Supporting Information

Synthesis of Selenium-Containing (*E*)-*N*-Propenolquinazolinones *via* $FeCl_3$-Mediated Cascade Reaction of Propargyl Quinazoline-4-yl Ethers with Diselenides

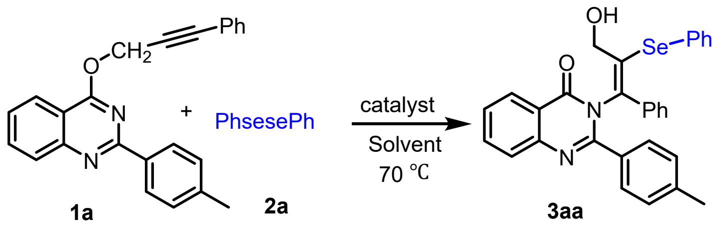
Xinqin Zhang, Qin Yang, Xiaofeng Zeng, Yang Fu, Qiuping Ding and Yiyuan Peng*

College of Chemistry and Materials Jiangxi Normal University, 99 Ziyang Avenue, Nanchang 330022, China

Contents

I. Optimization of reaction conditions for synthesis of products 3

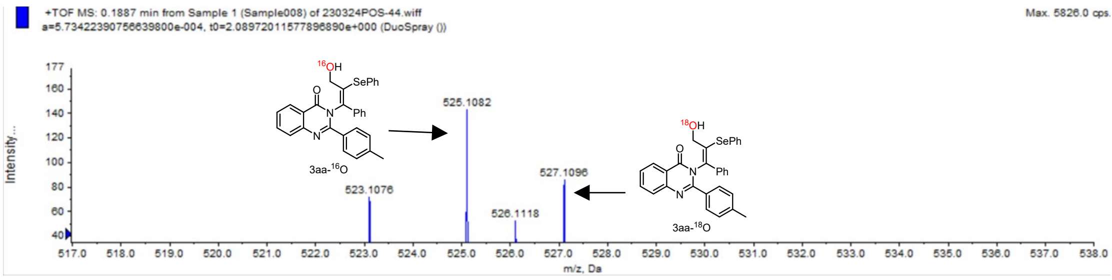
Table S1 Optimization of Reaction Conditions[a]



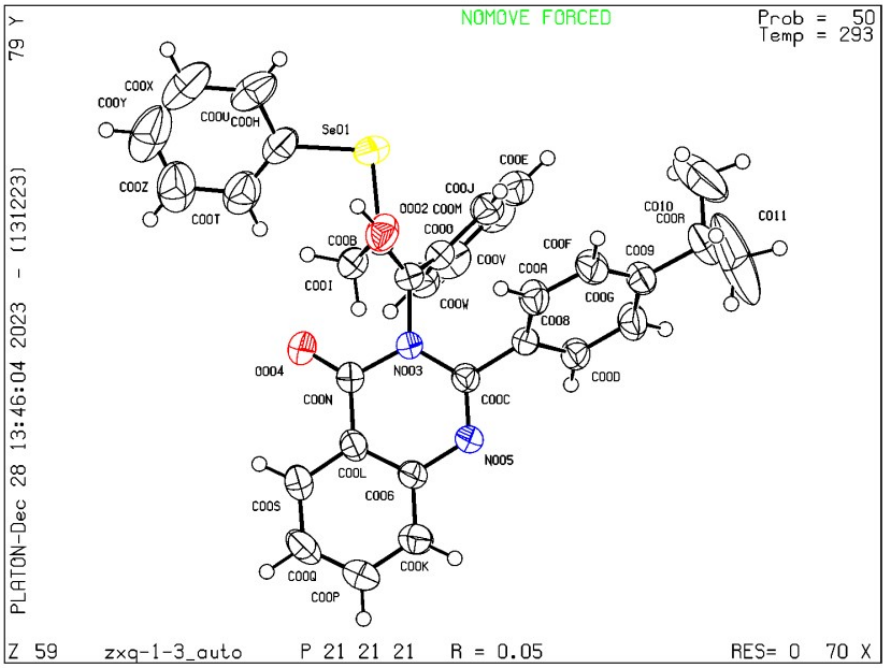
Entry	Catalyst (eq.)	solvent	Yield (%)[b]
1	$FeCl_3$ (2.0)	CH_2Cl_2	33
2[c]	$FeCl_3$ (2.0)	CH_2Cl_2	34
3	$FeCl_3$ (2.0)	DCE	30
4	$FeCl_3$ (2.0)	NMP	32
5	$FeCl_3$ (2.0)	Toluene	31
6	$FeCl_3$ (2.0)	DMSO	N.R.
7	$FeCl_3$ (2.0)	DMF	N.R.
8	$FeCl_3$ (2.0)	CH_3CN	N.R.
9	$FeCl_3$ (2.0)	CH_3OH	N.R.
10	$FeCl_3$ (2.0)	1,4-dioxane	60
11	$FeCl_3$ (2.0)	CH_3NO_2	78
12	CuI (2.0)	CH_3NO_2	No
13	$FeCl_3·6H_2O$ (2.0)	CH_3NO_2	90
14[c]	$FeCl_2·4H_2O$ (2.0)	CH_3NO_2	Trace
15[d]	$FeCl_2·4H_2O$ (2.0)	CH_3NO_2	63
16	$FeCl_3·6H_2O$ (2.5)	CH_3NO_2	91
17	$FeCl_3·6H_2O$ (1.5)	CH_3NO_2	70
18[e]	$FeCl_3·6H_2O$ (2.0)	CH_3NO_2	72
19[f]	$FeCl_3·6H_2O$ (2.0)	CH_3NO_2	85
20[g]	$FeCl_3·6H_2O$ (2.0)	CH_3NO_2	91
21[h]	$FeCl_3·6H_2O$ (2.0)	CH_3NO_2	90
22[i]	$FeCl_3·6H_2O$ (2.0)	CH_3NO_2	90
23[j]	$FeCl_3·6H_2O$ (2.0)	CH_3NO_2	85
24[K]	$FeCl_3·6H_2O$ (2.0)	CH_3NO_2/H_2O	89
25	-	CH_3NO_2	0

[a]Reaction conditions: **1a** (0.2 mmol), **2a** (0.2 mmol, 1.0 eq.), catalyst (0.4 mmol, 2.0 eq.), solvent (2.0 mL), under air atmosphere, at 70 °C for 2 h. [b] Yields based on isolated [c] The reaction was carried out under argon atmosphere. [d] 29 h. [e]at 60 °C. [f]at 80 °C. [g] 0.75 eq. of PhSeSePh was used. [h] 0.60 eq. of PhSeSePh was used. [i] 0.55 eq. of PhSeSePh was used. [j] 0.50 eq. of PhSeSePh was used. [K]20%-30% mL of water was added in the solvent of CH_3NO_2.

II. ^{18}O-Labeling Experiment



III. X-ray Single Crystal Diffraction Data of 3ca



Bond precision:	C-C = 0.0077 A	Wavelength=0.71073

Cell:	a=12.5627(11)	b=14.7048(7)	c=14.8441(7)
	alpha=90	beta=90	gamma=90
Temperature:	293 K		

	Calculated	Reported
Volume	2742.2(3)	2742.2(3)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C32 H28 N2 O2 Se	0.33(C32 H28 N2 O2 Se)
Sum formula	C32 H28 N2 O2 Se	C10.67 H9.33 N0.67 O0.67 Se0.33
Mr	551.52	183.84
Dx,g cm-3	1.336	1.336
Z	4	12
Mu (mm-1)	1.400	1.400
F000	1136.0	1136.0
F000'	1136.02	
h,k,lmax	17,20,20	17,18,20
Nref	7671[4266]	6380
Tmin,Tmax		0.313,1.000
Tmin'		

Correction method= # Reported T Limits: Tmin=0.313 Tmax=1.000
AbsCorr = MULTI-SCAN

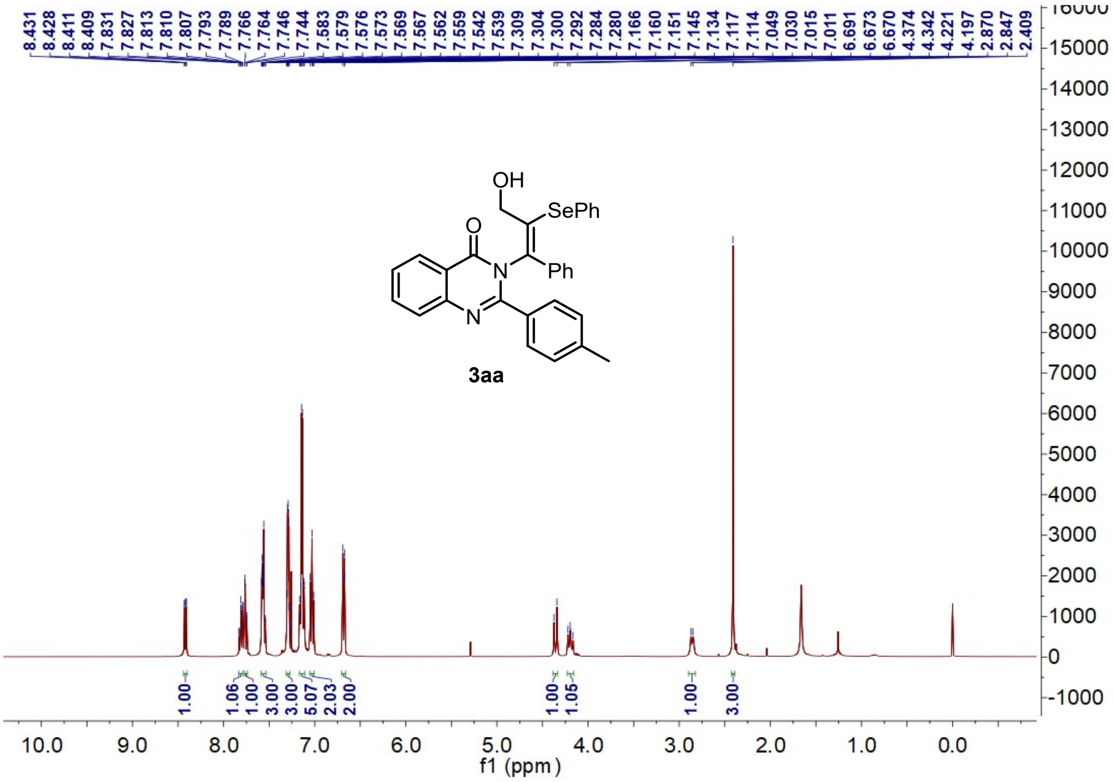
Data completeness= 1.50/0.83 Theta(max)= 29.521

R(reflections)= 0.0474(4030) wR2(reflections)= 0.0981(6380)

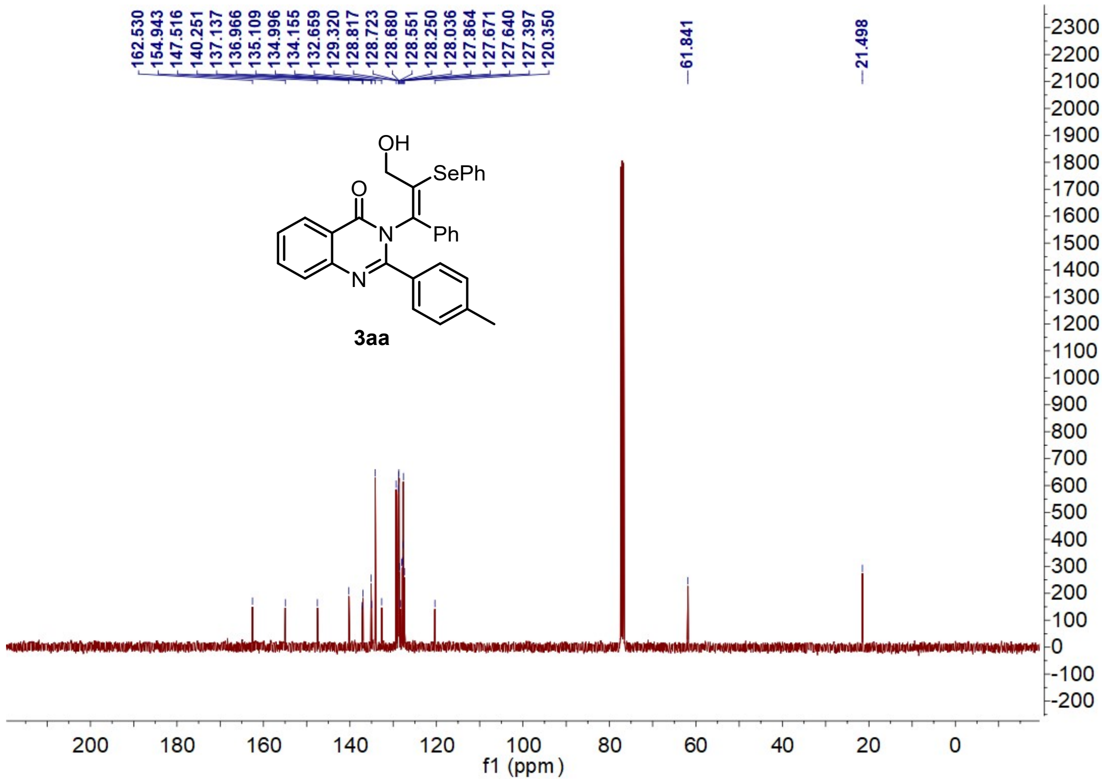
S = 0.998 Npar= 338

VI. Copies of NMR Spectra

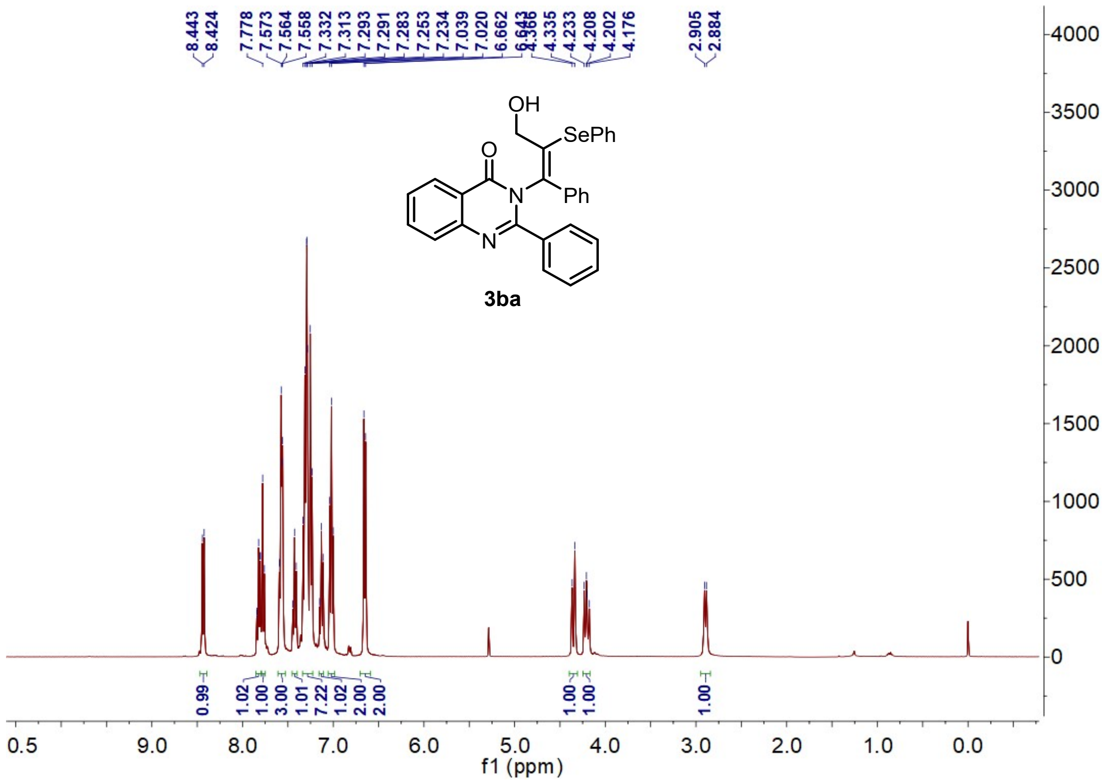
^{1}H-NMR of **3aa** ($CDCl_3$, 400 Hz)



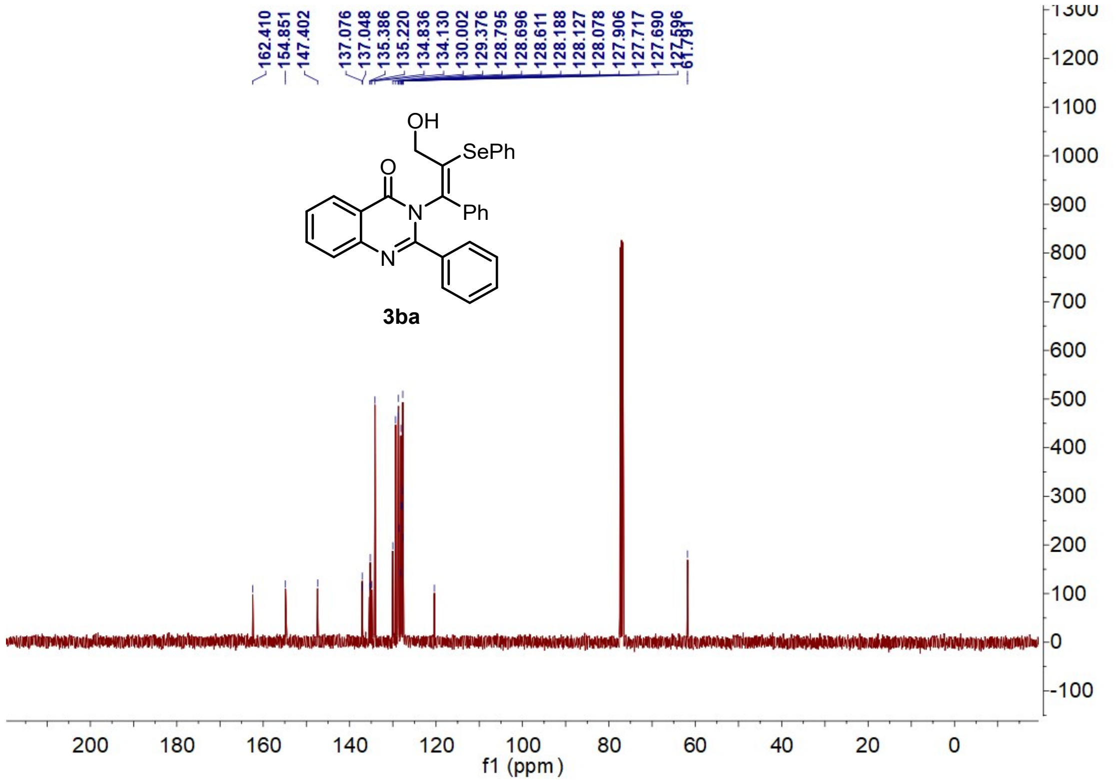
^{13}C-NMR of **3aa** ($CDCl_3$, 100 Hz)



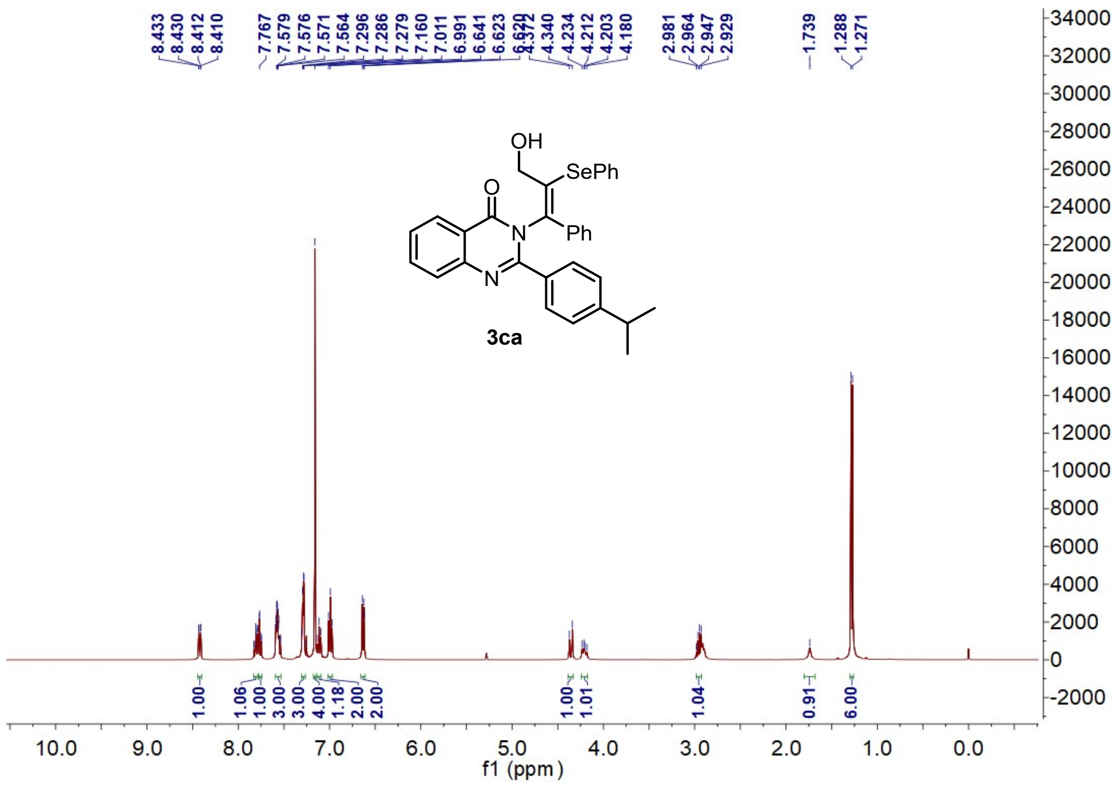
^{1}H-NMR of **3ba** ($CDCl_3$, 400 Hz)



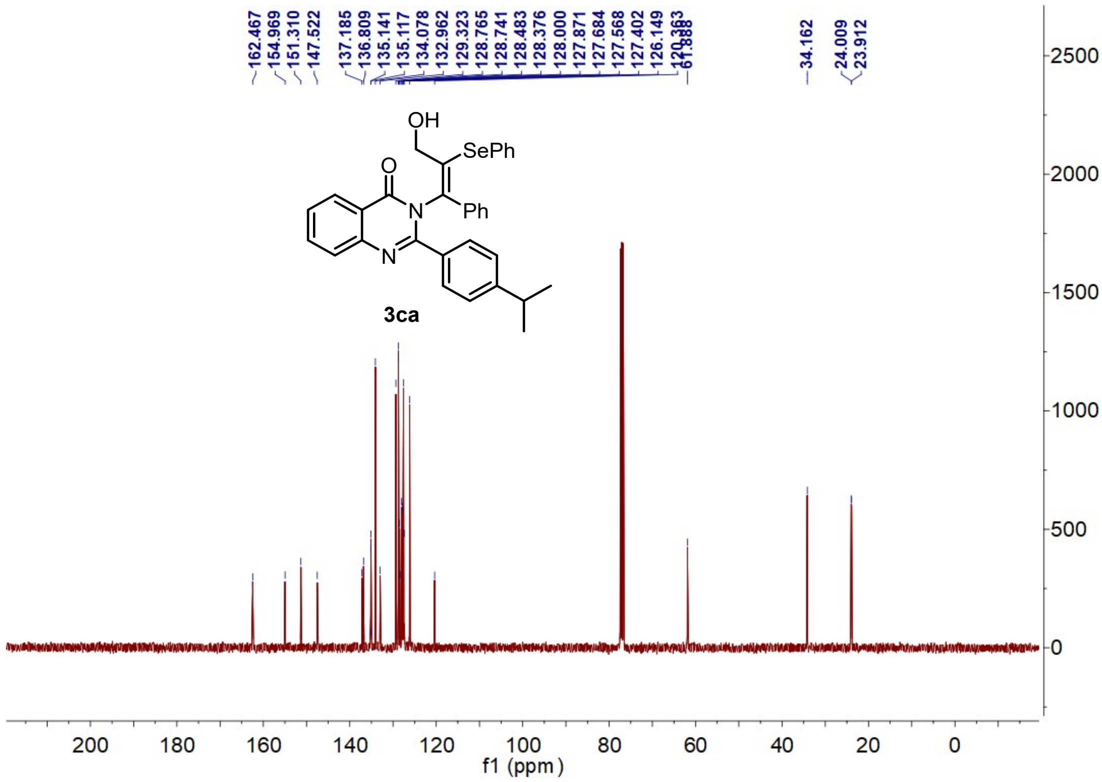
^{13}C-NMR of **3ba** ($CDCl_3$, 100 Hz)



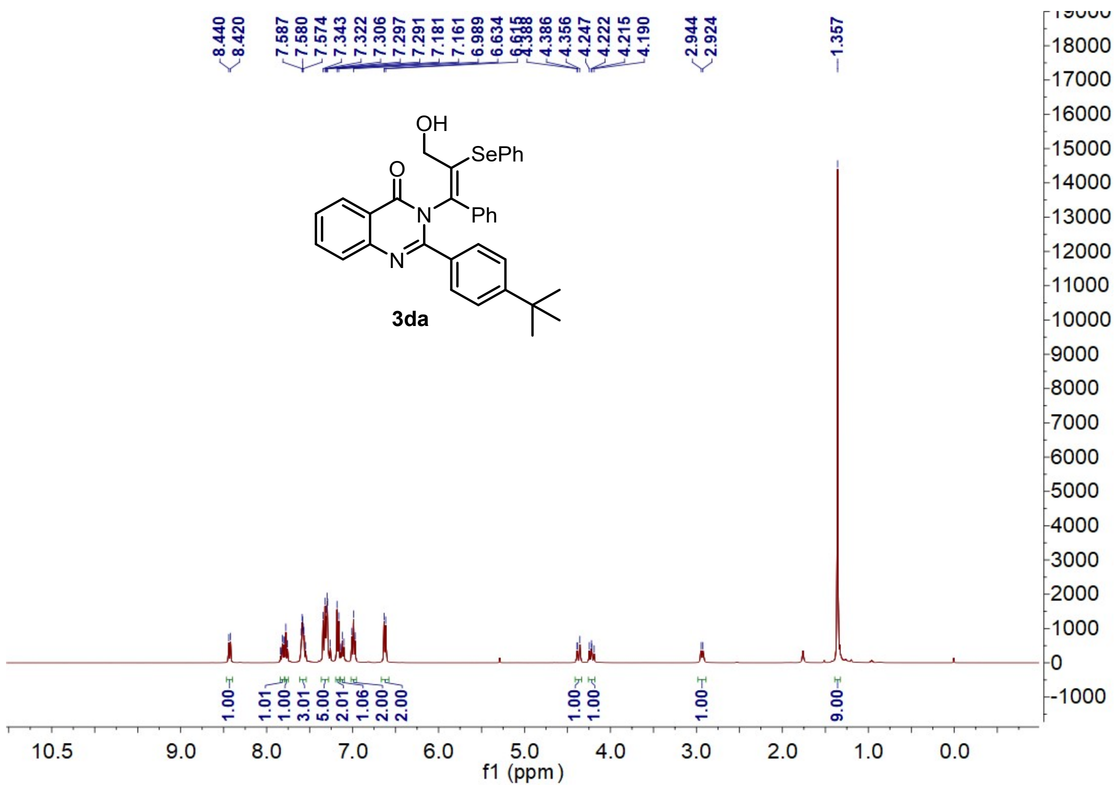
^{1}H-NMR of **3ca** ($CDCl_3$, 400 Hz)



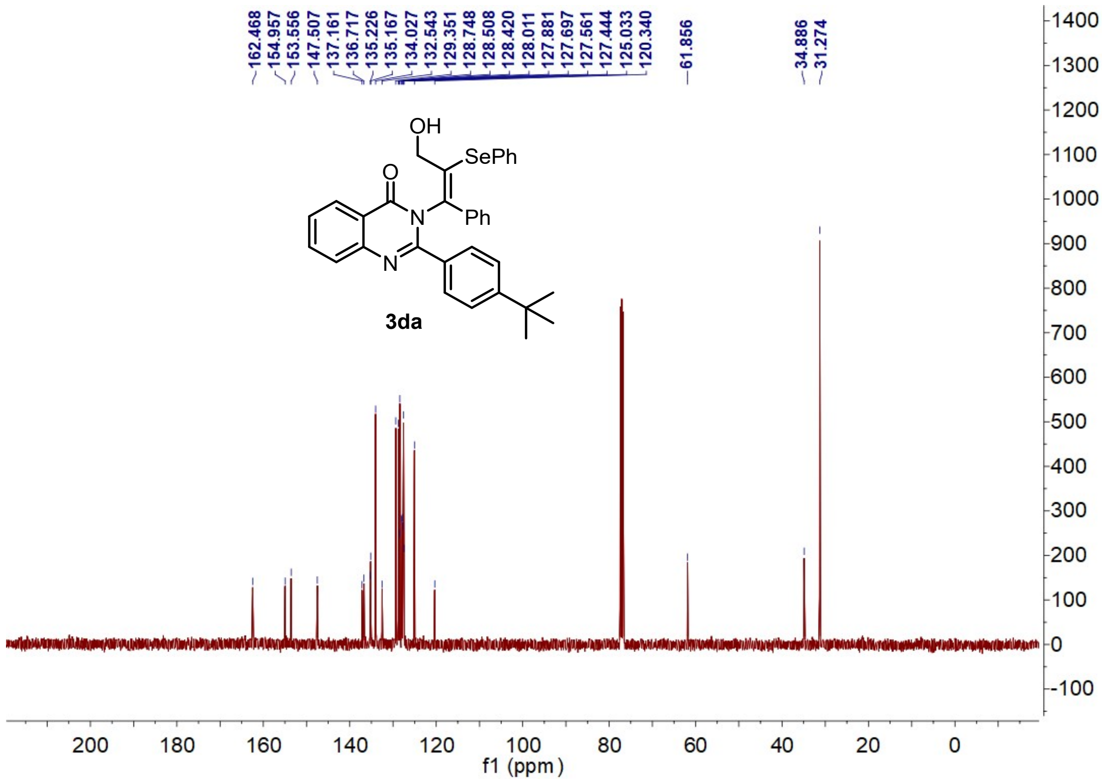
^{13}C-NMR of **3ca** ($CDCl_3$, 100 Hz)



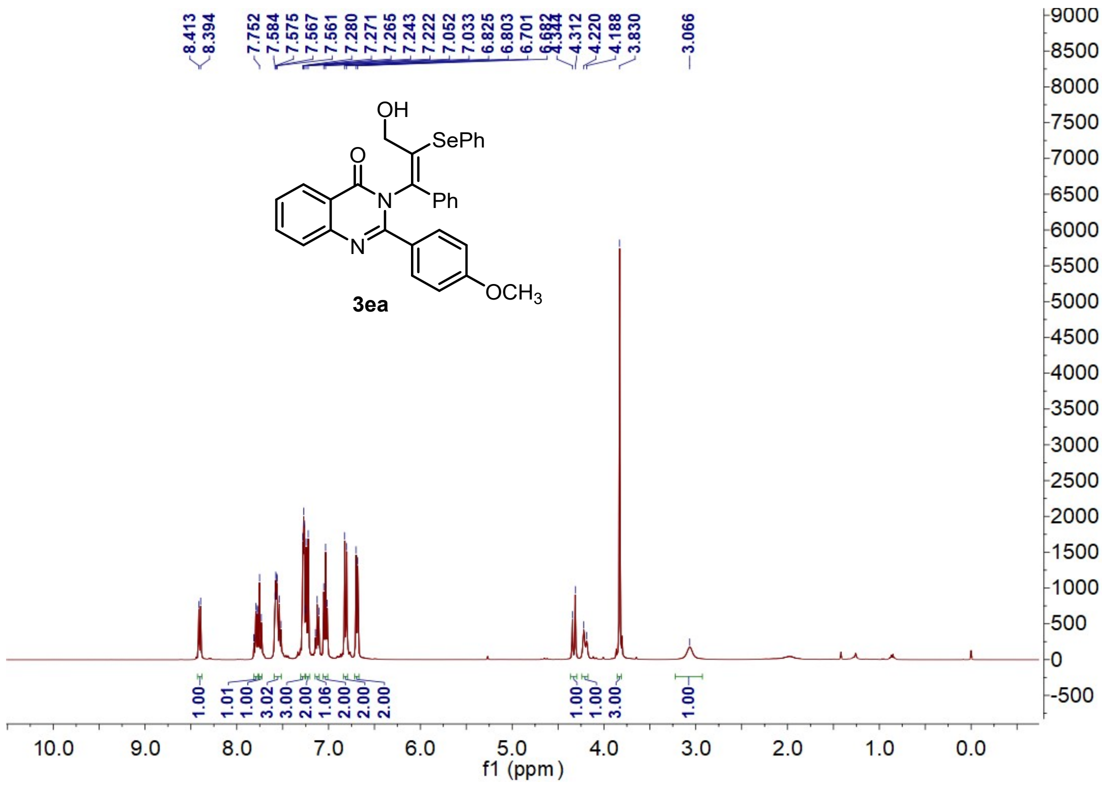
^{1}H-NMR of **3da** ($CDCl_3$, 400 Hz)



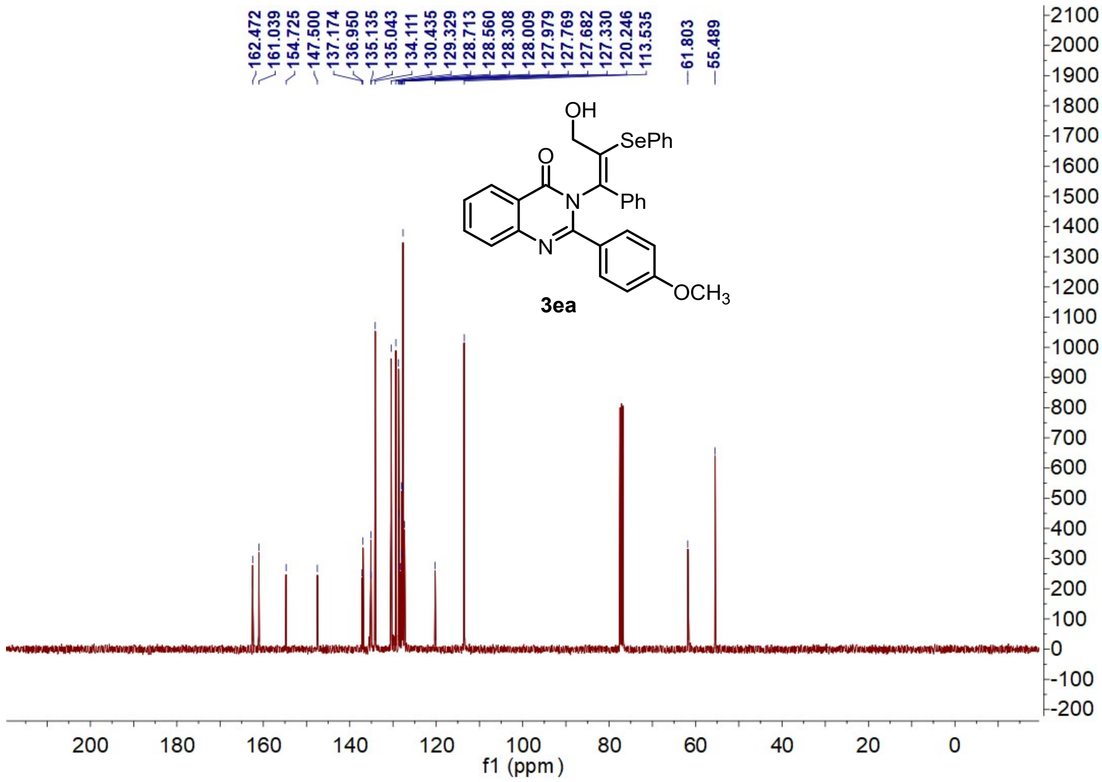
^{13}C-NMR of **3da** ($CDCl_3$, 100 Hz)



^{1}H-NMR of **3ea** ($CDCl_3$, 400 Hz)

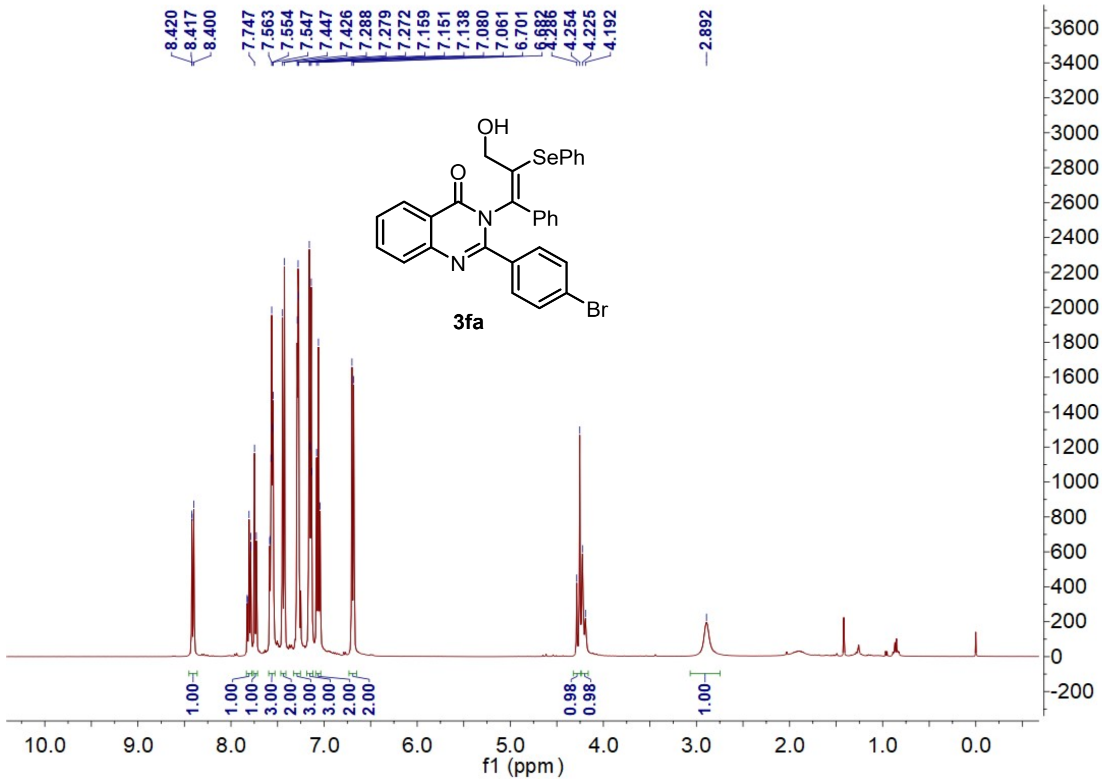


^{13}C-NMR of **3ea** ($CDCl_3$, 100 Hz)



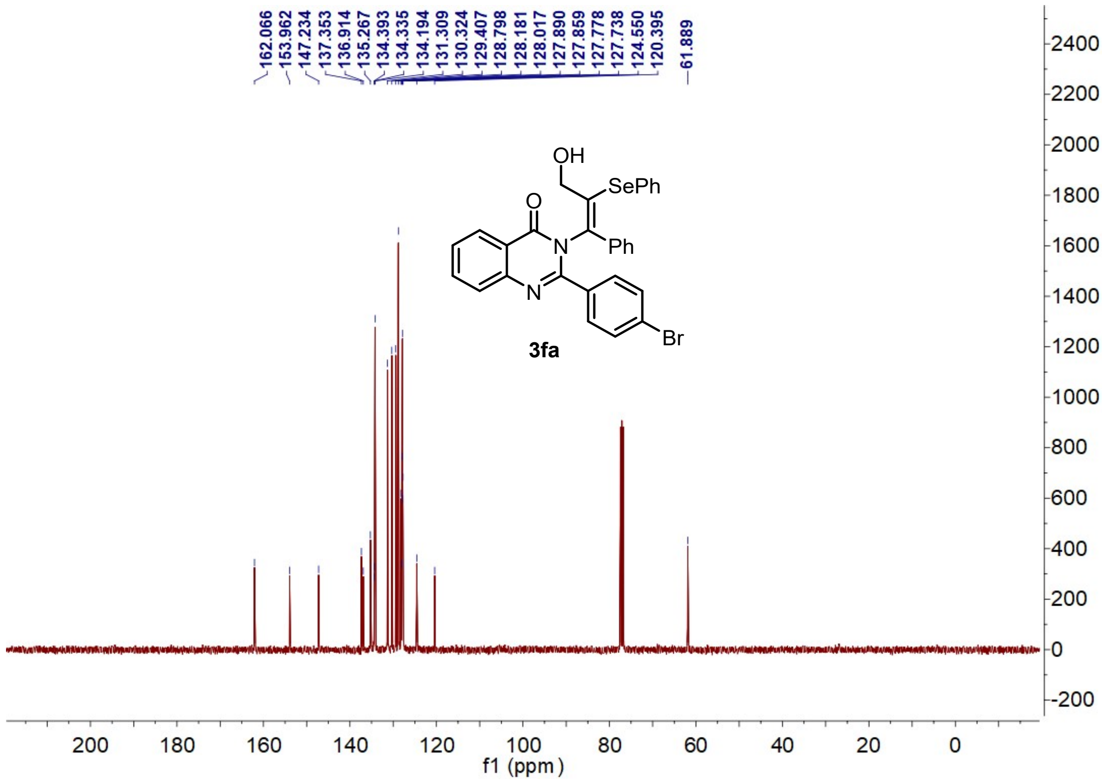
3ea

^{1}H-NMR of **3fa** ($CDCl_3$, 400 Hz)

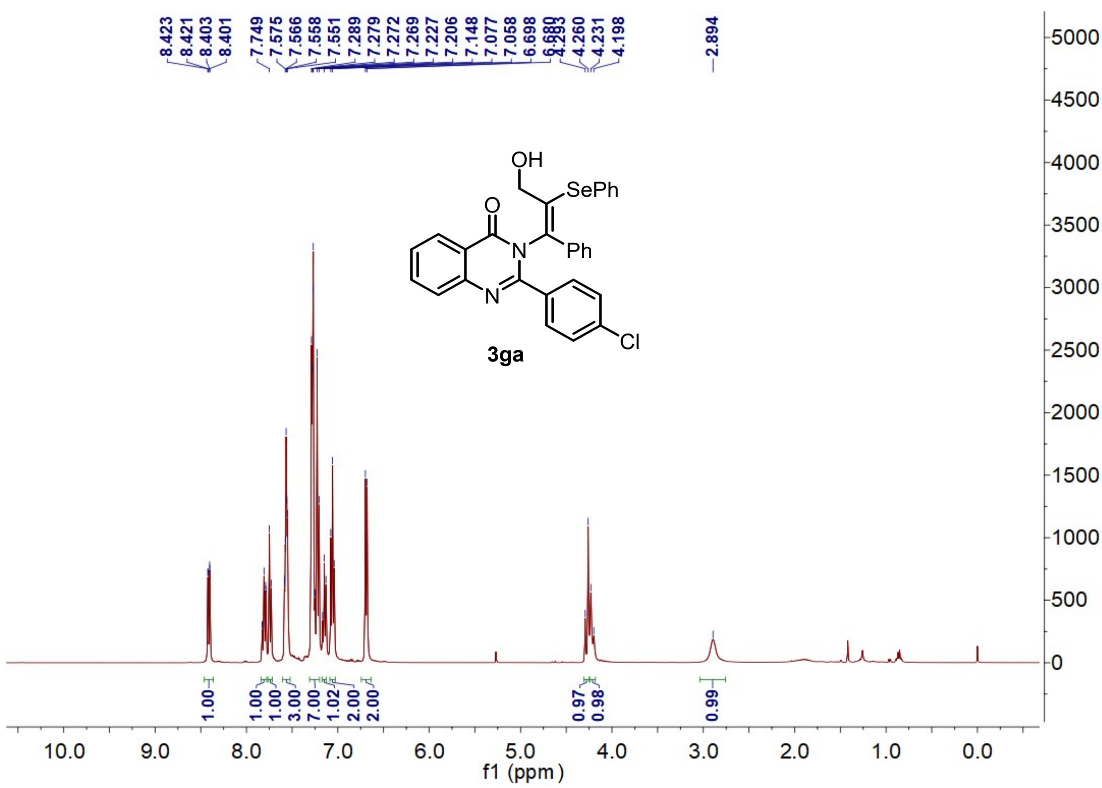


3fa

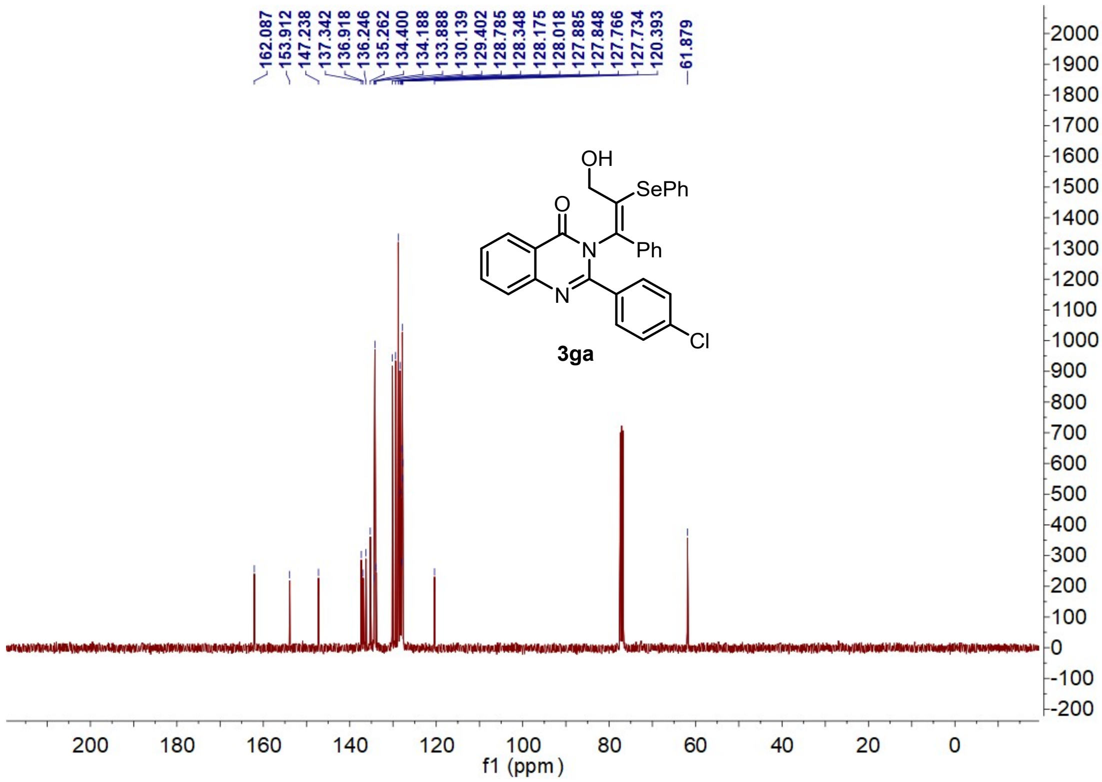
^{13}C-NMR of **3fa** ($CDCl_3$, 100 Hz)



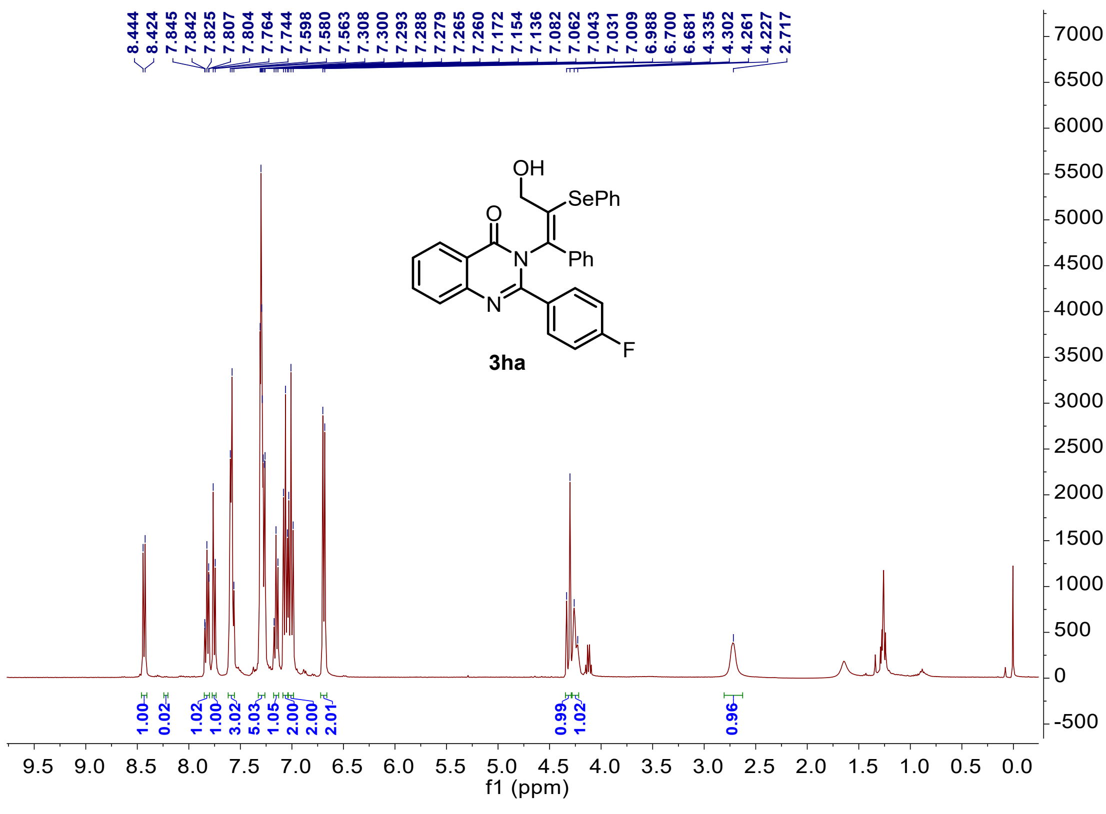
^{1}H-NMR of **3ga** ($CDCl_3$, 400 Hz)



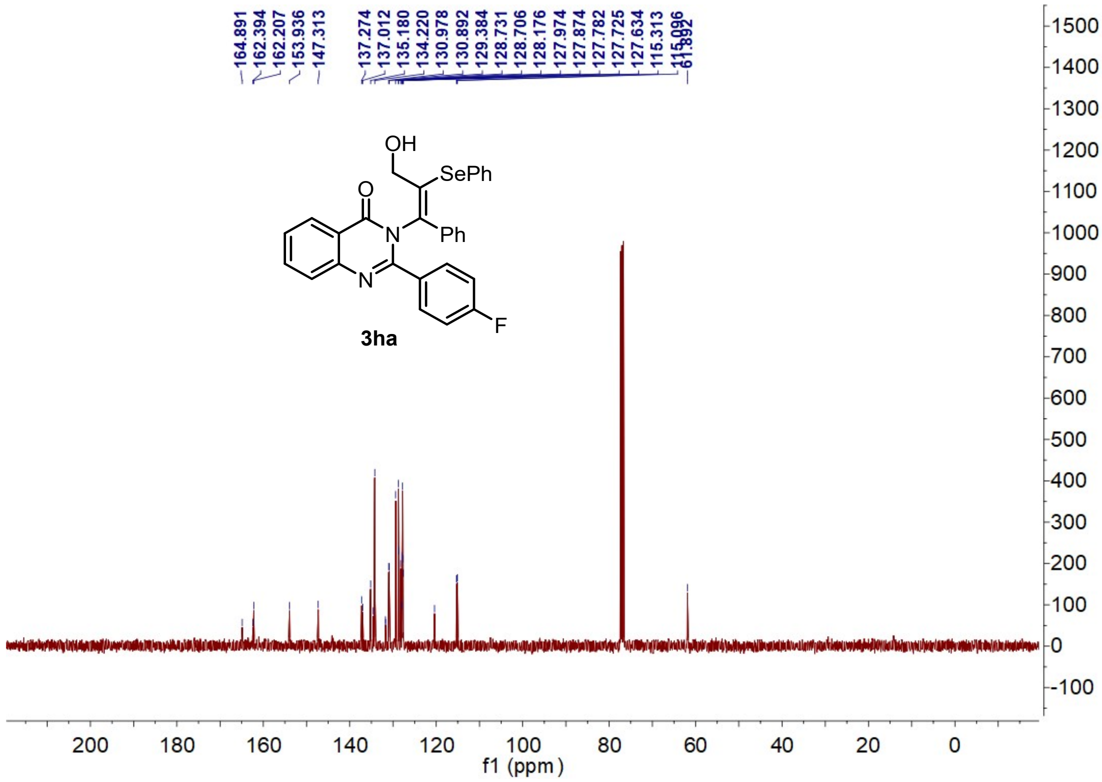
^{13}C-NMR of **3ga** ($CDCl_3$, 100 Hz)



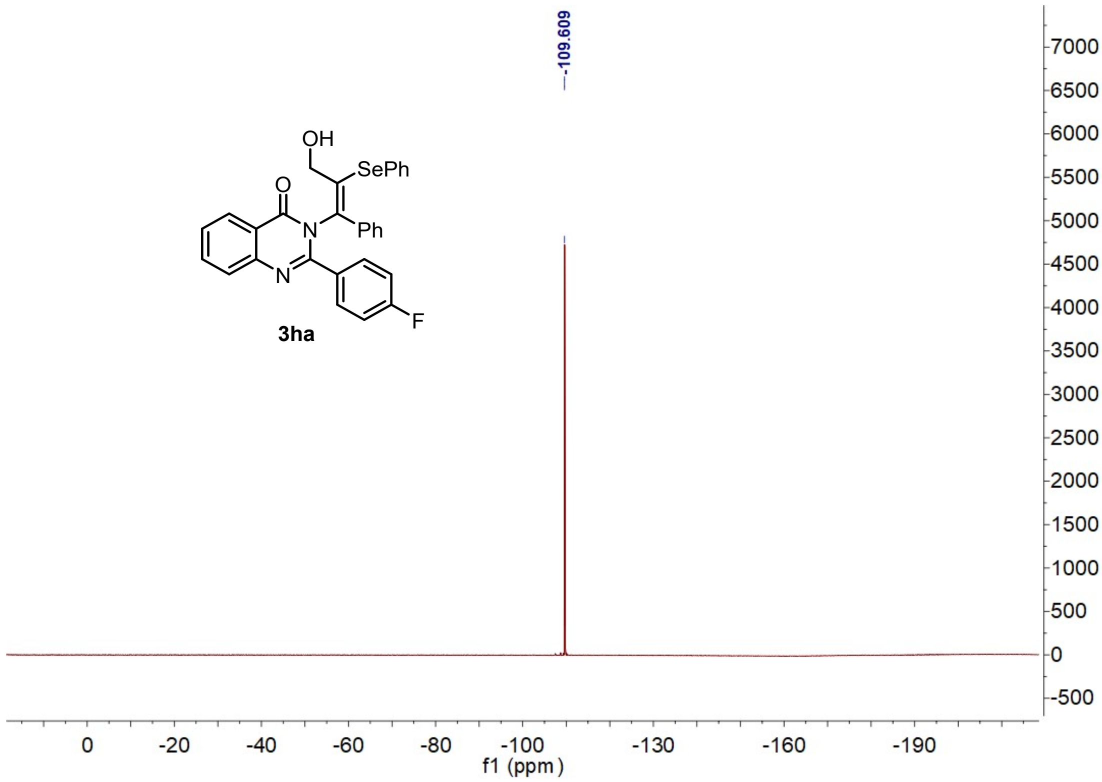
^{1}H-NMR of **3ha** ($CDCl_3$, 400 Hz)



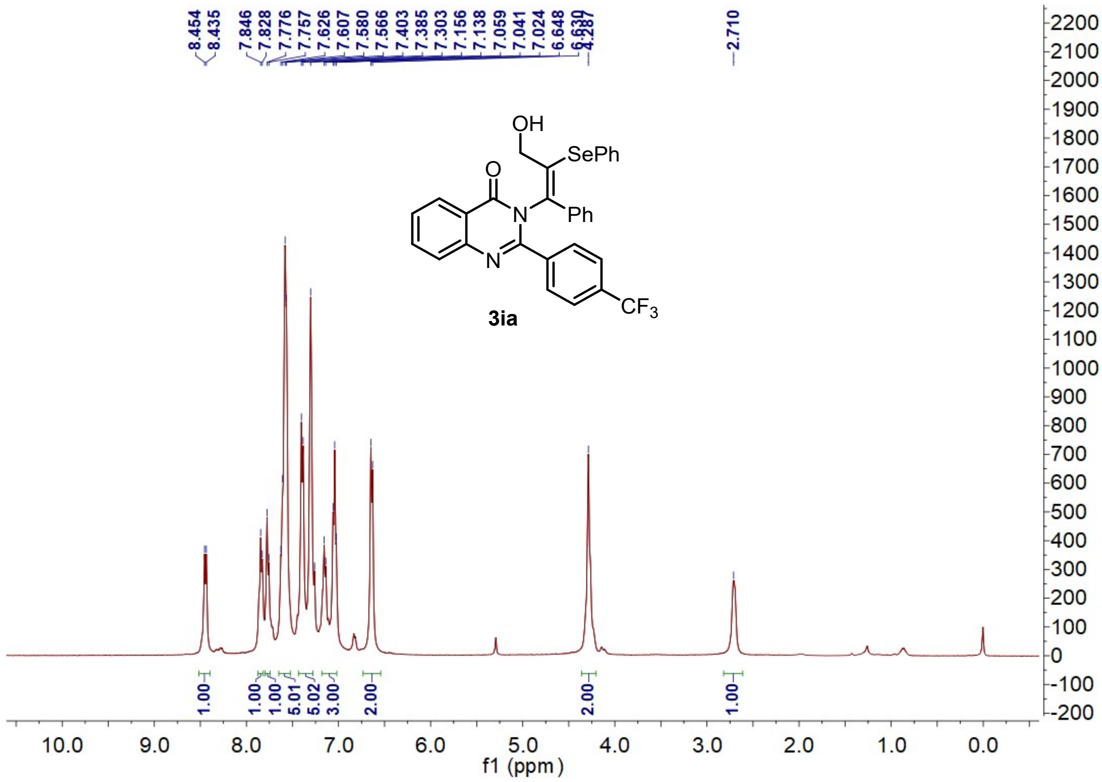
^{13}C-NMR of **3ha** ($CDCl_3$, 100 Hz)



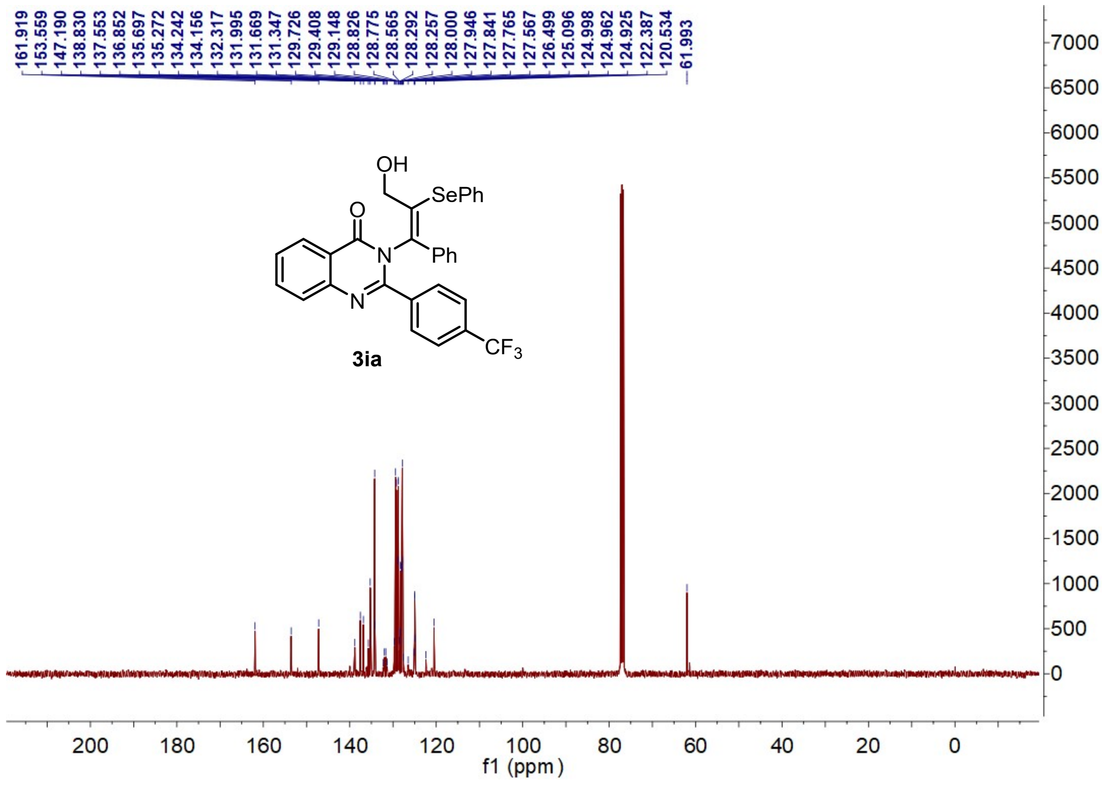
^{19}F-NMR of **3ha** ($CDCl_3$, 376 Hz)



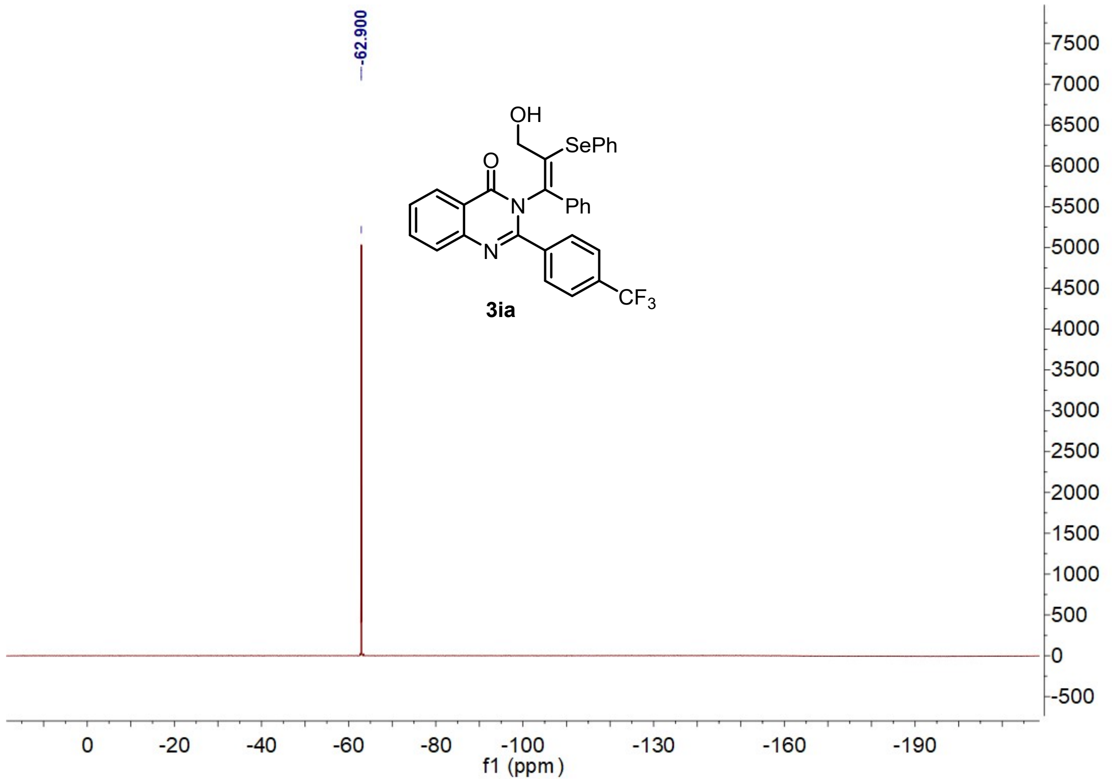
^{1}H-NMR of **3ia** ($CDCl_3$, 400 Hz)



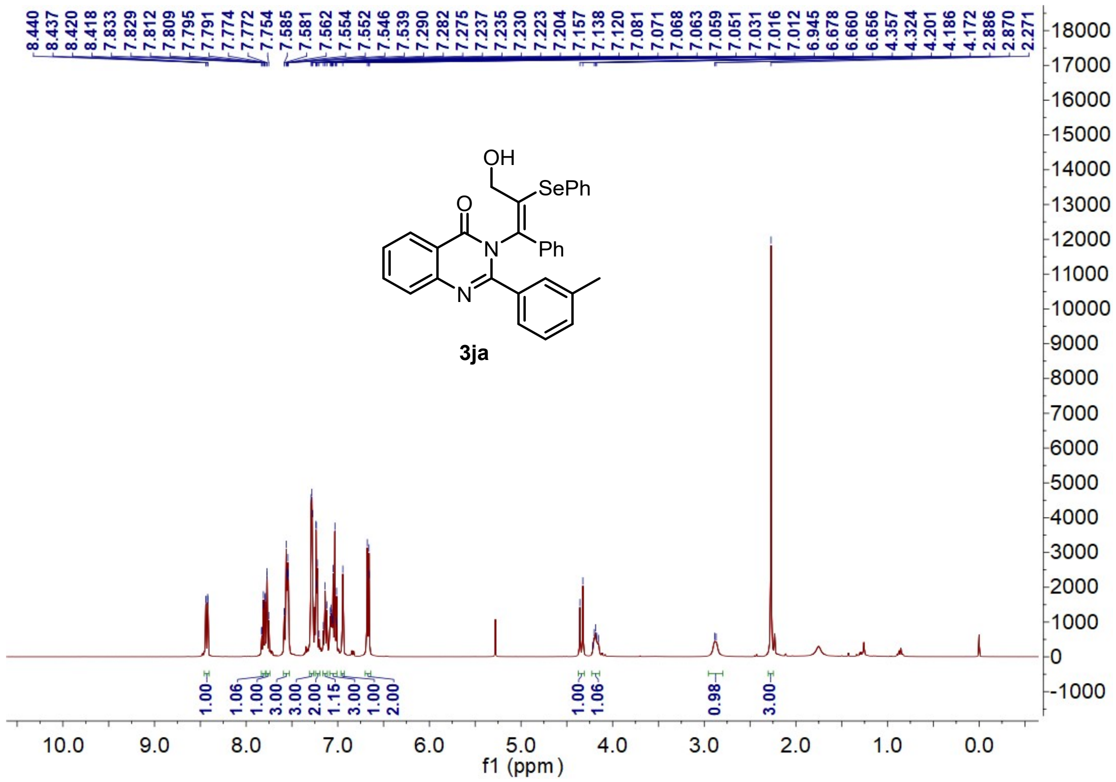
^{13}C-NMR of **3ia** ($CDCl_3$, 100 Hz)



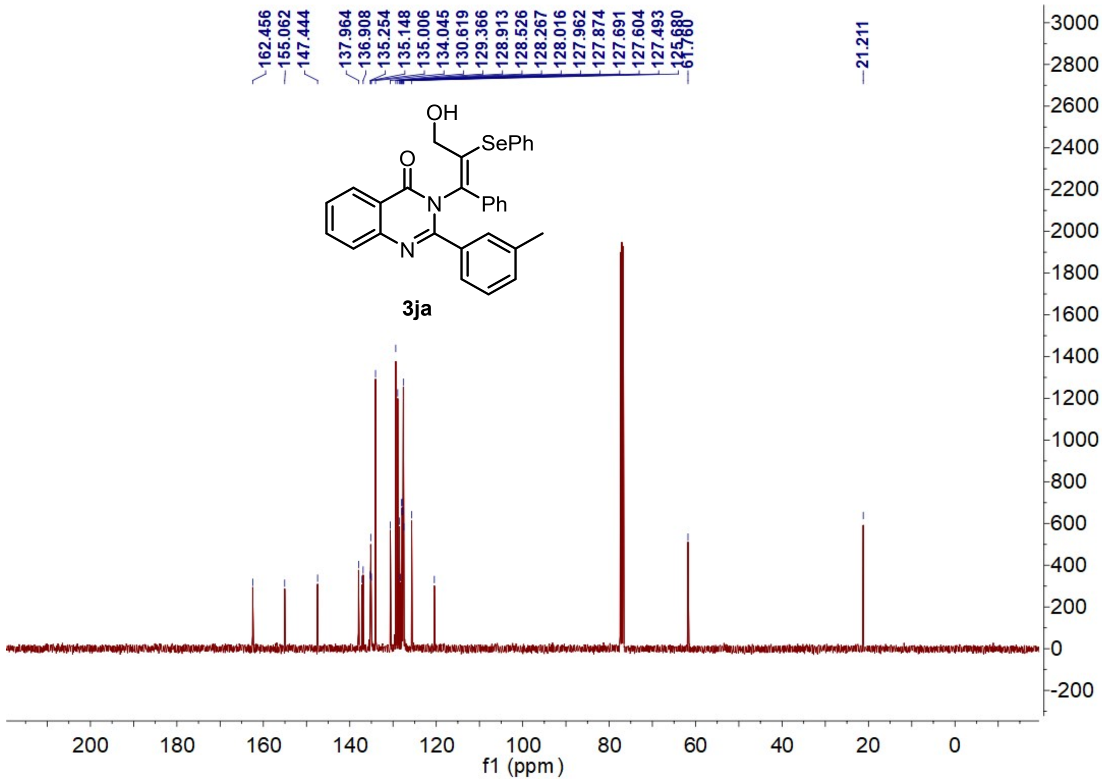
[19]F-NMR of **3ia** ($CDCl_3$, 376 Hz)



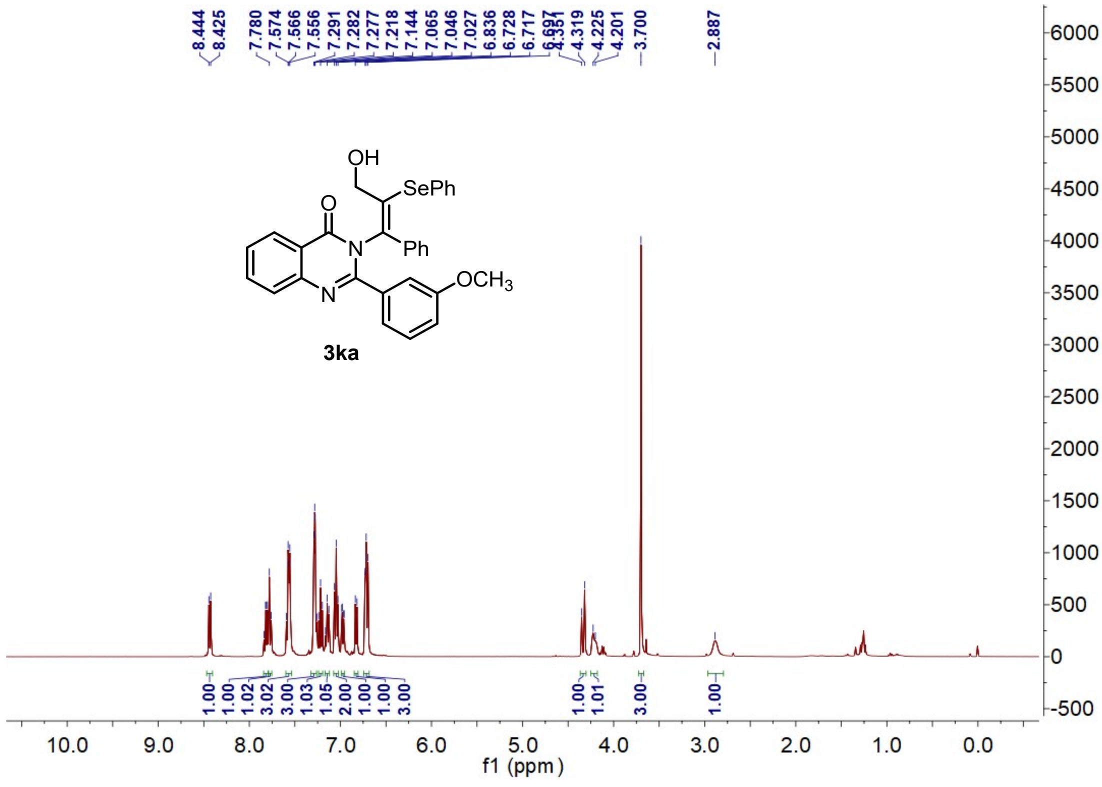
[1]H-NMR of **3ja** ($CDCl_3$, 400 Hz)



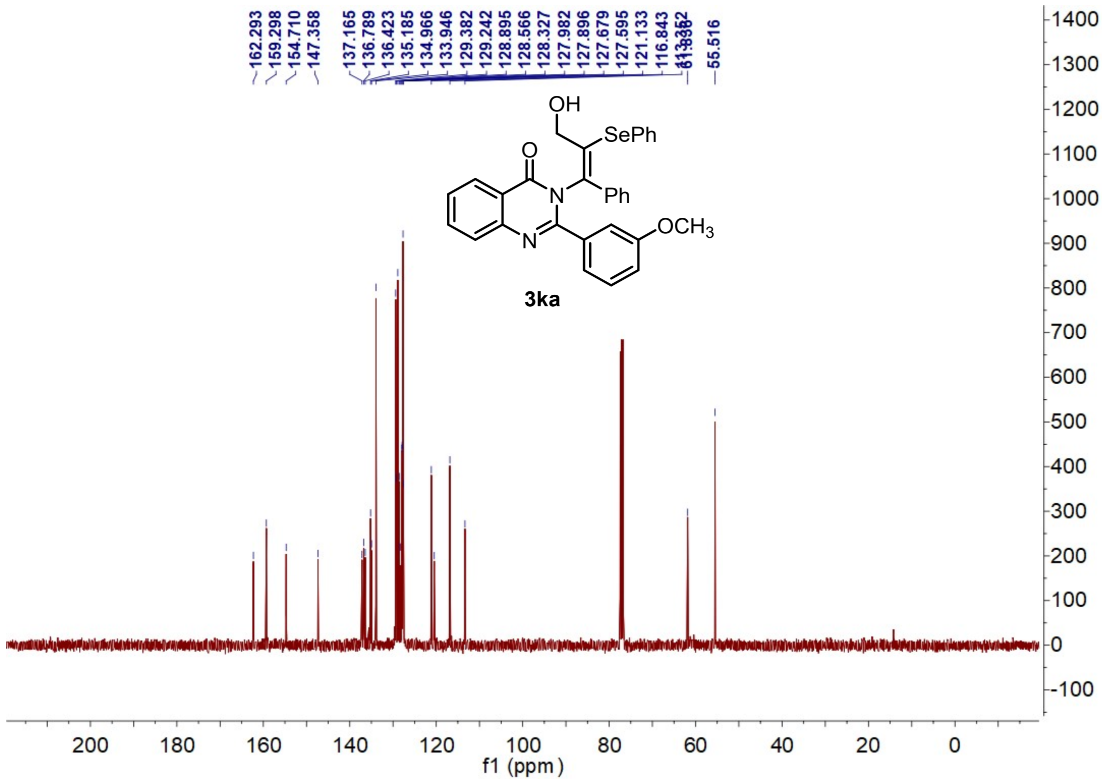
^{13}C-NMR of **3ja** ($CDCl_3$, 100 Hz)



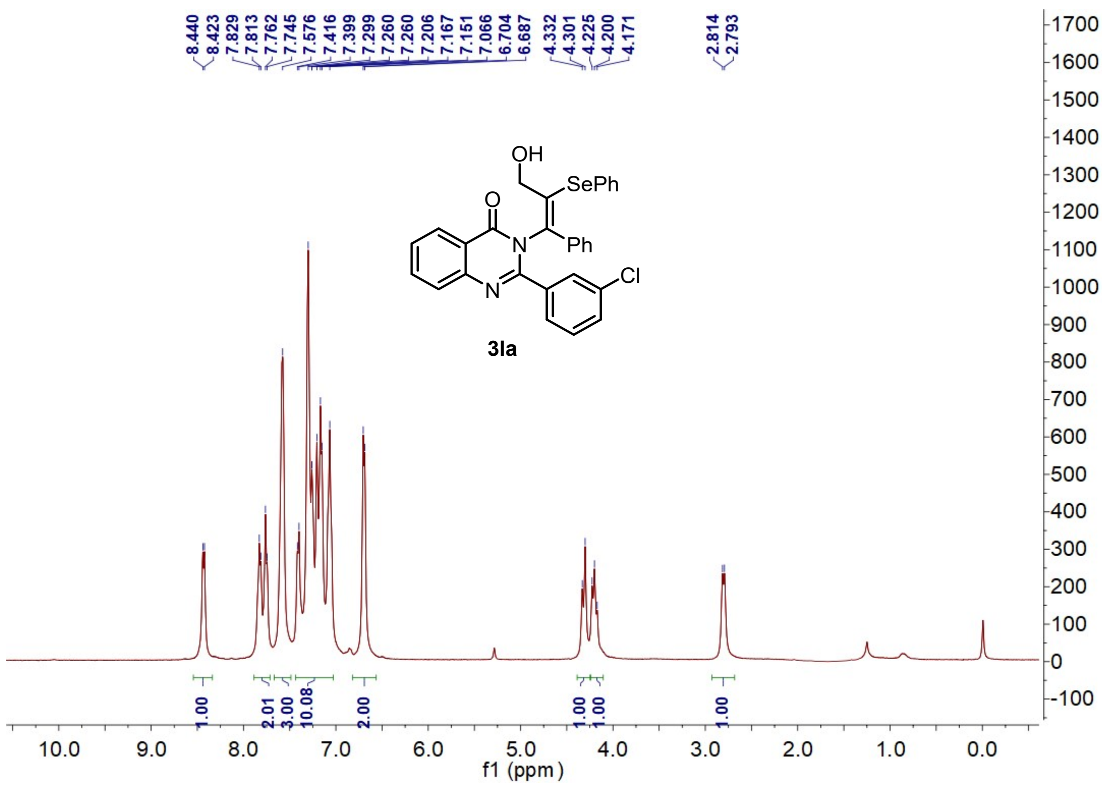
^{1}H-NMR of **3ka** ($CDCl_3$, 400 Hz)



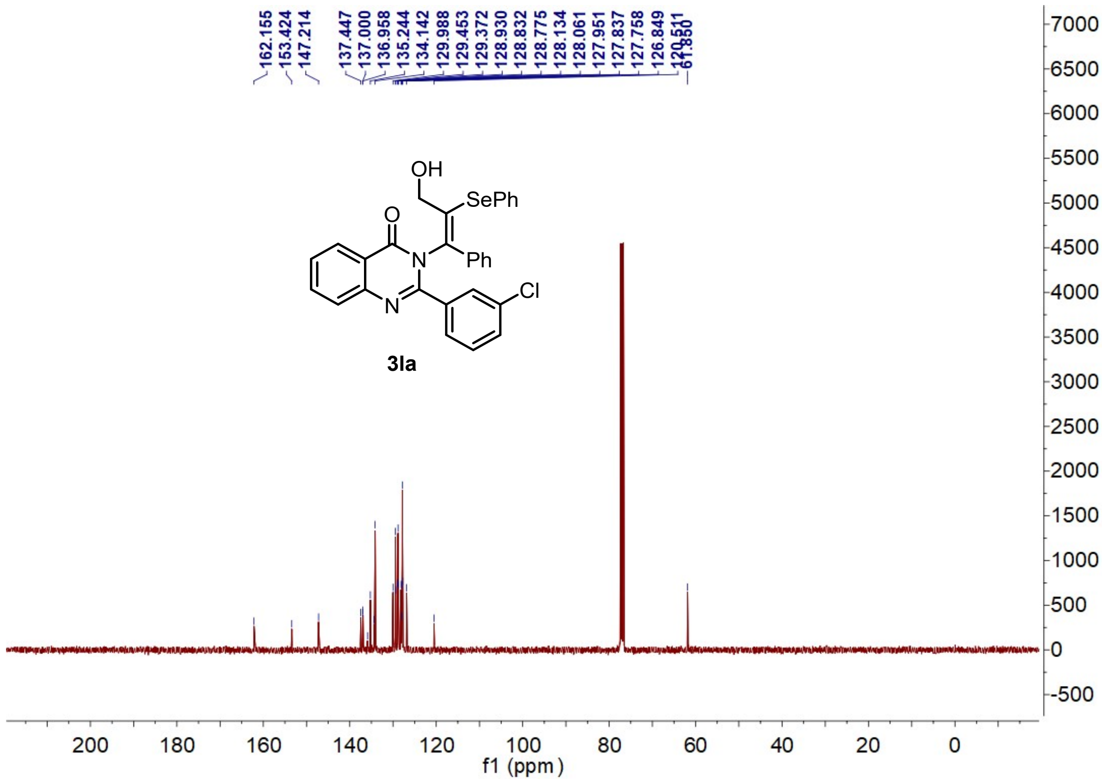
^{13}C-NMR of **3ka** ($CDCl_3$, 100 Hz)



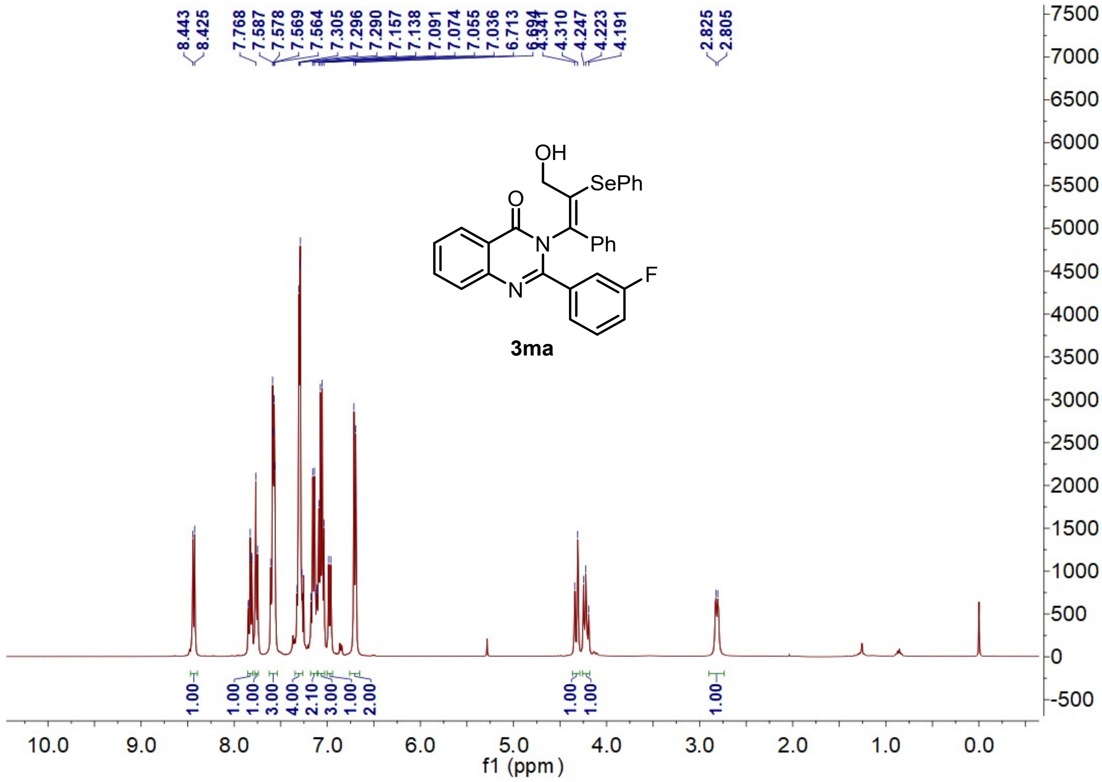
^{1}H-NMR of **3la** ($CDCl_3$, 400 Hz)



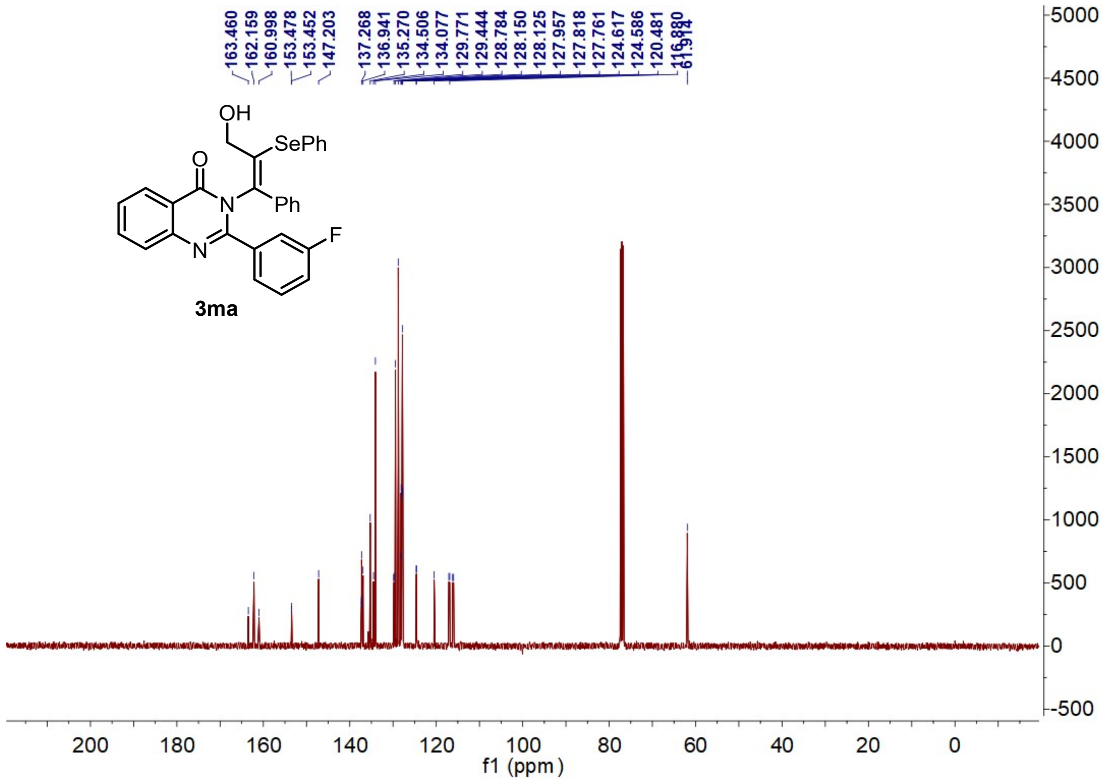
^{13}C-NMR of **3la** ($CDCl_3$, 100 Hz)



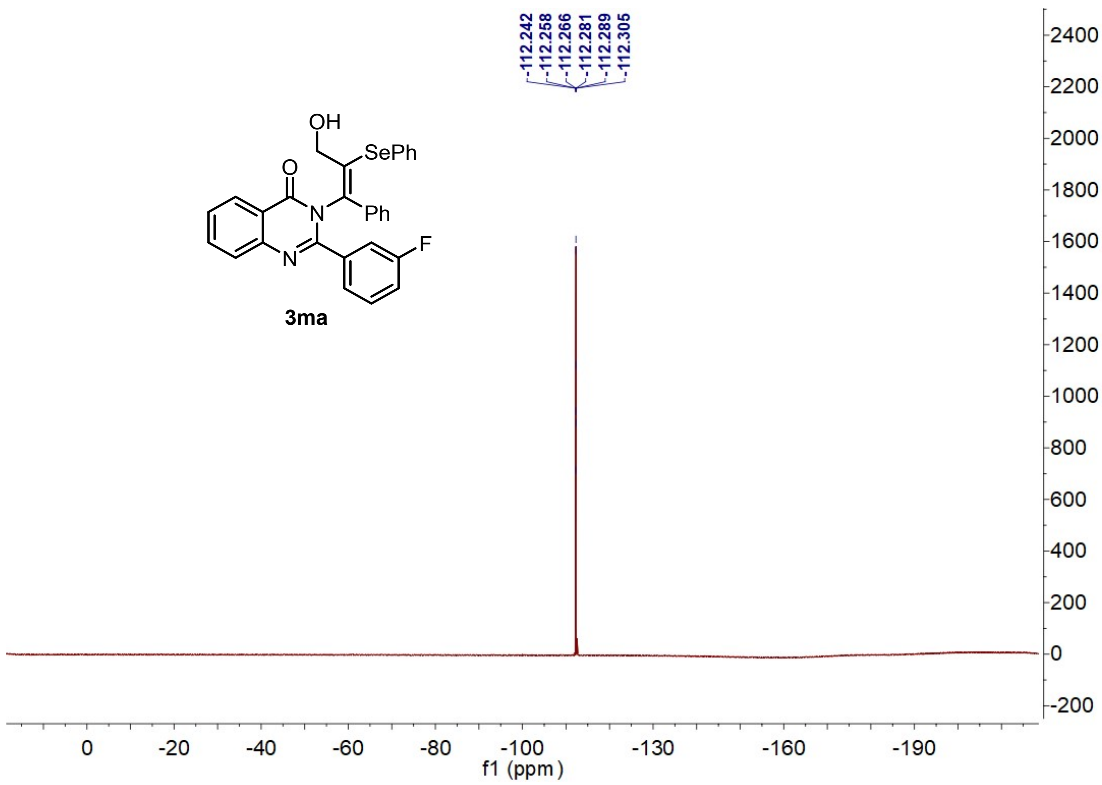
^{1}H-NMR of **3ma** ($CDCl_3$, 400 Hz)



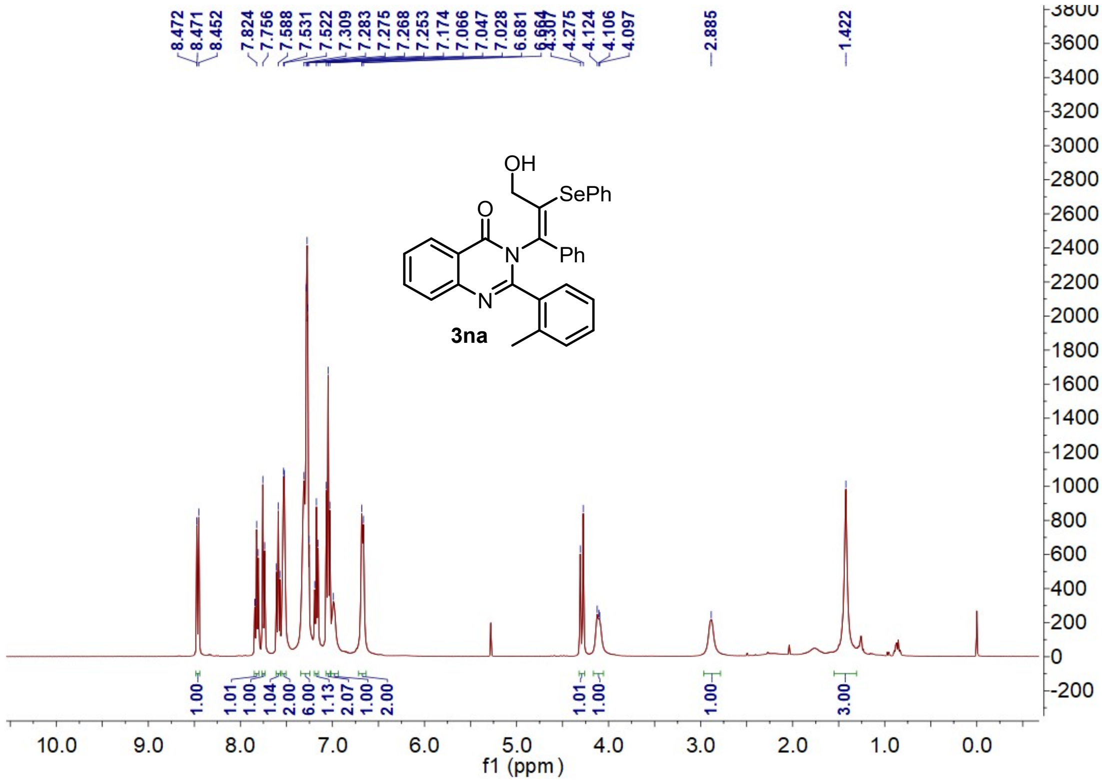
^{13}C-NMR of **3ma** ($CDCl_3$, 100 Hz)



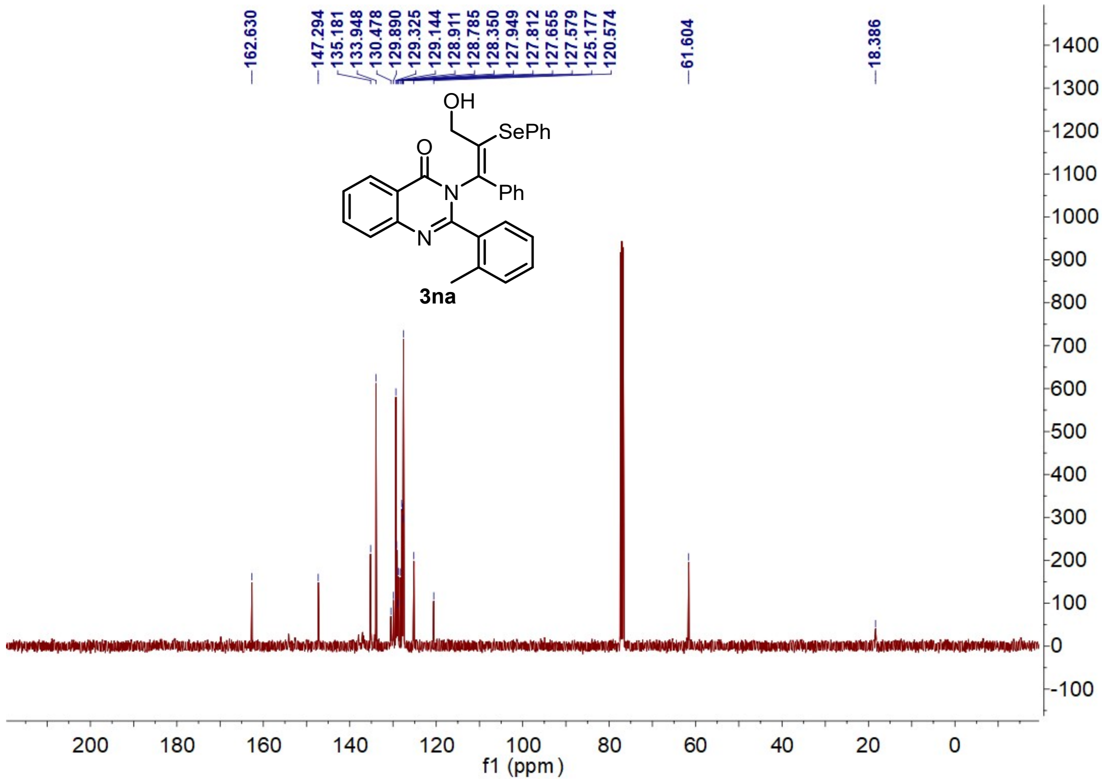
^{19}F-NMR of **3ma** ($CDCl_3$, 376 Hz)



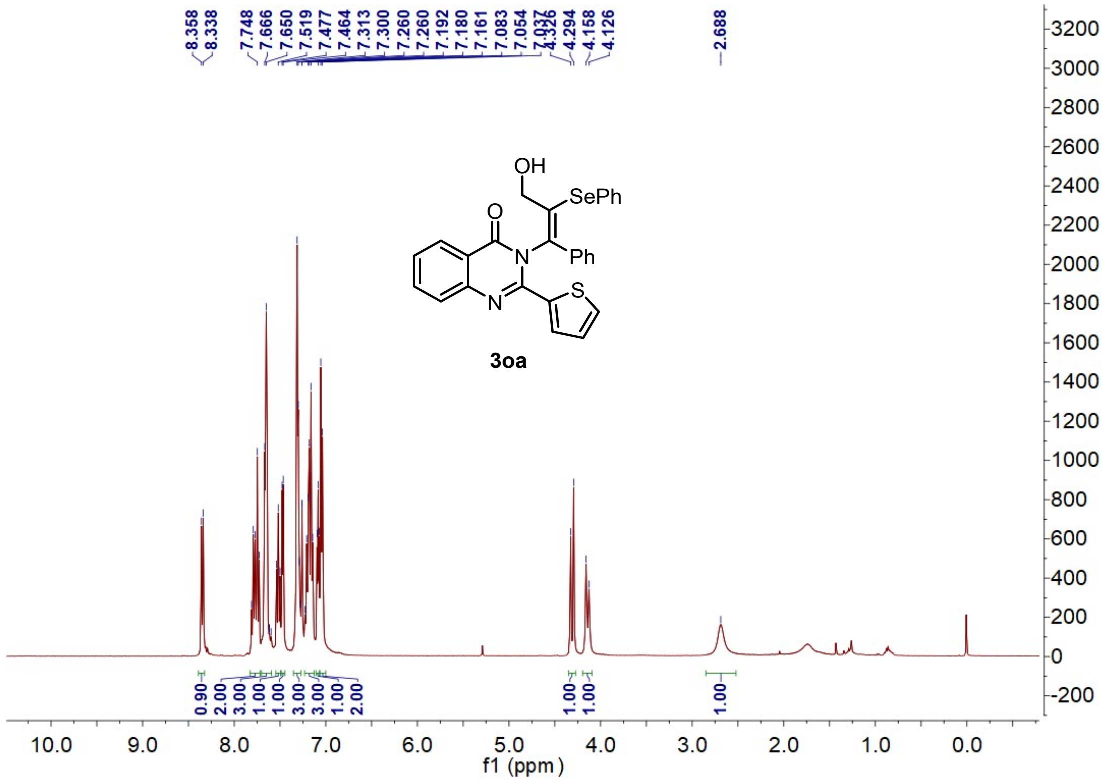
^{1}H-NMR of **3na** ($CDCl_3$, 400 Hz)



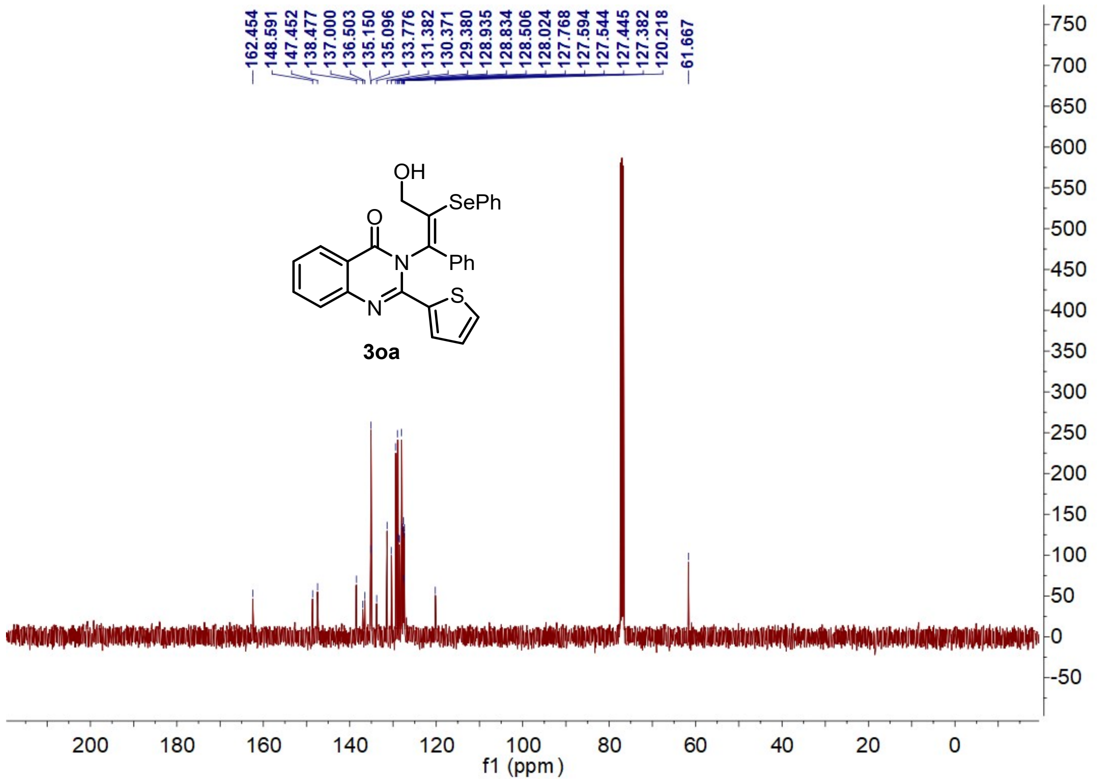
^{13}C-NMR of **3na** ($CDCl_3$, 100 Hz)



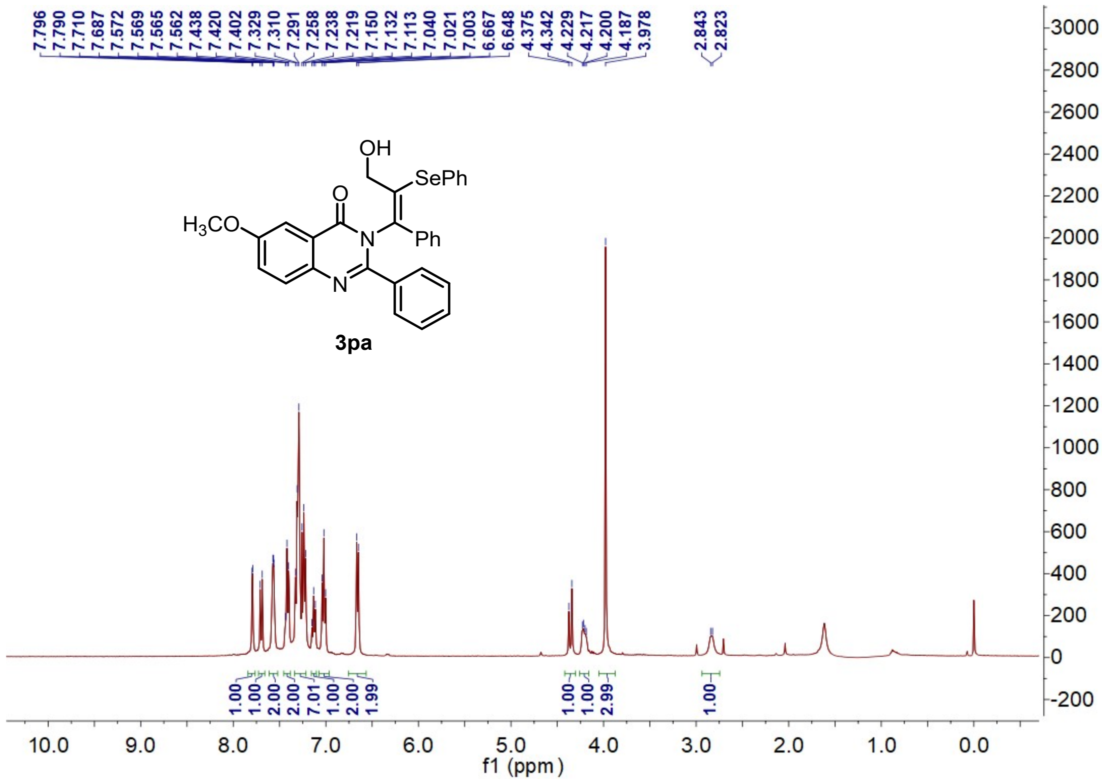
^{1}H-NMR of **3oa** ($CDCl_3$, 400 Hz)



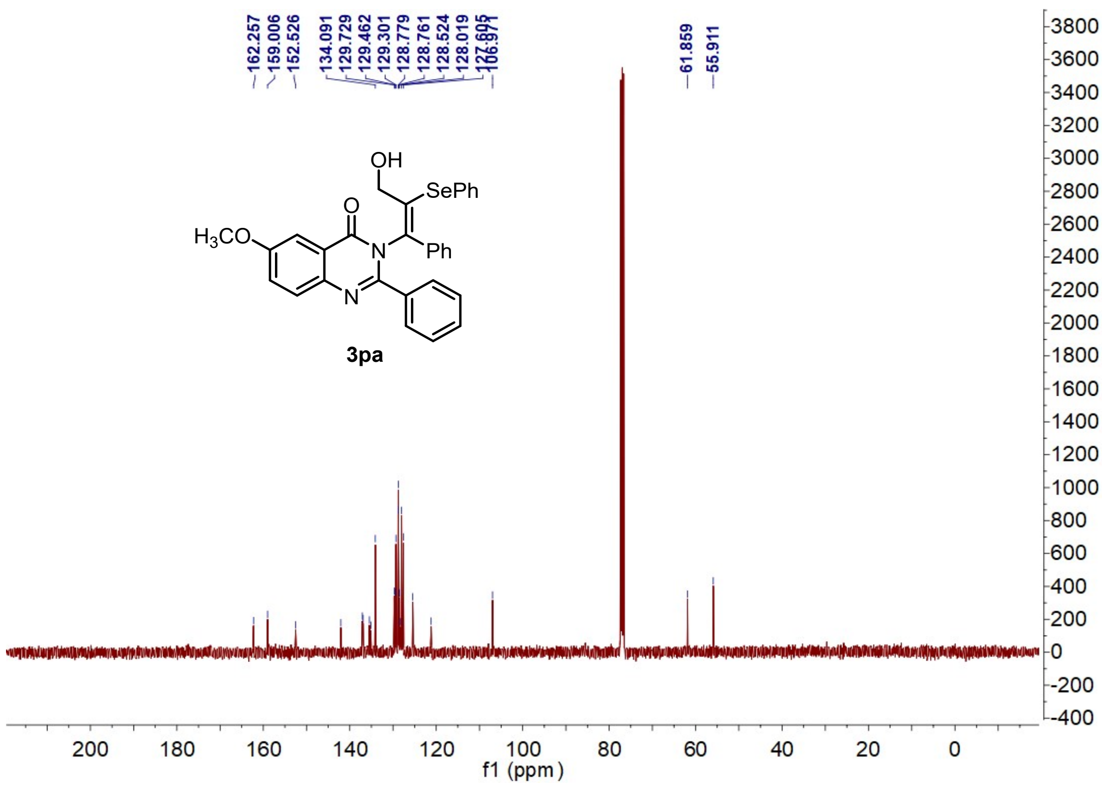
^{13}C-NMR of **3oa** (CDCl$_3$, 100 Hz)



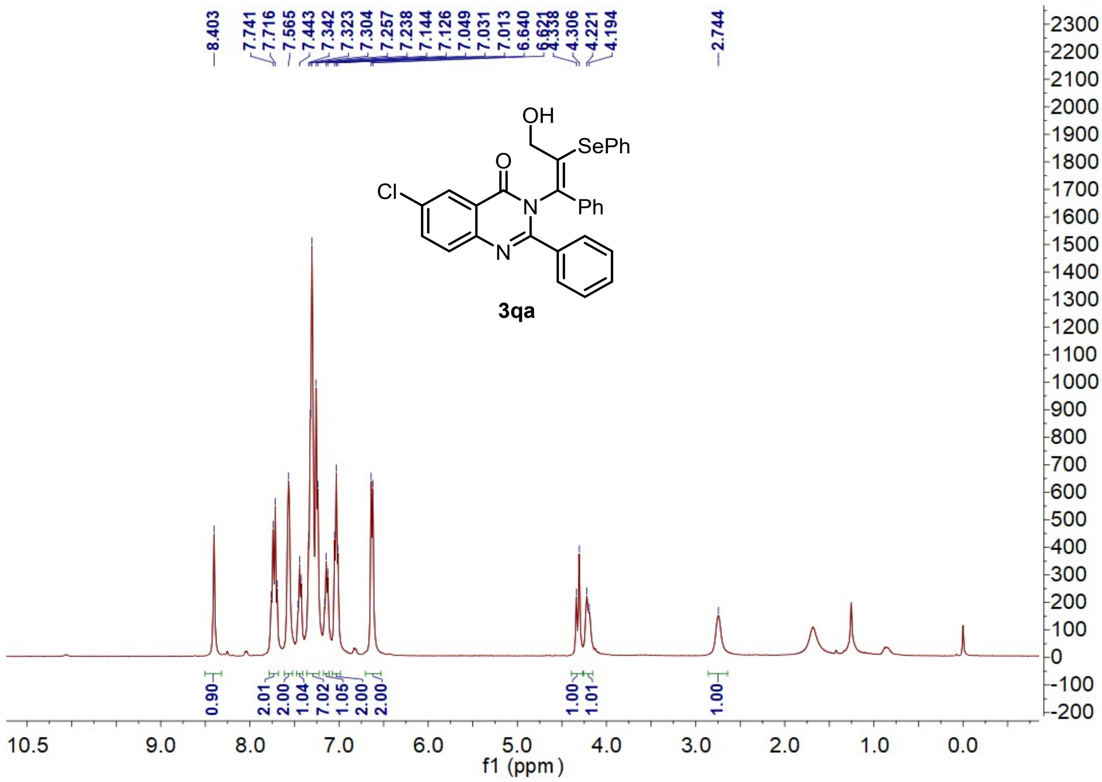
^{1}H-NMR of **3pa** (CDCl$_3$, 400 Hz)



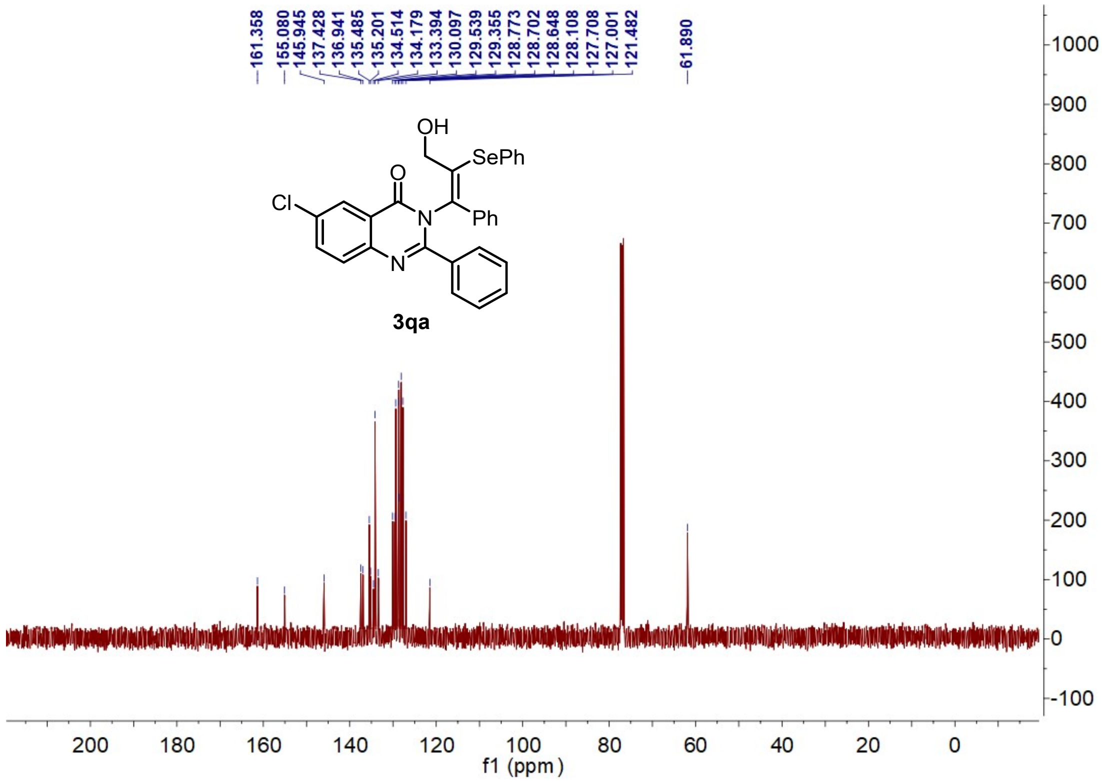
^{13}C-NMR of **3pa** ($CDCl_3$, 100 Hz)



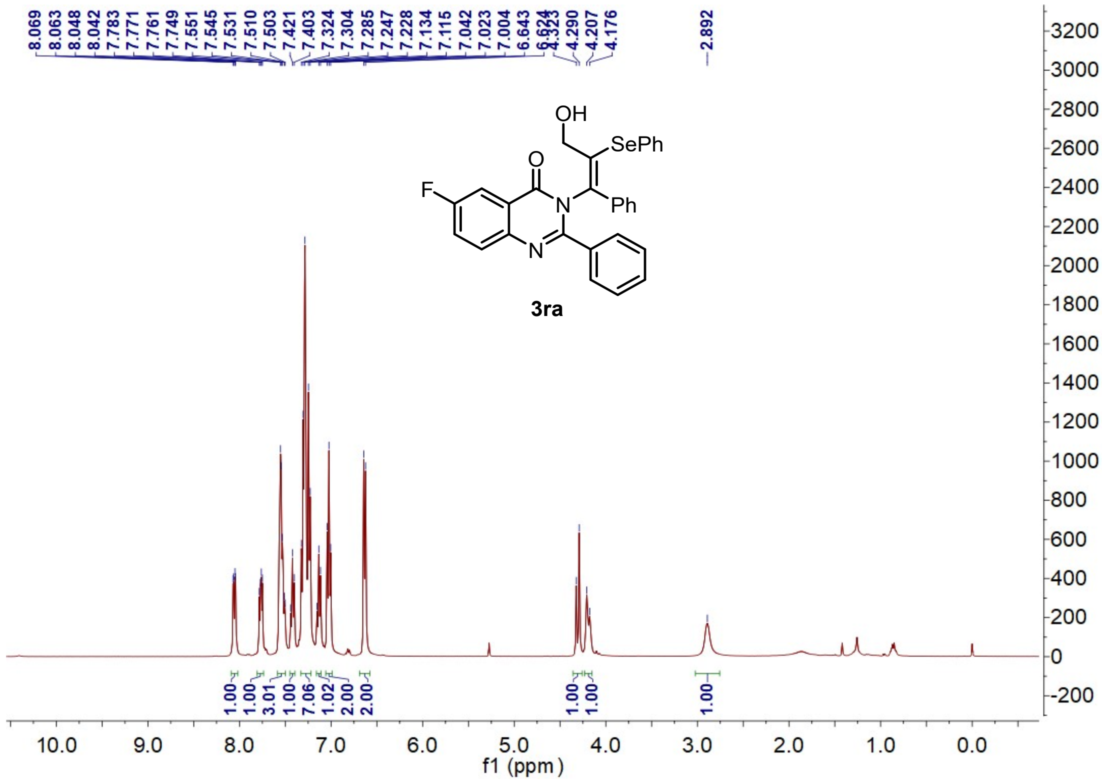
^{1}H-NMR of **3qa** ($CDCl_3$, 400 Hz)



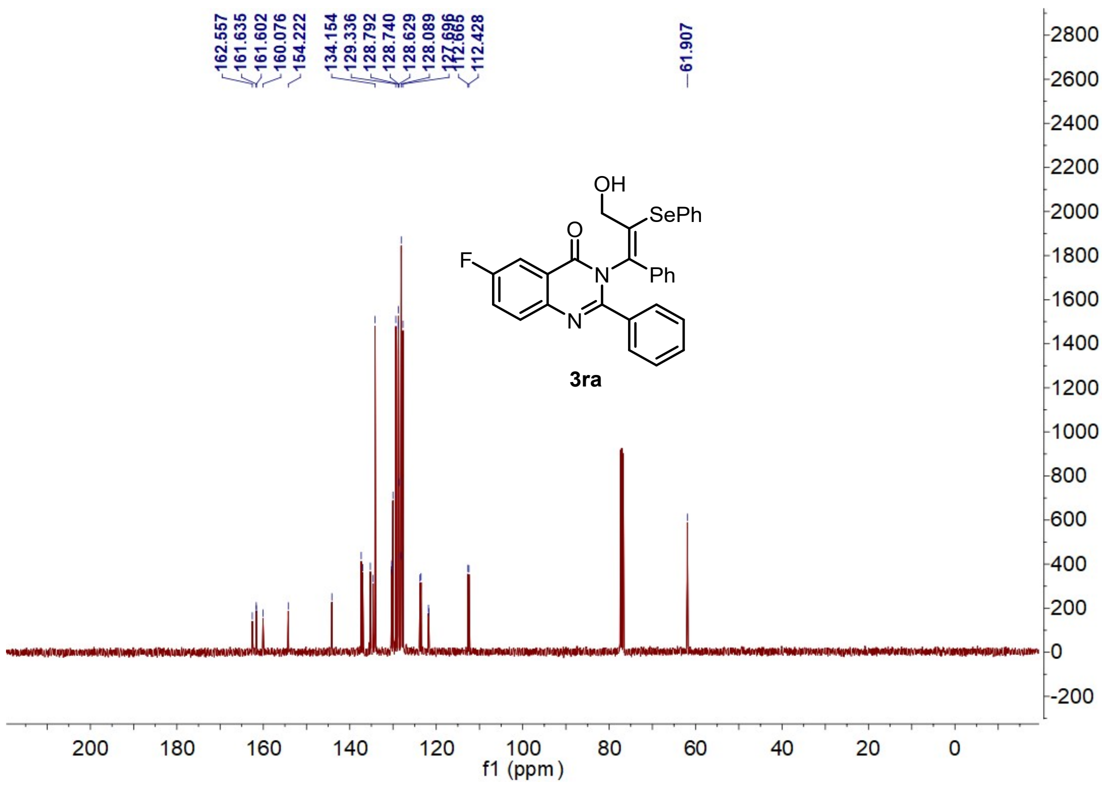
^{13}C-NMR of **3qa** ($CDCl_3$, 100 Hz)



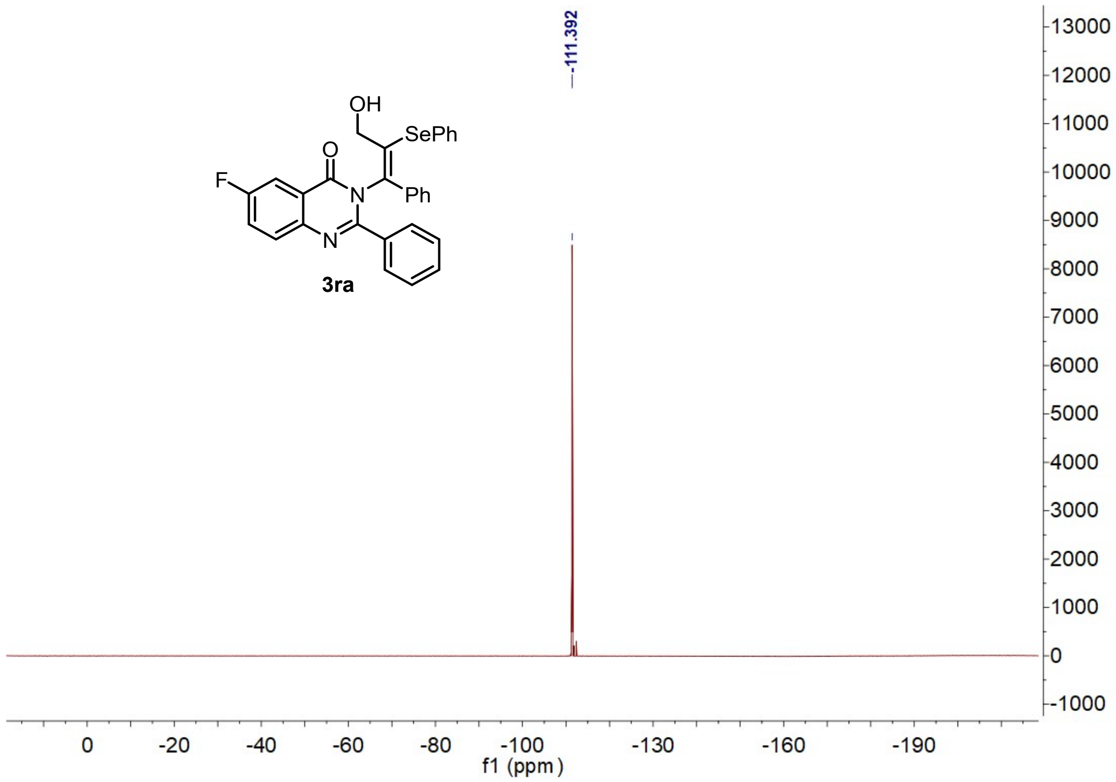
^{1}H-NMR of **3ra** ($CDCl_3$, 400 Hz)



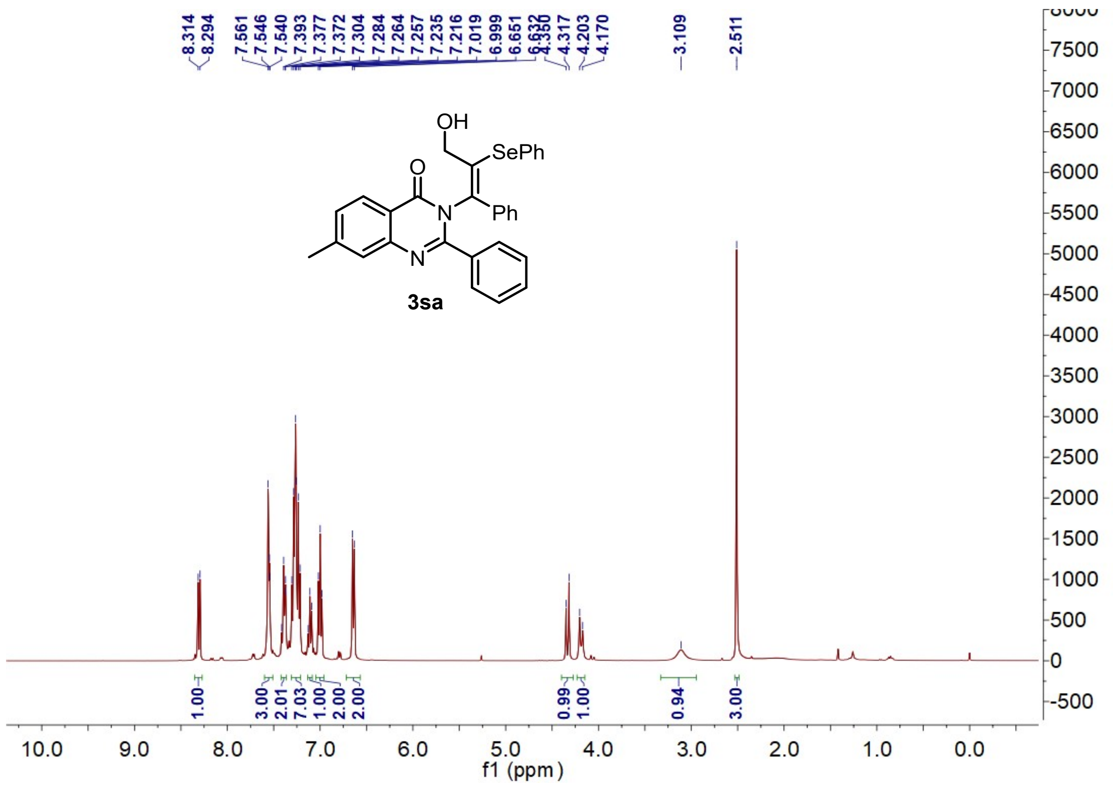
^{13}C-NMR of **3ra** ($CDCl_3$, 100 Hz)



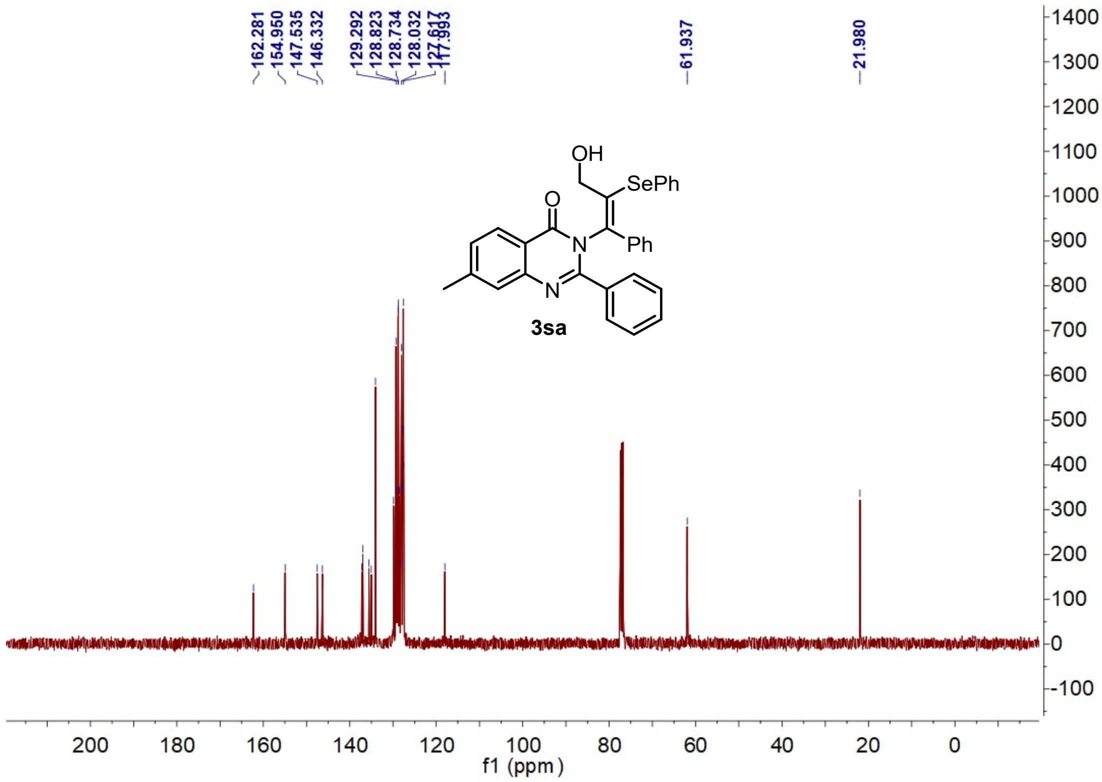
^{19}F-NMR of **3ra** ($CDCl_3$, 376 Hz)



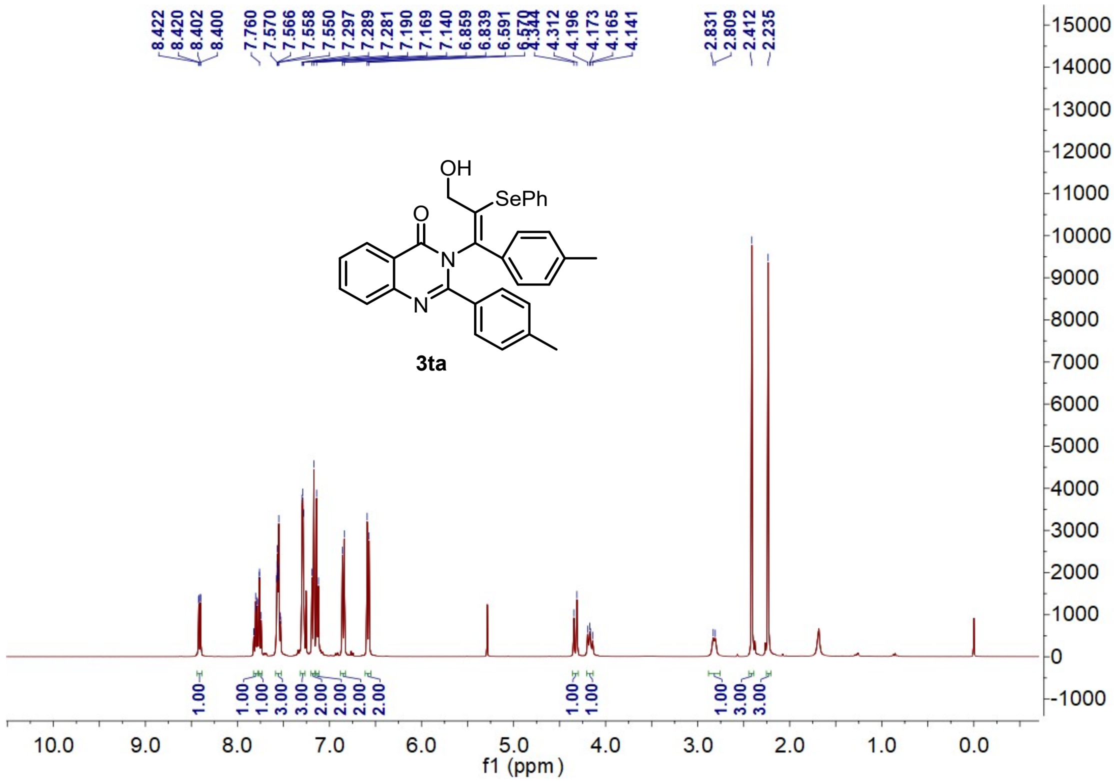
^{1}H-NMR of **3sa** ($CDCl_3$, 400 Hz)



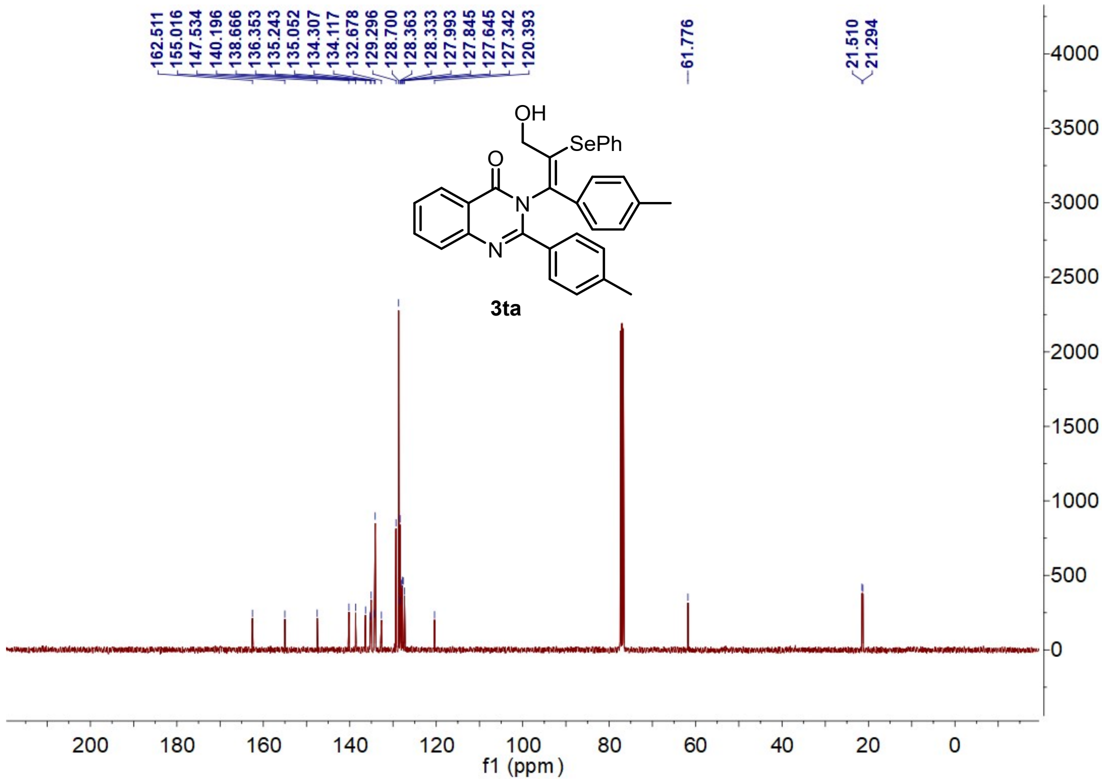
^{13}C-NMR of **3sa** ($CDCl_3$, 100 Hz)



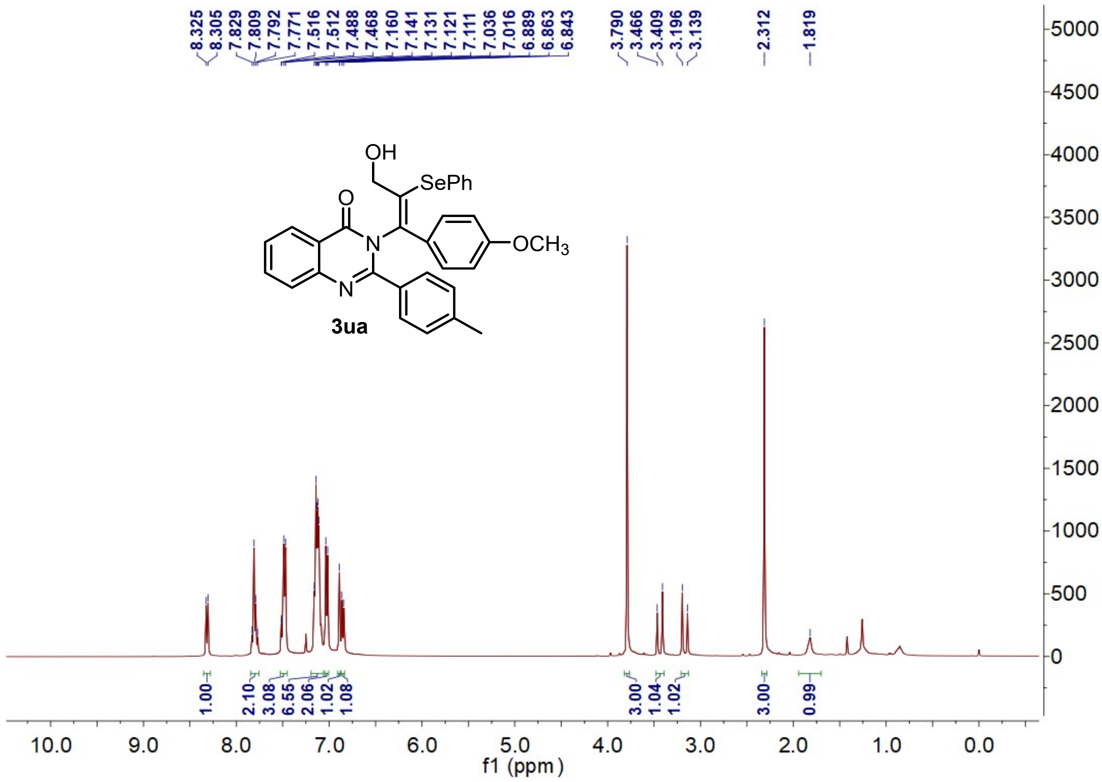
^{1}H-NMR of **3ta** ($CDCl_3$, 400 Hz)



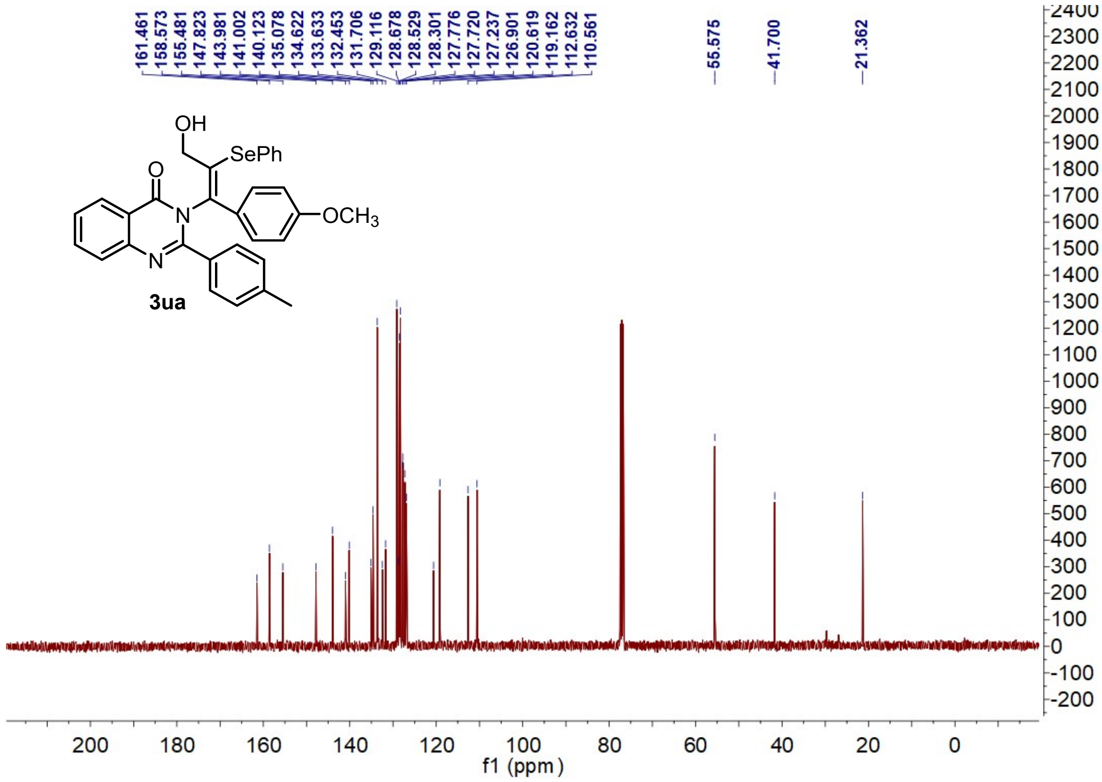
^{13}C-NMR of **3ta** ($CDCl_3$, 100 Hz)



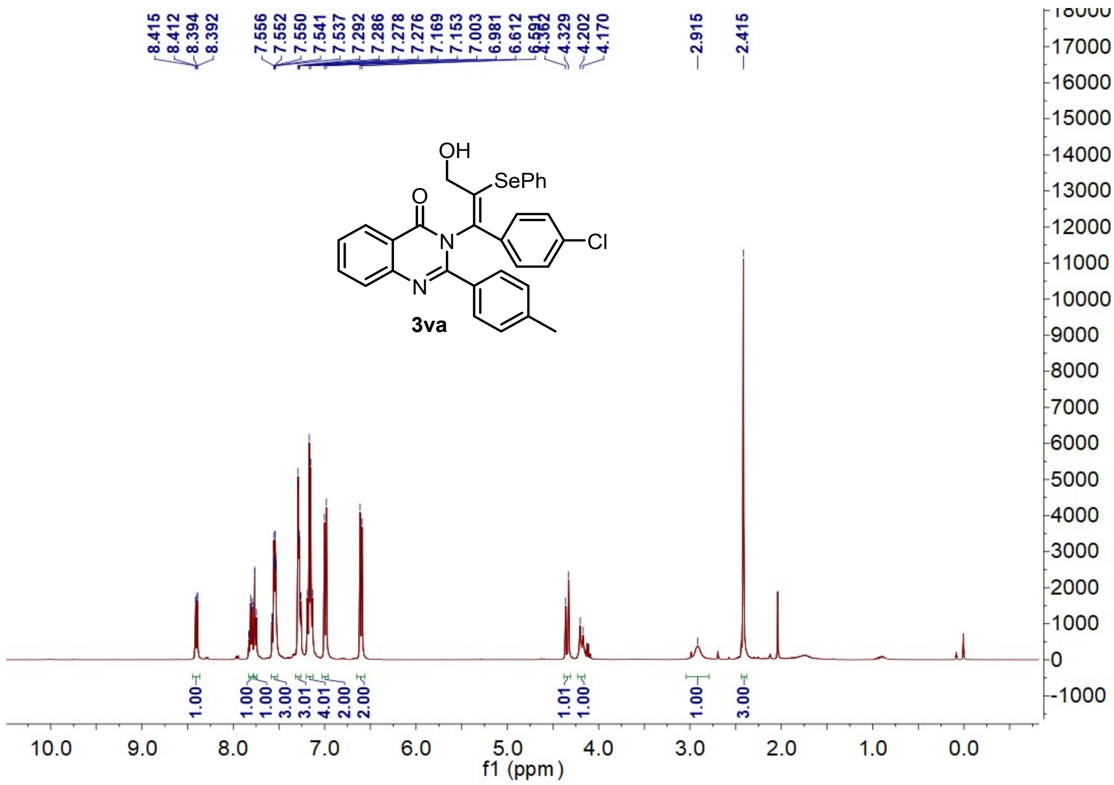
^{1}H-NMR of **3ua** ($CDCl_3$, 400 Hz)



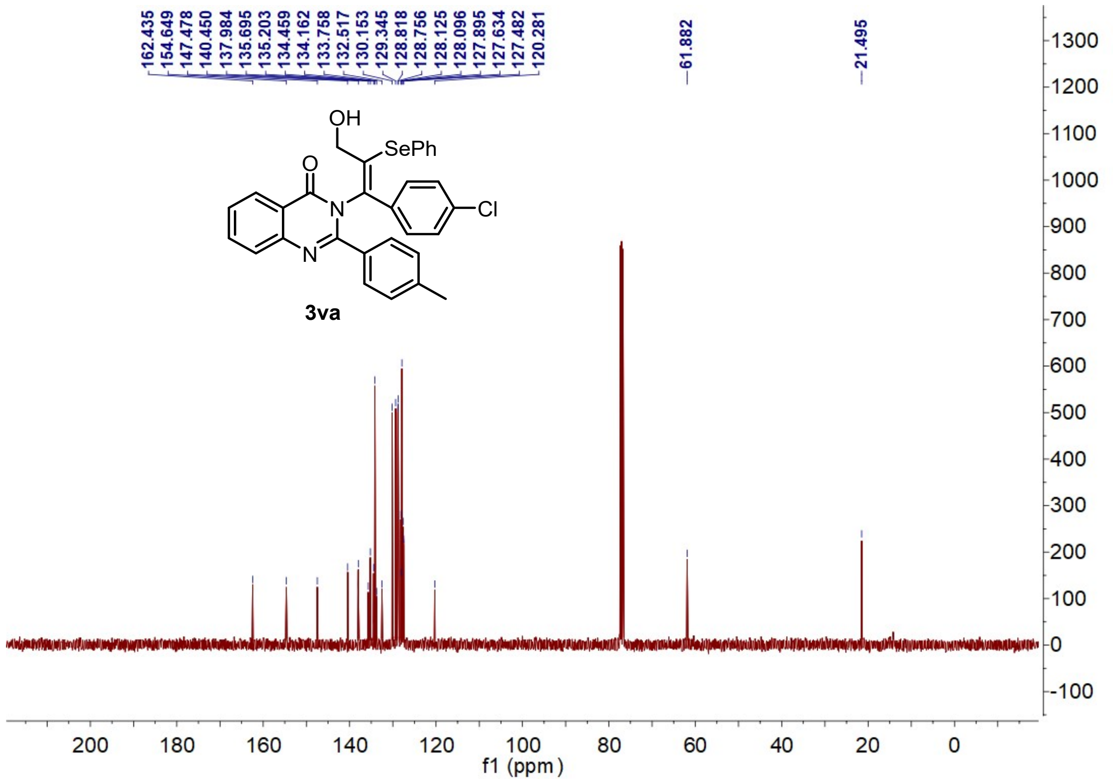
^{13}C-NMR of **3ua** ($CDCl_3$, 100 Hz)



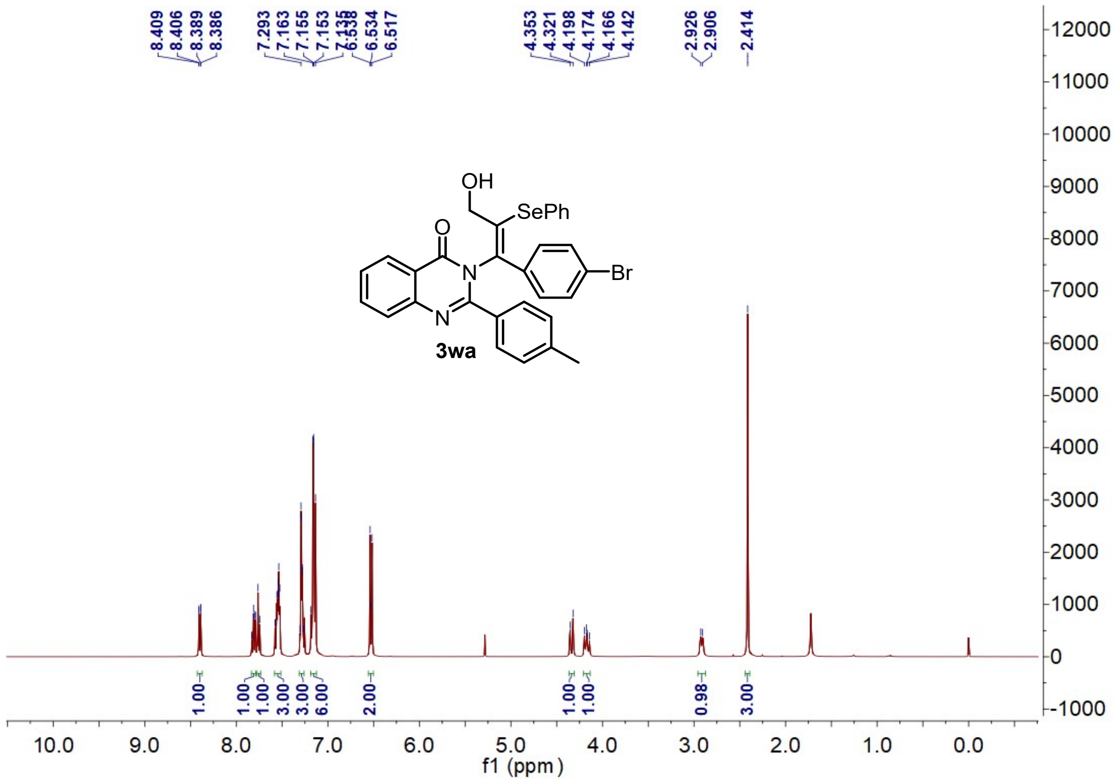
^{1}H-NMR of **3va** ($CDCl_3$, 400 Hz)



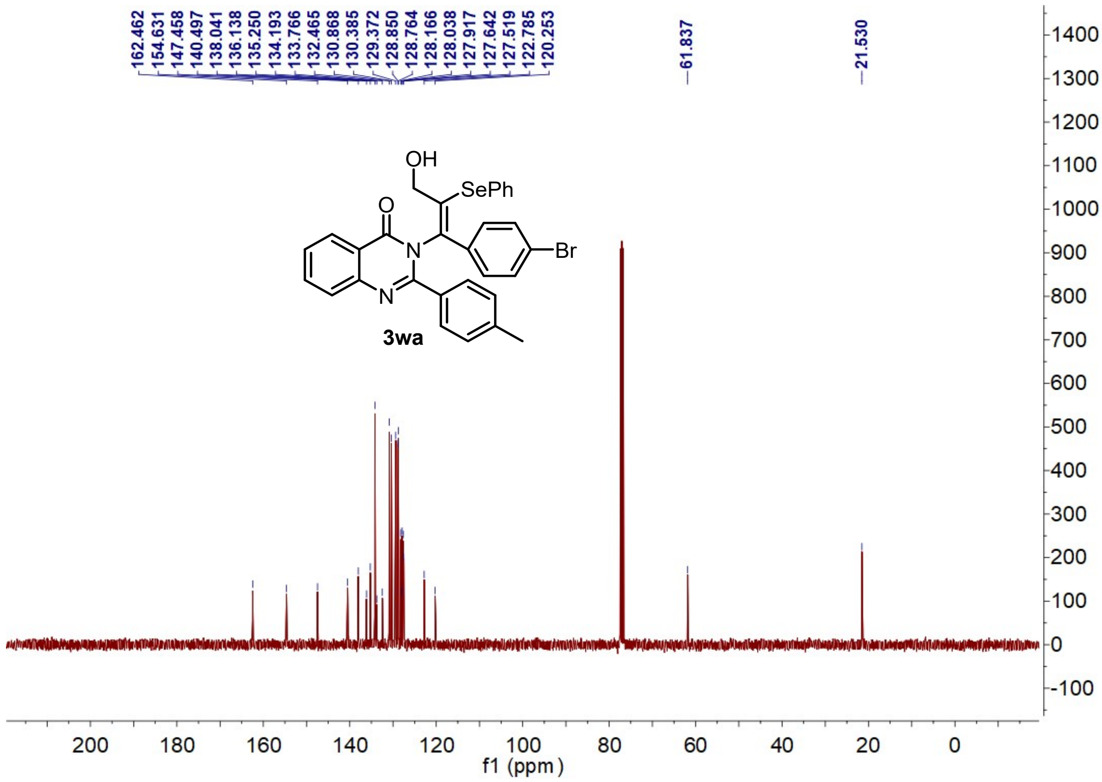
^{13}C-NMR of **3va** ($CDCl_3$, 100 Hz)



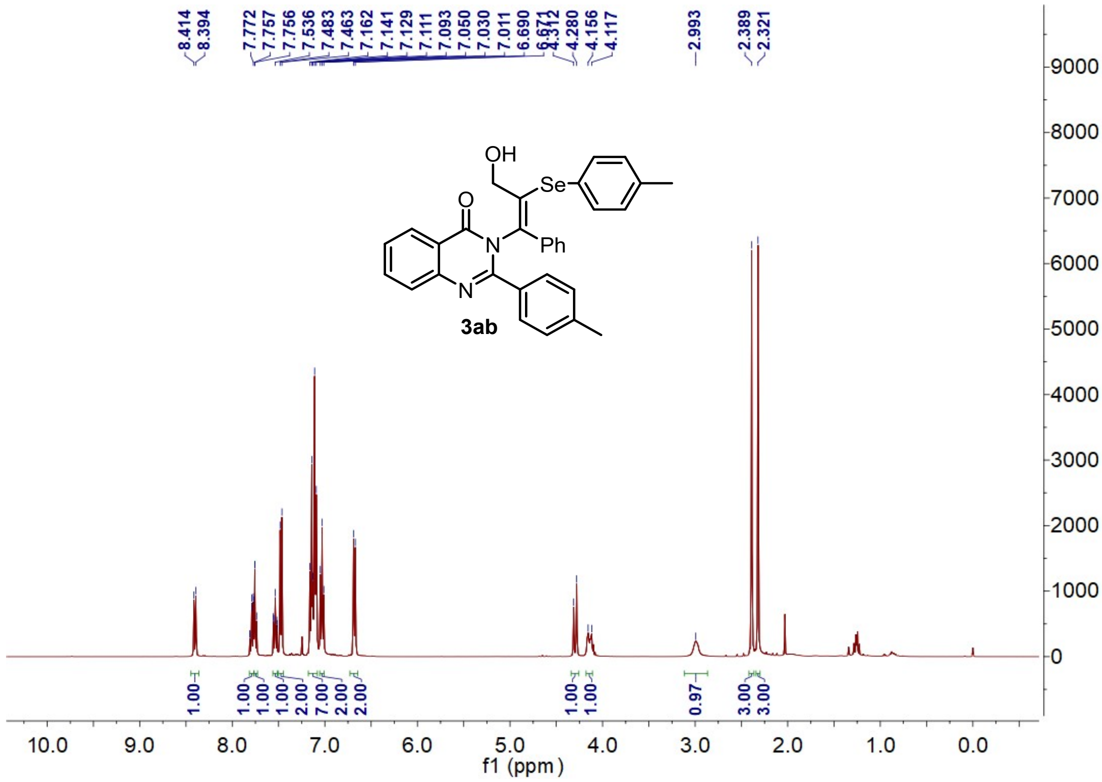
^{1}H-NMR of **3wa** ($CDCl_3$, 400 Hz)



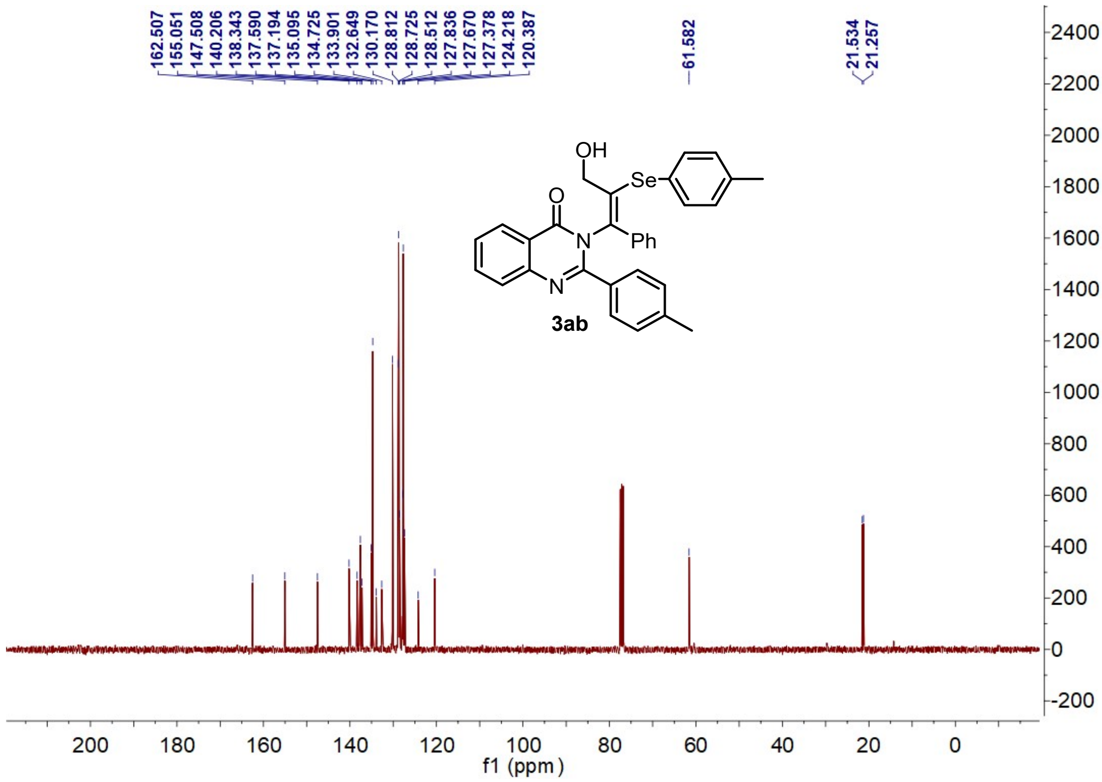
^{13}C-NMR of **3wa** ($CDCl_3$, 100 Hz)



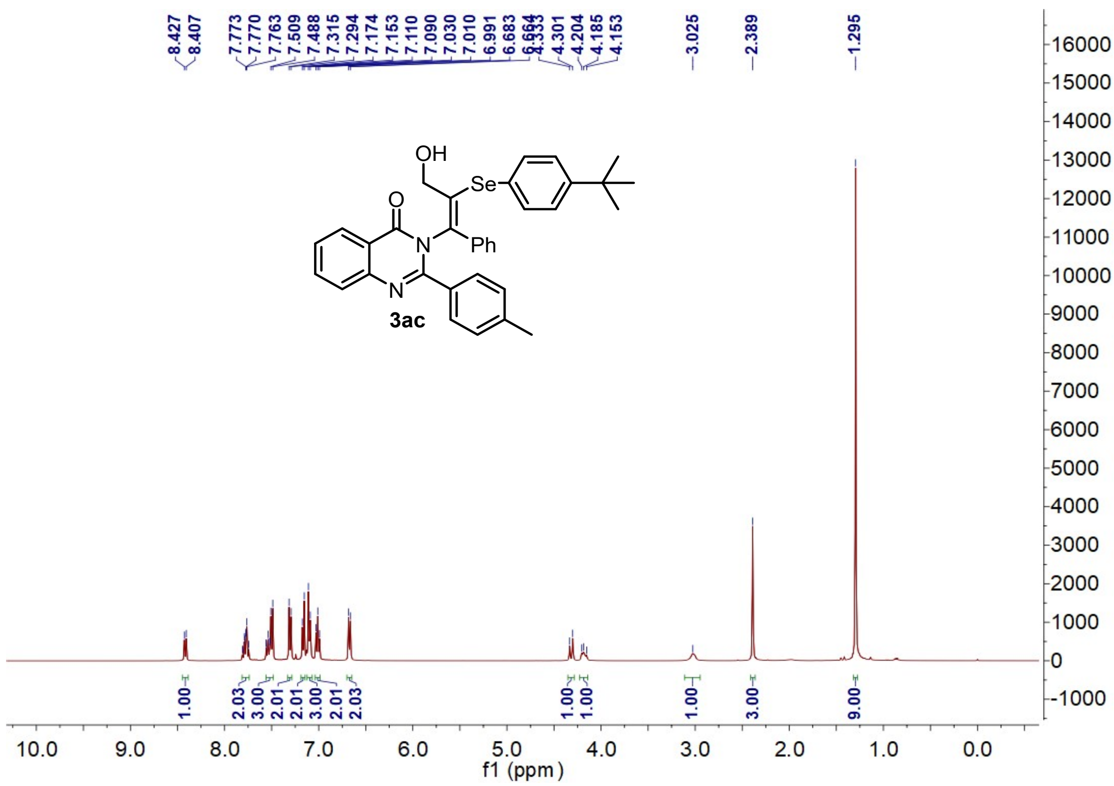
^{1}H-NMR of **3ab** ($CDCl_3$, 400 Hz)



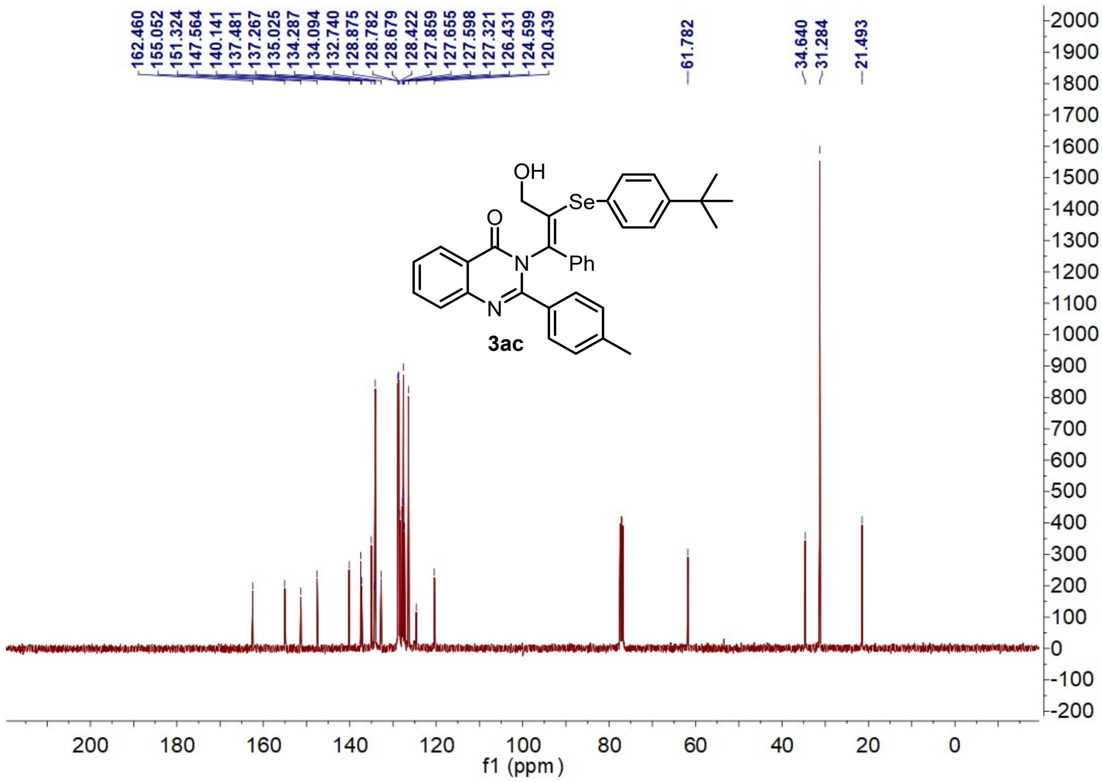
^{13}C-NMR of **3ab** ($CDCl_3$, 100 Hz)



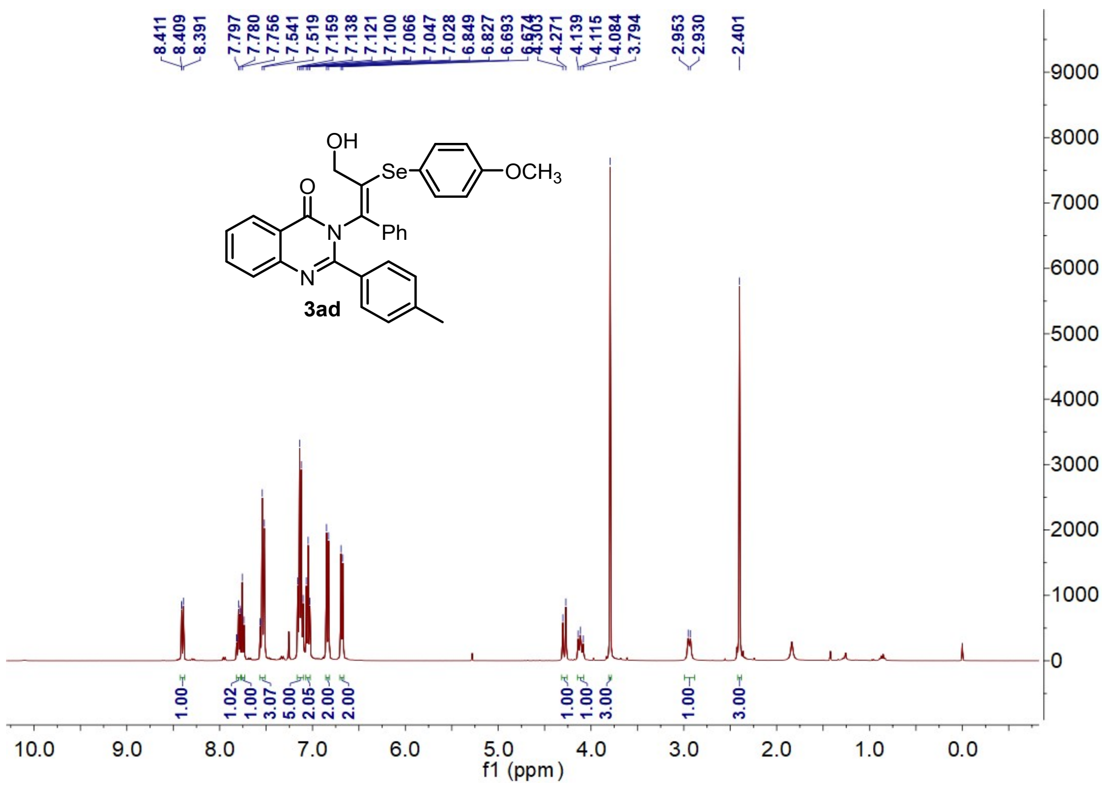
^{1}H-NMR of **3ac** ($CDCl_3$, 400 Hz)



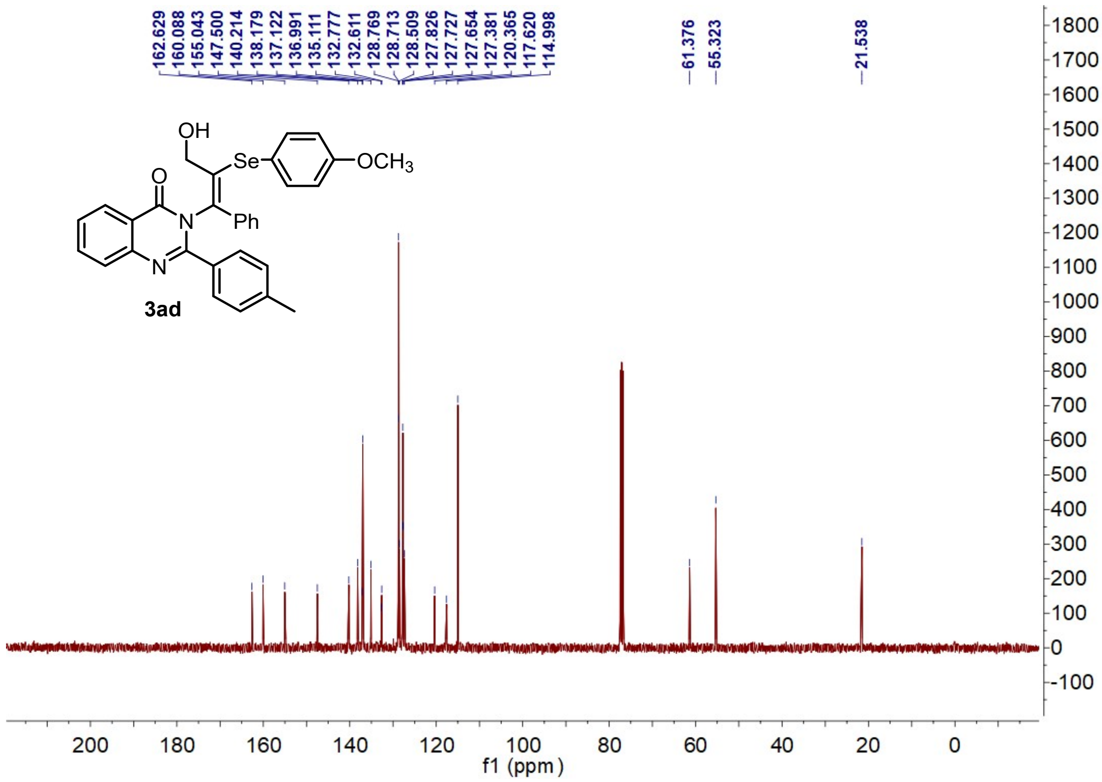
^{13}C-NMR of **3ac** ($CDCl_3$, 100 Hz)



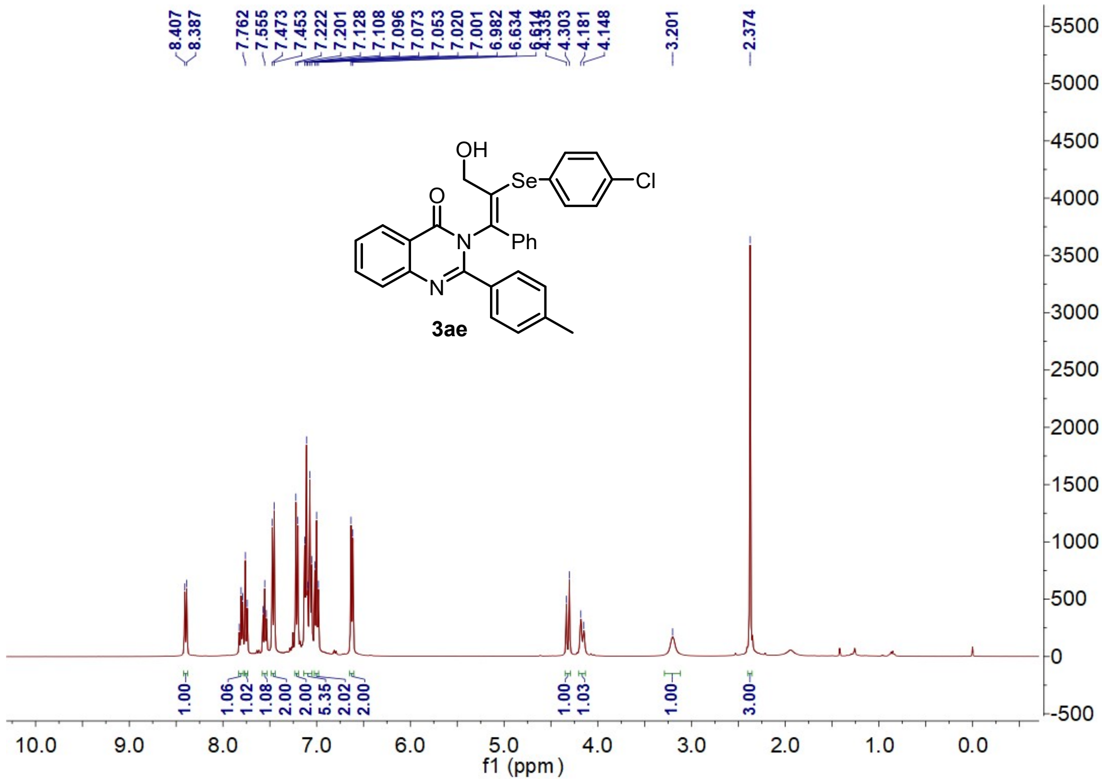
^{1}H-NMR of **3ad** ($CDCl_3$, 400 Hz)



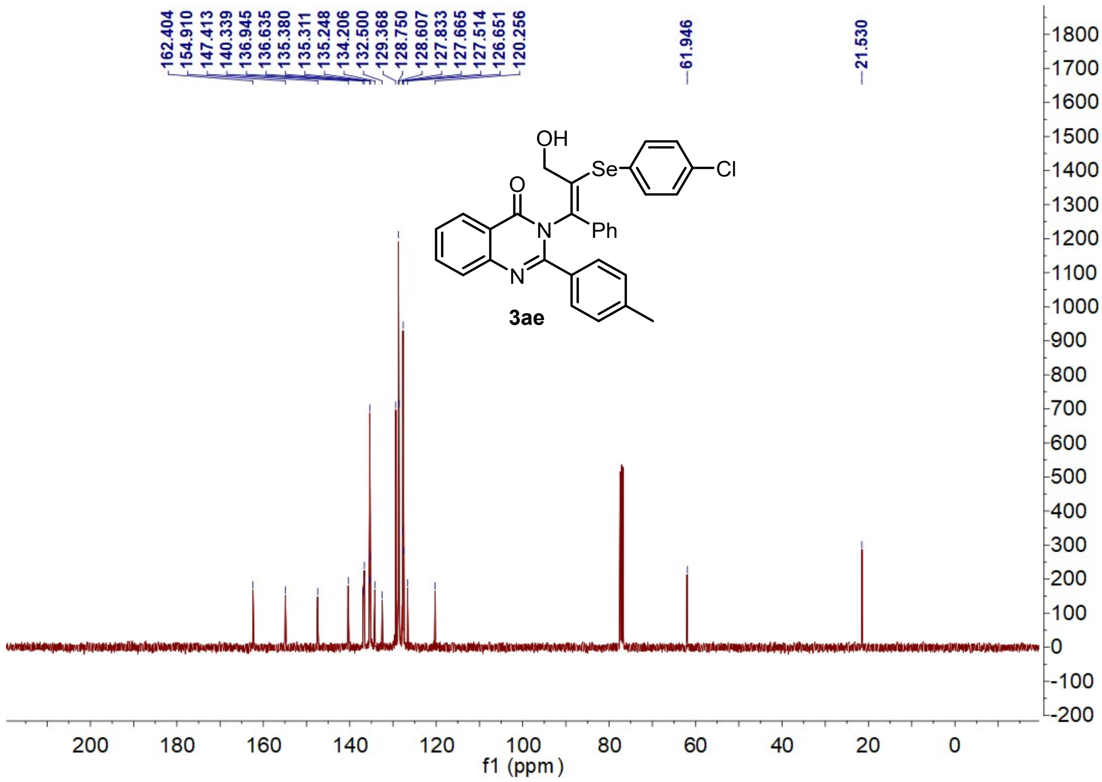
^{13}C-NMR of **3ad** ($CDCl_3$, 100 Hz)



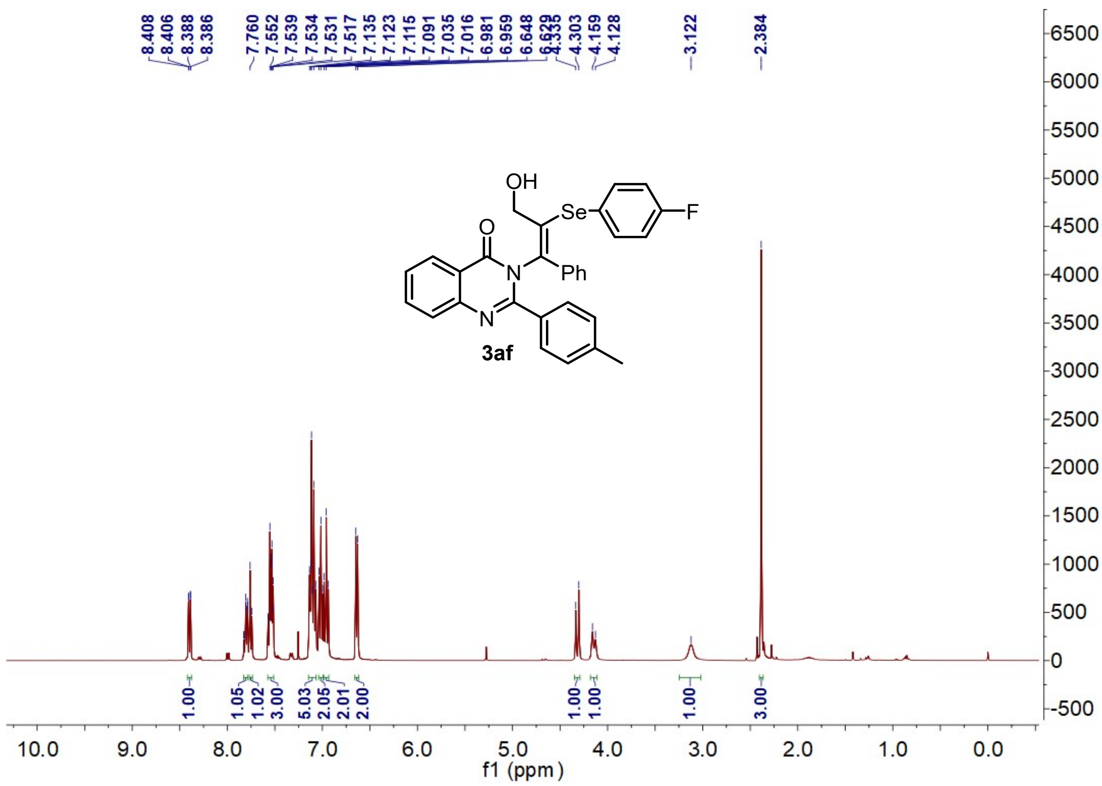
^{1}H-NMR of **3ae** ($CDCl_3$, 400 Hz)



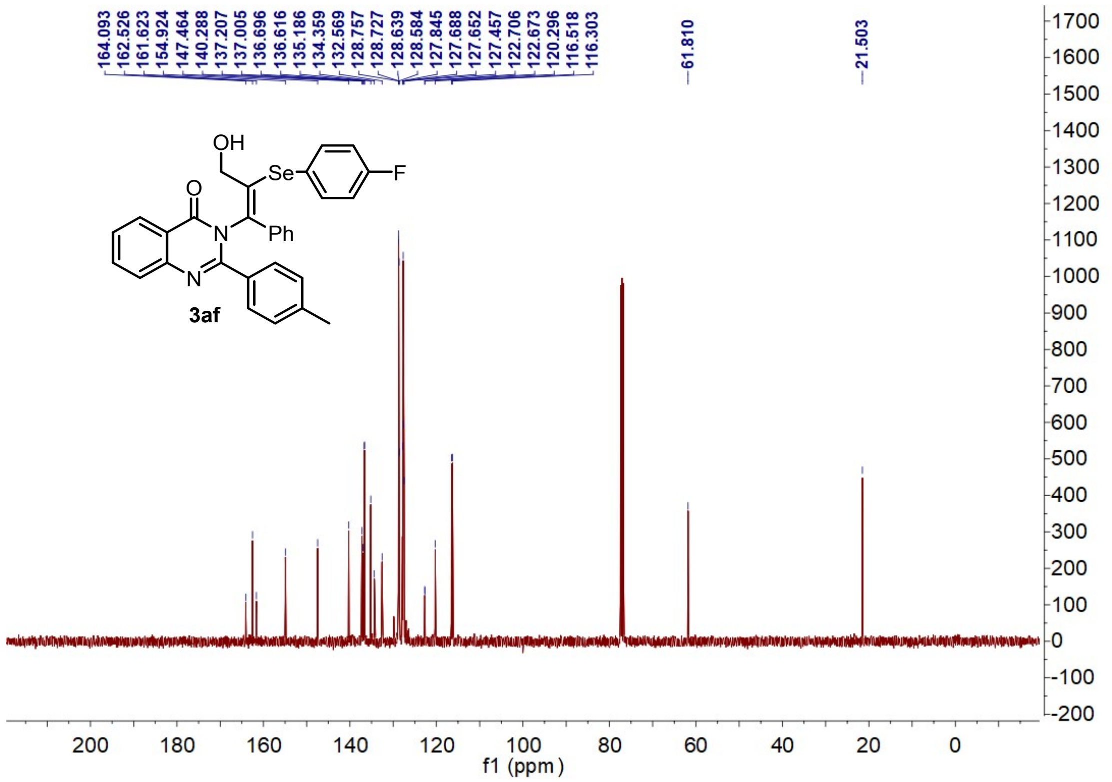
^{13}C-NMR of **3ae** ($CDCl_3$, 100 Hz)



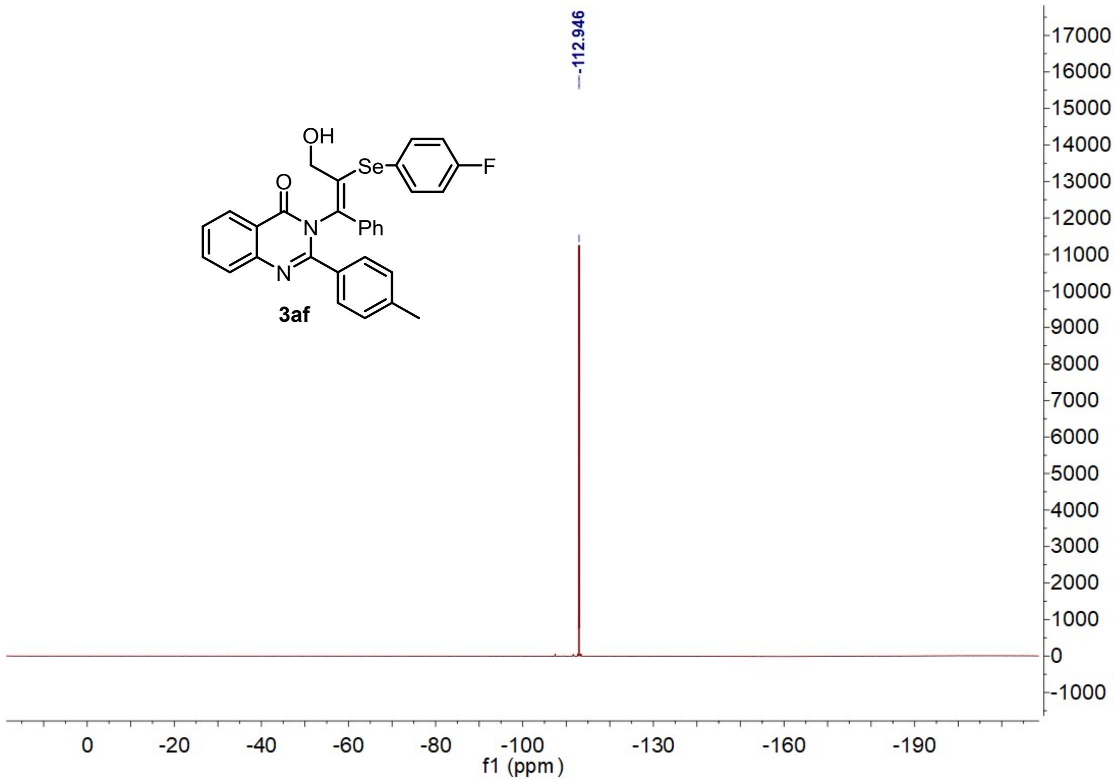
^{1}H-NMR of **3af** ($CDCl_3$, 400 Hz)



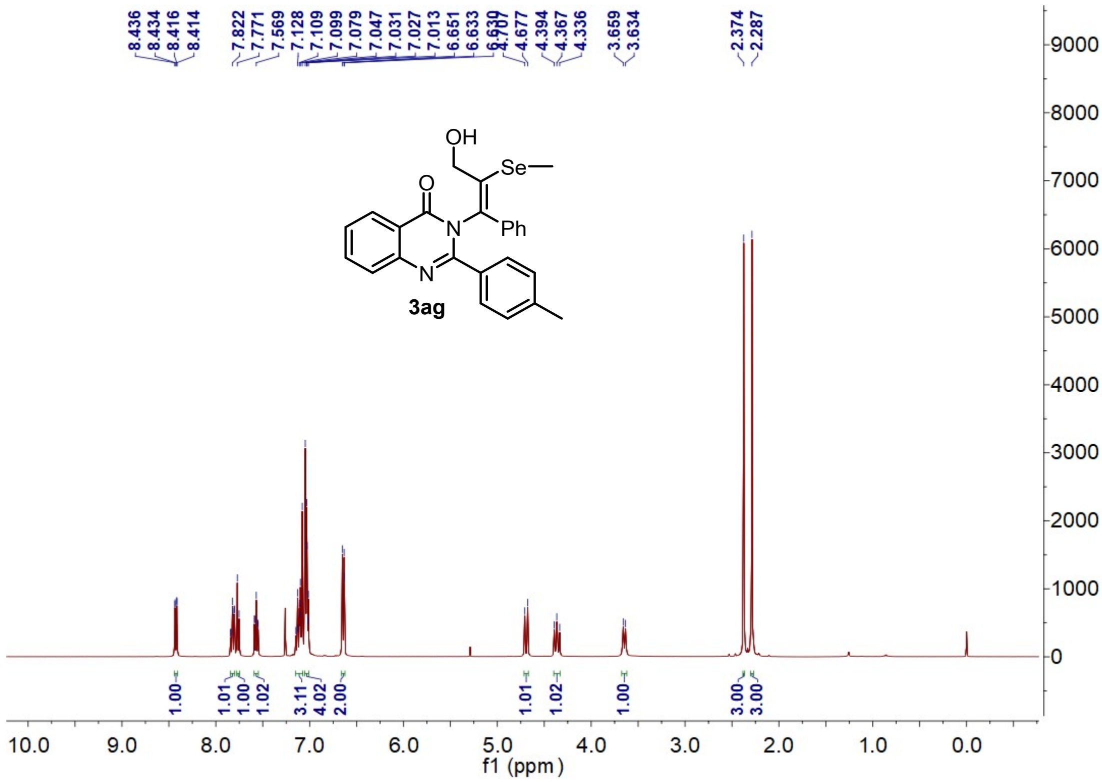
^{13}C-NMR of **3af** ($CDCl_3$, 100 Hz)



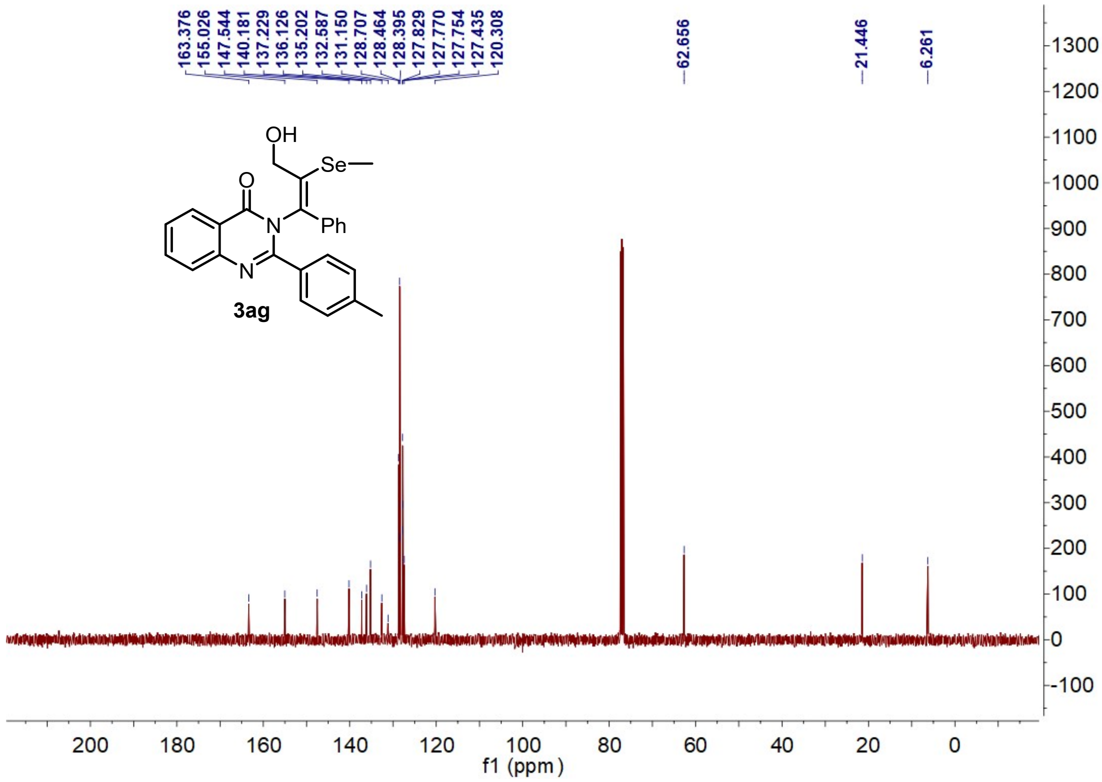
^{19}F-NMR of **3af** ($CDCl_3$, 376 Hz)



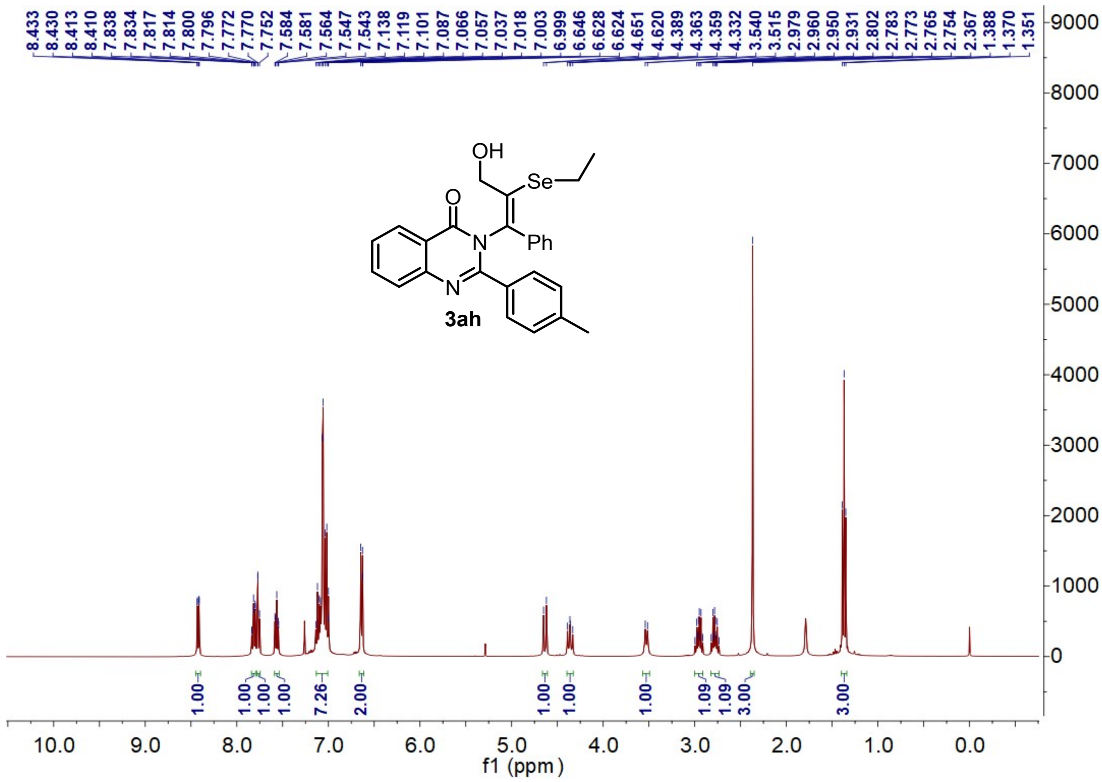
^{1}H-NMR of **3ag** ($CDCl_3$, 400 Hz)



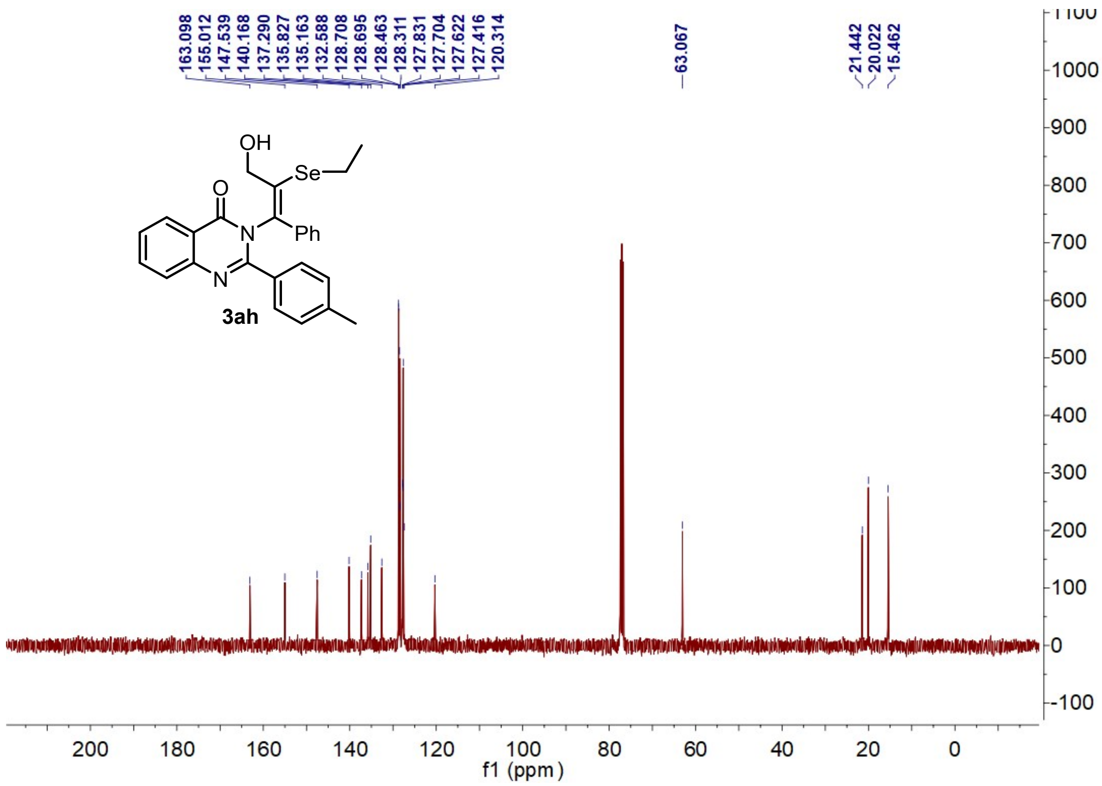
^{13}C-NMR of **3ag** ($CDCl_3$, 100 Hz)



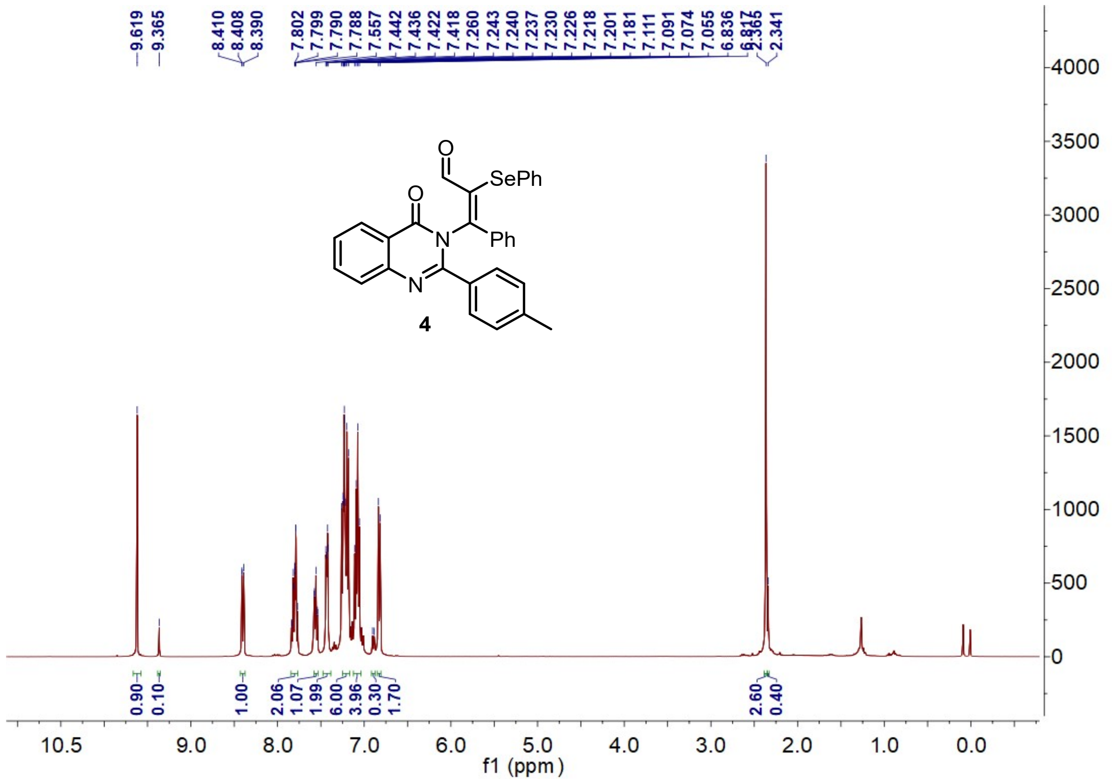
^{1}H-NMR of **3ah** ($CDCl_3$, 400 Hz)



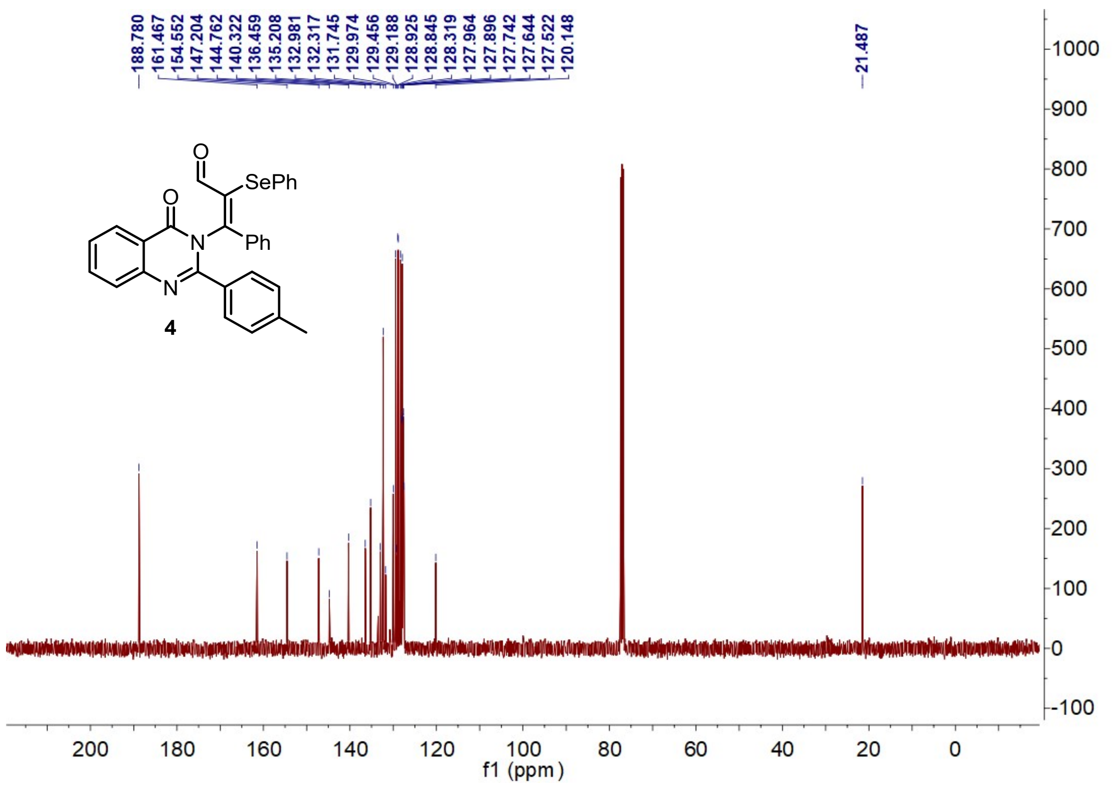
^{13}C-NMR of **3ah** ($CDCl_3$, 100 Hz)



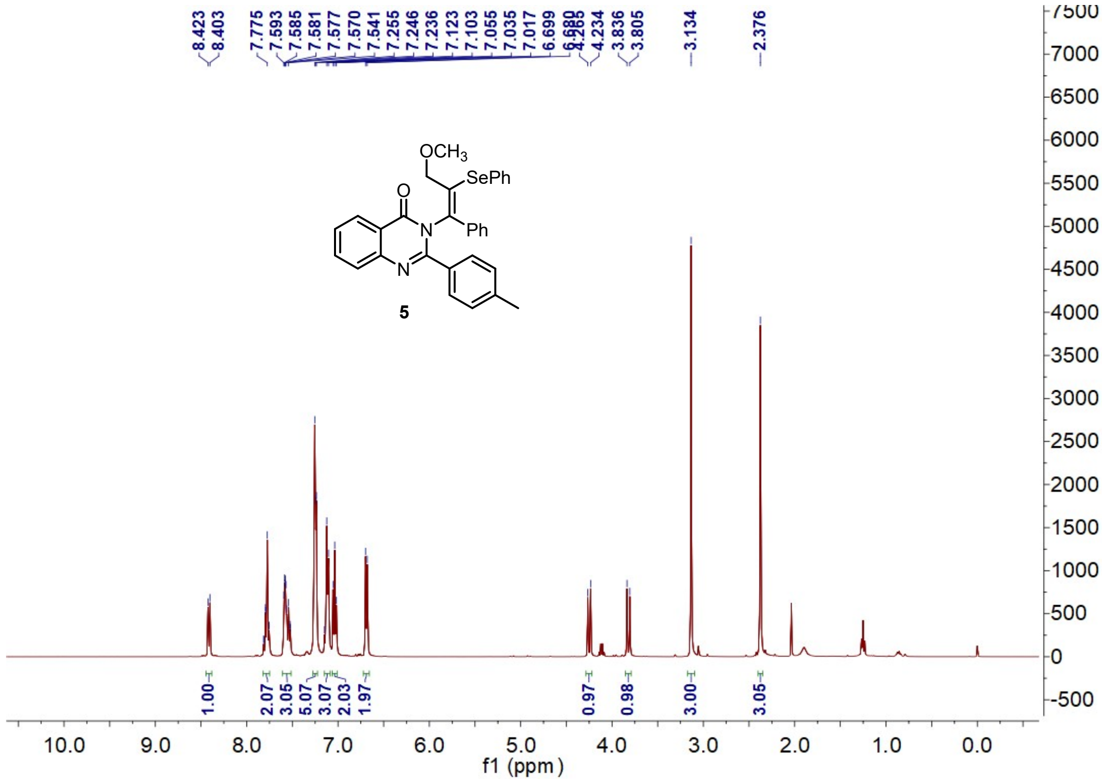
^{1}H-NMR of **4** ($CDCl_3$, 400 Hz)



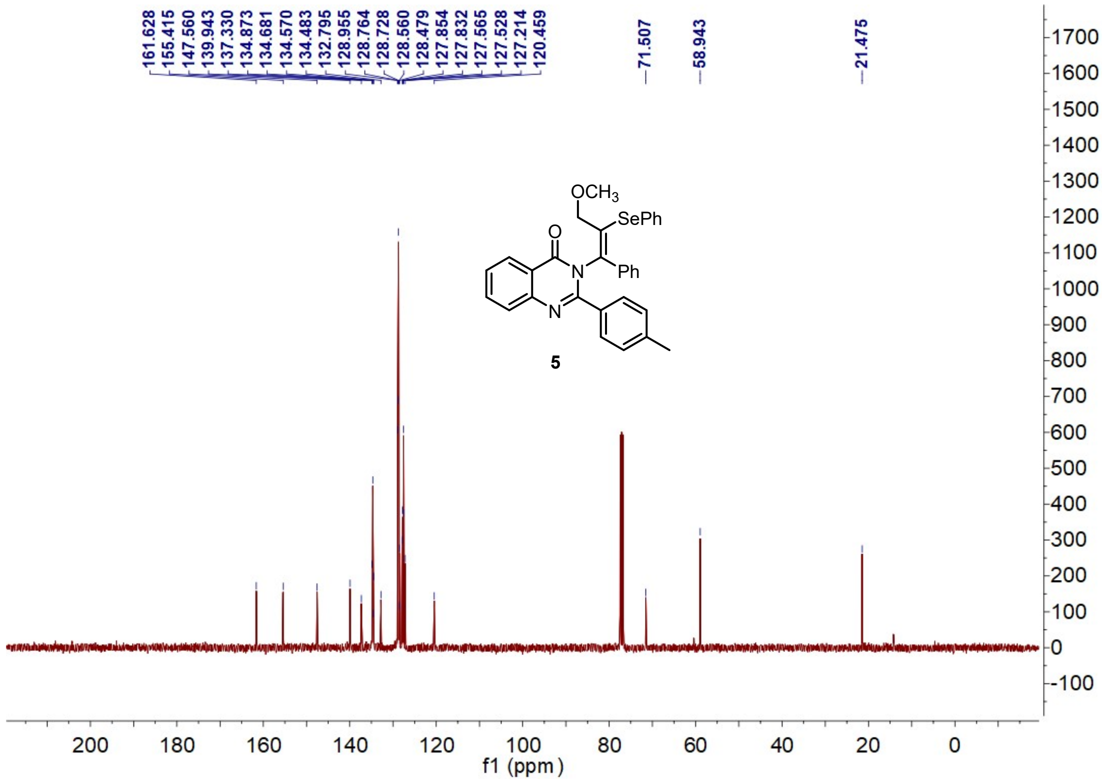
^{13}C-NMR of **4** ($CDCl_3$, 100 Hz)



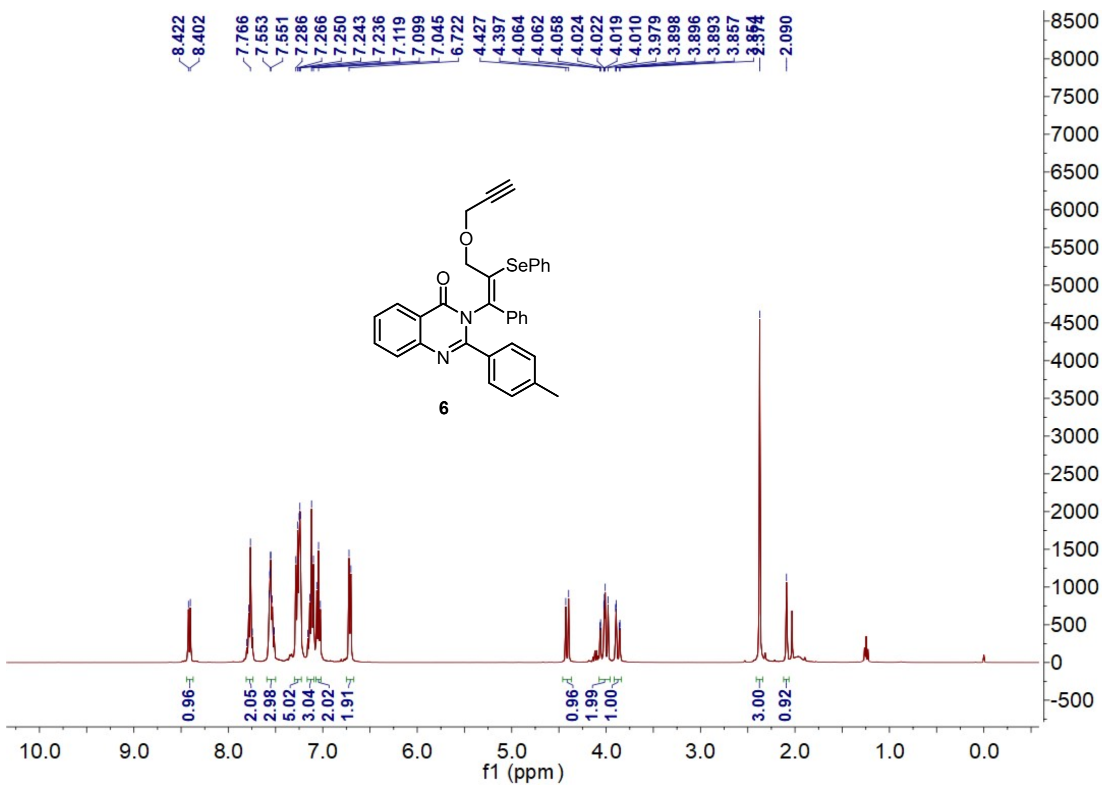
^{1}H-NMR of **5** ($CDCl_3$, 400 Hz)



^{13}C-NMR of **5** ($CDCl_3$, 100 Hz)



^{1}H-NMR of **6** ($CDCl_3$, 400 Hz)



^{13}C-NMR of **6** ($CDCl_3$, 100 Hz)