Supporting Information

Environmentally friendly Nafion-catalyzed synthesis of 3-substituted Isoquinoline by using hexamethyldisilazane as a nitrogen source under microwave irradiation

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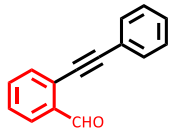
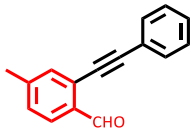
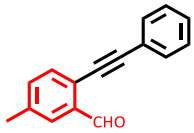
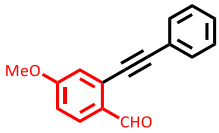
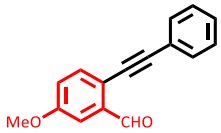
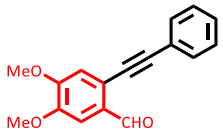
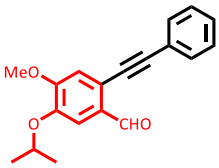
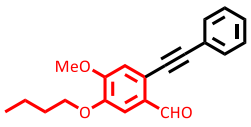
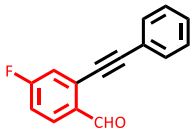
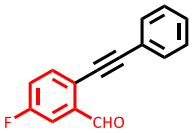
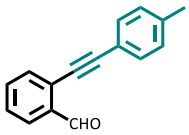
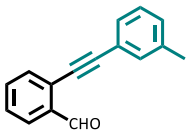
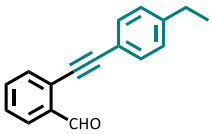
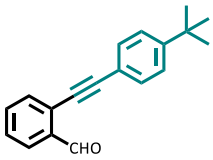
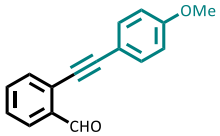
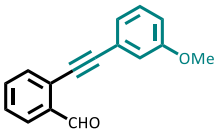
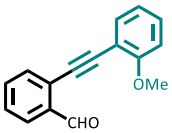
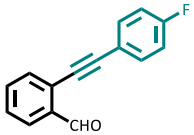
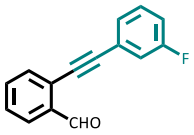
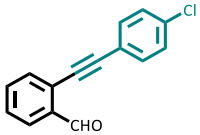
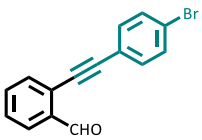
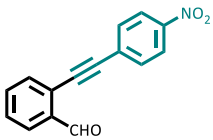
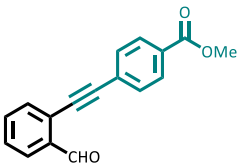
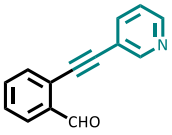
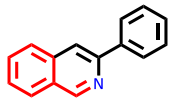
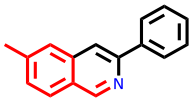
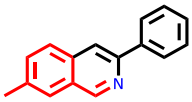
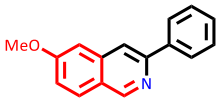
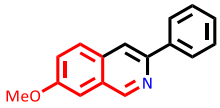
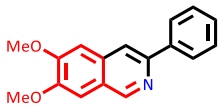
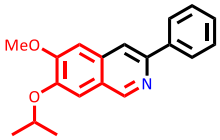
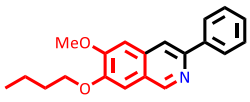
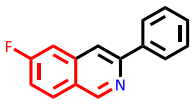
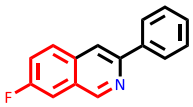
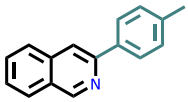
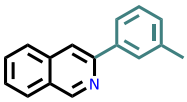
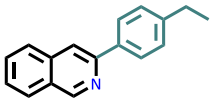
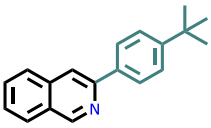
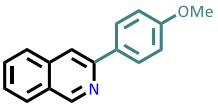
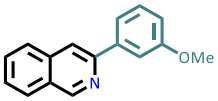
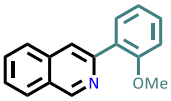
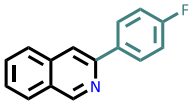
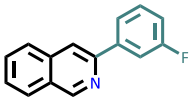
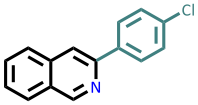
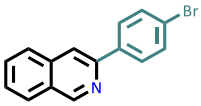
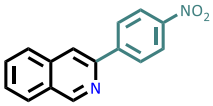
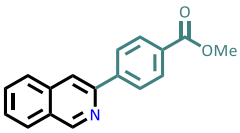
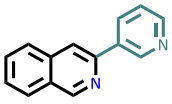
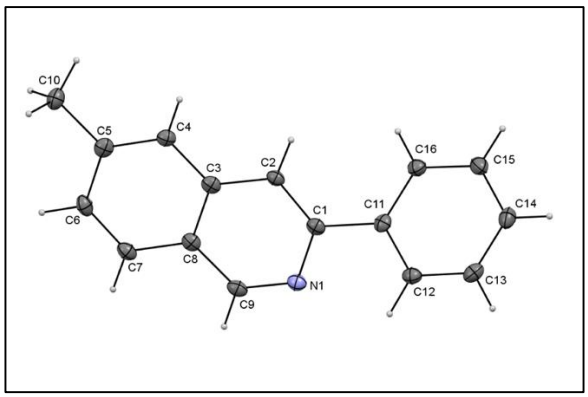
Total Pages of Supporting Information: 149.

Compound **2a** NMR (S-7~S-8) HRMS (S-102)	Compound **2b** NMR (S-9~S-10) HRMS (S-103)	Compound **2c** NMR (S-11~S-12) HRMS (S-104)	Compound **2d** NMR (S-13~S-14) HRMS (S-105)	Compound **2e** **NMR** (S-15~S-16) HRMS (S-106)
				
Compound **2f** NMR (S-17~S-18) HRMS (S-107)	Compound **2g** NMR (S-19~S-20) HRMS (S-108)	Compound **2h** NMR (S-21~S-22) HRMS (S-109)	Compound **2i** NMR (S-23~S-24) HRMS (S-110)	Compound **2j** NMR (S-25~S-26) HRMS (S-111)
				
Compound **2k** NMR (S-27~S-28) HRMS (S-112)	Compound **2l** NMR (S-29~S-30) HRMS (S-113)	Compound **2m** NMR (S-31~S-32) HRMS (S-114)	Compound **2n** NMR (S-33~S-34) HRMS (S-115)	Compound **2o** NMR (S-35~S-36) HRMS (S-116)
				
Compound **2p** NMR (S-37~S-38) HRMS (S-117)	Compound **2q** NMR (S-39~S-40) HRMS (S-118)	Compound **2r** NMR (S-41~S-42) HRMS (S-119)	Compound **2s** NMR (S-43~S-44) HRMS (S-120)	Compound **2t** NMR (S-45~S-46) HRMS (S-121)
				
Compound **2u** NMR (S-47~S-48) HRMS (S-122)	Compound **2v** NMR (S-49~S-50) HRMS (S-123)	Compound **2w** NMR (S-51~S-52) HRMS (S-124)	Compound **2x** NMR (S-53~S-54) HRMS (S-125)	
				

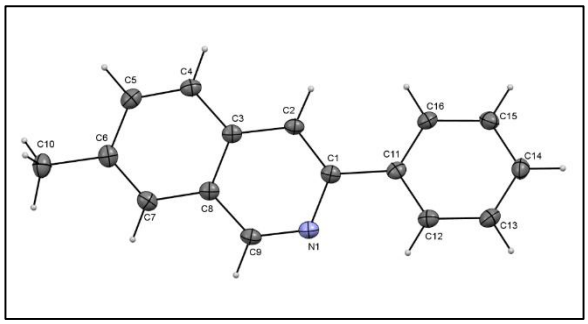
Compound **1a**	Compound **1b**	Compound **1c**	Compound **1d**	Compound **1e**
NMR (S-55~S-56)	NMR (S-57~S-58)	NMR (S-59~S-60)	NMR (S-61~S-62)	NMR (S-63~S-64)
HRMS (S-126)	HRMS (S-127)	HRMS (S-128)	HRMS (S-129)	HRMS (S-130)
				
Compound **1f**	Compound **1g**	Compound **1h**	Compound **1i**	Compound **1j**
NMR (S-65~S-66)	NMR (S-67~S-68)	NMR (S-69~S-70)	NMR (S-71~S-72)	NMR (S-73~S-74)
HRMS (S-131)	HRMS (S-132)	HRMS (S-133)	HRMS (S-134)	HRMS (S-135)
				
Compound **1k**	Compound **1l**	Compound **1m**	Compound **1n**	Compound **1o**
NMR (S-75~S-76)	NMR (S-77~S-78)	NMR (S-79~S-80)	NMR (S-81~S-82)	NMR (S-83~S-84)
HRMS (S-136)	HRMS (S-137)	HRMS (S-138)	HRMS (S-139)	HRMS (S-140)
				
Compound **1p**	Compound **1q**	Compound **1r**	Compound **1s**	Compound **1t**
NMR (S-85~S-86)	NMR (S-87~S-88)	NMR (S-89~S-90)	NMR (S-91~S-92)	NMR (S-93~S-94)
HRMS (S-141)	HRMS (S-142)	HRMS (S-143)	HRMS (S-144)	HRMS (S-145)
				
Compound **1u**	Compound **1v**	Compound **1w**	Compound **1x**	
NMR (S-95~S-96)	NMR (S-97~S-98)	NMR (S-99~S-100)	NMR (S-101~S-102)	
HRMS (S-146)	HRMS (S-147)	HRMS (S-148)	HRMS (S-149)	
				

Crystal data and structure refinement for compound **1b**
(the thermal ellipsoid was drawn at the 50% probability level)



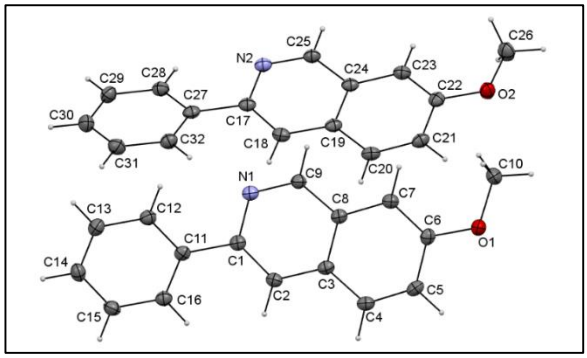
Identification code	i18487	
Empirical formula	C16 H13 N	
Formula weight	219.27	
Temperature	100.0(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 6.07430(10) Å	α= 90°.
	b = 7.29170(10) Å	β= 100.6020(10)°.
	c = 12.6835(2) Å	γ = 90°.
Volume	552.187(15) $Å^3$	
Z, Density (calculated)	2, 1.319 Mg/m^3	
Absorption coefficient	0.587 mm^{-1}	
F(000)	232	
Crystal size	0.200 x 0.180 x 0.165 mm^3	
Theta range for data collection	3.545 to 72.608°.	
Index ranges	-7<=h<=7, -8<=k<=9, -15<=l<=15	
Reflections collected	8632	
Independent reflections	2104 [R(int) = 0.0347]	
Completeness to theta = 67.679°	99.7 %	
Absorption correction	Numerical	
Max. and min. transmission	1 and 0.8369	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2104 / 1 / 155	
Goodness-of-fit on F^2	1.090	
Final R indices [I>2sigma(I)]	R1 = 0.0292, wR2 = 0.0800	
R indices (all data)	R1 = 0.0294, wR2 = 0.0801	
Absolute structure parameter	0.03(16)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.177 and -0.183 e.$Å^{-3}$	

Crystal data and structure refinement for compound **1c**
(the thermal ellipsoid was drawn at the 50% probability level)



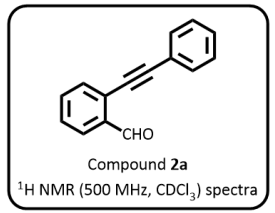
Identification code	i18488	
Empirical formula	C16 H13 N	
Formula weight	219.27	
Temperature	100.0(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 6.14730(10) Å	α= 90°.
	b = 7.40040(10) Å	β= 90°.
	c = 24.6690(3) Å	γ = 90°.
Volume	1122.25(3) Å ^{3}	
Z, Density (calculated)	4, 1.298 Mg/m^3	
Absorption coefficient	0.577 mm^{-1}	
F(000)	464	
Crystal size	0.153 x 0.125 x 0.095 mm^3	
Theta range for data collection	3.583 to 72.572°.	
Index ranges	-7<=h<=6, -9<=k<=9, -29<=l<=30	
Reflections collected	23354	
Independent reflections	2211 [R(int) = 0.0449]	
Completeness to theta = 67.679°	100.0 %	
Absorption correction	Numerical	
Max. and min. transmission	1 and 0.8162	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2211 / 0 / 155	
Goodness-of-fit on F^2	1.040	
Final R indices [I>2sigma(I)]	R1 = 0.0260, wR2 = 0.0664	
R indices (all data)	R1 = 0.0266, wR2 = 0.0666	
Absolute structure parameter	0.00(14)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.144 and -0.182 e.Å $^{-3}$	

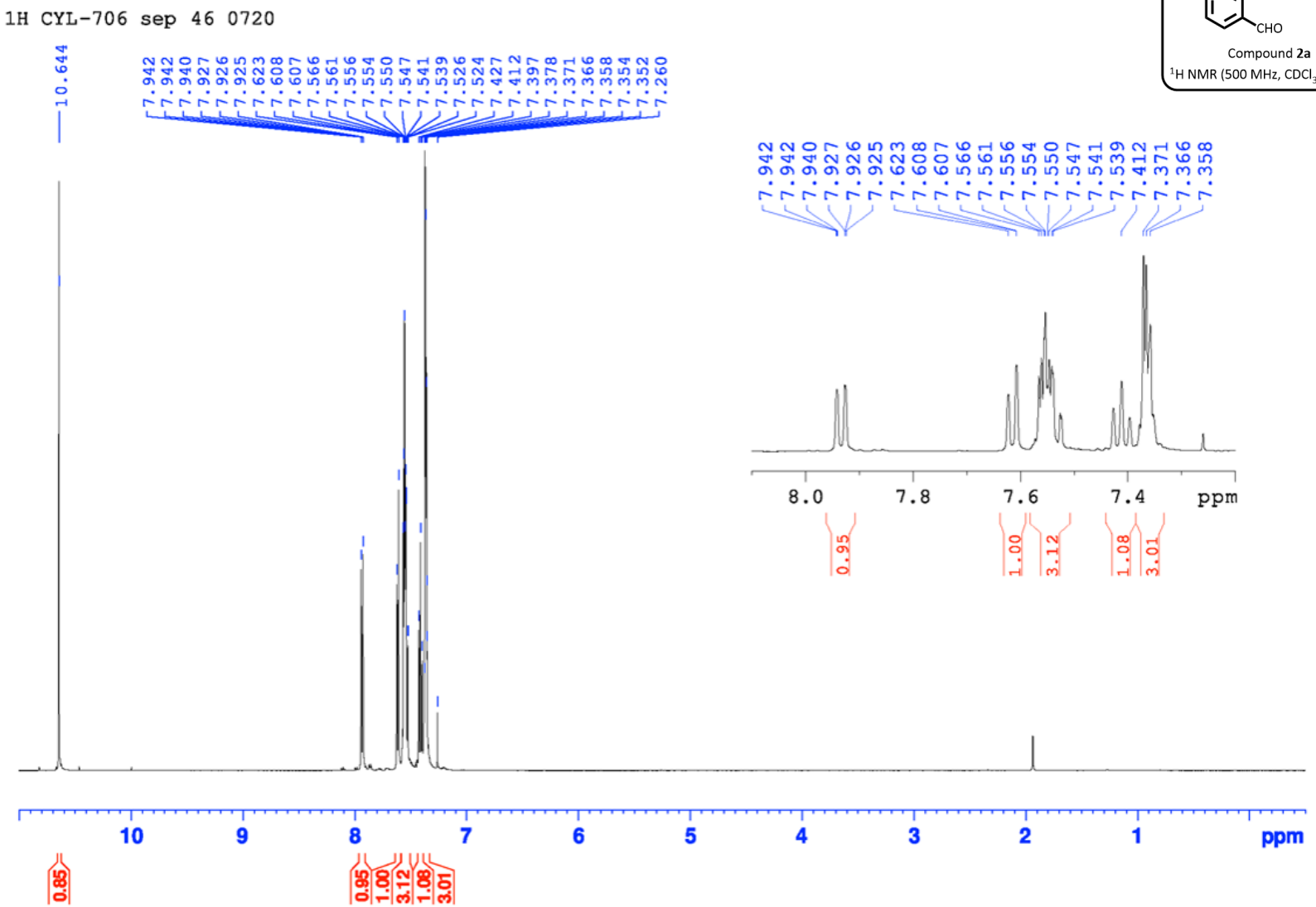
Crystal data and structure refinement for compound **1e**
(the thermal ellipsoid was drawn at the 50% probability level)



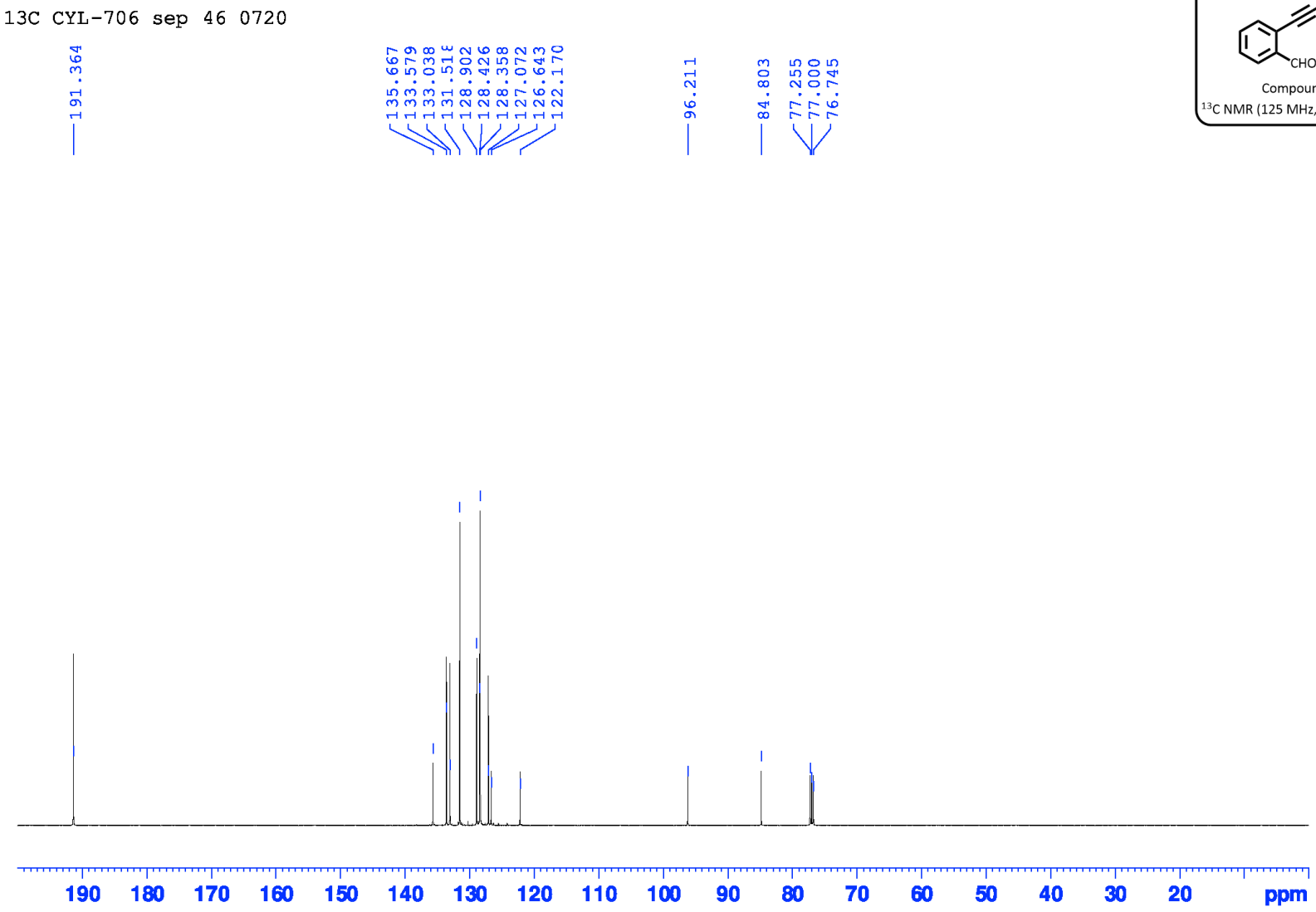
Identification code	i18491	
Empirical formula	C16 H13 N O	
Formula weight	235.27	
Temperature	100.0(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 12.0705(2) Å	α= 90°.
	b = 7.47590(10) Å	β= 97.4090(10)°.
	c = 26.1572(4) Å	γ = 90°.
Volume	2340.66(6) Å^3	
Z, Density (calculated)	8, 1.335 Mg/m^3	
Absorption coefficient	0.658 mm^{-1}	
F(000)	992	
Crystal size	0.120 x 0.101 x 0.094 mm^3	
Theta range for data collection	3.408 to 72.548°.	
Index ranges	-14<=h<=14, -8<=k<=9, -32<=l<=31	
Reflections collected	56392	
Independent reflections	4631 [R(int) = 0.0907]	
Completeness to theta = 67.679°	99.9 %	
Absorption correction	Numerical	
Max. and min. transmission	1 and 0.8211	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4631 / 0 / 327	
Goodness-of-fit on F^2	1.059	
Final R indices [I>2sigma(I)]	R1 = 0.0473, wR2 = 0.1201	
R indices (all data)	R1 = 0.0833, wR2 = 0.1289	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.412 and -0.194 e.Å^{-3}	

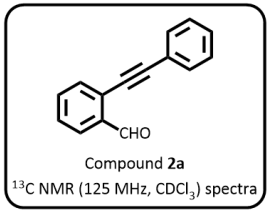
The ^{1}H NMR spectrum in $CDCl_3$ of compound 2a



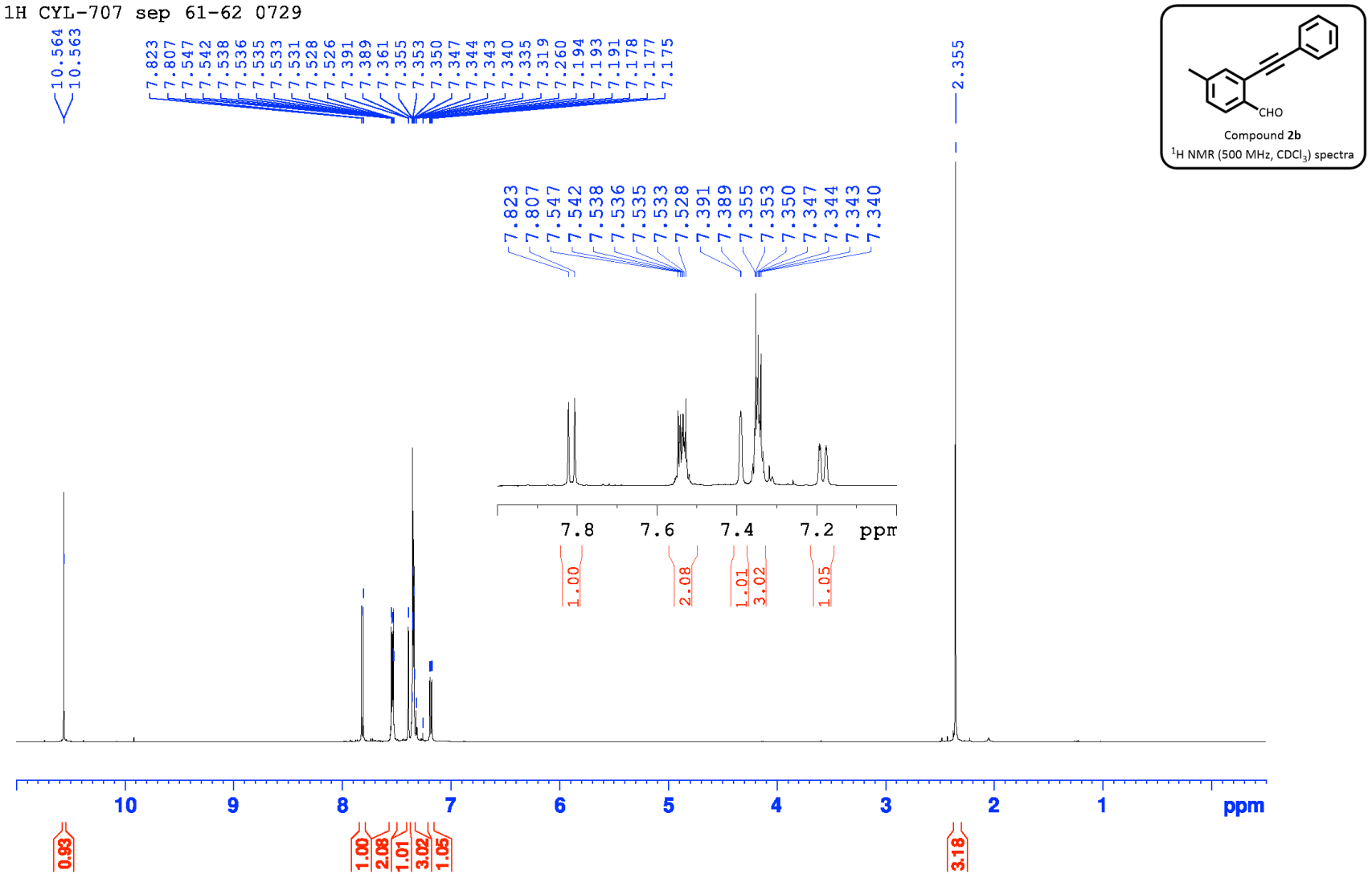


The ^{13}C NMR spectrum in $CDCl_3$ of compound 2a

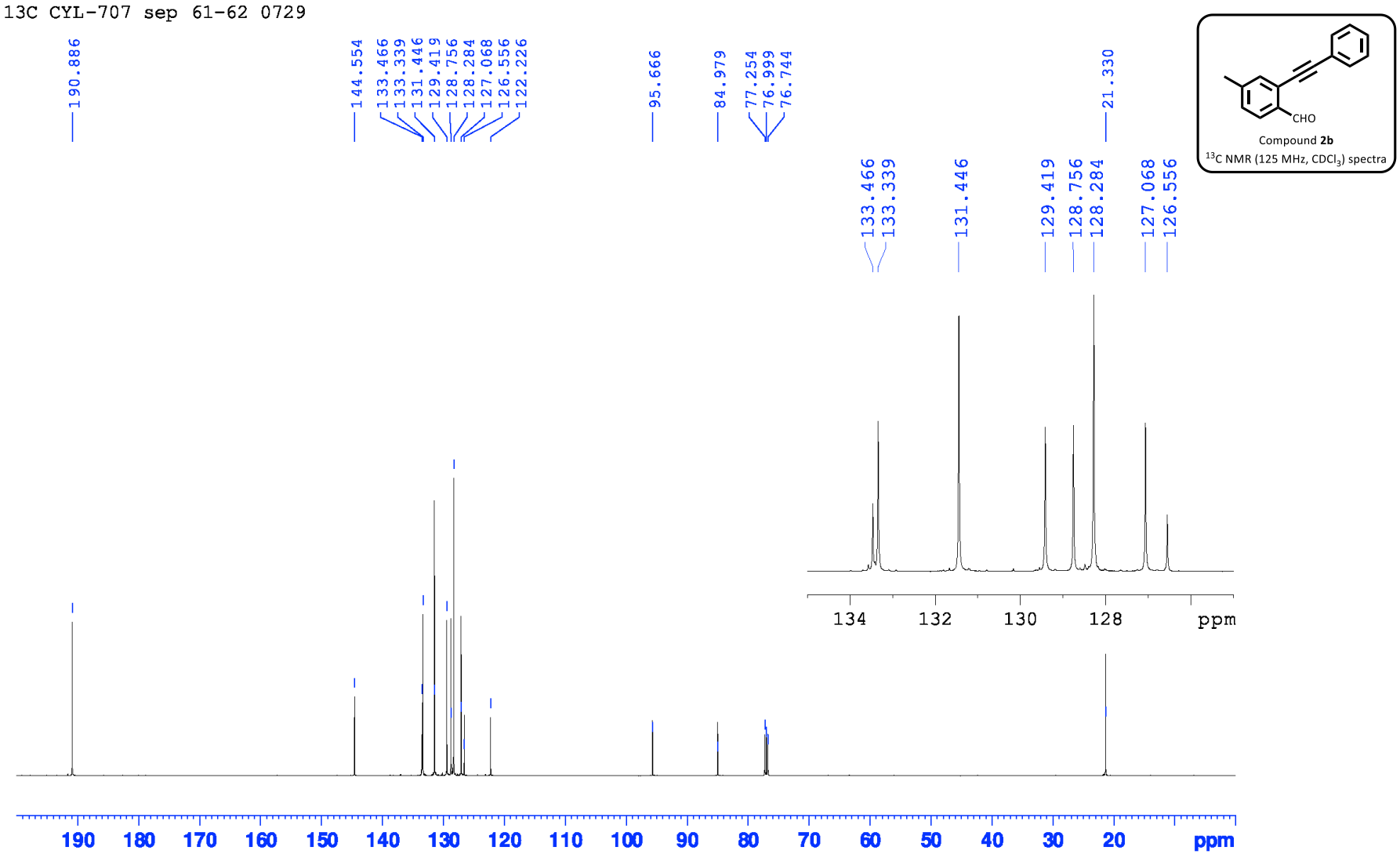




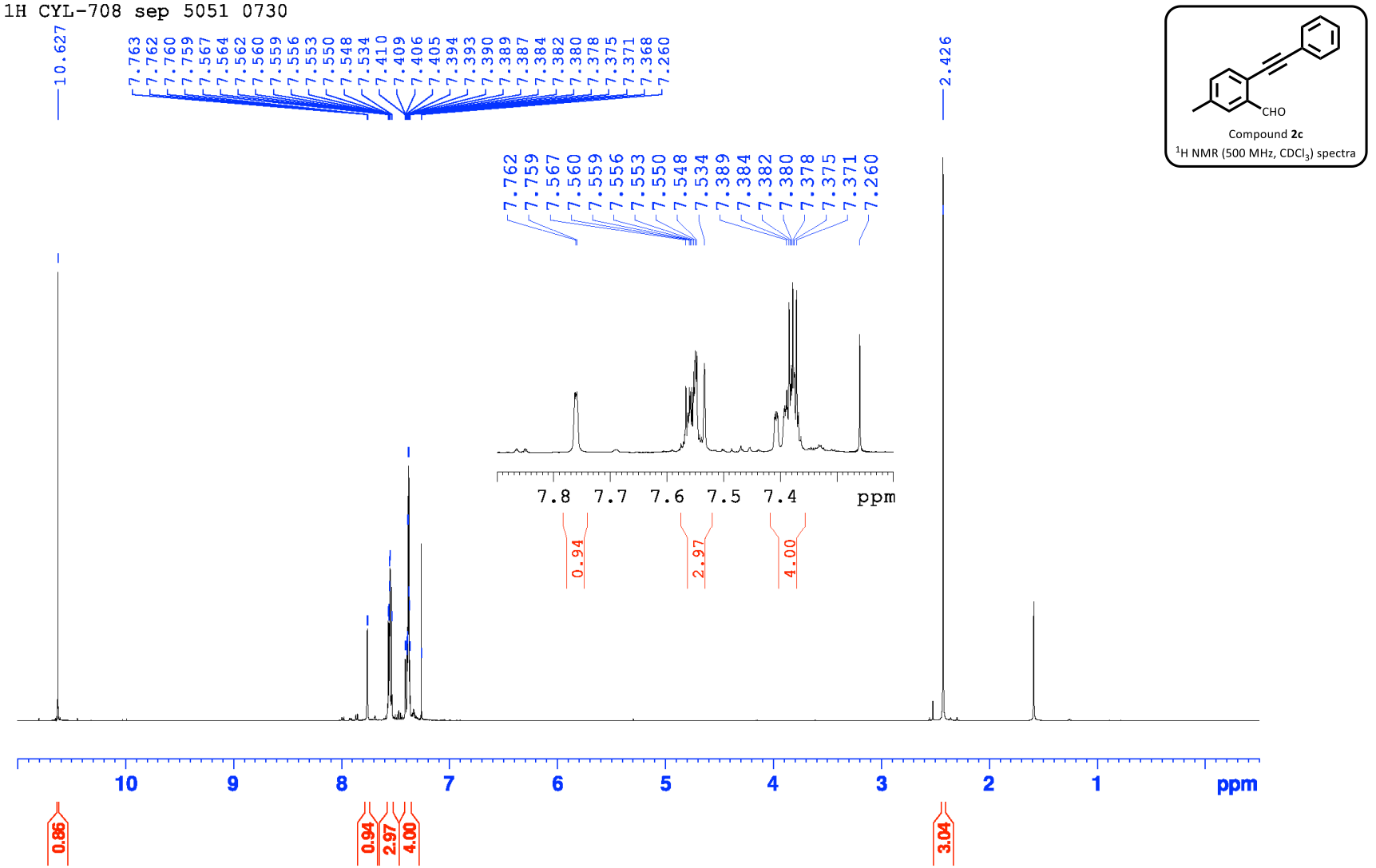
The ^{1}H NMR spectrum in $CDCl_3$ of compound 2b



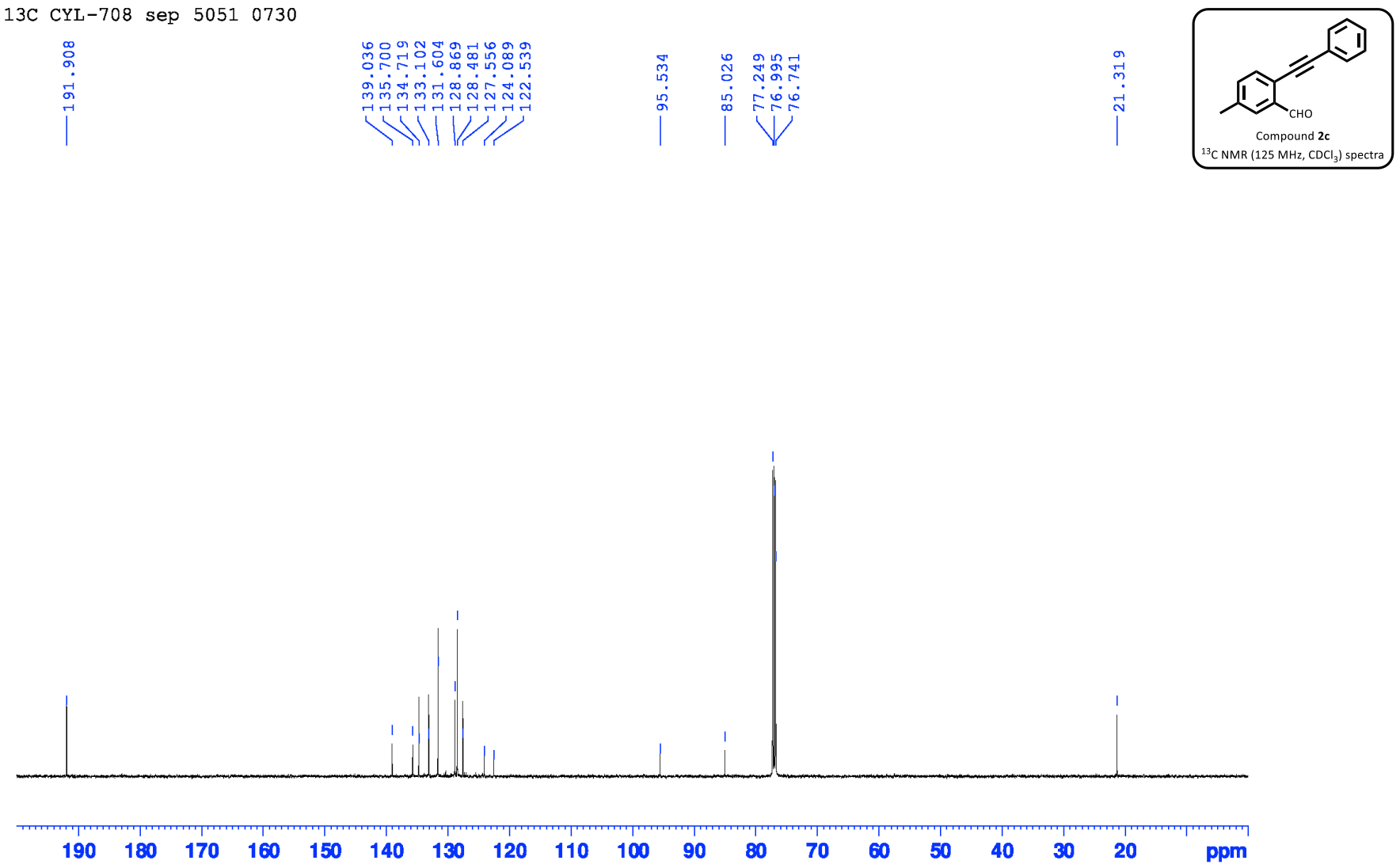
The ^{13}C NMR spectrum in $CDCl_3$ of compound 2b



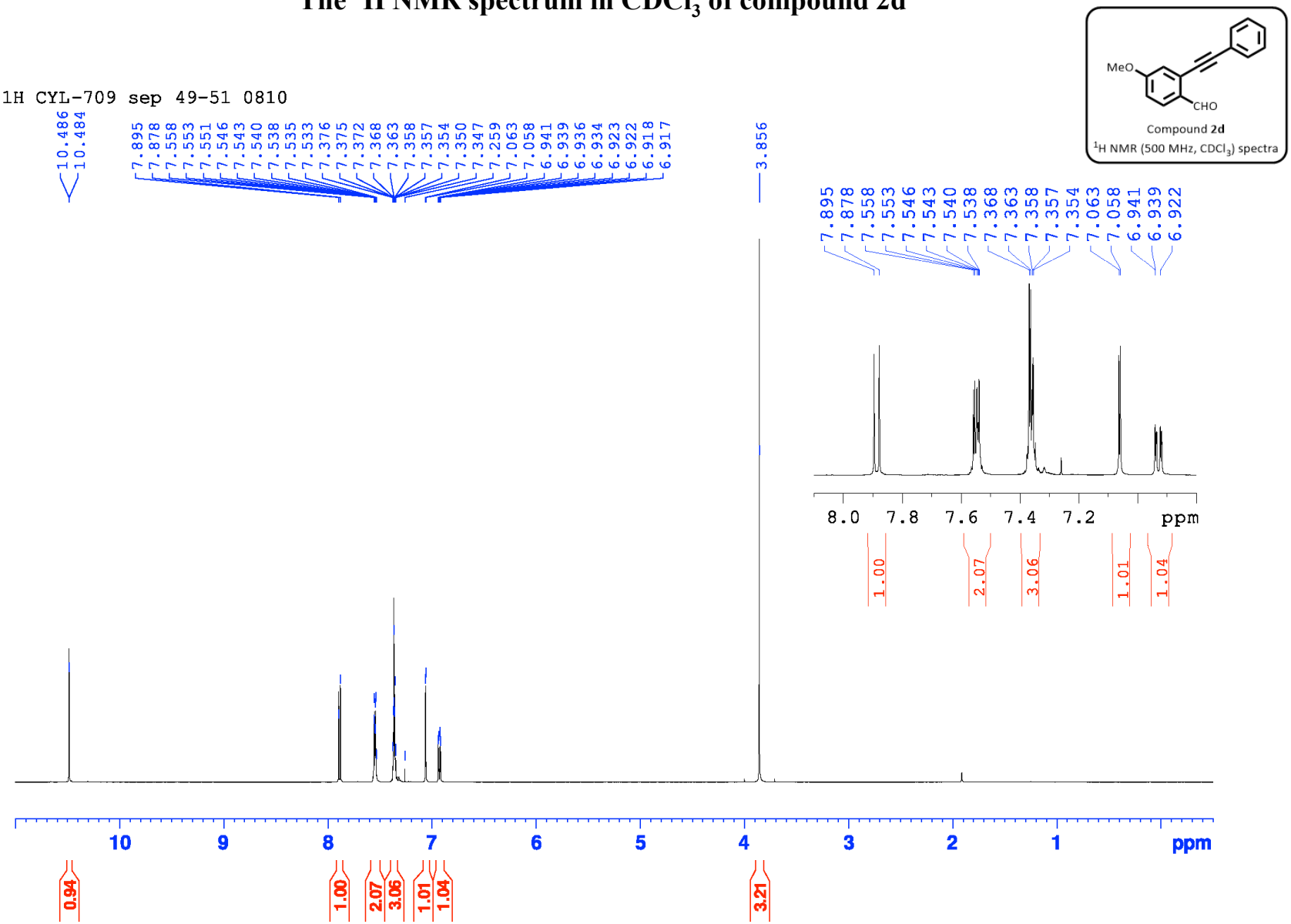
The ^{1}H NMR spectrum in $CDCl_3$ of compound 2c



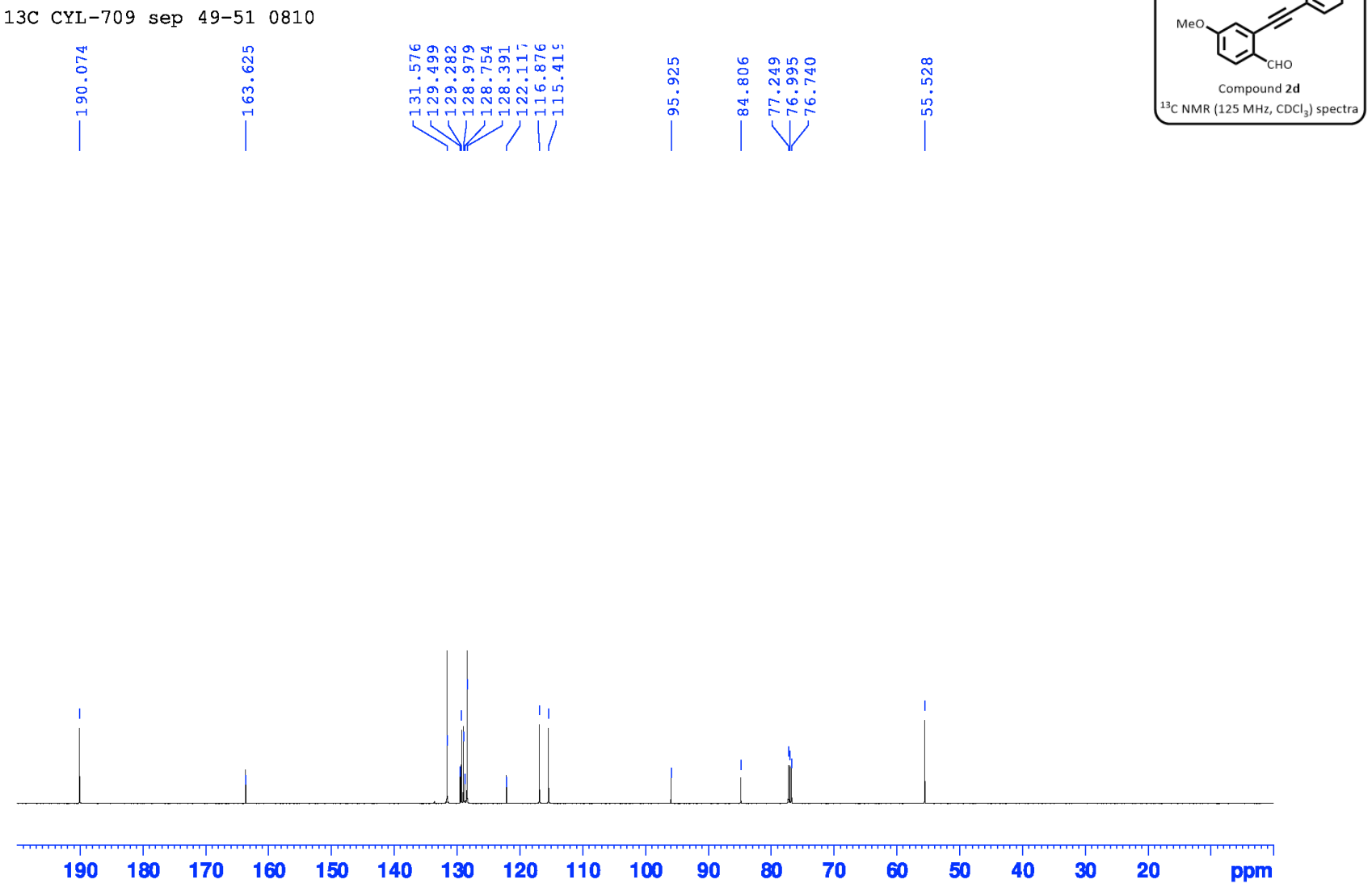
The ^{13}C NMR spectrum in $CDCl_3$ of compound 2c



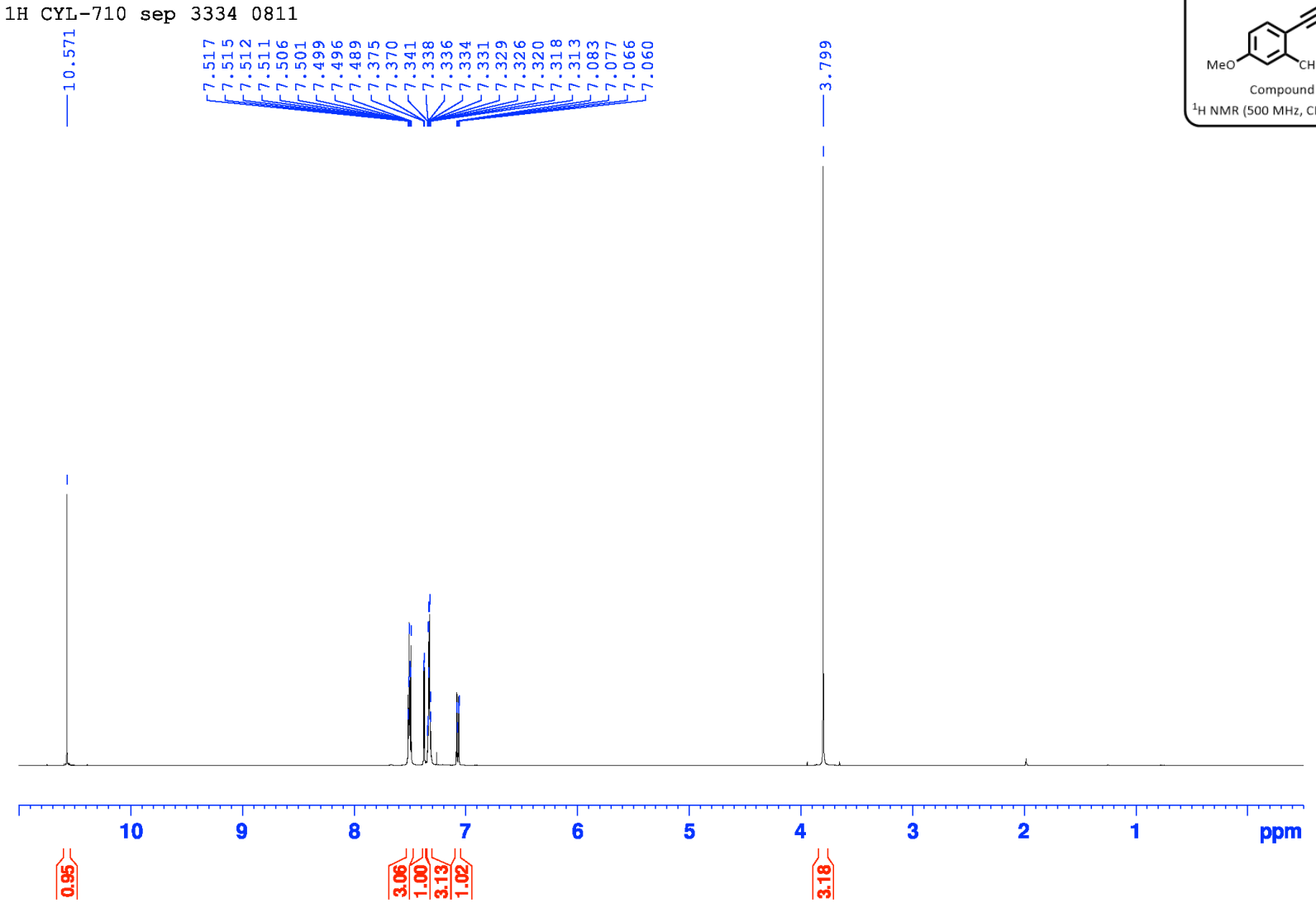
The ^{1}H NMR spectrum in $CDCl_3$ of compound 2d

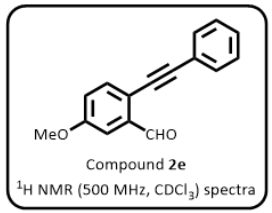


The ^{13}C NMR spectrum in $CDCl_3$ of compound 2d

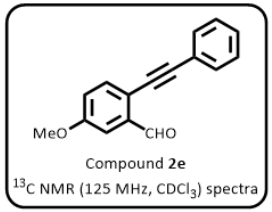


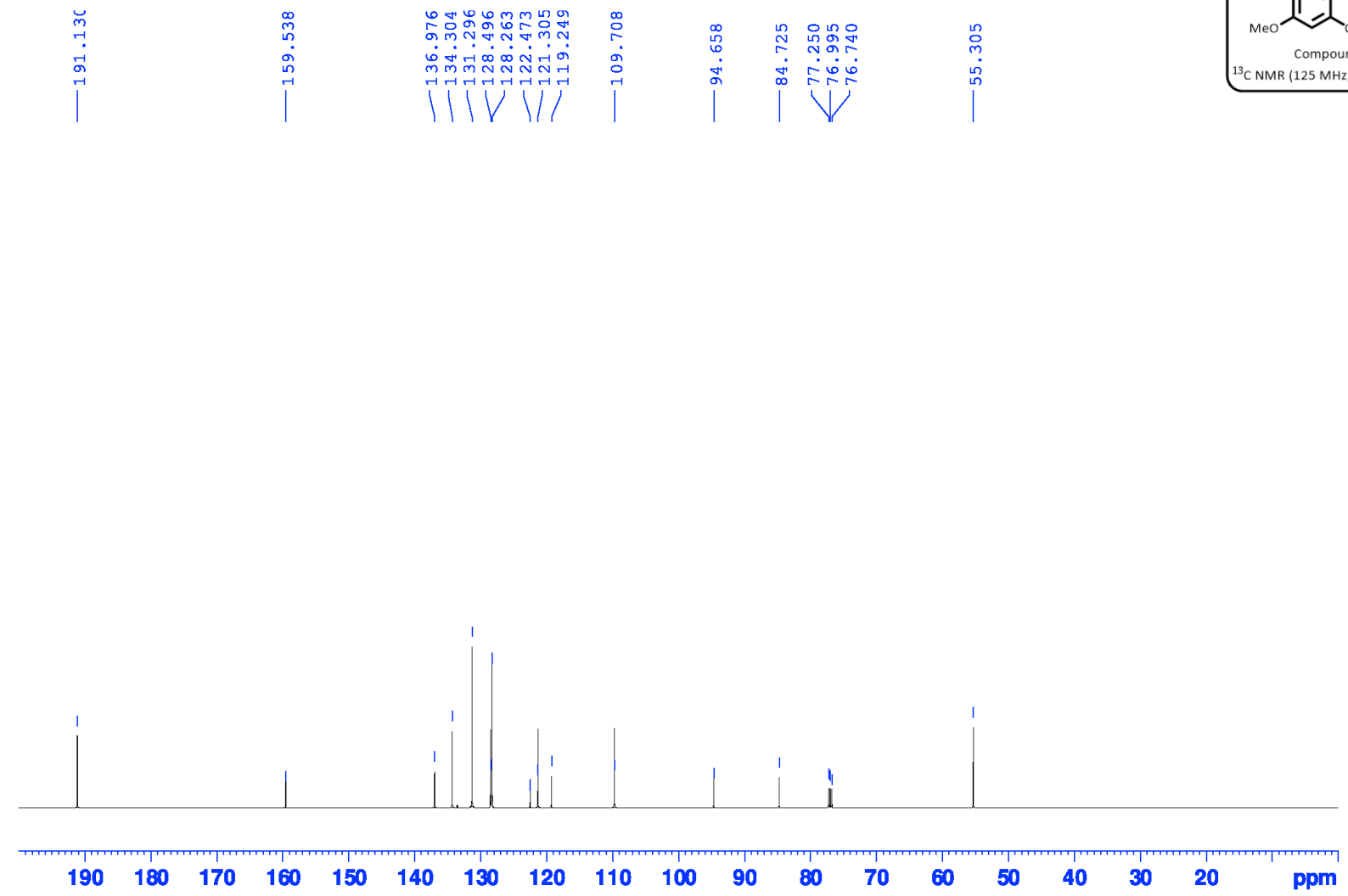
The ^{1}H NMR spectrum in $CDCl_3$ of compound 2e.



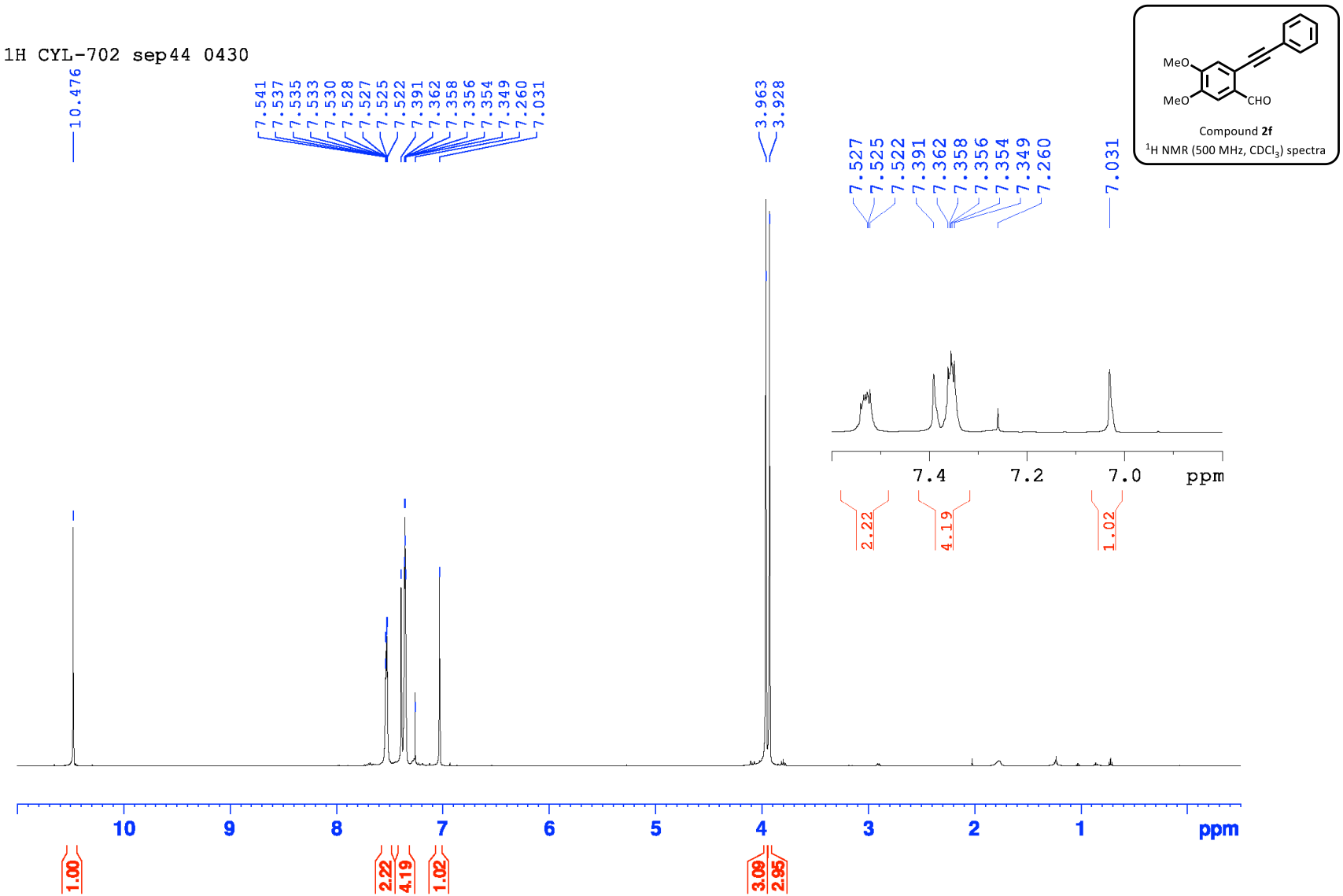


The ^{13}C NMR spectrum in $CDCl_3$ of compound 2e.

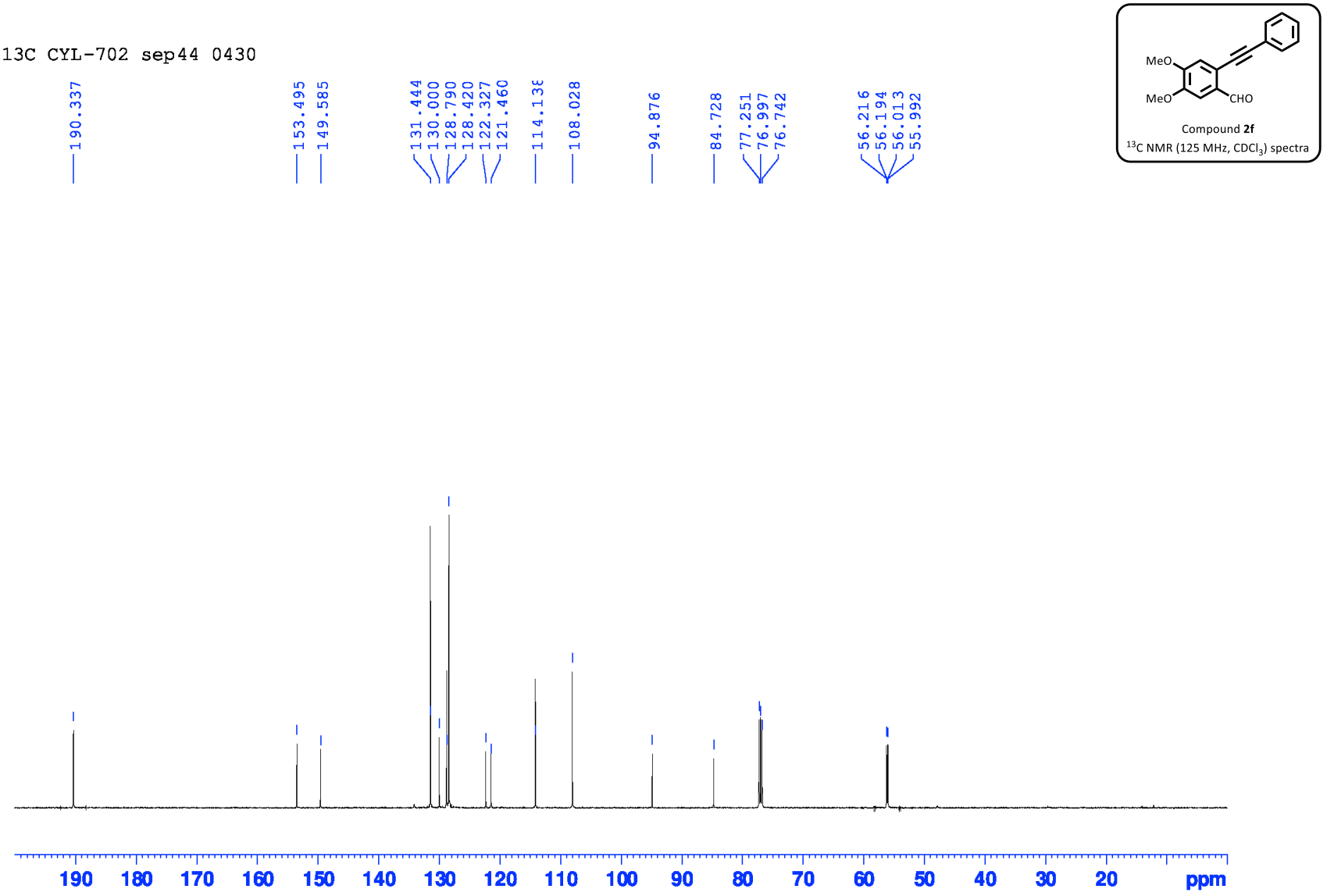




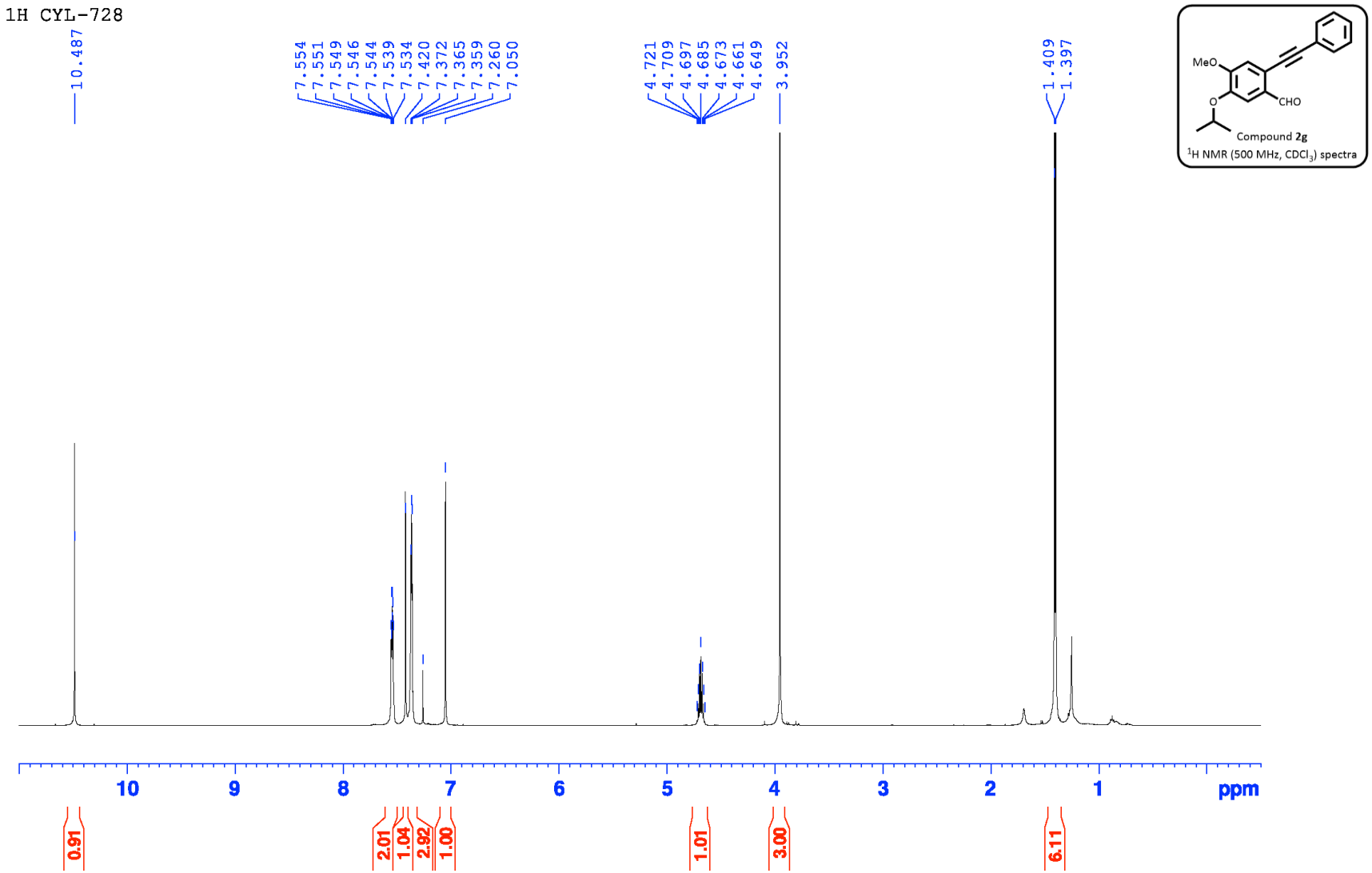
The ^{1}H NMR spectrum in $CDCl_3$ of compound 2f.



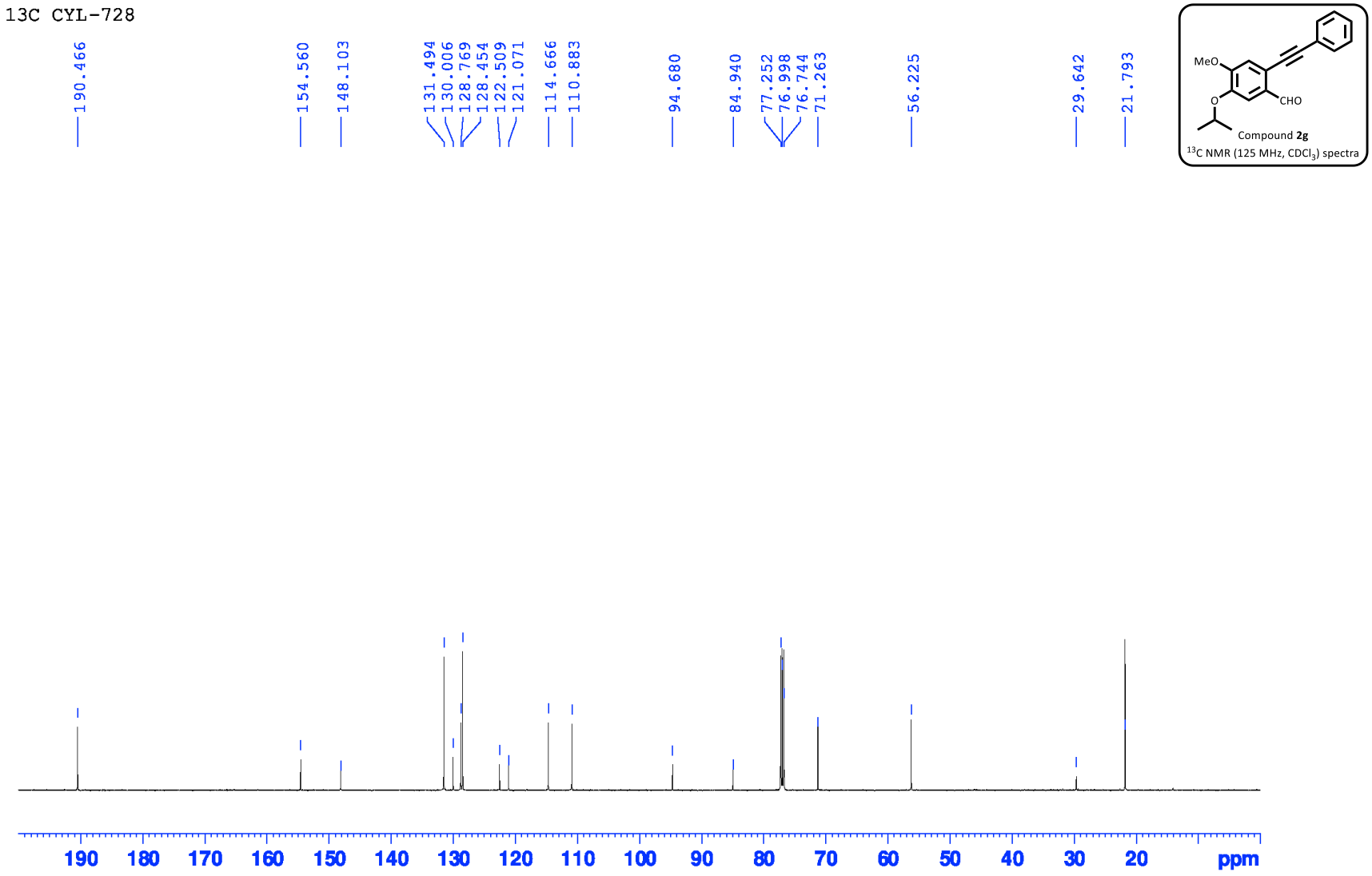
The ^{13}C NMR spectrum in $CDCl_3$ of compound 2f.



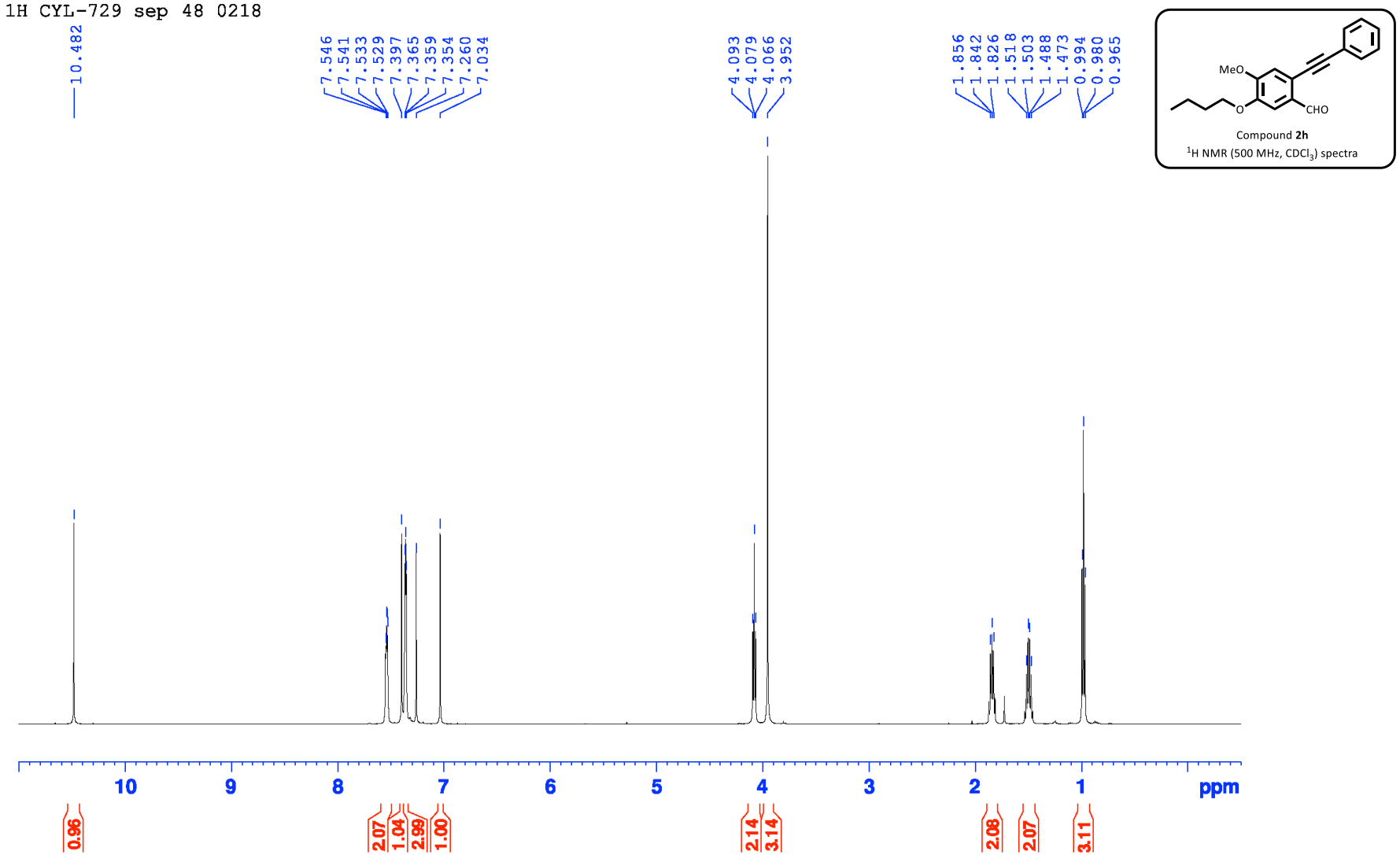
The ^{1}H NMR spectrum in $CDCl_3$ of compound 2g.



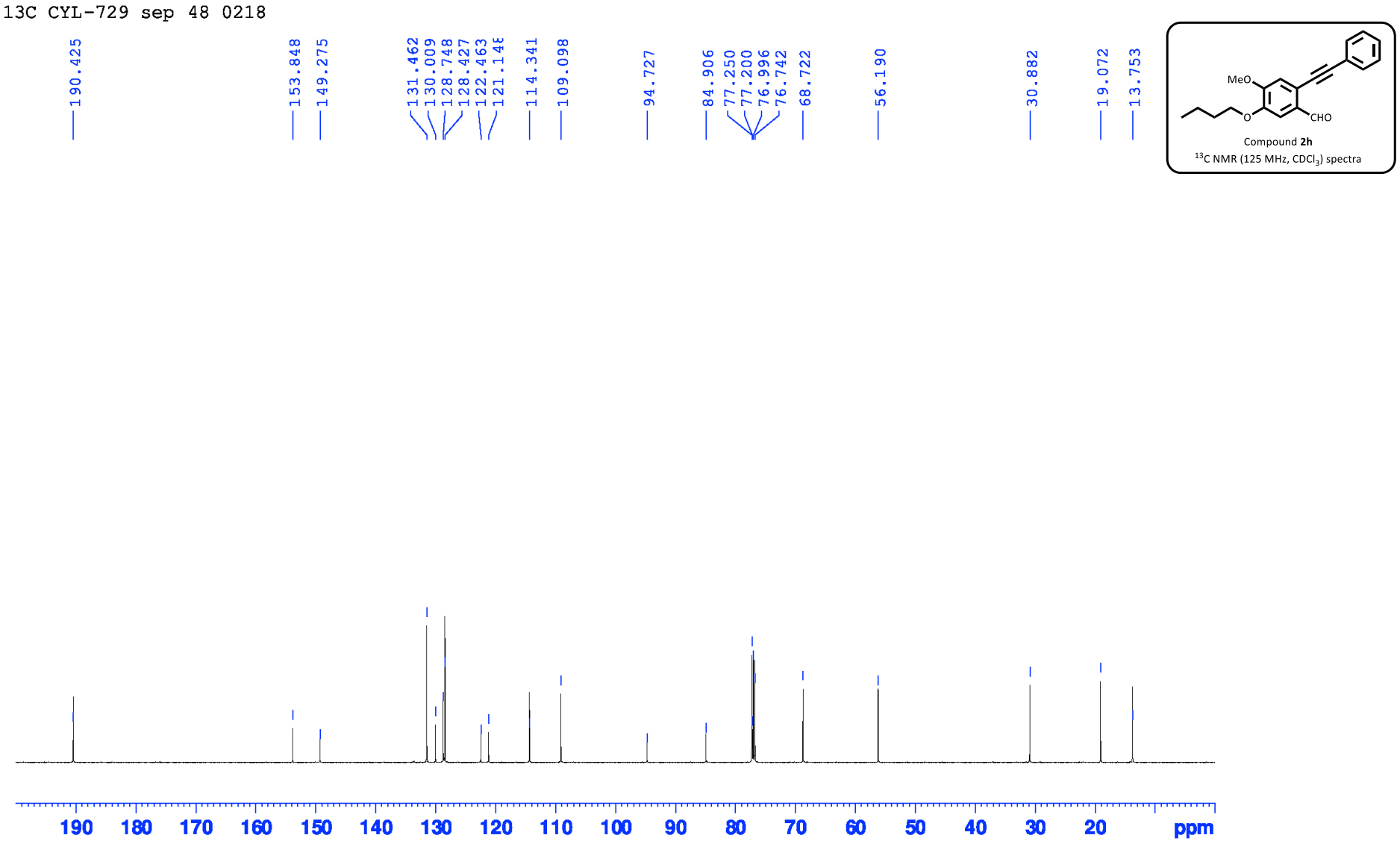
The ^{13}C NMR spectrum in $CDCl_3$ of compound 2g.



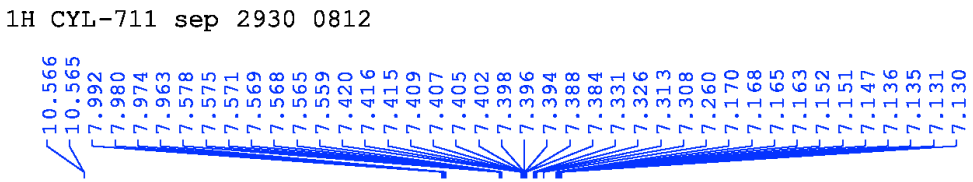
The ^{1}H NMR spectrum in $CDCl_3$ of compound 2h.

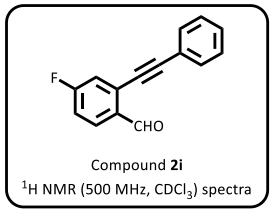


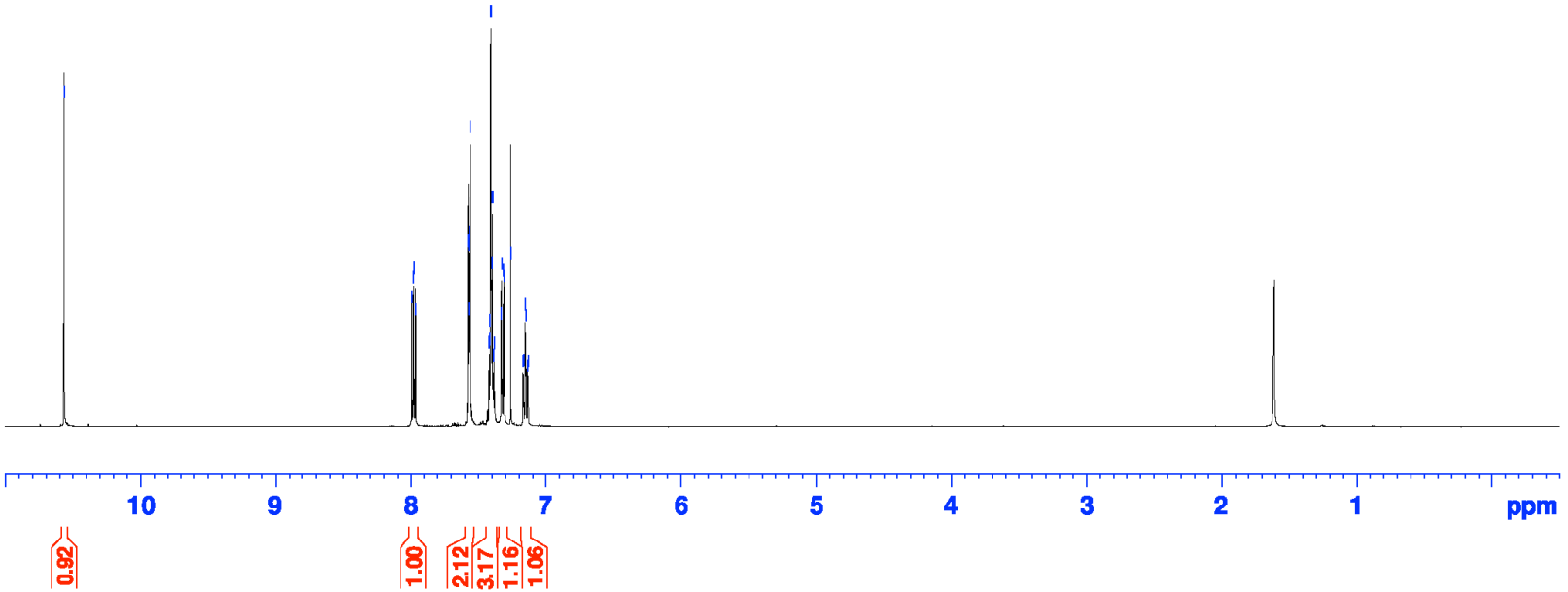
The ^{13}C NMR spectrum in $CDCl_3$ of compound 2h.



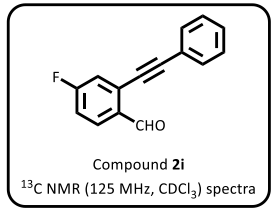
The ^{1}H NMR spectrum in $CDCl_3$ of compound 2i.

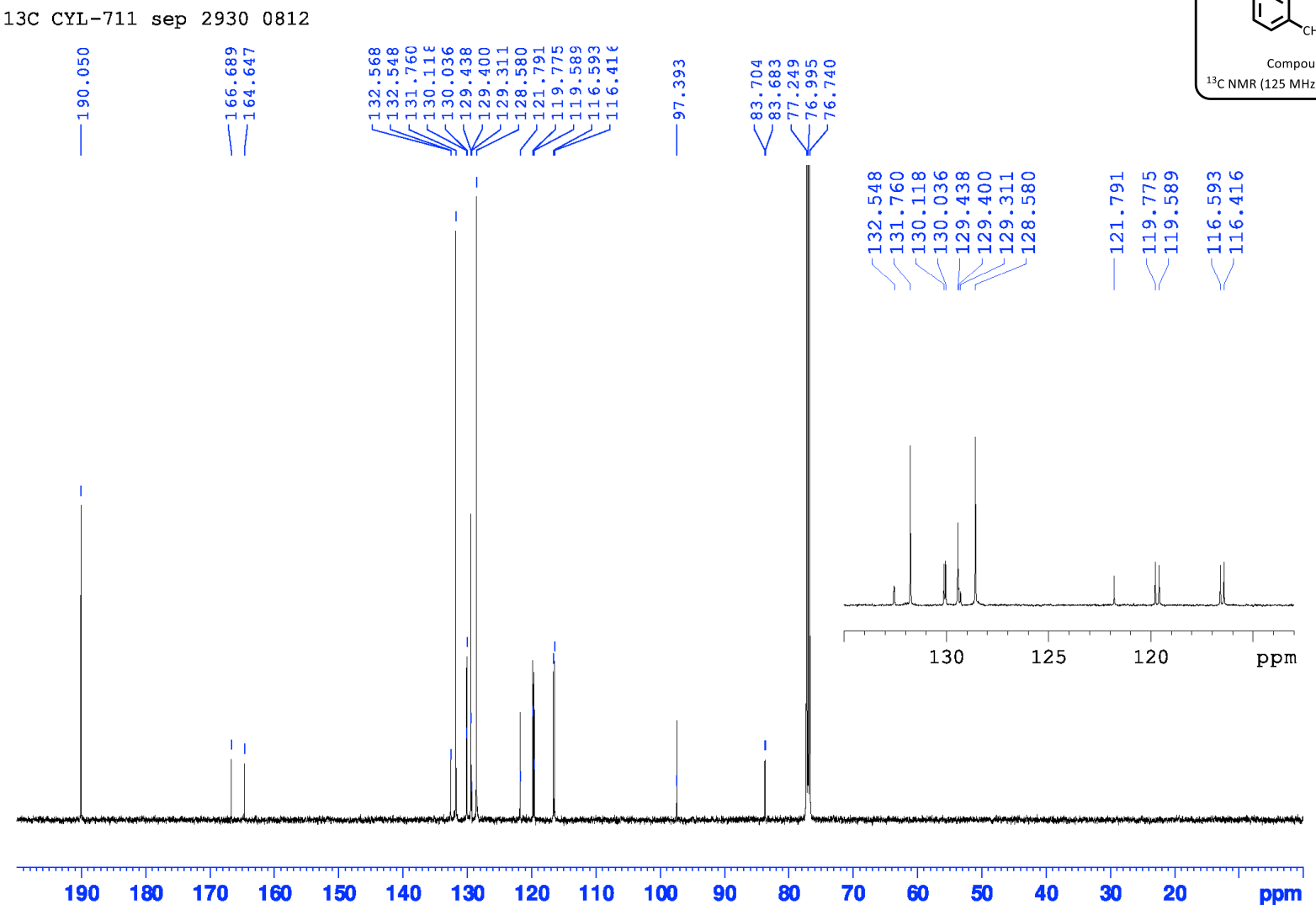




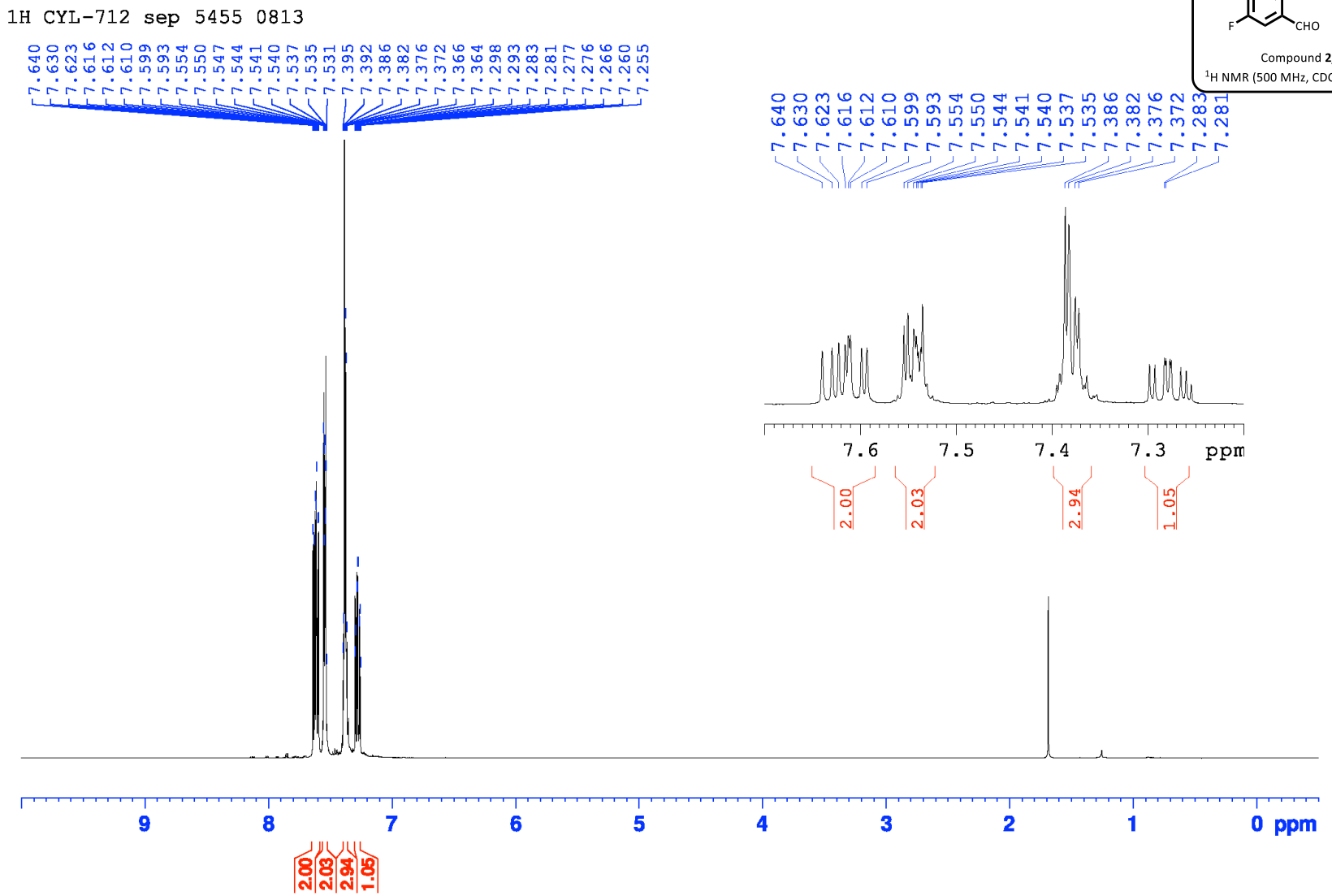


The ^{13}C NMR spectrum in $CDCl_3$ of compound 2i.

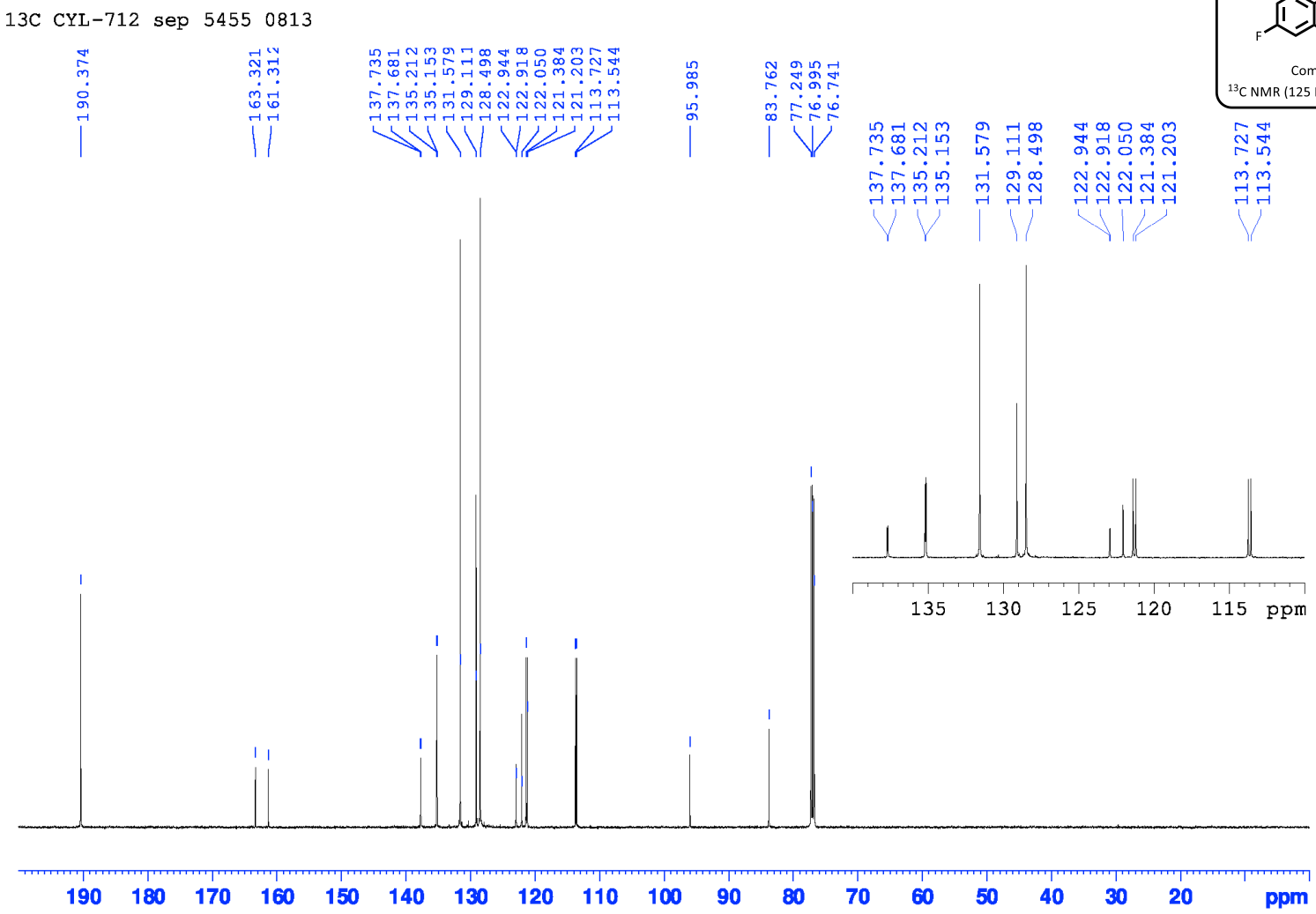




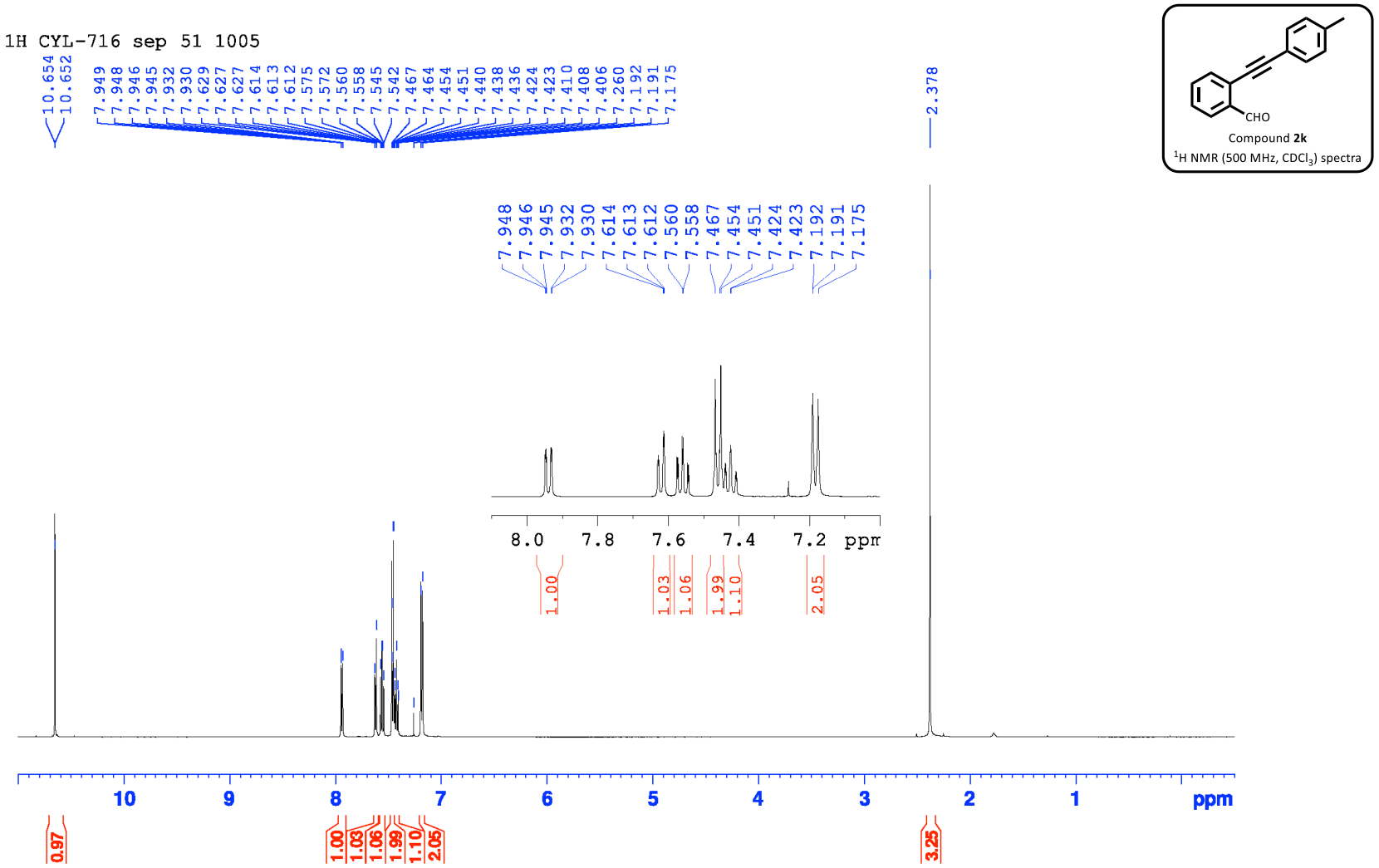
The ^{1}H NMR spectrum in $CDCl_3$ of compound 2j.



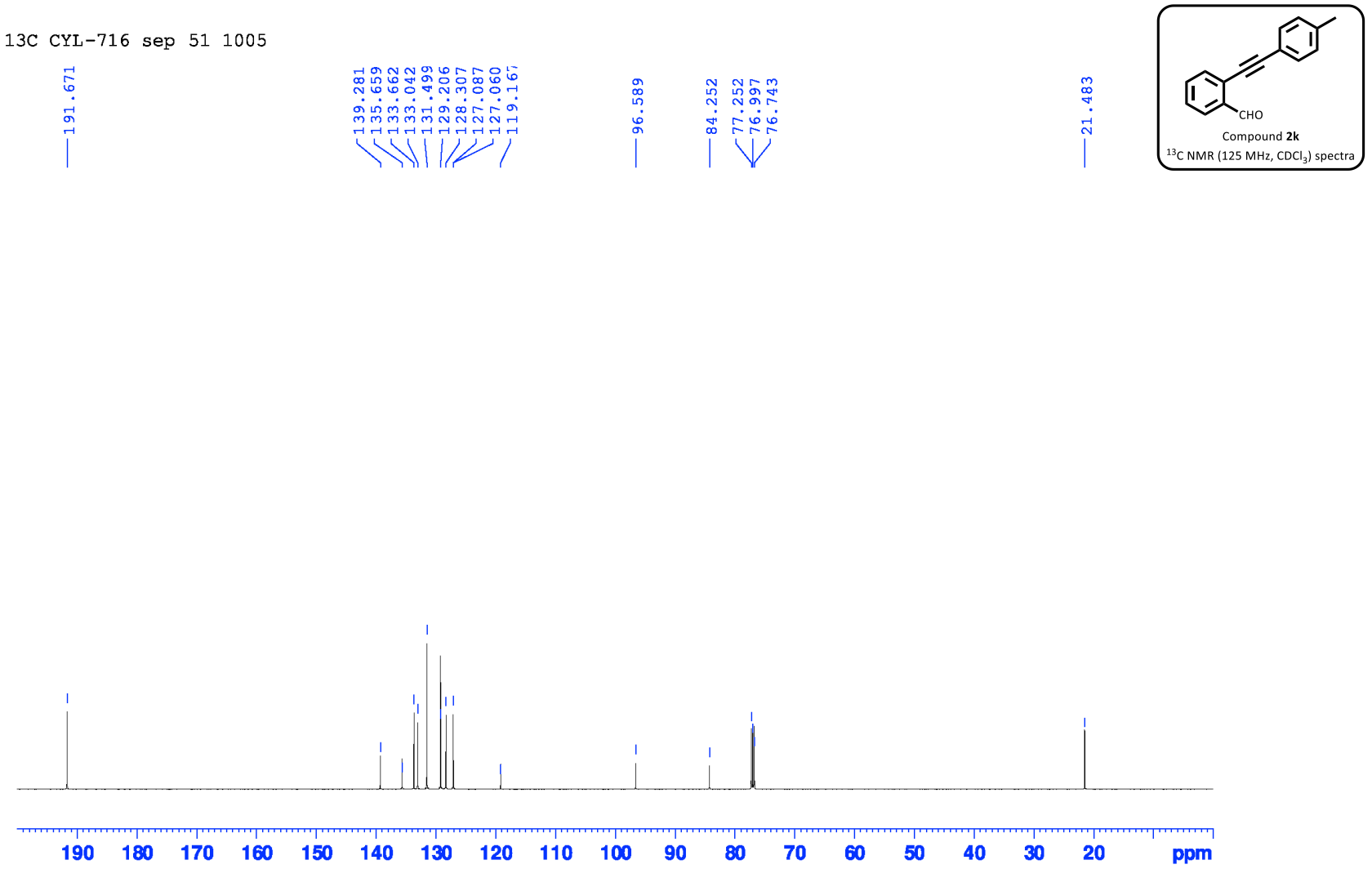
The ^{13}C NMR spectrum in $CDCl_3$ of compound 2j.



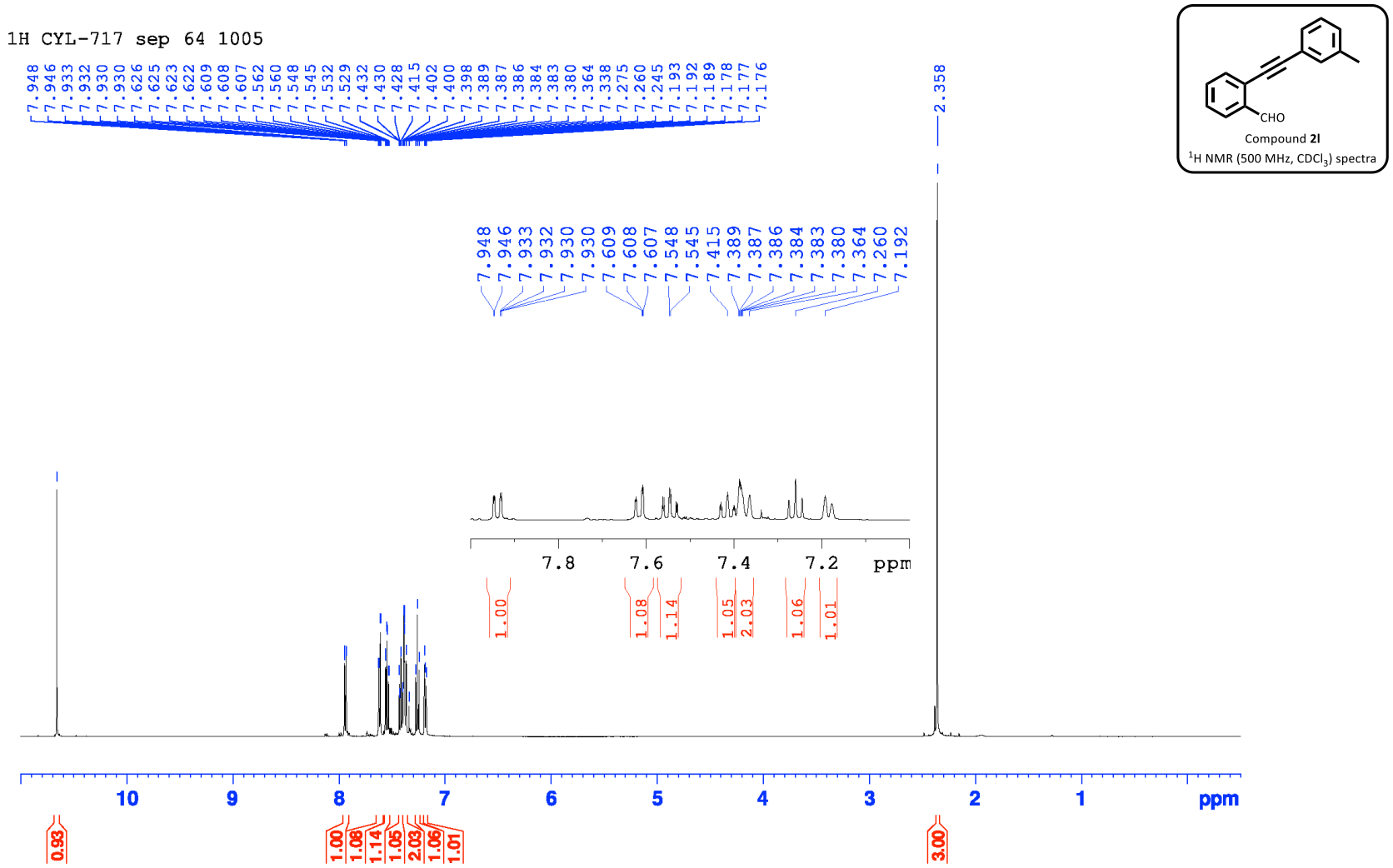
The ^{1}H NMR spectrum in $CDCl_3$ of compound 2k.



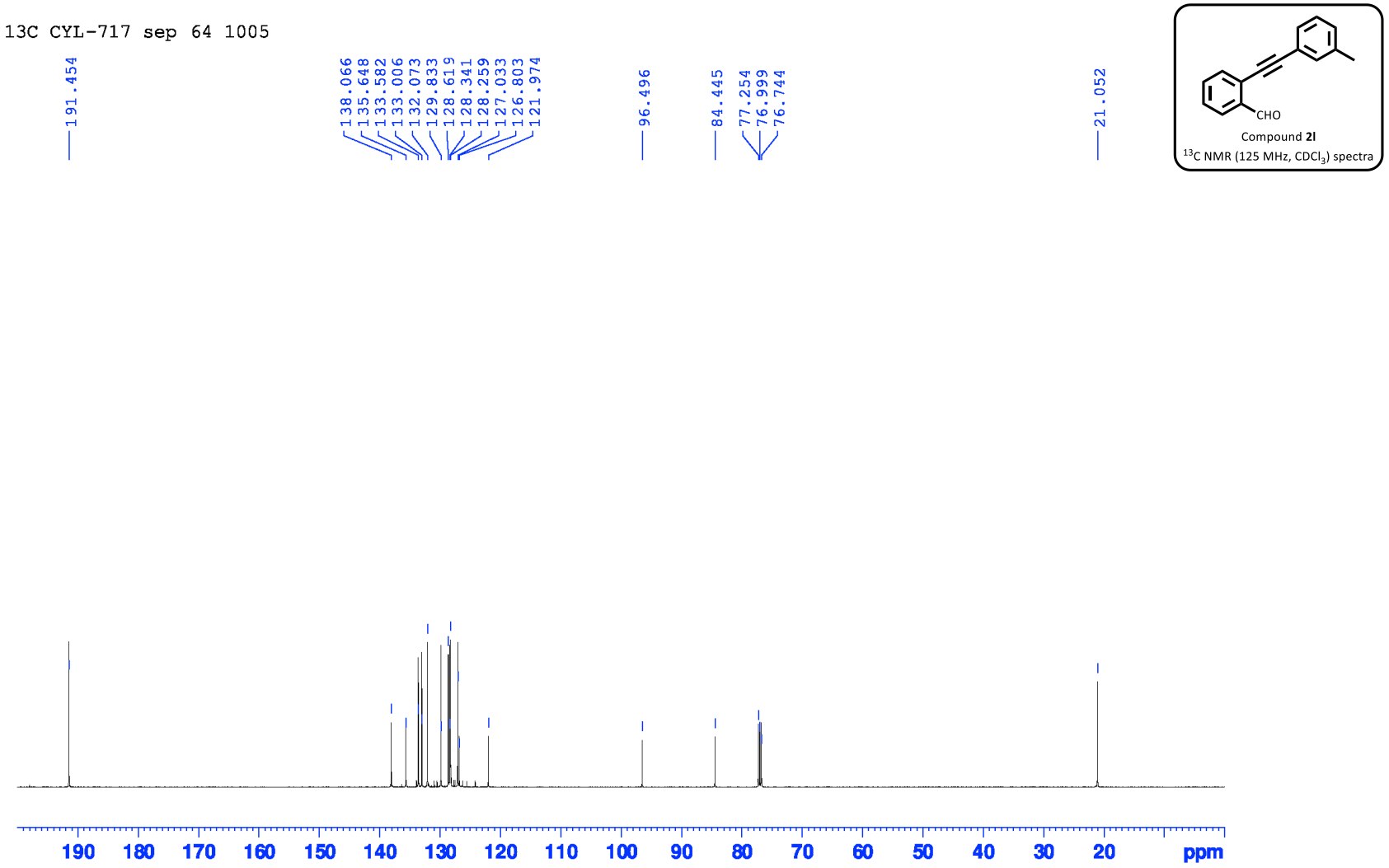
The ^{13}C NMR spectrum in $CDCl_3$ of compound 2k.



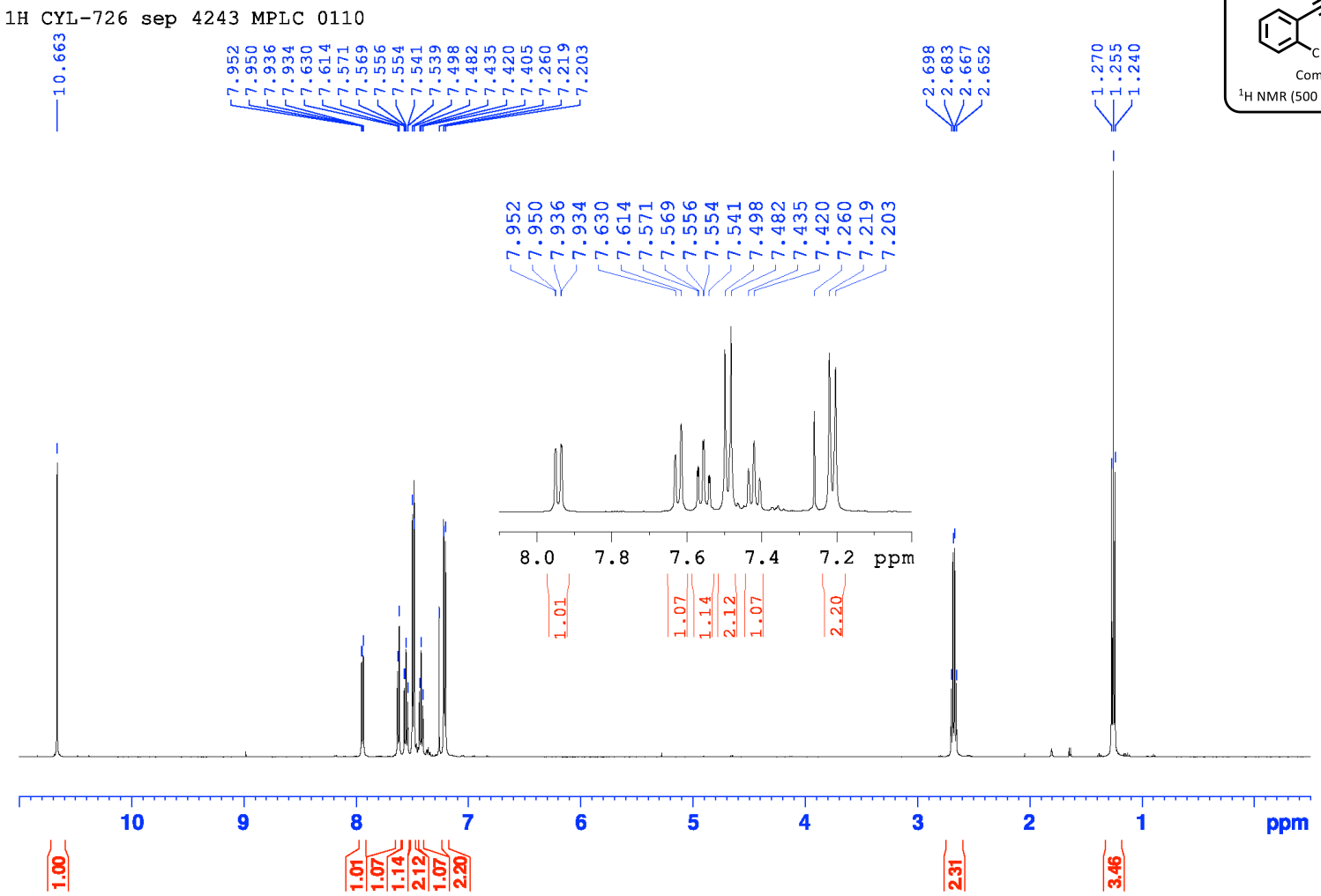
The ^{1}H NMR spectrum in $CDCl_3$ of compound 2l.

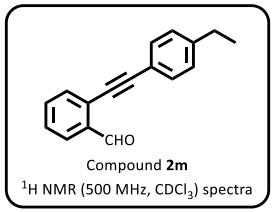


The ^{13}C NMR spectrum in $CDCl_3$ of compound 2l.

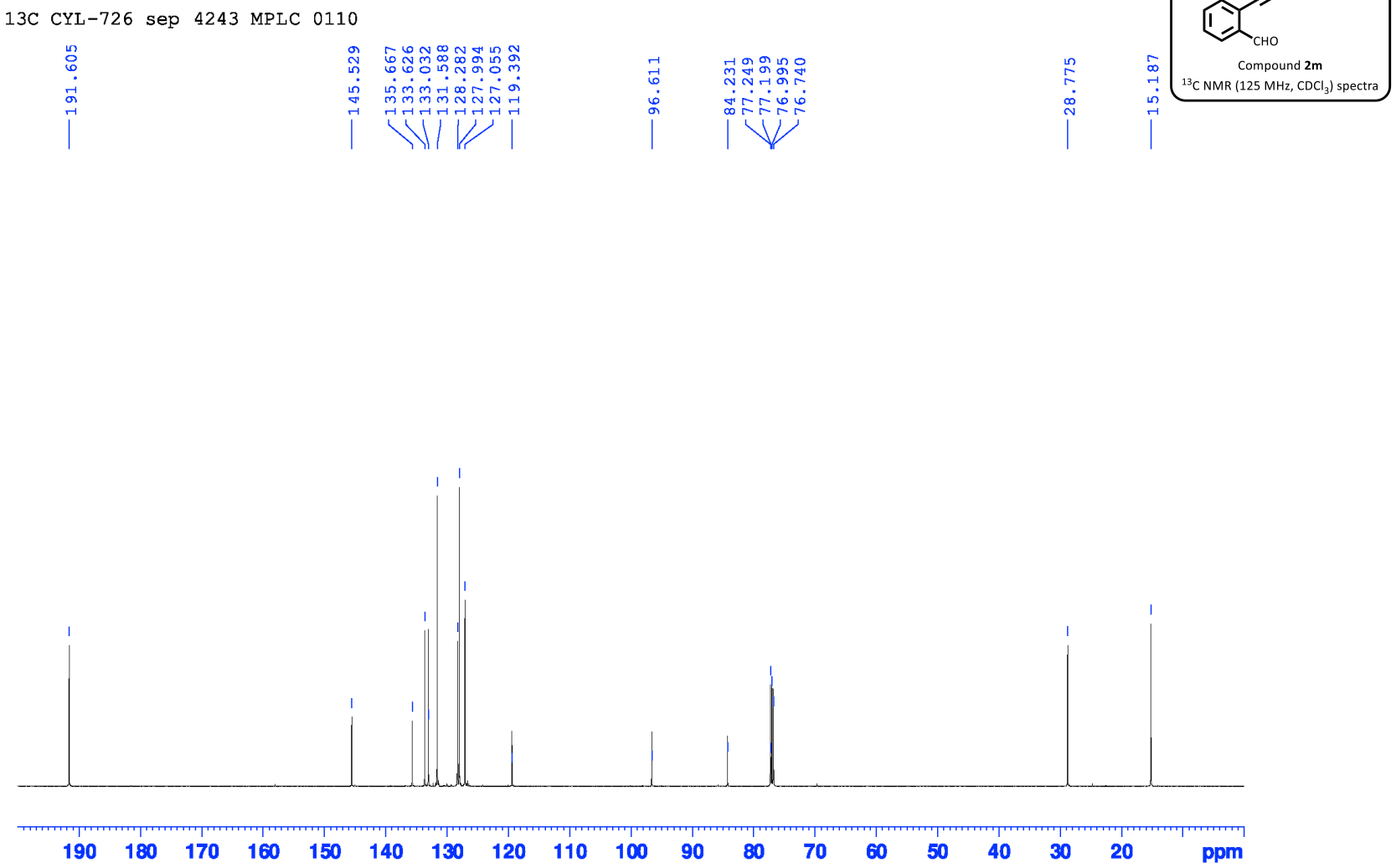


The ^{1}H NMR spectrum in $CDCl_3$ of compound 2m.

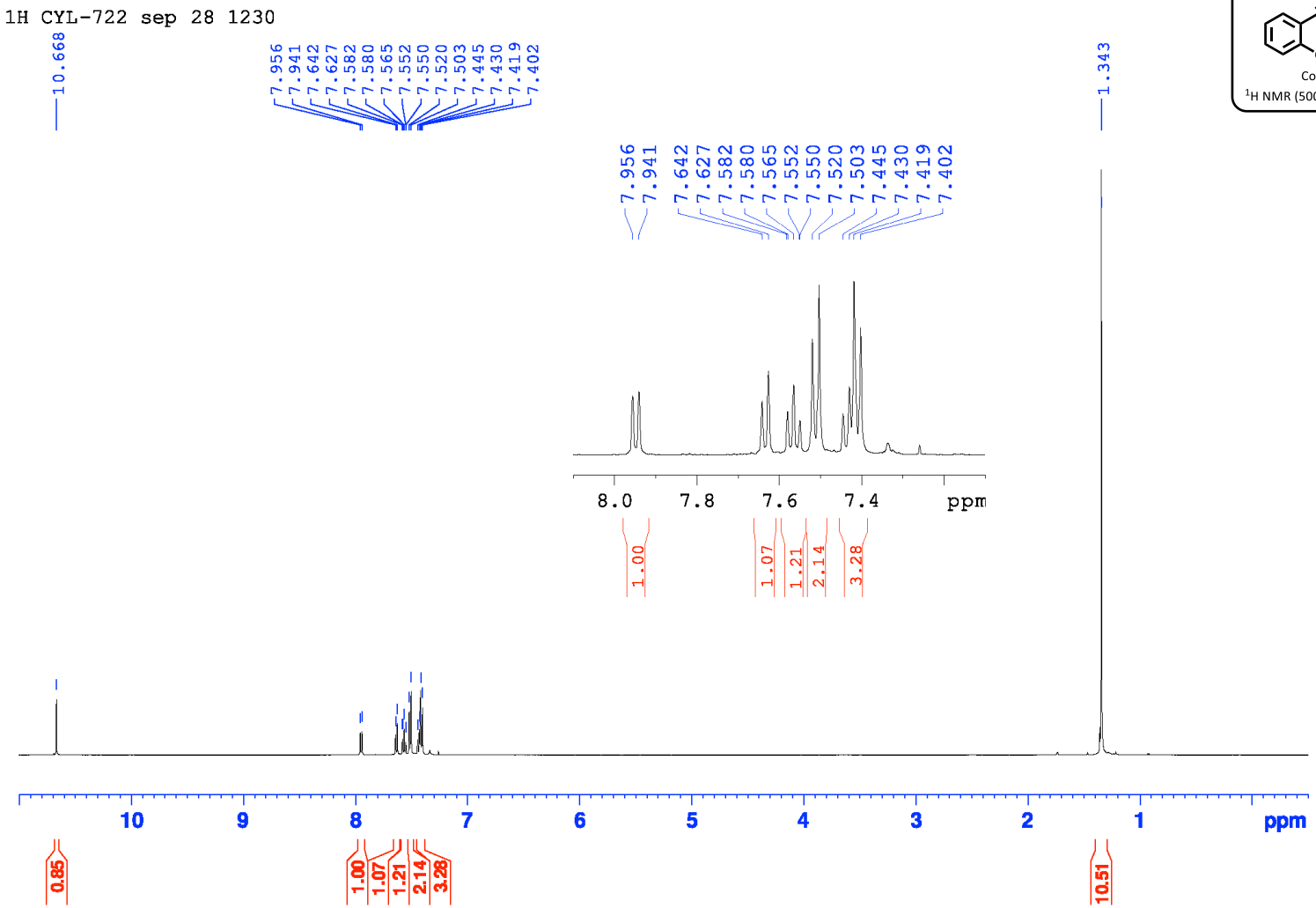


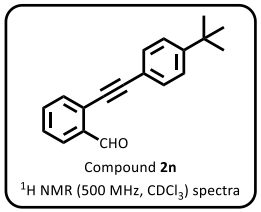


The ^{13}C NMR spectrum in $CDCl_3$ of compound 2m.

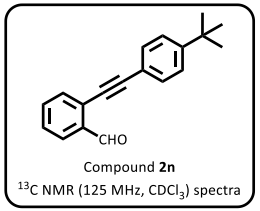


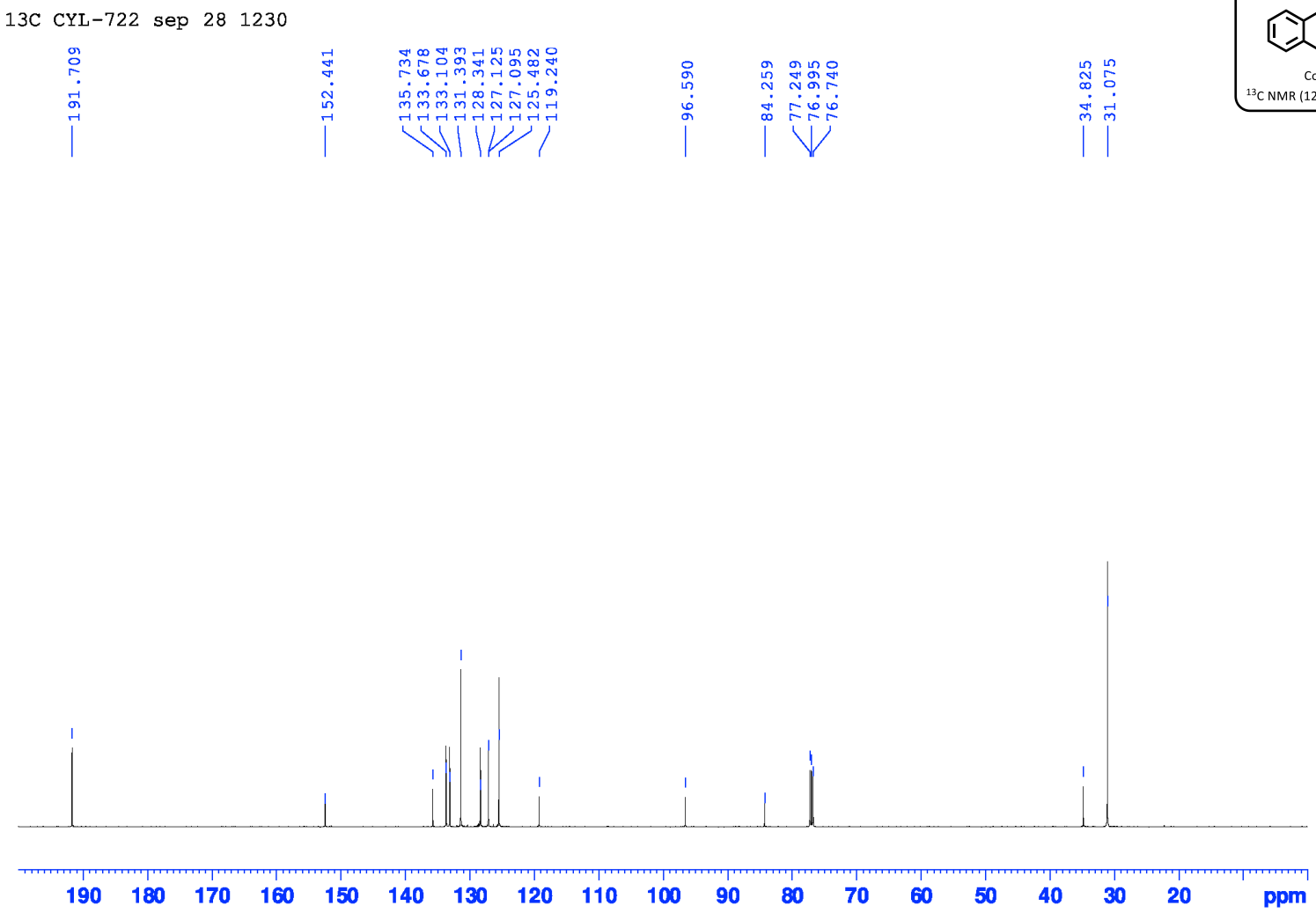
The ^{1}H NMR spectrum in $CDCl_3$ of compound 2n.



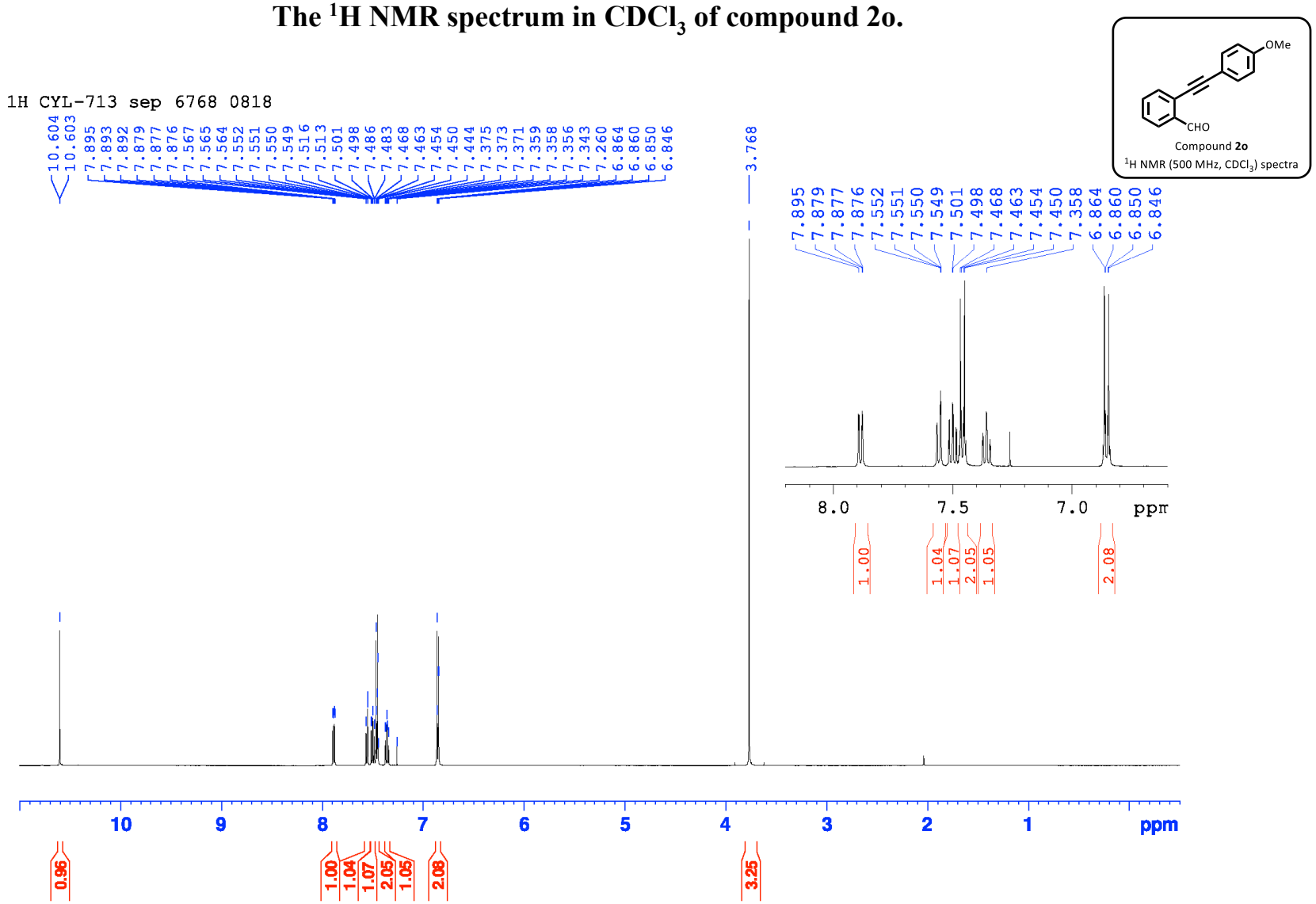


The ^{13}C NMR spectrum in $CDCl_3$ of Compound 2n.

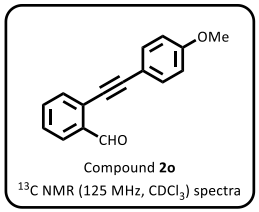


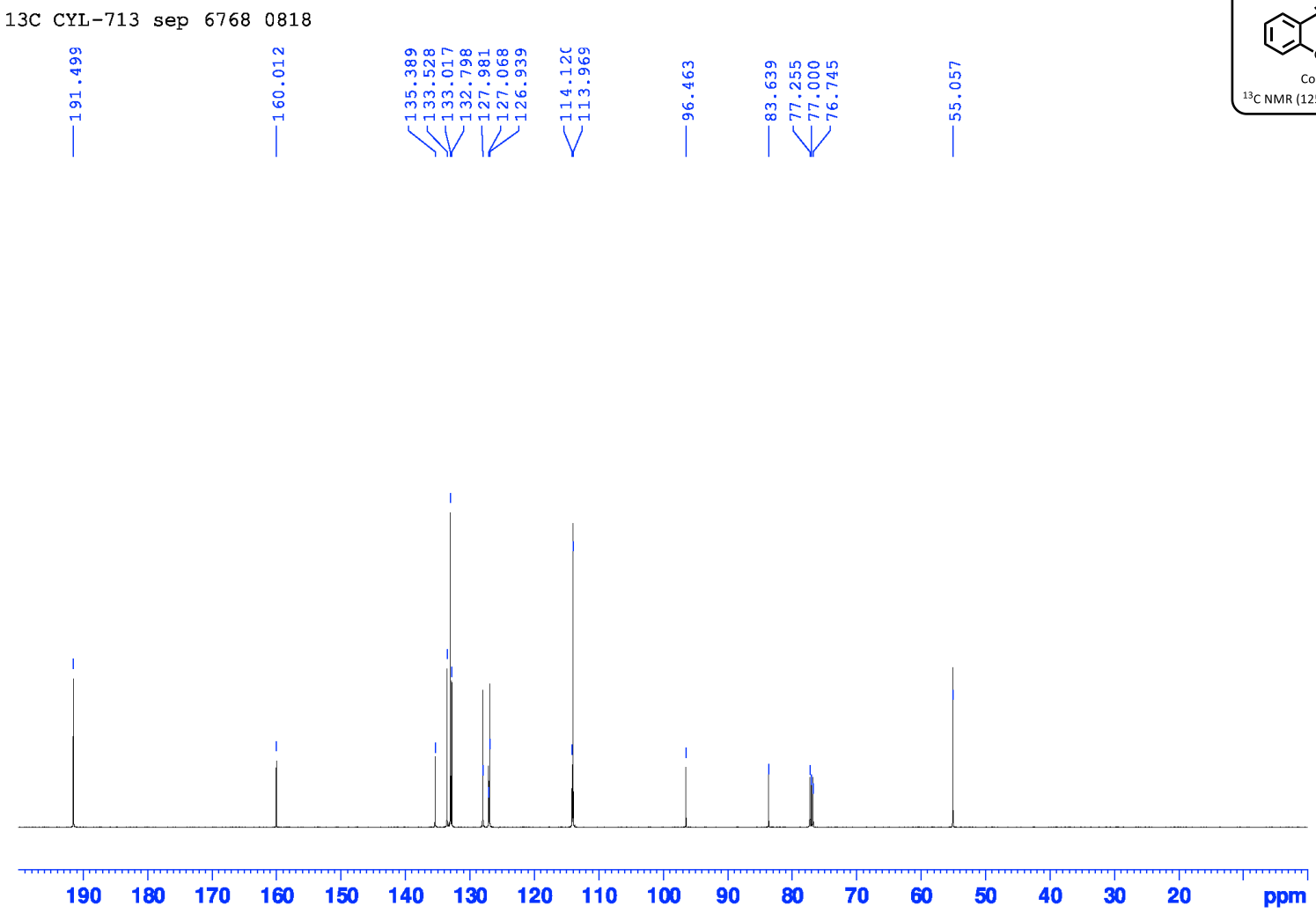


The ^{1}H NMR spectrum in $CDCl_3$ of compound 2o.

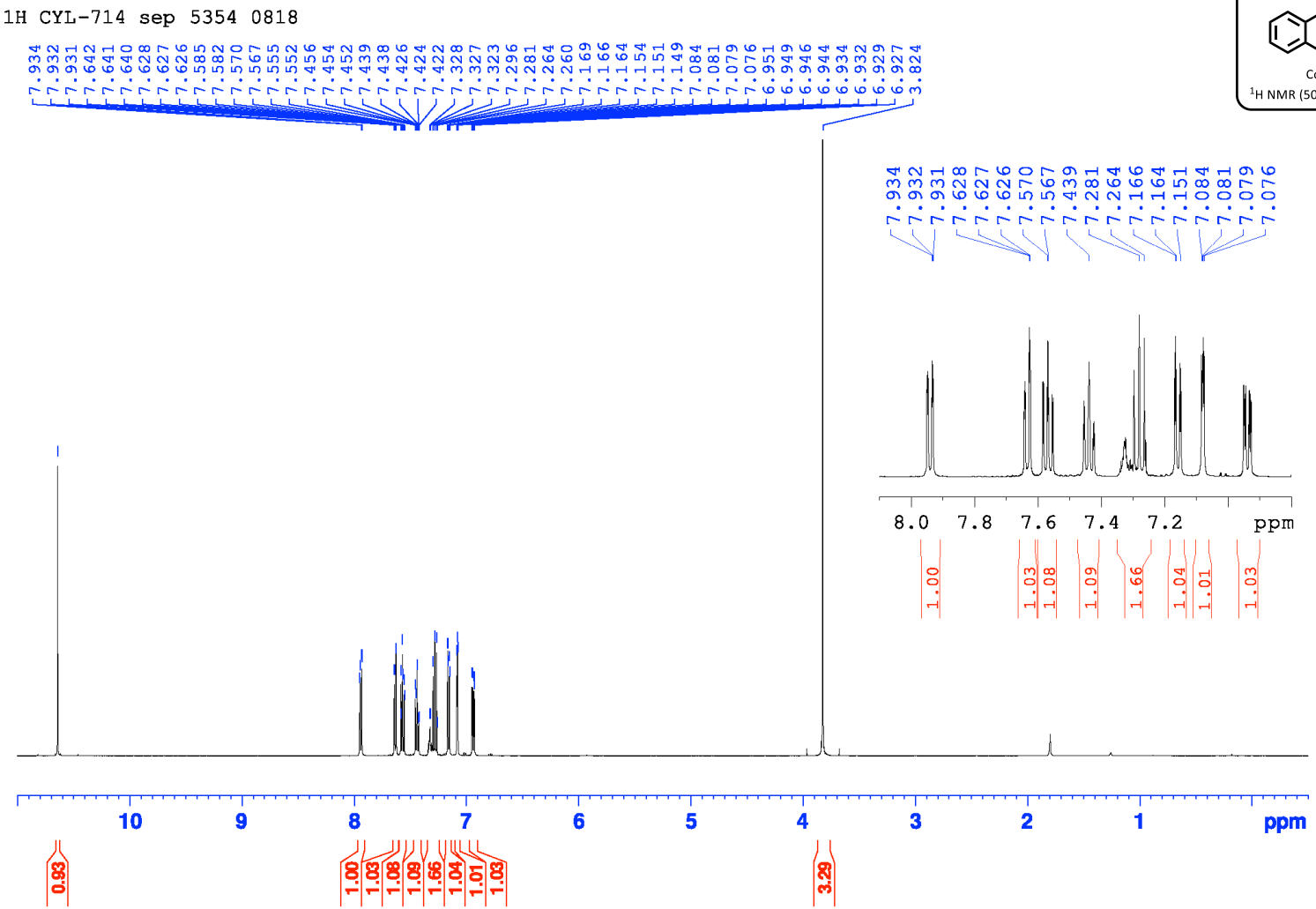


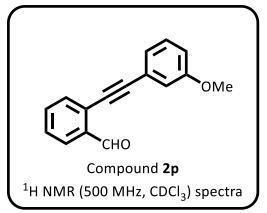
The ^{13}C NMR spectrum in $CDCl_3$ of compound 2o.



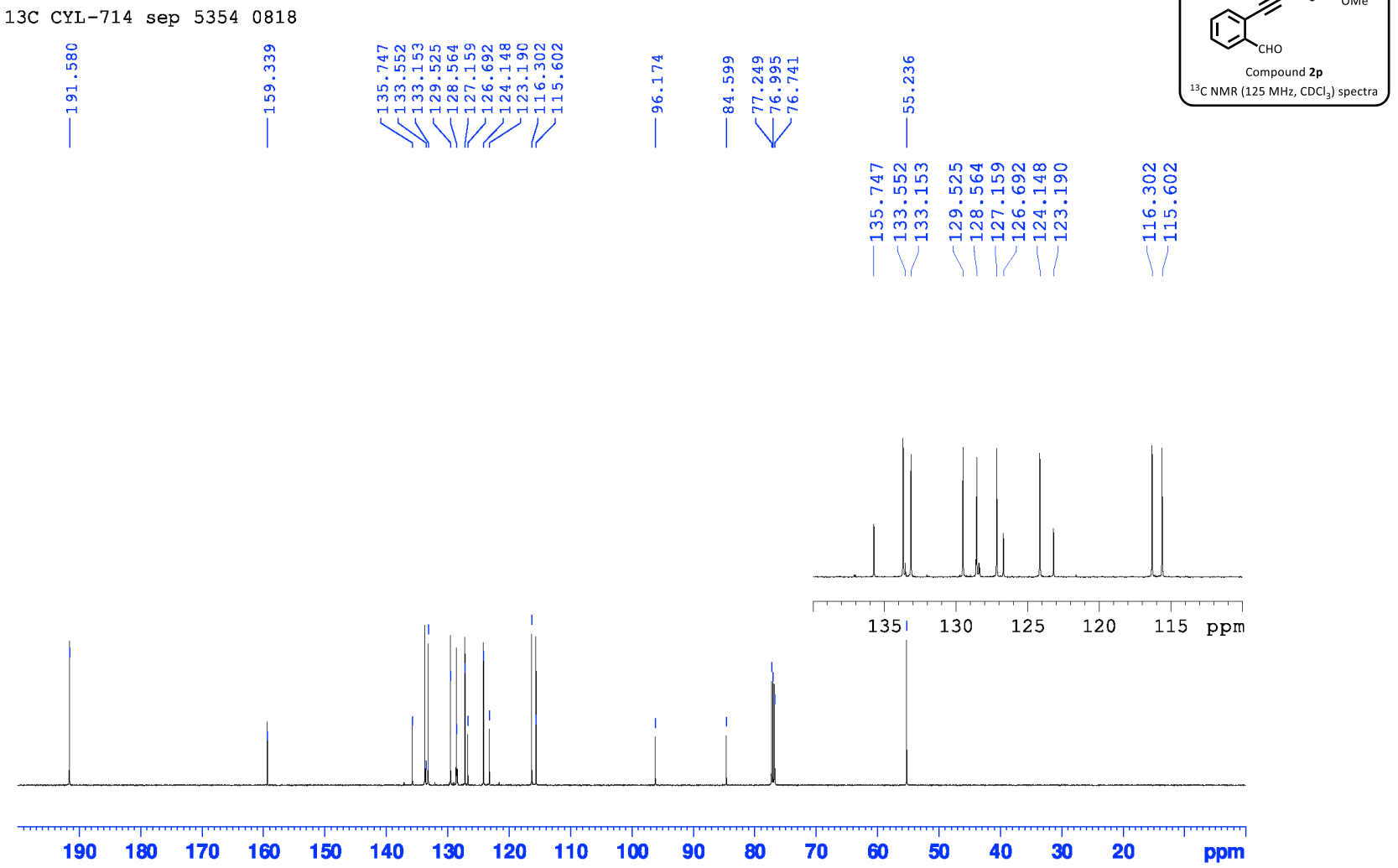


The ^{13}H NMR spectrum in $CDCl_3$ of compound 2p.

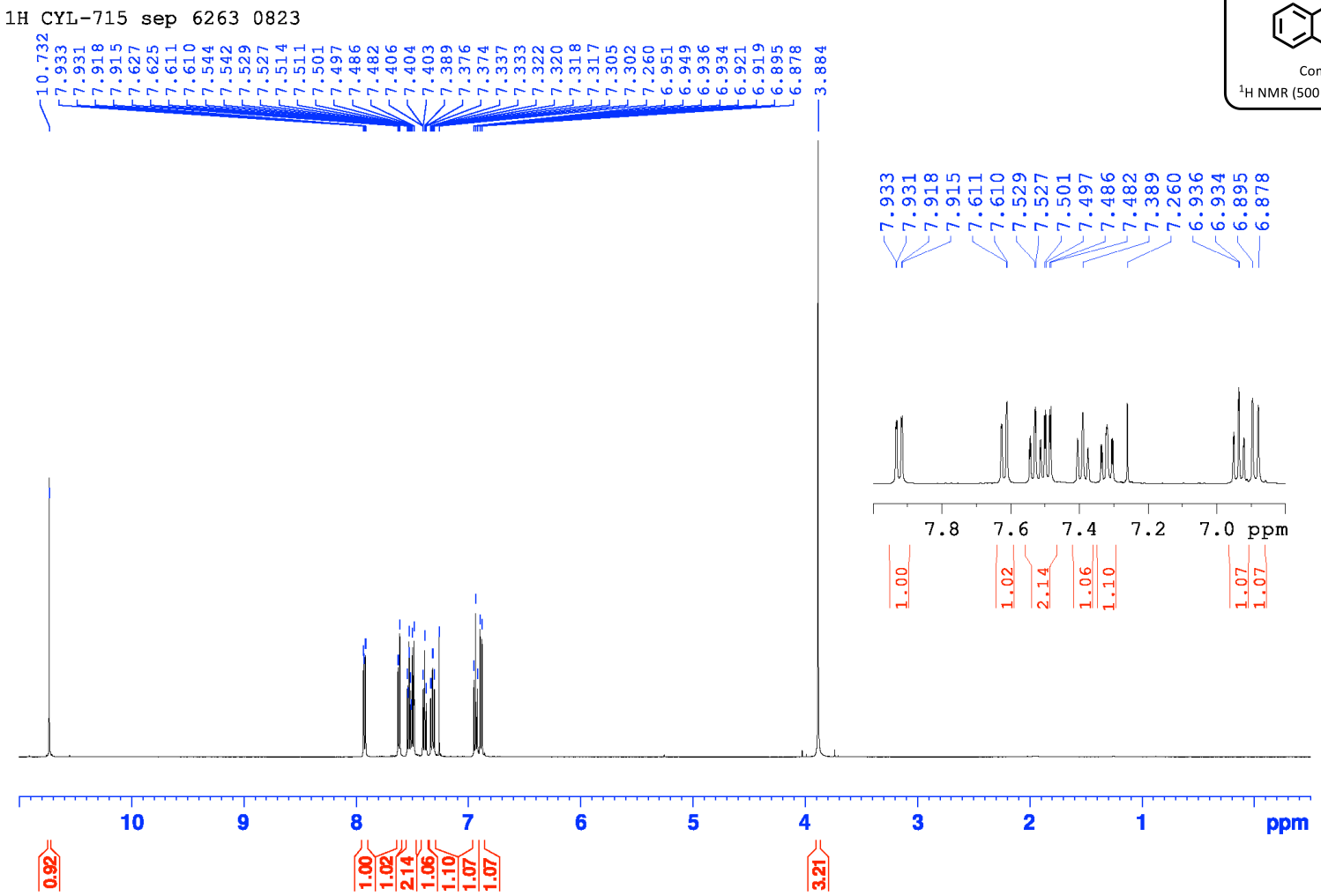


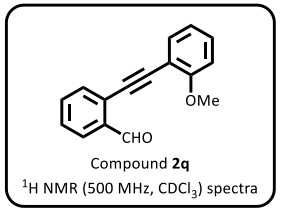


The ^{13}C NMR spectrum in $CDCl_3$ of compound 2p.

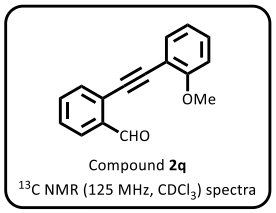


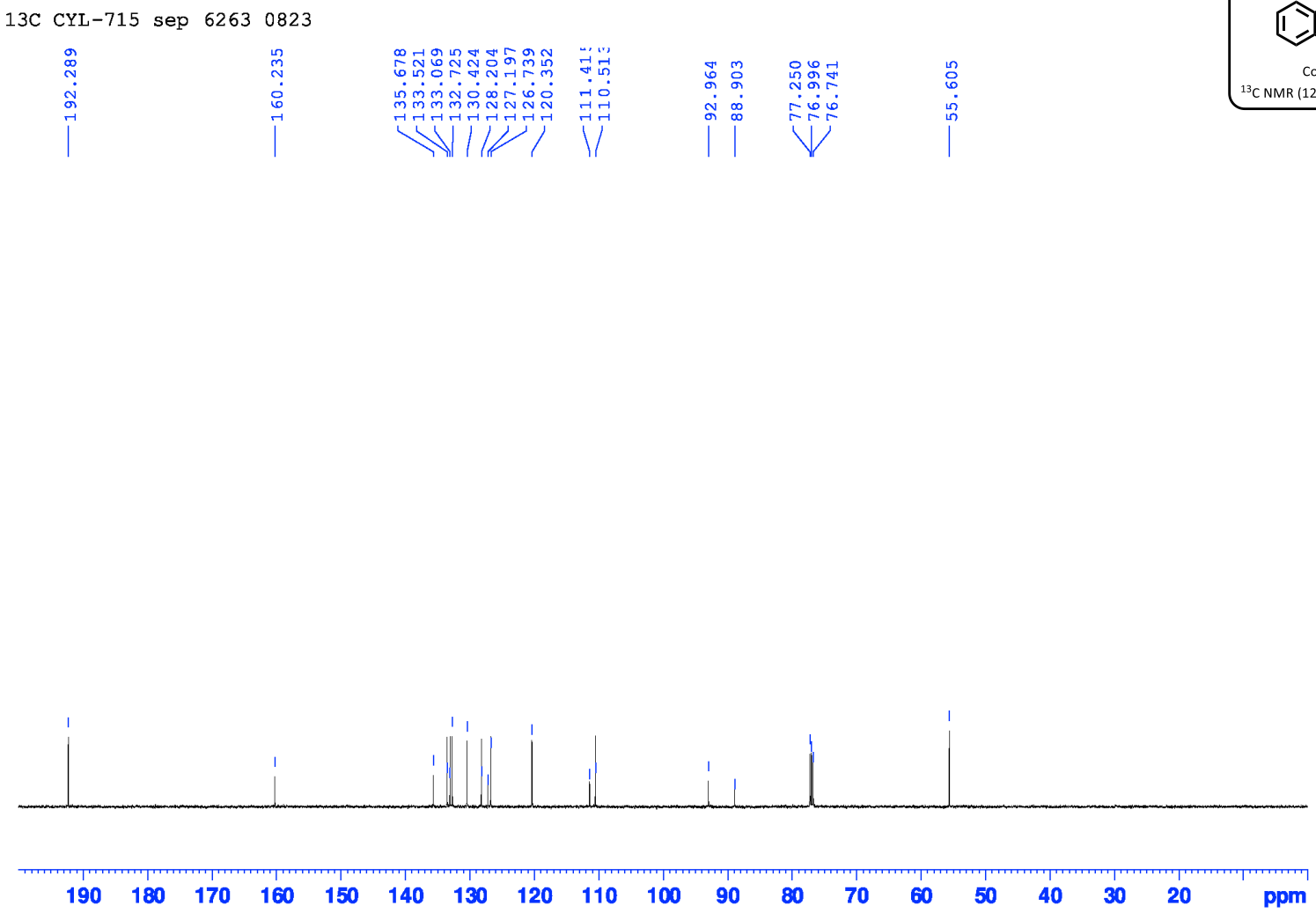
The ^{1}H NMR spectrum in $CDCl_3$ of compound 2q.



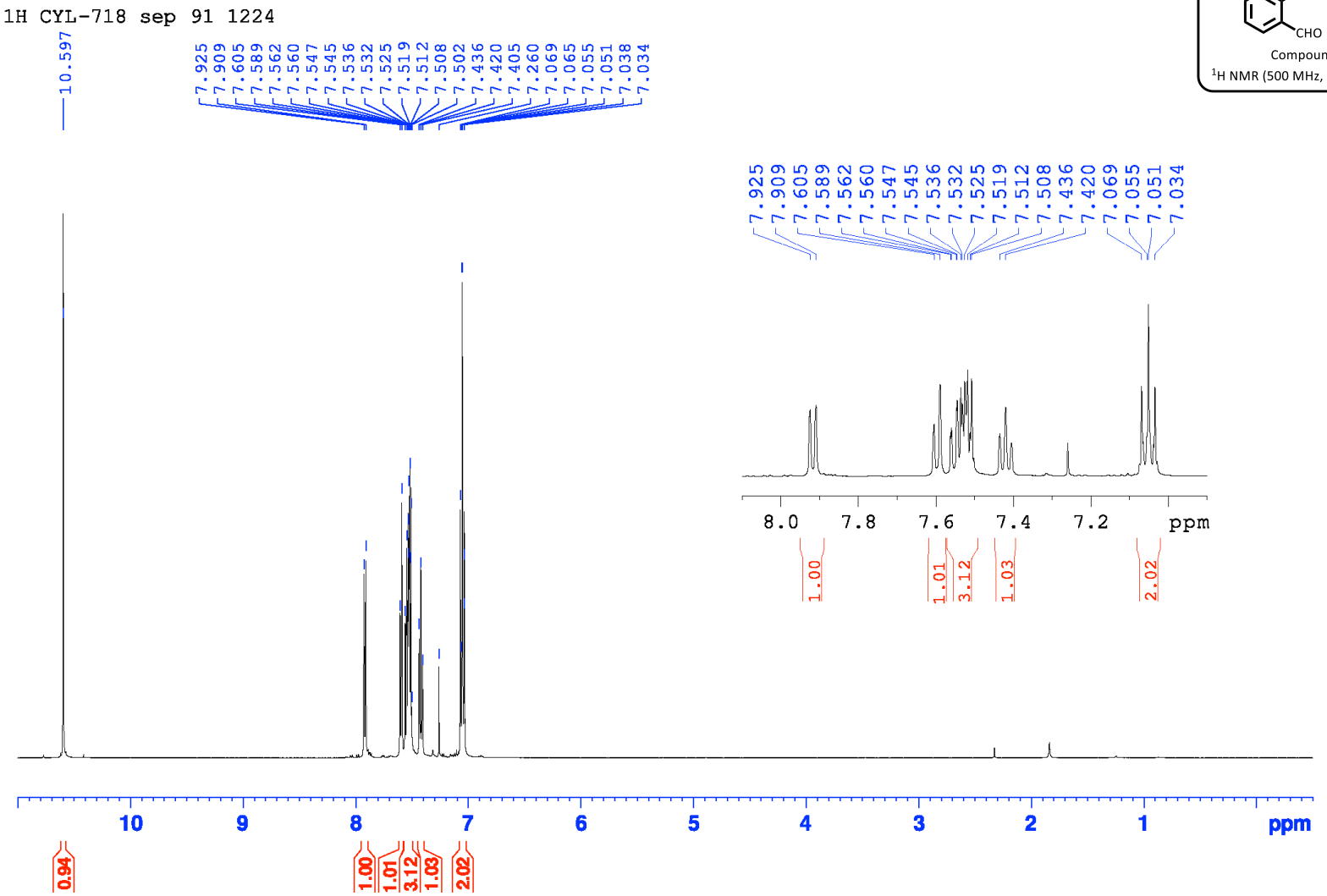


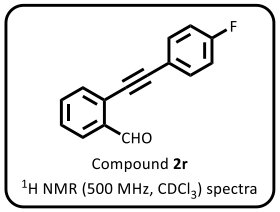
The ^{13}C NMR spectrum in $CDCl_3$ of compound 2q.



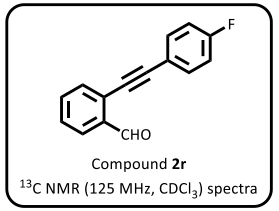


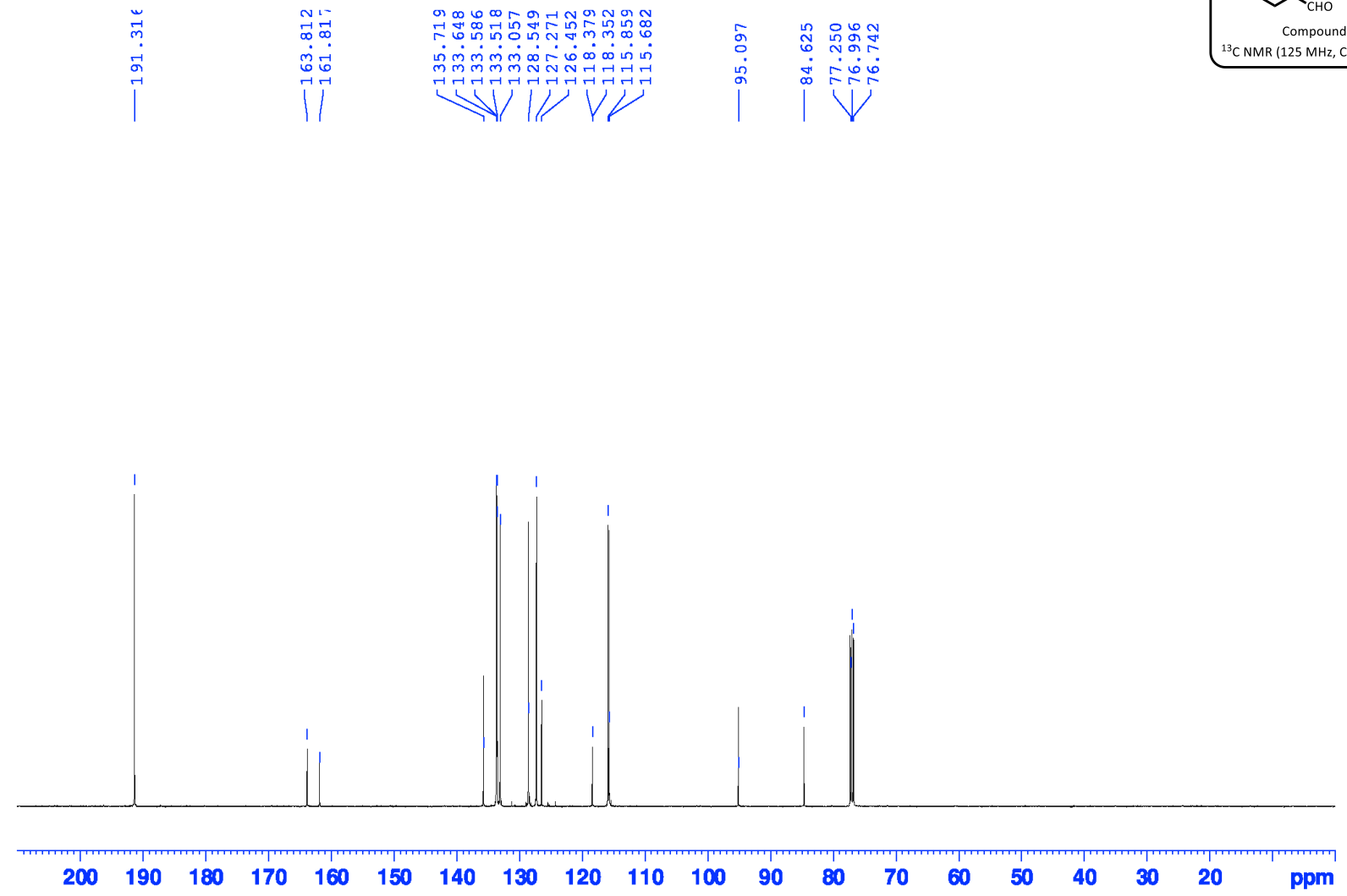
The ^{1}H NMR spectrum in $CDCl_3$ of compound 2r.



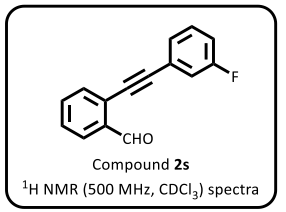


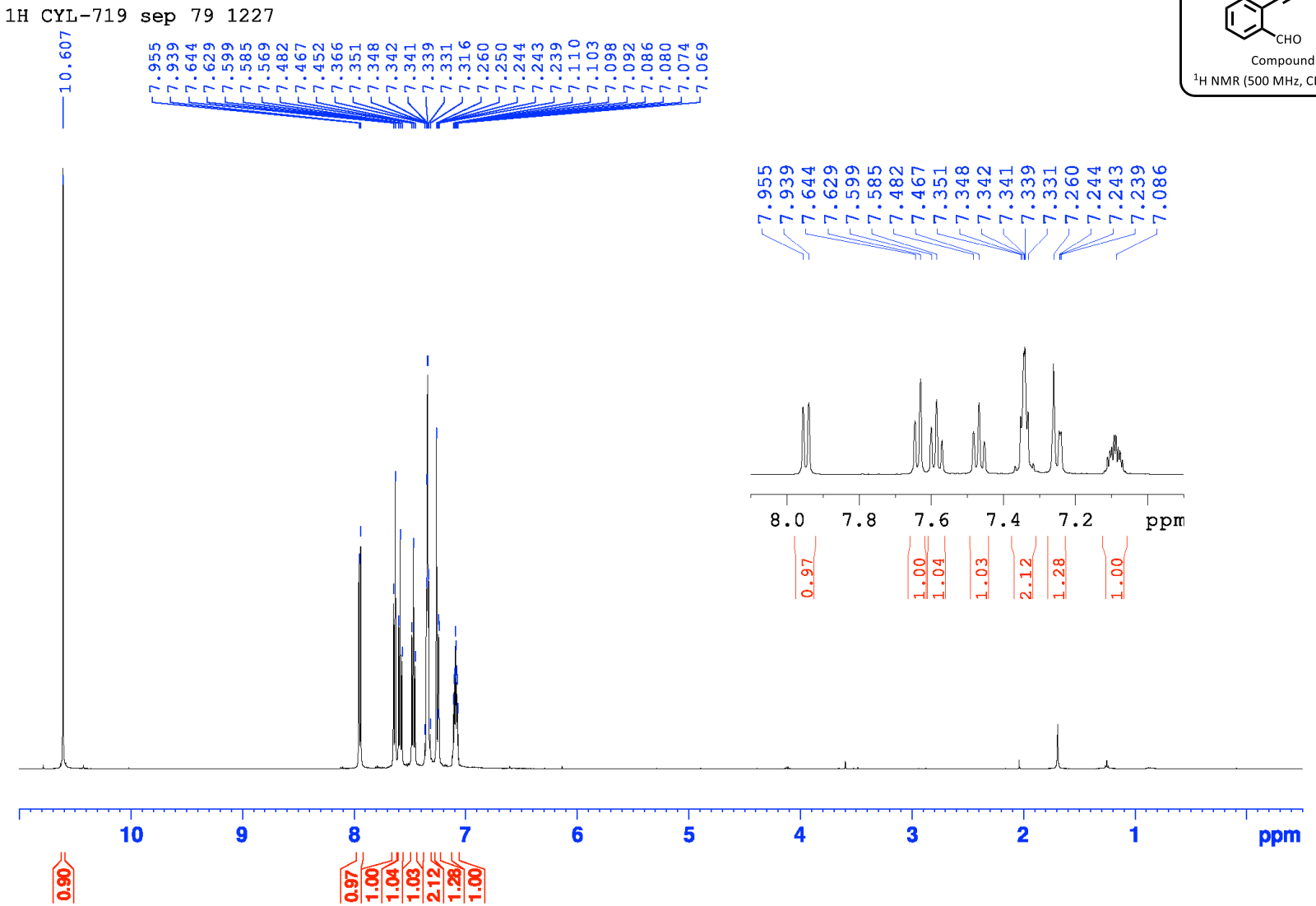
The ^{13}C NMR spectrum in $CDCl_3$ of compound 2r.



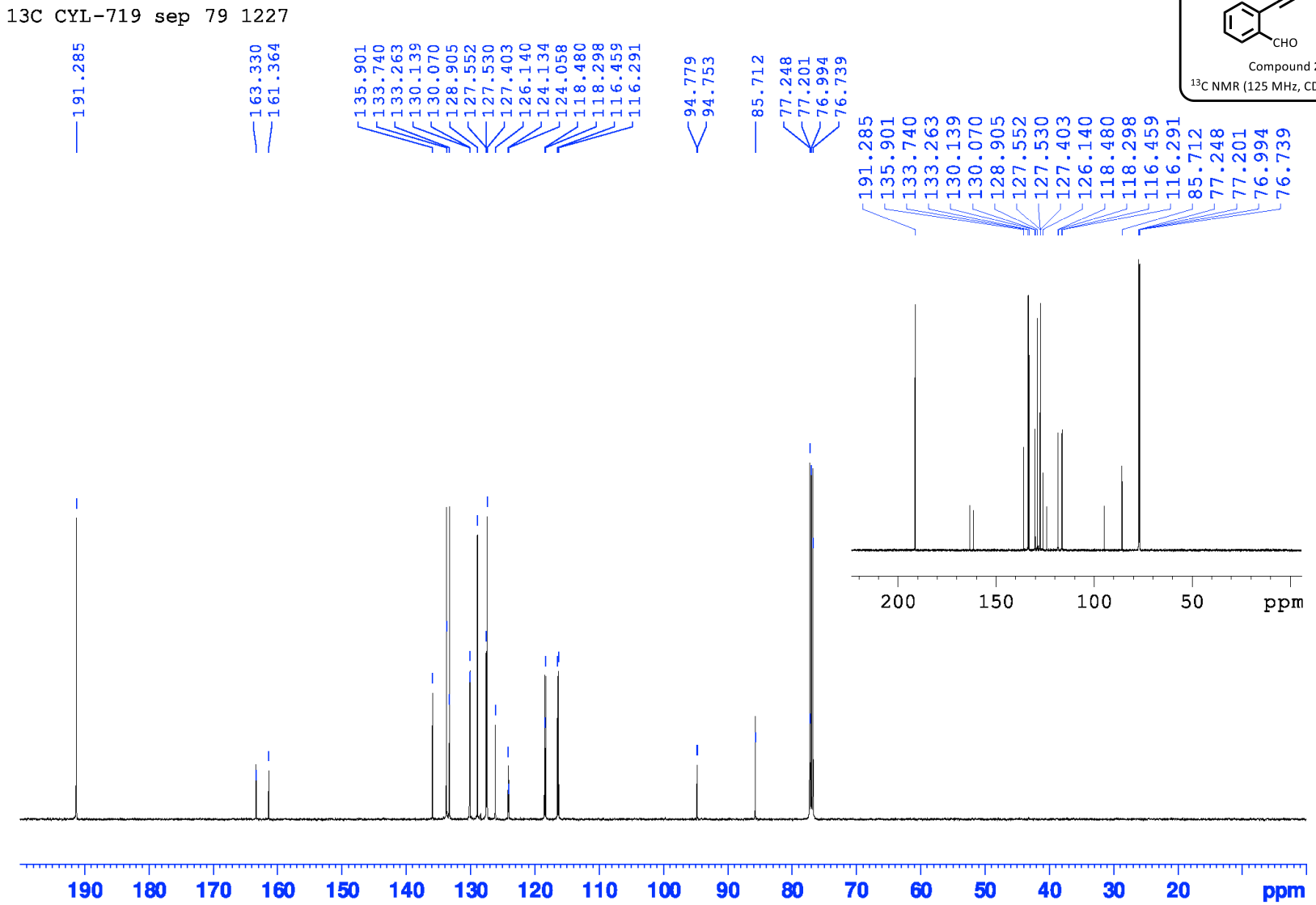


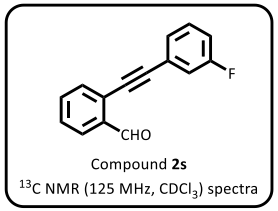
The ^{1}H NMR spectrum in $CDCl_3$ of compound 2s.



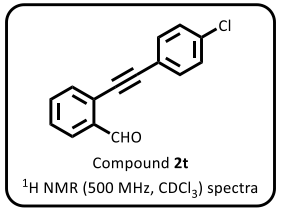


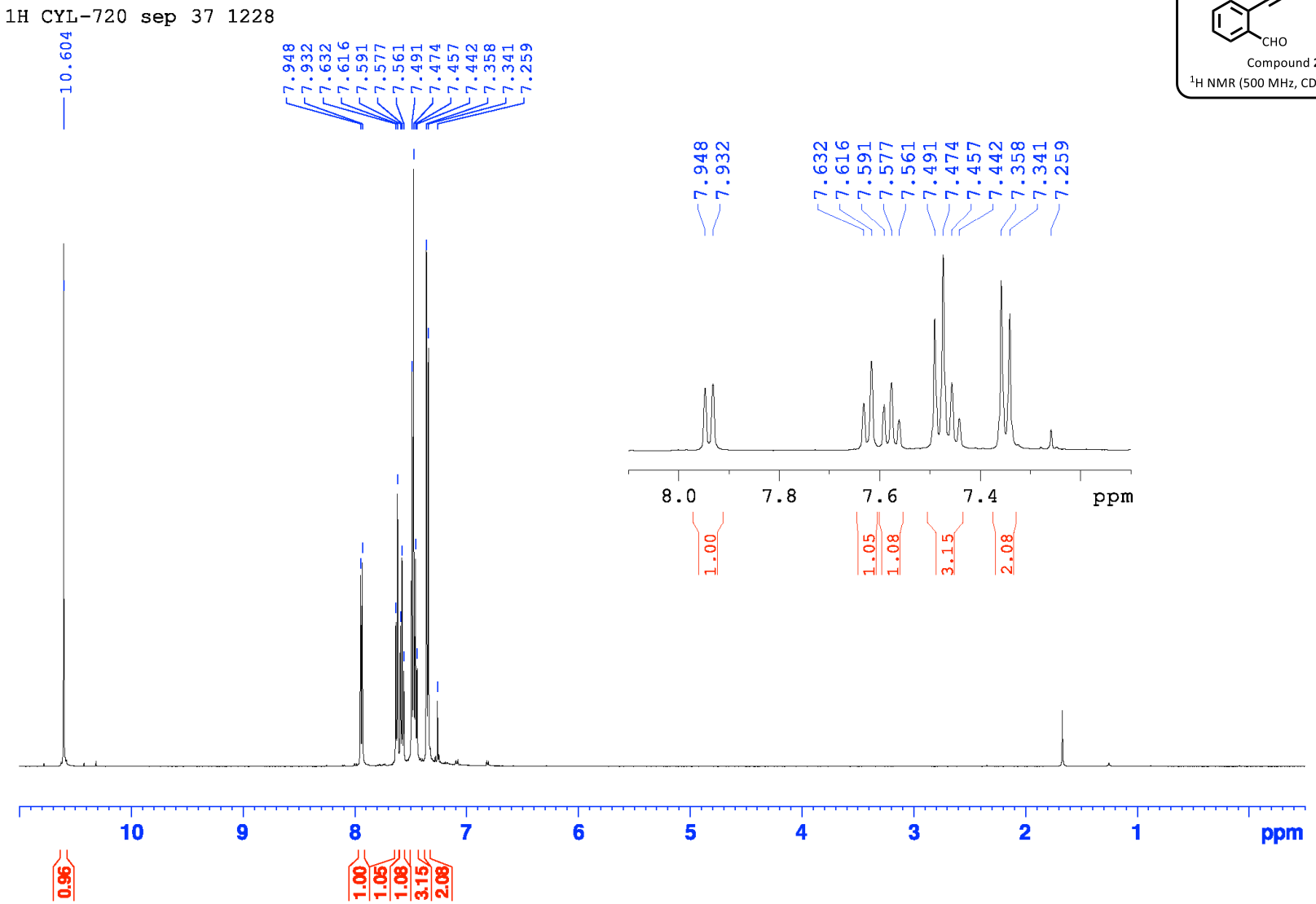
The ^{13}C NMR spectrum in $CDCl_3$ of compound 2s.



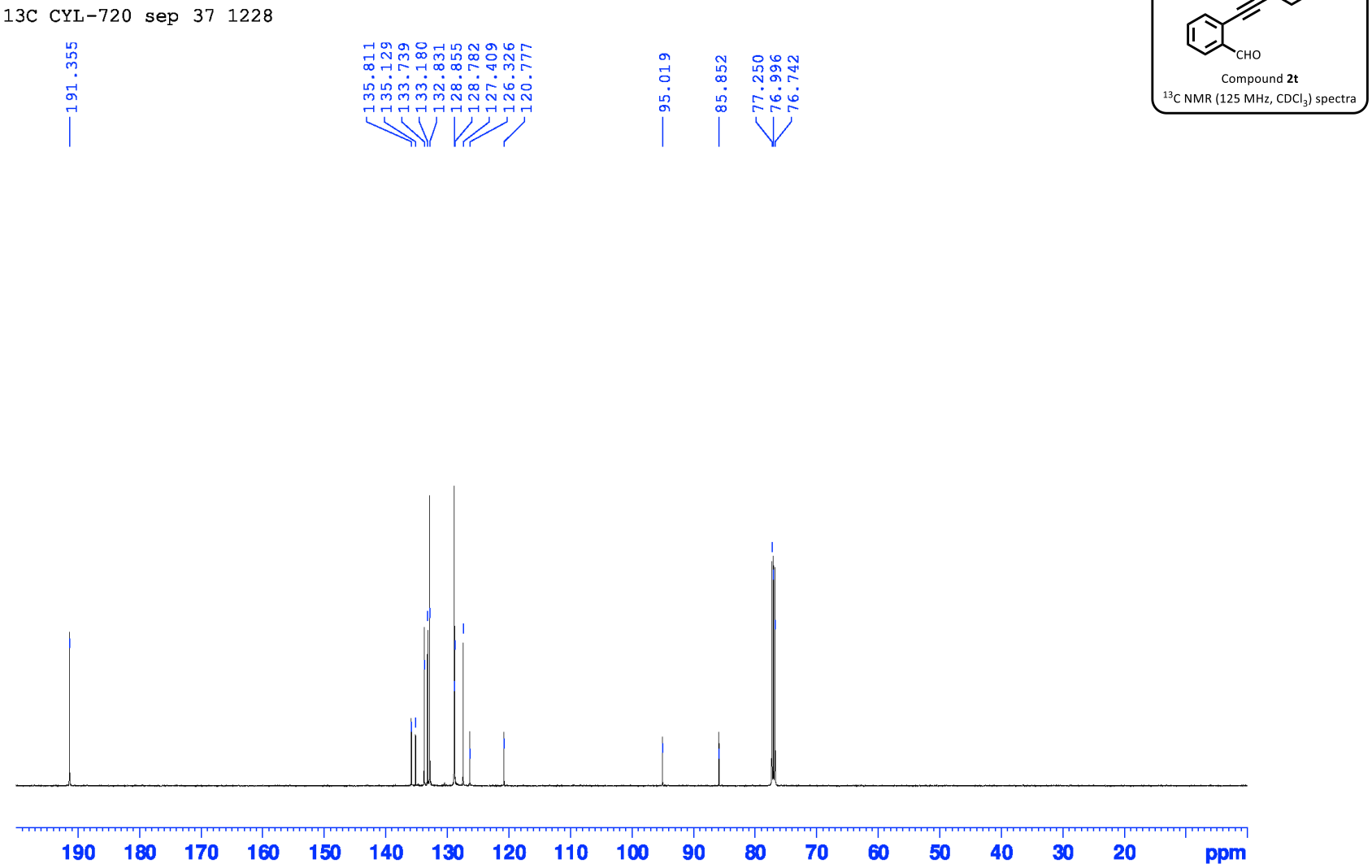


The ^{1}H NMR spectrum in $CDCl_3$ of compound 2t.

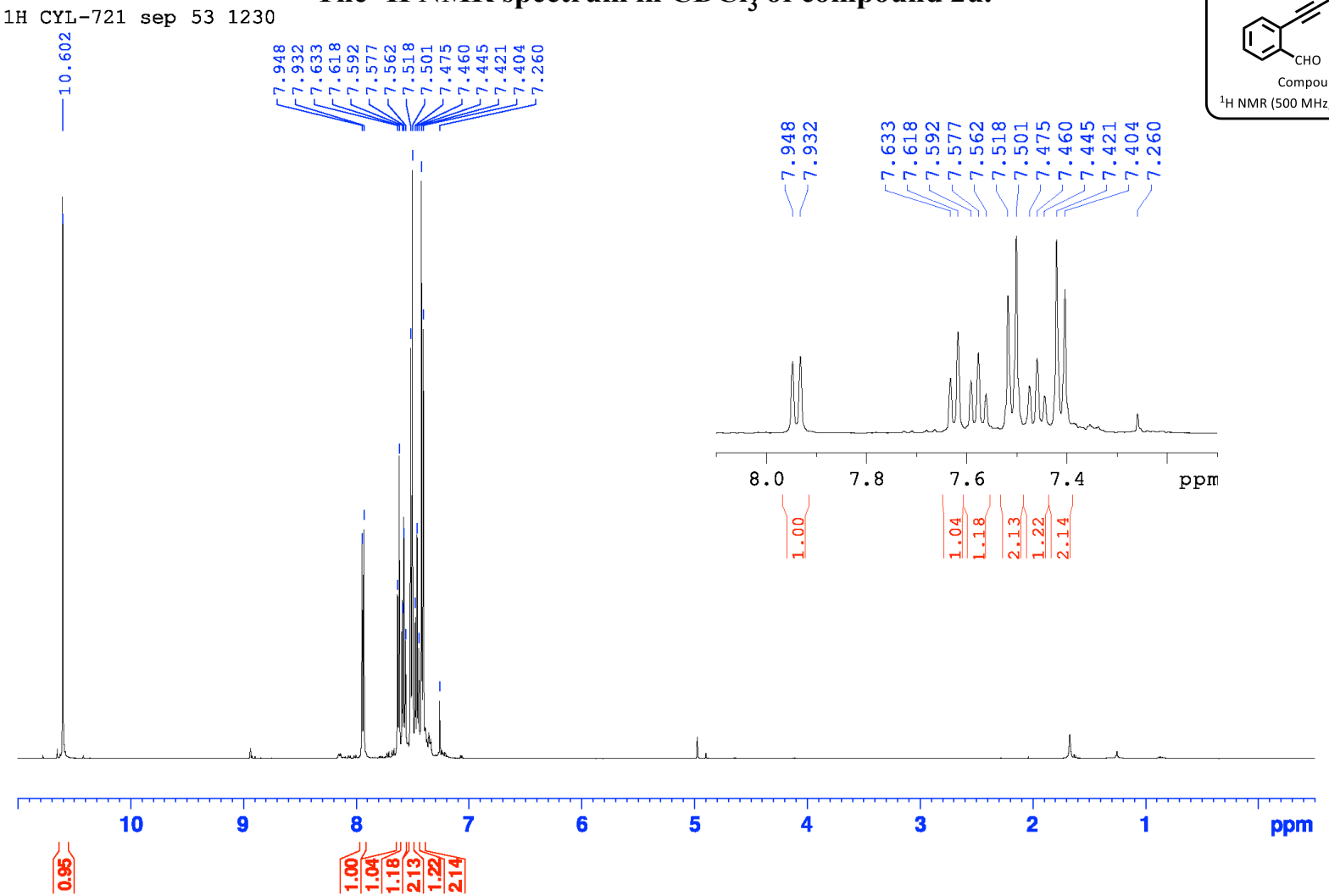


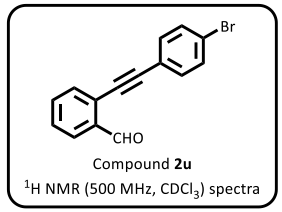


The ^{13}C NMR spectrum in $CDCl_3$ of compound 2t.

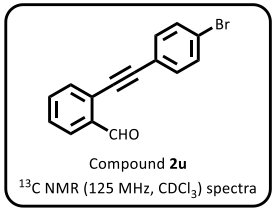


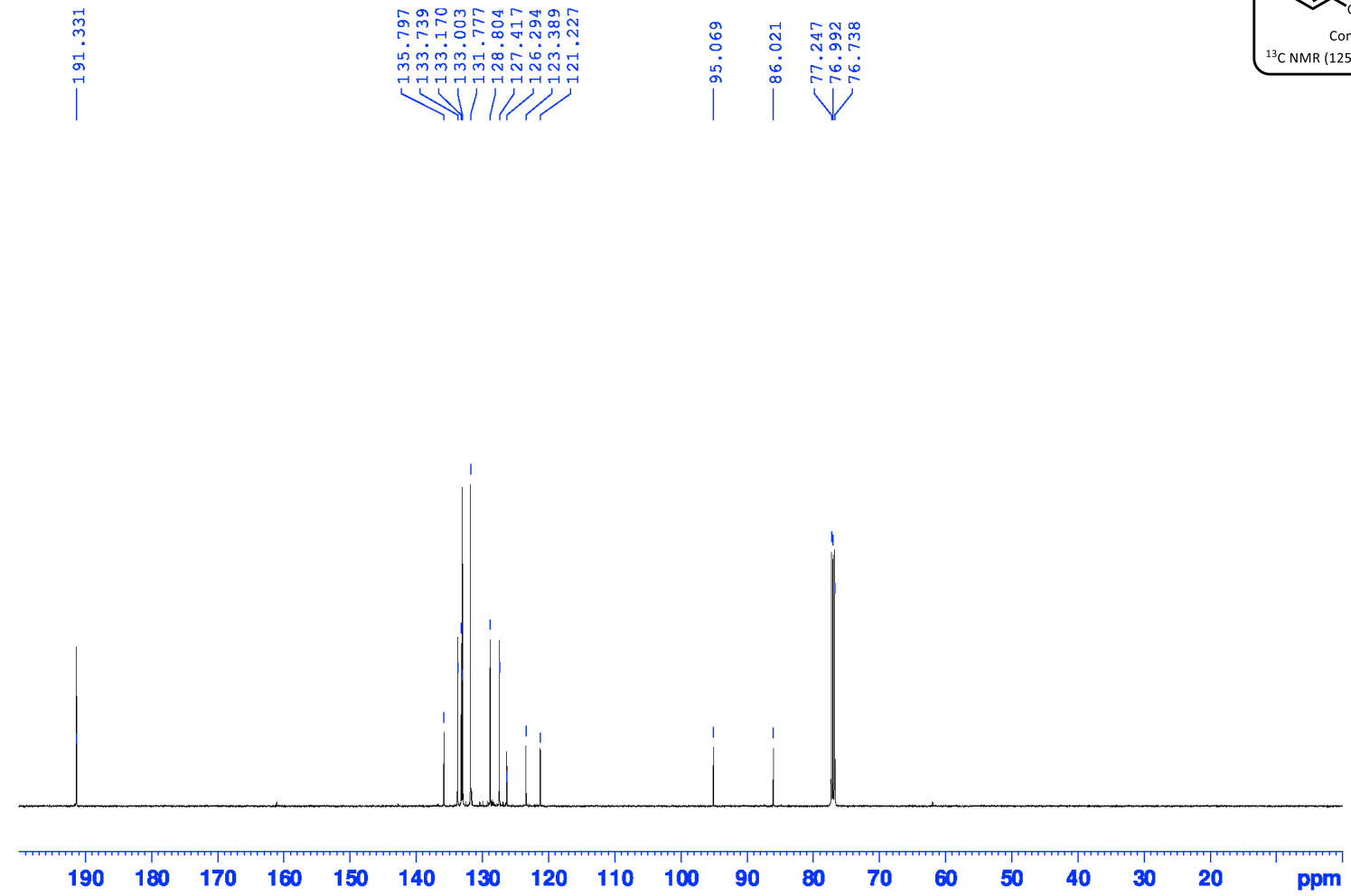
The ^{1}H NMR spectrum in $CDCl_3$ of compound 2u.



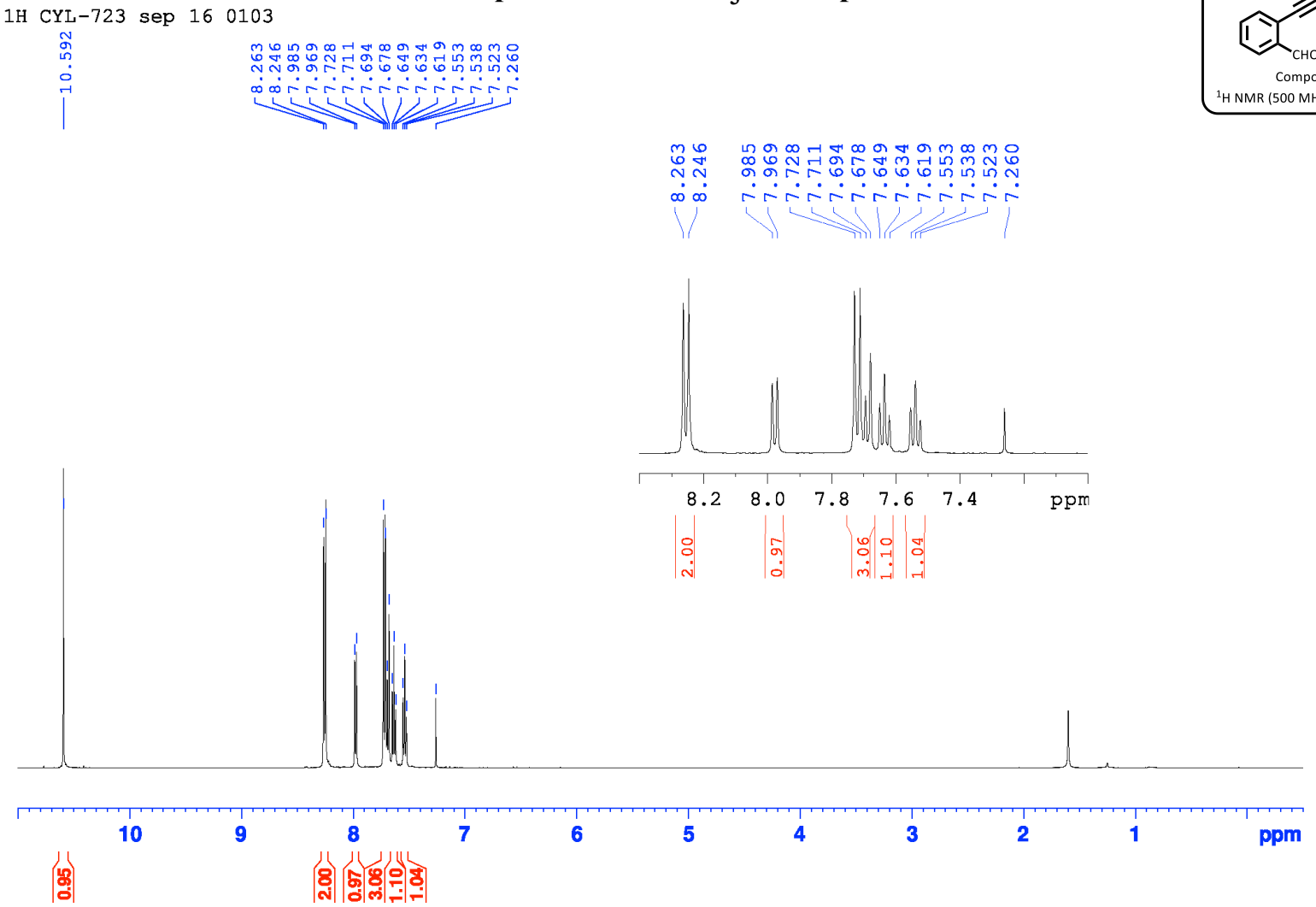


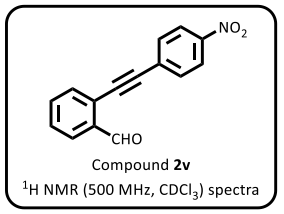
The ^{13}C NMR spectrum in $CDCl_3$ of compound 2u.





The ^{1}H NMR spectrum in $CDCl_3$ of compound 2v.

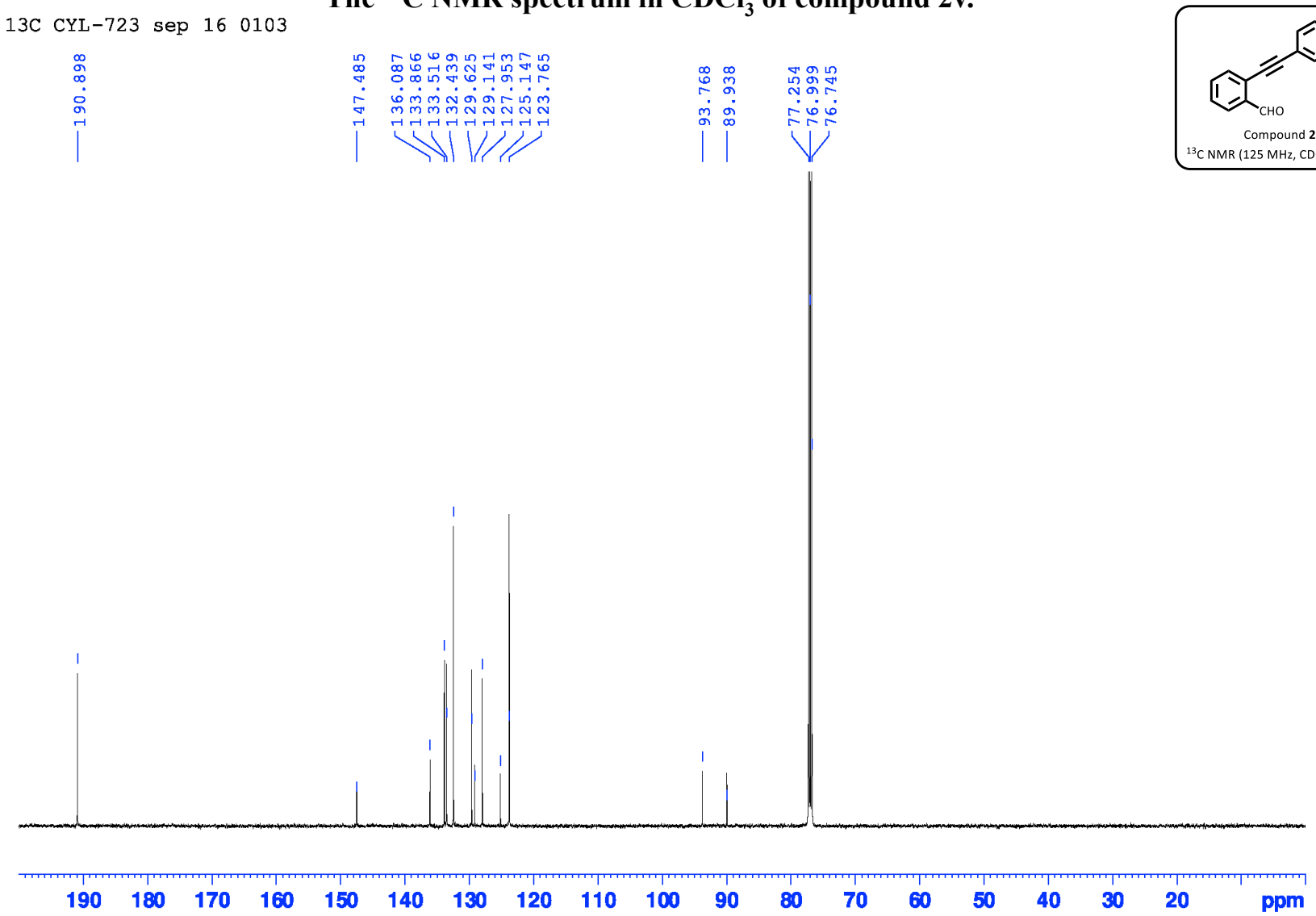




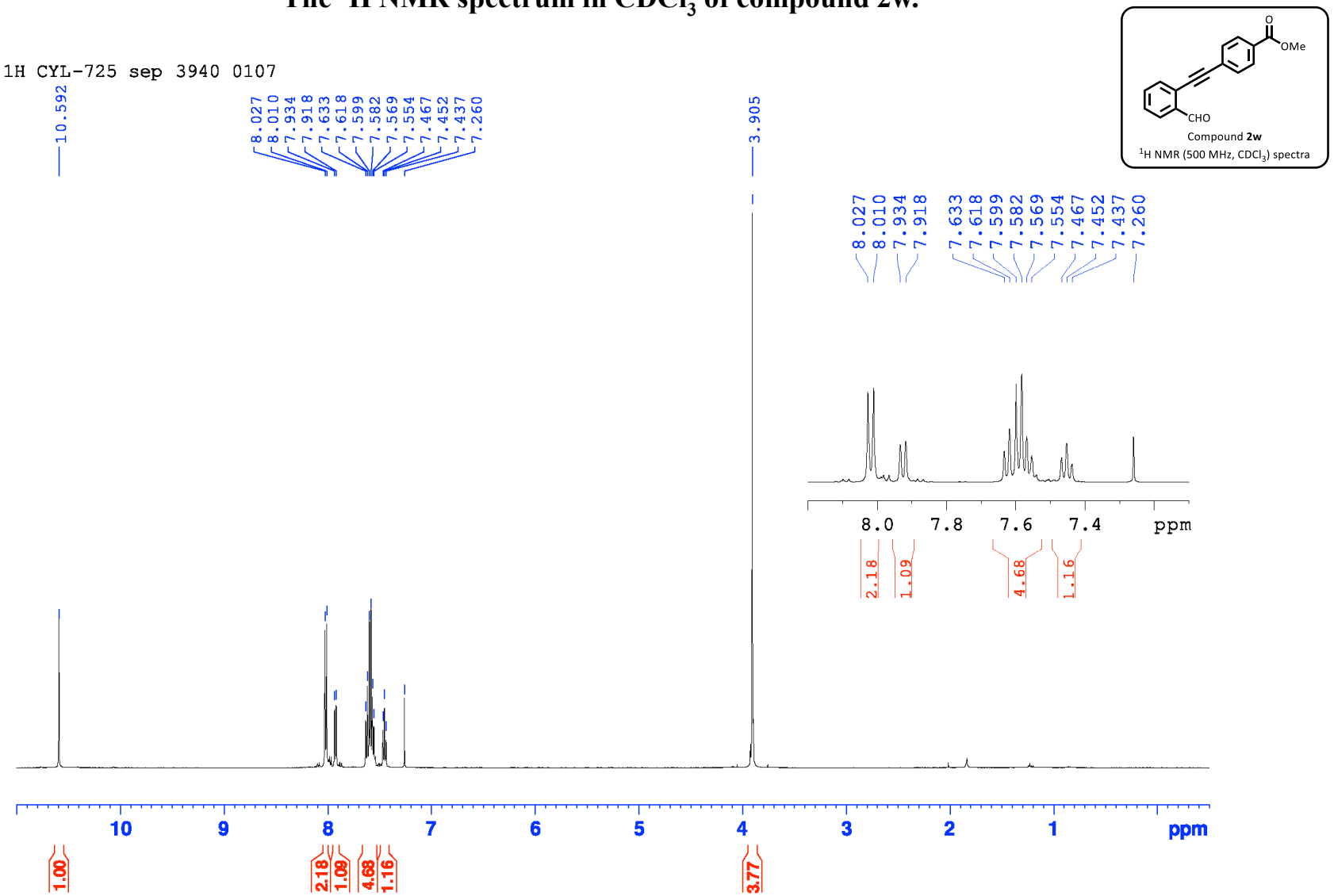
Compound **2v**

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

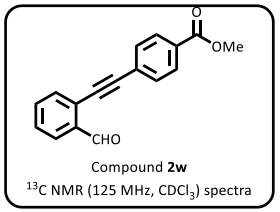
The ^{13}C NMR spectrum in $CDCl_3$ of compound 2v.



The ^{1}H NMR spectrum in $CDCl_3$ of compound 2w.

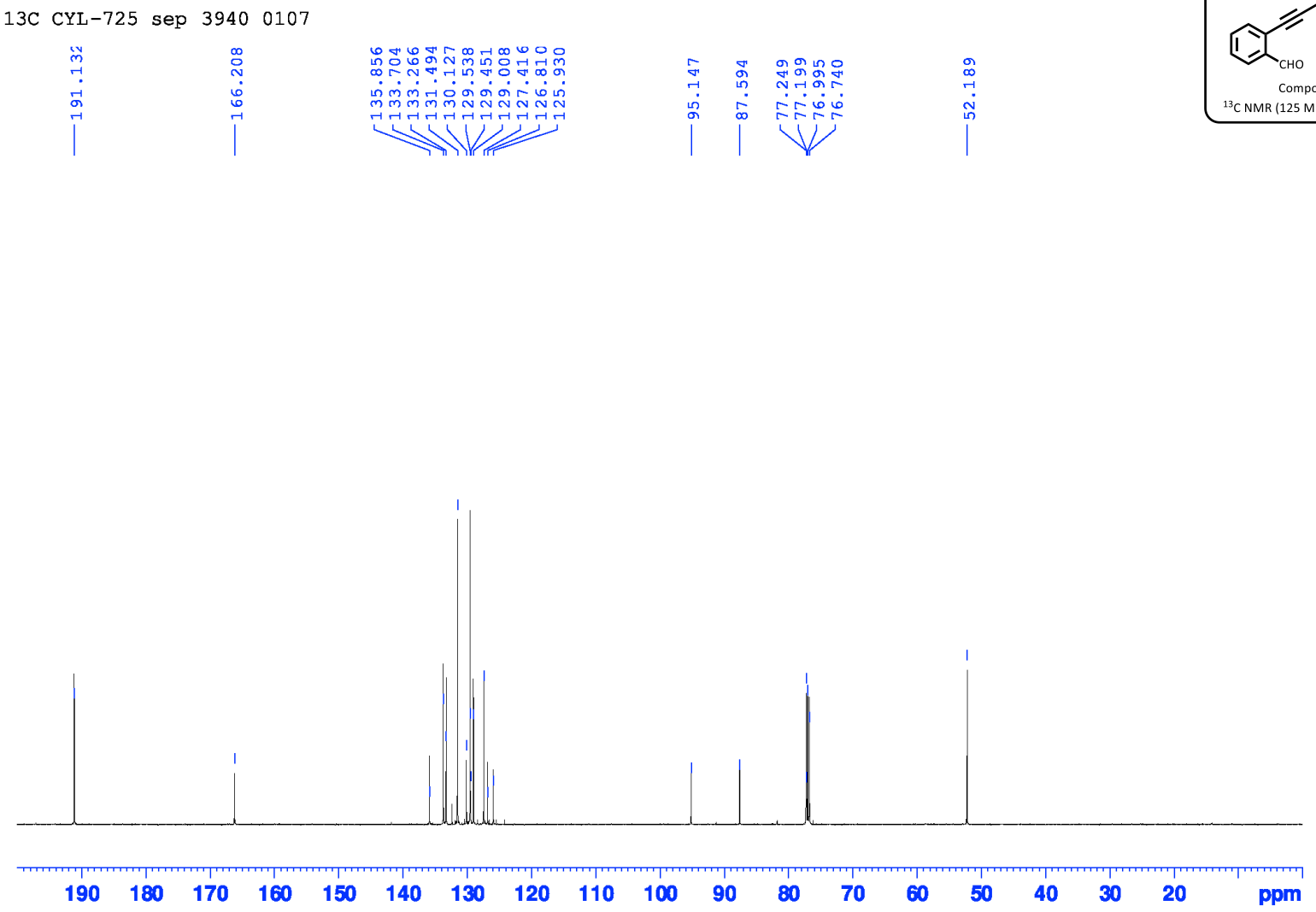


The ^{13}C NMR spectrum in $CDCl_3$ of compound 2w.

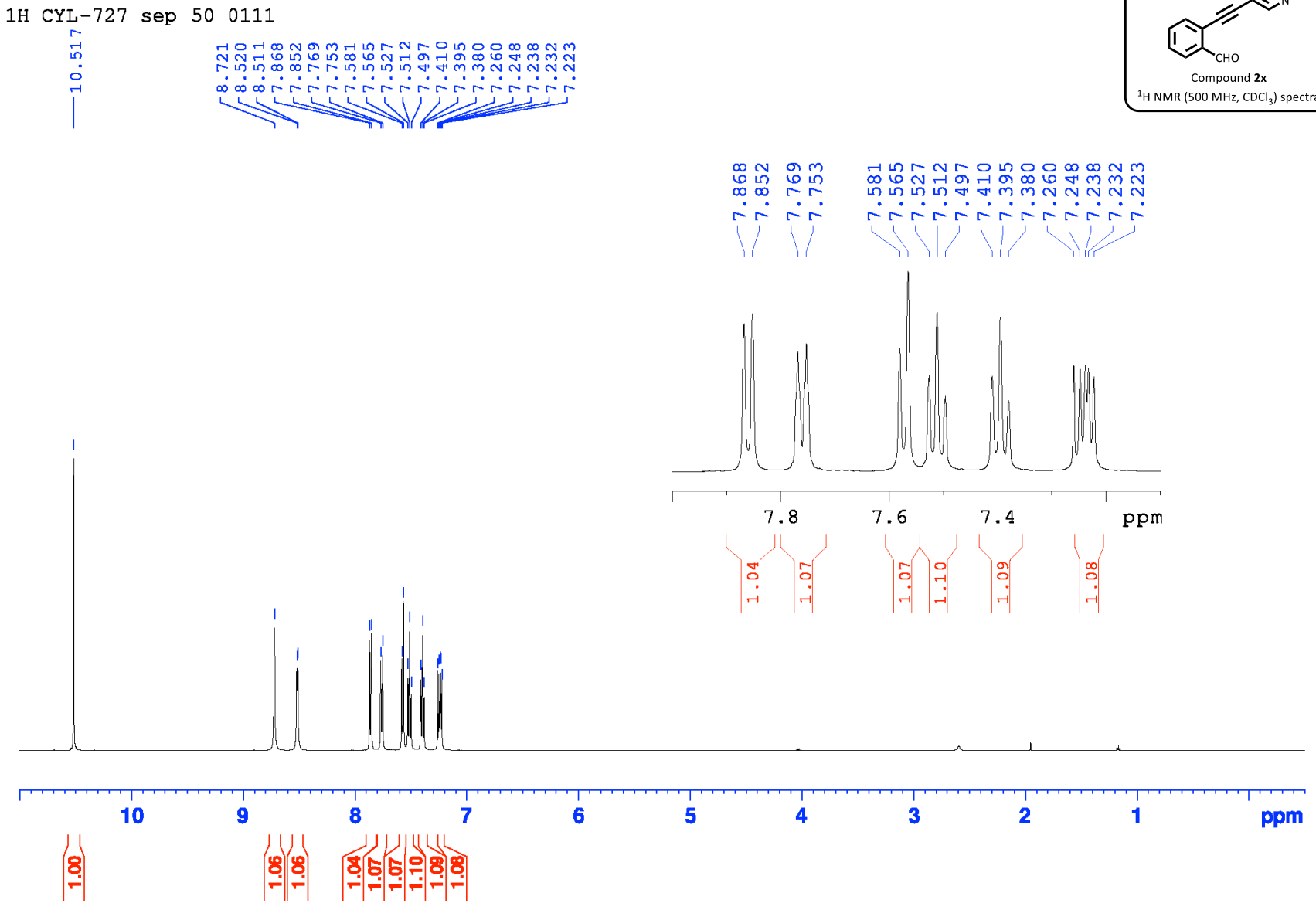


Compound **2w**

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



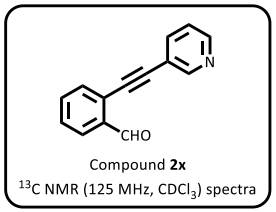
The ^{1}H NMR spectrum in $CDCl_3$ of compound 2x.

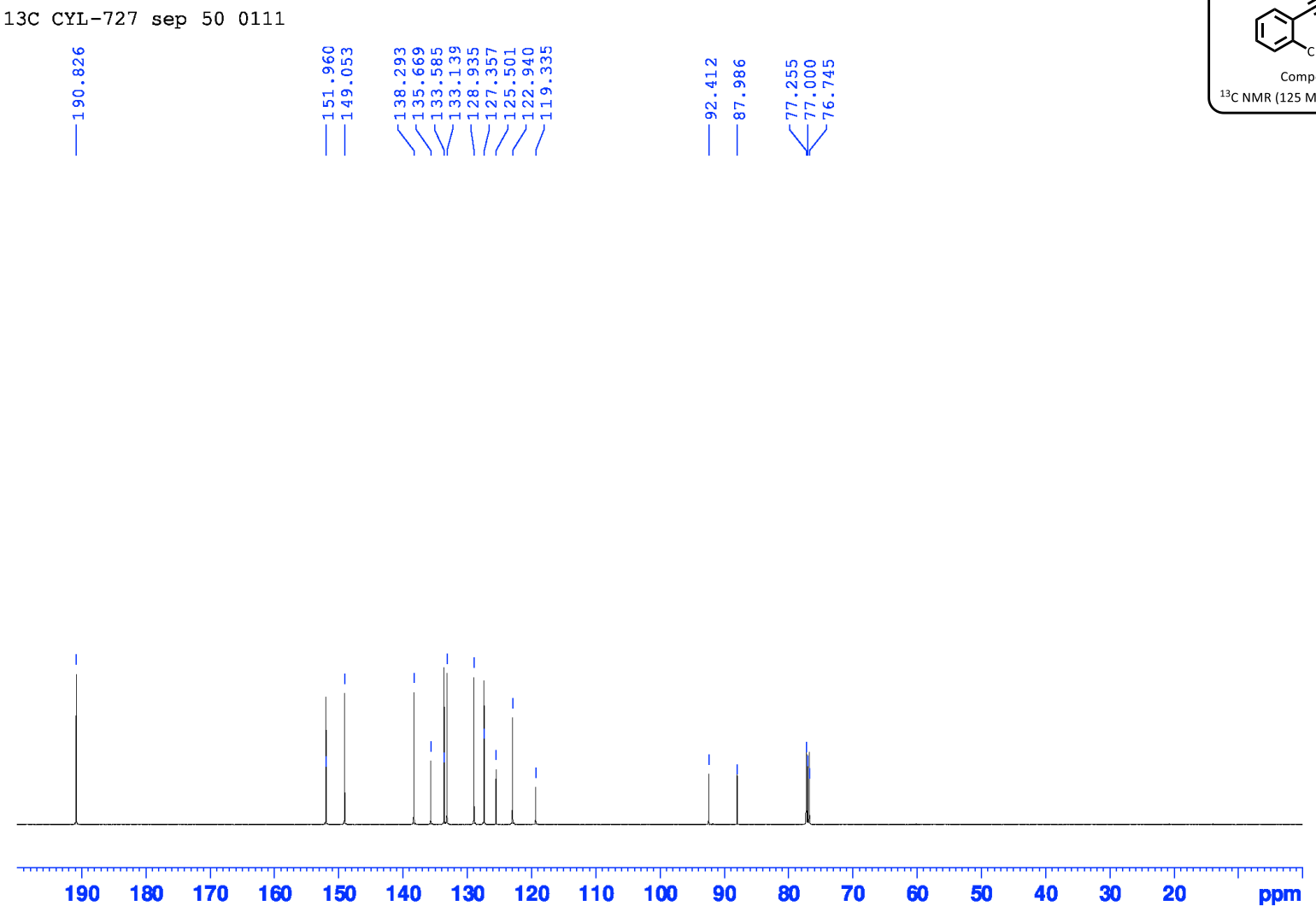


Compound **2x**

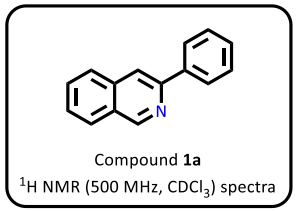
^{1}H NMR (500 MHz, $CDCl_3$) spectra

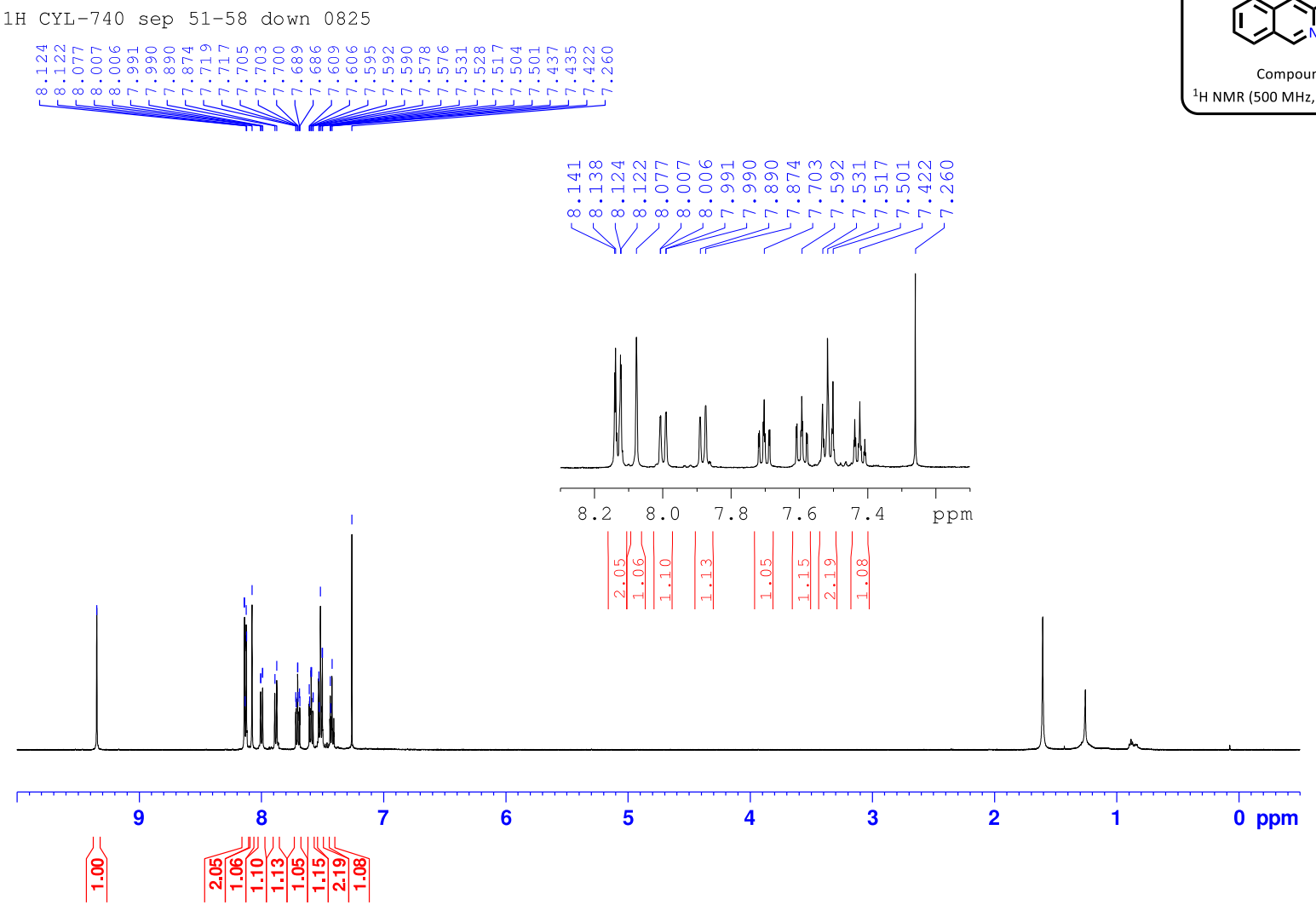
The ^{13}C NMR spectrum in $CDCl_3$ of compound 2x.



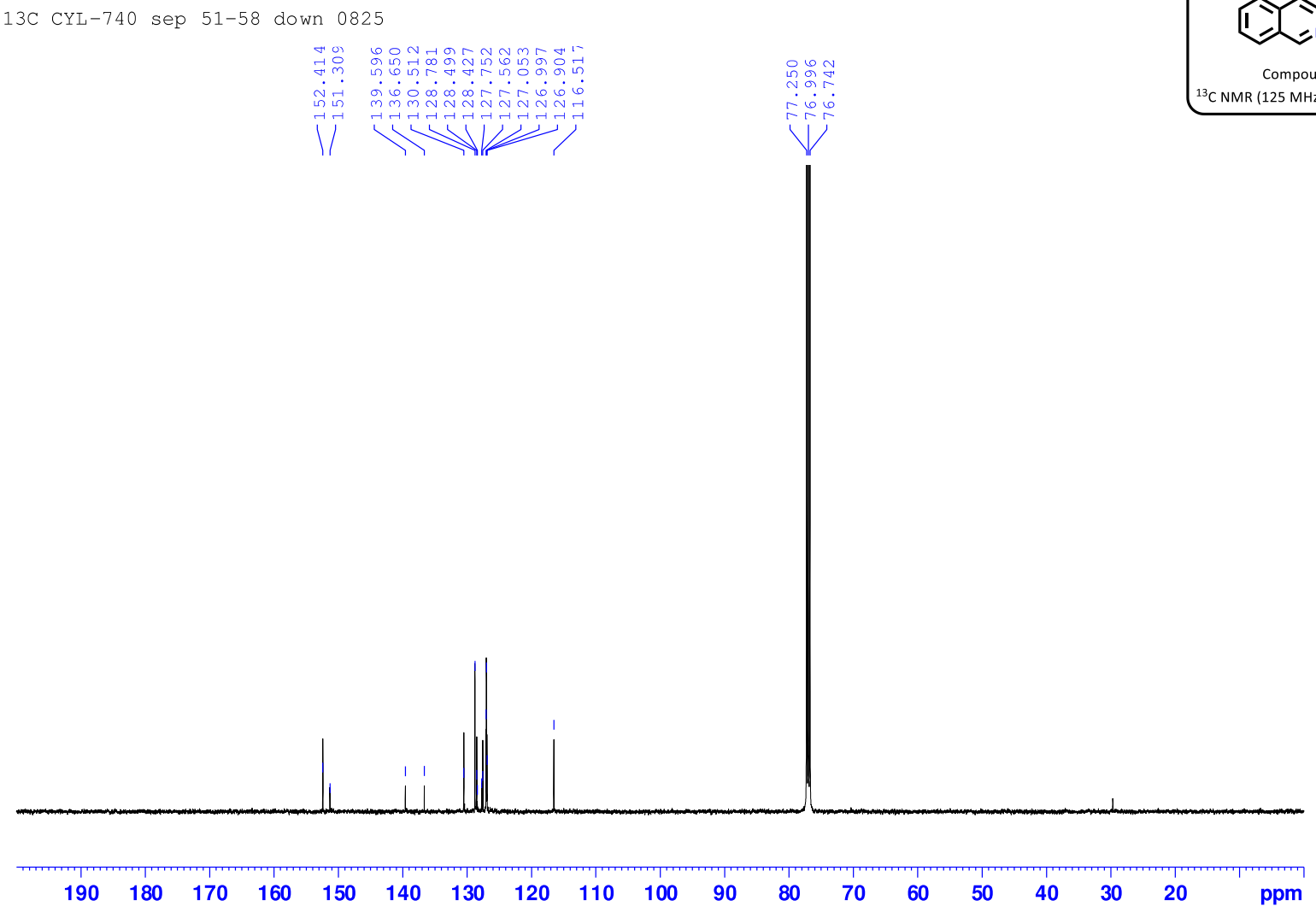


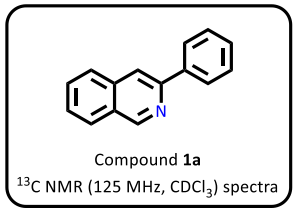
The ^{1}H NMR spectrum in $CDCl_3$ of compound 1a.



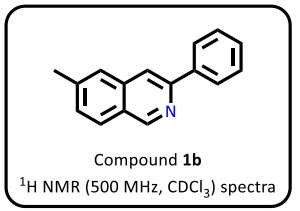


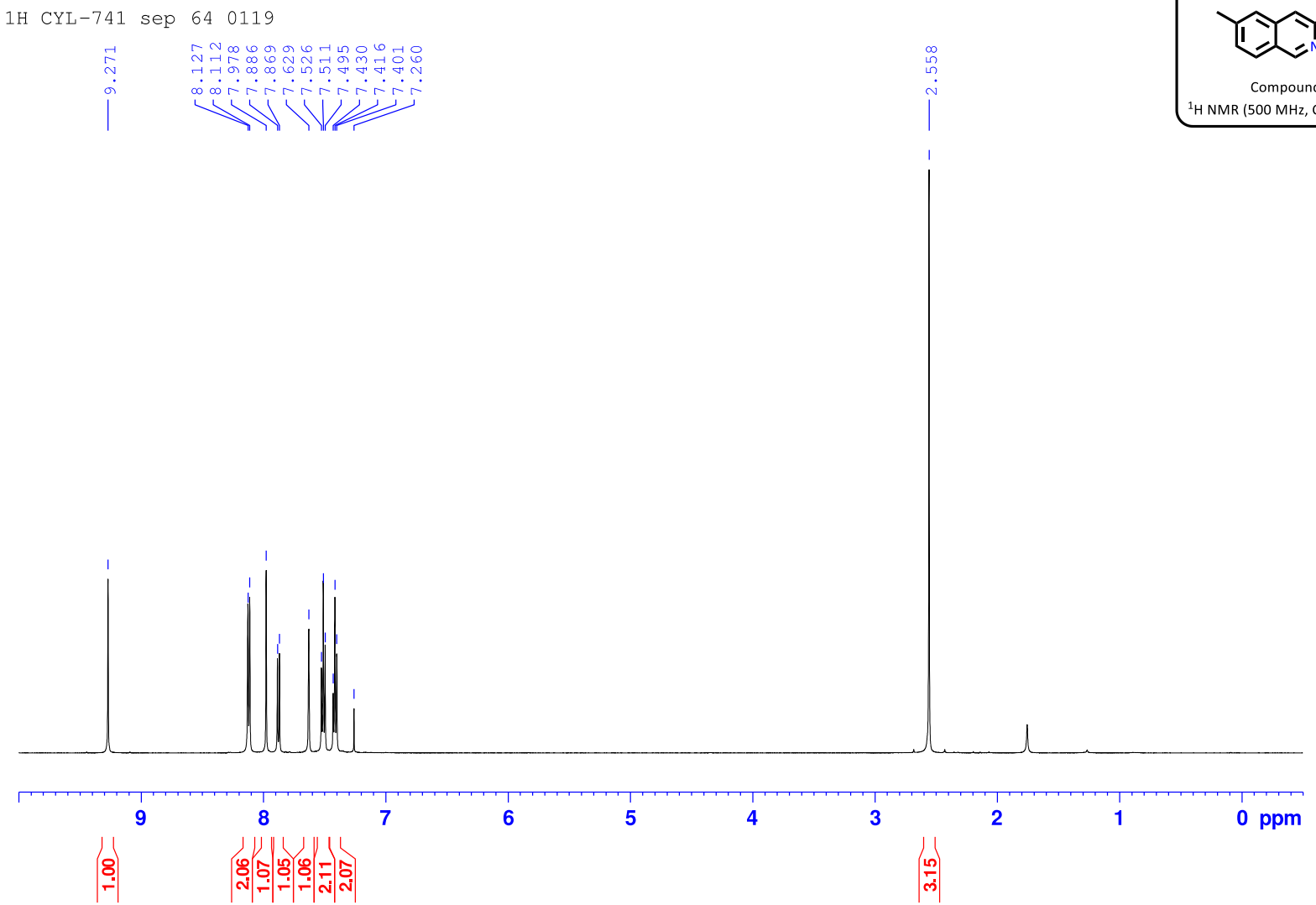
The ^{13}C NMR spectrum in $CDCl_3$ of compound 1a.



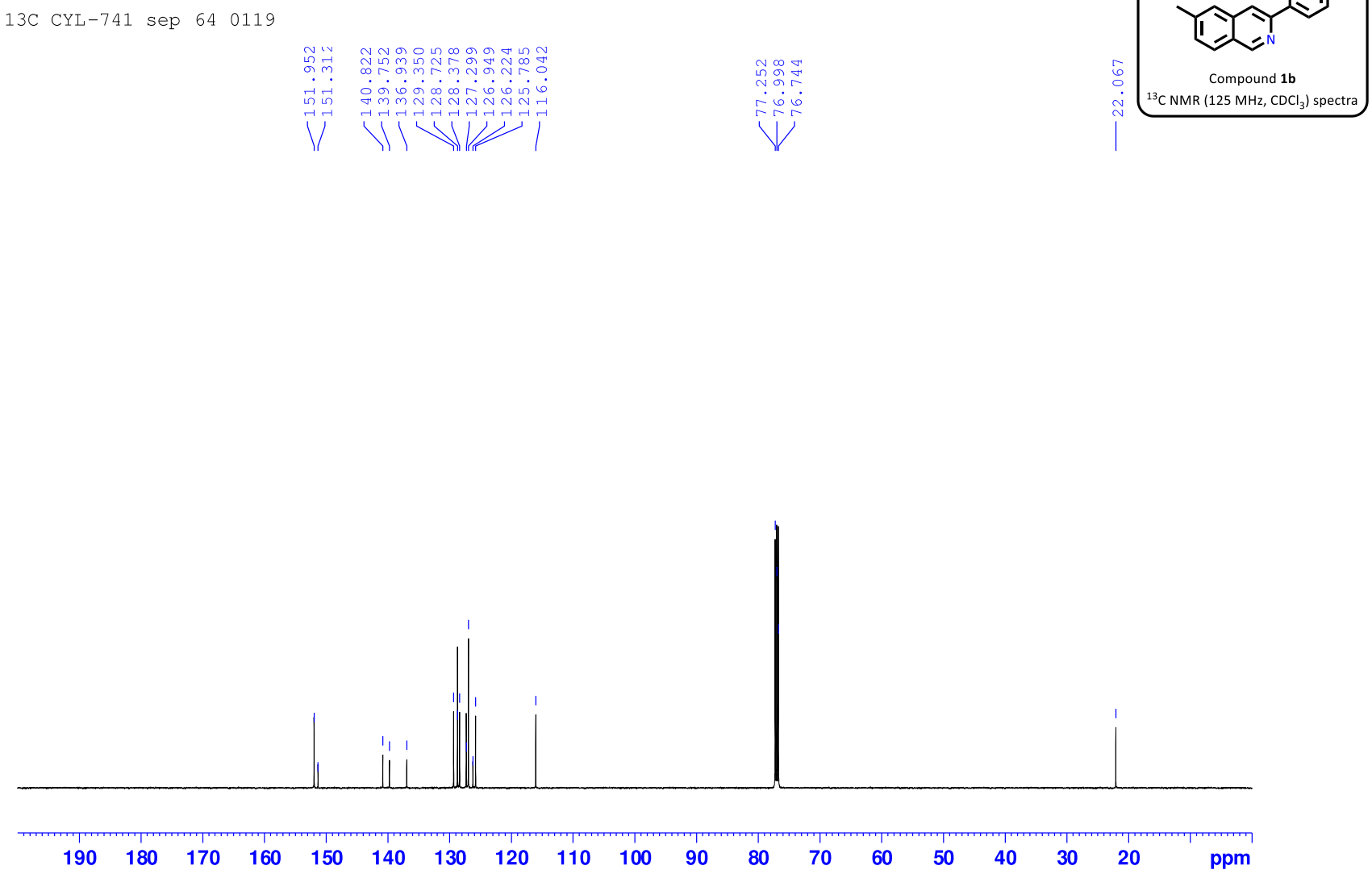


The ^{1}H NMR spectrum in $CDCl_3$ of compound 1b.

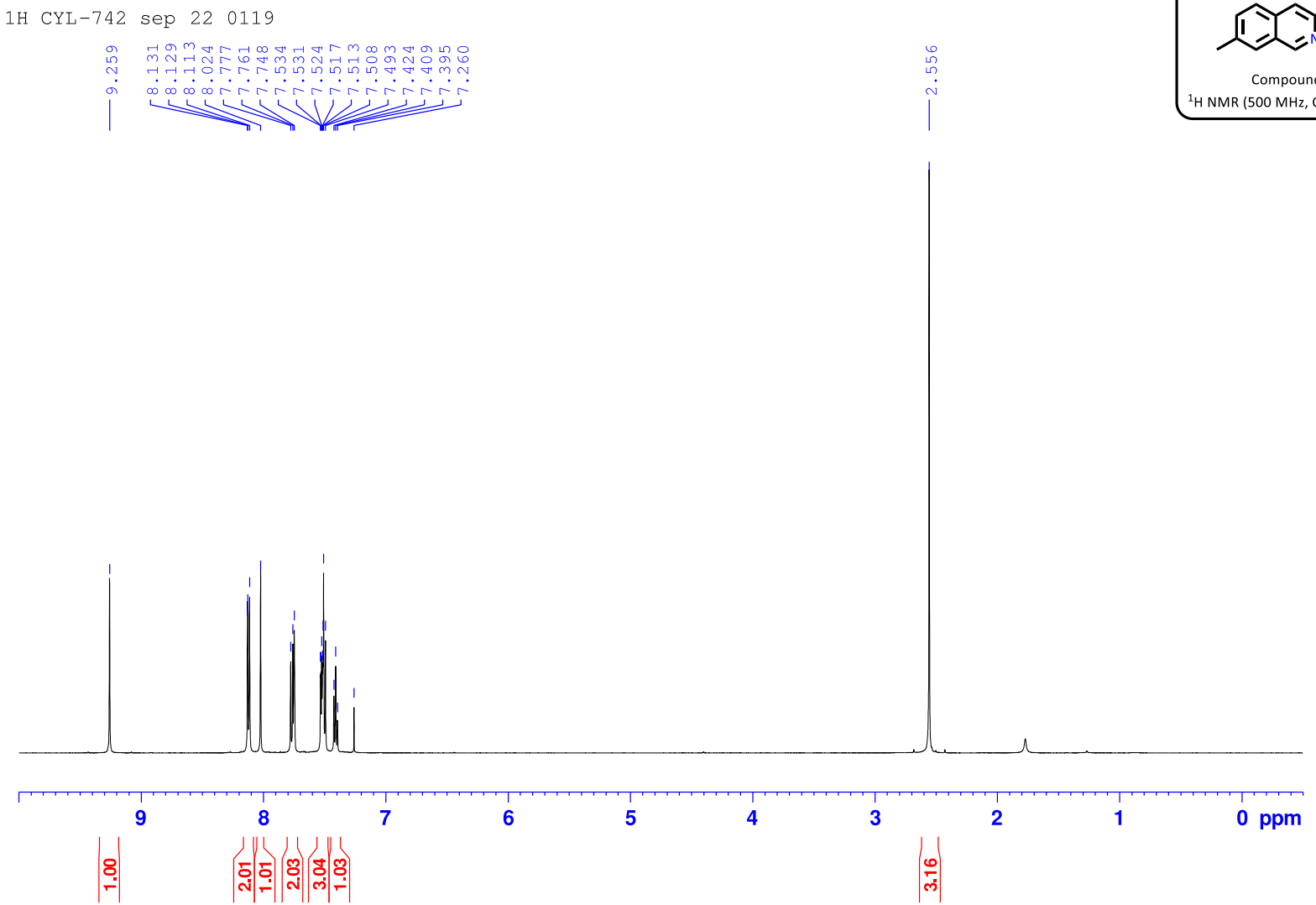


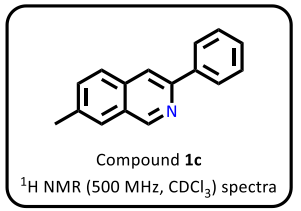


The ^{13}C NMR spectrum in $CDCl_3$ of compound 1b.

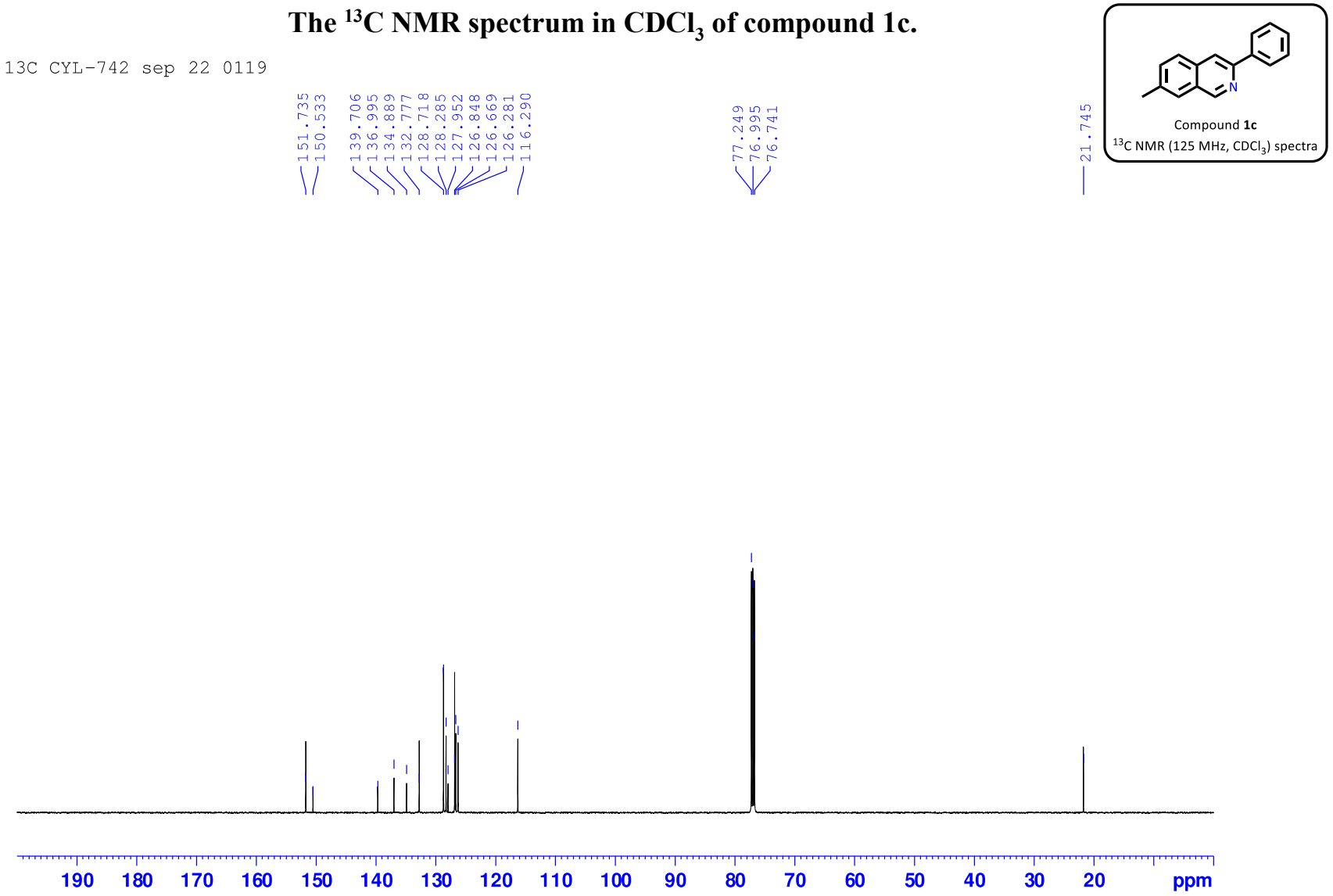


The ^{1}H NMR spectrum in $CDCl_3$ of compound 1c.

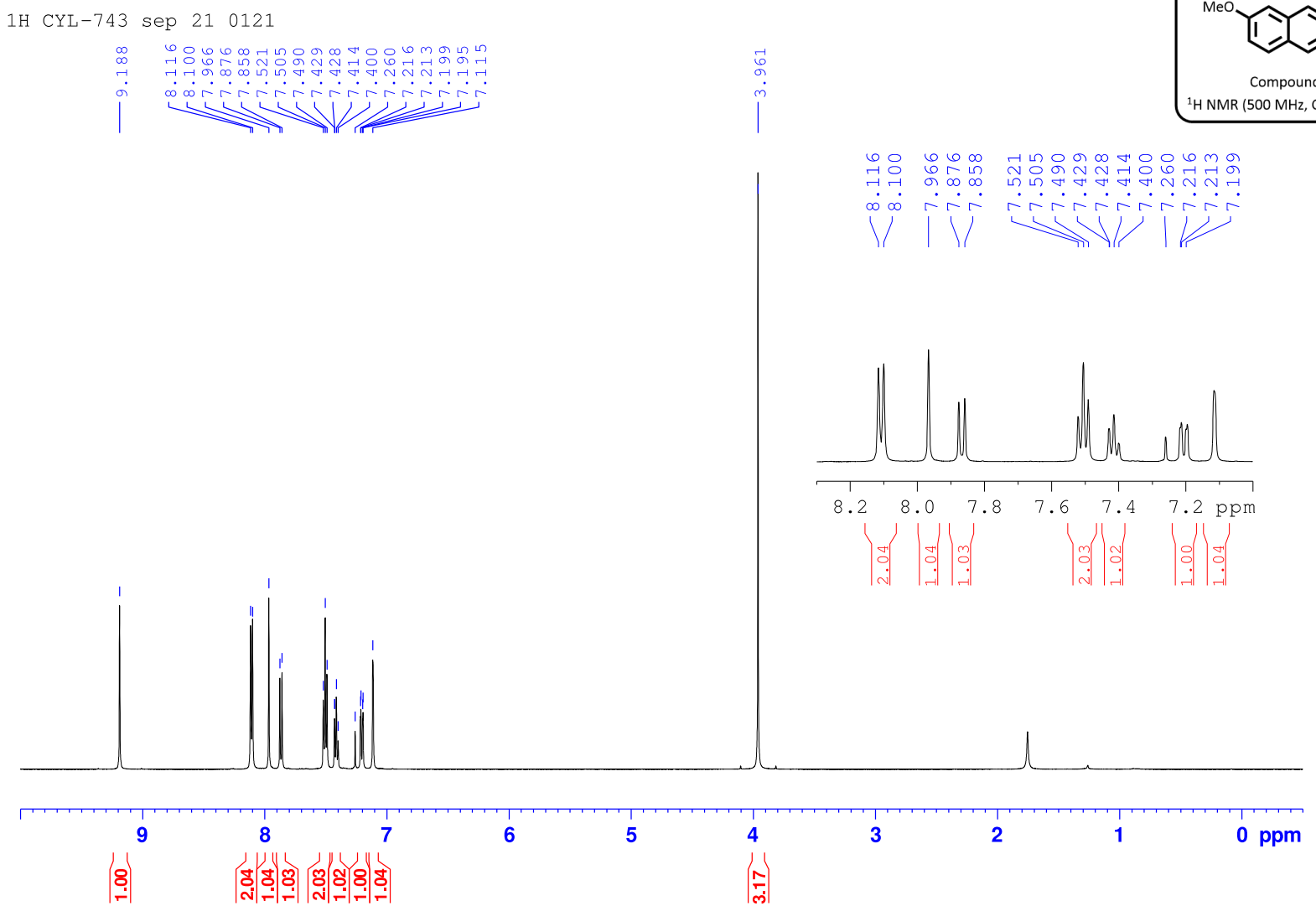




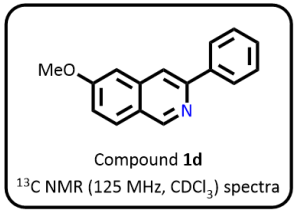
The ^{13}C NMR spectrum in $CDCl_3$ of compound 1c.

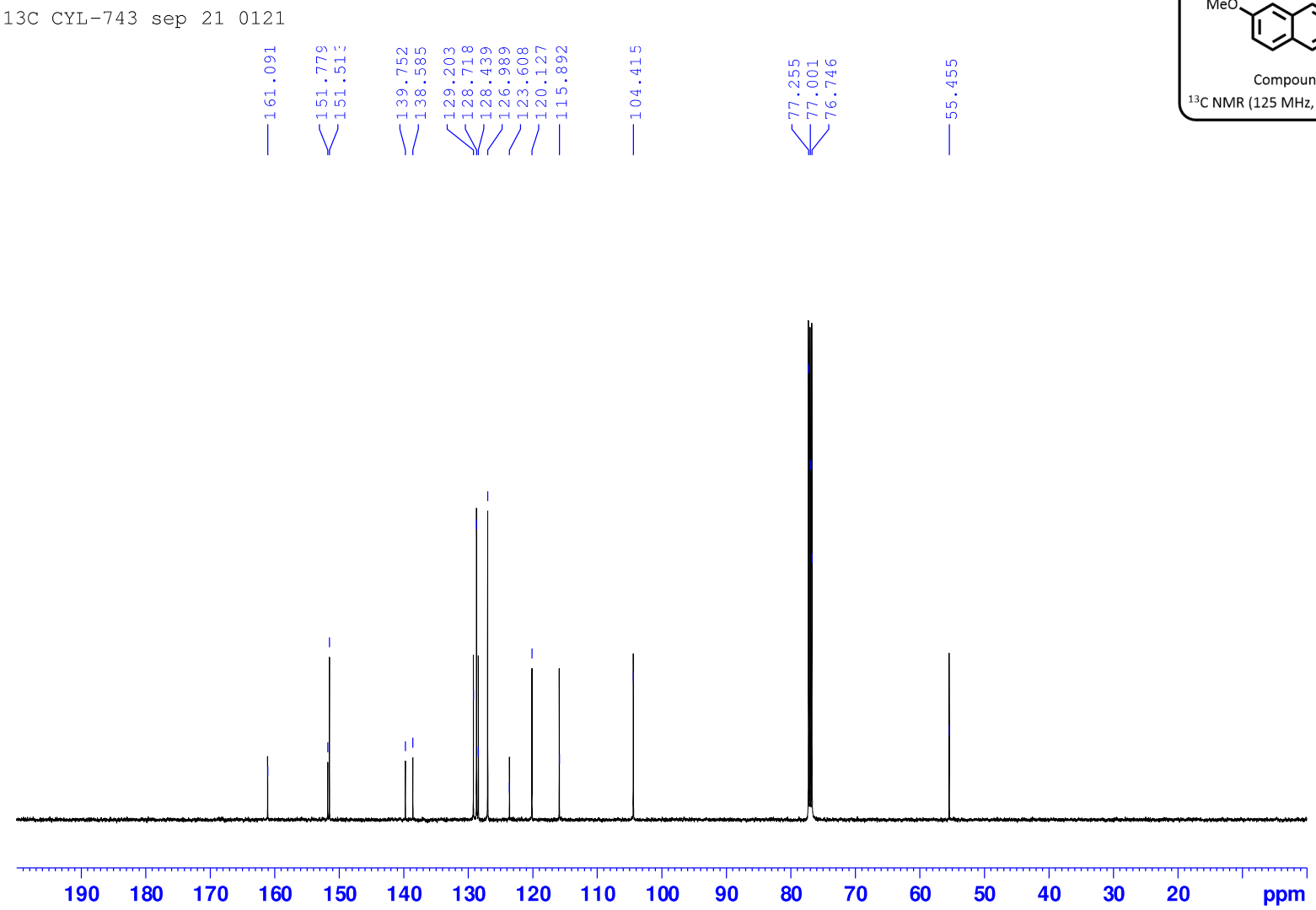


The ^{1}H NMR spectrum in $CDCl_3$ of compound 1d.

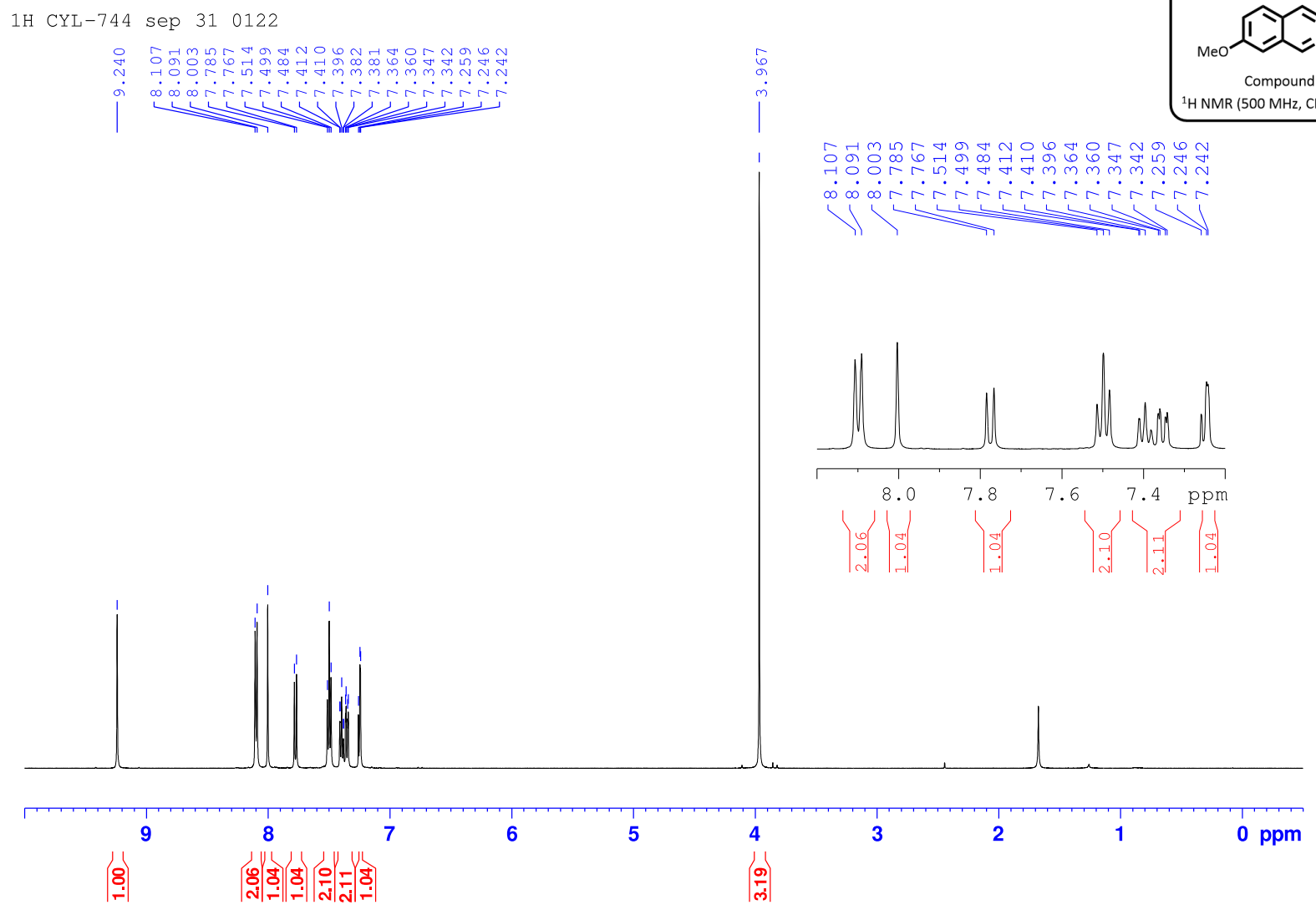


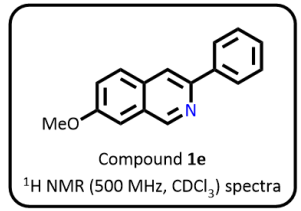
The ^{13}C NMR spectrum in $CDCl_3$ of compound 1d.



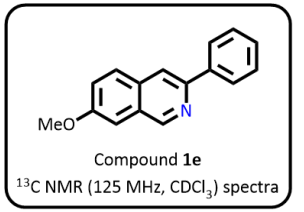


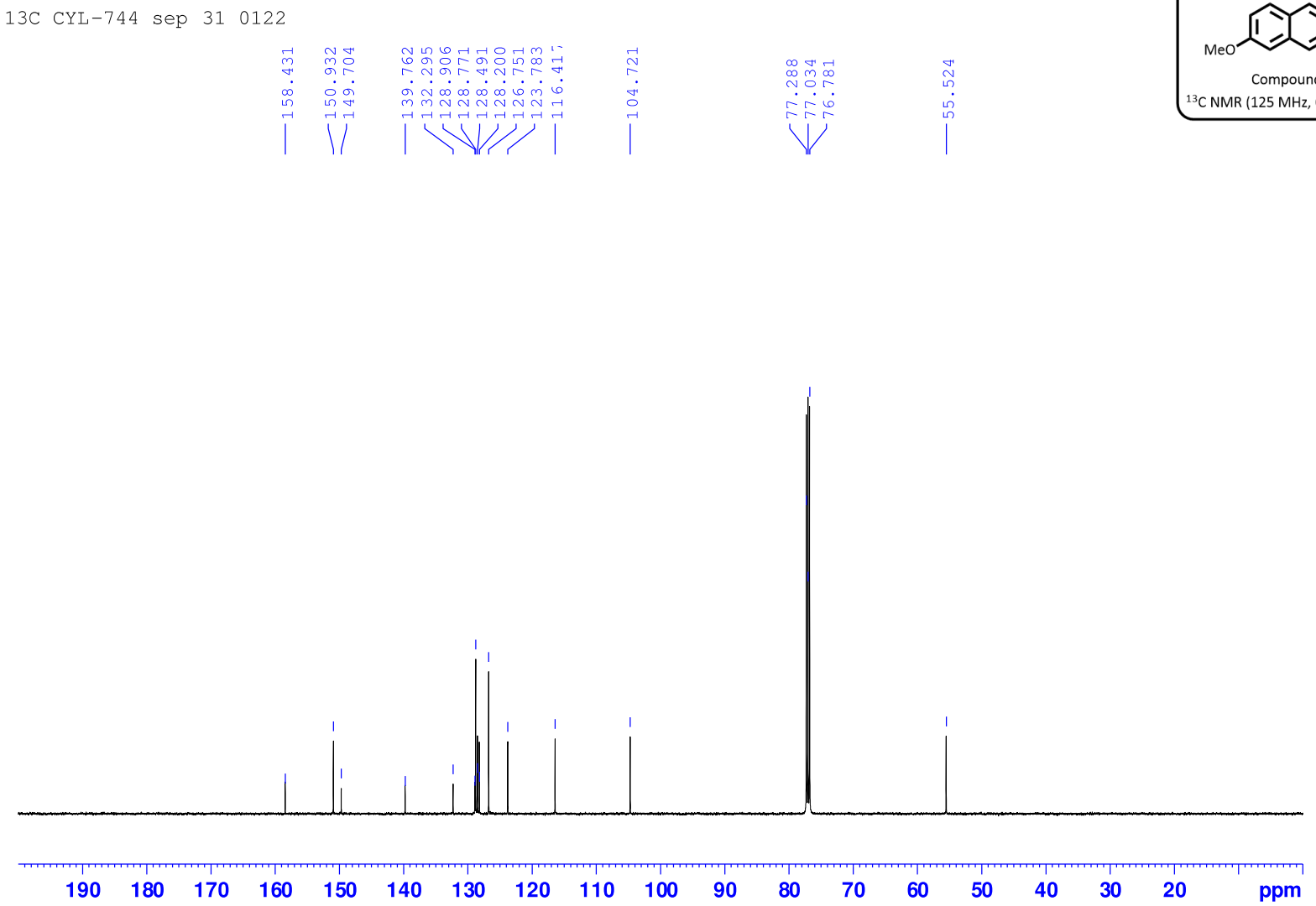
The ^{1}H NMR spectrum in $CDCl_3$ of compound 1e.



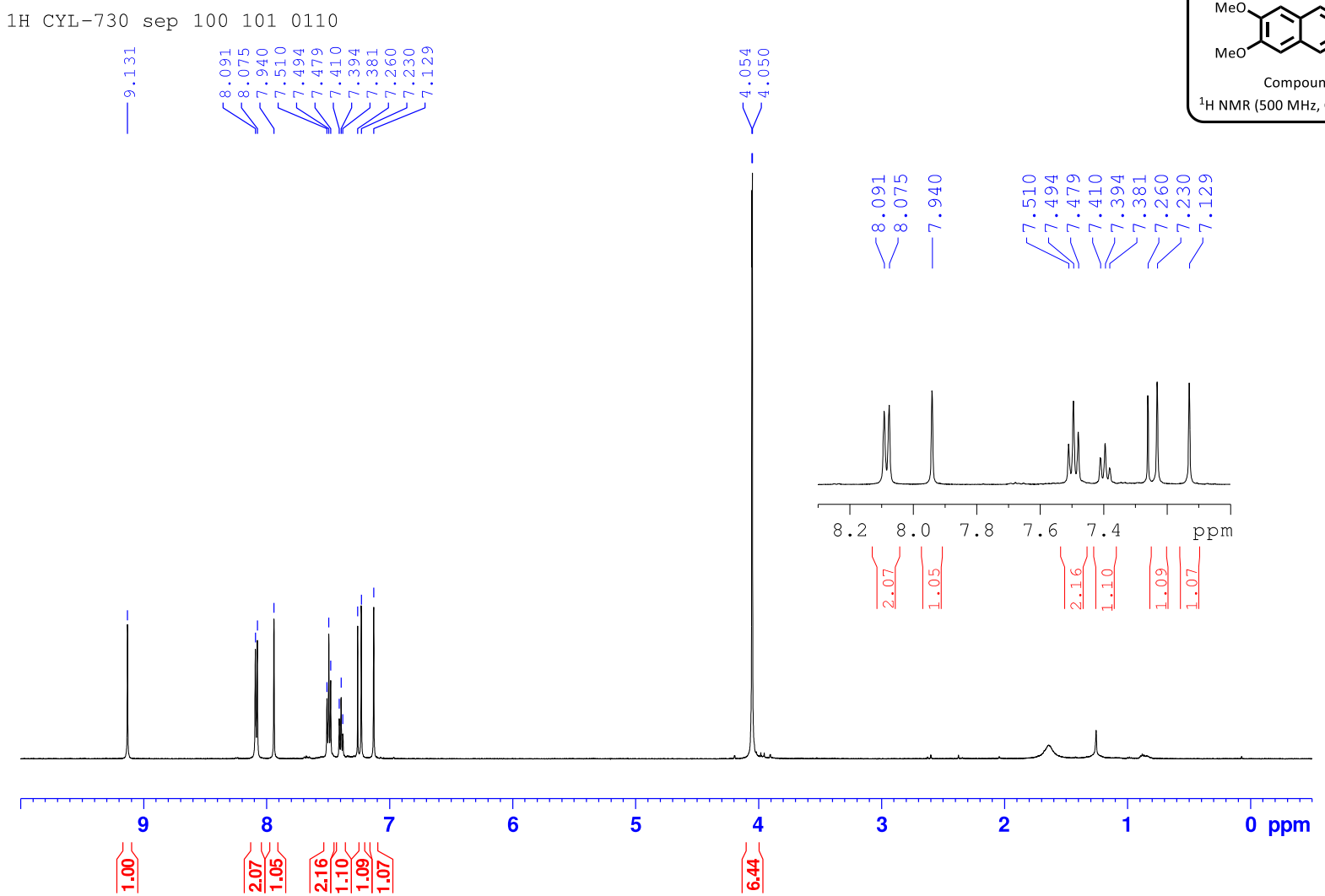


The ^{13}C NMR spectrum in $CDCl_3$ of compound 1e.

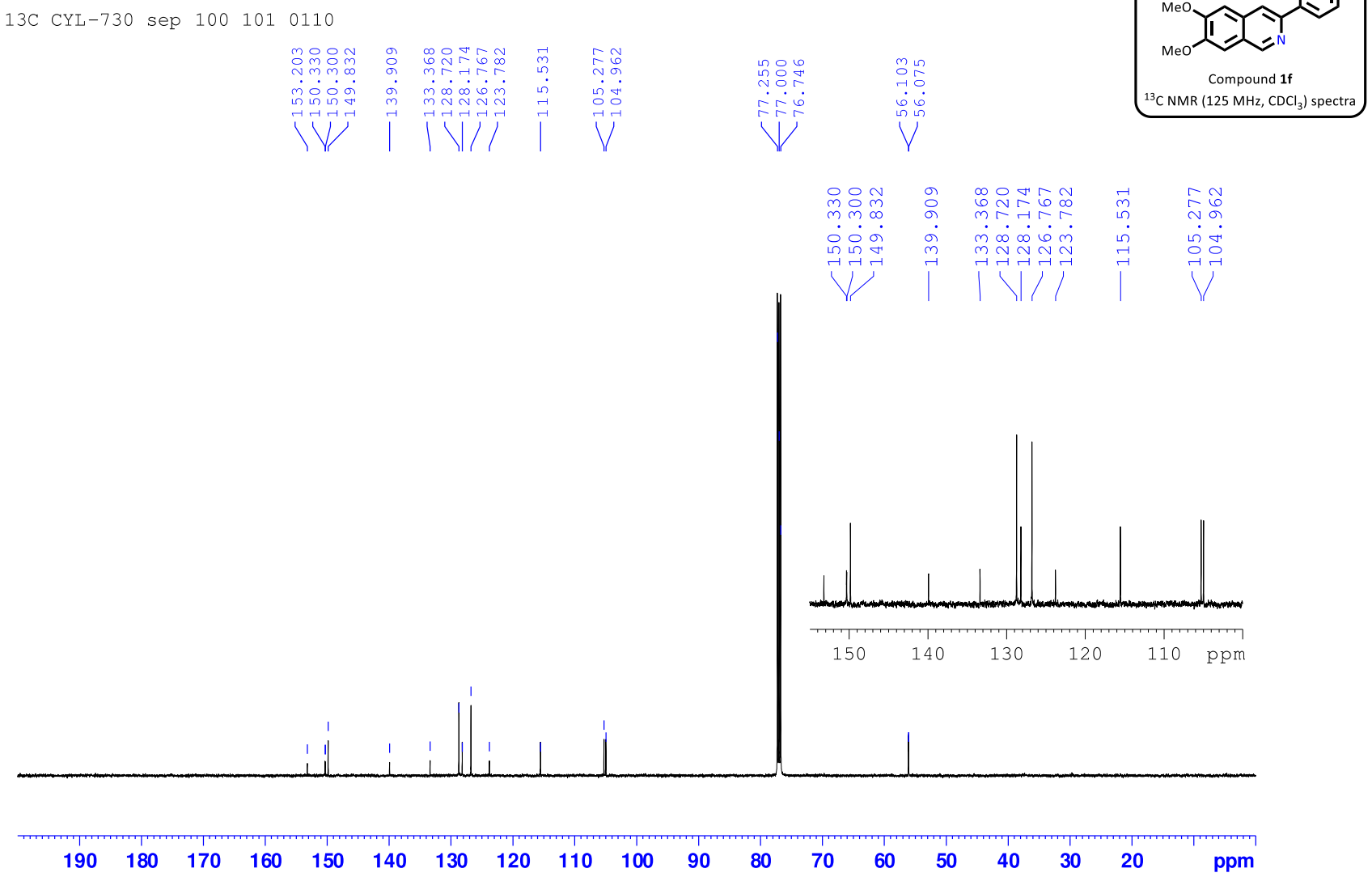




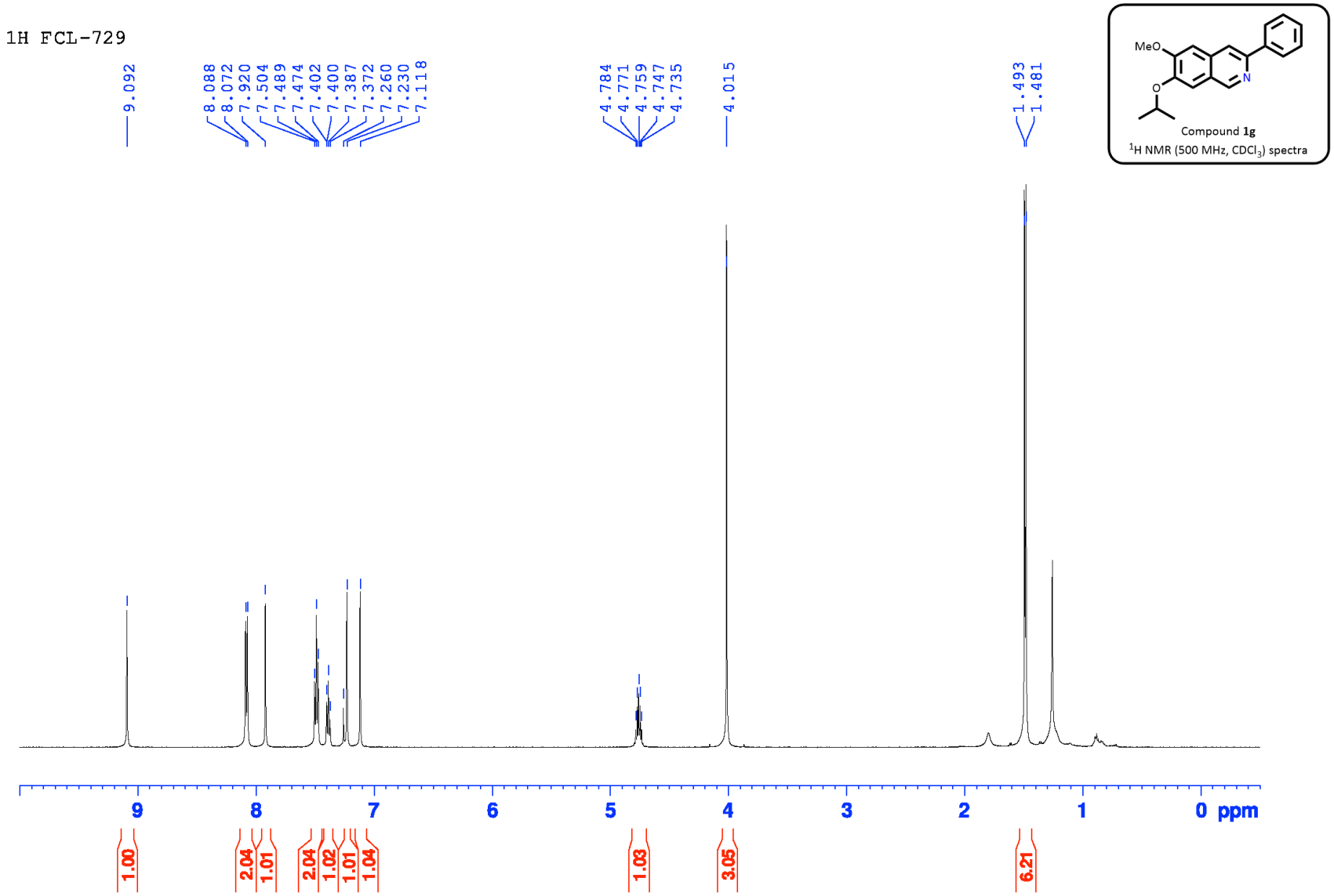
The ^{1}H NMR spectrum in $CDCl_3$ of compound 1f.



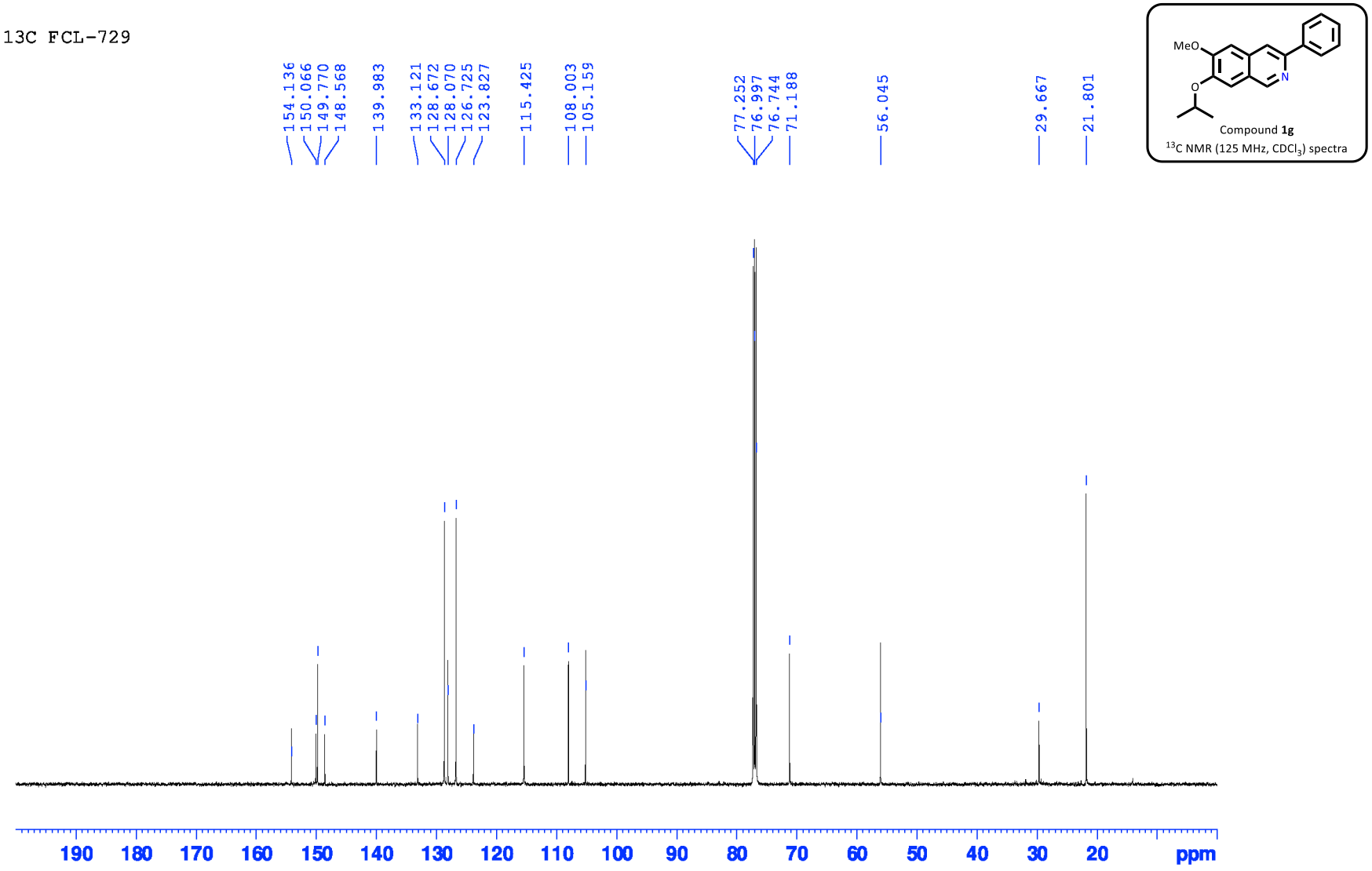
The ^{13}C NMR spectrum in $CDCl_3$ of compound 1f.



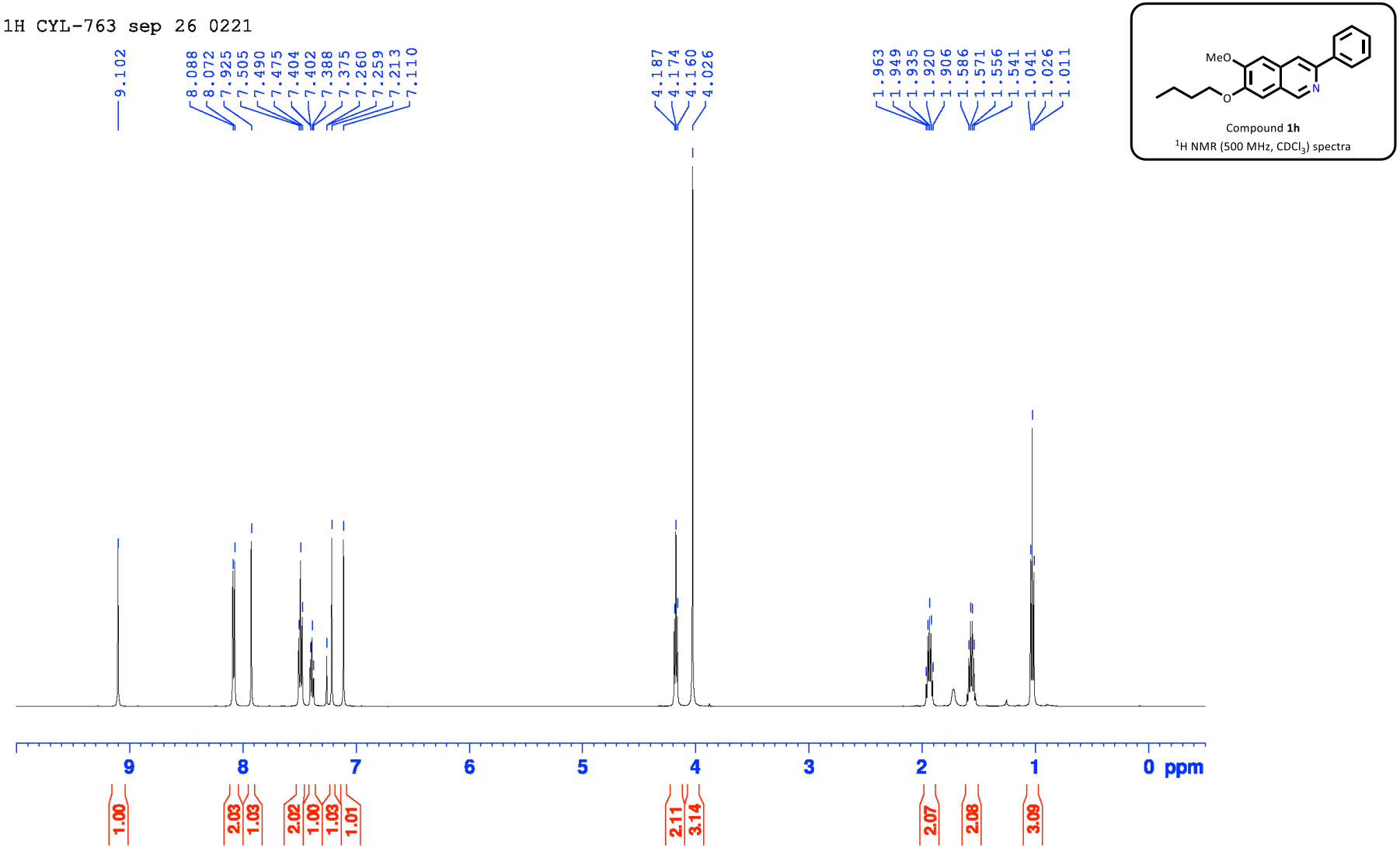
The ^{1}H NMR spectrum in $CDCl_3$ of compound 1g.



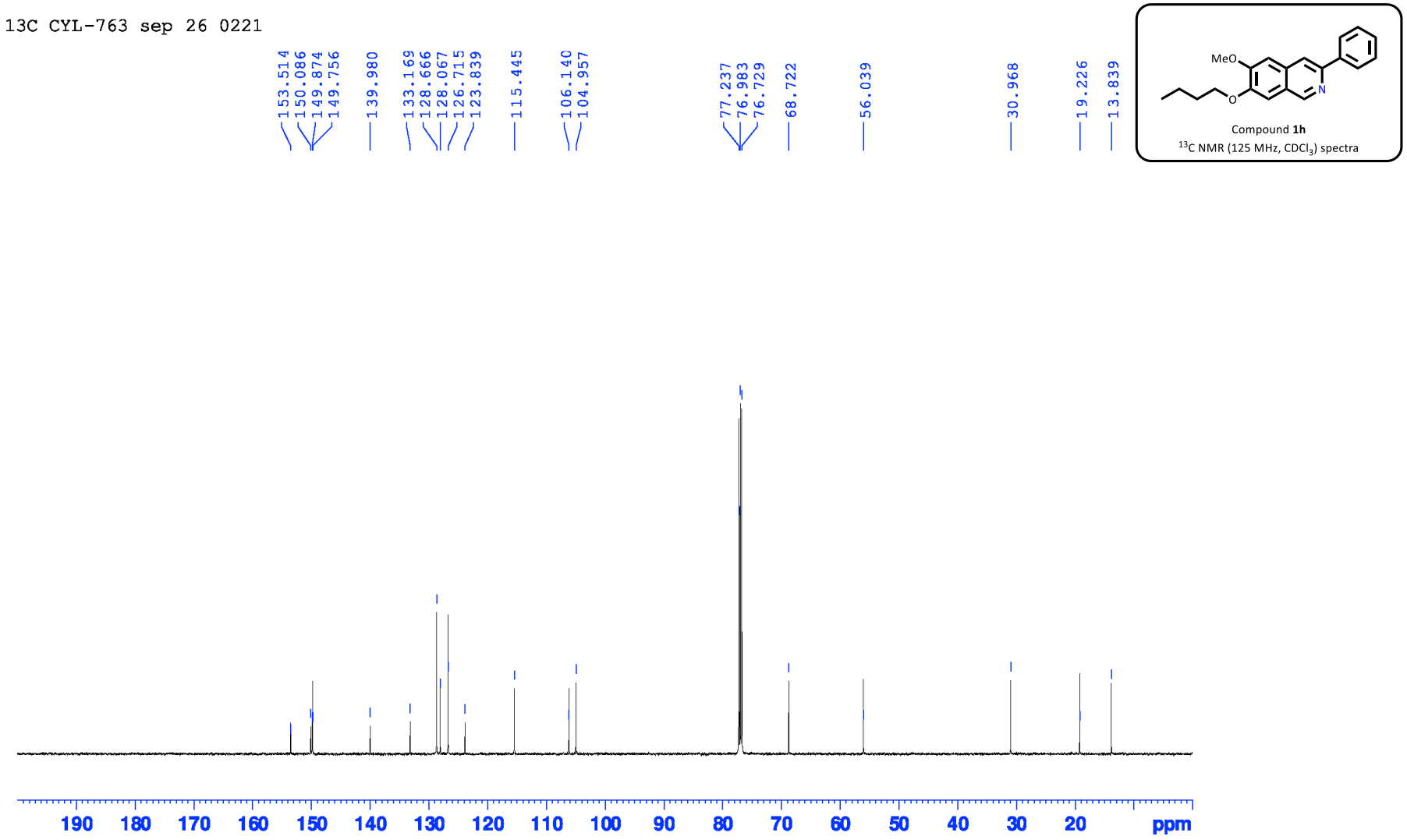
The ^{13}C NMR spectrum in $CDCl_3$ of compound 1g.



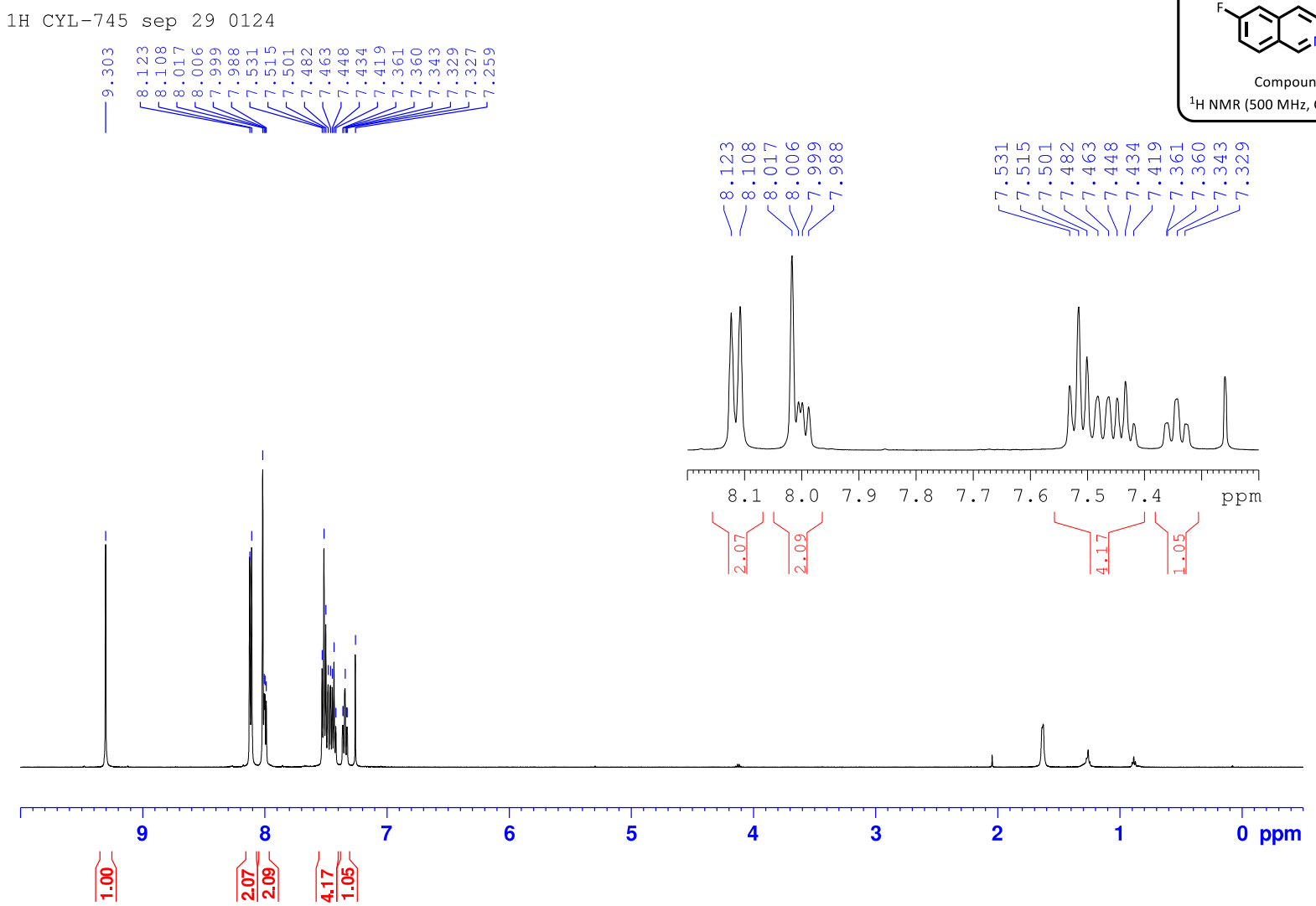
The ^{1}H NMR spectrum in $CDCl_3$ of compound 1h.

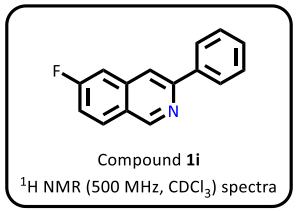


The ^{13}C NMR spectrum in $CDCl_3$ of compound 1h.

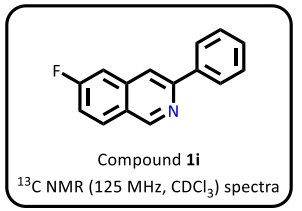


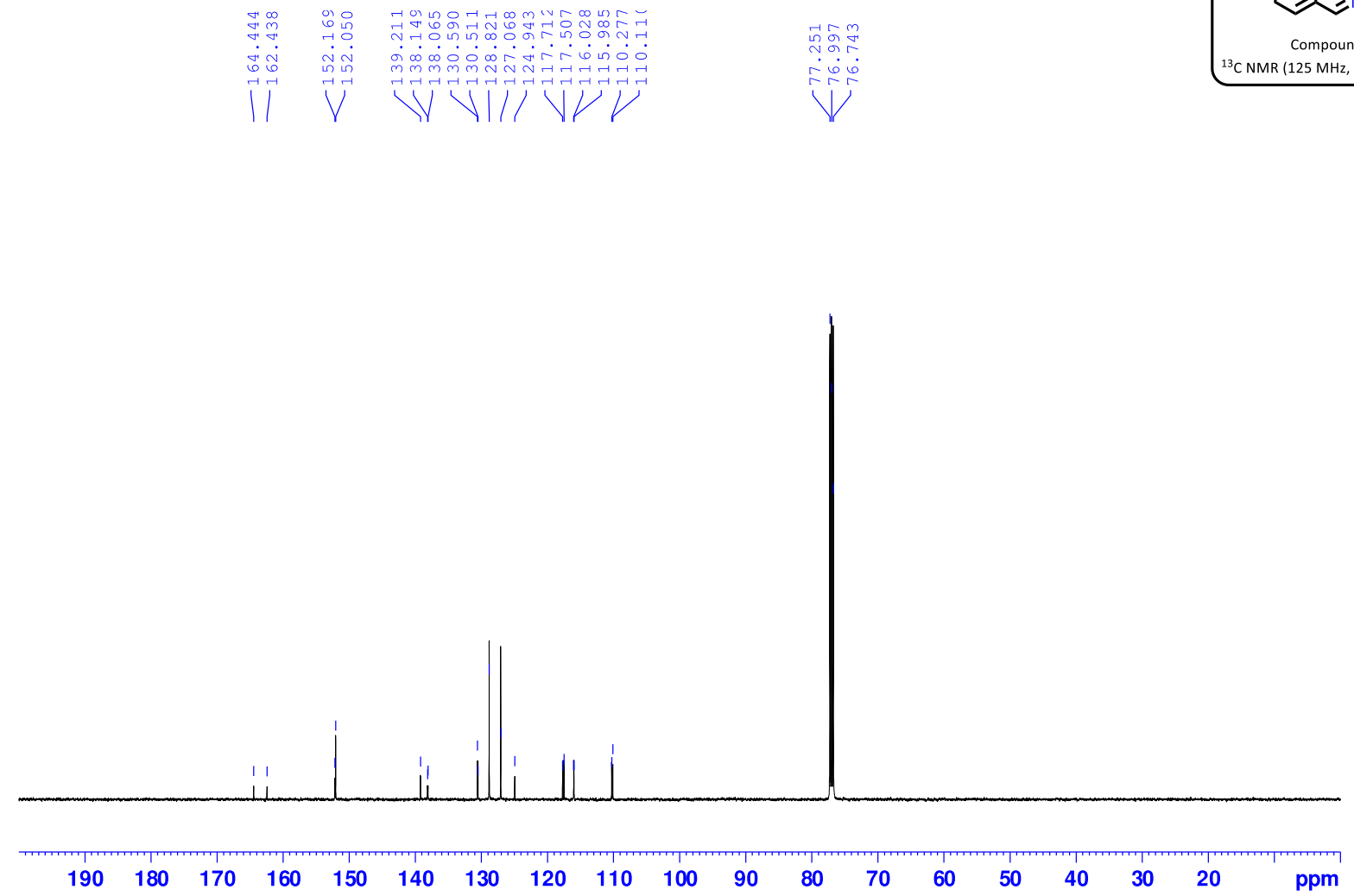
The ^{1}H NMR spectrum in $CDCl_3$ of compound 1i.



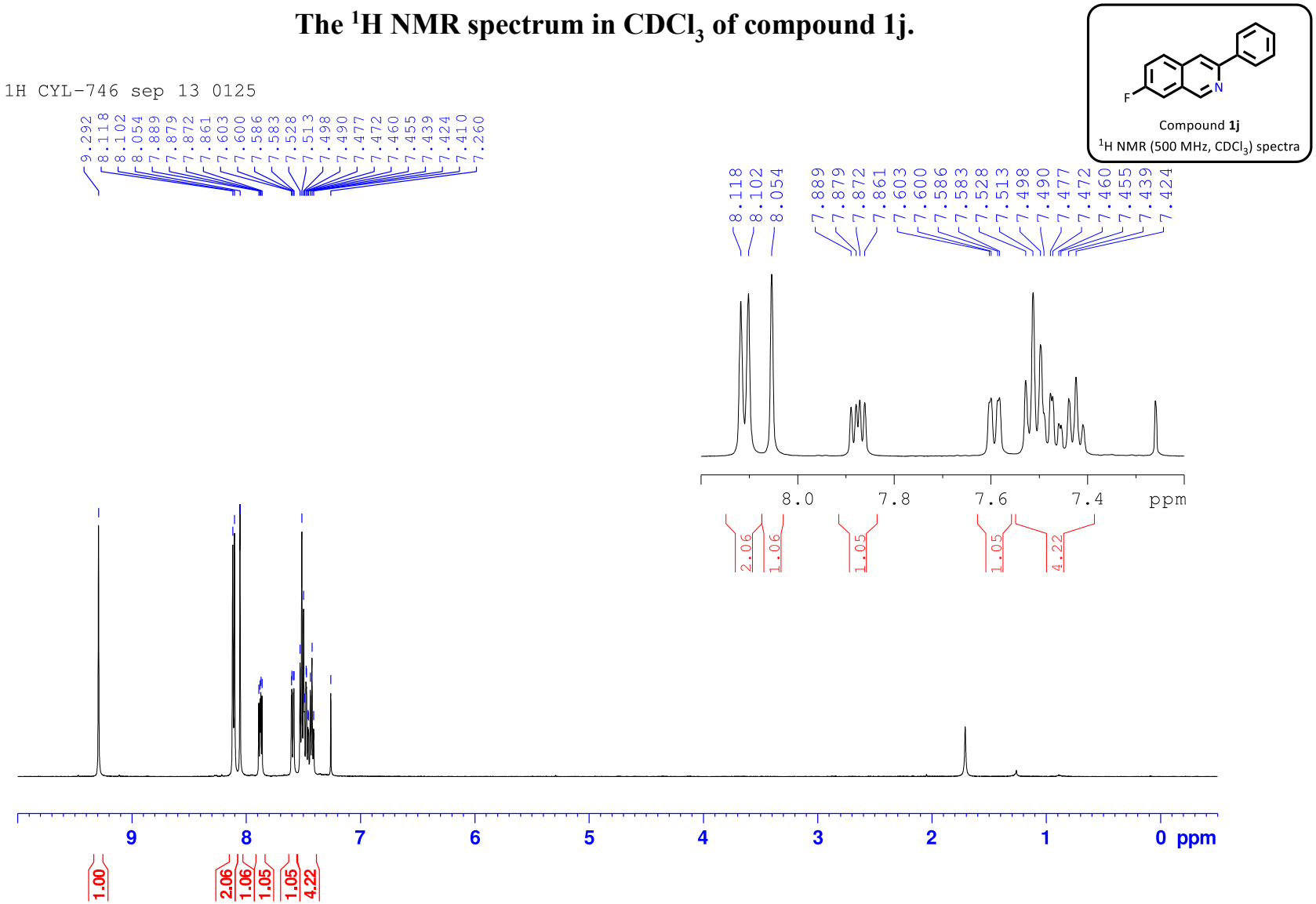


The ^{13}C NMR spectrum in $CDCl_3$ of compound 1i.

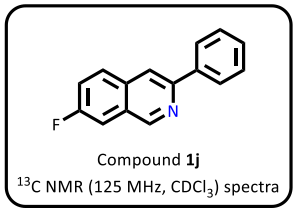


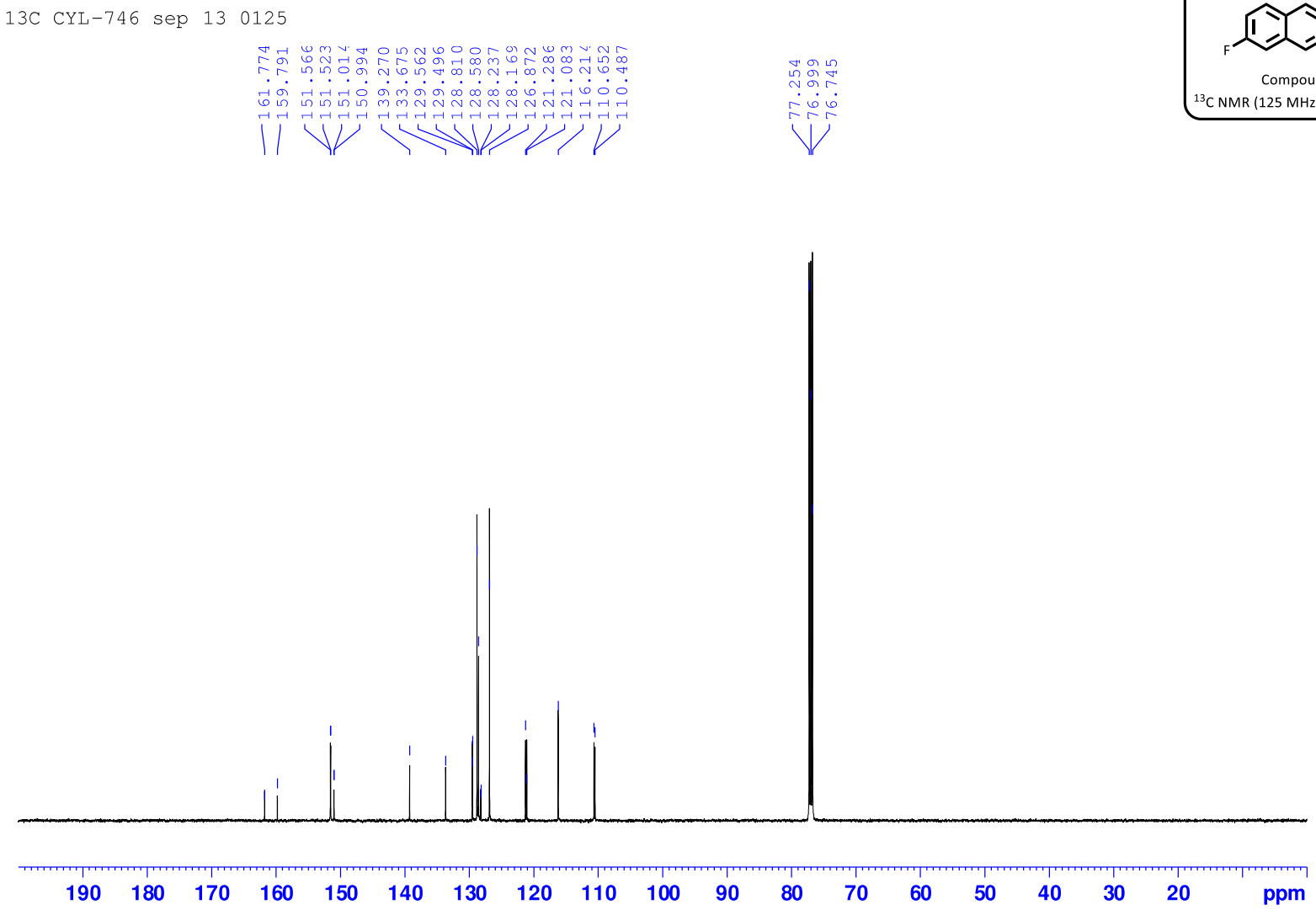


The ^{1}H NMR spectrum in $CDCl_3$ of compound 1j.

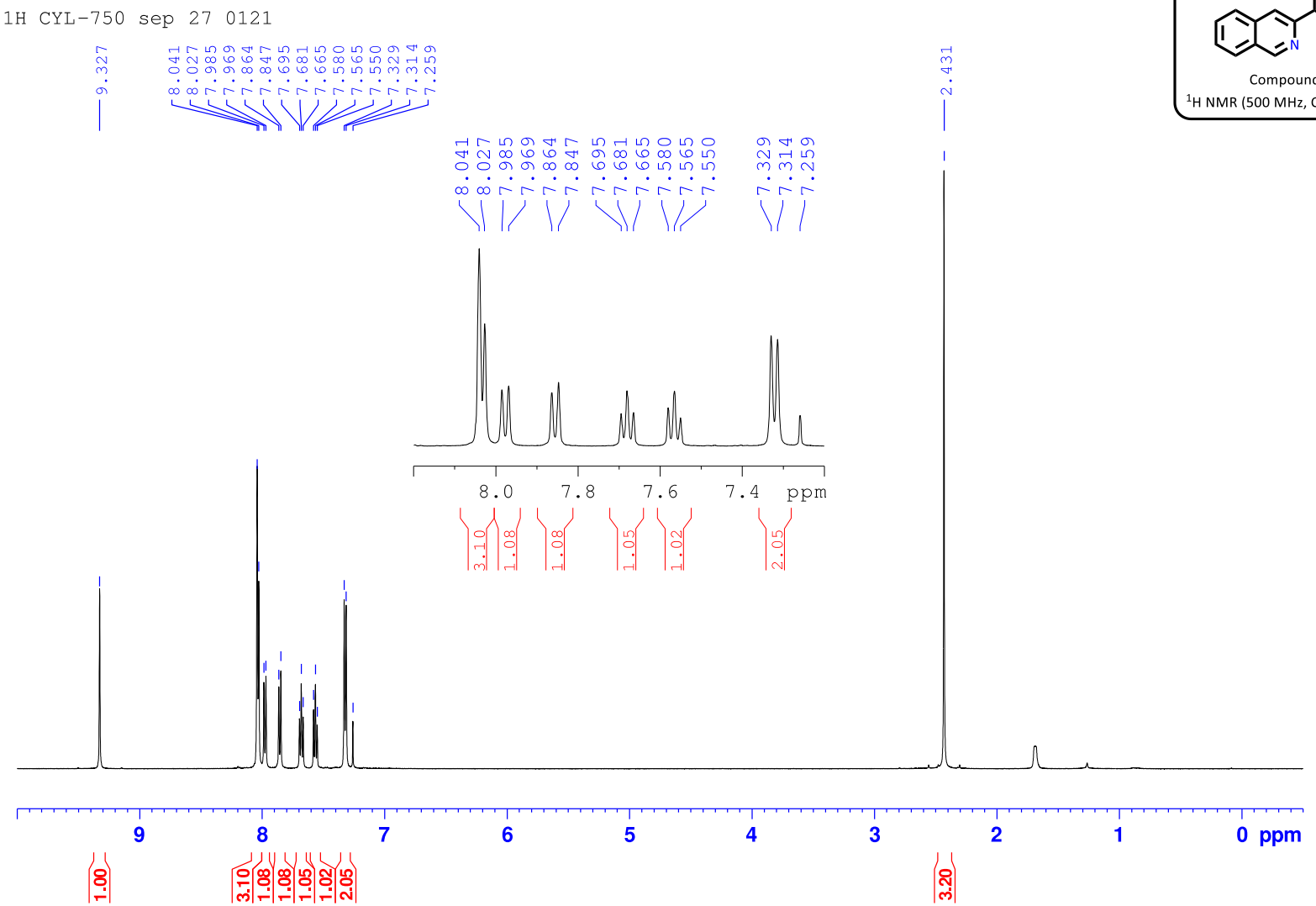


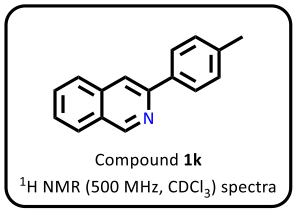
The ^{13}C NMR spectrum in $CDCl_3$ of compound 1j.





The ^{1}H NMR spectrum in $CDCl_3$ of compound 1k.

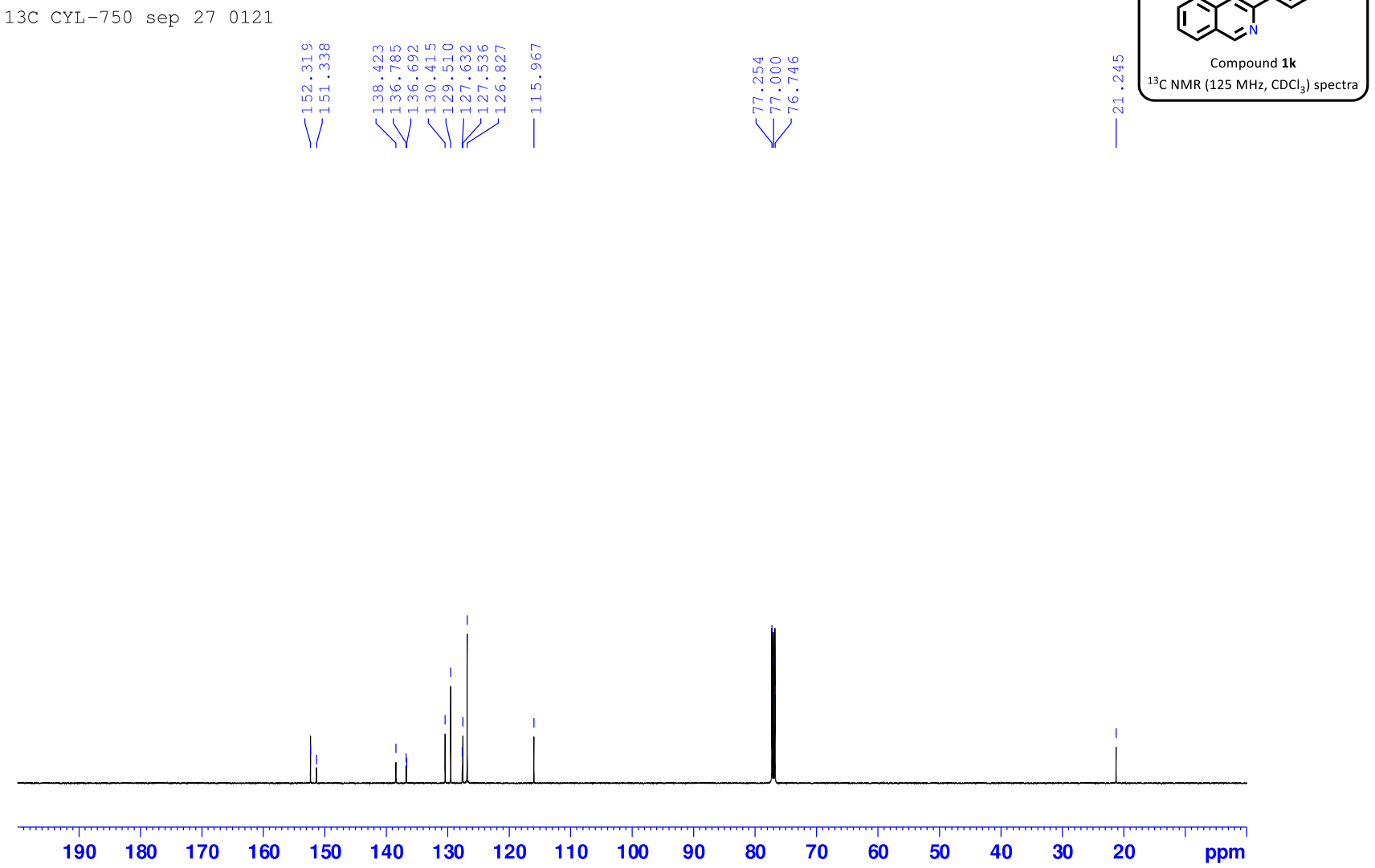




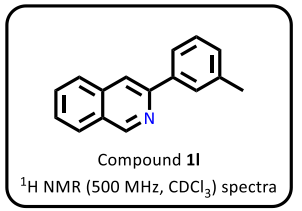
Compound **1k**

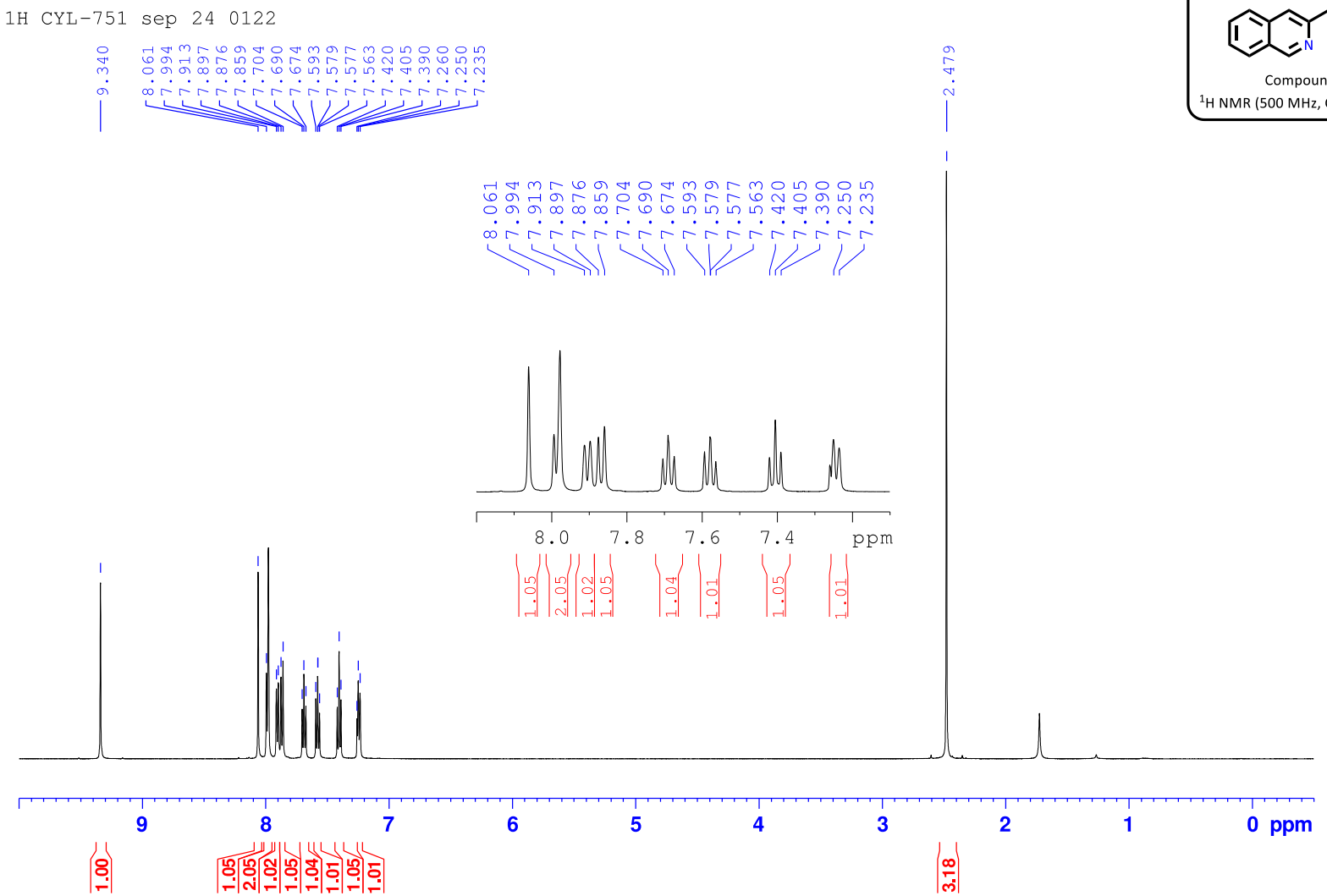
^{1}H NMR (500 MHz, $CDCl_3$) spectra

The ^{13}C NMR spectrum in $CDCl_3$ of compound 1k.

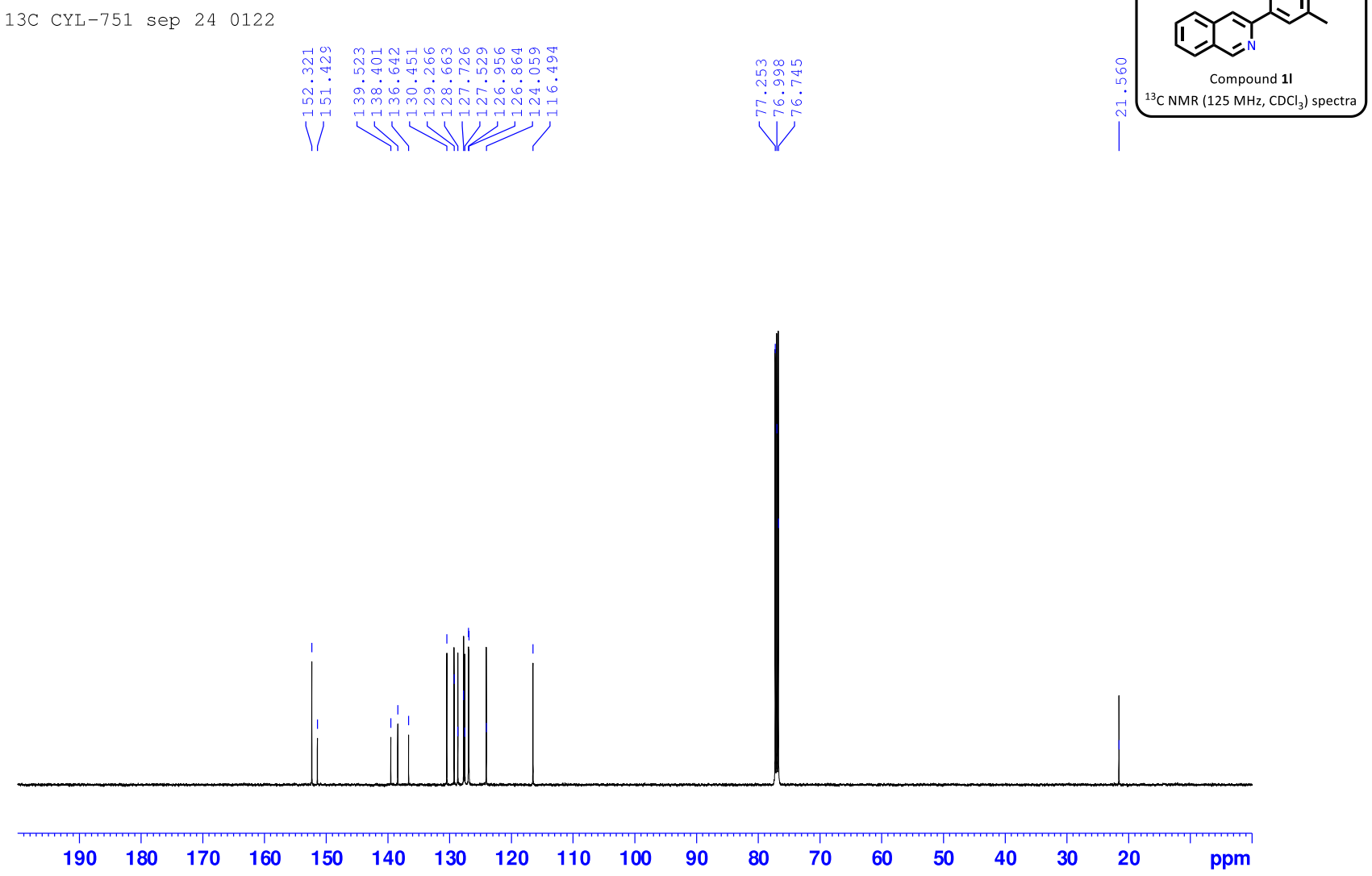


The ^{1}H NMR spectrum in $CDCl_3$ of compound 1l.

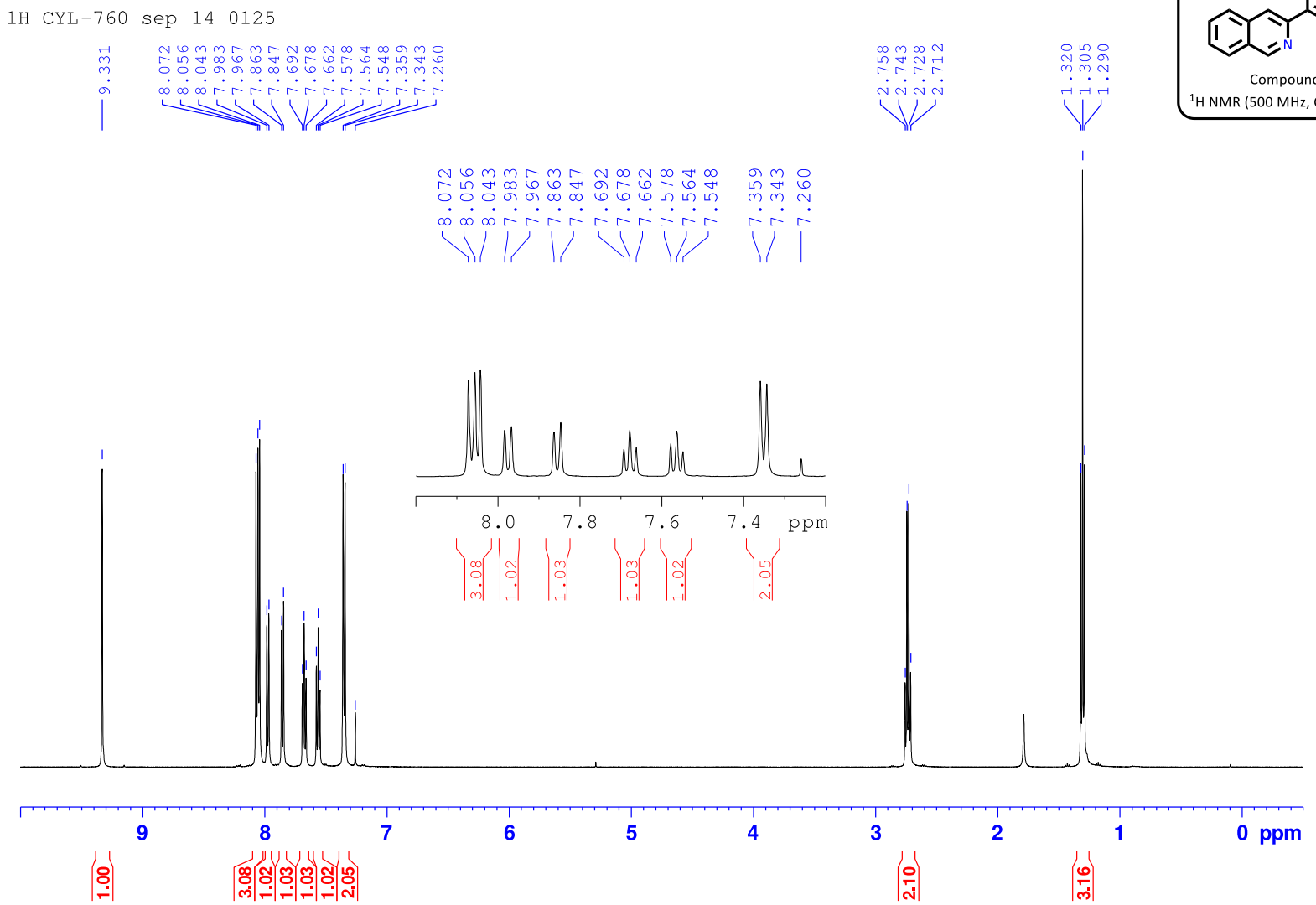


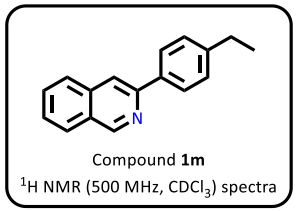


The ^{13}C NMR spectrum in $CDCl_3$ of compound 1l.

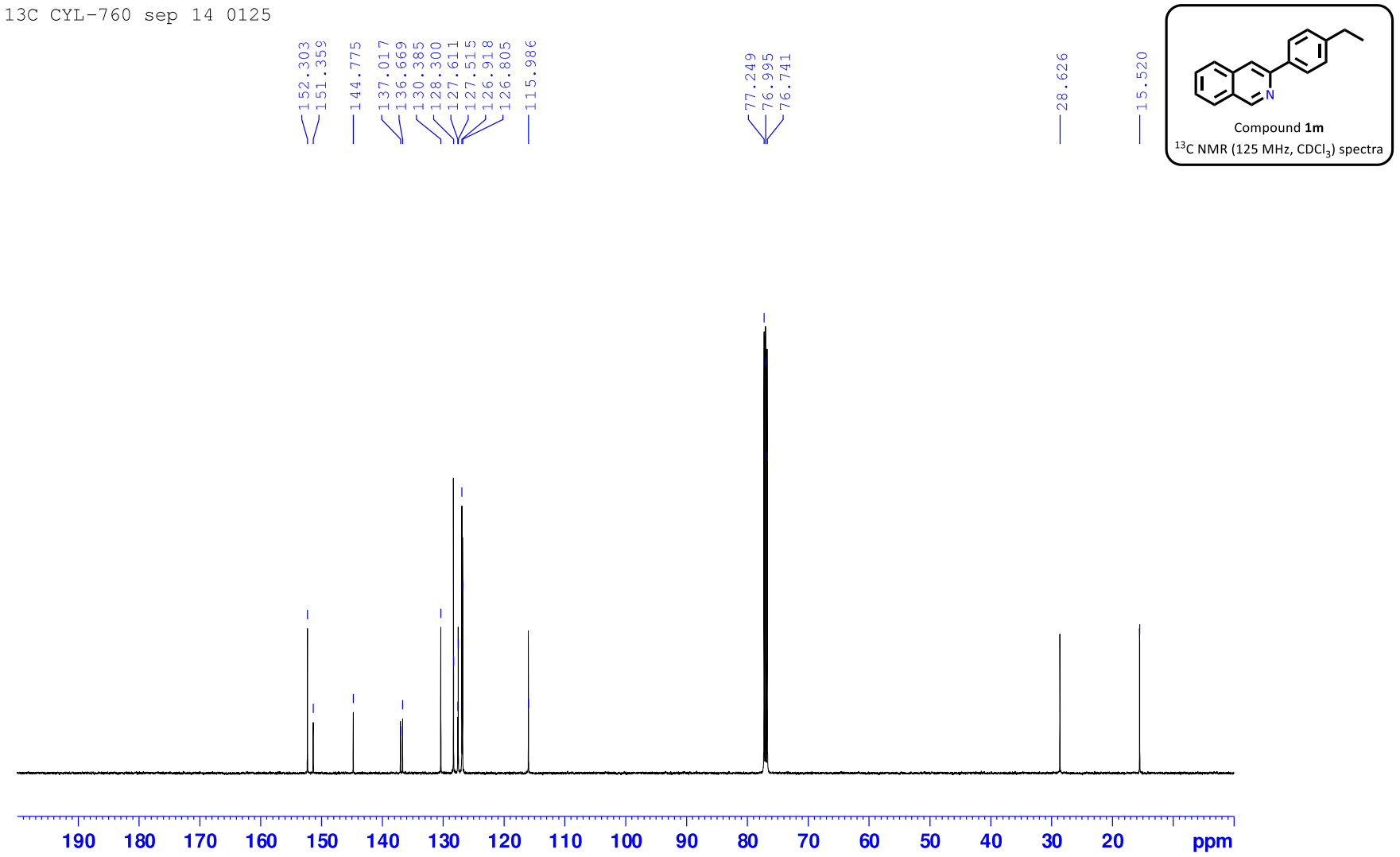


The ^{1}H NMR spectrum in $CDCl_3$ of compound 1m.

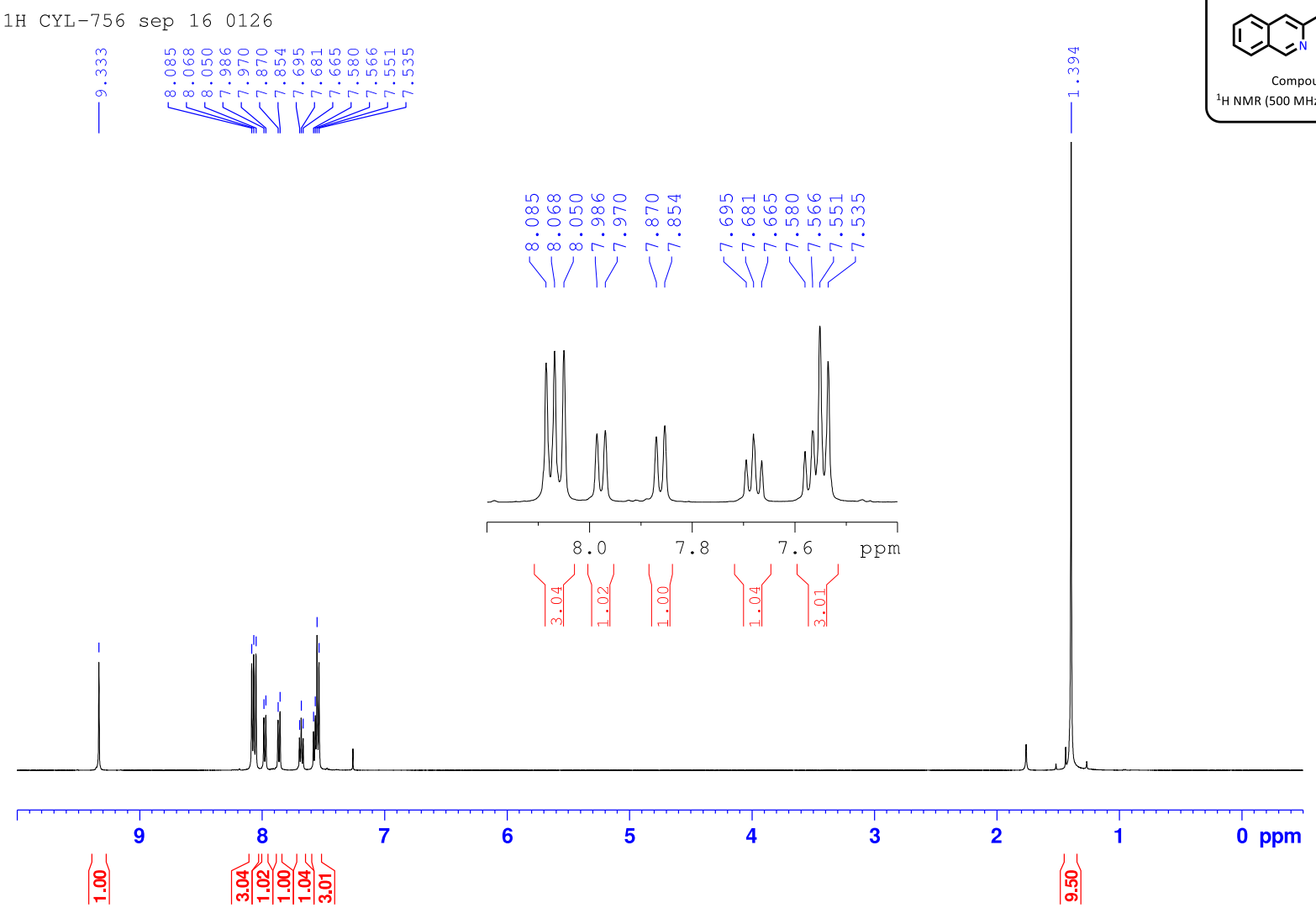


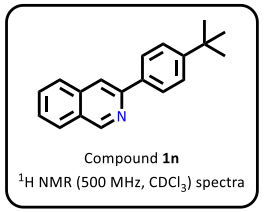


The ^{13}C NMR spectrum in $CDCl_3$ of compound 1m.

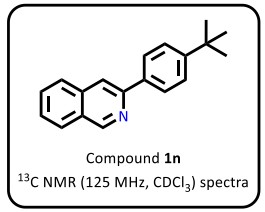


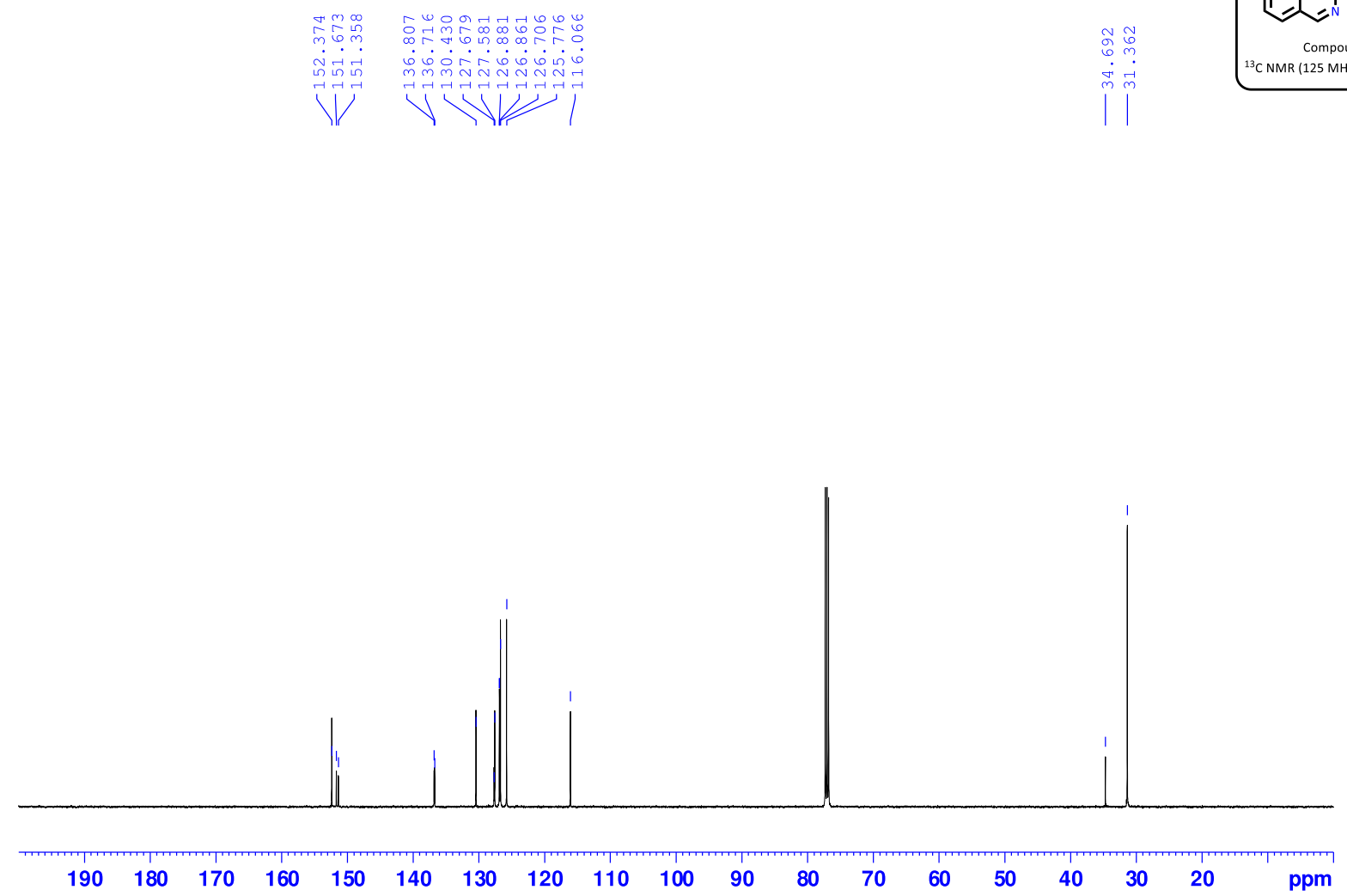
The ^{1}H NMR spectrum in $CDCl_3$ of compound 1n.



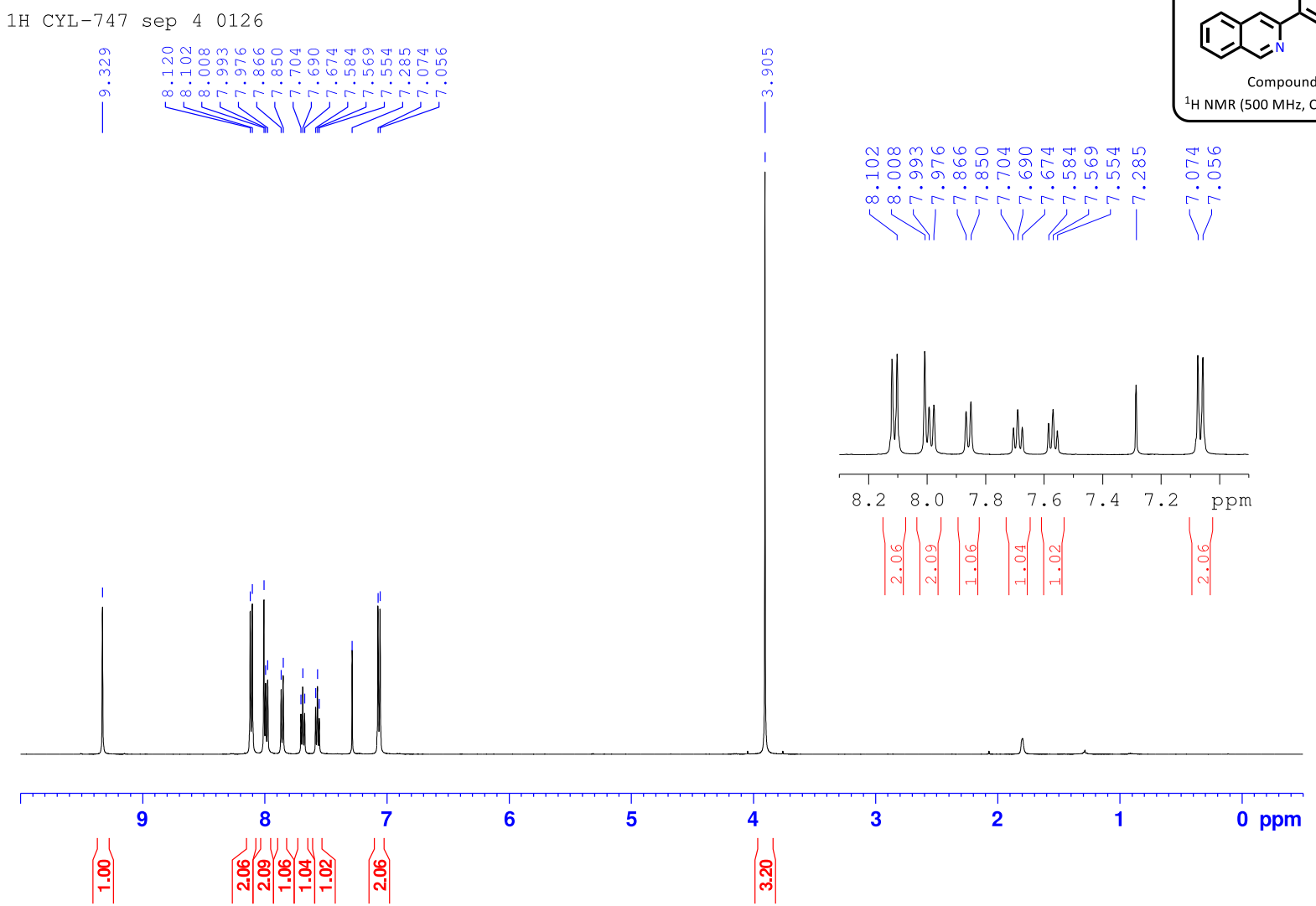


The ^{13}C NMR spectrum in $CDCl_3$ of compound 1n.

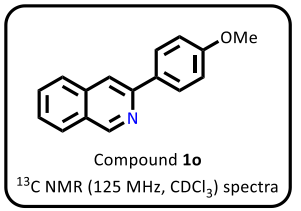


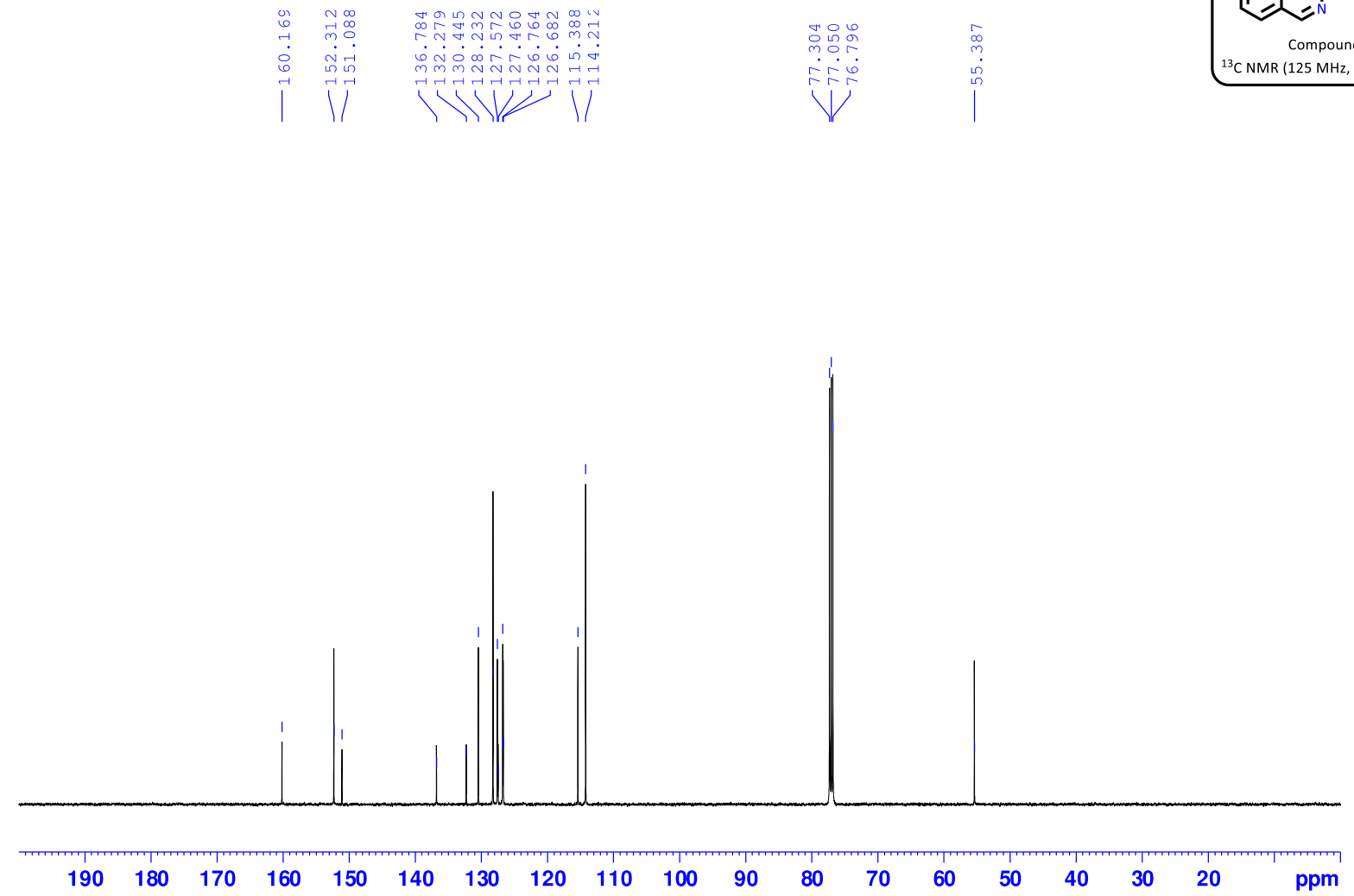


The ^{1}H NMR spectrum in $CDCl_3$ of compound 1o.

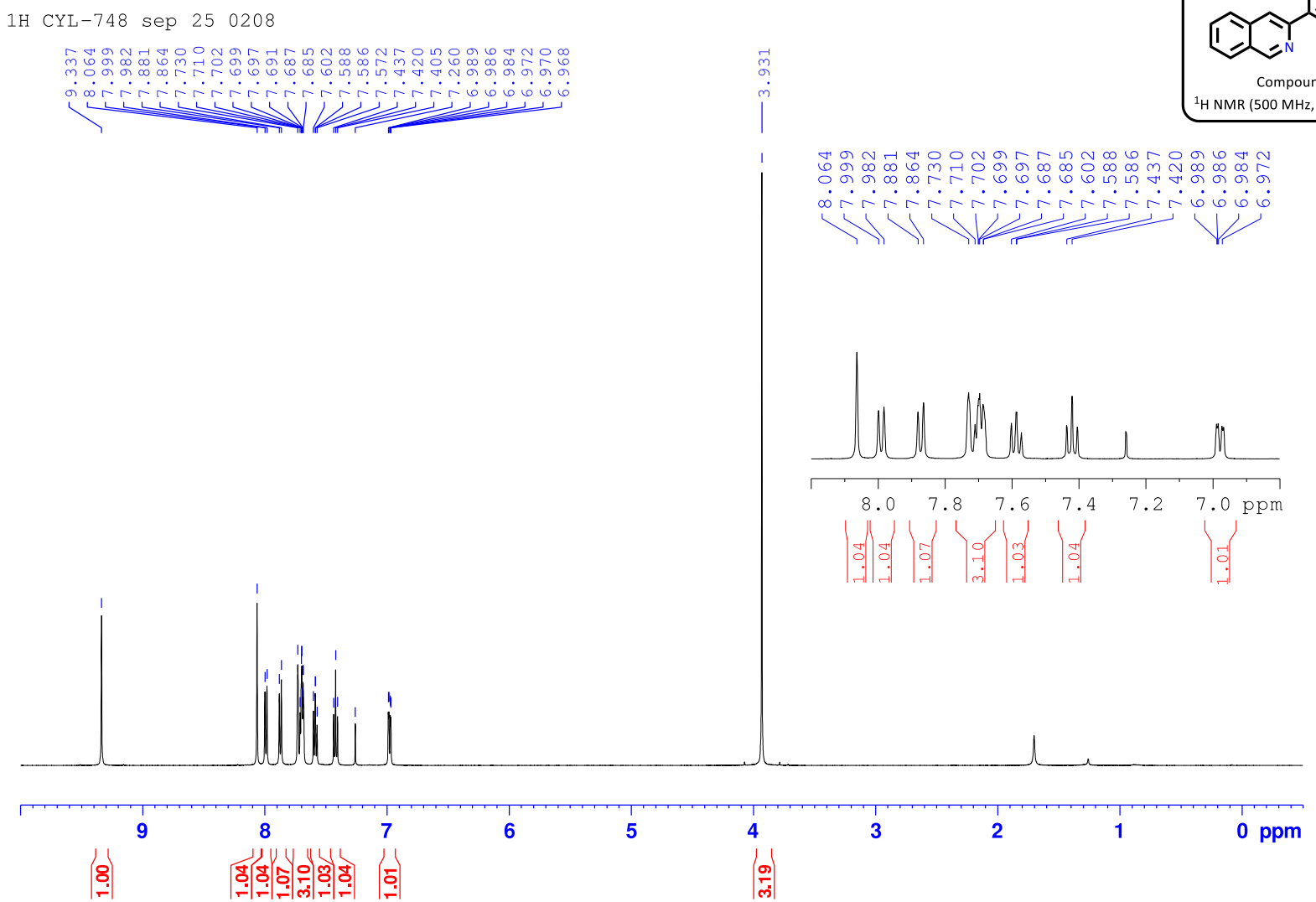


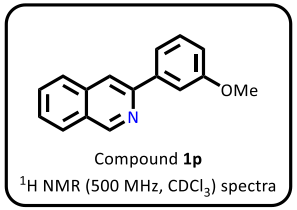
The ^{13}C NMR spectrum in $CDCl_3$ of compound 1o.



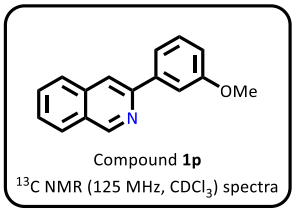


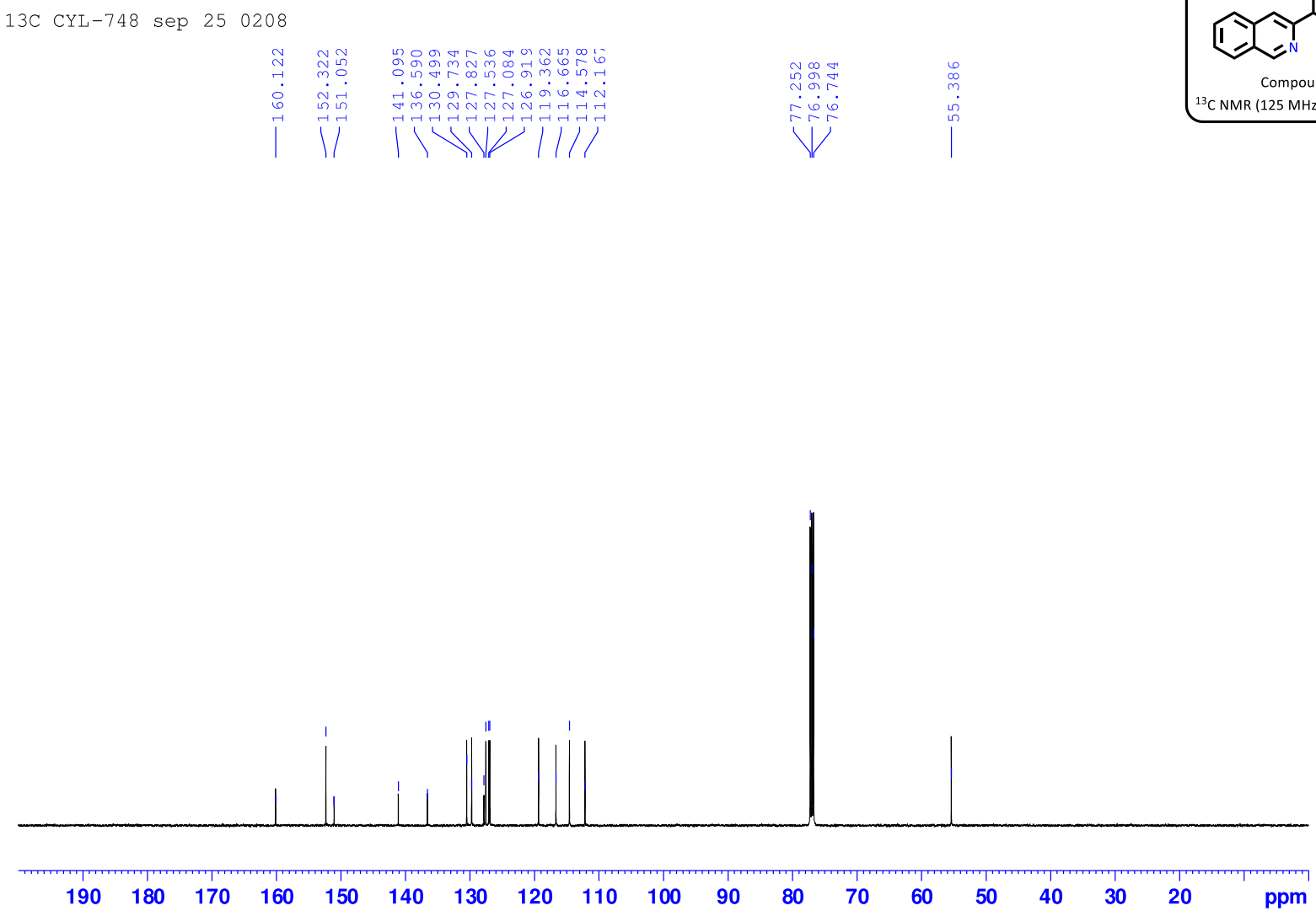
The ^{1}H NMR spectrum in $CDCl_3$ of compound 1p.



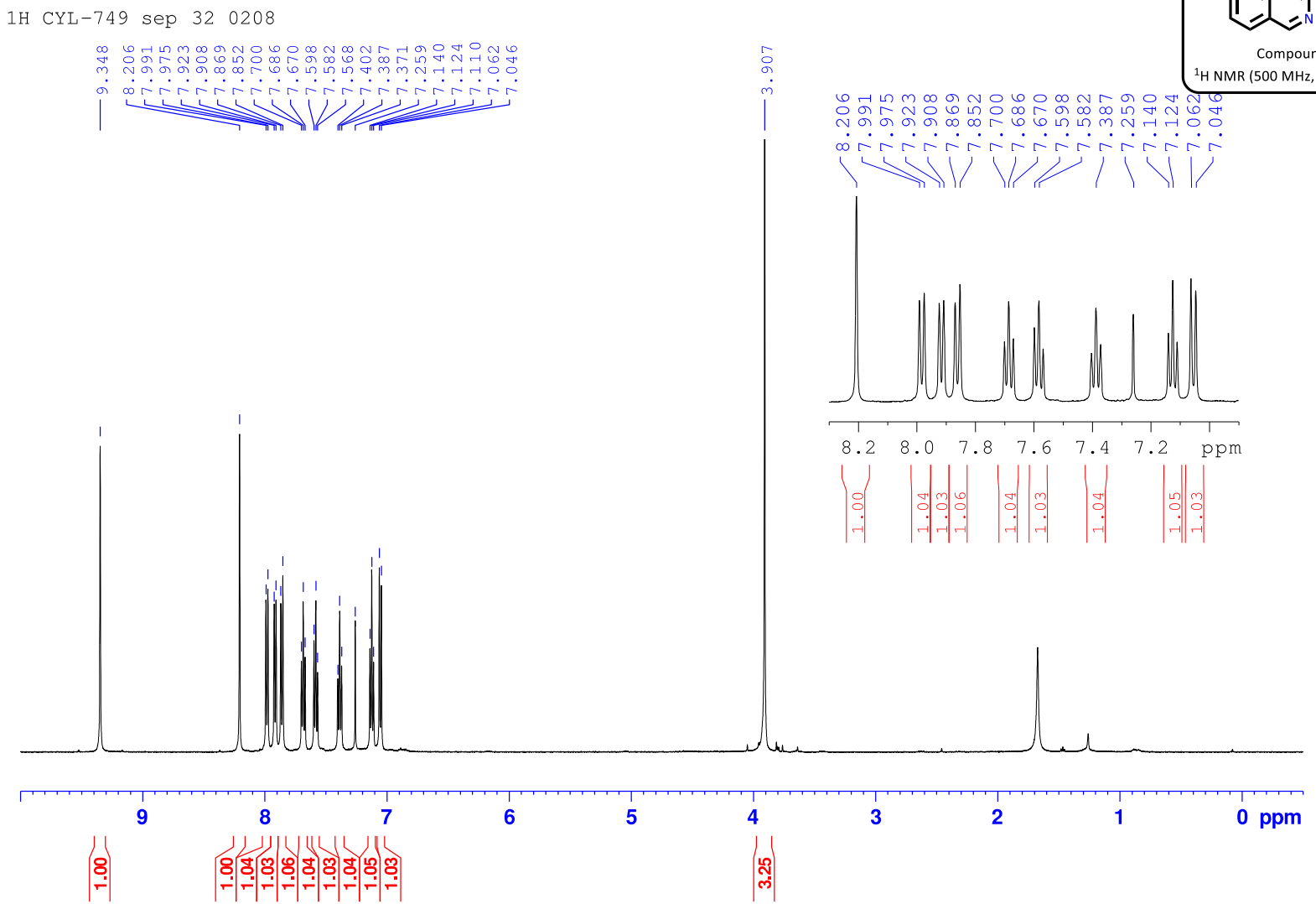


The ^{13}C NMR spectrum in $CDCl_3$ of compound 1p.

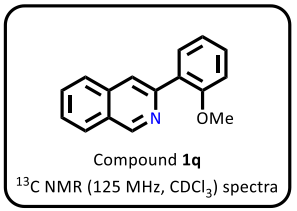


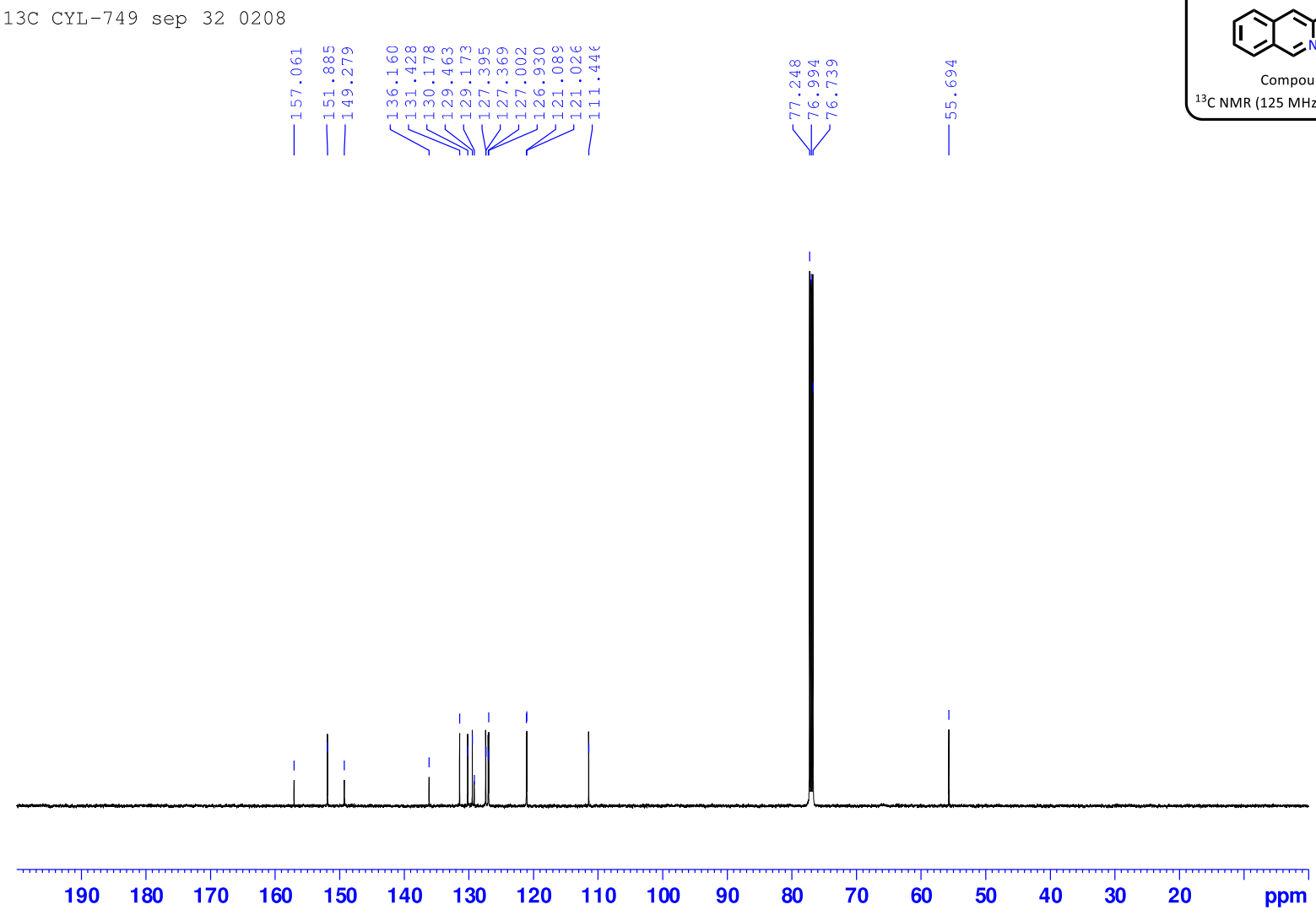


The ^{1}H NMR spectrum in $CDCl_3$ of compound 1q.

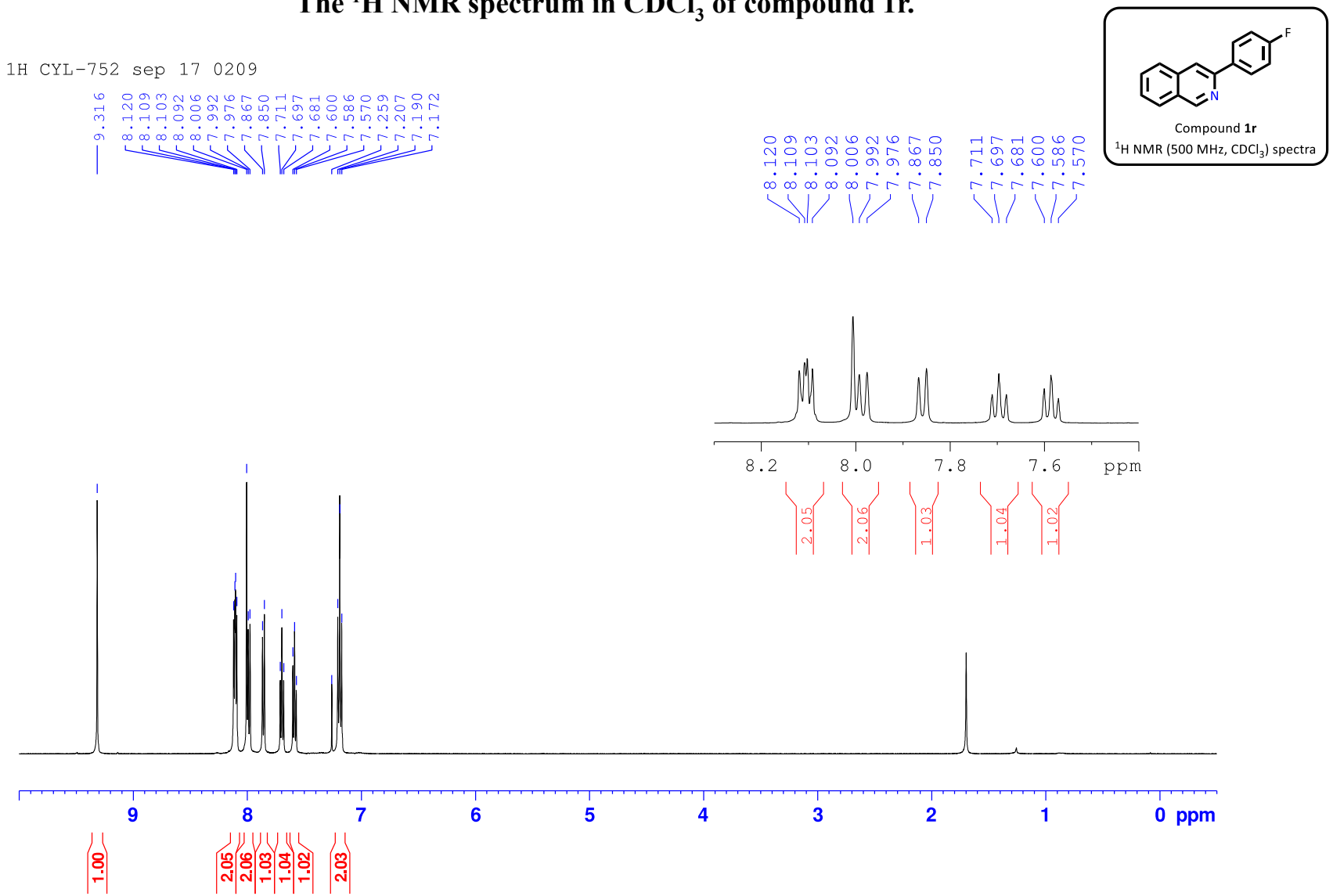


The ^{13}C NMR spectrum in $CDCl_3$ of compound 1q.

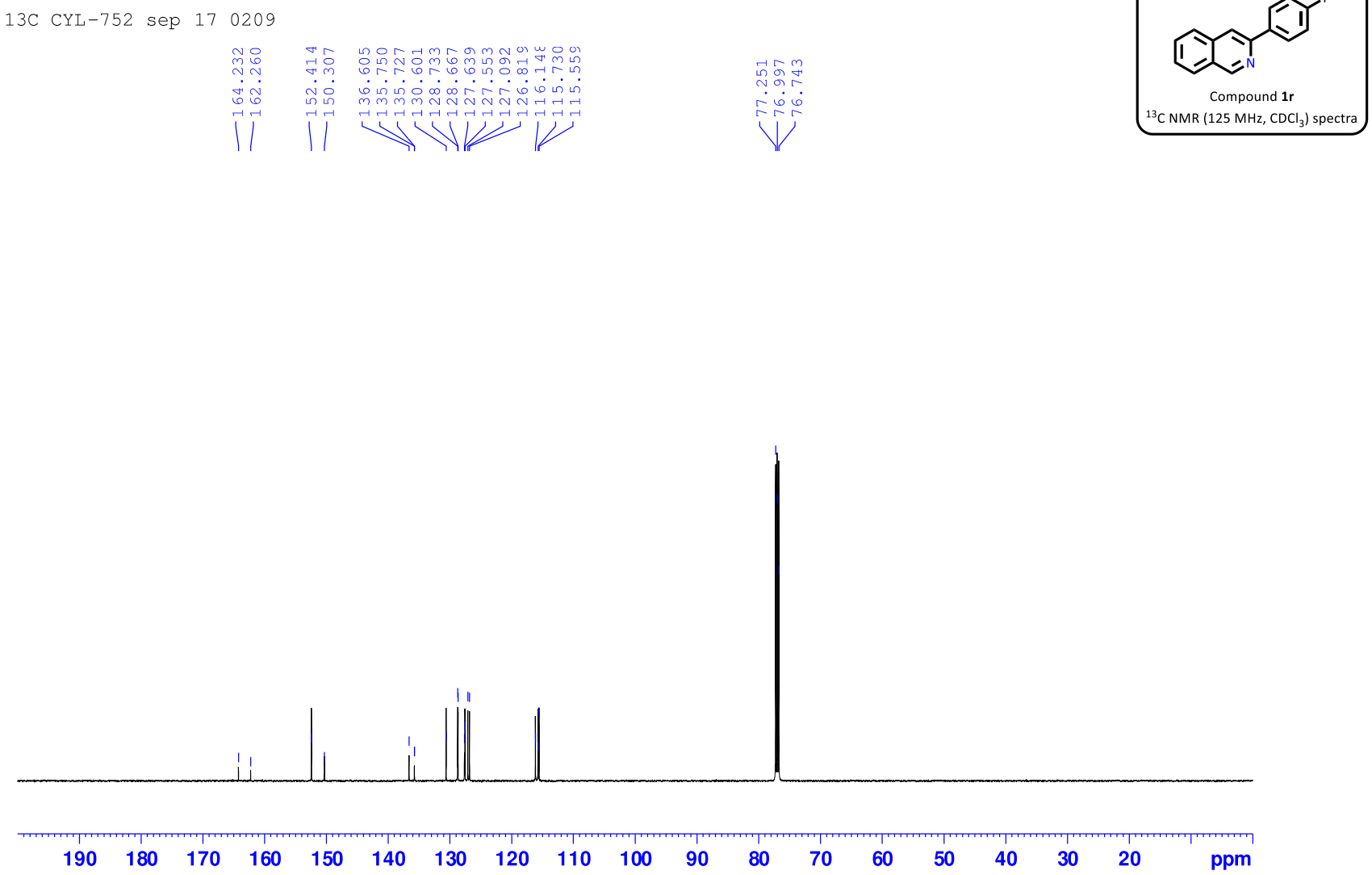




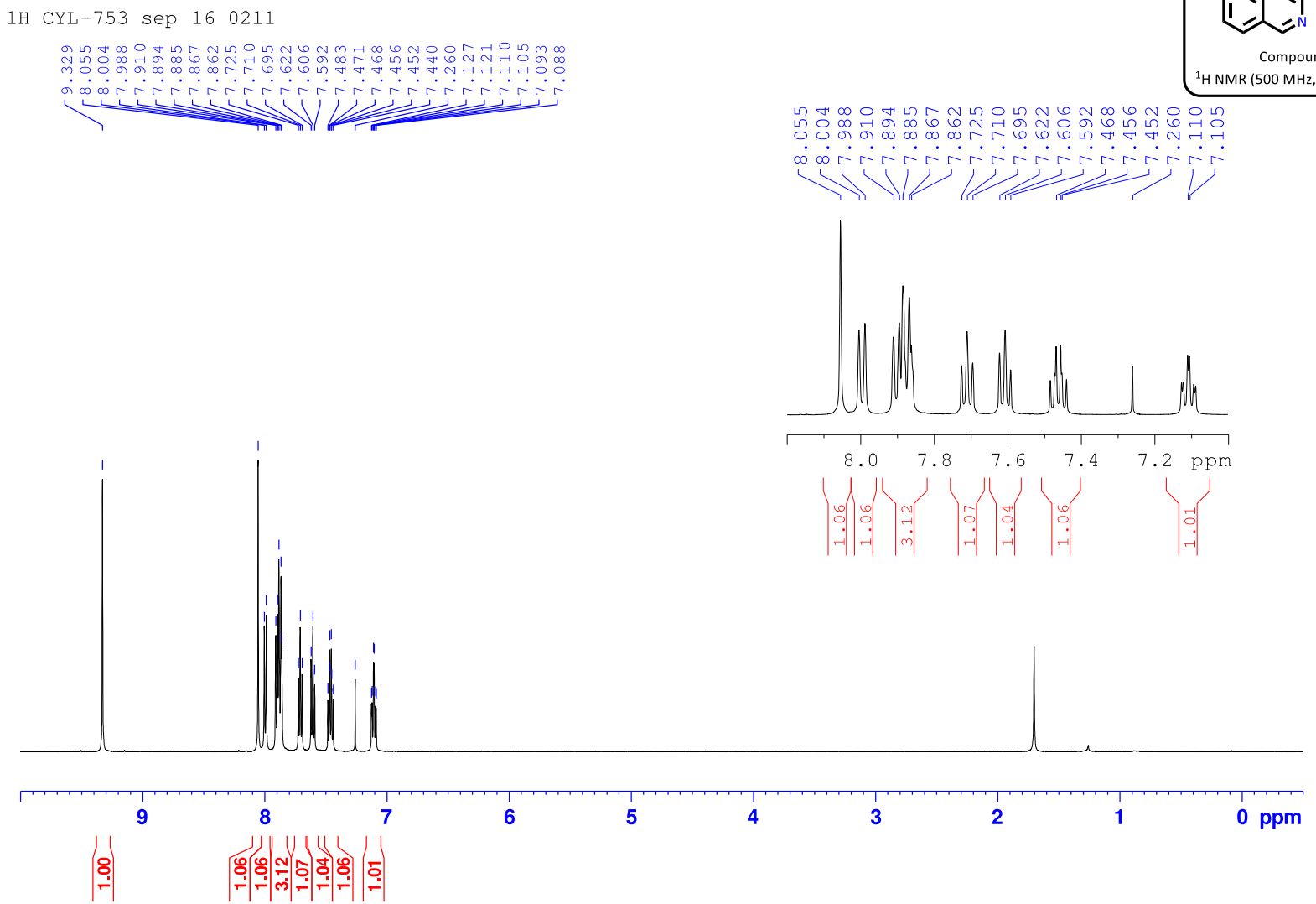
The ^{1}H NMR spectrum in $CDCl_3$ of compound 1r.

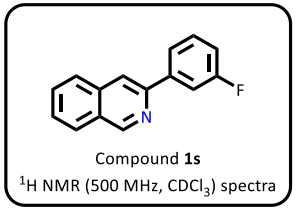


The ^{13}C NMR spectrum in $CDCl_3$ of compound 1r.

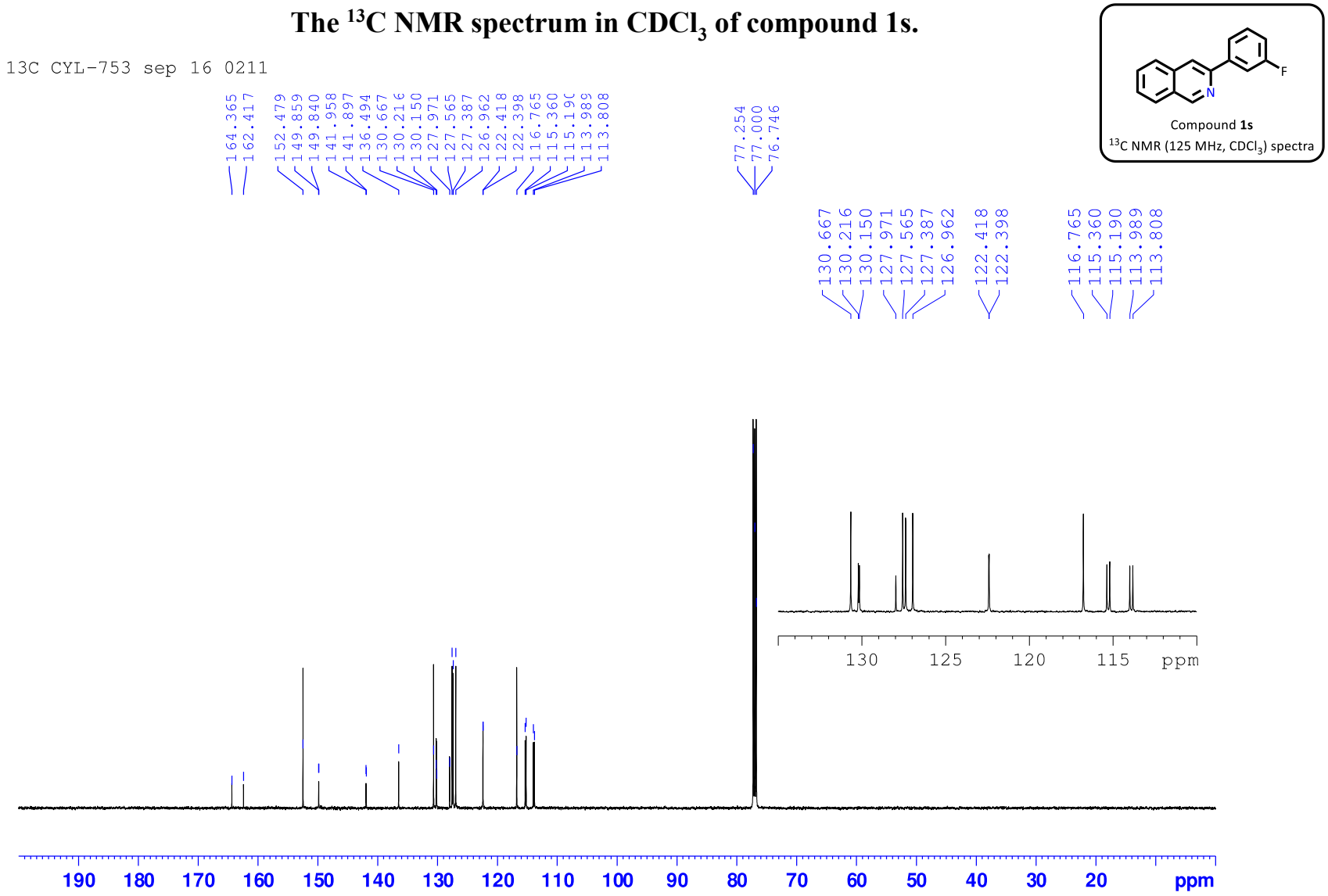


The ^{1}H NMR spectrum in $CDCl_3$ of compound 1s.

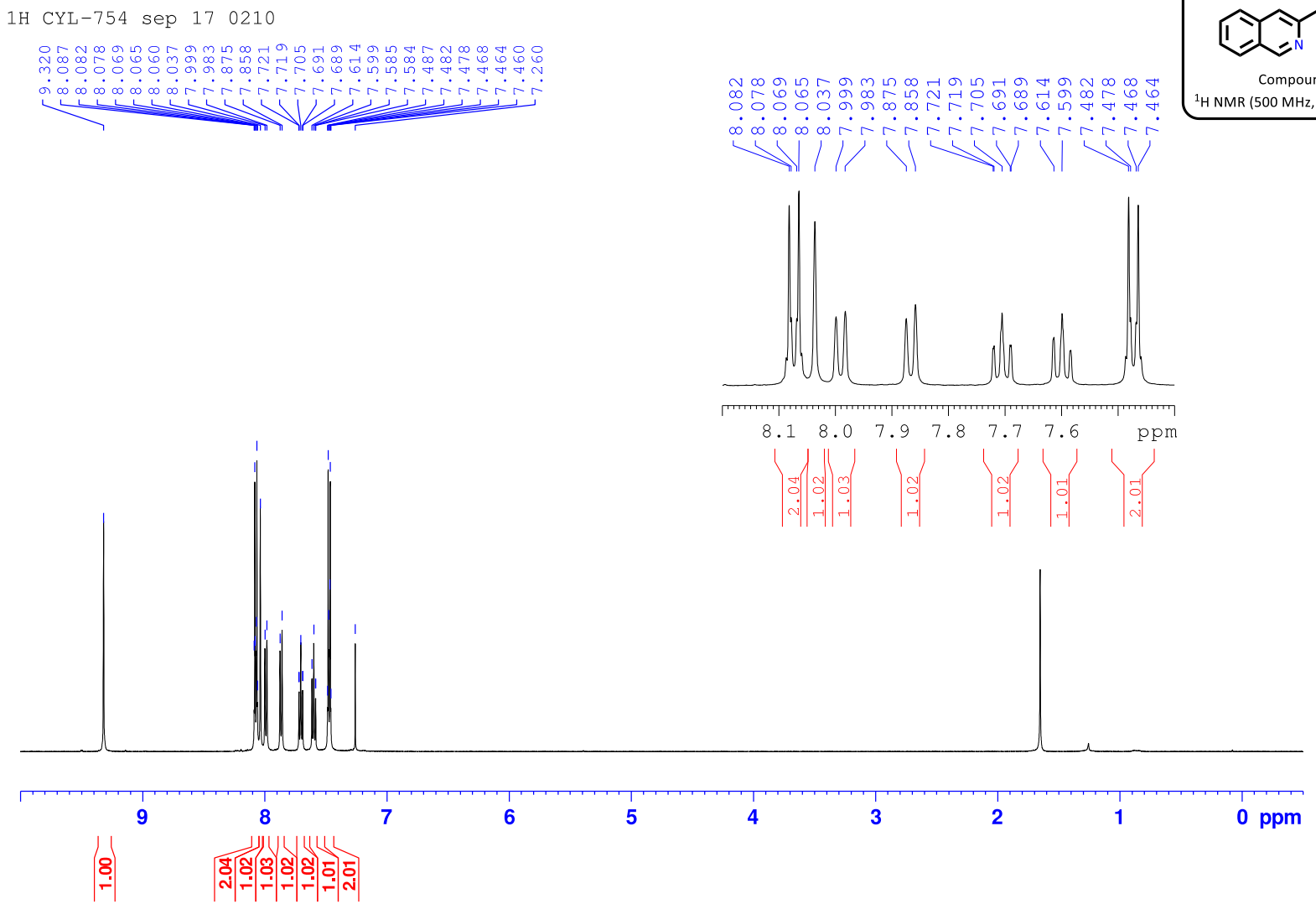


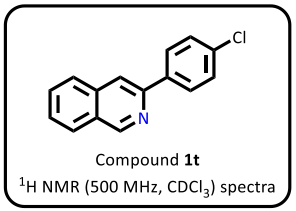


The ^{13}C NMR spectrum in $CDCl_3$ of compound 1s.

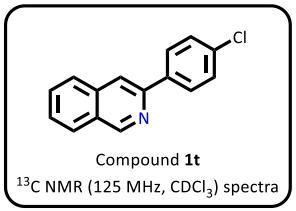


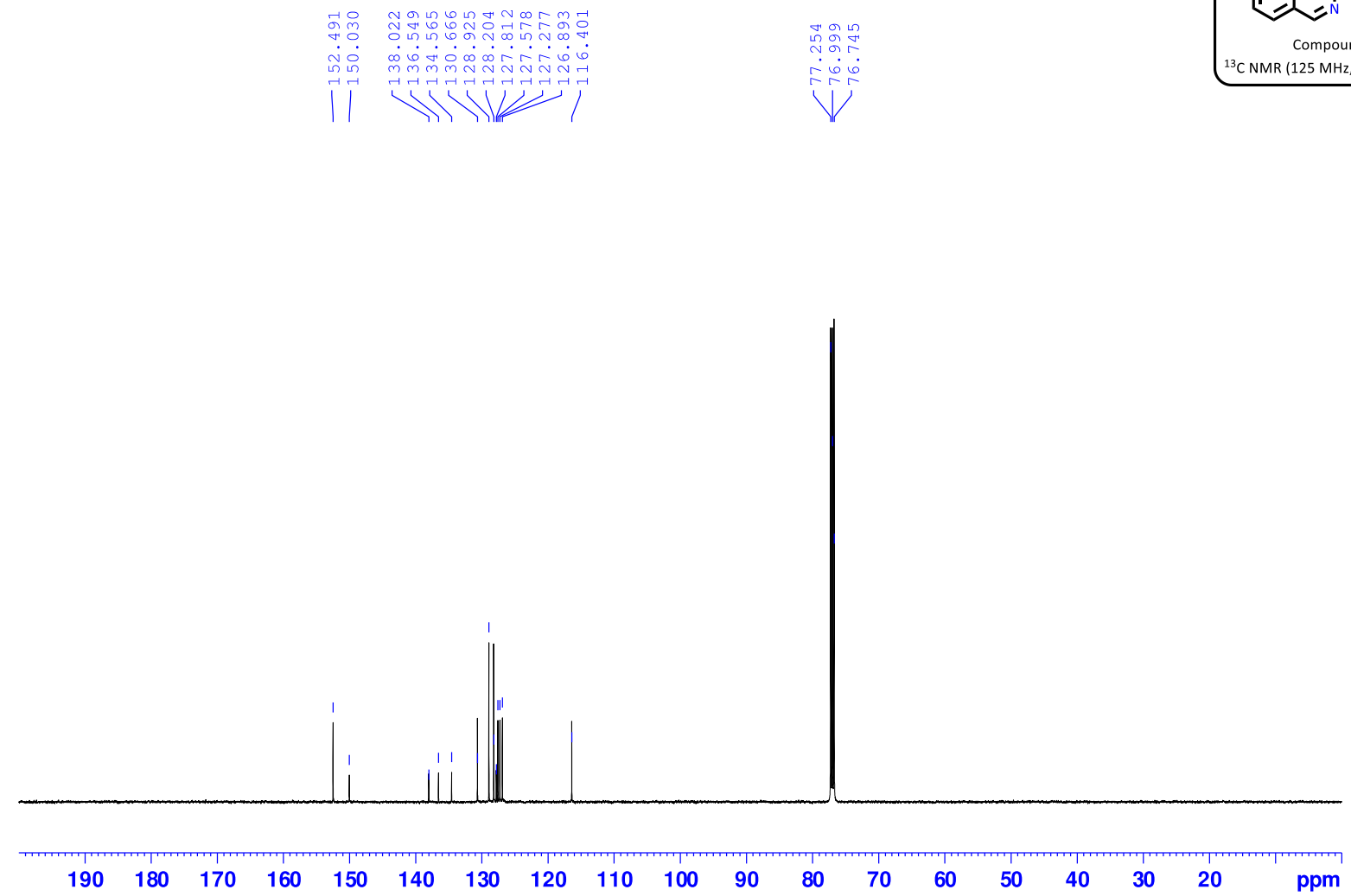
The ^{1}H NMR spectrum in $CDCl_3$ of compound 1t.



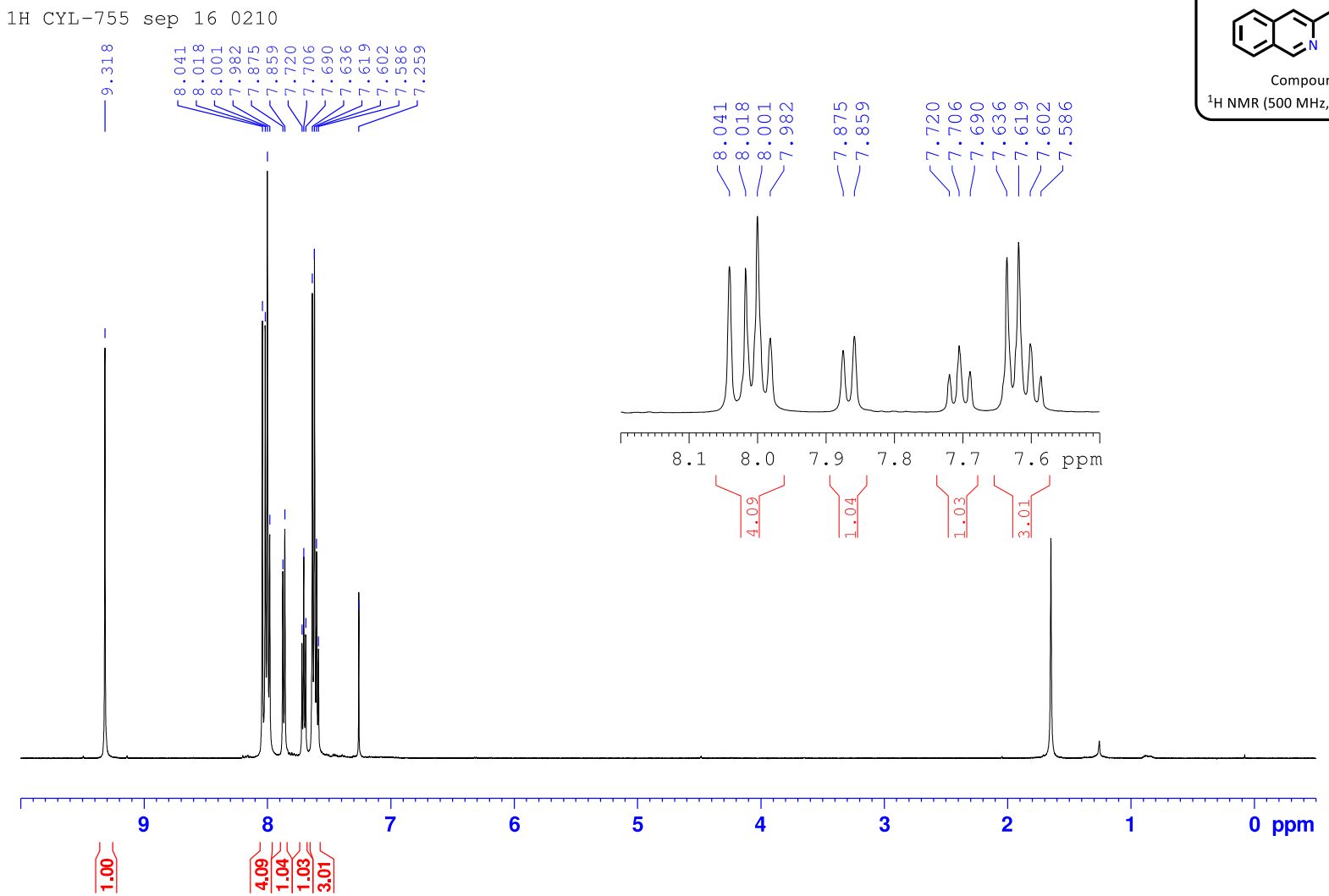


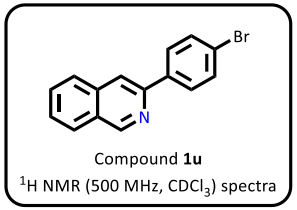
The ^{13}C NMR spectrum in $CDCl_3$ of compound 1t.





The ^{1}H NMR spectrum in $CDCl_3$ of compound 1u.

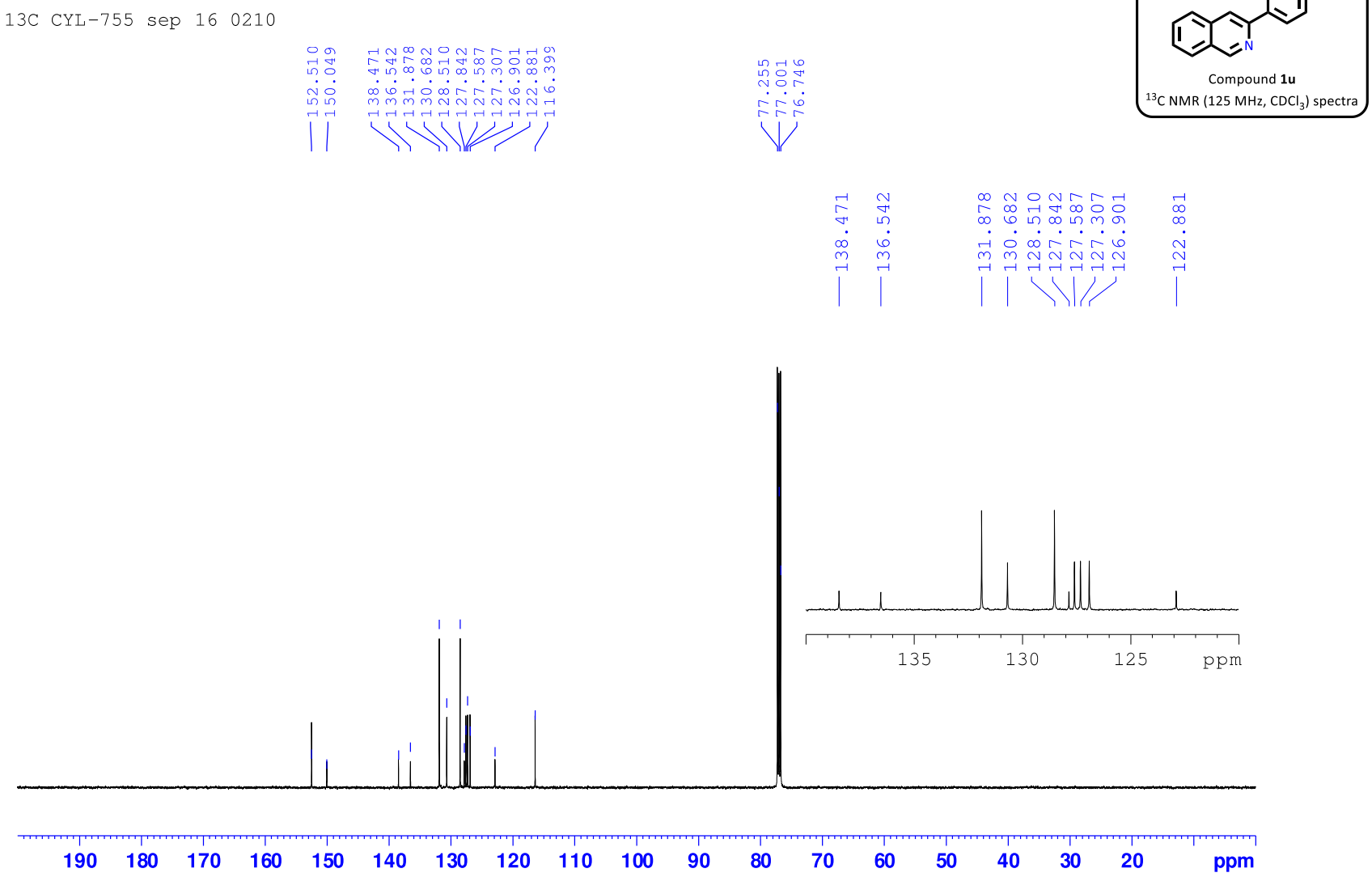




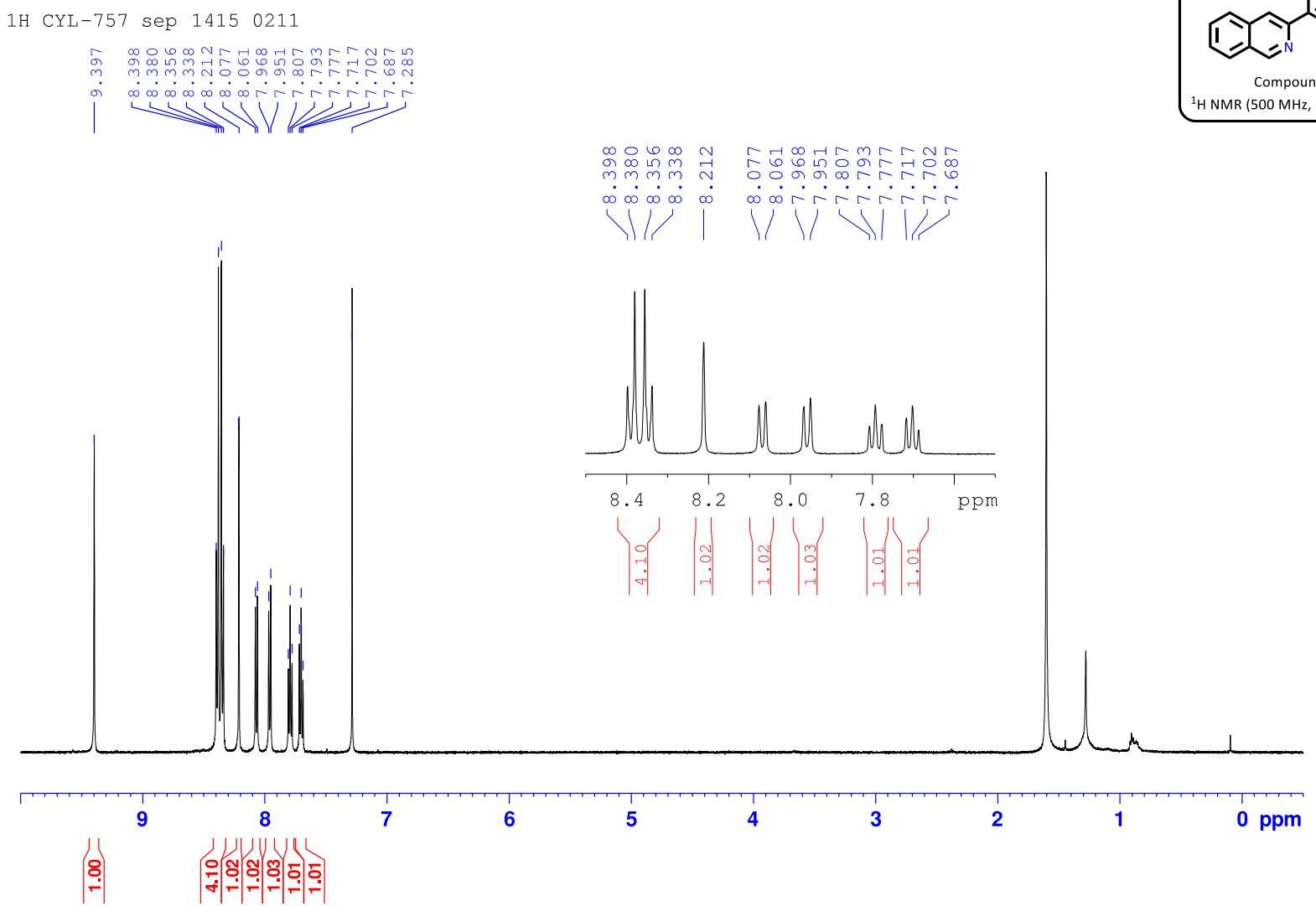
Compound **1u**

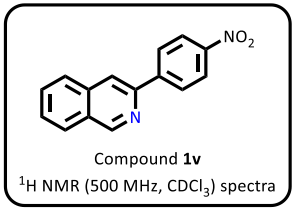
^{1}H NMR (500 MHz, $CDCl_3$) spectra

The ^{13}C NMR spectrum in $CDCl_3$ of compound 1u.

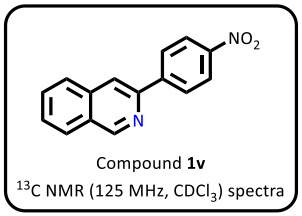


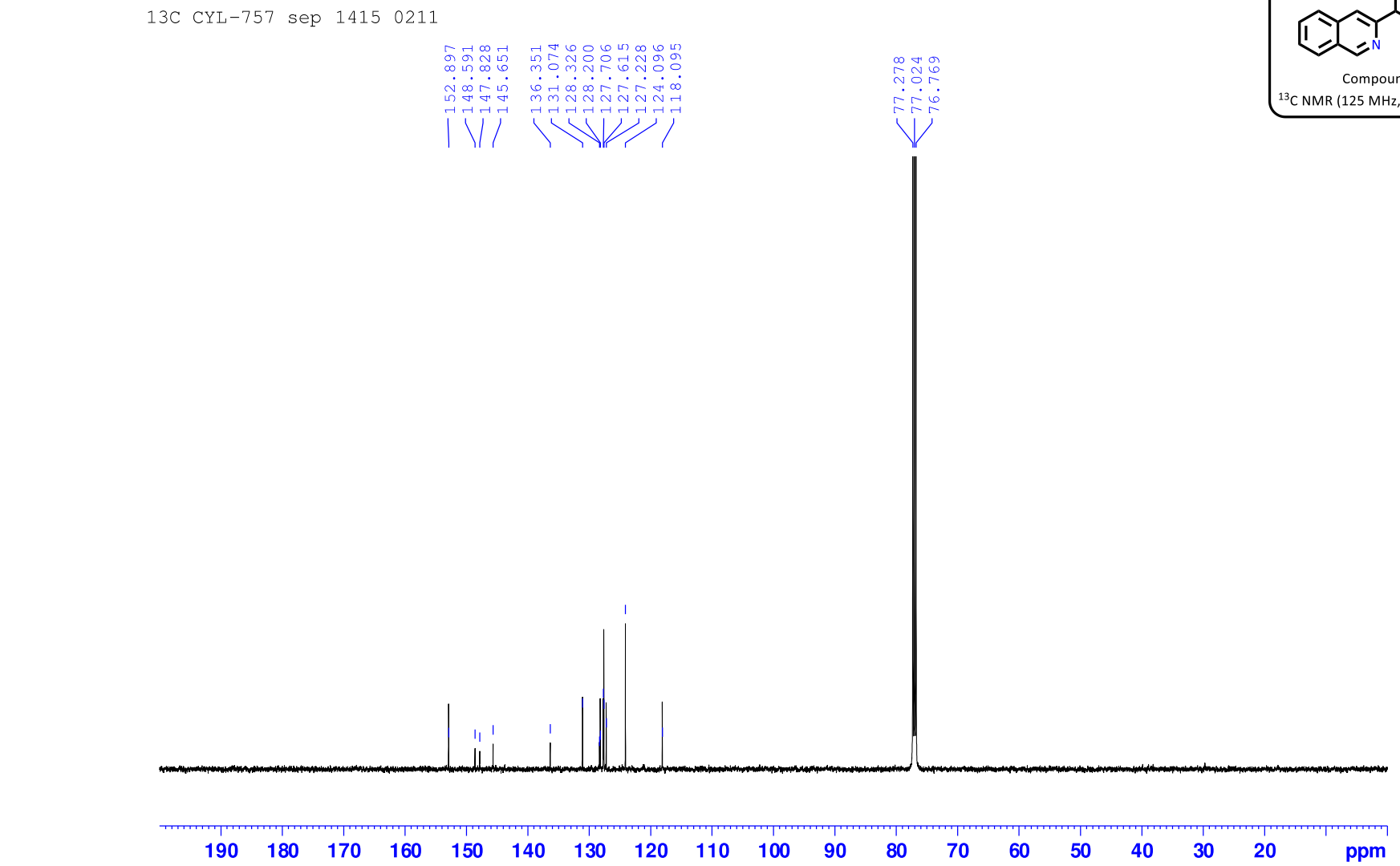
The ^{1}H NMR spectrum in $CDCl_3$ of compound 1v.





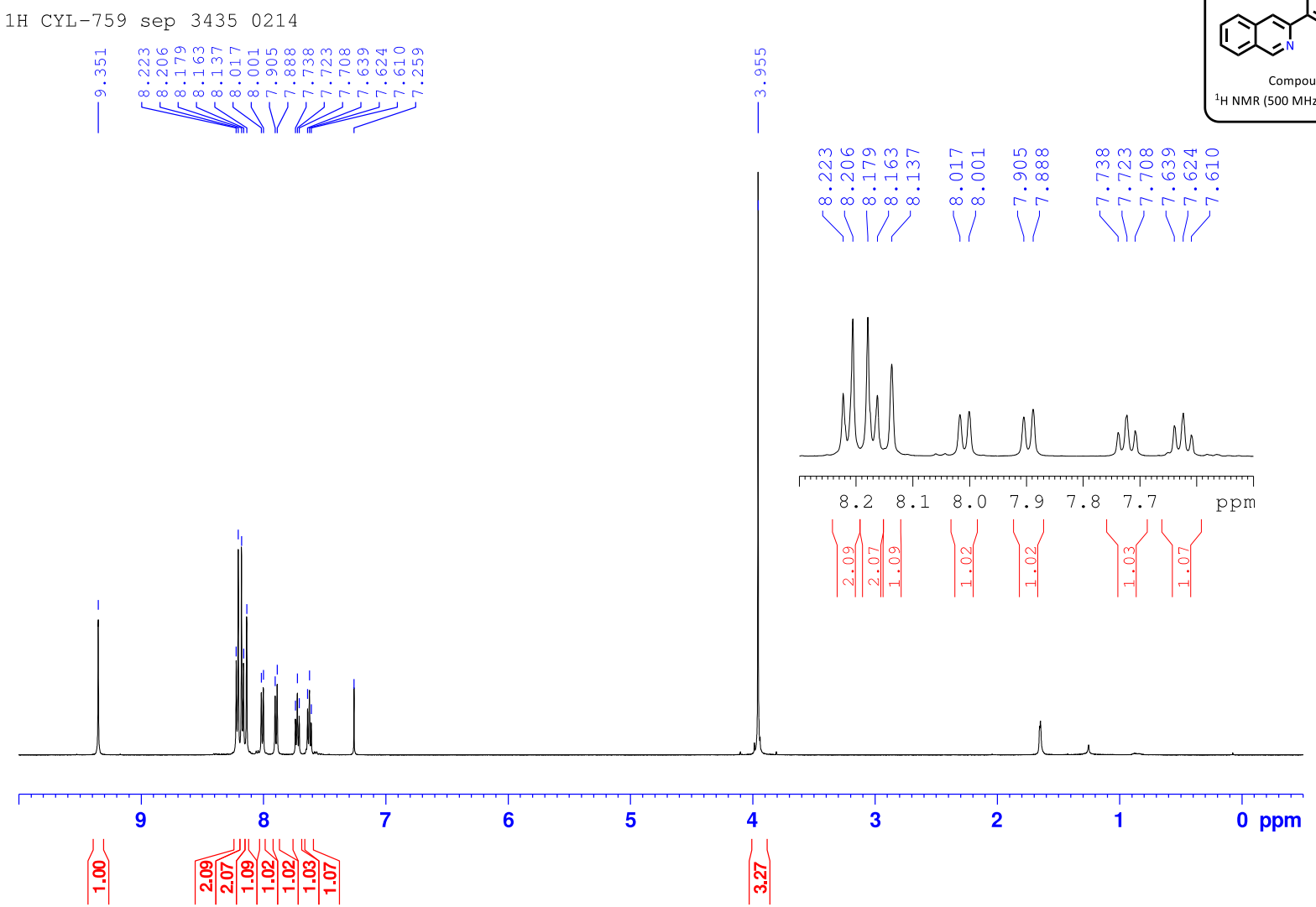
The ^{13}C NMR spectrum in $CDCl_3$ of compound 1v.

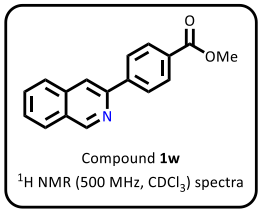




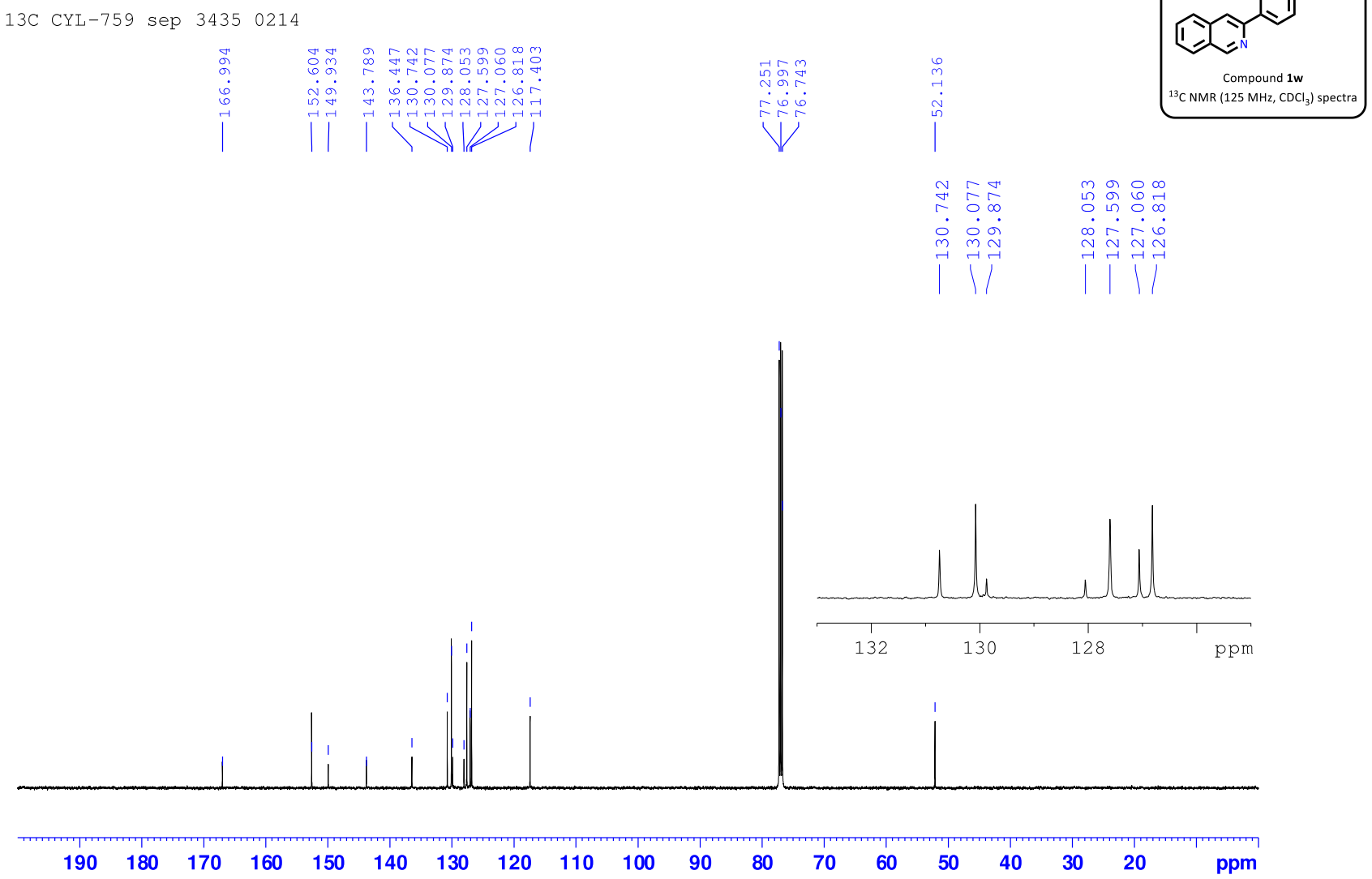
Z

The ^{1}H NMR spectrum in $CDCl_3$ of compound 1w.

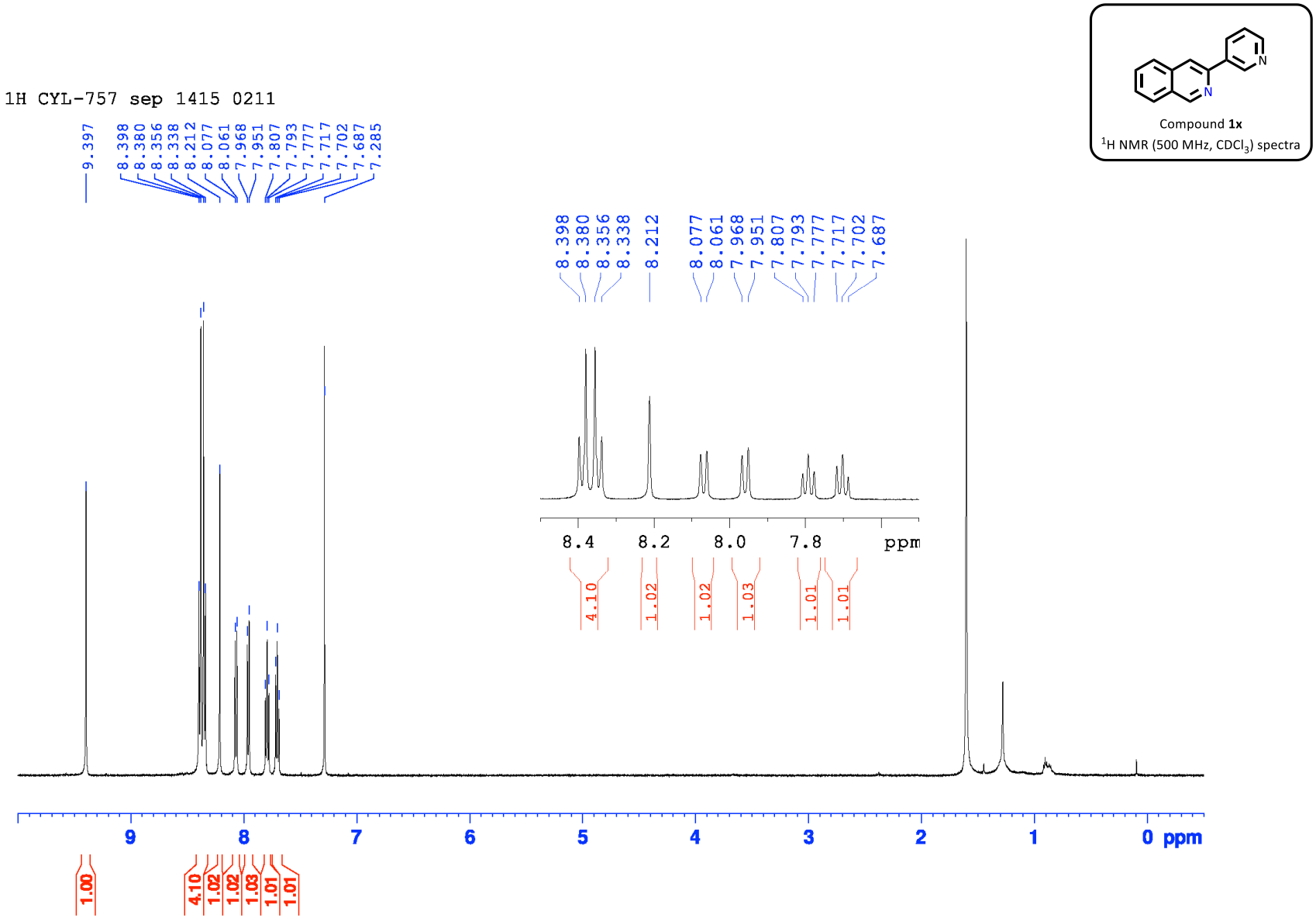




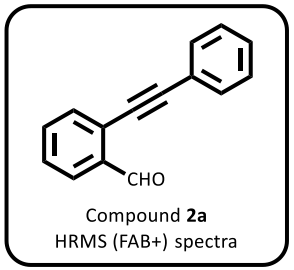
The ^{13}C NMR spectrum in $CDCl_3$ of compound 1w.



The ^{1}H NMR spectrum in $CDCl_3$ of compound 1x.

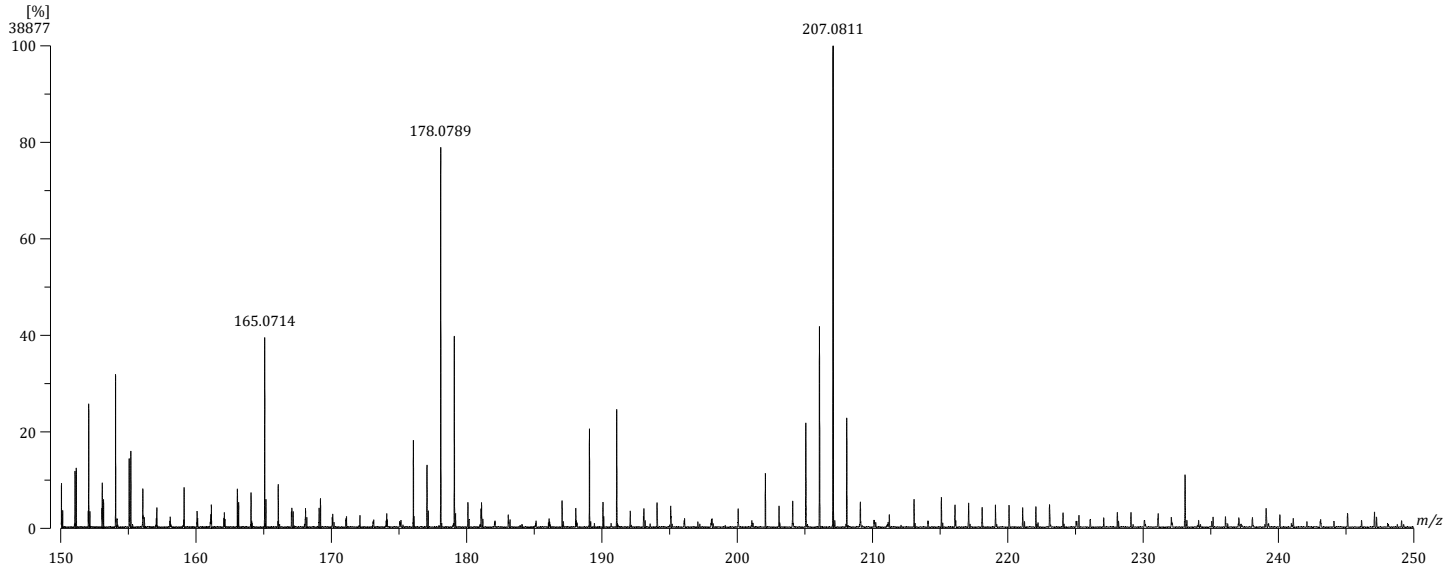


The high-resolution mass spectrum (FAB+) of compound 2a.



Compound **2a**
HRMS (FAB+) spectra

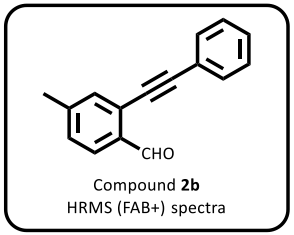
[Mass Spectrum]
Data : 20220421_CYL-706-HR-002 Date : 21-Apr-2022 17:23
Sample : CYL-706
Note : NBA
Ion Mode : FAB+
RT : 0.00 min Scan# : 1
Elements : C 1000/0, H 1000/0, O 1/1
Mass Tolerance : 50mmu
Unsaturation (U.S.) : -0.5 - 1000.0



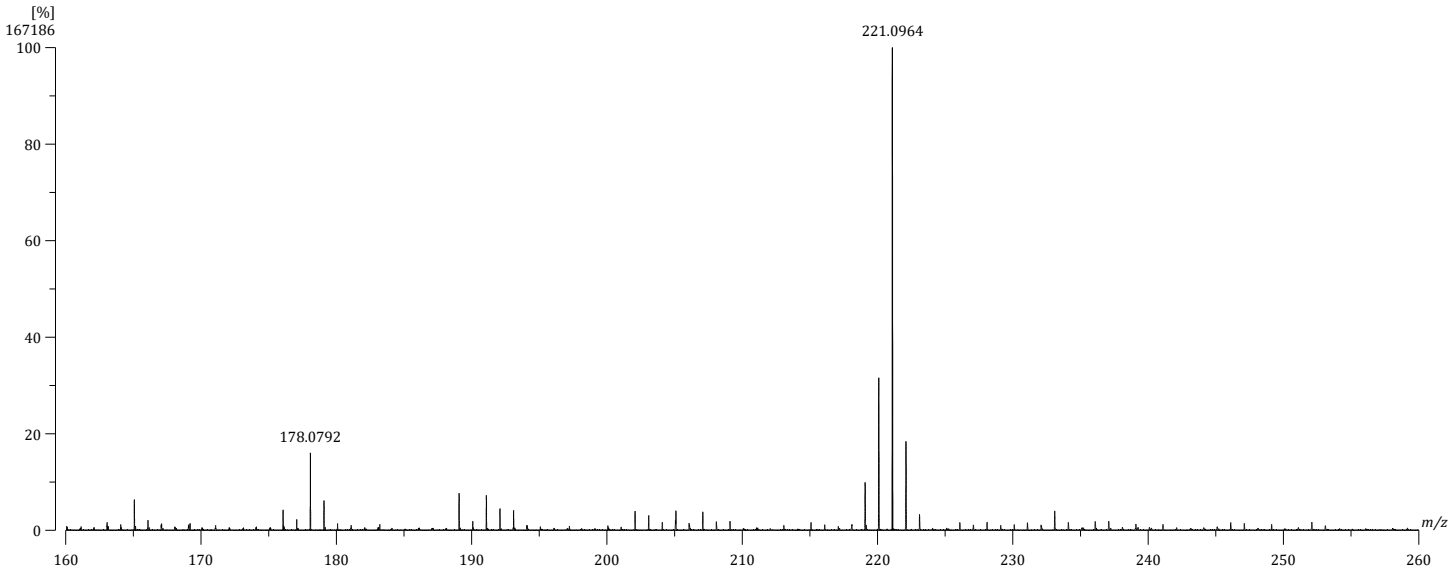
	Observed m/z	Int%
	207.0811	100.00

	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	O
1	207.0810	+0.5 / +0.1	10.5	15	11	1

The high-resolution mass spectrum (FAB+) of compound 2b.



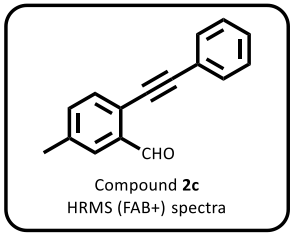
[Mass Spectrum]
Data : 20220421_CYL-707-HR-002 Date : 21-Apr-2022 17:37
Sample : CYL-707
Note : NBA
Ion Mode : FAB+
RT : 0.00 min Scan# : 1
Elements : C 1000/0, H 1000/0, O 1/1
Mass Tolerance : 50mmu
Unsaturation (U.S.) : -0.5 - 1000.0



Observed m/z	Int%
221.0964	100.00

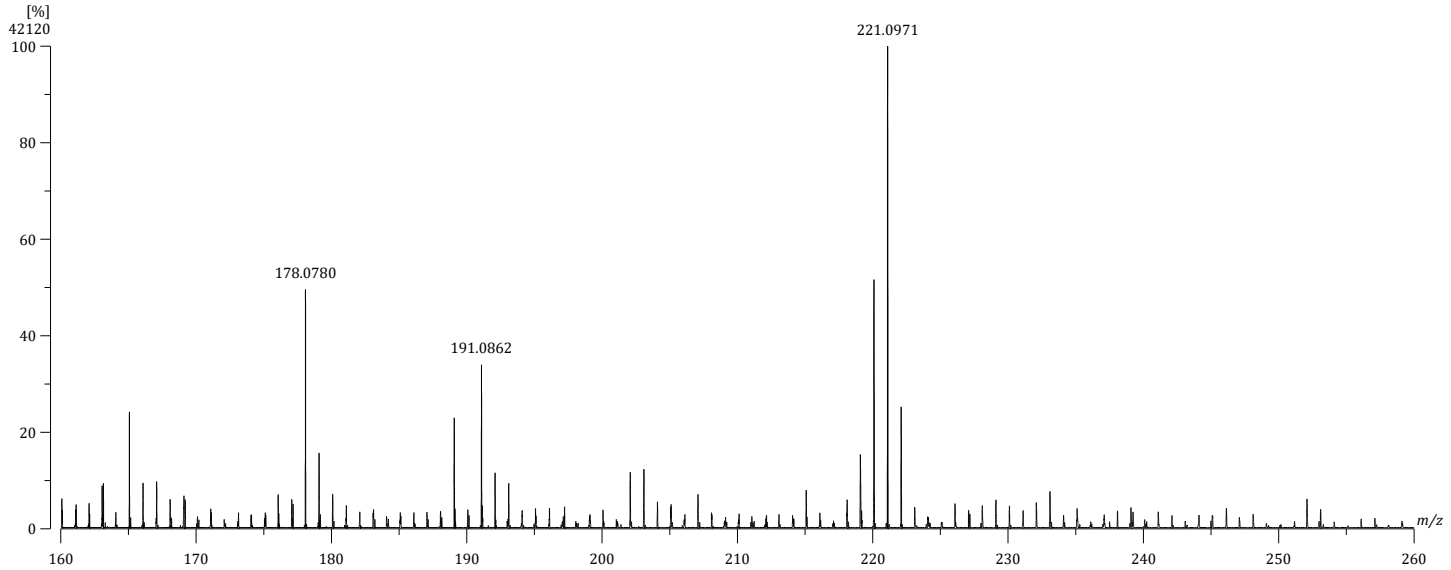
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	O
1	221.0966	-1.1 / -0.2	10.5	16	13	1

The high-resolution mass spectrum (FAB+) of compound 2c.



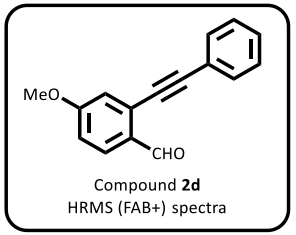
Compound **2c**
HRMS (FAB+) spectra

[Mass Spectrum]
Data : 20220421_CYL-708-HR-002 Date : 21-Apr-2022 17:43
Sample : CYL-708
Note : NBA
Ion Mode : FAB+
RT : 0.00 min Scan# : 1
Elements : C 1000/0, H 1000/0, O 1/1
Mass Tolerance : 50mmu
Unsaturation (U.S.) : -0.5 - 1000.0



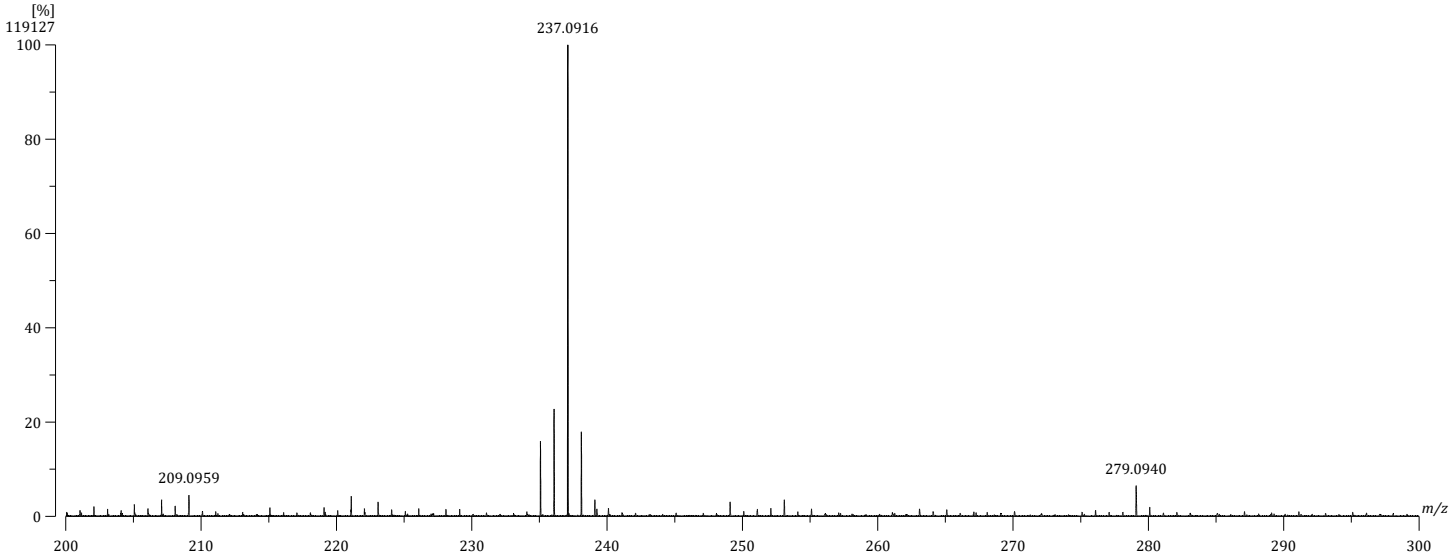
	Observed m/z	Int%					
	221.0971	100.00					
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	O	
1	221.0966	+2.1 / +0.5	10.5	16	13	1	

The high-resolution mass spectrum (FAB+) of compound 2d.



Compound **2d**
HRMS (FAB+) spectra

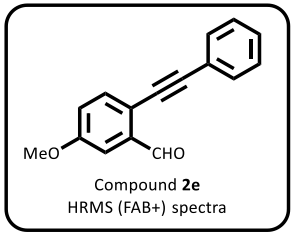
[Mass Spectrum]
Data : 20220421_CYL-709-HR-003 Date : 21-Apr-2022 17:50
Sample : CYL-709
Note : NBA
Ion Mode : FAB+
RT : 0.10 min Scan# : 2
Elements : C 1000/0, H 1000/0, O 2/2
Mass Tolerance : 50mmu
Unsaturation (U.S.) : -0.5 - 1000.0



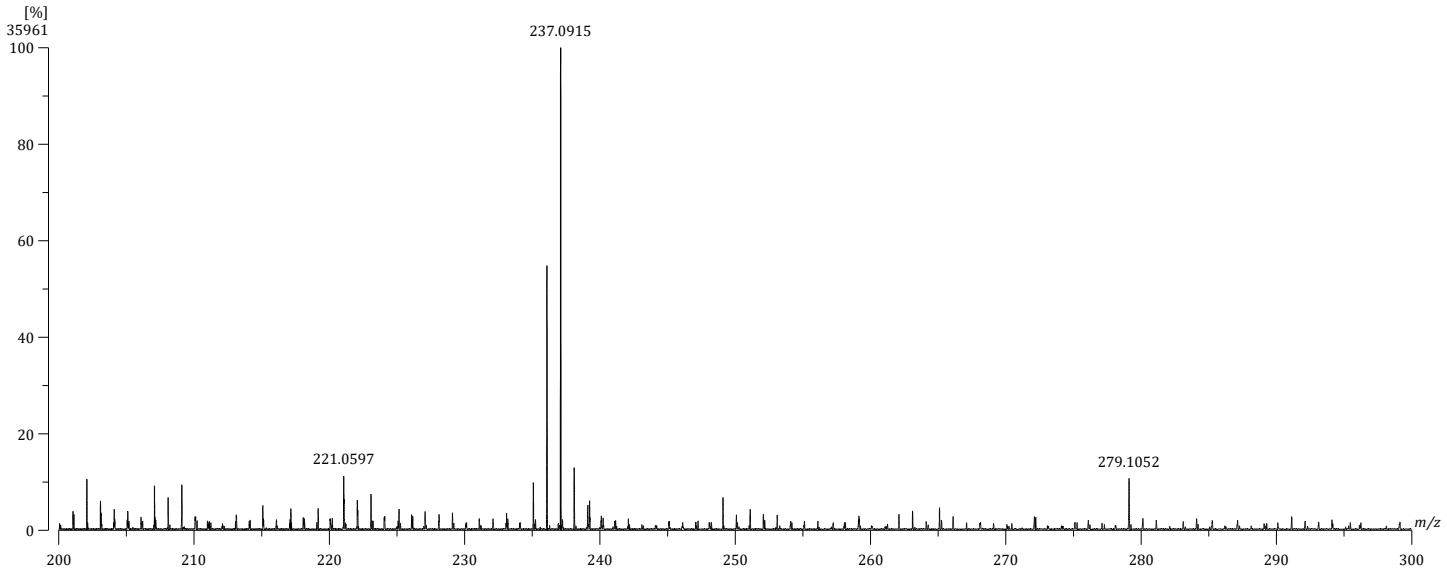
	Observed m/z	Int%
	237.0916	100.00

	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	O
1	237.0916	+0.2 / +0.0	10.5	16	13	2

The high-resolution mass spectrum (FAB+) of compound 2e.

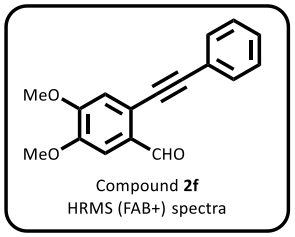


[Mass Spectrum]
Data : 20220422_CYL-710-HR-003 Date : 22-Apr-2022 11:22
Sample : CYL-710
Note : NBA
Ion Mode : FAB+
RT : 0.38 min Scan# : 5
Elements : C 1000/0, H 1000/0, O 2/2
Mass Tolerance : 50mmu
Unsaturation (U.S.) : -0.5 - 1000.0



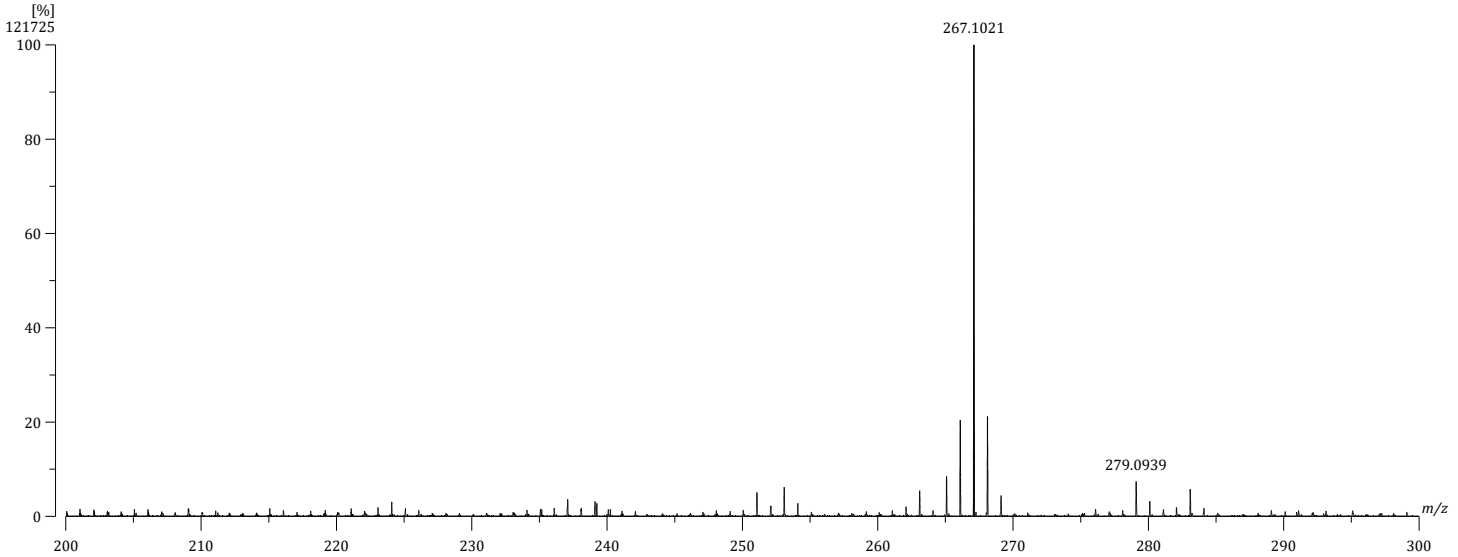
Observed m/z	Int%					
237.0915	100.00					
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	O
1	237.0916	-0.2 / -0.1	10.5	16	13	2

The high-resolution mass spectrum (FAB+) of compound 2f.



Compound **2f**
HRMS (FAB+) spectra

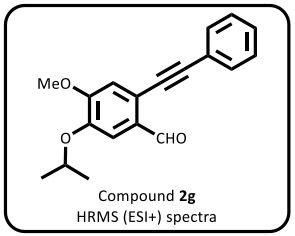
[Mass Spectrum]
Data : 20220422_CYL-701-2-HR-002 Date : 22-Apr-2022 11:29
Sample : CYL-701-2
Note : NBA
Ion Mode : FAB+
RT : 0.00 min Scan# : 1
Elements : C 1000/0, H 1000/0, O 3/3
Mass Tolerance : 50mmu
Unsaturation (U.S.) : -0.5 - 1000.0



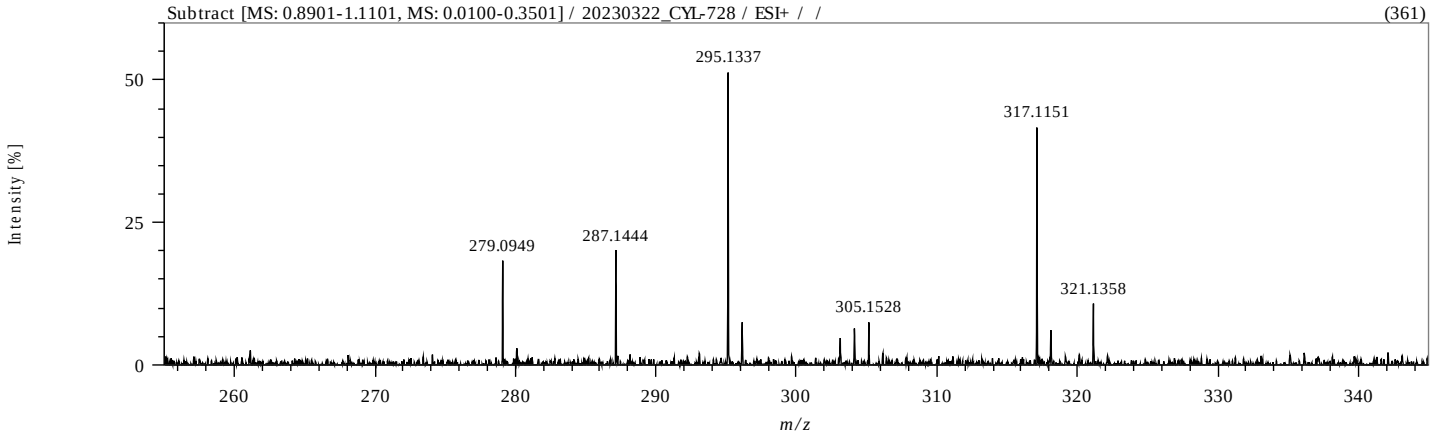
	Observed m/z	Int%
	267.1021	100.00

	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	O
1	267.1021	-0.1 / -0.0	10.5	17	15	3

The high-resolution mass spectrum (ESI+) of compound 2g.



Spectrum



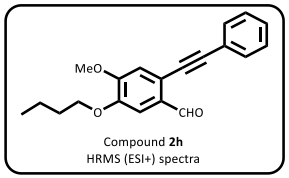
Elemental Composition

Parameters		Elements Set 1:				
Tolerance:	±5.00 ppm	Symbol	C	H	O	Na
Electron:	Odd/Even	Min	0	0	3	0
Charge:	+1	Max	100	400	3	1
DBE:	-99.0 - 999.0					

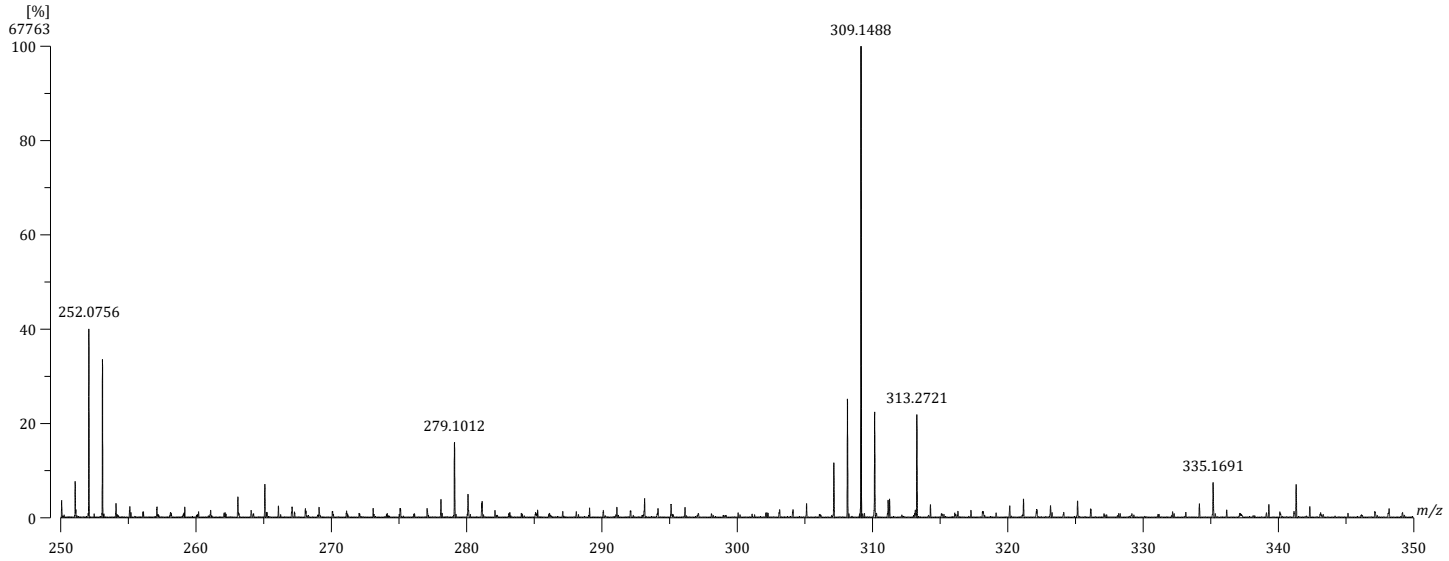
Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
295.13369	C19 H19 O3	295.13287	0.82	2.77	10.5
317.11506	C19 H18 O3 Na	317.11482	0.24	0.77	10.5

The high-resolution mass spectrum (FAB+) of compound 2h.

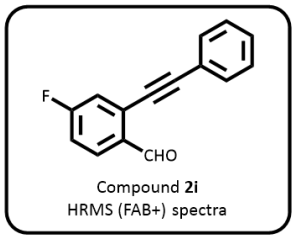


[Mass Spectrum]
Data : 20220421_CYL-729-HR-002 Date : 21-Apr-2022 16:57
Sample : CYL-729
Note : NBA
Ion Mode : FAB+
RT : 0.00 min Scan# : 1
Elements : C 1000/0, H 1000/0, O 3/3
Mass Tolerance : 50mmu
Unsaturation (U.S.) : -0.5 - 1000.0

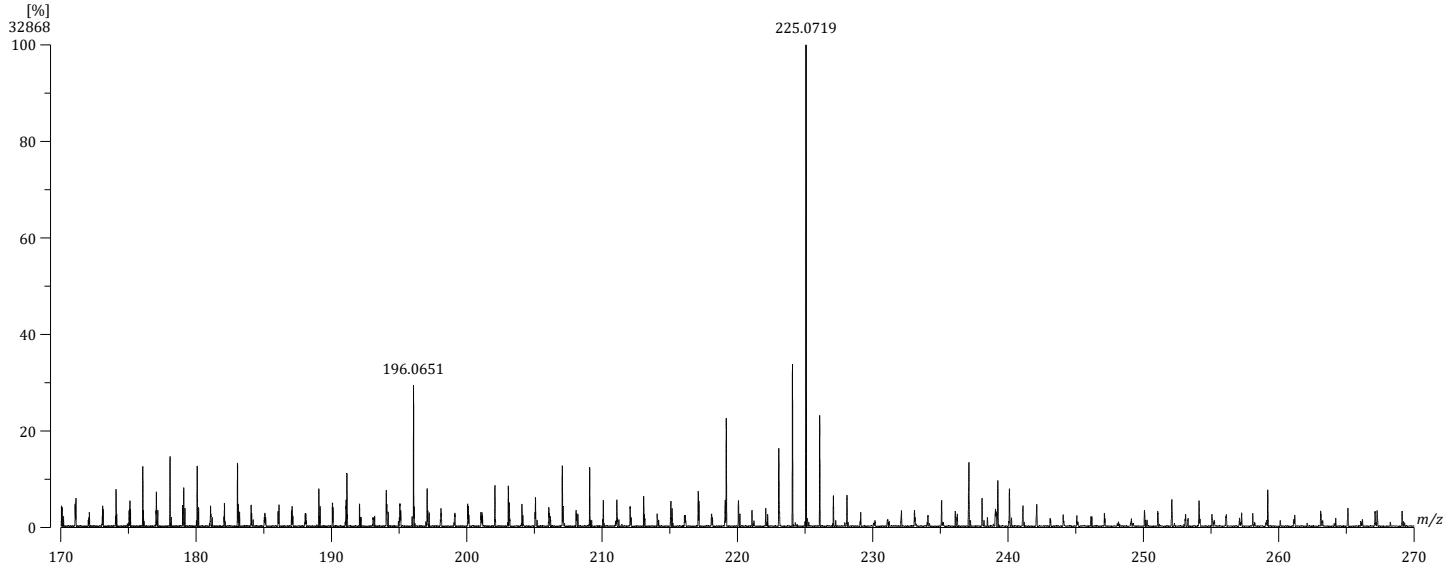


	Observed m/z	Int%				
	309.1488	100.00				
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	O
1	309.1491	-0.9 / -0.3	10.5	20	21	3

The high-resolution mass spectrum (FAB+) of compound 2i.



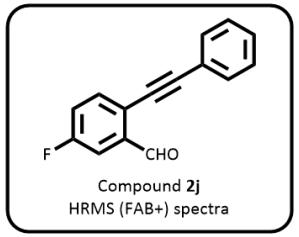
[Mass Spectrum]
Data : 20220422_CYL-711-HR-003 Date : 22-Apr-2022 12:30
Sample : CYL-711
Note : NBA
Ion Mode : FAB+
RT : 0.00 min Scan# : 1
Elements : C 1000/0, H 1000/0, F 1/1, O 1/1
Mass Tolerance : 50mmu
Unsaturation (U.S.) : -0.5 - 1000.0



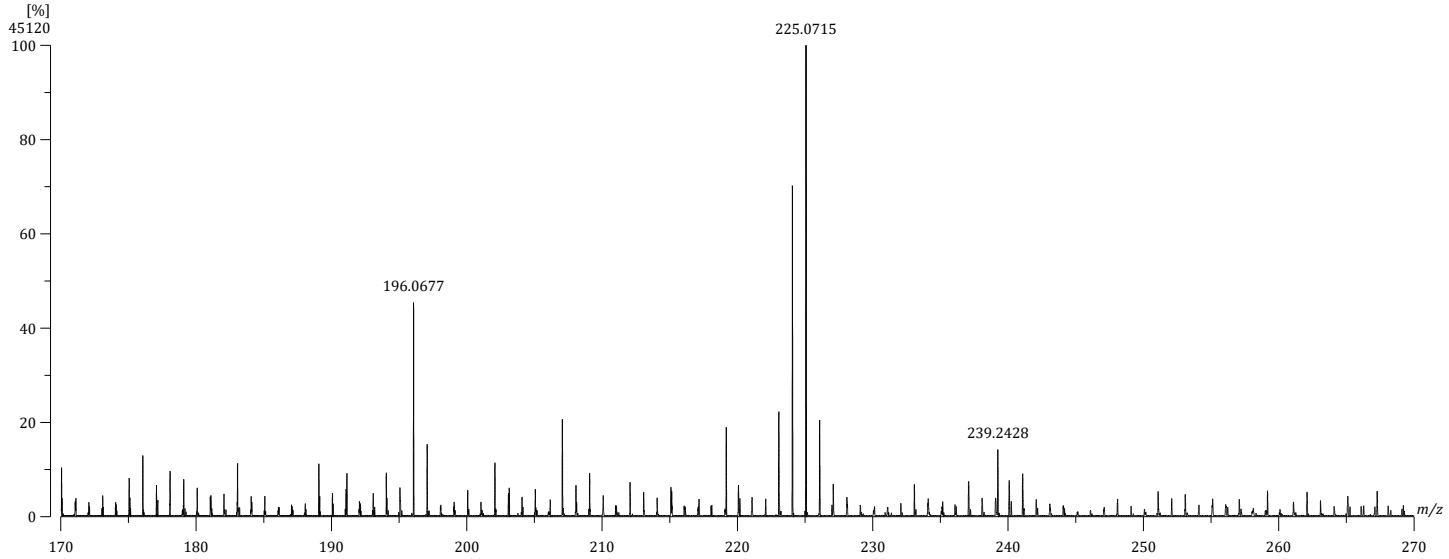
	Observed m/z	Int%
	225.0719	100.00

	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	F	O
1	225.0716	+1.5 / +0.3	10.5	15	10	1	1

The high-resolution mass spectrum (FAB+) of compound 2j.



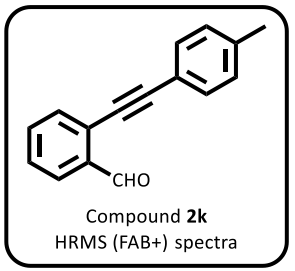
[Mass Spectrum]
Data : 20220422_CYL-712-HR-003 Date : 22-Apr-2022 12:22
Sample : CYL-712
Note : NBA
Ion Mode : FAB+
RT : 0.00 min Scan# : 1
Elements : C 1000/0, H 1000/0, F 1/1, O 1/1
Mass Tolerance : 50mmu
Unsaturation (U.S.) : -0.5 - 1000.0



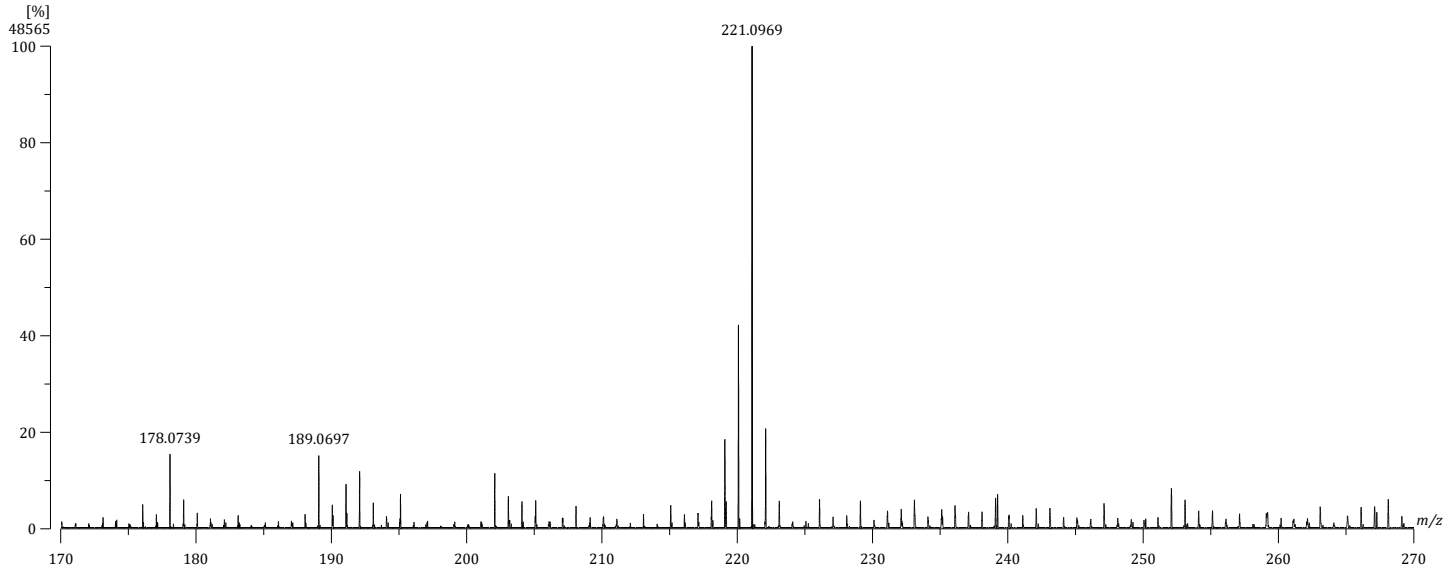
	Observed m/z	Int%
	225.0715	100.00

	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	F	O
1	225.0716	-0.3 / -0.1	10.5	15	10	1	1

The high-resolution mass spectrum (FAB+) of compound 2k.

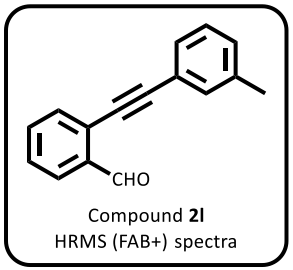


[Mass Spectrum]
Data : 20220422_CYL-716-HR-002 Date : 22-Apr-2022 11:57
Sample : CYL-716
Note : NBA
Ion Mode : FAB+
RT : 0.21 min Scan# : 3
Elements : C 1000/0, H 1000/0, O 1/1
Mass Tolerance : 50mmu
Unsaturation (U.S.) : -0.5 - 1000.0

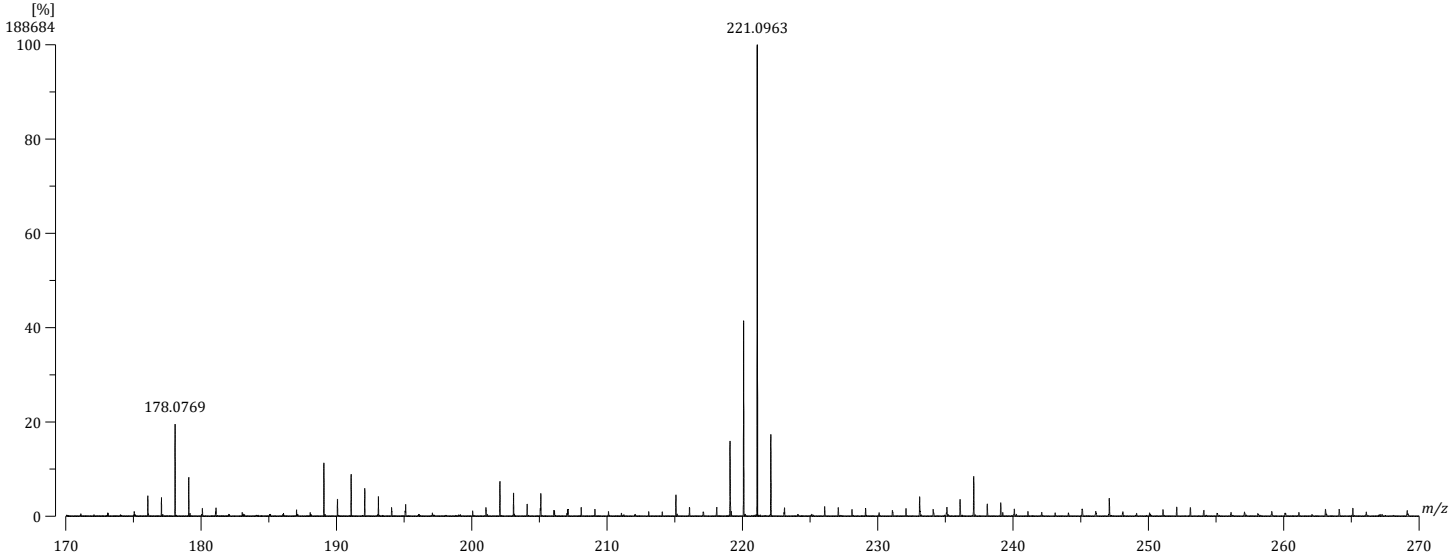


	Observed m/z	Int%					
	221.0969	100.00					
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	O	
1	221.0966	+1.2 / +0.3	10.5	16	13	1	

The high-resolution mass spectrum (FAB+) of compound 2l.

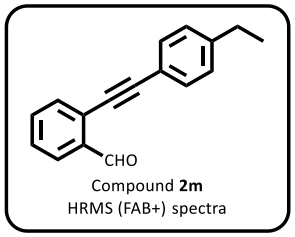


[Mass Spectrum]
Data : 20220422_CYL-717-HR-003 Date : 22-Apr-2022 11:47
Sample : CYL-717
Note : NBA
Ion Mode : FAB+
RT : 0.11 min Scan# : 2
Elements : C 1000/0, H 1000/0, O 1/1
Mass Tolerance : 50mmu
Unsaturation (U.S.) : -0.5 - 1000.0

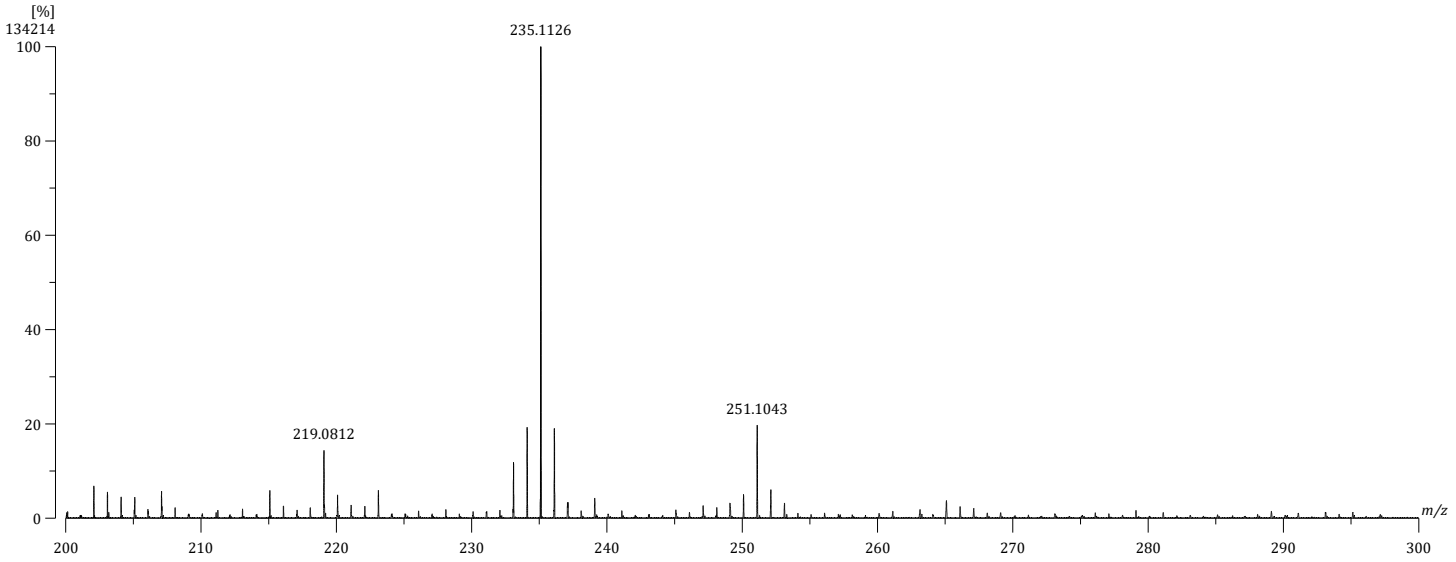


	Observed m/z	Int%				
	221.0963	100.00				
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	O
1	221.0966	-1.5 / -0.3	10.5	16	13	1

The high-resolution mass spectrum (FAB+) of compound 2m.

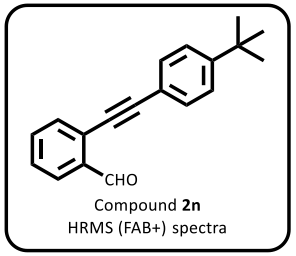


[Mass Spectrum]
Data : 20220422_CYL-726-HR-002 Date : 22-Apr-2022 11:36
Sample : CYL-726
Note : NBA
Ion Mode : FAB+
RT : 0.29 min Scan# : 4
Elements : C 1000/0, H 1000/0, O 1/1
Mass Tolerance : 50mmu
Unsaturation (U.S.) : -0.5 - 1000.0

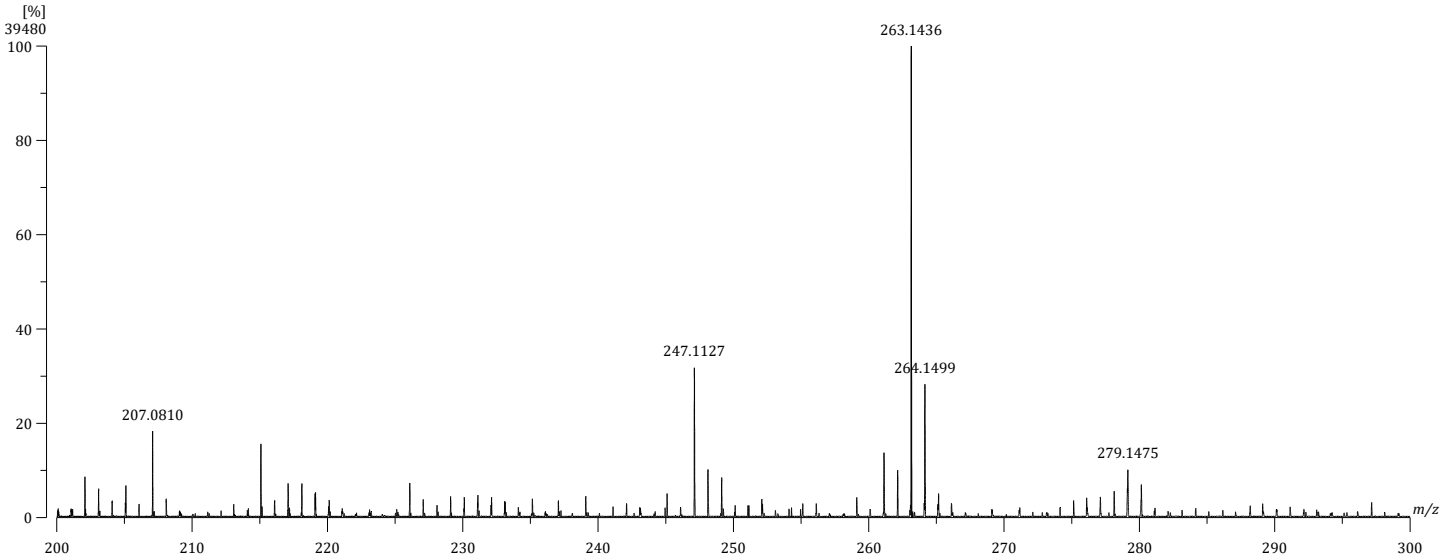


	Observed m/z	Int%					
	235.1126	100.00					
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	O	
1	235.1123	+1.3 / +0.3	10.5	17	15	1	

The high-resolution mass spectrum (FAB+) of compound 2n.

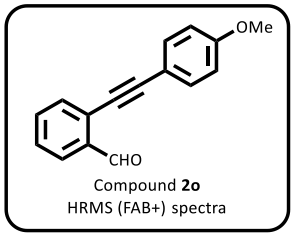


[Mass Spectrum]
Data : 20220421_CYL-722-HR-002 Date : 21-Apr-2022 17:16
Sample : CYL-722
Note : NBA
Ion Mode : FAB+
RT : 0.38 min Scan# : 5
Elements : C 1000/0, H 1000/0, O 1/1
Mass Tolerance : 50mmu
Unsaturation (U.S.) : -0.5 - 1000.0

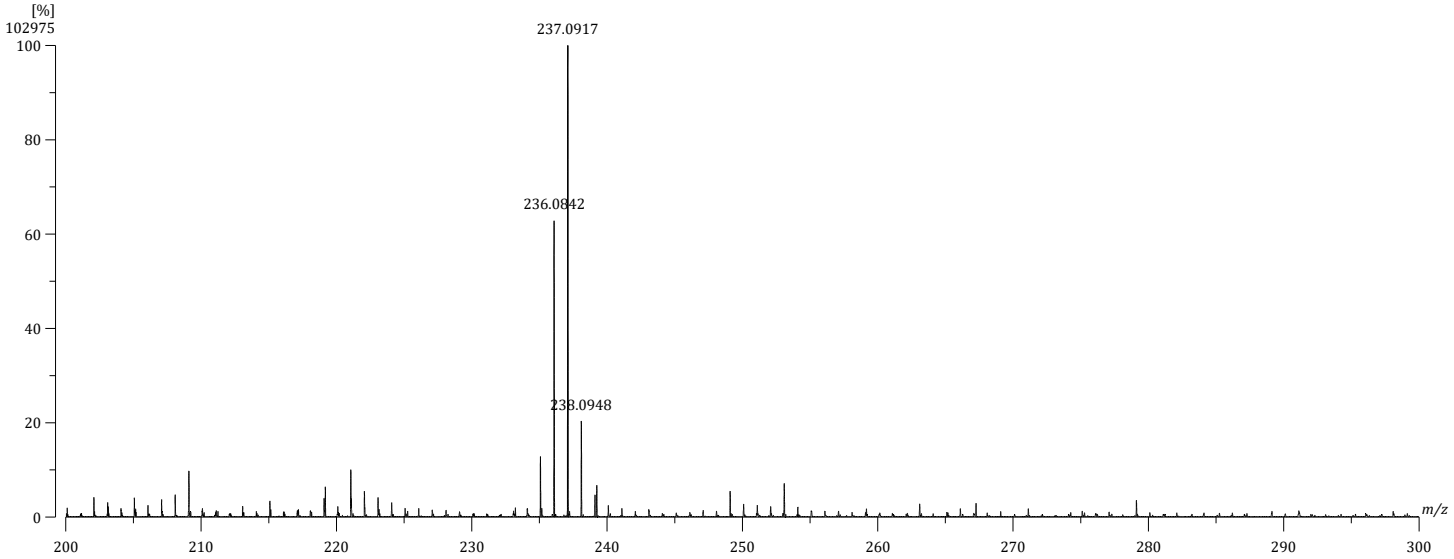


Observed m/z	Int%					
263.1436	100.00					
Estimated m/z	Err[ppm / mmu]	U.S.	C	H	O	
1 263.1436	+0.0 / +0.0	10.5	19	19	1	

The high-resolution mass spectrum (FAB+) of compound 2o.



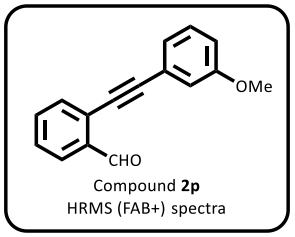
[Mass Spectrum]
Data : 20220421_CYL-713-HR-002 Date : 21-Apr-2022 17:10
Sample : CYL-713
Note : NBA
Ion Mode : FAB+
RT : 0.48 min Scan# : 6
Elements : C 1000/0, H 1000/0, O 2/2
Mass Tolerance : 50mmu
Unsaturation (U.S.) : -0.5 - 1000.0



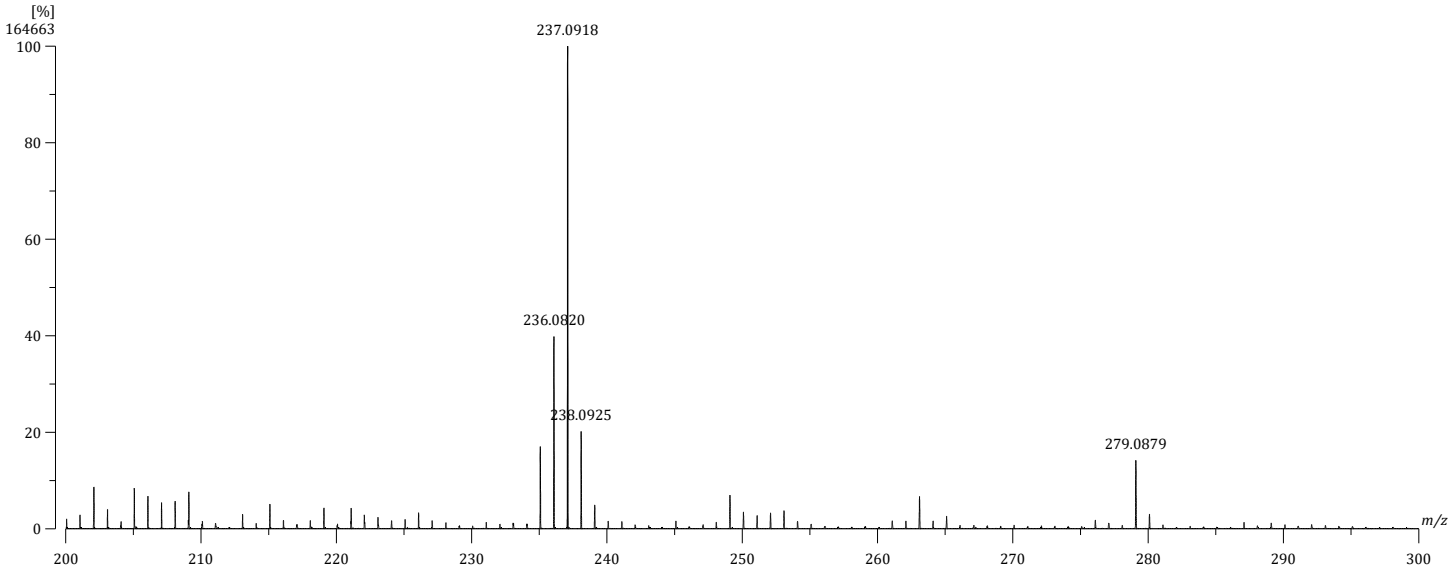
	Observed m/z	Int%
	237.0917	100.00

	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	O
1	237.0916	+0.6 / +0.1	10.5	16	13	2

The high-resolution mass spectrum (FAB+) of compound 2p.

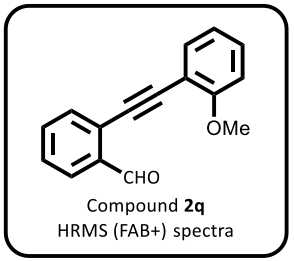


[Mass Spectrum]
Data : 20220421_CYL-714-HR-002 Date : 21-Apr-2022 17:03
Sample : CYL-714
Note : NBA
Ion Mode : FAB+
RT : 0.00 min Scan# : 1
Elements : C 1000/0, H 1000/0, O 2/2
Mass Tolerance : 50mmu
Unsaturation (U.S.) : -0.5 - 1000.0



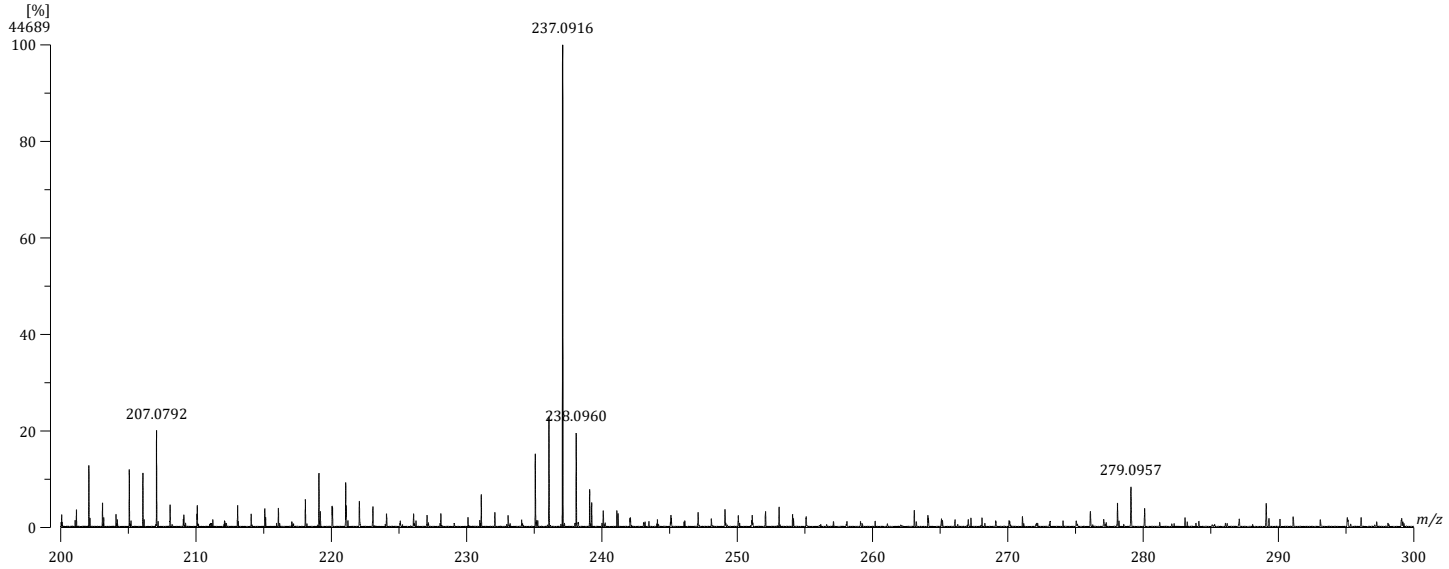
Observed m/z	Int%					
237.0918	100.00					
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	O
1	237.0916	+1.0 / +0.2	10.5	16	13	2

The high-resolution mass spectrum (FAB+) of compound 2q.



Compound **2q**
HRMS (FAB+) spectra

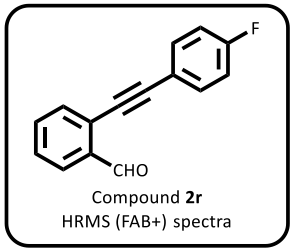
[Mass Spectrum]
Data : 20220421_CYL-715-HR-002 Date : 21-Apr-2022 16:50
Sample : CYL-715
Note : NBA
Ion Mode : FAB+
RT : 0.10 min Scan# : 2
Elements : C 1000/0, H 1000/0, O 2/2
Mass Tolerance : 50mmu
Unsaturation (U.S.) : -0.5 - 1000.0



	Observed m/z	Int%
	237.0916	100.00

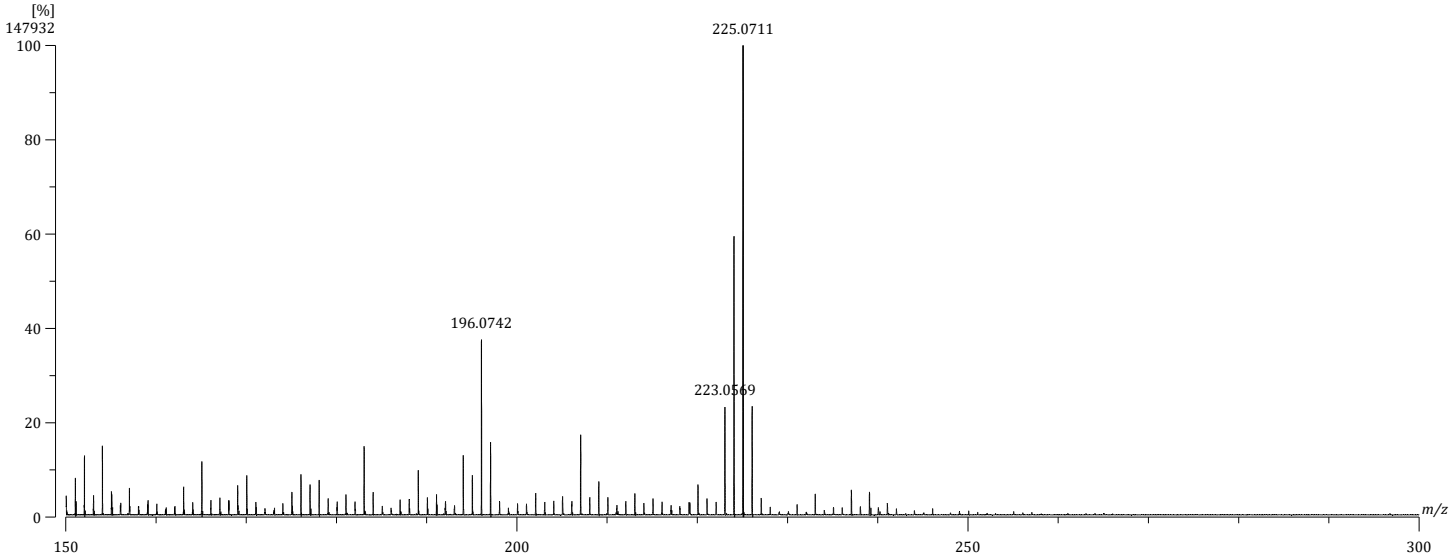
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	O
1	237.0916	+0.2 / +0.0	10.5	16	13	2

The high-resolution mass spectrum (FAB+) of compound 2r.



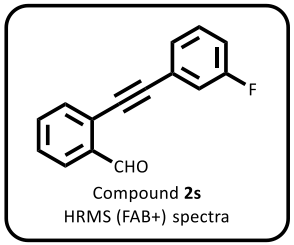
Compound **2r**
HRMS (FAB+) spectra

[Mass Spectrum]
Data : 20220420_CYL-718-HR-002 Date : 20-Apr-2022 16:55
Sample : CYL-718
Note : NBA
Ion Mode : FAB+
RT : 0.00 min Scan# : (1,6)
Elements : C 1000/0, H 1000/0, F 1/1, O 1/1
Mass Tolerance : 50mmu
Unsaturation (U.S.) : -0.5 - 1000.0

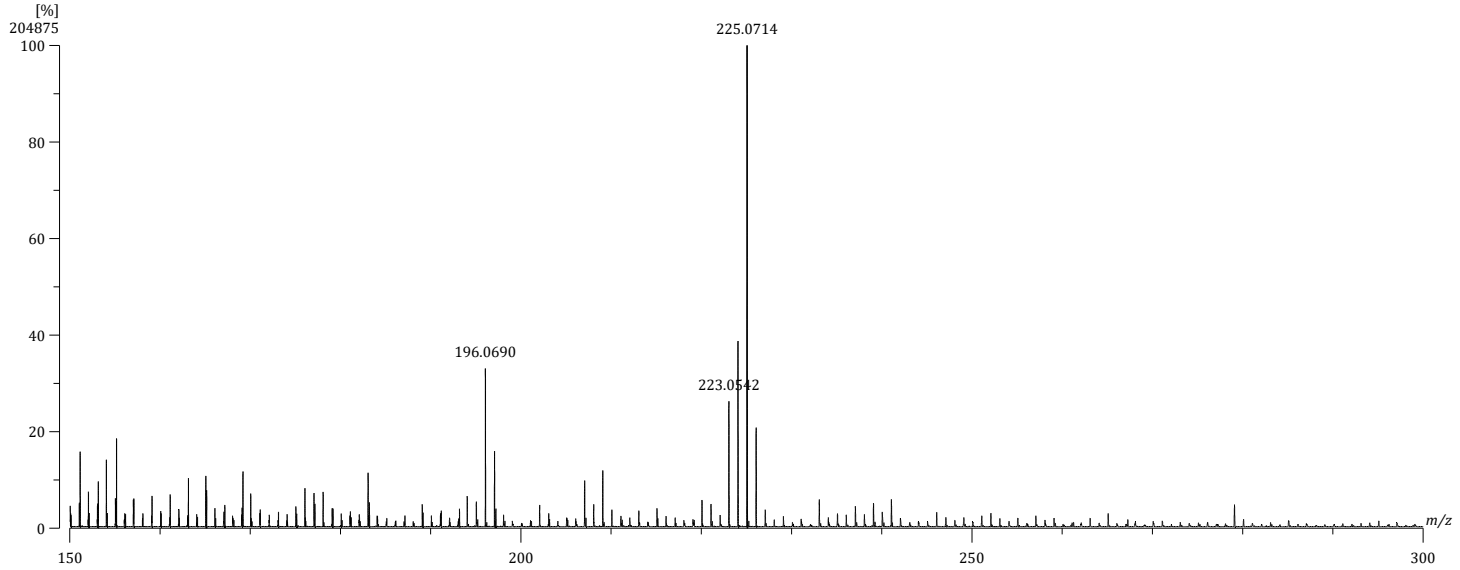


	Observed m/z	Int%						
	225.0711	100.00						
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	F	O	
1	225.0716	-2.1 / -0.5	10.5	15	10	1	1	

The high-resolution mass spectrum (FAB+) of compound 2s.



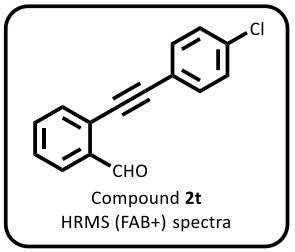
[Mass Spectrum]
Data : 20220421_CYL-719-HR-002 Date : 21-Apr-2022 16:21
Sample : CYL-719
Note : NBA
Ion Mode : FAB+
RT : 0.00 min Scan# : (1,6)
Elements : C 1000/0, H 1000/0, F 1/1, O 1/1
Mass Tolerance : 50mmu
Unsaturation (U.S.) : -0.5 - 1000.0



	Observed m/z	Int%
	225.0714	100.00

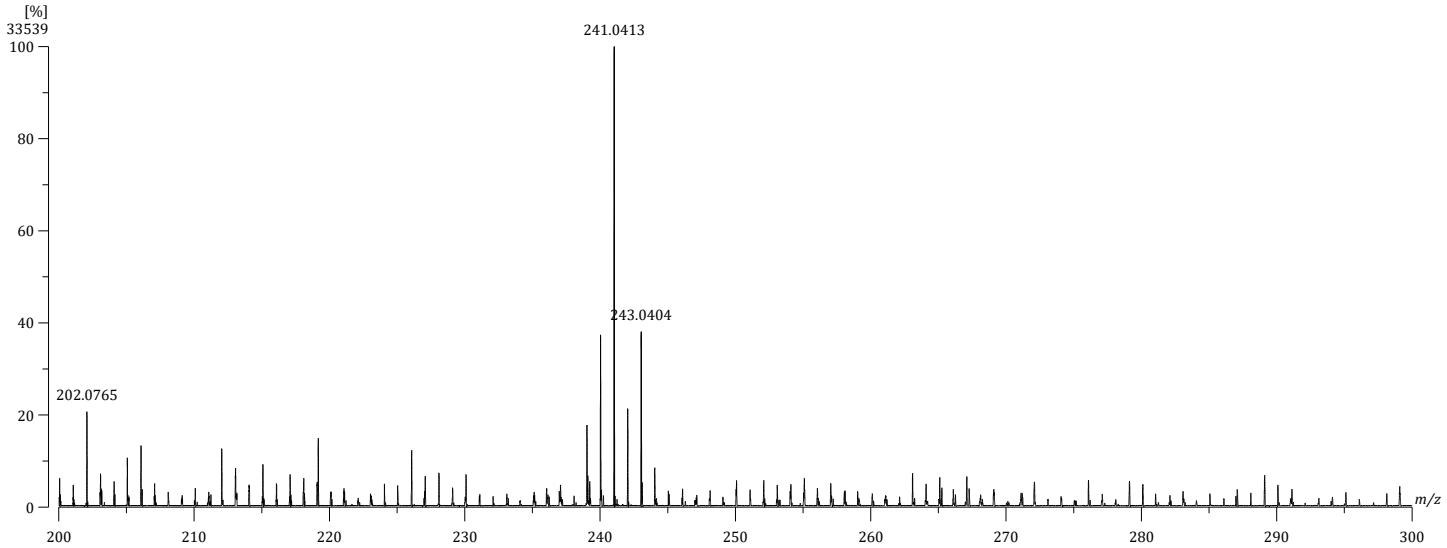
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	F	O
1	225.0716	-0.7 / -0.2	10.5	15	10	1	1

The high-resolution mass spectrum (FAB+) of compound 2t.



Compound **2t**
HRMS (FAB+) spectra

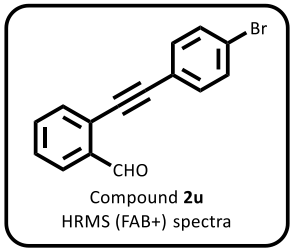
[Mass Spectrum]
Data : 20220421_CYL-720-HR-003 Date : 21-Apr-2022 16:14
Sample : CYL-720
Note : NBA
Ion Mode : FAB+
RT : 0.57 min Scan# : 7
Elements : C 1000/0, H 1000/0, 35Cl 1/0, 37Cl 1/0, O 1/1
Mass Tolerance : 5mmu
Unsaturation (U.S.) : -0.5 - 1000.0



	Observed m/z	Int%							
	241.0413	100.00							
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	35Cl	37Cl	O	
1	241.0420	-3.0 / -0.7	10.5	15	10	1	-	1	

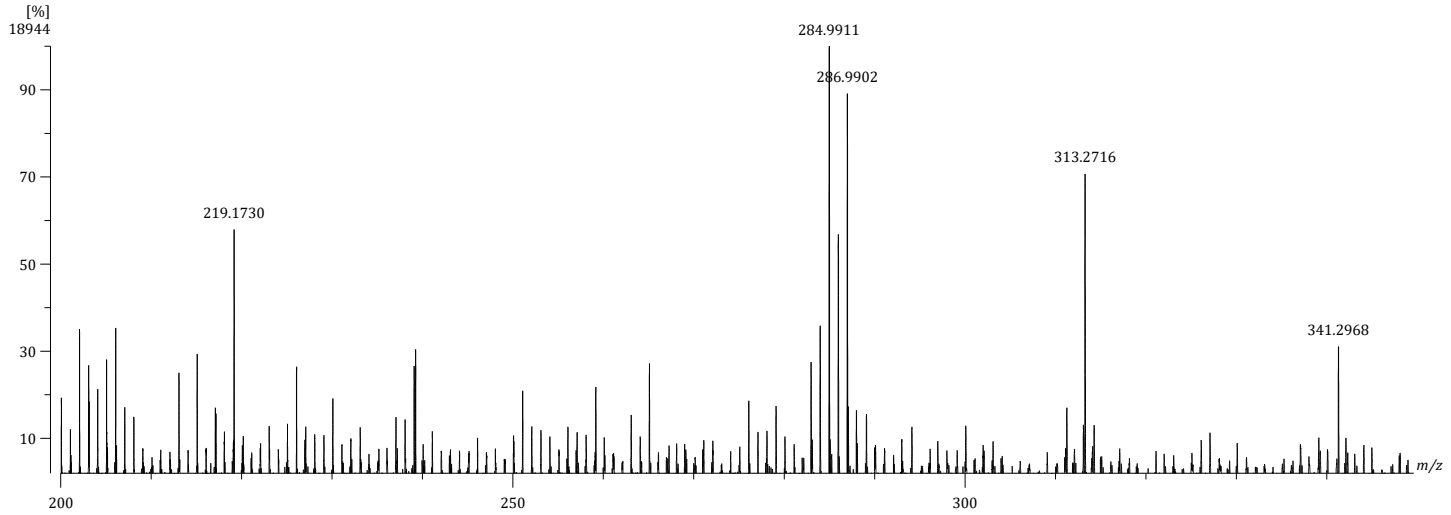
	Observed m/z	Int%							
	243.0404	38.07							
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	35Cl	37Cl	O	
2	243.0391	+5.5 / +1.3	10.5	15	10	-	1	1	

The high-resolution mass spectrum (FAB+) of compound 2u.



Compound **2u**
HRMS (FAB+) spectra

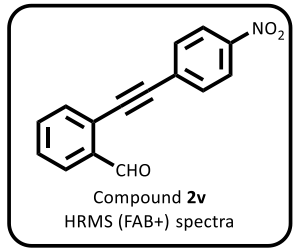
[Mass Spectrum]
Data : 20220420_CYL-721-HR-003 Date : 20-Apr-2022 17:10
Sample : CYL-721
Note : NBA
Ion Mode : FAB+
RT : 0.00 min Scan# : (1,3)
Elements : C 1000/0, H 1000/0, 79Br 1/0, 81Br 1/0, O 1/1
Mass Tolerance : 5mmu
Unsaturation (U.S.) : -0.5 - 1000.0



	Observed m/z	Int%							
	284.9911	100.00							
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	79Br	81Br	O	
1	284.9915	-1.4 / -0.4	10.5	15	10	1	-	1	

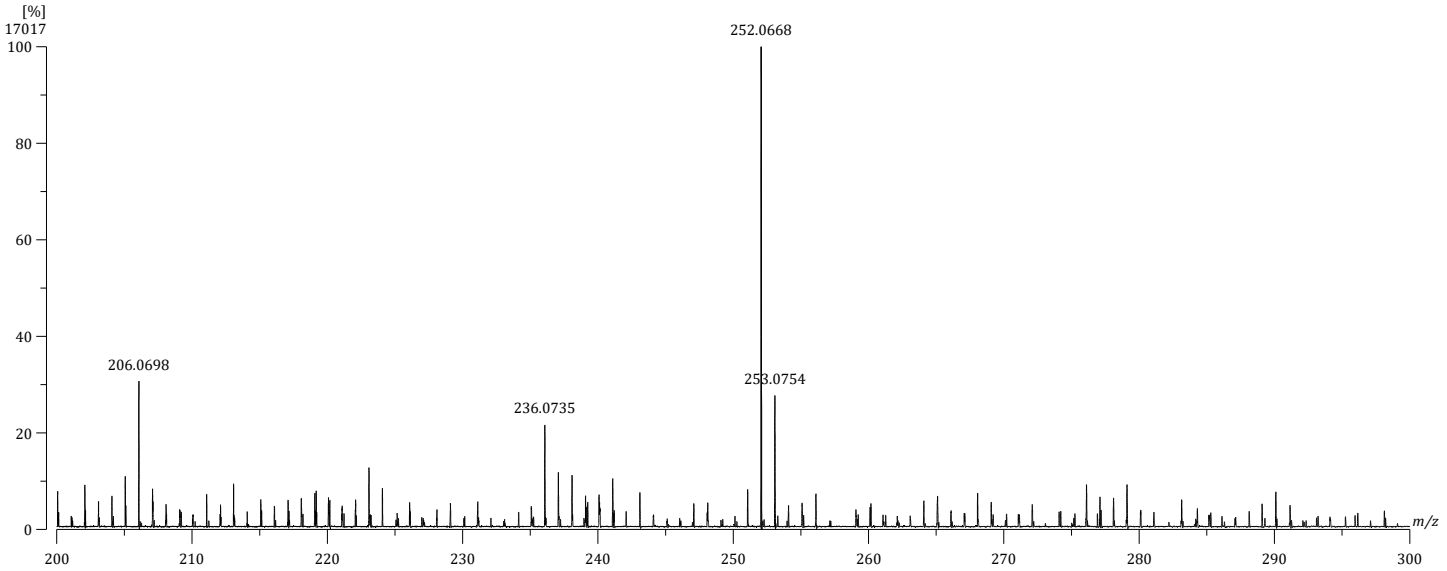
	Observed m/z	Int%							
	286.9902	89.08							
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	79Br	81Br	O	
2	286.9895	+2.6 / +0.7	10.5	15	10	-	1	1	

The high-resolution mass spectrum (FAB+) of compound 2v.



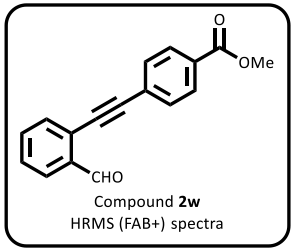
Compound **2v**
HRMS (FAB+) spectra

[Mass Spectrum]
Data : 20220421_CYL-723-HR-002 Date : 21-Apr-2022 16:28
Sample : CYL-723
Note : NBA
Ion Mode : FAB+
RT : 0.29 min Scan# : 4
Elements : C 1000/0, H 1000/0, N 1/1, O 3/3
Mass Tolerance : 50mmu
Unsaturation (U.S.) : -0.5 - 1000.0



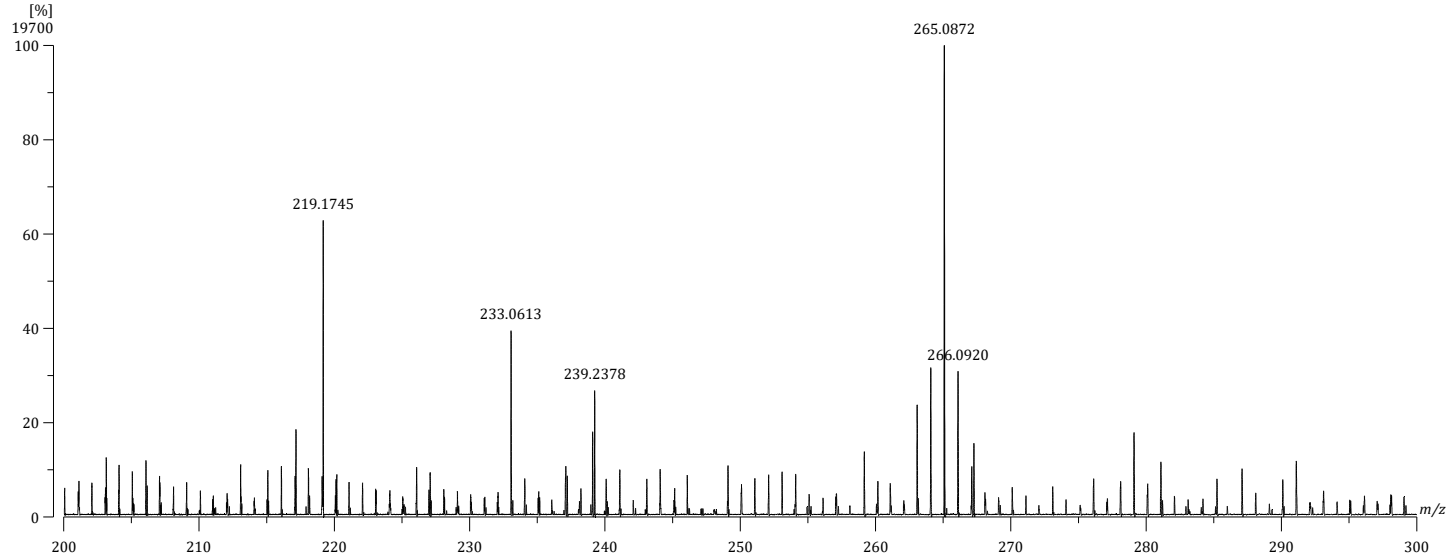
	Observed m/z	Int%					
	252.0668	100.00					
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	N	O
1	252.0661	+2.9 / +0.7	11.5	15	10	1	3

The high-resolution mass spectrum (FAB+) of compound 2w.



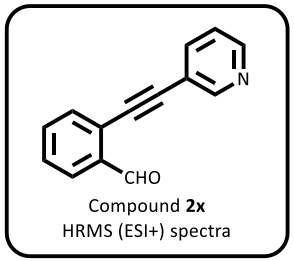
Compound **2w**
HRMS (FAB+) spectra

[Mass Spectrum]
Data : 20220421_CYL-725-HR-002 Date : 21-Apr-2022 16:43
Sample : CYL-725
Note : NBA
Ion Mode : FAB+
RT : 0.00 min Scan# : 1
Elements : C 1000/0, H 1000/0, O 3/3
Mass Tolerance : 50mmu
Unsaturation (U.S.) : -0.5 - 1000.0

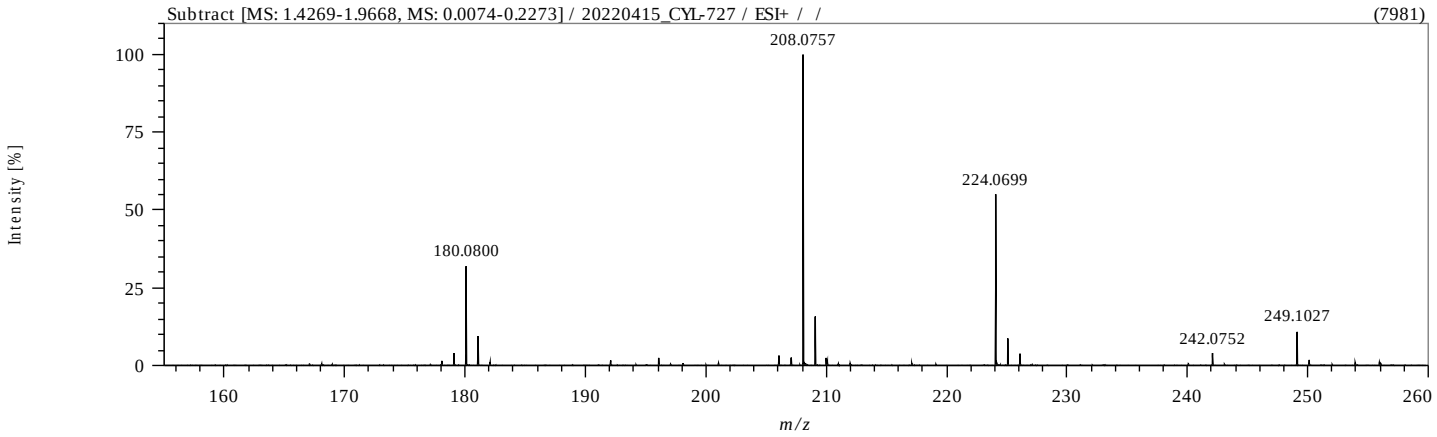


	Observed m/z	Int%				
	265.0872	100.00				
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	O
1	265.0865	+2.8 / +0.7	11.5	17	13	3

The high-resolution mass spectrum (ESI+) of compound 2x.



Spectrum



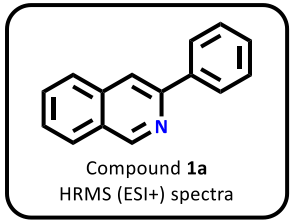
Elemental Composition

Parameters		Elements Set 1:				
Tolerance:	±10.00 ppm	Symbol	C	H	N	O
Electron:	Odd/Even	Min	0	0	1	1
Charge:	+1	Max	400	1000	2	1
DBE:	-99.0 - 999.0					

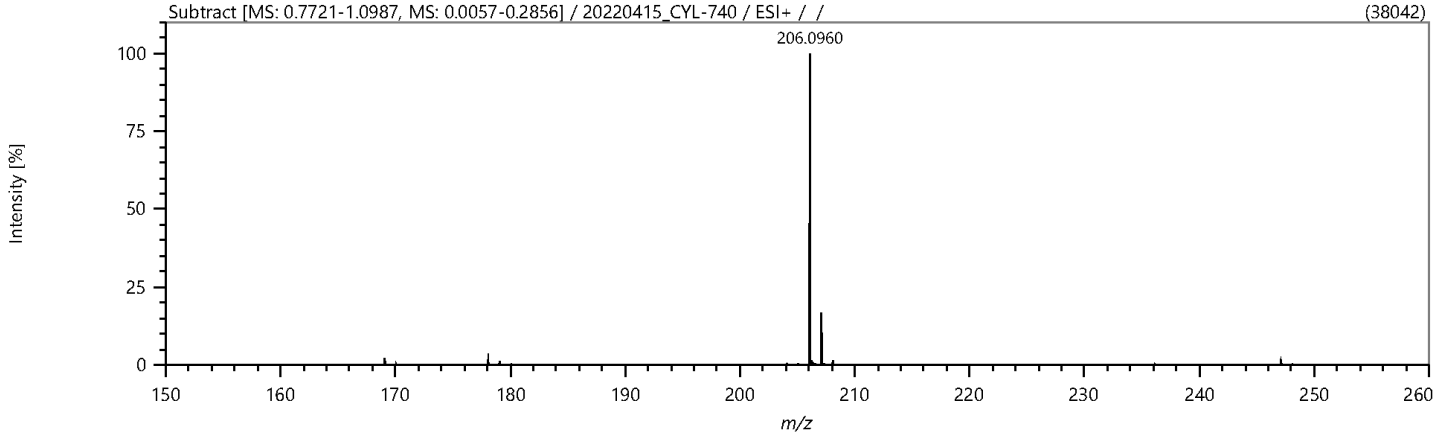
Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
208.07569	C14 H10 N O	208.07569	0.00	0.01	10.5

The high-resolution mass spectrum (ESI+) of compound 1a.



Spectrum



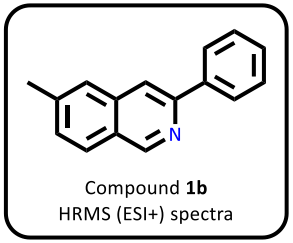
Elemental Composition

Parameters		Elements Set 1:			
Tolerance:	±10.00 ppm	Symbol	C	H	N
Electron:	Odd/Even	Min	0	0	1
Charge:	+1	Max	400	1000	2
DBE:	-99.0 - 999.0				

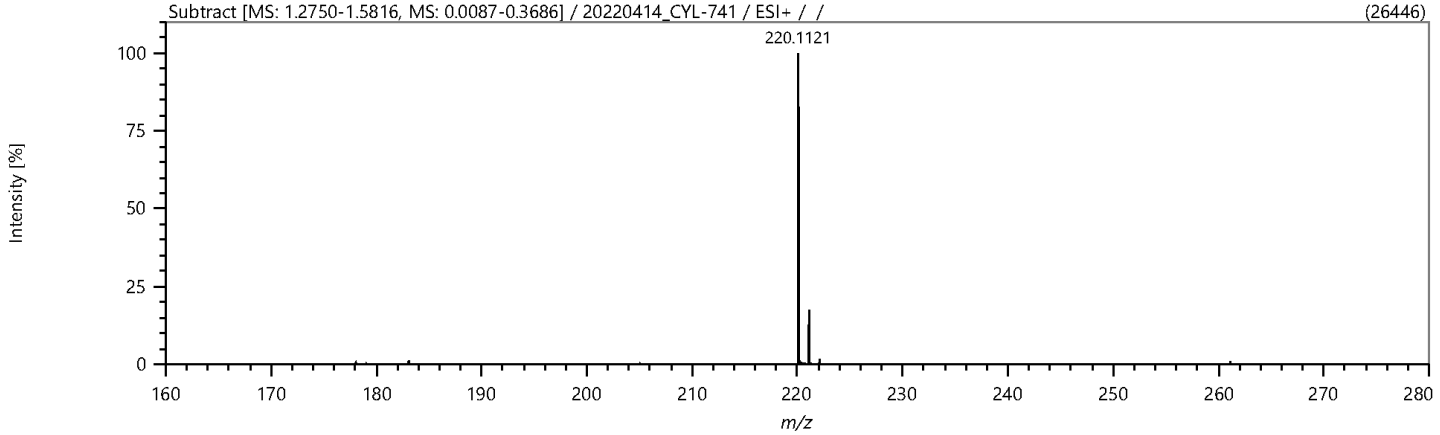
Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
206.09597	C15 H12 N	206.09643	-0.46	-2.23	10.5

The high-resolution mass spectrum (ESI+) of compound 1b.



Spectrum



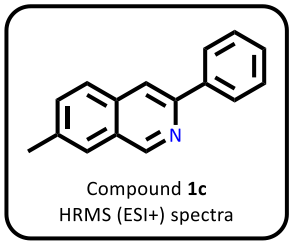
Elemental Composition

Parameters		Elements Set 1:			
Tolerance:	±20.00 ppm	Symbol	C	H	N
Electron:	Odd/Even	Min	0	0	1
Charge:	+1	Max	400	1000	2
DBE:	-99.0 - 999.0				

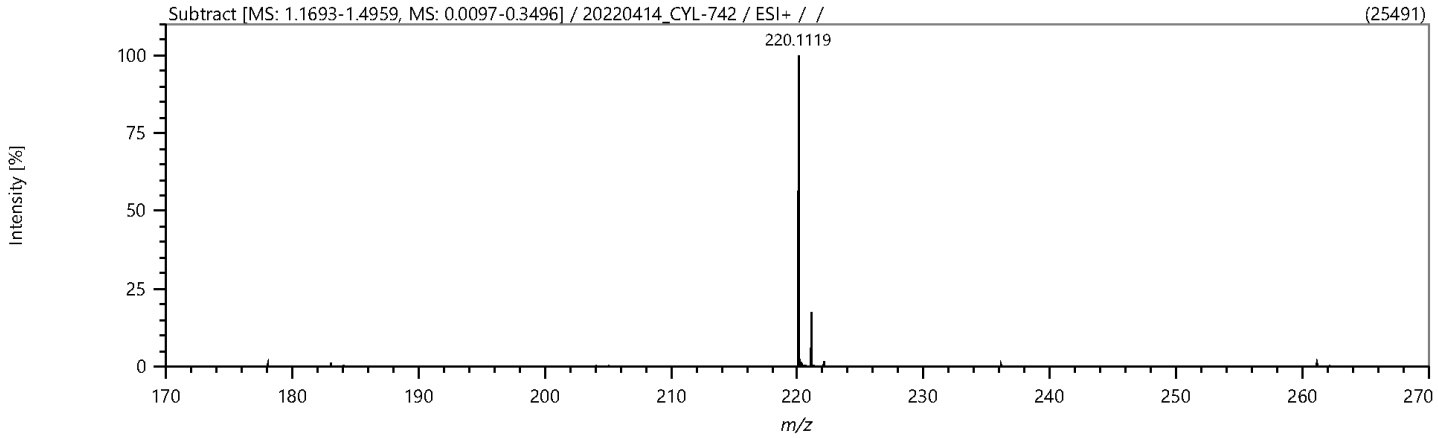
Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
220.11207	C16 H14 N	220.11208	-0.01	-0.04	10.5

The high-resolution mass spectrum (ESI+) of compound 1c.



Spectrum



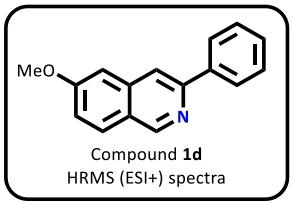
Elemental Composition

Parameters		Elements Set 1:			
Tolerance:	±20.00 ppm	Symbol	C	H	N
Electron:	Odd/Even	Min	0	0	1
Charge:	+1	Max	400	1000	1
DBE:	-99.0 - 999.0				

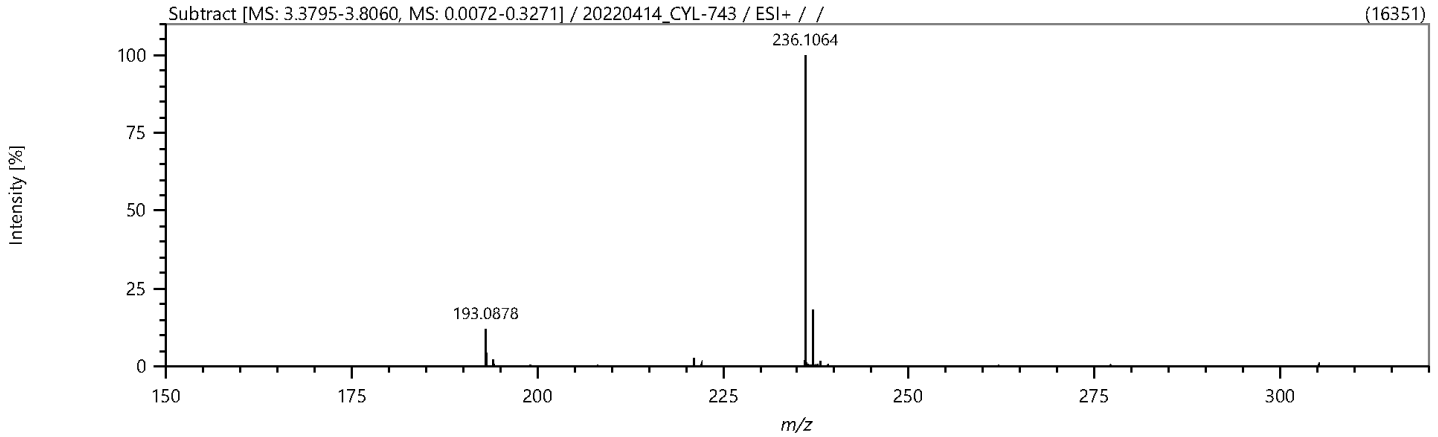
Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
220.11189	C16 H14 N	220.11208	-0.18	-0.82	10.5

The high-resolution mass spectrum (ESI+) of compound 1d.



Spectrum



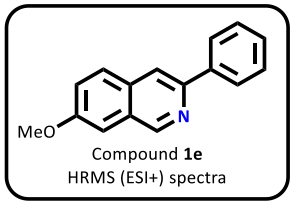
Elemental Composition

Parameters		Elements Set 1:				
Tolerance:	±20.00 ppm	Symbol	C	H	N	O
Electron:	Odd/Even	Min	0	0	1	1
Charge:	+1	Max	400	1000	1	1
DBE:	-99.0 - 999.0					

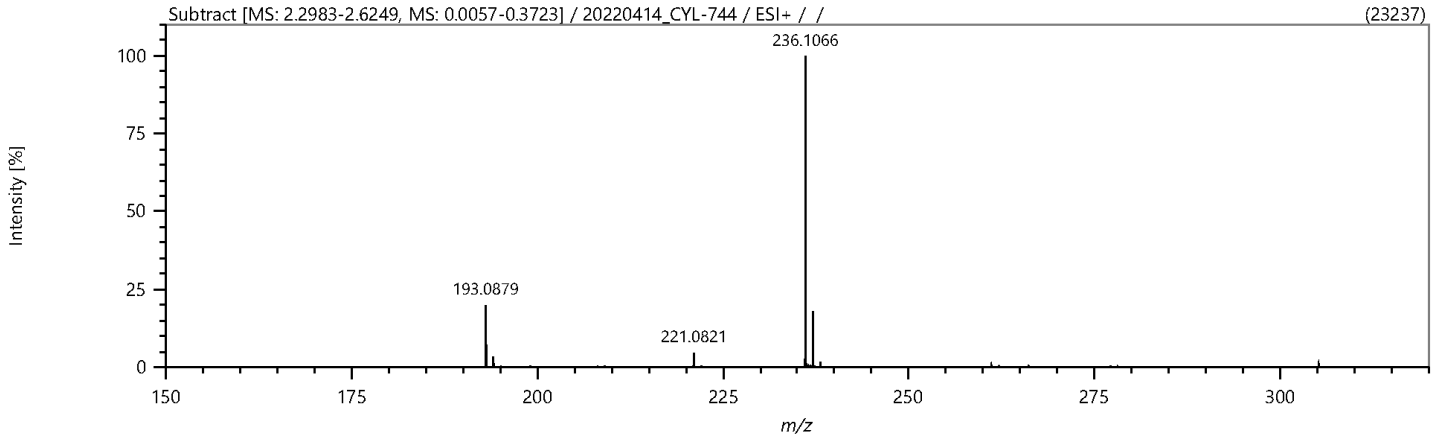
Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
236.10642	C16 H14 N O	236.10699	-0.57	-2.42	10.5

The high-resolution mass spectrum (ESI+) of compound 1e.



Spectrum



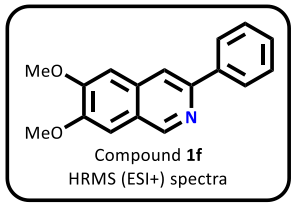
Elemental Composition

Parameters		Elements Set 1:				
Tolerance:	±20.00 ppm	Symbol	C	H	N	O
Electron:	Odd/Even	Min	0	0	1	1
Charge:	+1	Max	400	1000	1	2
DBE:	-99.0 - 999.0					

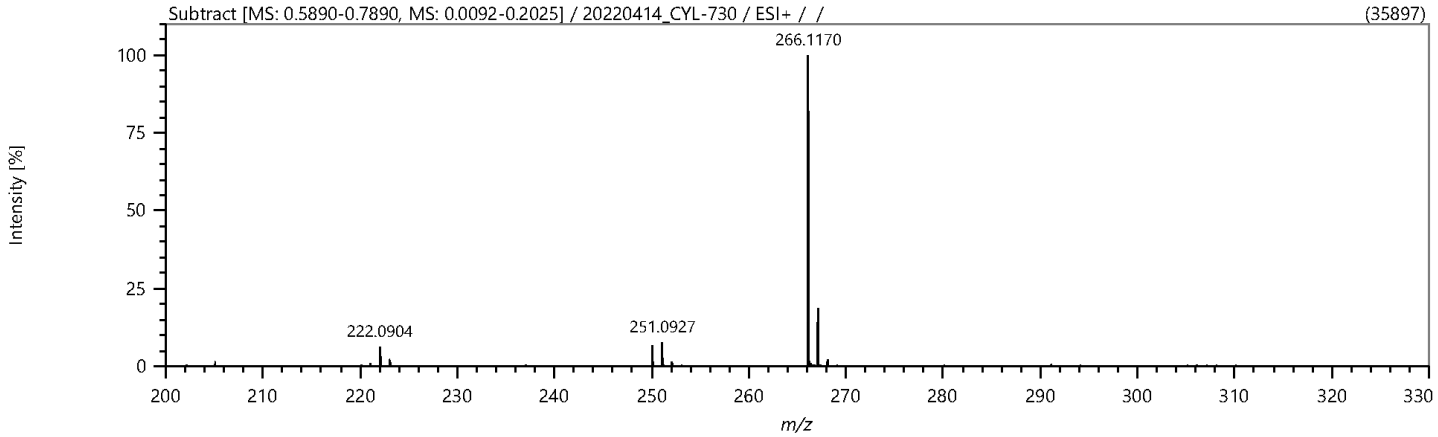
Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
236.10663	C16 H14 N O	236.10699	-0.36	-1.51	10.5

The high-resolution mass spectrum (ESI+) of compound 1f.



Spectrum



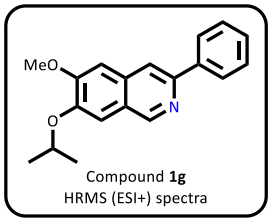
Elemental Composition

Parameters		Elements Set 1:				
Tolerance:	±20.00 ppm	Symbol	C	H	N	O
Electron:	Odd/Even	Min	0	0	1	2
Charge:	+1	Max	400	1000	1	2
DBE:	-99.0 - 999.0					

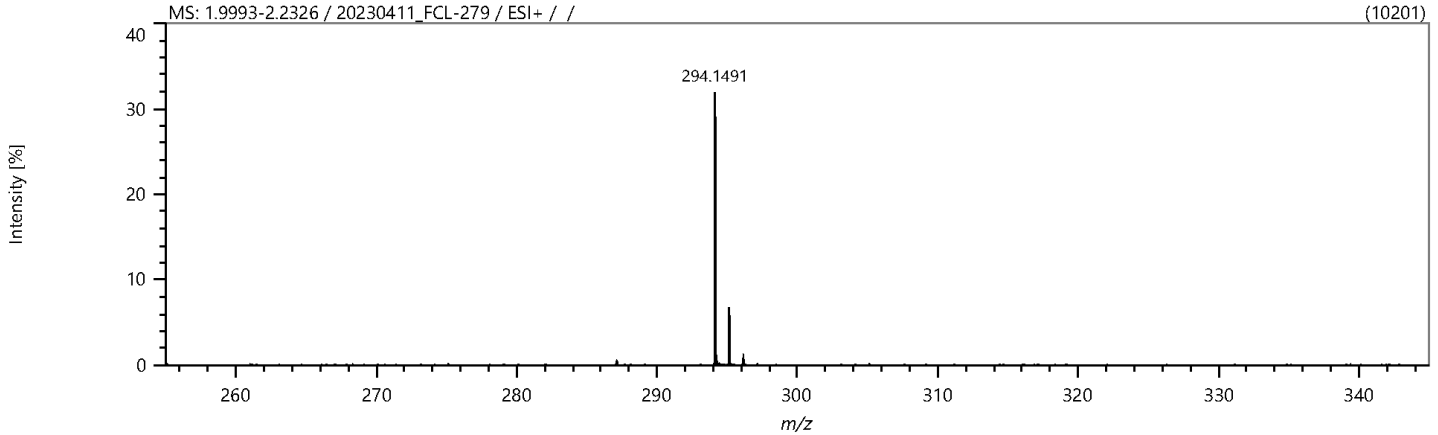
Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
266.11705	C17 H16 N O2	266.11756	-0.51	-1.91	10.5

The high-resolution mass spectrum (ESI+) of compound 1g.



Spectrum



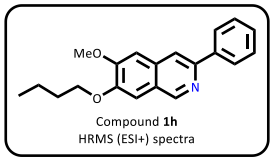
Elemental Composition

Parameters		Elements Set 1:					
Tolerance:	±5.00 ppm	Symbol	C	H	O	N	Na
Electron:	Odd/Even	Min	0	0	2	1	0
Charge:	+1	Max	100	400	2	1	1
DBE:	-99.0 - 999.0						

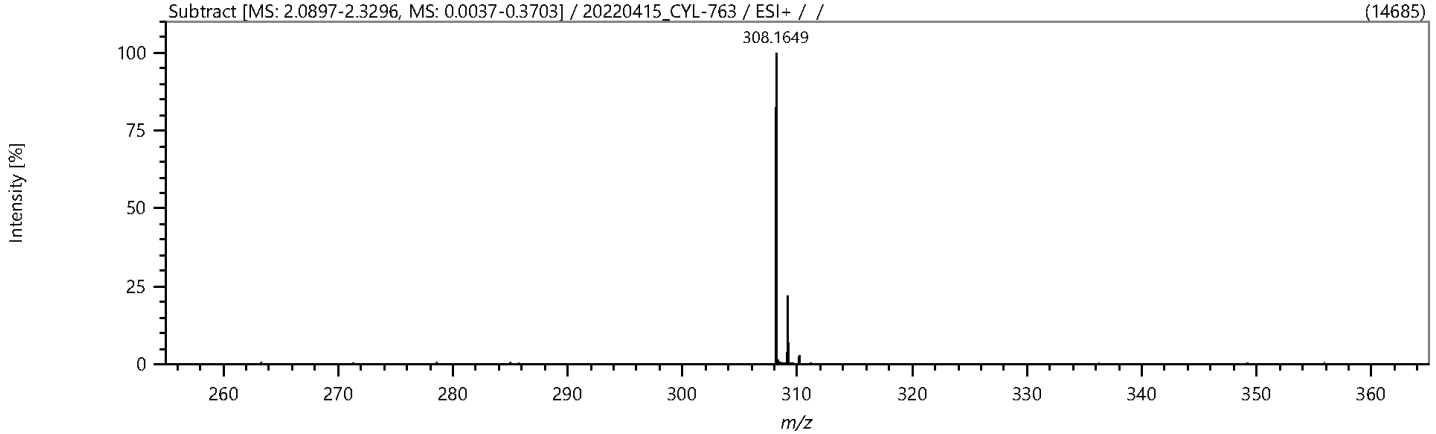
Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
294.14907	C19 H20 N O2	294.14886	0.21	0.72	10.5

The high-resolution mass spectrum (ESI+) of compound 1h.



Spectrum



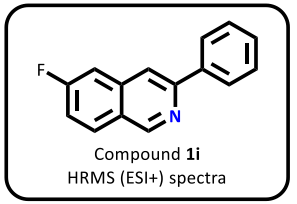
Elemental Composition

Parameters		Elements Set 1:				
Tolerance:	±10.00 ppm	Symbol	C	H	N	O
Electron:	Odd/Even	Min	0	0	1	1
Charge:	+1	Max	400	1000	2	2
DBE:	-99.0 - 999.0					

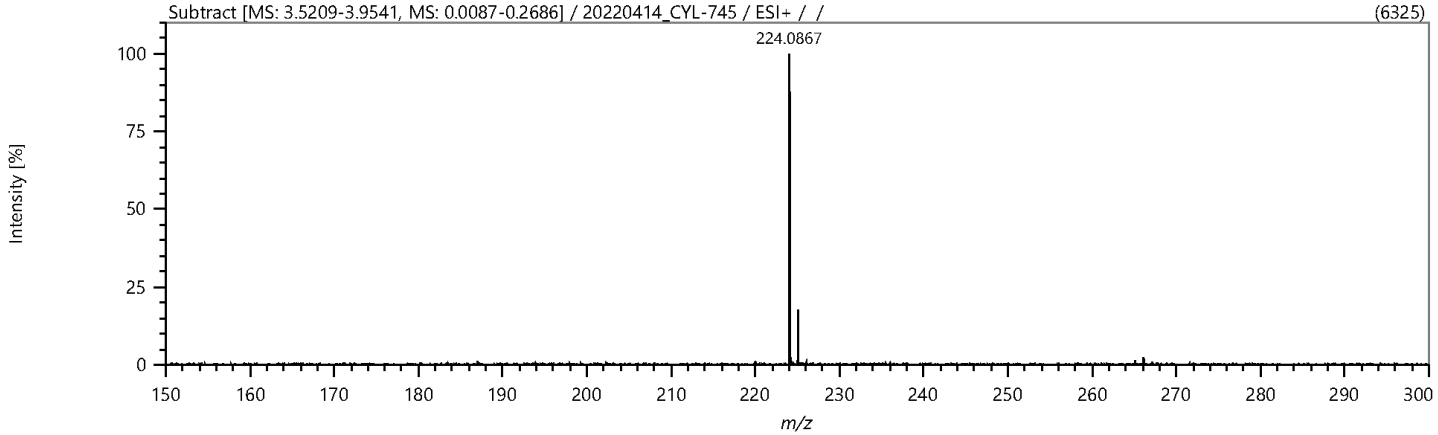
Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
308.16491	C20 H22 N O2	308.16451	0.41	1.33	10.5

The high-resolution mass spectrum (ESI+) of compound 1i.



Spectrum



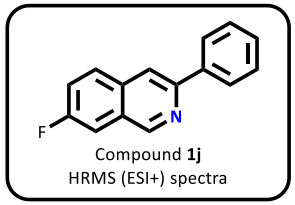
Elemental Composition

Parameters		Elements Set 1:				
Tolerance:	±20.00 ppm	Symbol	C	H	N	F
Electron:	Odd/Even	Min	0	0	1	1
Charge:	+1	Max	400	1000	1	1
DBE:	-99.0 - 999.0					

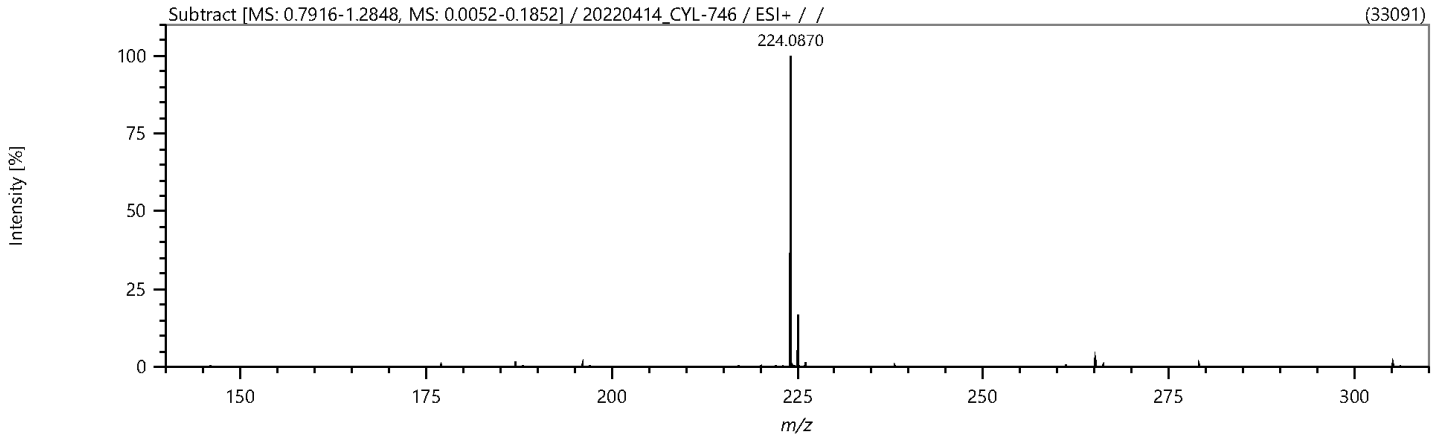
Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
224.08673	C15 H11 N F	224.08700	-0.27	-1.22	10.5

The high-resolution mass spectrum (ESI+) of compound 1j.



Spectrum



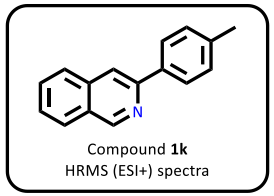
Elemental Composition

Parameters		Elements Set 1:				
Tolerance:	±20.00 ppm	Symbol	C	H	N	F
Electron:	Odd/Even	Min	0	0	1	1
Charge:	+1	Max	400	1000	1	1
DBE:	-99.0 - 999.0					

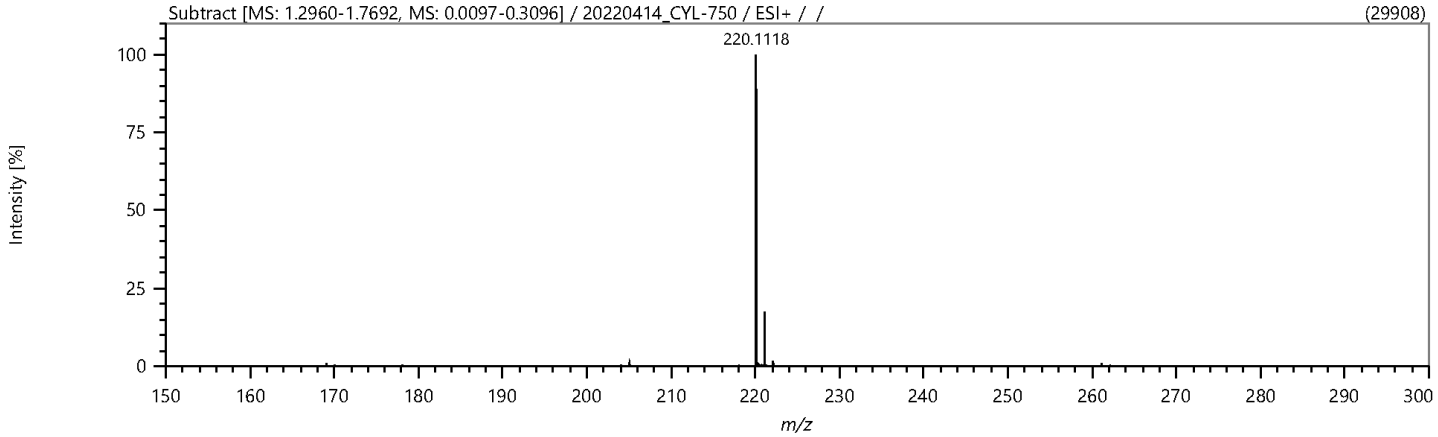
Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
224.08705	C15 H11 N F	224.08700	0.04	0.19	10.5

The high-resolution mass spectrum (ESI+) of compound 1k.



Spectrum



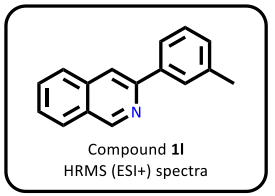
Elemental Composition

Parameters		Elements Set 1:			
Tolerance:	±20.00 ppm	Symbol	C	H	N
Electron:	Odd/Even	Min	0	0	1
Charge:	+1	Max	400	1000	1
DBE:	-99.0 - 999.0				

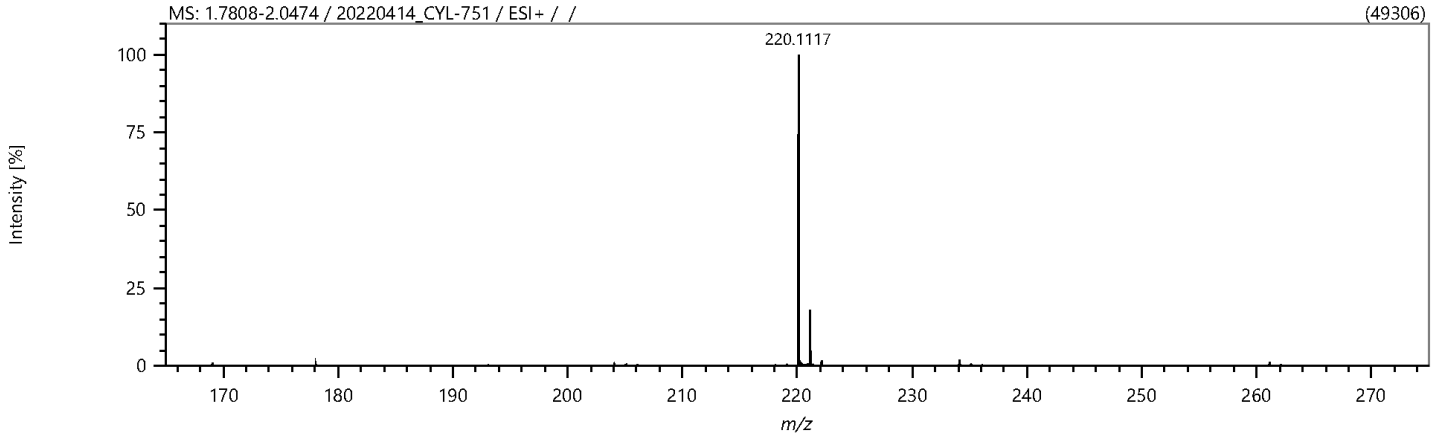
Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
220.11181	C16 H14 N	220.11208	-0.27	-1.23	10.5

The high-resolution mass spectrum (ESI+) of compound 1l.



Spectrum



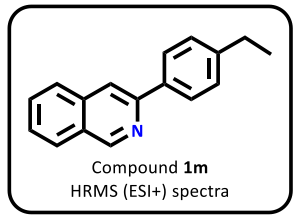
Elemental Composition

Parameters		Elements Set 1:			
Tolerance:	±20.00 ppm	Symbol	C	H	N
Electron:	Odd/Even	Min	0	0	1
Charge:	+1	Max	400	1000	1
DBE:	-99.0 - 999.0				

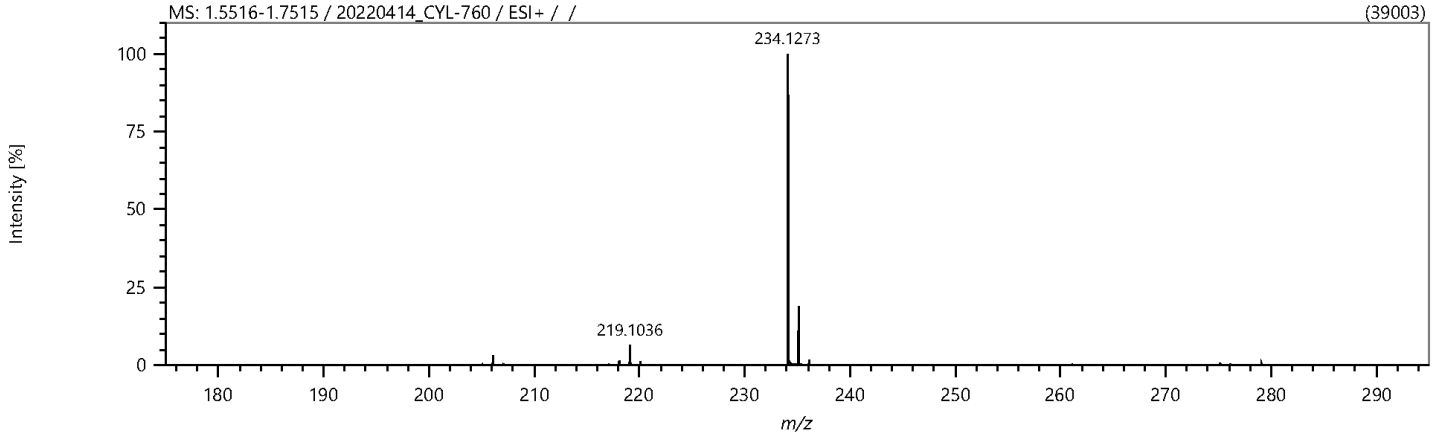
Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
220.11171	C16 H14 N	220.11208	-0.36	-1.64	10.5

The high-resolution mass spectrum (ESI+) of compound 1m.



Spectrum



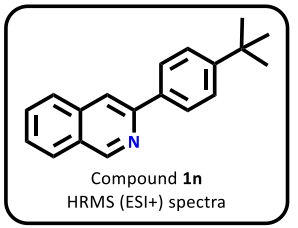
Elemental Composition

Parameters		Elements Set 1:			
Tolerance:	±20.00 ppm	Symbol	C	H	N
Electron:	Odd/Even	Min	0	0	1
Charge:	+1	Max	400	1000	1
DBE:	-99.0 - 999.0				

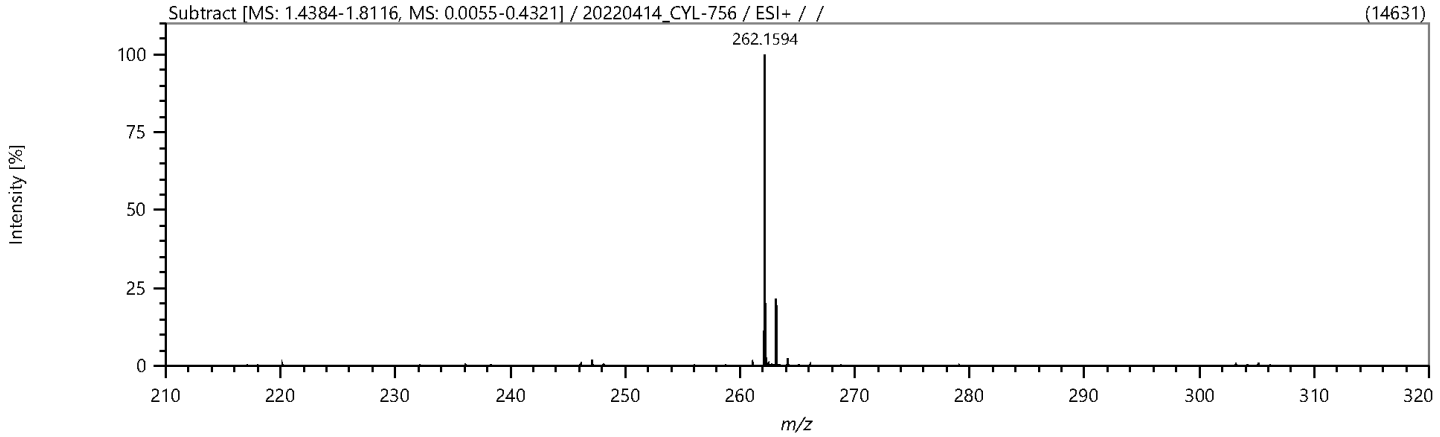
Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
234.12734	C17 H16 N	234.12773	-0.38	-1.64	10.5

The high-resolution mass spectrum (ESI+) of compound 1n.



Spectrum



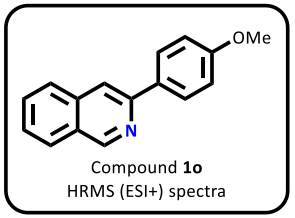
Elemental Composition

Parameters		Elements Set 1:			
Tolerance:	±20.00 ppm	Symbol	C	H	N
Electron:	Odd/Even	Min	0	0	1
Charge:	+1	Max	400	1000	1
DBE:	-99.0 - 999.0				

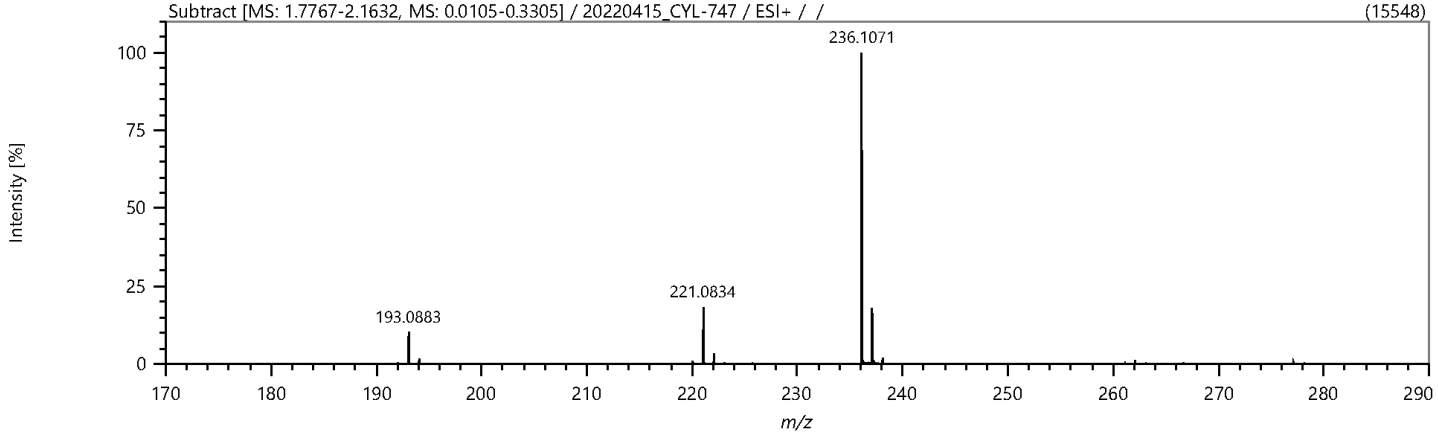
Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
262.15936	C19 H20 N	262.15903	0.33	1.26	10.5

The high-resolution mass spectrum (ESI+) of compound 1o.



Spectrum



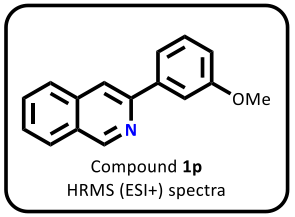
Elemental Composition

Parameters		Elements Set 1:				
Tolerance:	±10.00 ppm	Symbol	C	H	N	O
Electron:	Odd/Even	Min	0	0	1	1
Charge:	+1	Max	400	1000	2	2
DBE:	-99.0 - 999.0					

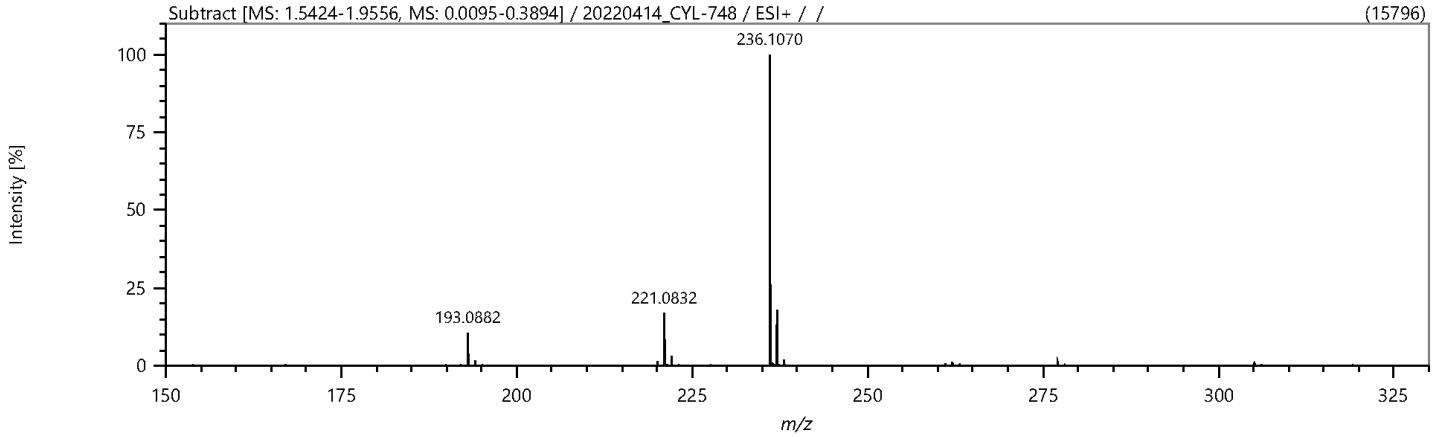
Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
236.10712	C16 H14 N O	236.10699	0.13	0.55	10.5

The high-resolution mass spectrum (ESI+) of compound 1p.



Spectrum



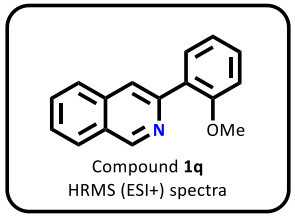
Elemental Composition

Parameters		Elements Set 1:				
Tolerance:	±10.00 ppm	Symbol	C	H	N	O
Electron:	Odd/Even	Min	0	0	1	1
Charge:	+1	Max	400	1000	2	1
DBE:	-99.0 - 999.0					

Results

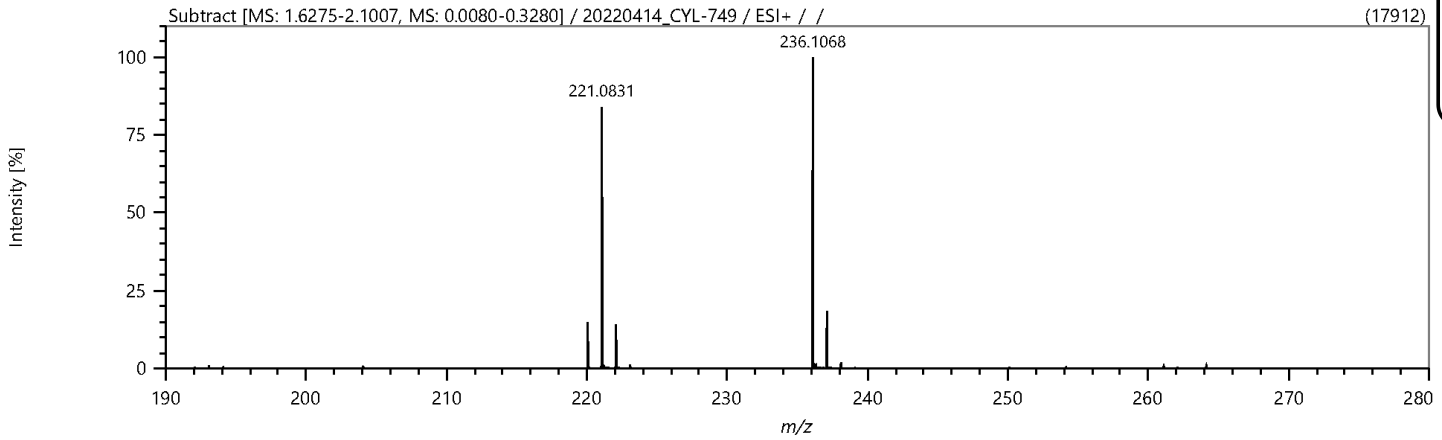
Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
236.10697	C16 H14 N O	236.10699	-0.02	-0.07	10.5

The high-resolution mass spectrum (ESI+) of compound 1q.



Compound **1q**
HRMS (ESI+) spectra

Spectrum



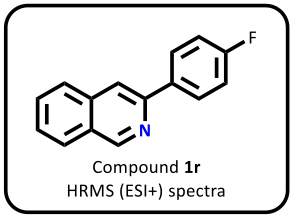
Elemental Composition

Parameters		Elements Set 1:				
Tolerance:	±10.00 ppm	Symbol	C	H	N	O
Electron:	Odd/Even	Min	0	0	1	1
Charge:	+1	Max	400	1000	2	2
DBE:	-99.0 - 999.0					

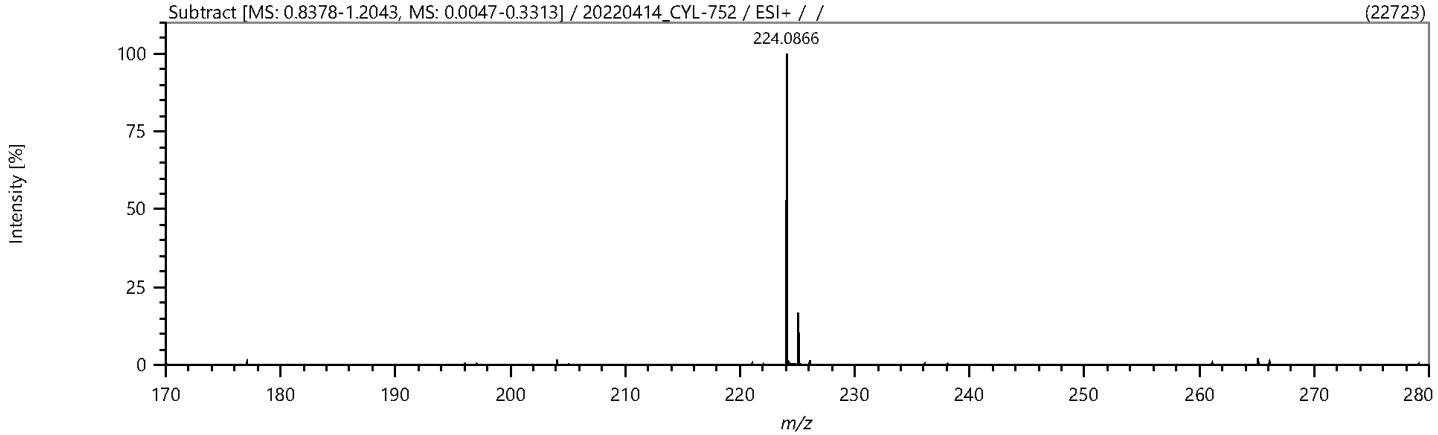
Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
236.10682	C16 H14 N O	236.10699	-0.17	-0.72	10.5

The high-resolution mass spectrum (ESI+) of compound 1r.



Spectrum



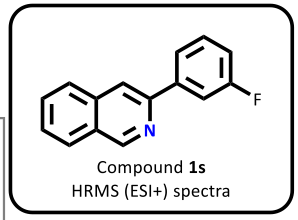
Elemental Composition

Parameters		Elements Set 1:				
Tolerance:	±10.00 ppm	Symbol	C	H	N	F
Electron:	Odd/Even	Min	0	0	1	1
Charge:	+1	Max	400	1000	2	1
DBE:	-99.0 - 999.0					

Results

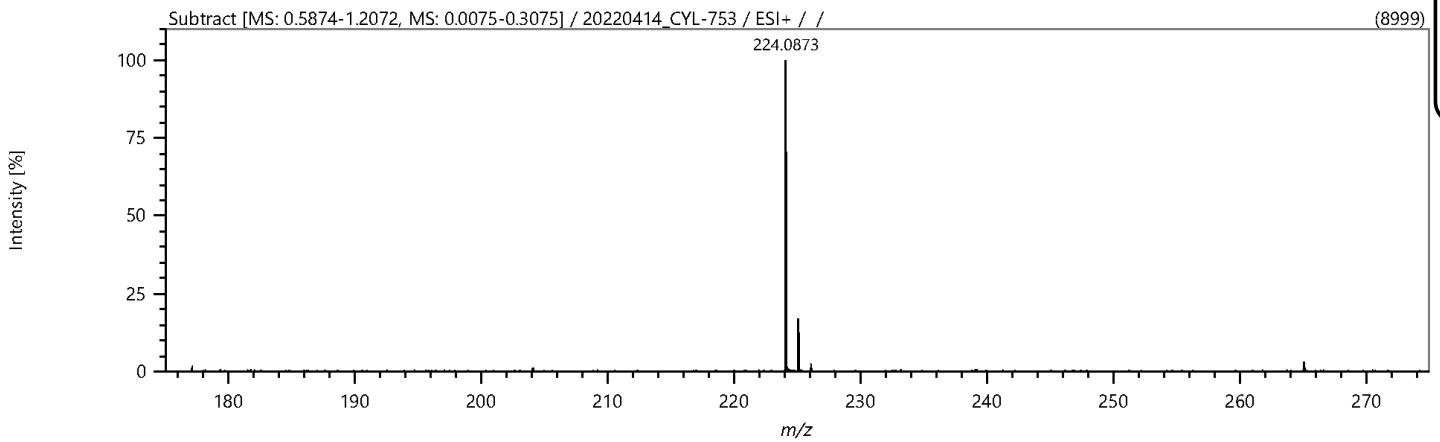
Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
224.08661	C15 H11 N F	224.08700	-0.40	-1.77	10.5

The high-resolution mass spectrum (ESI+) of compound 1s.



Compound **1s**
HRMS (ESI+) spectra

Spectrum



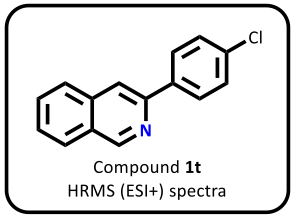
Elemental Composition

Parameters		Elements Set 1:				
Tolerance:	±10.00 ppm	Symbol	C	H	N	F
Electron:	Odd/Even	Min	0	0	1	1
Charge:	+1	Max	400	1000	2	2
DBE:	-99.0 - 999.0					

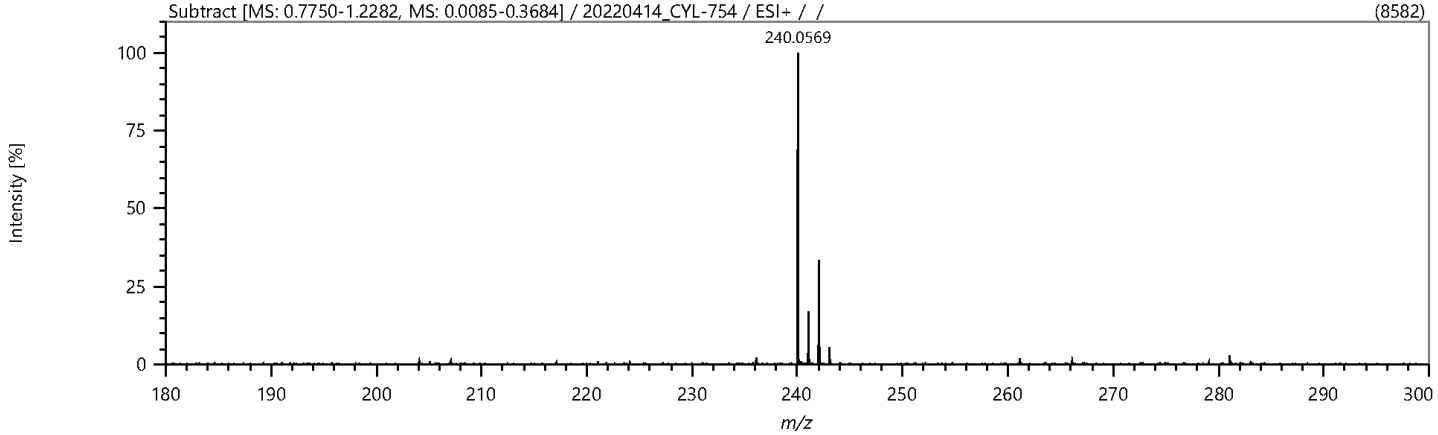
Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
224.08727	C15 H11 N F	224.08700	0.26	1.18	10.5

The high-resolution mass spectrum (ESI+) of compound 1t.



Spectrum



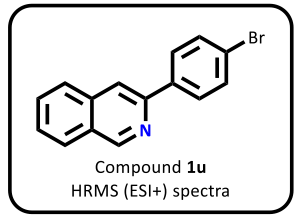
Elemental Composition

Parameters		Elements Set 1:				
Tolerance:	±10.00 ppm	Symbol	C	H	N	Cl
Electron:	Odd/Even	Min	0	0	1	1
Charge:	+1	Max	400	1000	2	1
DBE:	-99.0 - 999.0					

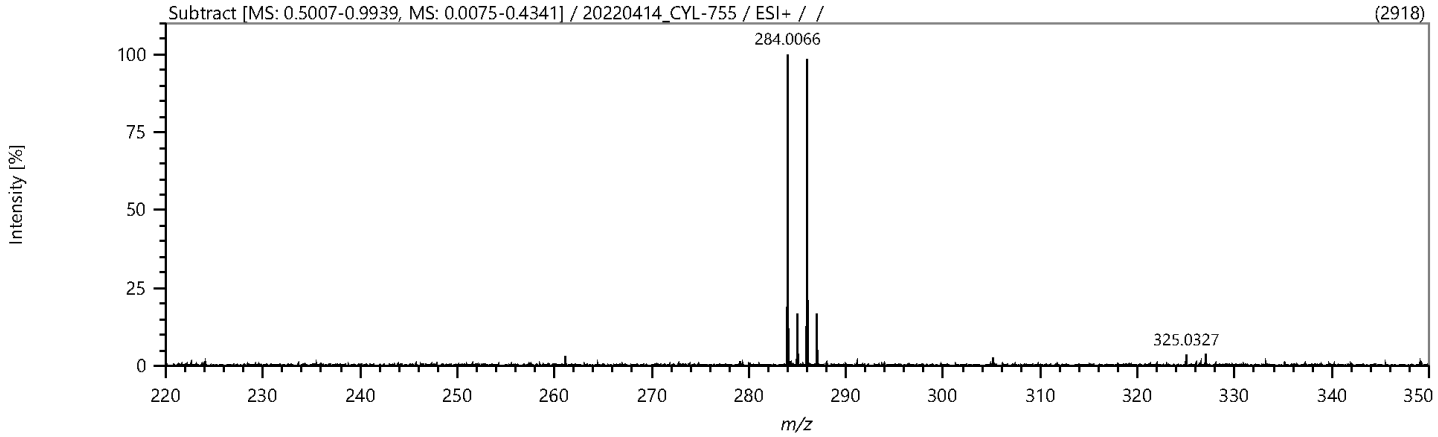
Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
240.05686	C15 H11 N Cl	240.05745	-0.59	-2.46	10.5

The high-resolution mass spectrum (ESI+) of compound 1u.



Spectrum



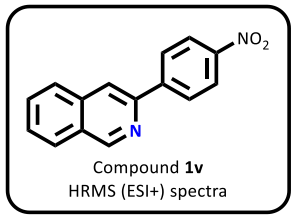
Elemental Composition

Parameters		Elements Set 1:				
Tolerance:	±10.00 ppm	Symbol	C	H	N	Br
Electron:	Odd/Even	Min	0	0	1	1
Charge:	+1	Max	400	1000	2	2
DBE:	-99.0 - 999.0					

Results

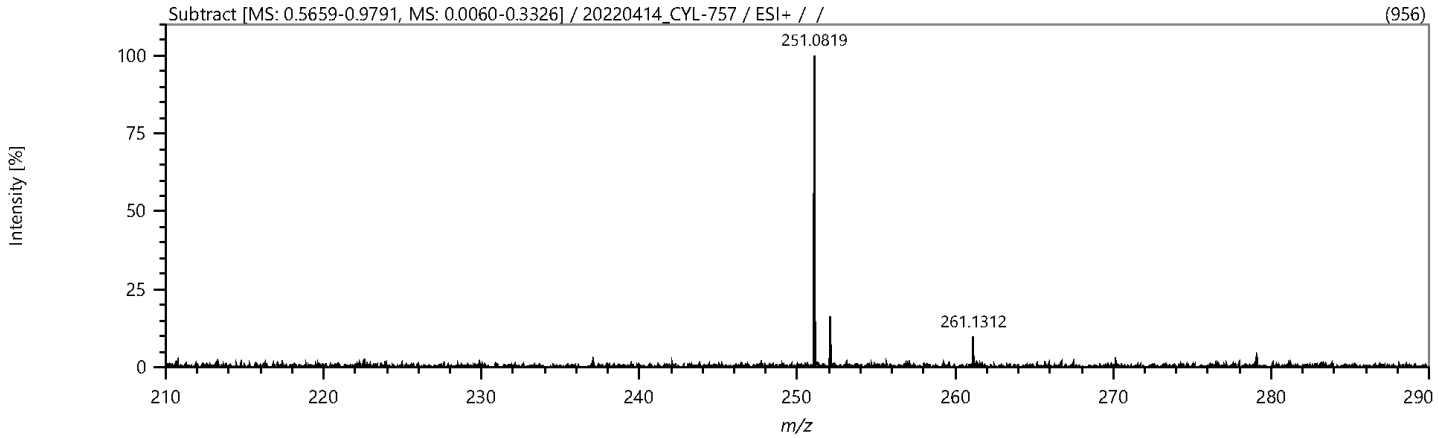
Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
284.00660	C15 H11 N Br	284.00694	-0.34	-1.19	10.5

The high-resolution mass spectrum (ESI+) of compound 1v.



Compound **1v**
HRMS (ESI+) spectra

Spectrum



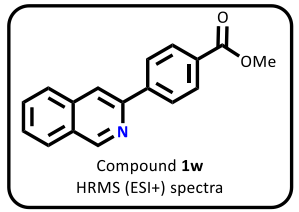
Elemental Composition

Parameters		Elements Set 1:				
Tolerance:	±10.00 ppm	Symbol	C	H	N	O
Electron:	Odd/Even	Min	0	0	1	1
Charge:	+1	Max	400	1000	2	2
DBE:	-99.0 - 999.0					

Results

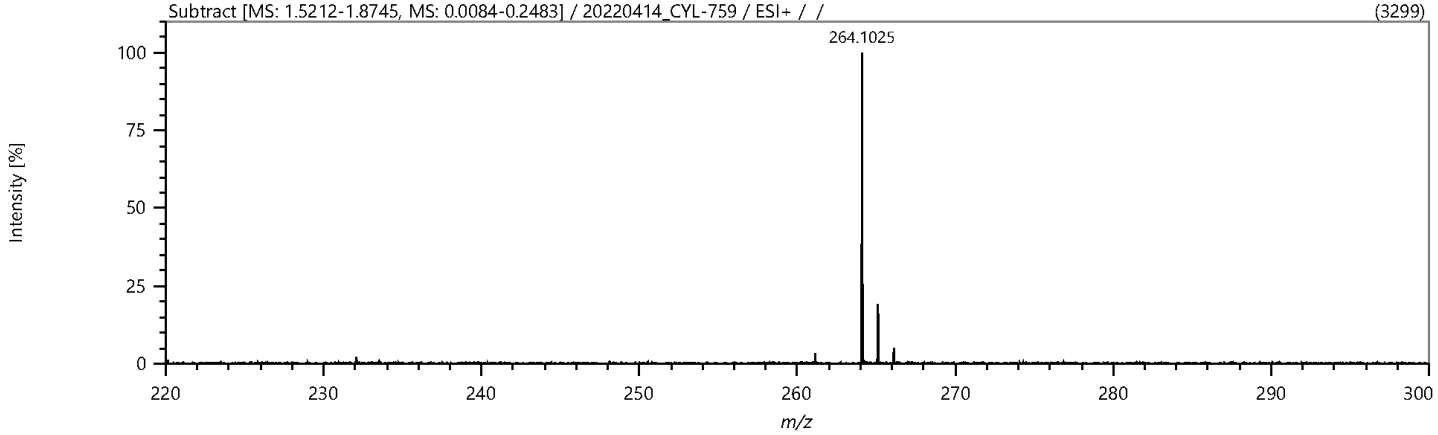
Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
251.08186	C15 H11 N2 O2	251.08150	0.35	1.40	11.5

The high-resolution mass spectrum (ESI+) of compound 1w.



Compound **1w**
HRMS (ESI+) spectra

Spectrum



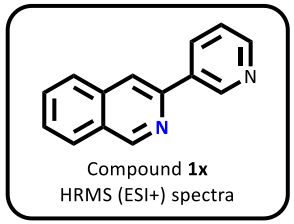
Elemental Composition

Parameters		Elements Set 1:				
Tolerance:	±10.00 ppm	Symbol	C	H	N	O
Electron:	Odd/Even	Min	0	0	1	2
Charge:	+1	Max	400	1000	2	2
DBE:	-99.0 - 999.0					

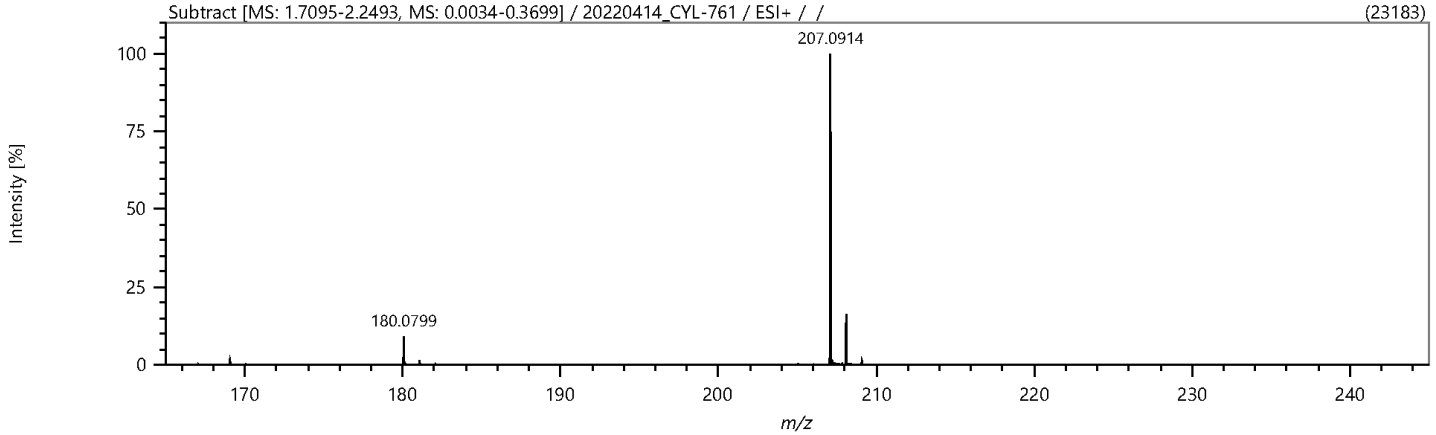
Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
264.10254	C17 H14 N O2	264.10191	0.64	2.42	11.5

The high-resolution mass spectrum (ESI+) of compound 1x.



Spectrum



Elemental Composition

Parameters		Elements Set 1:			
Tolerance:	±20.00 ppm	Symbol	C	H	N
Electron:	Odd/Even	Min	0	0	2
Charge:	+1	Max	400	1000	2
DBE:	-99.0 - 999.0				

Results

Mass	Formula	Calculated Mass	Mass Difference [mDa]	Mass Difference [ppm]	DBE
207.09140	C14 H11 N2	207.09167	-0.28	-1.33	10.5