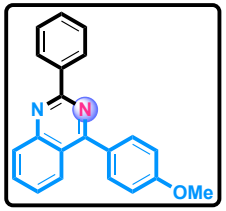


Compound 4j

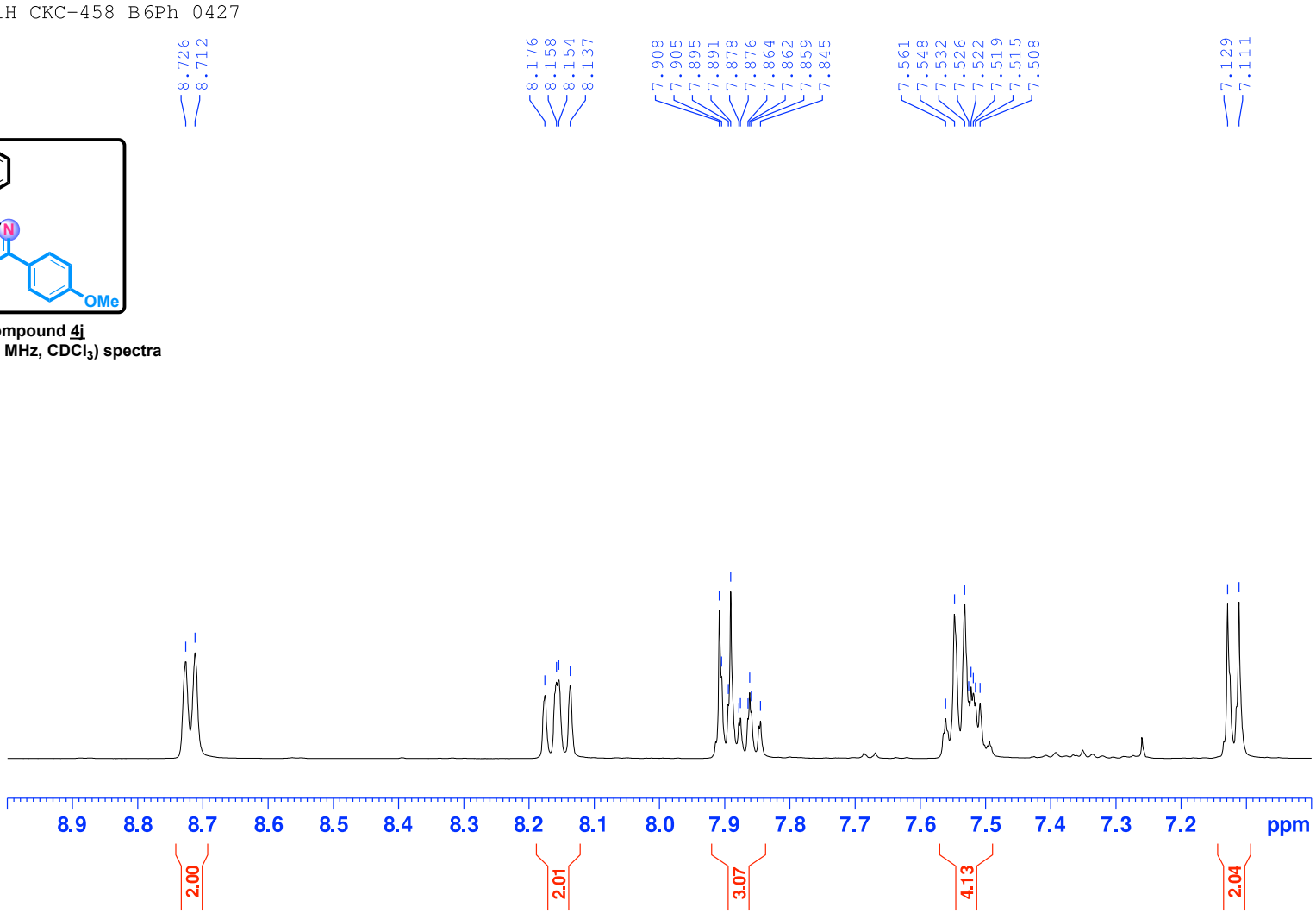


Compound 4j
^{1}H NMR (500 MHz, $CDCl_3$) spectra

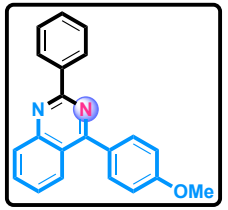
Compound 4j



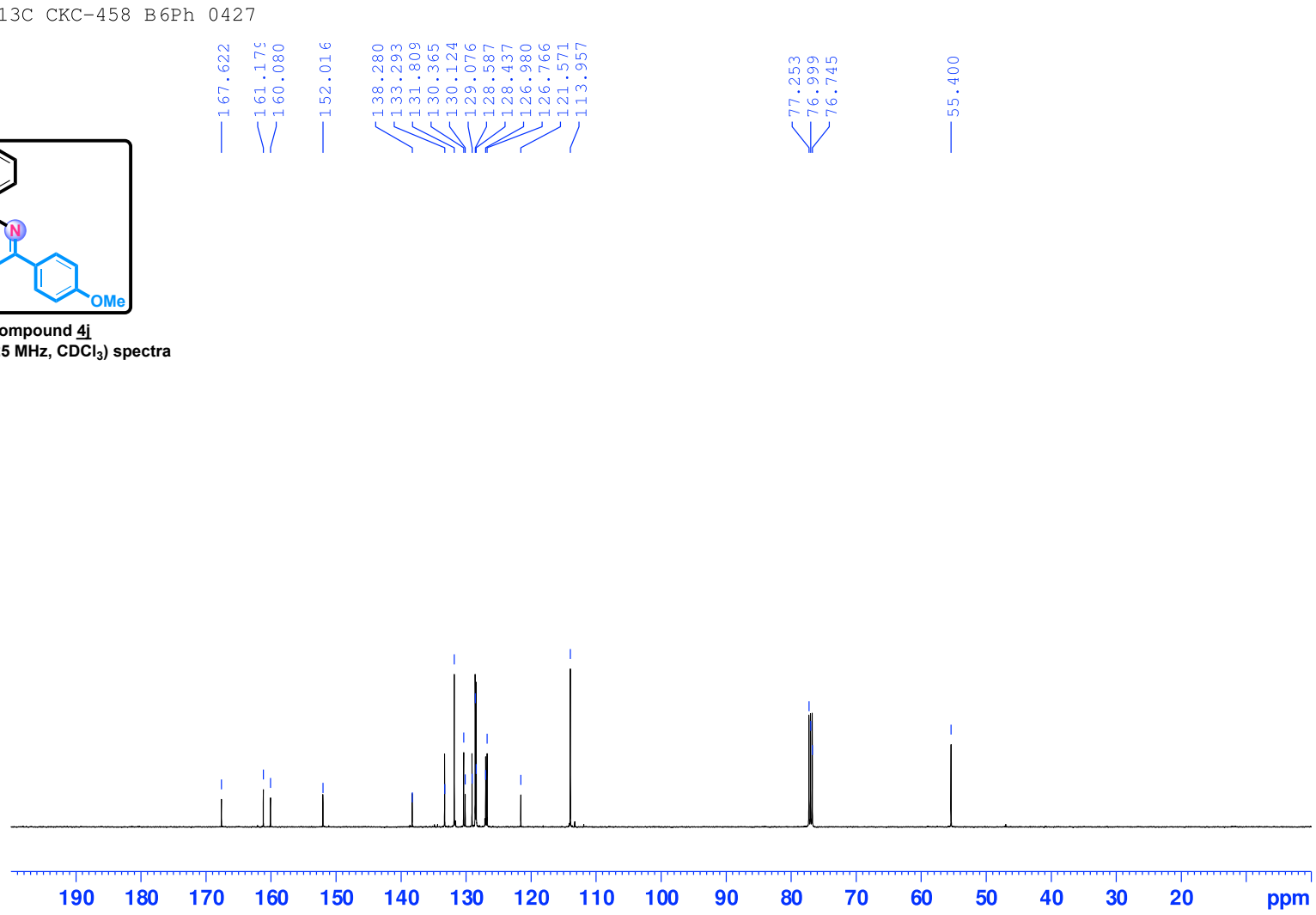
Compound 4j
^{1}H NMR (500 MHz, $CDCl_3$) spectra



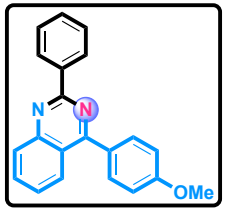
Compound 4j



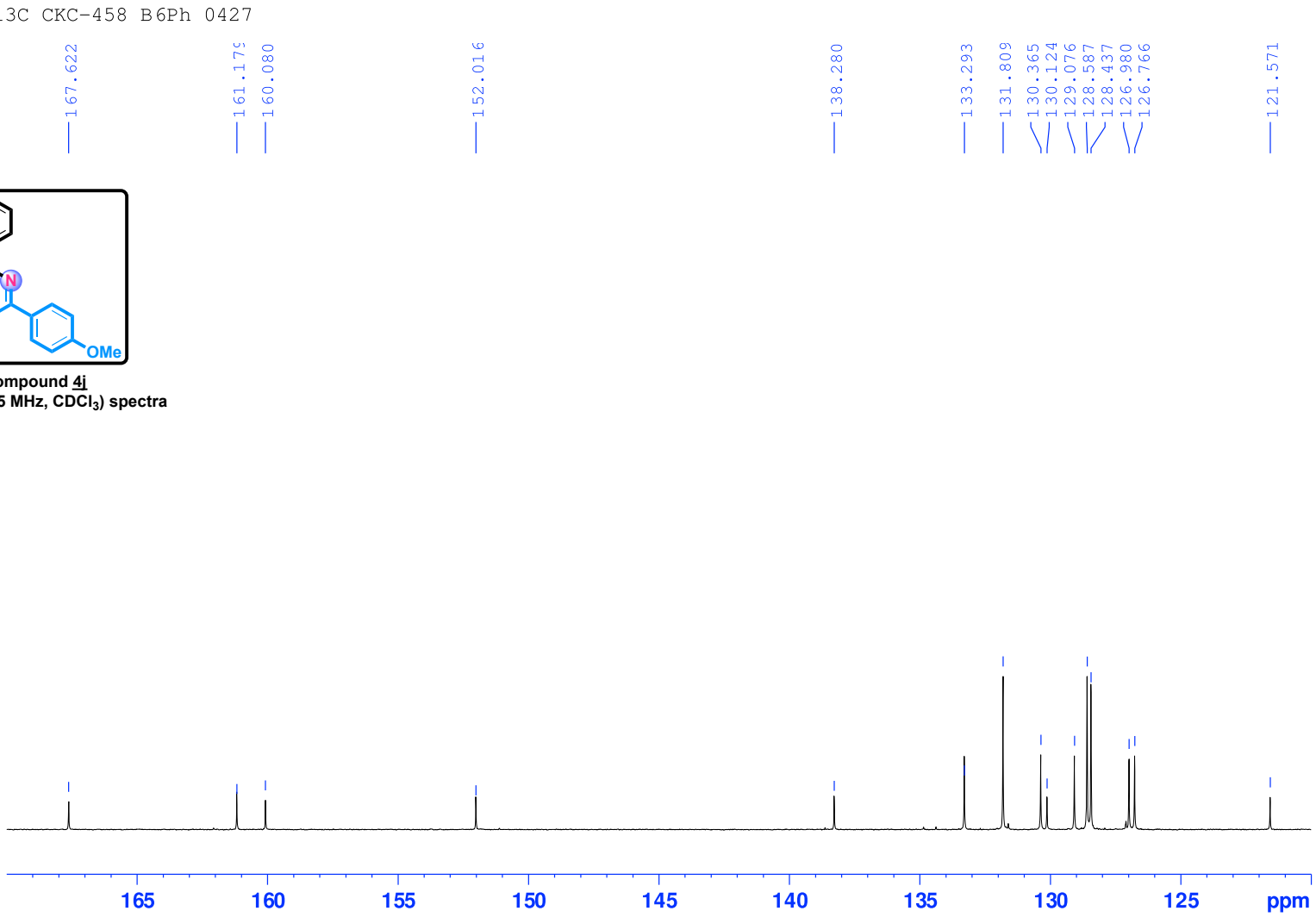
Compound 4j
^{13}C NMR (125 MHz, $CDCl_3$) spectra



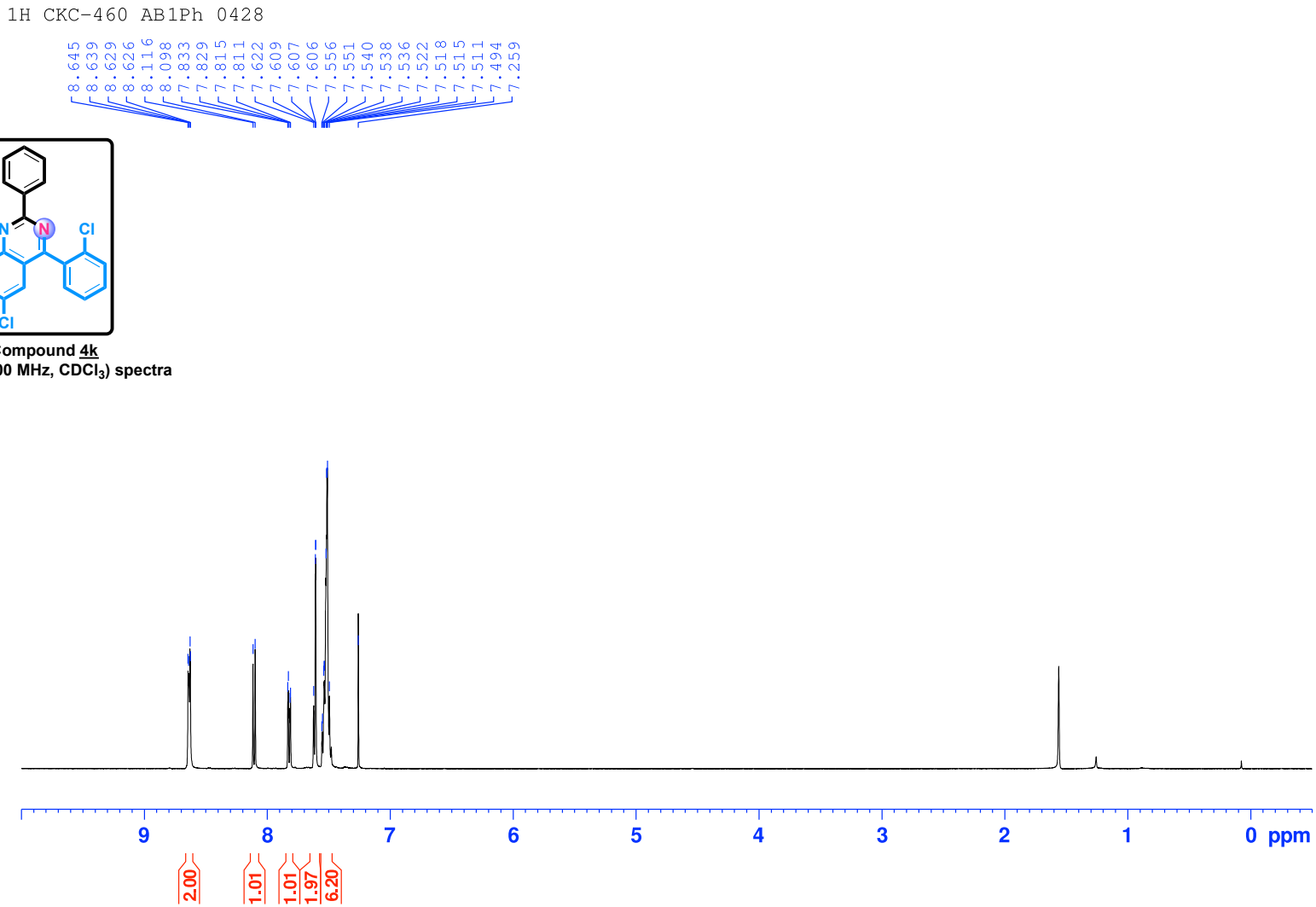
Compound 4j



Compound 4j
^{13}C NMR (125 MHz, $CDCl_3$) spectra

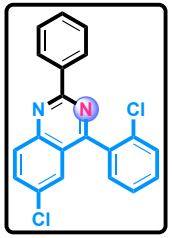


Compound 4k

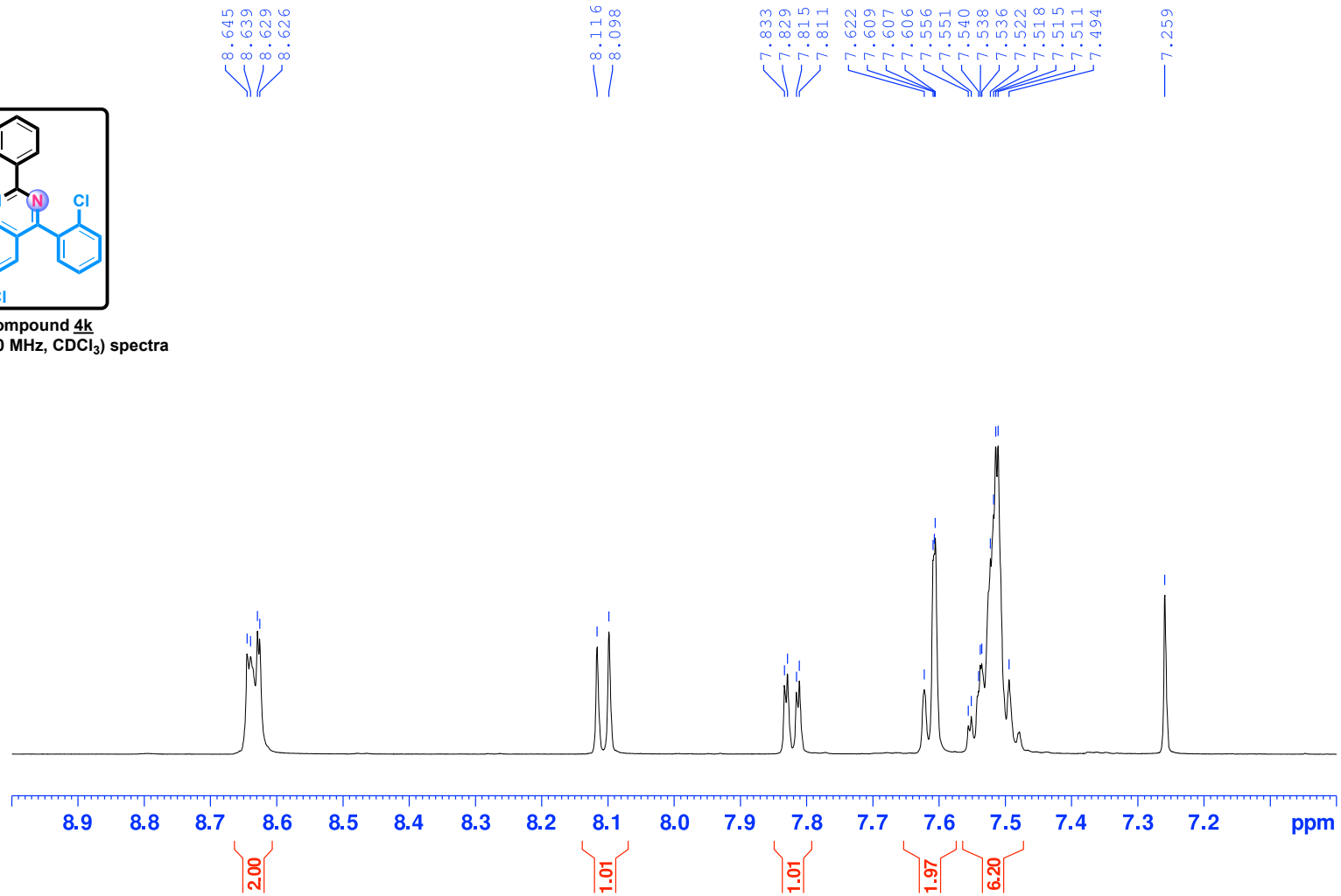


Compound 4k
^{1}H NMR (500 MHz, $CDCl_3$) spectra

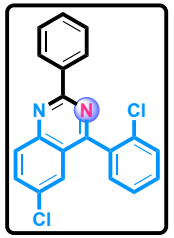
Compound 4k



Compound 4k
^{1}H NMR (500 MHz, $CDCl_3$) spectra

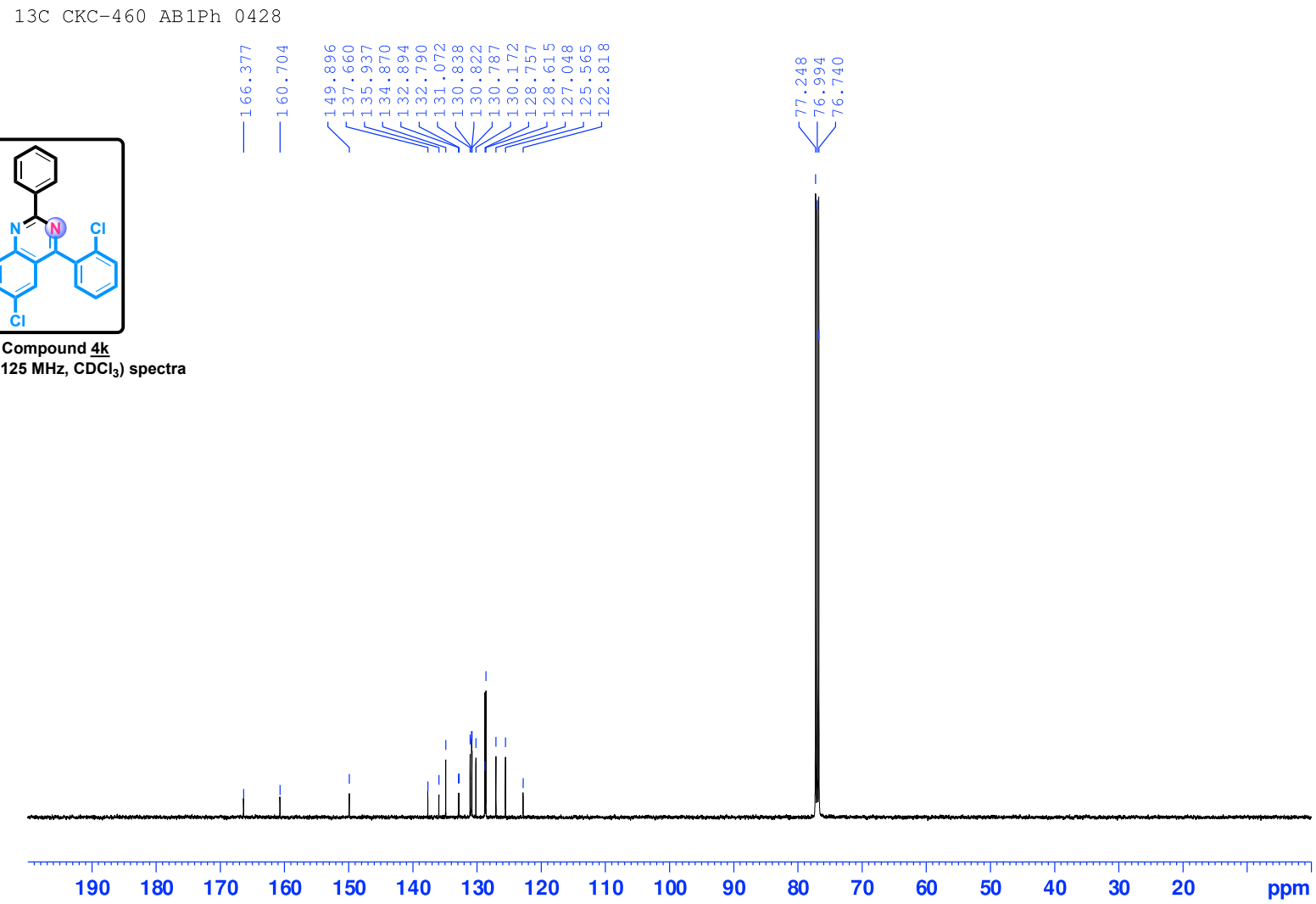


Compound 4k

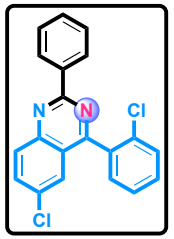


Compound 4k

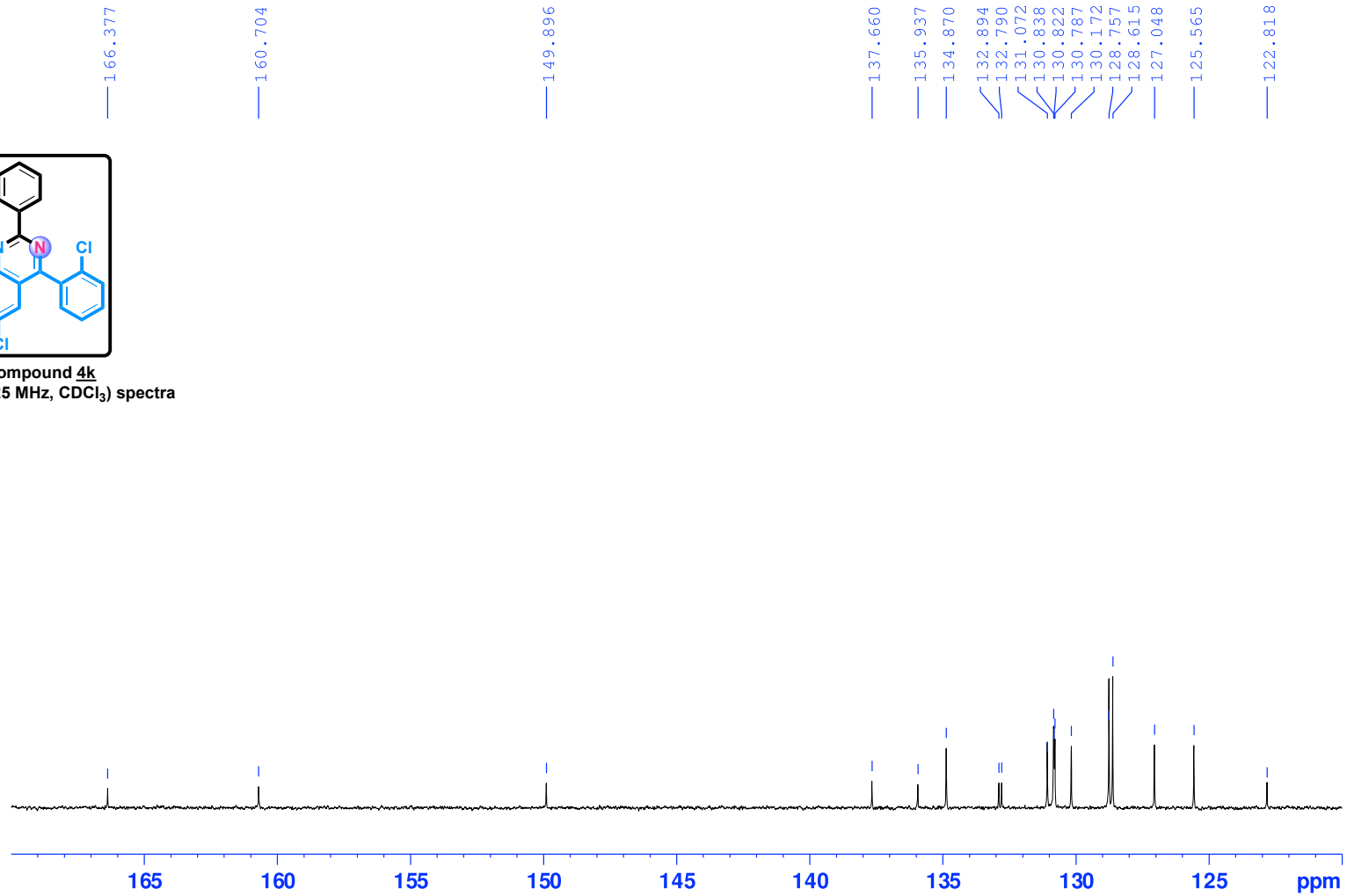
^{13}C NMR (125 MHz, $CDCl_3$) spectra



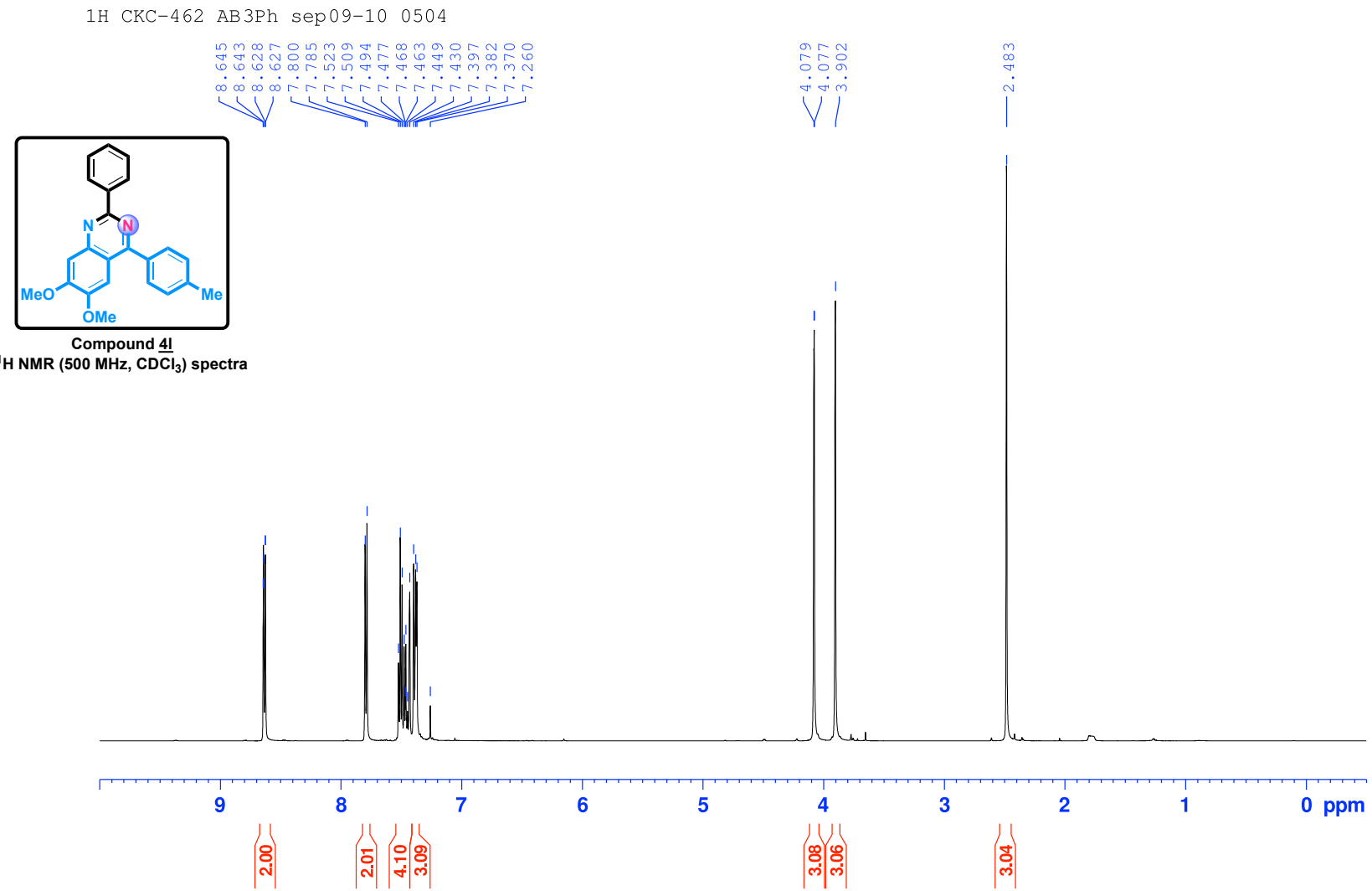
Compound 4k



Compound 4k
^{13}C NMR (125 MHz, $CDCl_3$) spectra

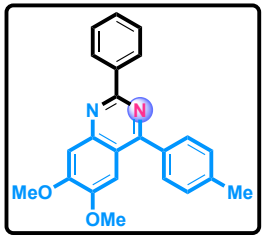


Compound 4l

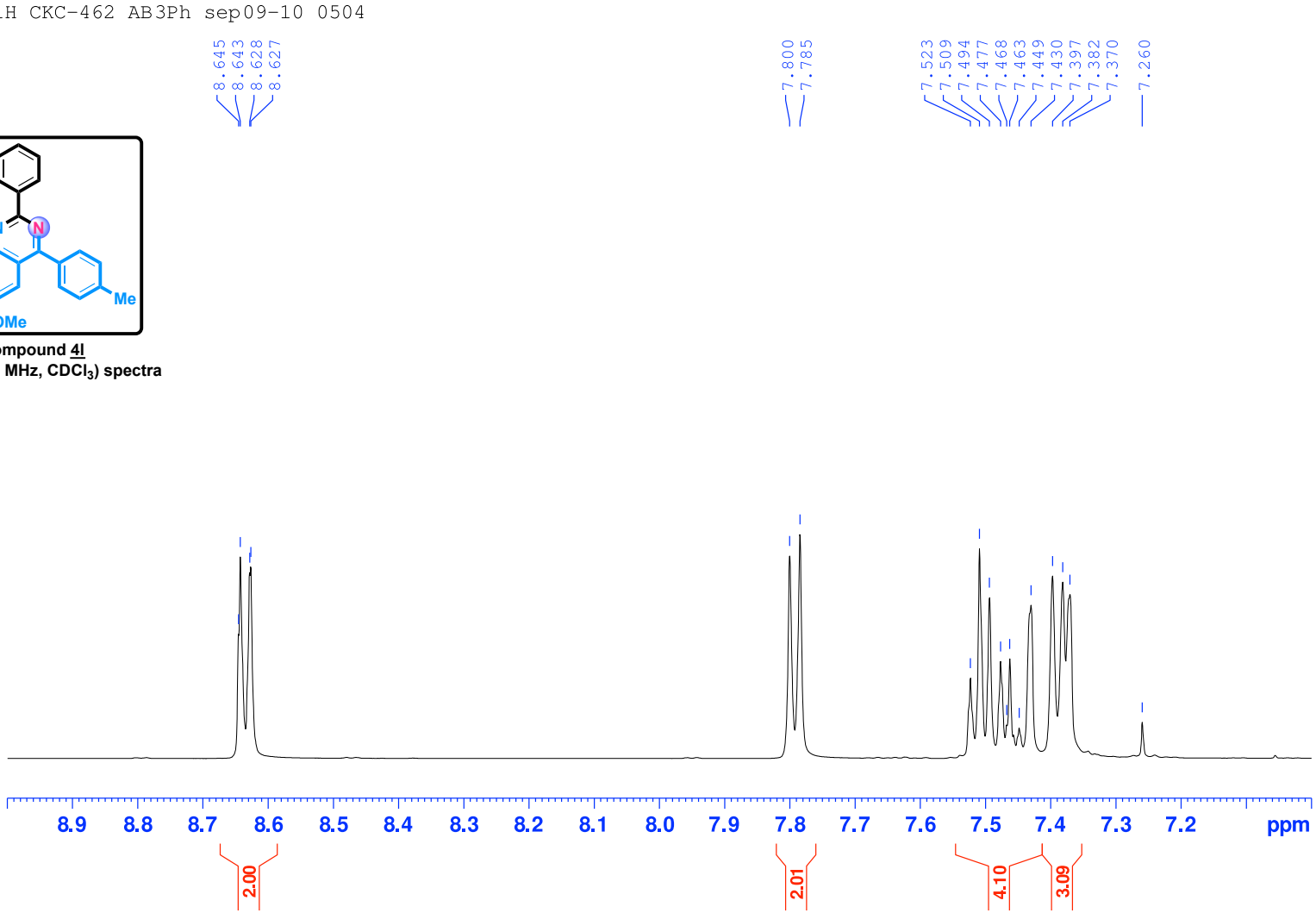


Compound 4l
^{1}H NMR (500 MHz, $CDCl_3$) spectra

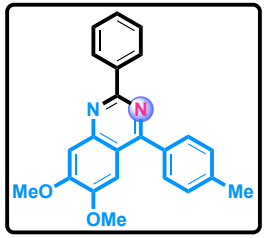
Compound 4l



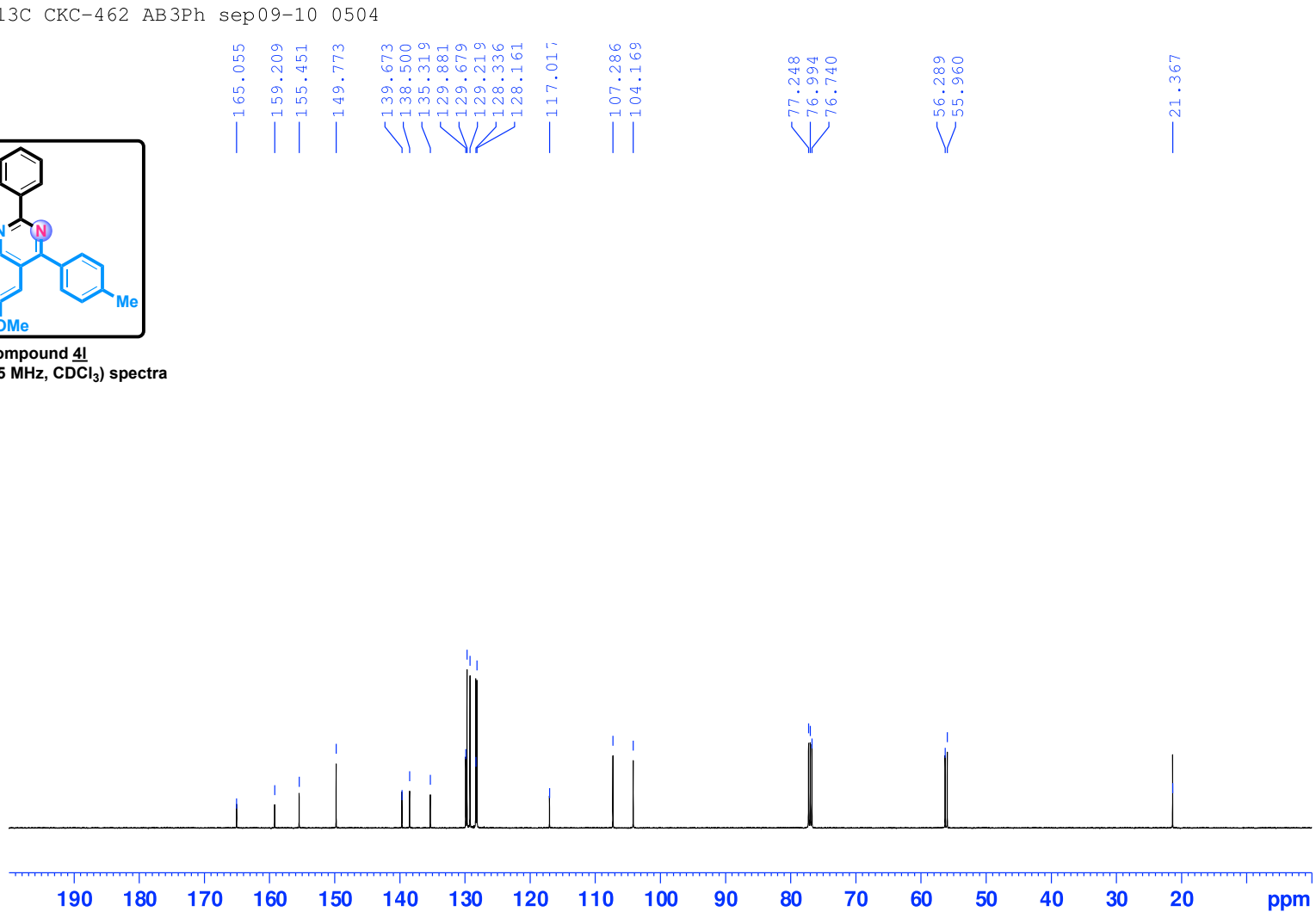
Compound 4l
^{1}H NMR (500 MHz, $CDCl_3$) spectra



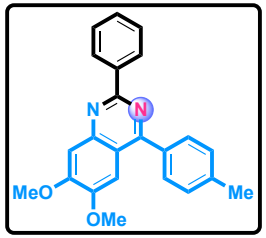
Compound 4l



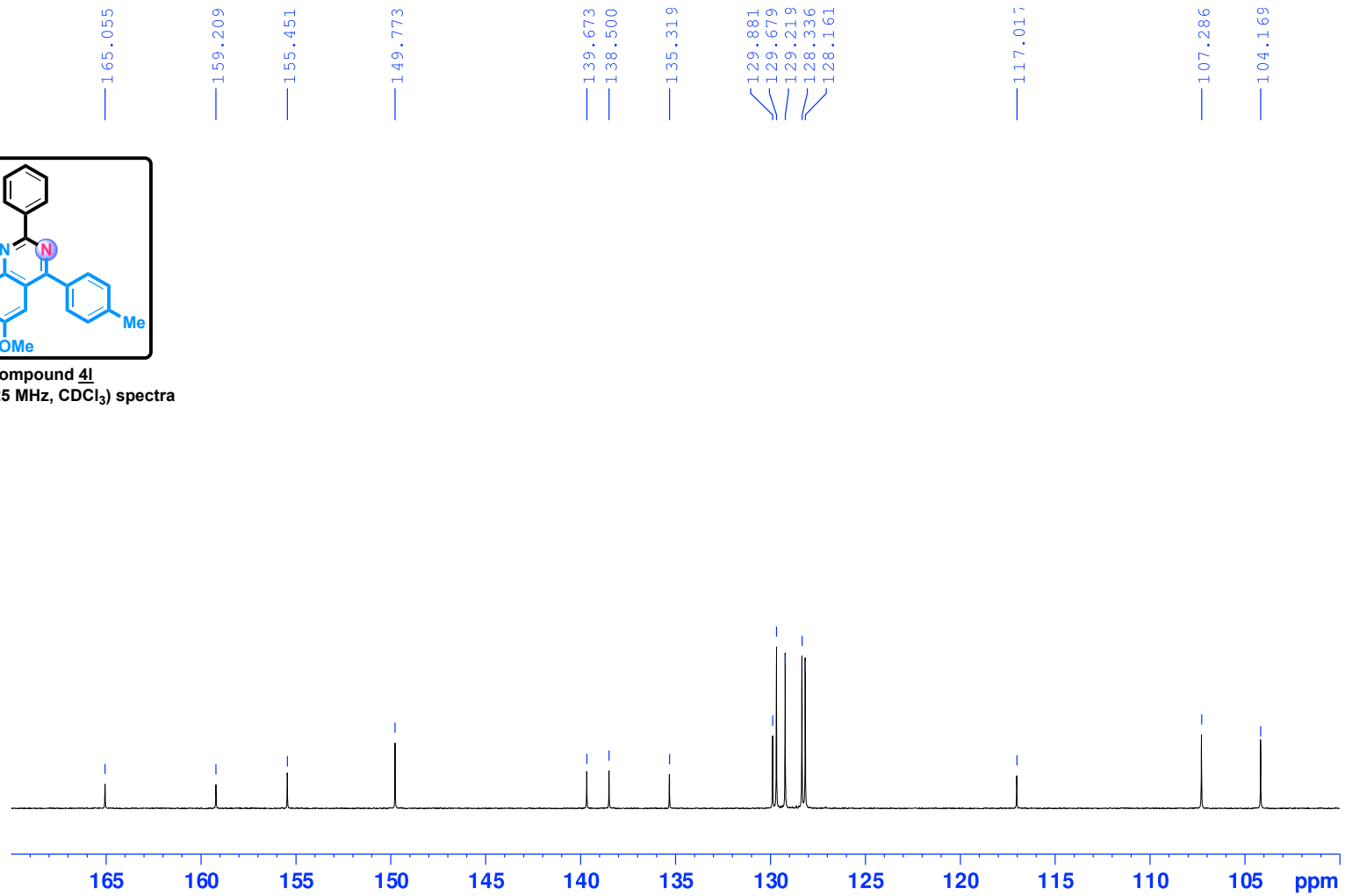
Compound 4l
^{13}C NMR (125 MHz, $CDCl_3$) spectra



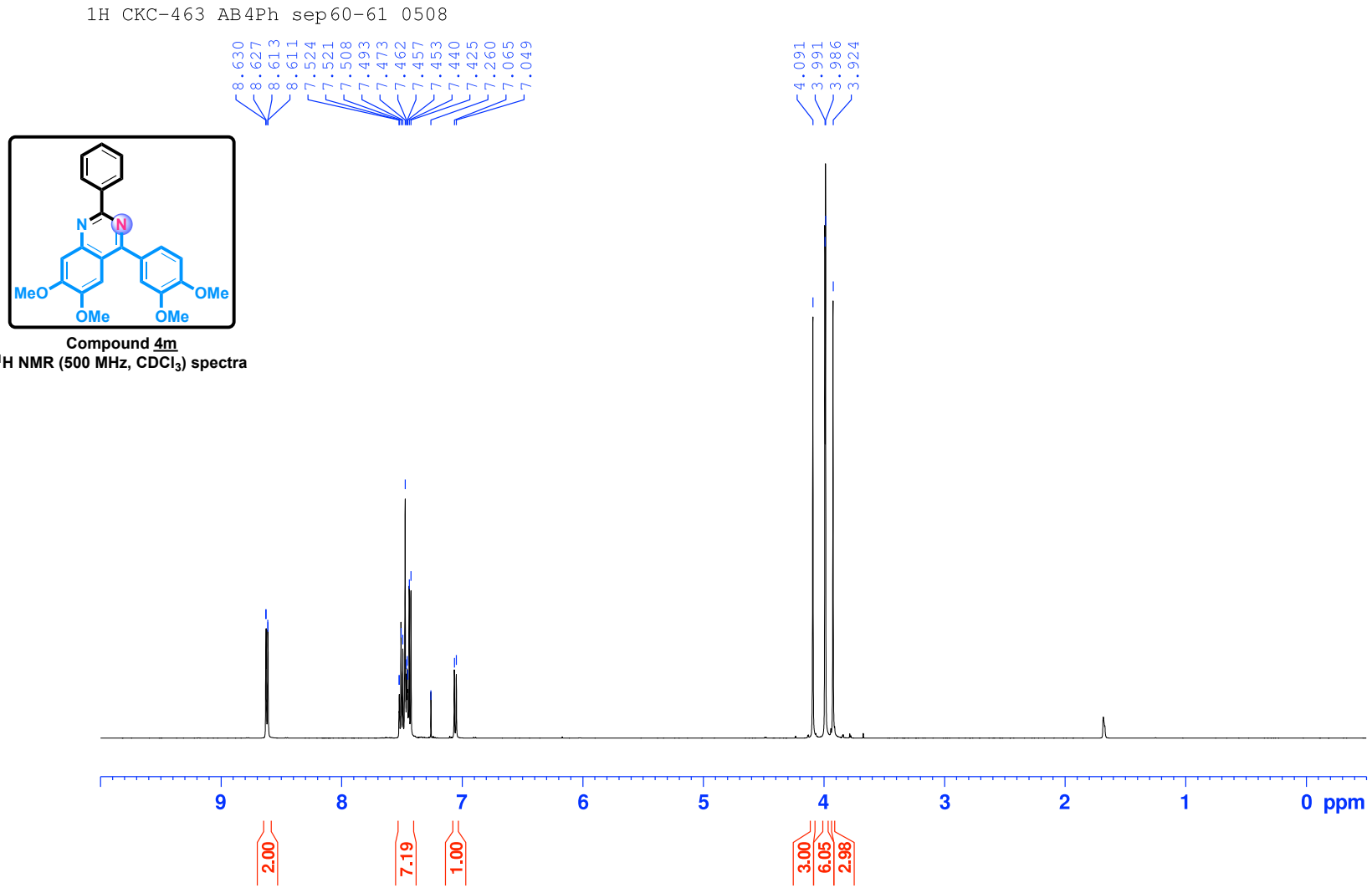
Compound 4l



Compound 4l
^{13}C NMR (125 MHz, $CDCl_3$) spectra

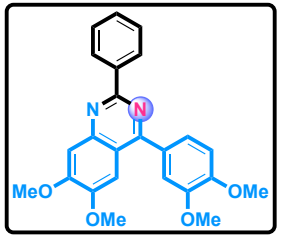


Compound 4m

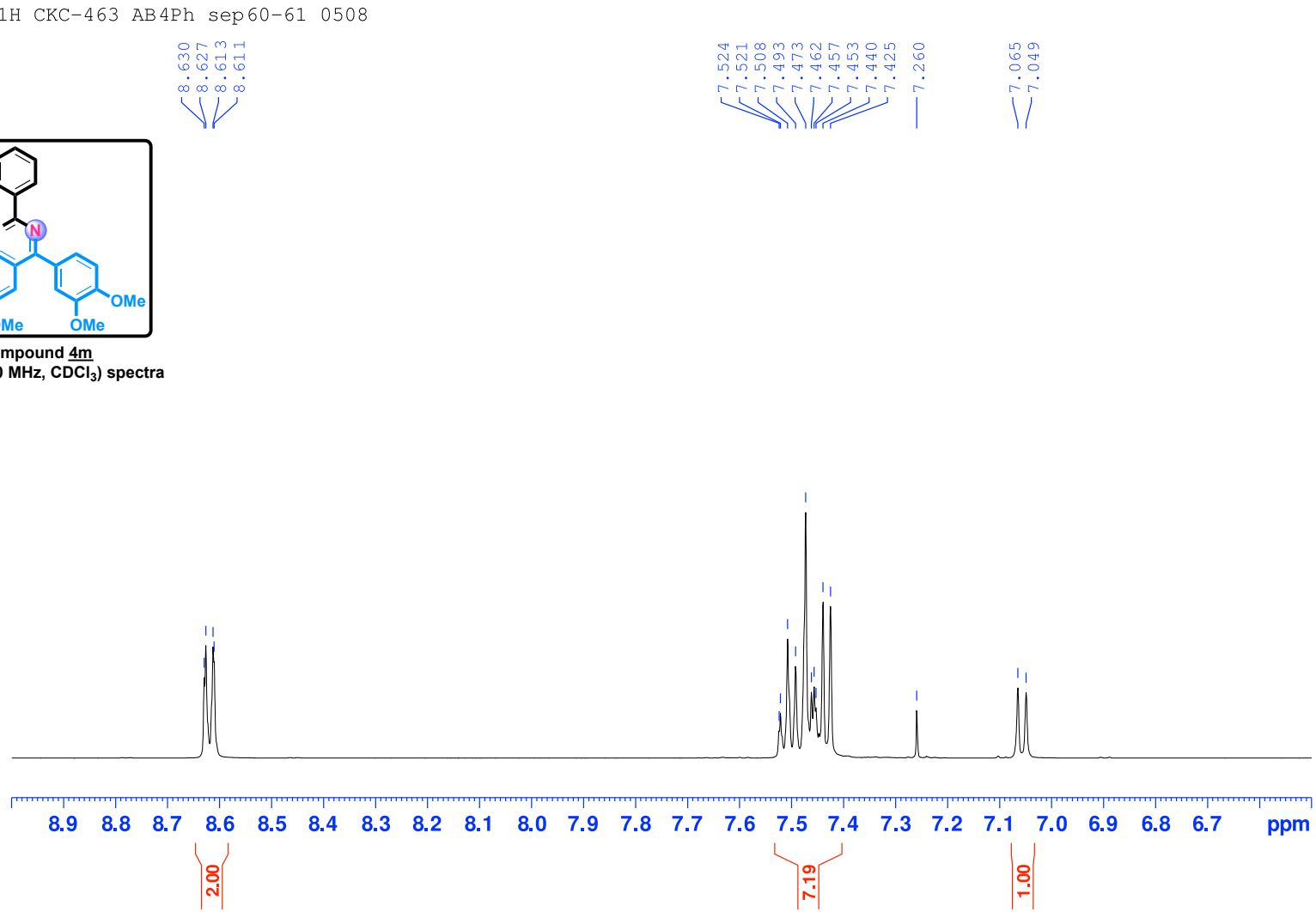


Compound 4m
^{1}H NMR (500 MHz, $CDCl_3$) spectra

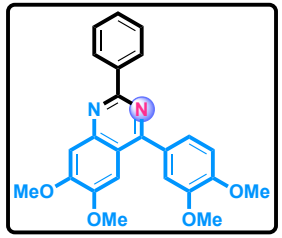
Compound 4m



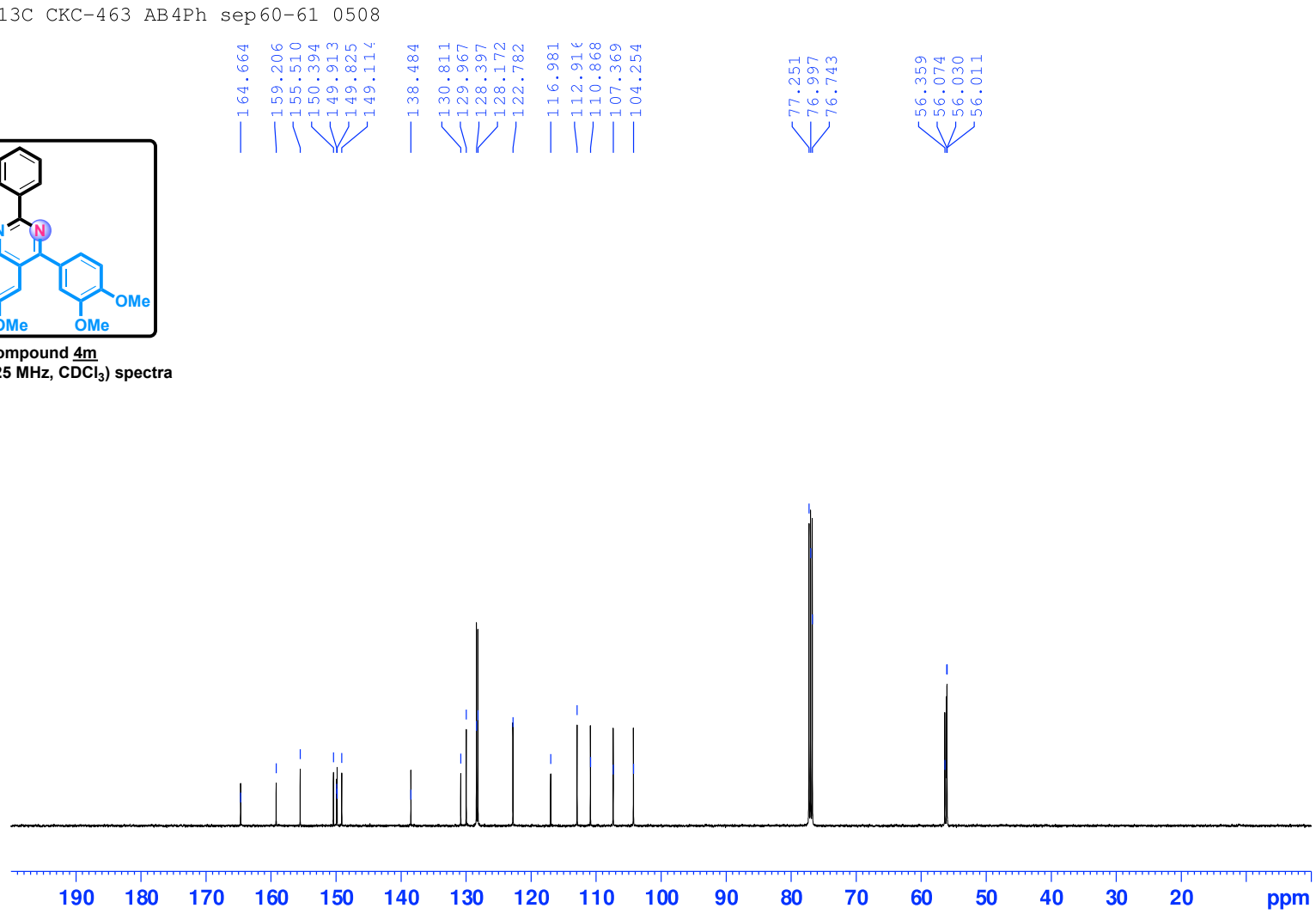
Compound 4m
^{1}H NMR (500 MHz, $CDCl_3$) spectra



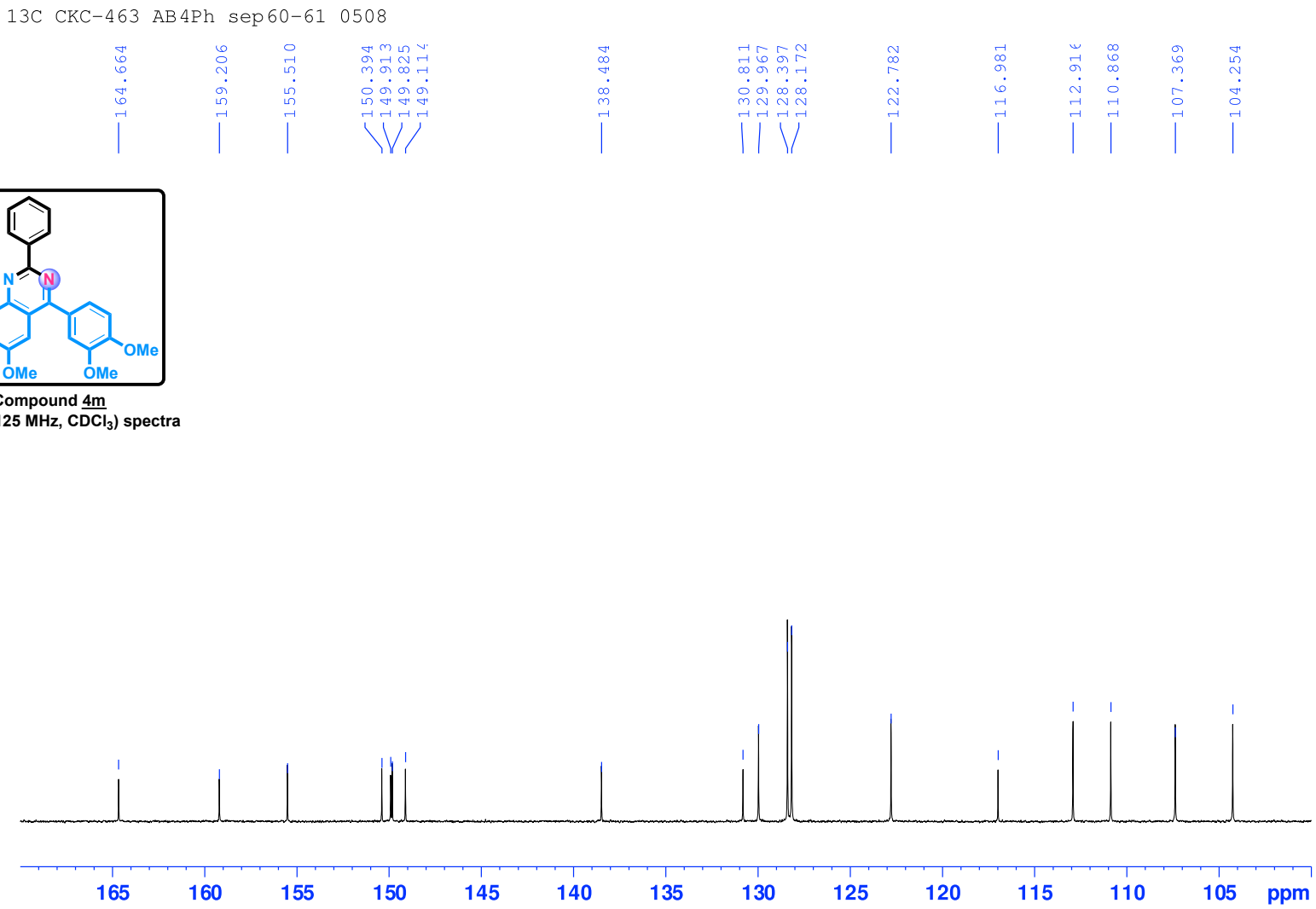
Compound 4m



Compound 4m
^{13}C NMR (125 MHz, $CDCl_3$) spectra

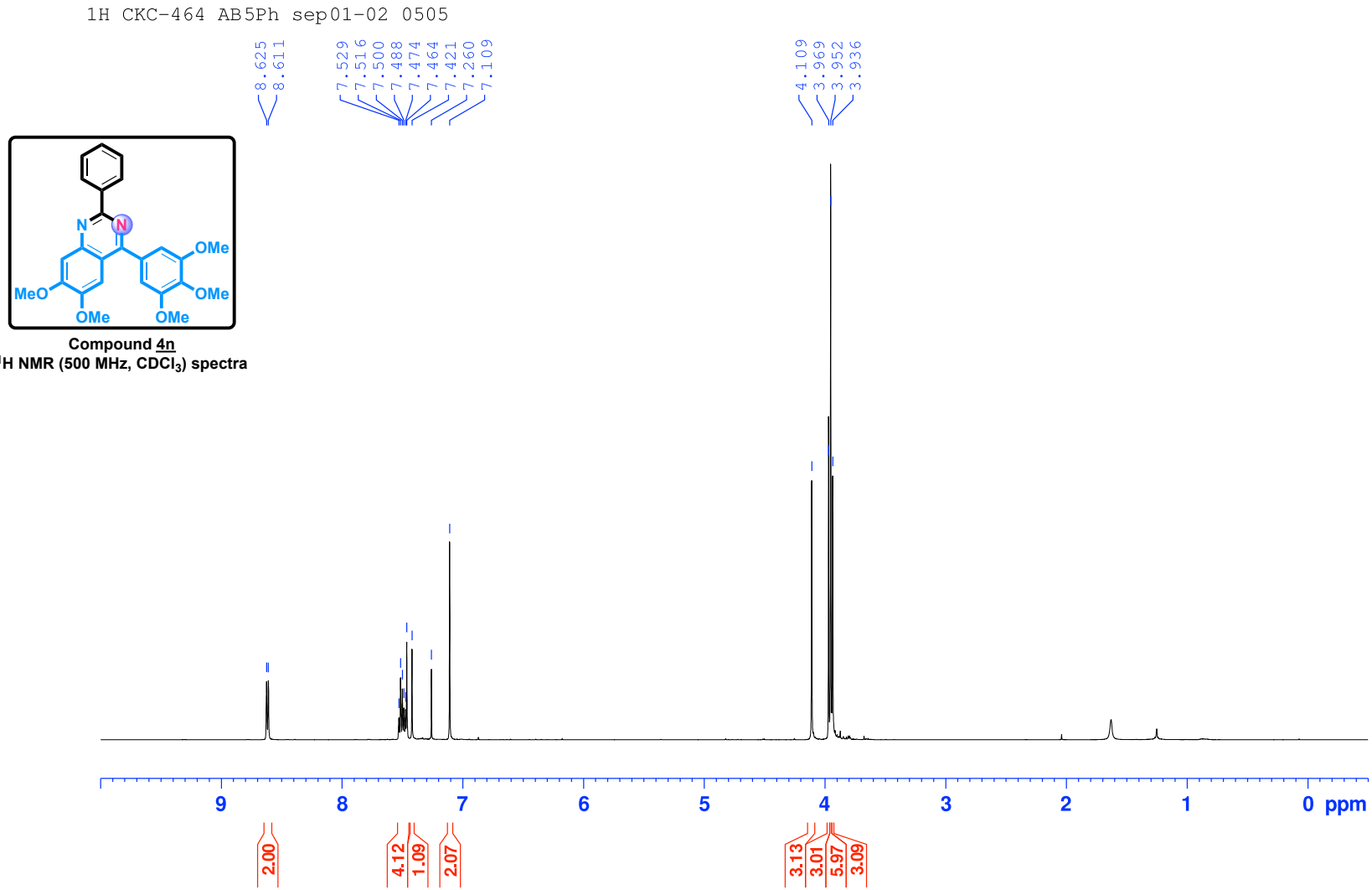


Compound 4m



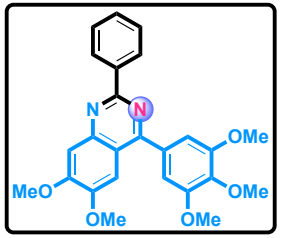
Compound 4m
^{13}C NMR (125 MHz, $CDCl_3$) spectra

Compound 4n

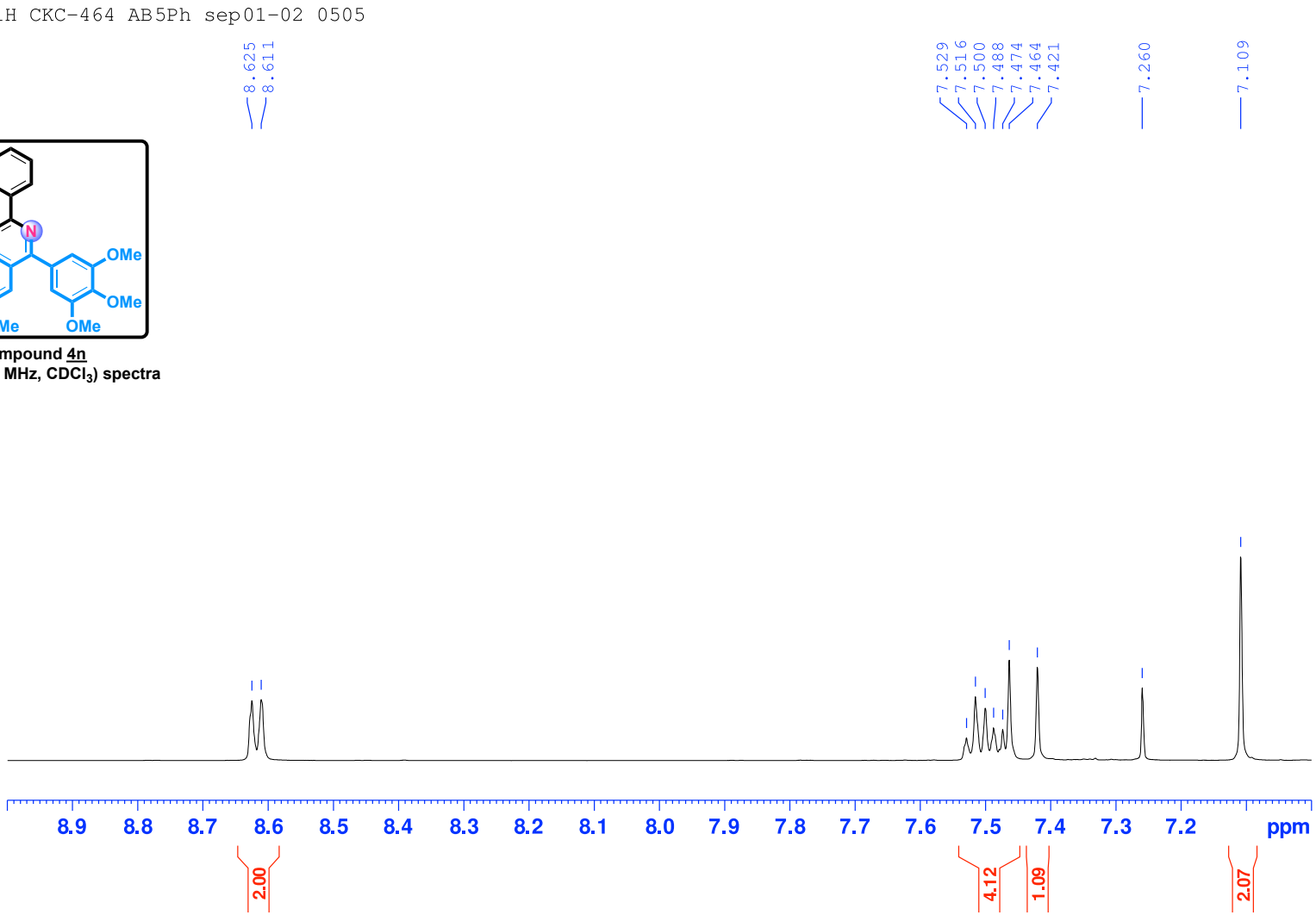


Compound 4n
^{1}H NMR (500 MHz, $CDCl_3$) spectra

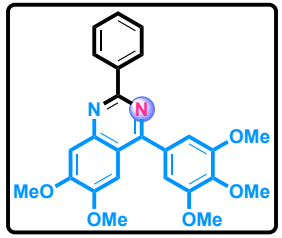
Compound 4n



Compound 4n
^{1}H NMR (500 MHz, $CDCl_3$) spectra

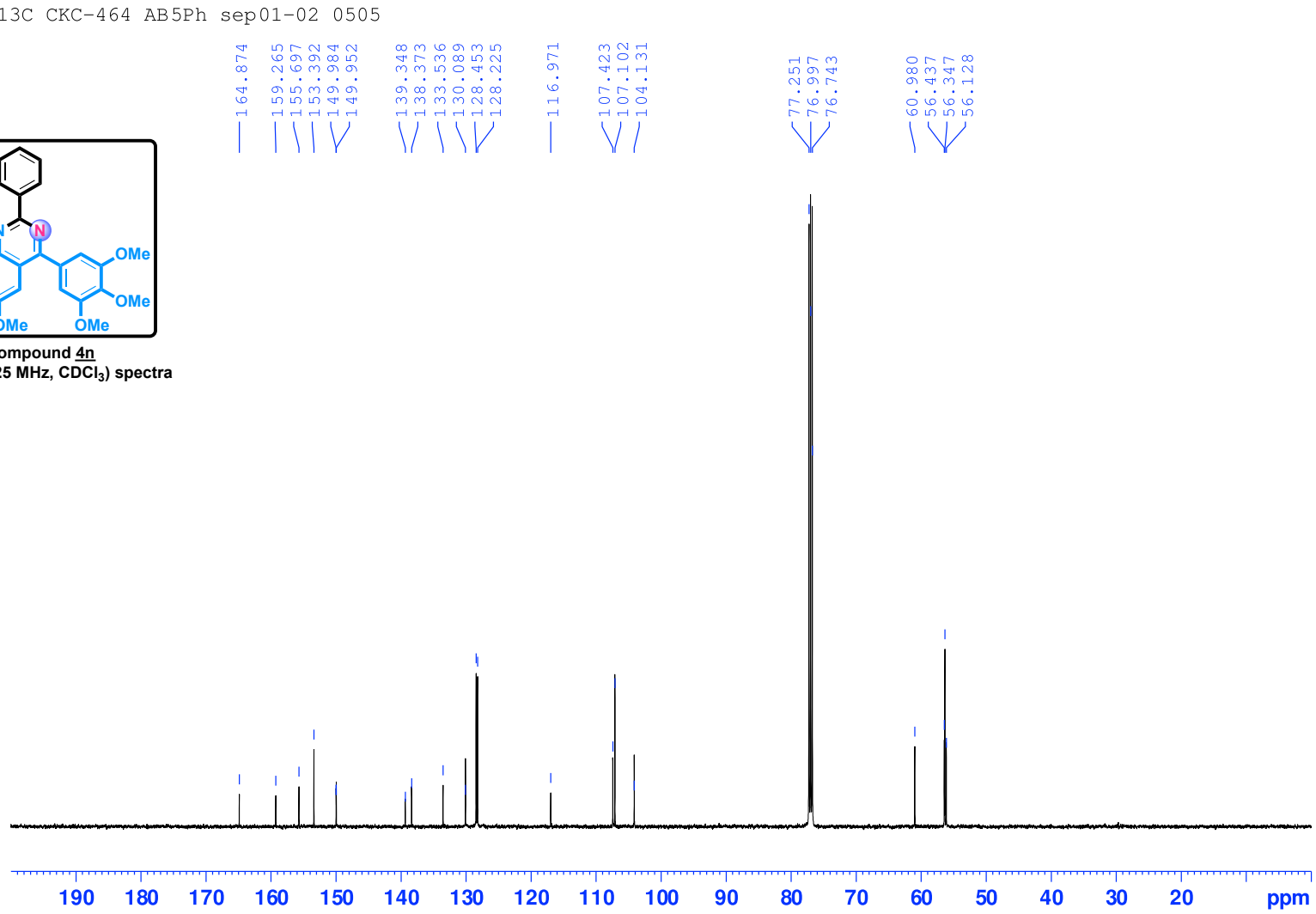


Compound 4n

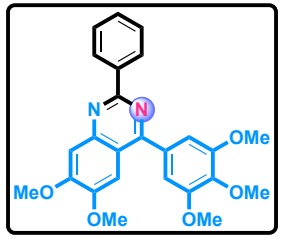


Compound 4n

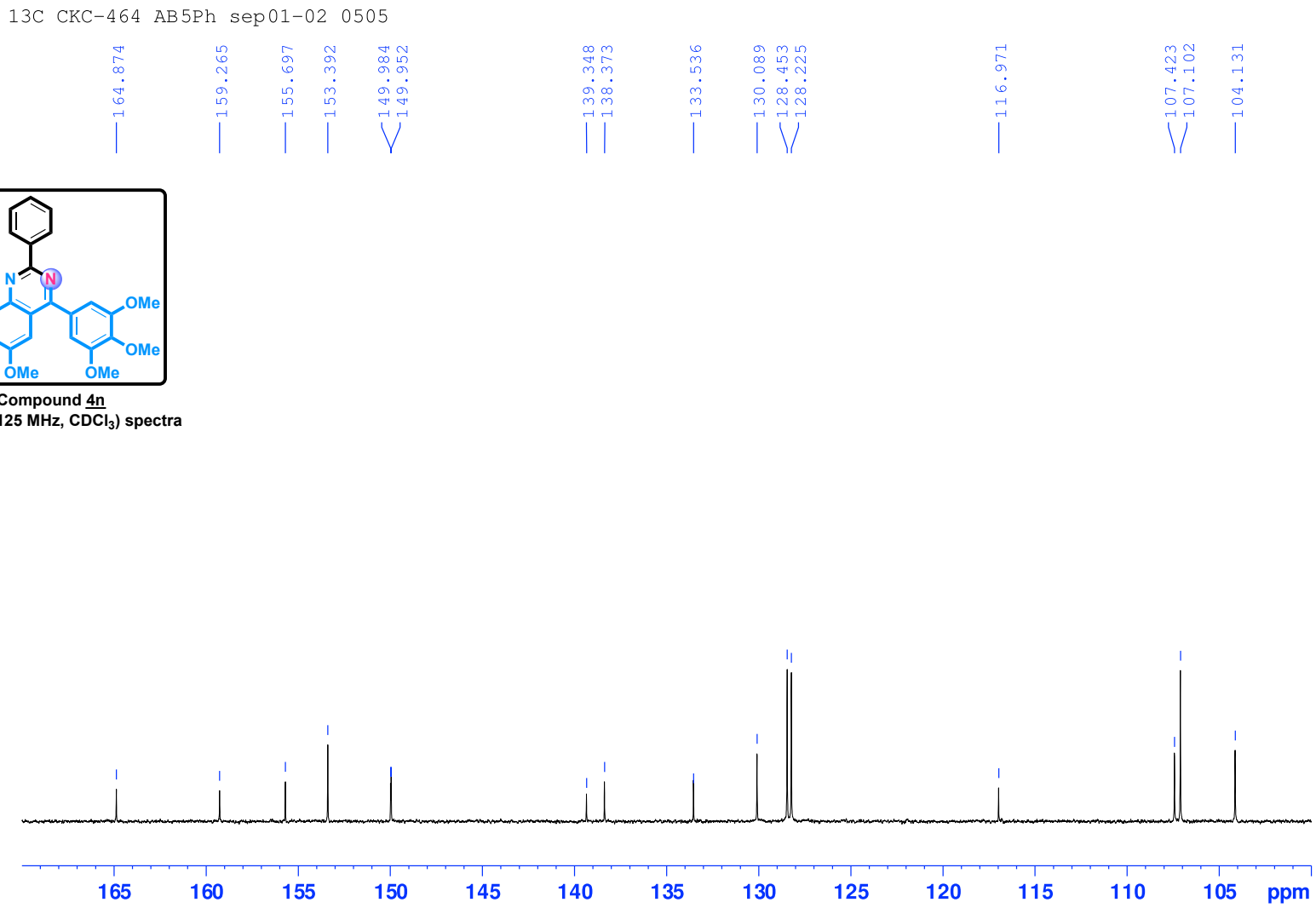
^{13}C NMR (125 MHz, $CDCl_3$) spectra



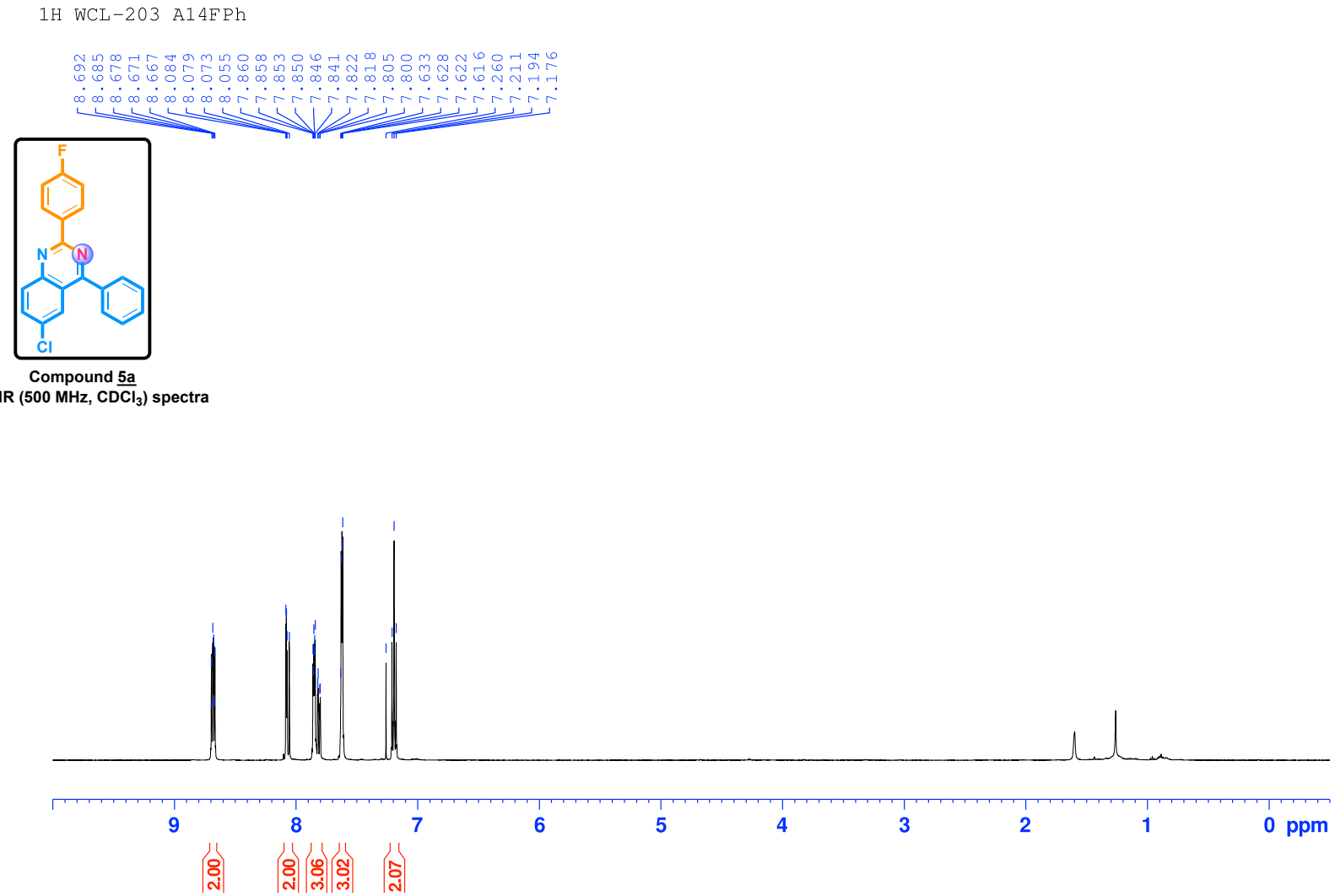
Compound 4n



Compound 4n
^{13}C NMR (125 MHz, $CDCl_3$) spectra

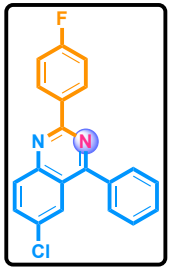


Compound 5a

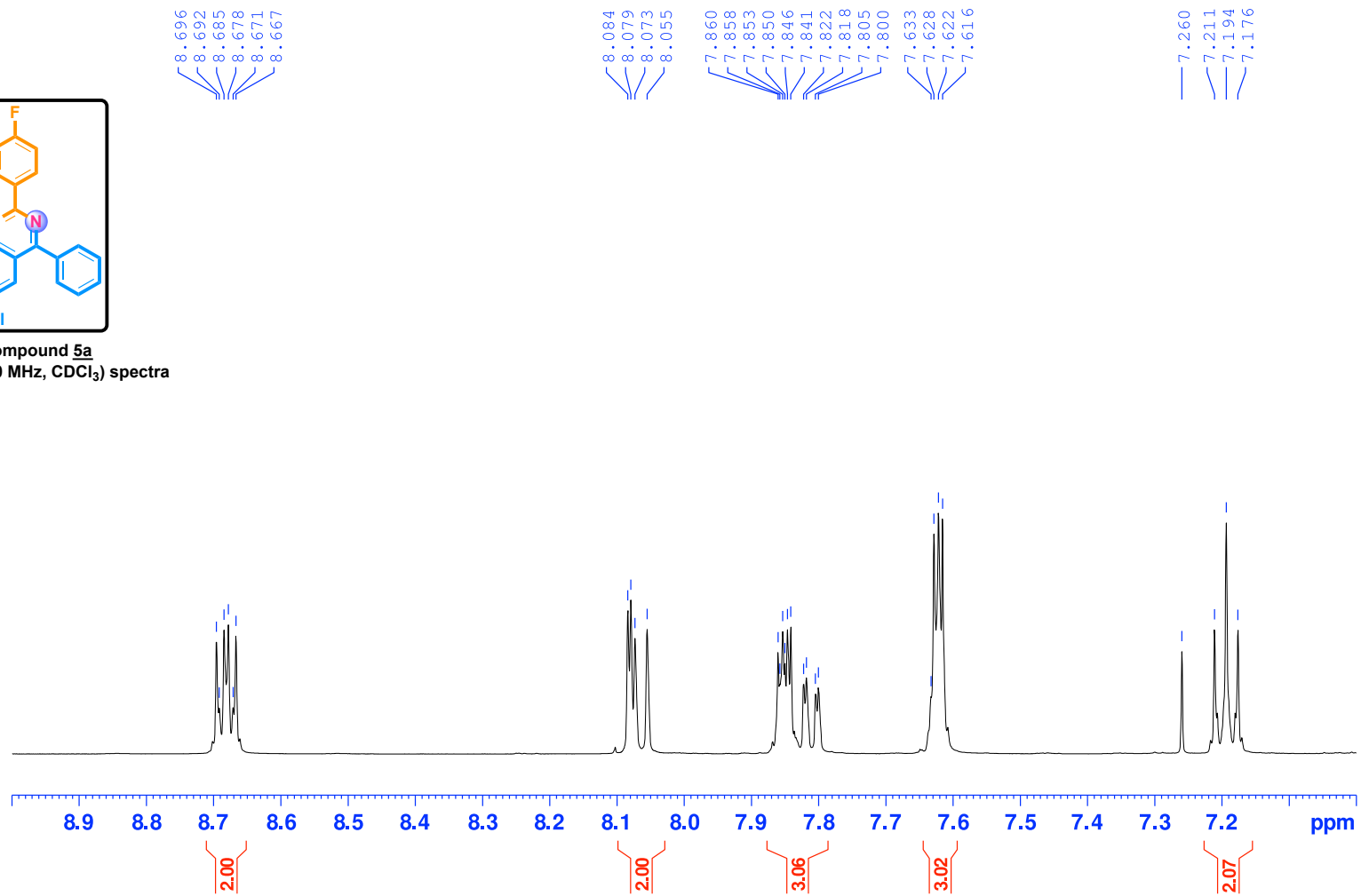


Compound 5a
^{1}H NMR (500 MHz, $CDCl_3$) spectra

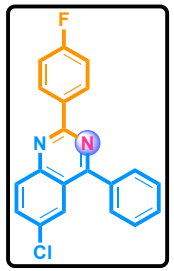
Compound 5a



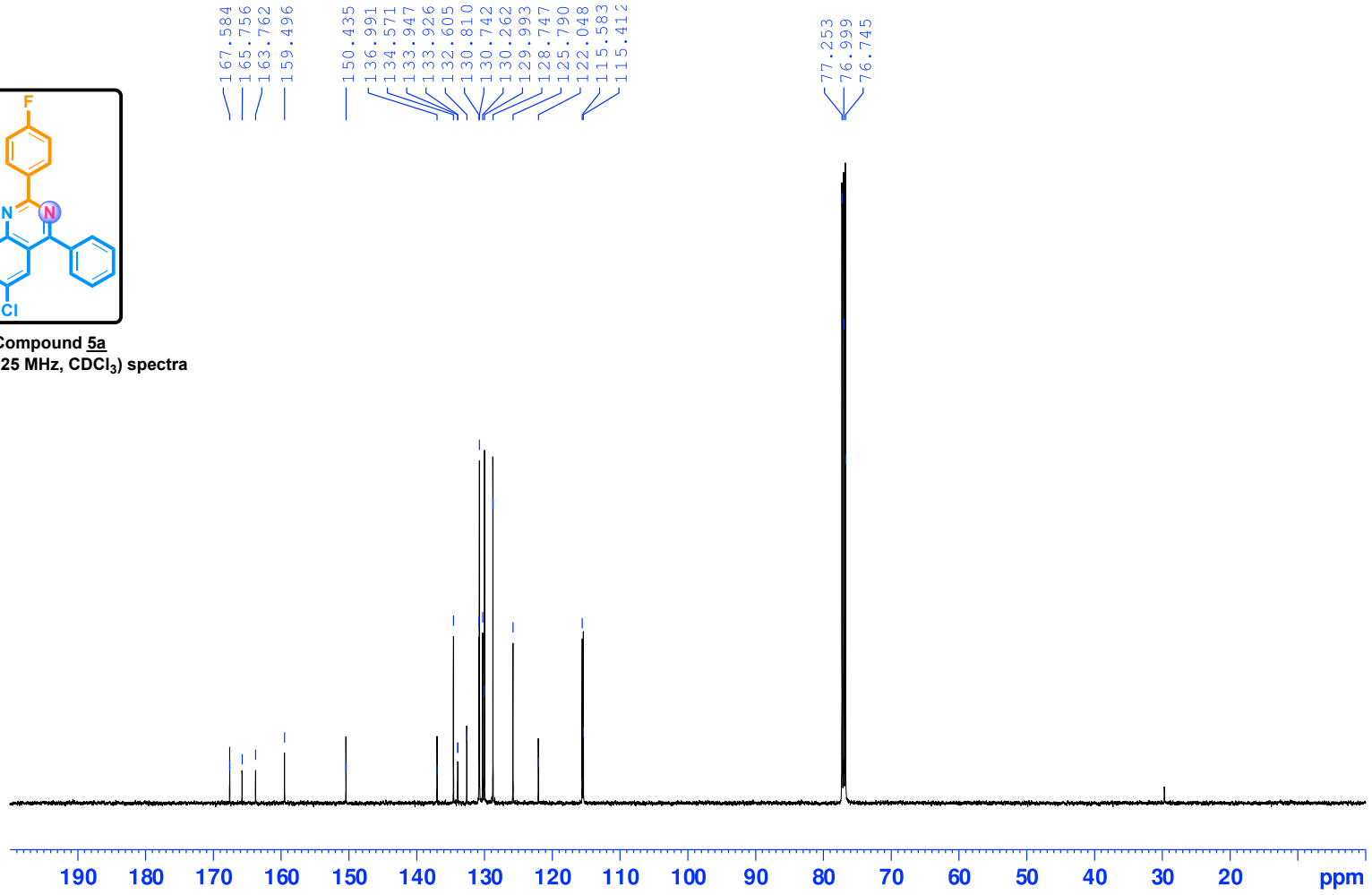
Compound 5a
^{1}H NMR (500 MHz, $CDCl_3$) spectra



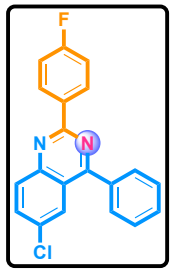
Compound 5a



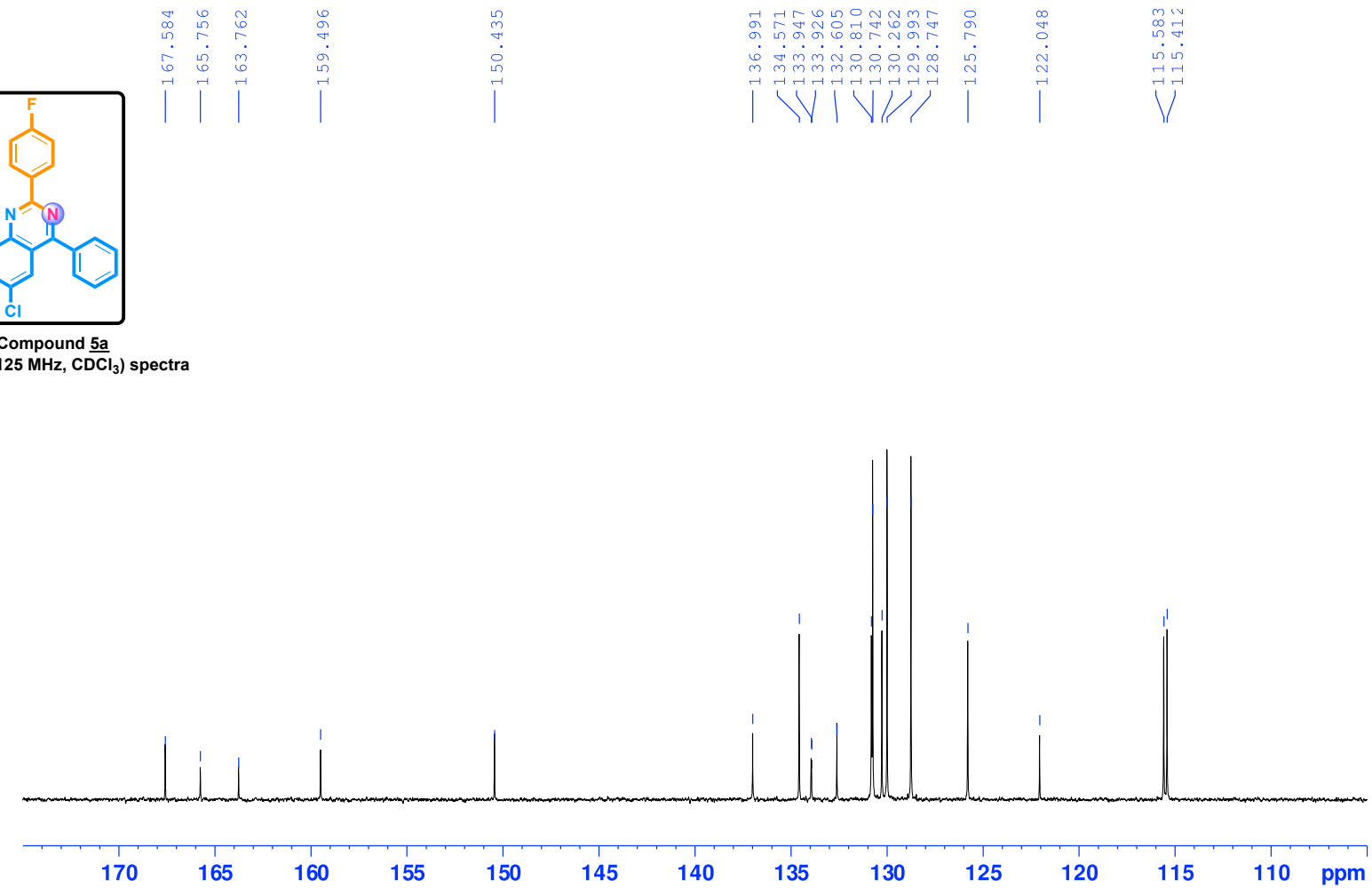
Compound 5a
^{13}C NMR (125 MHz, $CDCl_3$) spectra



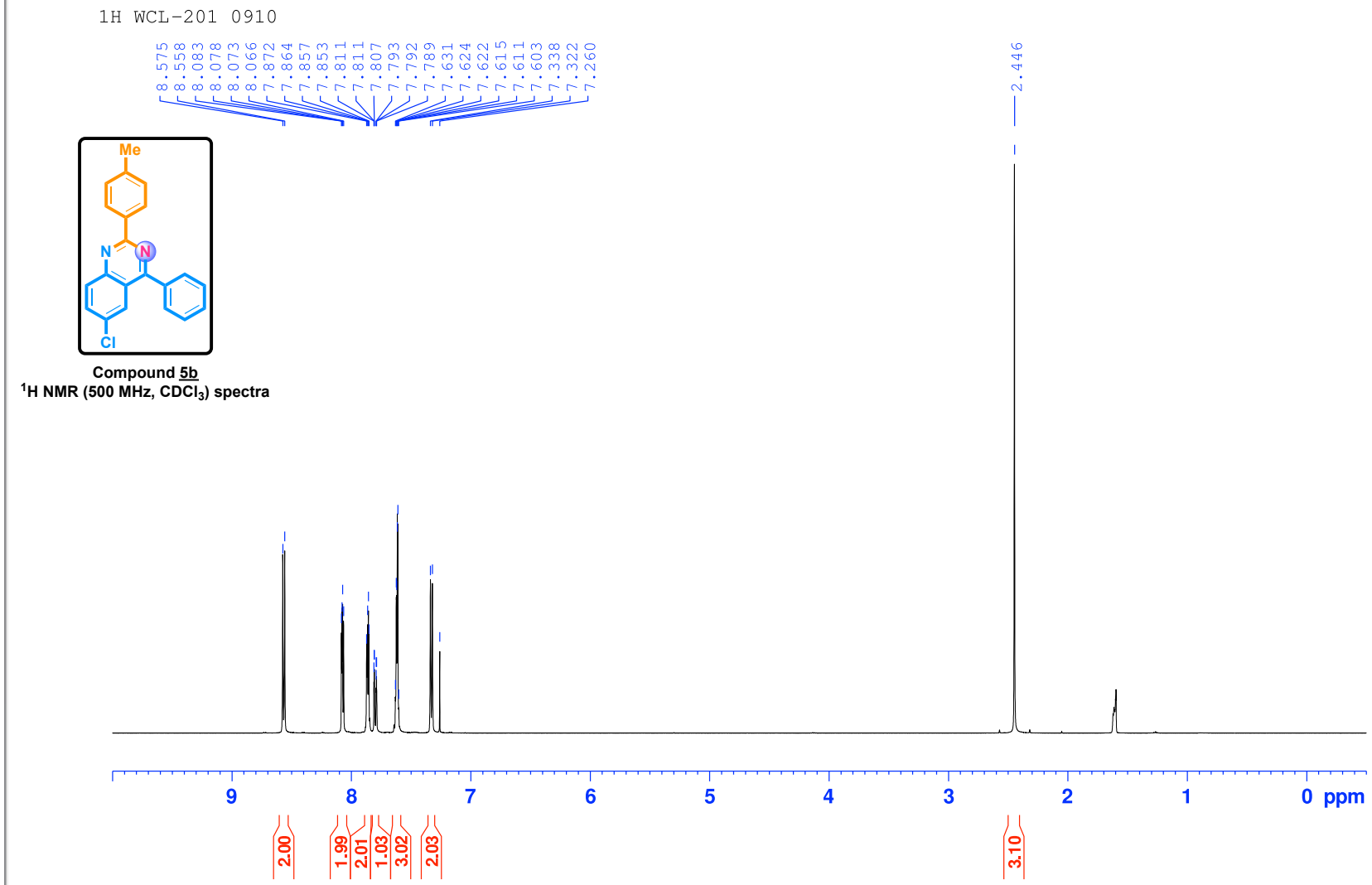
Compound 5a



Compound 5a
^{13}C NMR (125 MHz, $CDCl_3$) spectra

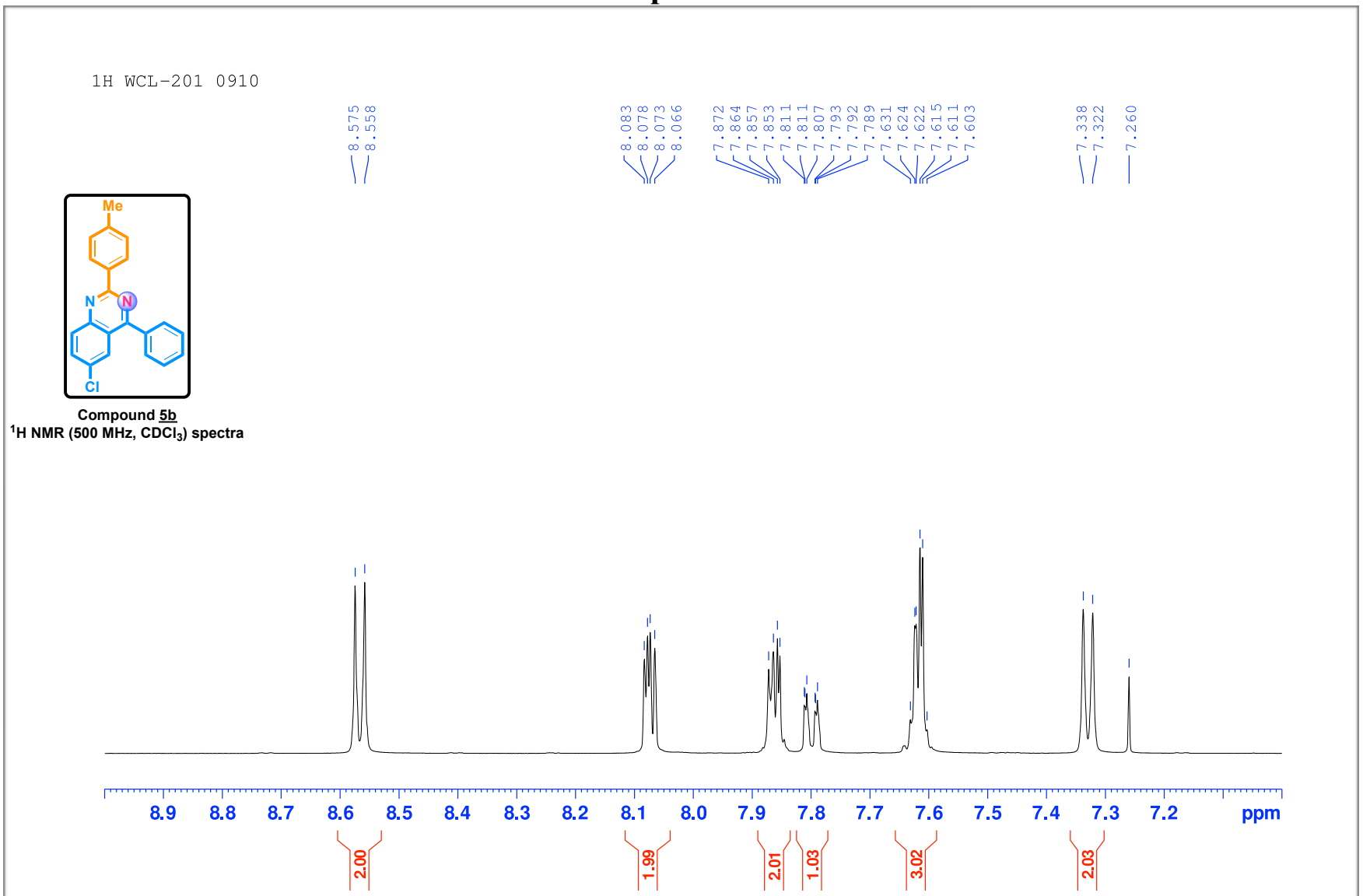


Compound 5b



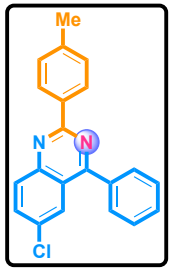
Compound 5b
^{1}H NMR (500 MHz, $CDCl_3$) spectra

Compound 5b

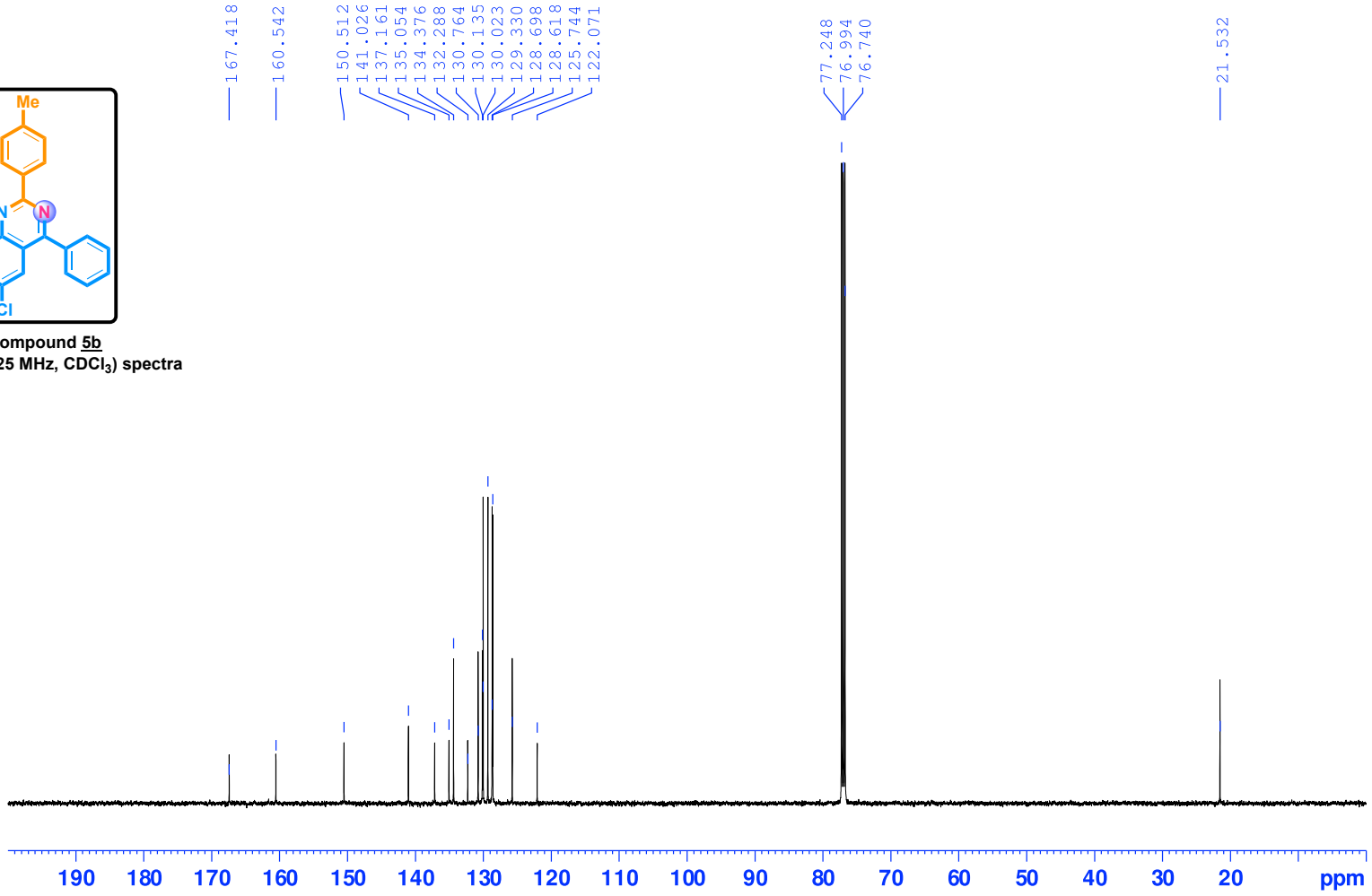


Compound 5b
^{1}H NMR (500 MHz, $CDCl_3$) spectra

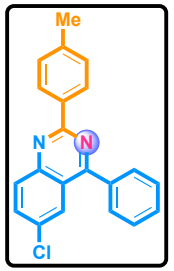
Compound 5b



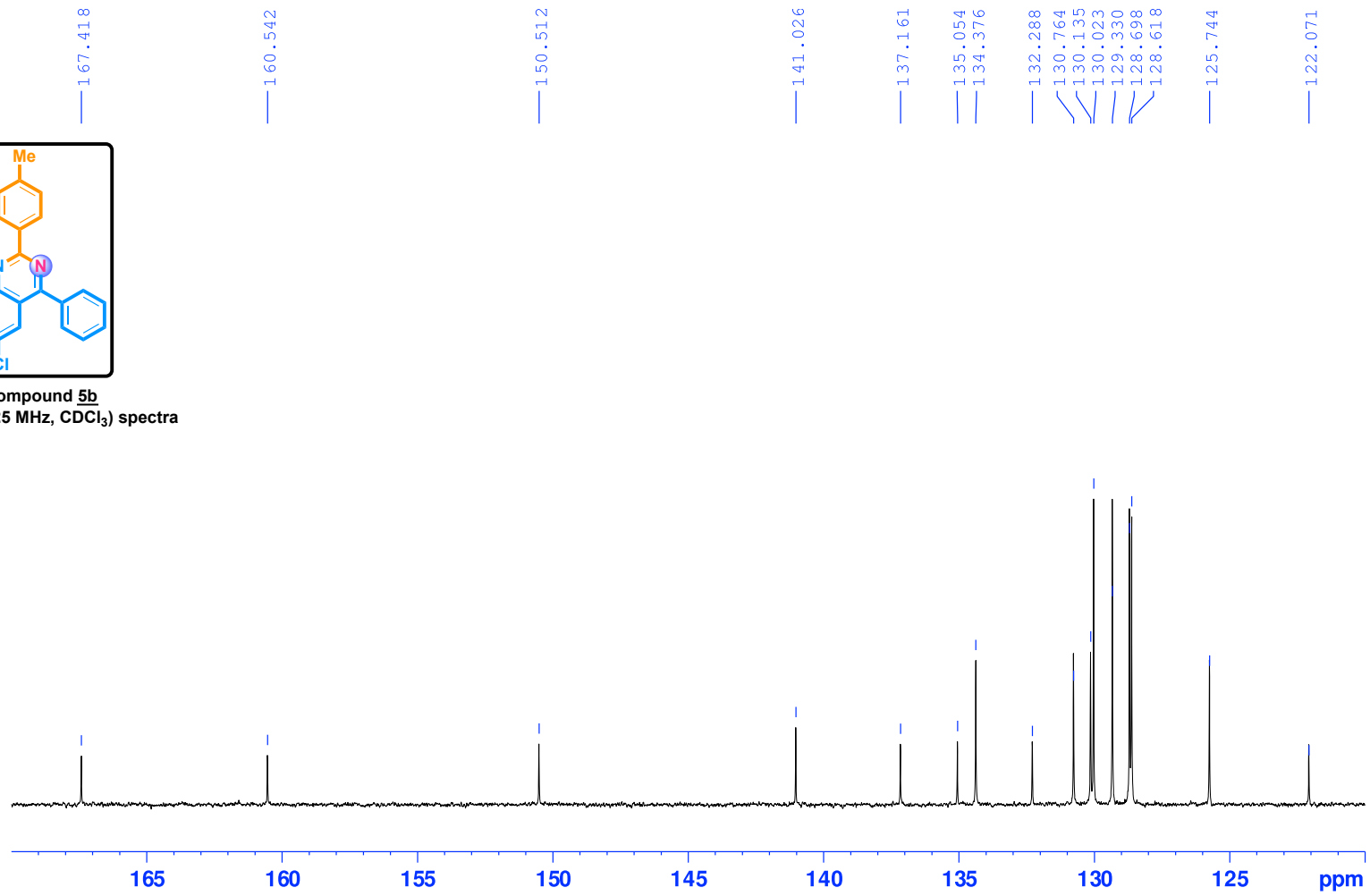
Compound 5b
^{13}C NMR (125 MHz, $CDCl_3$) spectra



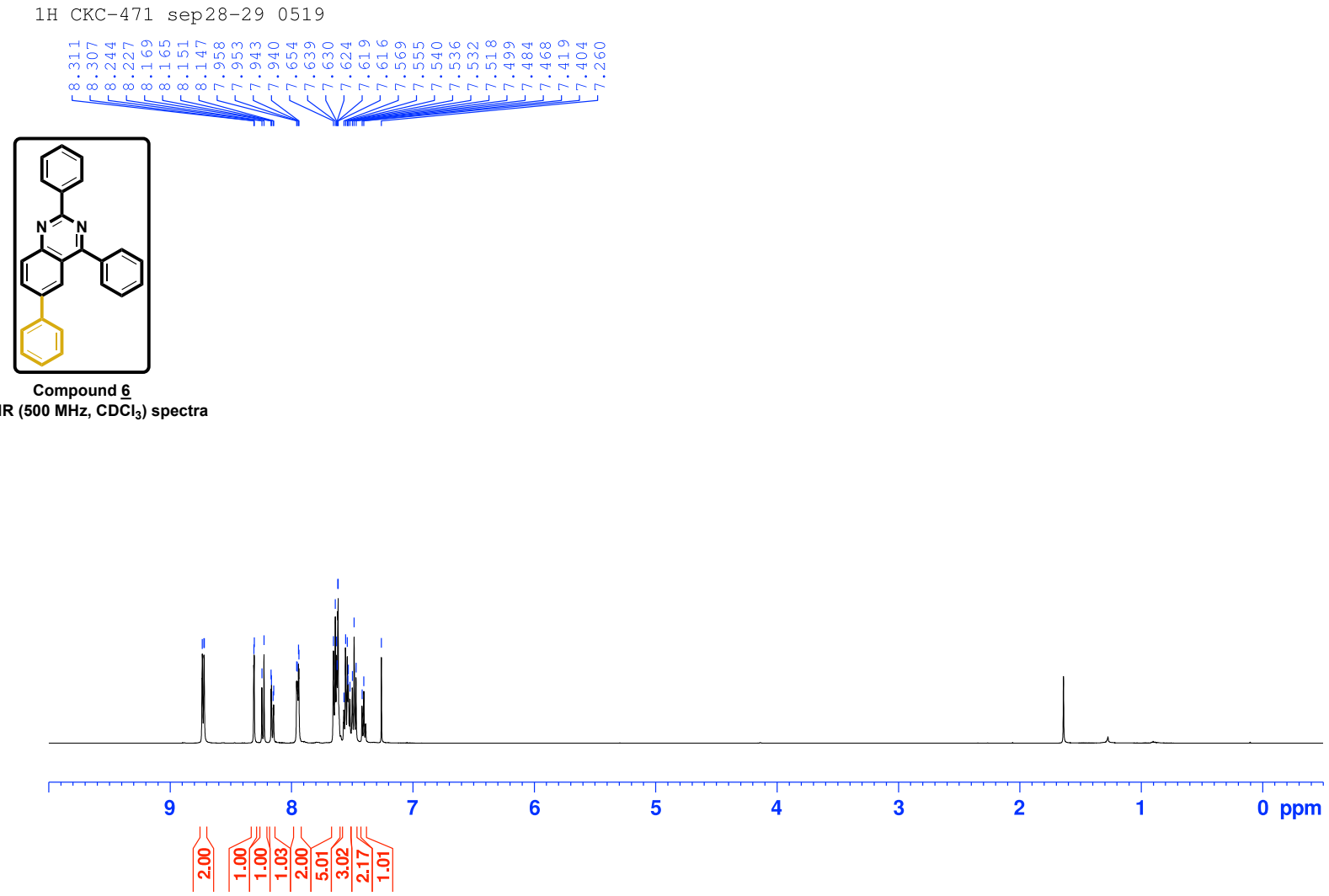
Compound 5b



Compound 5b
^{13}C NMR (125 MHz, $CDCl_3$) spectra

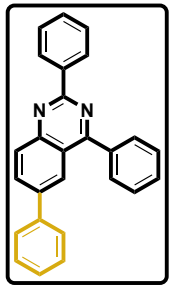


Compound 6

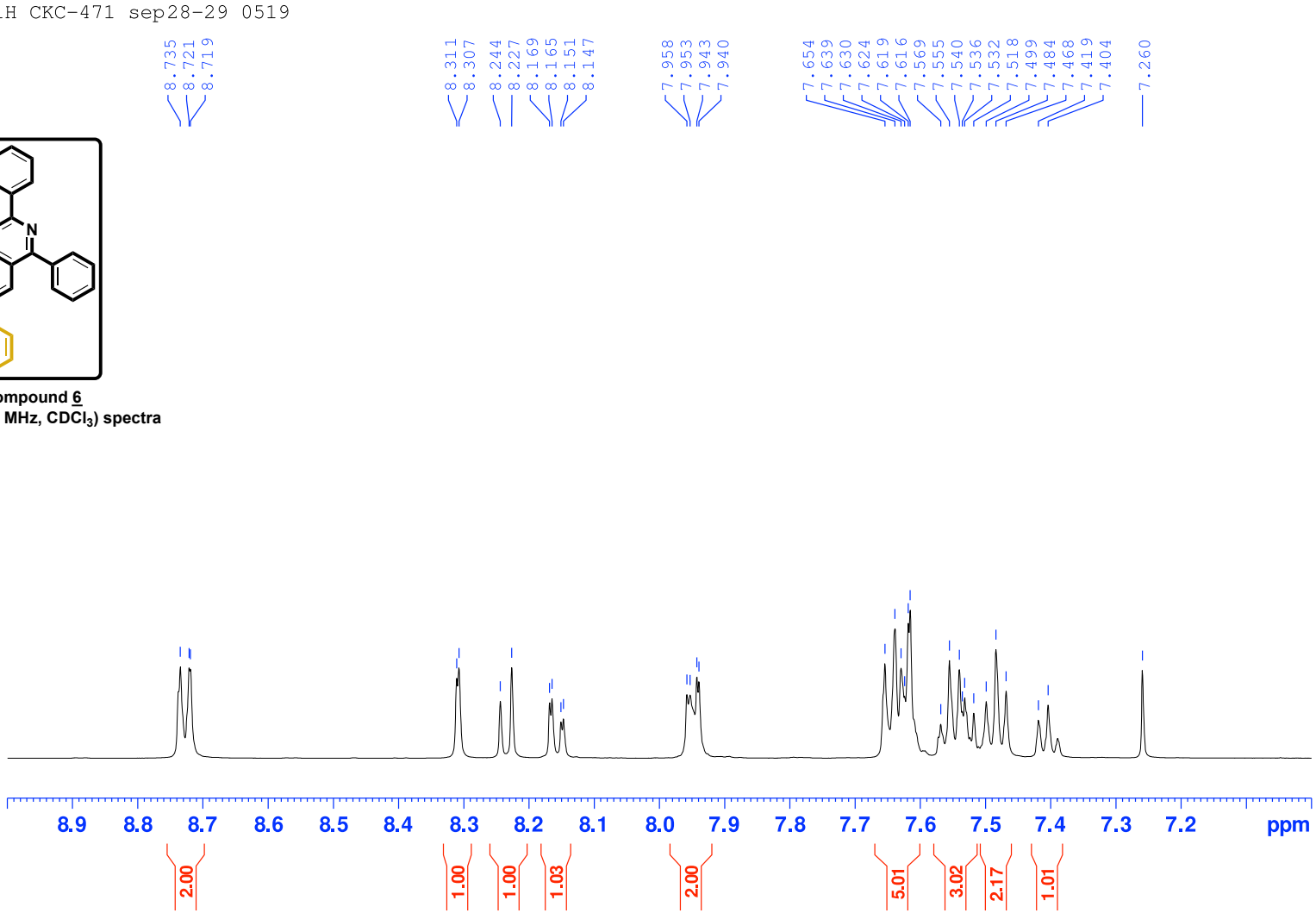


Compound 6
^{1}H NMR (500 MHz, $CDCl_3$) spectra

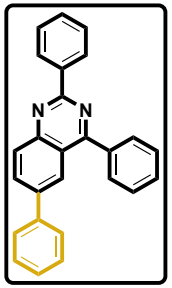
Compound 6



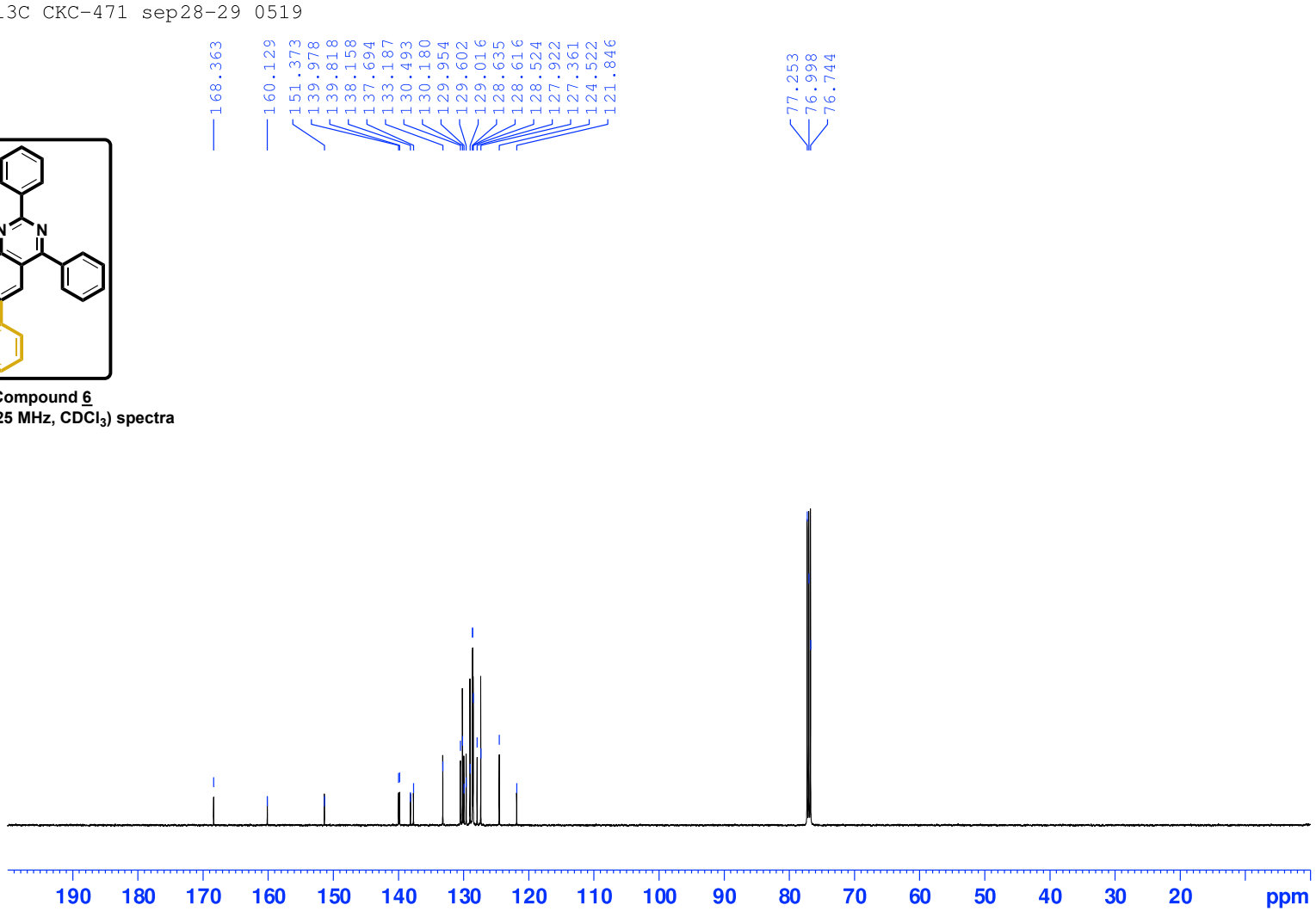
Compound 6
^{1}H NMR (500 MHz, $CDCl_3$) spectra



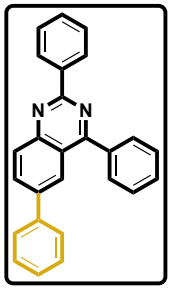
Compound 6



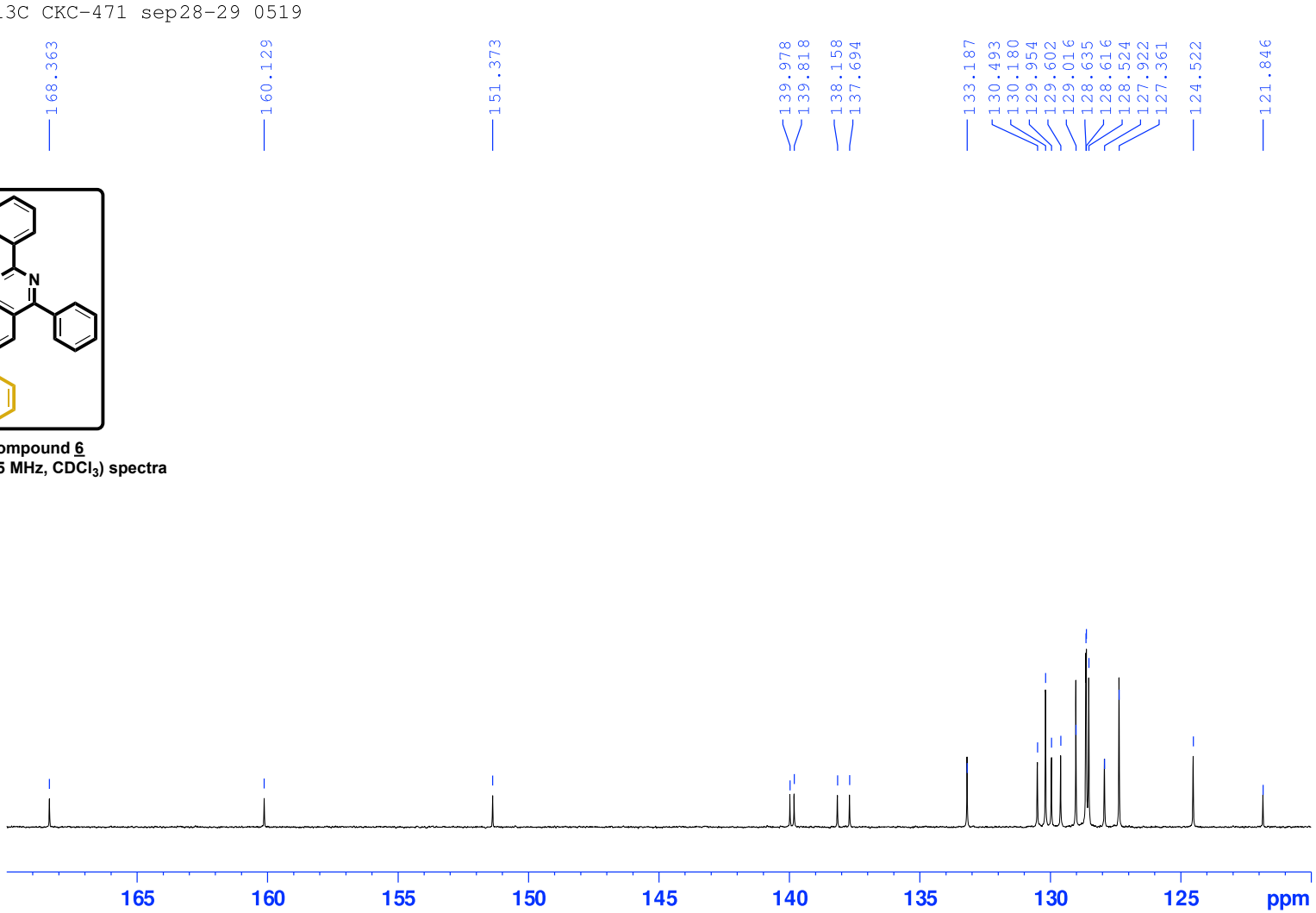
Compound 6
^{13}C NMR (125 MHz, $CDCl_3$) spectra



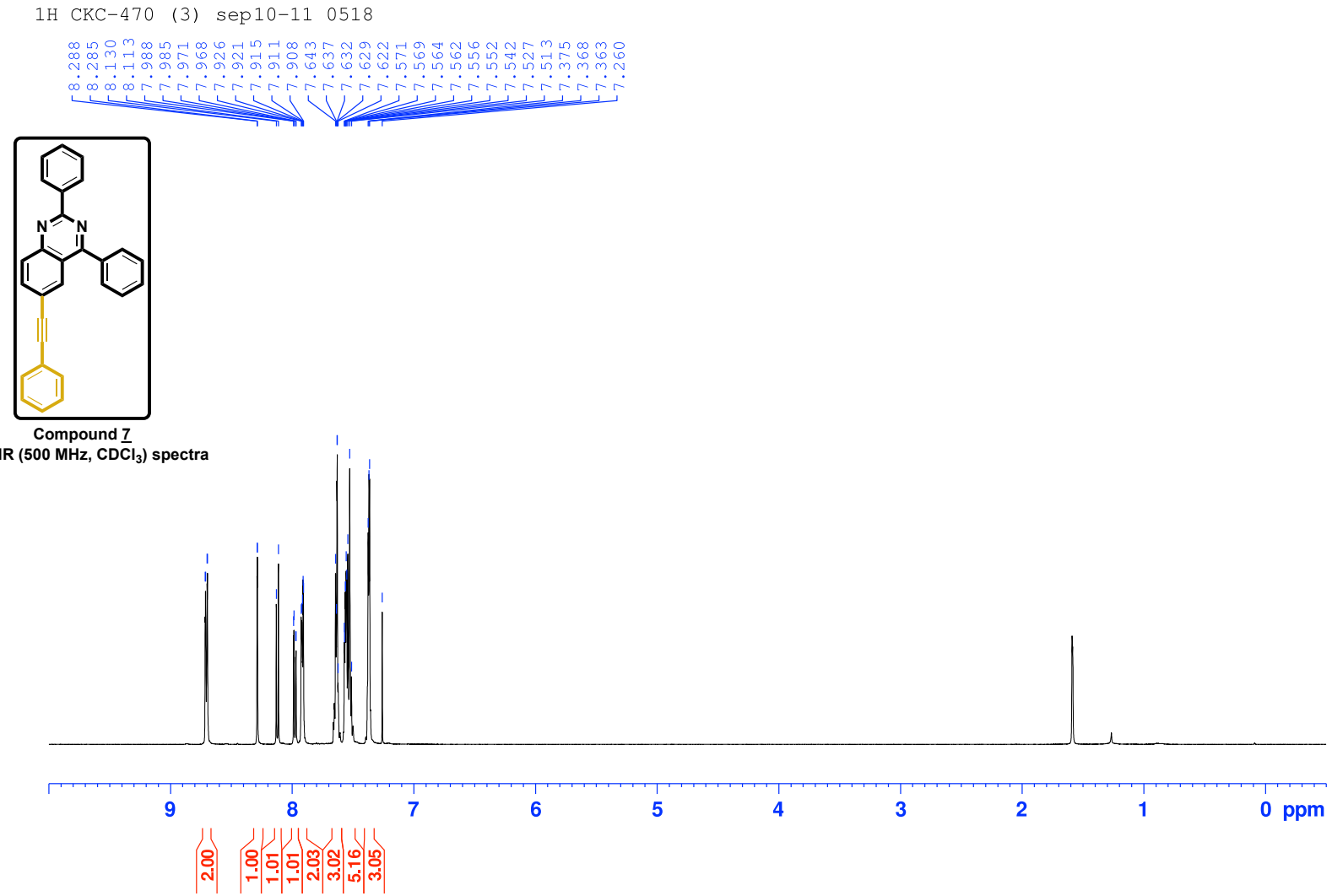
Compound 6



Compound 6
^{13}C NMR (125 MHz, $CDCl_3$) spectra



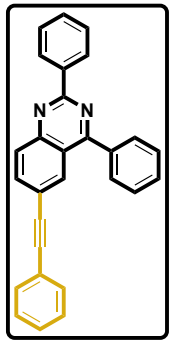
Compound 7



Compound 7

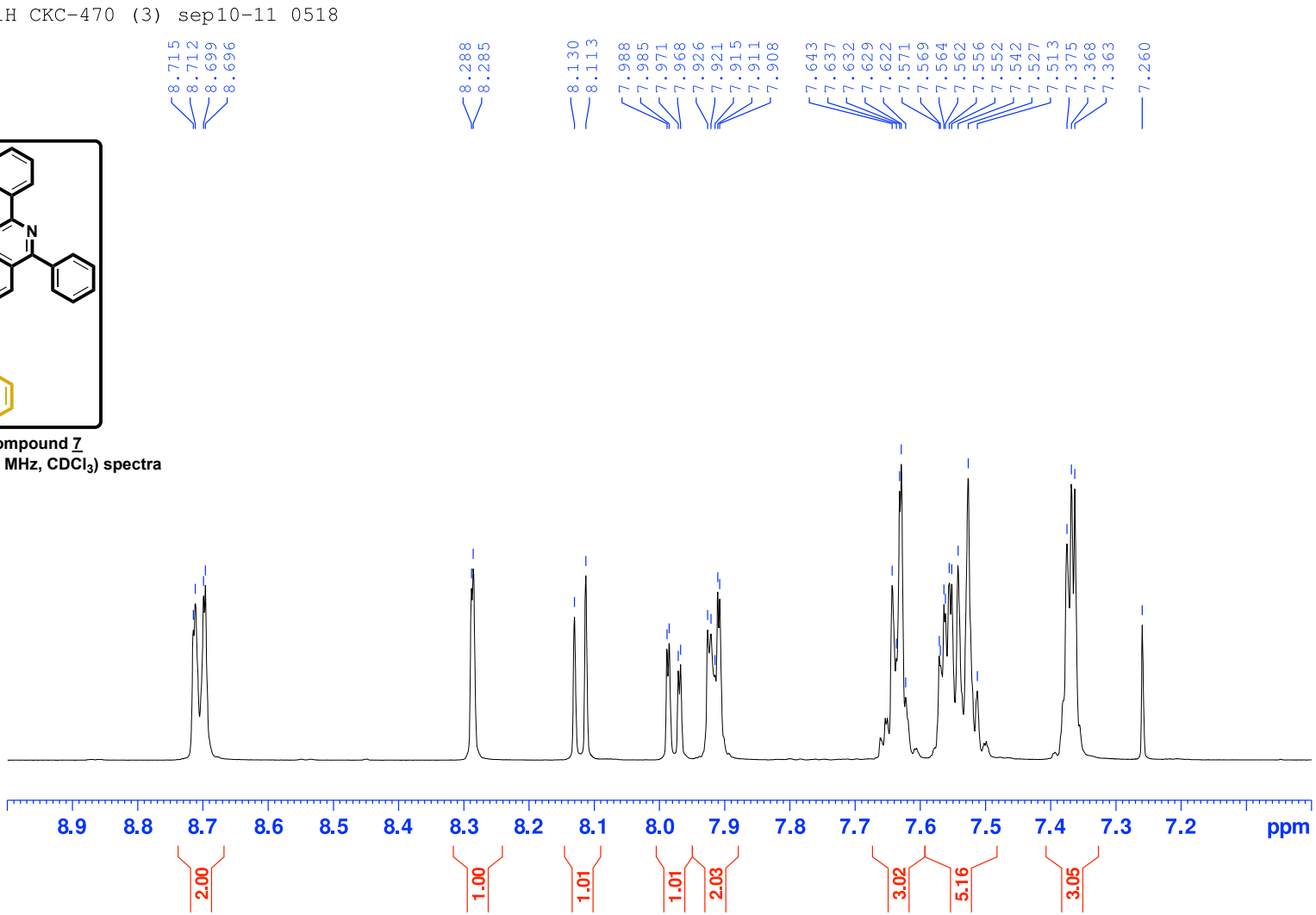
^{1}H NMR (500 MHz, $CDCl_3$) spectra

Compound 7

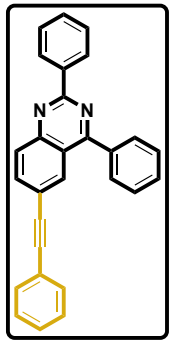


Compound 7

^{1}H NMR (500 MHz, $CDCl_3$) spectra

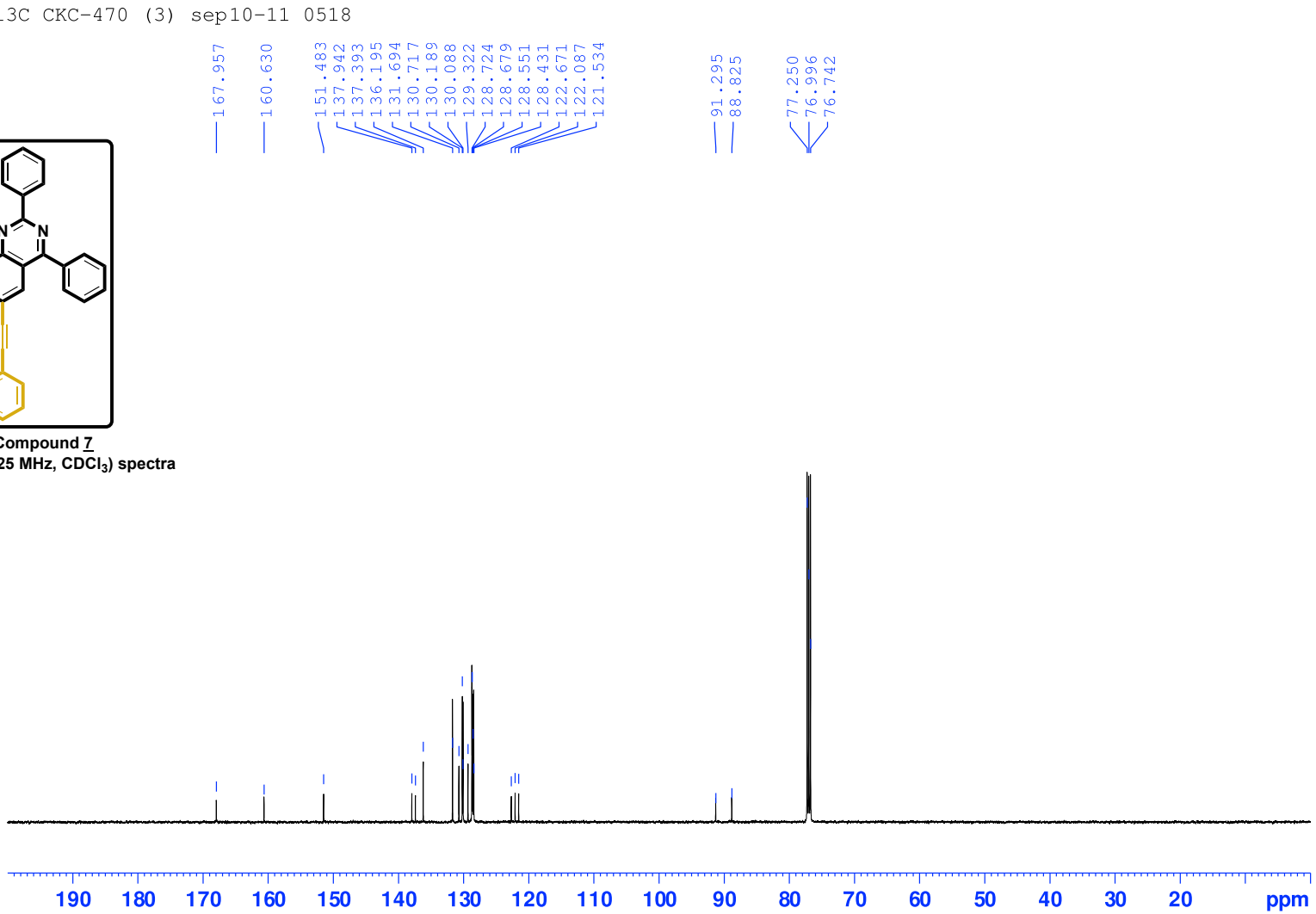


Compound 7

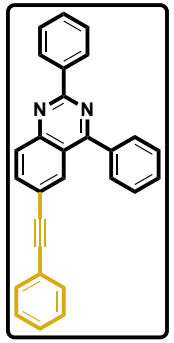


Compound 7

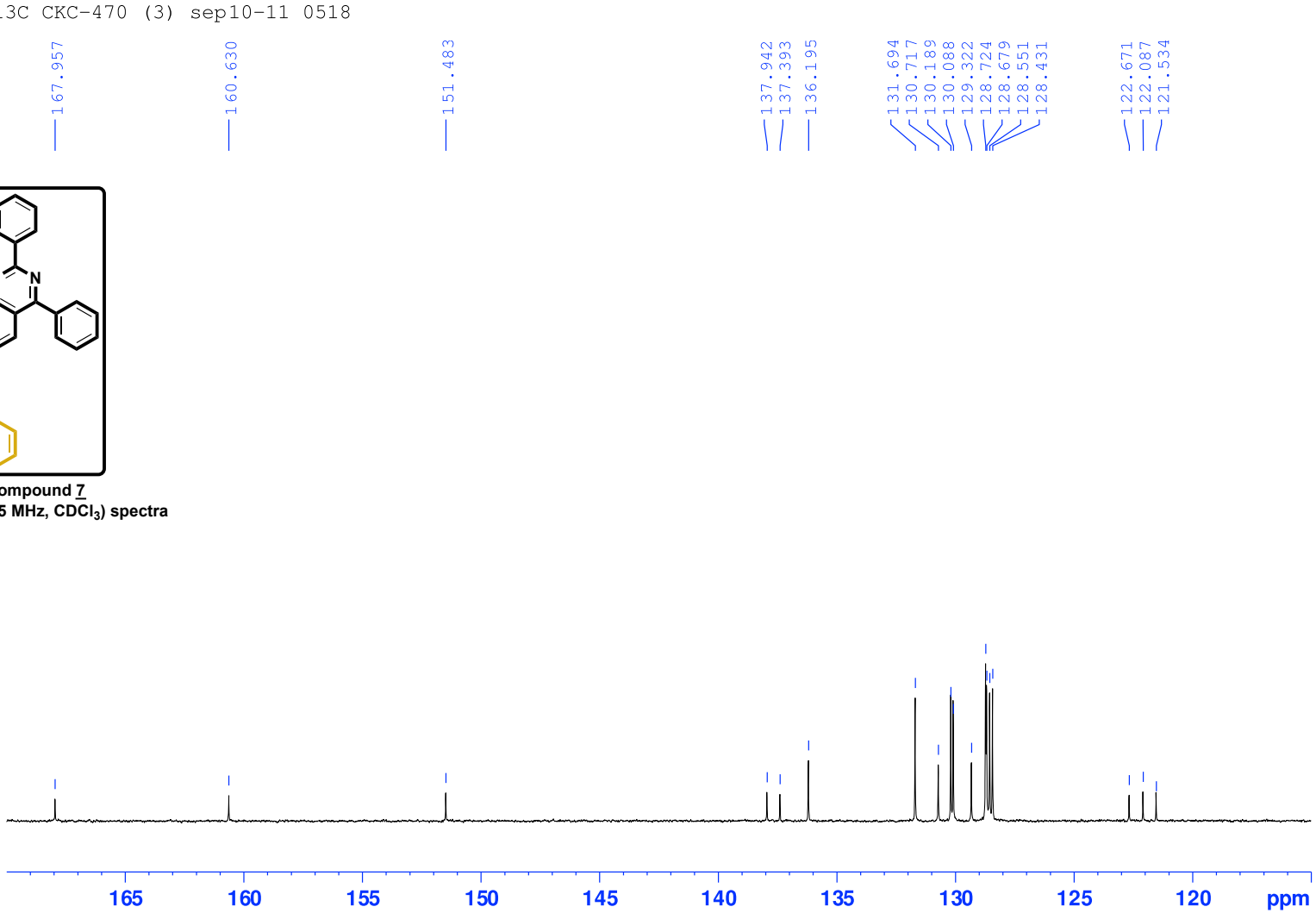
^{13}C NMR (125 MHz, $CDCl_3$) spectra



Compound 7

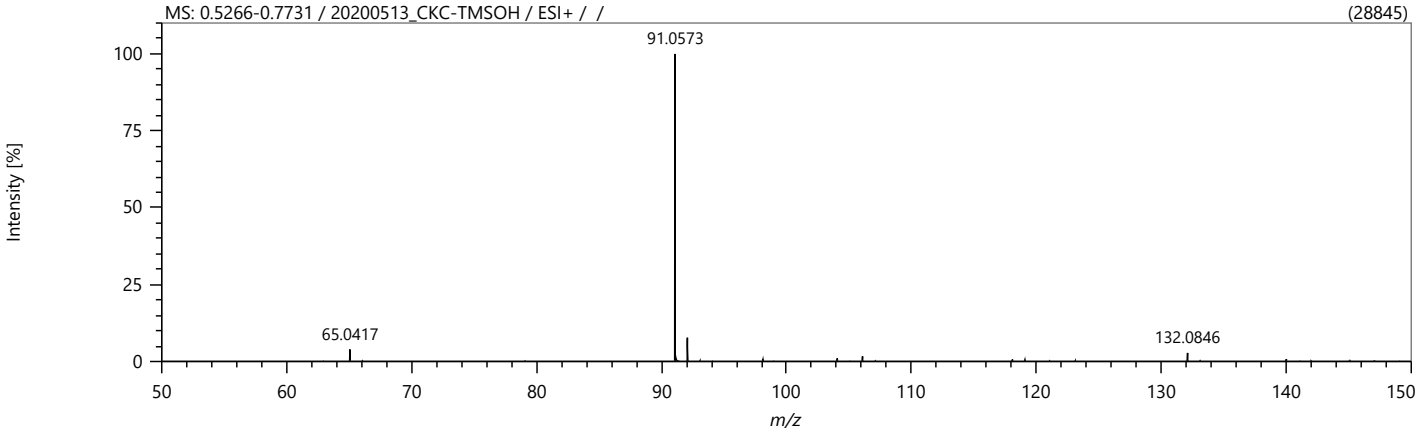


Compound 7
^{13}C NMR (125 MHz, $CDCl_3$) spectra



HRMS of TMSOH

Spectrum



Elemental Composition

Parameters	
Tolerance:	±100.00 ppm
Electron:	Odd/Even
Charge:	+1
DBE:	-99.0 - 999.0

Elements Set 1:

Symbol	C	H	O	N	Si
Min	0	0	1	0	1
Max	1000	4000	1	0	1

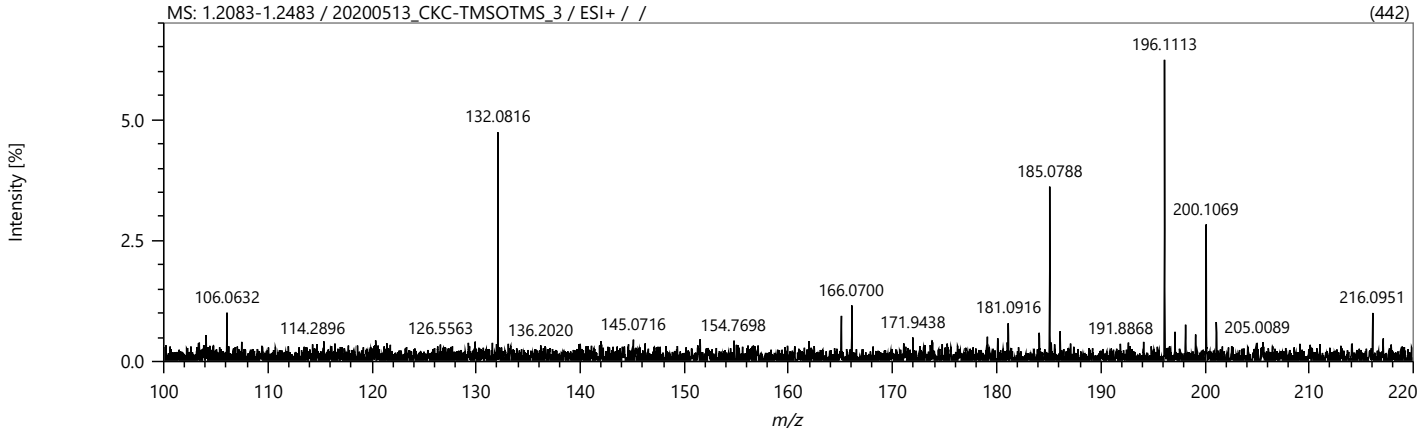
Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
91.05730	C3 H11 O Si	91.05737	-0.06	-0.70	-0.5

1 / 1

HRMS of TMSOTMS

Spectrum



Elemental Composition

Parameters	
Tolerance:	±100.00 ppm
Electron:	Odd/Even
Charge:	+1
DBE:	-99.0 - 999.0

Elements Set 1:

Symbol	C	H	O	N	Si	Na
Min	0	0	1	0	2	1
Max	1000	4000	1	0	2	1

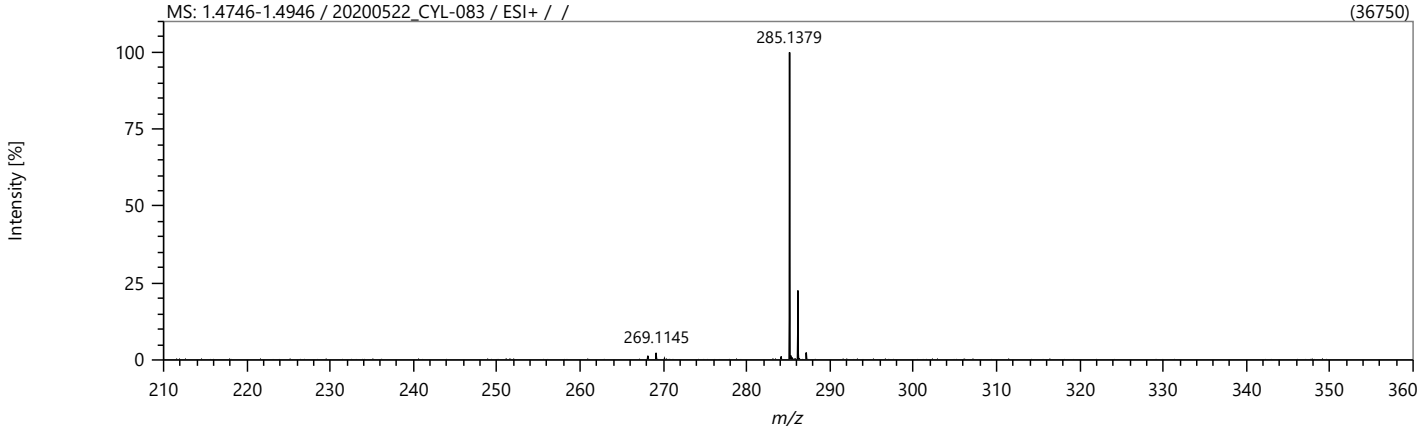
Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
185.07879	C6 H18 O Na Si2	185.07884	-0.05	-0.29	-0.5

1 / 1

HRMS of Intermediate E

Spectrum



Elemental Composition

Parameters	
Tolerance:	±10.00 ppm
Electron:	Odd/Even
Charge:	+1
DBE:	-99.0 - 999.0

Elements Set 1:

Symbol	C	H	Br	N	Na
Min	0	0	0	2	0
Max	1000	4000	0	2	0

Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
285.13787	C20 H17 N2	285.13862	-0.75	-2.63	13.5

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