# *Supporting Information for*

## [4+2] Cyclization of *para*-Quinone Methide Derivatives with Alkynes

Guang-Jian Mei*, Shao-Li Xu, Wen-Qin Zheng, Chen-Yu Bian and Feng Shi*

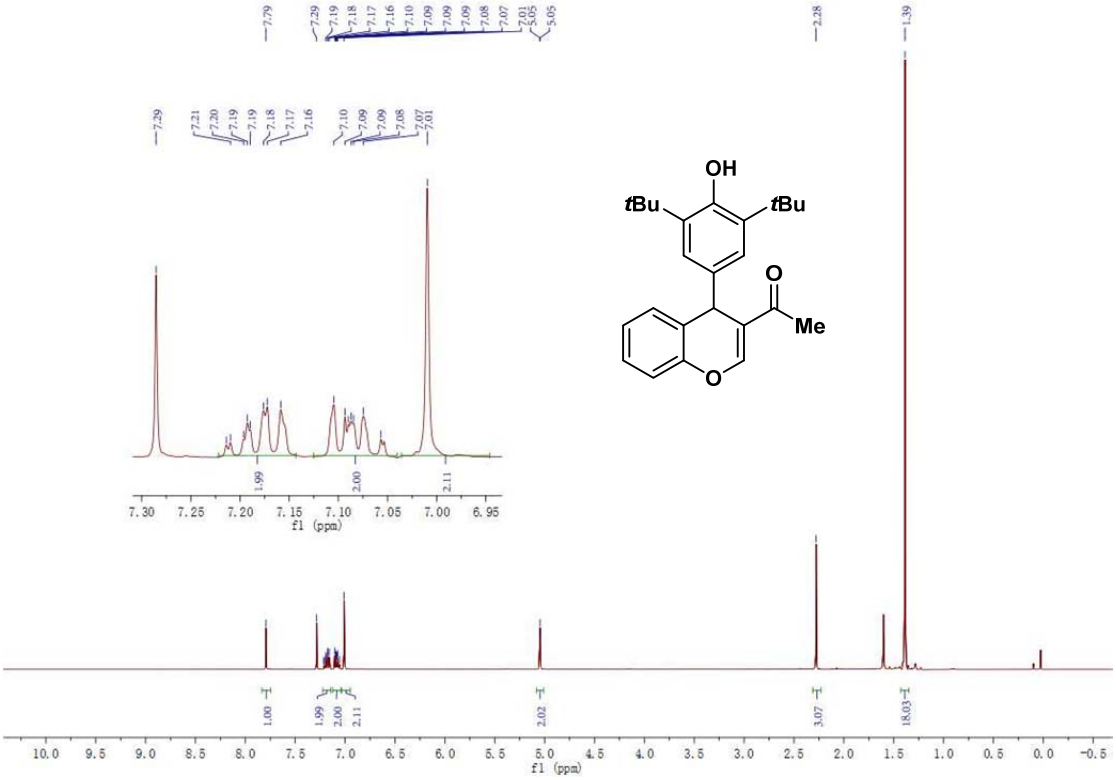
*School of Chemistry and Material Science, Jiangsu Normal University, Xuzhou 221116, China*

*E-mail: fshi@jsnu.edu.cn; guangjianM@jsnu.edu.cn*

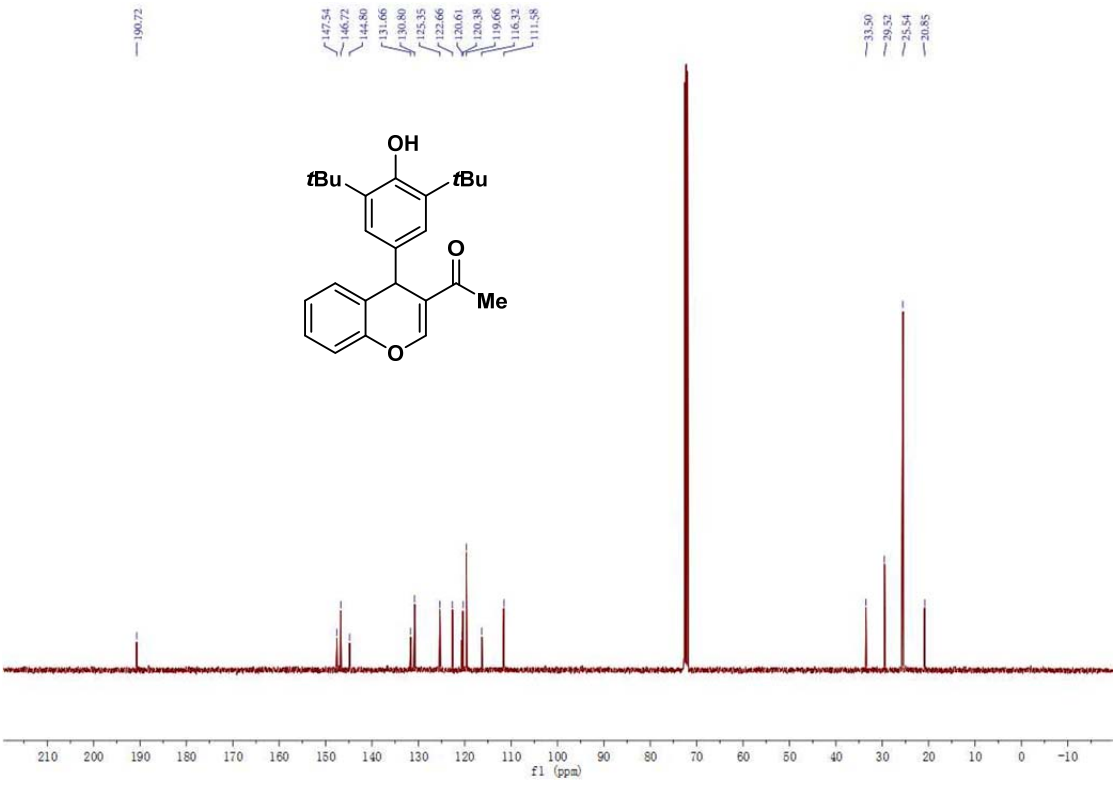
**Contents:**

## 1. Copies of NMR spectra

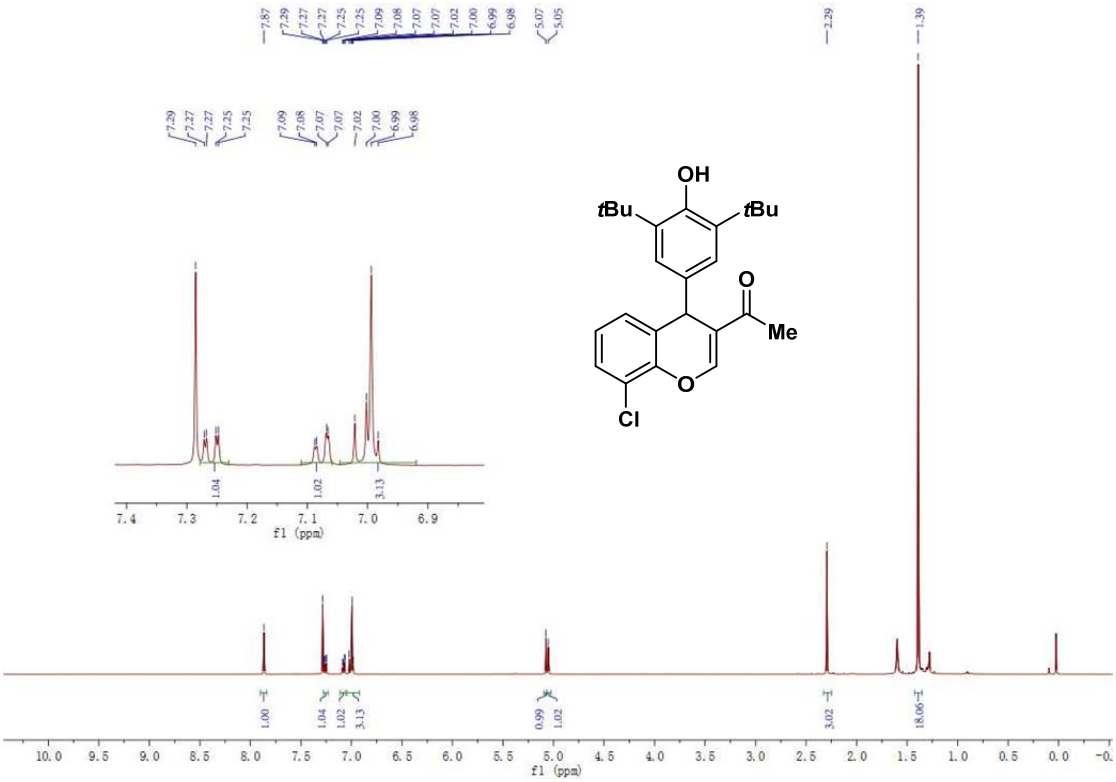
$^{1}$H NMR (400 MHz, $CDCl_3$) of compound **3aa**



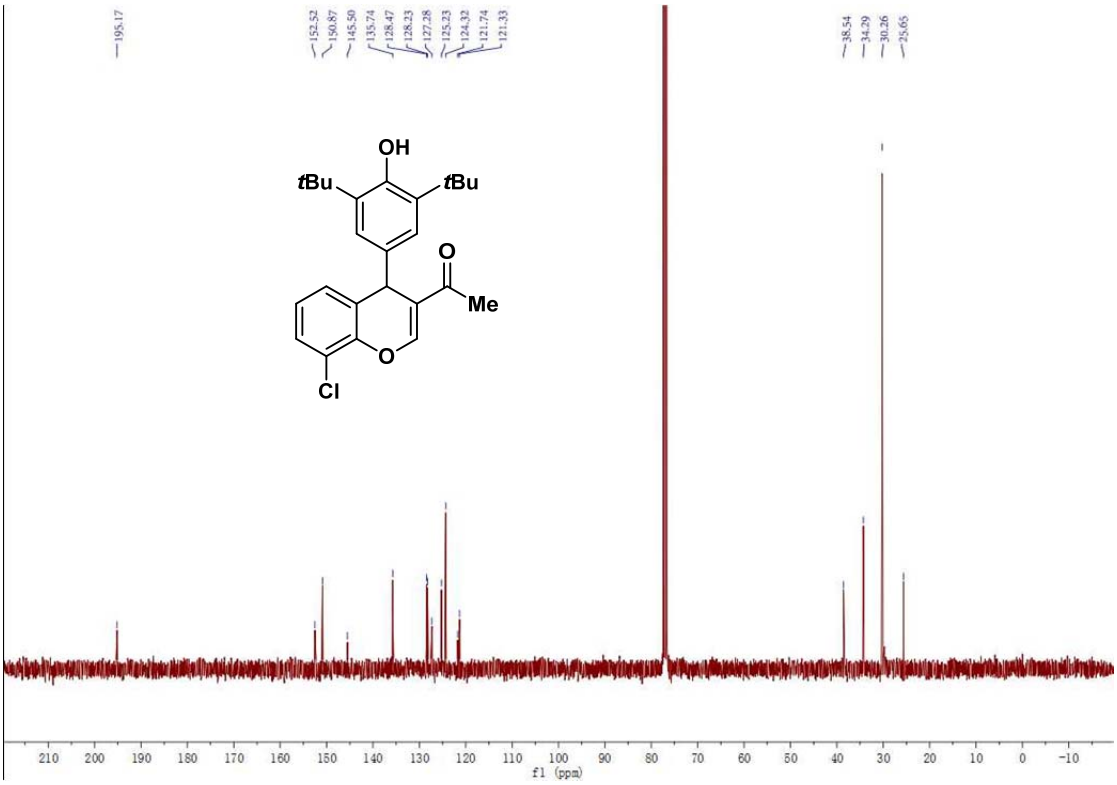

$^{13}$C NMR (100 MHz, $CDCl_3$) of compound **3aa**



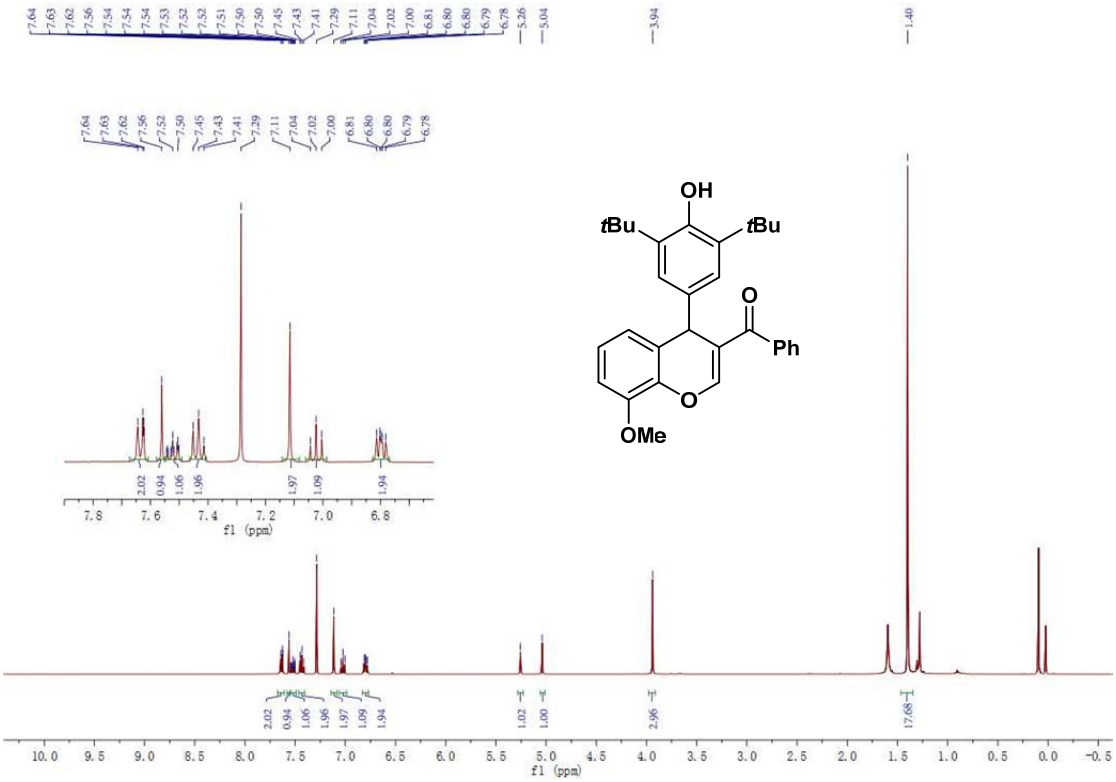
$^{1}$H NMR (400 MHz, $CDCl_3$) of compound **3ba**



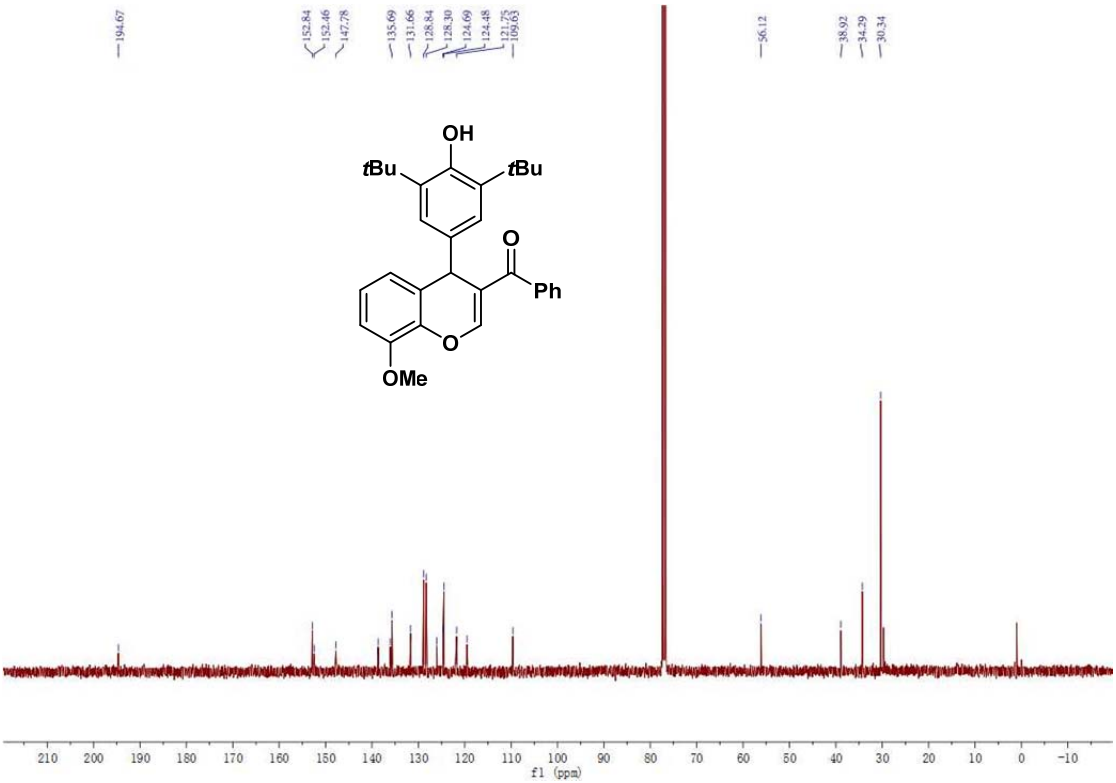

$^{13}$C NMR (100 MHz, $CDCl_3$) of compound **3ba**



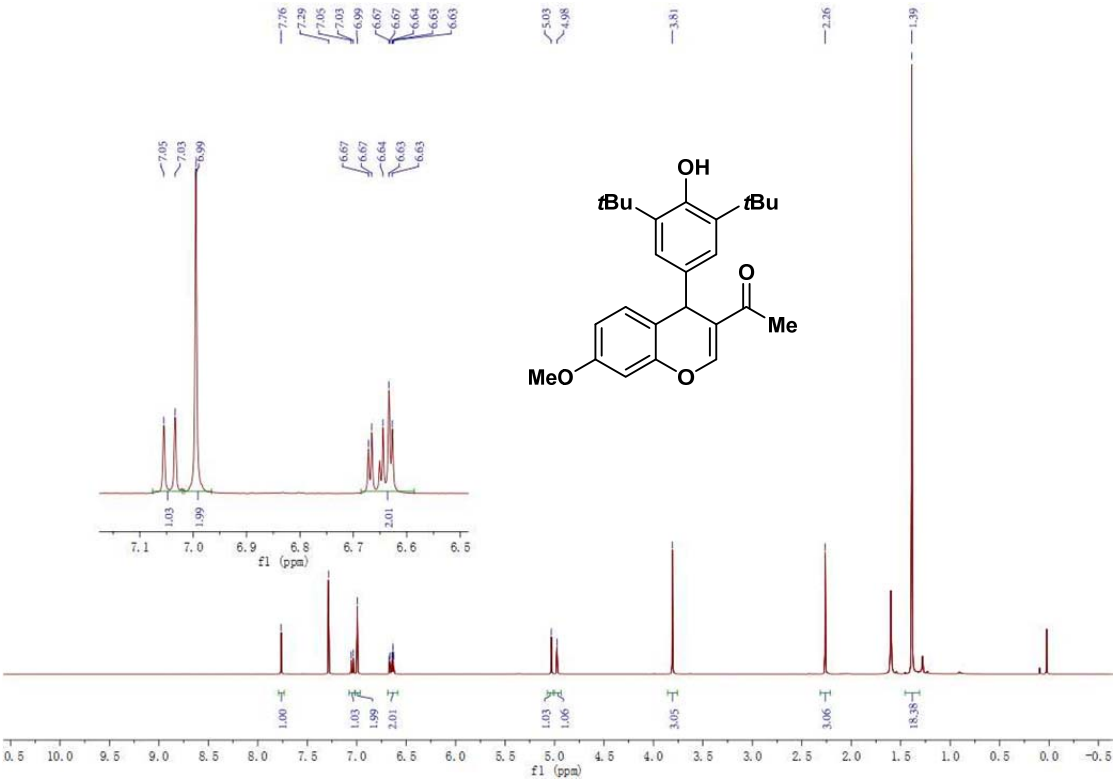
$^{1}$H NMR (400 MHz, $CDCl_3$) of compound **3cb**



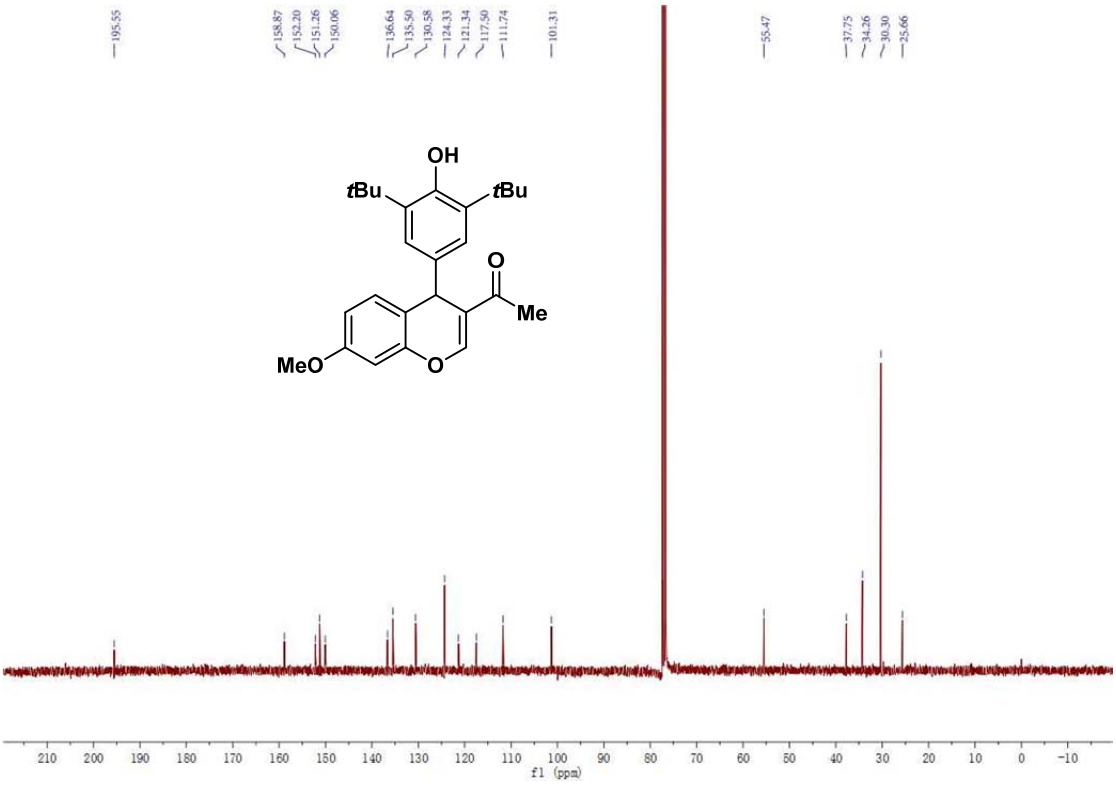

$^{13}$C NMR (100 MHz, $CDCl_3$) of compound **3cb**



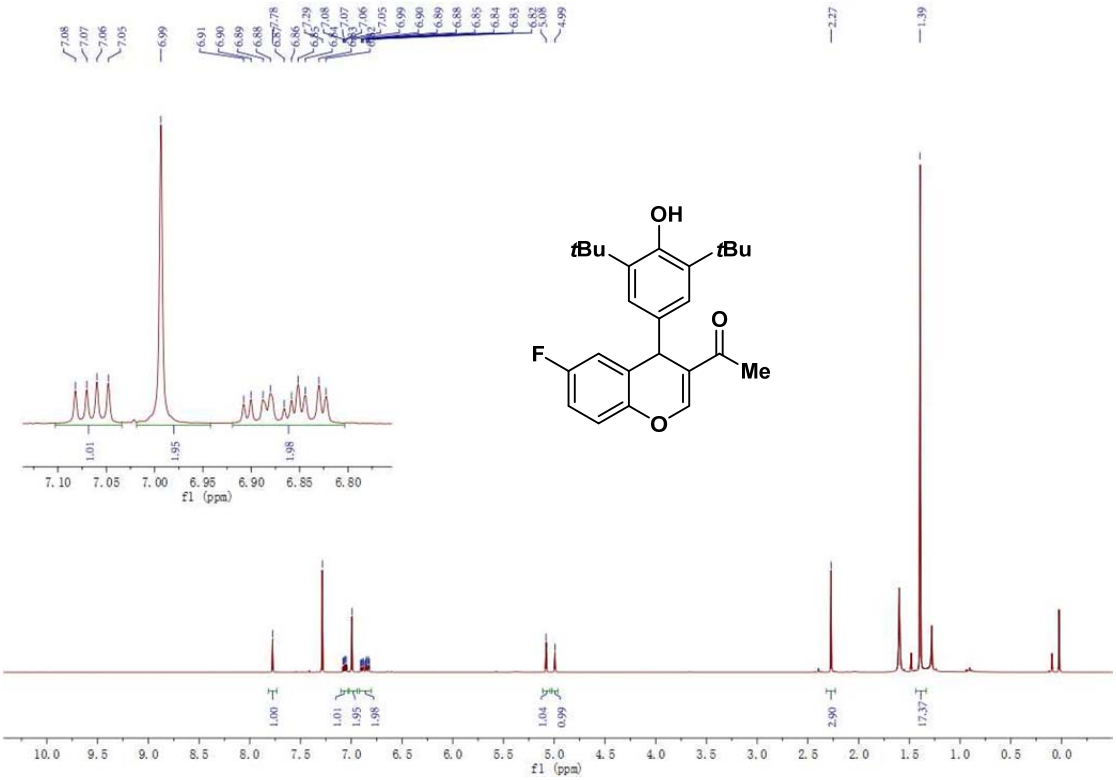
$^{1}$H NMR (400 MHz, $CDCl_3$) of compound **3da**



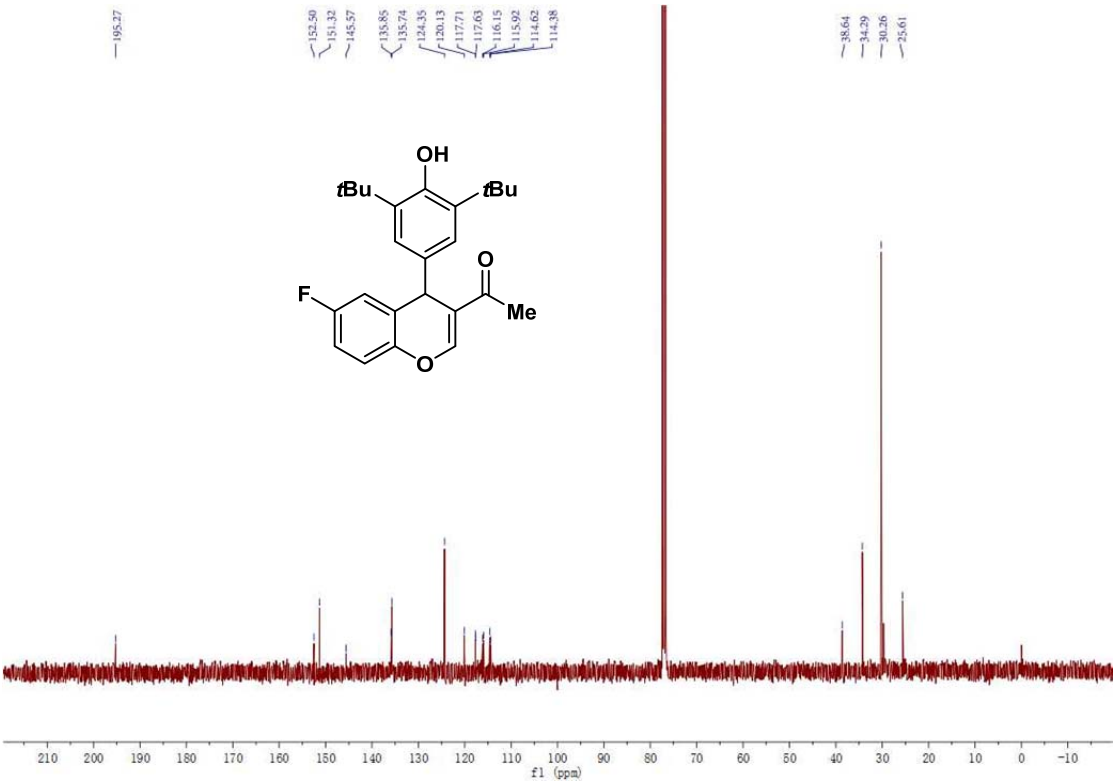

$^{13}$C NMR (100 MHz, $CDCl_3$) of compound **3da**



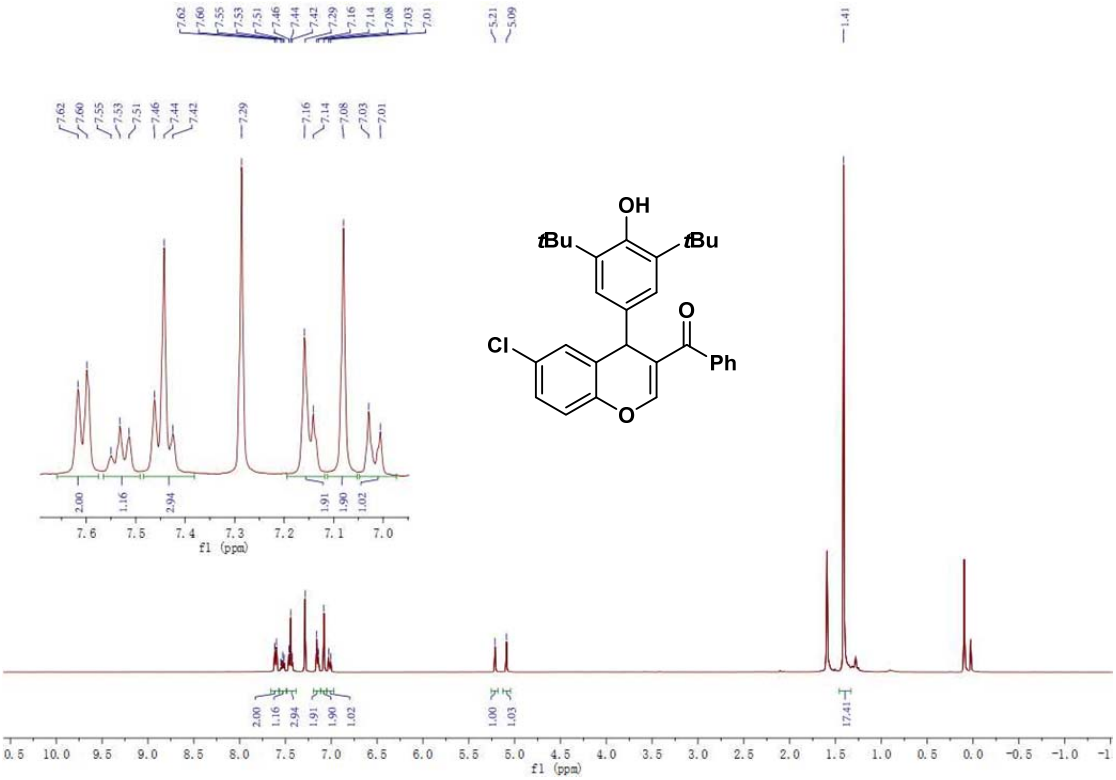
$^{1}$H NMR (400 MHz, $CDCl_3$) of compound **3ea**



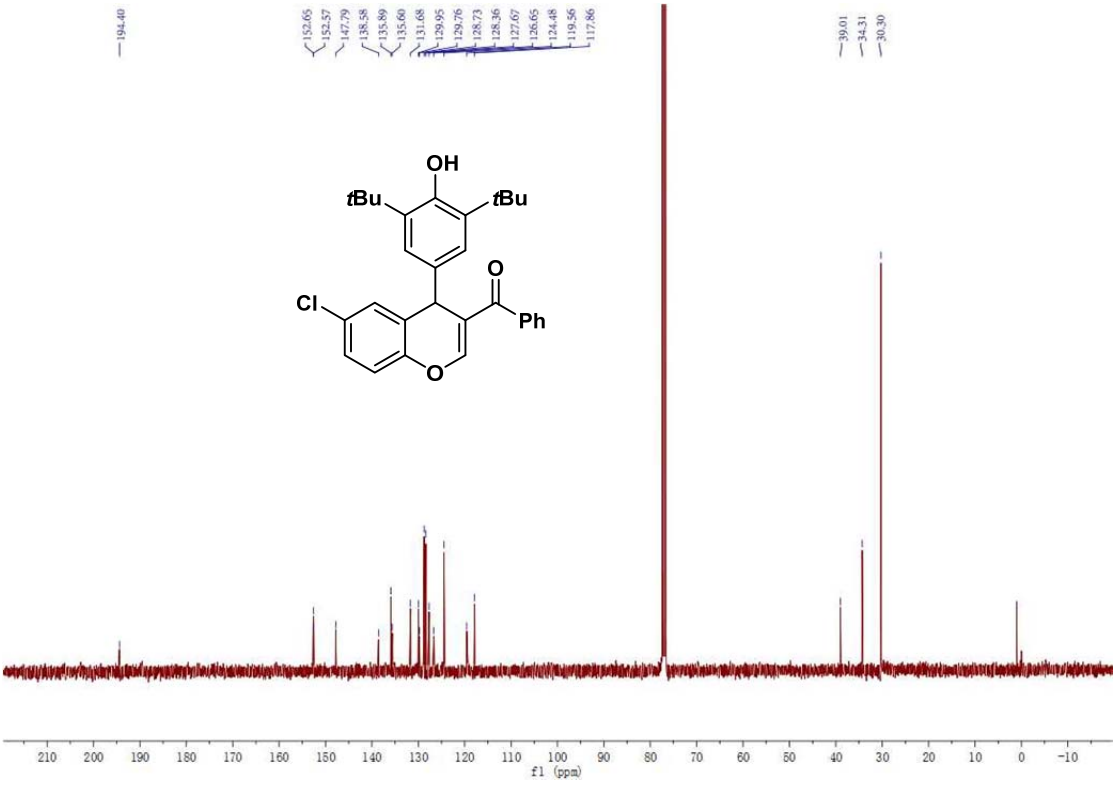

$^{13}$C NMR (100 MHz, $CDCl_3$) of compound **3ea**



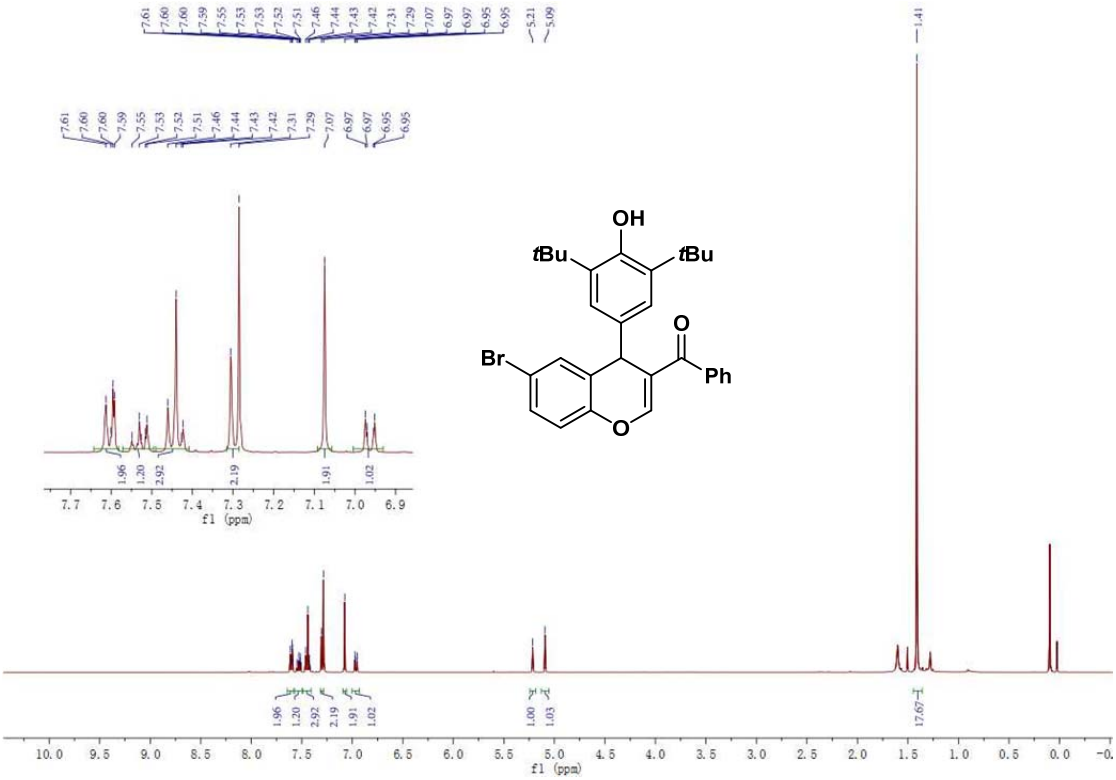
$^{1}$H NMR (400 MHz, $CDCl_3$) of compound **3fb**



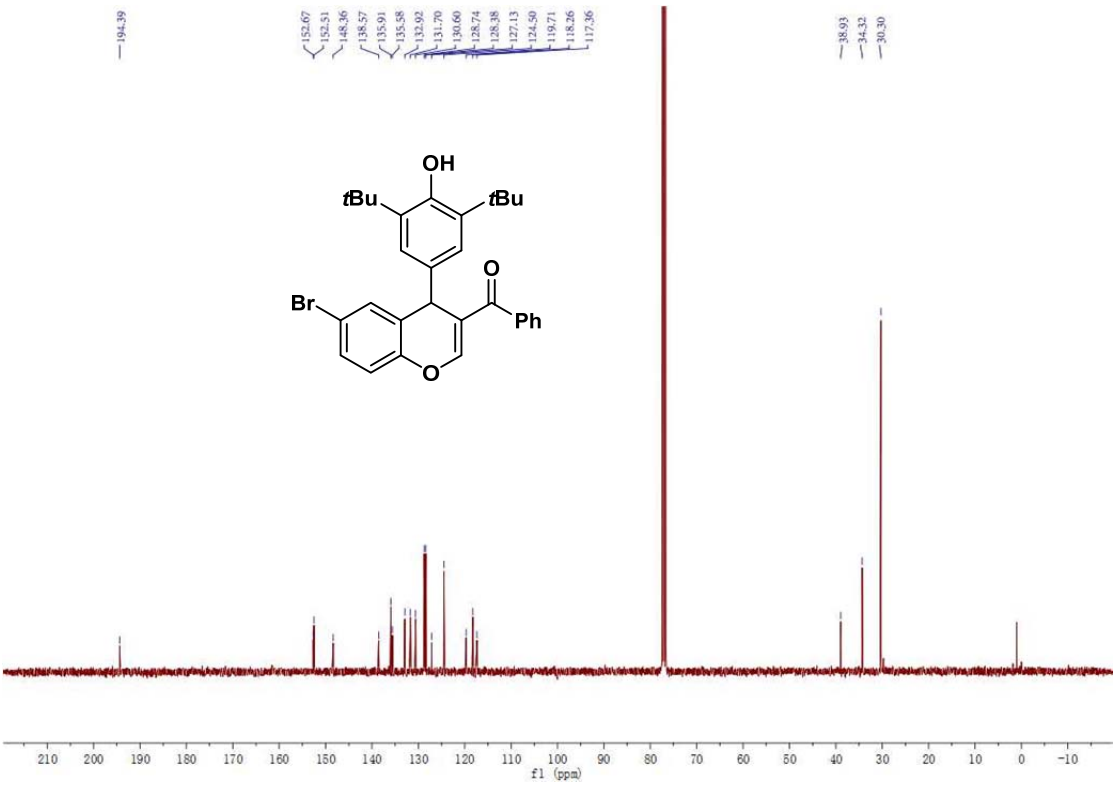

$^{13}$C NMR (100 MHz, $CDCl_3$) of compound **3fb**



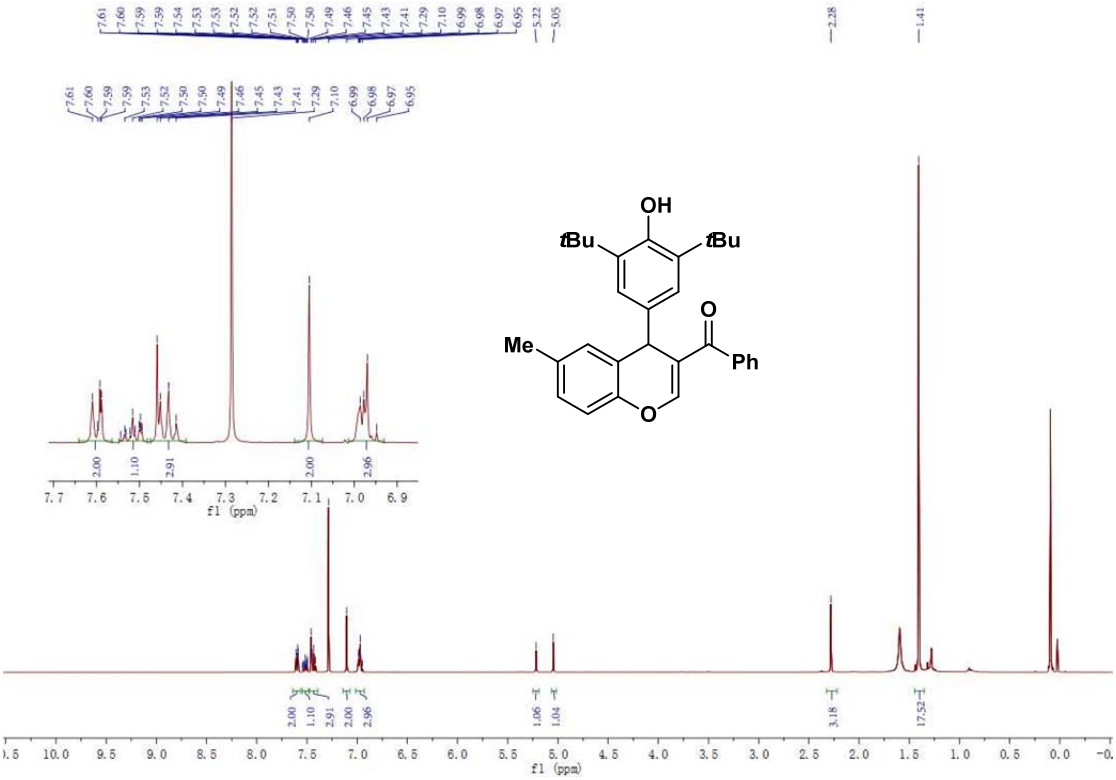
$^{1}$H NMR (400 MHz, $CDCl_3$) of compound **3gb**



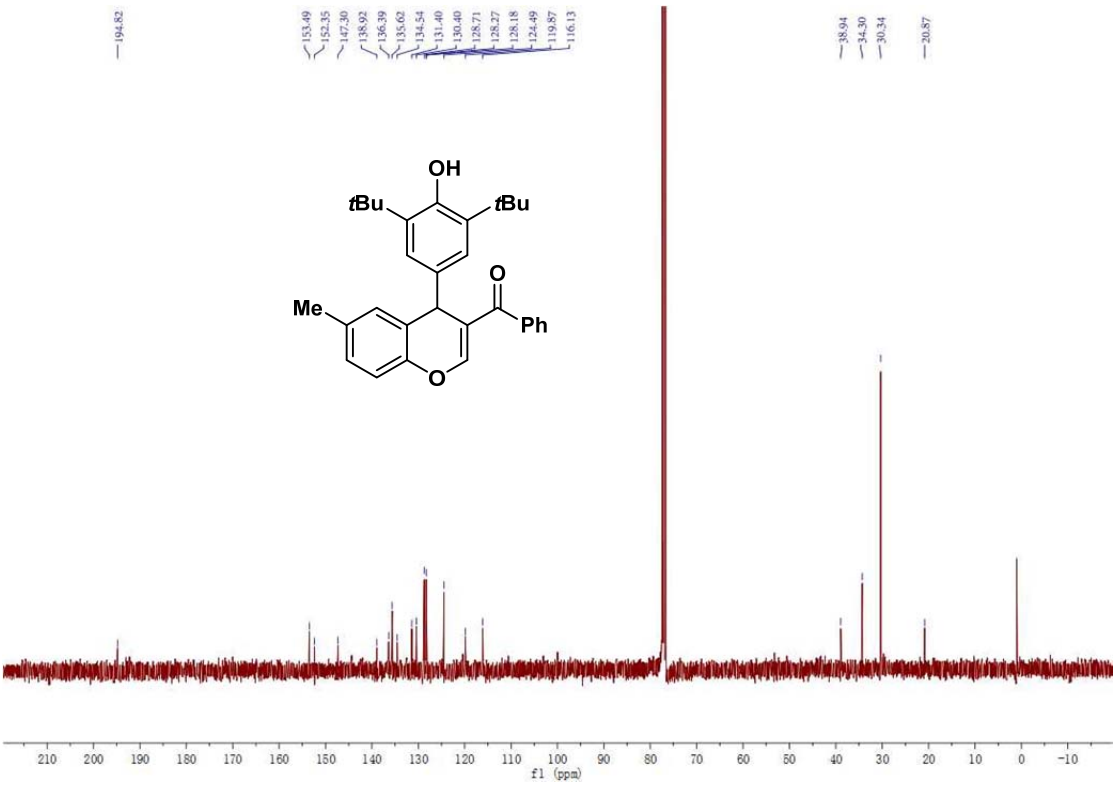

$^{13}$C NMR (100 MHz, $CDCl_3$) of compound **3gb**



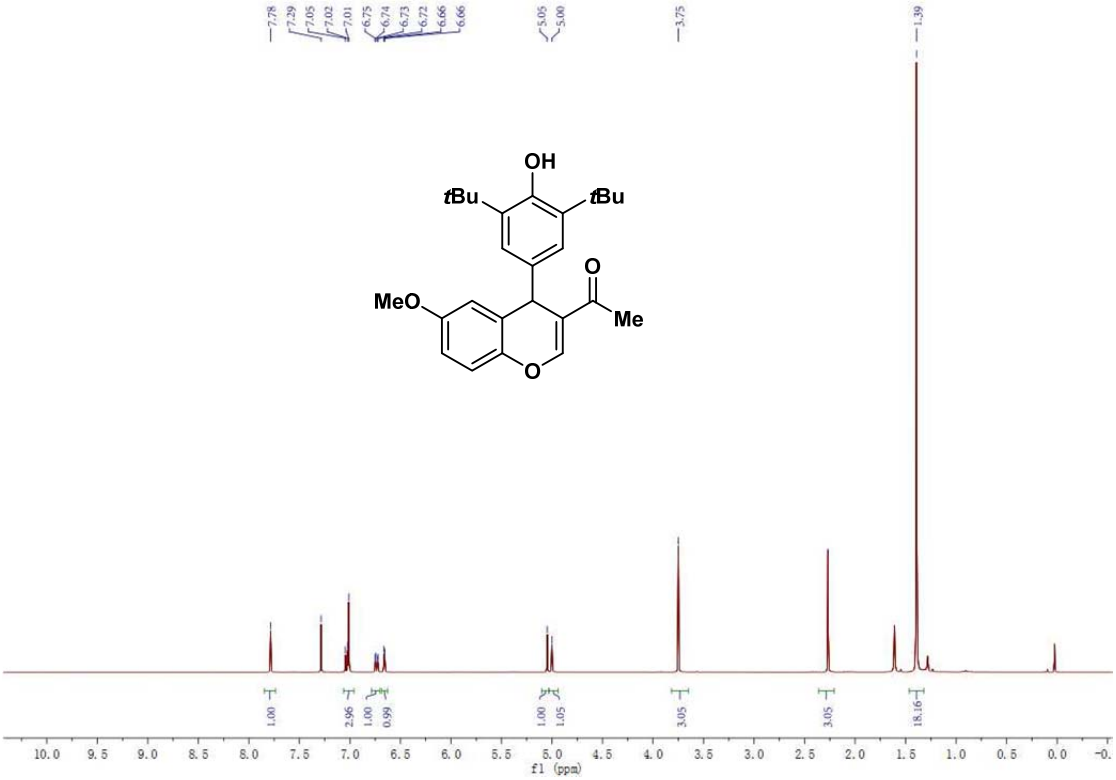
$^{1}$H NMR (400 MHz, $CDCl_3$) of compound **3hb**



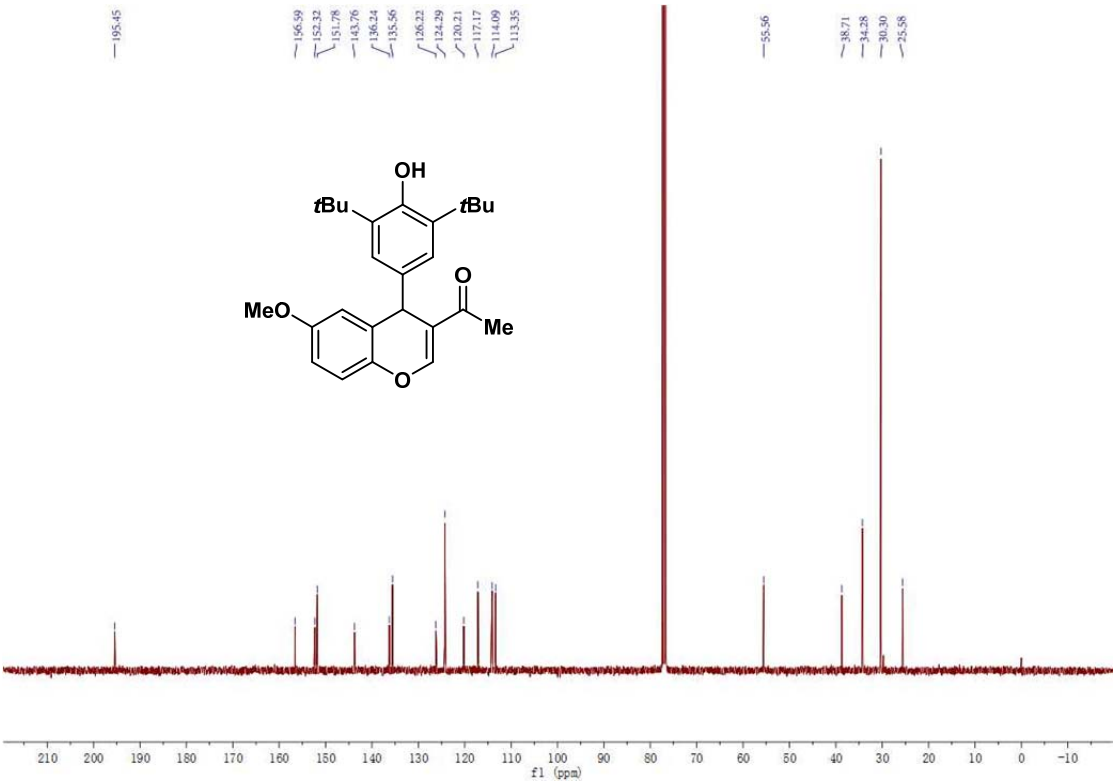

$^{13}$C NMR (100 MHz, $CDCl_3$) of compound **3hb**



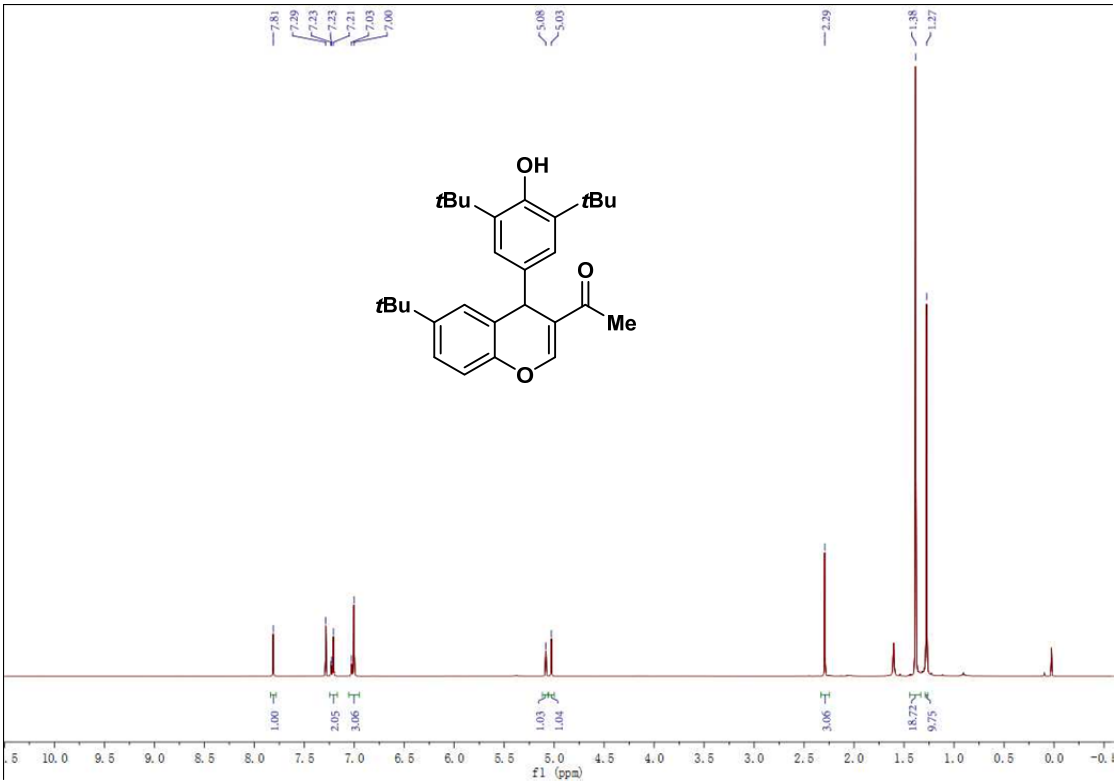
$^{1}$H NMR (400 MHz, $CDCl_3$) of compound **3ia**



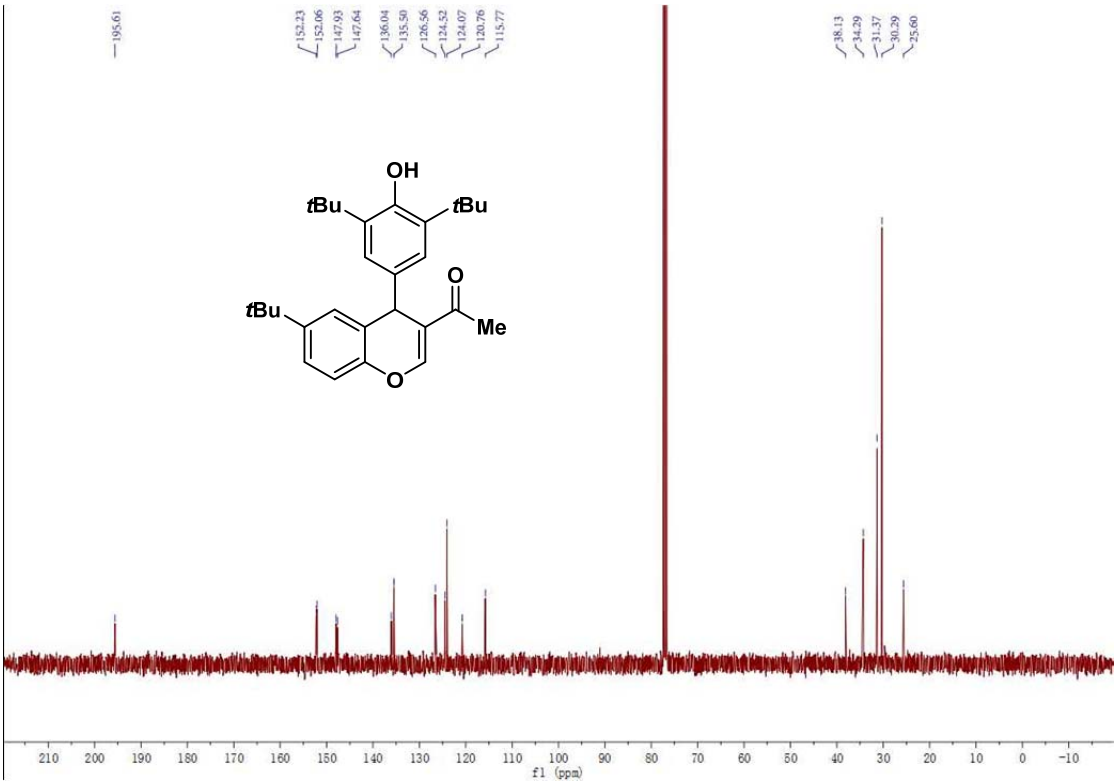

$^{13}$C NMR (100 MHz, $CDCl_3$) of compound **3ia**



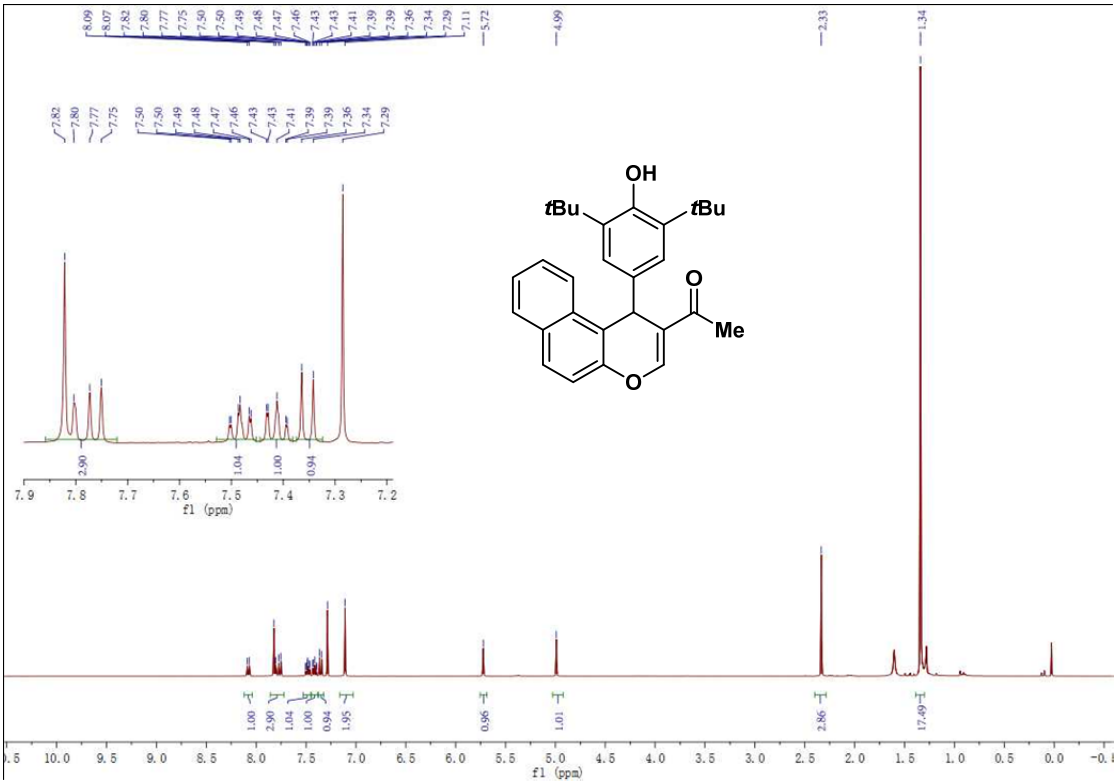
$^{1}$H NMR (400 MHz, $CDCl_3$) of compound **3ja**



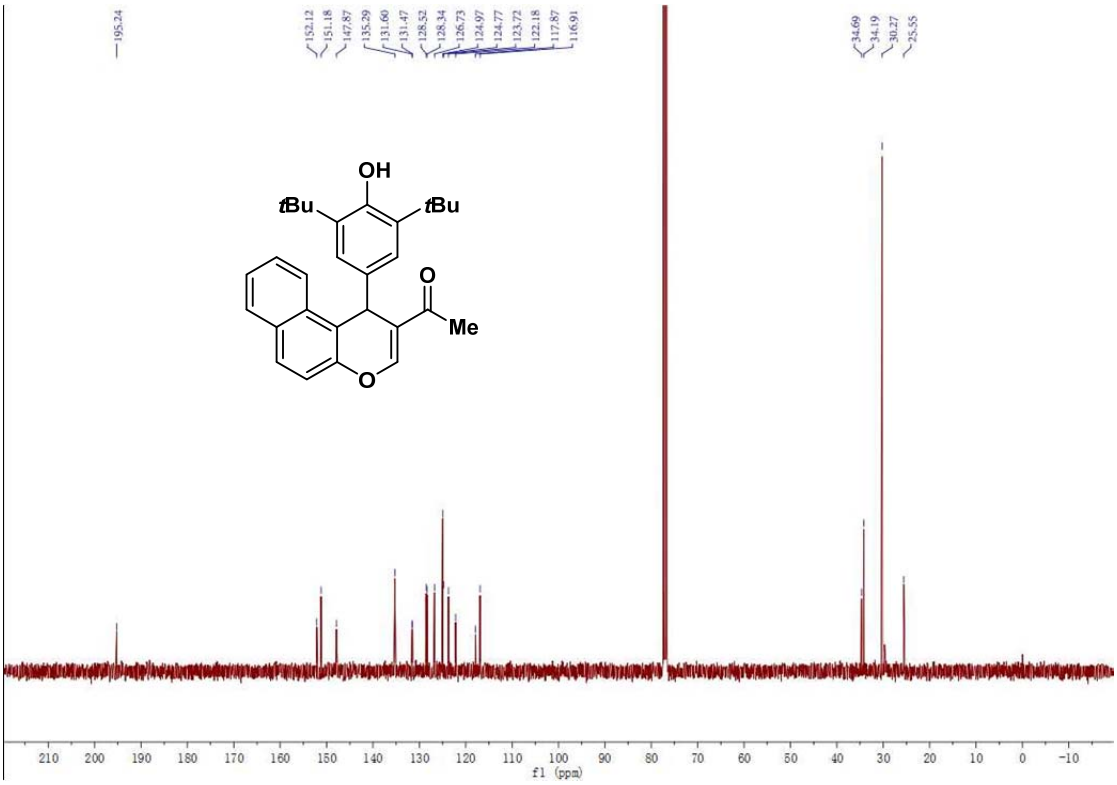

$^{13}$C NMR (100 MHz, $CDCl_3$) of compound **3ja**



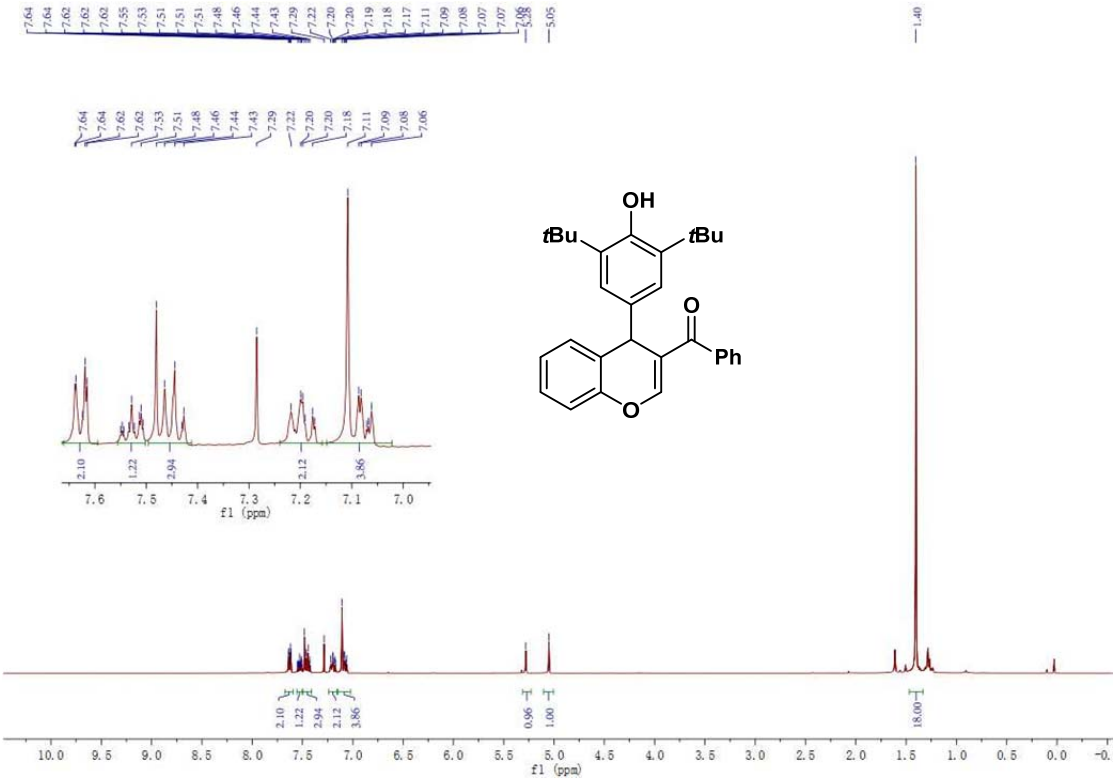
$^{1}$H NMR (400 MHz, $CDCl_3$) of compound **3ka**



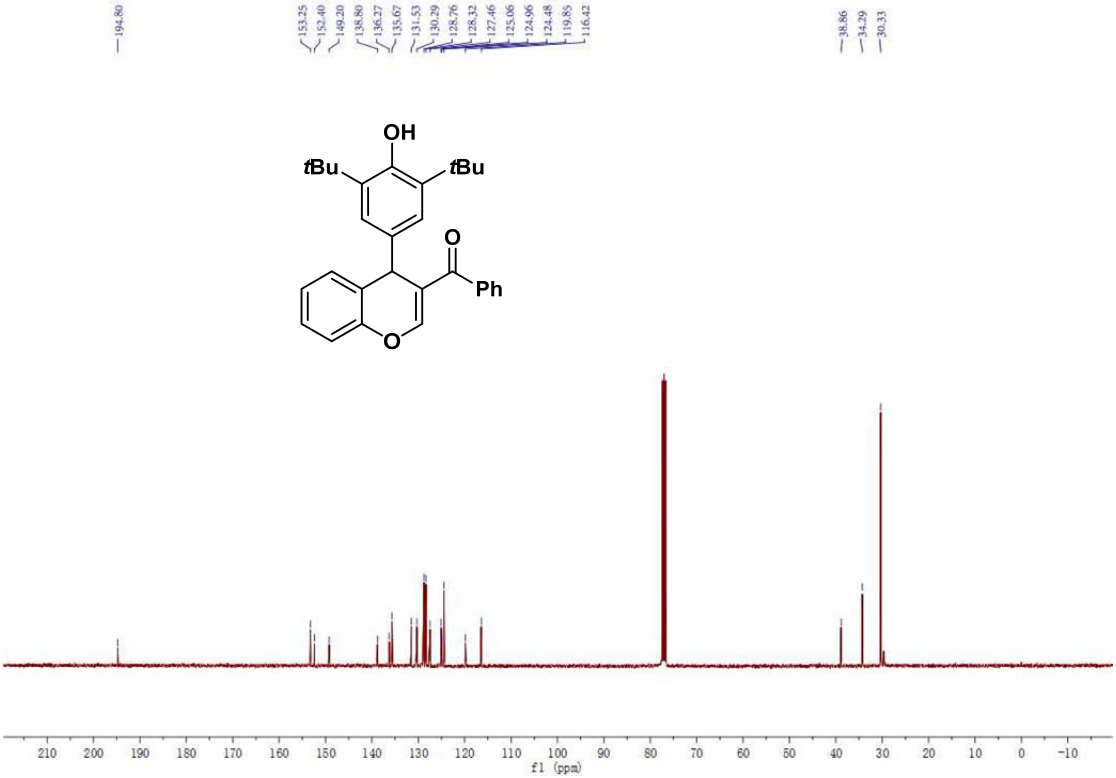

$^{13}$C NMR (100 MHz, $CDCl_3$) of compound **3ka**



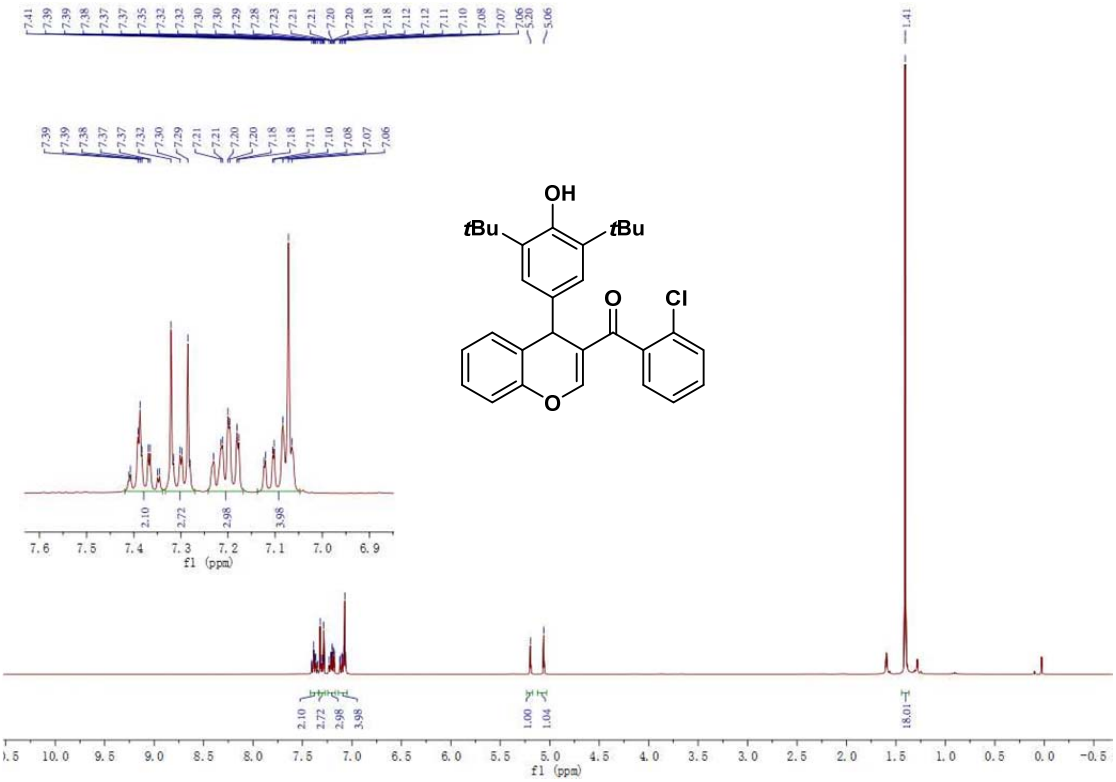
$^{1}$H NMR (400 MHz, $CDCl_3$) of compound **3ab**



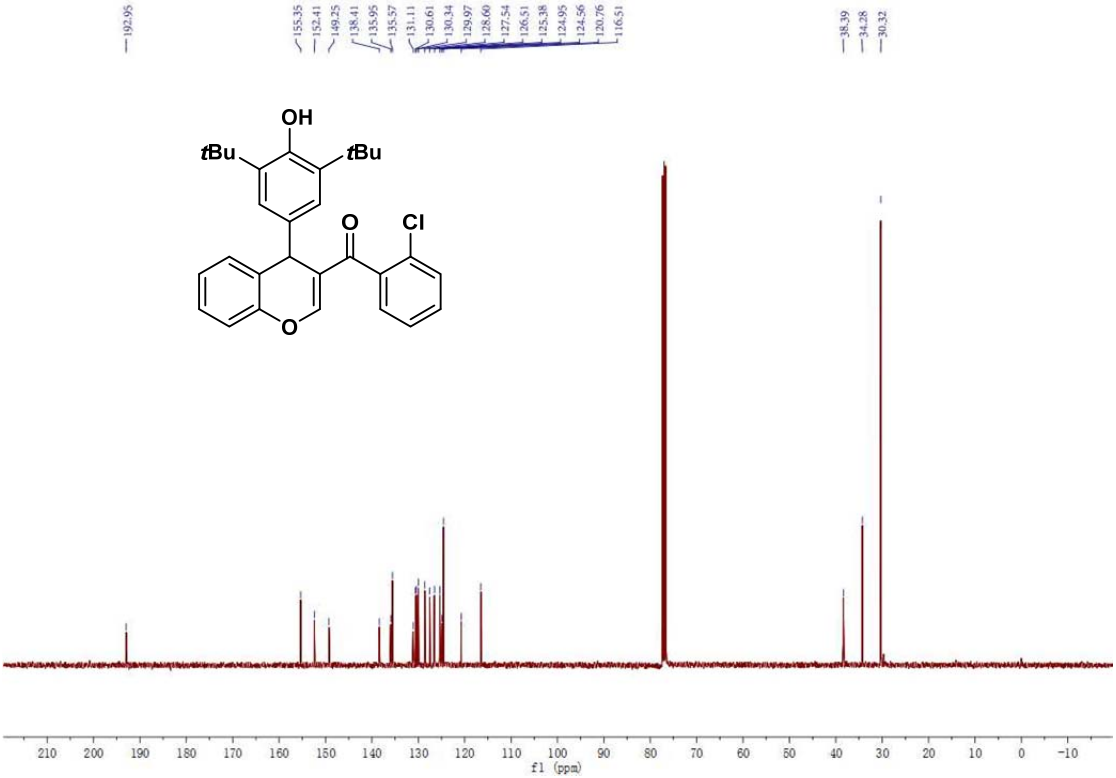

$^{13}$C NMR (100 MHz, $CDCl_3$) of compound **3ab**



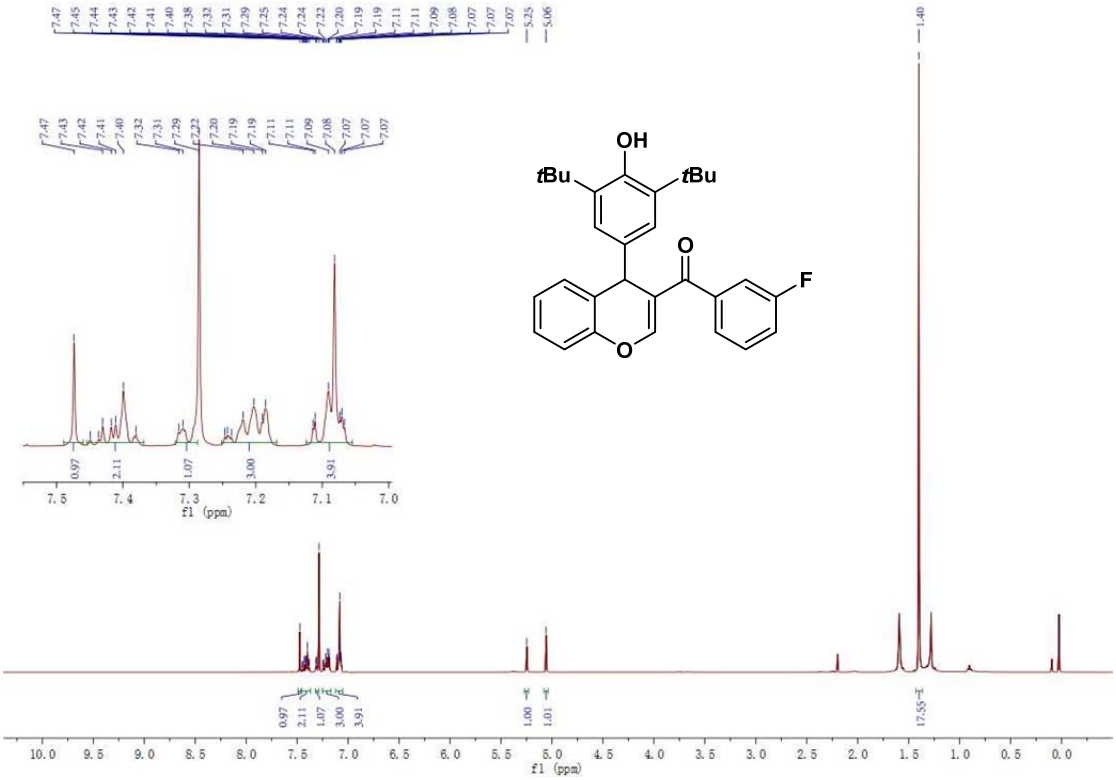
$^{1}$H NMR (400 MHz, $CDCl_3$) of compound **3ac**



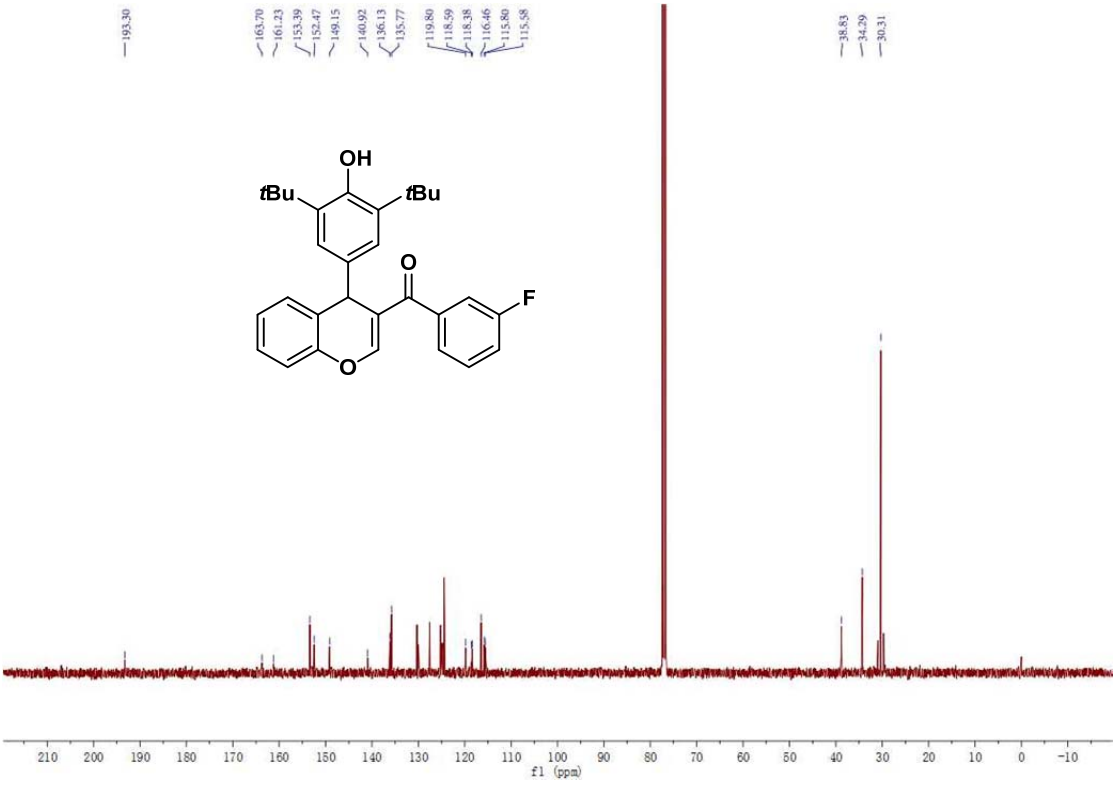

$^{13}$C NMR (100 MHz, $CDCl_3$) of compound **3ac**



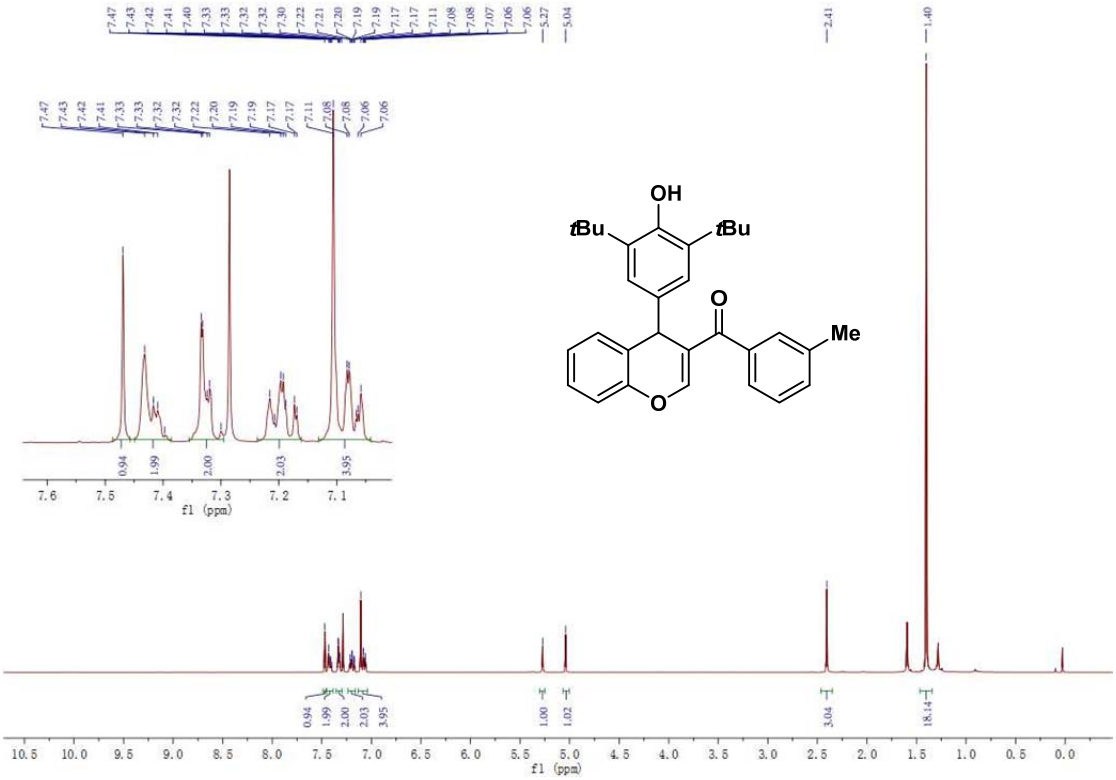
$^{1}$H NMR (400 MHz, $CDCl_3$) of compound **3ad**



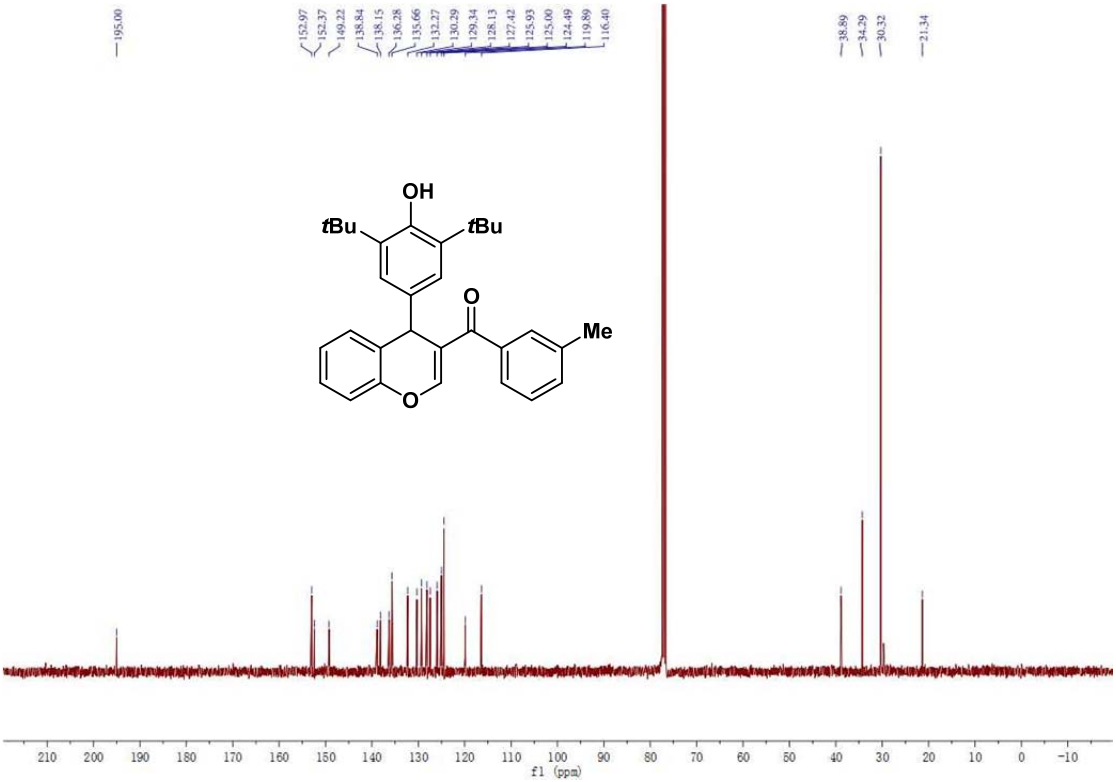

$^{13}$C NMR (100 MHz, $CDCl_3$) of compound **3ad**



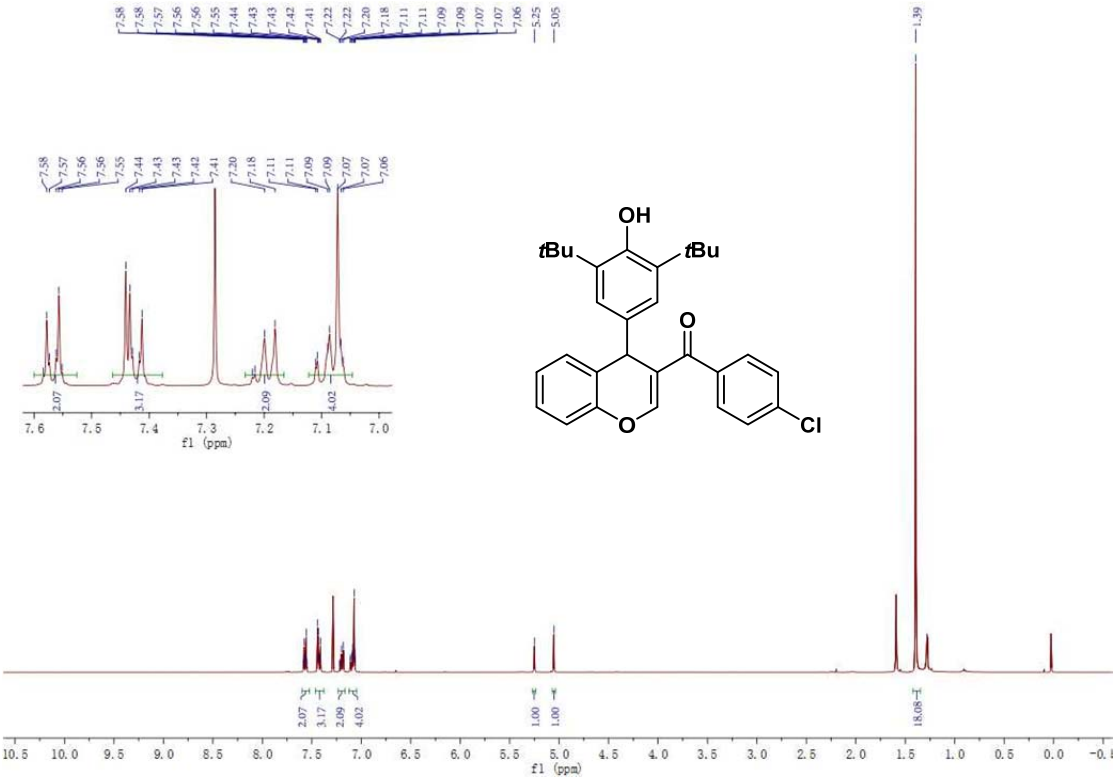
$^{1}$H NMR (400 MHz, $CDCl_3$) of compound **3ae**



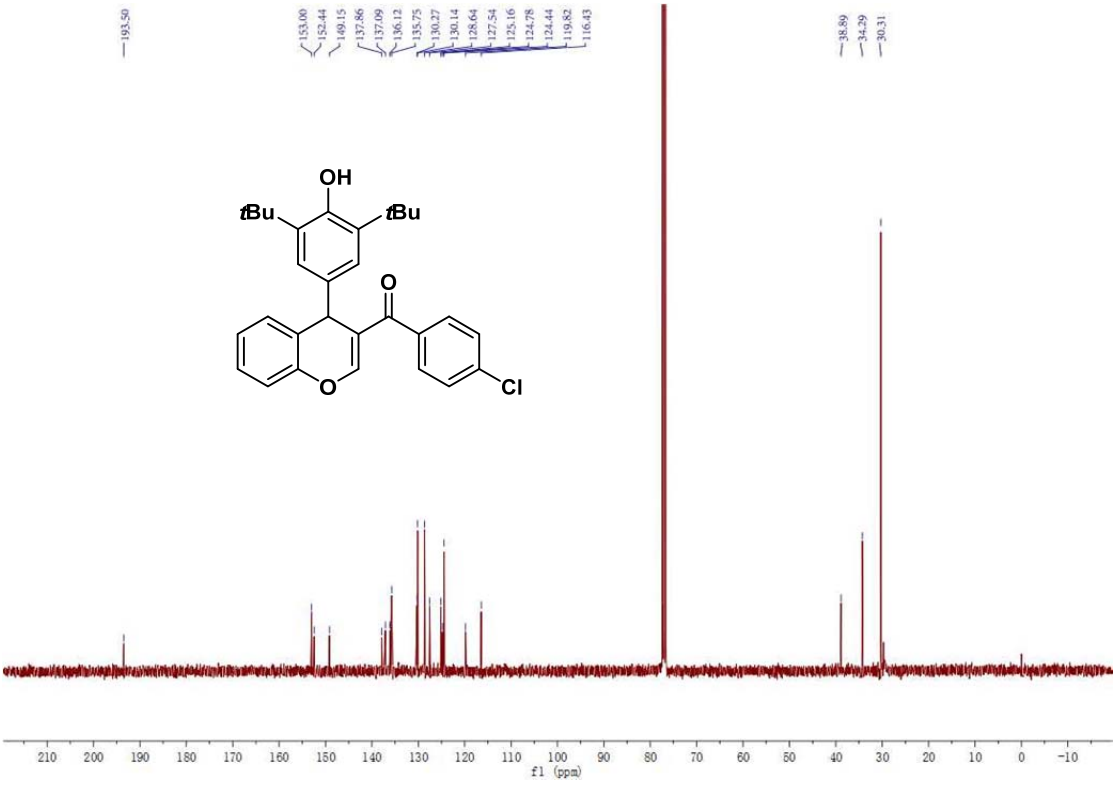

$^{13}$C NMR (100 MHz, $CDCl_3$) of compound **3ae**



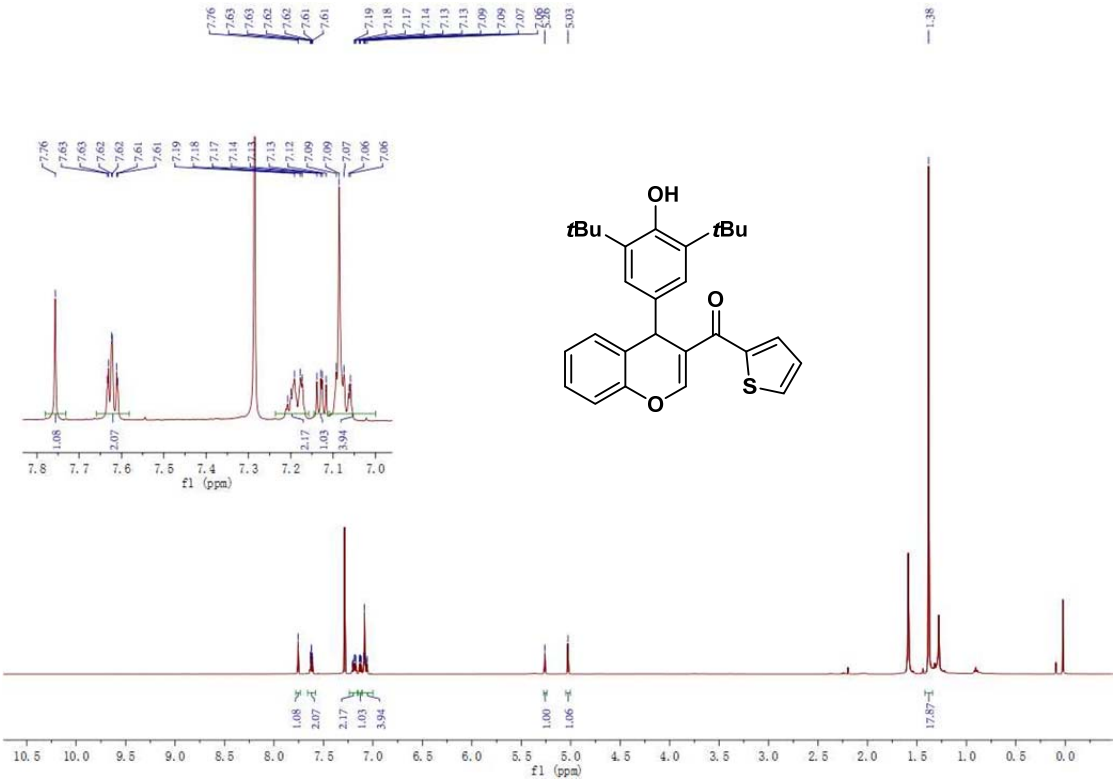
$^{1}$H NMR (400 MHz, $CDCl_3$) of compound **3af**



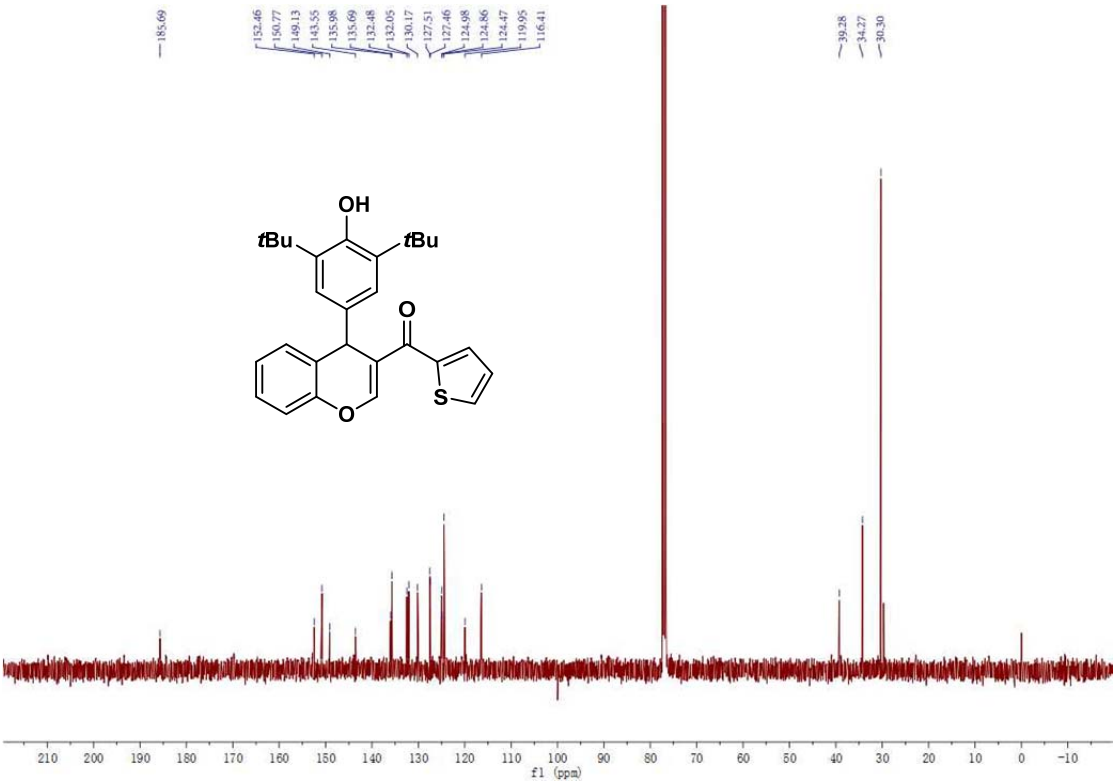

$^{13}$C NMR (100 MHz, $CDCl_3$) of compound **3af**



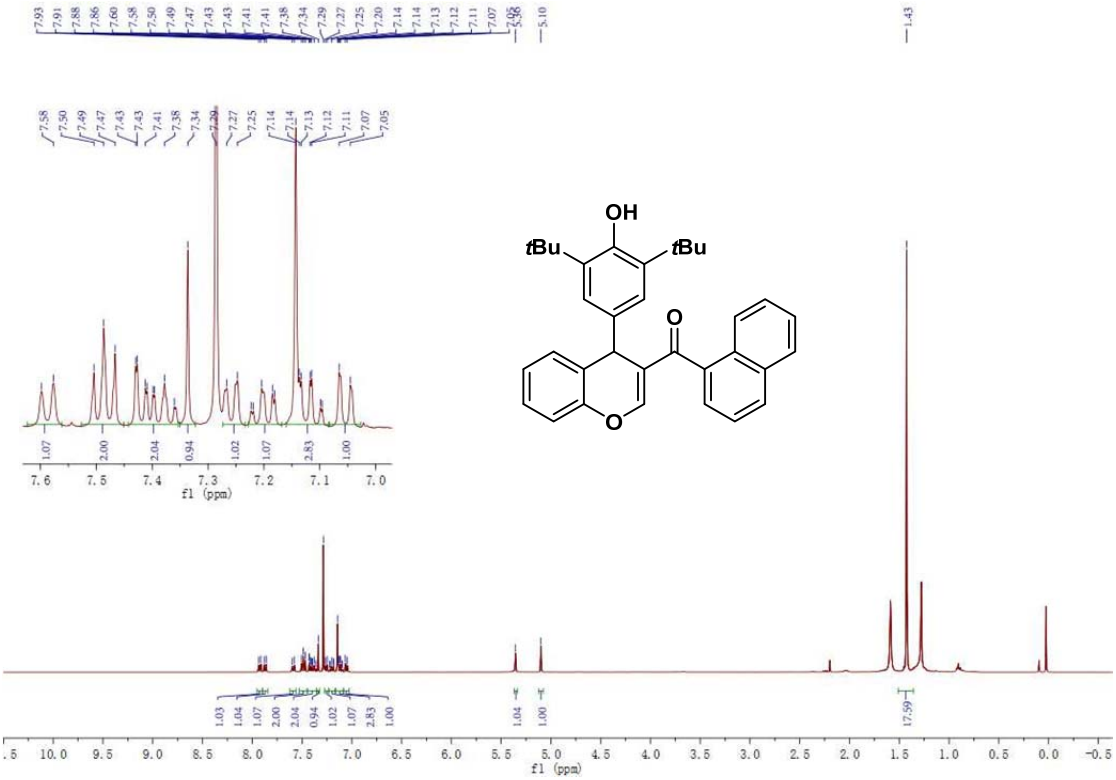
$^{1}$H NMR (400 MHz, $CDCl_3$) of compound **3ag**



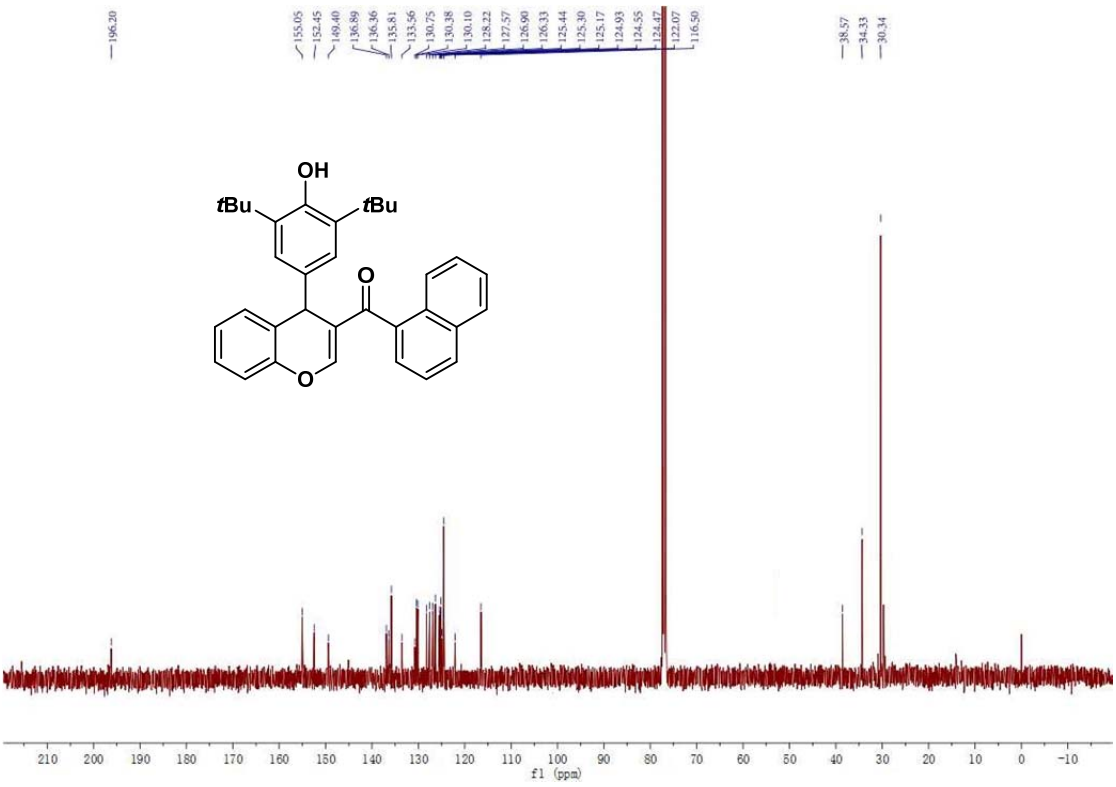

$^{13}$C NMR (100 MHz, $CDCl_3$) of compound **3ag**



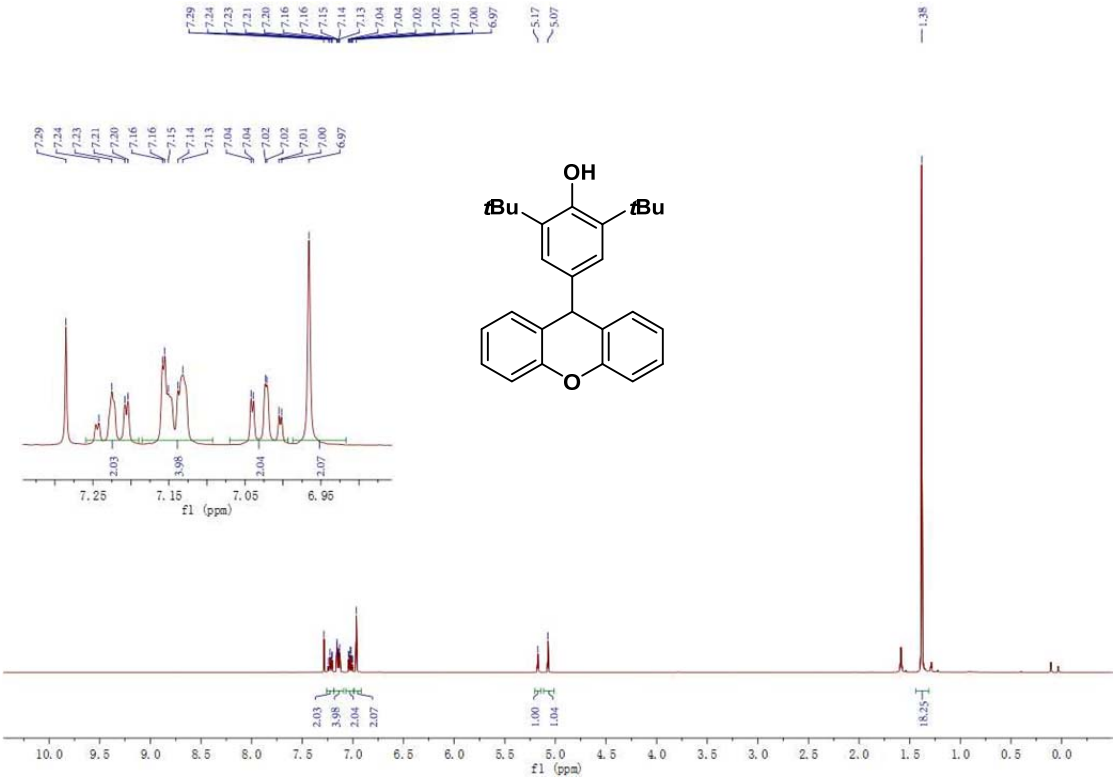
$^{1}$H NMR (400 MHz, $CDCl_3$) of compound **3ah**



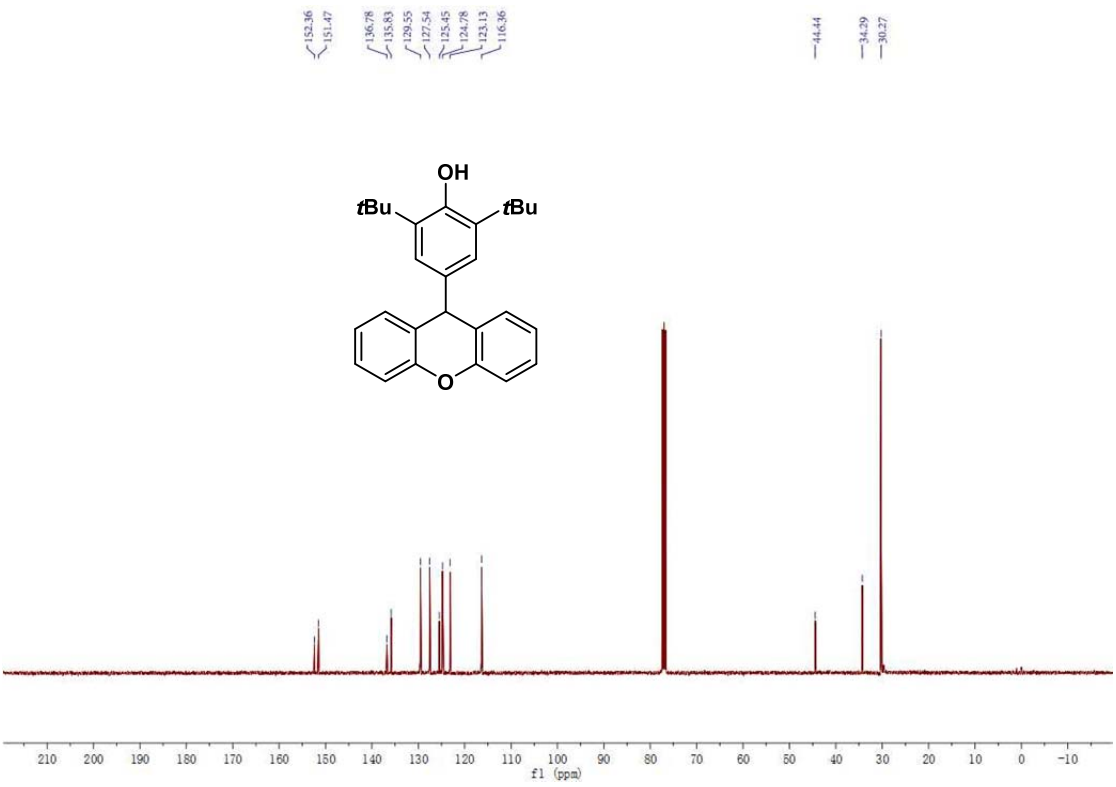

$^{13}$C NMR (100 MHz, $CDCl_3$) of compound **3ah**



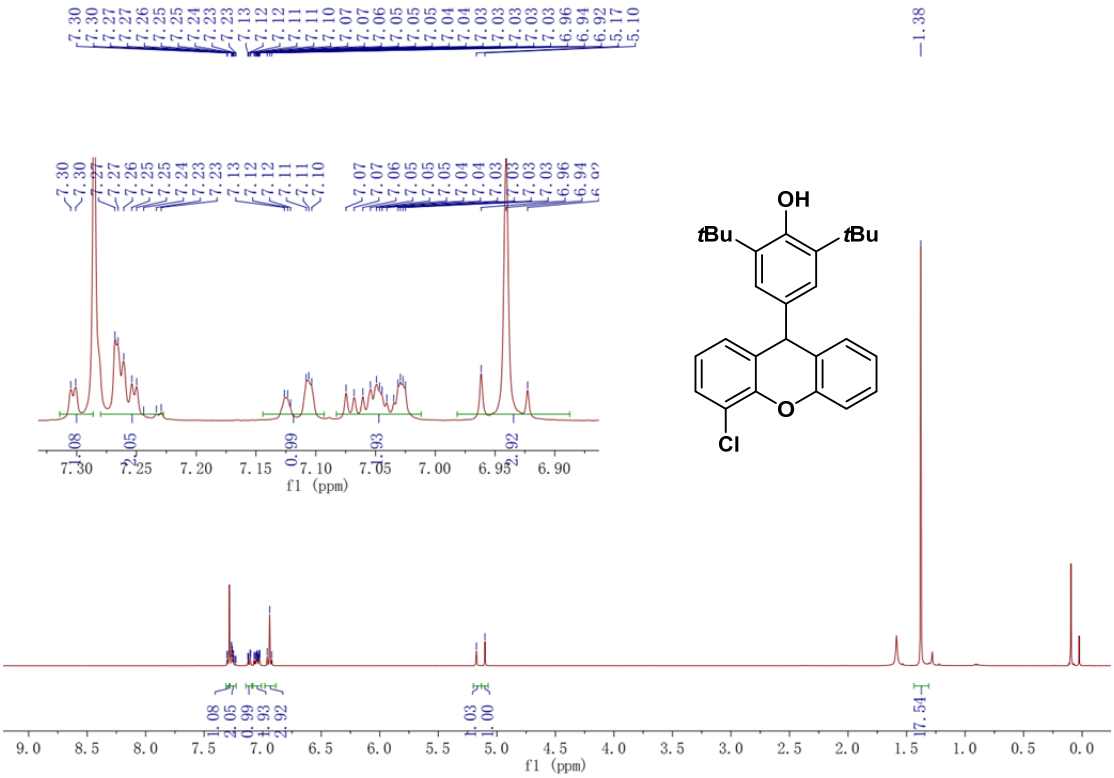
$^{1}$H NMR (400 MHz, $CDCl_3$) of compound **5a**



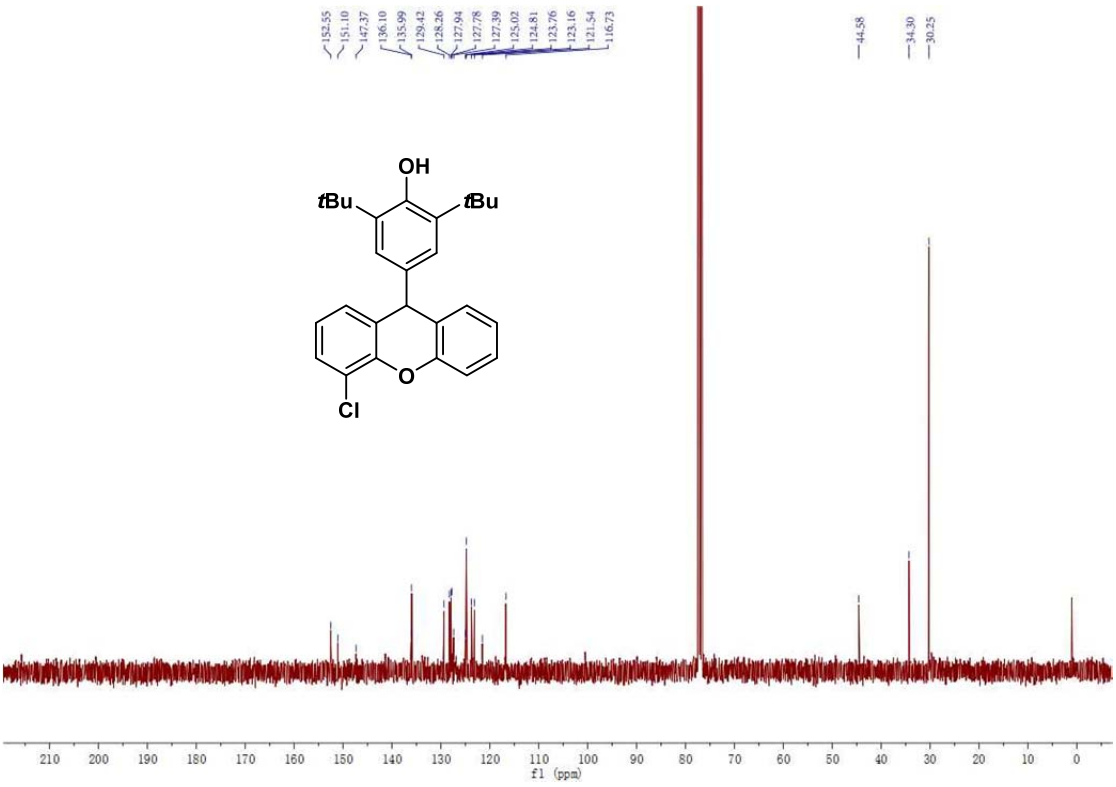

$^{13}$C NMR (100 MHz, $CDCl_3$) of compound **5a**



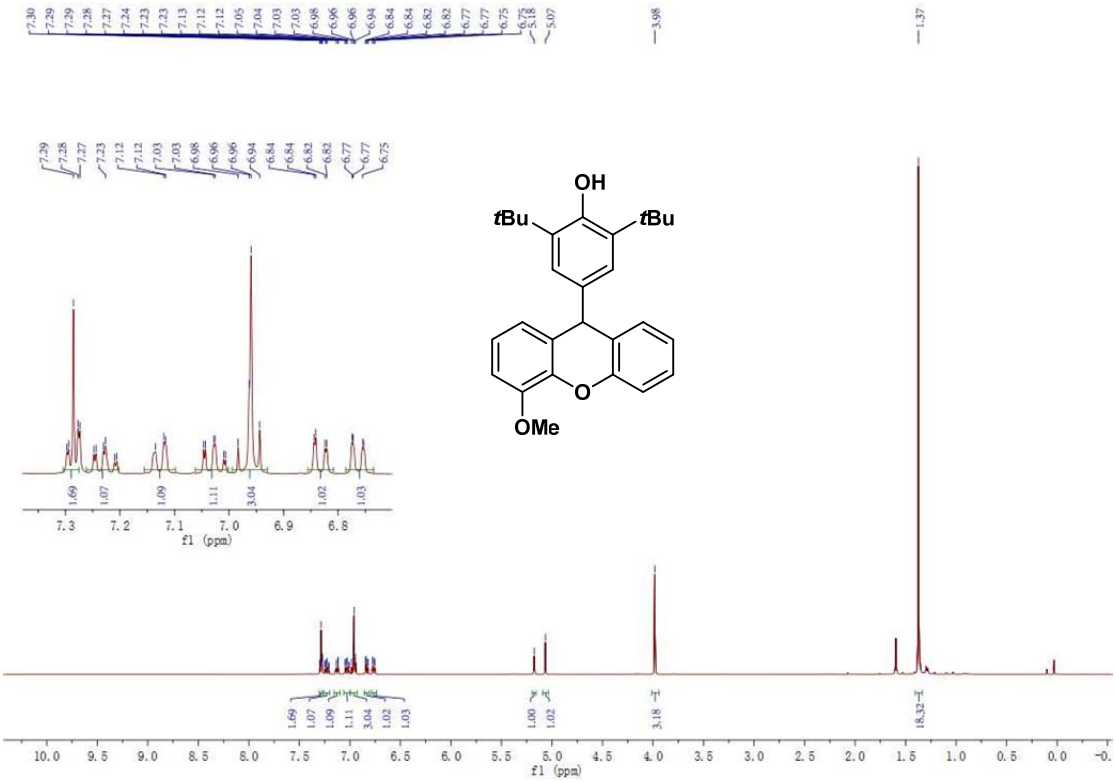
$^{1}$H NMR (400 MHz, $CDCl_3$) of compound **5b**



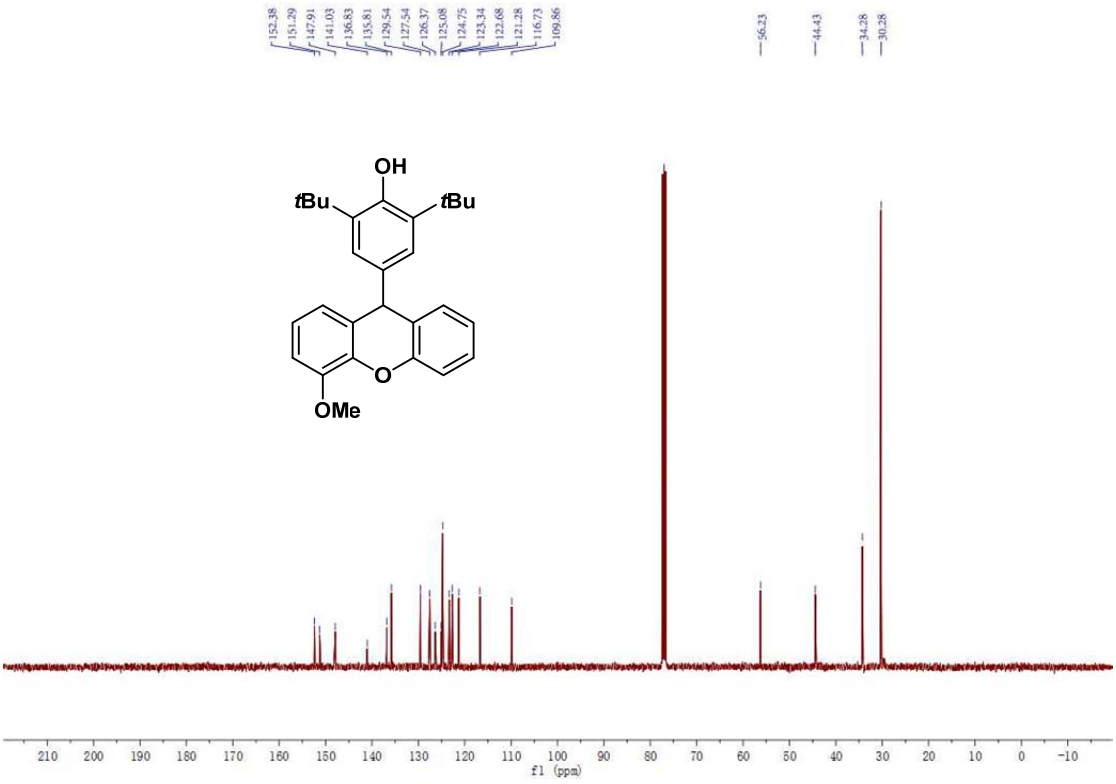

$^{13}$C NMR (100 MHz, $CDCl_3$) of compound **5b**



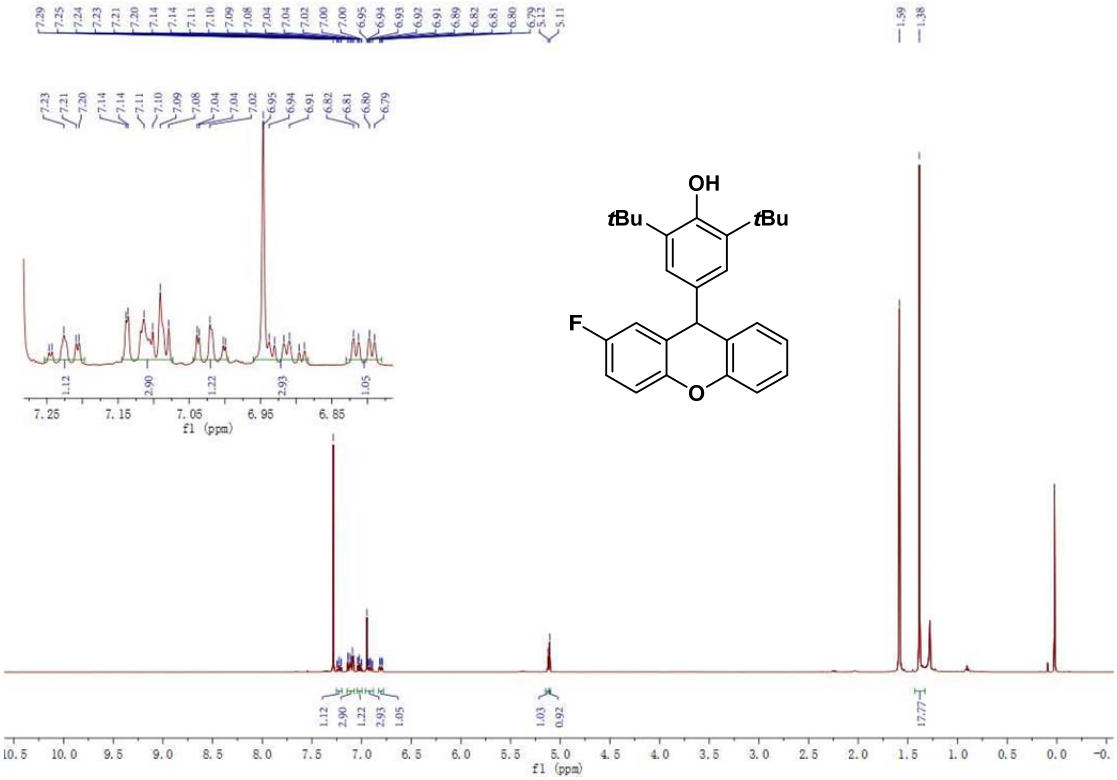
$^{1}$H NMR (400 MHz, $CDCl_3$) of compound **5c**



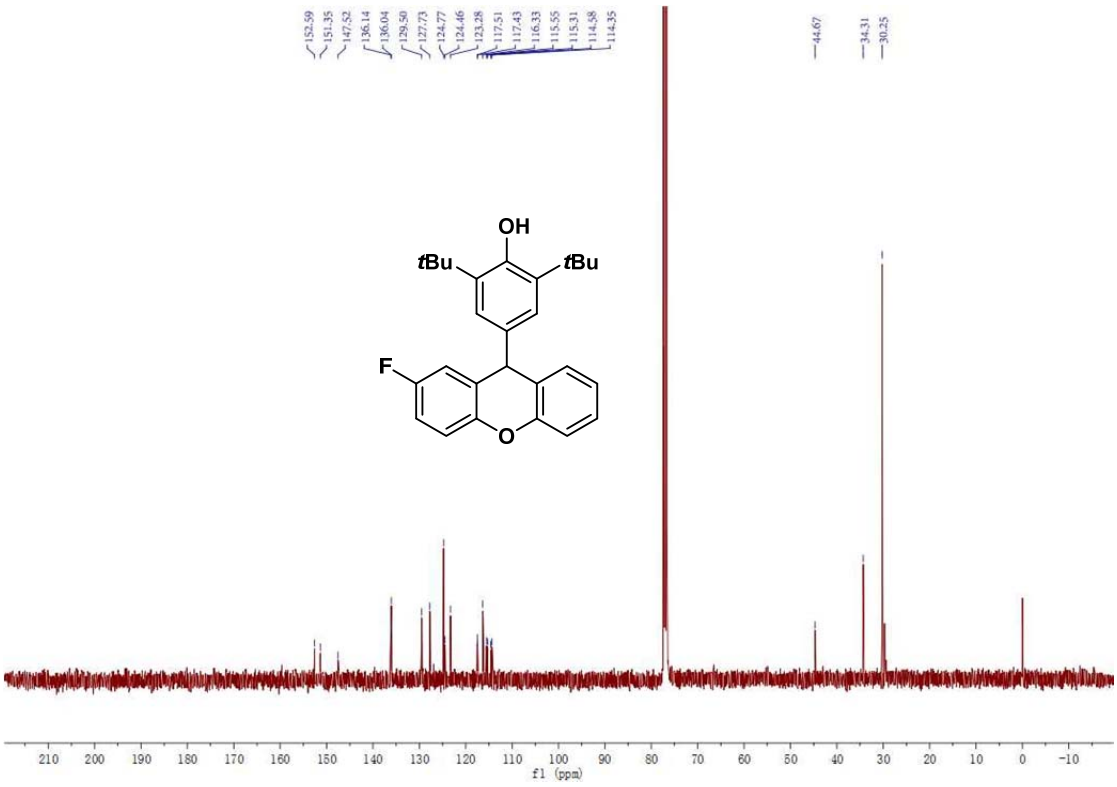

$^{13}$C NMR (100 MHz, $CDCl_3$) of compound **5c**



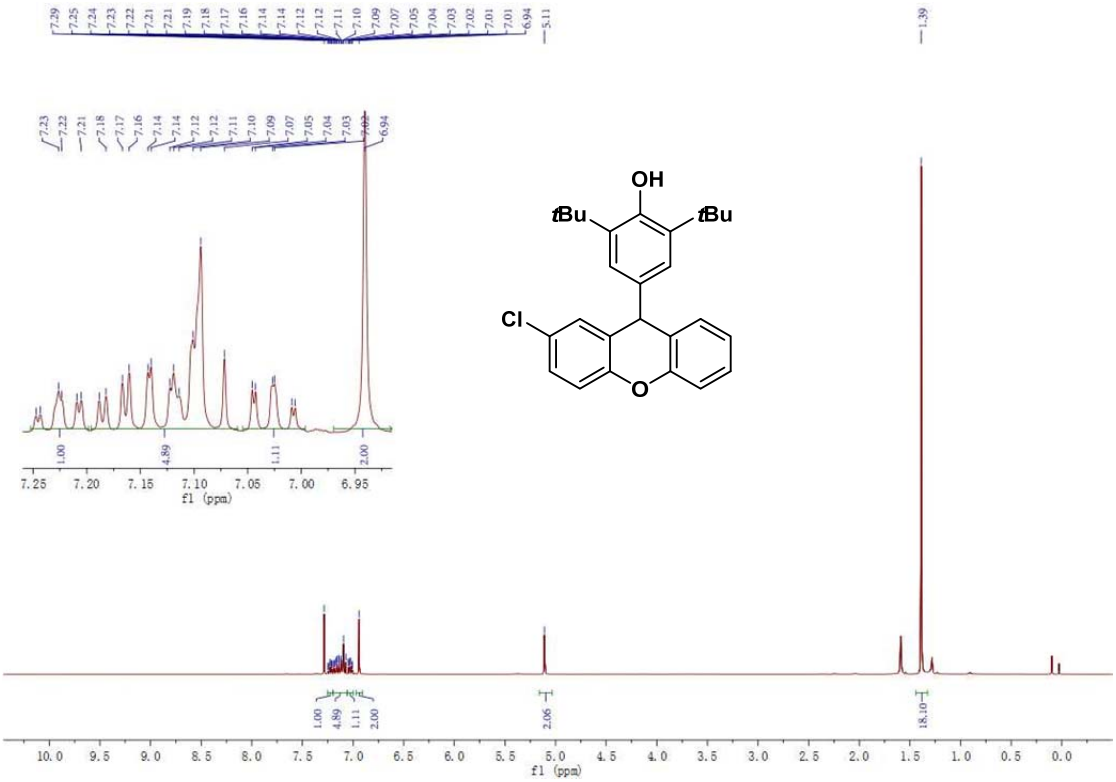
$^{1}$H NMR (400 MHz, $CDCl_3$) of compound **5e**



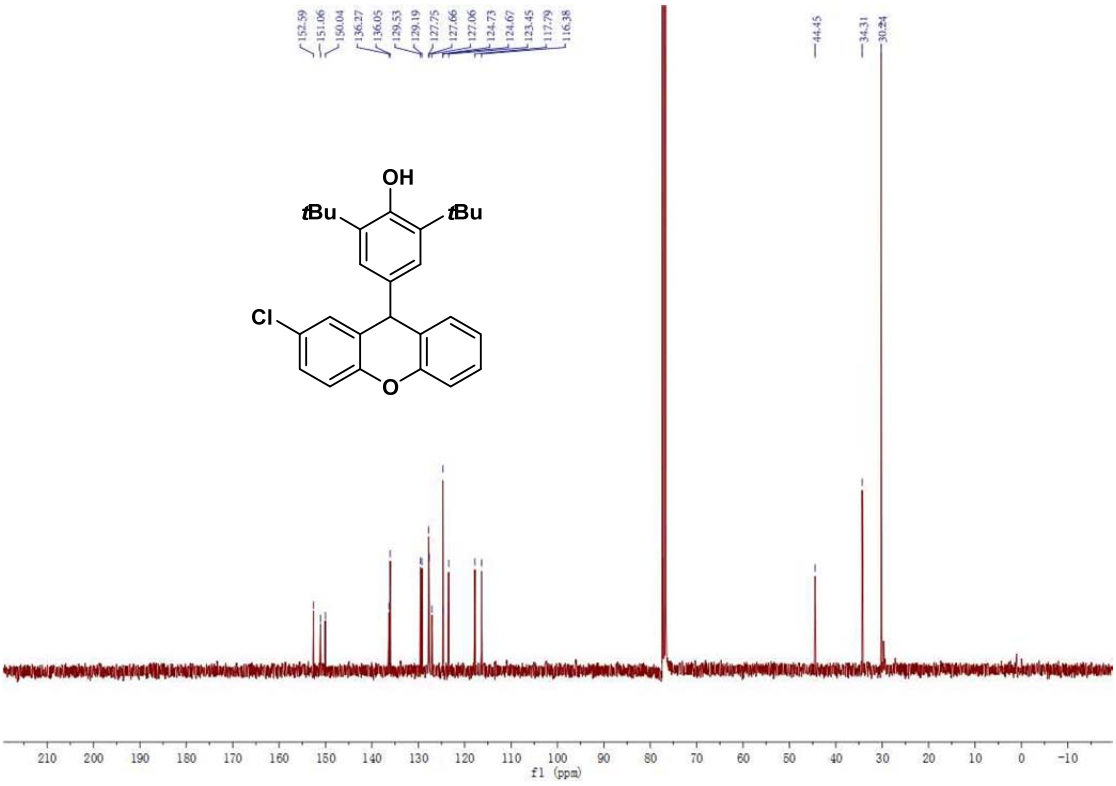

$^{13}$C NMR (100 MHz, $CDCl_3$) of compound **5e**



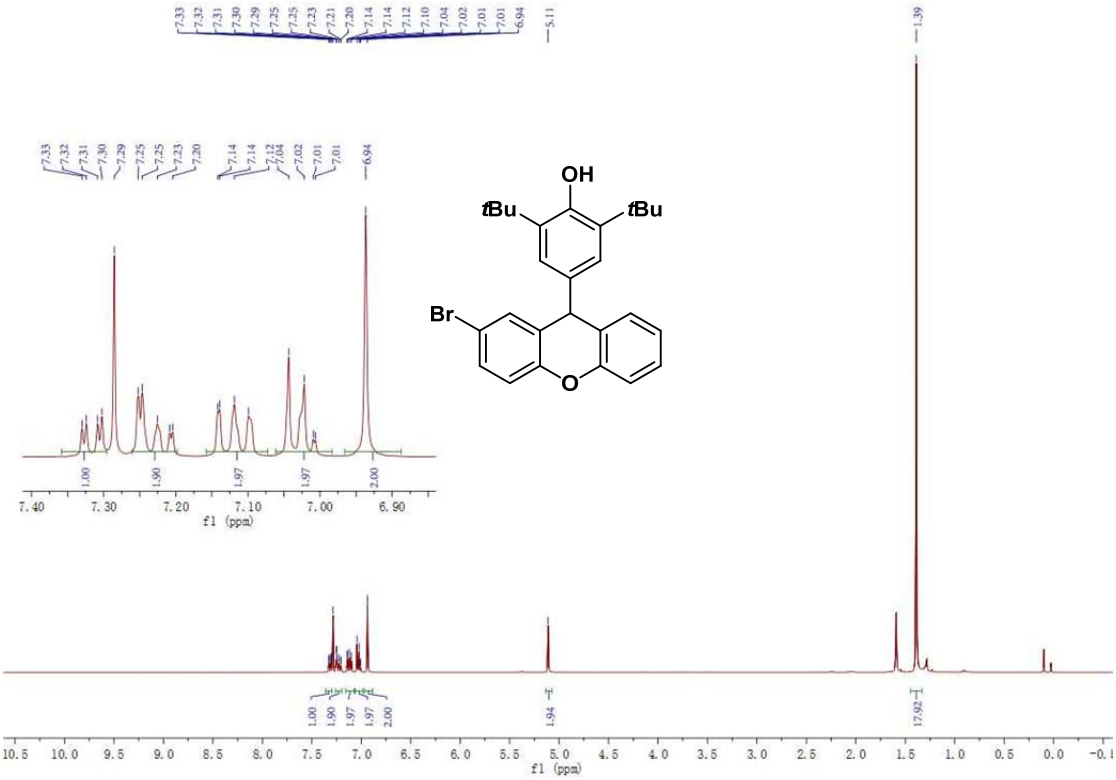
$^{1}$H NMR (400 MHz, $CDCl_3$) of compound **5f**



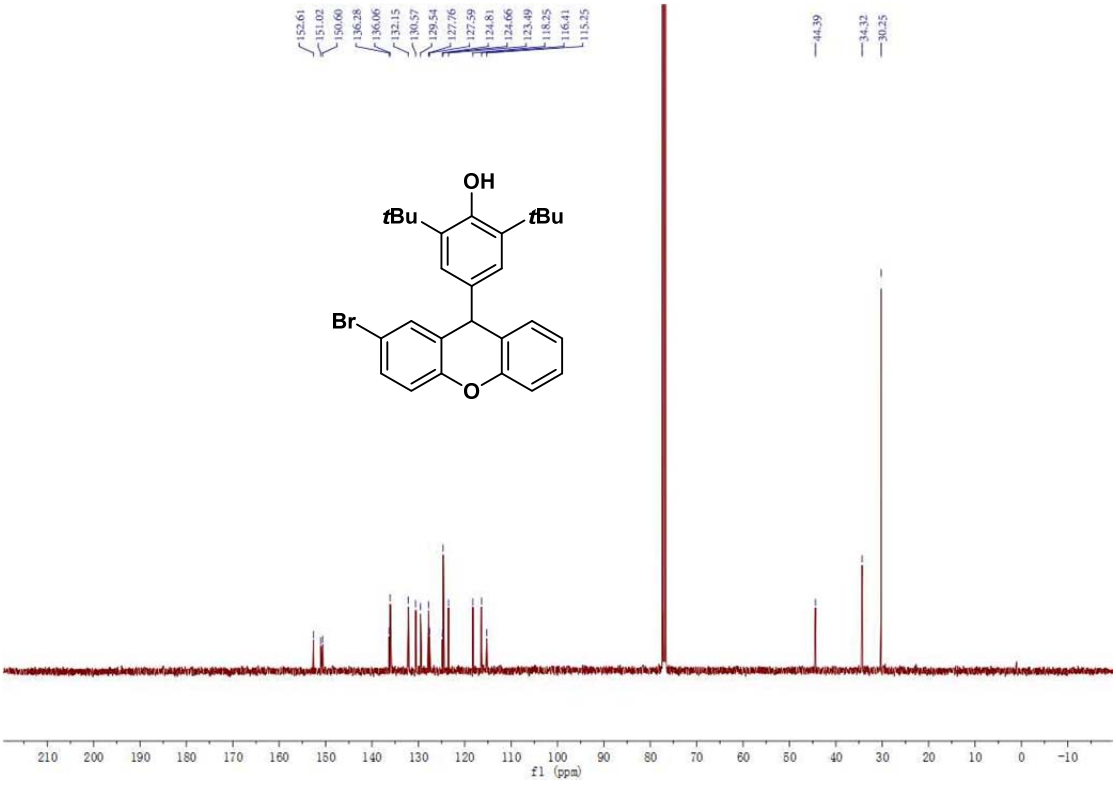

$^{13}$C NMR (100 MHz, $CDCl_3$) of compound **5f**



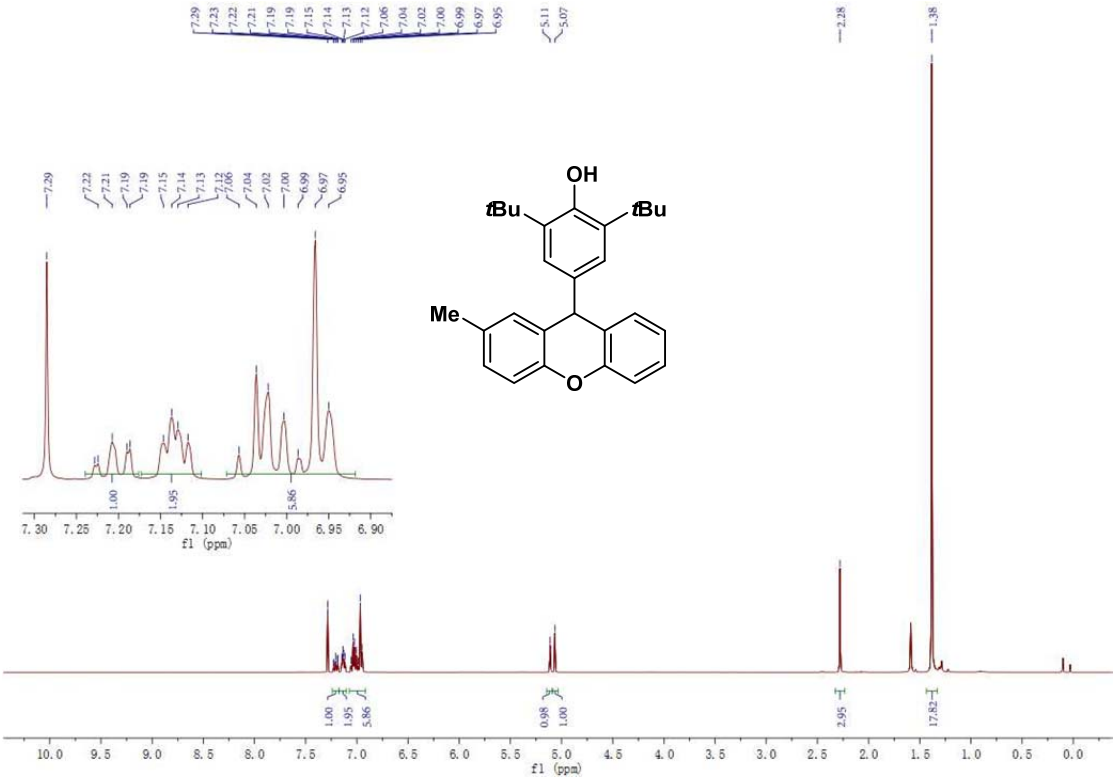
$^{1}$H NMR (400 MHz, $CDCl_3$) of compound **5g**



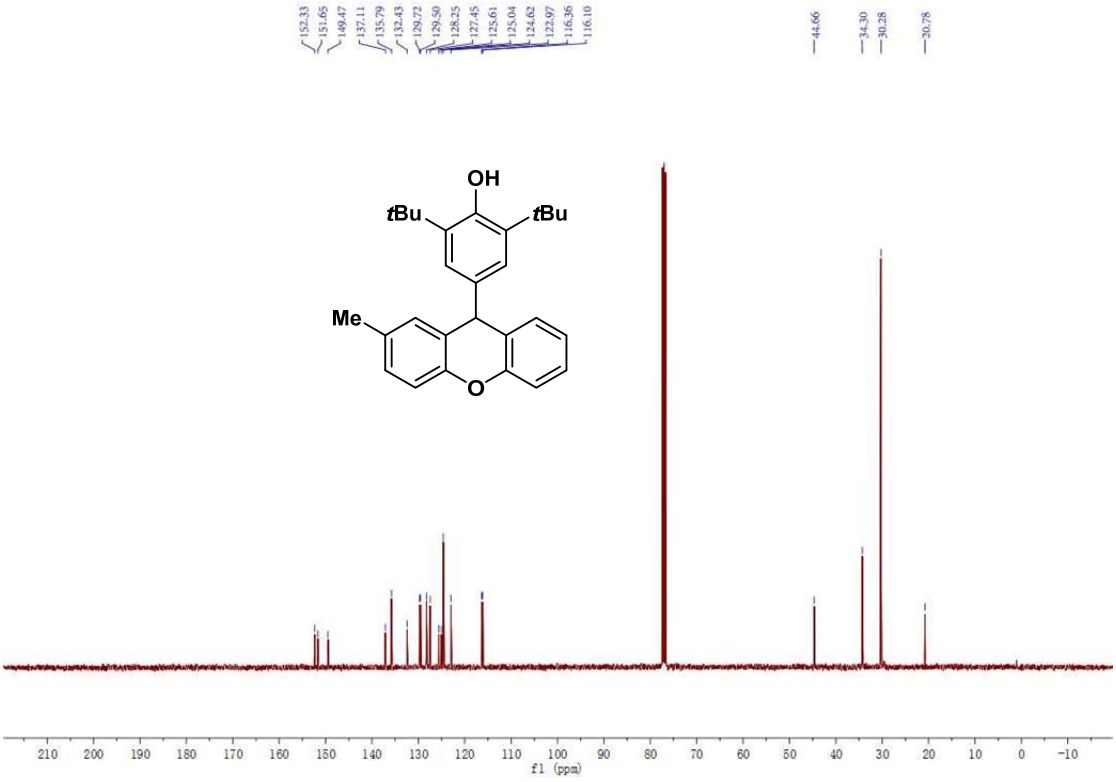

$^{13}$C NMR (100 MHz, $CDCl_3$) of compound **5g**



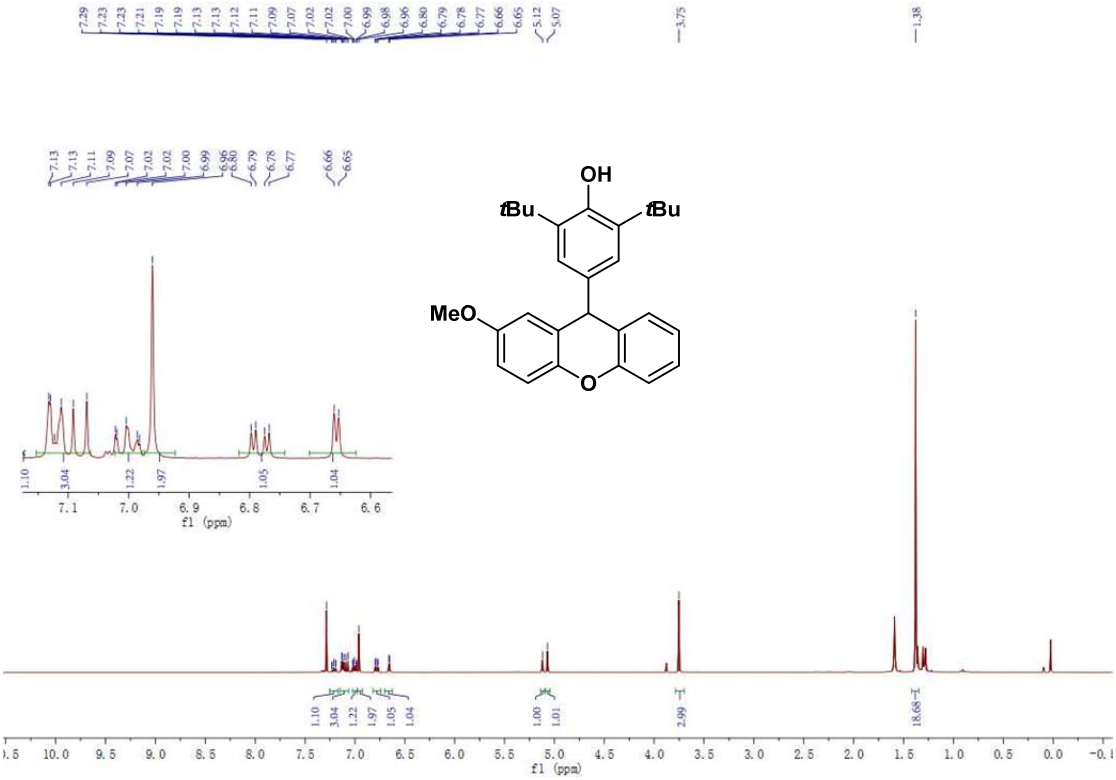
$^{1}$H NMR (400 MHz, $CDCl_3$) of compound **5h**



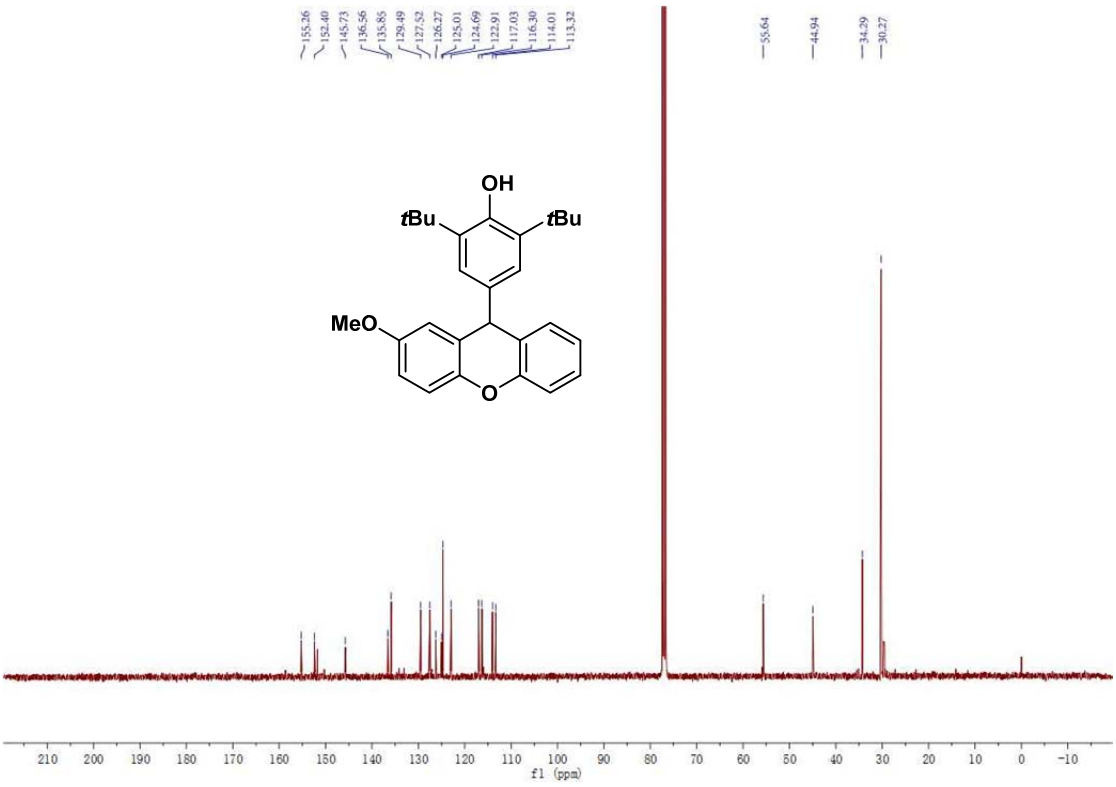

$^{13}$C NMR (100 MHz, $CDCl_3$) of compound **5h**



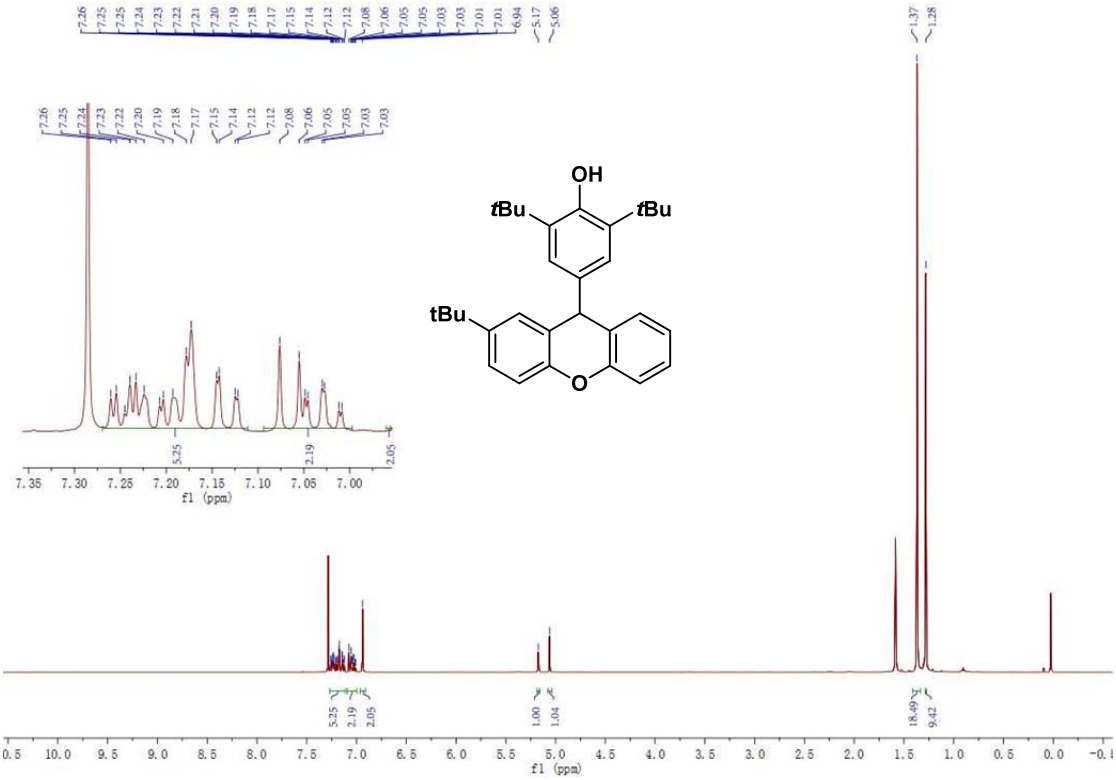
$^{1}$H NMR (400 MHz, $CDCl_3$) of compound **5i**



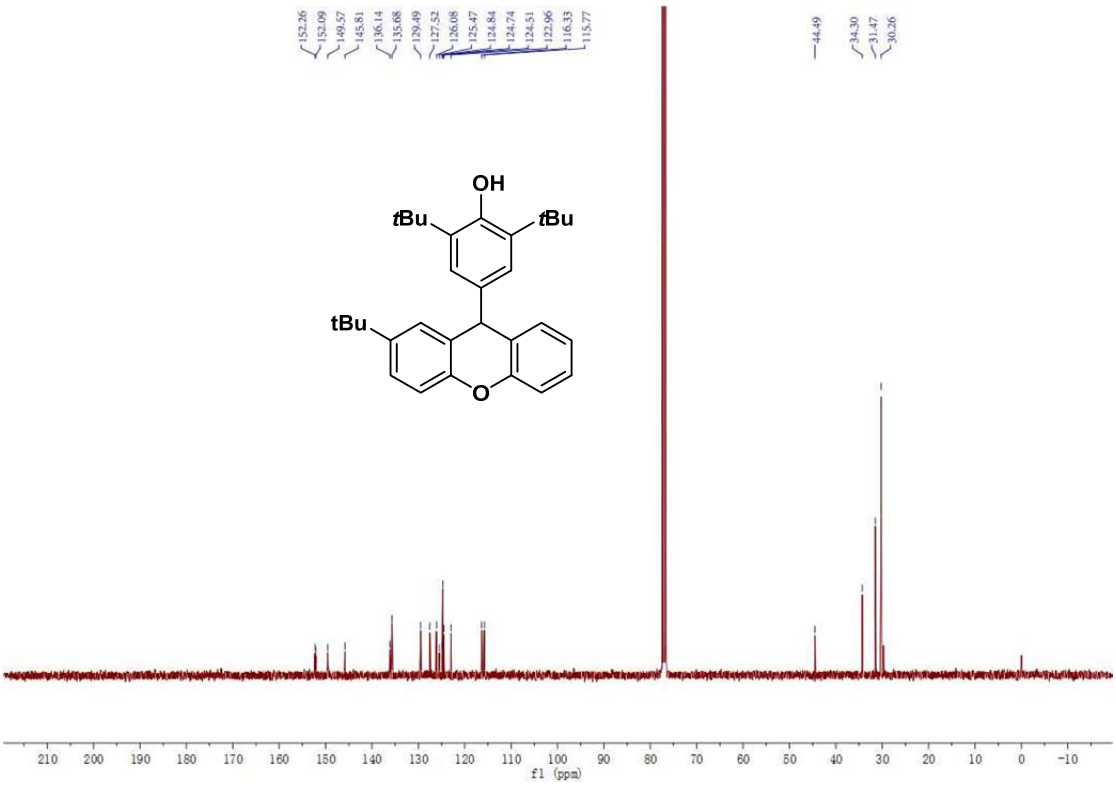

$^{13}$C NMR (100 MHz, $CDCl_3$) of compound **5i**



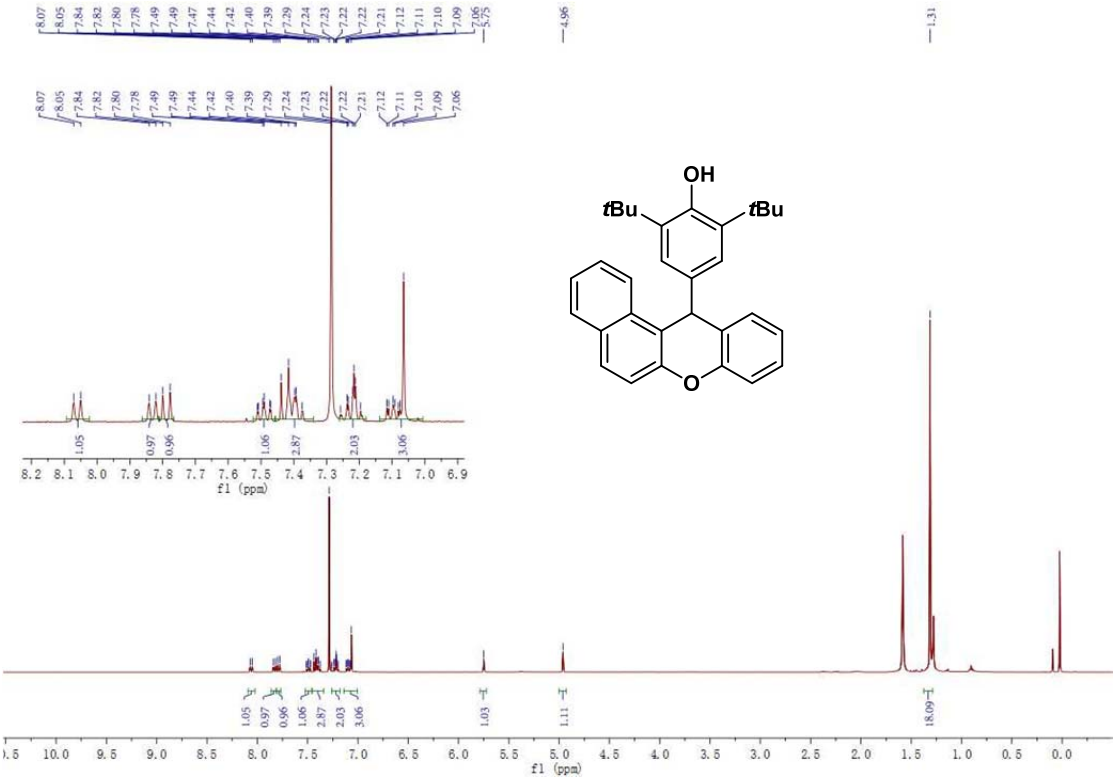
$^{1}$H NMR (400 MHz, $CDCl_3$) of compound **5j**



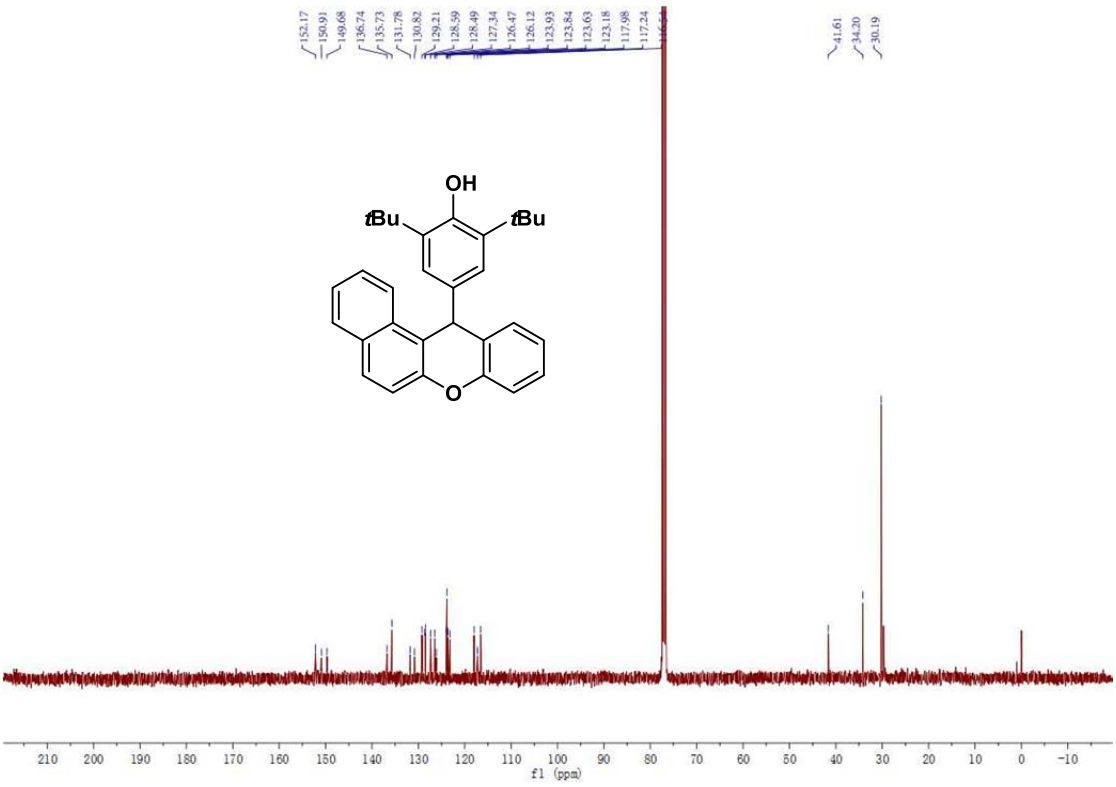

$^{13}$C NMR (100 MHz, $CDCl_3$) of compound **5j**



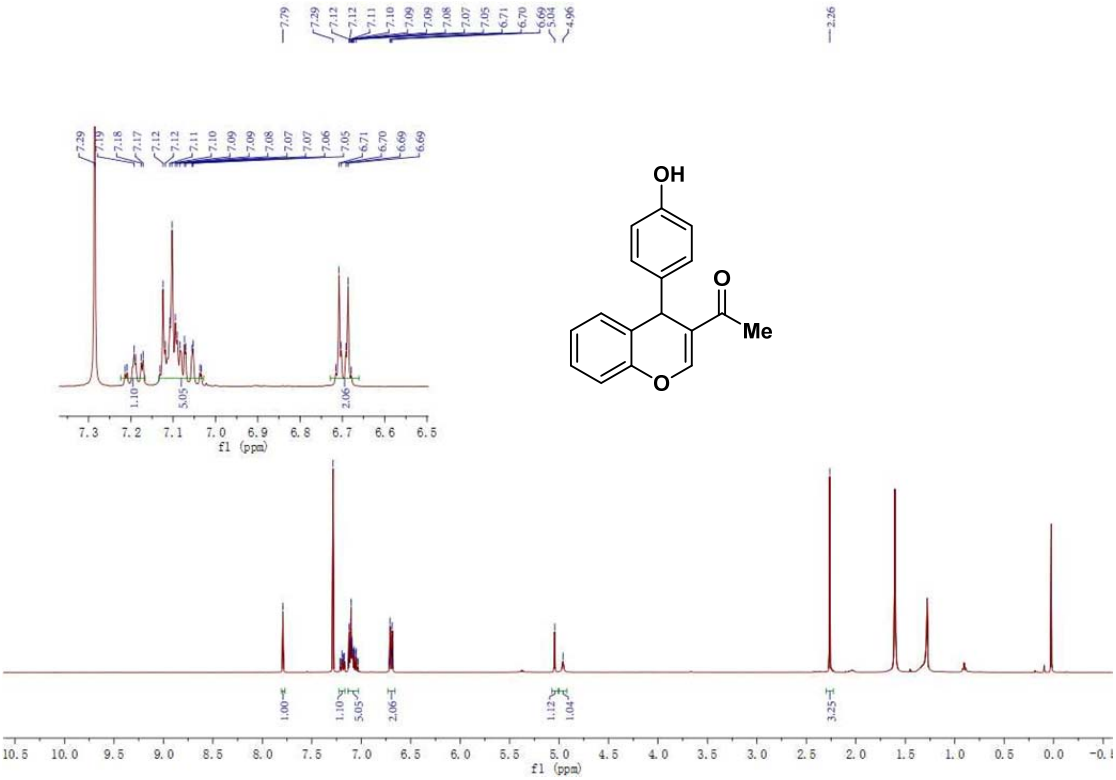
$^{1}$H NMR (400 MHz, $CDCl_3$) of compound **5k**



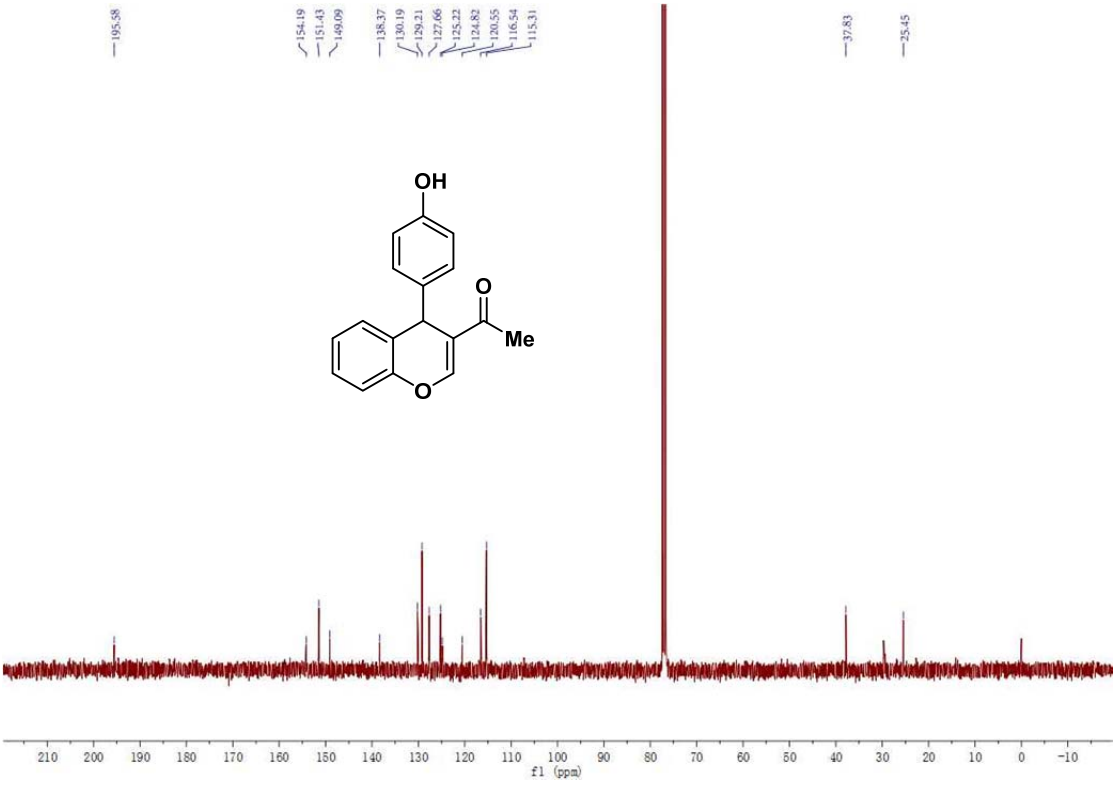

$^{13}$C NMR (100 MHz, $CDCl_3$) of compound **5k**



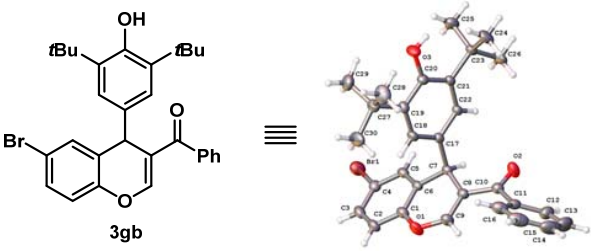
$^{1}$H NMR (400 MHz, $CDCl_3$) of compound **6**




$^{13}$C NMR (100 MHz, $CDCl_3$) of compound **6**

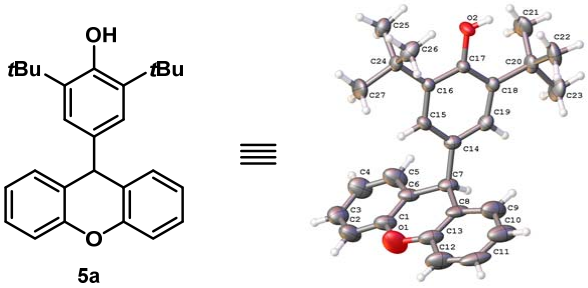


## 2. X-ray single crystal data for product 3gb and 5a




The thermal ellipsoid was drawn at the 30% probability level.

| | | |
|---|---|---|
| Empirical formula | C30 H31 Br O3 | |
| Formula weight | 519.46 | |
| Temperature | 296.15 K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | P 1 21/c 1 | |
| Unit cell dimensions | a = 16.1179(13) Å | α= 90°. |
| | b = 17.7380(14) Å | β= 105.4710(10)°. |
| | c = 9.6044(7) Å | γ = 90°. |
| Volume | 2646.4(4) $Å^3$ | |
| Z | 4 | |
| Density (calculated) | 1.304 $Mg/m^3$ | |
| Absorption coefficient | 1.581 $mm^{-1}$ | |
| F(000) | 1080 | |
| Theta range for data collection | 2.482 to 25.989°. | |
| Index ranges | -19<=h<=19, -21<=k<=16, -11<=l<=11 | |
| Reflections collected | 16087 | |
| Independent reflections | 5177 [R(int) = 0.0205] | |
| Completeness to theta = 25.242° | 99.7 % | |
| Absorption correction | Semi-empirical from equivalents | |
| Max. and min. transmission | 0.7457 and 0.6352 | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 5177 / 1 / 317 | |
| Goodness-of-fit on $F^2$ | 1.026 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0370, wR2 = 0.0907 | |
| R indices (all data) | R1 = 0.0504, wR2 = 0.0971 | |
| Extinction coefficient | n/a | |
| Largest diff. peak and hole | 0.399 and -0.433 $e.Å^{-3}$ | |




The thermal ellipsoid was drawn at the 30% probability level.

| | | |
|---|---|---|
| Empirical formula | C27 H30 O2 | |
| Formula weight | 386.51 | |
| Temperature | 296.15 K | |
| Wavelength | 0.71073 Å | |
| Crystal system | Monoclinic | |
| Space group | P 1 21/c 1 | |
| Unit cell dimensions | a = 10.046(3) Å | α= 90°. |
| | b = 10.897(3) Å | β= 97.917(14)°. |
| | c = 20.397(6) Å | γ = 90°. |
| Volume | 2211.6(11) $Å^3$ | |
| Z | 4 | |
| Density (calculated) | 1.161 $Mg/m^3$ | |
| Absorption coefficient | 0.071 $mm^{-1}$ | |
| F(000) | 832 | |
| Theta range for data collection | 2.668 to 25.991°. | |
| Index ranges | -12<=h<=12, -12<=k<=13, -25<=l<=22 | |
| Reflections collected | 13409 | |
| Independent reflections | 4339 [R(int) = 0.0672] | |
| Completeness to theta = 25.242° | 99.7 % | |
| Absorption correction | None | |
| Refinement method | Full-matrix least-squares on $F^2$ | |
| Data / restraints / parameters | 4339 / 0 / 272 | |
| Goodness-of-fit on $F^2$ | 0.926 | |
| Final R indices [I>2sigma(I)] | R1 = 0.0646, wR2 = 0.1656 | |
| R indices (all data) | R1 = 0.1221, wR2 = 0.1917 | |
| Extinction coefficient | n/a | |
| Largest diff. peak and hole | 0.220 and -0.293 $e.Å^{-3}$ | |