Anexo:

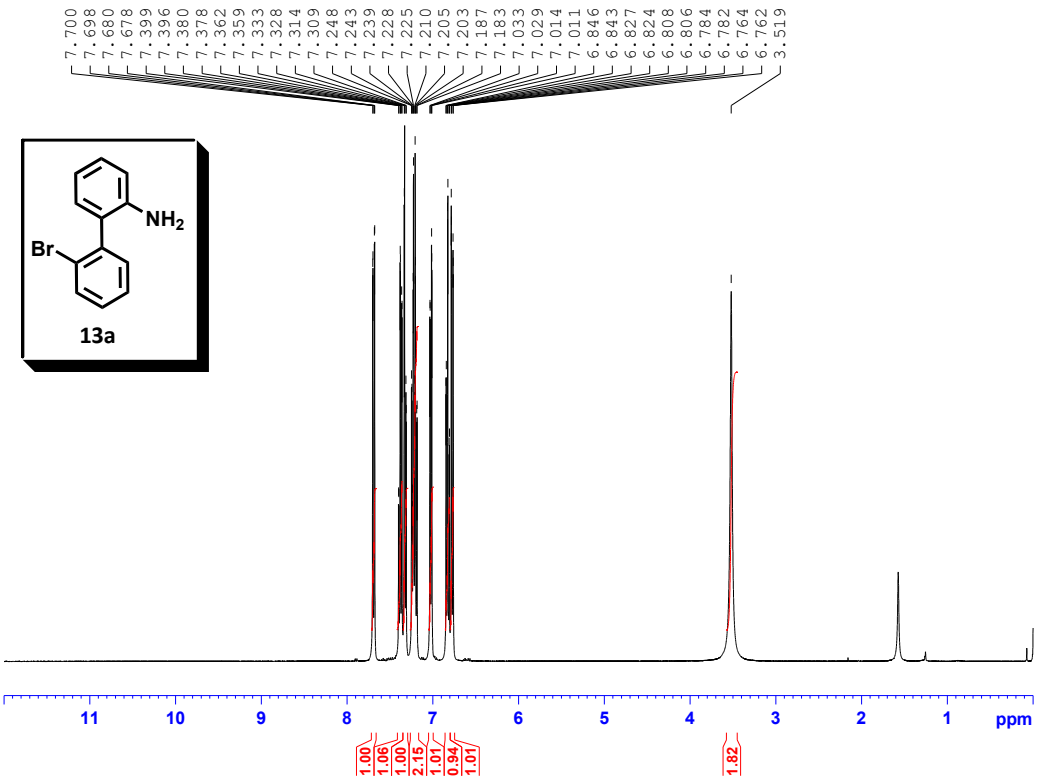
Material Complementario

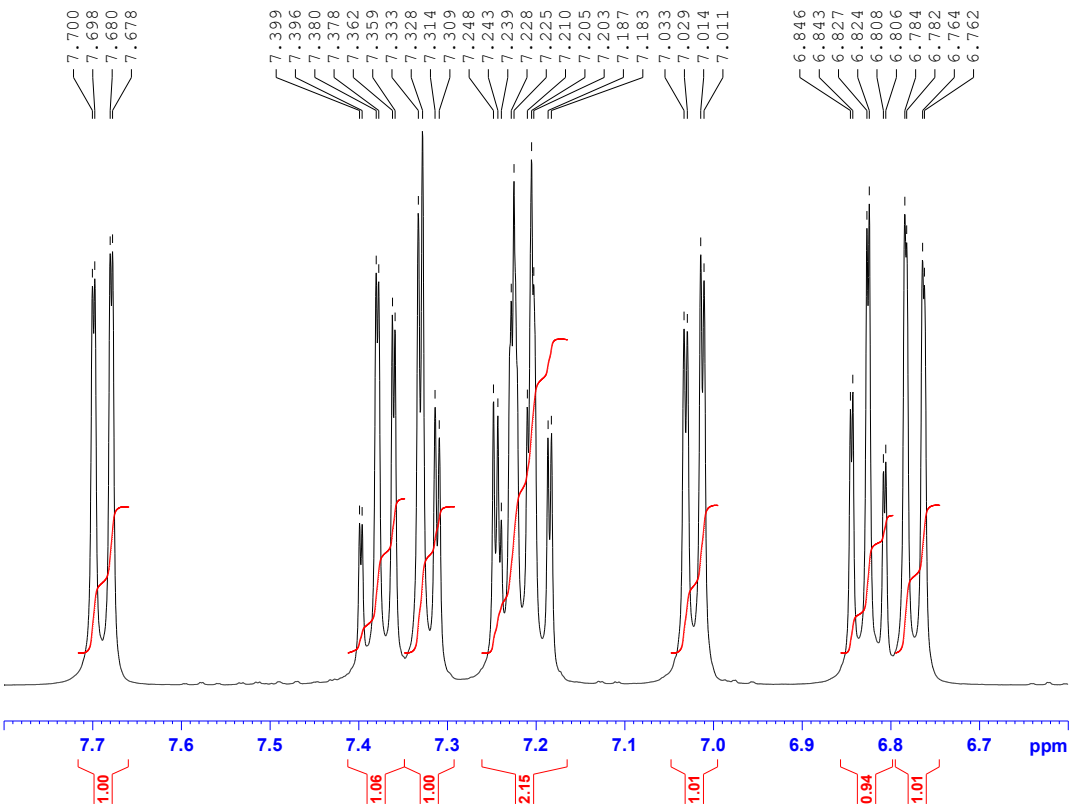
TABLA DE CONTENIDOS

A.1 CAPÍTULO II

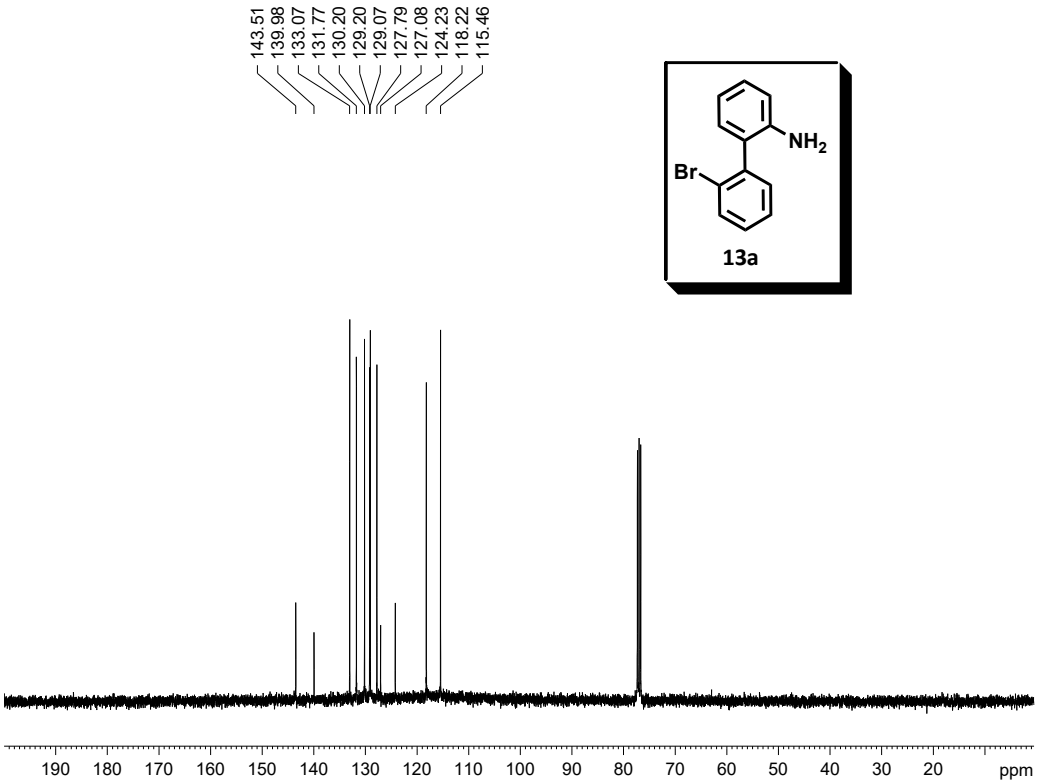
A.1.1 ESPECTROS DE RMN DE 2-HALO-BIFENIL-2-AMINAS

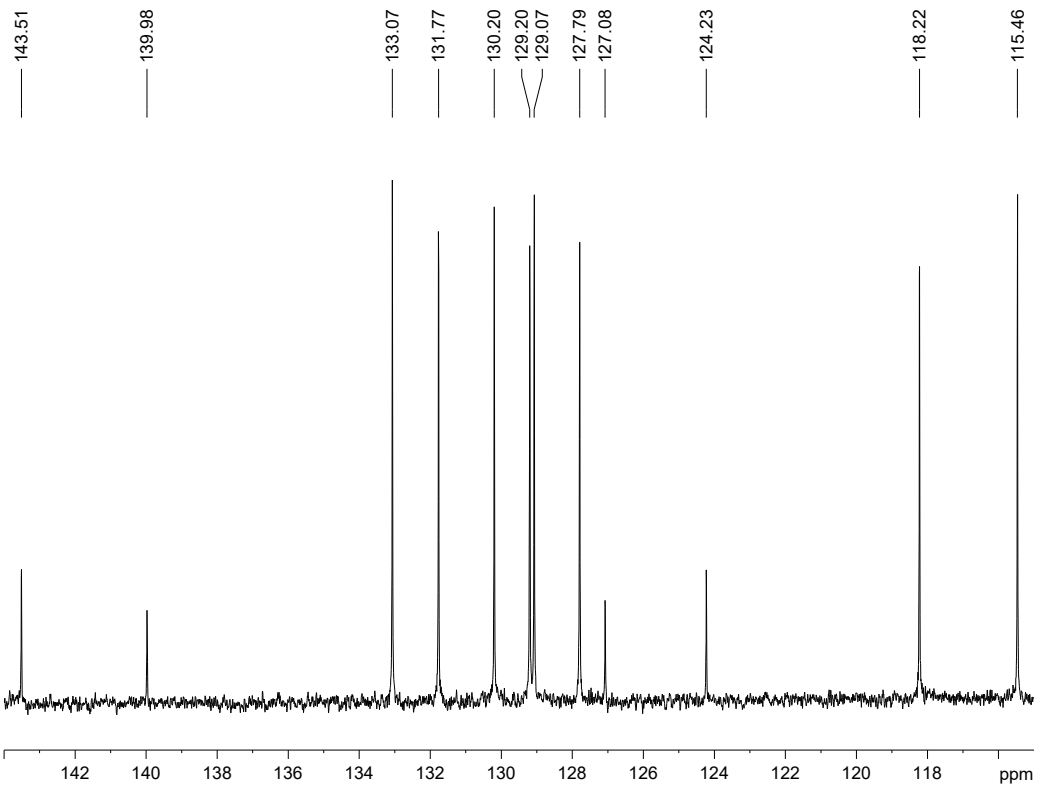
^{1}H-RMN ($CDCl_3$) 2'-Bromo-[1,1'-bifenil]-2-amina (13a)



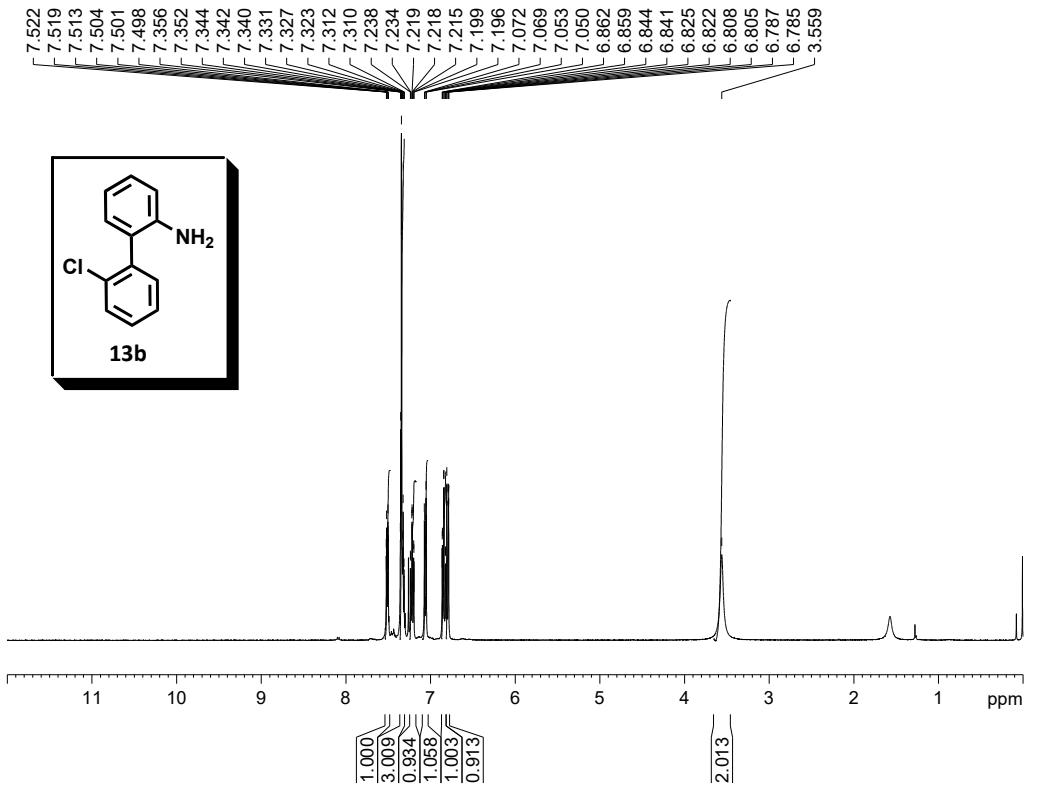


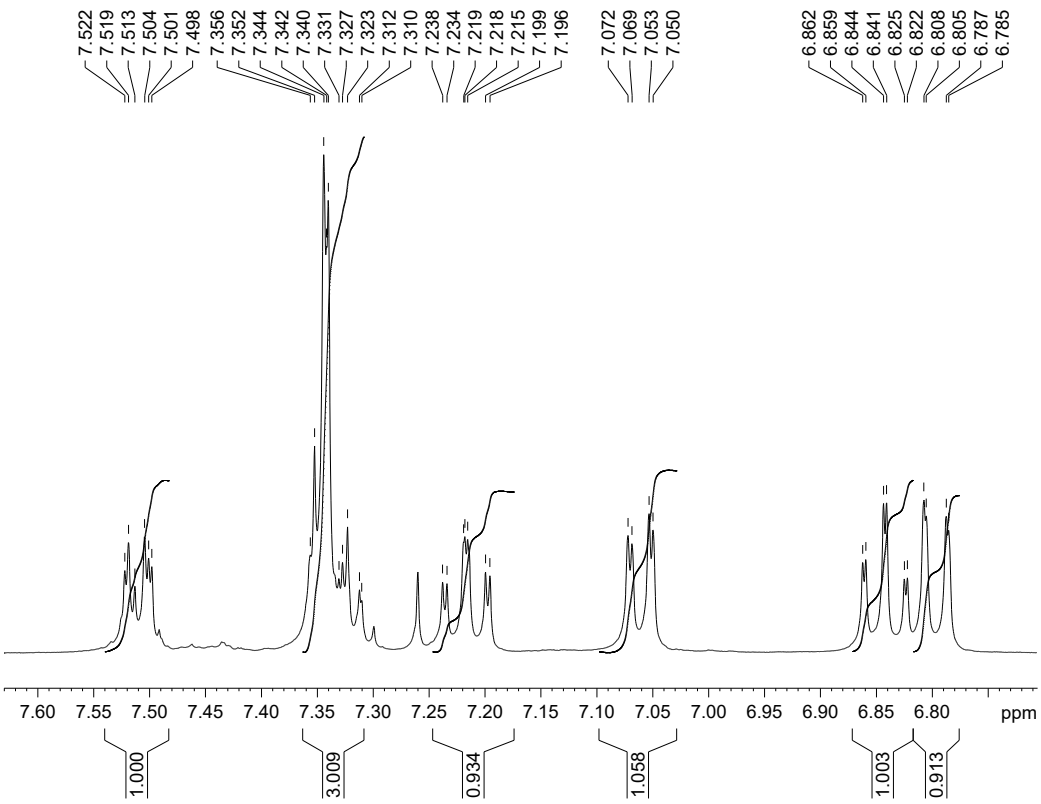
^{13}C-RMN ($CDCl_3$) 2'-Bromo-[1,1'-bifenil]-2-amina (13a)



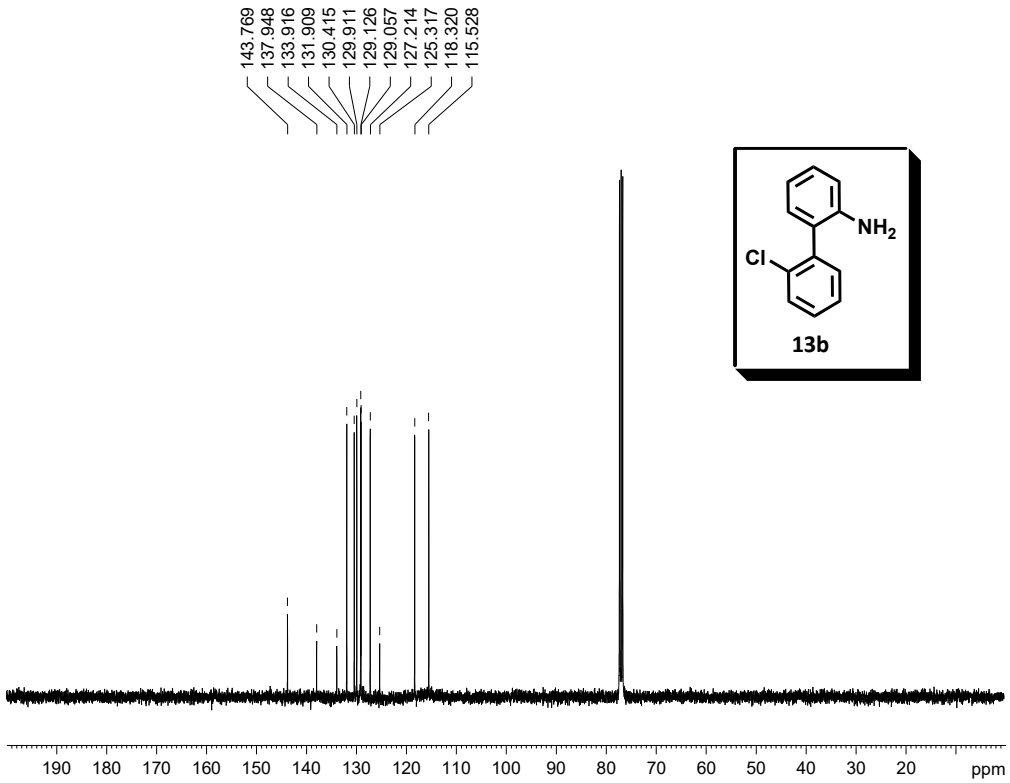


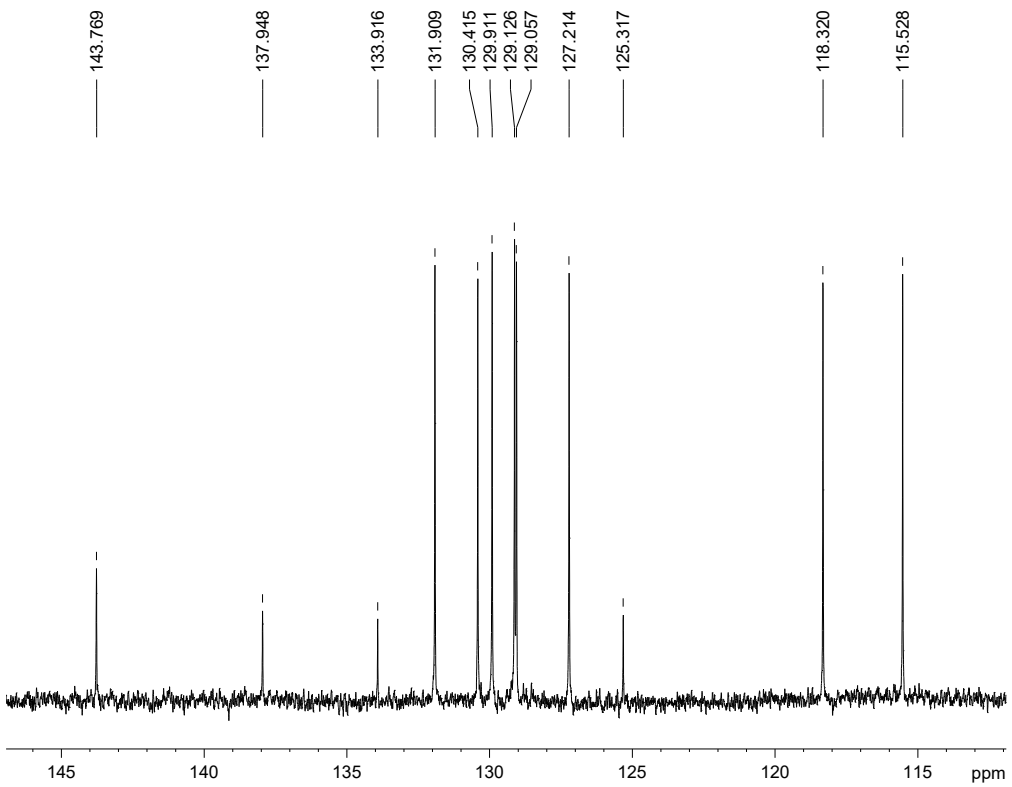
^{1}H-RMN ($CDCl_3$) 2'-Cloro-[1,1'-bifenil]-2-amina (13b)



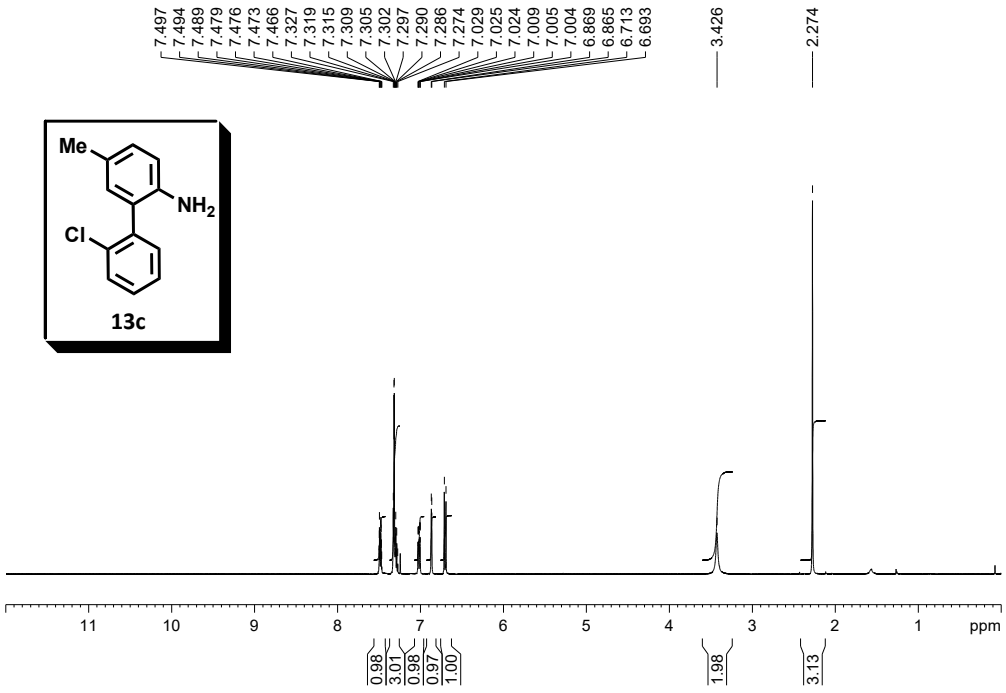


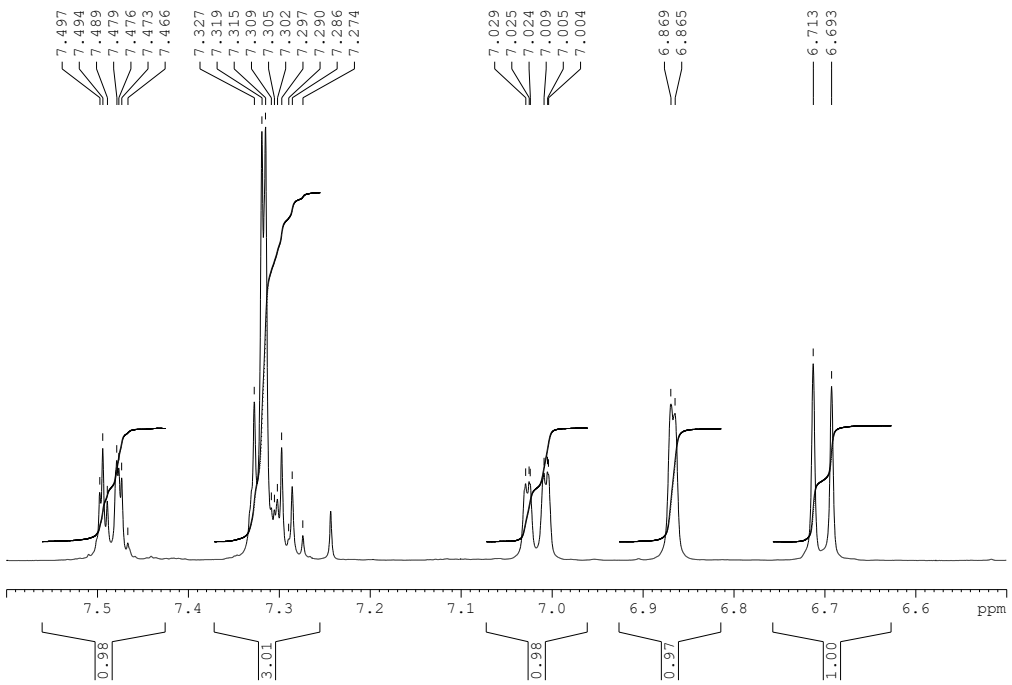
^{13}C-RMN ($CDCl_3$) 2'-Cloro-[1,1'-bifenil]-2-amina (13b)



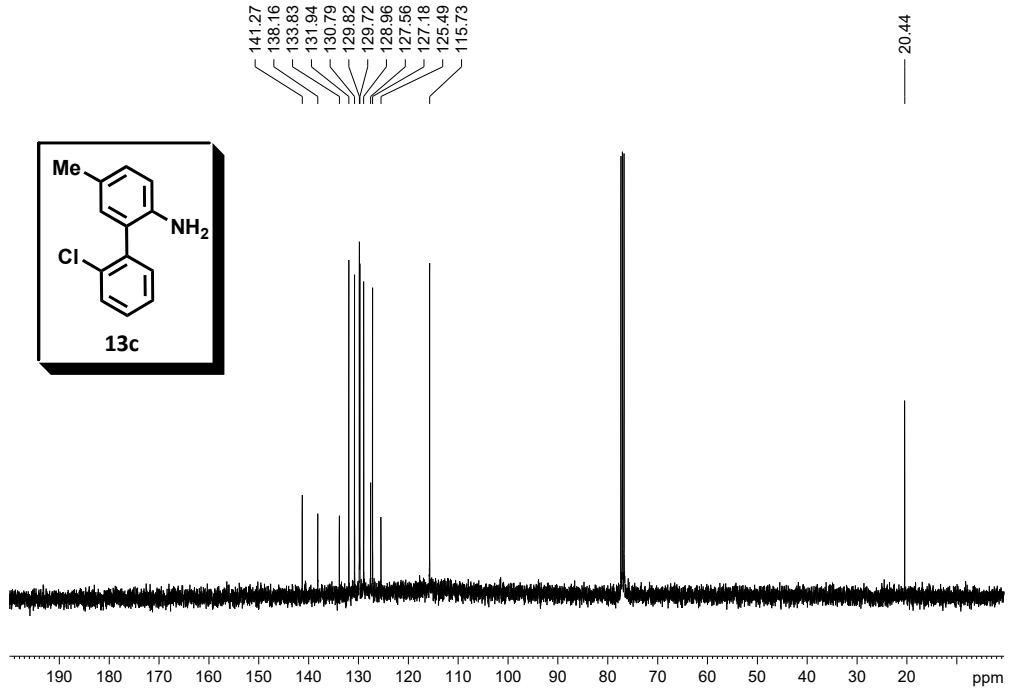


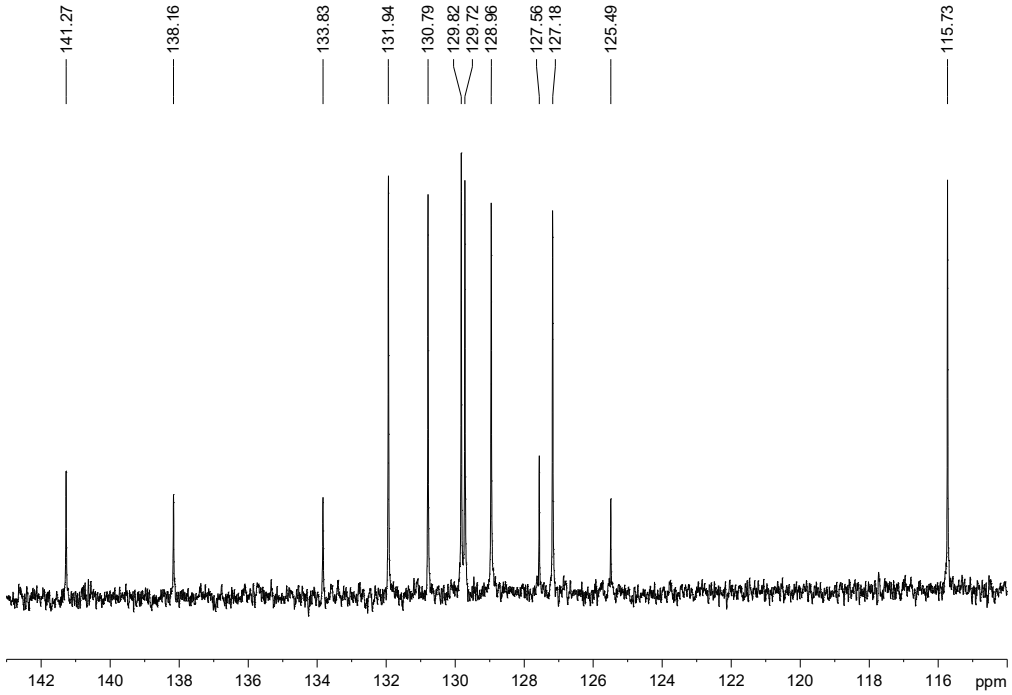
^{1}H-RMN ($CDCl_3$) 2'-Cloro-5-metil-[1,1'-bifenil]-2-amina (13c)



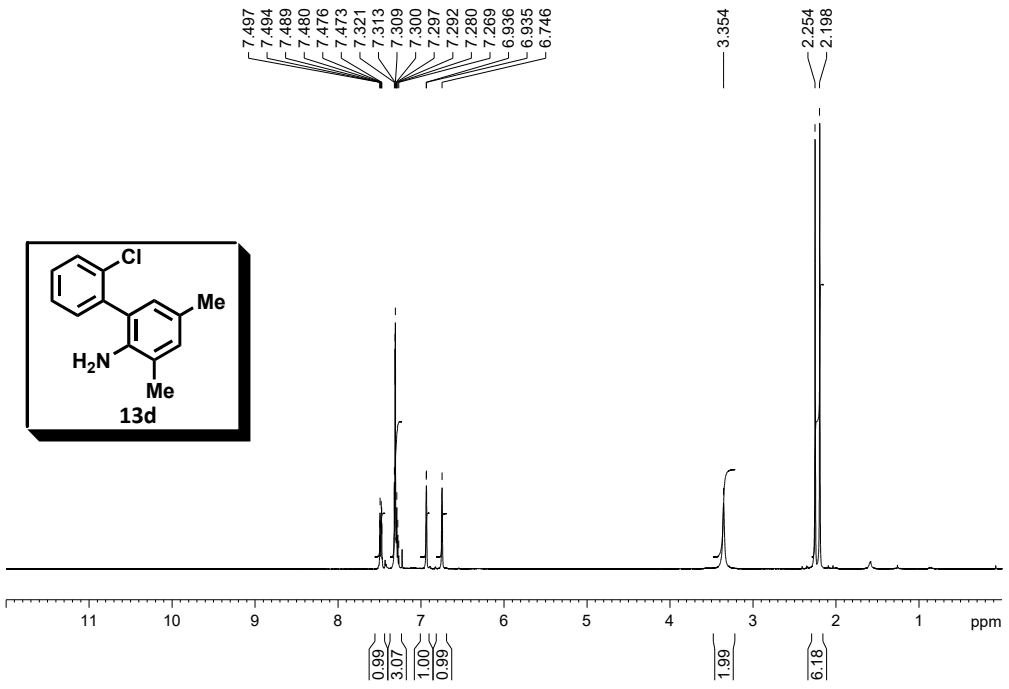


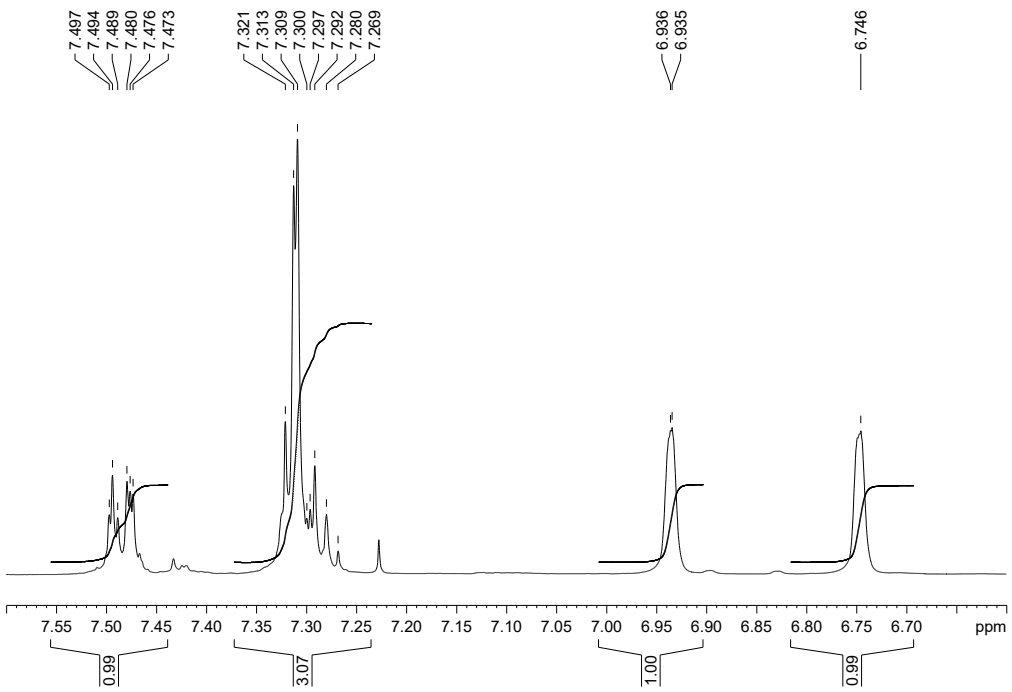
^{13}C-RMN ($CDCl_3$) 2'-Cloro-5-metil-[1,1'-bifenil]-2-amina (13c)



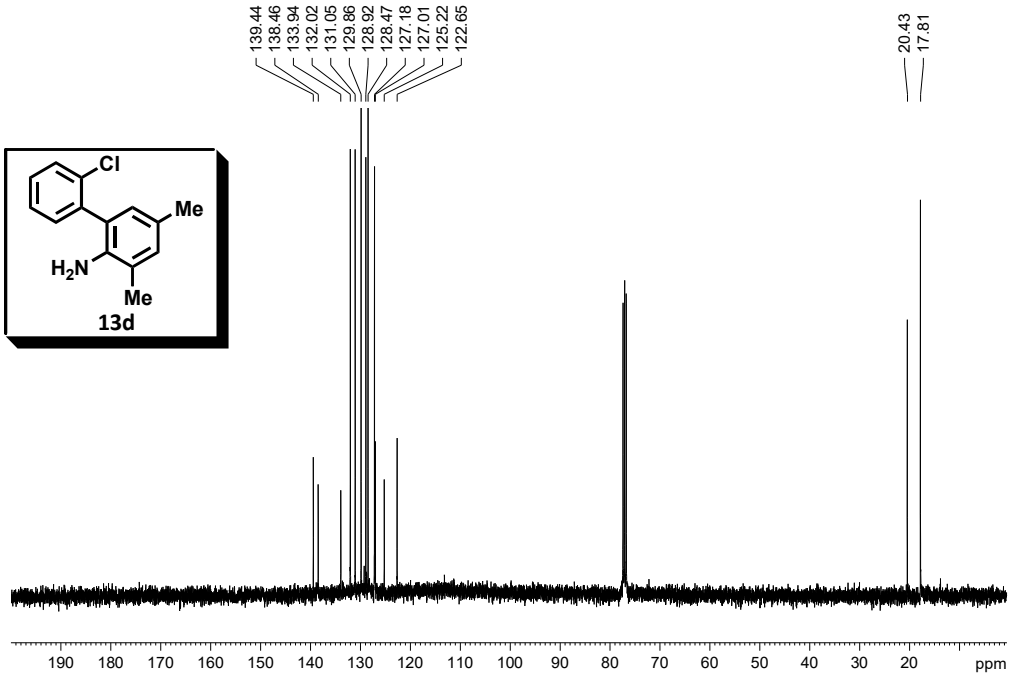


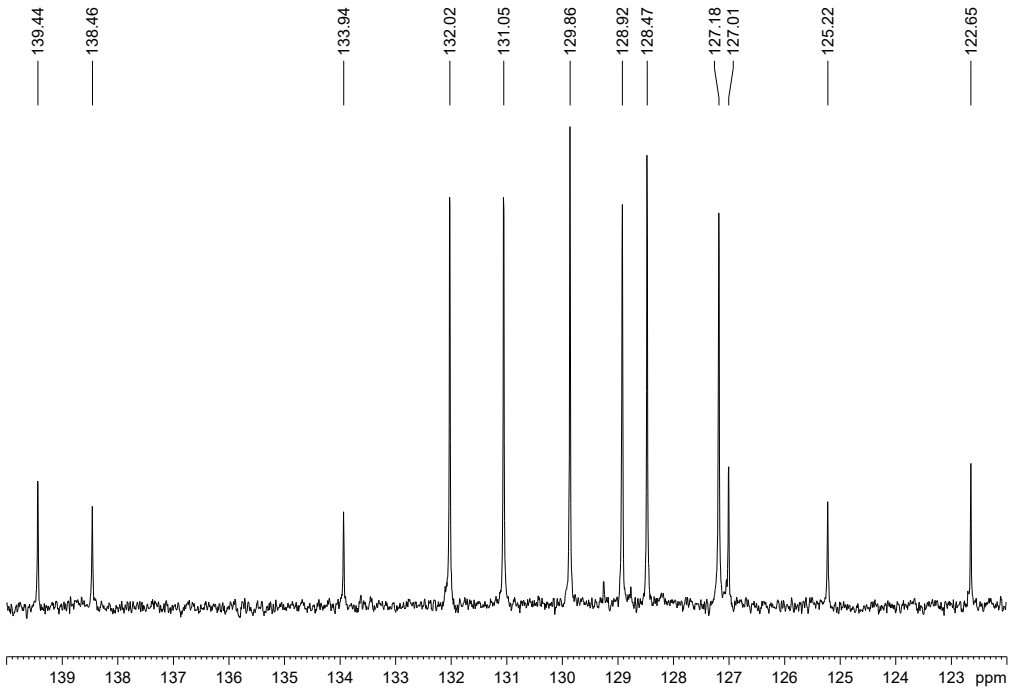
^{1}H-RMN ($CDCl_3$) 2'-Cloro-3,5-dimetil-[1,1'-bifenil]-2-amina (13d)



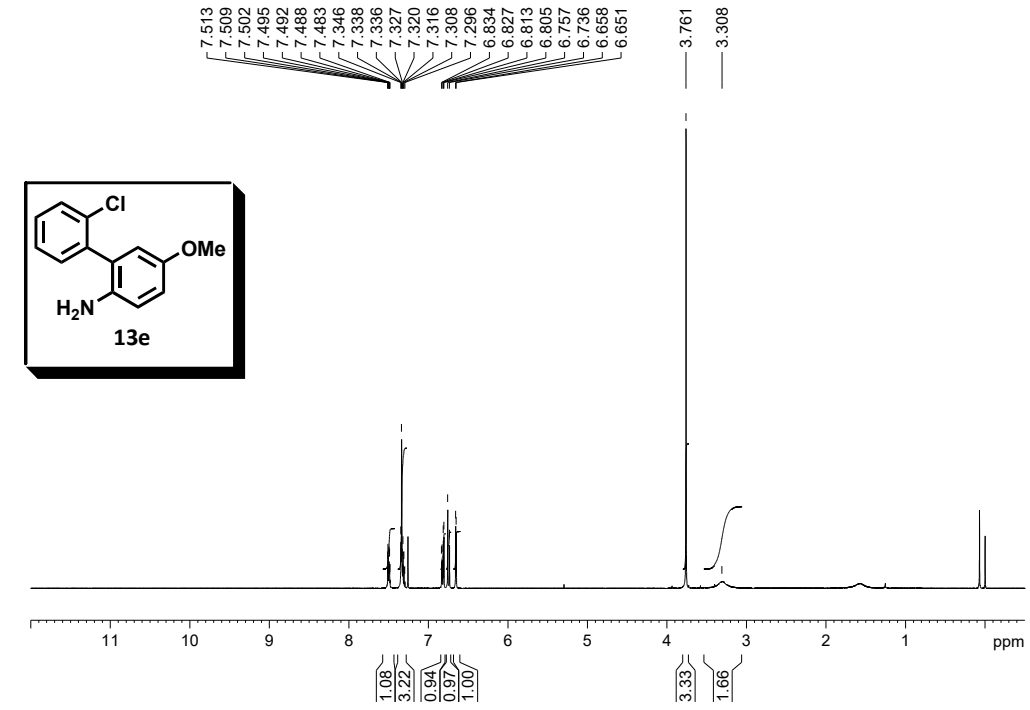


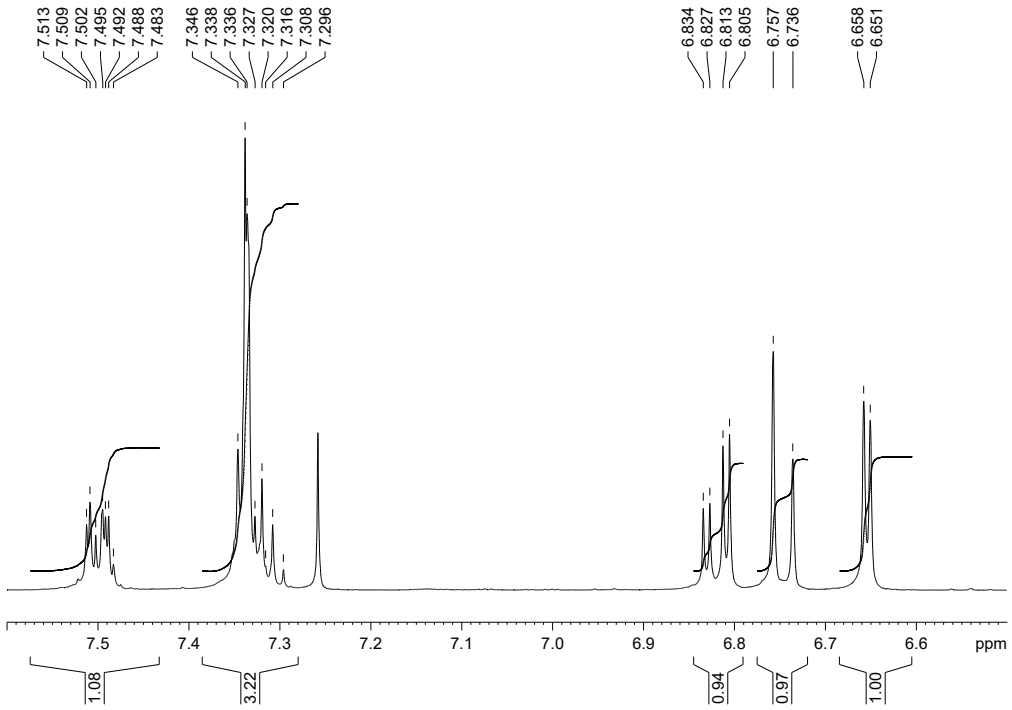
^{13}C-RMN ($CDCl_3$) 2'-Cloro-3,5-dimetil-[1,1'-bifenil]-2-amina (13d)



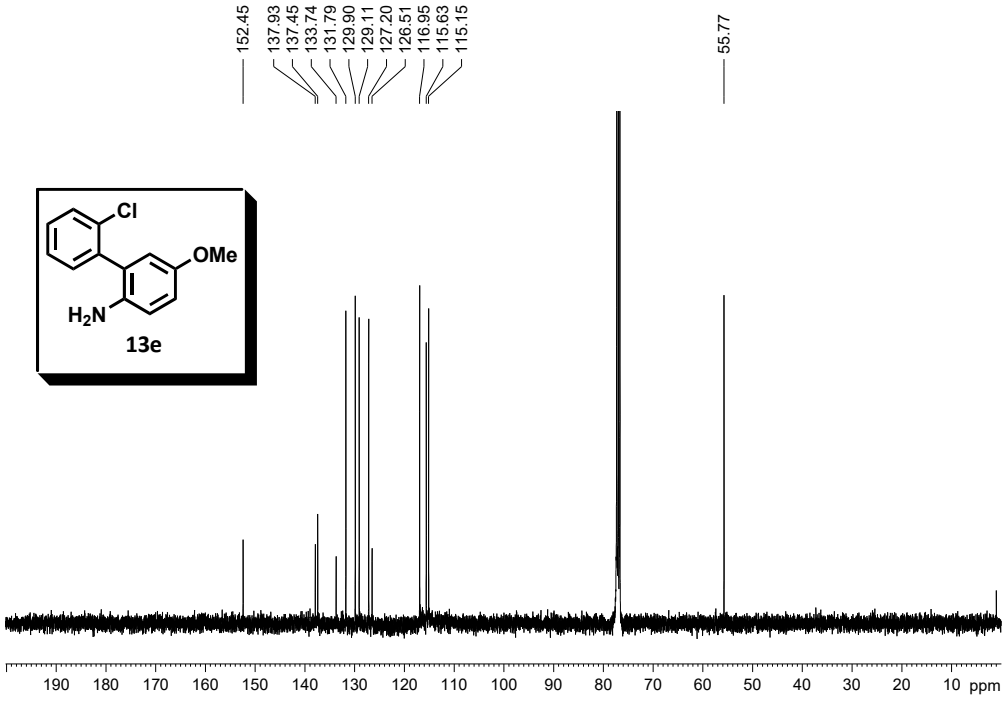


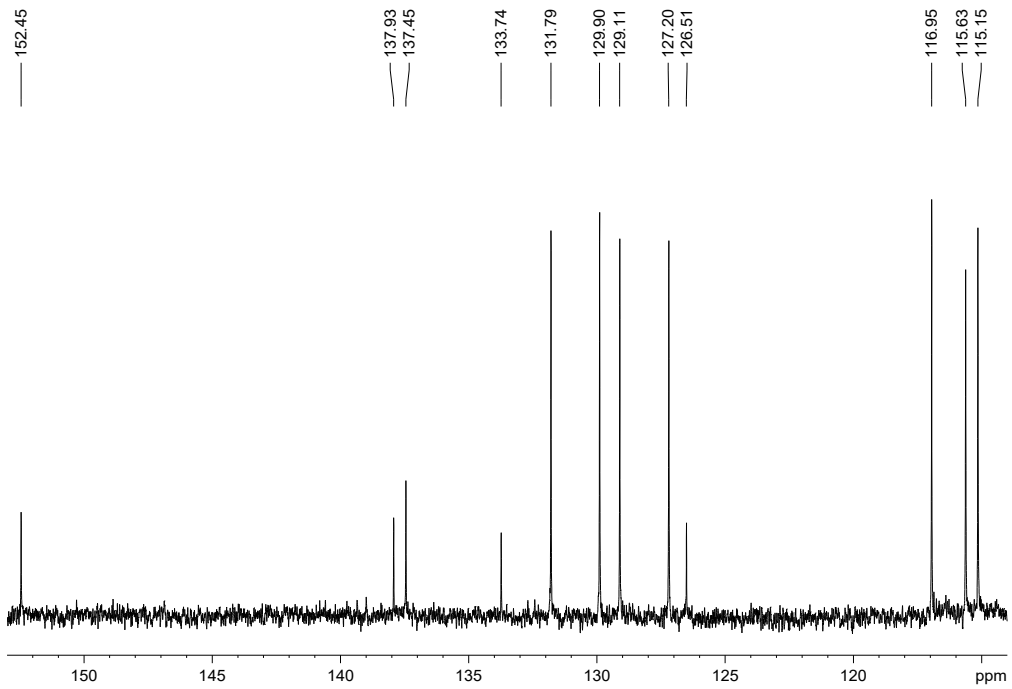
^{1}H-RMN ($CDCl_3$) 2'-Cloro-5-metoxi-[1,1'-bifenil]-2-amina (13e)



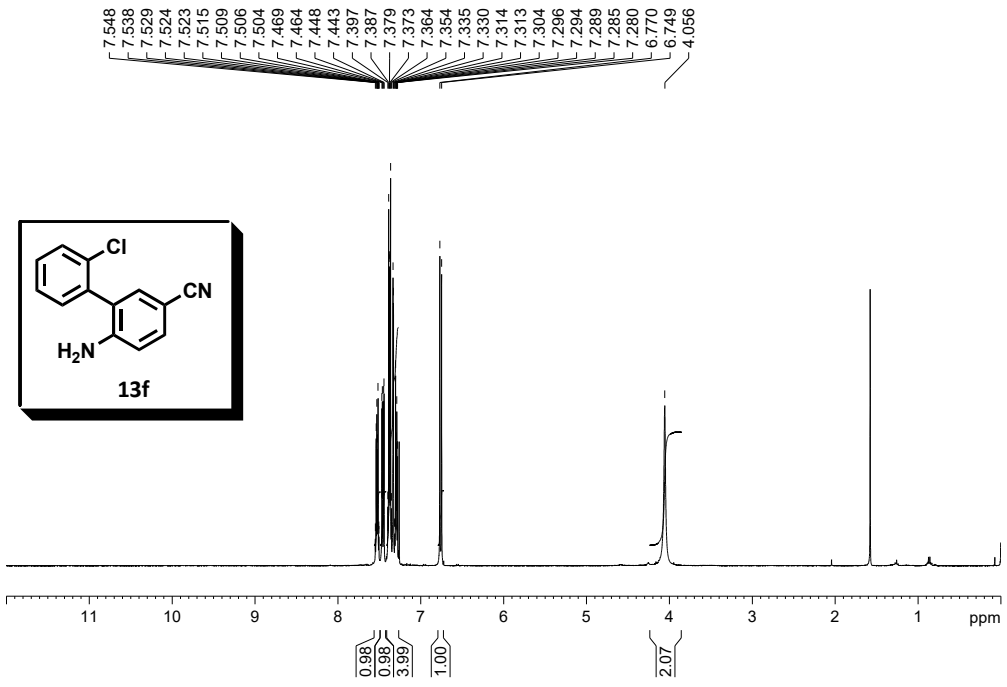


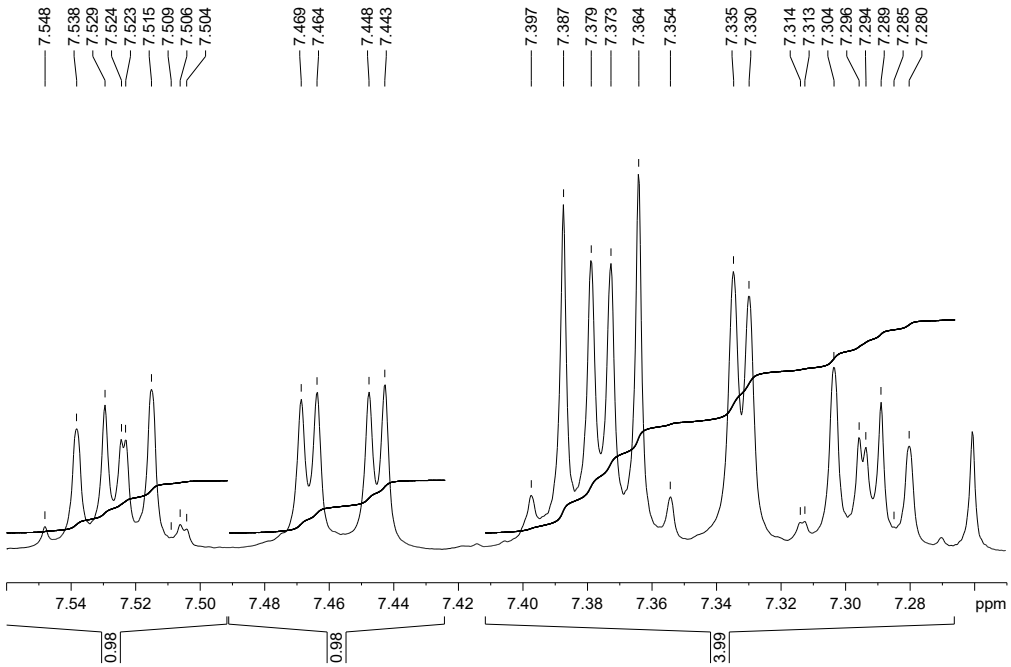
^{13}C-RMN ($CDCl_3$) 2'-Cloro-5-metoxi-[1,1'-bifenil]-2-amina (13e)



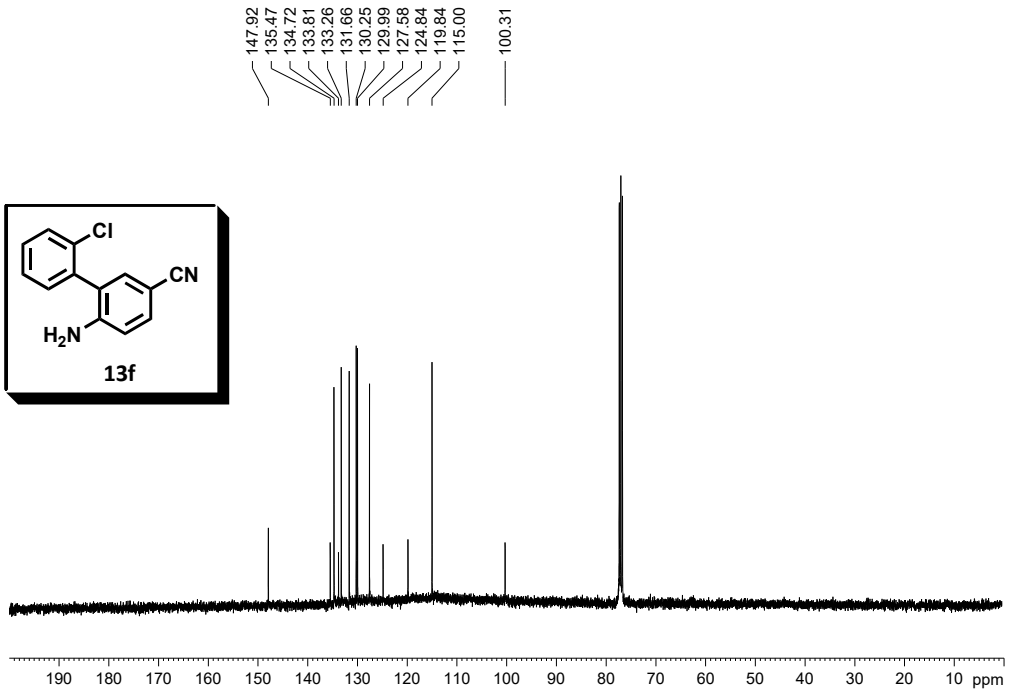


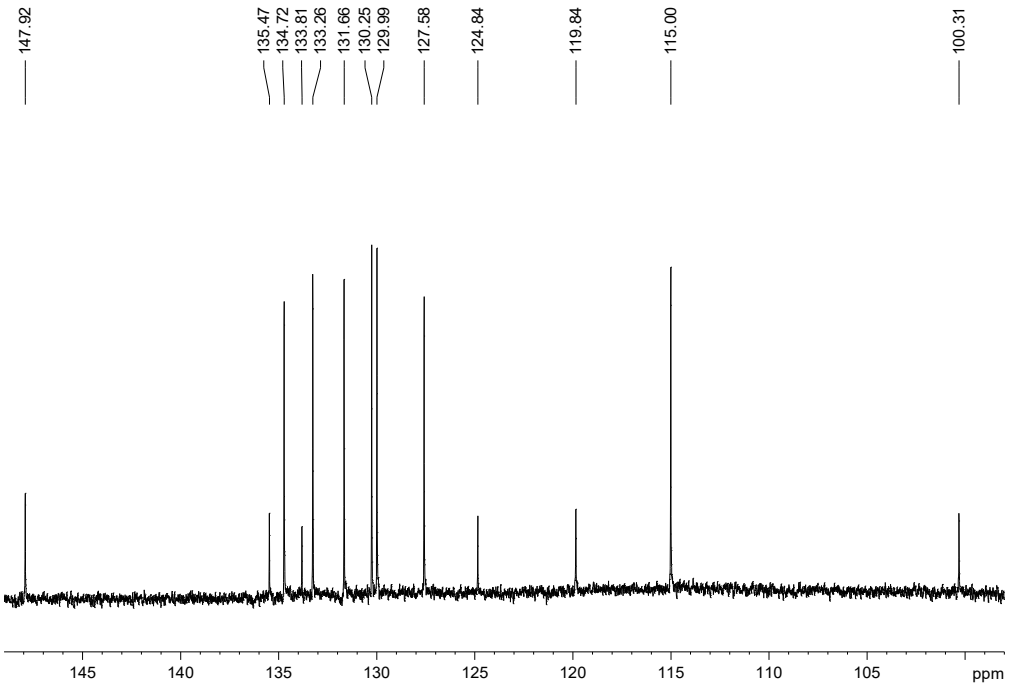
^{1}H-RMN ($CDCl_3$) 2'-Cloro-5-carbonitrilo-[1,1'-bifenil]-2-amina (13f)



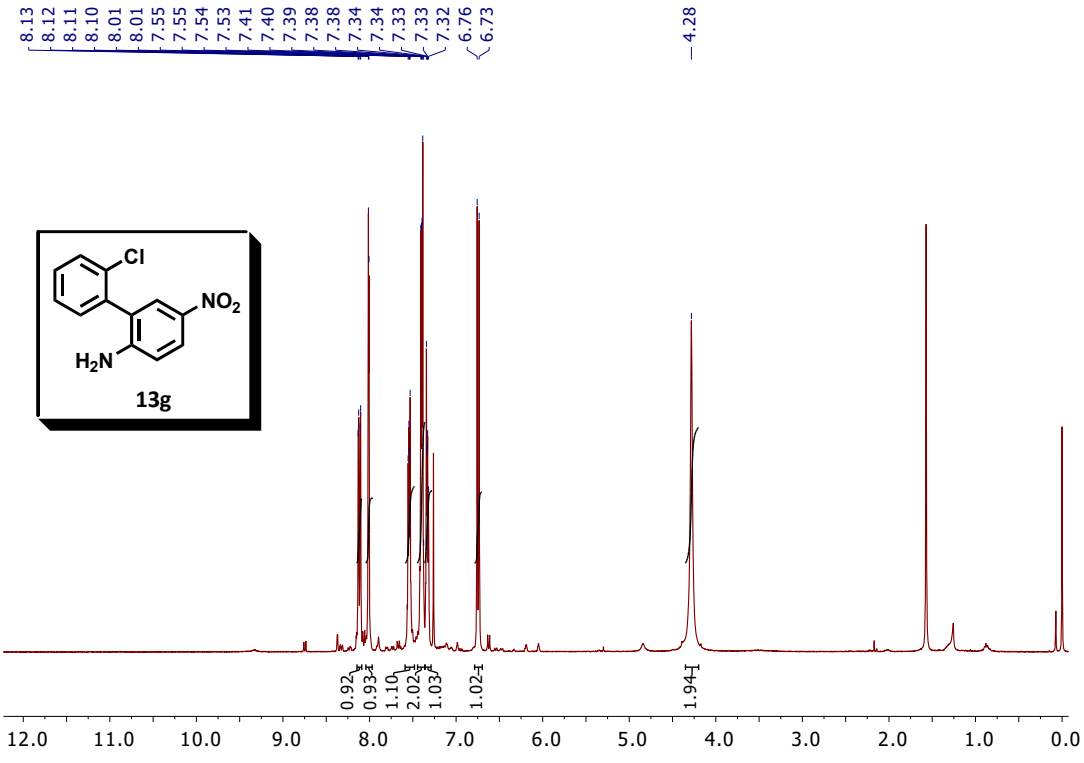


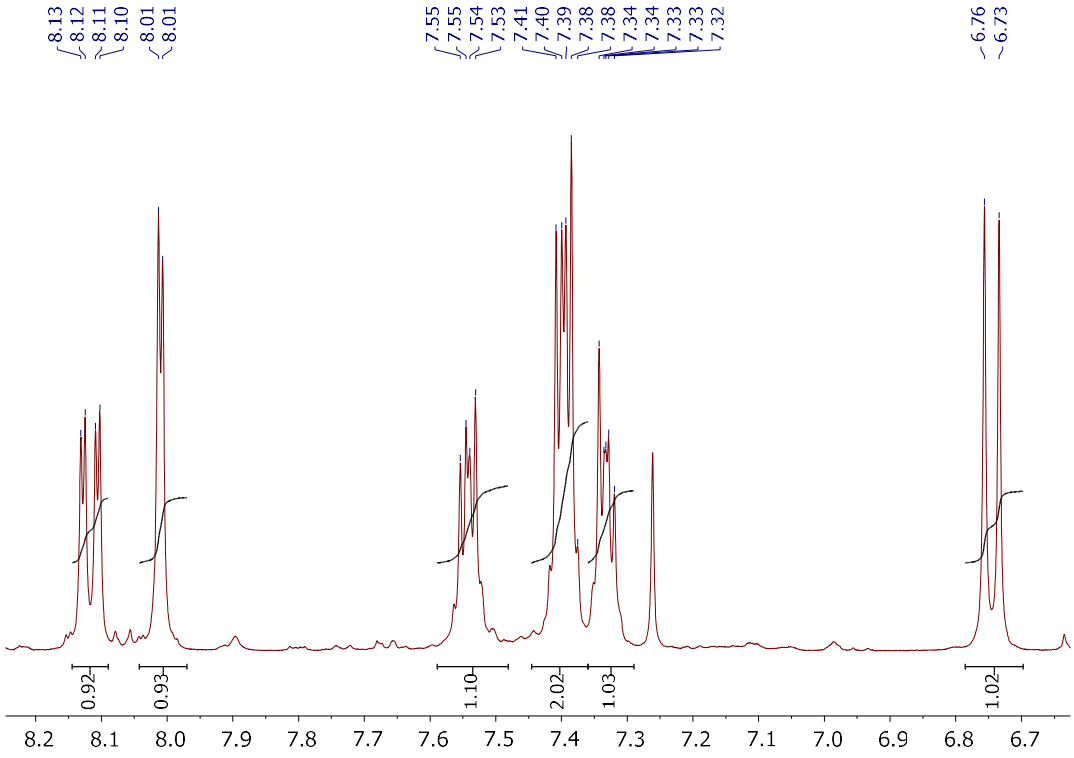
^{13}C-RMN ($CDCl_3$) 2'-Cloro-5-carbonitrilo-[1,1'-bifenil]-2-amina (13f)



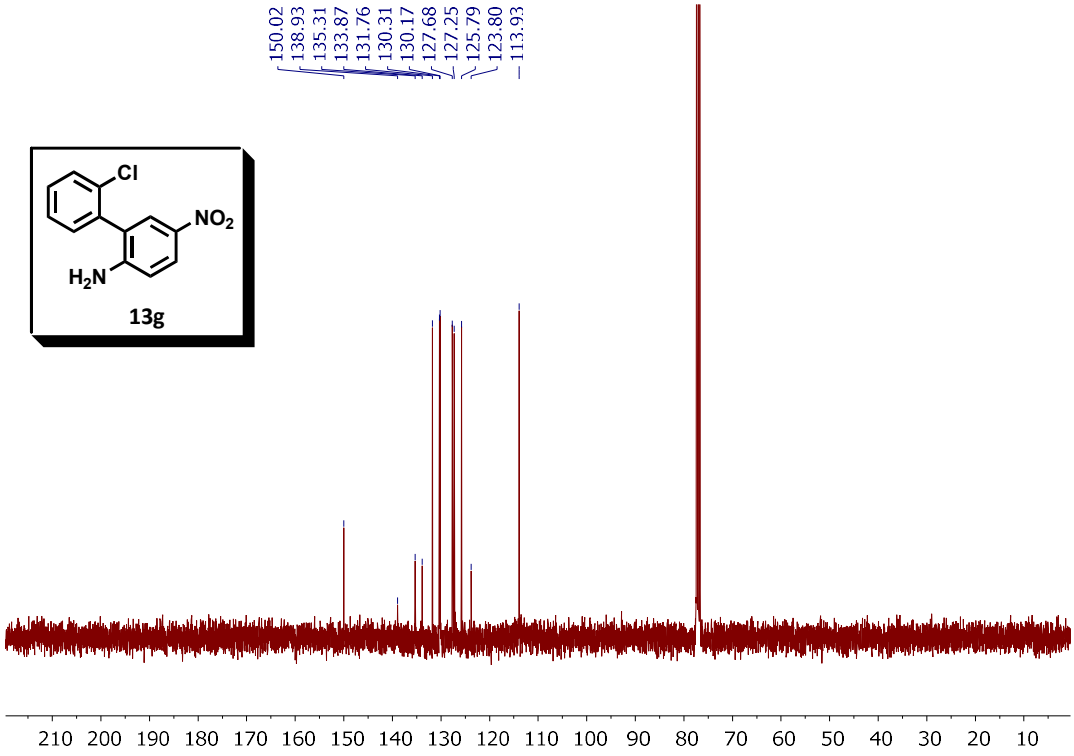


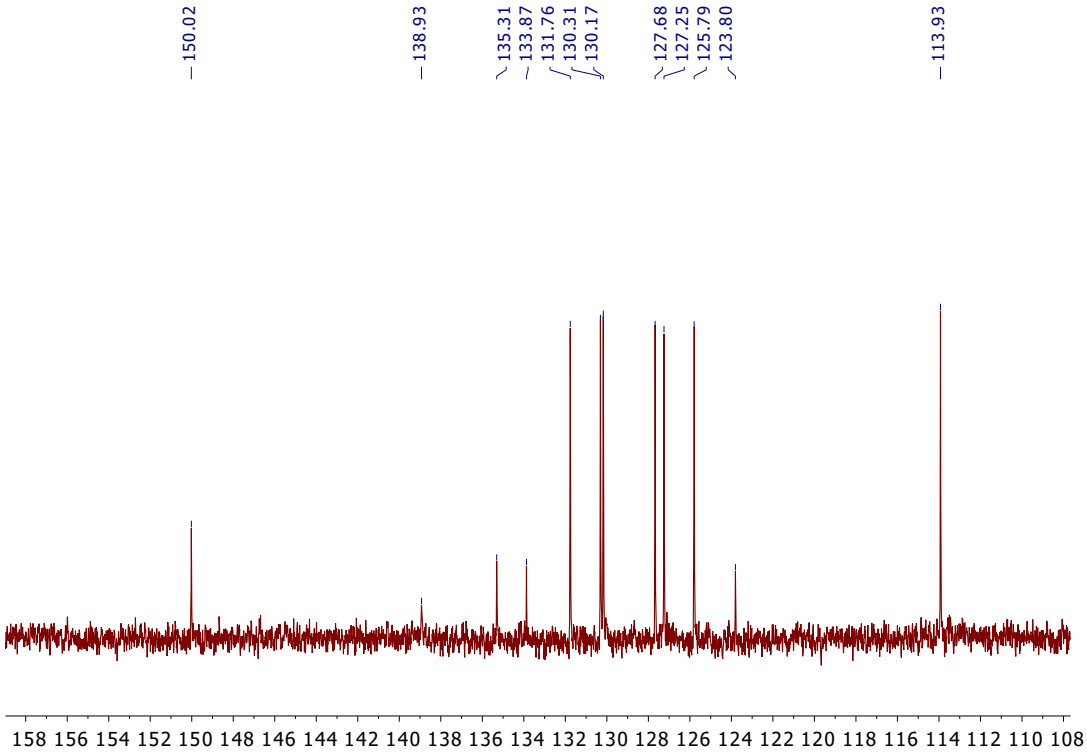
^{1}H-RMN ($CDCl_3$) 2'-Cloro-5-nitro-[1,1'-bifenil]-2-amina (13g)



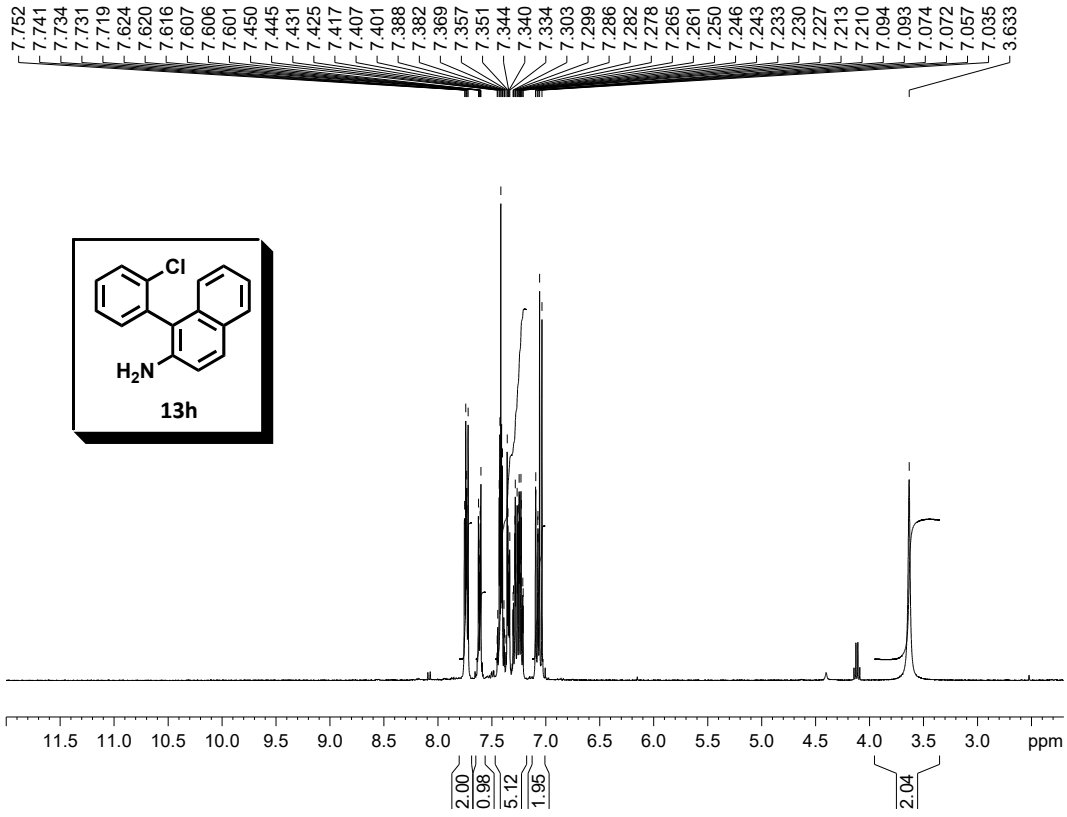


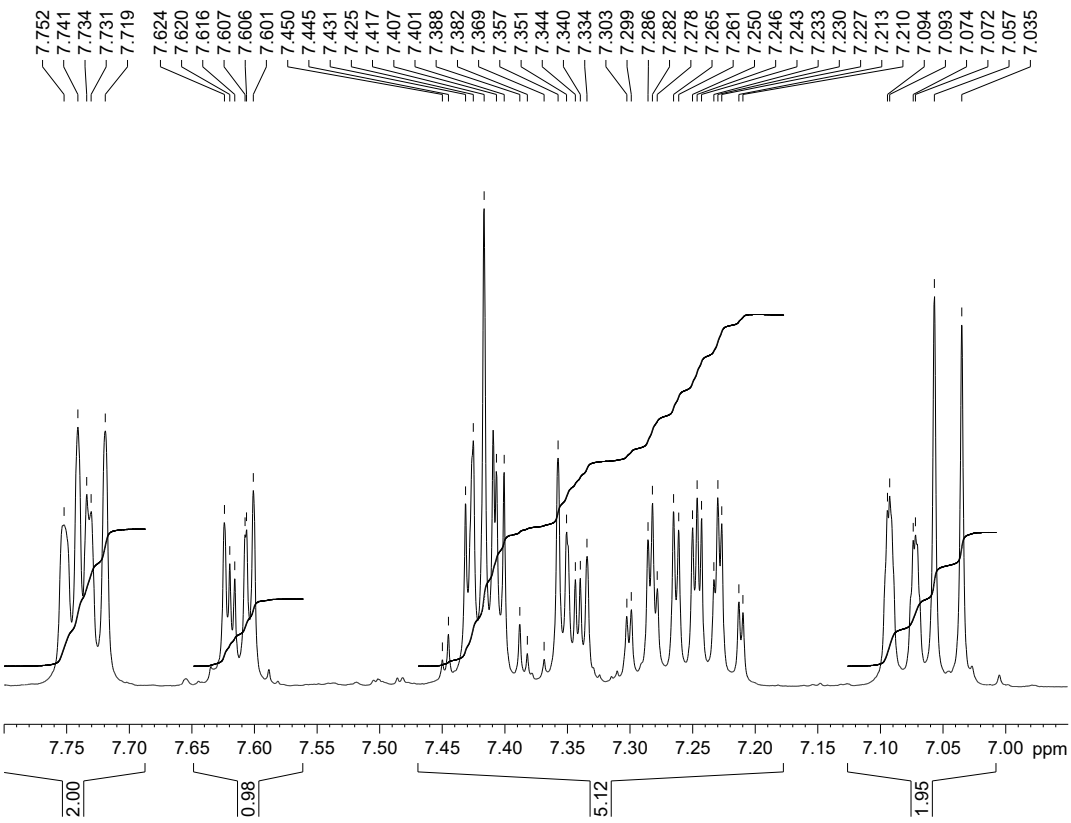
^{13}C-RMN ($CDCl_3$) 2'-Cloro-5-nitro-[1,1'-bifenil]-2-amina (13g)



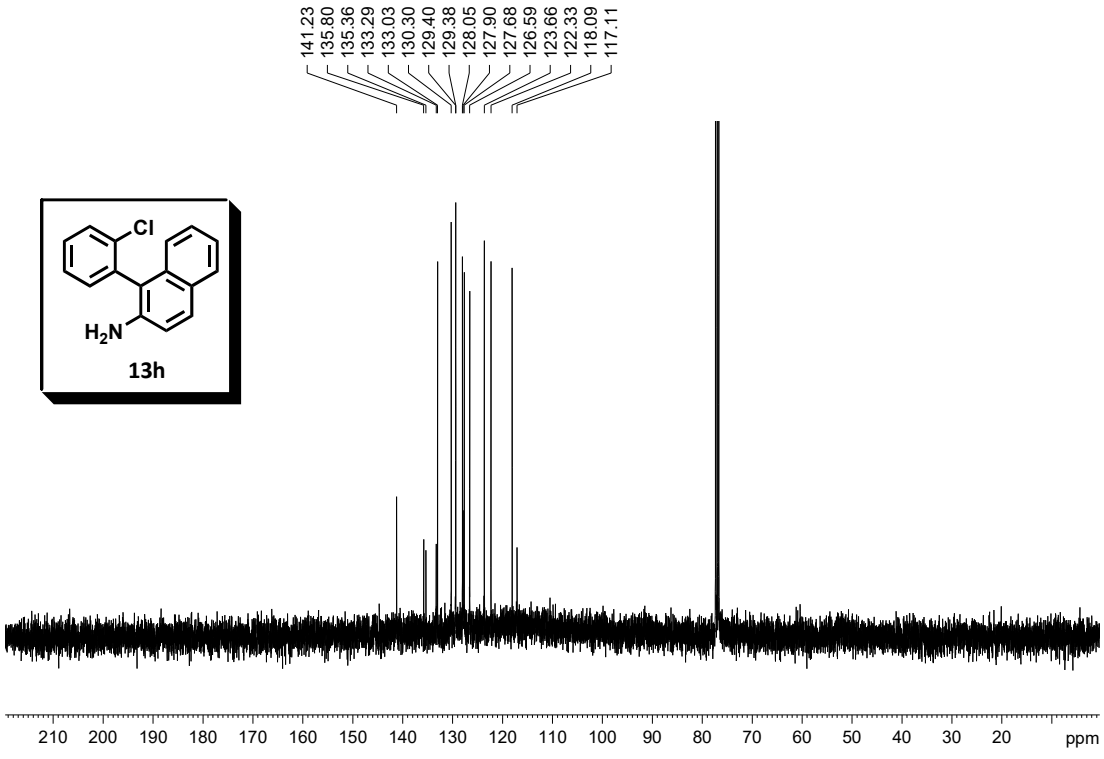


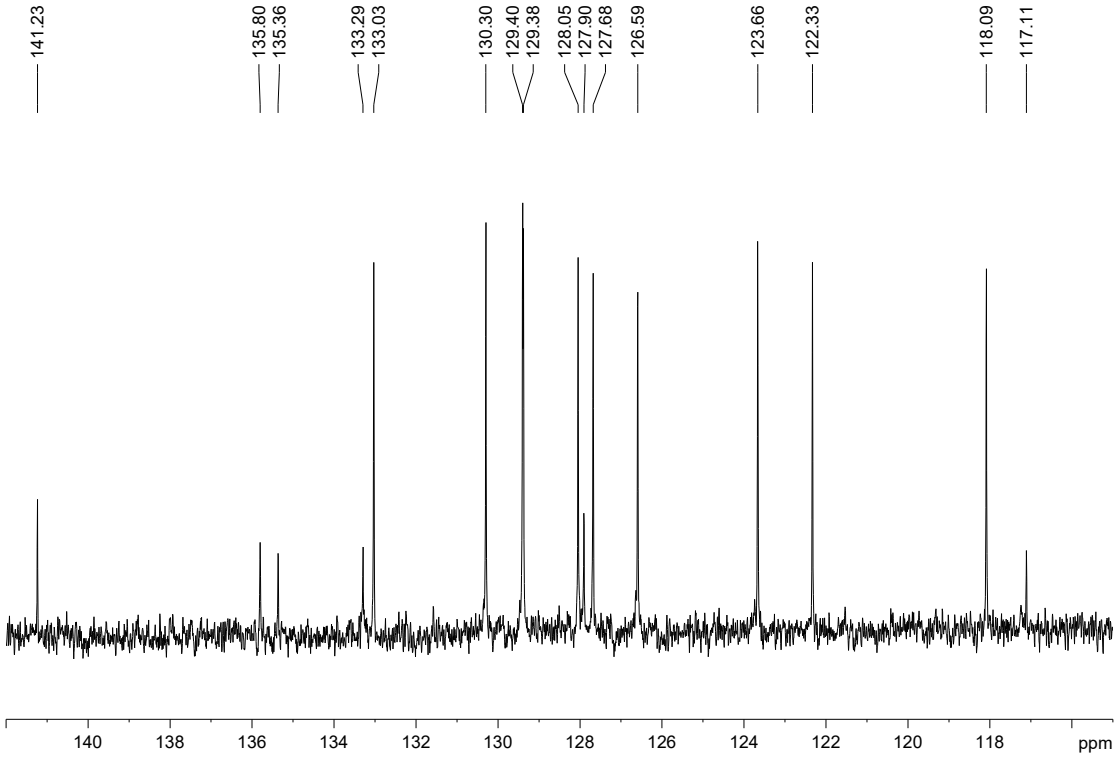
^{1}H-RMN ($CDCl_3$) 1-(2-Clorofenil)naftil-2-amina (13h)



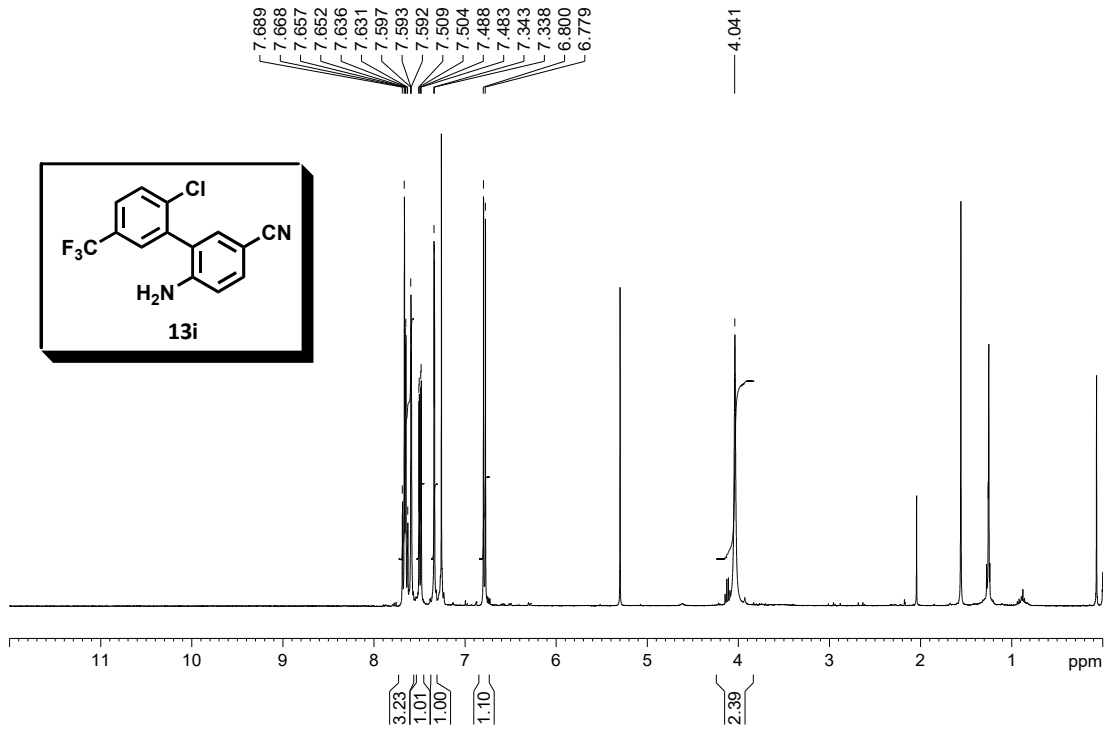


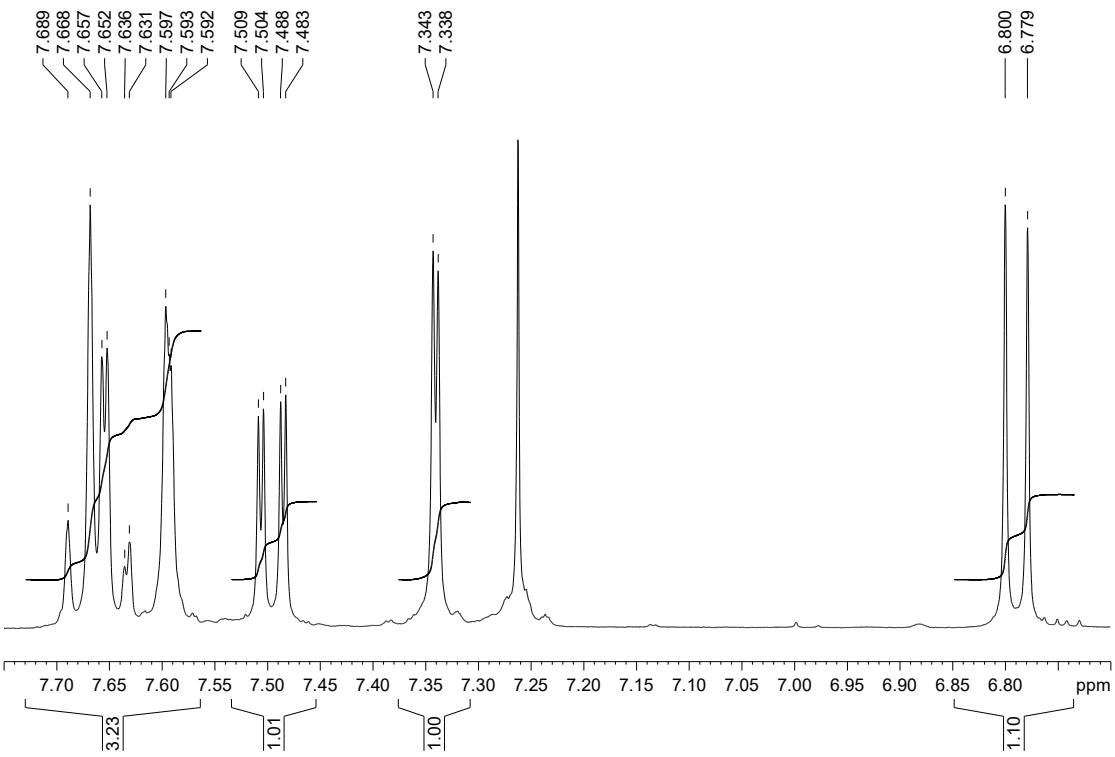
^{13}C-RMN ($CDCl_3$) 1-(2-Clorofenil)naftil-2-amina (13h)



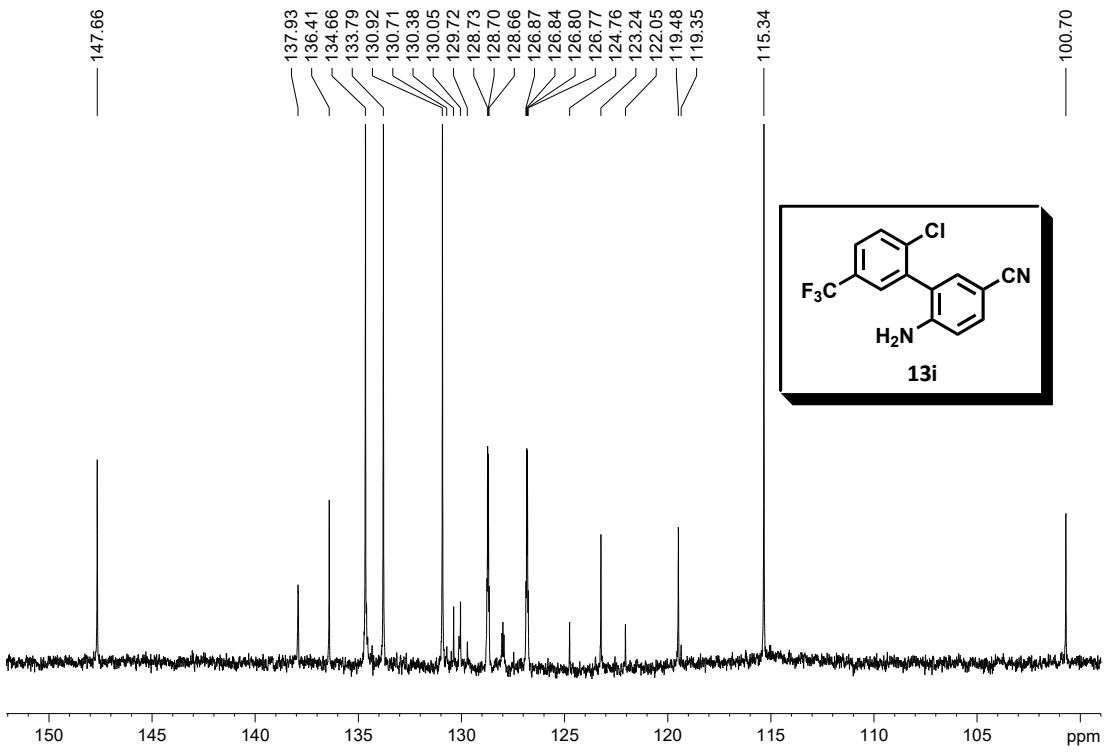


^{1}H-RMN ($CDCl_3$) 2'-Cloro-5´-trifluormetil-5-carbonitrilo-[1,1'-bifenil]-2-amina (13i)

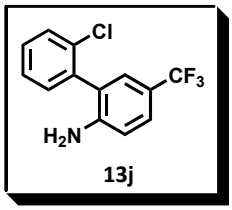




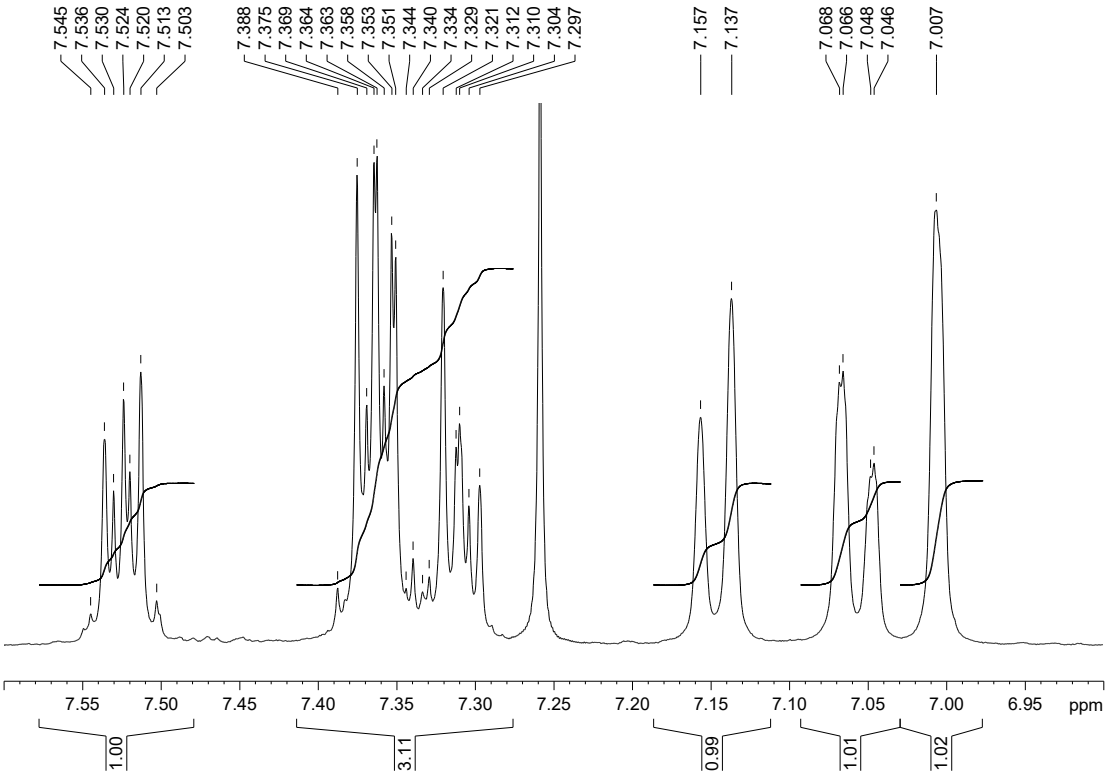
^{13}C-RMN ($CDCl_3$) 2'-Cloro-5´-trifluormetil-5-carbonitrilo-[1,1'-bifenil]-2-amina (13i)



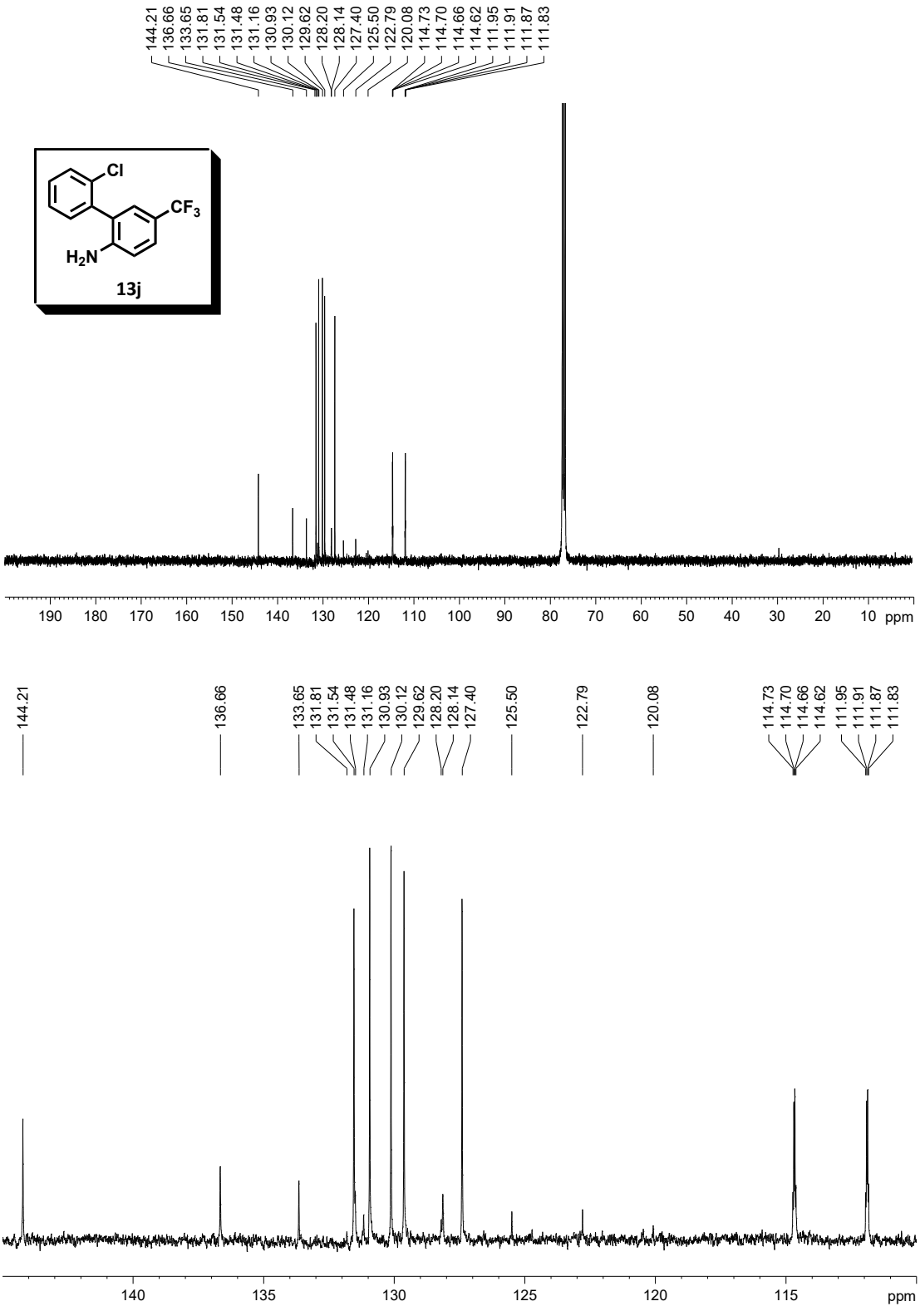
^{1}H-RMN ($CDCl_3$) 2'-Cloro-5-trifluormetil-[1,1'-bifenil]-2-amina (13j)

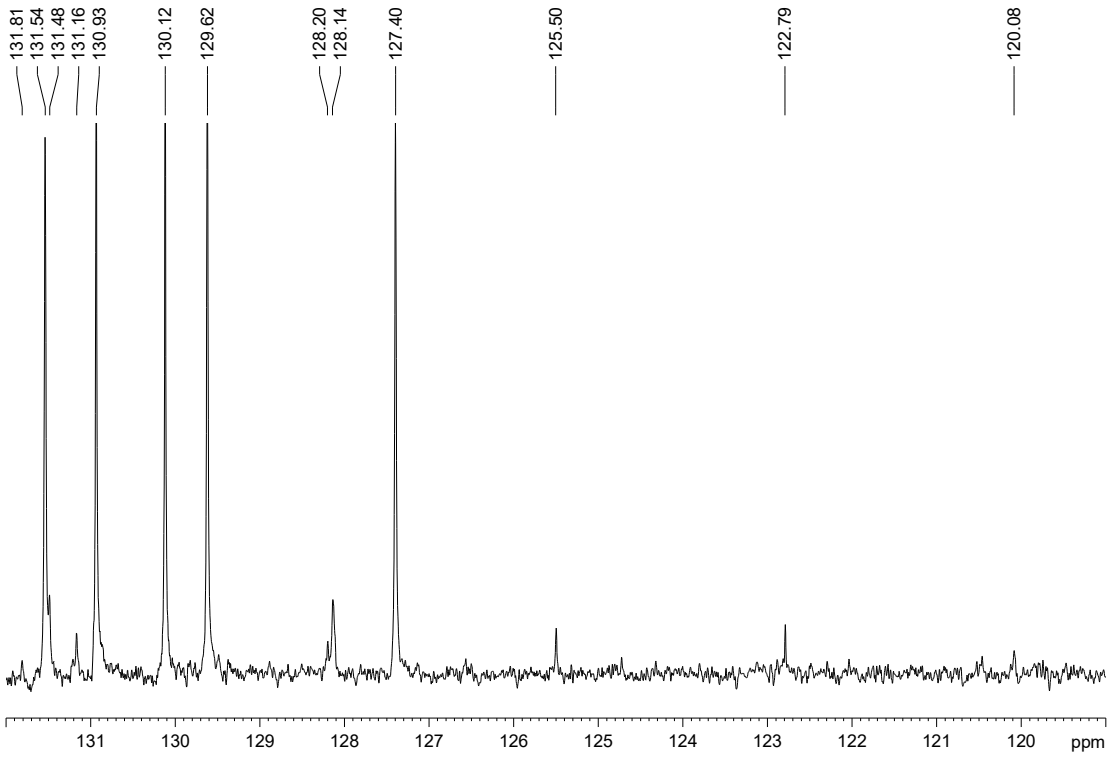


13j

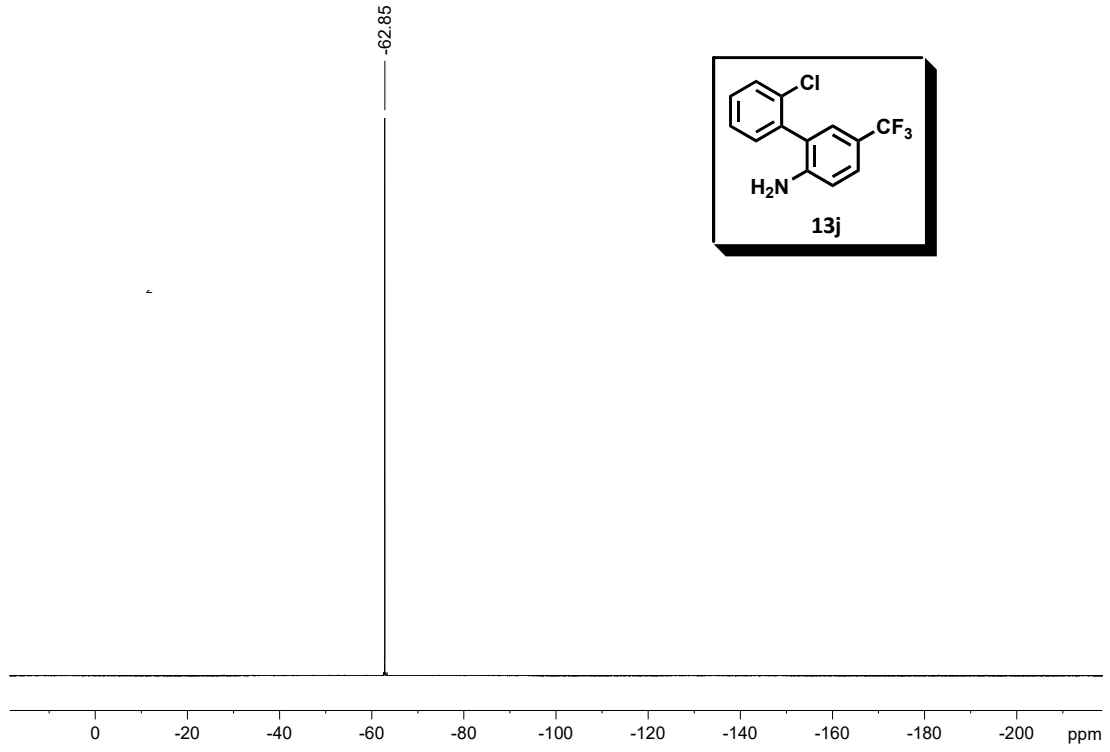


^{13}C-RMN ($CDCl_3$) 2'-Cloro-5-trifluormetil-[1,1'-bifenil]-2-amina (13j)

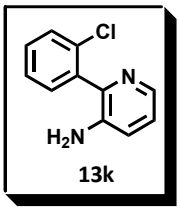




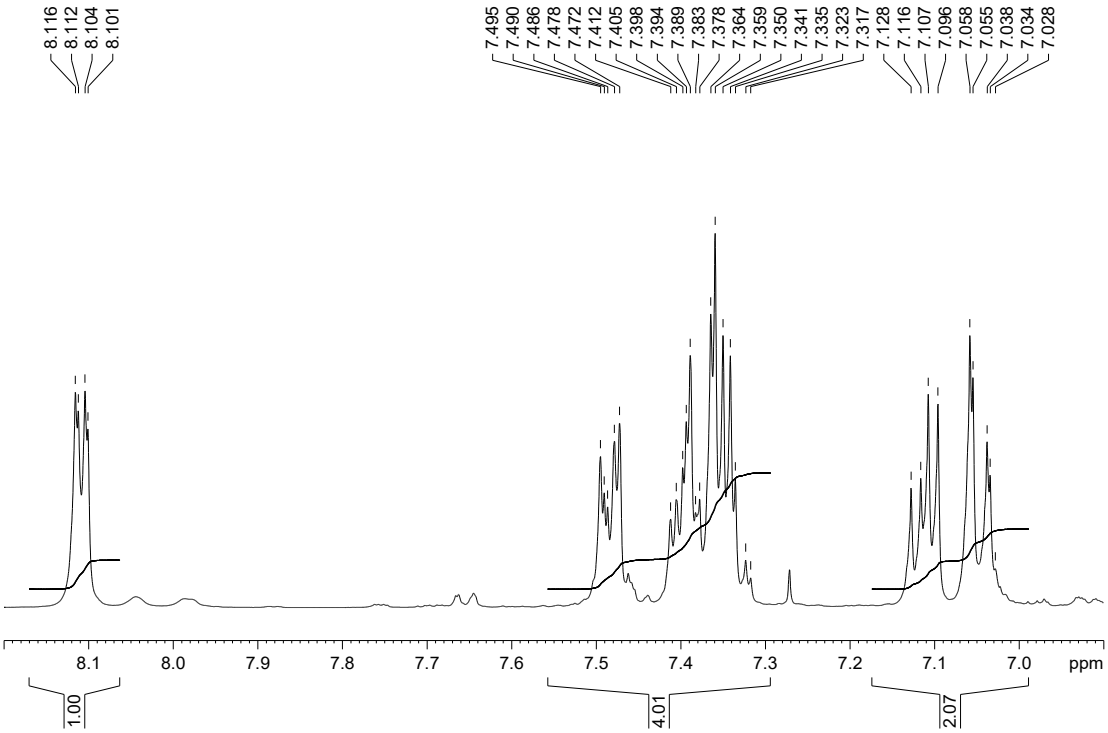
^{19}F - RMN ($CDCl_3$) 2'-Cloro-5-trifluormetil-[1,1'-bifenil]-2-amina (13j)



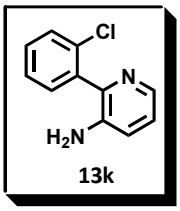
^{1}H-RMN ($CDCl_3$) 2-(2-Clorofenil)piridin-3-amina (13k)



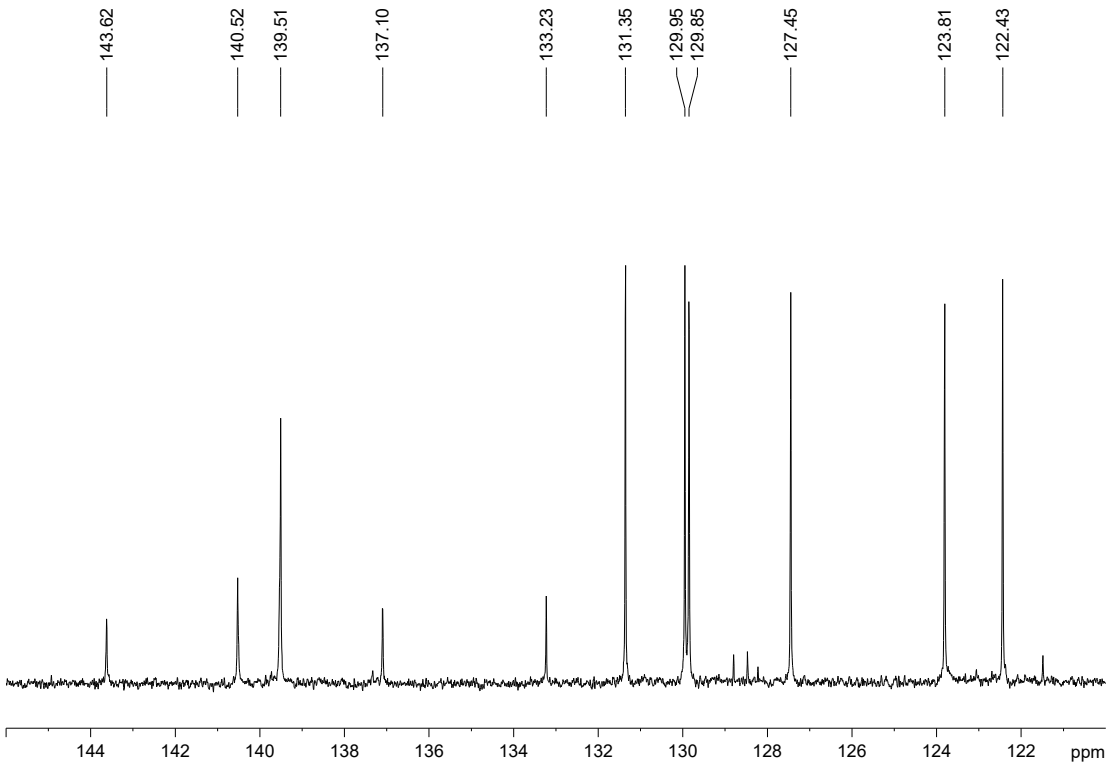
13k



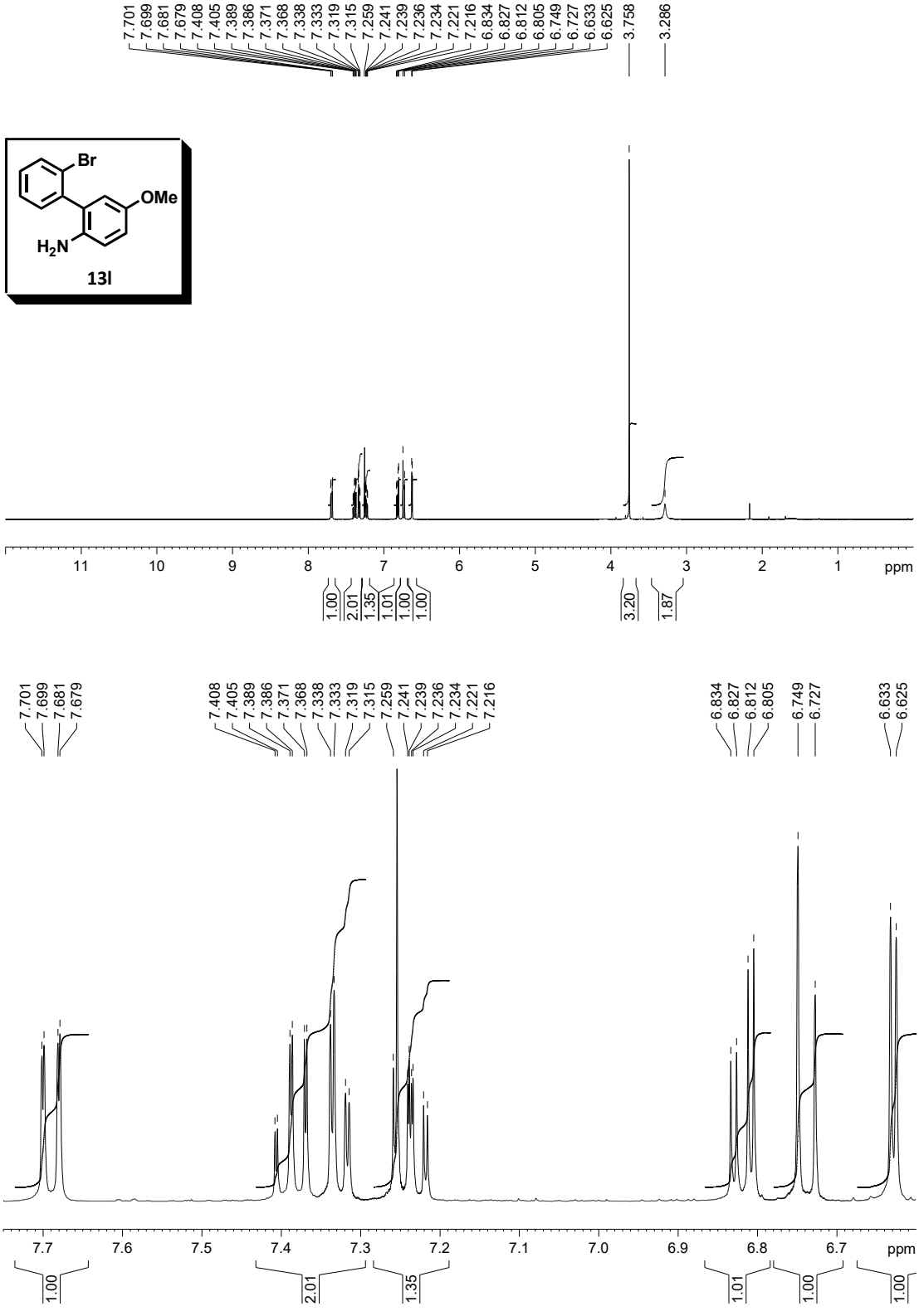
^{13}C-RMN ($CDCl_3$) 2-(2-Clorofenil)piridin-3-amina (13k)



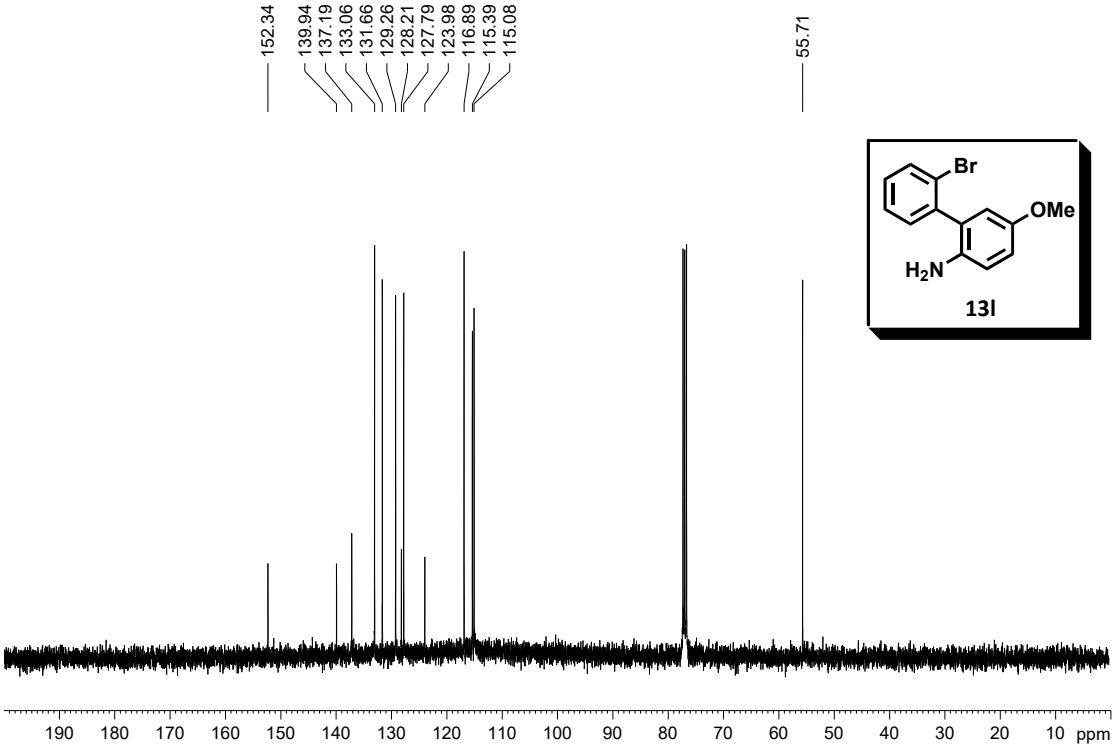
13k

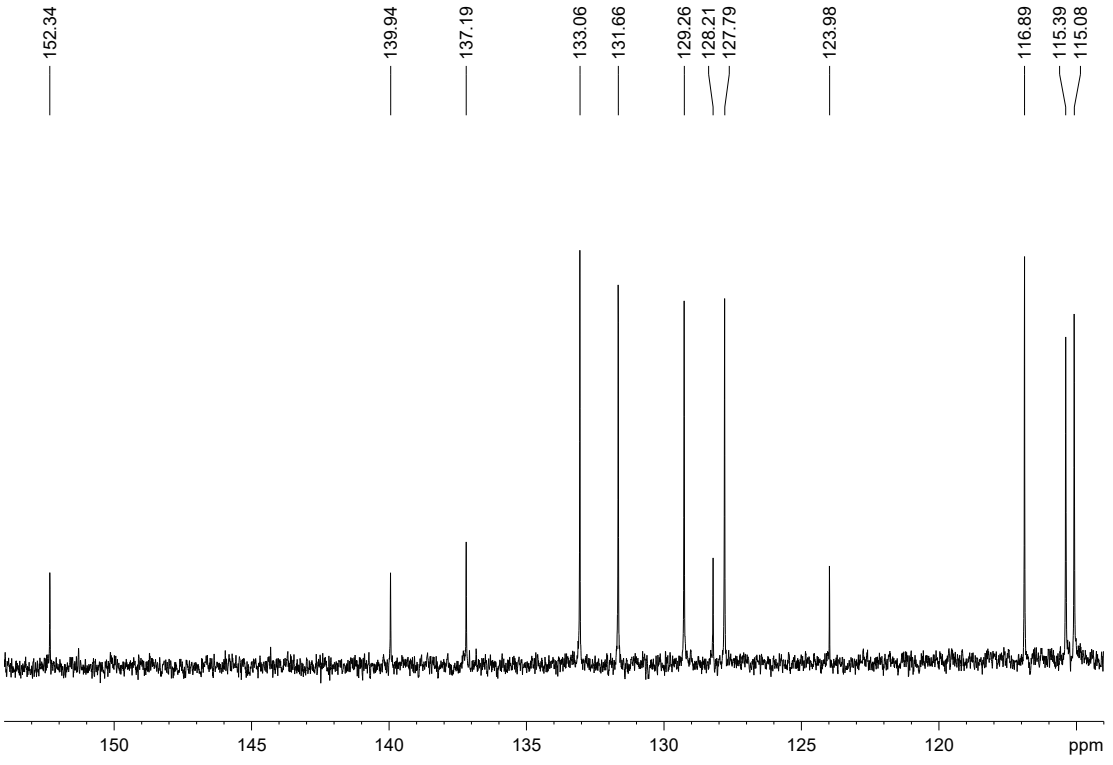


^{1}H-RMN ($CDCl_3$) 2'-Bromo-5-metoxi-[1,1'-bifenil]-2-amina (13l)

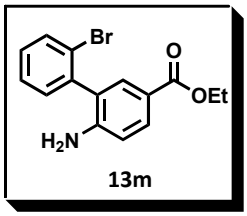


^{13}C-RMN ($CDCl_3$) 2'-Bromo-5-metoxi-[1,1'-bifenil]-2-amina (13l)

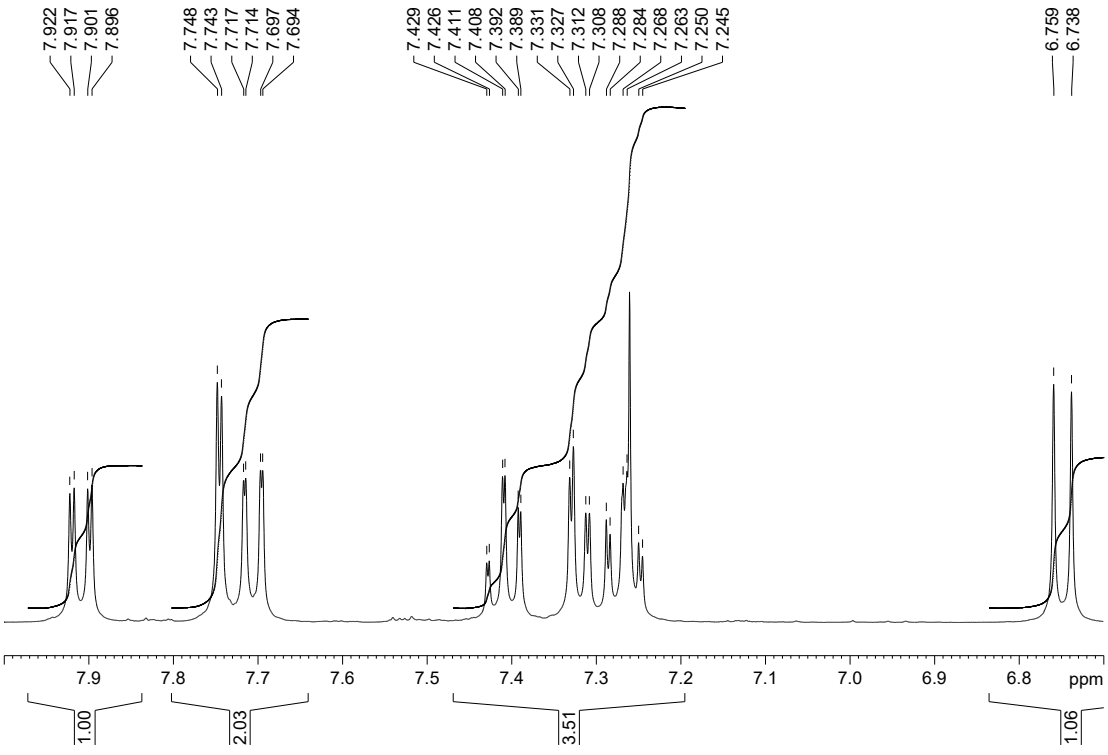




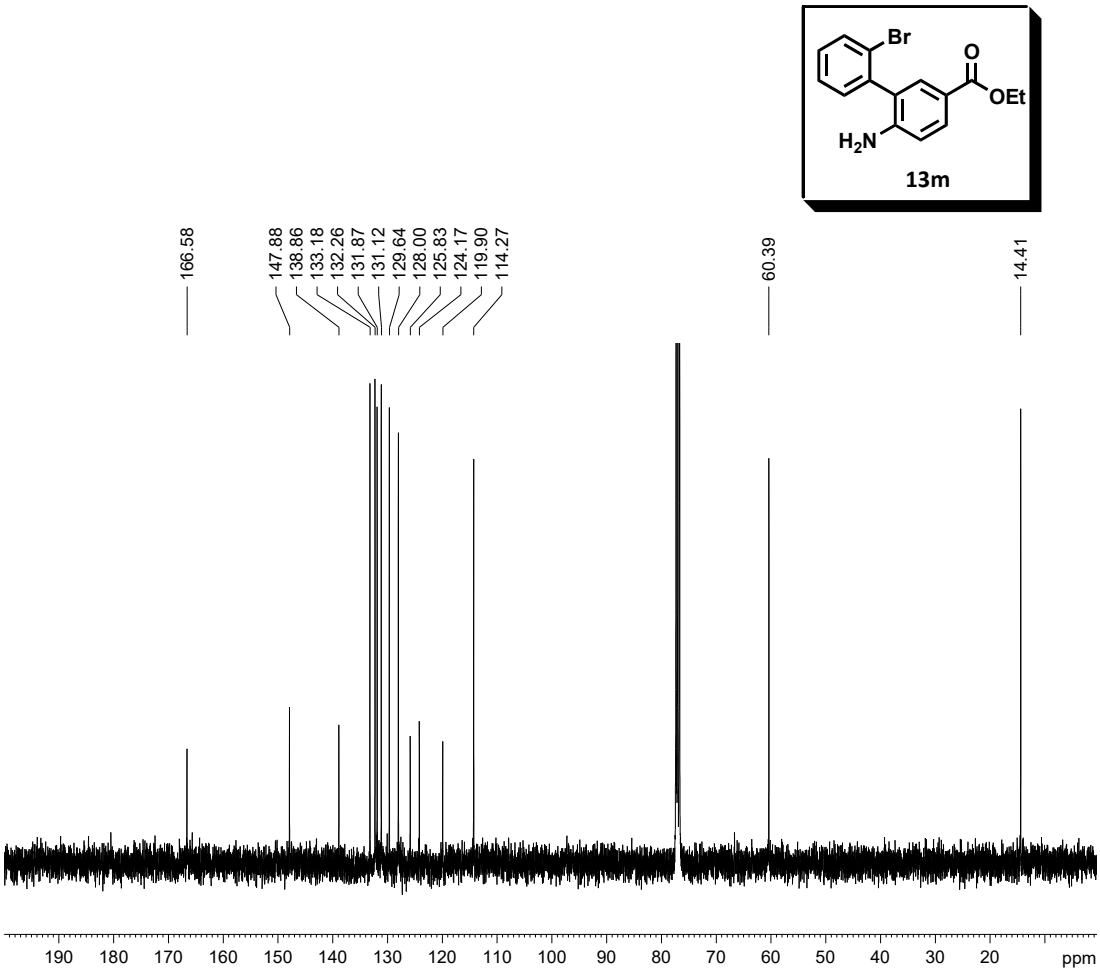
^{1}H-RMN ($CDCl_3$) 6-amino-2'-bromo-[1,1'-bifenil]-3-carboxilato de etilo (13m)



13m

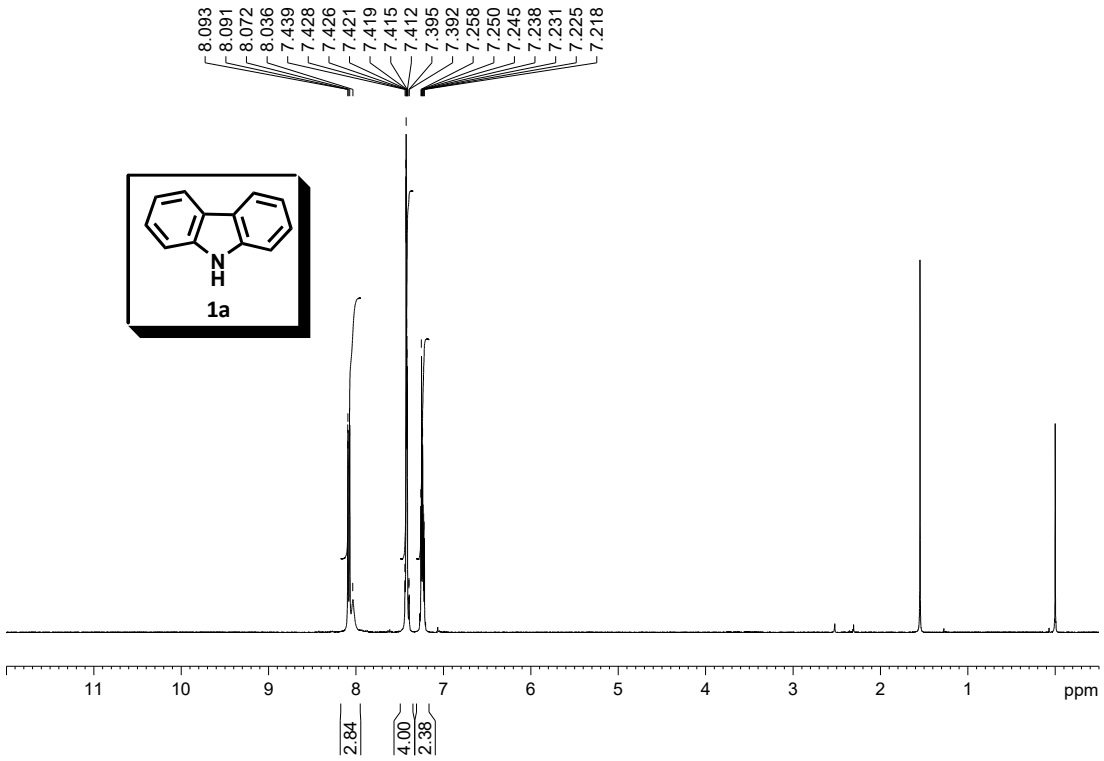


^{13}C-RMN ($CDCl_3$) 6-amino-2'-bromo-[1,1'-bifenil]-3-carboxilato de etilo (13m)



A.1.2 ESPECTROS DE RMN DE 9*H*-CARBAZOLES OBTENIDOS (PRODUCTOS CICLIZADOS)

^{1}H-RMN ($CDCl_3$) 9*H*-carbazol (1a)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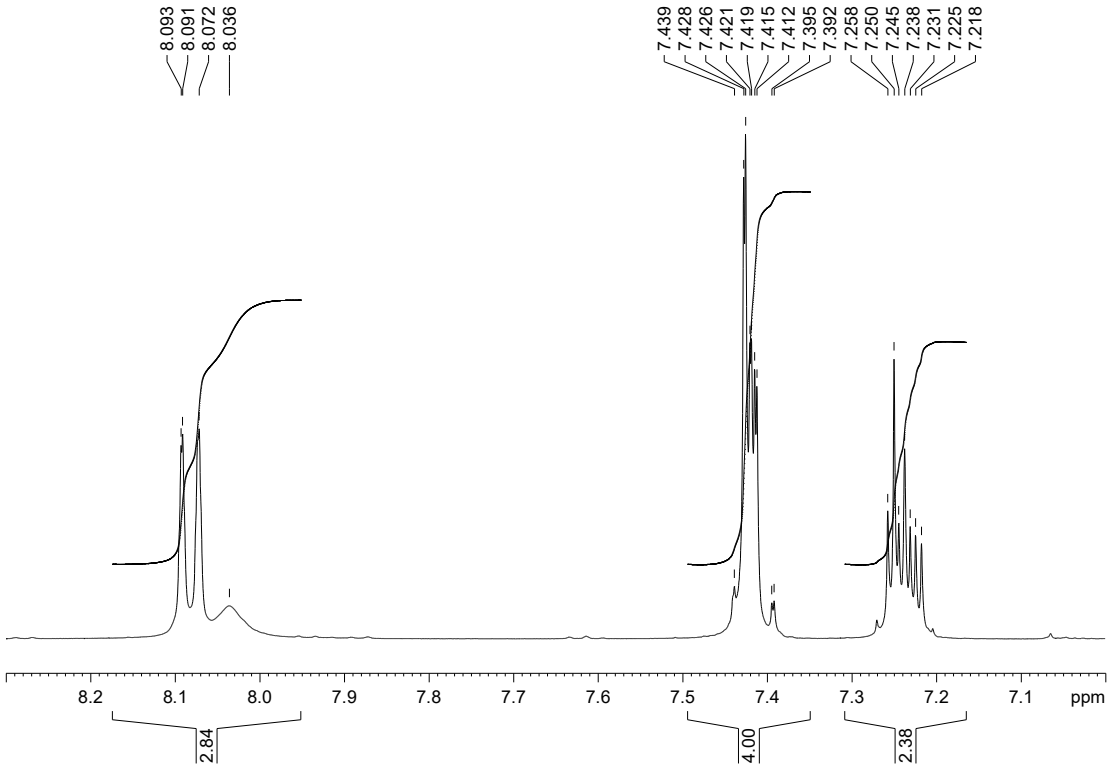
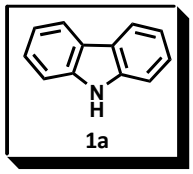
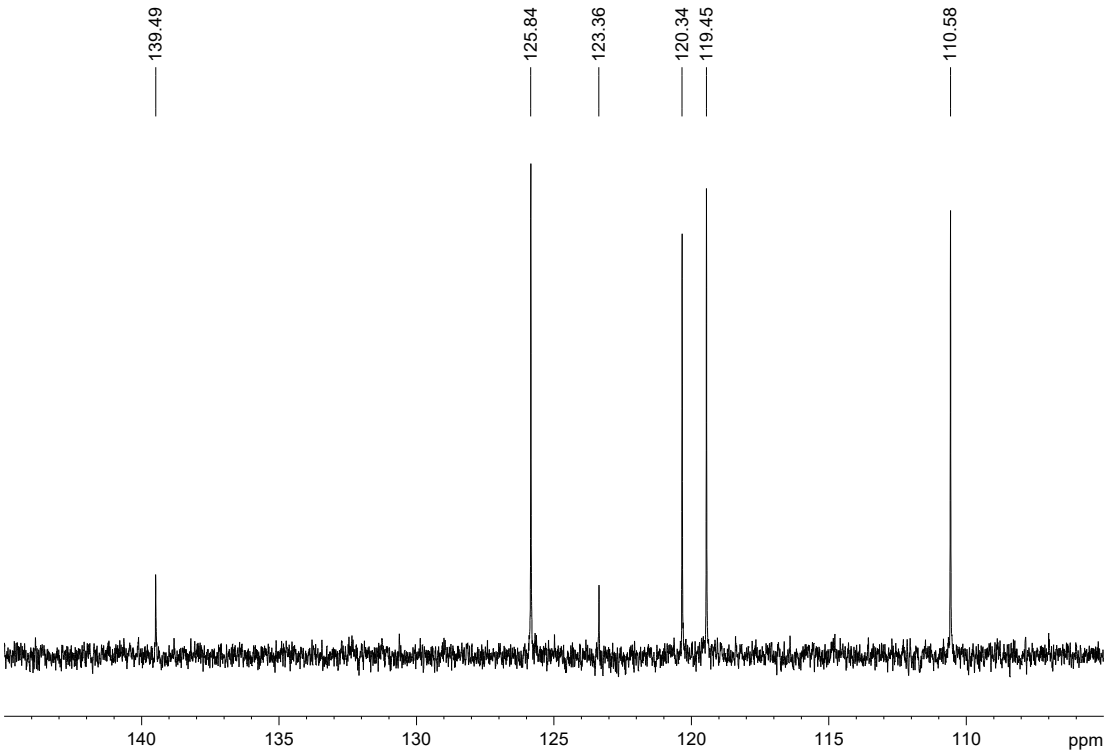
8.091
8.072
8.036
7.439
7.428
7.426
7.421
7.419
7.415
7.412
7.395
7.392
7.258
7.250
7.245
7.238
7.231
7.225
7.218
N
H
1a
11
10
9
8
7
6
5
4
3
2
1
ppm
2.84
4.00
2.38


8.093
8.091
8.072
8.036
7.439
7.428
7.426
7.421
7.419
7.415
7.412
7.395
7.392
7.258
7.250
7.245
7.238
7.231
7.225
7.218
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
ppm
2.84
4.00
2.38

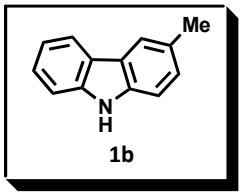
^{13}C-RMN ($CDCl_3$) 9*H*-carbazol (1a)

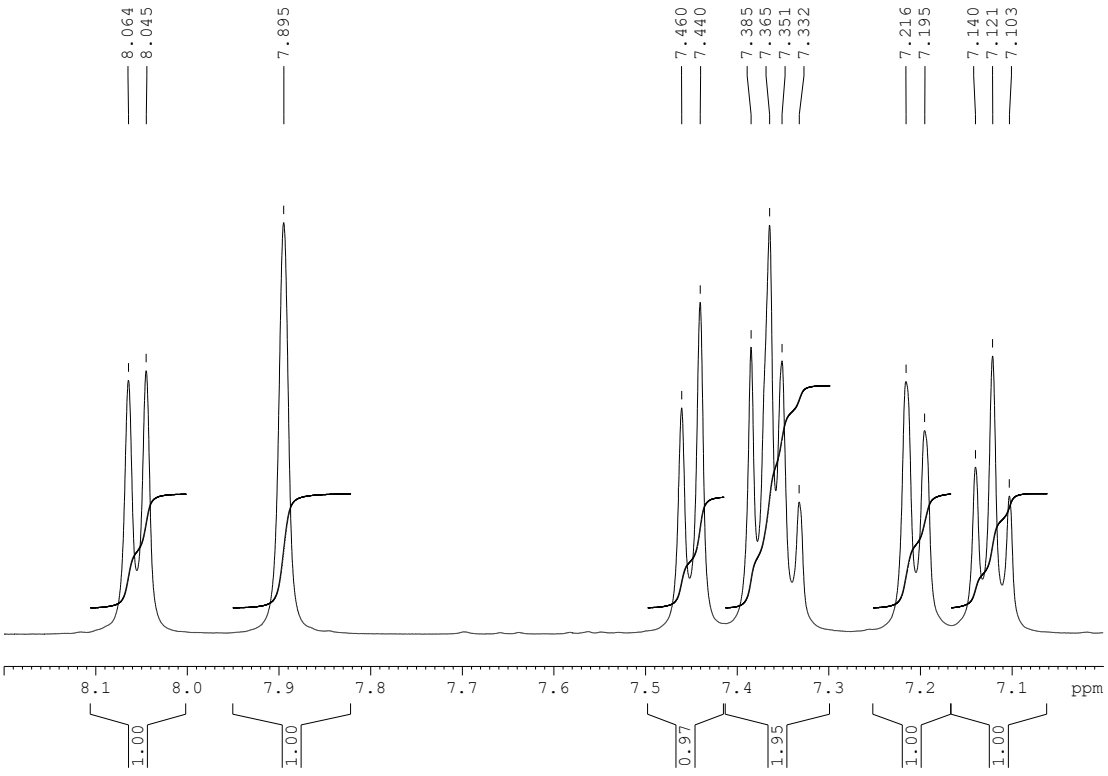


1a

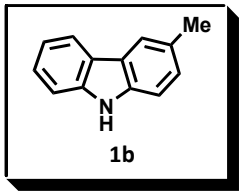


^{1}H-RMN (CD_3SOCD_3) 3-Metil-9*H*-carbazol (1b)

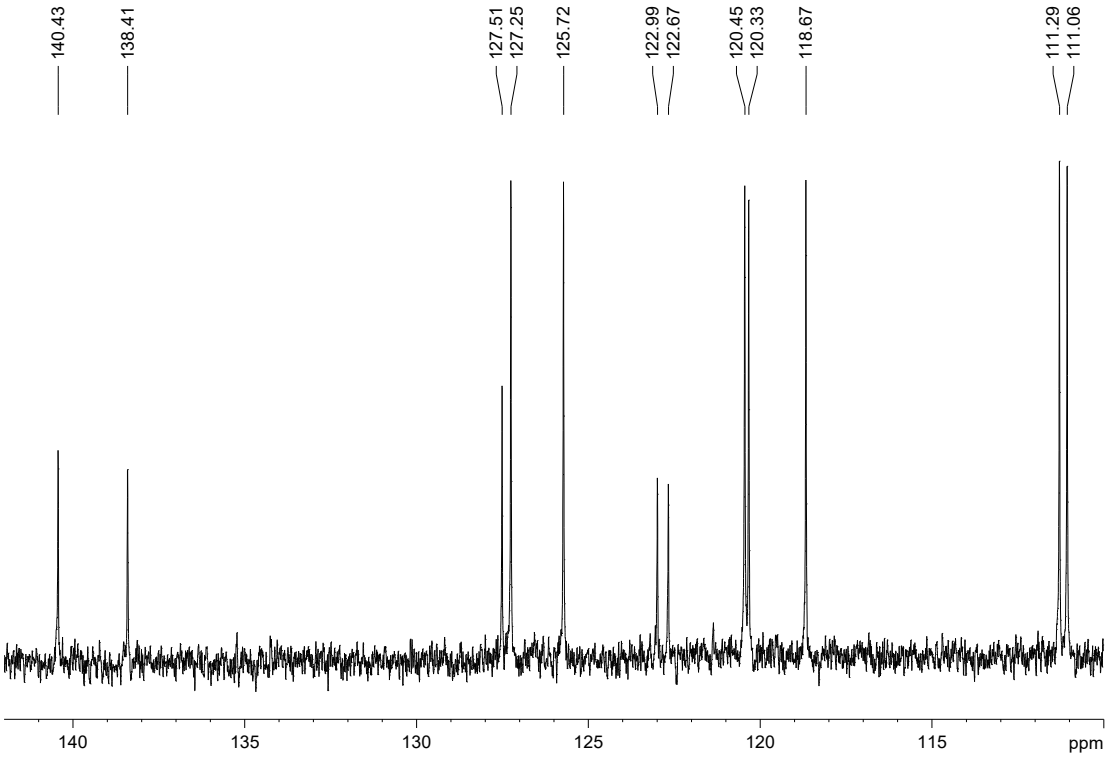




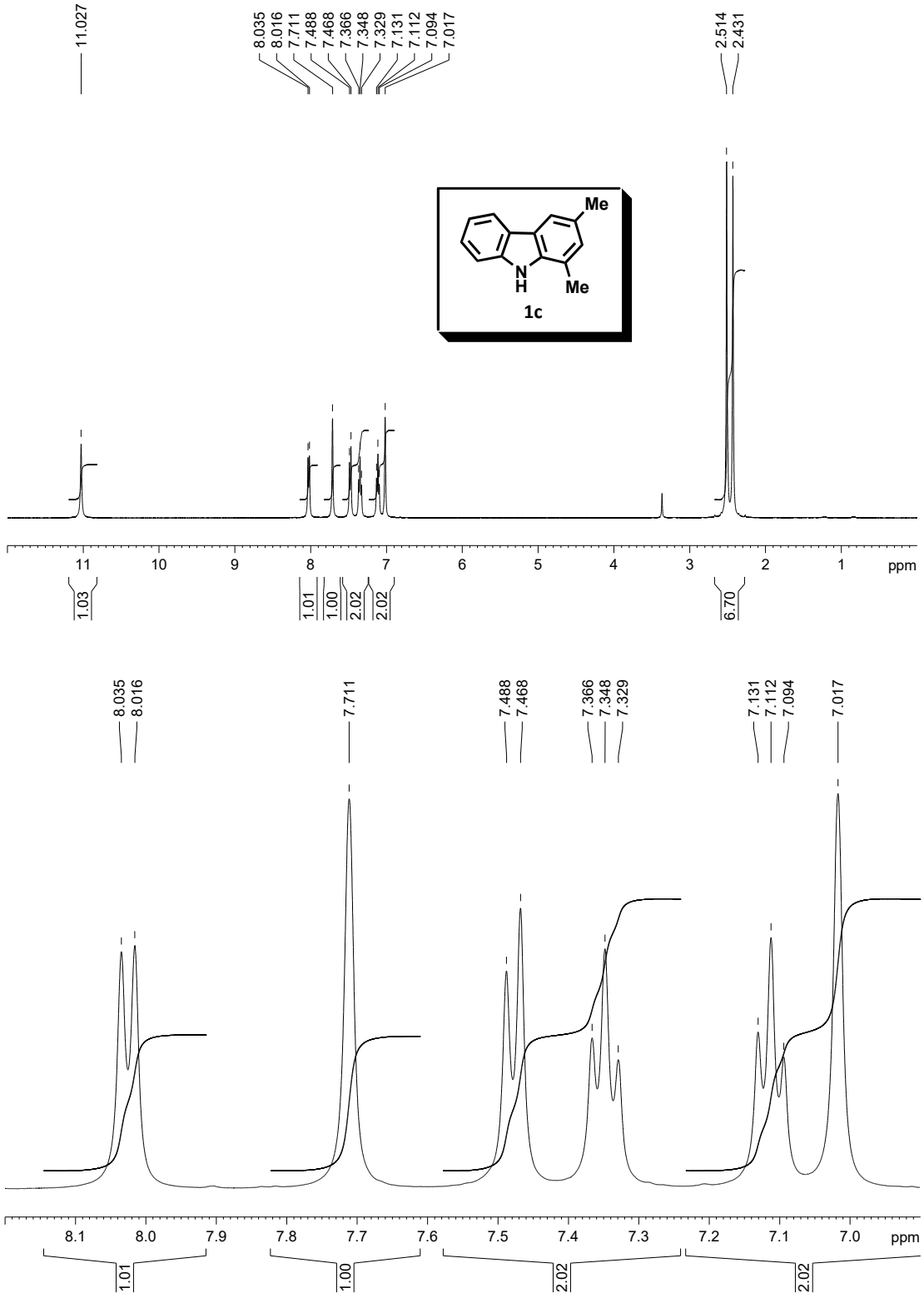
^{13}C-RMN (CD_3SOCD_3) 3-Metil-9*H*-carbazol (1b)



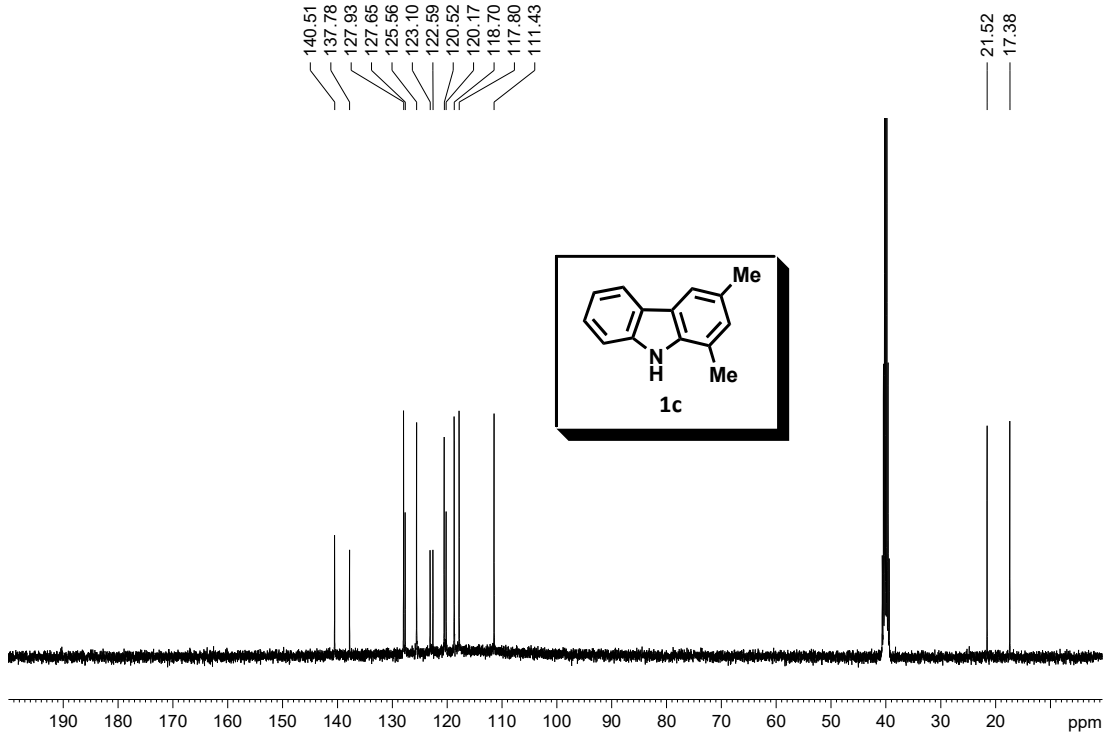
1b

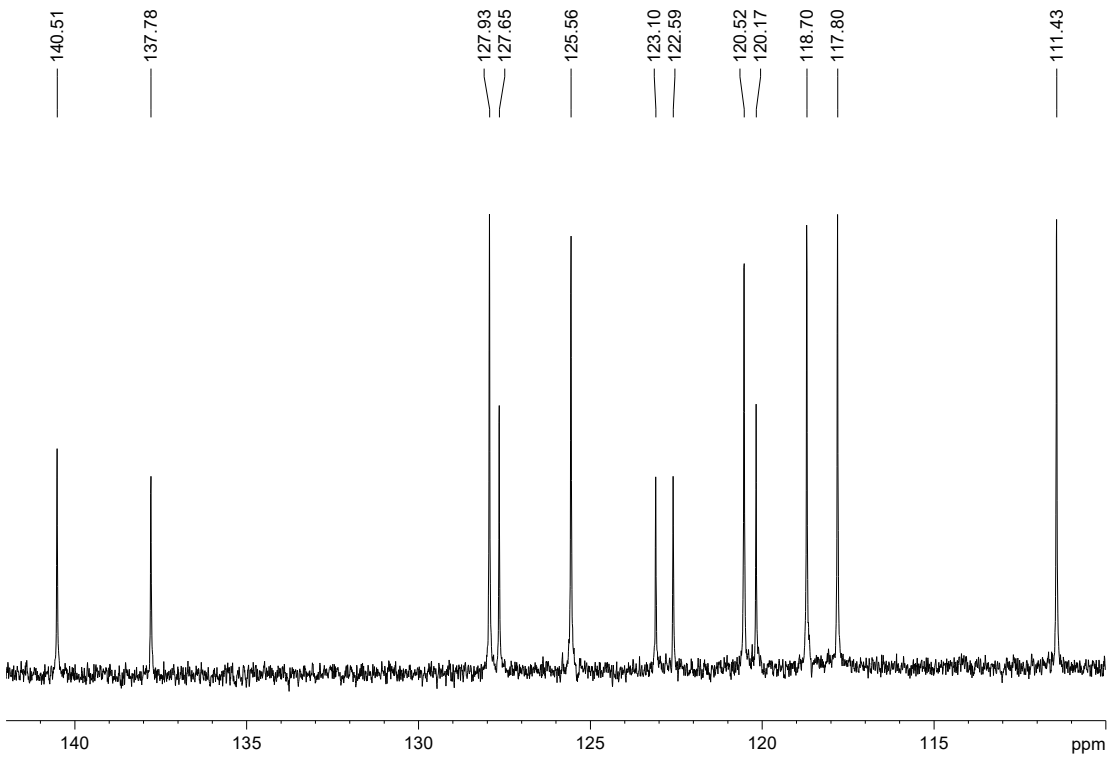


^{1}H-RMN (CD_3SOCD_3) 1,3-Dimetil-9*H*-carbazol (1c)

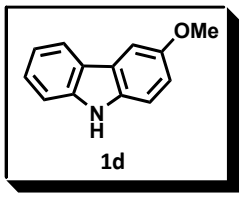


^{13}C-RMN (CD_3SOCD_3) 1,3-Dimetil-9*H*-carbazol (1c)

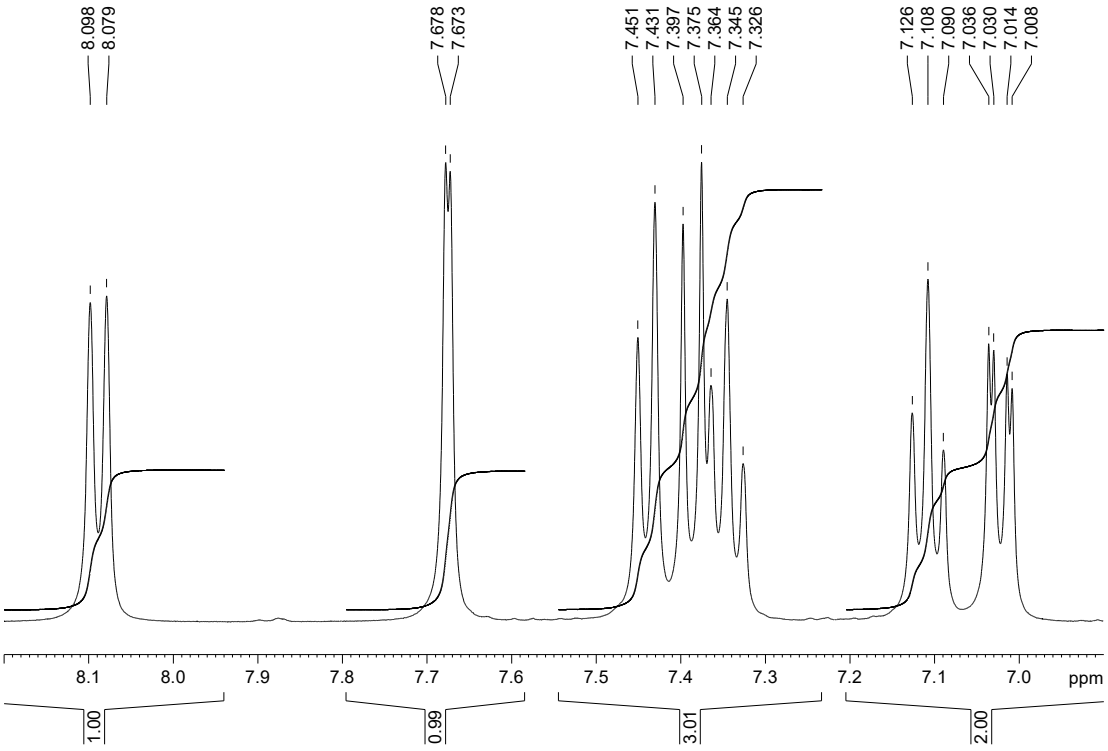




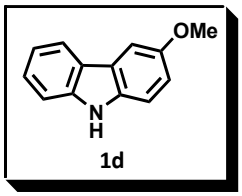
^{1}H-RMN (CD_3SOCD_3) 3-Metoxi-9H-carbazol (1d)



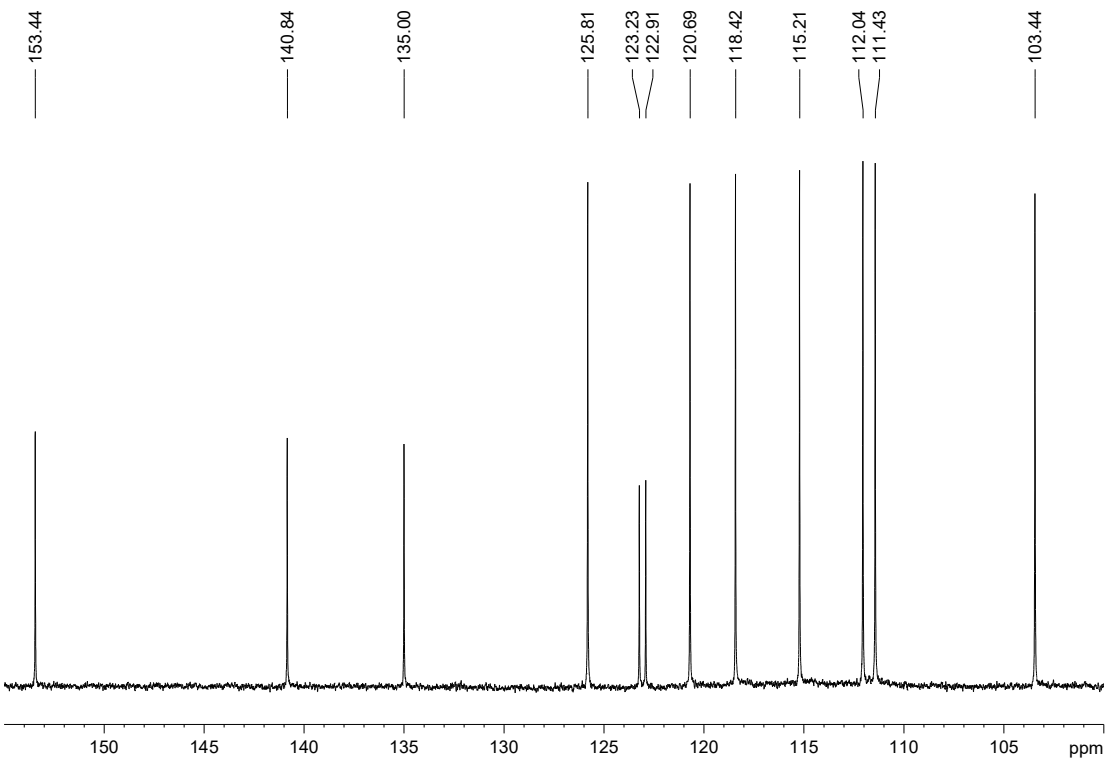
1d



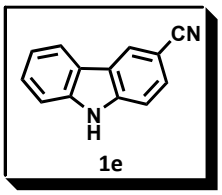
^{13}C-RMN (CD_3SOCD_3) 3-Metoxi-9H-carbazol (1d)



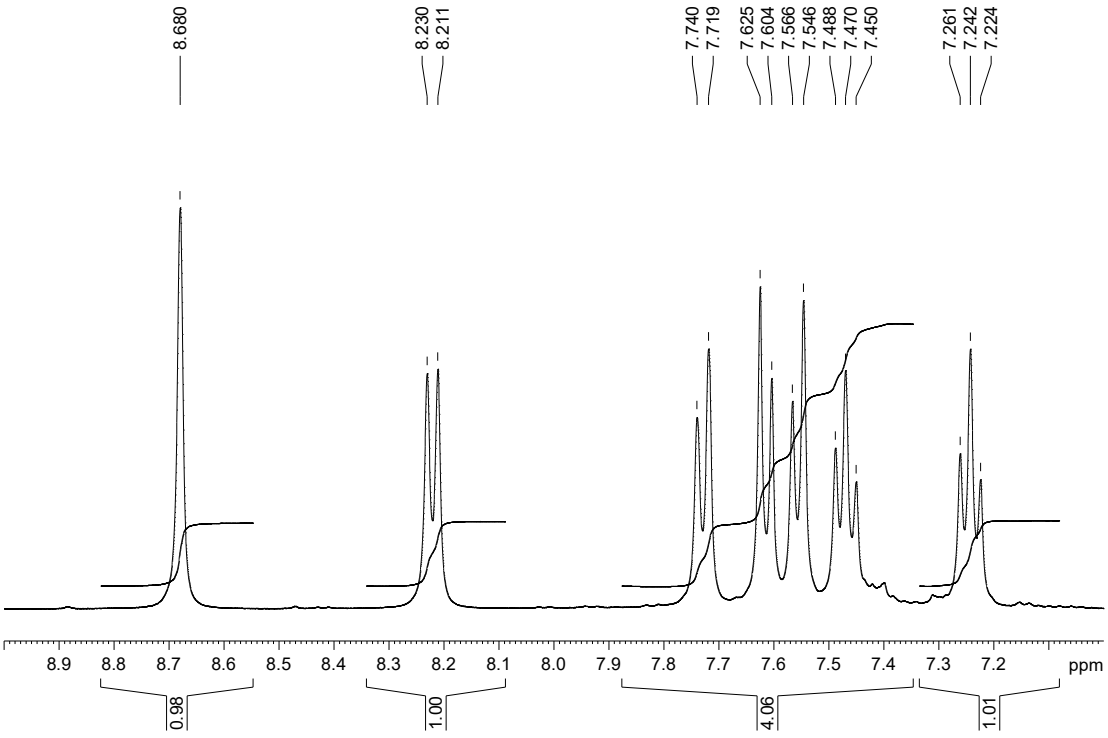
1d



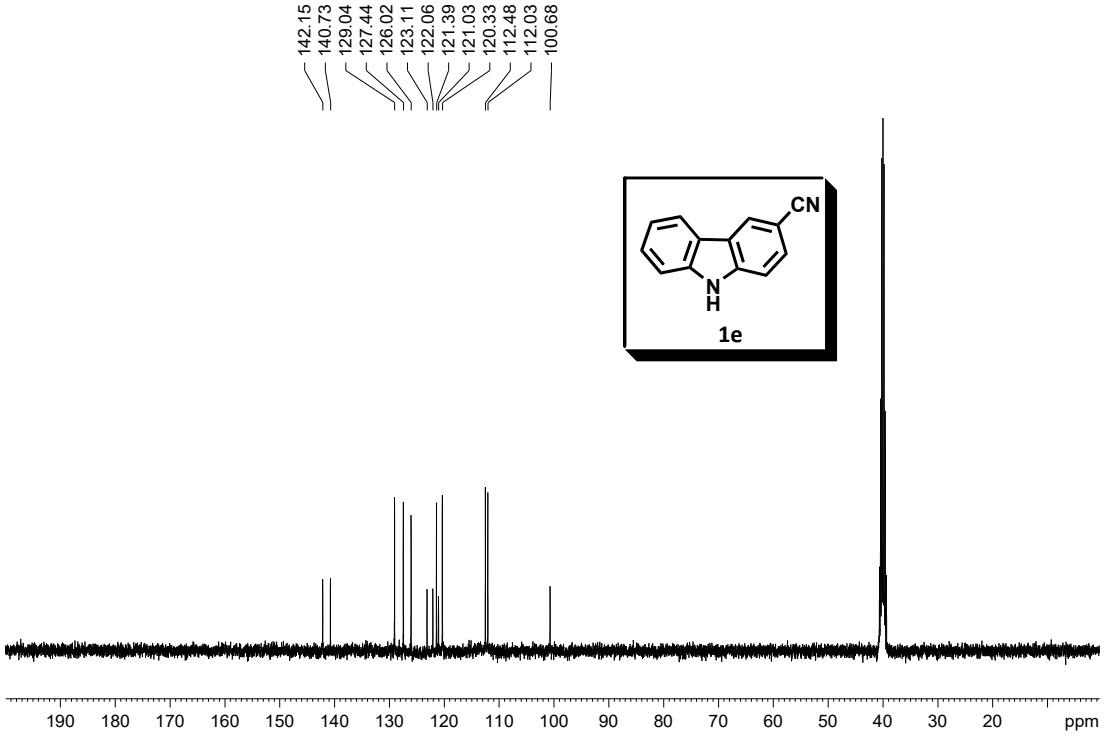
^{1}H-RMN (CD_3SOCD_3) 3-Carbonitrilo-9*H*-carbazol (1e)



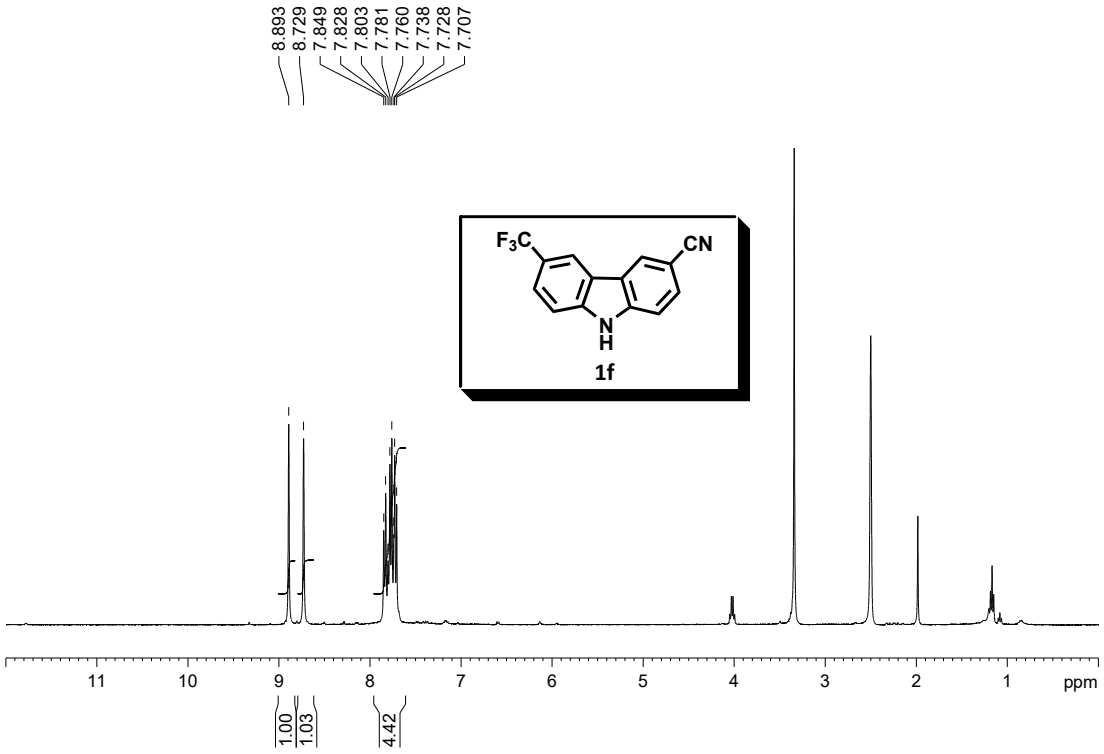
1e

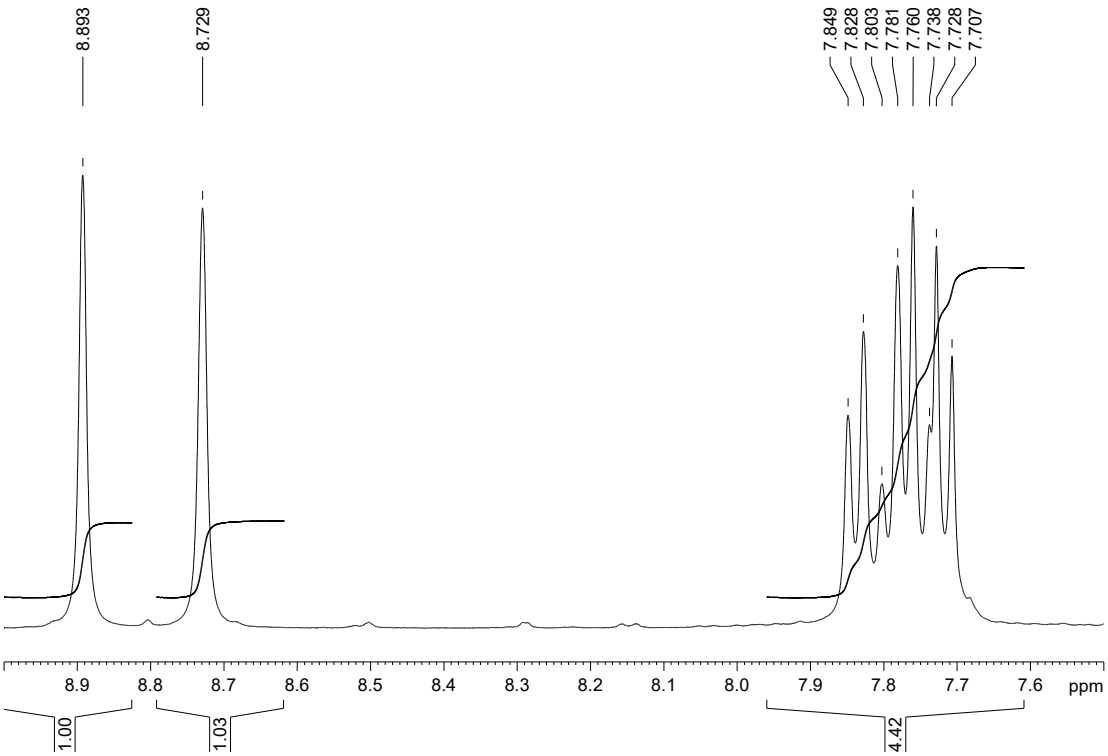


^{13}C-RMN (CD_3SOCD_3) 3-Carbonitrilo-9*H*-carbazol (1e)

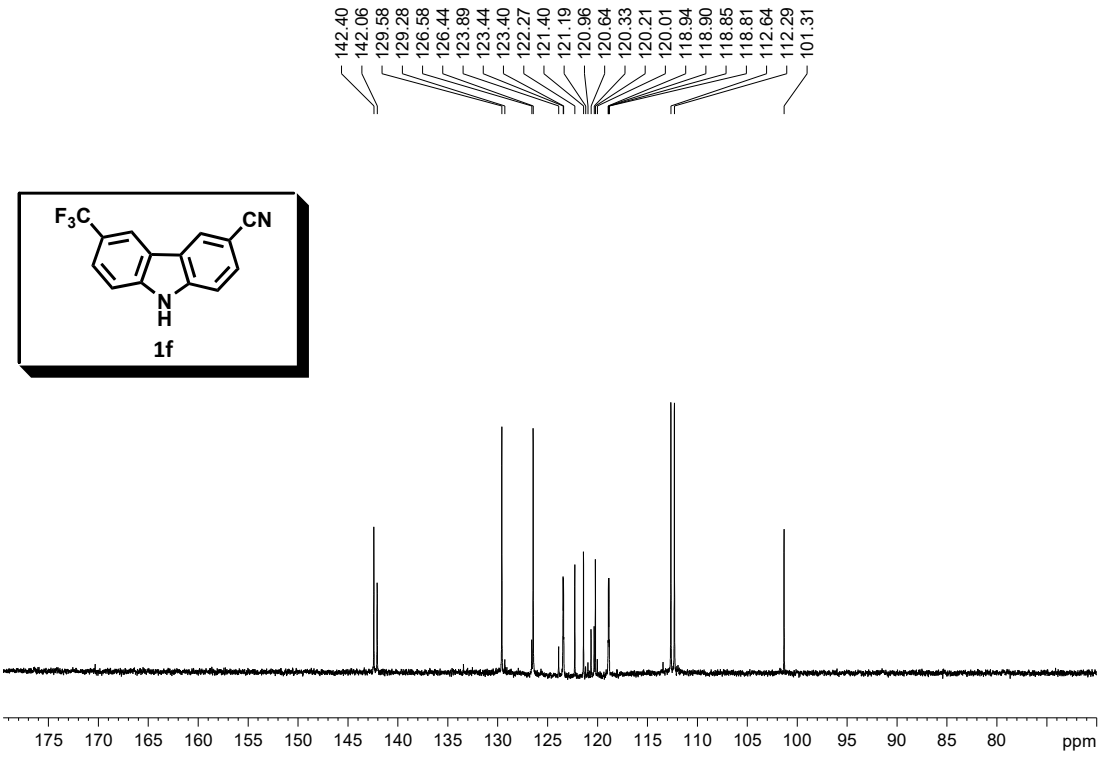


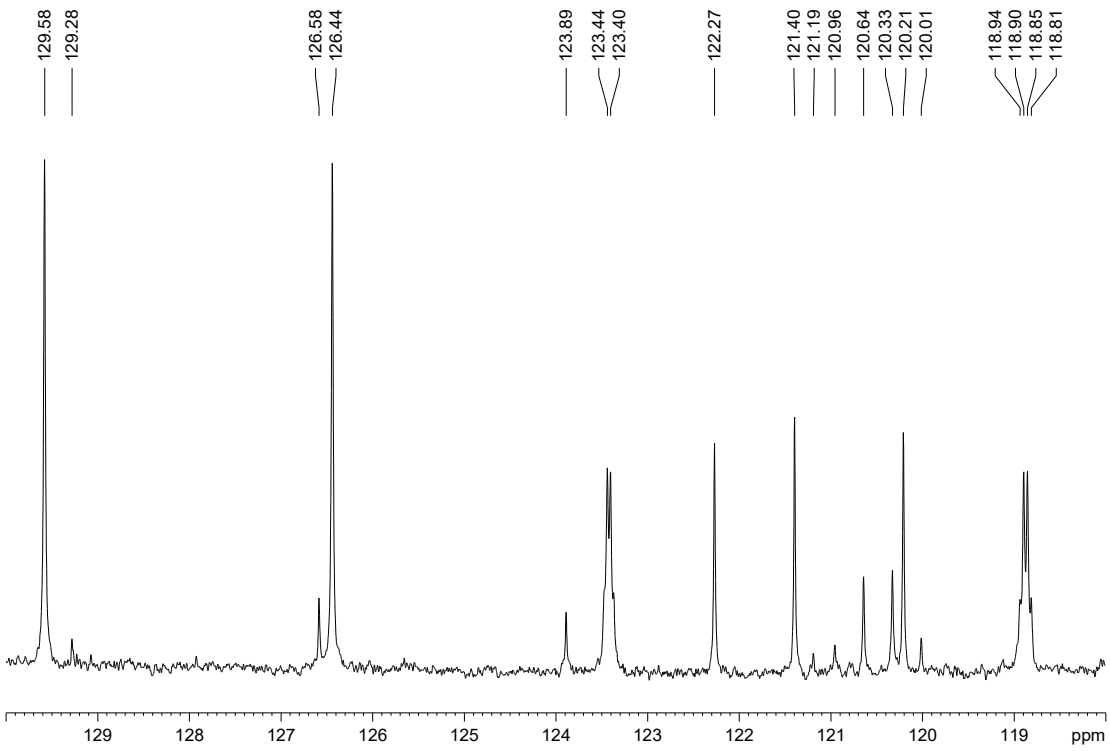
^{1}H-RMN (CD_3SOCD_3) 6-Trifluormetil-9*H*-carbazol-3-carbonitrilo (1f)



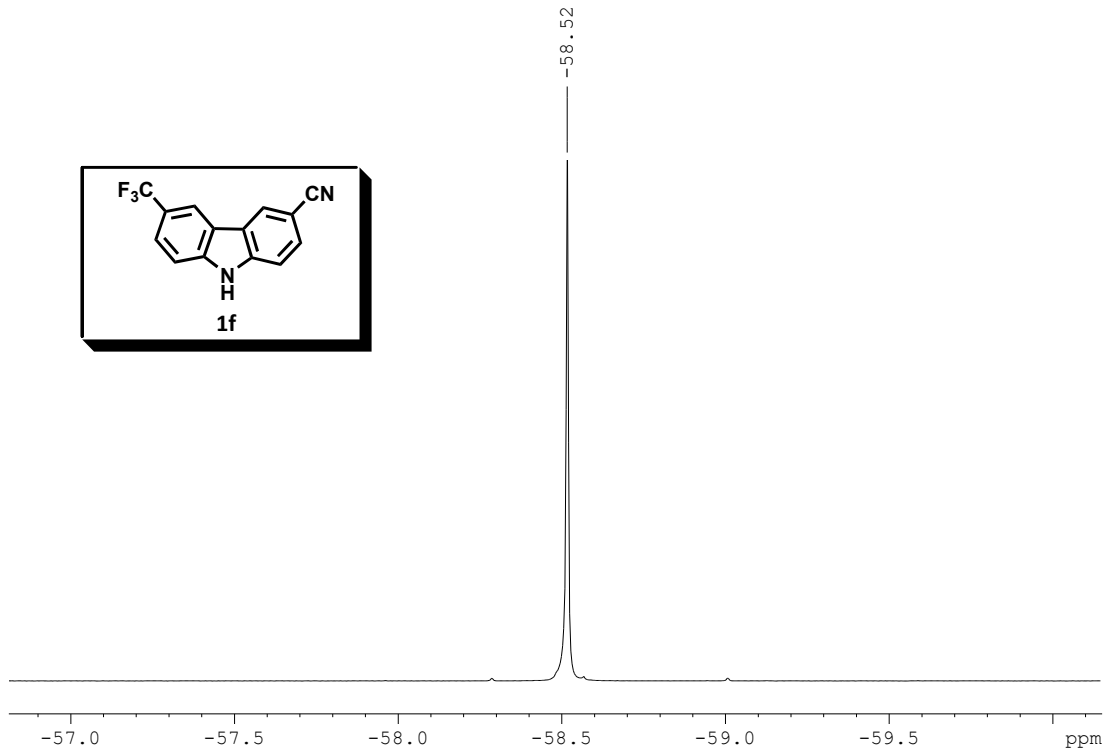


^{13}C-RMN (CD_3SOCD_3) 6-Trifluormetil-9*H*-carbazol-3-carbonitrilo (1f)

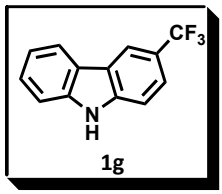




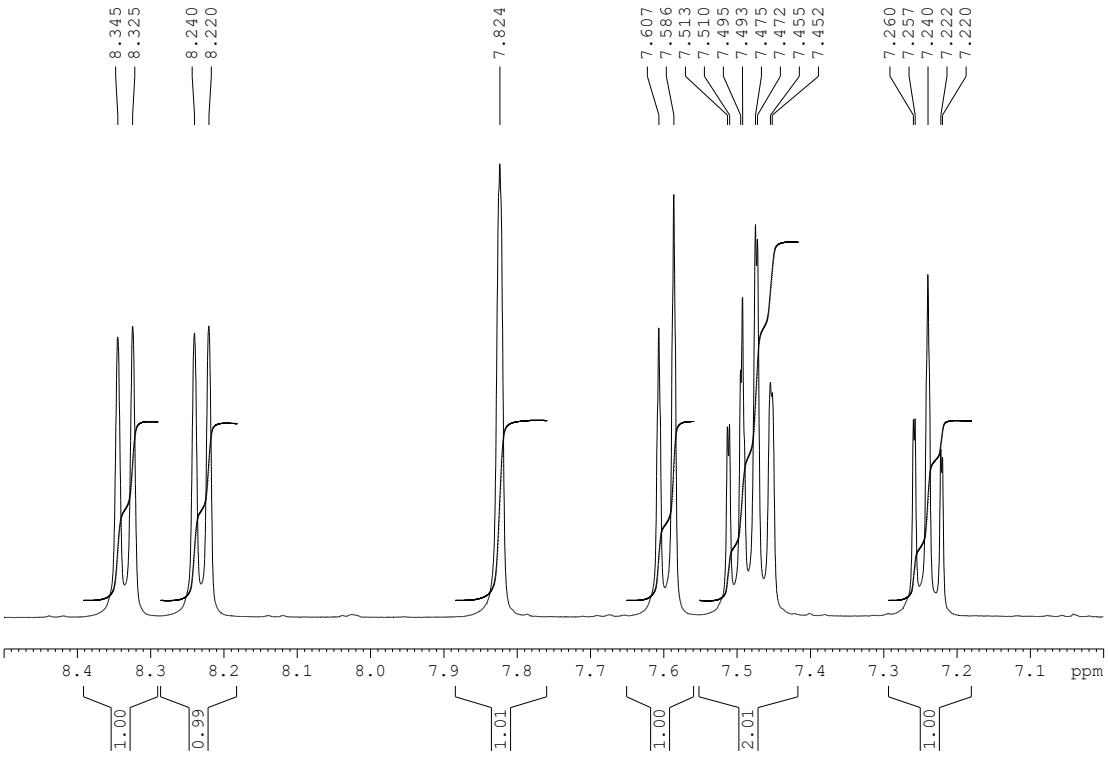
^{19}F - RMN (CD_3SOCD_3) 6-Trifluormetil-9*H*-carbazol-3-carbonitrilo (1f)



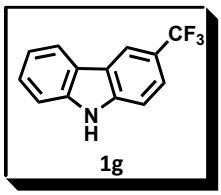
^{1}H-RMN (CD_3SOCD_3) 3-Trifluormetil-9*H*-carbazol (1g)



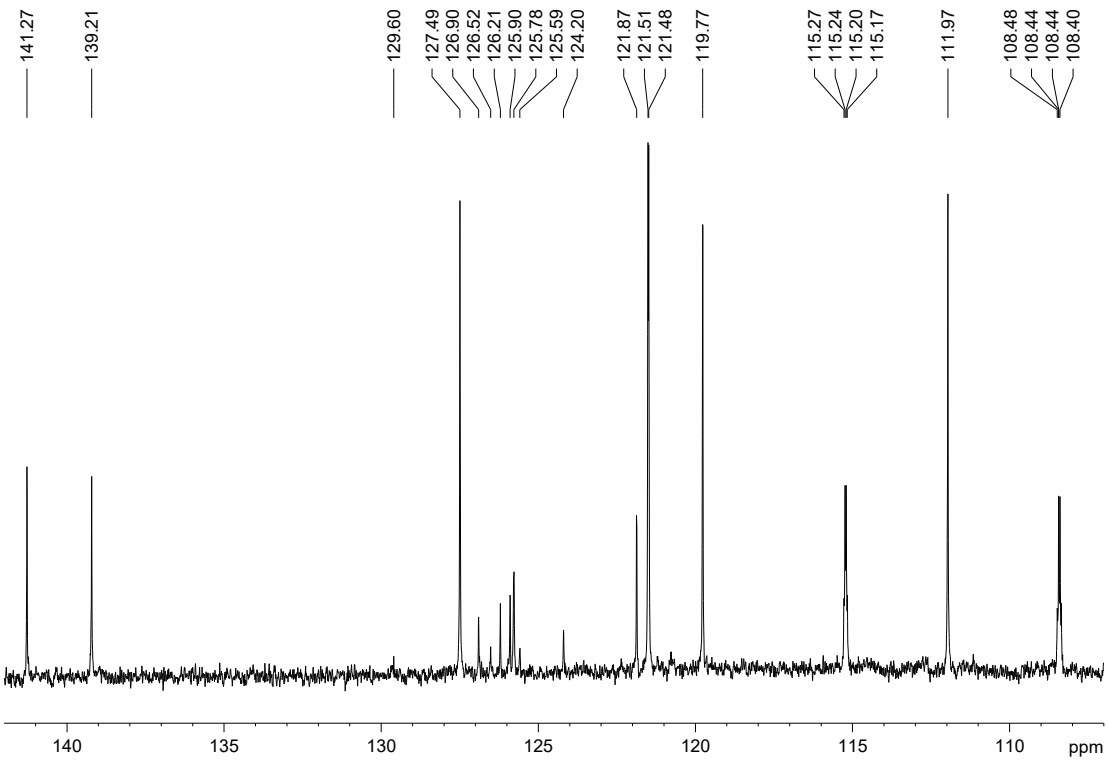
1g



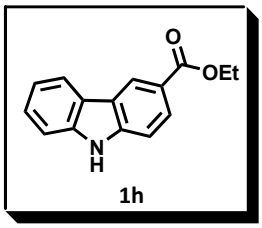
^{13}C-RMN (CD_3SOCD_3) 3-Trifluormetil-9*H*-carbazol (1g)



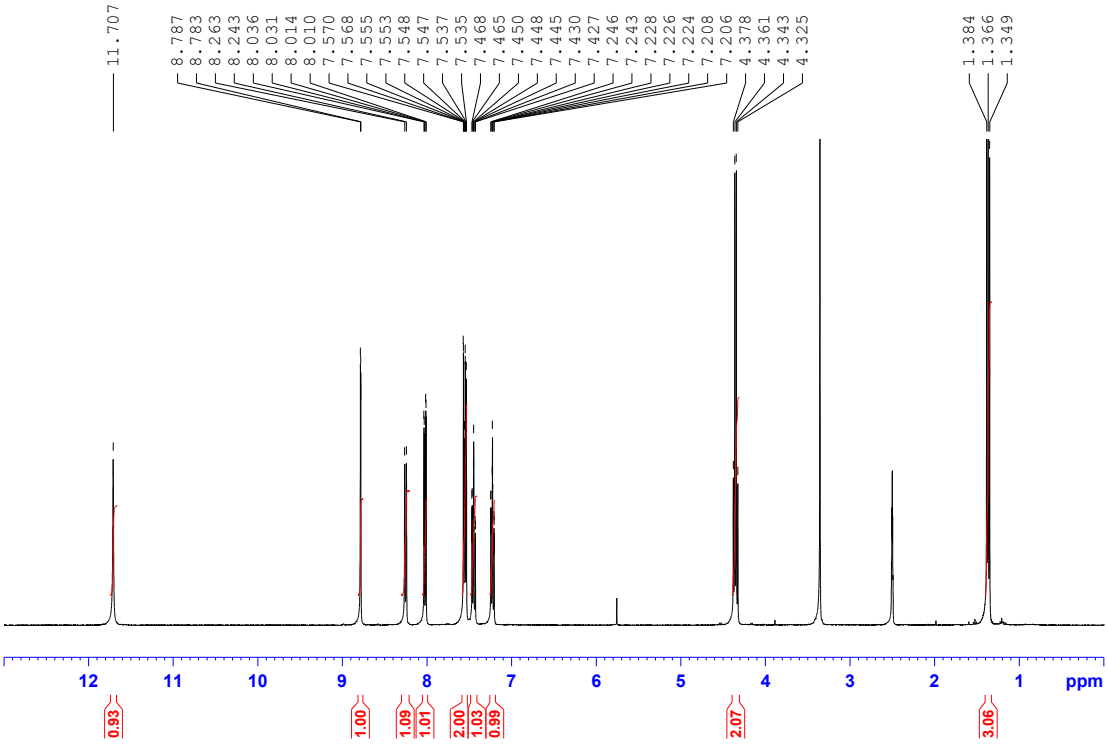
1g

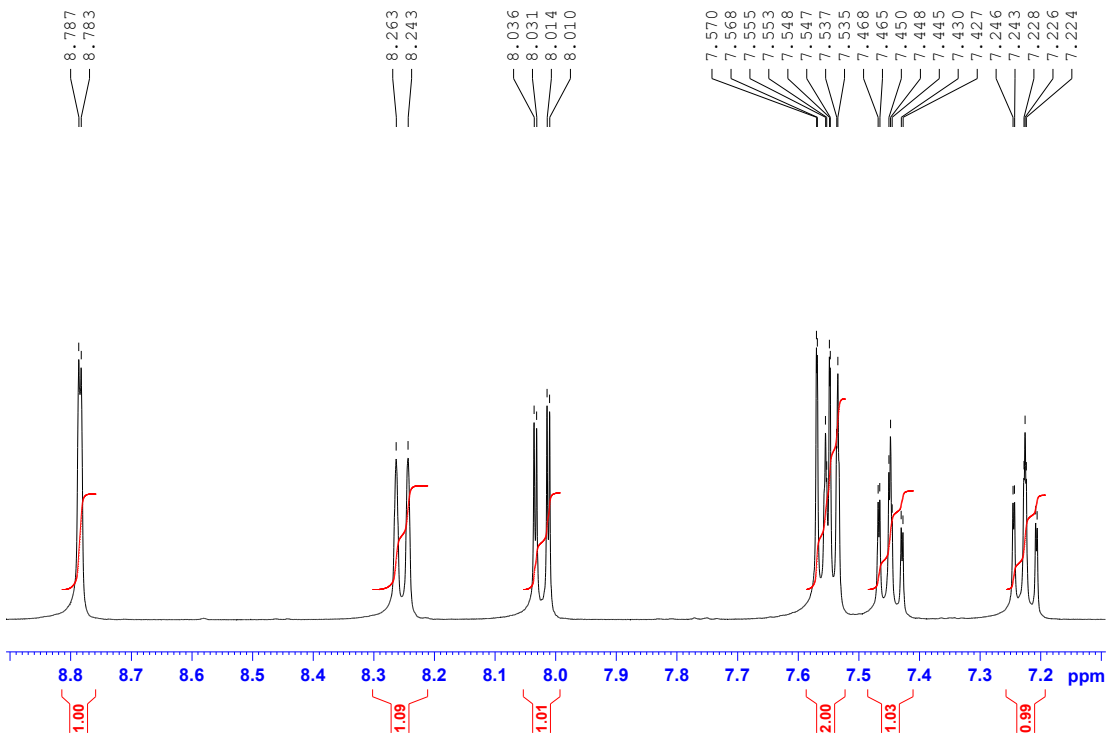


^{1}H-RMN (CD_3SOCD_3) 9*H*-carbazol-3-carboxilate de etilo (1h)

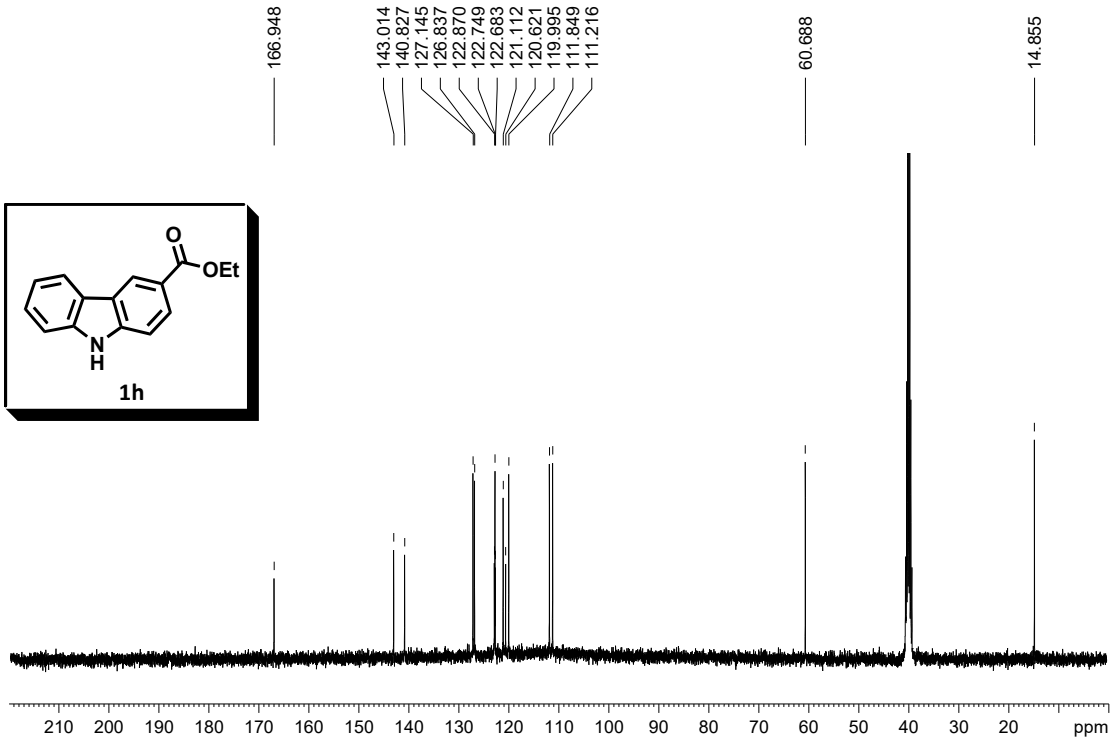


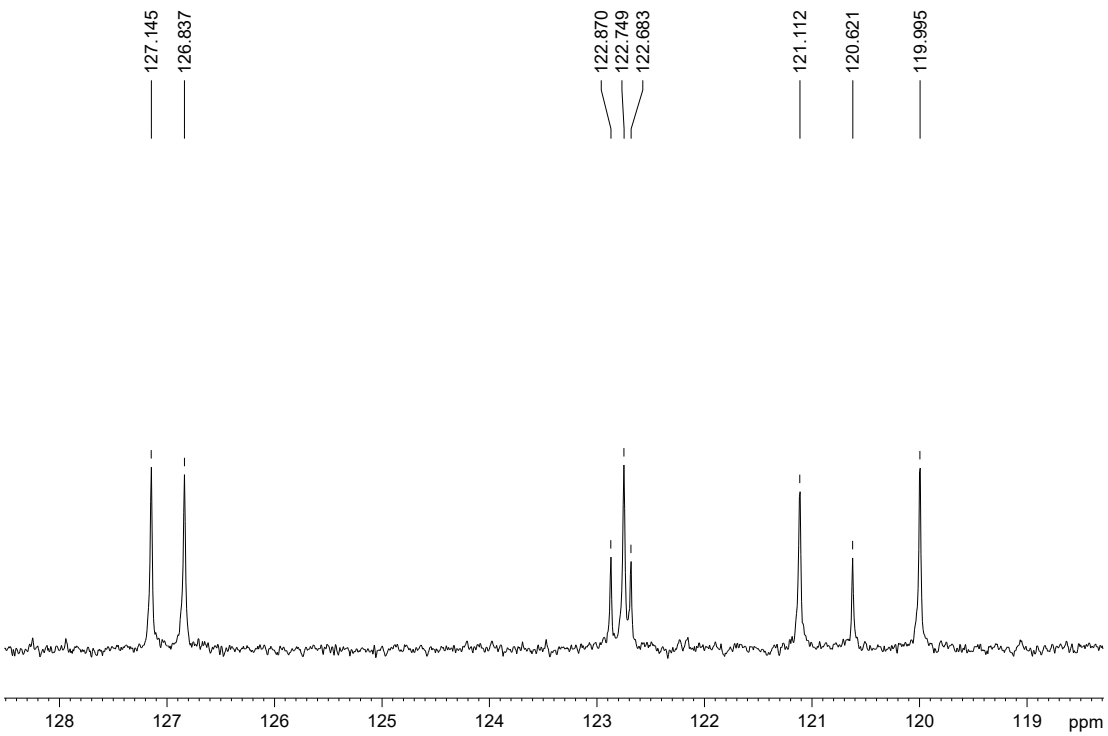
1h



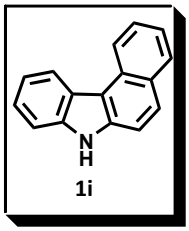


^{13}C-RMN (CD_3SOCD_3) 9*H*-carbazol-3-carboxilate de etilo (1h)

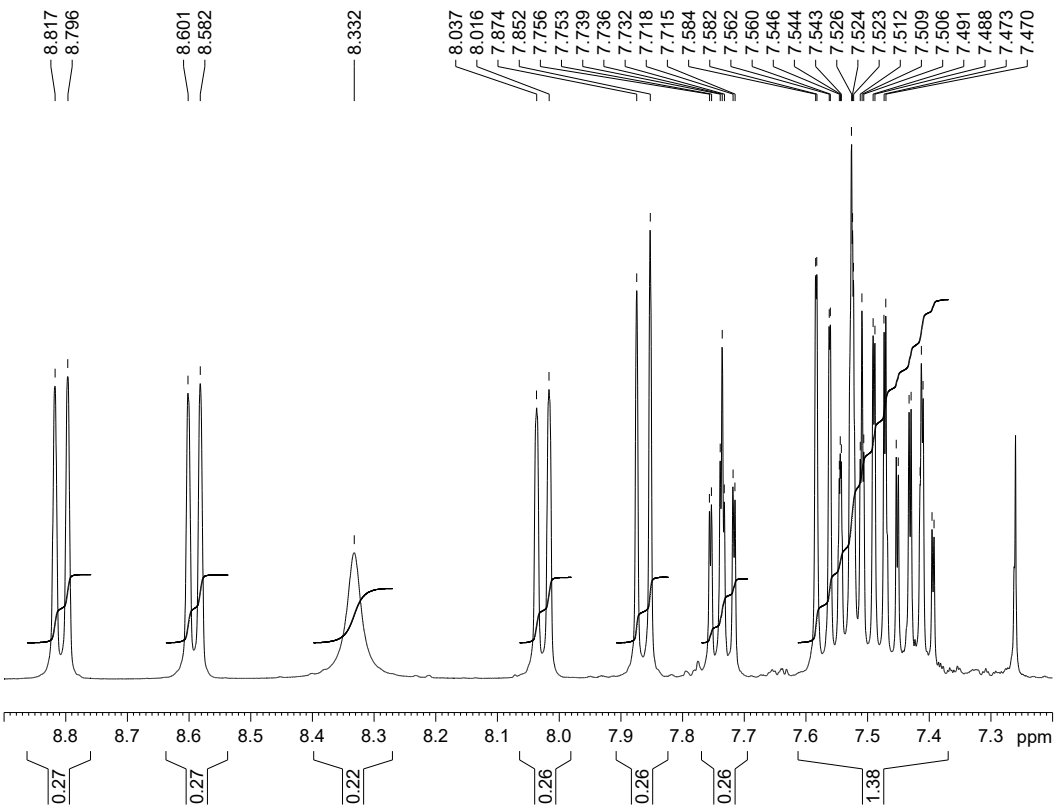




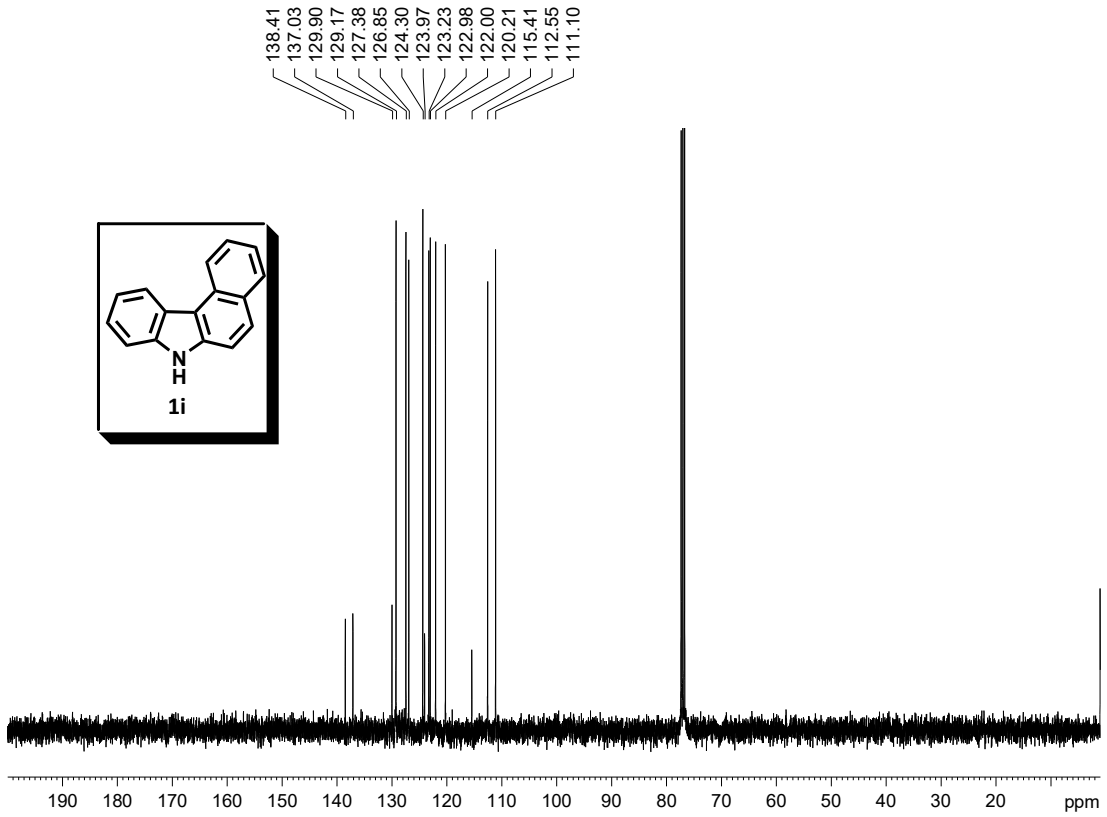
^{1}H-RMN ($CDCl_3$) 7*H*-Benzo[*c*]carbazol (1i)

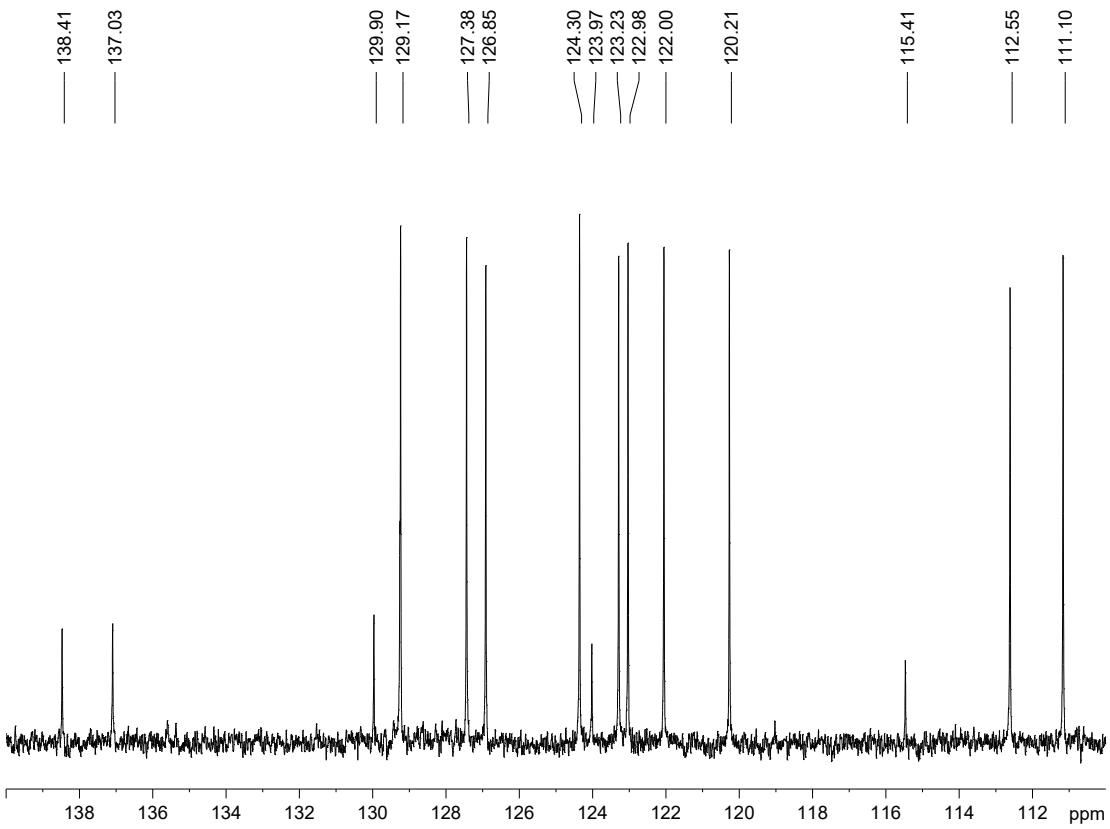


1i

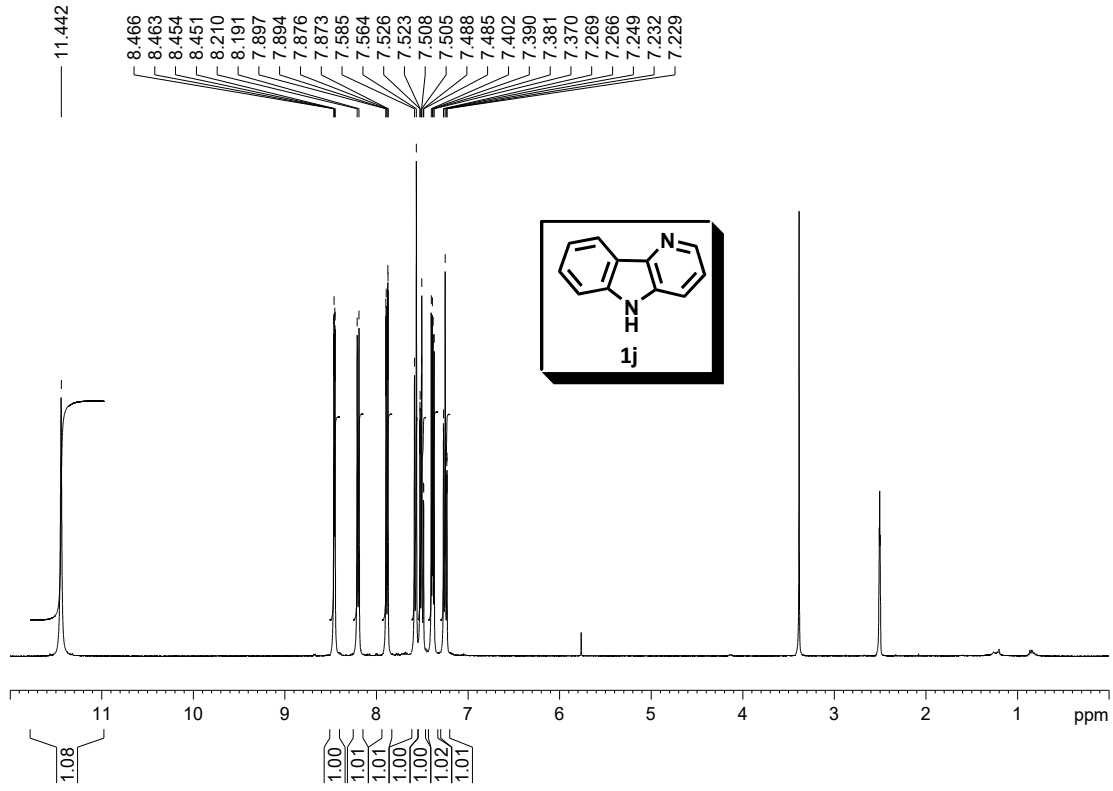


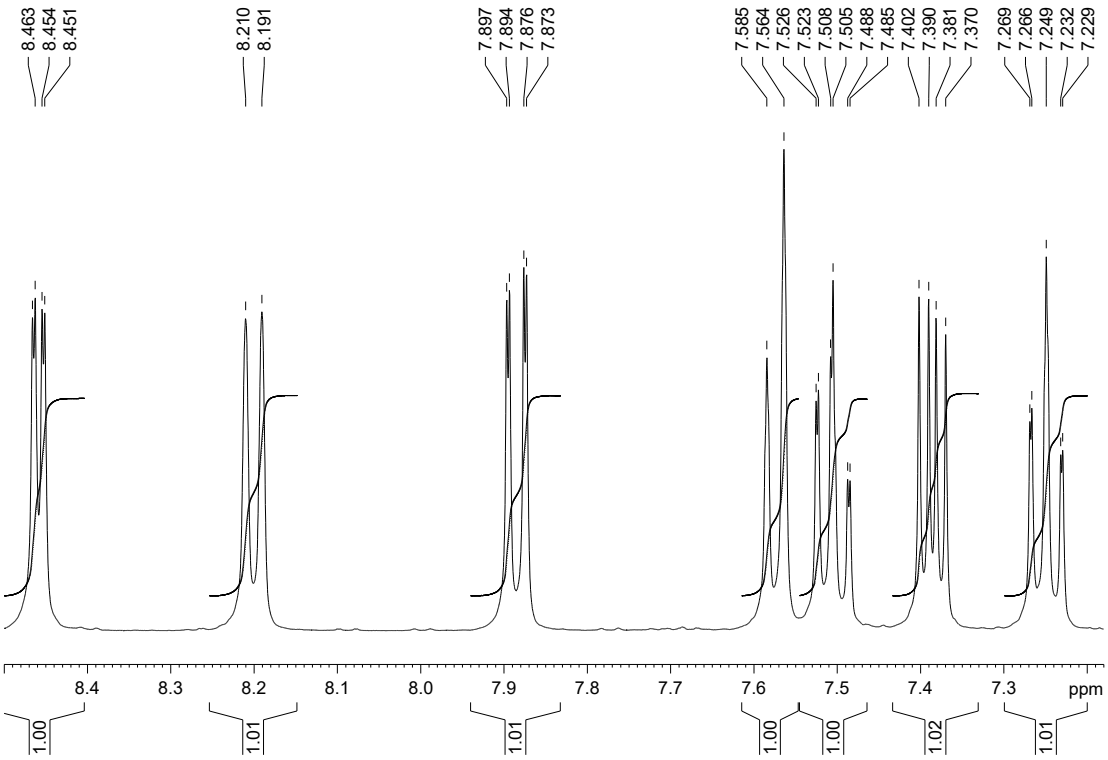
^{13}C-RMN ($CDCl_3$) 7*H*-Benzo[*c*]carbazol (1i)



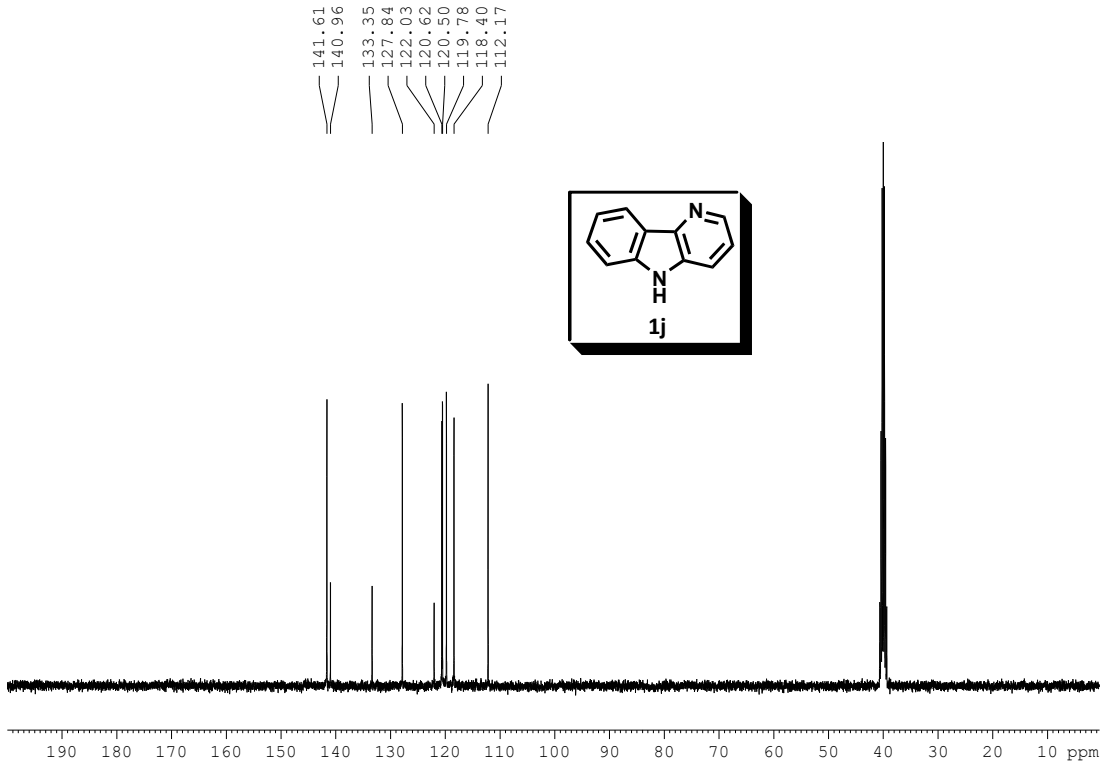


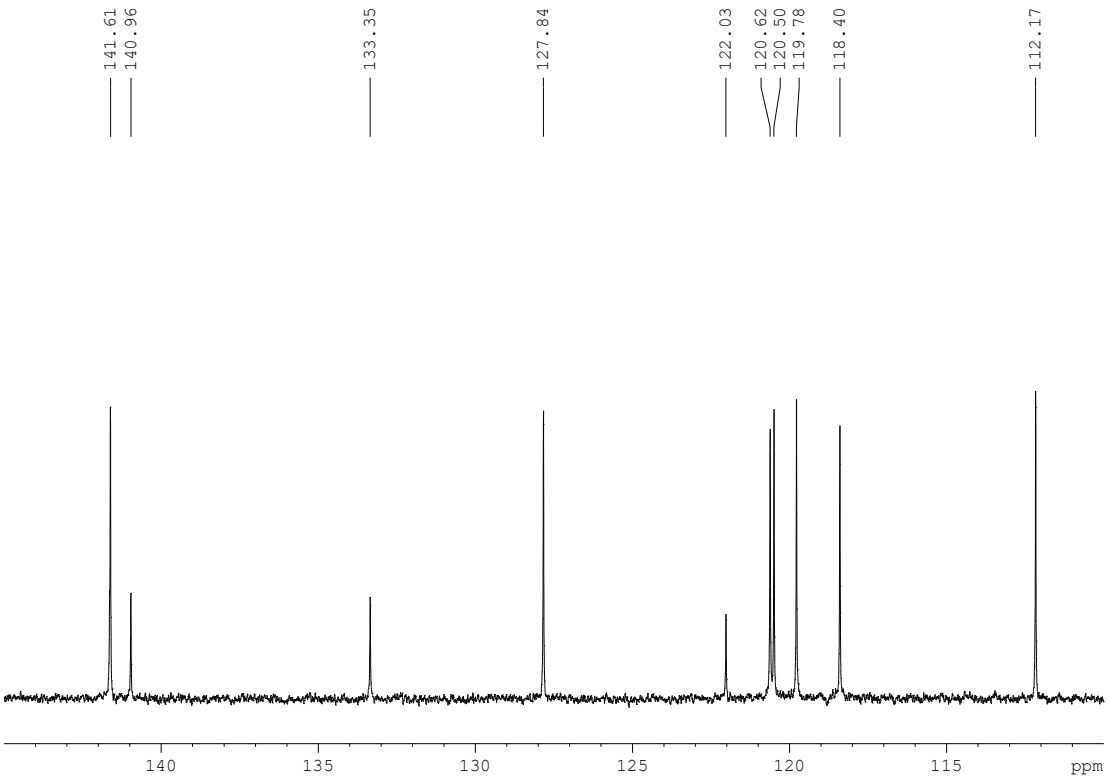
^{1}H-RMN (CD_3SOCD_3) 5*H*-Pirido[3,2-*b*]índole (1j)





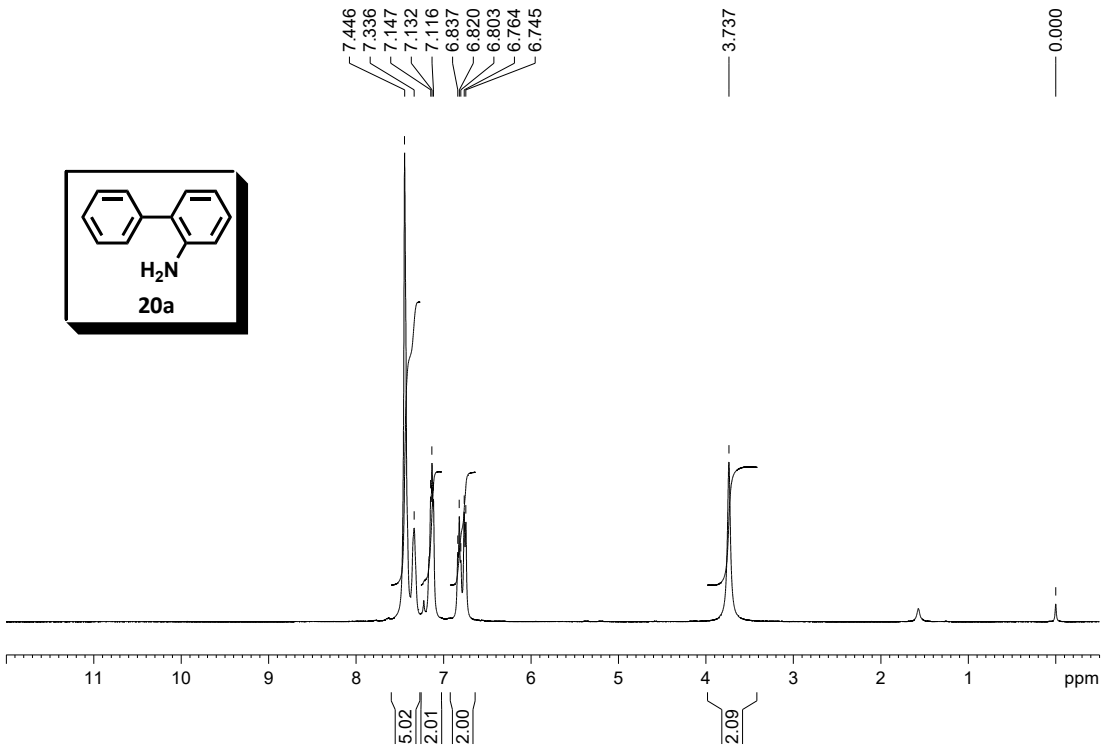
^{13}C-RMN (CD_3SOCD_3) 5*H*-Pirido[3,2-*b*]índole (1j)

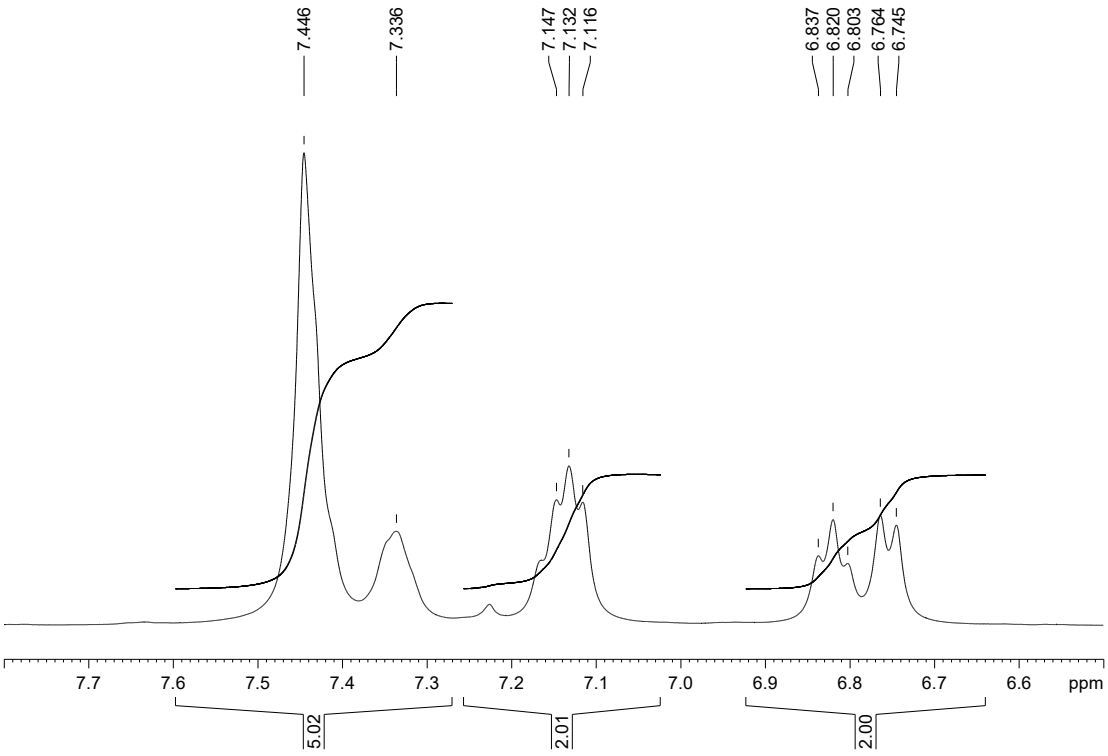




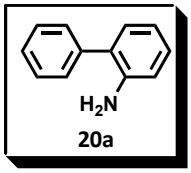
A.1.3 ESPECTROS DE RMN DE BIFENILAMINAS OBTENIDAS (PRODUCTOS DE REDUCCIÓN)

^{1}H-RMN ($CDCl_3$) [1,1'-Bifenil]-2-amina (20a)

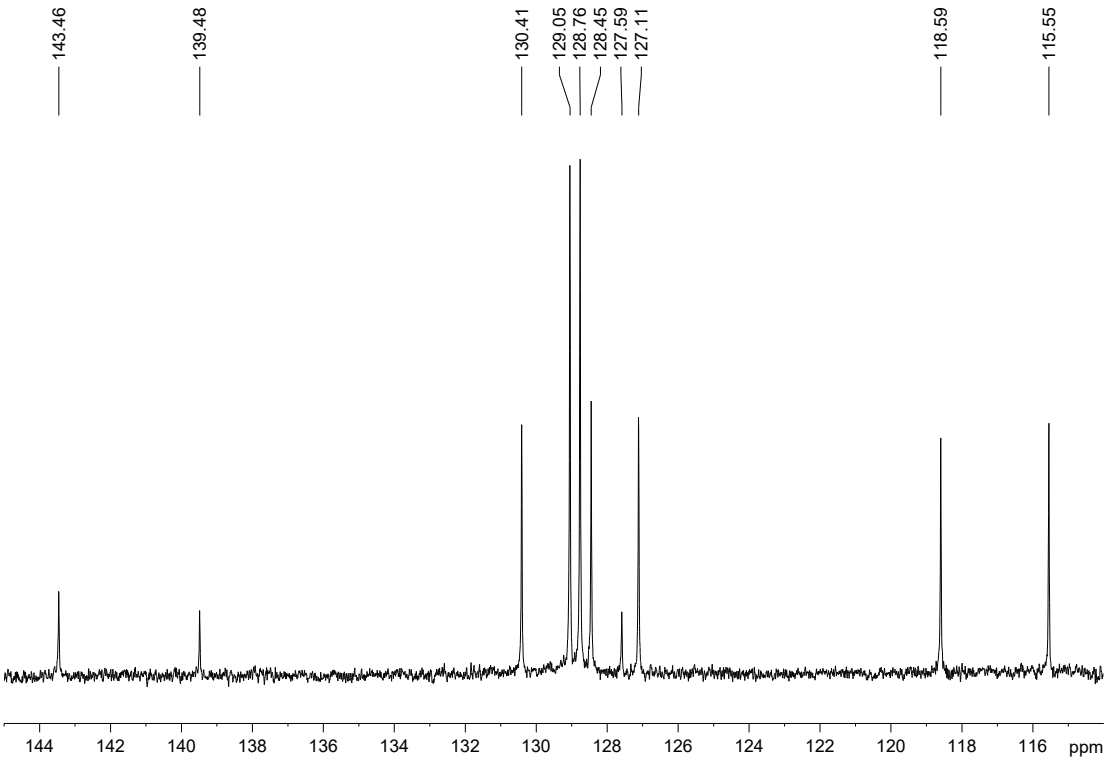

7.446
7.336
7.147
7.132
7.116
6.837
6.820
6.803
6.764
6.745
3.737
0.000
H2N
20a
11
10
9
8
7
6
5
4
3
2
1
ppm
5.02
2.01
2.00
2.09


7.446
7.336
7.147
7.132
7.116
6.837
6.820
6.803
6.764
6.745
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
ppm
5.02
2.01
2.00

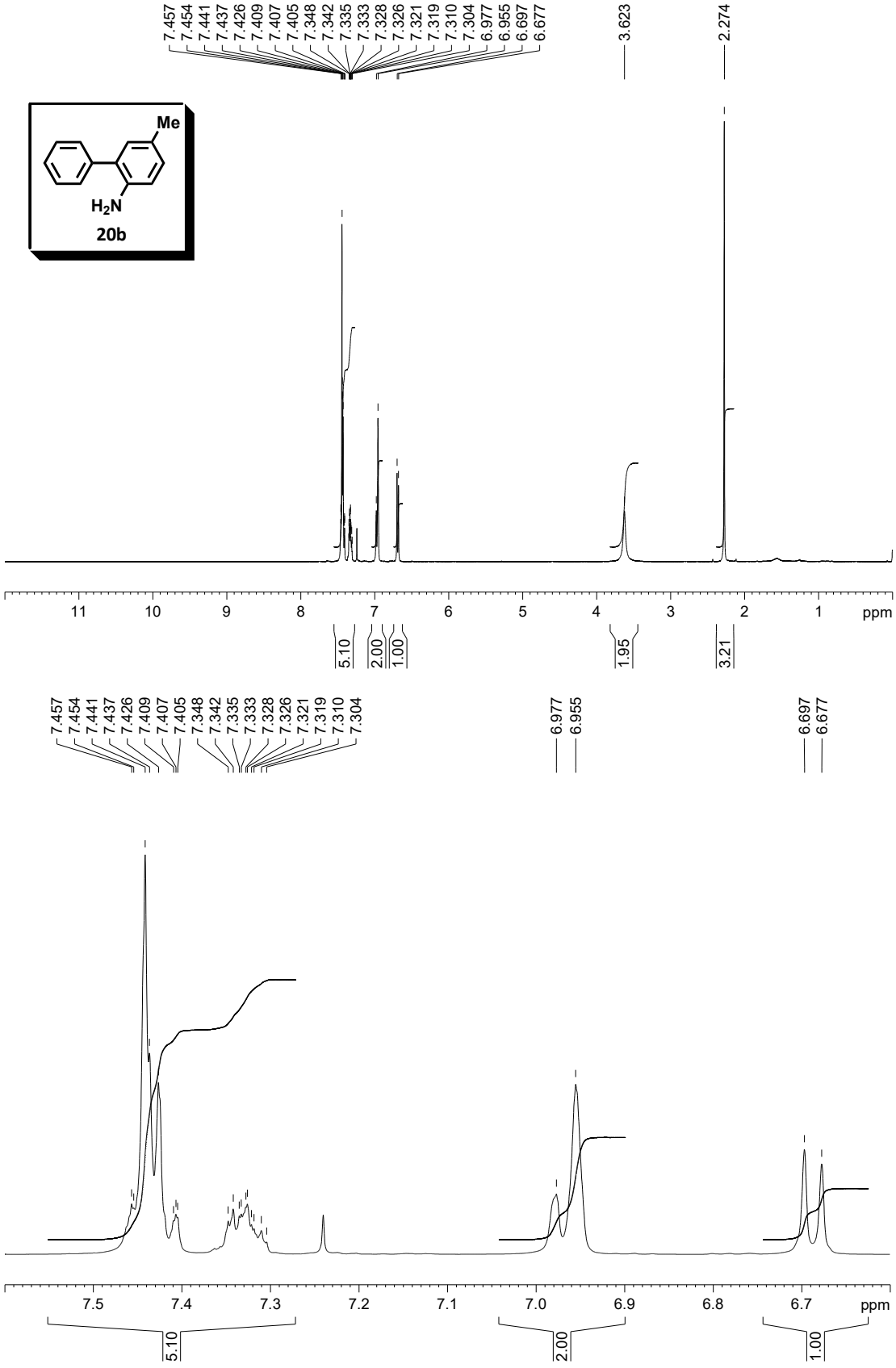
^{13}C-RMN ($CDCl_3$) [1,1'-Bifenil]-2-amina (20a)



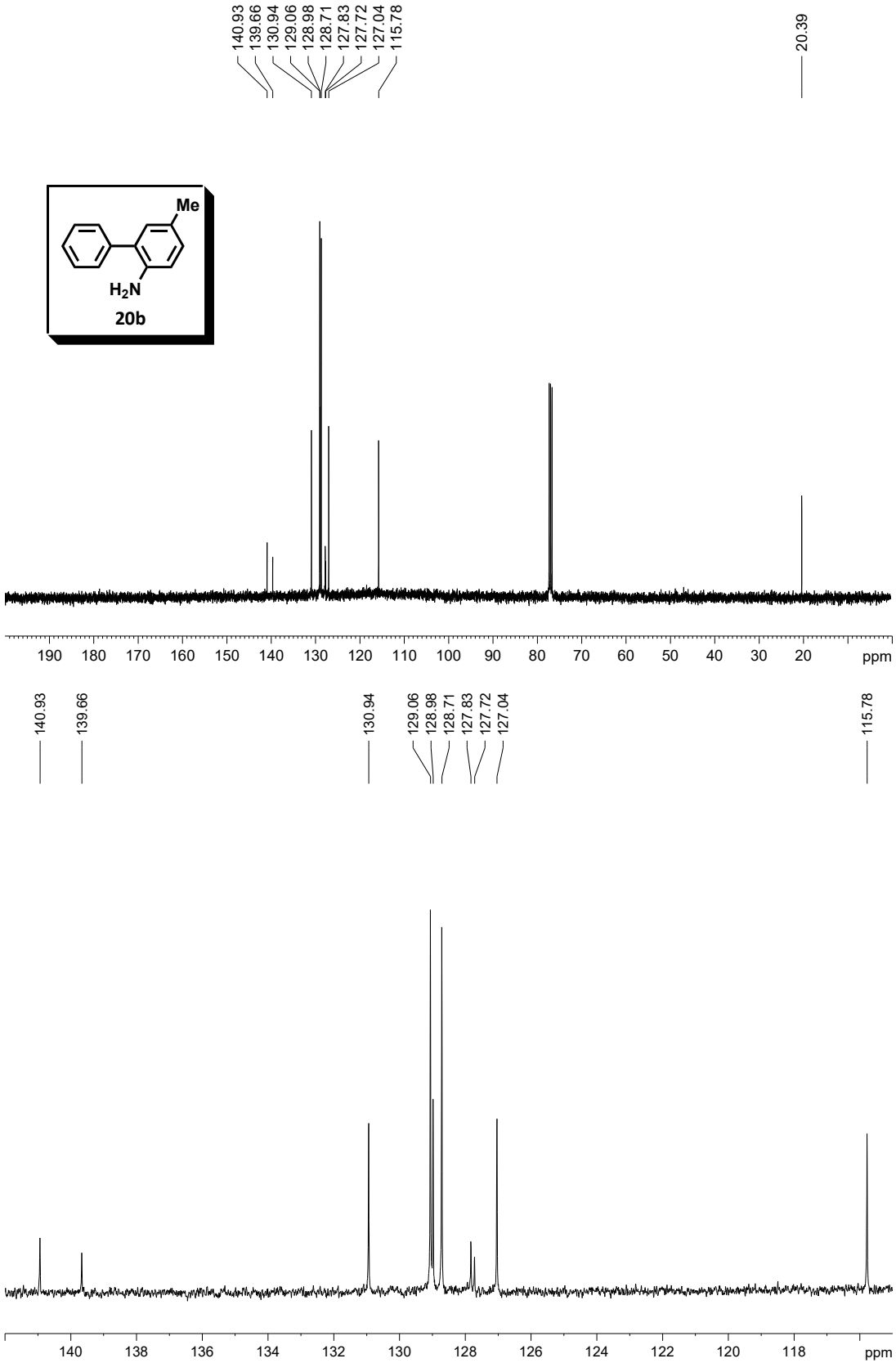
20a



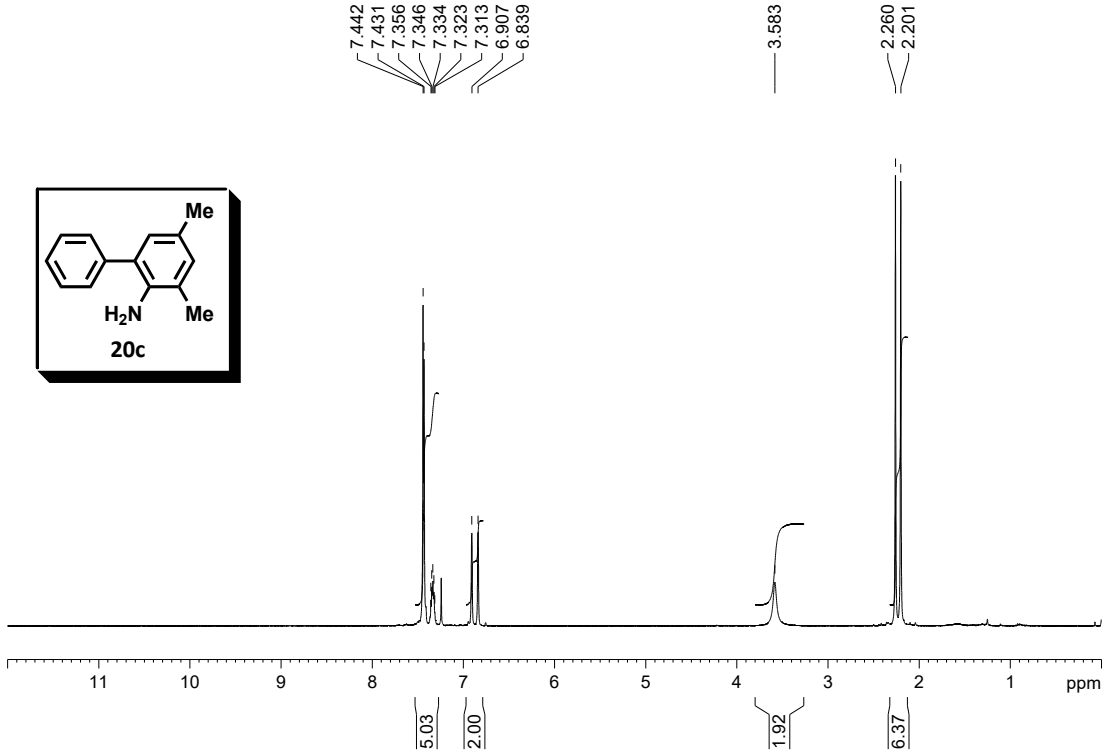
^{1}H-RMN ($CDCl_3$) 5-Metil-[1,1'-bifenil]-2-amina (20b)

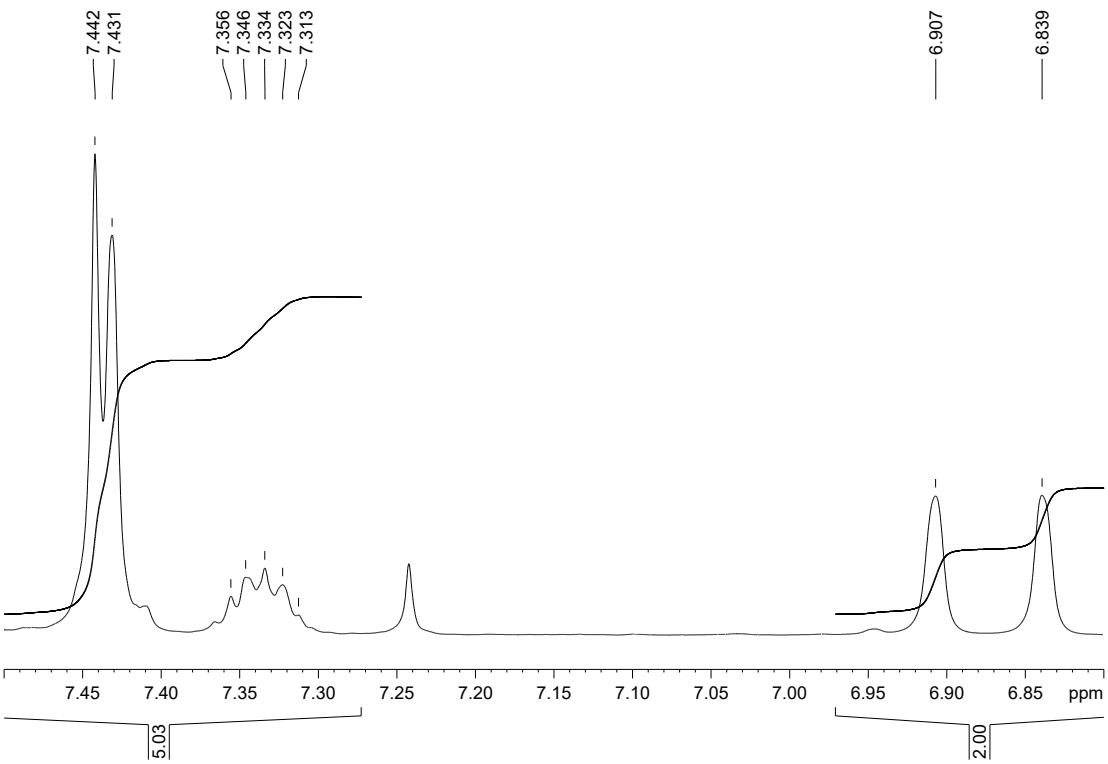


^{13}C-RMN ($CDCl_3$) 5-Metil-[1,1'-bifenil]-2-amina (20b)

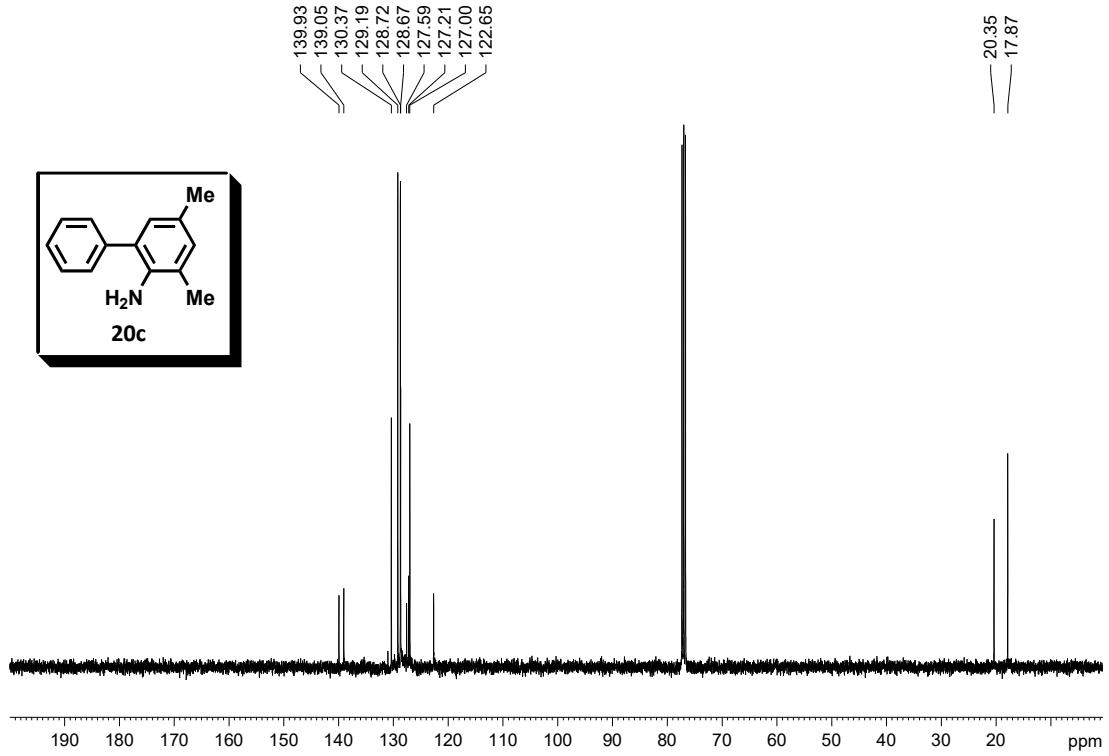


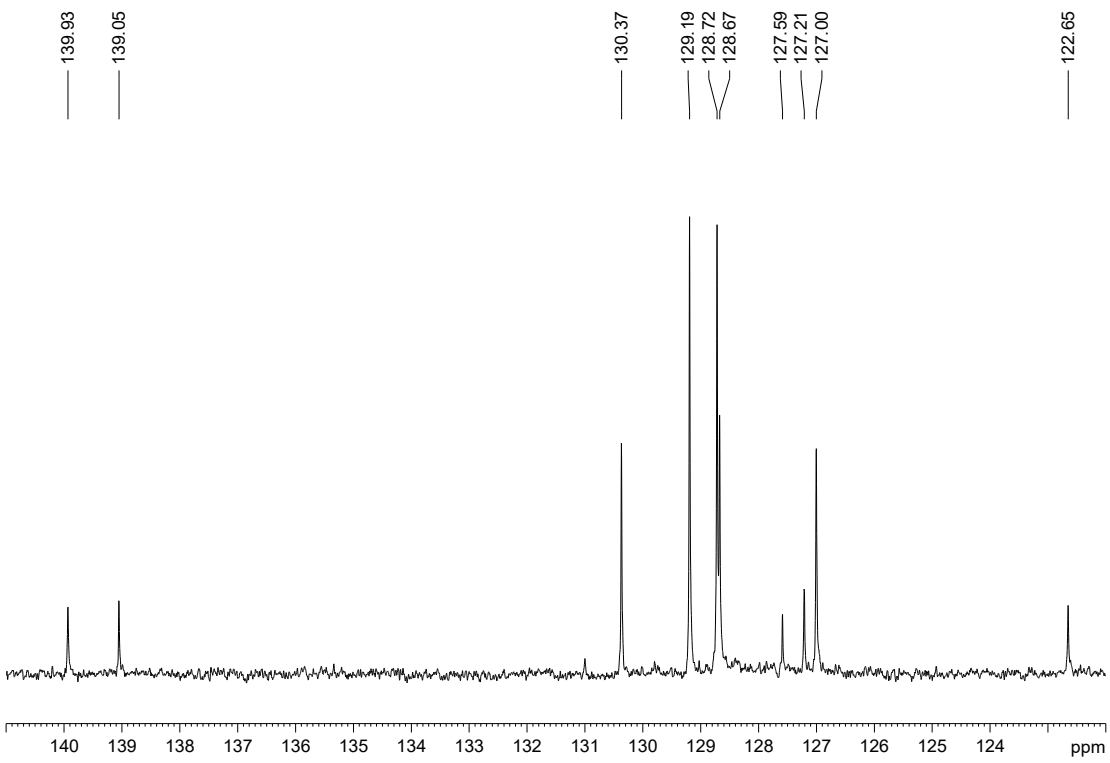
^{1}H-RMN ($CDCl_3$) 3,5-Dimetil-[1,1'-bifenil]-2-amina (20c)



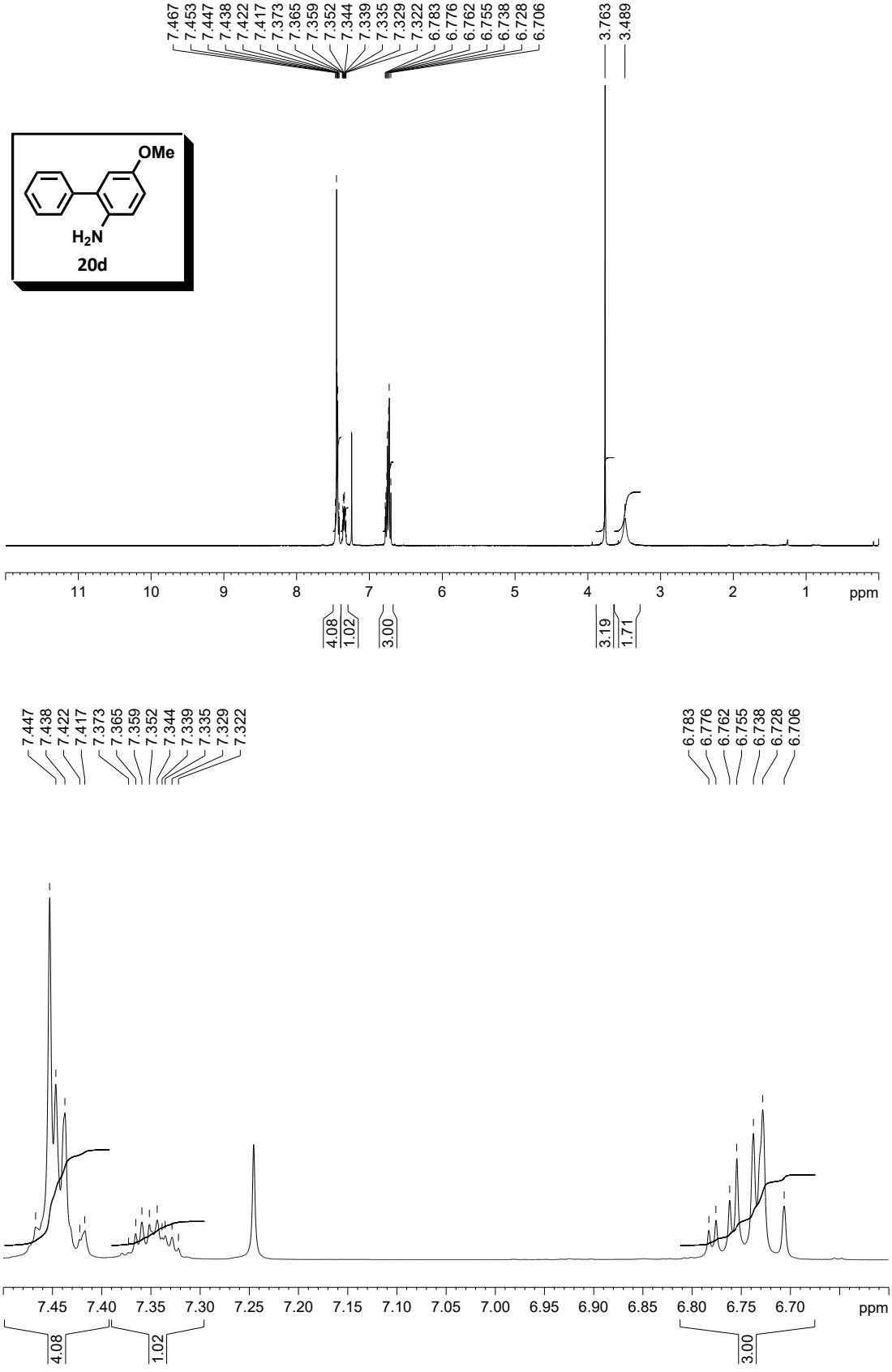


^{13}C-RMN ($CDCl_3$) 3,5-Dimetil-[1,1'-bifenil]-2-amina (20c)

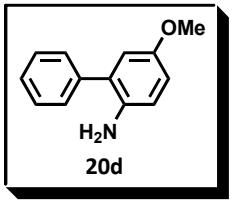


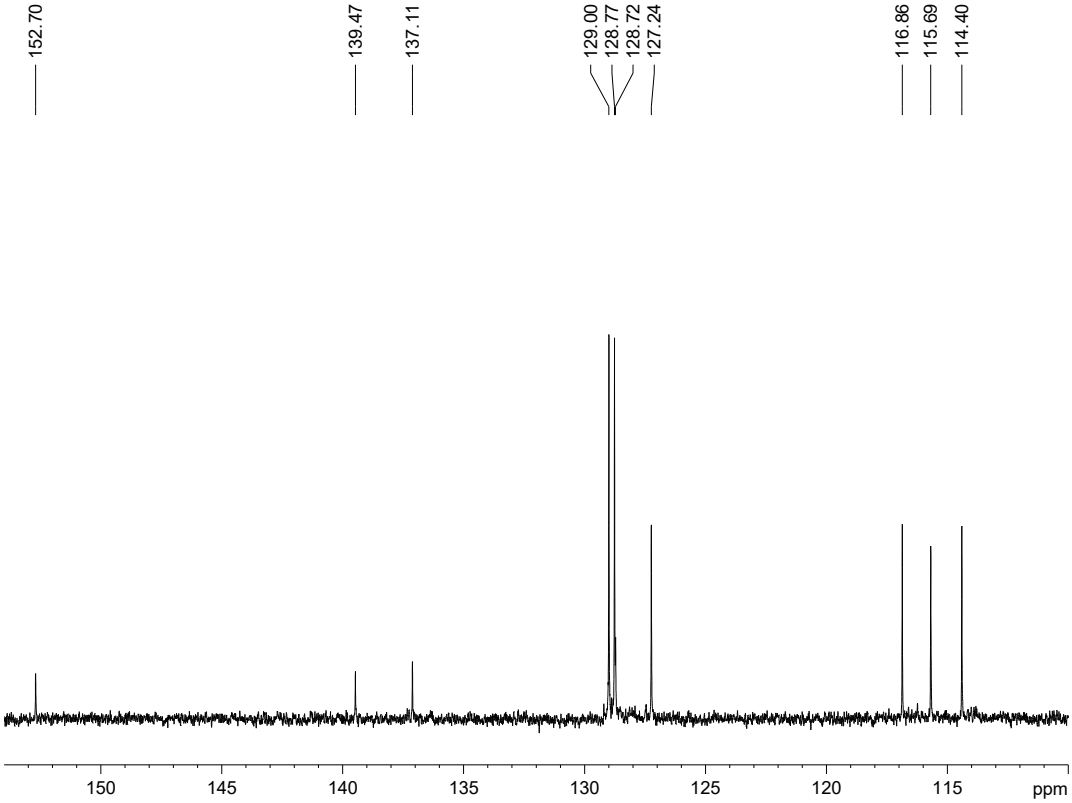


^{1}H-RMN ($CDCl_3$) 5-Metoxi-[1,1'-bifenil]-2-amina (20d)

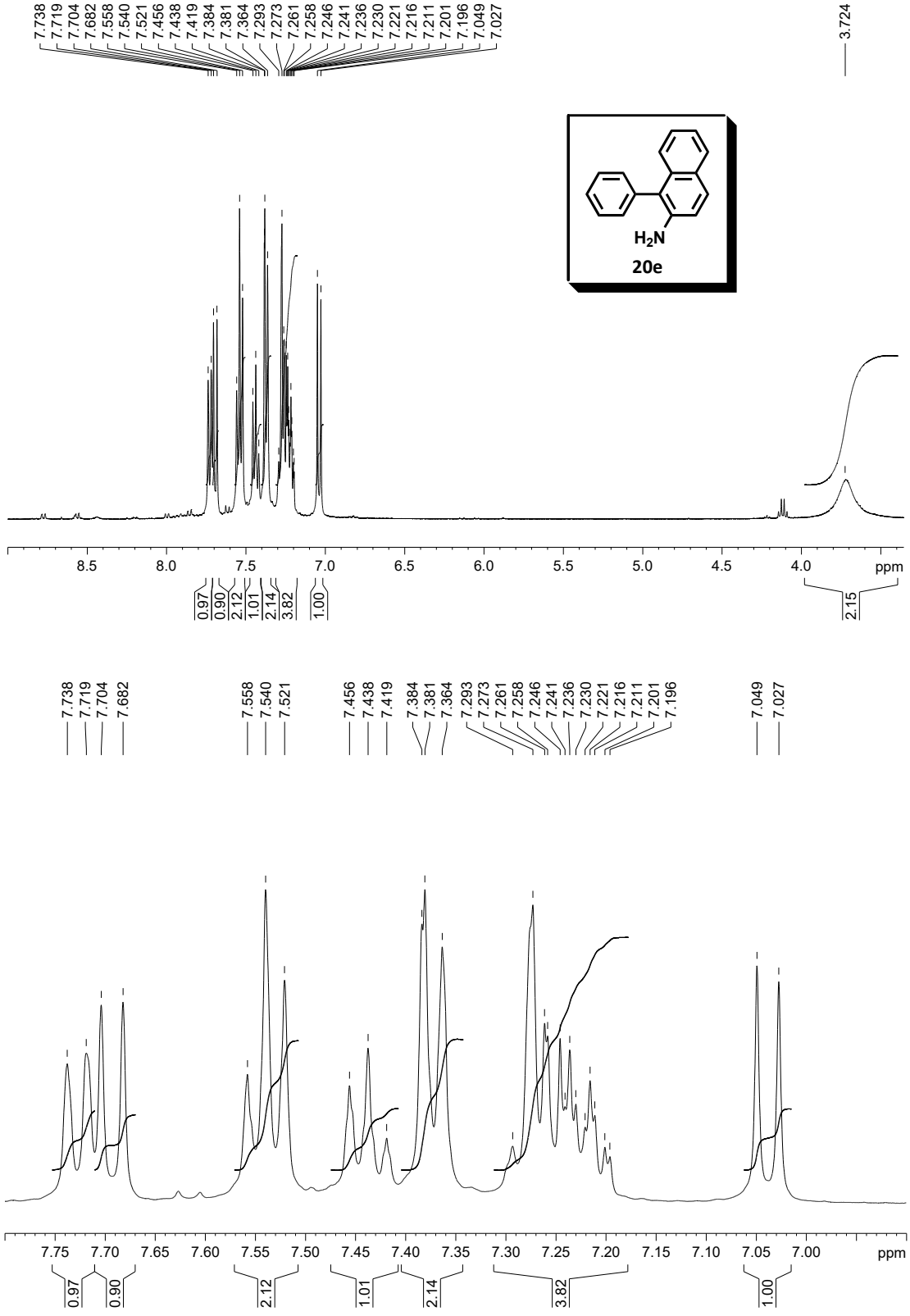


^{13}C-RMN ($CDCl_3$) 5-Metoxi-[1,1'-bifenil]-2-amina (20d)



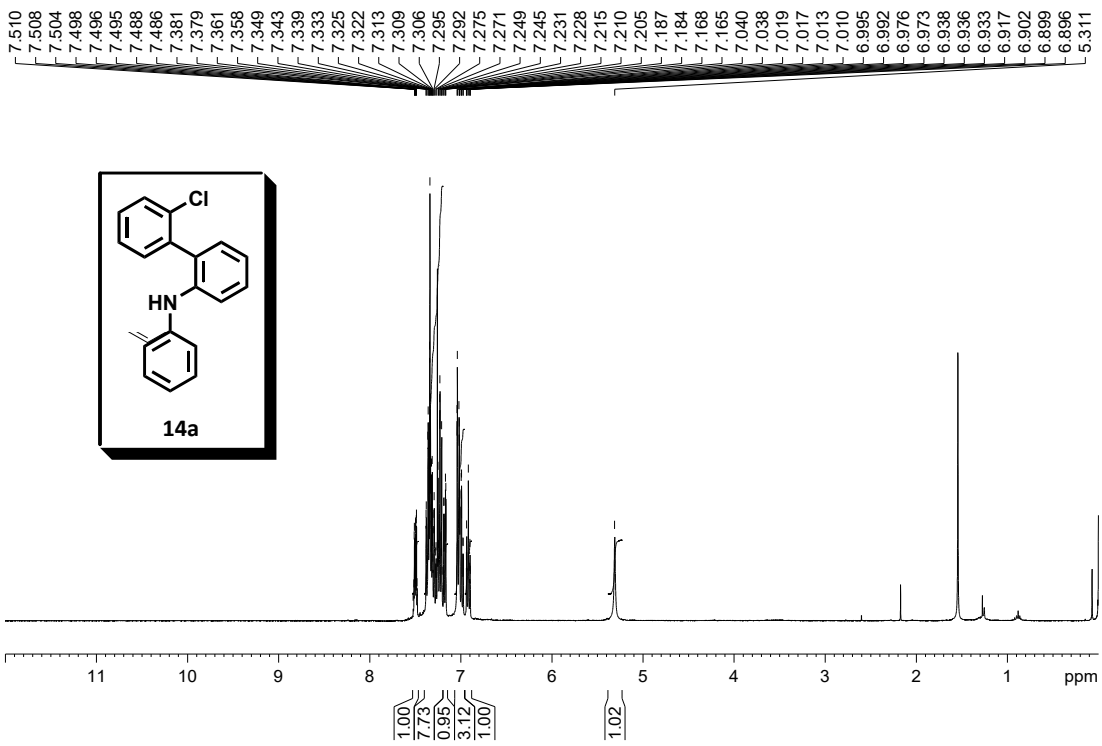


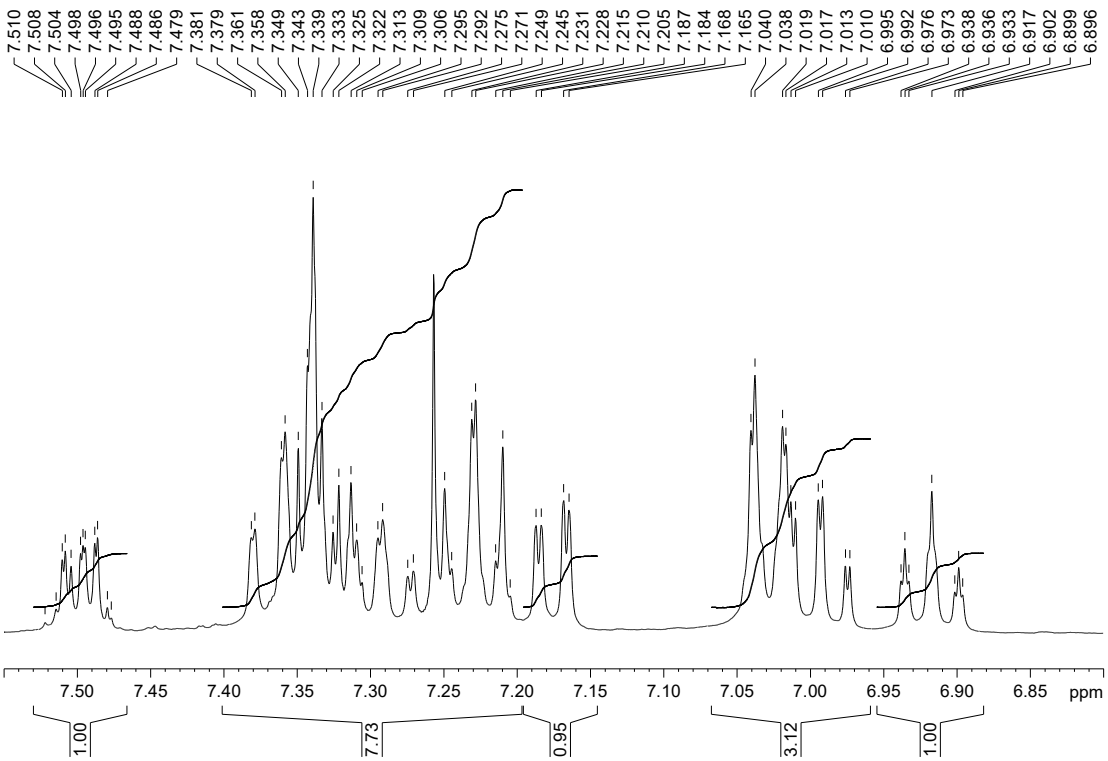
^{1}H-RMN ($CDCl_3$) 1-Fenilnaftalen-2-amina (20e)



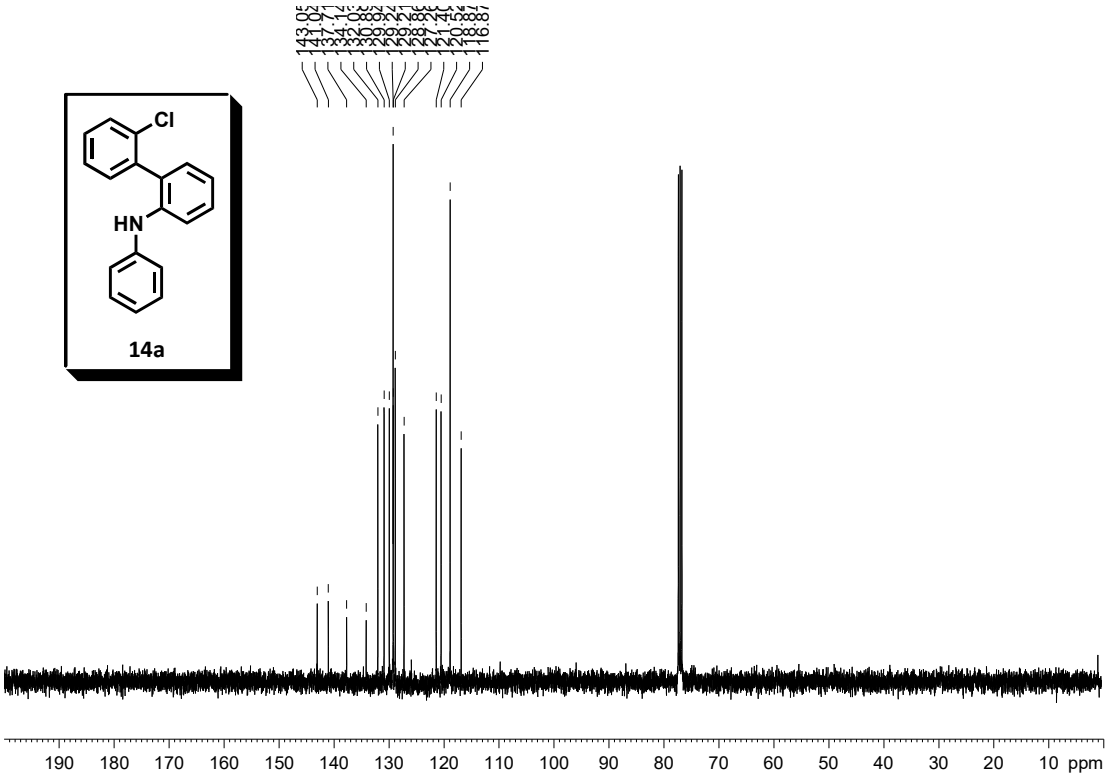
A.1.4 ESPECTROS DE RMN DE N-FENIL 2-HALO-BIFENIL-2-AMINAS OBTENIDAS

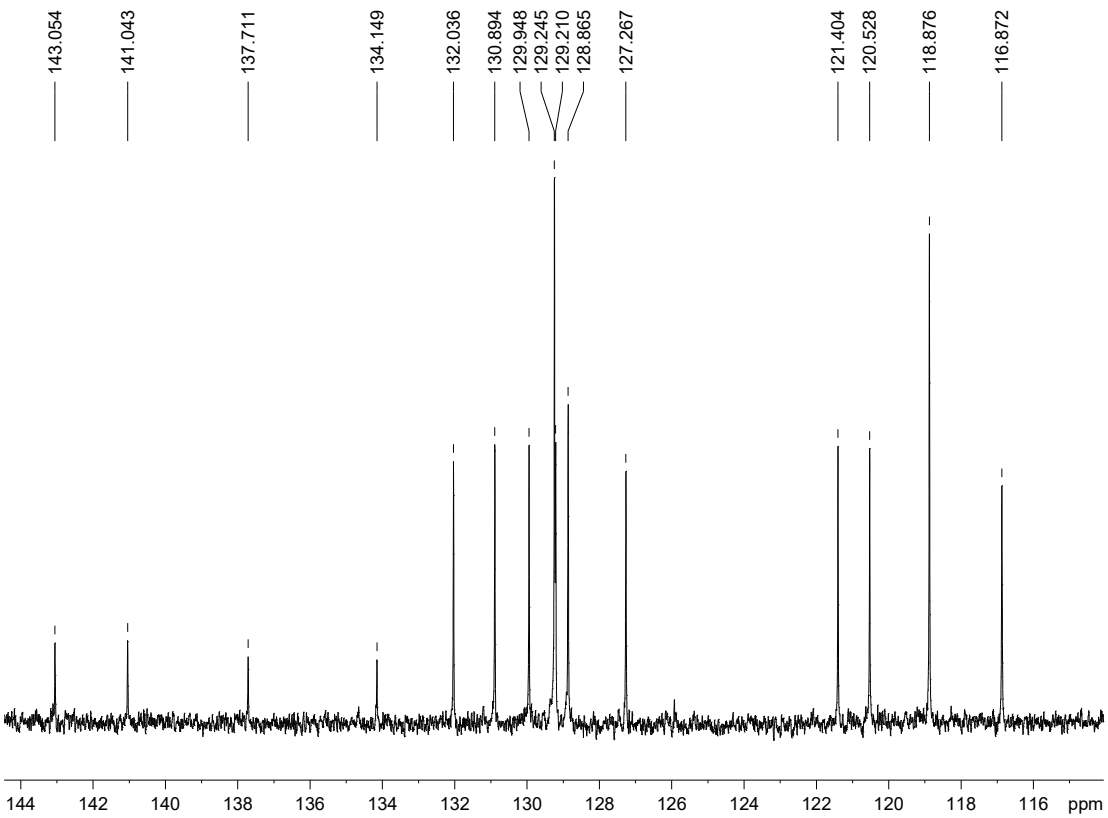
^{1}H-RMN ($CDCl_3$) *N*-fenil-2'-cloro-[1,1'-bifenil]-2-amina (14a)



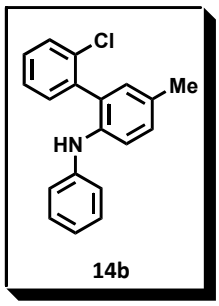


^{13}C-RMN ($CDCl_3$) *N*-fenil-2'-cloro-[1,1'-bifenil]-2-amina (14a)

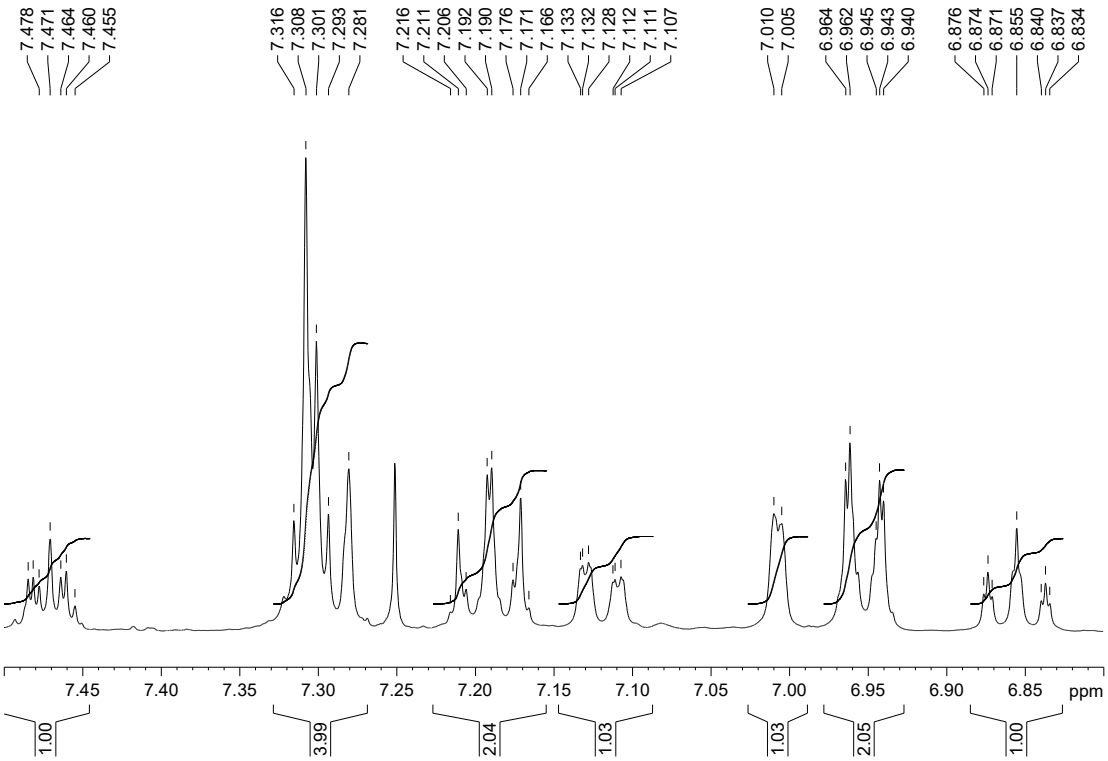




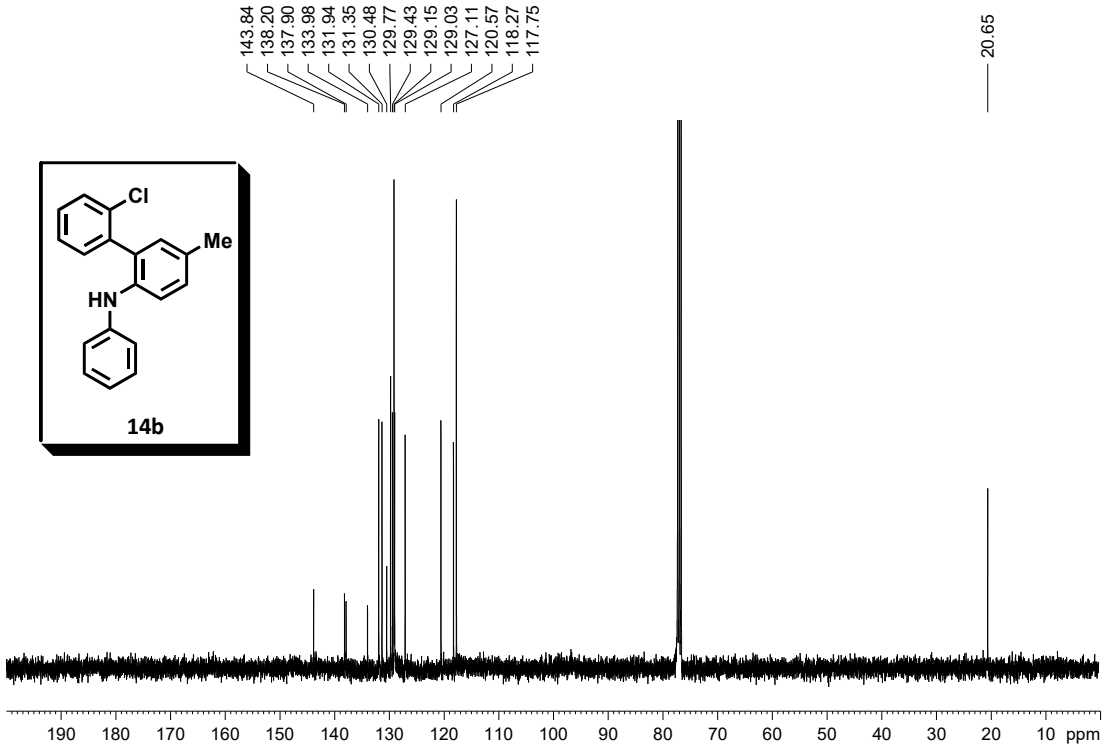
^{1}H-RMN ($CDCl_3$) *N*-fenil-2'-cloro-5-metil-[1,1'-bifenil]-2-amina (14b)

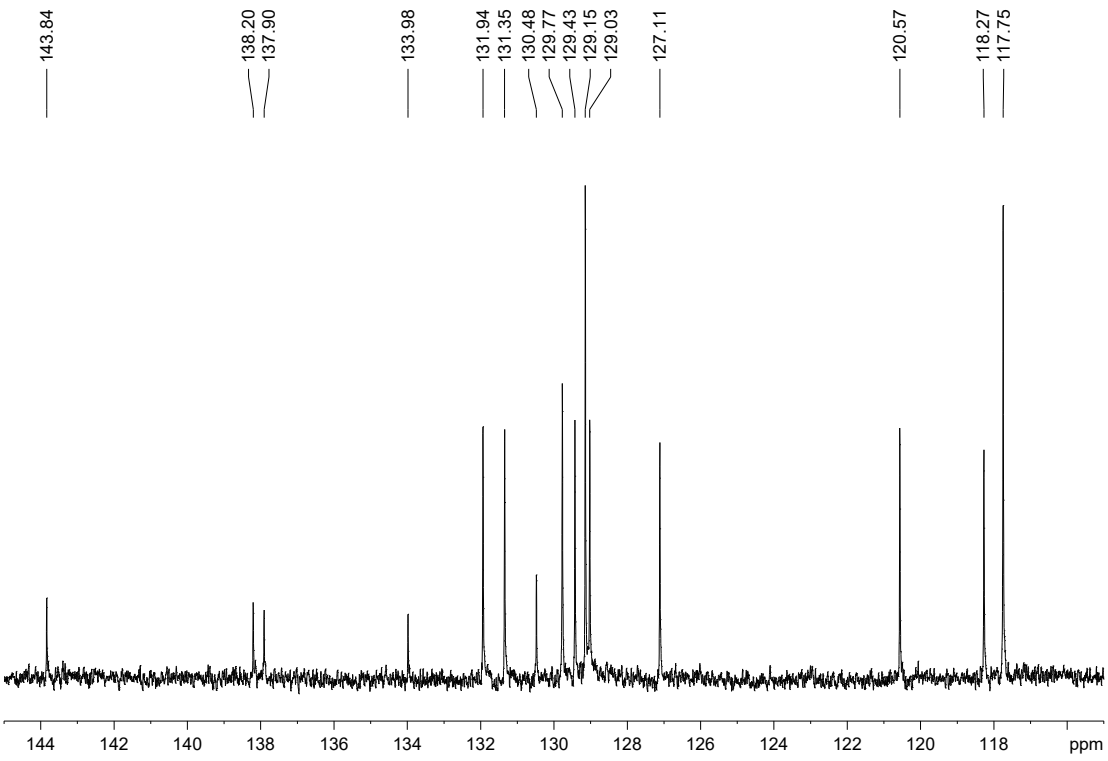


14b

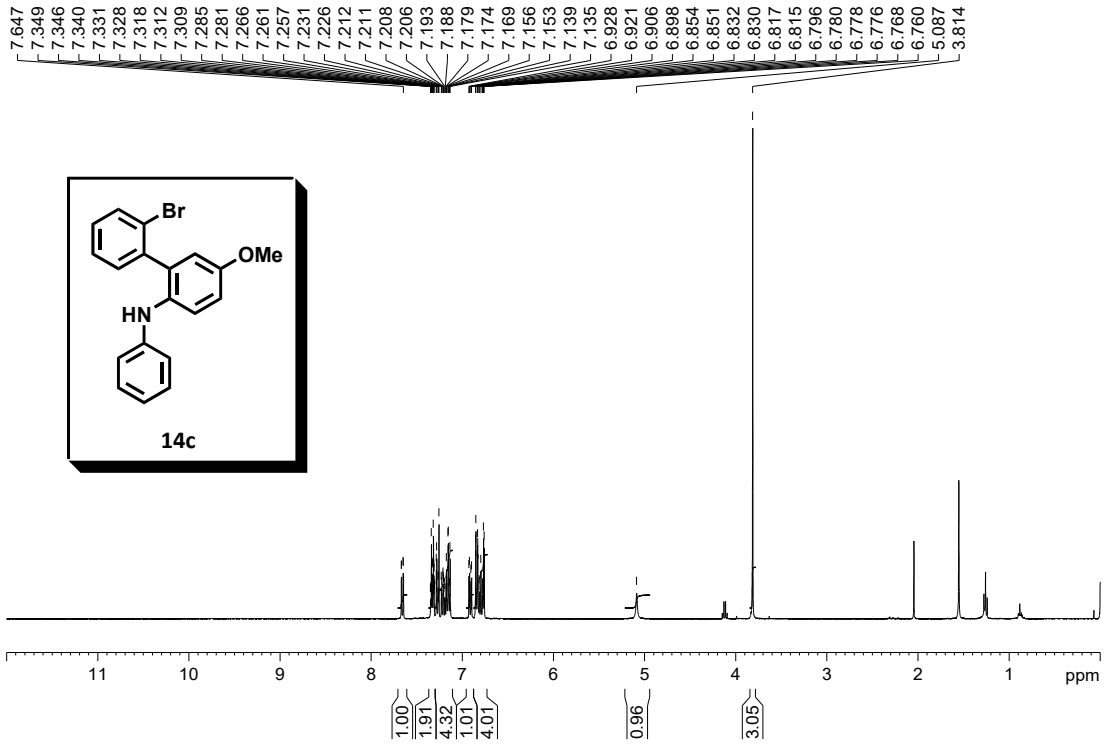


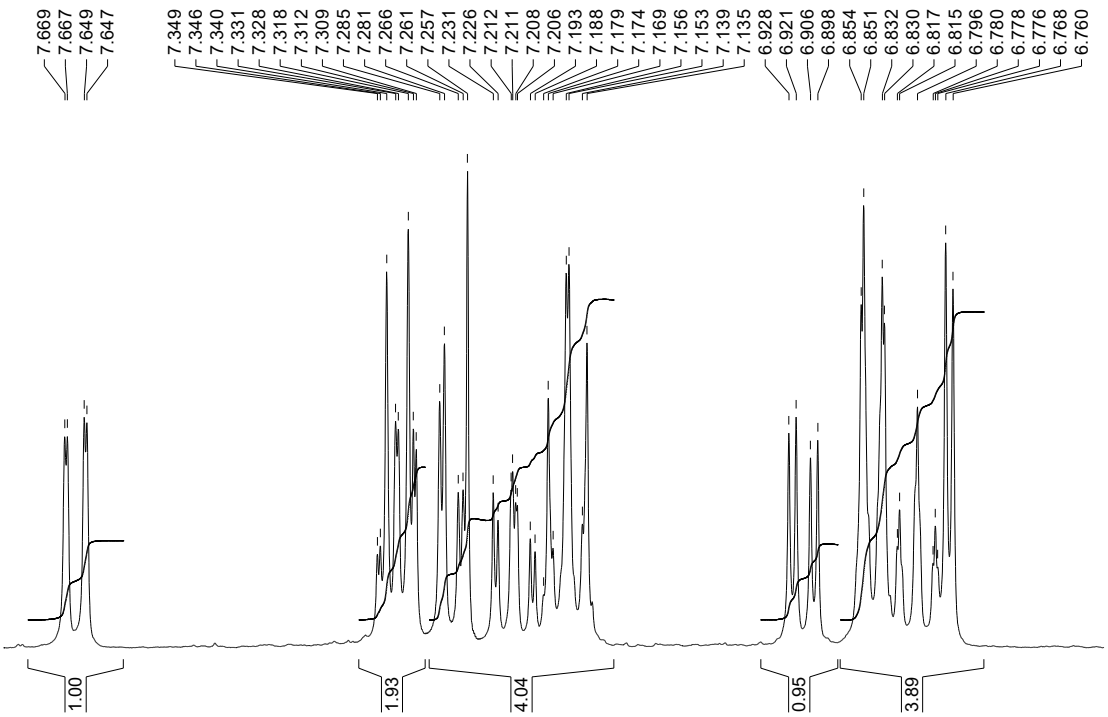
^{13}C-RMN ($CDCl_3$) *N*-fenil-2'-cloro-5-metil-[1,1'-bifenil]-2-amina (14b)



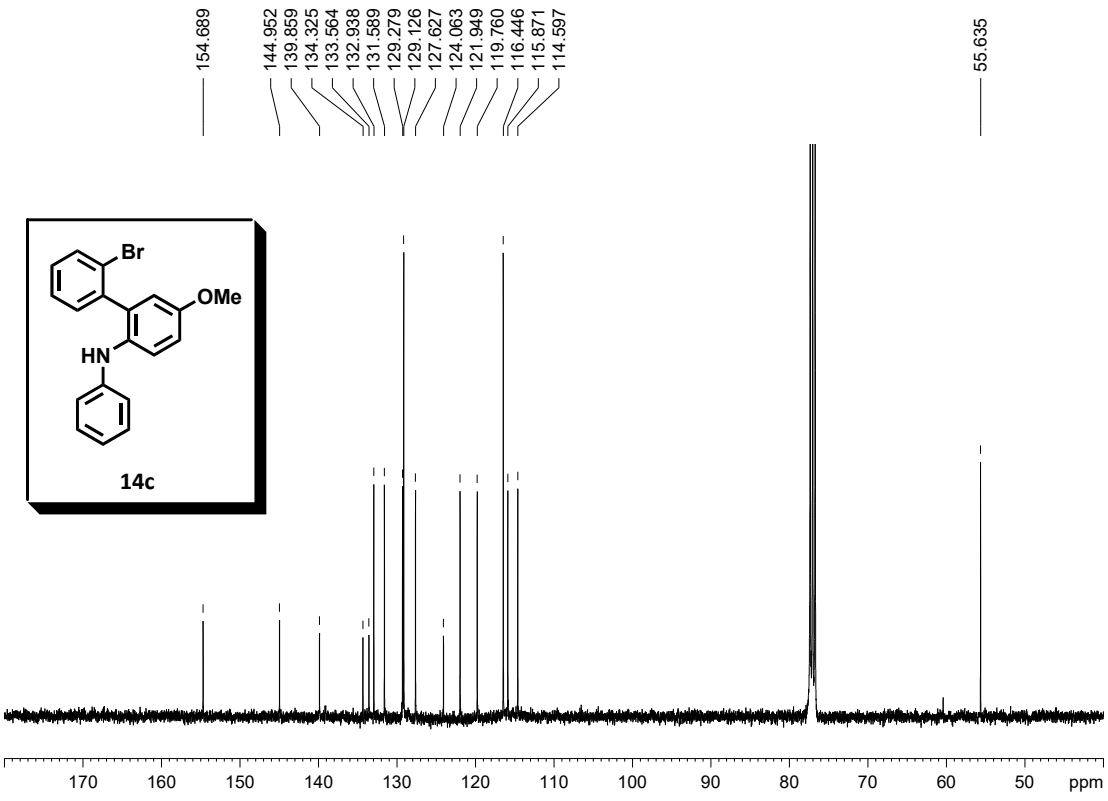


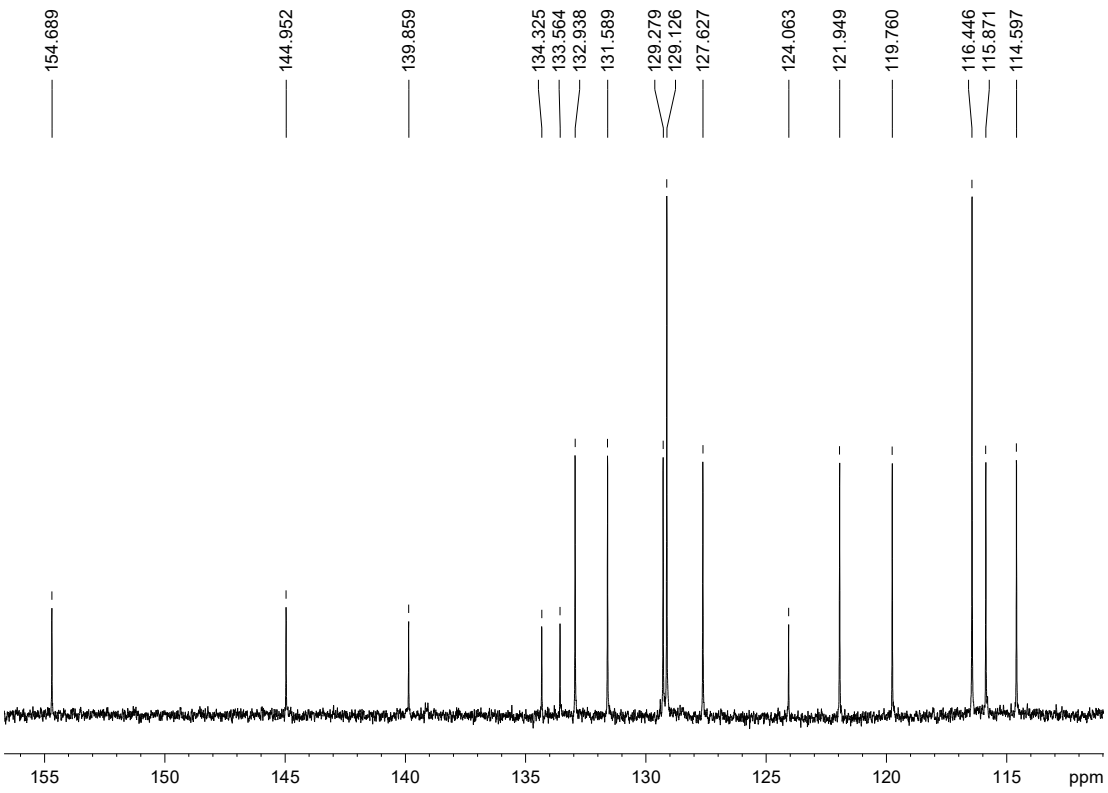
^{1}H-RMN ($CDCl_3$) *N*-fenil-2'-bromo-5-metoxi-[1,1'-bifenil]-2-amina (14c)



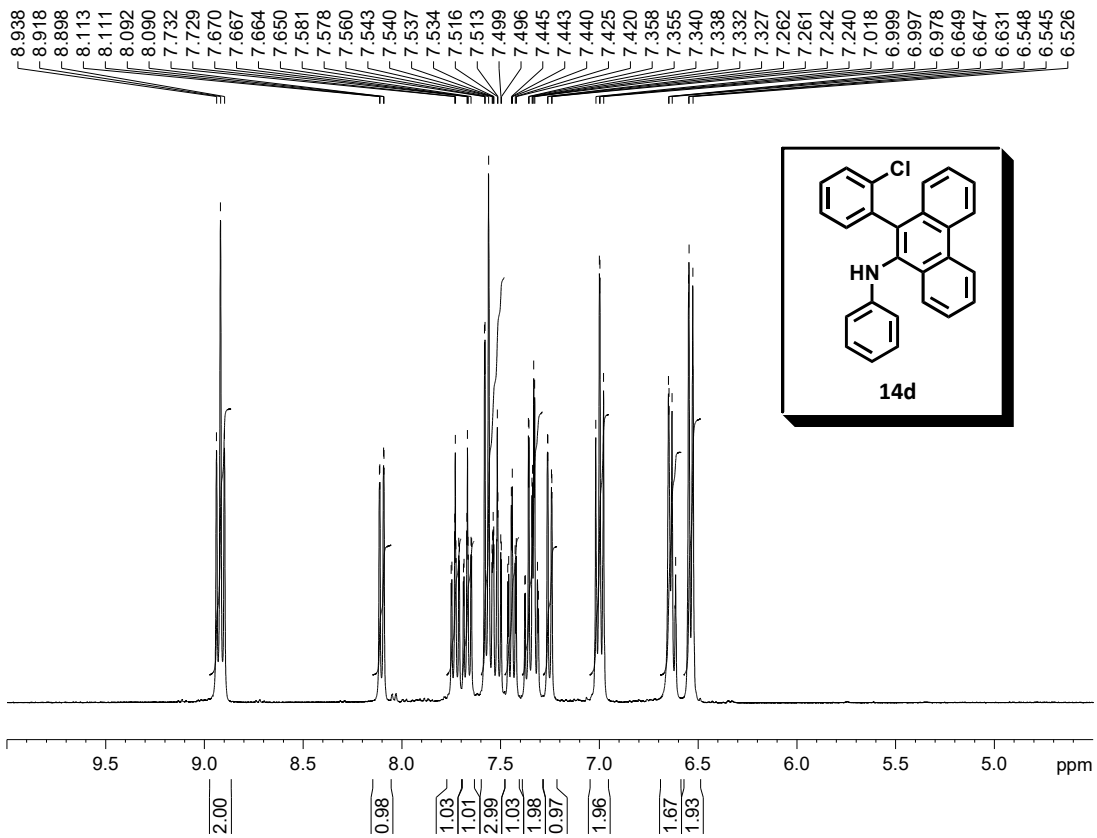


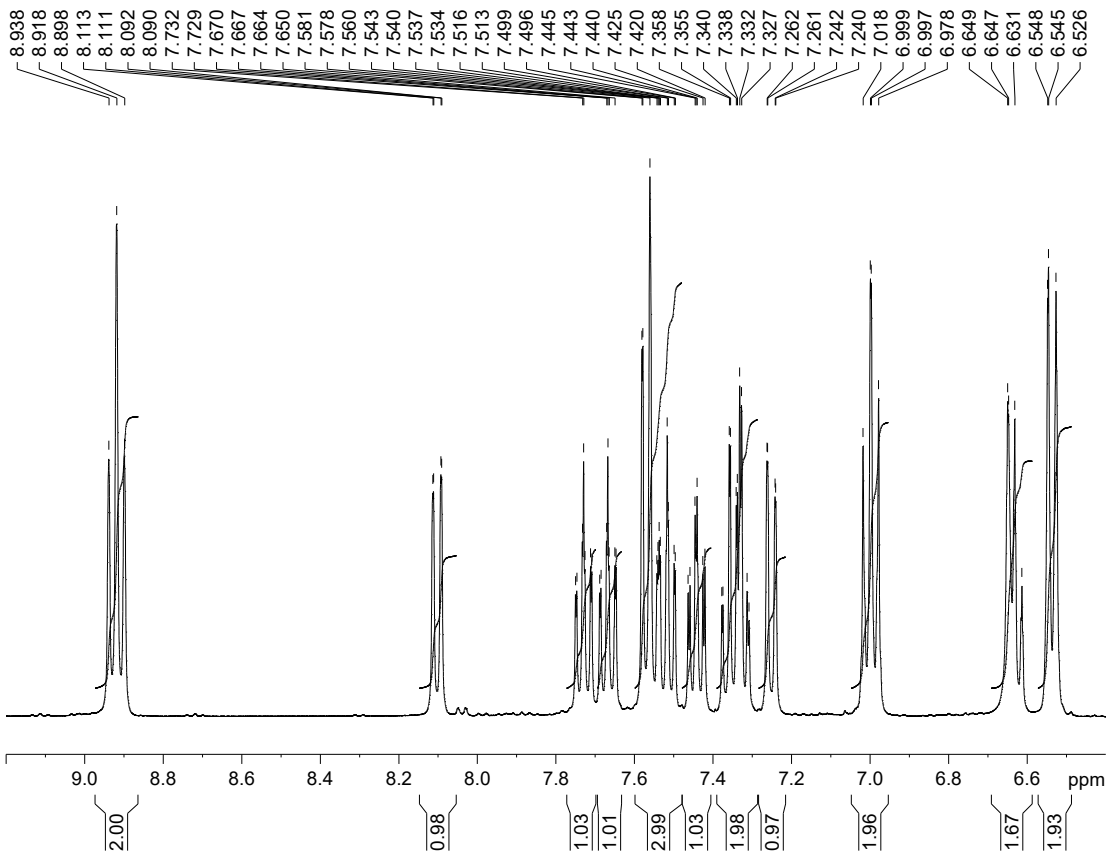
^{13}C-RMN ($CDCl_3$) *N*-fenil-2'-bromo-5-metoxi-[1,1'-bifenil]-2-amina (14c)





^{1}H-RMN (CD_3COCD_3) 10-(2-Clorofenil)-*N*-fenilfenantren-9-amina (14d)

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8.918
8.898
8.113
8.111
8.092
8.090
7.732
7.729
7.670
7.667
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7.650
7.581
7.578
7.560
7.543
7.540
7.537
7.534
7.516
7.513
7.499
7.496
7.445
7.443
7.440
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7.420
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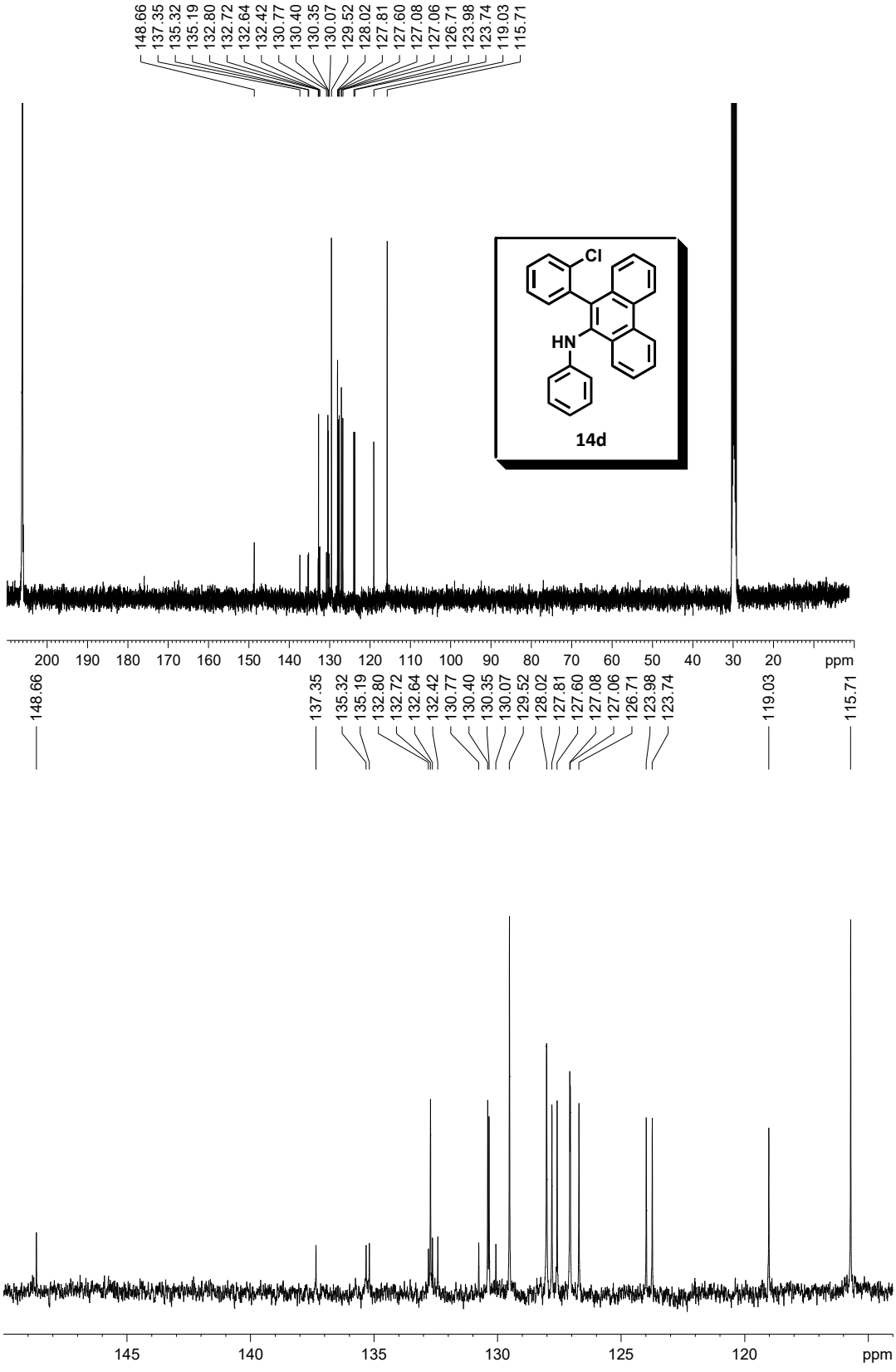
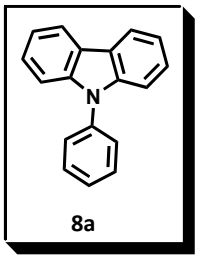
7.327
7.262
7.261
7.242
7.240
7.018
6.999
6.997
6.978
6.649
6.647
6.631
6.548
6.545
6.526
9.0
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
ppm
2.00
0.98
1.03
1.01
2.99
1.03
1.98
0.97
1.96
1.67
1.93

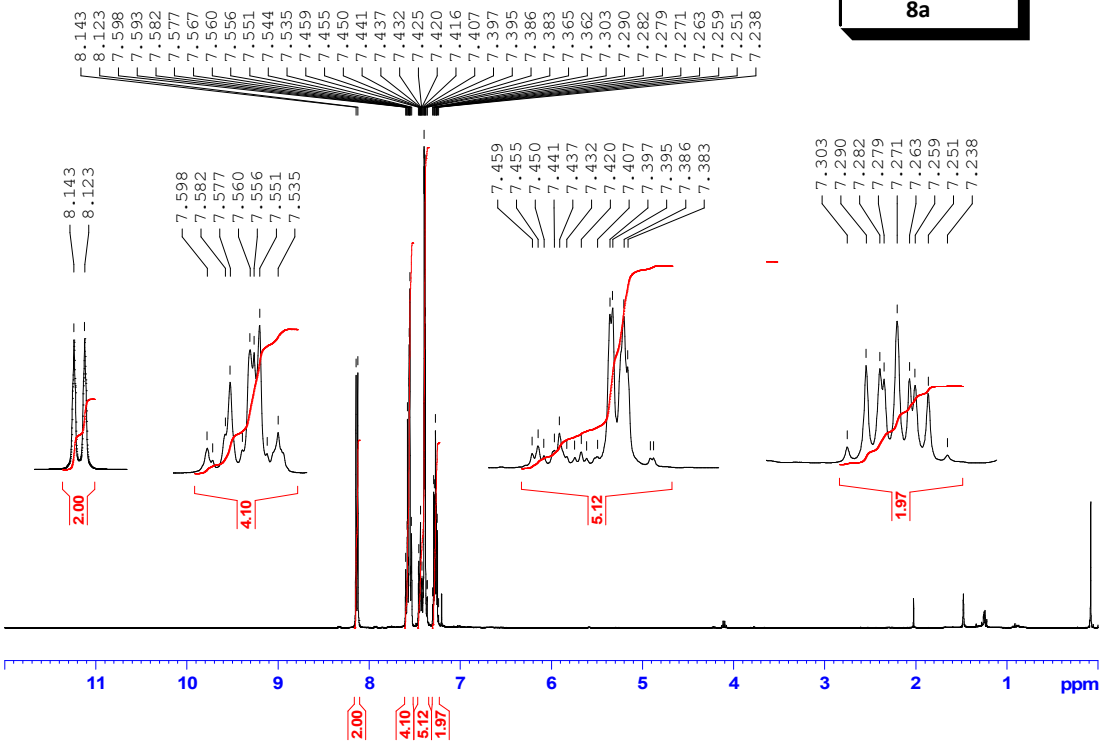
^{13}C-RMN (CD_3COCD_3) 10-(2-Clorofenil)-*N*-fenilfenantren-9-amina (14d)



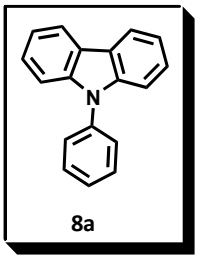
A.1.5 ESPECTROS DE RMN DE 9-FENIL-9*H*-CARBAZOLES OBTENIDOS

^{1}H-RMN ($CDCl_3$) 9-Fenil-9*H*-carbazol (8a)

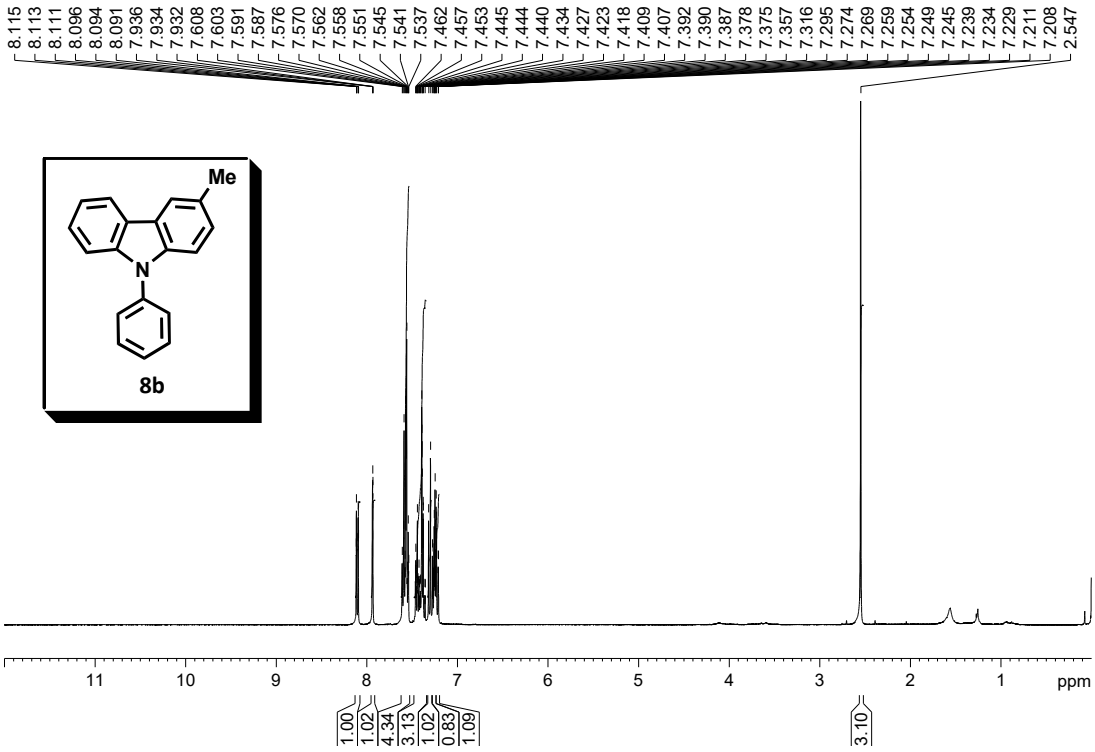


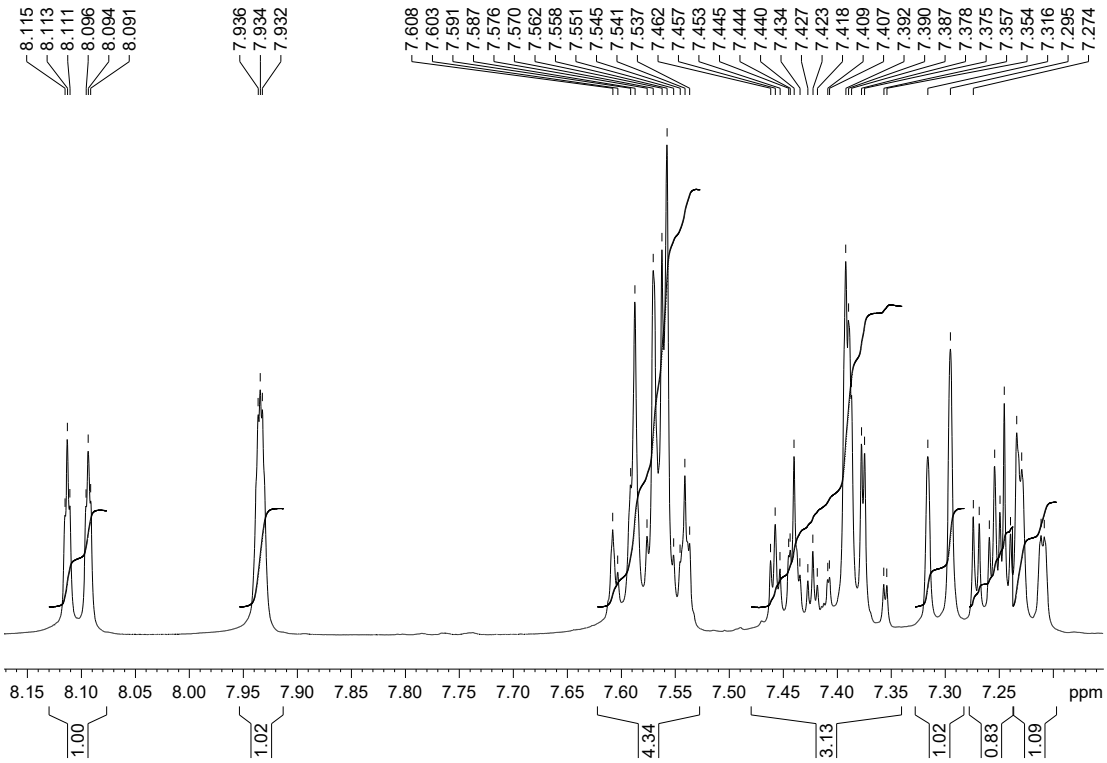


^{13}C-RMN ($CDCl_3$) 9-Fenil-9*H*-carbazol (8a)

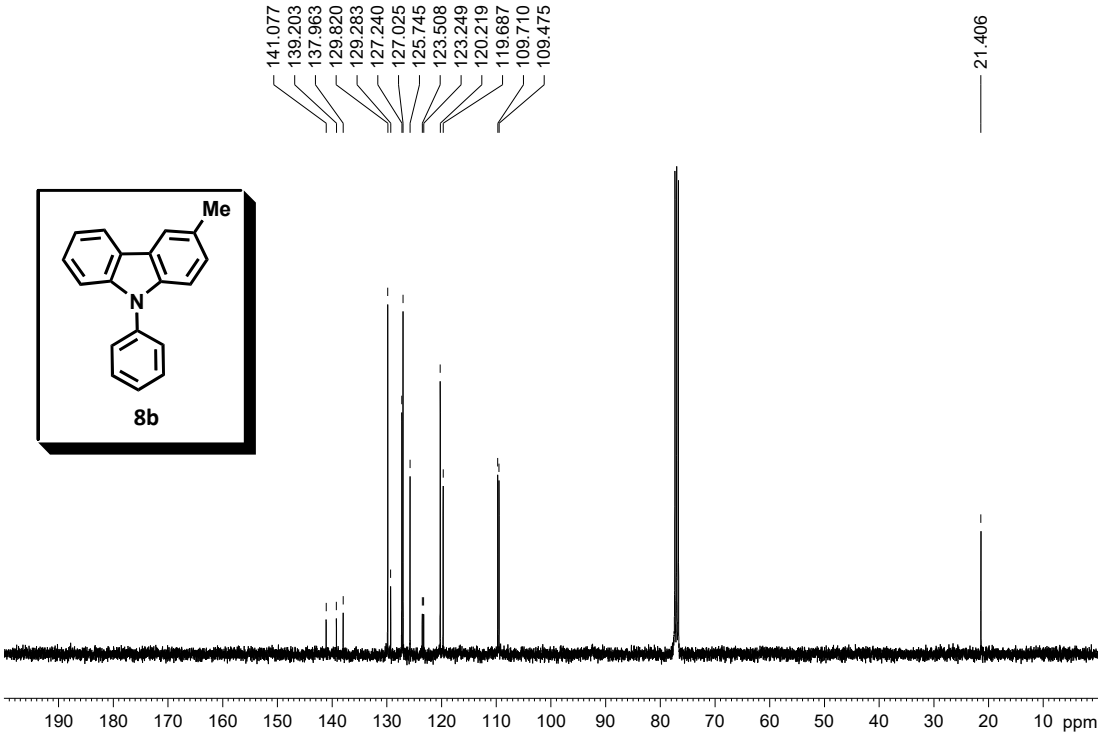


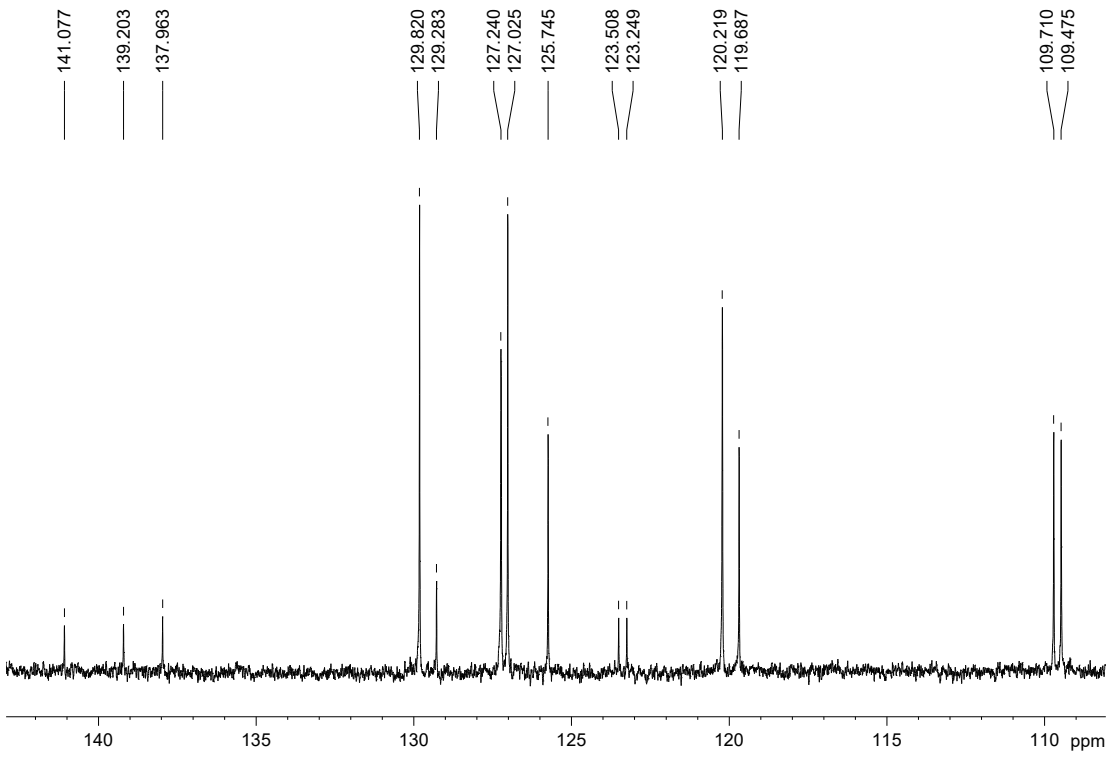
^{1}H-RMN ($CDCl_3$) 3-Metil-9-fenil-9*H*-carbazol (8b)



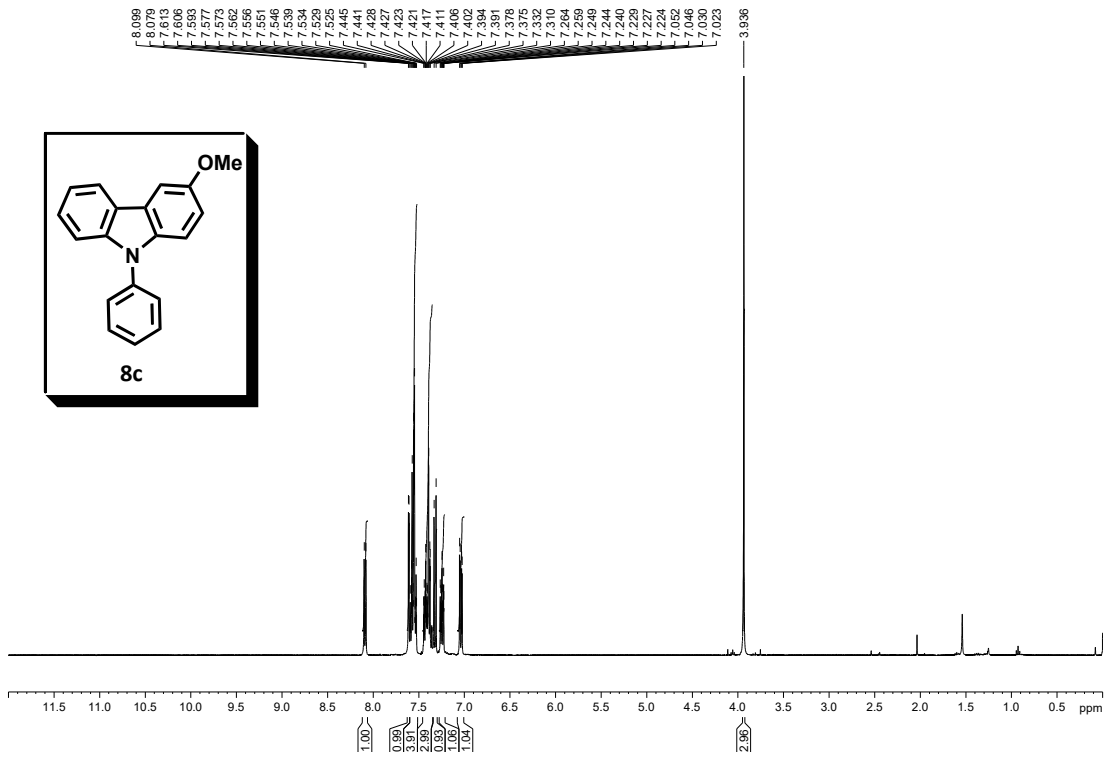


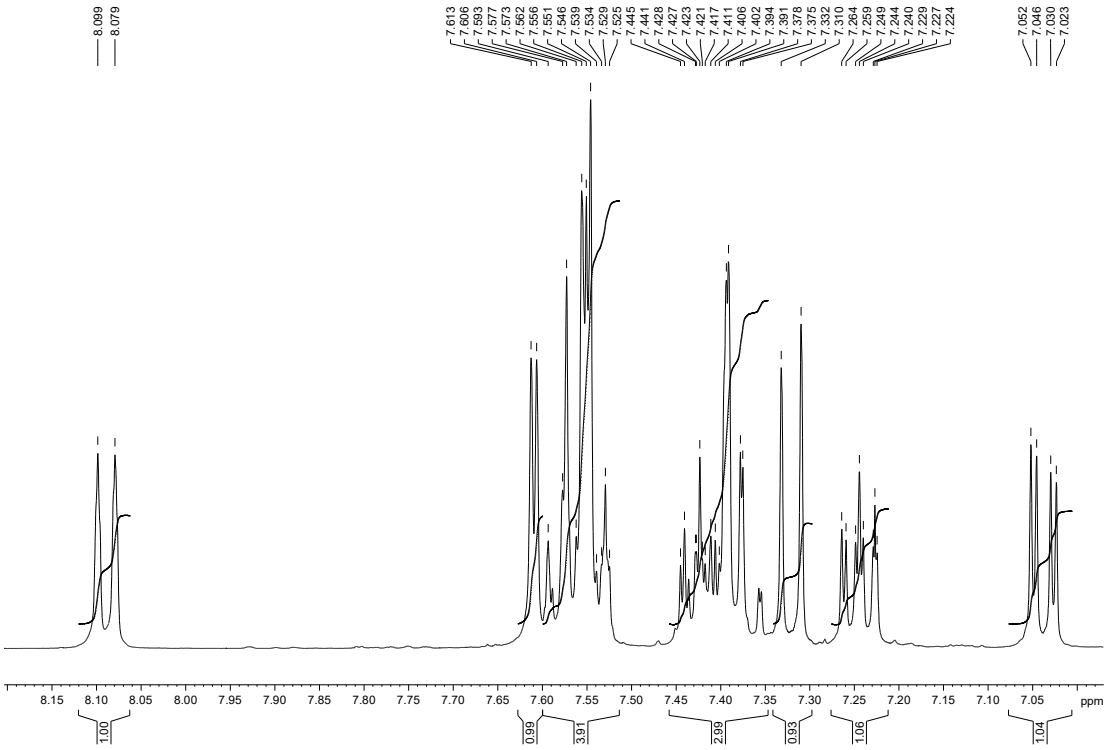
^{13}C-RMN ($CDCl_3$) 3-Metil-9-fenil-9*H*-carbazol (8b)



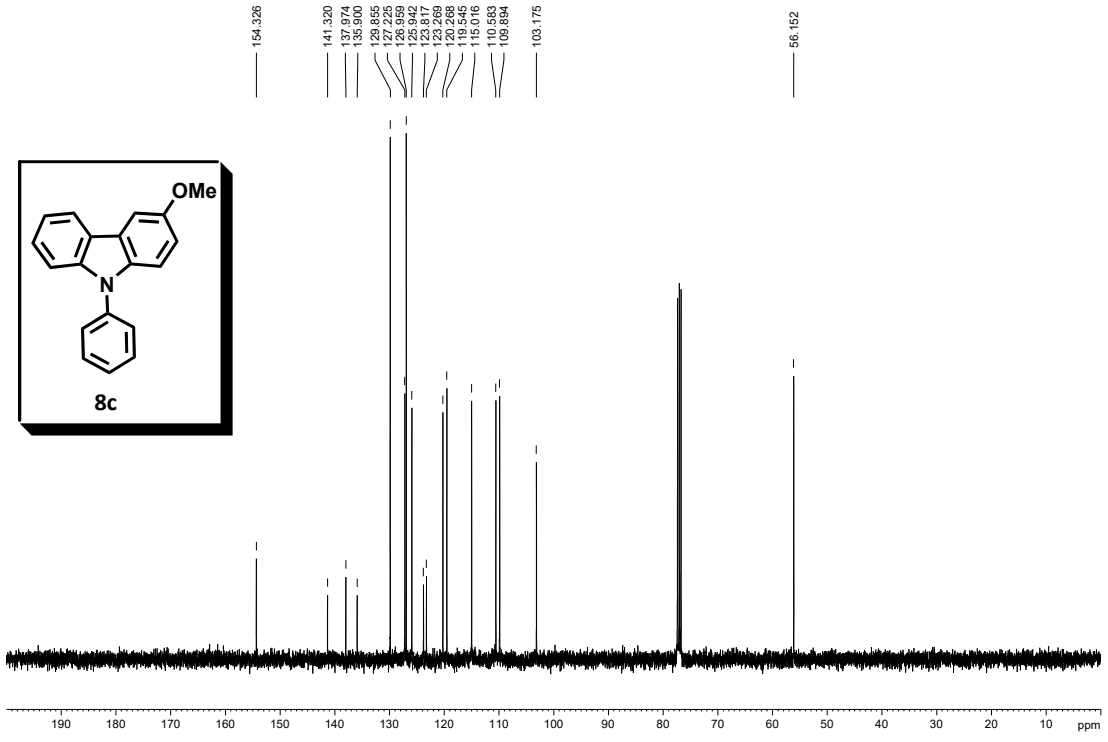


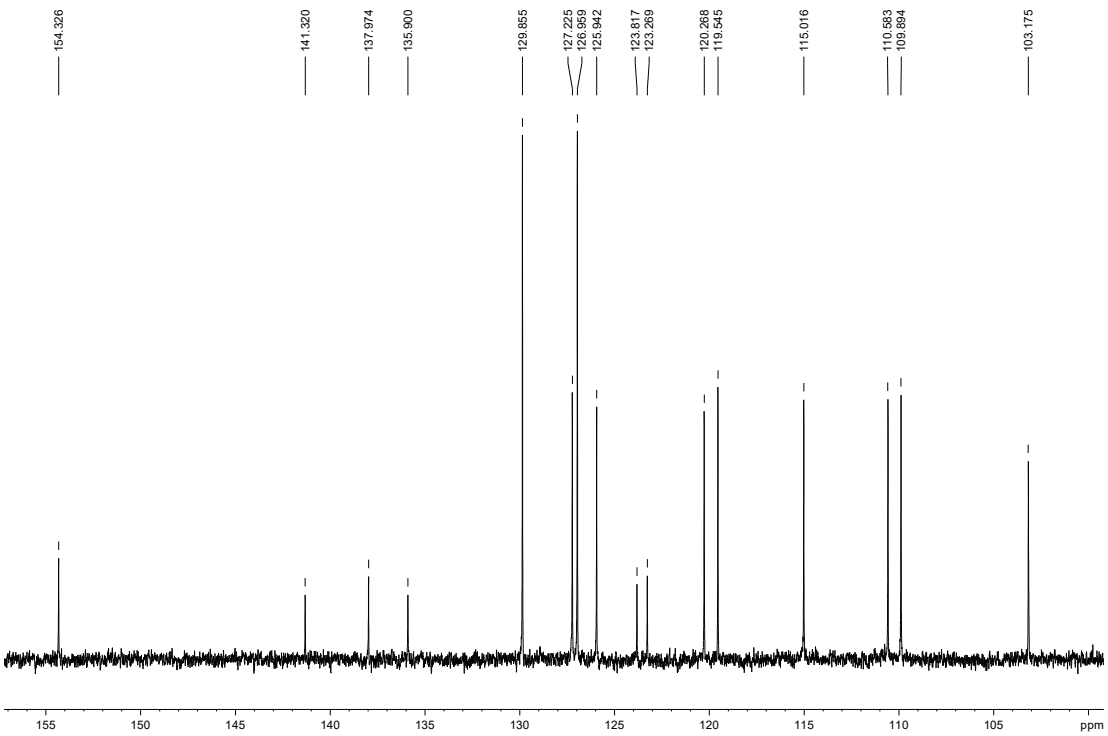
^{1}H-RMN ($CDCl_3$) 3-Metoxi-9-fenil-9*H*-carbazol (8c)



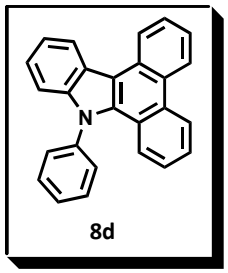


^{13}C-RMN ($CDCl_3$) 3-Metoxi-9-fenil-9*H*-carbazol (8c)

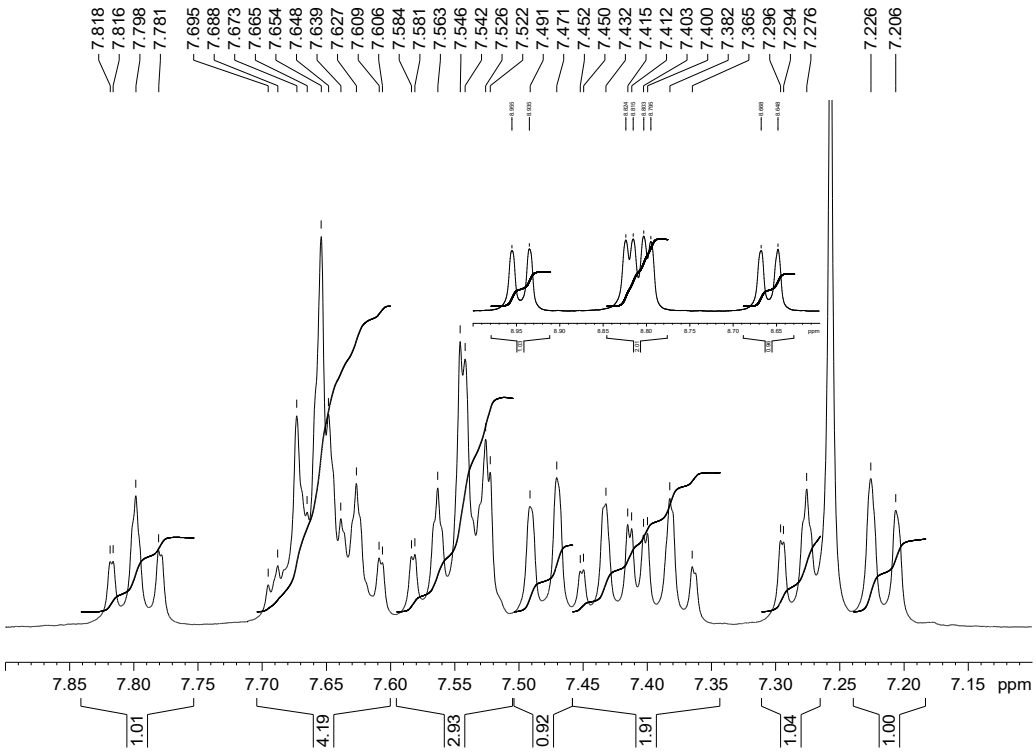




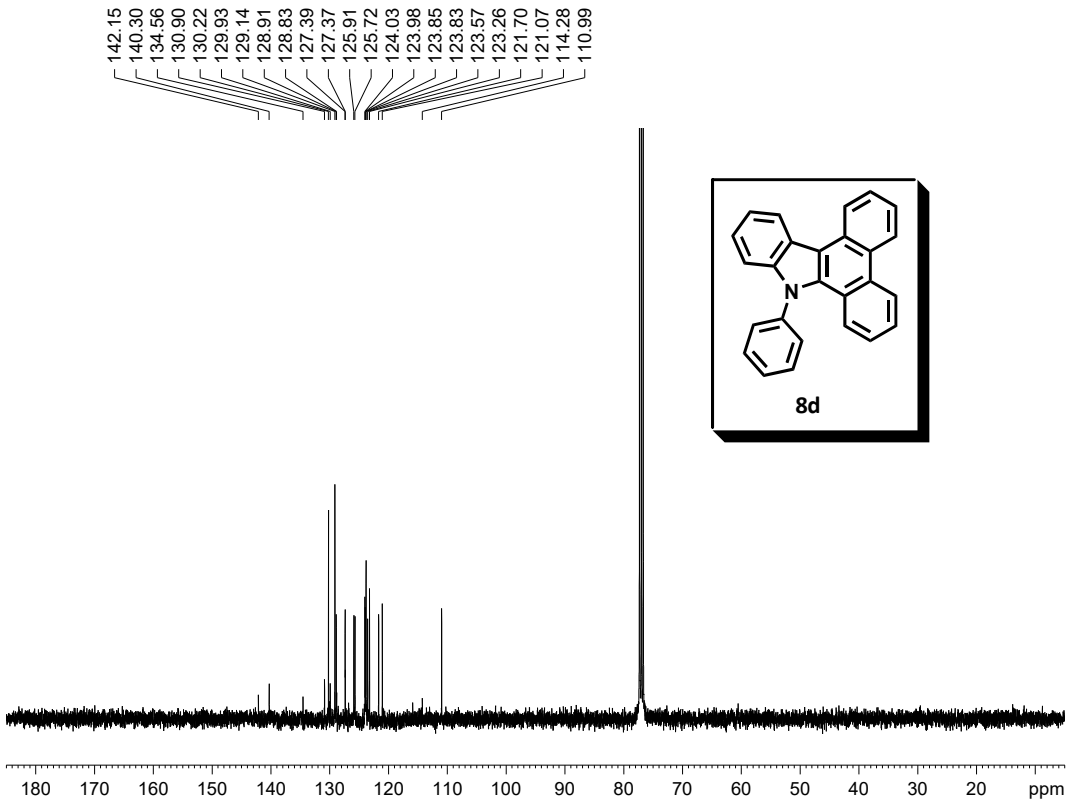
^{1}H-RMN ($CDCl_3$) 9-Fenil-9*H*-dibenzo[*a*,*c*]carbazol (8d)

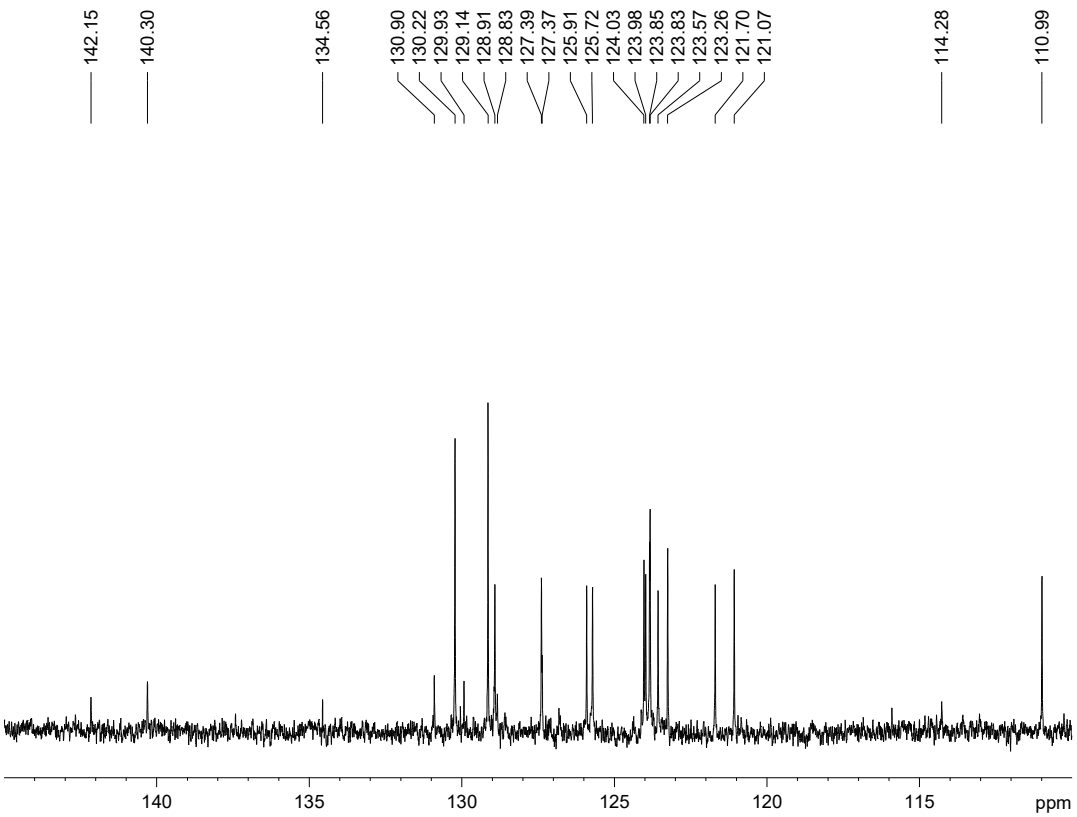


8d

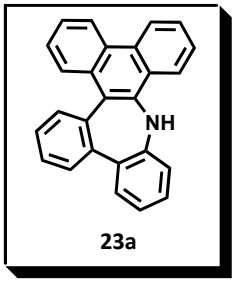


^{13}C-RMN ($CDCl_3$) 9-Fenil-9*H*-dibenzo[*a*,*c*]carbazol (8d)

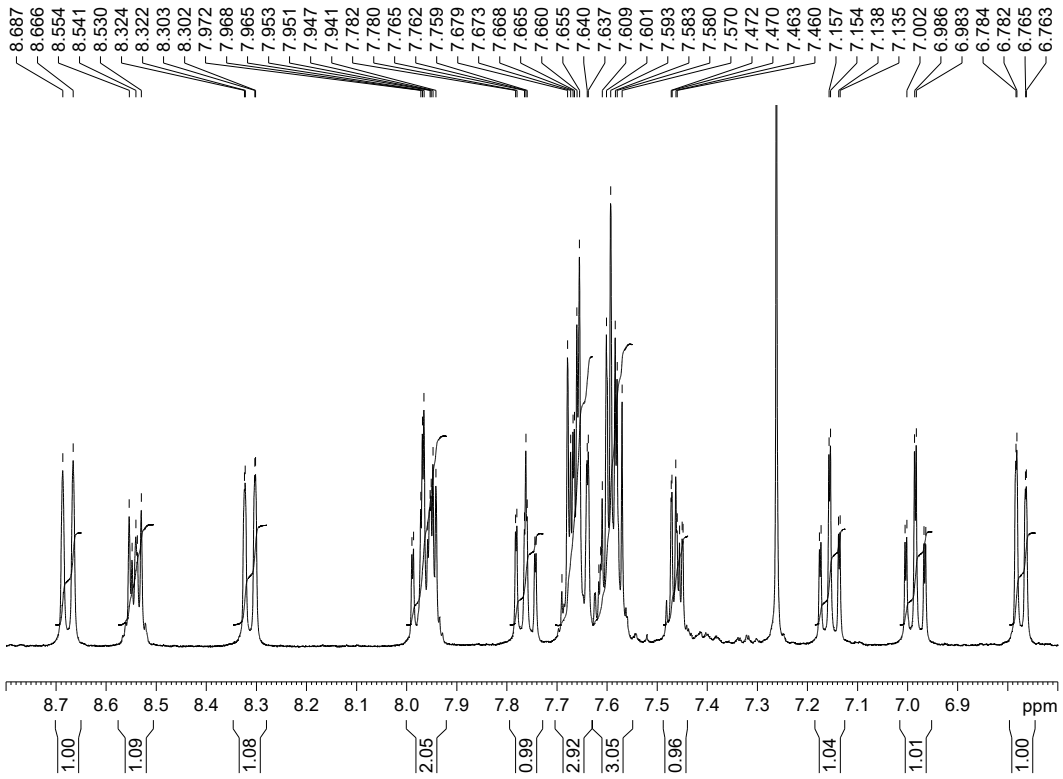




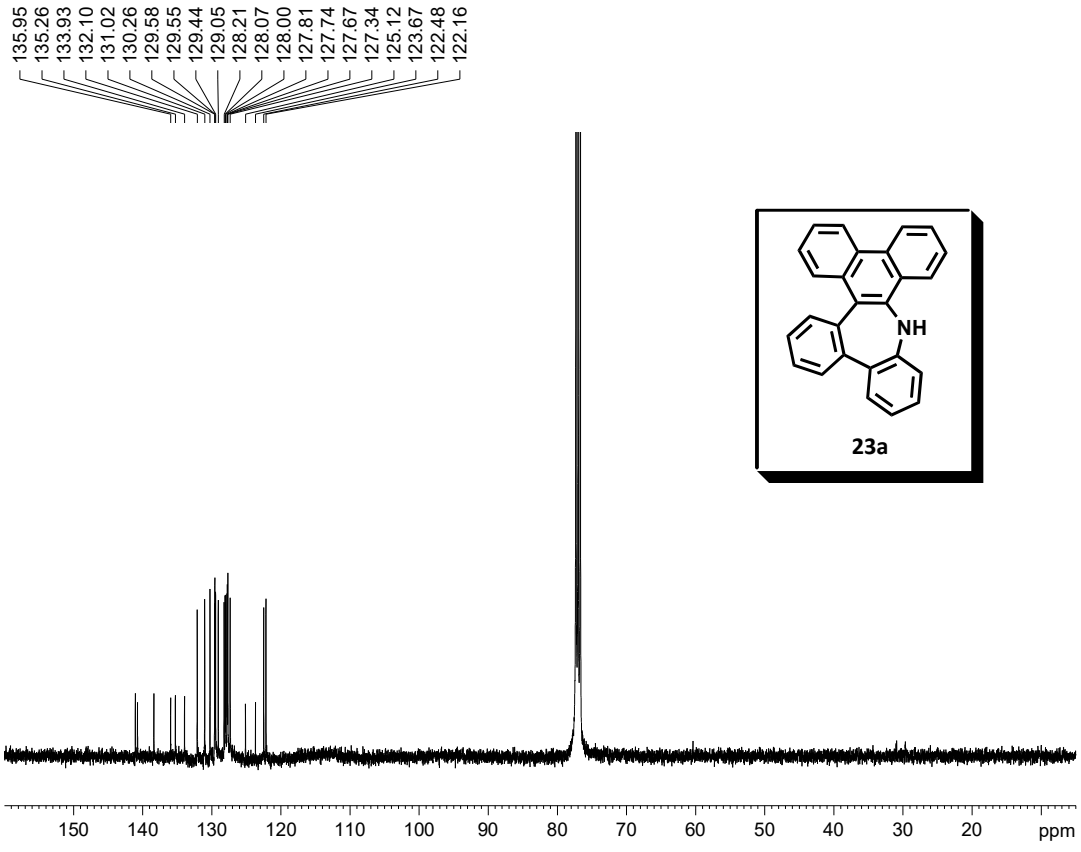
^{1}H-RMN ($CDCl_3$) 9*H*-Dibenzo[*b*,*d*]fenantro[9,10-*f*]acepina (23a)

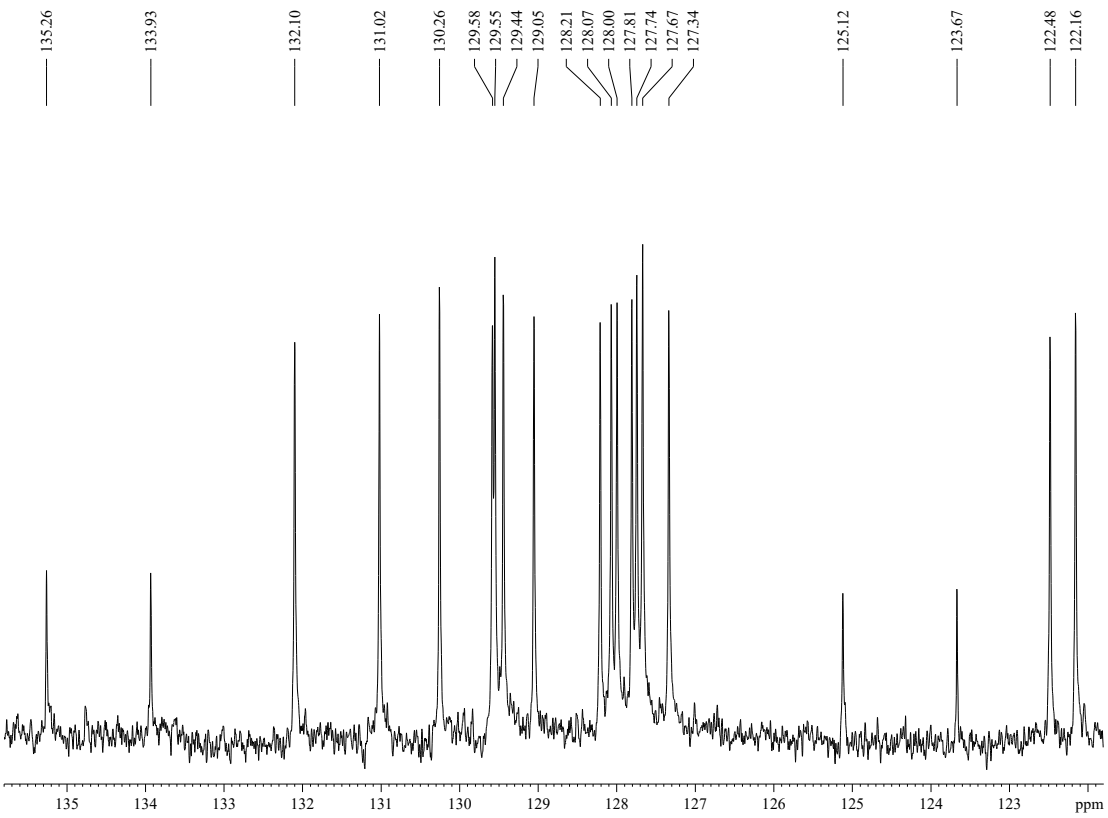


23a



^{13}C-RMN ($CDCl_3$) 9*H*-Dibenzo[*b*,*d*]fenantro[9,10-*f*]acepina (23a)





A.1.6 SECCIÓN DE CÁLCULOS TEÓRICOS

A 1.6.1 Estudio de aniónes de bifenlaminas

- Datos xyz de las especies **13b**$^{-}$ y (**13b**$^{-}$)* (Figura A.1.1)

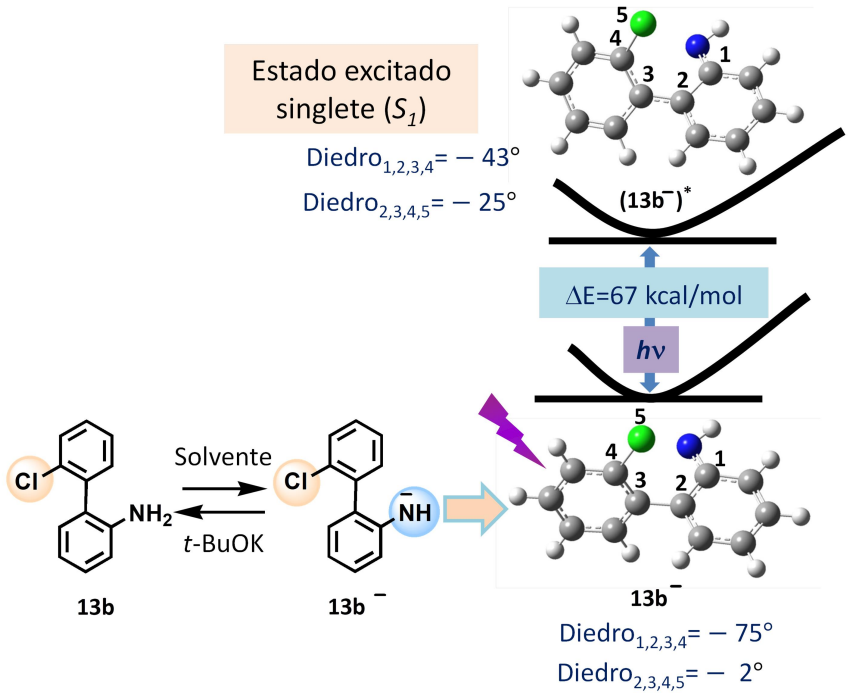


Figura A.1.1: Anión de la 2'-cloro-bifenil-2-amina **13b**$^-$

13b$^-$-anión

m06-2x/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -977.479088 a.u.

Carga = -1 Multiplicidad= 1

C	0.88533100	-0.43002500	-0.14430900
C	1.51223300	0.83790100	0.14302900
C	2.94865900	0.78700900	0.19948700
C	3.66994700	-0.36779400	-0.04426600
C	3.03185900	-1.57344100	-0.35944200
C	1.63502600	-1.57005100	-0.40359000
H	3.47782000	1.70943200	0.42991900
H	4.75541300	-0.33058400	0.00781000
H	3.59510400	-2.47810700	-0.55519800
H	1.10445400	-2.49156800	-0.63412600
C	-0.59603800	-0.50703900	-0.21386400
C	-1.41601300	-0.47401400	0.91849100
C	-1.24358200	-0.64050200	-1.44760700
C	-2.80099300	-0.55273200	0.84305600
C	-2.62885500	-0.72477500	-1.54991500
H	-0.63214900	-0.66897800	-2.34372900
C	-3.41171100	-0.67401700	-0.40129400
H	-3.39248200	-0.52905300	1.75081900

H	-3.09427000	-0.82720400	-2.52390300
H	-4.49209900	-0.73560800	-0.46500300
N	0.77929400	1.94055600	0.31516900
H	1.41247500	2.71919000	0.49984300
Cl	-0.69380700	-0.38678300	2.51458000

13b$^-$-exc-opt

TD-DFT m06-2x/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -977,372475 a.u.

Carga = -1 Multiplicidad= 1

C	0.85716400	-0.46344200	-0.22200300
C	1.50447100	0.73514200	0.32696700
C	2.92834900	0.73525200	0.46876200
C	3.70763000	-0.30692300	-0.01988700
C	3.08291800	-1.39317900	-0.66123000
C	1.69424200	-1.46541400	-0.76028200
H	3.39705400	1.62814400	0.87468000
H	4.78824500	-0.26998300	0.06103000
H	3.68803800	-2.19786900	-1.06575000
H	1.24144500	-2.34475300	-1.20699300
C	-0.57581900	-0.56851600	-0.23671700
C	-1.41117300	-0.18281000	0.86971300
C	-1.27423400	-1.11729100	-1.35757400
C	-2.78839700	-0.13457100	0.76607000
C	-2.64617400	-1.05248600	-1.46620300
H	-0.69332400	-1.52551700	-2.17960600
C	-3.42601200	-0.49639500	-0.42493200
H	-3.37651100	0.14620100	1.63503900
H	-3.12915500	-1.42744600	-2.36288800
H	-4.50348300	-0.42148600	-0.51207400
N	0.74726000	1.79731700	0.55452900
H	1.33754300	2.54230200	0.93151600
Cl	-0.74446100	-0.18446100	2.52379200

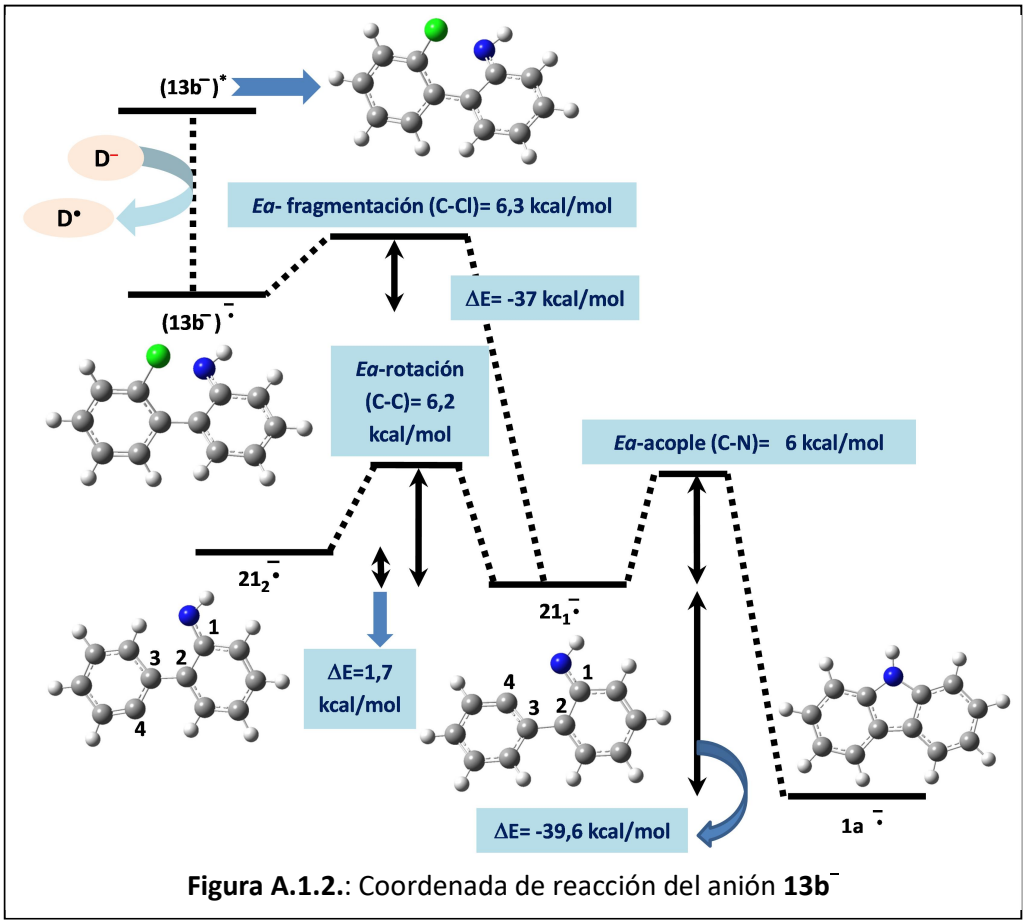


Figura A.1.2.: Coordenada de reacción del anión **13b**$^{-}$

13b-dianión-radical

m06-2x/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -977.519212 a.u.

Carga = -2 Multiplicidad= 2

C	0.86965400	-0.40969300	-0.14360200
C	1.53235200	0.79892200	0.34912900
C	2.96216800	0.74157000	0.39699300
C	3.70989900	-0.32471000	-0.10554700
C	3.06650700	-1.42956300	-0.66334400
C	1.66442600	-1.44886300	-0.65876900
H	3.48378700	1.61967500	0.77692800
H	4.79588200	-0.28059600	-0.06901100
H	3.62945400	-2.26767100	-1.06202100
H	1.15582700	-2.32947100	-1.04641400
C	-0.58096700	-0.51283800	-0.20914000
C	-1.47671700	-0.21967300	0.88043700
C	-1.25602200	-1.06271500	-1.35855000
C	-2.84446700	-0.22224600	0.76945400
C	-2.62588600	-1.04445200	-1.49865000

H	-0.64747200	-1.43954000	-2.17720300
C	-3.46487700	-0.53168900	-0.46920300
H	-3.44953100	-0.03370000	1.65223200
H	-3.06899800	-1.41880700	-2.41835300
H	-4.54371100	-0.51703800	-0.56658400
N	0.82432100	1.89346600	0.67096000
H	1.49031600	2.61892600	0.94406200
Cl	-0.82032800	-0.14747900	2.54215500

13b-radical

m06-2x/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -977.331966 a.u.

Carga = 0 Multiplicidad= 2

C	0.87050200	-0.45257200	-0.14979100
C	1.52686100	0.78866800	0.17595400
C	2.95875500	0.78966200	0.22537000
C	3.68584000	-0.34453200	-0.05588400
C	3.02515100	-1.53152200	-0.39742900
C	1.62672800	-1.57195900	-0.44193400
H	3.46171200	1.71759600	0.47896400
H	4.76863300	-0.31953400	-0.01840000
H	3.59523000	-2.42454000	-0.62444800
H	1.12411600	-2.49882800	-0.69679600
C	-0.61115800	-0.51749300	-0.21538500
C	-1.42124000	-0.42521400	0.91839600
C	-1.24154900	-0.70000500	-1.44901700
C	-2.80568100	-0.49457100	0.83658000
C	-2.62664500	-0.76738800	-1.55003700
H	-0.62638700	-0.77461400	-2.33937200
C	-3.40947300	-0.65974700	-0.40560700
H	-3.40116900	-0.42732900	1.73909700
H	-3.09112400	-0.90241000	-2.51981000
H	-4.48999000	-0.71109700	-0.47159800
N	0.78451000	1.87127000	0.38929100
H	1.39651900	2.66141100	0.60634700
Cl	-0.69452600	-0.27343900	2.50146800

13b-ET-C-Cl

m06-2x/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -977.499064 a.u.

Carga = -2 Multiplicidad= 2

C	0.85962300	-0.34429000	-0.36759500
C	1.44979900	0.80594000	0.30743200
C	2.87594600	0.74807300	0.48153300
C	3.67791300	-0.22298500	-0.08711100
C	3.10863200	-1.24325700	-0.85622600
C	1.71487400	-1.28667400	-0.94515500
H	3.32964800	1.51557500	1.10629200
H	4.75249200	-0.19509800	0.07791300
H	3.71883700	-2.01047200	-1.31954300
H	1.27079800	-2.14667300	-1.44063200
C	-0.56422300	-0.68173700	-0.20584400
C	-1.35373700	-0.09661900	0.82367900
C	-1.30049200	-1.47619200	-1.13764700
C	-2.72042600	0.08055400	0.68223200
C	-2.64460500	-1.22576300	-1.34977000
H	-0.82684100	-2.28103200	-1.69874400
C	-3.32254500	-0.28736700	-0.53075000
H	-3.31550400	0.44597300	1.52184400
H	-3.20129100	-1.82760300	-2.06356400
H	-4.17716600	0.26608000	-0.92173300
N	0.70969200	1.84618400	0.70983600
H	1.34887100	2.54076500	1.10096600
Cl	-0.98467800	-0.89156500	2.64854600

21-radical-anión

m06-2x/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -517.199236 a.u.

Carga = -1 Multiplicidad= 2

C	-0.66227100	-0.19066500	0.04769900
C	-1.40910900	1.04370000	-0.08992900
C	-2.84274800	0.89191100	-0.08240100
C	-3.46964400	-0.32524400	0.06916200
C	-2.72468000	-1.50547000	0.22553000
C	-1.33858100	-1.40424700	0.21068900
H	-3.44063200	1.79379900	-0.19558500
H	-4.55583400	-0.36553600	0.07433200
H	-3.21120100	-2.46333100	0.36735300
H	-0.75746300	-2.31021200	0.35707200
C	0.81013900	-0.15603400	0.03053900
C	1.53744100	0.99782700	0.29359200

C	1.60262800	-1.28812100	-0.26757000
C	2.90962400	1.10818300	0.29258000
C	2.99246900	-1.22988800	-0.26725300
H	1.12337900	-2.22586100	-0.52904900
C	3.66083500	-0.03810400	0.01460000
H	3.40173800	2.05273800	0.50501400
H	3.56013100	-2.12305600	-0.50623700
H	4.74494600	0.00230100	0.00801900
N	-0.79555800	2.21887300	-0.22285100
H	-1.50506500	2.94765100	-0.30819600

13b-ET-C-N

m06-2x/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -517.18972 a.u.

Carga = -1 Multiplicidad= 2

C	-0.69866200	-0.37429700	0.07984400
C	-1.21437900	0.94109900	-0.13745600
C	-2.61882600	1.09482300	-0.16587100
C	-3.45372100	-0.01090500	-0.03989800
C	-2.93525900	-1.29850700	0.12337800
C	-1.54994300	-1.46645500	0.18797800
H	-3.04388700	2.08487700	-0.30644300
H	-4.52972700	0.13392900	-0.06979500
H	-3.59902300	-2.15016900	0.22013800
H	-1.13290000	-2.45659600	0.35487100
C	0.76781900	-0.35561300	0.15839700
C	1.29577400	0.91964100	0.47223300
C	1.61279000	-1.41118700	-0.17819800
C	2.67047900	1.13367300	0.30290700
C	2.99529300	-1.20161400	-0.28140500
H	1.19854200	-2.39273700	-0.39763300
C	3.51110000	0.07554500	-0.07117400
H	3.11515800	2.10369900	0.51741300
H	3.65172900	-2.02125900	-0.55333000
H	4.57997200	0.24739900	-0.17392600
N	-0.27214400	1.90558100	-0.31486800
H	-0.57596700	2.83409300	-0.02850700

1a-radical-anión

m06-2x/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -517.26242 a.u.

Carga = -1 Multiplicidad= 2

C	1.20914700	-0.09771600	-0.48664600
C	1.83925200	-1.33623400	-0.13941300
C	3.21057400	-1.49788900	-0.09603300
C	4.02148600	-0.37066200	-0.41405800
C	3.43081300	0.84823500	-0.75440900
C	2.04388000	1.01587700	-0.79882400
H	3.65444200	-2.45204700	0.16926100
H	5.10167700	-0.46417000	-0.39097400
H	4.07083600	1.69347100	-0.99386500
H	1.61076700	1.97409700	-1.06750700
C	-0.18963400	-0.30179000	-0.43487900
C	-0.41247600	-1.66452800	-0.05457000
C	-1.32843600	0.52224900	-0.67584000
C	-1.67341200	-2.21034400	0.08879600
C	-2.60264100	-0.03404400	-0.53120000
H	-1.20843800	1.56039000	-0.96870400
C	-2.79366800	-1.36634700	-0.15807400
H	-1.80522800	-3.24801900	0.37790700
H	-3.47315000	0.58976900	-0.71693100
H	-3.79733500	-1.76414600	-0.05584700
N	0.83162400	-2.25660100	0.11577800
H	0.98151100	-3.21433400	0.38850000

13b-anión

B3LYP/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -977.720697 a.u.

Carga = -1 Multiplicidad= 1

C	0.86994	-0.31841	0.00009
C	1.65750	-0.04243	-1.18458
C	3.07910	0.02131	-0.95469
C	3.64988	-0.12326	0.29926
C	2.85755	-0.34865	1.43495
C	1.47258	-0.43912	1.25134
H	3.72052	0.20651	-1.81548
H	4.73171	-0.05664	0.39909
H	3.29870	-0.45959	2.42003
H	0.83513	-0.62741	2.11323
C	-0.61228	-0.43322	-0.09330
C	-1.28055	-1.54448	-0.62819

C	-1.43059	0.60395	0.38631
C	-2.66878	-1.62815	-0.69811
C	-2.82179	0.54369	0.33068
H	-0.94795	1.48187	0.80373
C	-3.44537	-0.57429	-0.21974
H	-3.13665	-2.51272	-1.11444
H	-3.41477	1.36910	0.71123
H	-4.52716	-0.63609	-0.27370
N	1.07343	0.15734	-2.37634
H	1.80525	0.34286	-3.06534
Cl	-0.35978	-2.95036	-1.19007

21_1-radical-anión

B3LYP/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -517.420144 a.u.

Carga = -1 Multiplicidad= 2

C	1.21534	-0.70043	-0.51756
C	2.06766	-1.03624	0.61086
C	3.48640	-0.92802	0.38015
C	4.01909	-0.52967	-0.82965
C	3.17966	-0.20724	-1.91178
C	1.80285	-0.30202	-1.72900
H	4.15102	-1.17429	1.20652
H	5.09931	-0.46788	-0.94314
H	3.59146	0.10110	-2.86727
H	1.16223	-0.06279	-2.57248
C	-0.24310	-0.79944	-0.35569
C	-0.81608	-1.29730	0.81587
C	-1.17867	-0.40346	-1.34869
C	-2.17063	-1.41844	1.05440
C	-2.55186	-0.51671	-1.14756
H	-0.83293	0.00801	-2.29199
C	-3.06653	-1.02400	0.05078
H	-2.54627	-1.81363	1.99622
H	-3.23006	-0.20012	-1.93477
H	-4.13934	-1.10800	0.20148
N	1.53941	-1.41421	1.77904
H	2.28127	-1.63051	2.44858

21_2-radical-anión

B3LYP/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -517.417379 a.u.

Carga = -1 Multiplicidad= 2

C	1.20997	-0.61461	-0.41674
C	2.09047	-1.77624	-0.34695
C	3.50298	-1.48098	-0.45751
C	4.01031	-0.21099	-0.62024
C	3.14490	0.89873	-0.68883
C	1.78142	0.66341	-0.58551
H	4.18661	-2.32725	-0.40643
H	5.08643	-0.06933	-0.69493
H	3.52894	1.90562	-0.81636
H	1.10094	1.51113	-0.63478
C	-0.25917	-0.68242	-0.32245
C	-1.06324	0.45680	-0.43516
C	-1.02130	-1.86372	-0.11031
C	-2.42598	0.54672	-0.36683
C	-2.41751	-1.83719	-0.02924
H	-0.47248	-2.79104	-0.01588
C	-3.13810	-0.65131	-0.15442
H	-2.94723	1.49460	-0.47111
H	-2.94875	-2.77074	0.13469
H	-4.22222	-0.64168	-0.09219
N	1.64155	-3.03084	-0.19478
H	2.45171	-3.65395	-0.17972

ET -CN-ciclización-13b-1a

B3LYP/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -517.412883 a.u.

Carga = -1 Multiplicidad= 2

C	1.22268	-0.24055	-0.35937
C	1.90905	-1.49547	-0.25209
C	3.32363	-1.48126	-0.30383
C	4.01400	-0.28705	-0.50681
C	3.33203	0.92631	-0.66020
C	1.93447	0.93755	-0.57825
H	3.87124	-2.41535	-0.20369
H	5.10033	-0.30257	-0.54653
H	3.88053	1.84983	-0.81695

H	1.40143	1.88238	-0.65548
C	-0.22826	-0.41631	-0.21417
C	-0.58715	-1.63211	0.42452
C	-1.21684	0.41031	-0.75752
C	-1.92372	-2.06089	0.36514
C	-2.56267	0.00382	-0.75214
H	-0.94583	1.35703	-1.22076
C	-2.90299	-1.24367	-0.22236
H	-2.23149	-2.99662	0.83151
H	-3.32622	0.64300	-1.18566
H	-3.94169	-1.57026	-0.23722
N	1.09610	-2.58575	-0.13635
H	1.50298	-3.35715	0.39069

ET-rotatción-21_1-21_2

B3LYP/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -517.412832 a.u.

Carga = -1 Multiplicidad= 2

C	1.23108	-0.58725	-0.42245
C	2.09047	-1.51371	0.28301
C	3.49878	-1.32194	0.04684
C	3.99748	-0.33238	-0.78617
C	3.13923	0.55056	-1.45665
C	1.76120	0.39689	-1.25324
H	4.19115	-1.99249	0.55447
H	5.07442	-0.24469	-0.91755
H	3.52364	1.32636	-2.11068
H	1.07203	1.06905	-1.76097
C	-0.25389	-0.68414	-0.26786
C	-0.96374	-0.00564	0.70287
C	-1.05186	-1.45512	-1.13829
C	-2.32638	-0.00475	0.89323
C	-2.44141	-1.50202	-1.00300
H	-0.56530	-2.01946	-1.92953
C	-3.08597	-0.78315	0.00542
H	-2.80426	0.56748	1.68280
H	-3.02591	-2.10230	-1.69331
H	-4.16676	-0.81936	0.10519
N	1.57648	-2.46393	1.08271
H	2.34975	-3.00331	1.47750

1a-radical-anión

B3LYP/6-311+g(d) scrf=(solvente=dmso,pcm)

Sum of electronic and zero-point Energies= -517.478905 a.u.

Carga = -1 Multiplicidad= 2

C	1.21295	-0.10815	-0.49005
C	1.84923	-1.34700	-0.14143
C	3.22729	-1.49690	-0.09646
C	4.03342	-0.36278	-0.41264
C	3.43571	0.85595	-0.75488
C	2.04380	1.01147	-0.80149
H	3.68071	-2.44768	0.17009
H	5.11553	-0.45008	-0.38593
H	4.07077	1.70721	-0.99153
H	1.60560	1.96870	-1.06998
C	-0.19224	-0.31016	-0.43853
C	-0.43121	-1.66808	-0.05823
C	-1.33072	0.52252	-0.67893
C	-1.69361	-2.21362	0.08930
C	-2.61103	-0.02604	-0.53136
H	-1.20759	1.56126	-0.97213
C	-2.81236	-1.36040	-0.15623
H	-1.83183	-3.25102	0.37988
H	-3.47838	0.60511	-0.71442
H	-3.81984	-1.75137	-0.05165
N	0.85274	-2.27895	0.11519
H	1.00267	-3.23475	0.39390

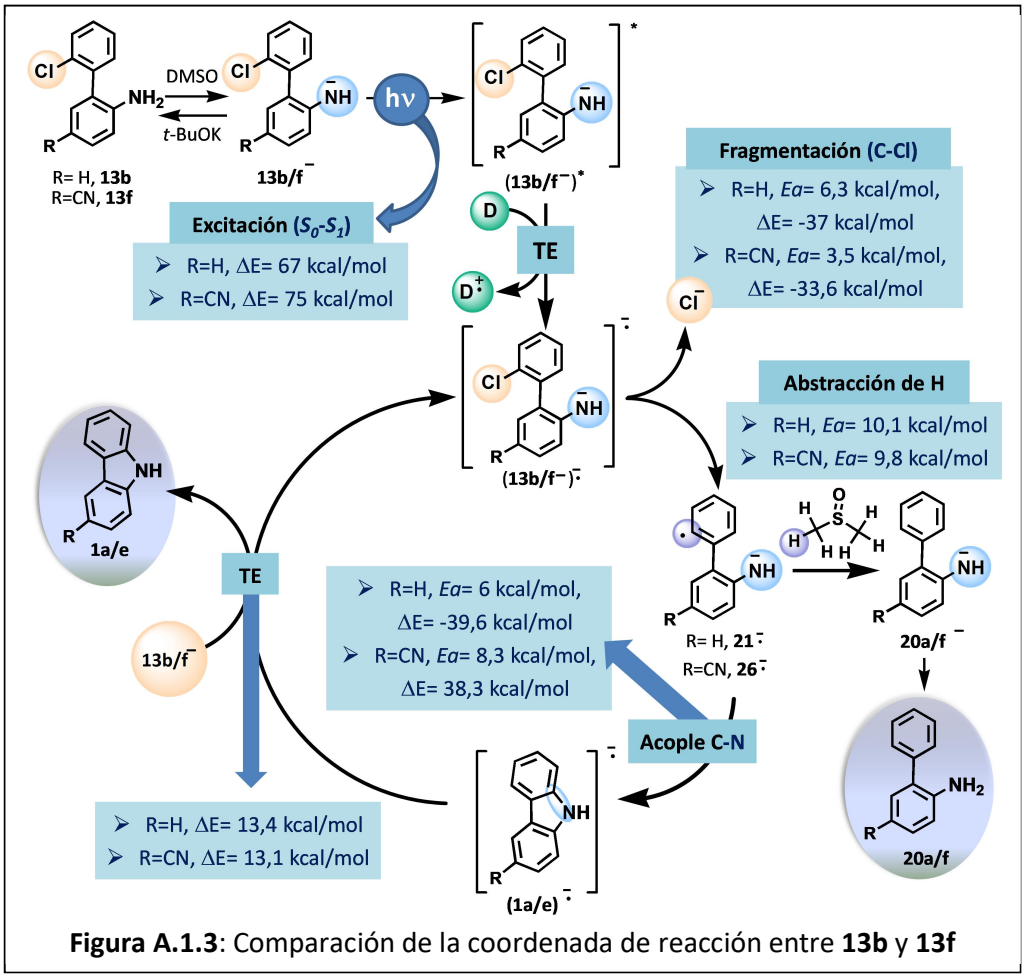


Figura A.1.3: Comparación de la coordenada de reacción entre **13b** y **13f**

13f⁻-anión

m06-2x/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -1069.743132 a.u.

Carga = -1 Multiplicidad= 1

C	0.88315300	-0.46116400	-0.14045800
C	1.51942400	0.81754500	0.13930200
C	2.96535500	0.77052100	0.21036000
C	3.68309800	-0.37369200	-0.01153700
C	3.03415800	-1.59163400	-0.31975000
C	1.62252900	-1.59411000	-0.37567300
H	3.48986900	1.69486300	0.43686000
H	4.76718400	-0.34948600	0.04602500
H	1.10533600	-2.52355700	-0.59816100
C	-0.59871100	-0.52775500	-0.21547900
C	-1.41545900	-0.46999100	0.91721400
C	-1.24105900	-0.66723900	-1.44980600
C	-2.80080500	-0.53213800	0.83976800
C	-2.62711100	-0.73531500	-1.55199500

H	-0.62818700	-0.71295900	-2.34403800
C	-3.40970100	-0.66115300	-0.40471600
H	-3.39363100	-0.48984700	1.74583700
H	-3.09289900	-0.84356300	-2.52496000
H	-4.49058000	-0.70996800	-0.46970800
N	0.79398800	1.90437500	0.29161000
H	1.41574300	2.69269400	0.47320300
Cl	-0.68882900	-0.36829500	2.50860000
C	3.77110400	-2.77485400	-0.55660900
N	4.37525200	-3.74425100	-0.75291100

13f⁻-exc-opt

TD-DFT m06-2x/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -1069,623601 a.u.

Carga = -1 Multiplicidad= 1

C	0.84430300	-0.49061900	-0.11888000
C	1.53271800	0.71036100	0.37206300
C	2.96325400	0.68673100	0.51827100
C	3.71715400	-0.39063000	0.07852800
C	3.05283800	-1.48304200	-0.52022900
C	1.65320200	-1.53753500	-0.62817800
H	3.45267500	1.58605200	0.87940000
H	4.79824000	-0.38486600	0.14353000
H	1.19282800	-2.42781400	-1.03914000
C	-0.58621900	-0.55641800	-0.17083700
C	-1.46904500	-0.09538200	0.86243400
C	-1.24223700	-1.17604900	-1.28310900
C	-2.84035600	-0.07108200	0.70500400
C	-2.61152600	-1.14207000	-1.44298200
H	-0.62867200	-1.61259300	-2.06430300
C	-3.43416700	-0.54447600	-0.47126500
H	-3.45956000	0.27485000	1.52610000
H	-3.05333900	-1.57589600	-2.33421300
H	-4.51000600	-0.50856400	-0.59207800
N	0.81831700	1.79927400	0.54409600
H	1.43059800	2.55032500	0.87038800
Cl	-0.86871400	0.16107900	2.50697200
C	3.83088900	-2.57038200	-1.02157200
N	4.45604700	-3.45222500	-1.42702300

13f-dianión-radical

m06-2x/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -1069.787386 a.u.

Carga = -2 Multiplicidad= 2

C	0.87901800	-0.45626300	-0.14496700
C	1.52607500	0.84544400	-0.04317500
C	2.97398800	0.81009500	-0.00942900
C	3.69686300	-0.35285300	-0.06144200
C	3.04543800	-1.60140600	-0.15933800
C	1.62848300	-1.60623300	-0.20363800
H	3.49840700	1.75909800	0.07109600
H	4.78180800	-0.31739100	-0.02589300
H	1.11065900	-2.55917700	-0.27845500
C	-0.60315500	-0.57163200	-0.21176000
C	-1.38562800	-0.81137000	0.88674700
C	-1.25801100	-0.47964300	-1.49258600
C	-2.80865900	-0.94775600	0.85289600
C	-2.68585700	-0.41388500	-1.52837700
H	-0.66389400	-0.22649800	-2.36390700
C	-3.43489200	-0.63767200	-0.39677400
H	-3.37508500	-1.02804100	1.77174100
H	-3.18802600	-0.20263700	-2.46944600
H	-4.51995800	-0.59783800	-0.44909000
N	0.82014100	1.95866800	0.02774100
H	1.46450900	2.74678200	0.10093700
Cl	-0.62963100	-0.95925900	2.49140600
C	3.78097700	-2.80626900	-0.21347200
N	4.38564900	-3.79523500	-0.25783400

13f-radical

m06-2x/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -1069.576068 a.u.

Carga = 0 Multiplicidad= 2

C	0.86947900	-0.47306700	-0.13201200
C	1.53614600	0.76917900	0.18404900
C	2.96961200	0.76431900	0.25144500
C	3.69496200	-0.36945000	-0.01017500
C	3.01900900	-1.55674500	-0.34797800
C	1.61457500	-1.59881700	-0.40537100
H	3.47738400	1.68947600	0.50160500

H	4.77683100	-0.35797500	0.03557800
H	1.11673300	-2.52873600	-0.65493700
C	-0.61121600	-0.53007700	-0.20785700
C	-1.42602200	-0.39810700	0.91849700
C	-1.23073900	-0.74353600	-1.44157600
C	-2.80992300	-0.45791900	0.82684600
C	-2.61543900	-0.80104300	-1.55041500
H	-0.60965000	-0.84885200	-2.32459100
C	-3.40489100	-0.65376200	-0.41516600
H	-3.41164300	-0.35996900	1.72227900
H	-3.07418900	-0.95880500	-2.51930000
H	-4.48522900	-0.69752100	-0.48807900
N	0.80089500	1.85432900	0.36830700
H	1.40846900	2.64870500	0.58235300
Cl	-0.70813800	-0.20823700	2.49994600
C	3.76870800	-2.74112400	-0.63387600
N	4.37349600	-3.69324100	-0.86659500

13f-ET-C-Cl

m06-2x/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -1069.784595 **a.u.**

Carga = -2 Multiplicidad= 2

C	0.87895600	-0.48158000	-0.14327600
C	1.50950500	0.82931300	-0.04804700
C	2.95780800	0.81196000	-0.01415900
C	3.69493900	-0.34217600	-0.06587100
C	3.05937200	-1.59880200	-0.16036900
C	1.64258200	-1.62250300	-0.20097700
H	3.47047900	1.76745900	0.06627000
H	4.77950500	-0.29318700	-0.03195800
H	1.13695900	-2.58218000	-0.27238800
C	-0.60043800	-0.61221200	-0.21657500
C	-1.40501100	-0.84783900	0.86293800
C	-1.25963400	-0.50832800	-1.49645000
C	-2.82165400	-0.90950000	0.85087000
C	-2.67991800	-0.37715400	-1.52821900
H	-0.65803900	-0.34900100	-2.38433300
C	-3.43996500	-0.55995000	-0.39578900
H	-3.38803700	-1.13870700	1.74320400
H	-3.17243500	-0.13483400	-2.46728800
H	-4.52083700	-0.45355300	-0.44282000

N	0.78936700	1.93323200	0.01927500
H	1.42311800	2.73011000	0.08943700
Cl	-0.59577400	-0.94244600	2.60147600
C	3.81019800	-2.79418300	-0.21407000
N	4.42817200	-3.77490900	-0.25789900

26-radical-anión

m06-2x/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -609.461902 a.u.

Carga = -1 Multiplicidad= 2

C	0.14308500	0.26361700	-0.01844500
C	0.49974000	1.67429400	-0.13911600
C	1.92277700	1.95141900	-0.16658300
C	2.87484200	0.97756000	-0.06299300
C	2.50133300	-0.38081800	0.07647000
C	1.13017400	-0.69551500	0.09547800
H	2.22822500	2.98903200	-0.26966300
H	3.92749800	1.24292000	-0.08106700
H	0.84785800	-1.73494400	0.23001300
C	-1.27939700	-0.13125500	0.00336600
C	-2.28798400	0.72420000	0.41874100
C	-1.71941000	-1.40955600	-0.39836400
C	-3.62926300	0.42527700	0.47684500
C	-3.06338300	-1.76628900	-0.34505800
H	-1.00228100	-2.12842400	-0.78213800
C	-4.02750300	-0.85920600	0.09304300
H	-4.35912900	1.15472000	0.81436100
H	-3.36268100	-2.75825200	-0.66530500
H	-5.07468400	-1.14097300	0.12612900
N	-0.42502100	2.60503400	-0.22212300
H	0.02654900	3.51632100	-0.30562400
C	3.47899400	-1.39483100	0.21672800
N	4.28155800	-2.22233400	0.33206600

13f-ET-C-N

m06-2x/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -609.448726 a.u.

Carga = -1 Multiplicidad= 2

C	-0.19036000	-0.00001300	0.06881900
C	-0.31879100	1.42400000	-0.12289300
C	-1.63147200	1.96960500	-0.18533000

C	-2.73405900	1.14408500	-0.12258100
C	-2.59298000	-0.25017700	0.02042100
C	-1.30100600	-0.80910600	0.12951900
H	-1.76078200	3.04060200	-0.30284100
H	-3.72965500	1.57118200	-0.18424700
H	-1.19264800	-1.87829100	0.28692700
C	1.22668900	-0.37016900	0.16514800
C	2.05736400	0.72296500	0.51103200
C	1.78188900	-1.59254200	-0.20248000
C	3.44376000	0.60007100	0.33847600
C	3.17302300	-1.73022100	-0.30133500
H	1.13647500	-2.43172600	-0.45141200
C	3.98958700	-0.62471300	-0.06216500
H	4.11194300	1.42499000	0.57496400
H	3.60711800	-2.67893400	-0.59707500
H	5.06770300	-0.72331400	-0.16407800
N	0.84380900	2.06995300	-0.21182400
H	0.80864900	3.07581900	-0.06309500
C	-3.74357500	-1.08174300	0.08316200
N	-4.67987200	-1.75909700	0.13198600

1e-radical-anión

m06-2x/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -609.522946 a.u.

Carga = -1 Multiplicidad= 2

C	1.15438900	-0.44141500	-0.87893000
C	1.81102800	-0.94024800	0.26959800
C	3.21008800	-0.94784600	0.41862000
C	3.96509800	-0.42798200	-0.64695900
C	3.34986700	0.07332400	-1.79643800
C	1.92975100	0.08888200	-1.95925200
H	3.68361100	-1.33874800	1.31068600
H	5.04769700	-0.41394600	-0.58045700
H	1.47442100	0.48206400	-2.85902900
C	-0.24060300	-0.60646200	-0.65766100
C	-0.40477200	-1.20686000	0.62902500
C	-1.40028900	-0.31212000	-1.41214200
C	-1.64599000	-1.51032100	1.15990700
C	-2.64717300	-0.61682500	-0.87758100

H	-1.31681600	0.14408700	-2.39367000
C	-2.78102500	-1.20808300	0.38894600
H	-1.73974900	-1.96641600	2.14026700
H	-3.54097900	-0.39183100	-1.45135600
H	-3.76758100	-1.43292400	0.77810000
N	0.86215300	-1.39192000	1.15899400
H	1.06288400	-1.79944200	2.05848600
C	4.18349900	0.58014300	-2.83277300
N	4.84700100	0.99561000	-3.68647400

1a

m06-2x/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -517.201129 a.u.

Carga = 0 Multiplicidad= 1

C	1.22685400	-0.09887300	-0.49101800
C	1.82650700	-1.33101600	-0.14362900
C	3.21325200	-1.48568300	-0.09823800
C	3.99260800	-0.38058700	-0.40798500
C	3.41390000	0.85183400	-0.75515000
C	2.03514100	0.99927600	-0.79814100
H	3.66331800	-2.43506600	0.16867000
H	5.07277600	-0.47206300	-0.38163900
H	4.05375000	1.69380100	-0.99251500
H	1.59088800	1.95197400	-1.06694600
C	-0.20668000	-0.30791300	-0.43726300
C	-0.40204600	-1.65619000	-0.06035500
C	-1.31525700	0.50981700	-0.67281500
C	-1.67961200	-2.20039700	0.08441500
C	-2.58750400	-0.02508000	-0.53096300
H	-1.18283500	1.54660800	-0.96376100
C	-2.76271500	-1.36783700	-0.15561000
H	-1.81846000	-3.23591400	0.37343000
H	-3.45687300	0.59604100	-0.71277200
H	-3.76662900	-1.76413600	-0.05122700
N	0.83085100	-2.25247600	0.11150700
H	0.98035700	-3.21090500	0.38447400

1e

m06-2x/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -609.449875 a.u.

Carga = 0 Multiplicidad= 1

C	1.17508800	-0.44328500	-0.87422800
C	1.82040500	-0.94682400	0.28383300
C	3.21246500	-0.94647000	0.41405400
C	3.95614700	-0.43602900	-0.63102300
C	3.32528100	0.06780000	-1.78868600
C	1.93632300	0.06825300	-1.91799600
H	3.69354500	-1.33486800	1.30337300
H	5.03739200	-0.41978100	-0.56764700
H	1.47088400	0.46007000	-2.81520200
C	-0.24865600	-0.60657100	-0.65852300
C	-0.39182400	-1.19933900	0.61463900
C	-1.38513400	-0.31003900	-1.41571200
C	-1.64393200	-1.50422700	1.14836900
C	-2.63307400	-0.60998900	-0.89123600
H	-1.29292800	0.14601000	-2.39560300
C	-2.75638600	-1.20129600	0.37769100
H	-1.74243000	-1.95982100	2.12692600
H	-3.52554500	-0.38553200	-1.46341600
H	-3.74388200	-1.42546800	0.76503200
N	0.86569100	-1.39224300	1.16024800
H	1.05108900	-1.80185100	2.06296400
C	4.13209100	0.58765000	-2.85213000
N	4.78389800	1.00457100	-3.70582200

13b-radical-anión-dmso

m06-2x/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -1070,286203 a.u.

Carga = -1 Multiplicidad= 2

C	-2.00765200	-0.53785700	0.02733800
C	-0.97445800	-1.54415900	-0.11822600
C	-1.44409900	-2.90689100	-0.13117900
C	-2.77132700	-3.24546000	0.00830300
C	-3.75375500	-2.25434300	0.17354400
C	-3.34369800	-0.92732800	0.17849900
H	-0.69930500	-3.69034500	-0.25338200
H	-3.05666300	-4.29435800	-0.00395200
H	-4.79781100	-2.51354500	0.30296800
H	-4.10011600	-0.16225900	0.32471500
C	-1.63606900	0.88700200	0.01870200
C	-0.32230000	1.31804100	0.15725800
C	-2.57245500	1.93440400	-0.14725800

C	0.10932700	2.62548900	0.15423100
C	-2.18634100	3.27018700	-0.14826100
H	-3.62136700	1.70485900	-0.30087100
C	-0.84737200	3.63324900	0.00371300
H	1.16124700	2.87323900	0.26823600
H	-2.94075400	4.03824900	-0.28268200
H	-0.55253200	4.67743000	-0.00244500
N	0.31008100	-1.20978300	-0.23619000
H	0.86279500	-2.06295500	-0.33870900
H	1.71443300	0.20696300	1.27850800
C	2.79915300	0.24904400	1.38644500
H	3.17651100	1.27260300	1.40202200
H	3.12327700	-0.28774100	2.27702800
S	3.50285900	-0.59908500	-0.03828800
O	5.01435100	-0.35104300	0.02383000
C	2.86431500	0.51906300	-1.29743800
H	1.77641100	0.44554200	-1.26373200
H	3.22289400	1.52673500	-1.08193900
H	3.24818600	0.17783200	-2.25793600

13f-radical-anión-dmso

m06-2x/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -1162.546320 a.u.

Carga = -1 Multiplicidad= 2

C	-2.05056300	-0.56404200	0.10301800
C	-1.00488000	-1.58400600	0.02616000
C	-1.47479600	-2.95279400	-0.04119000
C	-2.79797400	-3.28745900	0.00989800
C	-3.79016800	-2.28275000	0.12505900
C	-3.37887600	-0.93830100	0.16492300
H	-0.72658800	-3.73584000	-0.12844200
H	-3.09687000	-4.33029400	-0.03340500
H	-4.14389600	-0.17527900	0.26813300
C	-1.66877100	0.86493600	0.11346400
C	-0.40306300	1.29461900	0.48946200
C	-2.54482100	1.89212300	-0.28938400
C	0.04185800	2.59985100	0.51016000
C	-2.14528200	3.22249200	-0.29859300
H	-3.54167800	1.64493400	-0.63976900
C	-0.85729000	3.58789100	0.09254000
H	1.05542400	2.85259200	0.80995400

H	-2.84309300	3.98272800	-0.63238300
H	-0.55334100	4.62911300	0.07556200
N	0.26454700	-1.24135900	0.01209100
H	0.83733500	-2.08173100	-0.06154600
H	1.89265000	0.56607700	1.36977500
C	2.96181900	0.35930500	1.32036700
H	3.54937600	1.27756400	1.27585200
H	3.27188300	-0.24206400	2.17386600
S	3.29966900	-0.60998400	-0.16267300
O	4.82711400	-0.67293400	-0.27441300
C	2.79716000	0.63027500	-1.37417700
H	1.75419400	0.89451700	-1.20760400
H	3.45142100	1.49628600	-1.26161500
H	2.92707000	0.18884500	-2.36115700
C	-5.16235600	-2.62083600	0.20071300
N	-6.28476300	-2.90115200	0.25878600

13b-ET-abstracción-dmso

m06-2x/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -1070,268788 a.u.

Carga = -1 Multiplicidad= 2

C	1.62788300	-0.40460600	0.01211100
C	0.78993900	-1.33535100	0.73827100
C	1.18338700	-2.71405600	0.61348500
C	2.29406400	-3.11940500	-0.10127900
C	3.10990900	-2.19177600	-0.76253800
C	2.74992200	-0.84670100	-0.68593800
H	0.57563500	-3.45740300	1.12520800
H	2.53352900	-4.17890500	-0.14796700
H	3.97896400	-2.50572000	-1.32866300
H	3.35022200	-0.10604800	-1.20996000
C	1.31321800	1.04256400	0.02278100
C	0.03794900	1.52300400	-0.25690100
C	2.28954900	2.01869900	0.27778300
C	-0.30187500	2.85789000	-0.31758300
C	1.98320300	3.37891900	0.23926700
H	3.29991300	1.70071900	0.51896200
C	0.69162400	3.80763200	-0.05295500
H	-1.31172700	3.16840000	-0.56946700
H	2.76046300	4.10795000	0.44241500
H	0.45606200	4.86619100	-0.08113800

N	-0.25016000	-0.91358400	1.46088200
H	-0.67599600	-1.72613500	1.90853400
H	-0.88737300	0.57884800	-0.64733900
C	-1.65419500	-0.26332300	-1.24044400
H	-2.17103500	0.28162500	-2.03129300
H	-0.98824500	-1.04185400	-1.60620500
S	-2.86885100	-0.91504700	-0.09518600
O	-4.18093800	-1.00204900	-0.89152100
C	-3.04716900	0.56652400	0.92136900
H	-2.09309000	0.72862200	1.41956500
H	-3.32075300	1.39740700	0.26953300
H	-3.84261300	0.37118200	1.63921200

13f-ET-abstracción-dmso

m06-2x/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -1162,532153 a.u.

Carga = -1 Multiplicidad= 2

C	1.65201000	-0.38359900	-0.00011300
C	0.83564400	-1.31046600	0.77427800
C	1.21404600	-2.70304300	0.65368500
C	2.28636800	-3.12196100	-0.08608300
C	3.08699500	-2.19334900	-0.79058900
C	2.73434300	-0.82905700	-0.72470500
H	0.61892100	-3.43408300	1.19422600
H	2.52924600	-4.17912900	-0.13501800
H	3.32462700	-0.10744600	-1.28313800
C	1.32692100	1.06273300	0.00409100
C	0.05116000	1.52632900	-0.29472400
C	2.29208600	2.04224900	0.27565200
C	-0.30081900	2.85773800	-0.35619900
C	1.97263200	3.39942700	0.23475600
H	3.30077800	1.73121600	0.53167800
C	0.68125100	3.81445600	-0.07580000
H	-1.30998700	3.15986800	-0.61950700
H	2.73917400	4.13587600	0.45017700
H	0.43613400	4.87071500	-0.10578200
N	-0.15787600	-0.87240000	1.51882400
H	-0.58958900	-1.66814700	1.99002800
H	-0.86371900	0.57176700	-0.67853600
C	-1.64487900	-0.27466600	-1.25384800
H	-2.19606100	0.28461700	-2.01082300

H	-0.99241000	-1.04061500	-1.66772900
S	-2.80391000	-0.95975800	-0.07133600
O	-4.12300500	-1.13319400	-0.83608200
C	-3.02754000	0.53495400	0.91669600
H	-2.07763800	0.74676800	1.40477500
H	-3.33933300	1.34337700	0.25395000
H	-3.80645700	0.32336800	1.64780800
C	4.19558600	-2.61805200	-1.56030700
N	5.10442400	-2.96390400	-2.19039900

13b-ET-C-N-dmso

m06-2x/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -1070,278641 a.u.

Carga = -1 Multiplicidad= 2

C	-1.11225700	0.88655800	-0.25476000
C	-0.37336100	0.93226800	0.96864100
C	0.50698000	2.02218100	1.16022500
C	0.60623900	3.02782800	0.20597800
C	-0.15052500	2.99095700	-0.96906900
C	-1.00803300	1.91068200	-1.18918200
H	1.09876900	2.07285500	2.06964100
H	1.29168900	3.85272400	0.37713200
H	-0.05686500	3.77850700	-1.70824500
H	-1.57745300	1.85296300	-2.11348400
C	-1.94328900	-0.32279200	-0.31788600
C	-1.49614600	-1.35097800	0.54531700
C	-3.14683400	-0.45041900	-1.00860200
C	-2.34642300	-2.43651400	0.79496100
C	-3.96501900	-1.56906600	-0.79529800
H	-3.47347800	0.33565000	-1.68576500
C	-3.57515400	-2.53738200	0.12792600
H	-2.04287700	-3.24235000	1.46054800
H	-4.90864500	-1.66251600	-1.32208300
H	-4.21973000	-3.39342700	0.31339900
N	-0.62609400	-0.08620200	1.83177000
H	0.14980600	-0.30590800	2.45394300
H	1.44155500	0.74089300	-1.26043600
C	2.51968000	0.57728800	-1.25128000
H	2.83373700	-0.07960100	-2.06344800
H	3.03826600	1.53291000	-1.30966200
S	2.99220700	-0.20221200	0.30525500

O	4.44780300	-0.64199600	0.12038100
C	1.99767000	-1.69209900	0.11823800
H	0.93575800	-1.42894900	0.15163000
H	2.26872100	-2.17544800	-0.82149300
H	2.23866600	-2.34045000	0.96013500

20a-dmso

m06-2x/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -1070.292890 a.u.

Carga = -1 Multiplicidad= 2

C	-0.22407300	0.71863700	1.11918900
C	-0.02310600	-0.51761500	0.39898900
C	-0.31408600	-1.74453700	1.08443700
C	-0.81355100	-1.75296100	2.36418100
C	-1.03489700	-0.53959300	3.03356400
C	-0.73816600	0.67203500	2.40763300
H	-0.13830200	-2.67441900	0.55400000
H	-1.03259900	-2.69254900	2.85823500
H	-1.42051400	-0.54082600	4.04631000
H	-0.88375100	1.60033400	2.94984300
C	0.11750800	2.02463000	0.51248100
C	1.36234200	2.23392800	-0.09292800
C	-0.78658400	3.08989700	0.57935400
C	1.69247700	3.47813700	-0.61621100
C	-0.46024500	4.33259500	0.04477200
H	-1.75894000	2.93743100	1.03675800
C	0.78036400	4.53022800	-0.55478600
H	2.66486000	3.62826700	-1.07244800
H	-1.17694000	5.14475900	0.09516400
H	1.03675700	5.49868500	-0.96952500
N	0.38161700	-0.48384400	-0.86688600
H	0.49994200	-1.44454400	-1.19805700
H	2.07446900	1.41802500	-0.13170400
C	3.56717200	-1.51043600	1.47623200
H	4.65307500	-1.37676200	1.53423400
H	3.15702400	-1.97548000	2.37435100
S	3.11305200	-2.42808600	0.10737000
O	3.97360300	-3.71073300	-0.17465400
C	3.69618500	-1.33012400	-1.20967400
H	3.08695500	-0.42850900	-1.22839300
H	4.74171000	-1.08624100	-1.00862700

H	3.61308800	-1.86088900	-2.15737100

20e-dmso

m06-2x/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -1070.352174 a.u.

Carga = -1 Multiplicidad= 2

C	-0.42472800	0.37054900	1.40216200
C	-0.56259900	-0.64578600	0.40325800
C	-1.11962400	-1.88282900	0.66046100
C	-1.57432300	-2.14311900	1.98141300
C	-1.44588000	-1.16958300	2.97580300
C	-0.88026600	0.08180000	2.71857400
H	-1.20964000	-2.63044600	-0.12139900
H	-2.01863400	-3.10420400	2.21540800
H	-1.79717400	-1.39317400	3.97951100
H	-0.78943200	0.82037400	3.50894000
C	0.19836100	1.48482500	0.79321600
C	0.43132400	1.15096500	-0.57913600
C	0.60717600	2.77414400	1.25124100
C	1.04154100	2.01126800	-1.47303700
C	1.22633200	3.64014600	0.34640800
H	0.45190700	3.06984000	2.28376400
C	1.45150200	3.28881700	-0.98679000
H	1.20311600	1.72497200	-2.50763900
H	1.54880900	4.61913100	0.69126200
H	1.93523500	3.98831000	-1.65947600
N	-0.03223400	-0.14245300	-0.77671500
H	-0.02477300	-0.62919100	-1.65876100
H	3.03080100	1.60994300	0.36814200
C	3.61358200	0.92033700	0.98086200
H	4.65821400	0.88290600	0.66826100
H	3.53935900	1.20622200	2.02908600
S	2.91800700	-0.73698100	0.82908100
O	3.92014900	-1.66847100	1.52075700
C	3.22623700	-0.93624400	-0.93875100
H	2.71773500	-0.13679300	-1.47747000
H	4.30414400	-0.89856200	-1.10146500
H	2.83034900	-1.90642600	-1.23500900

***t*-BuO-anión**

m06-2x/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -232.99136 a.u.

Carga = -1 Multiplicidad= 1

C	1.75341800	-1.36455500	0.93276700
C	3.29732800	-1.32329100	0.86183100
H	1.35735500	-0.34402000	0.92627700
H	1.35640200	-1.88417500	0.05442500
H	1.37844600	-1.87225900	1.82924900
C	3.80350900	-2.78346600	0.89477500
C	3.80471500	-0.62148200	2.14223000
H	4.89831900	-2.79643600	0.88117300
H	3.46697700	-3.33548900	1.78054300
H	3.45007300	-3.31554600	0.00535100
H	3.47869900	-1.11775500	3.06399100
H	4.89943000	-0.59250400	2.13725100
H	3.44255100	0.41178800	2.16302500
O	3.72851700	-0.67097300	-0.26495000

***t*-BuO-radical**

m06-2x/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -232.828538 a.u.

Carga = 0 Multiplicidad= 2

C	1.73086800	-1.35912600	0.92761600
C	3.26022600	-1.37744900	0.90790800
H	1.36341200	-0.33156800	0.94725100
H	1.33597200	-1.85493000	0.03809600
H	1.35366700	-1.88462700	1.80751400
C	3.81589600	-2.80274700	0.89312700
C	3.81938400	-0.59915400	2.12439800
H	4.90718900	-2.78485000	0.88649100
H	3.47902200	-3.35477500	1.77325100
H	3.46968500	-3.33386900	0.00362300
H	3.48463100	-1.10802200	3.03050400
H	4.90952600	-0.58652800	2.10626800
H	3.44436900	0.42466600	2.13271000
O	3.74189100	-0.65718300	-0.17081800

A.1.6.2 Estudio de aniónes de *N*-fenil-bifenlaminas

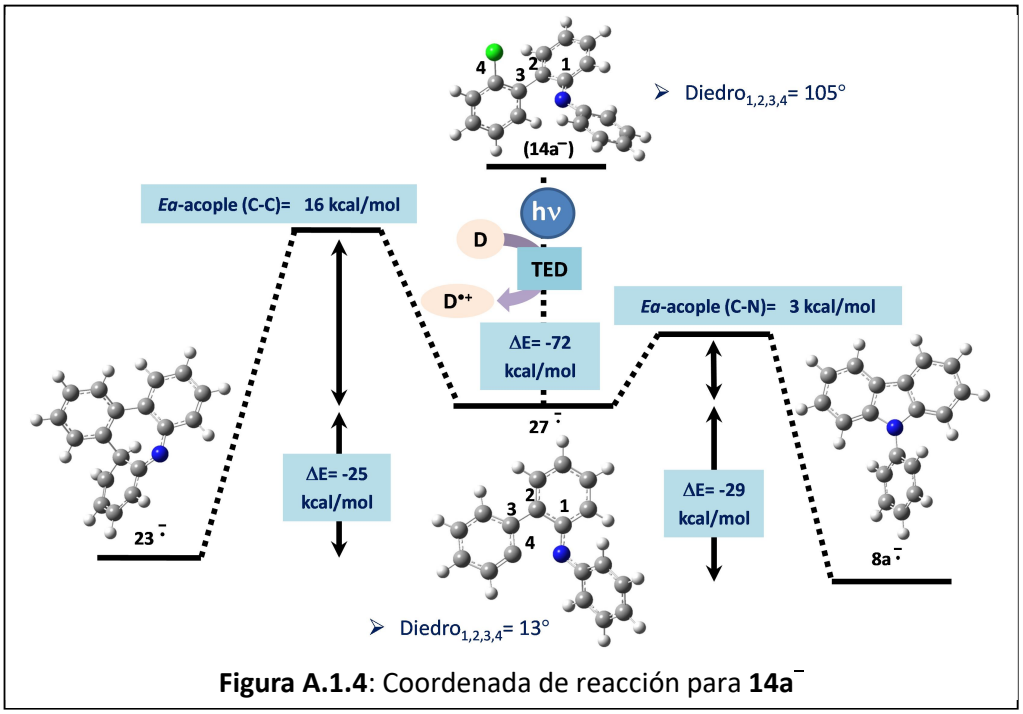


Figura A.1.4: Coordenada de reacción para **14a**$^{-}$

14a-anión

B3LYP/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -1208.748239 a.u.

Carga = -1 Multiplicidad= 1

C	0.95321	-1.37522	-0.45573
C	1.94206	-0.68703	-1.23782
C	3.29994	-1.02879	-0.95040
C	3.64333	-1.96562	0.01482
C	2.66141	-2.61850	0.76833
C	1.32369	-2.30931	0.51172
H	4.08752	-0.56287	-1.53202
H	4.69371	-2.19622	0.17819
H	2.92699	-3.34500	1.52931
H	0.54238	-2.80509	1.08283
C	-0.49478	-1.07357	-0.65238
C	-1.37861	-1.92545	-1.32514
C	-1.05009	0.10043	-0.11682
C	-2.73838	-1.64688	-1.46049
C	-2.40332	0.40143	-0.23708
H	-0.39126	0.78290	0.40989
C	-3.25313	-0.47622	-0.91169
H	-3.38221	-2.33904	-1.99042
H	-2.79480	1.31624	0.19566

H	-4.31043	-0.25506	-1.01238
N	1.53041	0.13482	-2.24178
Cl	-0.78051	-3.42084	-2.06855
C	2.29809	1.14083	-2.75643
C	3.28190	1.89427	-2.04774
C	2.04421	1.57176	-4.09205
C	3.94490	2.96932	-2.63252
H	3.50085	1.64085	-1.01603
C	2.71610	2.64293	-4.66772
H	1.29118	1.03349	-4.66197
C	3.68252	3.35918	-3.95020
H	4.67768	3.51801	-2.04480
H	2.48478	2.92469	-5.69229
H	4.20838	4.19492	-4.40057

27-radical-anión

B3LYP/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -748.449411 a.u.

Carga = -1 Multiplicidad= 2

C	1.02473	-0.98110	-0.05910
C	2.01419	-0.20911	-0.75845
C	3.37892	-0.52039	-0.50019
C	3.74806	-1.51452	0.39415
C	2.77525	-2.25967	1.07350
C	1.43178	-1.97994	0.83631
H	4.14738	0.05923	-1.00082
H	4.80308	-1.71088	0.56802
H	3.05972	-3.04654	1.76466
H	0.67980	-2.57256	1.34861
C	-0.39235	-0.68581	-0.33676
C	-0.72822	0.10707	-1.43571
C	-1.46344	-1.14579	0.46271
C	-2.02773	0.46691	-1.74724
C	-2.78301	-0.81615	0.15516
H	-1.27099	-1.74960	1.34509
C	-3.07779	-0.00973	-0.94783
H	-2.24916	1.09869	-2.60569
H	-3.58594	-1.18166	0.78859
H	-4.10791	0.24695	-1.18139
N	1.60572	0.83474	-1.53242

C	2.25186	1.25408	-2.66039
C	2.05905	2.59449	-3.09824
C	3.04609	0.42835	-3.50728
C	2.62109	3.07123	-4.27628
H	1.44891	3.24869	-2.48166
C	3.60430	0.91669	-4.68421
H	3.20584	-0.60939	-3.23419
C	3.40628	2.24219	-5.08663
H	2.44725	4.10411	-4.56754
H	4.19877	0.24902	-5.30342
H	3.84596	2.61612	-6.00560

ET-CN-ciclización 14a-8a

B3LYP/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -748.444578 a.u.

Carga = -1 Multiplicidad= 2

C	1.07713	-1.22845	-0.03231
C	2.02025	-0.38844	-0.70084
C	3.38950	-0.54484	-0.39794
C	3.80126	-1.50338	0.52516
C	2.87238	-2.32428	1.17735
C	1.51322	-2.17380	0.89857
H	4.12424	0.09174	-0.87947
H	4.86095	-1.61183	0.73979
H	3.20629	-3.07229	1.88945
H	0.78787	-2.80770	1.40192
C	-0.29397	-0.88269	-0.40267
C	-0.35108	-0.08128	-1.56469
C	-1.45723	-1.12429	0.33887
C	-1.53883	0.59345	-1.88720
C	-2.66214	-0.51141	-0.03061
H	-1.42743	-1.76327	1.21882
C	-2.68958	0.36761	-1.12268
H	-1.59878	1.23773	-2.76269
H	-3.56424	-0.69377	0.54549
H	-3.62338	0.85551	-1.39590
N	1.46769	0.58212	-1.50496
C	2.07064	1.11393	-2.61810
C	1.68749	2.41330	-3.04727
C	2.96599	0.39897	-3.46204
C	2.18288	2.96511	-4.22211

H	0.99463	2.97655	-2.42927
C	3.46128	0.96599	-4.63113
H	3.26457	-0.60708	-3.18693
C	3.08366	2.25510	-5.02802
H	1.87032	3.96477	-4.51287
H	4.14680	0.39096	-5.24883
H	3.47507	2.69168	-5.94109

8a-radical-anión

B3LYP/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -748.745614891 a.u.

Carga = -1 Multiplicidad= 2

C	-1.91499	0.78143	-0.03858
C	-0.53546	1.16553	-0.06838
C	-0.12772	2.48142	-0.21536
C	-1.13638	3.48540	-0.32743
C	-2.49072	3.13415	-0.29213
C	-2.90591	1.80501	-0.15113
H	0.92253	2.74988	-0.24659
H	-0.84487	4.52536	-0.43840
H	-3.24195	3.91665	-0.37724
H	-3.96311	1.55596	-0.13373
C	-1.96887	-0.62845	0.09213
C	-0.62253	-1.11531	0.13519
C	-3.03510	-1.57449	0.19516
C	-0.31629	-2.45807	0.28636
C	-2.72235	-2.93097	0.34072
H	-4.07032	-1.24656	0.16835
C	-1.39868	-3.38313	0.38941
H	0.71035	-2.80522	0.32605
H	-3.53111	-3.65460	0.41922
H	-1.18741	-4.44199	0.50325
N	0.23765	-0.00571	0.03704
C	1.65426	-0.06018	0.04353
C	2.33616	-0.85222	-0.88840
C	2.38743	0.67642	0.98205
C	3.72859	-0.91235	-0.87404
H	1.77215	-1.41384	-1.62434
C	3.78034	0.62594	0.98134
H	1.86278	1.28167	1.71254
C	4.45702	-0.17111	0.05719

H	4.24477	-1.53153	-1.60076
H	4.33683	1.20255	1.71332
H	5.54112	-0.21407	0.06259

ET-CC-ciclización-8a

B3LYP/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -748.423916 a.u.

Carga = -1 Multiplicidad= 2

C	1.54971	0.37159	0.04294
C	1.62983	-1.03132	-0.31675
C	2.94653	-1.59534	-0.40759
C	4.09270	-0.89121	-0.10585
C	4.00651	0.45343	0.29352
C	2.75193	1.04772	0.34263
H	3.00751	-2.63718	-0.71085
H	5.06098	-1.38064	-0.17826
H	4.89734	1.02995	0.52120
H	2.71056	2.10635	0.57525
C	0.29691	1.17385	-0.02968
C	-0.81917	0.85698	-0.81992
C	0.18862	2.40886	0.66376
C	-1.90248	1.69383	-1.01170
C	-0.89333	3.26847	0.49821
H	0.96884	2.70074	1.35898
C	-1.93915	2.93385	-0.36462
H	-2.73472	1.38615	-1.63891
H	-0.92216	4.20071	1.05469
H	-2.78130	3.60526	-0.50708
N	0.59832	-1.83306	-0.64252
C	-0.67248	-1.62702	-0.17834
C	-1.72636	-1.33694	-1.08675
C	-1.02204	-1.73580	1.19013
C	-3.06349	-1.32338	-0.66880
H	-1.48918	-1.29643	-2.14414
C	-2.34615	-1.64745	1.60777
H	-0.23356	-1.91977	1.91470
C	-3.38197	-1.45525	0.68078
H	-3.85185	-1.17422	-1.40156
H	-2.58207	-1.75555	2.66334
H	-4.41534	-1.42307	1.01178

23-radical anión (C-C)

B3LYP/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -748.485272 a.u.

Carga = -1 Multiplicidad= 2

C	1.59817	-0.73407	-0.10973
C	2.88775	-0.62866	-0.74063
C	4.02061	-0.96515	0.05921
C	3.92208	-1.31597	1.39212
C	2.66418	-1.37071	2.01205
C	1.53592	-1.09309	1.25106
H	4.99222	-0.92302	-0.42405
H	4.82188	-1.54167	1.95796
H	2.57027	-1.62549	3.06269
H	0.56059	-1.14022	1.72655
C	0.32867	-0.56845	-0.85503
C	0.16502	0.43897	-1.83551
C	-0.75050	-1.43534	-0.59663
C	-1.05184	0.52900	-2.52260
C	-1.95761	-1.32462	-1.27960
H	-0.62907	-2.22909	0.13317
C	-2.10987	-0.33681	-2.25272
H	-1.16698	1.30289	-3.27375
H	-2.76717	-2.01516	-1.06360
H	-3.04305	-0.24279	-2.79991
N	3.15087	-0.33180	-2.05243
C	2.41596	0.51926	-2.78263
C	1.30331	1.35589	-2.11975
C	2.66175	0.69722	-4.15551
C	0.94414	2.58662	-2.92293
H	1.69524	1.67515	-1.13965
C	2.08673	1.73993	-4.89607
H	3.37627	0.02586	-4.62707
C	1.27687	2.71107	-4.24265
H	0.34879	3.34923	-2.42657
H	2.32268	1.85220	-5.95007
H	0.94359	3.58452	-4.79997

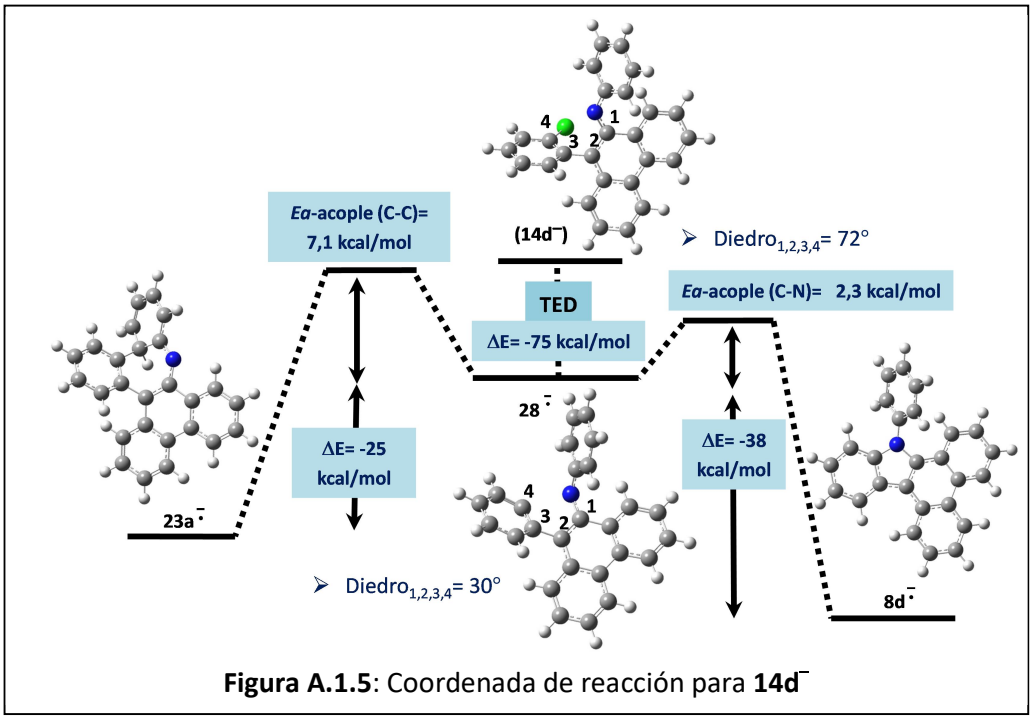


Figura A.1.5: Coordenada de reacción para **14d⁻**

14d-anión

B3LYP/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -1515.990135 a.u.

Carga = -1 Multiplicidad= 1

C	-4.30507	1.88615	1.93033
C	-4.37525	0.47994	1.93179
C	-3.23249	-0.27164	1.80900
C	-1.94749	0.33845	1.67203
C	-1.87949	1.76002	1.74778
C	-3.07296	2.50291	1.84368
C	-0.79605	-0.43416	1.43695
C	0.47848	0.17823	1.17273
C	0.58157	1.60708	1.53819
C	-0.58013	2.38140	1.77059
C	1.84314	2.20471	1.72772
C	1.96897	3.54381	2.05797
C	0.82030	4.32733	2.22161
C	-0.42915	3.75151	2.08949
C	-0.89759	-1.88939	1.37240
N	1.44722	-0.58244	0.68046
C	2.61678	-0.16629	0.08231
C	3.79772	-0.93880	0.28006
C	4.95560	-0.67160	-0.43516
C	5.00281	0.36628	-1.36568

C	3.86329	1.14325	-1.57149
C	2.69643	0.89459	-0.86418
C	-1.56717	-2.50010	0.29675
C	-1.67177	-3.88365	0.20083
C	-1.10404	-4.69800	1.18076
C	-0.43461	-4.12081	2.25577
H	-5.22504	2.47894	2.00172
H	-5.35497	-0.00959	2.02818
H	-3.29218	-1.37007	1.80625
H	-3.03370	3.60224	1.84389
H	2.75933	1.60105	1.62502
H	2.96330	3.98955	2.19410
H	0.91577	5.39360	2.46998
H	-1.31886	4.37369	2.25930
H	3.78270	-1.76592	1.00478
H	5.85090	-1.28709	-0.26299
H	5.92304	0.56861	-1.92702
H	3.88941	1.96529	-2.30186
H	1.80998	1.52395	-1.03321
H	-2.00423	-1.85603	-0.48096
H	-2.19489	-4.33640	-0.65303
H	-1.17911	-5.79096	1.10456
H	0.01897	-4.75936	3.02733
C	-0.33642	-2.72816	2.35302
Cl	0.47704	-2.08364	3.70647

28-radical-anión

B3LYP/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -1055.696407 a.u.

Carga = -1 Multiplicidad= 2

C	-4.39114	1.98669	2.07719
C	-4.41981	0.58278	2.06641
C	-3.24935	-0.13008	1.89812
C	-1.99320	0.51148	1.72855
C	-1.96141	1.93788	1.80977
C	-3.17862	2.63998	1.96392
C	-0.77017	-0.23649	1.53200
C	0.47304	0.39298	1.62526
C	0.52184	1.84744	1.76222
C	-0.67416	2.61829	1.78934

C	1.76576	2.51474	1.86857
C	1.84450	3.89084	1.94405
C	0.66674	4.65714	1.91851
C	-0.56137	4.02829	1.84996
C	-0.73627	-1.68572	1.22238
N	1.63167	-0.34819	1.67755
C	2.56282	-0.33994	0.68634
C	3.82907	-0.95464	0.91179
C	4.80370	-1.00515	-0.07528
C	4.58205	-0.44855	-1.34288
C	3.34577	0.15602	-1.59152
C	2.35695	0.20871	-0.61356
C	-1.66520	-2.34998	0.39215
C	-1.48916	-3.69183	0.04764
C	-0.38280	-4.40660	0.51077
C	0.56253	-3.75887	1.32161
C	0.35794	-2.43268	1.65610
H	-5.30703	2.55577	2.19920
H	-5.35871	0.05438	2.20097
H	-3.29025	-1.21073	1.92269
H	-3.17387	3.72181	2.01530
H	2.67024	1.92145	1.88971
H	2.81122	4.37823	2.02306
H	0.71748	5.74035	1.96537
H	-1.45249	4.64364	1.85020
H	4.01975	-1.38974	1.88912
H	5.75530	-1.48306	0.14468
H	5.34776	-0.48872	-2.11078
H	3.14492	0.58982	-2.56849
H	1.40348	0.67575	-0.84088
H	-2.50904	-1.81080	-0.02578
H	-2.21400	-4.17486	-0.60089
H	-0.24979	-5.45044	0.23803
H	1.43441	-4.30542	1.67633

8d-radical-anión

B3LYP/6-311+g(d) scrf=(solvente=dmso,pcm)

Sum of electronic and zero-point Energies= -1055.75748 a.u

Carga = -1 Multiplicidad= 2

C	-4.41491	2.25434	1.51720

C	-4.55584	0.88951	1.25480
C	-3.43487	0.07207	1.21802
C	-2.12559	0.56664	1.45255
C	-1.98413	1.97244	1.71721
C	-3.14274	2.77296	1.73343
C	-0.94838	-0.26593	1.38534
C	0.34193	0.35207	1.44415
C	0.51301	1.70610	1.79190
C	-0.65141	2.54572	1.95915
C	1.80149	2.29229	2.02576
C	1.93556	3.61095	2.40985
C	0.80135	4.42604	2.57665
C	-0.46421	3.87822	2.35275
C	-0.83888	-1.69598	1.28563
N	1.43769	-0.54384	1.33848
C	2.41291	-0.41810	0.32677
C	3.58496	-1.19188	0.41909
C	4.58109	-1.09681	-0.54793
C	4.44670	-0.21214	-1.62187
C	3.29490	0.57078	-1.71286
C	2.28625	0.47027	-0.75602
C	-1.76873	-2.78240	1.28732
C	-1.31811	-4.09926	1.17517
C	0.03806	-4.42689	1.07461
C	0.99585	-3.38494	1.11658
C	0.49586	-2.12237	1.21473
H	-5.28102	2.90817	1.54004
H	-5.53681	0.46418	1.06357
H	-3.57475	-0.96850	0.96695
H	-3.05287	3.83795	1.91218
H	2.68672	1.67755	1.91721
H	2.92728	4.01766	2.59066
H	0.90178	5.46215	2.88298
H	-1.32507	4.51948	2.50605
H	3.71152	-1.85527	1.26805
H	5.47480	-1.70656	-0.45490
H	5.22957	-0.13000	-2.36865
H	3.17477	1.26418	-2.54022
H	1.39438	1.08072	-0.83850
H	-2.83129	-2.61702	1.39933
H	-2.05515	-4.89772	1.17235

H	0.35779	-5.45843	0.97633
H	2.05964	-3.58637	1.07294

23a-radical-anión

B3LYP/6-311+g(d) scrf=(solvente=dmso,pcm)

Sum of electronic and zero-point Energies= -1055.743129 a.u

Carga = -1 Multiplicidad= 2

C	-3.71552	1.17060	3.60341
C	-3.53077	-0.13951	3.13351
C	-2.47118	-0.43315	2.29806
C	-1.54041	0.55763	1.87490
C	-1.72002	1.88201	2.38097
C	-2.81155	2.15157	3.23349
C	-0.41624	0.22313	1.02608
C	0.63884	1.14902	0.84511
C	0.41520	2.53807	1.29380
C	-0.75171	2.90830	2.01255
C	1.36972	3.53648	0.99276
C	1.18096	4.85752	1.35370
C	0.01675	5.22898	2.04350
C	-0.92426	4.26809	2.36375
C	-0.42368	-1.06112	0.28260
N	1.81412	0.94757	0.19776
C	2.46943	-0.22395	0.14795
C	1.97370	-1.43587	0.94868
C	3.02663	-2.50106	1.13045
C	4.16294	-2.52724	0.37548
C	4.46017	-1.48752	-0.55317
C	3.63587	-0.35811	-0.62393
C	-1.56282	-1.44119	-0.45577
C	-1.59135	-2.61069	-1.20739
C	-0.46834	-3.44036	-1.24109
C	0.67204	-3.07611	-0.52922
C	0.70783	-1.90211	0.23086
H	-4.54272	1.41035	4.26360
H	-4.21083	-0.92979	3.43768
H	-2.33310	-1.45618	1.97242
H	-2.95022	3.15033	3.62985
H	2.25953	3.23566	0.45613
H	1.92864	5.60317	1.10097

H	-0.14845	6.26406	2.32588
H	-1.81691	4.58040	2.89165
H	1.64715	-1.06783	1.93437
H	2.82188	-3.28841	1.85170
H	4.87215	-3.34304	0.50043
H	5.36277	-1.54089	-1.15407
H	3.91467	0.47896	-1.26008
H	-2.43360	-0.79405	-0.44998
H	-2.48207	-2.86828	-1.77251
H	-0.47855	-4.35660	-1.82378
H	1.55442	-3.70687	-0.55824

ET-CC-28-23a

B3LYP/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -1055.685510 a.u.

Carga = -1 Multiplicidad= 2

C	-3.89186	2.90700	0.17622
C	-2.63968	3.51774	0.00346
C	-1.49562	2.75034	-0.08657
C	-1.51398	1.32523	-0.00203
C	-2.80727	0.71260	0.09518
C	-3.95587	1.52526	0.20373
C	-0.30786	0.53088	-0.08808
C	-0.38087	-0.88136	-0.21597
C	-1.72336	-1.50596	-0.16227
C	-2.90052	-0.74016	0.02833
C	-1.83152	-2.91131	-0.25256
C	-3.05033	-3.55730	-0.16555
C	-4.21746	-2.80247	0.03005
C	-4.13630	-1.42610	0.12637
C	1.00832	1.21797	-0.18107
N	0.62941	-1.72919	-0.44157
C	1.93172	-1.57935	-0.04383
C	2.98222	-1.73136	-0.97992
C	4.31653	-1.74754	-0.58460
C	4.66811	-1.57420	0.75679
C	3.64589	-1.39294	1.69697
C	2.30970	-1.39415	1.31121
C	1.39255	2.24713	0.71402
C	2.59944	2.93182	0.58409

C	3.49261	2.61608	-0.44243
C	3.17644	1.56767	-1.31844
C	1.97482	0.92388	-1.13636
H	-4.79572	3.50150	0.26080
H	-2.56464	4.59908	-0.06974
H	-0.55399	3.25758	-0.24316
H	-4.93142	1.06326	0.29661
H	-0.91707	-3.47444	-0.38815
H	-3.10304	-4.63931	-0.23899
H	-5.18260	-3.29361	0.10818
H	-5.05373	-0.87133	0.27852
H	2.72156	-1.86950	-2.02503
H	5.09279	-1.88087	-1.33402
H	5.70886	-1.58321	1.06477
H	3.89596	-1.25984	2.74676
H	1.52970	-1.26501	2.05641
H	0.72564	2.50316	1.53165
H	2.84729	3.71396	1.29538
H	4.42815	3.15694	-0.55153
H	3.87113	1.26951	-2.09799

ET-CN-28-8d

B3LYP/6-311+g(d) scrf=(solvente=dmso,pcm)

Energía total con corrección de punto cero= -1055.692732 a.u.

Carga = -1 Multiplicidad= 2

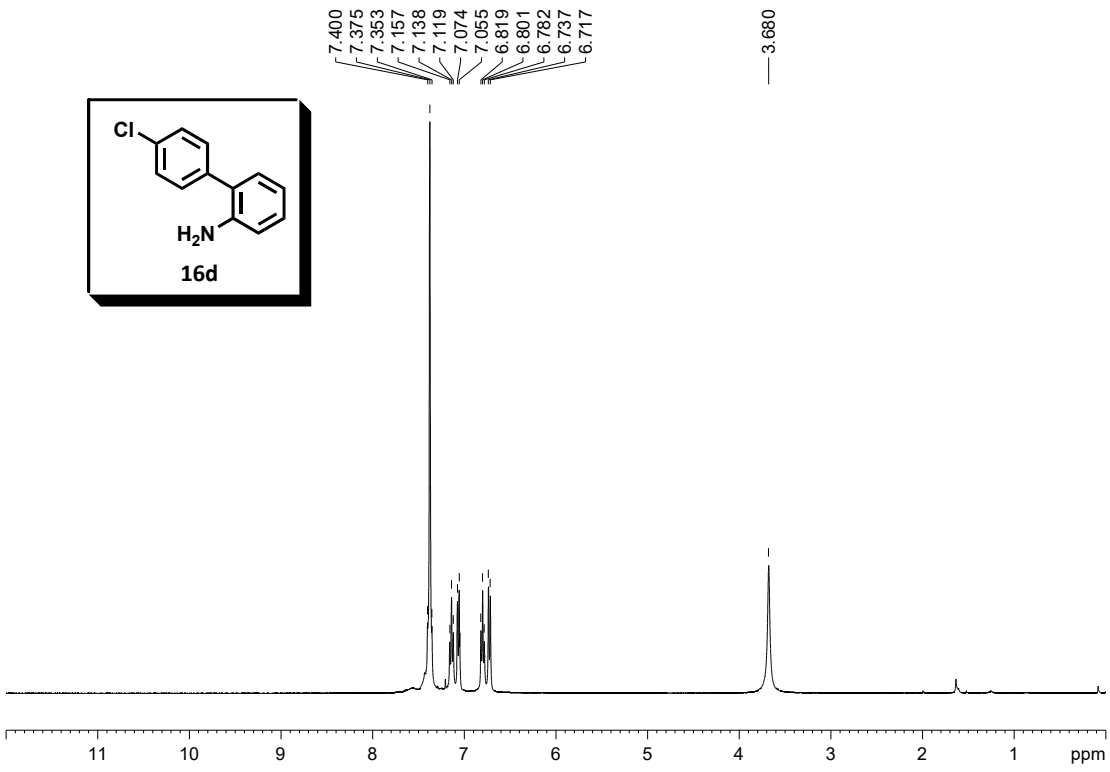
C	-4.43085	2.13990	1.99948
C	-4.52867	0.73849	1.98267
C	-3.38777	-0.02946	1.86025
C	-2.10099	0.55718	1.74476
C	-1.99767	1.98145	1.81855
C	-3.18647	2.73845	1.92974
C	-0.91279	-0.23813	1.58310
C	0.35270	0.34483	1.63565
C	0.48917	1.78045	1.77882
C	-0.67754	2.60088	1.82289
C	1.76180	2.39035	1.89868
C	1.89790	3.75958	2.00521
C	0.75333	4.57544	2.00047
C	-0.50119	4.00178	1.91870
C	-0.80654	-1.67877	1.30034

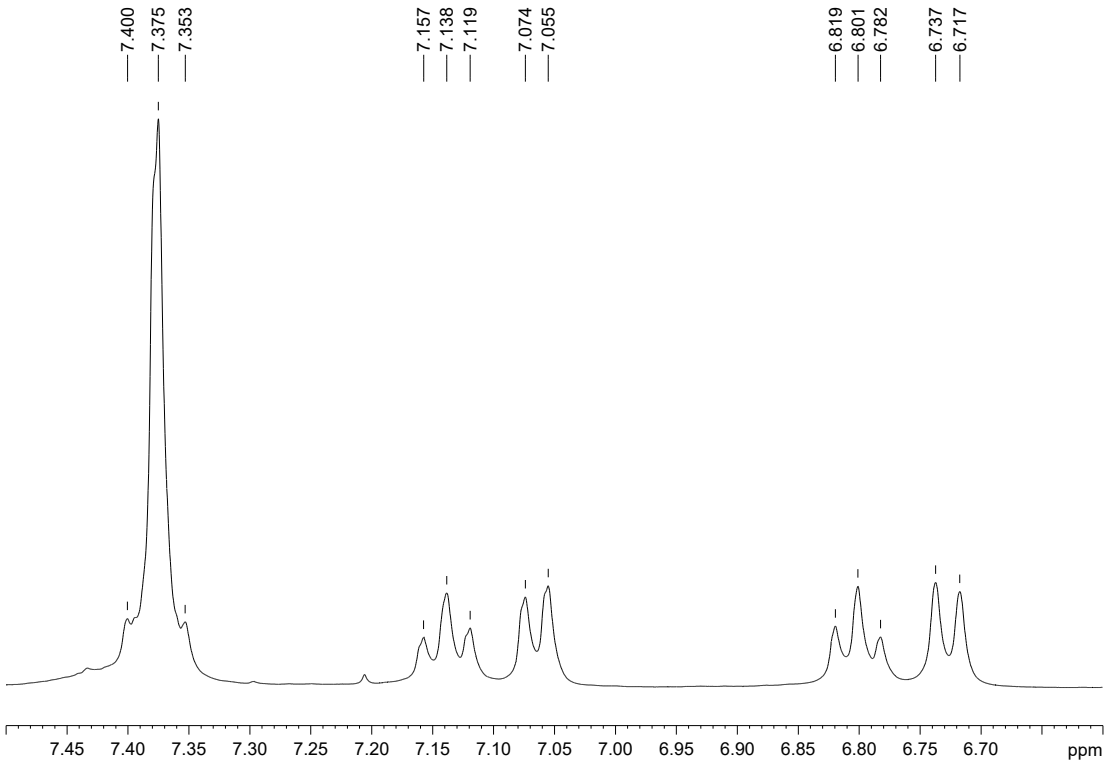
N	1.43982	-0.51719	1.62509
C	2.42239	-0.44888	0.65029
C	3.68441	-1.03926	0.90462
C	4.67634	-1.07247	-0.06950
C	4.45742	-0.51912	-1.33665
C	3.21181	0.05688	-1.61029
C	2.20877	0.08431	-0.64630
C	-1.67141	-2.48706	0.55008
C	-1.25383	-3.75606	0.11651
C	0.04124	-4.20329	0.40890
C	0.90821	-3.41779	1.17618
C	0.46583	-2.17916	1.66756
H	-5.32297	2.75157	2.08665
H	-5.49780	0.25785	2.07462
H	-3.47422	-1.10799	1.87726
H	-3.13707	3.81955	1.97472
H	2.64206	1.76077	1.90787
H	2.88426	4.20353	2.09601
H	0.85026	5.65382	2.07564
H	-1.36423	4.65554	1.93859
H	3.86940	-1.46127	1.88808
H	5.63539	-1.52771	0.16310
H	5.23564	-0.54072	-2.09262
H	3.01836	0.48499	-2.59061
H	1.24653	0.52842	-0.88212
H	-2.65274	-2.13135	0.25288
H	-1.92580	-4.37343	-0.47189
H	0.36495	-5.18172	0.05830
H	1.89366	-3.80320	1.43252

A.2 CAPÍTULO III

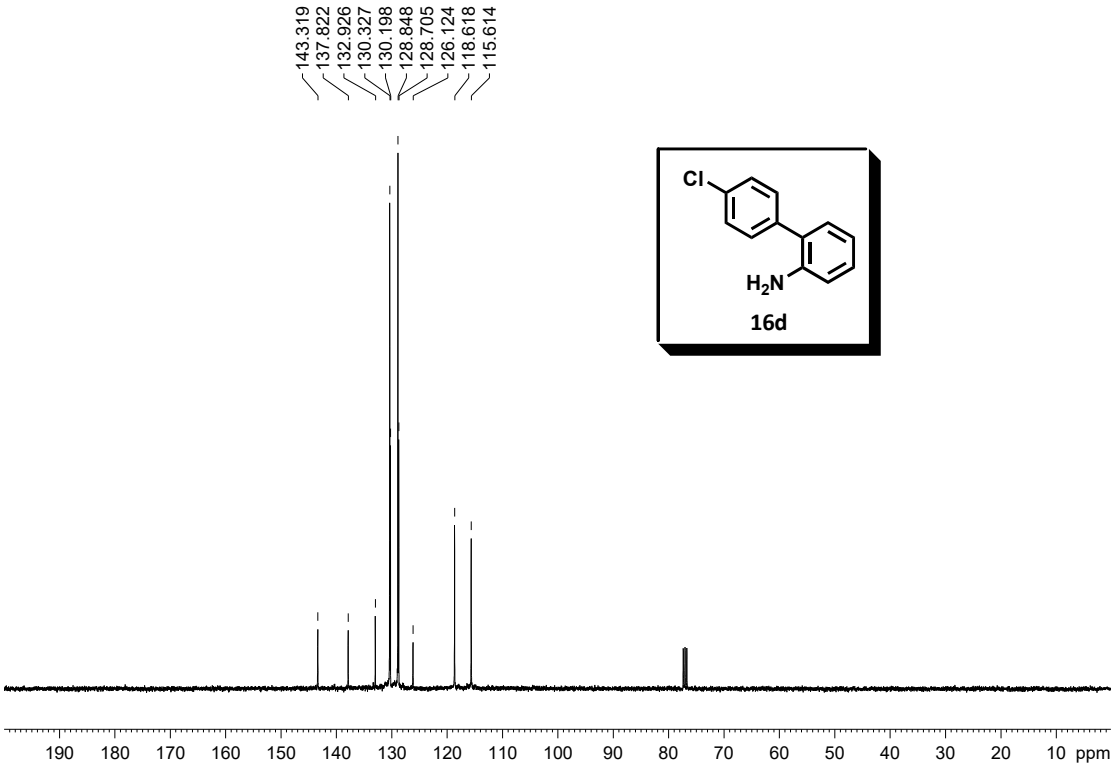
A.2.1 ESPECTROS DE RMN DE PRECURSORES Y PRODUCTOS

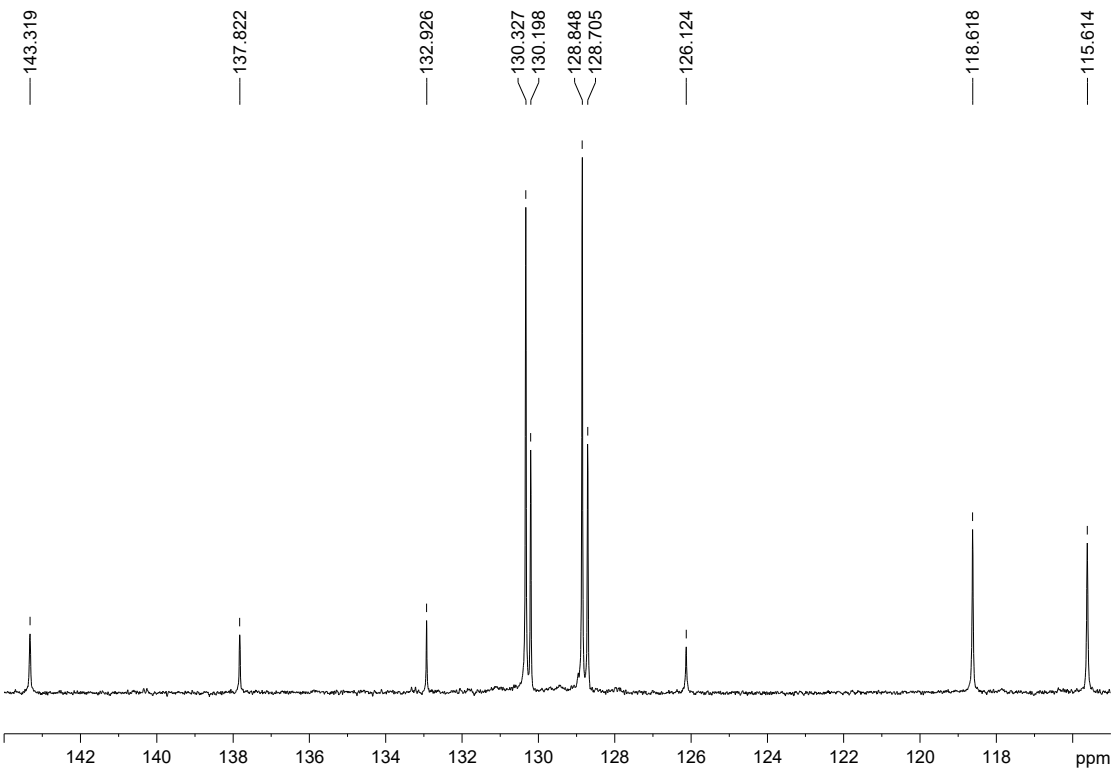
^{1}H-RMN ($CDCl_3$) 4´-cloro-[1,1'-bifenil]-2-amina (16d)


7.400
7.375
7.353
7.157
7.138
7.119
7.074
7.055
6.819
6.801
6.782
6.737
6.717
3.680
Cl
H2N
16d
11
10
9
8
7
6
5
4
3
2
1
ppm

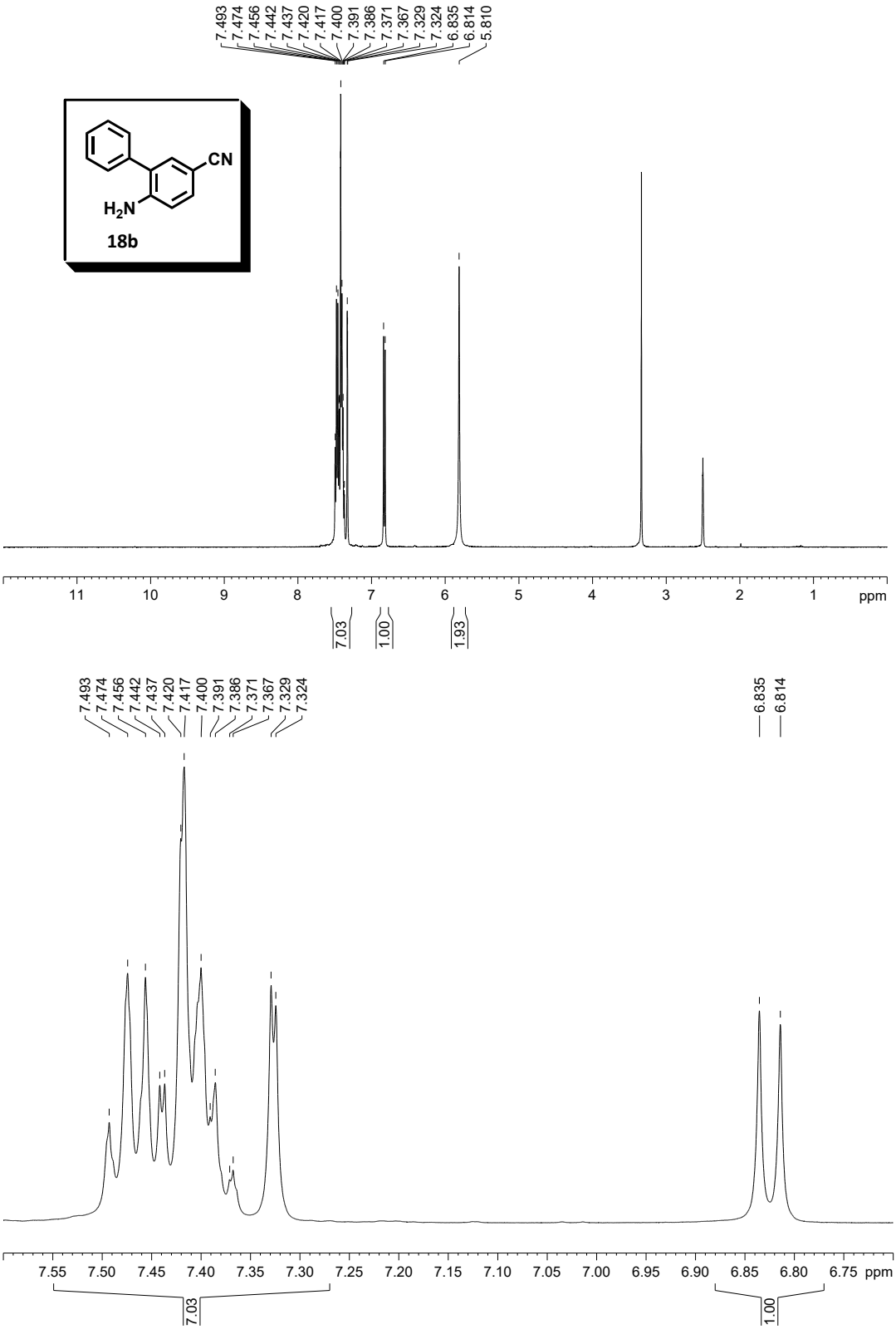

7.400
7.375
7.353
7.157
7.138
7.119
7.074
7.055
6.819
6.801
6.782
6.737
6.717
7.45
7.40
7.35
7.30
7.25
7.20
7.15
7.10
7.05
7.00
6.95
6.90
6.85
6.80
6.75
6.70
ppm

^{13}C-RMN ($CDCl_3$) 4´-cloro-[1,1'-bifenil]-2-amina (16d)

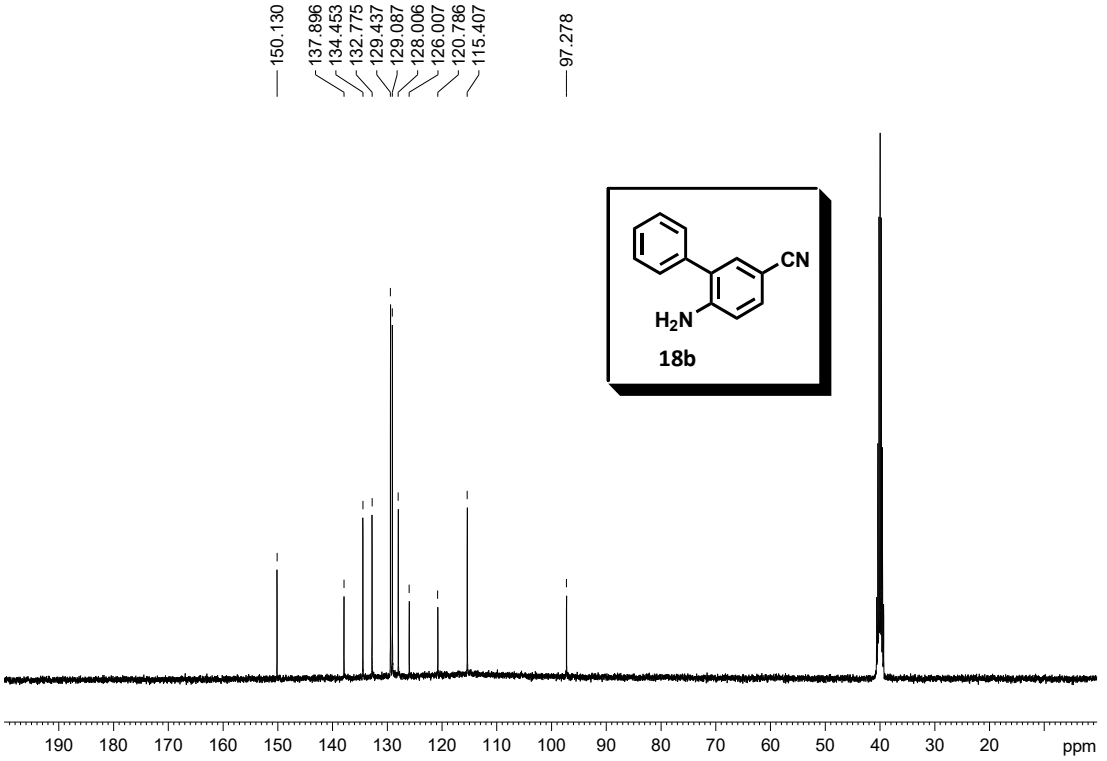


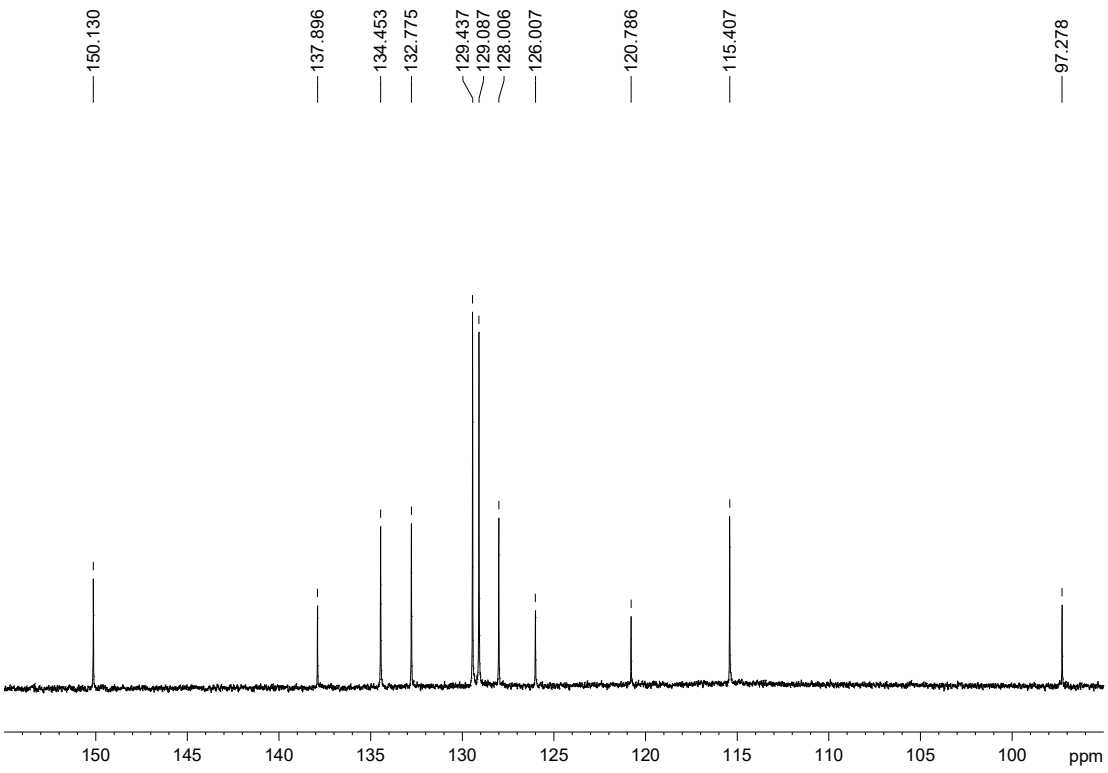


^{1}H-RMN (CD_3SOCD_3) 6-Amino-[1,1'-bifenil]-3-carbonitrilo (18b)



^{13}C-RMN (CD_3SOCD_3) 6-Amino-[1,1'-bifenil]-3-carbonitrilo (18b)

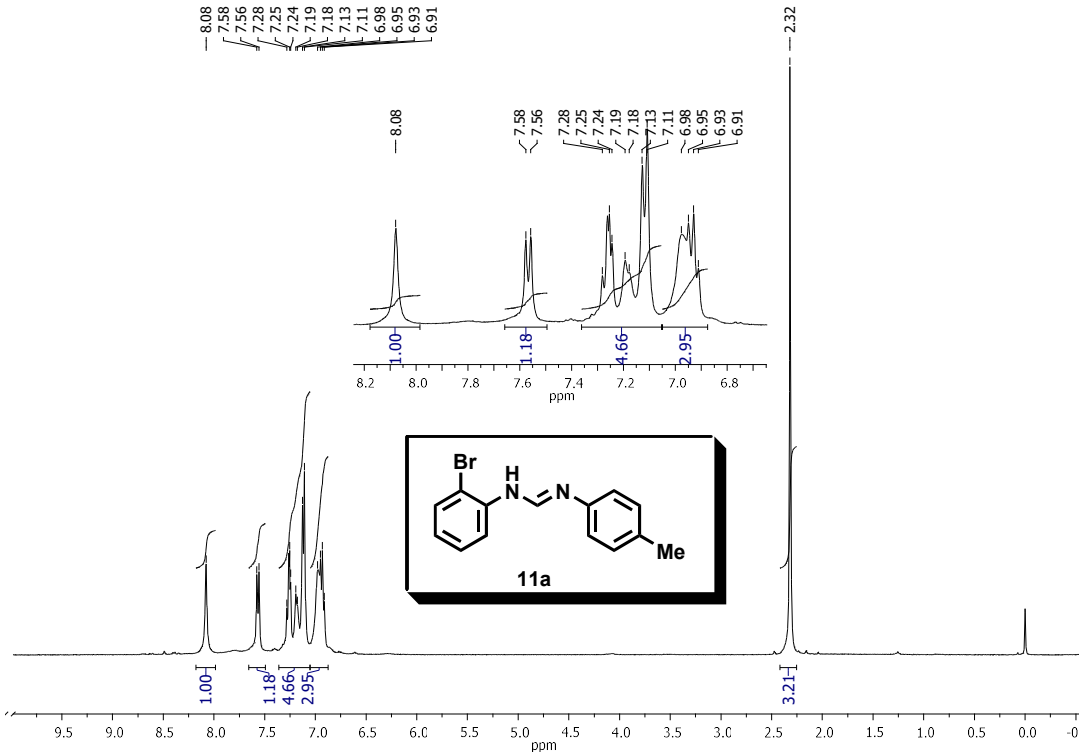




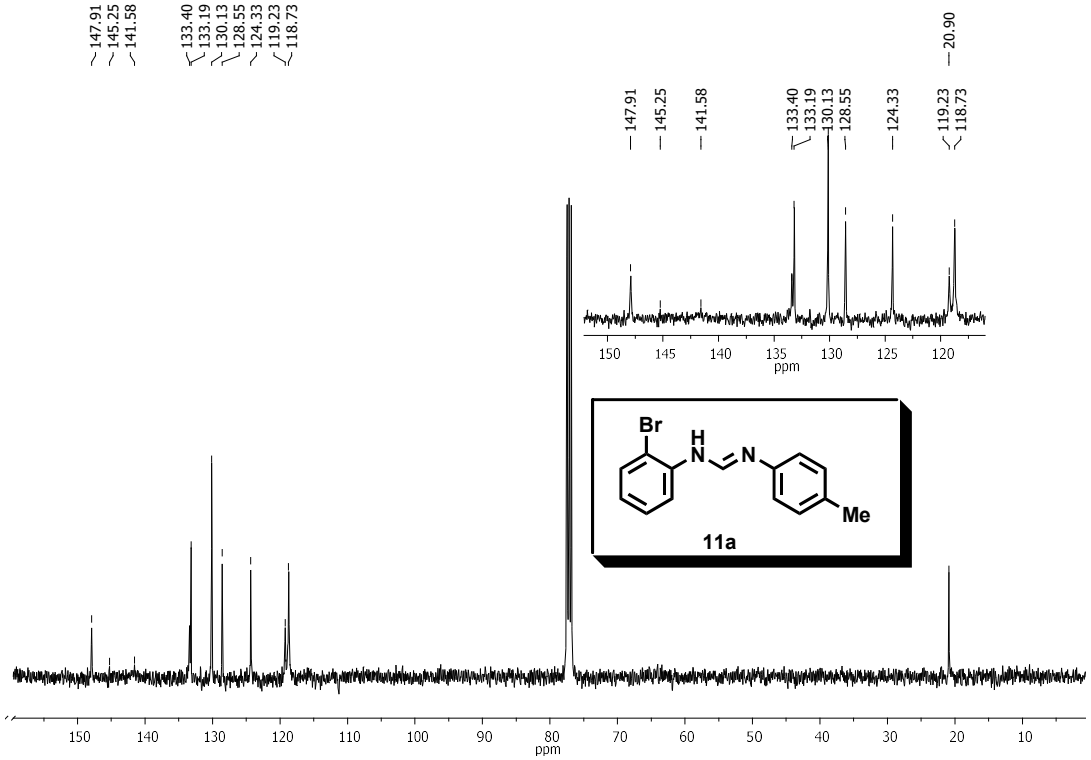
A.3 CAPÍTULO IV

A.3.1 ESPECTROS DE RMN DE PRECURSORES

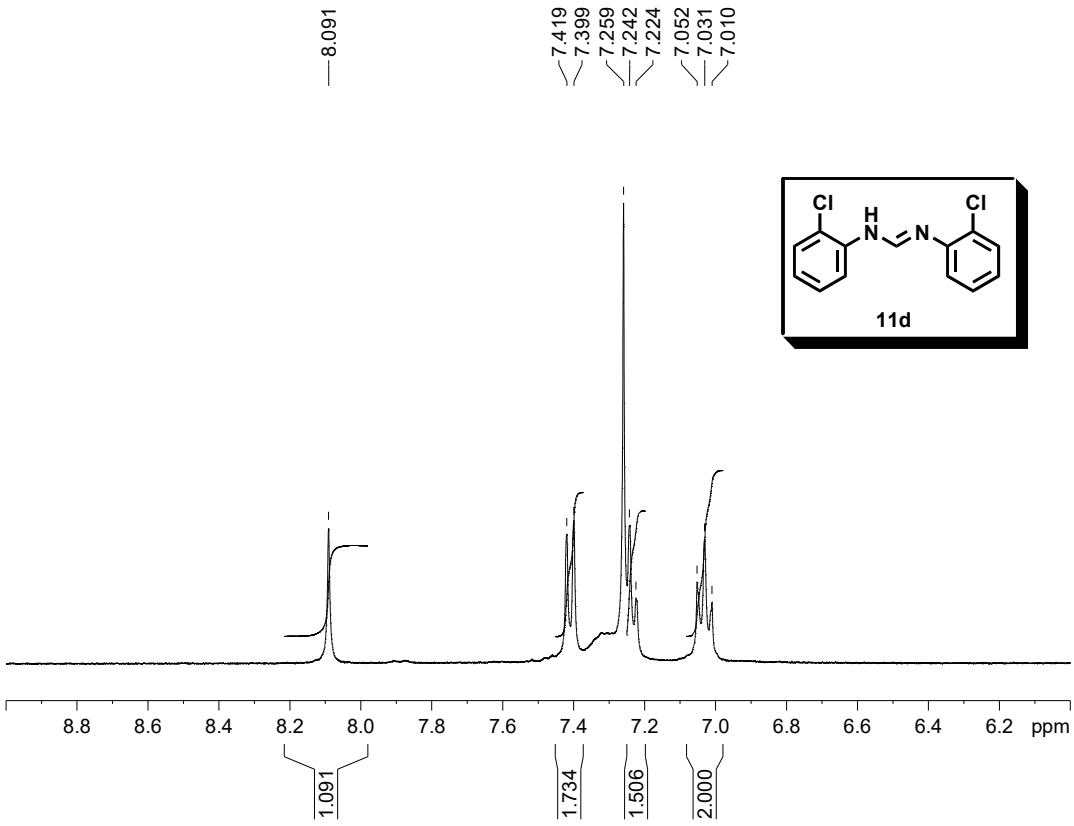
^{1}H-RMN ($CDCl_3$) *N*-(2-bromofenil)-*N*'-*p*-tolilformamidina (11a)



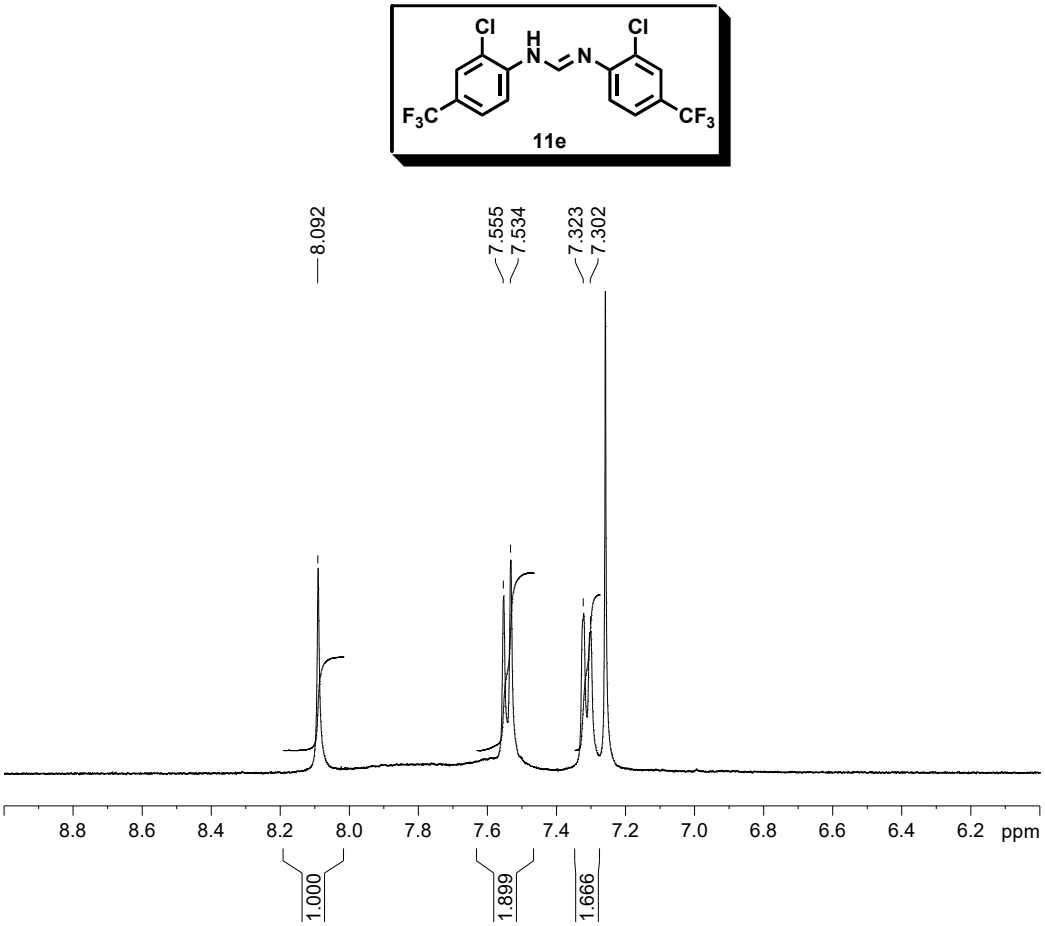
^{13}C-RMN ($CDCl_3$) *N*-(2-bromofenil)-*N*'-*p*-tolilformamidina (11a)



^{1}H-RMN ($CDCl_3$) *N*,*N*'-bis(2-clorofenil)formamidina (11d)

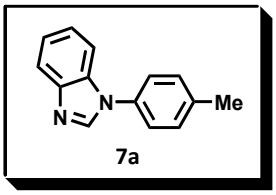


^{1}H-RMN ($CDCl_3$) *N*,*N*'-bis(2-cloro-4-(trifluormetil)fenil)formamidina (11e)

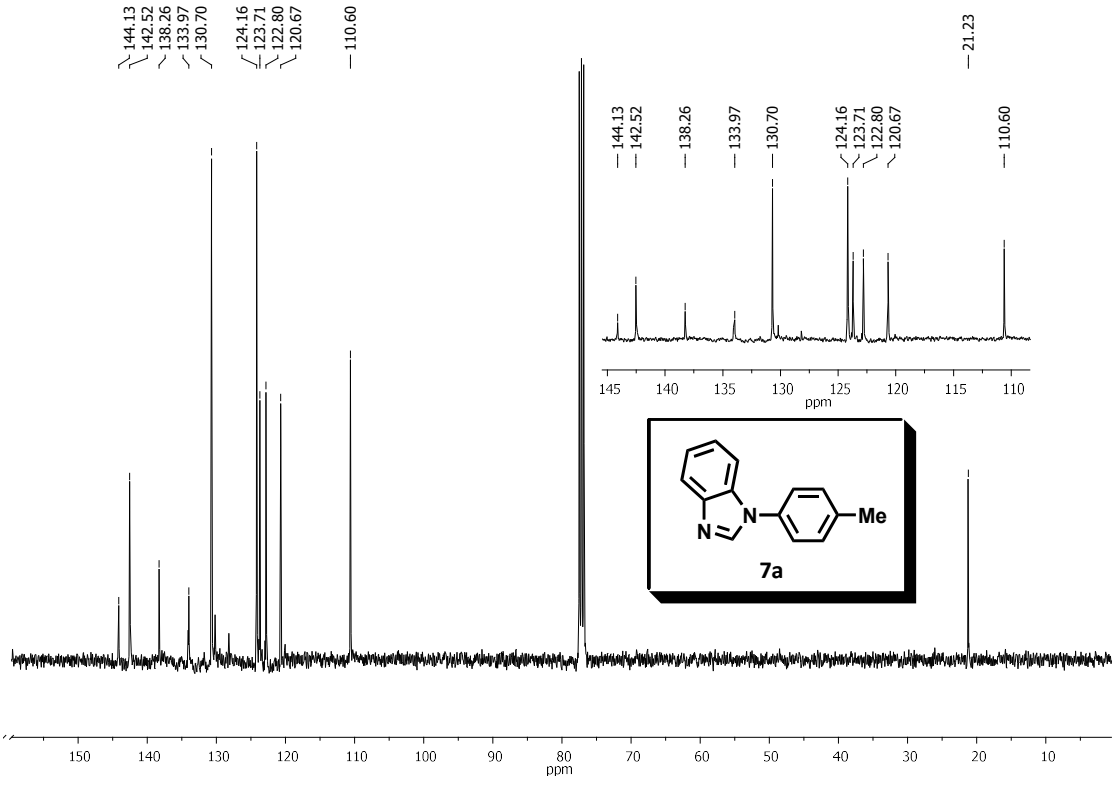


A.3.2 ESPECTROS DE RMN DE PRODUCTOS

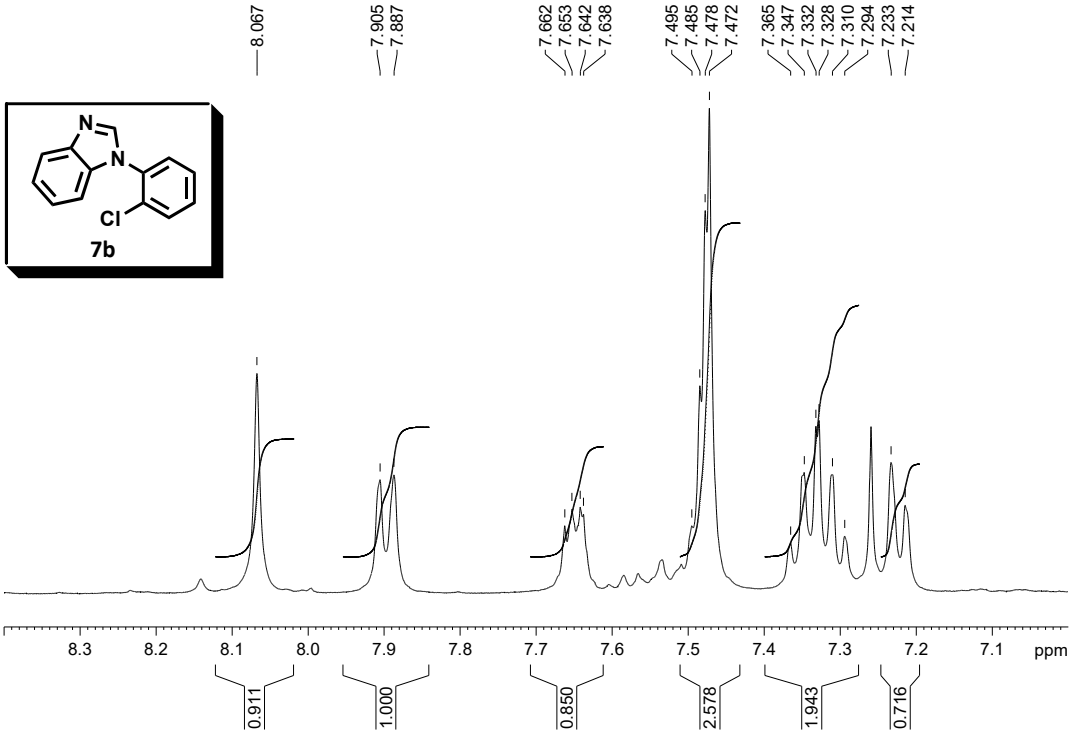
^{1}H-RMN ($CDCl_3$) 1-*p*-tolil-1*H*-benzo[*d*]imidazol (7a)



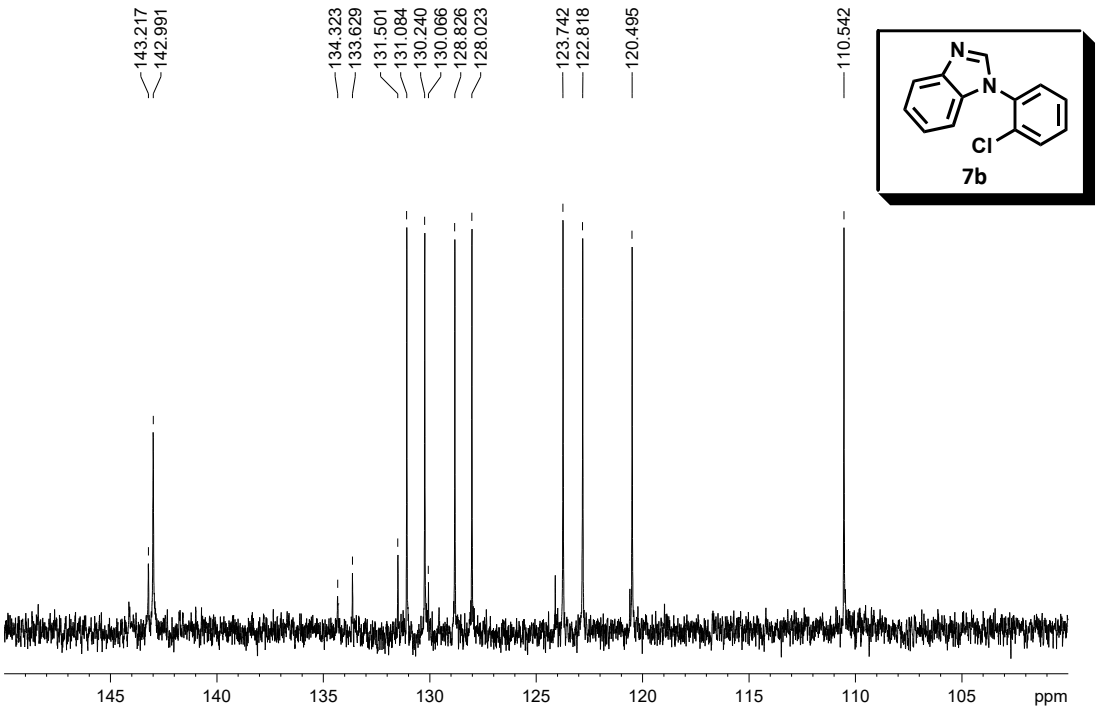
^{13}C-RMN ($CDCl_3$) 1-*p*-tolil-1*H*-benzo[*d*]imidazol (7a)



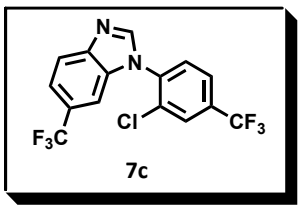
^{1}H-RMN ($CDCl_3$) 1-(2-Clorofenil)-1*H*-benzo[*d*]imidazol (7b)



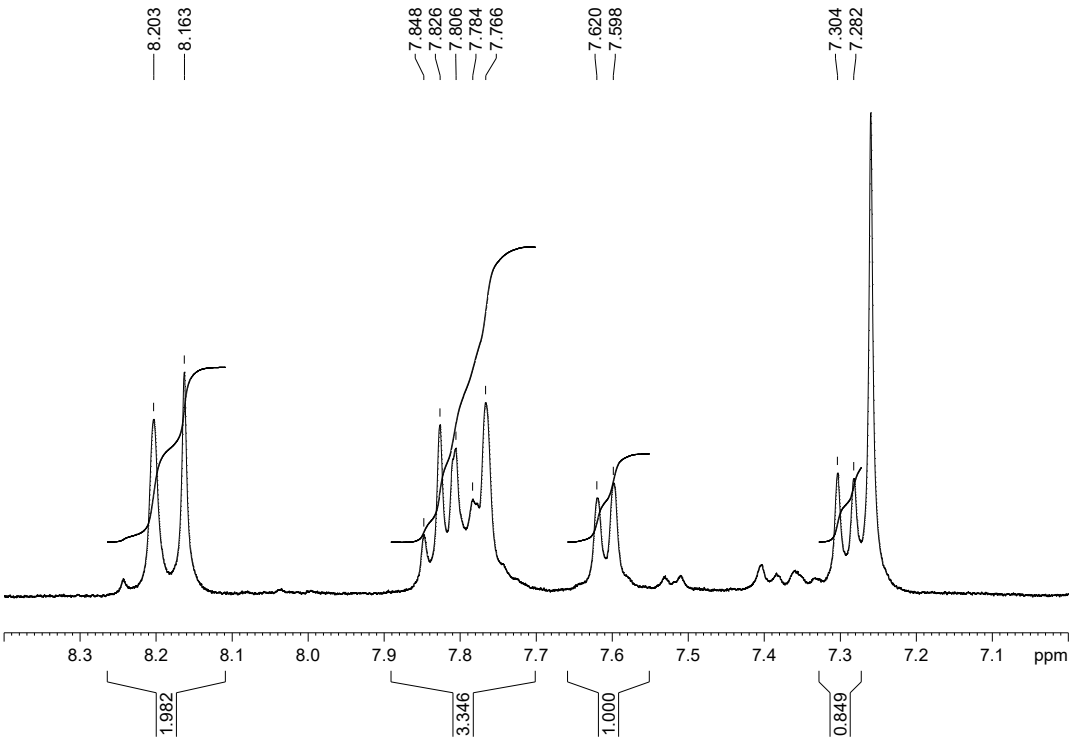
^{13}C-RMN ($CDCl_3$) 1-(2-Clorofenil)-1*H*-benzo[*d*]imidazol (7b)



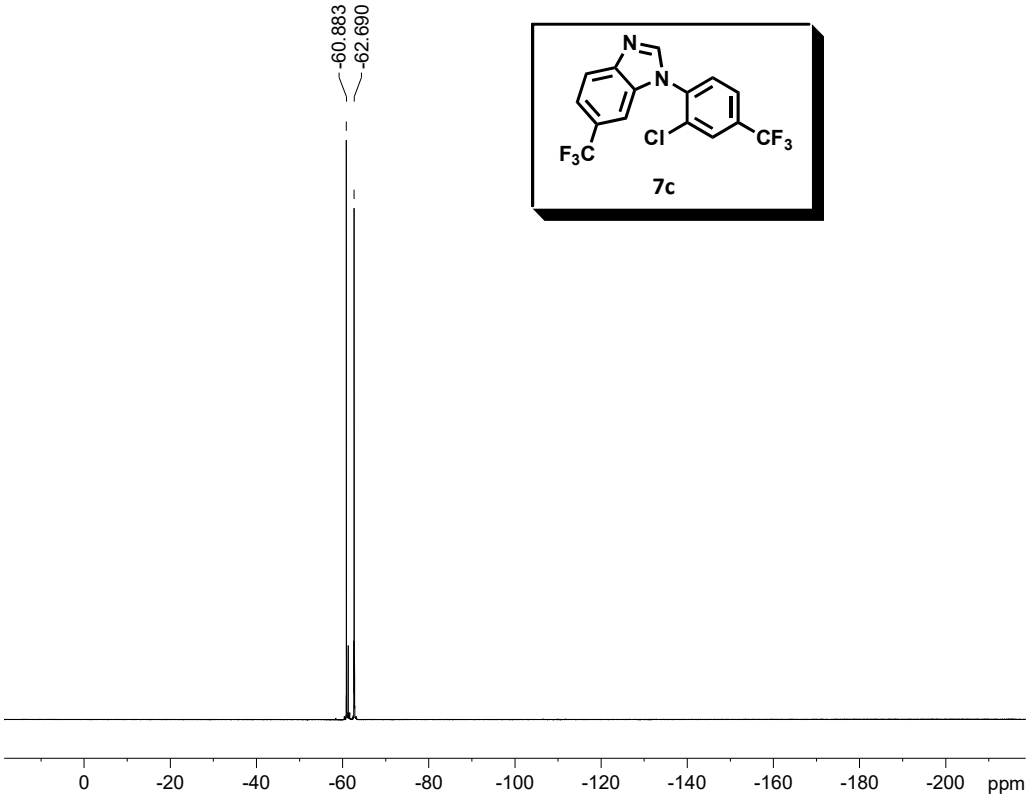
^{1}H-RMN ($CDCl_3$) 1-(2-Cloro-4-(trifluormetil)fenil)-6-(trifluormetil)-1*H*-benzo[*d*]imidazol (7c)



7c



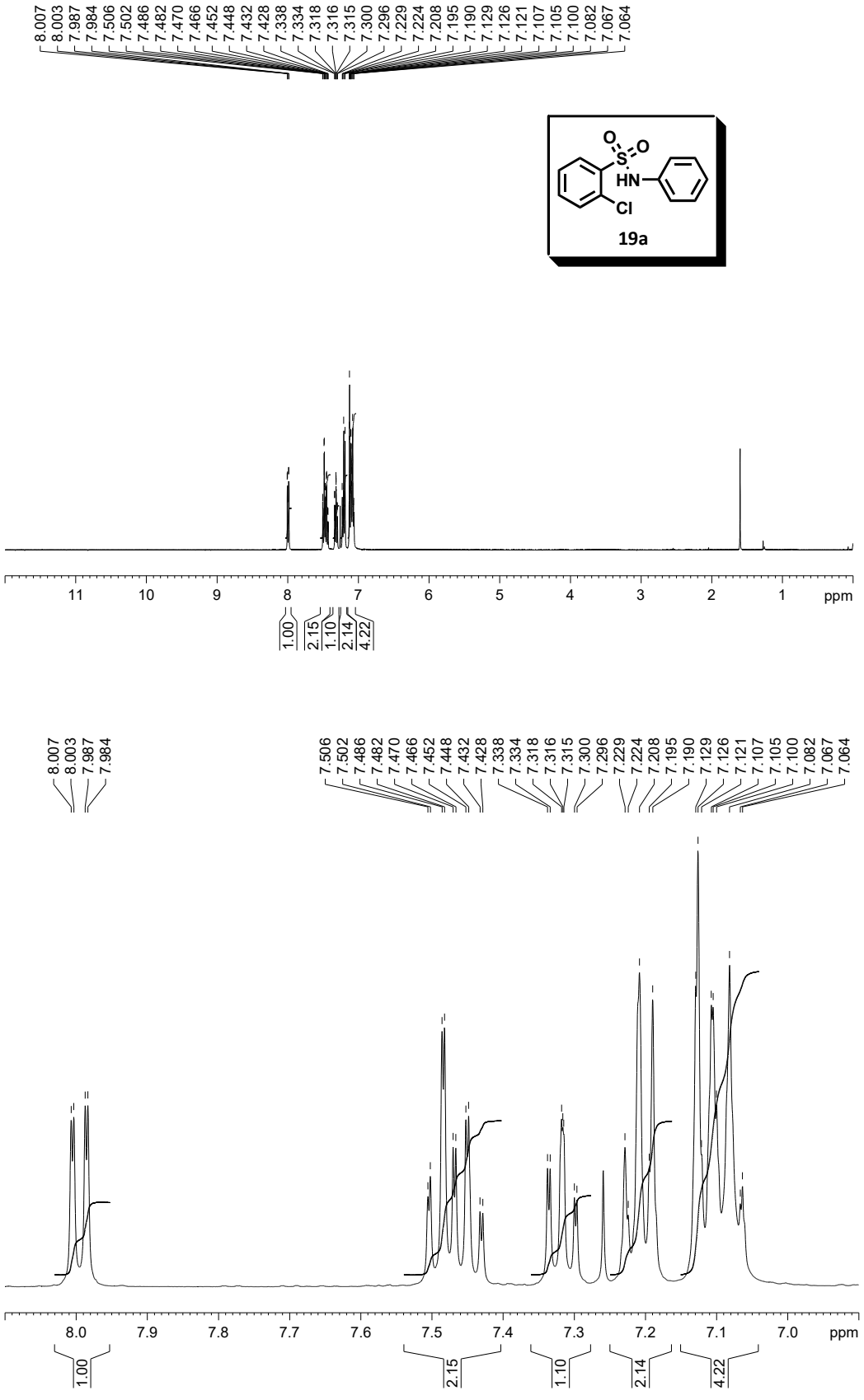
^{9}F-RMN ($CDCl_3$) 1-(2-Cloro-4-(trifluormetil)fenil)-6-(trifluormetil)-1*H*-benzo[*d*]imidazol (7c)



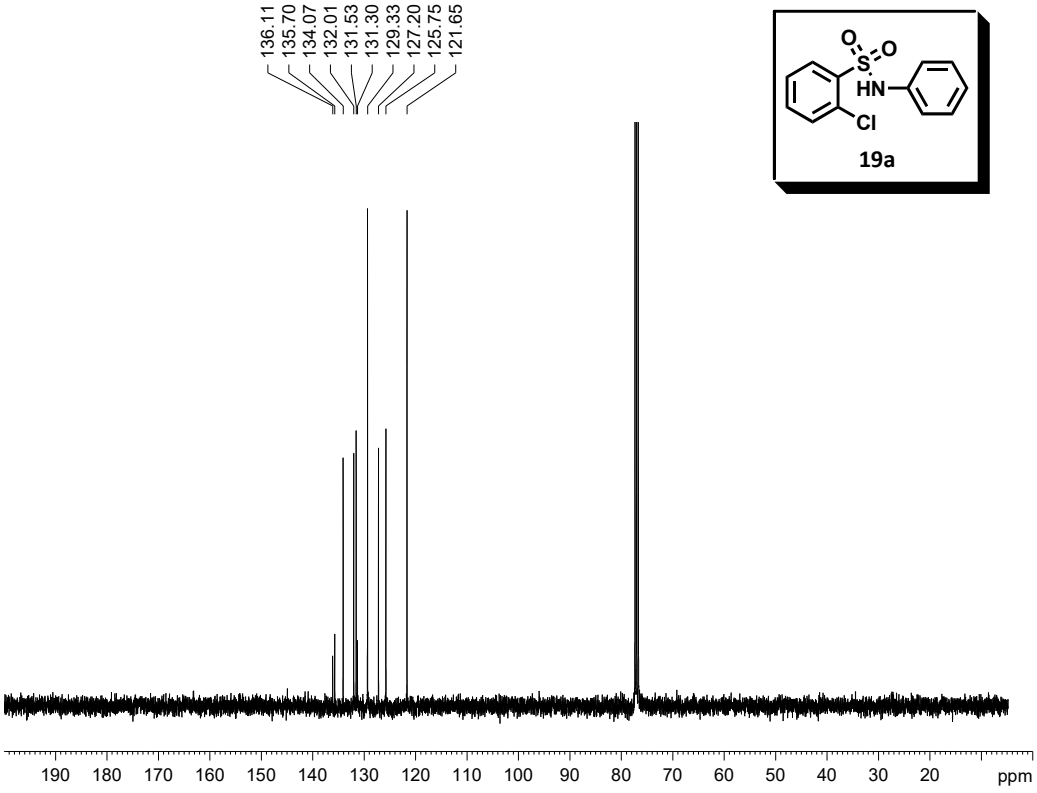
A.4 CAPÍTULO V

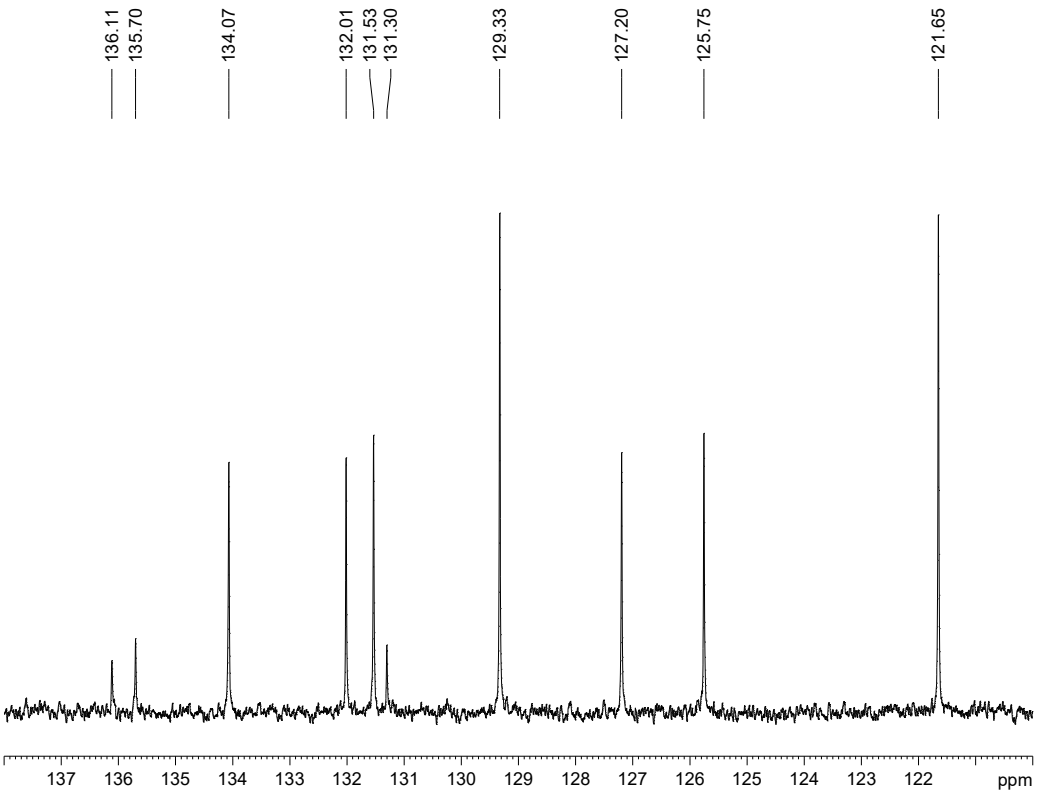
A.4.1 ESPECTROS DE RMN DE PRECURSORES: *N*-ARIL-*O*-HALO-SULFONAMIDAS

^{1}H-RMN ($CDCl_3$) 2-Cloro-*N*-fenilbencenosulfonamida (19a)

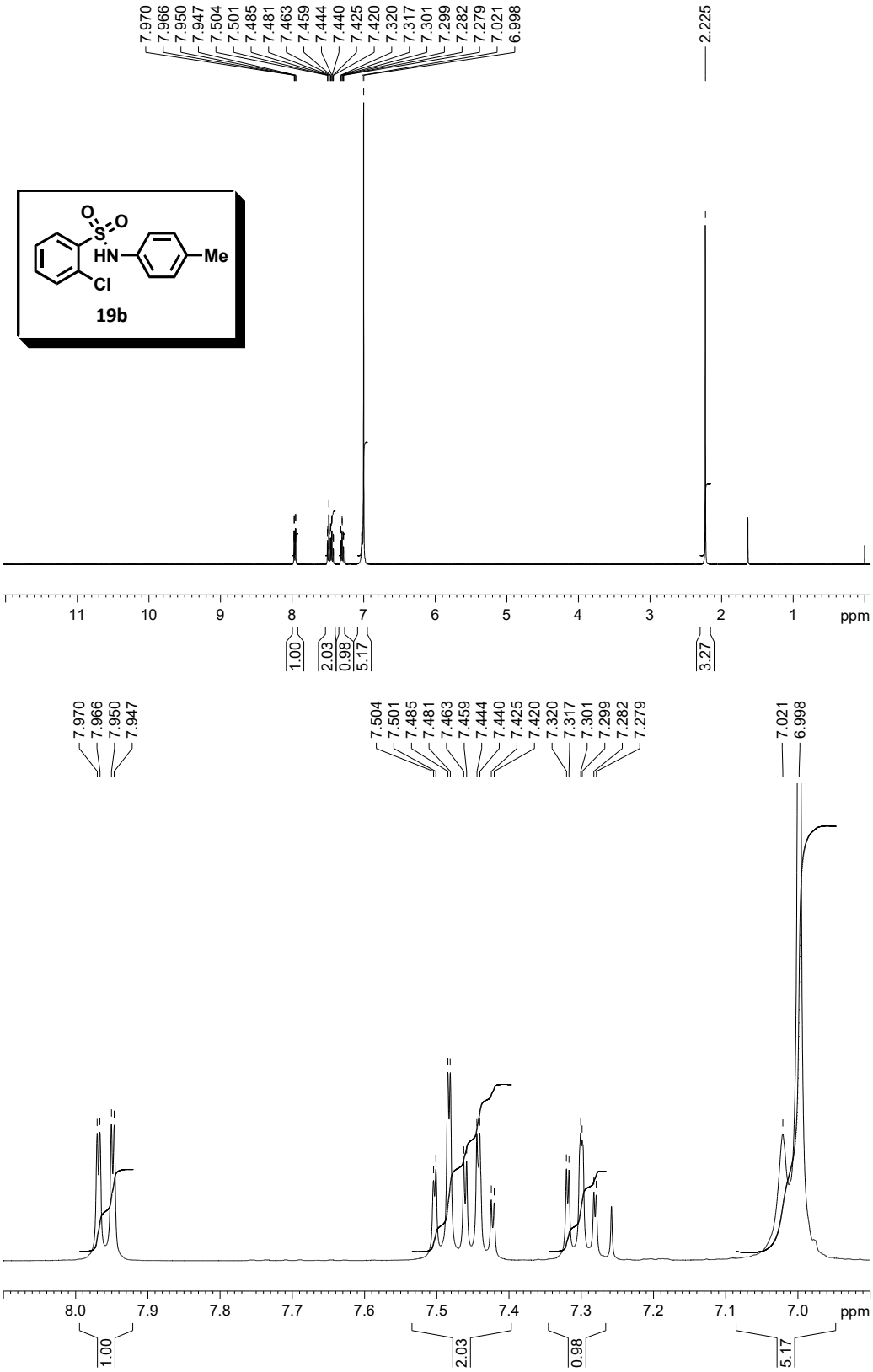


^{13}C-RMN ($CDCl_3$) 2-Cloro-*N*-fenilbencenosulfonamida (19a)

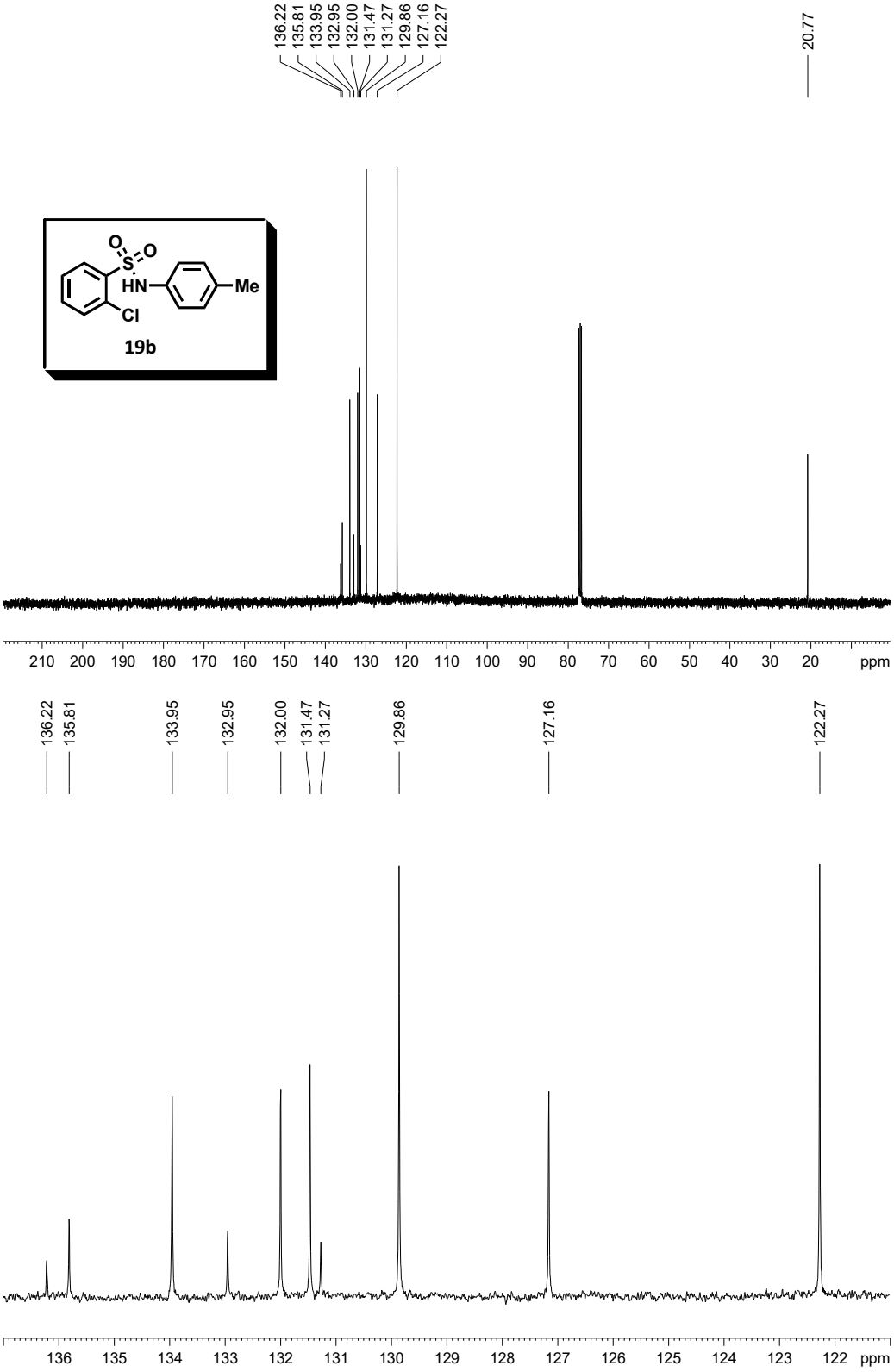




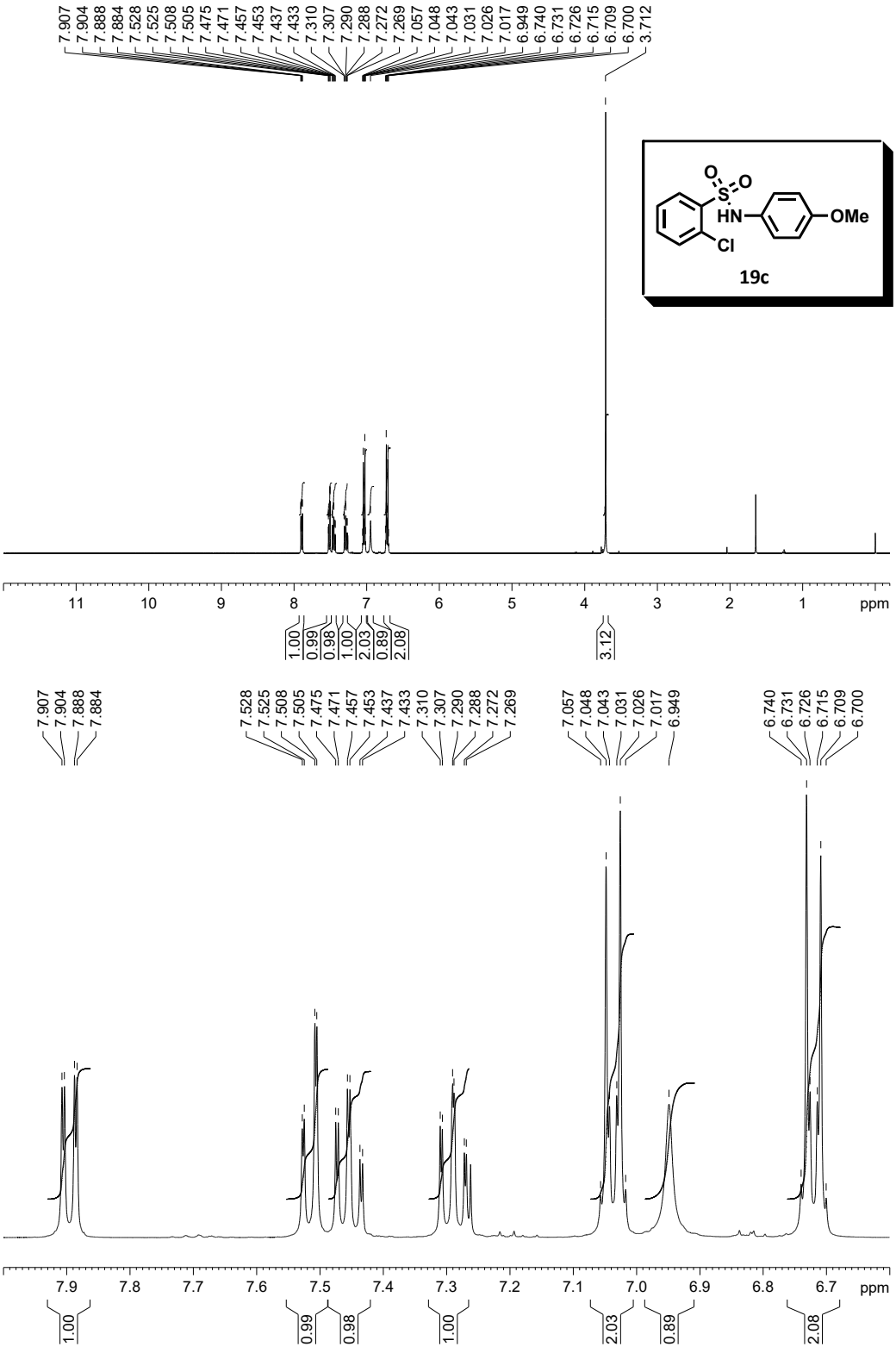
^{1}H-RMN ($CDCl_3$) 2-Cloro-*N*-(p-tolil)bencenosulfonamida (19b)



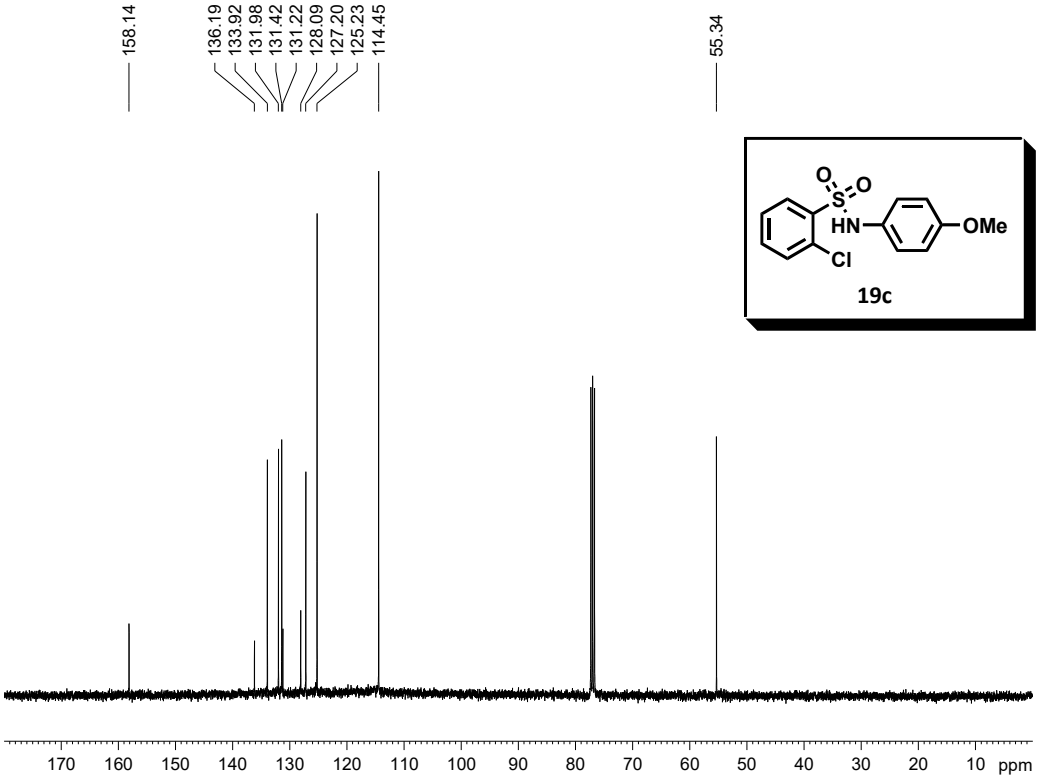
^{13}C-RMN ($CDCl_3$) 2-Cloro-*N*-(p-tolil)bencenosulfonamida (19b)

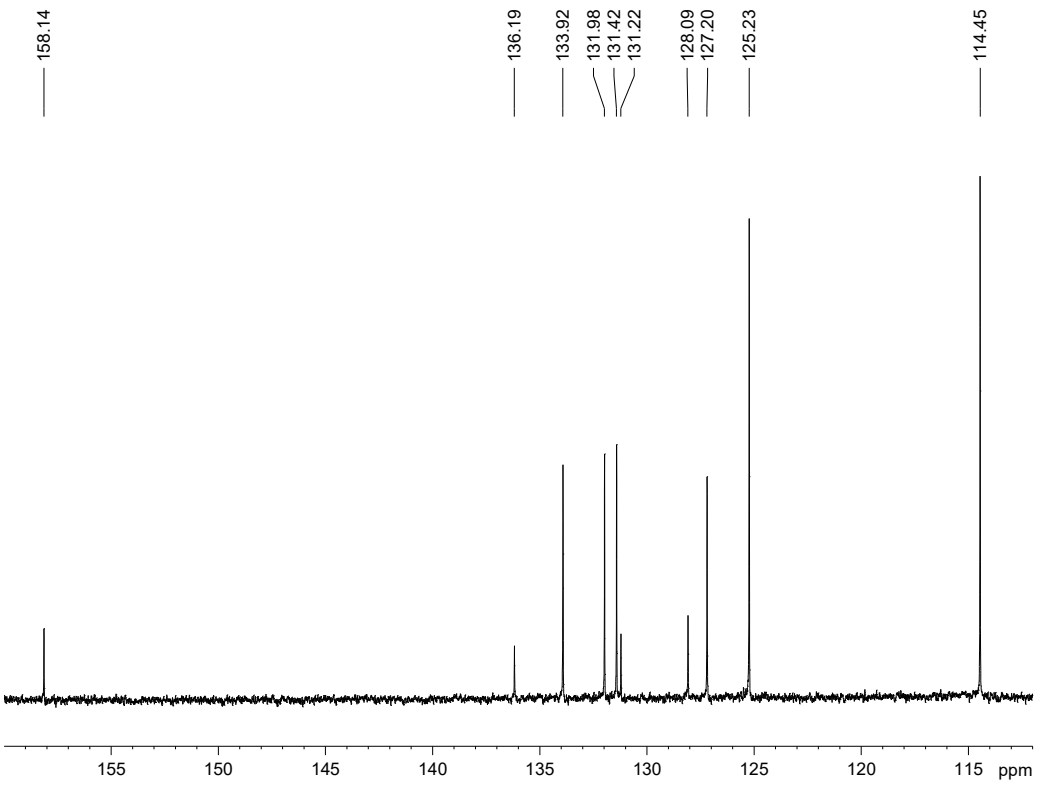


^{1}H-RMN ($CDCl_3$) 2-Cloro-*N*-(*p*-metoxifenil)bencenosulfonamida (19c)

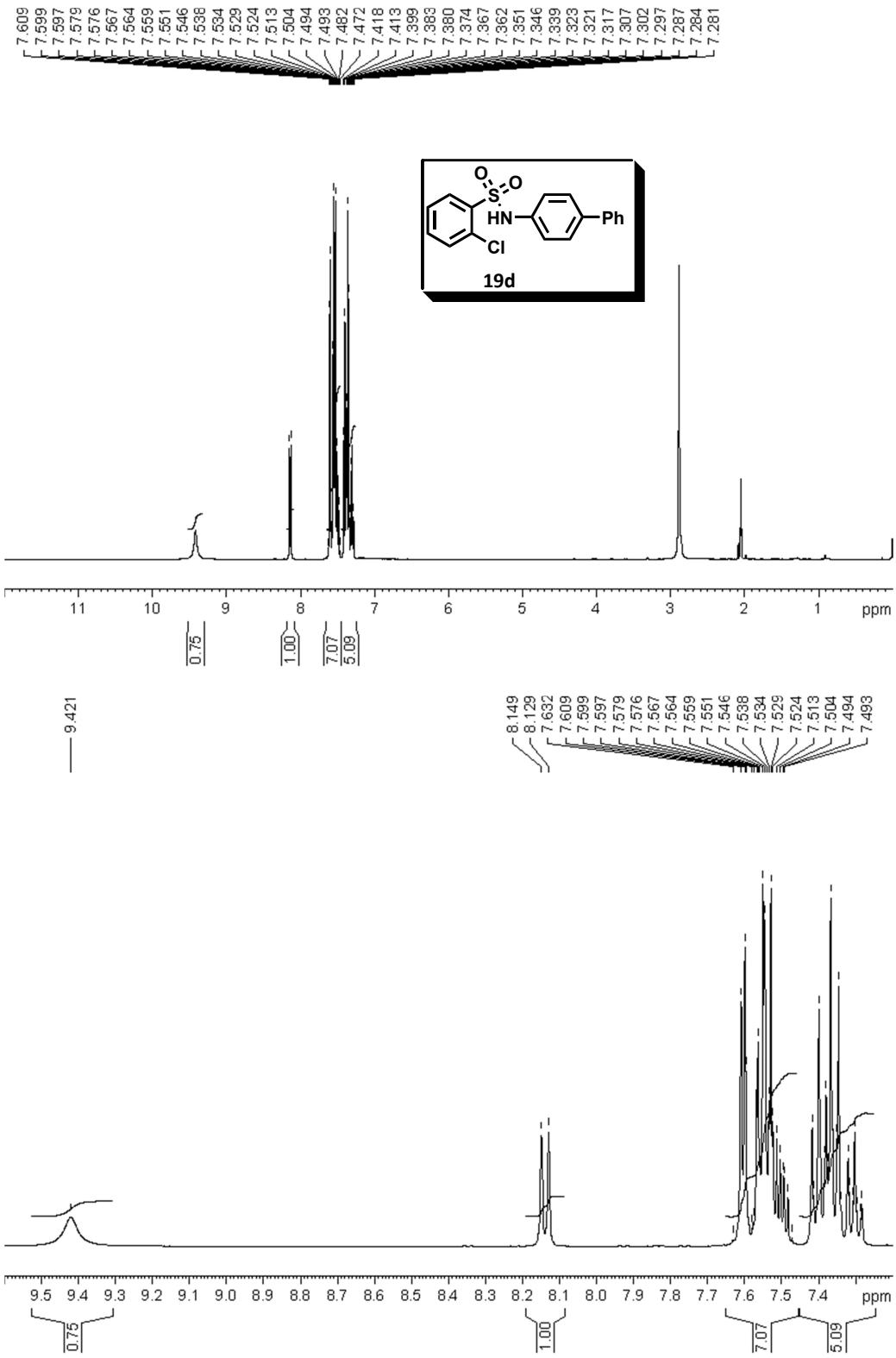


^{13}C-RMN ($CDCl_3$) 2-Cloro-*N*-(*p*-metoxifenil)bencenosulfonamida (19c)

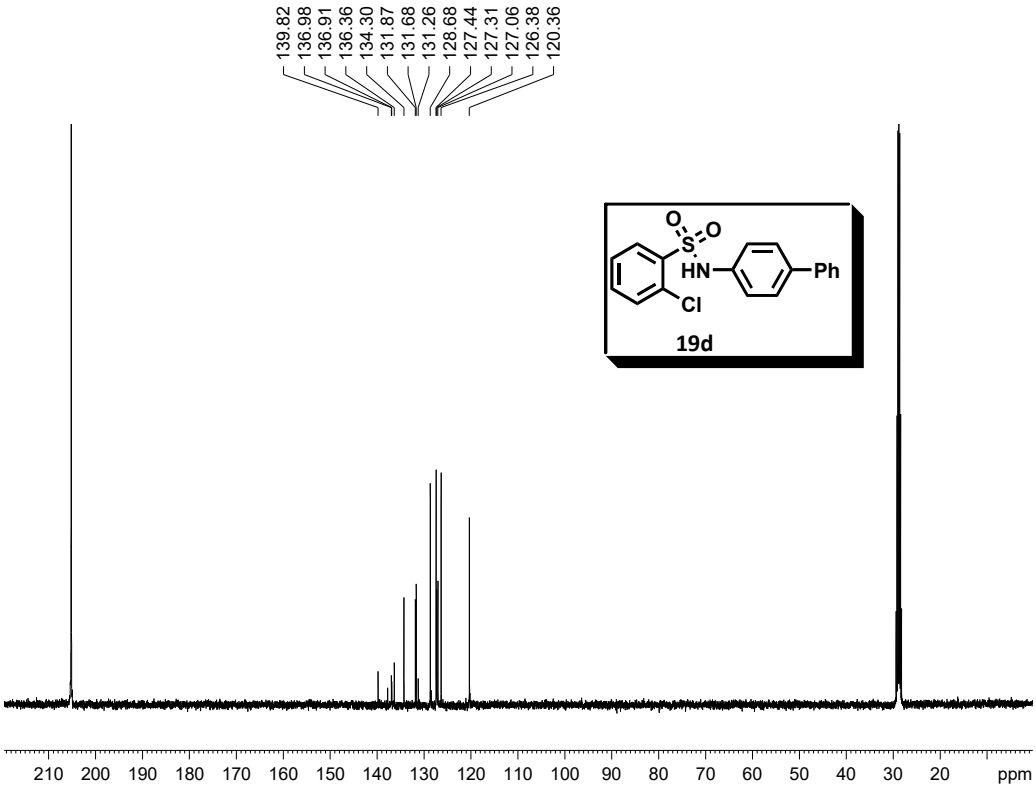


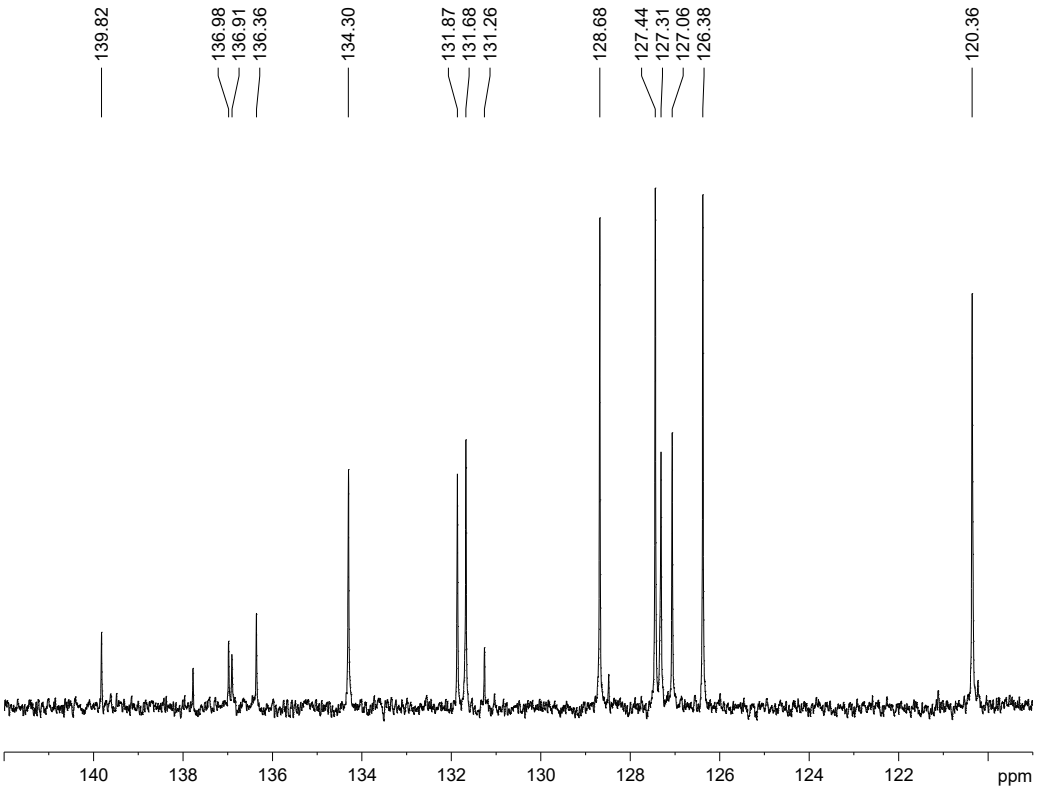


^{1}H-RMN ($CD_3C(O)CD_3$) *N*-([1,1'-bifenil]-4-il)-2-clorobencenosulfonamida (19d)

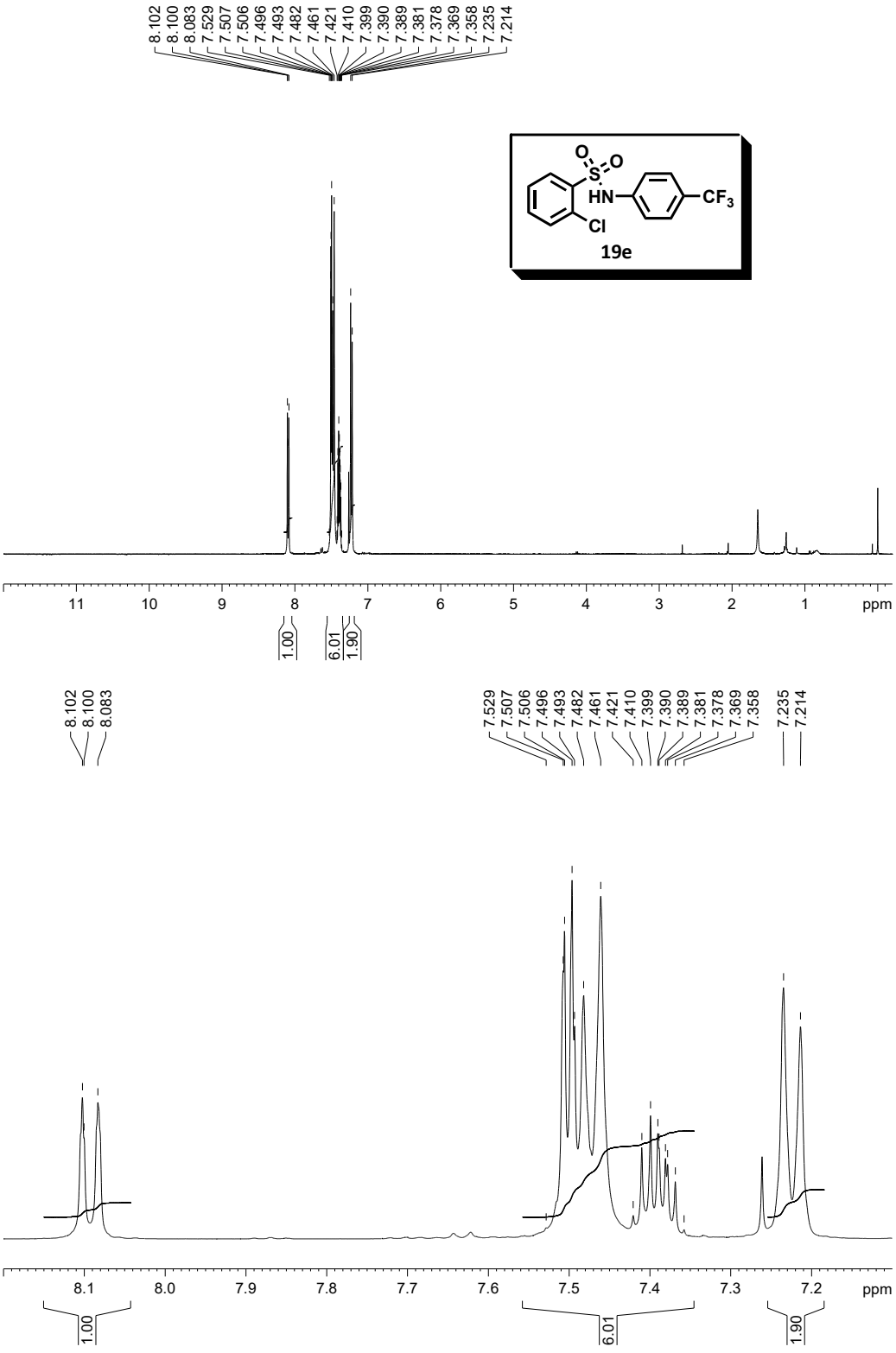


^{13}C-RMN ($CD_3C(O)CD_3$) *N*-([1,1'-bifenil]-4-il)-2-clorobencenosulfonamida (19d)

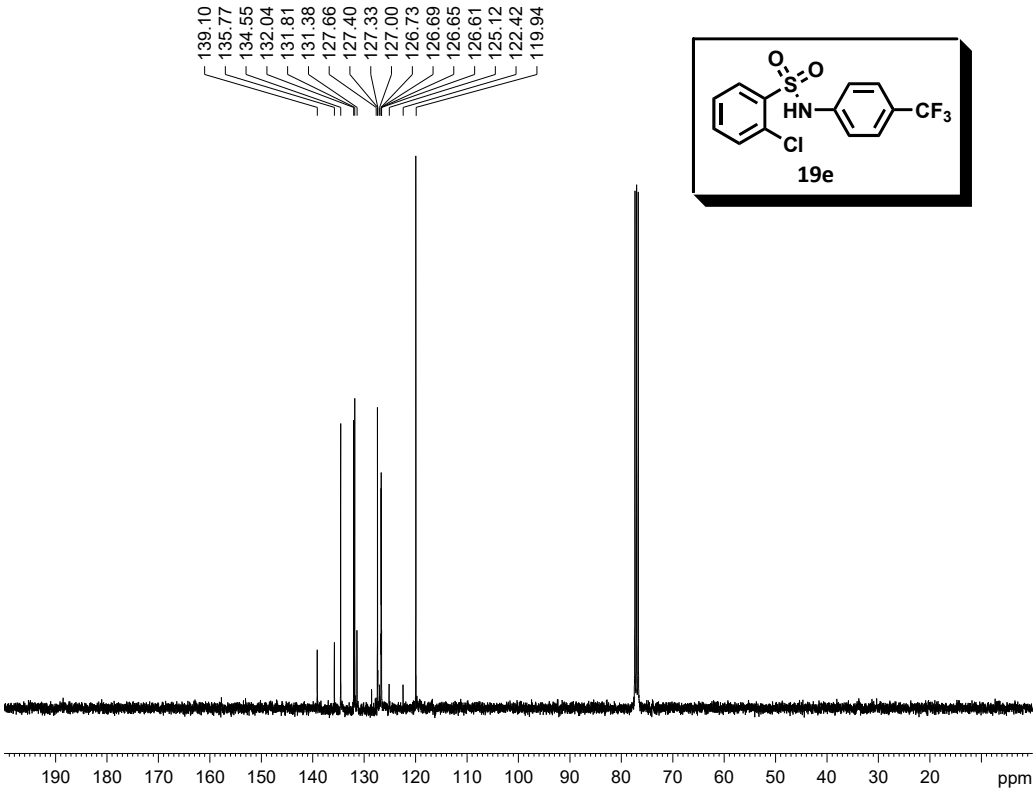


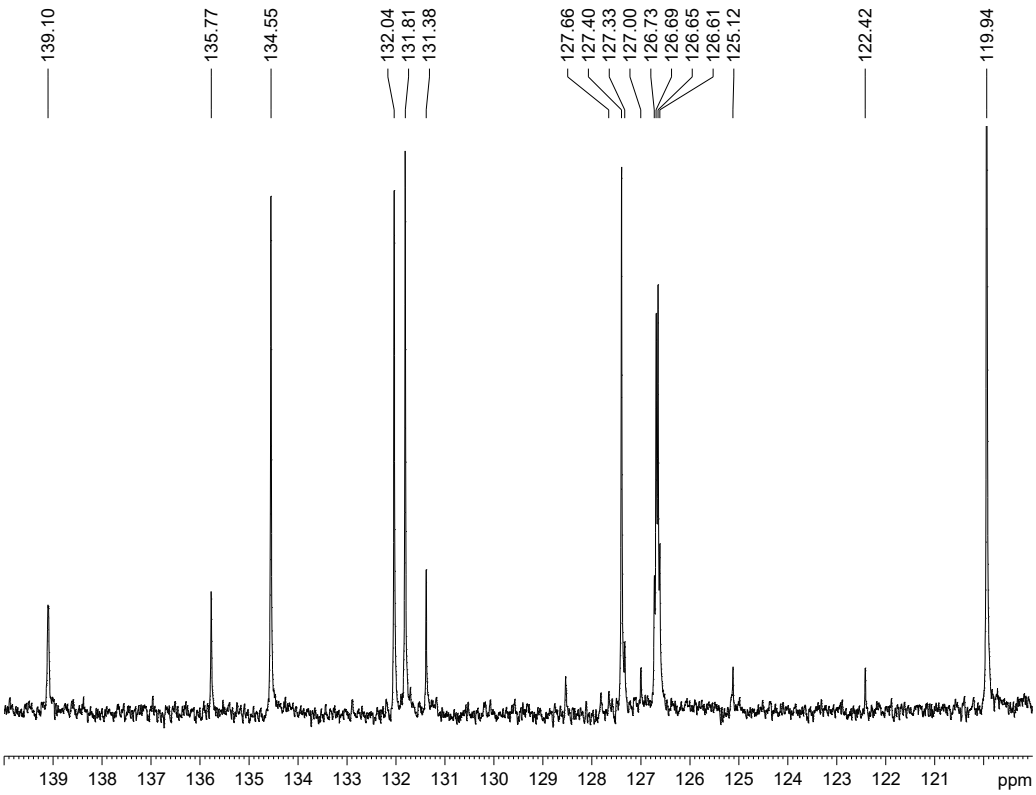


^{1}H-RMN ($CDCl_3$) 2-Cloro-*N*-(4-(trifluormetil)fenil)bencenosulfonamida (19e)

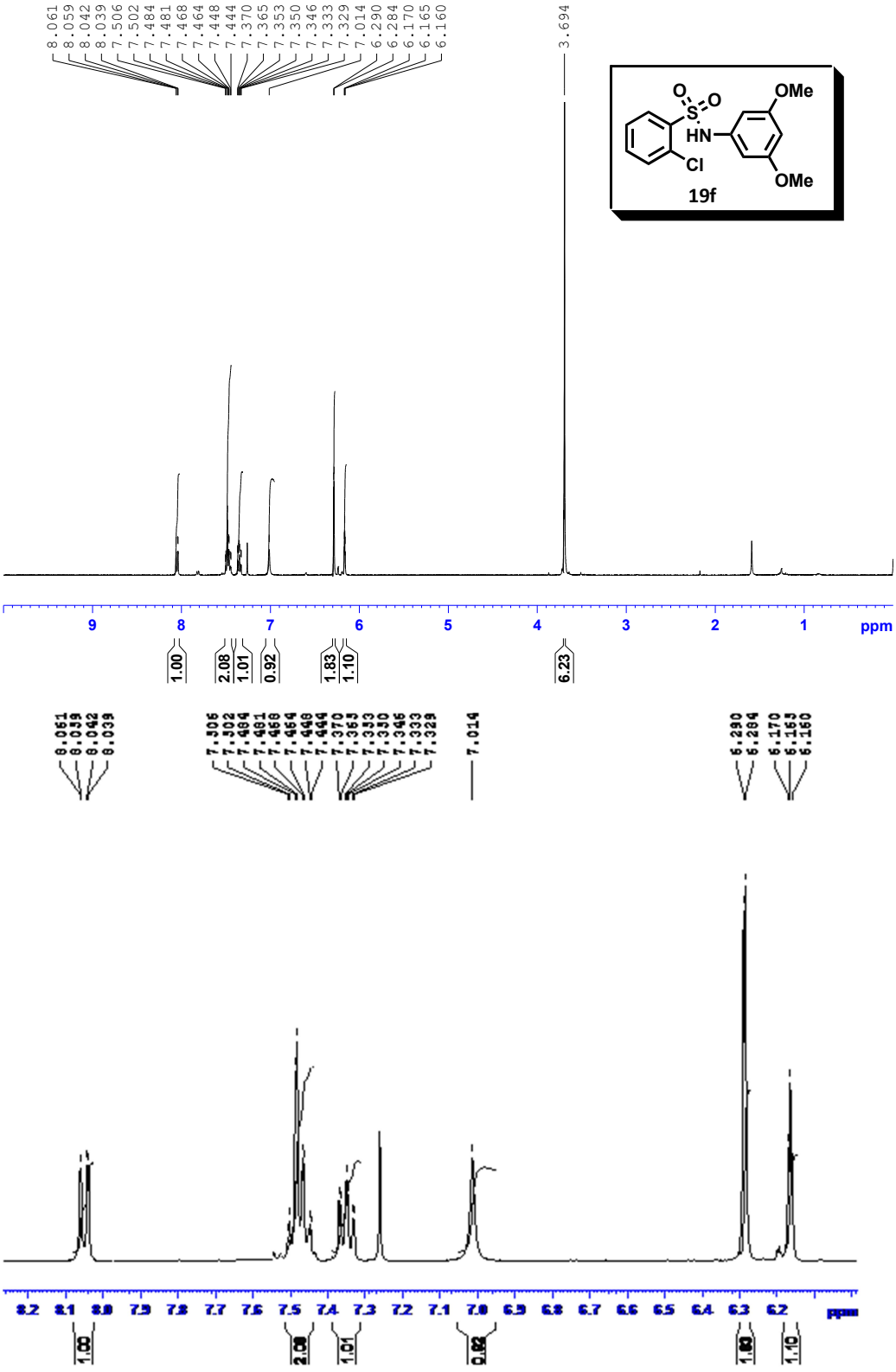


^{13}C-RMN ($CDCl_3$) 2-Cloro-*N*-(4-(trifluormetil)fenil)bencenosulfonamida (19e)

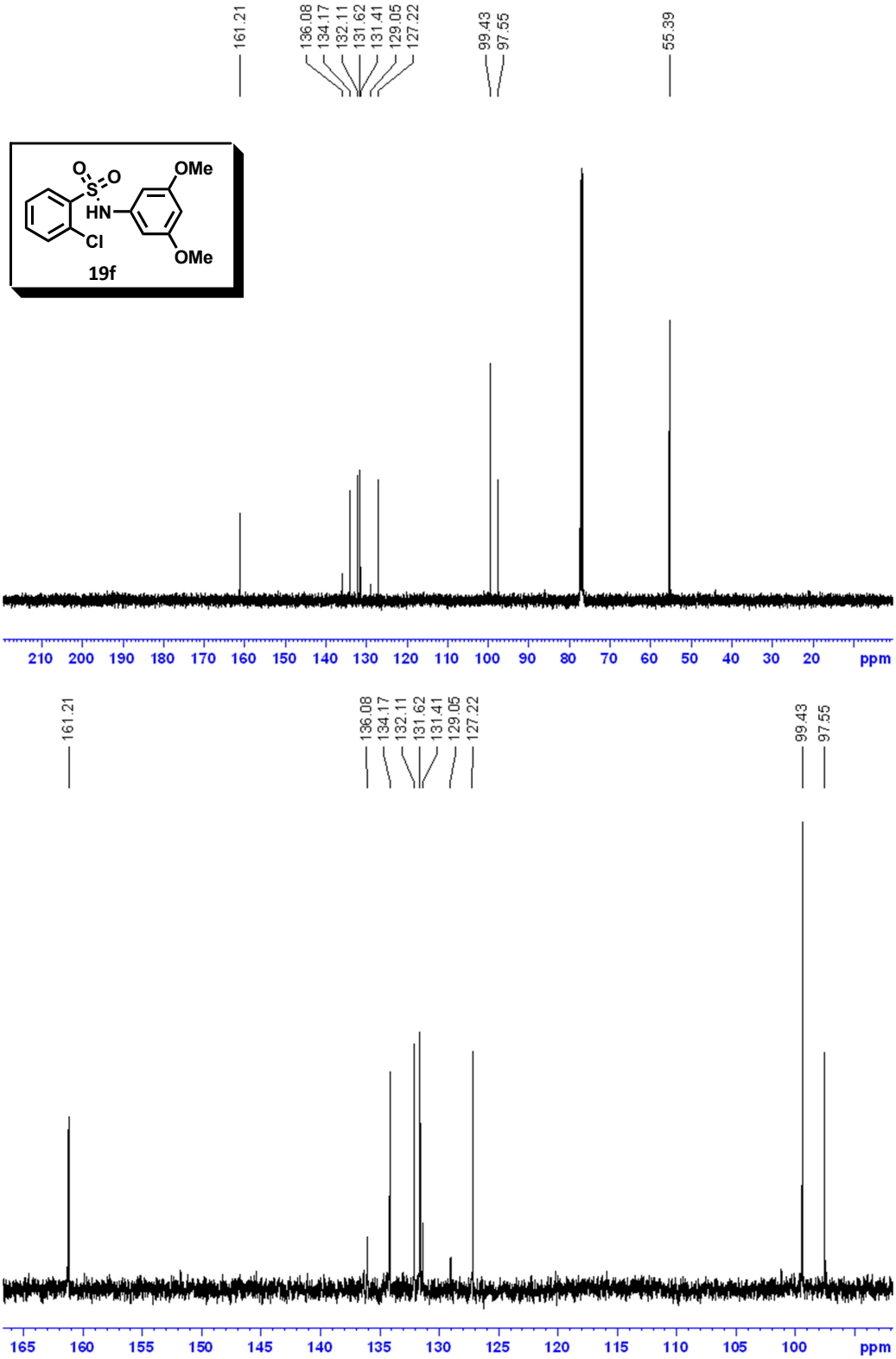




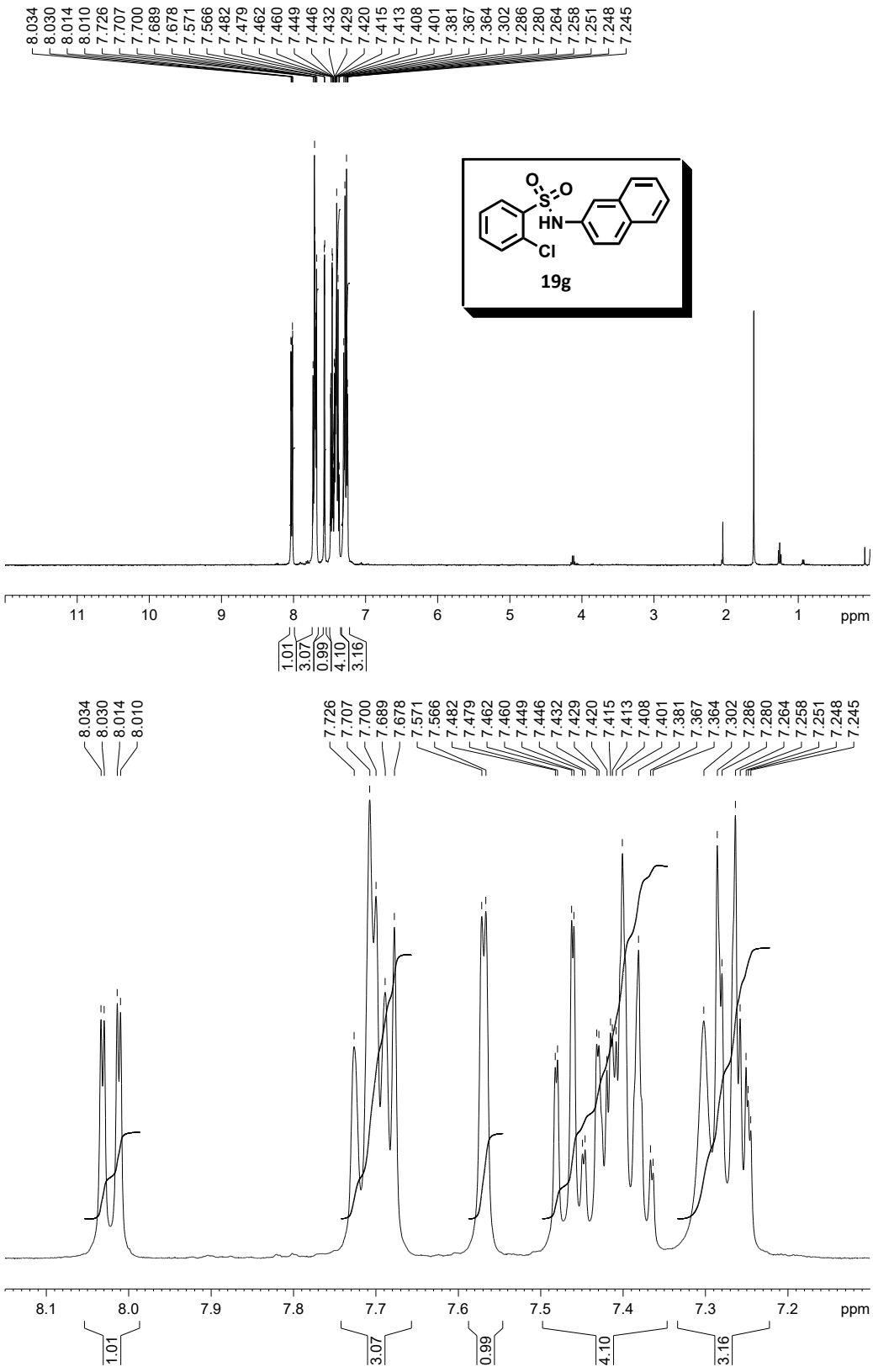
^{1}H-RMN ($CDCl_3$) 2-Cloro-*N*-(3,5-dimetoxifenil)bencenosulfonamida (19f)



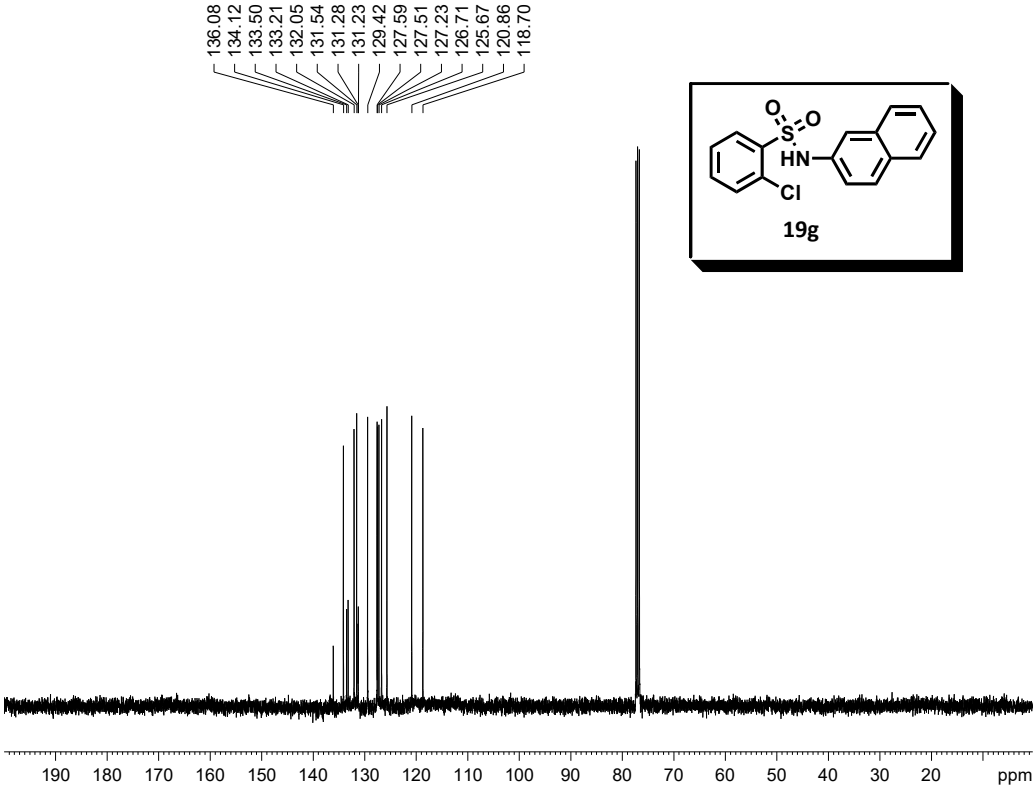
^{13}C-RMN ($CDCl_3$) 2-Cloro-*N*-(3,5-dimetoxifenil)bencenosulfonamida (19f)

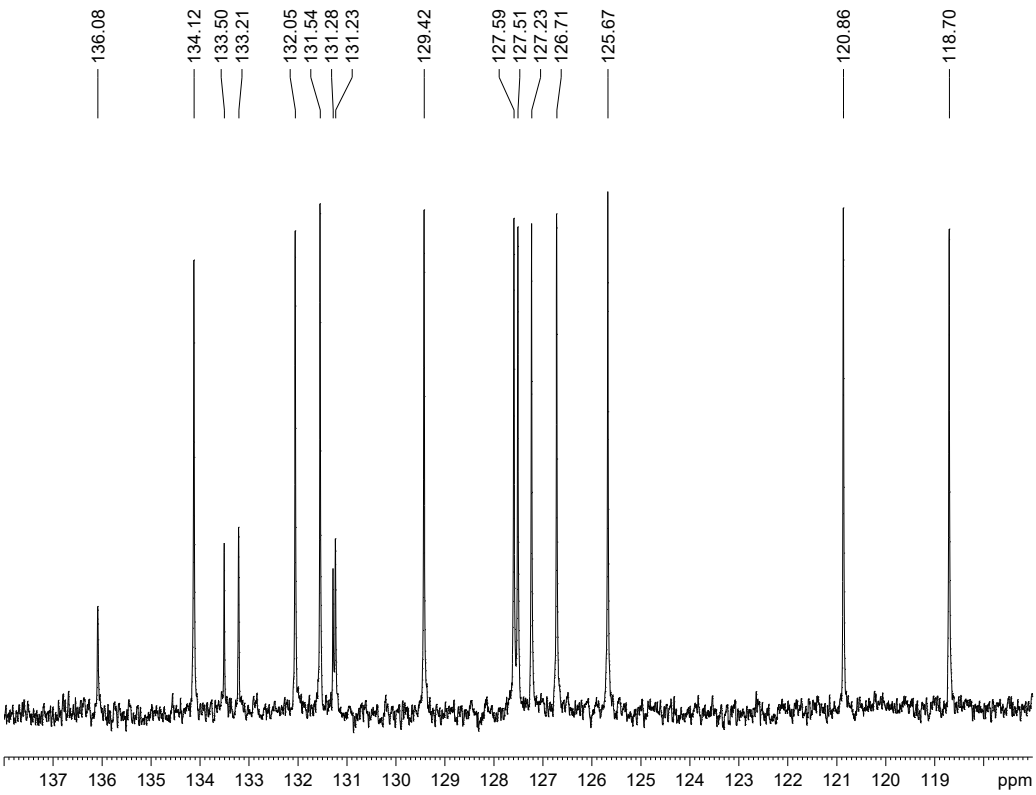


^{1}H-RMN ($CDCl_3$) 2-Cloro-*N*-(2-naftil)bencenosulfonamida (19g)

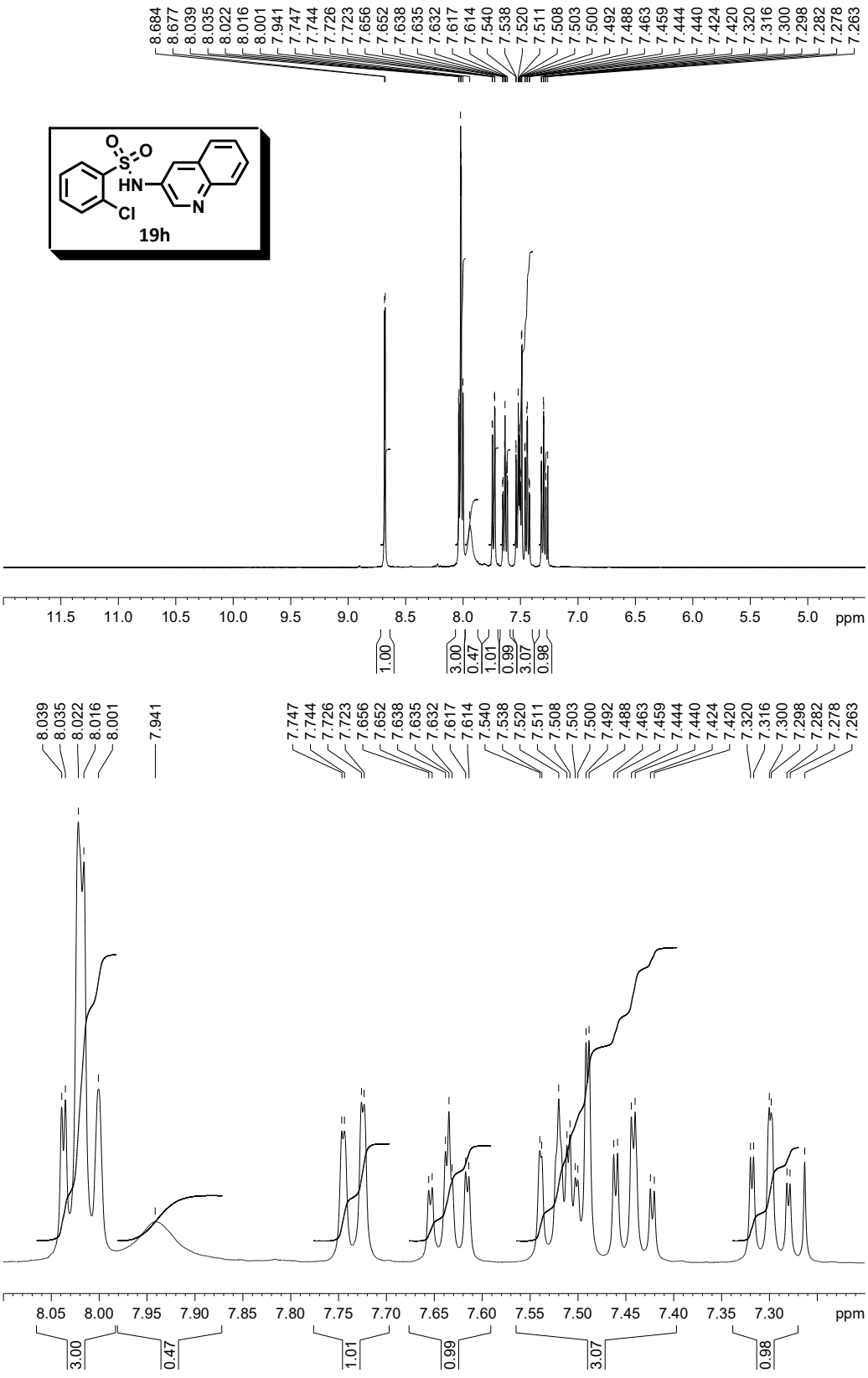


^{13}C-RMN ($CDCl_3$) 2-Cloro-*N*-(2-naftil)bencenosulfonamida (19g)

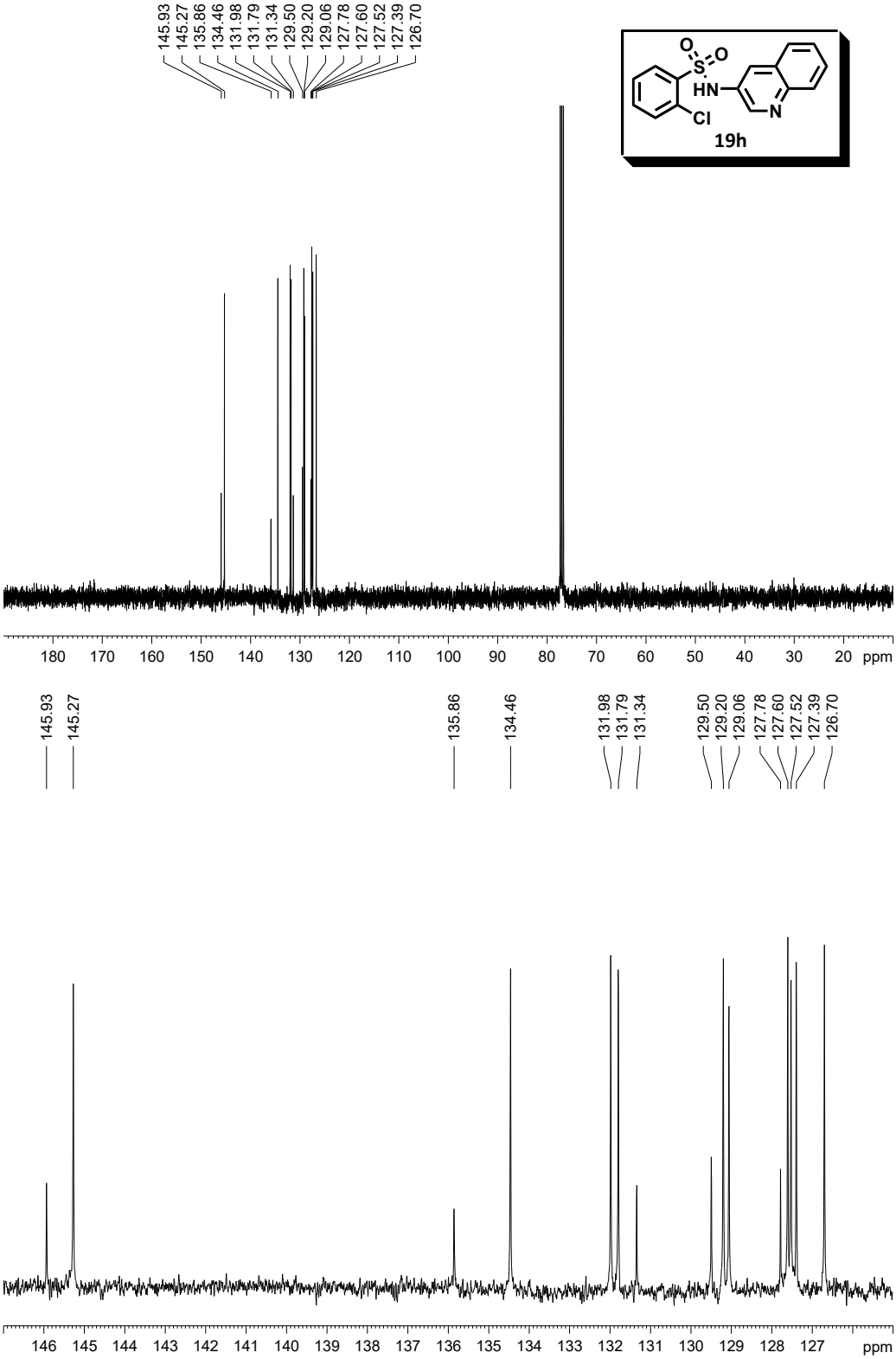




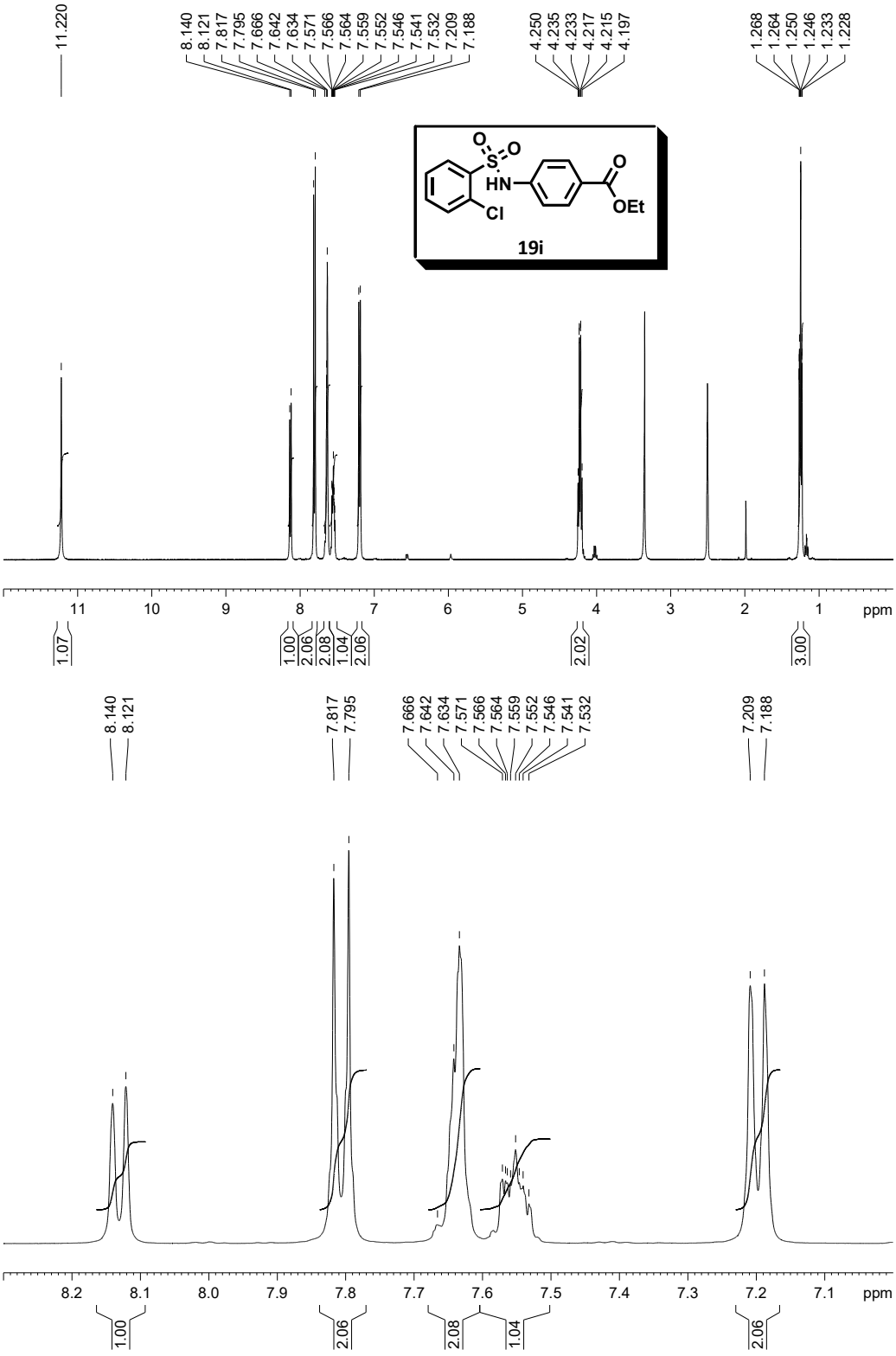
^{1}H-RMN ($CDCl_3$) 2-Cloro-*N*-(quinolin-3-il)bencenosulfonamida (19h)



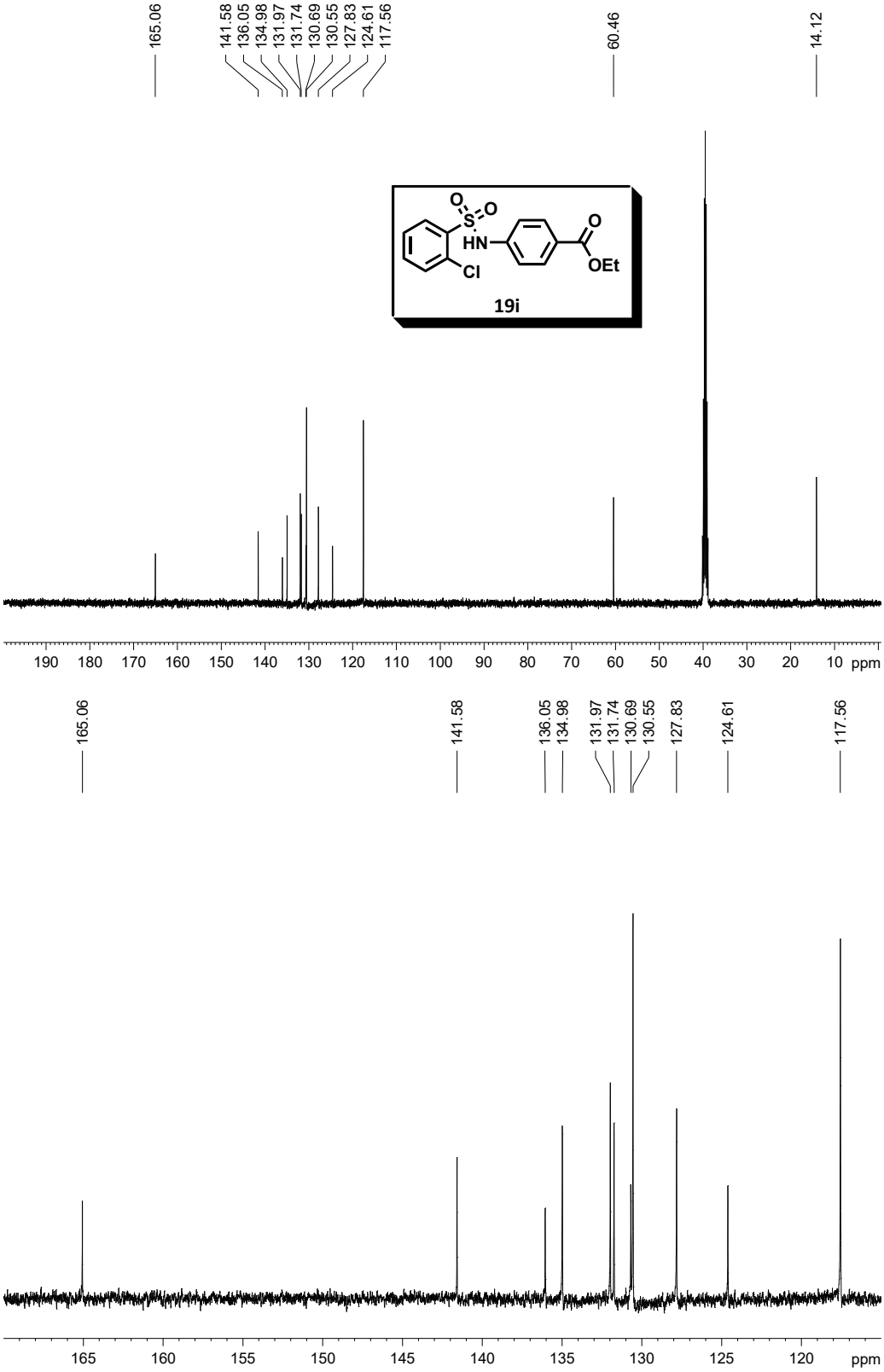
^{13}C-RMN ($CDCl_3$) 2-Cloro-*N*-(quinolin-3-il)bencenosulfonamida (19h)



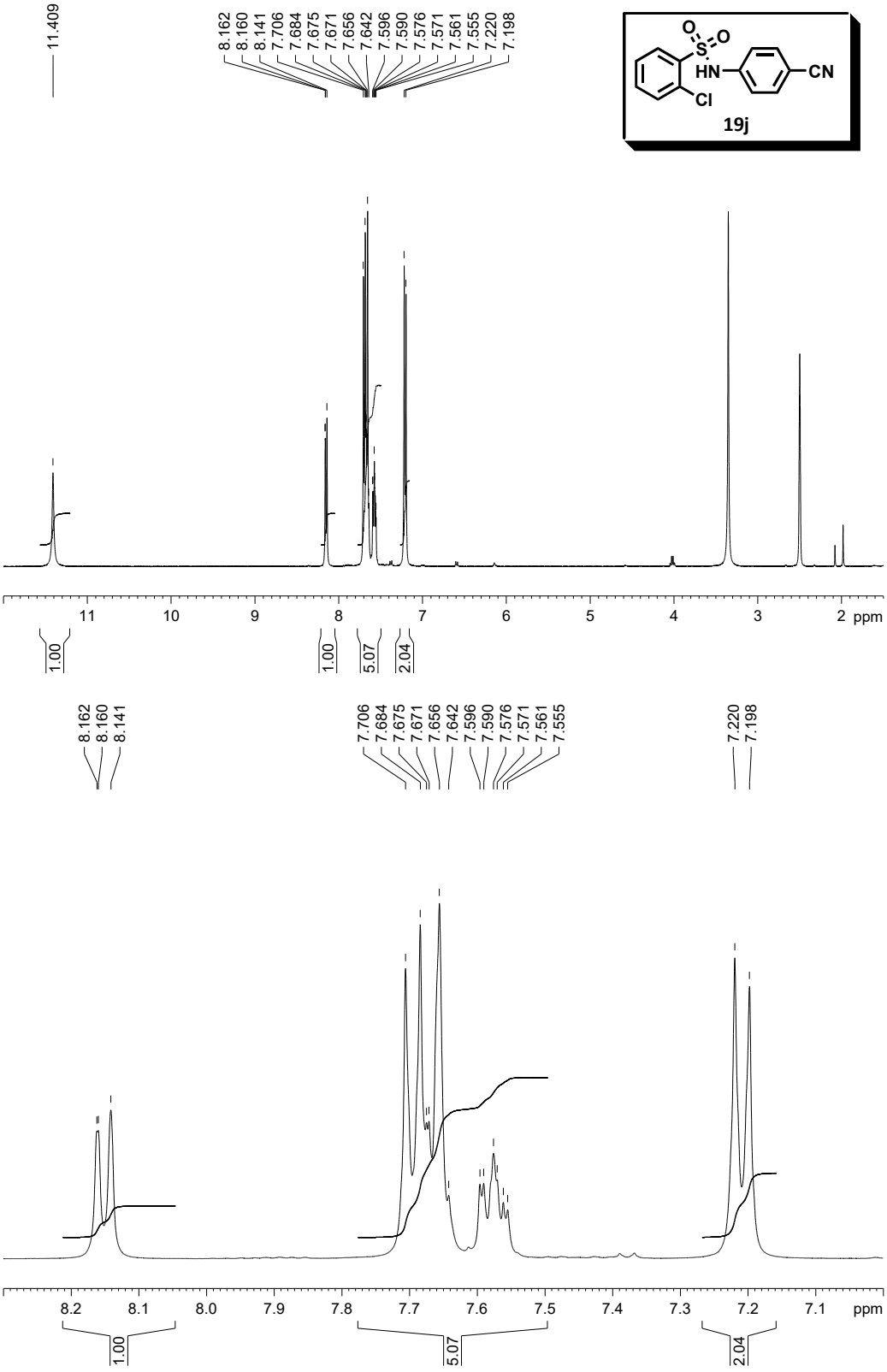
^{1}H-RMN (CD_3SOCD_3) 4-(2-Clorofenilsulfonamido)benzoato de etilo (19i)



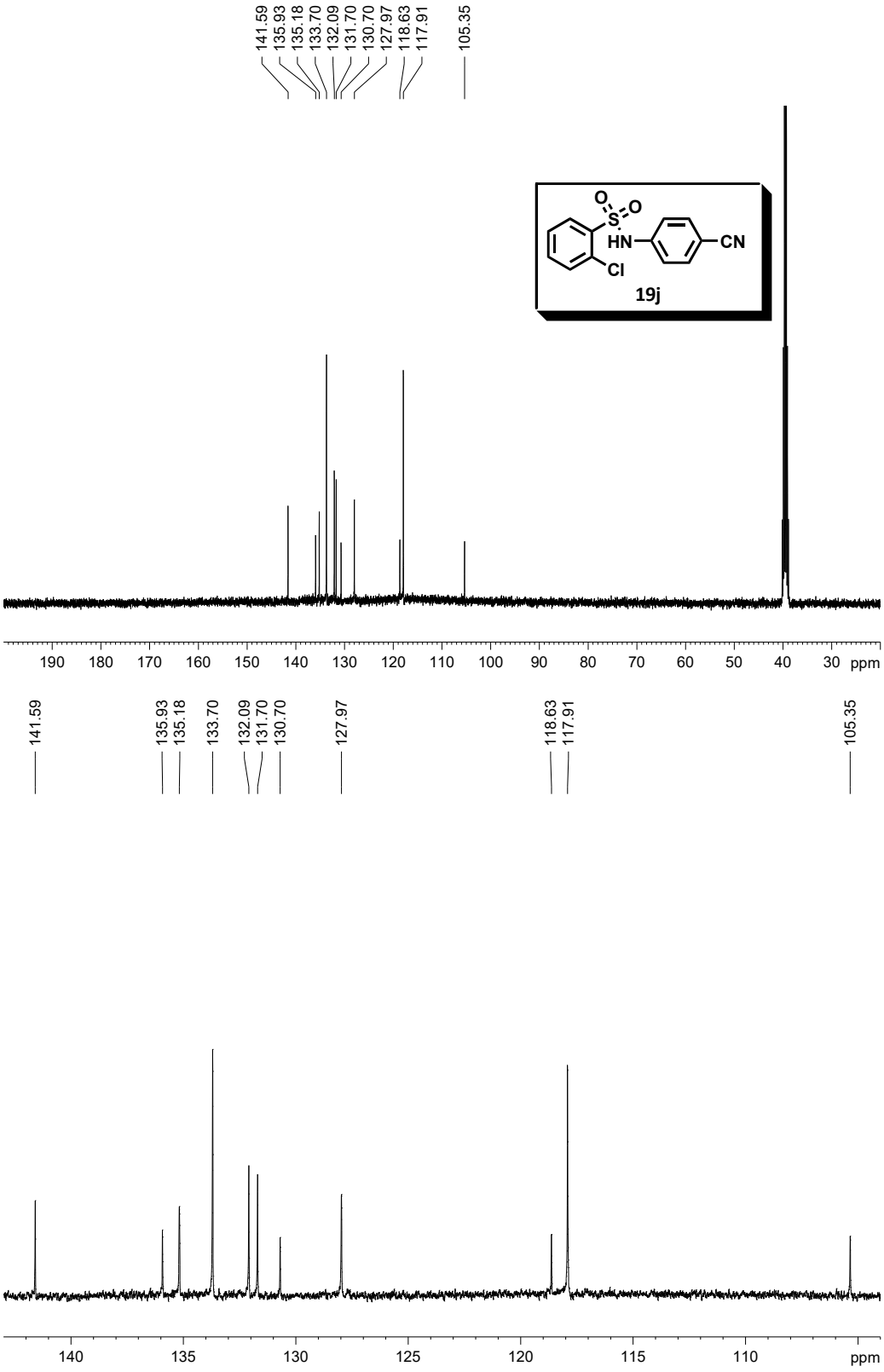
^{13}C-RMN (CD_3SOCD_3) 4-(2-Clorofenilsulfonamido)benzoato de etilo (19i)



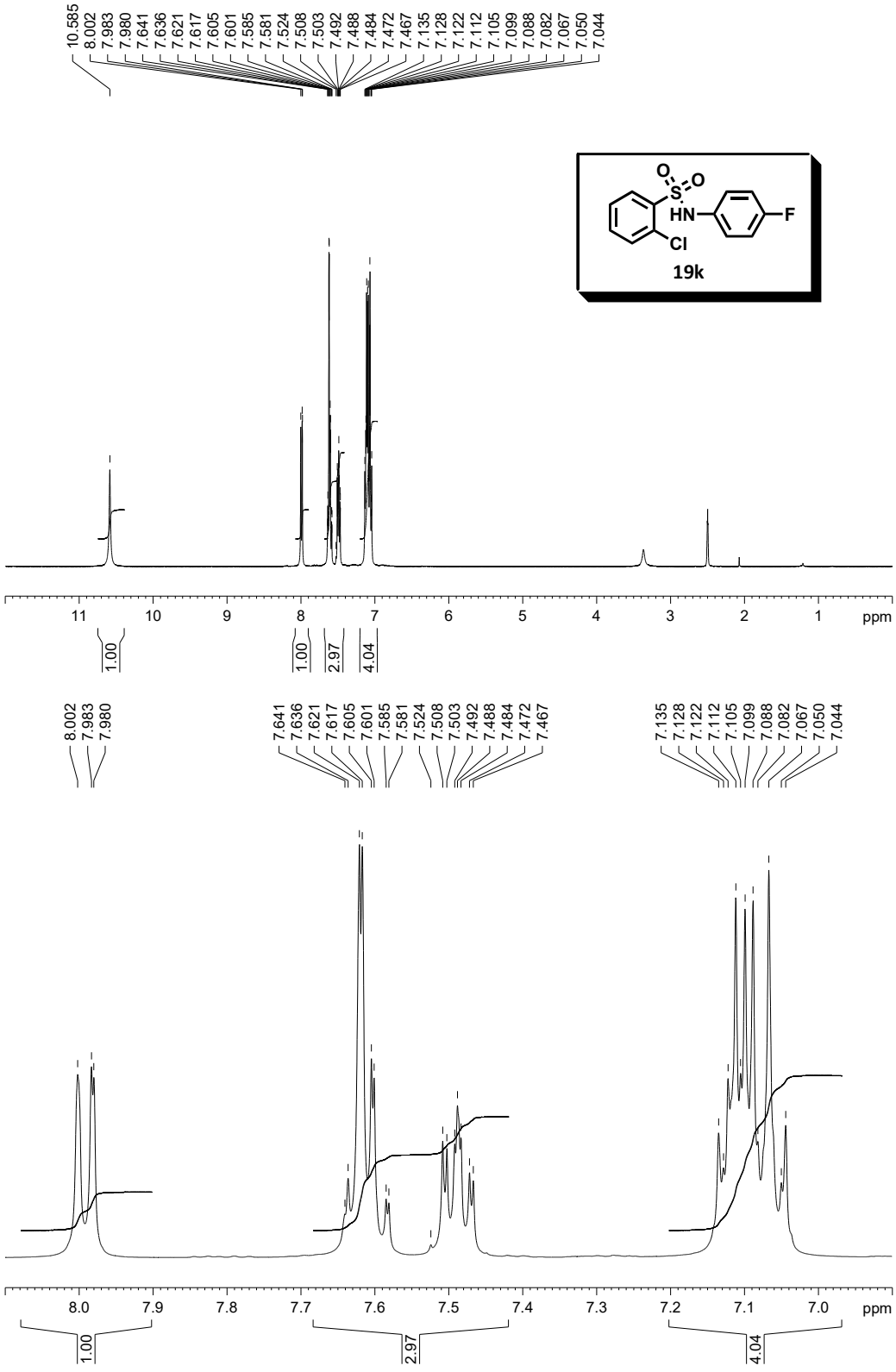
^{1}H-RMN (CD_3SOCD_3) 2-Cloro-*N*-(4-cianofenil)bencenosulfonamida (19j)



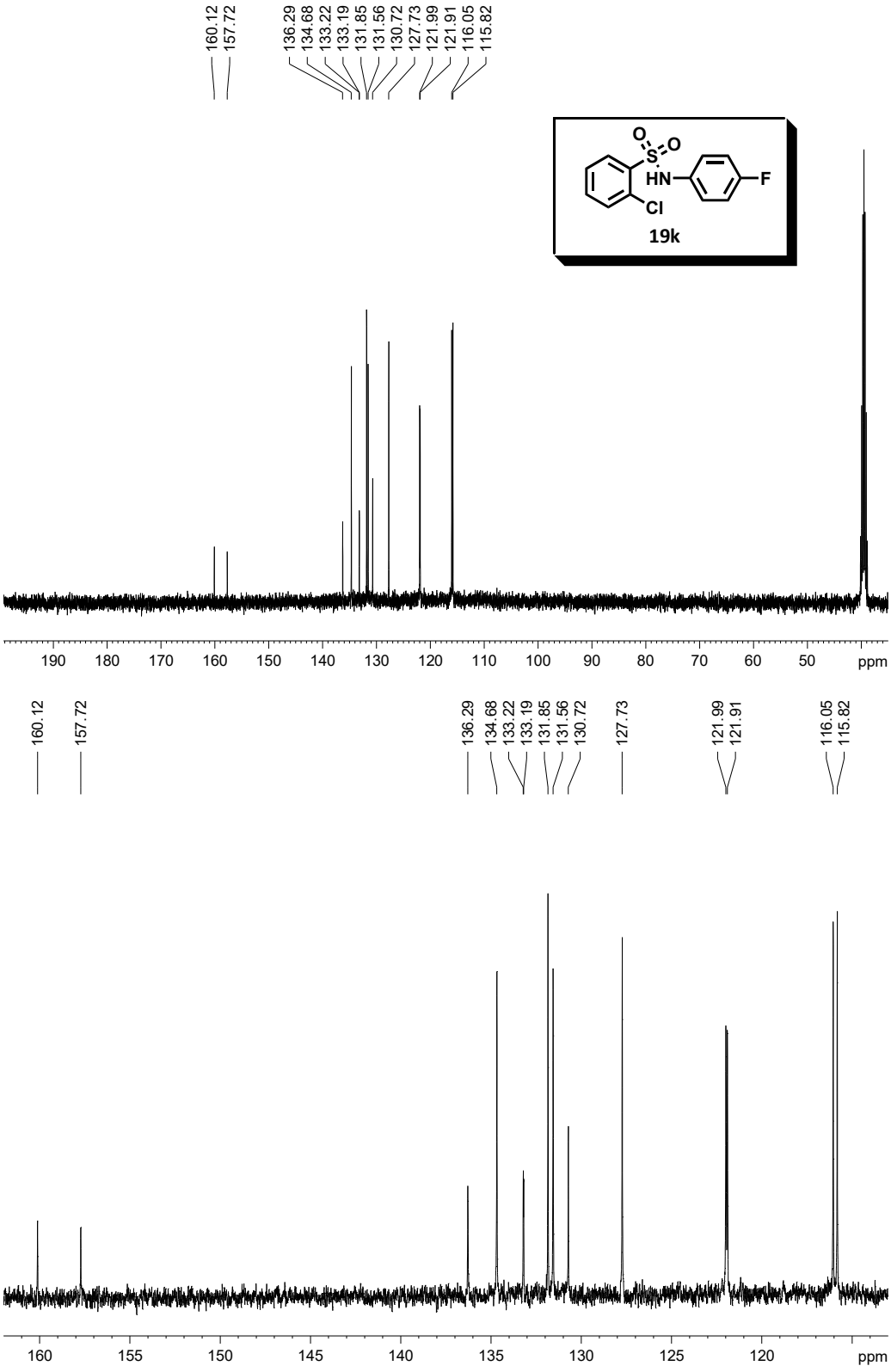
^{13}C-RMN (CD_3SOCD_3) 2-Cloro-*N*-(4-cianofenil)bencenosulfonamida (19j)



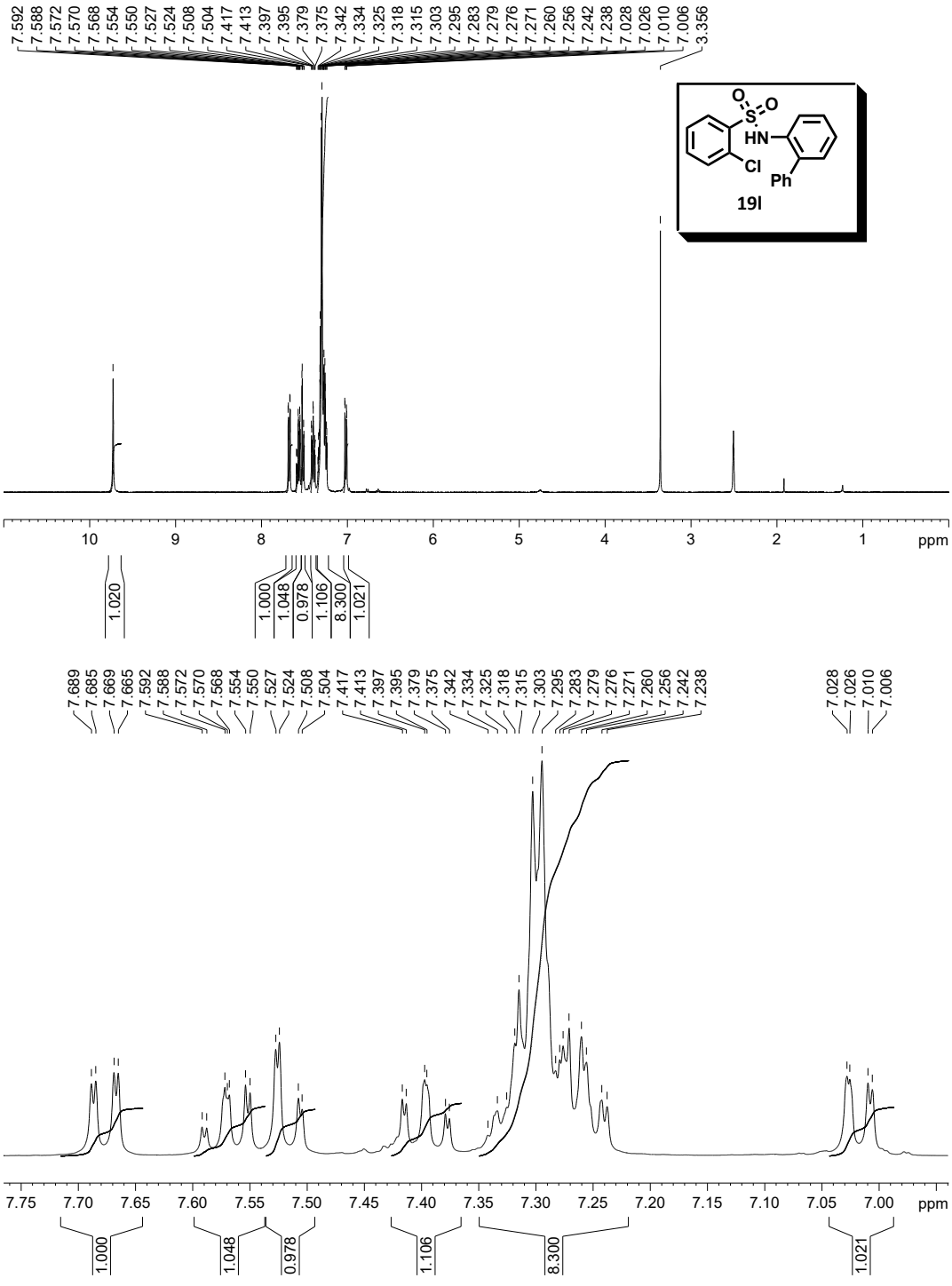
^{1}H-RMN (CD_3SOCD_3) 2-Cloro-*N*-(4-fluorfenil)bencenosulfonamida (19k)



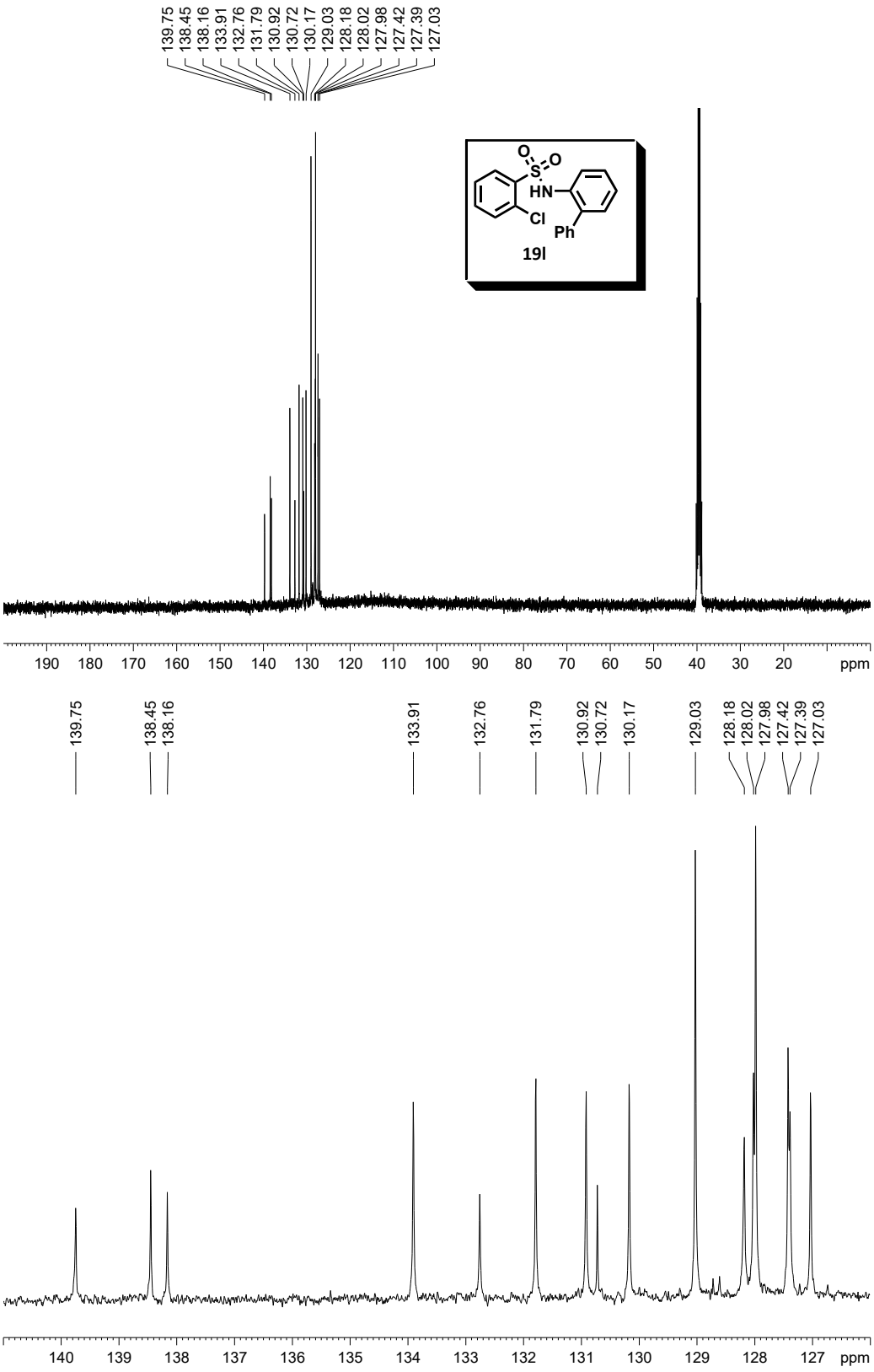
^{13}C-RMN (CD_3SOCD_3) 2-Cloro-*N*-(4-fluorfenil)bencenosulfonamida (19k)



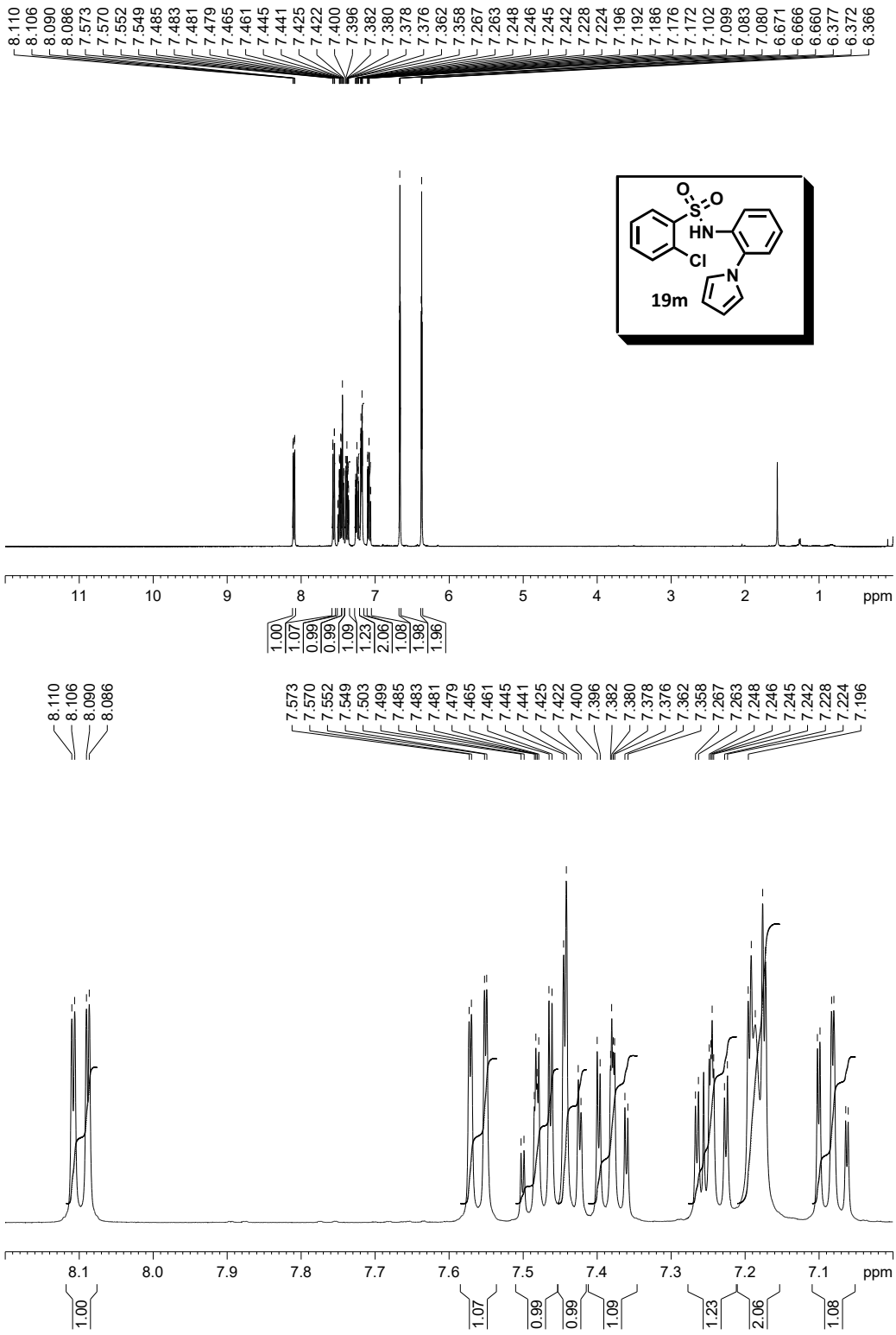
^{1}H-RMN (CD_3SOCD_3) *N*-([1,1'-Bifenil]-2-il)-2-clorobencenosulfonamida (19l)

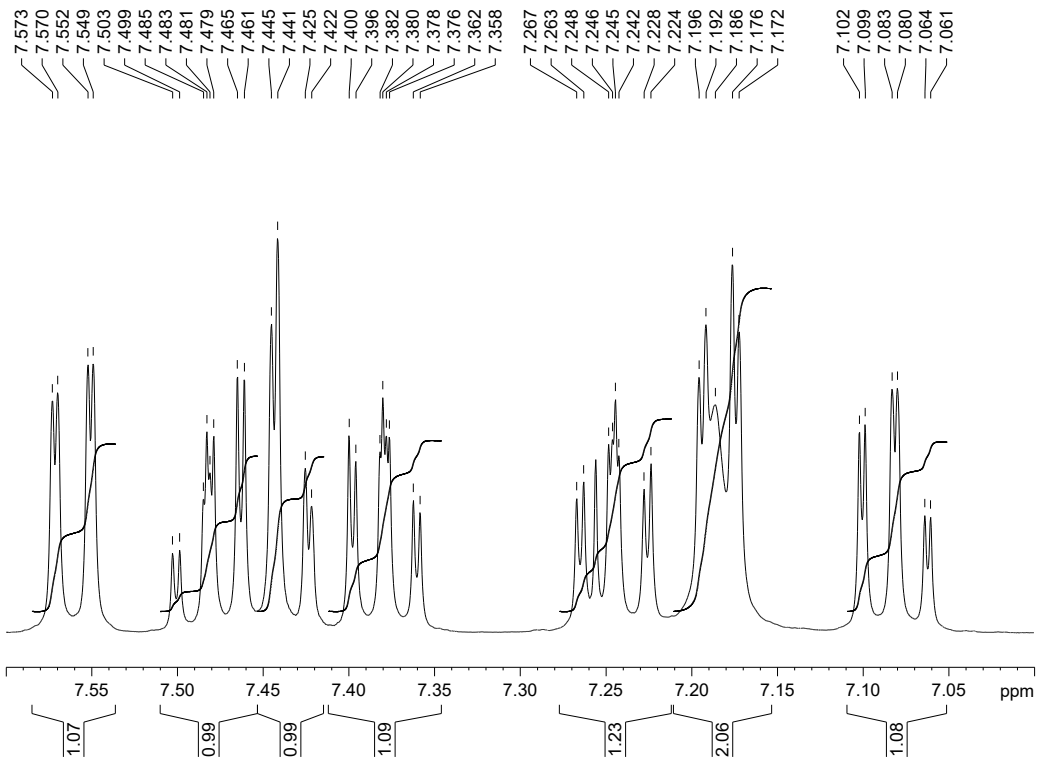


^{13}C-RMN (CD_3SOCD_3) *N*-([1,1'-Bifenil]-2-il)-2-clorobencenosulfonamida (19l)



^{1}H-RMN ($CDCl_3$) *N*-(2-(1*H*-Pirrol-1-il)fenil)-2-clorobencenosulfonamida (19m)

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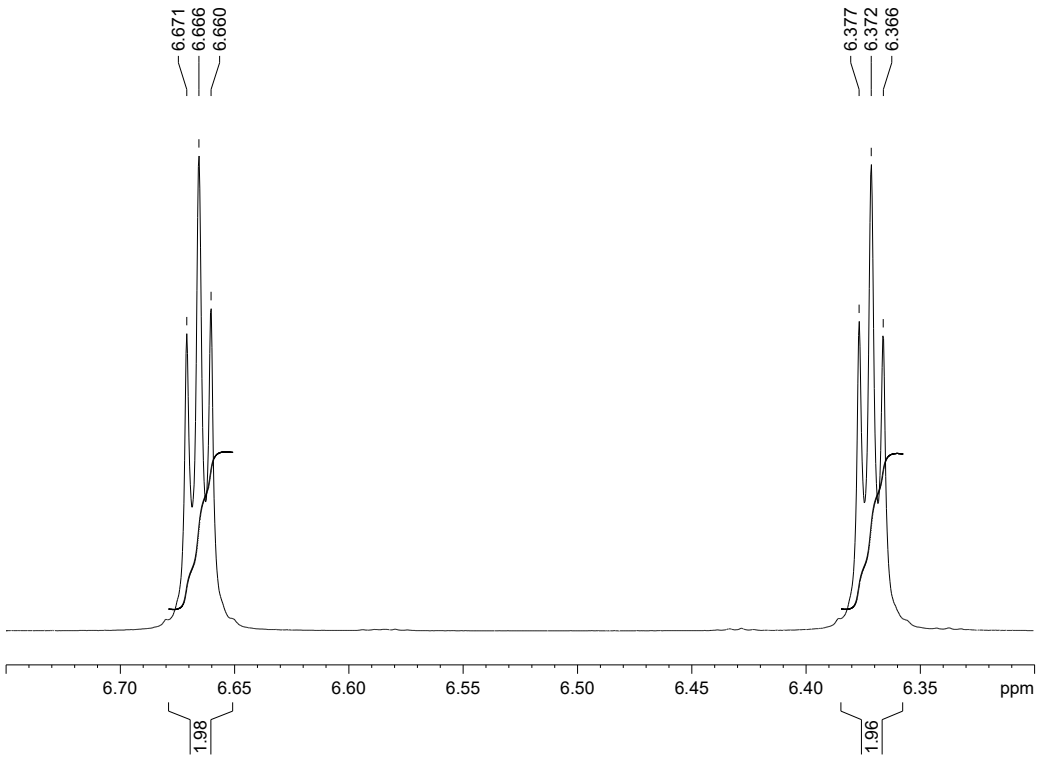
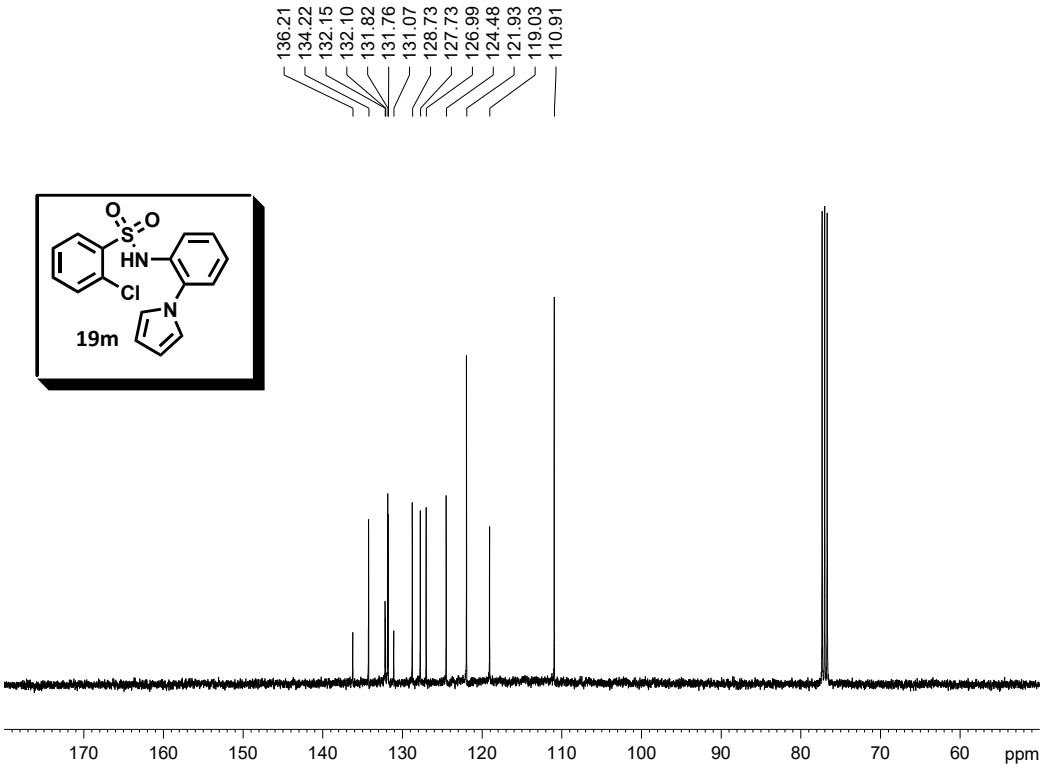
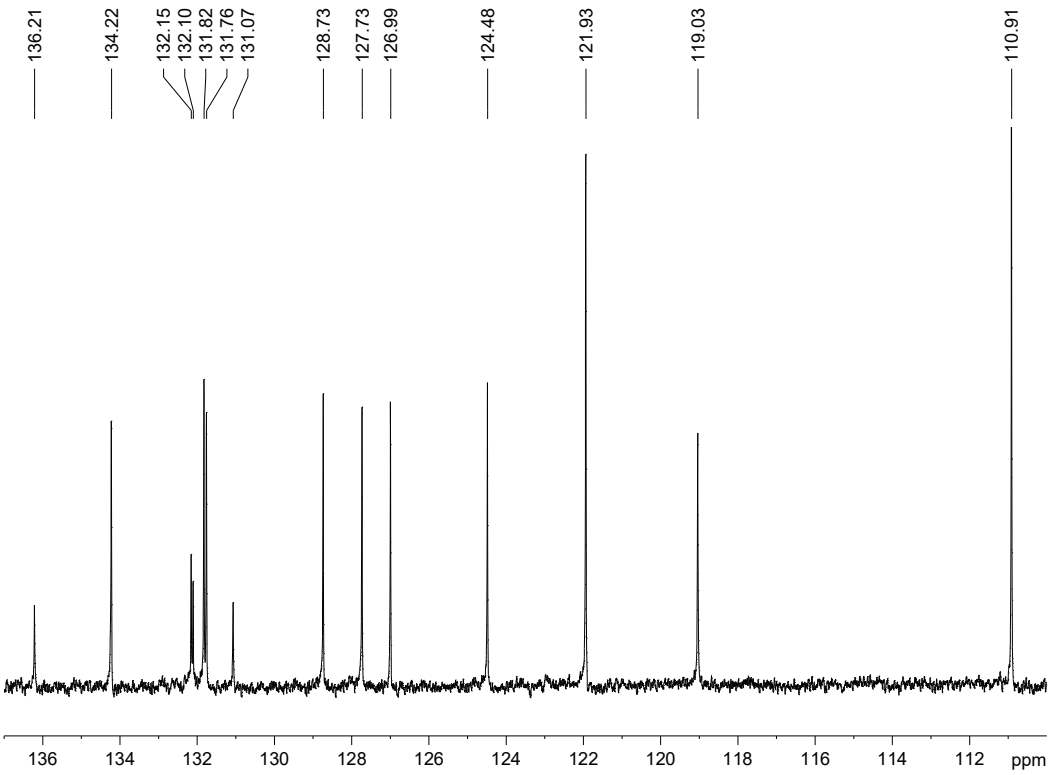
7.552
7.549
7.503
7.499
7.485
7.483
7.481
7.479
7.465
7.461
7.445
7.441
7.425
7.422
7.400
7.396
7.382
7.380
7.378
7.376
7.362
7.358
7.267
7.263
7.248
7.246
7.245
7.242
7.228
7.224
7.196
7.192
7.186
7.176
7.172
7.102
7.099
7.083
7.080
7.064
7.061
7.55
7.50
7.45
7.40
7.35
7.30
7.25
7.20
7.15
7.10
7.05
ppm
1.07
0.99
0.99
1.09
1.23
2.06
1.08

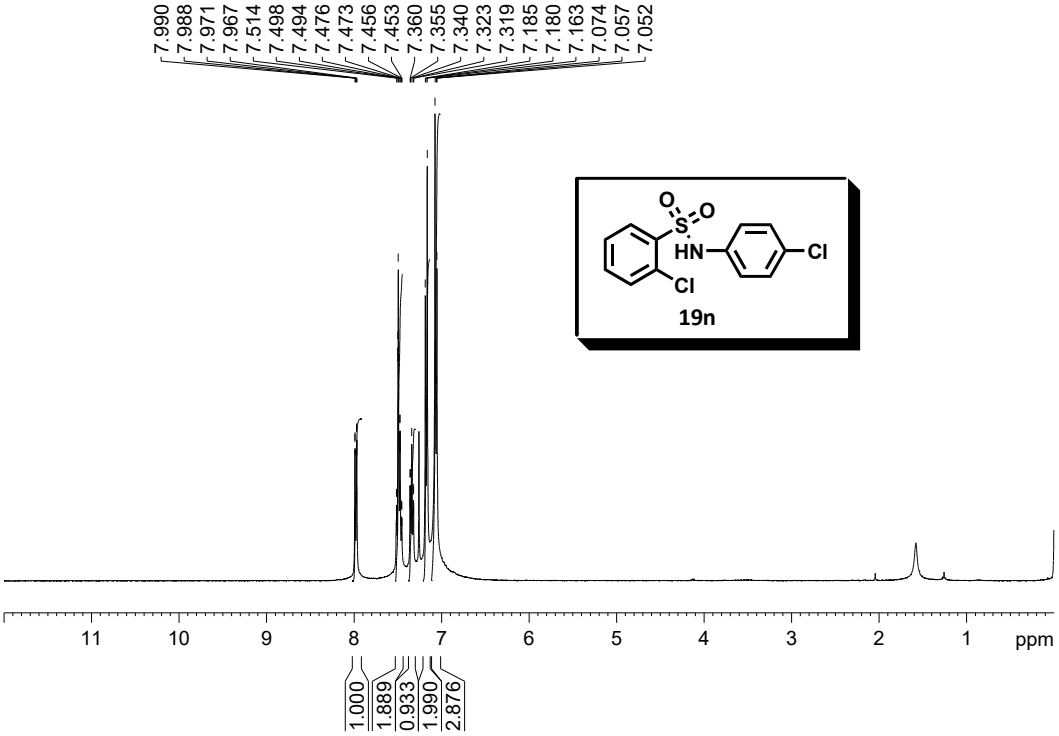

6.671
6.666
6.660
6.377
6.372
6.366
6.70
6.65
6.60
6.55
6.50
6.45
6.40
6.35
ppm
1.98
1.96

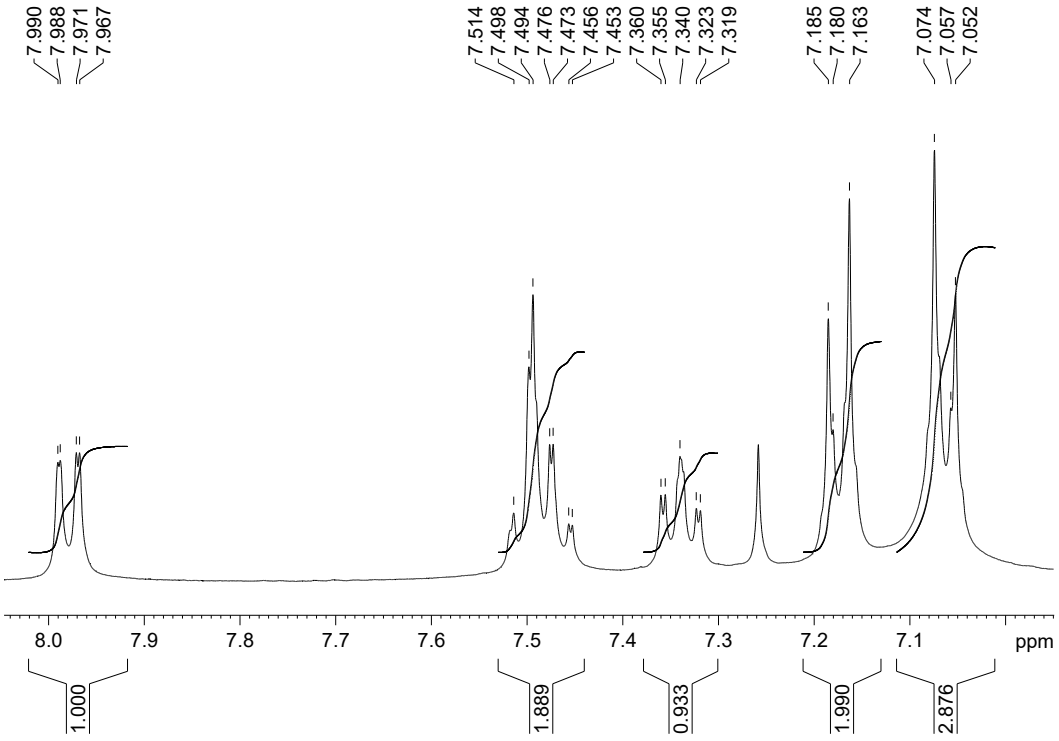
^{13}C-RMN ($CDCl_3$) *N*-(2-(1*H*-Pirrol-1-il)fenil)-2-clorobencenosulfonamida (19m)



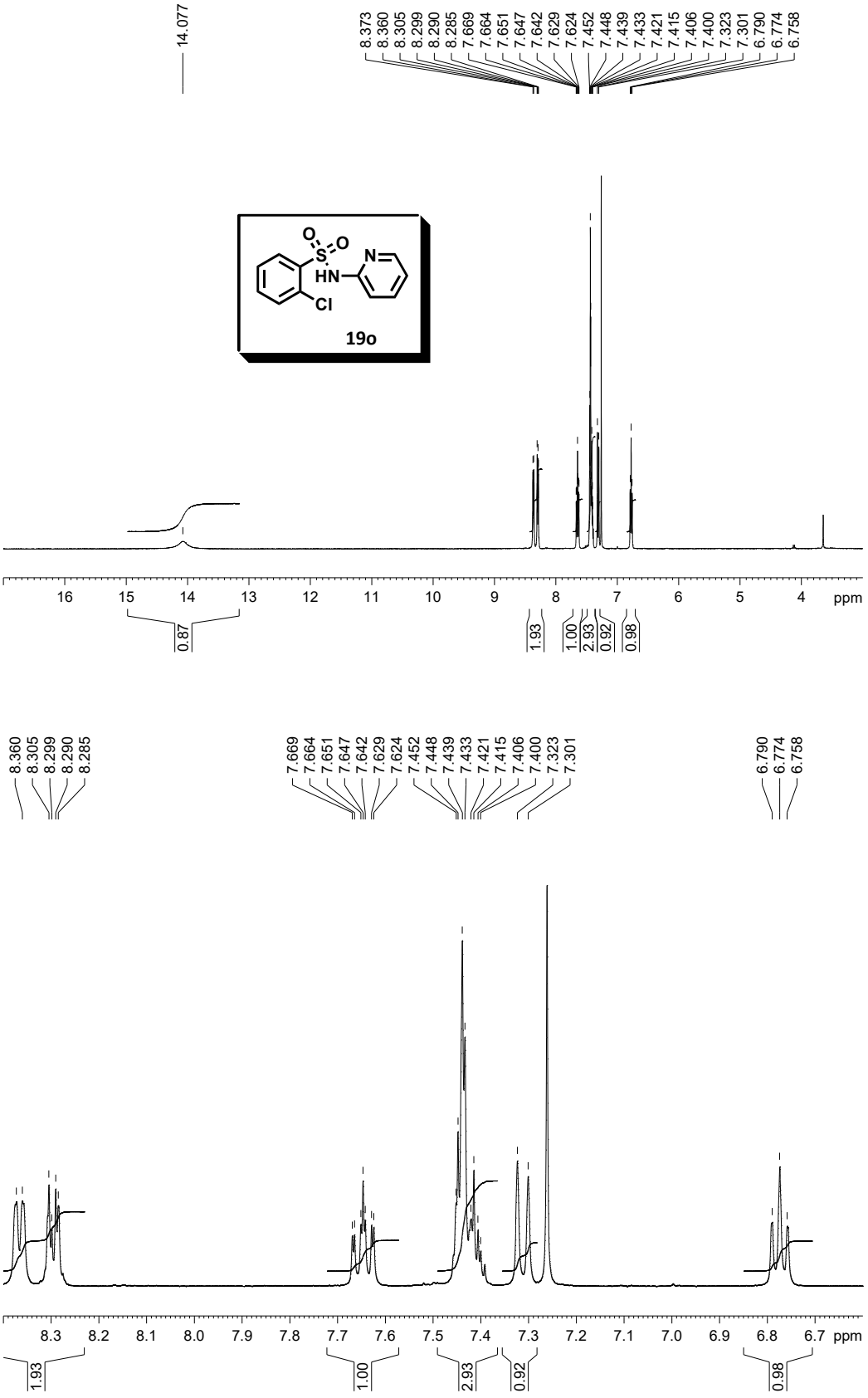


^{1}H-RMN ($CDCl_3$) 2-Cloro-*N*-(4-clorofenil)bencenosulfonamida (19n)

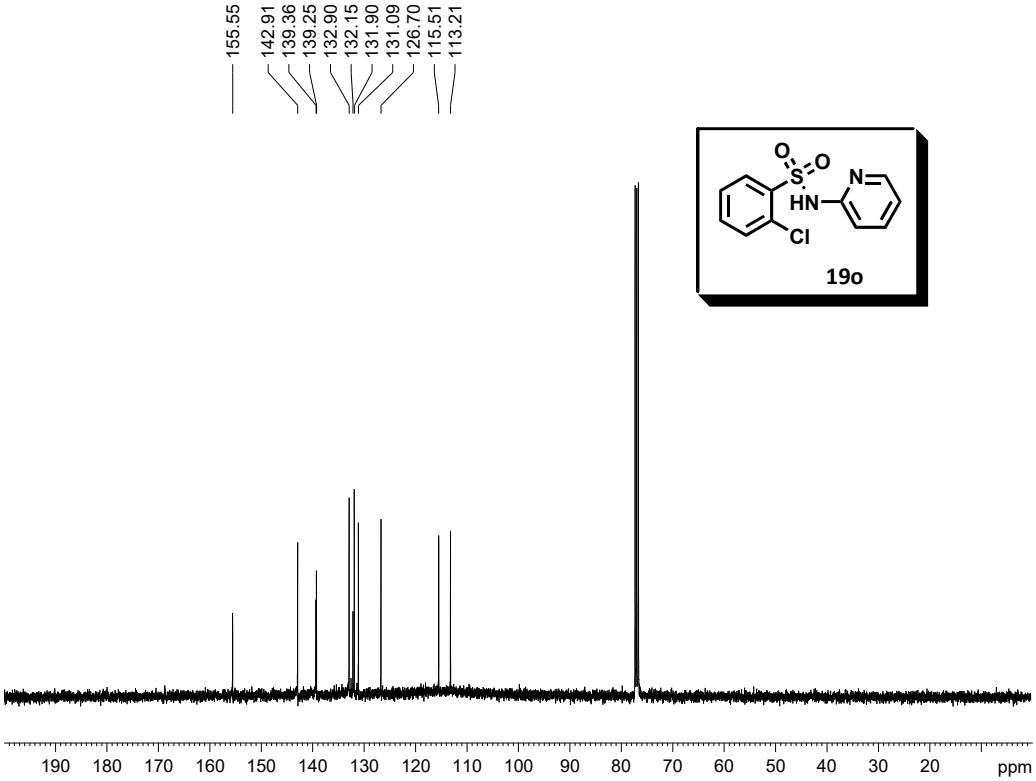


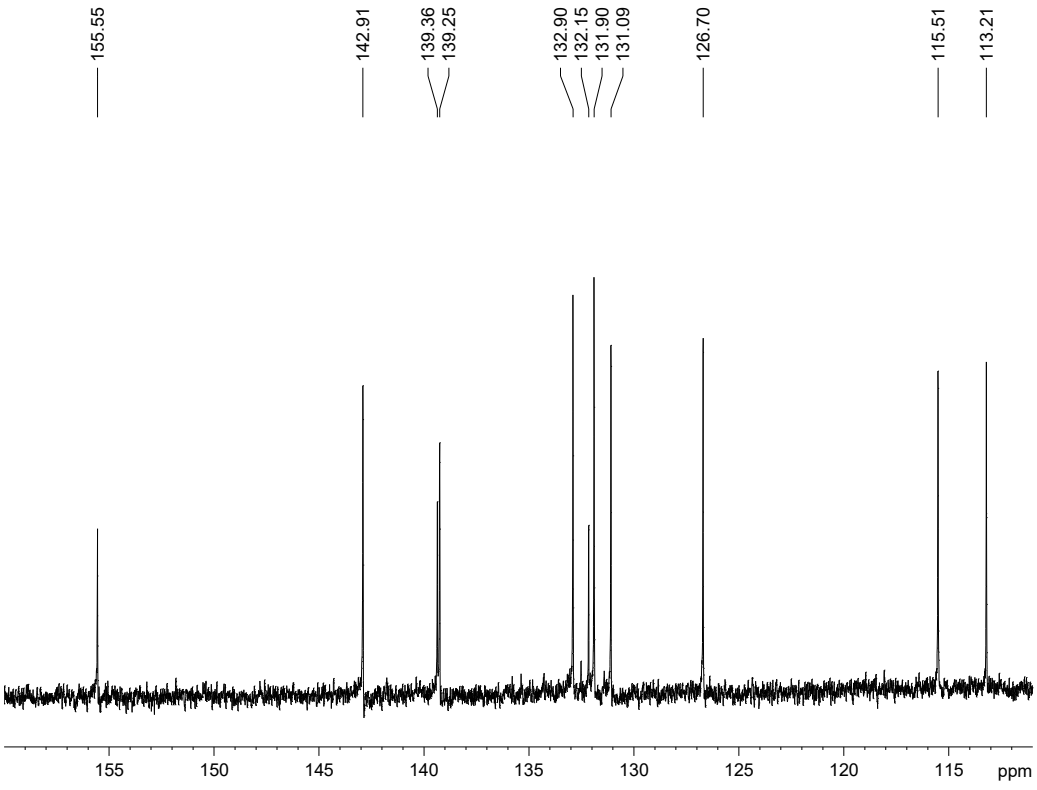


^{1}H-RMN ($CDCl_3$) 2-Cloro-*N*-(piridin-2il)-bencenosulfonamida (19o)

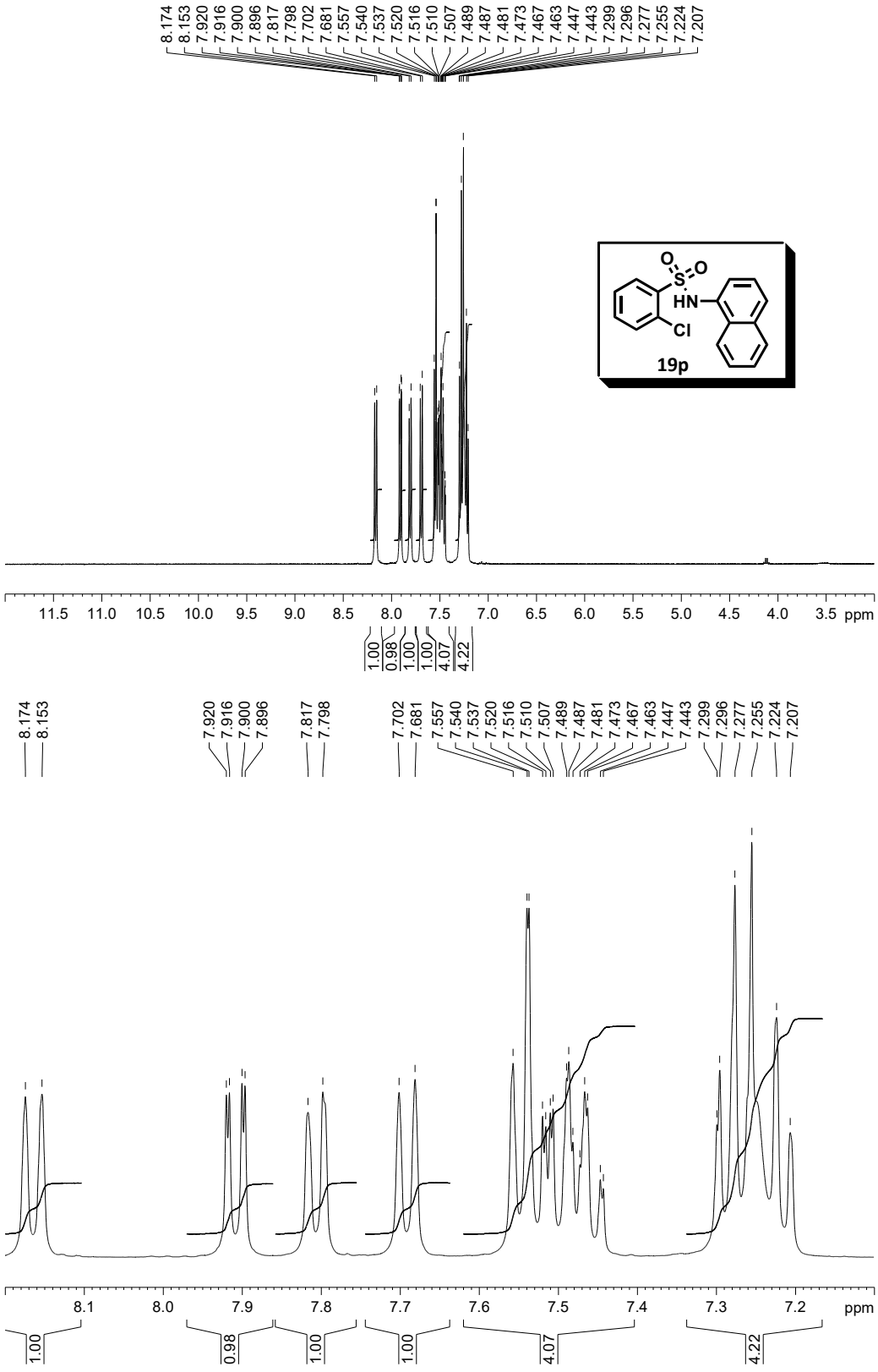


^{13}C-RMN ($CDCl_3$) 2-Cloro-*N*-(piridin-2il)-bencenosulfonamida (19o)

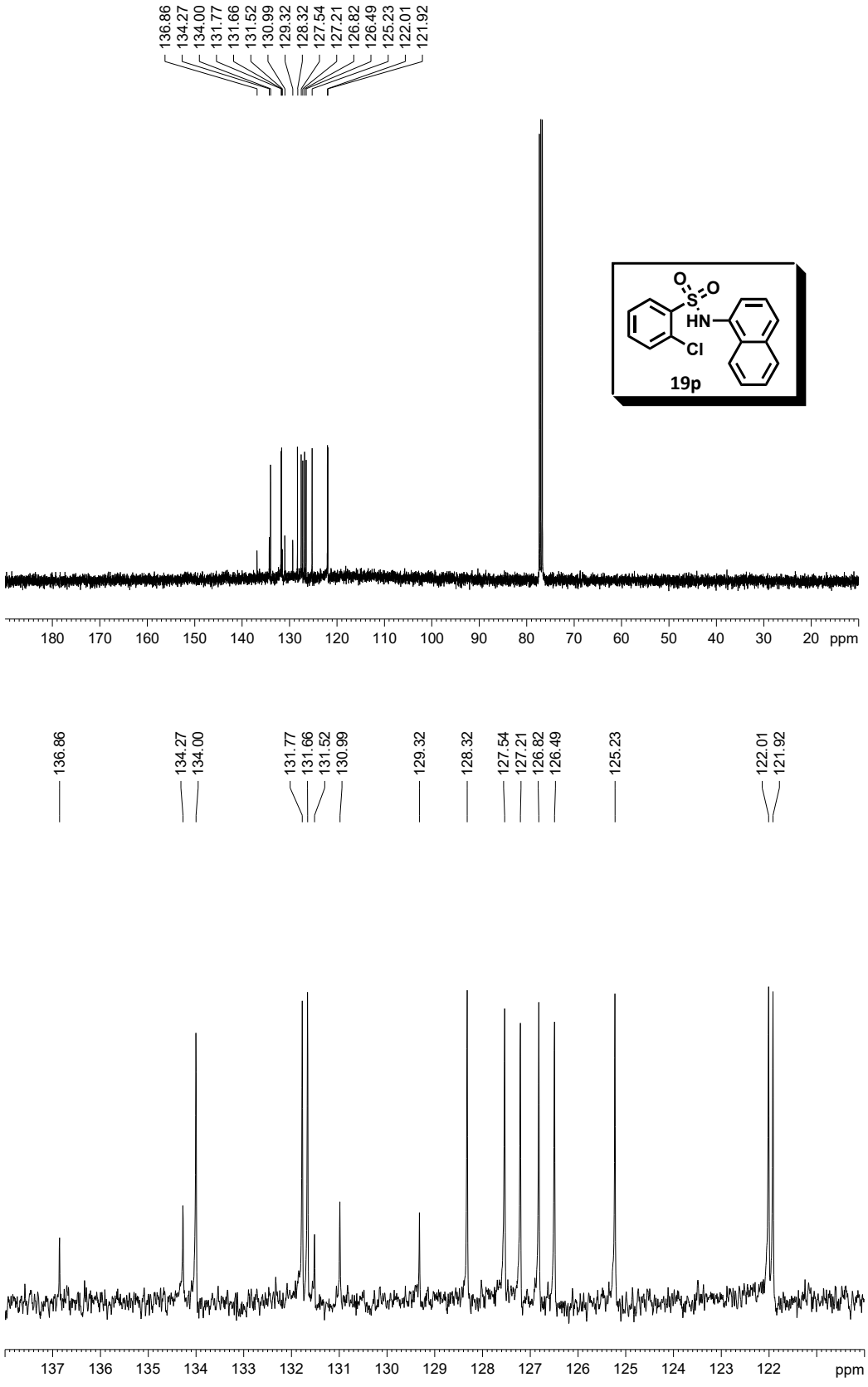




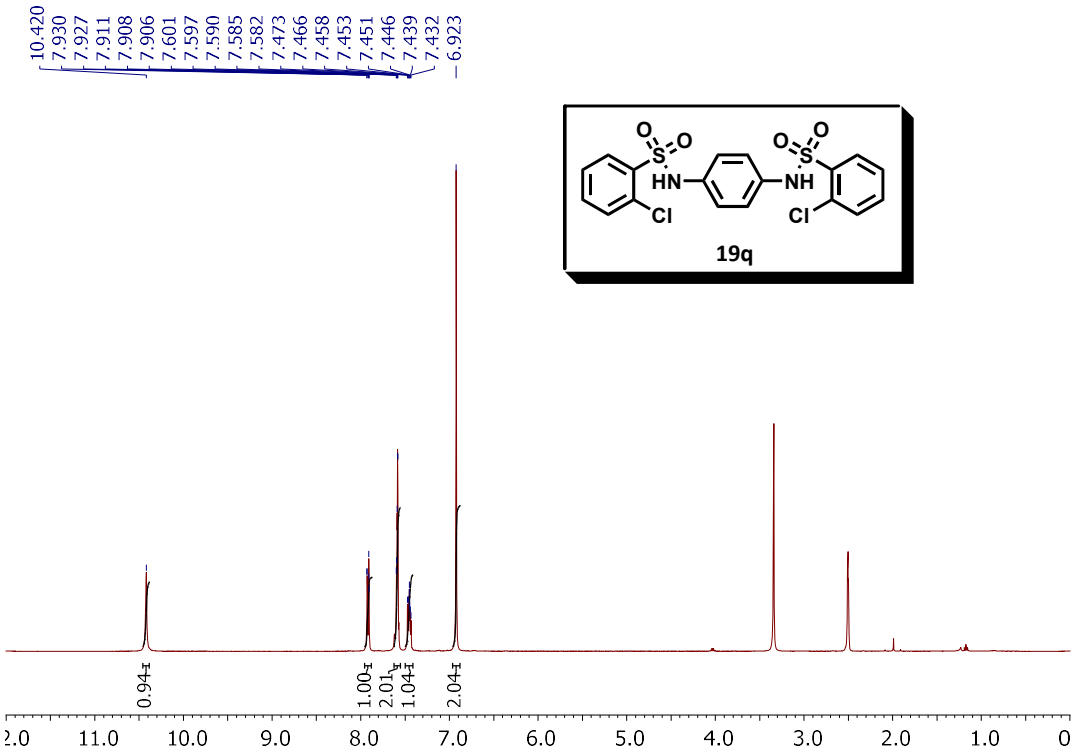
^{1}H-RMN ($CDCl_3$) 2-Cloro-*N*-(naftalen-1-il)-bencenosulfonamida (19p)

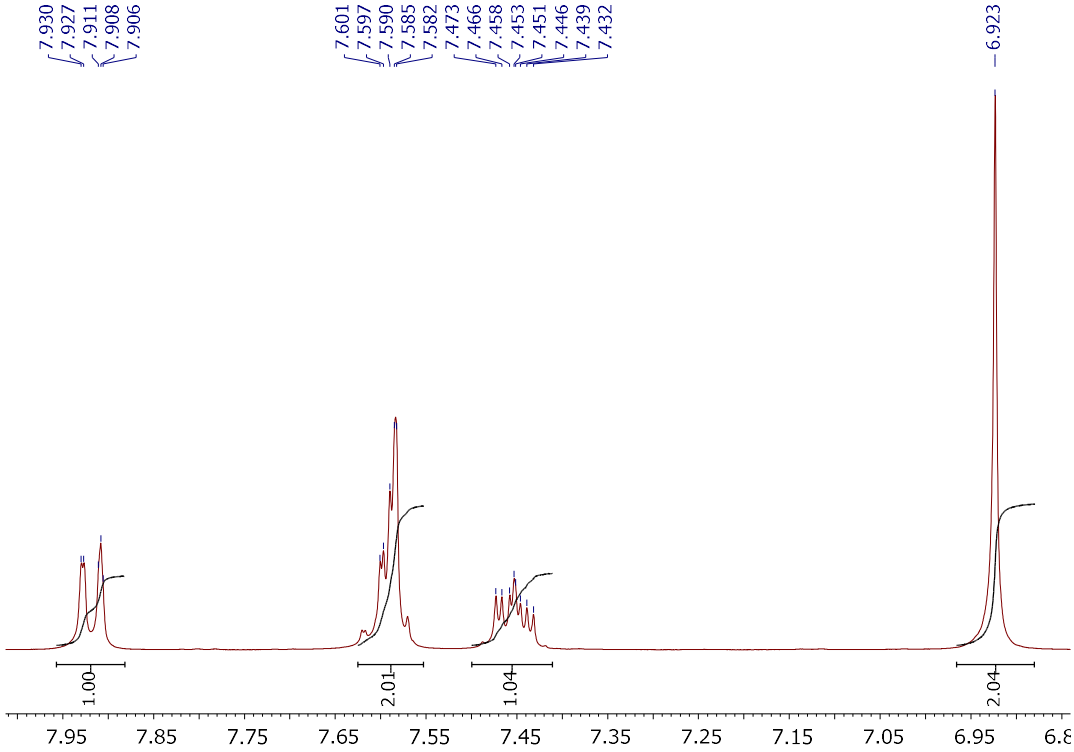


^{13}C-RMN ($CDCl_3$) 2-Cloro-*N*-(naftalen-1-il)-bencenosulfonamida (19p)

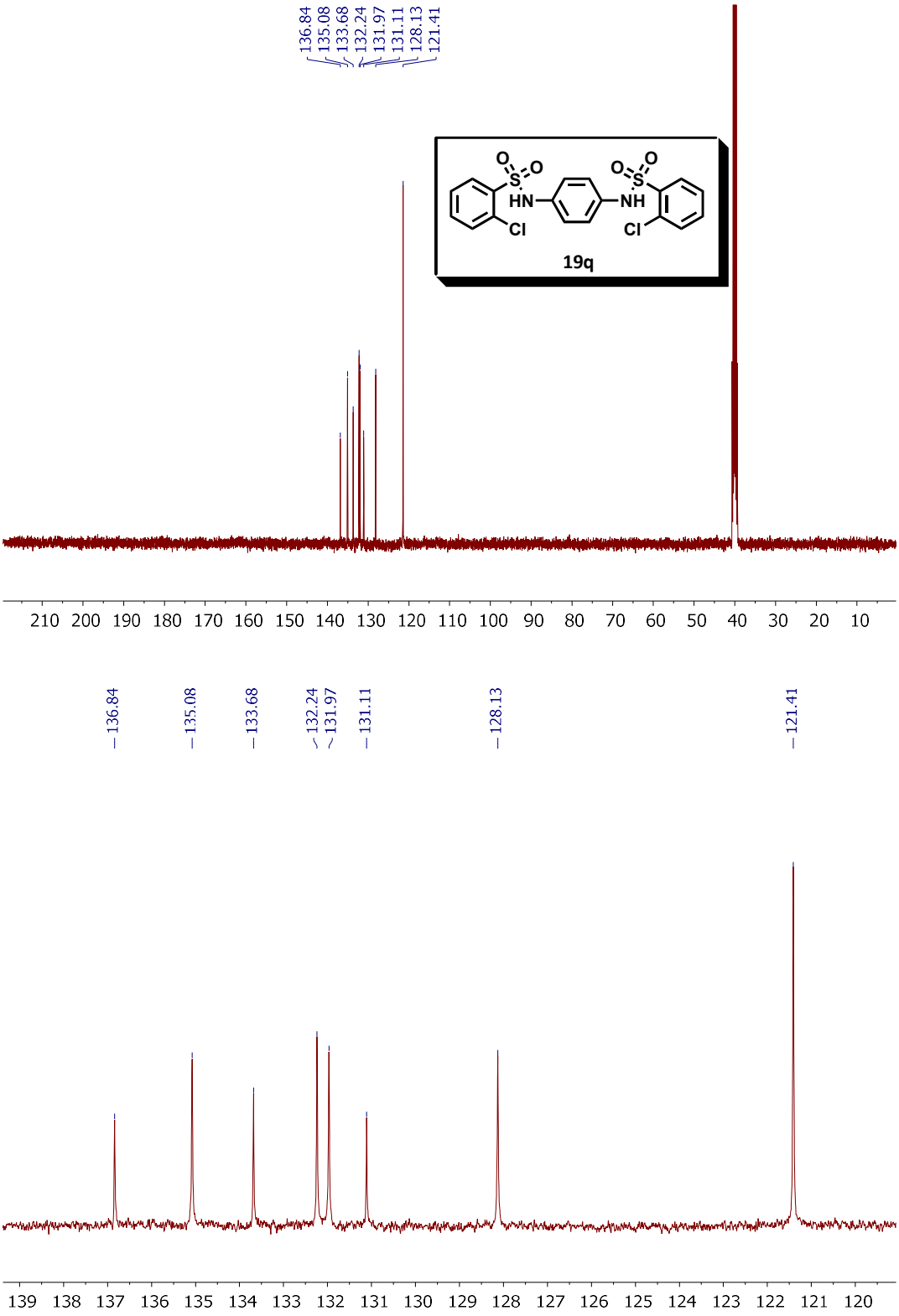


^{1}H-RMN (CD_3SOCD_3) *N,N'*-(1,4-Fenilen)bis(2-clorobenzenesulfonamide) (19q)

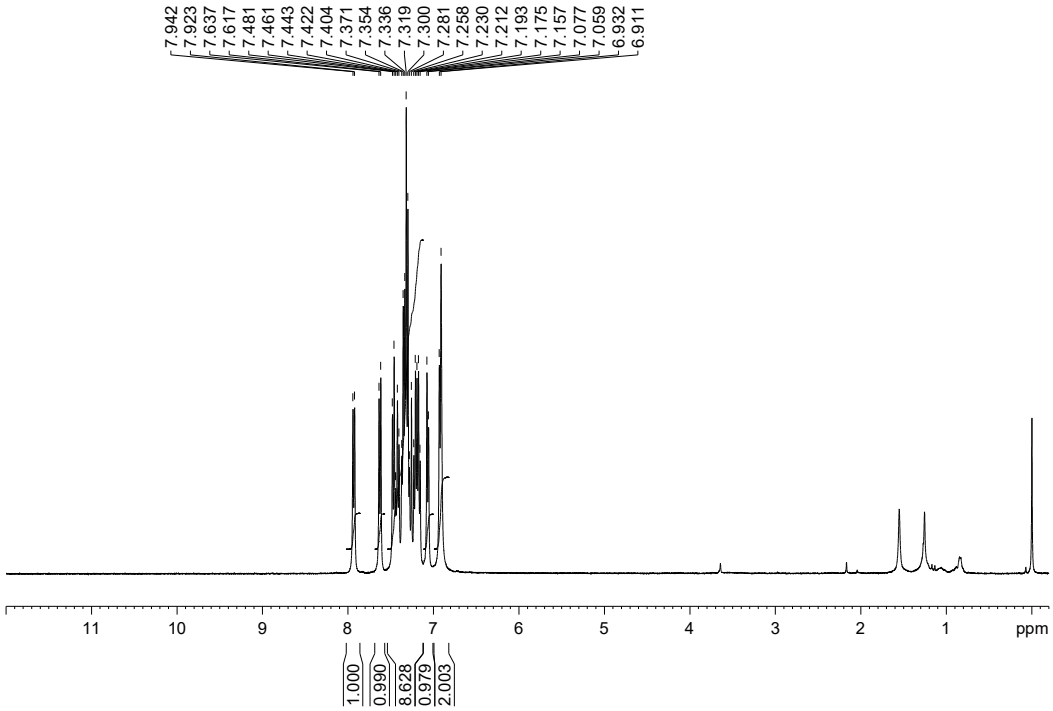


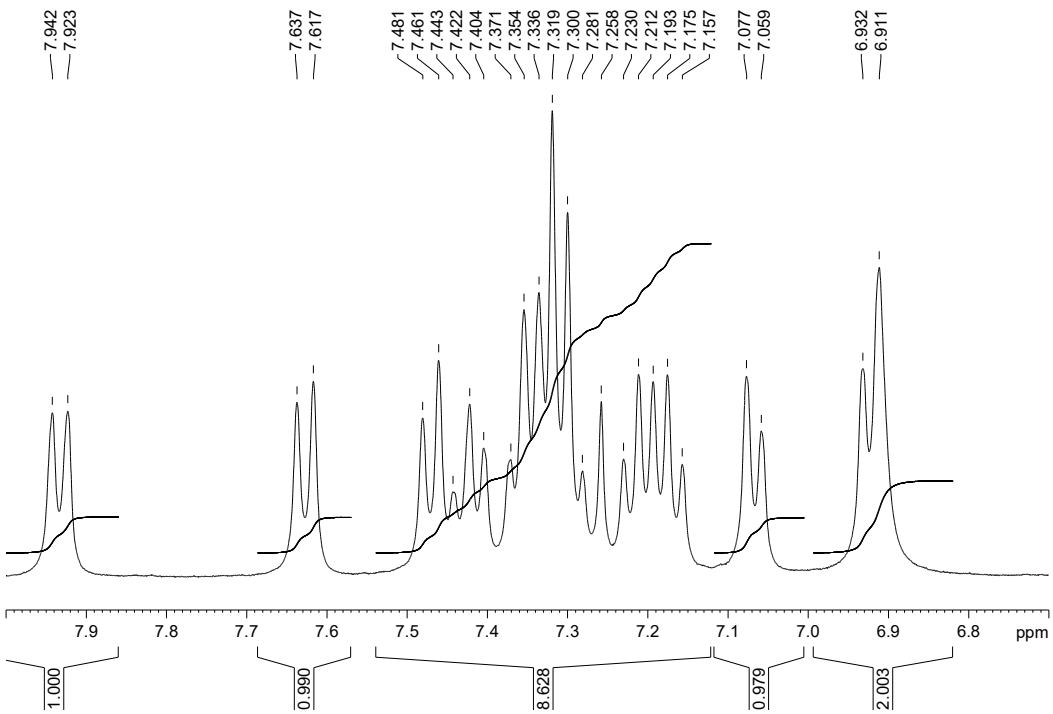


^{13}C-RMN (CD_3SOCD_3) *N,N'*-(1,4-Fenilen)bis(2-clorobenzenesulfonamide) (19q)

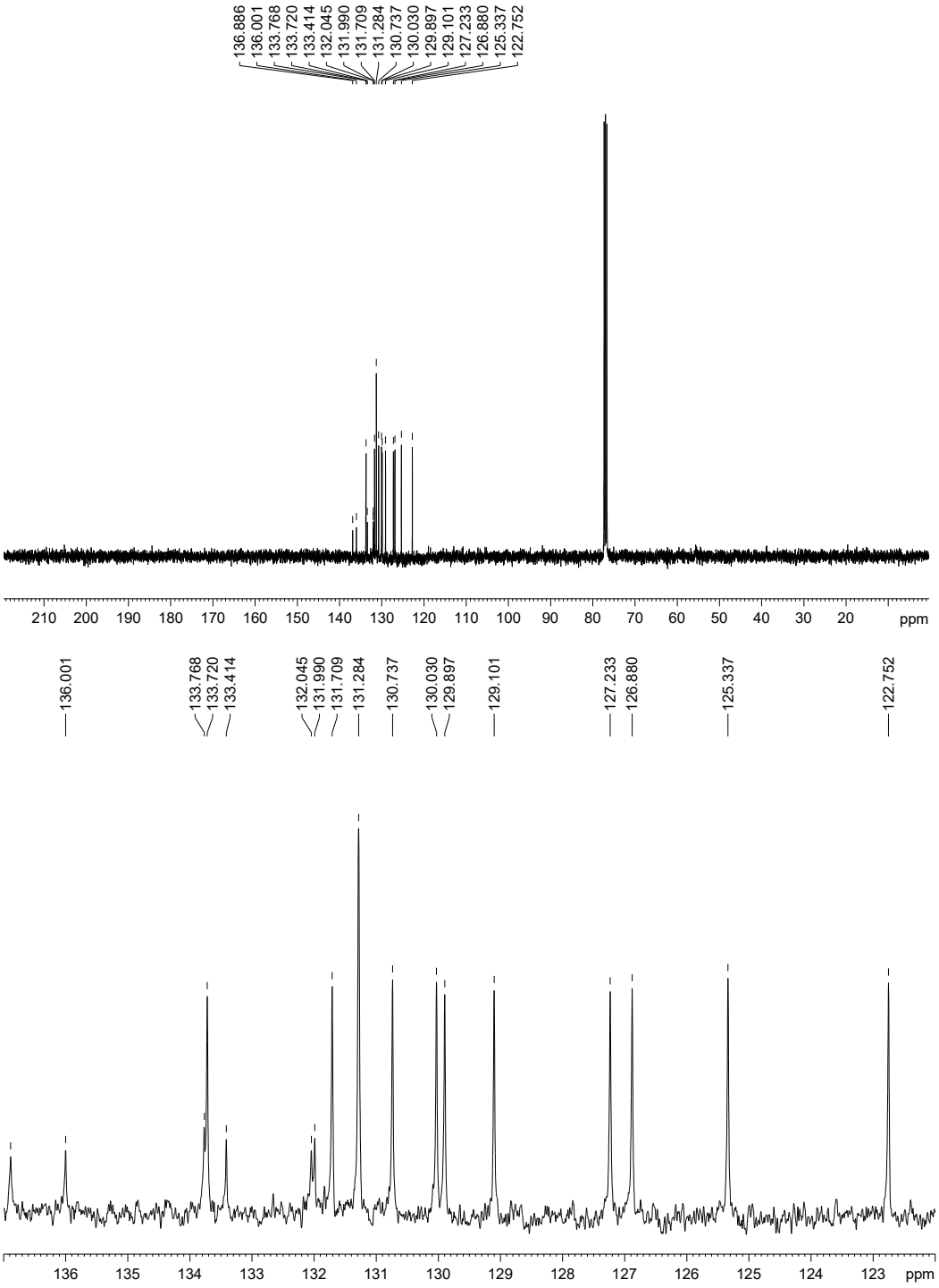


^{1}H-RMN ($CDCl_3$) *N*-([2-cloro-1,1'-Bifenil]-2-il)-2-clorobencenosulfonamida (19r)

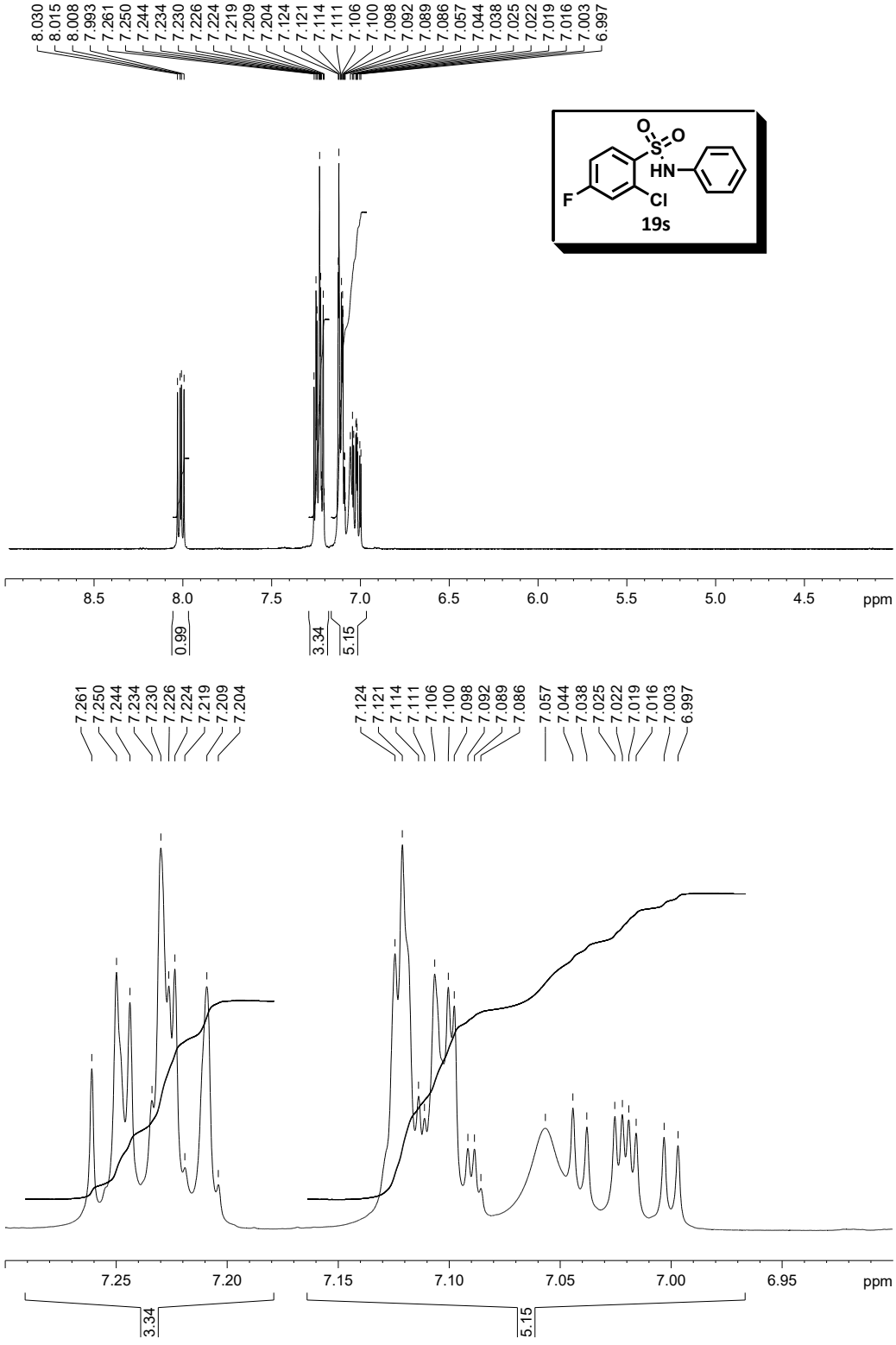




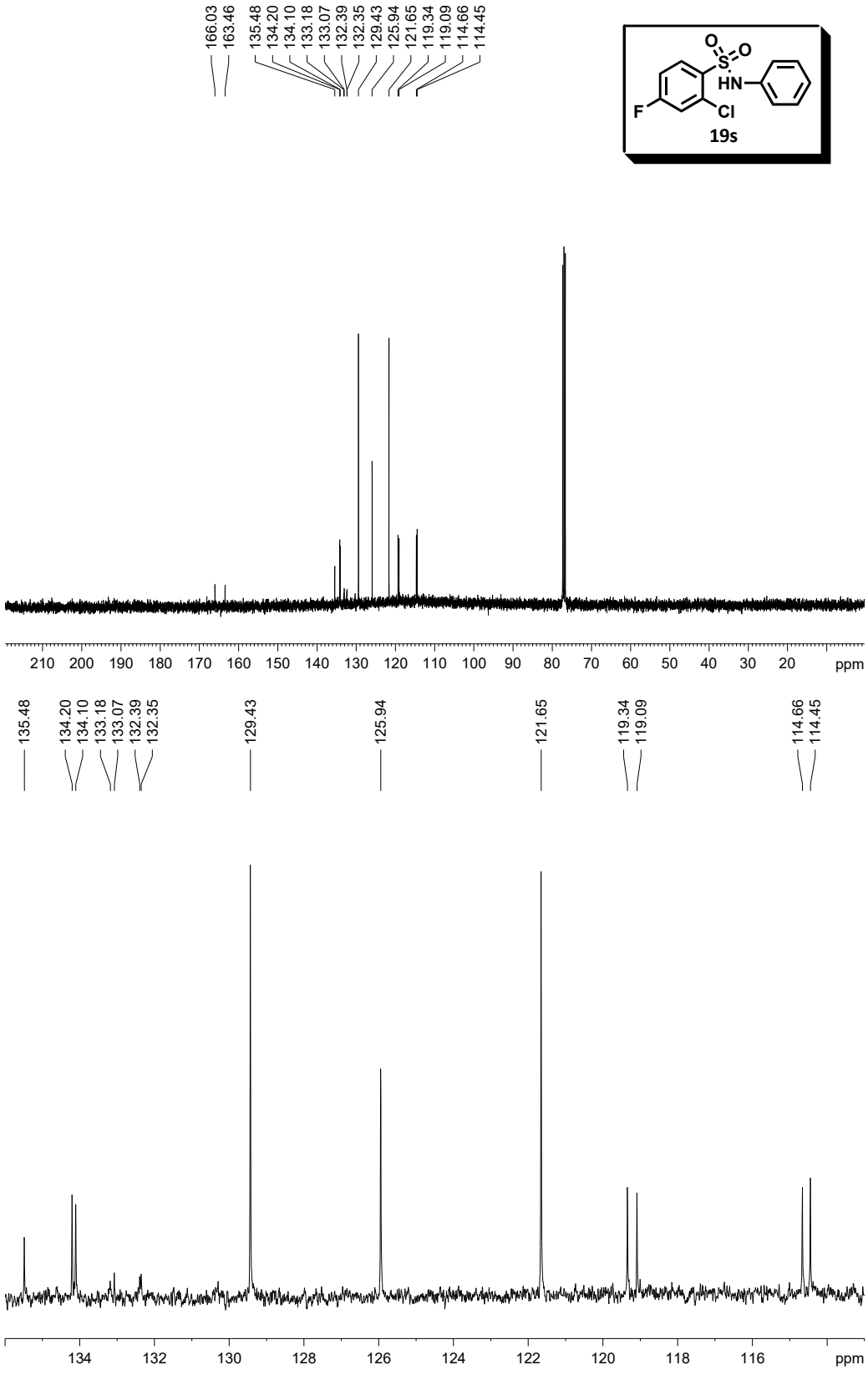
^{13}C-RMN ($CDCl_3$) *N*-([2-cloro-1,1'-Bifenil]-2-il)-2-clorobencenosulfonamida (19r)



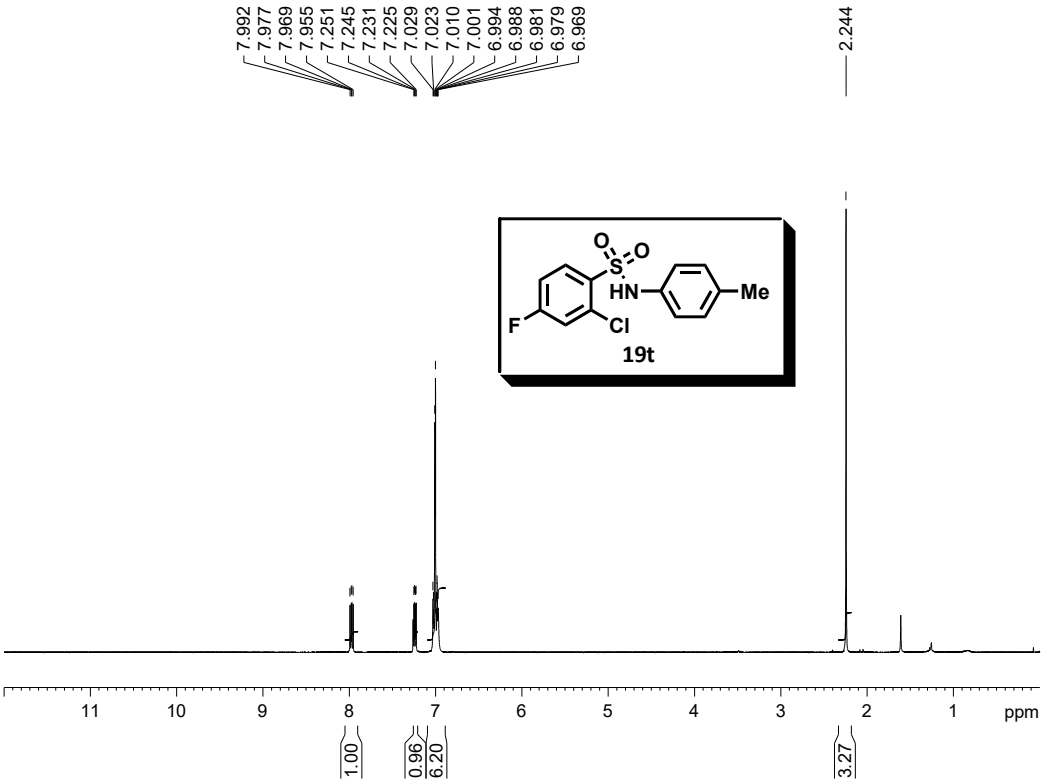
^{1}H-RMN ($CDCl_3$) 2-Cloro-4-fluor-*N*-fenilbencenosulfonamida (19s)

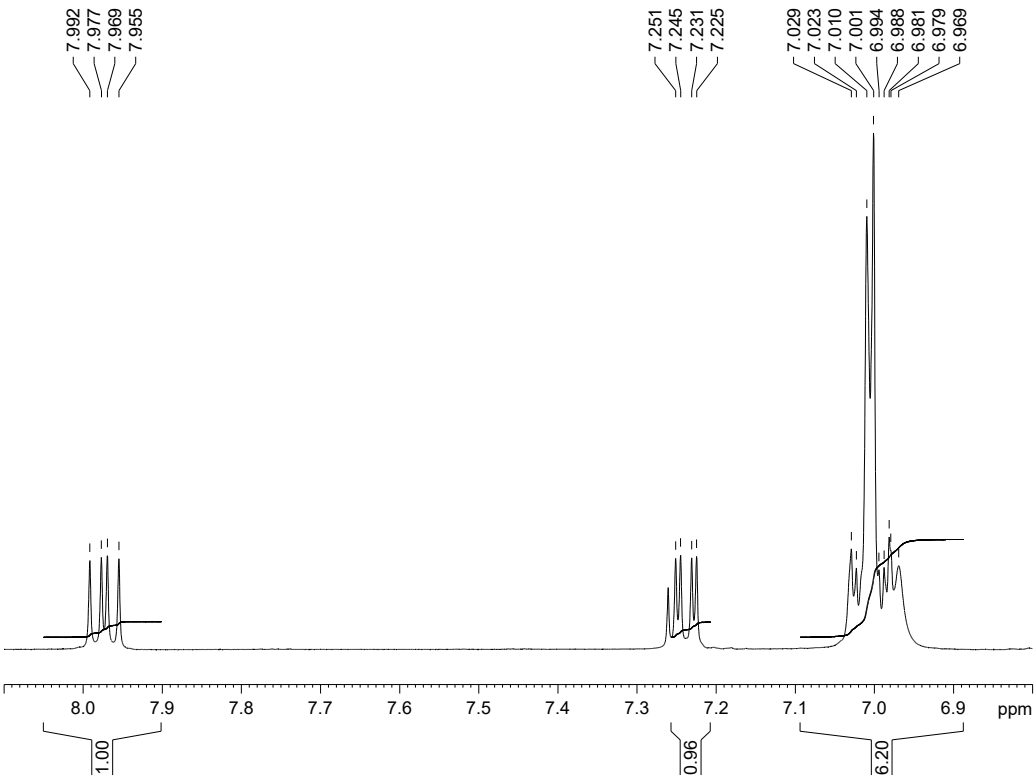


^{13}C-RMN ($CDCl_3$) 2-Cloro-4-fluor-*N*-fenilbencenosulfonamida (19s)

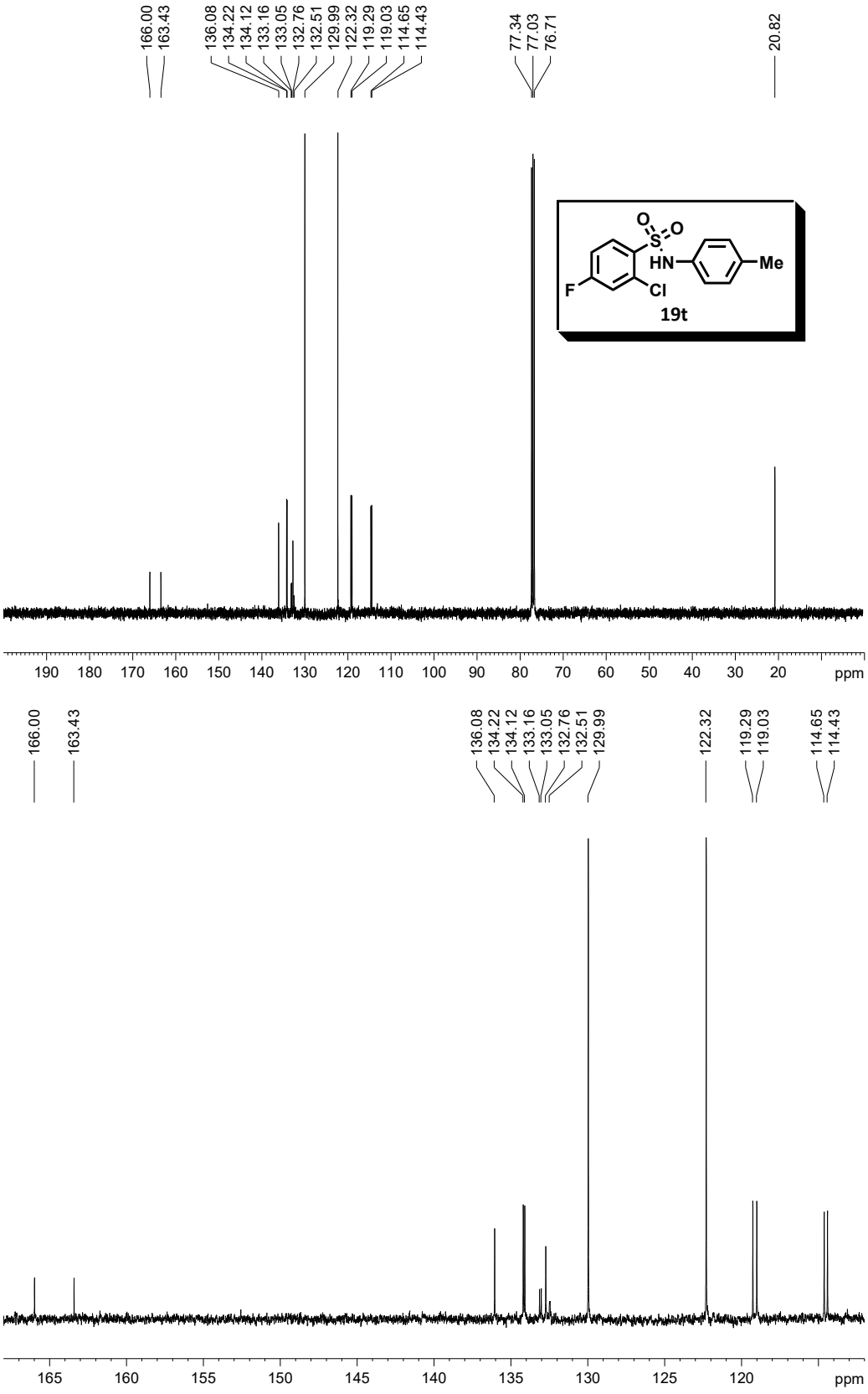


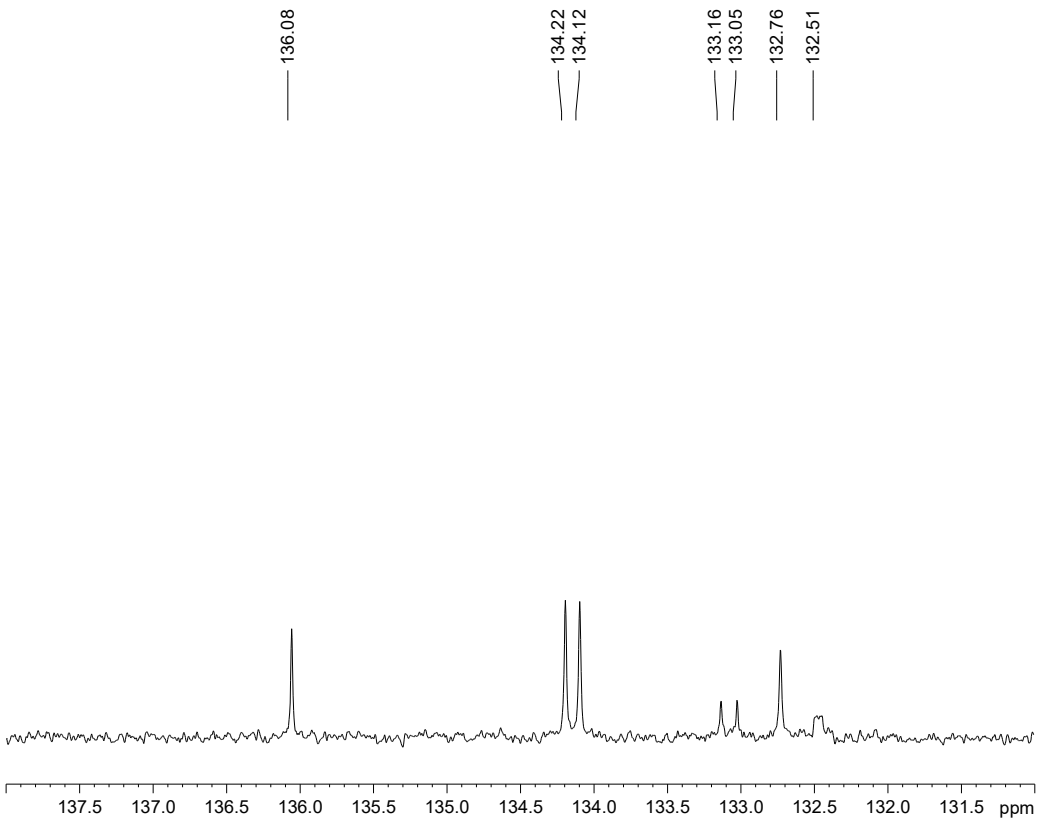
^{1}H-RMN ($CDCl_3$) 2-Cloro-4-fluor-*N*-(*p*-tolil)bencenosulfonamida (19t)



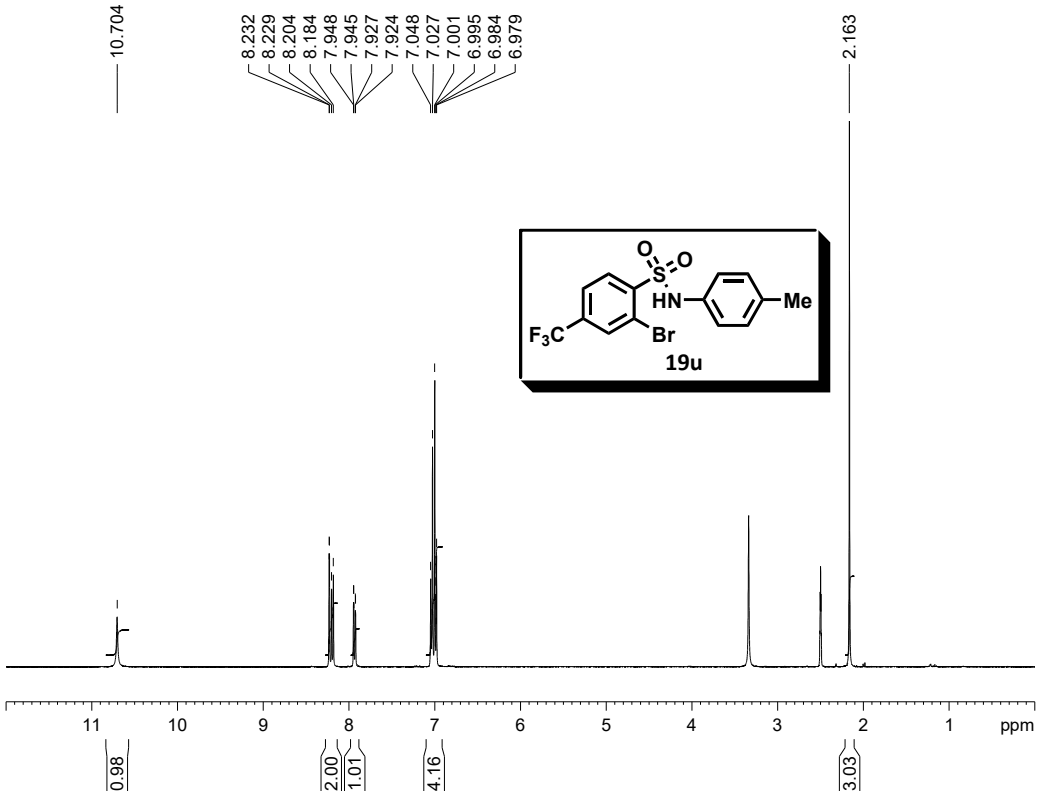


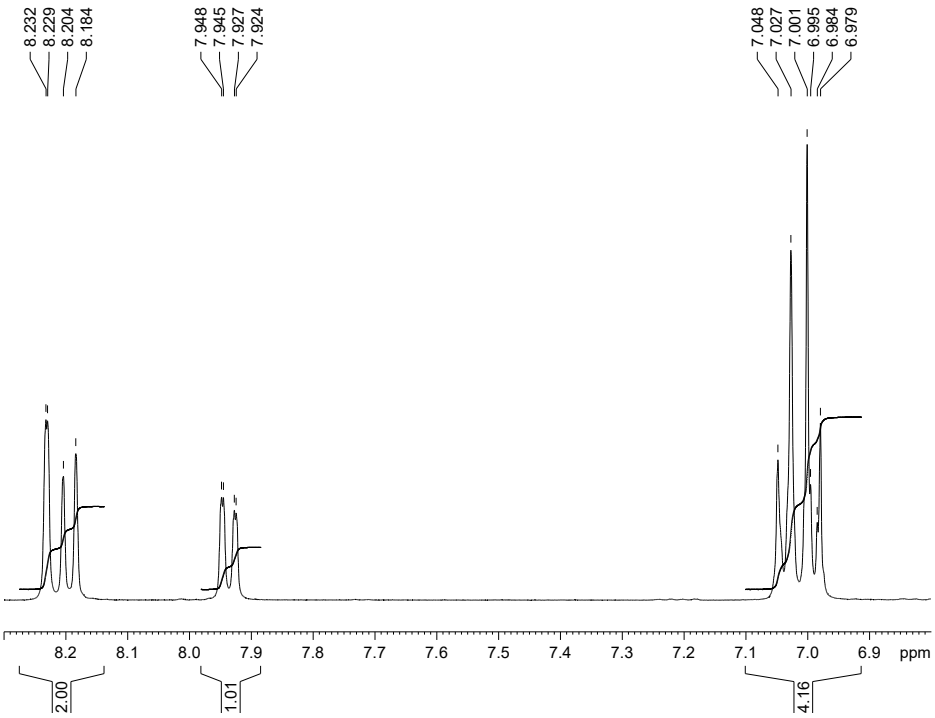
^{13}C-RMN ($CDCl_3$) 2-Cloro-4-fluor-*N*-(*p*-tolil)bencenosulfonamida (19t)



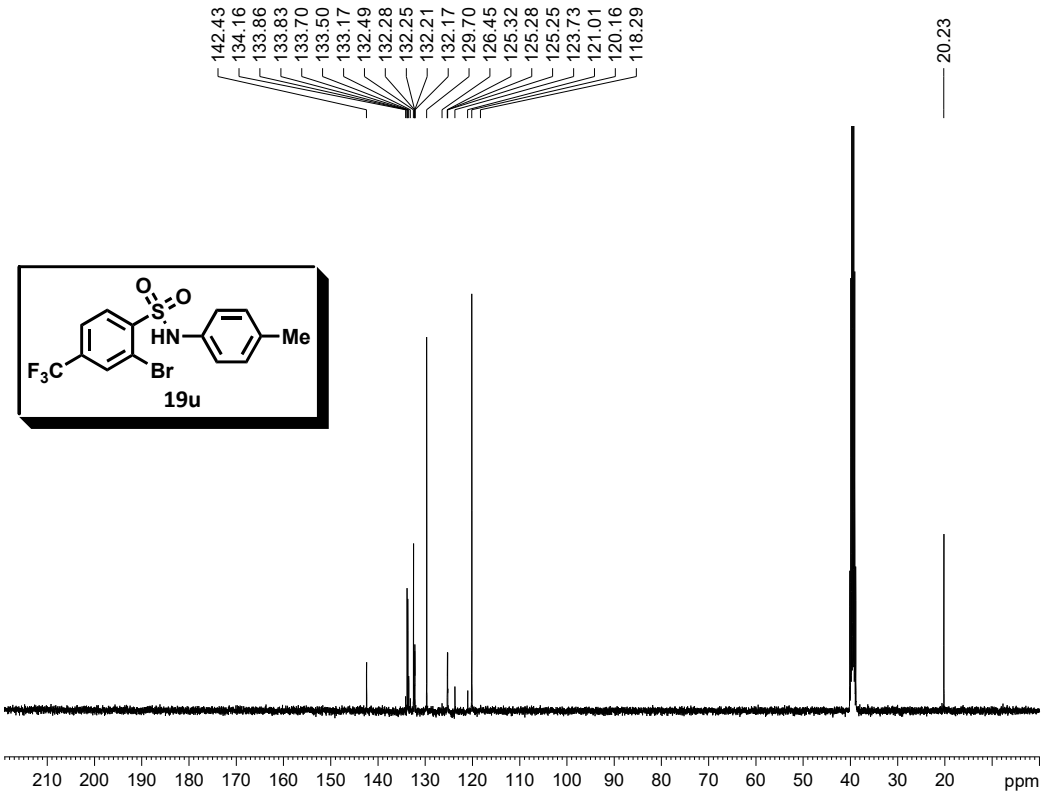


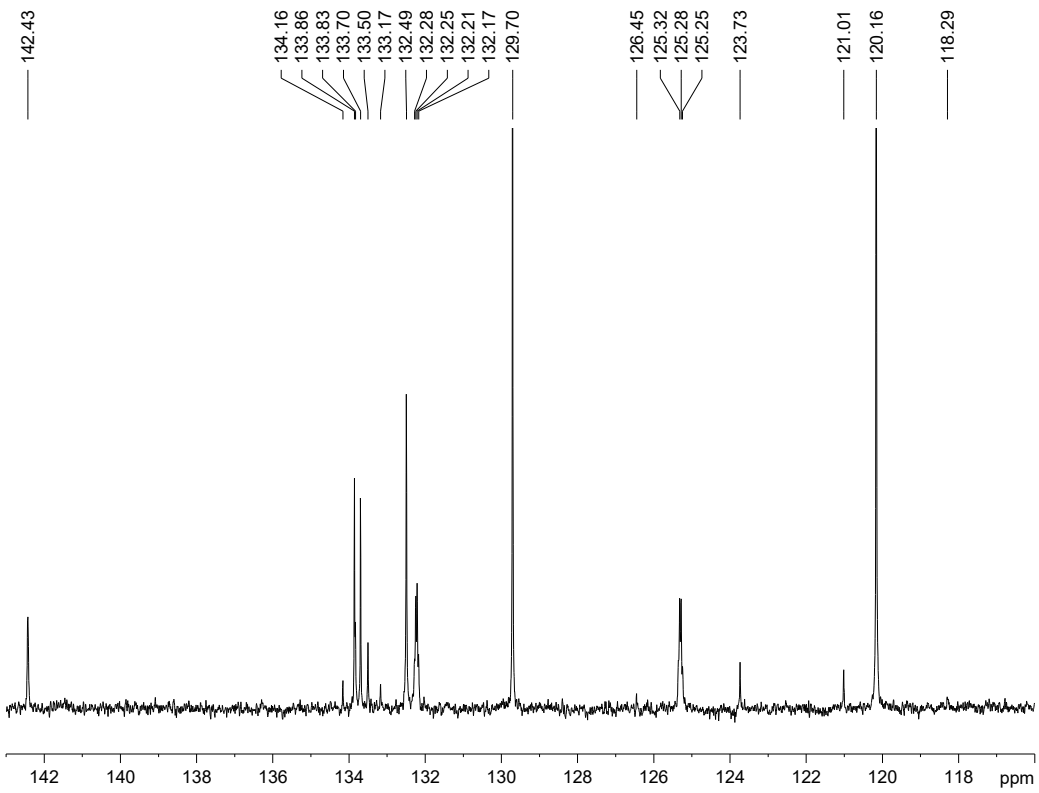
^{1}H-RMN (CD_3SOCD_3) 2-Bromo-*N*-(p-tolil)-4-(trifluormetil)-bencenosulfonamida (19u)

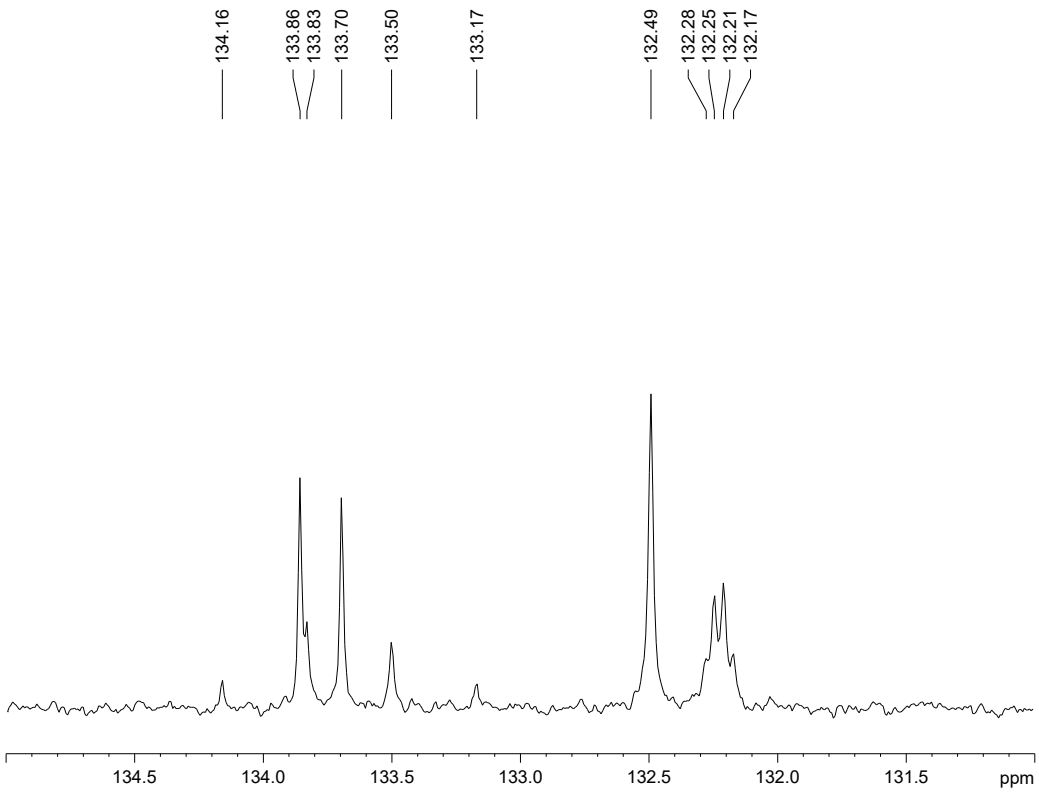




^{13}C-RMN (CD_3SOCD_3) 2-Bromo-*N*-(p-tolil)-4-(trifluormetil)-bencenosulfonamida (19u)




142.43
134.16
133.86
133.83
133.70
133.50
133.17
132.49
132.28
132.25
132.21
132.17
129.70
126.45
125.32
125.28
125.25
123.73
121.01
120.16
118.29
142
140
138
136
134
132
130
128
126
124
122
120
118
ppm


134.16
133.86
133.83
133.70
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133.17
132.49
132.28
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132.21
132.17
134.5
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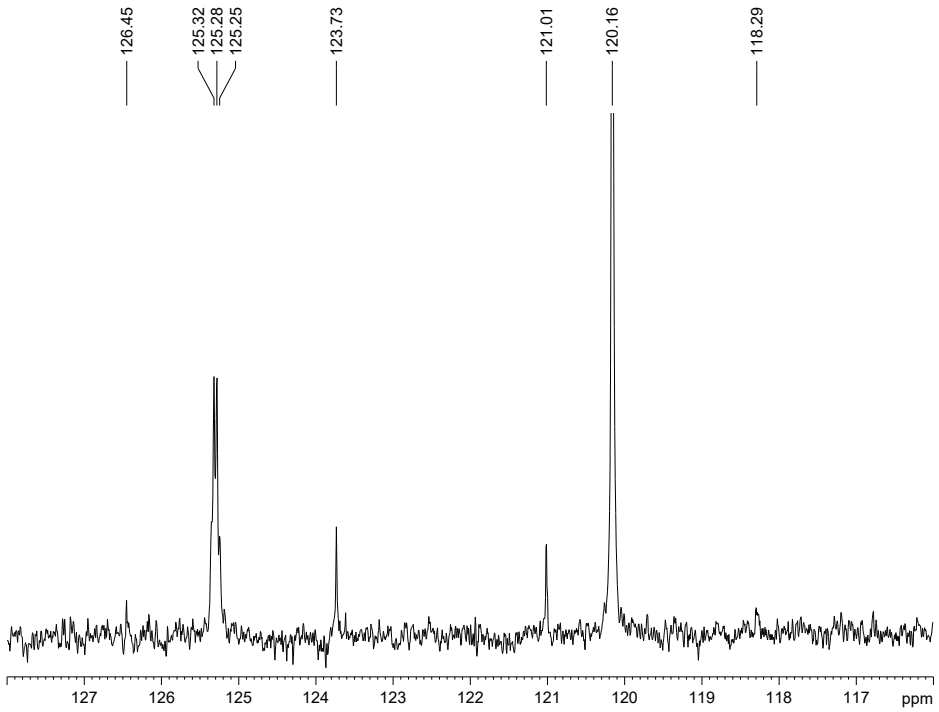
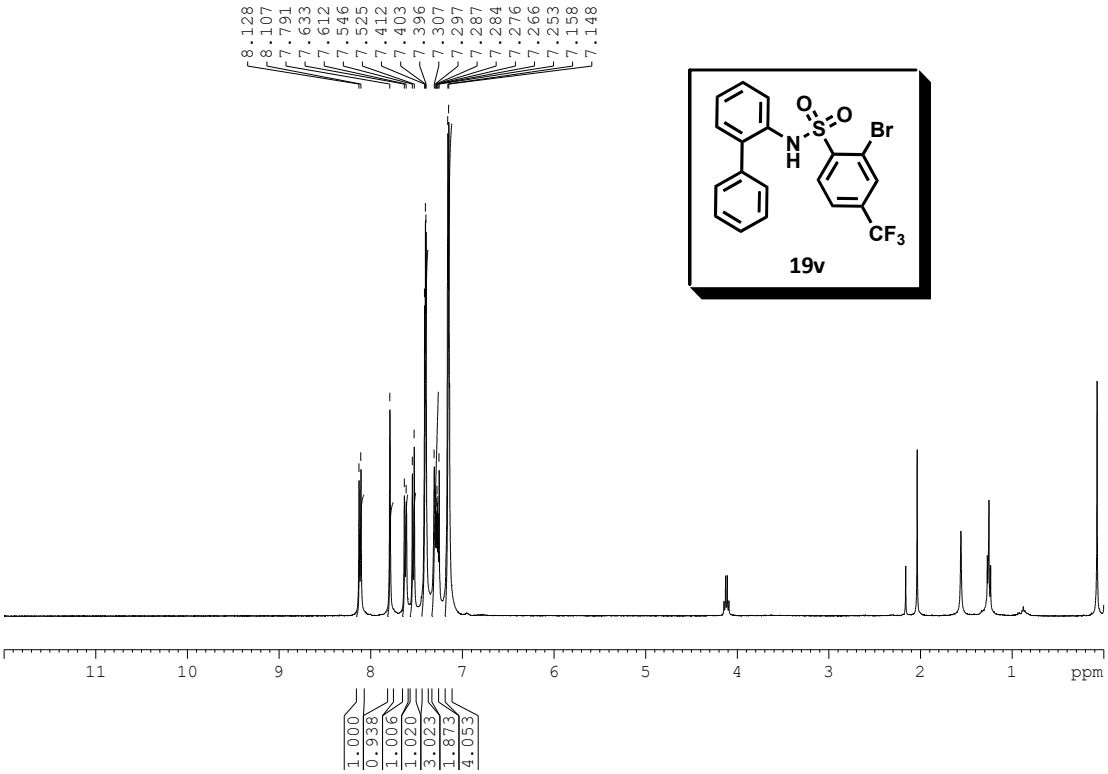
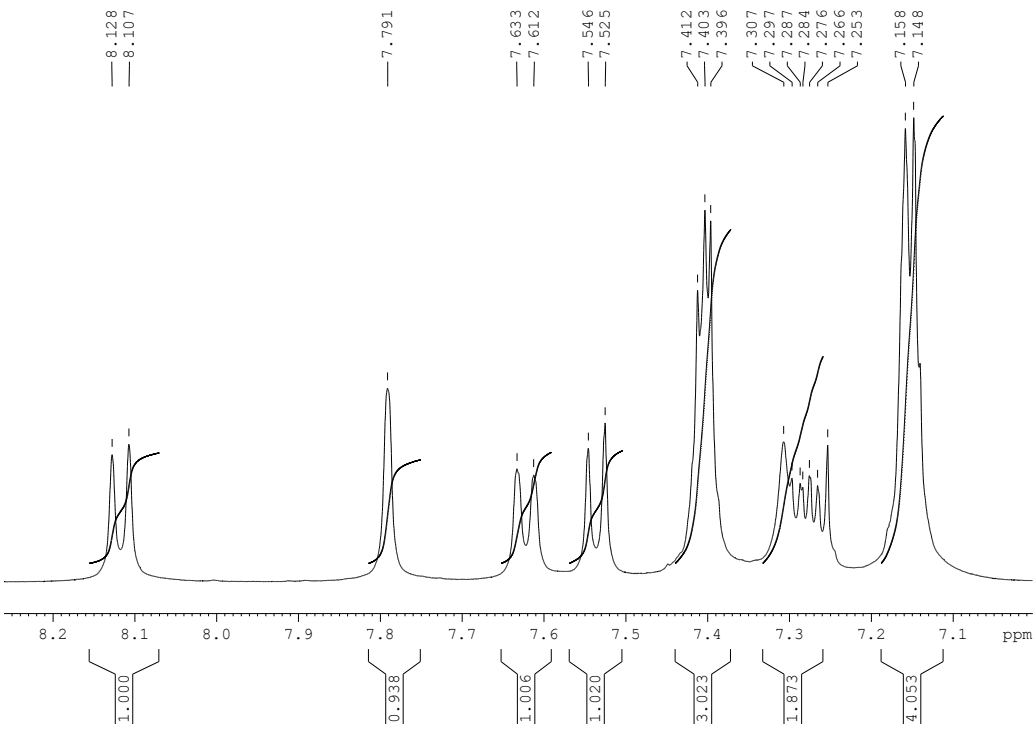
133.5
133.0
132.5
132.0
131.5
ppm

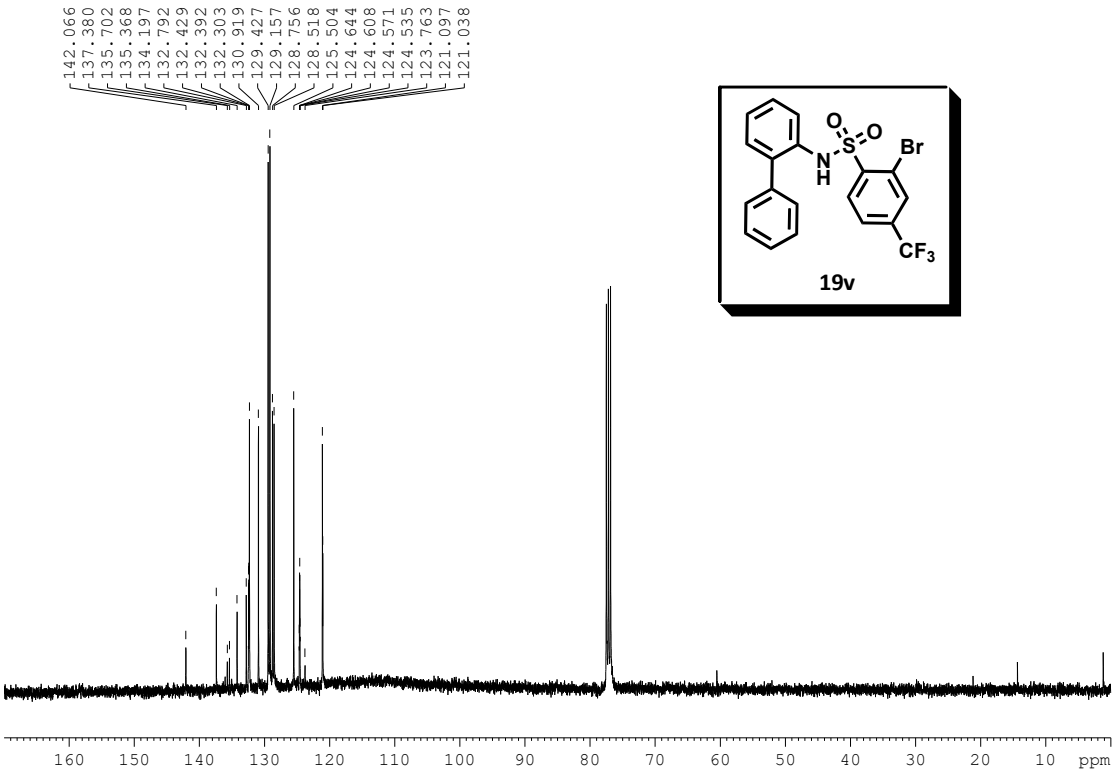


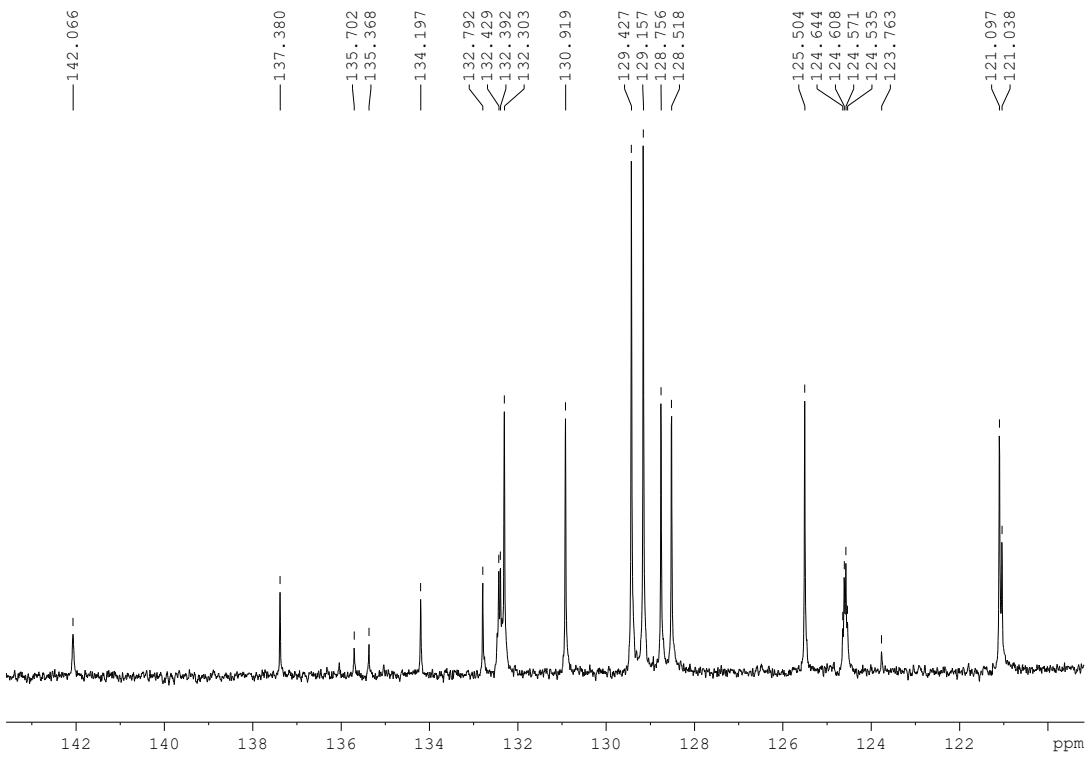
^{1}H-RMN (CD_3COCD_3) 2-Bromo- ***N*****-([1,1'-Bifenil]-2-il)-4-(trifluormetil)-bencenosulfonamida (19v)**

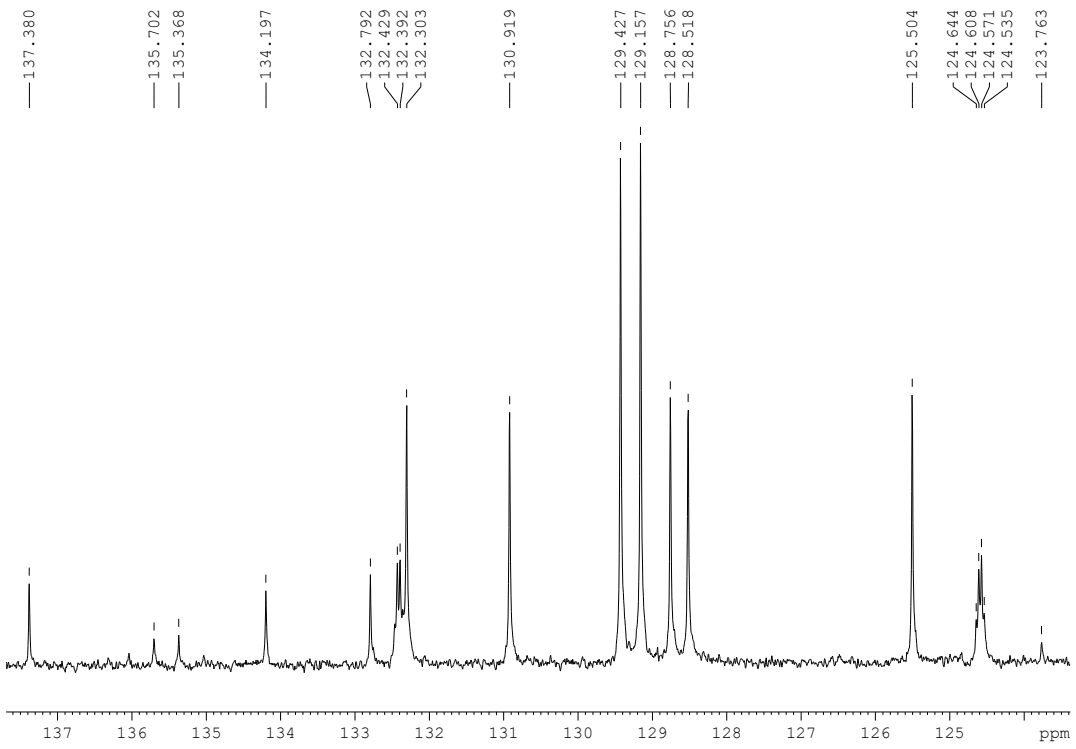




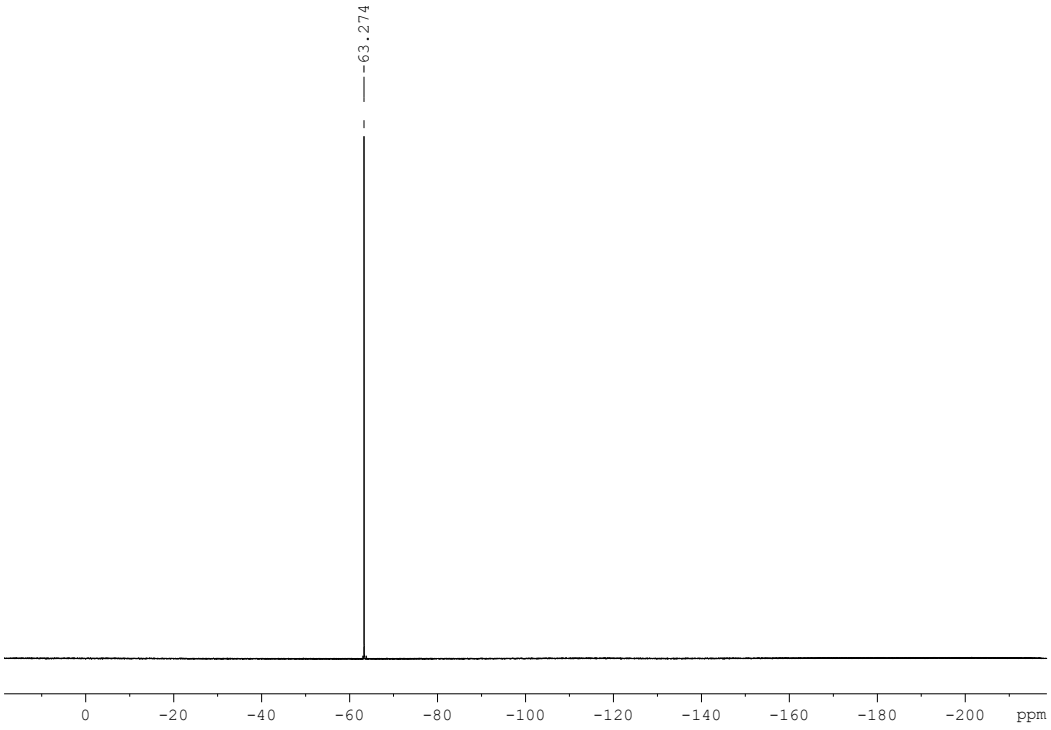
^{13}C-RMN (CD_3COCD_3) 2-Bromo- ***N*****-([1,1'-Bifenil]-2-il)-4-(trifluormetil)-bencenosulfonamida (19v)**




142.066
137.380
135.702
135.368
134.197
132.792
132.429
132.392
132.303
130.919
129.427
129.157
128.756
128.518
125.504
124.644
124.608
124.571
124.535
123.763
121.097
121.038
142
140
138
136
134
132
130
128
126
124
122
ppm

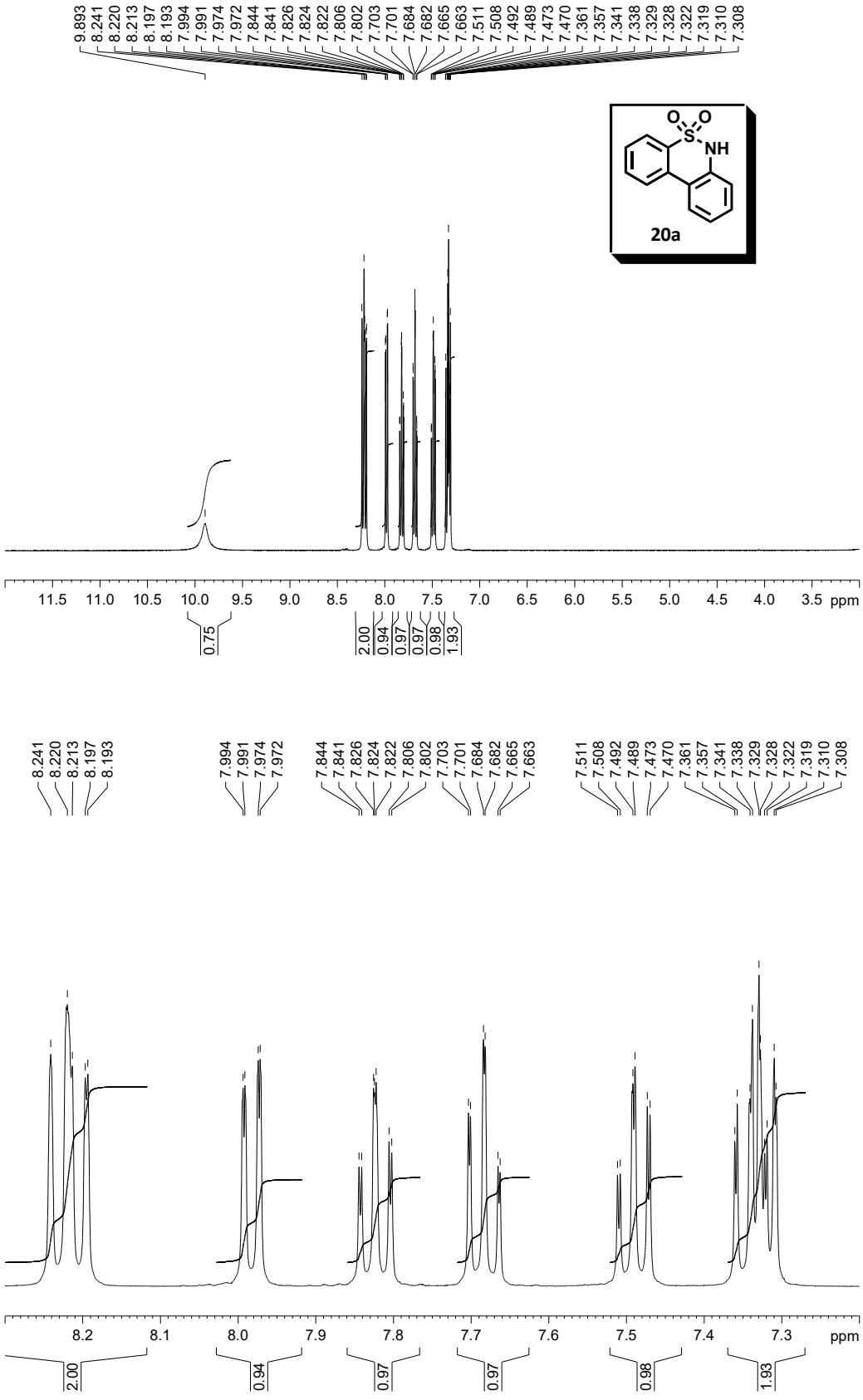

137.380
135.702
135.368
134.197
132.792
132.429
132.392
132.303
130.919
129.427
129.157
128.756
128.518
125.504
124.644
124.608
124.571
124.535
123.763
137
136
135
134
133
132
131
130
129
128
127
126
125
ppm

^{19}F-RMN (CD_3COCD_3) 2-Bromo- ***N*****-([1,1'-Bifenil]-2-il)-4-(trifluormetil)-bencenosulfonamida (19v)**

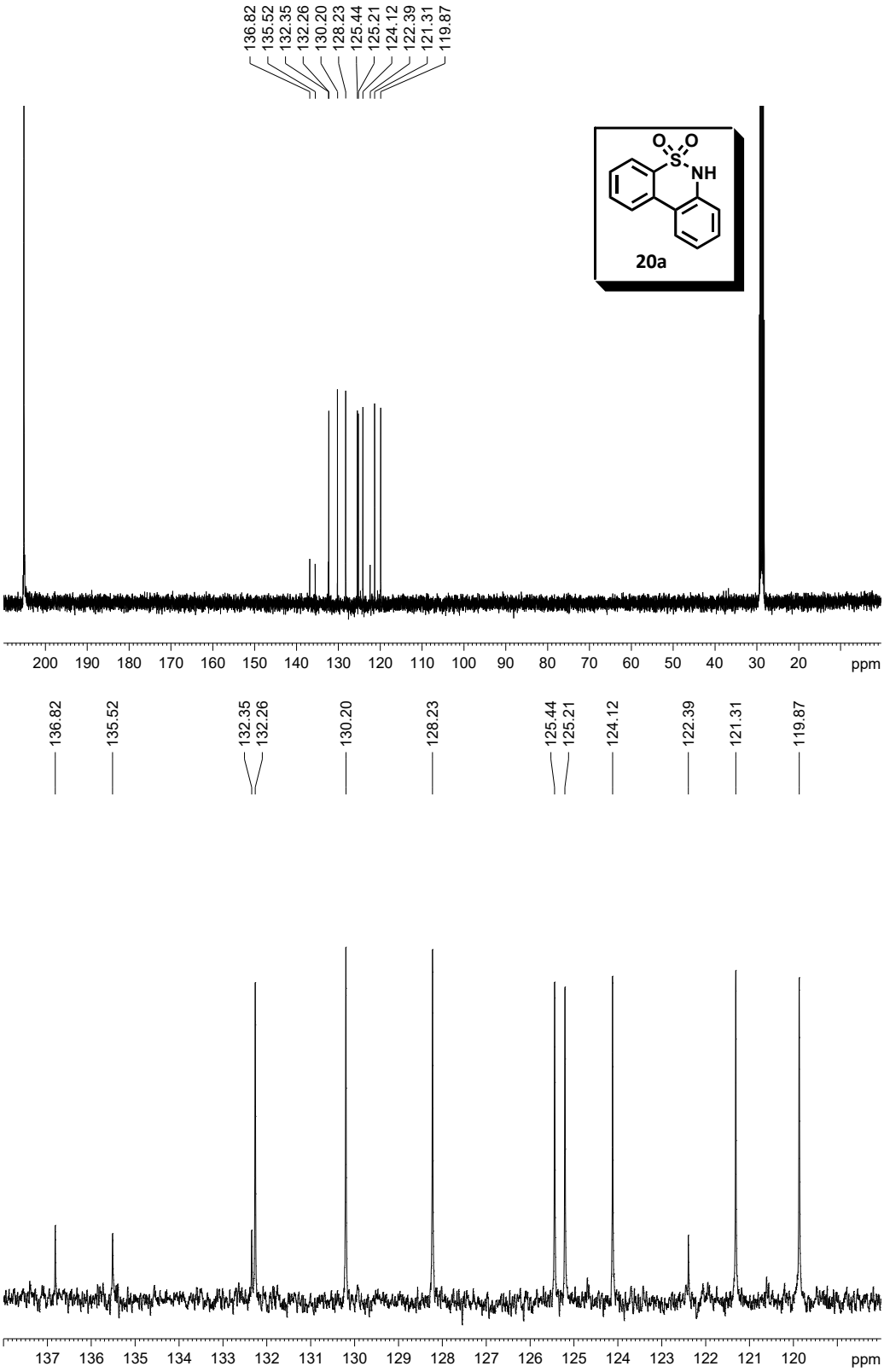


A.4.2 ESPECTROS DE RMN DE DIBENZOTIACINAS OBTENIDAS

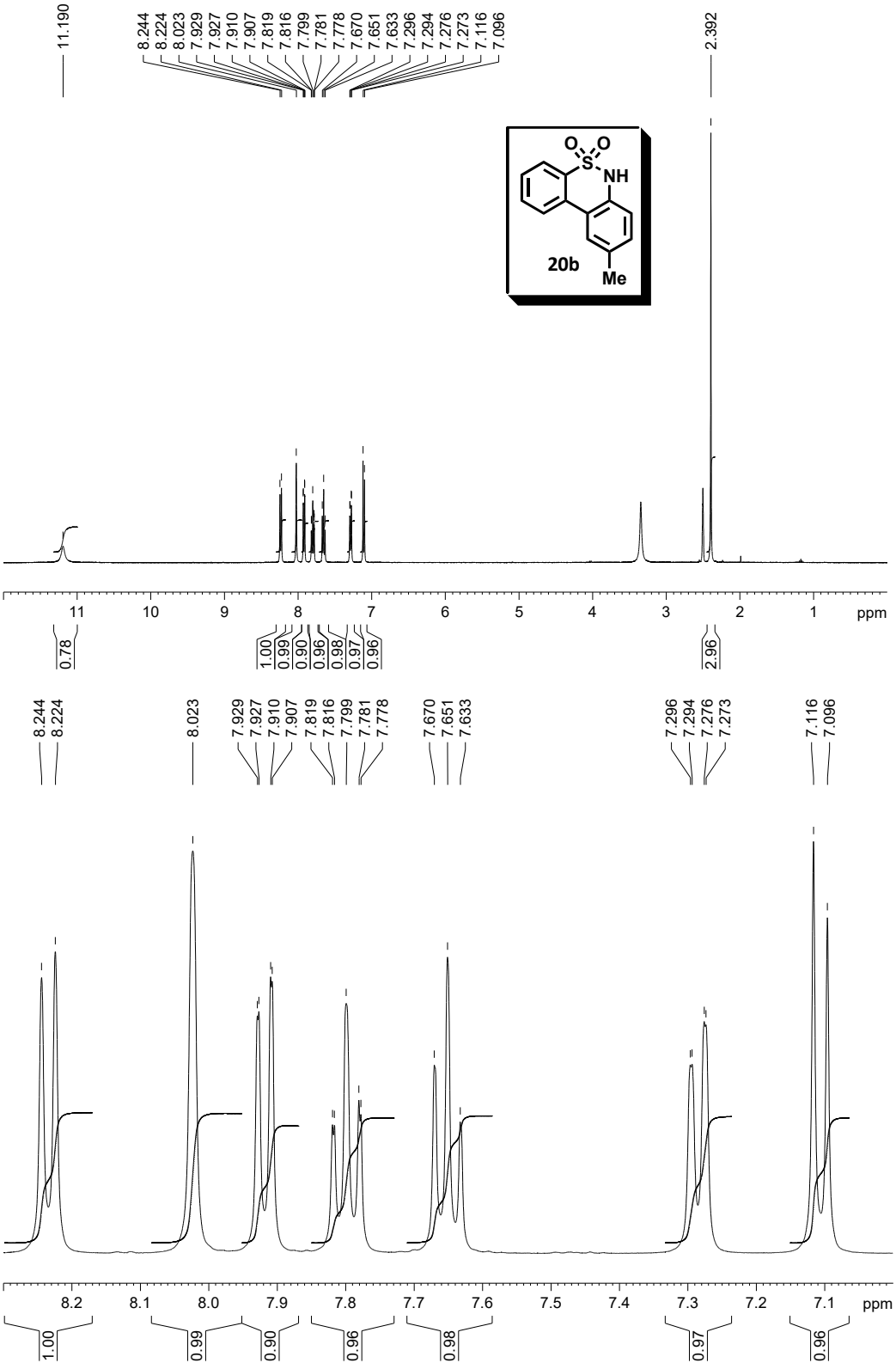
^{1}H-RMN (CD_3COCD_3) 6*H*-Dibenzo[*c*,*e*][1,2]tiacina 5;5-dioxido (20a)



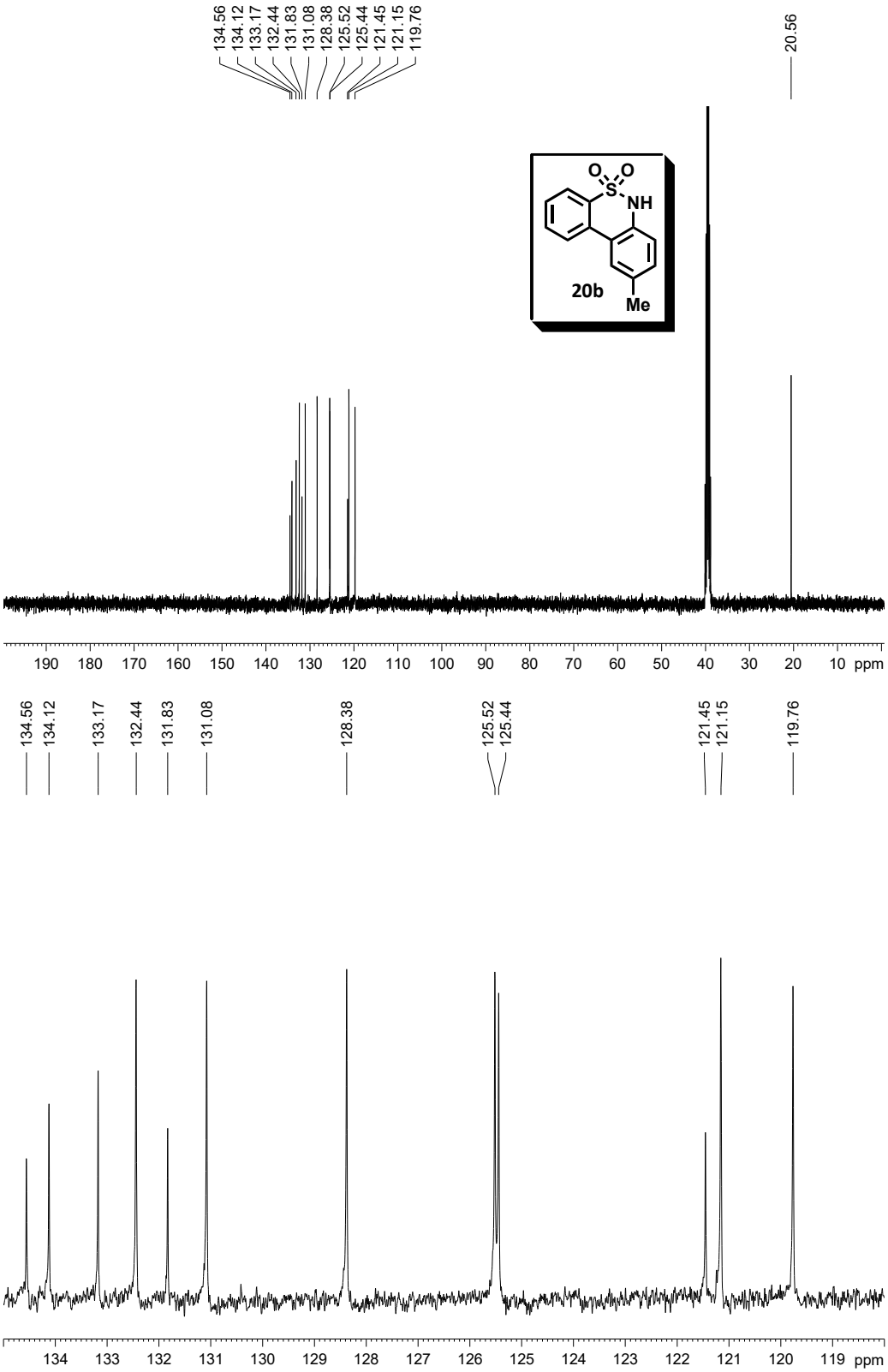
^{13}C-RMN (CD_3COCD_3) 6*H*-Dibenzo[*c*,*e*][1,2]tiacina 5;5-dioxido (20a)



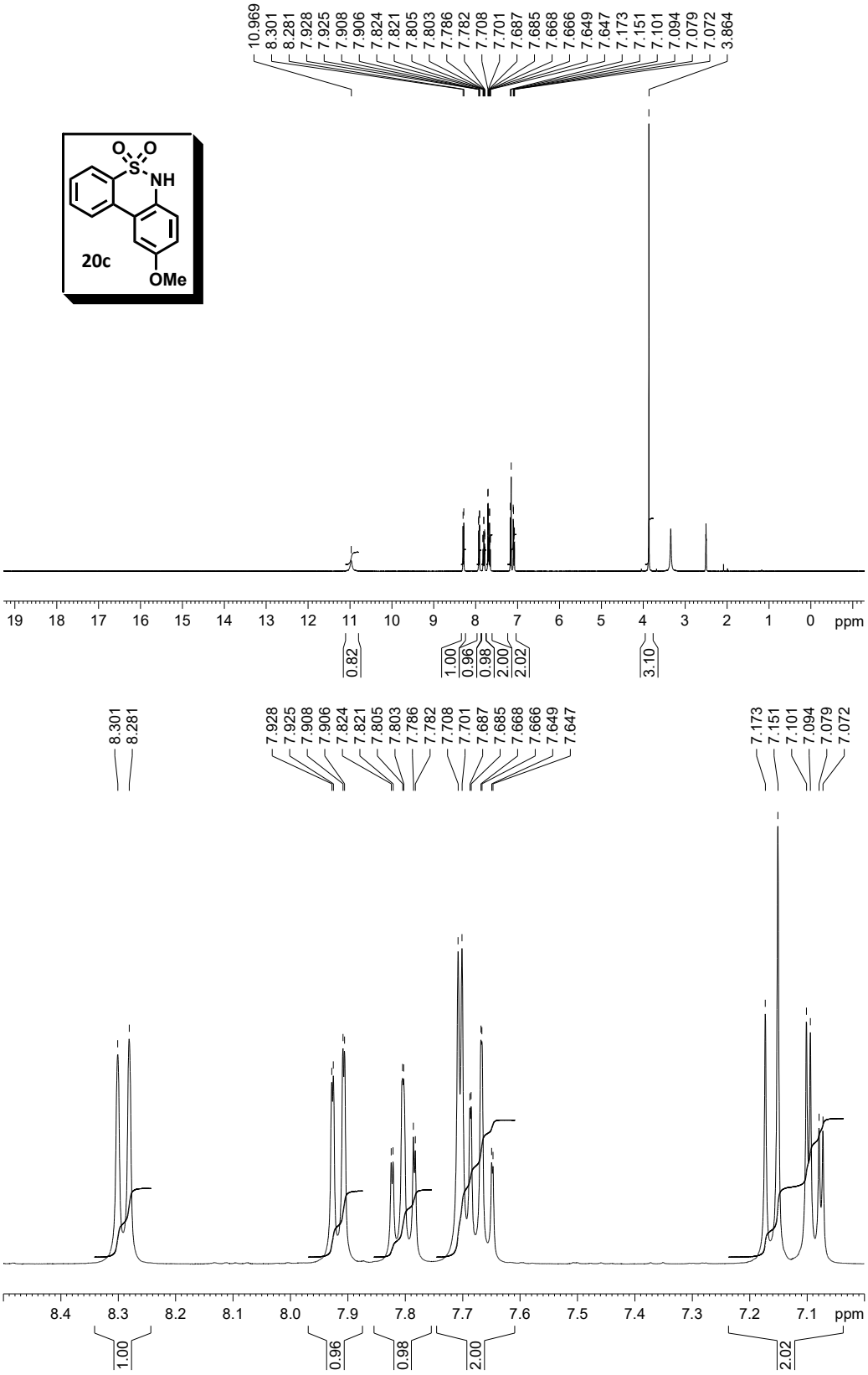
^{1}H-RMN (CD_3SOCD_3) 9-Metil-6*H*-Dibenzo[*c*,*e*][1,2]tiacina 5;5-dioxido (20b)



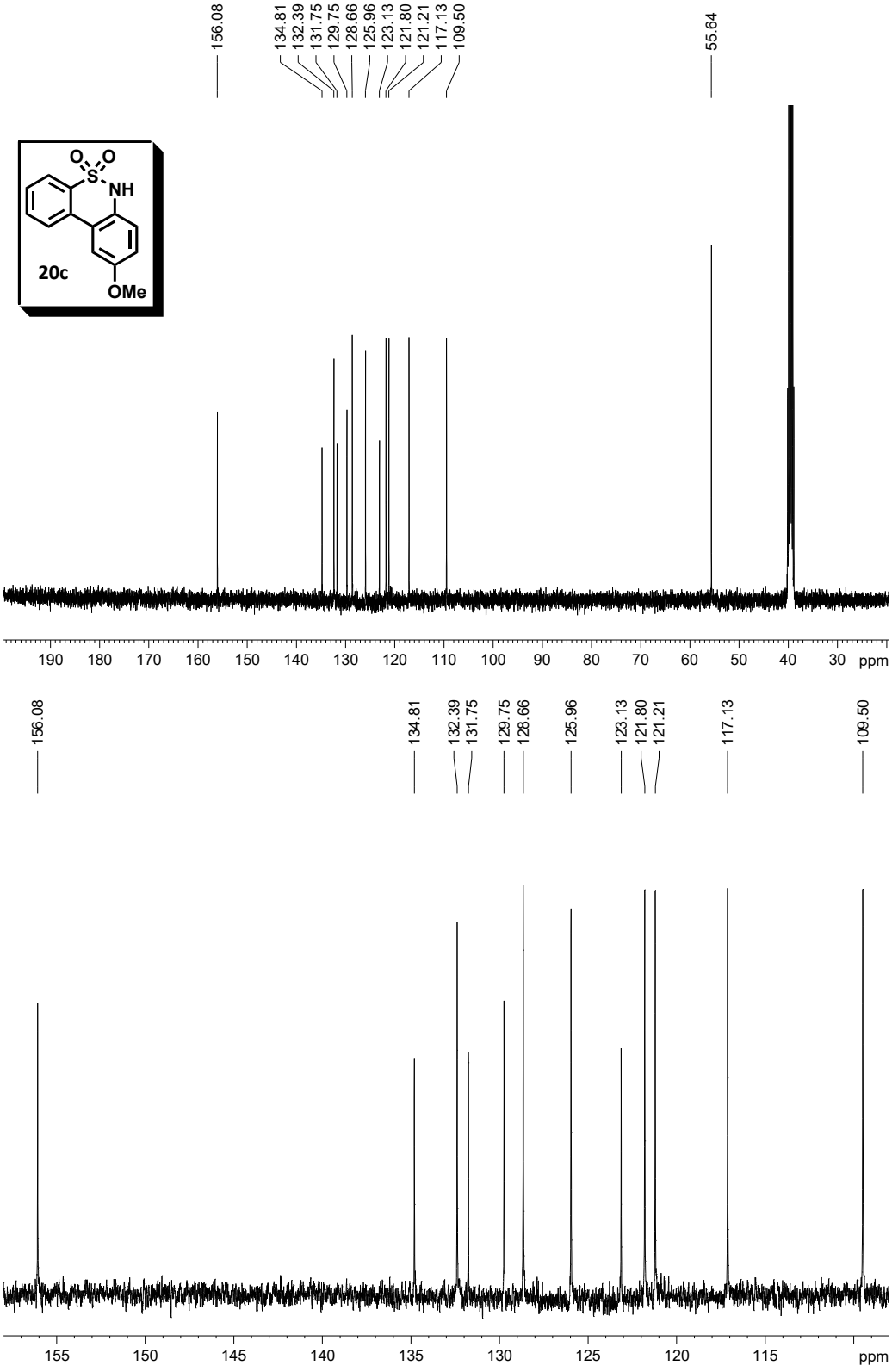
^{13}C-RMN (CD_3SOCD_3) 9-Metil-6*H*-Dibenzo[*c*,*e*][1,2]tiacina 5;5-dioxido (20b)



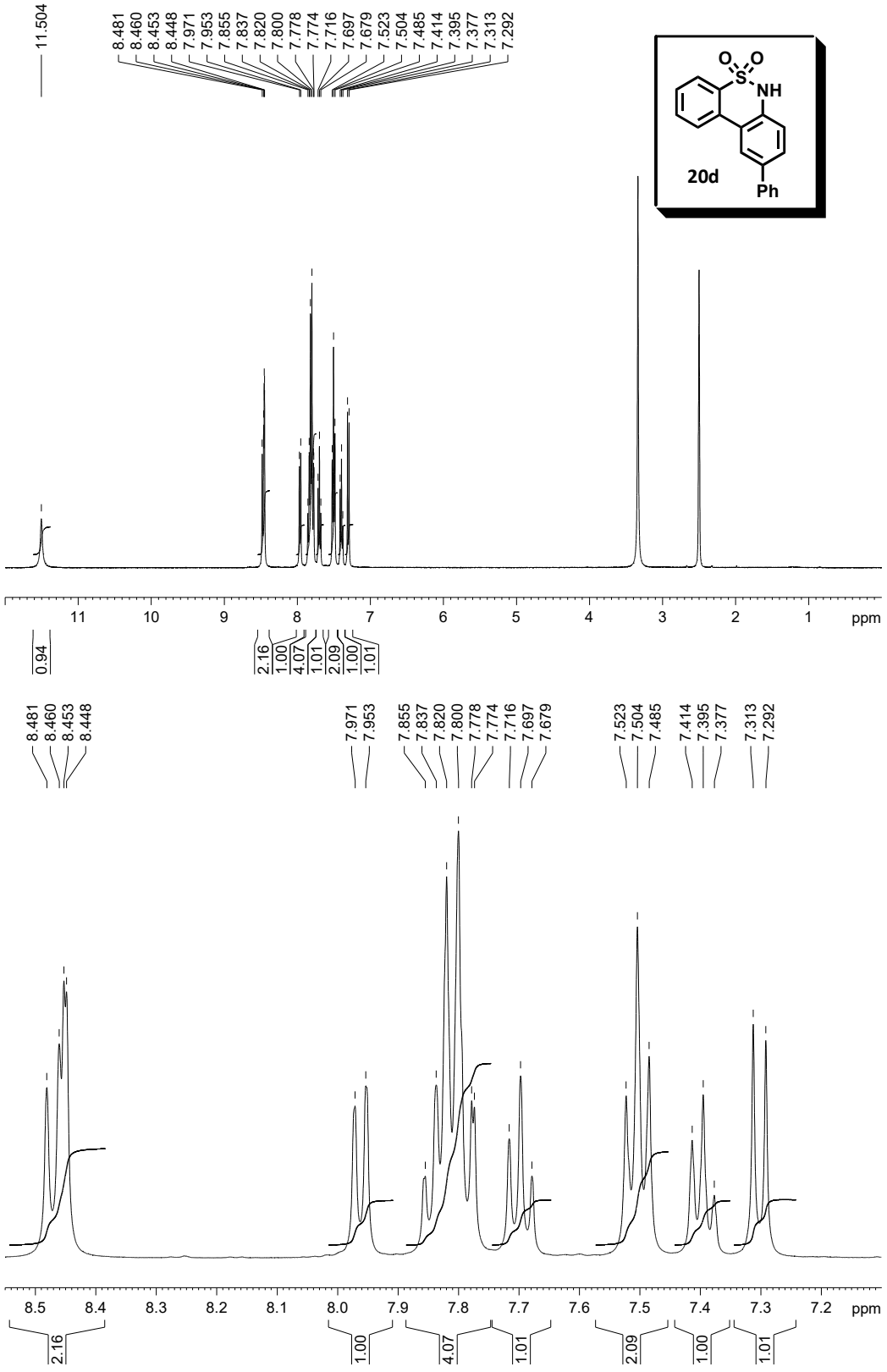
^{1}H-RMN (CD_3SOCD_3) 9-Metoxi-6*H*-Dibenzo[*c*,*e*][1,2]tiacina 5;5-dioxido (20c)



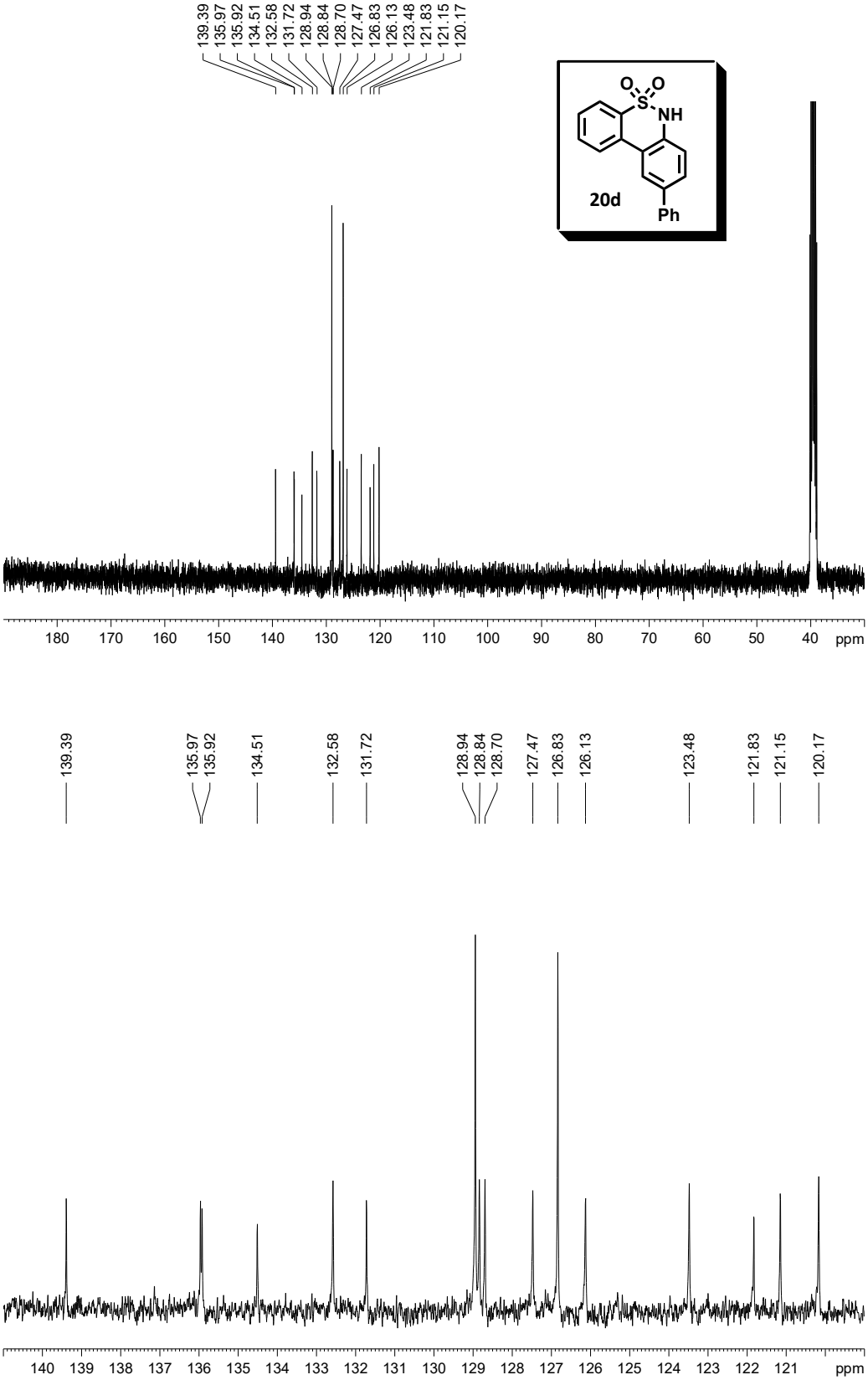
^{13}C-RMN (CD_3SOCD_3) 9-Metoxi-6*H*-Dibenzo[*c*,*e*][1,2]tiacina 5;5-dioxido (20c)



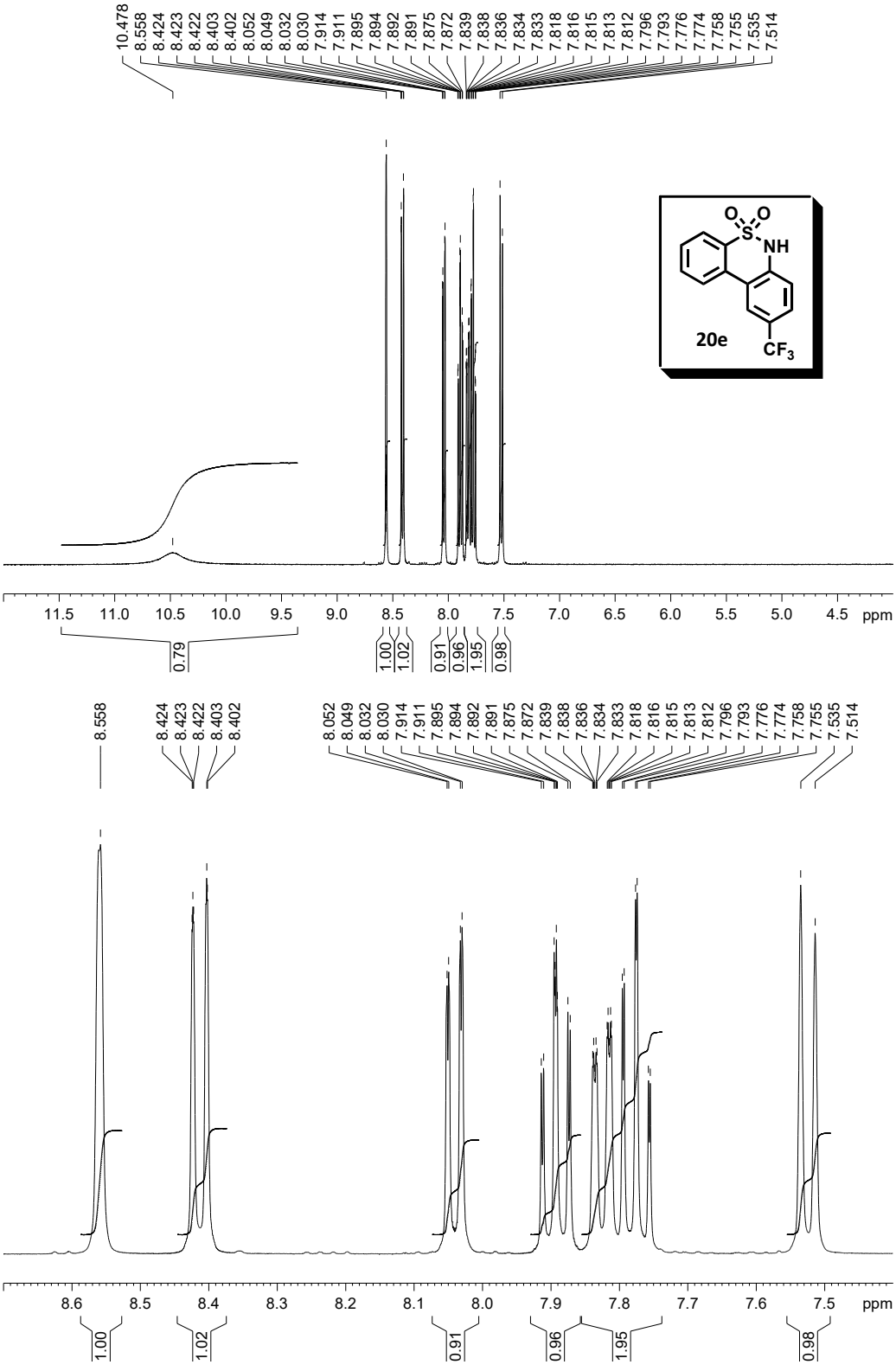
^{1}H-RMN (CD_3SOCD_3) 9-Fenil-6*H*-Dibenzo[*c*,*e*][1,2]tiacina 5;5-dioxido (20d)

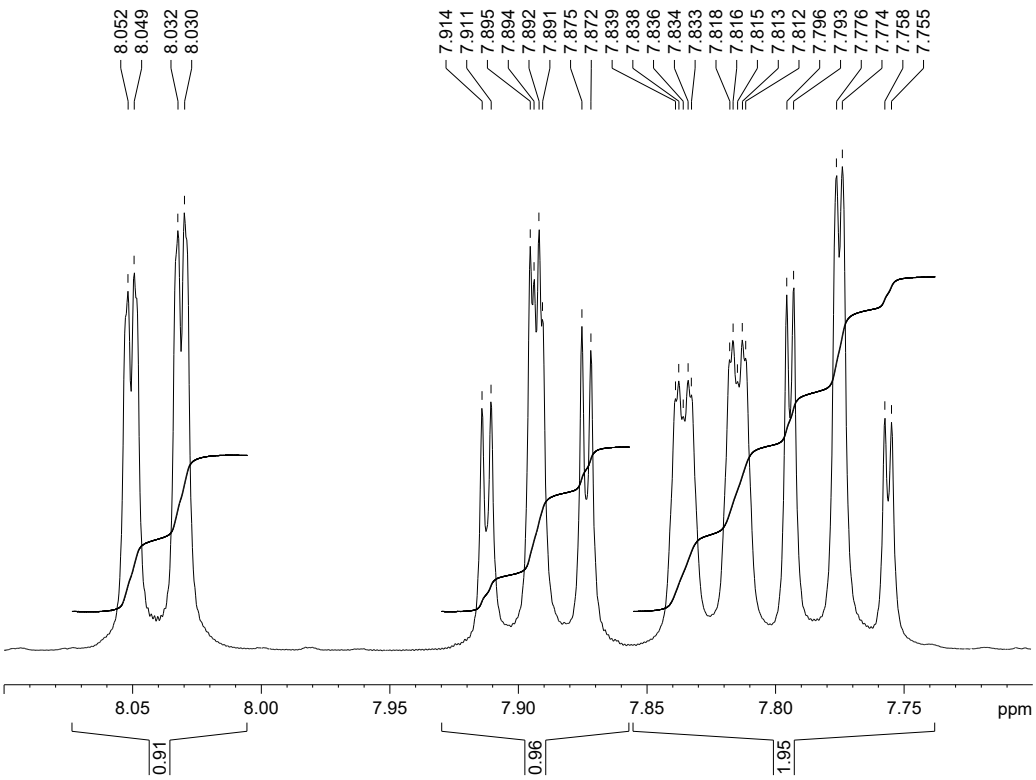


^{13}C-RMN (CD_3SOCD_3) 9-Fenil-6*H*-Dibenzo[*c*,*e*][1,2]tiacina 5;5-dioxido (20d)

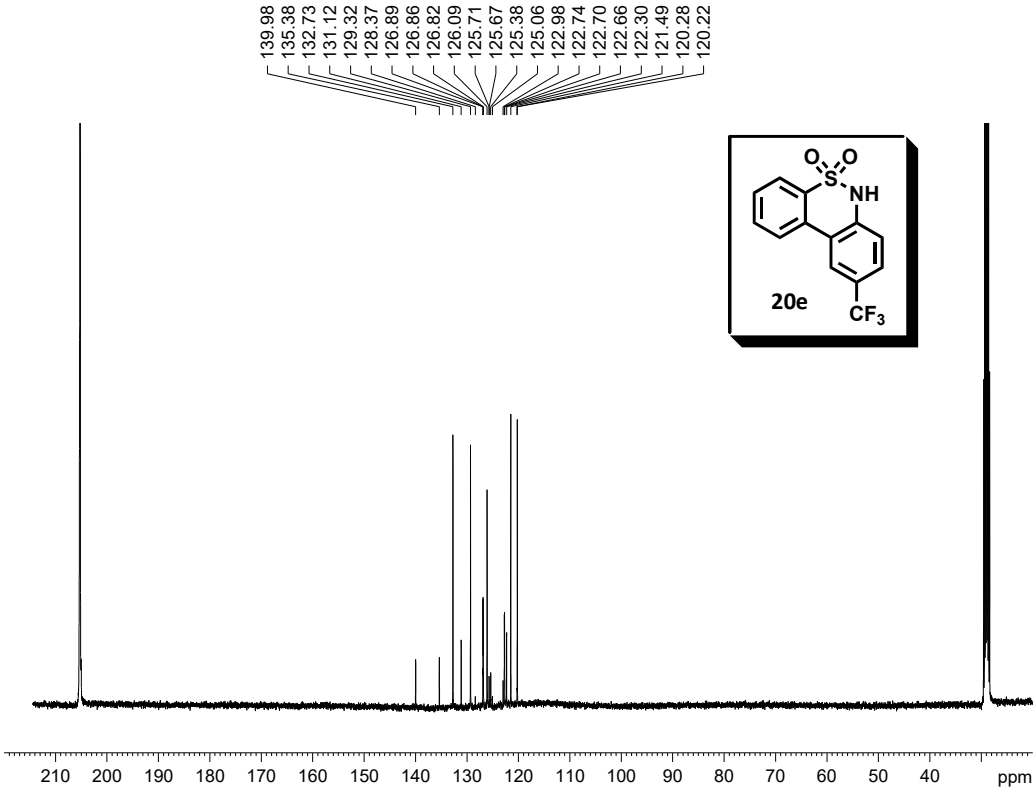


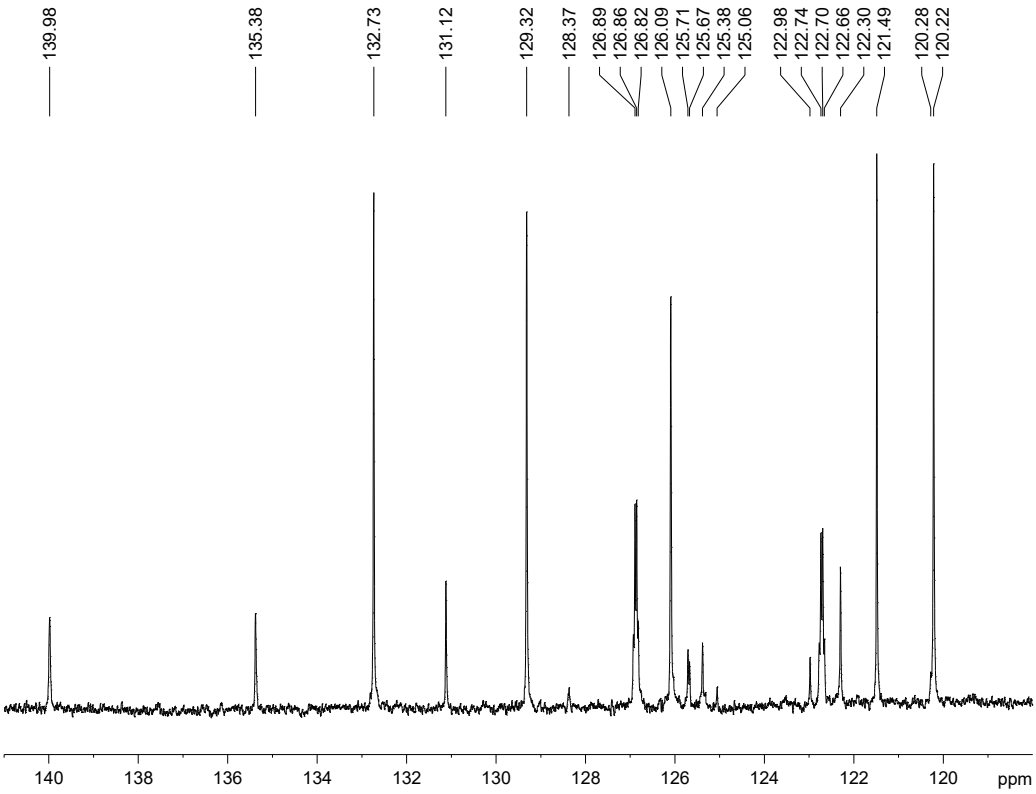
^{1}H-RMN (CD_3COCD_3) 9-Trifluormetil-6*H*-Dibenzo[*c*,*e*][1,2]tiacina 5;5-dioxido (20e)



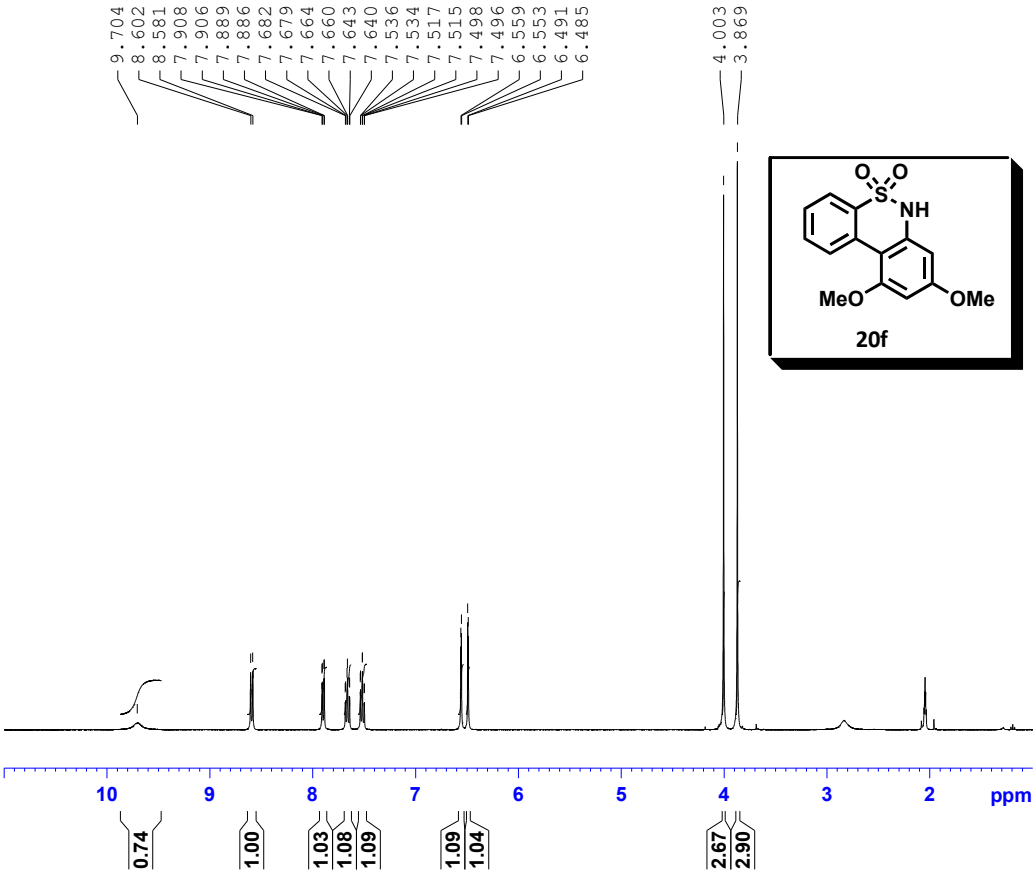


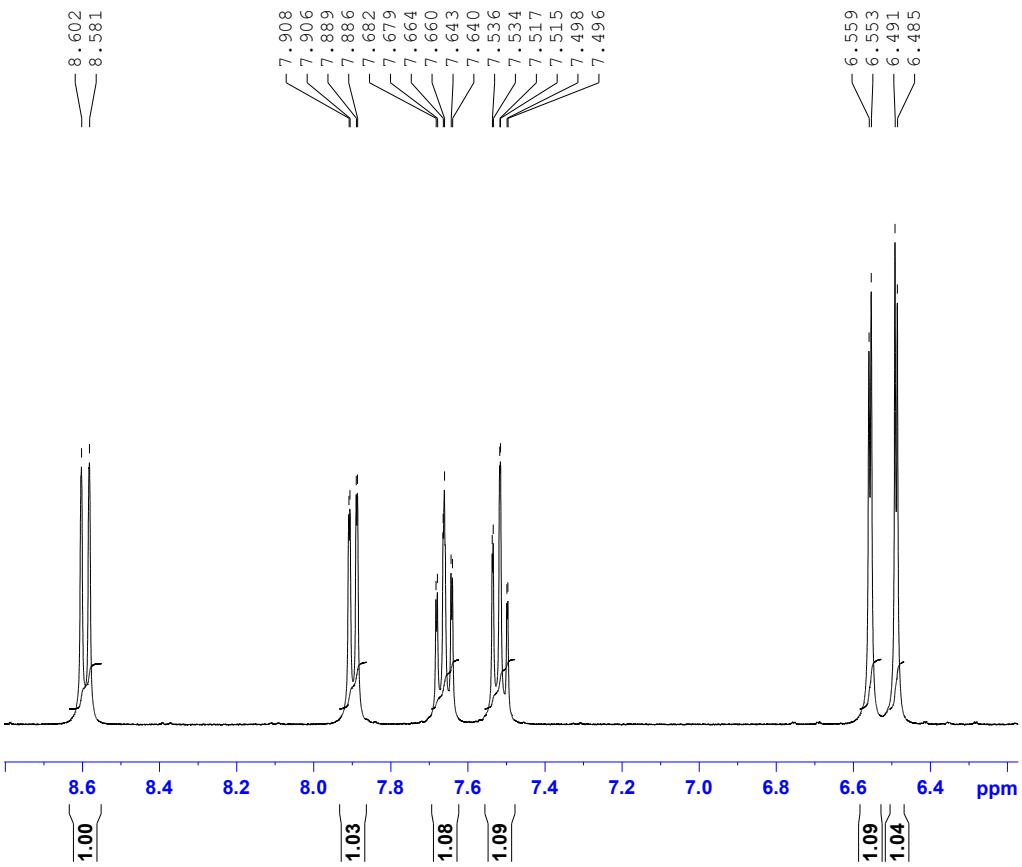
^{13}C-RMN (CD_3COCD_3) 9-Trifluormetil-6*H*-Dibenzo[*c*,*e*][1,2]tiacina 5;5-dioxido (20e)



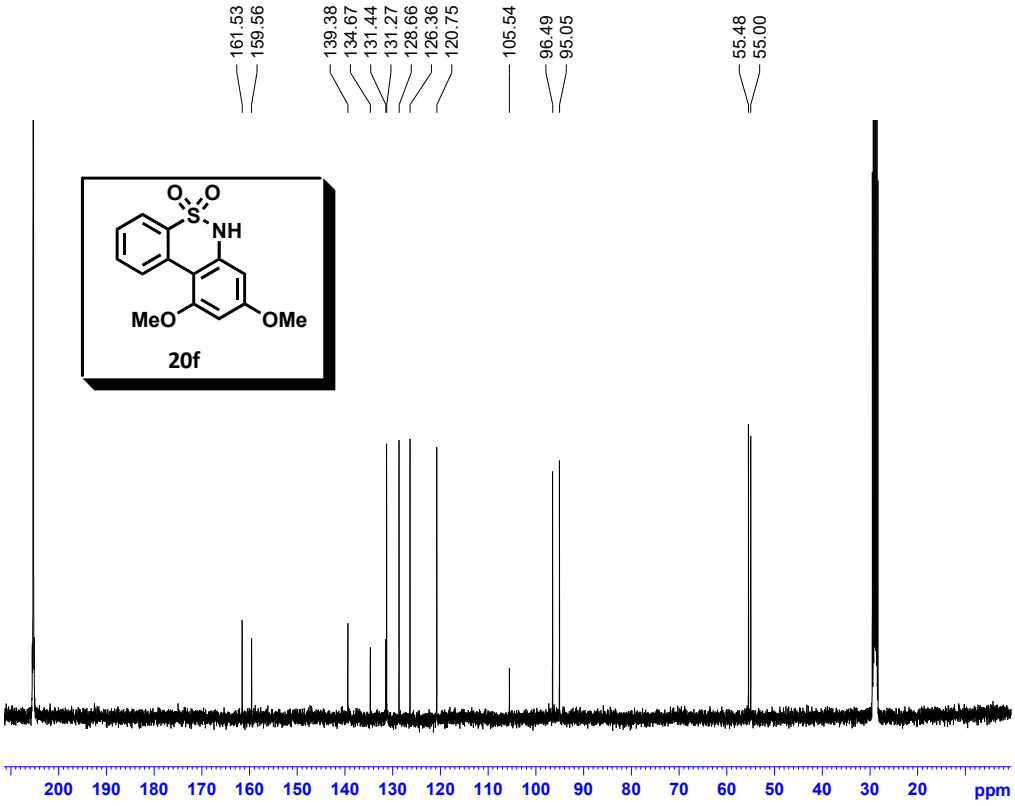


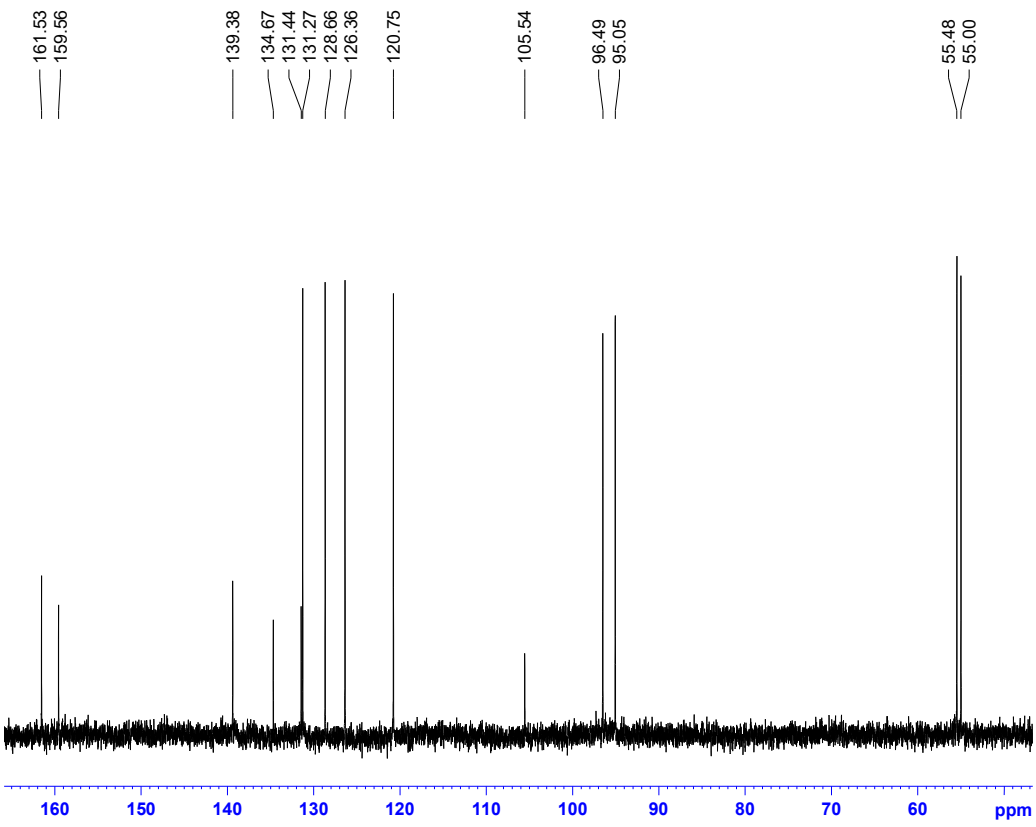
^{1}H-RMN (CD_3COCD_3) 8,10-*Di*-metoxi-6*H*-Dibenzo[*c*,*e*][1,2]tiacina 5;5-dioxido (20f)



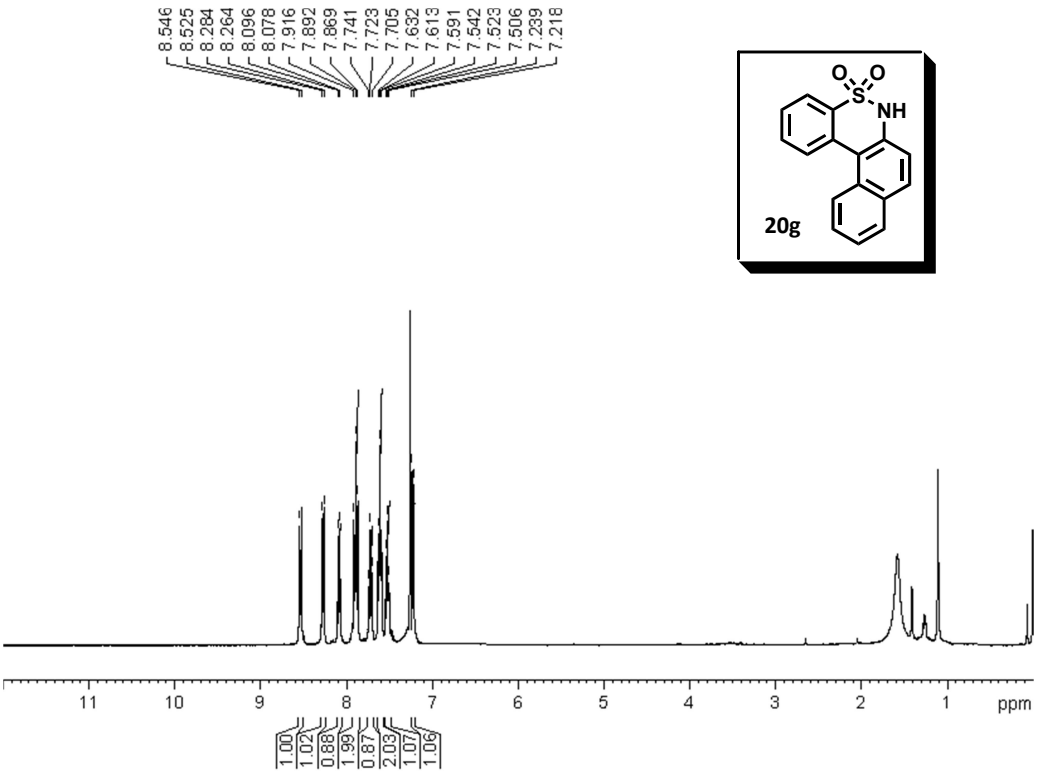


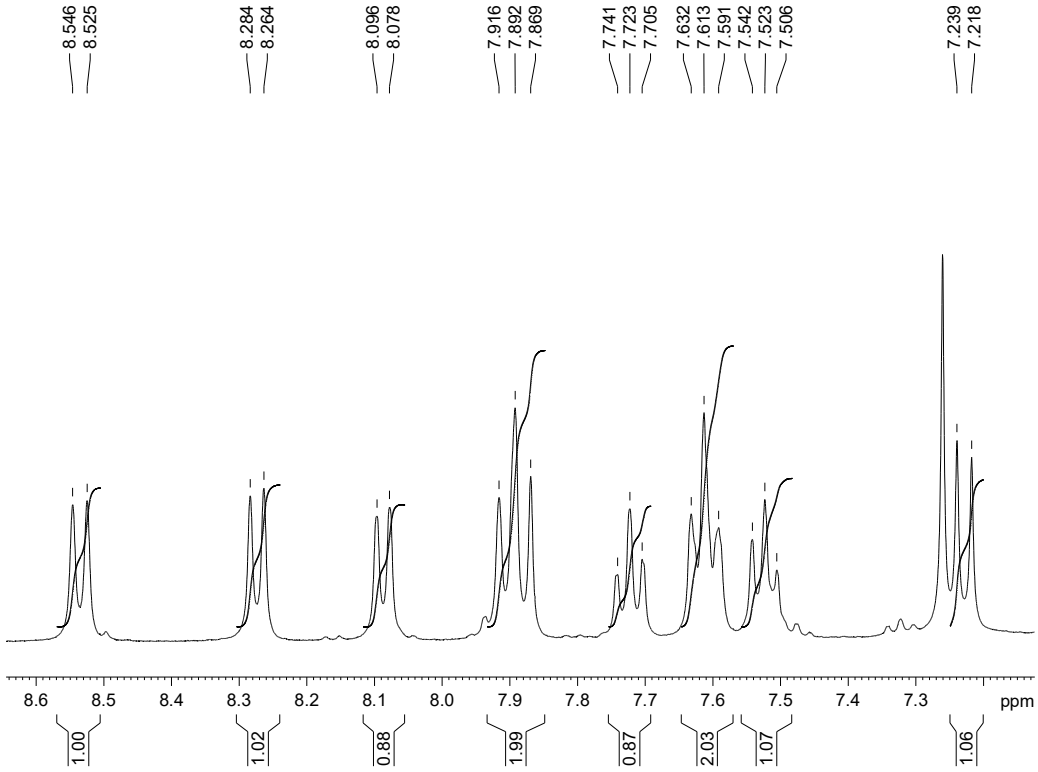
^{13}C-RMN (CD_3COCD_3) 8,10-*Di*-metoxi-6*H*-Dibenzo[*c*,*e*][1,2]tiacina 5;5-dioxido (20f)



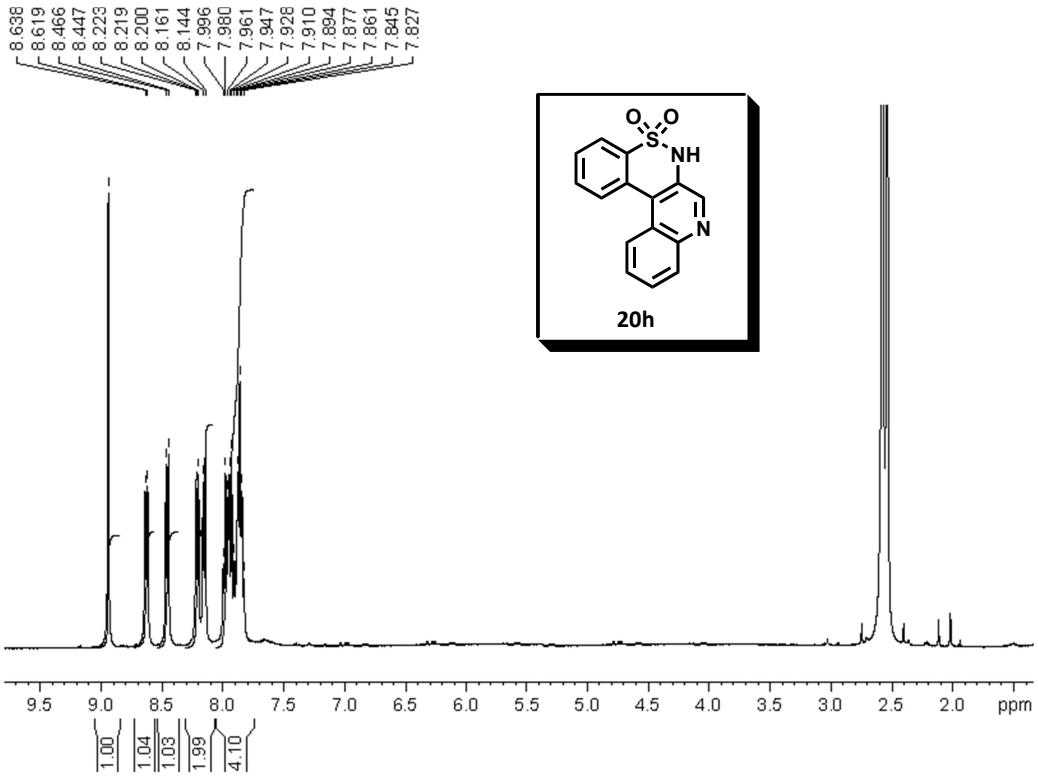


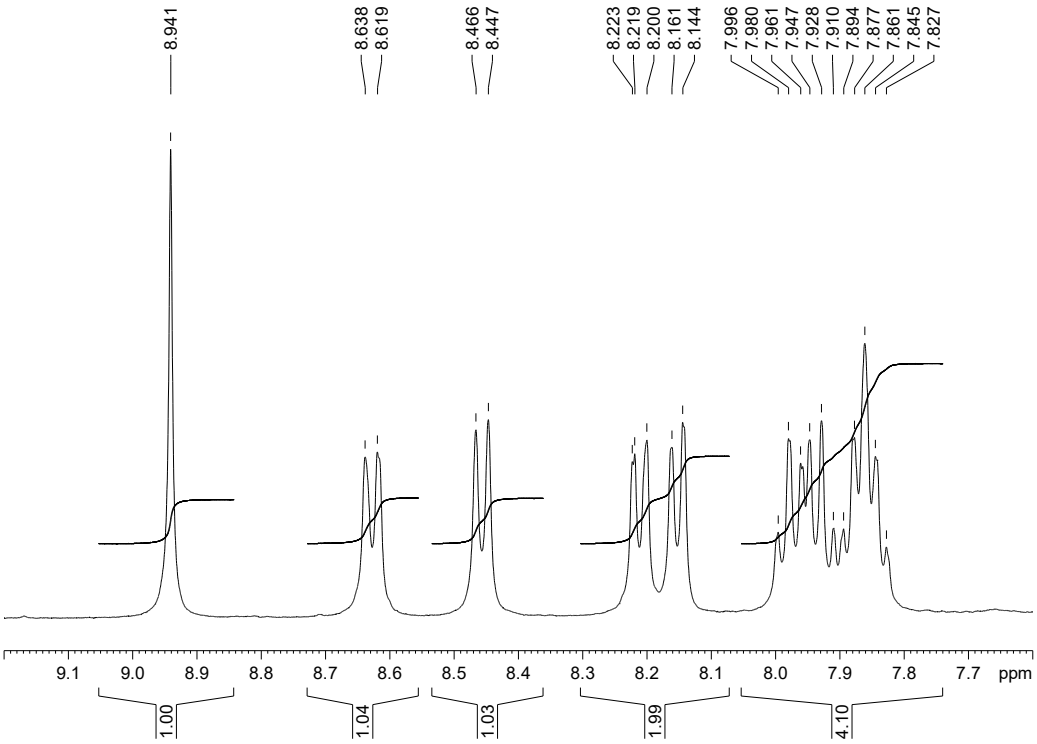
^{1}H-RMN ($CDCl_3$) 6*H*-Benzo[*e*]nafto[2,1-*c*][1,2]tiacina 5;5-dioxido (20g)



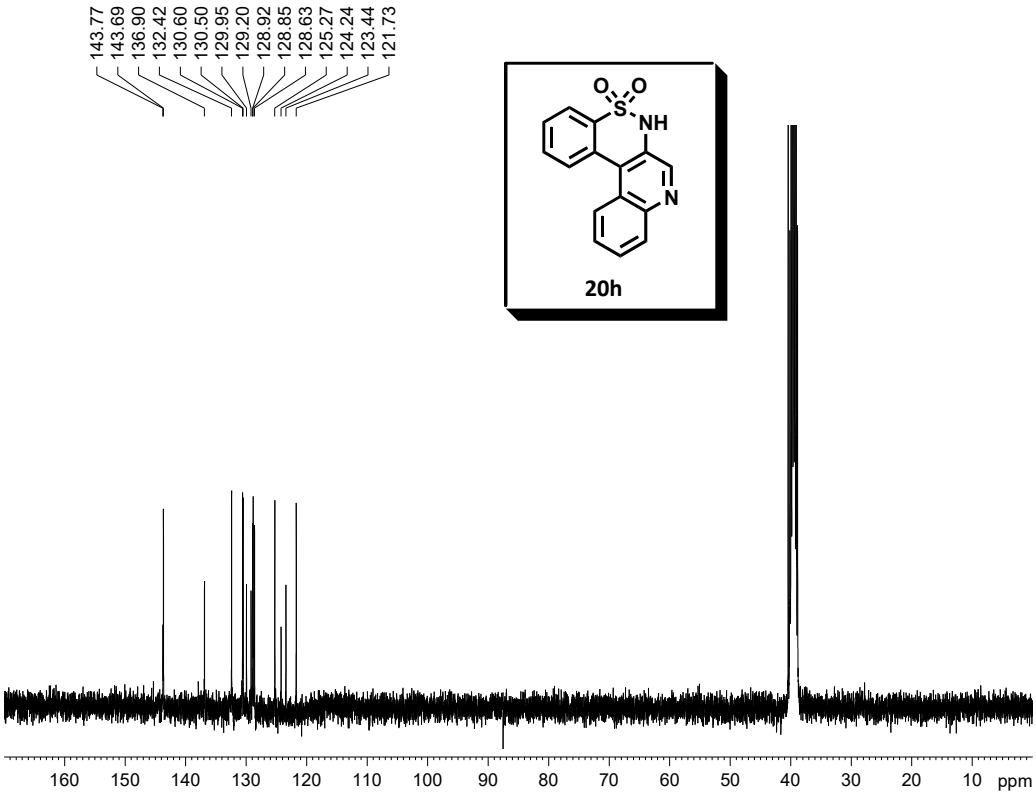


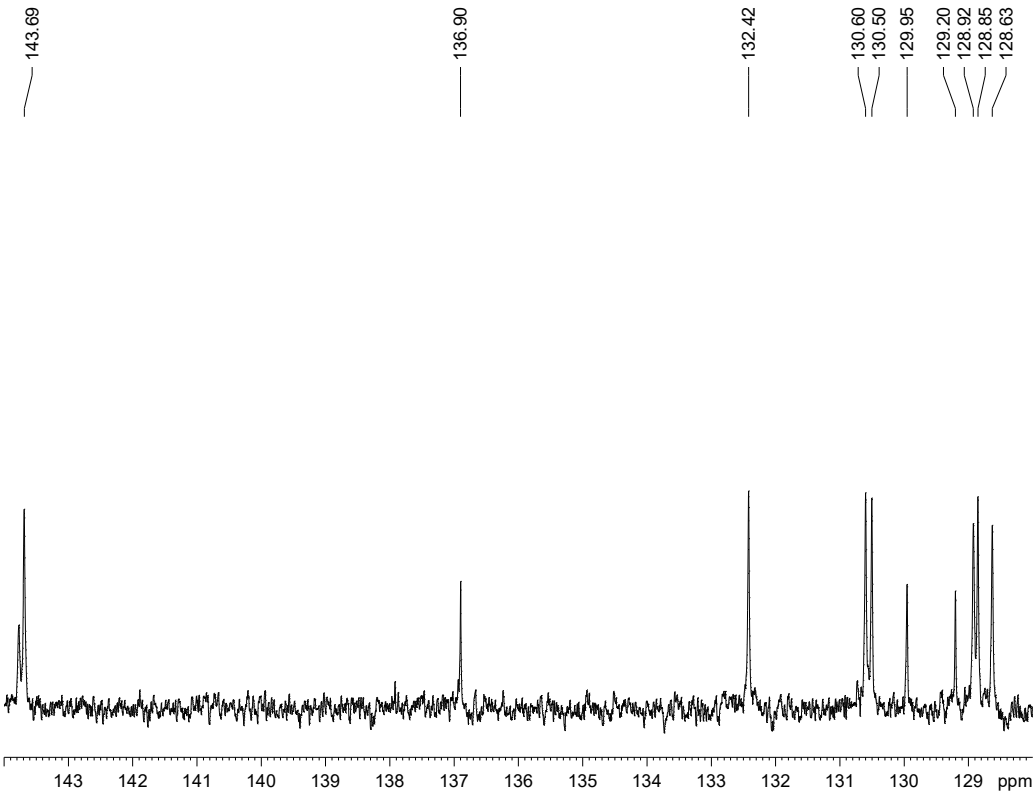
^{1}H-RMN (CD_3SOCD_3) 6*H*-Benzo[5,6][1,2]tiacino[3,4-*c*]quinolina *5,*5-dioxido (20h)



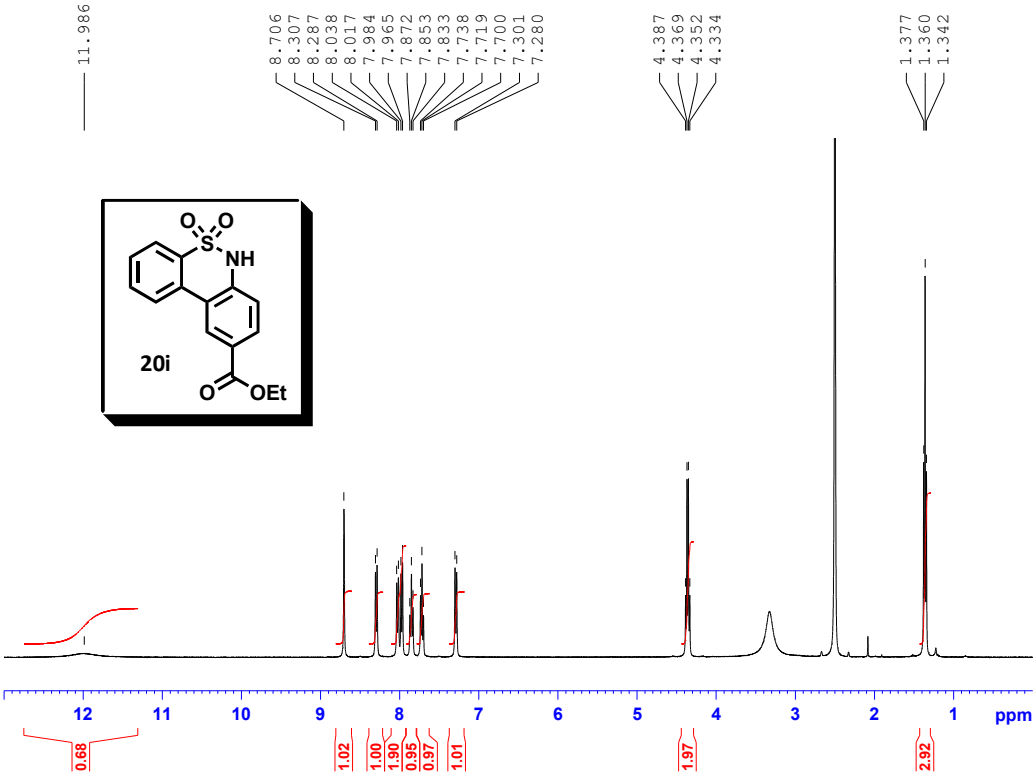


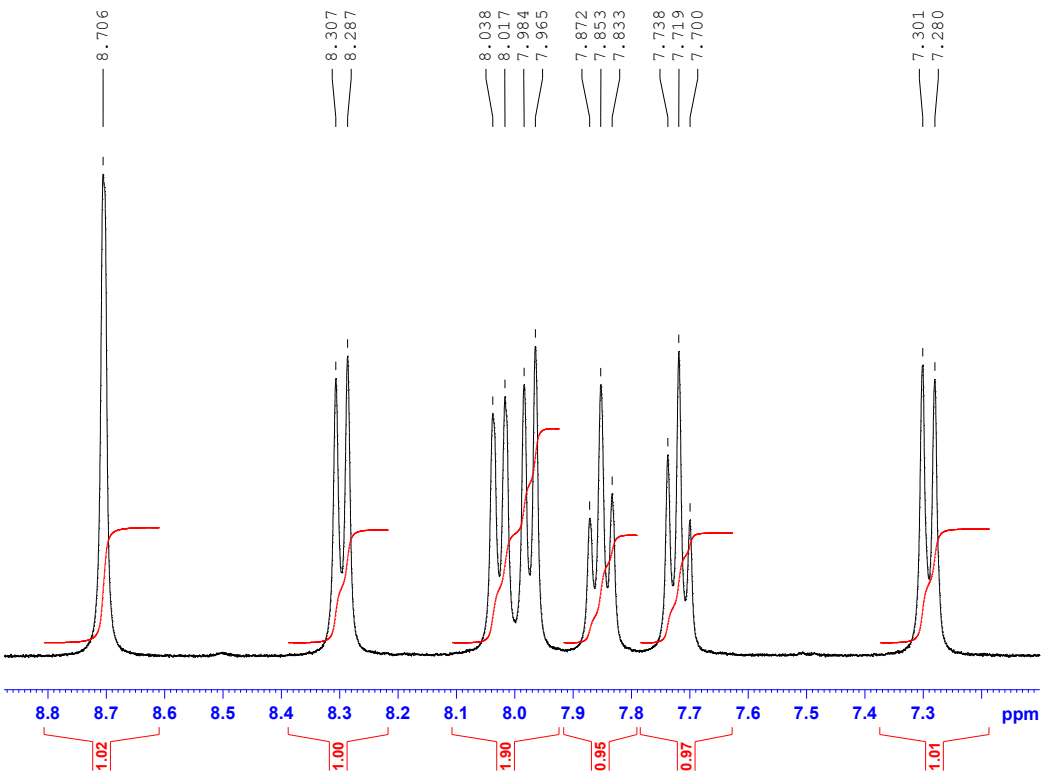
^{13}C-RMN (CD_3SOCD_3) 6*H*-Benzo[5,6][1,2]tiacino[3,4-*c*]quinolina *5,*5-dioxido (20h)



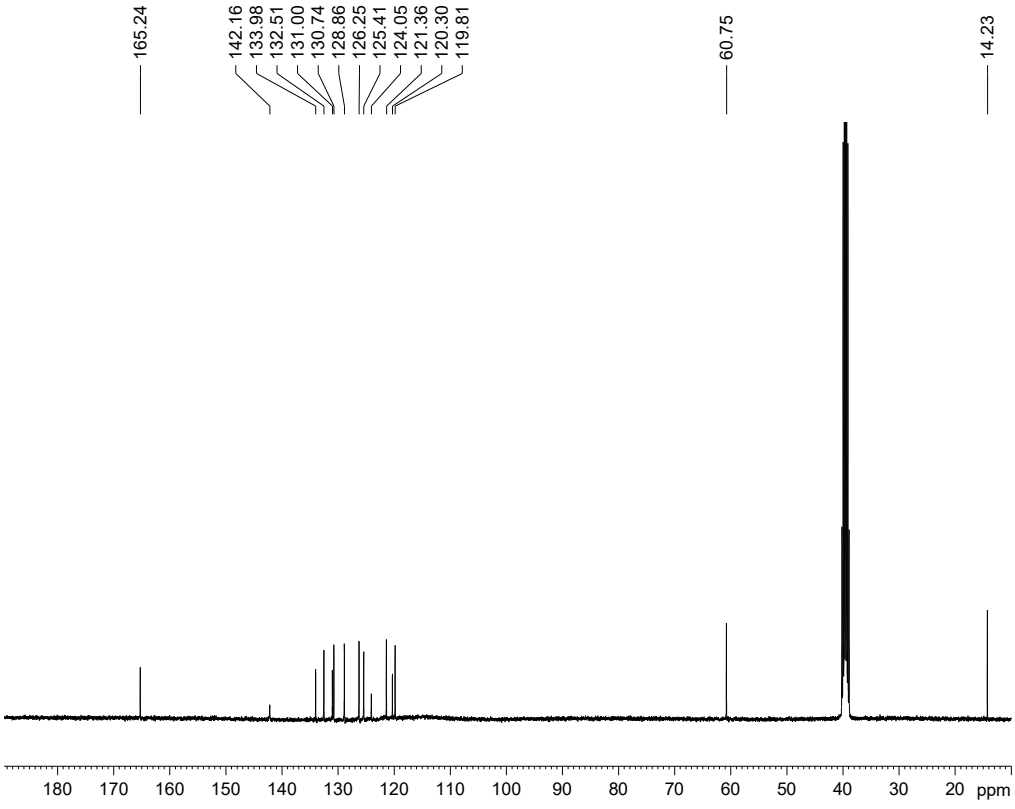


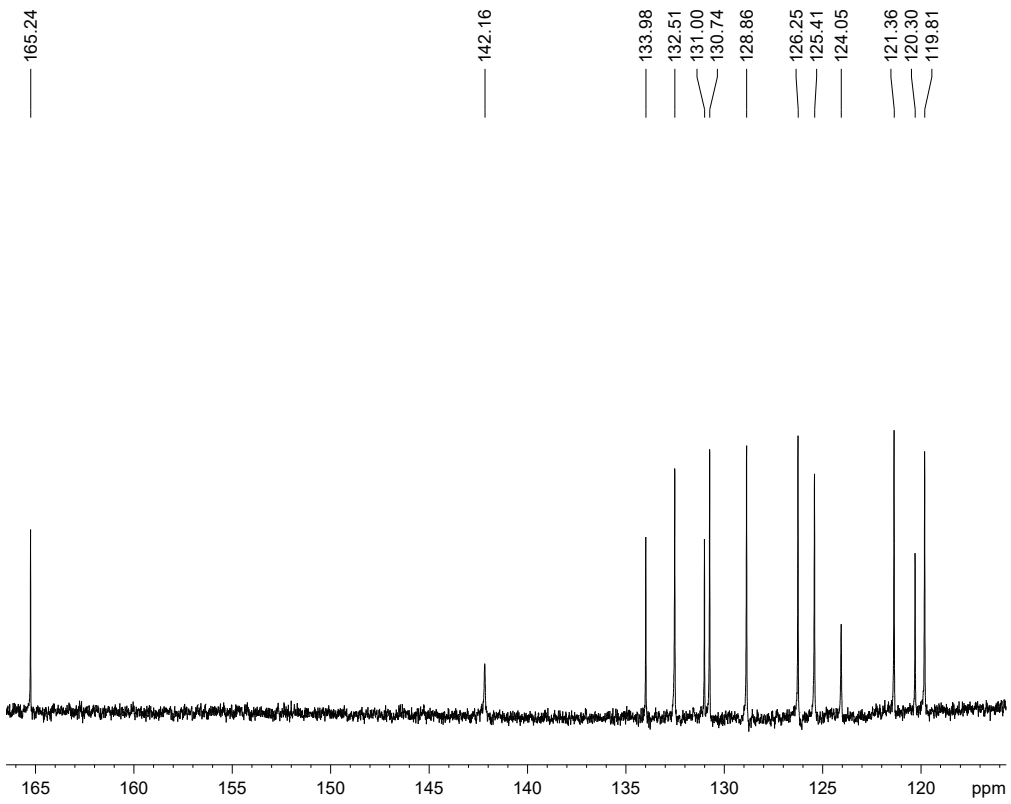
^{1}H-RMN (CD_3SOCD_3) 9-Carboxilato de etilo -6*H*-Dibenzo[*c*,*e*][1,2]tiacina 5;5-dioxido (20i)



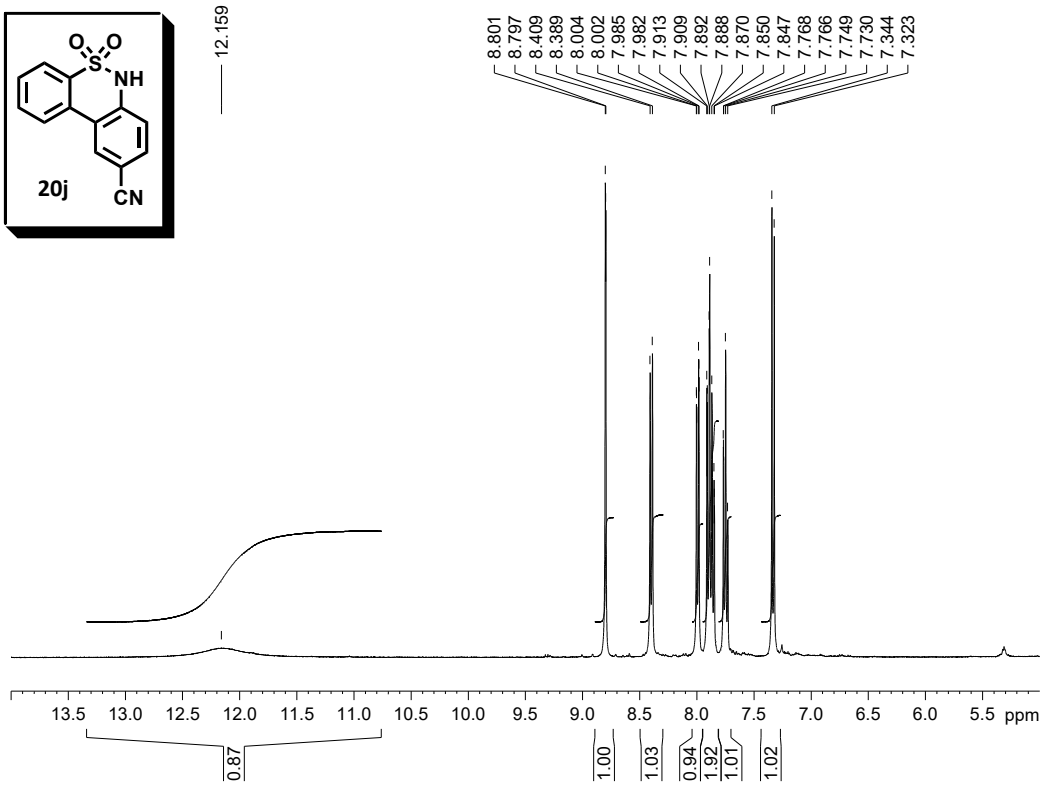


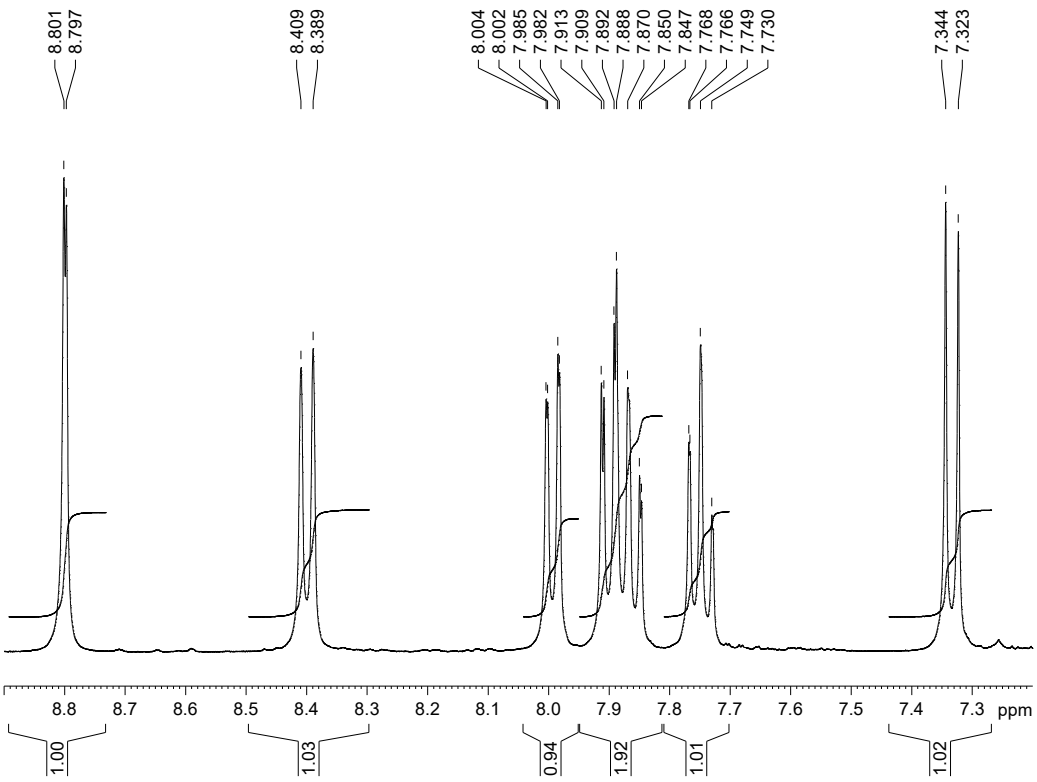
^{13}C-RMN (CD_3SOCD_3) 9-Carboxilato de etilo -6*H*-Dibenzo[*c*,*e*][1,2]tiacina 5;5-dioxido (20i)



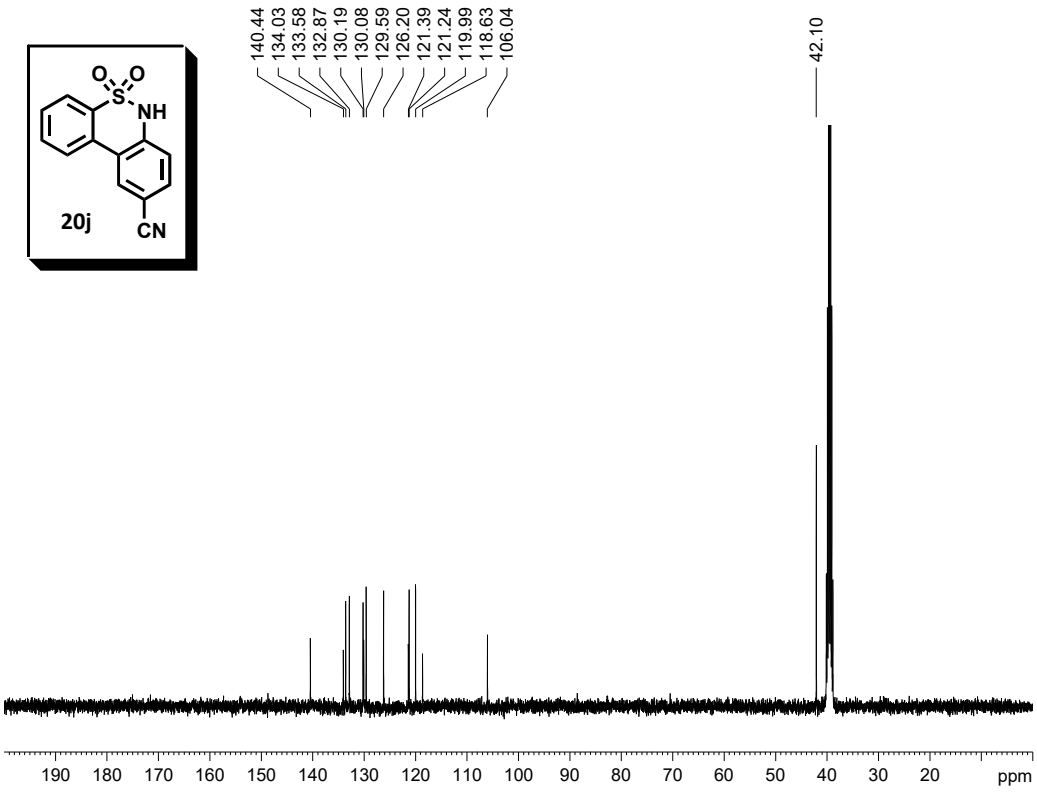


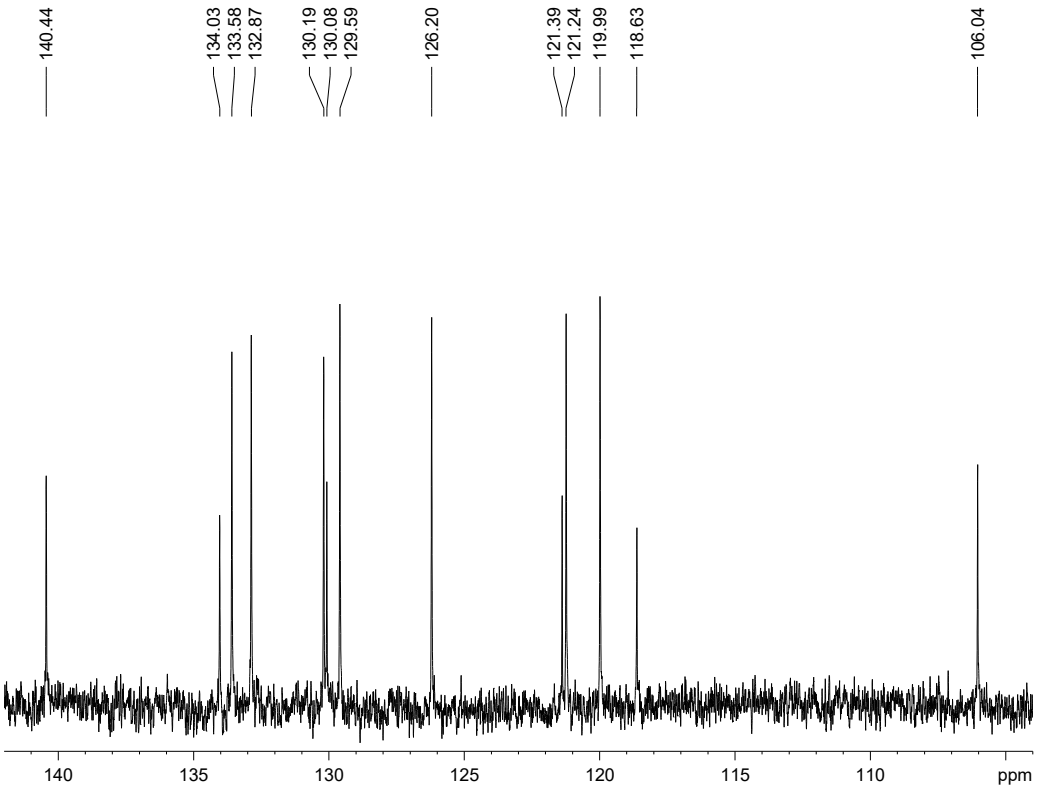
^{1}H-RMN (CD_3SOCD_3) 9-Ciano-6*H*-dibenzo[*c*,*e*][1,2]tiacina 5;5-dioxido (20j)



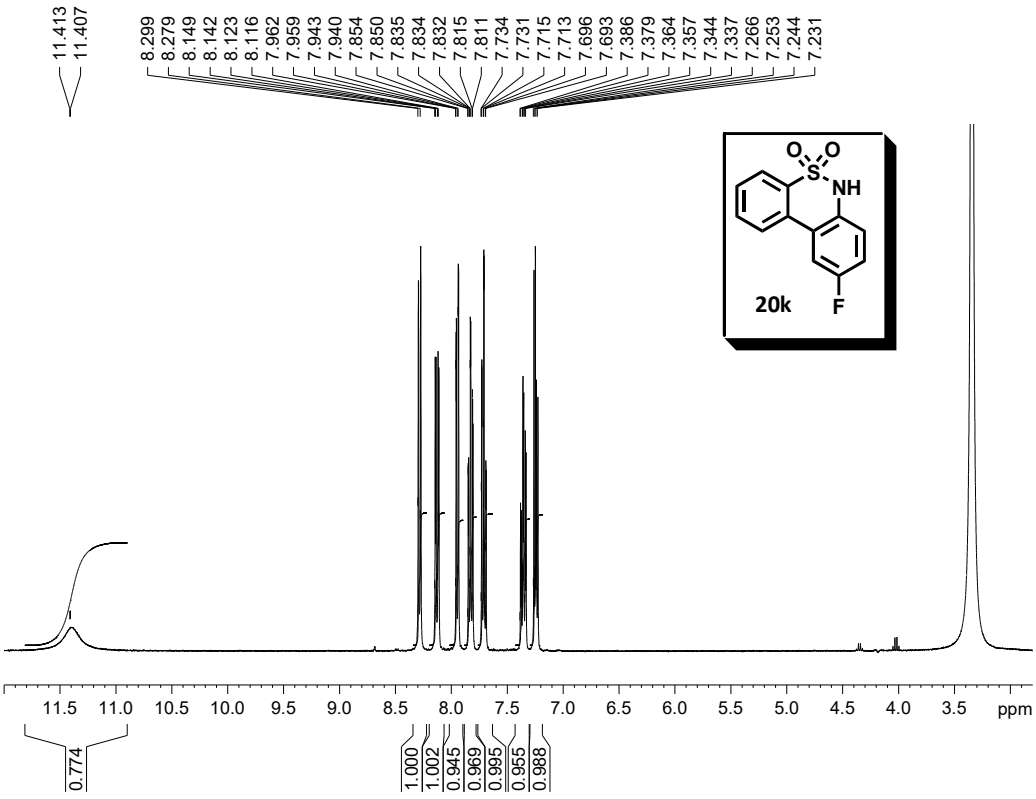


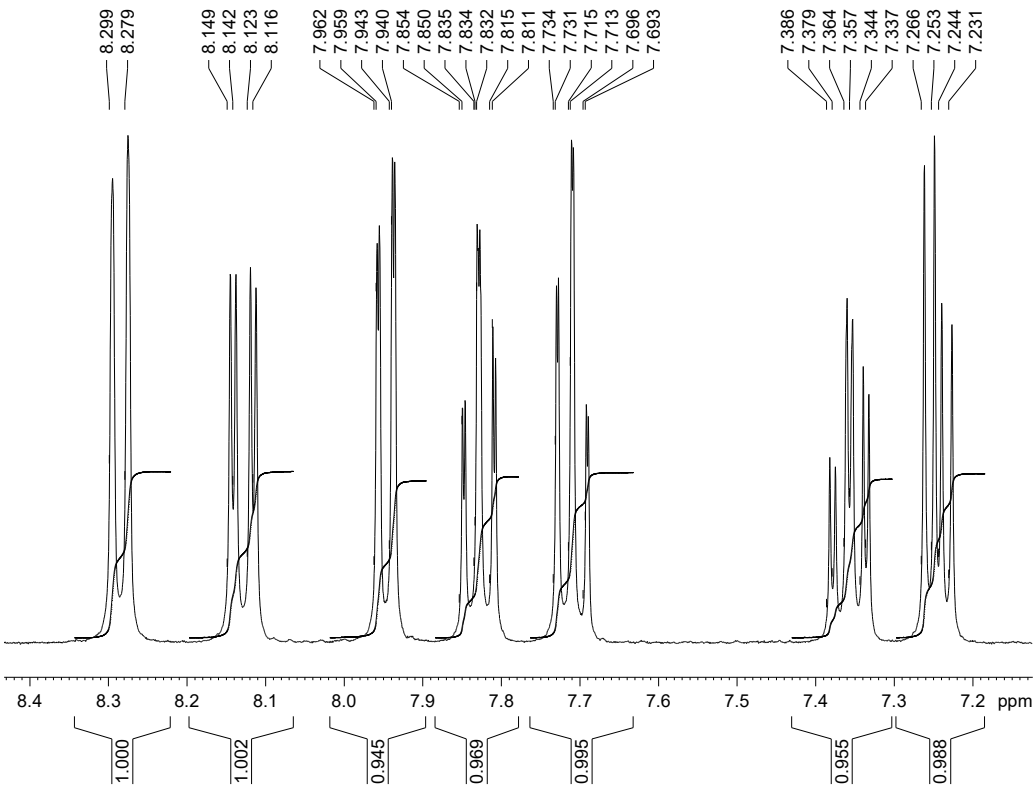
^{13}C-RMN (CD_3SOCD_3) 9-Ciano-6*H*-dibenzo[*c*,*e*][1,2]tiacina 5;5-dioxido (20j)



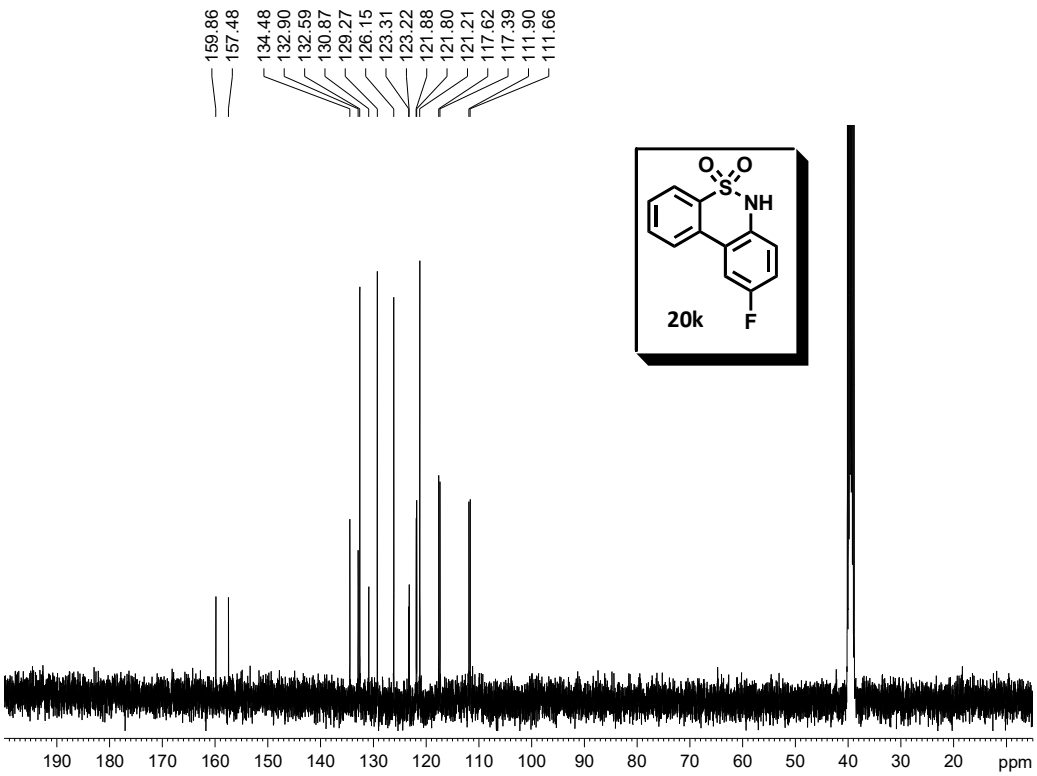


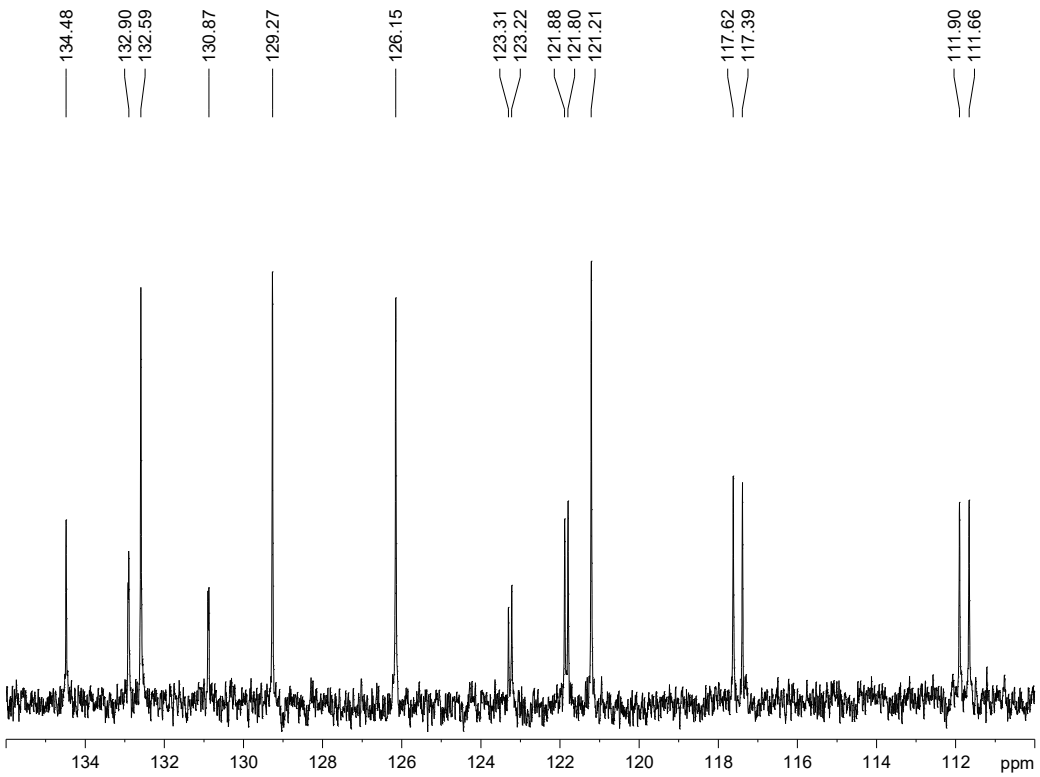
^{1}H-RMN (CD_3SOCD_3) 9-Fluor-6*H*-Dibenzo[*c*,*e*][1,2]tiacina 5;5-dioxido (20k)



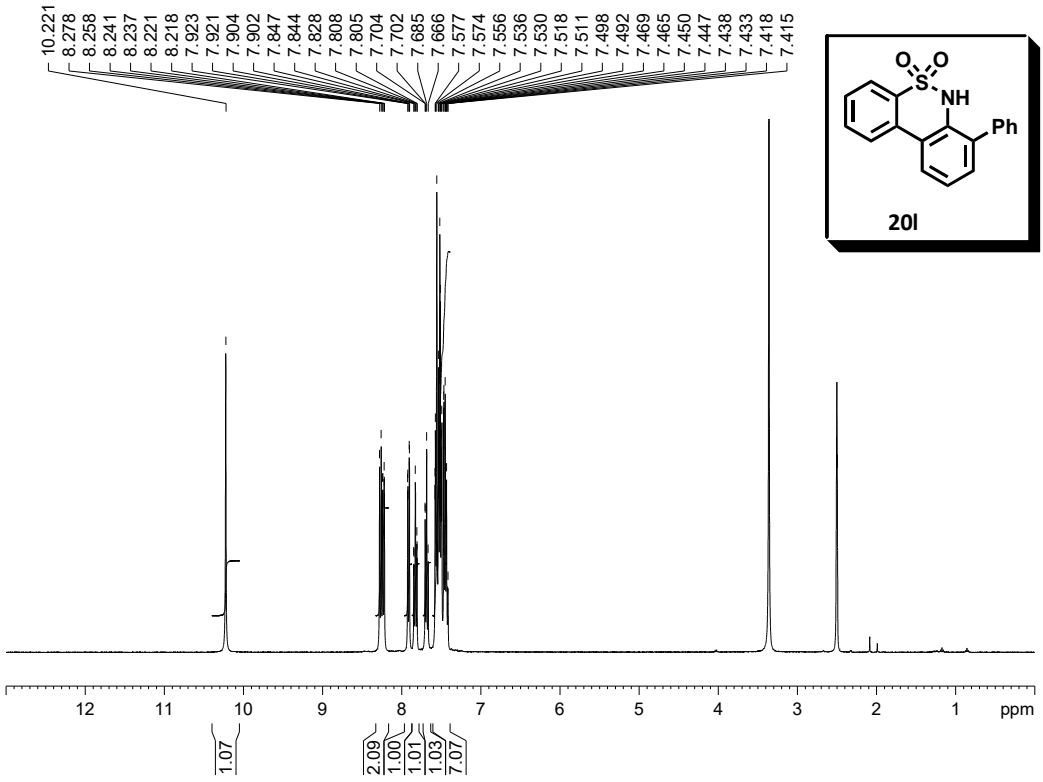


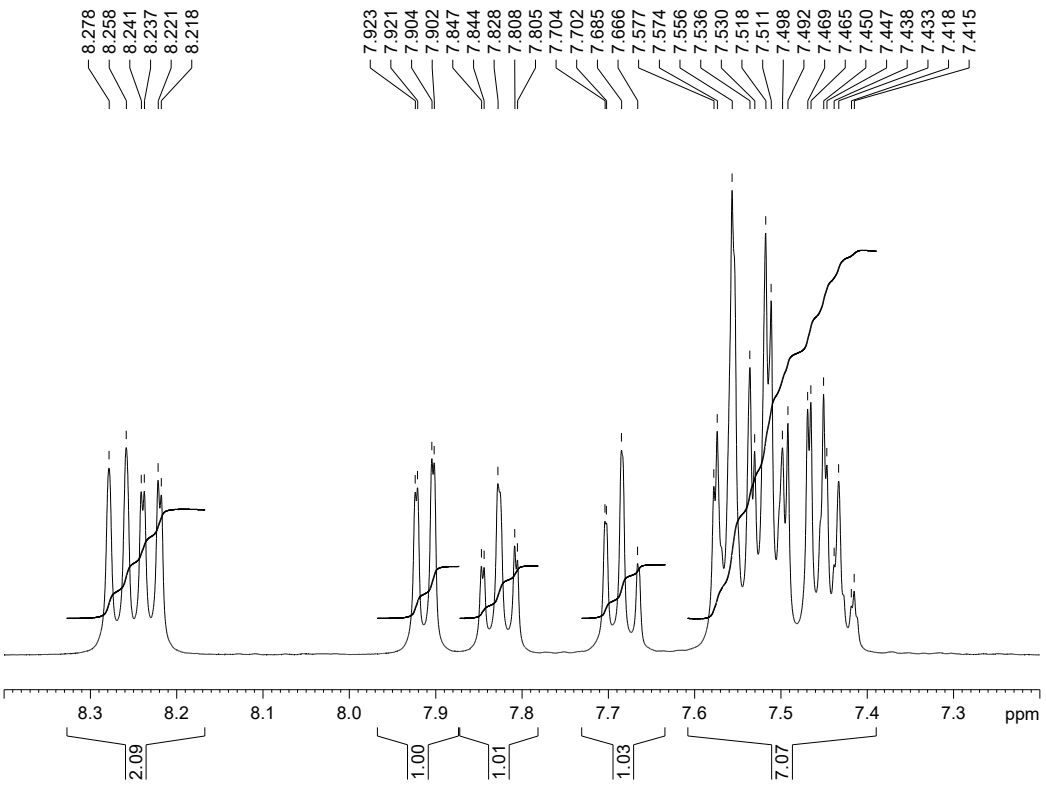
^{13}C-RMN (CD_3SOCD_3) 9-Fluor-6*H*-Dibenzo[*c*,*e*][1,2]tiacina 5;5-dioxido (20k)



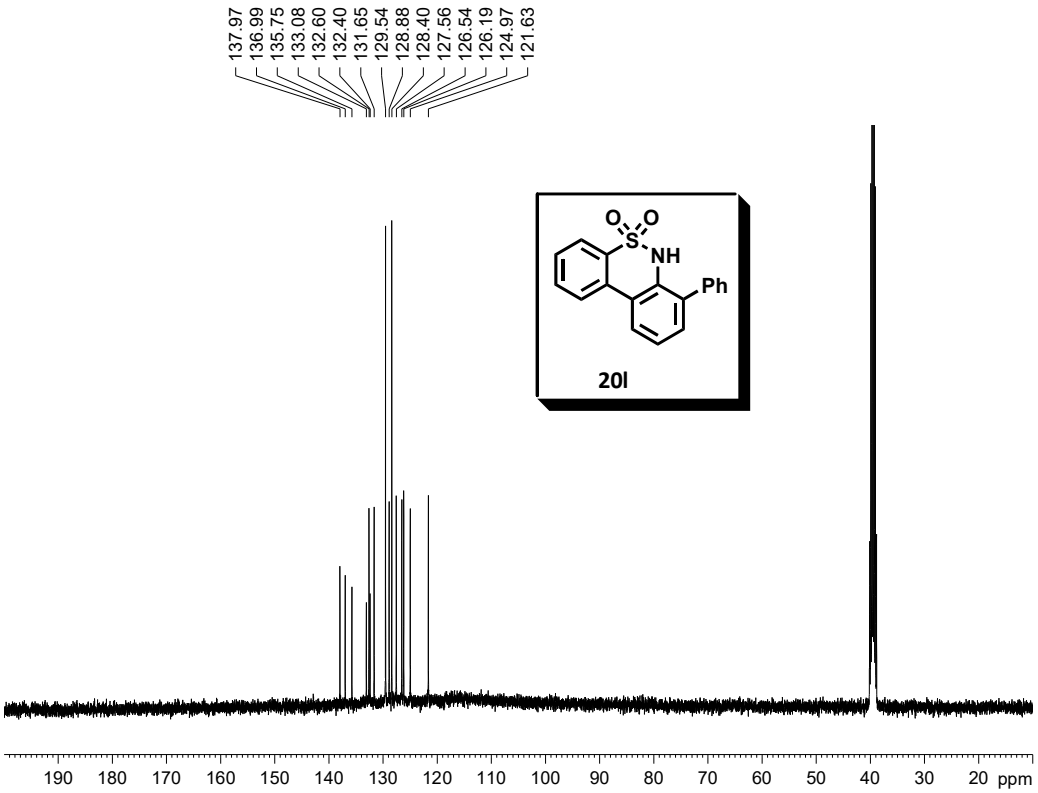


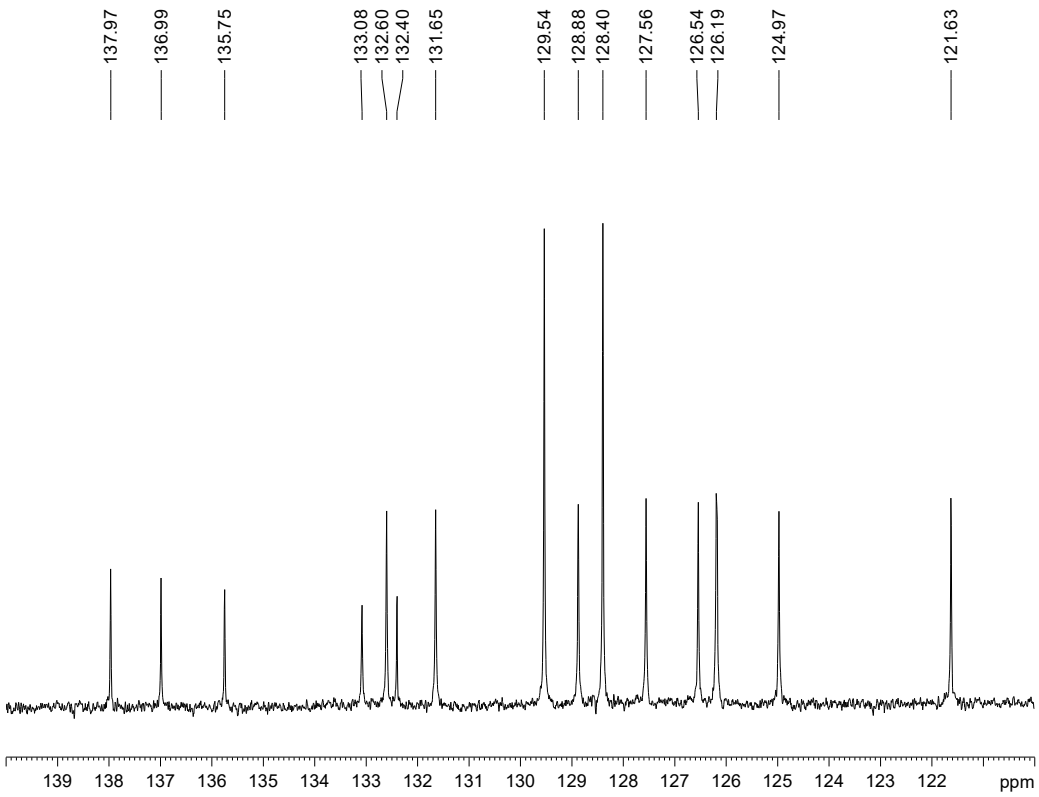
^{1}H-RMN (CD_3SOCD_3) 7-Fenil-6*H*-Dibenzo[*c*,*e*][1,2]tiacina 5;5-dioxido (20l)



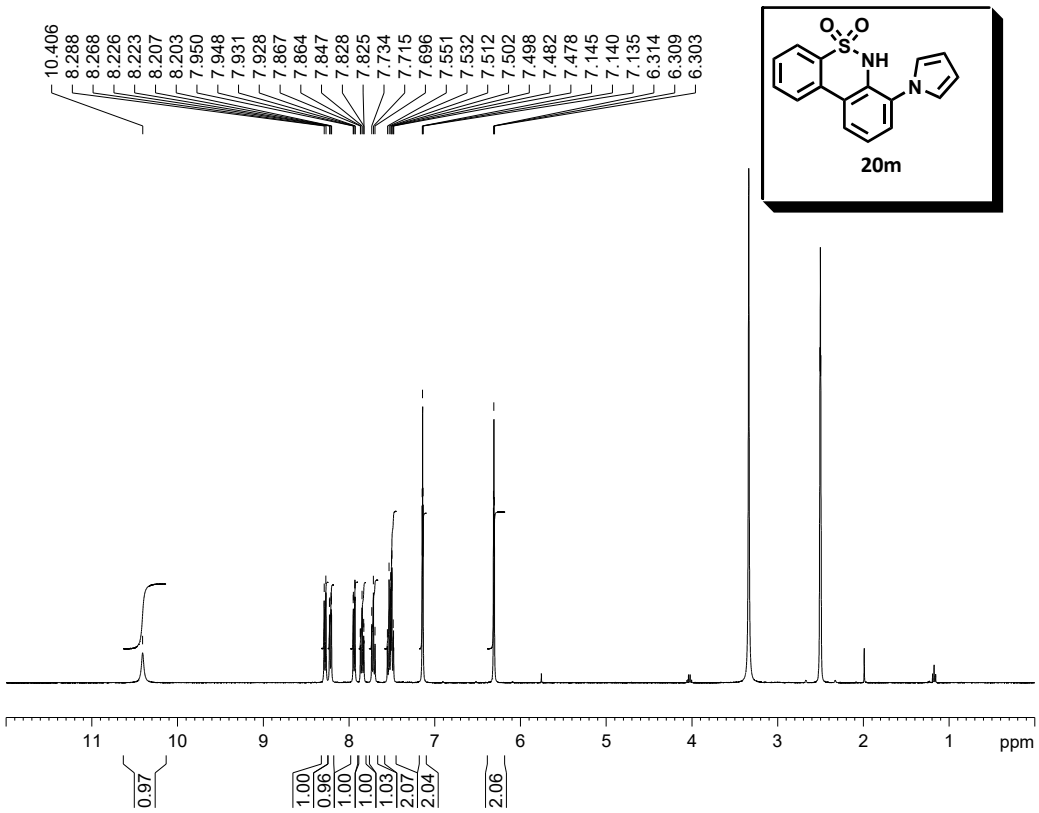


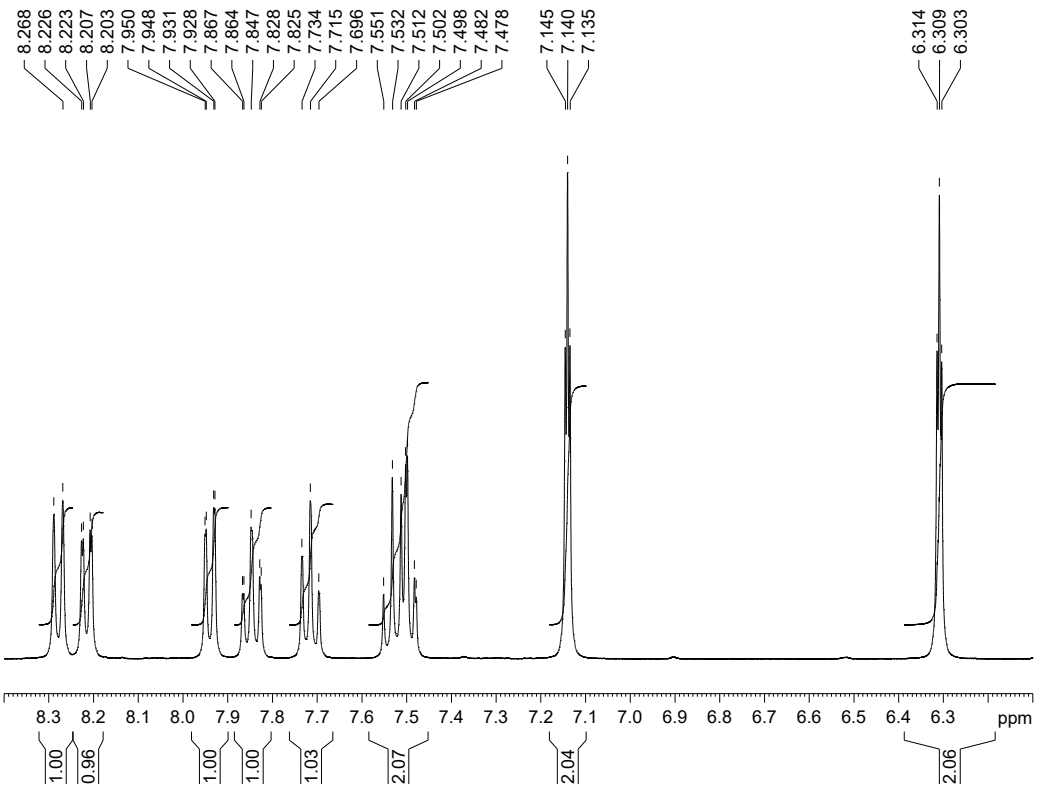
^{13}C-RMN (CD_3SOCD_3) 7-Fenil-6*H*-Dibenzo[*c*,*e*][1,2]tiacina 5;5-dioxido (20l)



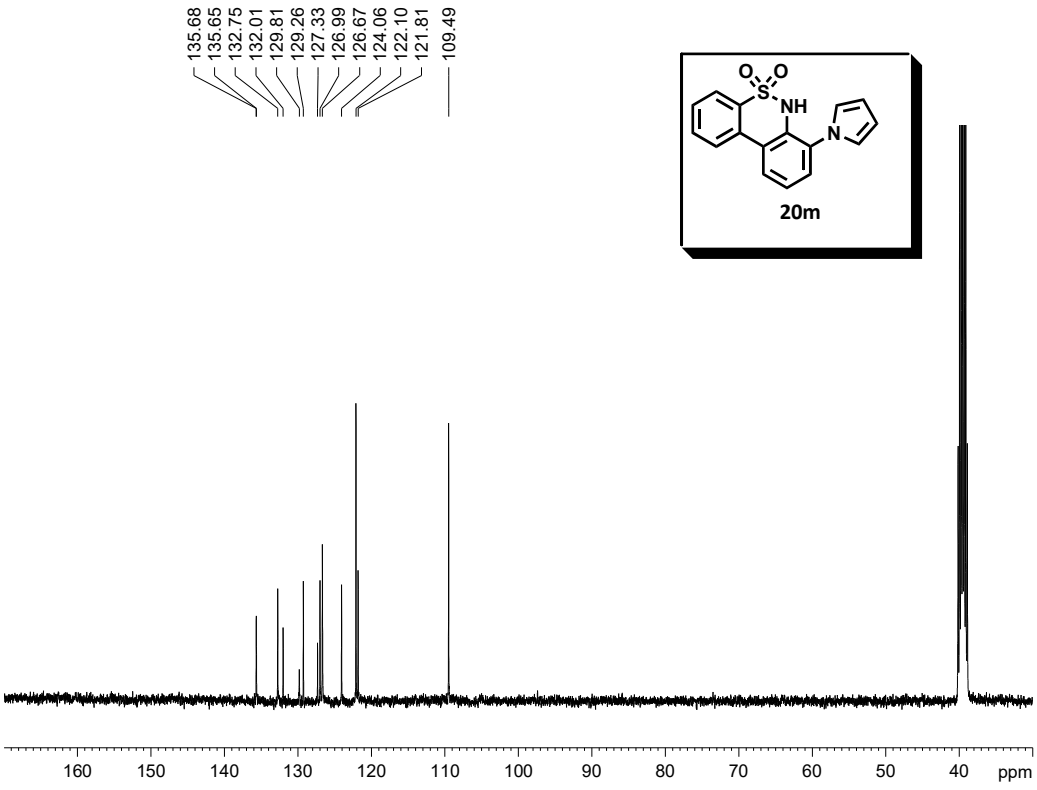


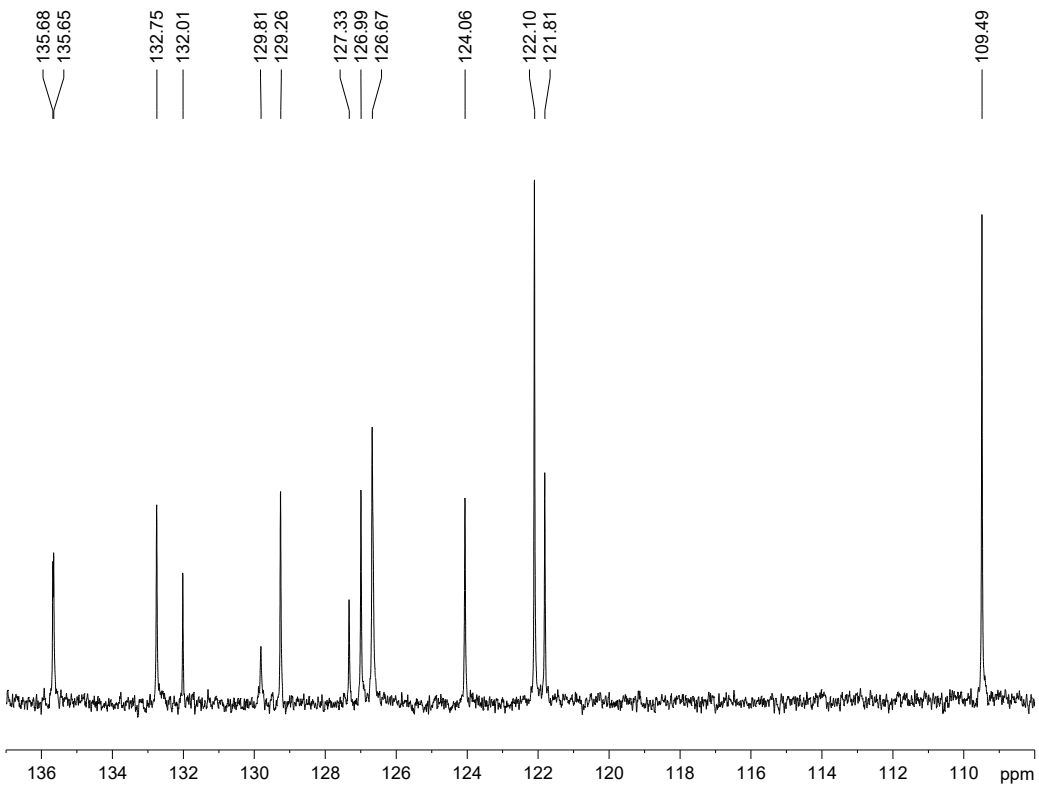
^{1}H-RMN (CD_3SOCD_3) 7-(1*H*-Pirrol-1-il)-6*H*-Dibenzo[*c*,*e*][1,2]tiacina 5;5-dioxido (20m)



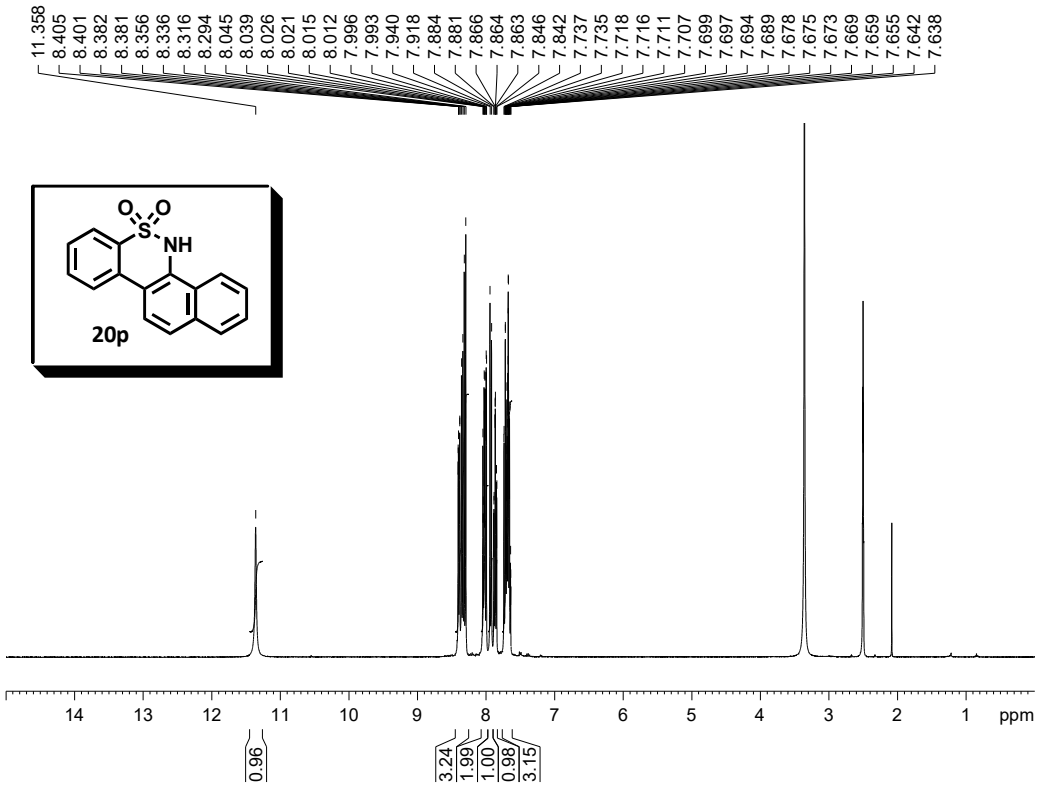


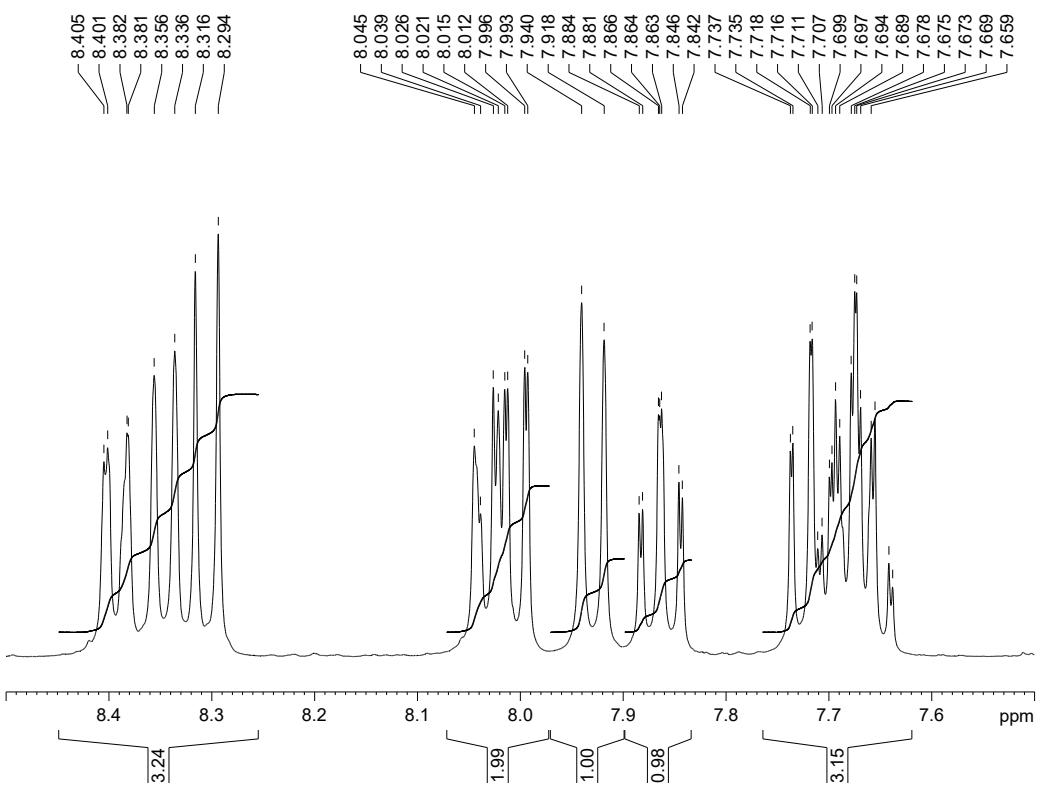
^{13}C-RMN (CD_3SOCD_3) 7-(1*H*-Pirrol-1-il)-6*H*-Dibenzo[*c*,*e*][1,2]tiacina 5;5-dioxido (20m)

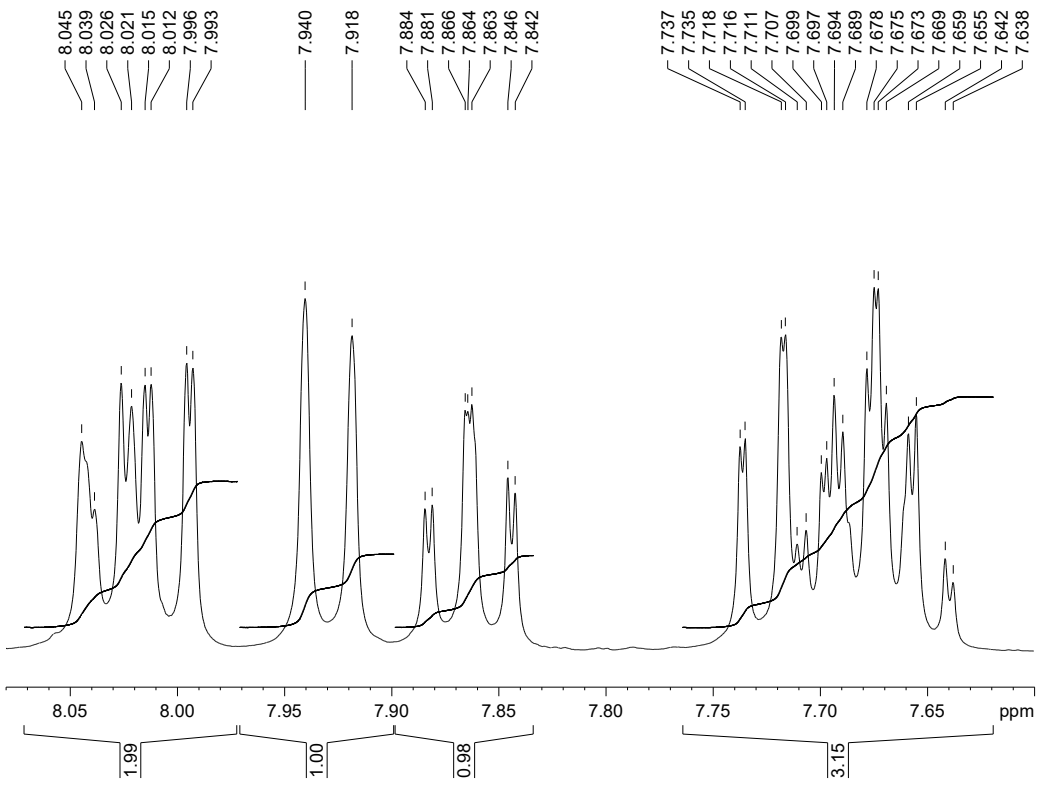




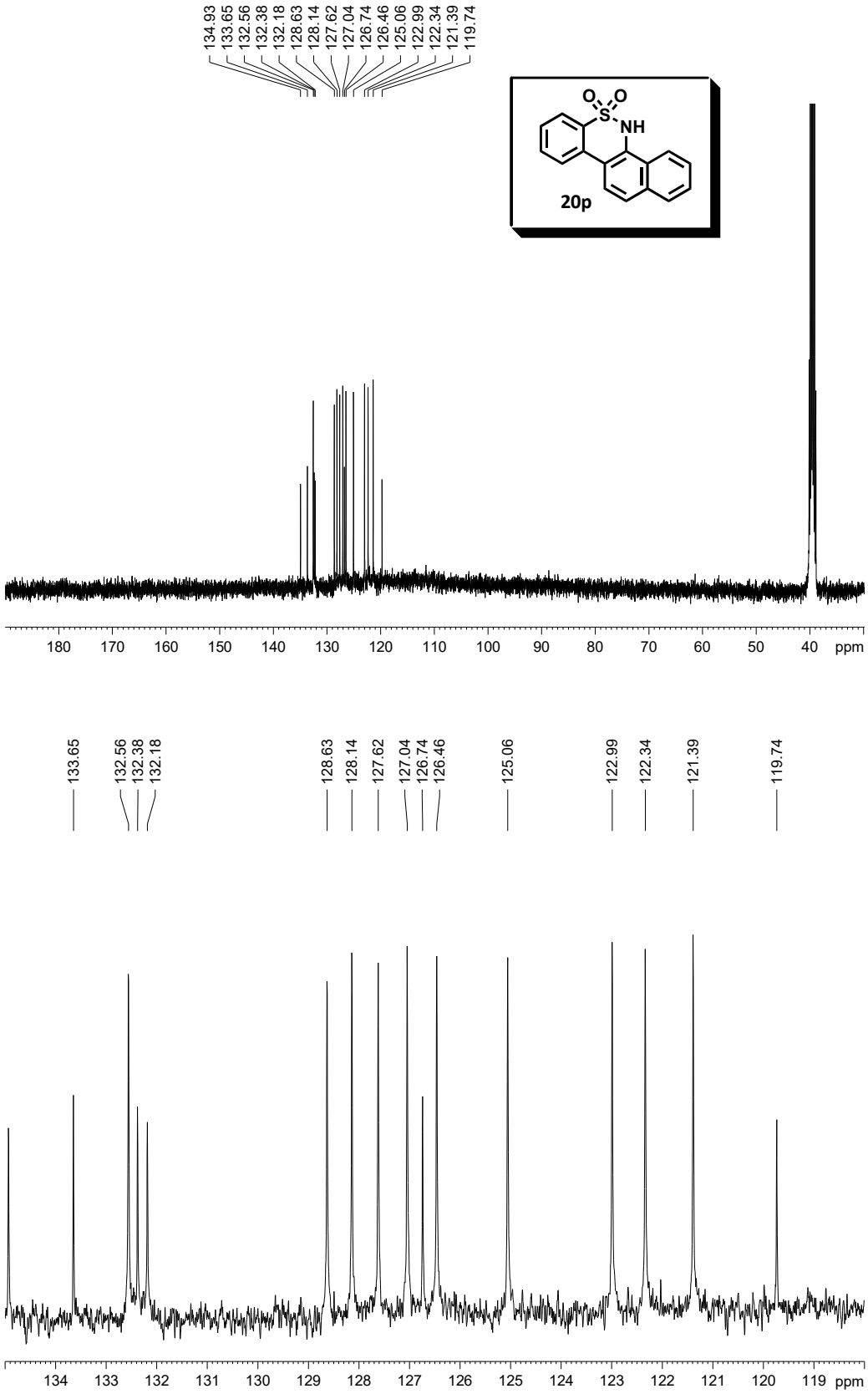
^{1}H-RMN (CD_3SOCD_3) 5*H*-Benzo[*e*]nafto[1,2-*c*][1,2]tiacina 5;5-dioxido (20p)



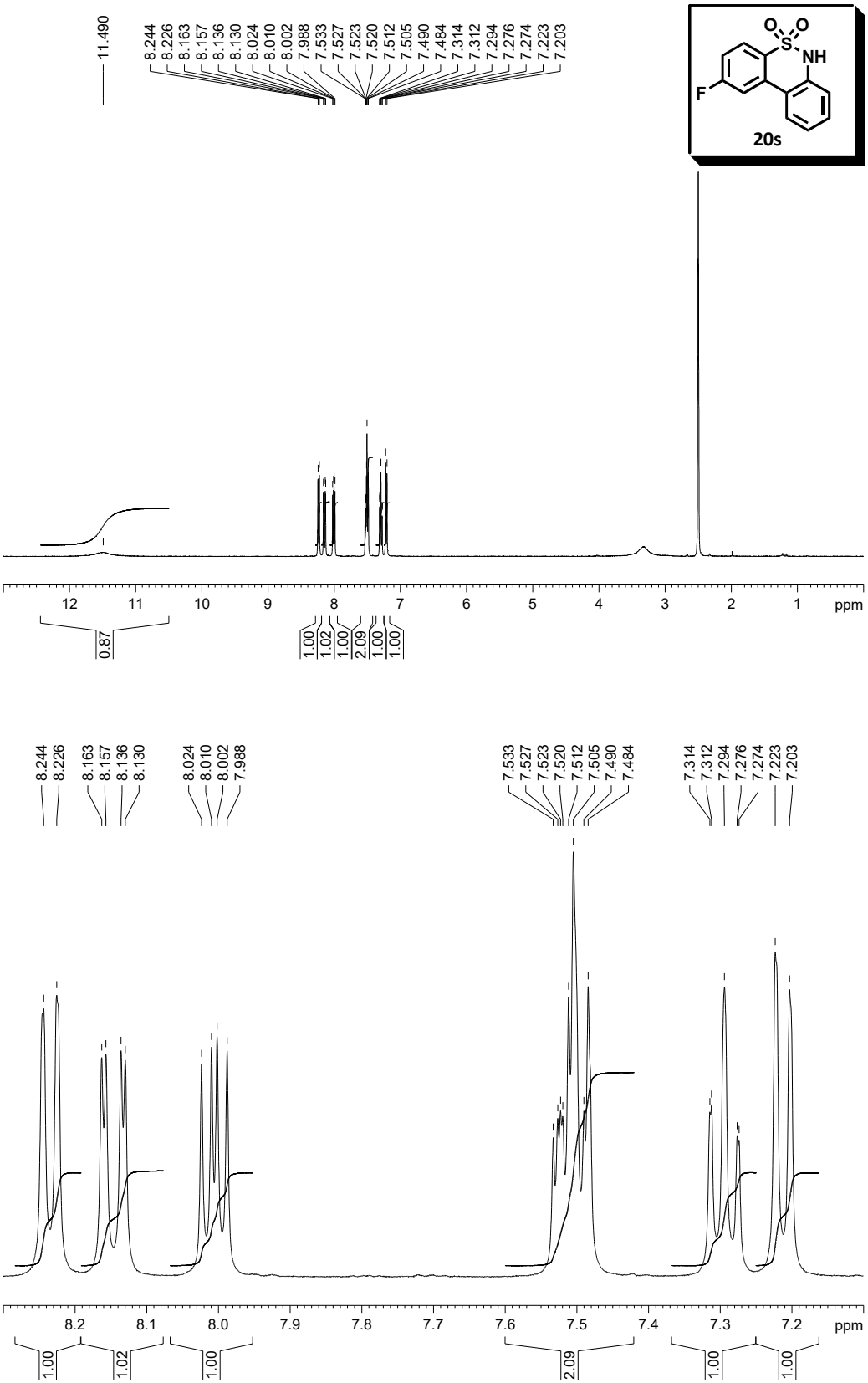

8.405
8.401
8.382
8.381
8.356
8.336
8.316
8.294
8.045
8.039
8.026
8.021
8.015
8.012
7.996
7.993
7.940
7.918
7.884
7.881
7.866
7.864
7.863
7.846
7.842
7.737
7.735
7.718
7.716
7.711
7.707
7.699
7.697
7.694
7.689
7.678
7.675
7.673
7.669
7.659
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
ppm
3.24
1.99
1.00
0.98
3.15

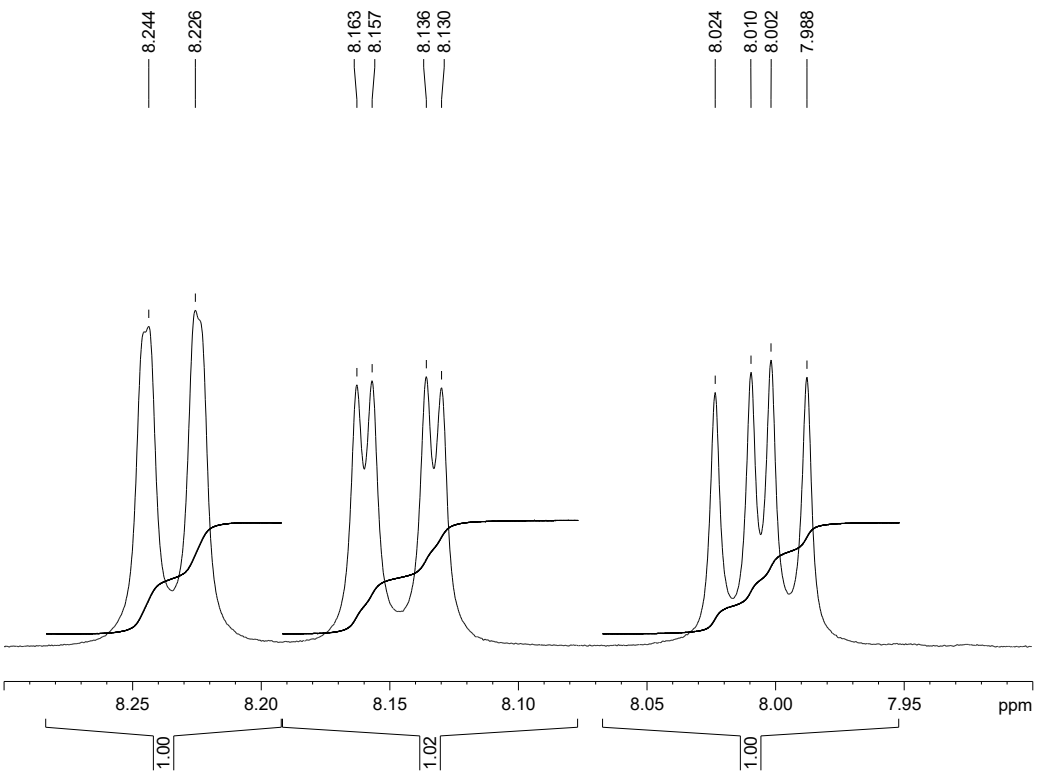

8.045
8.039
8.026
8.021
8.015
8.012
7.996
7.993
7.940
7.918
7.884
7.881
7.866
7.864
7.863
7.846
7.842
7.737
7.735
7.718
7.716
7.711
7.707
7.699
7.697
7.694
7.689
7.678
7.675
7.673
7.669
7.659
7.655
7.642
7.638
8.05
8.00
7.95
7.90
7.85
7.80
7.75
7.70
7.65
ppm
1.99
1.00
0.98
3.15

^{13}C-RMN (CD_3SOCD_3) 5*H*-Benzo[*e*]nafto[1,2-*c*][1,2]tiacina 5;5-dioxido (20p)

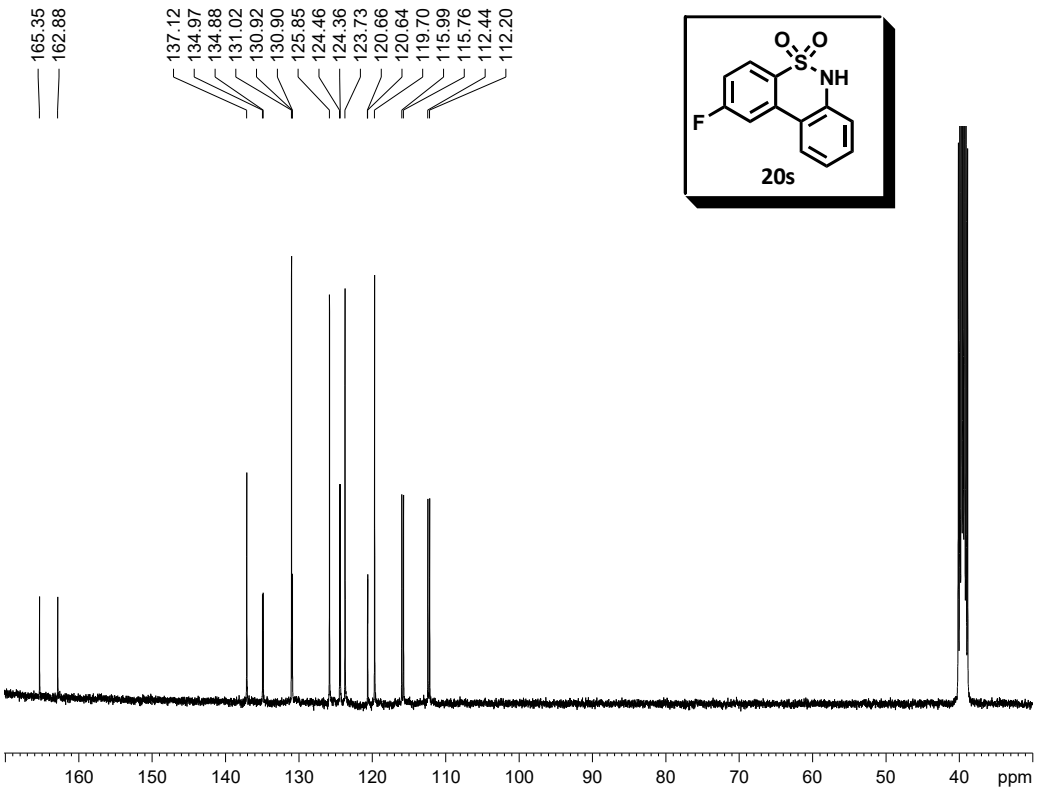


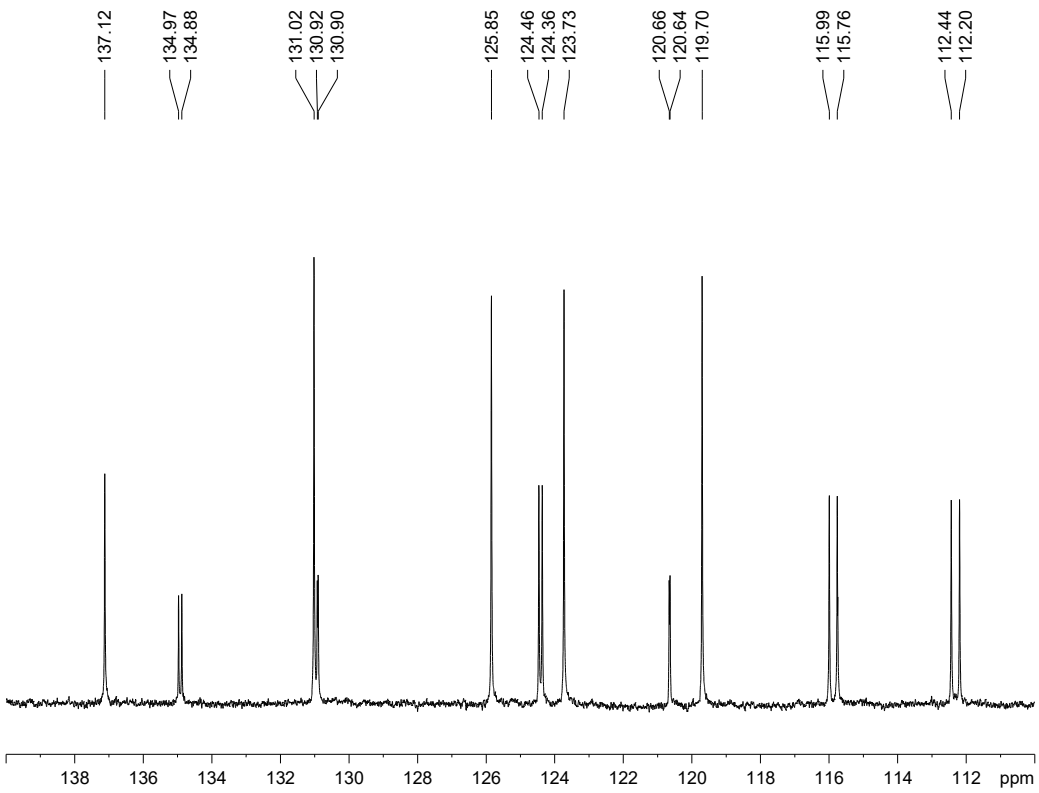
^{1}H-RMN (CD_3SOCD_3) 2-Fluor-6*H*-dibenzo[*c*,*e*][1,2]tiacina 5,5-dioxido (20s)



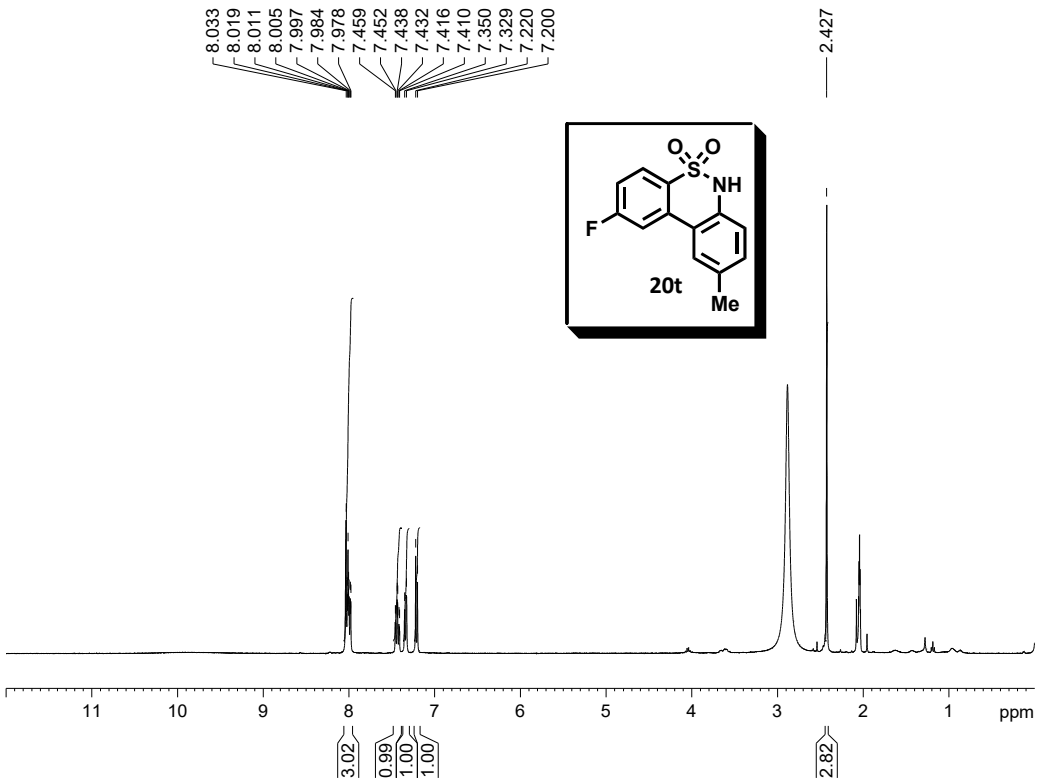


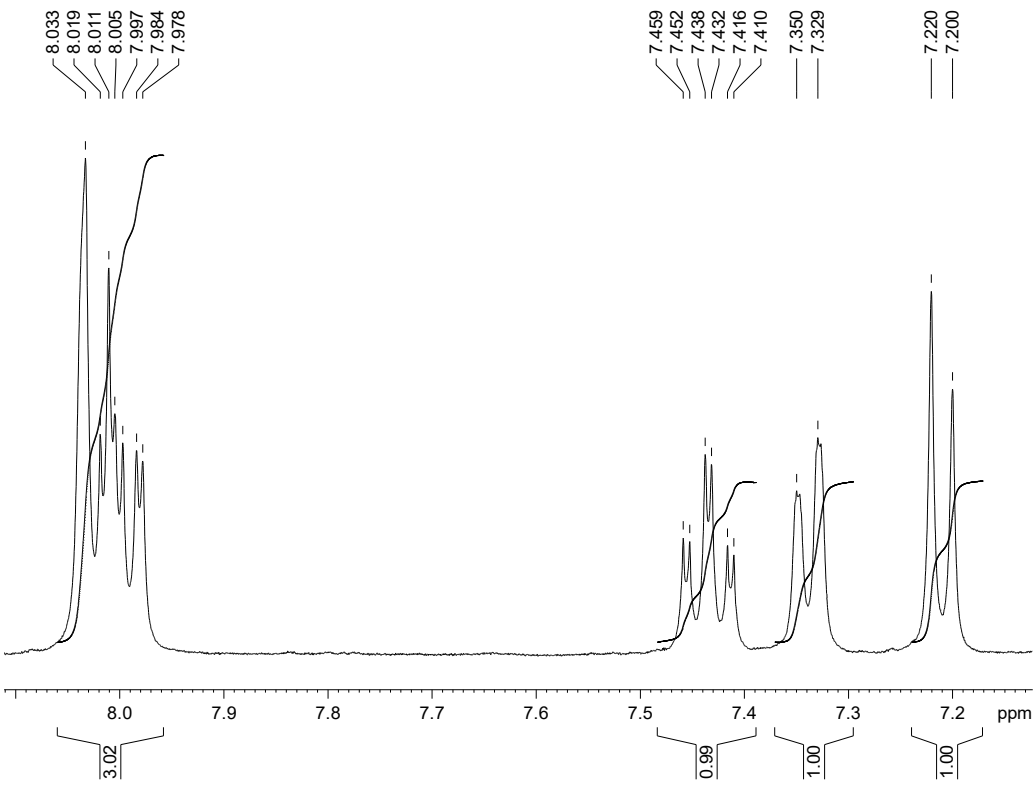
^{13}C-RMN (CD_3SOCD_3) 2-Fluor-6*H*-dibenzo[*c*,*e*][1,2]tiacina 5,5-dioxido (20s)



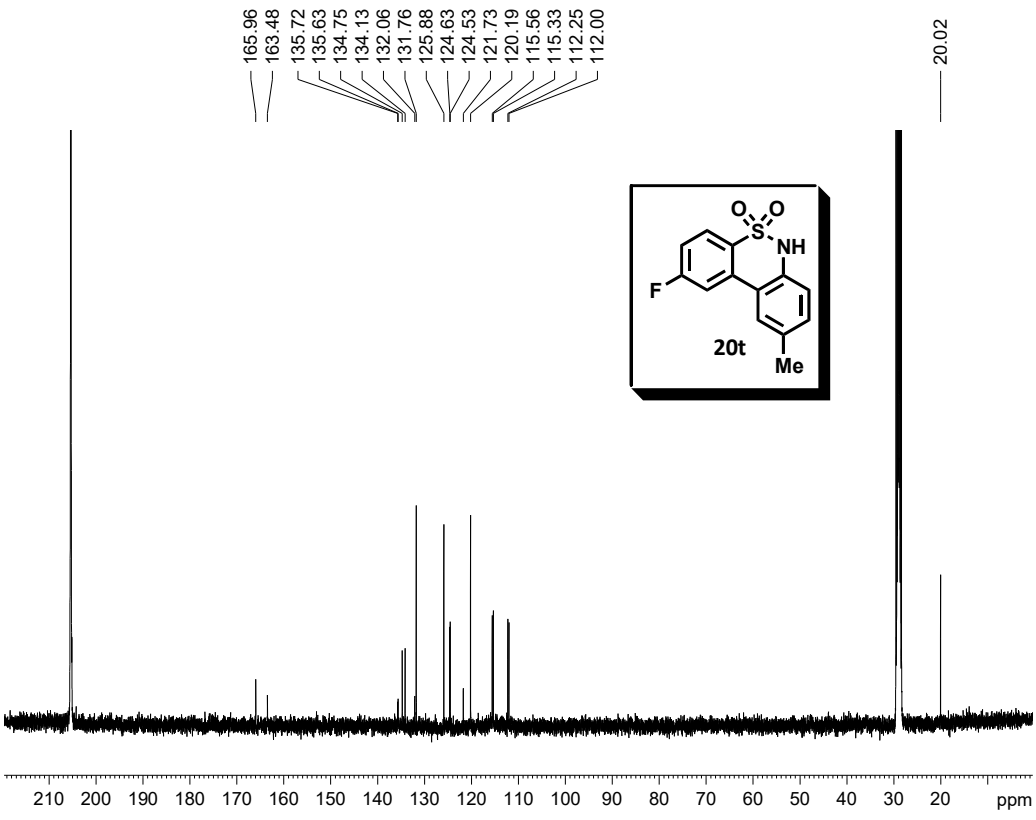


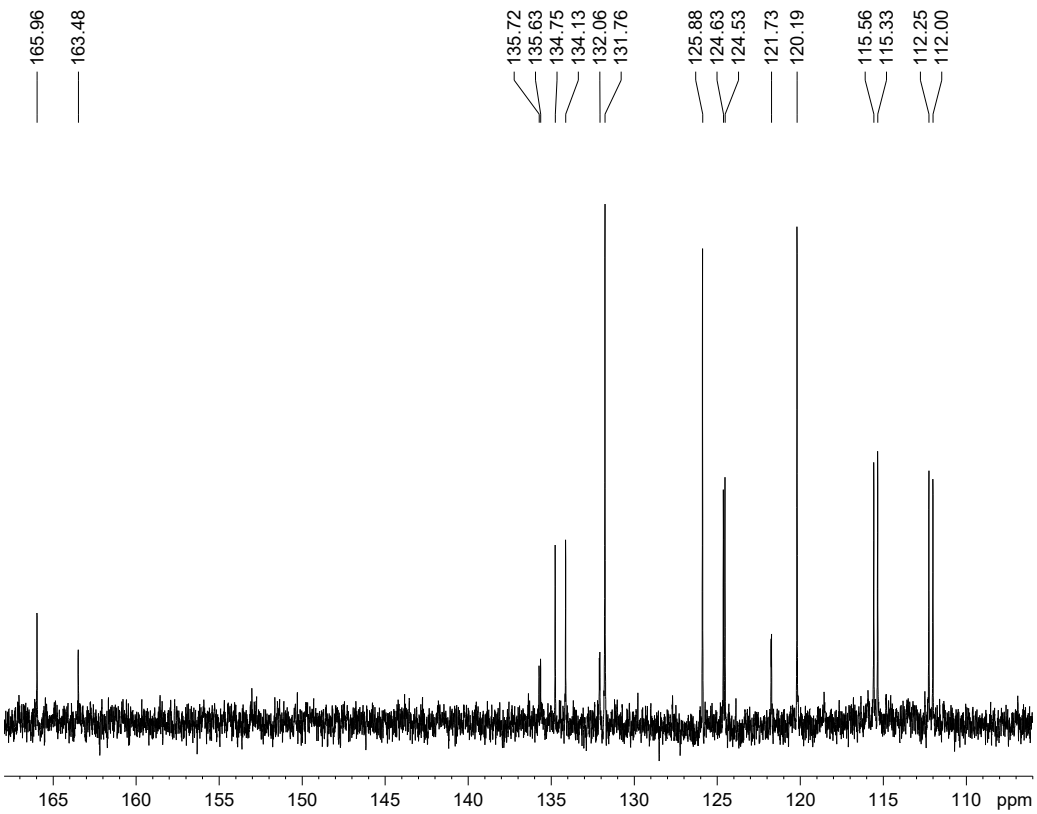
^{1}H-RMN (CD_3COCD_3) 2-Fluor-9-metil-6*H*-dibenzo[*c*,*e*][1,2]tiacina 5,5-dioxido (20t)



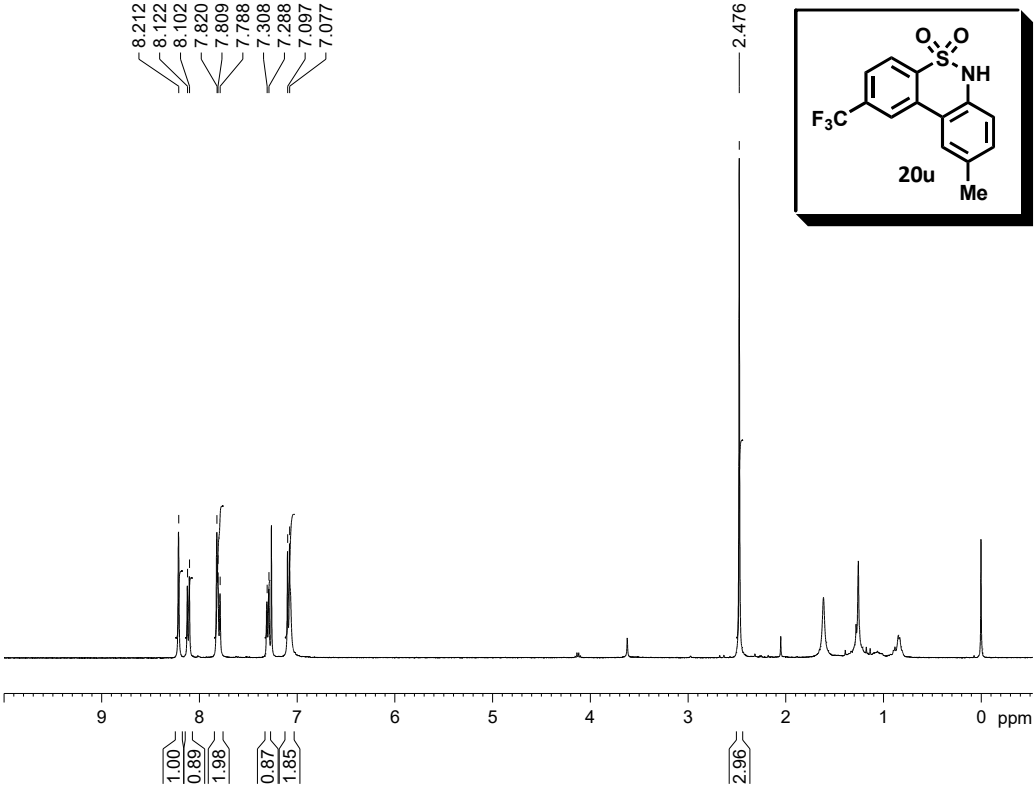


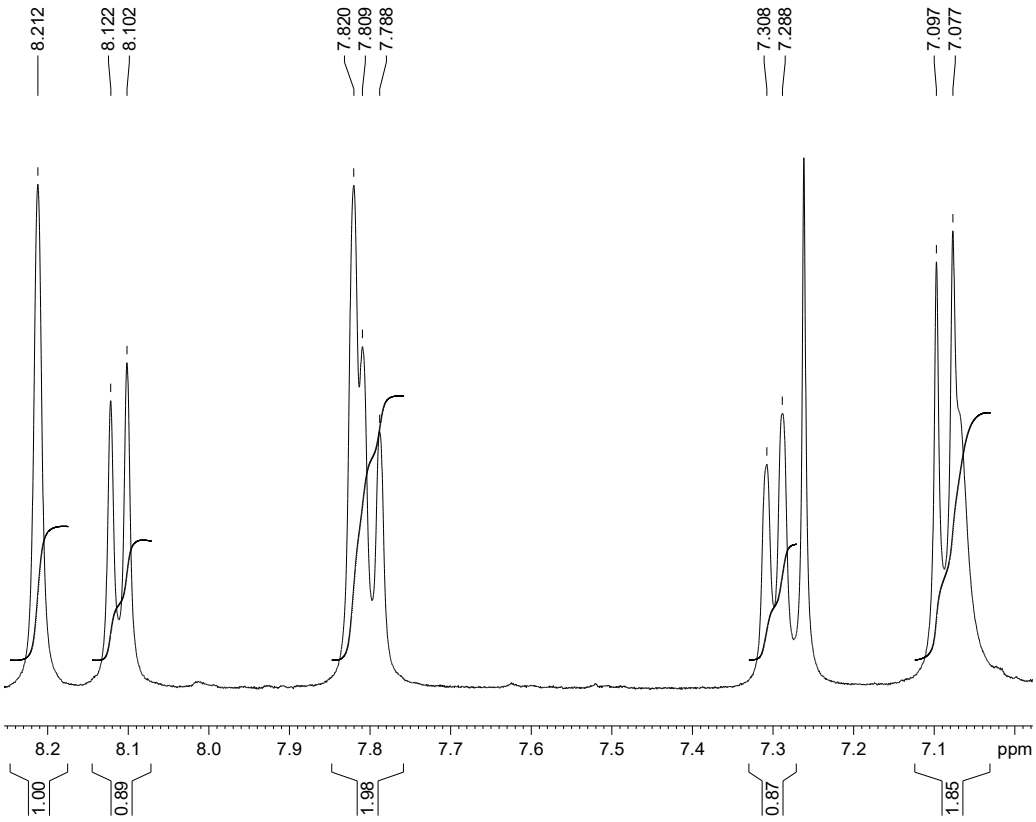
^{13}C-RMN (CD_3COCD_3) 2-Fluor-9-metil-6*H*-dibenzo[*c*,*e*][1,2]tiacina 5,5-dioxido (20t)



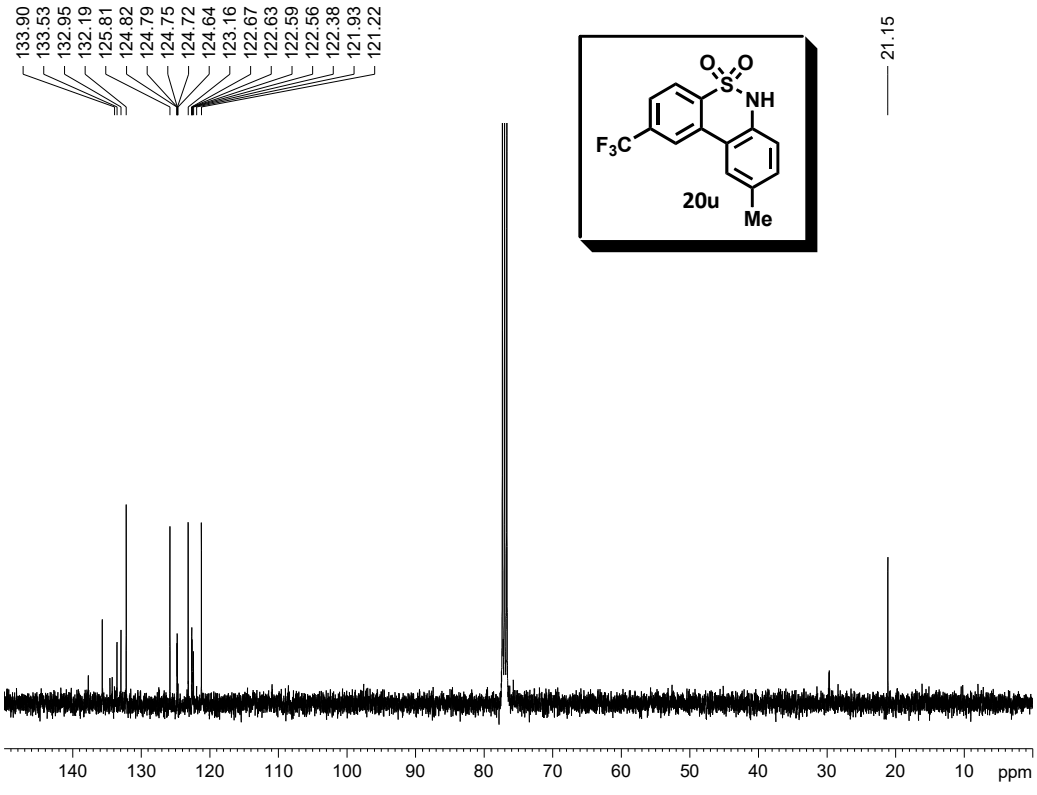


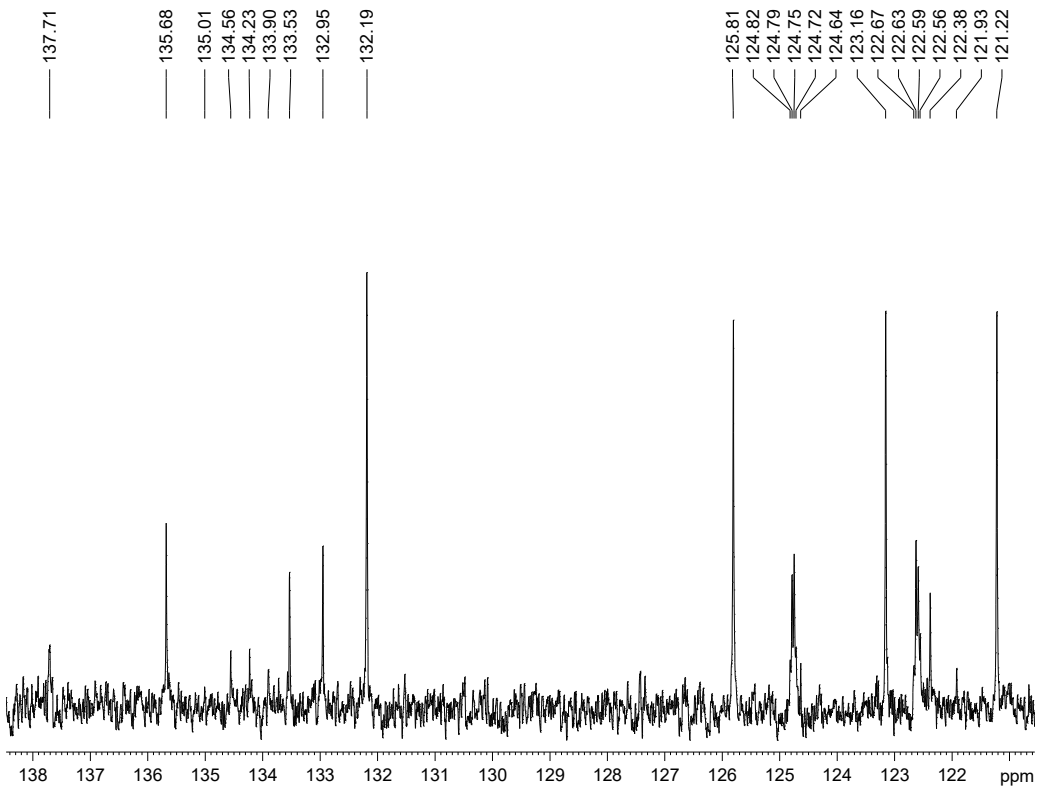
^{1}H-RMN ($CDCl_3$) 9-Metil-2-(trifluormetil)-6*H*-dibenzo[*c*,*e*][1,2]tiacina 5,5-dioxido (20u)



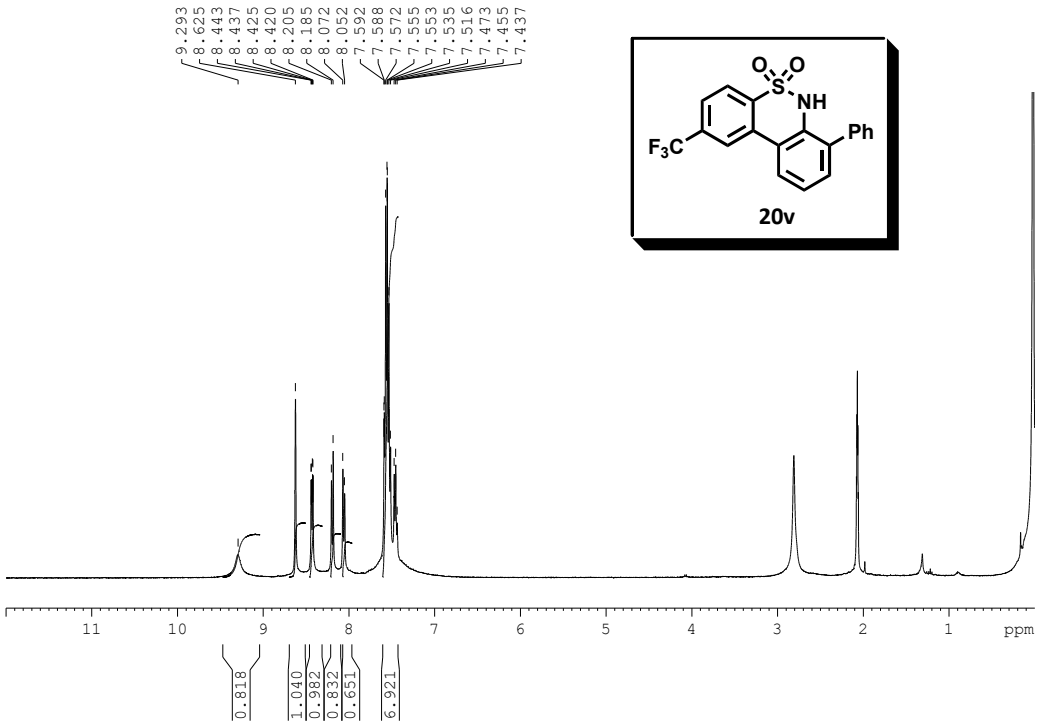


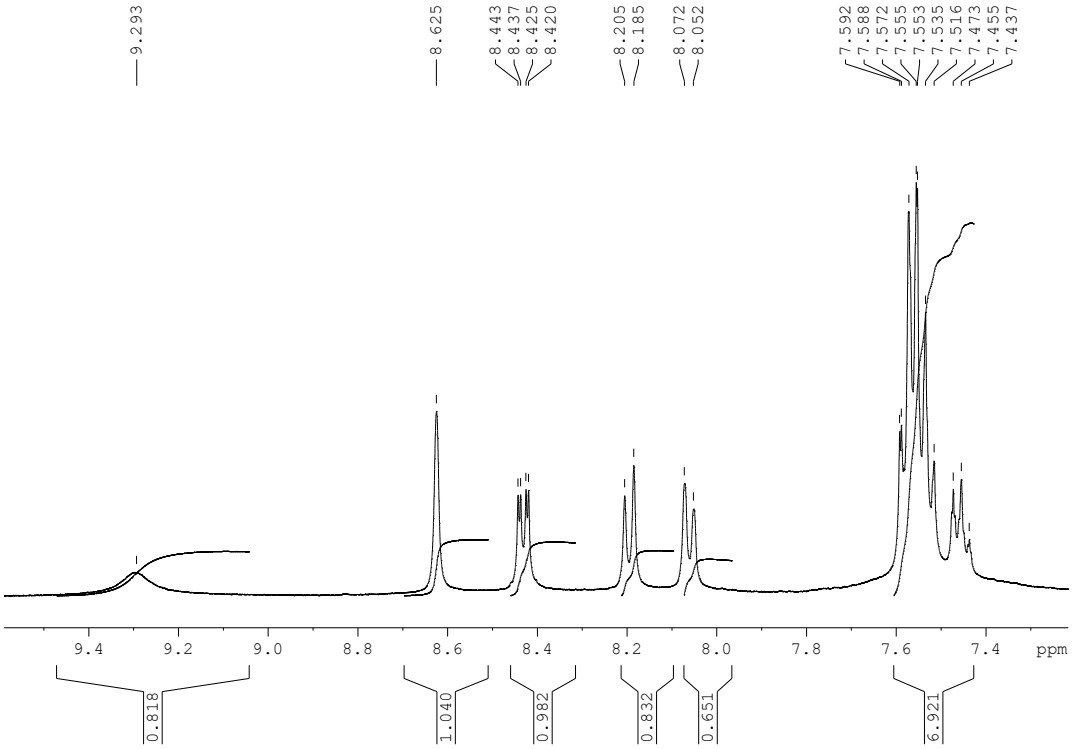
^{13}C-RMN ($CDCl_3$) 9-Metil-2-(trifluormetil)-6*H*-dibenzo[*c*,*e*][1,2]tiacina 5,5-dioxido (20u)



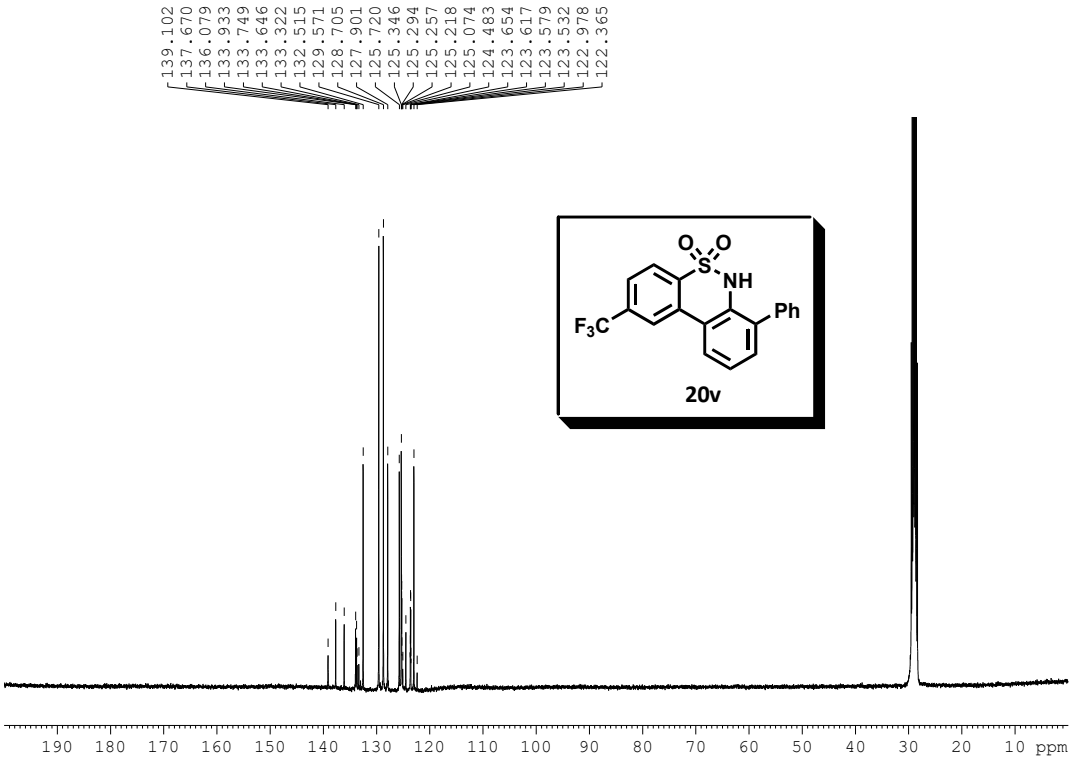


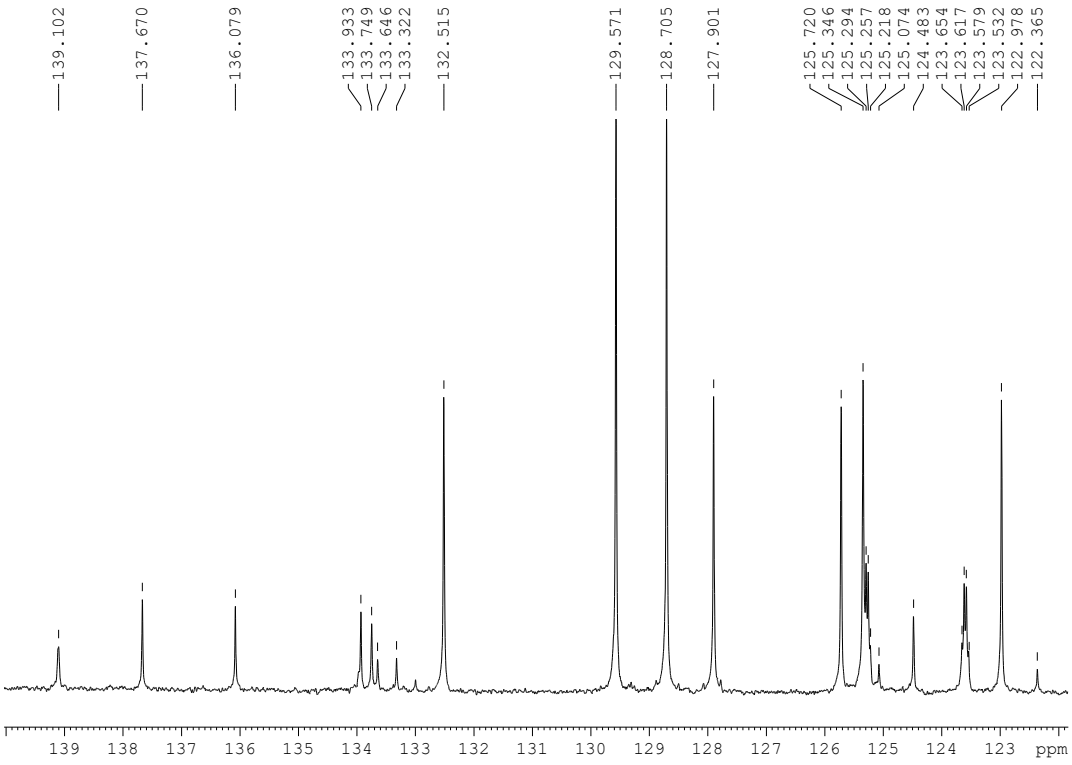
^{1}H-RMN (CD_3COCD_3) 7-Fenil-2-(trifluormetil)-6*H*-dibenzo[*c*,*e*][1,2]tiacina 5,5-dioxido (20u)



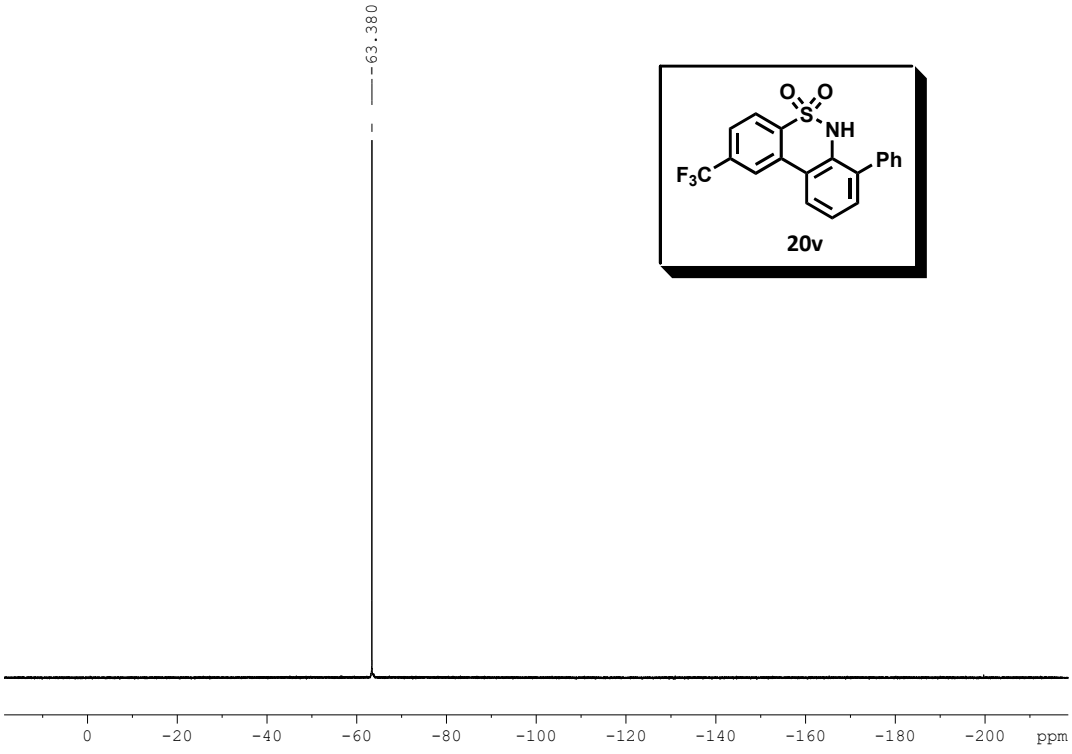


^{13}C-RMN (CD_3COCD_3) 7-Fenil-2-(trifluormetil)-6*H*-dibenzo[*c*,*e*][1,2]tiacina 5,5-dioxido (20u)



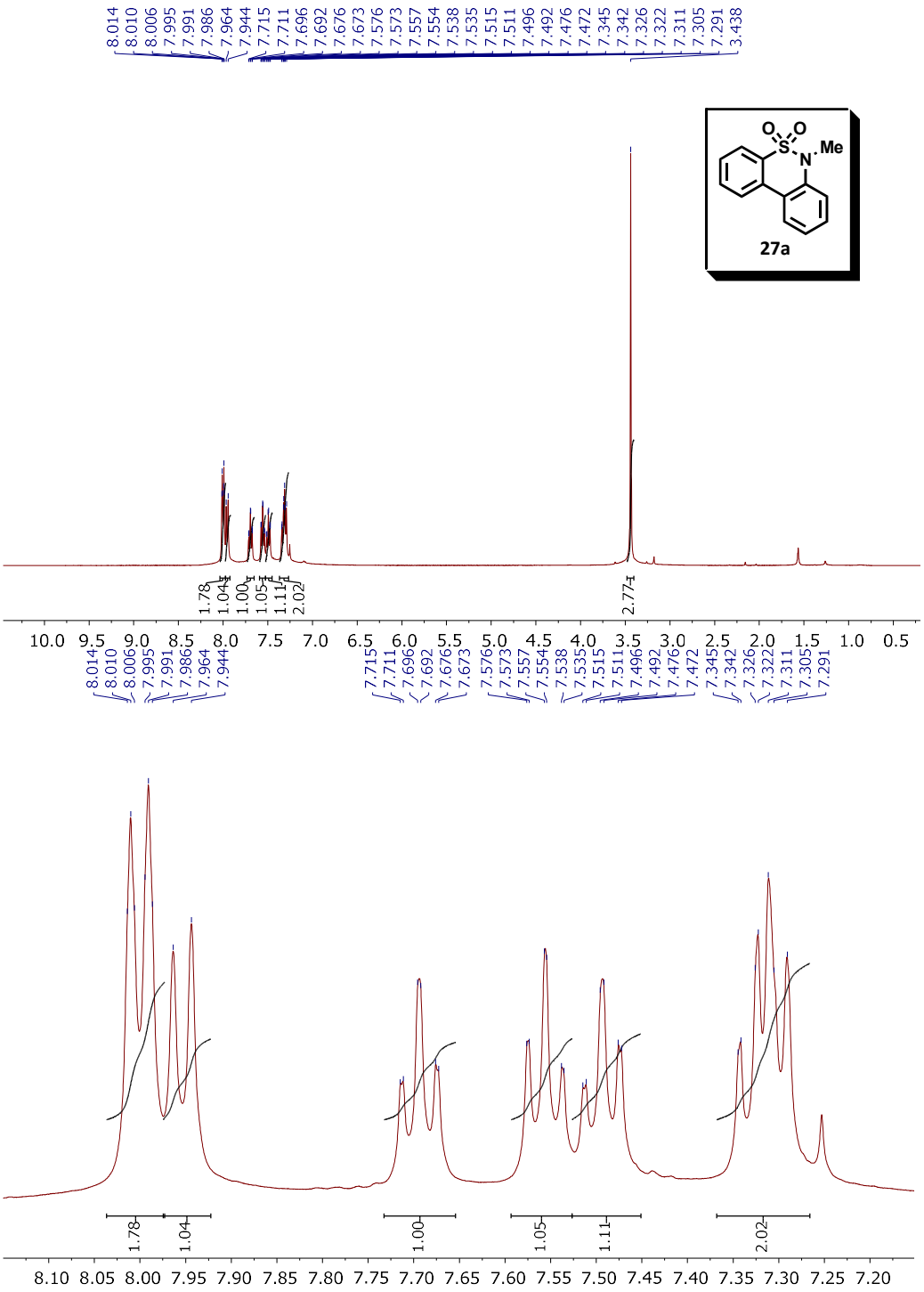


^{19}F-RMN (CD_3COCD_3) 7-Fenil-2-(trifluormetil)-6*H*-dibenzo[*c*,*e*][1,2]tiacina 5,5-dioxido (20u)

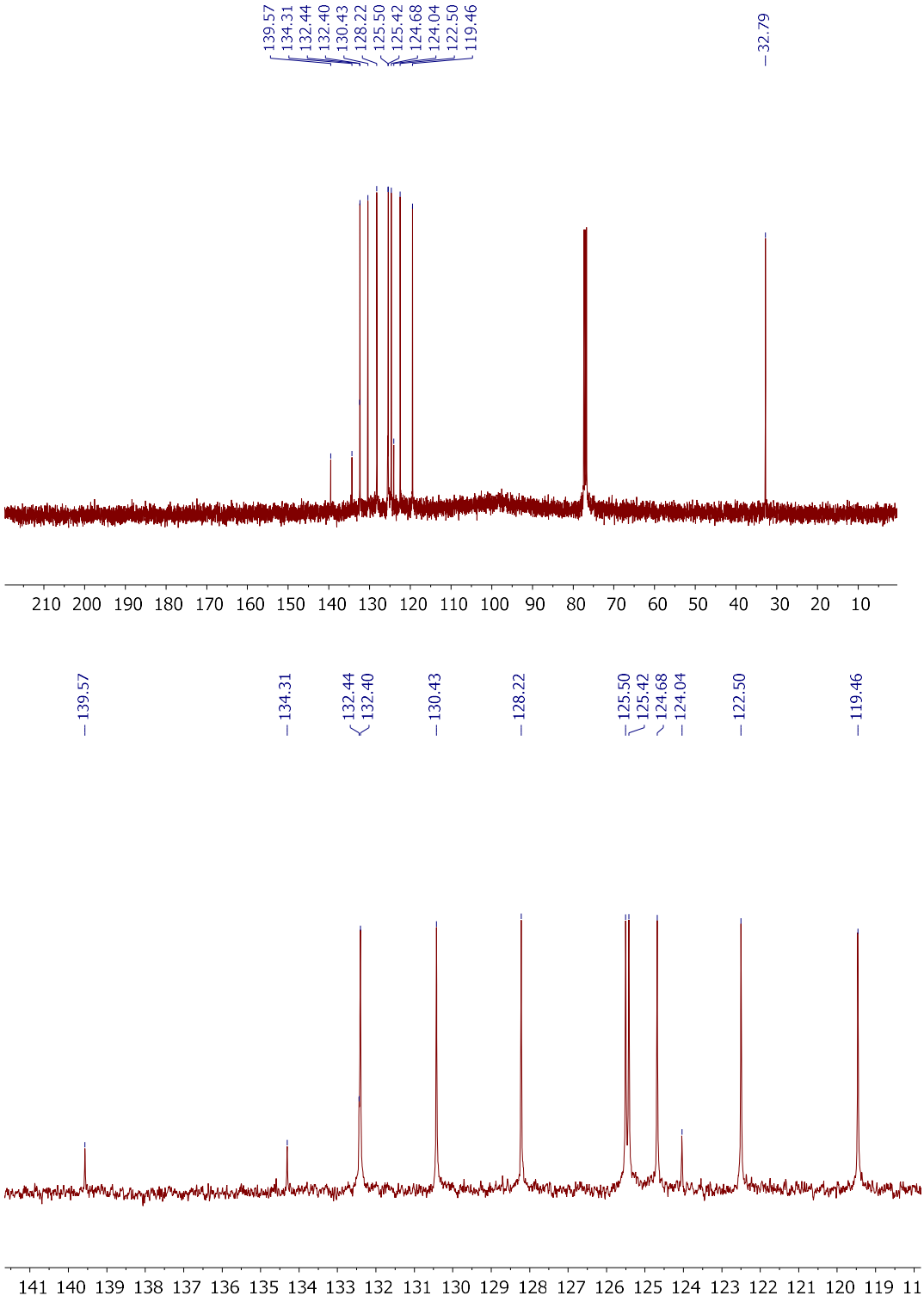


A.4.3 ESPECTROS DE RMN DE DIBENZOTIACINAS DERIVATIZADAS

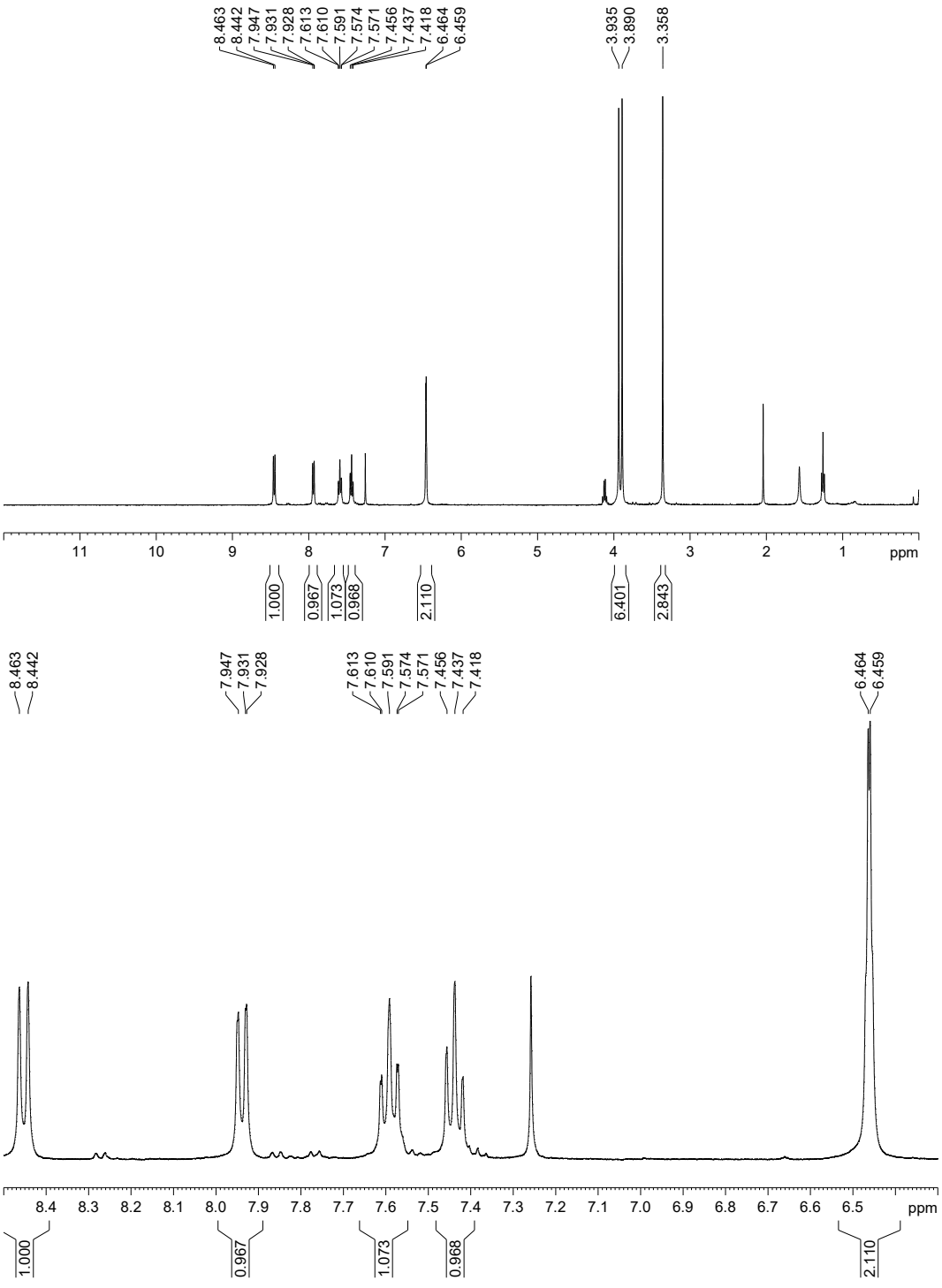
^{1}H-RMN ($CDCl_3$) 6-Metil-6*H*-dibenzo[*c,e*][1,2]tiacina 5,5-dióxido (27a)



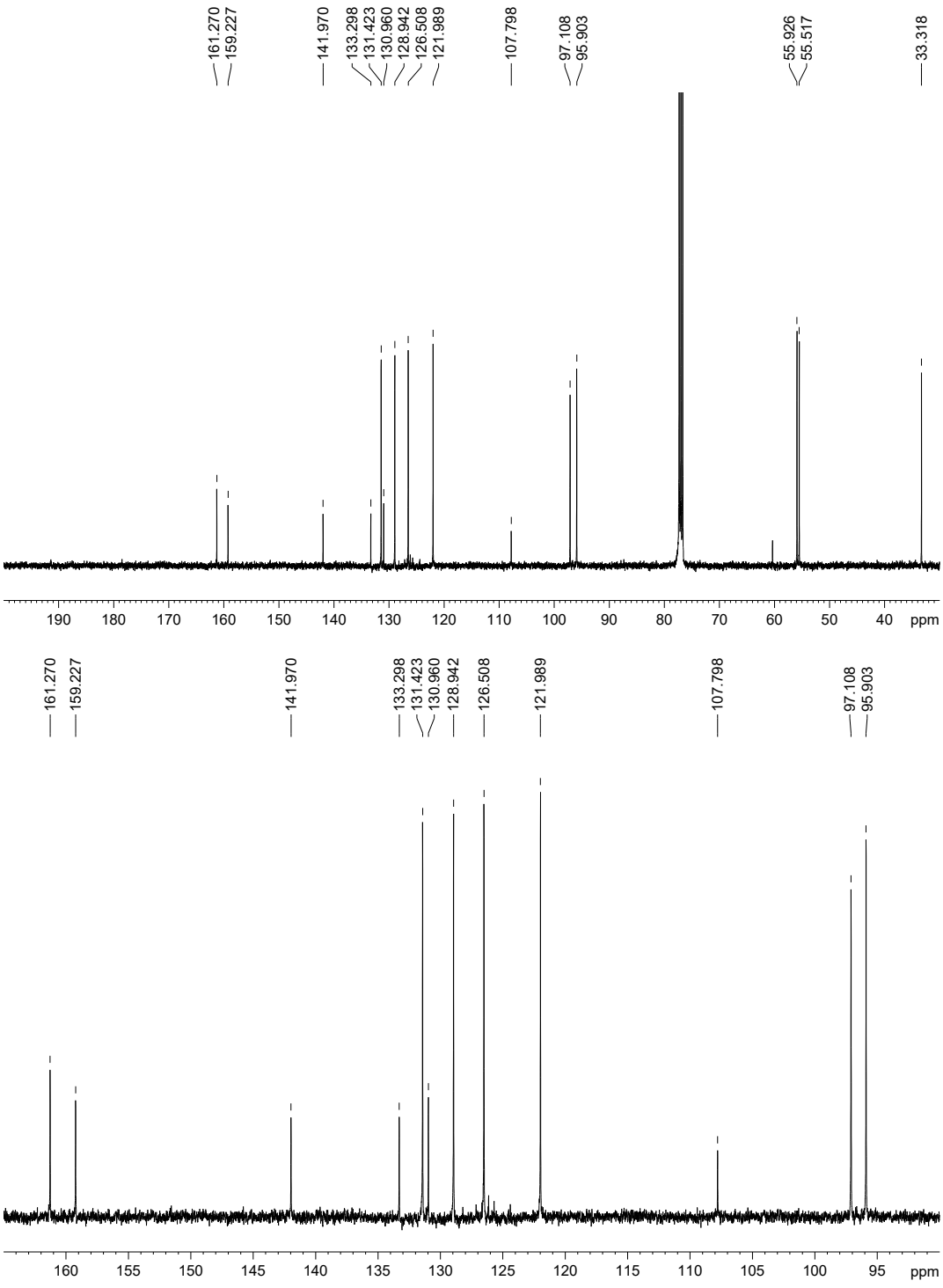
^{13}C-RMN ($CDCl_3$) 6-Metil-6*H*-dibenzo[*c,e*][1,2]tiacina 5,5-dióxido (27a)



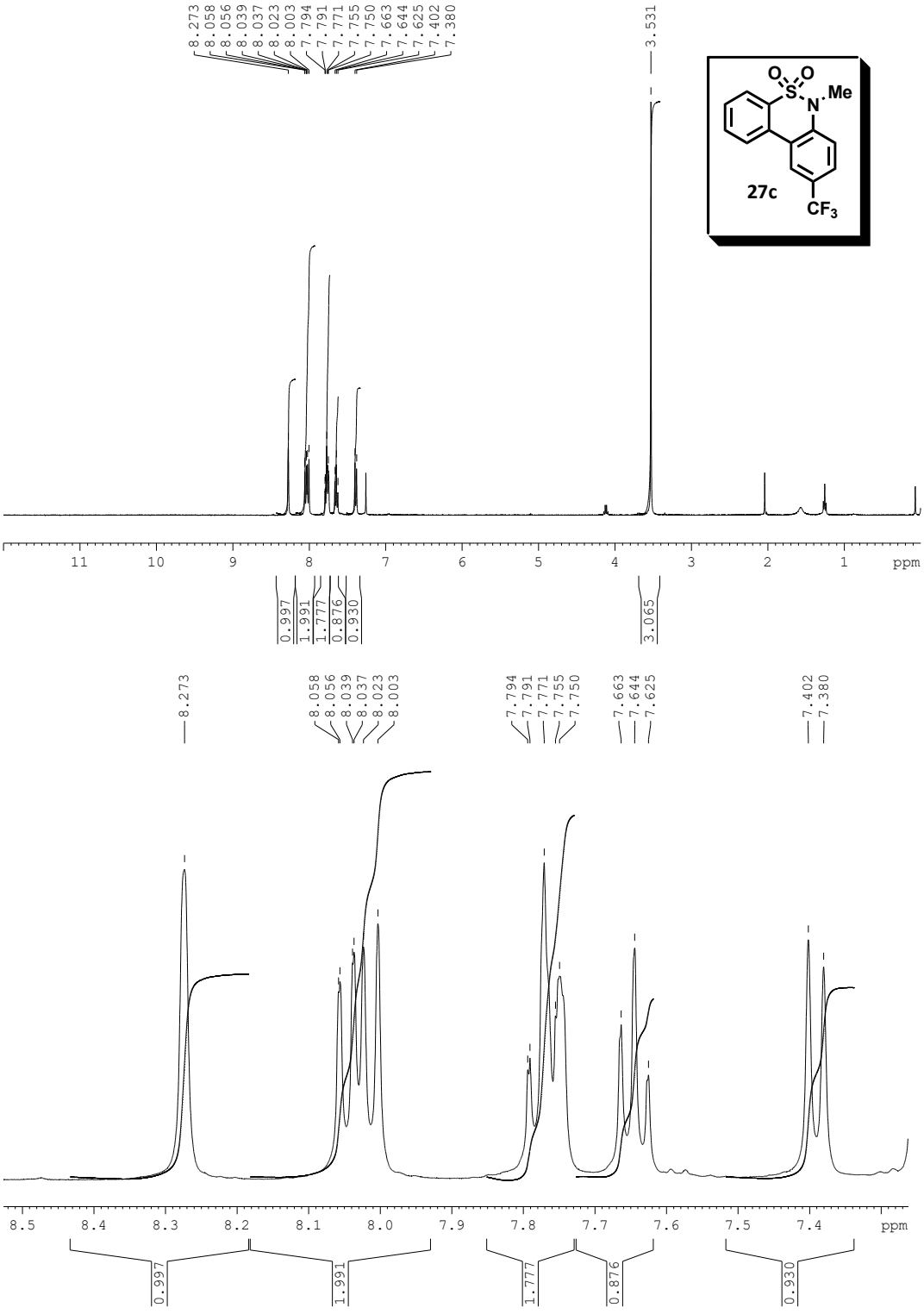
^{1}H-RMN ($CDCl_3$) 6-Metil-8,10-*di*-metoxi-6*H*-Dibenzo[*c*,*e*][1,2]tiacina 5,5-dioxido (27b)



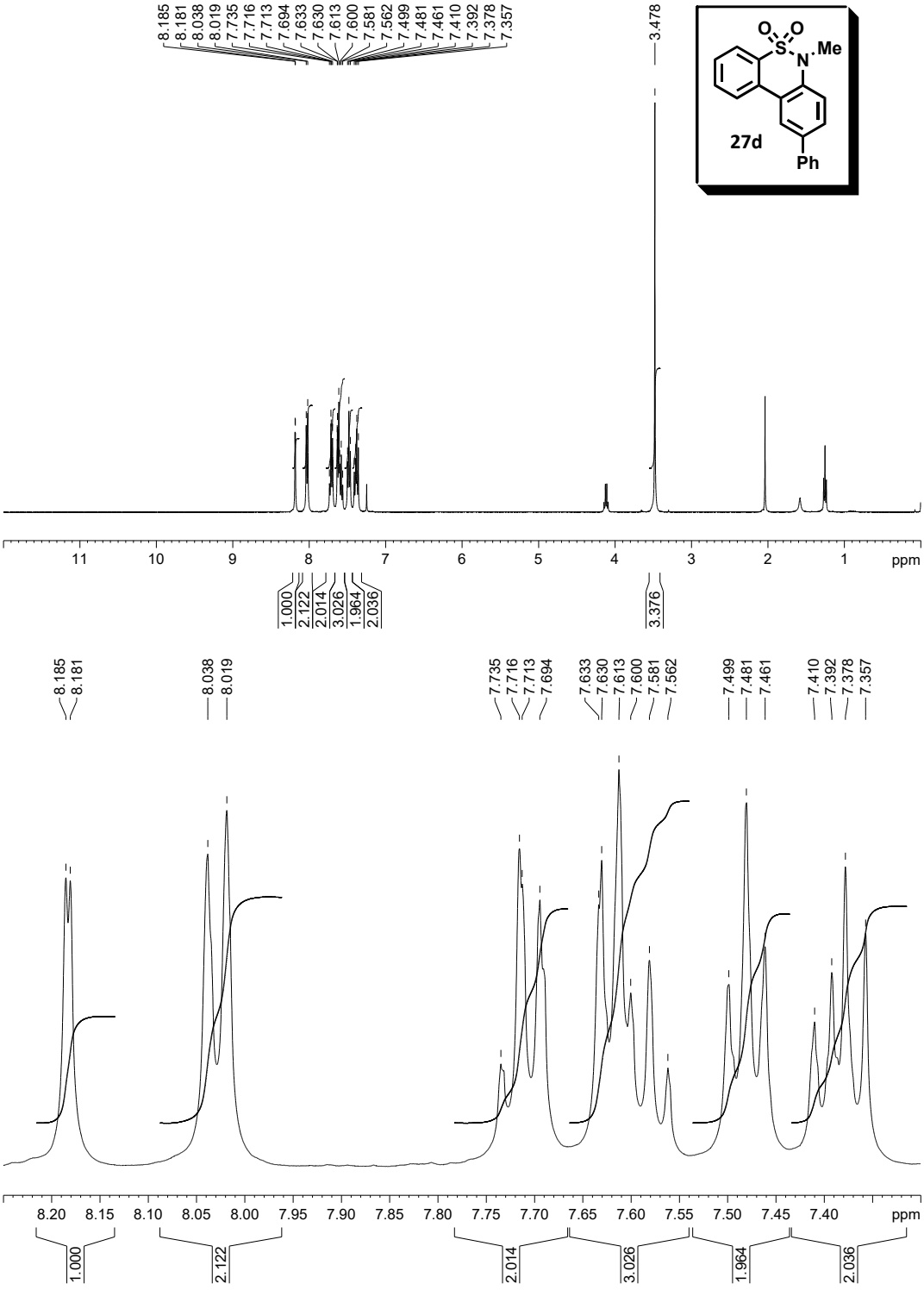
^{13}C-RMN ($CDCl_3$) 6-Metil-8,10-*di*-metoxi-6*H*-Dibenzo[*c*,*e*][1,2]tiacina 5,5-dioxido (27b)



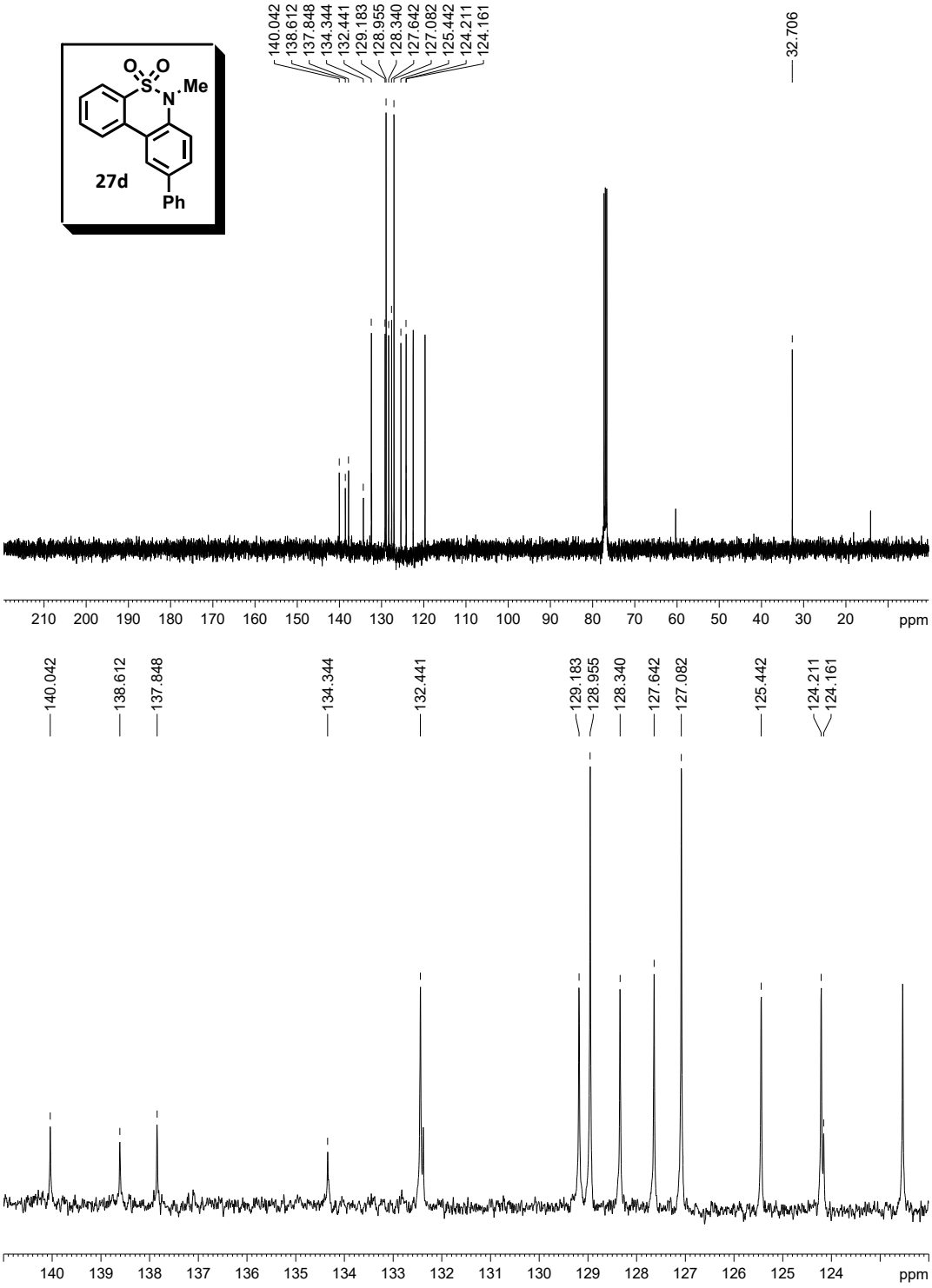
^{1}H-RMN ($CDCl_3$) 6-Metil-9-trifluormetil-6*H*-Dibenzo[*c*,*e*][1,2]tiacina 5,5-dioxido (27c)



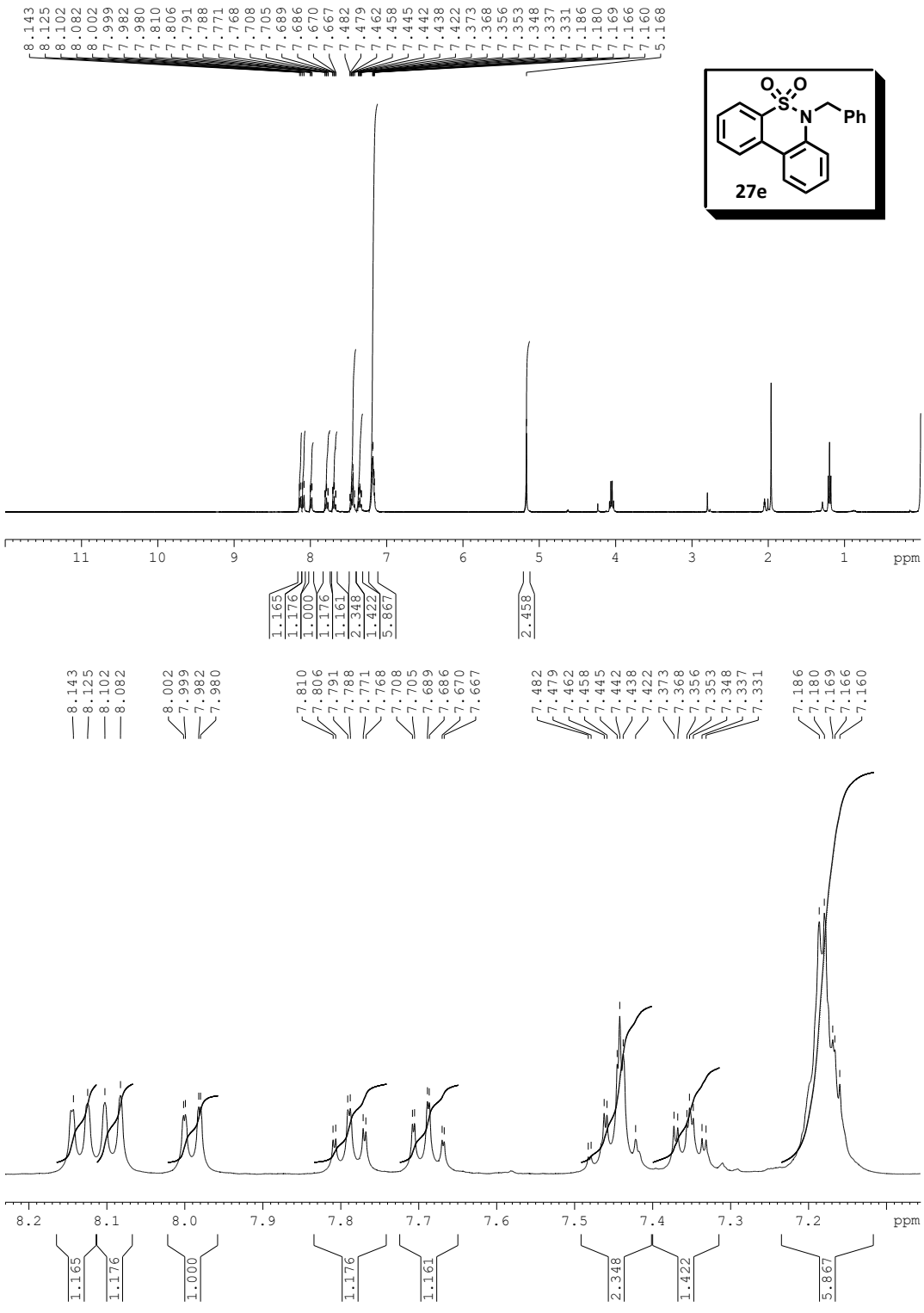
^{1}H-RMN ($CDCl_3$) 9-Fenil-6-Metil-6*H*-Dibenzo[*c*,*e*][1,2]tiacina 5,5-dioxido (27d)



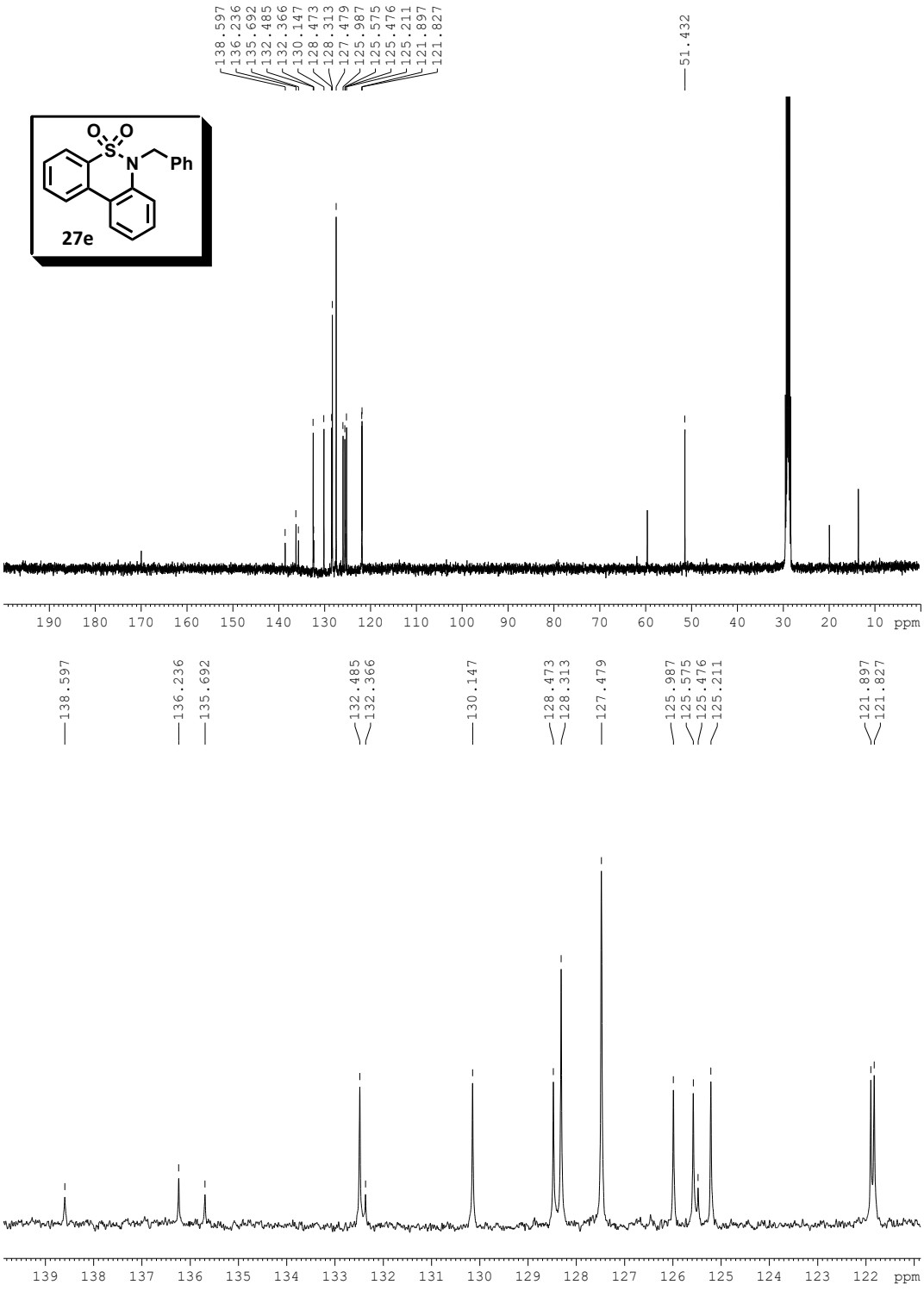
^{13}C-RMN ($CDCl_3$) 9-Fenil-6-Metil-6*H*-Dibenzo[*c*,*e*][1,2]tiacina 5,5-dioxido (27d)



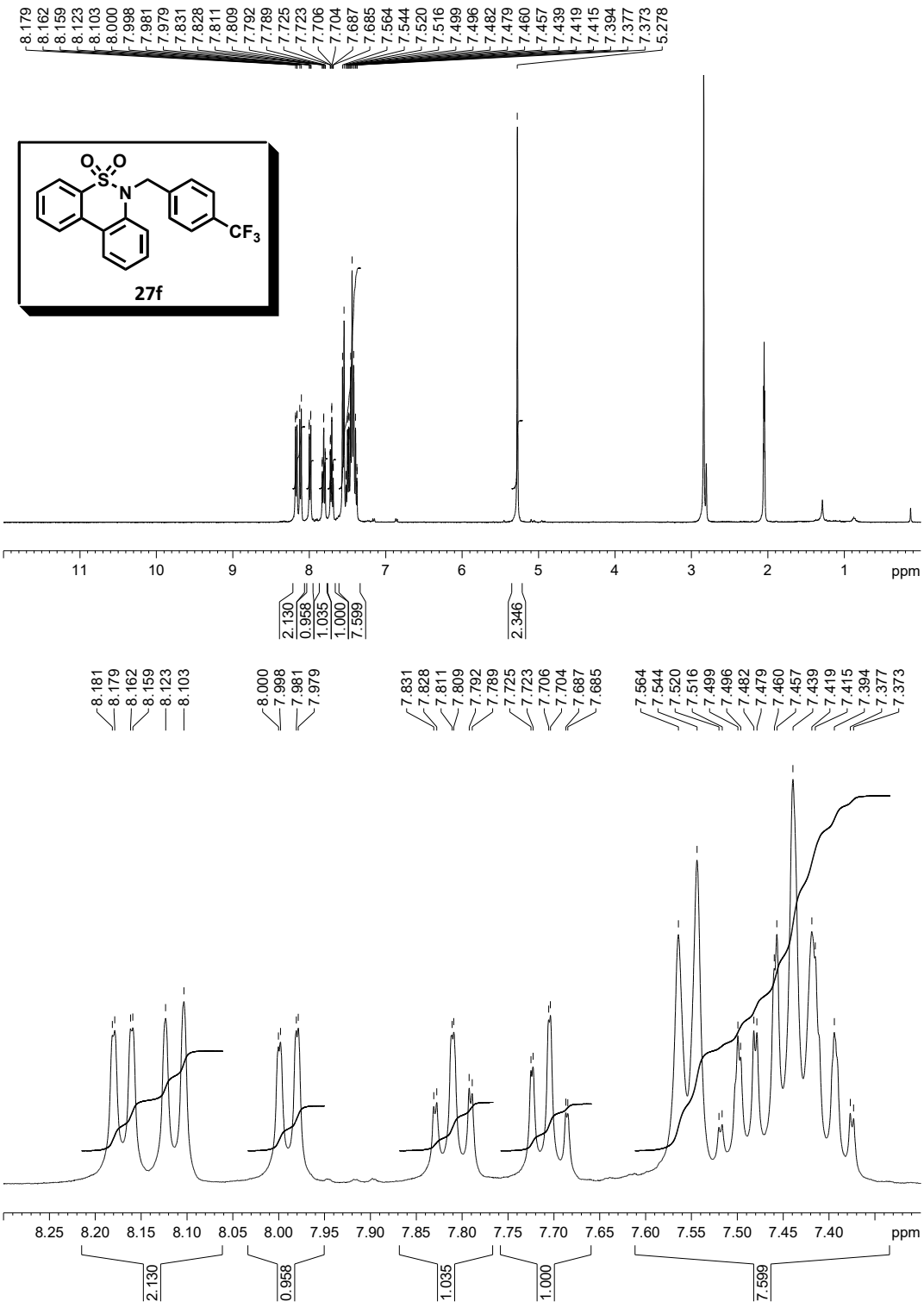
^{1}H-RMN (CD_3COCD_3) 6-Bencil-6*H*-dibenzo[*c,e*][1,2]tiacina 5,5-dióxido (27e)



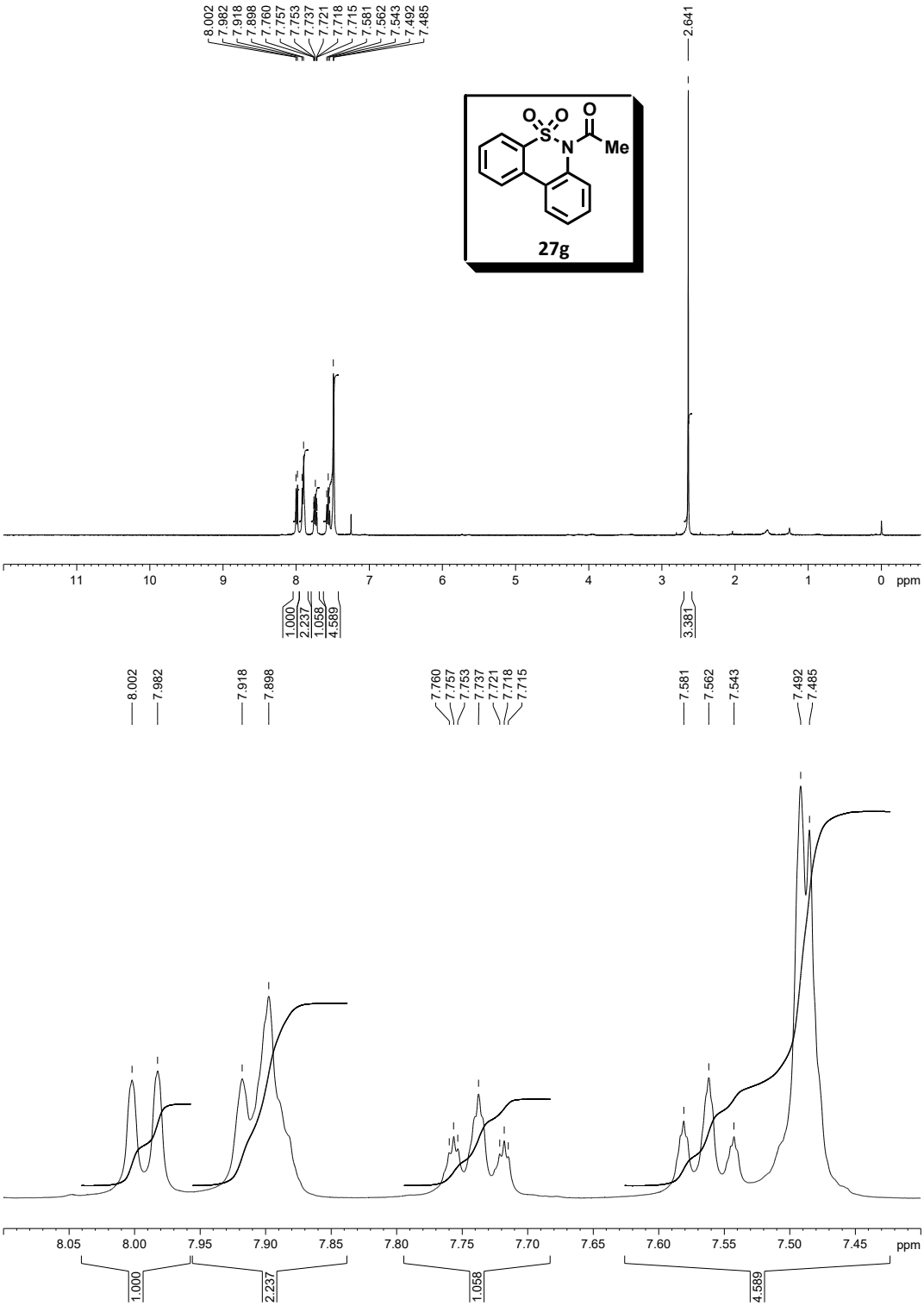
^{13}C-RMN (CD_3COCD_3) 6-Bencil-6*H*-dibenzo[*c,e*][1,2]tiacina 5,5-dióxido (27e)



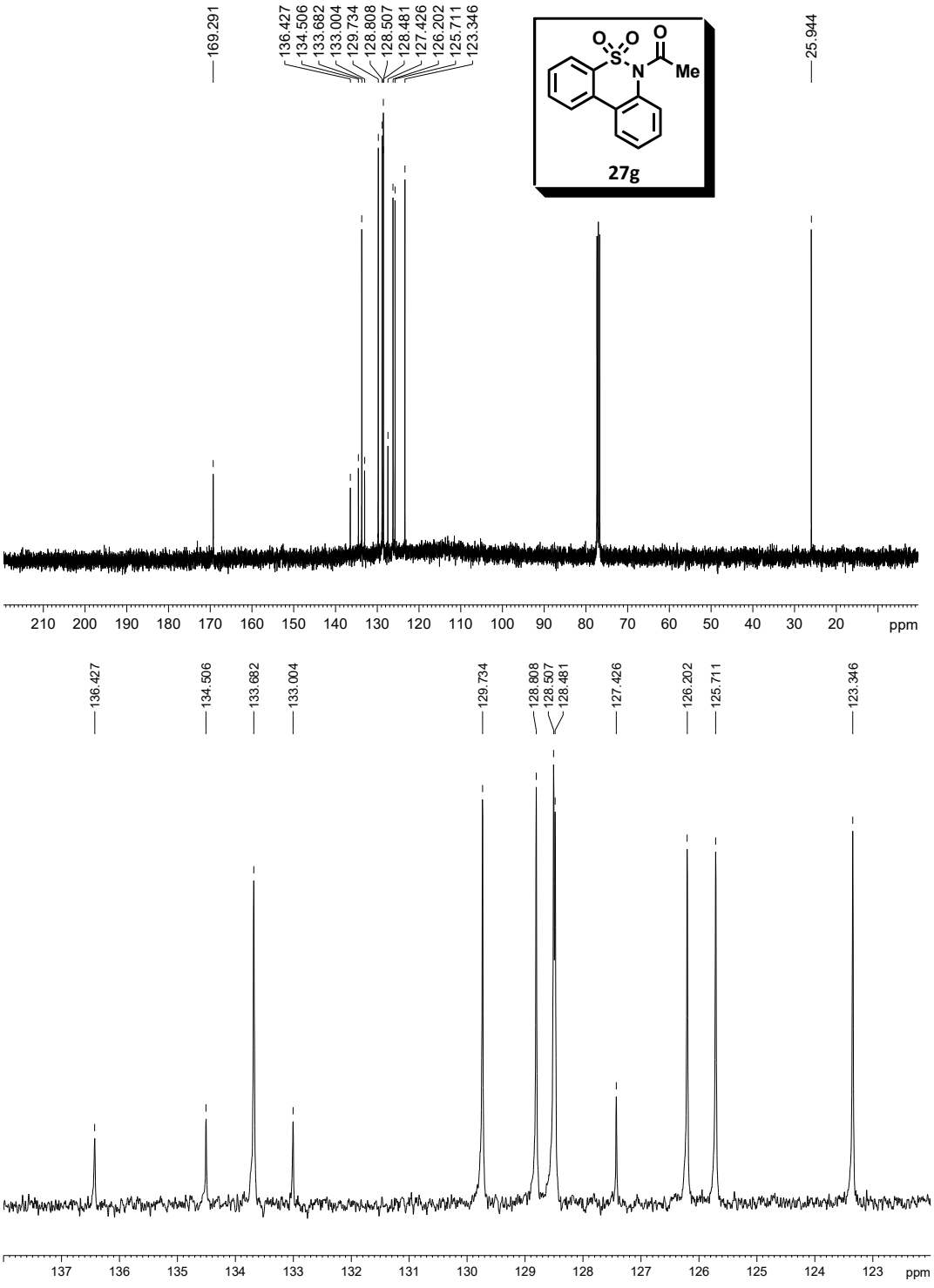
^{1}H-RMN (CD_3COCD_3) 6-(4-Trifluormetil-bencil)-6*H*-dibenzo[*c,e*][1,2]tiacina 5,5-dióxido (27f)



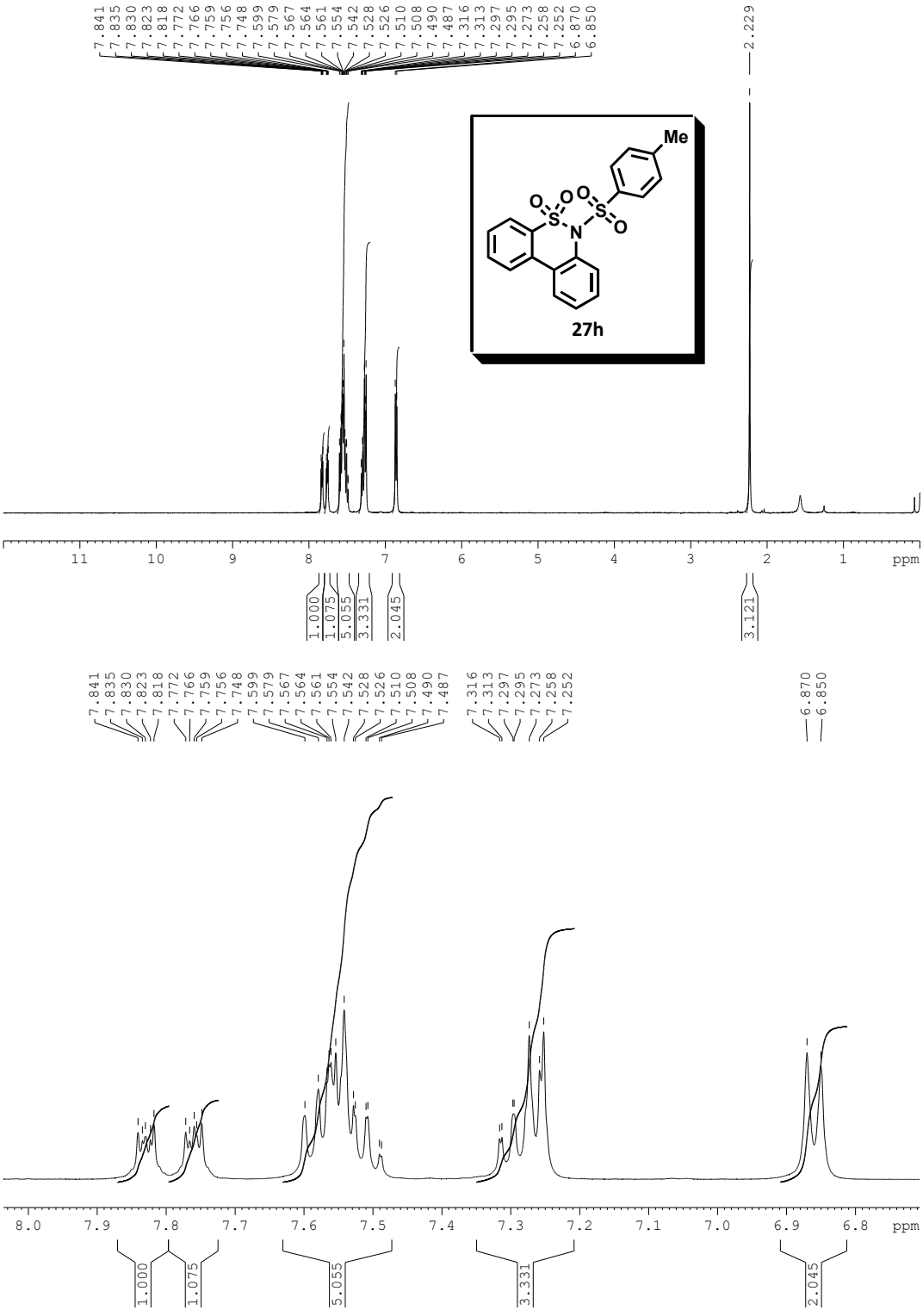
^{1}H-RMN ($CDCl_3$) 6-Acetil-6*H*-dibenzo[*c*,*e*][1,2]tiacina 5,5-dióxido (27g)



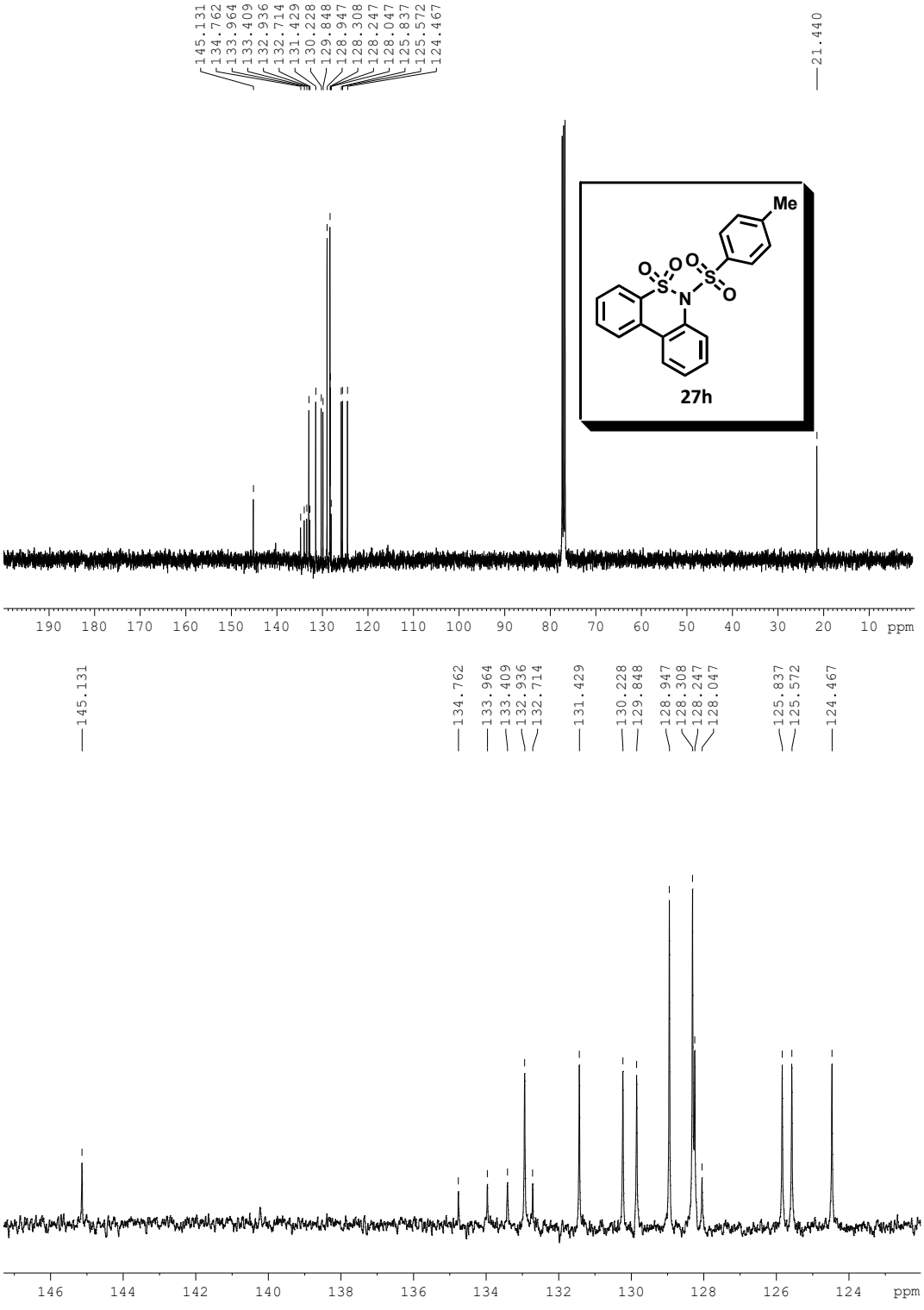
^{13}C-RMN ($CDCl_3$) 6-Acetil-6*H*-dibenzo[*c*,*e*][1,2]tiacina 5,5-dióxido (27g)



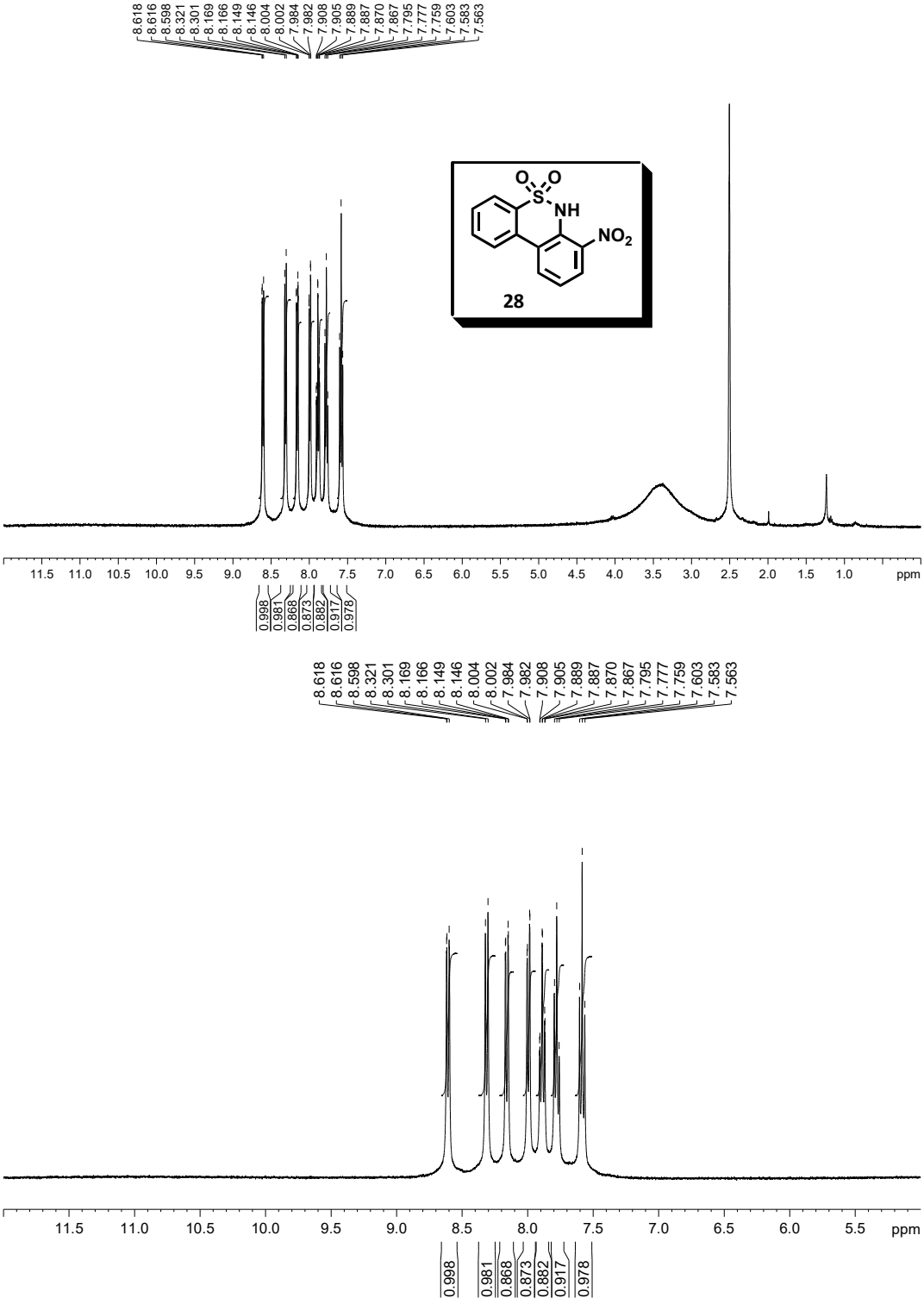
^{1}H-RMN ($CDCl_3$) 6-Tosil-6*H*-dibenzo[*c,e*][1,2]tiacina 5,5-dióxido (27h)

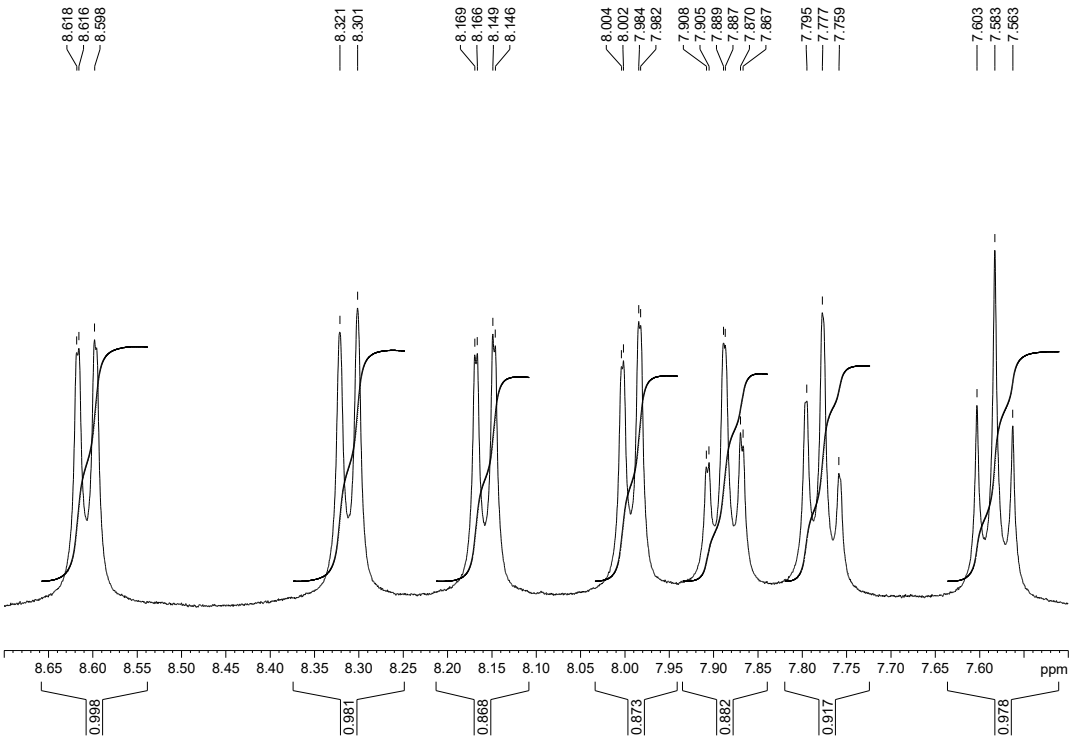


^{13}C-RMN ($CDCl_3$) 6-Tosil-6*H*-dibenzo[*c,e*][1,2]tiacina 5,5-dióxido (27h)

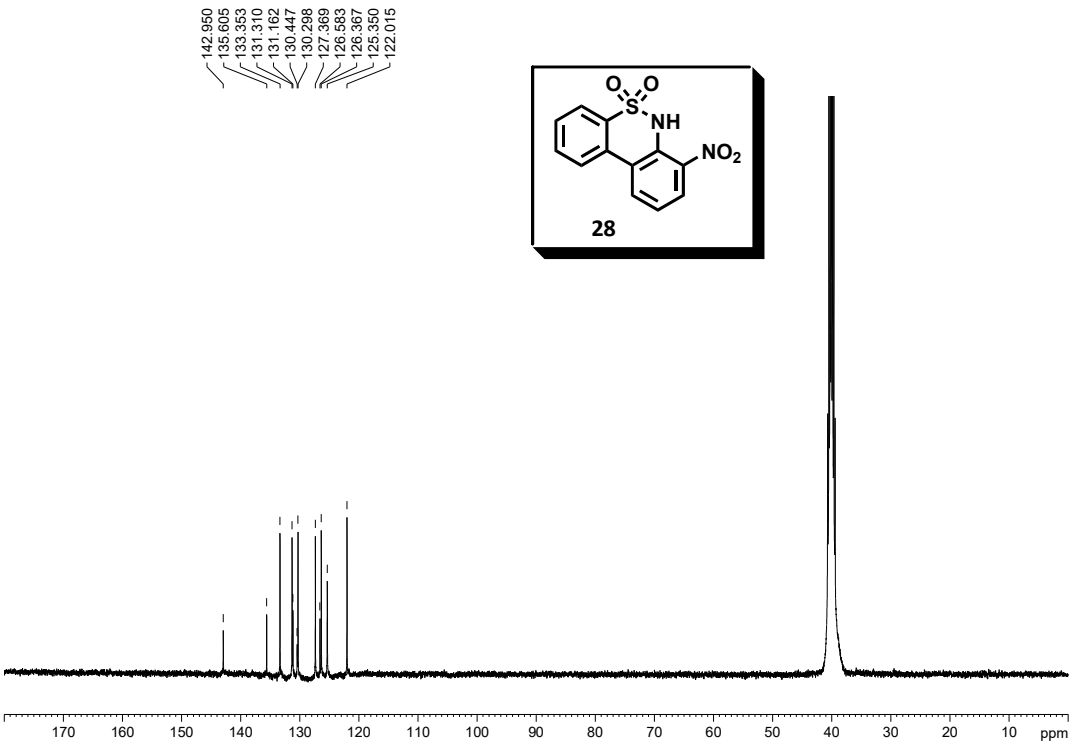


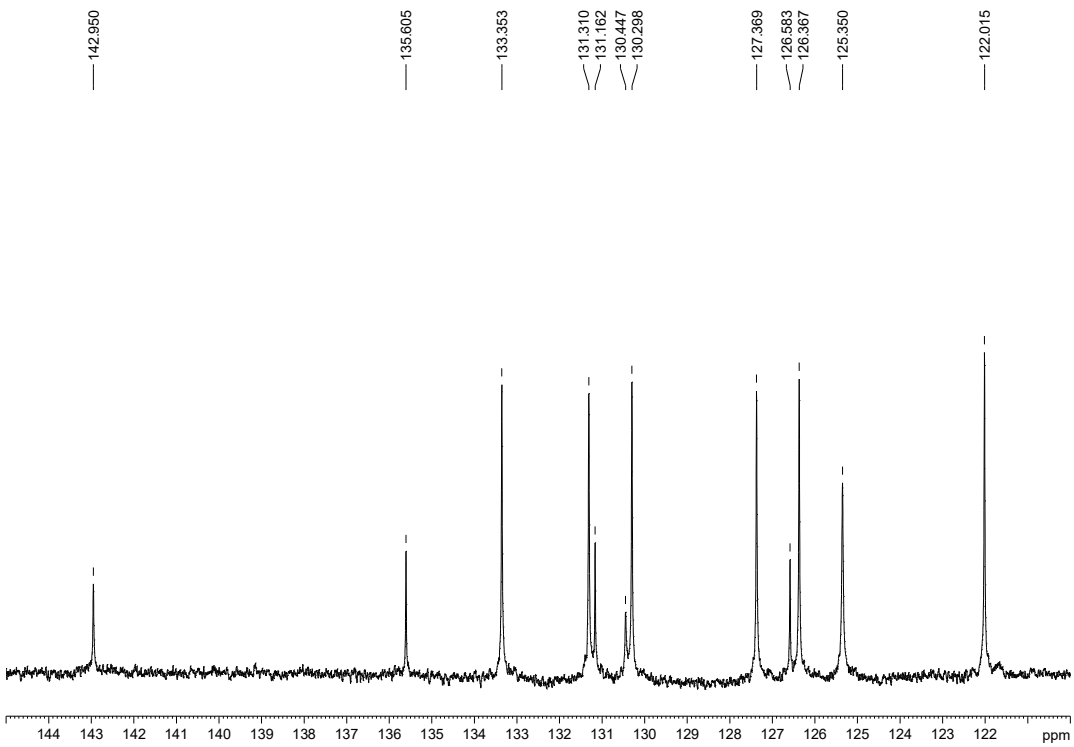
^{1}H-RMN (CD_3SOCD_3) 7-Nitro-6*H*-dibenzo[*c*,*e*][1,2]tiacina 5,5-dioxido (28)



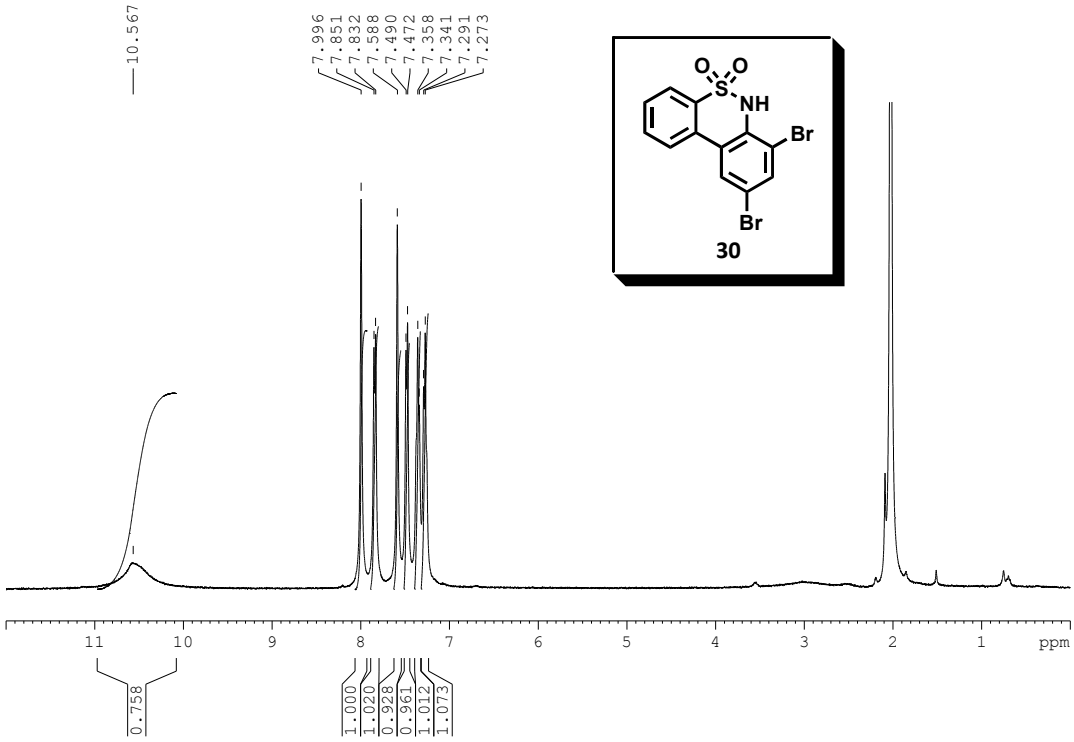


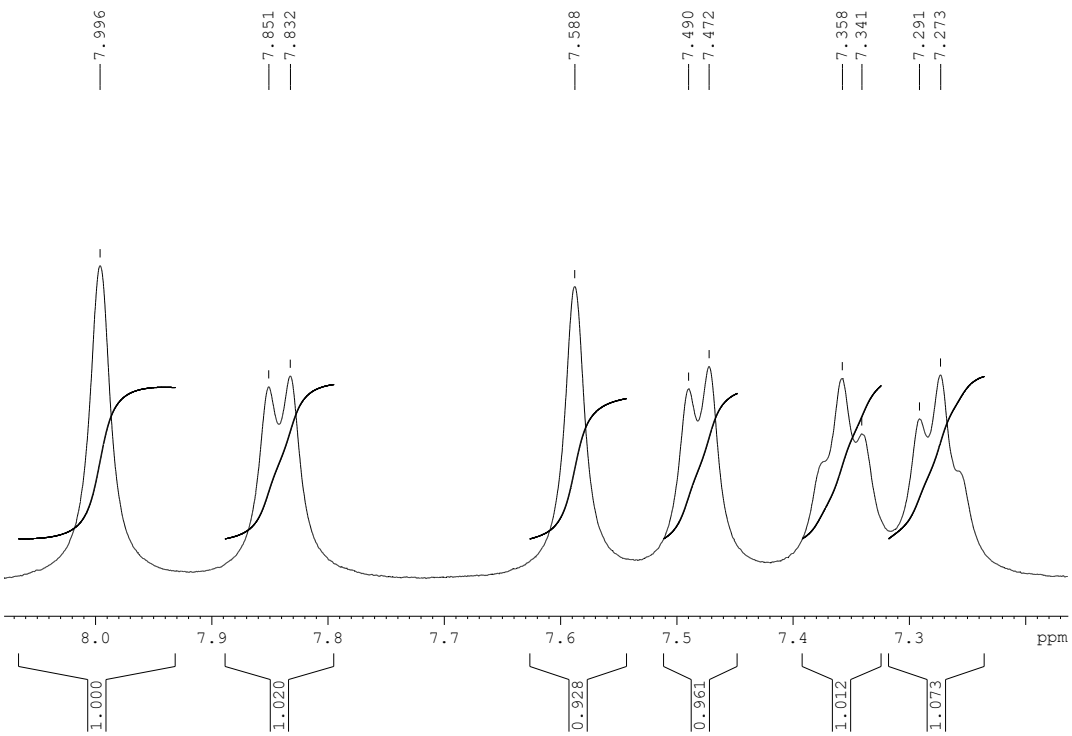
^{13}C-RMN (CD_3SOCD_3) 7-Nitro-6*H*-dibenzo[*c*,*e*][1,2]tiacina 5,5-dioxido (28)

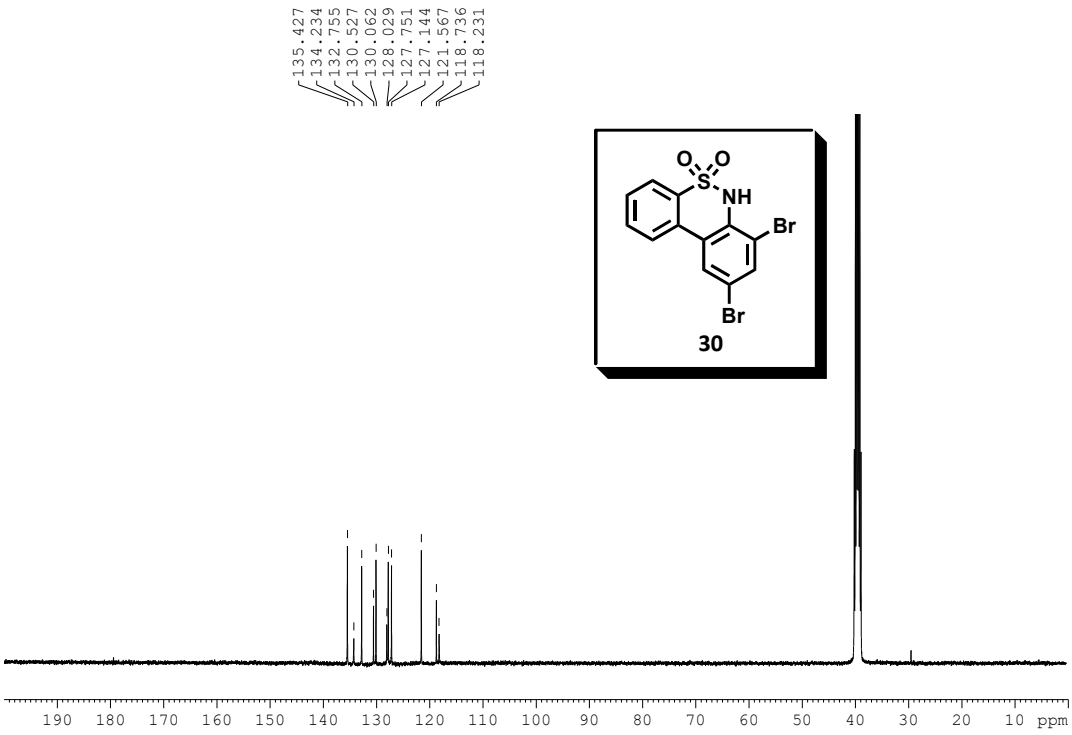


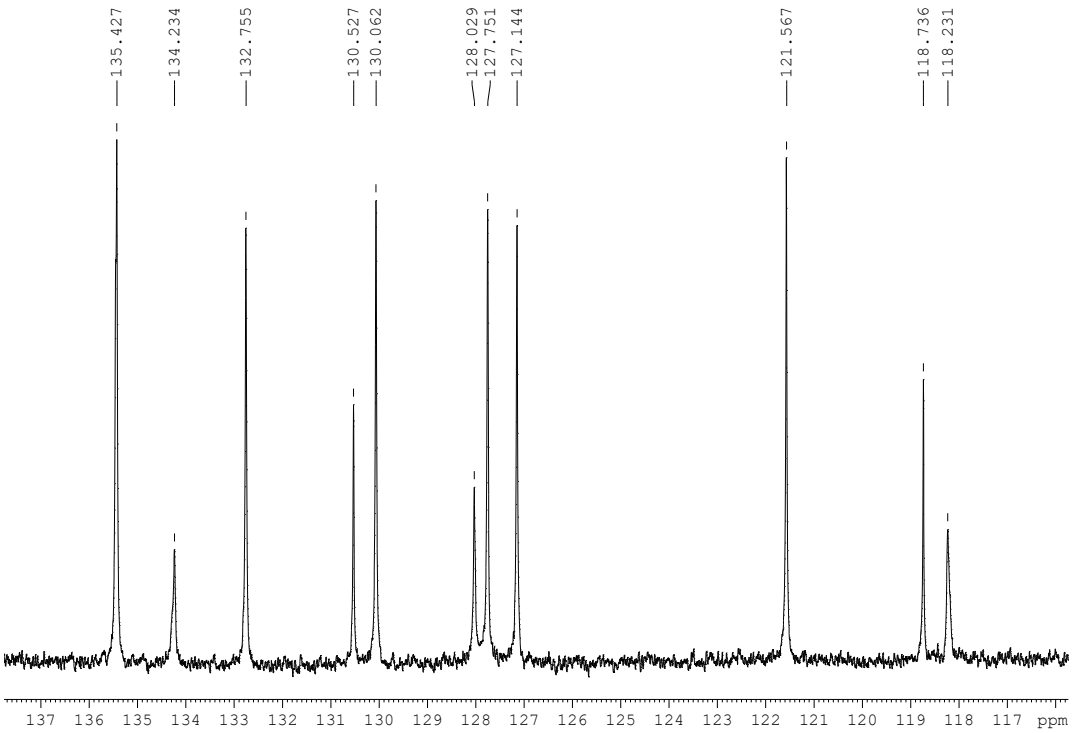


^{1}H-RMN (CD_3SOCD_3) 7,9-Dibromo-6*H*-dibenzo[*c*,*e*][1,2]tiacina 5,5-dioxido (30)




7.996
7.851
7.832
7.588
7.490
7.472
7.358
7.341
7.291
7.273
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
ppm
1.000
1.020
0.928
0.961
1.012
1.073

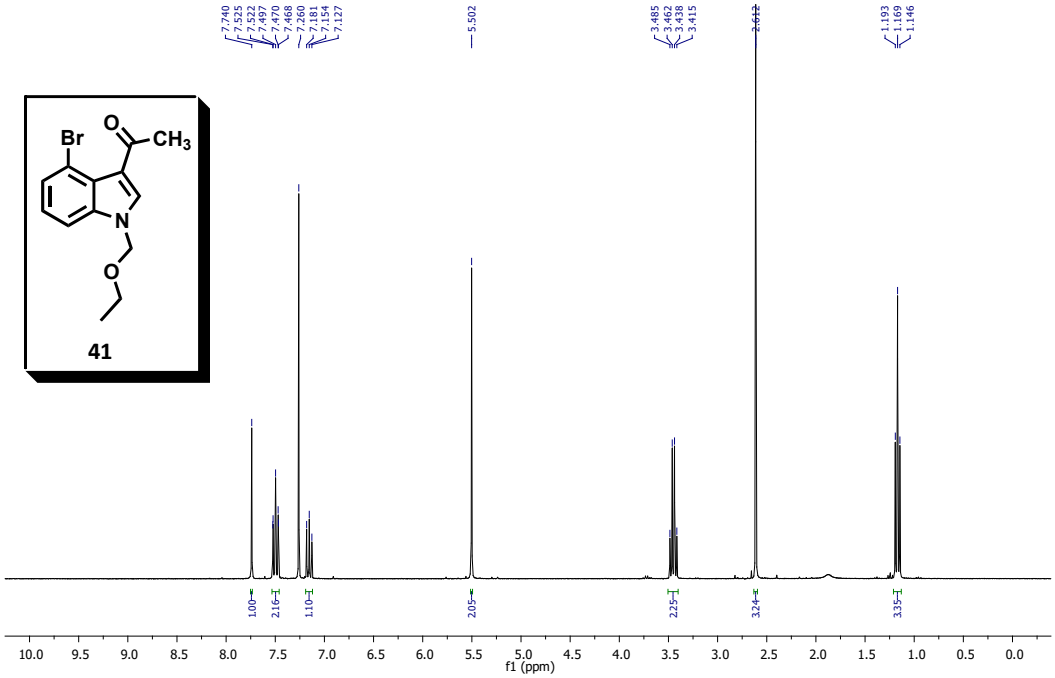

135.427
134.234
132.755
130.527
130.062
128.029
127.751
127.144
121.567
118.736
118.231
O
O
S
NH
Br
Br
30
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm



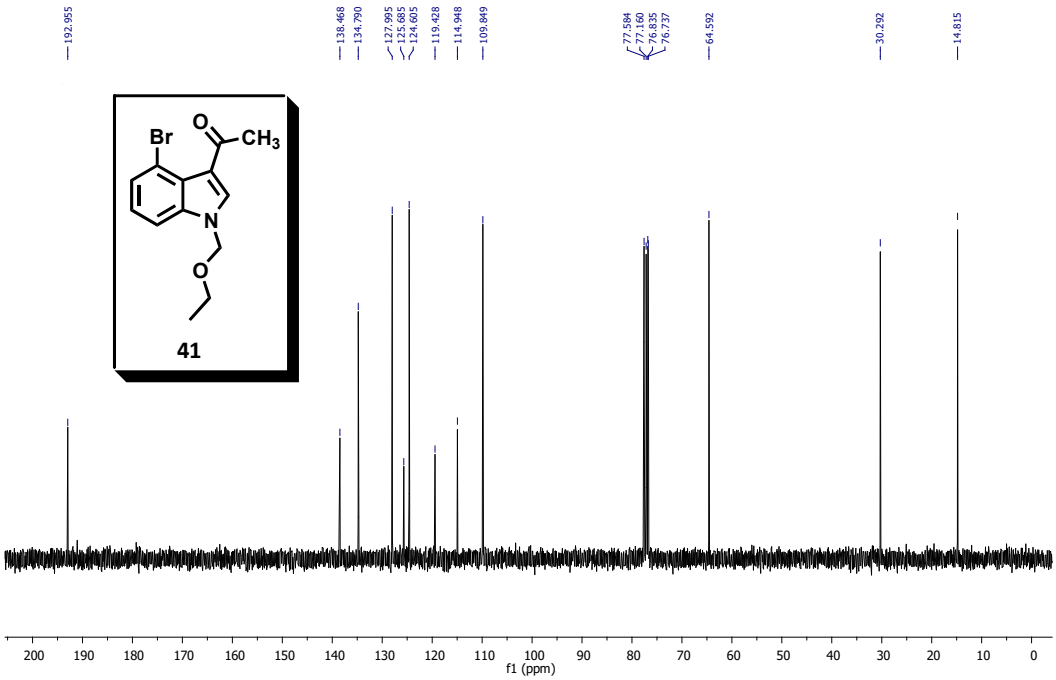
A.5 CAPÍTULO VI

A.5.1 ESPECTROS DE RMN DE INDOL Y AZAINDOL ACETILADOS Y PROTEGIDOS

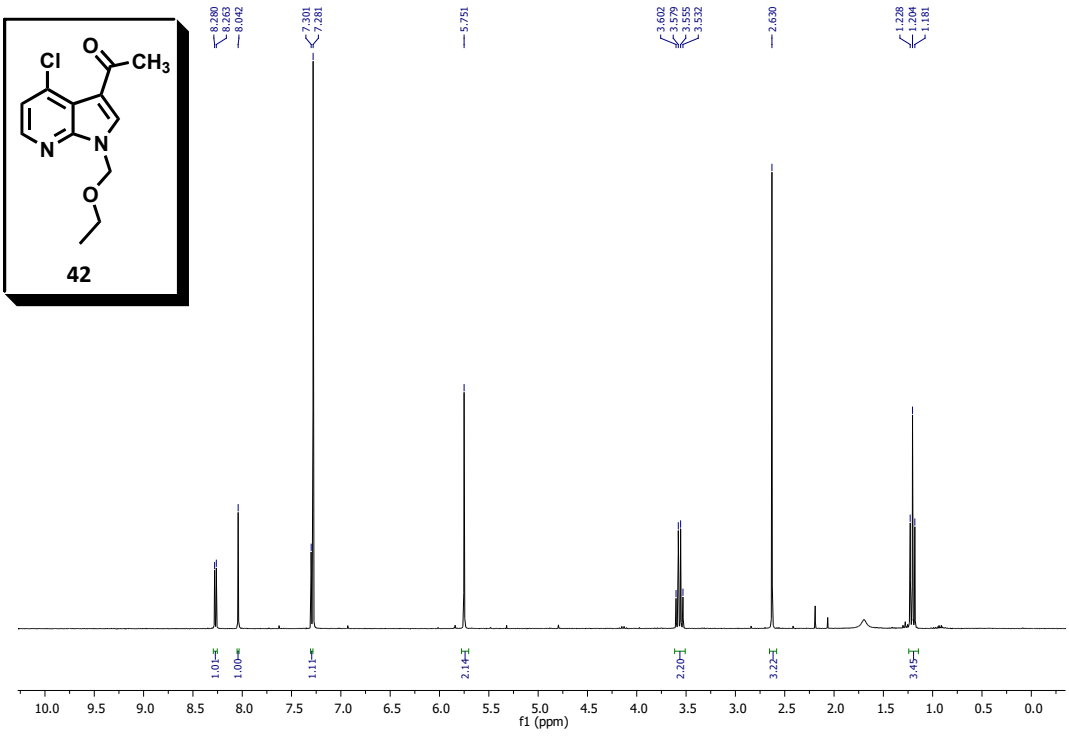
^{1}H-RMN ($CDCl_3$) 3-Acetil-4-bromo-1-etoximetil-indol (41)



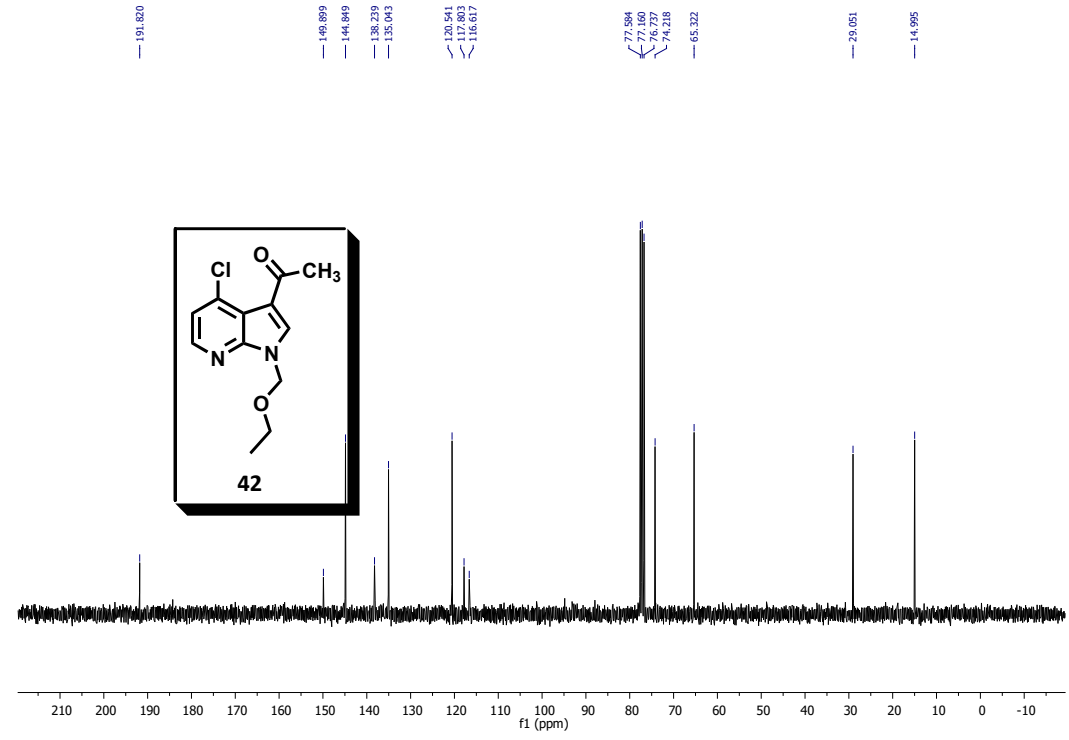
^{13}C-RMN ($CDCl_3$) 3-Acetil-4-bromo-1-etoximetil-indol (41)



^{1}H-RMN ($CDCl_3$) 3-Acetil-4-cloro-1-etoximetil-7-azaindol (42)

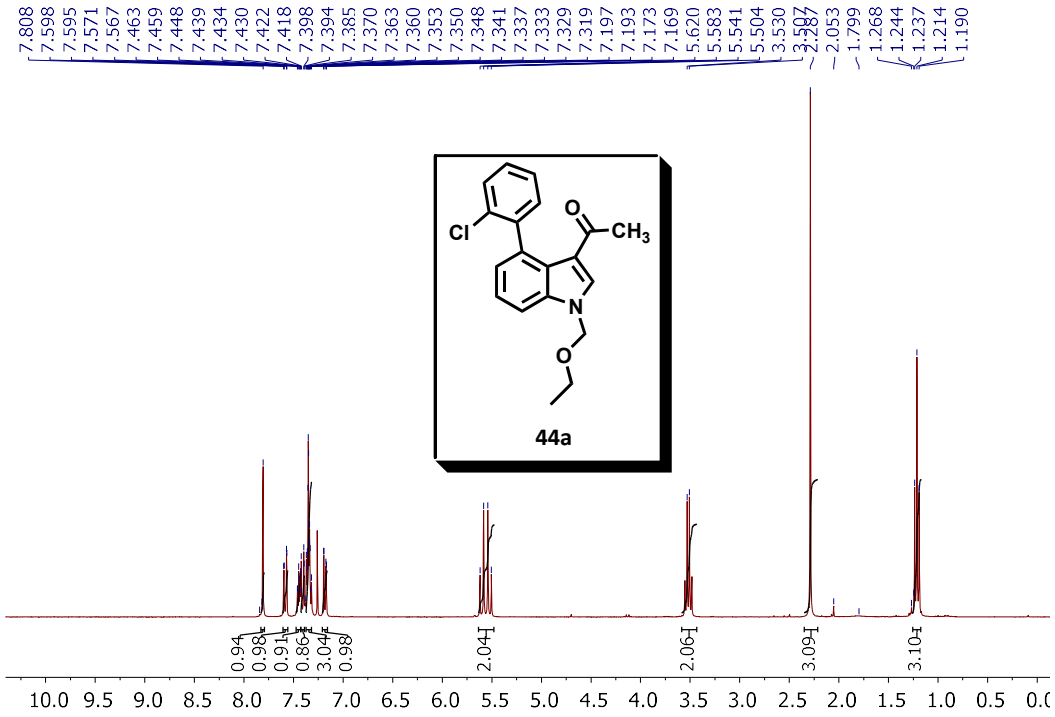


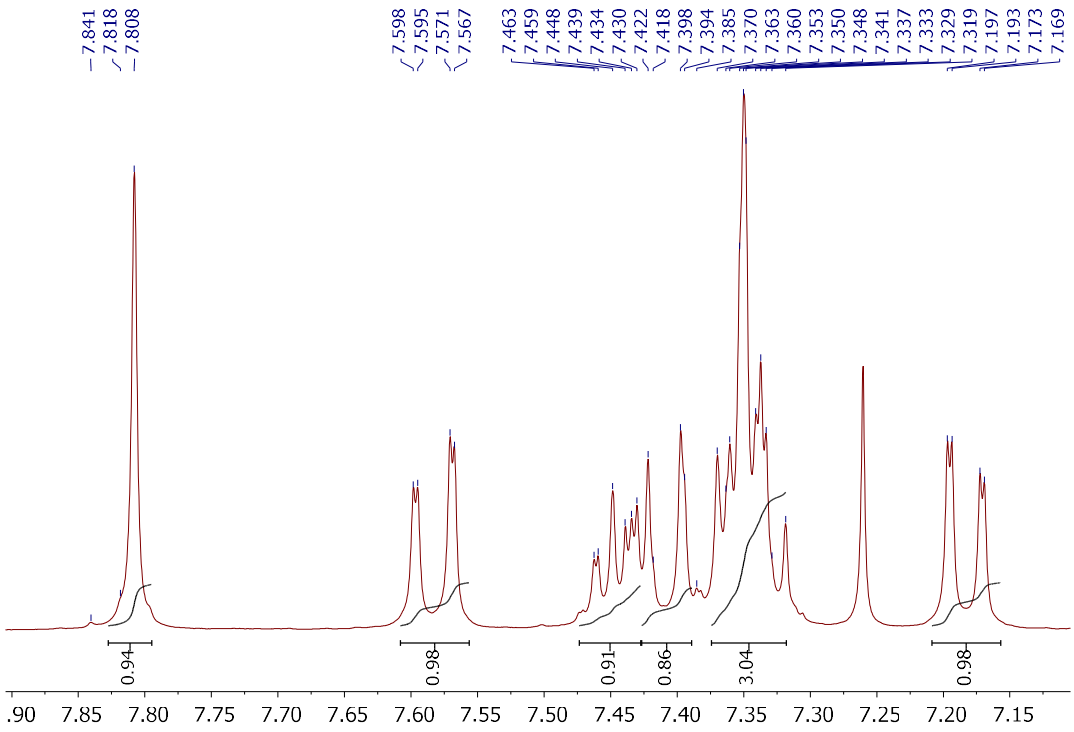
^{13}C-RMN ($CDCl_3$) 3-Acetil-4-bromo-1-etoximetil-indol (41)

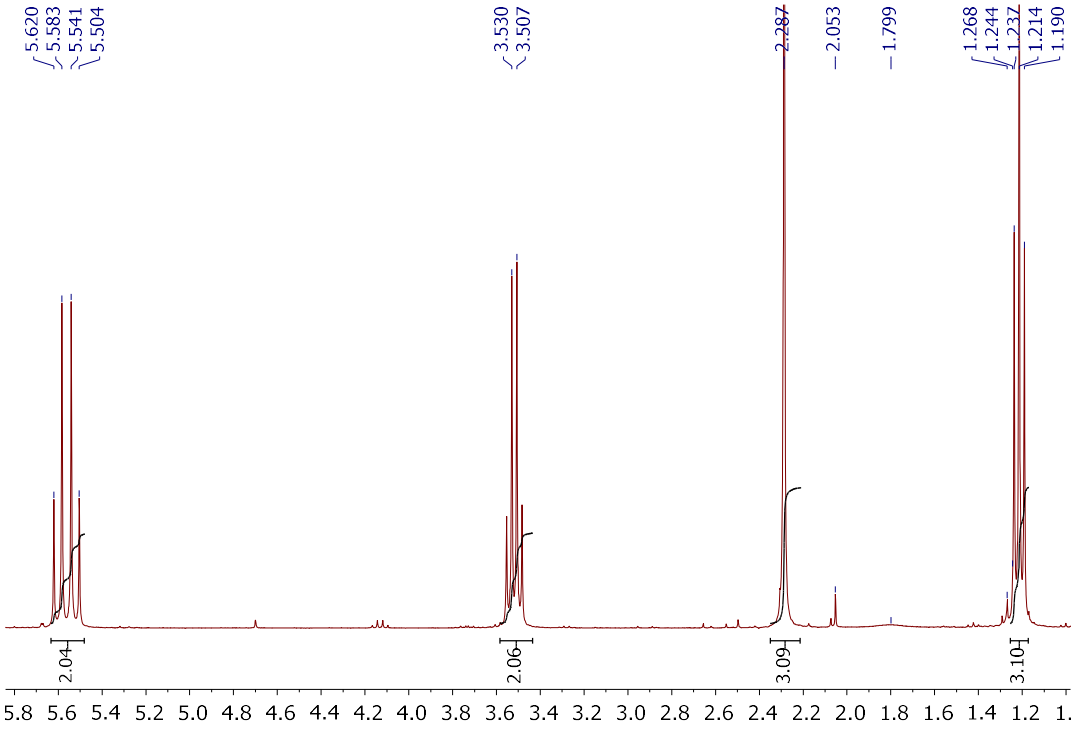


A.5.2 ESPECTROS DE RMN DE PRECURSORES DE CIERRE DE ANILLO

^{1}H-RMN ($CDCl_3$) 3-Acetil-4-(2-Clorofenil)-1-etoximetil-indol (44a)



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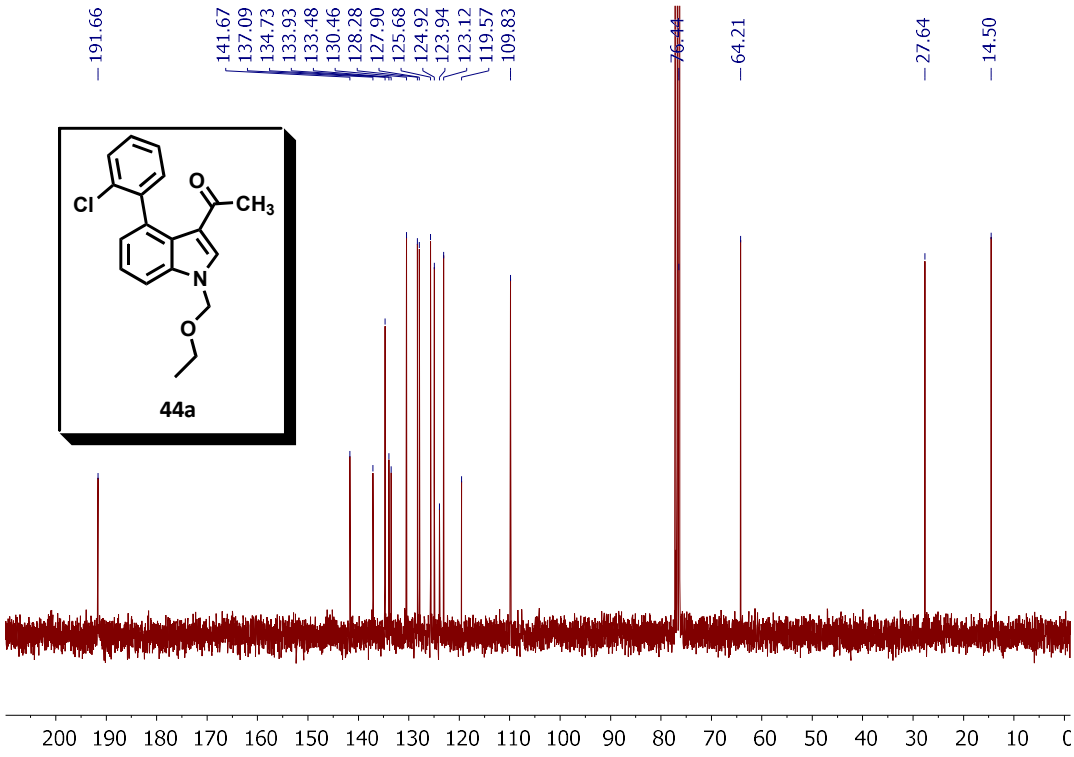
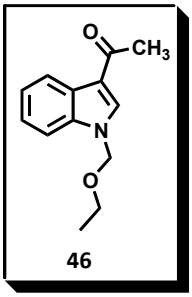
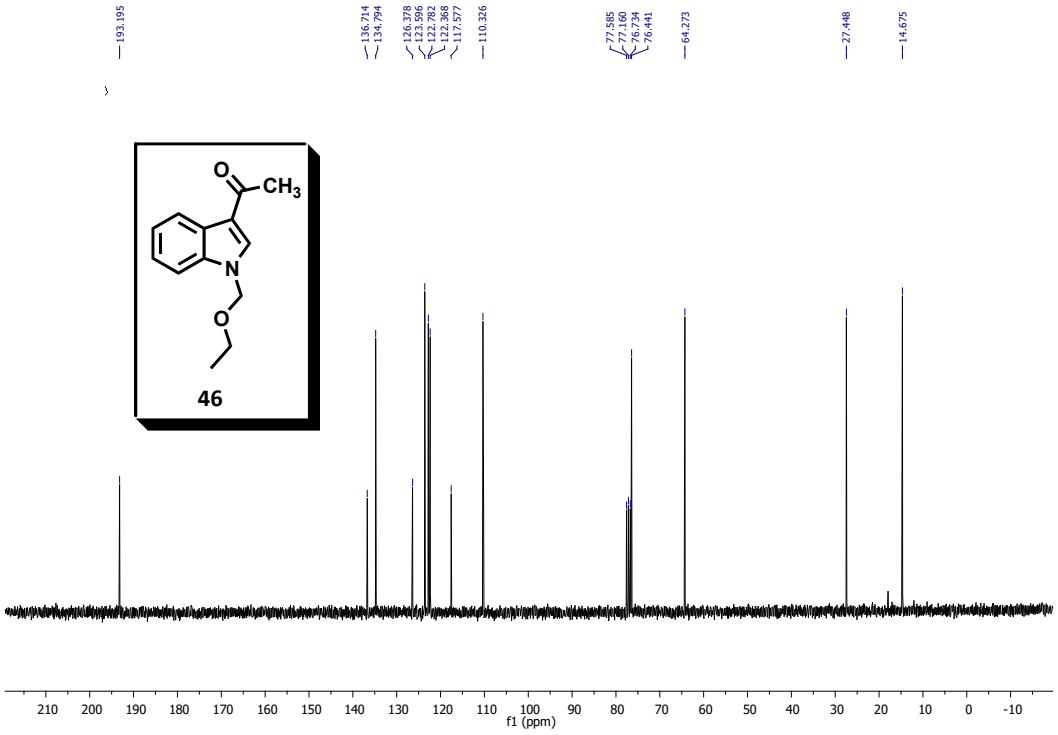
5.541
5.504
3.530
3.507
2.287
2.053
1.799
1.268
1.244
1.232
1.214
1.190
2.04
2.06
3.09
3.10
5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.


191.66
141.67
137.09
134.73
133.93
133.48
130.46
128.28
127.90
125.68
124.92
123.94
123.12
119.57
109.83
76.44
64.21
27.64
14.50
Cl
O
CH3
N
O
44a
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

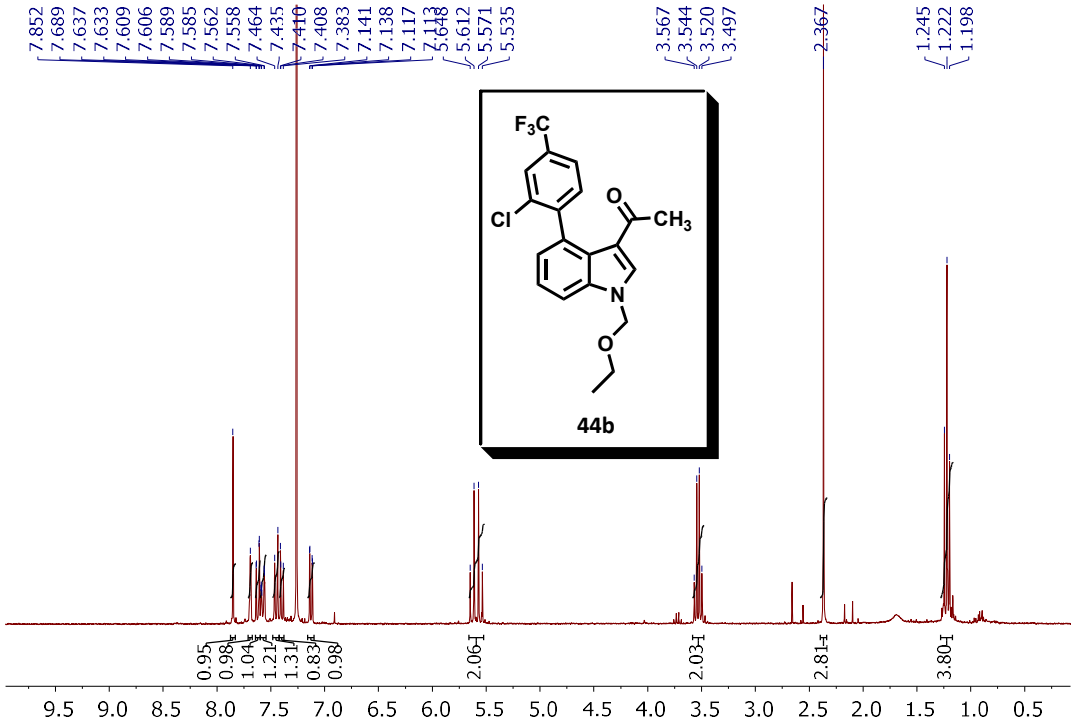
^{1}H-RMN ($CDCl_3$) 3-Acetil-1-etoximetil-indol (46)

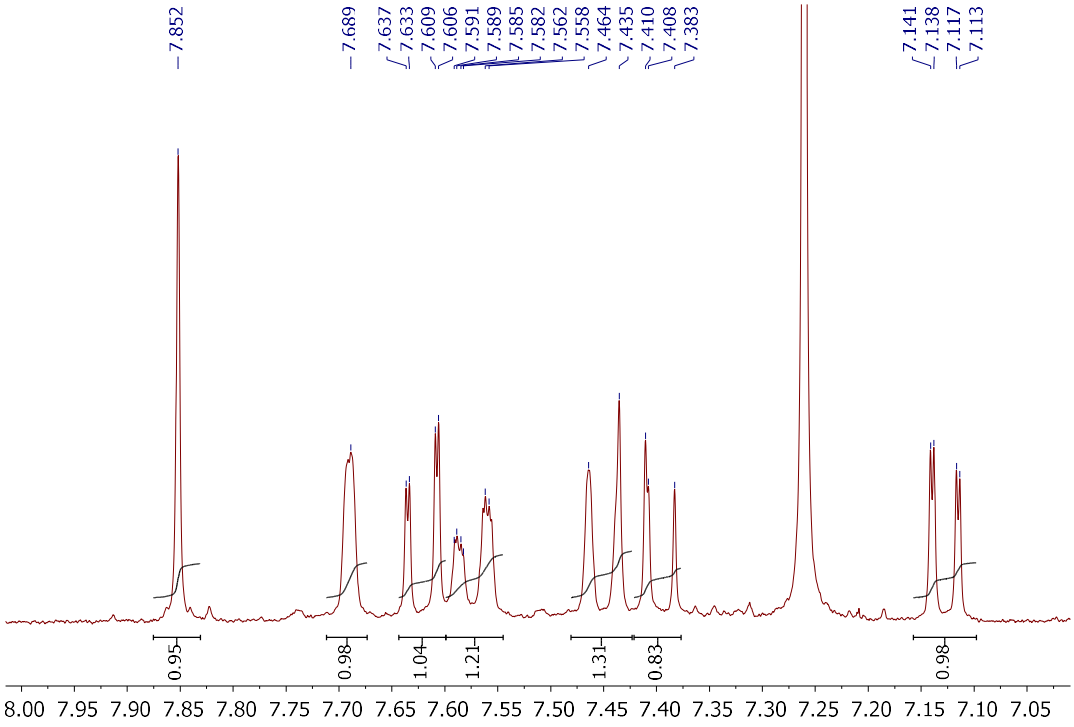


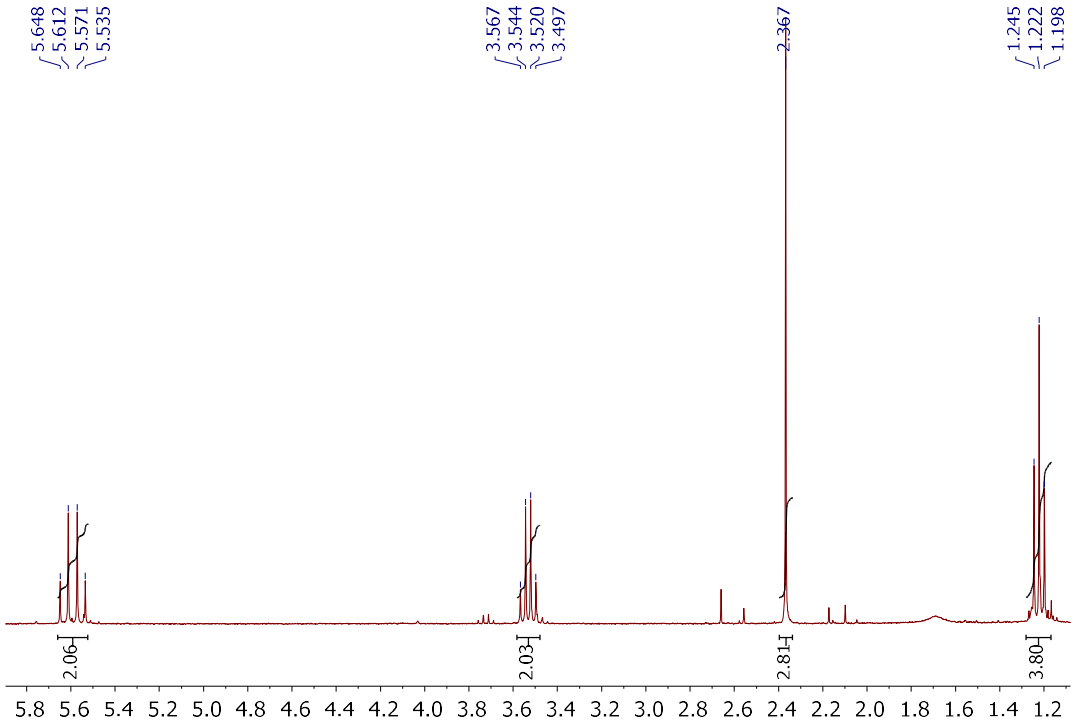
^{13}C-RMN ($CDCl_3$) 3-Acetil-1-etoximetil-indol (46)



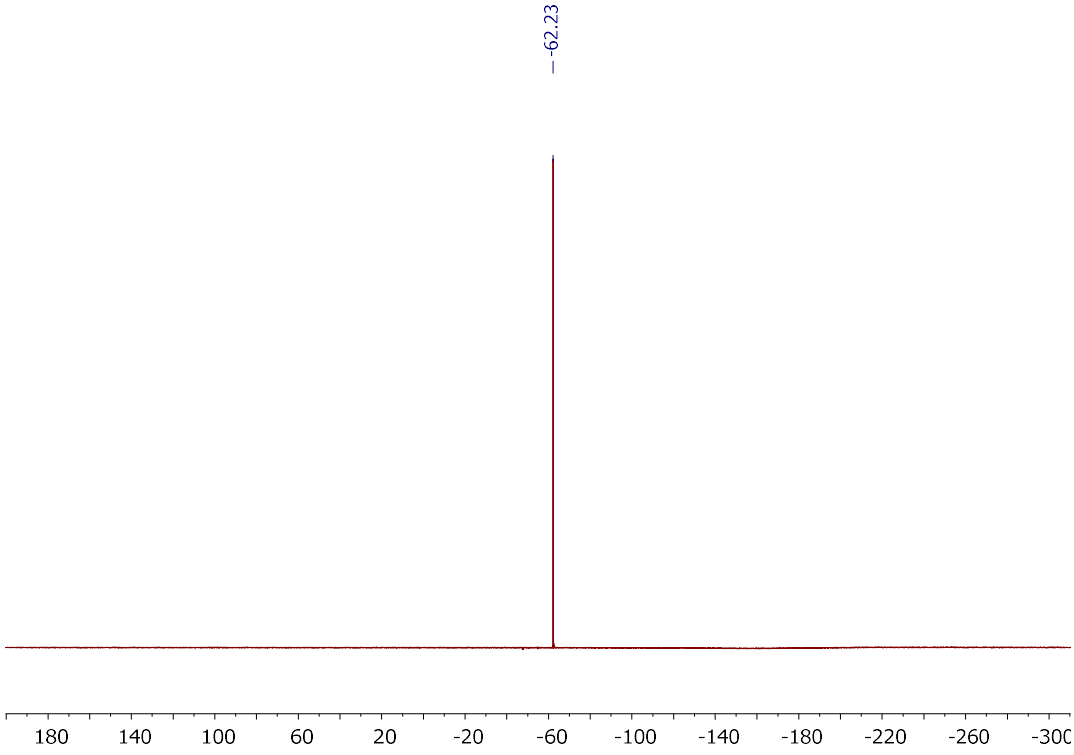
^{1}H-RMN ($CDCl_3$) 3-Acetil-4-(2-cloro-4-trifluormetil-fenil)-1-etoximetil-indol (44b)



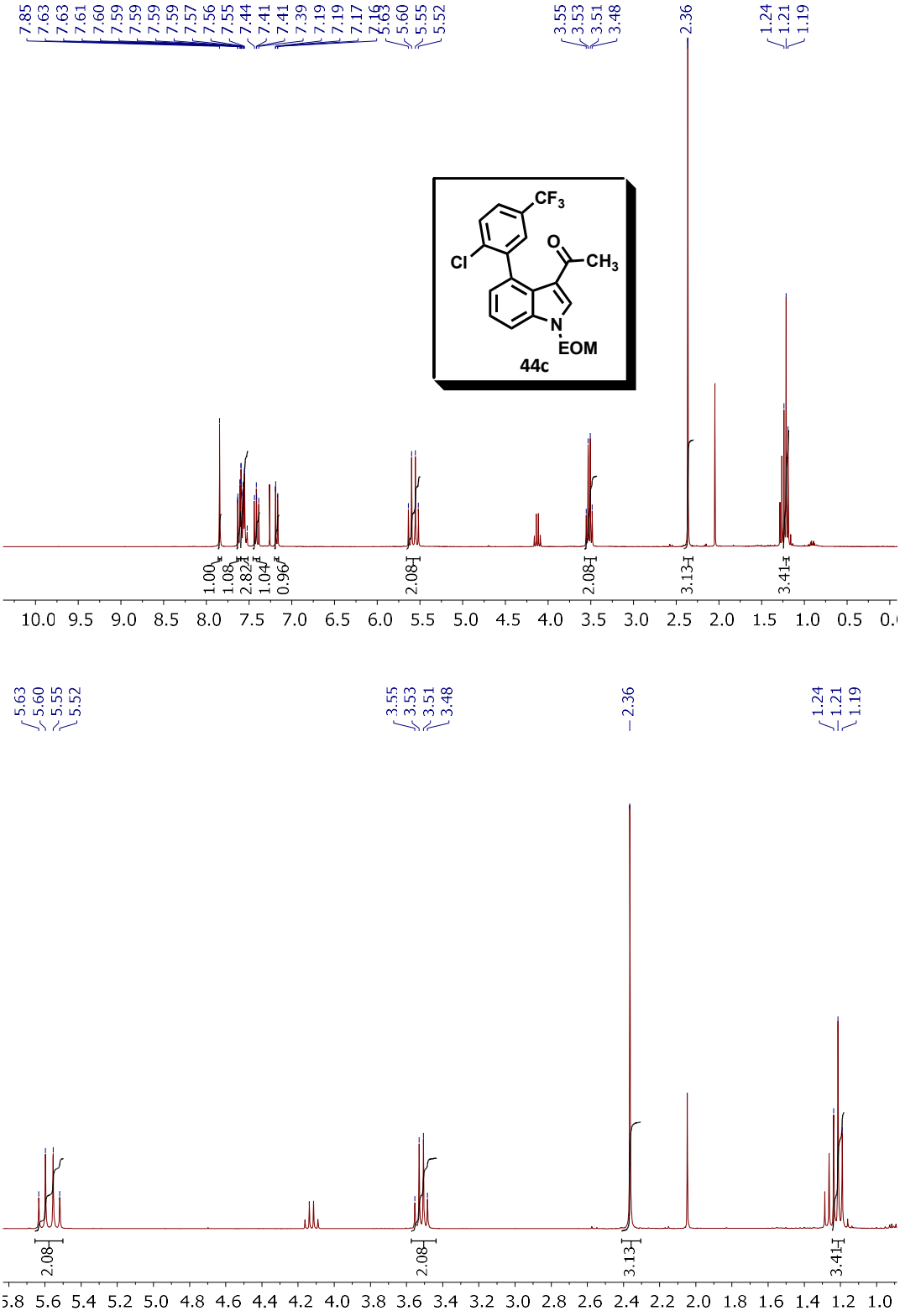


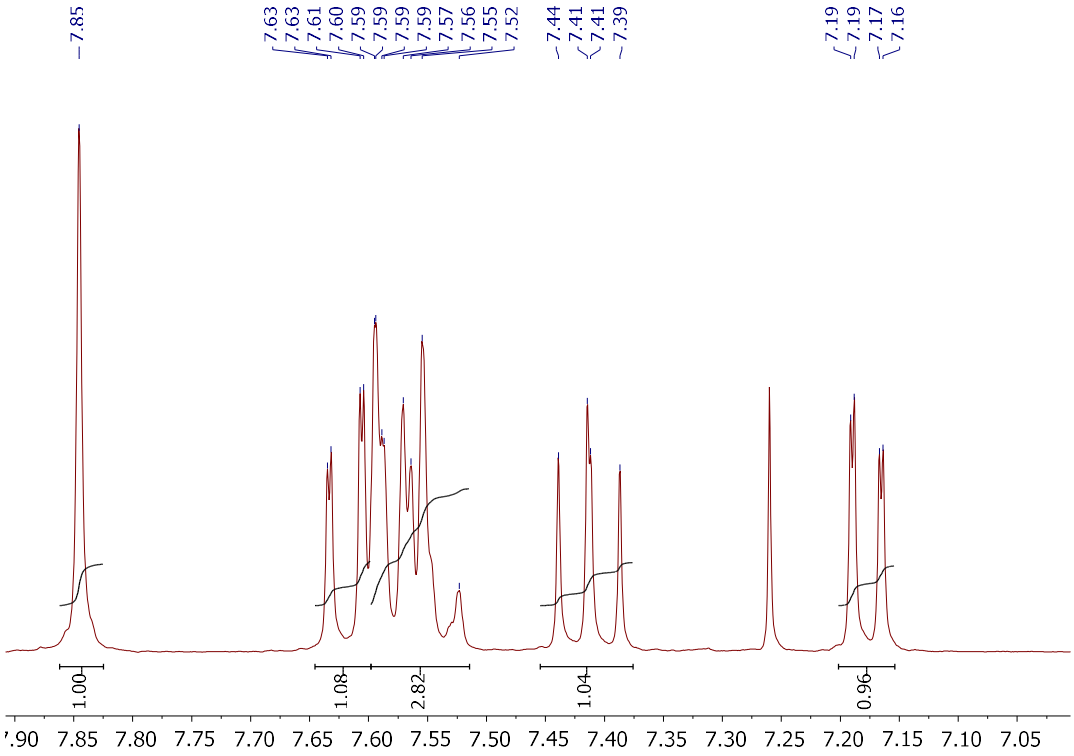


^{19}F-RMN ($CDCl_3$) 3-Acetil-4-(2-cloro-4-trifluormetil-fenil)-1-etoximetil-indol (44b)

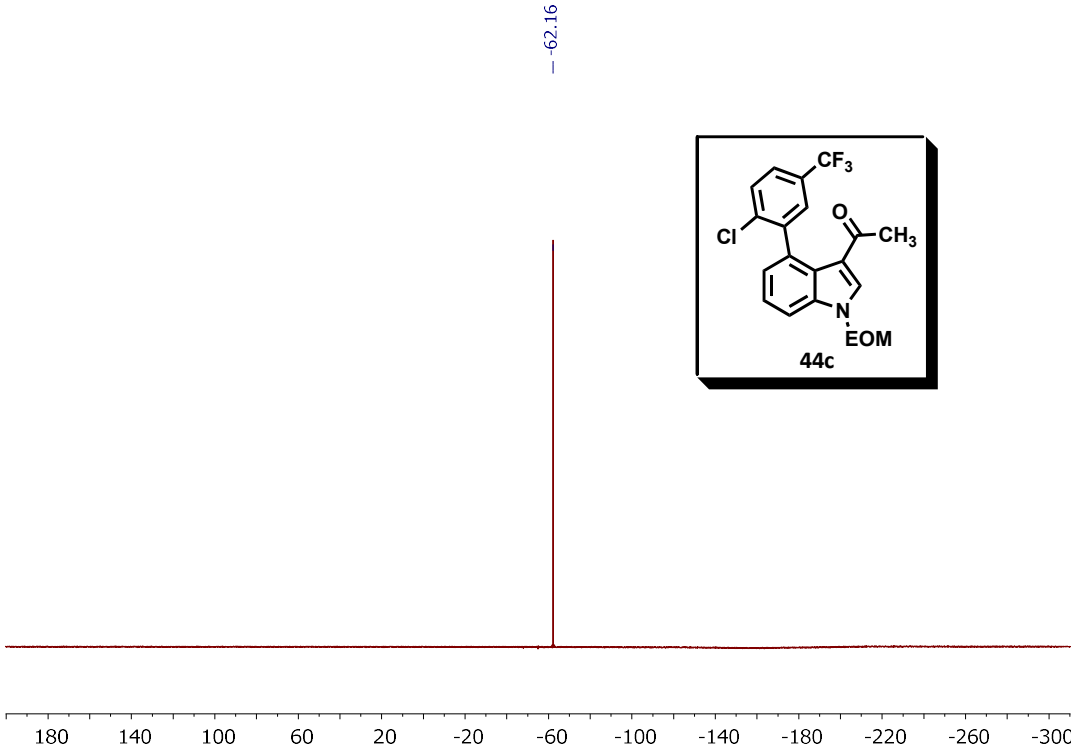


^{1}H-RMN ($CDCl_3$) 3-Acetil-4-(2-cloro-5-trifluormetil-fenil)-1-etoximetil-indol (44c)

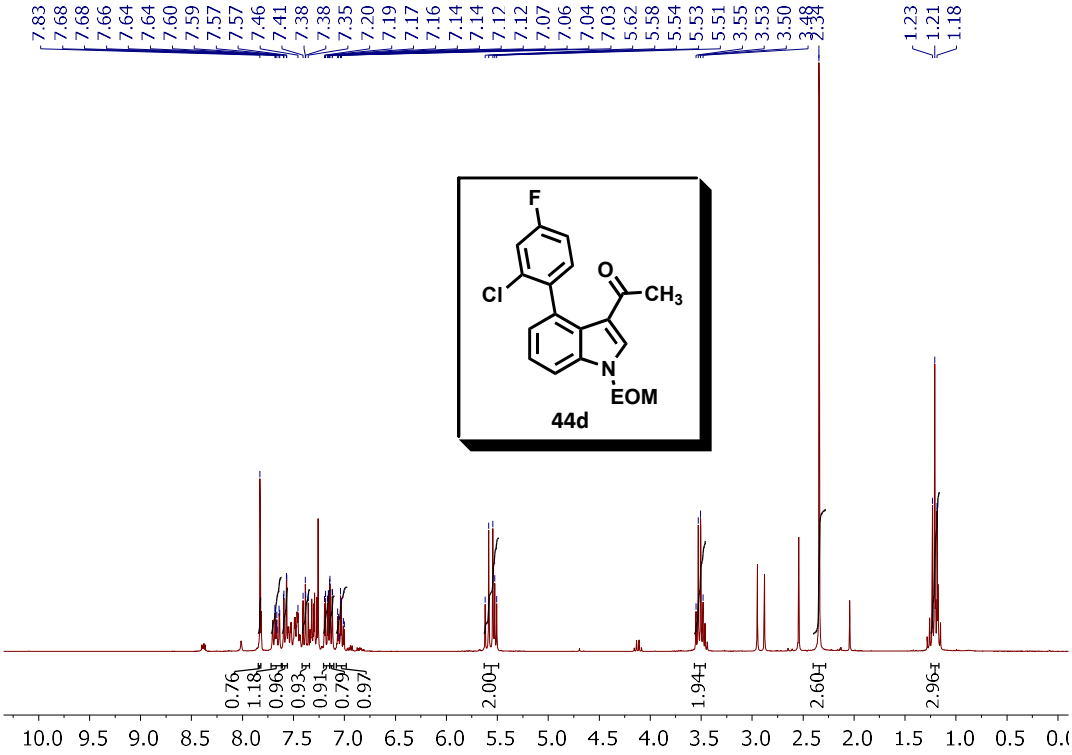


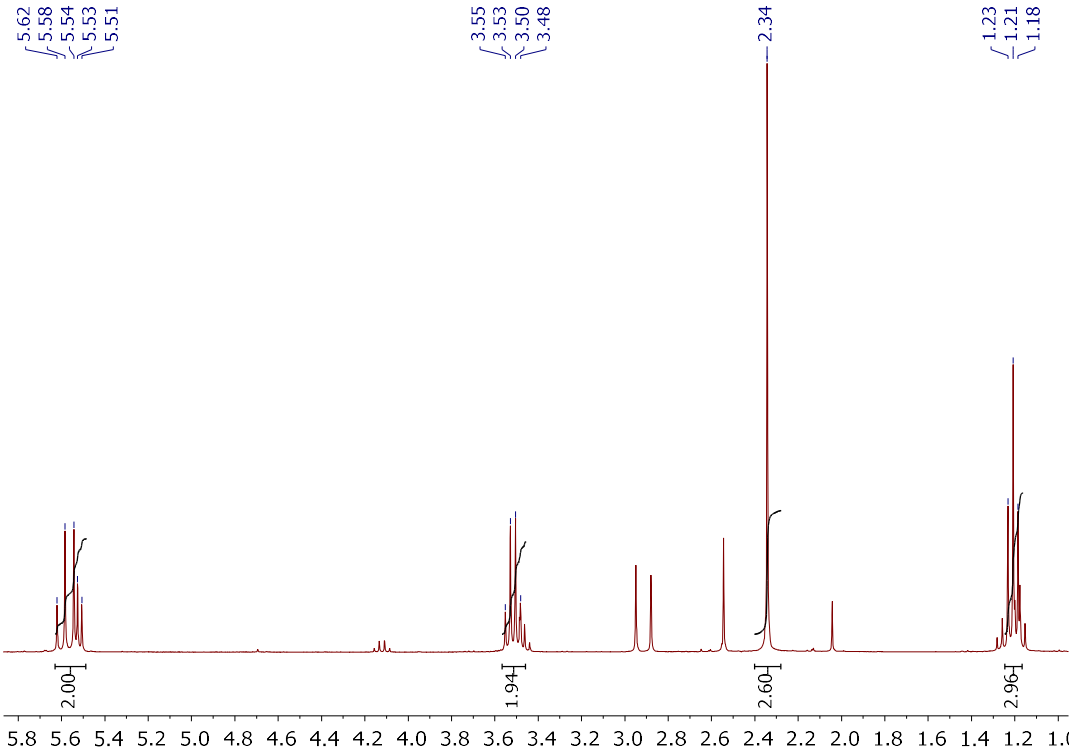


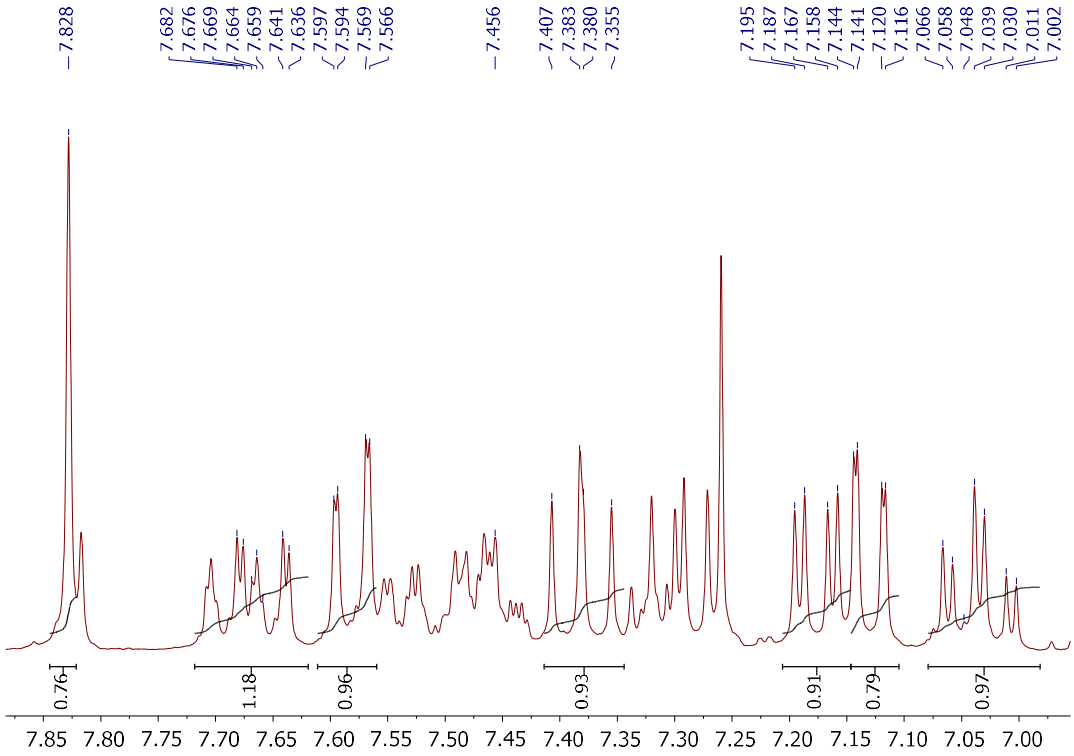
^{19}F-RMN ($CDCl_3$) 3-Acetil-4-(2-cloro-5-trifluormetil-fenil)-1-etoximetil-indol (44c)



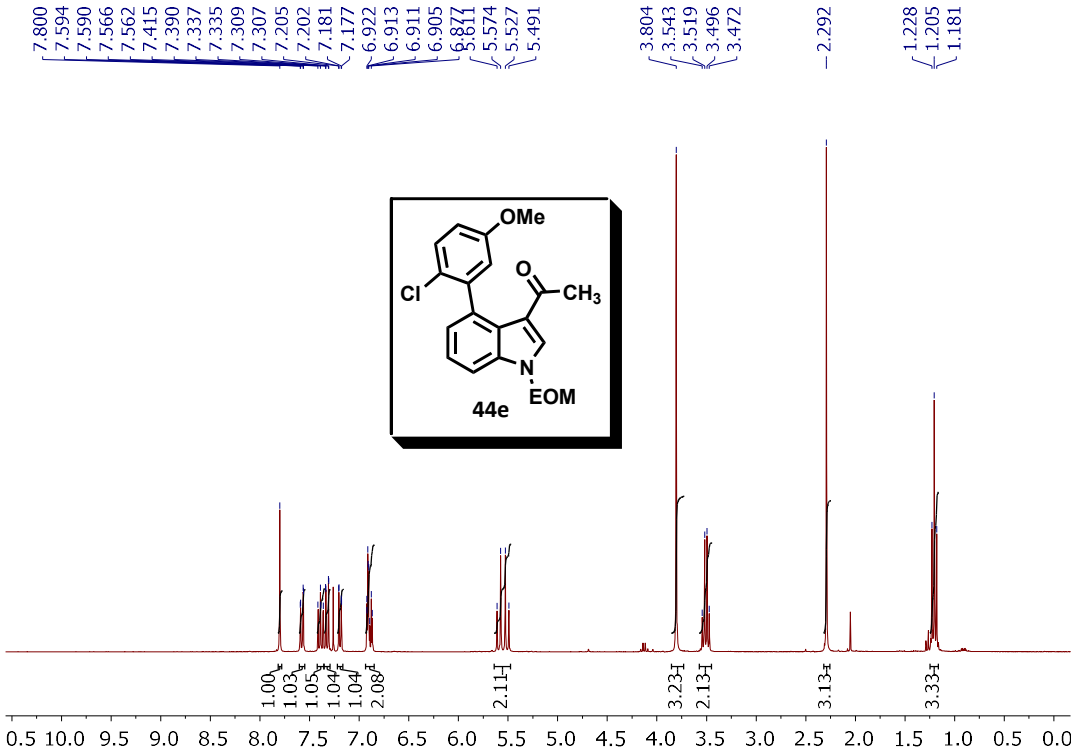
^{1}H-RMN ($CDCl_3$) 3-Acetil-4-(2-cloro-4-fluor-fenil)-1-etoximetil-indol (44d)

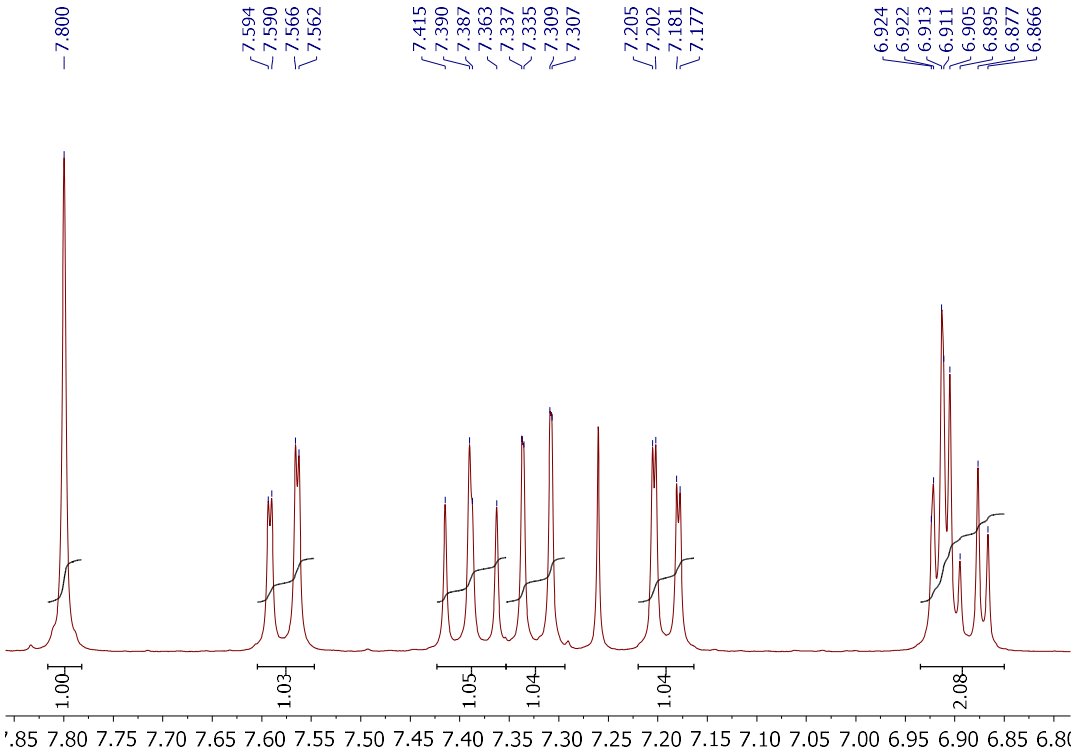






^{1}H-RMN ($CDCl_3$) 3-Acetil-4-(2-cloro-5-metoxi-fenil)-1-etoximetil-indol (44e)

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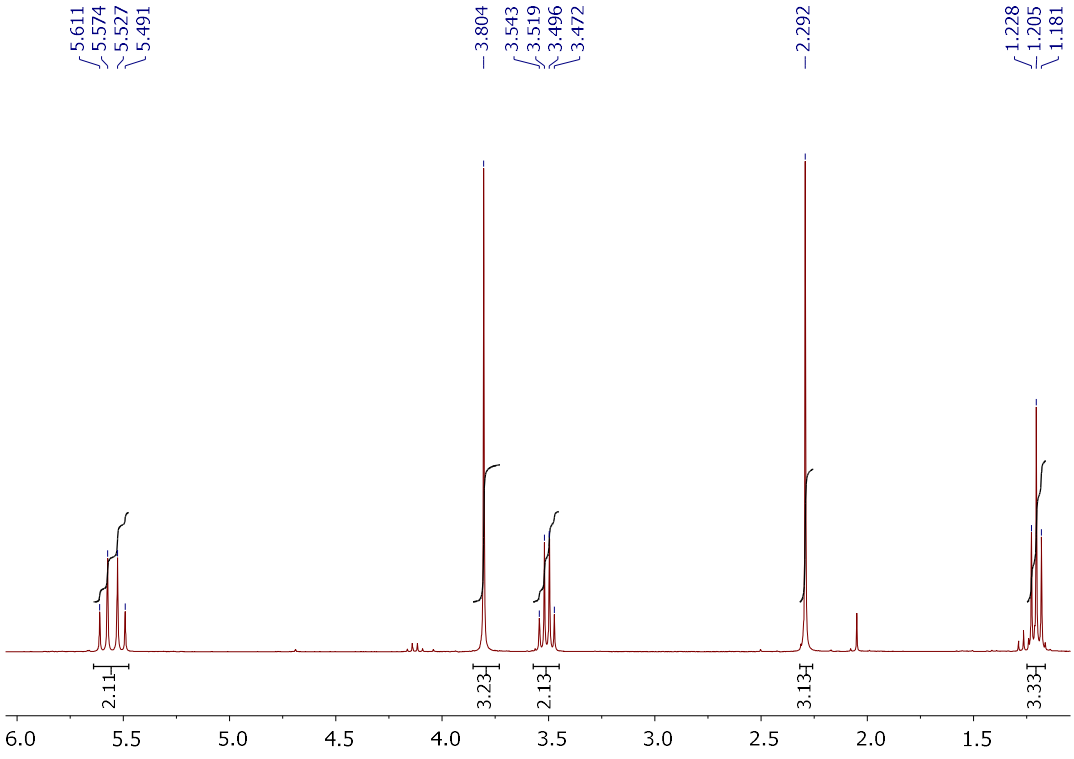
7.387
7.363
7.337
7.335
7.309
7.307
7.205
7.202
7.181
7.177
6.924
6.922
6.913
6.911
6.905
6.895
6.877
6.866
1.00
1.03
1.05
1.04
1.04
2.08
7.85 7.80 7.75 7.70 7.65 7.60 7.55 7.50 7.45 7.40 7.35 7.30 7.25 7.20 7.15 7.10 7.05 7.00 6.95 6.90 6.85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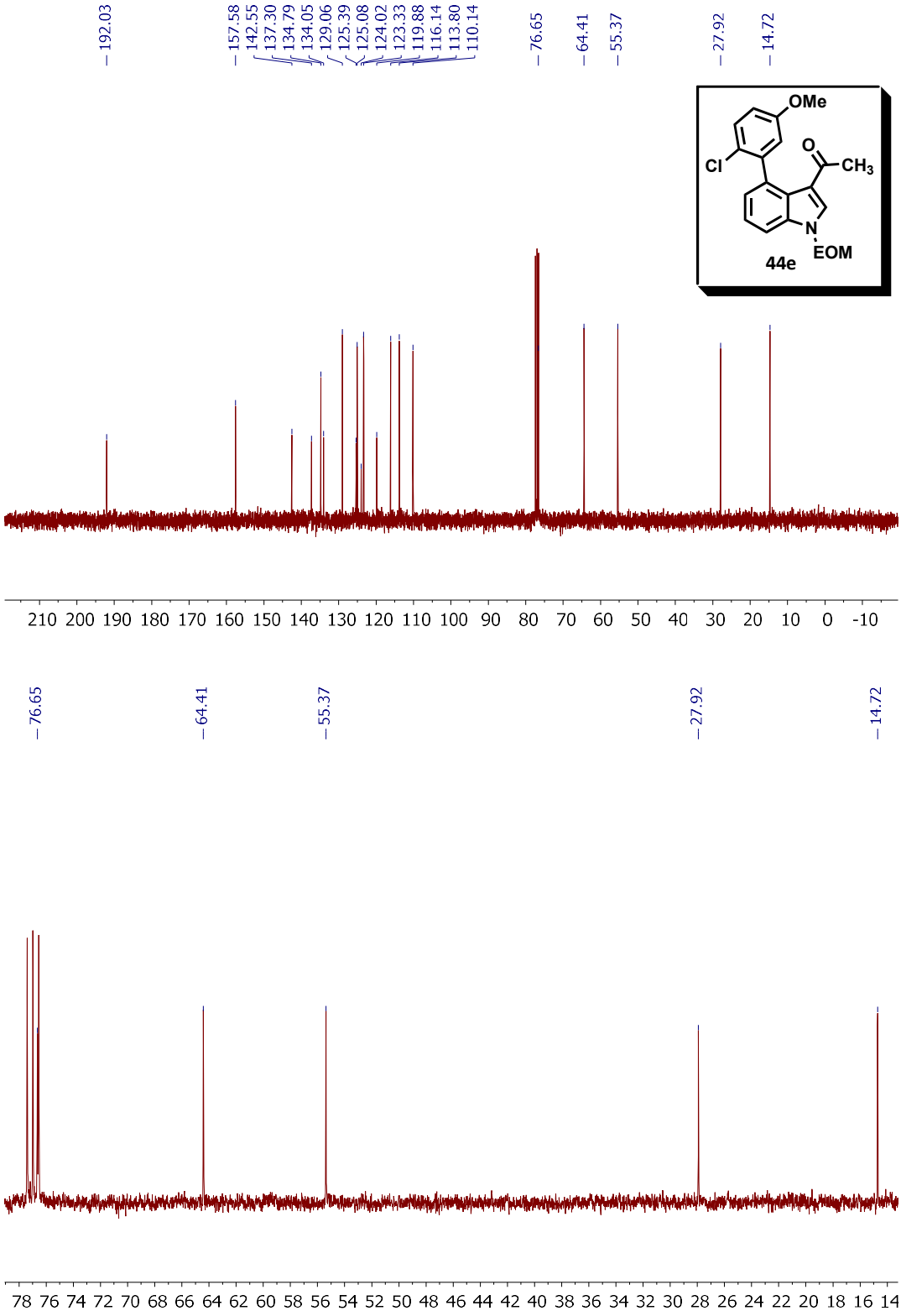
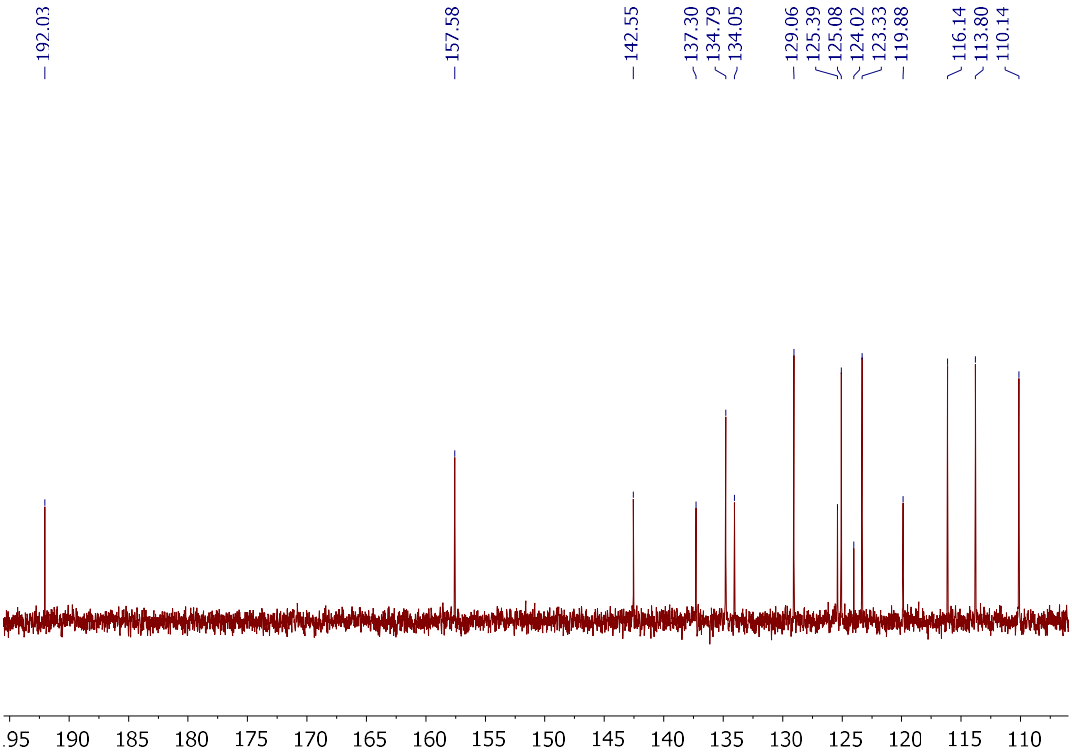
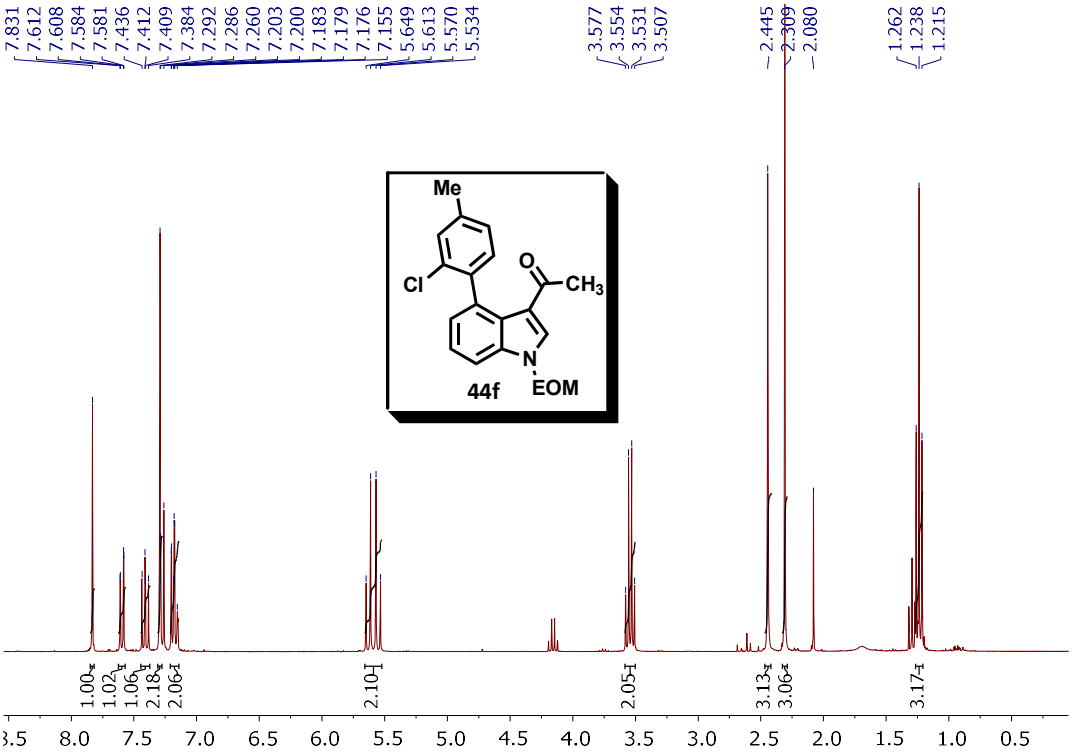
3.543
3.519
3.496
3.472
2.292
1.228
1.205
1.181
2.11
3.23
2.13
3.13
3.33
6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5

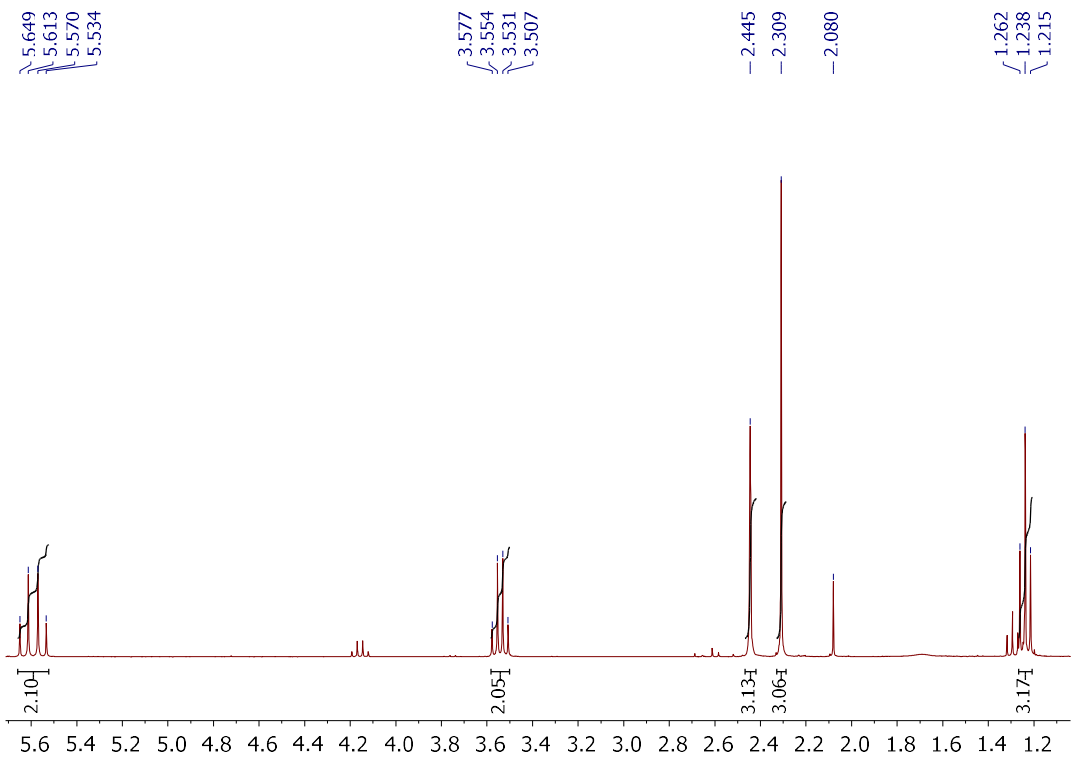
^{13}C-RMN ($CDCl_3$) 3-Acetil-4-(2-cloro-5-metoxi-fenil)-1-etoximetil-indol (44e)





^{1}H-RMN ($CDCl_3$) 3-Acetil-4-(2-cloro-4-metil-fenil)-1-etoximetil-indol (44f)

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3.507
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2.309
2.080
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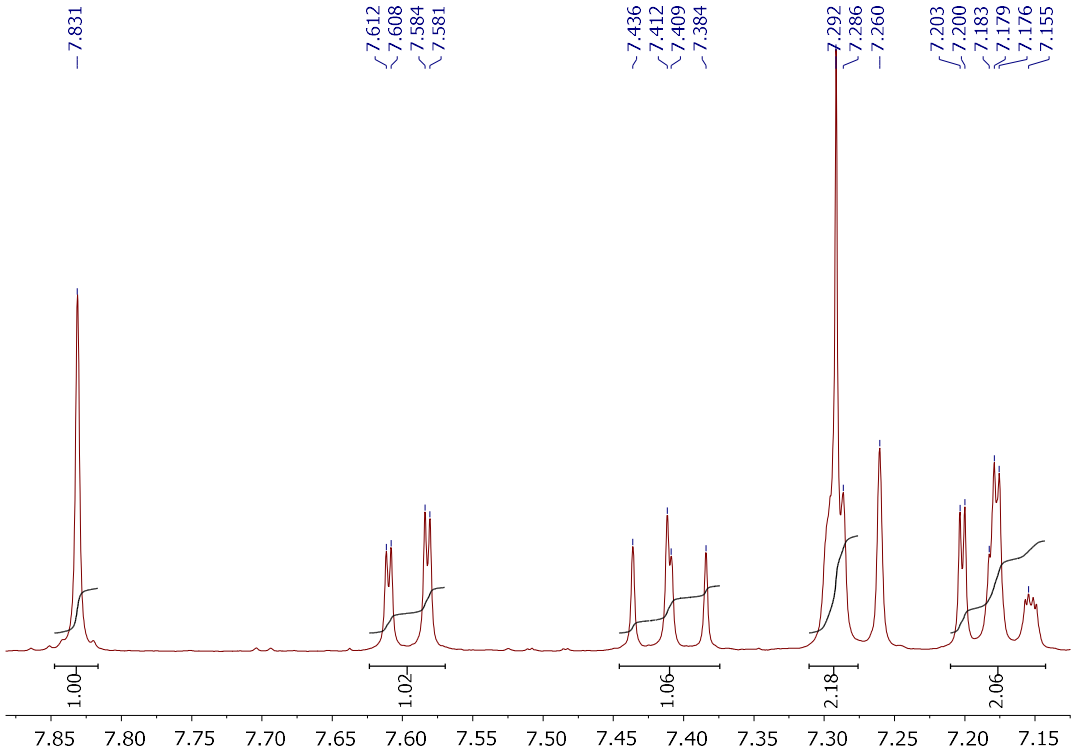
1.238
1.215
2.10
2.05
3.13
3.06
3.17
5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2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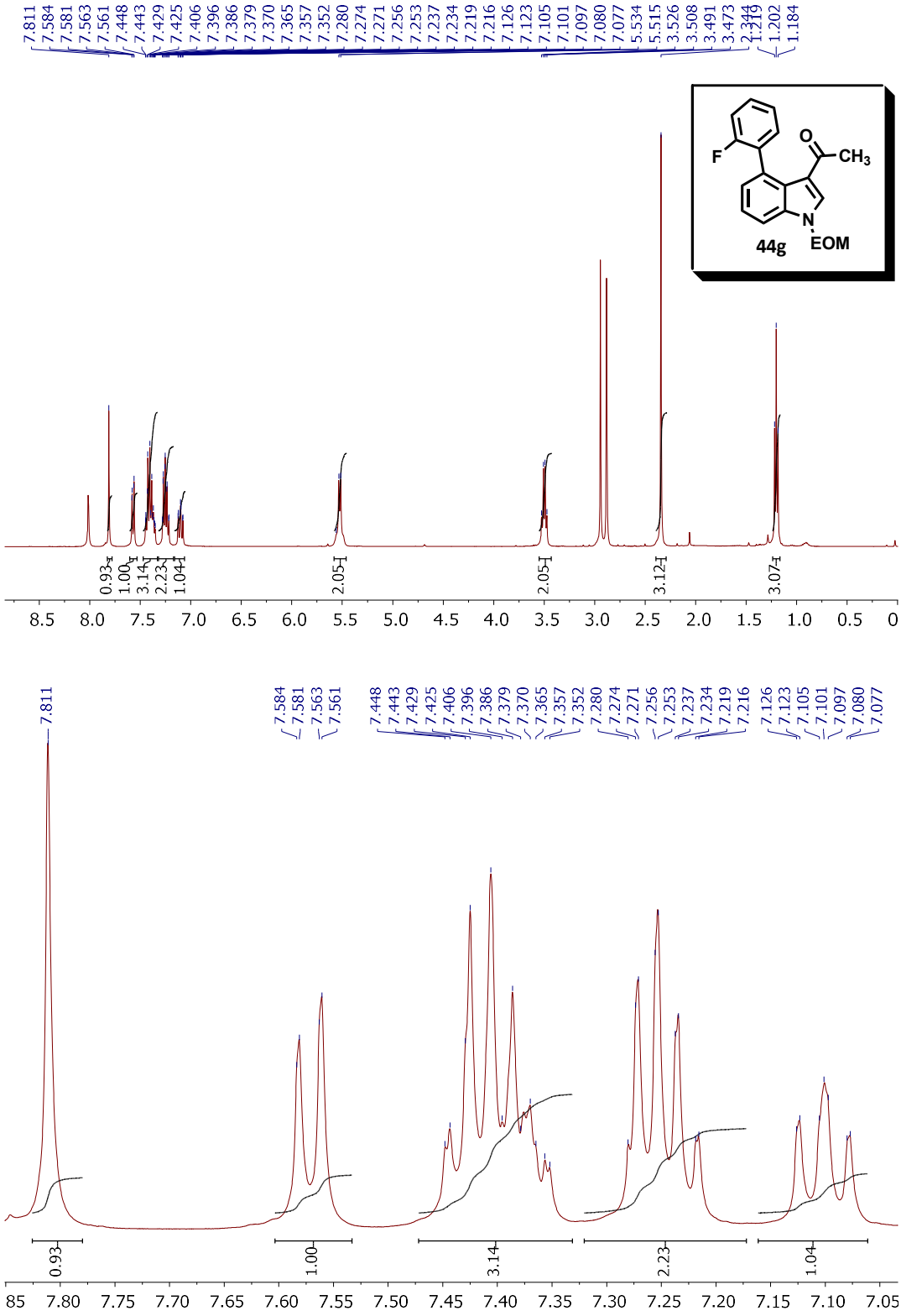
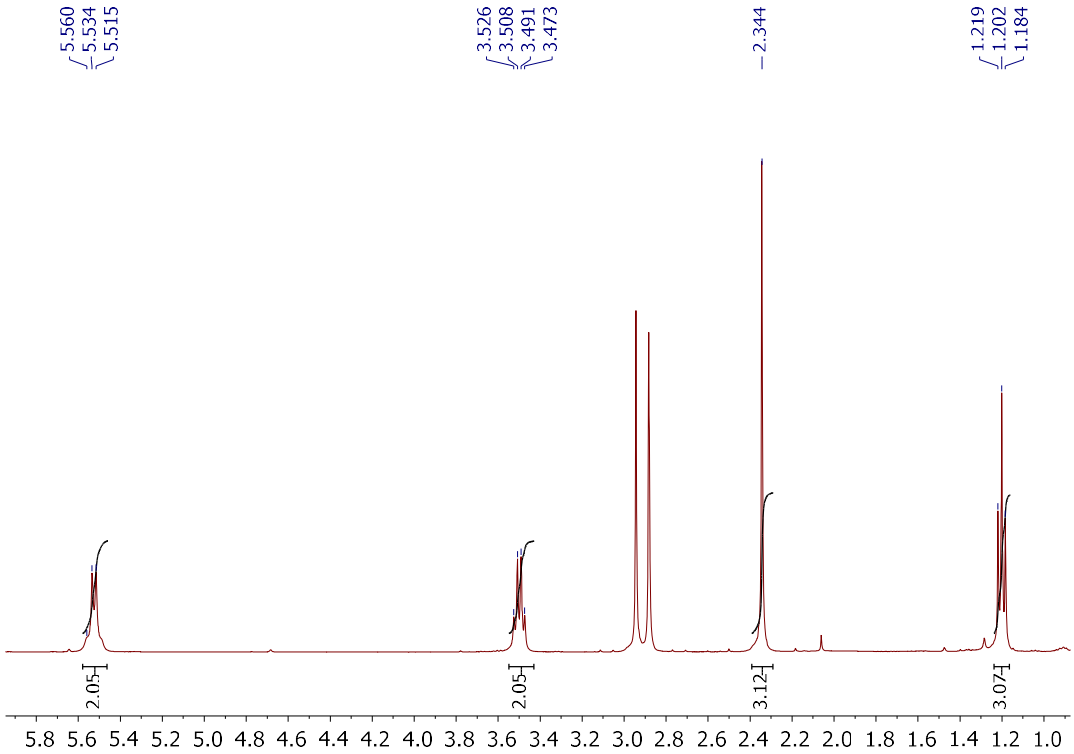
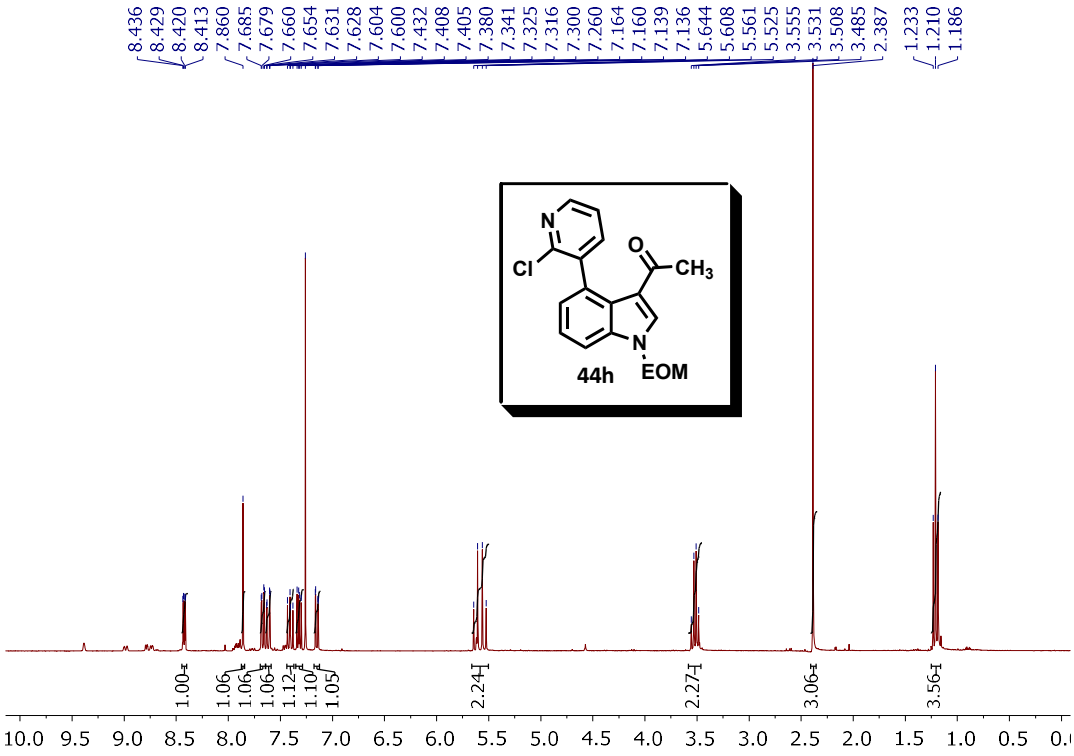
7.200
7.183
7.179
7.176
7.155
1.00
1.02
1.06
2.18
2.06
7.85 7.80 7.75 7.70 7.65 7.60 7.55 7.50 7.45 7.40 7.35 7.30 7.25 7.20 7.15

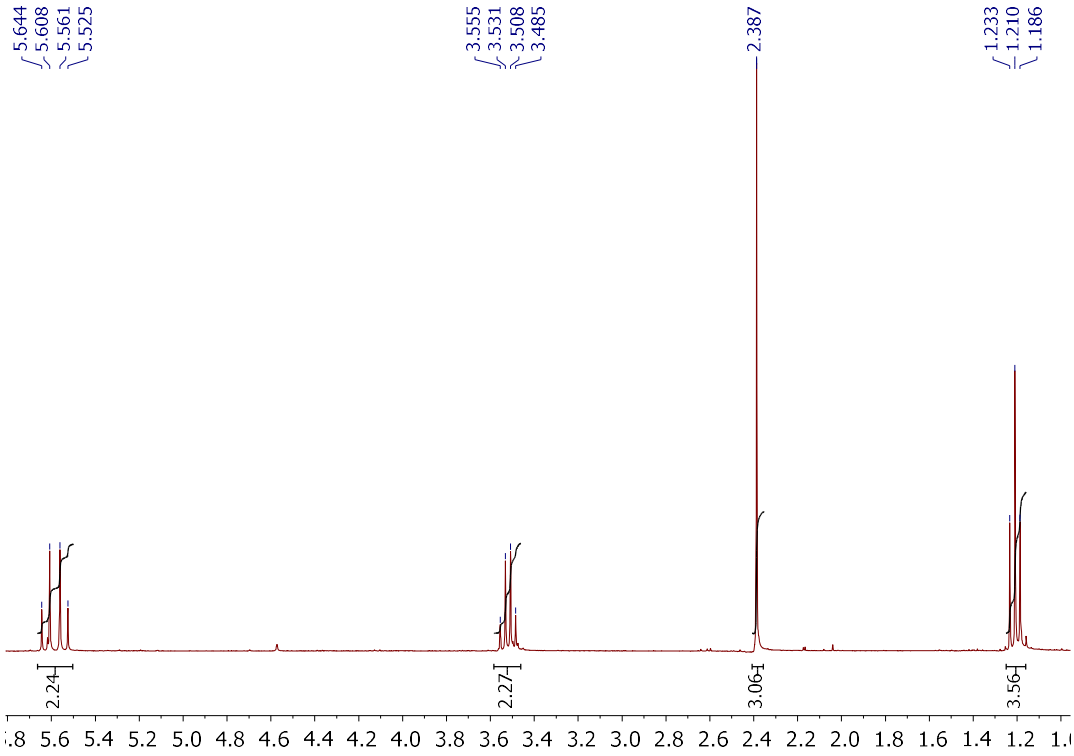
^{1}H-RMN ($CDCl_3$) 3-Acetil-4-(2-fluorfenil)-1-etoximetil-indol (44g)

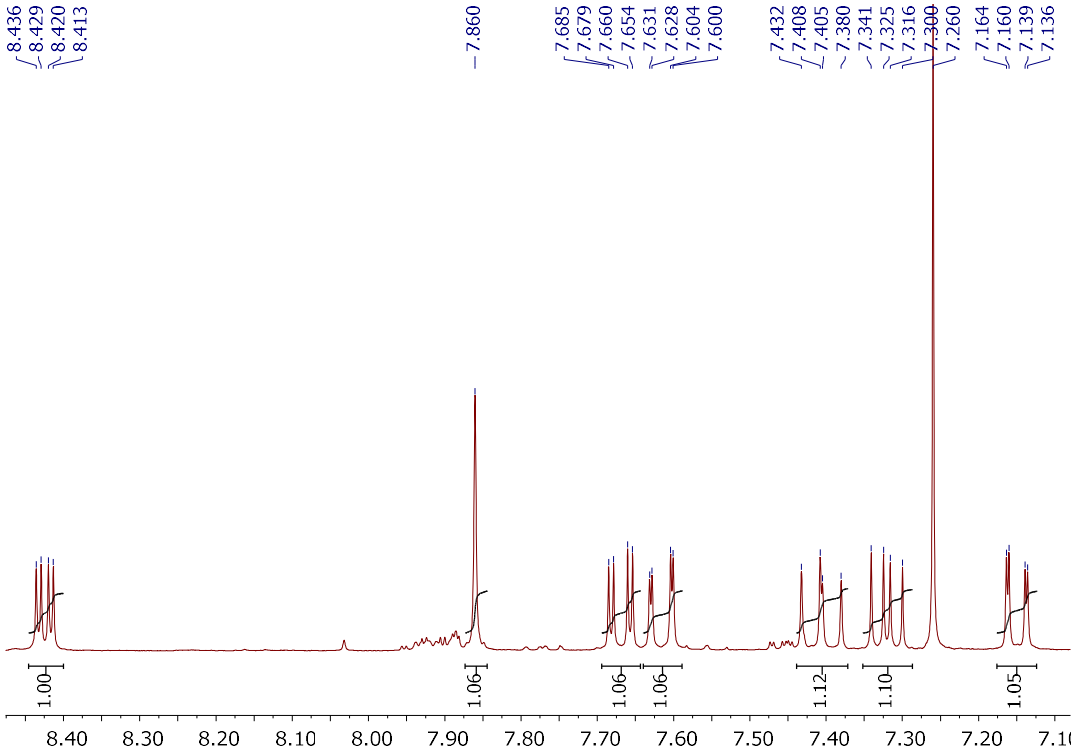




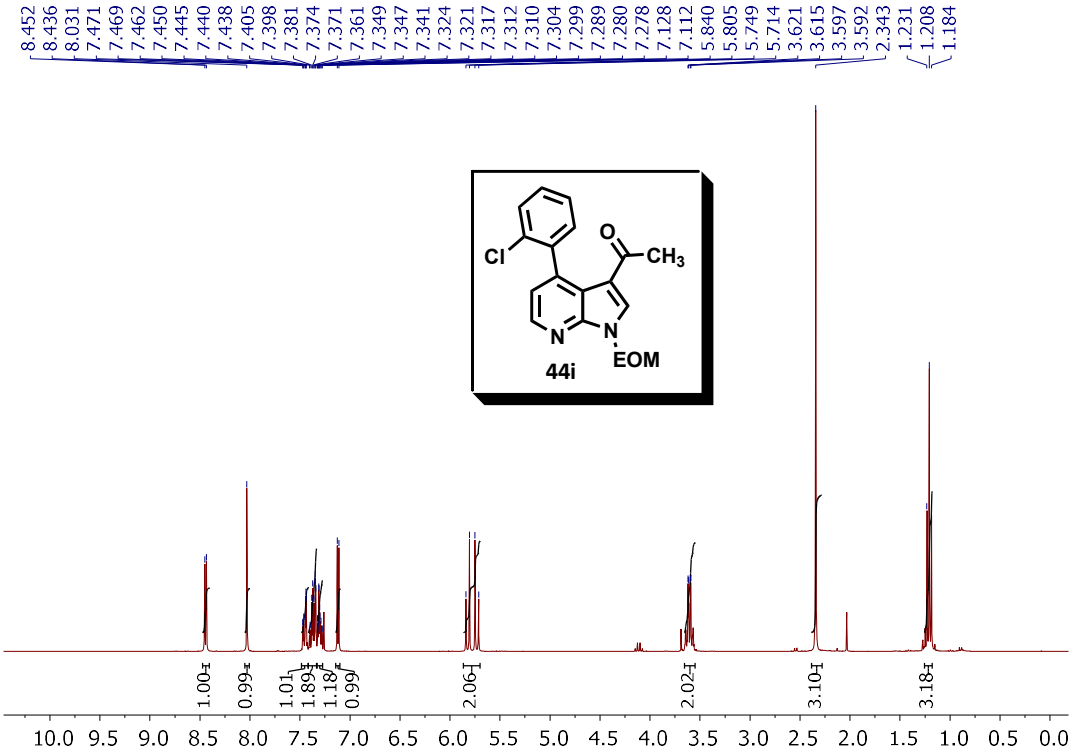
^{1}H-RMN ($CDCl_3$) 3-Acetil-4-(2-cloro-3-piridinil)-1-etoximetil-indol (44h)

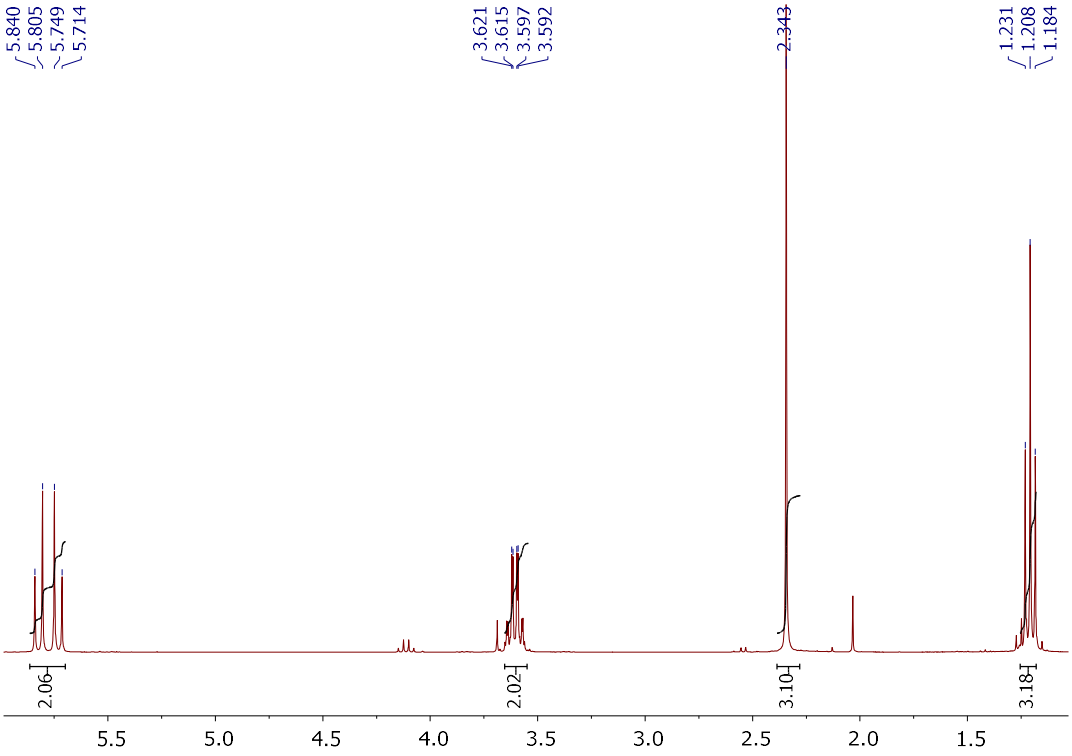


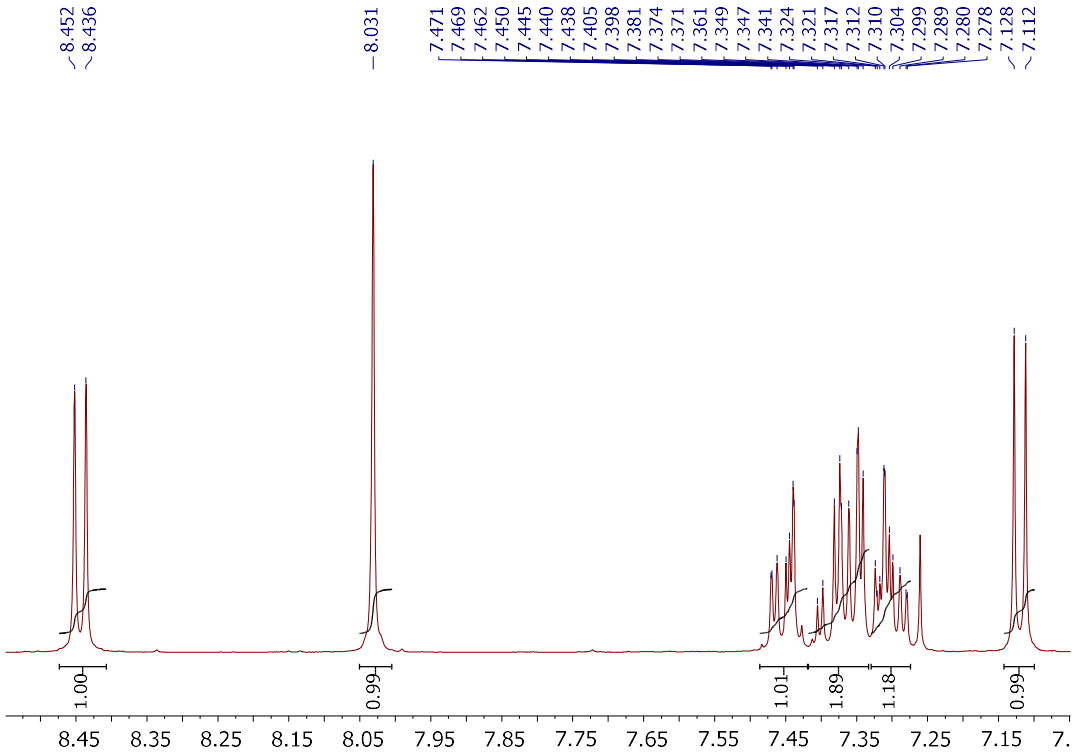

5.644
5.608
5.561
5.525
3.555
3.531
3.508
3.485
2.387
1.233
1.210
1.186
2.24
2.27
3.06
3.56
5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2


8.436
8.429
8.420
8.413
7.860
7.685
7.679
7.660
7.654
7.631
7.628
7.604
7.600
7.432
7.408
7.405
7.380
7.341
7.325
7.316
7.300
7.260
7.164
7.160
7.139
7.136
1.00
1.06
1.06
1.06
1.12
1.10
1.05
8.40 8.30 8.20 8.10 8.00 7.90 7.80 7.70 7.60 7.50 7.40 7.30 7.20

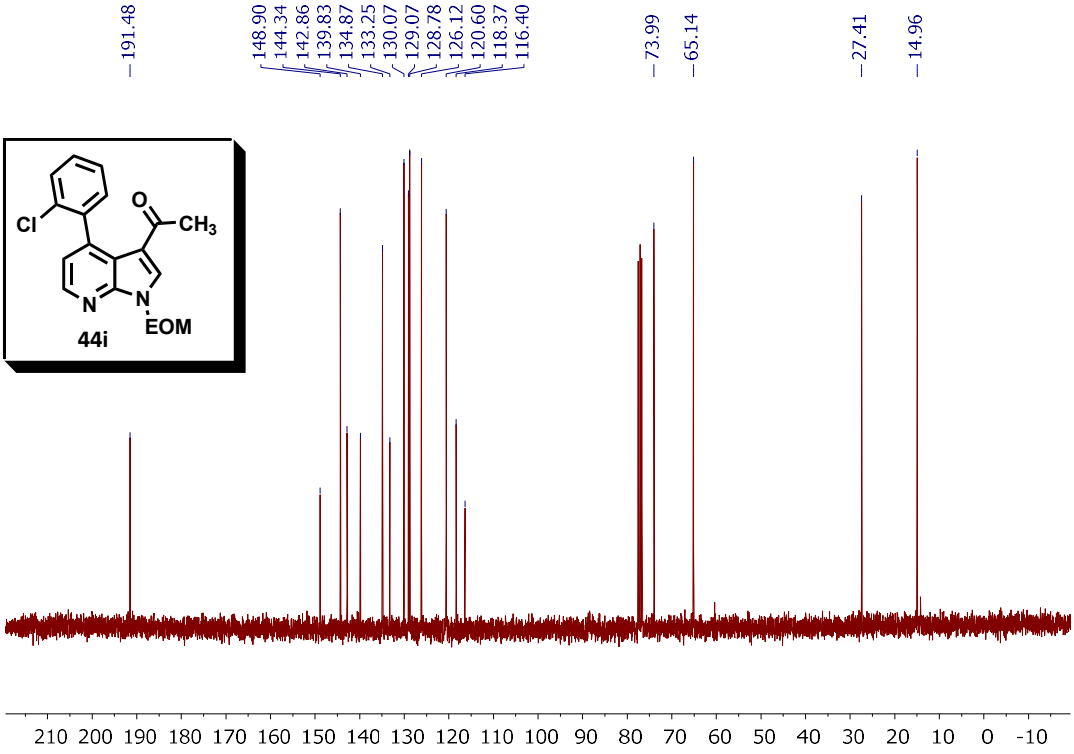
^{1}H-RMN ($CDCl_3$) 3-Acetil-4-(2-clorofenil)-1-etoximetil-7-azaindol (44i)

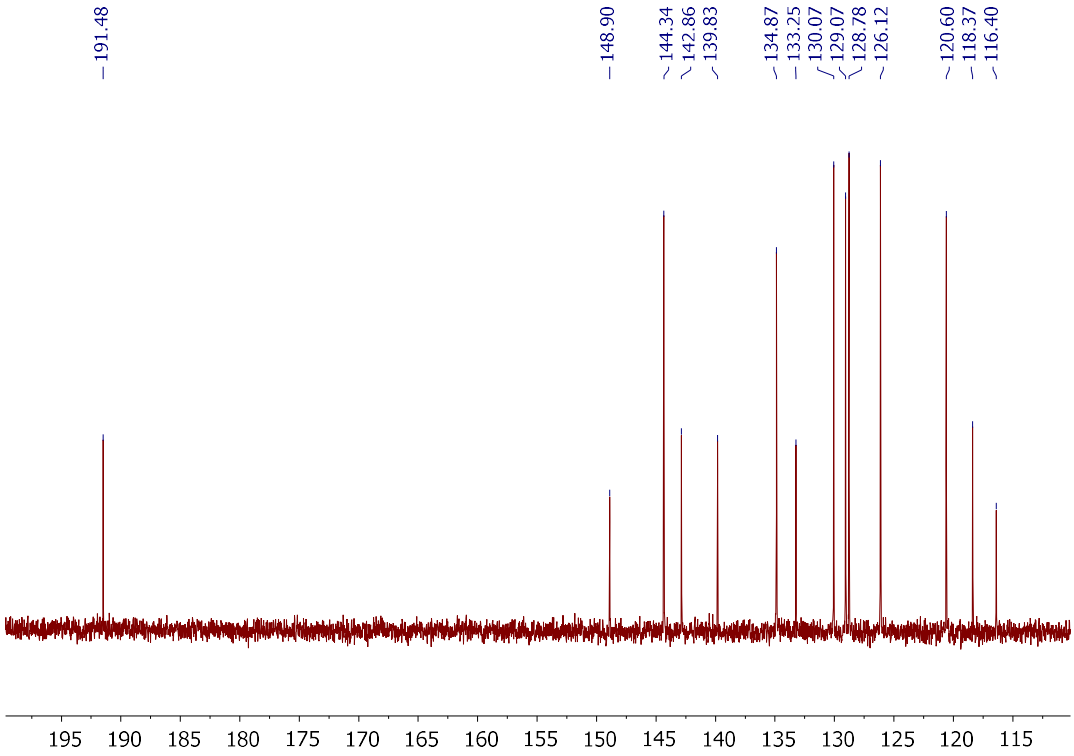




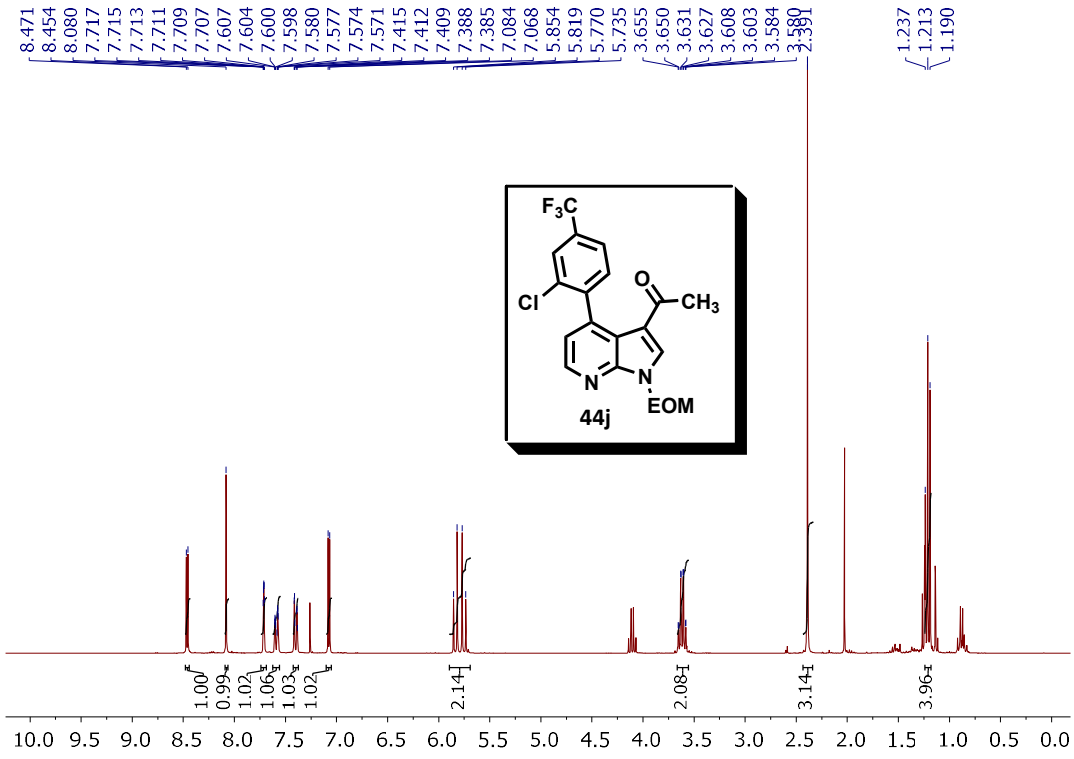


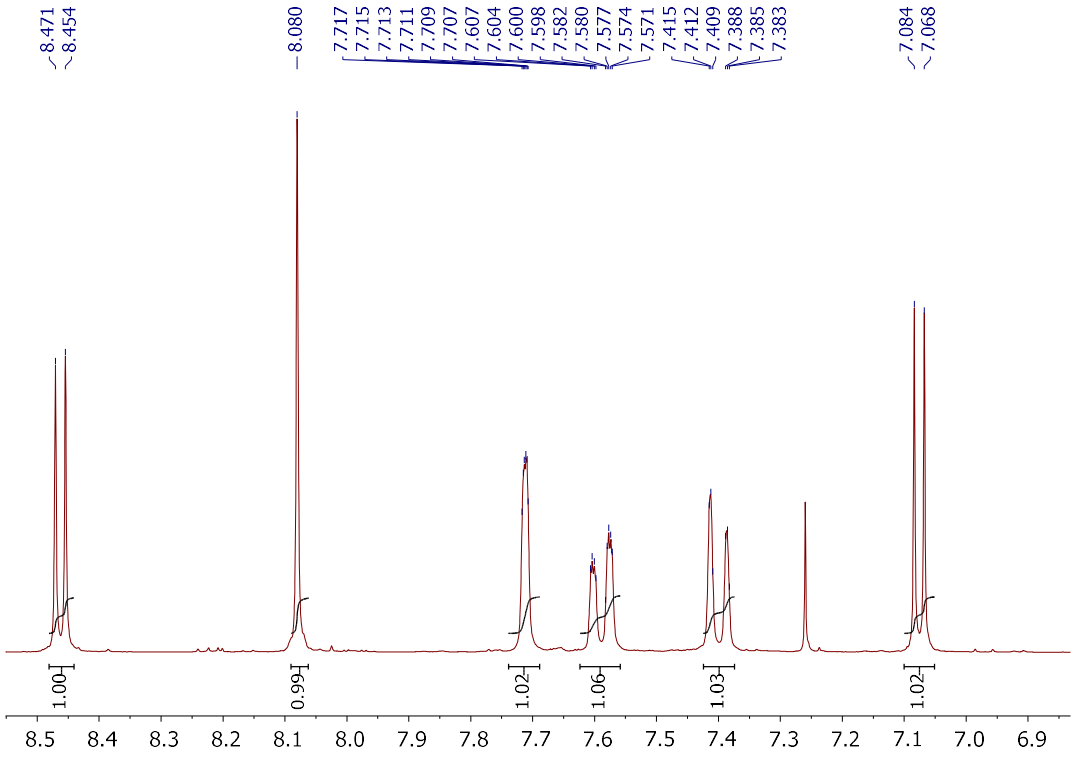
^{13}C-RMN ($CDCl_3$) 3-Acetil-4-(2-clorofenil)-1-etoximetil-7-azaindol (44i)

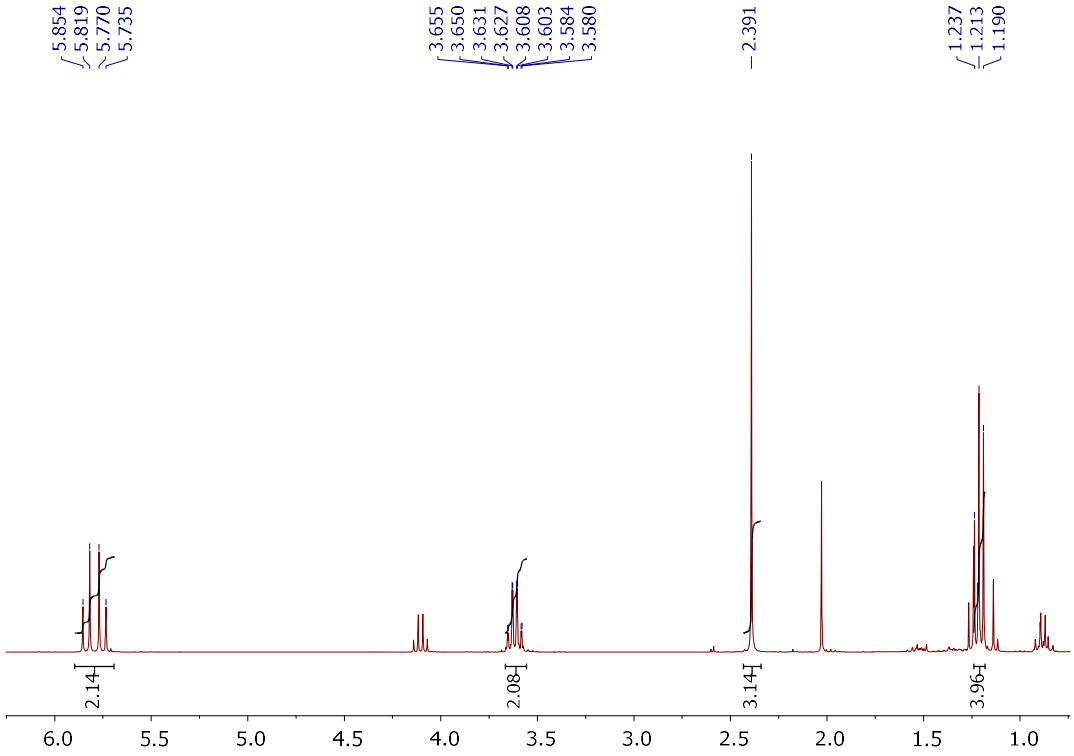




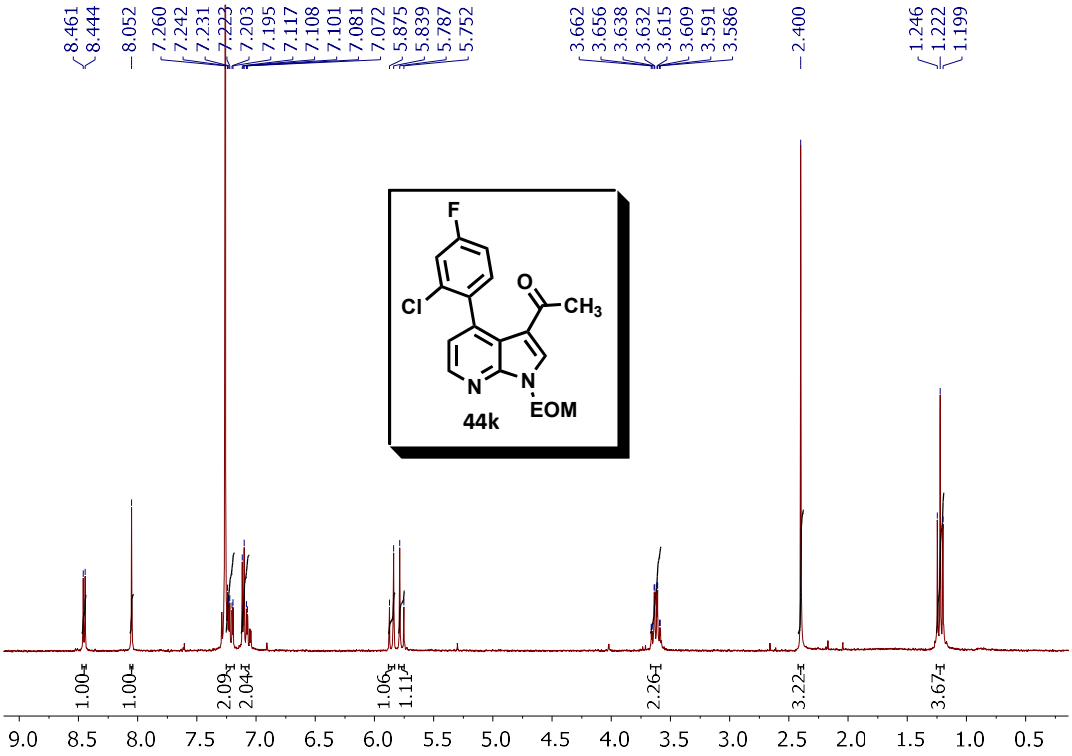
^{1}H-RMN ($CDCl_3$) 3-Acetil-4-(2-cloro-4-trifluormetil-fenil)-1-etoximetil-7-azaindol (44j)

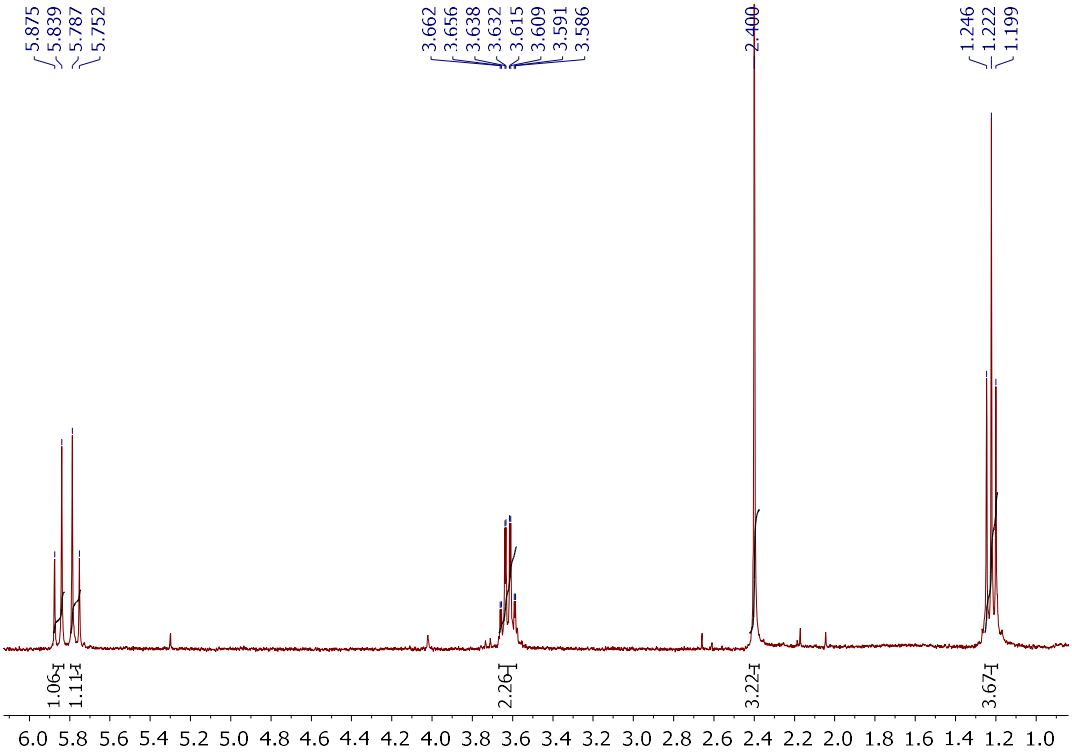


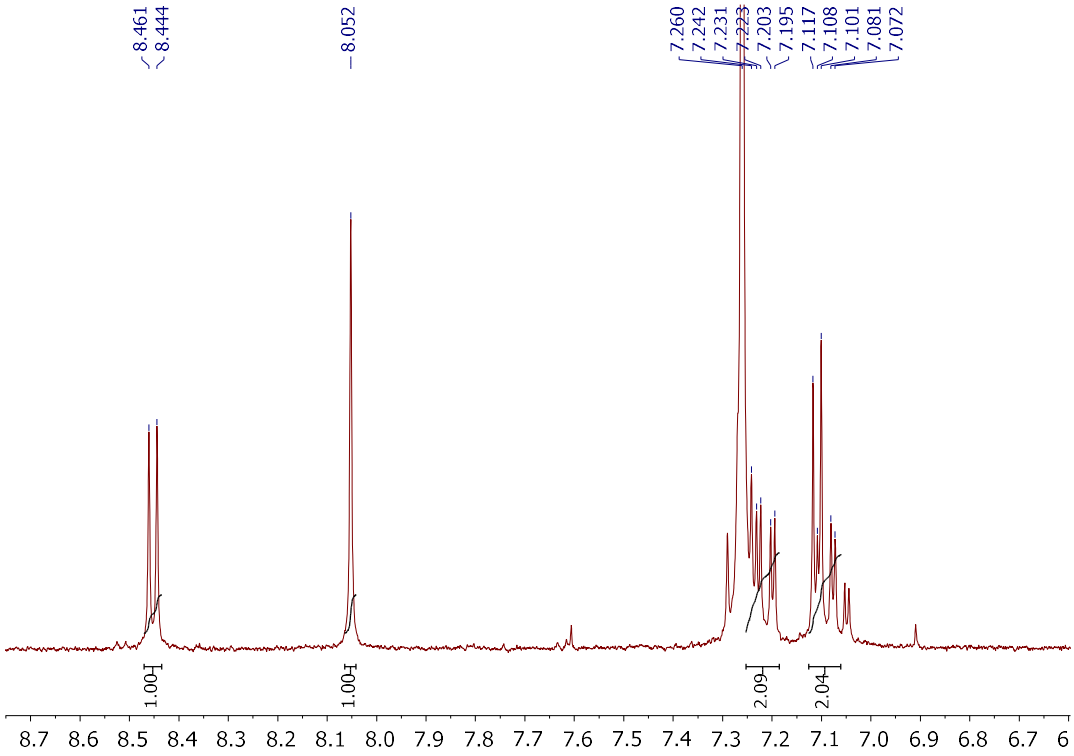

8.471
8.454
8.080
7.717
7.715
7.713
7.711
7.709
7.707
7.607
7.604
7.600
7.598
7.582
7.580
7.577
7.574
7.571
7.415
7.412
7.409
7.388
7.385
7.383
7.084
7.068
1.00
0.99
1.02
1.06
1.03
1.02
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9


5.854
5.819
5.770
5.735
3.655
3.650
3.631
3.627
3.608
3.603
3.584
3.580
2.391
1.237
1.213
1.190
2.14
2.08
3.14
3.96
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0

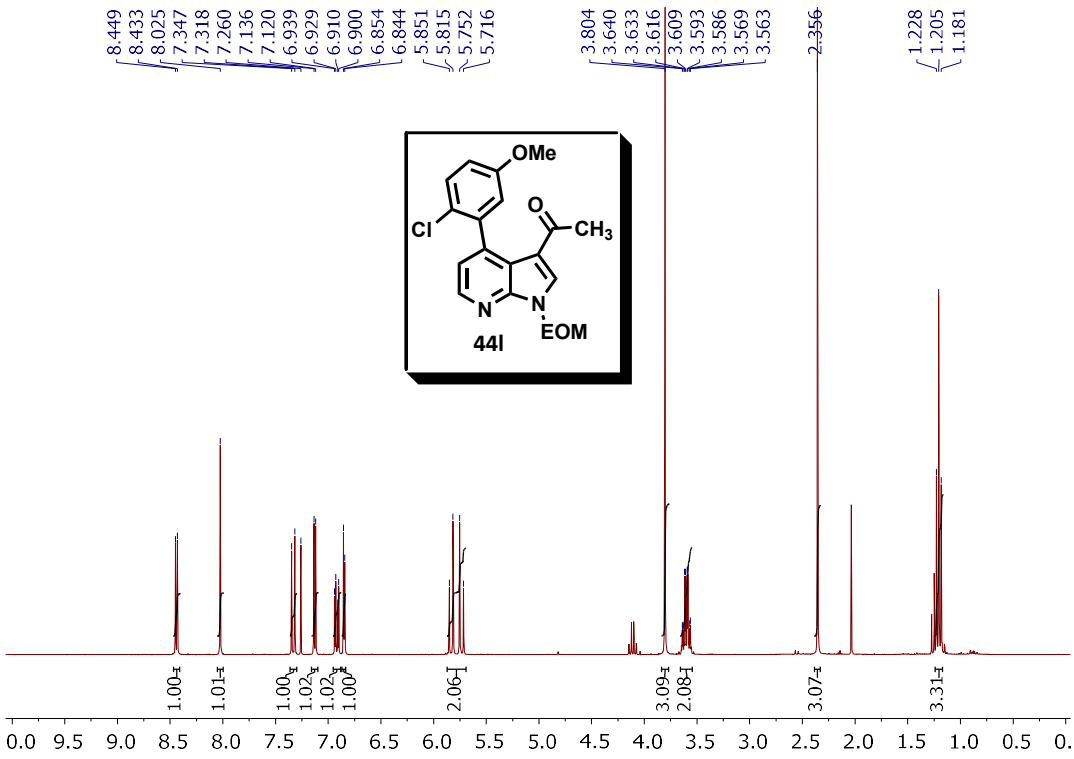
^{1}H-RMN ($CDCl_3$) 3-Acetil-4-(2-cloro-4-fluor-fenil)-1-etoximetil-7-azaindol (44k)

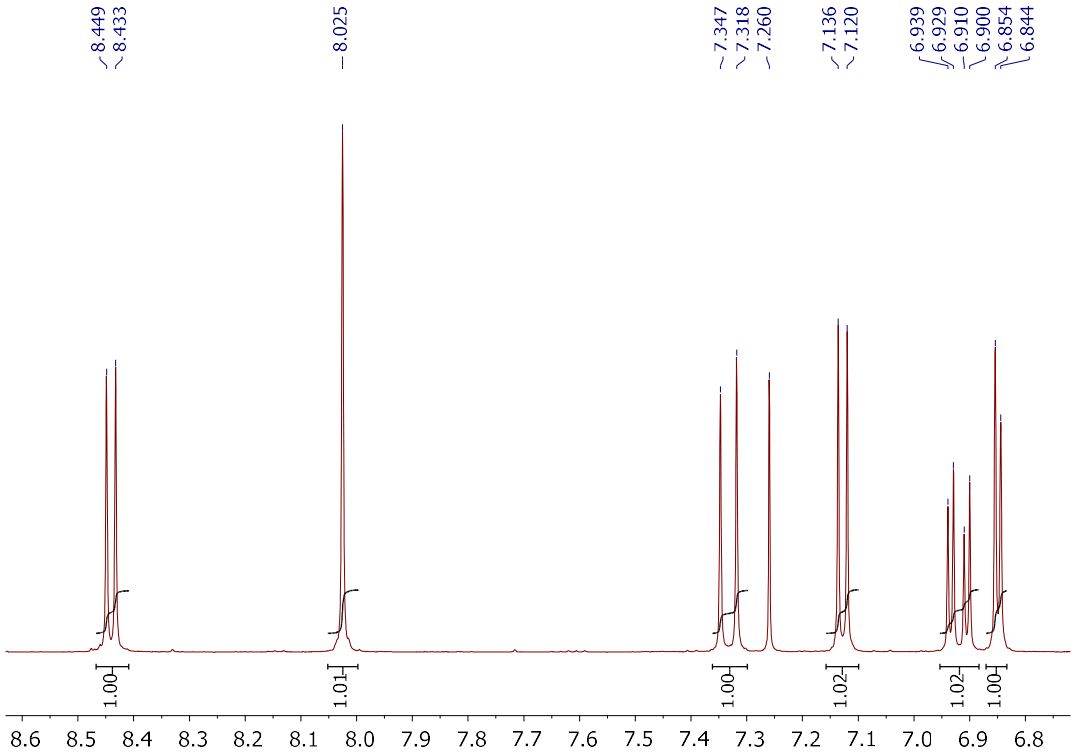


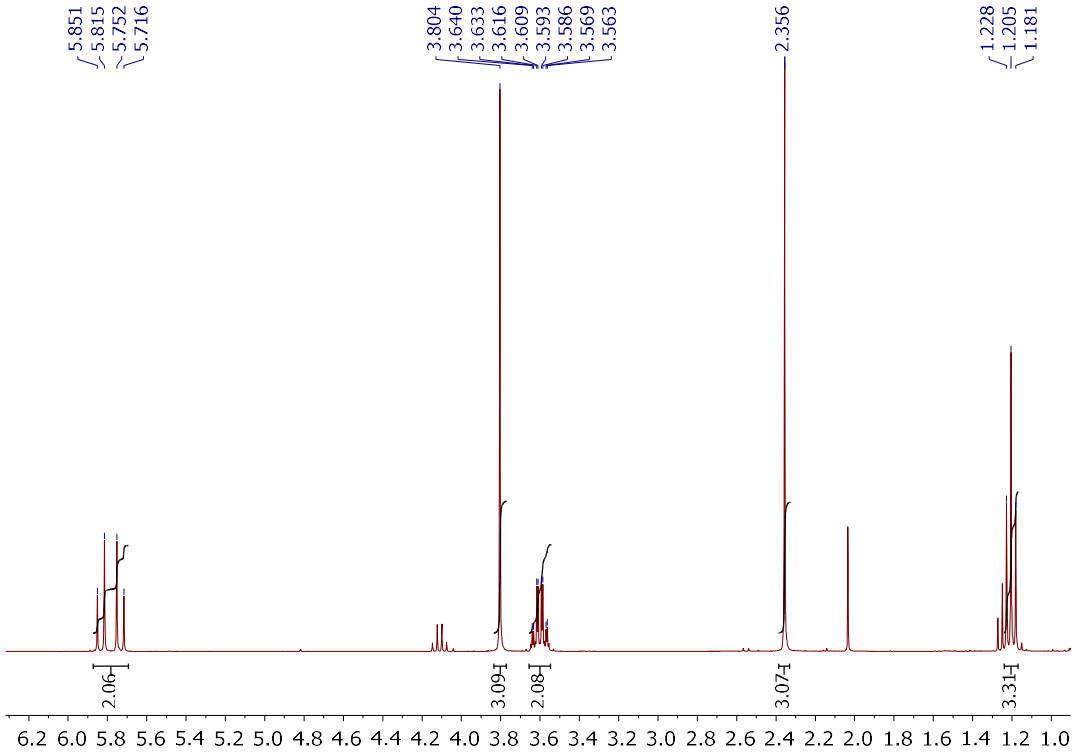




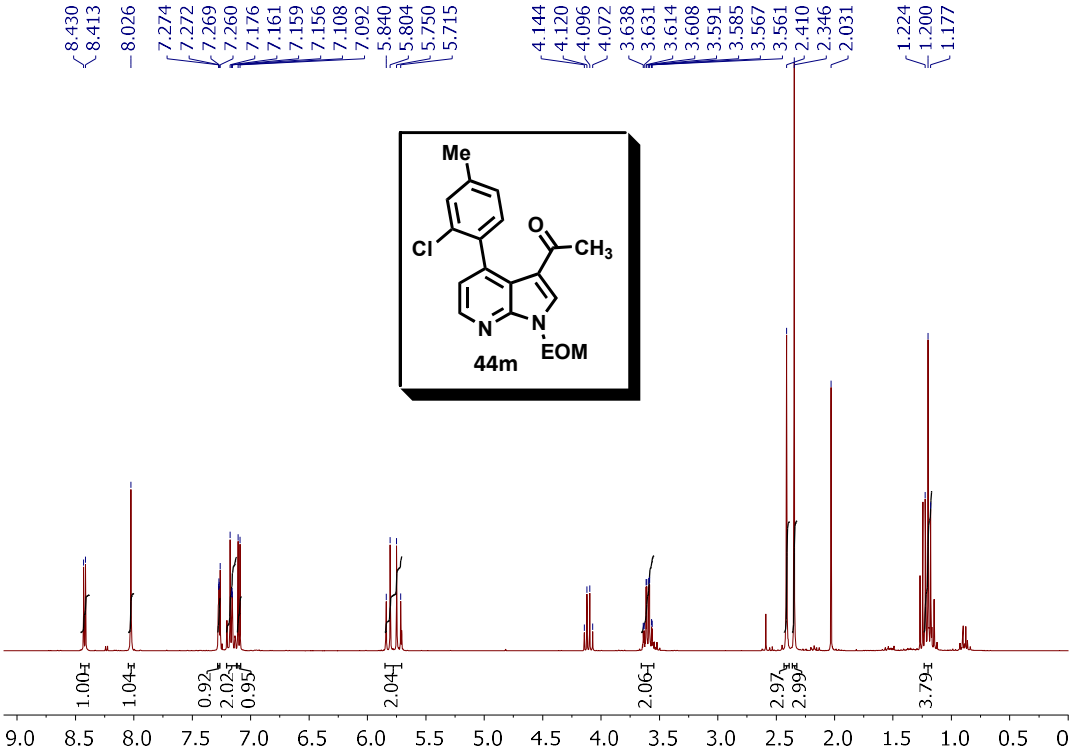
^{1}H-RMN ($CDCl_3$) 3-Acetil-4-(2-cloro-5-metoxi-fenil)-1-etoximetil-7-azaindol (44l)

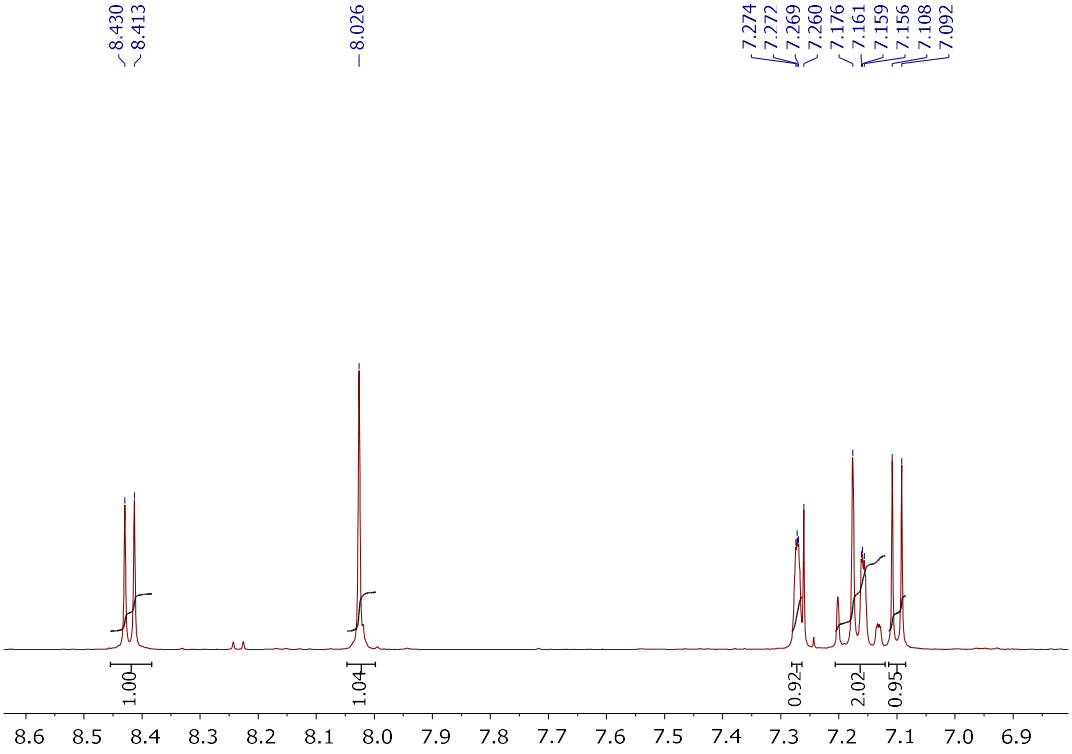


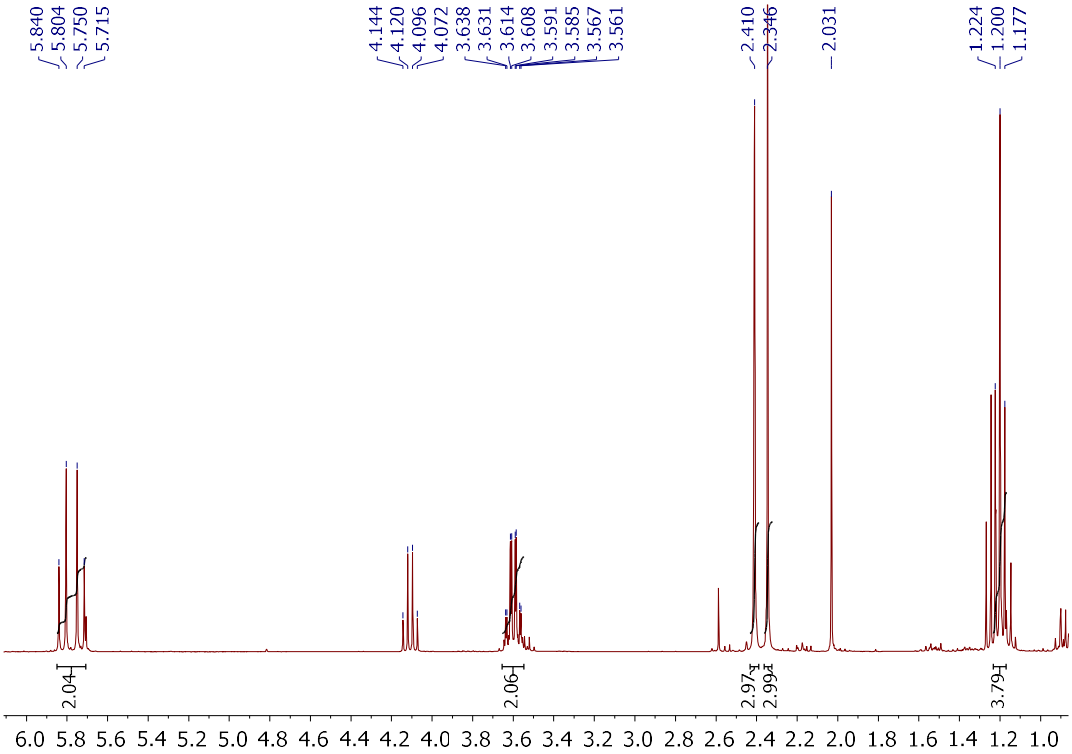

8.449
8.433
8.025
7.347
7.318
7.260
7.136
7.120
6.939
6.929
6.910
6.900
6.854
6.844
1.00
1.01
1.00
1.02
1.02
1.00
8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8


5.851
5.815
5.752
5.716
3.804
3.640
3.633
3.616
3.609
3.593
3.586
3.569
3.563
2.356
1.228
1.205
1.181
2.06
3.09
2.08
3.07
3.31
6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0

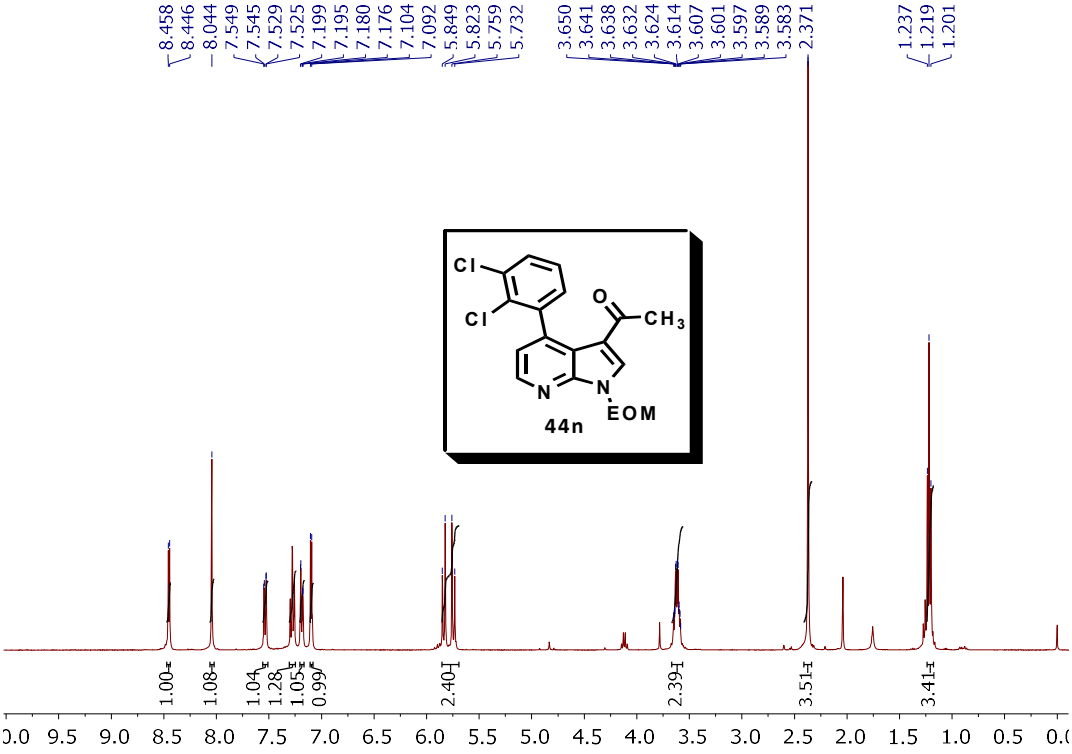
^{1}H-RMN ($CDCl_3$) 3-Acetil-4-(2-cloro-4-metil-fenil)-1-etoximetil-7-azaindol (44m)

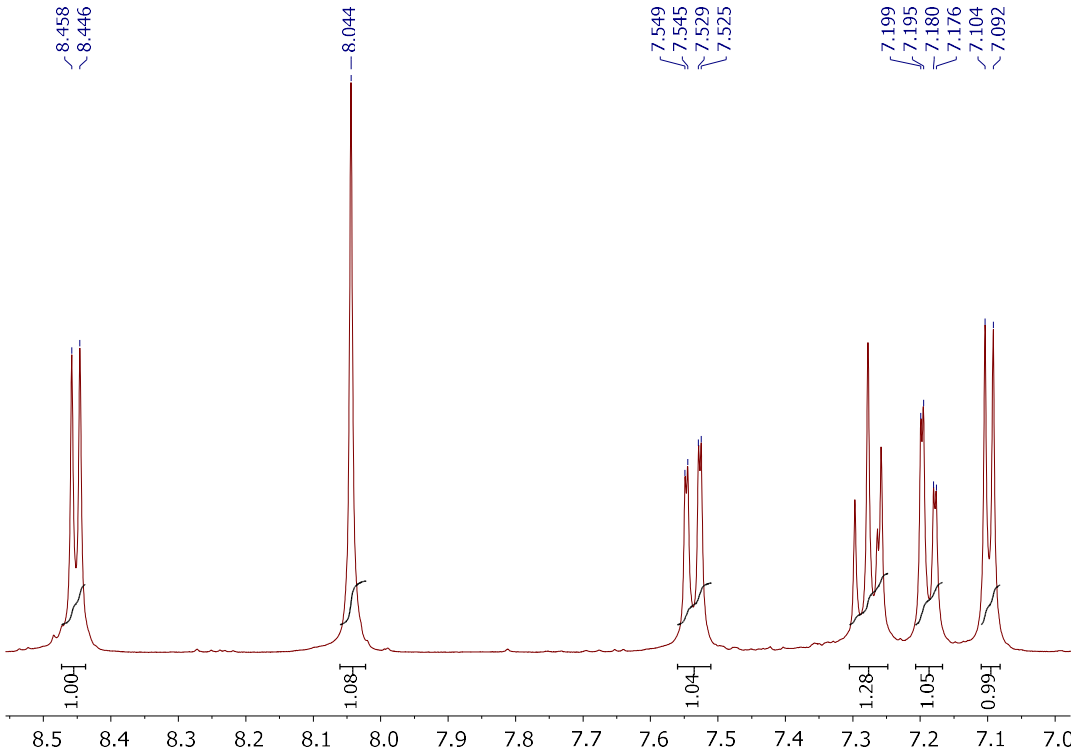


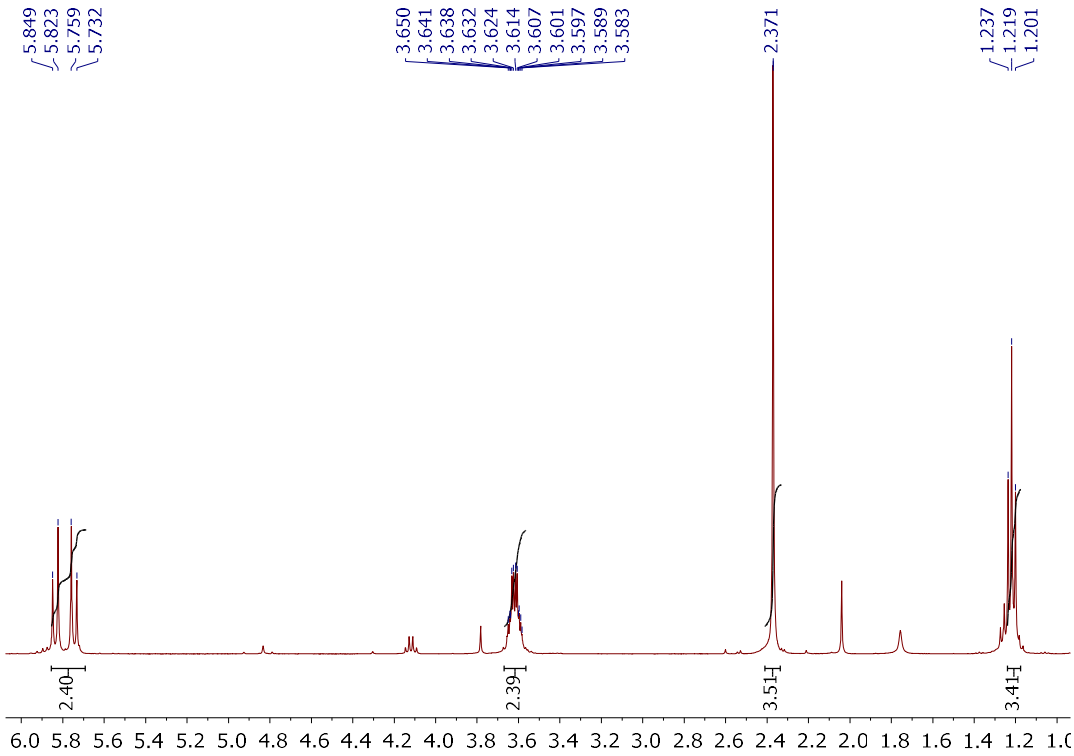




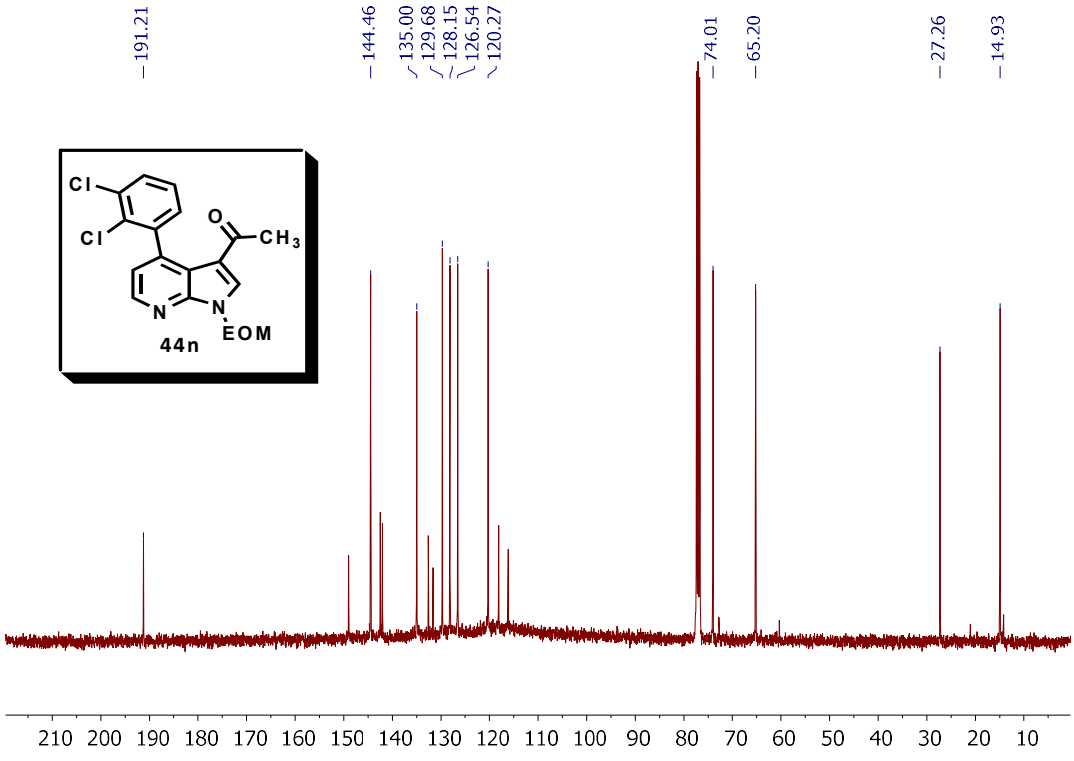
^{1}H-RMN ($CDCl_3$) 3-Acetil-4-(2,3-dicloro-fenil)-1-etoximetil-7-azaindol (44n)

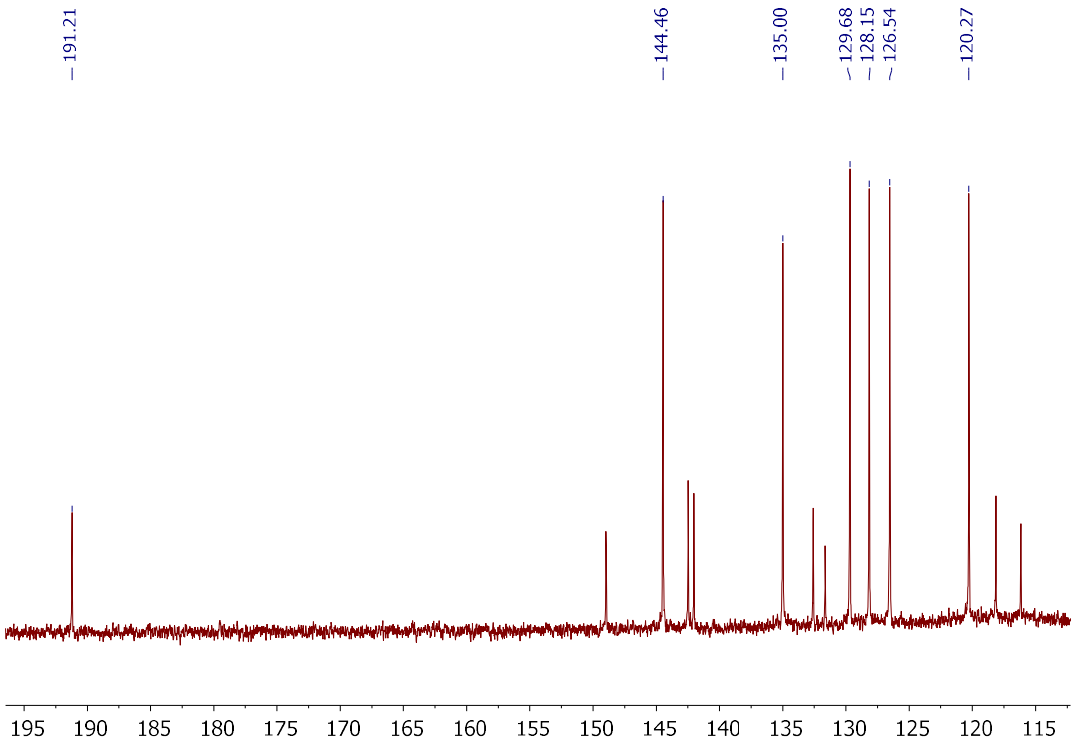



8.458
8.446
8.044
7.549
7.545
7.529
7.525
7.199
7.195
7.180
7.176
7.104
7.092
1.00
1.08
1.04
1.28
1.05
0.99
8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0

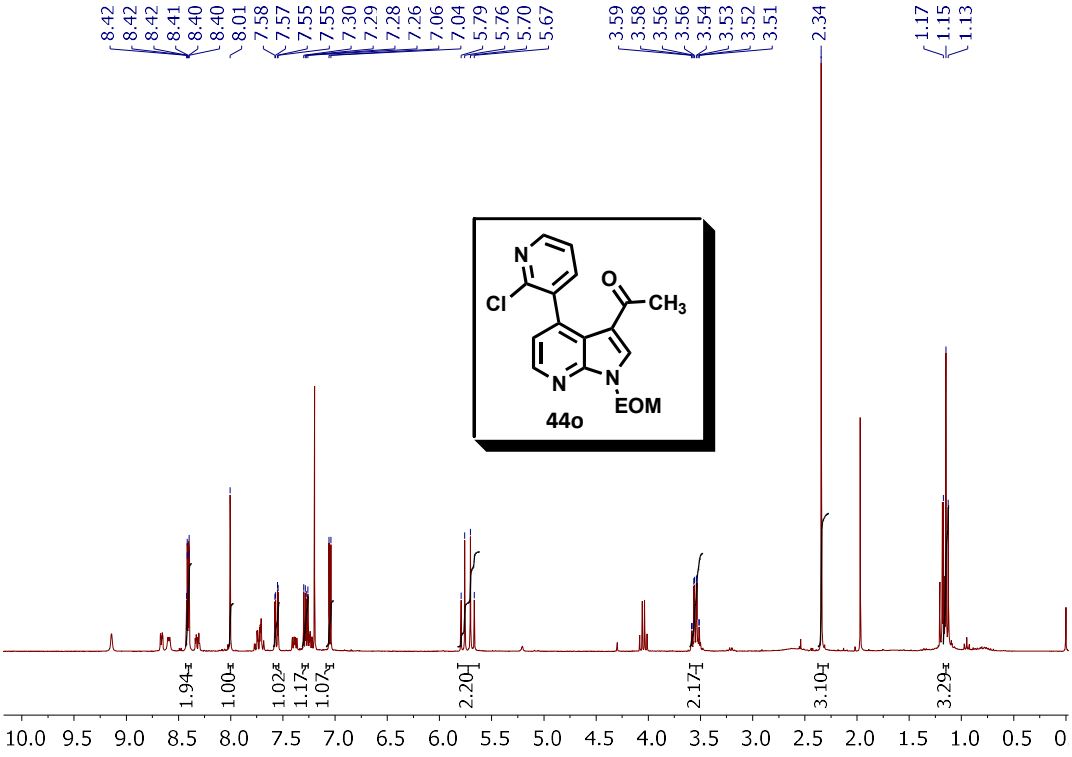

5.849
5.823
5.759
5.732
3.650
3.641
3.638
3.632
3.624
3.614
3.607
3.601
3.597
3.589
3.583
2.371
1.237
1.219
1.201
2.40
2.39
3.51
3.41
6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0

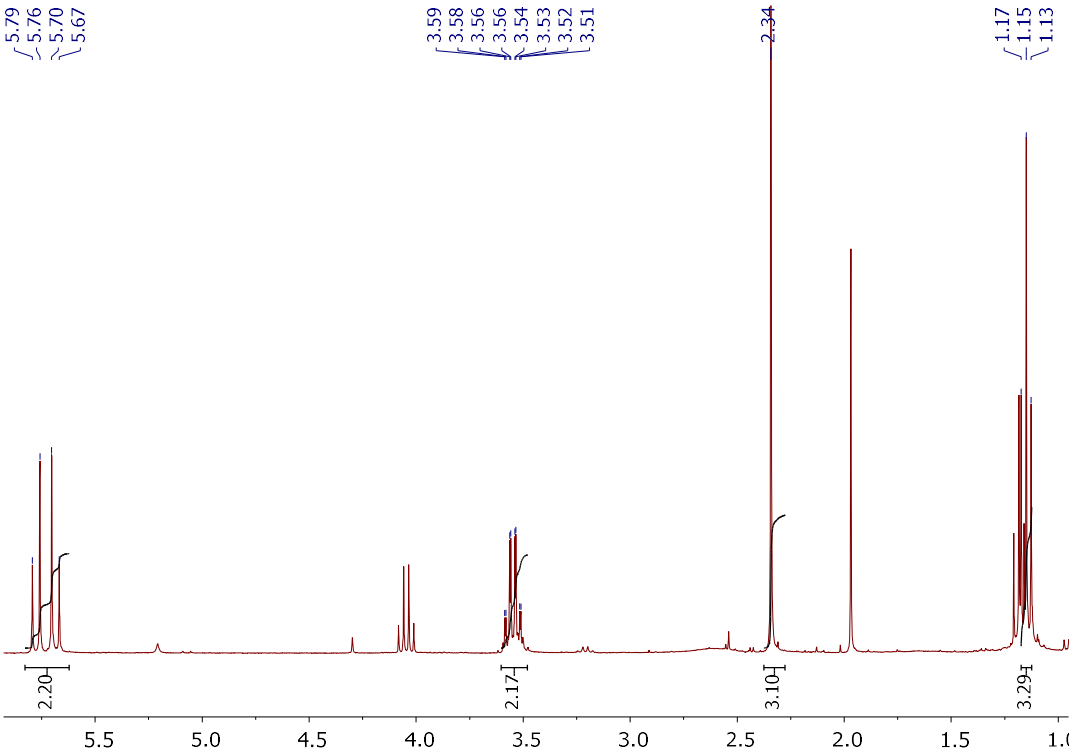
^{13}C-RMN ($CDCl_3$) 3-Acetil-4-(2,3-dicloro-fenil)-1-etoximetil-7-azaindol (44n)

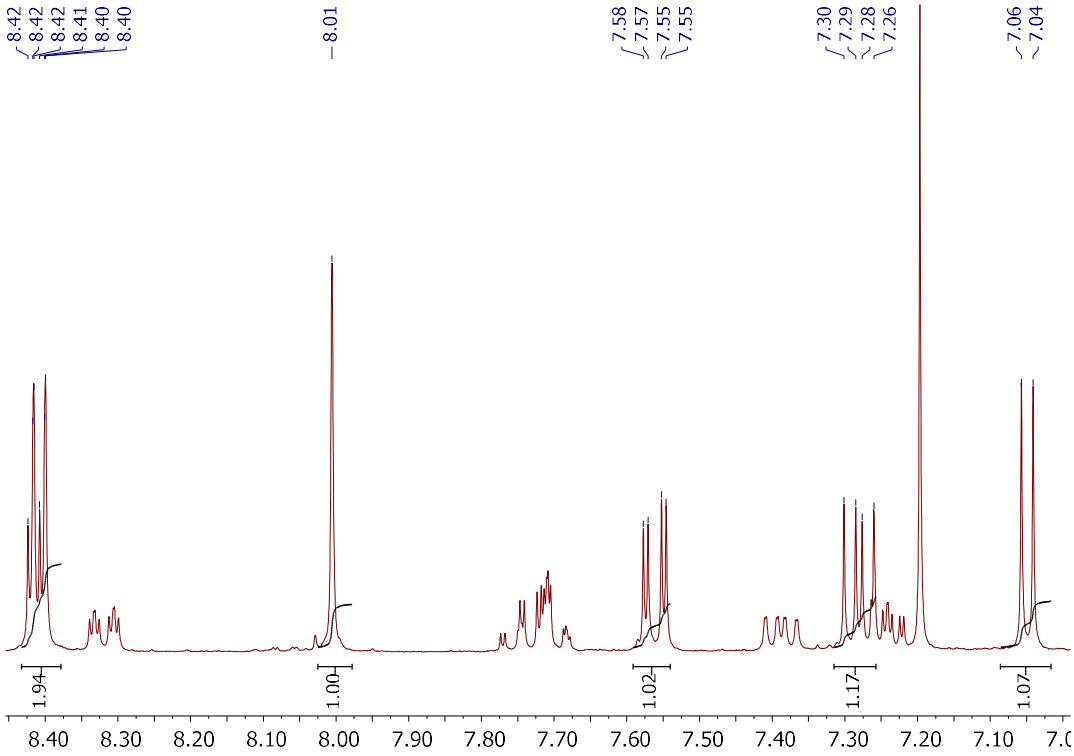




^{1}H-RMN ($CDCl_3$) 3-Acetil-4-(2-cloro-3-piridinil)-1-etoximetil-7-azaindol (44o)

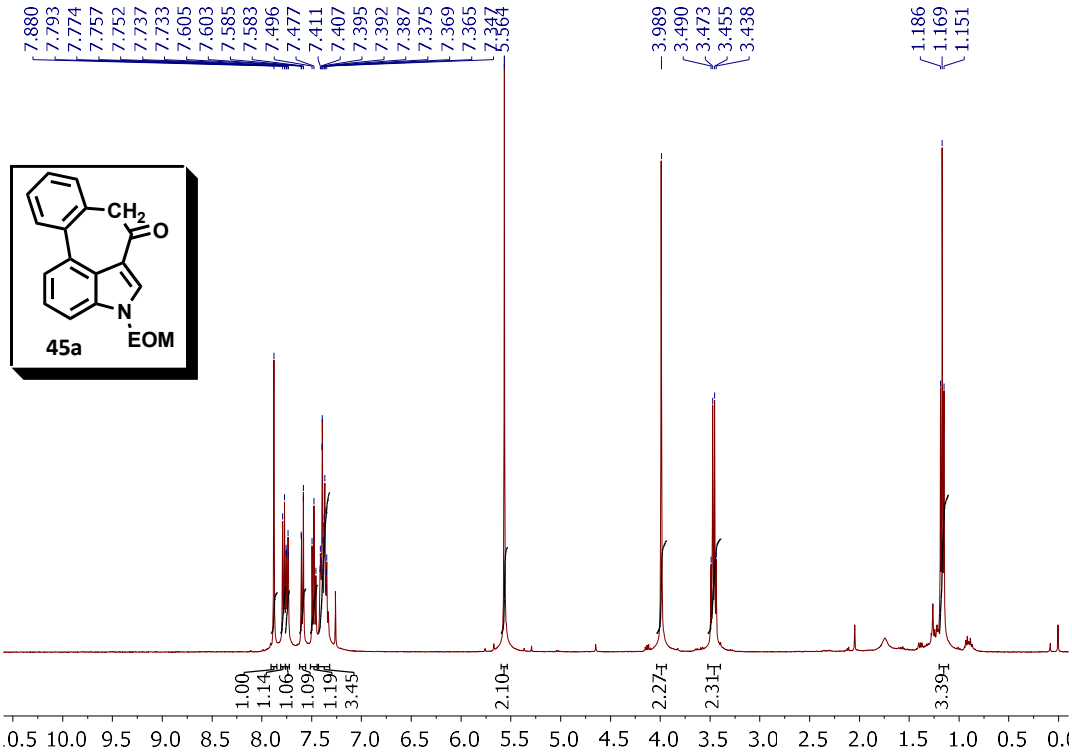


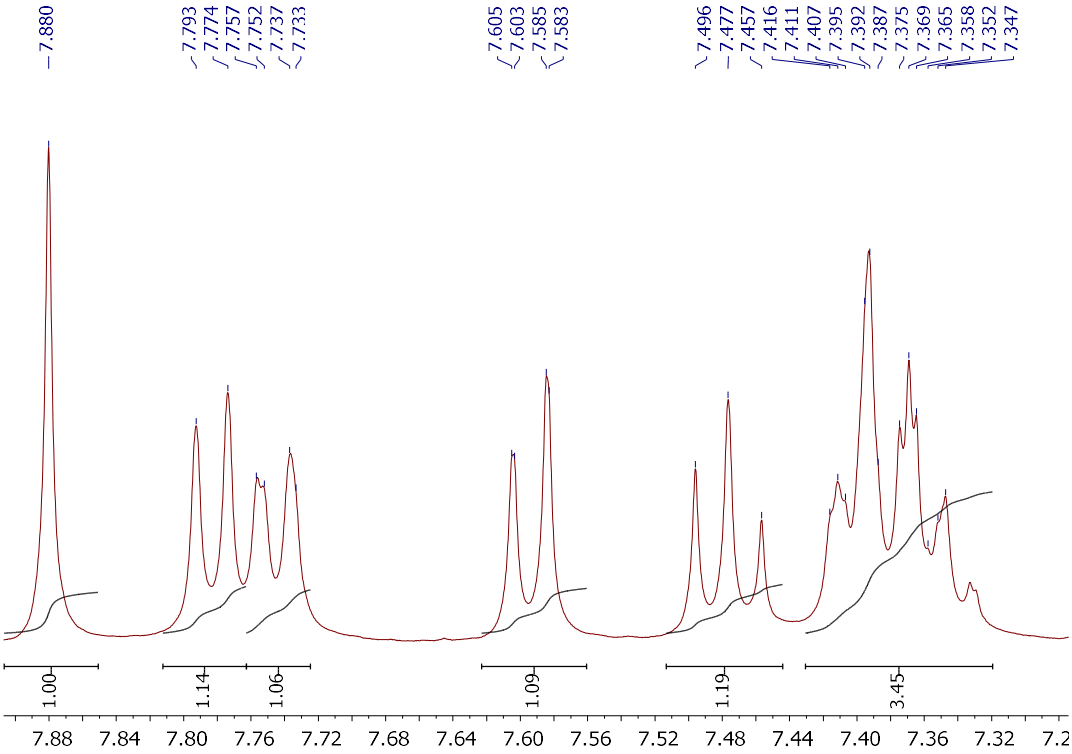


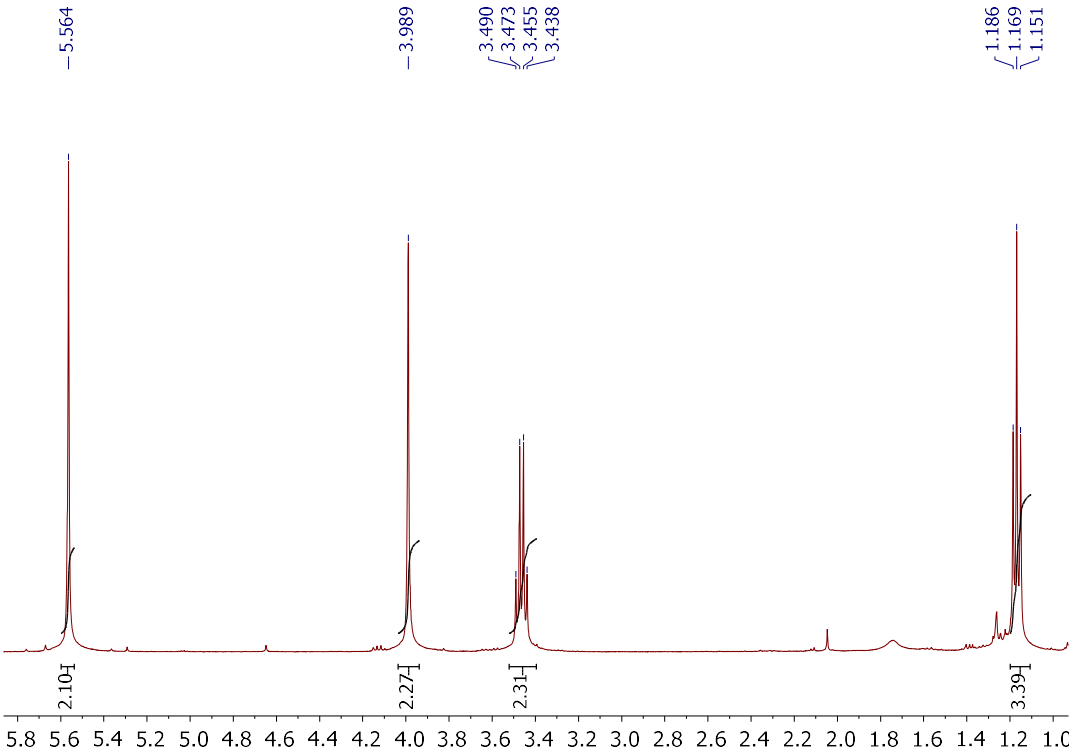


A.5.3 ESPECTROS DE RMN DE PRODUCTOS DE CIERRE DE ANILLO

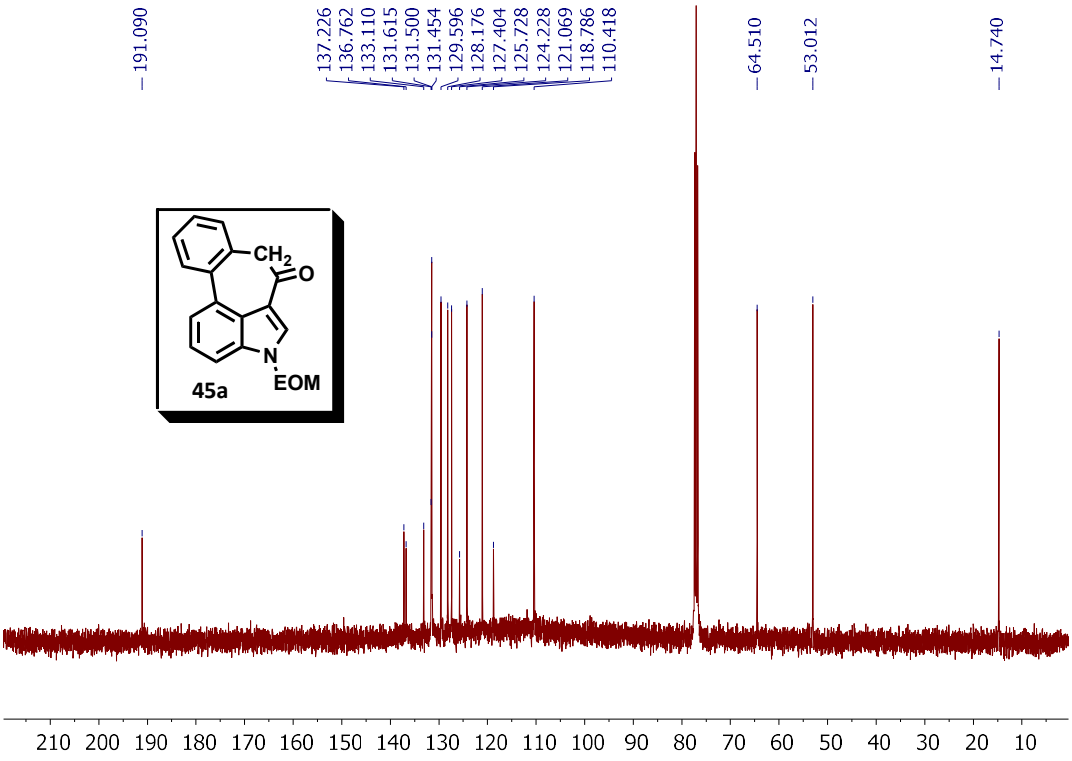
^{1}H-RMN ($CDCl_3$) 4-(Etoximetil)-4,7-dihidro-6*H*-3,4-azadibenzo[*cd*,*f*]azulen-6-ona (45a)


7.880
7.793
7.774
7.757
7.752
7.737
7.733
7.605
7.603
7.585
7.583
7.496
7.477
7.411
7.407
7.395
7.392
7.387
7.375
7.369
7.365
7.347
5.584
3.989
3.490
3.473
3.455
3.438
1.186
1.169
1.151
CH2
O
N
EOM
45a
1.00
1.14
1.06
1.09
1.19
3.45
2.10
2.27
2.31
3.39
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5

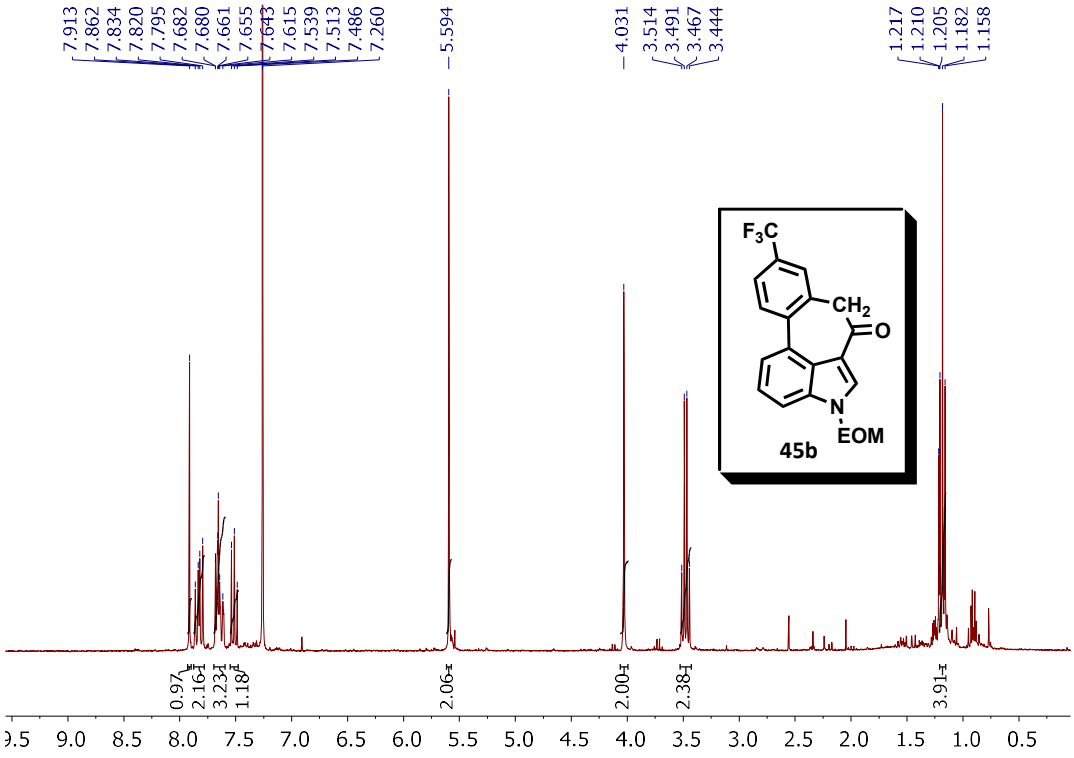

7.880
7.793
7.774
7.757
7.752
7.737
7.733
7.605
7.603
7.585
7.583
7.496
7.477
7.457
7.416
7.411
7.407
7.395
7.392
7.387
7.375
7.369
7.365
7.358
7.352
7.347
1.00
1.14
1.06
1.09
1.19
3.45
7.88 7.84 7.80 7.76 7.72 7.68 7.64 7.60 7.56 7.52 7.48 7.44 7.40 7.36 7.32

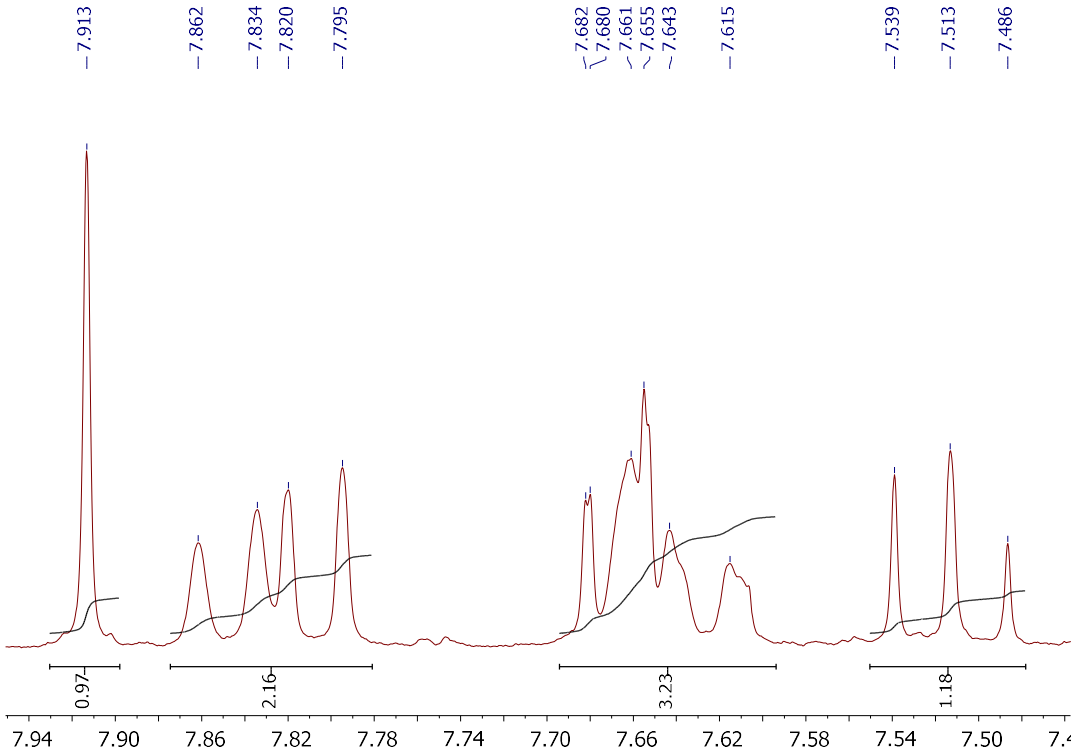


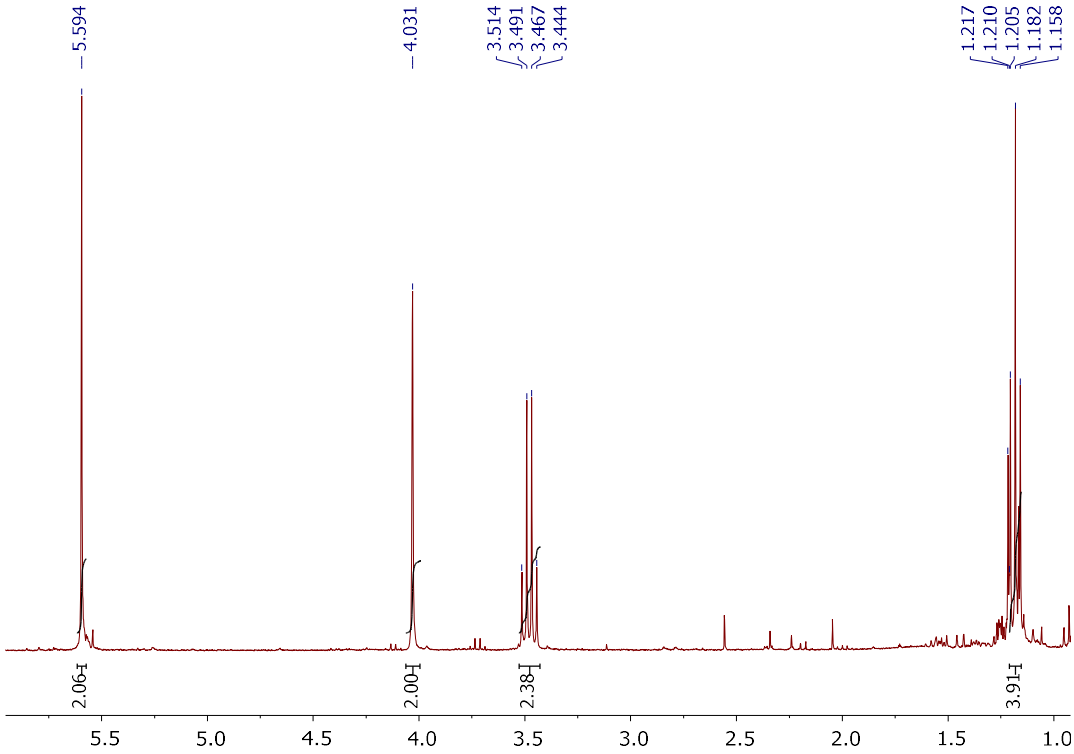
^{13}C-RMN ($CDCl_3$) 4-(Etoximetil)-4,7-dihidro-6*H*-3,4-azadibenzo[*cd*,*f*]azulen-6-ona (45a)



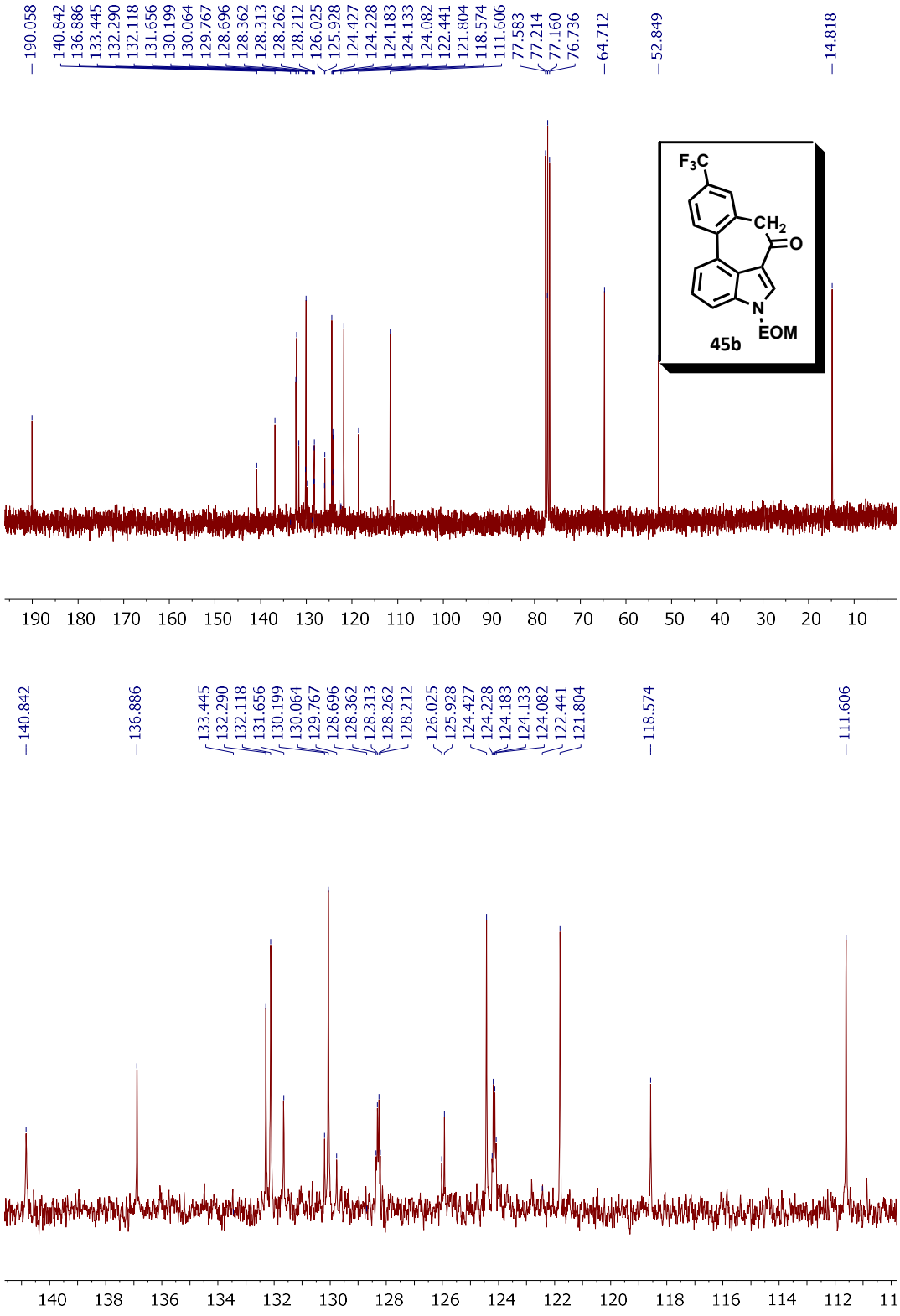
^{1}H-RMN ($CDCl_3$) 4-(Etoximetil)-9-trifluormetil-4,7-dihidro-6*H*-3,4-azadibenzo[*cd*,*f*]azulen-6-ona (45b)



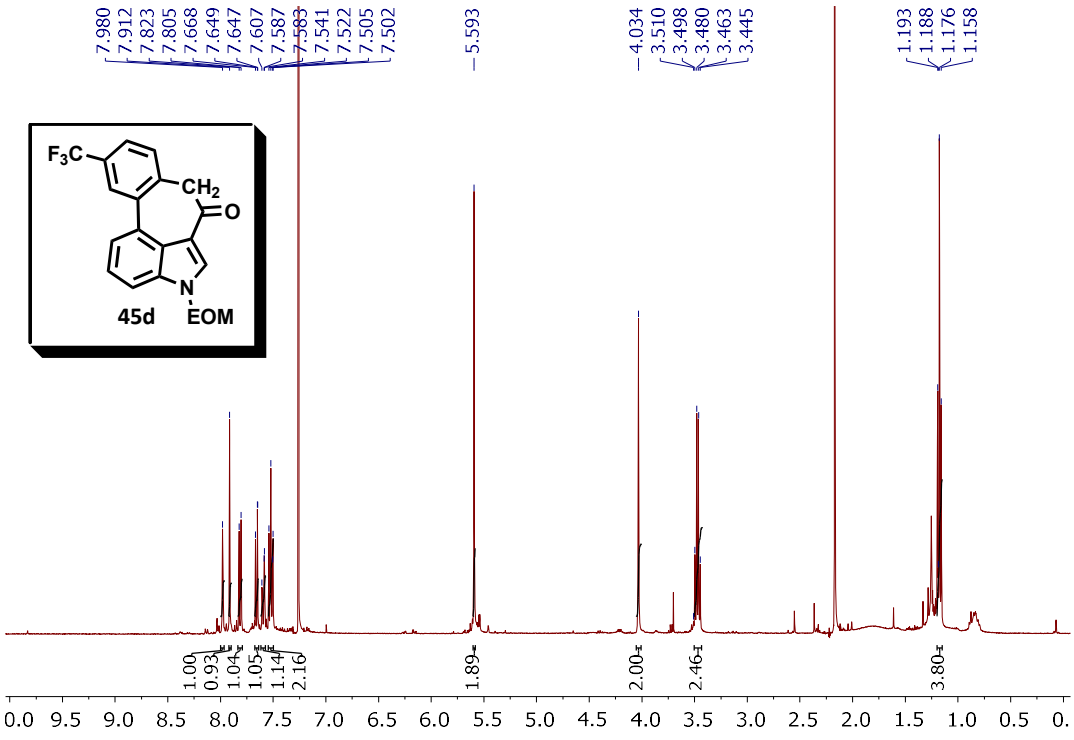

7.913
7.862
7.834
7.820
7.795
7.682
7.680
7.661
7.655
7.643
7.615
7.539
7.513
7.486
0.97
2.16
3.23
1.18
7.94
7.90
7.86
7.82
7.78
7.74
7.70
7.66
7.62
7.58
7.54
7.50

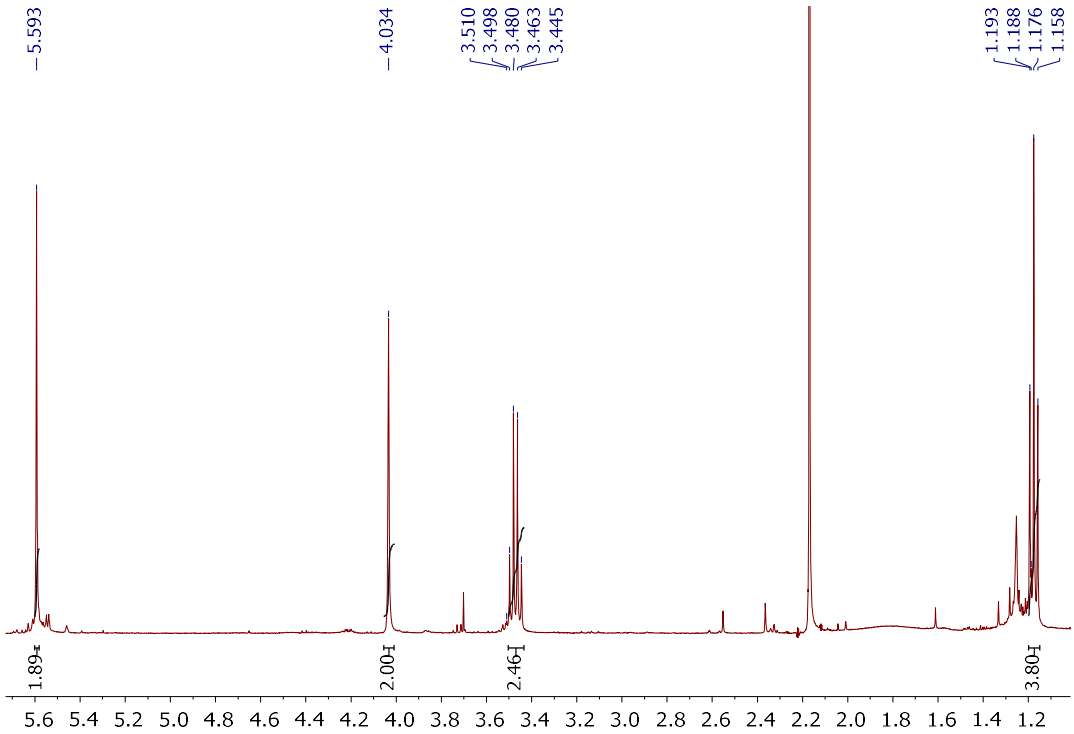

5.594
4.031
3.514
3.491
3.467
3.444
1.217
1.210
1.205
1.182
1.158
2.06
2.00
2.38
3.91
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0

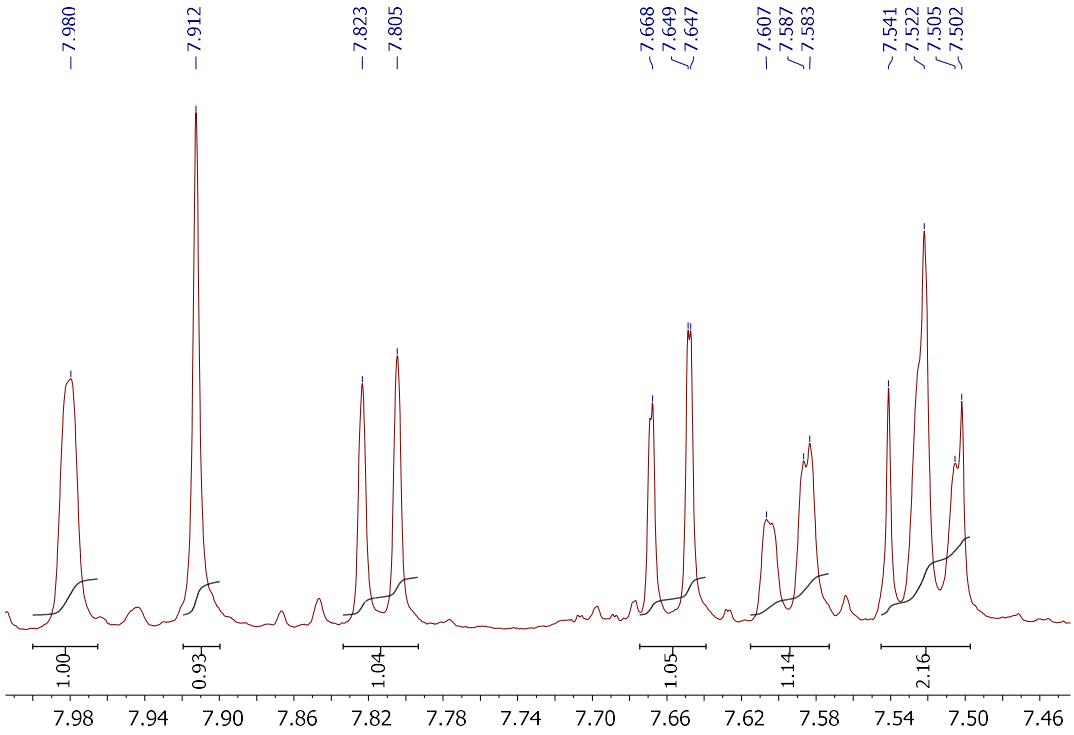
^{13}C-RMN ($CDCl_3$) 4-(Etoximetil)-9-trifluormetil-4,7-dihidro-6*H*-3,4-azadibenzo[*cd*,*f*]azulen-6-ona (45b)



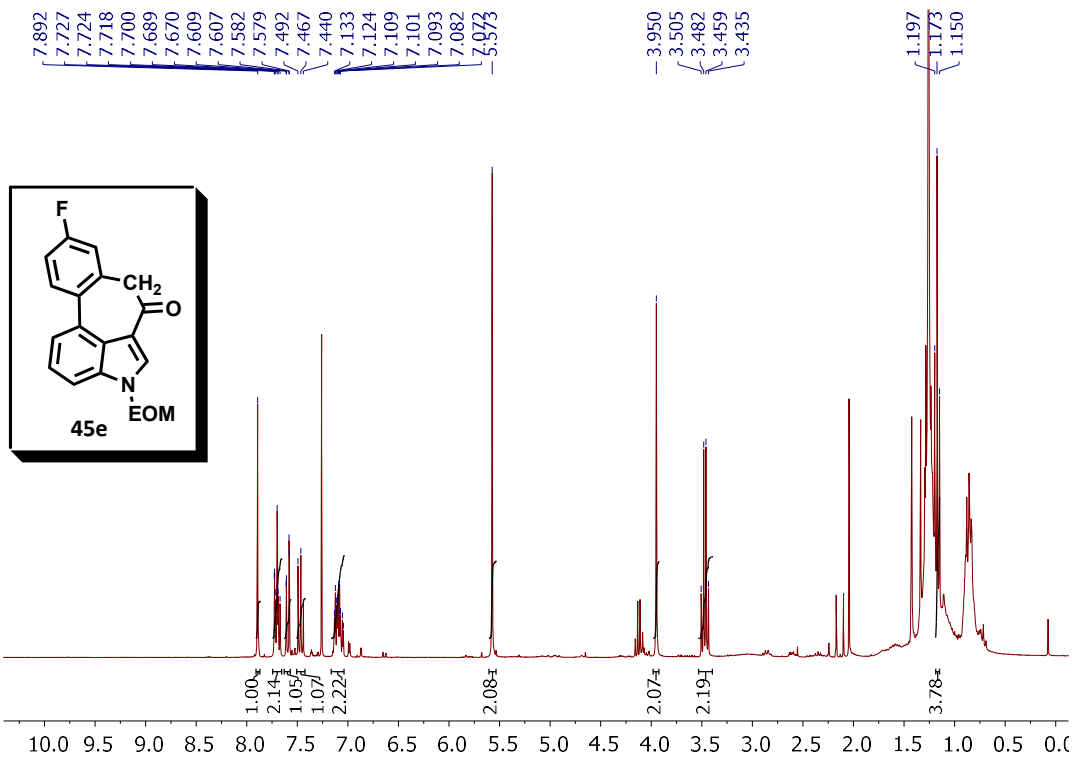
^{1}H-RMN ($CDCl_3$) 4-(Etoximetil)-10-trifluormetil-4,7-dihidro-6*H*-3,4-azadibenzo[*cd*,*f*]azulen-6-ona (45d)







^{1}H-RMN ($CDCl_3$) 4-(Etoximetil)-9-fluor-4,7-dihidro-6*H*-3,4-azadibenzo[*cd*,*f*]azulen-6-ona (45e)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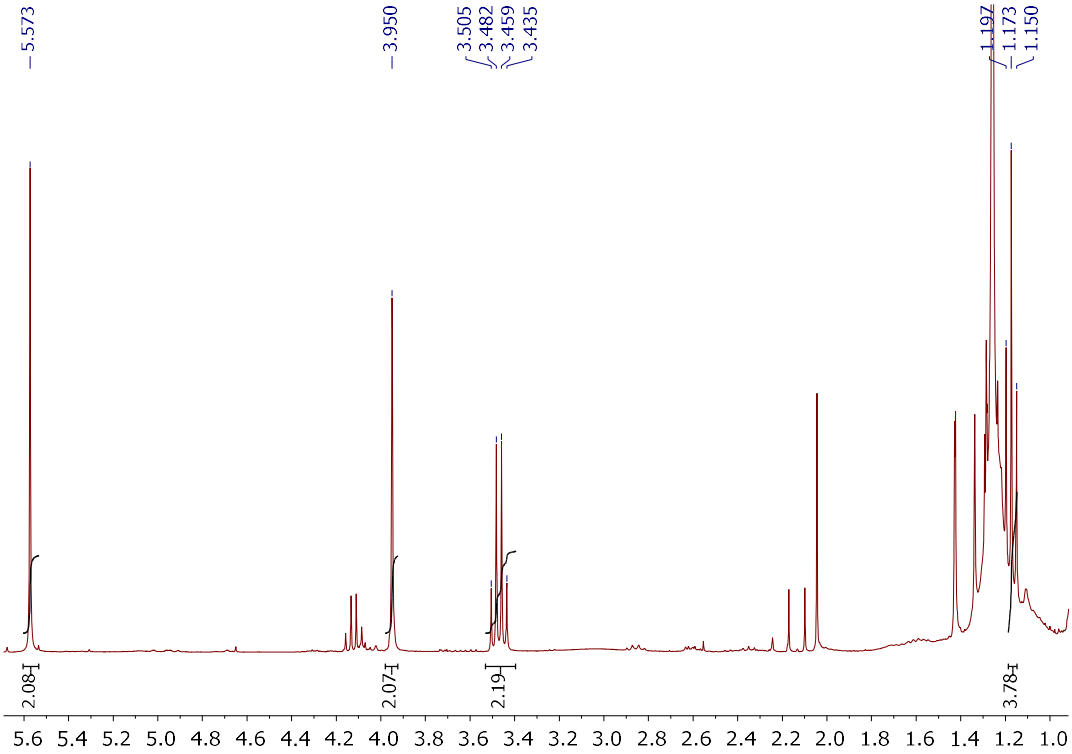
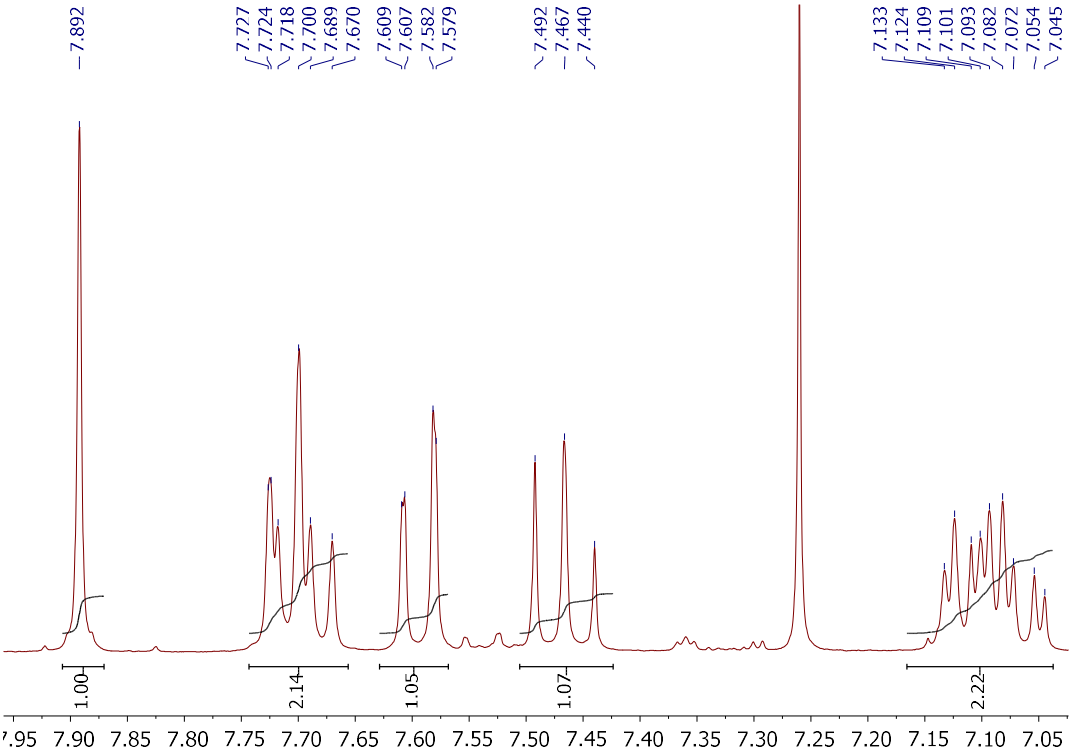
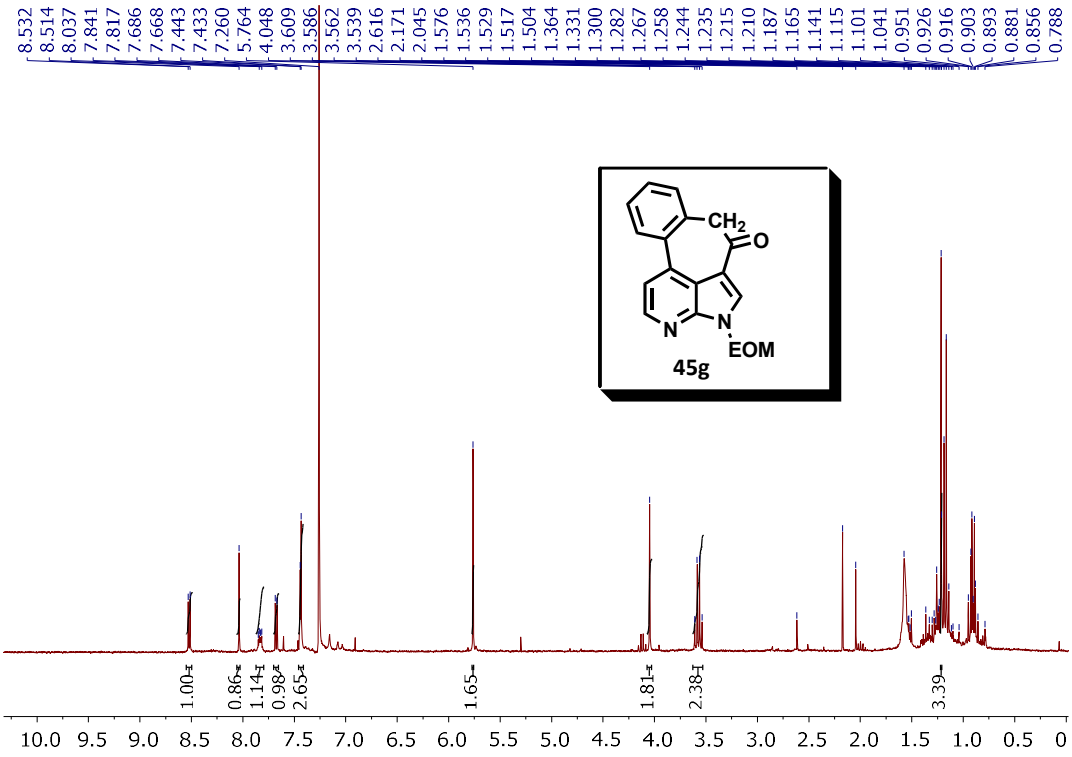
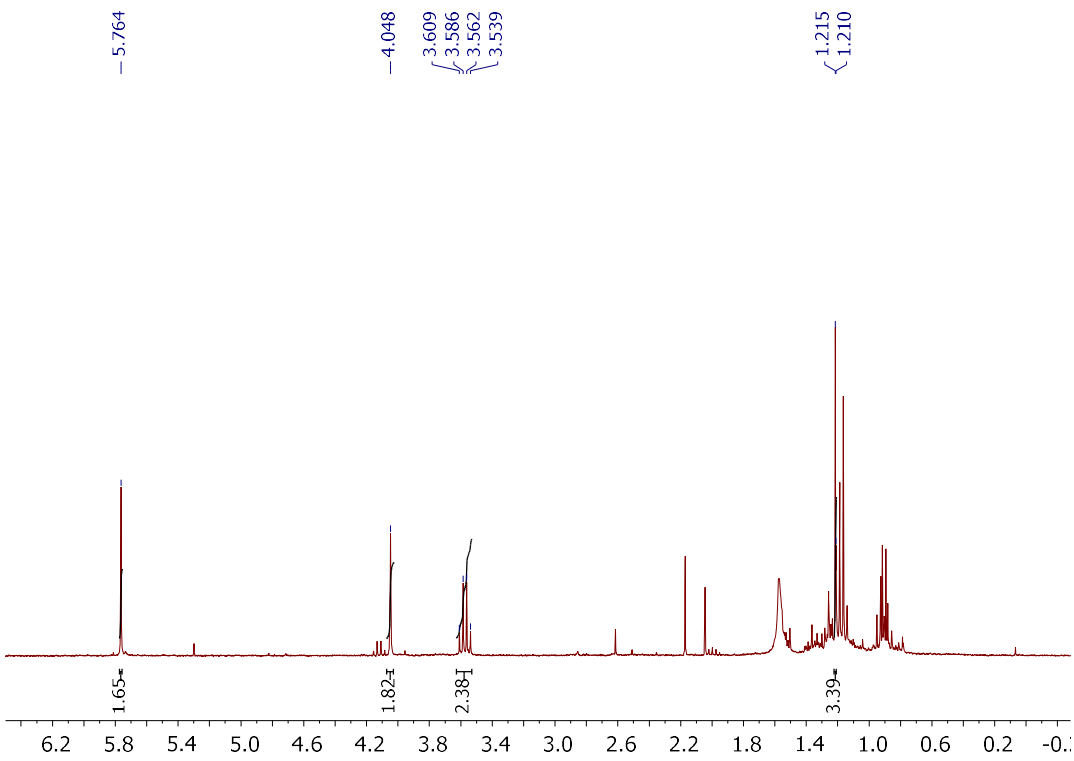
7.727
7.724
7.718
7.700
7.689
7.670
7.609
7.607
7.582
7.579
7.492
7.467
7.440
7.133
7.124
7.109
7.101
7.093
7.082
7.072
5.573
3.950
3.505
3.482
3.459
3.435
1.197
1.173
1.150
F
CH2
O
N
EOM
45e
1.00
2.14
1.05
1.07
2.22
2.08
2.07
2.19
3.78
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

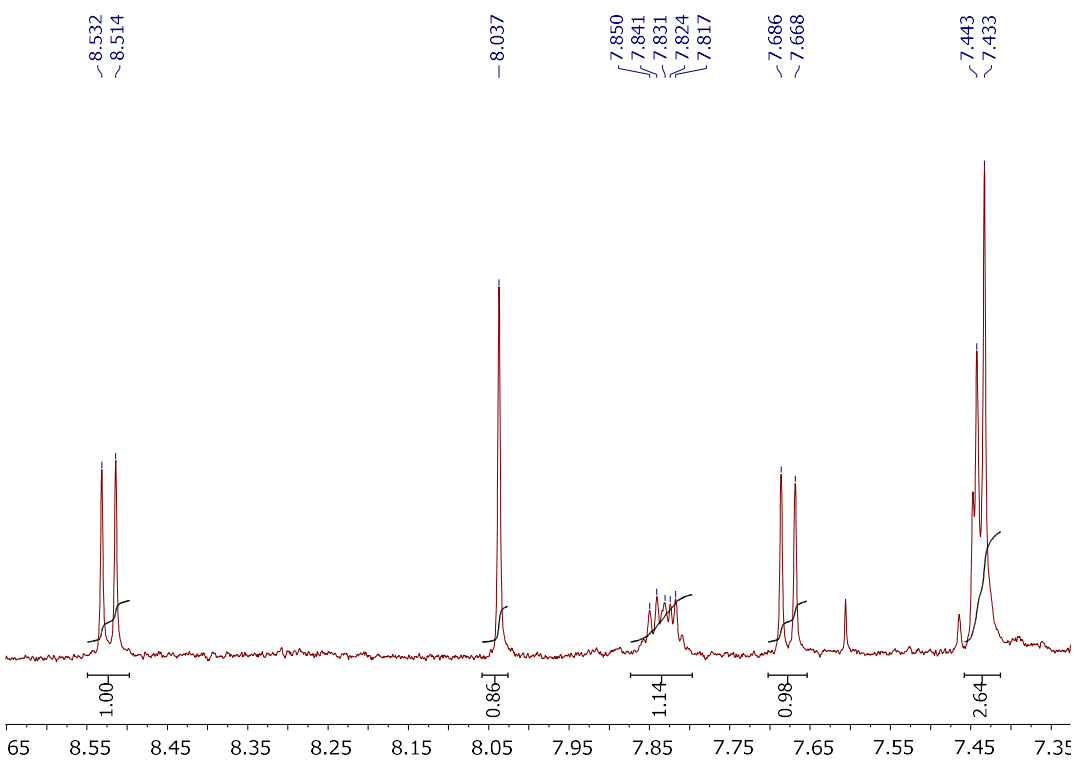

5.573
3.950
3.505
3.482
3.459
3.435
1.197
1.173
1.150
2.08
2.07
2.19
3.78
5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0



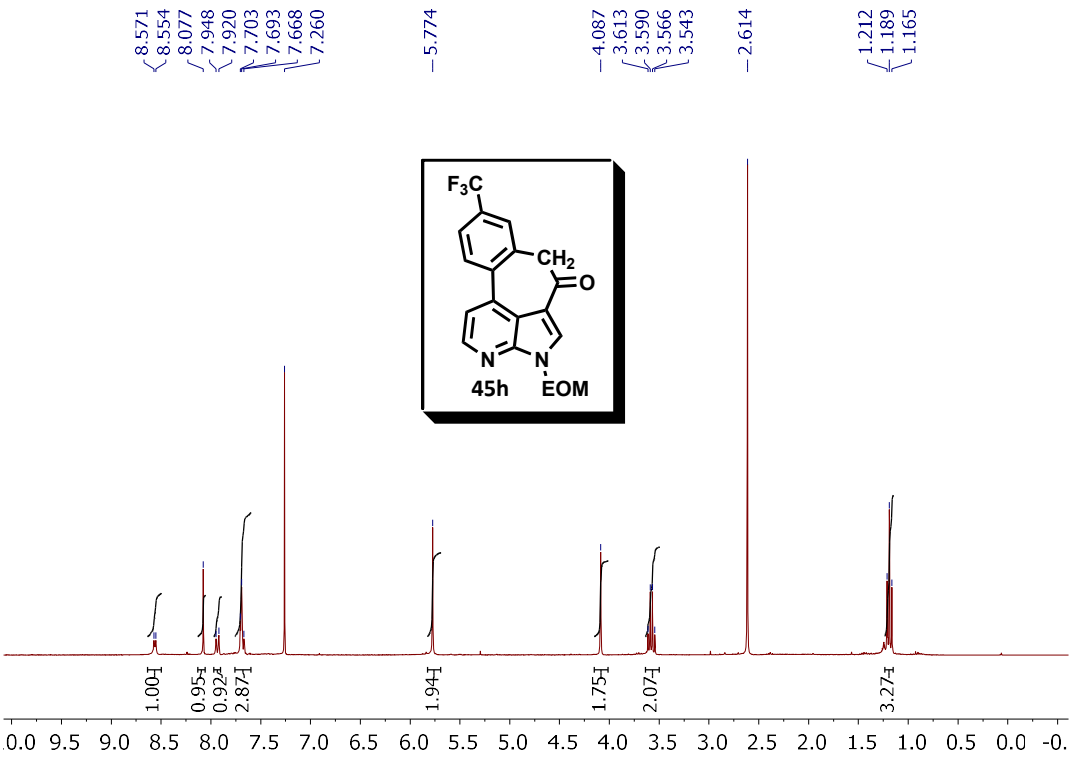
^{1}H-RMN ($CDCl_3$) 4-(Etoximetil)-4,7-dihidro-6*H*-3,4-diazadibenzo[*cd*,*f*]azulen-6-ona (45g)

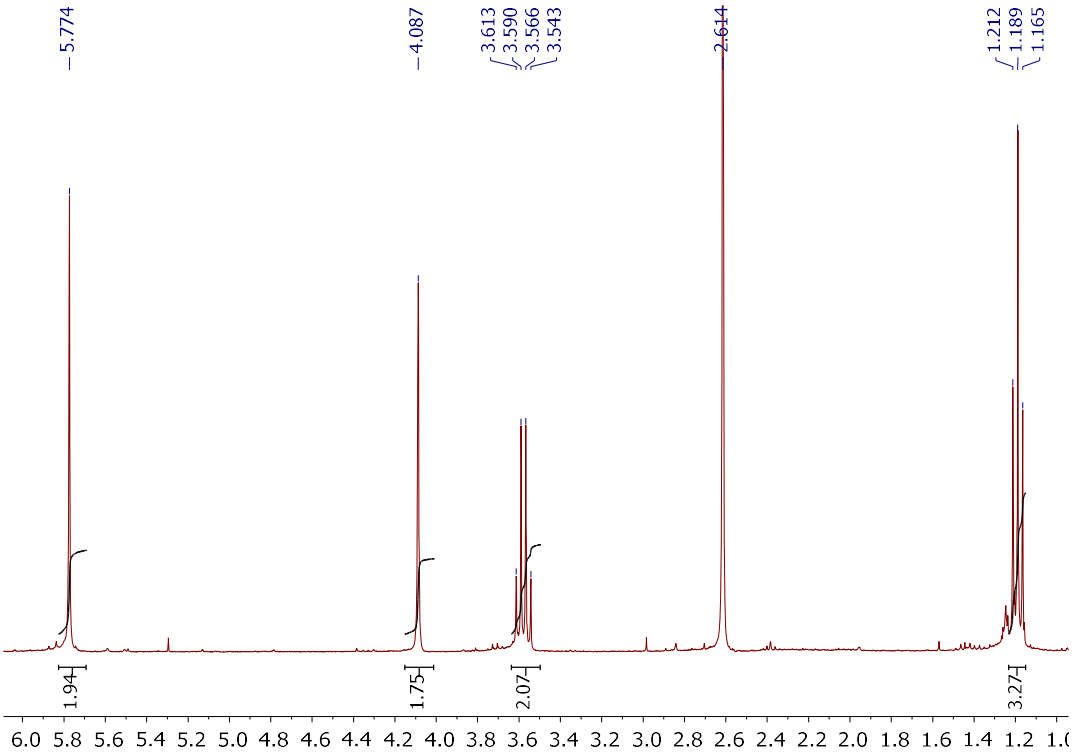


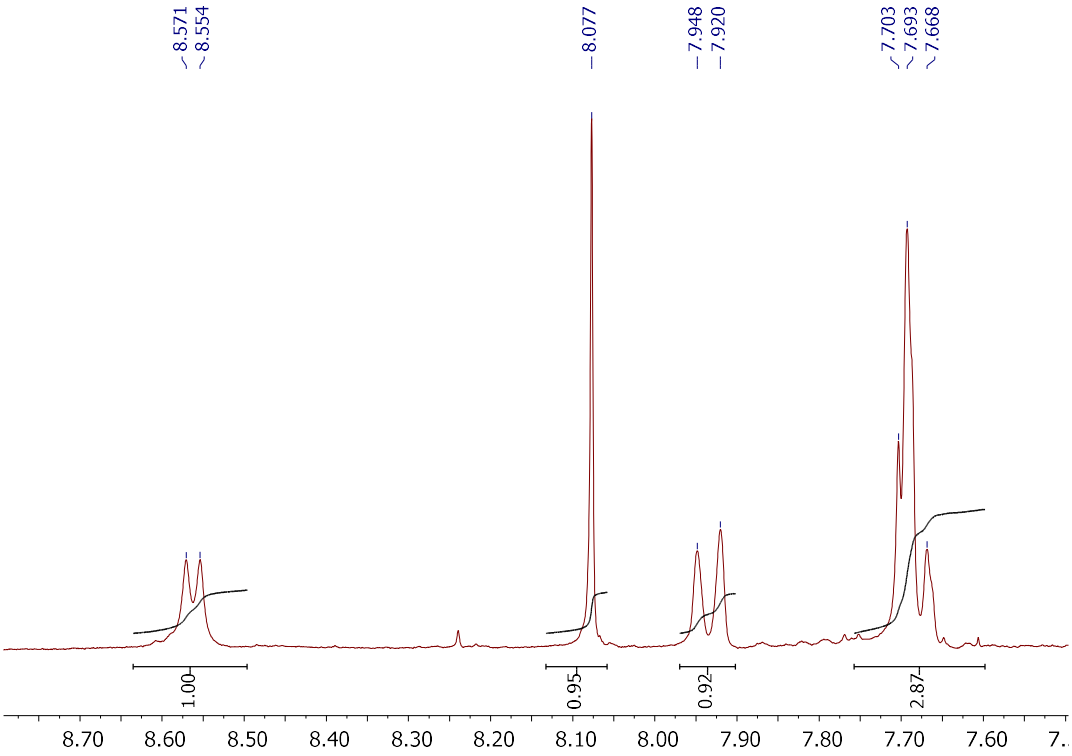

5.764
4.048
3.609
3.586
3.562
3.539
1.215
1.210
1.65
1.82
2.38
3.39
6.2
5.8
5.4
5.0
4.6
4.2
3.8
3.4
3.0
2.6
2.2
1.8
1.4
1.0
0.6
0.2


8.532
8.514
8.037
7.850
7.841
7.831
7.824
7.817
7.686
7.668
7.443
7.433
1.00
0.86
1.14
0.98
2.64
8.55
8.45
8.35
8.25
8.15
8.05
7.95
7.85
7.75
7.65
7.55
7.45

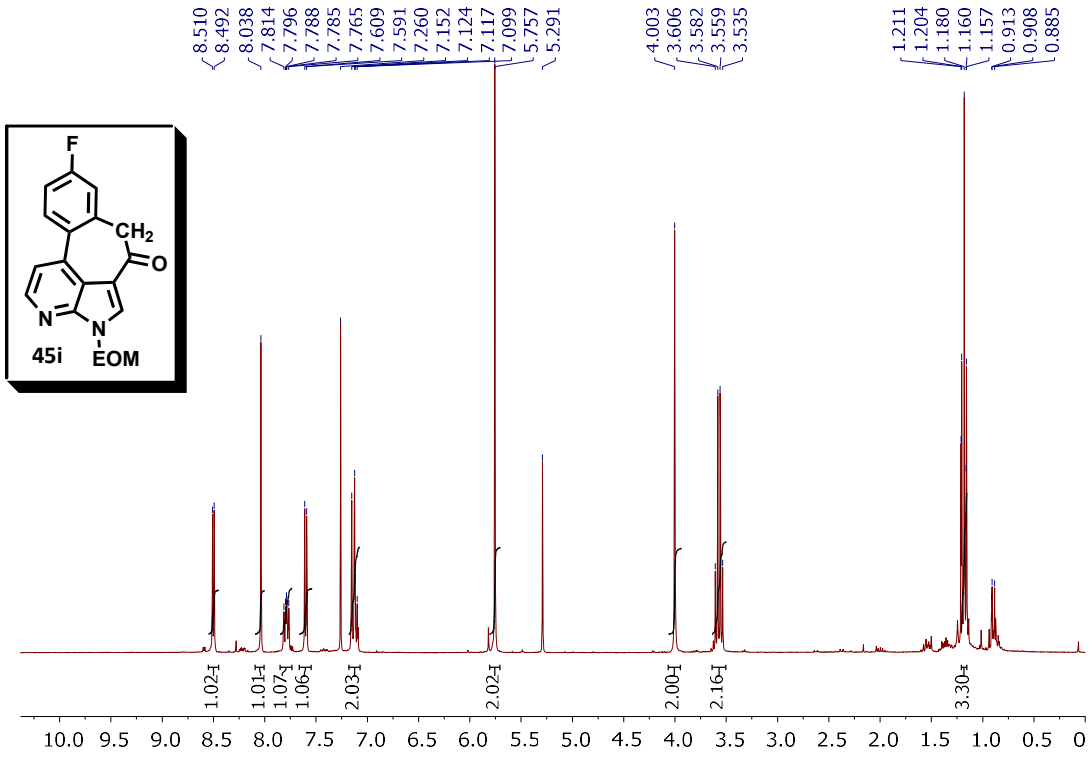
^{1}H-RMN ($CDCl_3$) 4-(Etoximetil)-9-trifluormetil-4,7-dihidro-6*H*-3,4-diazadibenzo[*cd*,*f*]azulen-6-ona (45h)

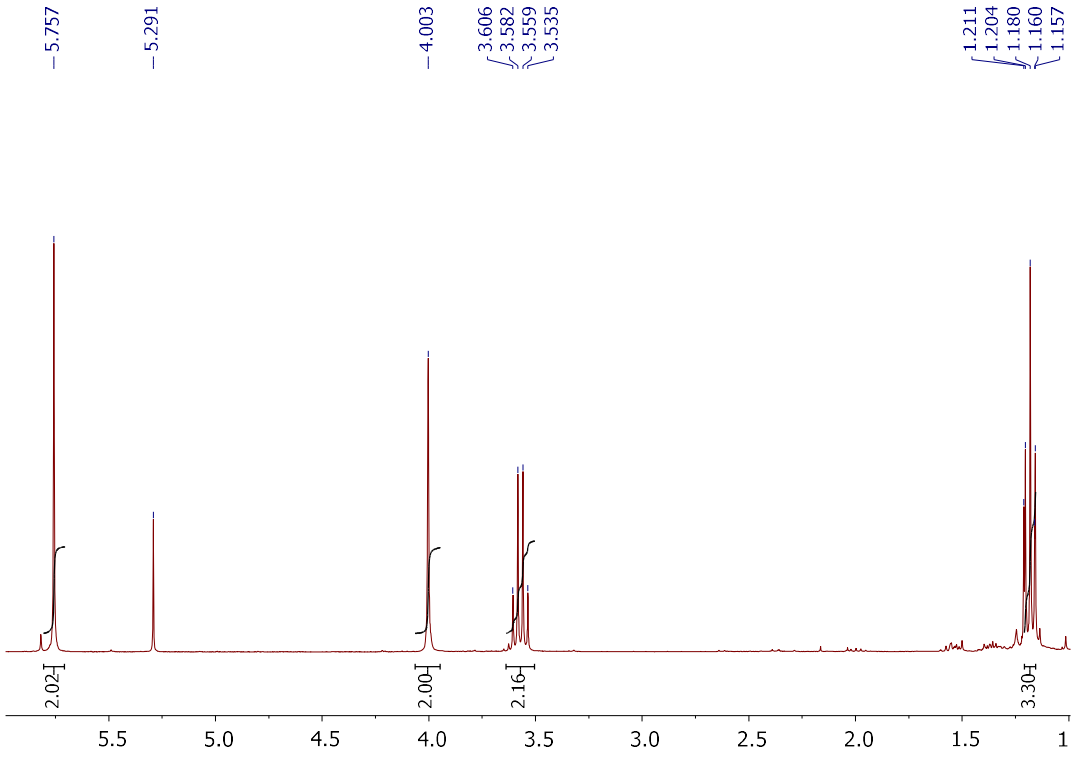


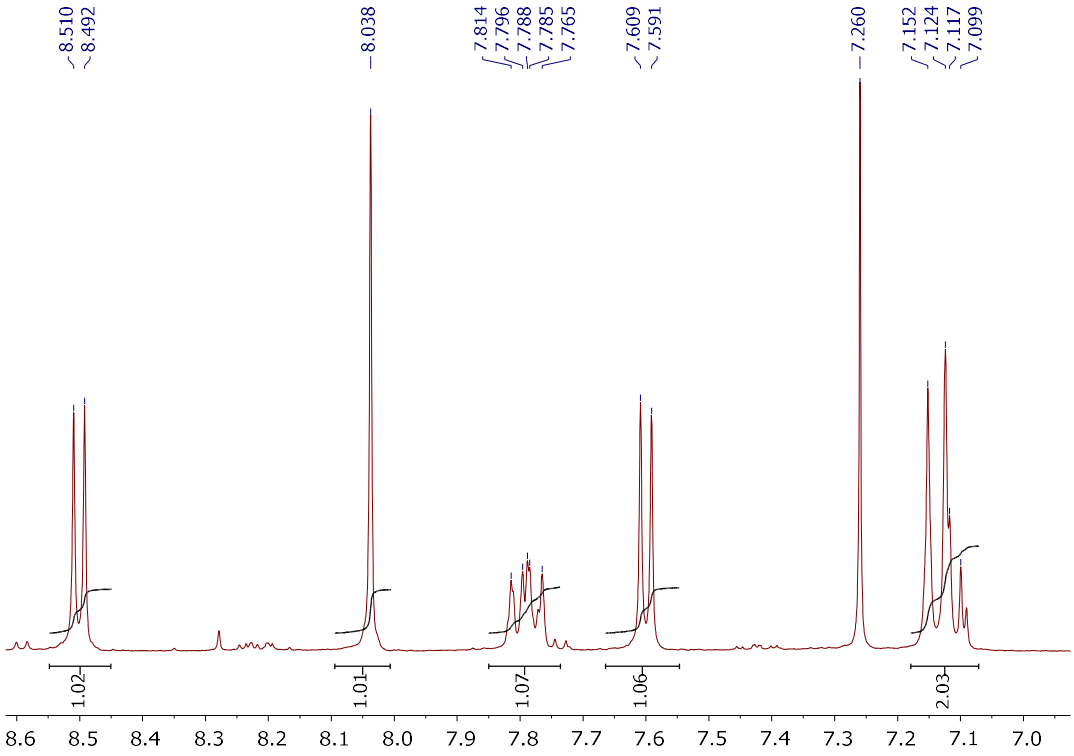




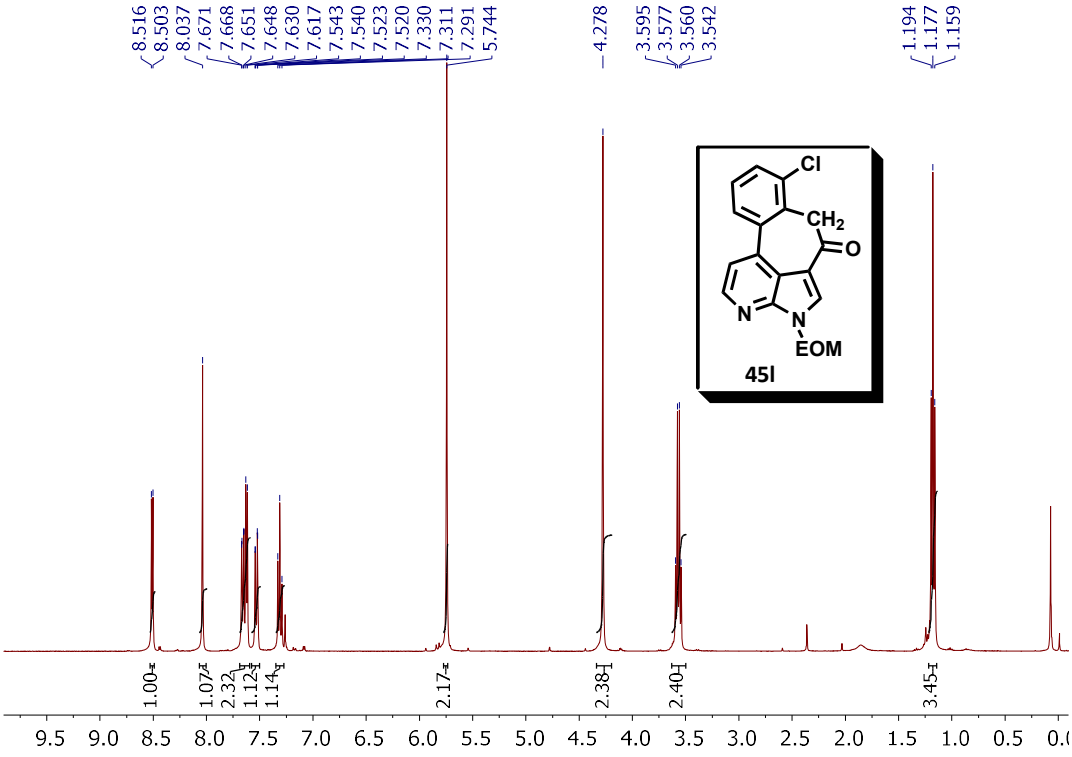
^{1}H-RMN ($CDCl_3$) 4-(Etoximetil)-4,7-dihidro-6*H*-3,4-diazadibenzo[*cd*,*f*]azulen-6-ona (45g)

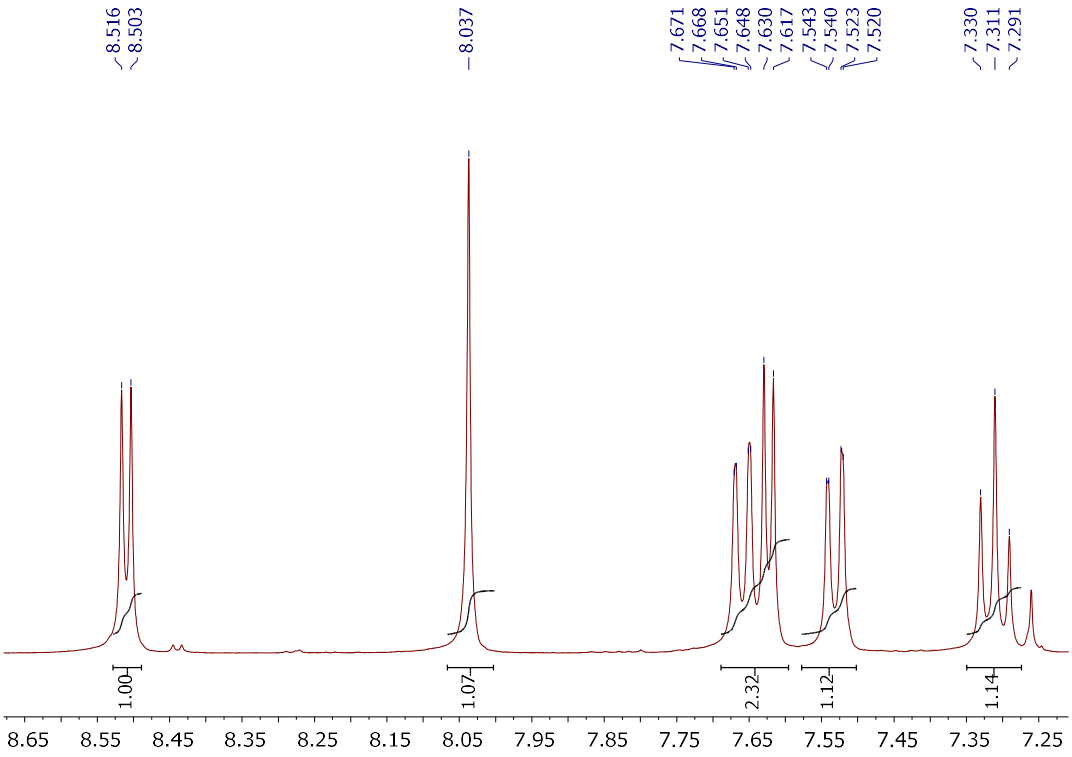


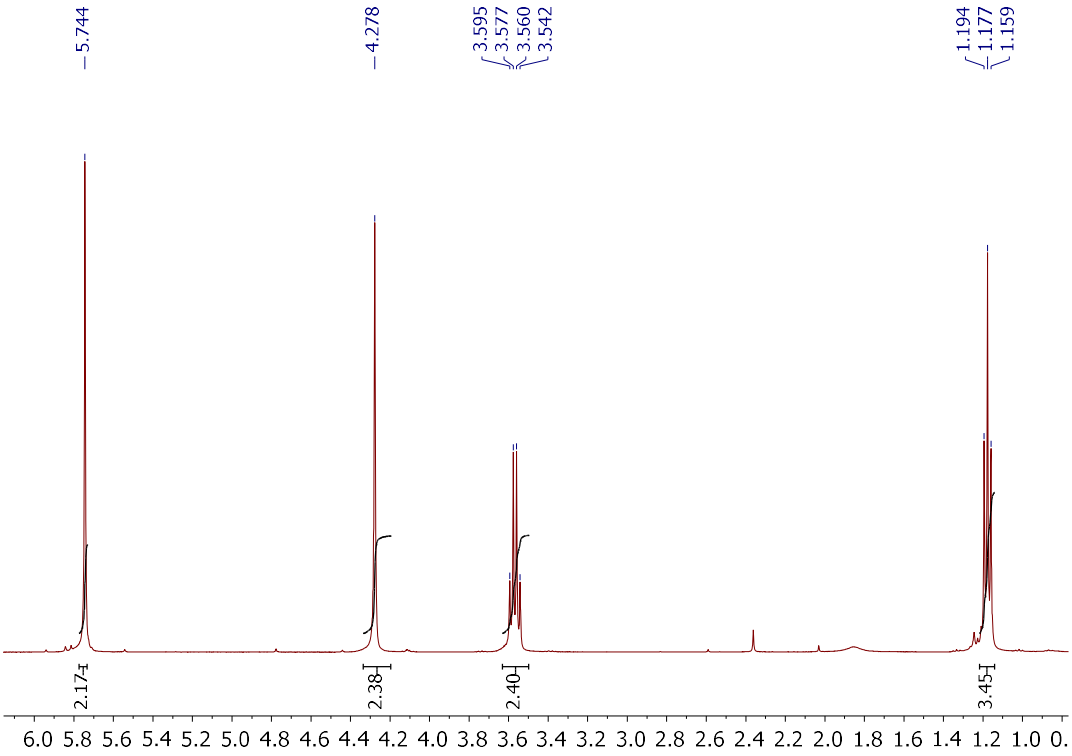

5.757
5.291
4.003
3.606
3.582
3.559
3.535
1.211
1.204
1.180
1.160
1.157
2.02
2.00
2.16
3.30
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1


8.510
8.492
8.038
7.814
7.796
7.788
7.785
7.765
7.609
7.591
7.260
7.152
7.124
7.117
7.099
1.02
1.01
1.07
1.06
2.03
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0

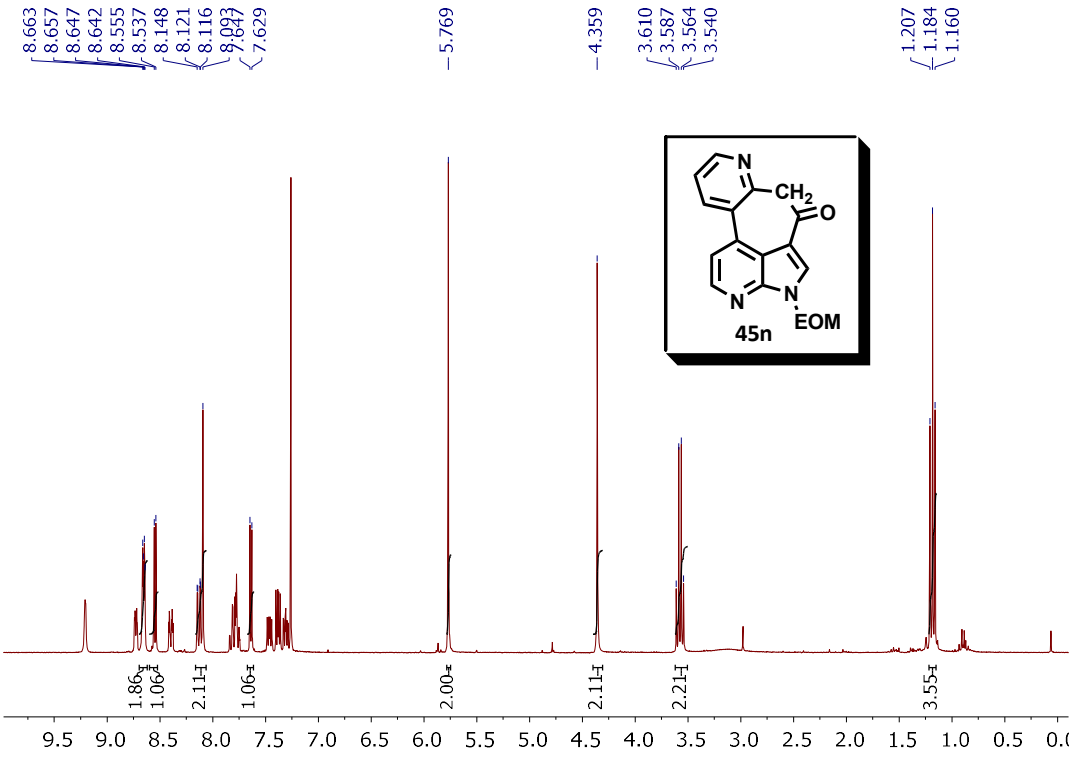
^{1}H-RMN ($CDCl_3$) 4-(Etoximetil)-8-cloro-4,7-dihidro-6*H*-3,4-diazadibenzo[*cd*,*f*]azulen-6-ona (45l)

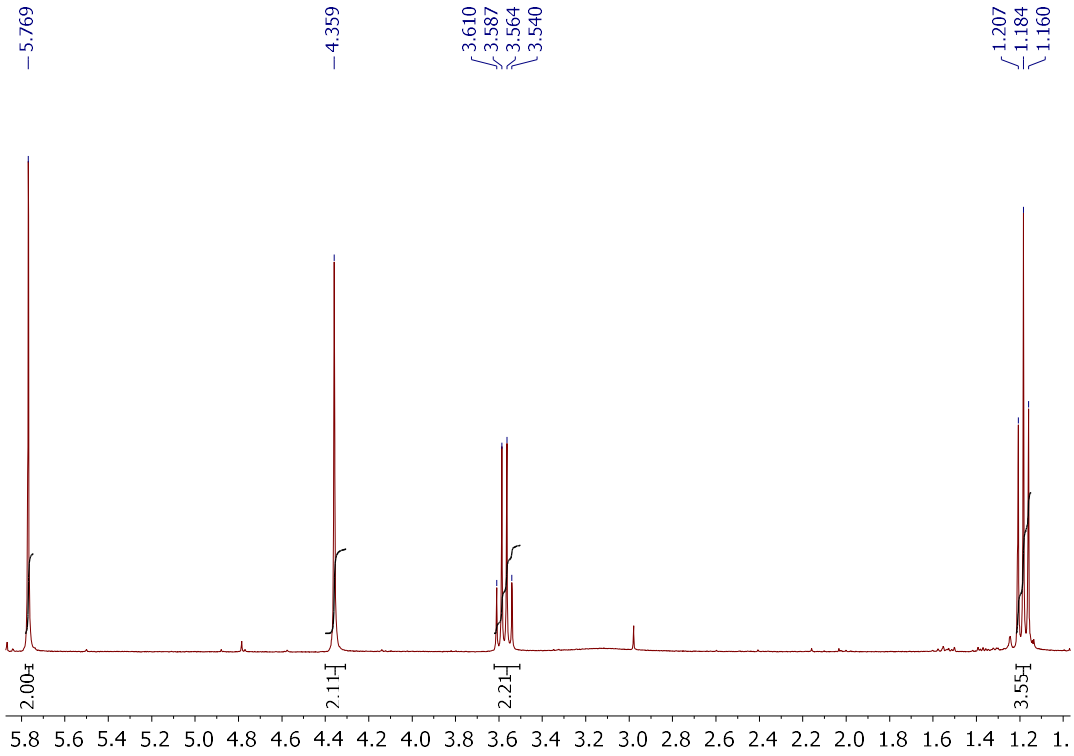






^{1}H-RMN ($CDCl_3$) 4-(Etoximetil)-4,7-dihidro-6*H*-3,4-triazadibenzo[*cd*,*f*]azulen-6-ona (45n)

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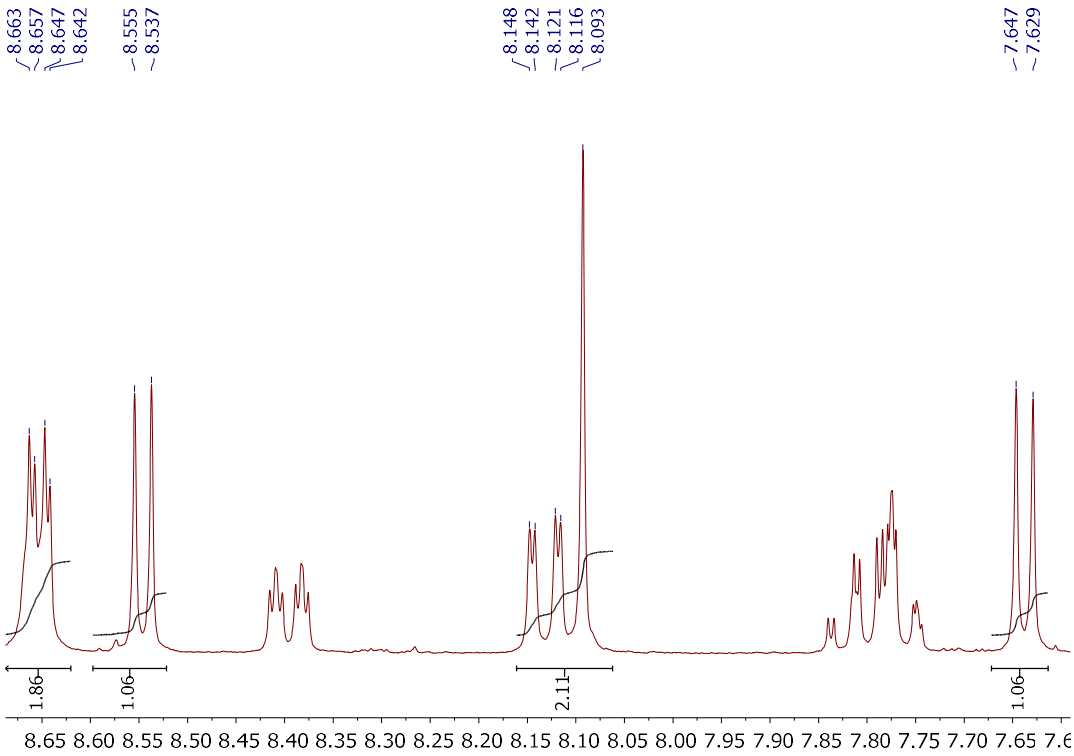
4.359
3.610
3.587
3.564
3.540
1.207
1.184
1.160
2.00
2.11
2.21
3.55
5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.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8.657
8.647
8.642
8.555
8.537
8.148
8.142
8.121
8.116
8.093
7.647
7.629
1.86
1.06
2.11
1.06
8.65 8.60 8.55 8.50 8.45 8.40 8.35 8.30 8.25 8.20 8.15 8.10 8.05 8.00 7.95 7.90 7.85 7.80 7.75 7.70 7.65 7.6