

## Table of Contents

|  |    |
|--|----|
| 1. General information .....                                       | 1  |
| 2. Faradaic efficiency .....                                       | 2  |
| 3. Preparation of the starting materials .....                     | 2  |
| 3.1 General procedure for the synthesis of alkynes .....           | 2  |
| 3.2 General procedure for the synthesis of sulfoxonium ylides..... | 4  |
| 3. General preparation of 1,4-dicarbonyl Z-alkenes .....           | 6  |
| 4. Molecular structure and crystallographic data .....             | 7  |
| 5. Computational studies Computational details .....               | 10 |
| 6. Optimization of reaction conditions.....                        | 26 |
| 7. Gram-scale reaction .....                                       | 27 |
| 8. Synthetic Application.....                                      | 28 |
| 9. Cyclic voltammetry study .....                                  | 30 |
| 10. Control experiment .....                                       | 35 |
| 10.1 Radical trapping experiment .....                             | 35 |
| 10.2 <sup>18</sup> O-labeling experenments.....                    | 37 |
| 10.3 Inert atmosphere and No H <sub>2</sub> O.....                 | 38 |
| 10.4 Intermediate detection.....                                   | 39 |
| 11. NMR Spectra for the Obtained Compound.....                     | 40 |
| 12. References .....   | 59 |
| 13. NMR Spectra .....  | 60 |

## 1. General information

All reactions were carried out in sealed air using oven dried glassware. 1,1,1,3,3,3-hexafluoro-2-propanol, 1,2-dichloroethane, tetrabutylammonium perchlorate, and graphite felt are all available from commercial sources. Deionized water is obtained by ultra pure water machine. The electrochemical instrument is HONGSHENGFENG DPS-305BM. Column chromatography was performed on silica gel (200-300 mesh). NMR spectra were recorded in CDCl<sub>3</sub> on 500 MHz spectrometers. <sup>1</sup>H NMR chemical shifts (δ) are reported in parts per million relative to tetramethylsilane (0 ppm). The following abbreviations are used for multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublets, dt = doublet of triplets, and m = multiplet. HRMS were obtained on an Ultima Global spectrometer with an ESI source. Melting points are uncorrected.

## 2. Faradaic efficiency

The current efficiency c.e. (coulombic yield) for the products were given according to the following Faraday efficiency formula. They were presented in Table 2 and Scheme 2 in the main text.

$$\eta = \frac{z_p \cdot N_p \cdot F}{I \cdot t} \times 100\%$$

$\eta$ : Faradaic efficiency in percent [%],  $z_p$ : Number of electrons per product [-],  $N_p$ : Number of mols of the product [mol],  $F$ : Faraday constant [96 485 sA mol<sup>-1</sup>],  $I$ : Current [mA],  $t$ : Time [s]

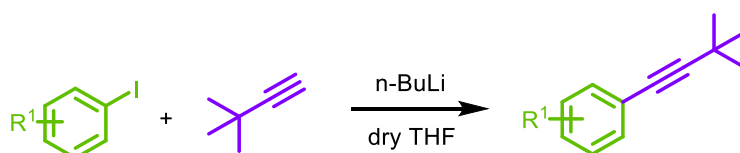
The calculation of the current efficiency of **3a** is as follows:

$$\eta = \frac{2 \cdot 0.84 \cdot 0.1 \cdot 96485}{5 \cdot 2.25 \cdot 3600} \times 100\% = 40\%$$

## 3. Preparation of the starting materials

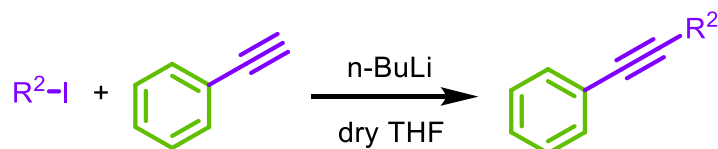
### 3.1 General procedure for the synthesis of alkynes

The compounds **1a-5a** were prepared according to previously described methods.<sup>[1]</sup>



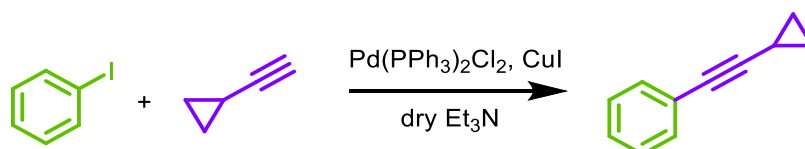
To a flame-dried round-bottom flask under N<sub>2</sub> was added alkyne (5.0 mmol, 1.0 eq.) followed by dry THF (25.0 mL, 0.2 M). Cool the flask to 0 °C. *n*-Butyllithium (4.0 mL, 2.5 M in hexanes, 10.0 mmol, 2.0 eq.) was added slowly and the reaction was allowed to stir for 1 hour. Iodoalkane (21.0 mmol, 2.1 eq.) was added at -20 °C and the reaction was allowed to stir at room temperature for 3 ~ 5 hour (when most of alkyne was consumed as detected by TLC). The reaction was quenched with a saturated solution of ammonium chloride and extracted with ethyl acetate. The organics were dried over MgSO<sub>4</sub> and the solvents were removed under reduced pressure. The residue was purified by silica chromatography to afford the corresponding compounds **1a-5a**.

The compounds **6a-8a**, **12a** were prepared according to previously described methods.<sup>[1]</sup>



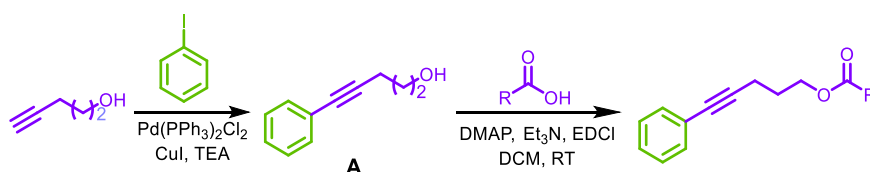
To a flame-dried round-bottom flask under  $N_2$  was added alkyne (5.0 mmol, 1.0 eq.) followed by dry THF (25.0 mL, 0.2 M). Cool the flask to  $0\text{ }^\circ\text{C}$ . *n*-Butyllithium (4.0 mL, 2.5 M in hexanes, 10.0 mmol, 2.0 eq.) was added slowly and the reaction was allowed to stir for 1 hour. Iodoalkane (21.0 mmol, 2.1 eq.) was added at  $-20\text{ }^\circ\text{C}$  and the reaction was allowed to stir at room temperature for 3 ~ 5 hour (when most of alkyne was consumed as detected by TLC). The reaction was quenched with a saturated solution of ammonium chloride and extracted with ethyl acetate. The organics were dried over  $MgSO_4$  and the solvents were removed under reduced pressure. The residue was purified by silica chromatography to afford the corresponding compounds **6a-8a**, **12a**.

The compounds **9a** were prepared according to previously described methods.<sup>[1]</sup>



To a 50 mL flame-dried round-bottom flask, under  $N_2$ , was added  $PdCl_2(PPh_3)_2$  (0.05 mmol, 0.01 eq.),  $CuI$  (0.1 mmol, 0.02 eq.), iodobenzene (5.0 mmol, 1.0 eq.), cyclopropyl acetylene (6.0 mmol, 1.2 eq.) and dry  $Et_3N$  (10.0 mL), the reaction was allowed to stir at room temperature. The reaction was stirred overnight checked by TLC. The reaction is filtered over celite, washing with dichloromethane. The solvent was removed and the residue purified by flash column chromatography on silica gel to give compounds **9a**.

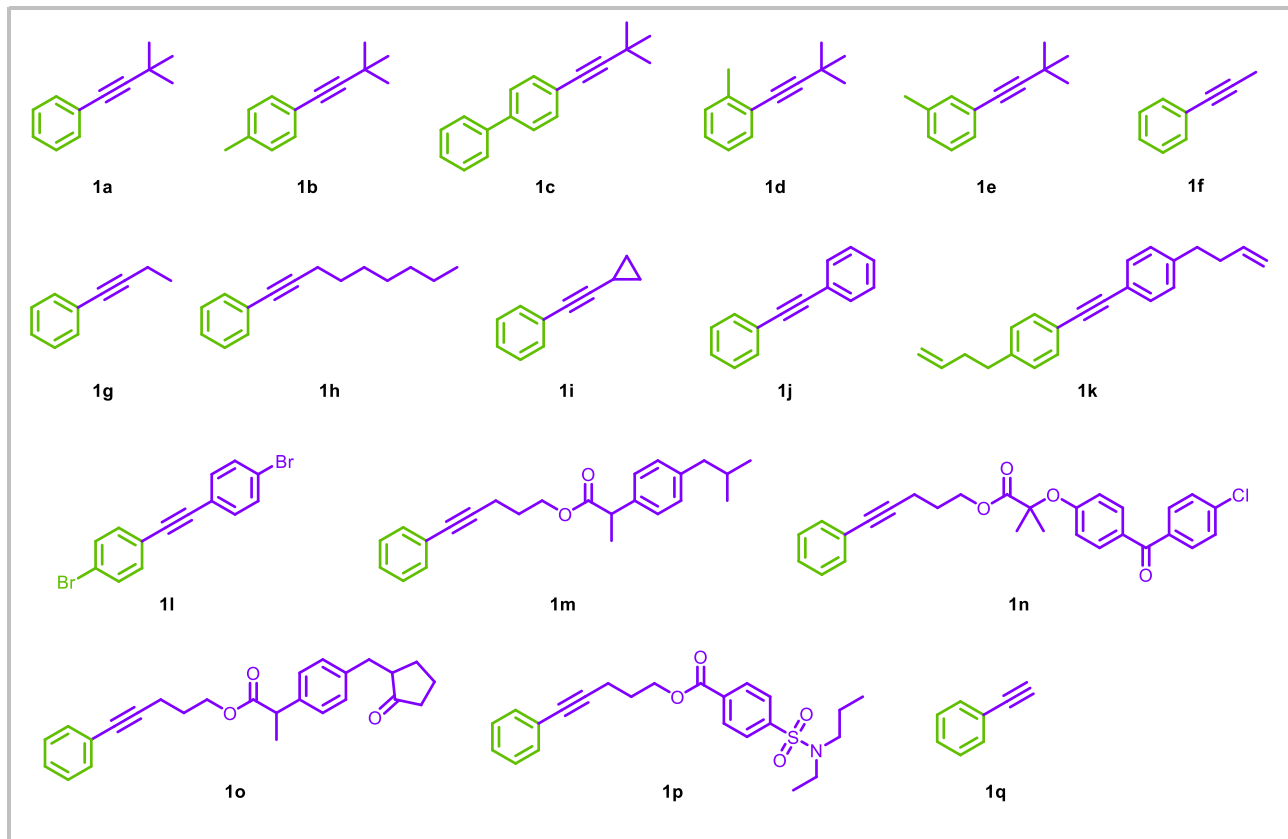
The compounds **13a-16a** were prepared according to previously described methods.<sup>[1]</sup>



**Step 1:** To a 50 mL flame-dried round-bottom flask, under  $N_2$ , was added  $PdCl_2(PPh_3)_2$  (0.05 mmol, 0.01 eq.),  $CuI$  (0.1 mmol, 0.02 eq.), iodobenzene (6.0 mmol, 1.2 eq.), alkynol (5.0 mmol, 1.0 eq.) and dry  $Et_3N$  (10.0 mL), the reaction was allowed to stir at room temperature. The reaction was stirred overnight checked by TLC. The reaction is filtered over celite, washing with dichloromethane. The solvent was removed and the residue purified by flash column chromatography on silica gel to give compounds **A**.

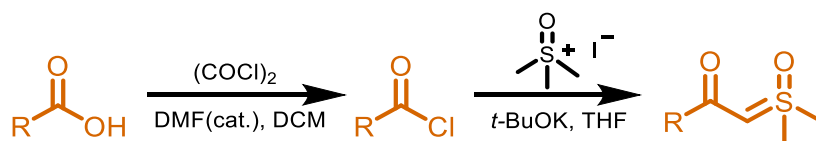
**Step 2:** To a solution of compound **A** (2.0 mmol, 1.0 eq.), DMAP (4-dimethylaminopyridine) (0.4 mmol, 0.2 eq.) and  $Et_3N$  (6.0 mmol, 3.0 eq.) in DCM (20.0 mL) at room temperature were added EDCI (1-ethyl-3-(3-dimethylamino)propyl)-carbodiimide hydrochloride) (4.0 mmol, 2.0 eq.)

and pent-4-yn-1-ol (12.0 mmol, 1.2 eq.). The reaction mixture was stirred at room temperature for 6 h before quenched with H<sub>2</sub>O (30.0 mL) and extracted 3 times with DCM (10.0 mL). The combined organic layer was dried over MgSO<sub>4</sub>. The filtrate was concentrated in vacuo and the residue was purified by chromatography on silica gel, eluting with hexanes/EtOAc 15:1 (v/v) to afford **13a-16a**.



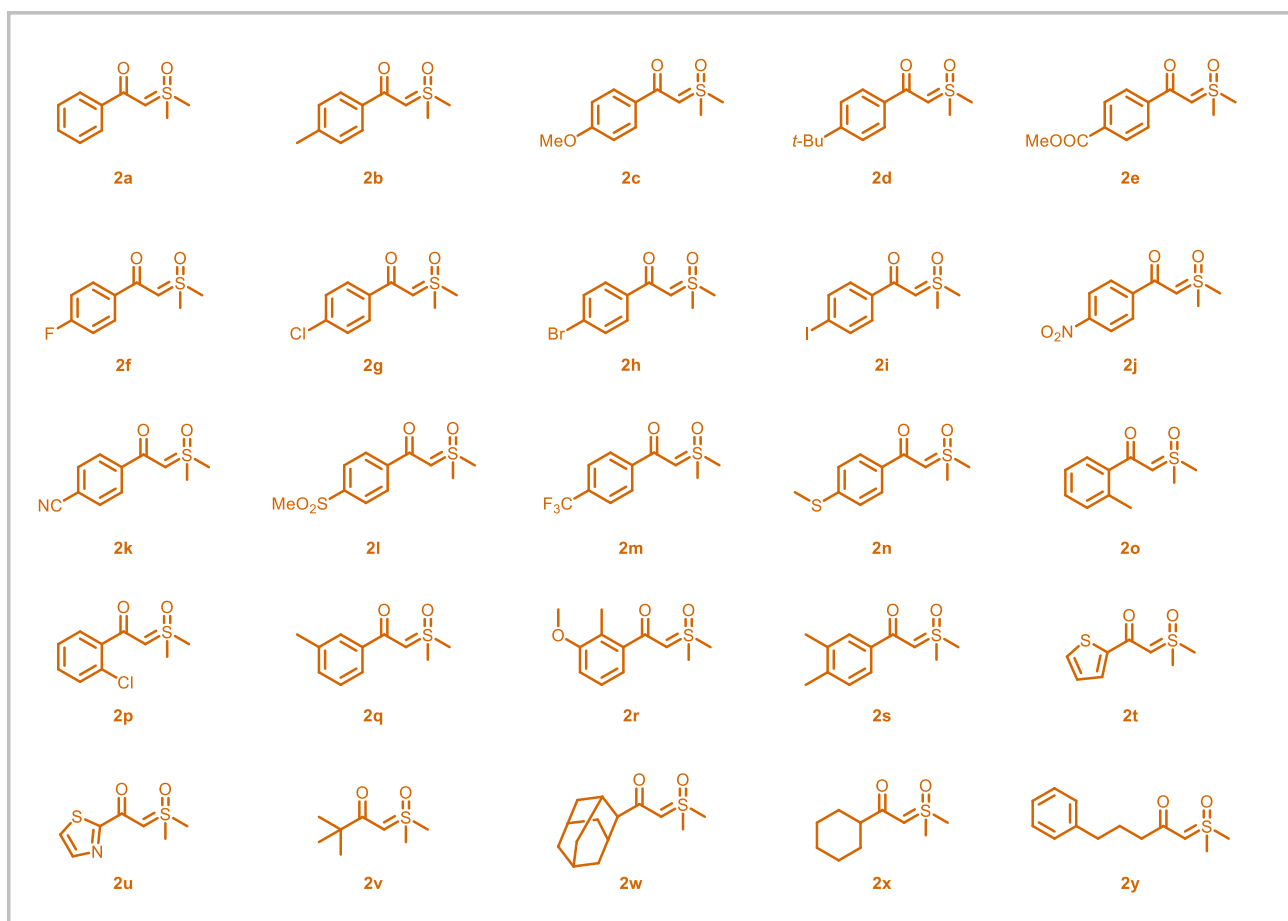
## 2.2 General procedure for the synthesis of sulfoxonium ylides

The compounds **2a-2y** were prepared according to previously described methods. <sup>[2,3]</sup>



**Step 1:** A round-bottom flask (25.0 mL) was charged with benzoic acid (7.0 mmol, 1.0 eq.), dry DCM (21.0 mL) and catalytic amount of DMF (3.0 drops). The reaction mixture was cooled to 0 °C and stirred for 10 minutes. Then, (COCl)<sub>2</sub> (10.5 mmol, 1.5 eq.) was added dropwise to the reaction mixture and stirred at 25 °C for 4~5 h. The resulting mixture was concentrated under reduced pressure to afford acid chloride quantitatively which was used directly without further purification for the next step.

**Step 2:** To a stirred solution of potassium *tert*-butoxide (7.0 mmol) in THF (80.0 mL) was added trimethylsulfoxonium iodide (9.9 g, 45.0 mmol) at room temperature. The resulting mixture was refluxed for 2 h, and then cooled to 0 °C, which was followed by addition of benzoyl chloride (2.1 g, 15.0 mmol) in THF (10.0 mL). The reaction was allowed to room temperature and stirred for another 4 hours. Next, the solvent was evaporated, water (60.0 mL) and ethyl acetate (40.0 mL) were then added to the resulting slurry. The layers were separated and the aqueous layer was extracted with ethyl acetate and the organic layers were combined. The organic solution was dried over anhydrous MgSO<sub>4</sub>, filtered, and evaporated to dryness.



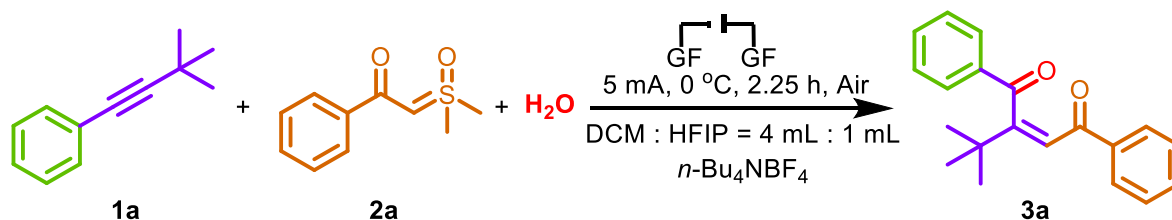
### 3. General preparation of 1,4-dicarbonyl Z-alkenes



Figure S1. Components required for the reaction



Figure S2. Typical reaction set up

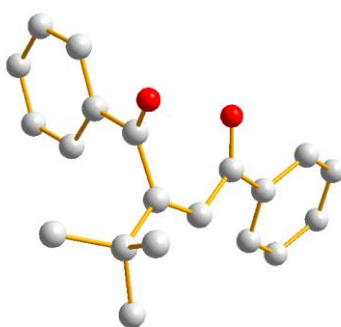


In an undivided cell (10 mL) equipped with a stir bar, **1a** (0.1 mmol, 1.0 eq.), **2a** (0.2 mmol, 2.0 eq.),  $\text{H}_2\text{O}$  (0.1 mmol, 1.0 eq.) and  $n\text{-Bu}_4\text{NBF}_4$  (0.4 mmol, 4.0 eq.) were combined and added. The flask was equipped with a rubber stopper, a graphite felt anode (1.0 cm x 1.0 cm x 0.5 cm) and a graphite felt cathode (1.0 cm x 1.0 cm x 0.5 cm). Then DCM (4.0 mL) and 1,1,1,3,3,3-Hexafluoro-2-propanol (HFIP) (1.0 mL) and were injected respectively into the flask

via syringes. The reaction mixture was stirred and electrolyzed in air for 2.25 hours at a constant current of 0 °C and 5 mA. After the reaction was complete, the residue was purified by column chromatography using petroleum ether and ethyl acetate as eluent, to afford the desired product **3a**.

#### 4. Molecular structure and crystallographic data

Single-crystals of compound **3a** was grown from recrystallization by diffusion volatilization of hexane (69 °C)/dichloromethane (v/v, 3/1) at room temperature for 4 days. Single-crystal *X-ray* diffraction studies for compound **3a** was carried out on a XtaLAB AFC10 (RCD3): fixed-chi single diffractometer with mirror-monochromated Mo K $\alpha$  radiation. Cell parameters were obtained by global refinement of the positions of all collected reflections. Intensities were S15 corrected for Lorentz and polarization effects and empirical absorption. The structures were solved by direct methods and refined by full-matrix least squares on F<sup>2</sup>. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were placed in calculated positions. Structure solution and refinement were performed by using the SHELXL package. Displacement ellipsoid was drawn at the 50% probability level. The *X-ray* crystallographic files, in CIF format, are available from the Cambridge Crystallographic Data Centre on quoting the deposition number CCDC 2340616 for **3a**. Copies of this information may be obtained free of charge from The Director, CCDC, 12 Union Road, Cambridge CB2 IEZ, UK (Fax: +44-1223-336033; e-mail: deposit@ccdc.cam.ac.uk or www: <http://www.ccdc.cam.ac.uk>)



**Figure S3.** Crystallographic structure of **3a**

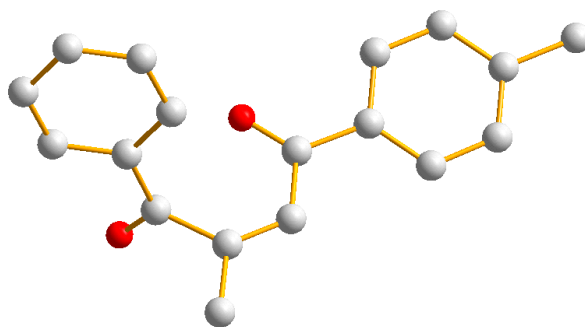
*X-Ray* crystallographic data compound **3a**

|                     |  |
|---------------------|--|
| Identification code | MX13731  |
| Empirical formula   | C <sub>20</sub> H <sub>20</sub> O <sub>2</sub> |
| Formula weight      | 292.36   |
| Temperature/K       | 297.27(10)                                     |
| Crystal system      | monoclinic                                     |
| Space group         | P21/n  |



|   |   |
|---|---|
| a/Å   | 10.7659(4)  |
| b/Å   | 14.5214(5)  |
| c/Å   | 11.4358(5)  |
| $\alpha$ /°                                 | 90  |
| $\beta$ /°                                  | 110.658(5)  |
| $\gamma$ /°                                 | 90  |
| Volume/Å <sup>3</sup>                       | 1672.87(12)   |
| Z   | 4   |
| $\rho$ calcg/cm <sup>3</sup>                | 1.161   |
| $\mu$ /mm <sup>-1</sup>                     | 0.074   |
| F(000)                                      | 624.0   |
| Crystal size/mm <sup>3</sup>                | 0.32 × 0.28 × 0.25  |
| Radiation                                   | Mo K $\alpha$ ( $\lambda$ = 0.71073)                          |
| 2 $\Theta$ range for data collection/°      | 4.728 to 60.42  |
| Index ranges                                | -12 ≤ h ≤ 15, -16 ≤ k ≤ 19, -15 ≤ l ≤ 16                      |
| Reflections collected                       | 13131   |
| Independent reflections                     | 4101 [R <sub>int</sub> = 0.0143, R <sub>sigma</sub> = 0.0162] |
| Data/restraints/parameters                  | 4101/0/202  |
| Goodness-of-fit on F <sup>2</sup>           | 1.090   |
| Final R indexes [I ≥ 2 $\sigma$ (I)]        | R <sub>1</sub> = 0.0537, wR <sub>2</sub> = 0.1632             |
| Final R indexes [all data]                  | R <sub>1</sub> = 0.0644, wR <sub>2</sub> = 0.1706             |
| Largest diff. peak/hole / e Å <sup>-3</sup> | 0.34/-0.25  |

Single-crystals of compound **3al** was grown from recrystallization by diffusion volatilization of petroleum ether (60-90 °C)/dichloromethane (v/v, 3/1) at room temperature for 5 days. Single-crystal *X-ray* diffraction studies for compound **3al** was carried out on a XtaLAB AFC10 (RCD3): fixed-chi single diffractometer with mirror-monochromated Mo K $\alpha$  radiation. Cell parameters were obtained by global refinement of the positions of all collected reflections. Intensities were S15 corrected for Lorentz and polarization effects and empirical absorption. The structures were solved by direct methods and refined by full-matrix least squares on F<sup>2</sup>. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were placed in calculated positions. Structure solution and refinement were performed by using the SHELXL package. Displacement ellipsoid was drawn at the 50% probability level. The *X-ray* crystallographic files, in CIF format, are available from the Cambridge Crystallographic Data Centre on quoting the deposition number CCDC 2179302 for **3al**. Copies of this information may be obtained free of charge from The Director, CCDC, 12 Union Road, Cambridge CB2 IEZ, UK (Fax: +44-1223-336033; e-mail: deposit@ccdc.cam.ac.uk or www: <http://www.ccdc.cam.ac.uk>)



**Figure S4.** Crystallographic structure of **3al**

*X-Ray* crystallographic data compound **3al**

|                                    |   |
|------------------------------------|---|
| Identification code                | MX10483   |
| Empirical formula                  | C <sub>18</sub> H <sub>16</sub> O <sub>2</sub>                |
| Formula weight                     | 264.31  |
| Temperature/K                      | 170.01(10)  |
| Crystal system                     | orthorhombic  |
| Space group                        | Pbca  |
| a/Å                                | 8.2970(3)   |
| b/Å                                | 11.4089(5)  |
| c/Å                                | 29.4395(11)   |
| α/°                                | 90  |
| β/°                                | 90  |
| γ/°                                | 90  |
| Volume/Å <sup>3</sup>              | 2786.73(19)   |
| Z                                  | 8   |
| ρ <sub>calc</sub> /cm <sup>3</sup> | 1.260   |
| μ/mm <sup>-1</sup>                 | 0.081   |
| F(000)                             | 1120.0  |
| Crystal size/mm <sup>3</sup>       | 0.28 × 0.21 × 0.08  |
| Radiation                          | Mo Kα (λ = 0.71073)   |
| 2θ range for data collection/°     | 5.536 to 62.172   |
| Index ranges                       | -11 ≤ h ≤ 9, -15 ≤ k ≤ 14, -30 ≤ l ≤ 42                       |
| Reflections collected              | 16298   |
| Independent reflections            | 3902 [R <sub>int</sub> = 0.0226, R <sub>sigma</sub> = 0.0220] |
| Data/restraints/parameters         | 3902/0/183  |
| Goodness-of-fit on F <sup>2</sup>  | 1.056   |
| Final R indexes [I ≥ 2σ (I)]       | R <sub>1</sub> = 0.0410, wR <sub>2</sub> = 0.1103             |

|  |                                  |
|--|----------------------------------|
| Final R indexes [all data]                     | $R_1 = 0.0509$ , $wR_2 = 0.1158$ |
| Largest diff. peak/hole / $e \text{ \AA}^{-3}$ | 0.36/-0.19                       |

## 5. Computational studies Computational details

In this work, geometry optimizations and frequency calculation of all structures including reactants, intermediates, transition states, and products were computed with Gaussian 16, Revision A. 03 package, which was based on M06-2X density functional and 6-31G(d) basis set. All the stationary structures and transition state structures (TSs) were identified by no imaginary frequency and a single imaginary frequency. Meanwhile, Intrinsic Reaction Coordinate (IRC) calculations were used for all the TSs. The solvent effect of Dichloromethane (DCM) was evaluated through the SMD method based upon M06-2X density functional and 6-311++G(d,p) basis set. All reported energies are free energies at a concentration of 1 M and a temperature of 298.15 K.<sup>[4,5]</sup>

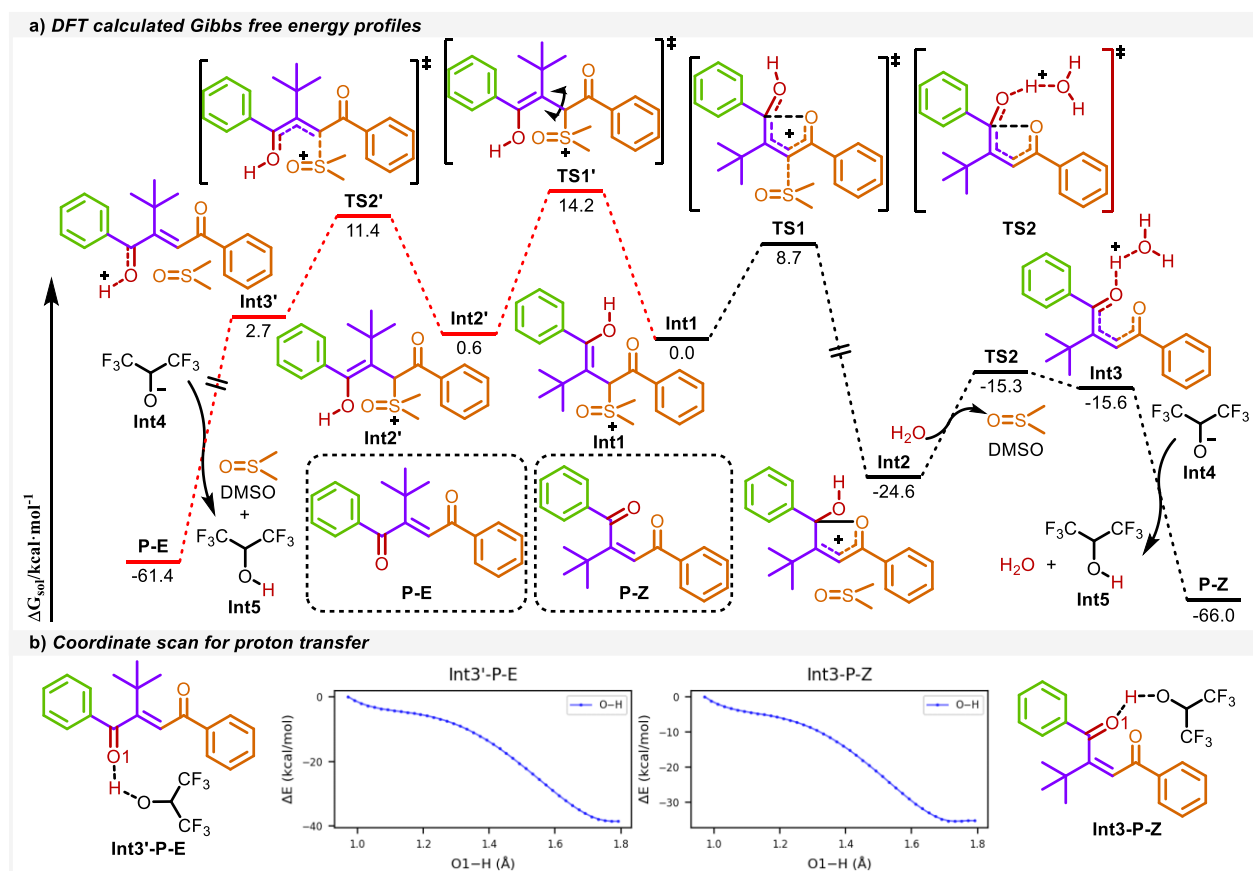


Figure S5. DFT calculations

## Cartesian coordinates of the optimized structures:

### Int1

E = -1477.921714 a.u.

1 1

|   |             |             |            |
|---|-------------|-------------|------------|
| O | 0.39910500  | 27.54090400 | 4.89306300 |
| O | 3.13484900  | 27.78344500 | 5.42831000 |
| C | -0.55132400 | 26.06553700 | 6.47166200 |
| C | -0.69010300 | 24.74141200 | 6.90284300 |
| H | -0.05642800 | 23.94672700 | 6.52810900 |
| C | -1.67466200 | 24.41563000 | 7.82858900 |
| H | -1.78553400 | 23.38841400 | 8.15341700 |
| C | -2.51734300 | 25.40279800 | 8.32738700 |
| C | -2.39011600 | 26.72126600 | 7.89207800 |
| H | -3.05439500 | 27.48669300 | 8.27454100 |
| C | -1.41719300 | 27.05107200 | 6.96304100 |
| H | -1.31059300 | 28.06746100 | 6.60283000 |
| C | 0.47910700  | 26.50758300 | 5.49465200 |
| C | 1.70720300  | 25.56298600 | 5.23099500 |
| H | 1.31442200  | 24.55932700 | 5.06167000 |
| C | 2.57077600  | 25.98838100 | 4.07490600 |
| C | 2.58225500  | 25.01362600 | 2.89172600 |
| C | 3.12779300  | 27.20463300 | 4.17240600 |
| C | 3.73256600  | 28.06785300 | 3.13283000 |
| C | 2.89552300  | 28.70181600 | 2.21367400 |
| H | 1.82904500  | 28.50316800 | 2.24215100 |
| C | 3.43455500  | 29.57586600 | 1.27693700 |
| H | 2.78589300  | 30.06599900 | 0.56082900 |
| C | 4.80427100  | 29.81841400 | 1.25938500 |
| C | 5.63785200  | 29.20209600 | 2.18881600 |
| C | 5.10213800  | 28.33819800 | 3.13519700 |
| H | 6.70383400  | 29.39521000 | 2.17482100 |
| H | 5.74942200  | 27.85185900 | 3.85858800 |
| H | 5.22401500  | 30.49364200 | 0.52320000 |
| C | 3.45008500  | 25.46840600 | 1.71268500 |
| H | 3.04069200  | 26.33796100 | 1.20130100 |
| H | 4.47146200  | 25.70162600 | 2.01974500 |
| H | 3.49927700  | 24.65411100 | 0.98672900 |
| C | 3.15226400  | 23.66079800 | 3.36376700 |
| H | 4.21859800  | 23.74701900 | 3.59137800 |
| H | 2.64676300  | 23.24106700 | 4.23919200 |
| H | 3.05481000  | 22.92181100 | 2.56595500 |
| C | 1.14168200  | 24.82370900 | 2.38361900 |

|   |             |             |            |
|---|-------------|-------------|------------|
| H | 1.13652800  | 24.15749600 | 1.51833900 |
| H | 0.47632600  | 24.37672300 | 3.12867100 |
| H | 0.71059100  | 25.77989000 | 2.07889300 |
| H | -3.28163700 | 25.14403500 | 9.05078700 |
| H | 3.17566000  | 28.74342600 | 5.33282400 |
| S | 2.62372200  | 25.19321400 | 6.80586000 |
| O | 2.31517600  | 23.84613100 | 7.29016800 |
| C | 4.37598100  | 25.34183900 | 6.50164400 |
| H | 4.84162800  | 24.94105400 | 7.40267600 |
| H | 4.60554600  | 24.71485300 | 5.64223100 |
| H | 4.62933100  | 26.38368200 | 6.32677900 |
| C | 2.25776400  | 26.43186400 | 8.04532600 |
| H | 2.26323300  | 27.41241400 | 7.57580700 |
| H | 1.28244700  | 26.17583900 | 8.45650800 |
| H | 3.03153100  | 26.34010900 | 8.80751200 |

**TS1'**

E = -1477.899741 a.u.

1 1

|   |            |             |            |
|---|------------|-------------|------------|
| O | 0.96897400 | 25.29574500 | 5.76504000 |
| O | 4.05621900 | 28.54037100 | 5.79407100 |
| C | 2.30043700 | 23.50390400 | 6.53719800 |
| C | 1.24013000 | 22.60273500 | 6.38515500 |
| H | 0.32440500 | 22.94670100 | 5.91901000 |
| C | 1.37009600 | 21.29427900 | 6.82400100 |
| H | 0.55103600 | 20.59735500 | 6.69509500 |
| C | 2.55305100 | 20.87840700 | 7.42963800 |
| C | 3.61057500 | 21.76954000 | 7.59071600 |
| H | 4.53173800 | 21.44178100 | 8.05678700 |
| C | 3.48971500 | 23.07683800 | 7.14119500 |
| H | 4.33895500 | 23.74196900 | 7.25475600 |
| C | 2.06209800 | 24.89525900 | 6.07874300 |
| C | 3.19505000 | 25.95739100 | 6.08390400 |
| H | 4.12930700 | 25.61250700 | 6.53550300 |
| C | 3.38491300 | 26.59110600 | 4.70328500 |
| C | 3.48745800 | 25.61367200 | 3.50178600 |
| C | 3.65951600 | 27.90646400 | 4.63922500 |
| C | 3.53887700 | 28.82488800 | 3.48830400 |
| C | 2.31498500 | 28.93785100 | 2.82687000 |
| H | 1.48240500 | 28.31809400 | 3.14212000 |
| C | 2.17257000 | 29.84592700 | 1.78494900 |

|   |            |             |            |
|---|------------|-------------|------------|
| H | 1.22209200 | 29.93490100 | 1.27261200 |
| C | 3.24776500 | 30.64338000 | 1.40568900 |
| C | 4.46323900 | 30.54823900 | 2.07865900 |
| C | 4.60705200 | 29.65026400 | 3.12758500 |
| H | 5.29793700 | 31.17278300 | 1.78356000 |
| H | 5.55433800 | 29.56428800 | 3.65020400 |
| H | 3.13678000 | 31.34745500 | 0.58948000 |
| C | 2.15113000 | 25.00258700 | 3.03665500 |
| H | 1.78420000 | 24.20911300 | 3.68717600 |
| H | 1.37126500 | 25.76113800 | 2.95421000 |
| H | 2.29568800 | 24.55577400 | 2.05065900 |
| C | 4.14283600 | 26.27007500 | 2.27183000 |
| H | 3.48200400 | 26.95910600 | 1.75021700 |
| H | 5.06292200 | 26.79828800 | 2.52840700 |
| H | 4.40085400 | 25.47653400 | 1.56825700 |
| C | 4.45164900 | 24.48041200 | 3.91423500 |
| H | 4.60161800 | 23.80713800 | 3.06827400 |
| H | 5.42965200 | 24.87995900 | 4.19797700 |
| H | 4.07427400 | 23.86494600 | 4.73108600 |
| H | 2.65402900 | 19.85579900 | 7.77370900 |
| H | 3.76194300 | 29.46135100 | 5.77050100 |
| S | 2.55084600 | 27.13332000 | 7.41697000 |
| O | 1.70803800 | 28.25165200 | 7.01493200 |
| C | 1.63059500 | 26.11373000 | 8.57186200 |
| H | 2.16994100 | 25.19186000 | 8.79013600 |
| H | 1.51272000 | 26.72475900 | 9.46663700 |
| H | 0.66211700 | 25.91003700 | 8.12081600 |
| C | 3.97144000 | 27.56416100 | 8.43446200 |
| H | 4.26211800 | 26.68116500 | 9.00325000 |
| H | 4.76849900 | 27.92228600 | 7.79260400 |
| H | 3.62120500 | 28.35163000 | 9.10286300 |

## Int2'

E = -1477.922297 a.u.

1 1

|   |            |             |            |
|---|------------|-------------|------------|
| O | 1.20532700 | 24.38613100 | 7.49867100 |
| O | 3.87220200 | 28.23511000 | 6.24508900 |
| C | 3.34327600 | 23.72253000 | 6.73633700 |
| C | 3.06023800 | 22.36186500 | 6.89103700 |
| H | 2.04573700 | 22.05803000 | 7.12046300 |
| C | 4.07110200 | 21.42530100 | 6.74055000 |
| H | 3.85110800 | 20.36977700 | 6.84349800 |

|   |             |             |            |
|---|-------------|-------------|------------|
| C | 5.37011800  | 21.84527600 | 6.46451100 |
| C | 5.66135300  | 23.20110500 | 6.33753600 |
| H | 6.67681000  | 23.52167500 | 6.13879900 |
| C | 4.64975700  | 24.14188000 | 6.46231300 |
| H | 4.88384400  | 25.19474300 | 6.34888200 |
| C | 2.22438100  | 24.67205800 | 6.90957000 |
| C | 2.42868200  | 26.10507800 | 6.41456400 |
| H | 3.11028000  | 26.55171600 | 7.14625200 |
| C | 2.89439700  | 26.48133600 | 5.04678900 |
| C | 2.37165000  | 25.76699700 | 3.78398600 |
| C | 3.68886000  | 27.57824700 | 5.05906700 |
| C | 4.42244800  | 28.19690500 | 3.93236300 |
| C | 4.05892300  | 29.47932900 | 3.51321000 |
| H | 3.21066600  | 29.97454900 | 3.97586500 |
| C | 4.75072600  | 30.08606200 | 2.47333700 |
| H | 4.45506800  | 31.07026600 | 2.13034000 |
| C | 5.81775200  | 29.42669400 | 1.86904700 |
| C | 6.19978500  | 28.16283600 | 2.30774100 |
| C | 5.50352500  | 27.54488800 | 3.34003200 |
| H | 7.03974700  | 27.65805600 | 1.84573500 |
| H | 5.79782500  | 26.56136400 | 3.68954900 |
| H | 6.35609900  | 29.90181900 | 1.05759500 |
| C | 0.94968400  | 25.24348100 | 4.04937400 |
| H | 0.89207000  | 24.53248800 | 4.87753900 |
| H | 0.25869800  | 26.07544100 | 4.21795200 |
| H | 0.59249900  | 24.71166800 | 3.16611400 |
| C | 2.24127600  | 26.72393600 | 2.58387400 |
| H | 1.73275700  | 27.64825100 | 2.86815100 |
| H | 3.19897500  | 26.97828900 | 2.13386800 |
| H | 1.64531900  | 26.23414600 | 1.81076300 |
| C | 3.25903200  | 24.57988200 | 3.37333300 |
| H | 2.89513200  | 24.16571200 | 2.42966500 |
| H | 4.29290100  | 24.89353100 | 3.21956100 |
| H | 3.25347200  | 23.77679600 | 4.11126800 |
| H | 6.16096200  | 21.11265300 | 6.35327000 |
| H | 4.53944400  | 28.92277400 | 6.13322100 |
| S | 0.87794300  | 27.15196000 | 6.83011400 |
| O | 0.76949900  | 28.26830000 | 5.89083800 |
| C | -0.69921800 | 26.29450700 | 6.95143400 |
| H | -0.75040000 | 25.76116400 | 7.89490200 |
| H | -1.43091500 | 27.10029400 | 6.87523000 |
| H | -0.79262300 | 25.60435200 | 6.11862400 |

|   |            |             |            |
|---|------------|-------------|------------|
| C | 1.18525800 | 27.69771400 | 8.50170500 |
| H | 1.33494200 | 26.82054400 | 9.13229100 |
| H | 2.07910300 | 28.31973800 | 8.45751500 |
| H | 0.32580100 | 28.28167300 | 8.82953000 |

**TS2'**

E = -1477.895959 a.u.

1 1

|   |            |             |             |
|---|------------|-------------|-------------|
| O | 3.65869400 | 23.42271500 | 5.35724100  |
| O | 1.58328600 | 27.89499300 | 4.56599100  |
| C | 2.72809800 | 24.16049400 | 7.39590100  |
| C | 2.70852300 | 25.24741100 | 8.27477400  |
| H | 2.98537300 | 26.24242100 | 7.94171900  |
| C | 2.38774700 | 25.05116000 | 9.61243800  |
| H | 2.39866600 | 25.88909000 | 10.29925900 |
| C | 2.06371000 | 23.77692700 | 10.07083300 |
| C | 2.08364200 | 22.69230500 | 9.19731000  |
| H | 1.83588100 | 21.70042200 | 9.55549100  |
| C | 2.42826500 | 22.87908800 | 7.86497600  |
| H | 2.44819400 | 22.04743600 | 7.17048600  |
| C | 3.06019800 | 24.28518000 | 5.94381700  |
| C | 2.55626800 | 25.53873900 | 5.25178600  |
| H | 2.32971100 | 26.33536900 | 5.95021800  |
| C | 2.67149500 | 25.91676700 | 3.92191300  |
| C | 2.91523800 | 24.99853300 | 2.69809400  |
| C | 2.46020000 | 27.31804100 | 3.76622700  |
| C | 3.15997600 | 28.19558100 | 2.83689900  |
| C | 2.45713800 | 29.20516000 | 2.16164000  |
| H | 1.37756400 | 29.28025800 | 2.25430700  |
| C | 3.13560100 | 30.05139400 | 1.29944200  |
| H | 2.59329400 | 30.80940200 | 0.74796800  |
| C | 4.51343000 | 29.91800100 | 1.13746500  |
| C | 5.21749800 | 28.93623000 | 1.83112100  |
| C | 4.54415500 | 28.06453300 | 2.67294300  |
| H | 6.29085400 | 28.85169100 | 1.71447400  |
| H | 5.08235000 | 27.30977500 | 3.23328100  |
| H | 5.04158900 | 30.58605900 | 0.46752400  |
| C | 4.37039800 | 24.52203700 | 2.57175600  |
| H | 5.04106000 | 25.34715000 | 2.32536900  |
| H | 4.72212500 | 24.02817600 | 3.47341400  |



|   |             |             |             |
|---|-------------|-------------|-------------|
| H | 4.43401300  | 23.80523800 | 1.74969200  |
| C | 1.96900000  | 23.78730000 | 2.83695700  |
| H | 2.12156600  | 23.20739900 | 3.74160600  |
| H | 0.92087300  | 24.09441500 | 2.79696000  |
| H | 2.13549200  | 23.11891400 | 1.99013700  |
| C | 2.51534900  | 25.68501500 | 1.37712100  |
| H | 2.46035700  | 24.92064100 | 0.60068600  |
| H | 1.52658600  | 26.15279500 | 1.43736200  |
| H | 3.23099700  | 26.43219500 | 1.03618700  |
| H | 1.80510600  | 23.62810300 | 11.11264400 |
| H | 1.64907000  | 28.86154600 | 4.51554700  |
| S | 0.14734000  | 24.60240700 | 5.74104600  |
| O | -0.07489400 | 23.17061700 | 5.39190600  |
| C | -0.59737300 | 24.91993100 | 7.35452000  |
| H | -1.65165200 | 24.64645400 | 7.30570100  |
| H | -0.07468000 | 24.28366100 | 8.06861700  |
| H | -0.46771300 | 25.96903200 | 7.62007600  |
| C | -0.91411000 | 25.63409000 | 4.71095600  |
| H | -0.91682300 | 26.65135300 | 5.10076800  |
| H | -0.50713100 | 25.62146000 | 3.70002300  |
| H | -1.91475700 | 25.20179400 | 4.71167700  |

### Int3'

E = -1477.916694 a.u.

1 1

|   |            |             |             |
|---|------------|-------------|-------------|
| O | 3.50855200 | 23.71885100 | 5.31894400  |
| O | 2.01021800 | 28.38682000 | 4.32325100  |
| C | 2.69382500 | 24.54638000 | 7.37239600  |
| C | 2.03891900 | 25.55059400 | 8.09287600  |
| H | 1.71410000 | 26.46158400 | 7.60663500  |
| C | 1.73838100 | 25.35951000 | 9.43567600  |
| H | 1.22292400 | 26.13652800 | 9.98759900  |
| C | 2.09187300 | 24.17050900 | 10.06866400 |
| C | 2.75362900 | 23.17140200 | 9.35859600  |
| H | 3.03501700 | 22.24878500 | 9.85196500  |
| C | 3.05455600 | 23.35944400 | 8.01715400  |
| H | 3.56361700 | 22.59143800 | 7.44736600  |
| C | 3.01061200 | 24.64426100 | 5.91681800  |
| C | 2.78675000 | 25.96050100 | 5.22387600  |
| H | 2.77089000 | 26.81872900 | 5.88469300  |
| C | 2.74450900 | 26.20579100 | 3.89199200  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 2.57897100  | 25.24001500 | 2.69567500  |
| C | 2.81177000  | 27.63594300 | 3.63634600  |
| C | 3.73975100  | 28.26497600 | 2.71718500  |
| C | 3.36694200  | 29.42421000 | 2.01500000  |
| H | 2.35165200  | 29.80638600 | 2.07412300  |
| C | 4.27407100  | 30.02514000 | 1.16062700  |
| H | 3.98430500  | 30.89911900 | 0.59079100  |
| C | 5.55732700  | 29.49400900 | 1.02650100  |
| C | 5.93563000  | 28.35649500 | 1.73531900  |
| C | 5.02652400  | 27.72848200 | 2.57247100  |
| H | 6.93881200  | 27.96133900 | 1.63509800  |
| H | 5.31346500  | 26.85711000 | 3.14892200  |
| H | 6.26681600  | 29.97231300 | 0.36154800  |
| C | 3.87433900  | 24.51270200 | 2.30631400  |
| H | 4.59710800  | 25.18834300 | 1.84414100  |
| H | 4.32889900  | 24.02034900 | 3.16346400  |
| H | 3.63401100  | 23.74908500 | 1.56238700  |
| C | 1.49193800  | 24.21204200 | 3.06886500  |
| H | 1.84601100  | 23.49894800 | 3.80852700  |
| H | 0.60566900  | 24.70823100 | 3.46523300  |
| H | 1.22341300  | 23.65447100 | 2.16911000  |
| C | 2.05429300  | 26.00833400 | 1.46625400  |
| H | 1.75694900  | 25.28655900 | 0.70452900  |
| H | 1.16736400  | 26.60505000 | 1.70681700  |
| H | 2.80398400  | 26.65592900 | 1.00994700  |
| H | 1.85516900  | 24.02479300 | 11.11631700 |
| H | 2.21149500  | 29.33176600 | 4.21753500  |
| S | -0.88279100 | 25.10958900 | 6.57898900  |
| O | 0.25539100  | 25.56560700 | 5.67409000  |
| C | -0.52093100 | 23.39493100 | 7.02683300  |
| H | -0.15489200 | 22.88272000 | 6.13588500  |
| H | 0.24513900  | 23.40005800 | 7.80033600  |
| H | -1.42493400 | 22.92009400 | 7.40830500  |
| C | -2.25003400 | 24.75699800 | 5.45105700  |
| H | -3.09658100 | 24.35545800 | 6.00757700  |
| H | -2.52768700 | 25.70017800 | 4.98439000  |
| H | -1.90824200 | 24.05171500 | 4.69348800  |

**P-E**

E = -924.420552 a.u.

0 1

|   |            |             |            |
|---|------------|-------------|------------|
| O | 3.07695500 | 23.85947600 | 7.43017000 |
| O | 5.28409500 | 28.29371500 | 6.71305300 |
| C | 3.94333600 | 22.72506600 | 5.55014500 |
| C | 3.45066100 | 21.49519800 | 5.99199900 |
| H | 2.96479800 | 21.45149000 | 6.95967000 |
| C | 3.58609800 | 20.36519100 | 5.20042300 |
| H | 3.20673500 | 19.41116700 | 5.54789300 |
| C | 4.20968400 | 20.45693900 | 3.95757200 |
| C | 4.69616000 | 21.67961700 | 3.50869400 |
| H | 5.17789800 | 21.75080500 | 2.54040700 |
| C | 4.56513400 | 22.81266700 | 4.30375100 |
| H | 4.94413300 | 23.76481700 | 3.94704300 |
| C | 3.75477900 | 23.92285400 | 6.42959000 |
| C | 4.47960500 | 25.17157600 | 6.04293900 |
| H | 5.53082100 | 25.01372900 | 5.80351300 |
| C | 4.01748900 | 26.42671300 | 6.02058900 |
| C | 2.59133700 | 26.93268700 | 6.23274600 |
| C | 5.08833900 | 27.48009400 | 5.84117500 |
| C | 5.90295800 | 27.48245400 | 4.58264300 |
| C | 7.07602100 | 28.23948000 | 4.56080800 |
| H | 7.36279000 | 28.77405500 | 5.45893700 |
| C | 7.84655300 | 28.29767400 | 3.40925800 |
| H | 8.76233300 | 28.87732100 | 3.39855500 |
| C | 7.43977100 | 27.61536900 | 2.26450100 |
| C | 6.26197500 | 26.87608500 | 2.27339700 |
| C | 5.49650000 | 26.80379100 | 3.43211900 |
| H | 5.93826900 | 26.35814300 | 1.37790700 |
| H | 4.57356500 | 26.23406800 | 3.43859800 |
| H | 8.03980000 | 27.66539900 | 1.36283200 |
| C | 1.54782300 | 25.95041500 | 5.68136600 |
| H | 1.77946000 | 25.66180300 | 4.65130200 |
| H | 1.46087300 | 25.05043600 | 6.28507500 |
| H | 0.56862400 | 26.43520600 | 5.67728700 |
| C | 2.36750100 | 27.15457000 | 7.73802300 |
| H | 2.46195500 | 26.21031400 | 8.27547600 |
| H | 3.09766700 | 27.86196900 | 8.13433800 |
| H | 1.36437000 | 27.55879800 | 7.90427400 |
| C | 2.40944200 | 28.26835700 | 5.48791300 |
| H | 1.37454000 | 28.60156200 | 5.58949000 |
| H | 3.05139000 | 29.05252400 | 5.88966800 |
| H | 2.62007200 | 28.16223500 | 4.41867200 |
| H | 4.31518200 | 19.57306200 | 3.33850500 |

**TS1**

E = -1477.903446 a.u.

1 1

|   |             |             |            |
|---|-------------|-------------|------------|
| O | 0.67127800  | 27.94895800 | 5.11426100 |
| O | 3.35079500  | 27.66891600 | 5.32006100 |
| C | -0.37220700 | 26.39259900 | 6.55482600 |
| C | -0.76794500 | 25.06545100 | 6.76234700 |
| H | -0.39362400 | 24.25284600 | 6.15008300 |
| C | -1.66443400 | 24.75970400 | 7.77859900 |
| H | -1.97148300 | 23.73214100 | 7.93035500 |
| C | -2.16259800 | 25.76948100 | 8.59710200 |
| C | -1.77892800 | 27.09255300 | 8.38930700 |
| H | -2.17465100 | 27.87904900 | 9.02051100 |
| C | -0.89641700 | 27.40430300 | 7.36592900 |
| H | -0.59954800 | 28.42965700 | 7.17933600 |
| C | 0.59019900  | 26.80651100 | 5.49591000 |
| C | 1.46975300  | 25.73471900 | 4.85994100 |
| H | 0.98409900  | 24.76964600 | 4.74530900 |
| C | 2.47501200  | 26.01878800 | 3.95036600 |
| C | 2.83605000  | 24.96708100 | 2.87043100 |
| C | 3.10488200  | 27.27648200 | 4.08284900 |
| C | 3.52357100  | 28.16258900 | 3.00834300 |
| C | 2.65895700  | 28.37410000 | 1.92771300 |
| H | 1.69854100  | 27.87231300 | 1.90901300 |
| C | 3.01847600  | 29.26560600 | 0.92941500 |
| H | 2.34570400  | 29.44947700 | 0.10092200 |
| C | 4.24278400  | 29.92775900 | 0.99655400 |
| C | 5.10488700  | 29.72039200 | 2.07163400 |
| C | 4.74178300  | 28.85232100 | 3.08908800 |
| H | 6.05849000  | 30.23216100 | 2.11098400 |
| H | 5.42561500  | 28.66302100 | 3.91099400 |
| H | 4.52597600  | 30.61404400 | 0.20722800 |
| C | 4.08287200  | 25.33649600 | 2.05517200 |
| H | 3.91595800  | 26.16105100 | 1.36290500 |
| H | 4.92926800  | 25.59423900 | 2.69896600 |
| H | 4.37855500  | 24.47092400 | 1.45971800 |
| C | 3.14417500  | 23.63288800 | 3.57918500 |
| H | 4.06283900  | 23.69298500 | 4.16707600 |
| H | 2.34781200  | 23.28302900 | 4.23862300 |
| H | 3.29832800  | 22.85847600 | 2.82515800 |

|   |             |             |            |
|---|-------------|-------------|------------|
| C | 1.65061000  | 24.75927700 | 1.91593800 |
| H | 1.90073900  | 23.99868400 | 1.17313500 |
| H | 0.75584300  | 24.42144200 | 2.44451400 |
| H | 1.40059200  | 25.67608000 | 1.37872500 |
| H | -2.85696000 | 25.52579900 | 9.39268500 |
| H | 3.53181500  | 28.62113800 | 5.35160700 |
| S | 2.40256300  | 24.80427000 | 6.95954800 |
| O | 2.16782000  | 23.33300200 | 6.97166800 |
| C | 4.17256000  | 25.12303800 | 6.87838000 |
| H | 4.65974700  | 24.38204300 | 7.51222200 |
| H | 4.49285100  | 25.00145500 | 5.84456400 |
| H | 4.37604000  | 26.13773700 | 7.21370300 |
| C | 2.05488500  | 25.48153700 | 8.59783100 |
| H | 2.18814200  | 26.56320700 | 8.57237800 |
| H | 1.02036600  | 25.23439300 | 8.83106900 |
| H | 2.73086800  | 25.01167200 | 9.31264300 |

## Int2

E = -1477.963664 a.u.

l 1

|   |             |             |            |
|---|-------------|-------------|------------|
| O | 1.70748500  | 28.48067500 | 4.76640900 |
| O | 3.88964600  | 28.97765000 | 4.22820900 |
| C | 0.38988400  | 27.50340500 | 6.45956300 |
| C | 0.11039600  | 26.37852300 | 7.25691200 |
| H | 0.68741400  | 25.46252200 | 7.15817200 |
| C | -0.91790800 | 26.45264500 | 8.18251300 |
| H | -1.14603300 | 25.59565700 | 8.80406100 |
| C | -1.65843100 | 27.62498600 | 8.31470600 |
| C | -1.38156800 | 28.74217100 | 7.52313300 |
| H | -1.96531600 | 29.64701600 | 7.63673200 |
| C | -0.36017800 | 28.68684600 | 6.59584200 |
| H | -0.13041000 | 29.54223300 | 5.97236500 |
| C | 1.45233500  | 27.44128500 | 5.49868800 |
| C | 2.31404600  | 26.33609600 | 5.19685500 |
| H | 2.27659600  | 25.37296200 | 5.69537200 |
| C | 3.16181700  | 26.72835500 | 4.22175600 |
| C | 4.21696400  | 25.88732300 | 3.55843200 |
| C | 2.84629300  | 28.17537700 | 3.85921400 |
| C | 2.34668900  | 28.37454900 | 2.44330500 |
| C | 1.10955100  | 27.85934000 | 2.05684400 |
| H | 0.47325500  | 27.35763400 | 2.77896500 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 0.68835900  | 27.98627100 | 0.74165600  |
| H | -0.27393500 | 27.58790200 | 0.44350600  |
| C | 1.49965900  | 28.62574400 | -0.19330900 |
| C | 2.73062700  | 29.13998300 | 0.19163200  |
| C | 3.15899600  | 29.01225000 | 1.51019000  |
| H | 3.36466700  | 29.63786900 | -0.53198900 |
| H | 4.13331900  | 29.39278100 | 1.79547400  |
| H | 1.16915300  | 28.72223900 | -1.22055800 |
| C | 5.50200800  | 26.69011900 | 3.30525200  |
| H | 5.33980900  | 27.50633400 | 2.60113000  |
| H | 5.90346200  | 27.11105700 | 4.22809500  |
| H | 6.25092200  | 26.02196200 | 2.87562800  |
| C | 4.52944800  | 24.67828500 | 4.44981700  |
| H | 4.88152000  | 24.99227400 | 5.43540200  |
| H | 3.65449900  | 24.03918900 | 4.58701900  |
| H | 5.31322100  | 24.07918800 | 3.98331200  |
| C | 3.65898800  | 25.37525800 | 2.20928600  |
| H | 4.38605100  | 24.68187000 | 1.78066400  |
| H | 2.71752900  | 24.83901300 | 2.34766400  |
| H | 3.49889600  | 26.18152800 | 1.49320500  |
| H | -2.46134100 | 27.67242900 | 9.04161300  |
| H | 3.71334900  | 29.88730100 | 3.95247400  |
| S | 2.59449600  | 22.47559400 | 7.21261800  |
| O | 1.96737700  | 23.80585400 | 6.82308100  |
| C | 1.21936700  | 21.30959000 | 7.29585300  |
| H | 1.56495600  | 20.35741200 | 7.69785900  |
| H | 0.43509100  | 21.73965800 | 7.91842000  |
| H | 0.85388700  | 21.17067700 | 6.28016000  |
| C | 2.90620600  | 22.59464100 | 8.98660800  |
| H | 3.24047500  | 21.63028800 | 9.36871500  |
| H | 3.68889800  | 23.33790500 | 9.12654400  |
| H | 1.99095300  | 22.91846800 | 9.48182300  |

## TS2

E = -1001.209946 a.u.

1 1

|   |            |             |            |
|---|------------|-------------|------------|
| O | 1.50972100 | 28.77859700 | 4.67147000 |
| O | 4.06920700 | 28.95544700 | 4.02469000 |
| C | 0.37648900 | 27.69302500 | 6.43994300 |
| C | 0.40872600 | 26.67856600 | 7.40426100 |
| H | 1.18094200 | 25.91932400 | 7.39115600 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | -0.53855600 | 26.65641300 | 8.41756200  |
| H | -0.50663500 | 25.87793000 | 9.16975300  |
| C | -1.52743900 | 27.63386500 | 8.46490600  |
| C | -1.56746800 | 28.64523600 | 7.50601700  |
| H | -2.34178000 | 29.40151500 | 7.54680300  |
| C | -0.61583400 | 28.68030800 | 6.50158500  |
| H | -0.63387400 | 29.45741700 | 5.74715600  |
| C | 1.37310200  | 27.76719800 | 5.36227000  |
| C | 2.25197000  | 26.61719400 | 5.03880800  |
| H | 2.14780000  | 25.66939200 | 5.54552600  |
| C | 3.16208300  | 26.80429000 | 4.07594200  |
| C | 4.15989300  | 25.76830600 | 3.56320700  |
| C | 3.22049600  | 28.17253700 | 3.47235700  |
| C | 2.64118300  | 28.45845700 | 2.16418000  |
| C | 1.51179800  | 27.74980200 | 1.73005100  |
| H | 1.04234000  | 27.02627500 | 2.38742500  |
| C | 0.99215700  | 27.99046400 | 0.47165800  |
| H | 0.11368700  | 27.45368700 | 0.13582300  |
| C | 1.60666700  | 28.92196900 | -0.36642600 |
| C | 2.73394600  | 29.61974600 | 0.05537000  |
| C | 3.25037600  | 29.39762100 | 1.32334100  |
| H | 3.21221700  | 30.33258800 | -0.60467900 |
| H | 4.13789000  | 29.93033500 | 1.64295900  |
| H | 1.20491800  | 29.09946500 | -1.35719700 |
| C | 5.56282800  | 26.39521400 | 3.49776500  |
| H | 5.61758300  | 27.20290100 | 2.76392200  |
| H | 5.87332900  | 26.79201000 | 4.46626500  |
| H | 6.27974900  | 25.63014700 | 3.19505800  |
| C | 4.18775300  | 24.55700300 | 4.49833500  |
| H | 4.44670500  | 24.84240200 | 5.52044600  |
| H | 3.23231900  | 24.02748800 | 4.50908000  |
| H | 4.94300600  | 23.85187300 | 4.14804700  |
| C | 3.74646700  | 25.30242800 | 2.15374500  |
| H | 4.43064000  | 24.51385400 | 1.83352500  |
| H | 2.73430300  | 24.89129500 | 2.14964500  |
| H | 3.79881500  | 26.10435600 | 1.41608500  |
| H | -2.27107800 | 27.60905000 | 9.25288600  |
| H | 3.86582300  | 29.92571500 | 3.81871000  |
| O | 2.94848500  | 31.19589900 | 3.77785100  |
| H | 3.18040400  | 32.06266100 | 4.12156400  |
| H | 2.08700000  | 30.93498100 | 4.12618300  |

### Int3

E = -1001.210140 a.u.

1 1

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 1.42003800  | 28.83410000 | 4.67576200  |
| O | 4.06743500  | 28.93935800 | 4.00892700  |
| C | 0.36809800  | 27.69773900 | 6.45985300  |
| C | 0.47395300  | 26.70408800 | 7.43987400  |
| H | 1.28362400  | 25.98469800 | 7.42190900  |
| C | -0.44493700 | 26.65445700 | 8.47876400  |
| H | -0.35452400 | 25.89269200 | 9.24331700  |
| C | -1.47983200 | 27.58223200 | 8.53592500  |
| C | -1.59260600 | 28.57319500 | 7.56196700  |
| H | -2.40170000 | 29.29179000 | 7.60976600  |
| C | -0.66836100 | 28.63683000 | 6.53321100  |
| H | -0.74147600 | 29.39994400 | 5.76786900  |
| C | 1.33225200  | 27.81183200 | 5.34943200  |
| C | 2.21627300  | 26.66248700 | 5.00568700  |
| H | 2.09101100  | 25.71668700 | 5.51282500  |
| C | 3.14525100  | 26.79952700 | 4.05161900  |
| C | 4.12247500  | 25.71824900 | 3.58650200  |
| C | 3.27451000  | 28.14095600 | 3.41150600  |
| C | 2.69868600  | 28.44208900 | 2.11599800  |
| C | 1.58478400  | 27.71766800 | 1.66230700  |
| H | 1.13925800  | 26.96014900 | 2.29700000  |
| C | 1.04780600  | 27.99310000 | 0.41882800  |
| H | 0.18064300  | 27.44724200 | 0.06888700  |
| C | 1.63037300  | 28.97304900 | -0.38595900 |
| C | 2.74312200  | 29.68655200 | 0.05254400  |
| C | 3.27500000  | 29.43200900 | 1.30575900  |
| H | 3.19515500  | 30.43619700 | -0.58465400 |
| H | 4.15041100  | 29.97615200 | 1.63937500  |
| H | 1.21516700  | 29.17774200 | -1.36598100 |
| C | 5.54278400  | 26.30808200 | 3.55268100  |
| H | 5.63993400  | 27.10168700 | 2.80713400  |
| H | 5.83390900  | 26.71418000 | 4.52350700  |
| H | 6.25049700  | 25.52206200 | 3.28402600  |
| C | 4.09093300  | 24.52531000 | 4.54384700  |
| H | 4.33194400  | 24.82225000 | 5.56703600  |
| H | 3.12112900  | 24.02263300 | 4.53945100  |
| H | 4.83481200  | 23.79307900 | 4.22611500  |
| C | 3.73940400  | 25.23710200 | 2.17457700  |



|   |             |             |            |
|---|-------------|-------------|------------|
| H | 4.41796000  | 24.43255000 | 1.88355300 |
| H | 2.72118600  | 24.84195900 | 2.14996600 |
| H | 3.82494000  | 26.02583500 | 1.42557000 |
| H | -2.20152100 | 27.53471300 | 9.34302200 |
| H | 3.84264200  | 29.91589300 | 3.81160500 |
| O | 2.90021100  | 31.13176800 | 3.79927000 |
| H | 3.10815800  | 31.98387500 | 4.19164500 |
| H | 2.05934100  | 30.81045900 | 4.15320500 |

**P-Z**

E = -924.425766 a.u.

0 1

|   |             |             |             |
|---|-------------|-------------|-------------|
| O | 0.62153800  | 28.93763400 | 5.13342200  |
| O | 3.30670000  | 29.86621900 | 3.68168800  |
| C | -0.14345100 | 27.09628200 | 6.38838800  |
| C | -0.07653700 | 25.72139000 | 6.61982100  |
| H | 0.73140900  | 25.13026000 | 6.20438000  |
| C | -1.06691100 | 25.08807200 | 7.36268500  |
| H | -1.01448400 | 24.01867100 | 7.53134200  |
| C | -2.12190400 | 25.82595200 | 7.88670000  |
| C | -2.19614300 | 27.19784600 | 7.65568500  |
| H | -3.02094200 | 27.77274400 | 8.06073100  |
| C | -1.21636700 | 27.82753000 | 6.90372500  |
| H | -1.25988200 | 28.89062500 | 6.69876600  |
| C | 0.87198400  | 27.83426900 | 5.56857100  |
| C | 2.18601600  | 27.18267400 | 5.31380800  |
| H | 2.45671600  | 26.33729100 | 5.93350500  |
| C | 3.03536900  | 27.62836800 | 4.38124800  |
| C | 4.41102600  | 27.02061200 | 4.11899800  |
| C | 2.70164500  | 28.83374700 | 3.52080500  |
| C | 1.71952000  | 28.66852300 | 2.40090900  |
| C | 1.10814400  | 27.44959700 | 2.10886700  |
| H | 1.31809000  | 26.57552000 | 2.71548300  |
| C | 0.22181600  | 27.35227000 | 1.04224300  |
| H | -0.25259400 | 26.40362700 | 0.81872800  |
| C | -0.05786000 | 28.47171400 | 0.26660100  |
| C | 0.55018000  | 29.69105300 | 0.55645600  |
| C | 1.43706400  | 29.78839000 | 1.61797000  |
| H | 0.32883500  | 30.56455500 | -0.04608900 |
| H | 1.92112500  | 30.72561300 | 1.86534500  |
| H | -0.75167600 | 28.39567000 | -0.56321100 |

|   |             |             |            |
|---|-------------|-------------|------------|
| C | 5.48276800  | 27.96361500 | 4.69723800 |
| H | 5.43805700  | 28.95095000 | 4.24035100 |
| H | 5.34814500  | 28.08303200 | 5.77463200 |
| H | 6.47348200  | 27.53641000 | 4.51761400 |
| C | 4.55913400  | 25.64470800 | 4.77225300 |
| H | 4.51919300  | 25.70370300 | 5.86228600 |
| H | 3.78483700  | 24.95145500 | 4.43234800 |
| H | 5.52979700  | 25.22006500 | 4.50673200 |
| C | 4.62972300  | 26.87616600 | 2.60317300 |
| H | 5.61553800  | 26.44428000 | 2.41531000 |
| H | 3.88151200  | 26.22106600 | 2.14937200 |
| H | 4.58851700  | 27.84135300 | 2.09338200 |
| H | -2.88935600 | 25.33209300 | 8.47210300 |

#### Int4

E = -789.211285 a.u.

-1 1

|   |              |             |             |
|---|--------------|-------------|-------------|
| C | -10.25461800 | 10.97677700 | -5.04458000 |
| H | -9.69573200  | 9.98856800  | -5.04456500 |
| C | -9.66972100  | 11.67471100 | -6.30001700 |
| C | -9.66975000  | 11.67473400 | -3.78914200 |
| O | -11.55429000 | 10.95876000 | -5.04459900 |
| F | -10.04813900 | 12.95870100 | -6.42515700 |
| F | -8.30994100  | 11.68047100 | -6.37606300 |
| F | -10.08506700 | 11.04578200 | -7.41557900 |
| F | -10.04811300 | 12.95874900 | -3.66407200 |
| F | -8.30997400  | 11.68043200 | -3.71303300 |
| F | -10.08517900 | 11.04587000 | -2.67357600 |

#### Int5

E = -789.775551 a.u.

0 1

|   |              |             |             |
|---|--------------|-------------|-------------|
| C | -10.13814400 | 10.99276000 | -5.04458100 |
| H | -9.71572400  | 9.98324900  | -5.04456500 |
| C | -9.65480500  | 11.67665000 | -6.32056700 |
| C | -9.65484300  | 11.67667600 | -3.76859500 |
| O | -11.53354000 | 11.01824500 | -5.04460600 |
| H | -11.88470700 | 10.12561600 | -5.04456800 |
| F | -10.09313200 | 12.92587200 | -6.41393700 |
| F | -8.32161200  | 11.69178300 | -6.38857300 |

|   |              |             |             |
|---|--------------|-------------|-------------|
| F | -10.11043600 | 10.99556200 | -7.37589900 |
| F | -10.09315300 | 12.92590700 | -3.67527300 |
| F | -8.32165200  | 11.69178900 | -3.70053800 |
| F | -10.11052500 | 10.99562100 | -2.71326300 |

## H<sub>2</sub>O

E = -76.398884 a.u.

0 1

|   |            |             |            |
|---|------------|-------------|------------|
| O | 4.44610400 | 29.59052700 | 4.21007000 |
| H | 5.40528700 | 29.61583100 | 4.21007000 |
| H | 4.14977500 | 30.50314000 | 4.21007000 |

## DMSO

E = -553.136082 a.u.

0 1

|   |            |             |            |
|---|------------|-------------|------------|
| S | 2.90498700 | 25.34141200 | 6.78556300 |
| O | 3.00132300 | 24.09855600 | 7.62211400 |
| C | 4.61251500 | 25.79872200 | 6.37718100 |
| H | 5.19775900 | 25.77621800 | 7.29682200 |
| H | 4.98784000 | 25.04320800 | 5.68901700 |
| H | 4.64623800 | 26.78167100 | 5.90697400 |
| C | 2.61994900 | 26.70270900 | 7.95060000 |
| H | 2.69691900 | 27.66550600 | 7.44514700 |
| H | 1.61660600 | 26.57162200 | 8.35230800 |
| H | 3.34885000 | 26.61580600 | 8.75677400 |

## 6. Optimization of reaction conditions

**Table S1.** Screening of solvents

| Entry | Deviation from standard conditions <sup>a</sup> | Yield (%) <sup>b</sup> |
|-------|---|------------------------|
| 1     | 5 mL CHCl <sub>3</sub>                          | NR <sup>c</sup>        |
| 2     | 5 mL ethyl acetate                              | Trace                  |
| 3     | 5 mL MeCN                                       | 21%                    |
| 4     | 5 mL THF  | Trace                  |
| 5     | 5 mL DCE  | 6%                     |
| 6     | 5 mL MeNO <sub>2</sub>                          | 8%                     |

<sup>a</sup>Reaction conditions: GF anode (1.0 cm x 1.0 cm x 0.5 cm), GF cathode (1.0 cm x 1.0 cm x 0.5 cm), undivided cell, constant current = 5 mA, **1a** (0.1 mmol, 1.0 eq.), **2a** (0.2 mmol, 2.0 eq.), H<sub>2</sub>O

(0.1 mmol, 1.0 eq.) electrolyte (4.0 eq.), DCM = 4.0 mL, HFIP = 1.0 mL, 5 mA, 0 °C, Air, 2.25 h (4.20 F·mol<sup>-1</sup>), <sup>b</sup>Isolated yields.

**Table S2.** Screening of quantity of electrolyte

| Entry | Deviation from standard conditions <sup>a</sup>     | Yield (%) <sup>b</sup> |
|-------|---|------------------------|
| 1     | 0.2 mmol <i>n</i> -Bu <sub>4</sub> NBF <sub>4</sub> | 65%                    |

<sup>a</sup>Reaction conditions: GF anode (1.0 cm x 1.0 cm x 0.5 cm), GF cathode (1.0 cm x 1.0 cm x 0.5 cm), undivided cell, constant current = 5 mA, **1a** (0.1 mmol, 1.0 eq.), **2a** (0.2 mmol, 2.0 eq.), H<sub>2</sub>O (0.1 mmol, 1.0 eq.) electrolyte (4.0 eq.), DCM = 4.0 mL, HFIP = 1.0 mL, 5 mA, 0 °C, Air, 2.25 h (4.20 F·mol<sup>-1</sup>), <sup>b</sup>Isolated yields.

**Table S3.** Screening of experimental response time

| Entry | Deviation from standard conditions <sup>a</sup> | Yield (%) <sup>b</sup> |
|-------|---|------------------------|
| 1     | 2 h   | 76%                    |
| 2     | 2.5 h   | 62%                    |

<sup>a</sup>Reaction conditions: GF anode (1.0 cm x 1.0 cm x 0.5 cm), GF cathode (1.0 cm x 1.0 cm x 0.5 cm), undivided cell, constant current = 5 mA, **1a** (0.1 mmol, 1.0 eq.), **2a** (0.2 mmol, 2.0 eq.), H<sub>2</sub>O (0.1 mmol, 1.0 eq.) electrolyte (4.0 eq.), DCM = 4.0 mL, HFIP = 1.0 mL, 5 mA, 0 °C, Air, 2.25 h (4.20 F·mol<sup>-1</sup>), <sup>b</sup>Isolated yields.

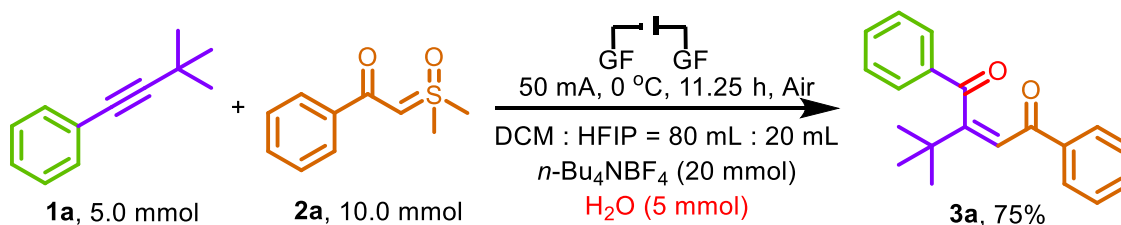
## 7. Gram-scale reaction



**Figure S6.** Components required for gram-scale reaction



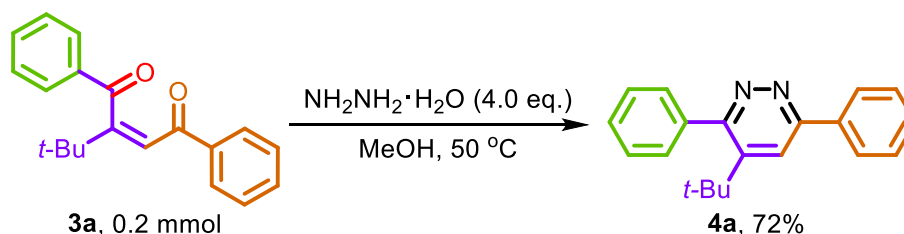
**Figure S7.** Typical reaction set up for gram-scale reaction



To the mixed solution of DCM (80.0 mL), HFIP (20.0 mL), H<sub>2</sub>O (5.0 mmol, 1.0 eq.), alkyne **1a** (5.0 mmol, 1.0 eq.), sulfoxonium ylide **2a** (10.0 mmol, 2.0 eq.) and tetrabutylammonium tetrafluoroborate (20.0 mmol, 4.0 eq.) were added. Equipped with graphite felt (2.0 cm × 1.0 cm × 0.5 cm) as anode, graphite felt (2.0 cm × 1.0 cm × 0.5 cm) as cathode, non-separating electrolytic cell device. The reaction mixture was stirred at constant current of 50 mA at 0 °C in the air for 15 hours. After the reaction (monitored by TLC), the reaction system was dried with anhydrous MgSO<sub>4</sub>, filtered, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography and eluted with petroleum ether and ethyl acetate (PE/ EA = 20:1).

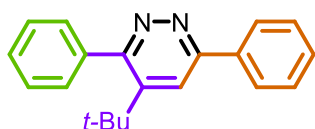
## 8. Synthetic Application

### a) Synthesis of Product **4a**



A flame-dried Schlenk-tube equipped with a magnetic stir bar was charged with **3a** (58.5 mg, 0.2 mmol, 1.0 eq.), sealed with a septum, and degassed by alternating vacuum evacuation and nitrogen

backfilling (three times) before MeOH (2.0 mL) was added. Then, hydrazinium hydroxide solution (wt.% = 85%, 45.6  $\mu$ L, 0.8 mmol, 4.0 eq.) were added successively by micro-syringe. The reaction mixture was then stirred at 50 °C for 5 h. After the reaction was complete, the solvent was removed under reduced pressure with the aid of a rotary evaporator. The crude residue was purified by silica gel column chromatography (PE:EtOAc = 10:1) to afford the desired product **4a** as a white solid in 72% yield (41.5 mg).<sup>[6]</sup>



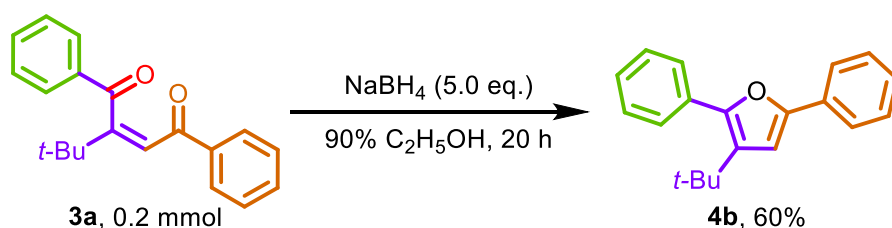
**4-(tert-butyl)-3,6-diphenylpyridazine (4a)**

41.5 mg, 72% yield.

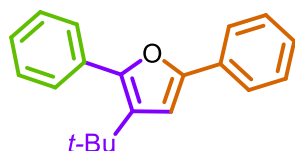
<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  8.13 (d,  $J$  = 7.0 Hz, 2H), 7.92 (s, 1H), 7.56 – 7.51 (m, 3H), 7.47 – 7.45 (m, 3H), 7.42 (dd,  $J$  = 6.1, 2.5 Hz, 2H),

1.27 (s, 9H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  161.2, 158.1, 148.4, 140.7, 136.8, 129.8, 129.0, 128.3, 127.8, 127.2, 121.8, 35.4, 31.2. HRMS (ESI-TOF, [M + H<sup>+</sup>]): calcd for C<sub>20</sub>H<sub>20</sub>N<sub>2</sub> 289.1699, found 289.1703

b) Synthesis of Product **4b**



1,4-dicarbonyl Z-alkene **3a** (0.2 mmol, 58.5 mg) was added to a flask containing ethanol (90%) in an ice bath at 0 °C. NaBH<sub>4</sub> (1.0 mmol, 38.0 mg) was added and the mixture was kept stirring at 0 °C for 1 h. After that time, the ice bath was removed and the mixture was stirred at room temperature overnight. Water (40 mL) and aqueous HCl (2.0 M) were added to the mixture until pH 7 was reached. The resulting aqueous phase was washed with ethyl acetate (3 x 20.0 mL) and the combined organic phases were dried over MgSO<sub>4</sub> and filtered off. The organic solvent was removed under vacuum and the residue was purified by column chromatography using petroleum ether and ethyl acetate (100:1 v/v) as eluent. (33.1 mg, 60% yield).<sup>[6]</sup>



**3-(tert-butyl)-2,5-diphenylfuran (4b)**

33.1 mg, 60% yield.

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  7.68 (d,  $J$  = 7.3 Hz, 2H), 7.55 (dd,  $J$  = 7.7, 1.8 Hz, 2H), 7.45 – 7.34 (m, 5H), 7.25 – 7.23 (m, 1H), 6.74 (s, 1H), 1.27

(s, 9H). <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)  $\delta$  151.4, 148.2, 133.8, 132.8, 130.9, 130.4, 128.6, 128.6, 128.5, 128.2, 127.8, 127.0, 123.6, 106.8, 31.8, 30.7. HRMS (ESI-TOF, [M + H<sup>+</sup>]): calcd for C<sub>20</sub>H<sub>20</sub>O 277.1587, found 277.1583

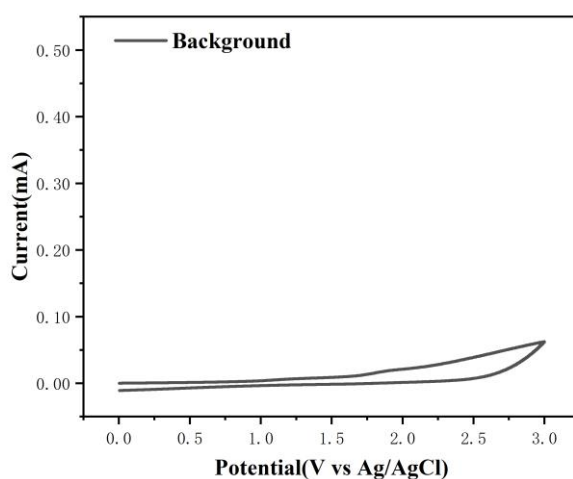
## 9. Cyclic voltammetry study

The cyclic voltammetry experiments were carried out with a computer-controlled electrochemical analyzer for electrochemical measurements. The data was collected with the CS300H potentiostat (Wuhan Coster Instrument Co., LTD).

**Working electrode:** The working electrode is a 3 mm diameter glassy carbon working electrode. Polished with 0.05  $\mu\text{m}$  aluminum oxide and then sonicated in distilled water and ethanol before measurements.

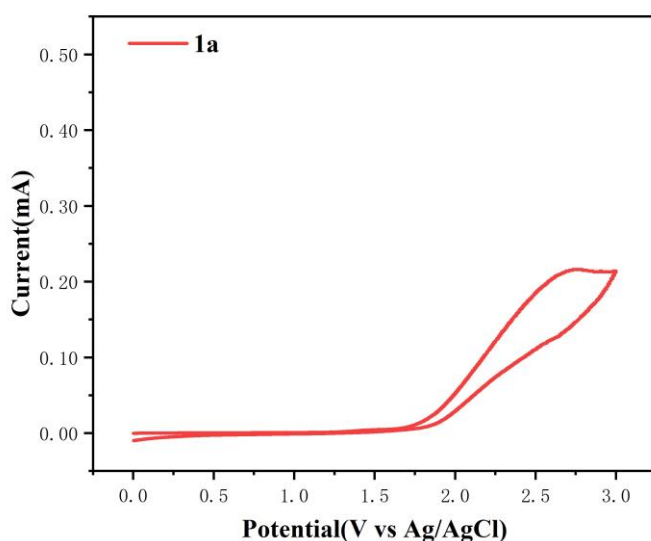
**Reference electrode:** The reference electrode is SCE (saturated aqueous KCl) that was washed with water and ethanol before measurements.

**Counter electrode:** The counter electrode is a platinum wire that was polished with 0.05  $\mu\text{m}$  aluminum oxide and then sonicated in distilled water and ethanol before measurements.



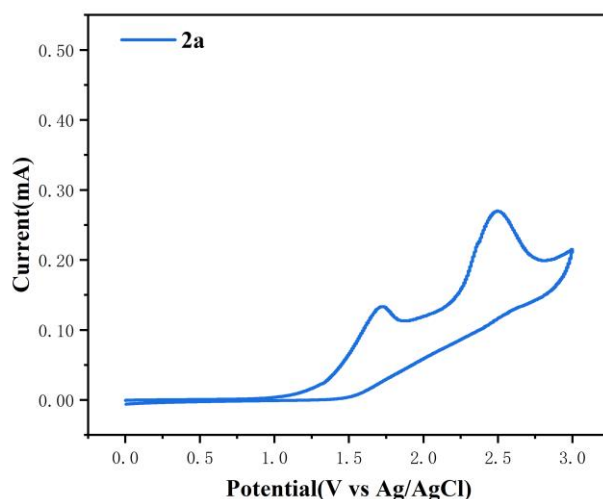
**Figure S8.** Cyclic voltammogram of **blank** sample

**General procedure for cyclic voltammetry (CV):** Cyclic voltammogram of **blank** sample was performed in a three-electrode cell at room temperature. The working electrode was a steady glassy carbon, the counter electrode was a platinum wire, and the reference was an Ag/AgCl electrode submerged in saturated aqueous KCl solution. A solution of *n*-Bu<sub>4</sub>NBF<sub>4</sub> (0.1 mmol) in 4.0 mL DCM, 1.0 mL HFIP, and 1.8  $\mu\text{L}$  H<sub>2</sub>O was subject to cyclic voltammetry experiment. The scan rate was 100 mV/s, ranging from 0.0 V to 3.0 V.



**Figure S9.** Cyclic voltammogram of **1a** sample

**General procedure for cyclic voltammetry (CV):** Cyclic voltammogram of **1a** sample was performed in a three-electrode cell at room temperature. The working electrode was a steady glassy carbon, the counter electrode was a platinum wire, and the reference was an Ag/AgCl electrode submerged in saturated aqueous KCl solution. A solution of **1a** (0.1 mmol) and *n*-Bu<sub>4</sub>NBF<sub>4</sub> (0.1 mmol) in 4.0 mL DCM, 1.0 mL HFIP, and 1.8 μL H<sub>2</sub>O was subject to cyclic voltammetry experiment. The scan rate was 100 mV/s, ranging from 0.0 V to 3.0 V.

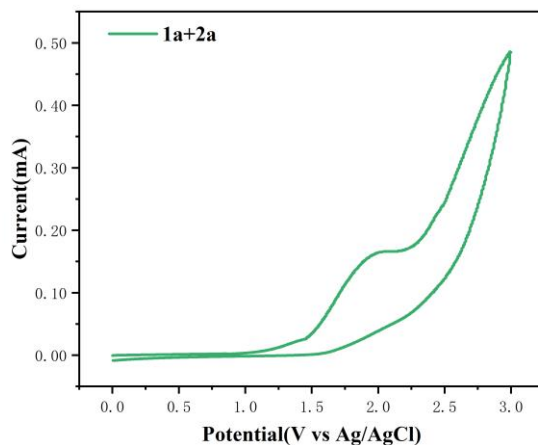


**Figure S10.** Cyclic voltammogram of **2a** sample

**General procedure for cyclic voltammetry (CV):** Cyclic voltammogram of **2a** sample was performed in a three-electrode cell at room temperature. The working electrode was a steady glassy carbon, the counter electrode was a platinum wire, and the reference was an Ag/AgCl electrode

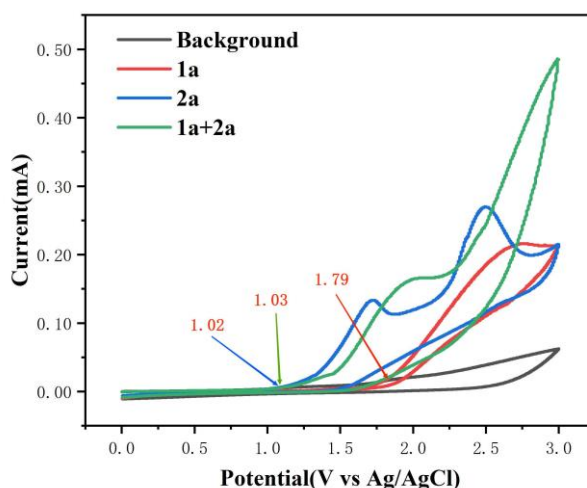


submerged in saturated aqueous KCl solution. A solution of **2a** (0.1 mmol) and *n*-Bu<sub>4</sub>NBF<sub>4</sub> (0.1 mmol) in 4.0 mL DCM, 1.0 mL HFIP, and 1.8 μL H<sub>2</sub>O was subject to cyclic voltammetry experiment. The scan rate was 100 mV/s, ranging from 0.0 V to 3.0 V.

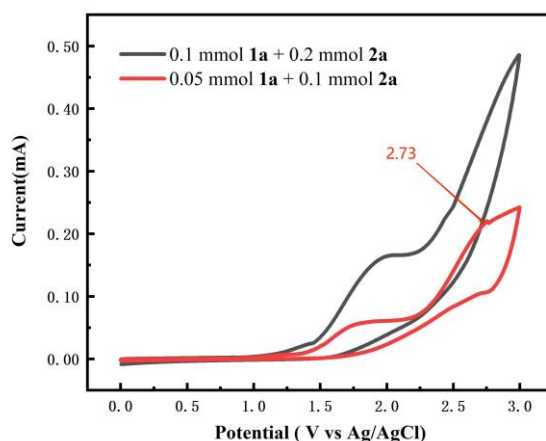


**Figure S11.** Cyclic voltammogram of **1a+2a** sample

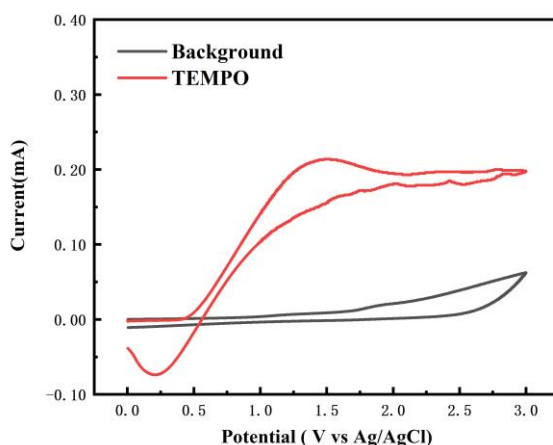
**General procedure for cyclic voltammetry (CV):** Cyclic voltammogram of **1a+2a** sample was performed in a three-electrode cell at room temperature. The working electrode was a steady glassy carbon, the counter electrode was a platinum wire, and the reference was an Ag/AgCl electrode submerged in saturated aqueous KCl solution. A solution of **1a** (0.1 mmol), **2a** (0.2 mmol) and *n*-Bu<sub>4</sub>NBF<sub>4</sub> (0.1 mmol) in 4.0 mL DCM, 1.0 mL HFIP, and 1.8 μL H<sub>2</sub>O was subject to cyclic voltammetry experiment. The scan rate was 100 mV/s, ranging from 0.0 V to 3.0 V.



**Figure S12.** Cyclic voltammograms of **blank**, **1a**, **2a**, and **1a+2a**

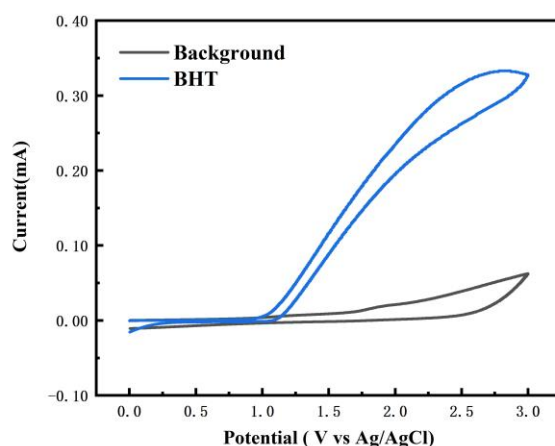


**Figure S13.** Cyclic voltammograms of **1a+2a**, and 0.5 eq. (**1a+2a**)



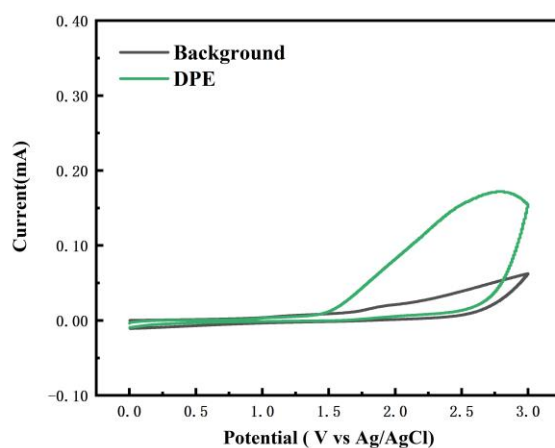
**Figure S14.** Cyclic voltammograms of **TEMPO**

**General procedure for cyclic voltammetry (CV):** Cyclic voltammogram of **TEMPO** sample was performed in a three-electrode cell at room temperature. The working electrode was a steady glassy carbon, the counter electrode was a platinum wire, and the reference was an Ag/AgCl electrode submerged in saturated aqueous KCl solution. A solution of **TEMPO** (0.1 mmol) and *n*-Bu<sub>4</sub>NBF<sub>4</sub> (0.1 mmol) in 4.0 mL DCM, 1.0 mL HFIP, and 1.8  $\mu$ L H<sub>2</sub>O was subject to cyclic voltammetry experiment. The scan rate was 100 mV/s, ranging from 0.0 V to 3.0 V.



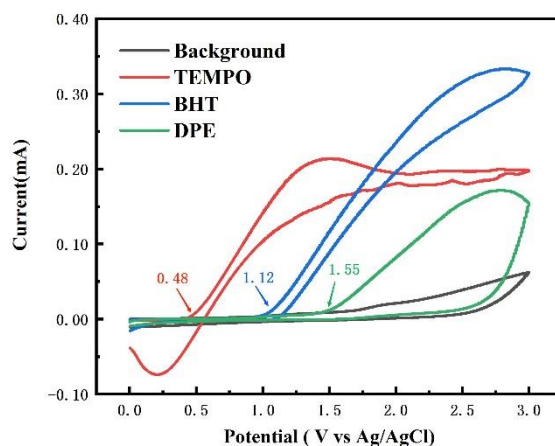
**Figure S15.** Cyclic voltammograms of **BHT**

**General procedure for cyclic voltammetry (CV):** Cyclic voltammogram of **BHT** sample was performed in a three-electrode cell at room temperature. The working electrode was a steady glassy carbon, the counter electrode was a platinum wire, and the reference was an Ag/AgCl electrode submerged in saturated aqueous KCl solution. A solution of **BHT** (0.1 mmol) and *n*-Bu<sub>4</sub>NBF<sub>4</sub> (0.1 mmol) in 4.0 mL DCM, 1.0 mL HFIP, and 1.8 μL H<sub>2</sub>O was subject to cyclic voltammetry experiment. The scan rate was 100 mV/s, ranging from 0.0 V to 3.0 V.



**Figure S16.** Cyclic voltammograms of **DPE**

**General procedure for cyclic voltammetry (CV):** Cyclic voltammogram of **DPE** sample was performed in a three-electrode cell at room temperature. The working electrode was a steady glassy carbon, the counter electrode was a platinum wire, and the reference was an Ag/AgCl electrode submerged in saturated aqueous KCl solution. A solution of **DPE** (0.1 mmol) and *n*-Bu<sub>4</sub>NBF<sub>4</sub> (0.1 mmol) in 4.0 mL DCM, 1.0 mL HFIP, and 1.8 μL H<sub>2</sub>O was subject to cyclic voltammetry experiment. The scan rate was 100 mV/s, ranging from 0.0 V to 3.0 V.

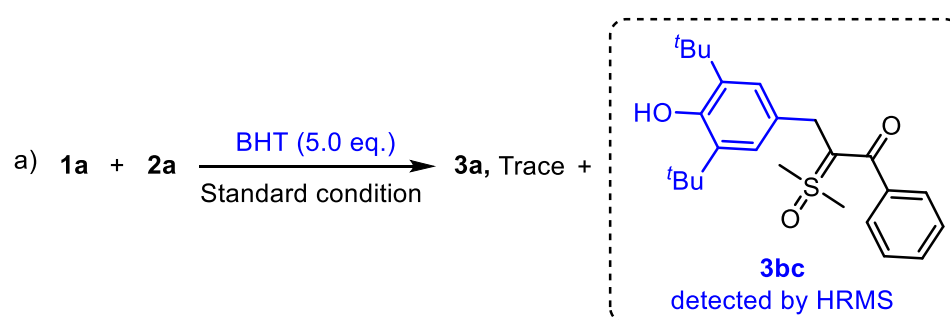


**Figure S17.** Cyclic voltammograms of **TEMPO**, **BHT**, **DPE**

The cyclic voltammetry in terms of **TEMPO**, **BHT** and **1,1-diphenylethylene (DPE)** was conducted and the results showed that the onset potential of **TEMPO** was 0.75 V, which was lower than that of **2a** (1.03 V), indicating that **TEMPO** was firstly oxidized. However, the fact that the onset potential of **BHT** was 1.12 V and the onset potential of **1,1-diphenylethylene** was 1.55 V, which was higher than that of **2a** (1.03 V), indicated that **2a** was first oxidized through the electrochemical reaction.

## 10. Control experiment

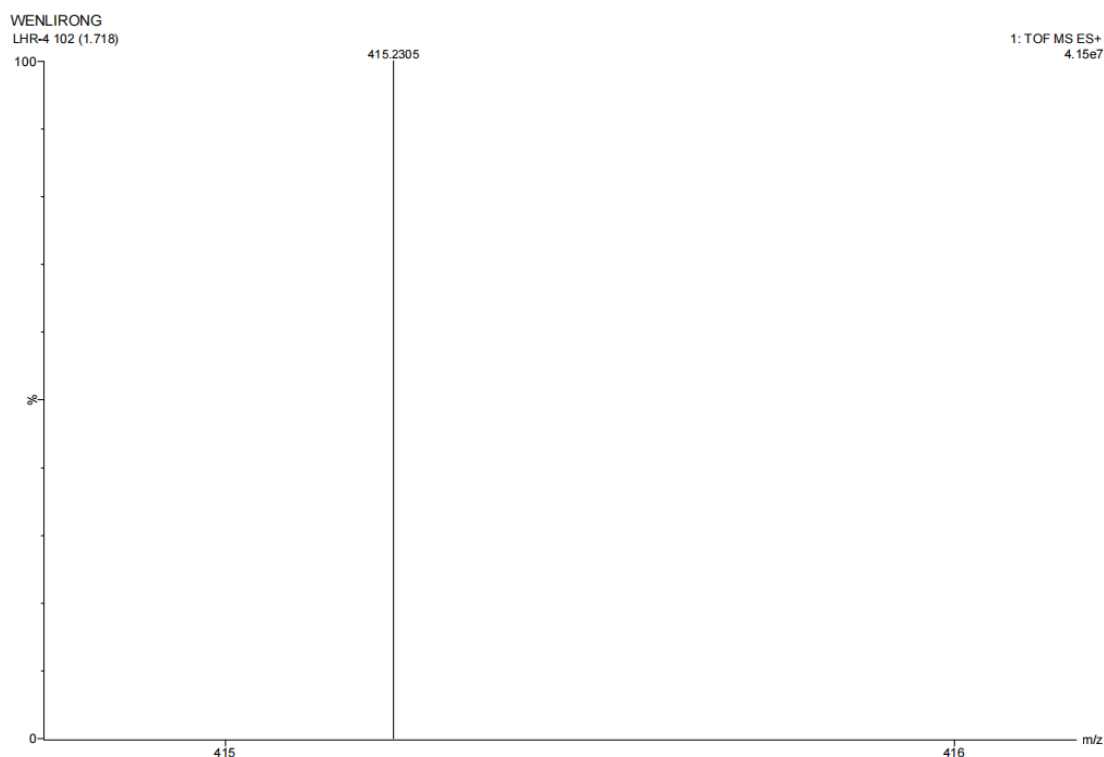
### 10.1 Radical trapping experiment



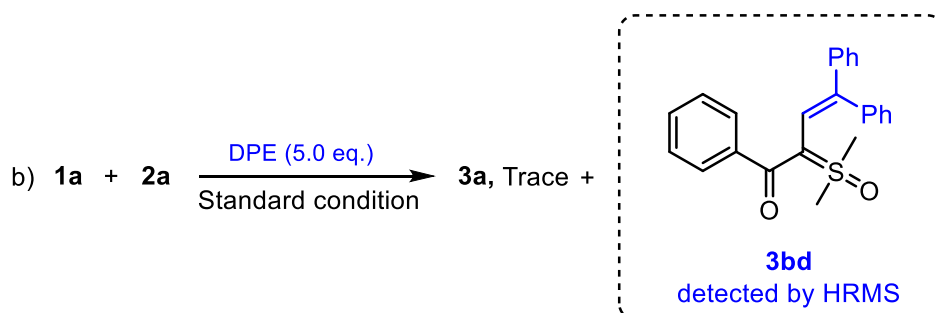
In an undivided cell (10 mL) equipped with a stir bar, **1a** (0.1 mmol, 1.0 eq.), **2a** (0.2 mmol, 2.0 eq.),  $\text{H}_2\text{O}$  (0.1 mmol, 1.0 eq.), butylated hydroxytoluene (BHT) (0.5 mmol, 5.0 eq.) and  $n\text{-Bu}_4\text{NBF}_4$  (0.4 mmol, 4.0 eq.) were combined and added. The flask was equipped with a rubber stopper, a graphite felt anode (1.0 cm x 1.0 cm x 0.5 cm) and a graphite felt cathode (1.0 cm x 1.0 cm x 0.5 cm). Then DCM (4.0 mL) and 1,1,1,3,3,3-Hexafluoro-2-propanol (HFIP) (1.0 mL) and were injected respectively into the flask via syringes. The reaction mixture was stirred and

electrolyzed in air for 2.25 hours at a constant current of 0 °C and 5 mA. After the reaction was complete, no product **3a** was gained. **3bc** detected by HRMS.

HRMS (ESI-TOF, [M + H<sup>+</sup>]): calcd for C<sub>25</sub>H<sub>34</sub>O<sub>3</sub>S 415.2301, found 415.2305

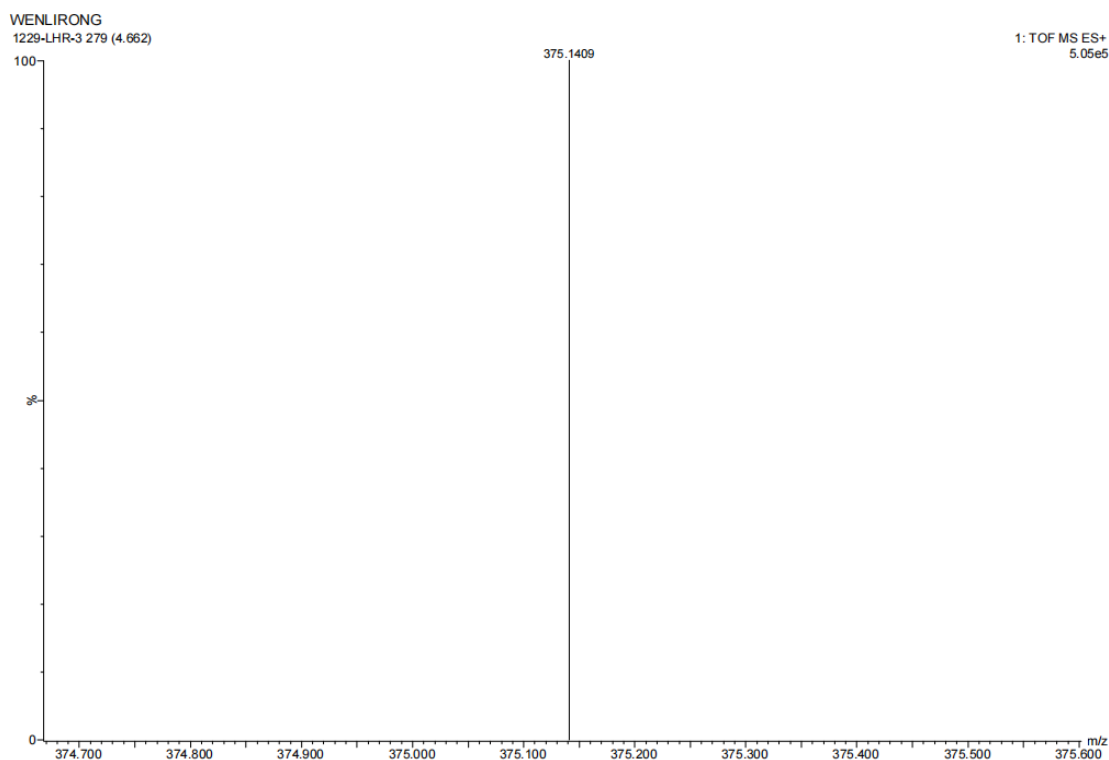


**Figure S18.** HRMS of **3bc**



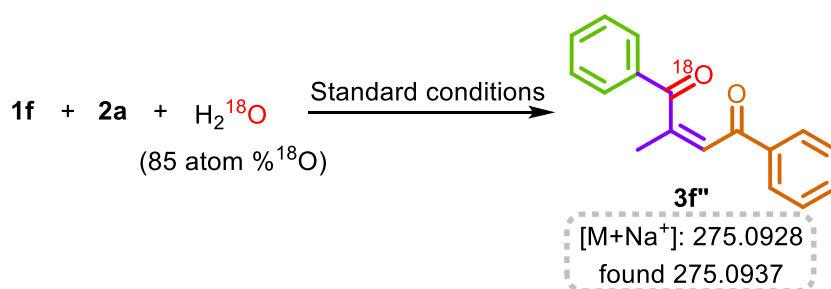
In an undivided cell (10 mL) equipped with a stir bar, **1a** (0.1 mmol, 1.0 eq.), **2a** (0.2 mmol, 2.0 eq.), H<sub>2</sub>O (0.1 mmol, 1.0 eq.), butylated 1,1-diphenylethylene (DPE) (0.5 mmol, 5.0 eq.) and *n*-Bu<sub>4</sub>NBF<sub>4</sub> (0.4 mmol, 4.0 eq.) were combined and added. The flask was equipped with a rubber stopper, a graphite felt anode (1.0 cm x 1.0 cm x 0.5 cm) and a graphite felt cathode (1.0 cm x 1.0 cm x 0.5 cm). Then DCM (4.0 mL) and 1,1,1,3,3,3-Hexafluoro-2-propanol (HFIP) (1.0 mL) and were injected respectively into the flask via syringes. The reaction mixture was stirred and electrolyzed in air for 2.25 hours at a constant current of 0 °C and 5 mA. After the reaction was complete, no product **3a** was gained. **3bd** detected by HRMS.

HRMS (ESI-TOF, [M + H<sup>+</sup>]): calcd for C<sub>24</sub>H<sub>22</sub>O<sub>2</sub>S 375.1413, found 375.1409



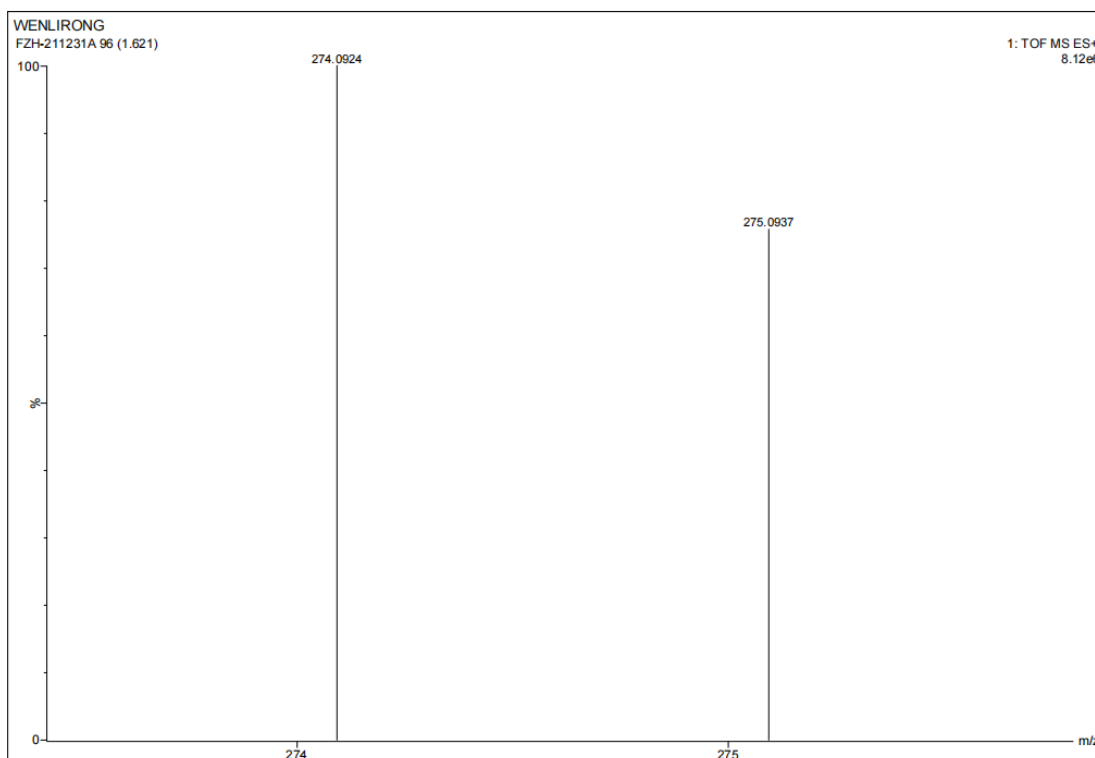
**Figure S19.** HRMS of **3bd**

## 10.2 $^{18}\text{O}$ -labeling experiments



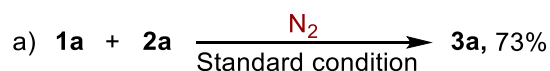
In an undivided cell (10 mL) equipped with a stir bar, **1f** (0.1 mmol, 1.0 eq.), **2a** (0.2 mmol, 2.0 eq.),  $\text{H}_2^{18}\text{O}$  (0.1 mmol, 1.0 eq.), and *n*-Bu<sub>4</sub>NBF<sub>4</sub> (0.4 mmol, 4.0 eq.) were combined and added. The flask was equipped with a rubber stopper, a graphite felt anode (1.0 cm x 1.0 cm x 0.5 cm) and a graphite felt cathode (1.0 cm x 1.0 cm x 0.5 cm). Then DCM (4.0 mL) and 1,1,1,3,3,3-Hexafluoro-2-propanol (HFIP) (1.0 mL) and were injected respectively into the flask via syringes. The reaction mixture was stirred and electrolyzed in air for 2.25 hours at a constant current of 0 °C and 5 mA. After the reaction was complete, the residue was purified by column chromatography using petroleum ether and ethyl acetate as eluent, to afford the desired product **3f''**. **3f''** detected by HRMS.

HRMS (ESI-TOF, [M + Na<sup>+</sup>]): calcd for C<sub>17</sub>H<sub>14</sub>O<sup>18</sup>O 275.0928, found 275.0937



**Figure S20.** HRMS of **3f''**

### 10.3 Inert atmosphere and No H<sub>2</sub>O

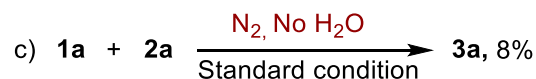


In an undivided cell (10 mL) equipped with a stir bar, **1a** (0.1 mmol, 1.0 eq.), **2a** (0.2 mmol, 2.0 eq.), H<sub>2</sub>O (0.1 mmol, 1.0 eq.), and *n*-Bu<sub>4</sub>NBF<sub>4</sub> (0.4 mmol, 4.0 eq.) were combined and added. The flask was equipped with a rubber stopper, a graphite felt anode (1.0 cm x 1.0 cm x 0.5 cm) and a graphite felt cathode (1.0 cm x 1.0 cm x 0.5 cm). Then DCM (4.0 mL) and 1,1,1,3,3,3-Hexafluoro-2-propanol (HFIP) (1.0 mL) were injected respectively into the flask via syringes. The reaction mixture was stirred and electrolyzed in N<sub>2</sub> for 2.25 hours at a constant current of 0 °C and 5 mA. After the reaction was complete, the residue was purified by column chromatography using petroleum ether and ethyl acetate as eluent, to afford the desired product **3a**.

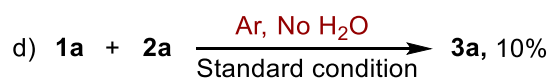


In an undivided cell (10 mL) equipped with a stir bar, **1a** (0.1 mmol, 1.0 eq.), **2a** (0.2 mmol, 2.0 eq.), H<sub>2</sub>O (0.1 mmol, 1.0 eq.), and *n*-Bu<sub>4</sub>NBF<sub>4</sub> (0.4 mmol, 4.0 eq.) were combined and added. The flask was equipped with a rubber stopper, a graphite felt anode (1.0 cm x 1.0 cm x 0.5 cm) and a graphite felt cathode (1.0 cm x 1.0 cm x 0.5 cm). Then DCM (4.0 mL) and

1,1,1,3,3,3-Hexafluoro-2-propanol (HFIP) (1.0 mL) and were injected respectively into the flask via syringes. The reaction mixture was stirred and electrolyzed in Argon (Ar) for 2.25 hours at a constant current of 0 °C and 5 mA. After the reaction was complete, the residue was purified by column chromatography using petroleum ether and ethyl acetate as eluent, to afford the desired product **3a**.

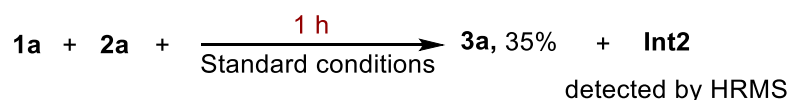


In an undivided cell (10 mL) equipped with a stir bar, **1a** (0.1 mmol, 1.0 eq.), **2a** (0.2 mmol, 2.0 eq.), and *n*-Bu<sub>4</sub>NBF<sub>4</sub> (0.4 mmol, 4.0 eq.) were combined and added. The flask was equipped with a rubber stopper, a graphite felt anode (1.0 cm x 1.0 cm x 0.5 cm) and a graphite felt cathode (1.0 cm x 1.0 cm x 0.5 cm). Then DCM (4.0 mL) and 1,1,1,3,3,3-Hexafluoro-2-propanol (HFIP) (1.0 mL) and were injected respectively into the flask via syringes. The reaction mixture was stirred and electrolyzed in N<sub>2</sub> for 2.25 hours at a constant current of 0 °C and 5 mA. After the reaction was complete, the residue was purified by column chromatography using petroleum ether and ethyl acetate as eluent, to afford the desired product **3a**.



In an undivided cell (10 mL) equipped with a stir bar, **1a** (0.1 mmol, 1.0 eq.), **2a** (0.2 mmol, 2.0 eq.), and *n*-Bu<sub>4</sub>NBF<sub>4</sub> (0.4 mmol, 4.0 eq.) were combined and added. The flask was equipped with a rubber stopper, a graphite felt anode (1.0 cm x 1.0 cm x 0.5 cm) and a graphite felt cathode (1.0 cm x 1.0 cm x 0.5 cm). Then DCM (4.0 mL) and 1,1,1,3,3,3-Hexafluoro-2-propanol (HFIP) (1.0 mL) and were injected respectively into the flask via syringes. The reaction mixture was stirred and electrolyzed in Argon (Ar) for 2.25 hours at a constant current of 0 °C and 5 mA. After the reaction was complete, the residue was purified by column chromatography using petroleum ether and ethyl acetate as eluent, to afford the desired product **3a**.

#### 10.4 Intermediate detection



In an undivided cell (10 mL) equipped with a stir bar, **1a** (0.1 mmol, 1.0 eq.), **2a** (0.2 mmol, 2.0 eq.), H<sub>2</sub>O (0.1 mmol, 1.0 eq.), and *n*-Bu<sub>4</sub>NBF<sub>4</sub> (0.4 mmol, 4.0 eq.) were combined and added. The flask was equipped with a rubber stopper, a graphite felt anode (1.0 cm x 1.0 cm x 0.5 cm) and a graphite felt cathode (1.0 cm x 1.0 cm x 0.5 cm). Then DCM (4.0 mL) and 1,1,1,3,3,3-Hexafluoro-2-propanol (HFIP) (1.0 mL) and were injected respectively into the flask via syringes. The reaction mixture was stirred and electrolyzed in air for 1 hours at a constant current of 0 °C and 5 mA. After the reaction was complete, the residue was purified by column



chromatography using petroleum ether and ethyl acetate as eluent, to afford the desired product **3a**. **Int2** detected by HRMS.

HRMS (ESI-TOF,  $[M^+]$ ): calcd for  $C_{20}H_{21}O_2^+$  293.1536, found 293.1537

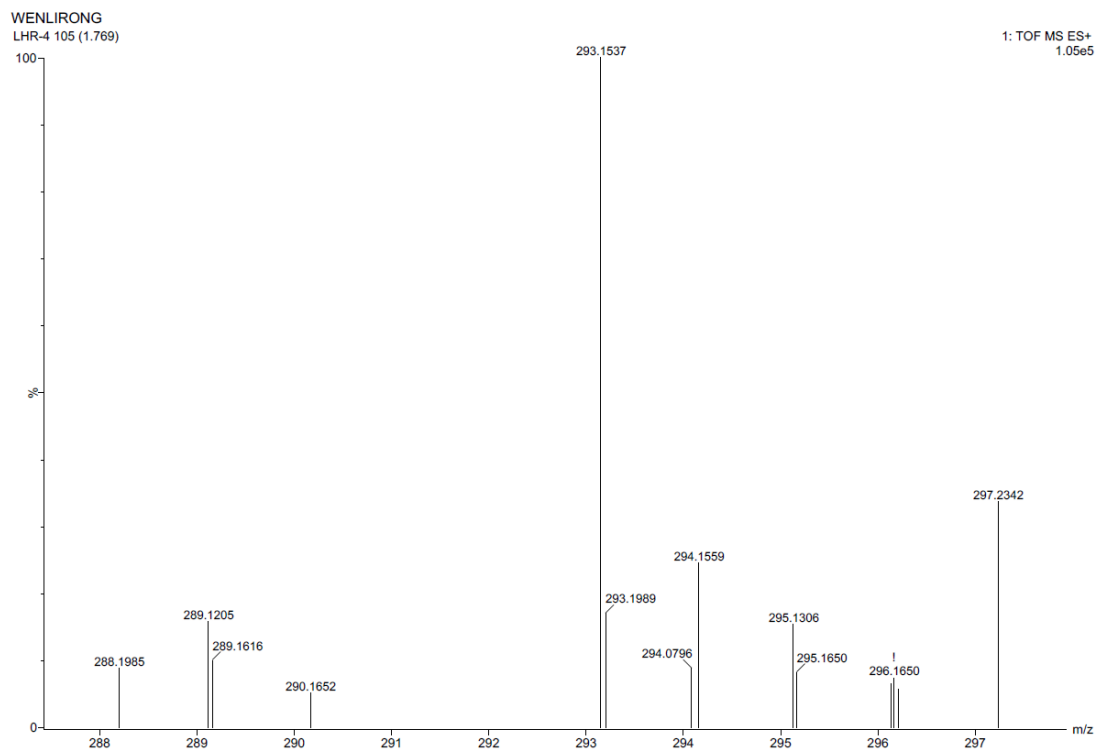
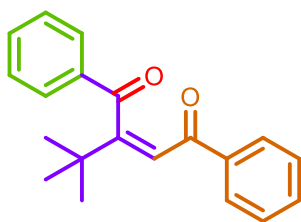


Figure S21. HRMS of Int2

## 11. NMR Spectra for the Obtained Compound



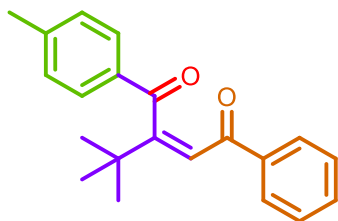
### (Z)-2-(tert-butyl)-1,4-diphenylbut-2-ene-1,4-dione (**3a**)

24.5 mg, 84% yield.

$^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  7.97 – 7.91 (m, 4H), 7.58 (t,  $J = 7.4$  Hz, 1H), 7.53 (t,  $J = 7.4$  Hz, 1H), 7.49 – 7.43 (m, 4H), 7.29 (s, 1H), 1.31 (s, 9H).

$^{13}C$  NMR (125 MHz,  $CDCl_3$ )  $\delta$  198.9, 188.5, 167.8, 137.3, 136.4, 132.9, 132.6, 128.4, 128.3, 128.2, 128.1, 120.3, 36.5, 29.6.

HRMS (ESI-TOF,  $[M + Na^+]$ ): calcd for  $C_{20}H_{20}O_2$  315.1356, found 315.1359



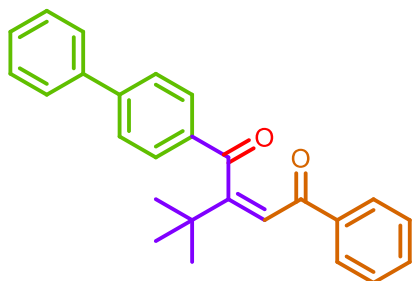
**(Z)-2-(tert-butyl)-4-phenyl-1-(p-tolyl)but-2-ene-1,4-dione (3b)**

21.8 mg, 71% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.90 (d,  $J = 7.3$  Hz, 2H), 7.80 (d,  $J = 7.9$  Hz, 2H), 7.54 (t,  $J = 7.4$  Hz, 1H), 7.44 (t,  $J = 7.6$  Hz, 2H), 7.23 (s, 1H), 7.21 (d,  $J = 8.0$  Hz, 2H), 2.37 (s, 3H), 1.27 (s, 9H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  198.8, 188.7, 168.1, 143.6, 137.6, 134.3, 133.0, 129.3, 128.7, 128.6, 128.5, 128.4, 120.3, 36.7, 29.9, 21.7.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{21}\text{H}_{22}\text{O}_2$  307.1693, found 307.1693



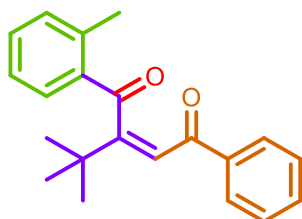
**(Z)-1-([1,1'-biphenyl]-4-yl)-2-(tert-butyl)-4-phenylbut-2-ene-1,4-dione (3c)**

22.9 mg, 62% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.99 (d,  $J = 8.2$  Hz, 2H), 7.93 (d,  $J = 7.4$  Hz, 2H), 7.64 (d,  $J = 8.6$  Hz, 2H), 7.60 (d,  $J = 7.0$  Hz, 2H), 7.55 (d,  $J = 7.5$  Hz, 1H), 7.47 – 7.43 (m, 4H), 7.37 (t,  $J = 7.3$  Hz, 1H), 7.29 (s, 1H), 1.32 (s, 9H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  198.8, 188.8, 168.1, 145.6, 140.1, 137.6, 135.5, 133.2, 128.9, 128.9, 128.7, 128.6, 128.5, 128.1, 127.4, 127.3, 120.5, 36.8, 29.9.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{26}\text{H}_{24}\text{O}_2$  369.1849, found 369.1855



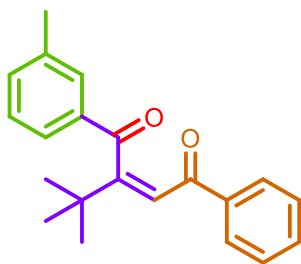
**(Z)-2-(tert-butyl)-4-phenyl-1-(o-tolyl)but-2-ene-1,4-dione (3d)**

23.3 mg, 76% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.79 (d,  $J = 7.6$  Hz, 2H), 7.51 (d,  $J = 8.5$  Hz, 1H), 7.45 (t,  $J = 7.4$  Hz, 1H), 7.35 (t,  $J = 7.7$  Hz, 2H), 7.25 (t,  $J = 7.5$  Hz, 1H), 7.17 (d,  $J = 7.2$  Hz, 1H), 7.09 (s, 1H), 7.06 (t,  $J = 7.6$  Hz, 1H), 2.67 (s, 3H), 1.21 (s, 9H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  201.0, 189.2, 169.2, 140.3, 137.7, 135.2, 133.0, 132.3, 131.9, 131.7, 128.6, 128.5, 125.3, 120.7, 36.9, 30.2, 22.2.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{21}\text{H}_{22}\text{O}_2$  307.1693, found 307.1687



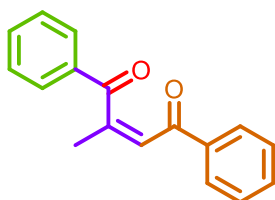
**(Z)-2-(tert-butyl)-4-phenyl-1-(m-tolyl)but-2-ene-1,4-dione (3e)**

21.3 mg, 70% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.87 (dd,  $J = 8.4, 1.4$  Hz, 2H), 7.76 (s, 1H), 7.60 (d,  $J = 7.5$  Hz, 1H), 7.52 (t,  $J = 7.4$  Hz, 1H), 7.41 (t,  $J = 7.6$  Hz, 2H), 7.29 (d,  $J = 7.8$  Hz, 1H), 7.24 (d,  $J = 3.8$  Hz, 1H), 7.22 (s, 1H), 2.35 (s, 3H), 1.25 (s, 9H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  199.3, 188.7, 168.2, 138.4, 137.6, 136.6, 133.8, 133.1, 128.6, 128.5, 128.5, 128.4, 125.9, 120.4, 36.7, 29.9, 21.4.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{21}\text{H}_{22}\text{O}_2$  307.1693, found 307.1698



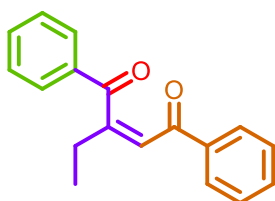
**(Z)-2-methyl-1,4-diphenylbut-2-ene-1,4-dione (3f)**

15.3 mg, 61% yield. The spectra matched with the previous report.<sup>[7]</sup>

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.93 – 7.91 (m, 4H), 7.55 (t,  $J = 7.4$  Hz, 2H), 7.46 – 7.43 (m, 4H), 7.16 (s, 1H), 2.25 (s, 3H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  199.4, 188.1, 156.3, 136.9, 134.5, 133.3, 133.3, 128.8, 128.7, 128.6, 128.4, 122.9, 22.2.

HRMS (ESI-TOF,  $[\text{M} + \text{Na}^+]$ ): calcd for  $\text{C}_{17}\text{H}_{14}\text{O}_2$  273.0886, found 273.0889



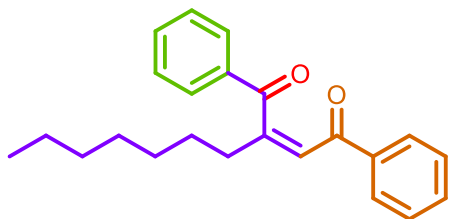
**(Z)-2-ethyl-1,4-diphenylbut-2-ene-1,4-dione (3g)**

16.4 mg, 62% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.92 – 7.90 (m, 4H), 7.54 (q,  $J = 7.5$  Hz, 2H), 7.46 – 7.42 (m, 4H), 7.12 (s, 1H), 2.57 (q,  $J = 6.6$  Hz, 2H), 1.25 (t,  $J = 7.4$  Hz, 3H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  199.3, 188.3, 161.6, 137.2, 135.2, 133.1, 128.7, 128.6, 128.6, 128.4, 121.1, 28.7, 11.6.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{18}\text{H}_{16}\text{O}_2$  265.1223, found 265.1225



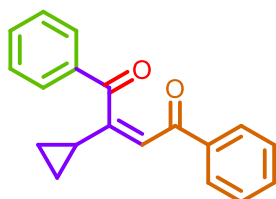
**(Z)-2-heptyl-1,4-diphenylbut-2-ene-1,4-dione (3h)**

16.3 mg, 49% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.91 (d,  $J = 7.8$  Hz, 4 H), 7.57 – 7.52 (m, 2H), 7.46 – 7.42 (m, 4H), 7.11 (s, 1H), 2.51 (t,  $J = 7.8$  Hz, 2H), 1.66 – 1.59 (m, 2H), 1.39 – 1.36 (m, 2H), 1.32 – 1.25 (m, 6H), 0.88 (t,  $J = 6.7$  Hz, 2H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  199.2, 188.3, 160.5, 137.2, 135.1, 133.1, 128.7, 128.6, 128.6, 128.4, 121.9, 35.7, 31.7, 29.2, 28.9, 27.2, 22.6, 14.0.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{23}\text{H}_{26}\text{O}_2$  335.2006, found 335.2008



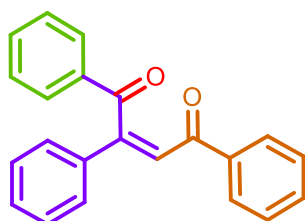
**(Z)-2-cyclopropyl-1,4-diphenylbut-2-ene-1,4-dione (3i)**

18.8 mg, 68% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.94 (d,  $J = 7.7$  Hz, 2H), 7.90 (d,  $J = 7.7$  Hz, 2H), 7.54 (t,  $J = 7.5$  Hz, 2H), 7.46 – 7.42 (m, 4H), 7.14 (s, 1H), 1.91 – 1.85 (m, 1H), 1.03 – 1.01 (m, 2H), 0.89 – 0.87 (m, 2H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  197.3, 187.5, 162.9, 137.3, 135.7, 133.2, 133.0, 128.7, 128.6, 128.5, 128.4, 119.9, 16.9, 9.0.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{19}\text{H}_{16}\text{O}_2$  277.1223, found 277.1222



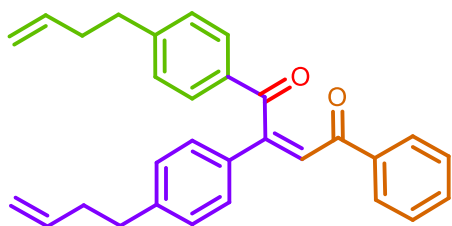
**(Z)-1,2,4-triphenylbut-2-ene-1,4-dione (3j)**

23.2 mg, 74% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.01 – 7.97 (m, 4H), 7.64 (s, 1H), 7.61 (dd,  $J = 8.0, 1.7$  Hz, 2H), 7.59 – 7.56 (m, 1H), 7.54 – 7.51 (m, 1H), 7.47 (t,  $J = 7.7$  Hz, 2H), 7.44 – 7.41 (m, 5H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  197.5, 188.2, 156.4, 137.3, 136.1, 134.8, 133.3, 133.3, 130.7, 129.2, 128.8, 128.7, 128.6, 127.3, 121.0.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{22}\text{H}_{16}\text{O}_2$  313.1223, found 313.1224



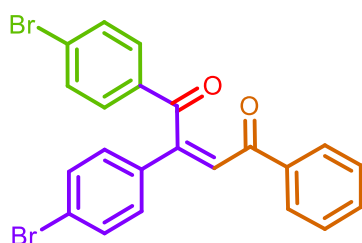
**(Z)-1,2-bis(4-(but-3-en-1-yl)phenyl)-4-phenylbut-2-ene-1,4-dione (3k)**

23.6 mg, 56% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.99 (d,  $J = 7.0$  Hz, 2H), 7.90 (d,  $J = 8.2$  Hz, 2H), 7.61 (s, 1H), 7.59 – 7.52 (m, 3H), 7.46 (t,  $J = 7.7$  Hz, 2H), 7.23 (t,  $J = 7.9$  Hz, 4H), 5.88 – 5.78 (m, 2H), 5.06 – 4.97 (m, 4H), 2.74 – 2.70 (m, 4H), 2.39 – 2.33 (m, 4H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  197.4, 188.2, 156.5, 147.8, 145.1, 137.6, 137.5, 134.2, 133.2, 132.5, 129.3, 128.9, 128.9, 128.7, 128.6, 127.3, 119.9, 115.4, 115.3, 35.5, 35.2, 35.1, 34.9.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{30}\text{H}_{28}\text{O}_2$  421.2162, found 421.2168



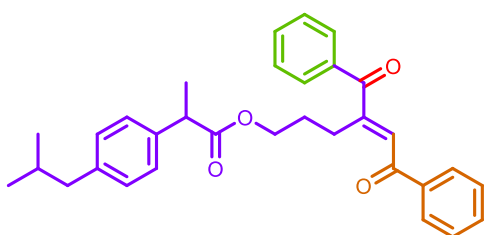
**(Z)-1,2-bis(4-bromophenyl)-4-phenylbut-2-ene-1,4-dione (3l)**

23.4 mg, 50% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.99 – 7.96 (m, 2H), 7.80 (d,  $J = 8.6$  Hz, 2H), 7.62 (s, 1H), 7.60 – 7.54 (m, 5H), 7.50 – 7.43 (m, 4H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  196.1, 188.1, 154.6, 137.0, 134.7, 133.7, 133.3, 132.6, 132.2, 130.1, 128.8, 128.7, 128.7, 125.6, 121.5.

HRMS (ESI-TOF,  $[\text{M} + \text{Na}^+]$ ): calcd for  $\text{C}_{22}\text{H}_{14}\text{Br}_2\text{O}_2$  490.9253, found 490.9252



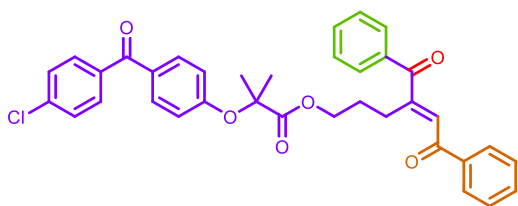
**(E)-4-benzoyl-6-oxo-6-phenylhex-4-en-1-yl 2-(4-isobutylphenyl) propanoate (3m)**

15.8 mg, 33% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.89 – 7.86 (m, 4H), 7.64 – 7.56 (m, 2H), 7.53 – 7.42 (m, 4H), 7.17 (d,  $J = 8.0$  Hz, 2H), 7.05 (d,  $J = 5.6$  Hz, 2H), 7.03 (s, 1H), 4.19 – 4.13 (m, 1H), 4.10 – 4.04 (m, 1H), 3.65 (q,  $J = 7.1$  Hz, 1H), 2.88 – 2.83 (m, 2H), 2.40 (d,  $J = 7.2$  Hz, 2H), 1.90 – 1.84 (m, 2H), 1.83 – 1.77 (m, 1H), 1.46 (d,  $J = 7.2$  Hz, 3H), 0.87 (d,  $J = 6.6$  Hz, 6H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  197.8, 191.5, 174.7, 152.4, 140.4, 137.8, 137.4, 136.5, 133.6, 133.3, 130.9, 129.8, 129.2, 128.8, 128.7, 128.5, 127.2, 64.1, 45.1, 45.0, 30.1, 27.6, 26.0, 22.4, 18.4.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{32}\text{H}_{34}\text{O}_4$  483.2530, found 483.2527



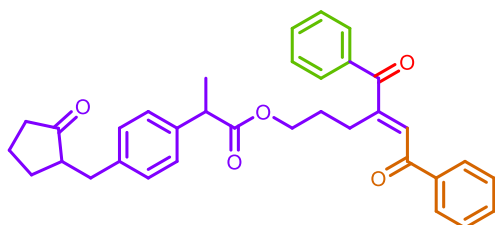
**(E)-4-benzoyl-6-oxo-6-phenylhex-4-en-1-yl  
2-(4-(4-chlorobenzoyl)phenoxy)-2-methylpropanoate (3n)**

25.0 mg, 42% yield.

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.85 – 7.83 (m, 4H), 7.68 (dd, *J* = 8.6, 3.3 Hz, 4H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.49 (t, *J* = 7.7 Hz, 2H), 7.46 – 7.41 (m, 4H), 7.08 (s, 1H), 6.85 (d, *J* = 8.8 Hz, 2H), 4.25 (t, *J* = 6.4 Hz, 2H), 2.85 – 2.82 (m, 2H), 1.93 – 1.87 (m, 2H), 1.67 (s, 6H).

<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 197.7, 194.2, 191.4, 173.5, 159.7, 152.1, 138.3, 137.3, 136.4, 136.4, 133.7, 133.4, 132.0, 131.2, 131.1, 130.3, 129.8, 128.9, 128.7, 128.5, 128.5, 117.4, 79.5, 65.2, 27.7, 25.9, 25.5.

HRMS (ESI-TOF, [M + H<sup>+</sup>]): calcd for C<sub>36</sub>H<sub>31</sub>ClO<sub>6</sub> 595.1882, found 595.1884



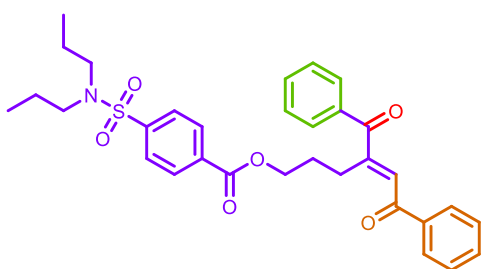
**(E)-4-benzoyl-6-oxo-6-phenylhex-4-en-1-yl 2-(4-((2-oxocyclopentyl)methyl)phenyl)propanoate (3o)**

20.4 mg, 39% yield.

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.88 (d, *J* = 8.2 Hz, 4H), 7.62 (t, *J* = 7.3 Hz, 1H), 7.57 (d, *J* = 7.3 Hz, 1H), 7.53 – 7.45 (m, 4H), 7.18 (d, *J* = 8.0 Hz, 2H), 7.07 (d, *J* = 4.5 Hz, 2H), 7.06 (s, 1H), 4.19 – 4.13 (m, 1H), 4.10 – 4.04 (m, 1H), 3.65 (q, *J* = 7.2 Hz, 1H), 3.09 (dd, *J* = 13.9, 4.0 Hz, 1H), 2.88 – 2.83 (m, 2H), 2.48 – 2.43 (m, 1H), 2.43 – 2.28 (m, 2H), 2.14 – 2.06 (m, 2H), 1.95 – 1.83 (m, 3H), 1.74 – 1.63 (m, 2H), 1.45 (d, *J* = 7.2 Hz, 3H).

<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 197.7, 191.5, 174.6, 152.4, 138.7, 138.4, 137.4, 136.5, 133.7, 133.3, 130.9, 129.8, 129.0, 128.8, 128.7, 128.5, 127.6, 64.2, 51.0, 45.1, 38.2, 35.2, 29.2, 27.6, 26.0, 20.5, 18.4.

HRMS (ESI-TOF, [M + H<sup>+</sup>]): calcd for C<sub>34</sub>H<sub>34</sub>O<sub>5</sub> 523.2479, found 523.2481



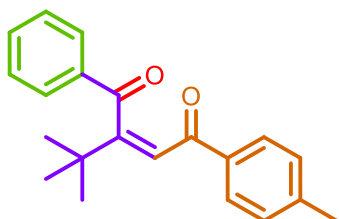
**(E)-4-benzoyl-6-oxo-6-phenylhex-4-en-1-yl 4-(N,N-dipropylsulfamoyl)benzoate (3p)**

22.5 mg, 40% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.13 (d,  $J = 8.2$  Hz, 2H), 7.90 – 7.84 (m, 6H), 7.63 (t,  $J = 7.4$  Hz, 1H), 7.57 (t,  $J = 7.4$  Hz, 1H), 7.51 (t,  $J = 7.6$  Hz, 2H), 7.45 (t,  $J = 7.7$  Hz, 2H), 7.13 (s, 1H), 4.41 (t,  $J = 6.3$  Hz, 2H), 3.12 – 3.08 (m, 4H), 3.02 (t,  $J = 7.8$  Hz, 2H), 2.09 – 2.03 (m, 2H), 1.58 – 1.52 (m, 4H), 0.87 (t,  $J = 7.4$  Hz, 6H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  197.8, 191.6, 165.2, 152.0, 144.1, 137.3, 136.4, 133.7, 133.6, 133.4, 131.4, 130.3, 129.8, 128.9, 128.7, 128.5, 126.9, 65.0, 50.0, 27.7, 26.0, 22.0, 11.2.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{32}\text{H}_{35}\text{NO}_6\text{S}$  562.2258, found 562.2264



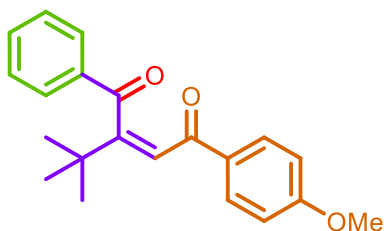
**(Z)-2-(tert-butyl)-1-phenyl-4-(p-tolyl)but-2-ene-1,4-dione (3q)**

23.3 mg, 76% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.90 (d,  $J = 7.5$  Hz, 2H), 7.81 (d,  $J = 7.9$  Hz, 2H), 7.49 (t,  $J = 7.4$  Hz, 1H), 7.40 (t,  $J = 7.6$  Hz, 2H), 7.24 (s, 2H), 7.23 (s, 1H), 2.40 (s, 3H), 1.27 (s, 9H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  199.2, 188.3, 167.4, 144.0, 136.8, 135.1, 132.7, 129.3, 128.6, 128.5, 128.3, 120.6, 36.7, 29.9, 21.7.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{21}\text{H}_{22}\text{O}_2$  307.1693, found 307.1693



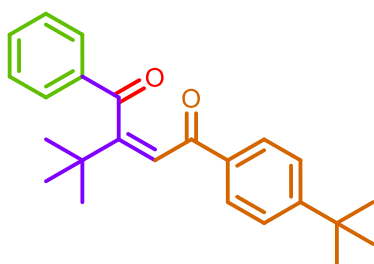
**(Z)-2-(tert-butyl)-4-(4-methoxyphenyl)-1-phenylbut-2-ene-1,4-dione (3r)**

26.6 mg, 83% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.90 (d,  $J = 9.0$  Hz, 4H), 7.49 (t,  $J = 7.3$  Hz, 1H), 7.40 (t,  $J = 7.5$  Hz, 2H), 7.22 (s, 1H), 6.91 (d,  $J = 9.0$  Hz, 2H), 3.85 (s, 3H), 1.26 (s, 9H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  199.4, 187.2, 167.0, 163.6, 136.8, 132.8, 130.9, 130.5, 128.5, 128.3, 120.5, 113.8, 55.5, 36.6, 29.9.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{21}\text{H}_{22}\text{O}_3$  323.1642, found 323.1649



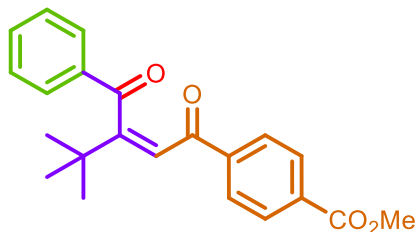
**(Z)-2-(tert-butyl)-4-(4-(tert-butyl)phenyl)-1-phenylbut-2-ene-1,4-dione (3s)**

23.0 mg, 66% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.90 (d,  $J = 7.1$  Hz, 2H), 7.85 (d,  $J = 8.5$  Hz, 2H), 7.51 – 7.44 (m, 3H), 7.39 (t,  $J = 7.5$  Hz, 2H), 7.26 (s, 1H), 1.32 (s, 9H), 1.27 (s, 9H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  199.3, 188.3, 167.5, 156.9, 136.7, 135.0, 132.8, 128.5, 128.5, 128.3, 125.6, 120.6, 36.7, 35.1, 31.1, 29.9.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{24}\text{H}_{28}\text{O}_2$  349.2162, found 349.2161



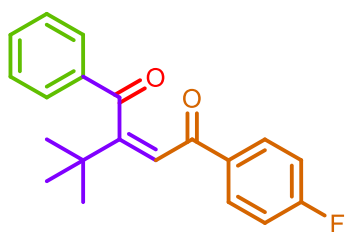
**methyl (Z)-4-(3-benzoyl-4,4-dimethylpent-2-enoyl) benzoate (3t)**

23.5 mg, 67% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.09 (d,  $J = 8.3$  Hz, 2H), 7.93 (d,  $J = 8.2$  Hz, 2H), 7.89 (d,  $J = 7.2$  Hz, 2H), 7.52 (t,  $J = 7.3$  Hz, 1H), 7.42 (t,  $J = 7.6$  Hz, 2H), 7.23 (s, 1H), 3.94 (s, 3H), 1.28 (s, 9H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  198.8, 188.2, 169.3, 166.1, 140.8, 136.5, 133.8, 133.0, 129.8, 128.6, 128.3, 128.3, 120.2, 52.4, 36.9, 29.8.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{22}\text{H}_{22}\text{O}_4$  351.1591, found 351.1594



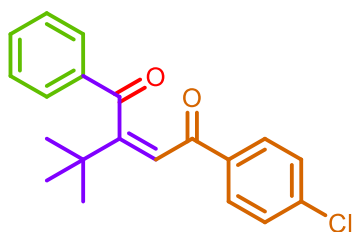
**(Z)-2-(tert-butyl)-4-(4-fluorophenyl)-1-phenylbut-2-ene-1,4-dione (3u)**

25.2 mg, 81% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.94 – 7.88 (m, 1H), 7.51 (t,  $J = 7.4$  Hz, 1H), 7.41 (t,  $J = 7.6$  Hz, 2H), 7.20 (s, 1H), 7.11 (t,  $J = 8.5$  Hz, 2H), 1.27 (s, 9H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  197.9, 186.2, 167.3, 163.7 (d,  $J = 255.1$  Hz), 135.7, 133.0 (d,  $J = 3.0$  Hz), 131.9, 130.1 (d,  $J = 9.4$  Hz), 127.5, 127.3, 119.2, 114.7 (d,  $J = 21.9$  Hz), 35.7, 28.9.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{20}\text{H}_{19}\text{FO}_2$  311.1442, found 311.1438



**(Z)-2-(tert-butyl)-4-(4-chlorophenyl)-1-phenylbut-2-ene-1,4-dione (3v)**

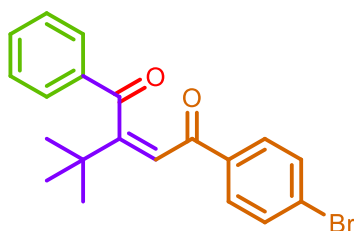
21.9 mg, 67% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.89 (d,  $J = 6.9$  Hz, 2H), 7.83 (d,  $J = 8.6$  Hz, 2H), 7.51 (t,  $J = 7.3$  Hz, 1H), 7.43 (d,  $J = 5.7$  Hz, 2H), 7.41 (d,  $J = 6.6$  Hz, 2H), 7.19 (s, 1H), 1.27 (s, 9H).



$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  198.9, 187.5, 168.7, 139.6, 136.6, 135.9, 132.9, 129.9, 128.9, 128.6, 128.3, 120.1, 36.8, 29.8.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{20}\text{H}_{19}\text{ClO}_2$  327.1146, found 327.1141



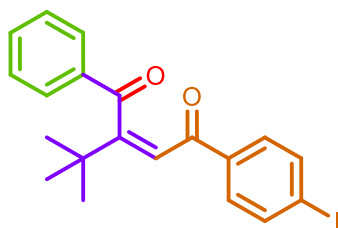
**(Z)-4-(4-bromophenyl)-2-(tert-butyl)-1-phenylbut-2-ene-1,4-dione (3w)**

23.6 mg, 74% yield.

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.88 (d,  $J = 7.0$  Hz, 2H), 7.75 (d,  $J = 8.6$  Hz, 2H), 7.58 (d,  $J = 8.5$  Hz, 2H), 7.53 – 7.49 (m, 1H), 7.41 (t,  $J = 7.7$  Hz, 2H), 7.17 (s, 1H), 1.27 (s, 9H).

$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  198.9, 187.7, 168.8, 136.6, 136.3, 132.9, 131.9, 130.0, 128.6, 128.3, 120.0, 36.8, 29.8.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{20}\text{H}_{19}\text{BrO}_2$  371.0641, found 371.0639



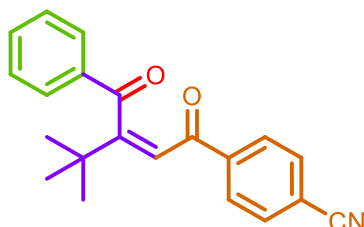
**(Z)-2-(tert-butyl)-4-(4-iodophenyl)-1-phenylbut-2-ene-1,4-dione (3x)**

22.1 mg, 53% yield.

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.91 (d,  $J = 7.5$  Hz, 2H), 7.83 (d,  $J = 8.1$  Hz, 2H), 7.62 (d,  $J = 8.0$  Hz, 2H), 7.54 (t,  $J = 7.4$  Hz, 1H), 7.44 (t,  $J = 7.5$  Hz, 2H), 7.20 (s, 1H), 1.30 (s, 9H).

$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  198.9, 188.0, 168.8, 137.9, 136.8, 136.6, 132.9, 129.8, 128.6, 128.3, 119.9, 101.1, 36.8, 29.9.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{20}\text{H}_{19}\text{IO}_2$  419.0502, found 419.0505



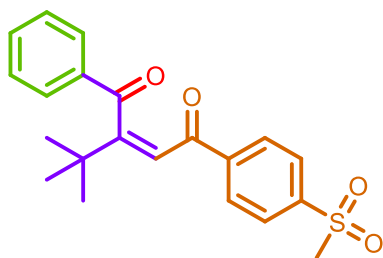
**(Z)-4-(3-benzoyl-4,4-dimethylpent-2-enoyl) benzonitrile (3y)**

21.6 mg, 65% yield.

$^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.96 (d,  $J = 8.5$  Hz, 2H), 7.88 (d,  $J = 7.6$  Hz, 2H), 7.73 (d,  $J = 8.2$  Hz, 2H), 7.53 (t,  $J = 7.4$  Hz, 1H), 7.42 (t,  $J = 7.6$  Hz, 2H), 7.18 (s, 1H), 1.28 (s, 9H).

$^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )  $\delta$  198.6, 187.5, 170.4, 140.6, 136.4, 133.1, 132.5, 128.8, 128.6, 128.3, 119.6, 117.8, 116.3, 37.0, 29.8.

HRMS (ESI-TOF,  $[M + H^+]$ ): calcd for  $C_{21}H_{19}NO_2$  318.1489, found 318.1490



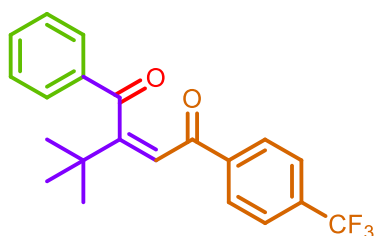
**(Z)-2-(tert-butyl)-4-(4-(methylsulfonyl)phenyl)-1-phenylbut-2-ene-1,4-dione (3z)**

23.2 mg, 63% yield.

$^1H$  NMR (500 MHz, Chloroform-*d*)  $\delta$  8.05 – 7.99 (m, 4H), 7.88 (d,  $J = 7.4$  Hz, 2H), 7.52 (t,  $J = 7.3$  Hz, 1H), 7.42 (t,  $J = 7.6$  Hz, 2H), 7.21 (s, 1H), 3.05 (s, 3H), 1.28 (s, 9H).

$^{13}C$  NMR (125 MHz,  $CDCl_3$ )  $\delta$  198.7, 187.6, 170.5, 144.1, 141.6, 136.3, 133.2, 129.3, 128.7, 128.3, 127.8, 119.8, 44.3, 37.1, 29.8.

HRMS (ESI-TOF,  $[M + H^+]$ ): calcd for  $C_{21}H_{22}O_4S$  371.1312, found 371.1310



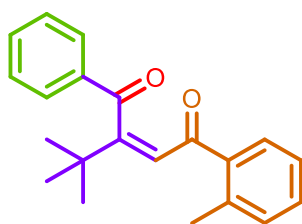
**(Z)-2-(tert-butyl)-1-phenyl-4-(4-(trifluoromethyl)phenyl)but-2-ene-1,4-dione (3aa)**

23.7 mg, 66% yield.

$^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  7.98 (d,  $J = 8.0$  Hz, 2H), 7.89 (d,  $J = 7.7$  Hz, 2H), 7.70 (d,  $J = 8.0$  Hz, 2H), 7.53 (t,  $J = 7.5$  Hz, 1H), 7.43 (t,  $J = 7.6$  Hz, 2H), 7.22 (s, 1H), 1.29 (s, 9H).

$^{13}C$  NMR (125 MHz,  $CDCl_3$ )  $\delta$  198.7, 187.8, 169.7, 140.3, 136.5, 134.3 (q,  $J = 32.7$  Hz), 133.0, 128.7, 128.6, 128.3, 125.7 (q,  $J = 3.8$  Hz), 123.6 (d,  $J = 272.7$  Hz), 120.0, 36.9, 29.8.

HRMS (ESI-TOF,  $[M + H^+]$ ): calcd for  $C_{21}H_{19}F_3O_2$  361.1410, found 361.1411



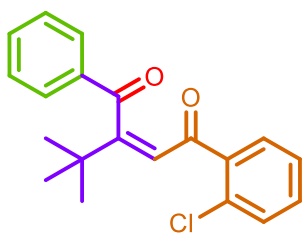
**(Z)-2-(tert-butyl)-1-phenyl-4-(o-tolyl) but-2-ene-1,4-dione (3ab)**

19.4 mg, 63% yield.

$^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  7.90 (d,  $J = 7.5$  Hz, 2H), 7.57 (d,  $J = 7.6$  Hz, 1H), 7.51 (t,  $J = 7.4$  Hz, 1H), 7.41 (t,  $J = 7.7$  Hz, 2H), 7.34 (t,  $J = 7.4$  Hz, 1H), 7.24 (d,  $J = 7.5$  Hz, 1H), 7.17 (d,  $J = 7.5$  Hz, 1H), 6.96 (s, 1H), 2.29 (s, 3H), 1.26 (s, 9H).

$^{13}C$  NMR (125 MHz,  $CDCl_3$ )  $\delta$  198.9, 192.9, 166.2, 138.5, 138.1, 136.7, 132.9, 131.6, 131.3, 128.6, 128.5, 128.4, 125.5, 124.4, 36.6, 29.8, 20.5.

HRMS (ESI-TOF,  $[M + H^+]$ ): calcd for  $C_{21}H_{22}O_2$  307.1693, found 307.1698



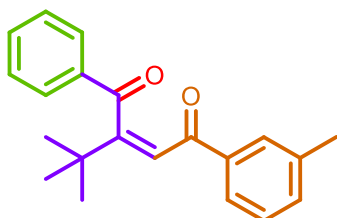
**(Z)-2-(tert-butyl)-4-(2-chlorophenyl)-1-phenylbut-2-ene-1,4-dione (3ac)**

25.5 mg, 78% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.96 (d,  $J = 7.3$  Hz, 2H), 7.52 (t,  $J = 7.3$  Hz, 1H), 7.45 – 7.38 (m, 5H), 7.29 – 7.27 (m, 1H), 7.02 (s, 1H), 1.26 (s, 9H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  198.6, 190.8, 166.4, 138.9, 136.4, 133.0, 132.2, 131.5, 130.4, 130.2, 128.5, 128.4, 127.1, 124.6, 36.7, 29.6.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{20}\text{H}_{19}\text{ClO}_2$  327.1146, found 327.1149



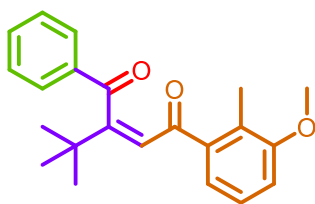
**(Z)-2-(tert-butyl)-1-phenyl-4-(m-tolyl)but-2-ene-1,4-dione (3ad)**

21.0 mg, 69% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.90 (d,  $J = 7.6$  Hz, 2H), 7.71 (d,  $J = 9.7$  Hz, 2H), 7.50 (t,  $J = 7.3$  Hz, 1H), 7.40 (t,  $J = 7.6$  Hz, 2H), 7.35 – 7.31 (m, 2H), 7.25 (s, 1H), 2.38 (s, 3H), 1.28 (s, 9H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  199.2, 188.9, 167.8, 138.5, 137.5, 136.7, 133.9, 132.8, 129.0, 128.6, 128.5, 128.3, 125.7, 120.7, 36.8, 29.9, 21.4.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{21}\text{H}_{22}\text{O}_2$  307.1693, found 307.1695



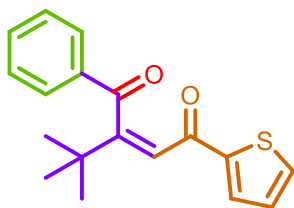
**(Z)-2-(tert-butyl)-4-(3-methoxy-2-methylphenyl)-1-phenylbut-2-ene-1,4-dione (3ae)**

16.8 mg, 50% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.91 (d,  $J = 7.2$  Hz, 2H), 7.51 (t,  $J = 7.4$  Hz, 1H), 7.42 (t,  $J = 7.5$  Hz, 2H), 7.20 (t,  $J = 7.9$  Hz, 1H), 7.07 (d,  $J = 7.6$  Hz, 1H), 6.93 (d,  $J = 8.1$  Hz, 1H), 6.88 (s, 1H), 3.82 (s, 3H), 2.14 (s, 3H), 1.24 (s, 9H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  198.9, 193.4, 166.3, 158.1, 140.6, 136.6, 132.9, 128.5, 128.3, 126.2, 126.1, 124.9, 120.0, 112.6, 55.7, 36.7, 29.8, 12.7.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{22}\text{H}_{24}\text{O}_3$  337.1798, found 337.1796



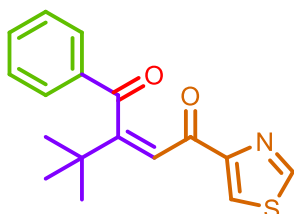
**(Z)-2-(tert-butyl)-1-phenyl-4-(thiophen-2-yl)but-2-ene-1,4-dione (3af)**

13.1 mg, 44% yield.

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.91 – 7.88 (m, 2H), 7.78 (dd, *J* = 3.8, 1.1 Hz, 1H), 7.63 (dd, *J* = 4.9, 1.1 Hz, 1H), 7.53 – 7.49 (m, 1H), 7.42 (t, *J* = 7.4 Hz, 2H), 7.14 (dd, *J* = 4.8, 3.9 Hz, 1H), 7.07 (s, 1H), 1.26 (s, 9H).

<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 198.8, 180.9, 167.8, 144.8, 136.7, 134.4, 132.9, 132.2, 128.6, 128.3, 128.2, 120.5, 36.7, 29.8.

HRMS (ESI-TOF, [M + H<sup>+</sup>]): calcd for C<sub>18</sub>H<sub>18</sub>O<sub>2</sub>S 299.1100, found 299.1110



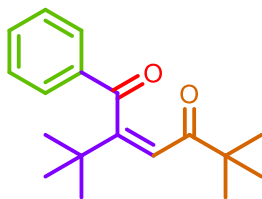
**(Z)-2-(tert-butyl)-1-phenyl-4-(thiazol-5-yl)but-2-ene-1,4-dione (3ag)**

18.0 mg, 60% yield.

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.97 (s, 1H), 8.51 (s, 1H), 7.88 (d, *J* = 6.7 Hz, 2H), 7.53 (t, *J* = 7.4 Hz, 1H), 7.43 (t, *J* = 7.7 Hz, 2H), 7.02 (s, 1H), 1.27 (s, 9H).

<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 198.3, 180.6, 169.7, 159.7, 147.0, 140.8, 136.4, 133.2, 128.7, 128.3, 120.1, 36.9, 29.8.

HRMS (ESI-TOF, [M + H<sup>+</sup>]): calcd for C<sub>17</sub>H<sub>17</sub>NO<sub>2</sub>S 300.1053, found 300.1053



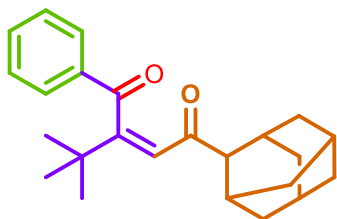
**(Z)-2-(tert-butyl)-5,5-dimethyl-1-phenylhex-2-ene-1,4-dione (3ah)**

16.0 mg, 59% yield.

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.82 (d, *J* = 7.5 Hz, 2H), 7.50 (t, *J* = 7.2 Hz, 1H), 7.41 (t, *J* = 7.6 Hz, 2H), 6.74 (s, 1H), 1.19 (s, 9H), 1.11 (s, 9H).

<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 202.4, 198.3, 165.3, 135.6, 131.7, 127.4, 127.1, 119.1, 42.2, 35.3, 28.8, 25.1.

HRMS (ESI-TOF, [M + H<sup>+</sup>]): calcd for C<sub>18</sub>H<sub>24</sub>O<sub>2</sub> 273.1849, found 273.1853



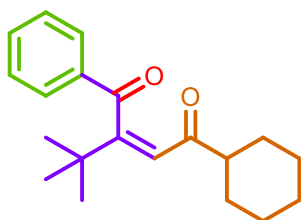
**(Z)-4-(adamantan-2-yl)-2-(tert-butyl)-1-phenylbut-2-ene-1,4-dione (3ai)**

18.1 mg, 52% yield.

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.81 (d, *J* = 7.2 Hz, 2H), 7.49 (t, *J* = 7.4 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 2H), 6.77 (s, 1H), 2.03 (t, *J* = 3.4 Hz, 3H), 1.75 (d, *J* = 3.0 Hz, 7H), 1.72 (s, 2H), 1.68 – 1.65 (m, 3H), 1.19 (s, 9H).

<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 202.9, 199.4, 166.1, 136.6, 132.6, 128.4, 128.2, 119.7, 45.5, 37.9, 36.5, 36.4, 29.8, 27.8.

HRMS (ESI-TOF, [M + H<sup>+</sup>]): calcd for C<sub>24</sub>H<sub>30</sub>O<sub>2</sub> 351.2319, found 351.2321



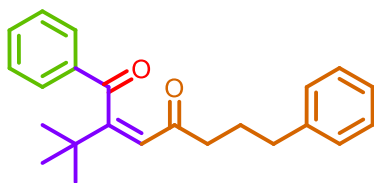
**(Z)-2-(tert-butyl)-4-cyclohexyl-1-phenylbut-2-ene-1,4-dione (3aj)**

15.8 mg, 53% yield.

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.82 (d, *J* = 7.6 Hz, 2H), 7.50 (t, *J* = 7.3 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 2H), 6.52 (s, 1H), 2.41 – 2.36 (m, 1H), 1.81 – 1.73 (m, 4H), 1.67 – 1.61 (m, 1H), 1.25 – 1.21 (m, 4H), 1.19 (s, 9H).

<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 201.5, 199.1, 165.8, 136.6, 132.7, 128.4, 128.2, 123.0, 50.6, 36.2, 29.8, 28.1, 25.8, 25.6.

HRMS (ESI-TOF, [M + H<sup>+</sup>]): calcd for C<sub>20</sub>H<sub>26</sub>O<sub>2</sub> 299.2006, found 299.2006



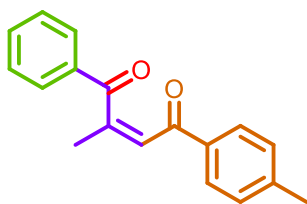
**(Z)-2-(tert-butyl)-1,7-diphenylhept-2-ene-1,4-dione (3ak)**

11.7 mg, 35% yield.

<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 7.83 (d, *J* = 7.7 Hz, 2H), 7.51 (t, *J* = 7.1 Hz, 1H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.27 – 7.24 (m, 2H), 7.18 (d, *J* = 6.5 Hz, 1H), 7.11 (d, *J* = 7.5 Hz, 2H), 6.40 (s, 1H), 2.54 (t, *J* = 7.5 Hz, 2H), 2.47 (t, *J* = 7.3 Hz, 2H), 1.86 – 1.80 (m, 2H), 1.17 (s, 9H).

<sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) δ 199.1, 198.5, 165.6, 141.5, 136.7, 132.8, 128.5, 128.4, 128.3, 128.3, 125.9, 123.7, 42.4, 36.1, 34.9, 29.7, 24.9.

HRMS (ESI-TOF, [M + H<sup>+</sup>]): calcd for C<sub>23</sub>H<sub>26</sub>O<sub>2</sub> 335.2006, found 335.2008



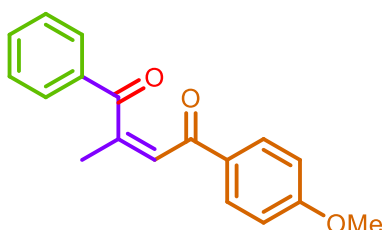
**(Z)-2-methyl-1-phenyl-4-(p-tolyl) but-2-ene-1,4-dione (3al)**

17.7 mg, 67% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.92 (d,  $J = 7.6$  Hz, 2H), 7.82 (d,  $J = 8.0$  Hz, 2H), 7.54 (t,  $J = 7.3$  Hz, 1H), 7.44 (t,  $J = 7.6$  Hz, 2H), 7.24 (d,  $J = 7.9$  Hz, 2H), 7.15 (s, 1H), 2.40 (s, 3H), 2.24 (s, 3H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  199.4, 187.7, 155.7, 144.1, 134.6, 134.5, 133.2, 129.3, 128.7, 128.7, 128.4, 123.0, 22.1, 21.7.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{18}\text{H}_{16}\text{O}_2$  265.1223, found 265.1245



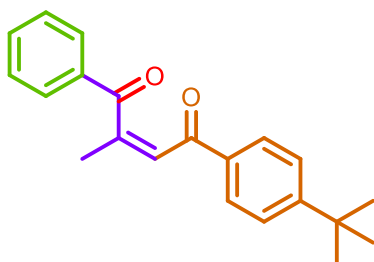
**(Z)-4-(4-methoxyphenyl)-2-methyl-1-phenylbut-2-ene-1,4-dione (3am)**

17.9 mg, 64% yield. The spectra matched with the previous report.<sup>[7]</sup>

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.90 – 7.86 (m, 4H), 7.60 (t,  $J = 7.4$  Hz, 1H), 7.50 (t,  $J = 7.8$  Hz, 2H), 7.07 (s, 1H), 6.93 (d,  $J = 8.9$  Hz, 2H), 3.87 (s, 3H), 2.31 (s, 2H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  198.4, 190.7, 163.9, 148.0, 136.4, 133.0, 131.4, 131.0, 130.6, 129.8, 128.6, 114.0, 55.5, 15.8.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{18}\text{H}_{16}\text{O}_3$  281.1172, found 281.1195



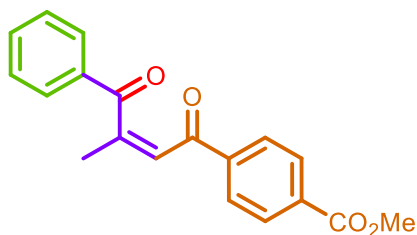
**(Z)-4-(4-(tert-butyl) phenyl)-2-methyl-1-phenylbut-2-ene-1,4-dione (3an)**

18.1 mg, 59% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.92 (d,  $J = 8.3$  Hz, 2H), 7.86 (d,  $J = 8.4$  Hz, 2H), 7.54 (t,  $J = 7.4$  Hz, 1H), 7.47 – 7.44 (m, 4H), 7.16 (s, 1H), 2.25 (s, 3H), 1.33 (s, 9H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  198.7, 186.8, 156.2, 154.8, 133.4, 133.2, 132.3, 127.8, 127.6, 127.4, 124.6, 122.0, 34.1, 30.0, 21.1.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{21}\text{H}_{22}\text{O}_2$  307.1693, found 307.1694



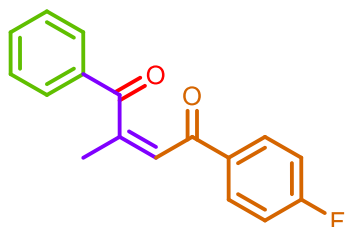
**Methyl (Z)-4-(3-methyl-4-oxo-4-phenylbut-2-enoyl)benzoate (3ao)**

18.8 mg, 61% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.10 (d,  $J = 8.4$  Hz, 2H), 7.95 (d,  $J = 8.5$  Hz, 2H), 7.91 (d,  $J = 8.0$  Hz, 2H), 7.56 (t,  $J = 7.4$  Hz, 1H), 7.46 (t,  $J = 7.6$  Hz, 2H), 7.15 (s, 1H), 3.94 (s, 3H), 2.28 (s, 3H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  199.1, 187.6, 166.2, 157.6, 140.2, 134.3, 133.9, 133.5, 129.9, 128.9, 128.4, 128.4, 122.6, 52.5, 22.3.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{19}\text{H}_{16}\text{O}_4$  309.1121, found 309.1120



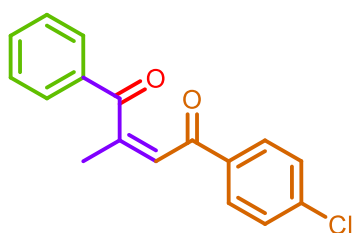
**(Z)-4-(4-fluorophenyl)-2-methyl-1-phenylbut-2-ene-1,4-dione (3ap)**

15.0 mg, 56% yield. The spectra matched with the previous report.<sup>[7]</sup>

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.99 – 7.93 (m, 4H), 7.58 (t,  $J = 7.6$  Hz, 1H), 7.48 (t,  $J = 7.4$  Hz, 2H), 7.16 – 7.12 (m, 3H), 2.28 (s, 3H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  199.3, 186.6, 165.8 (d,  $J = 255.3$  Hz), 156.7, 134.5, 133.4, 133.3 (d,  $J = 2.9$  Hz), 131.3, 131.2, 128.8, 128.8, 128.4, 122.6, 115.9, 115.7, 22.2.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{17}\text{H}_{13}\text{FO}_2$  269.0972, found 269.0990



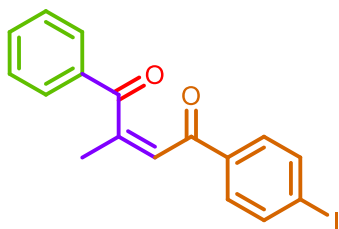
**(Z)-4-(4-chlorophenyl)-2-methyl-1-phenylbut-2-ene-1,4-dione (3aq)**

17.4 mg, 61% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.91 (d,  $J = 7.6$  Hz, 2H), 7.85 (d,  $J = 8.3$  Hz, 2H), 7.56 (t,  $J = 7.1$  Hz, 1H), 7.45 (t,  $J = 7.7$  Hz, 2H), 7.41 (d,  $J = 8.5$  Hz, 2H), 7.10 (s, 1H), 2.26 (s, 3H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  199.2, 186.9, 157.1, 139.8, 135.2, 134.4, 133.4, 130.0, 129.0, 128.8, 128.4, 122.4, 22.3.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{17}\text{H}_{13}\text{ClO}_2$  285.0677, found 285.0699



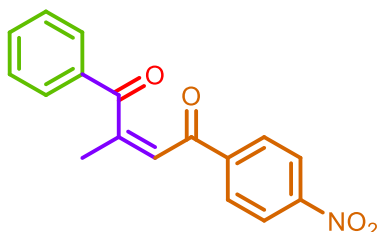
**(Z)-4-(4-iodophenyl)-2-methyl-1-phenylbut-2-ene-1,4-dione (3ar)**

23.7 mg, 63% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.90 (d,  $J = 7.7$  Hz, 2H), 7.80 (d,  $J = 7.5$  Hz, 2H), 7.61 (d,  $J = 8.2$  Hz, 2H), 7.55 (t,  $J = 7.1$  Hz, 1H), 7.45 (t,  $J = 7.5$  Hz, 2H), 7.08 (s, 1H), 2.25 (s, 3H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  199.2, 187.4, 157.2, 138.0, 136.2, 134.4, 133.4, 129.9, 128.8, 128.4, 122.3, 101.4, 22.3.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{17}\text{H}_{13}\text{IO}_2$  377.0033, found 377.0046



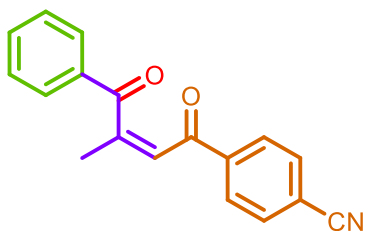
**(Z)-2-methyl-4-(4-nitrophenyl)-1-phenylbut-2-ene-1,4-dione (3as)**

14.8 mg, 50% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.29 (d,  $J = 5.4$  Hz, 2H), 8.06 (d,  $J = 7.1$  Hz, 2H), 7.91 (d,  $J = 5.7$  Hz, 2H), 7.59 (t,  $J = 5.8$  Hz, 1H), 7.47 (t,  $J = 5.3$  Hz, 2H), 7.13 (s, 1H), 2.30 (s, 3H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  198.7, 186.6, 159.0, 150.3, 141.5, 134.2, 133.7, 129.5, 128.9, 128.4, 123.9, 122.1, 22.5.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{17}\text{H}_{13}\text{NO}_4$  296.0917, found 296.0940



**(Z)-4-(3-methyl-4-oxo-4-phenylbut-2-enoyl) benzonitrile (3at)**

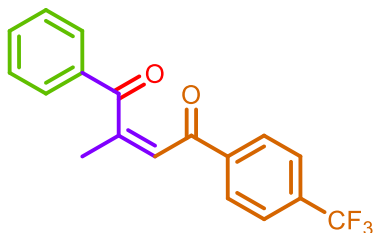
12.4 mg, 45% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.98 (d,  $J = 8.2$  Hz, 2H), 7.90 (d,  $J = 7.0$  Hz, 2H), 7.74 (d,  $J = 8.1$  Hz, 2H), 7.58 (t,  $J = 7.4$  Hz, 1H), 7.46 (t,  $J = 7.7$  Hz, 2H), 7.10 (s, 1H), 2.28 (s, 3H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  198.8, 186.8, 158.6, 140.0, 134.2, 133.6, 132.6, 132.5, 128.9, 128.4, 122.1, 117.8, 116.4, 22.4.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{18}\text{H}_{13}\text{NO}_2$  276.1019, found 276.1019





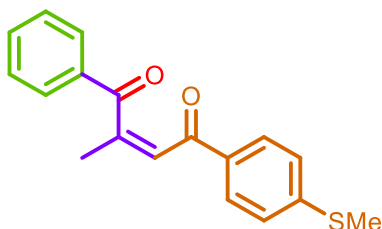
**(Z)-2-methyl-1-phenyl-4-(4-(trifluoromethyl) phenyl) but-2-ene-1,4-dione (3au)**

18.1 mg, 57% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.01 (d,  $J = 8.0$  Hz, 2H), 7.91 (d,  $J = 7.5$  Hz, 2H), 7.71 (d,  $J = 8.0$  Hz, 2H), 7.57 (t,  $J = 7.3$  Hz, 1H), 7.46 (t,  $J = 7.6$  Hz, 2H), 7.14 (s, 1H), 2.29 (s, 3H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  199.0, 187.2, 158.0, 139.6, 134.6, 134.3, 134.3, 133.6, 128.9 (d,  $J = 5.8$  Hz), 128.4, 125.7 (q,  $J = 3.7$  Hz), 123.5 (d,  $J = 272.8$  Hz), 122.3, 22.4.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{18}\text{H}_{13}\text{F}_3\text{O}_2$  319.0940, found 319.0961



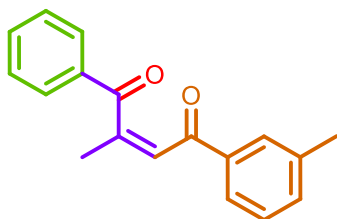
**(Z)-2-methyl-4-(4-(methylthio) phenyl)-1-phenylbut-2-ene-1,4-dione (3av)**

18.9 mg, 64% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.07 (d,  $J = 8.2$  Hz, 2H), 8.02 (d,  $J = 8.2$  Hz, 2H), 7.90 (d,  $J = 7.1$  Hz, 2H), 7.58 (t,  $J = 7.2$  Hz, 1H), 7.47 (t,  $J = 7.5$  Hz, 2H), 7.13 (s, 1H), 3.06 (s, 3H), 2.29 (s, 3H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  198.8, 186.9, 158.6, 144.2, 141.0, 134.2, 133.6, 129.3, 128.9, 128.4, 127.8, 122.2, 44.3, 22.4.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{18}\text{H}_{16}\text{O}_2\text{S}$  297.0944, found 297.0945



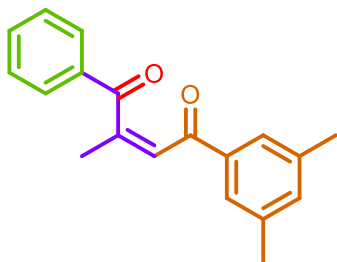
**(Z)-2-methyl-1-phenyl-4-(m-tolyl) but-2-ene-1,4-dione (3aw)**

18.2 mg, 69% yield. The spectra matched with the previous report.<sup>[7]</sup>

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.92 (d,  $J = 7.7$  Hz, 2H), 7.72 (d,  $J = 2.2$  Hz, 2H), 7.54 (t,  $J = 7.3$  Hz, 1H), 7.44 (t,  $J = 7.7$  Hz, 2H), 7.37 – 7.33 (m, 2H), 7.15 (s, 1H), 2.37 (s, 3H), 2.25 (s, 3H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  199.4, 188.3, 156.1, 138.5, 136.9, 134.6, 134.0, 133.3, 129.2, 128.8, 128.5, 128.4, 125.8, 123.1, 22.2, 21.3.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{18}\text{H}_{16}\text{O}_2$  265.1223, found 265.1227



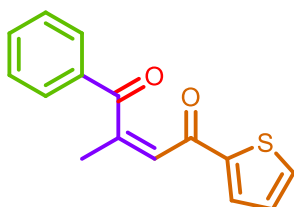
**(Z)-4-(3,5-dimethylphenyl)-2-methyl-1-phenylbut-2-ene-1,4-dione (3ax)**

15.6 mg, 56% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.92 – 7.90 (m, 2H), 7.53 (d,  $J = 7.1$  Hz, 3H), 7.44 (t,  $J = 7.7$  Hz, 2H), 7.18 (s, 1H), 7.14 (d,  $J = 1.7$  Hz, 1H), 2.34 (s, 6H), 2.25 (s, 3H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  199.4, 188.4, 155.8, 138.3, 137.0, 134.9, 134.6, 133.2, 128.7, 128.4, 126.4, 123.2, 22.1, 21.2.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{19}\text{H}_{18}\text{O}_2$  279.1380, found 279.1378



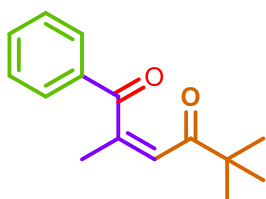
**(Z)-2-methyl-1-phenyl-4-(thiophen-2-yl) but-2-ene-1,4-dione (3ay)**

13.6 mg, 53% yield. The spectra matched with the previous report.<sup>[7]</sup>

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.87 (d,  $J = 7.6$  Hz, 2H), 7.68 (d,  $J = 4.8$  Hz, 1H), 7.63 – 7.62 (m, 2H), 7.51 (t,  $J = 7.7$  Hz, 2H), 7.13 – 7.11 (m, 1H), 7.04 (d,  $J = 1.7$  Hz, 1H), 2.44 (s, 3H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{DCI}_3$ )  $\delta$  198.1, 183.5, 150.6, 145.6, 136.0, 134.7, 133.3, 132.3, 129.8, 128.7, 128.6, 128.4, 16.1.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{15}\text{H}_{12}\text{O}_2\text{S}$  257.0631, found 257.0631



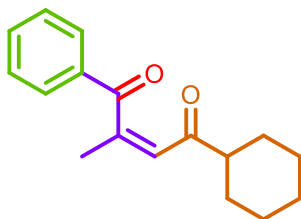
**(Z)-2,5,5-trimethyl-1-phenylhex-2-ene-1,4-dione (3az)**

15.9 mg, 69% yield.

$^1\text{H NMR}$  (500 MHz,  $\text{CDCl}_3$ )  $\delta$  7.85 (d,  $J = 7.6$  Hz, 2H), 7.54 (t,  $J = 7.0$  Hz, 1H), 7.44 (t,  $J = 7.5$  Hz, 2H), 6.64 (s, 1H), 2.13 (s, 3H), 1.12 (s, 9H).

$^{13}\text{C NMR}$  (125 MHz,  $\text{CDCl}_3$ )  $\delta$  202.9, 199.6, 154.9, 134.4, 133.2, 128.7, 128.3, 122.5, 42.8, 26.0, 21.8.

HRMS (ESI-TOF,  $[\text{M} + \text{H}^+]$ ): calcd for  $\text{C}_{15}\text{H}_{18}\text{O}_2$  231.1380, found 231.1380



**(Z)-4-cyclohexyl-2-methyl-1-phenylbut-2-ene-1,4-dione (3ba)**

11.2 mg, 46% yield.

**<sup>1</sup>H NMR** (500 MHz, CDCl<sub>3</sub>) δ 7.88 (d, *J* = 7.7 Hz, 2H), 7.57 (t, *J* = 7.2 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 2H), 6.48 (s, 1H), 2.42 – 2.26 (m, 1H), 2.14 (s, 3H), 1.85 – 1.82 (m, 2H), 1.79 – 1.77 (m, 2H), 1.67 (d, *J* = 12.2 Hz, 1H), 1.29 – 1.25 (m, 4H), 1.20 – 1.15 (m, 1H).

**<sup>13</sup>C NMR** (125 MHz, CDCl<sub>3</sub>) δ 201.1, 199.6, 154.2, 134.4, 133.3, 128.7, 128.3, 125.3, 50.1, 27.9, 25.7, 25.5, 21.7.

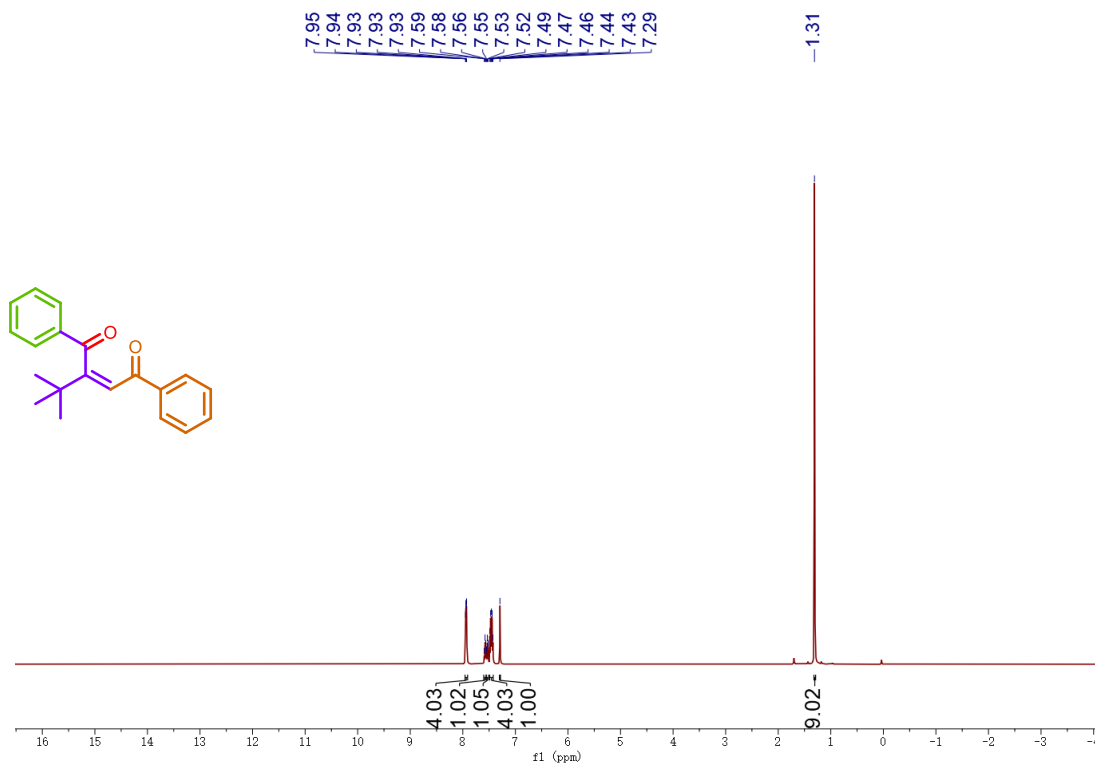
HRMS (ESI-TOF, [M + H<sup>+</sup>]): calcd for C<sub>17</sub>H<sub>20</sub>O<sub>2</sub> 257.1536, found 257.1537

## 12. References

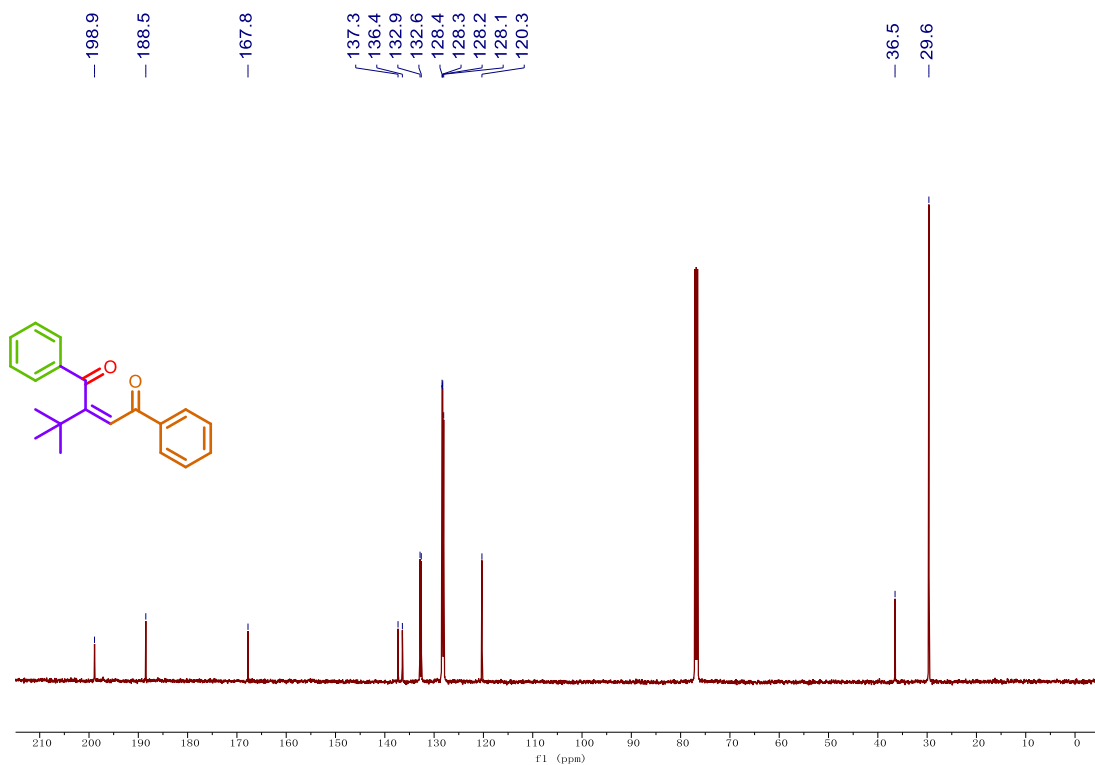
- [1] M.-Q. Ping, M.-Z. Guo, R.-T. Li, Z.-C. Wang, C. Ma, L.-R. Wen, S.-F. Ni, W.-S. Guo, M. Li and L.-B. Zhang, *Org. Lett.*, 2022, **24**, 7410-7415.
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- [4] Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2016**.
- [5] A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B.*, 2009, **113**, 6378-6396.
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- [7] Y. He, Z. Zheng, Q. Liu, G. Song, N. Sun and X.-Y. Chai, *J. Org. Chem.*, 2018, **83**, 12514-12526.

## 13. NMR Spectra

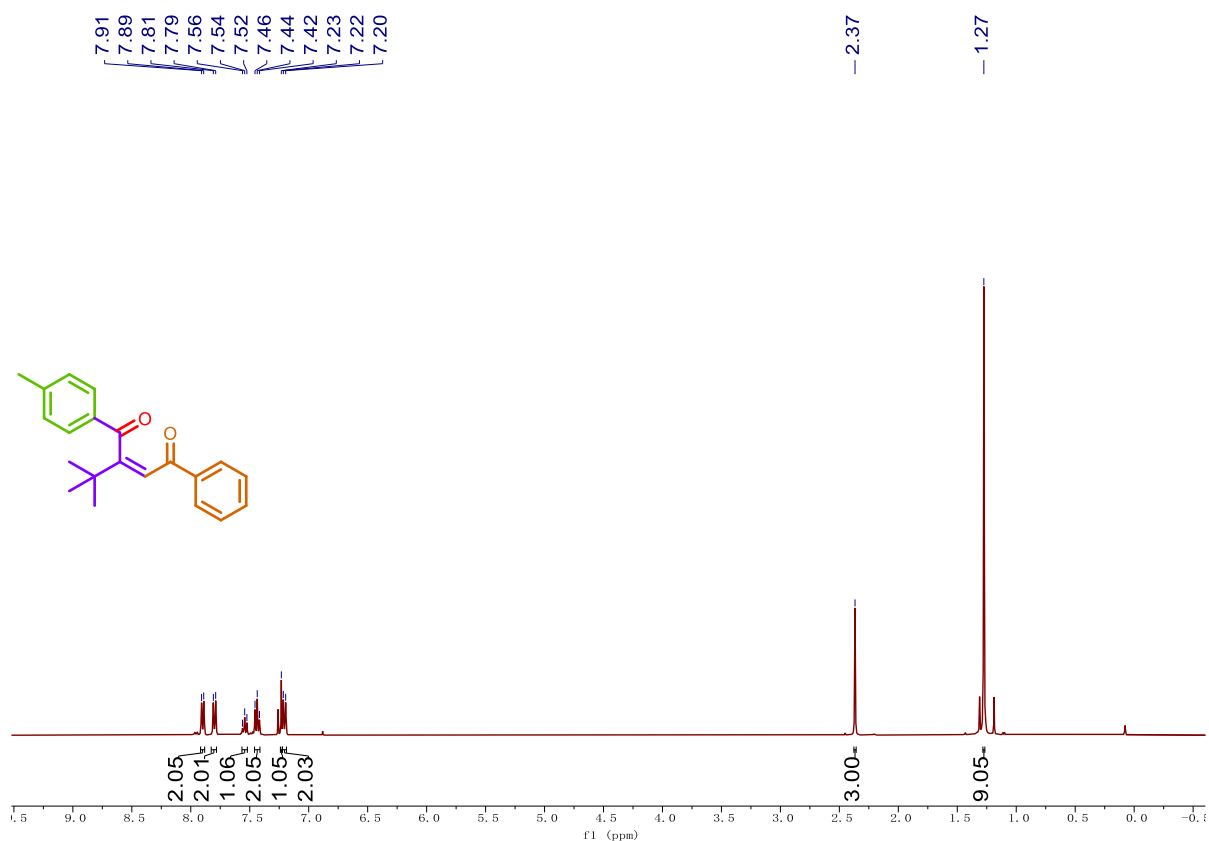
Compound 3a:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )



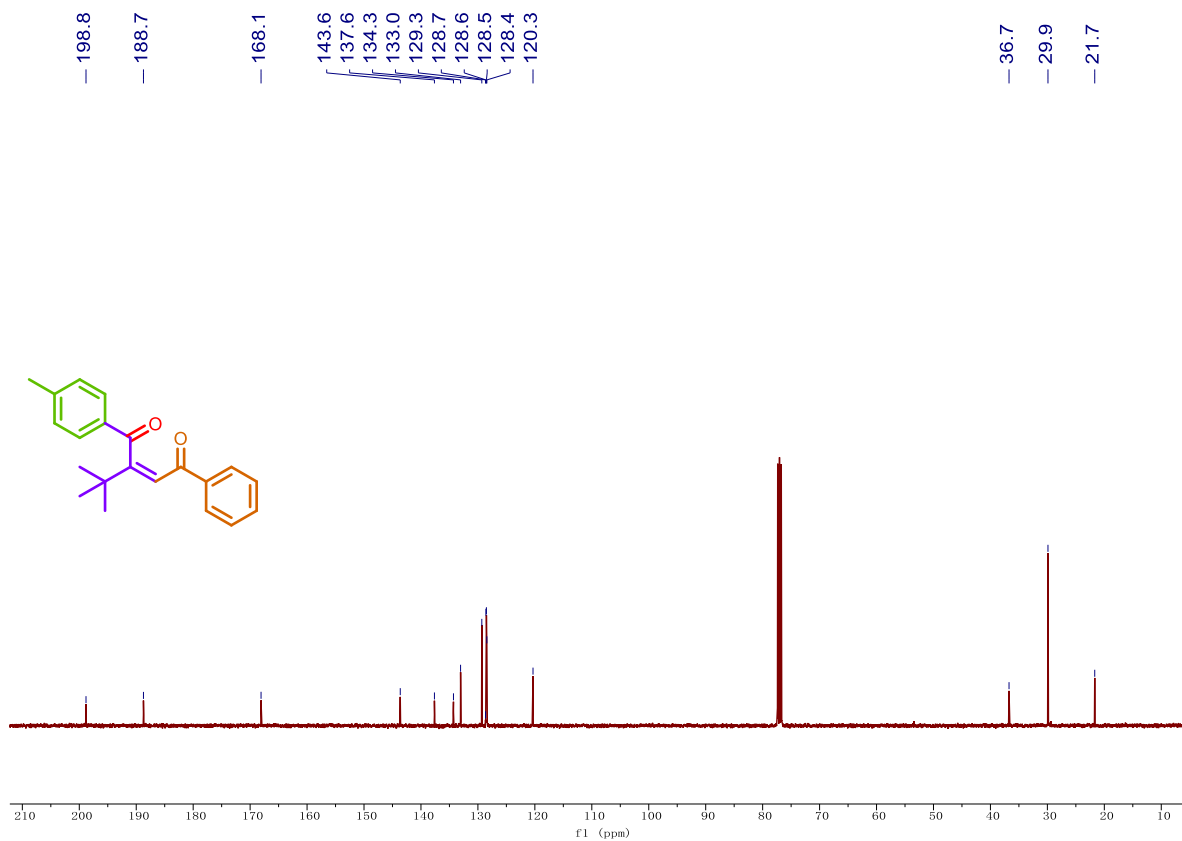
Compound 3a:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )



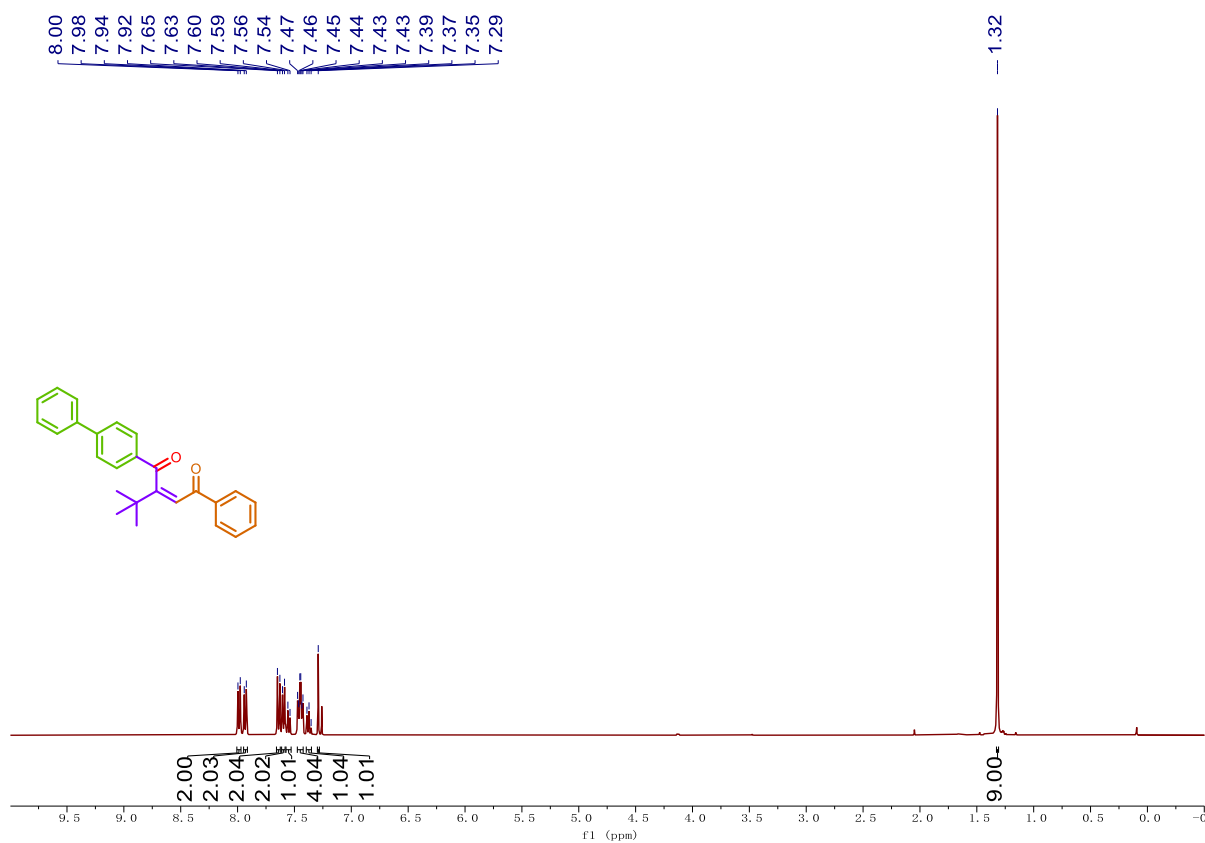
**Compound 3b: <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)**



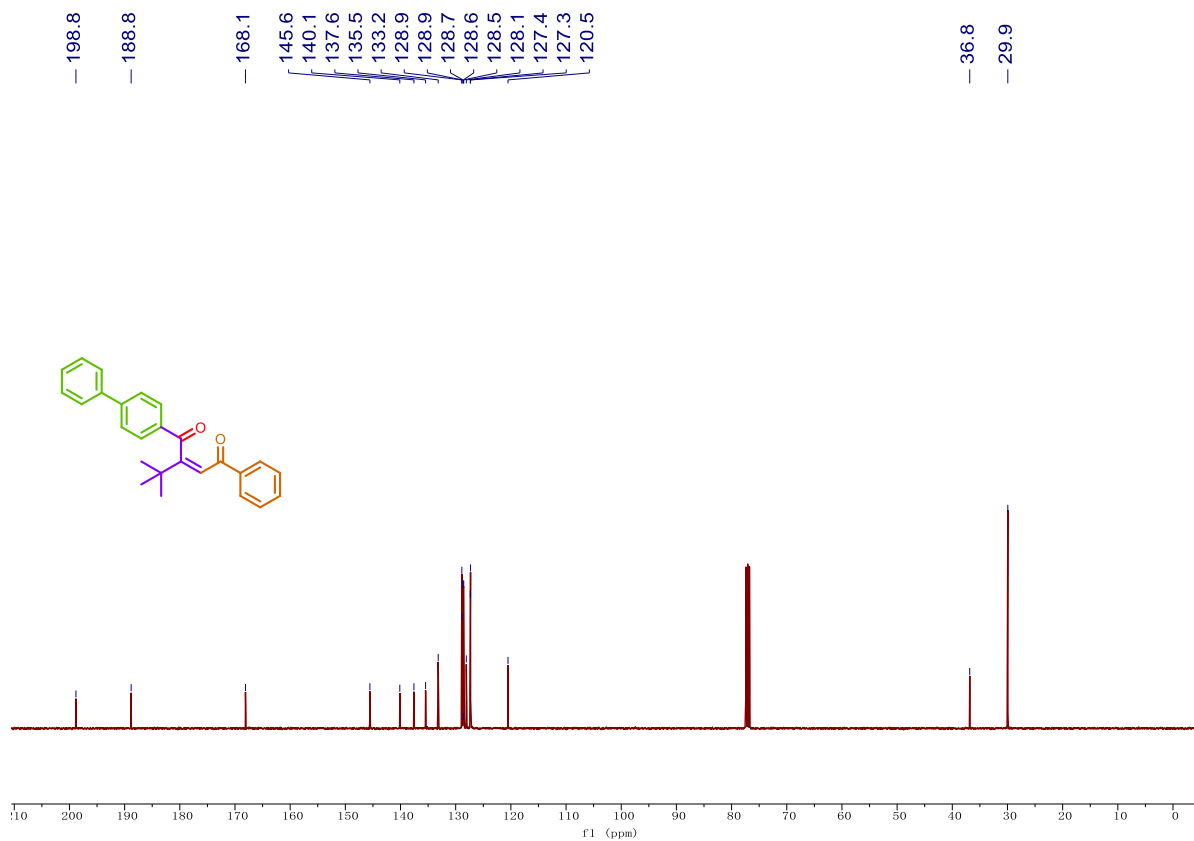
**Compound 3b: <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)**



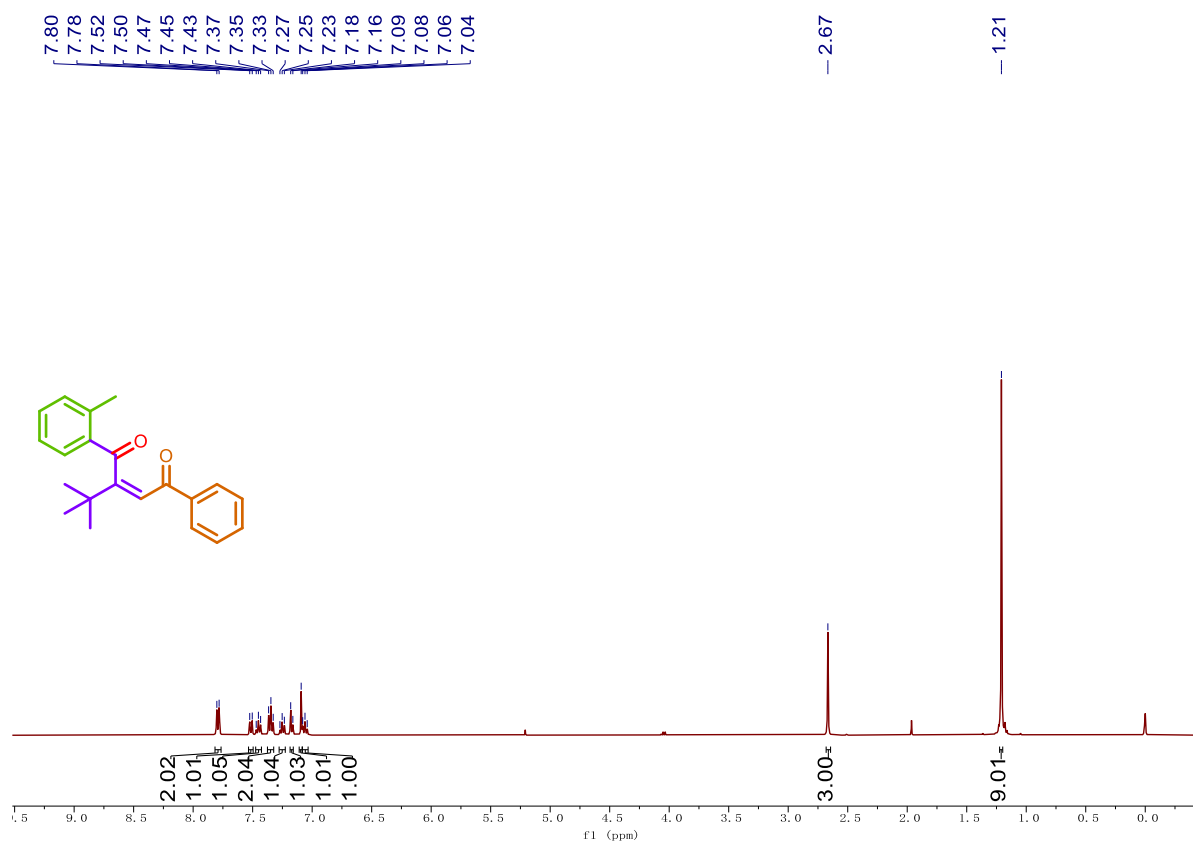
**Compound 3c:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )**



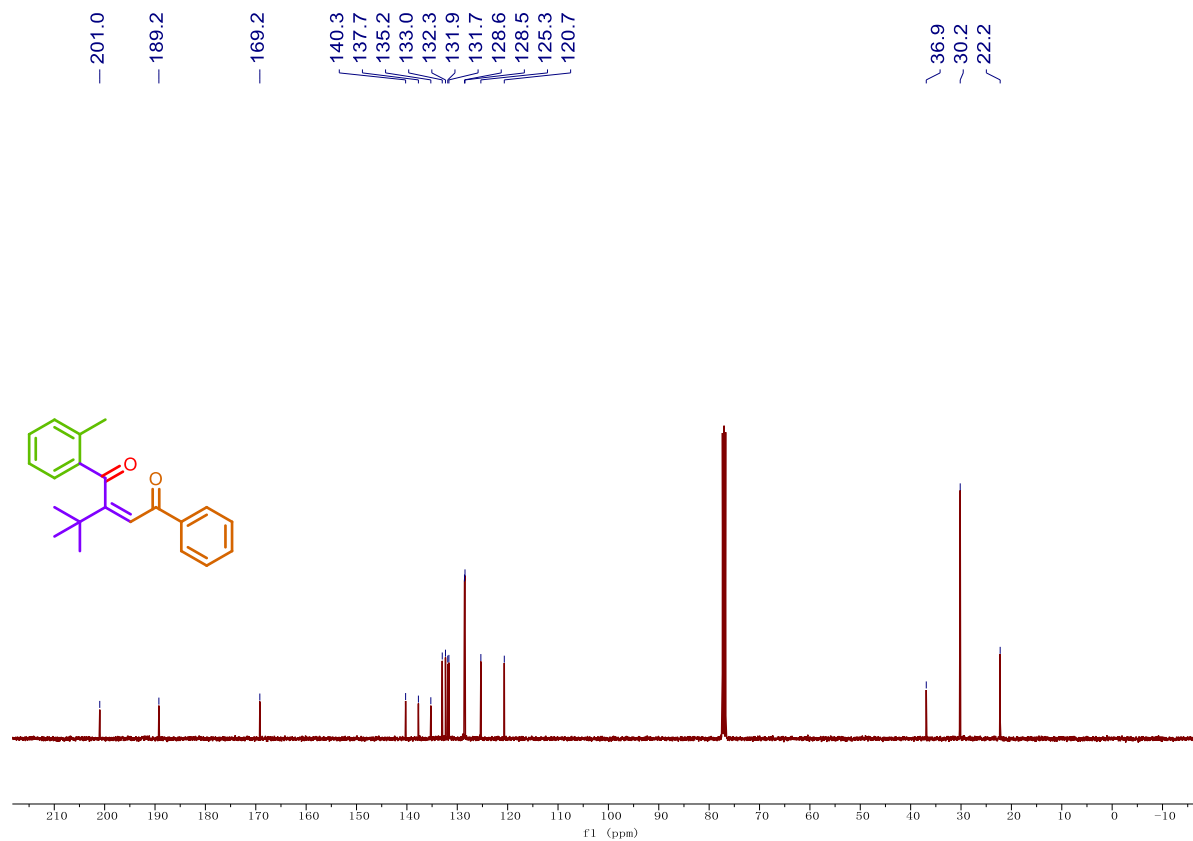
**Compound 3c:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )**



**Compound 3d:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )**

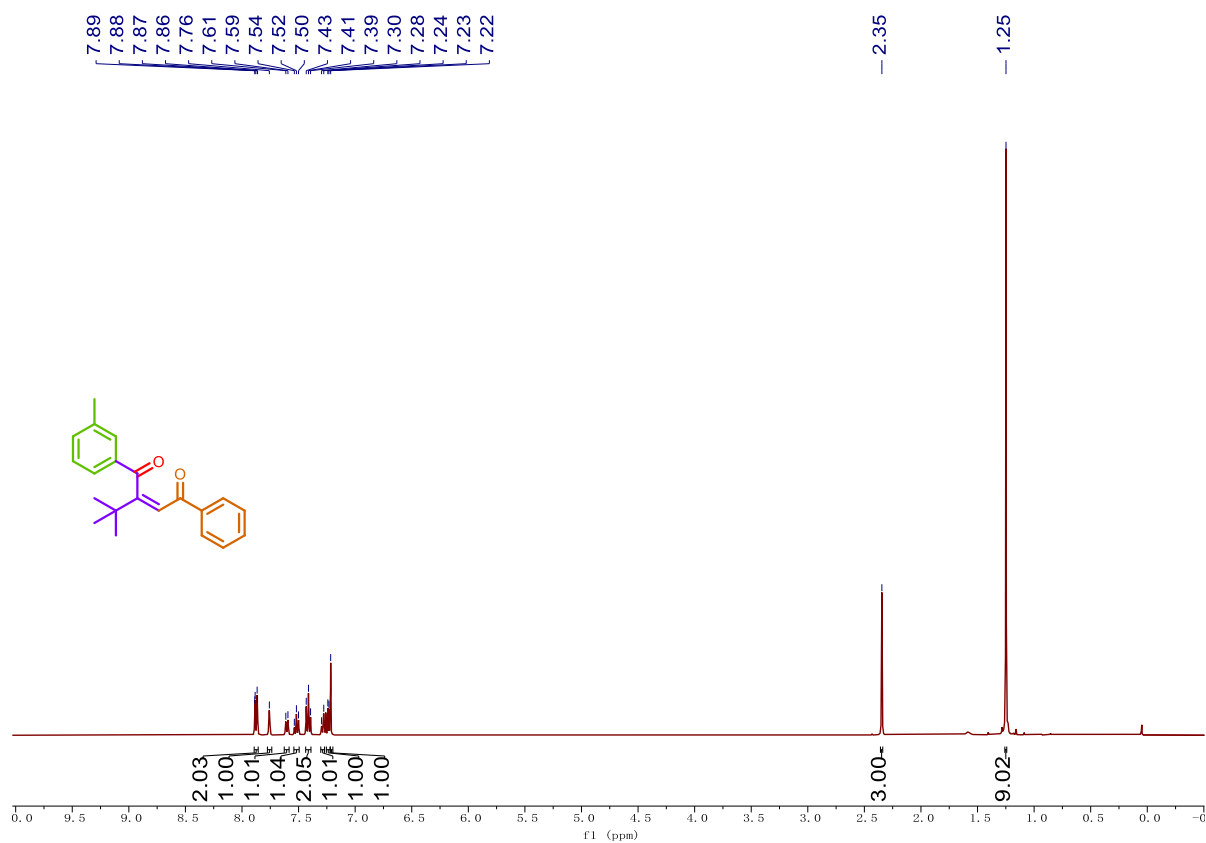


**Compound 3d:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )**

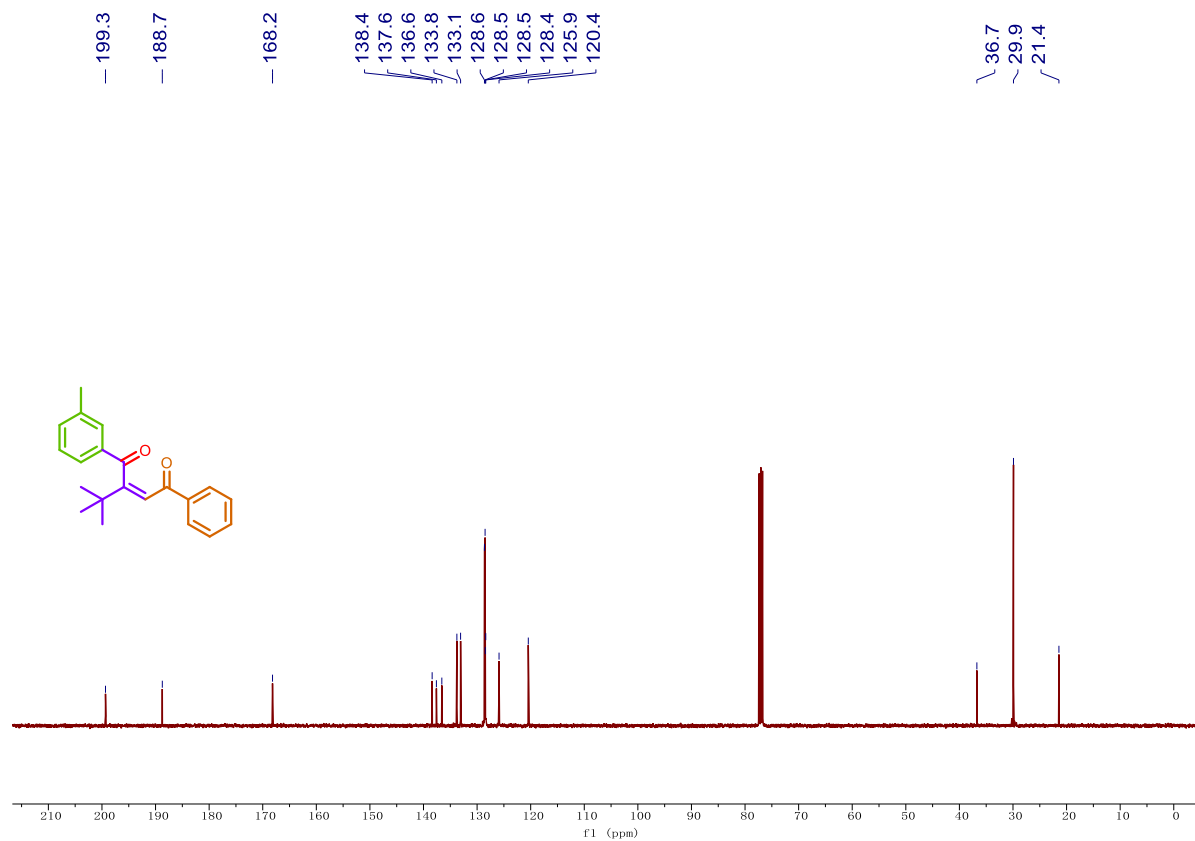




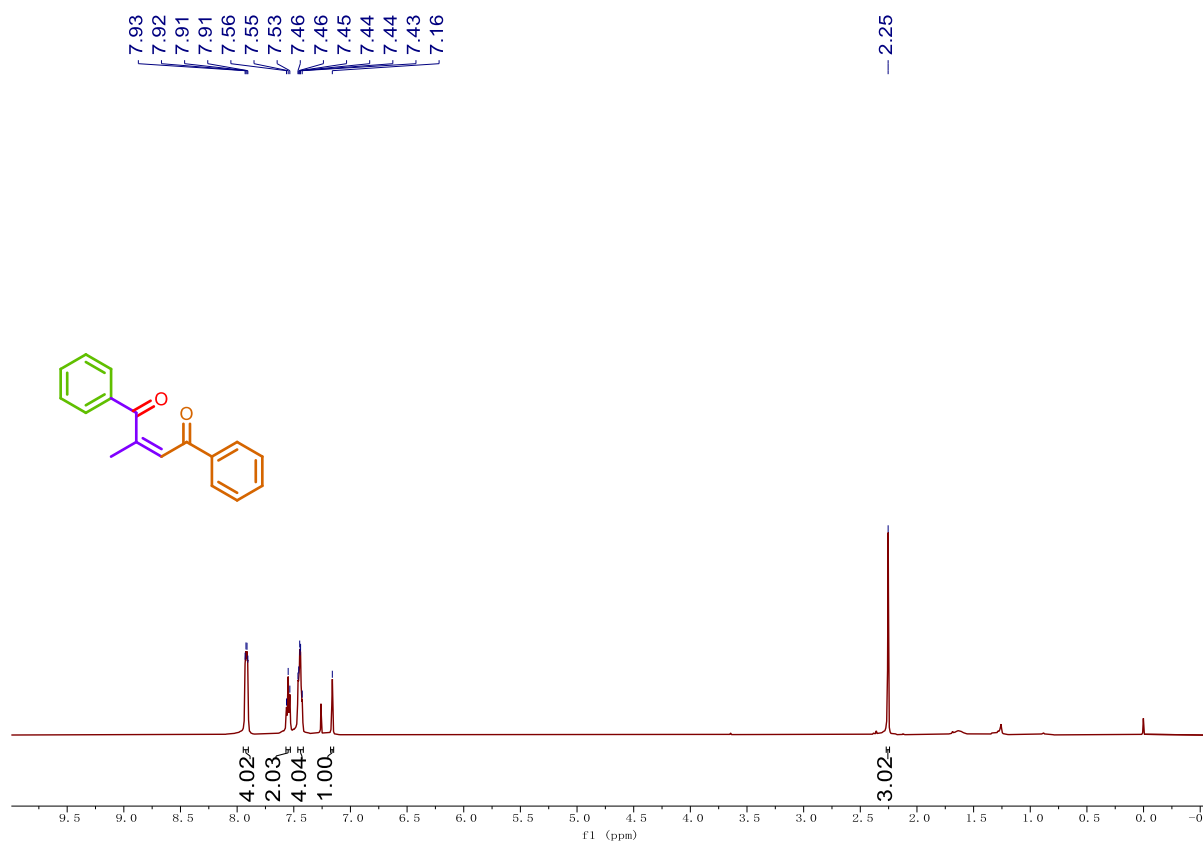
**Compound 3e:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )**



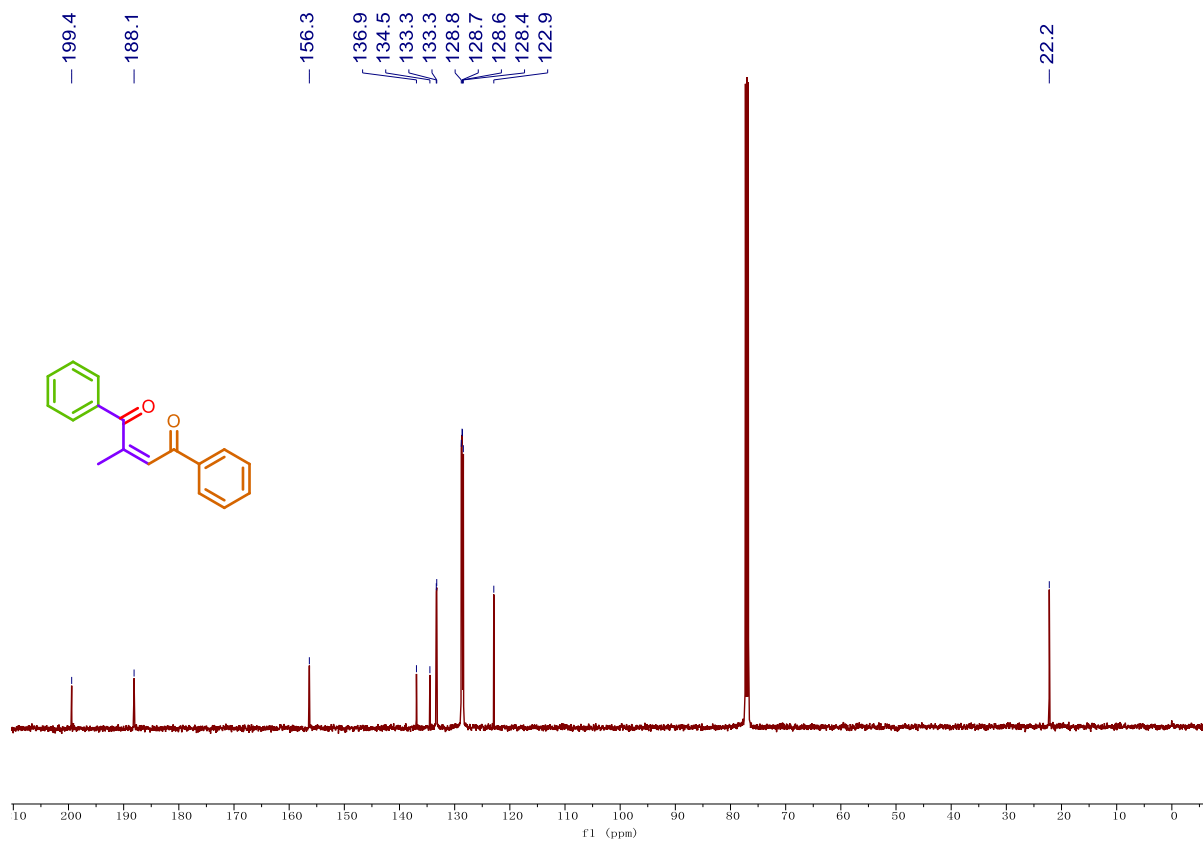
**Compound 3e:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )**



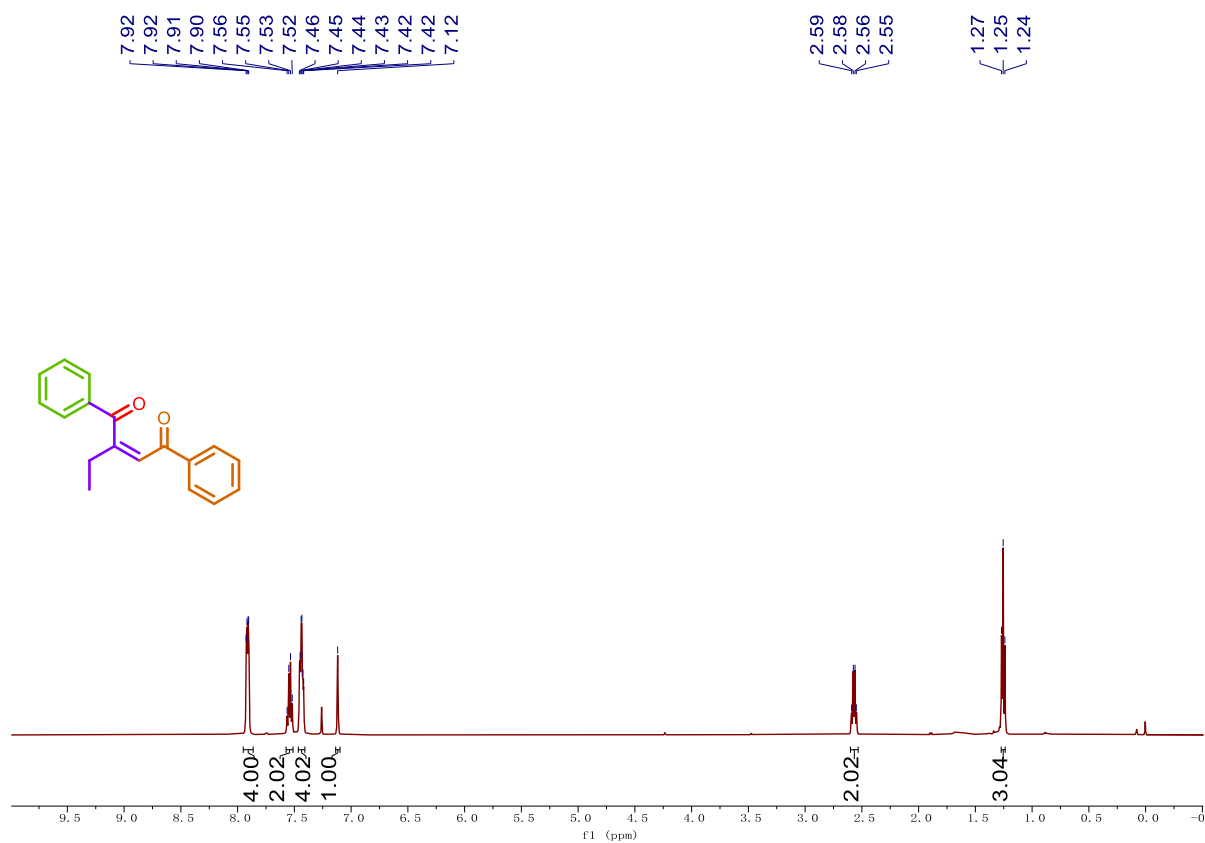
Compound 3f:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )



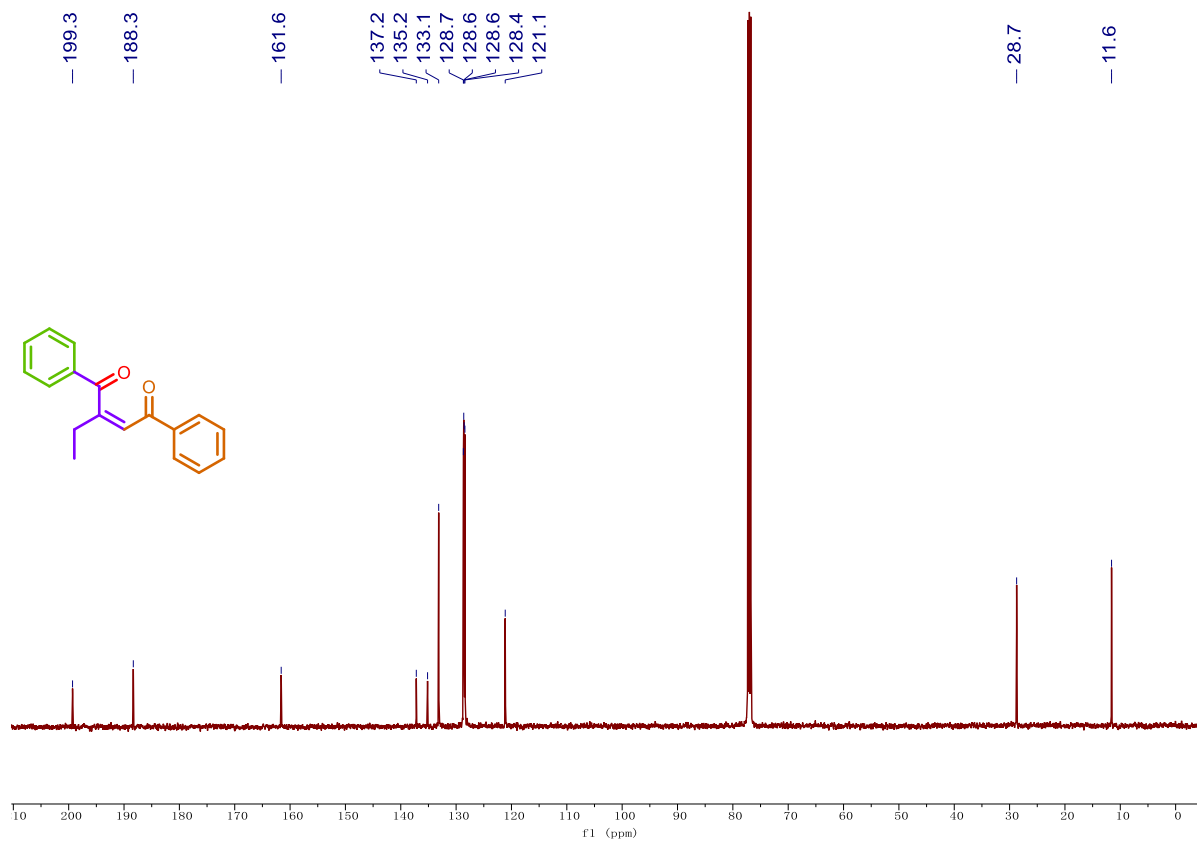
Compound 3f:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )



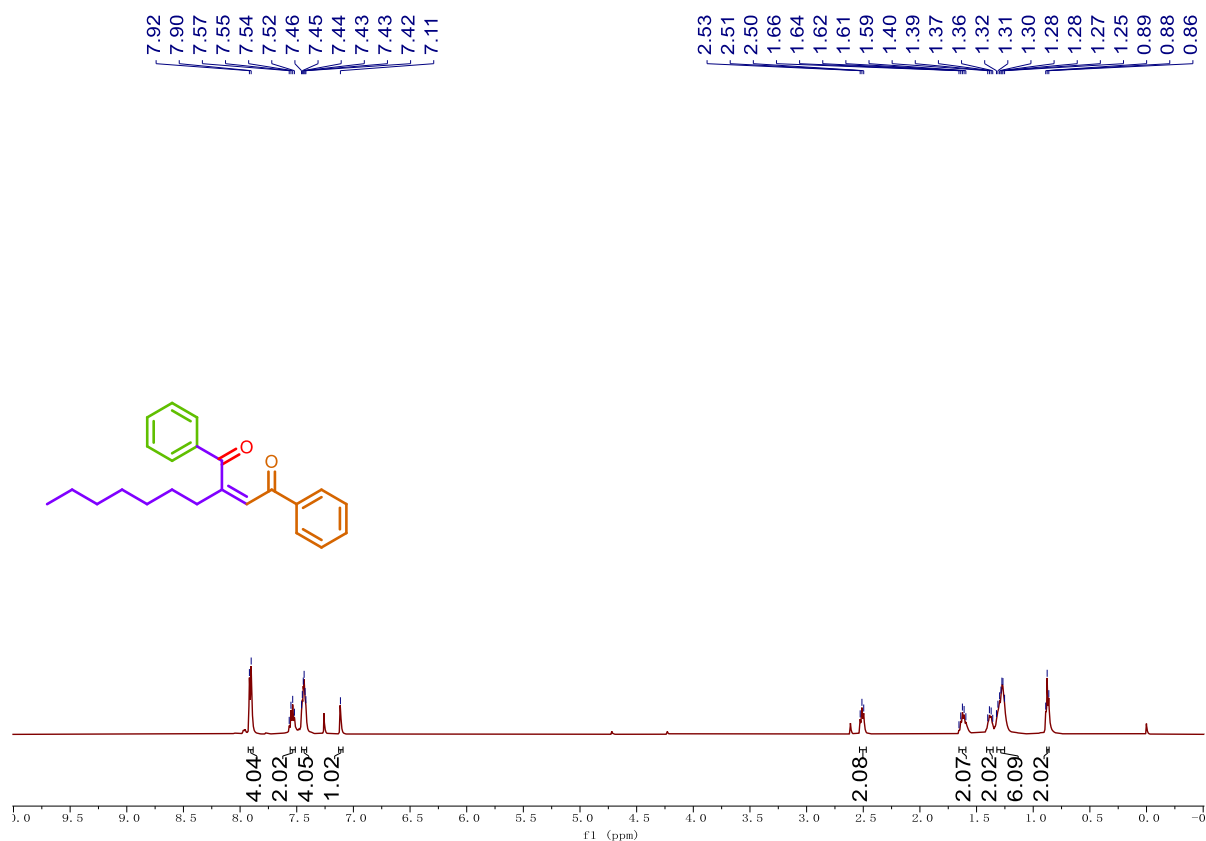
Compound 3g:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )



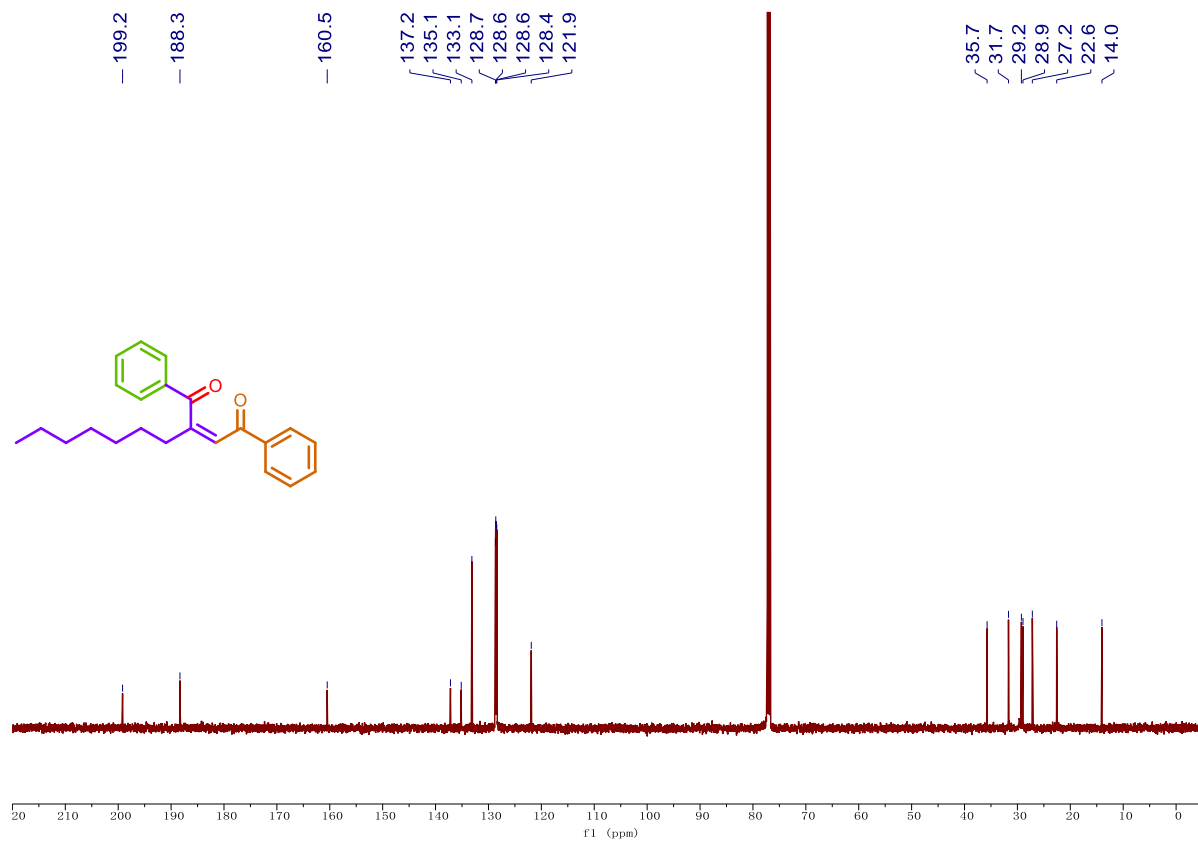
Compound 3g:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )



**Compound 3h:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )**



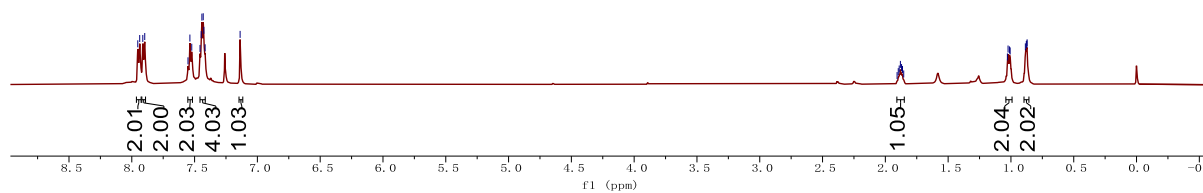
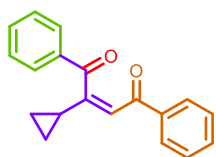
**Compound 3h:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )**



**Compound 3i:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )**

7.95  
7.94  
7.91  
7.90  
7.55  
7.54  
7.52  
7.46  
7.45  
7.44  
7.43  
7.43  
7.42  
7.14

1.91  
1.90  
1.89  
1.88  
1.87  
1.86  
1.85  
1.03  
1.02  
1.01  
1.01  
0.89  
0.88  
0.87  
0.87



**Compound 3i:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )**

197.3

187.5

162.9

137.3

135.7

133.2

133.0

128.7

128.6

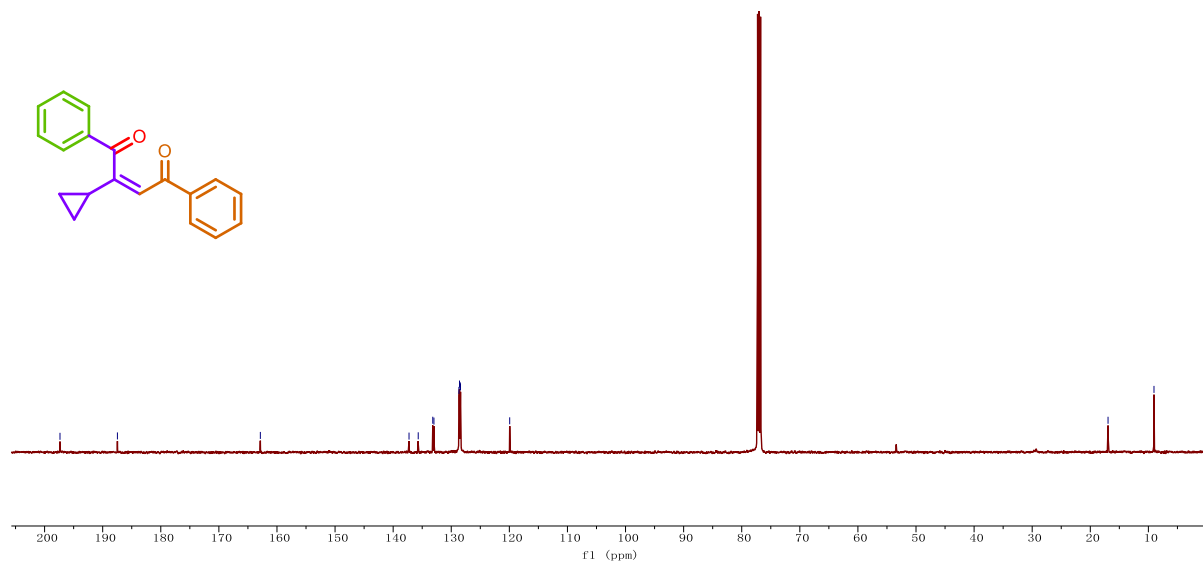
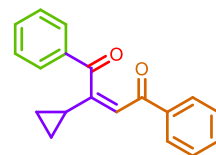
128.5

128.4

119.9

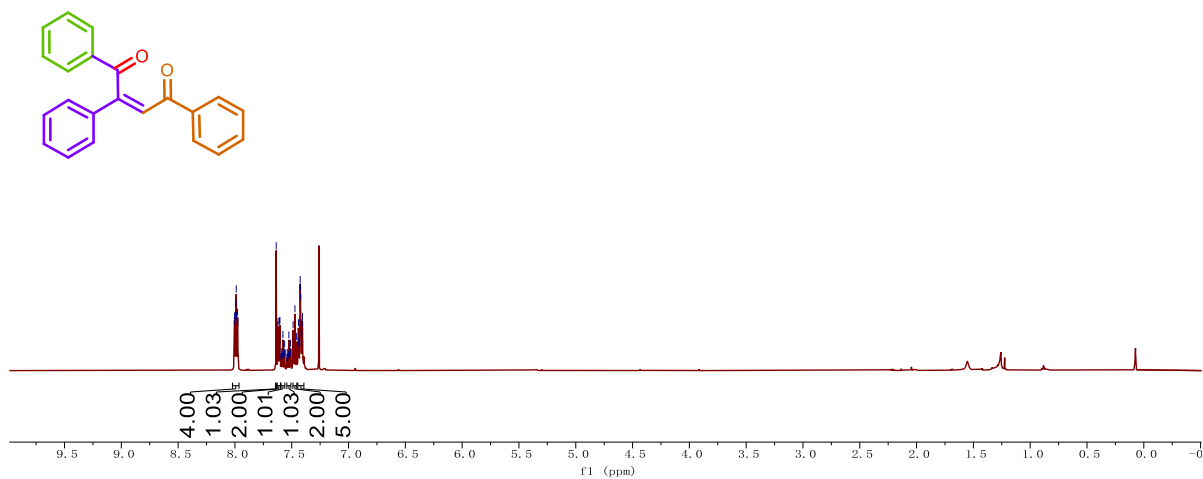
16.9

9.0



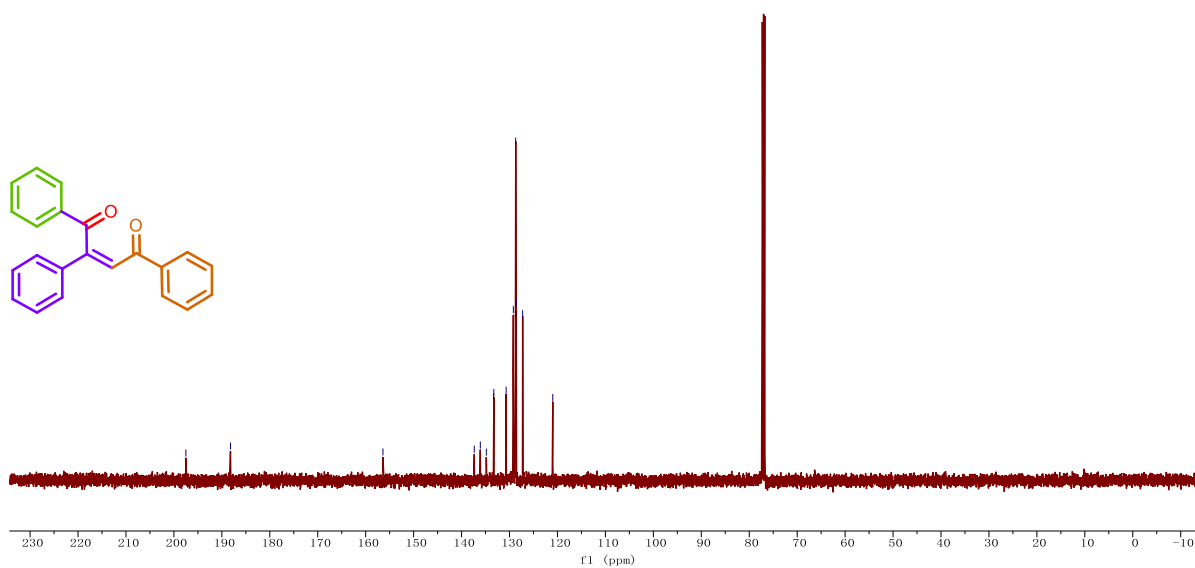
**Compound 3j:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )**

8.01  
8.00  
7.99  
7.99  
7.99  
7.99  
7.98  
7.97  
7.64  
7.62  
7.62  
7.61  
7.60  
7.59  
7.59  
7.58  
7.58  
7.57  
7.56  
7.56  
7.54  
7.54  
7.54  
7.53  
7.53  
7.52  
7.51  
7.51  
7.51  
7.49  
7.47  
7.46  
7.44  
7.44  
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7.42  
7.42  
7.41  
7.41  
7.41  
7.41

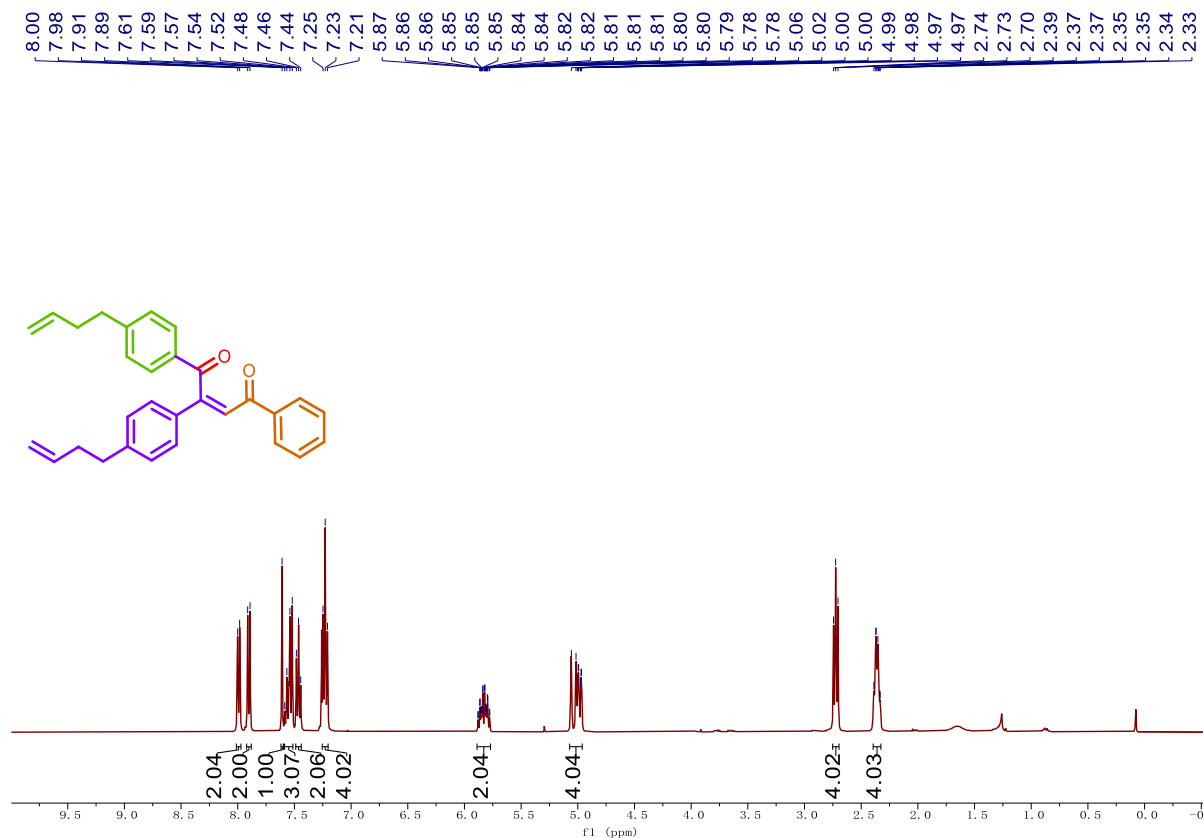


**Compound 3j:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )**

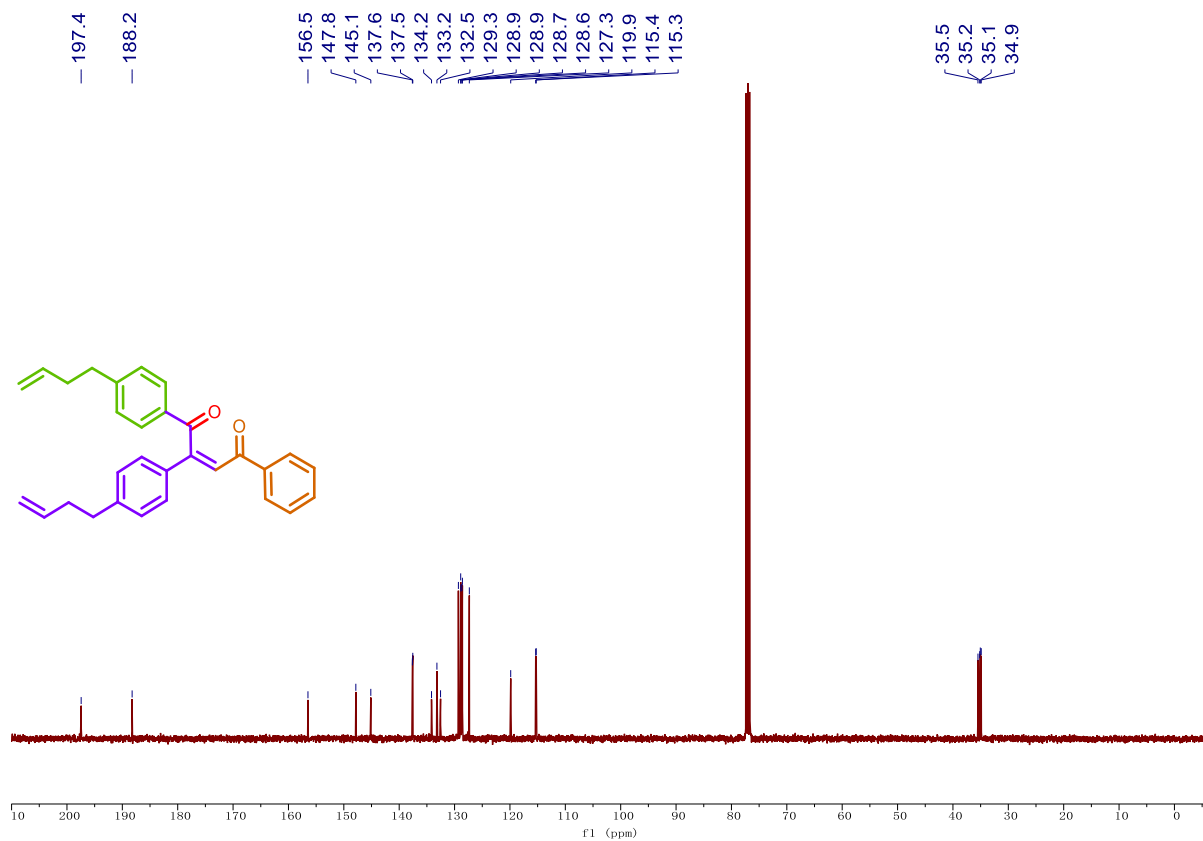
197.5  
188.2  
156.4  
137.3  
136.1  
134.8  
133.3  
133.3  
133.3  
130.7  
129.2  
128.8  
128.7  
128.6  
127.3  
121.0



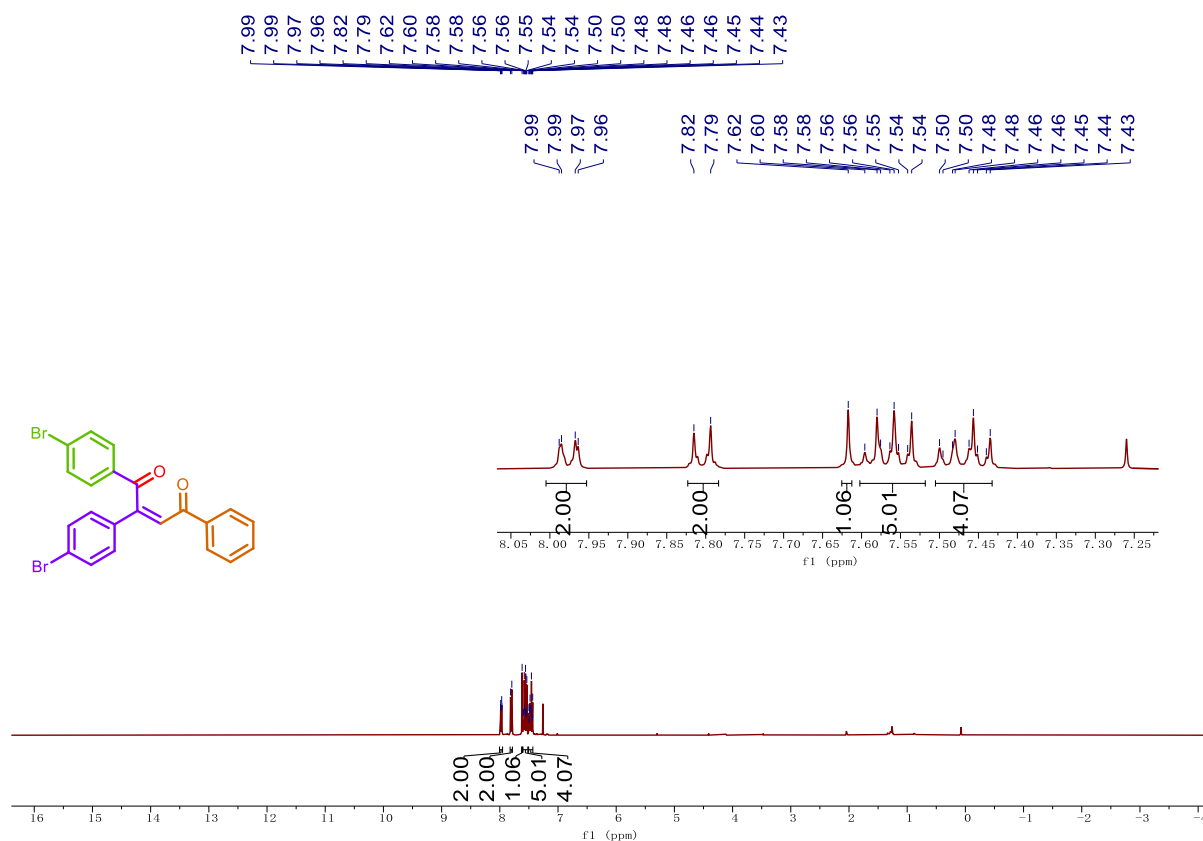
**Compound 3k: <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)**



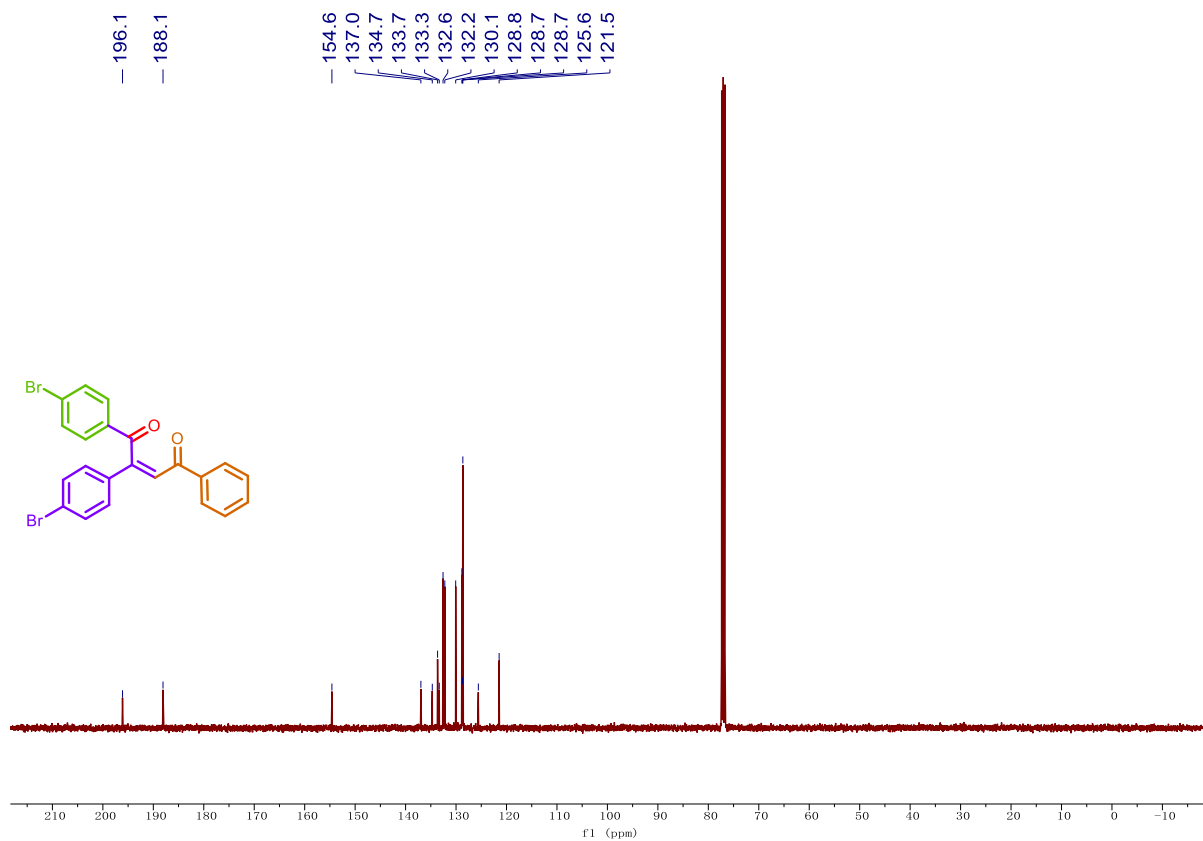
**Compound 3k: <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)**



**Compound 3l:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )**

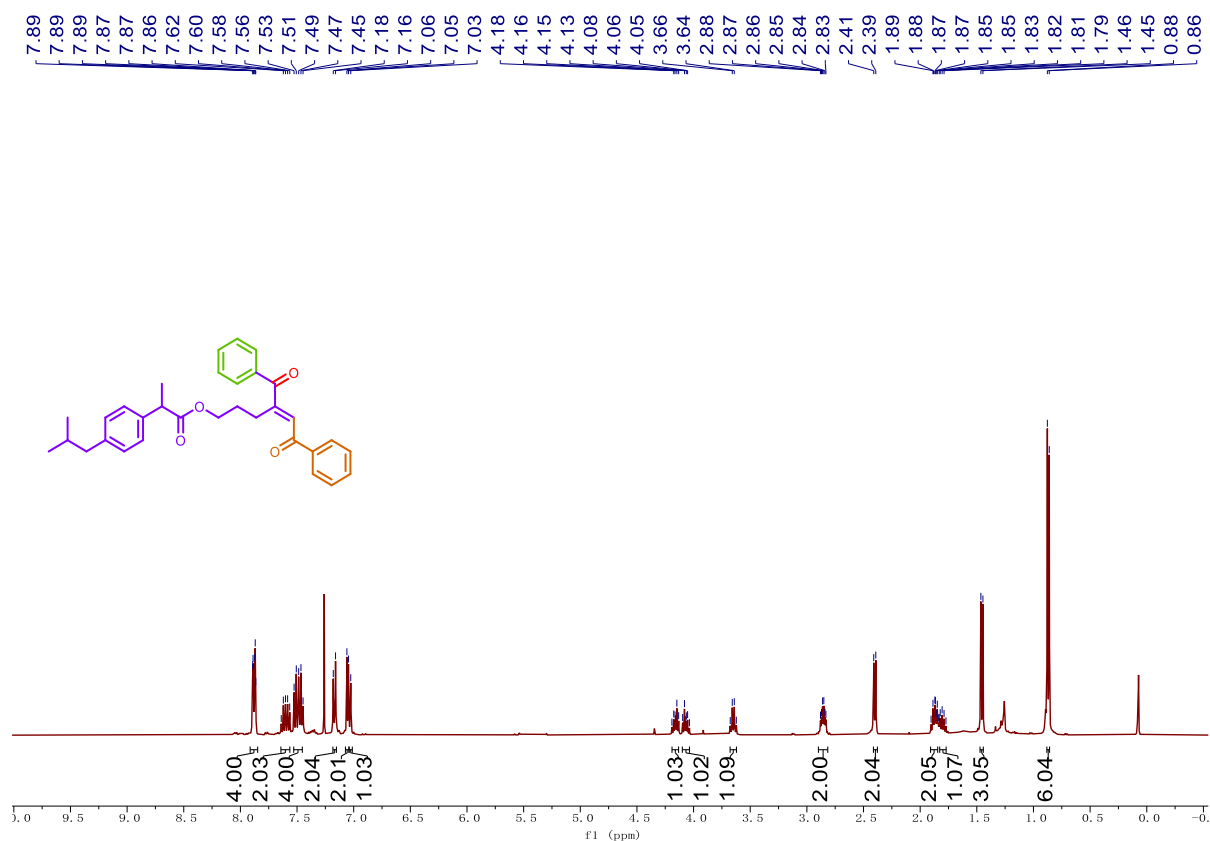


**Compound 3l:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )**

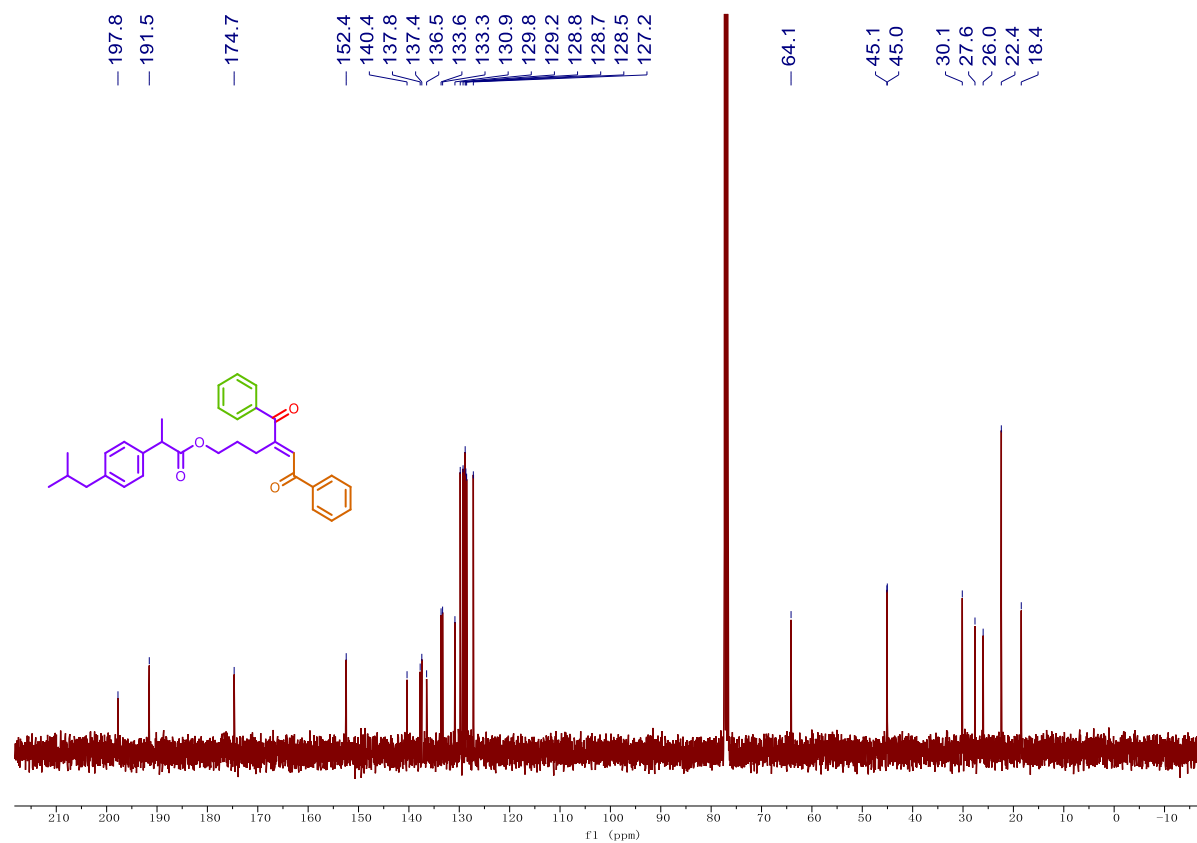




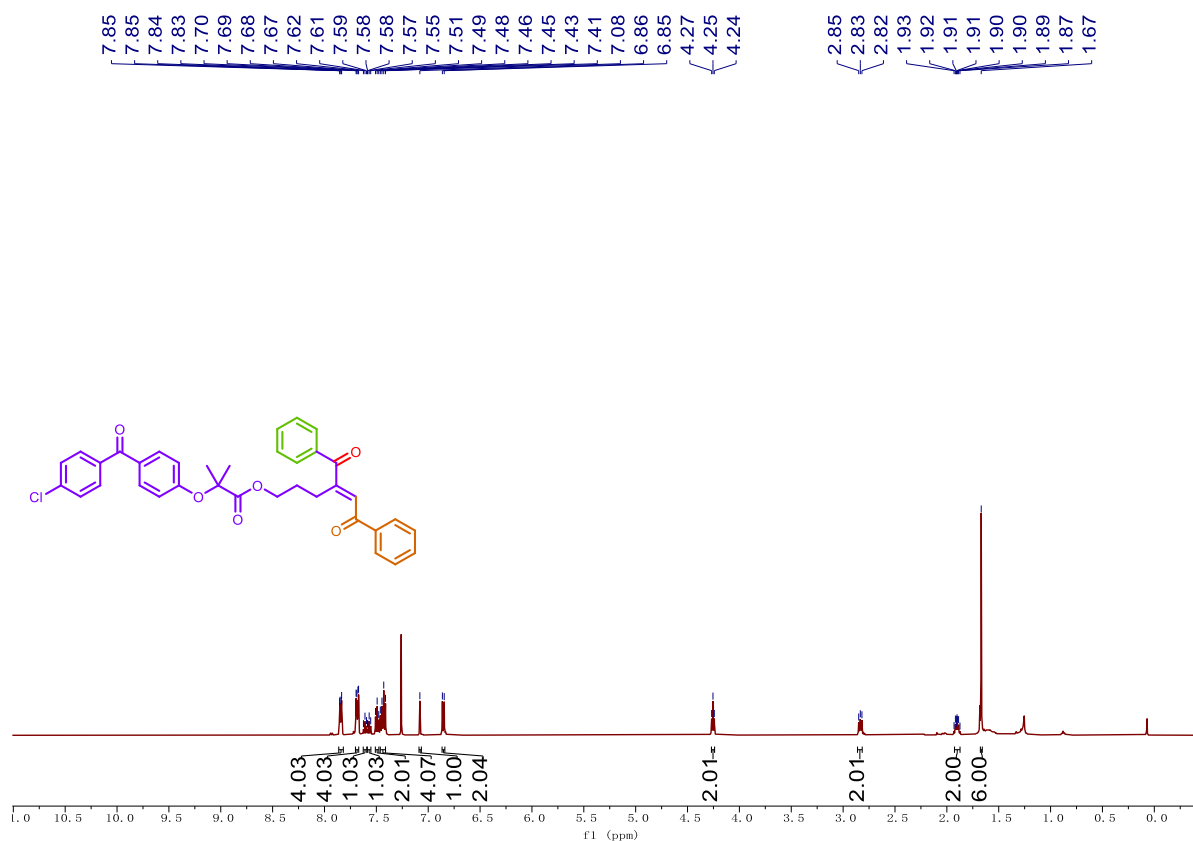
**Compound 3m:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )**



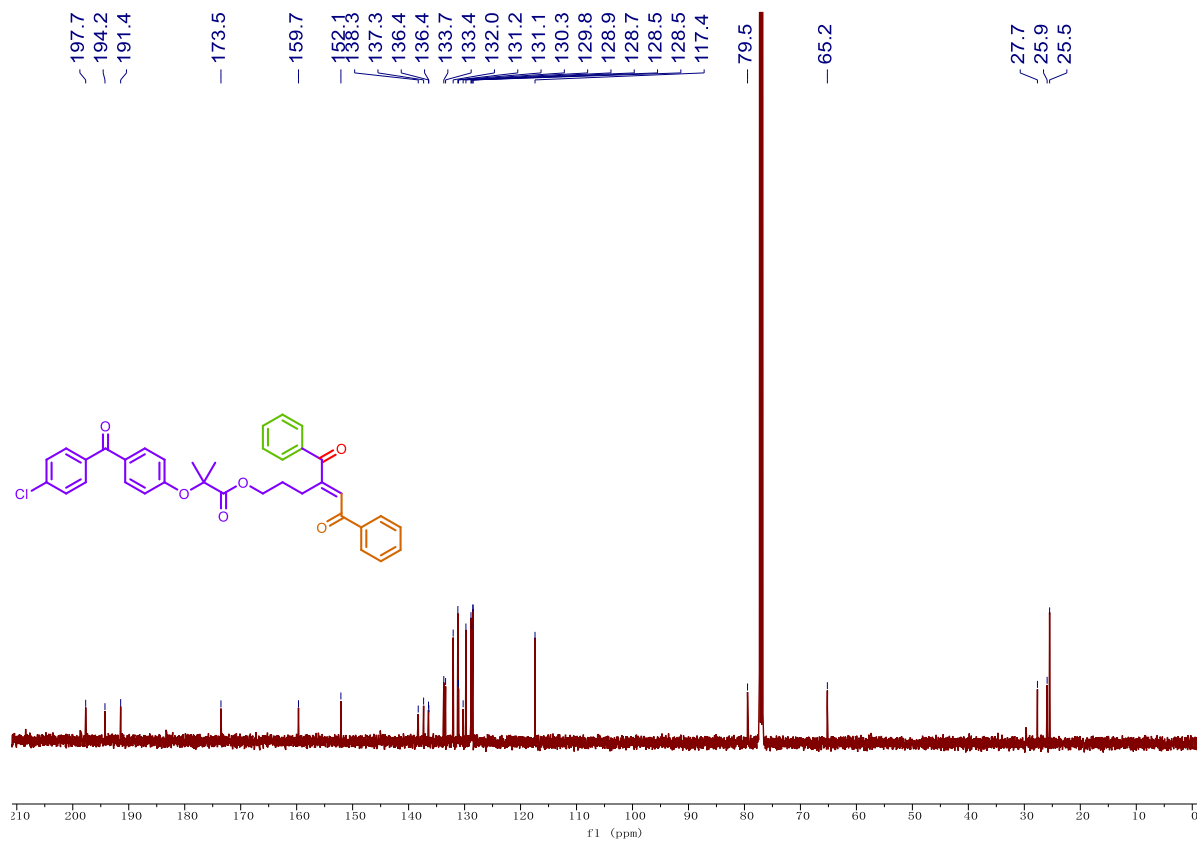
**Compound 3m:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )**



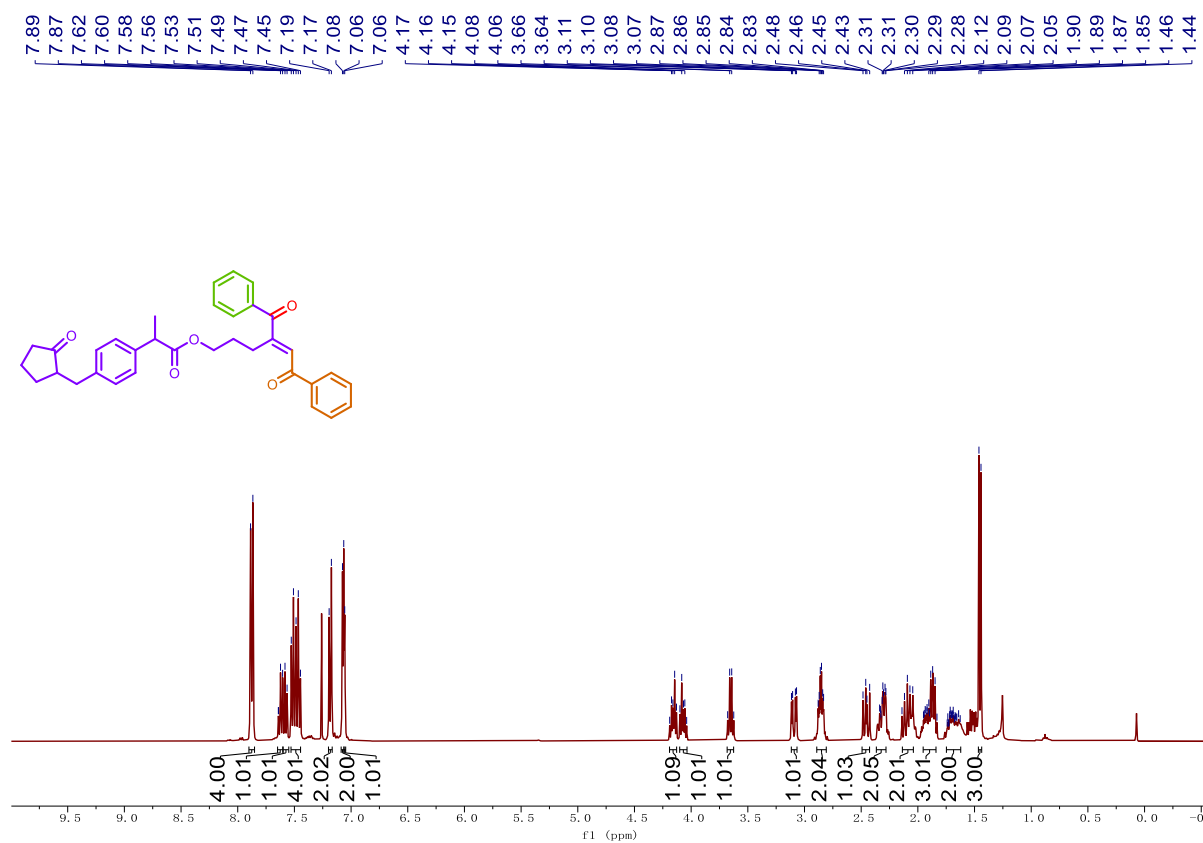
**Compound 3n: <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)**



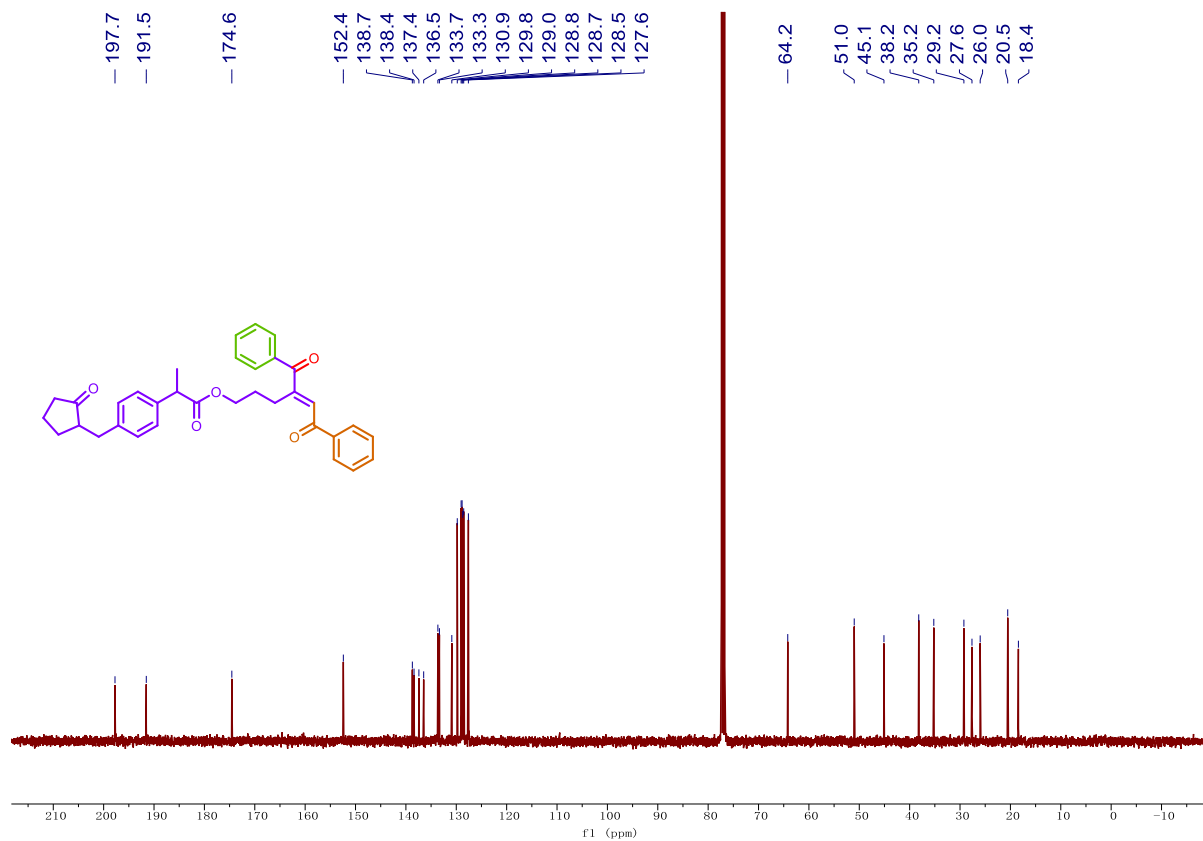
**Compound 3n: <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>)**



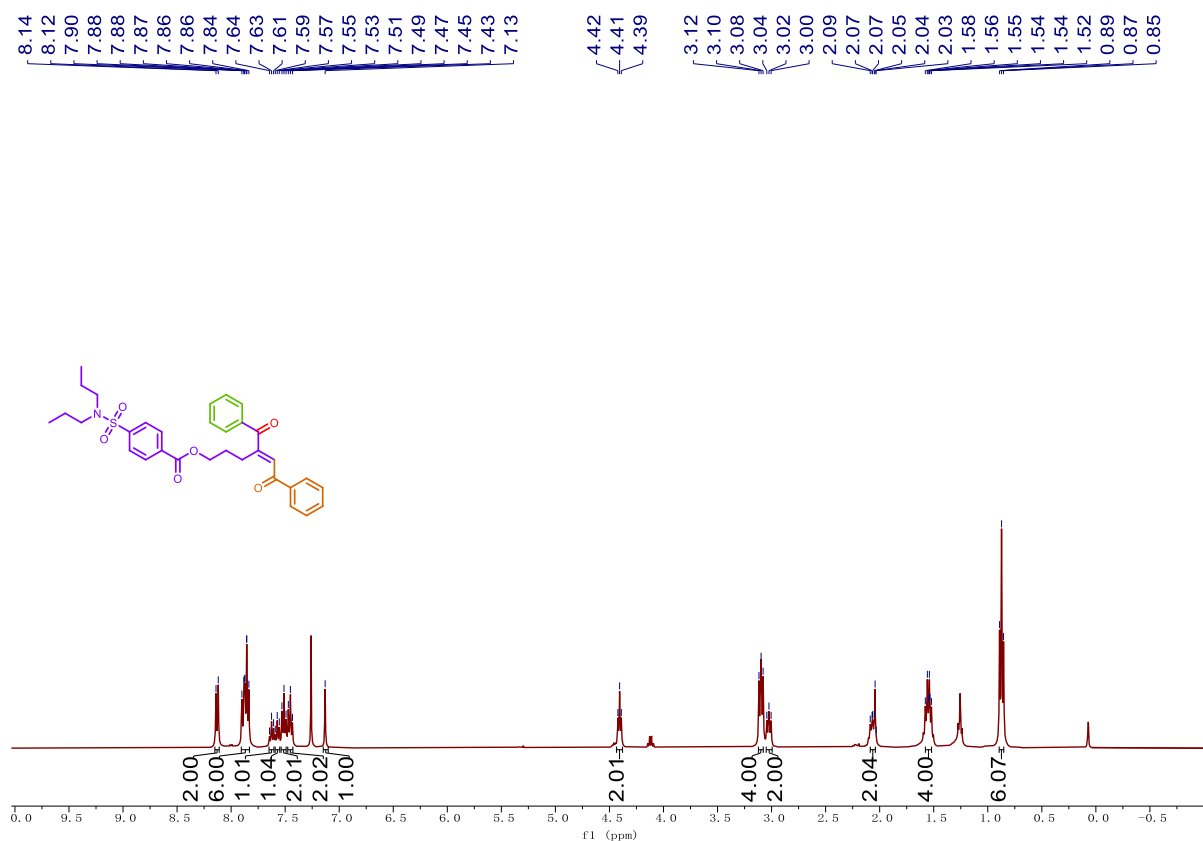
**Compound 3o:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )**



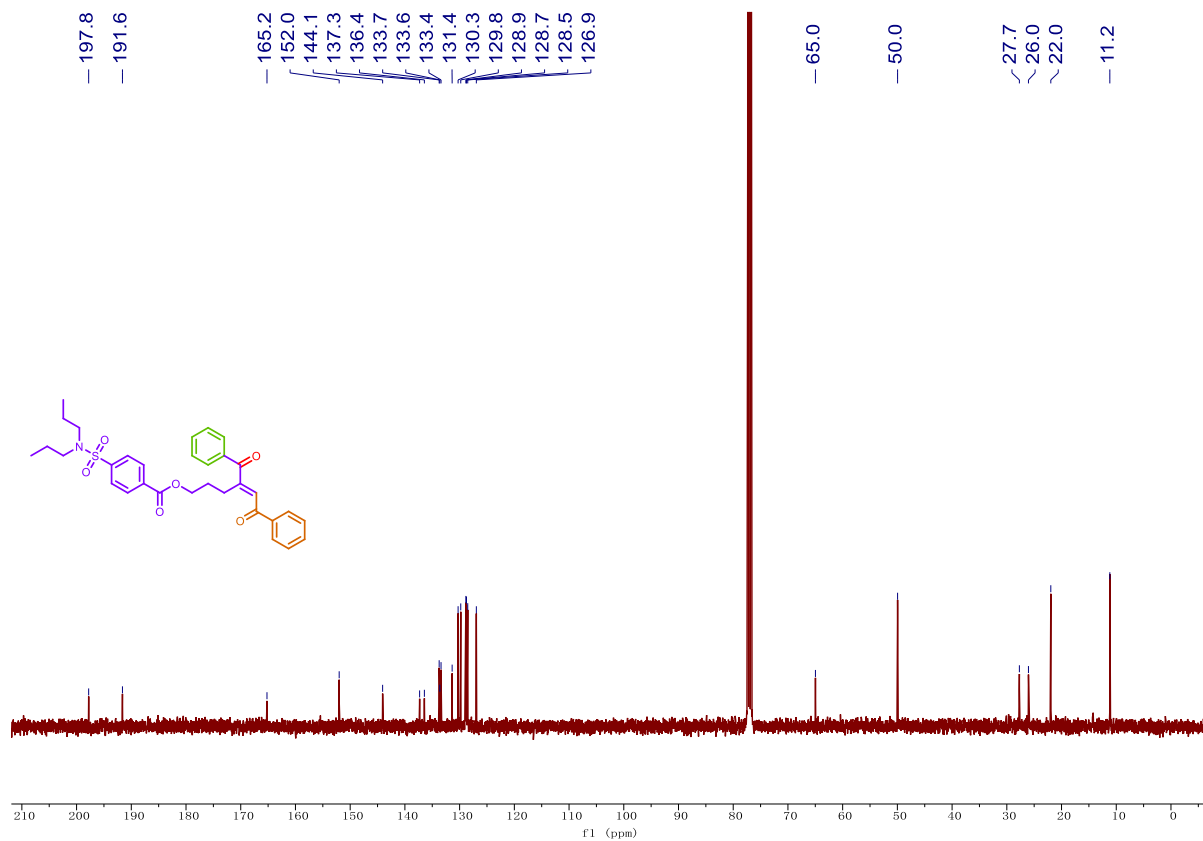
**Compound 3o:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )**



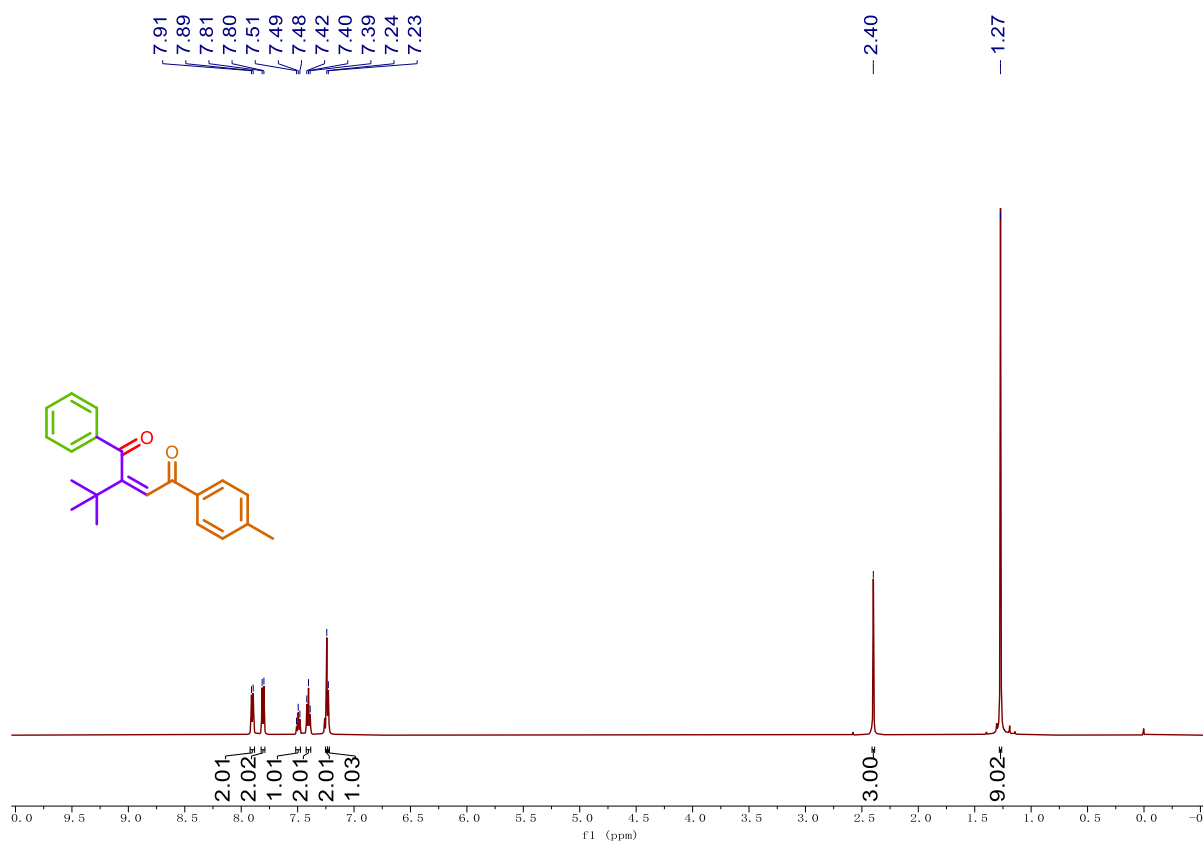
**Compound 3p:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )**



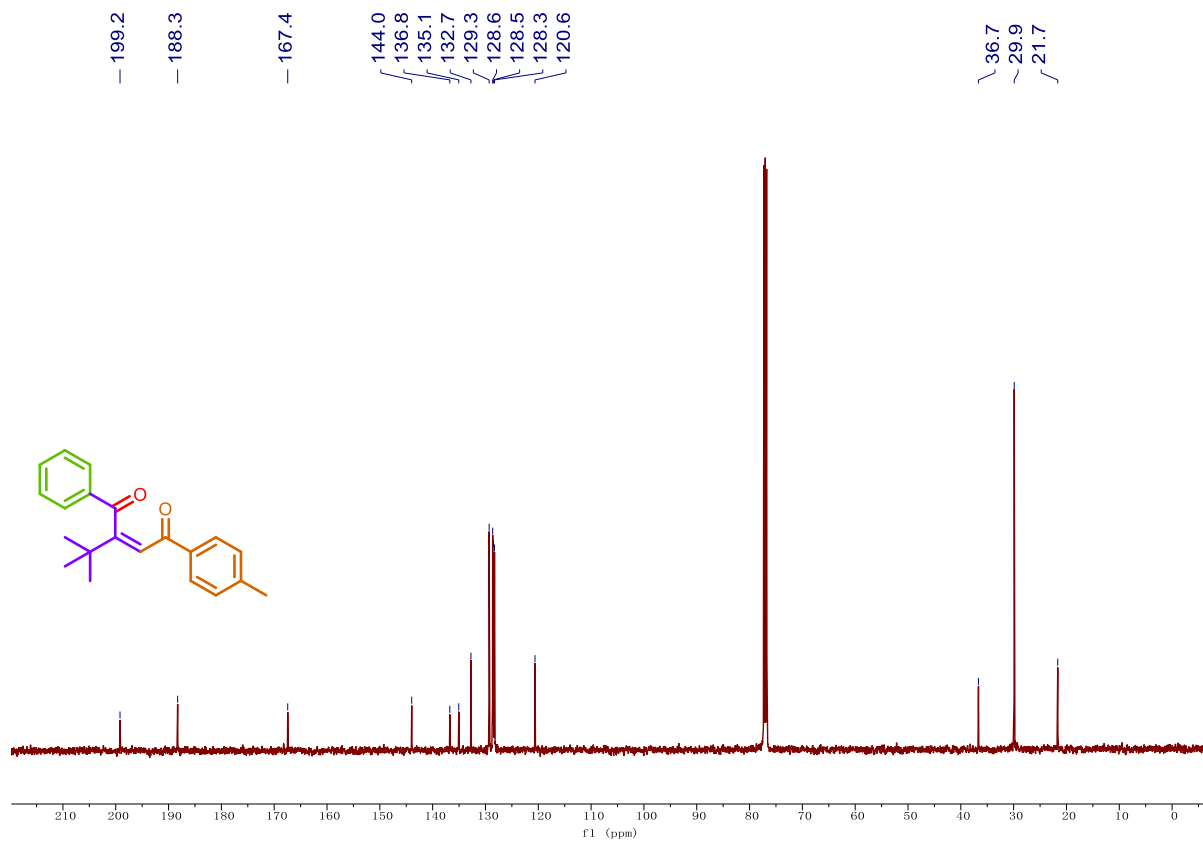
**Compound 3p:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )**



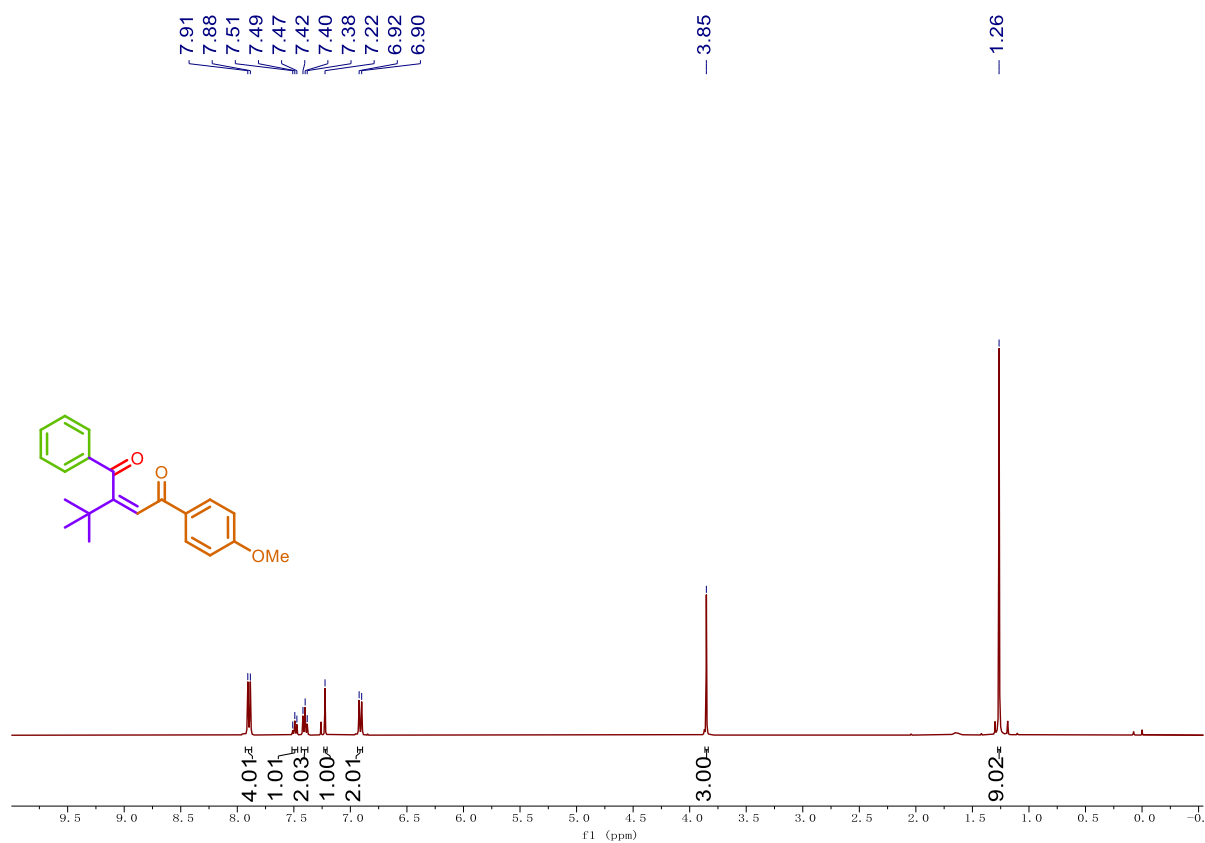
Compound 3q:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )



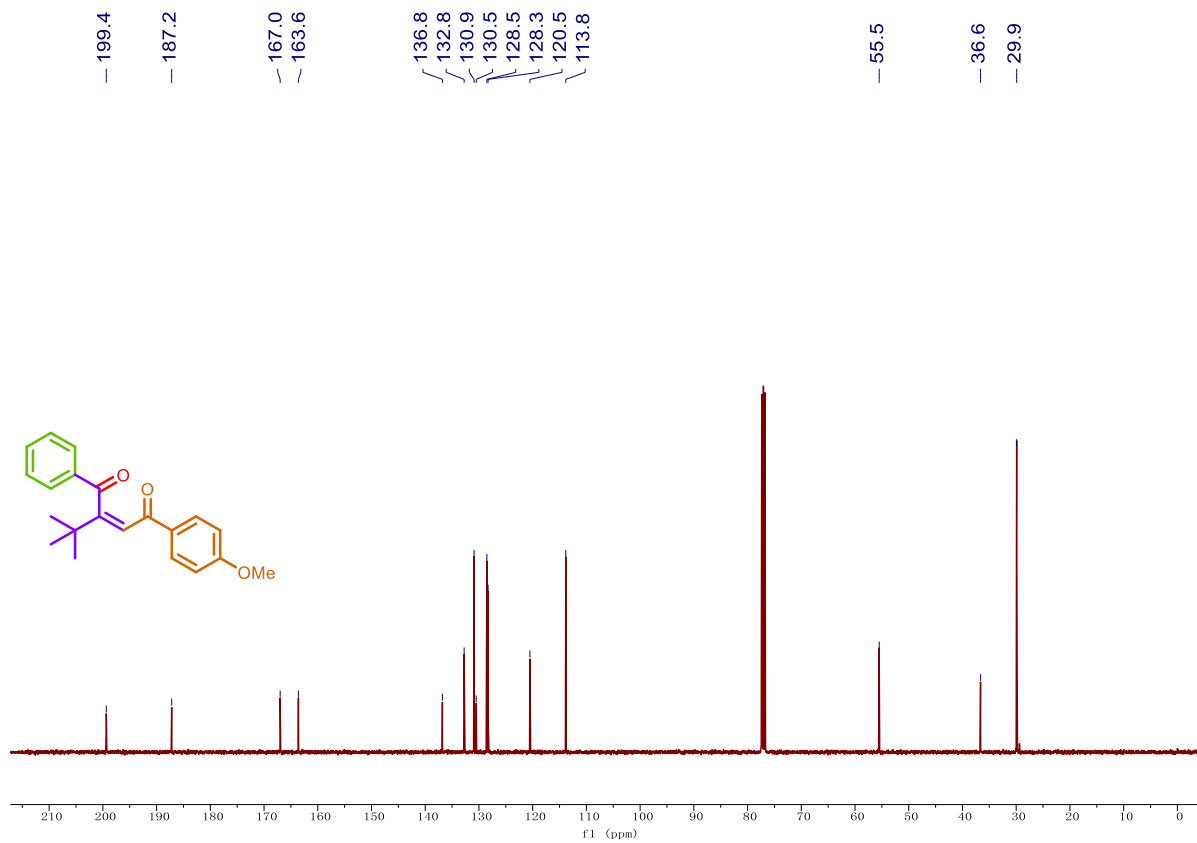
Compound 3q:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )



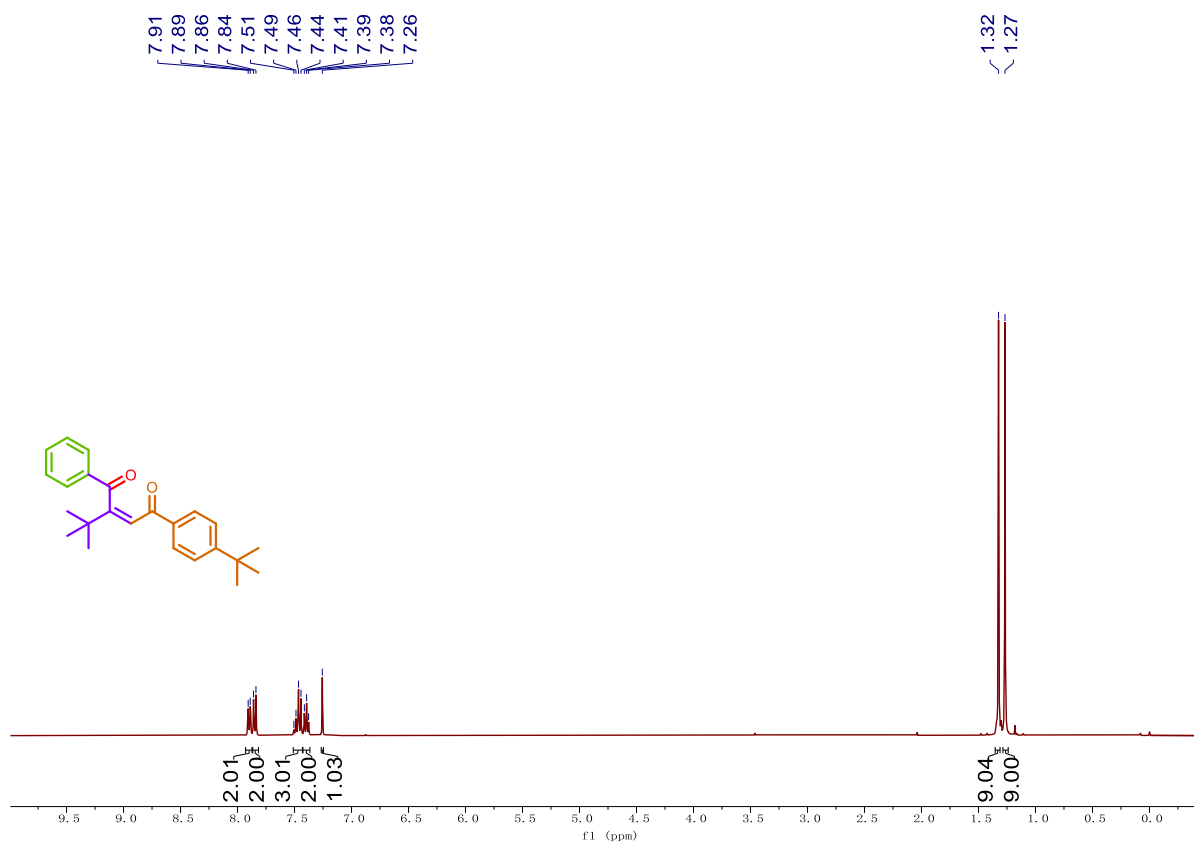
**Compound 3r:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )**



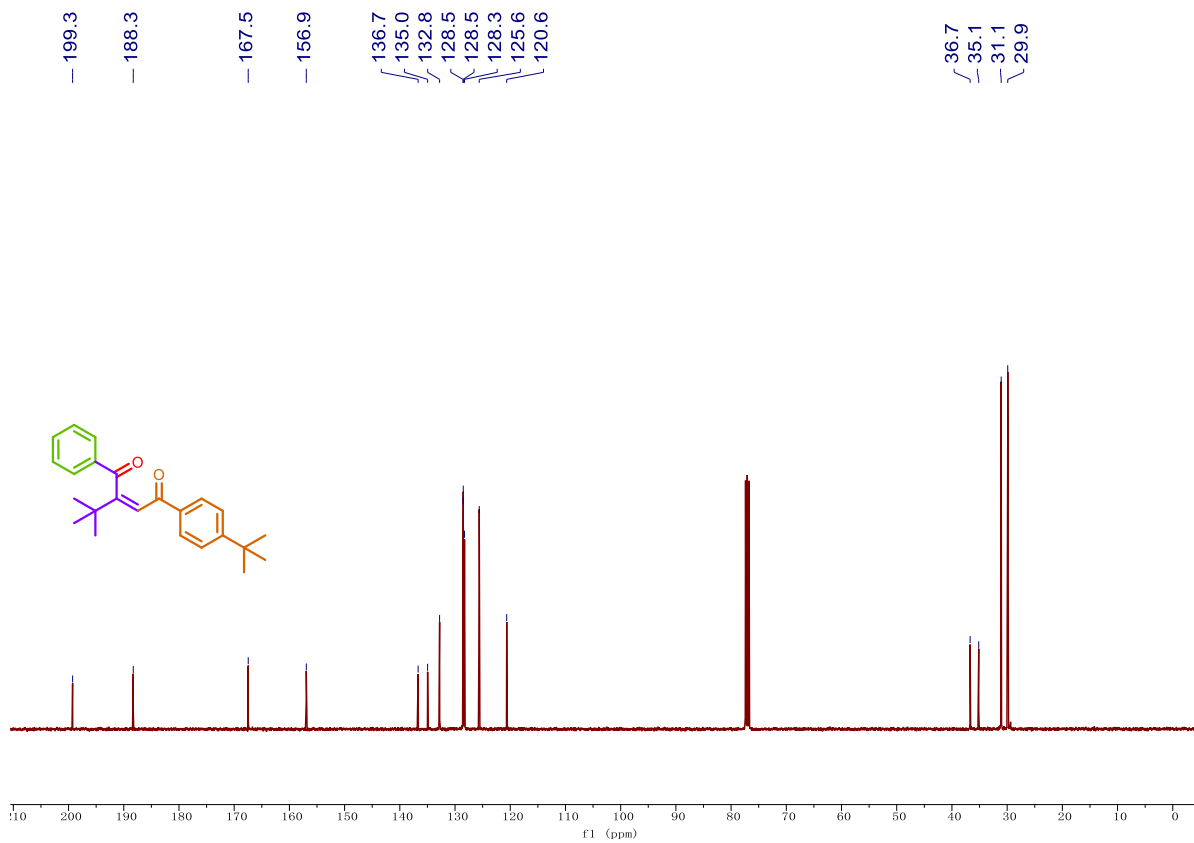
**Compound 3r:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )**



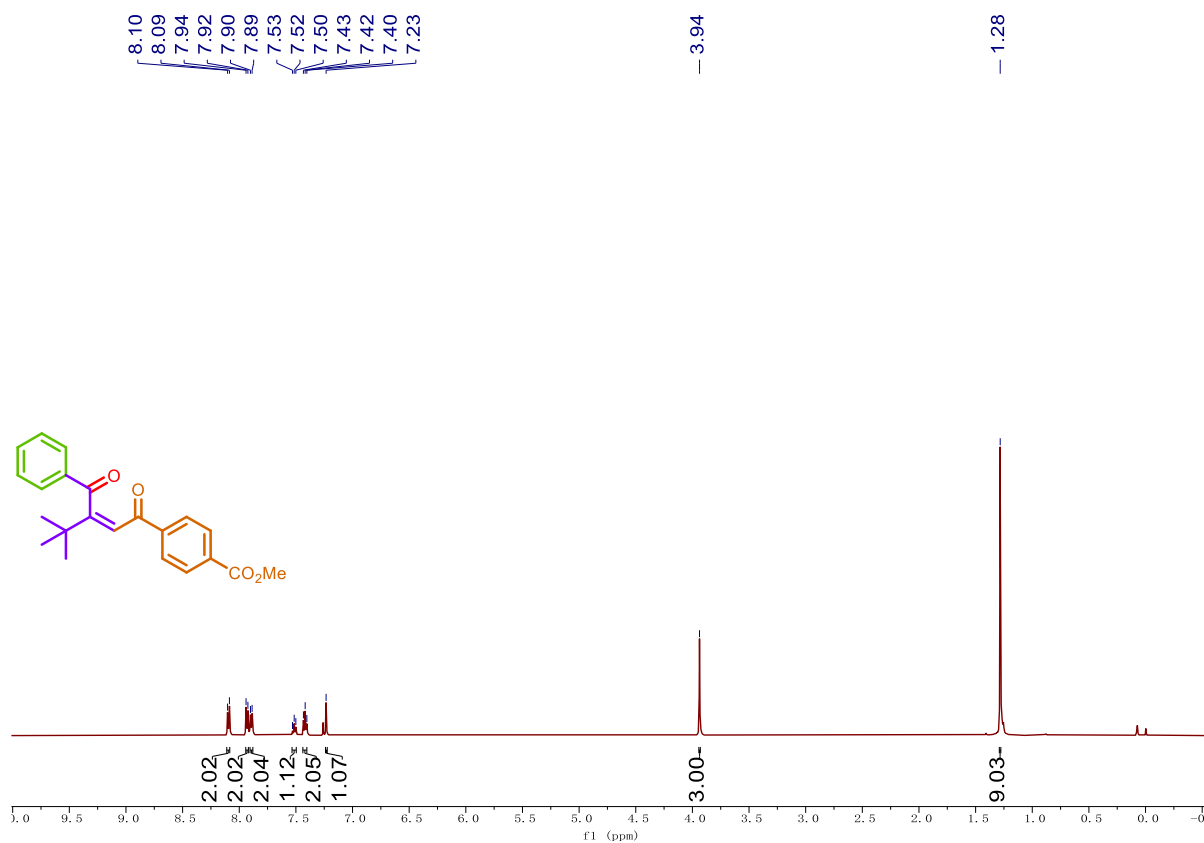
Compound 3s:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )



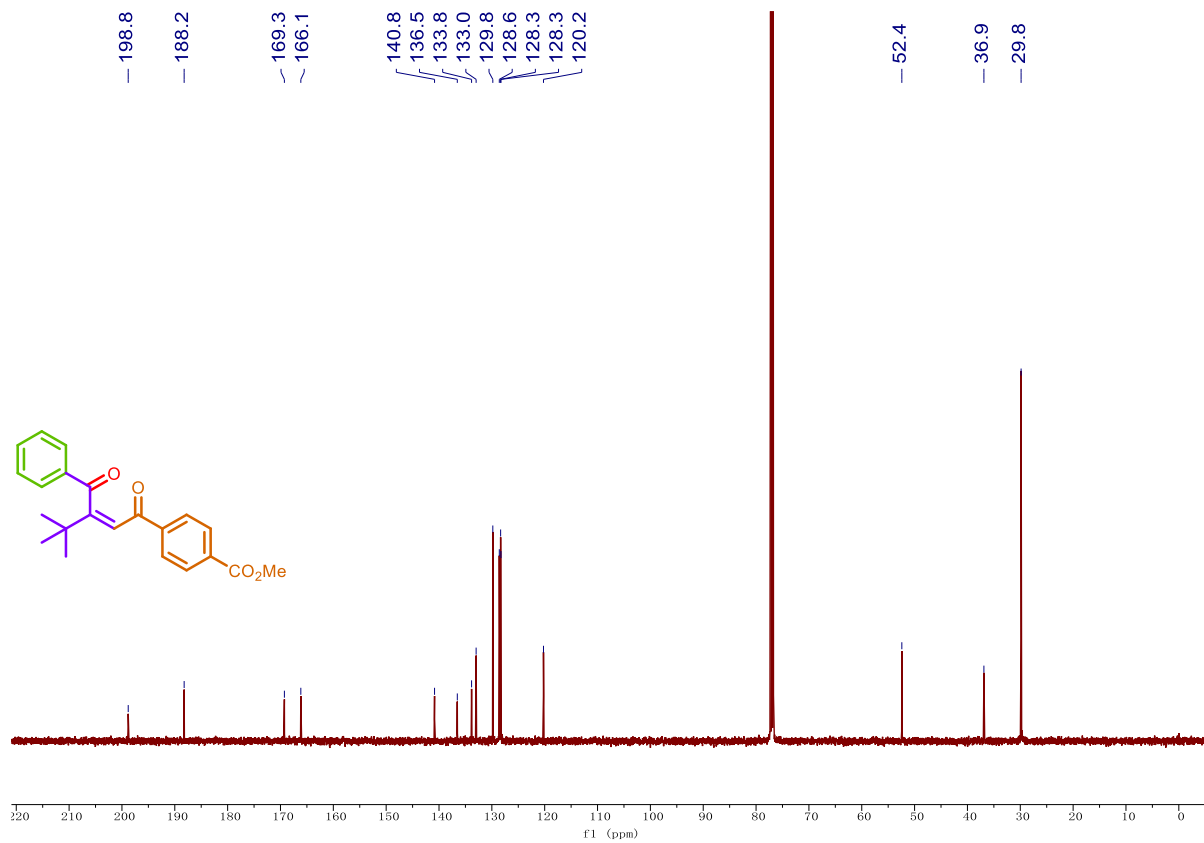
Compound 3s:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )



**Compound 3t:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )**

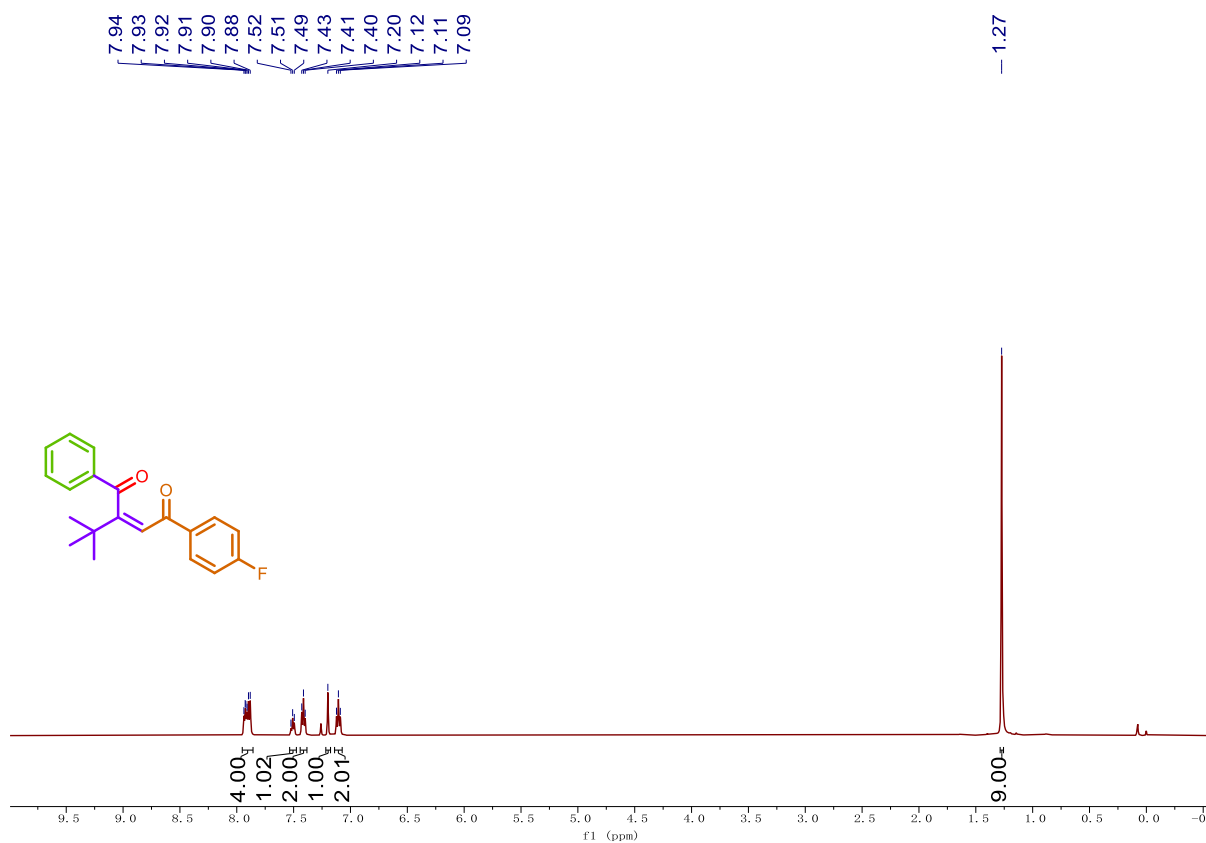


**Compound 3t:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )**

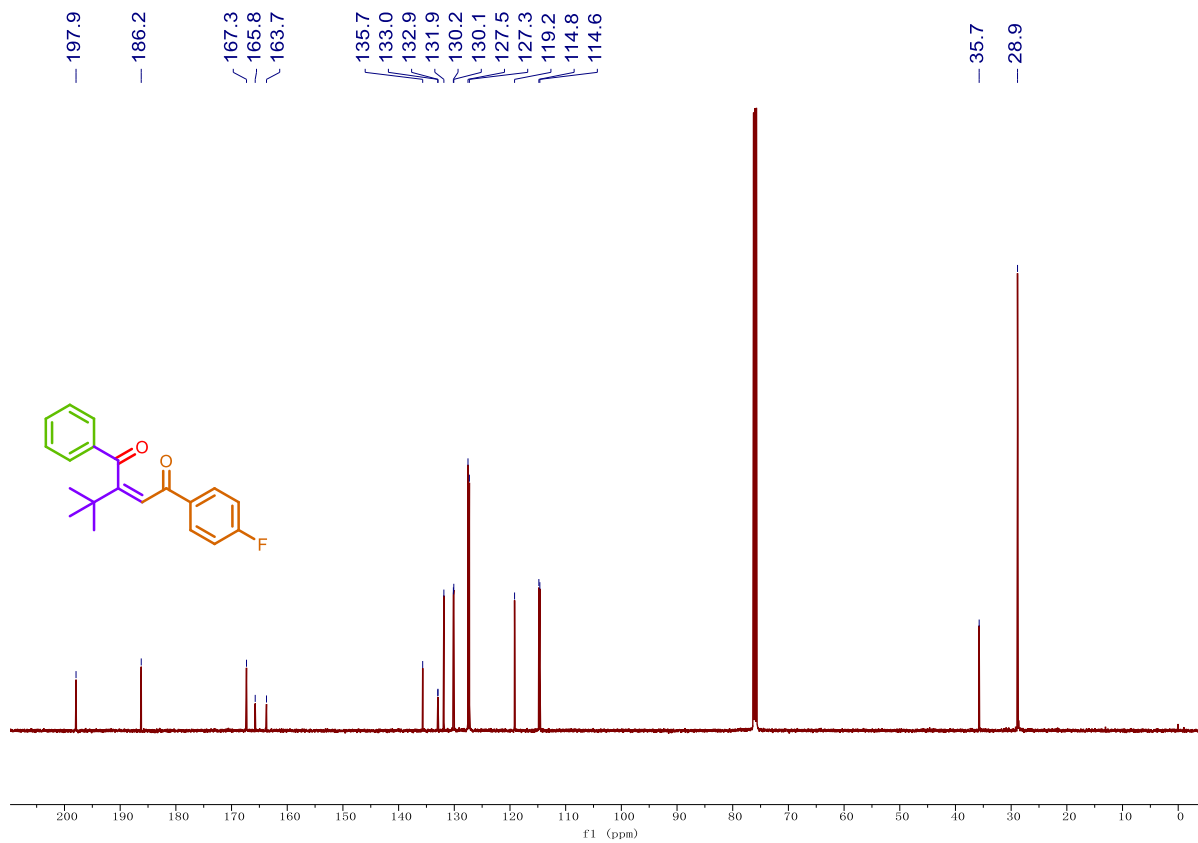




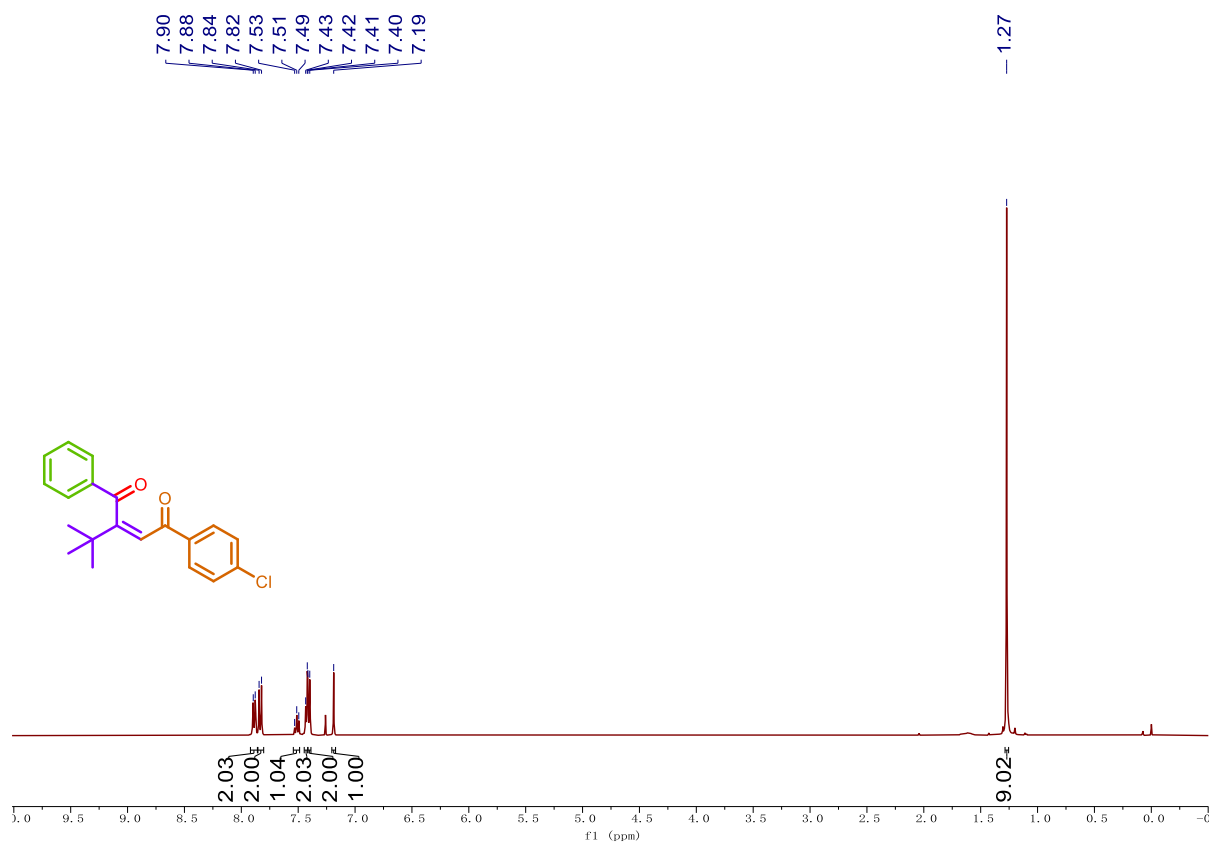
Compound 3u:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )



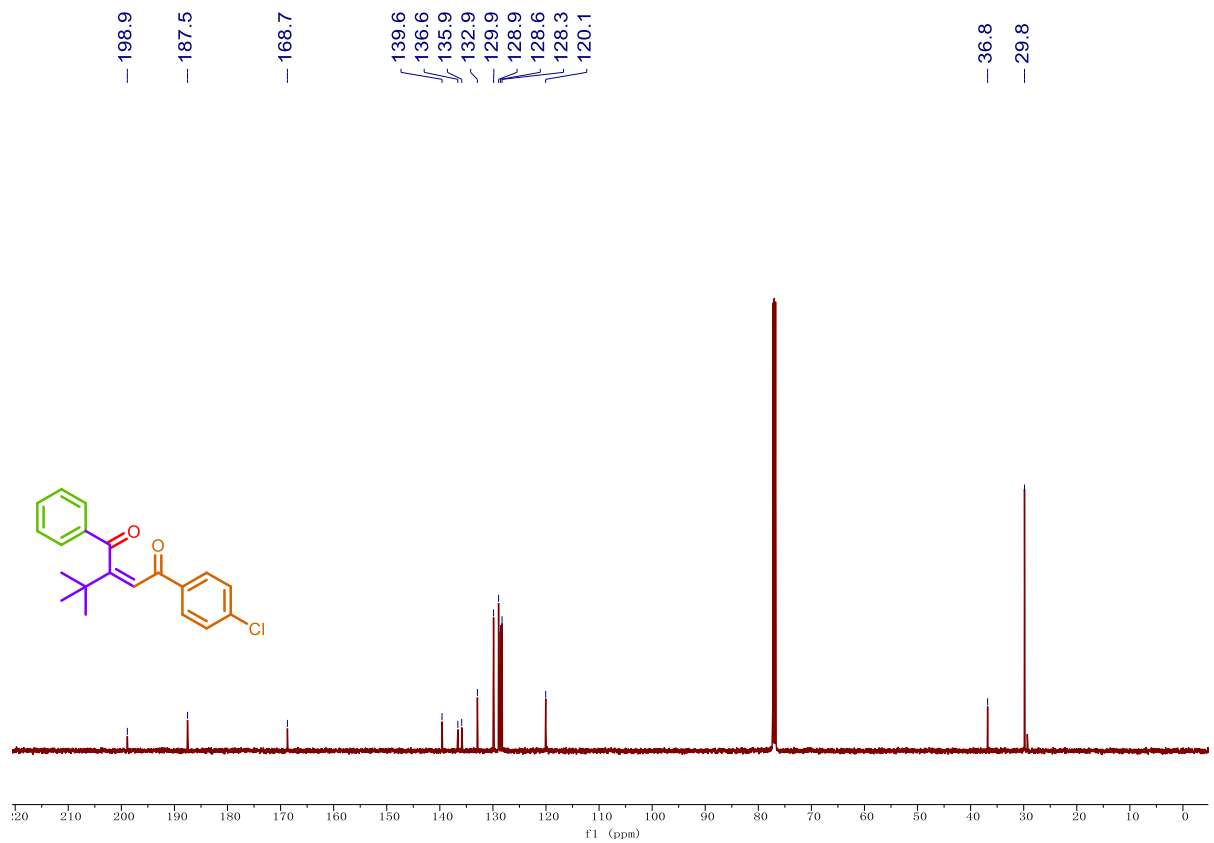
Compound 3u:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )



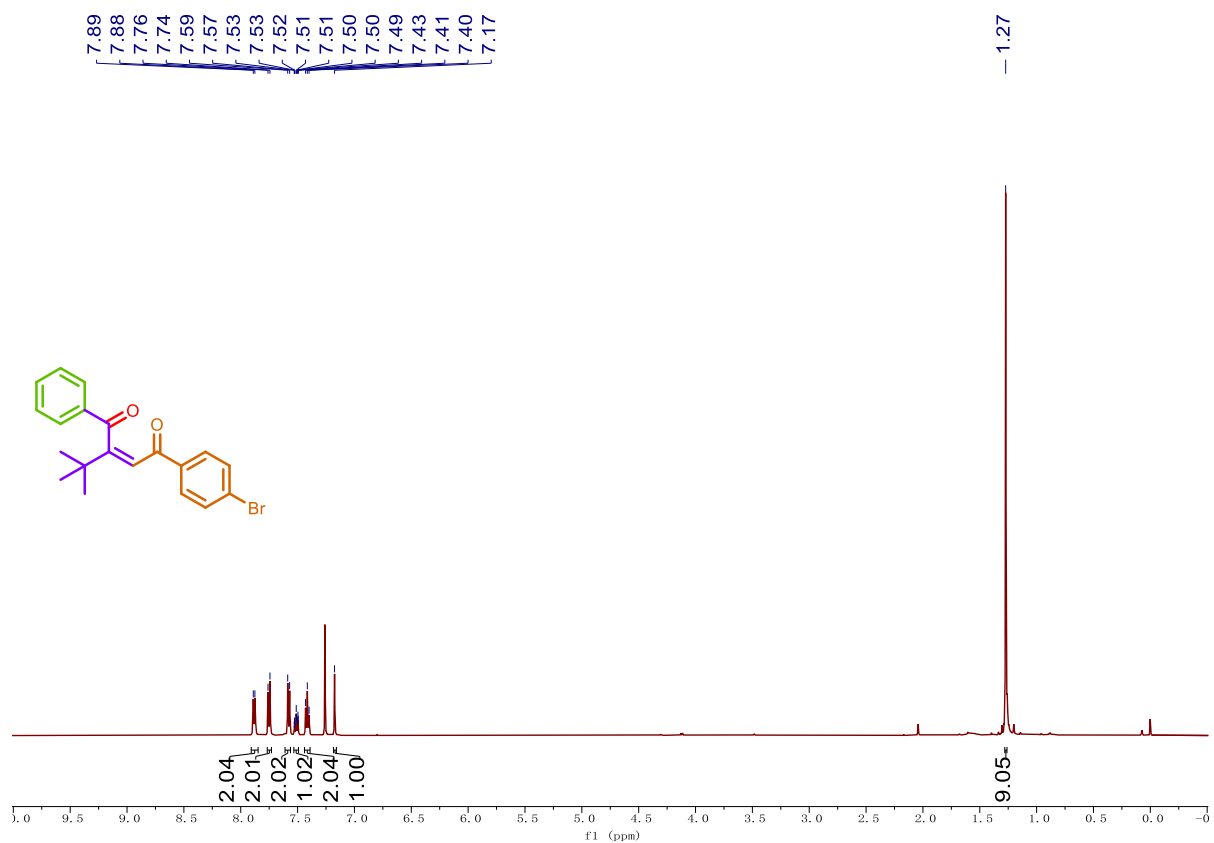
Compound 3v:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )



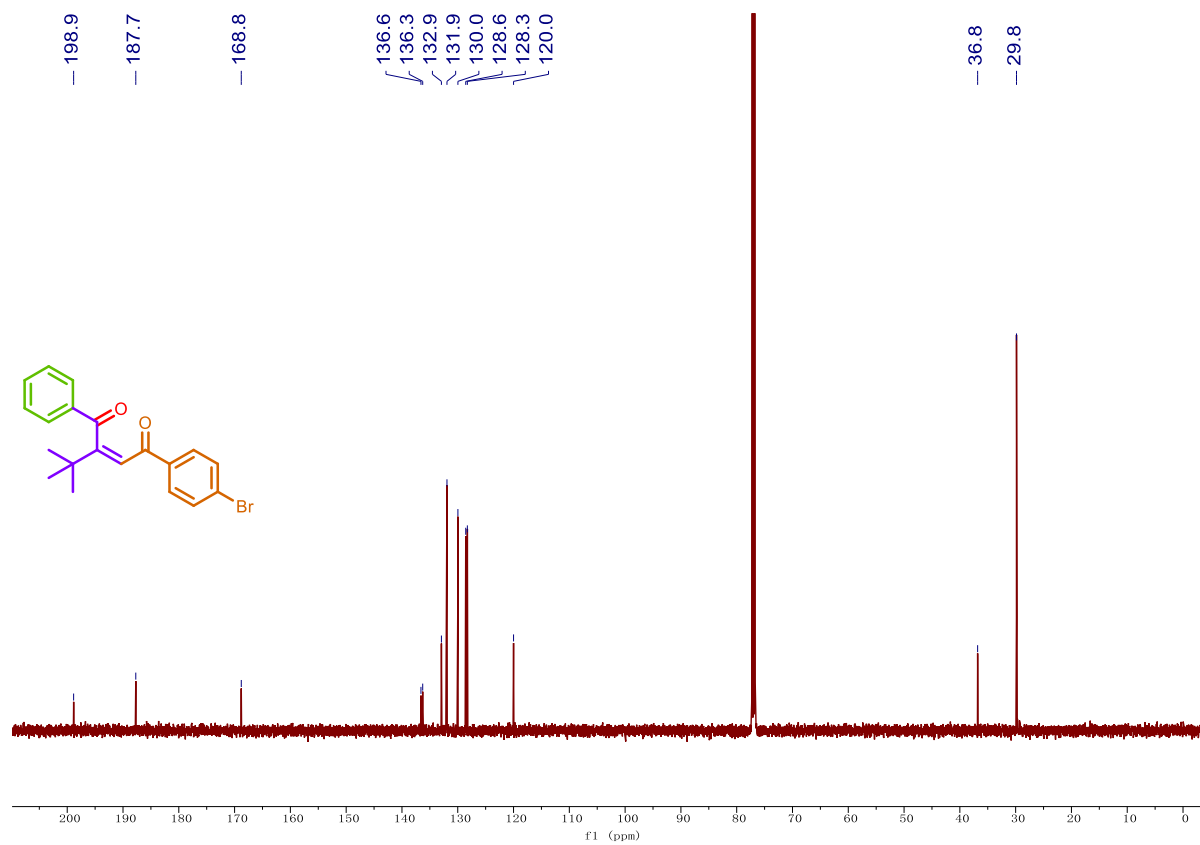
Compound 3v:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )



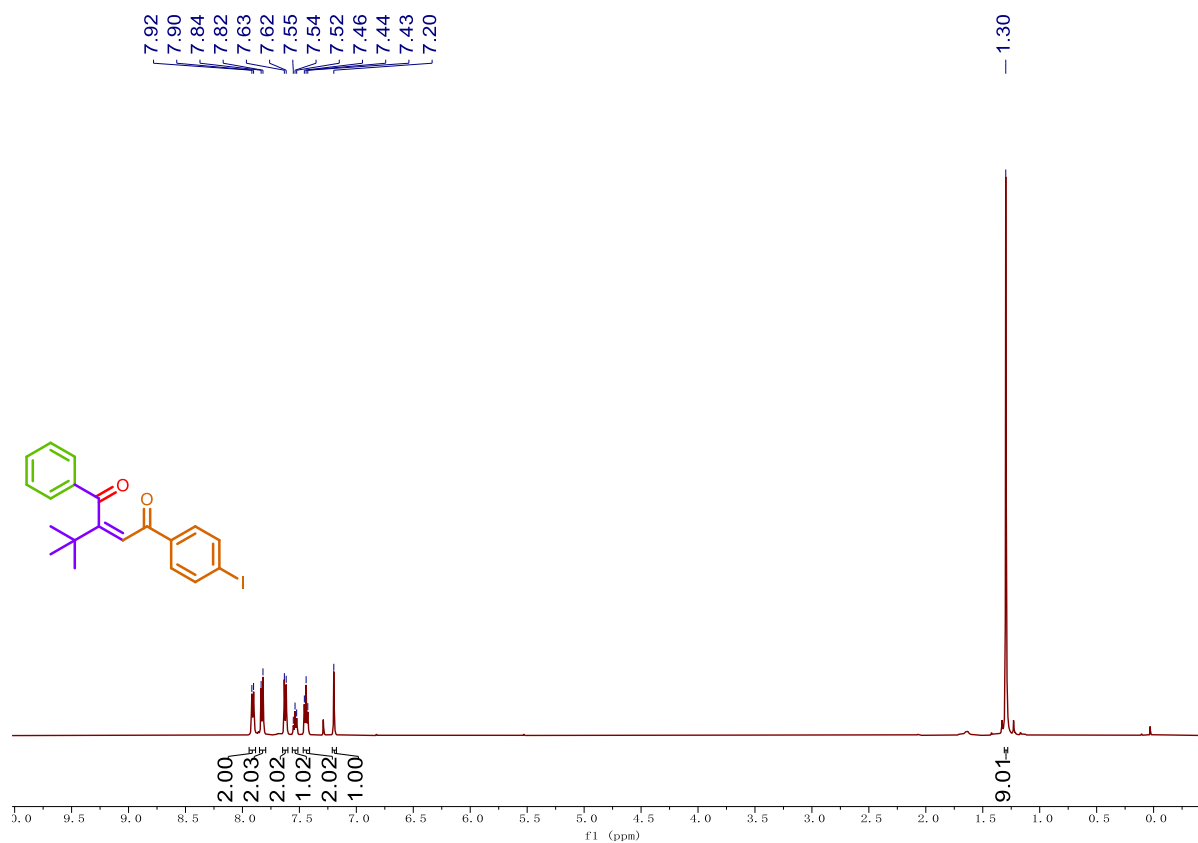
Compound 3w:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )



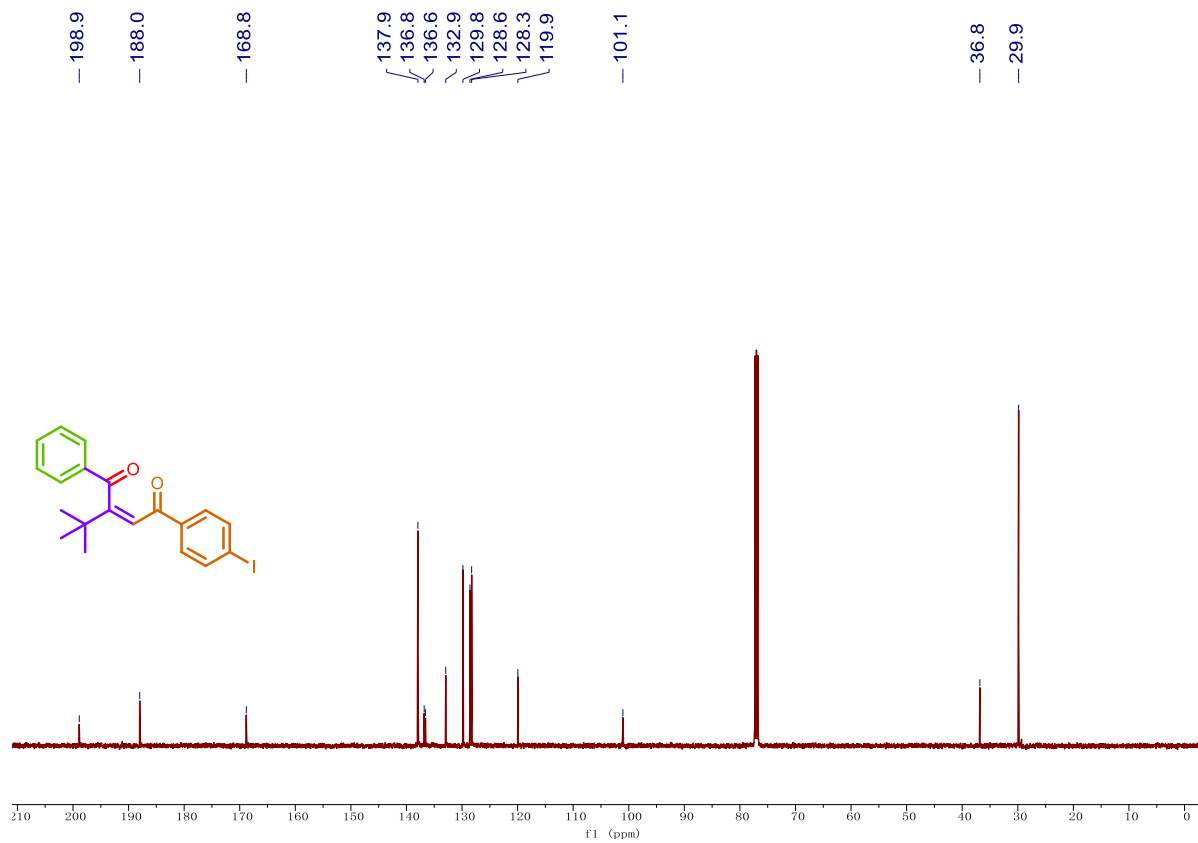
Compound 3w:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )



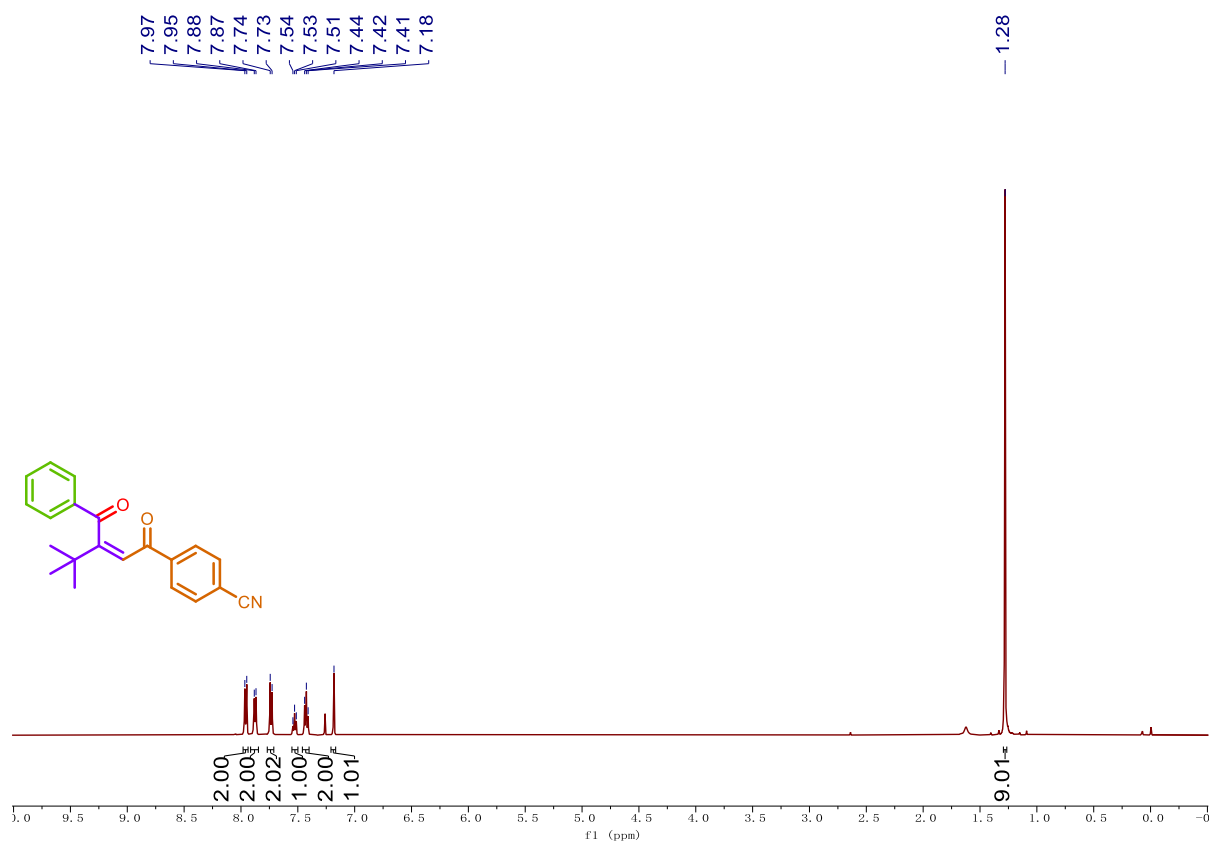
Compound 3x:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )



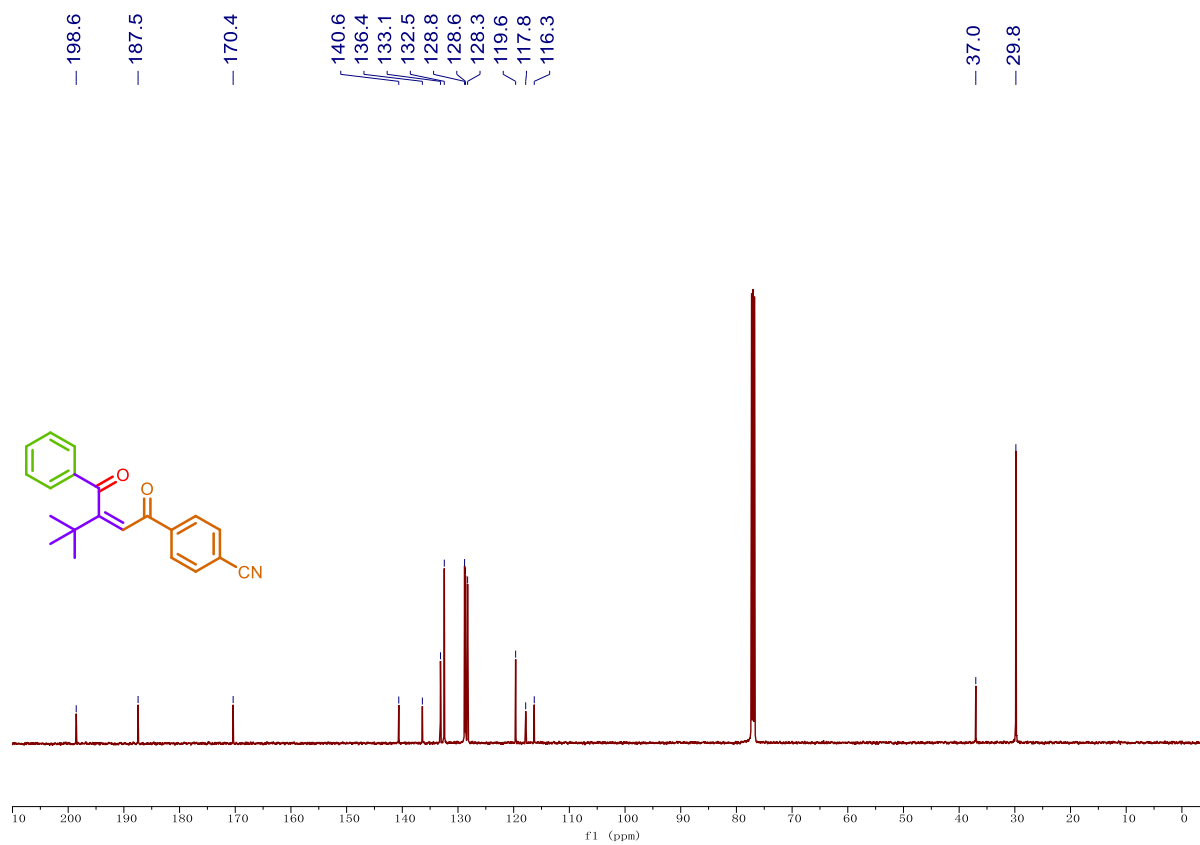
Compound 3x:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )



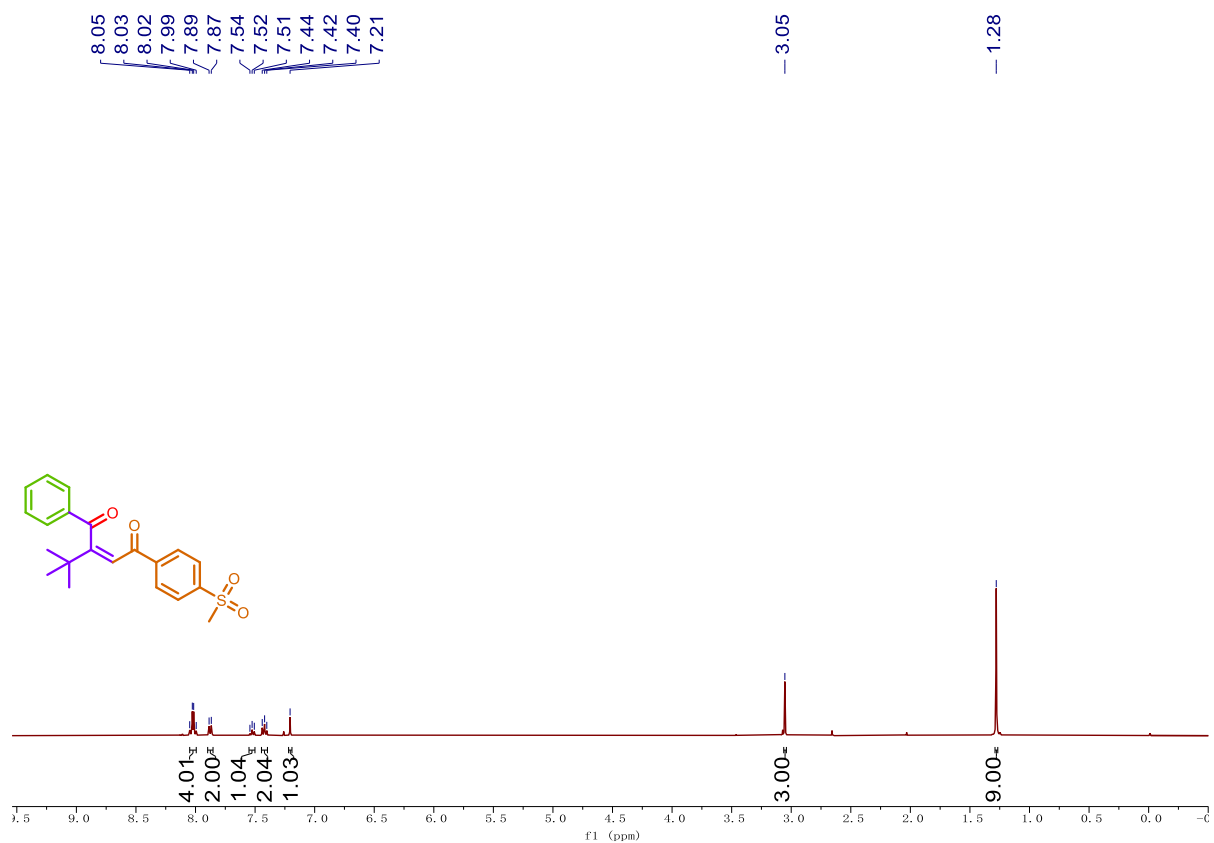
Compound 3y:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )



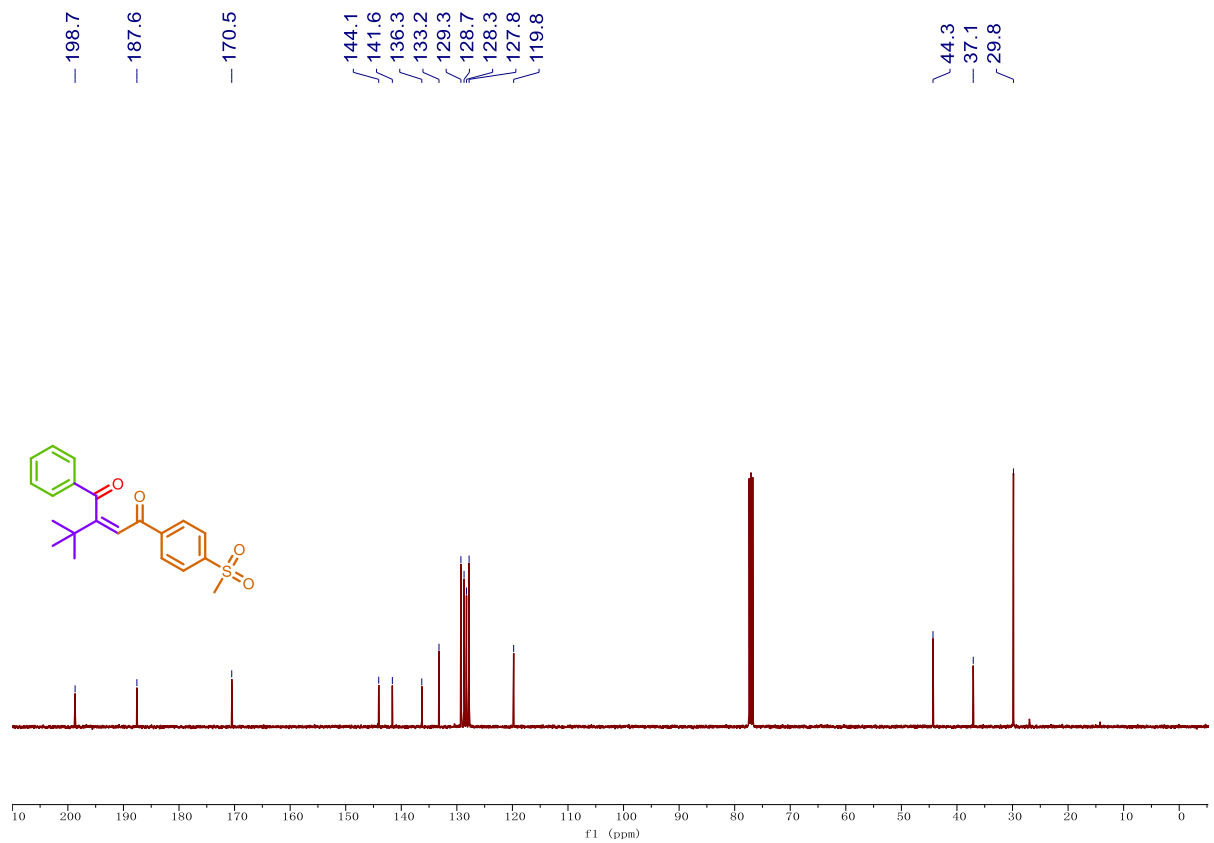
Compound 3y:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )



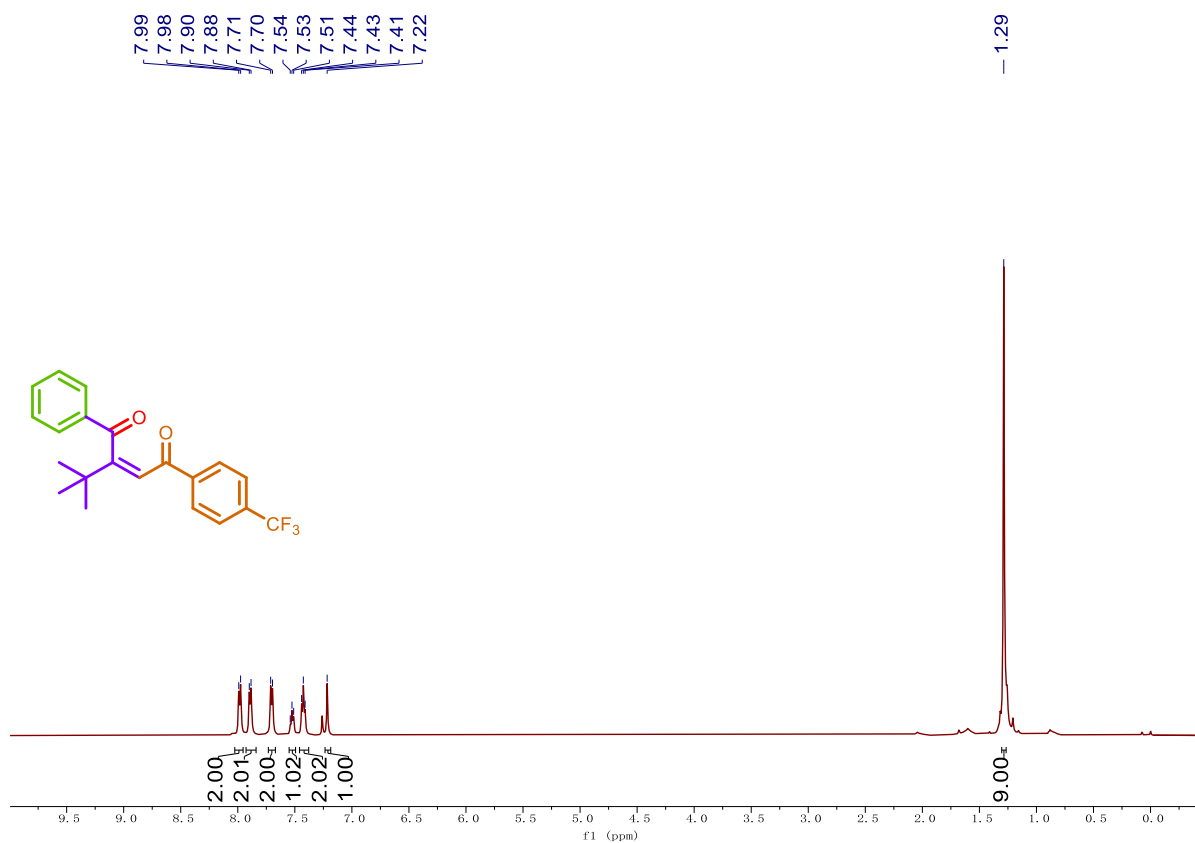
Compound 3z:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )



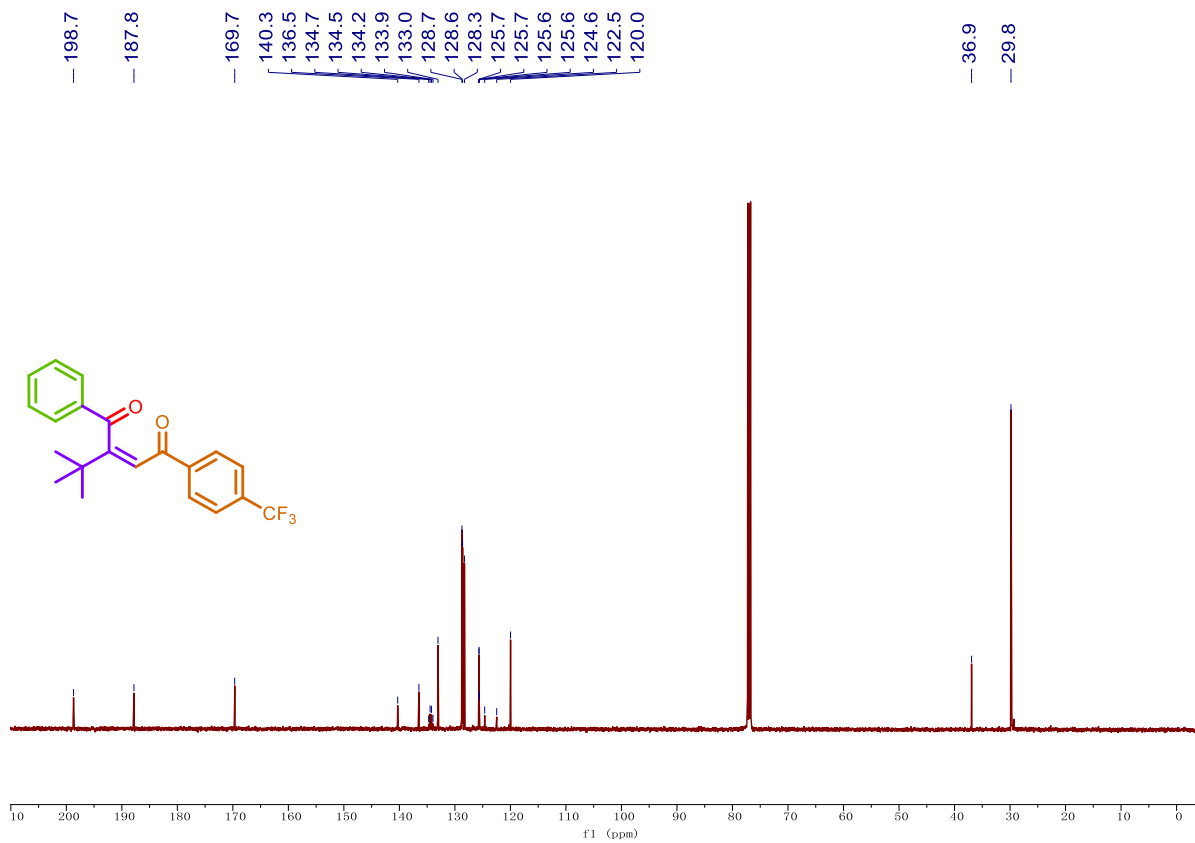
Compound 3z:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )



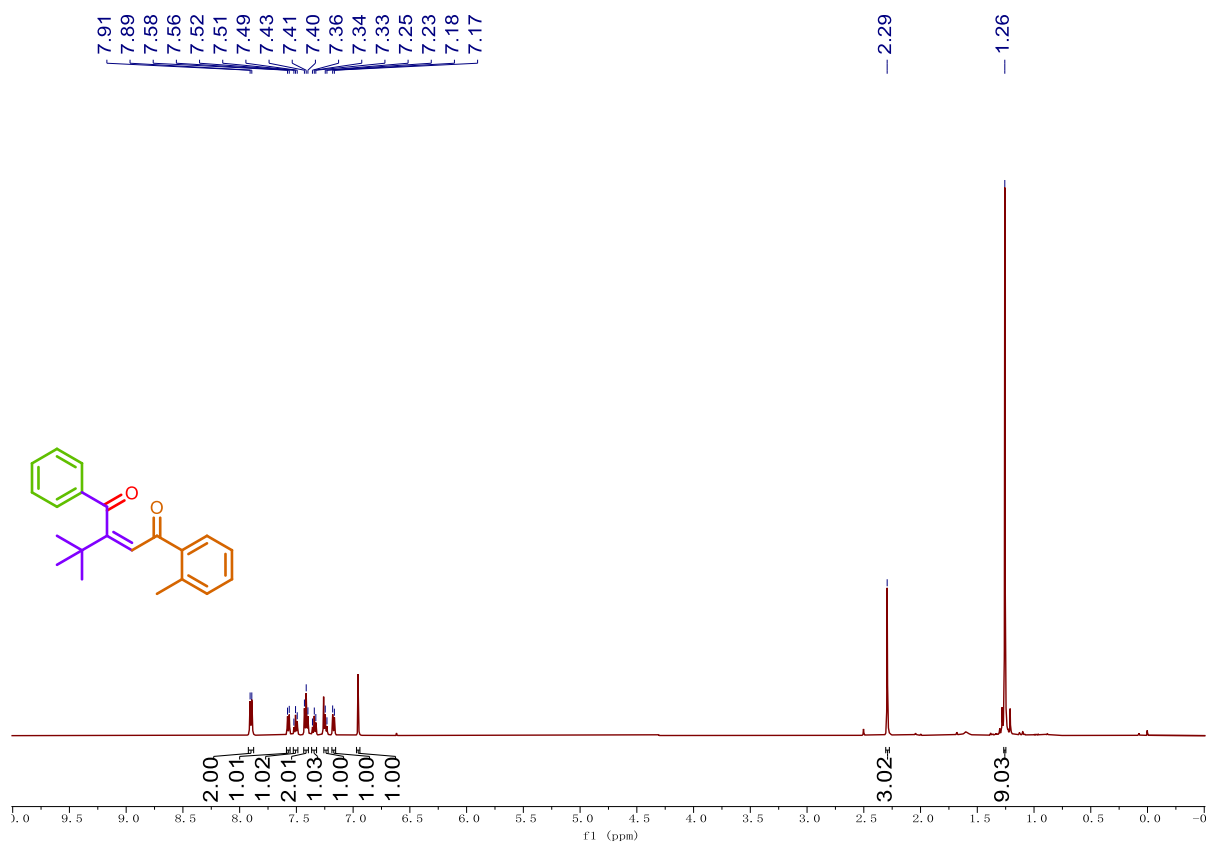
**Compound 3aa:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )**



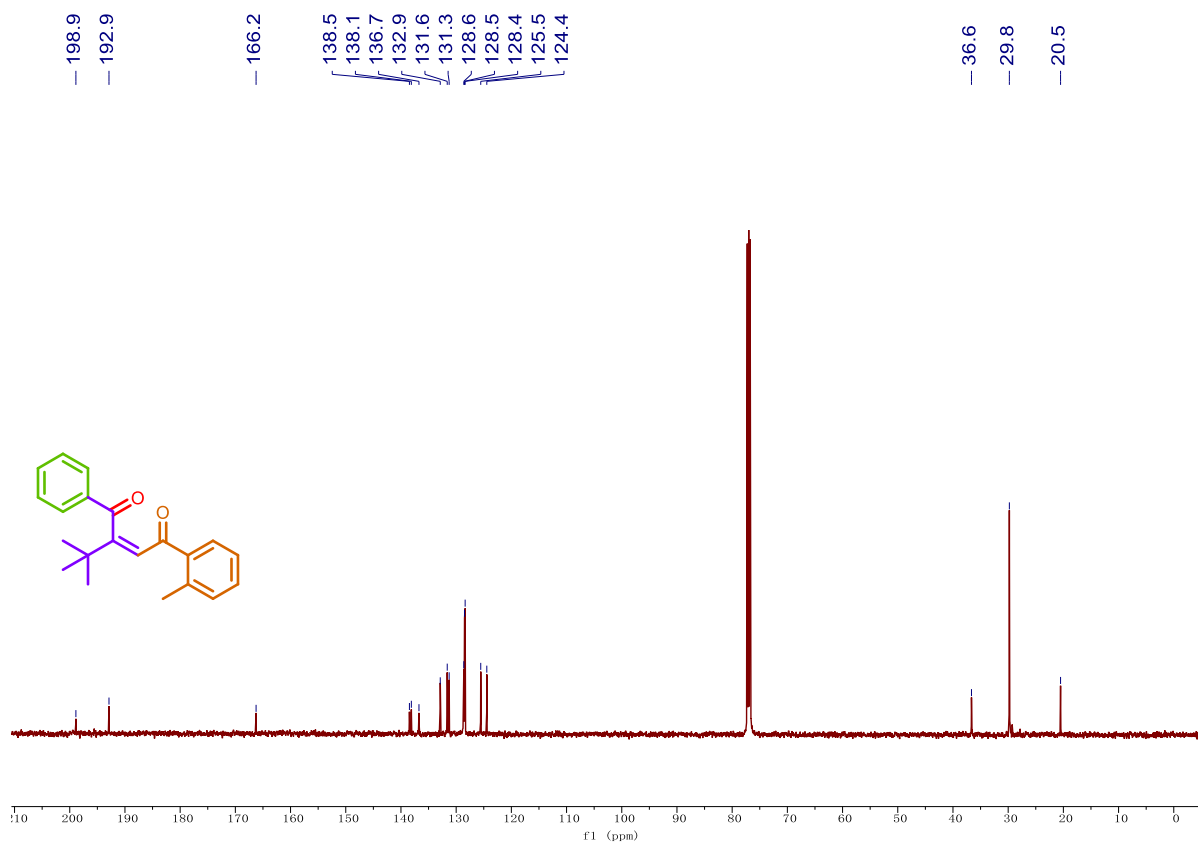
**Compound 3aa:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )**



**Compound 3ab:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )**

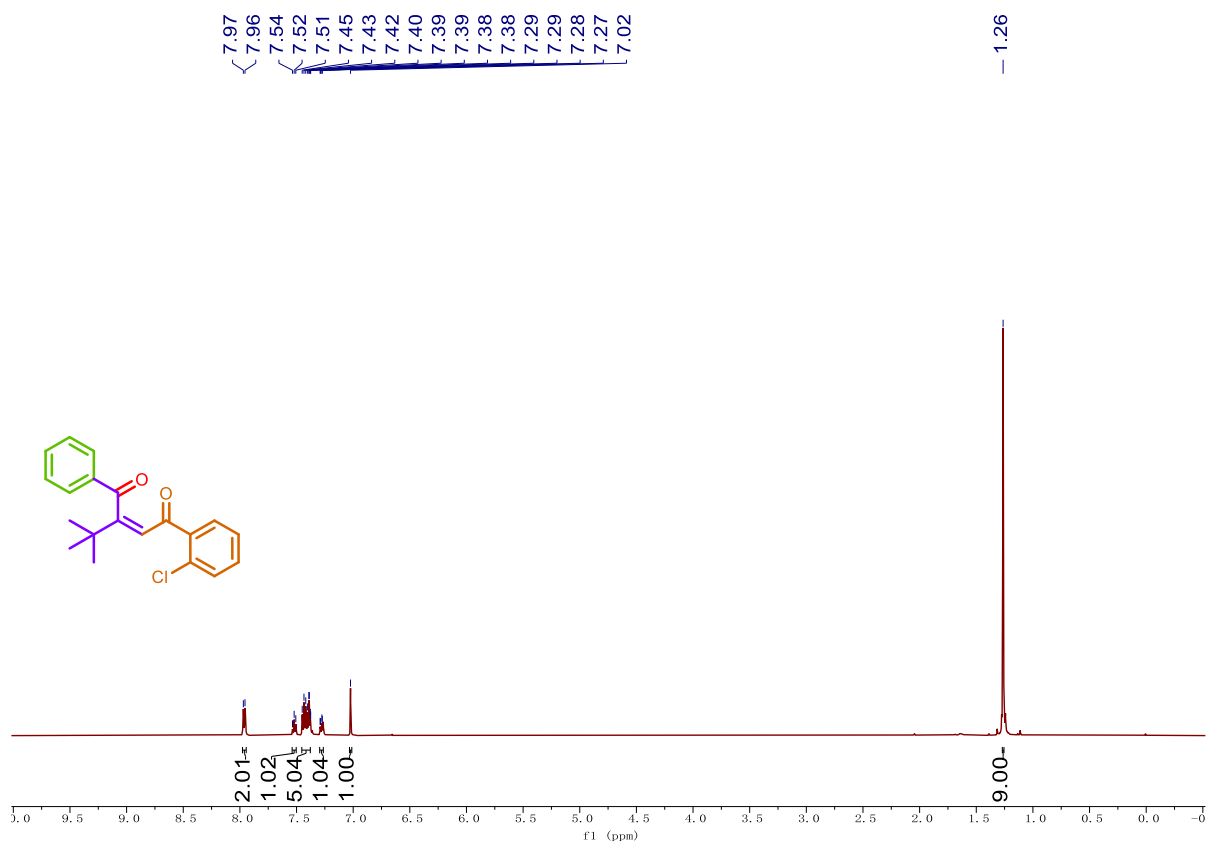


**Compound 3ab:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )**

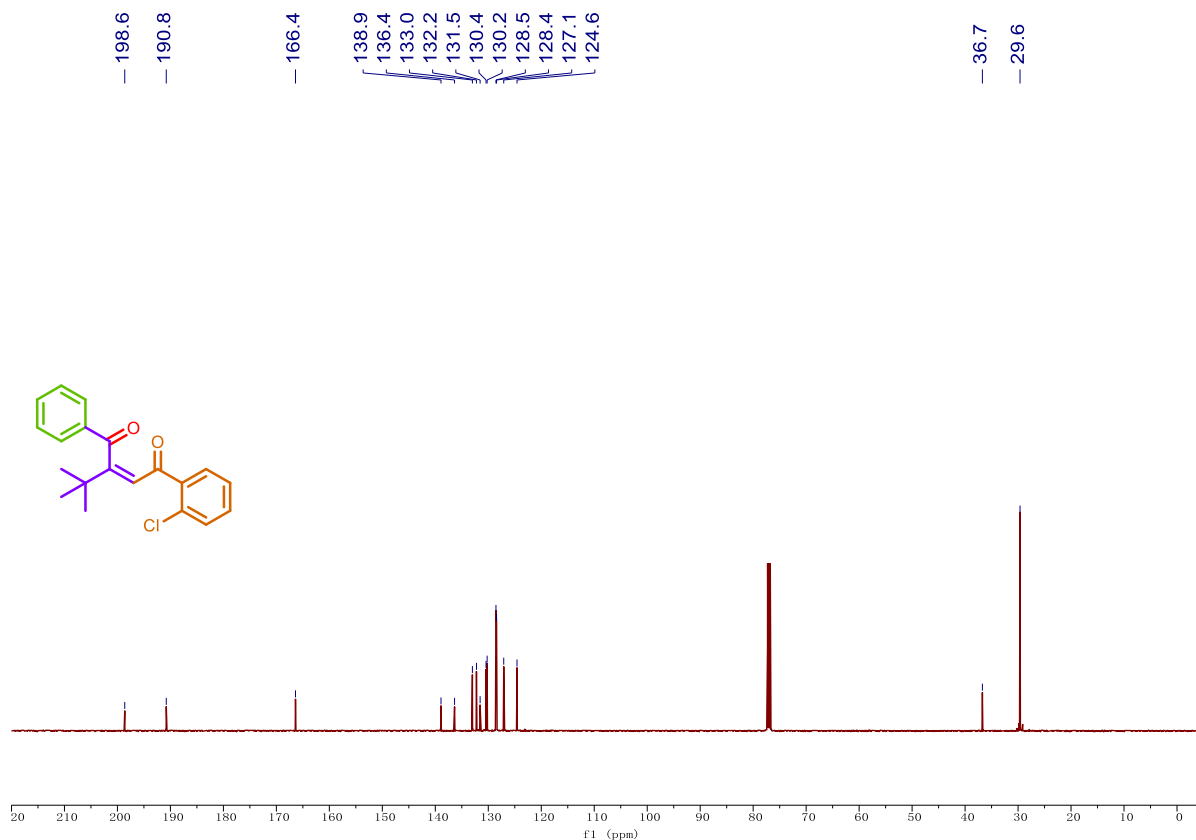




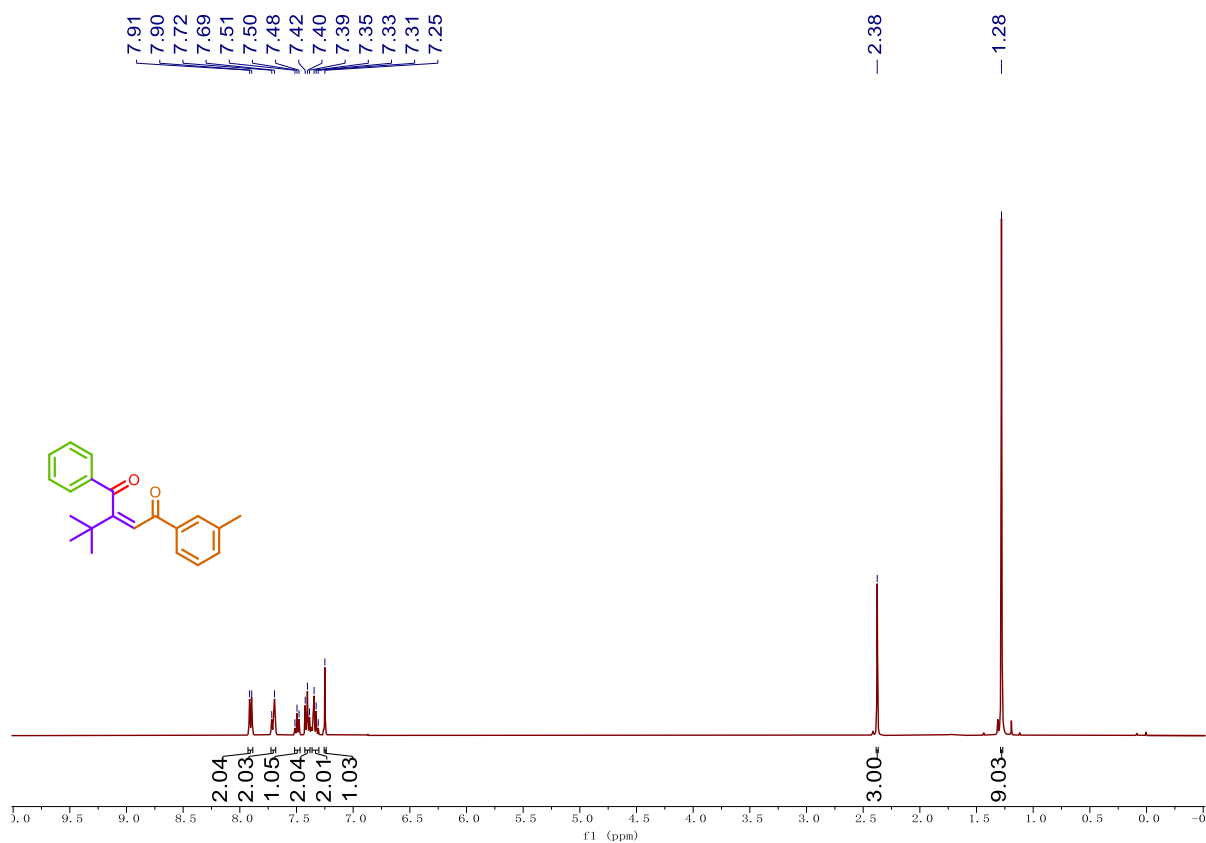
**Compound 3ac:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )**



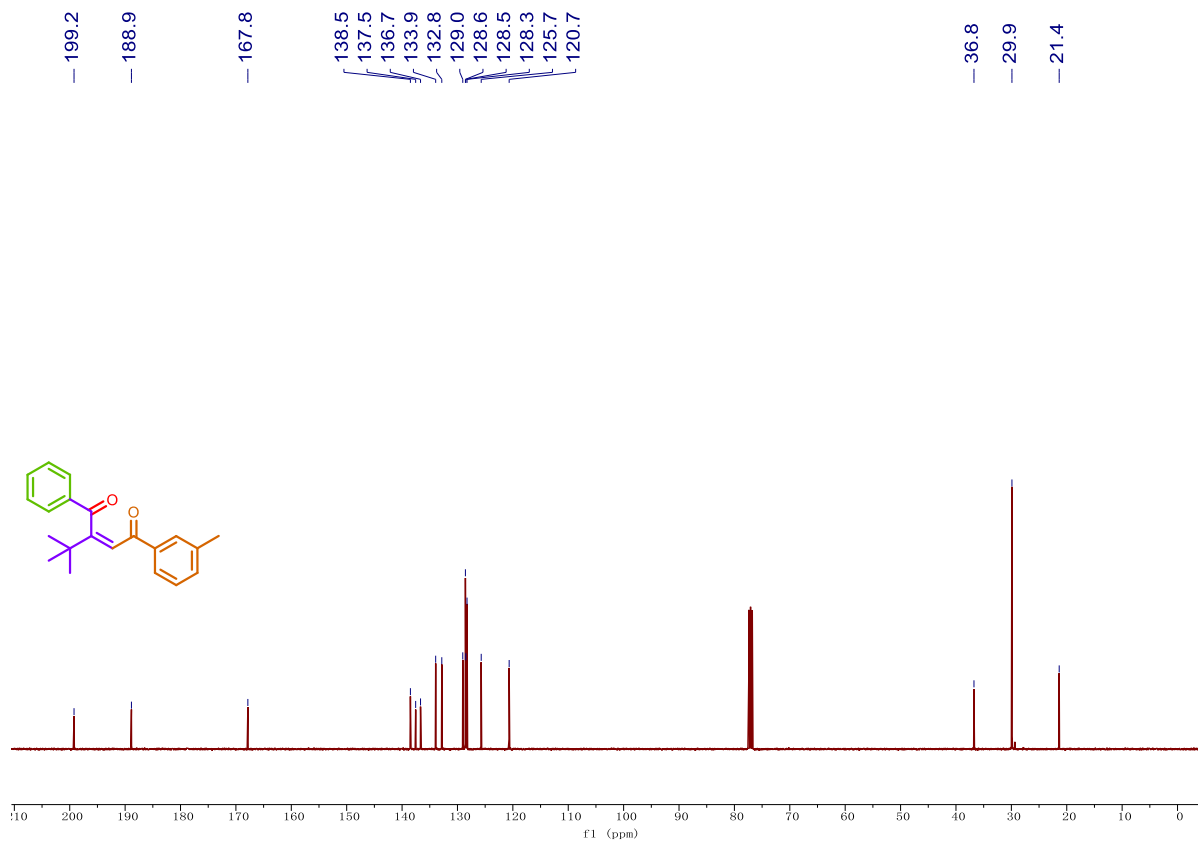
**Compound 3ac:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )**



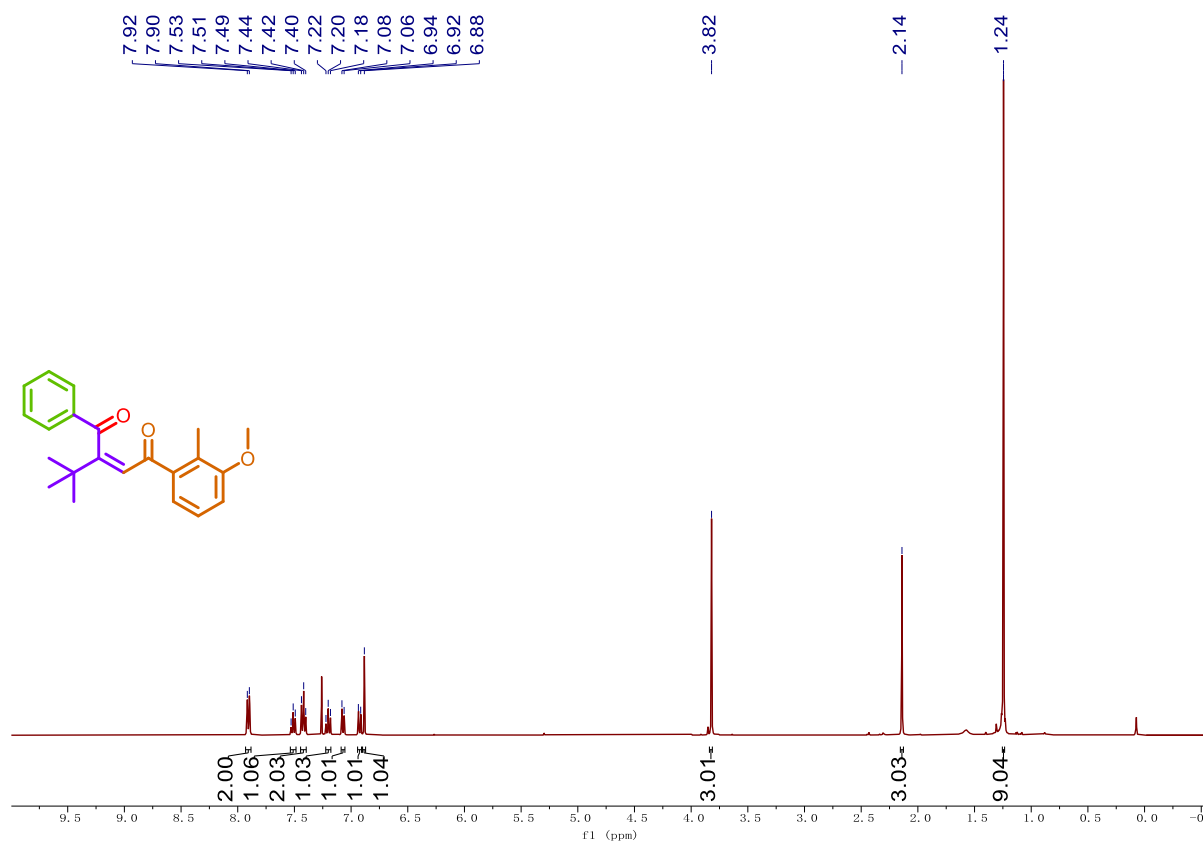
**Compound 3ad:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )**



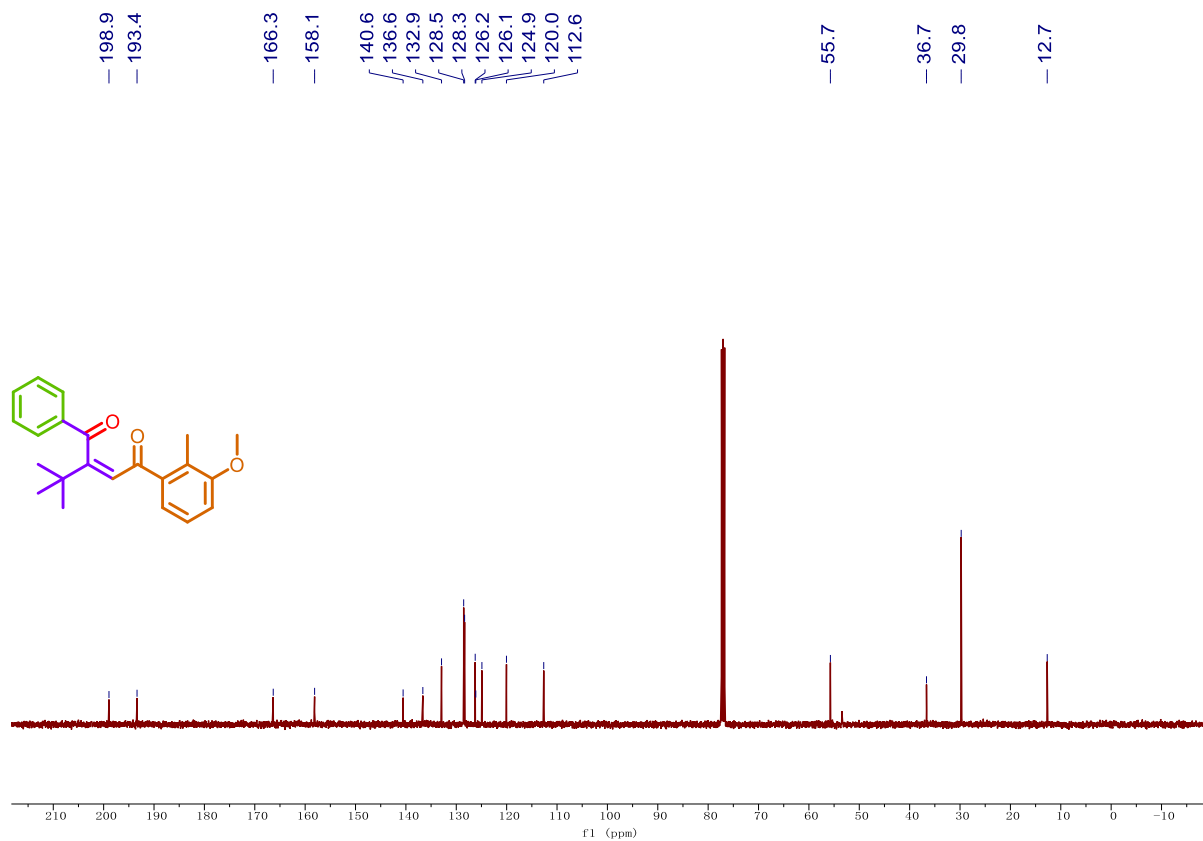
**Compound 3ad:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )**



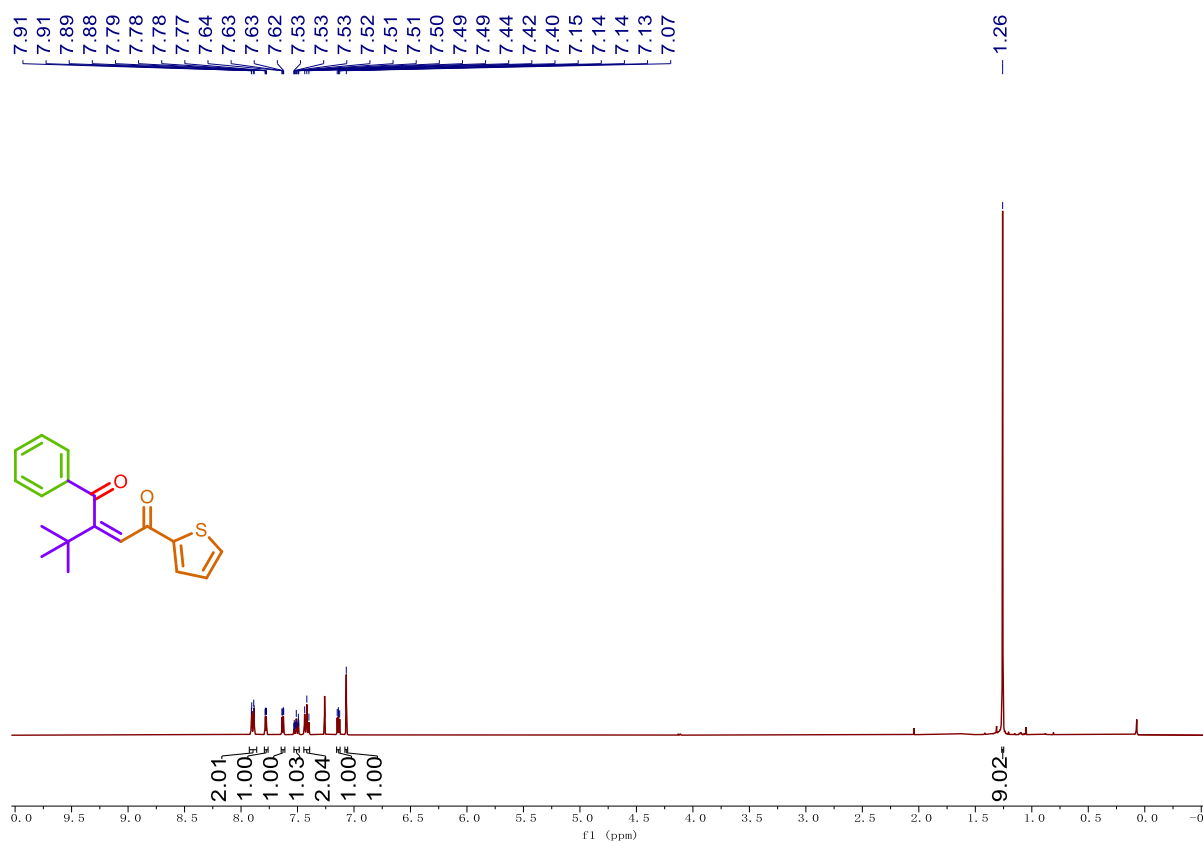
**Compound 3ae:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )**



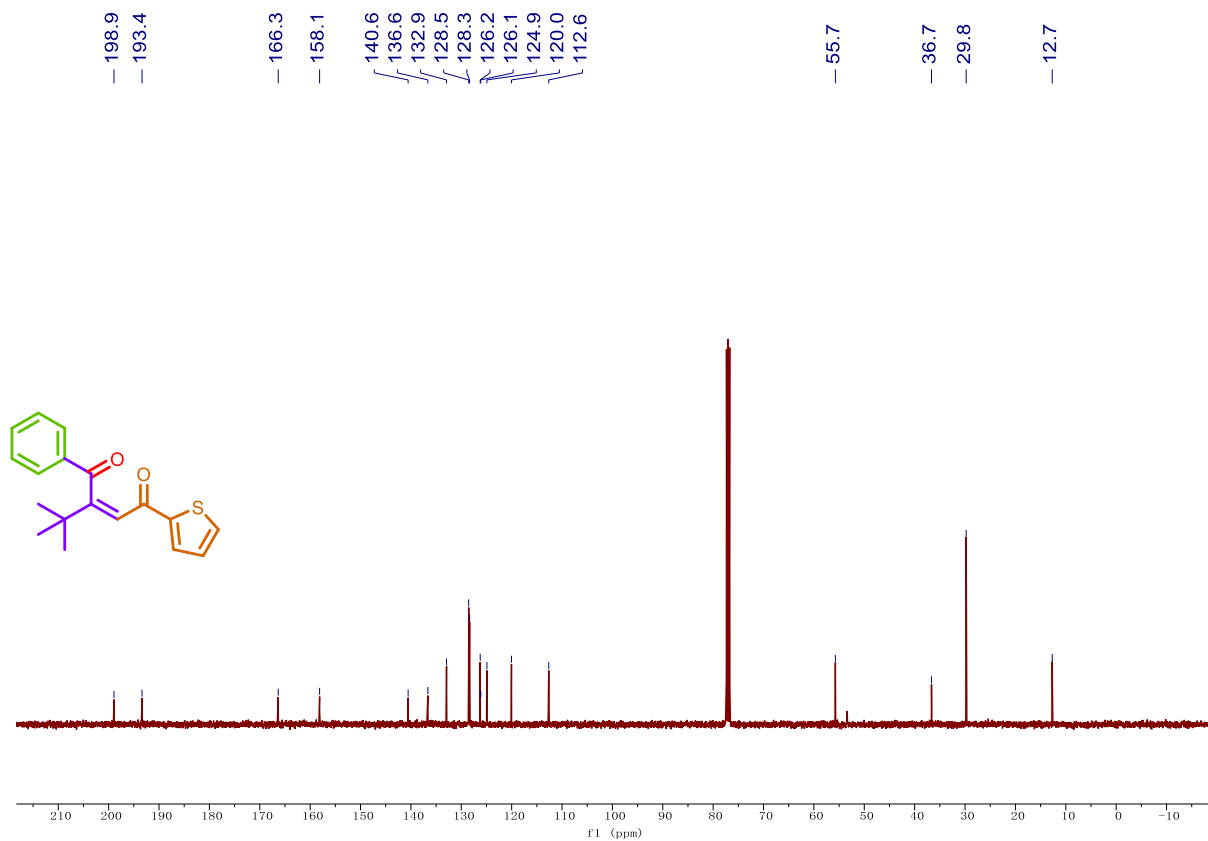
**Compound 3ae:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )**



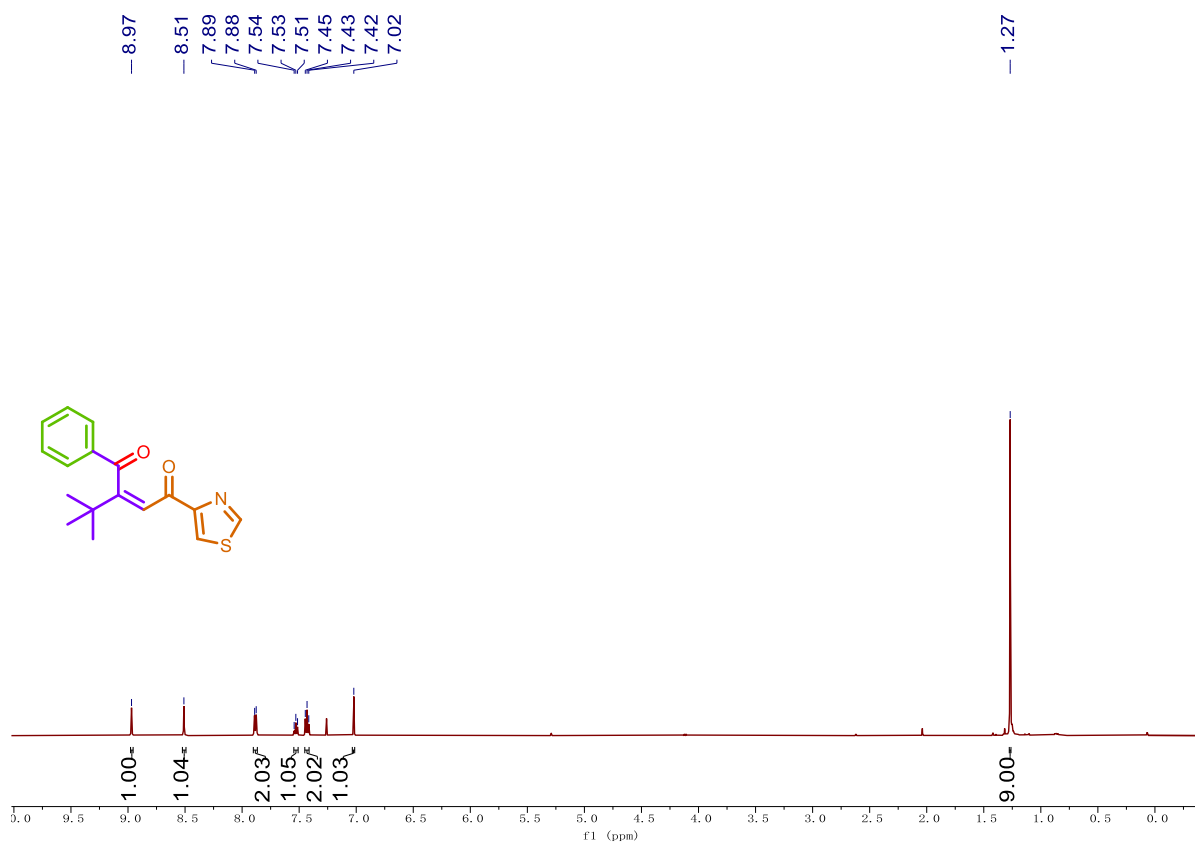
**Compound 3af:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )**



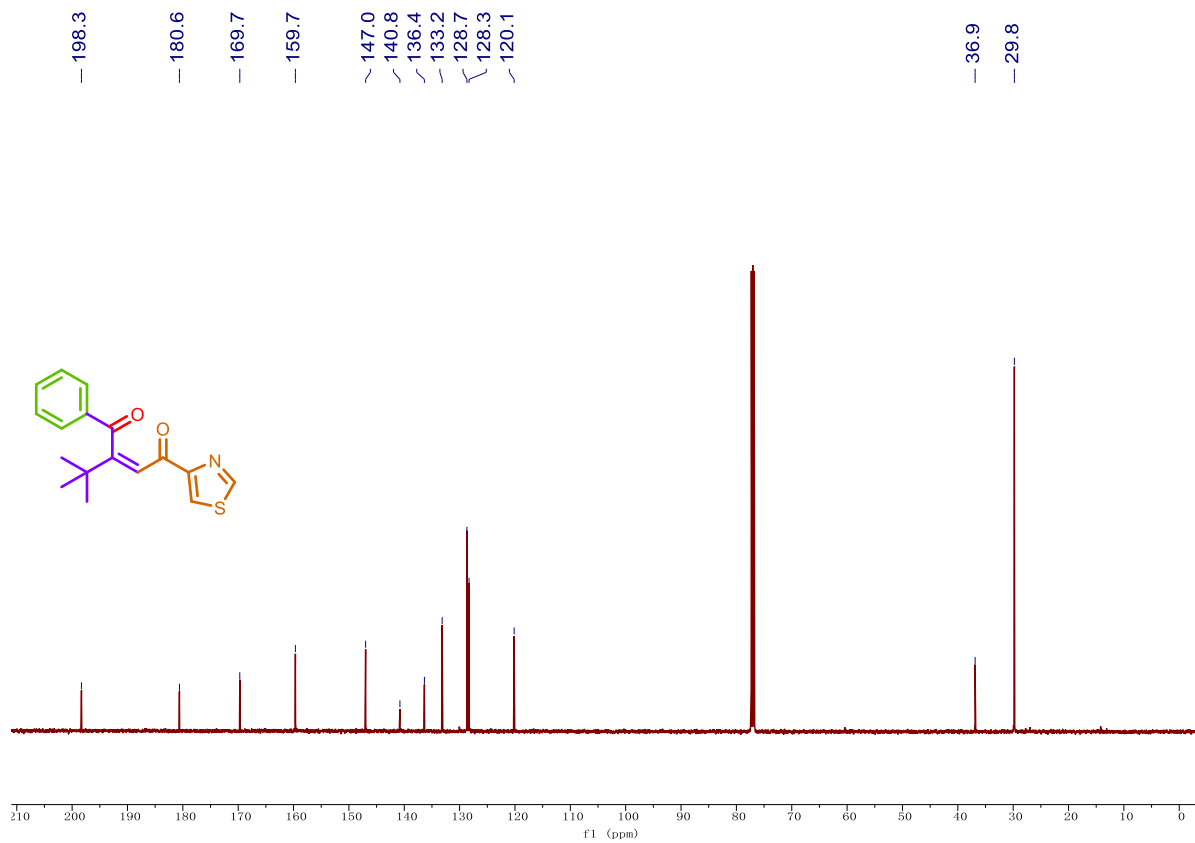
**Compound 3af:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )**



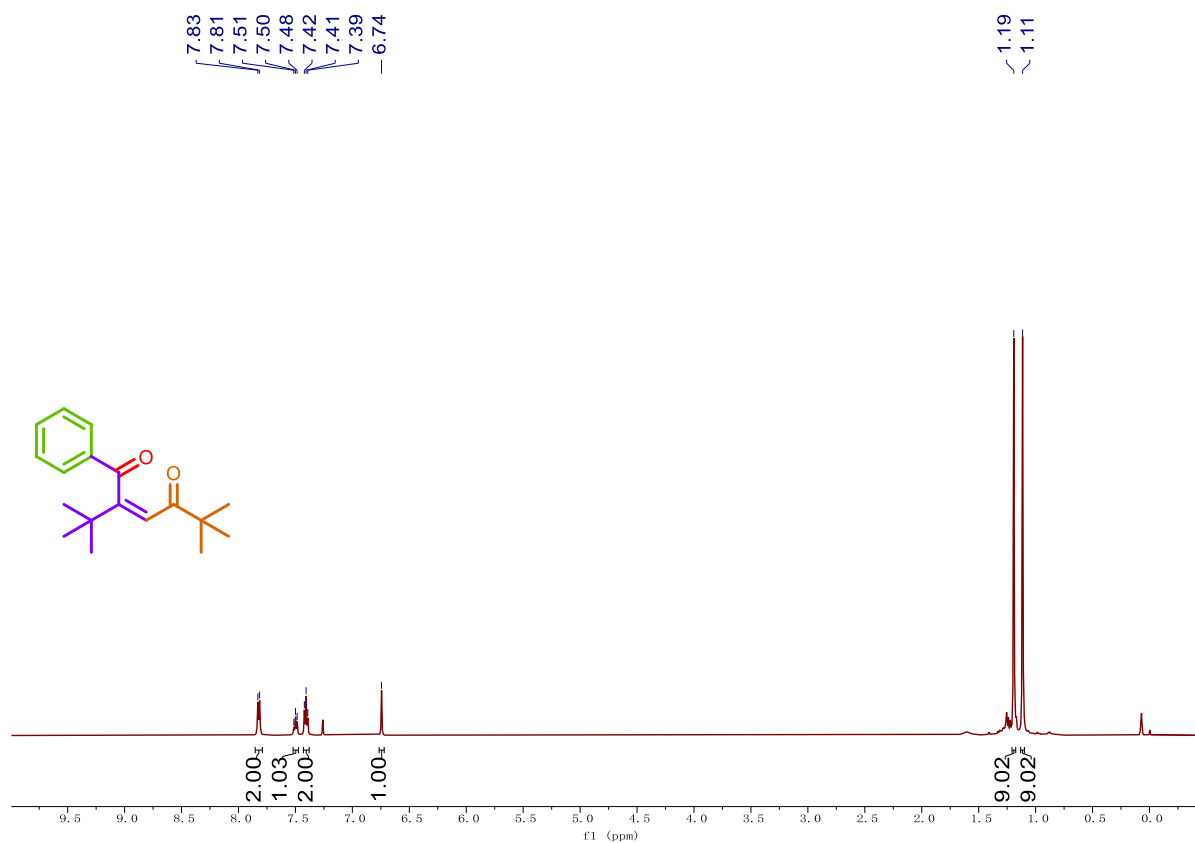
Compound 3ag:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )



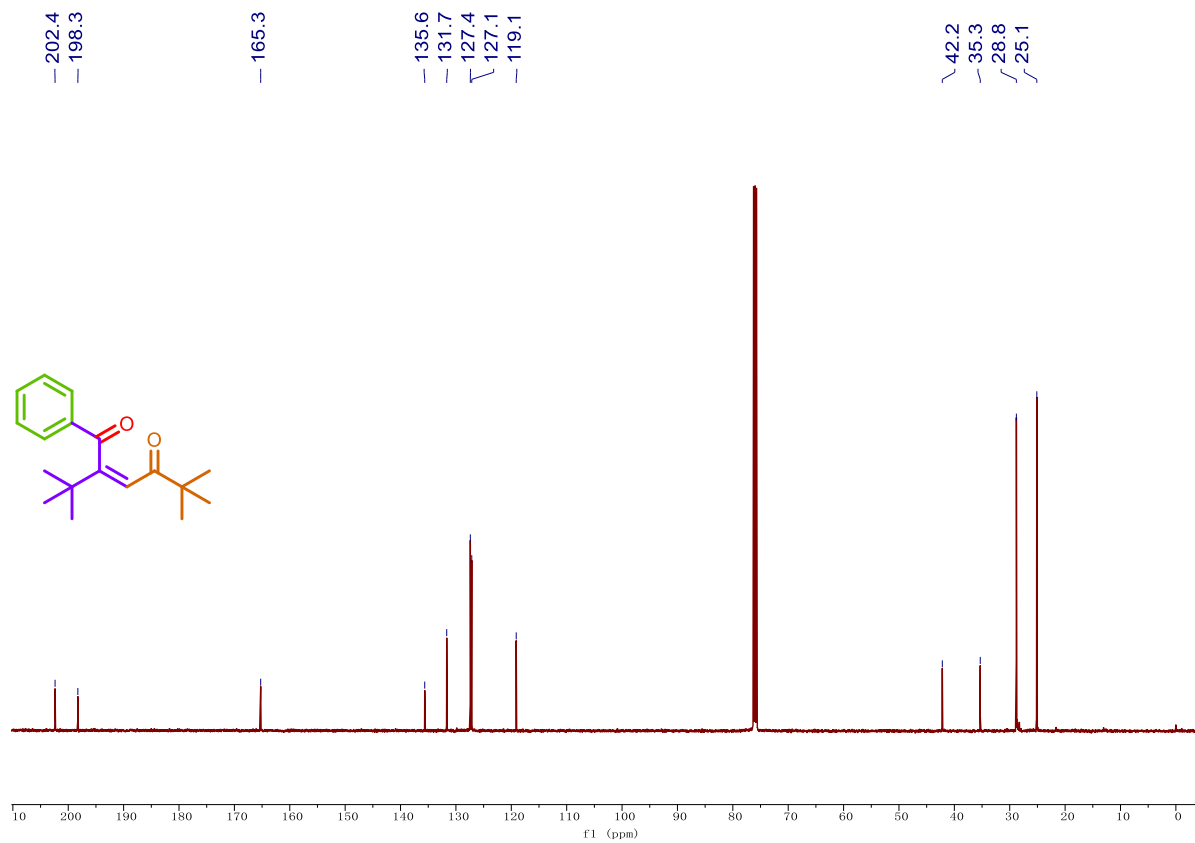
Compound 3ag:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )



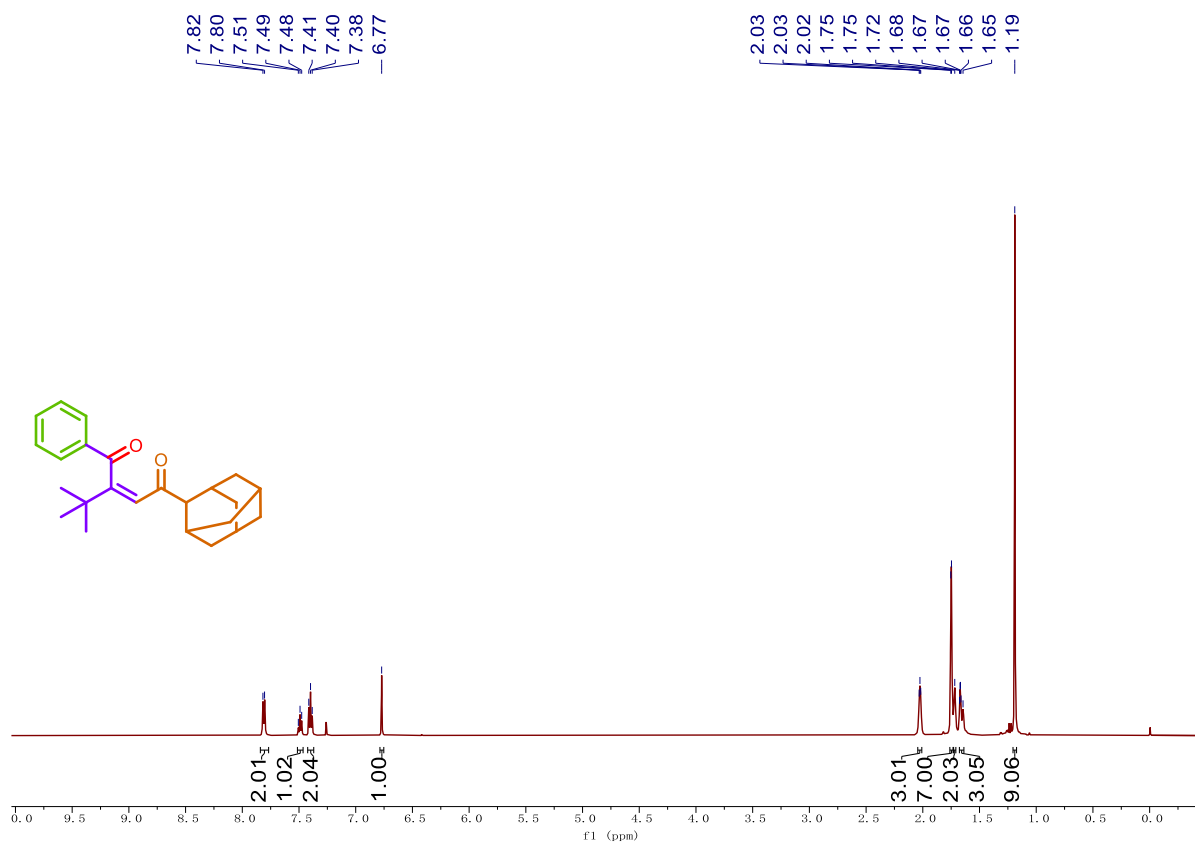
Compound 3ah:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )



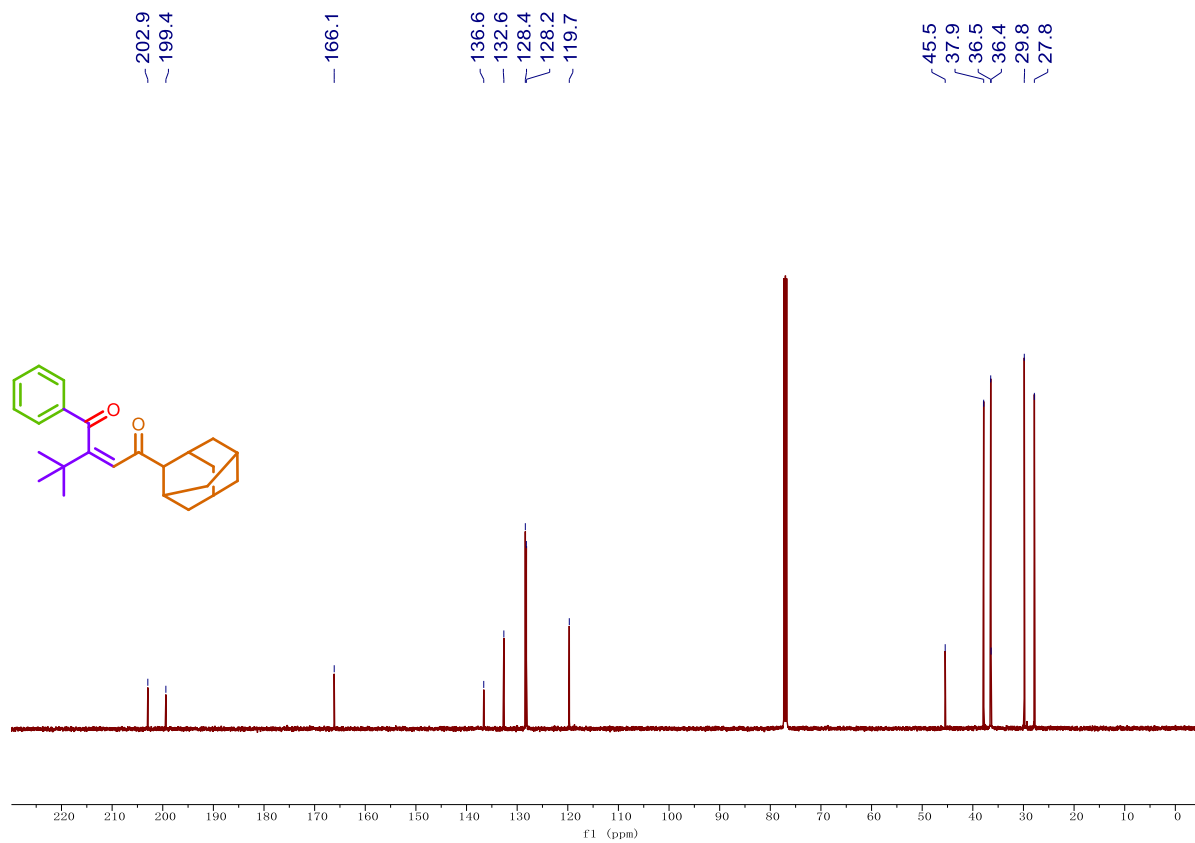
Compound 3ah:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )



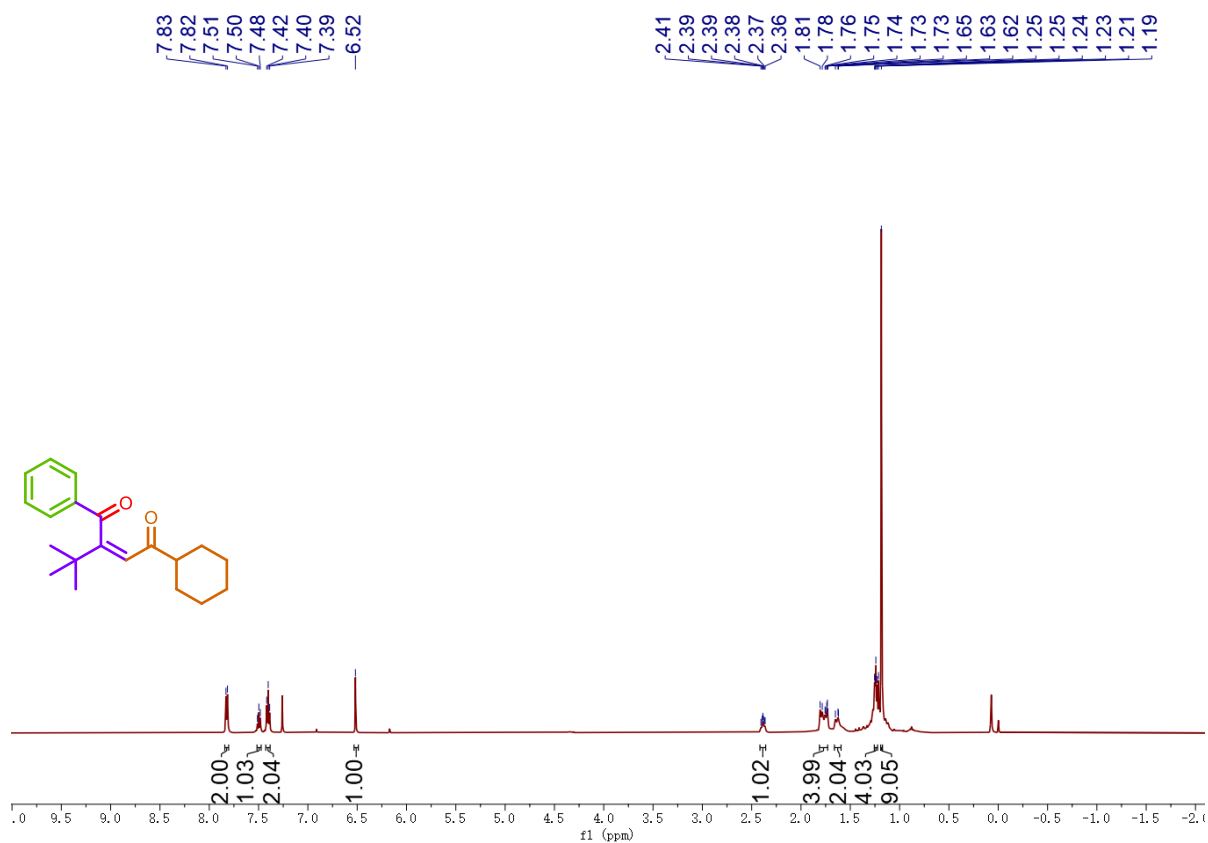
Compound 3ai:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )



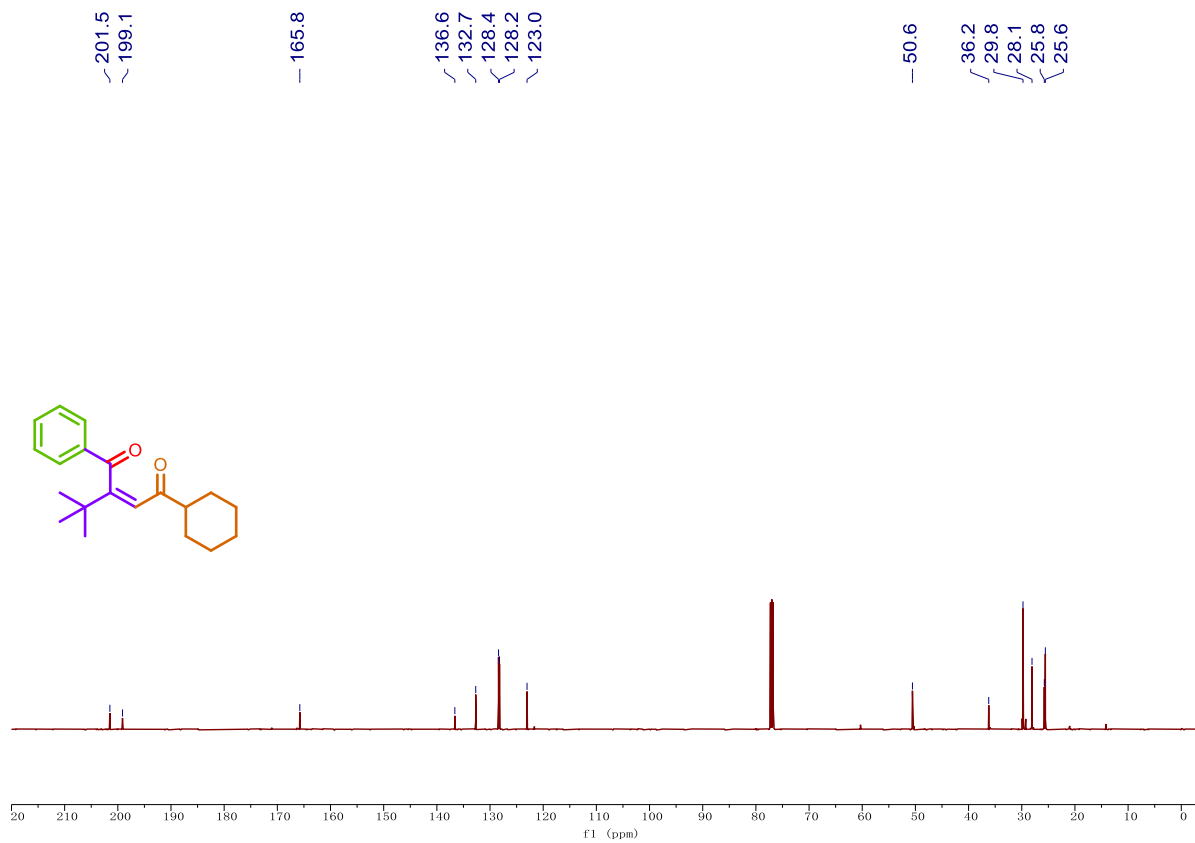
Compound 3ai:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )



**Compound 3aj:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )**

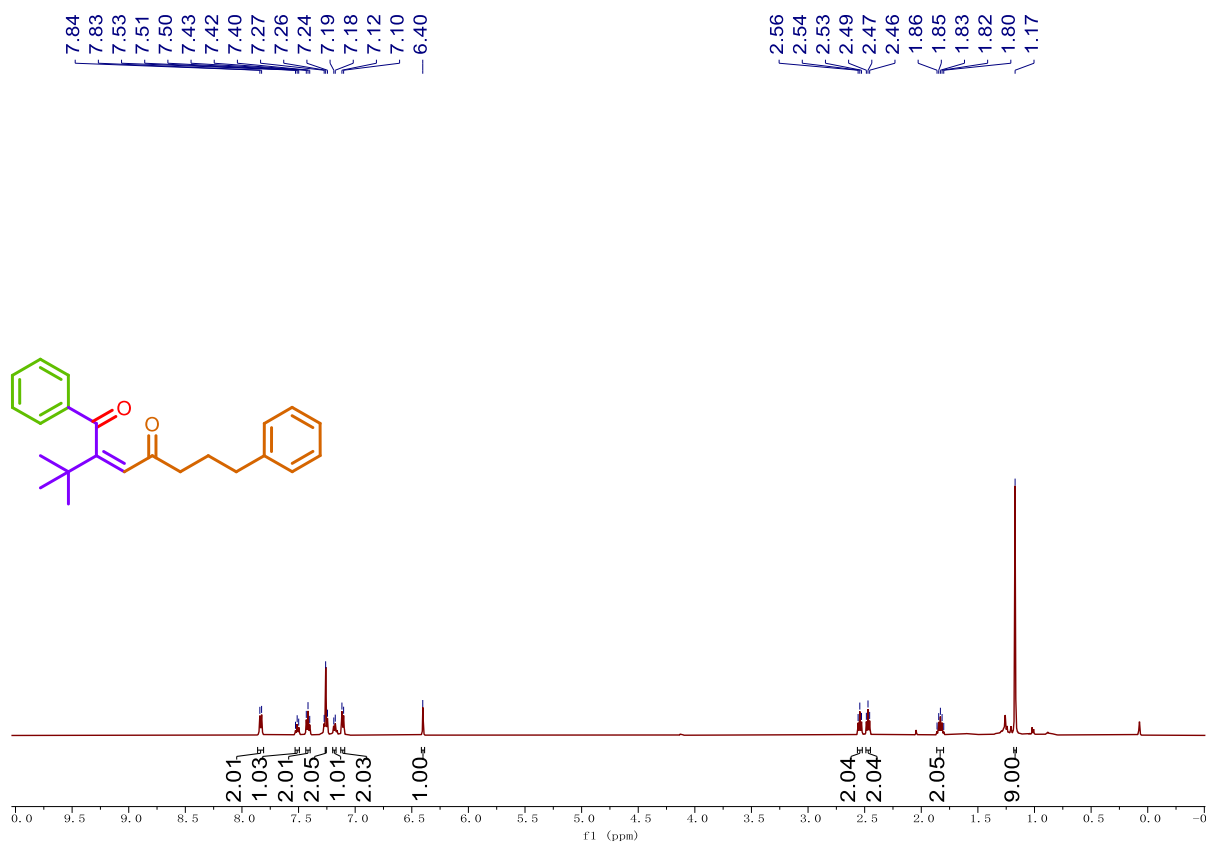


**Compound 3aj:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )**

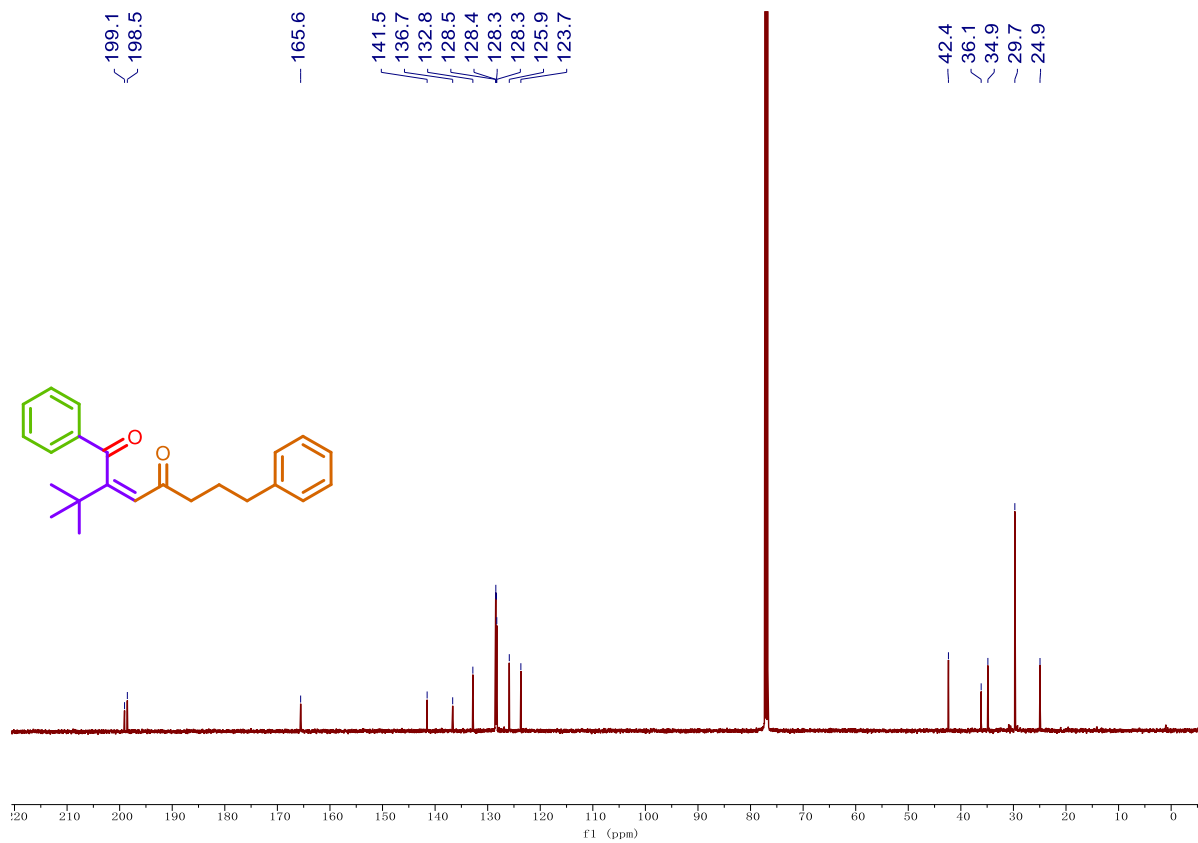




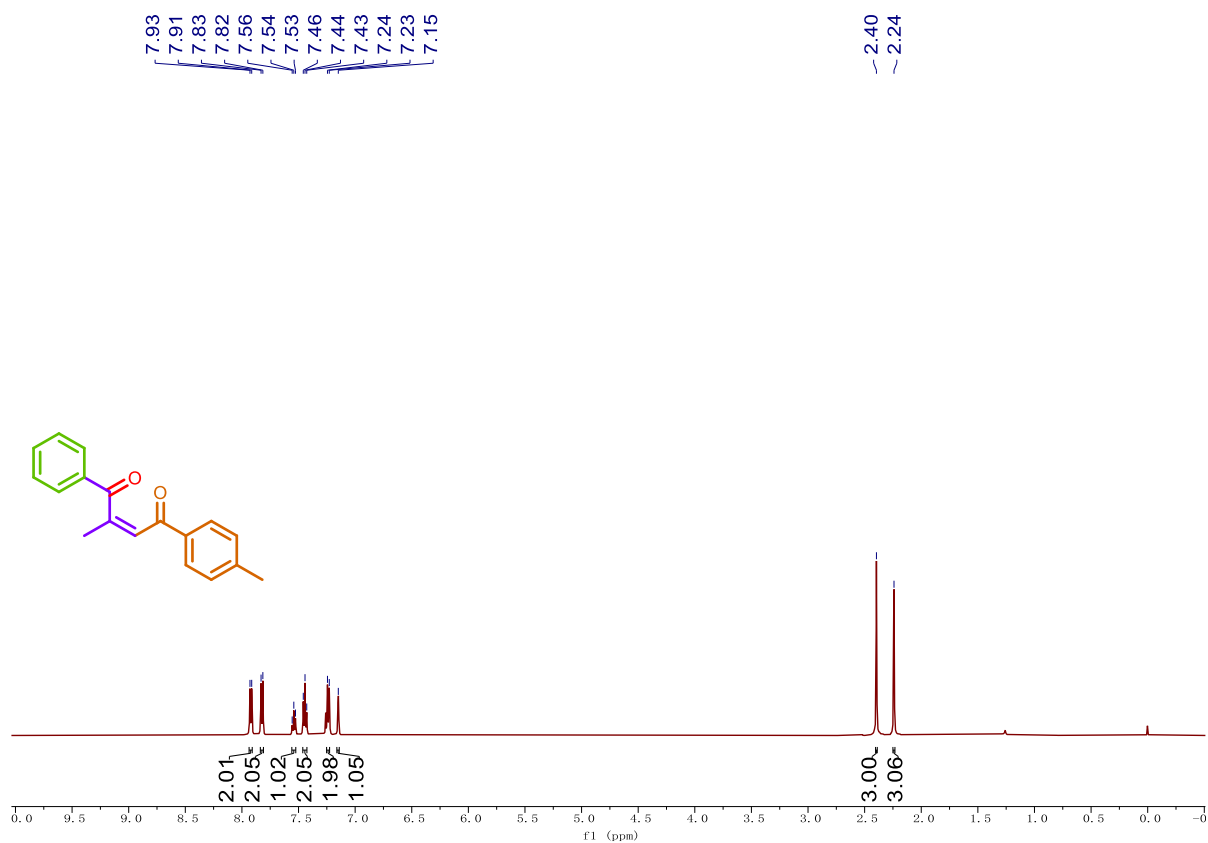
Compound 3ak:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )



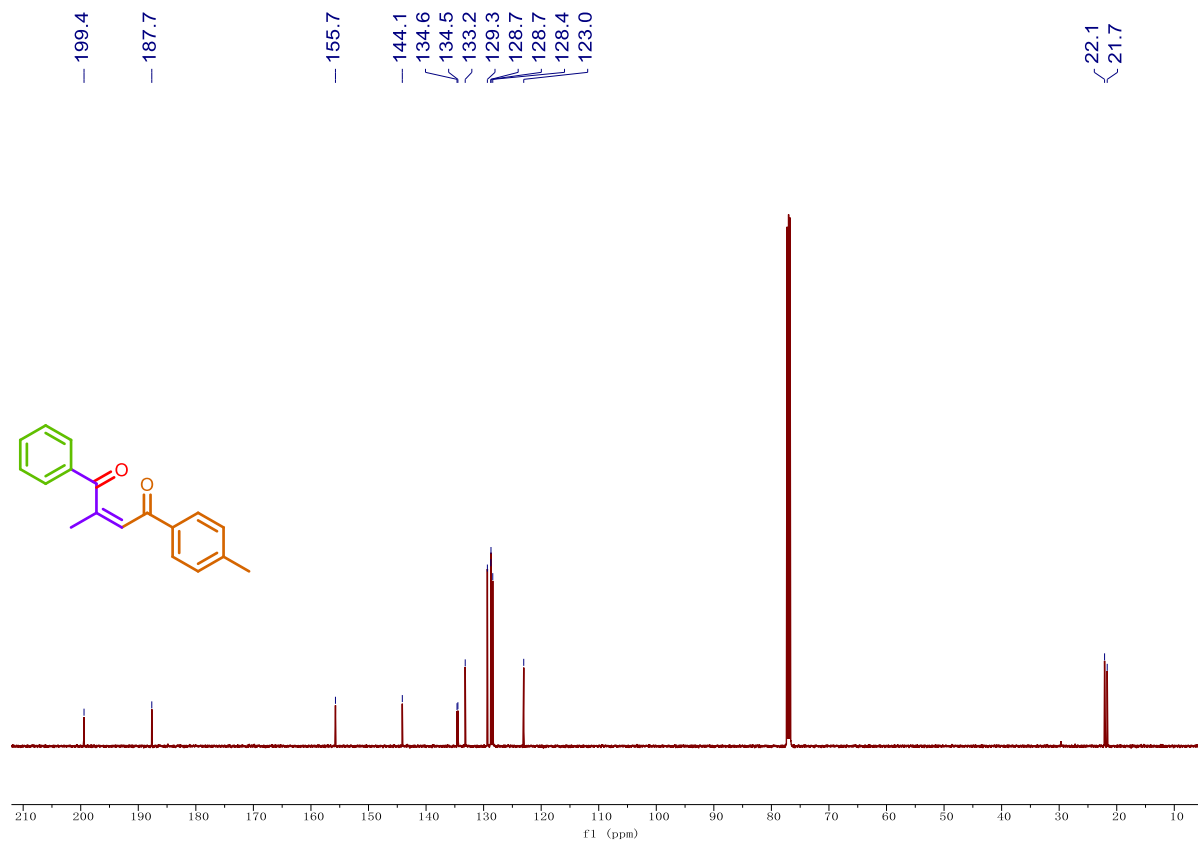
Compound 3ak:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )



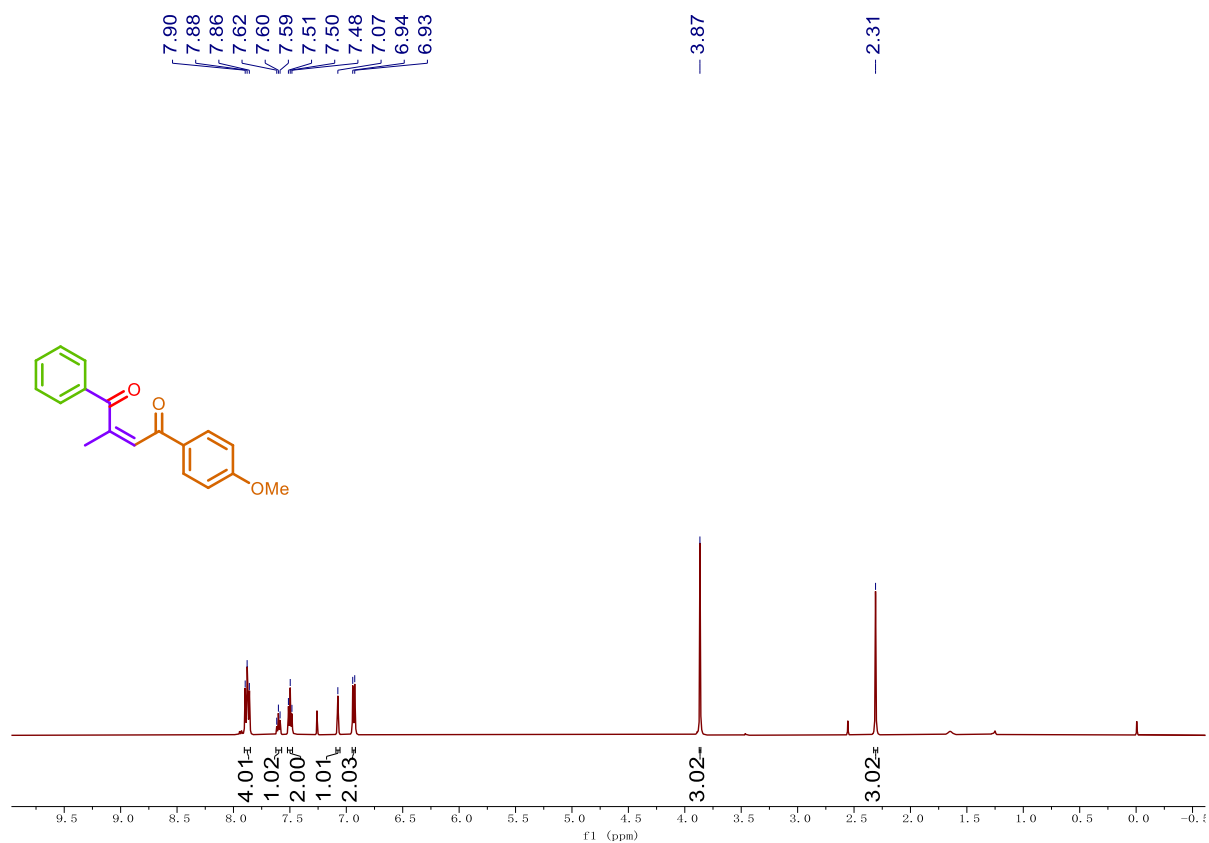
Compound 3al:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )



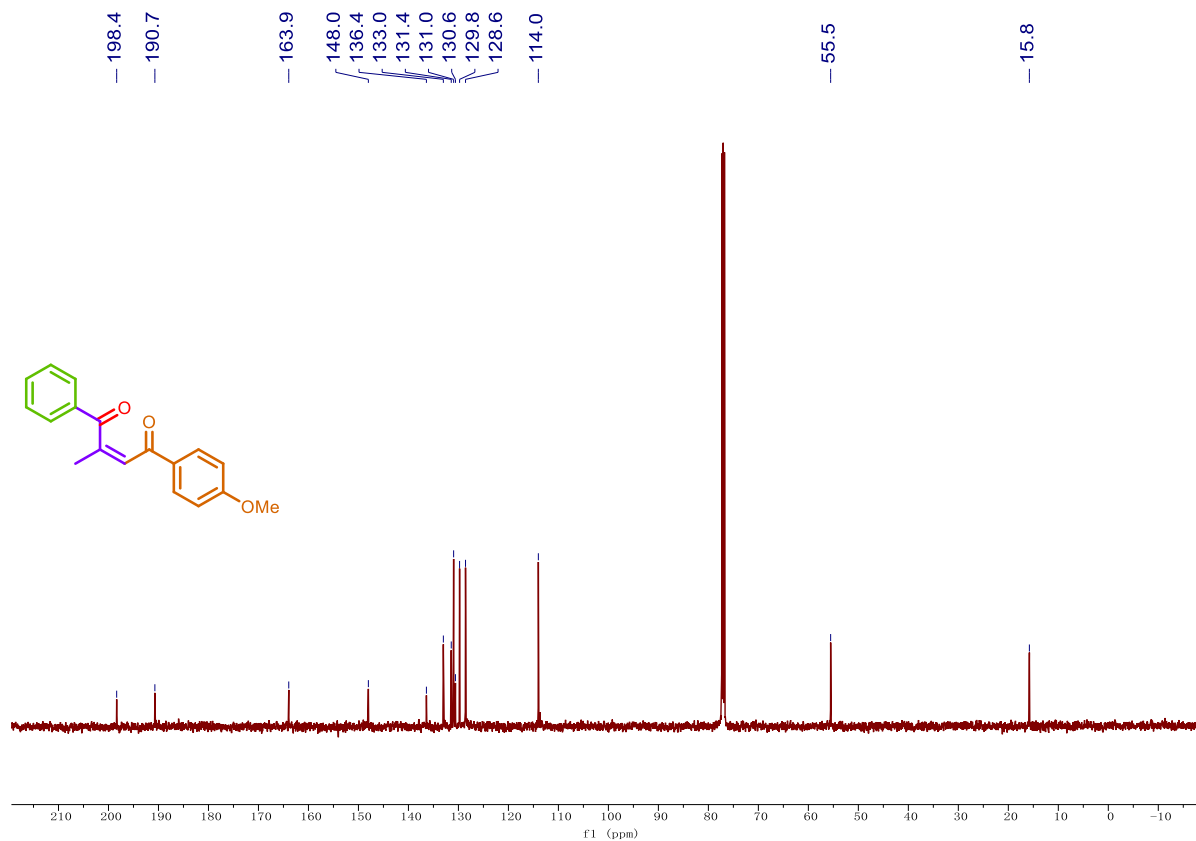
Compound 3al:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )



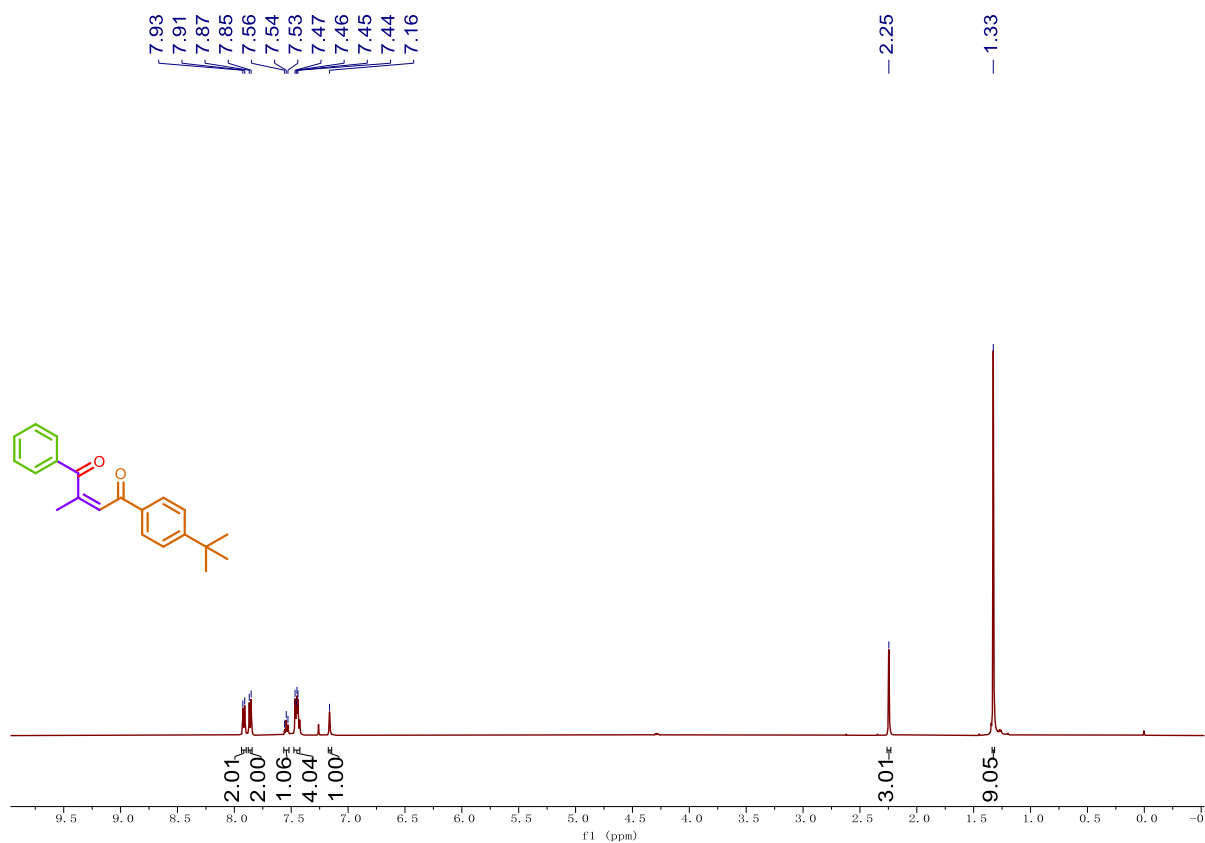
Compound 3am:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )



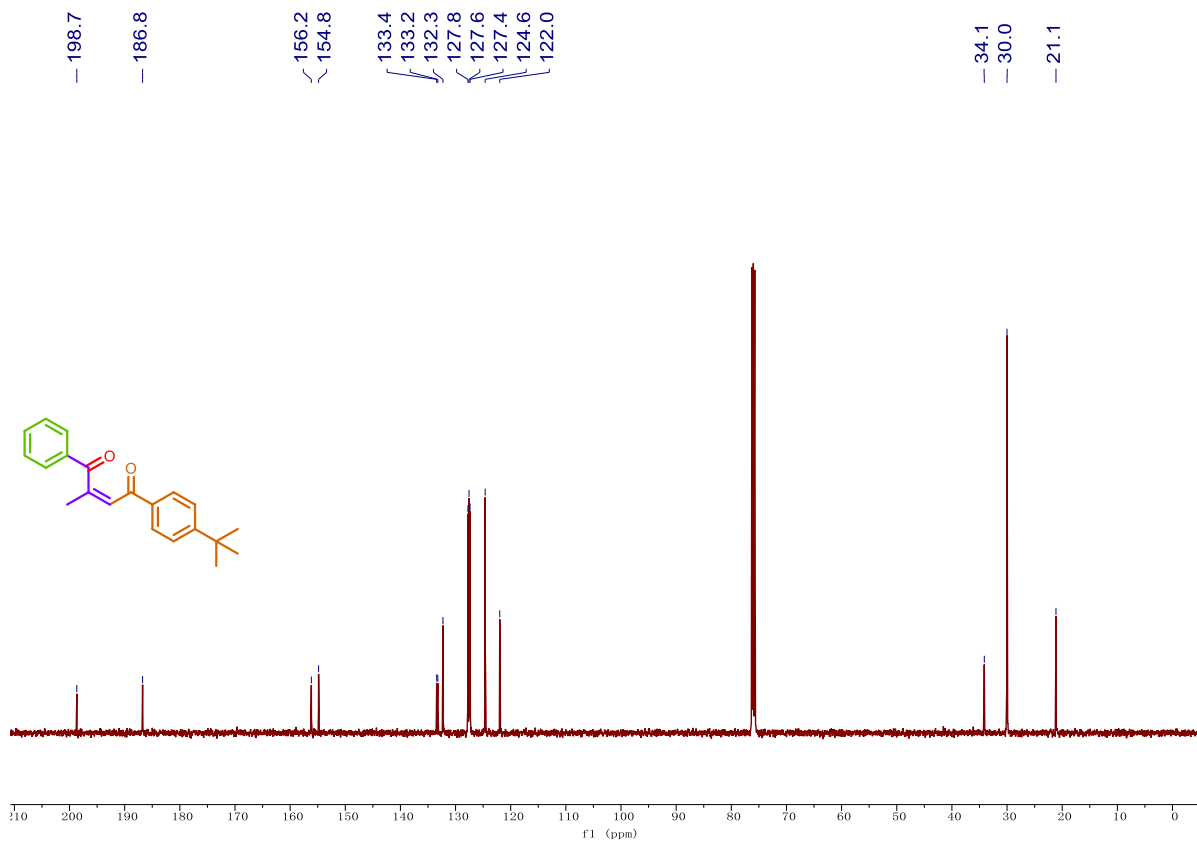
Compound 3am:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )



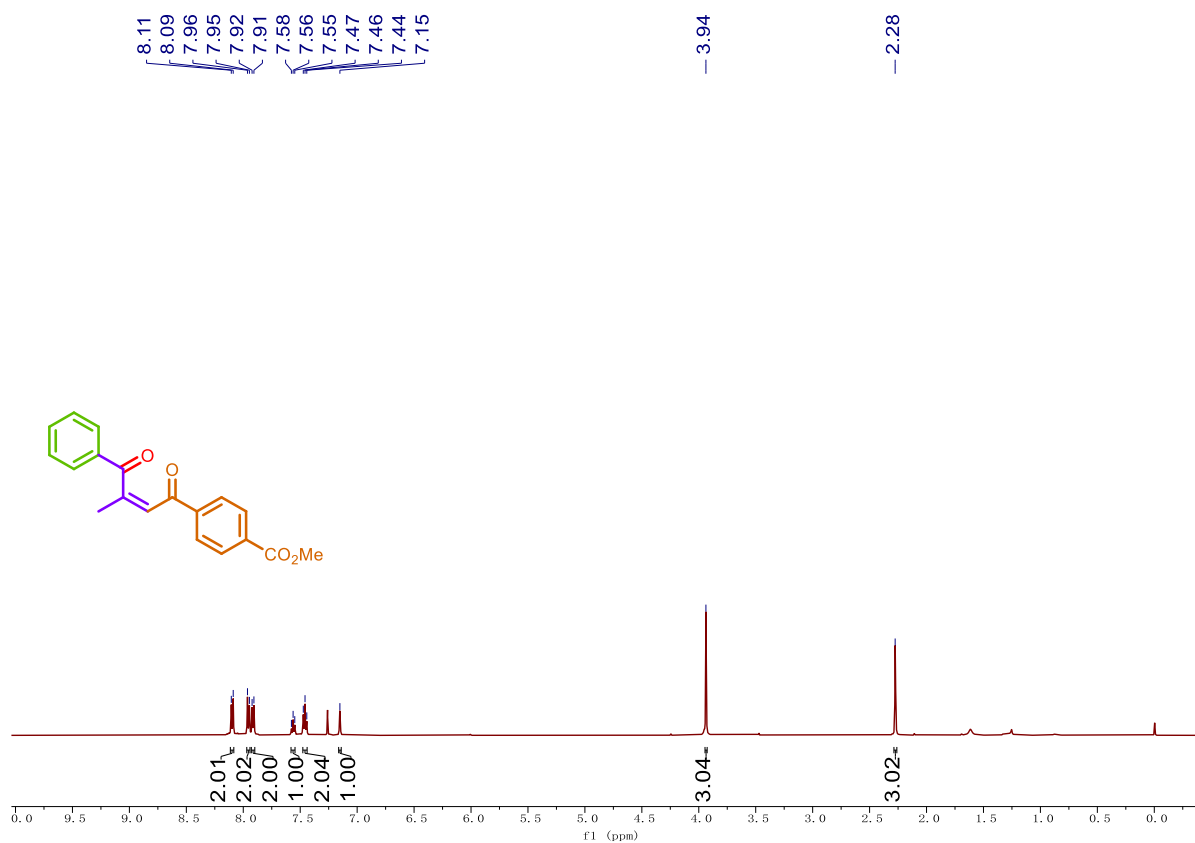
**Compound 3an:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )**



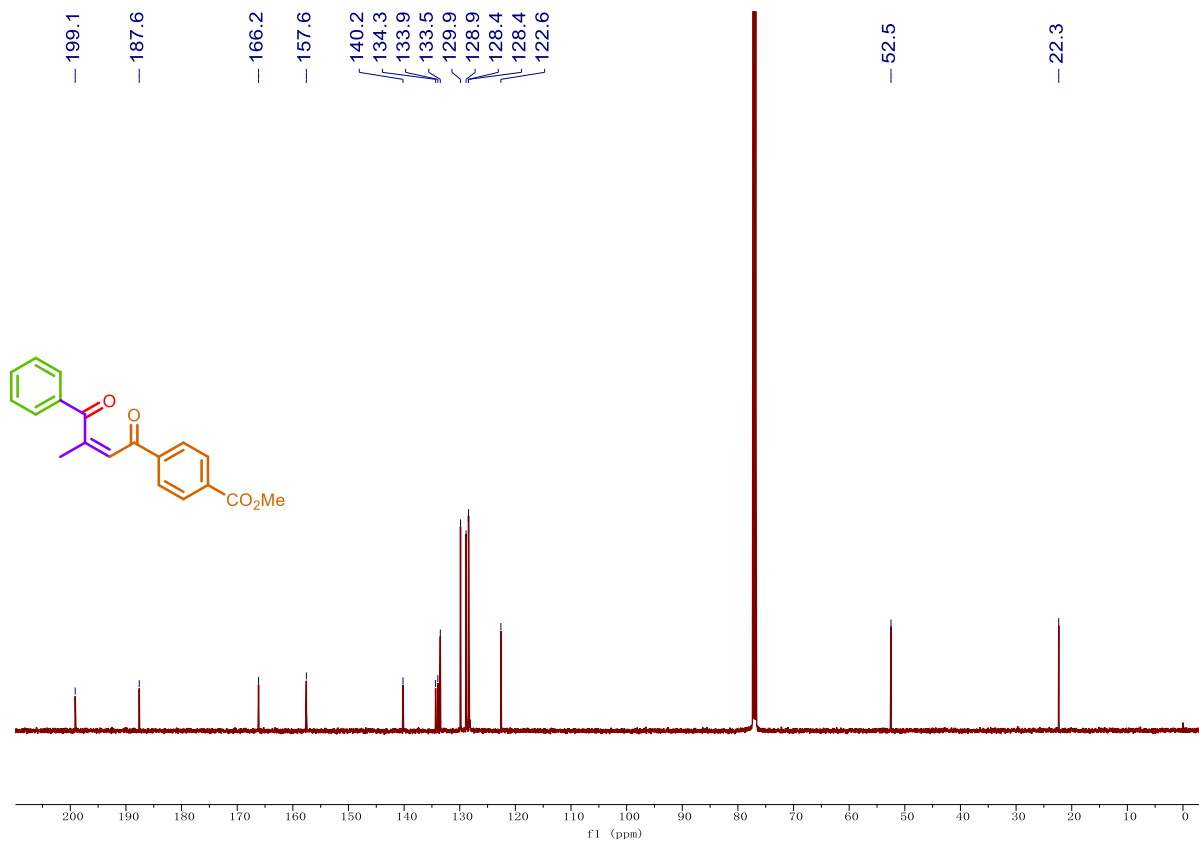
**Compound 3an:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )**



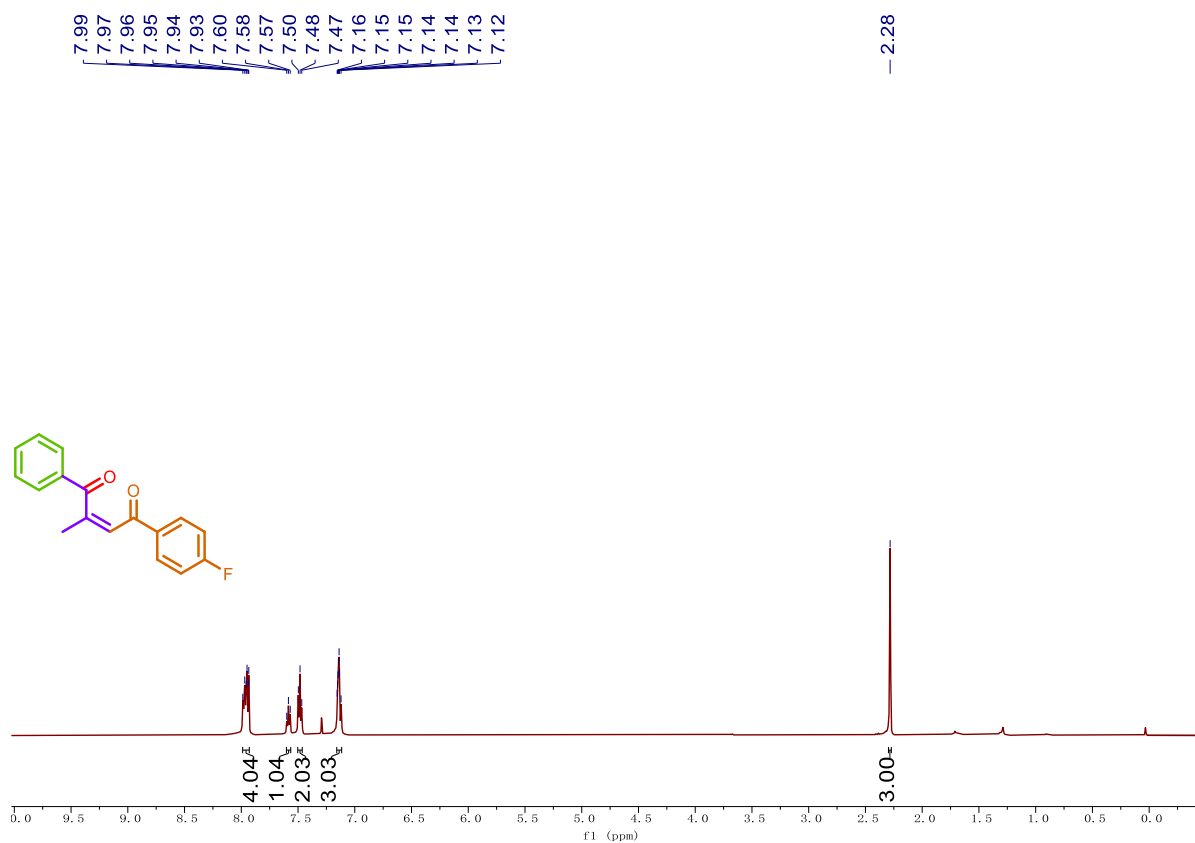
**Compound 3ao:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )**



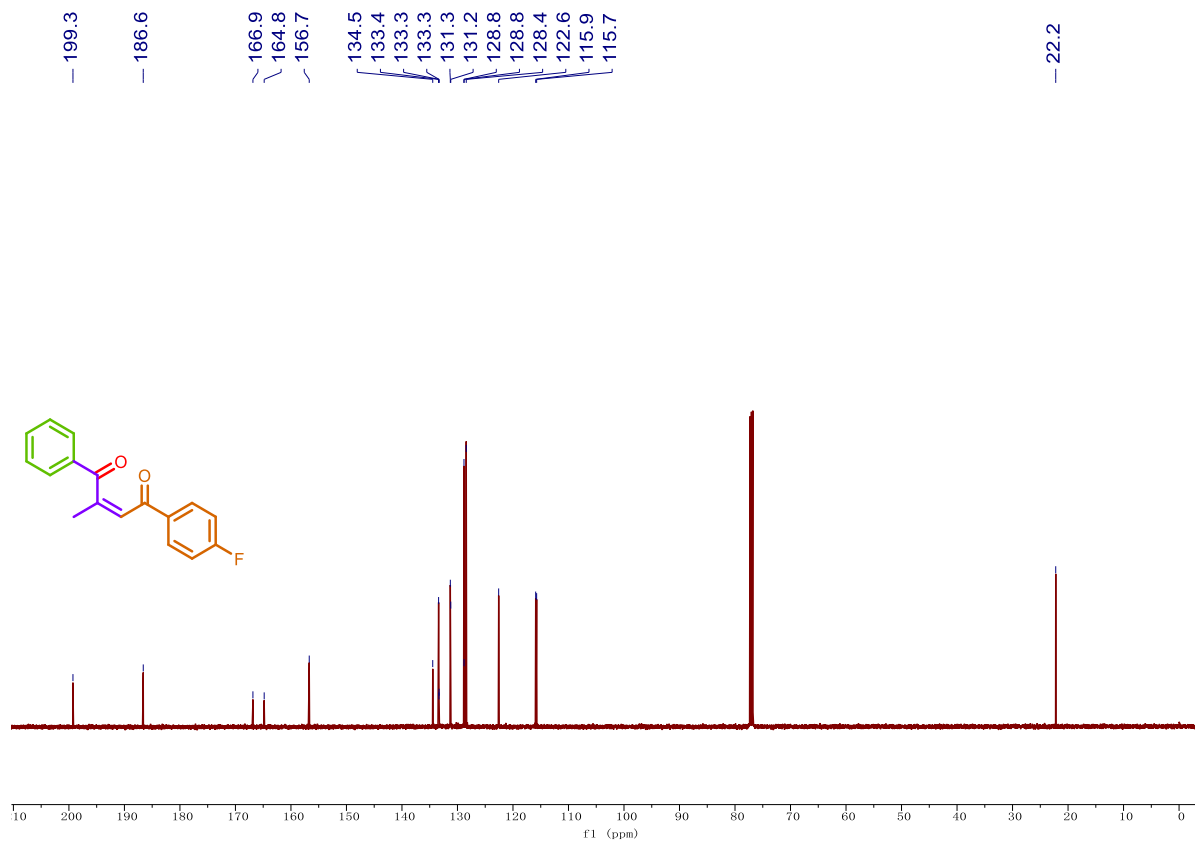
**Compound 3ao:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )**



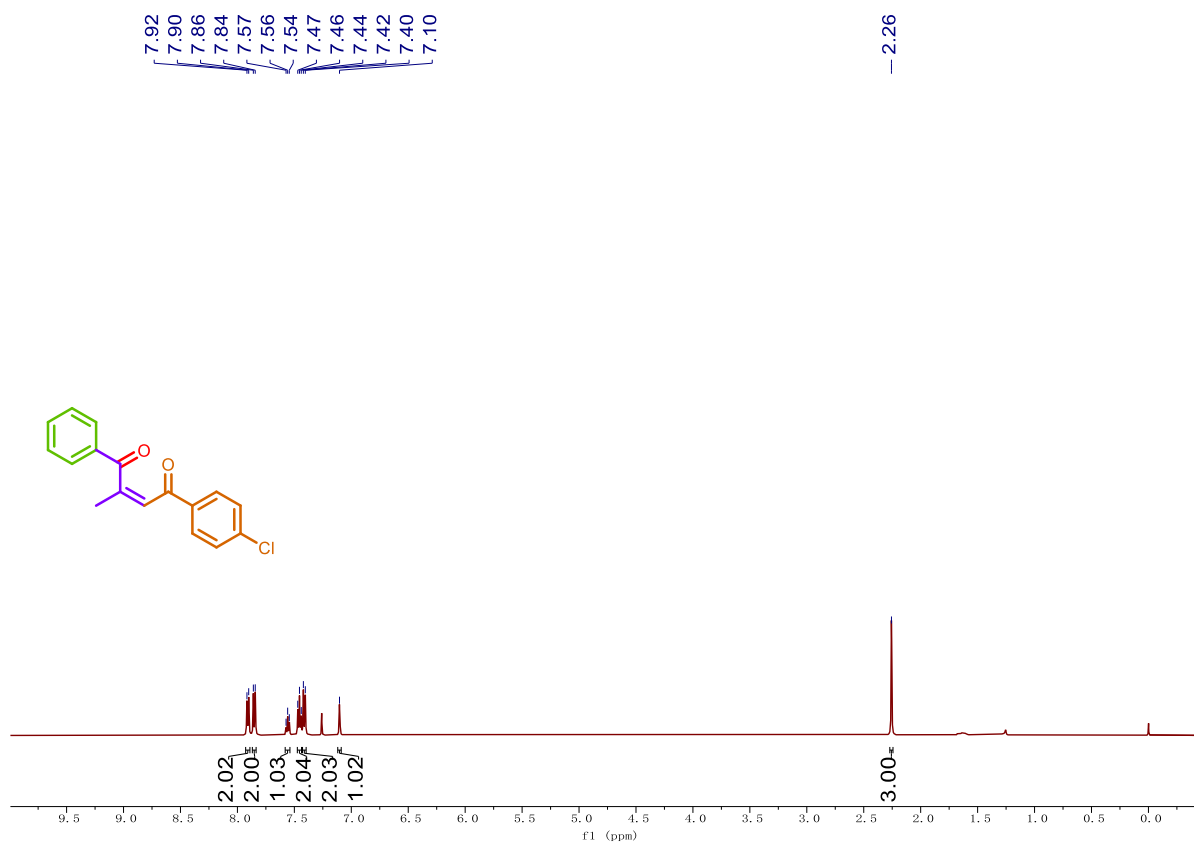
**Compound 3ap:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )**



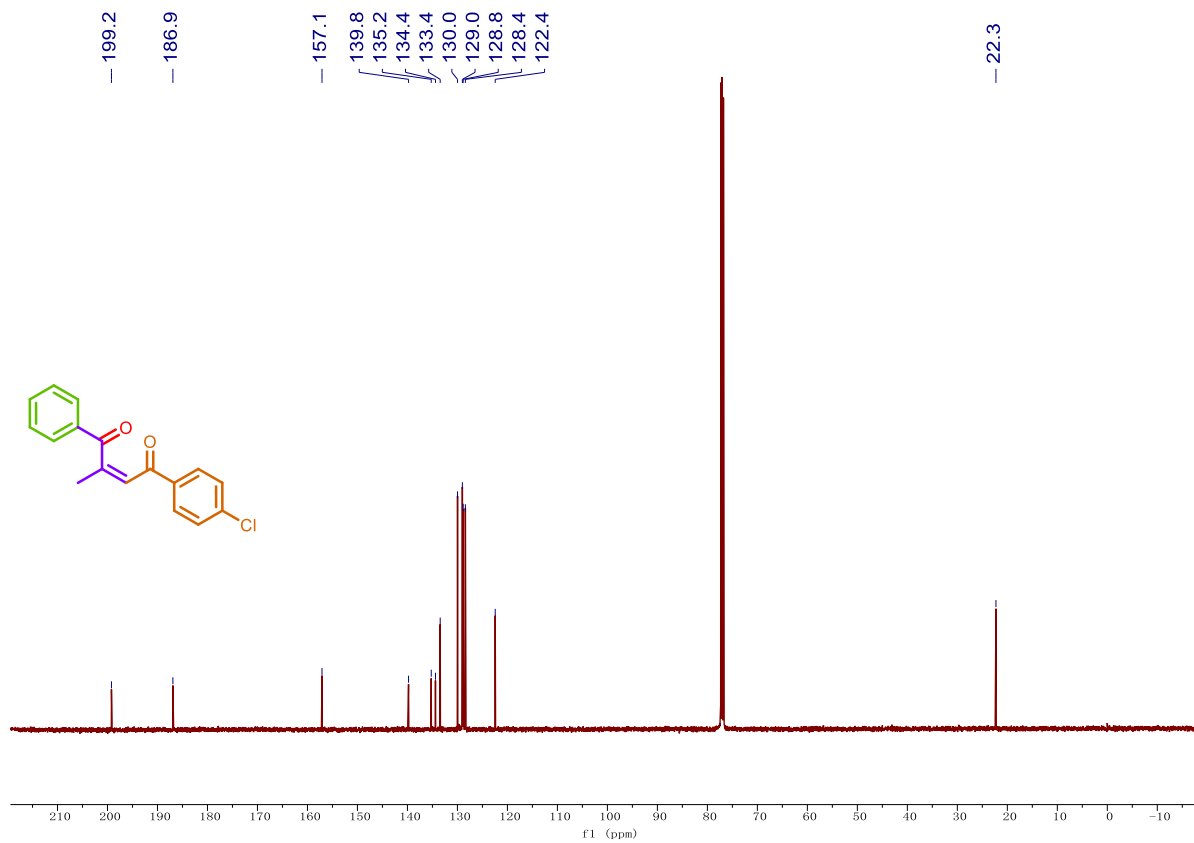
**Compound 3ap:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )**



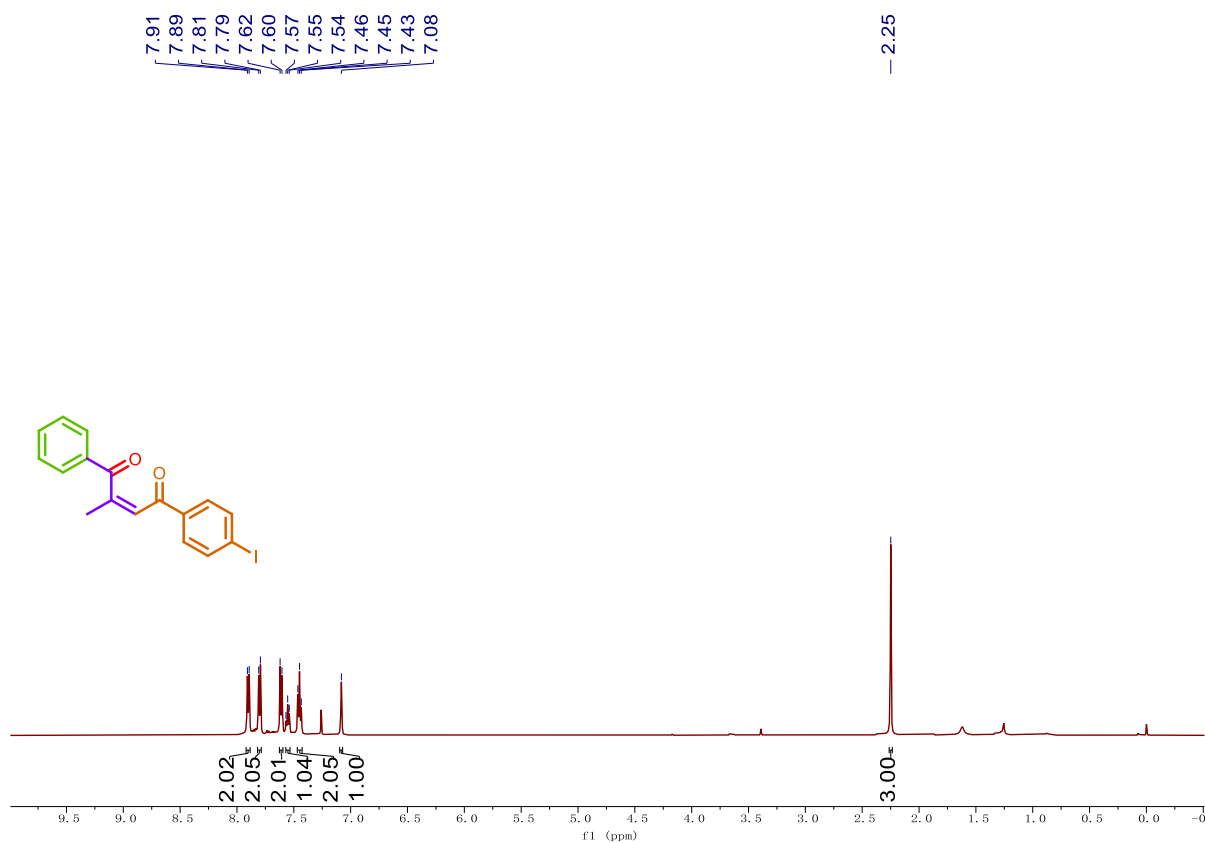
Compound 3aq:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )



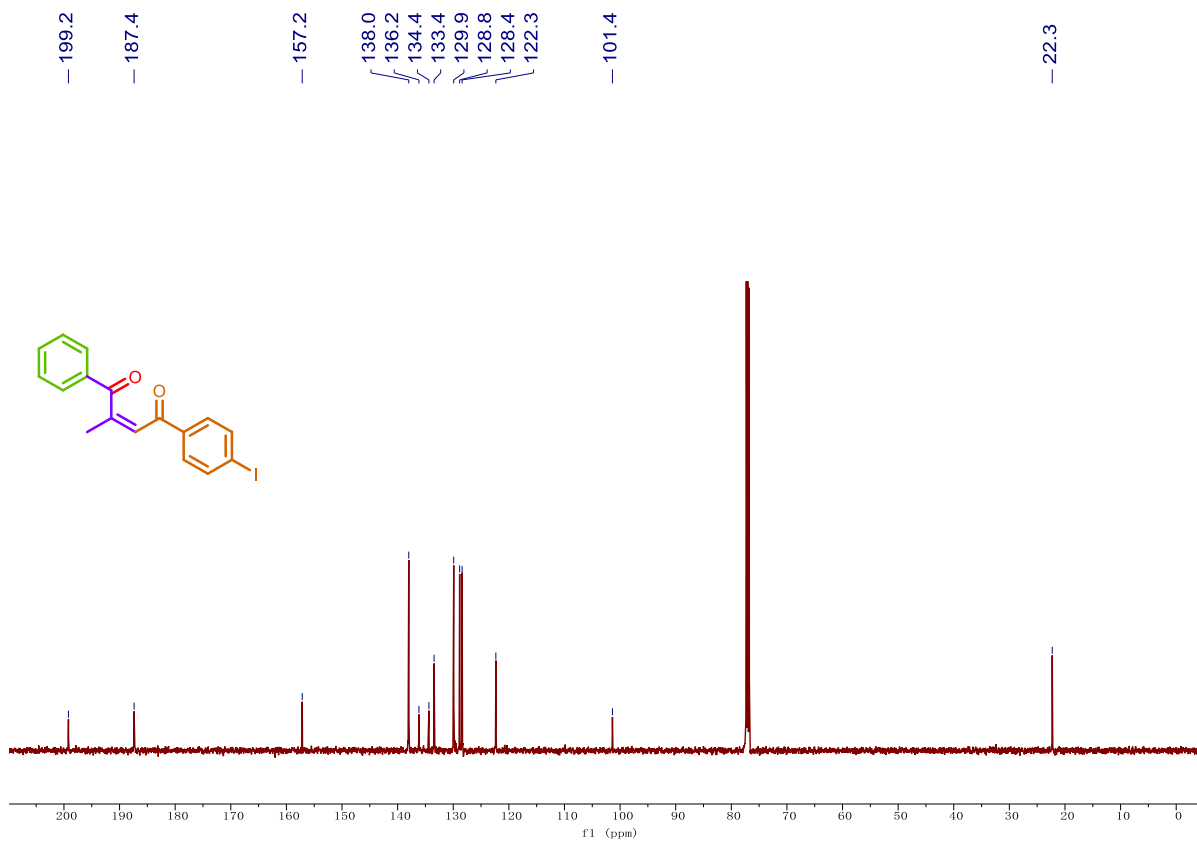
Compound 3aq:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )



Compound 3ar:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )

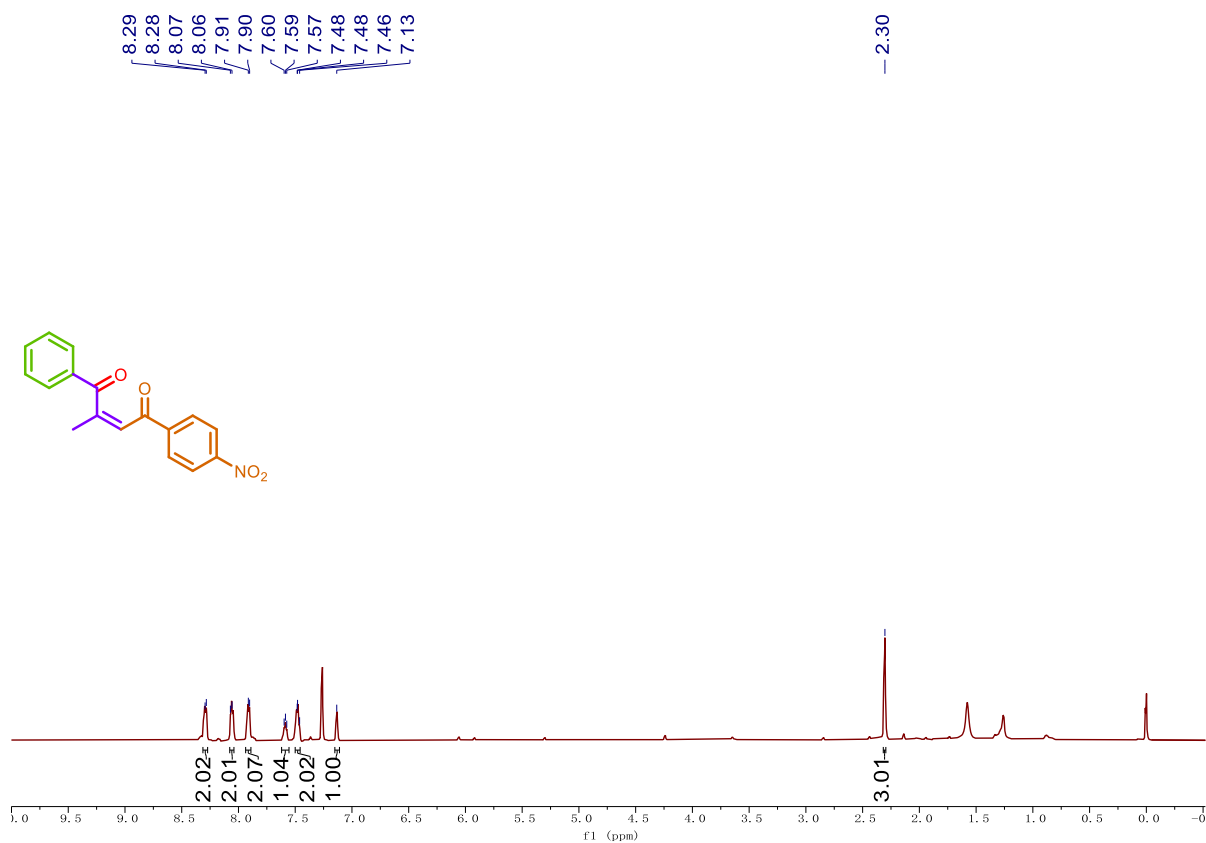


Compound 3ar:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )

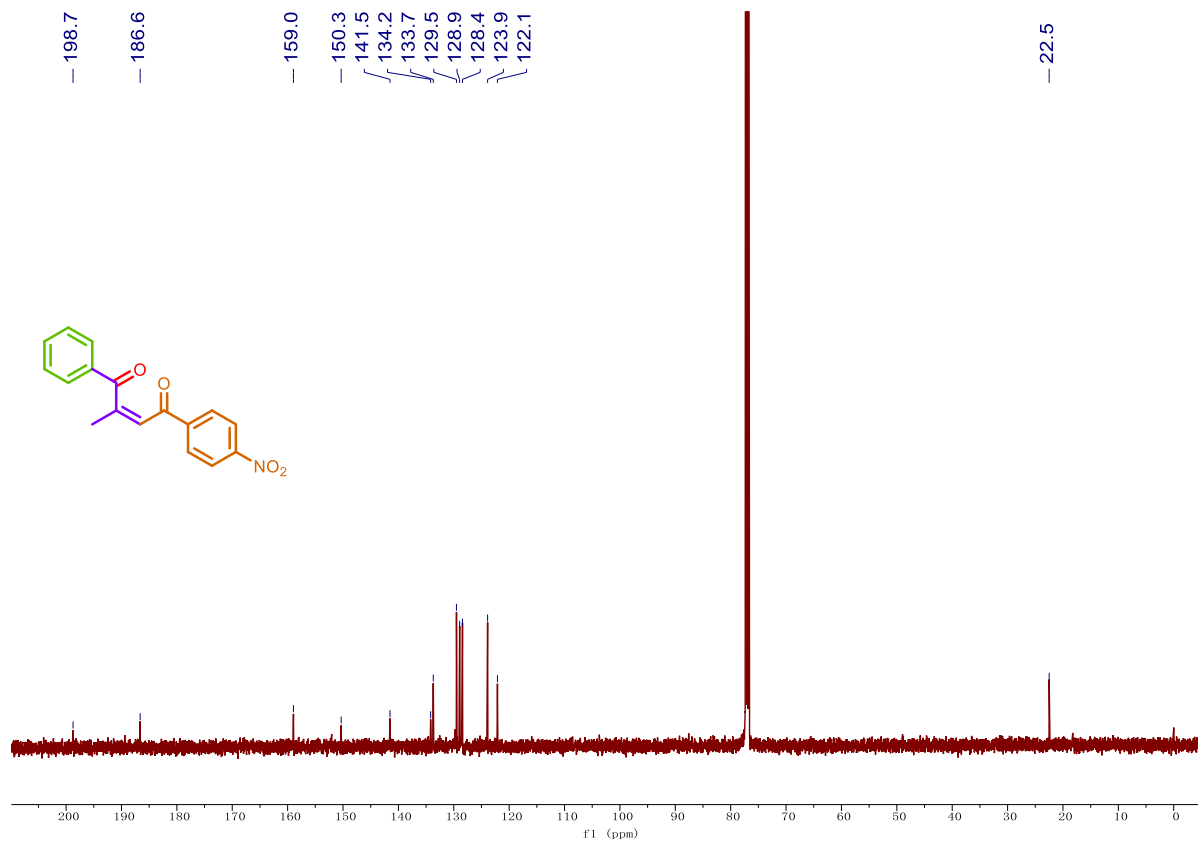




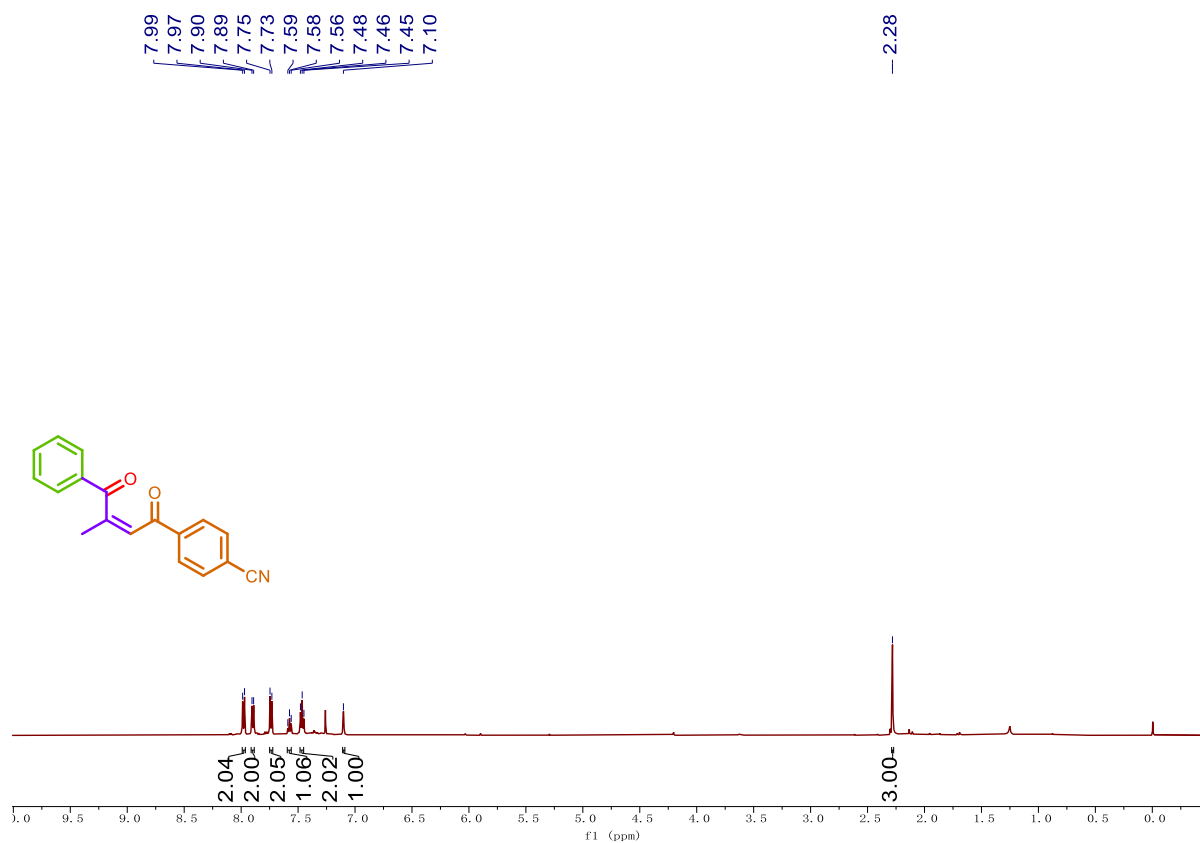
Compound 3as:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )



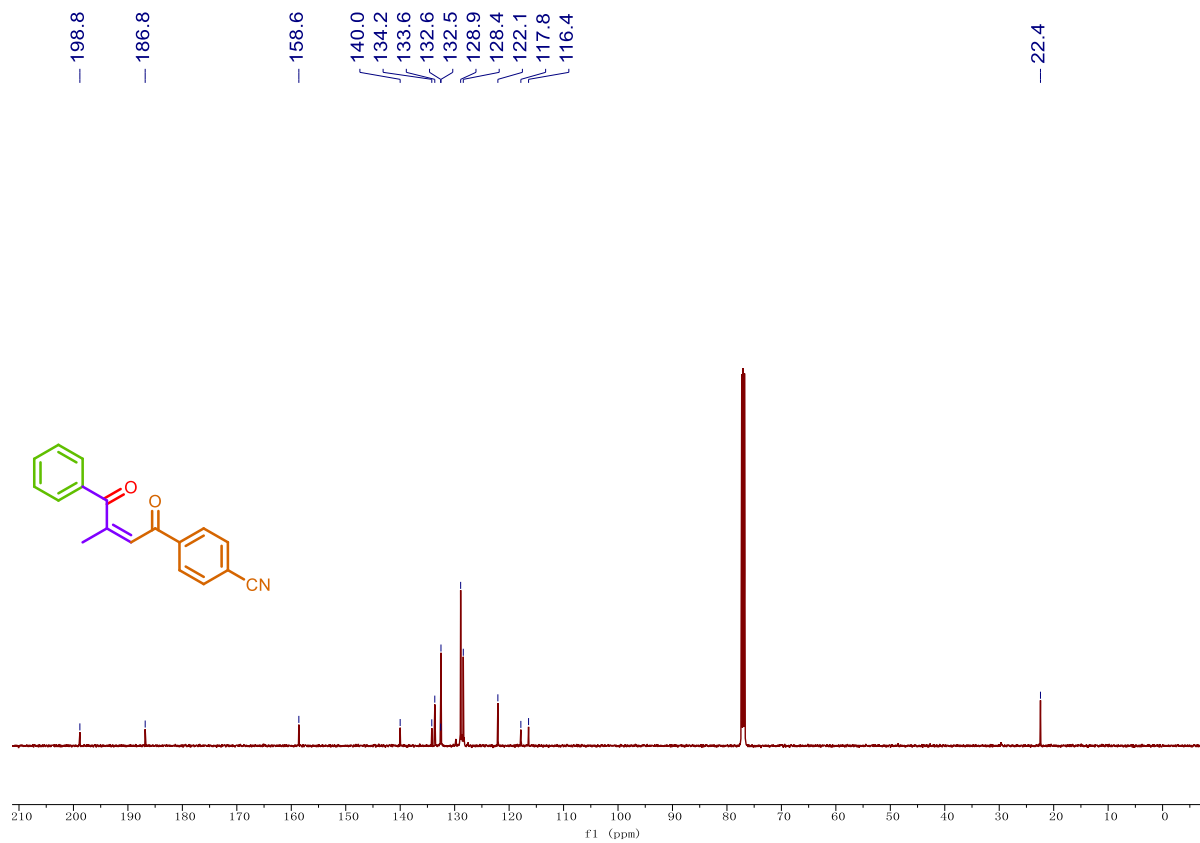
Compound 3as:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )



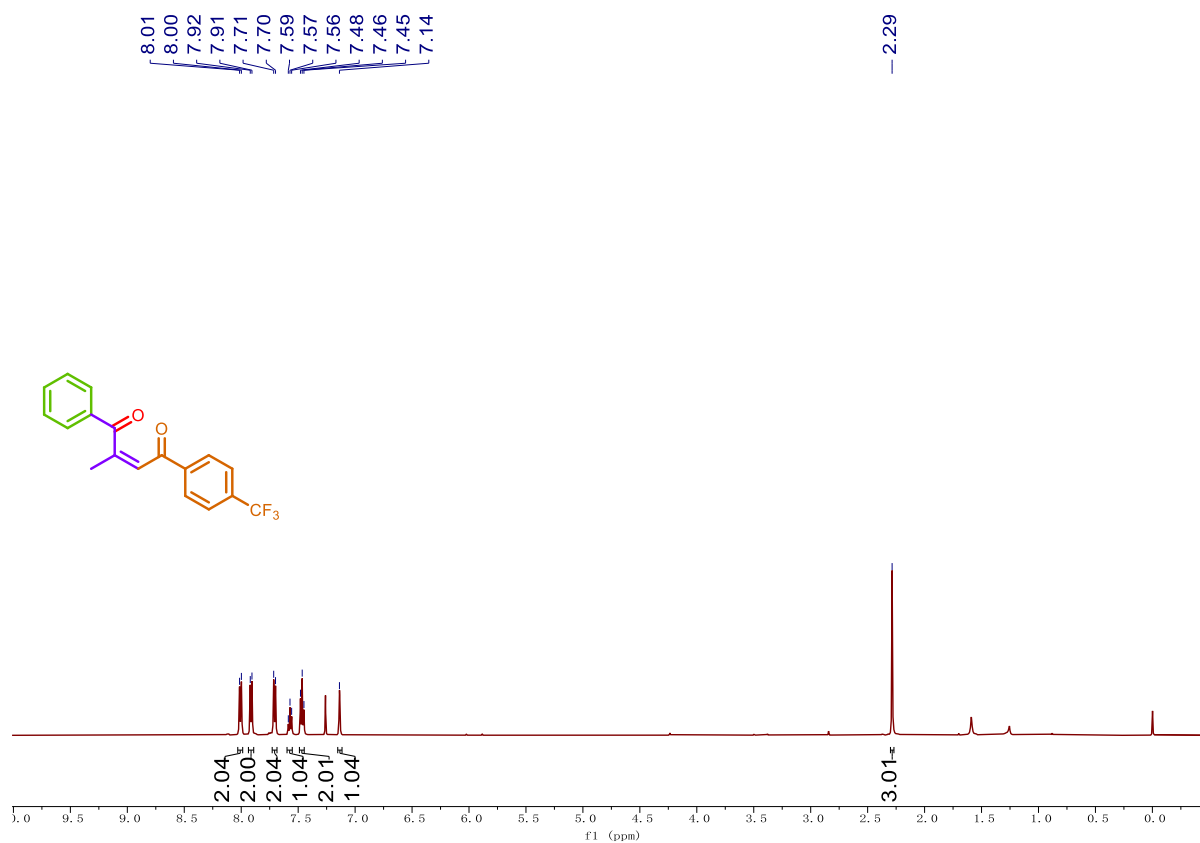
**Compound 3at:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )**



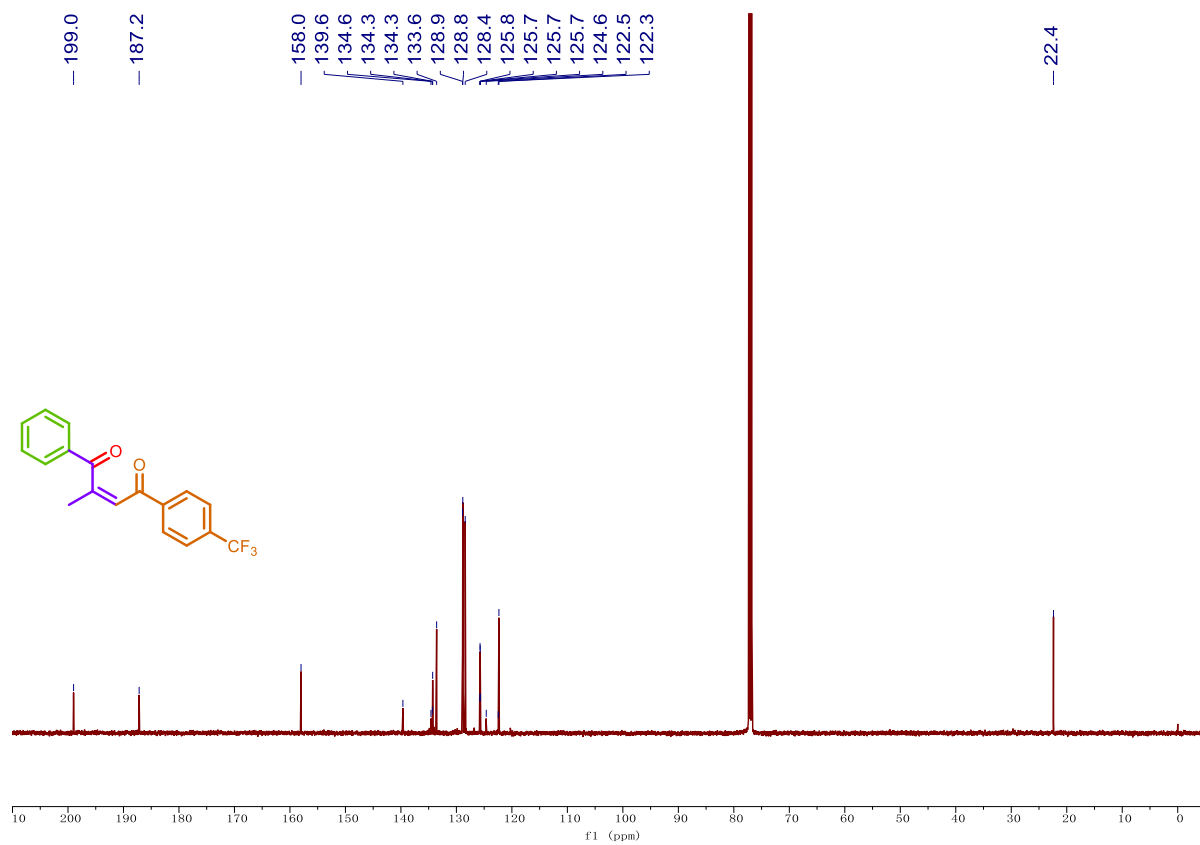
**Compound 3at:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )**



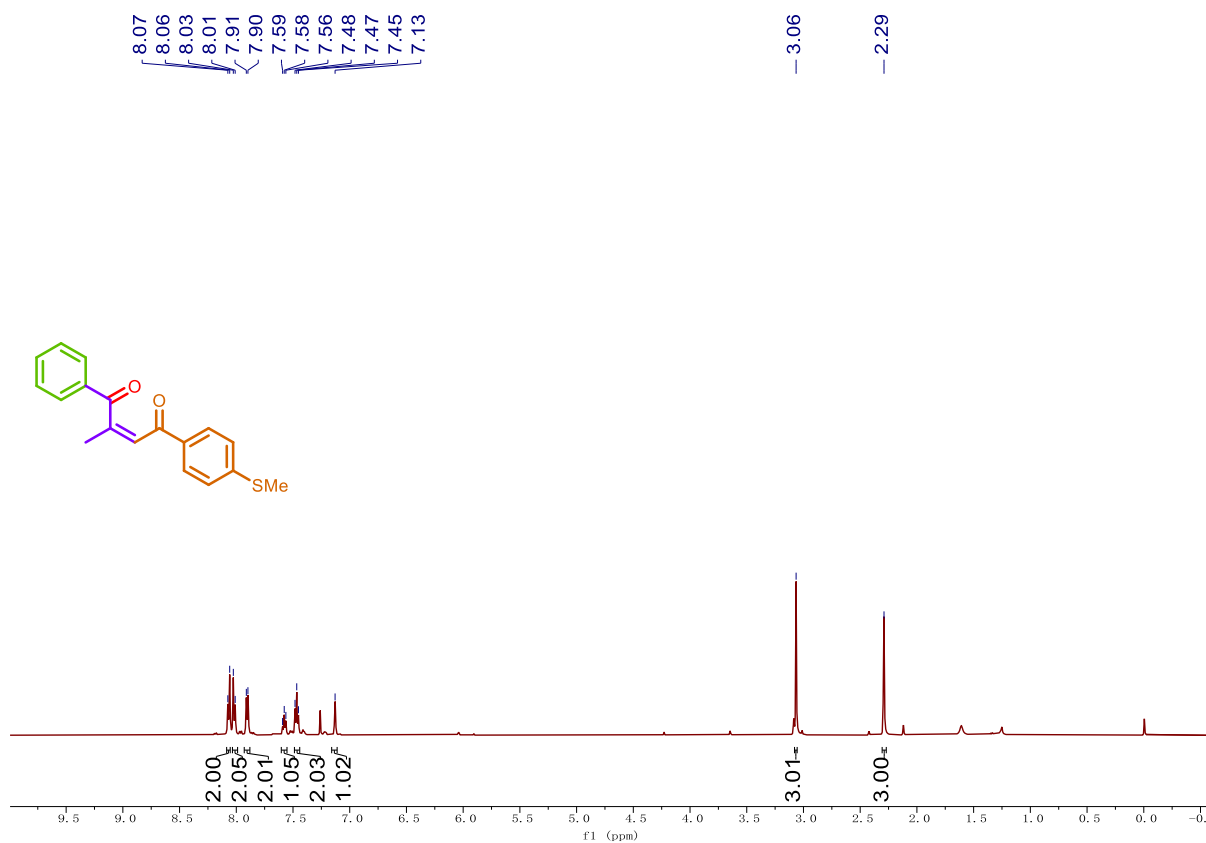
Compound 3au:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )



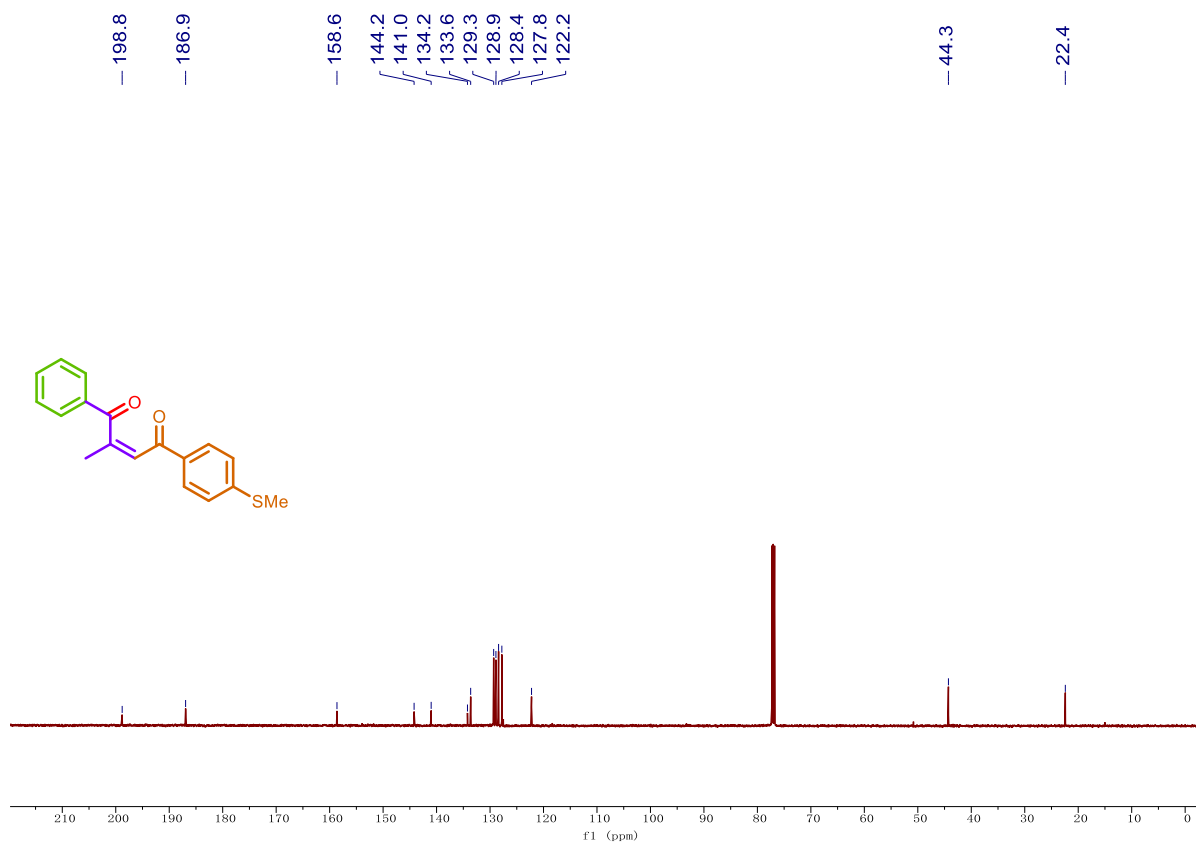
Compound 3au:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )



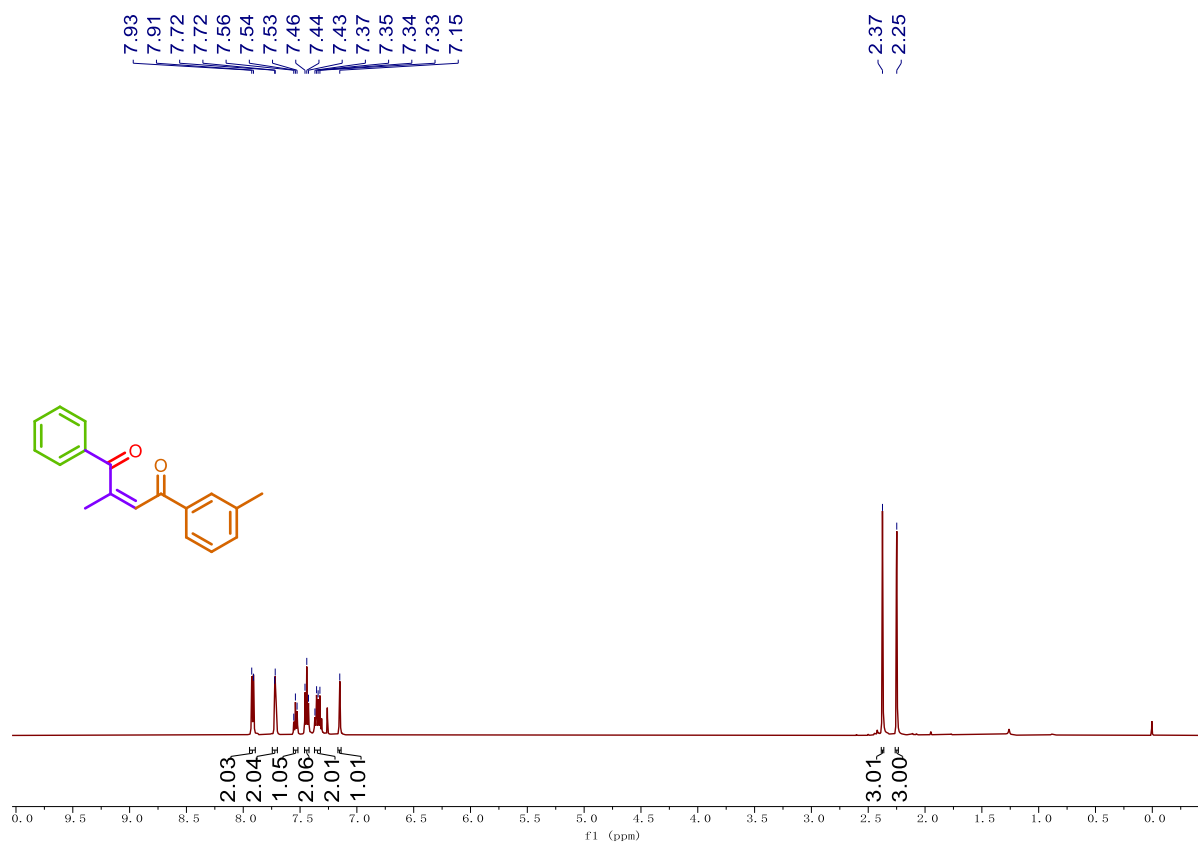
**Compound 3av:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )**



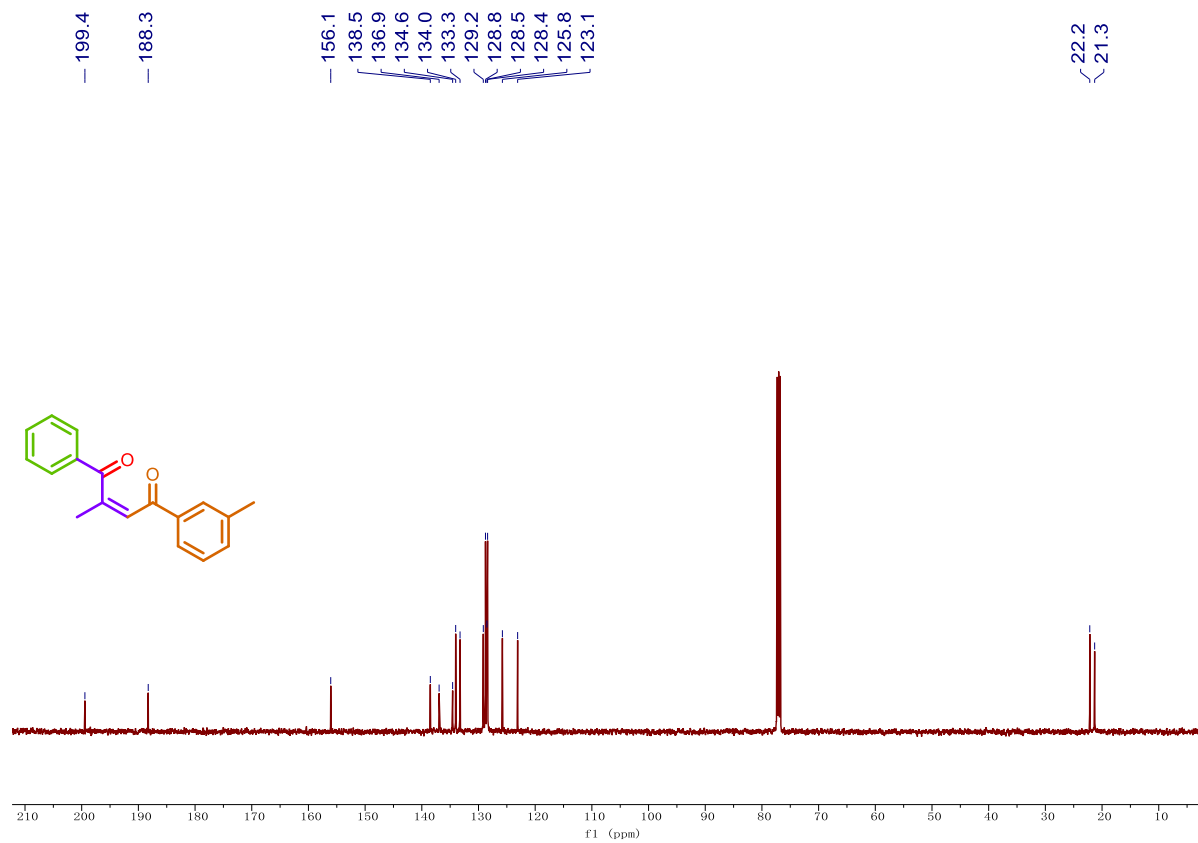
**Compound 3av:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )**



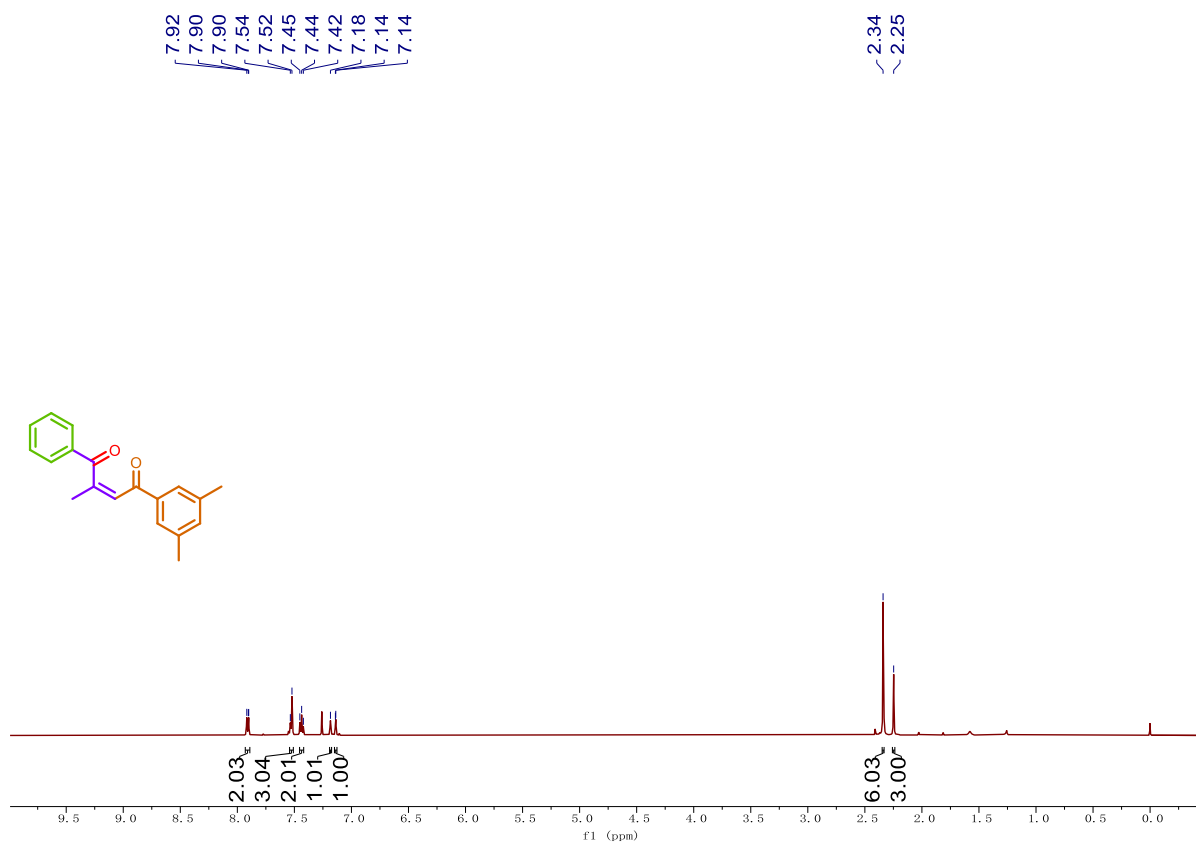
Compound 3aw:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )



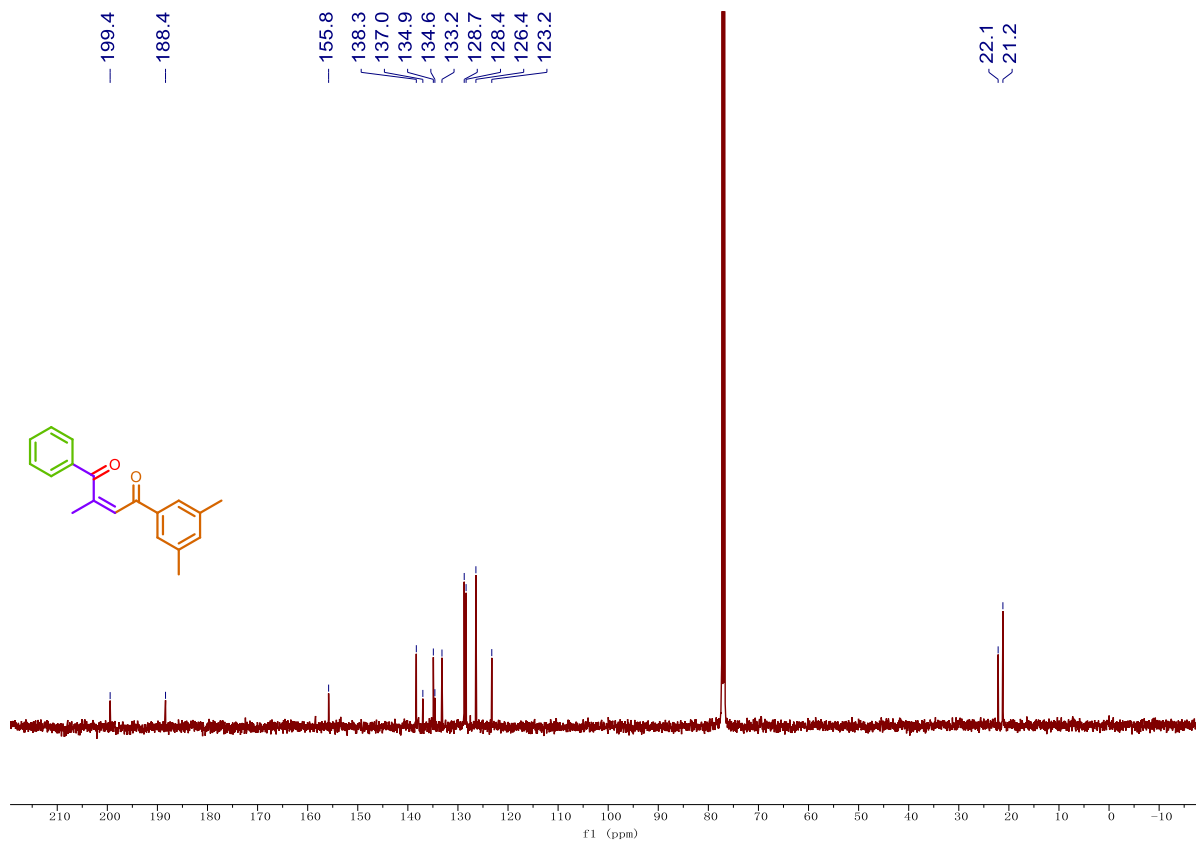
Compound 3aw:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )



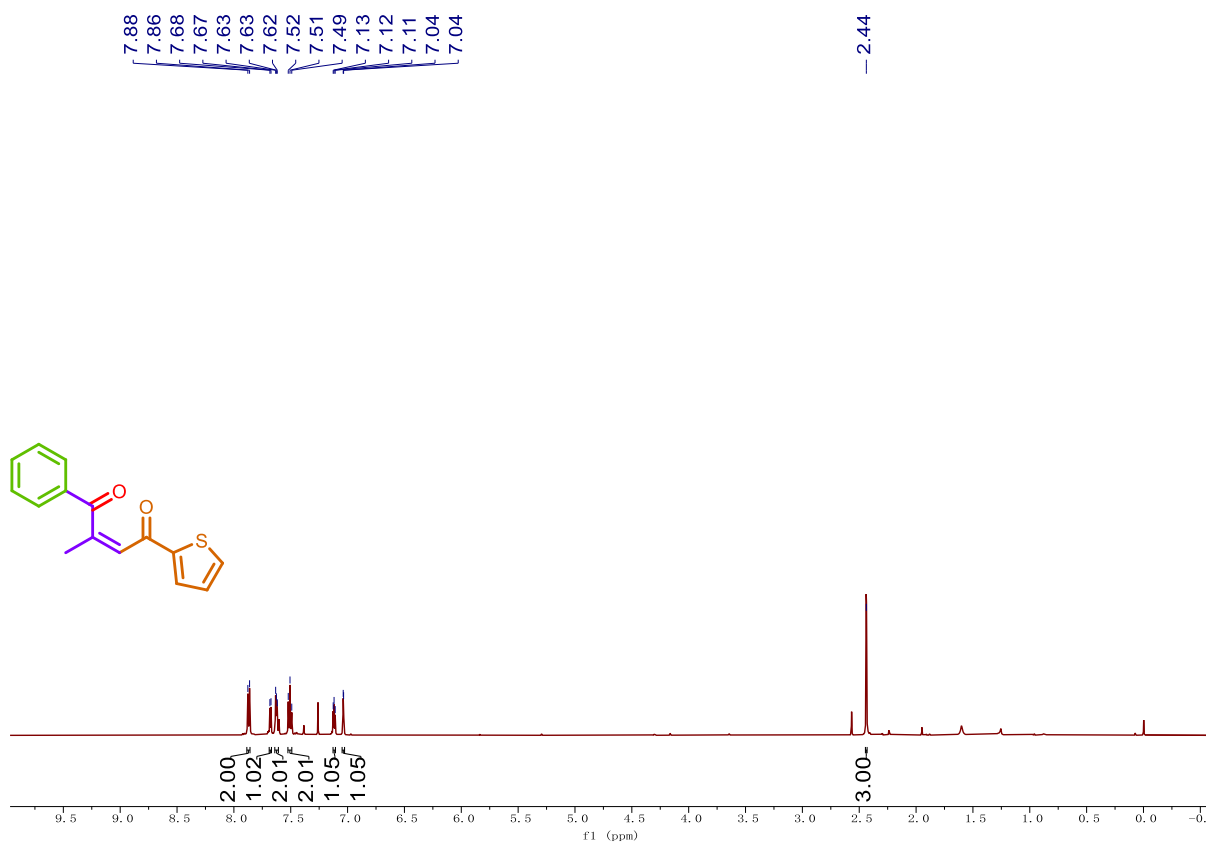
Compound 3ax:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )



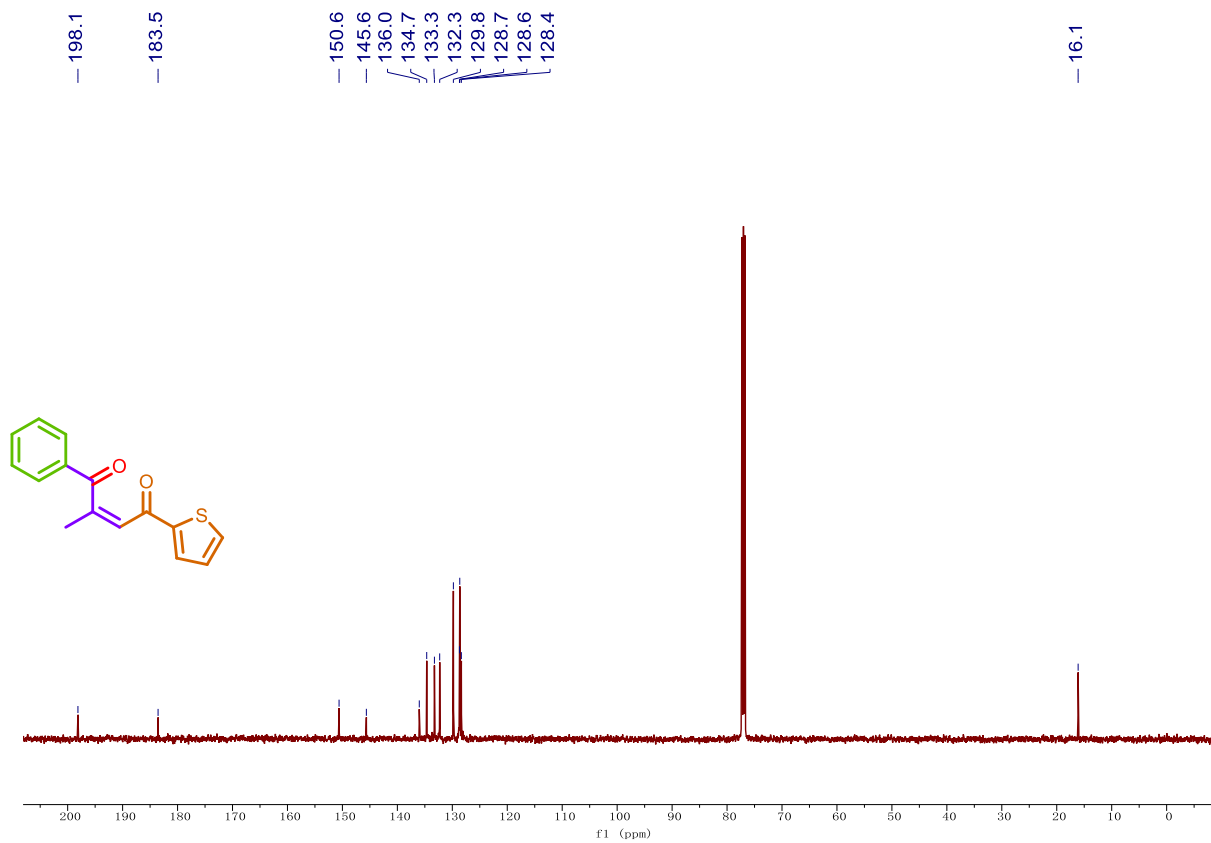
Compound 3ax:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )



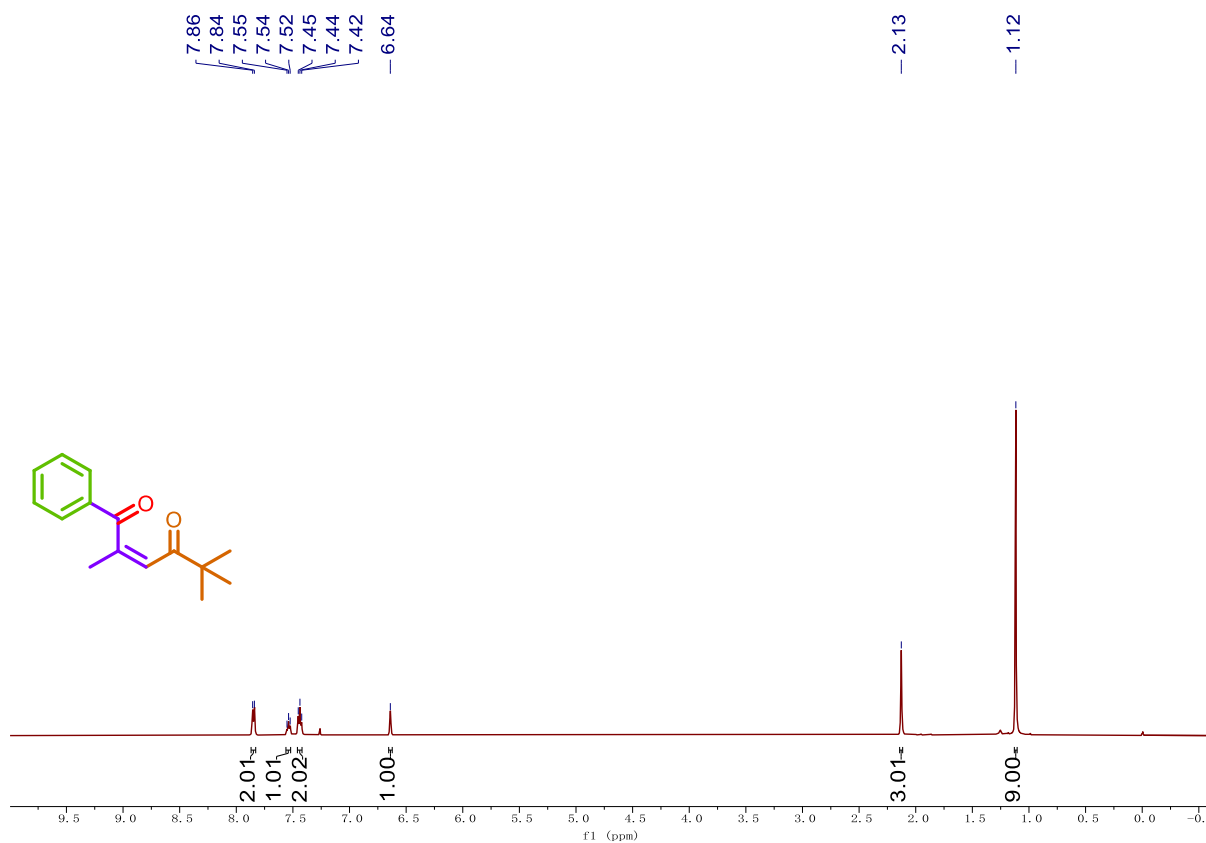
Compound 3ay:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )



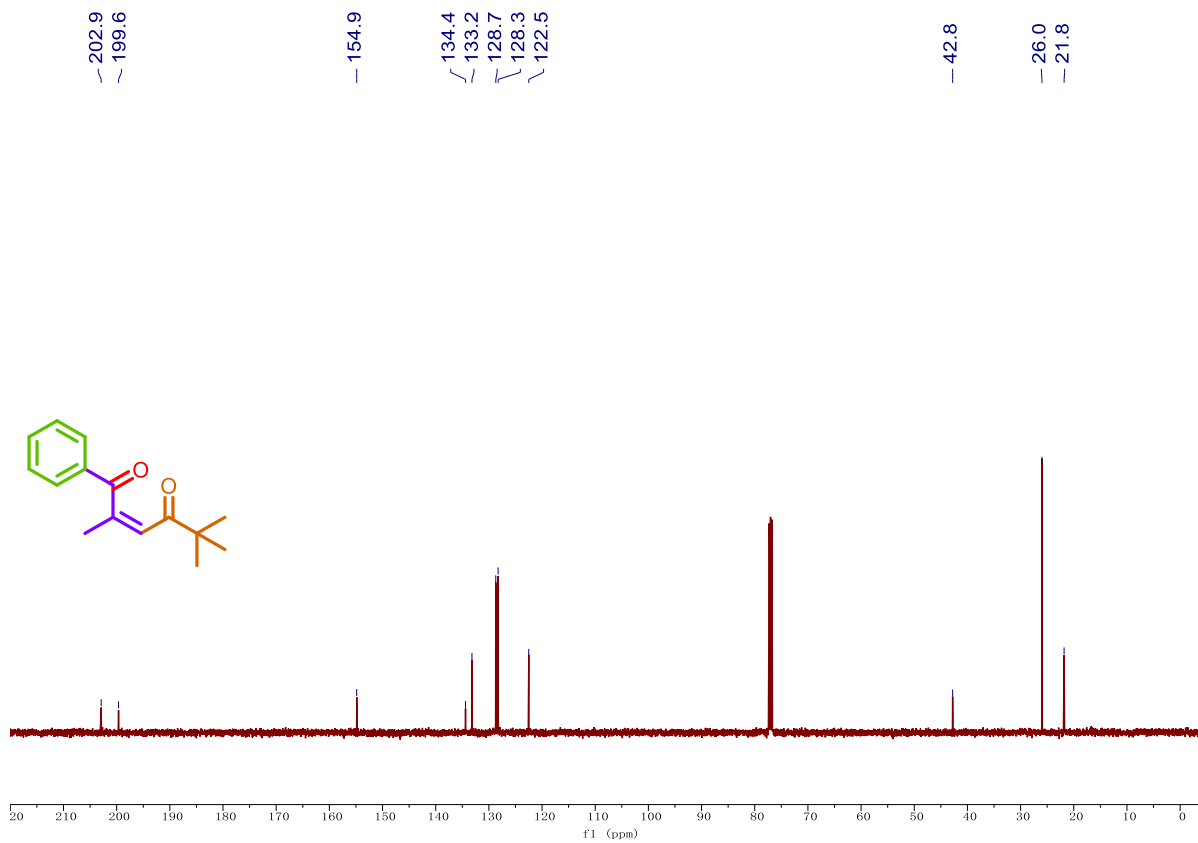
Compound 3ay:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )



Compound 3az:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )

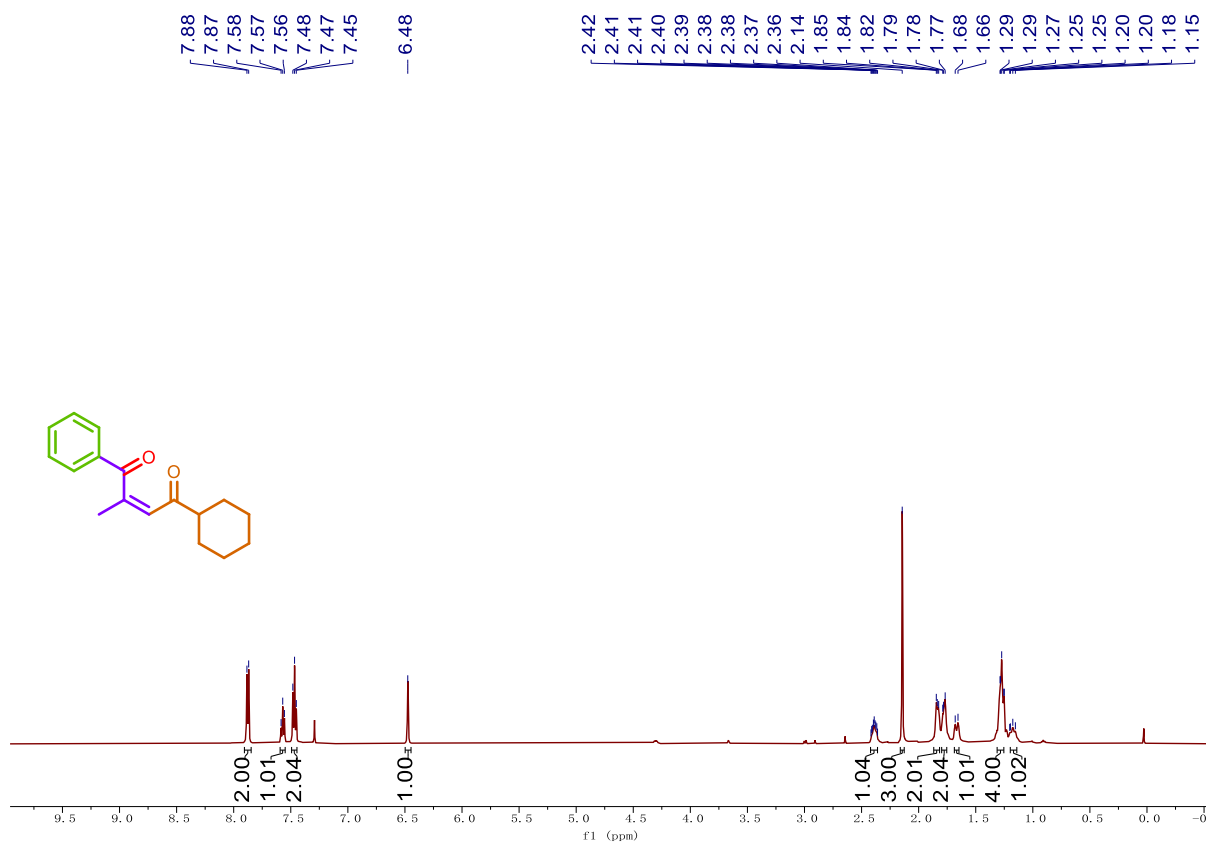


Compound 3az:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )

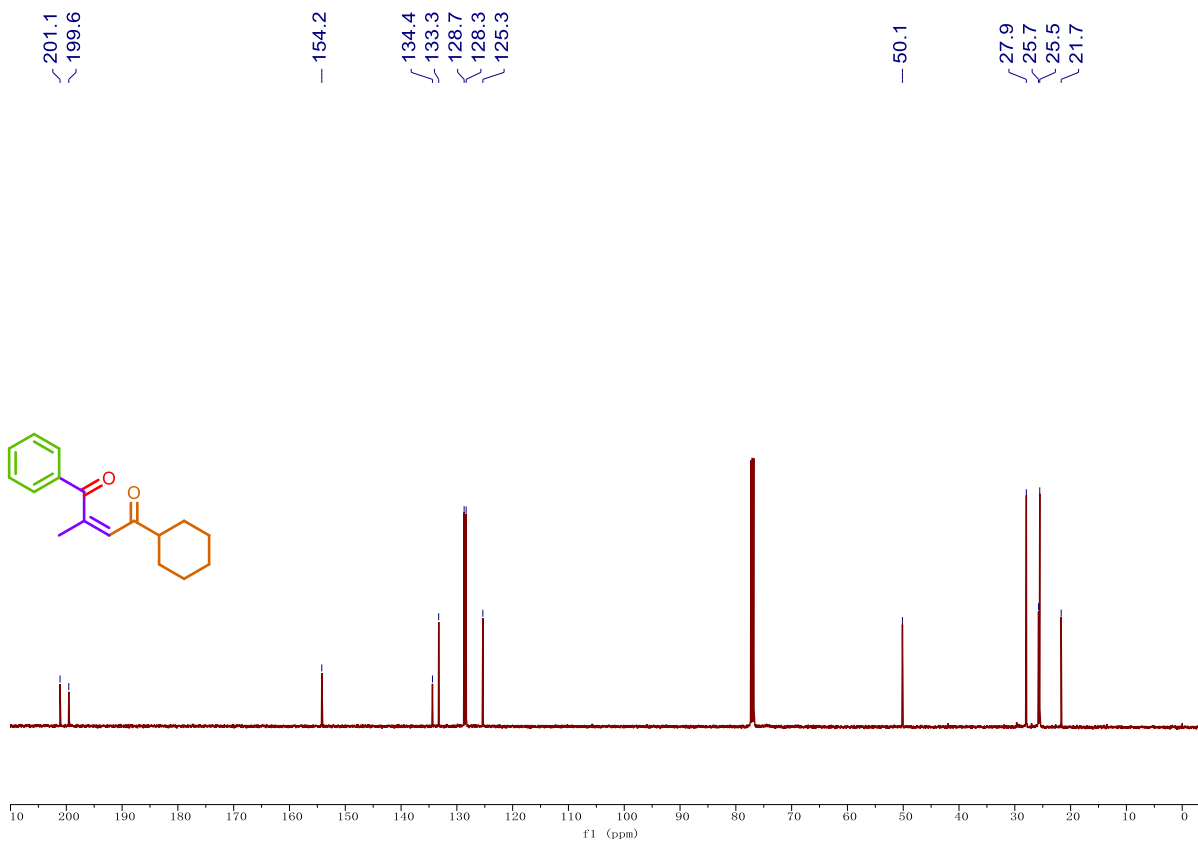




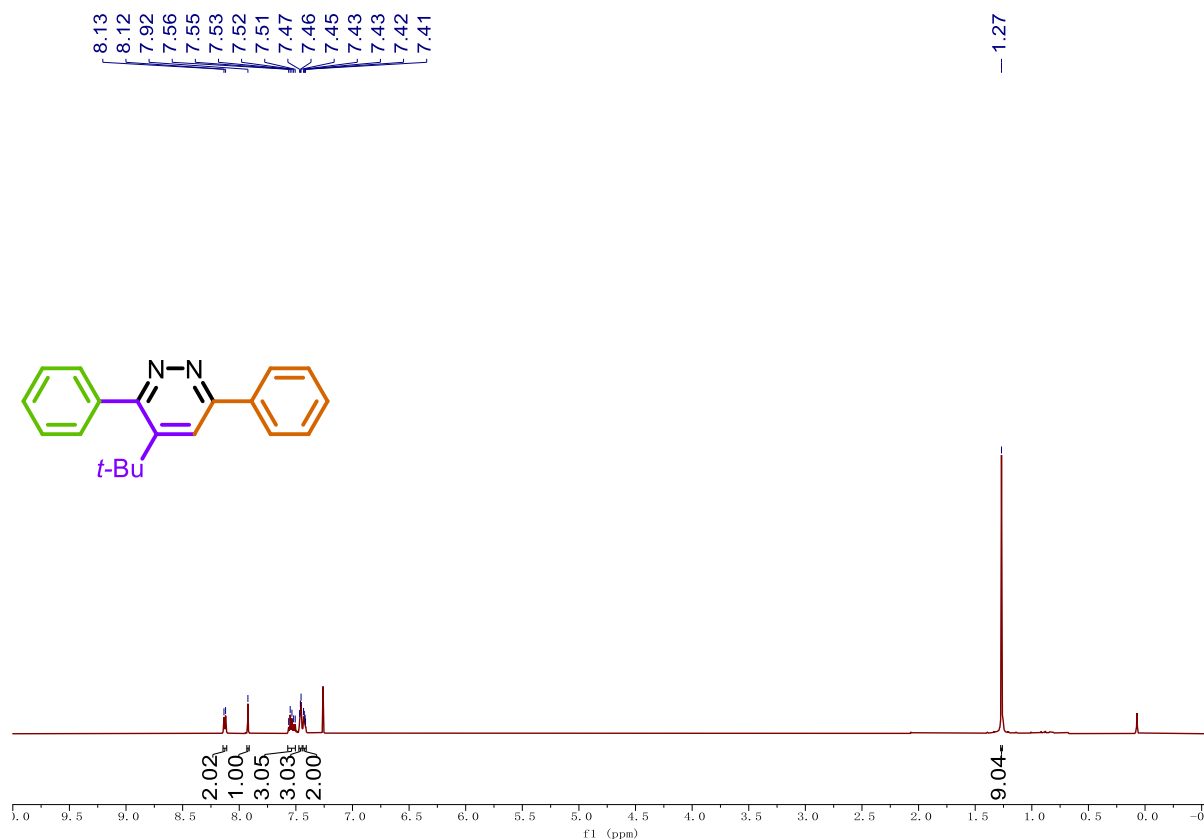
Compound 3ba:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )



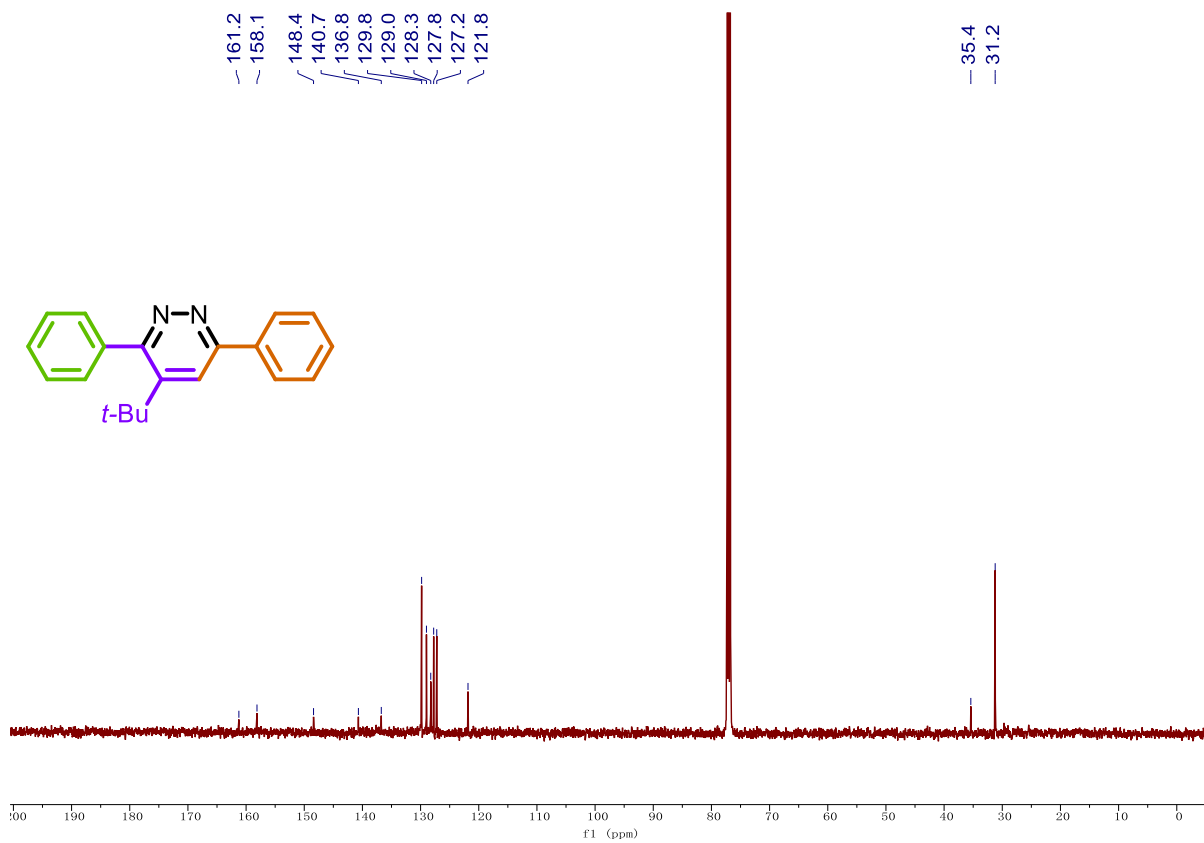
Compound 3ba:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )



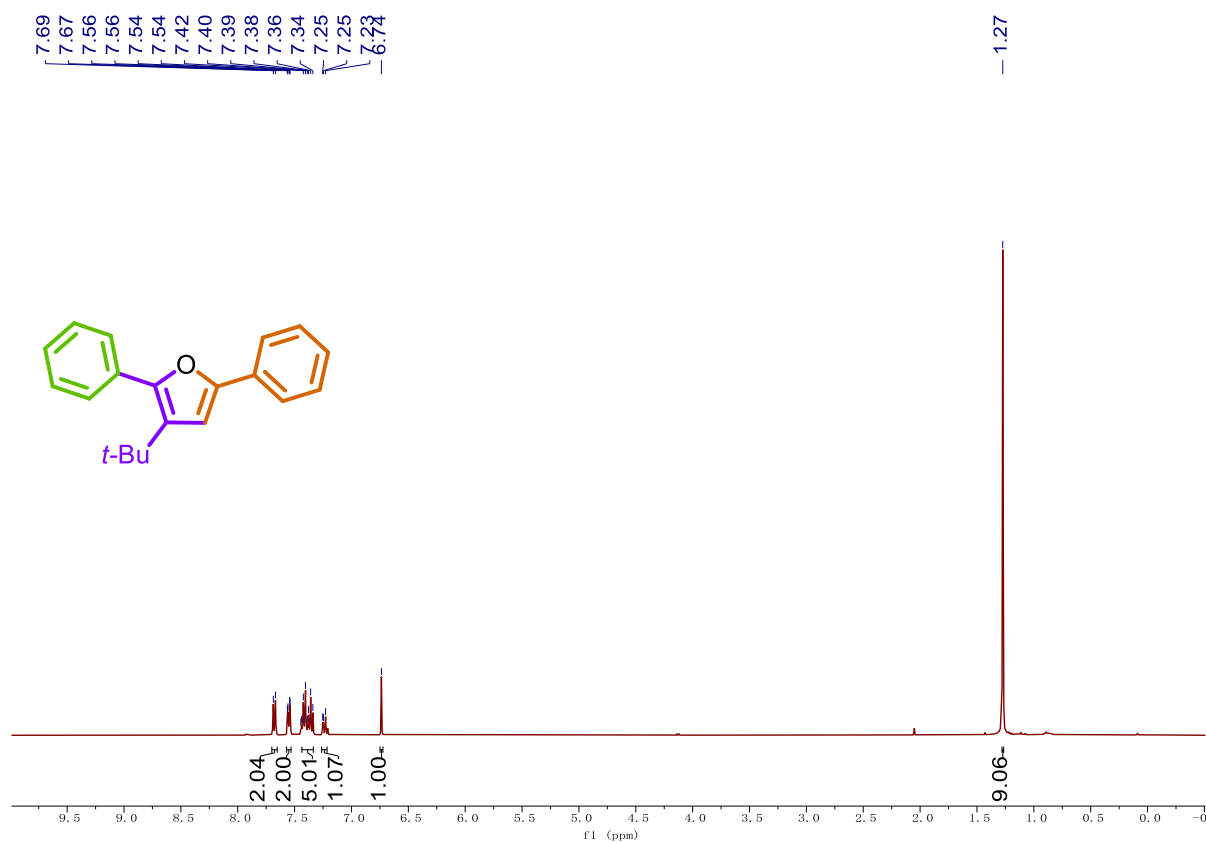
**Compound 4a:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )**



**Compound 4a:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )**



**Compound 4b:  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )**



**Compound 4b:  $^{13}\text{C}$  NMR (125 MHz,  $\text{CDCl}_3$ )**

