

Supporting Information

A Palladium-Catalyzed Method for the Synthesis of 2-(α -Styryl)-2,3-dihydroquinazolin-4-ones and 3-(α -Styryl)-3,4-dihydro-1,2,4-benzothiadiazine-1,1-dioxide: Access to 2-(α -Styryl)-quinazolin-4(3H)-ones and 3-(α -Styryl)-1,2,4-benzothiadiazine-1,1-dioxides

*Priyanka Kundu, Amrita Mondal, Chinmay Chowdhury**

Organic & Medicinal Chemistry Division, CSIR-Indian Institute of Chemical Biology, 4, Raja S.C. Mullick Road, Kolkata-700032, India.

chinmay@iicb.res.in

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1. X-ray diffraction analysis of products **9aa** (Table 2), **9bd** (Table 2), **23g** (Table 3), **7d** (Scheme 4):

a)

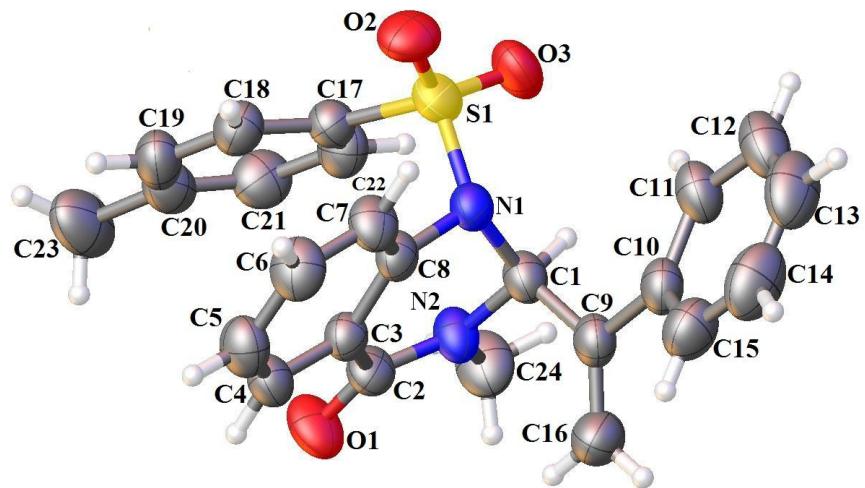


Figure S1: ORTEP¹ diagram of product **9aa** (Drawn at 50% probability)

b)

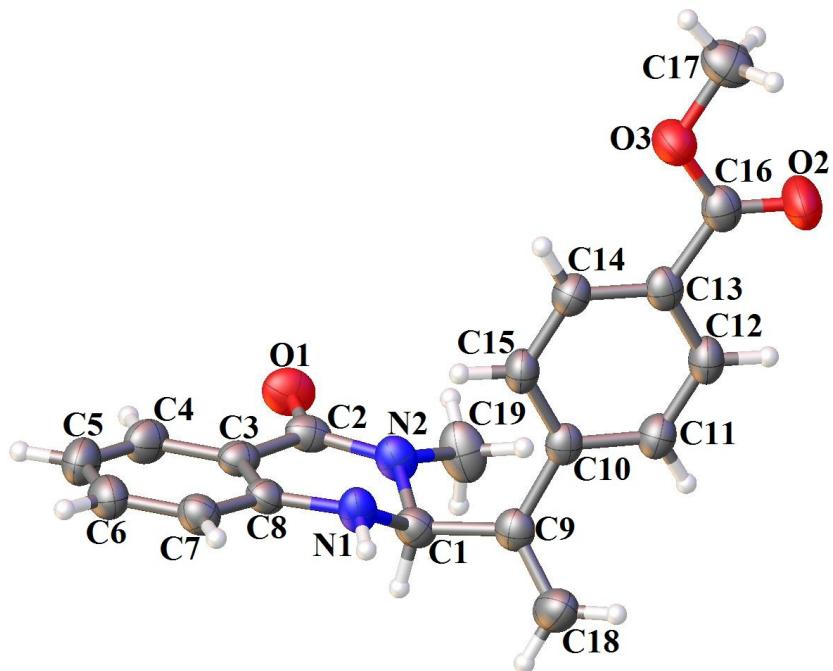


Figure S2: ORTEP¹ diagram of product **9bd** (Drawn at 50% probability)

c)

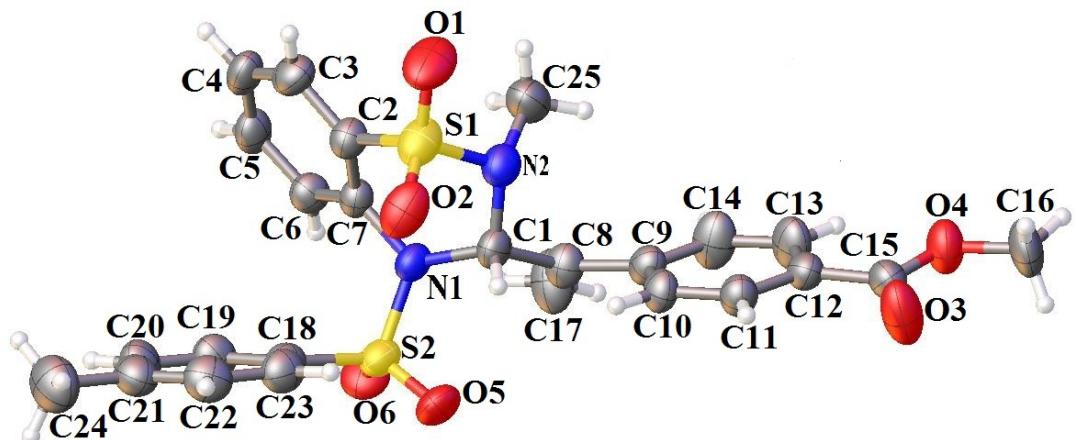


Figure S4: ORTEP¹ diagram of product **23g** (Drawn at 50% probability)

d)

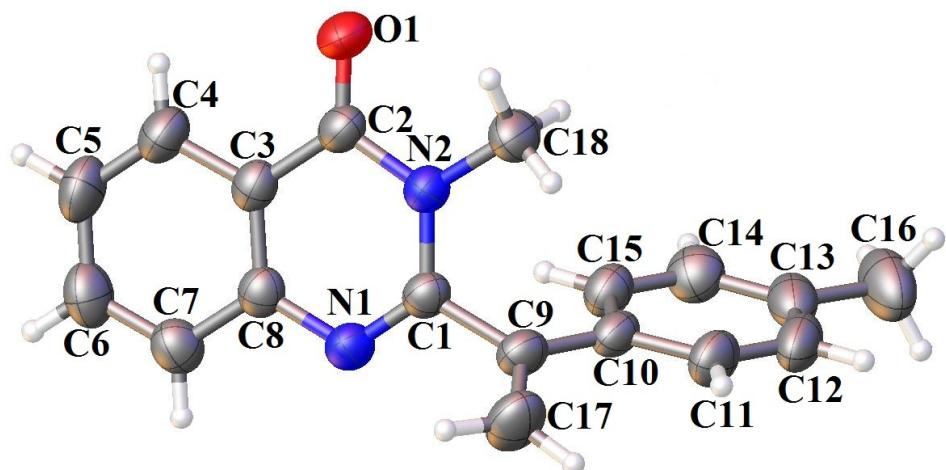


Figure S5: ORTEP¹ diagram of product **7d** (Drawn at 50% probability)

Reference

1. Dolomanov, O.V.; Bourhis, L.J.; Gildea, R.J.; Howard, J.A.K.; Puschman, H. *OLEX2:A complete structure solution, refinement and analysis program*(2009). *J. Appl. Cryst.* **2009**, *42*, 339.

2. Table S1: Important crystal data of products **9aa**, **9bd**

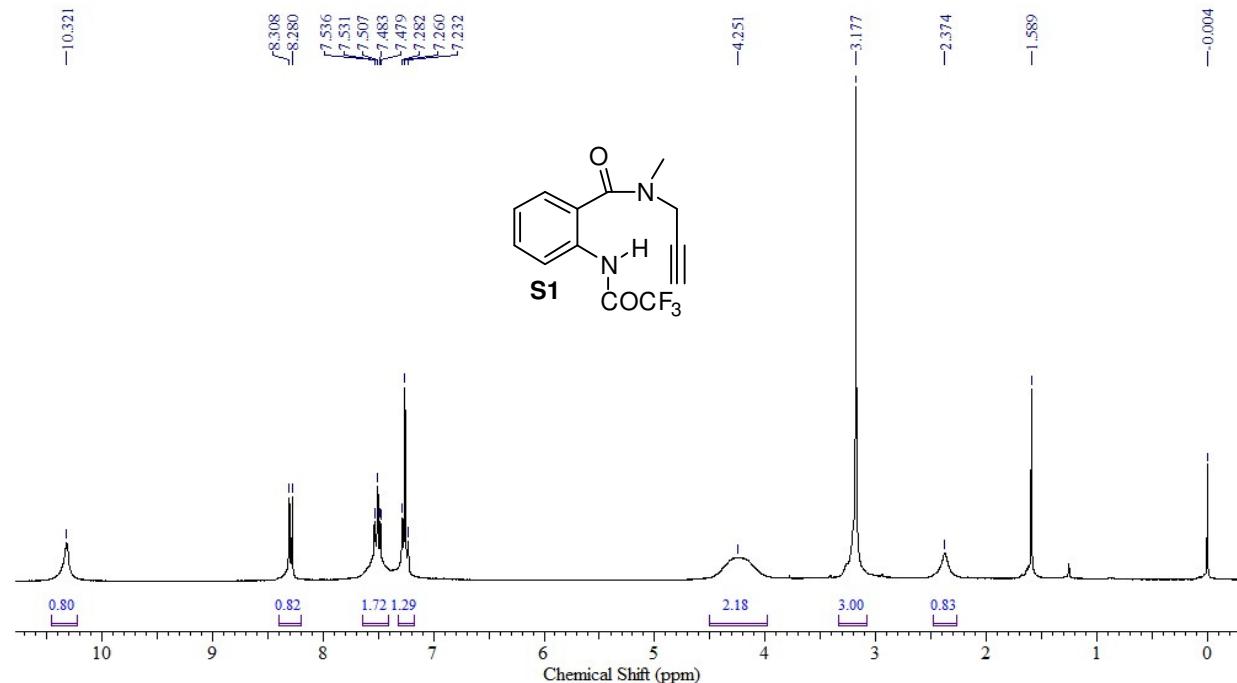
	9aa	9bd
CCDC deposition number	1477128	1477129
Empirical Formula	C ₂₄ H ₂₂ N ₂ O ₃ S	C ₁₉ H ₁₈ N ₂ O ₃
Formula weight	418.49	322.35
Temperature (K)	293.15	293.15
Wavelength	0.71073	0.71073
Crystal System	triclinic	monoclinic
Space Group	P -1	P 1 21/c 1
Unit Cell Dimension	a=8.0522(11) Å b=11.3712(17) Å c=12.2775(19) Å α=82.627(10)° β=81.964(10)° γ=77.726(9)°	a=7.0264(13) Å b=14.456(3) Å c=15.504(3) Å α=90° β=93.110(12)° γ=90°
Volume Å ³	1082.0(3)	1572.5(5)
Z	2	4
Density Calculated g/cm ³	1.284	1.362
Absorption coefficient(Mu) mm ⁻¹	0.177	0.093
F(000)	440	680
Theta range for data collection	1.842 -27.343°	2.631-26.345°
Index ranges	-10<=h<=10 -14<=k<=14 -15<=l<=15	-9<=h<=6 -18<=k<=18 -19<=l<=20
Reflection Collected	19686	14492
Independent Reflections	4854	3501
	[R(int) = 0.0614]	[R(int) = 0.0433]
Completeness to the theta=25.44°	99.0%	97.9%
Absorption Correction	Multi-scan	Multi-scan
Max. and min. transmission	1 and 0.800955	1 and 0.678785
Refinement method	Full-matrix least-squares on F ²	Full-matrix least-squares on F ²
Data/Restraints/parameter	4854/0/279	3501/0/219
s		
Goodness of fit on F ²	0.992	1.027
Final R indices [I>=2sigma(I)]	R ₁ =0.0511 wR ₂ =0.1313	R ₁ = 0.0458 wR ₂ = 0.1105
R indices (all data)	R ₁ = 0.1128 wR ₂ = 0.1597	R ₁ = 0.0718 wR ₂ = 0.1281
Largest difference peak and hole [e.Å ⁻³]	0.239 and - 0.257	0.231 and -0.236

3. Table S2: Important crystal data of compounds **23g** and **7d**

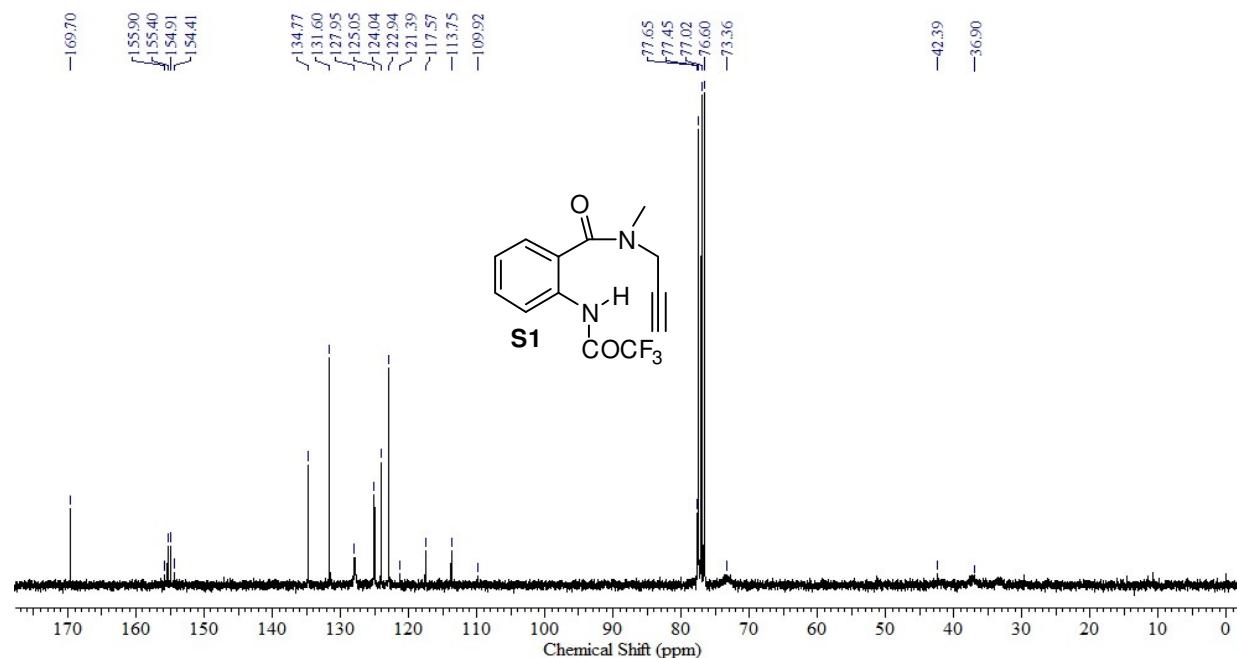
	23g	7d
CCDC deposition number	1477130	1477127
Empirical Formula	C ₂₅ H ₂₄ N ₂ O ₆ S ₂	C ₁₈ H ₁₆ N ₂ O
Formula weight	512.58	276.33
Temperature (K)	293.15	293.15
Wavelength	0.71073	0.71073
Crystal System	monoclinic	monoclinic
Space Group	P 1 21/c 1	P 1 21/c 1
Unit Cell Dimension	a= 12.154(5) Å b=22.713(8) Å c=8.812(3) Å α= 90° β=100.95(2)° γ=90°	a= 14.6277(13) Å b= 11.2274(10) Å c= 9.0326(7) Å α=90° β= 92.402(4)° γ=90°
Volume Å ³	2388.2(15)	1482.1(2)
Z	4	4
Density Calculated g/cm ³	1.426	1.238
Absorption coefficient(Mu) mm ⁻¹	0.268	0.078
F(000)	1072	584
Theta range for data collection	2.48 - 25.78 °	2.288 - 27.372 °
Index ranges	-15<=h<=15 -29<=k<=25 -11<=l<=10	-18<=h<=18 -14<=k<=14 -11<=l<=11
Reflection Collected	30599	13422
Independent Reflections	5399	3340[R(int)= 0.0413] [R(int) = 0.0950]
Completeness to the theta=25.44°	97.1%	98.6%
Absorption Correction	Multi-scan	Multi-scan
Max. and min. transmission	1 and 0.587357	1 and 0.753884
Refinement method	Full-matrix least-squares on F ²	Full-matrix least-squares on F ²
Data/Restraints/parameter	5399/0/319	3340/0/192
Goodness of fit on F ²	0.941	1.030
Final R indices [I>=2sigma(I)]	R ₁ = 0.0540 wR ₂ = 0.1442	R ₁ = 0.0451 wR ₂ = 0.1135
R indices (all data)	R ₁ = 0.1002 wR ₂ = 0.1713	R ₁ = 0.0719 wR ₂ = 0.1377
Largest difference peak and hole [e.Å ⁻³]	0.235 and -0.348	0.199 and -0.156

4) NMR spectra of acetylene **S1**:

¹H NMR (CDCl₃, 300 MHz) spectrum of **S1**:

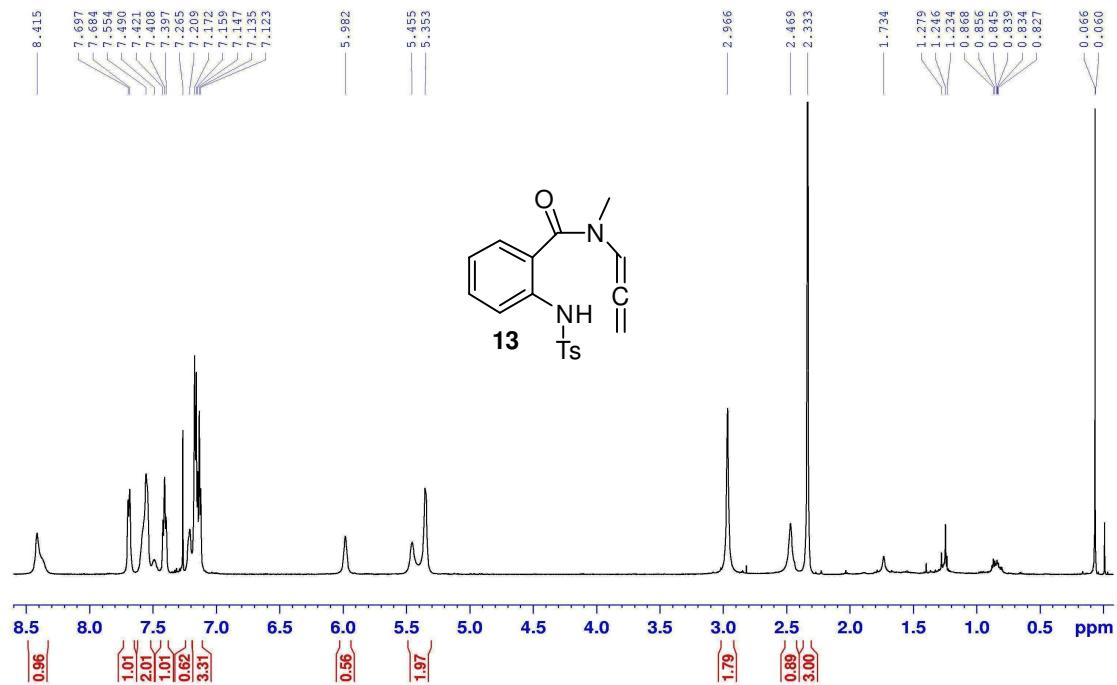


¹³C NMR (CDCl₃, 75 MHz) spectrum of compound **S1**:

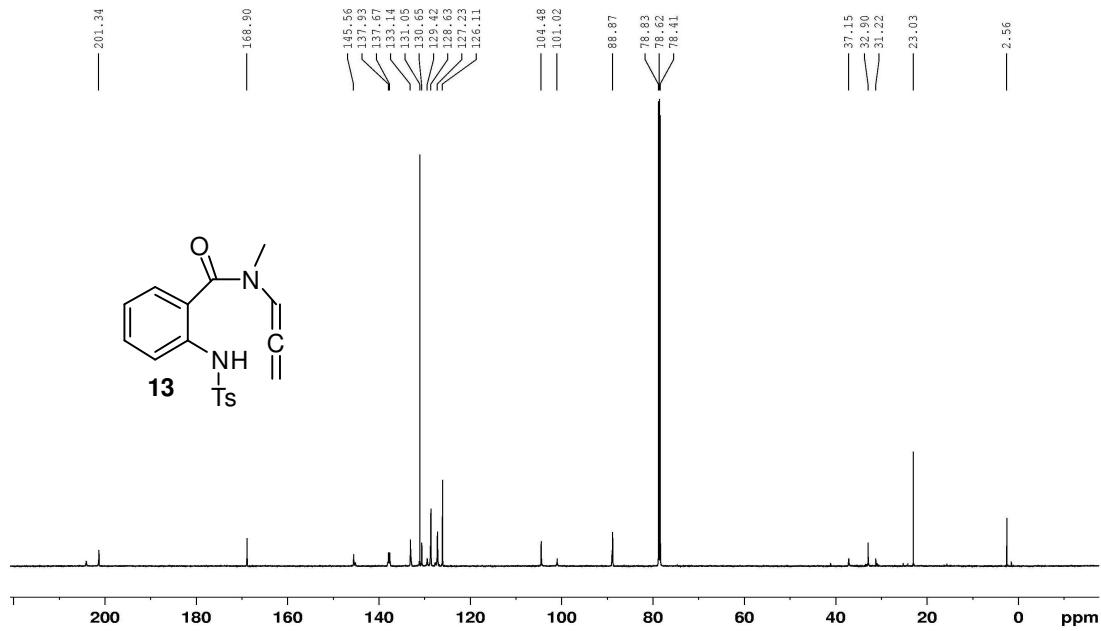


5) NMR spectra of allenes **13**, **14**, **15**:

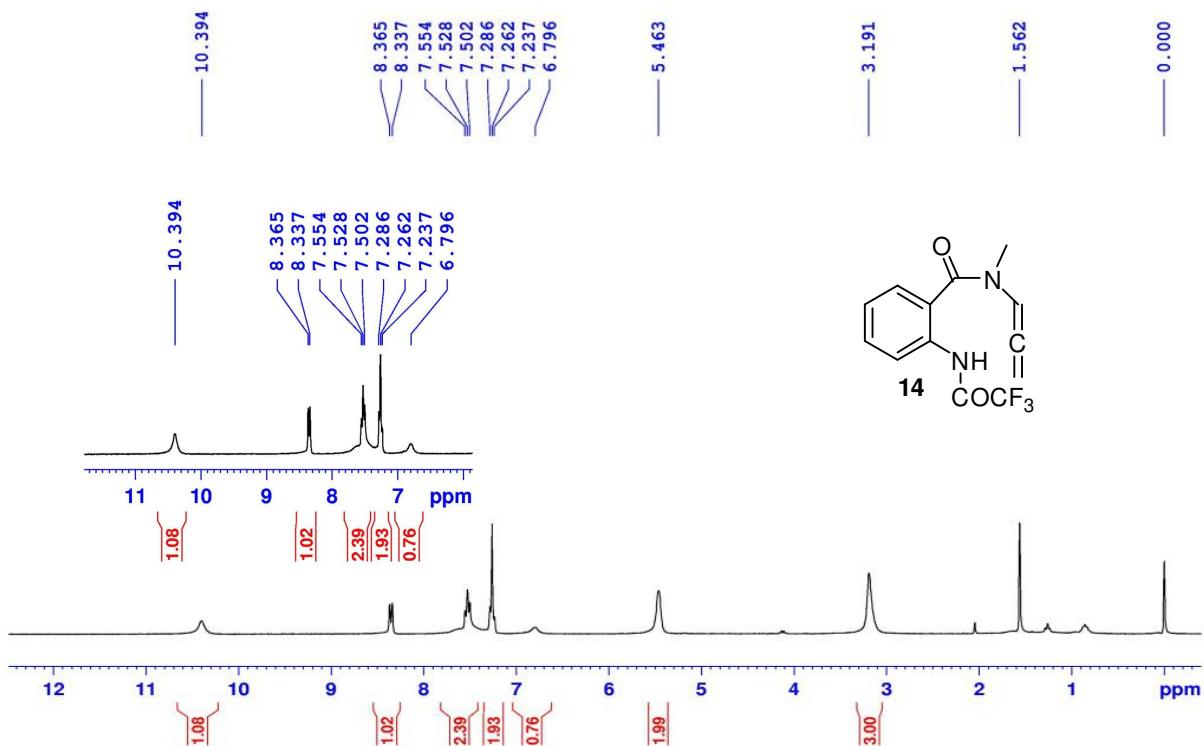
^1H NMR (CDCl_3 , 600 MHz) spectrum of compound **13**:



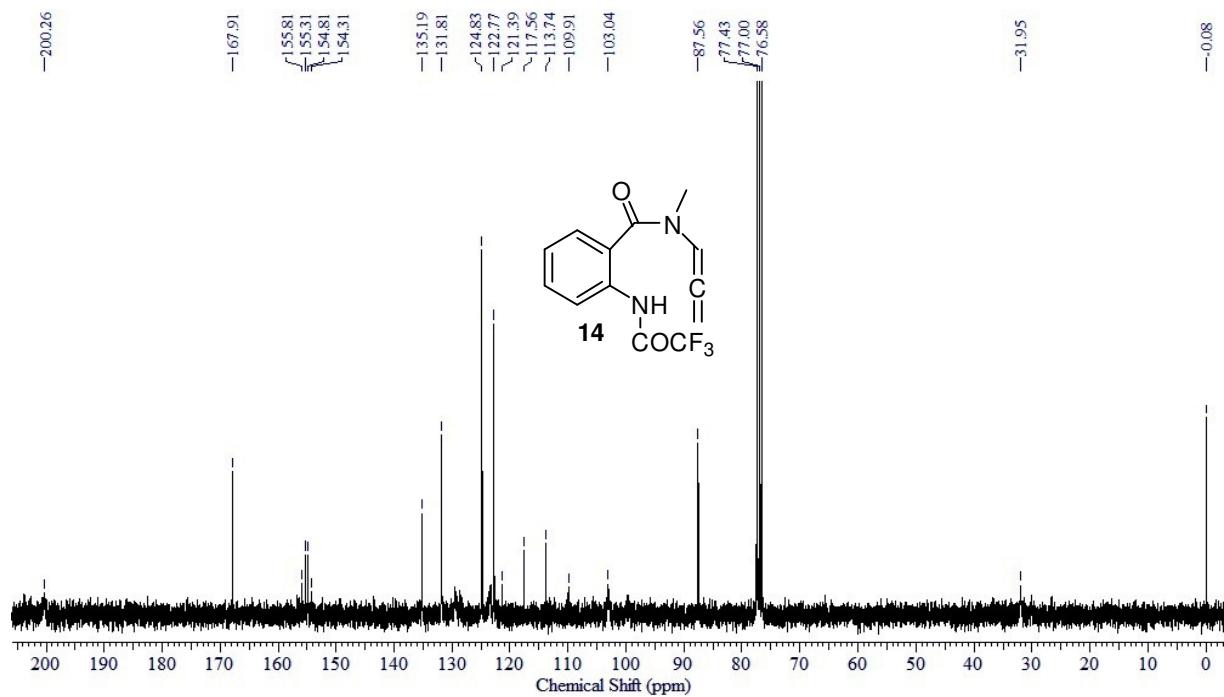
^{13}C NMR (CDCl_3 , 150 MHz) spectrum of compound **13**:



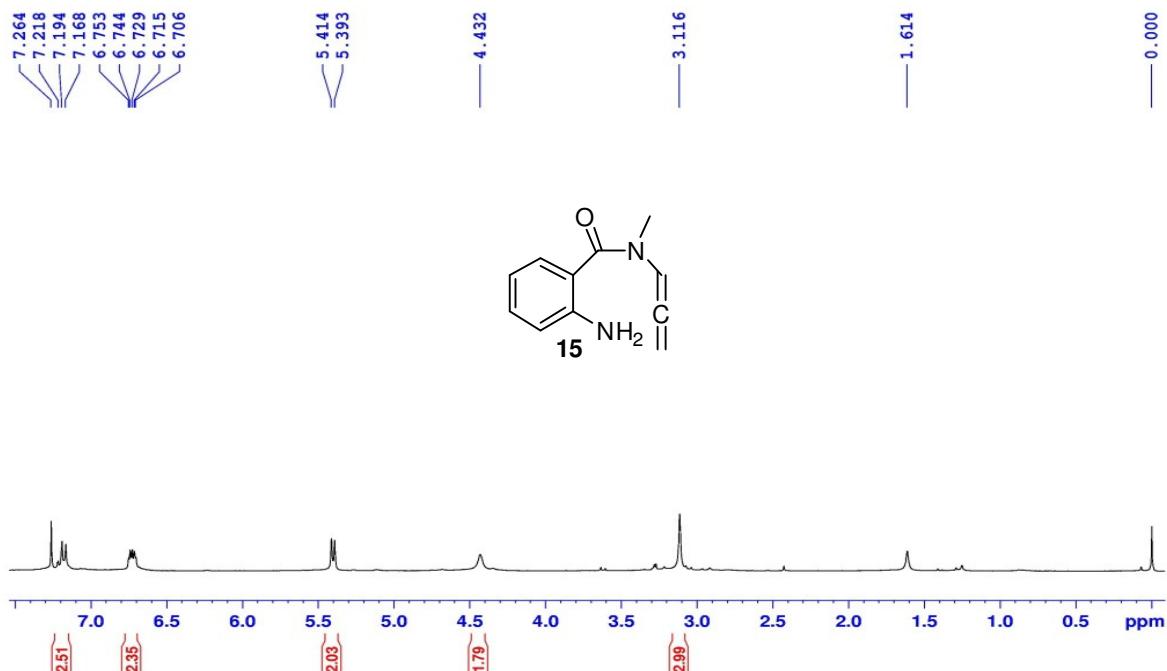
¹H NMR (CDCl_3 , 300 MHz) spectrum of compound **14**:



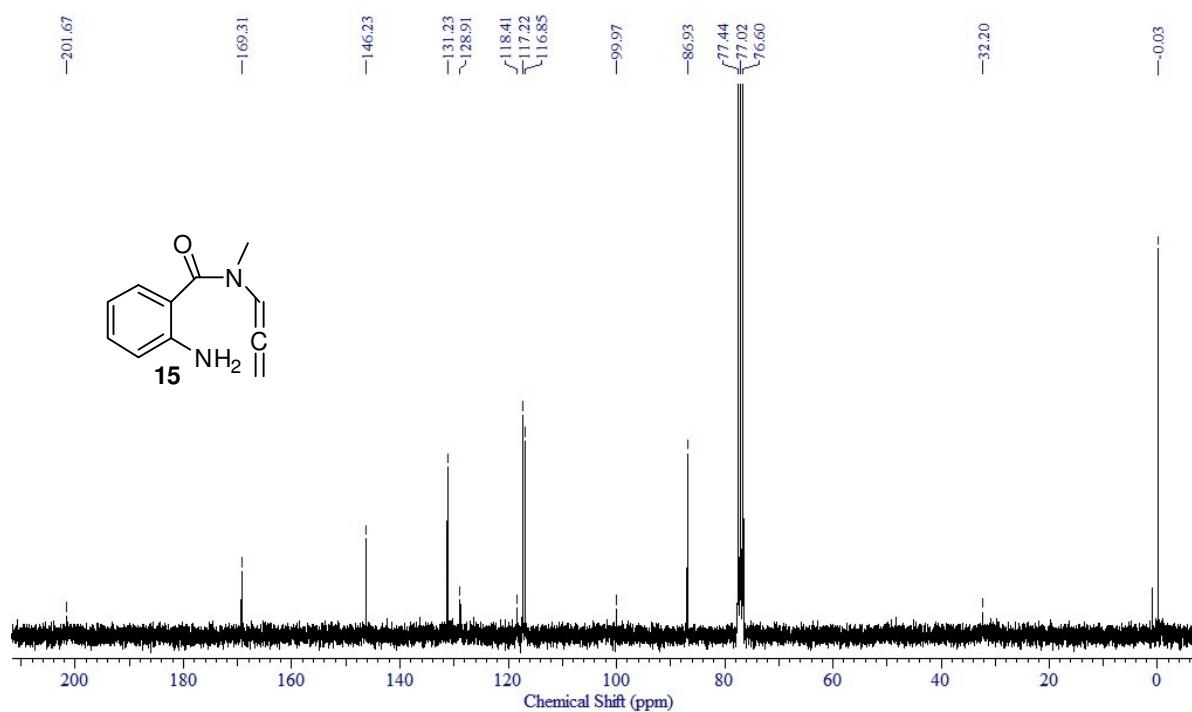
¹³C NMR (CDCl_3 , 75 MHz) spectrum of compound **14**:



¹H NMR (CDCl_3 , 300 MHz) spectrum of compound **15**:

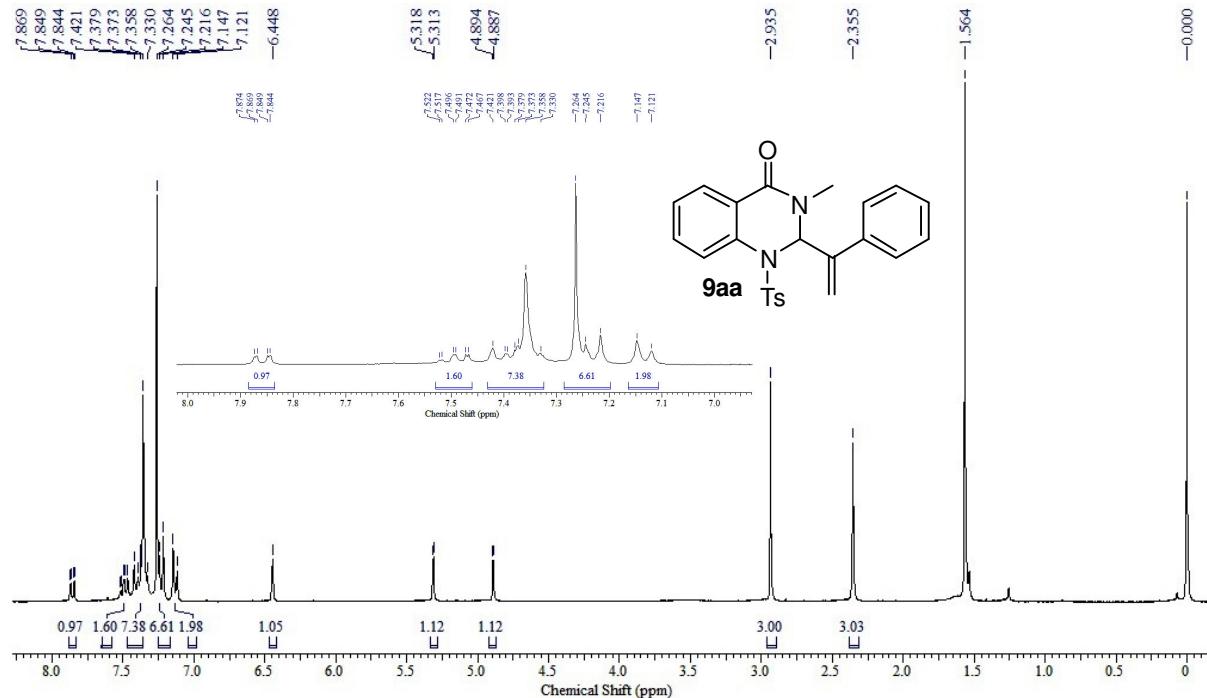


¹³C NMR (CDCl_3 , 75 MHz) spectrum of compound **15**:

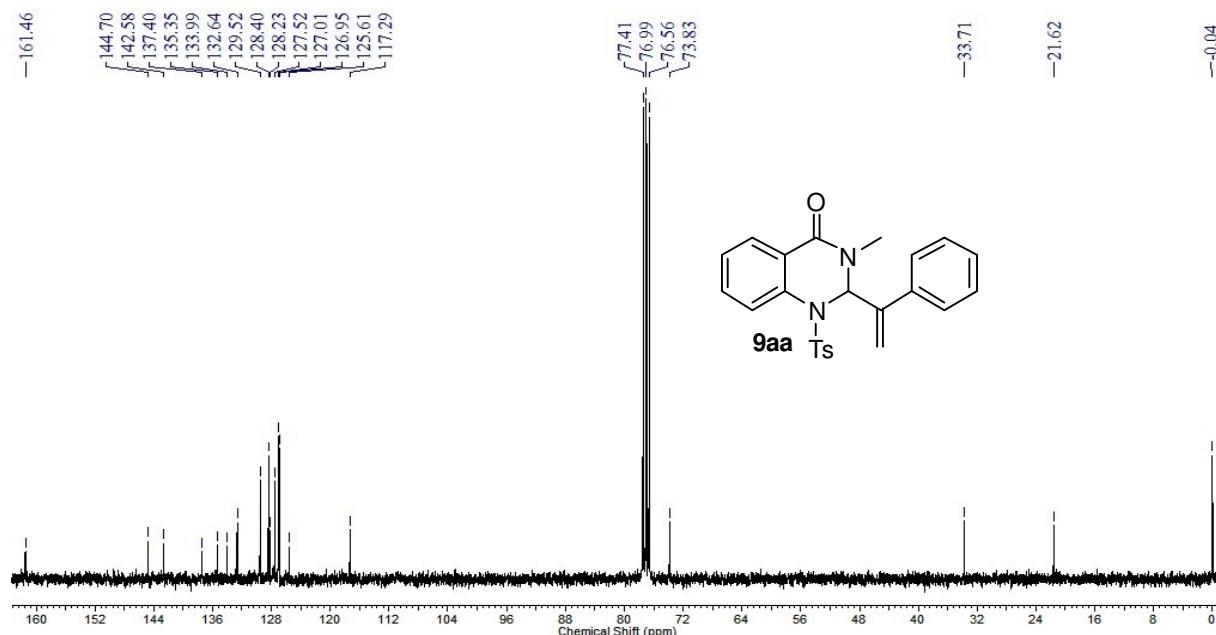


6) NMR spectra of products **9aa-9al** (Table 2):

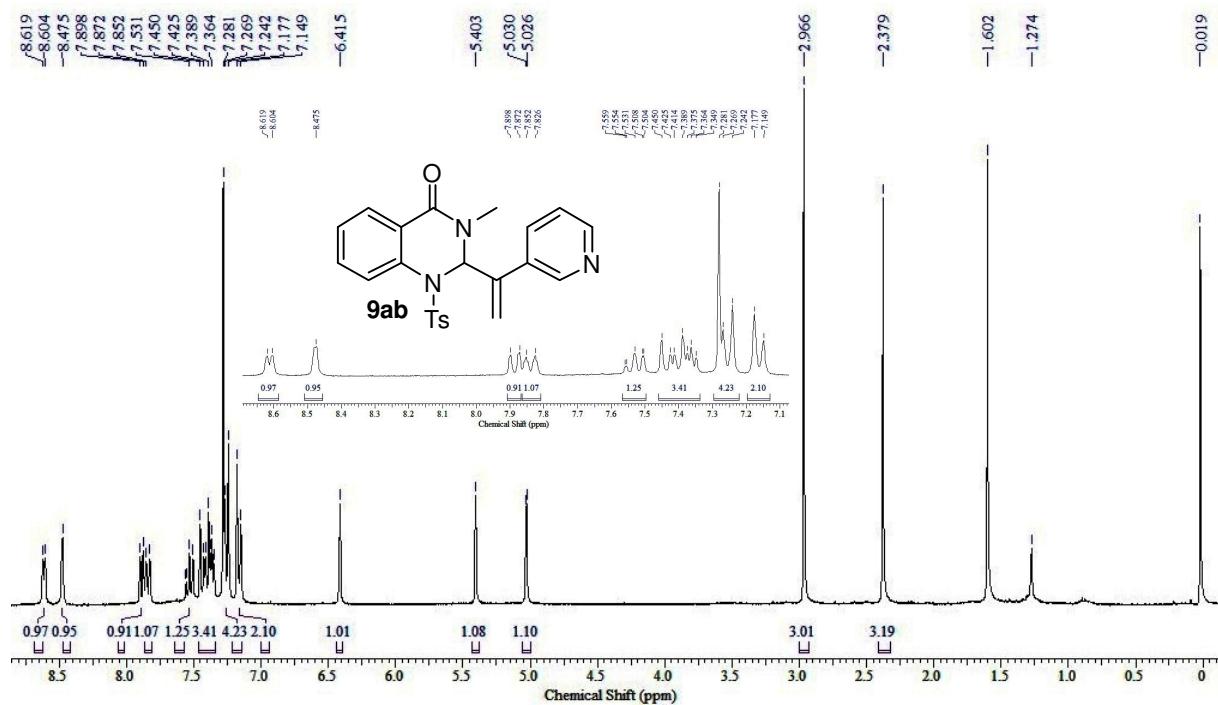
¹H NMR (CDCl₃, 300 MHz) spectrum of product **9aa**:



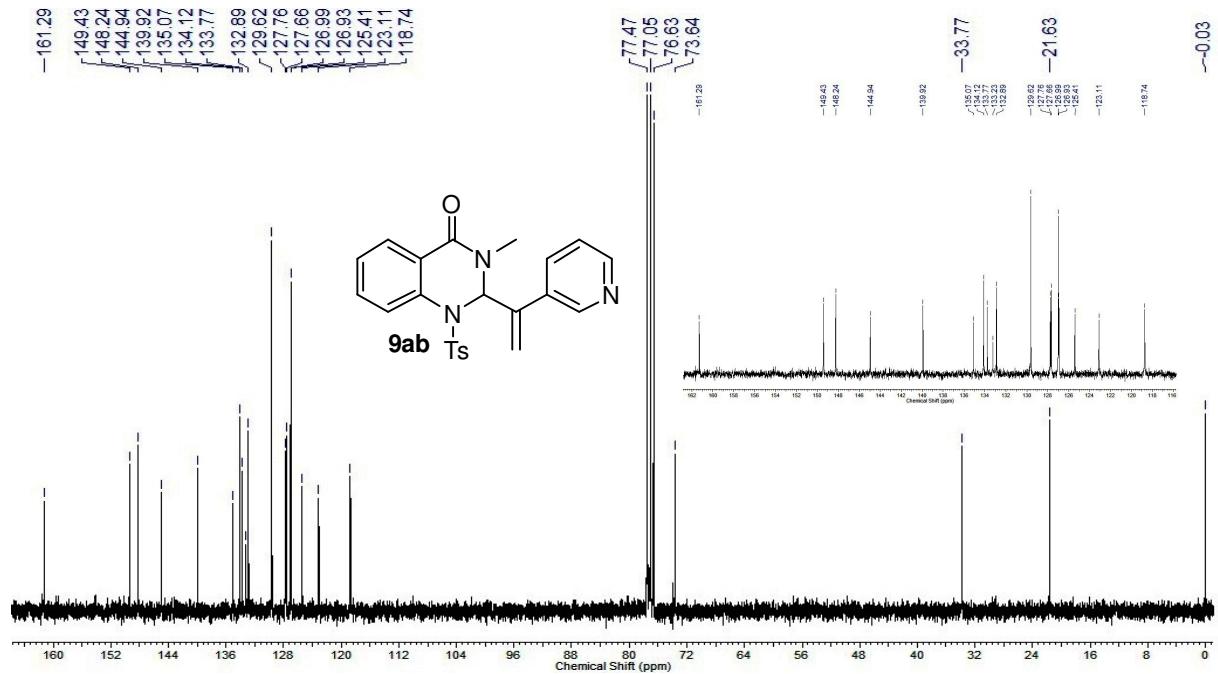
¹³C NMR (CDCl_3 , 75 MHz) spectrum of product **9aa**:



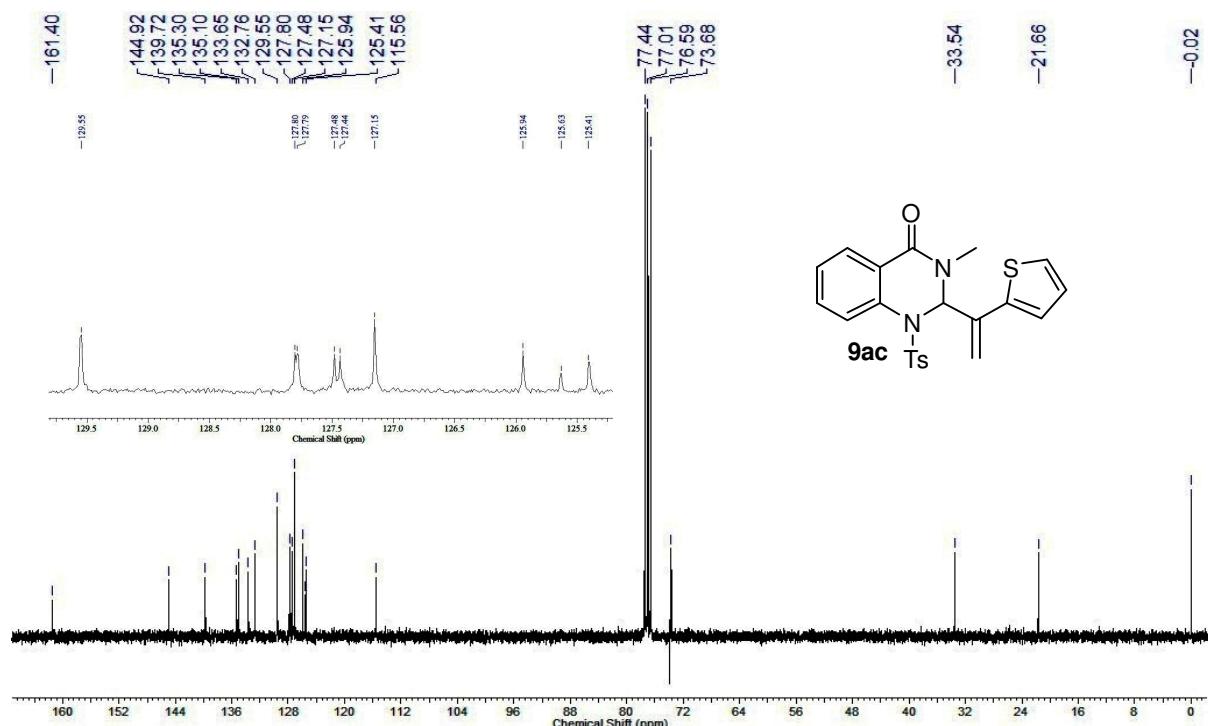
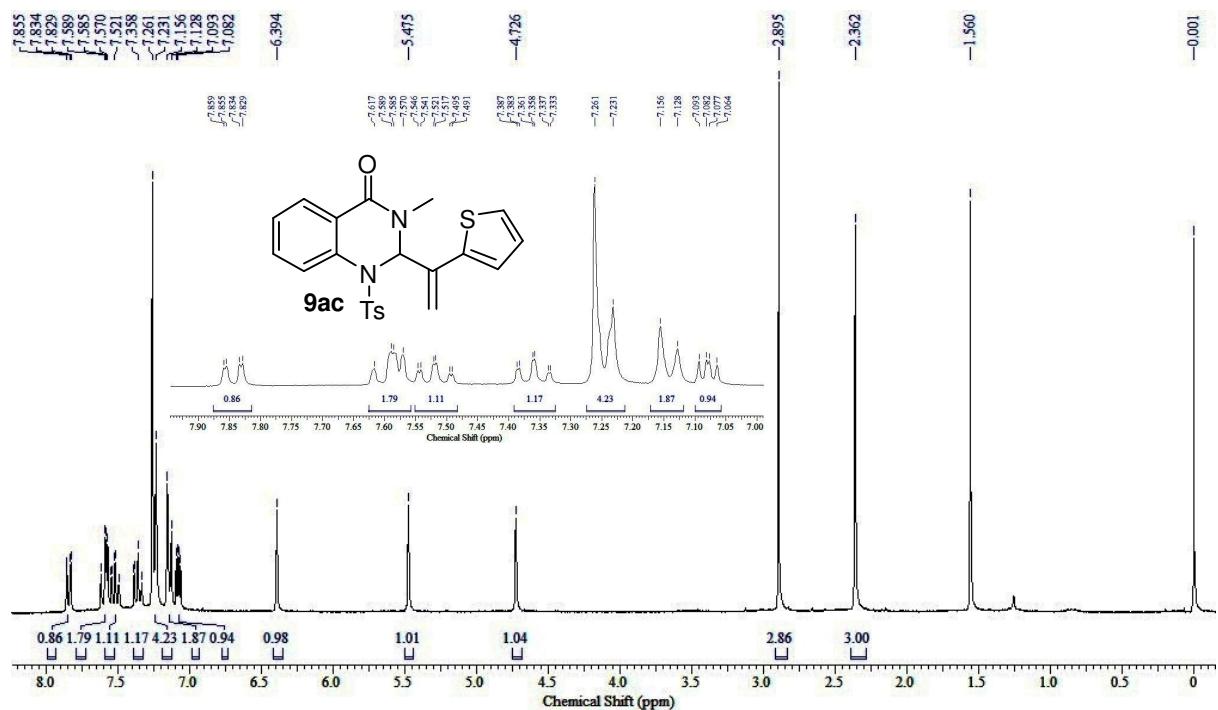
¹H NMR (CDCl_3 , 300 MHz) spectrum of product **9ab**:



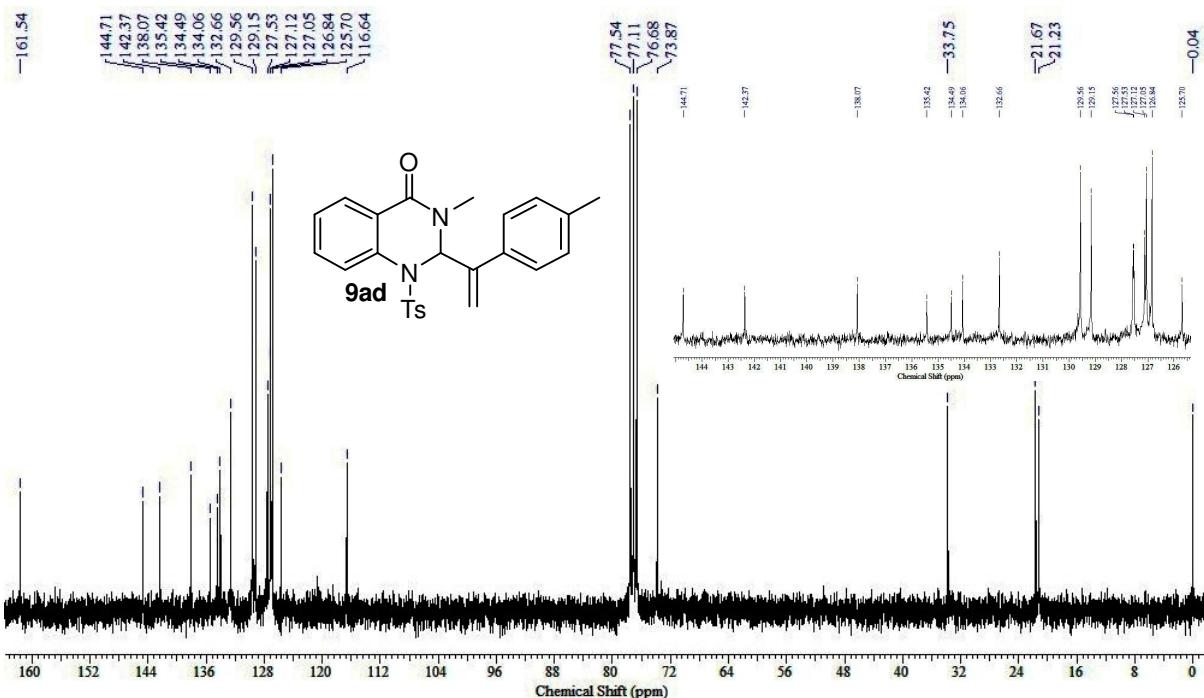
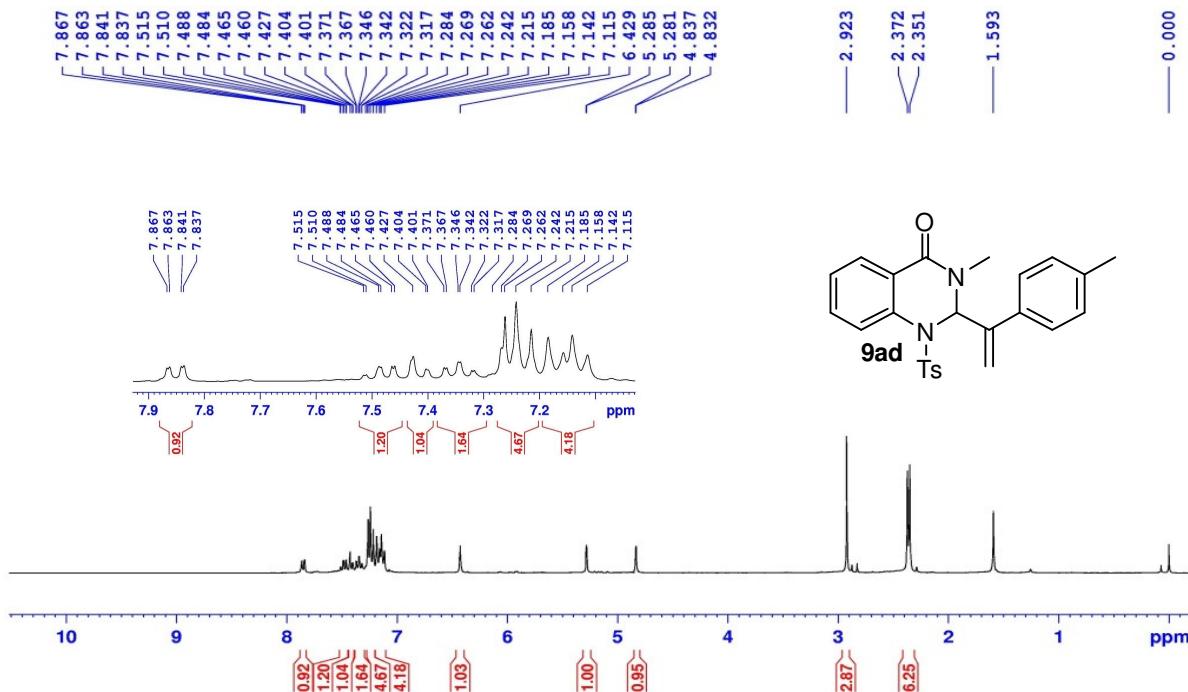
¹³C NMR (CDCl_3 , 75 MHz) spectrum of product **9ab**:



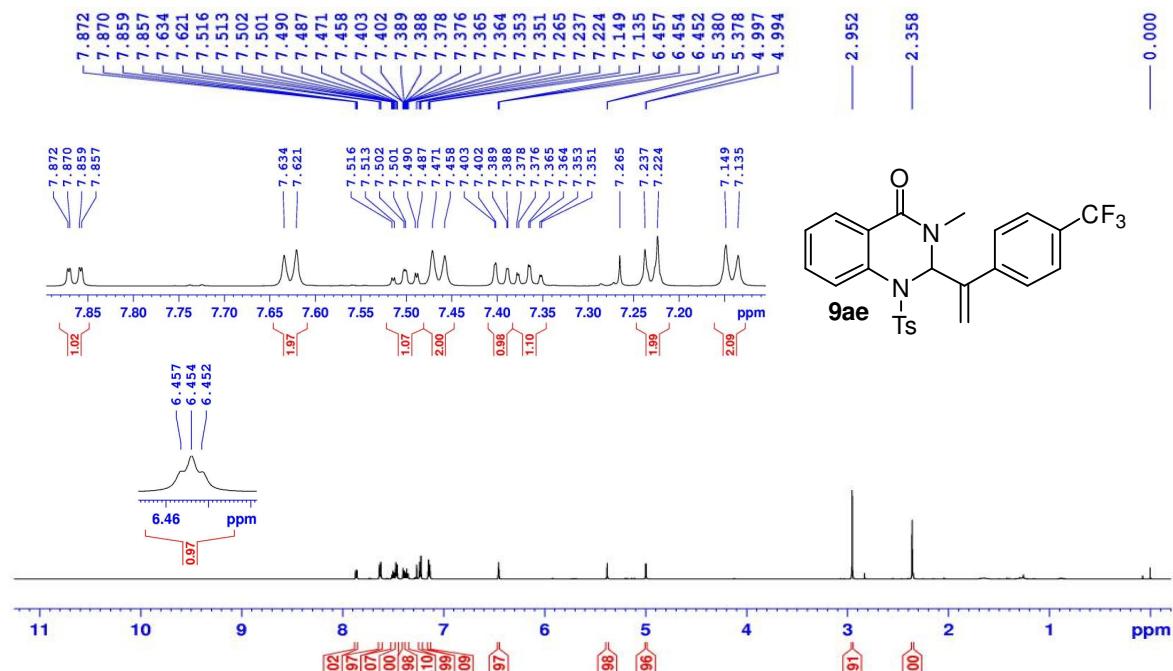
¹H NMR (CDCl_3 , 300 MHz) spectrum of product **9ac**:



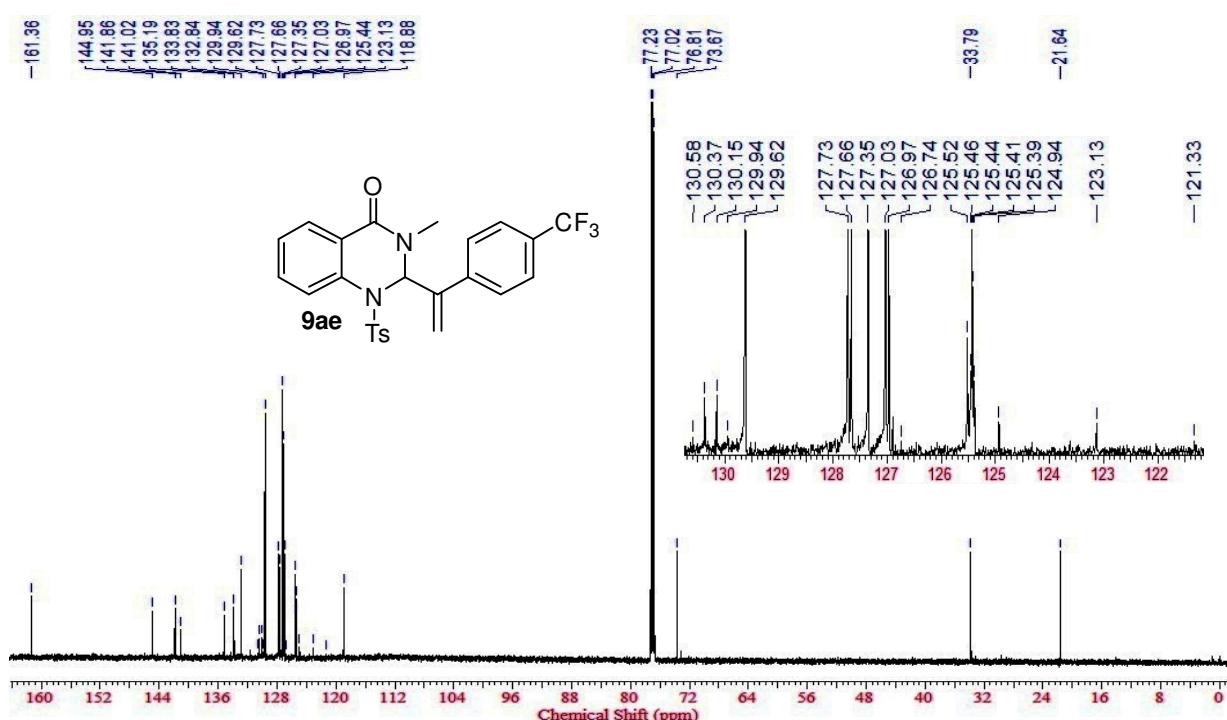
¹H NMR (CDCl_3 , 300 MHz) spectrum of product **9ad**:



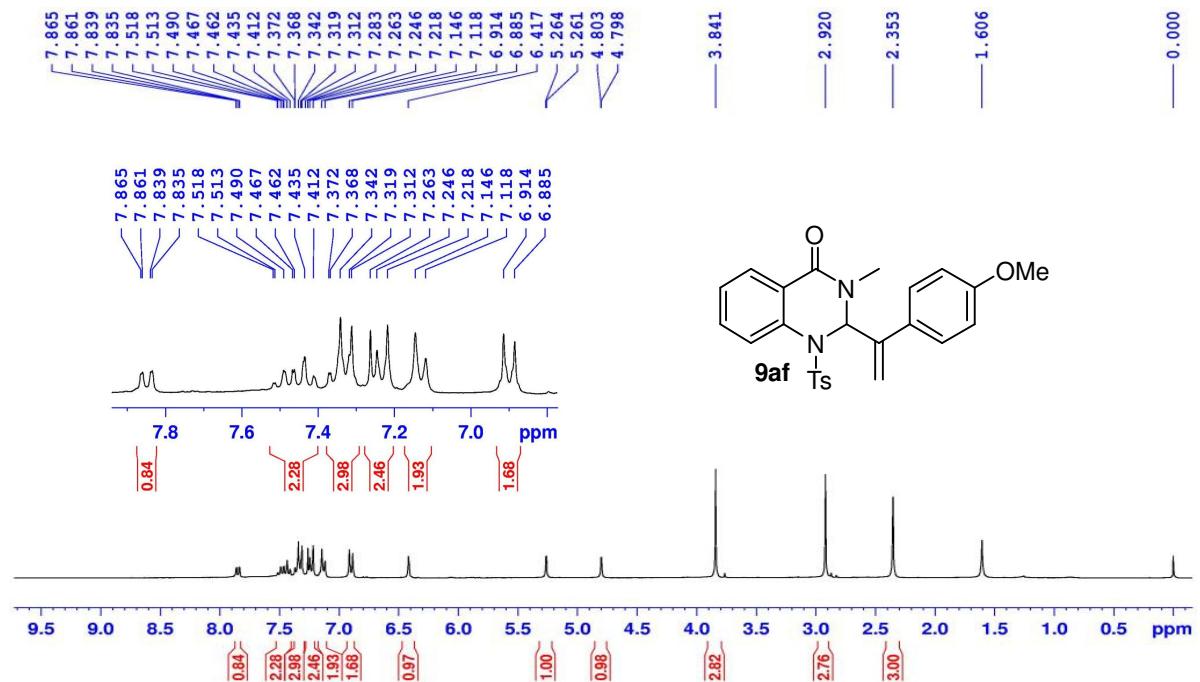
¹H NMR (CDCl₃, 600 MHz) spectrum of product **9ae**:



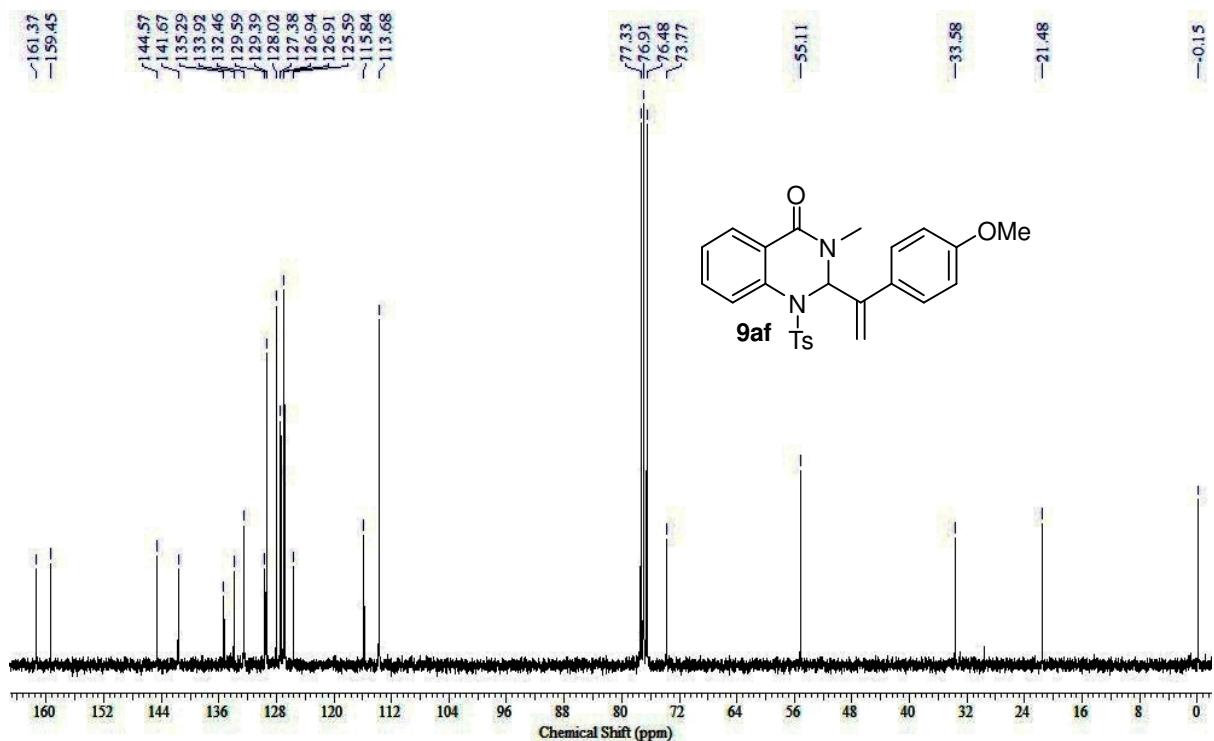
¹³C NMR (CDCl_3 , 150 MHz) spectrum of product **9ae**:



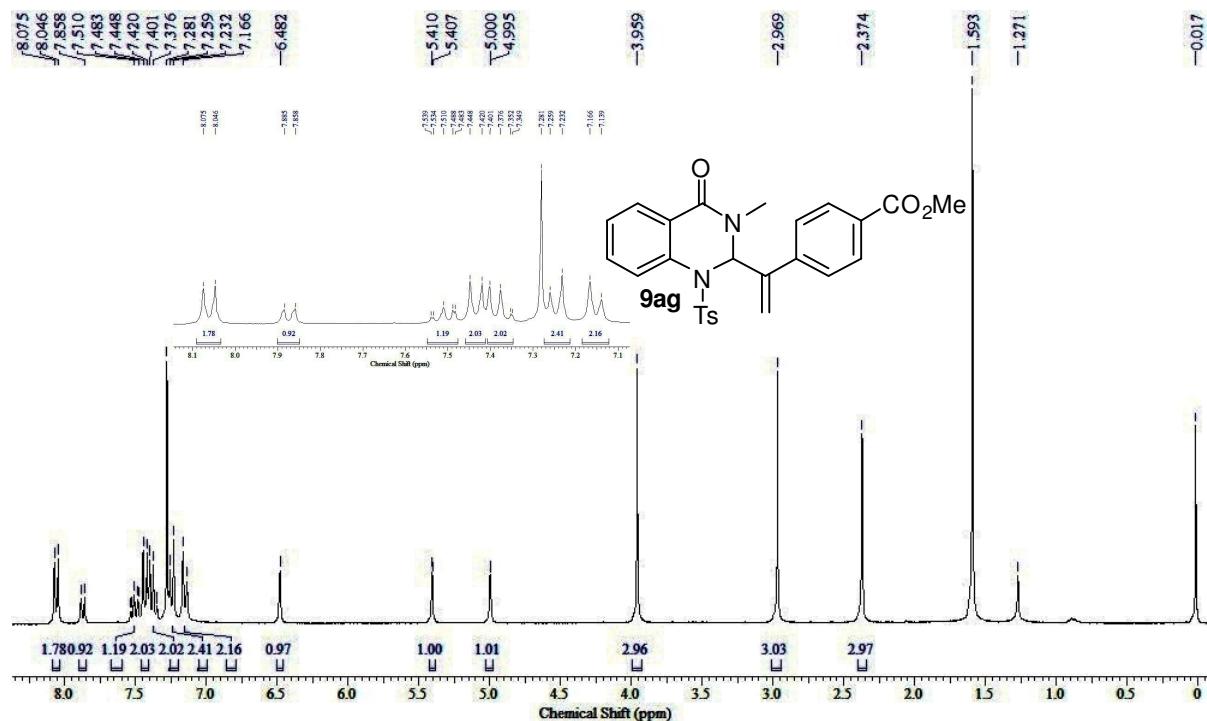
¹H NMR (CDCl_3 , 300 MHz) spectrum of product **9af**:



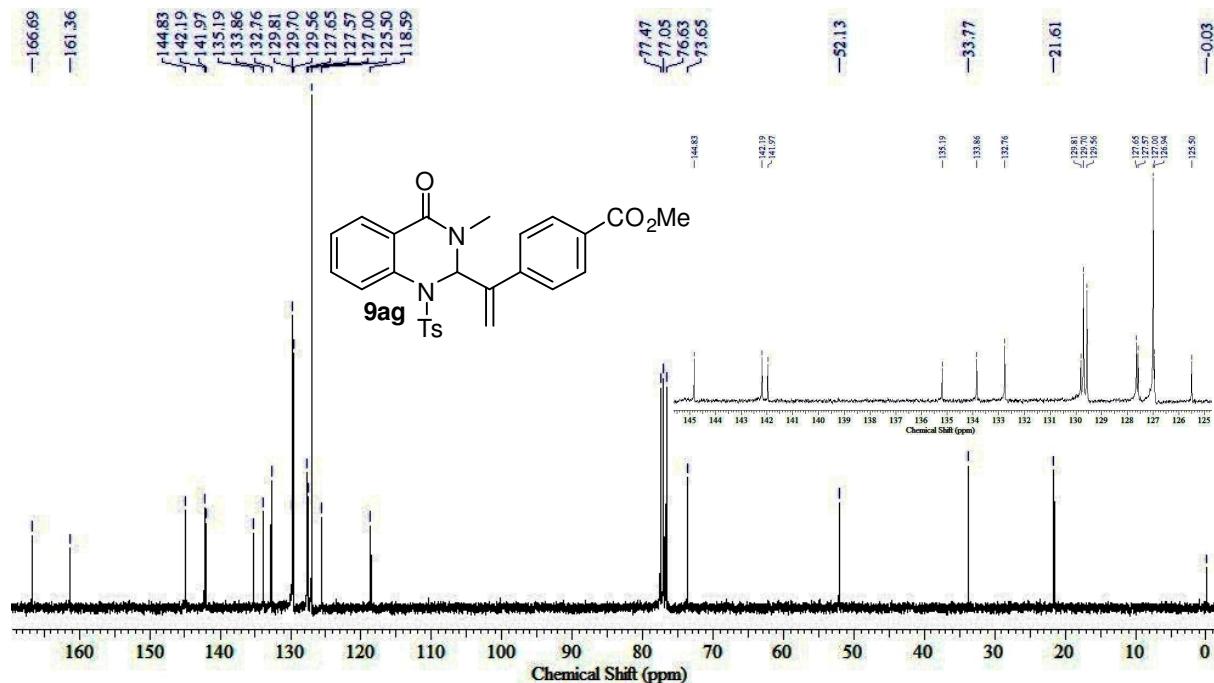
¹³C NMR (CDCl_3 , 75 MHz) spectrum of product **9af**:



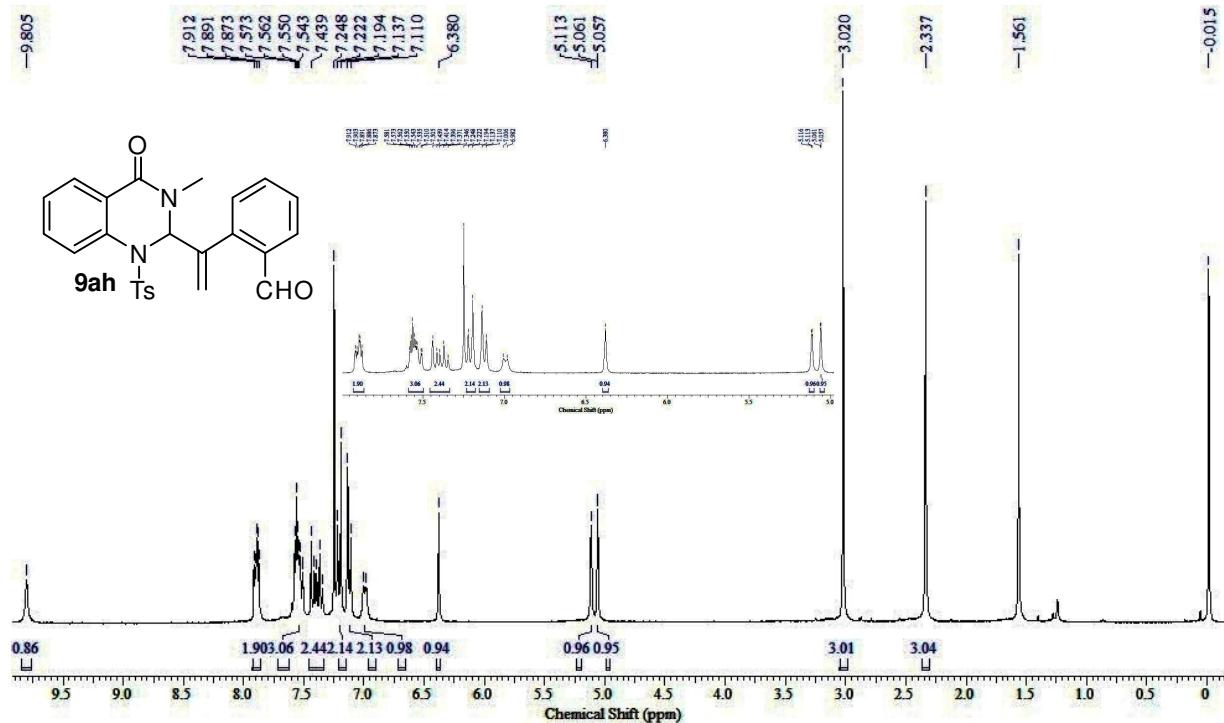
¹H NMR (CDCl_3 , 300 MHz) spectrum of product **9ag**:



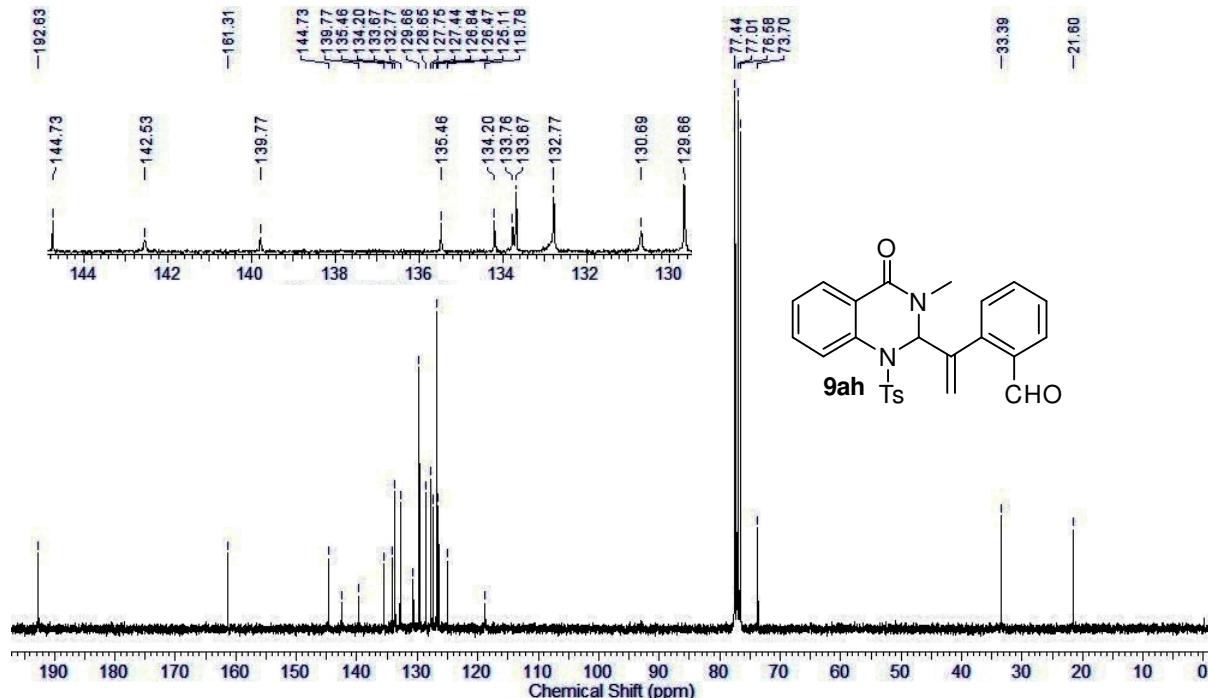
¹³C NMR (CDCl_3 , 75 MHz) spectrum of product **9ag**:



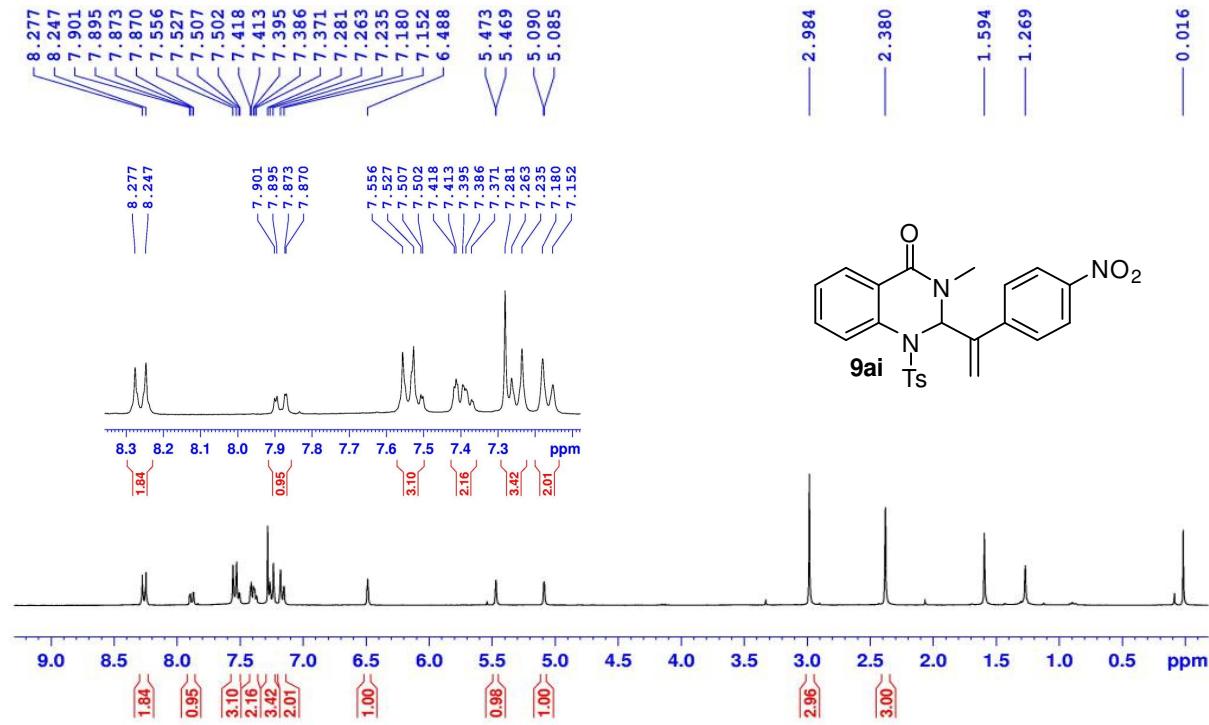
¹H NMR (CDCl_3 , 300 MHz) spectrum of product **9ah**:



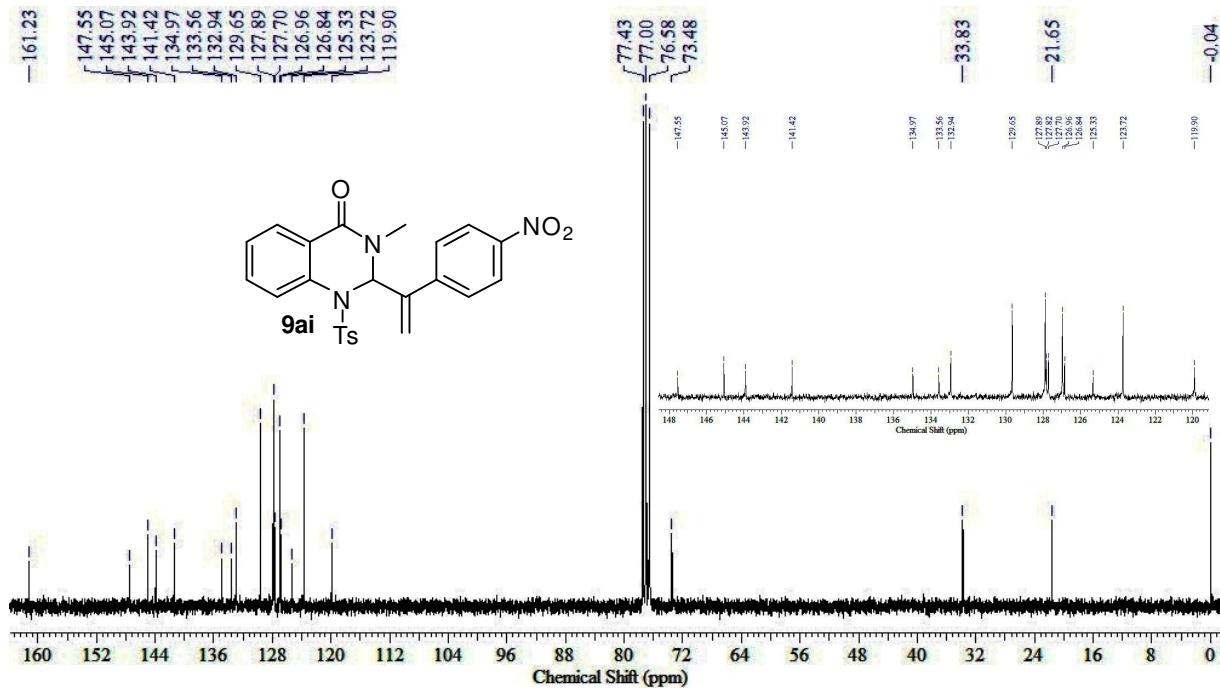
¹³C NMR (CDCl_3 , 75 MHz) spectrum of product **9ah**:



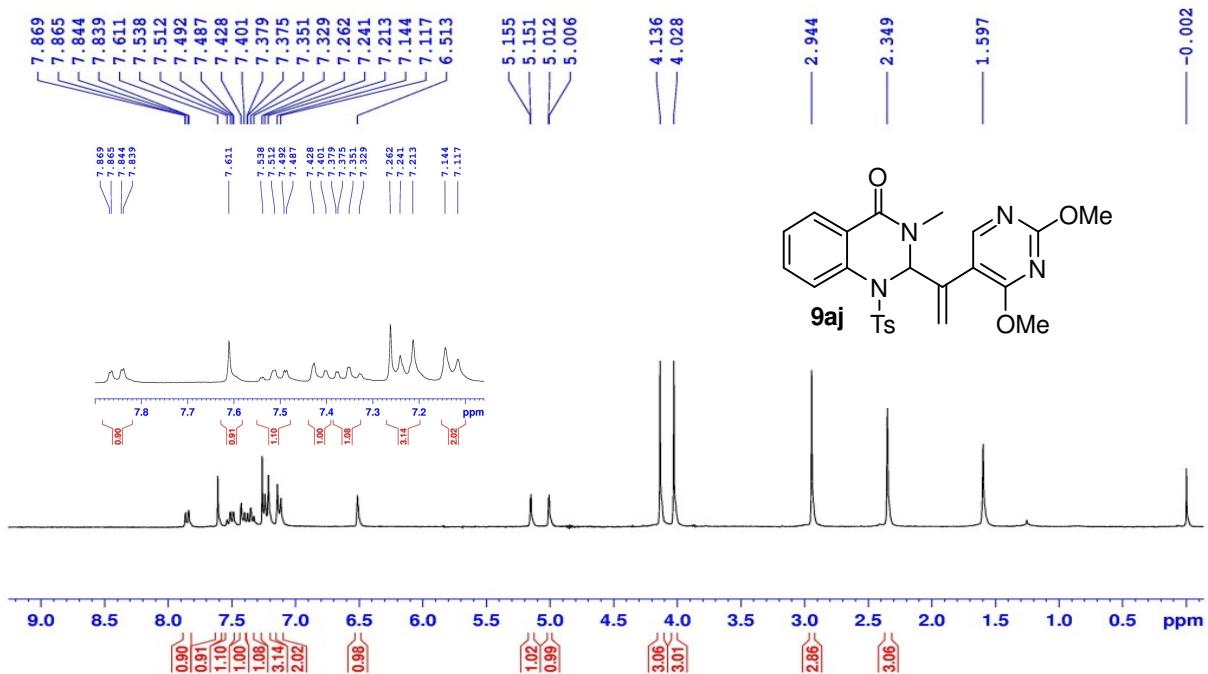
¹H NMR (CDCl_3 , 300 MHz) spectrum of product **9ai**:



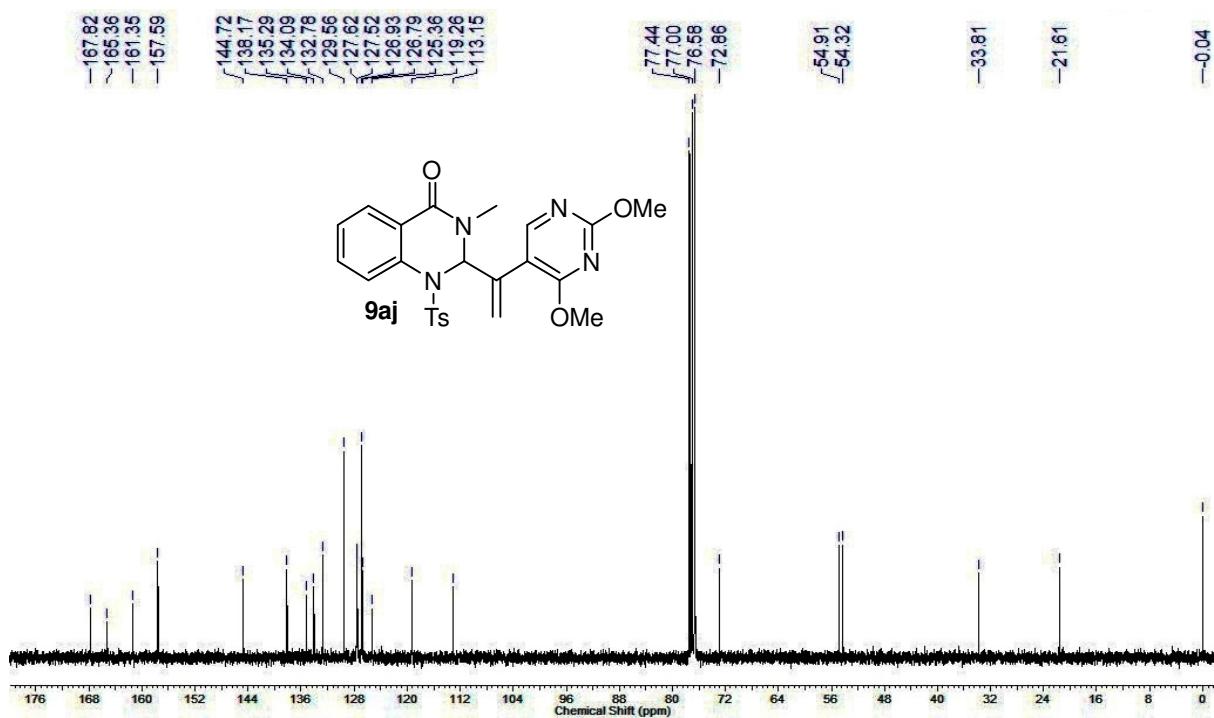
¹³C NMR (CDCl₃, 75 MHz) spectrum of product **9ai**:



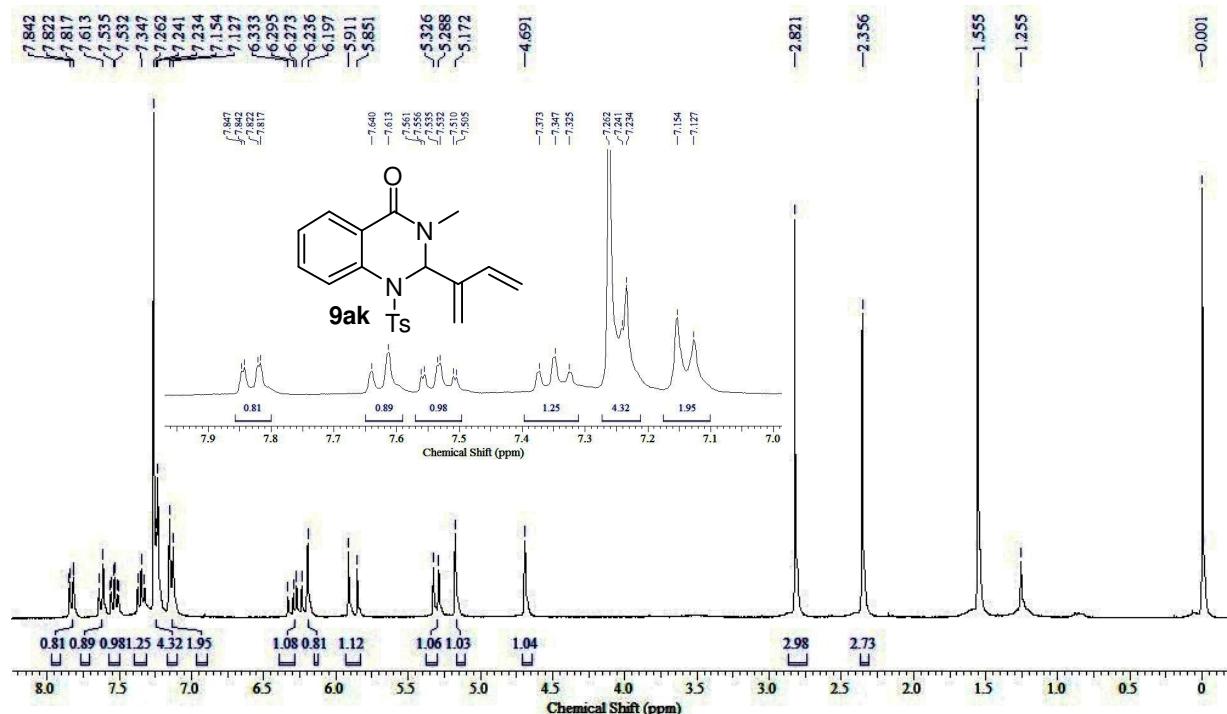
¹H NMR (CDCl_3 , 300 MHz) spectrum of product **9aj**:



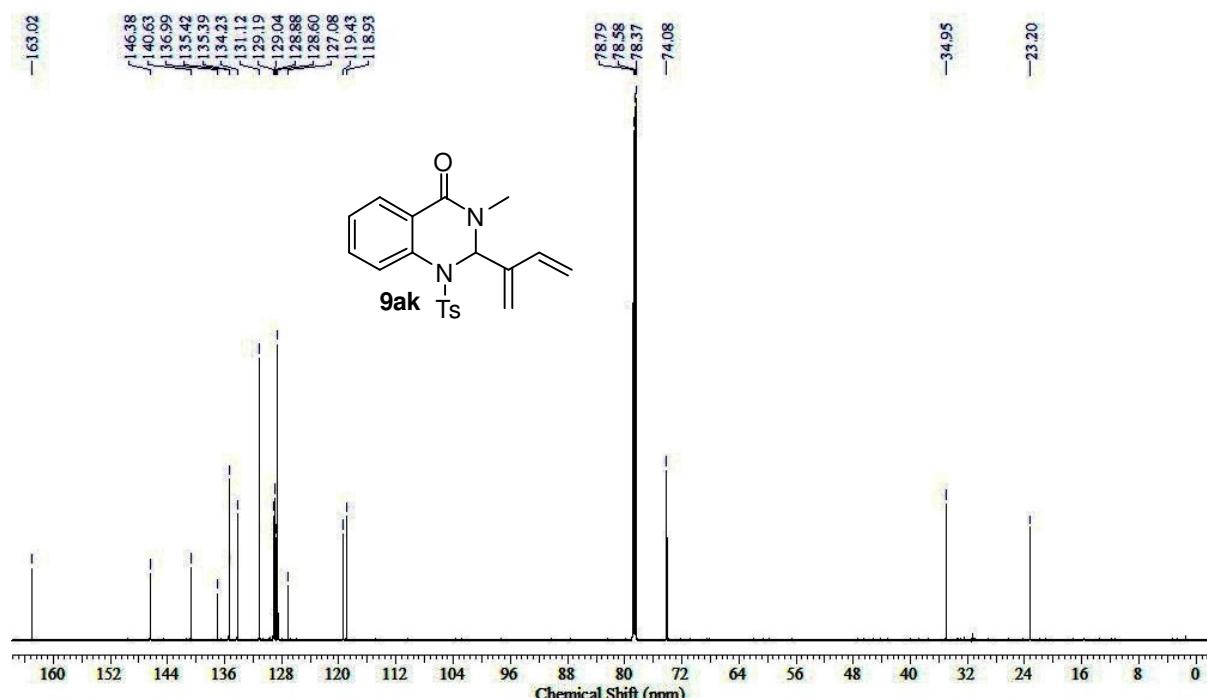
¹³C NMR (CDCl_3 , 75 MHz) spectrum of product **9aj**:



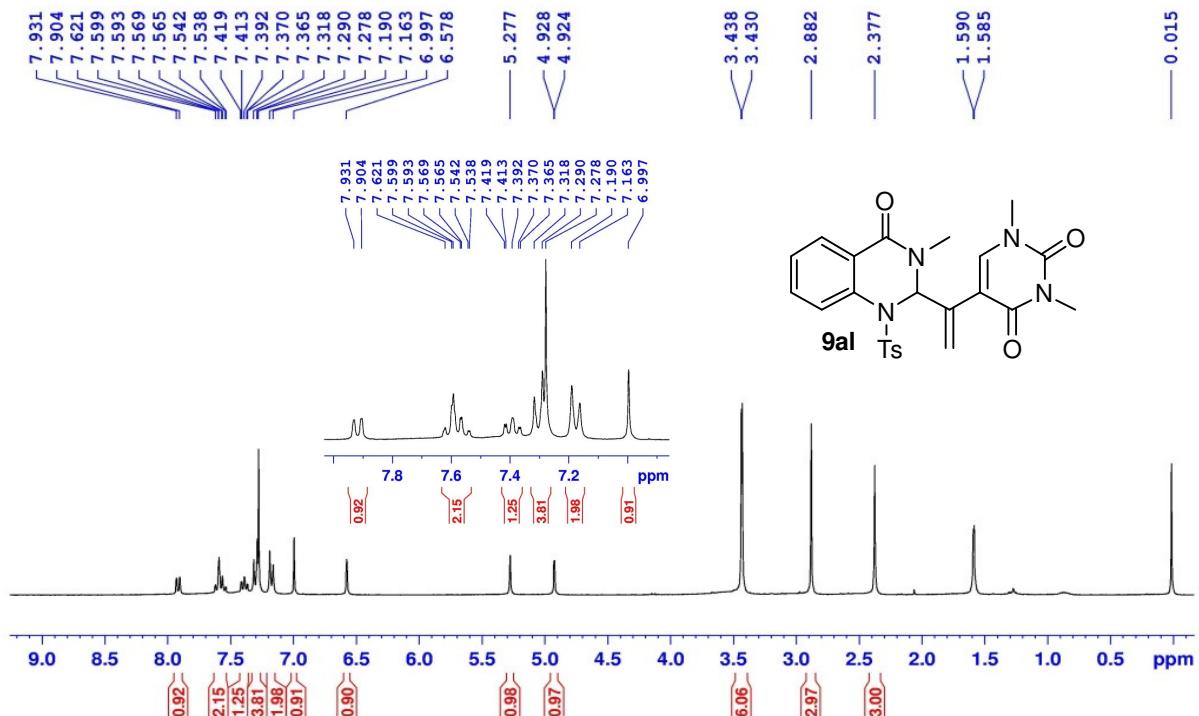
¹H NMR (CDCl_3 , 300 MHz) spectrum of product **9ak**:



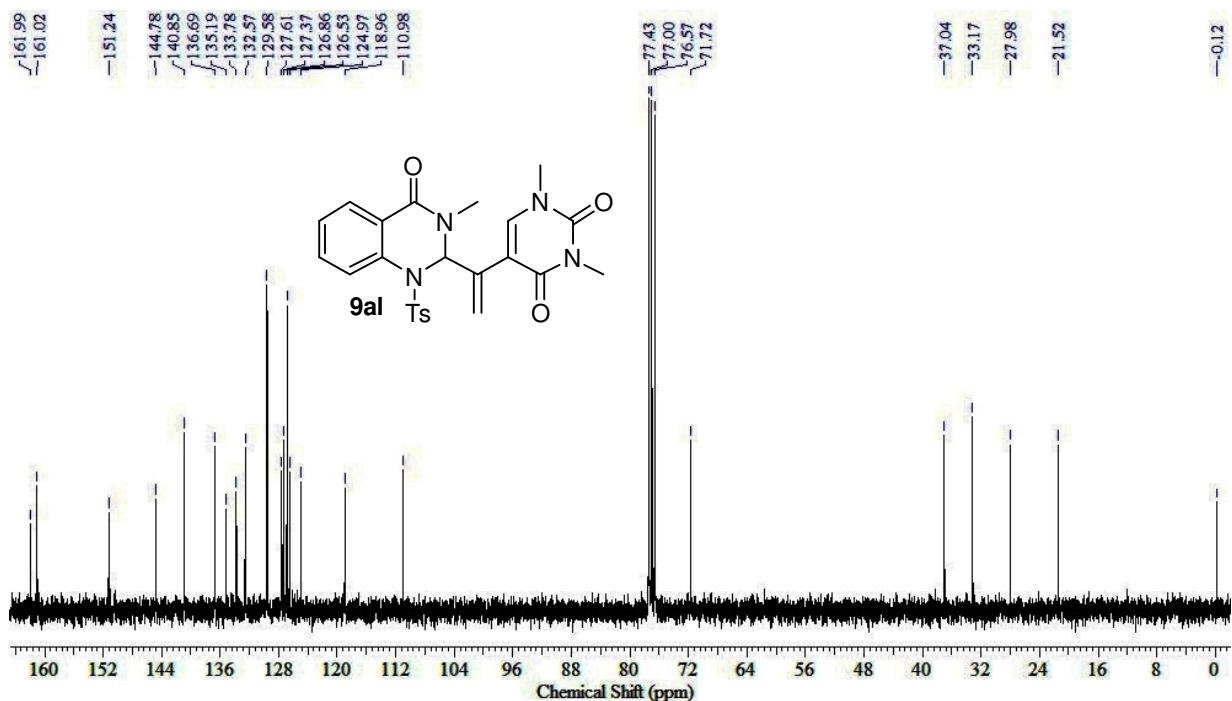
¹³C NMR (CDCl_3 , 150 MHz) spectrum of product **9ak**:



¹H NMR (CDCl_3 , 300 MHz) spectrum of product **9al**:

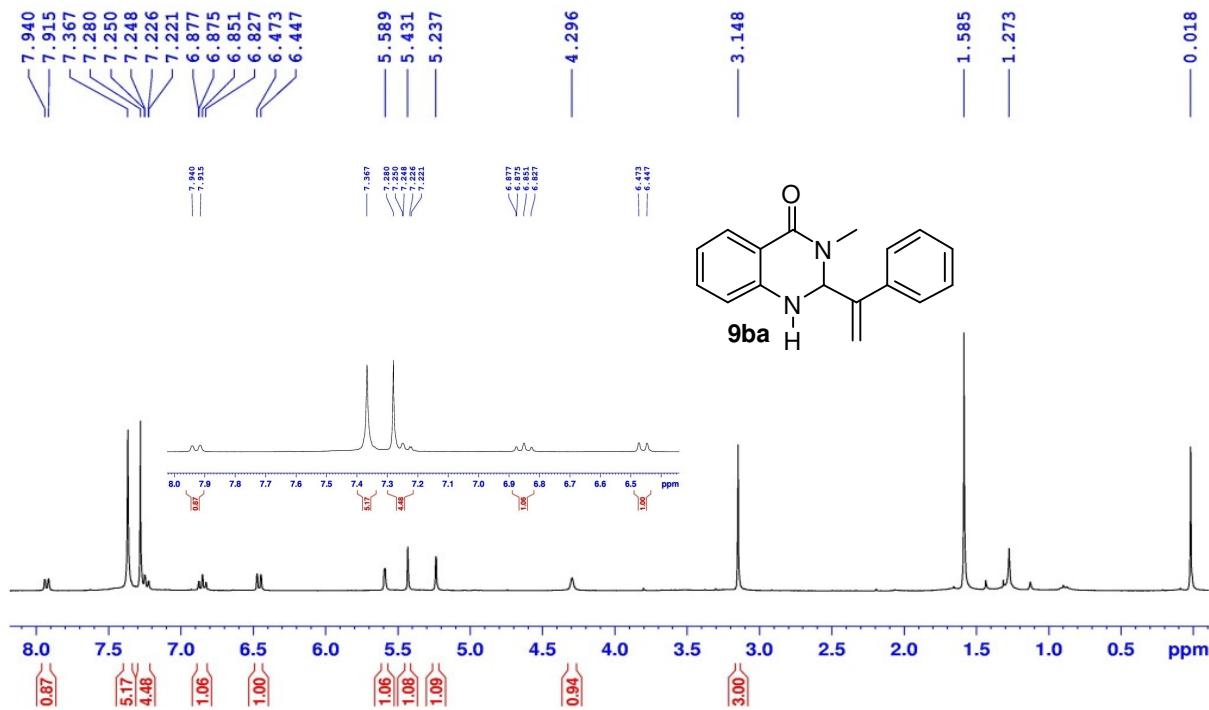


¹³C NMR (CDCl₃, 75 MHz) spectrum of product **9al**:

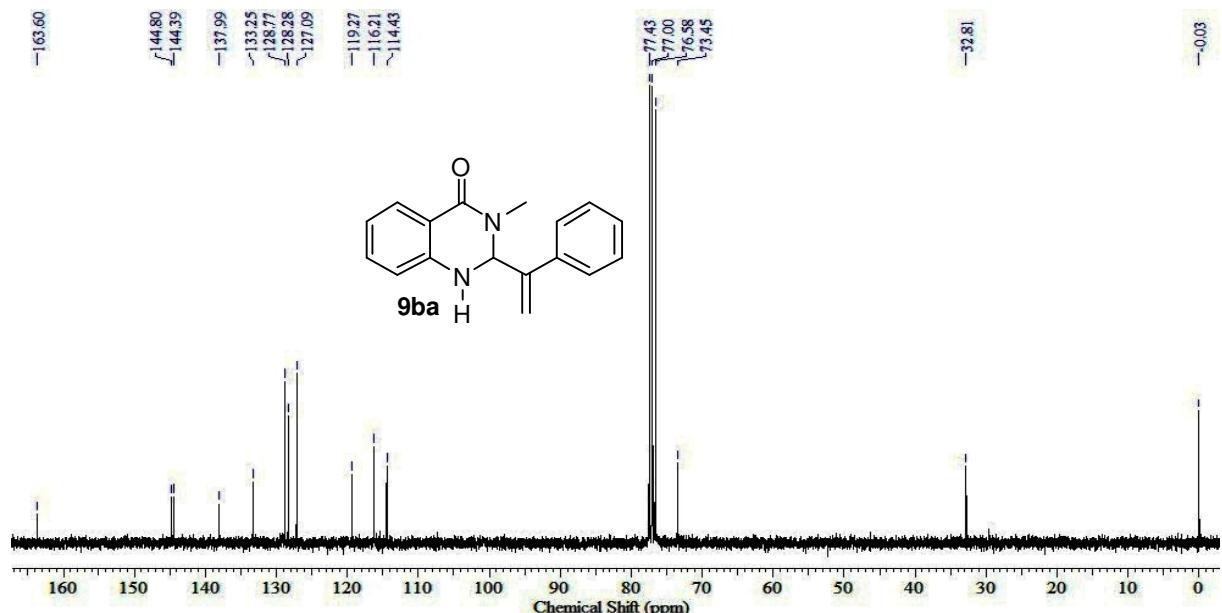


7) NMR spectra of products **9ba-9be** (Table 2):

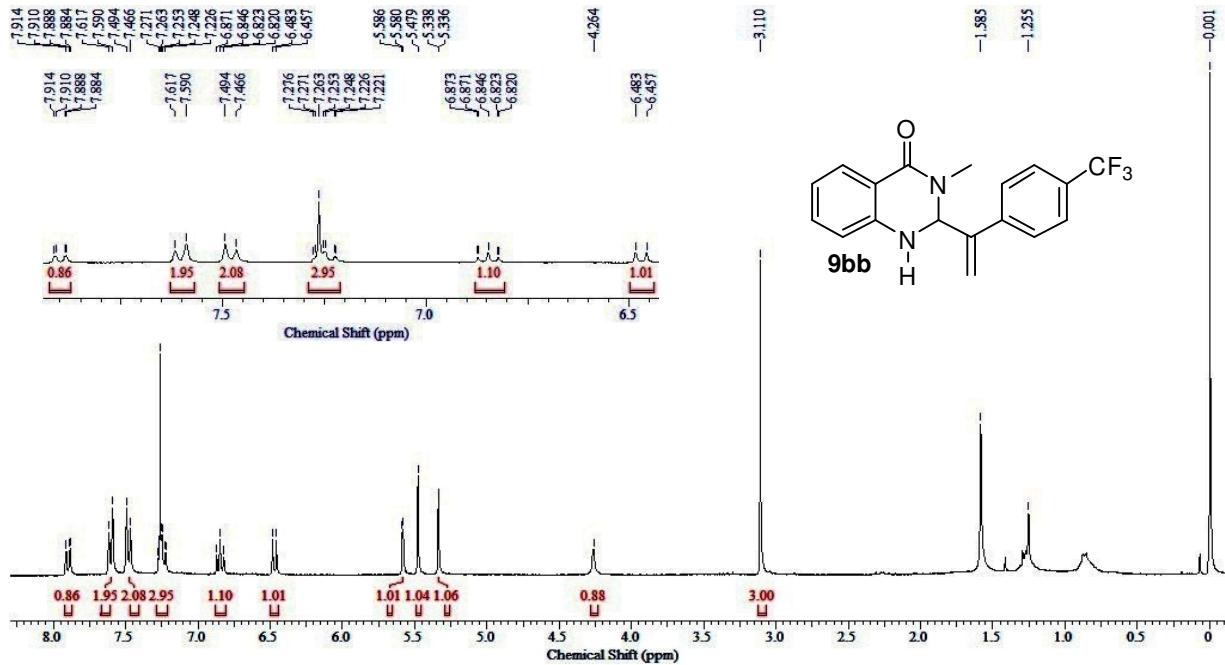
¹H NMR (CDCl_3 , 300 MHz) spectrum of product **9ba**:



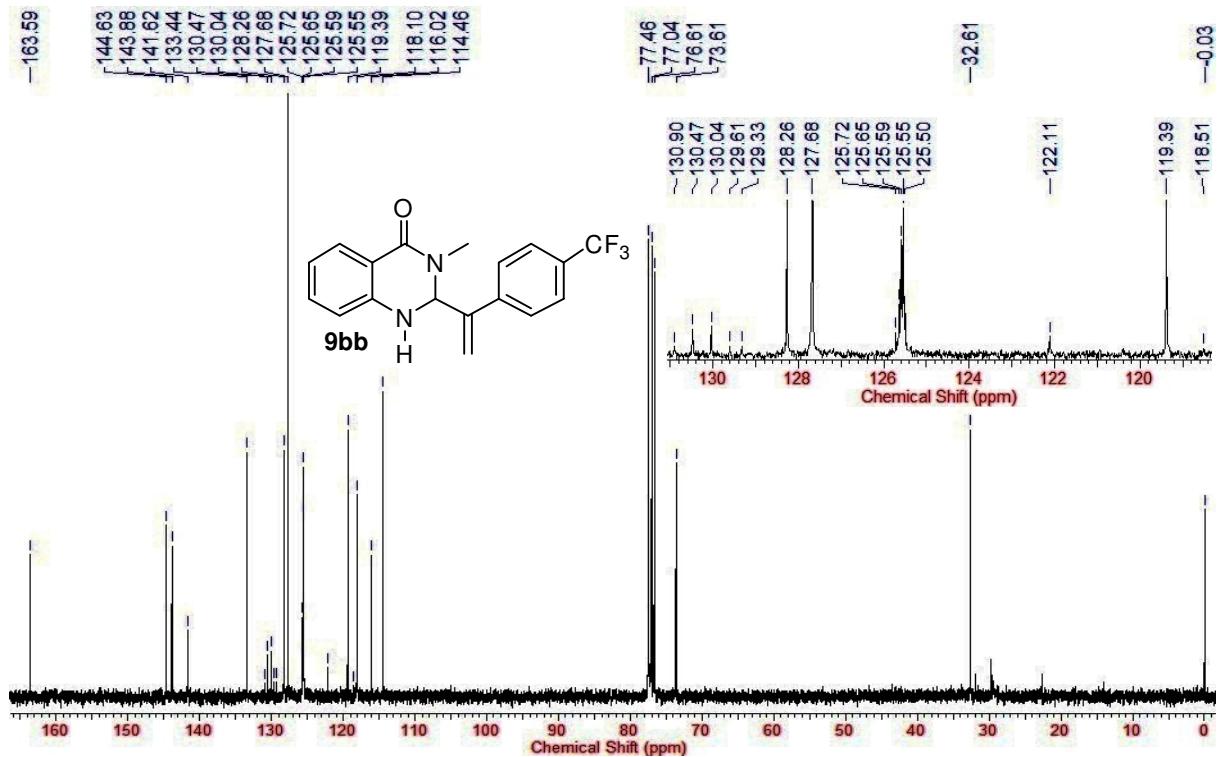
¹³C NMR (CDCl_3 , 75 MHz) spectrum of product **9ba**:



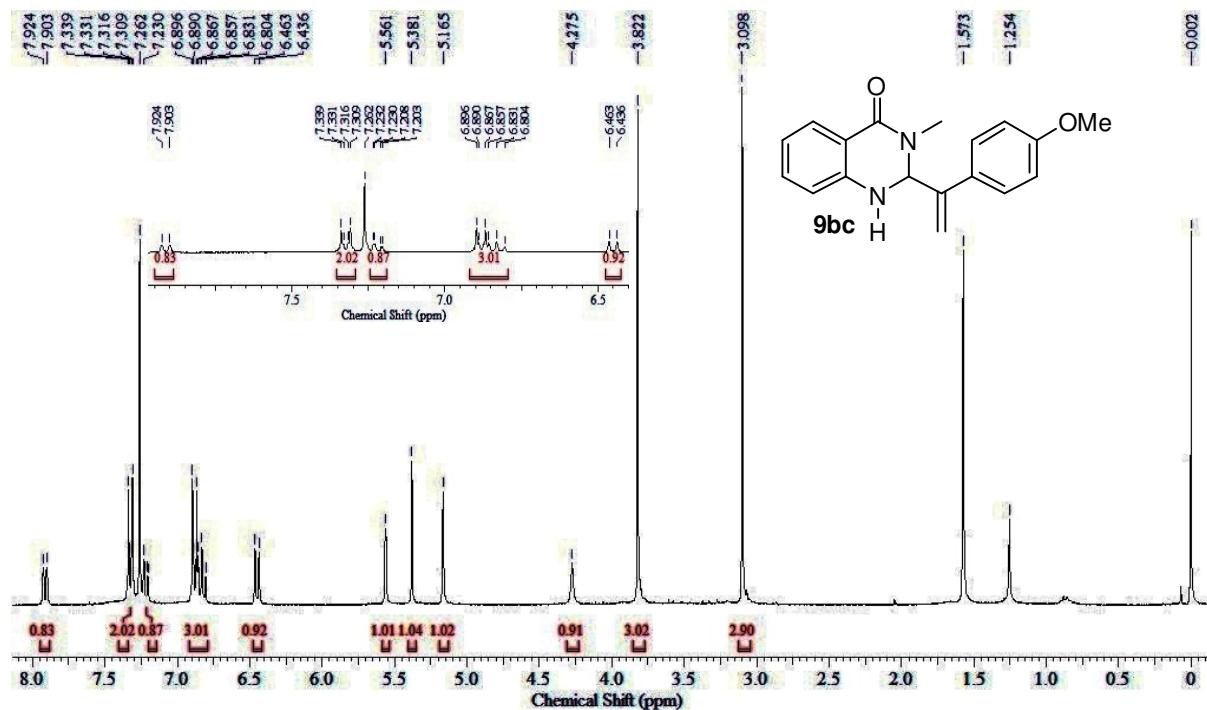
¹H NMR (CDCl₃, 300 MHz) spectrum of product 9bb:



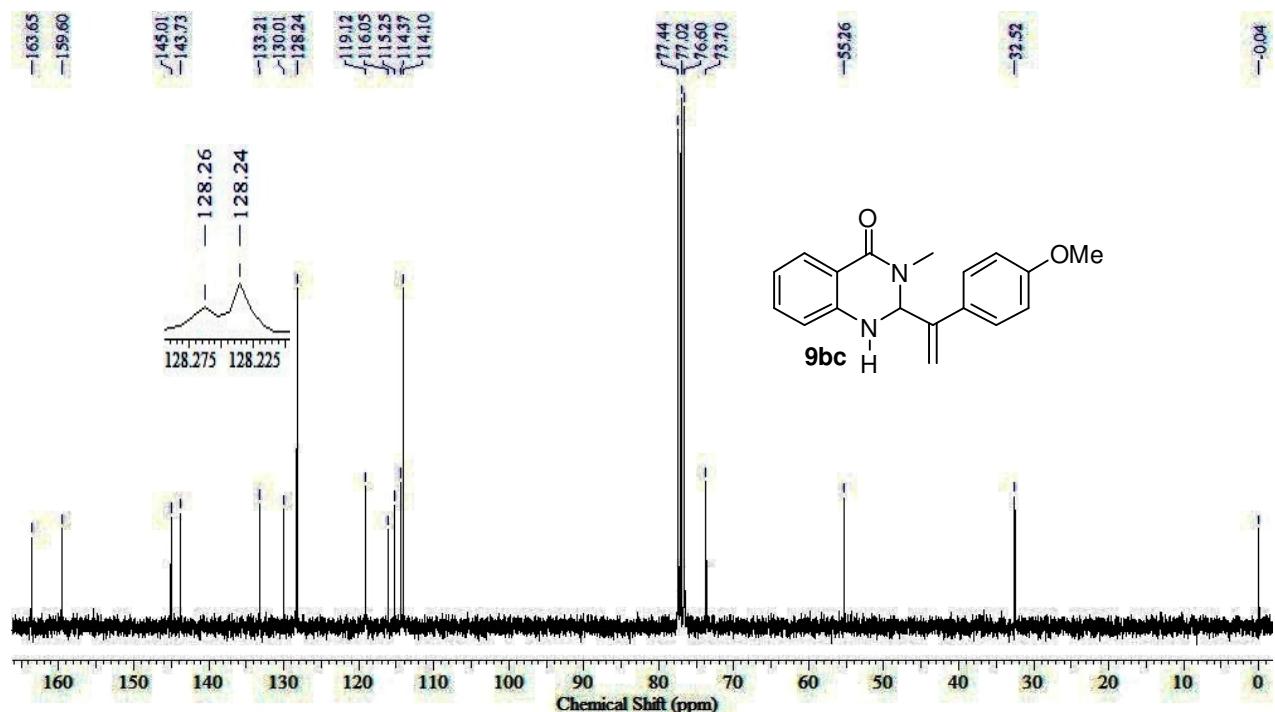
¹³C NMR (CDCl₃, 75 MHz) spectrum of product **9bb**:



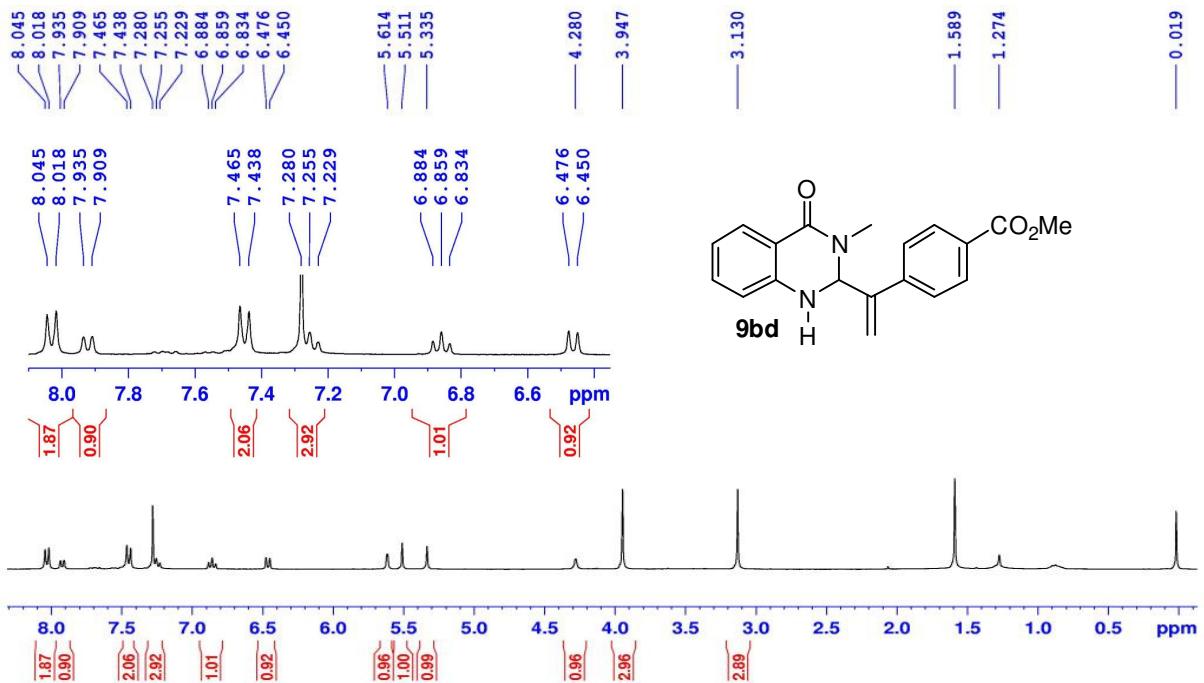
¹H NMR (CDCl₃, 300 MHz) spectrum of product **9bc**:



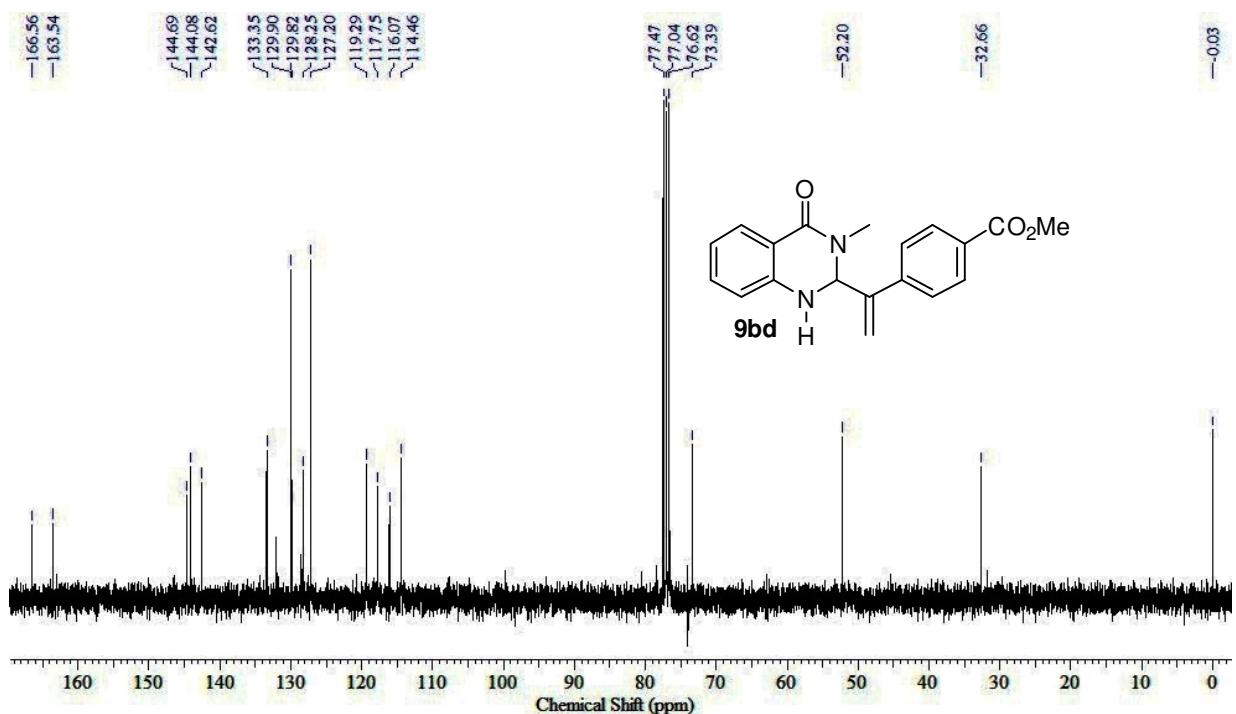
¹³C NMR (CDCl_3 , 75 MHz) spectrum of product **9bc**:



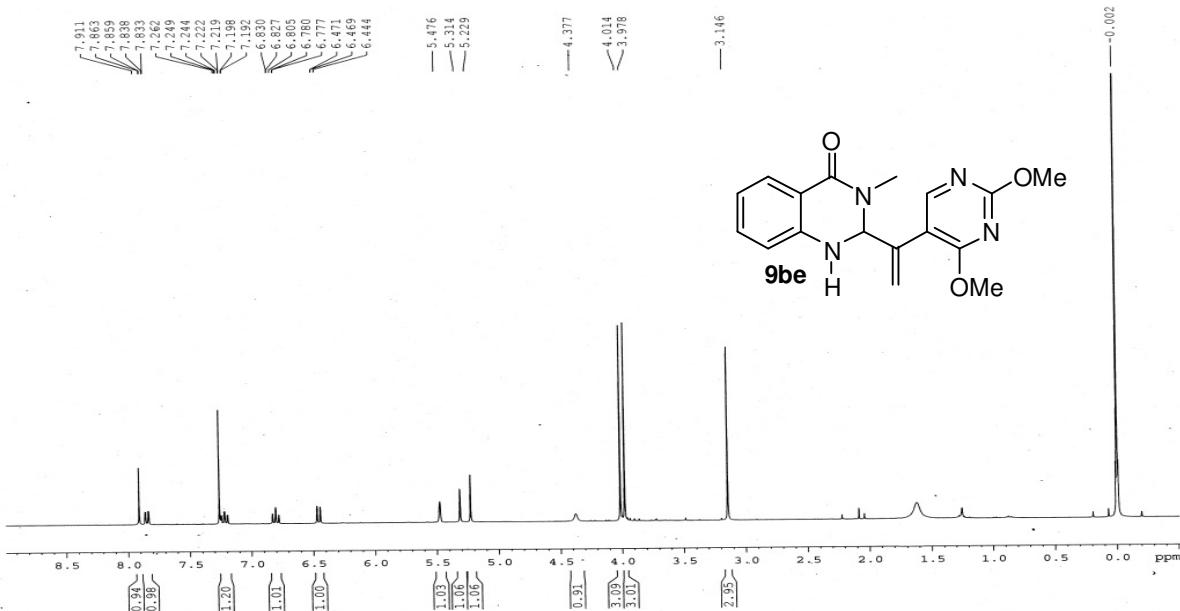
¹H NMR (CDCl₃, 300 MHz) spectrum of product 9bd:



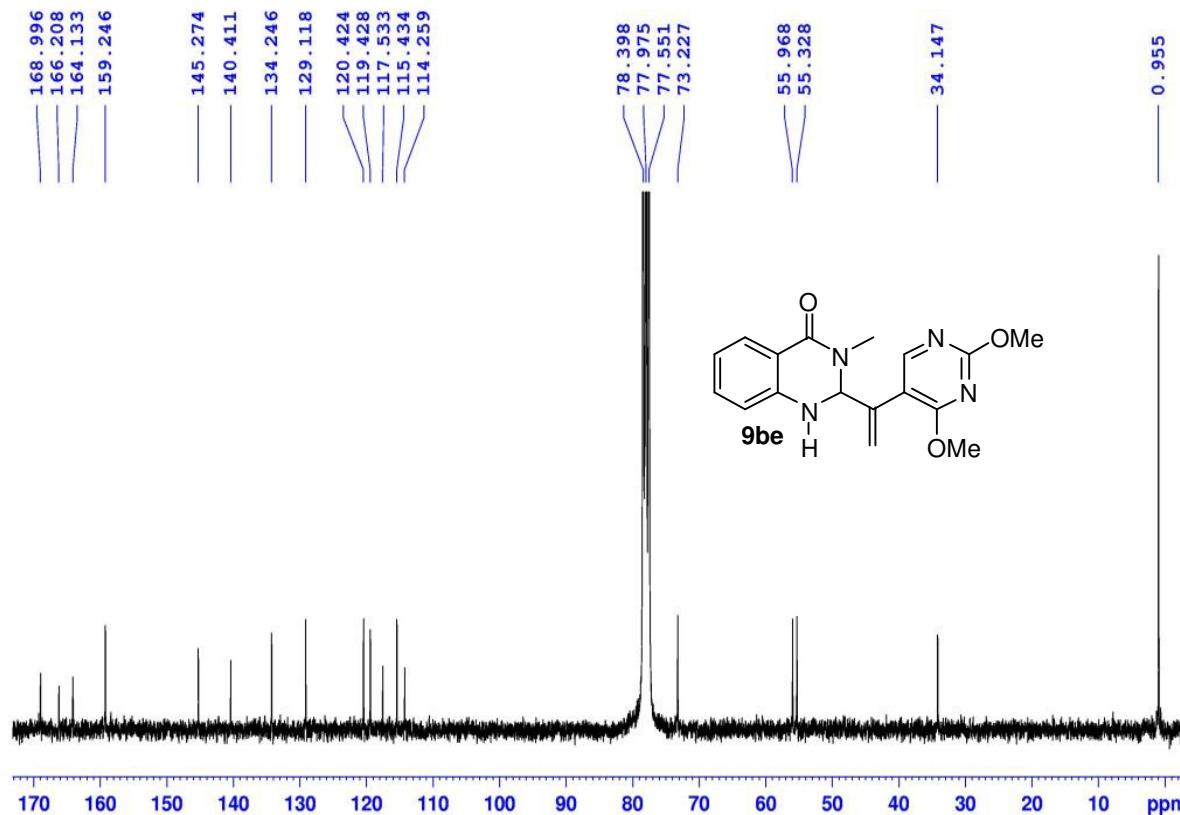
¹³C NMR (CDCl₃, 75 MHz) spectrum of product **9bd**:



¹H NMR (CDCl_3 , 300 MHz) spectrum of product **9be**:

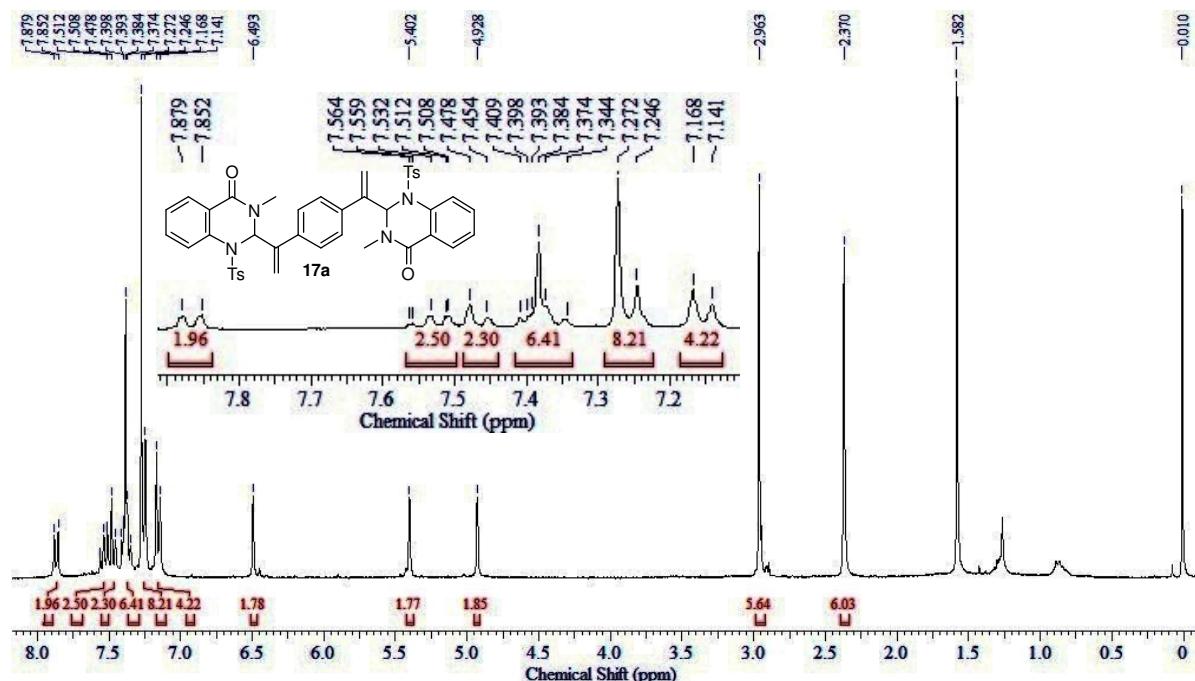


¹³C NMR (CDCl_3 , 75 MHz) spectrum of product **9be**:

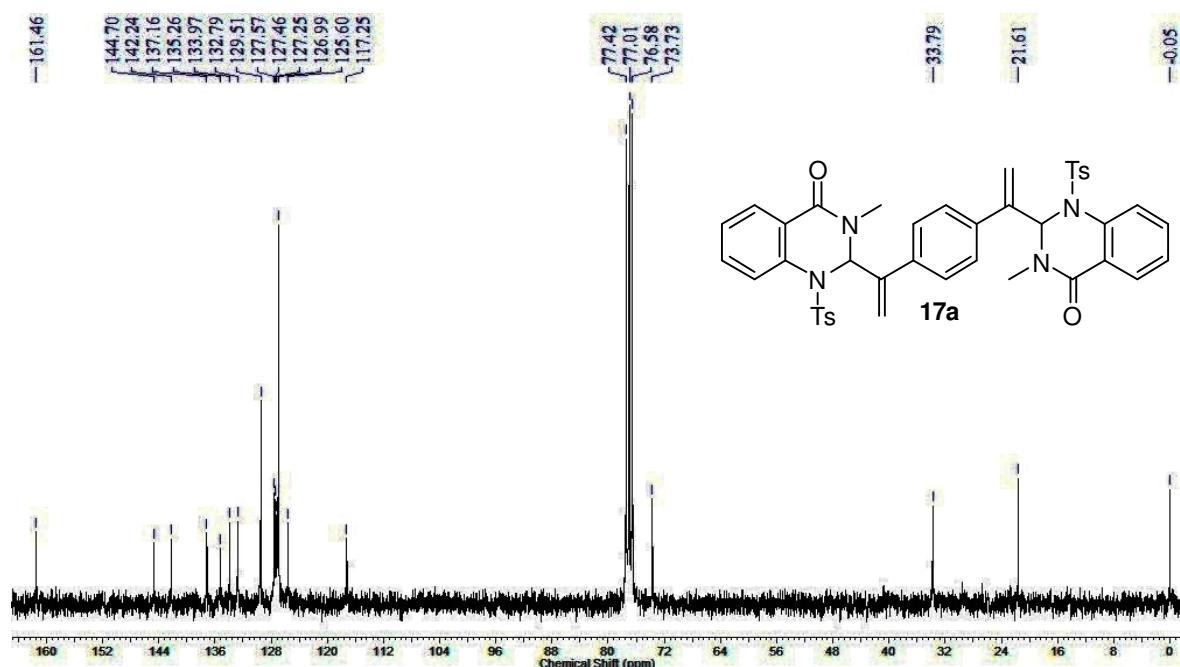


8) NMR and HRMS spectra of bis-heteroannulated products **17a**, **17b** (scheme 2):

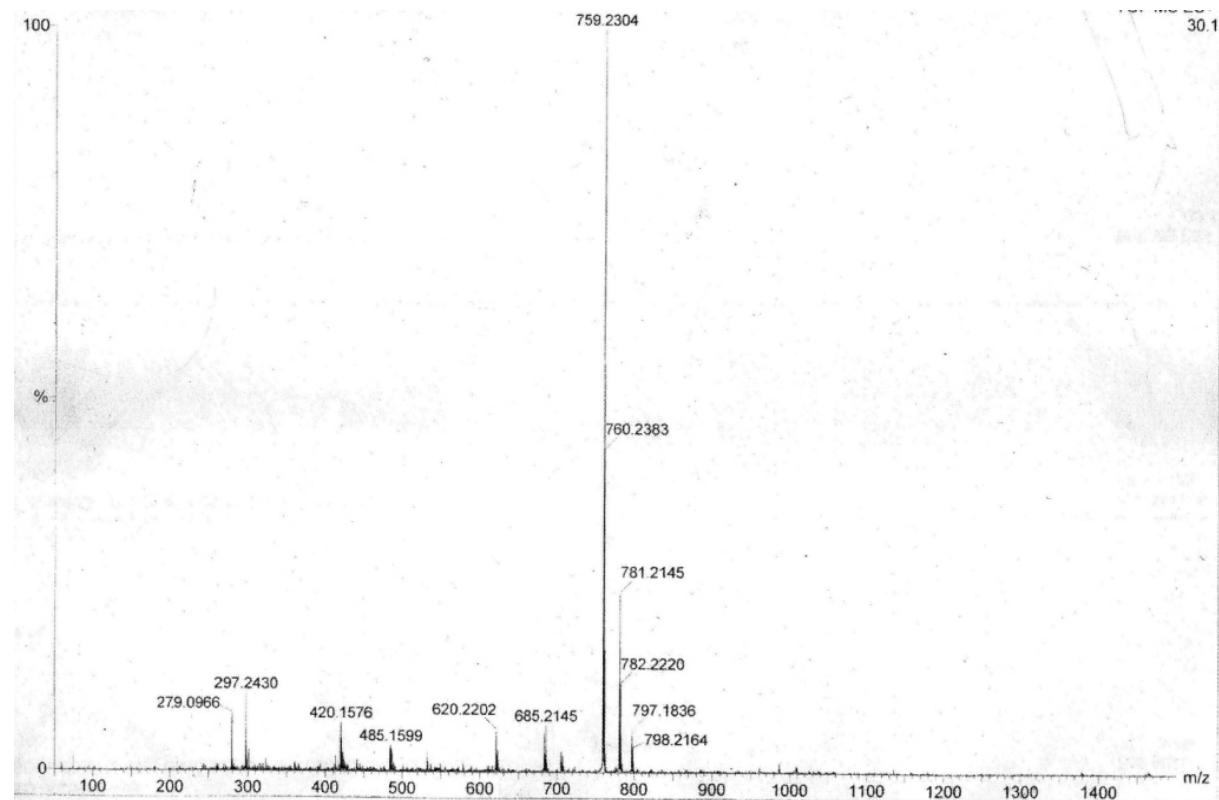
¹H NMR (CDCl_3 , 300 MHz) spectrum of bis-heteroannulated product **17a**:



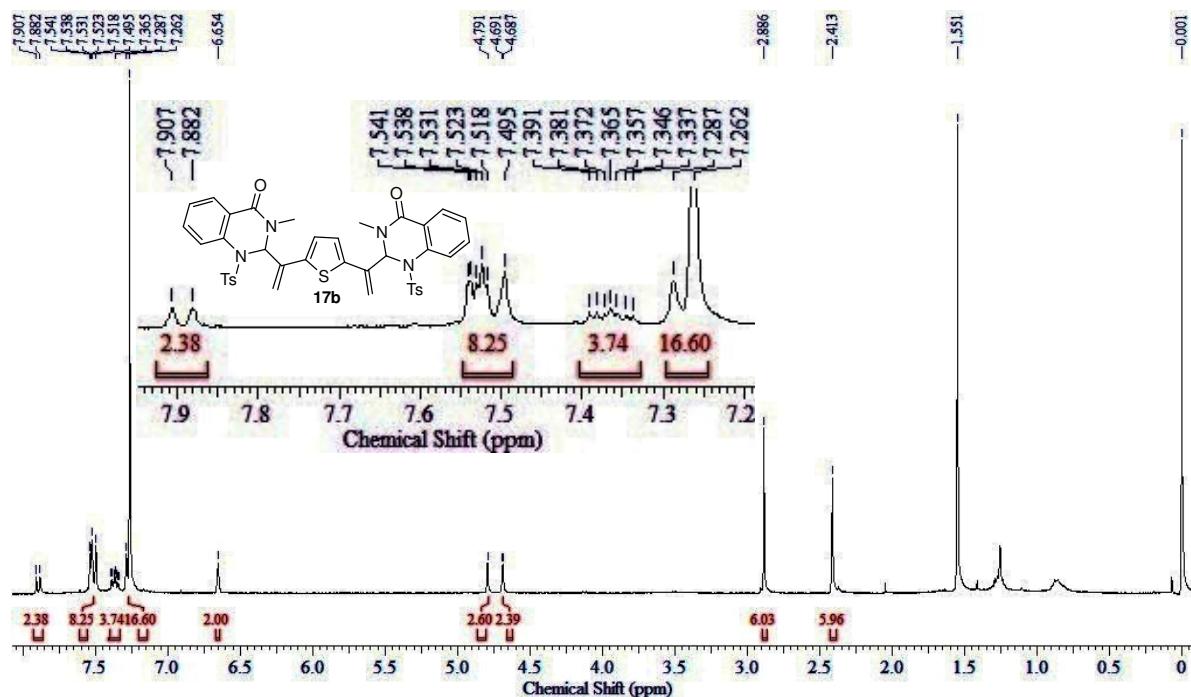
¹³C NMR (CDCl_3 , 75 MHz) spectrum of bis-heteroannulated product **17a**:



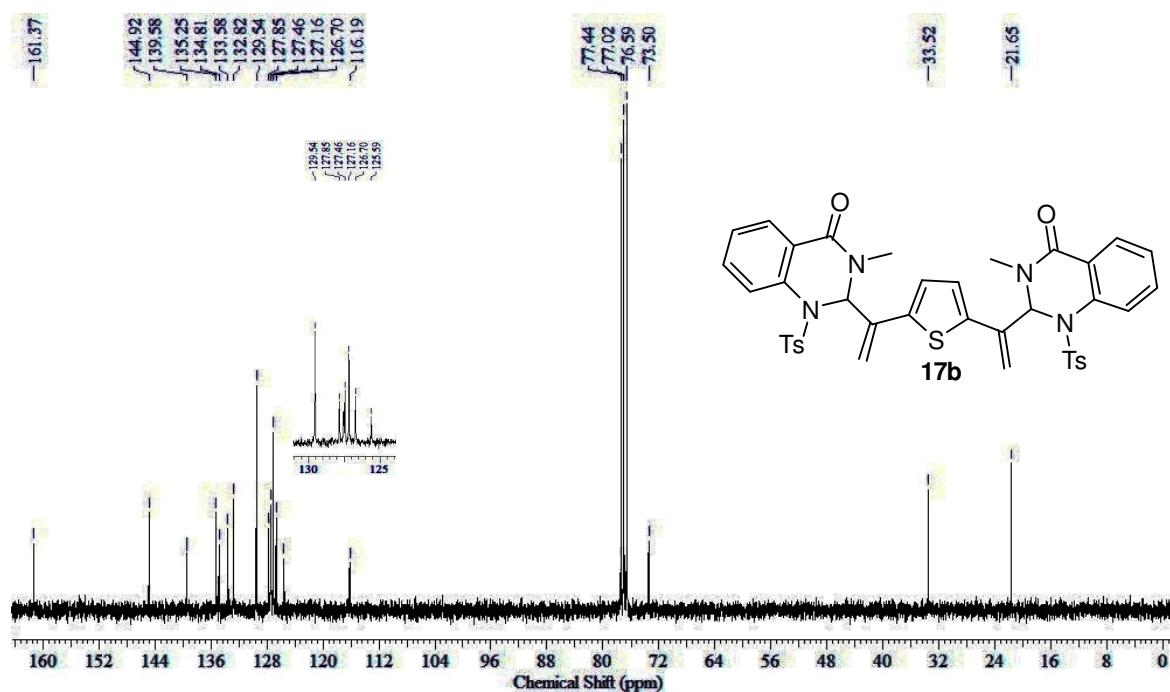
HRMS spectra of product **17a**:



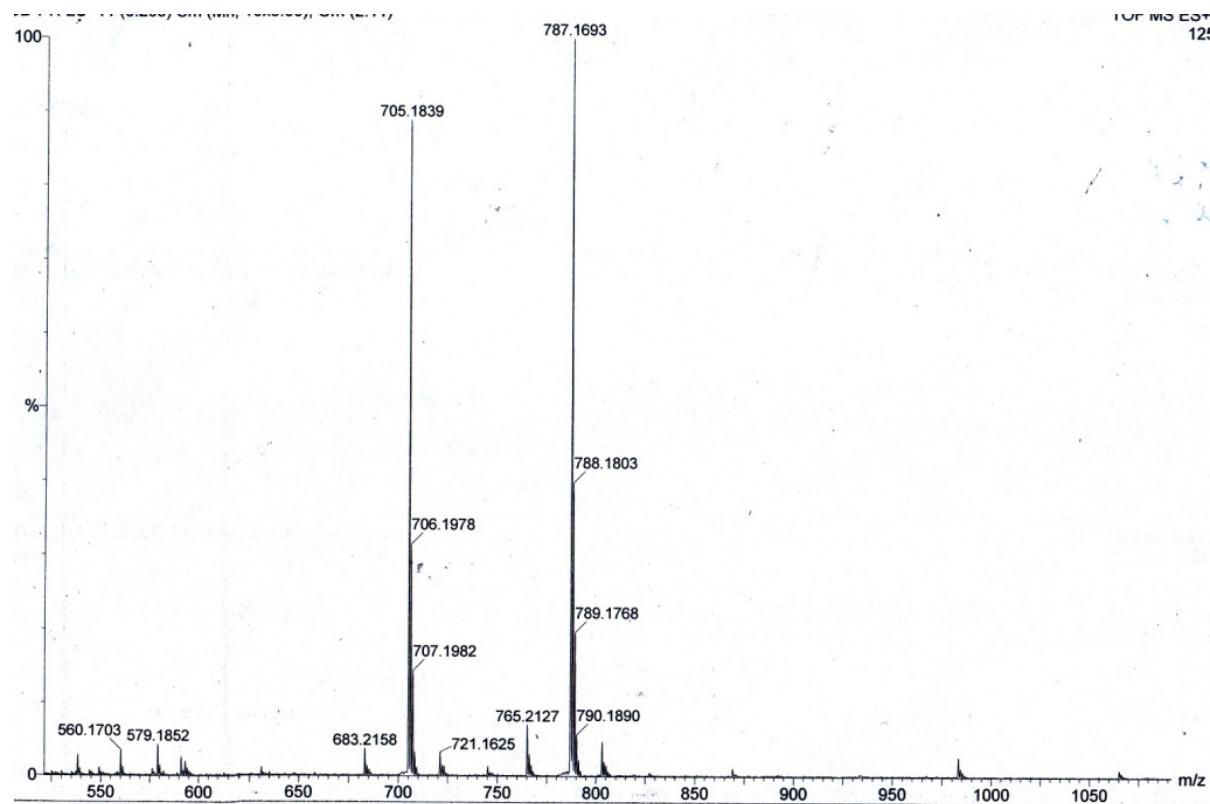
¹H NMR (CDCl_3 , 300 MHz) spectrum of bis-heteroannulated product **17b**:



¹³C NMR (CDCl_3 , 75 MHz) spectrum of bis-heteroannulated product **17b**:

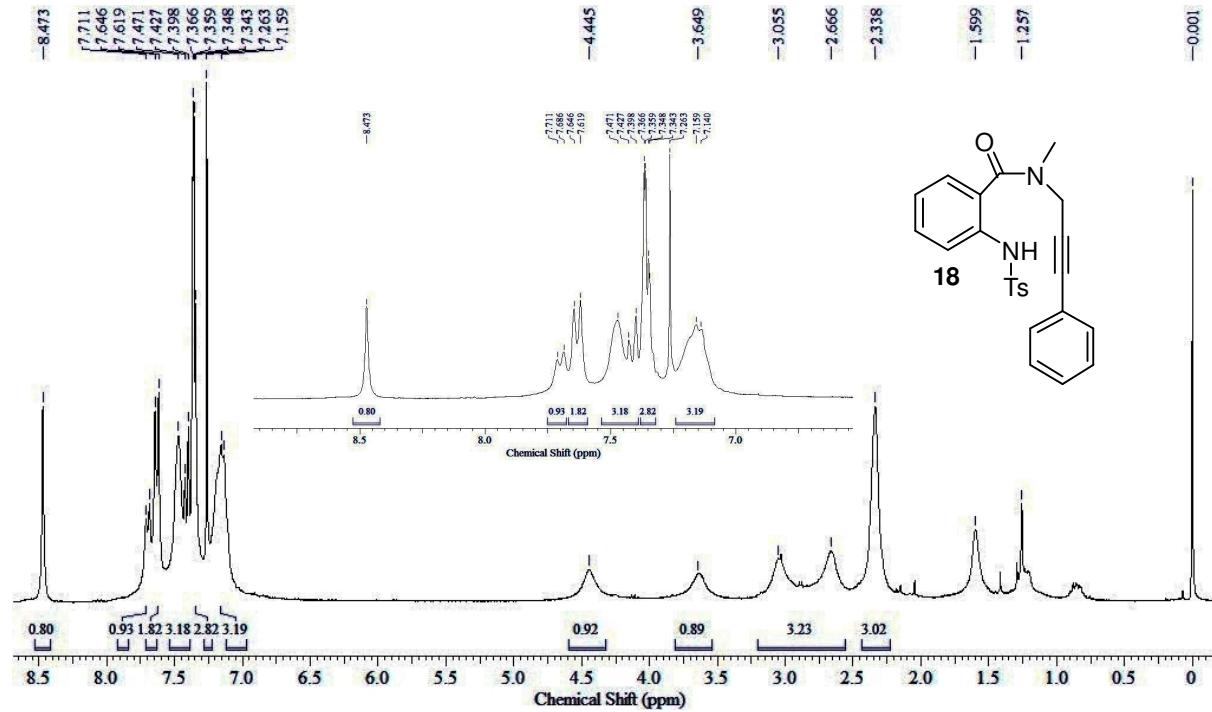


HRMS spectra of product **17b**:

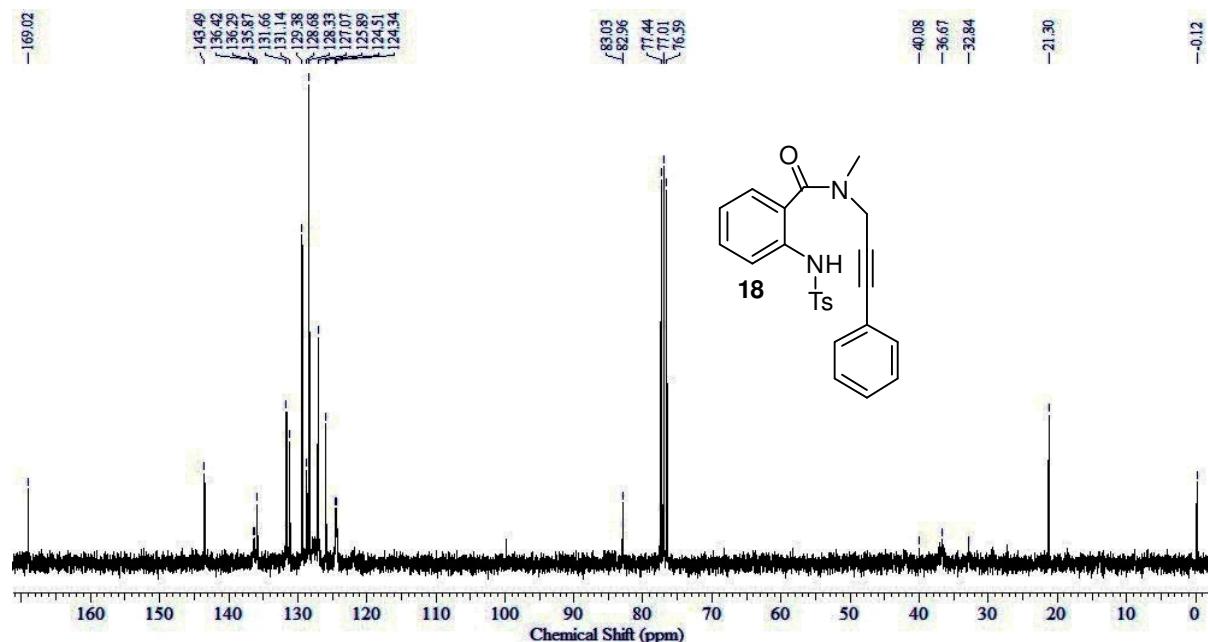


9) NMR spectra of **18**, **20** (scheme 3):

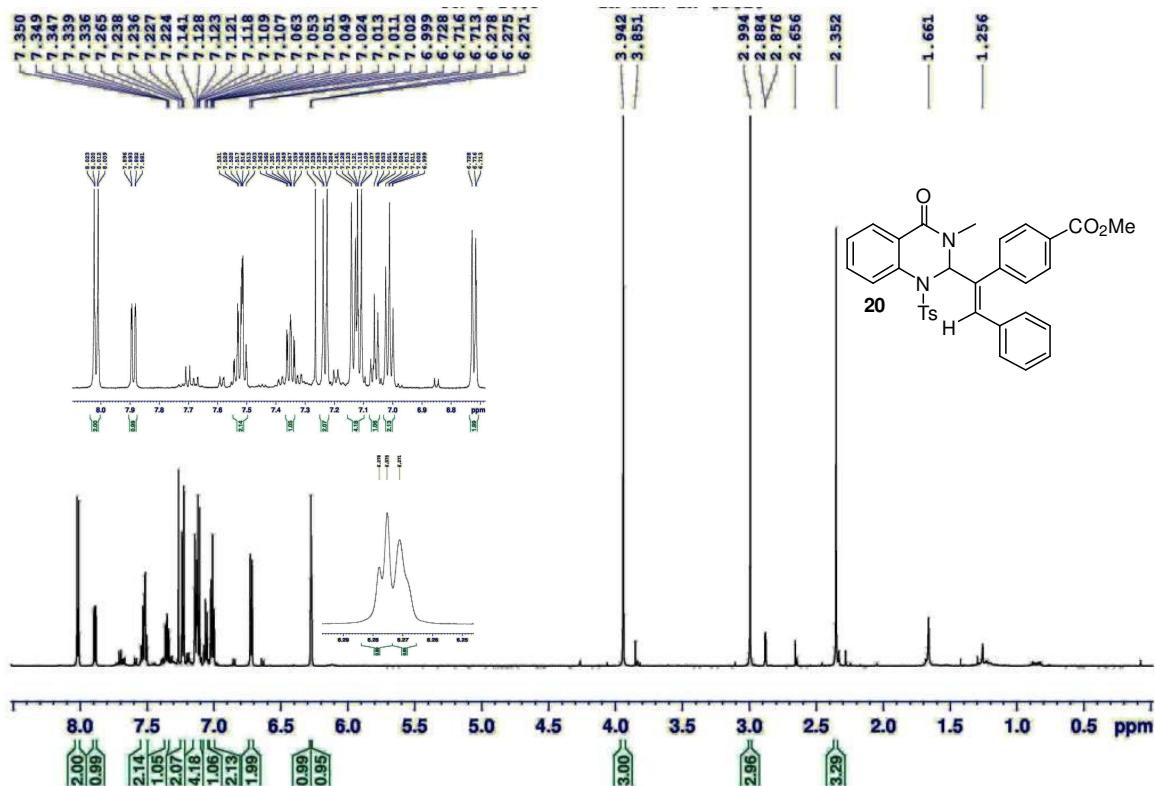
^1H NMR (CDCl_3 , 300 MHz) spectrum of starting acetylene **18**:



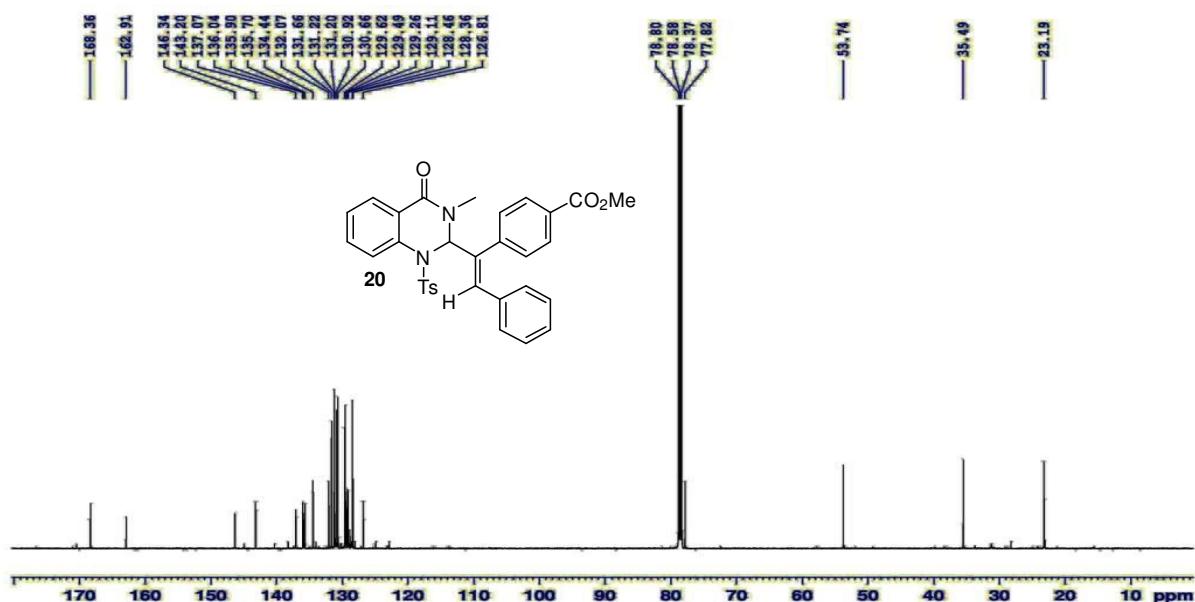
^{13}C NMR (CDCl_3 , 75 MHz) spectrum of starting acetylene **18**:



¹H NMR (CDCl_3 , 600 MHz) spectrum of product **20**:

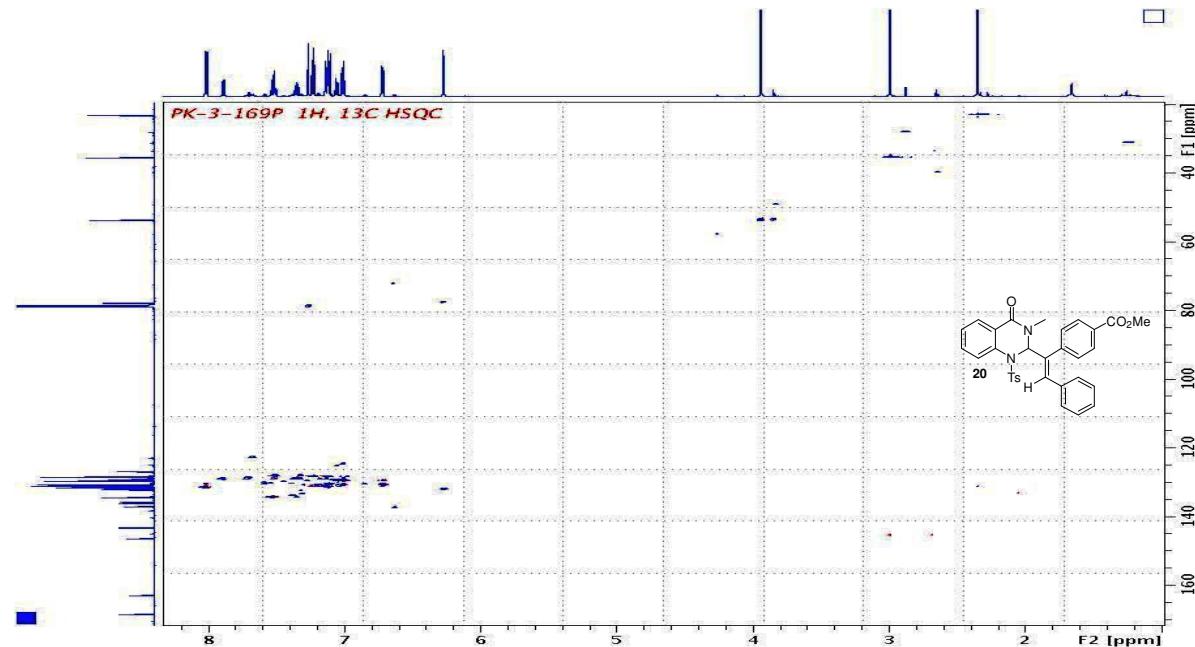


¹³C NMR (CDCl_3 , 150 MHz) spectrum of product **20**:

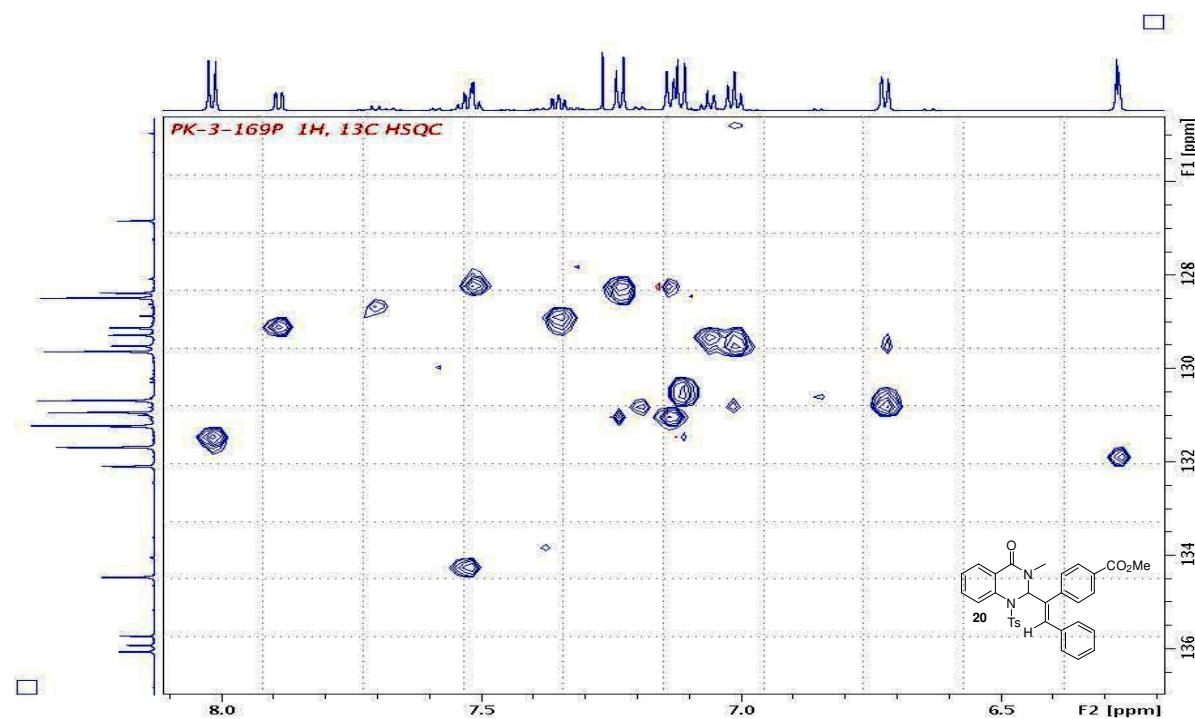


2D NMR spectra of **20**

HSQC spectrum of product **20**:



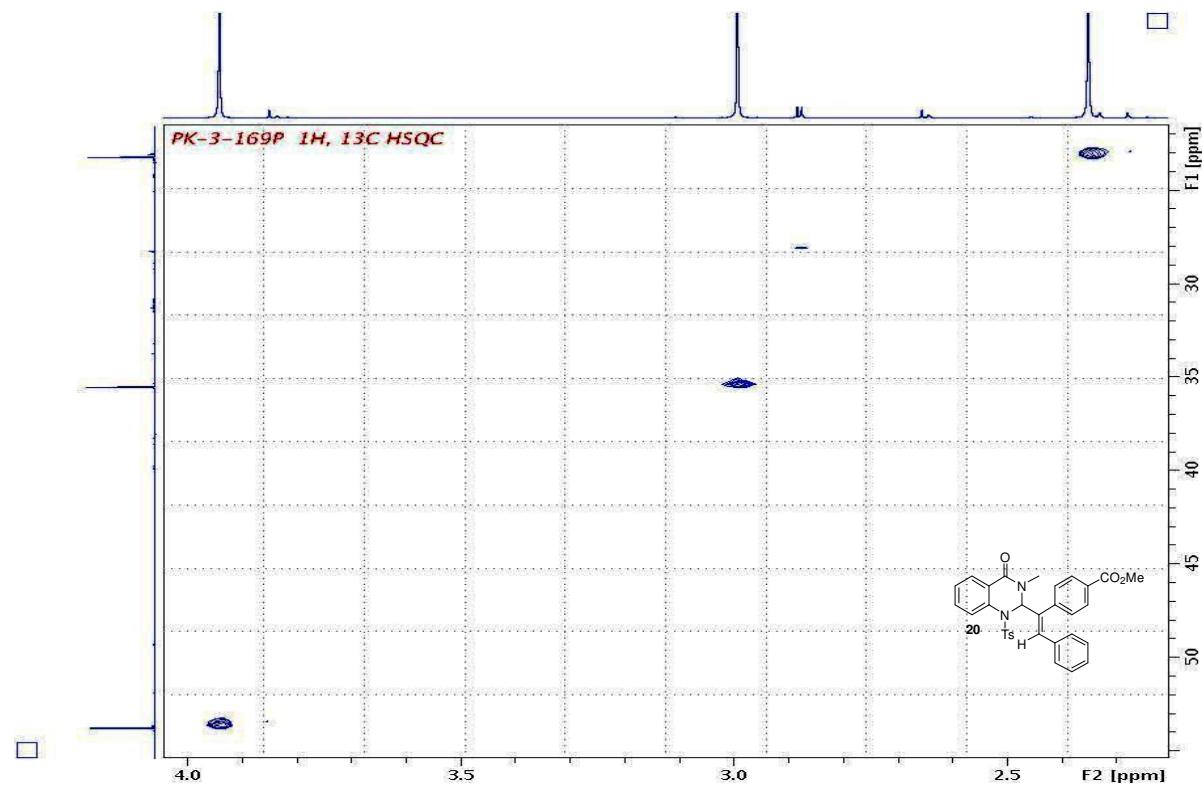
Expansion 1:



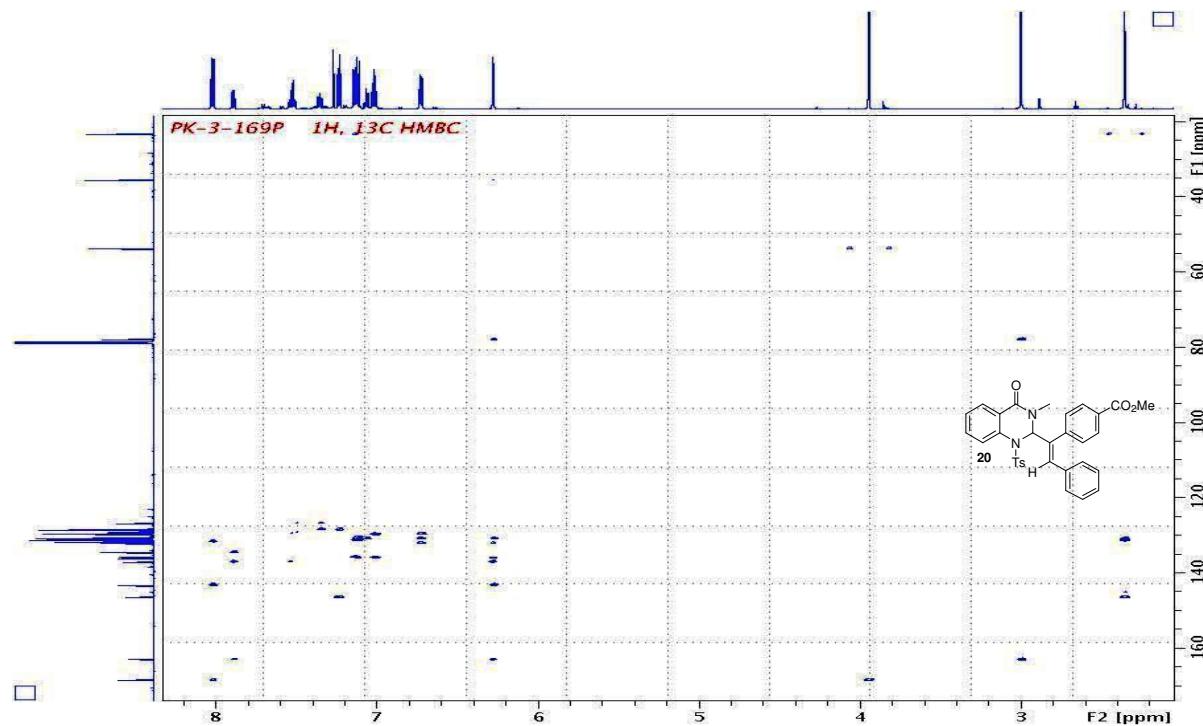
Expansion 2:



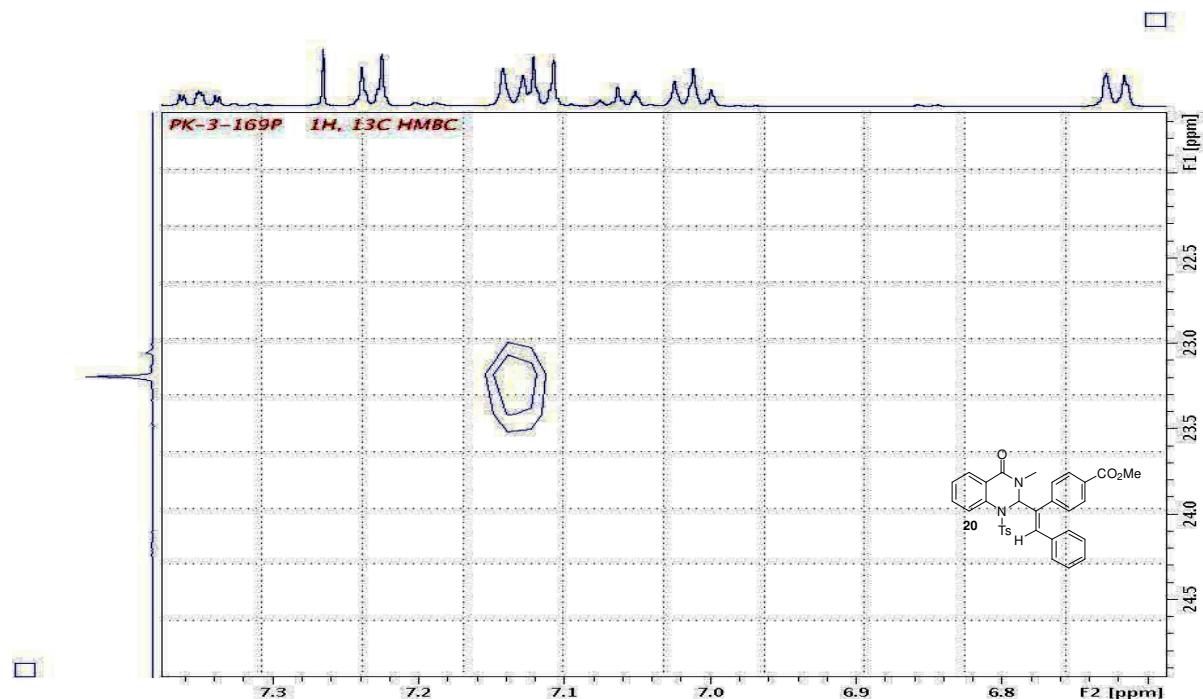
Expansion 3:



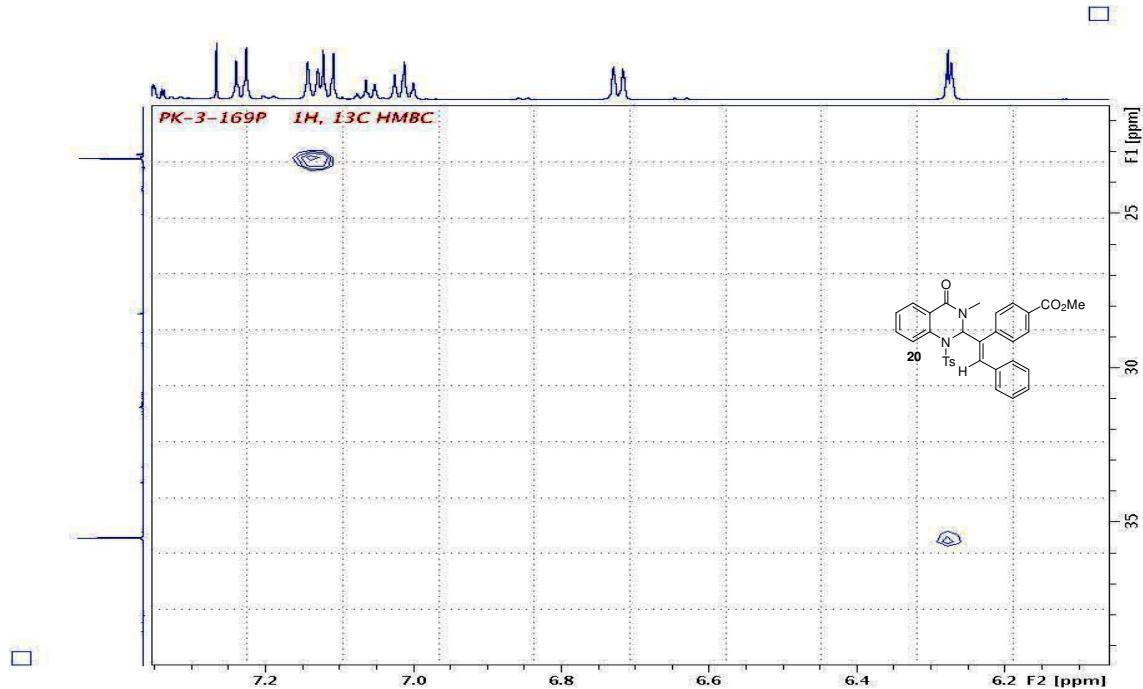
HMBC spectrum of product **20**:



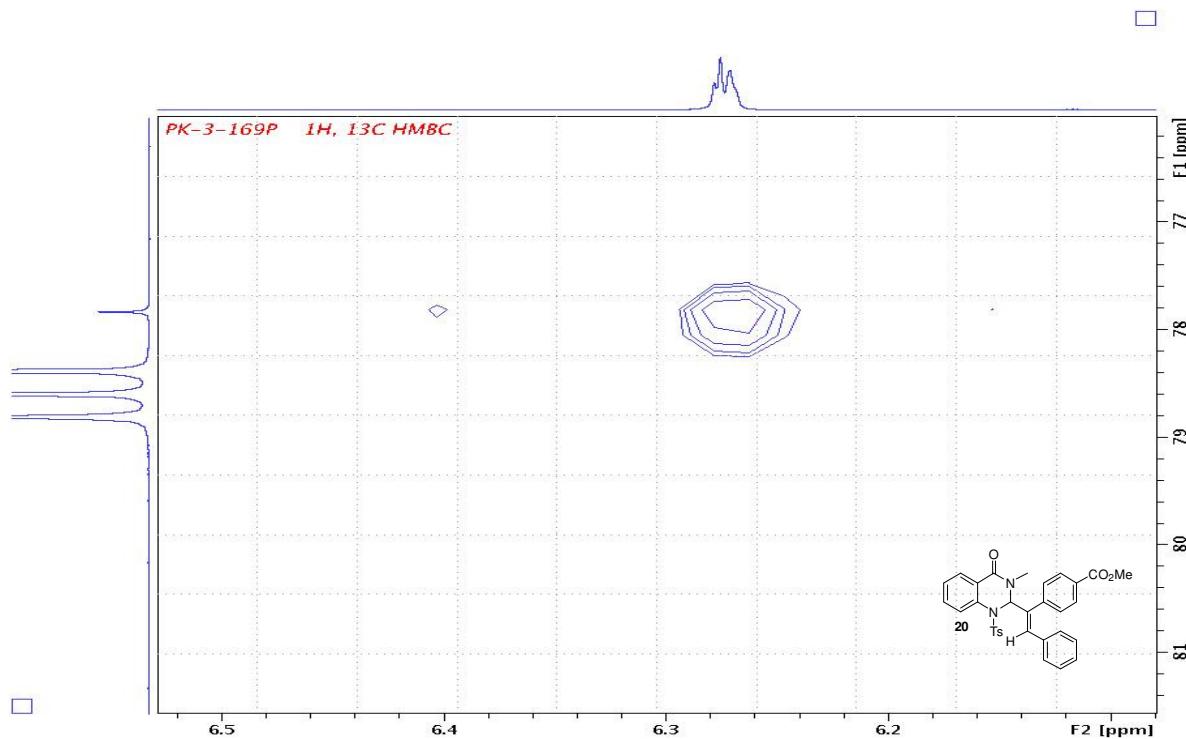
Expansion 1:



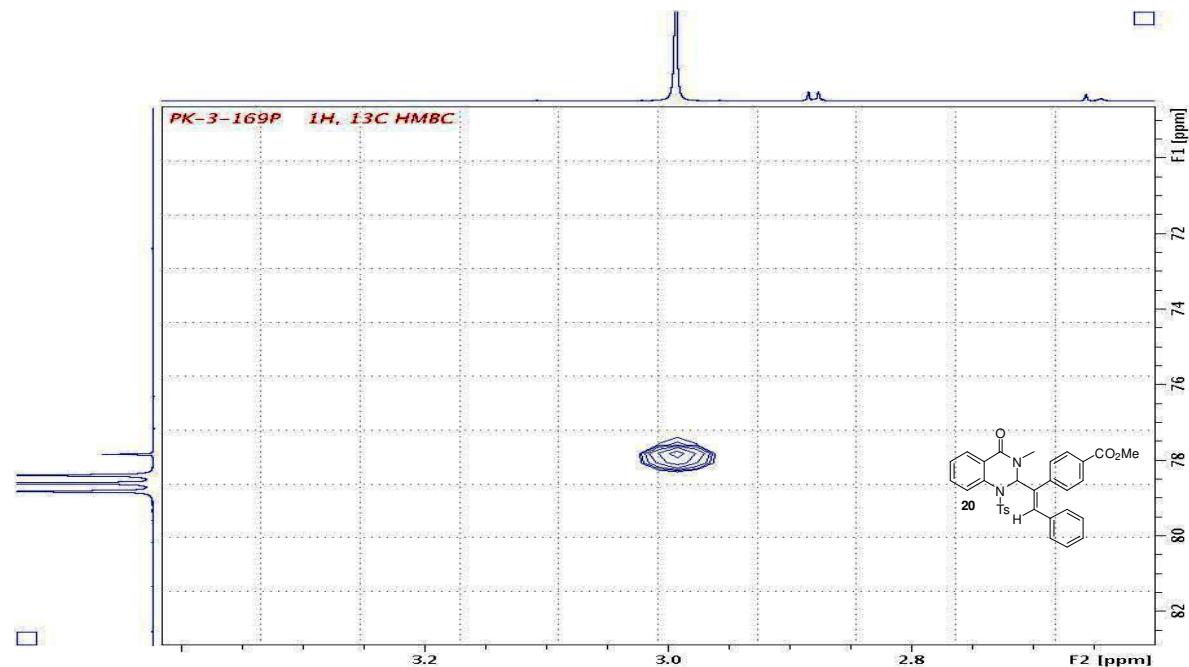
Expansion 2:



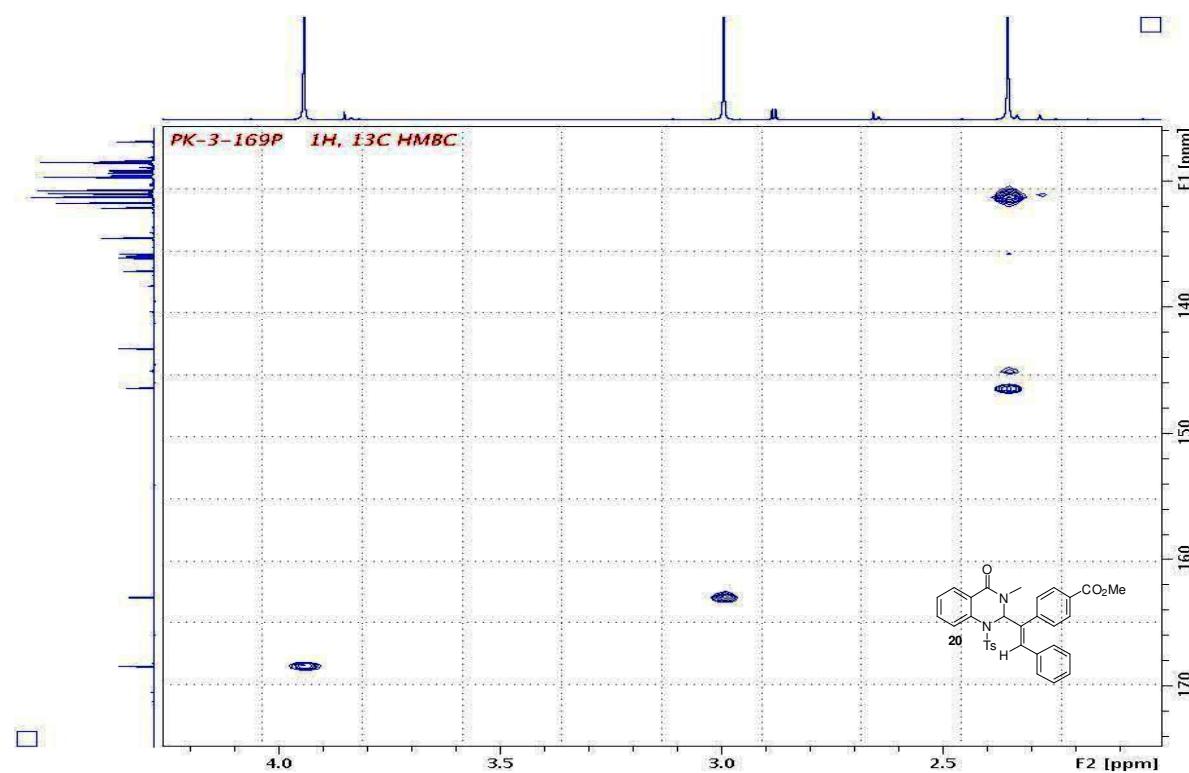
Expansion 3:



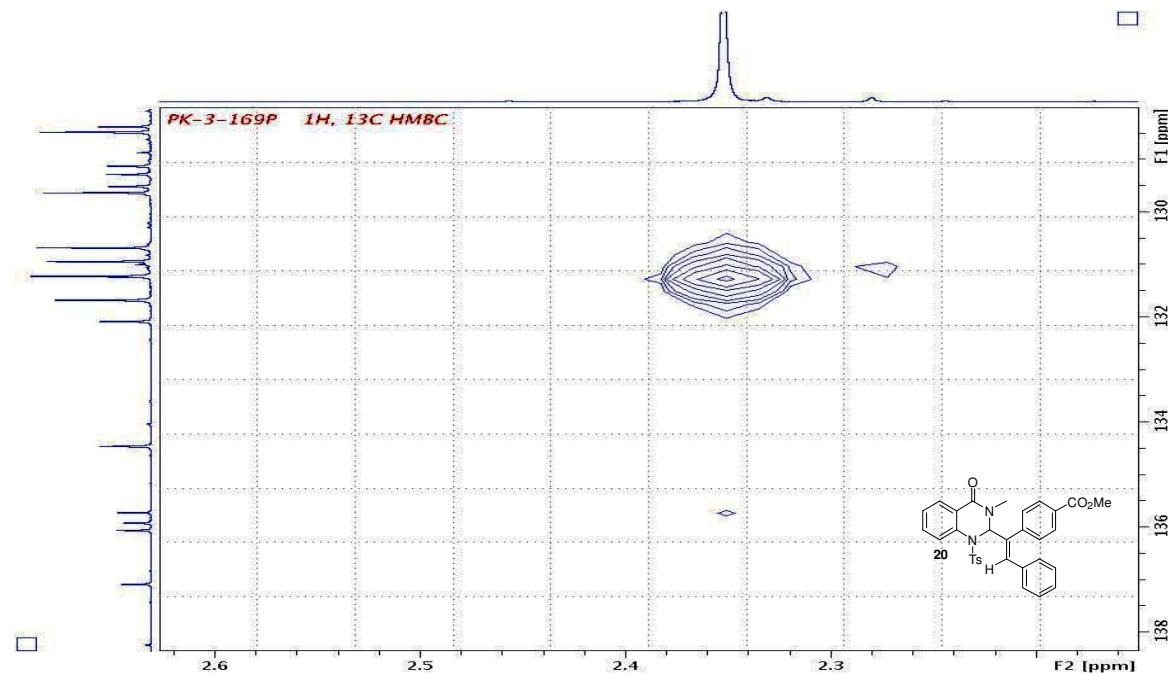
Expansion 4:



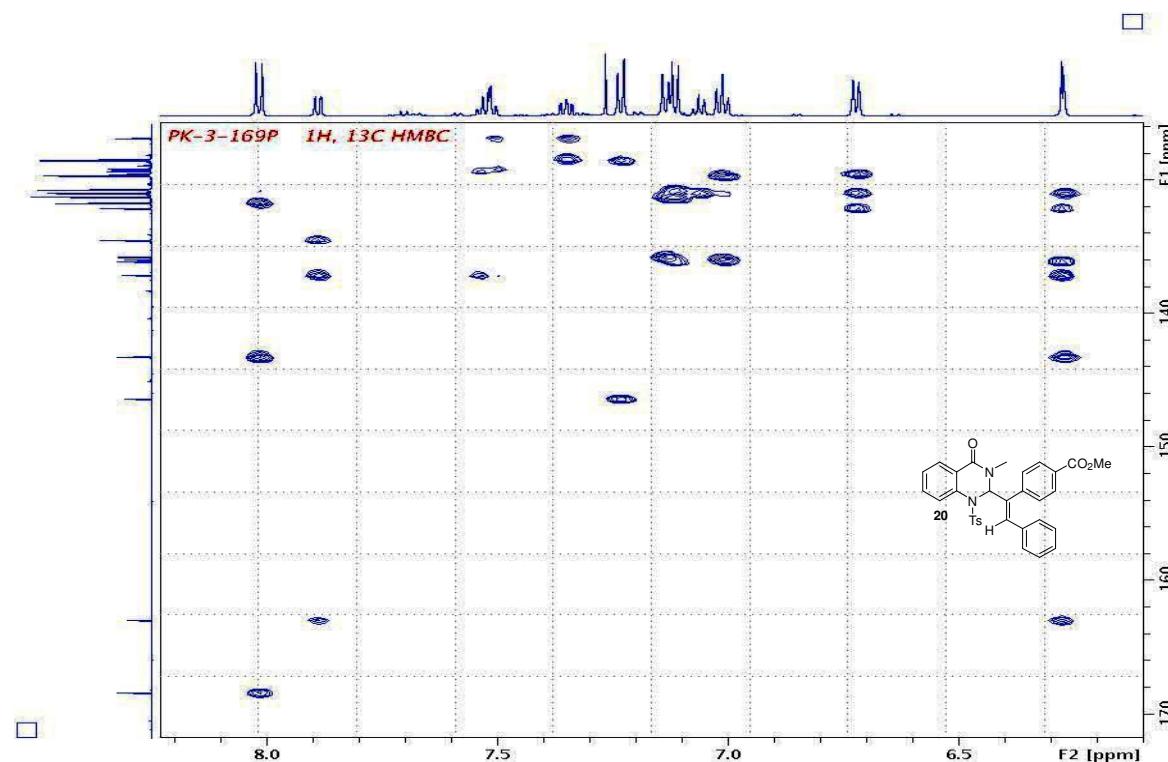
Expansion 5:



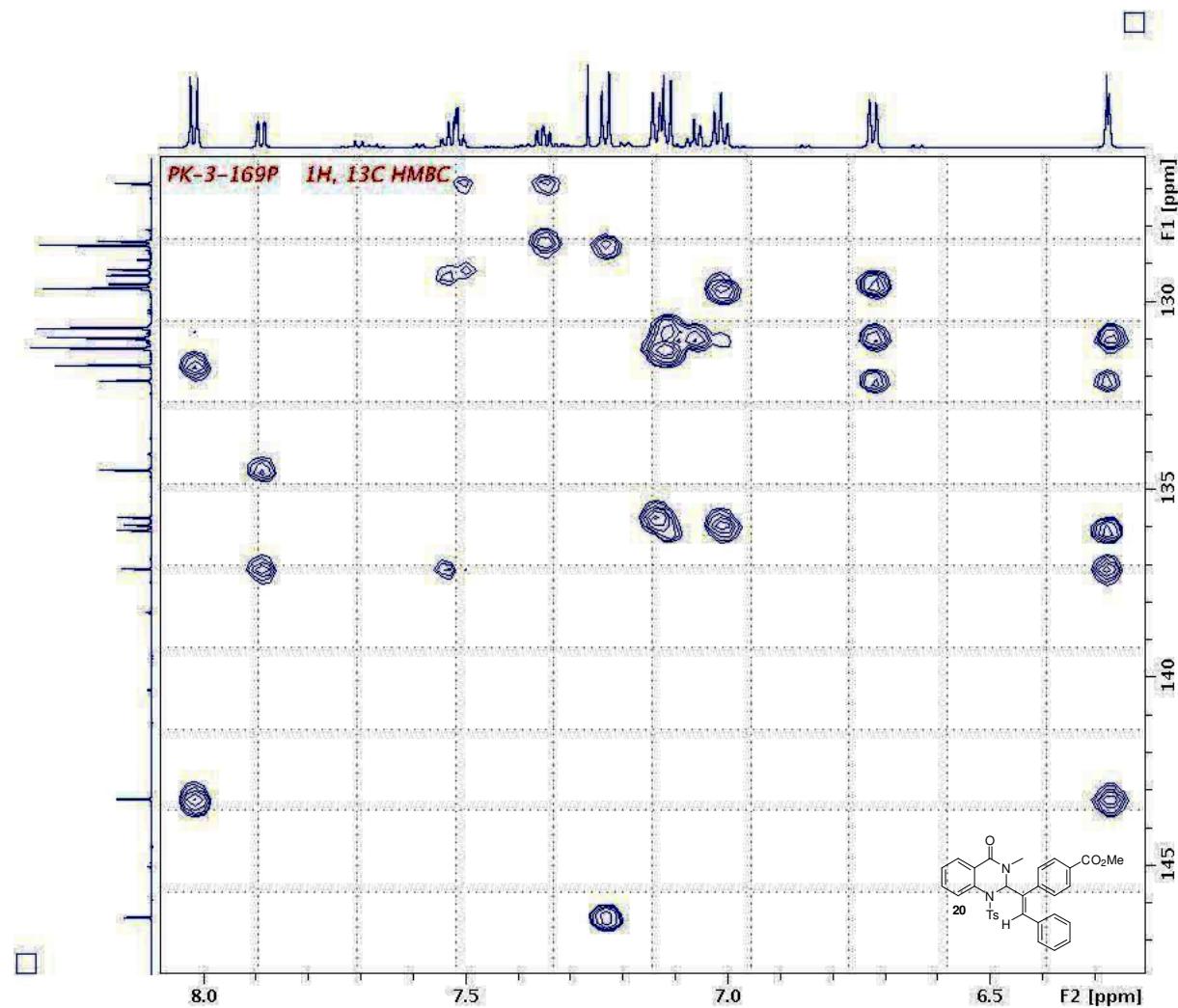
Expansion 6:



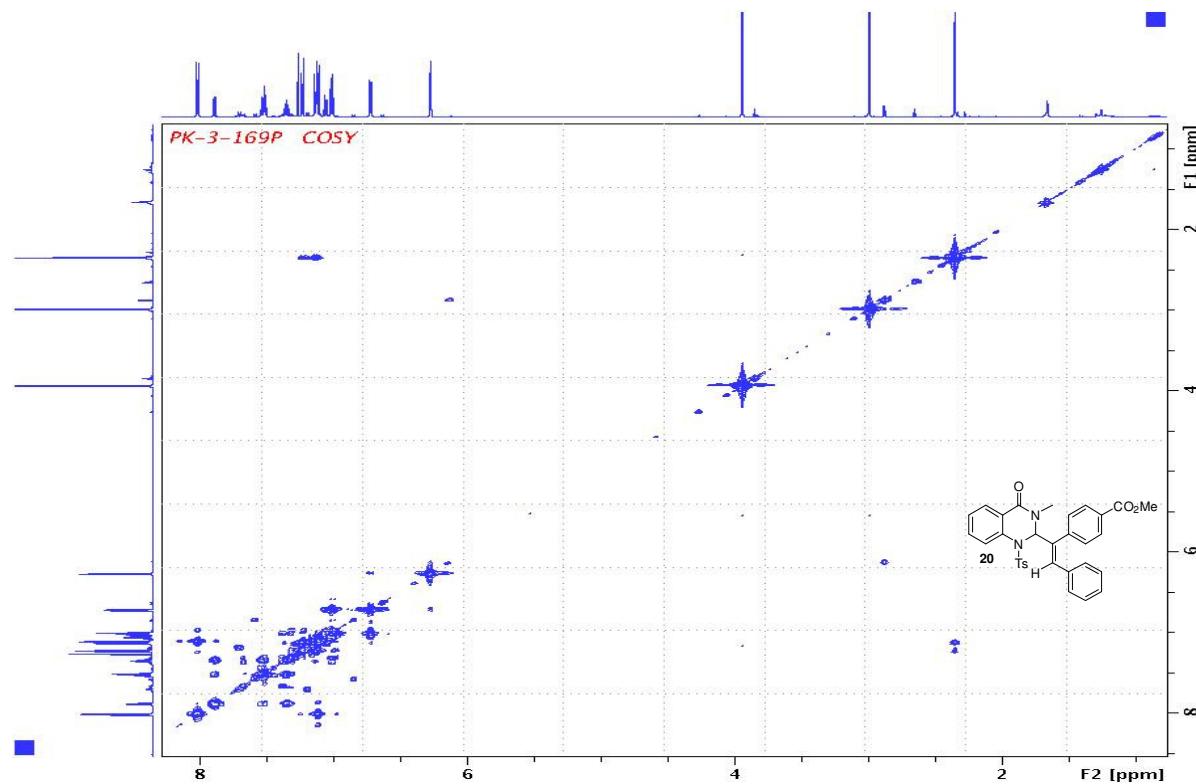
Expansion 7:



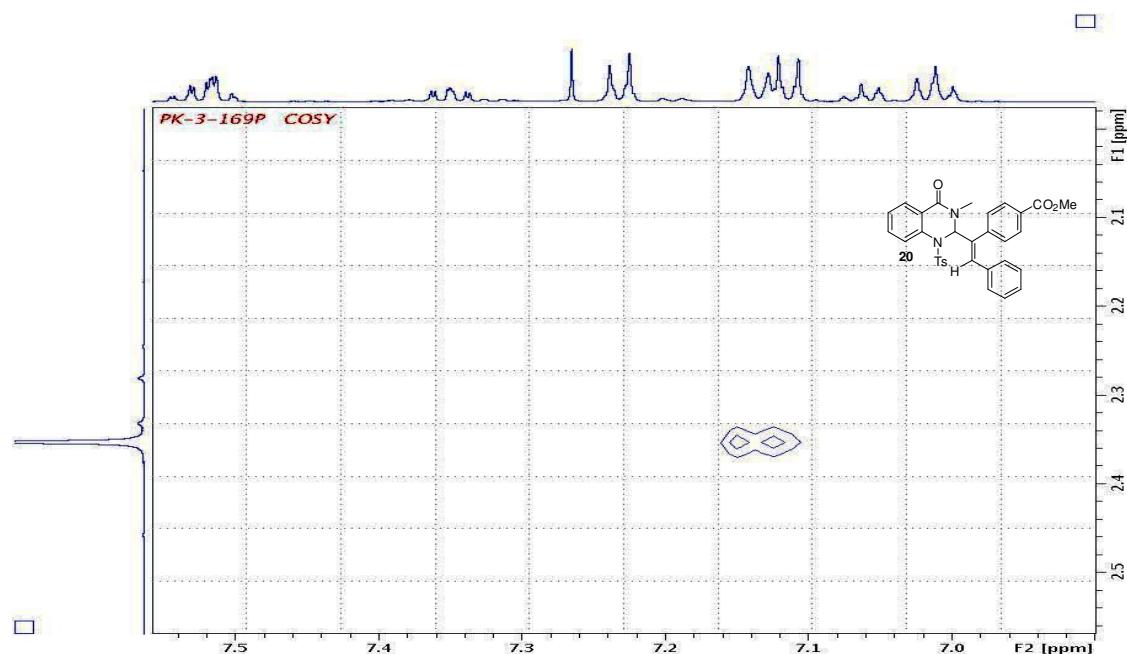
Expansion 8:



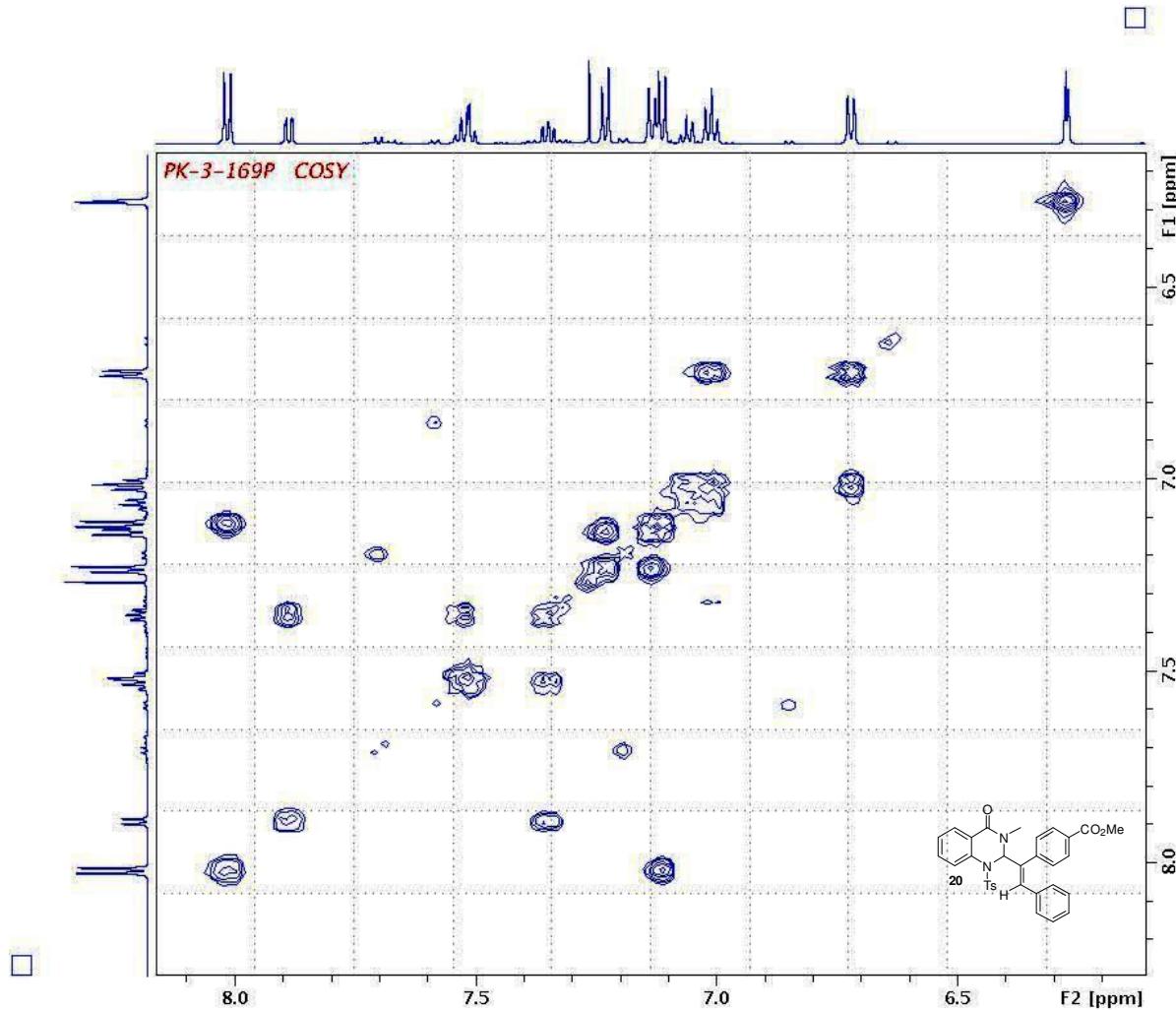
COSY spectrum of product **20**:



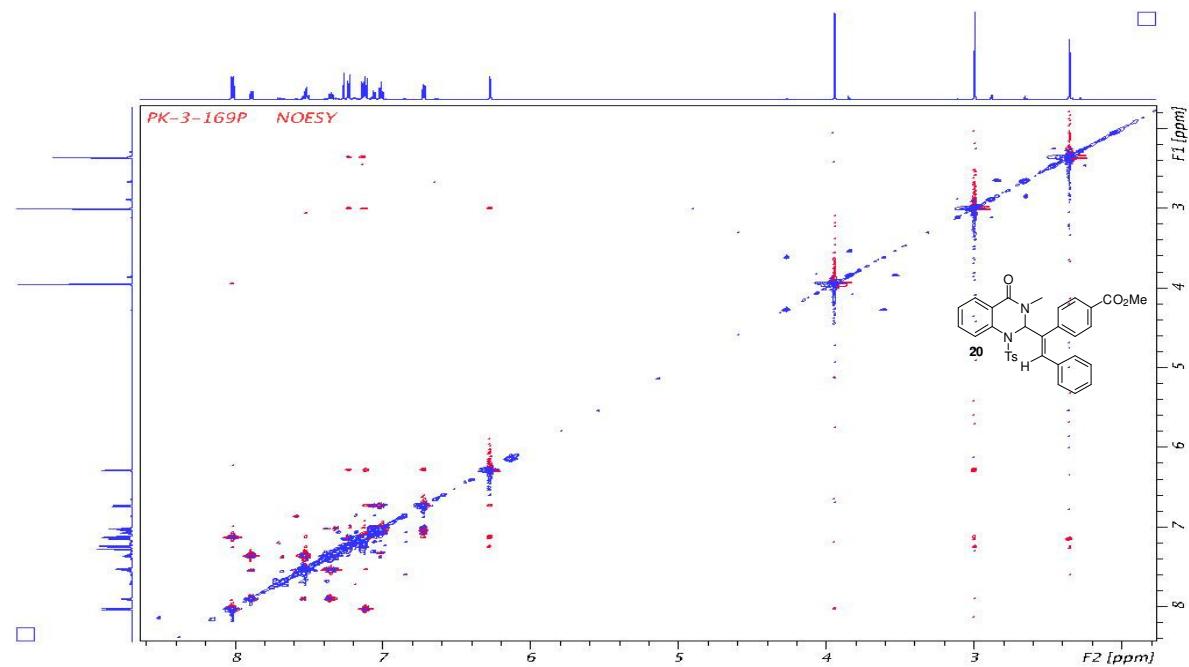
Expansion 1:



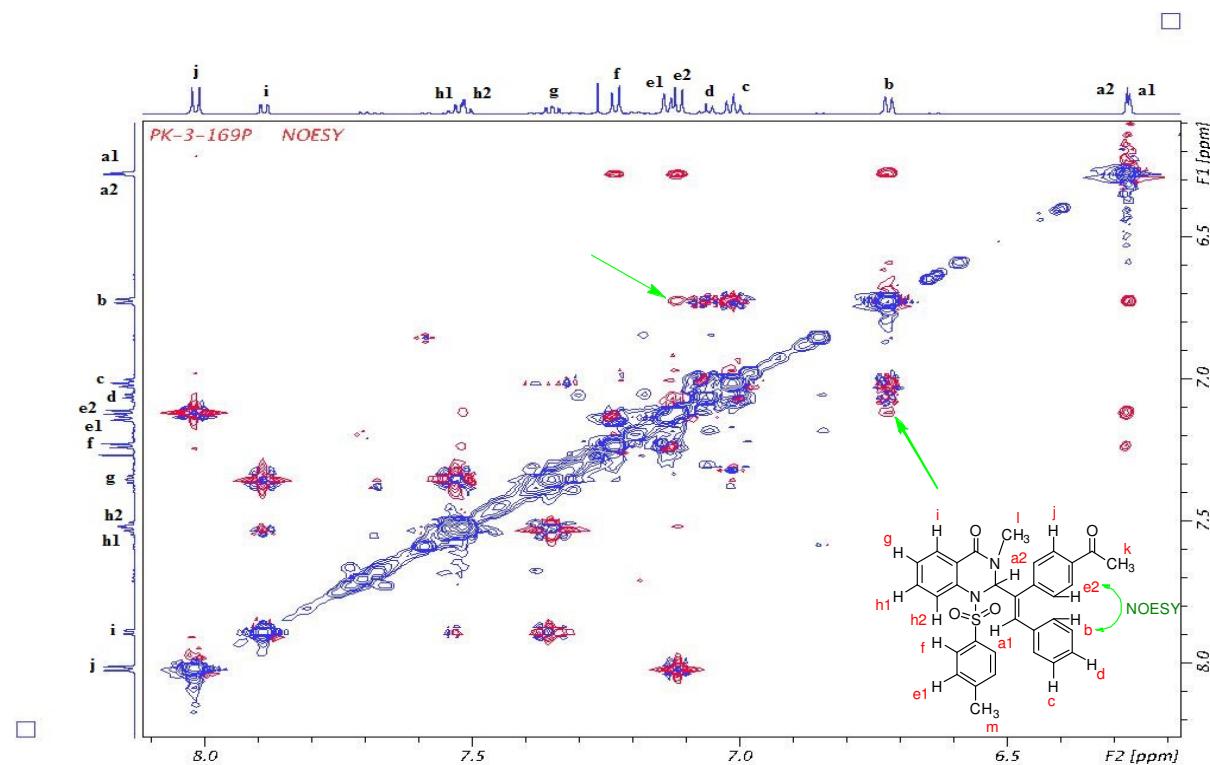
Expansion 2:



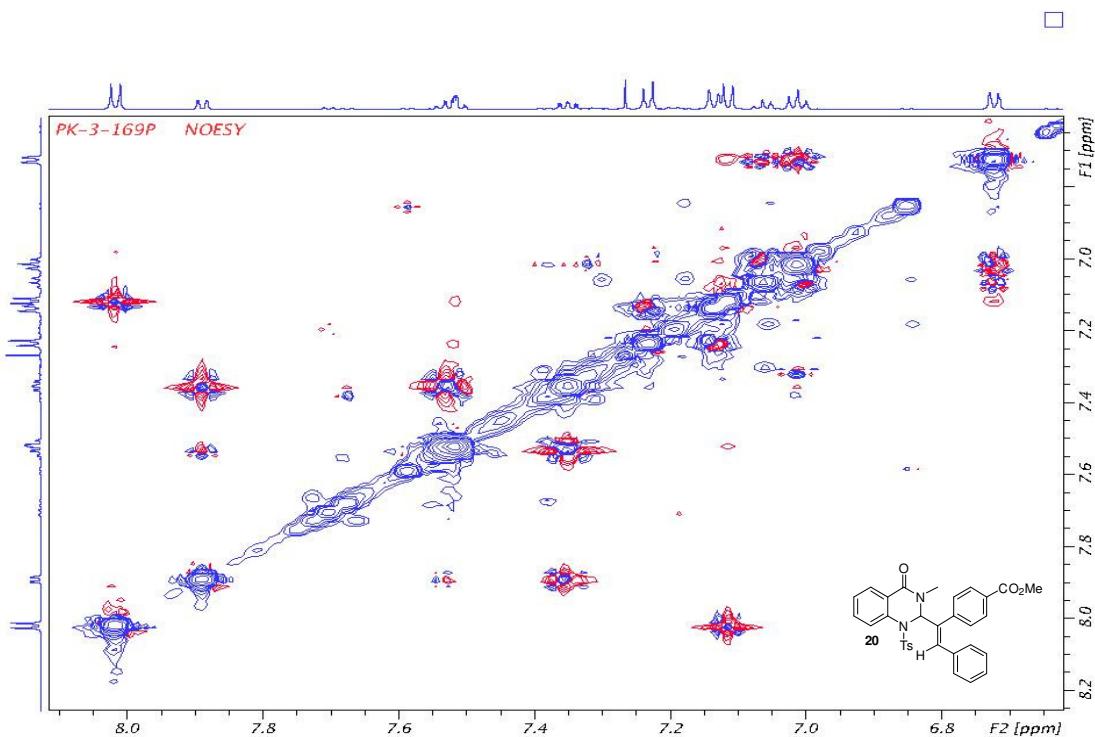
NOESY spectrum of product **20**:



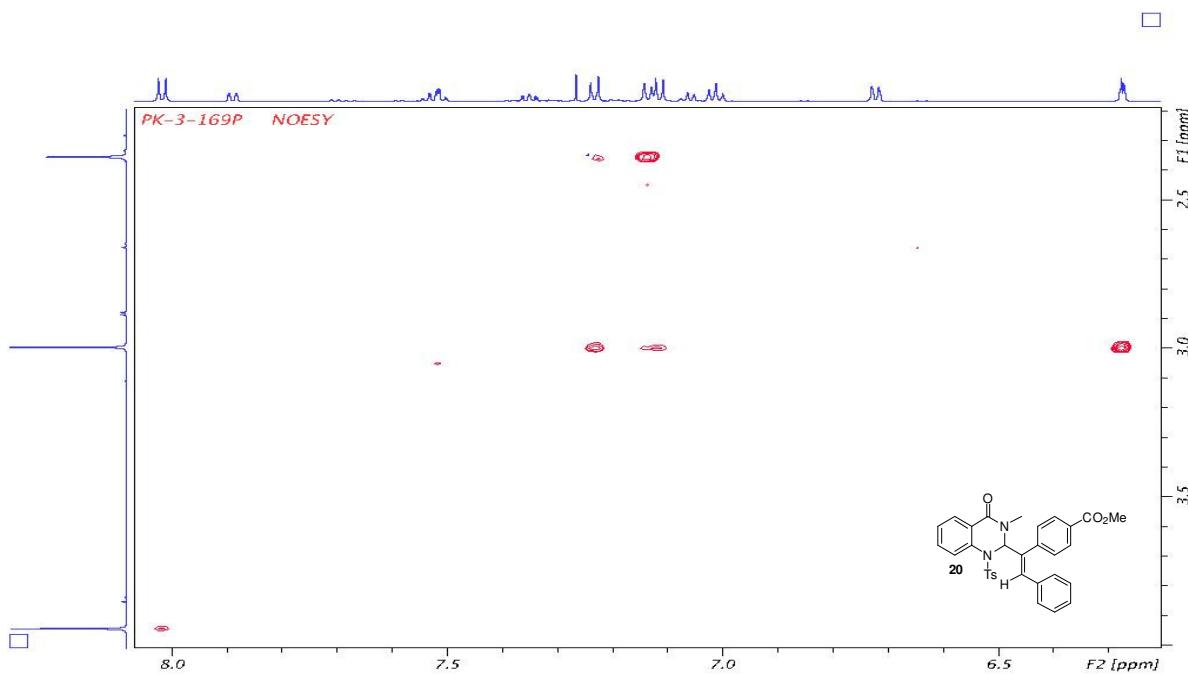
Expansion 1:



Expansion 2:

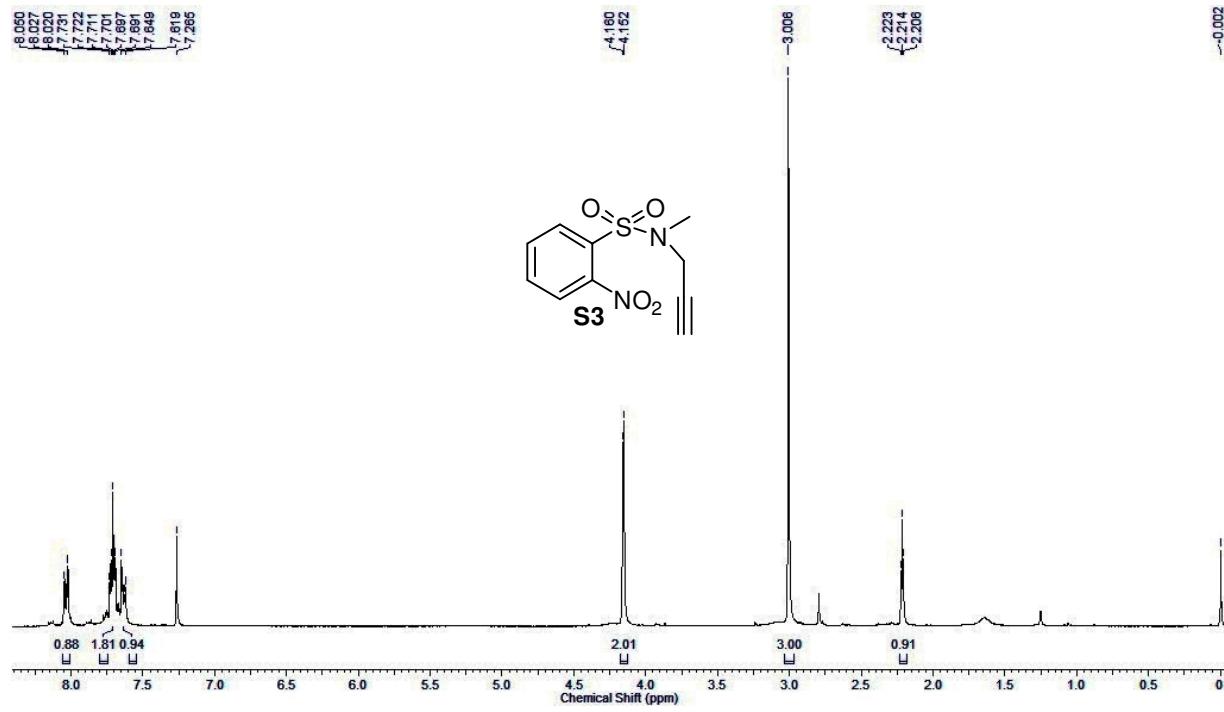


Expansion 3:

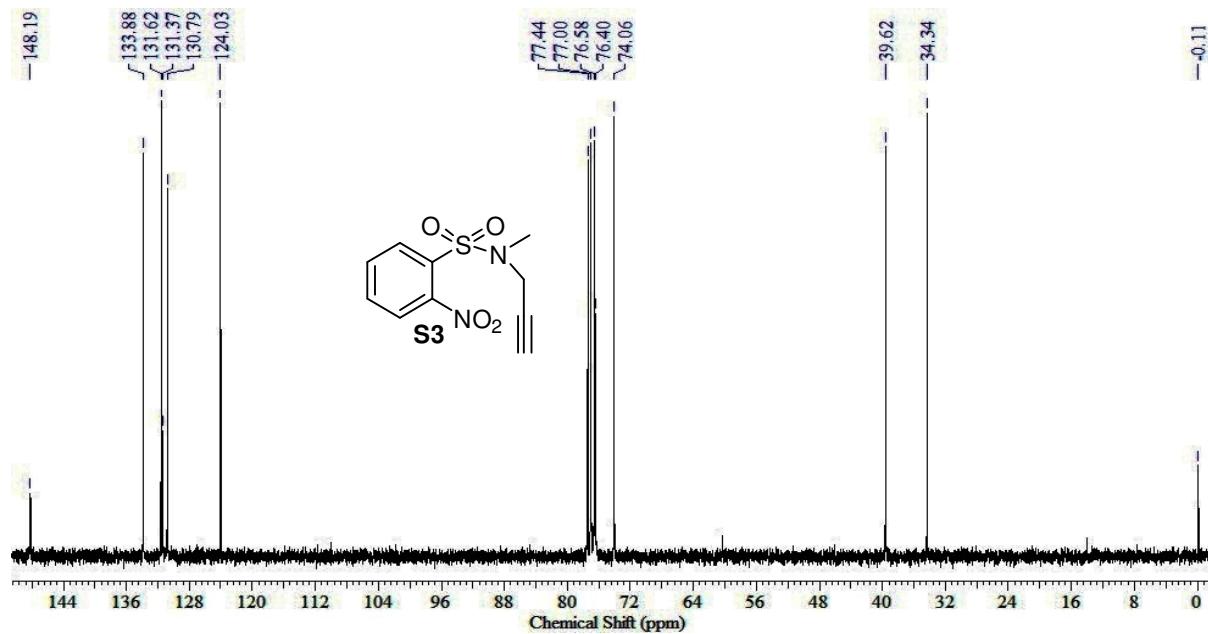


10) NMR spectra of starting substrates **S3**, **S4**, **21** (table 3):

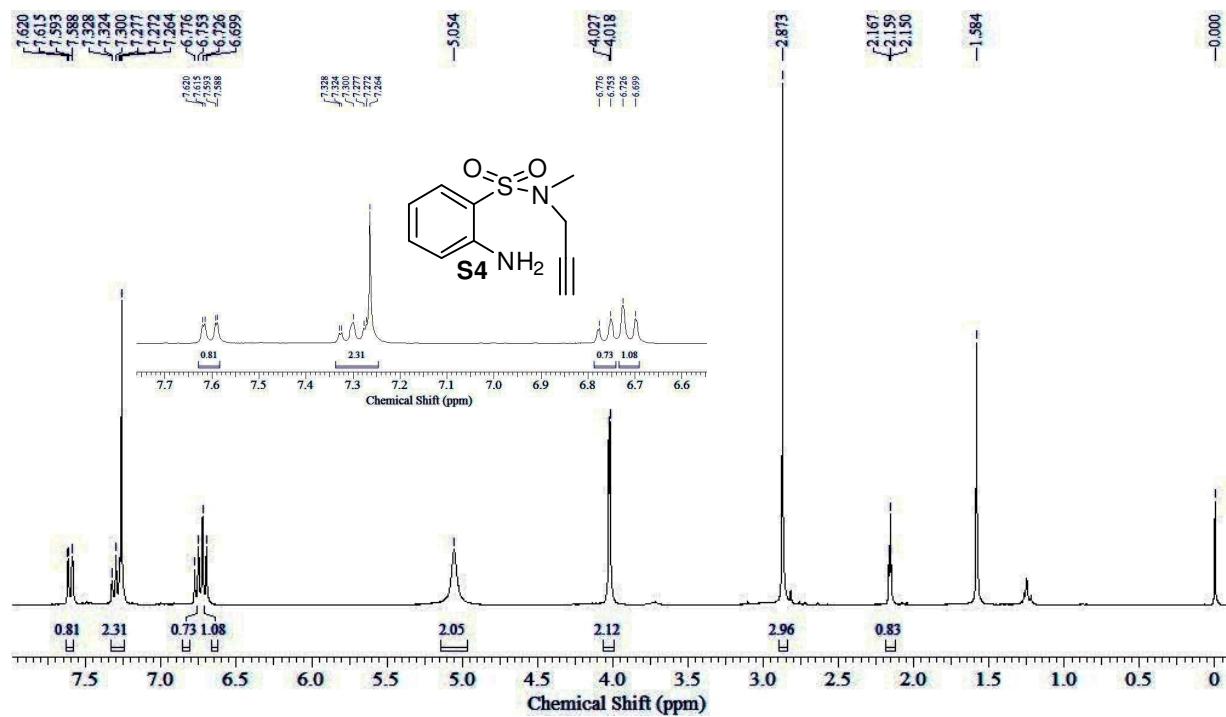
¹H NMR (CDCl_3 , 300 MHz) spectrum of starting substrate **S3**:



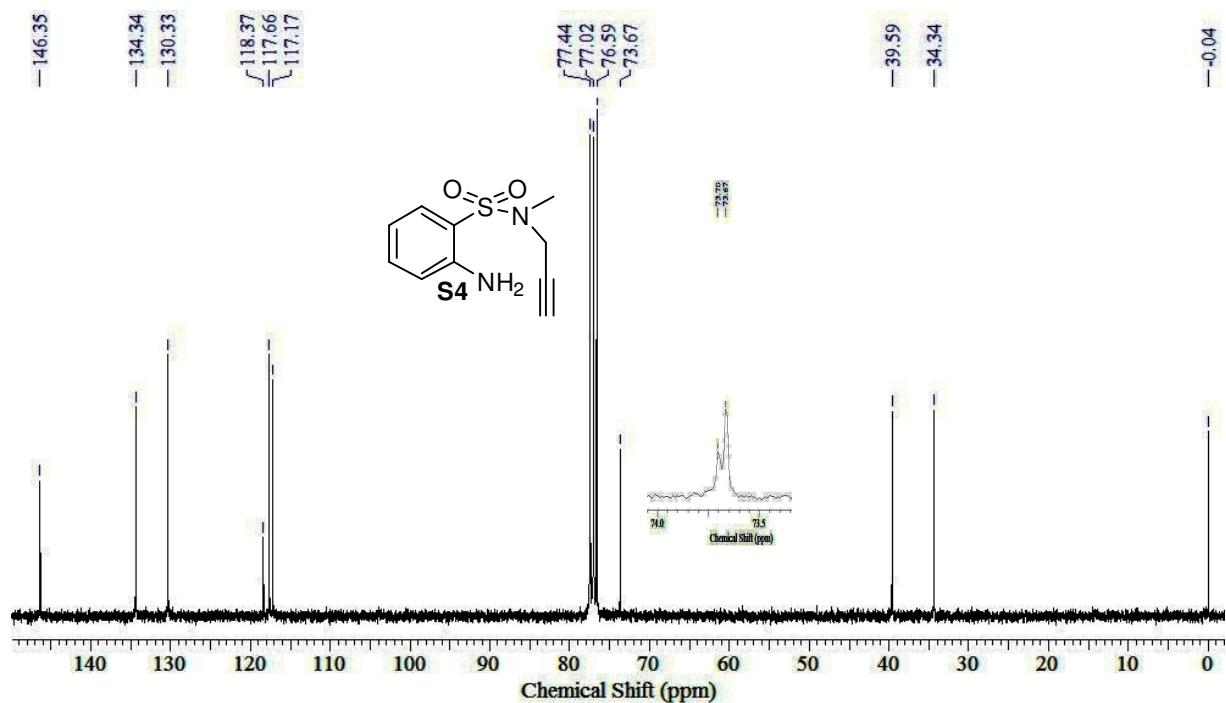
¹³C NMR (CDCl_3 , 75 MHz) spectrum of starting substrate **S3**:



¹H NMR (CDCl_3 , 300 MHz) spectrum of starting substrate S4:

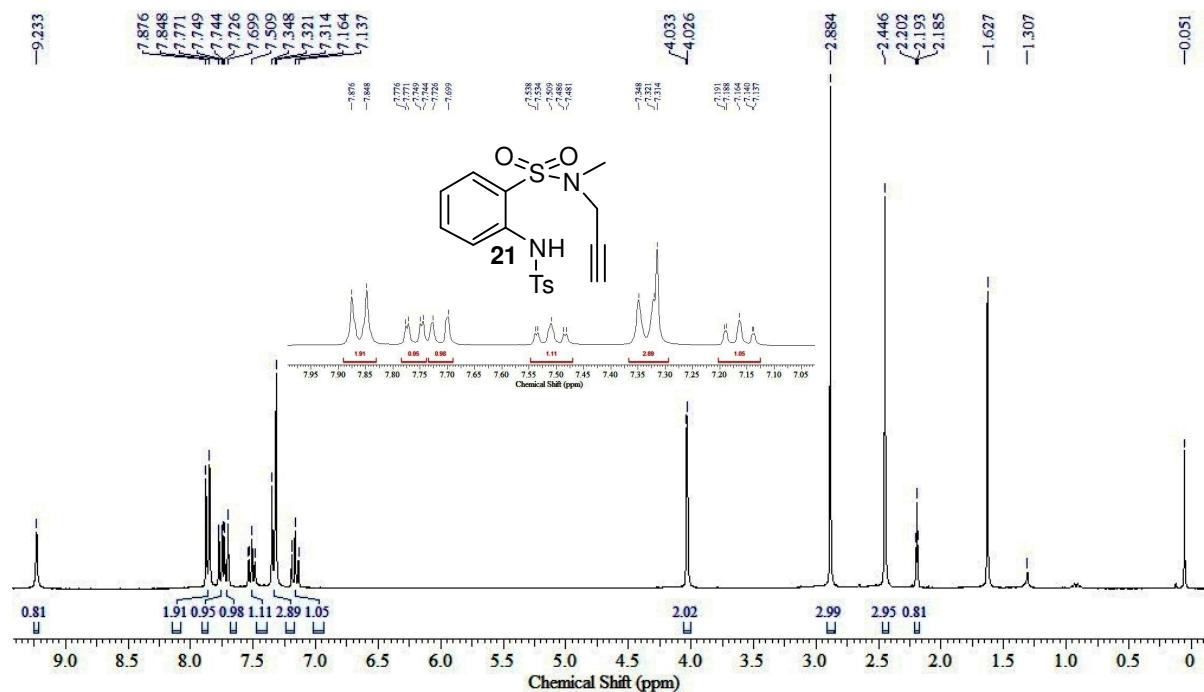


¹³C NMR (CDCl_3 , 75 MHz) spectrum of starting substrate S4:

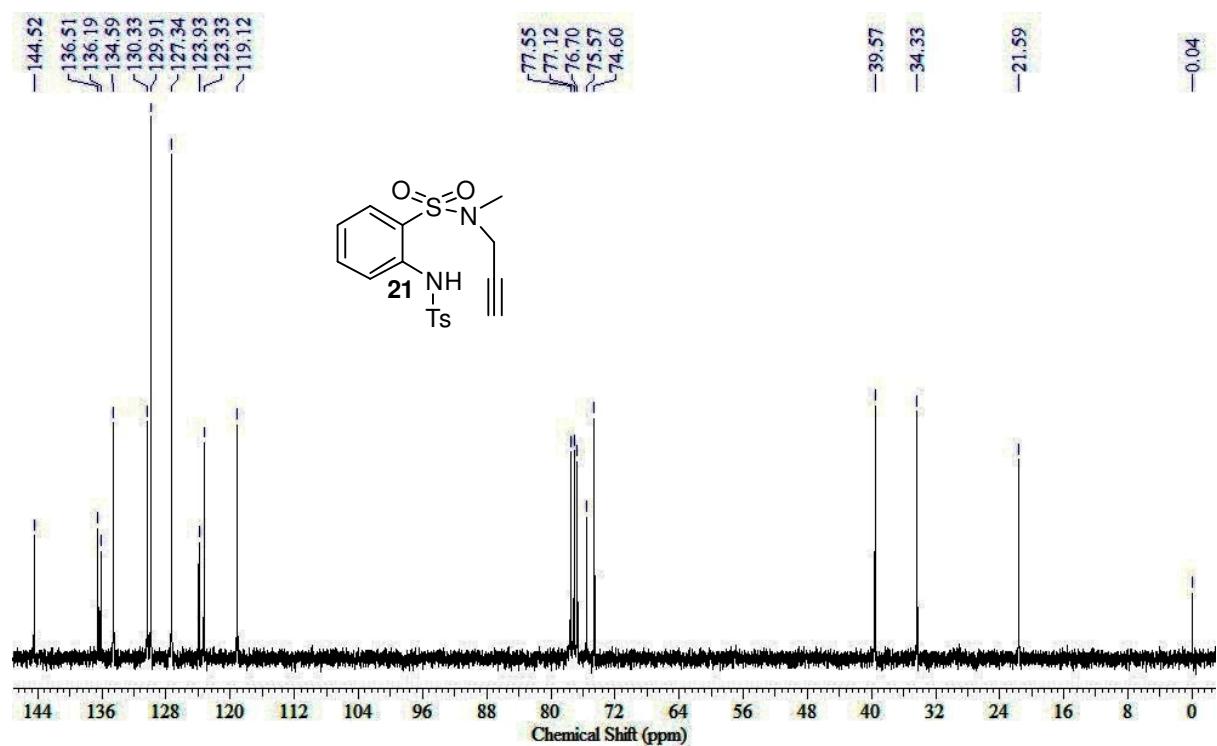


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¹H NMR (CDCl_3 , 300 MHz) spectrum of starting substrate **21**:

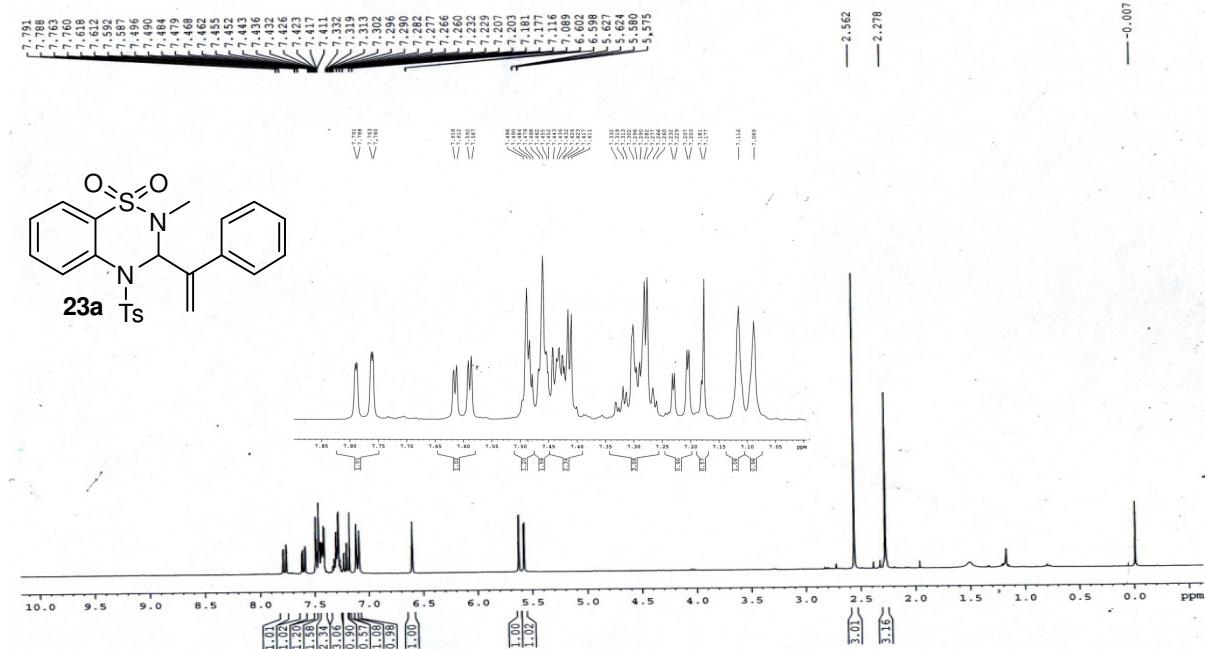


¹³C NMR (CDCl_3 , 75 MHz) spectrum of starting substrate **21**:

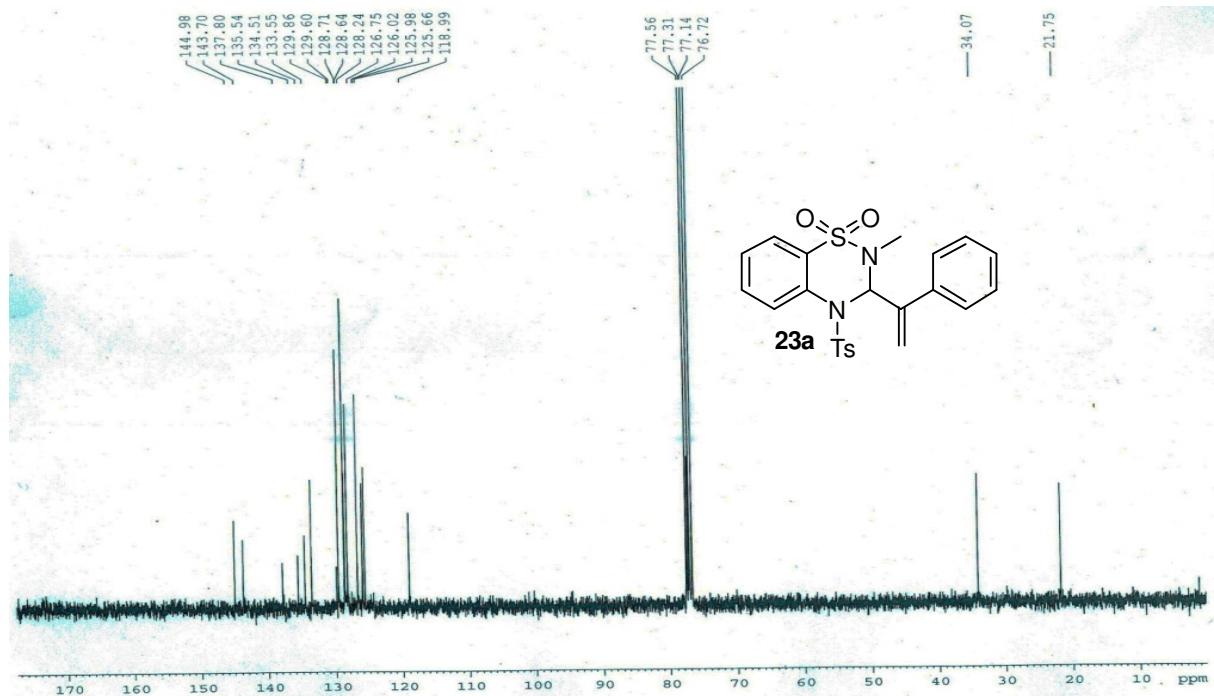


11) NMR spectra of products **23**:

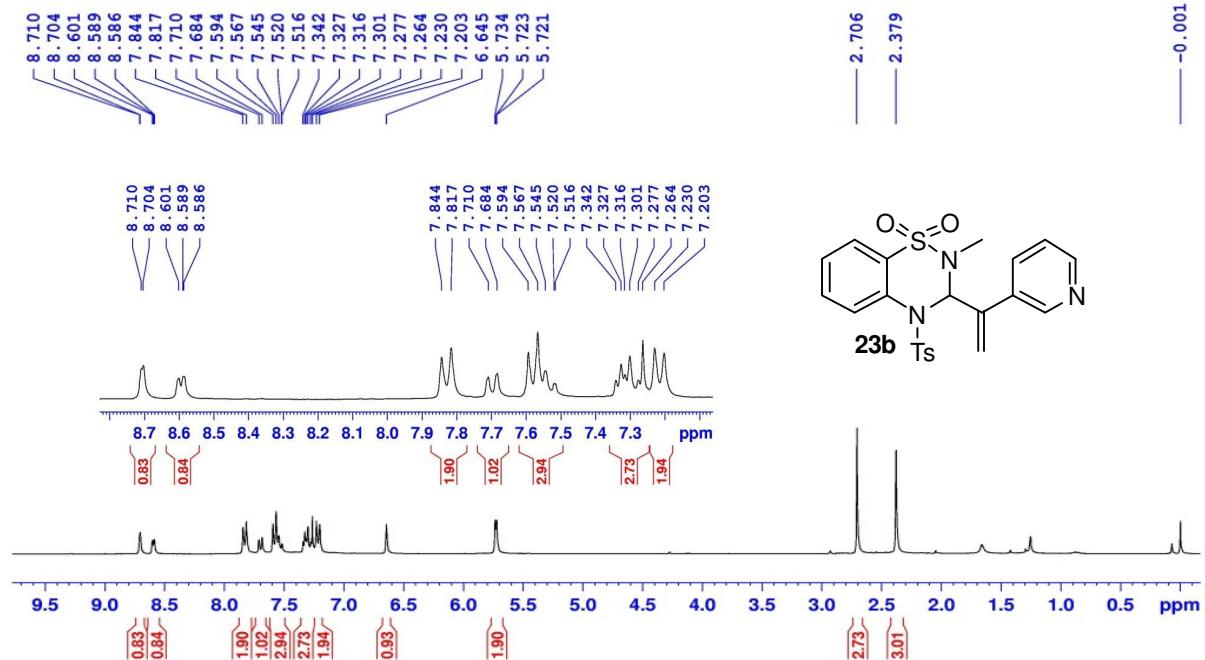
¹H NMR (CDCl₃, 300 MHz) spectrum of product **23a**:



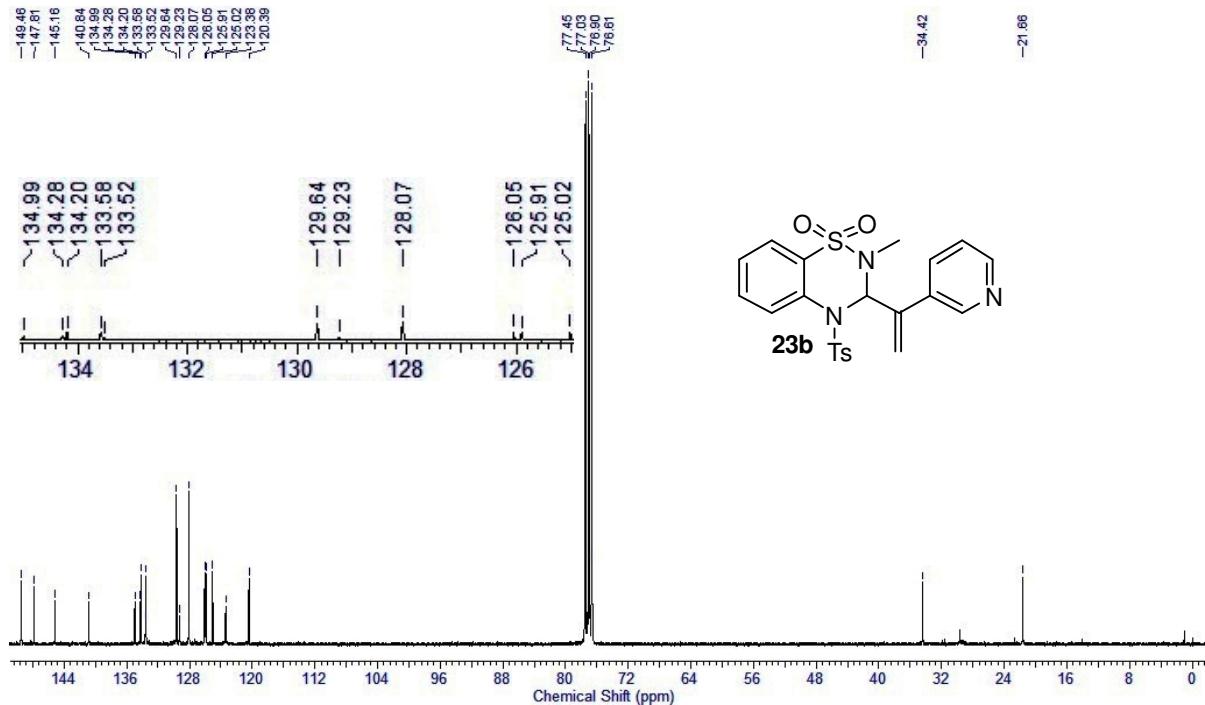
¹³C NMR (CDCl₃, 75 MHz) spectrum of product **23a**:



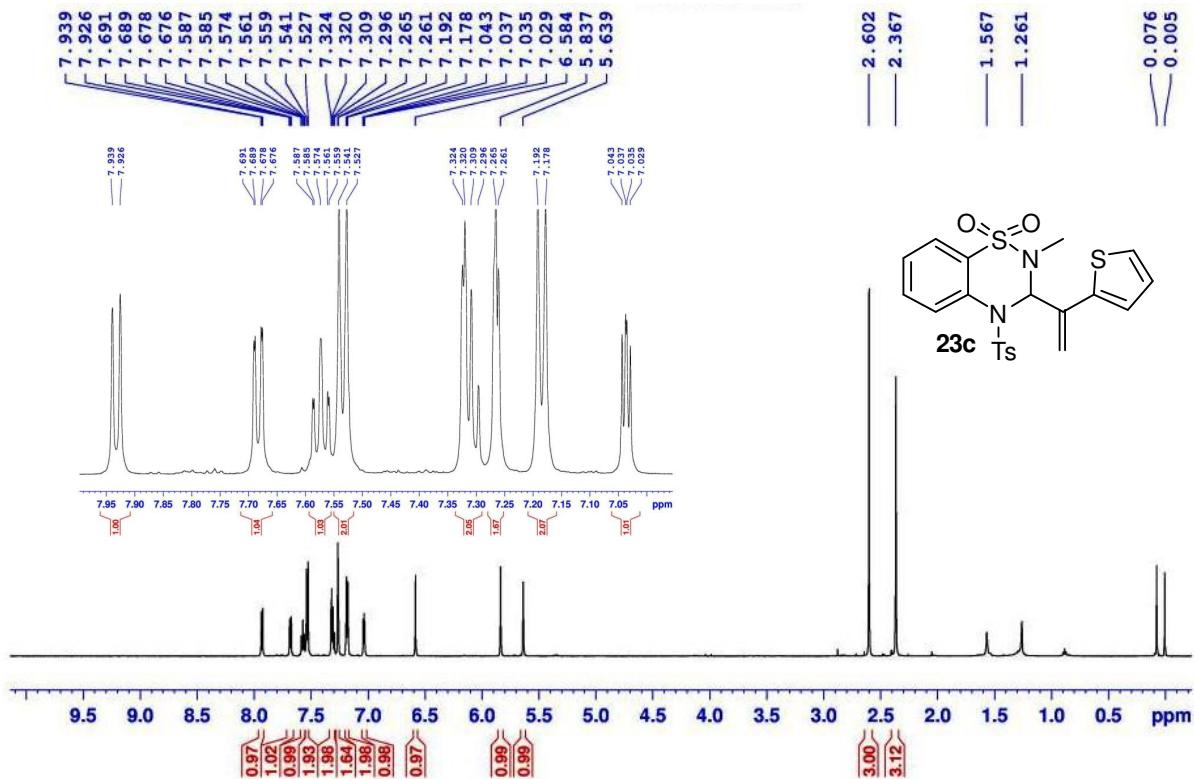
¹H NMR (CDCl_3 , 300 MHz) spectrum of product **23b**:



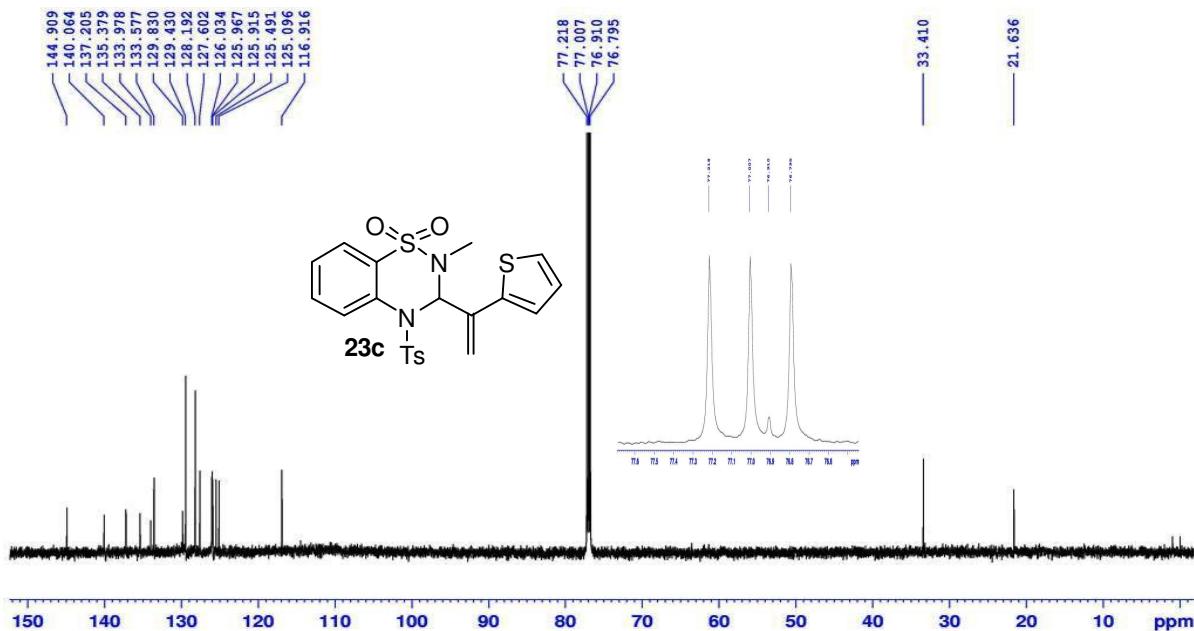
¹³C NMR (CDCl_3 , 75 MHz) spectrum of product **23b**:



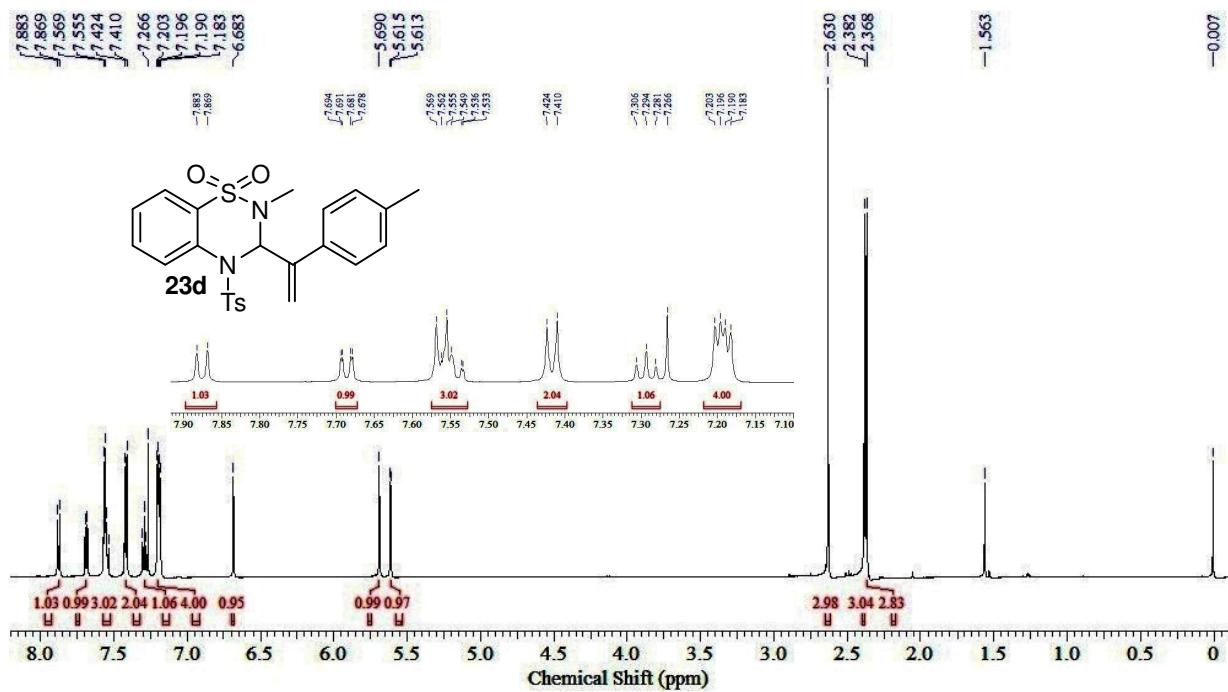
¹H NMR (CDCl_3 , 600 MHz) spectrum of product **23c**:



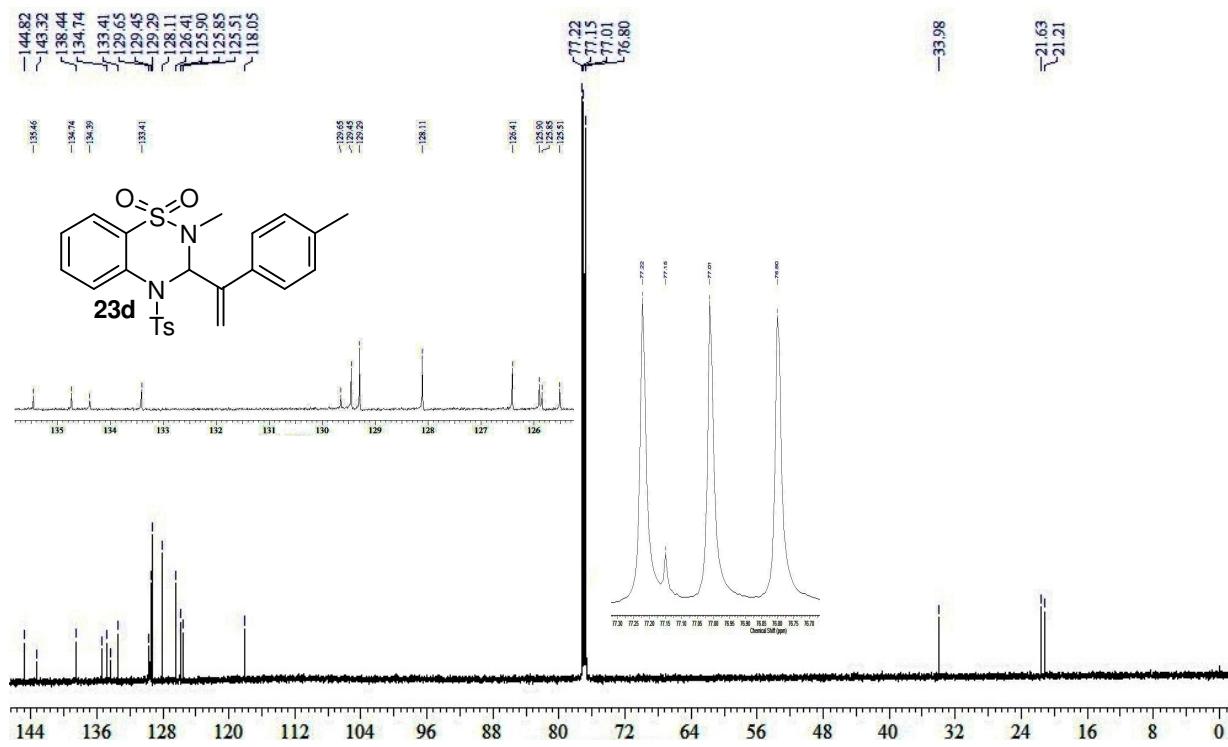
¹³C NMR (CDCl_3 , 150 MHz) spectrum of product **23c**:



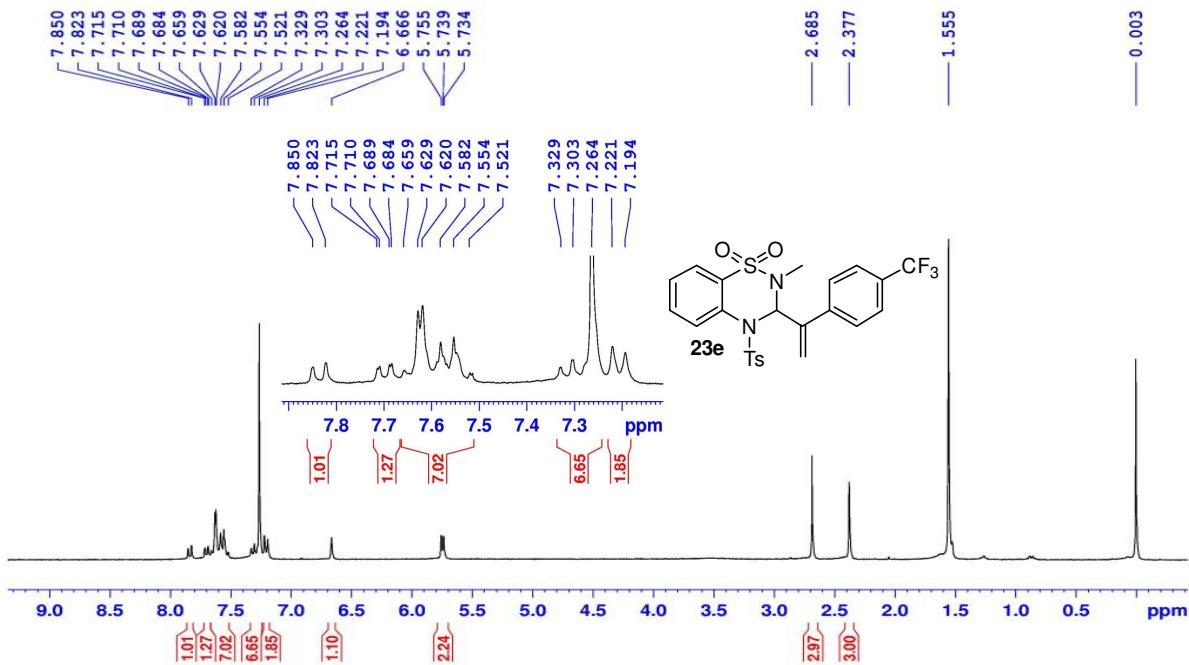
¹H NMR (CDCl_3 , 600 MHz) spectrum of product **23d**:



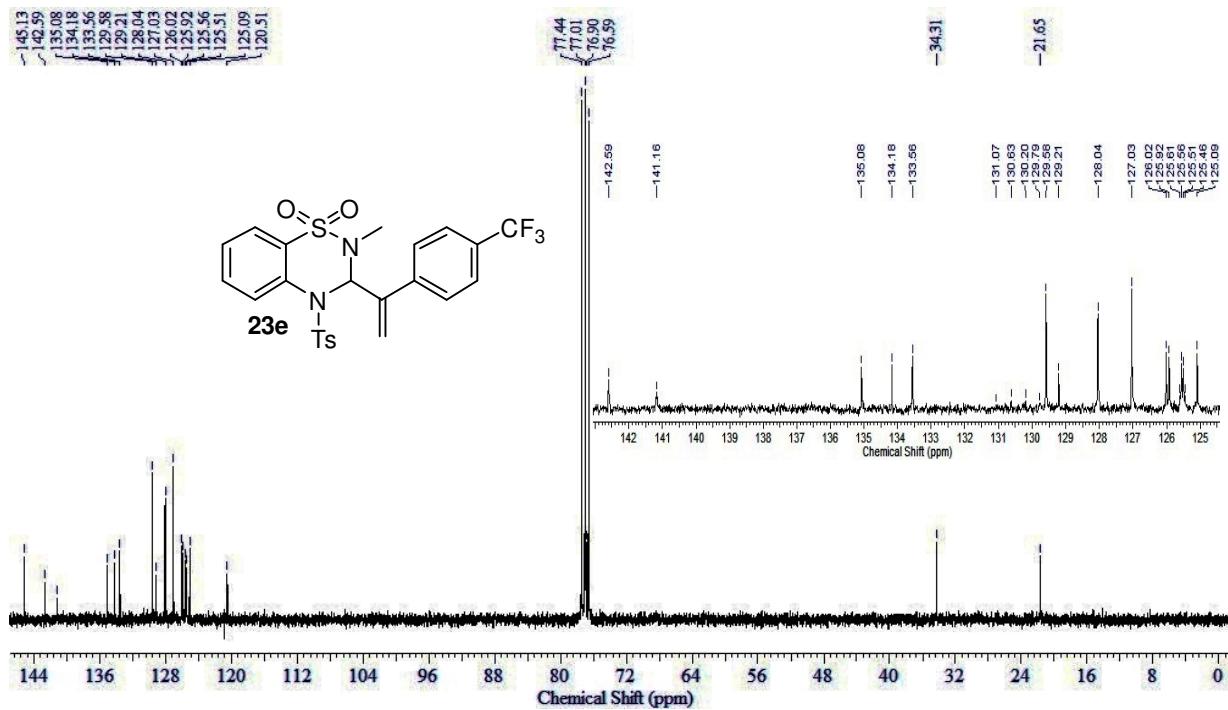
¹³C NMR (CDCl_3 , 150 MHz) spectrum of product **23d**:



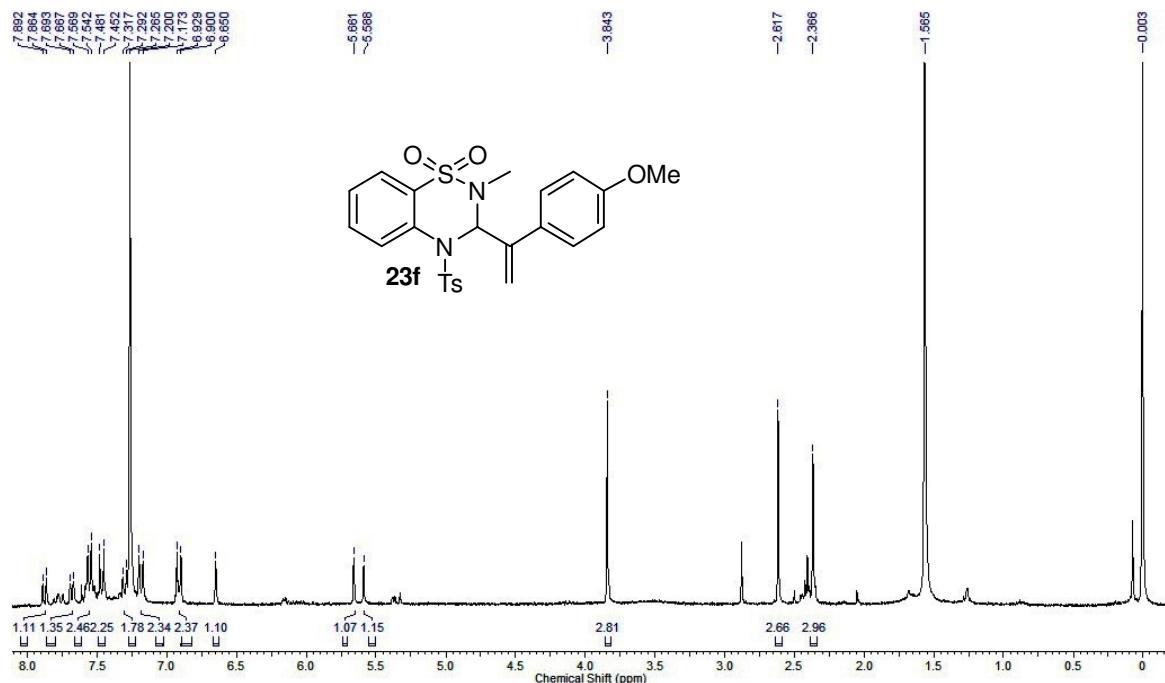
¹H NMR (CDCl_3 , 300 MHz) spectrum of product **23e**:



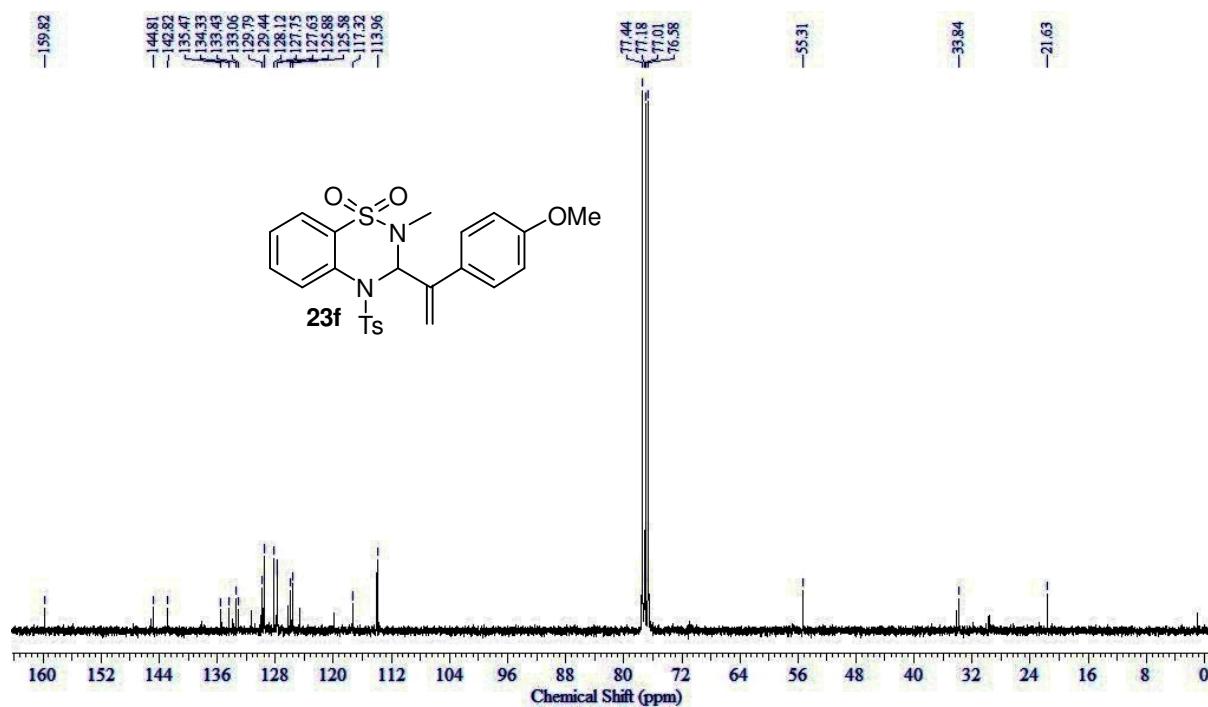
¹³C NMR (CDCl_3 , 75 MHz) spectrum of product **23e**:



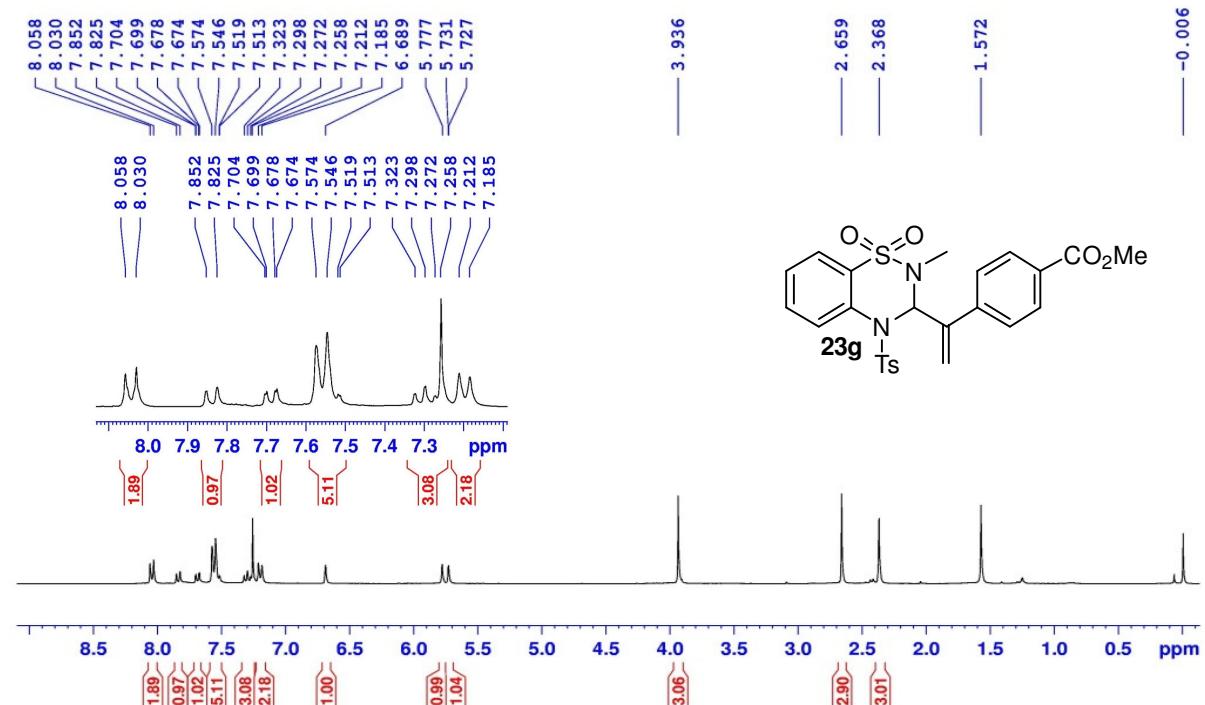
¹H NMR (CDCl_3 , 300 MHz) spectrum of product **23f**:



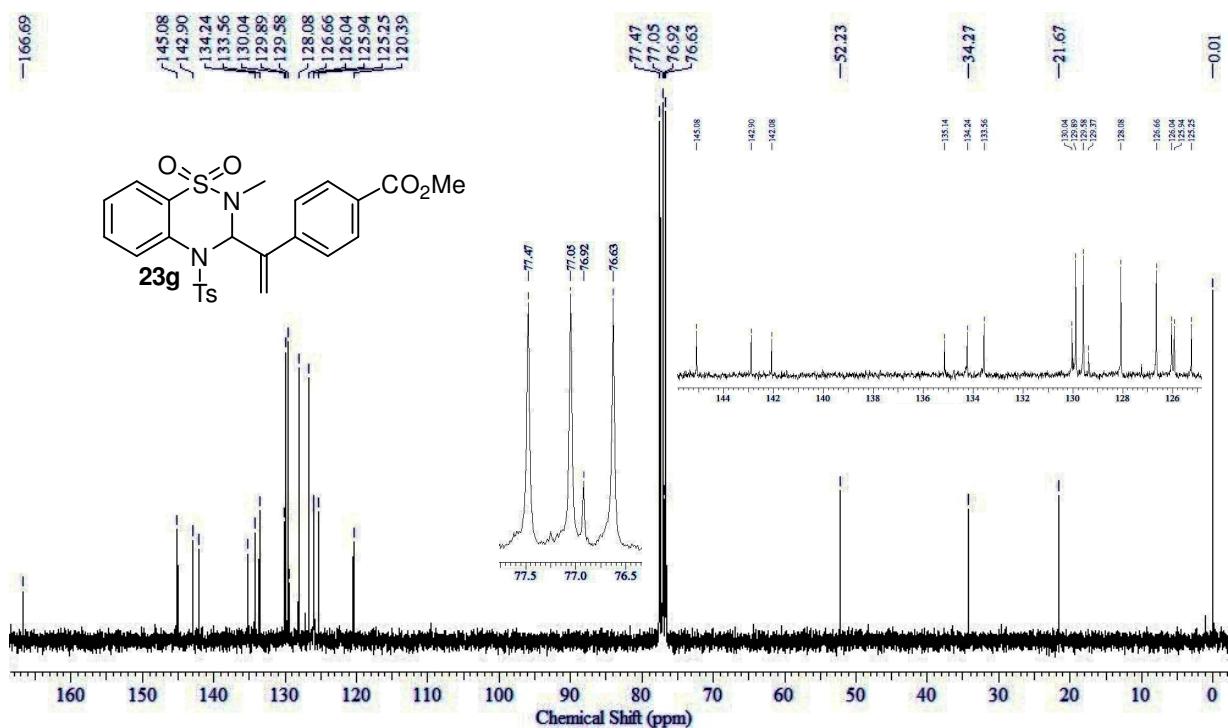
¹³C NMR (CDCl_3 , 75 MHz) spectrum of product **23f**:



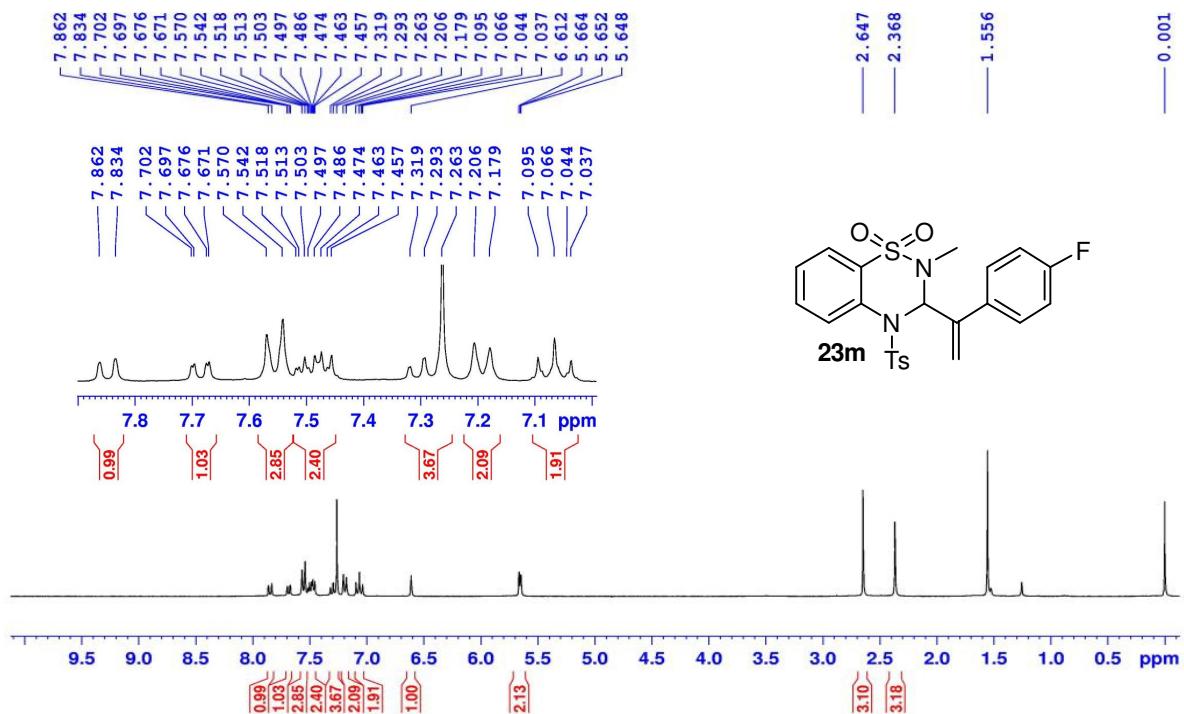
¹H NMR (CDCl₃, 300 MHz) spectrum of product **23g**:



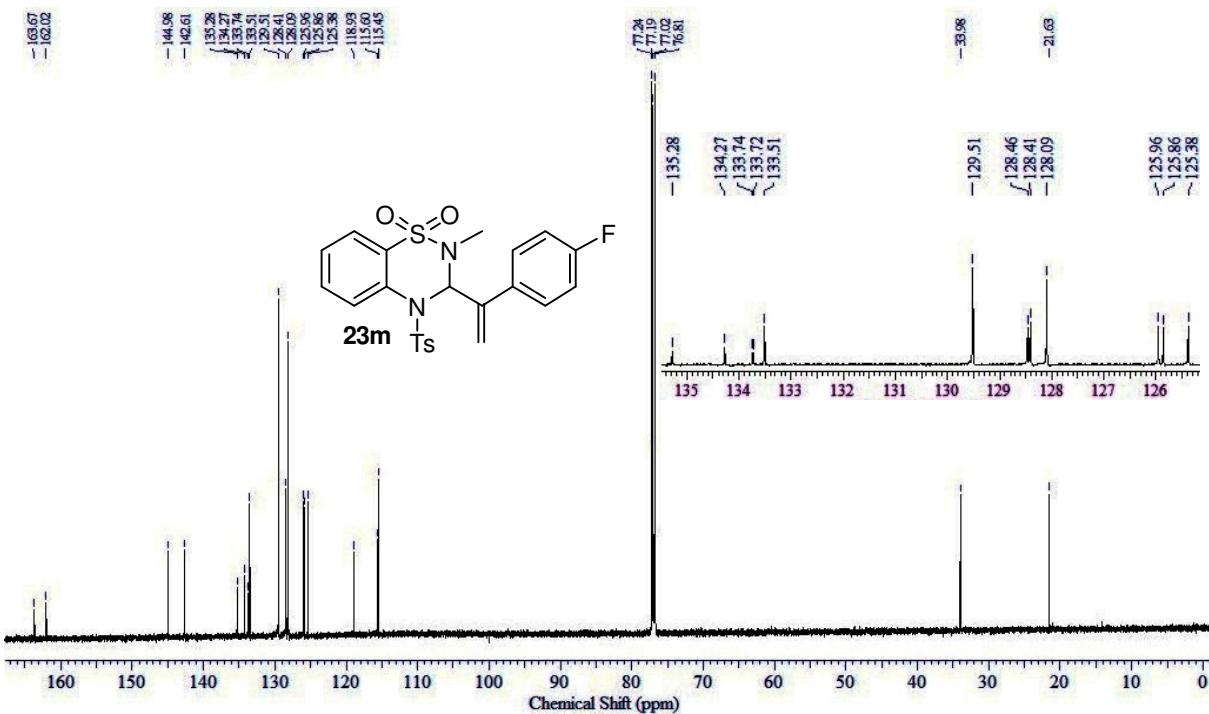
¹³C NMR (CDCl₃, 75 MHz) spectrum of product **23g**:



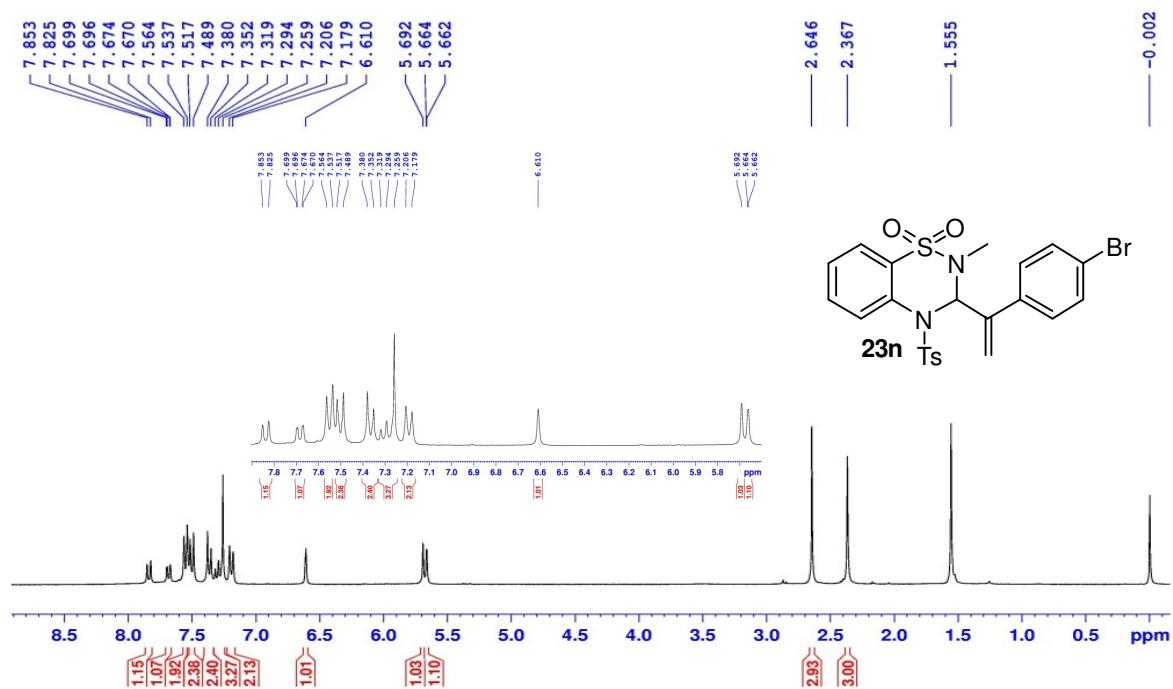
¹H NMR (CDCl_3 , 300 MHz) spectrum of product **23m**:



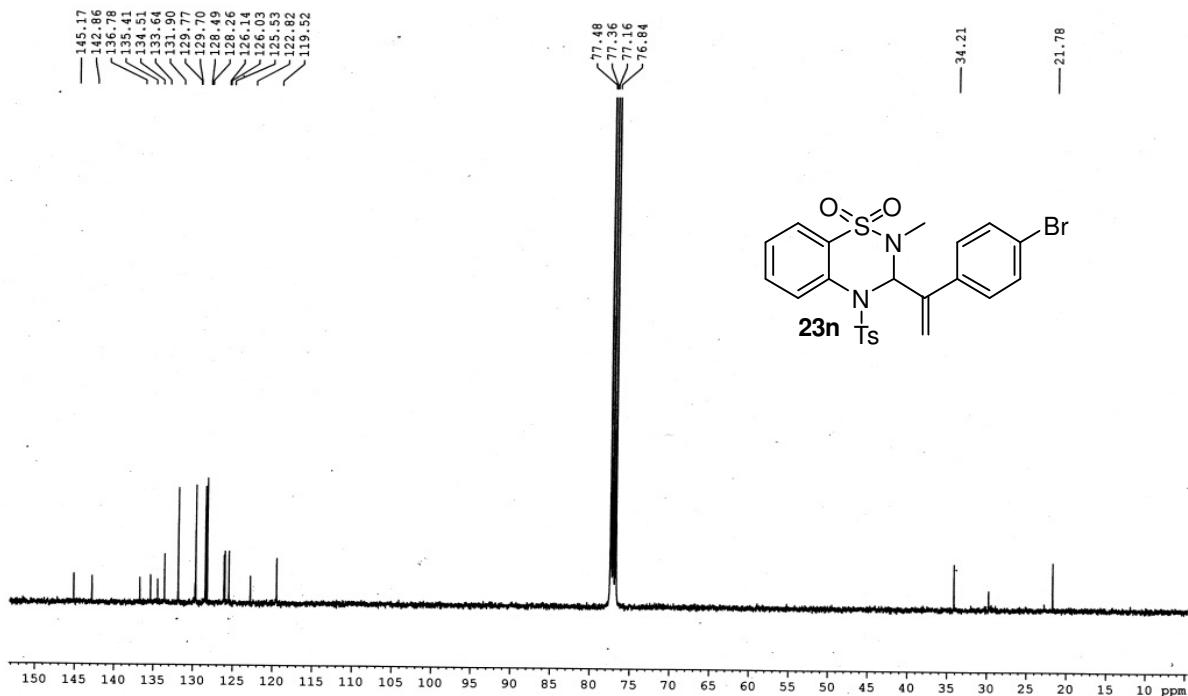
¹³C NMR (CDCl₃, 150 MHz) spectrum of product **23m**:



¹H NMR (CDCl_3 , 300 MHz) spectrum of product **23n**:

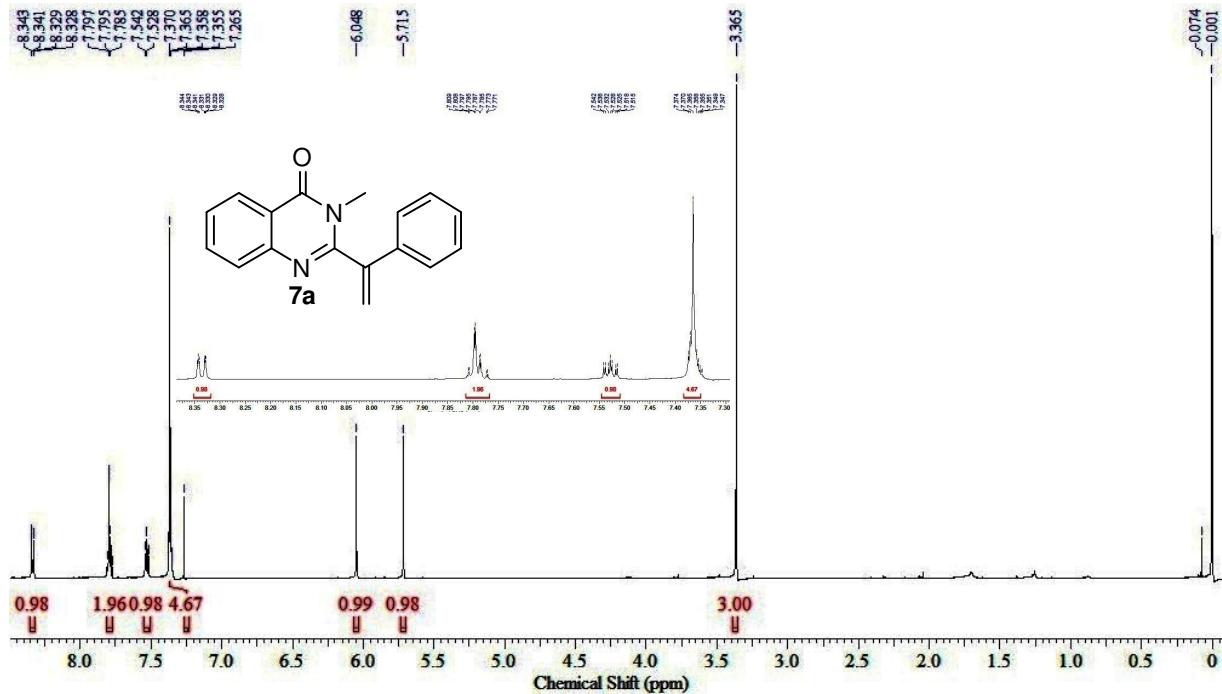


¹³C NMR (CDCl_3 , 100 MHz) spectrum of product **23n**:

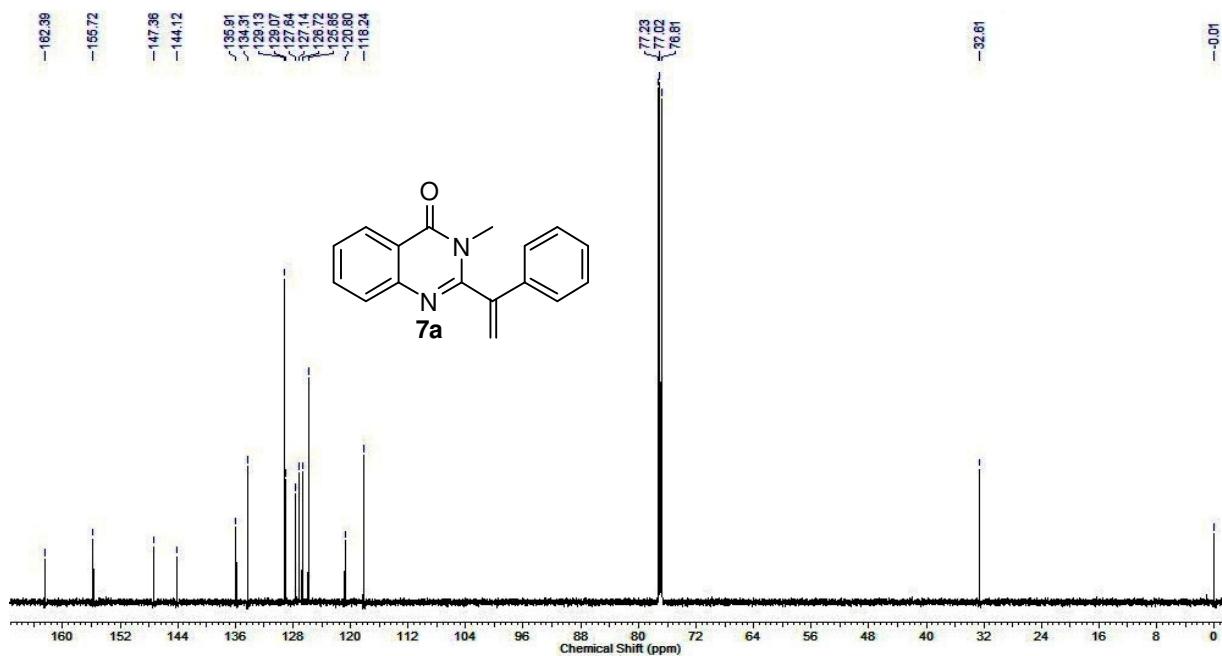


12) NMR spectra of products **7a-7f**, **8a-8b** (scheme 4):

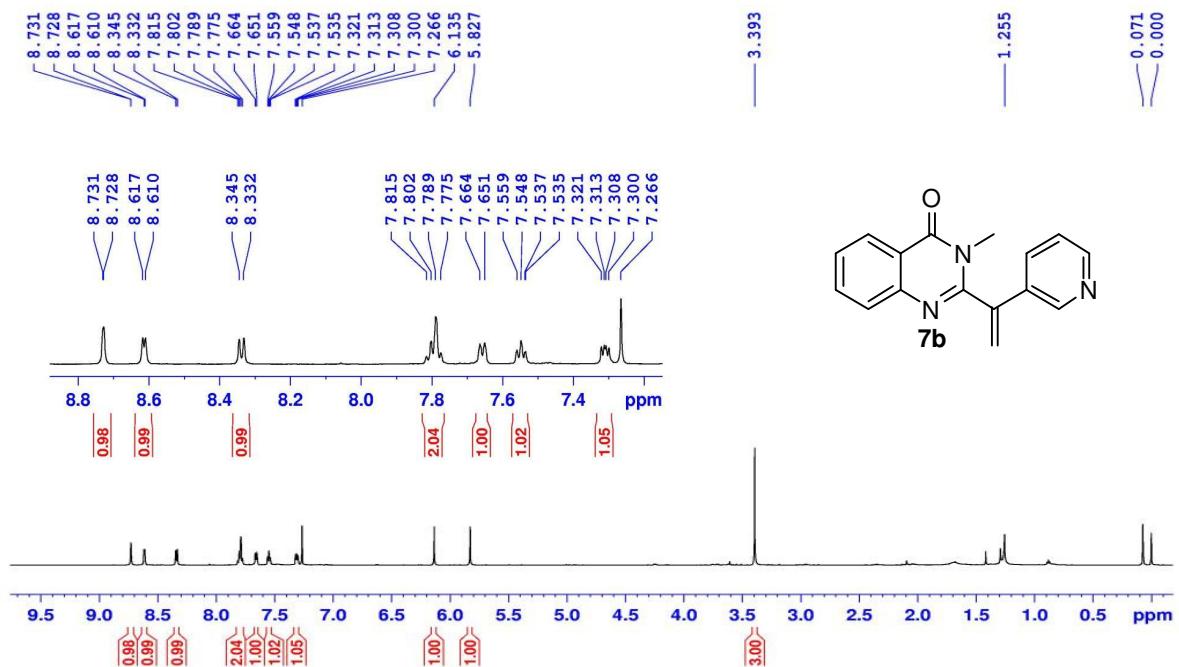
¹H NMR (CDCl_3 , 600 MHz) spectrum of product **7a**:



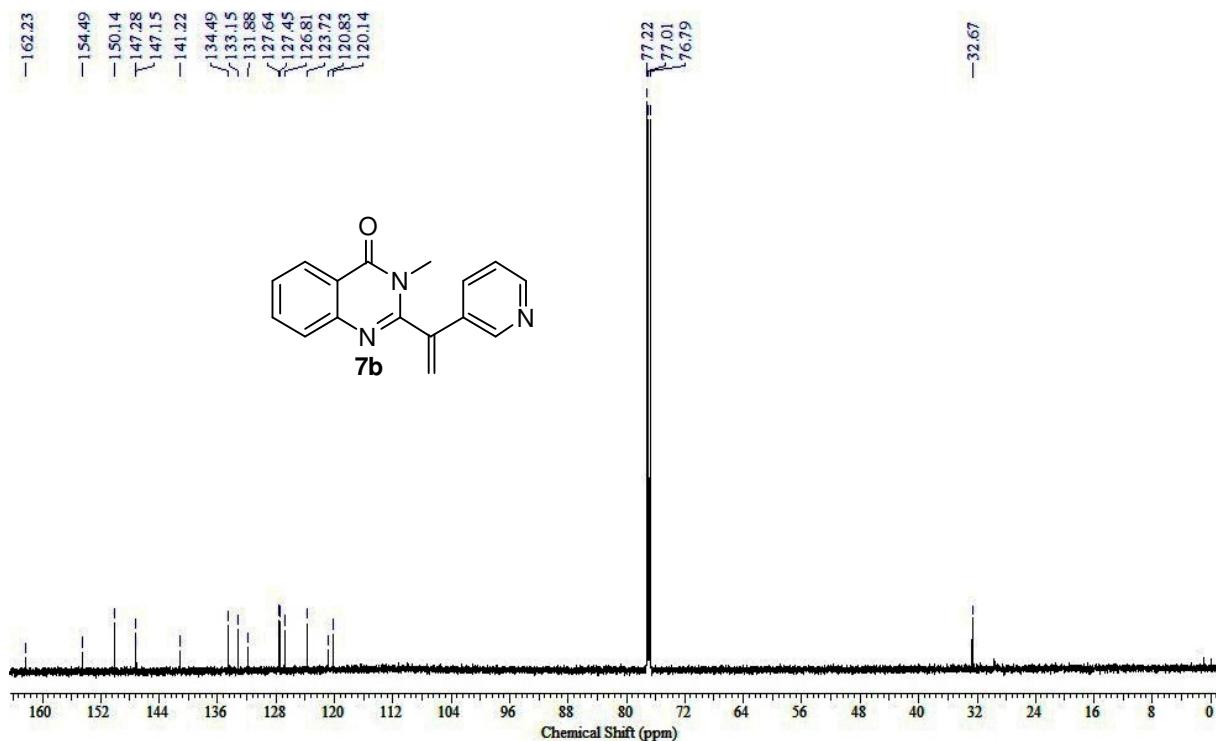
¹³C NMR (CDCl_3 , 150 MHz) spectrum of product **7a**:



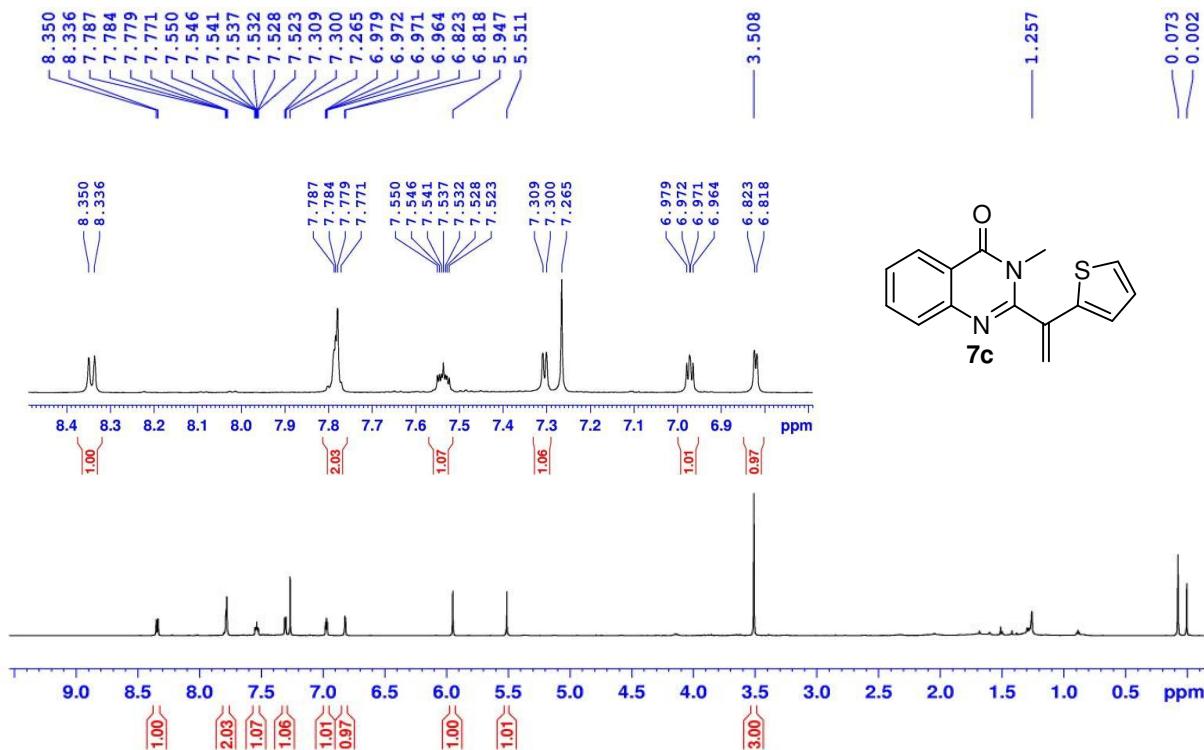
¹H NMR (CDCl₃, 600 MHz) spectrum of product 7b:



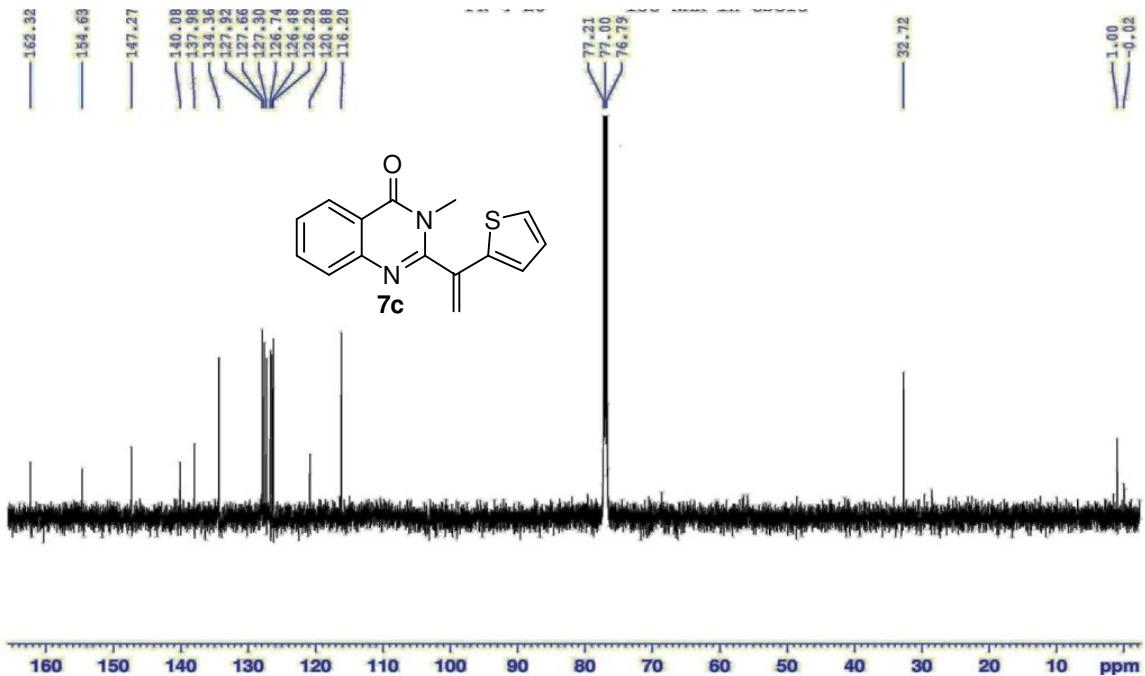
¹³C NMR (CDCl₃, 150 MHz) spectrum of product 7b:



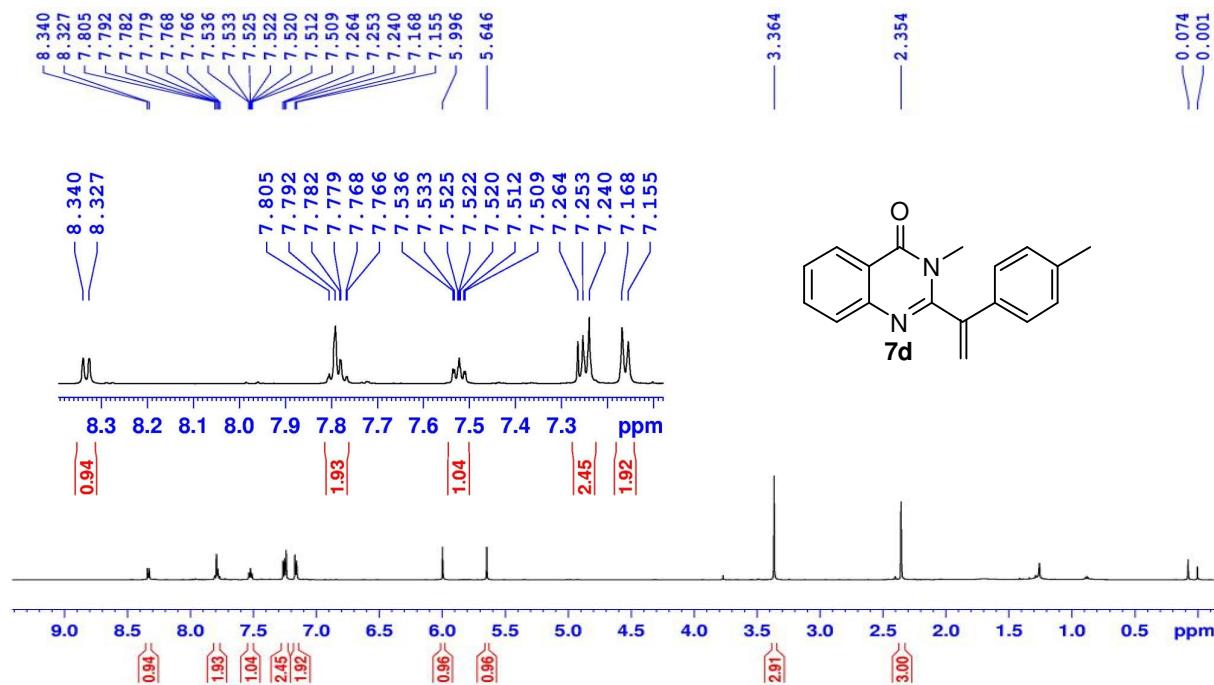
¹H NMR (CDCl₃, 600 MHz) spectrum of product 7c:



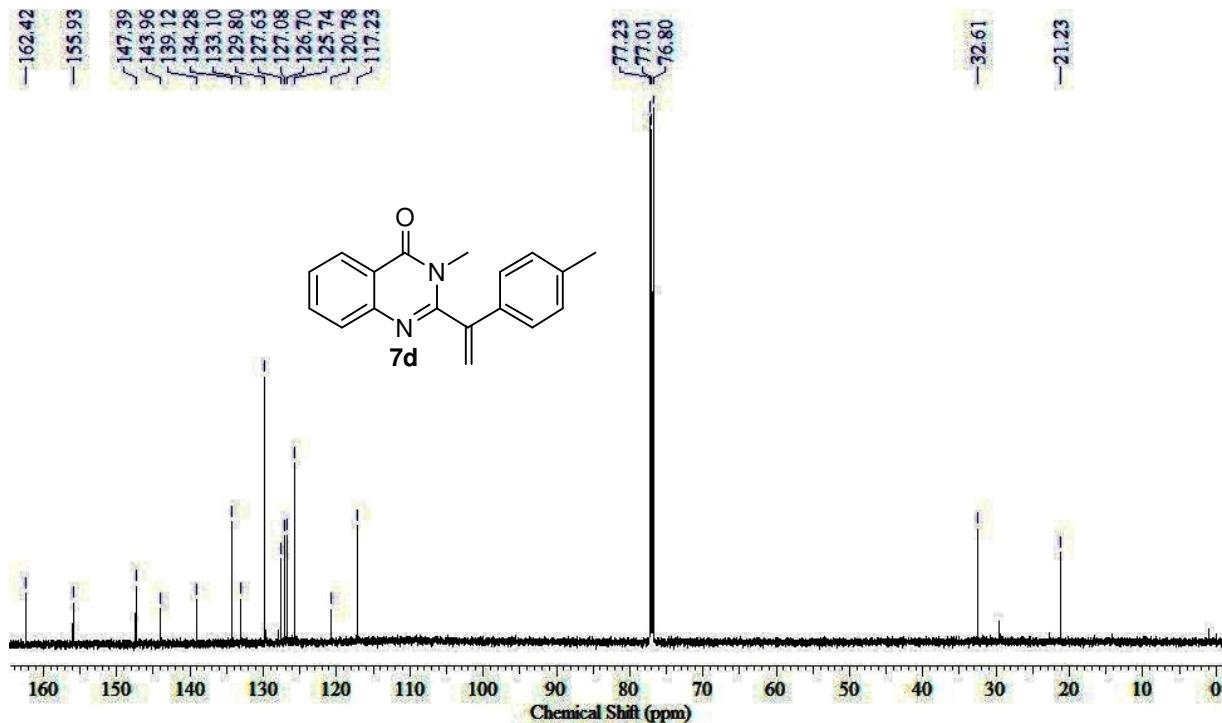
¹³C NMR (CDCl₃, 150 MHz) spectrum of product 7c:



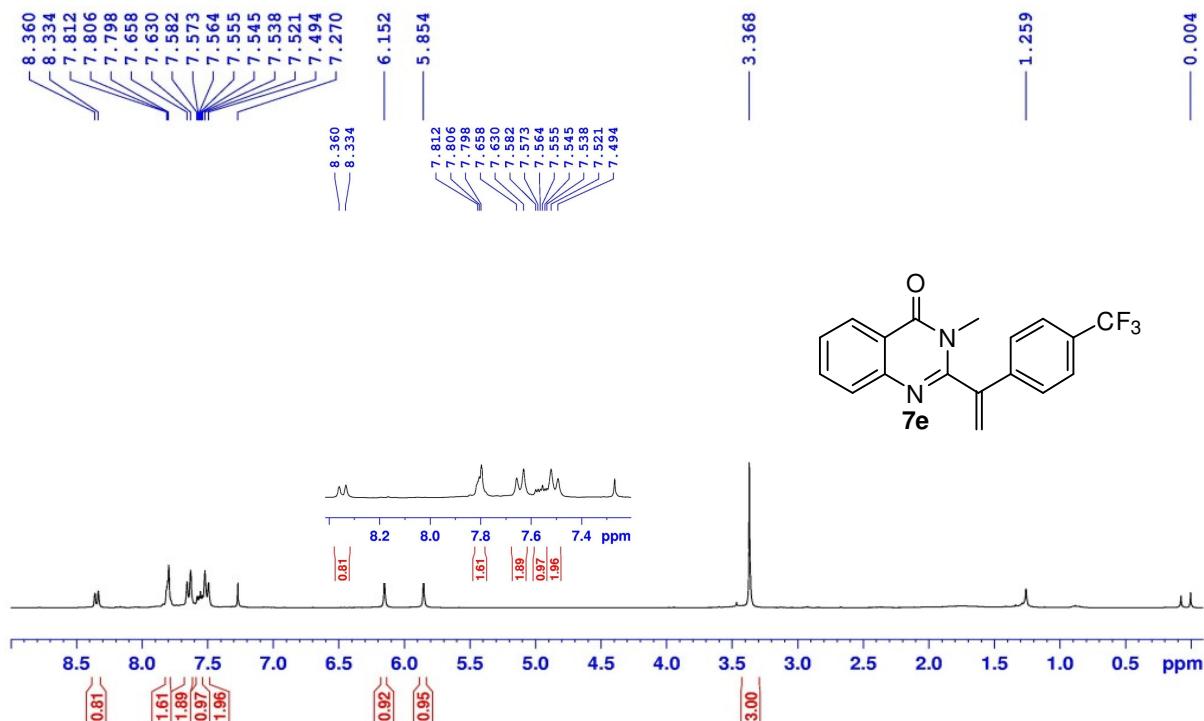
¹H NMR (CDCl_3 , 600 MHz) spectrum of product **7d**:



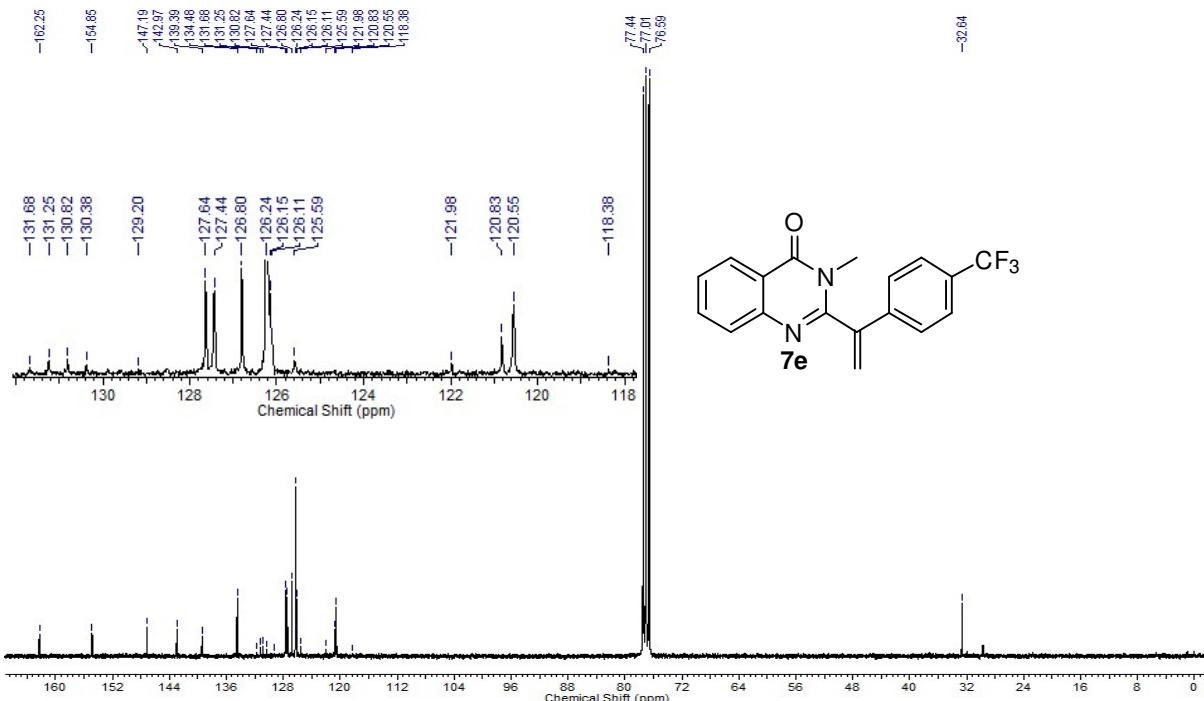
¹³C NMR (CDCl_3 , 150 MHz) spectrum of product **7d**:



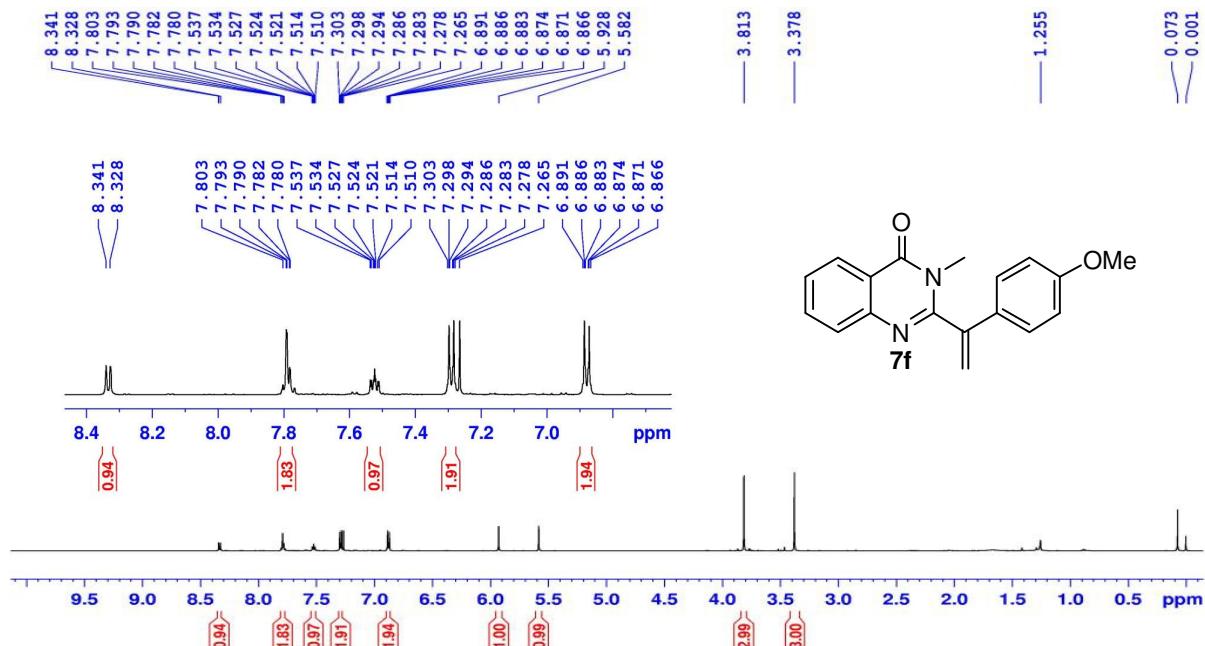
¹H NMR (CDCl₃, 300 MHz) spectrum of product 7e:



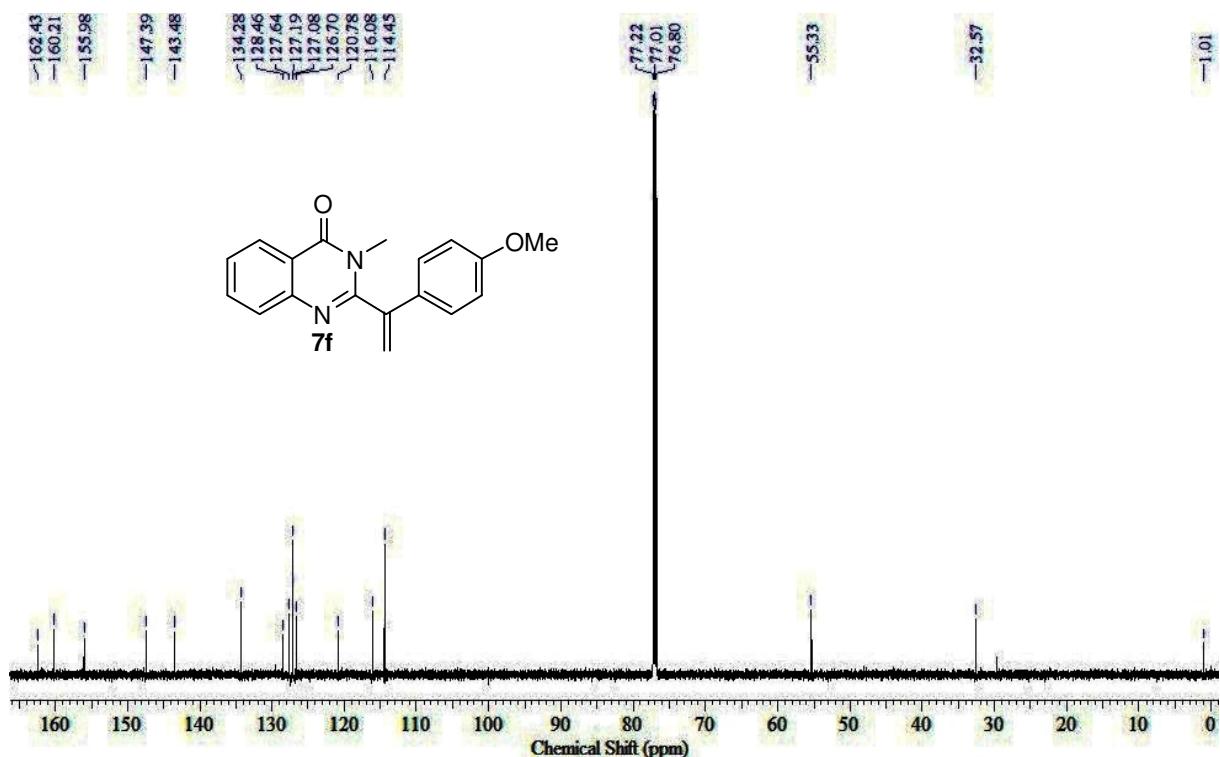
¹³C NMR (CDCl₃, 75 MHz) spectrum of product 7e:



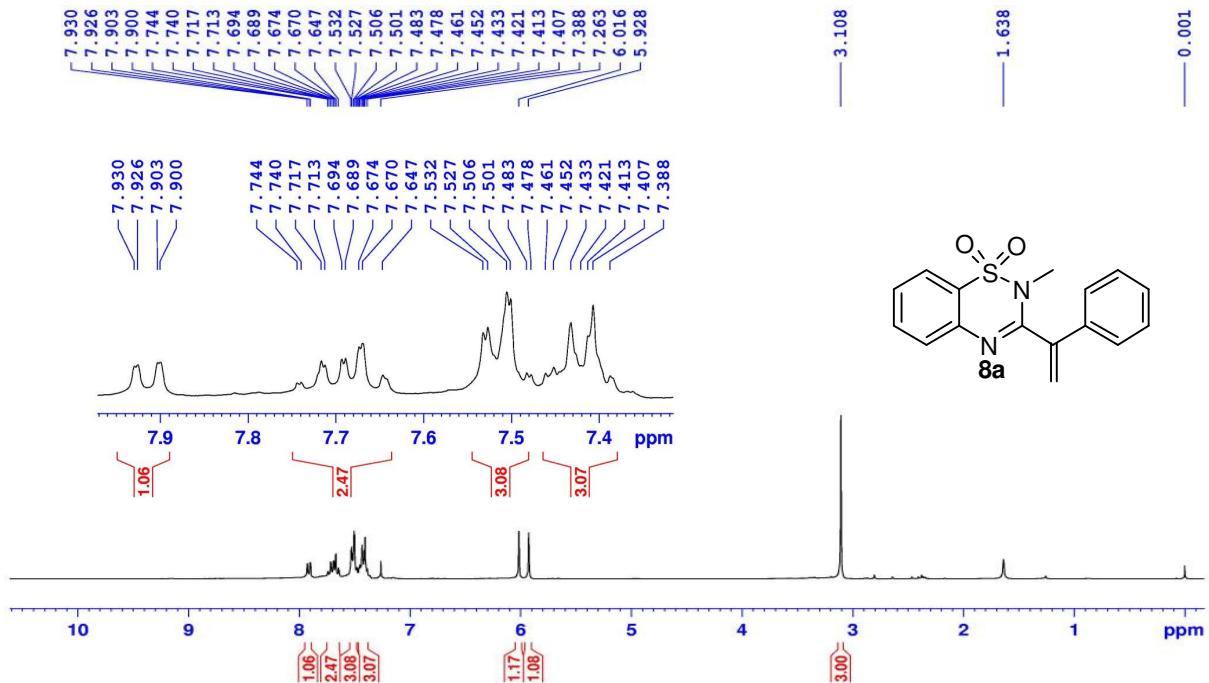
¹H NMR (CDCl₃, 600 MHz) spectrum of product 7f:



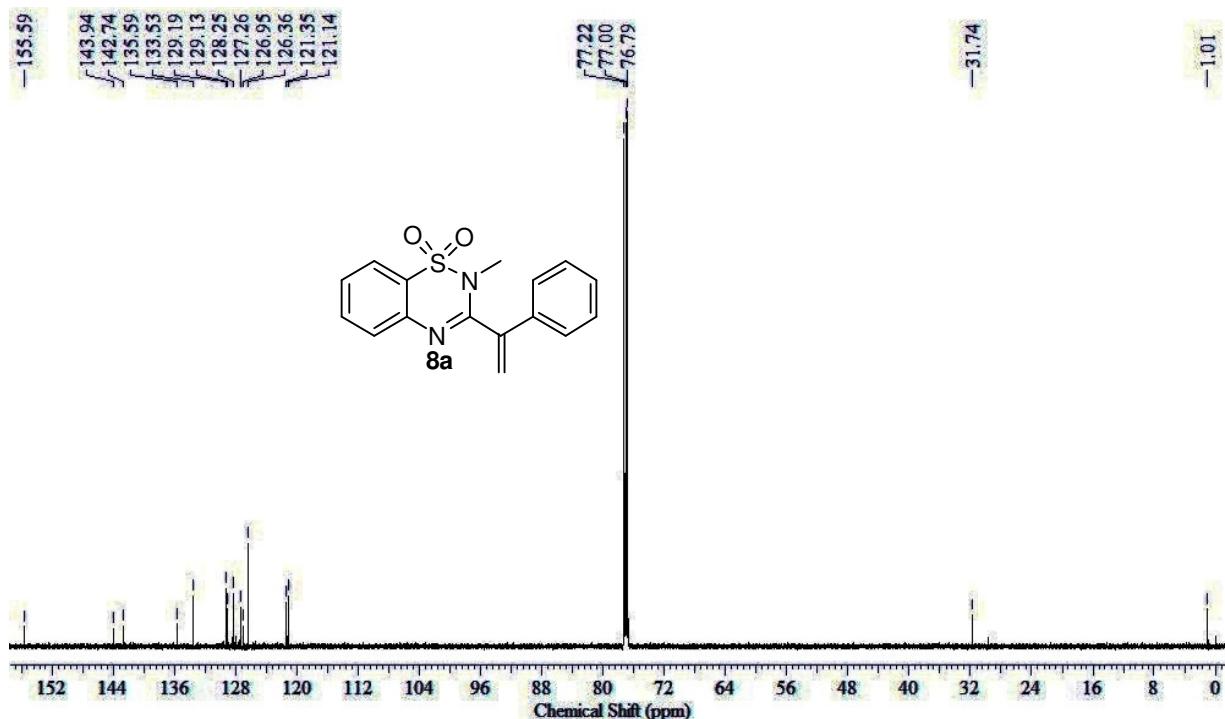
¹³C NMR (CDCl₃, 150 MHz) spectrum of product **7f**:



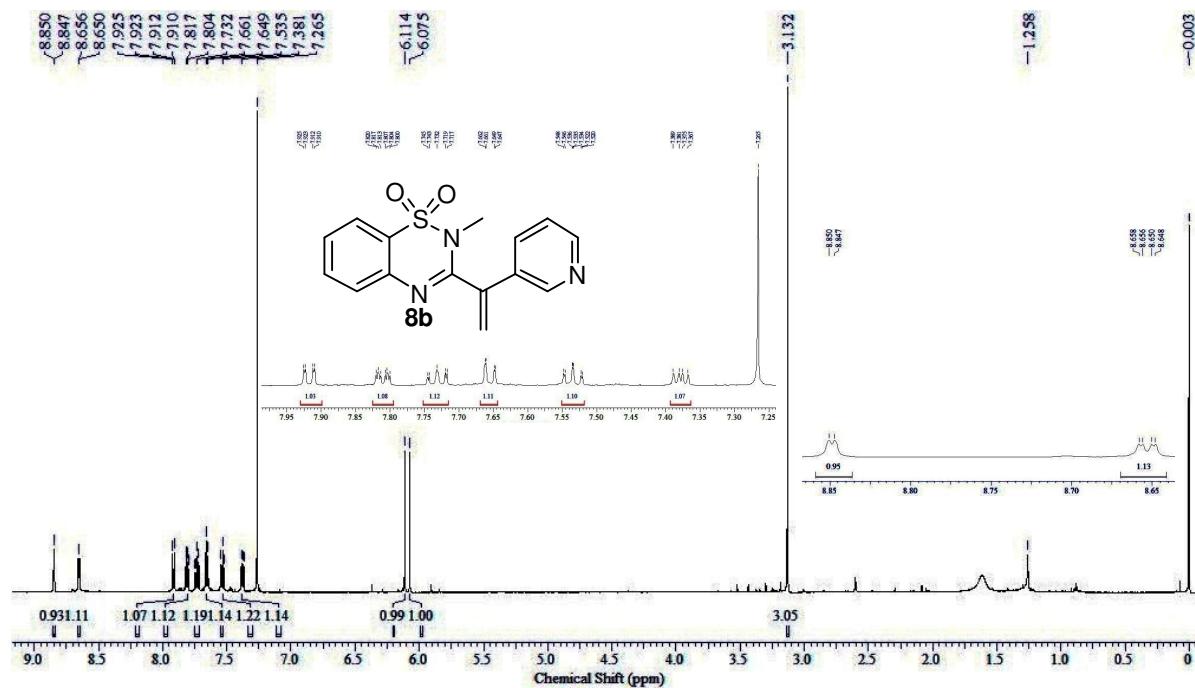
¹H NMR (CDCl_3 , 300 MHz) spectrum of product **8a**:



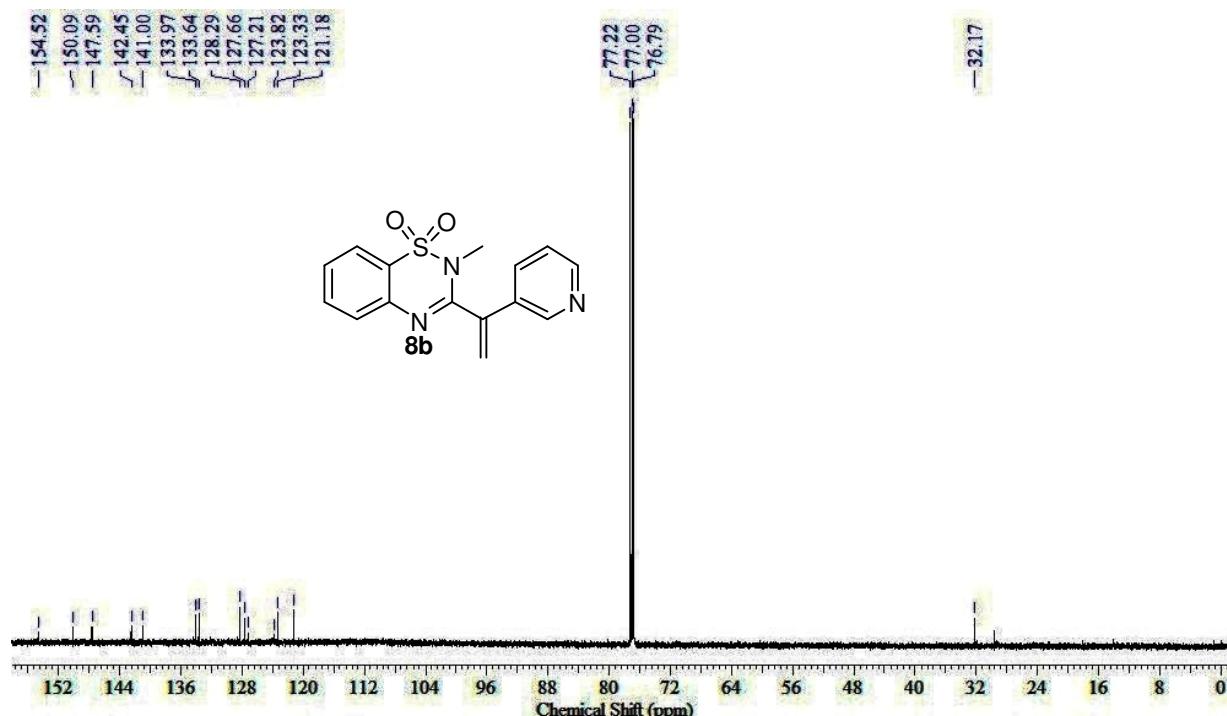
¹³C NMR (CDCl_3 , 150 MHz) spectrum of product **8a**:



¹H NMR (CDCl_3 , 600 MHz) spectrum of product **8b**:

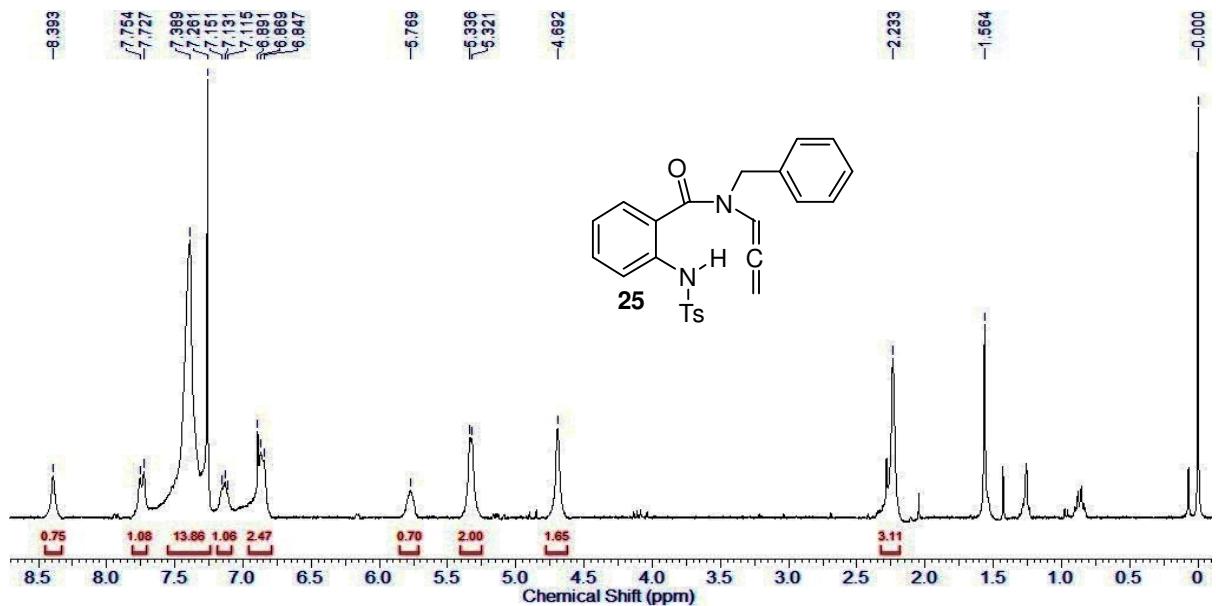


¹³C NMR (CDCl_3 , 150 MHz) spectrum of product **8b**:

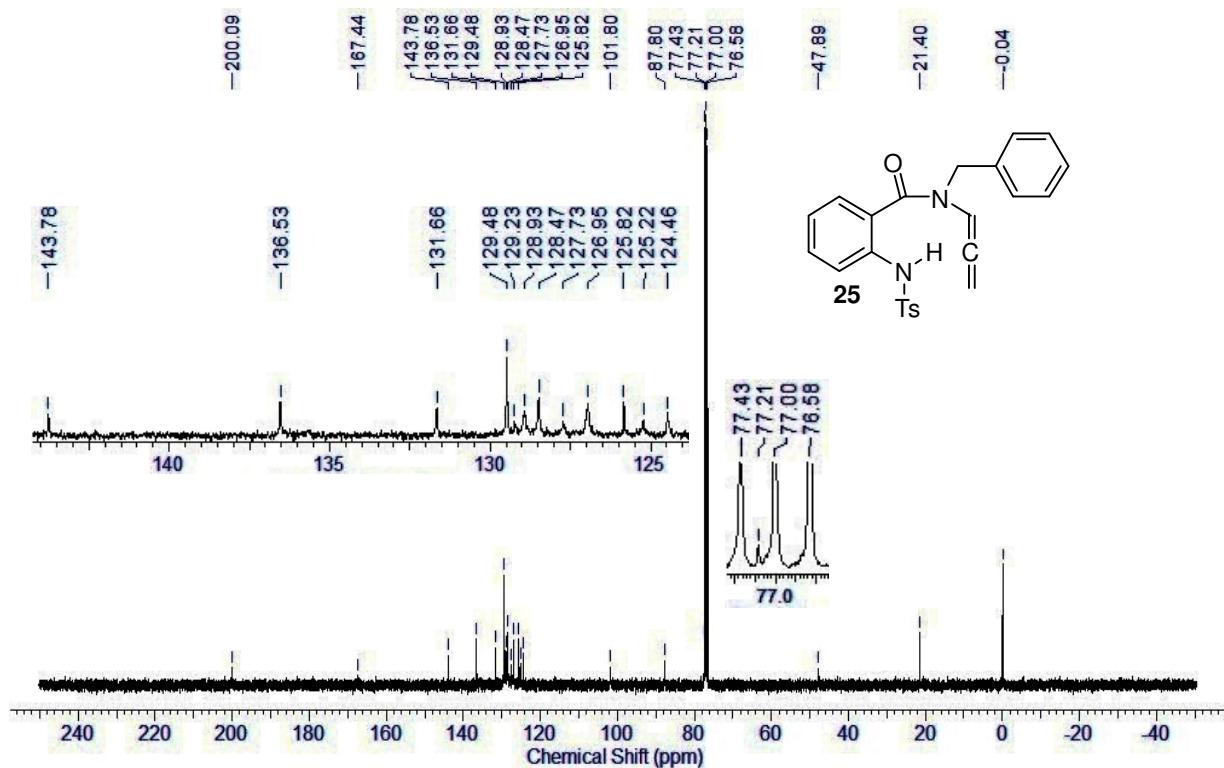


13) NMR spectra of allene **25** (scheme 5):

¹H NMR (CDCl_3 , 300 MHz) spectrum of compound 25:

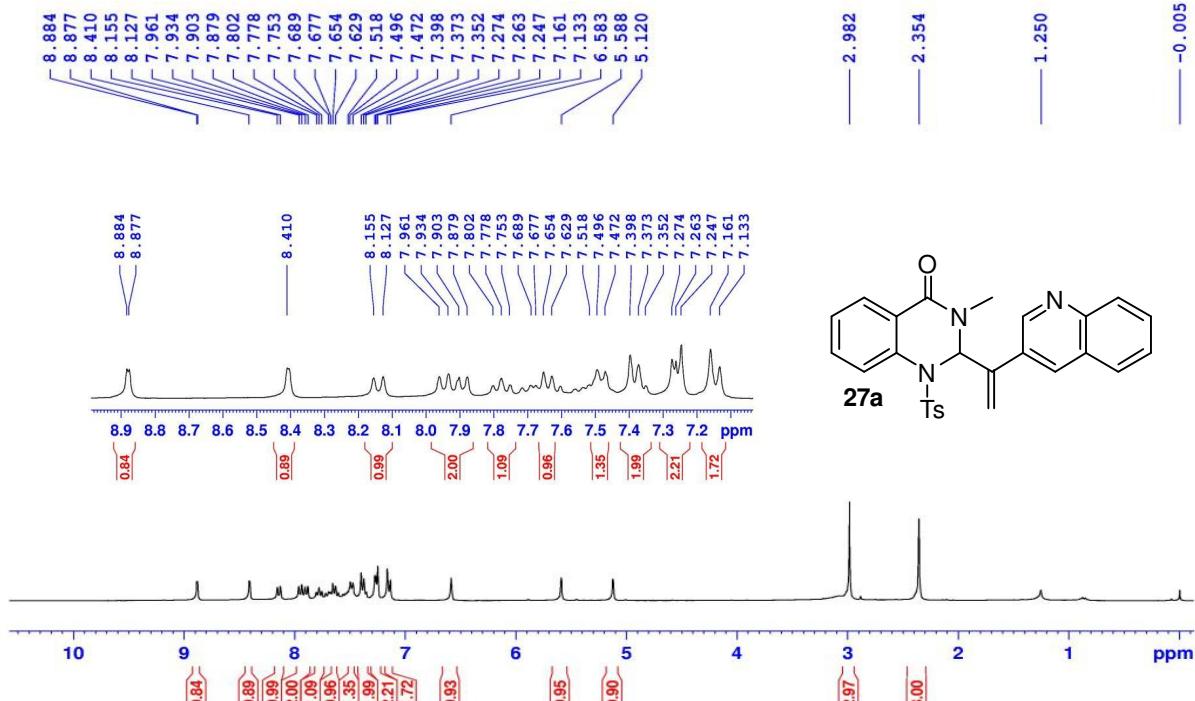


¹³C NMR (CDCl₃, 75 MHz) spectrum of compound 25:

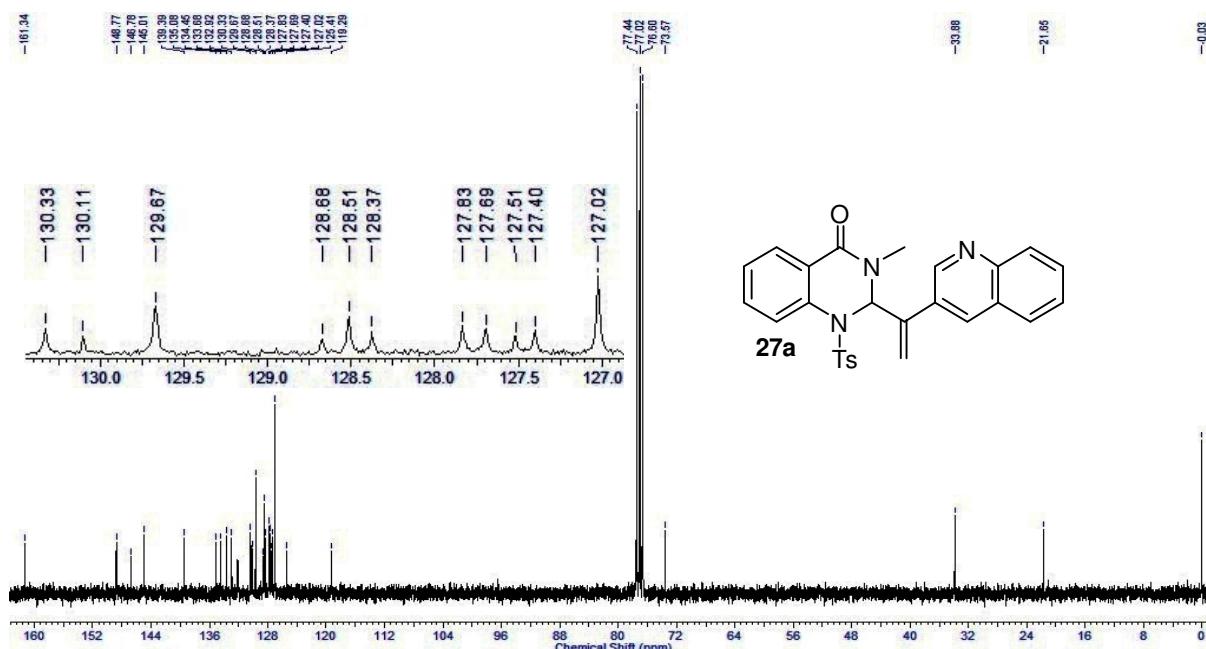


14) NMR spectra of products **27a-27c** (scheme 5):

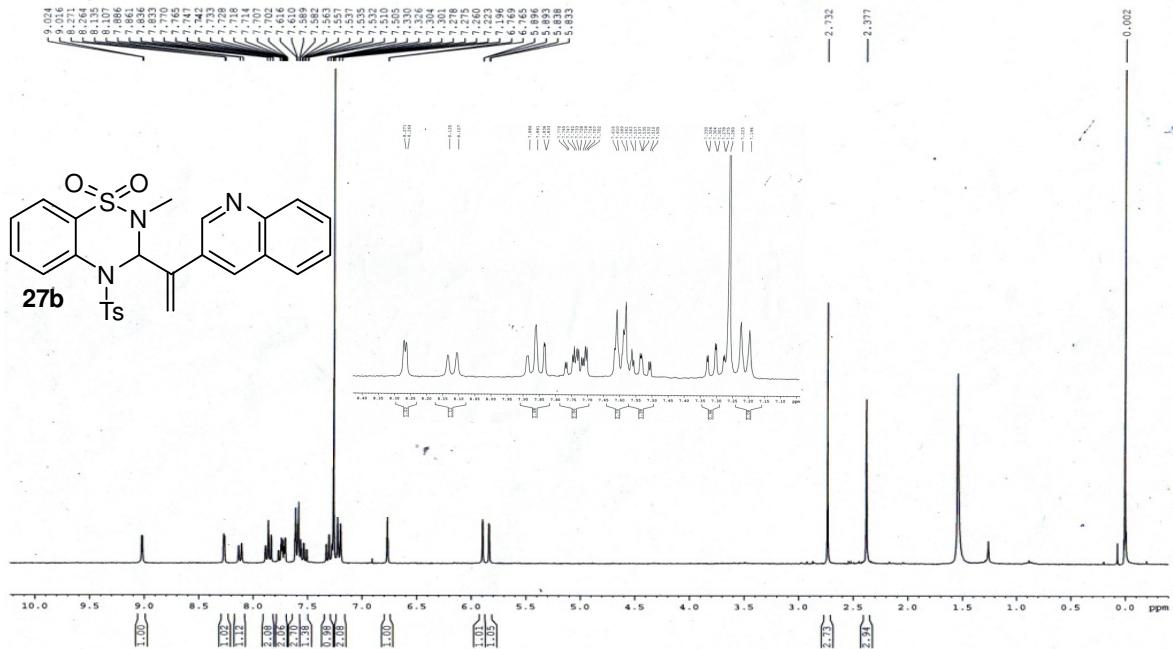
¹H NMR (CDCl₃, 300 MHz) spectrum of product **27a**:



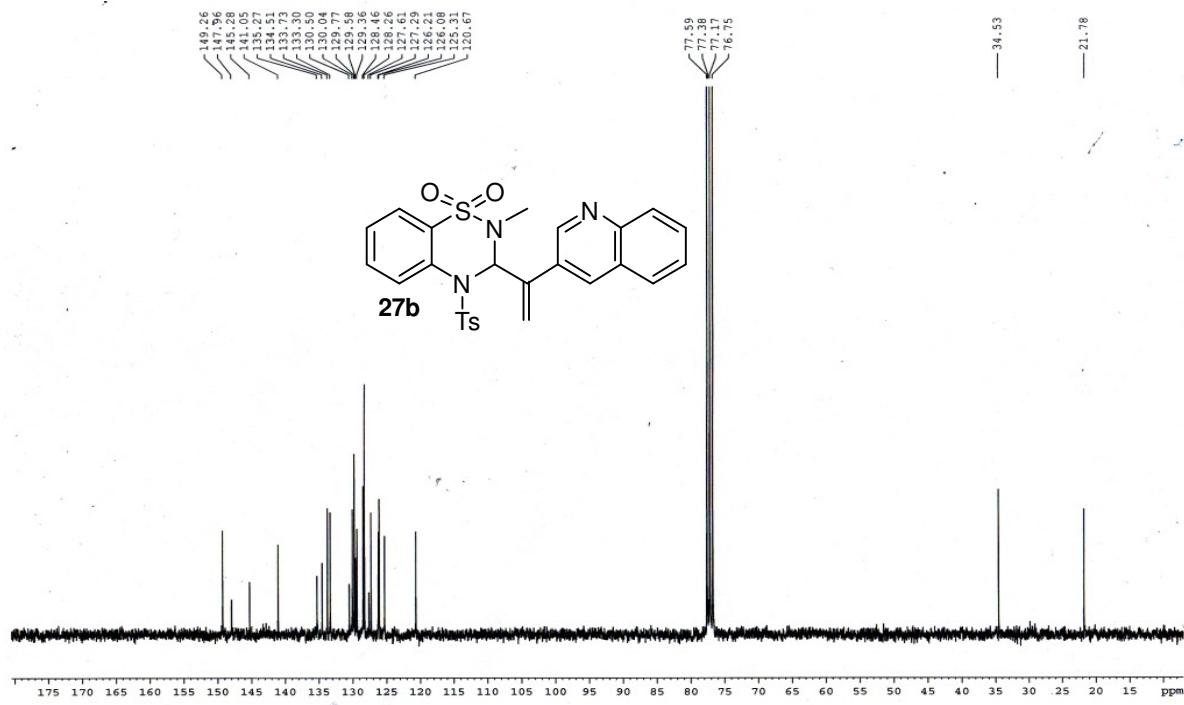
¹³C NMR (CDCl_3 , 75 MHz) spectrum of product **27a**:



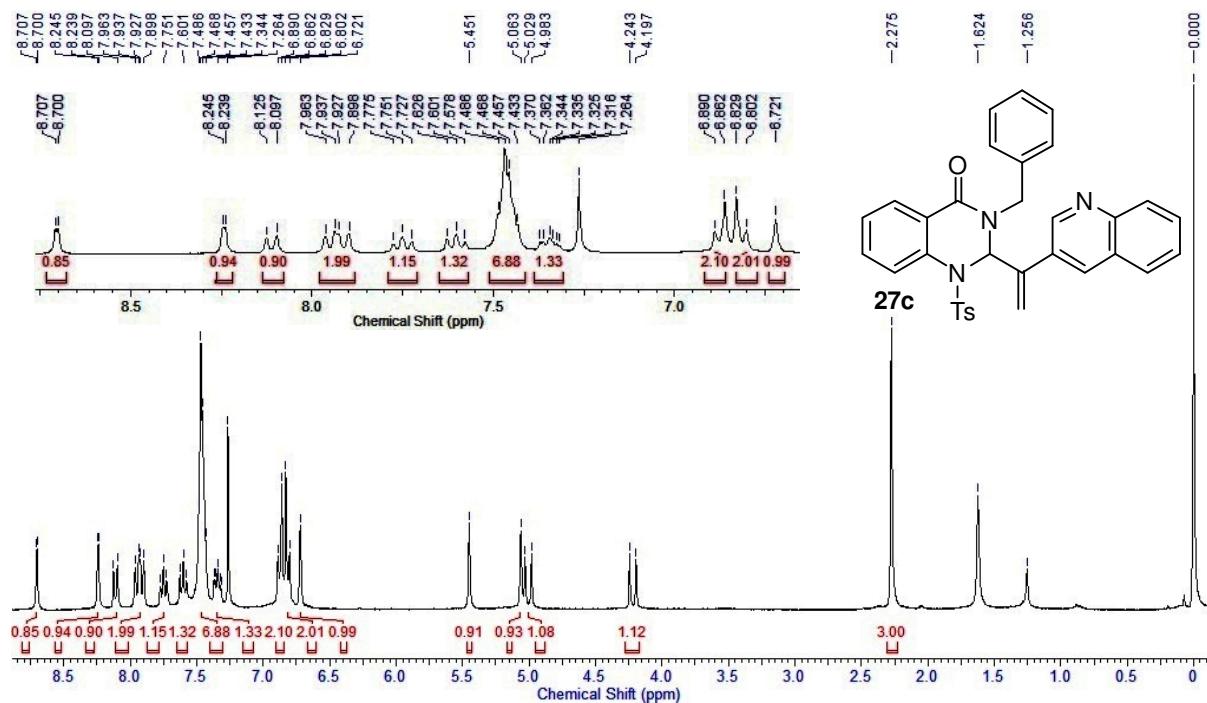
¹H NMR (CDCl_3 , 300 MHz) spectrum of product **27b**:



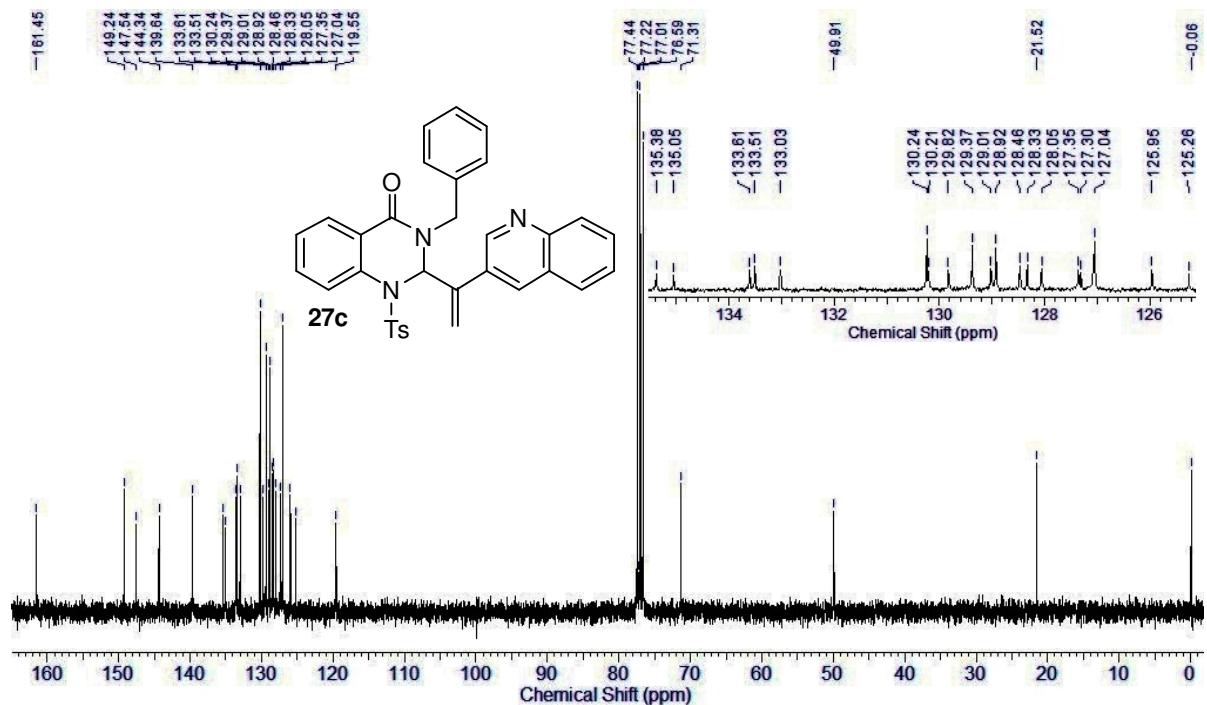
¹³C NMR (CDCl₃, 75 MHz) spectrum of product **27b**:



¹H NMR (CDCl_3 , 300 MHz) spectrum of product **27c**:

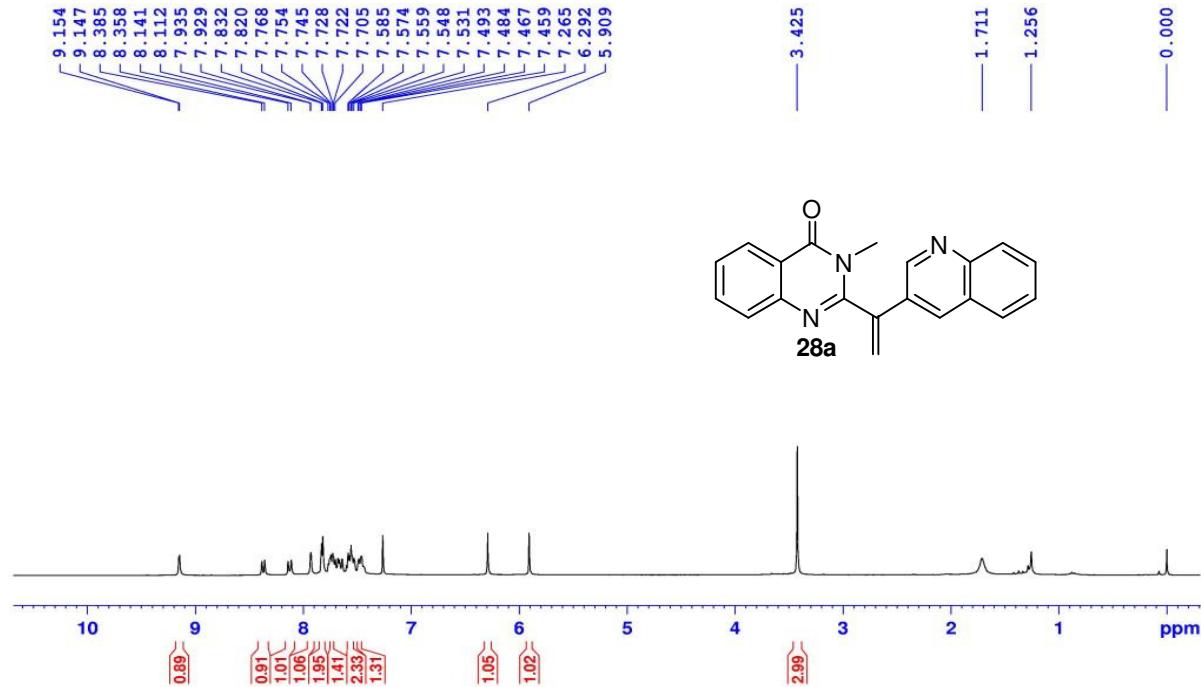


¹³C NMR (CDCl_3 , 75 MHz) spectrum of product **27c**:

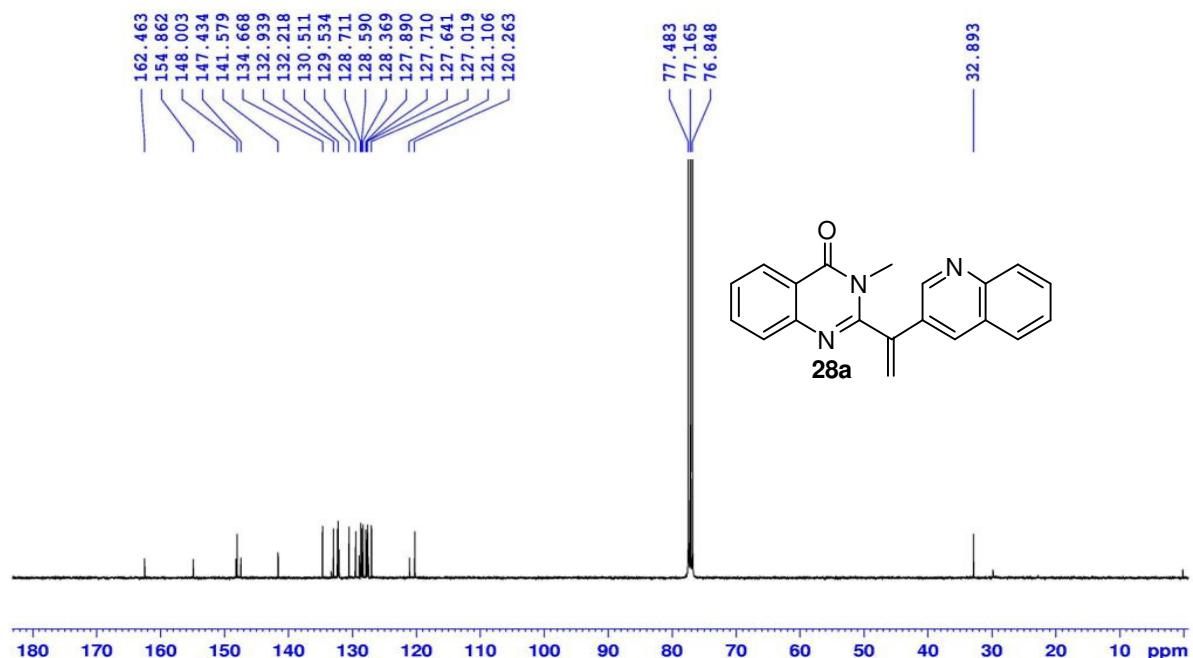


15) NMR spectra of products **28a**-**28c** (scheme 5):

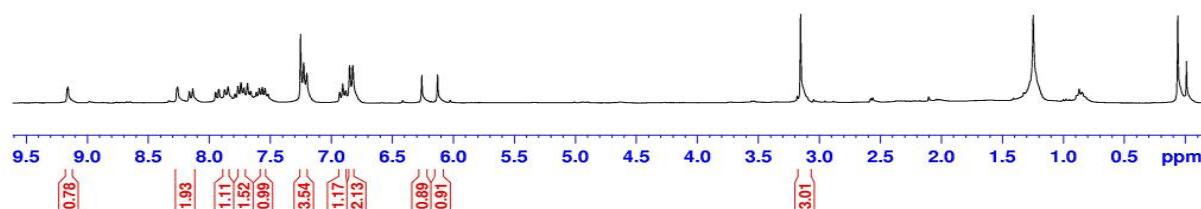
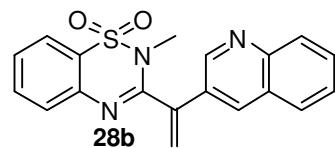
¹H NMR (CDCl_3 , 300 MHz) spectrum of product **28a**:



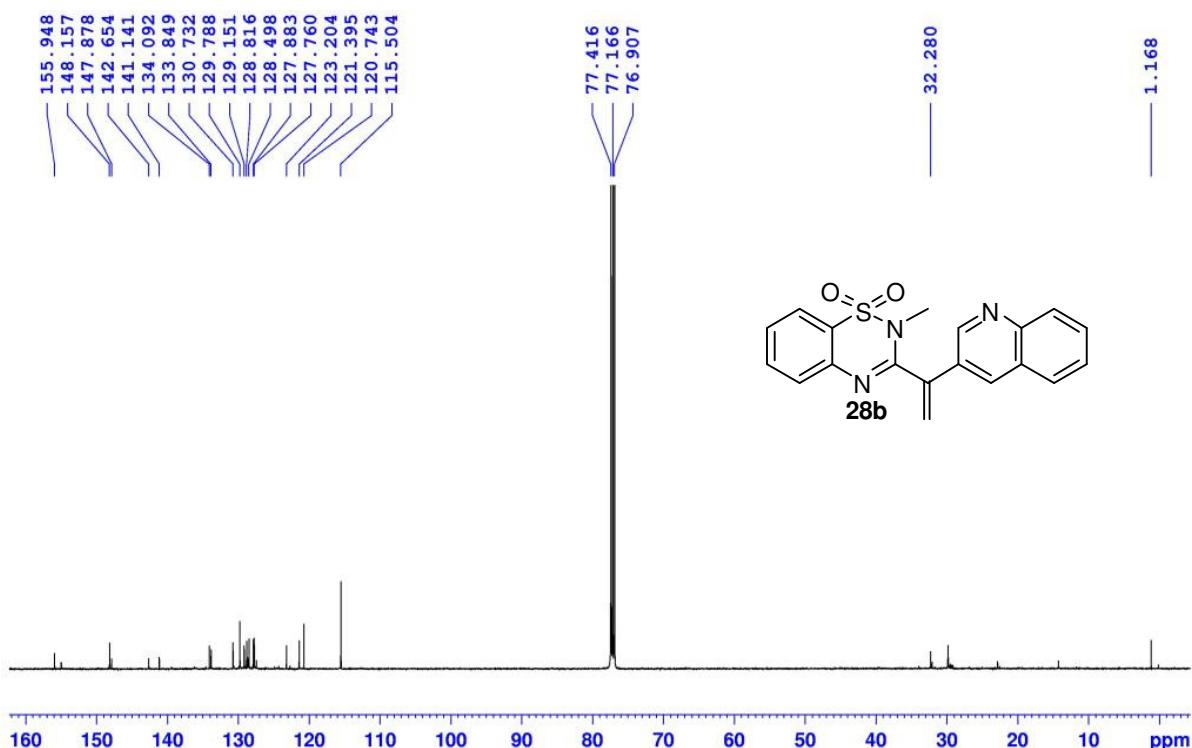
¹³C NMR (CDCl_3 , 100 MHz) spectrum of product **28a**:



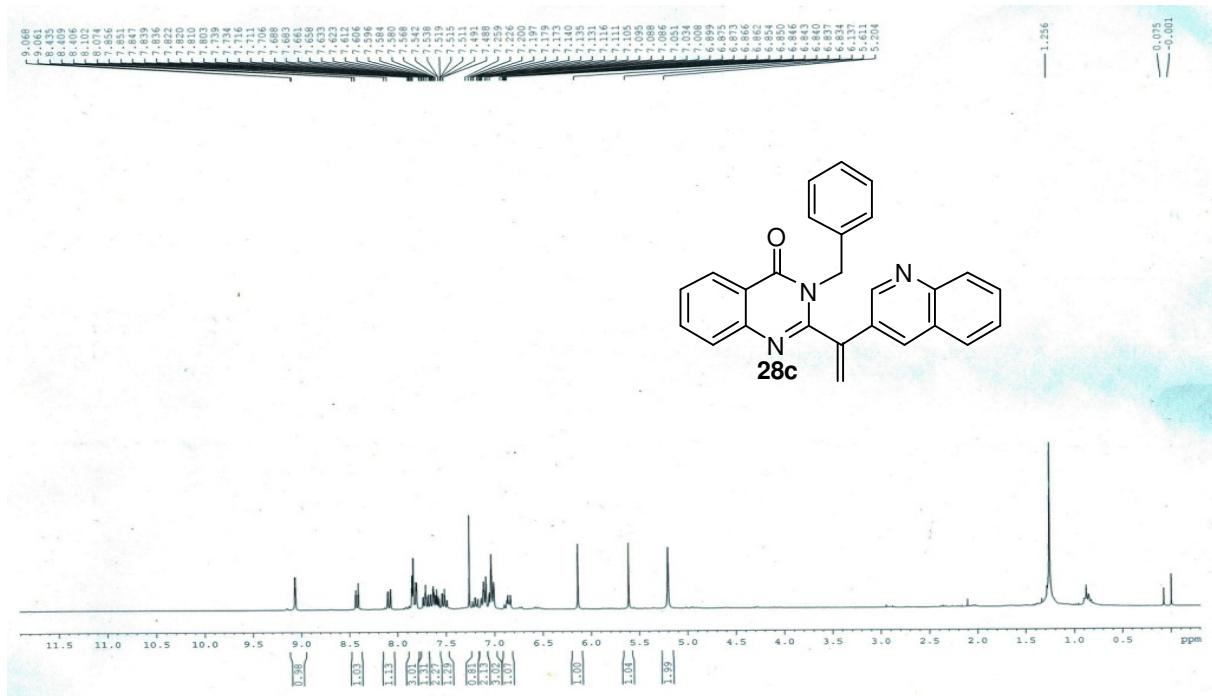
¹H NMR (CDCl_3 , 300 MHz) spectrum of product **28b**:



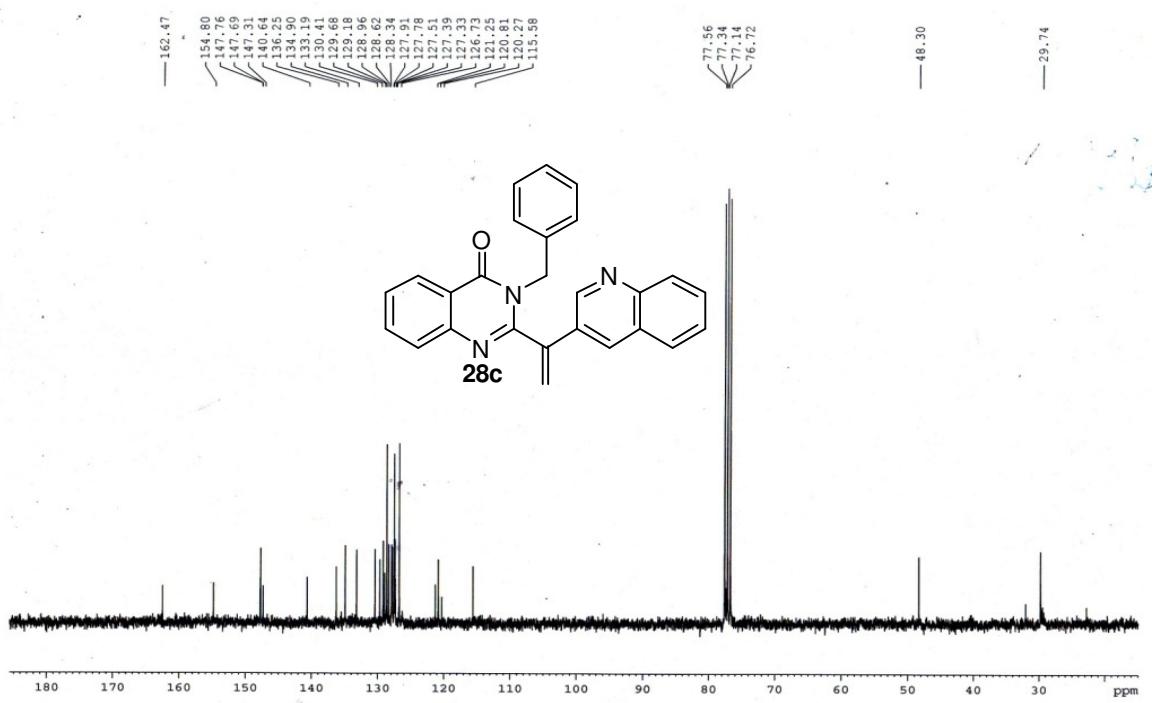
¹³C NMR (CDCl_3 , 100 MHz) spectrum of product **28b**:



¹H NMR (CDCl₃, 300 MHz) spectrum of product **28c**:



¹³C NMR (CDCl_3 , 75 MHz) spectrum of product **28c**:



HRMS spectrum of product **8a**:

