

Supporting Information

Visible Light-mediated Hydrogen Atom Transfer and Proton Transfer for the Conversion of (2-Vinylaryl)methanol Derivatives to Arylaldehydes or Aryl Ketones

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Table of Contents

1. General remarks	2
2. General procedures for the synthesis of substrates 1	4
3. General procedure for the synthesis of 2	13
4. Mechanistic Investigations	14
5. Transformation of the products	20
6. Spectroscopic data of substrates 1	22
7. Spectroscopic data of products.....	92
8. Computational details.....	175
9. References	205

1. General remarks

^1H , ^{13}C and ^{19}F NMR spectra were recorded at 400 MHz, 100 MHz and 376 MHz, respectively. HRMS spectra were recorded by EI, ESI, FI method. Infrared spectra were recorded on a Perkin-Elmer PE-983 spectrometer with absorption in cm^{-1} . Mass spectra were recorded by EI, ESI, and HRMS was measured on an Agilent Technologies 6224 TOF LC/MS instrument and a Waters Micromass GCT Permier. Melting points were determined on a digital melting point apparatus and temperatures were uncorrected. The employed solvents were dried up by standard methods when necessary. Commercially obtained reagents were used without further purification. All reactions were monitored by TLC plate analysis with silica gel coated plates (Huanghai GF254). Flash column chromatography was performed by using 300-400 mesh silica gel eluting with ethyl acetate and petroleum ether at increased pressure.

Reaction setup

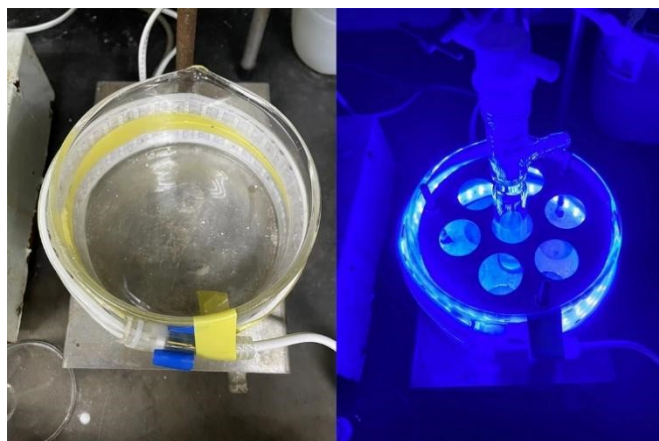
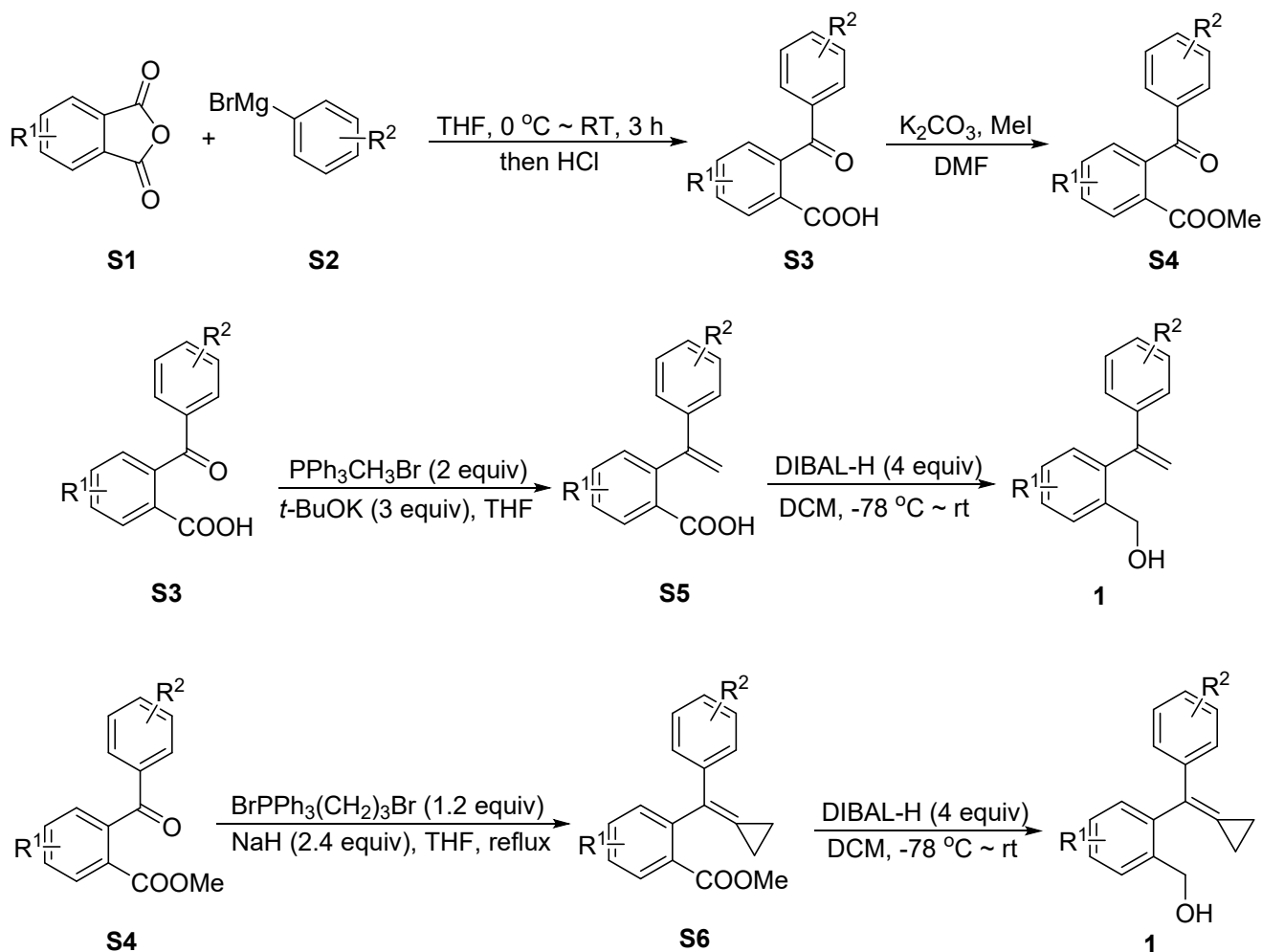


Figure S1. 5 W LEDs strip and reaction setup

As depicted in the picture, reactions were carried out in oven-dried sealed tubes. The reaction temperature was maintained at room temperature by a water bath and a fan.

2. General procedures for the synthesis of substrates 1

Synthesis of substrates **1a-1h**, **1j-1z**, and **1ai**.^{1,2}



S1 (10.0 mmol) and dry tetrahydrofuran (THF, 40.0 mL) were added to a Schlenk flask under argon atmosphere. Then Grignard's reagent **S2** (1.2 equiv) was added dropwise at 0 °C. The resulting mixture was stirred at room temperature for 3 h before quenching with a HCl (1.0 M) solution and extracted three times with ethyl acetate (EtOAc). The combine organic phase was dried over anhydrous Na_2SO_4 . The organic phase was concentrated under reduced pressure and purified by a silica gel column chromatography to obtain the corresponding carboxylic acids (**S3**).

MeI (2.0 equiv) and K_2CO_3 (1.5 equiv) were added to a solution of **S3** (1.0 equiv) in *N,N*-dimethylformamide (DMF). The resulting mixture was stirred at room temperature for 3 h before EtOAc was added and washed three times with water. The organic phase was dried over anhydrous

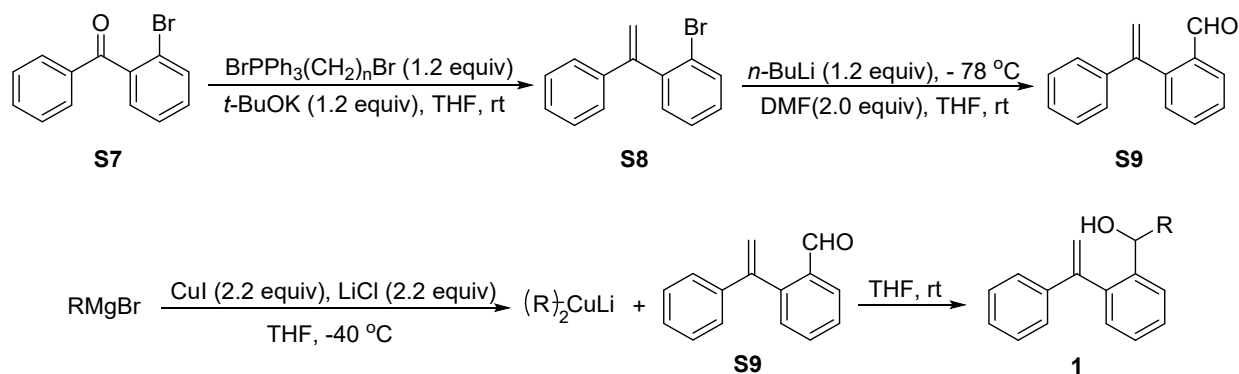
Na₂SO₄ and concentrated under reduced pressure to obtain the corresponding crude products (**S4**).

Methyltriphenylphosphonium bromide (10.0 mmol, 2.0 equiv) and dry THF (50 mL) were added to a Schlenk flask under argon atmosphere and then *t*-BuOK (1.0 M in THF, 15 mL, 3.0 equiv) was added dropwise. The resulting mixture was stirred at room temperature for 30 minutes, then **S3** (5.0 mmol) was added and stirred for 16 h. The mixture was quenched with a NaOH (10%, 50 mL) solution, then the aqueous phase was acidified with a HCl (1.0 M) solution to pH = 1 and extracted three times with EtOAc. The combine organic phase was dried over anhydrous Na₂SO₄. The organic phase was concentrated under reduced pressure and purified by a silica gel column chromatography to obtain the corresponding carboxylic acids (**S5**).

3-bromopropyltriphenylphosphonium bromide (6.0 mmol, 1.2 equiv) and NaH (12.0 mmol, 1.2 equiv) were added to a Schlenk flask under argon atmosphere and then dry THF was added. The mixture was stirred at 75 °C for 2 h and then a solution of compound **S4** (5.0 mmol, 1.0 equiv) in 5.0 mL THF was added. The reaction mixture was stirred at 75 °C overnight before quenching with a HCl (1.0 M) solution and extracted three times with EtOAc. The combine organic phase was dried over anhydrous Na₂SO₄. The organic phase was concentrated under reduced pressure and purified by a silica gel column chromatography to obtain the corresponding products **S6**.

DIBAL-H (1.0 M, 4.0 equiv) was added slowly to a solution of **S5** or **S6** (1.0 equiv) in dry dichloromethane (DCM) at -78 °C under argon atmosphere. After that, the reaction mixture was stirred at room temperature for 3 h and quenching with 10 mL of H₂O, 30.0 mL of 15% NaOH, 10 mL of H₂O sequence. The resulting mixture was stirred at room temperature for 1 h and extracted three times with EtOAc. The combine organic phase was dried over anhydrous Na₂SO₄. The organic phase was concentrated under reduced pressure and purified by a silica gel column chromatography to obtain the corresponding products **1**.

Synthesis of substrates **1ac-1ah**

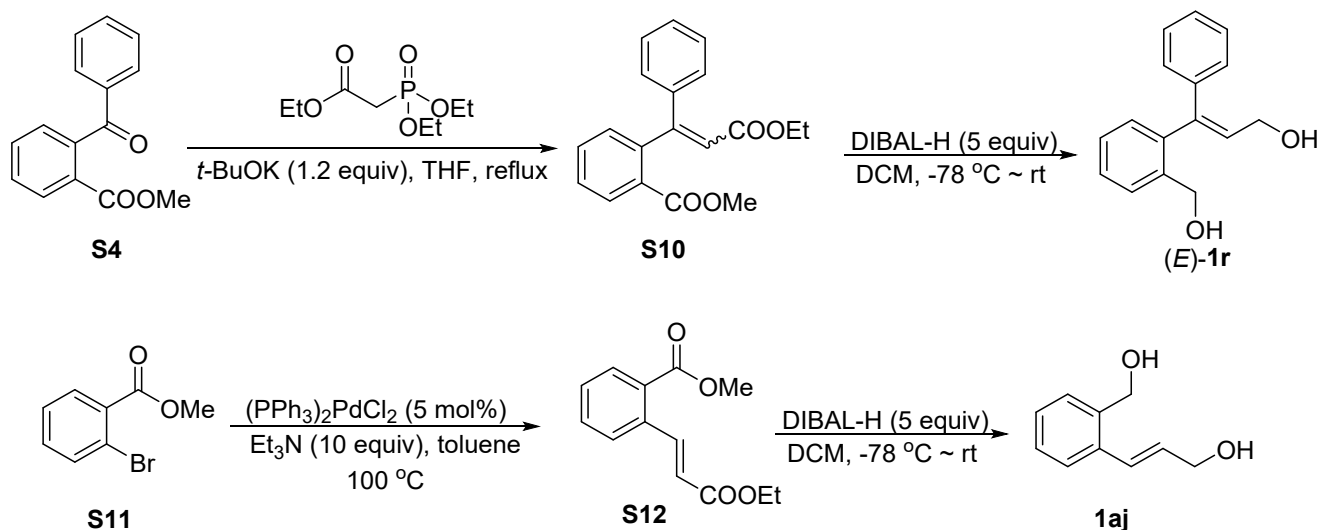


S8 were synthesized according to the previous literature.^[2] Alkyltriphenylphosphonium bromide (24.0 mmol, 1.2 equiv) and dry THF (50.0 mL) were added to a Schlenk flask under argon atmosphere and then *t*-BuOK (1.0 M in THF, 24 mL, 1.2 equiv) was added dropwise. The resulting mixture was stirred at room temperature for 30 minutes before **S3** (20.0 mmol) was added. The reaction mixture was stirred at rt for 2 h before quenching with a HCl (1.0 M) solution and extracted three times with EtOAc. The combine organic phase was dried over anhydrous Na₂SO₄. The organic phase was concentrated under reduced pressure and purified by a silica gel column chromatography to obtain the corresponding product **S8**.

n-BuLi (2.4 M, 1.2 equiv) was added slowly to a solution of **S8** (1.0 equiv) in dry THF at -78 °C under argon atmosphere. The mixture was stirred at -78 °C for 30 minutes and then DMF (5.0 mmol, 1.0 equiv) was added. The reaction was stirred at rt for 2 h before quenching with a HCl (1.0 M) solution and extracted three times with EtOAc. The combine organic phase was dried over anhydrous Na₂SO₄. The organic phase was concentrated under reduced pressure and purified by a silica gel column chromatography to obtain the corresponding products **S9**.

CuI (2.2 equiv), LiCl (2.2 equiv) and dry THF (30.0 mL) were added to a Schlenk flask under argon atmosphere. The resulting mixture was stirred at -40 °C for 30 minutes, then a solution of **S9** (1.0 equiv) in dry THF was added. The reaction mixture was stirred at rt for 2 h before quenching with a saturated NH₄Cl solution and extracted three times with EtOAc. The combine organic phase was dried over anhydrous Na₂SO₄. The organic phase was concentrated under reduced pressure and purified by a silica gel column chromatography to obtain the corresponding products **1**.

Synthesis of substrates **1r** and **1aj**³

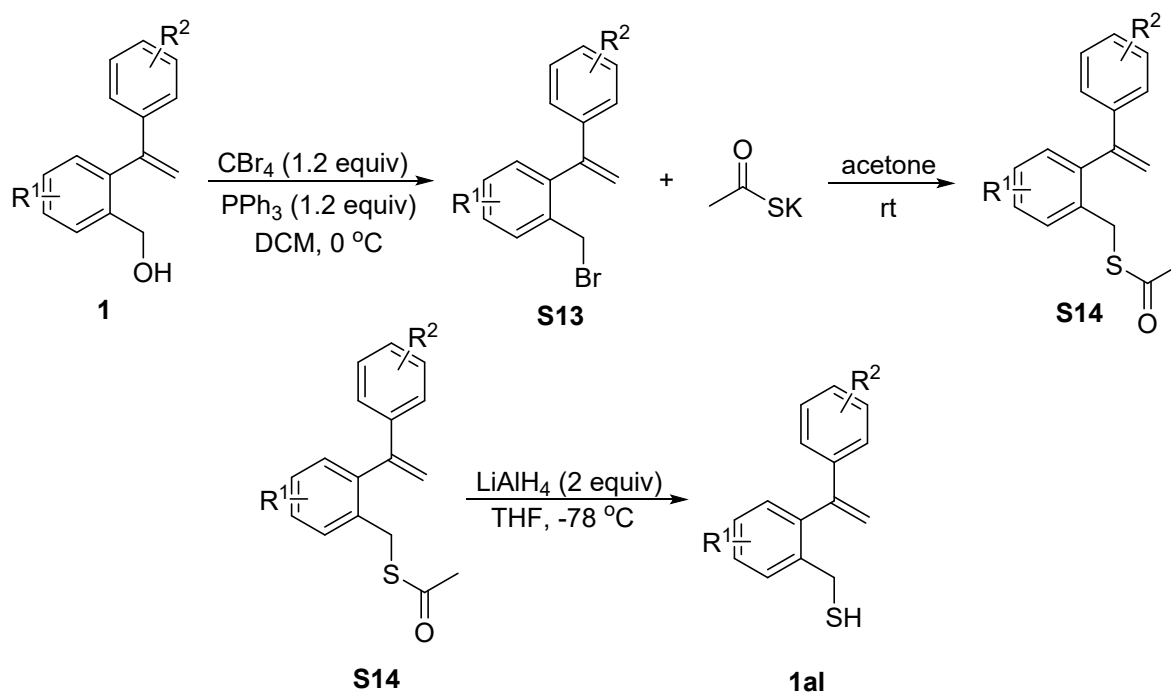


Phosphate ester and dry THF were added to a Schlenk flask under argon atmosphere and then *t*-BuOK (1.0 M in THF) was added dropwise. The resulting mixture was stirred at room temperature for 30 minutes before **S4** was added. The reaction mixture was stirred at 75 °C overnight before quenching with a HCl (1.0 M) solution and extracted three times with EtOAc. The combine organic phase was dried over anhydrous Na₂SO₄. The organic phase was concentrated under reduced pressure and purified by a silica gel column chromatography to obtain the corresponding products **S10**.

(PPh₃)₂PdCl₂, Et₃N, **S11**, and dry toluene (30.0 mL) were added to a Schlenk flask under argon atmosphere. The reaction mixture was stirred at 75 °C overnight. The organic phase was concentrated under reduced pressure and purified by a silica gel column chromatography to obtain the corresponding products **S12**.

DIBAL-H (1.0 M, 5.0 equiv) was added slowly to a solution of **S10** or **S12** (1.0 equiv) in dry dichloromethane (DCM) at -78 °C under argon atmosphere. After that, the reaction mixture was stirred at room temperature for 3 h and quenching with 10 mL of H₂O, 30.0 mL of 15% NaOH, 10 mL of H₂O sequence. The resulting mixture was stirred at room temperature for 1 h and extracted three times with EtOAc. The combine organic phase was dried over anhydrous Na₂SO₄. The organic phase was concentrated under reduced pressure and purified by a silica gel column chromatography to obtain the corresponding products **1r** or **1aj**.

Synthesis of substrate **1al**

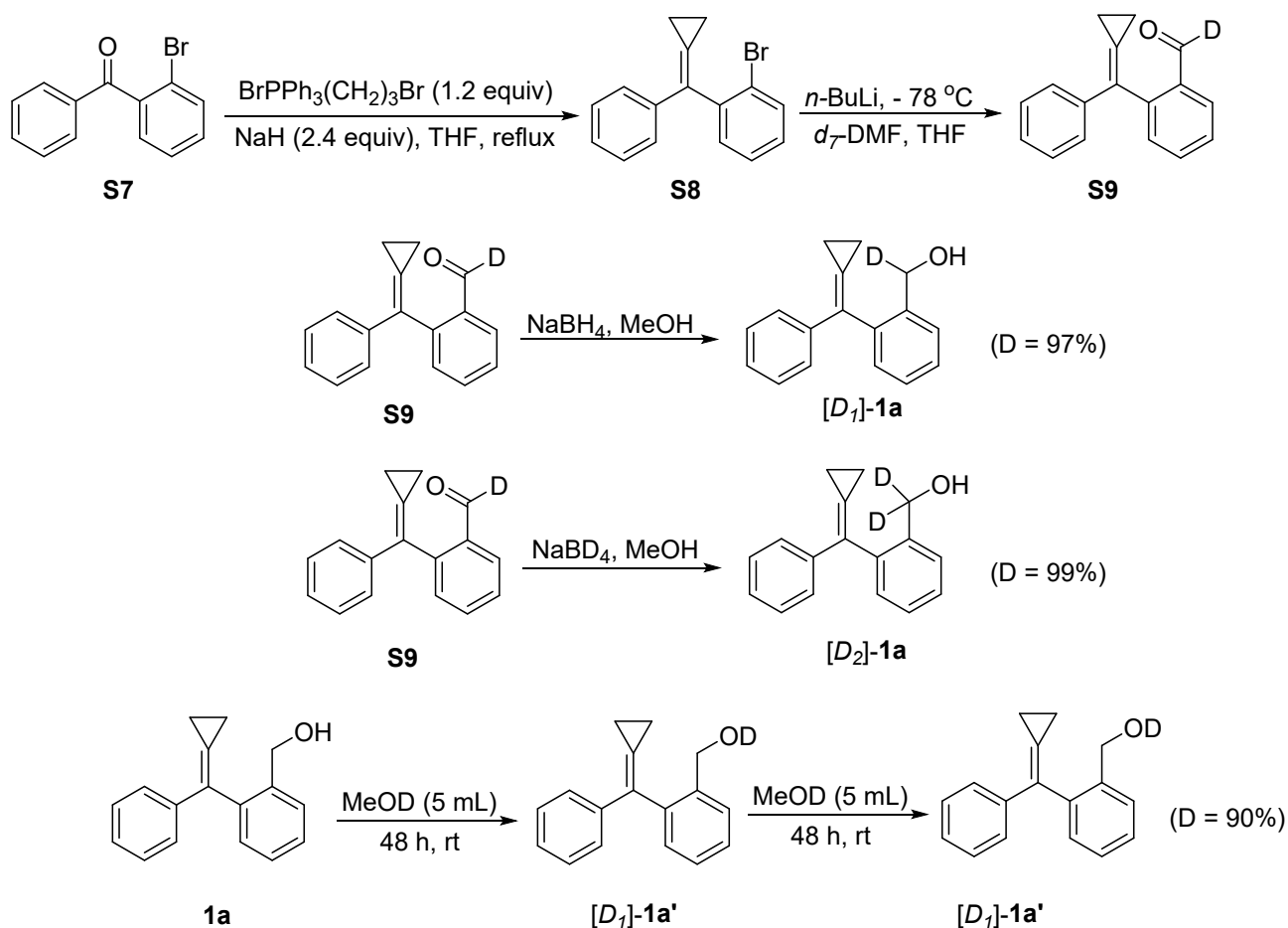


1 (5.0 mmol), CBr_4 (6.0 mmol, 1.2 equiv) and dry DCM (10 mL) were added to a Schlenk flask under argon atmosphere and then PPh_3 (1.0 M in DCM , 6.0 mL, 1.2 equiv) was added dropwise at $-0\text{ }^\circ\text{C}$. The reaction mixture was stirred at $0\text{ }^\circ\text{C}$ for 2 h before quenching with H_2O and extracted three times with EtOAc . The combine organic phase was dried over anhydrous Na_2SO_4 . The organic phase was concentrated under reduced pressure and purified by a silica gel column chromatography to obtain the corresponding product **S13**.

S13 (4.0 mmol), potassium thioacetate (4.8 mmol, 1.2 equiv), and acetone (20 mL) were added to a Schlenk flask under argon atmosphere. The reaction mixture was stirred at rt overnight before quenching with H_2O and extracted three times with EtOAc . The combine organic phase was dried over anhydrous Na_2SO_4 . The organic phase was concentrated under reduced pressure and purified by a silica gel column chromatography to obtain the corresponding products **S14**.

LiAlH_4 (1.0 M, 2.0 equiv) was added slowly to a solution of **S14** (1.0 equiv) in dry THF at $-78\text{ }^\circ\text{C}$ under argon atmosphere. After that, the reaction mixture was stirred at $-78\text{ }^\circ\text{C}$ for 3 h and quenching with 10 mL of H_2O , 30.0 mL of 15% NaOH , 10 mL of H_2O sequence. The resulting mixture was stirred at room temperature for 1 h and extracted three times with EtOAc . The combine organic phase was dried over anhydrous Na_2SO_4 . The organic phase was concentrated under reduced pressure and purified by a silica gel column chromatography to obtain the corresponding product **1al**.

Synthesis of the deuterated substrates.⁴



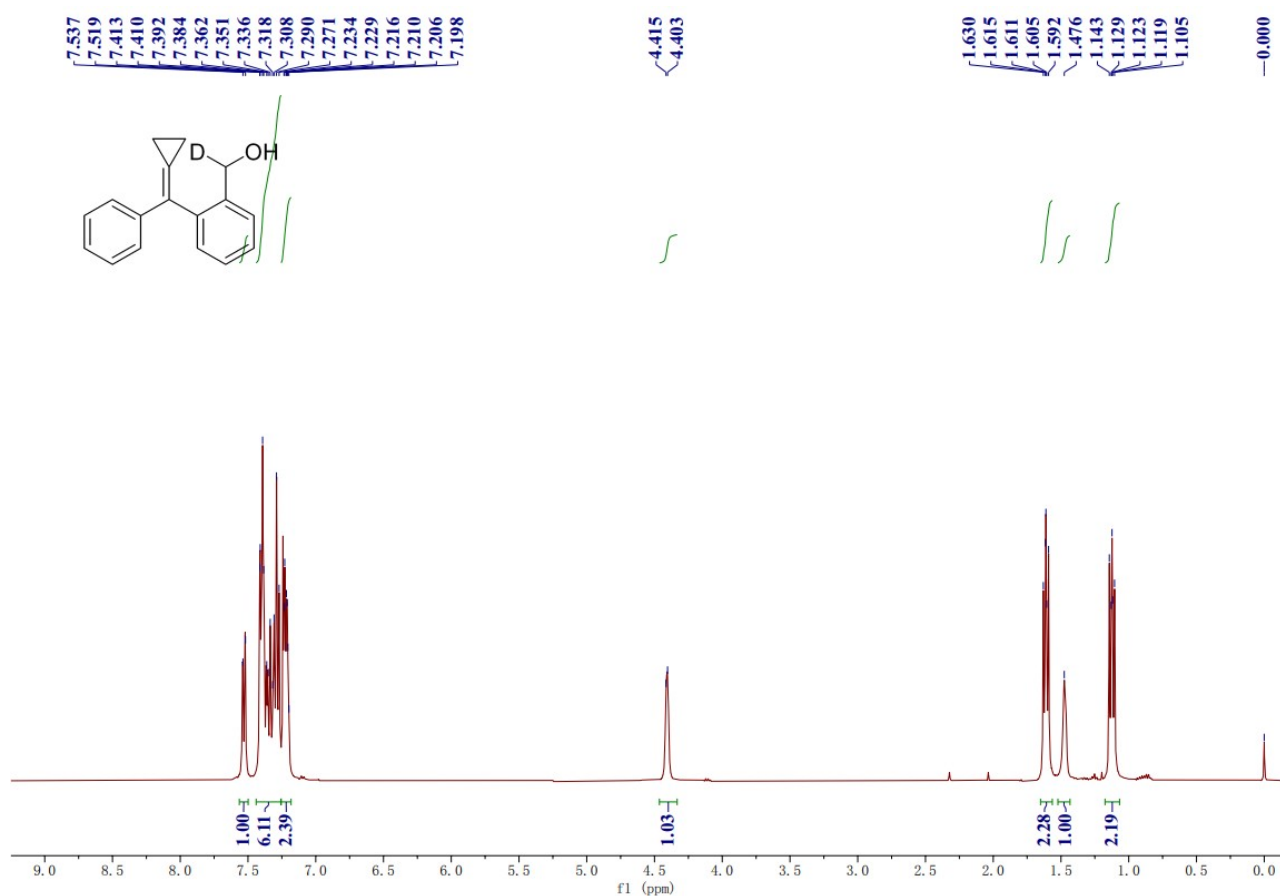
3-bromopropyltriphenylphosphonium bromide (6.0 mmol, 1.2 equiv) and NaH (12.0 mmol, 1.2 equiv) were added to a Schlenk flask under argon atmosphere and then dry THF was added. The mixture was stirred at 75 °C for 2 h and then a solution of compound **S7** (5.0 mmol, 1.0 equiv) in 5 mL THF was added. The reaction mixture was stirred at 75 °C overnight before quenching with a HCl (1.0 M) solution and extracted three times with EtOAc. The combine organic phase was dried over anhydrous Na₂SO₄. The organic phase was concentrated under reduced pressure and purified by a silica gel column chromatography to obtain the corresponding product **S8**.

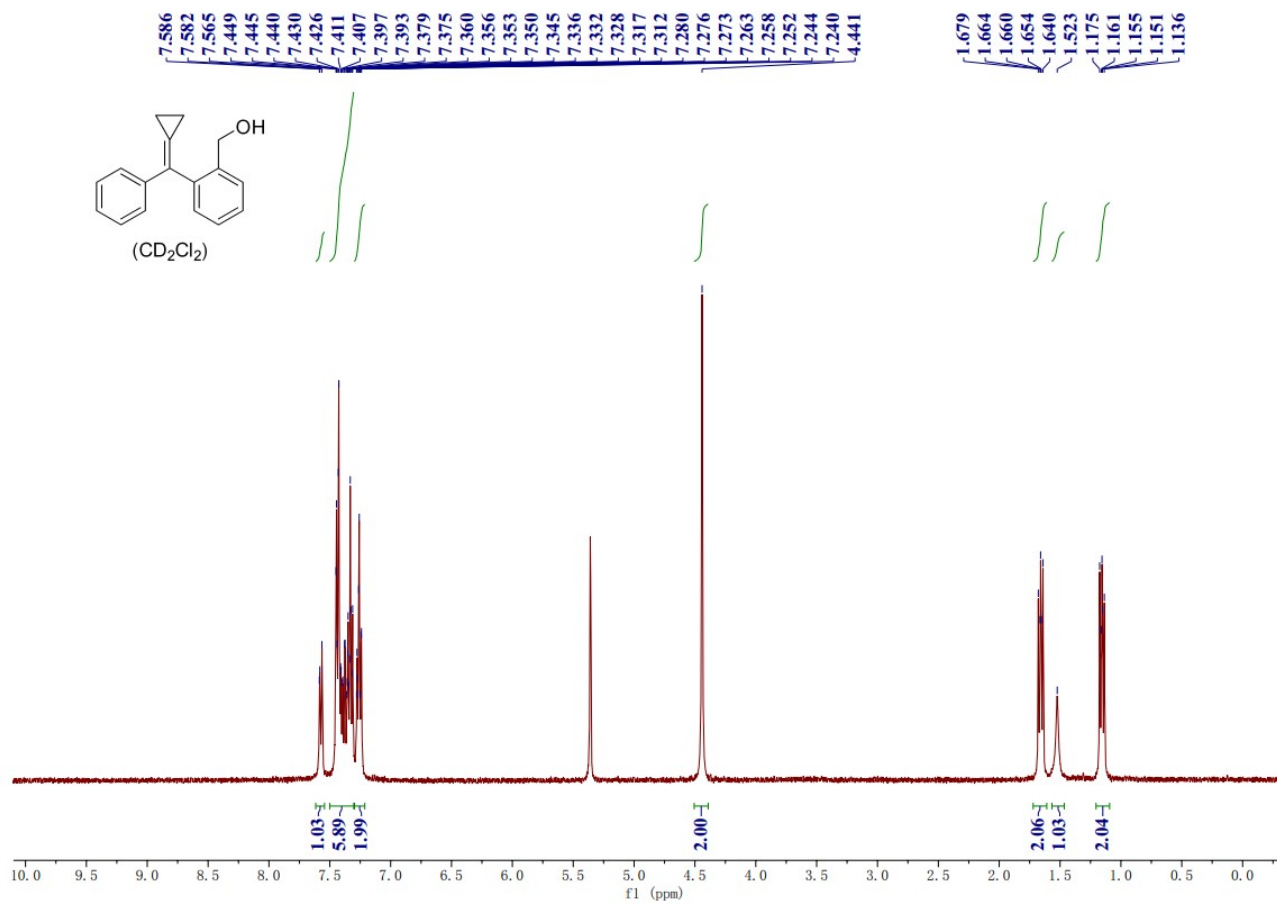
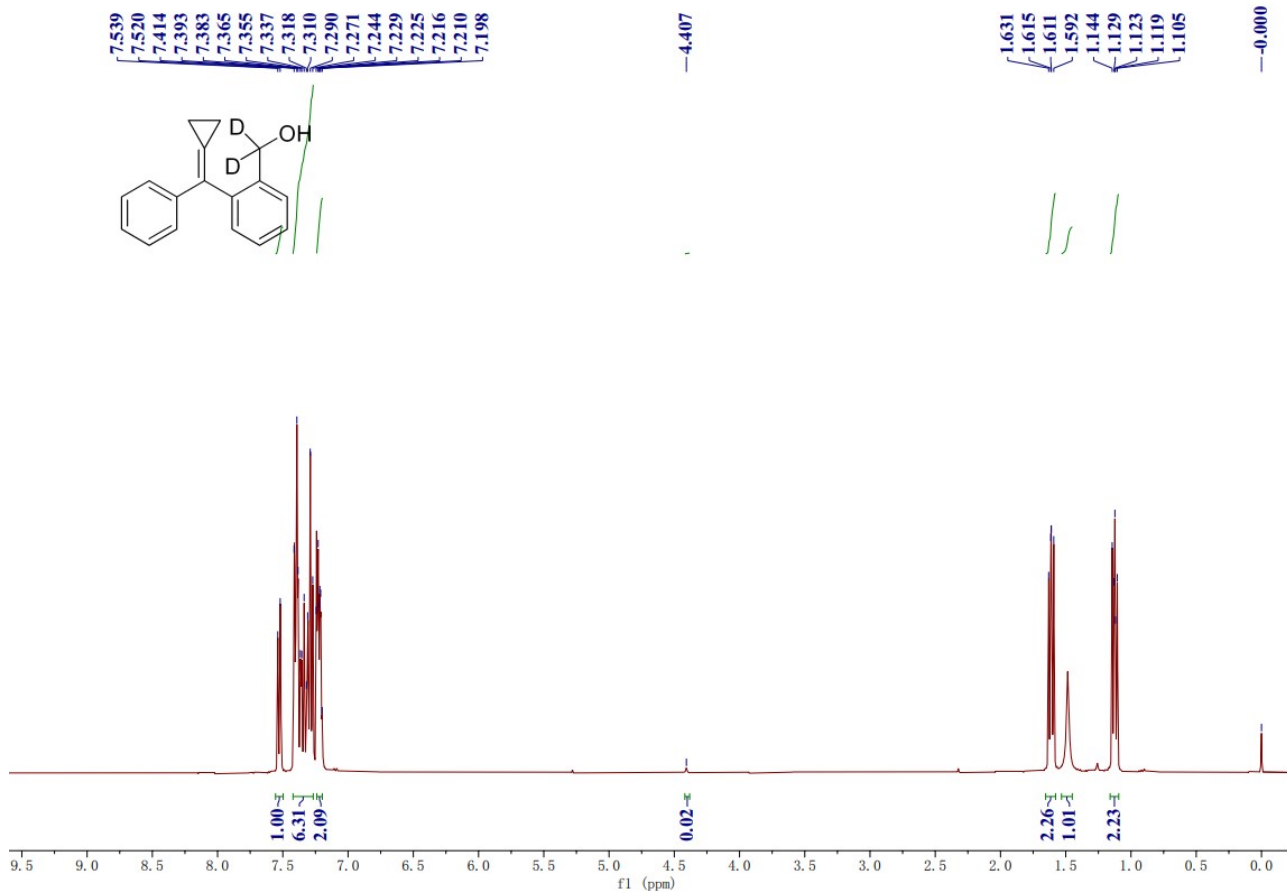
S8 (4.0 mmol) and dry tetrahydrofuran (THF, 10 mL) were added to a Schlenk flask under argon atmosphere, then *n*-BuLi (2.4 M, 1.2 equiv) was added dropwise at -78 °C. The mixture was stirred at -78 °C for 1 h, and then *d*₇-DMF was added slowly. Afterward, the reaction mixture was stirred at rt for 3 h before quenching with H₂O and extracted three times with EtOAc. The combine organic phase was dried over anhydrous Na₂SO₄. The organic phase was concentrated under reduced pressure and purified by a silica gel column chromatography to obtain the corresponding product **S9**.

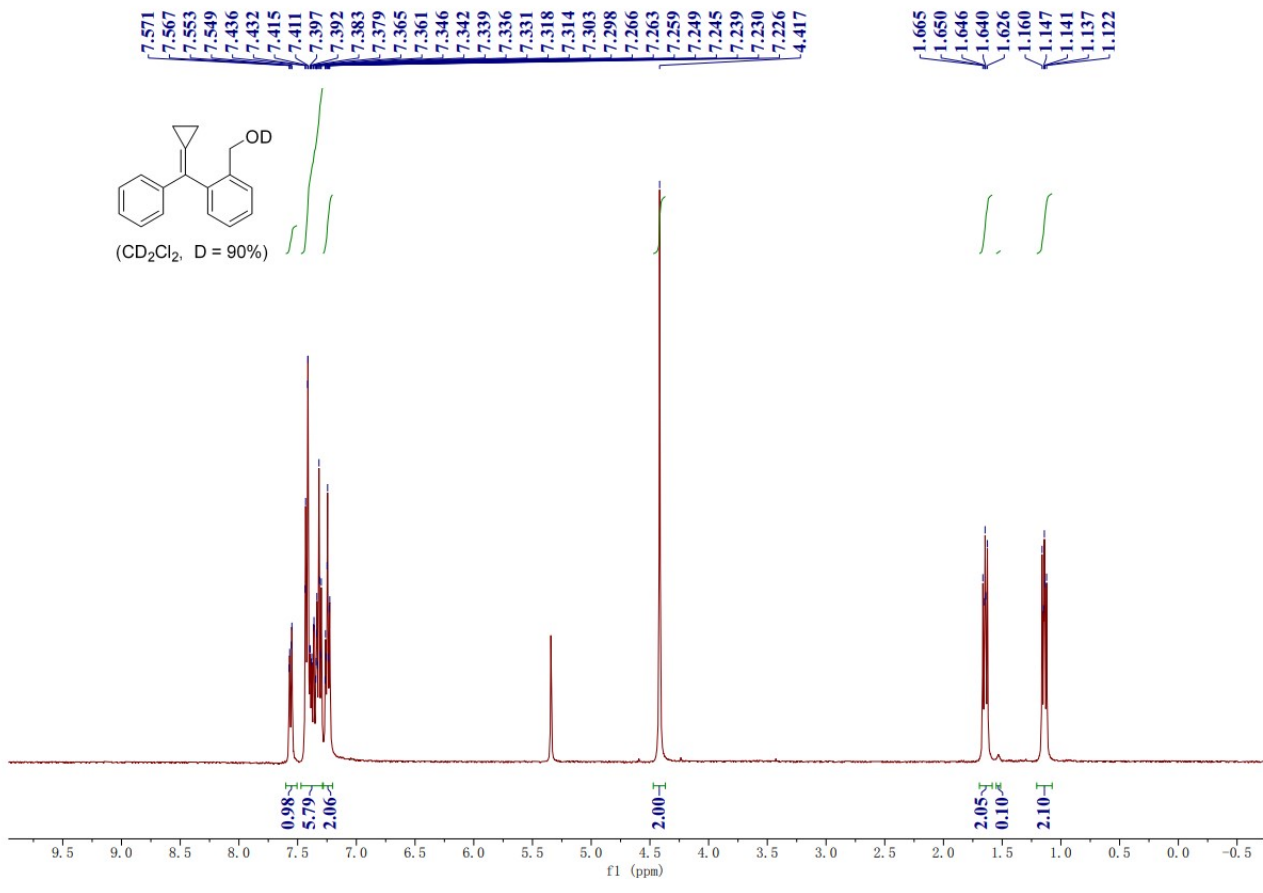
NaBH₄ (1.2 equiv) was added slowly to a solution of **S9** (1.0 equiv) in MeOH at 0 °C. After that, the reaction mixture was stirred at room temperature for 3 h before quenching with H₂O and extracted three times with EtOAc. The combine organic phase was dried over anhydrous Na₂SO₄. The organic phase was concentrated under reduced pressure and purified by a silica gel column chromatography to obtain the deuterated product [*D*₁]-**1a** with 97% D content.

NaBD₄ (1.2 equiv) was added slowly to a solution of **S9** (1.0 equiv) in MeOH at 0 °C. After that, the reaction mixture was stirred at room temperature for 3 h before quenching with H₂O and extracted three times with EtOAc. The combine organic phase was dried over anhydrous Na₂SO₄. The organic phase was concentrated under reduced pressure and purified by a silica gel column chromatography to obtain the deuterated product [*D*₂]-**1a** with 99% D content.

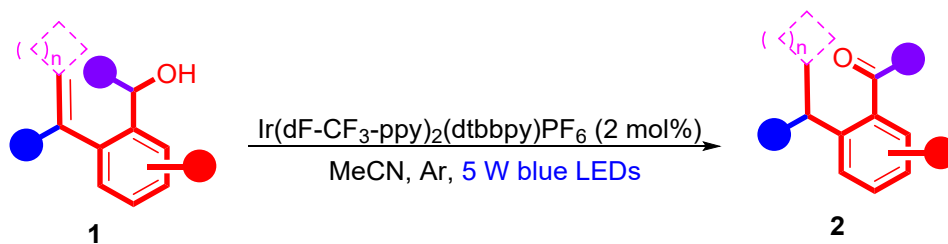
(2-(cyclopropylidene(phenyl)methyl)phenyl)methanol **1a** (2.0 mmol) was added to MeOD (5 mL) in a Schlenk tube and the mixture was stirred at room temperature for 48 h. The reaction solvent was removed by reduced pressure distillation. Repeat the above operation to obtain deuterated product [*D*₁]-**1a'** with 90% D content.







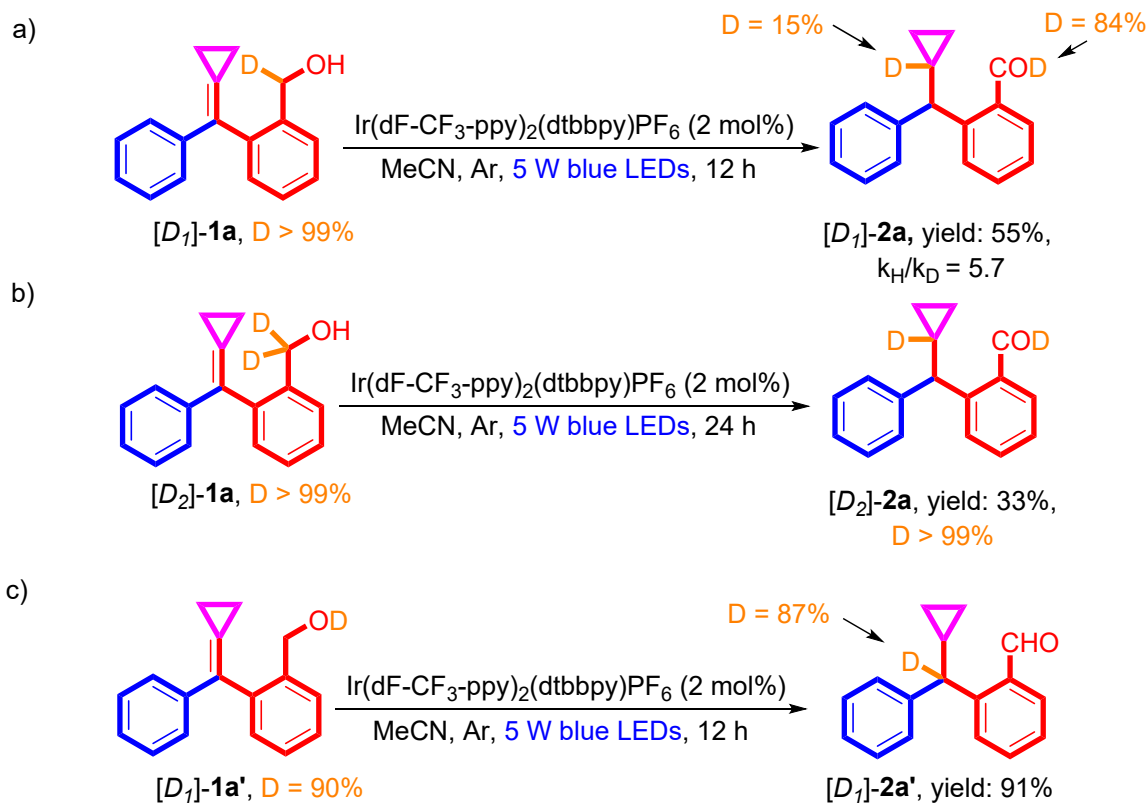
3. General procedure for the synthesis of 2



To a 10.0 mL sealed tube were added substrate **1** (0.20 mmol, 1.0 equiv), Ir(dF-CF₃-ppy)₂(dtbbpy)PF₆ (0.004 mmol, 0.02 equiv), and CH₃CN (2.0 mL), then the resulting mixture was bubbled with argon for 15 minutes. The resulting mixture was stirred upon irradiation of 5 W blue LEDs at rt for 3 - 48 hours. Then, the solvent was removed under vacuum and the residue was purified by a silica gel column chromatography (petroleum ether : ethyl acetate = 10 : 1) to give the desired products **2** in 24 - 96% yields.

4. Mechanistic Investigations

4.1 Deuterium labeling experiment



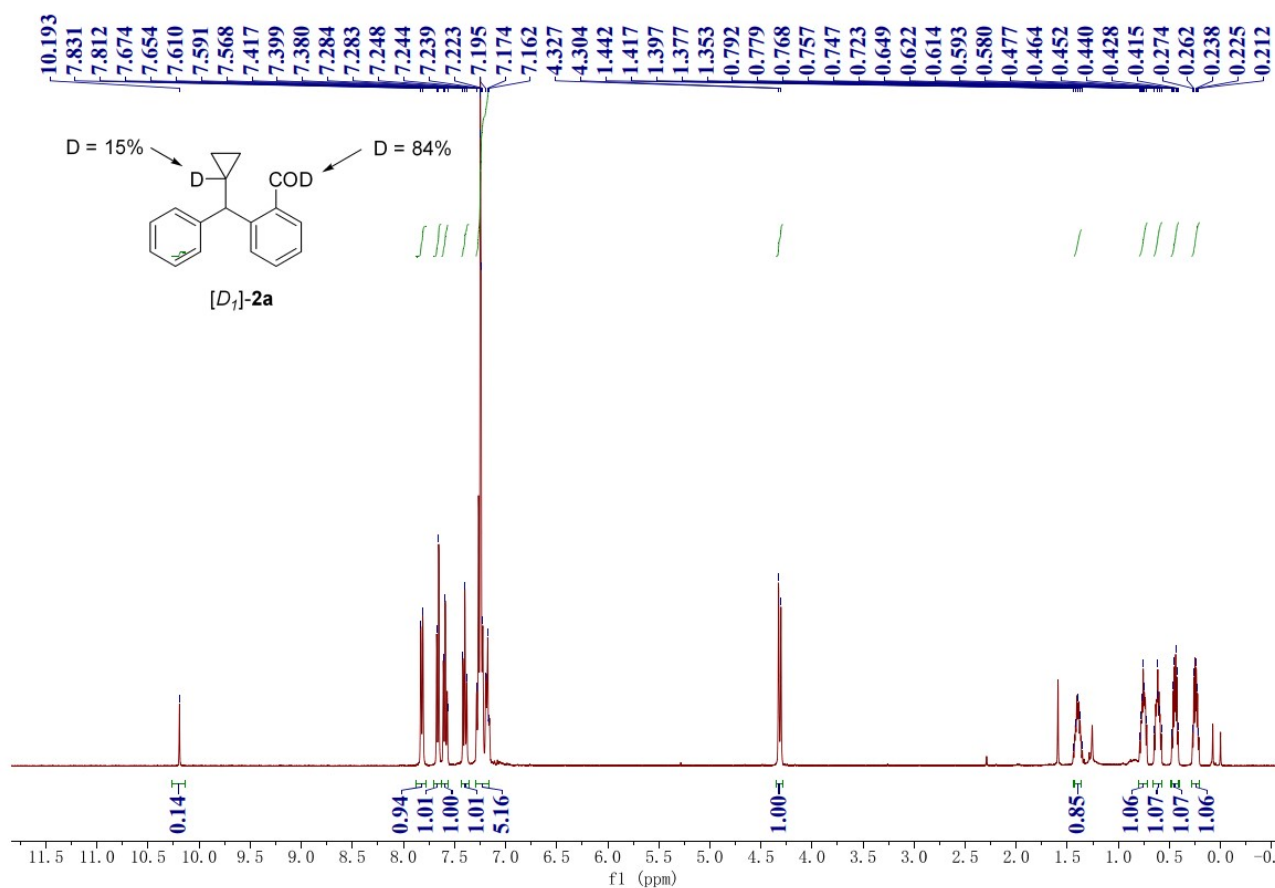
Experimental procedure:

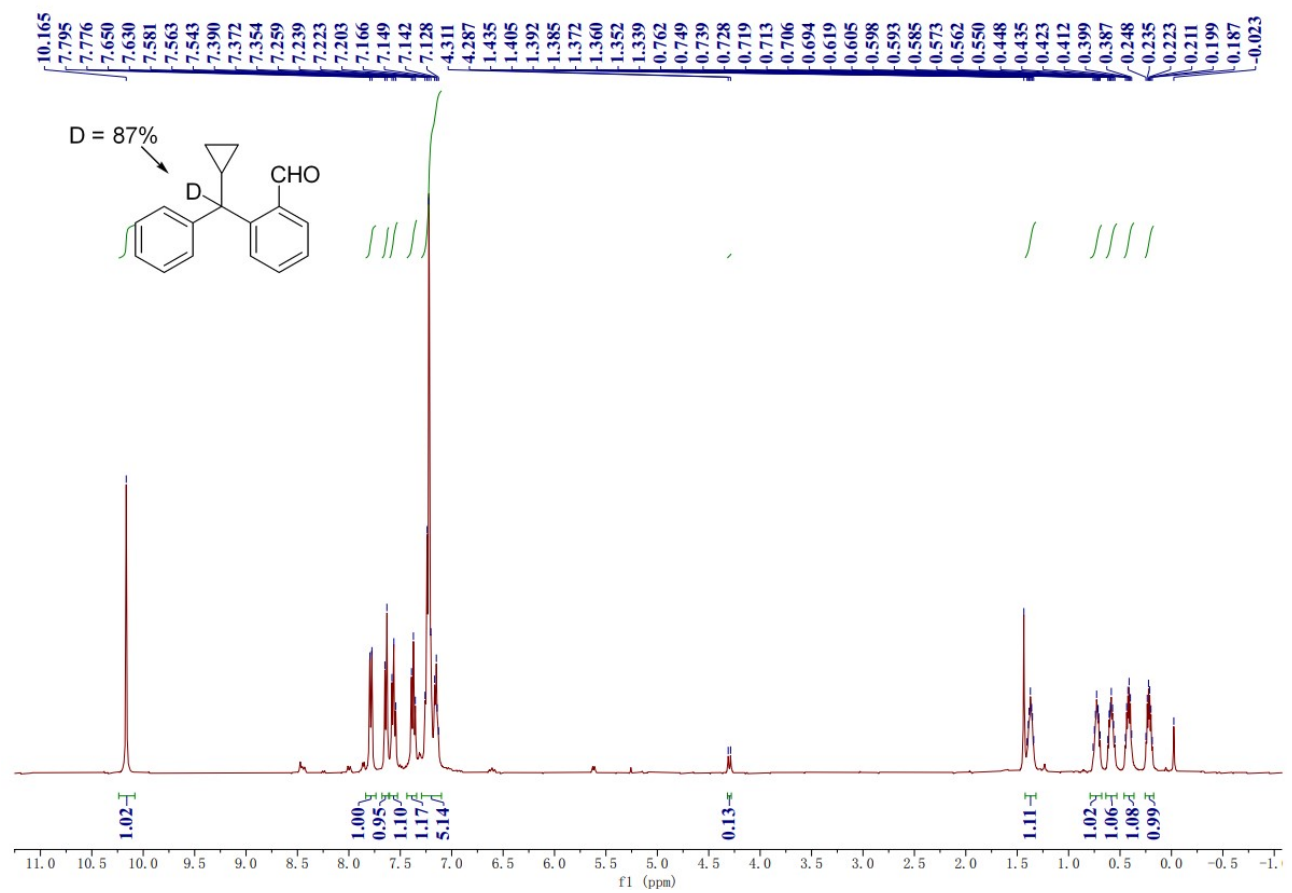
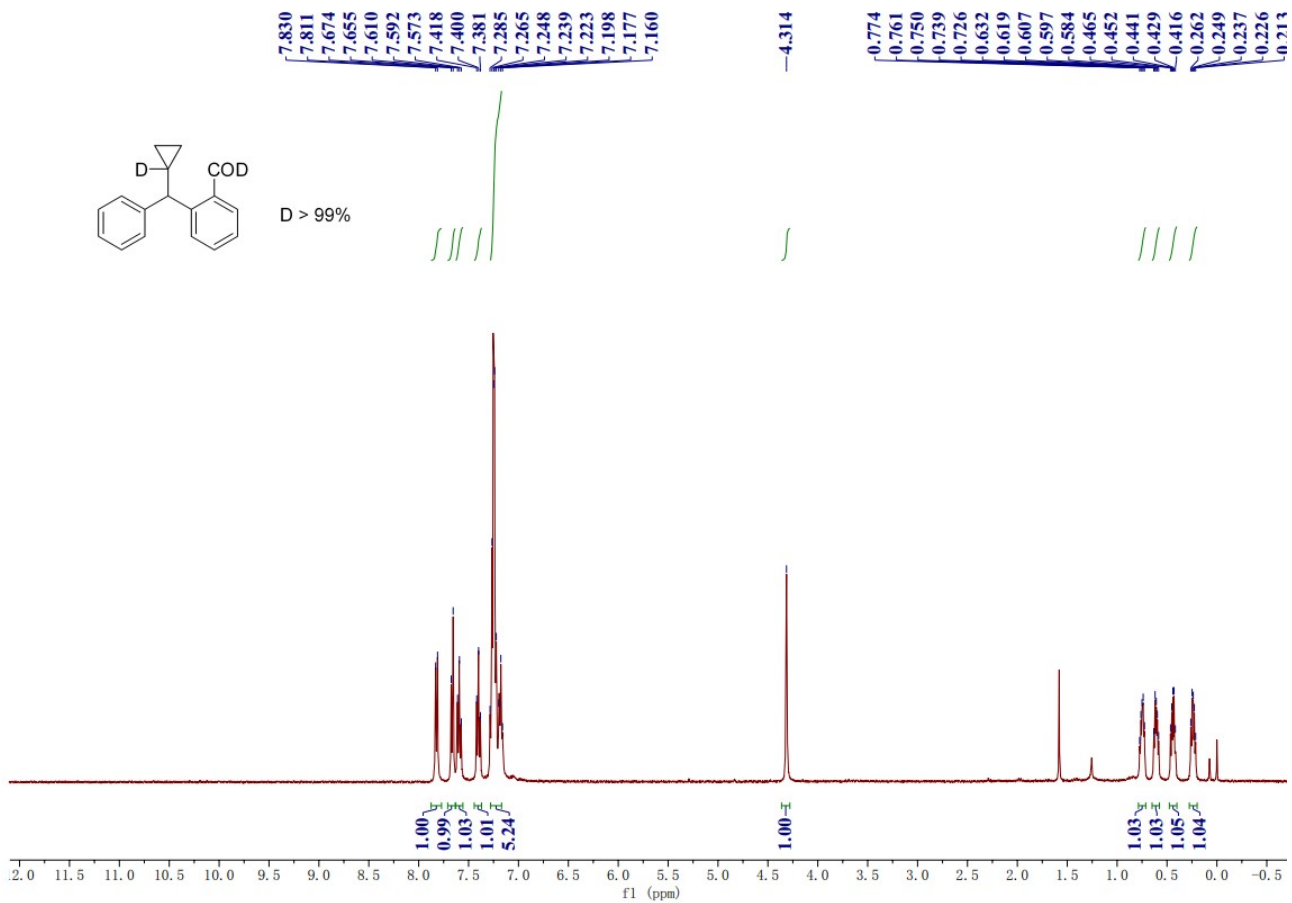
a) To a 10.0 mL sealed tube were added substrate [D_1]-**1a** (0.20 mmol, 1.0 equiv), Ir(dF-CF₃-ppy)₂(dtbbpy)PF₆ (0.004 mmol, 0.02 equiv), and CH₃CN (2.0 mL), then the resulting mixture was bubbled with argon for 15 minutes. The resulting mixture was stirred upon irradiation of 5 W blue LEDs at rt for 12 hours. Then, the solvent was removed under vacuum and the residue was purified by a silica gel column chromatography (petroleum ether: ethyl acetate = 10 : 1) to give the desired product [D_1]-**2a** in 55% yield.

b) To a 10.0 mL sealed tube were added substrate [D_2]-**1a** (0.20 mmol, 1.0 equiv), Ir(dF-CF₃-ppy)₂(dtbbpy)PF₆ (0.004 mmol, 0.02 equiv), and CH₃CN (2.0 mL), then the resulting mixture was bubbled with argon for 15 minutes. The resulting mixture was stirred upon irradiation of 5 W blue LEDs at rt for 24 hours. Then, the solvent was removed under vacuum and the residue was purified

by a silica gel column chromatography (petroleum ether: ethyl acetate = 10 : 1) to give the desired product $[D_2]$ -**2a** in 50% yield with 99% D content.

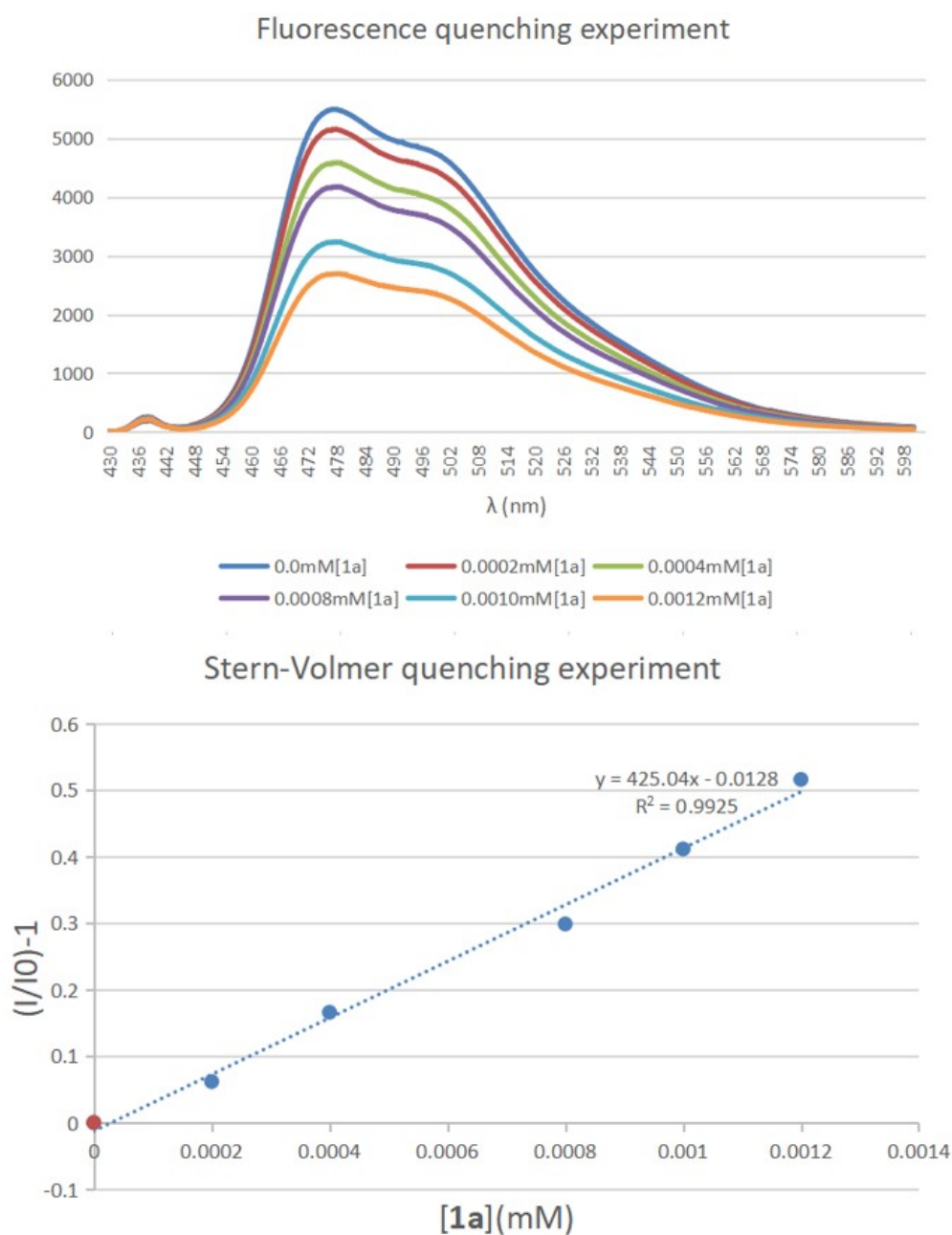
c) To a 10.0 mL sealed tube were added substrate $[D_1]$ -**1a'** (0.20 mmol, 1.0 equiv), Ir(dF-CF₃-ppy)₂(dtbbpy)PF₆ (0.004 mmol, 0.02 equiv), and CH₃CN (2.0 mL), then the resulting mixture was bubbled with argon for 15 minutes. The resulting mixture was stirred upon irradiation of 5 W blue LEDs at rt for 24 hours. Then, the solvent was removed under vacuum and the residue was purified by a silica gel column chromatography (petroleum ether: ethyl acetate = 10 : 1) to give the desired product $[D_1]$ -**2a'** in 91% yield with 87% D content.





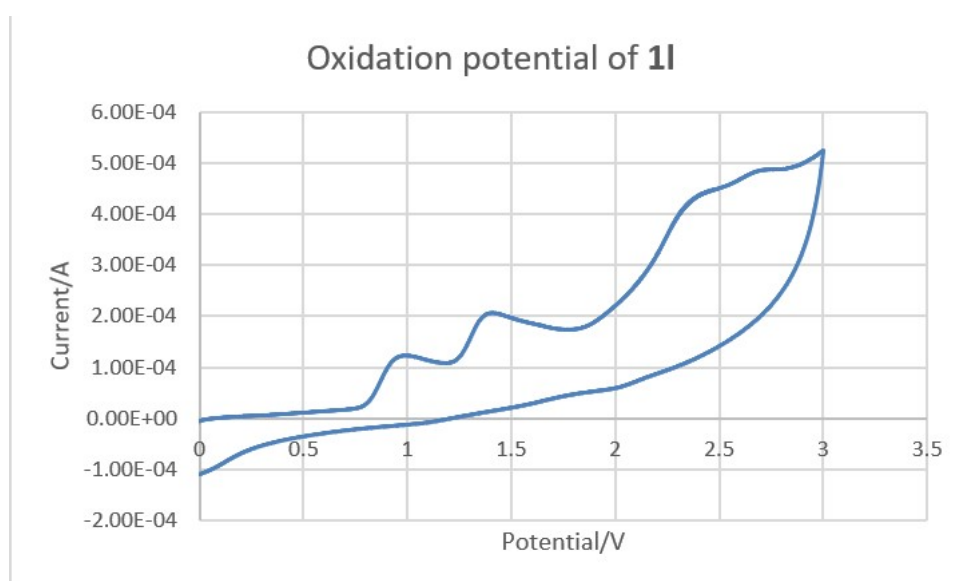
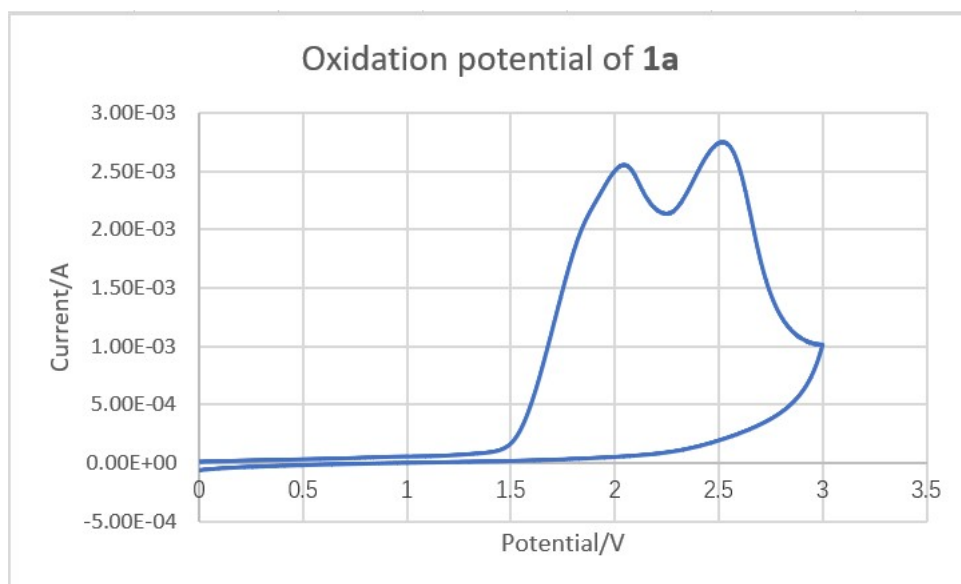
4.2 Luminescence quenching experiments (Stern-Volmer studies).

Emission intensities were recorded using a Hitachi F-4600 FL spectrophotometer with a 10 nm band width. Different concentration of **1a** solutions were prepared and added to a 1 cm path length quartz cuvette fitted with a Teflon® septum under argon atmosphere. In this experiment, the appropriate amount of **1a** was added to a 0.001 M photocatalyst solution in MeCN under an argon atmosphere and the emission from the sample was collected. The photocatalyst was excited at 435 nm and the emission intensity is collected at 430-600 nm.



4.3 Cyclic Voltammetry Experiments

Cyclic Voltammogram was recorded by the CH Instruments Electrochemical Workstation model CHI760E used a Pt as counter electrode, a glassy carbon as working electrode and a saturated glycerol electrode as reference electrode. A solution of the substrates **1a** or **1l** in MeCN (0.1 M) was tested with 0.1 M Bu₄NPF₆ as the supporting electrolyte. Scan rate = 0.1 V/s.



4.3 Quantum Yield and Light on/off Experiments

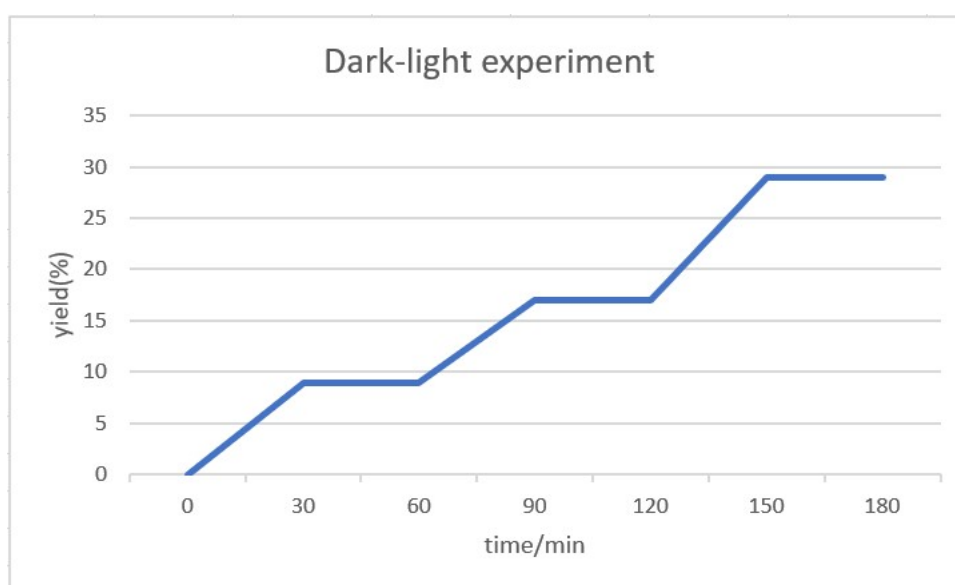
To further investigate whether the reaction involved a chain process, we measured the quantum yield of the reaction of **1a**.

$$\phi = \frac{n_x}{n_p} = \frac{n_x}{\frac{\Delta E \times S \times t}{N_A h \nu}} = \frac{n_x \times N_A \times h \times c}{\Delta E \times S \times t \times \lambda}$$

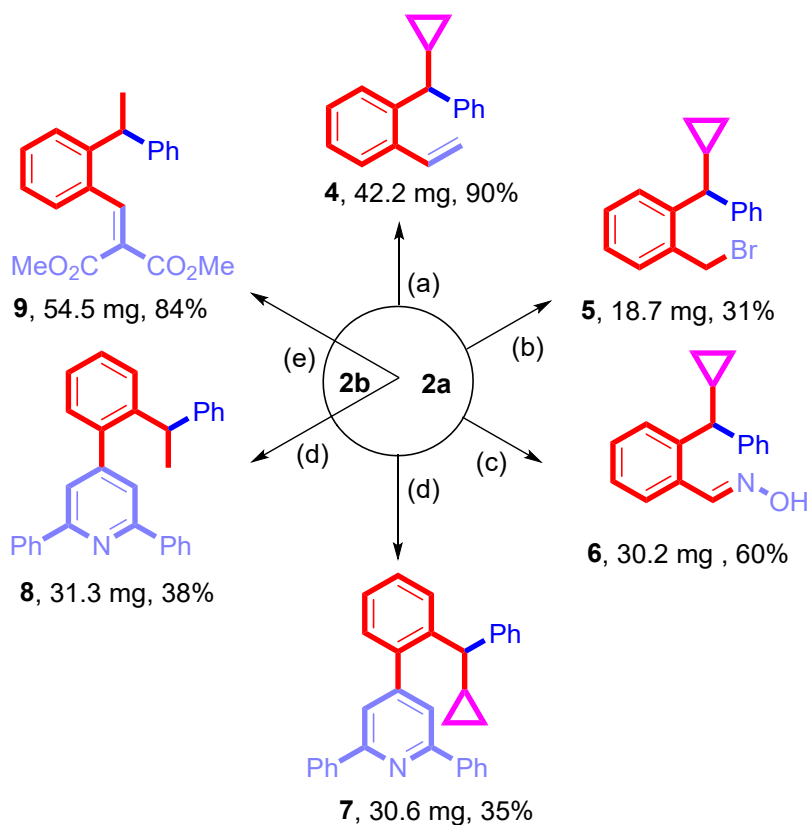
n_x is the amount of photochemical or photophysical events x occurred during irradiation, n_p is the number of photons absorbed by the reactant. E is the radiant power. S is the irradiated area. t is the irradiated time. N_A is the Avogadro constant. h is the Planck constant. ν is the frequency of incident light. n_x was analyzed by ^1H NMR, ΔE was measured by ILT1400 Portable Radiometer/Photometer.⁵

To a cuvette were added substrate **1** (0.20 mmol, 1.0 equiv), Ir(dF-CF₃-ppy)₂(dtbbpy)PF₆ (0.004 mmol, 0.02 equiv), and CH₃CN (2.0 mL), then the resulting mixture was bubbled with argon for 15 minutes. The resulting mixture was stirred upon irradiation of 100 W blue LEDs at rt for 30 min. The reaction mixture was concentrated in *vacuo* and analyzed by ^1H NMR spectrum using 1,3,5-trimethoxybenzene as an internal standard. The quantum yield is calculated to be 0.13.

In the control experiment shown below, successive intervals of irradiation and dark periods. The result was that the reaction process was completely interrupted in the absence of light and resumed with further light, demonstrating that continuous light is necessary for the **1a** to **2a** conversion process.



5. Transformation of the products



(a) Methyltriphenylphosphonium bromide (0.40 mmol, 2.0 equiv) and dry THF (5.0 mL) were added to a flame-dried Schlenk tube under argon atmosphere and then *t*-BuOK (1.0 M in THF, 0.4 mL, 2.0 equiv) was added dropwise. The resulting mixture was stirred at room temperature for 30 minutes, then **2a** (0.2 mmol) was added and stirred for 3 h before quenching with a HCl (1.0 M) solution and extracted three times with EtOAc. The combine organic phase was dried over anhydrous Na₂SO₄. The organic phase was concentrated under reduced pressure and purified by a silica gel column chromatography to obtain the corresponding product **4**.

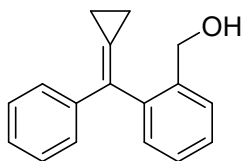
(b) To a flame-dried Schlenk tube were added **2a** (0.20 mmol, 1.0 equiv), phenylsilane (0.24 mmol, 1.2 equiv), boron tribromide (0.24 mmol, 1.2 equiv, 0.24 mL 1.0 M solution in DCM) and anhydrous DCM (0.6 mL) under argon. The resulting mixture was stirred for 3 h before quenching with a solution of pinacol (0.6 mmol, 3.0 equiv) in Et₃N (1.0 mL). The organic phase was concentrated under reduced pressure and purified by a silica gel column chromatography to obtain the corresponding product **5**.

(c) To a flame-dried Schlenk tube were added **2a** (0.20 mmol, 1.0 equiv), $\text{NH}_2\text{OH}\cdot\text{HCl}$ (0.24 mmol, 1.2 equiv), CH_3COONa (0.24 mmol, 1.2 equiv) and $\text{HCOOH}/\text{H}_2\text{O}$ (2.0 mL, 3 : 2) and the resulting mixture was stirred at 80 °C for 3 h. The organic phase was concentrated under reduced pressure and purified by a silica gel column chromatography to obtain the corresponding product **6**

(d) To a flame-dried Schlenk tube were added **2a** (0.20 mmol, 1.0 equiv) or **2b** (0.20 mmol, 1.0 equiv), phenylacetophenone (0.60 mmol, 3.0 equiv), NH_4I (0.40 mmol, 2 equiv), DMSO (0.60 mmol, 3.0 equiv) and PhCl (0.8 mL) and the resulting mixture was stirred at 130 °C for 12 h under molecular oxygen (1.0 atm). The organic phase was concentrated under reduced pressure and purified by a silica gel column chromatography to obtain the corresponding products **7** or **8**.

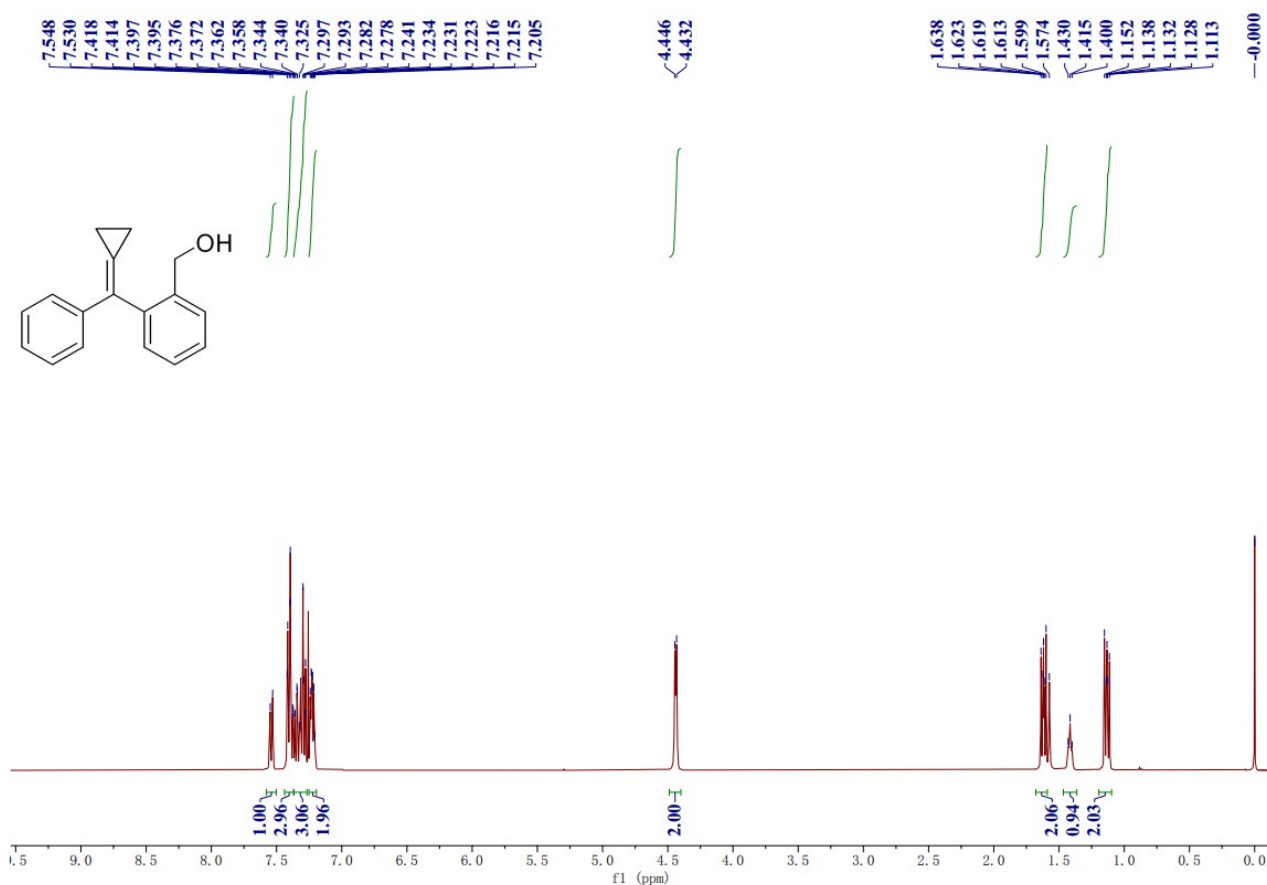
(e) To a flame-dried Schlenk tube were added **2b** (0.20 mmol, 1.0 equiv), dimethyl malonate (0.40 mmol, 2 equiv) AcOH (0.02 mmol, 10 mol%), piperazine (0.02 mmol, 10 mol%), and toluene (2.0 mL) and the resulting mixture was stirred at 100 °C for 12 h. The organic phase was concentrated under reduced pressure and purified by a silica gel column chromatography to obtain the corresponding product **9**.

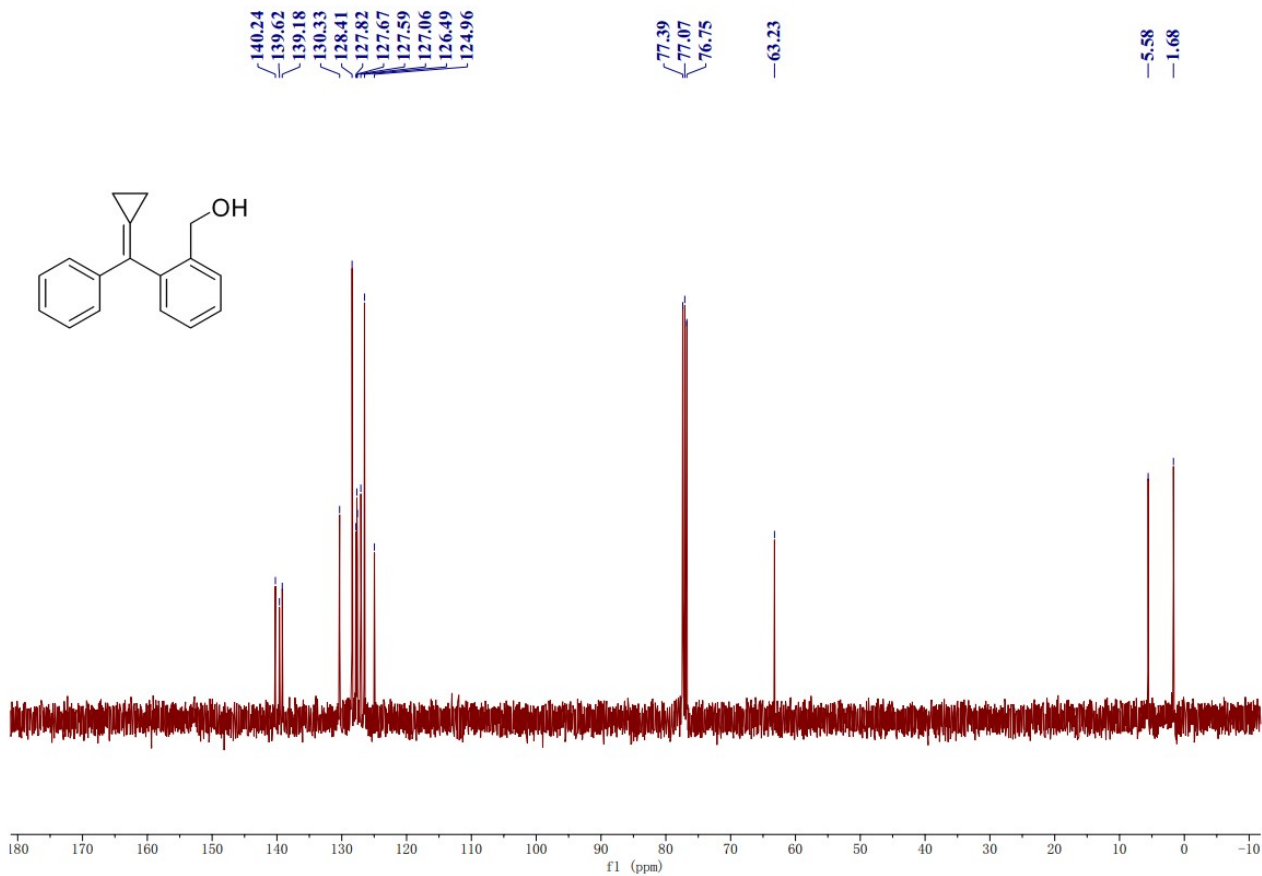
6. Spectroscopic data of substrates 1

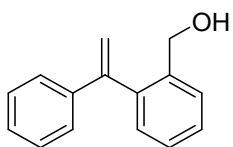


(2-(cyclopropylidene(phenyl)methyl)phenyl)methanol (1a)

A white solid, M.P.: 116-118 °C, 2100 mg, 82% yield. ¹H NMR (CDCl₃, TMS, 400 MHz) δ 7.54 (d, *J* = 7.2 Hz, 1H), 7.42 -7.37 (m, 3H), 7.34-7.27 (m, 3H), 7.24-7.20 (m, 2H), 4.44 (d, *J* = 6.0 Hz, 2H), 1.64-1.57 (m, 2H) 1.42 (t, *J* = 6.0 Hz, 1H), 1.15-1.11 (m, 2H). ¹³C NMR (CDCl₃, TMS, 100 MHz) δ 140.2, 139.6, 139.2, 130.3, 128.4, 127.8, 127.7, 127.6, 127.1, 126.5, 125.0, 77.4, 77.1, 76.8, 63.2, 5.6, 1.7. IR (acetone) ν 3274, 3050, 2923, 1596, 1490, 1442, 1364, 1158, 1004, 835 cm⁻¹. HRMS (EI) Calcd. for C₁₇H₁₆O (M⁺): 238.1196, Found: 238.1194.

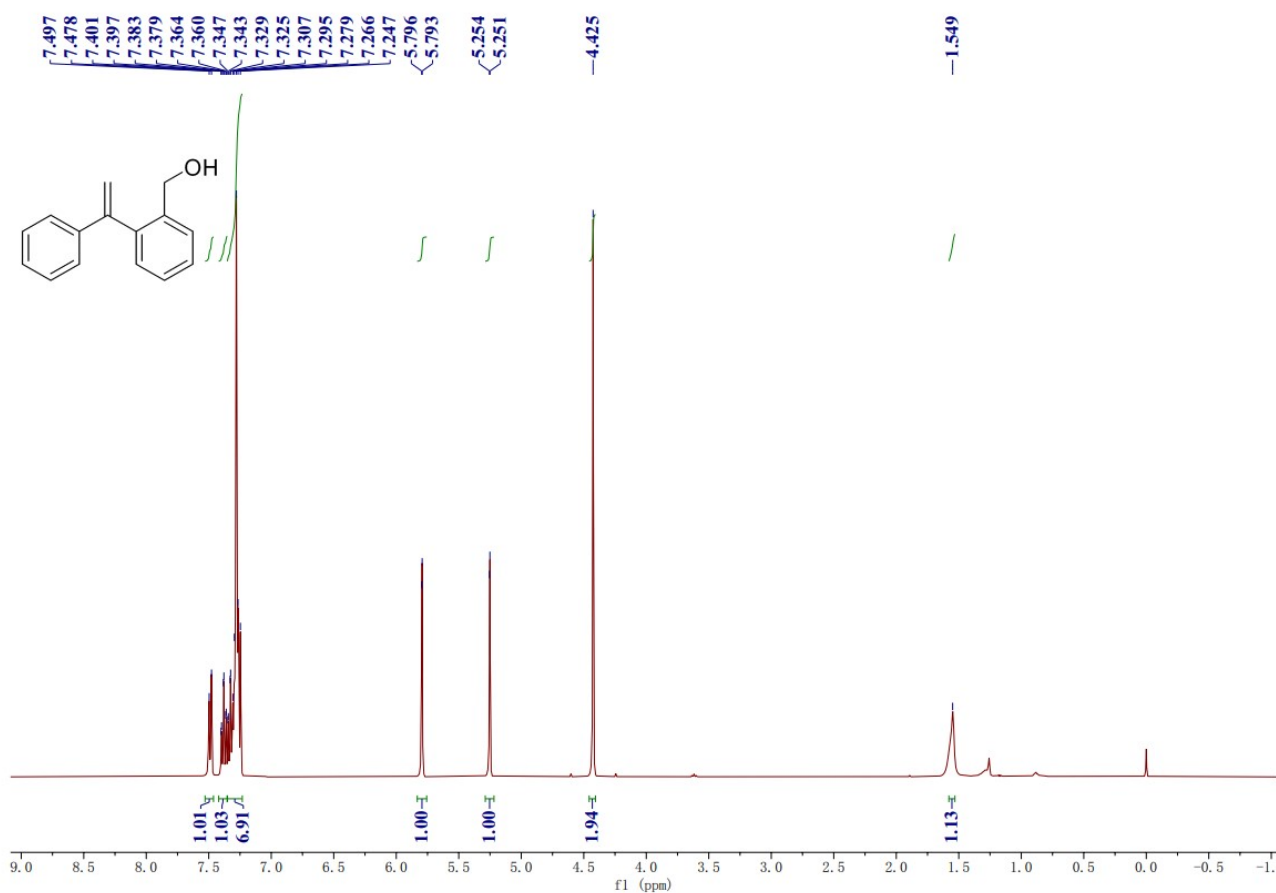


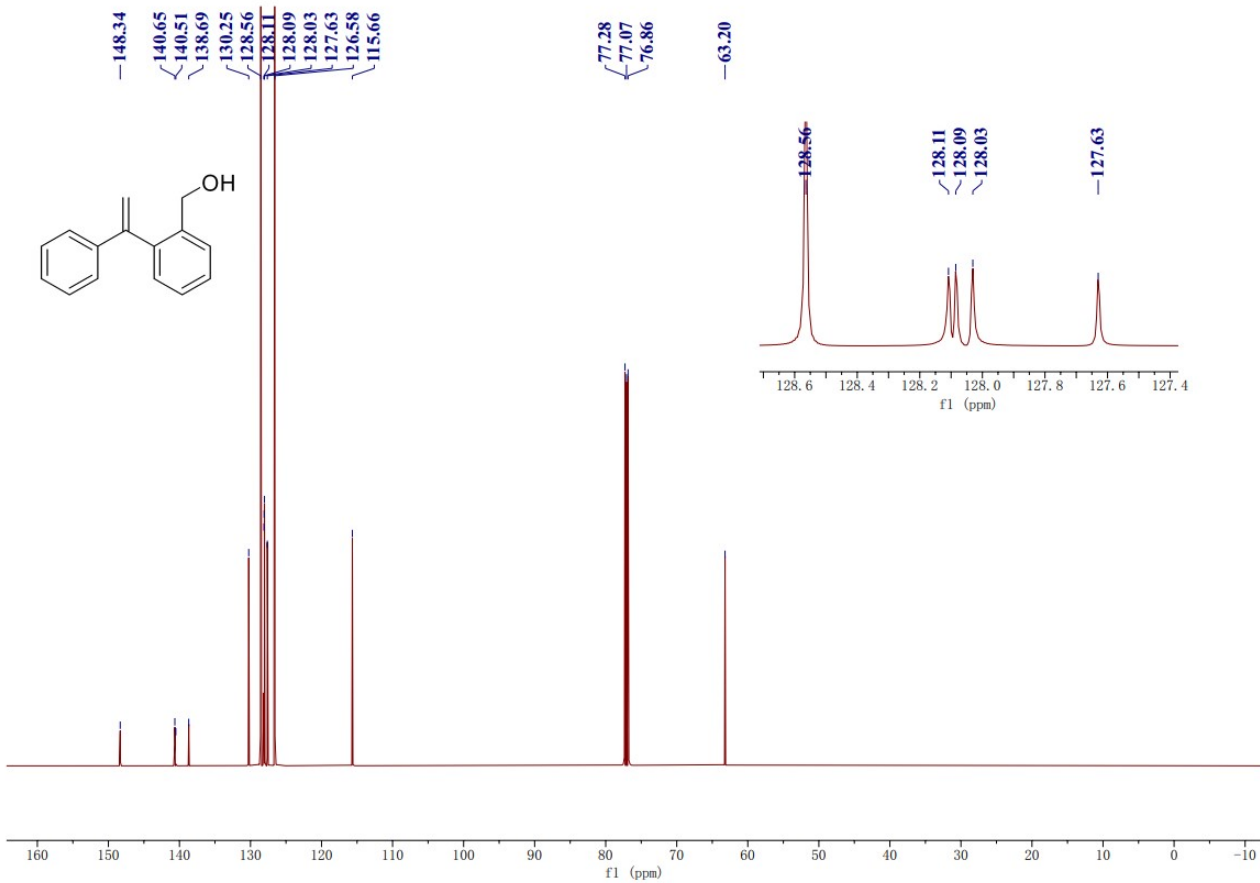


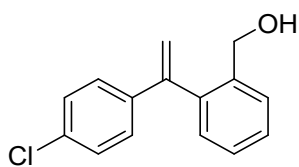


(2-(1-phenylvinyl)phenyl)methanol (1b)

This is a known compound and its spectroscopic data are consistent with those in the previous literature.¹ CAS number: 71264-86-3. A colorless oil. 908 mg, 80% yield. ¹H NMR (CDCl₃, TMS, 400 MHz) δ 7.49 (d, *J* = 7.6 Hz, 1H), 7.40-7.36 (m, 1H), 7.35-7.25 (m, 7H), 5.79 (d, *J* = 1.4 Hz, 1H), 5.25 (d, *J* = 1.4 Hz, 1H), 4.43 (s, 2H), 1.55 (br, 1H). ¹³C NMR (CDCl₃, TMS, 150 MHz) δ 148.3, 140.6, 140.5, 138.7, 130.2, 128.6, 128.1, 128.1, 128.0, 127.6, 126.6, 115.7, 63.2.

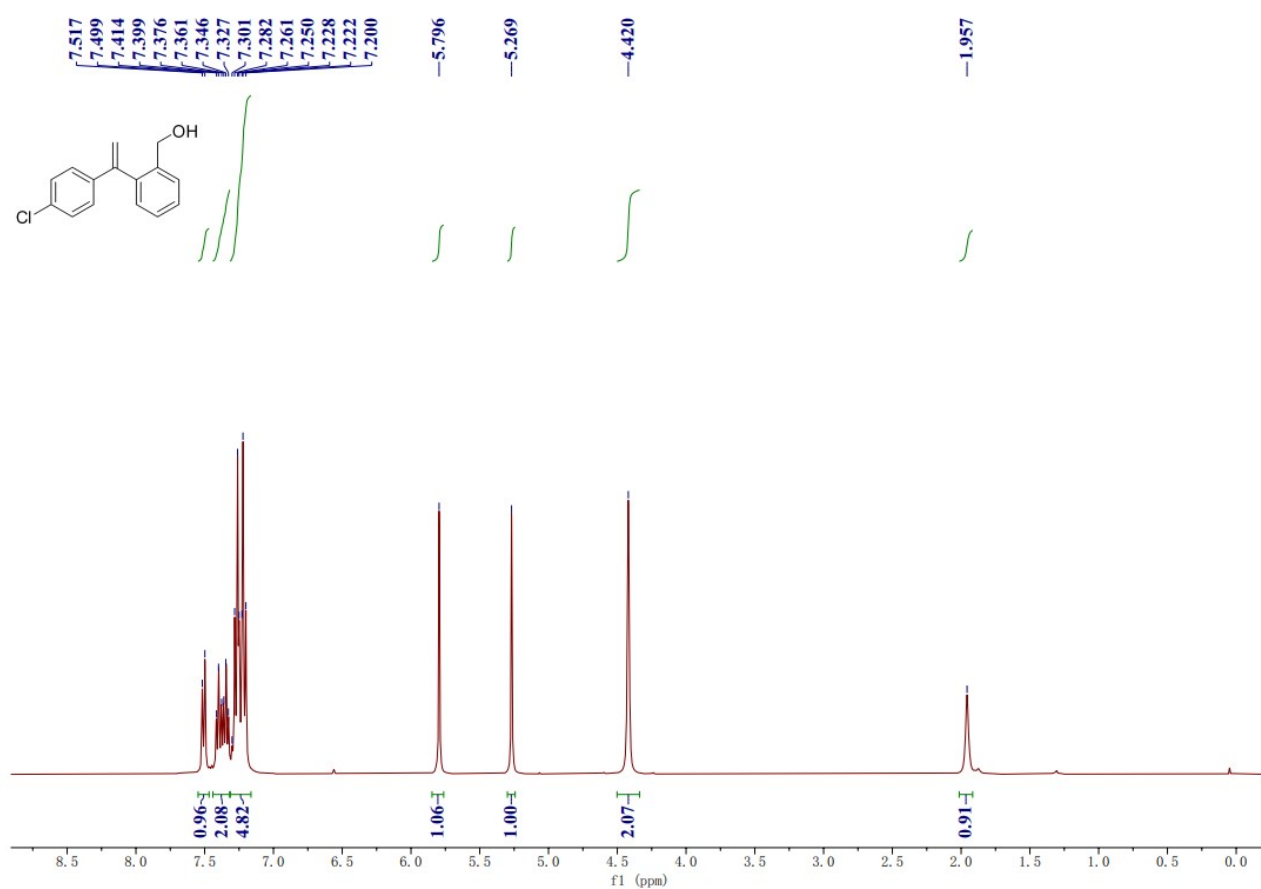


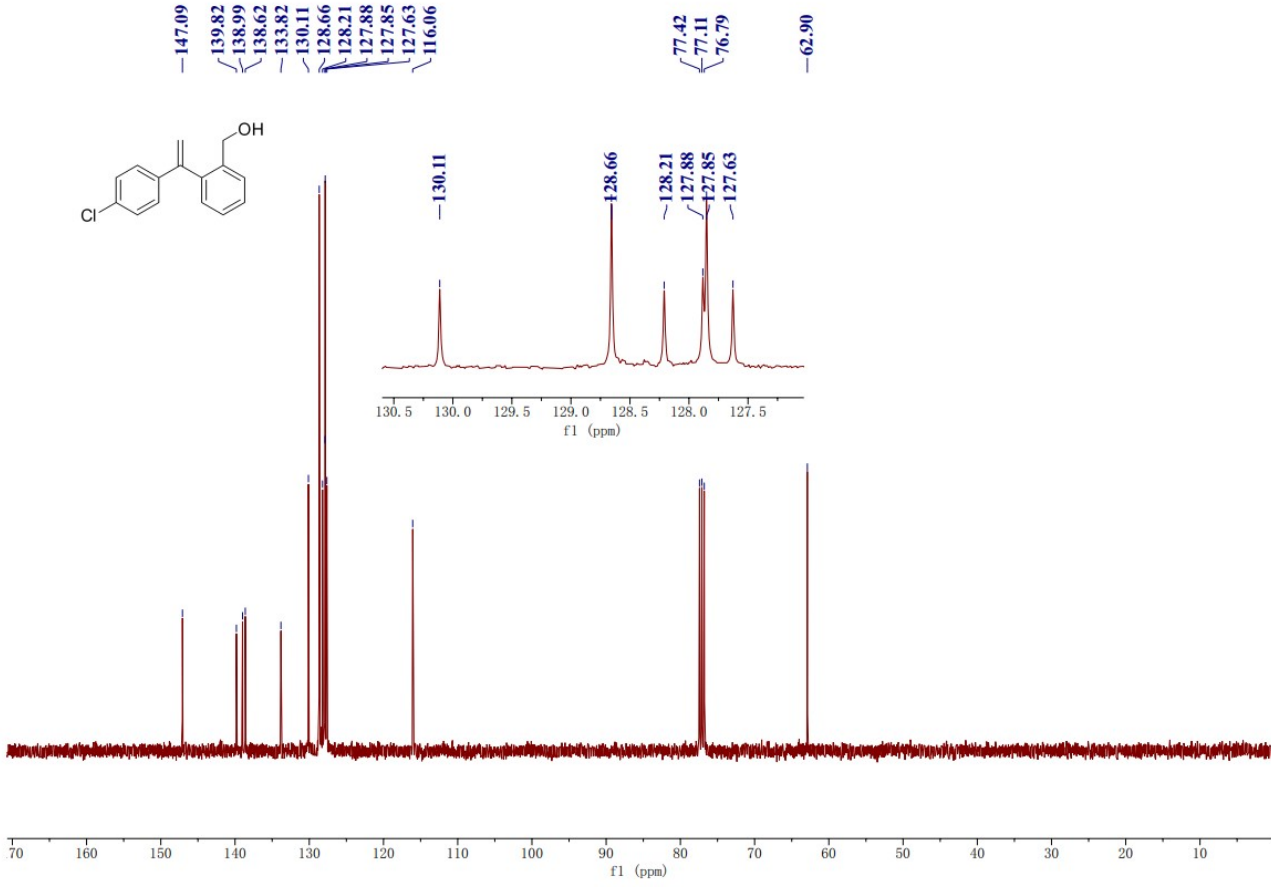


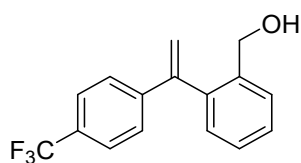


(2-(1-(4-chlorophenyl)vinyl)phenyl)methanol (1c)

This is a known compound and its spectroscopic data are consistent with those in the previous literature.¹ CAS number: 98216-74-1. A colorless oil. 843 mg, 71% yield. ¹H NMR (CDCl₃, TMS, 400 MHz) δ 7.51 (d, *J* = 7.6 Hz, 1H), 7.41-7.33 (m, 2H), 7.30-7.20 (m, 5H), 5.80 (s, 1H), 5.27 (s, 1H), 4.42 (s, 2H), 1.96 (s, 1H). ¹³C NMR (CDCl₃, TMS, 100 MHz) δ 147.1, 139.8, 139.0, 138.6, 133.8, 130.1, 128.7, 128.2, 127.88, 127.85, 127.6, 116.1, 62.9.

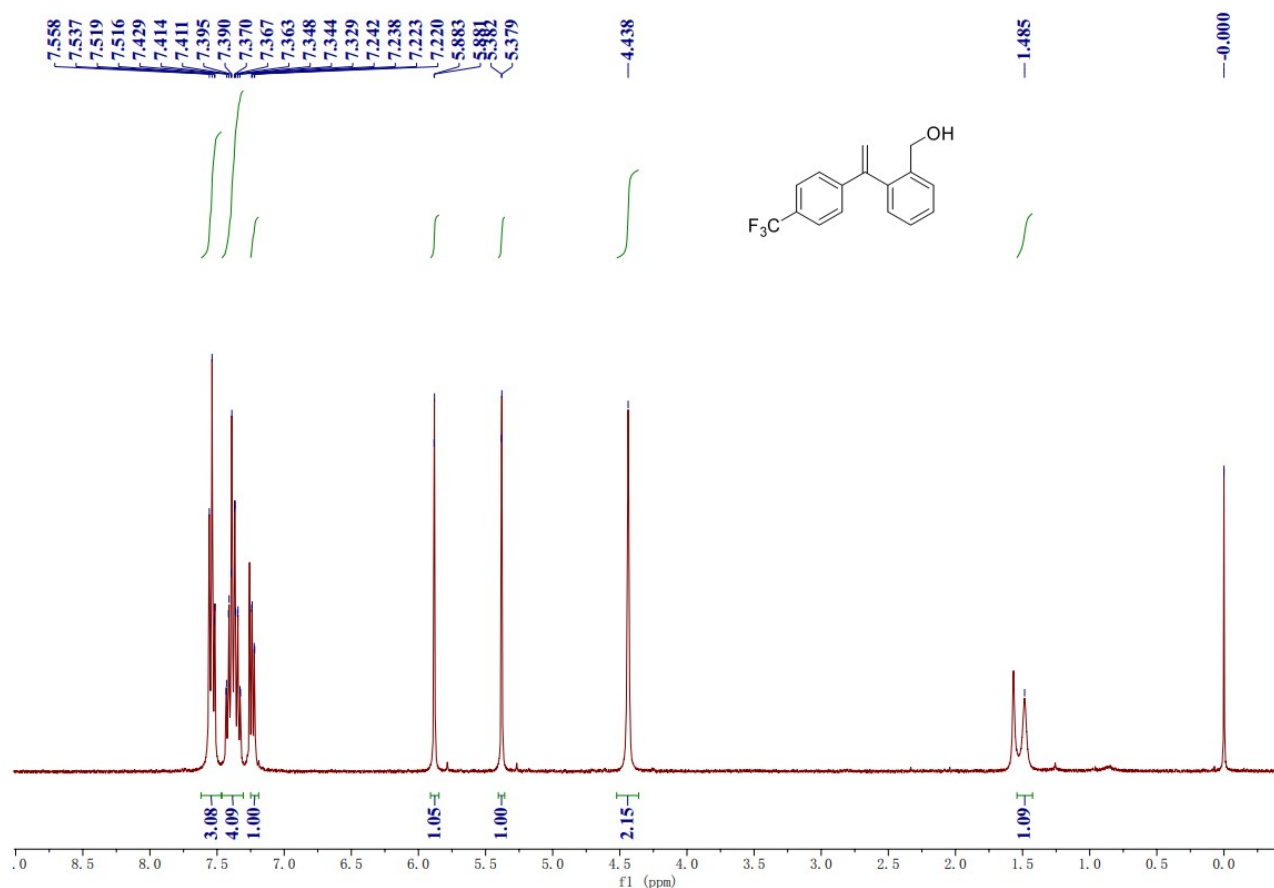


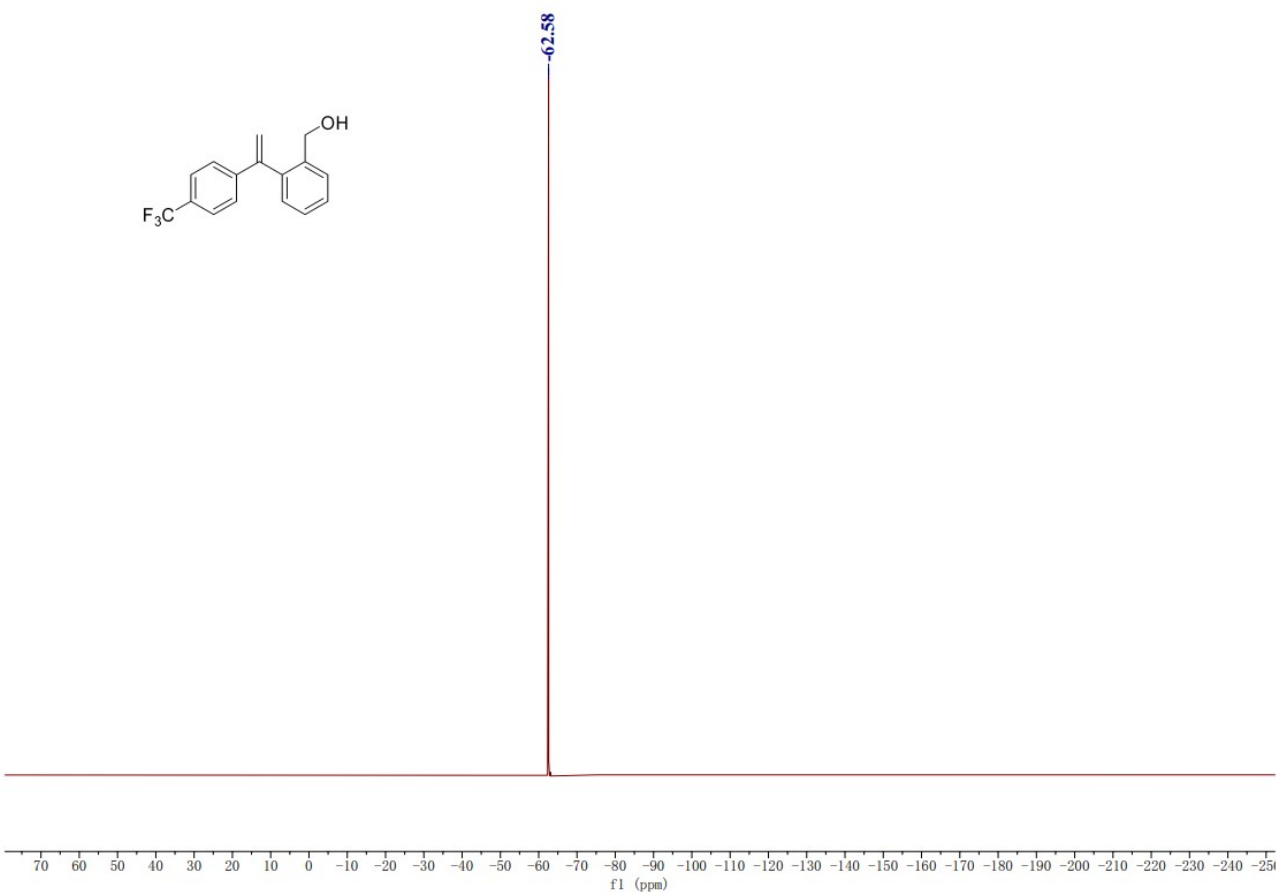
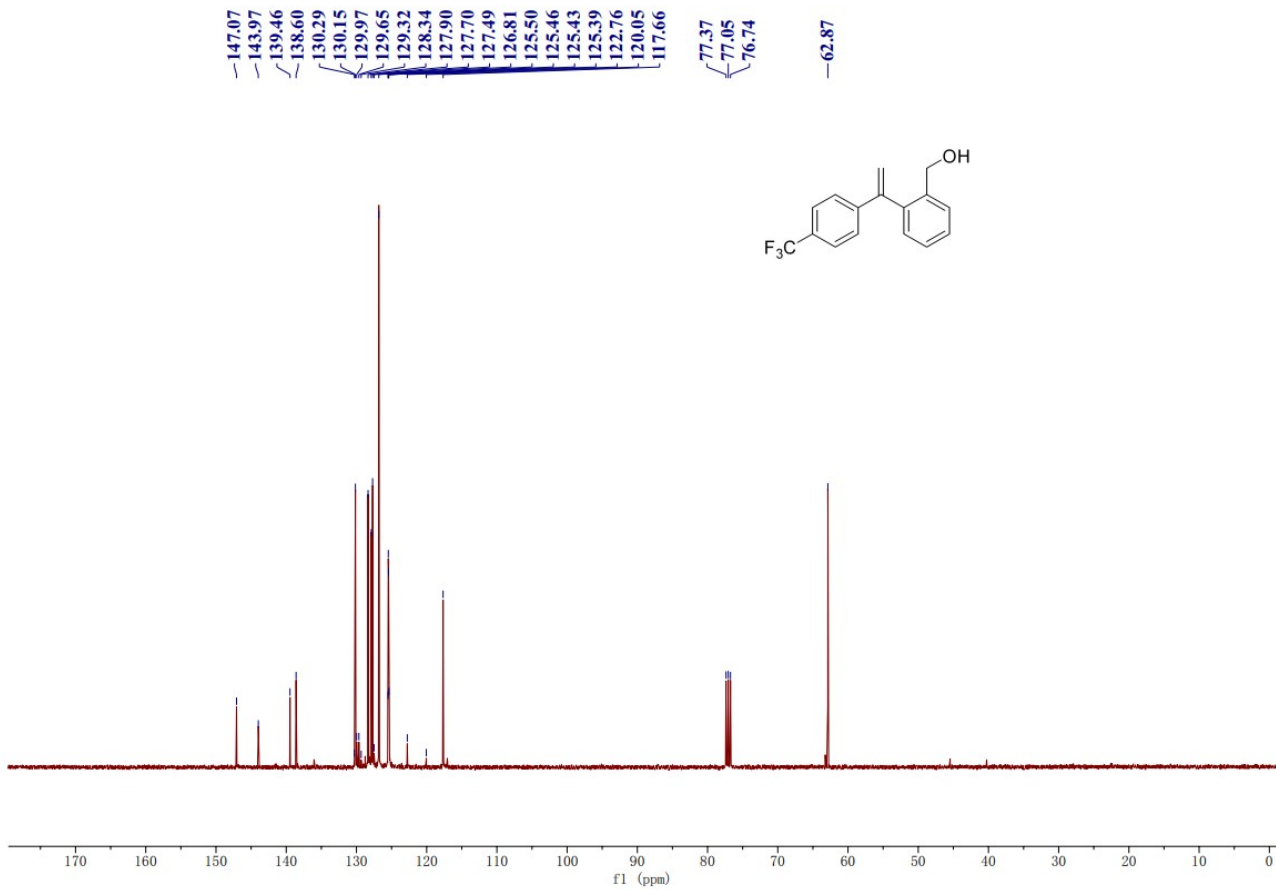


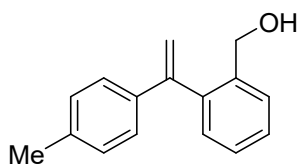


(2-(1-(4-(trifluoromethyl)phenyl)vinyl)phenyl)methanol (1d)

This is a known compound and its spectroscopic data are consistent with those in the previous literature.⁴ CAS number: 345295-66-1. A colorless oil. 608 mg, 78% yield. ¹H NMR (CDCl₃, TMS, 400 MHz) δ 7.56-7.52 (m, 3H), 7.43-7.33 (m, 4H), 7.24-7.22 (m, 1H), 5.88 (d, *J* = 1.2 Hz, 1H), 5.38 (d, *J* = 1.2 Hz, 1H), 4.44 (s, 2H), 1.49 (s, 1H). ¹³C NMR (CDCl₃, TMS, 100 MHz) δ 147.1, 144.0, 139.5, 138.6, 130.2, 129.8 (q, *J* = 32.4 Hz), 128.3, 127.9, 127.7, 126.8, 125.5 (q, *J* = 3.8 Hz), 123.8 (q, *J* = 271.0 Hz), 117.7, 62.9. ¹⁹F NMR (CDCl₃, CFCl₃, 376 MHz) δ -62.6.

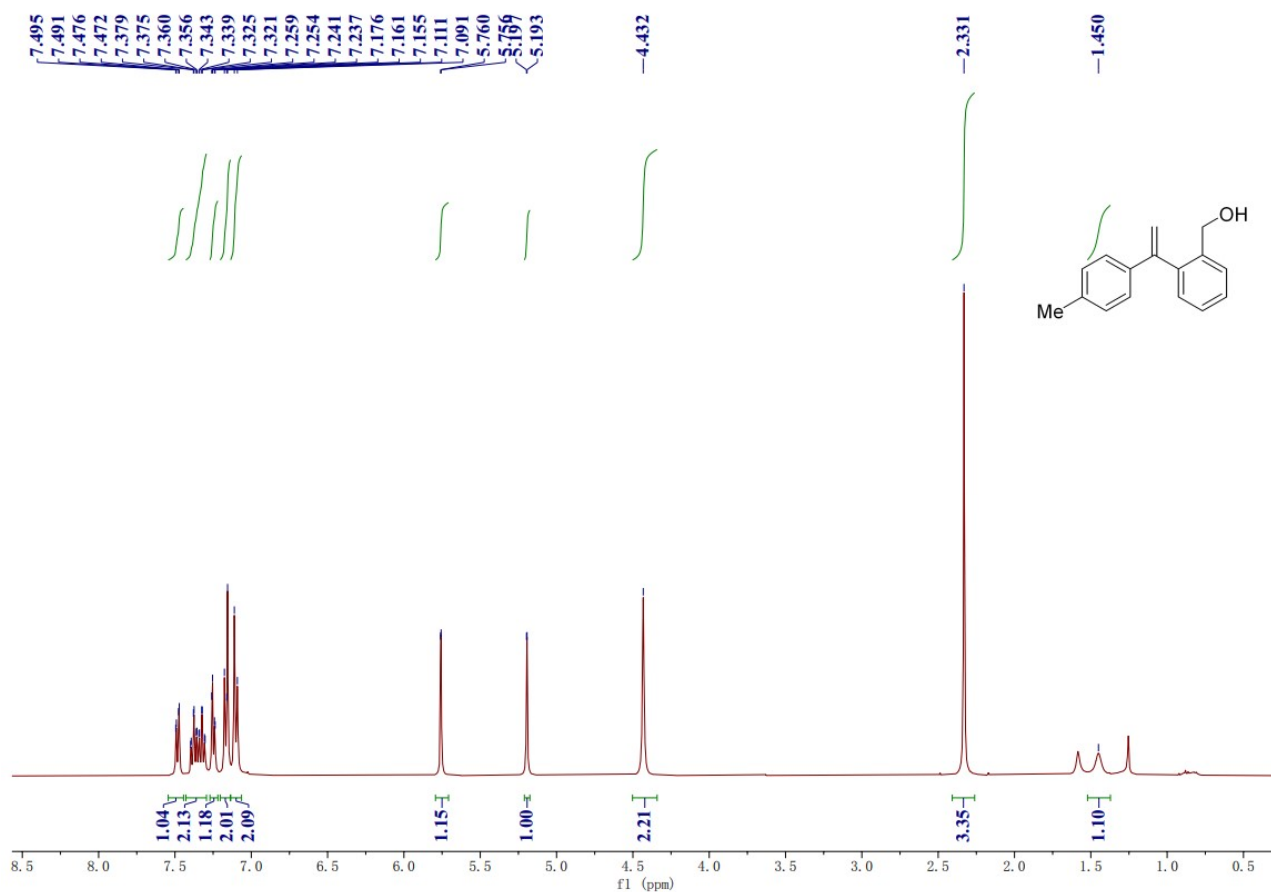


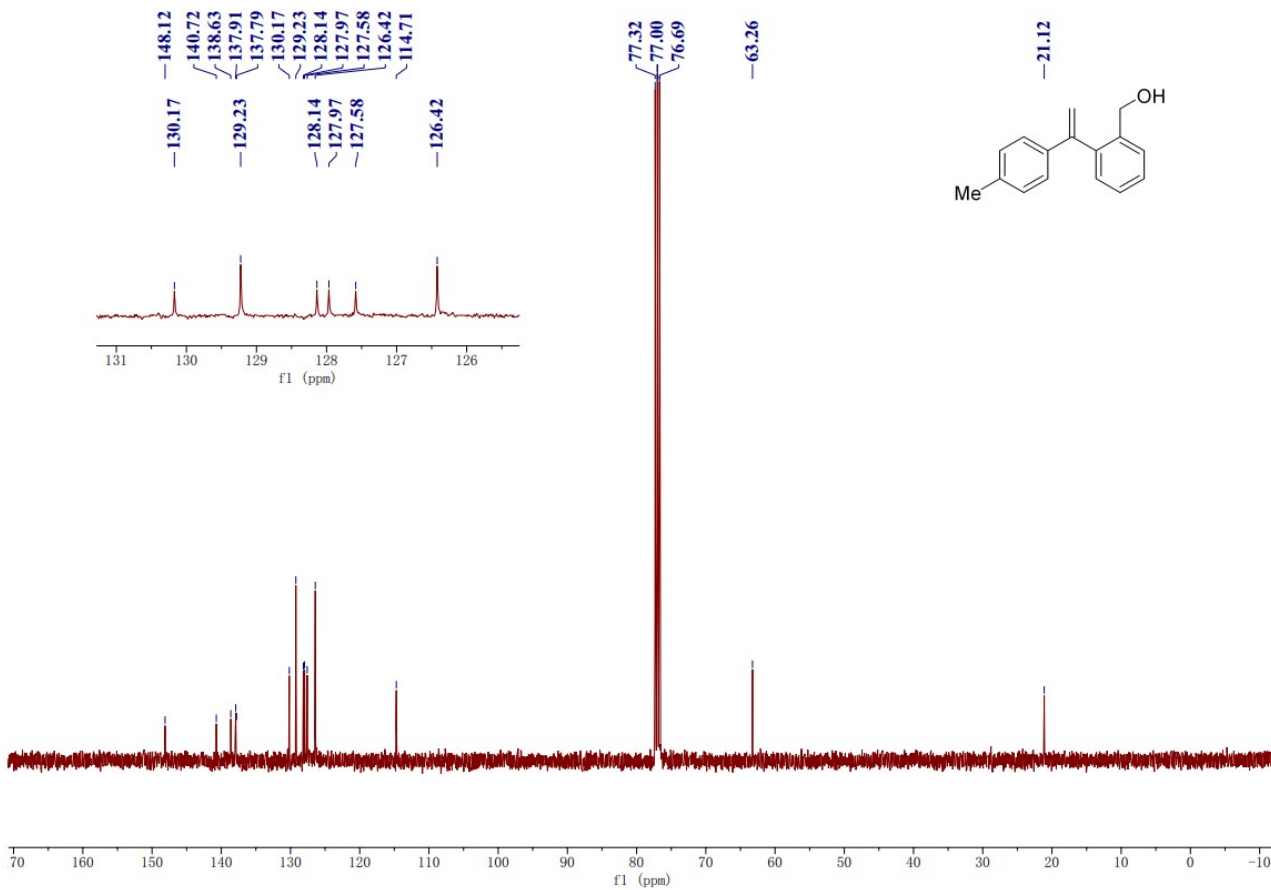


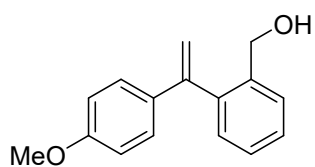


(2-(1-(p-tolyl)vinyl)phenyl)methanol (1e)

This is a known compound and its spectroscopic data are consistent with those in the previous literature.^[1] CAS number: 2001050-08-2. A colorless oil. 704 mg, 80% yield. ¹H NMR (CDCl₃, TMS, 400 MHz) δ 7.48 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.40-7.32 (m, 2H), 7.26-7.24 (m, 1H), 7.17 (d, *J* = 8.4 Hz, 2H), 7.10 (d, *J* = 8.0 Hz, 2H), 5.76 (d, *J* = 1.4 Hz, 1H), 5.19 (d, *J* = 1.4 Hz, 1H), 4.43 (s, 2H), 2.33 (s, 3H), 1.45 (s, 1H). ¹³C NMR (CDCl₃, TMS, 100 MHz) δ 148.1, 140.7, 138.6, 137.9, 137.8, 130.2, 129.2, 128.1, 128.0, 127.6, 126.4, 114.7, 63.3, 21.1.

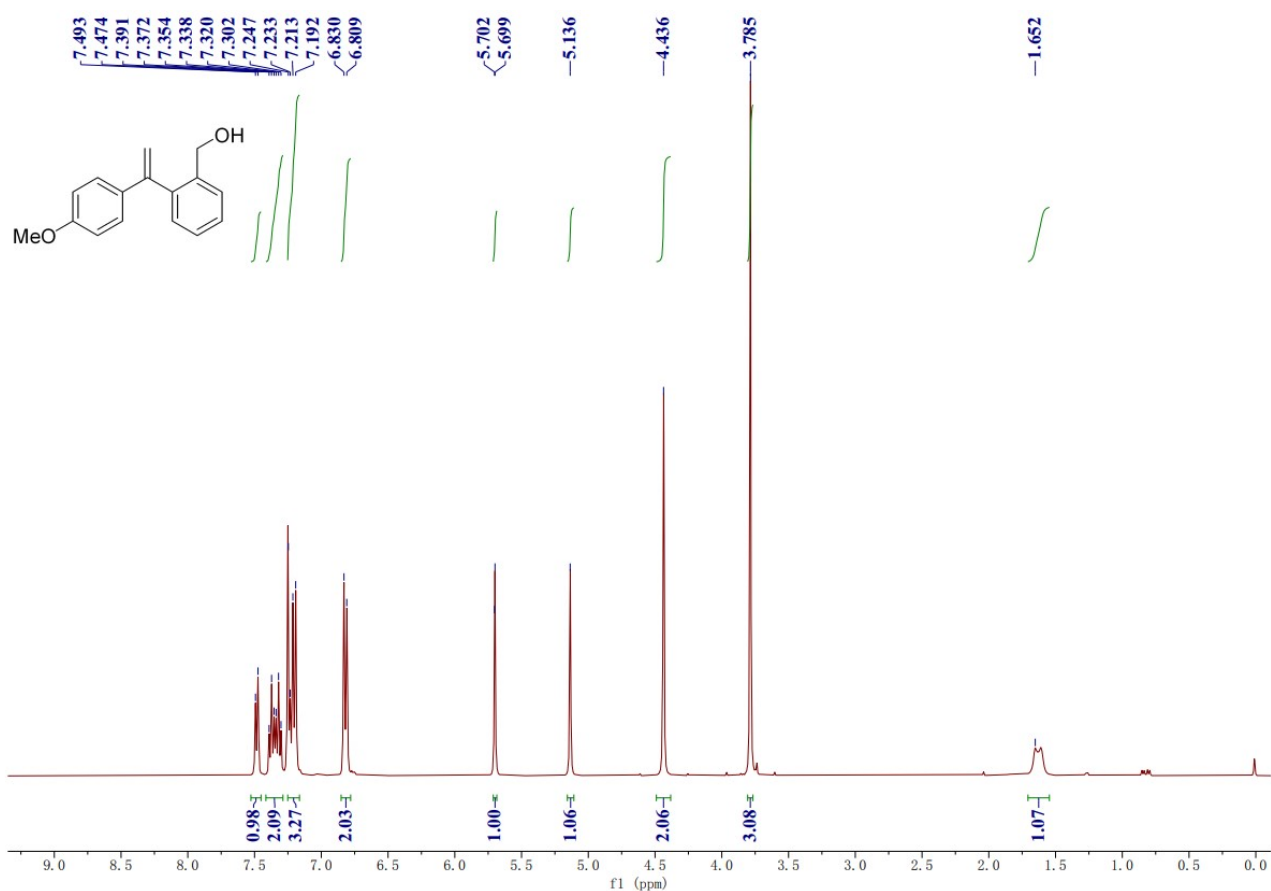


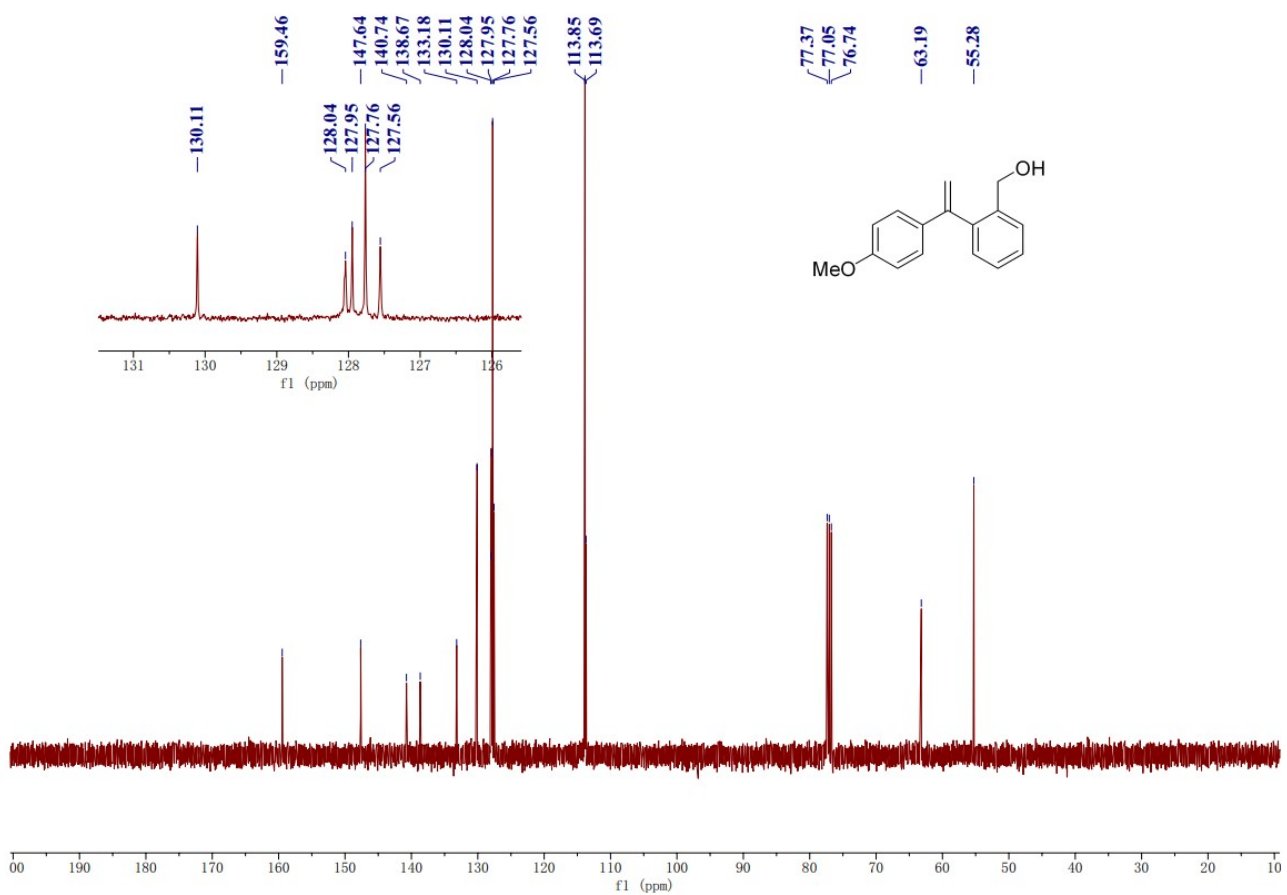


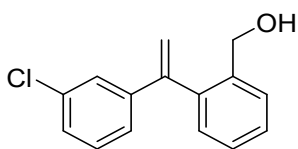


(2-(1-(4-methoxyphenyl)vinyl)phenyl)methanol (1f)

This is a known compound and its spectroscopic data are consistent with those in the previous literature.⁶ CAS number: 2001050-09-3. A white solid. 765 mg, 87% yield. ¹H NMR (CDCl₃, TMS, 400 MHz) δ 7.48 (d, *J* = 7.6 Hz, 1H), 7.39-7.30 (m, 2H), 7.25-7.19 (m, 3H), 6.82 (d, *J* = 8.4 Hz, 2H), 5.70 (s, 1H), 5.14 (s, 1H), 4.44 (s, 2H), 3.79 (s, 3H), 1.65 (br, 1H). ¹³C NMR (CDCl₃, TMS, 100 MHz) δ 159.5, 147.6, 140.7, 138.7, 133.2, 130.1, 128.0, 127.9, 127.8, 127.6, 113.9, 113.7, 63.2, 55.3.

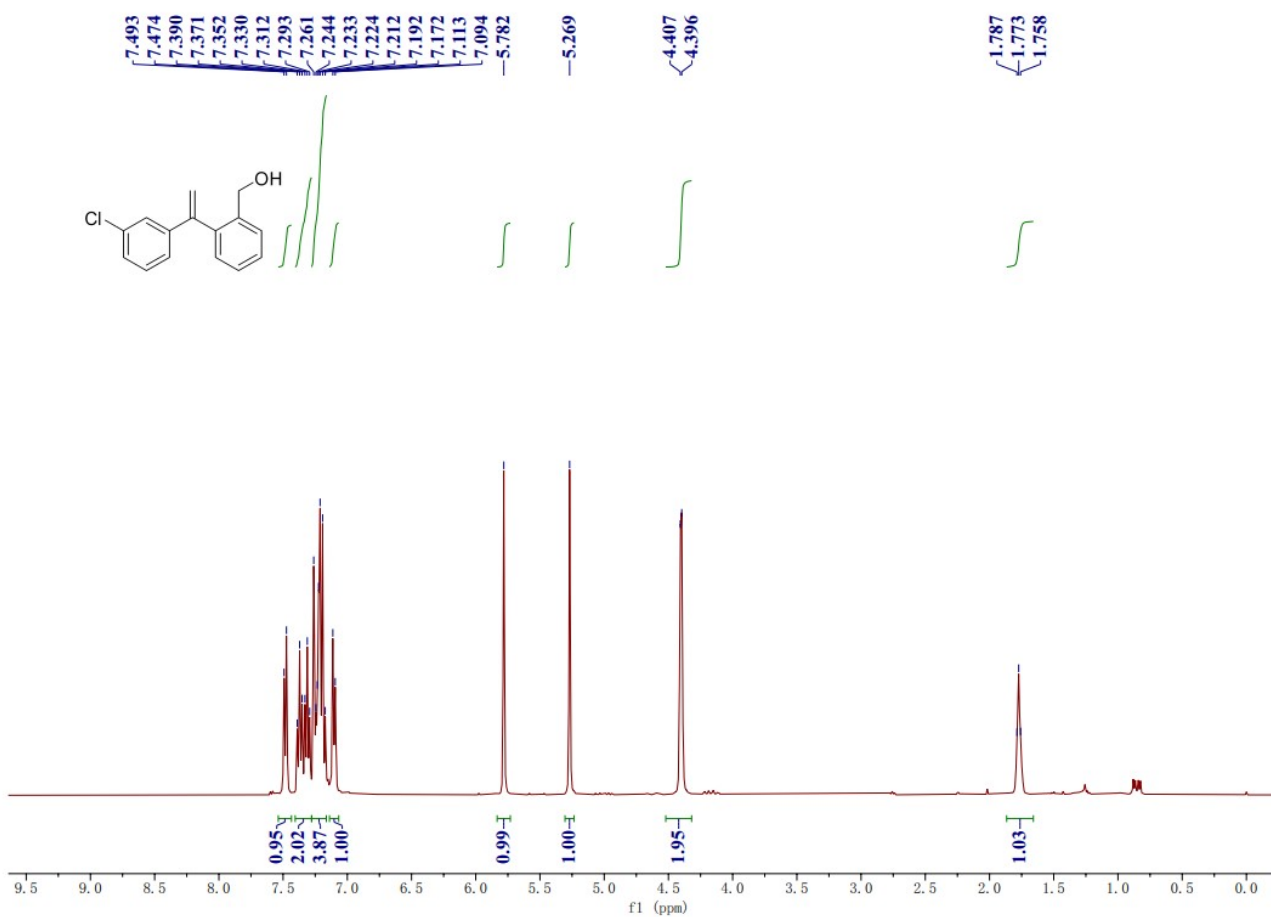


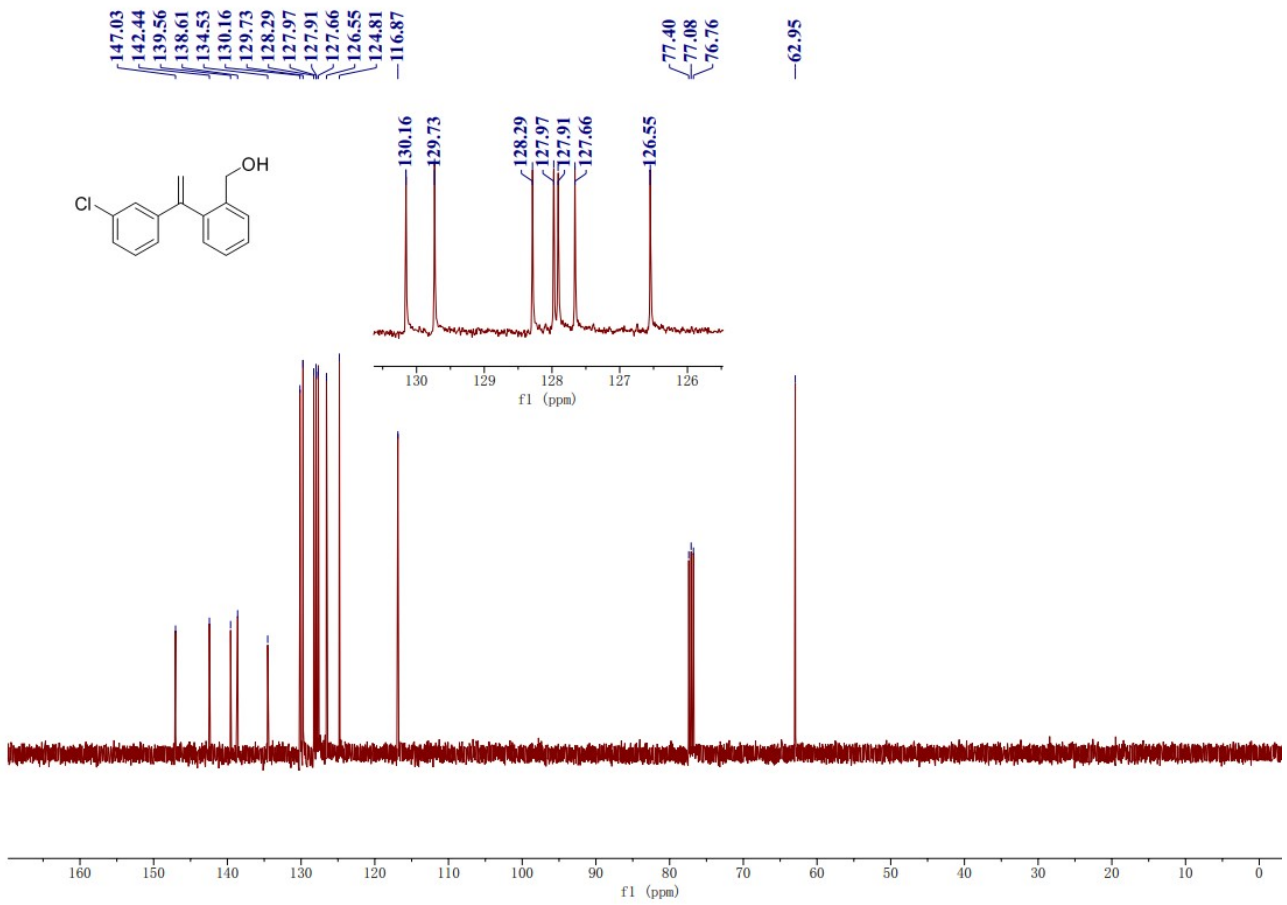


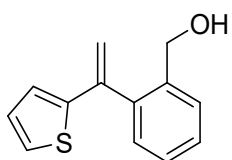


(2-(1-(3-chlorophenyl)vinyl)phenyl)methanol (1g)

A colorless oil, 450 mg, 84% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.48 (d, $J = 7.6$ Hz, 1H), 7.39-7.29 (m, 2H), 7.26-7.17 (m, 4H), 7.10 (d, $J = 7.6$ Hz, 1H), 5.78 (s, 1H), 5.27 (s, 1H), 4.40 (d, $J = 4.4$ Hz, 2H), 1.77 (br, 1H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 147.0, 142.4, 139.6, 138.6, 134.5, 130.2, 129.7, 128.3, 128.0, 127.9, 127.7, 126.5, 124.8, 116.9, 63.0. IR (acetone) ν 3376, 3054, 2971, 1597, 1493, 1444, 1189, 1073, 904, 695 cm^{-1} . HRMS (EI) Calcd. for $\text{C}_{21}\text{H}_{18}\text{O}$ (M^+): 244.0649, Found: 244.0647.

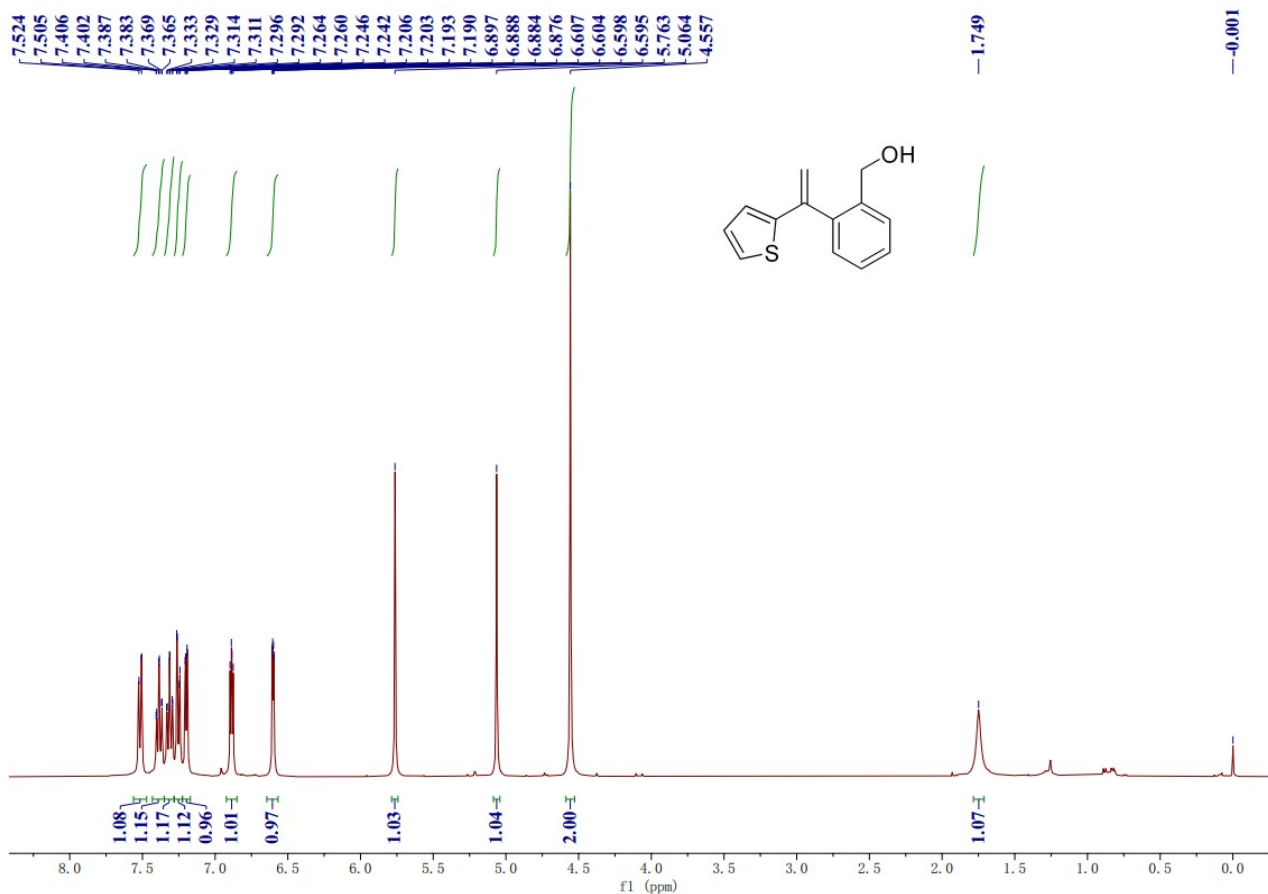


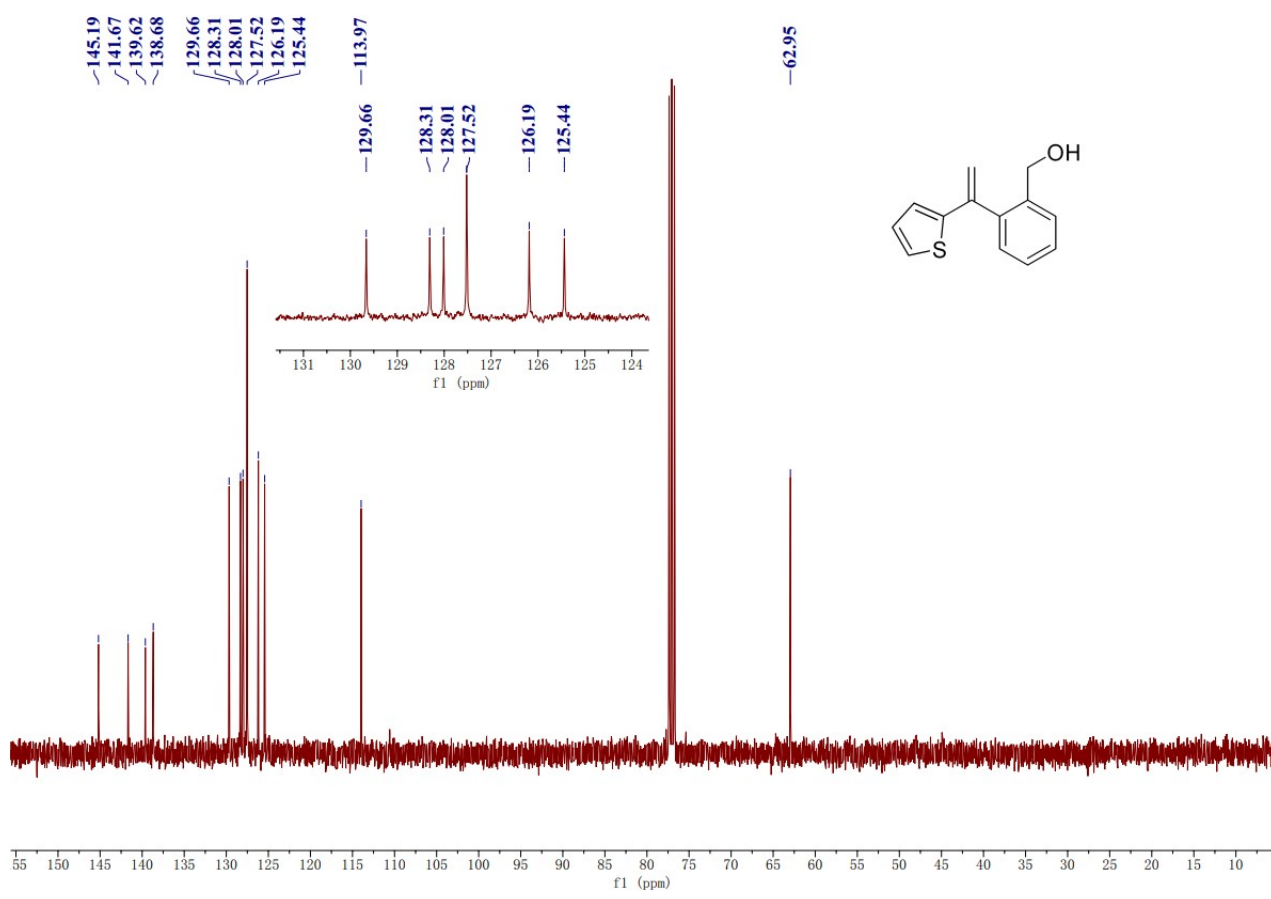


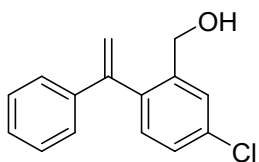


(2-(1-(thiophen-2-yl)vinyl)phenyl)methanol (1h)

This is a known compound and its spectroscopic data are consistent with those in the previous literature.¹ CAS number: 2712651-65-3. A white solid, 810 mg, 81% yield. ¹H NMR (CDCl₃, TMS, 400 MHz) δ 7.51 (d, *J* = 7.6 Hz, 1H), 7.41-7.36 (m, 1H), 7.33-7.29 (m, 1H), 7.25 (d, *J* = 7.4, 1H), 7.20 (d, *J* = 5.2, 1H), 6.90-6.88 (m, 1H), 6.61-6.60 (m, 1H), 5.76 (s, 1H), 5.06 (s, 1H), 4.56 (s, 2H), 1.75 (s, 1H). ¹³C NMR (CDCl₃, TMS, 100 MHz) δ 145.2, 141.7, 139.6, 138.7, 129.7, 128.3, 128.0, 127.5, 126.2, 125.4, 114.0, 63.0.

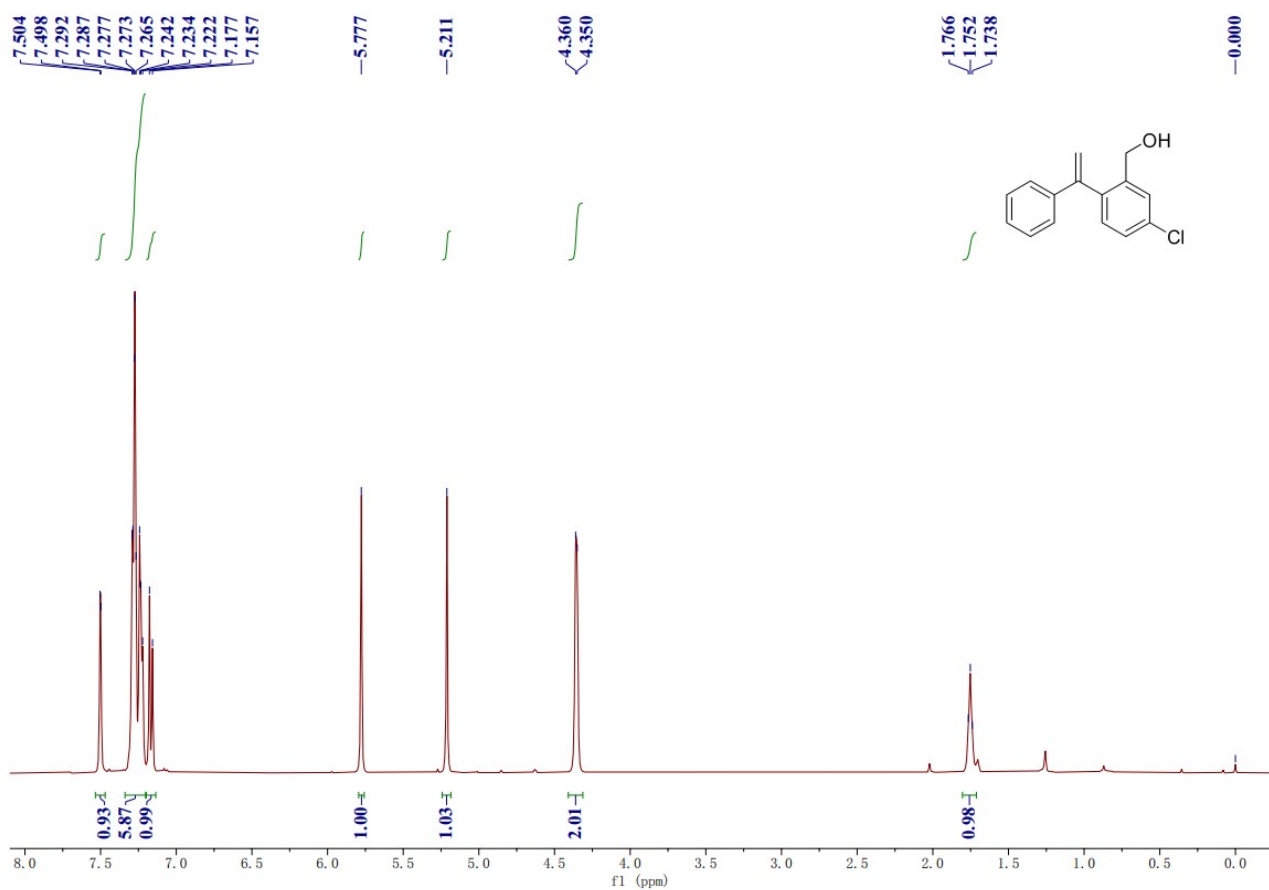


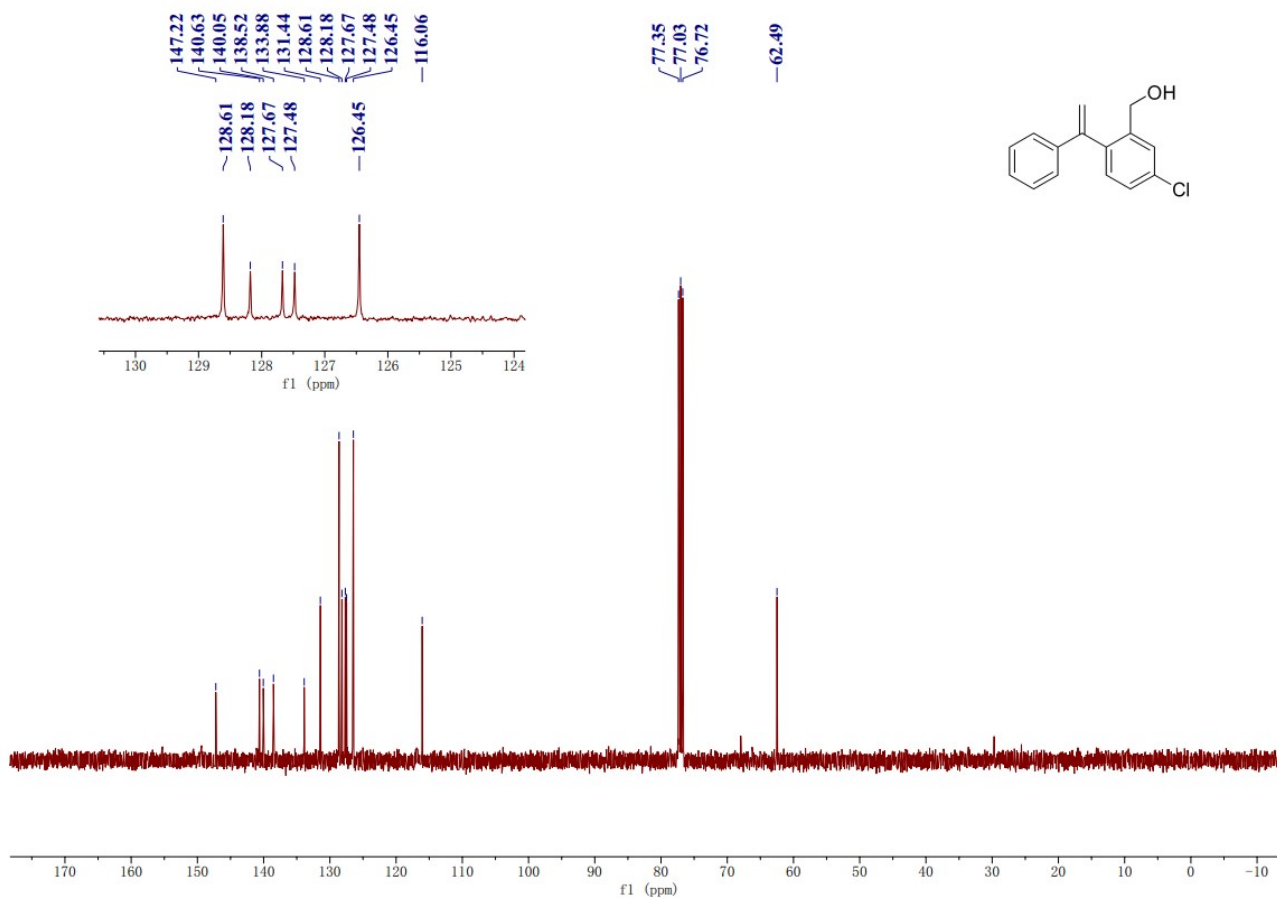


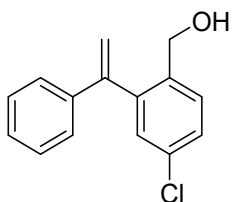


(5-chloro-2-(1-phenylvinyl)phenyl)methanol (1i)

A colorless oil, 572 mg, 86% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.50 (d, $J = 2.3$ Hz, 1H), 7.29-7.22 (m, 6H), 7.17 (d, $J = 8.1$ Hz, 1H), 5.78 (s, 1H), 5.21 (s, 1H), 4.40 (d, $J = 4.1$ Hz, 2H), 1.75 (br, 1H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 147.0, 142.4, 139.6, 138.6, 134.5, 130.2, 129.7, 128.3, 128.0, 127.9, 127.7, 126.5, 124.8, 116.9, 77.4, 77.1, 76.8, 63.0. IR (acetone) ν 3382, 3056, 2973, 1594, 1494, 1478, 1403, 1190, 908, 879 cm^{-1} . HRMS (EI) Calcd. for $\text{C}_{15}\text{H}_{13}\text{ClO}$ (M^+): 244.0649, Found: 244.0643.

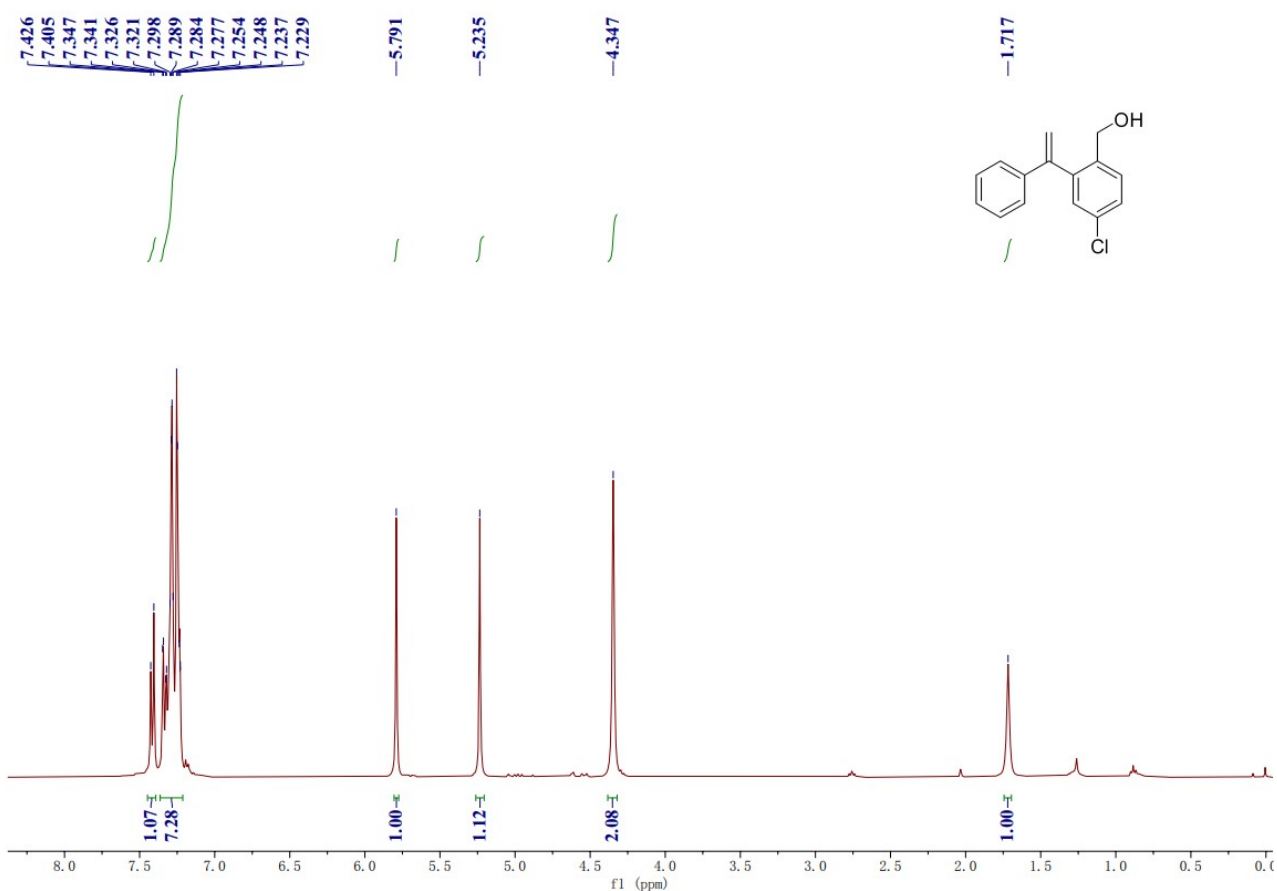


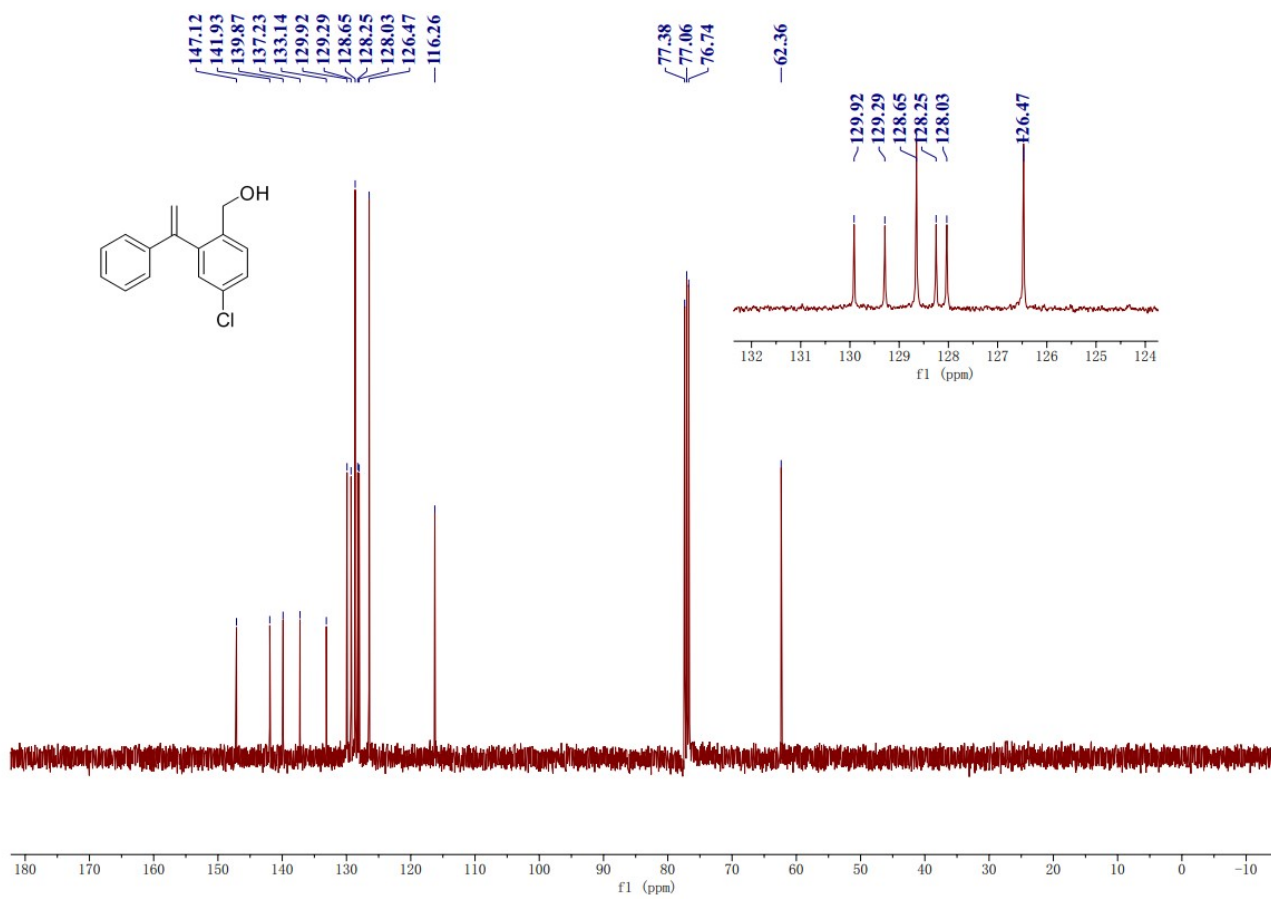


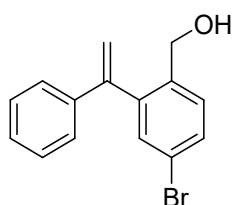


(4-chloro-2-(1-phenylvinyl)phenyl)methanol (1j)

This is a known compound and its spectroscopic data are consistent with those in the previous literature.⁶ CAS number: 2191304-69-3. A colorless oil, 491 mg, 76% yield. ¹H NMR (CDCl₃, TMS, 400 MHz) δ 7.42 (d, *J* = 8.2 Hz, 1H), 7.35-7.23 (m, 7H), 5.79 (s, 1H), 5.24 (s, 1H), 4.35 (s, 2H), 1.72 (s, 1H). ¹³C NMR (CDCl₃, TMS, 100 MHz) δ 147.1, 141.9, 139.9, 137.2, 133.1, 129.9, 129.3, 128.6, 128.2, 128.0, 126.5, 116.3, 62.4.

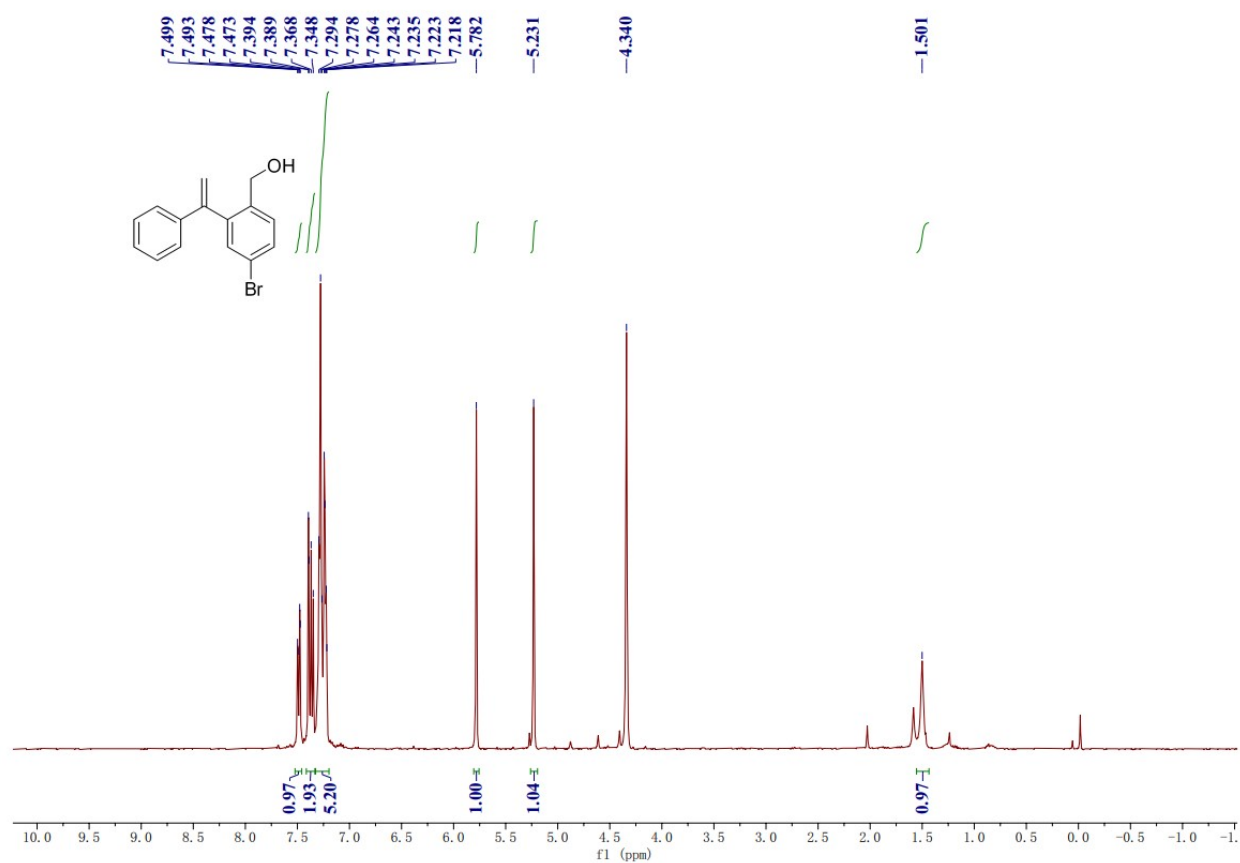


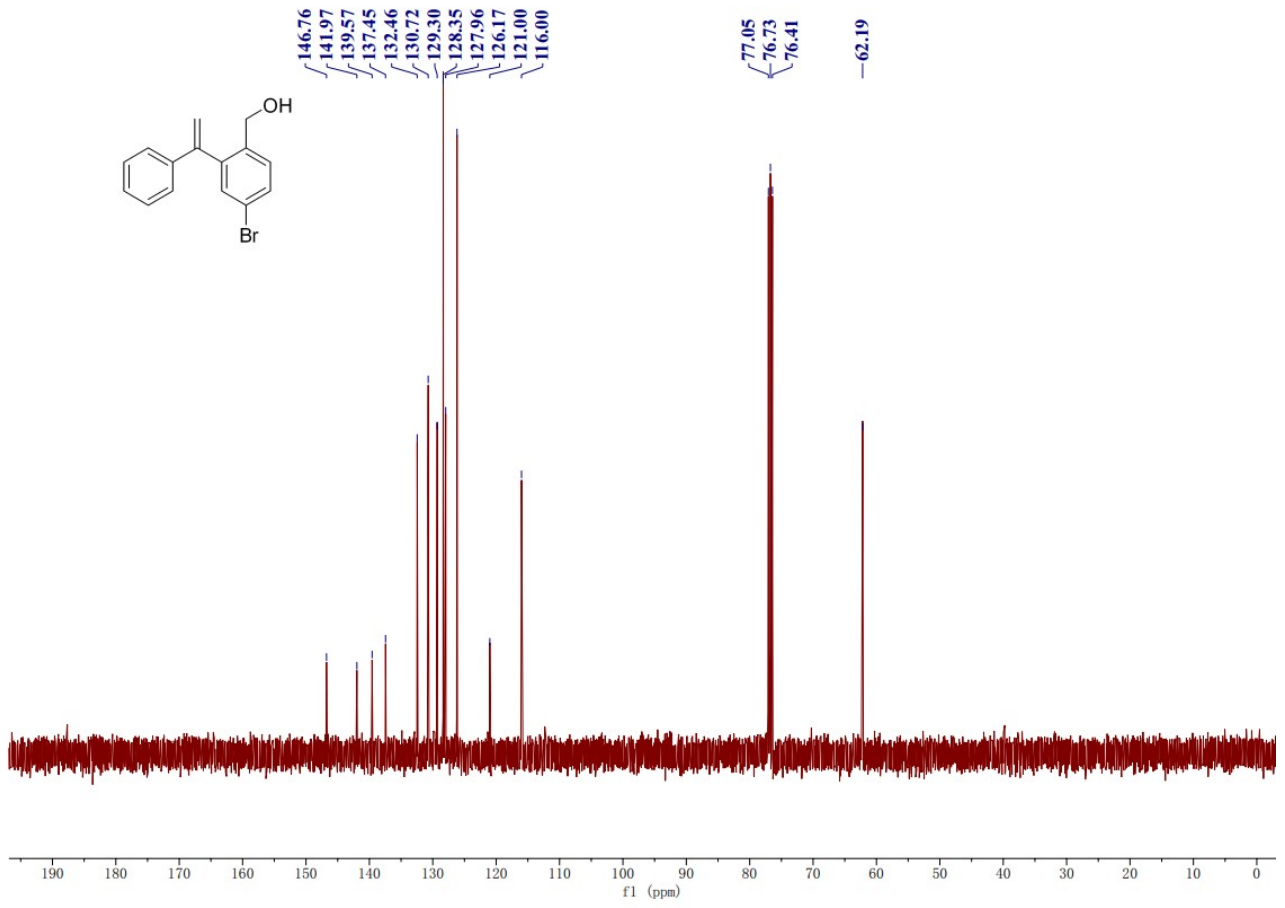


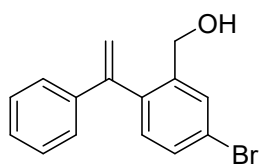


(4-bromo-2-(1-phenylvinyl)phenyl)methanol (1k)

This is a known compound and its spectroscopic data are consistent with those in the previous literature.⁴ CAS number: 2821886-40-0. A colorless oil, 481 mg, 73% yield. ¹H NMR (CDCl₃, TMS, 400 MHz) δ 7.49 (d, *J* = 8.2 Hz, 1H), 7.40-7.35 (m, 2H), 7.30-7.22 (m, 5H), 5.78 (s, 1H), 5.23 (s, 1H), 4.34 (s, 2H), 1.50 (br, 1H). ¹³C NMR (CDCl₃, TMS, 100 MHz) δ 146.8, 142.0, 139.6, 137.4, 132.5, 130.7, 129.3, 128.4, 128.0, 126.2, 121.0, 116.0, 62.2.

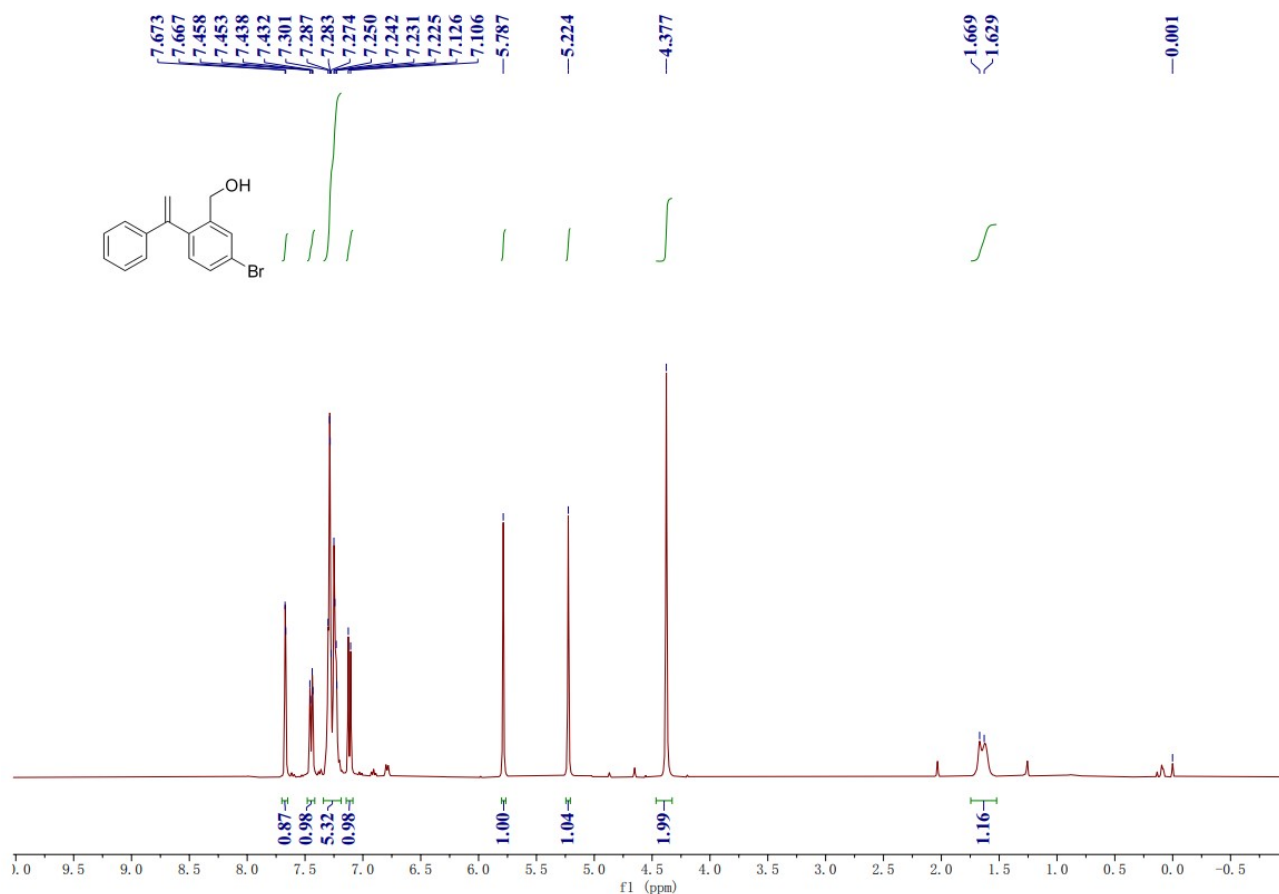


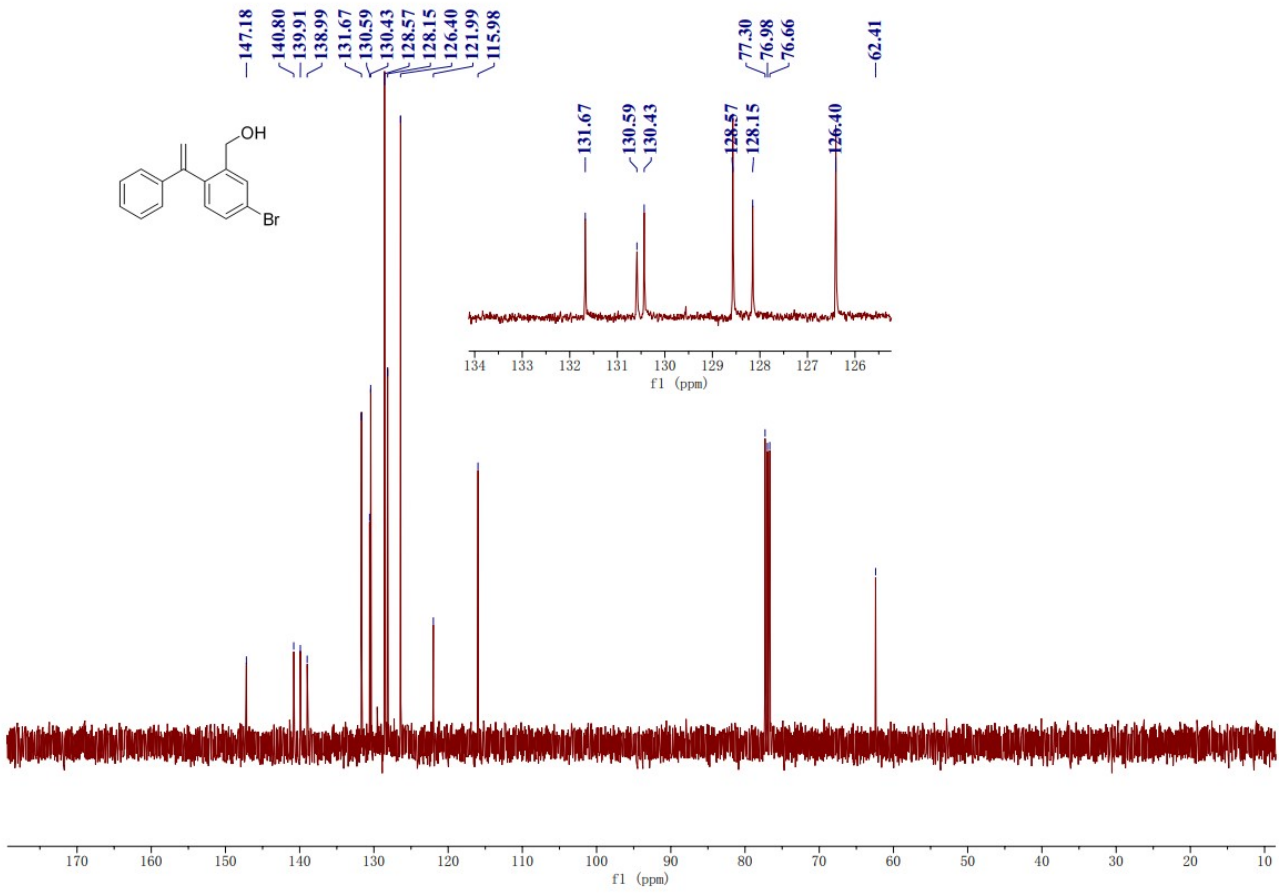


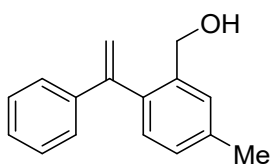


(5-bromo-2-(1-phenylvinyl)phenyl)methanol (11)

A colorless oil, 451 mg, 70% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.67 (d, $J = 2.2$ Hz, 1H), 7.45 (dd, $J = 8.1, 2.2$ Hz, 1H), 7.30-7.23 (m, 5H), 7.12 (d, $J = 8.0$ Hz, 1H), 5.79 (s, 1H), 5.22 (s, 1H), 4.38 (s, 2H), 1.67-1.63 (br, 1H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 147.2, 140.8, 139.9, 139.0, 131.7, 130.6, 130.4, 128.6, 128.2, 126.4, 122.0, 116.0, 62.4. IR (acetone) ν 3330, 3081, 2926, 1613, 1493, 1477, 1397, 908, 864, 706 cm^{-1} . HRMS (EI) Calcd. for $\text{C}_{15}\text{H}_{13}\text{BrO}$ (M^+): 288.0144, Found: 288.0138.

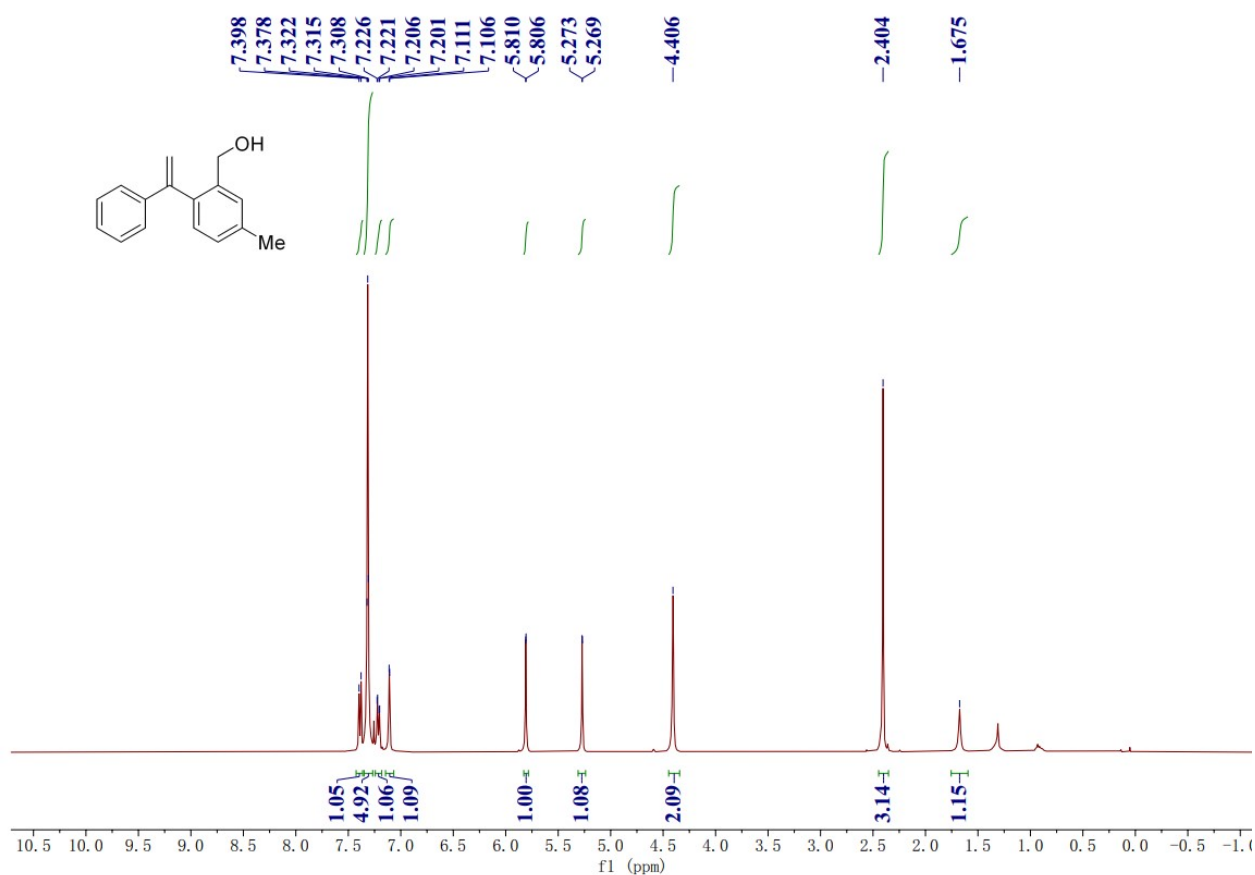


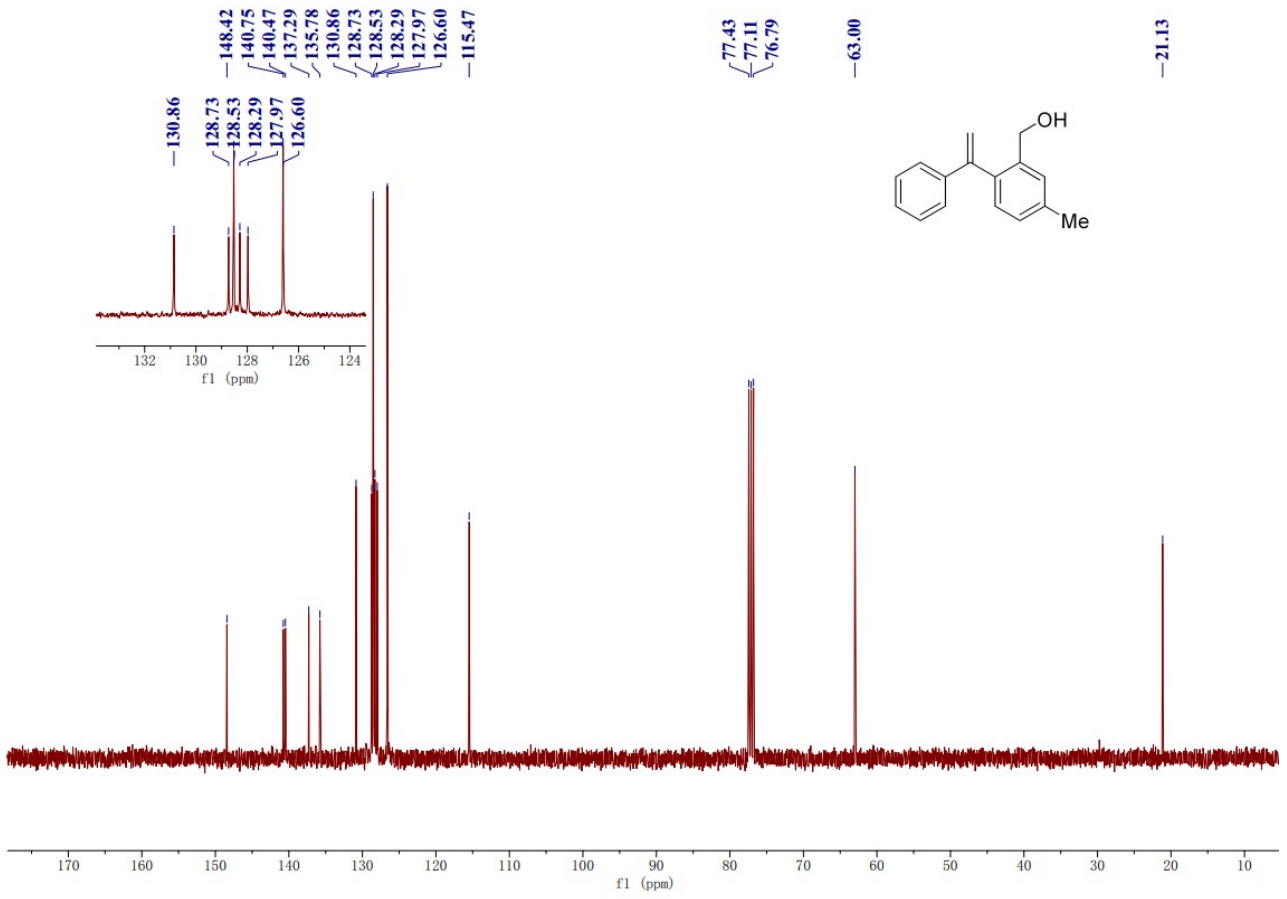


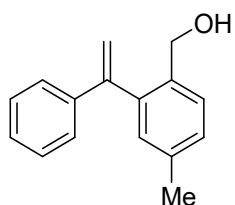


(5-methyl-2-(1-phenylvinyl)phenyl)methanol (1m)

This is a known compound and its spectroscopic data are consistent with those in the previous literature.⁴ CAS number: 2821886-39-7. A colorless oil, 231 mg, 82% yield. ¹H NMR (CDCl₃, TMS, 400 MHz) δ 7.39 (d, *J* = 7.8 Hz, 1H), 7.32-7.31 (m, 5H), 7.21 (dd, *J* = 7.8, 1.9 Hz, 1H), 7.11 (d, *J* = 1.9 Hz, 1H), 5.81 (d, *J* = 1.4 Hz, 1H), 5.27 (d, *J* = 1.4 Hz, 1H), 4.41 (s, 2H), 2.40 (s, 3H), 1.67 (br, 1H). ¹³C NMR (CDCl₃, TMS, 100 MHz) δ 148.4, 140.8, 140.5, 137.3, 135.8, 130.9, 128.7, 128.5, 128.3, 128.0, 126.6, 115.5, 63.0, 21.1.

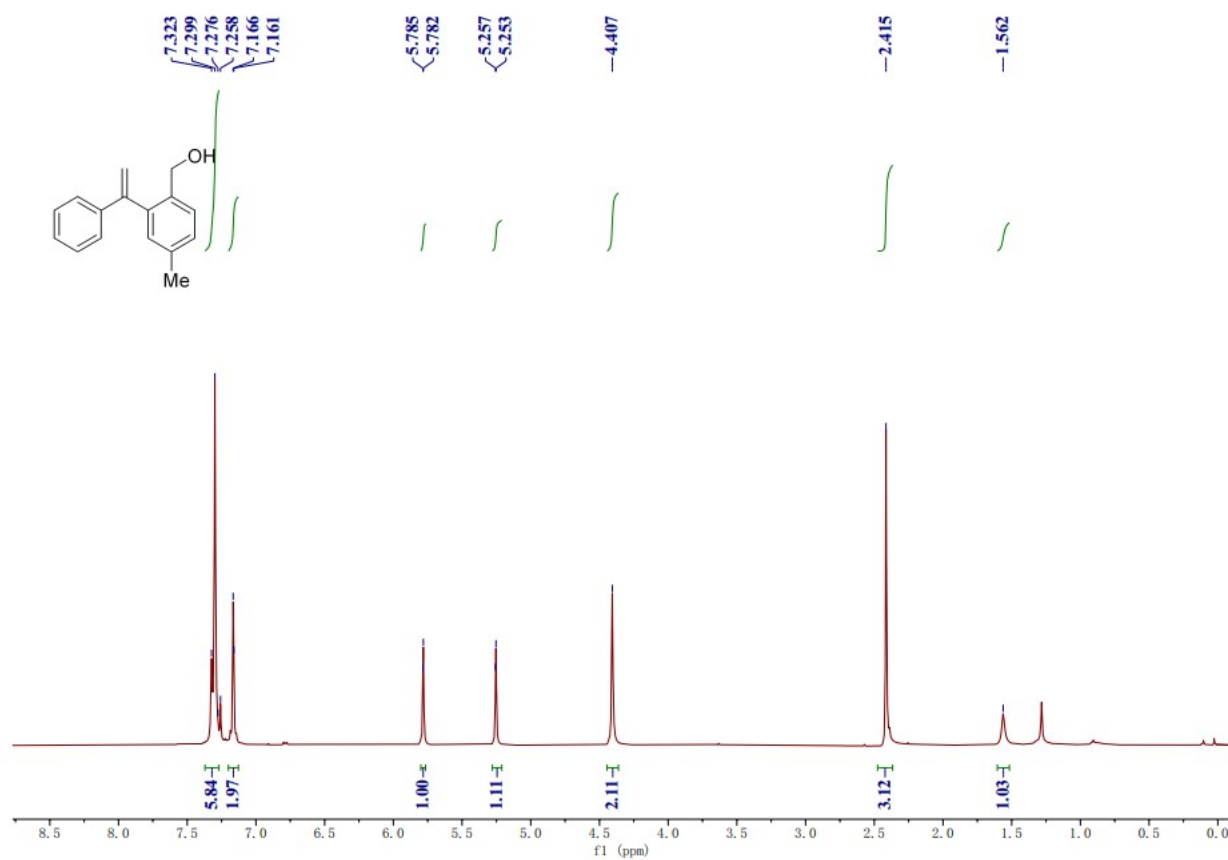


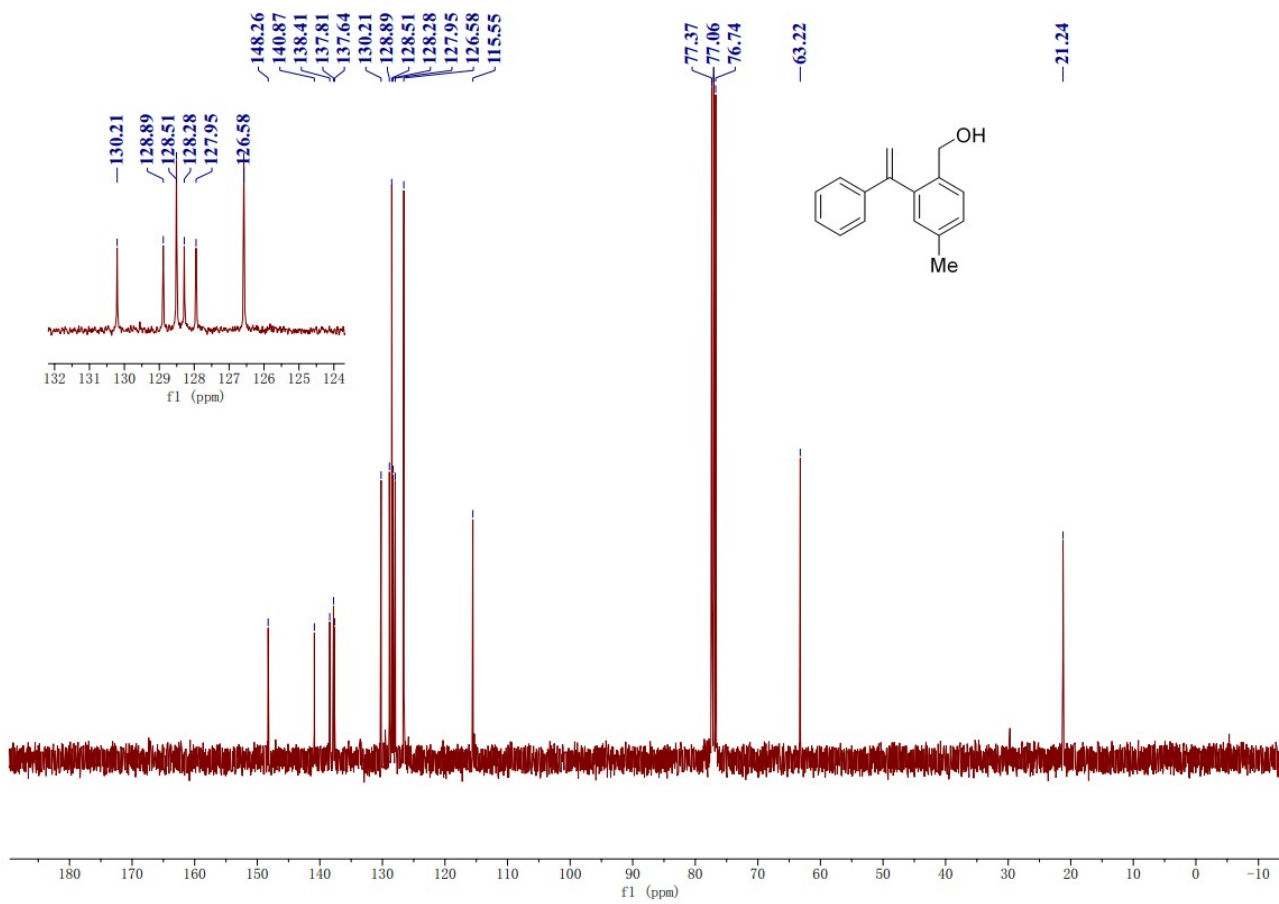


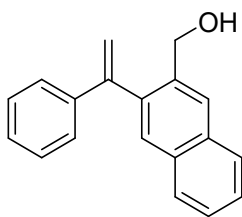


(4-methyl-2-(1-phenylvinyl)phenyl)methanol (1n)

A colorless oil, 161 mg, 78% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.32-7.26 (m, 6H), 7.17-7.16 (m, 2H), 5.78 (d, $J = 1.4$ Hz, 1H), 5.25 (d, $J = 1.4$ Hz, 1H), 4.41 (s, 2H), 2.42 (s, 3H), 1.56 (br, 1H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 148.3, 140.9, 138.4, 137.8, 137.6, 130.2, 128.9, 128.5, 128.3, 127.9, 126.6, 115.5, 63.2, 21.2. IR (acetone) ν 3351, 3052, 2923, 1581, 1493, 1445, 1027, 906, 819, 780 cm^{-1} . HRMS (EI) Calcd. for $\text{C}_{16}\text{H}_{16}\text{O}$ (M^+): 244.1196, Found: 244.1198.

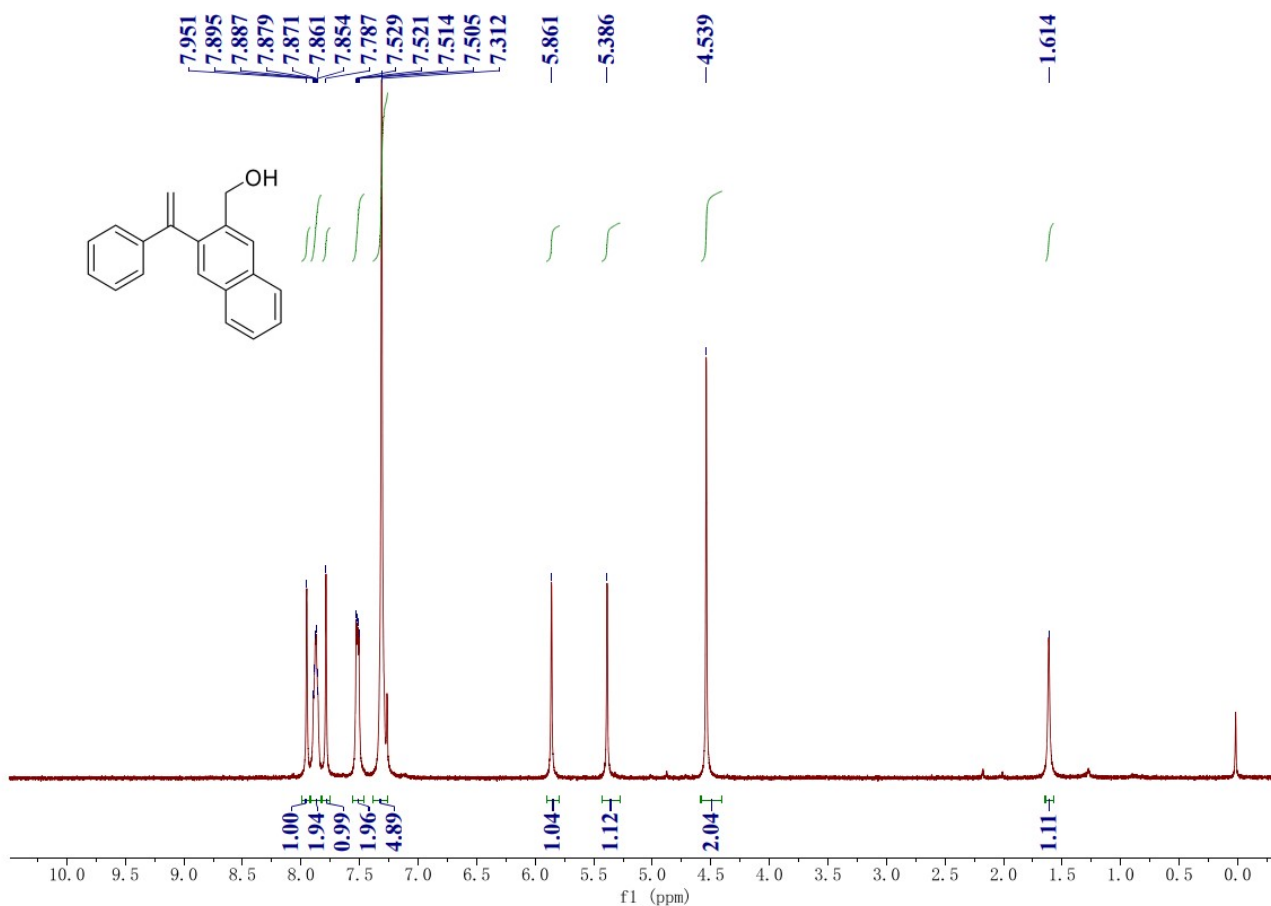


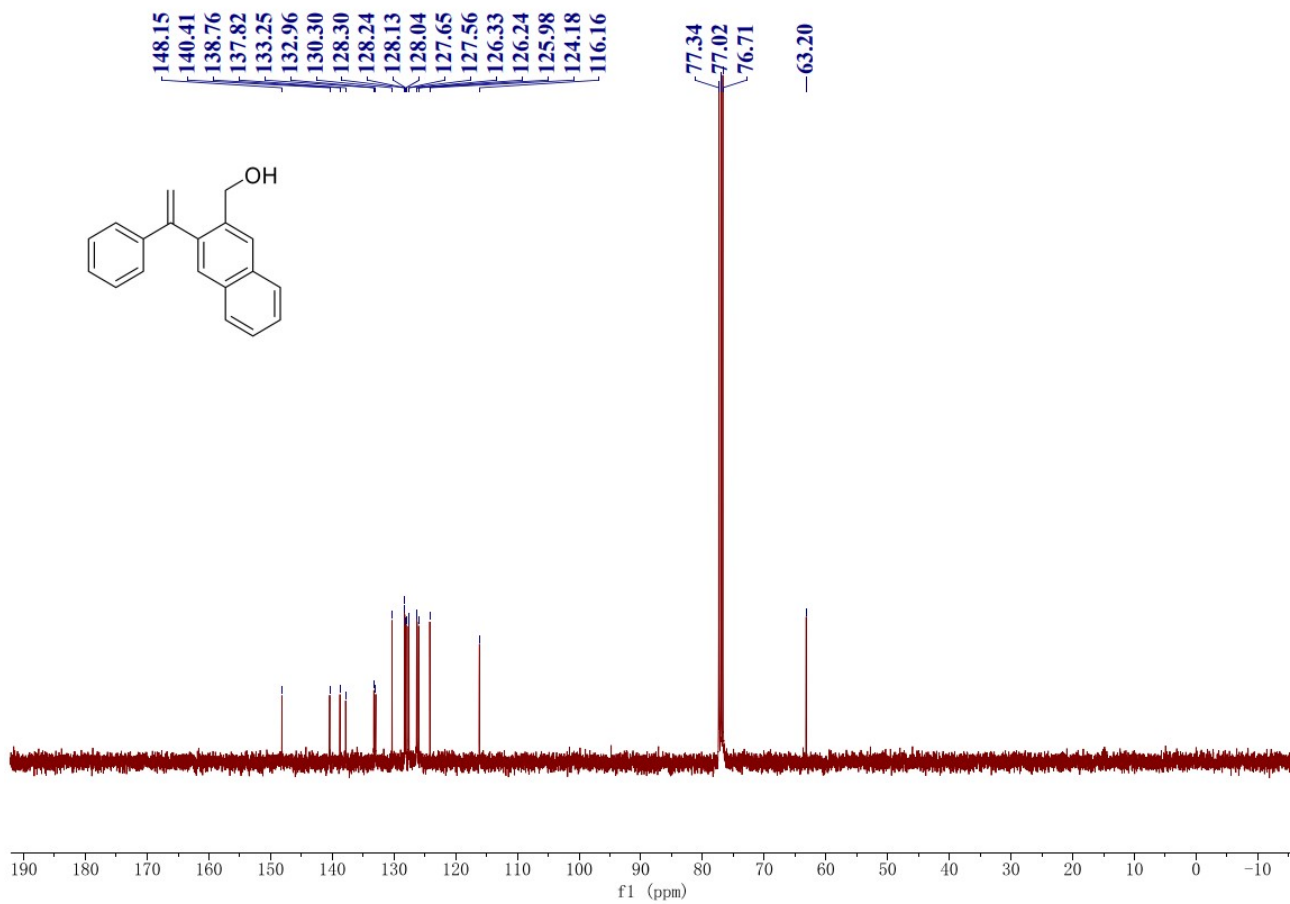


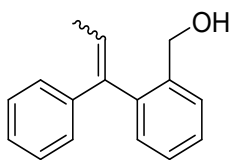


(3-(1-phenylvinyl)naphthalen-2-yl)methanol (1o)

A white solid, M.P.: 110-112 °C, 332 mg, 87% yield. ¹H NMR (CDCl₃, TMS, 400 MHz) δ 7.95 (s, 1H), 7.90-7.85 (m, 2H), 7.79 (s, 1H), 7.53-7.51 (m, 2H), 7.31 (s, 5H), 5.86 (s, 1H), 5.39 (s, 1H), 4.54 (s, 2H), 1.61 (br, 1H). ¹³C NMR (CDCl₃, TMS, 100 MHz) δ 148.2, 140.4, 138.8, 137.8, 133.3, 133.0, 130.3, 128.3, 128.2, 128.1, 128.0, 127.7, 127.6, 126.3, 126.2, 126.0, 124.2, 116.2, 63.2. IR (acetone) ν 3367, 3056, 2925, 1600, 1508, 1492, 1444, 1039, 880, 699 cm⁻¹. HRMS (EI) Calcd. for C₁₉H₁₆O (M⁺): 260.1196, Found: 260.1202.

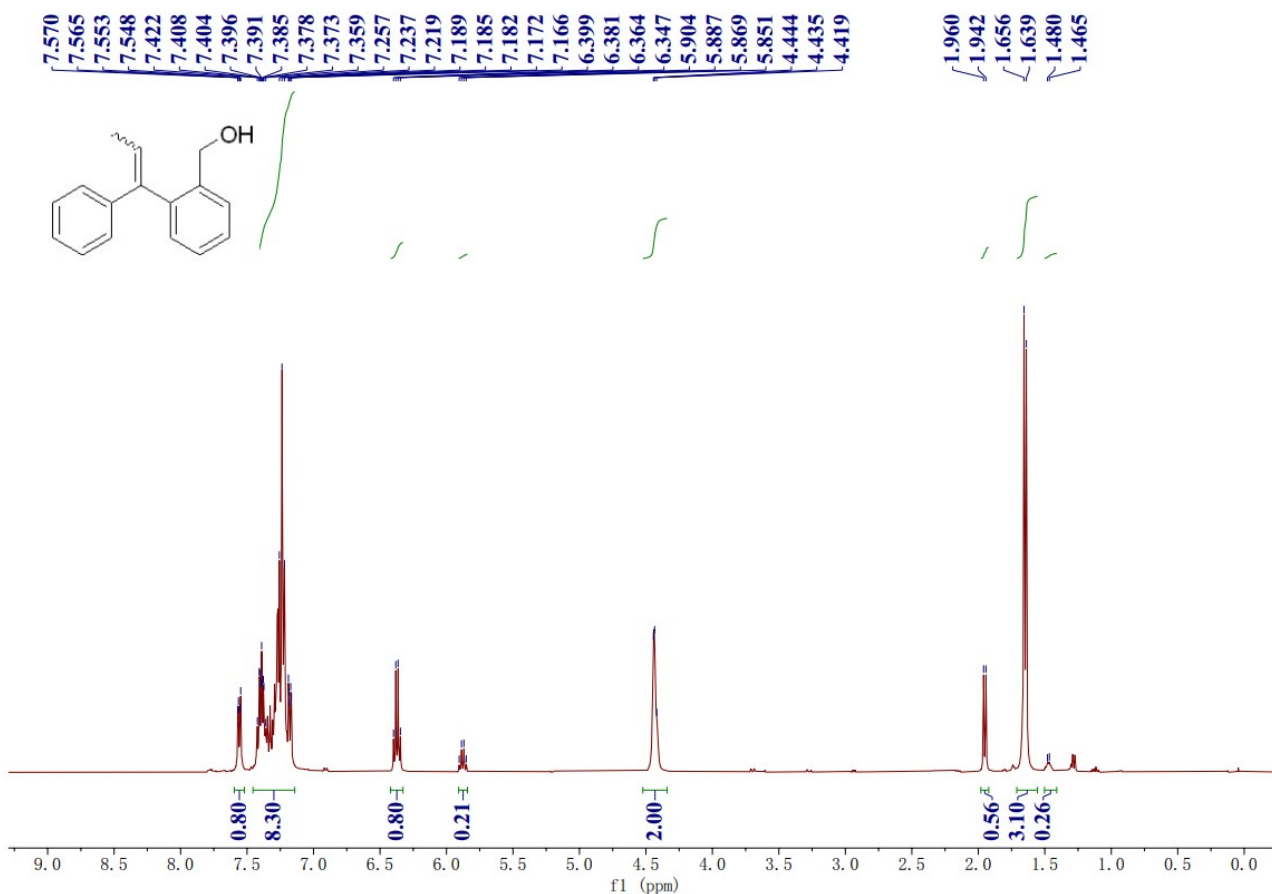


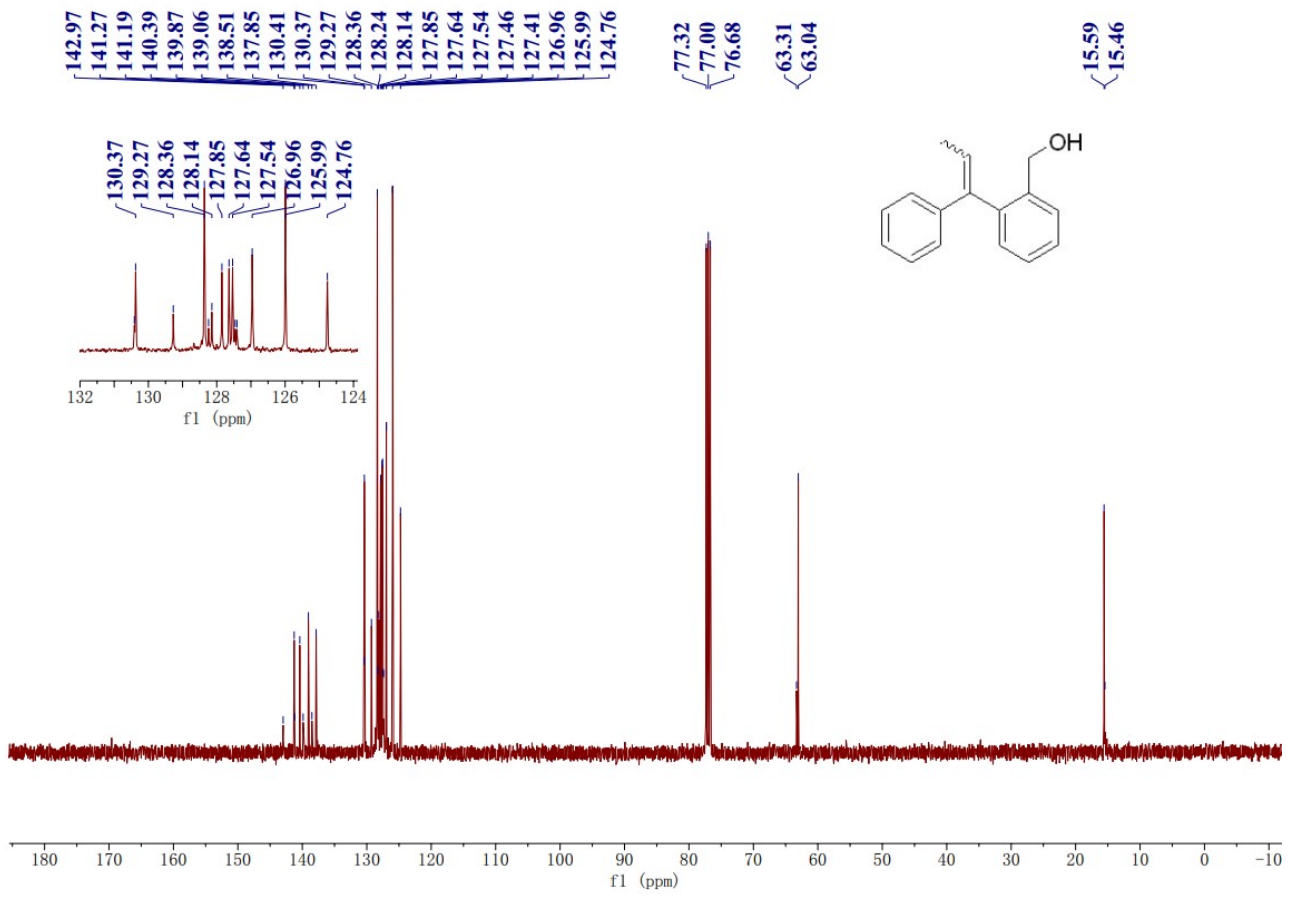


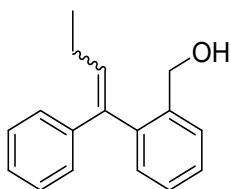


(2-(1-phenylprop-1-en-1-yl)phenyl)methanol (1p)

A yellow oil, 107 mg, 63% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.56 (dd, $J = 6.8, 2.1$ Hz, 0.8H), 7.42-7.17 (m, 8.3H), 6.37 (q, $J = 7.0$ Hz, 0.8H), 5.88 (q, $J = 7.2$ Hz, 0.21H), 4.44-4.20 (m, 2H), 1.95 (d, $J = 7.2$ Hz, 0.56H), 1.65 (d, $J = 6.8$ Hz, 3.1H), 1.47 (br, 0.26H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 143.0, 141.3, 141.2, 140.4, 139.9, 139.1, 138.5, 137.9, 130.4, 129.3, 128.4, 128.2, 128.1, 127.9, 127.6, 127.54, 127.46, 127.4, 127.0, 126.0, 124.8, 63.3, 63.0, 15.6, 15.5. IR (acetone) ν 3333, 3058, 2932, 1495, 1445, 1379, 1198, 1030, 870, 698 cm^{-1} . HRMS (EI) Calcd. for $\text{C}_{16}\text{H}_{16}\text{O}$ (M^+): 224.1196, Found: 224.1196.

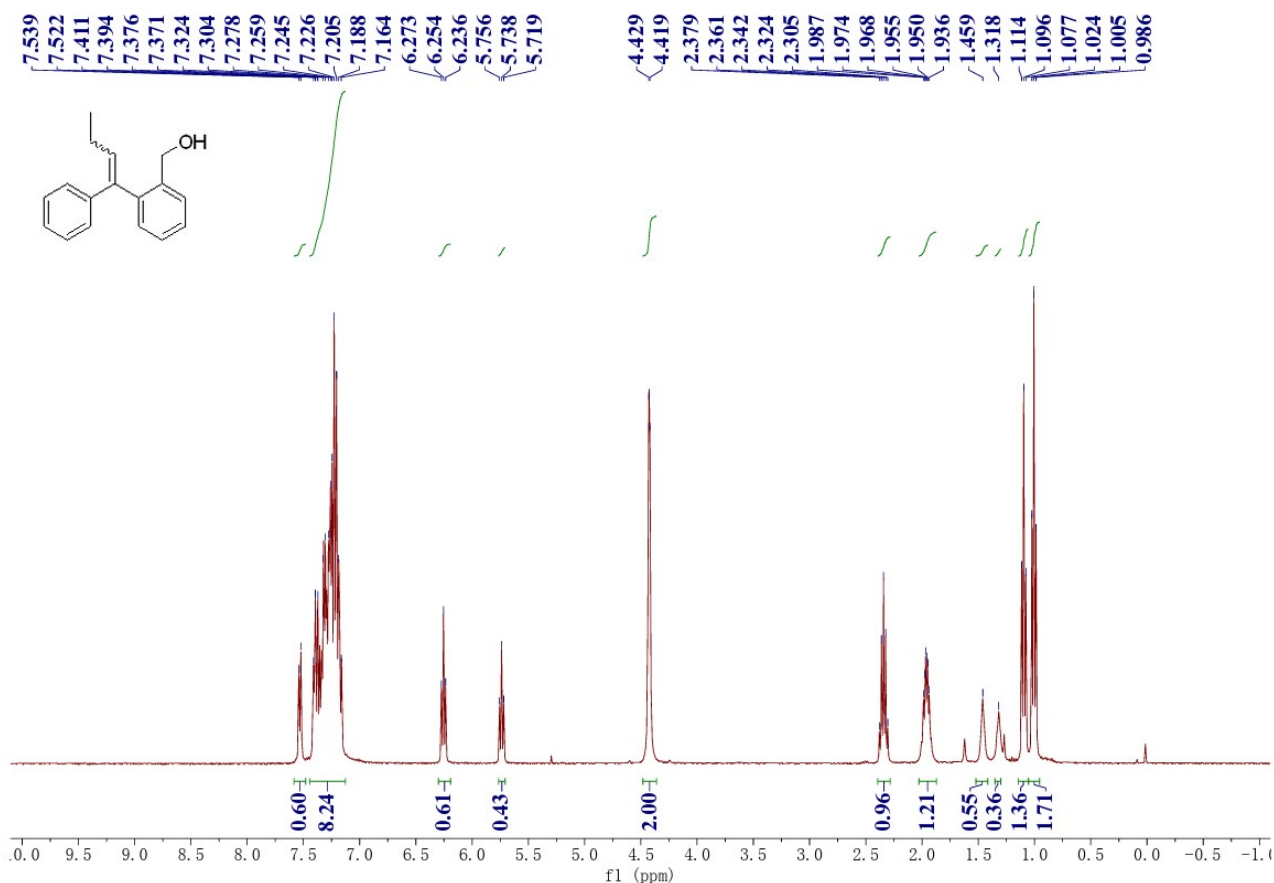


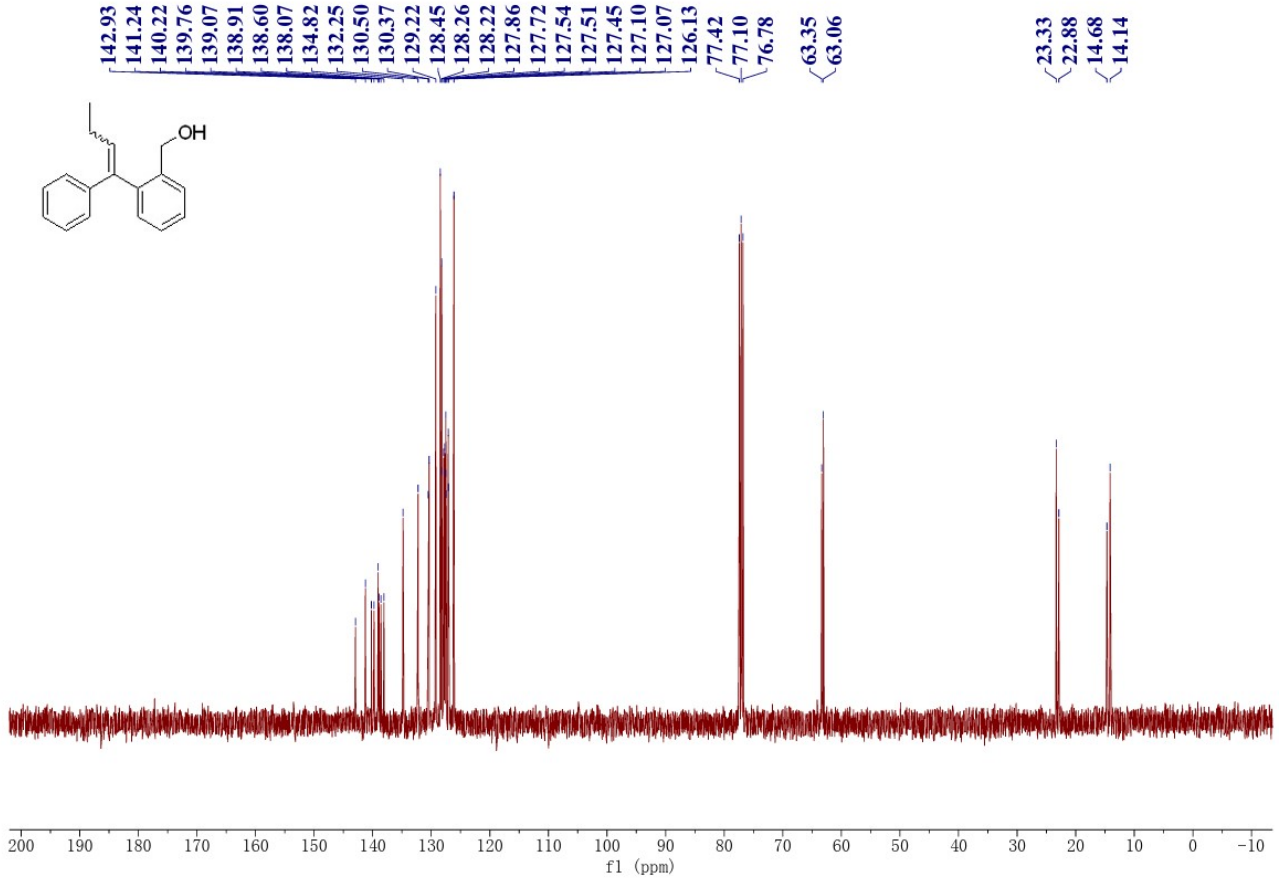


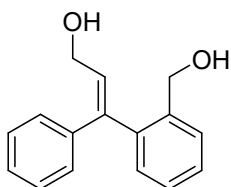


(2-(1-phenylbut-1-en-1-yl)phenyl)methanol (1q)

A colorless oil. 131 mg, 68% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.53 (d, $J = 6.8$ Hz, 0.60H), 7.41-7.16 (m, 8.24H), 6.25 (t, $J = 7.4$ Hz, 0.61H), 5.74 (t, $J = 7.4$ Hz, 0.43H), 4.42 (d, $J = 4.0$ Hz, 2H), 2.38-2.31 (m, 0.96H), 1.99-1.94 (m, 1.21H), 1.46 (br, 0.55), 1.32 (br, 0.36), 1.10 (t, $J = 7.6$ Hz, 1.36H), 1.01 (t, $J = 7.6$ Hz, 1.71H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 142.9, 141.2, 140.2, 139.8, 139.1, 138.9, 138.6, 138.1, 134.8, 132.2, 130.5, 130.4, 129.2, 128.4, 128.3, 128.2, 127.9, 127.7, 127.54, 127.51, 127.45, 127.1, 127.1, 126.1, 63.4, 63.1, 23.3, 22.9, 14.7, 14.1. IR (acetone) ν 3333, 3059, 2930, 1493, 1444, 1374, 1195, 1031, 869, 699 cm^{-1} . HRMS (EI) Calcd. for $\text{C}_{17}\text{H}_{16}$ ($\text{M}-\text{H}_2\text{O}$) $^+$: 220.1247, Found: 220.1245.

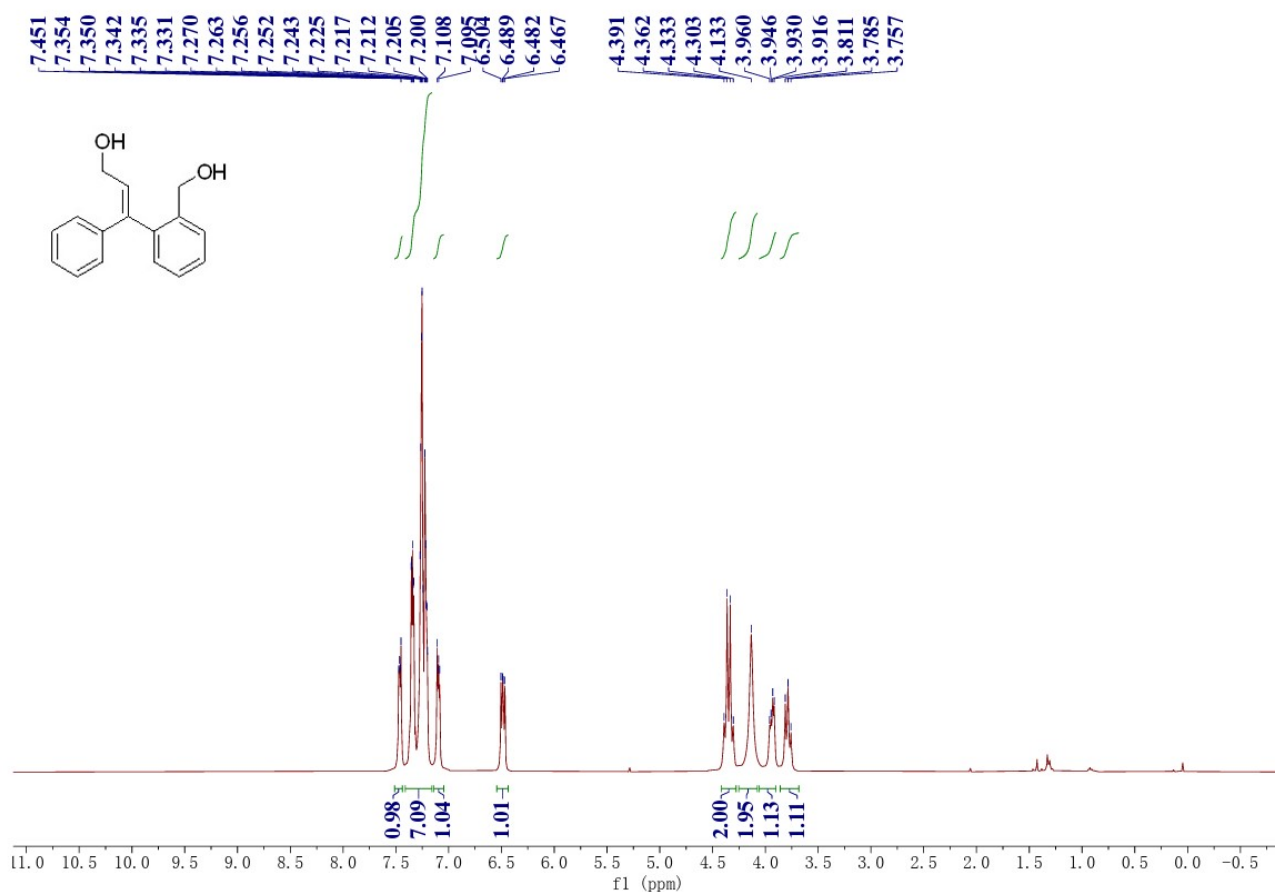


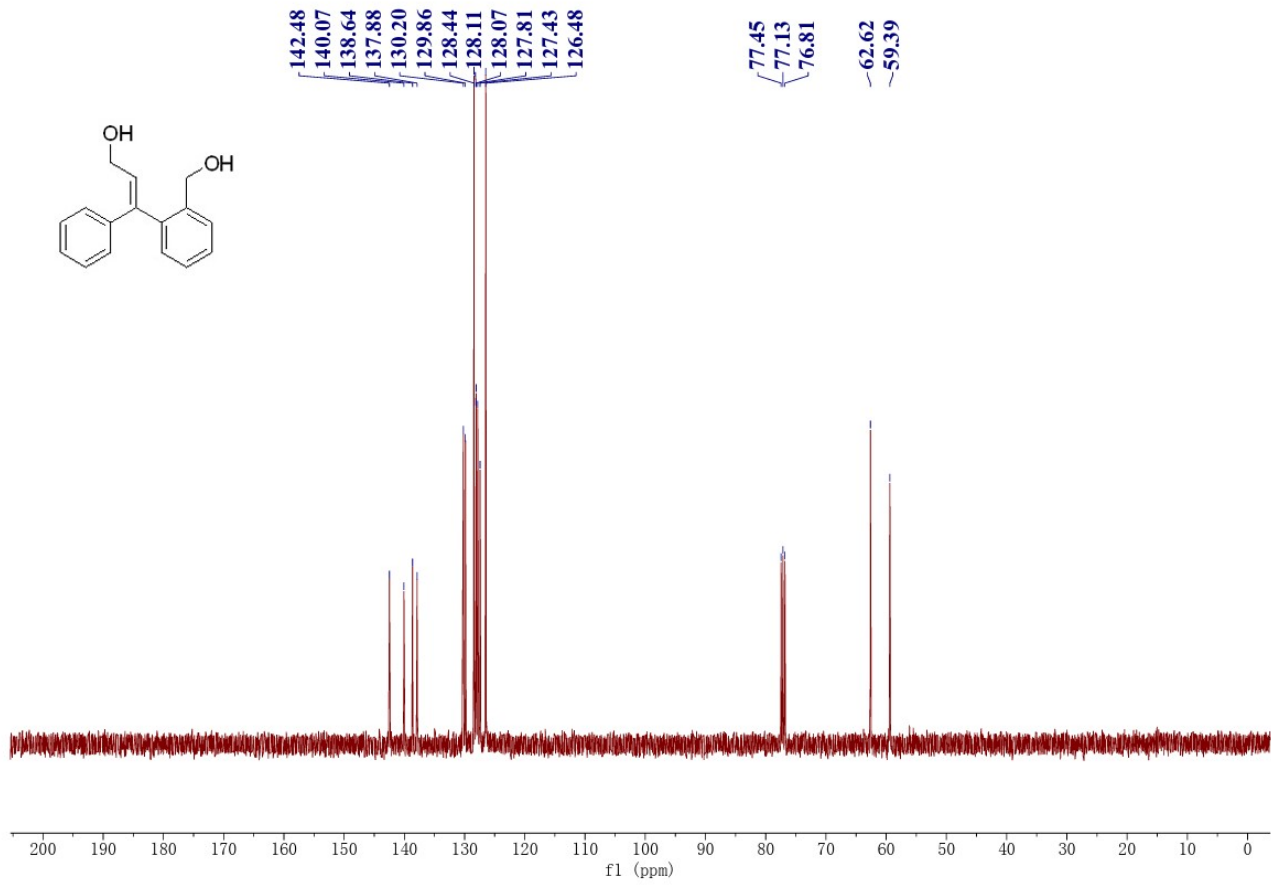


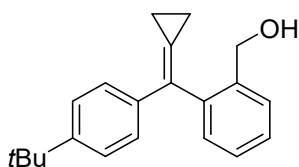


(E)-3-(2-(hydroxymethyl)phenyl)-3-phenylprop-2-en-1-ol (1r)

A colorless oil, 256 mg, 78% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.47-7.45 (m, 1H), 7.35-7.20 (m, 7H), 7.11-7.09 (m, 1H), 6.49 (dd, $J = 9.0, 6.0$ Hz, 1H), 4.35 (q, $J = 11.6$ Hz, 2H), 4.13 (s, 2H), 3.96-3.92 (m, 1H), 3.81-3.76 (m, 1H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 142.5, 140.1, 138.6, 137.9, 130.2, 129.9, 128.4, 128.11, 128.07, 127.8, 127.4, 126.5, 62.6, 59.4. IR (acetone) ν 3312, 3027, 2924, 2877, 1492, 1445, 1198, 1109, 964, 695 cm^{-1} . Calcd. for $\text{C}_{16}\text{H}_{14}\text{O}$ (M- H_2O) $^+$: 222.1039, Found: 222.1038.

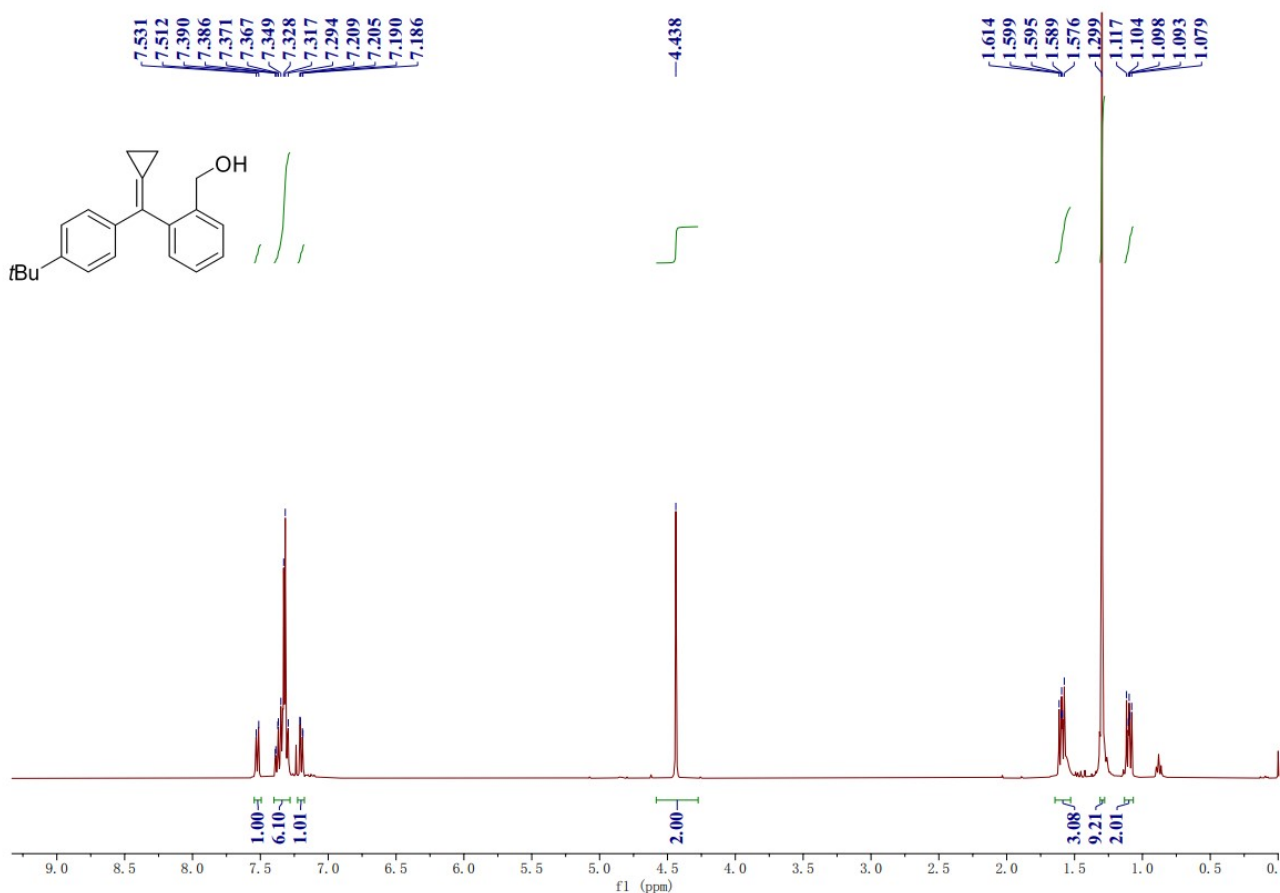


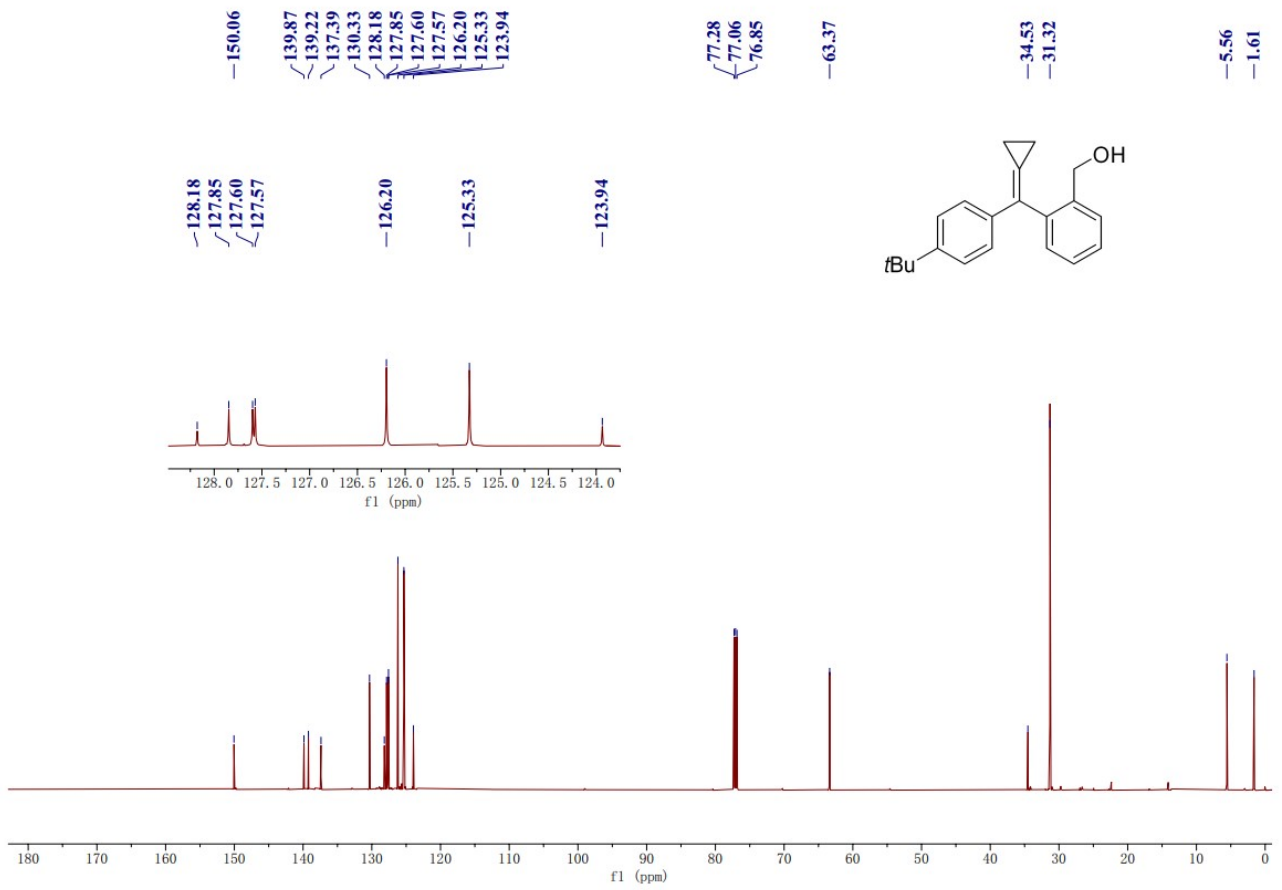


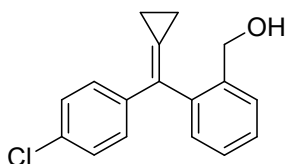


(2-((4-(tert-butyl)phenyl)(cyclopropylidene)methyl)phenyl)methanol (1s)

A colorless oil. 381 mg, 81% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.52 (d, $J = 7.6$ Hz, 1H), 7.39-7.29 (m, 6H), 7.21-7.19 (m, 1H), 4.44 (s, 2H), 1.61-1.58 (m, 3H), 1.30 (s, 9H), 1.12-1.08 (m, 2H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 150.1, 139.9, 139.2, 137.4, 130.3, 128.2, 127.9, 127.60, 127.57, 126.2, 125.3, 123.9, 63.4, 34.5, 31.3, 5.6, 1.6. IR (acetone) ν 3367, 2962, 2903, 1518, 1461, 1363, 1228, 1019, 836, 759 cm^{-1} . HRMS (EI) Calcd. for $\text{C}_{21}\text{H}_{24}\text{O}$ (M^+): 292.1822, Found: 292.1817.

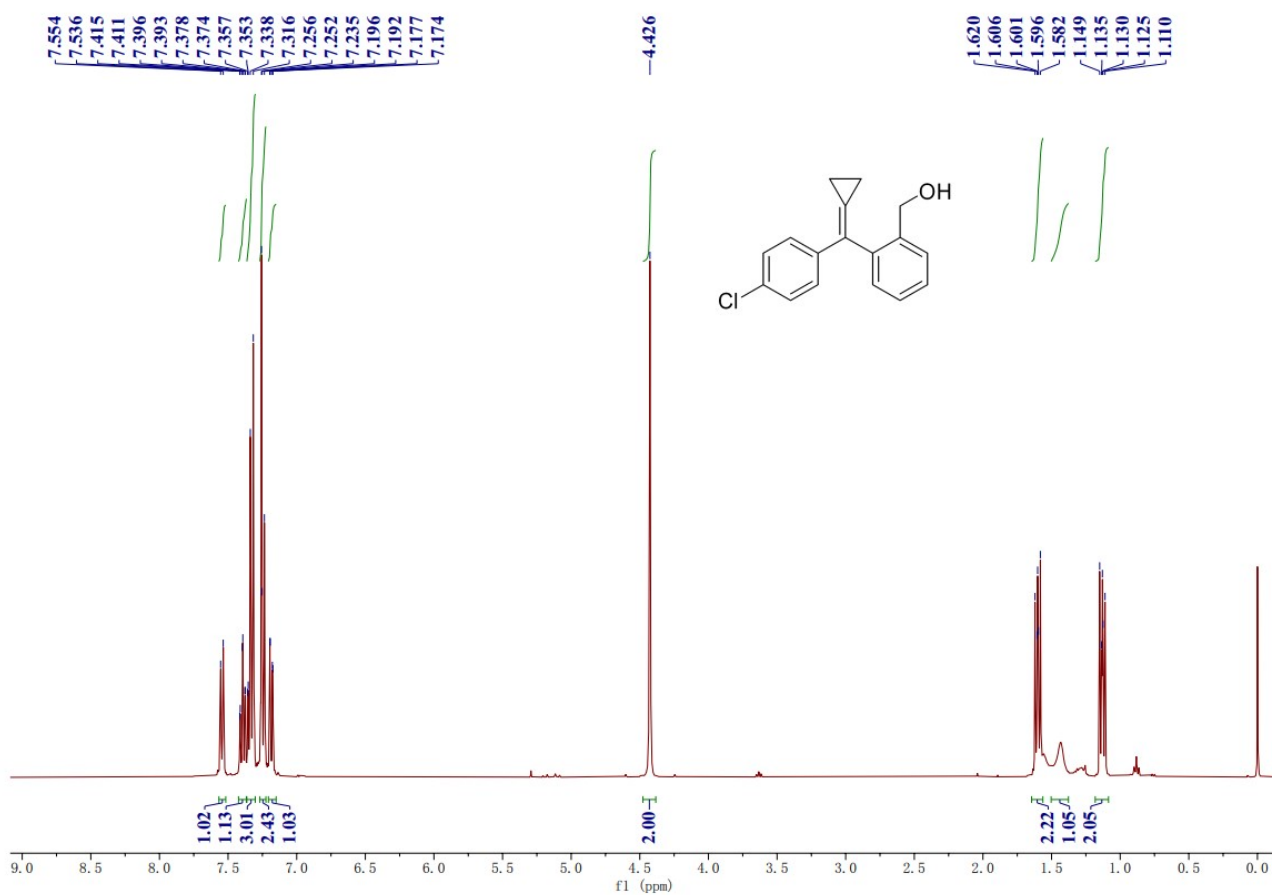


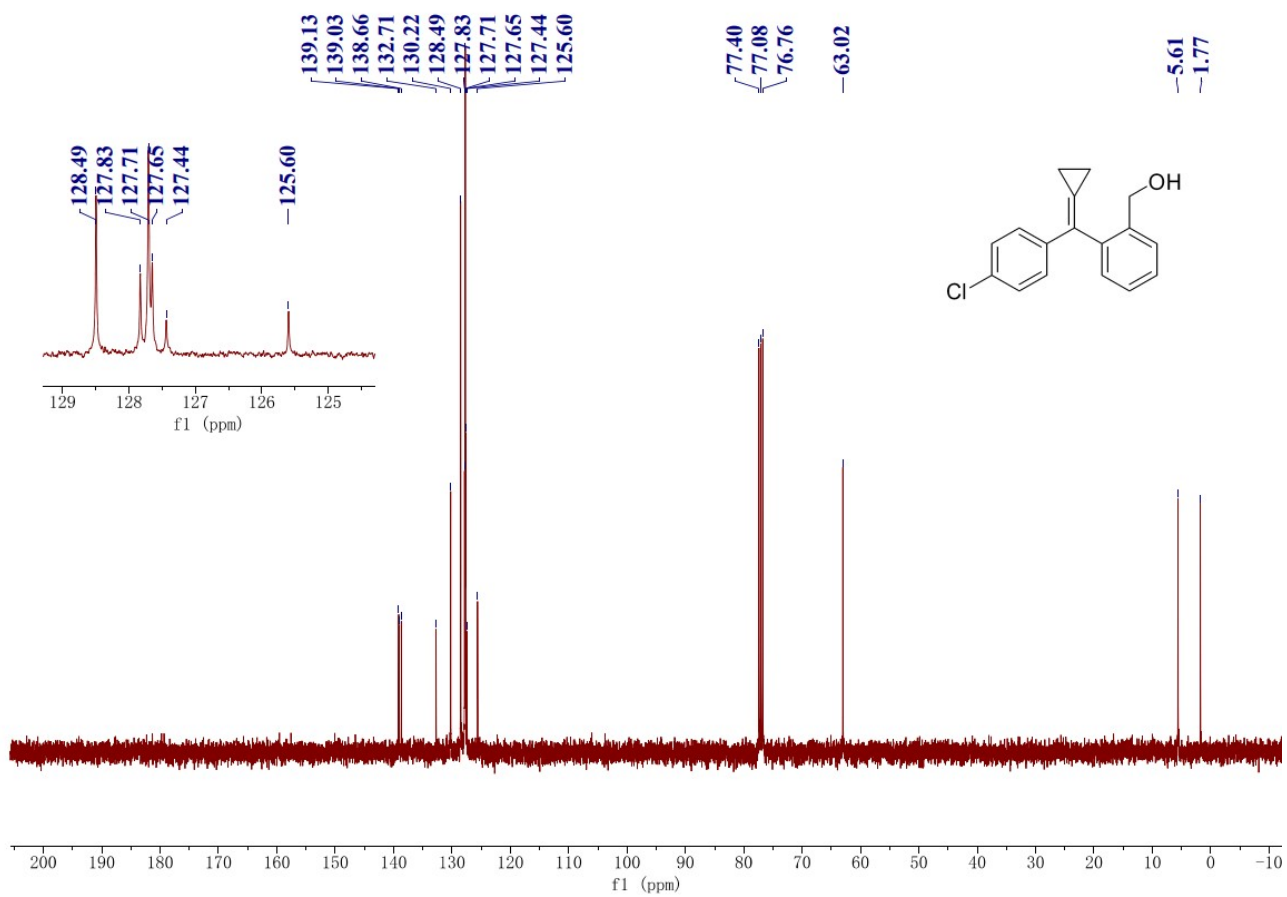


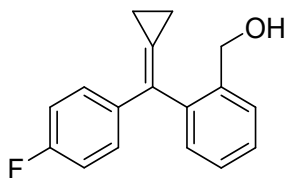


(2-((4-chlorophenyl)(cyclopropylidene)methyl)phenyl)methanol (1t)

A colorless oil. 306 mg, 81% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.54 (d, $J = 7.2$ Hz 1H), 7.42-7.37 (m, 1H), 7.36-7.32 (m, 3H), 7.26-7.24 (m, 2H), 7.20-7.17 (m, 1H), 4.43 (s, 2H), 1.62-1.58 (m, 2H), 1.50 (br, 1H), 1.14-1.11 (m, 2H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 139.1, 139.0, 138.7, 132.7, 130.2, 128.5, 127.8, 127.7, 127.6, 127.4, 125.6, 77.4, 77.1, 76.8, 63.0, 5.6, 1.8. IR (acetone) ν 3312, 3048, 2972, 1489, 1448, 1399, 1189, 1092, 903, 760 cm^{-1} . HRMS (EI) Calcd. for $\text{C}_{17}\text{H}_{15}\text{ClO}$ (M^+): 270.0806, Found: 270.0801.

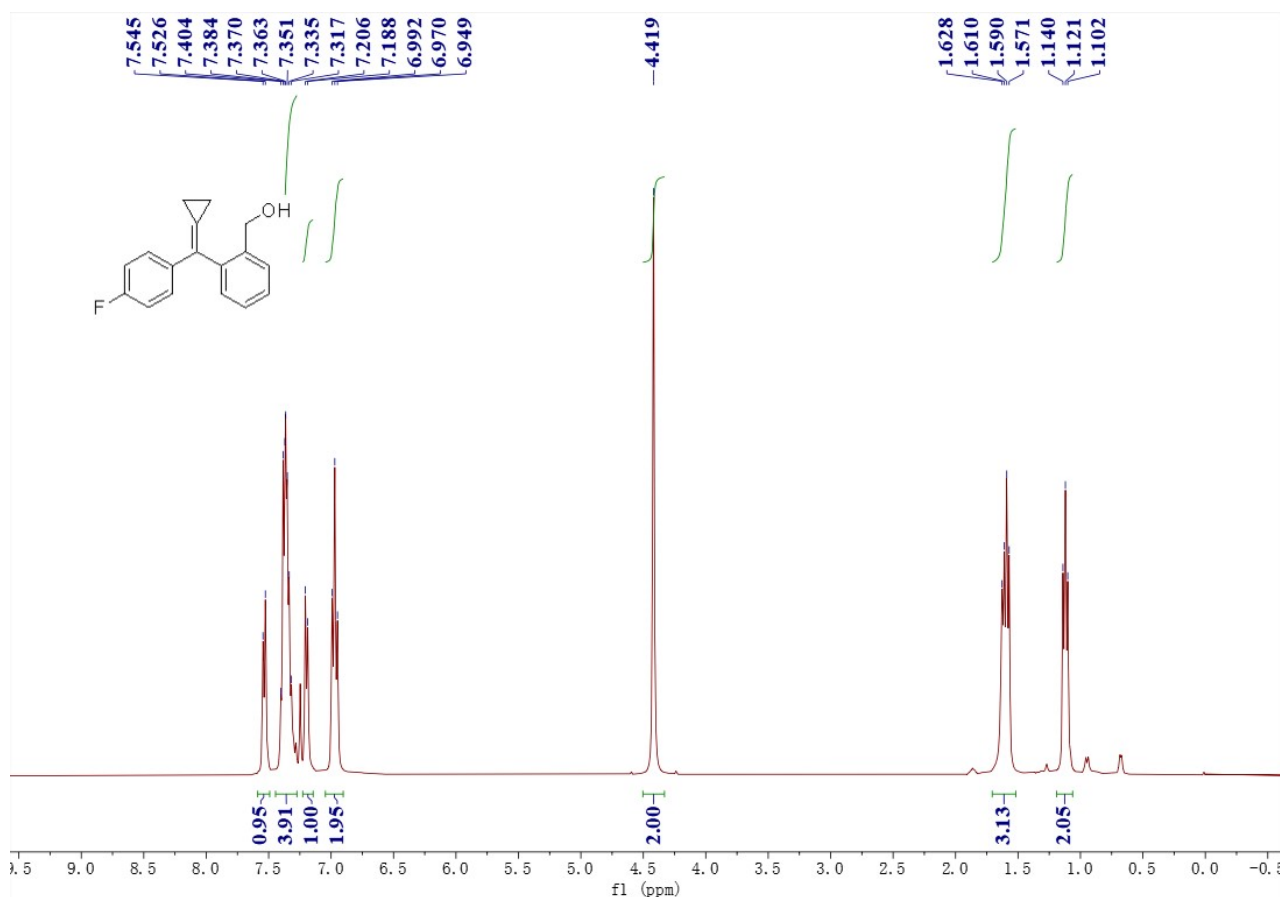


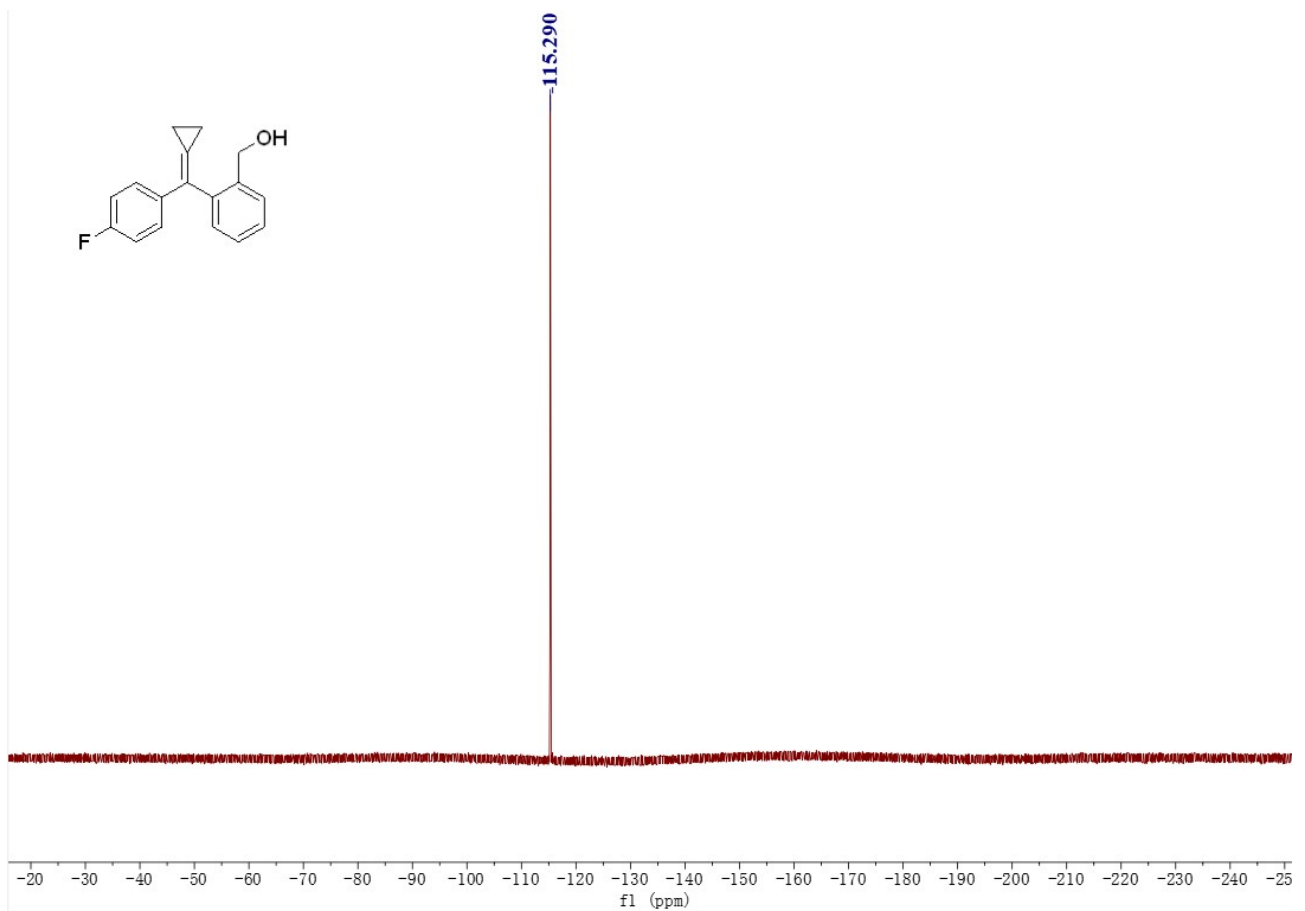
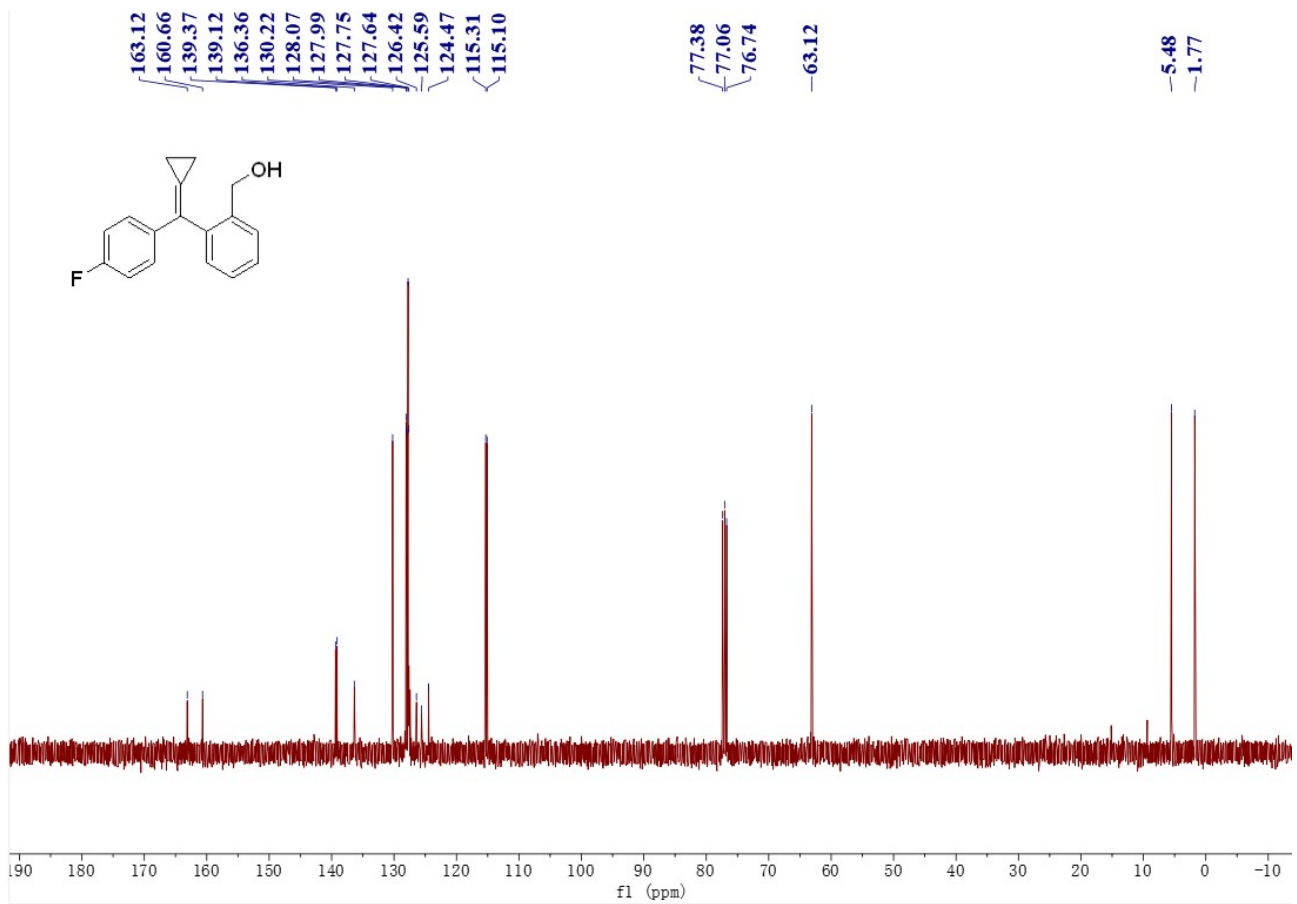


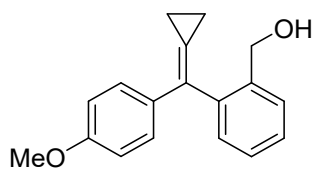


(2-(cyclopropylidene(4-fluorophenyl)methyl)phenyl)methanol (1u)

A colorless oil, 401 mg, 87% yield ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.54 (d, $J = 7.4$ Hz, 1H), 7.40-7.32 (m, 4H), 7.20 (d, $J = 7.4$ Hz, 1H), 6.97 (t, $J = 8.6$ Hz, 2H), 4.42 (s, 2H), 1.63-1.57 (m, 3H), 1.14-1.10 (m, 2H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 161.9 (d, $J = 248.5$ Hz), 139.2 (d, $J = 25.0$ Hz), 136.4, 130.2, 128.1, 128.0, 127.8, 127.6, 126.4, 125.6, 124.5, 115.2 (d, $J = 21.0$ Hz), 63.1, 5.5, 1.8. ^{19}F NMR (376 MHz, CDCl_3) δ -115.3. IR (acetone) ν 3369, 3025, 2972, 1482, 1445, 1224, 1189, 1100, 904, 757 cm^{-1} . HRMS (EI) Calcd. for $\text{C}_{17}\text{H}_{15}\text{FO}$ (M^+): 254.1101, Found: 254.1104.

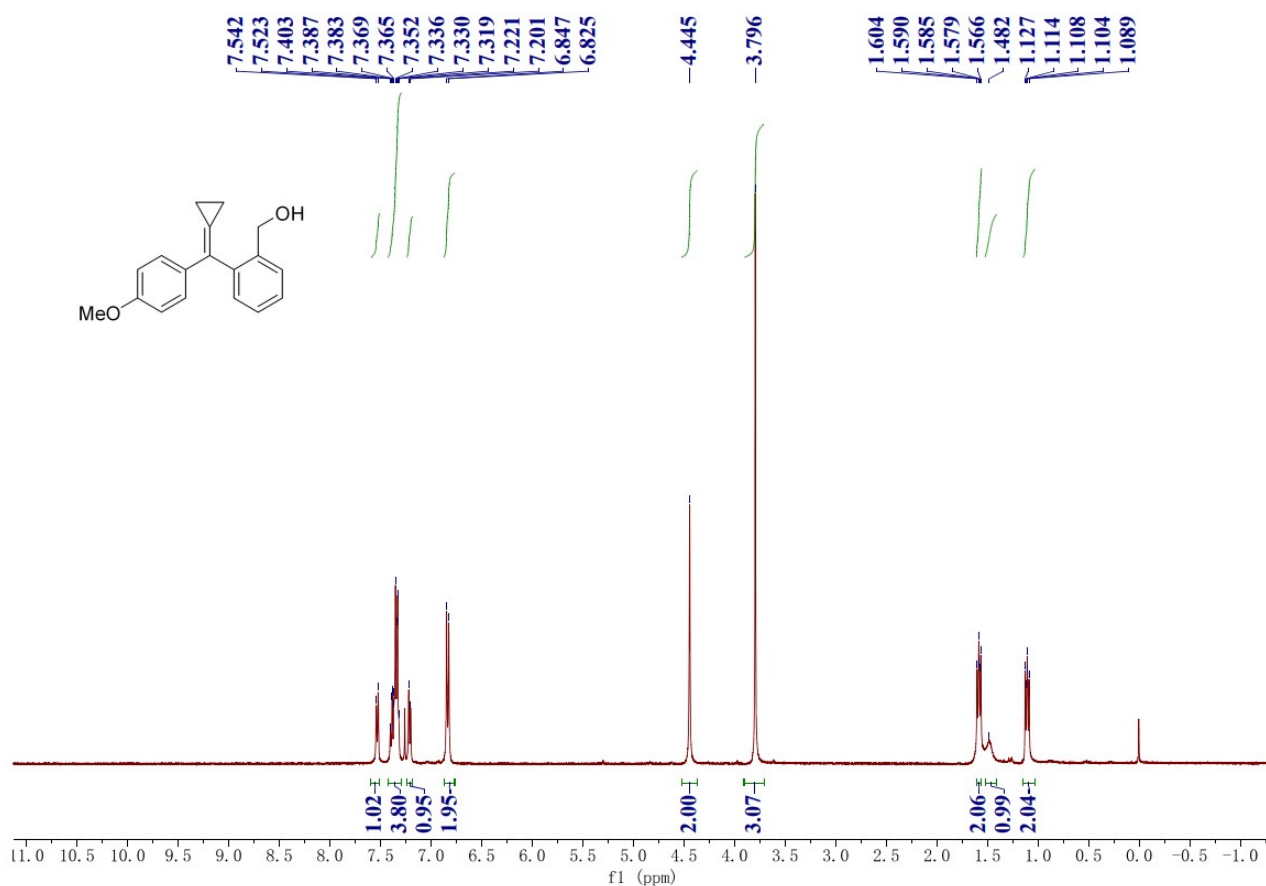


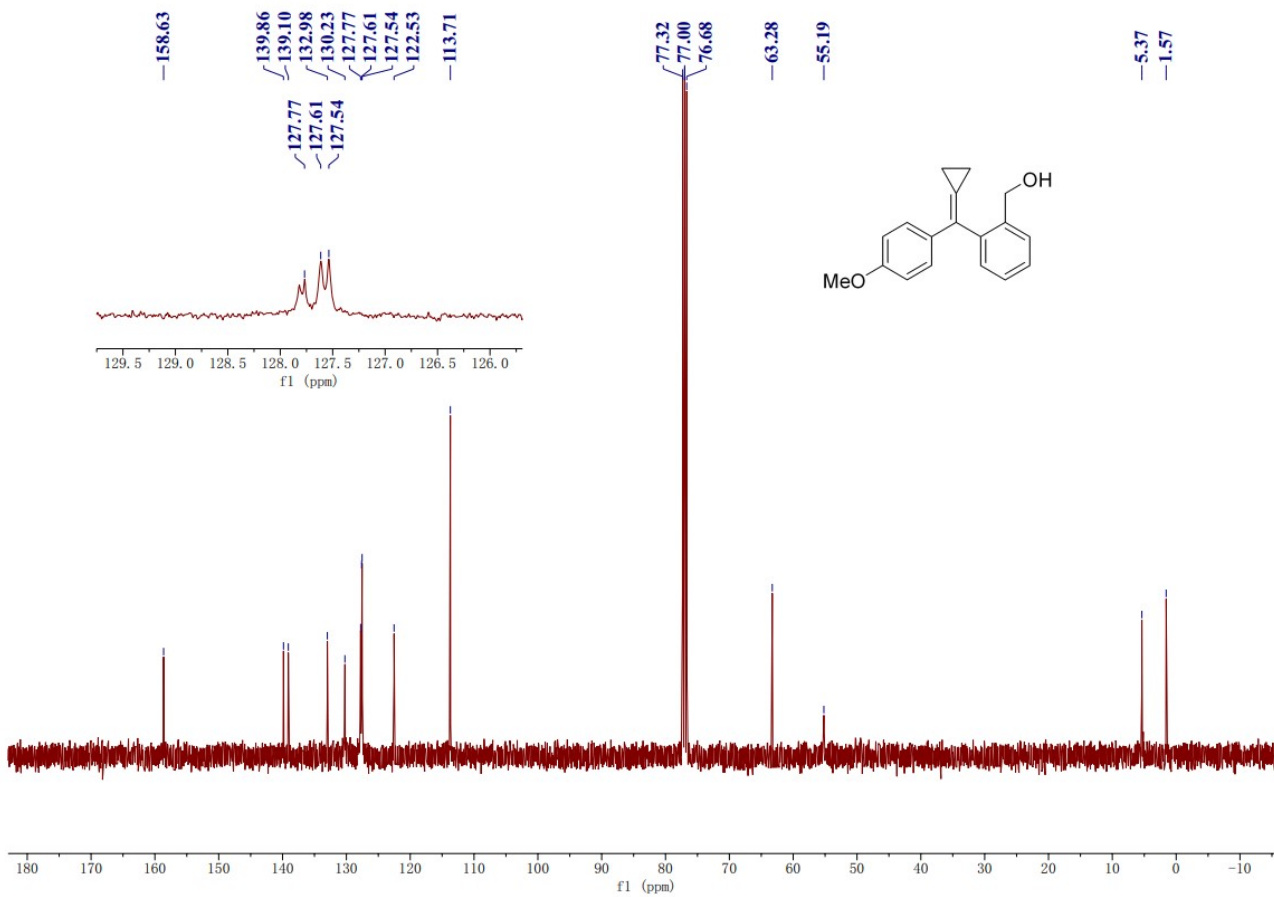


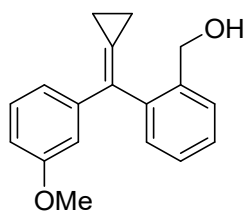


(2-(cyclopropylidene(4-methoxyphenyl)methyl)phenyl)methanol (1v)

A white solid, M.P.: 106-108 °C, 391 mg, 72% yield, ¹H NMR (CDCl₃, TMS, 400 MHz) δ 7.53 (d, *J* = 7.6 Hz, 1H), 7.40-7.32 (m, 4H), 7.21 (d, *J* = 9.0 Hz, 1H), 6.84 (d, *J* = 8.6 Hz, 2H), 4.44 (s, 2H), 3.80 (s, 3H), 1.60-1.57 (m, 2H), 1.48 (br, 1H), 1.13-1.09 (m, 2H). ¹³C NMR (CDCl₃, TMS, 100 MHz) δ 158.6, 139.9, 139.1, 133.0, 130.2, 127.80, 127.77, 127.61, 127.5, 122.5, 113.7, 63.3, 55.2, 5.4, 1.6. IR (acetone) ν 3382, 2933, 1604, 1577, 1452, 1300, 1176, 1032, 756, 700 cm⁻¹. HRMS (FI) Calcd. for C₁₈H₁₈O₂ (M⁺): 266.1301, Found: 266.1305.

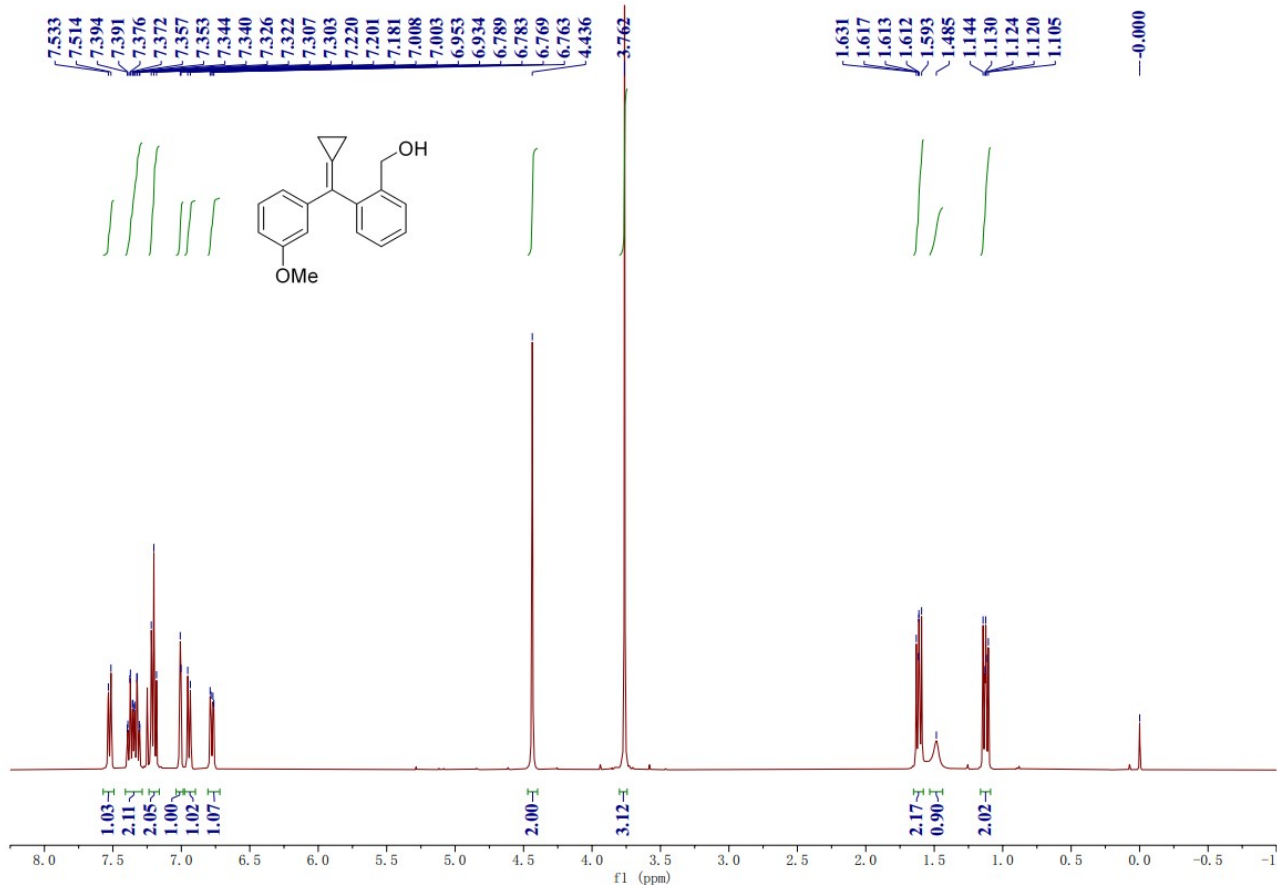


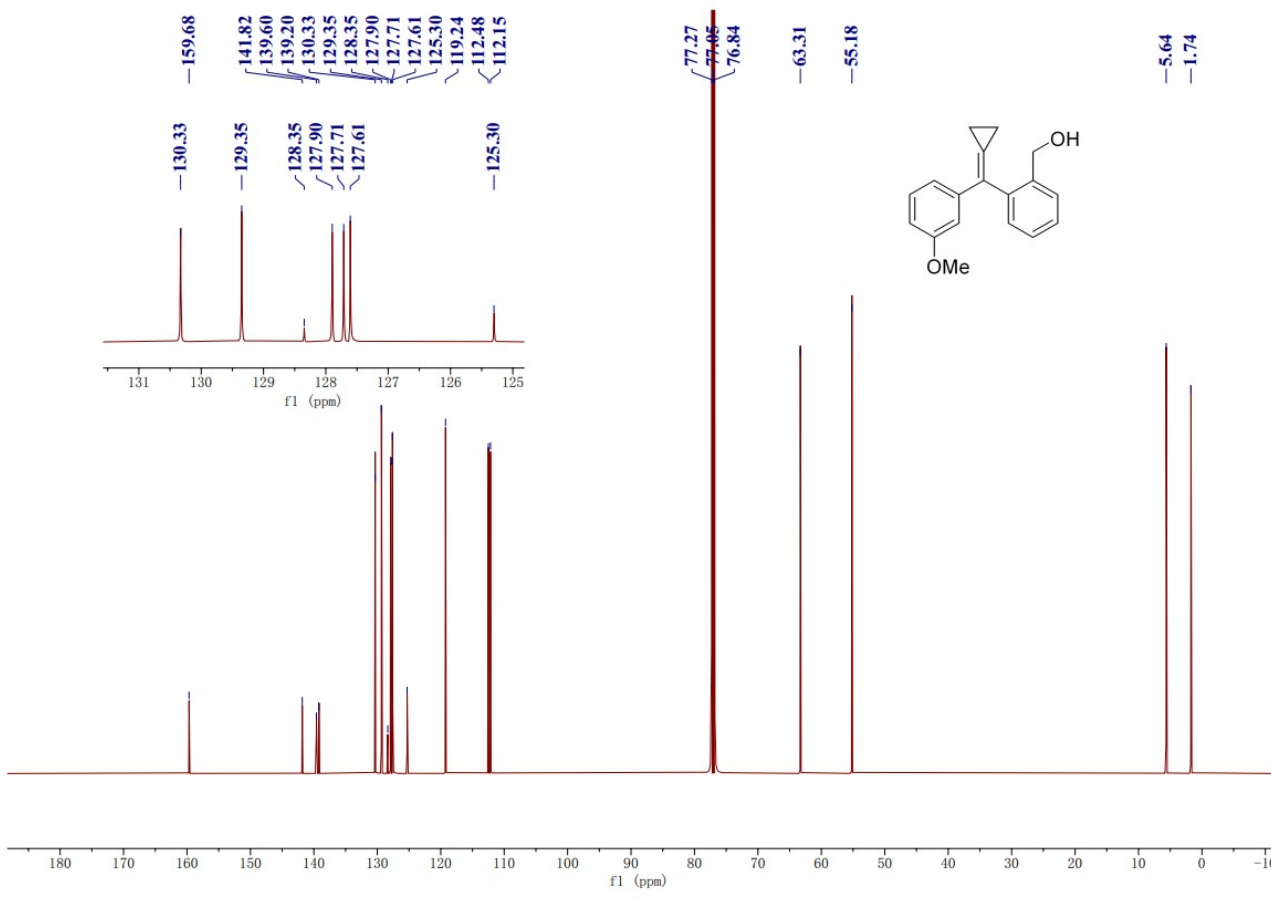


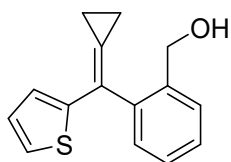


(2-(cyclopropylidene(3-methoxyphenyl)methyl)phenyl)methanol (1w)

A colorless oil, 208 mg, 73% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.52 (d, $J = 7.6$ Hz, 1H), 7.39-7.30 (m, 2H), 7.22-7.17 (m, 2H), 7.01-7.00 (m, 1H), 6.94 (d, $J = 7.8$ Hz, 1H), 6.79-6.76 (m, 1H), 4.44 (s, 2H), 3.76 (s, 3H), 1.63-1.59 (m, 2H), 1.49 (br, 1H), 1.14-1.11 (m, 2H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 159.7, 141.8, 139.6, 139.2, 130.3, 129.3, 128.3, 127.9, 127.7, 127.6, 125.3, 119.2, 112.5, 112.2, 63.3, 55.2, 5.6, 1.7. IR (acetone) ν 3383, 2969, 1596, 1577, 1463, 1287, 1162, 1039, 752, 697 cm^{-1} . HRMS (EI) Calcd. for $\text{C}_{18}\text{H}_{18}\text{O}_2$ (M^+): 266.1301, Found: 266.1298.

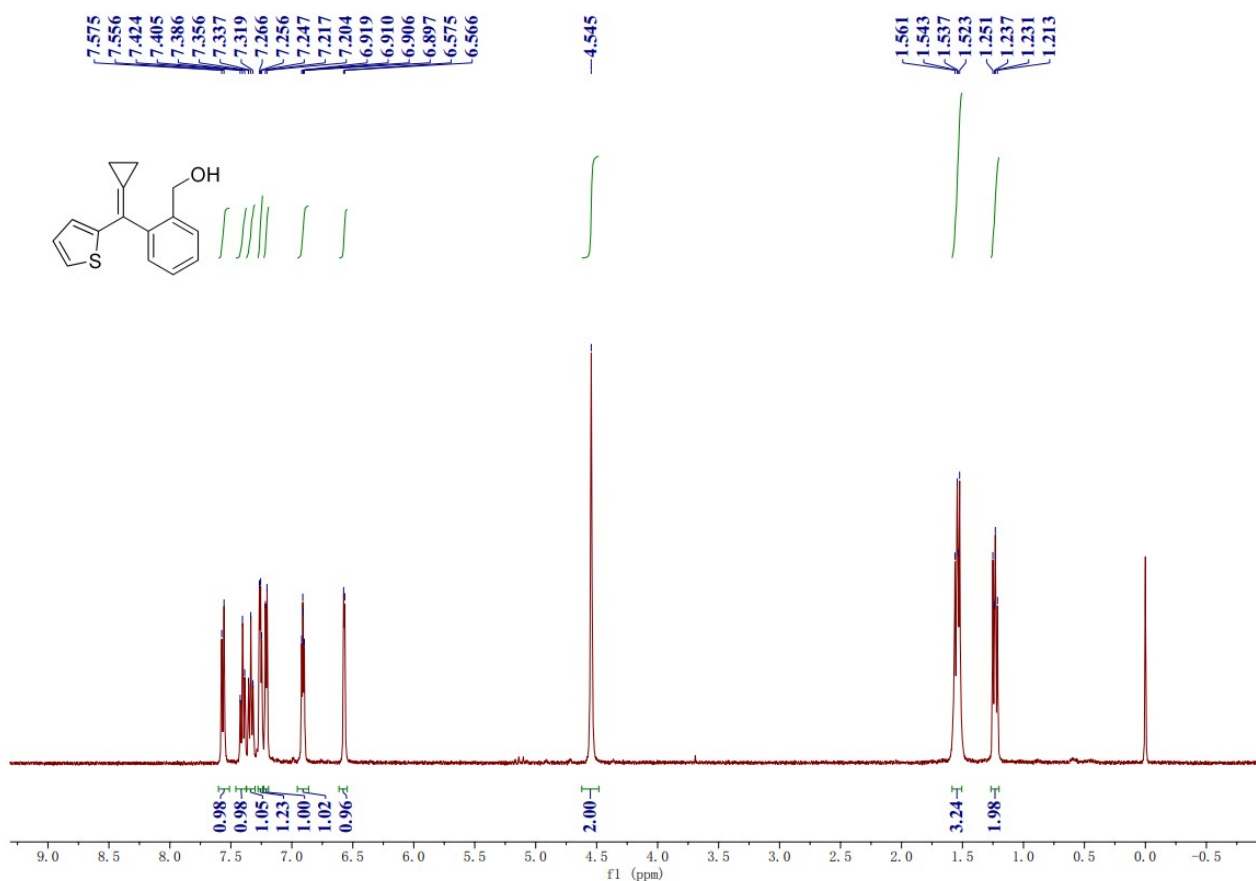


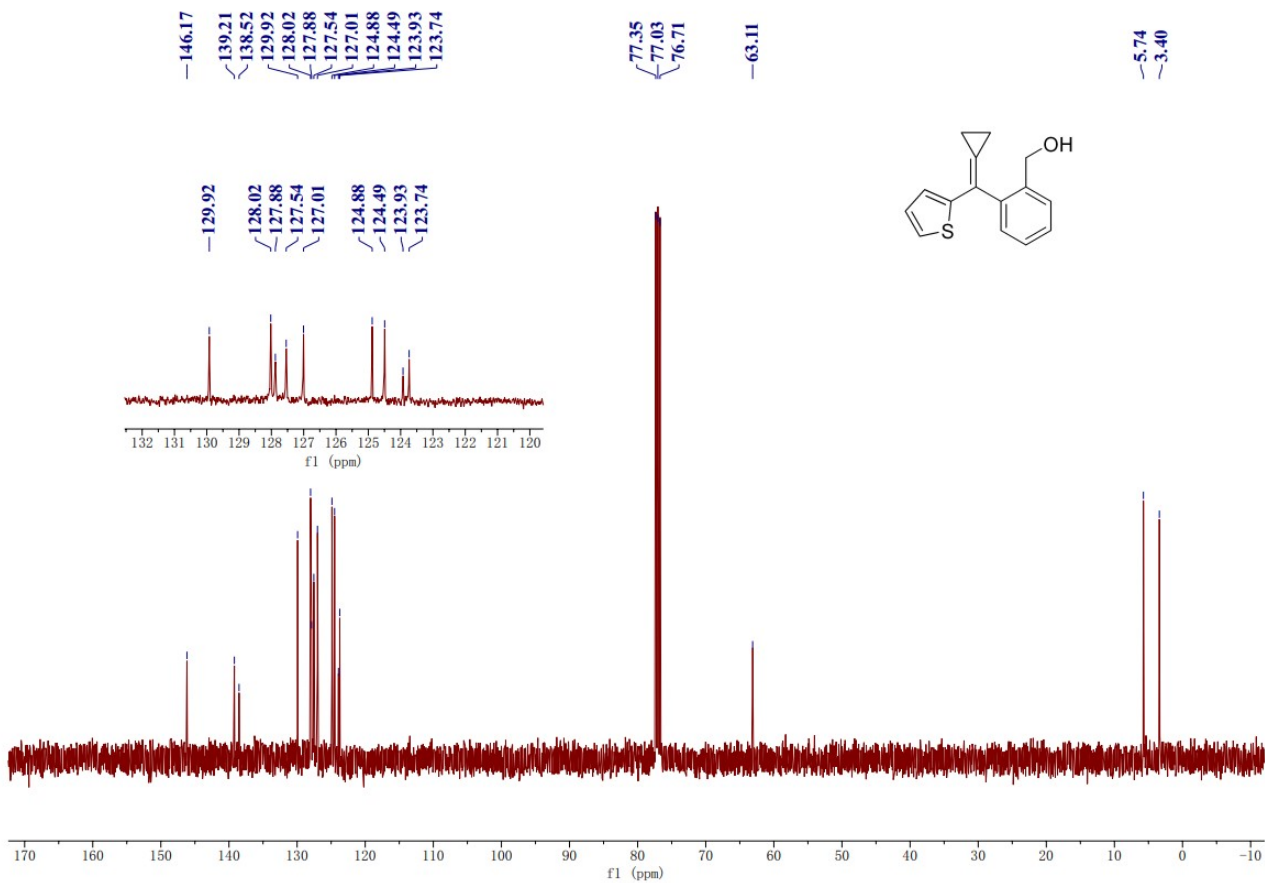


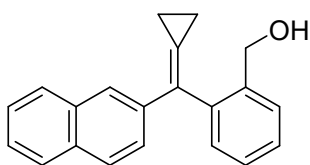


(2-(cyclopropylidene(thiophen-2-yl)methyl)phenyl)methanol (1x)

A white solid, M.P.: 105-108 °C, 290 mg, 73% yield. ¹H NMR (CDCl₃, TMS, 400 MHz) δ 7.57 (d, *J* = 7.6 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.34 (t, *J* = 7.4 Hz, 1H), 7.29-7.18 (m, 3H), 6.92-6.90 (m, 1H), 6.57 (d, *J* = 3.6 Hz, 1H), 4.54 (s, 2H), 1.56-1.52 (m, 3H), 1.25-1.21 (m, 2H). ¹³C NMR (CDCl₃, TMS, 100 MHz) δ 146.2, 139.2, 138.5, 129.9, 128.0, 127.9, 127.5, 127.0, 124.9, 124.5, 123.9, 123.7, 63.1, 5.7, 3.4. IR (acetone) ν 3336, 3067, 2970, 1600, 1484, 1234, 1032, 844, 753, 697 cm⁻¹. HRMS (EI) Calcd. for C₁₅H₁₄OS (M⁺): 242.0760, Found: 242.0762.

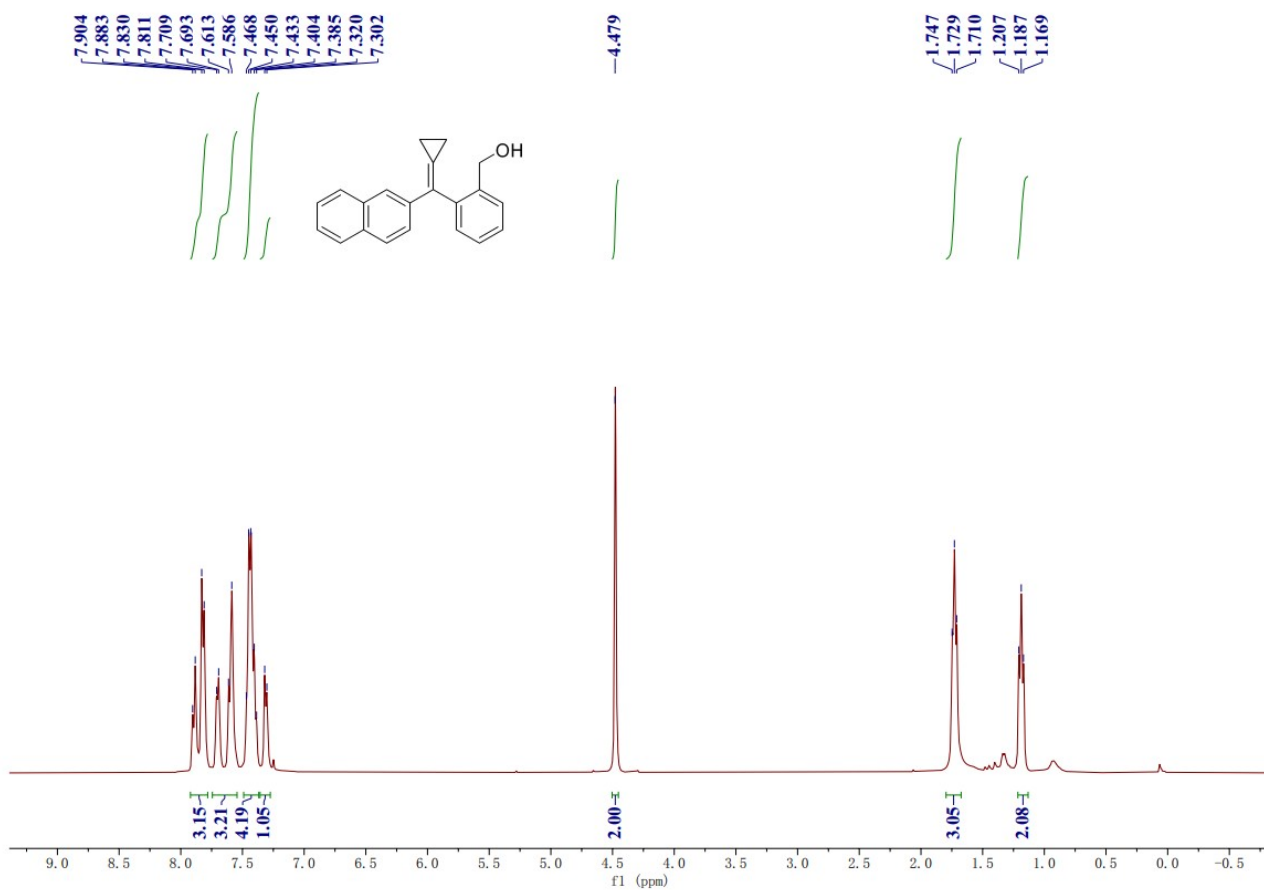


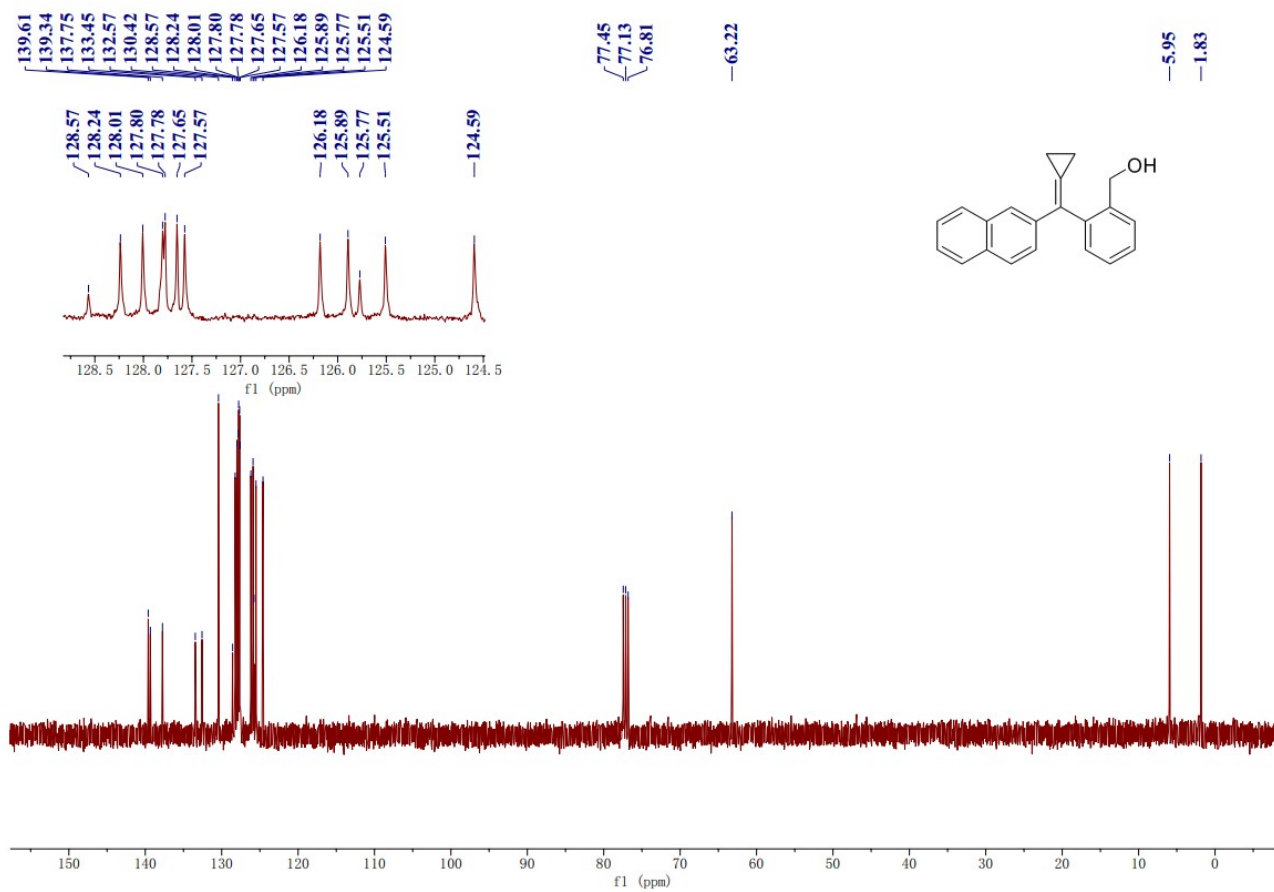


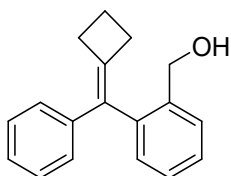


(2-(cyclopropylidene(naphthalen-2-yl)methyl)phenyl)methanol (1y)

A yellow solid, M.P.: 125-128 °C, 408 mg, 89% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.91-7.81 (m, 3H), 7.71-7.60 (m, 3H), 7.47-7.39 (m, 4H), 7.32-7.30 (m, 1H), 4.48 (s, 2H), 1.75-1.71 (m, 3H), 1.21-1.17 (m, 2H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) 139.6, 139.3, 137.7, 133.5, 132.6, 130.4, 128.6, 128.2, 128.0, 127.80, 127.78, 127.7, 127.6, 126.2, 125.9, 125.8, 125.5, 124.6, 63.2, 5.9, 1.8. IR (acetone) ν 3380, 3056, 2974, 1600, 1505, 1485, 1193, 1037, 866, 749 cm^{-1} . HRMS (EI) Calcd. for $\text{C}_{21}\text{H}_{18}\text{O}$ (M^+): 286.1352, Found: 286.1354.

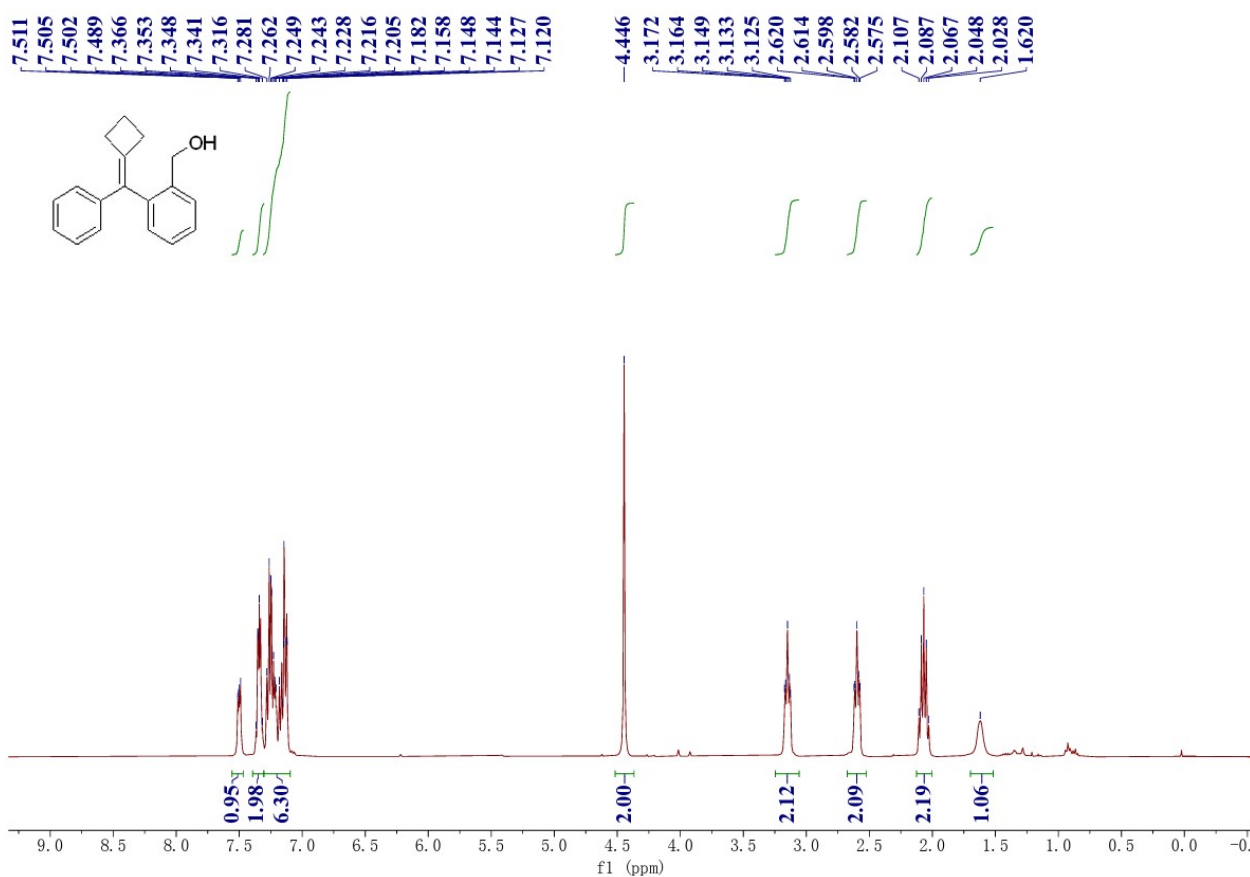


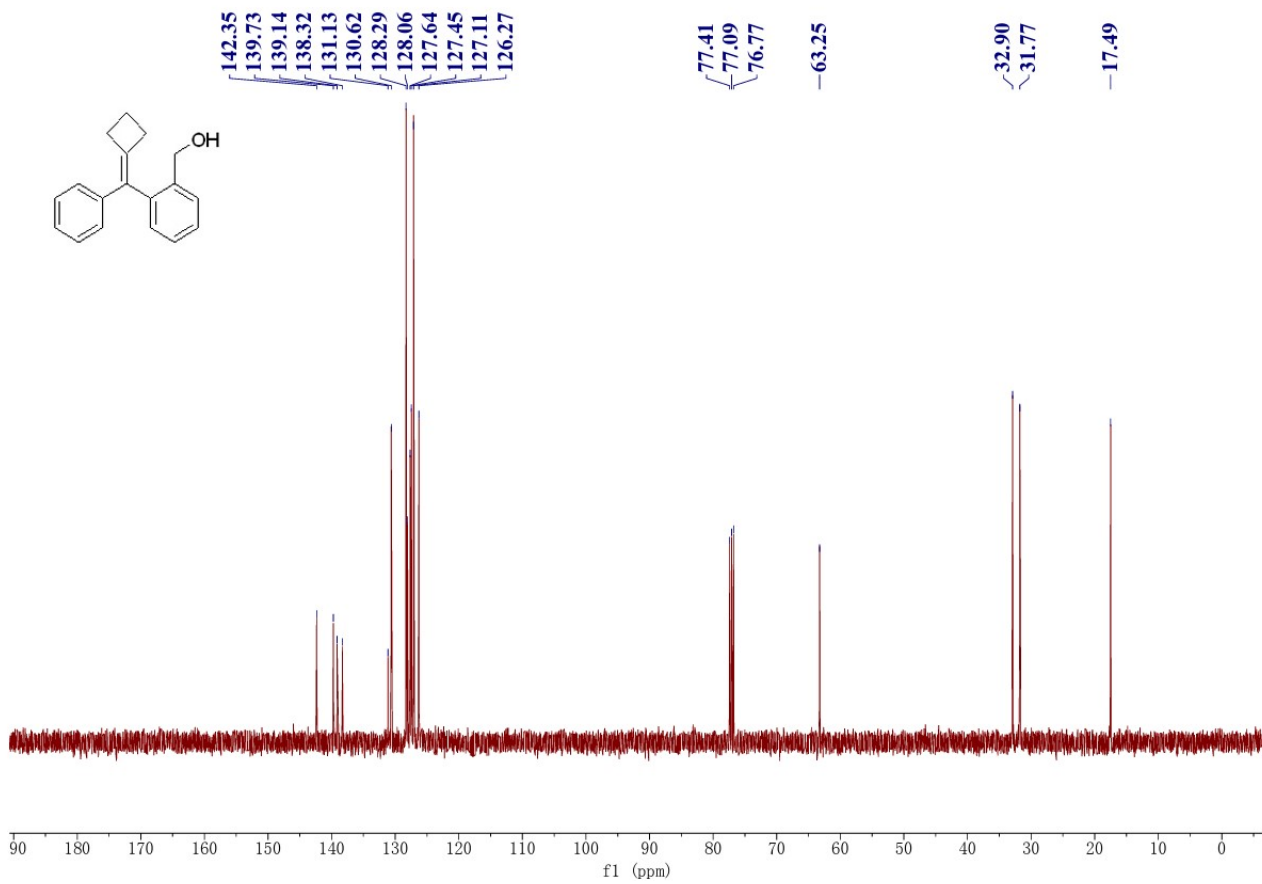


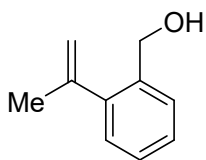


(2-(cyclobutylidene(phenyl)methyl)phenyl)methanol (1z)

A white solid, M.P.: 115-117 °C, 150 mg, 85% yield. ¹H NMR (CDCl₃, TMS, 400 MHz) δ 7.51-7.49 (m, 1H), 7.37-7.34 (m, 2H), 7.32-7.12 (m, 6H), 4.45 (s, 2H), 3.17-3.13 (m, 2H), 2.62-2.58 (m, 2H), 2.11-2.03 (m, 2H), 1.62 (br, 1H). ¹³C NMR (CDCl₃, TMS, 100 MHz) δ 142.3, 139.7, 139.1, 138.3, 131.1, 130.6, 128.3, 128.1, 127.6, 127.5, 127.1, 126.3, 63.2, 32.9, 31.8, 17.5. IR (acetone) ν 3344, 3056, 2951, 1494, 1443, 1412, 1197, 1032, 901, 695 cm⁻¹. HRMS (EI) Calcd. for C₁₈H₁₆O₂ (M-H₂O)⁺: 232.1247, Found: 232.1248.

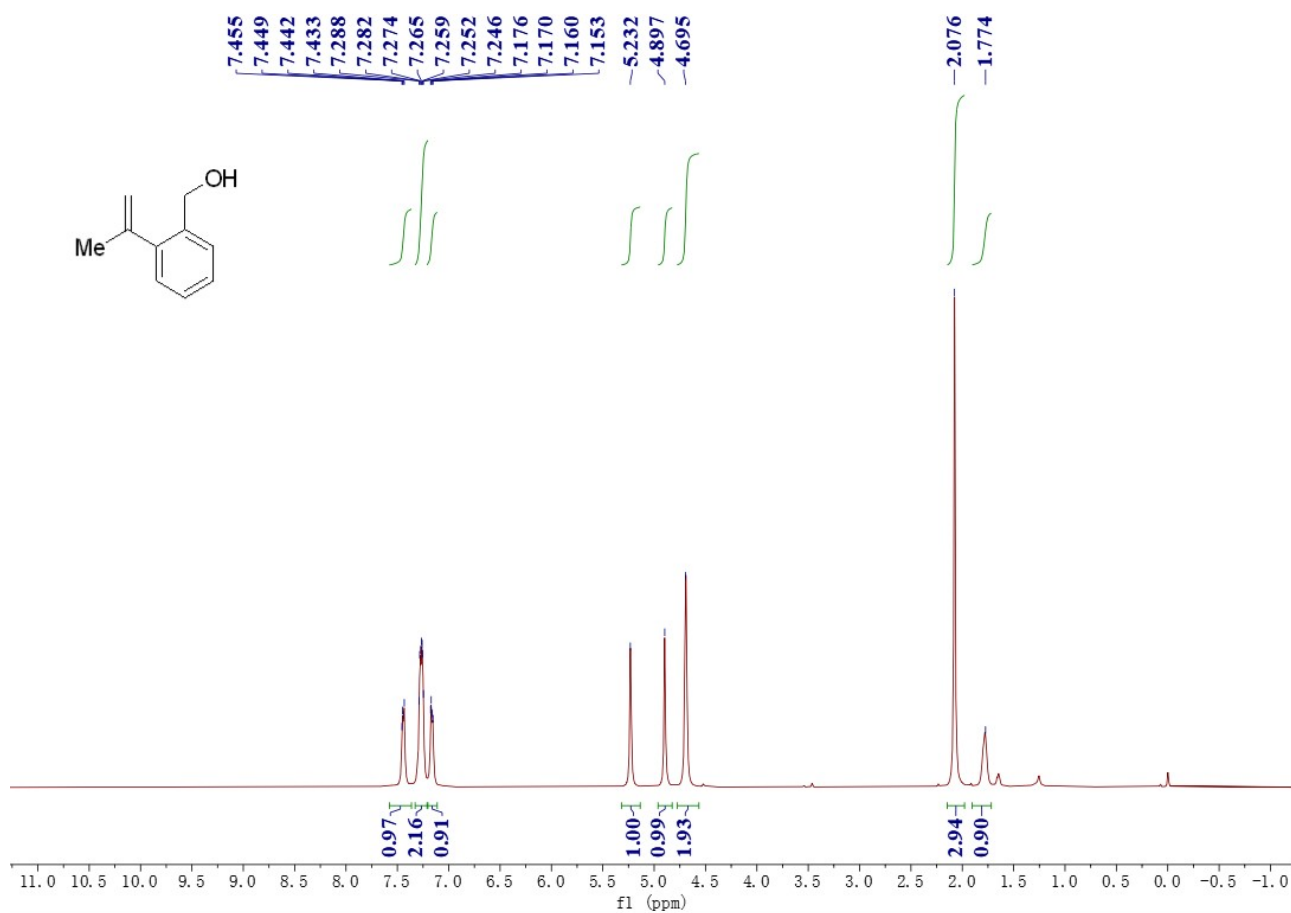


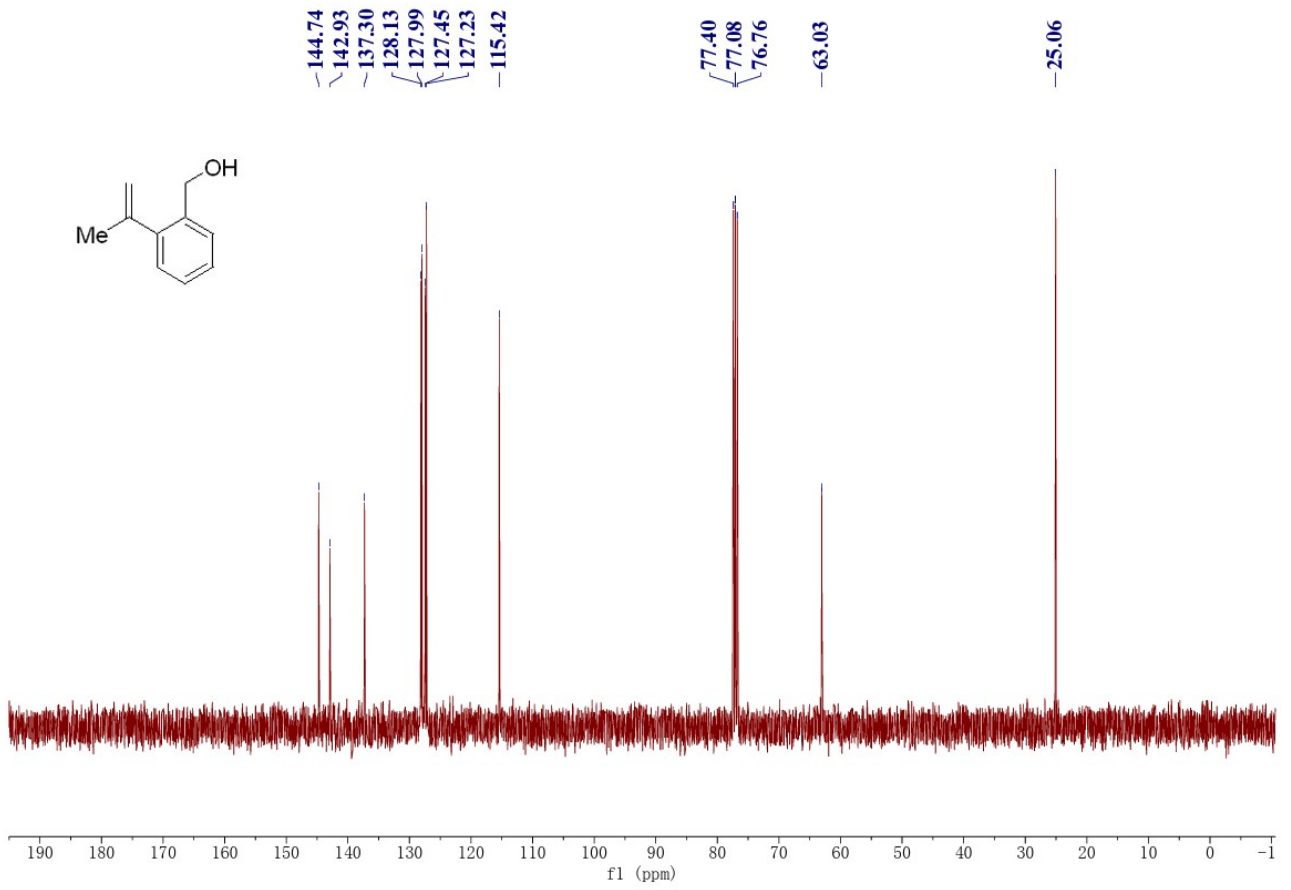
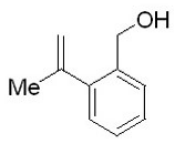


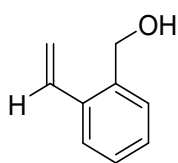


(2-(prop-1-en-2-yl)phenyl)methanol (1aa)

This is a known compound and its spectroscopic data are consistent with those in the previous literature.⁶ CAS number: 180092-32-4. A colorless oil, 501 mg, 90% yield. ¹H NMR (CDCl₃, TMS, 400 MHz) δ 7.46-7.43 (m, 1H), 7.29-7.25 (m, 2H), 7.18-7.15 (m, 1H), 5.23 (s, 1H), 4.90 (s, 1H), 4.70 (s, 2H), 2.08 (s, 3H), 1.77 (br, 1H). ¹³C NMR (CDCl₃, TMS, 100 MHz) δ 144.7, 142.9, 137.3, 128.1, 128.0, 127.5, 127.2, 115.4, 63.0, 25.1.

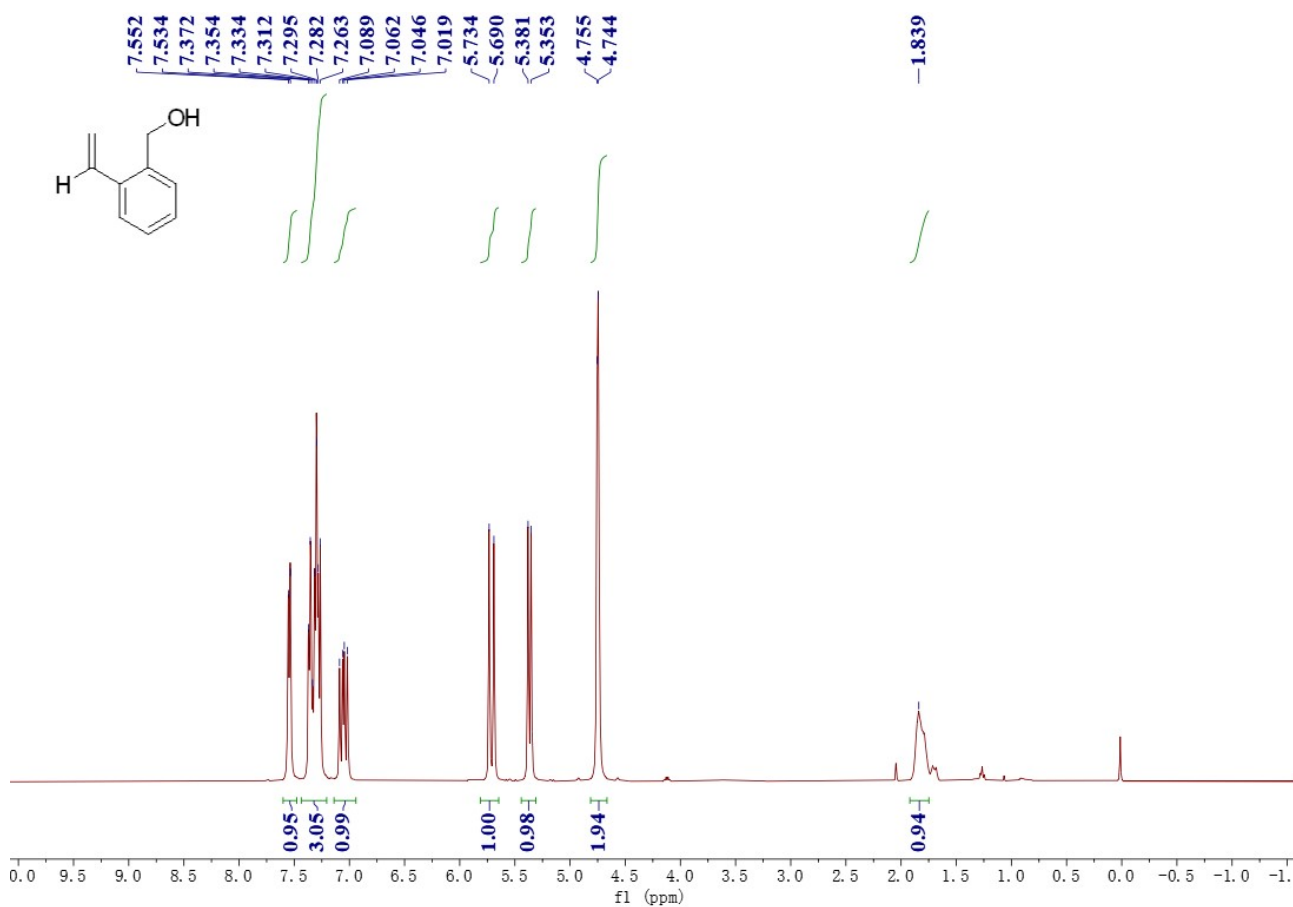


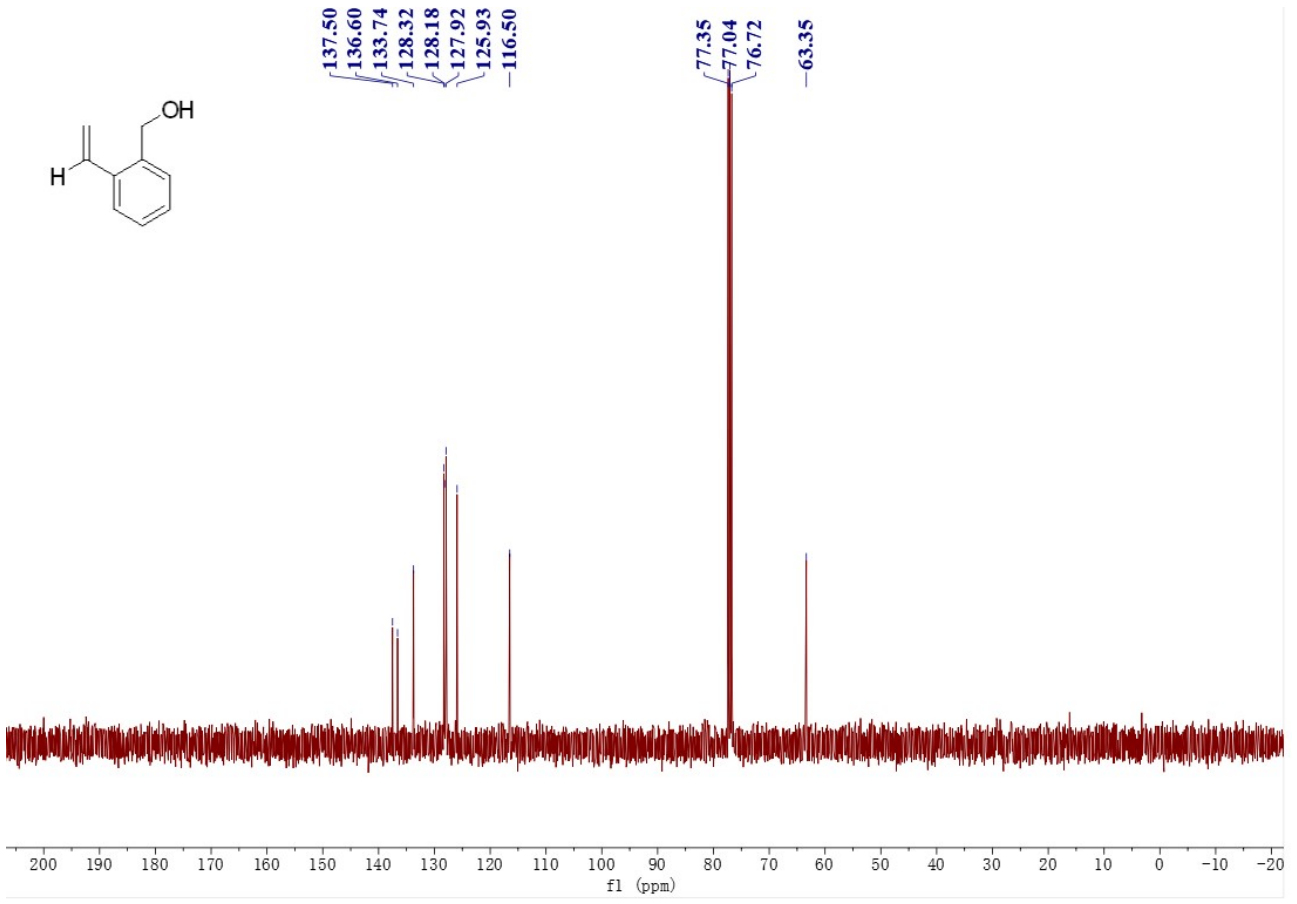
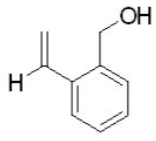


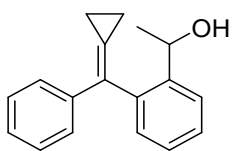


(2-vinylphenyl)methanol (1ab)

This is a known compound and its spectroscopic data are consistent with those in the previous literature.⁸ CAS number: 35106-82-2. A colorless oil, 601 mg, 93% yield. ¹H NMR (CDCl₃, TMS, 400 MHz) δ 7.54 (d, *J* = 7.2 Hz, 1H), 7.37-7.26 (m, 3H), 7.05 (dd, *J* = 17.4, 10.8 Hz, 2H), 5.71 (d, *J* = 17.4 Hz, 1H), 5.37 (d, *J* = 10.8 Hz, 1H), 4.75 (d, *J* = 4.6 Hz, 2H), 1.84 (br, 1H). ¹³C NMR (CDCl₃, TMS, 100 MHz) δ 137.5, 136.6, 133.7, 128.3, 128.2, 127.9, 125.9, 116.5, 63.4.

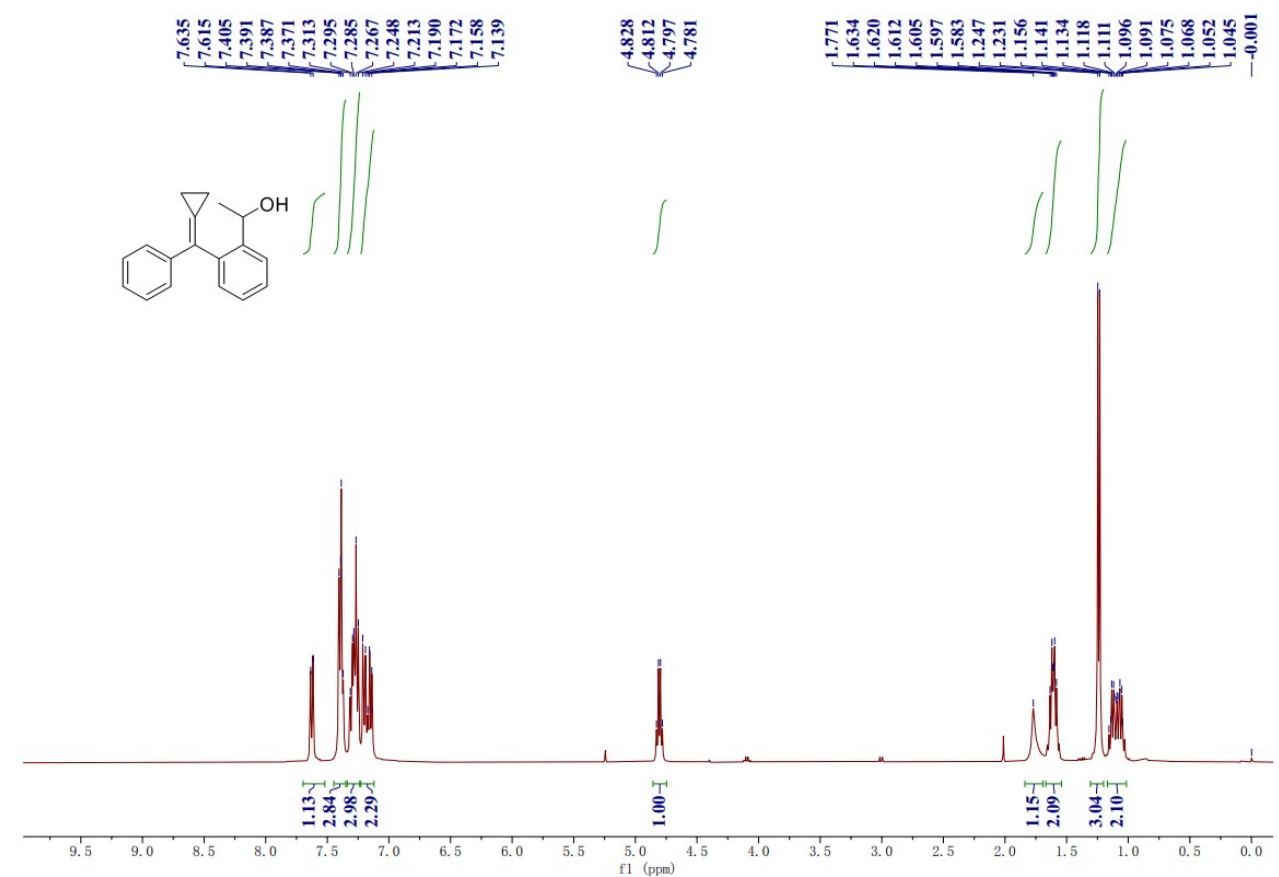


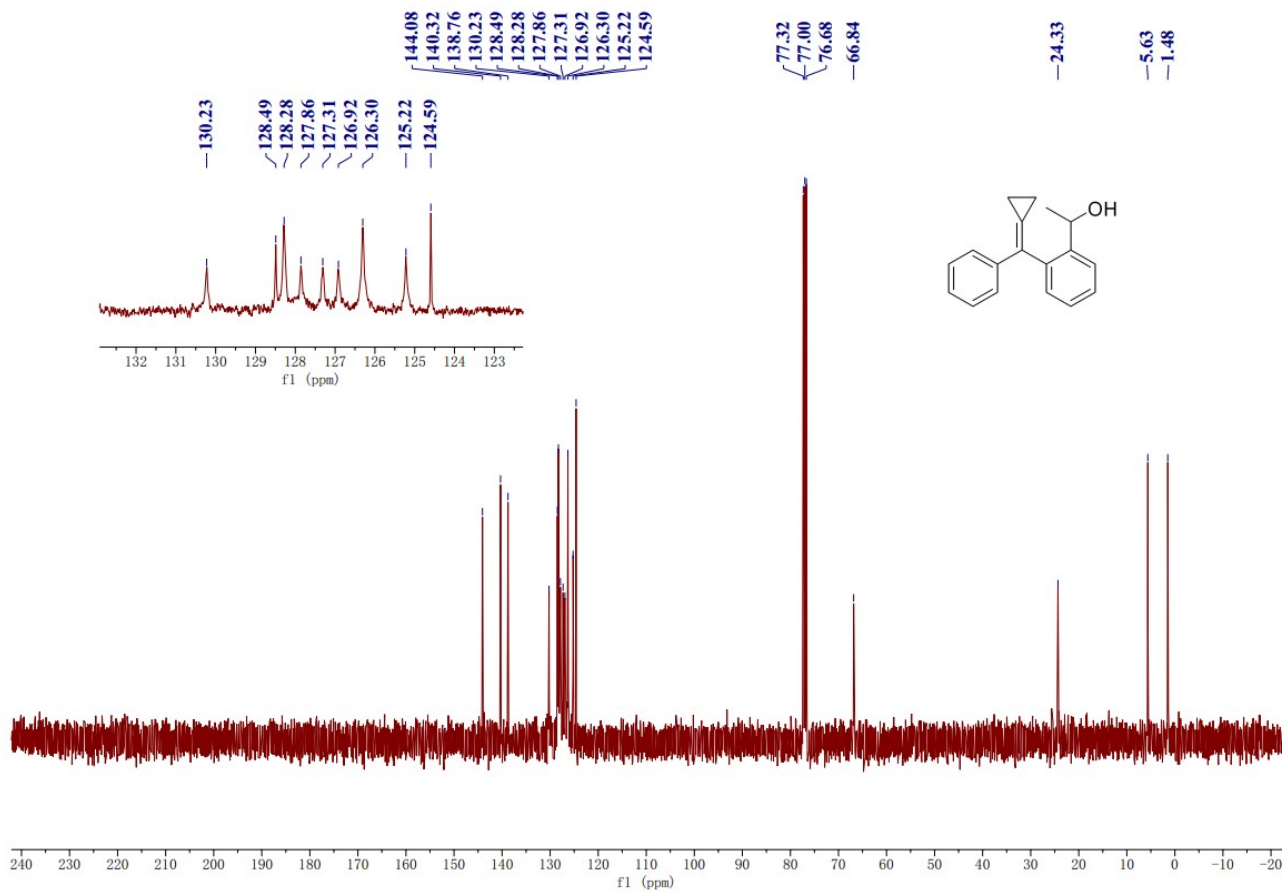


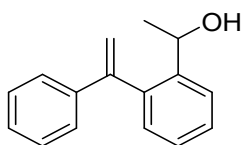


1-(2-(cyclopropylidene(phenyl)methyl)phenyl)ethan-1-ol (1ac)

A white solid, M.P.: 115-118 °C, 327 mg, 89% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.62 (d, $J = 7.8$ Hz, 1H), 7.41-7.37 (m, 3H), 7.31-7.25 (m, 3H), 7.21-7.14 (m, 2H), 4.80 (q, $J = 6.4$ Hz, 2H), 1.77 (br, 1H), 1.63-1.58 (m, 2H), 1.24 (d, $J = 6.4$ Hz, 3H), 1.16-1.05 (m, 2H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 144.1, 140.3, 138.8, 130.2, 128.5, 128.3, 127.9, 127.3, 126.9, 126.3, 125.2, 124.6, 66.8, 24.3, 5.6, 1.5. IR (acetone) ν 3376, 3054, 2971, 1597, 1493, 1444, 1189, 1073, 904, 695 cm^{-1} . HRMS (EI) Calcd. for $\text{C}_{18}\text{H}_{18}\text{O}$ (M^+): 250.1352, Found: 250.1355.

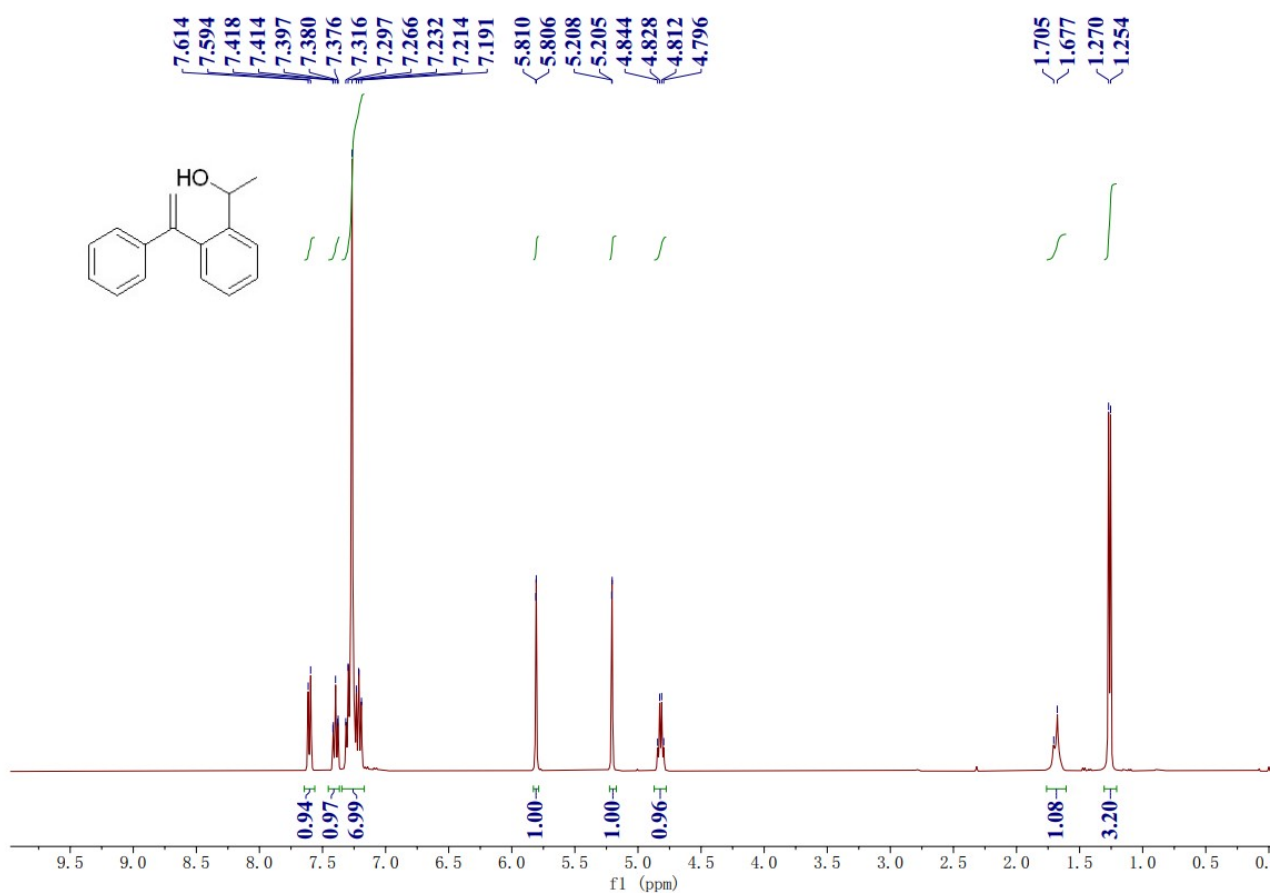


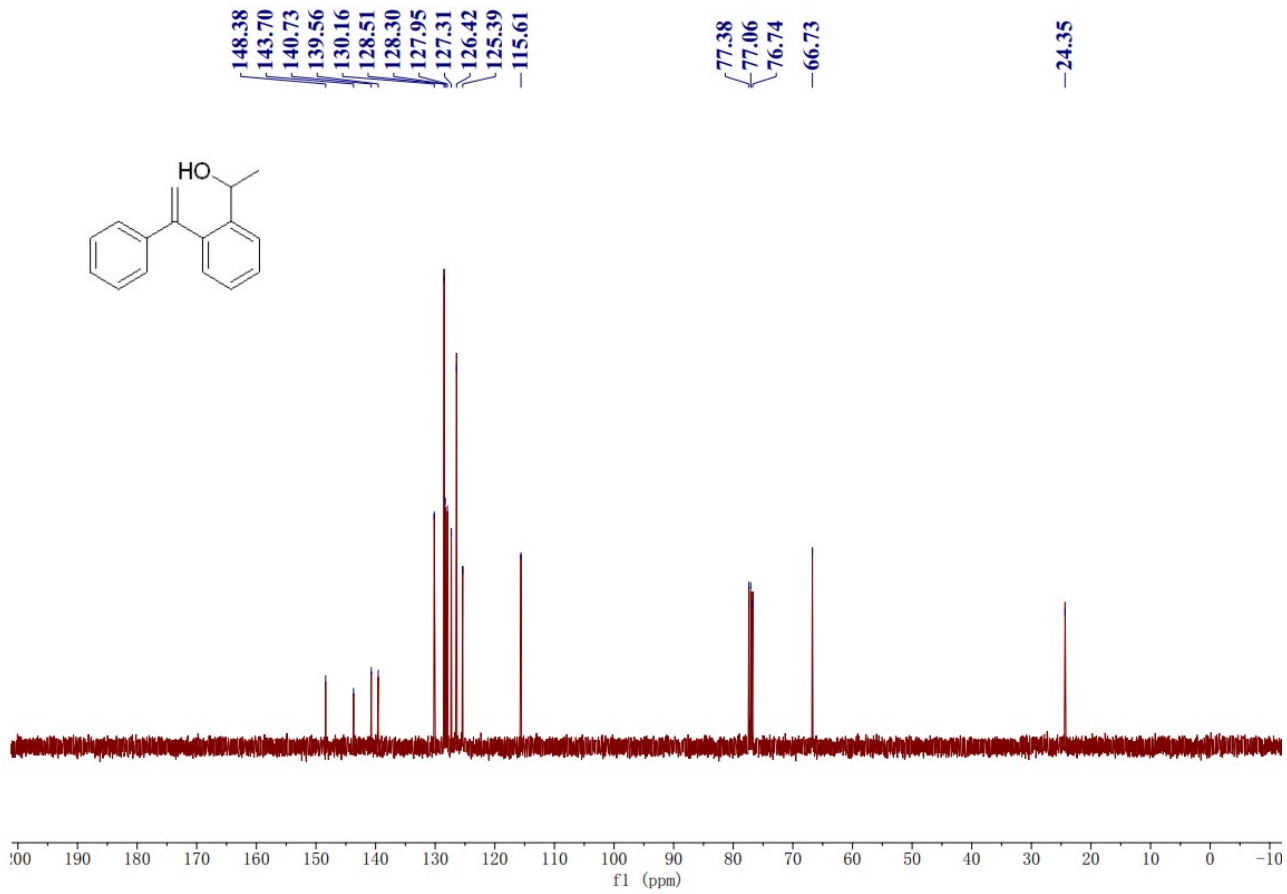
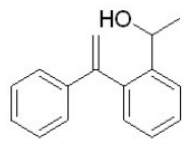


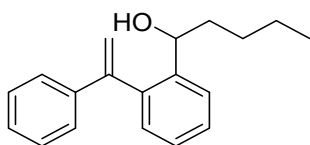


1-(2-(1-phenylvinyl)phenyl)ethan-1-ol (1ad)

This is a known compound and its spectroscopic data are consistent with those in the previous literature.⁸ CAS number: 2597348-95-1. A white solid, 331 mg, 79% yield. ¹H NMR (CDCl₃, TMS, 400 MHz) δ 7.60 (d, *J* = 7.8 Hz, 1H), 7.42-7.38 (m, 1H), 7.32-7.19 (m, 7H), 5.81 (d, *J* = 1.4 Hz, 1H), 5.21 (d, *J* = 1.4 Hz, 1H), 4.82 (q, *J* = 6.4 Hz, 1H), 1.68 (br, 1H), 1.26 (d, *J* = 6.4 Hz, 3H). ¹³C NMR (CDCl₃, TMS, 100 MHz) δ 148.4, 143.7, 140.7, 139.6, 130.2, 128.5, 128.3, 128.0, 127.3, 126.4, 125.4, 115.6, 66.7, 24.3.

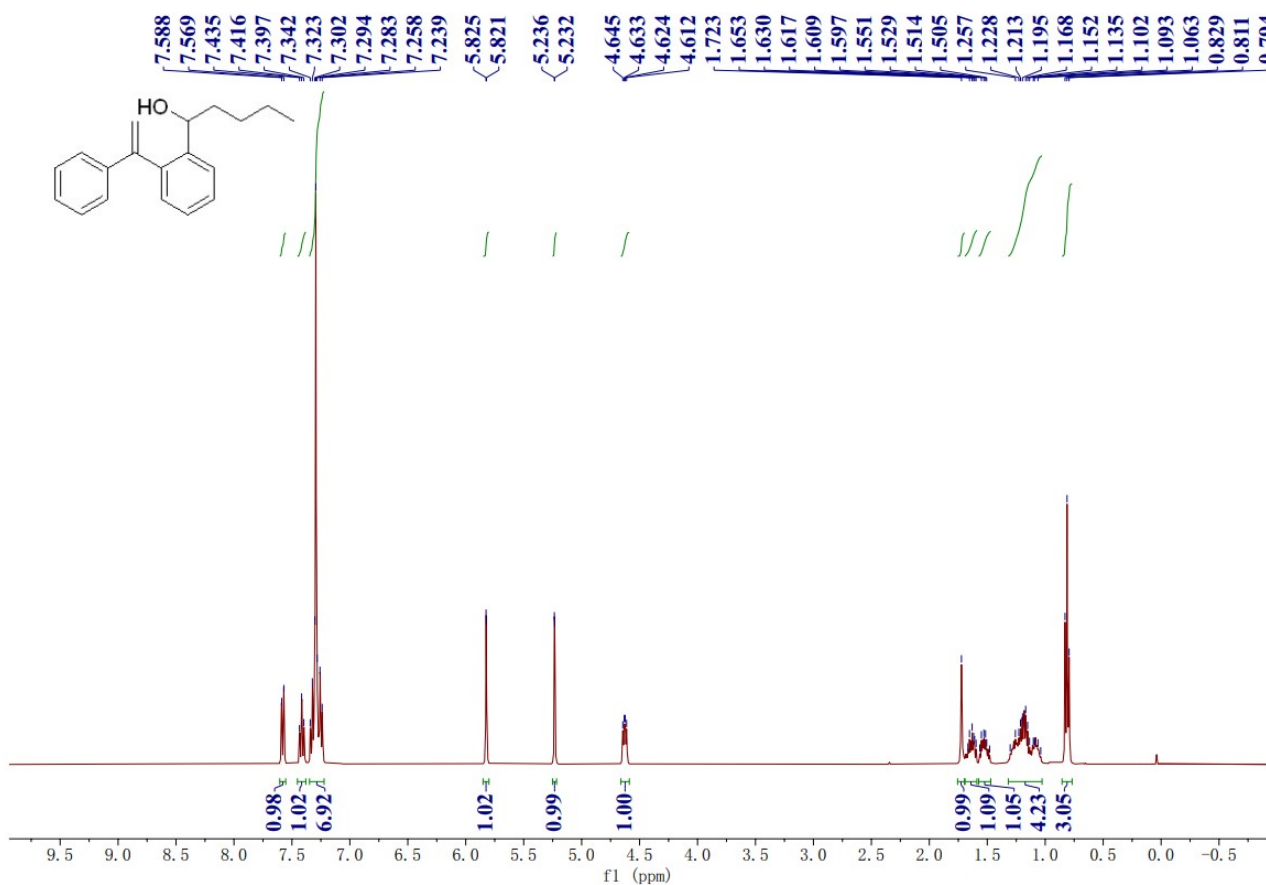


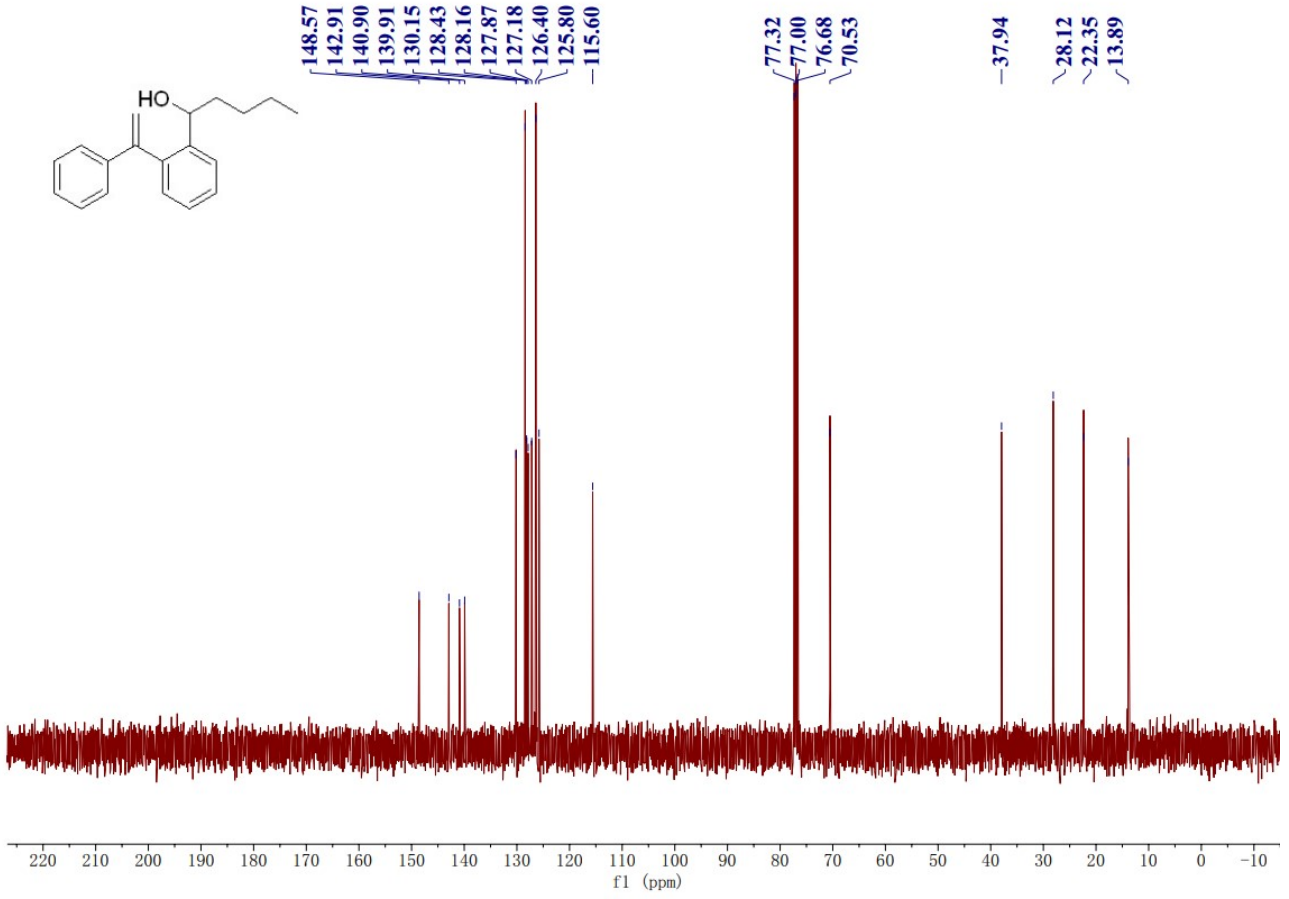
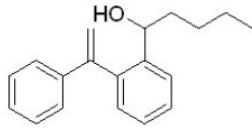


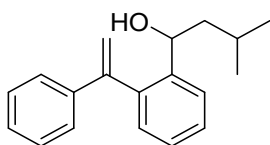


1-(2-(1-phenylvinyl)phenyl)pentan-1-ol (1ae)

This is a known compound and its spectroscopic data are consistent with those in the previous literature.⁹ CAS number: 2111919-00-5. A colorless oil, 310 mg, 88% yield. ¹H NMR (CDCl₃, TMS, 400 MHz) δ 7.58 (d, *J* = 7.8 Hz, 1H), 7.42 (t, *J* = 7.5 Hz, 1H), 7.34-7.24 (m, 7H), 5.82 (d, *J* = 1.4 Hz, 1H), 5.23 (d, *J* = 1.4 Hz, 1H), 4.63 (dd, *J* = 8.3, 4.9 Hz, 1H), 1.72 (br, 1H), 1.67-1.60 (m, 1H), 1.57-1.48 (m, 1H), 1.30-1.04 (m, 4H), 0.81 (t, *J* = 7.1 Hz, 3H). ¹³C NMR (CDCl₃, TMS, 100 MHz) δ 148.6, 142.9, 140.9, 139.9, 130.2, 128.4, 128.2, 127.9, 127.2, 126.4, 125.8, 115.6, 70.5, 37.9, 28.1, 22.4, 13.9.

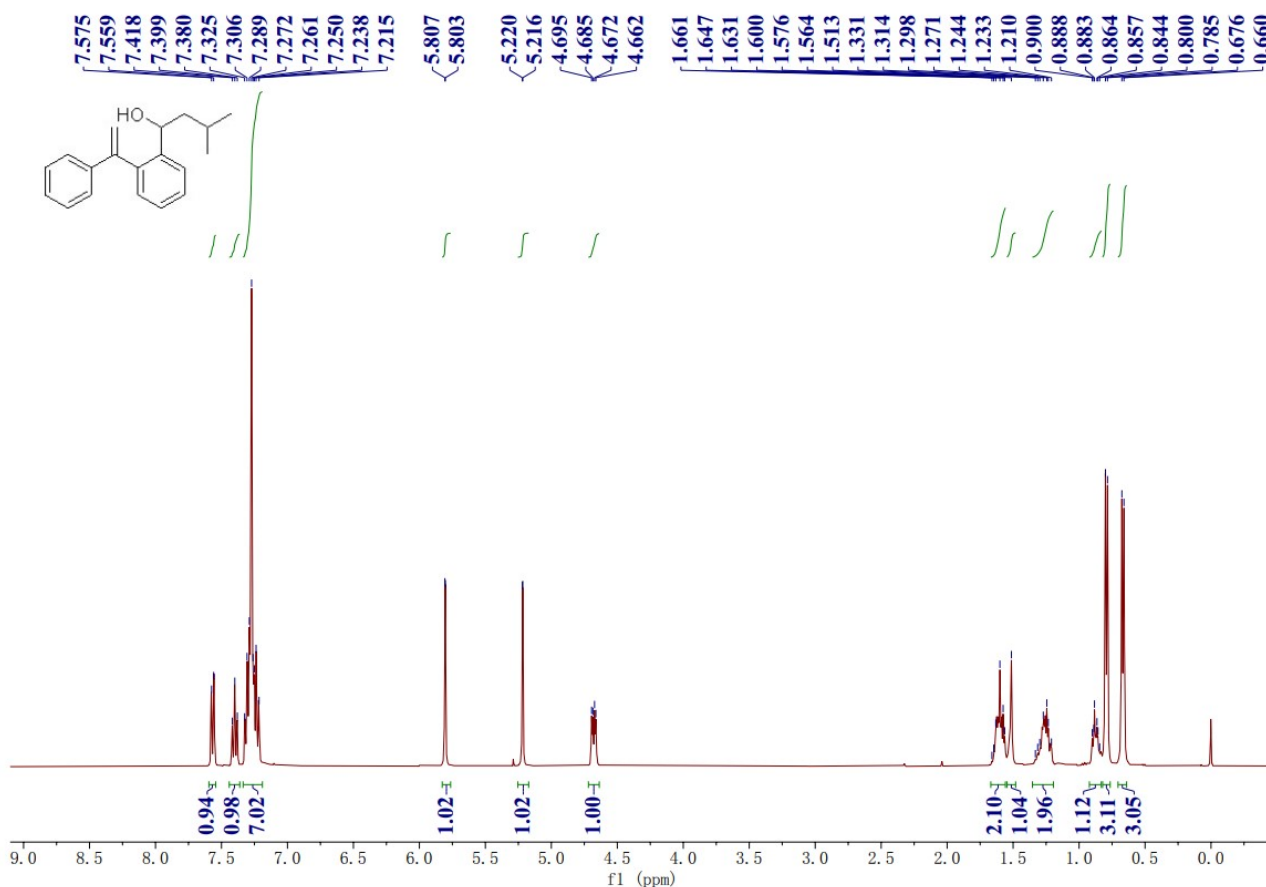


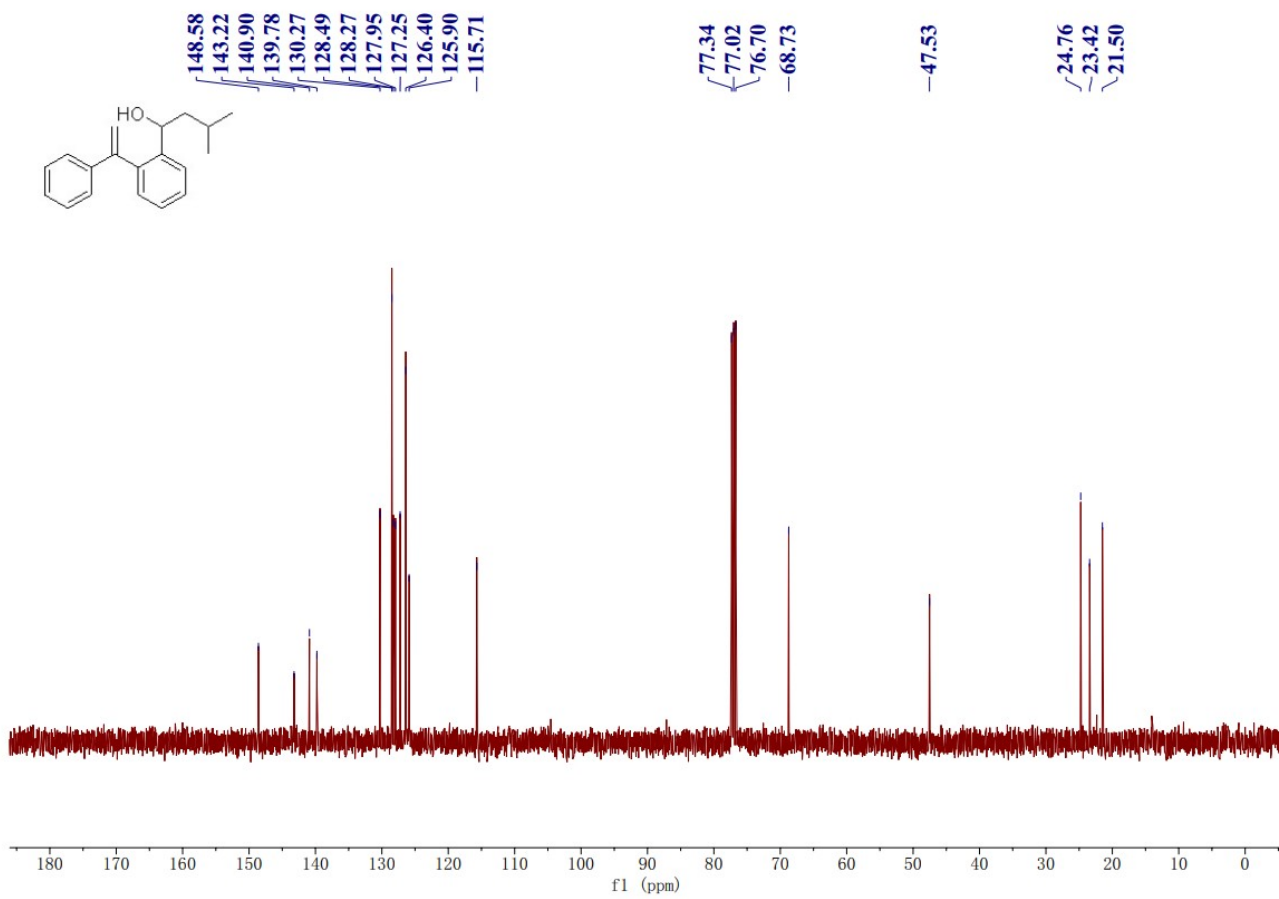


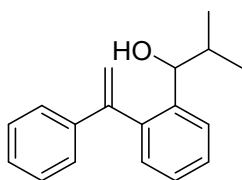


3-methyl-1-(2-(1-phenylvinyl)phenyl)butan-1-ol (1af)

This is a known compound and its spectroscopic data are consistent with those in the previous literature.¹⁰ CAS number: 1632462-81-7. A colorless oil, 345 mg, 87% yield. ¹H NMR (CDCl₃, TMS, 400 MHz) δ 7.57 (d, *J* = 6.4 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.34-7.22 (m, 7H), 5.80 (d, *J* = 1.4 Hz, 1H), 5.22 (d, *J* = 1.4 Hz, 1H), 4.68 (dd, *J* = 9.0, 3.9 Hz, 1H), 1.66-1.56 (m, 2H), 1.51 (br, 1H), 1.33-1.21 (m, 2H), 0.90-0.84 (m, 1H) 0.79 (d, *J* = 6.2 Hz, 3H), 0.67 (d, *J* = 6.2 Hz, 3H). ¹³C NMR (CDCl₃, TMS, 100 MHz) δ 148.6, 143.2, 140.9, 139.8, 130.3, 128.5, 128.3, 127.9, 127.2, 126.4, 125.9, 115.7, 68.7, 47.5, 24.8, 23.4, 21.5.

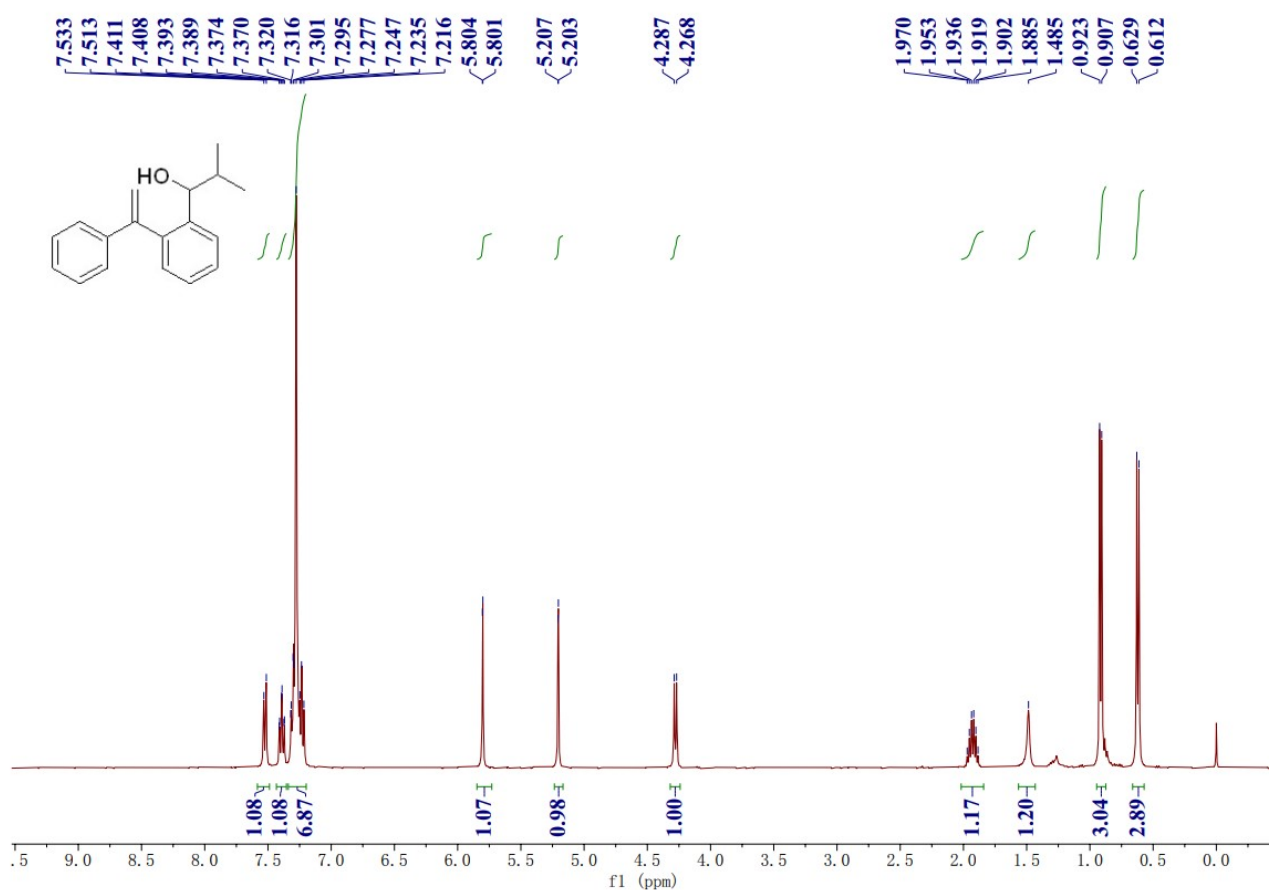


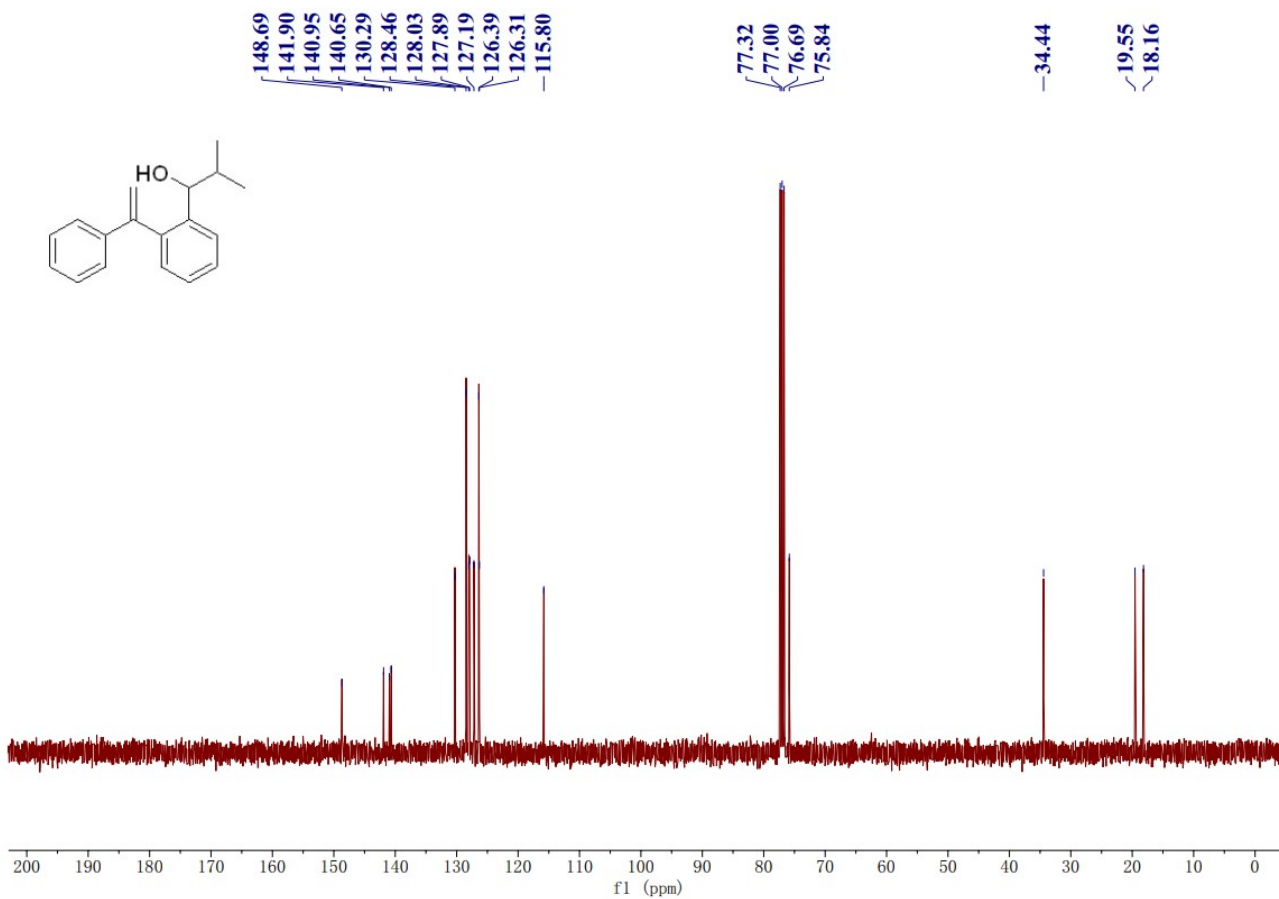


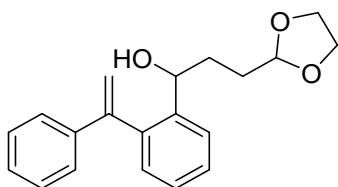


2-methyl-1-(2-(1-phenylvinyl)phenyl)propan-1-ol (1ag)

A colorless oil, 201 mg, 81% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.52 (d, $J = 7.8$ Hz, 1H), 7.41-7.37 (m, 1H), 7.32-7.22 (m, 7H), 5.80 (d, $J = 1.4$ Hz, 1H), 5.21 (d, $J = 1.4$ Hz, 1H), 4.28 (d, $J = 7.6$ Hz, 1H), 1.97-1.89 (m, 1H), 1.49 (br, 1H), 0.91 (d, $J = 6.6$ Hz, 3H), 0.62 (d, $J = 6.8$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 148.7, 141.9, 141.0, 140.6, 130.3, 128.5, 128.0, 127.9, 127.2, 126.4, 126.3, 115.8, 75.8, 34.4, 19.6, 18.2. IR (acetone) ν 3449, 3057, 2929, 1613, 1573, 1493, 1444, 1027, 904, 709 cm^{-1} . HRMS (EI) Calcd. for $\text{C}_{18}\text{H}_{18}$ ($\text{M}-\text{H}_2\text{O}$) $^+$: 234.1403, Found: 234.1403.

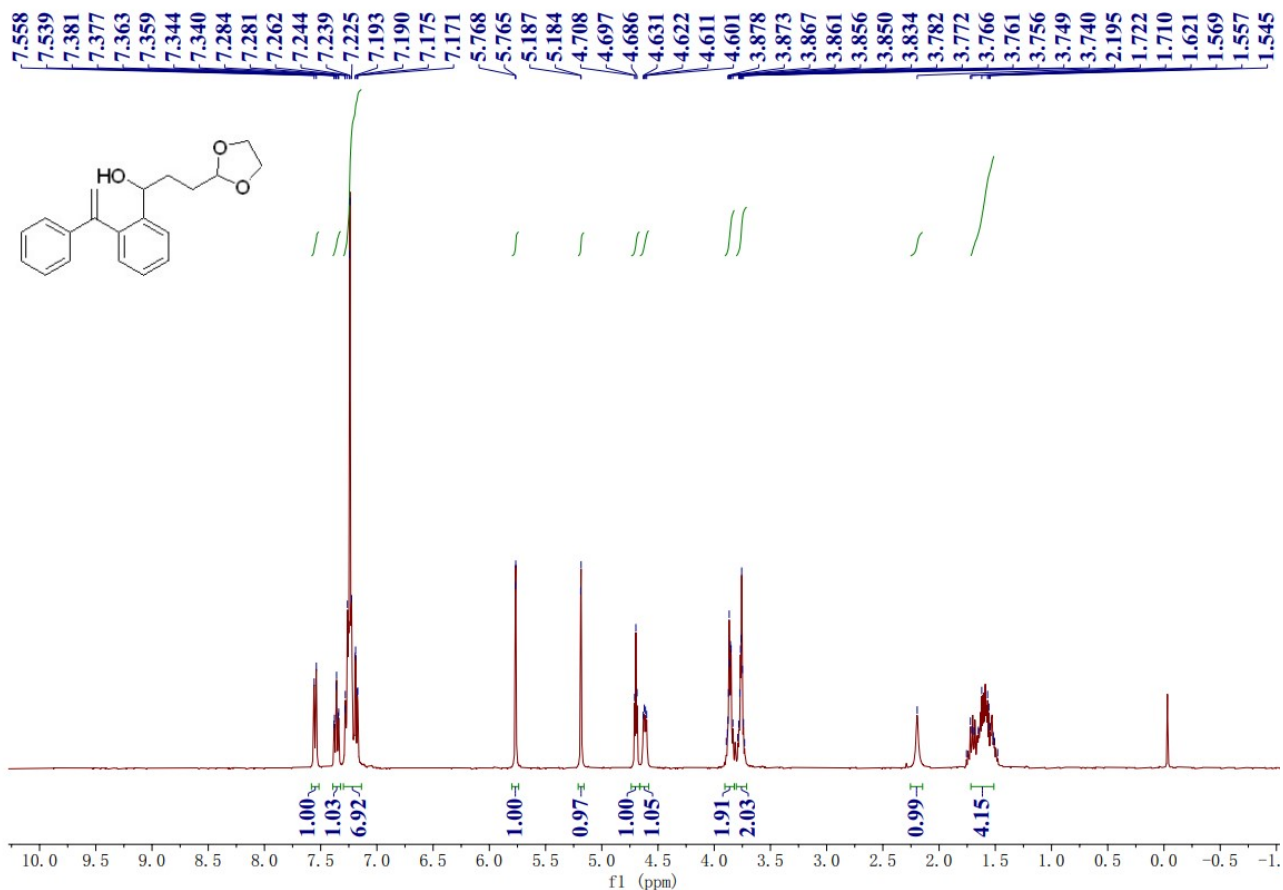


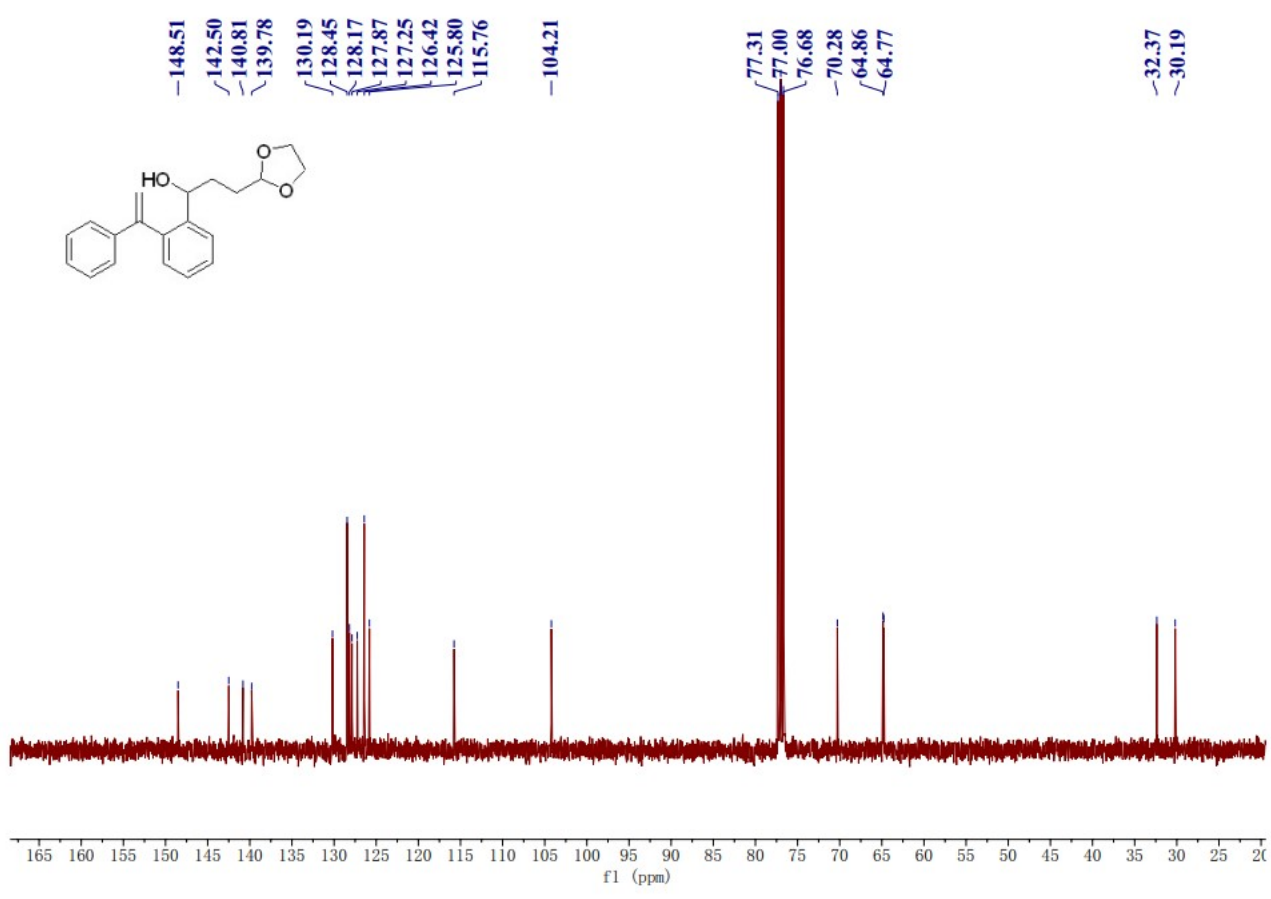


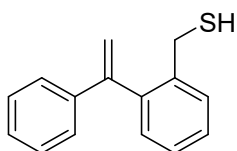


3-(1,3-dioxolan-2-yl)-1-(2-(1-phenylvinyl)phenyl)propan-1-ol (1ah)

A colorless oil, 340 mg, 80% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.55 (d, $J = 7.7$ Hz, 1H), 7.36 (td, $J = 7.5$, 1.5 Hz, 1H), 7.28-7.17 (m, 7H), 5.77 (d, $J = 1.4$ Hz, 1H), 5.19 (d, $J = 1.4$ Hz, 1H), 4.70 (t, $J = 4.3$ Hz, 1H), 4.62 (dd, $J = 8.3$, 4.0 Hz, 1H), 3.90-3.83 (m, 2H), 3.79-3.73 (m, 2H), 2.19 (br, 1H), 1.76-1.48 (m, 4H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 148.5, 142.5, 140.8, 139.8, 130.2, 128.4, 128.2, 127.9, 127.2, 126.4, 125.8, 115.8, 104.2, 70.3, 64.9, 64.8, 32.4, 30.2. IR (acetone) ν 3425, 3059, 2928, 1614, 1573, 1494, 1407, 1322, 906, 770 cm^{-1} . HRMS (FI) Calcd. for $\text{C}_{20}\text{H}_{22}\text{O}_3$ (M^+): 310.1563, Found: 310.1560.

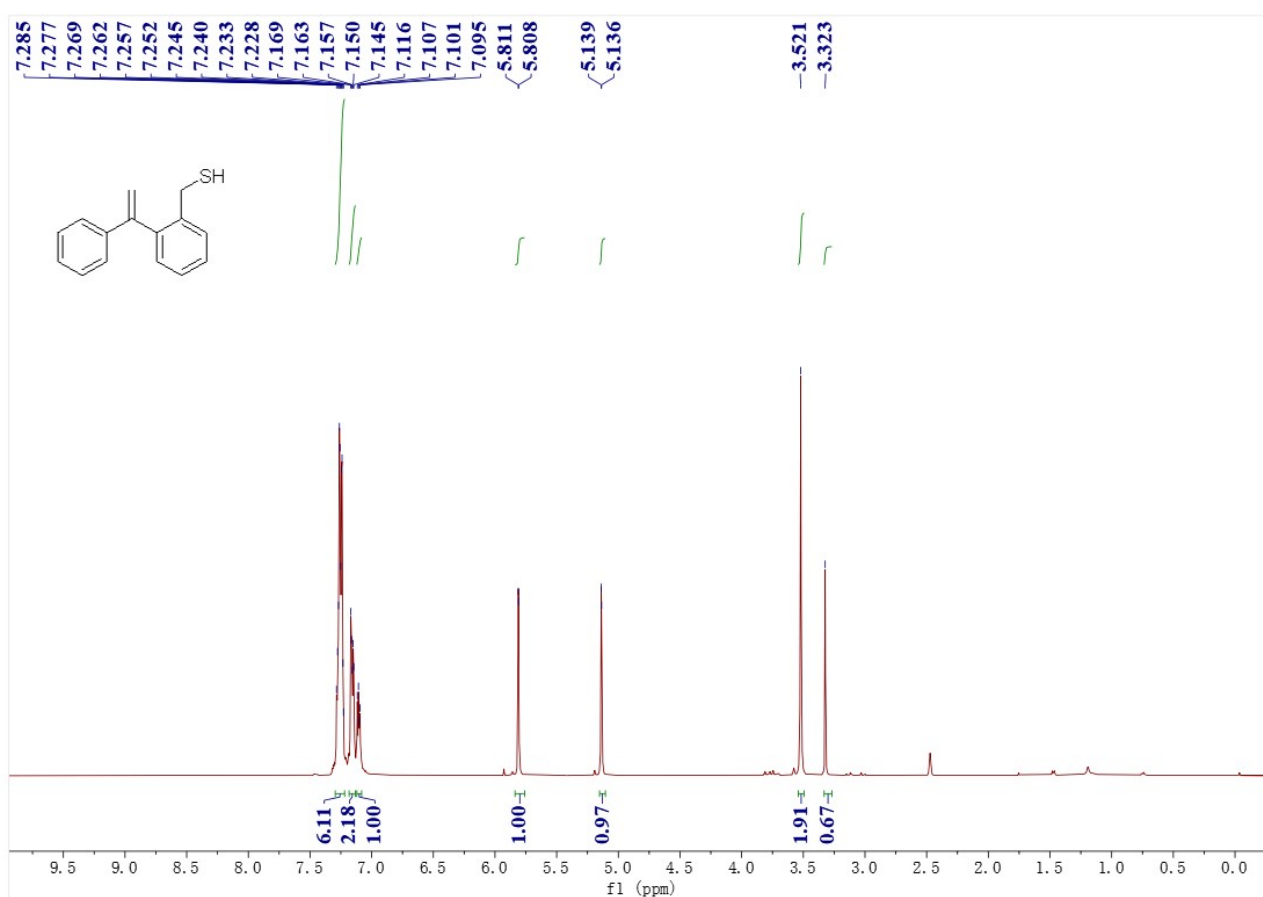


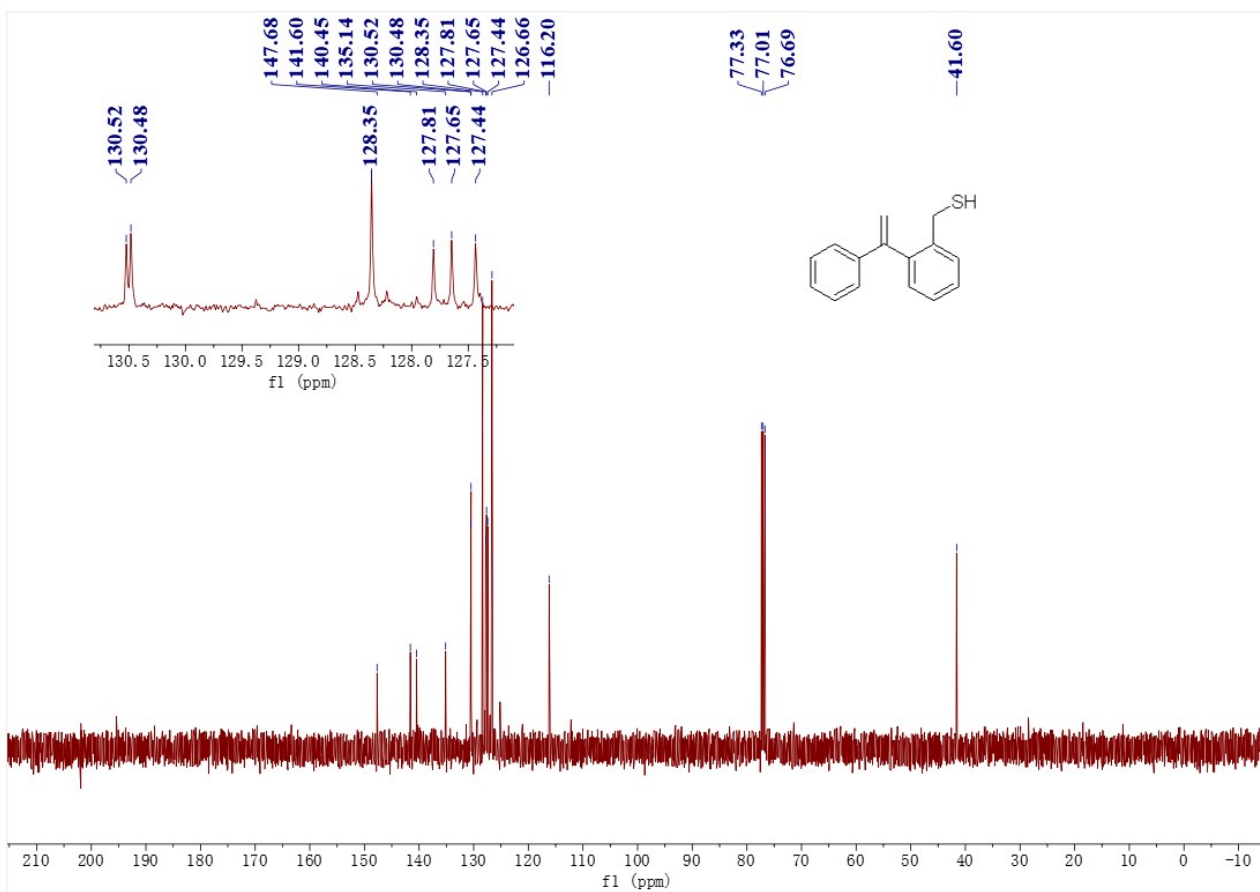




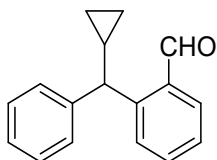
(2-(1-phenylvinyl)phenyl)methanethiol (1a)

A colorless oil, 203 mg, 68% yield. ^1H NMR (DMSO- d_6 , TMS, 400 MHz) δ 7.34-7.20 (m, 6H), 7.18-7.14 (m, 2H), 7.13-7.07 (m, 1H), 5.81 (d, $J = 1.2$ Hz, 1H), 5.14 (d, $J = 1.2$ Hz, 1H), 3.52 (s, 2H), 3.32 (s, 1H). ^{13}C NMR (CDCl $_3$, TMS, 100 MHz) δ 147.7, 141.6, 140.5, 135.1, 130.52, 130.48, 128.4, 127.8, 127.6, 127.4, 126.7, 116.2, 41.6. IR (acetone) ν 3400, 3058, 2929, 1610, 1551, 1493, 1407, 1321, 906, 777 cm^{-1} . HRMS (EI) Calcd. for C $_{15}$ H $_{14}$ S (M $^+$): 226.0811, Found: 226.0807.



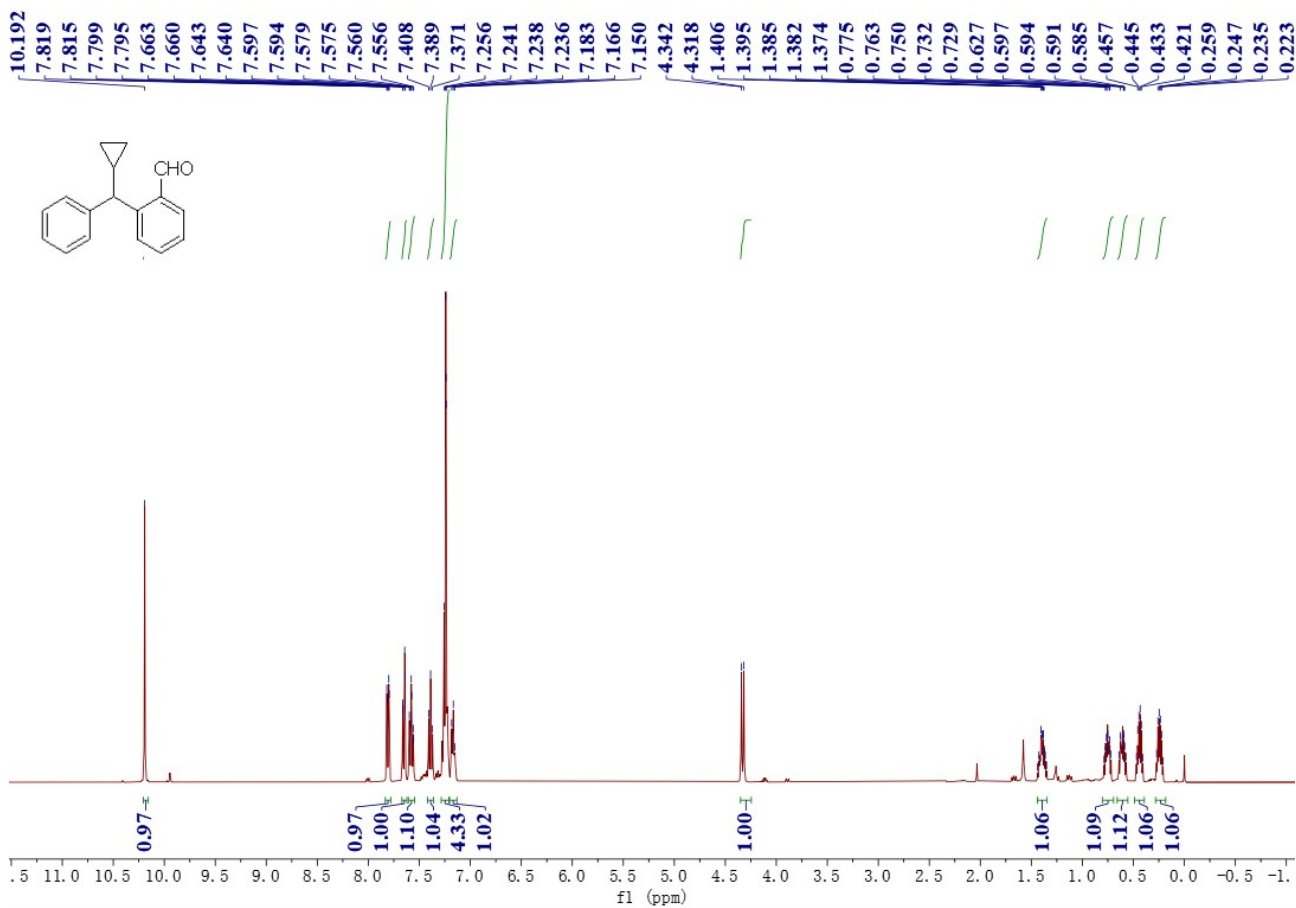


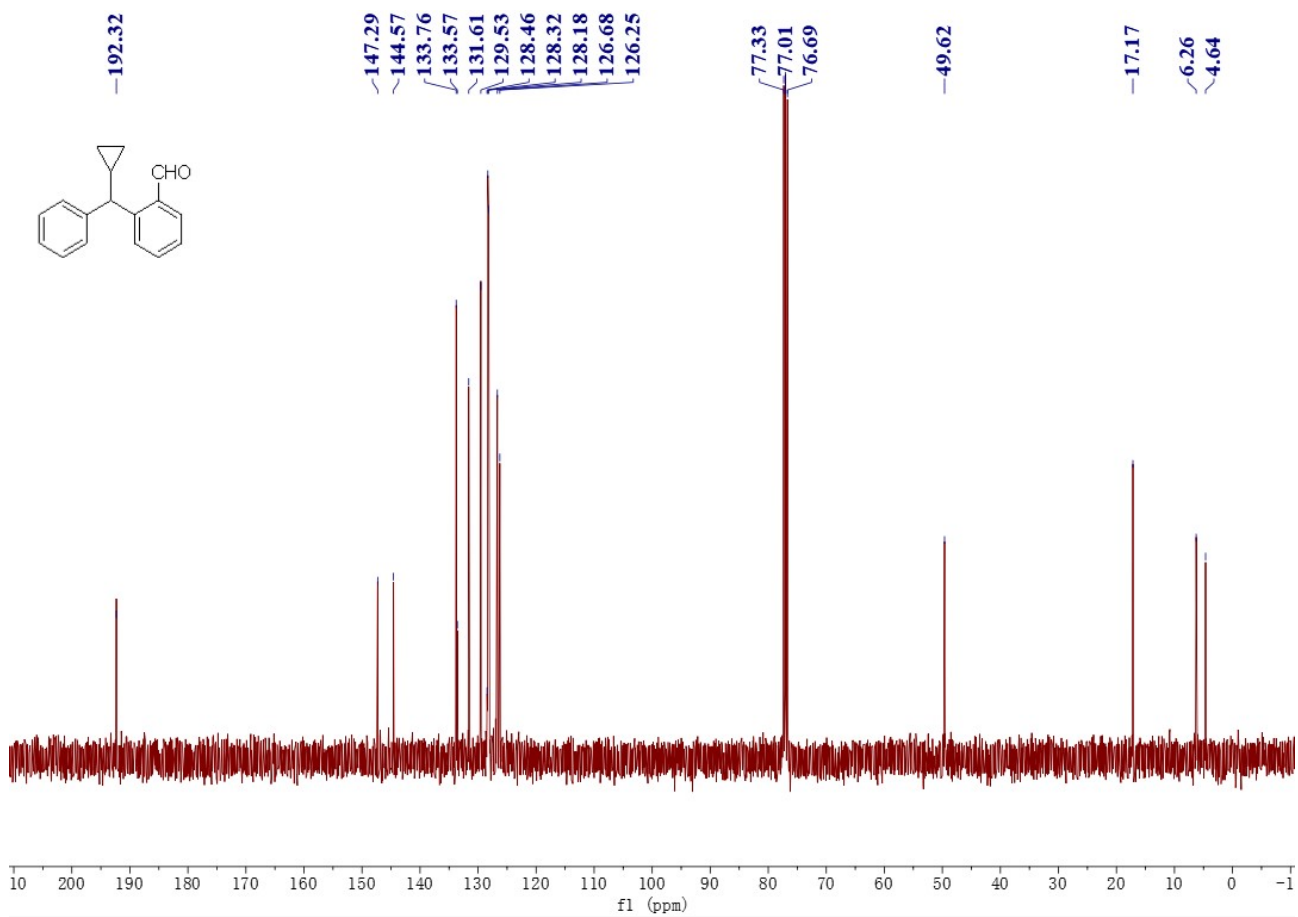
7. Spectroscopic data of products

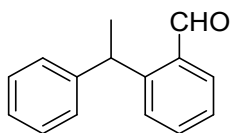


2-(cyclopropyl(phenyl)methyl)benzaldehyde (2a)

A white solid, M.P.: 67-69 °C, 44.4 mg, 94% yield. ¹H NMR (CDCl₃, TMS, 400 MHz) δ 10.19 (s, 1H), 7.81 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.65 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.58 (td, *J* = 7.6, 1.6 Hz, 1H), 7.39 (t, *J* = 7.6 Hz, 1H), 7.26-7.24 (m, 4H), 7.18-7.15 (m, 1H), 4.33 (d, *J* = 9.4 Hz, 1H), 1.44-1.35 (m, 1H), 0.79-0.72, (m, 1H), 0.64-0.57 (m, 1H), 0.47-0.41 (m, 1H), 0.27-0.21 (m, 1H). ¹³C NMR (CDCl₃, TMS, 100 MHz) δ 192.3, 147.3, 144.6, 133.8, 133.6, 131.6, 129.5, 128.5, 128.3, 128.2, 126.7, 126.2, 49.6, 17.2, 6.3, 4.6. IR (acetone) ν 3064, 3001, 2860, 1690, 1597, 1493, 1451, 1200, 871, 751 cm⁻¹. Calcd. for C₁₇H₁₆O (M⁺): 236.1196, Found: 236.1202.

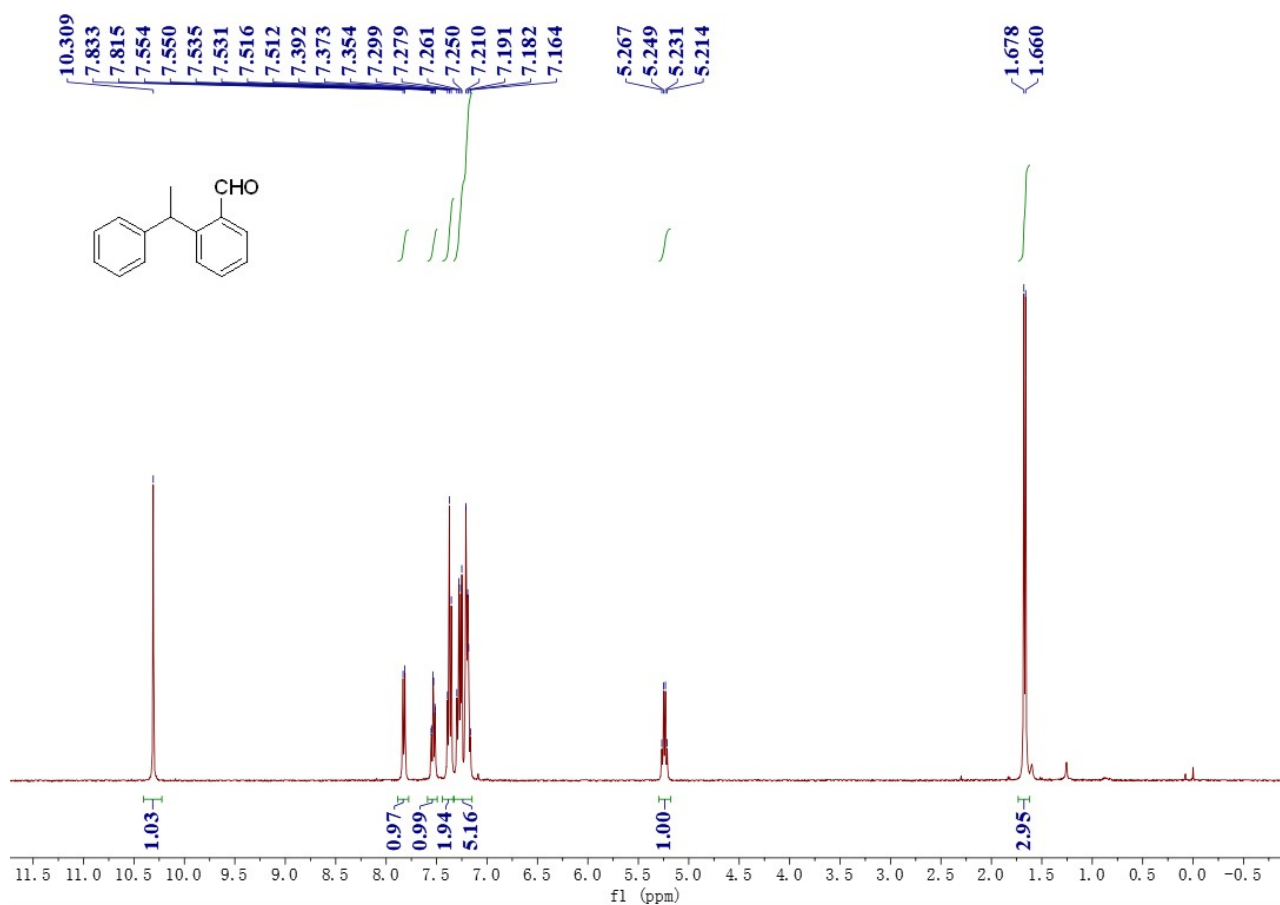


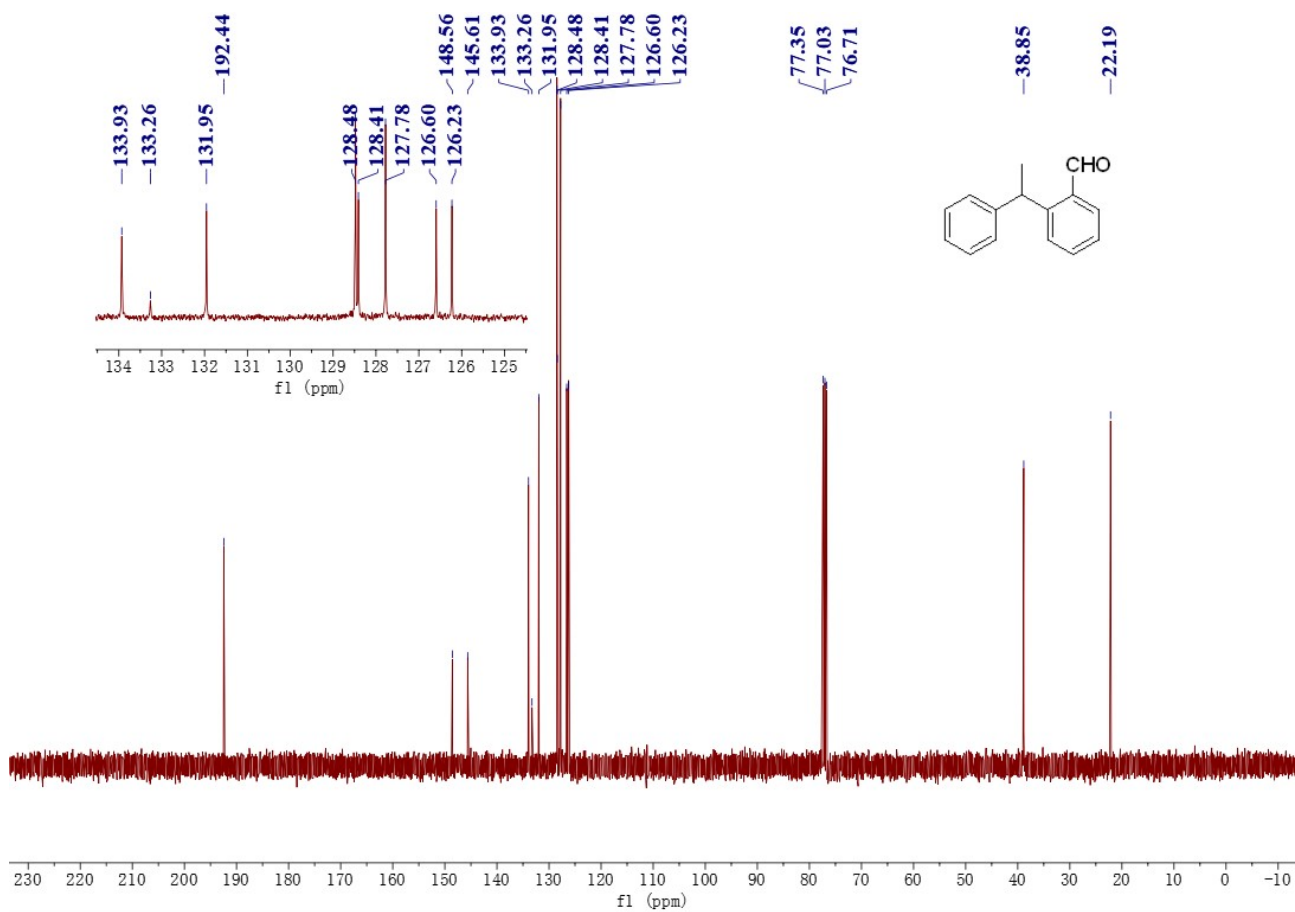


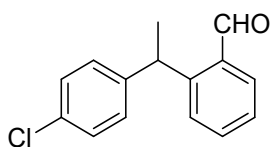


2-(1-phenylethyl)benzaldehyde (2b)

This is a known compound and its spectroscopic data are consistent with those in the previous literature.¹¹ CAS number: 61608-90-0. A colorless oil. 35.3 mg, 84% yield. ¹H NMR (CDCl₃, TMS, 400 MHz) δ 10.31 (s, 1H), 7.82 (d, *J* = 7.2 Hz, 1H), 7.53 (td, *J* = 7.6, 1.6 Hz, 1H), 7.37 (t, *J* = 7.6 Hz, 2H), 7.30-7.16 (m, 5H), 5.24 (q, *J* = 7.2 Hz, 1H), 1.67 (d, *J* = 7.2 Hz, 3H). ¹³C NMR (CDCl₃, TMS, 100 MHz) δ 192.4, 148.6, 145.6, 133.9, 133.3, 132.0, 128.5, 128.4, 127.8, 126.6, 126.2, 38.9, 22.2.

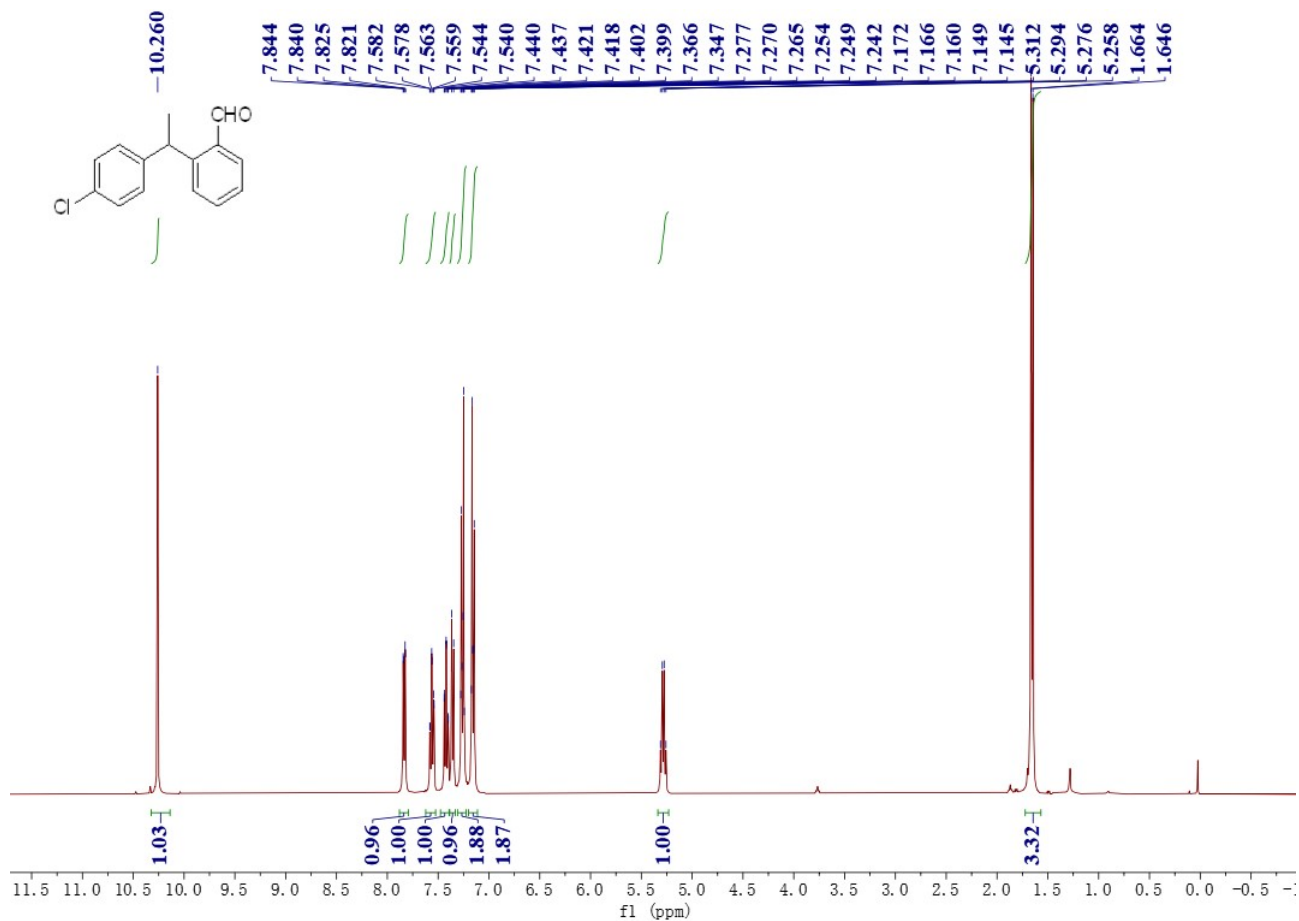


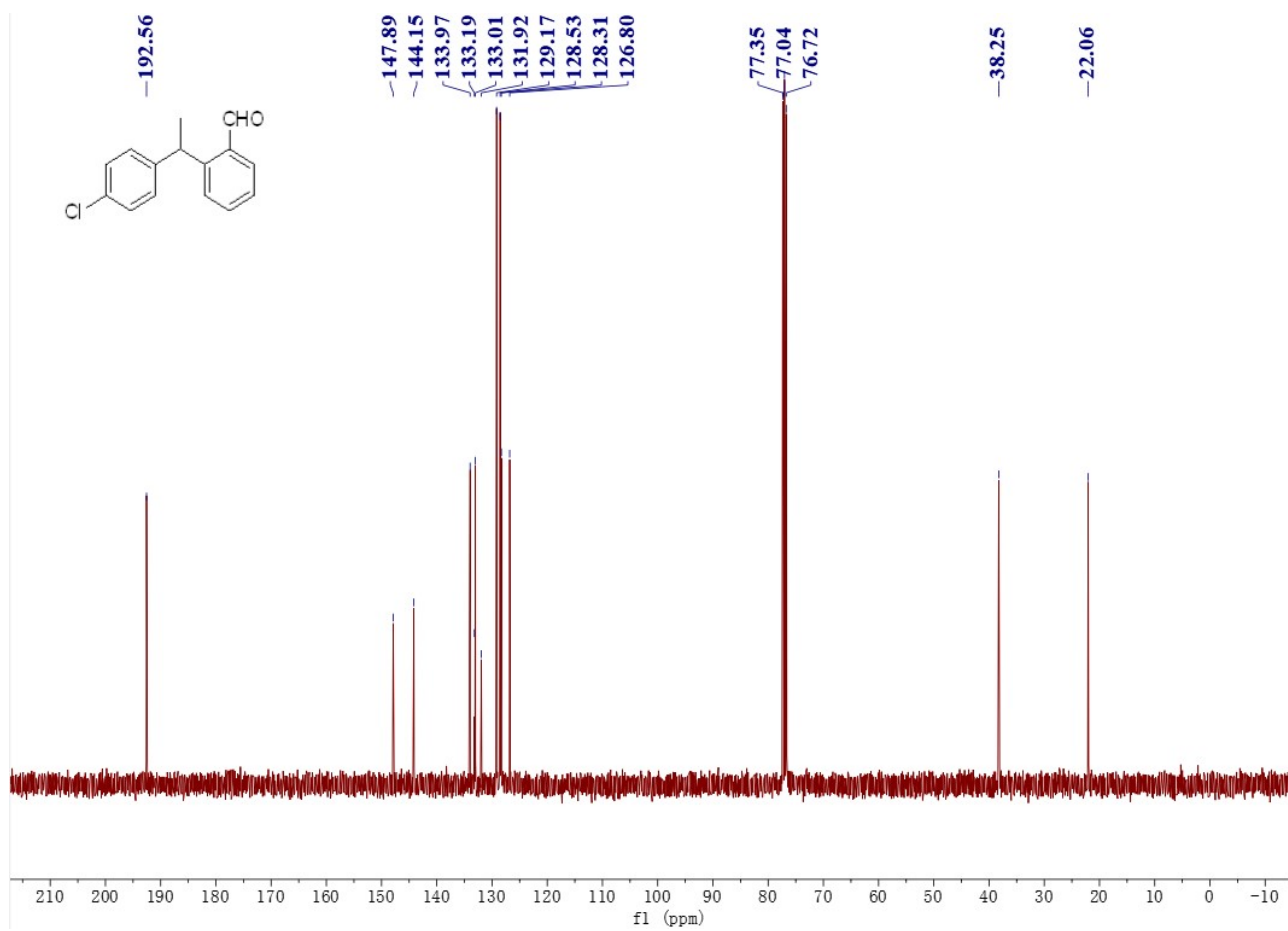


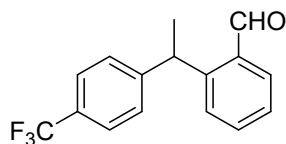


2-(1-(4-chlorophenyl)ethyl)benzaldehyde (2c)

A colorless oil. 47.0 mg, 96% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 10.26 (s, 1H), 7.83 (dd, $J = 7.6, 1.6$ Hz, 1H), 7.56 (td, $J = 7.6, 1.6$ Hz, 1H), 7.42 (td, $J = 7.6, 1.2$ Hz, 1H), 7.36 (d, $J = 7.8$ Hz, 1H), 7.28-7.24 (m, 2H), 7.17-7.15 (m, 2H), 5.28 (q, $J = 7.2$ Hz, 1H), 1.66 (d, $J = 7.2$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 192.6, 147.9, 144.2, 134.0, 133.2, 133.0, 131.9, 129.2, 128.5, 128.3, 126.8, 38.2, 22.1. IR (acetone) ν 3061, 2962, 2876, 1693, 1598, 1489, 1396, 1197, 908, 835 cm^{-1} . Calcd. for $\text{C}_{15}\text{H}_{13}\text{ClO}$ (M^+): 244.0649, Found: 244.0650.

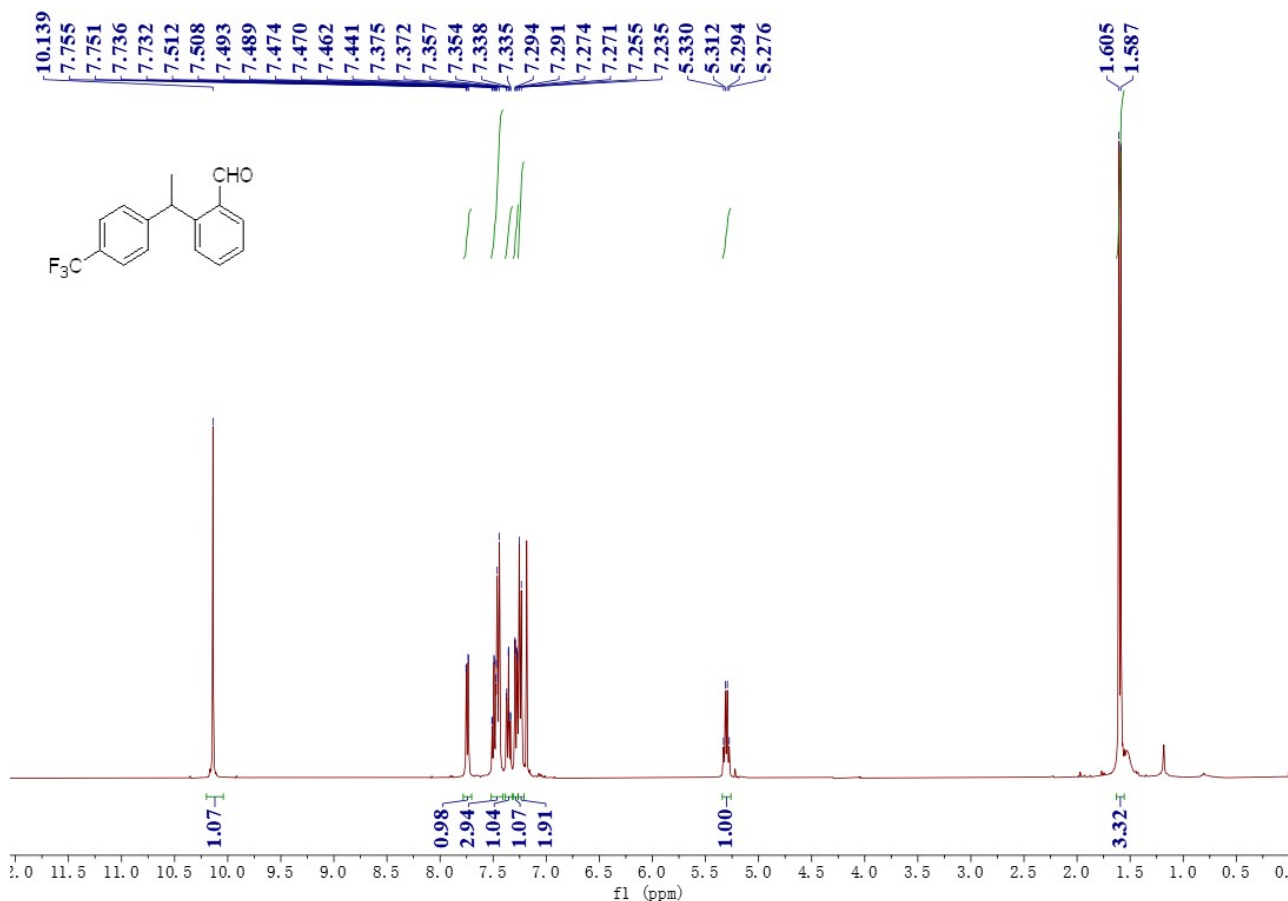


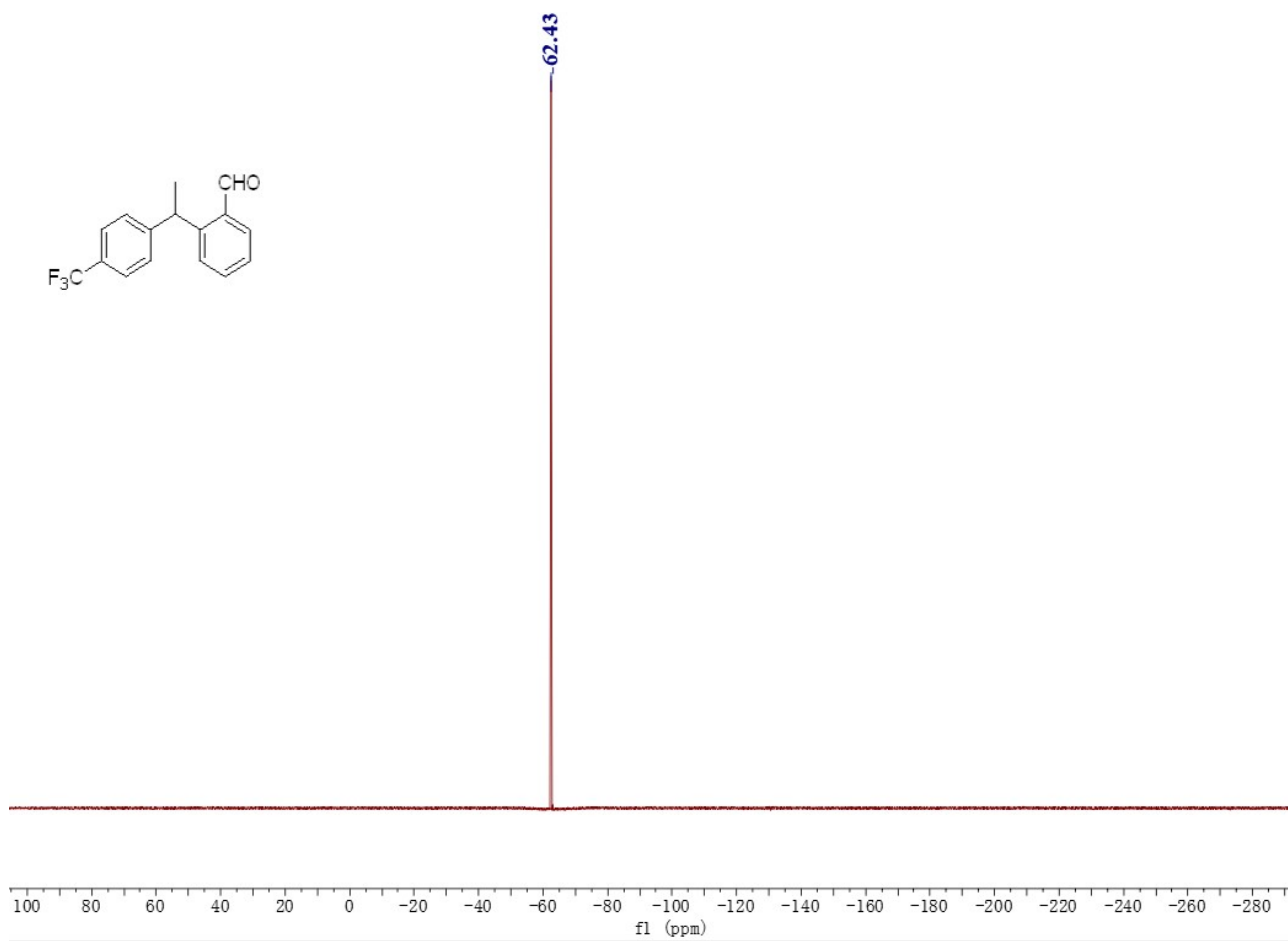
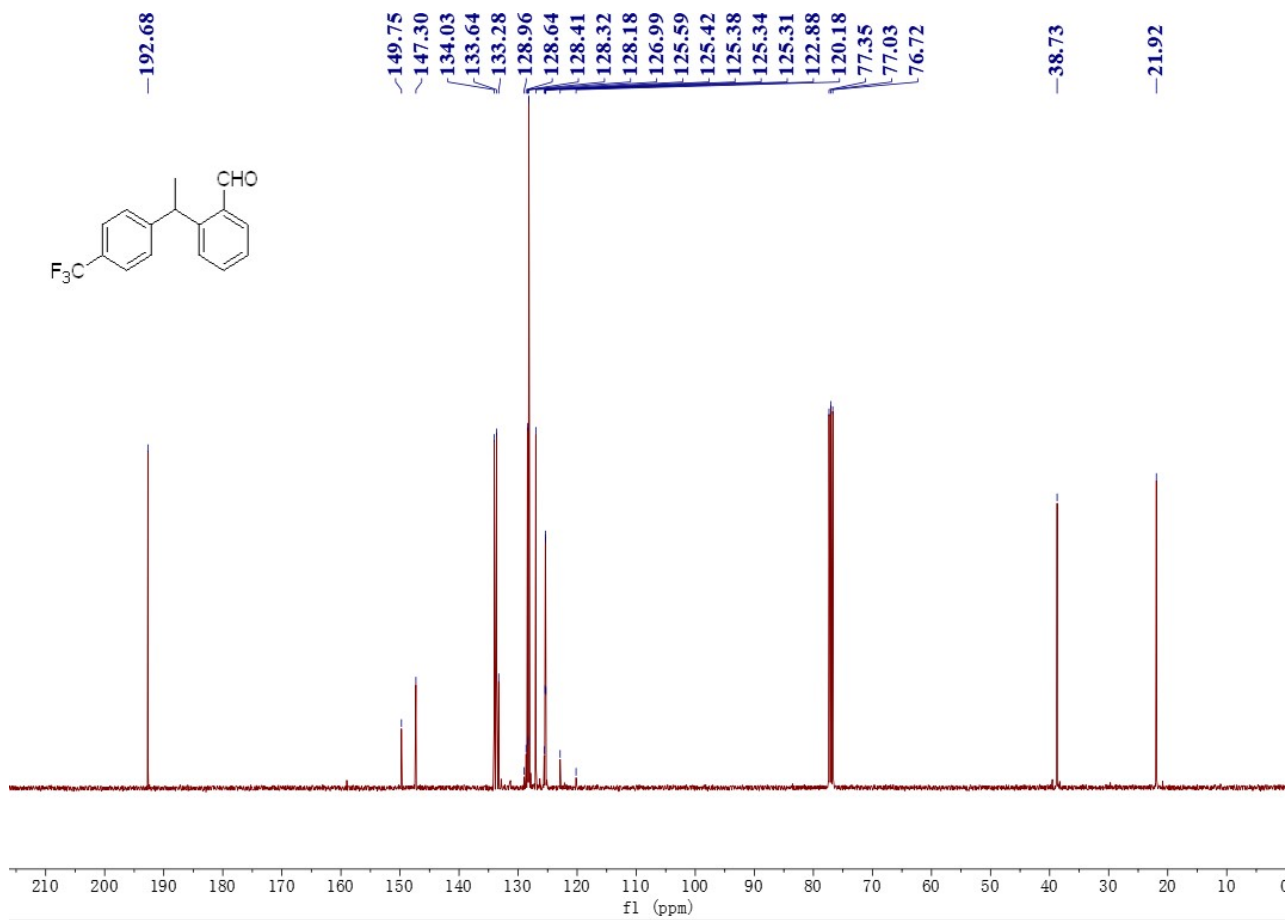


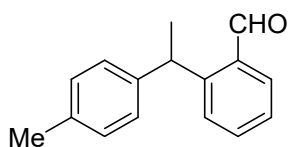


2-(1-(4-(trifluoromethyl)phenyl)ethyl)benzaldehyde (2d)

A colorless oil. 40.6 mg, 73% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 10.14 (s, 1H), 7.74 (dd, $J = 7.6, 1.6$ Hz, 1H), 7.51-7.44 (m, 3H), 7.36 (td, $J = 7.6, 1.2$ Hz, 1H), 7.28 (dd, $J = 7.8, 1.2$ Hz, 1H), 7.24 (d, $J = 8.0$ Hz, 2H), 5.30 (q, $J = 7.2$ Hz, 1H), 1.60 (d, $J = 7.2$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 192.7, 149.8, 147.3, 134.0, 133.6, 133.3, 128.5 (d, $J = 32.2$ Hz), 128.4, 128.2, 127.0, 125.3 (d, $J = 4.0$ Hz), 124.2 (q, $J = 273.6$ Hz), 38.7, 21.9. ^{19}F NMR (376 MHz, CDCl_3) δ -62.4. IR (acetone) ν 3076, 2870, 2735, 1689, 1571, 1452, 1293, 1186, 864, 695. Calcd. for $\text{C}_{16}\text{H}_{13}\text{OF}_3$ (M^+): 278.0913, Found: 278.0908.

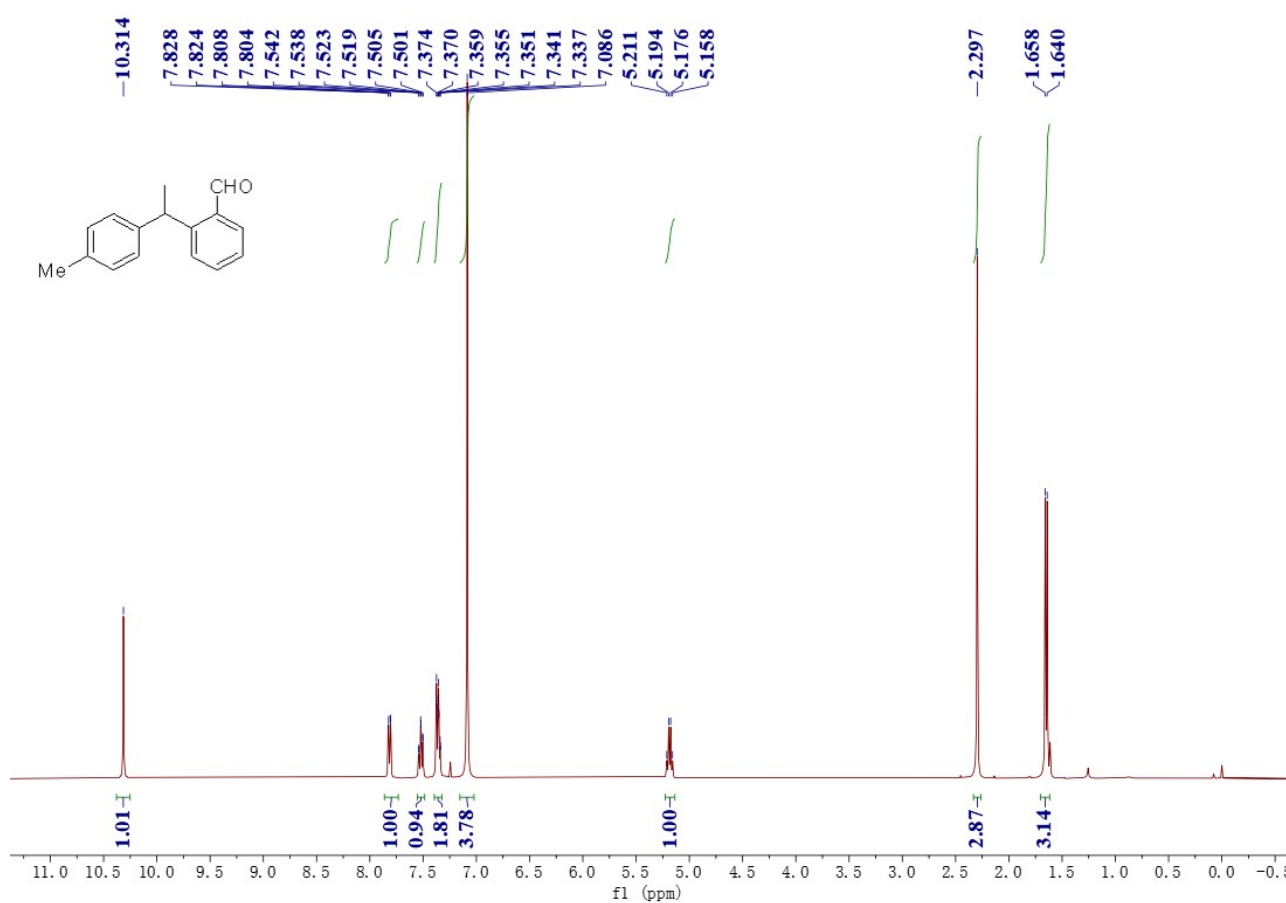


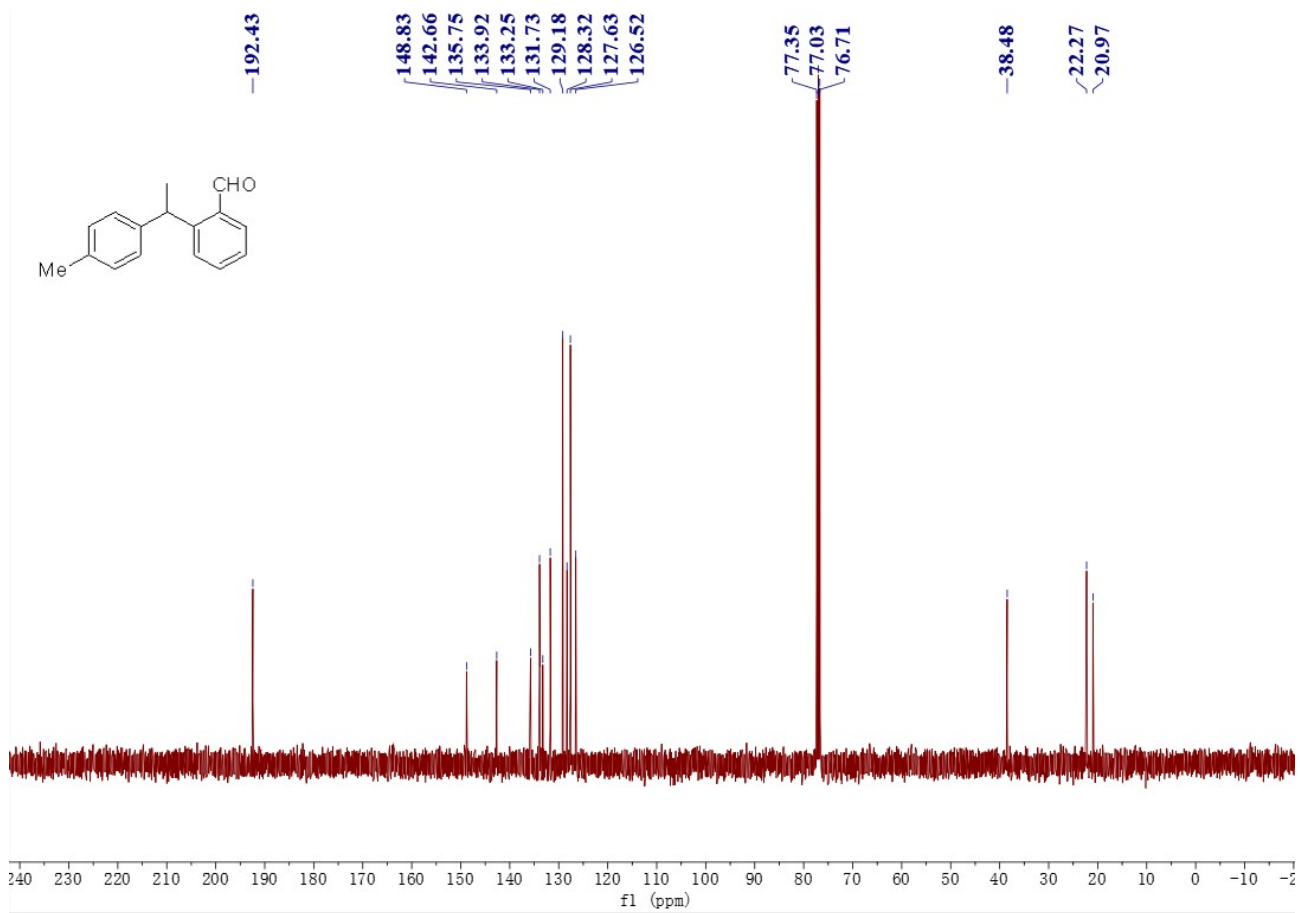


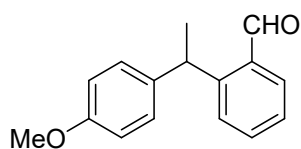


2-(1-(p-tolyl)ethyl)benzaldehyde (2e)

A colorless oil. 40.8 mg, 91% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 10.31 (s, 1H), 7.83-7.80 (m, 1H), 7.52 (td, $J = 7.6, 1.6$ Hz, 1H), 7.37-7.34 (m, 2H), 7.09 (s, 4H), 5.18 (q, $J = 7.2$ Hz, 1H), 2.30 (s, 3H), 1.65 (d, $J = 7.2$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 192.4, 148.8, 142.7, 135.7, 133.9, 133.3, 131.7, 129.2, 128.3, 127.6, 126.5, 38.5, 22.3, 21.0. IR (acetone) ν 2967, 2873, 1692, 1598, 1511, 1486, 1246, 1031, 825, 748 cm^{-1} . Calcd. for $\text{C}_{16}\text{H}_{16}\text{O}$ (M^+): 224.1196, Found: 224.1207.

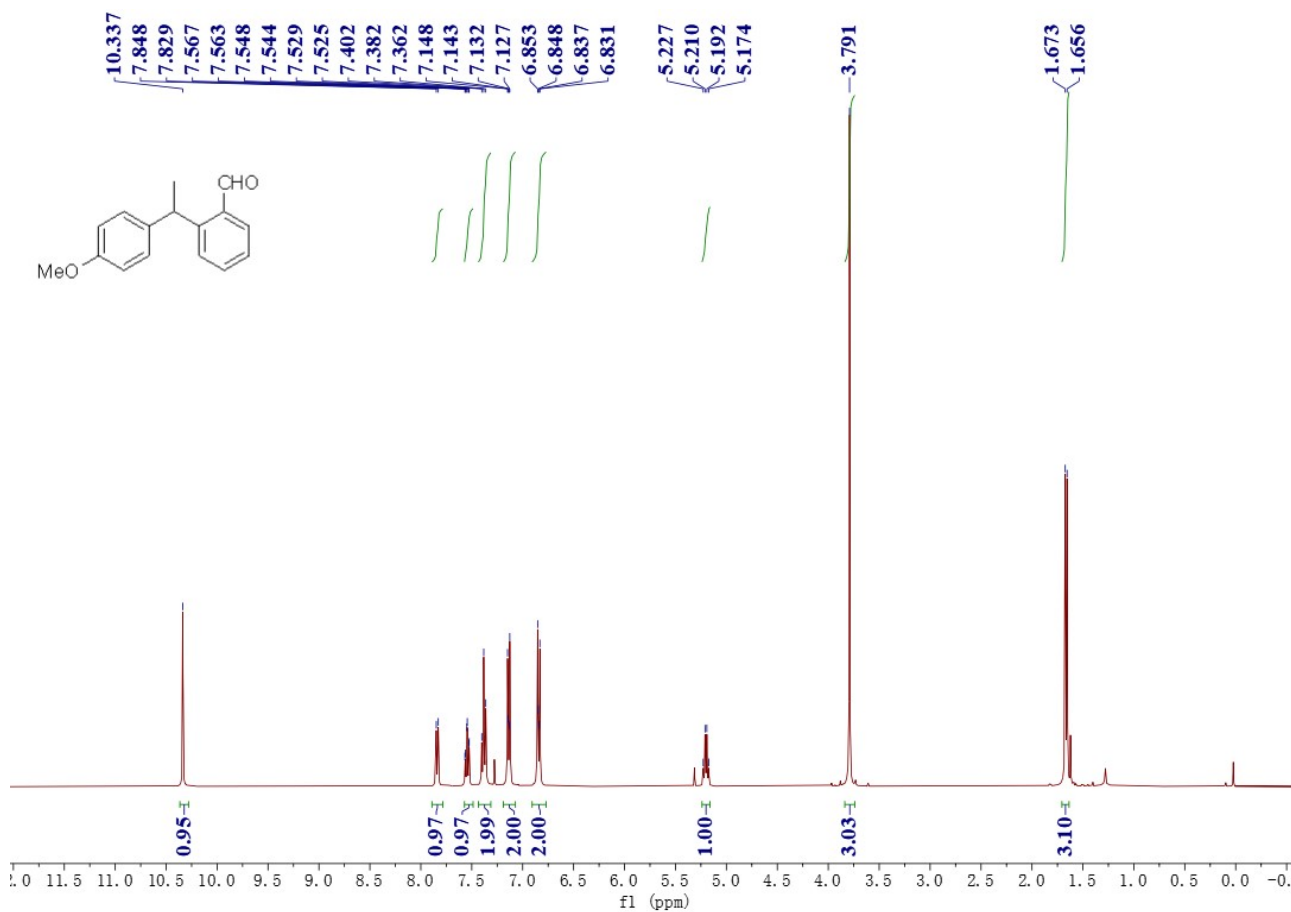


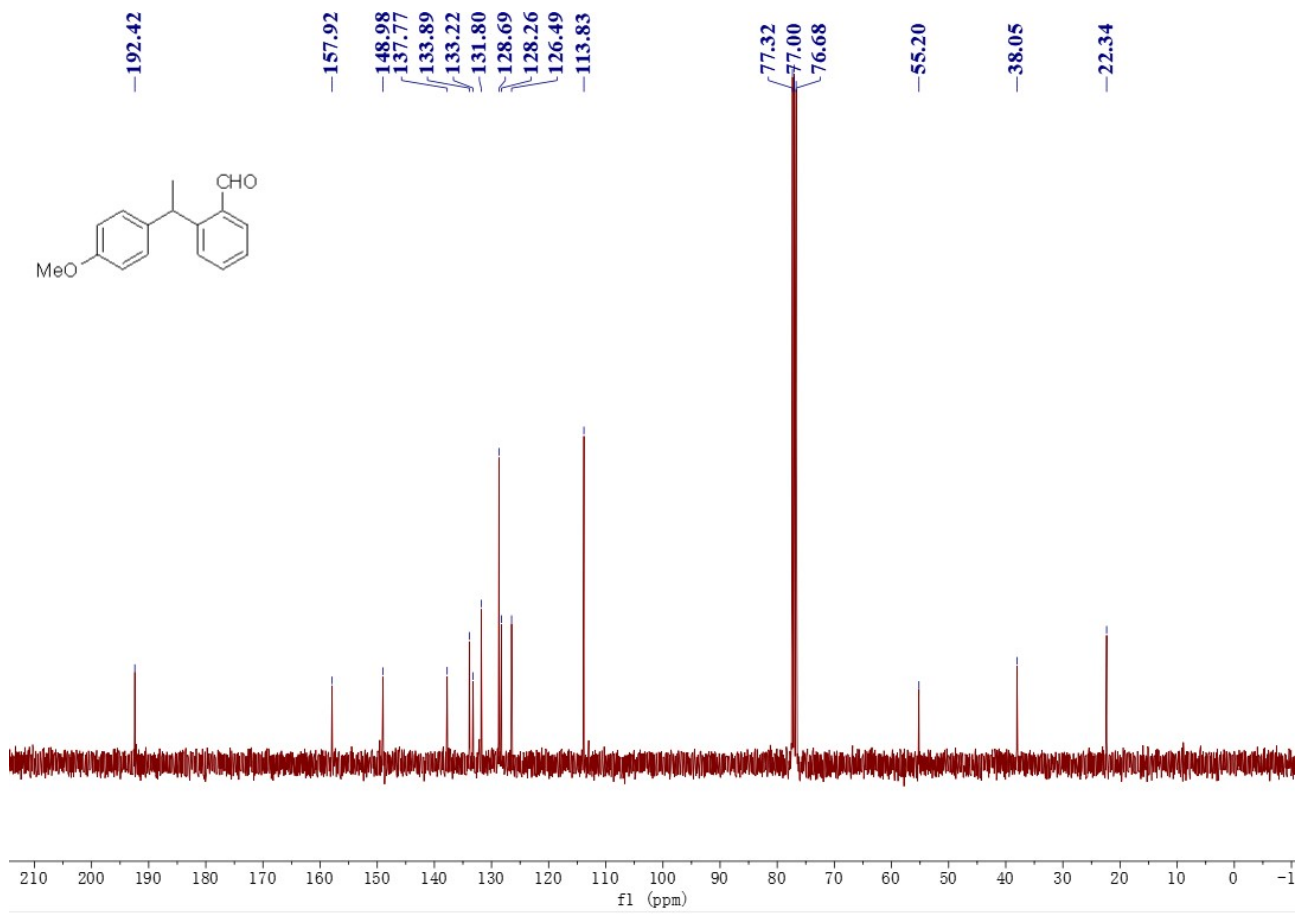


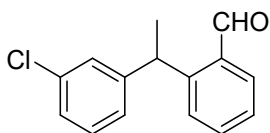


2-(1-(4-methoxyphenyl)ethyl)benzaldehyde (2f)

A colorless oil. 31.2 mg, 65% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 10.34 (s, 1H), 7.84 (d, $J = 7.6$ Hz, 1H), 7.55 (td, $J = 7.6, 1.6$ Hz, 1H), 7.38 (t, $J = 8.0$ Hz, 2H), 7.15-7.13 (m, 2H), 6.85-6.83 (m, 2H), 5.20 (q, $J = 7.2$ Hz, 1H), 3.79 (s, 3H), 1.66 (d, $J = 7.2$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 192.4, 157.9, 149.0, 137.8, 133.9, 133.2, 131.8, 128.7, 128.3, 126.5, 113.8, 55.2, 38.0, 22.3. IR (acetone) ν 2966, 2831, 1690, 1598, 1489, 1453, 1245, 1029, 831, 769 cm^{-1} . HRMS (EI) calcd. for $\text{C}_{16}\text{H}_{16}\text{O}_2$ (M^+): 240.1145, Found: 240.1143.

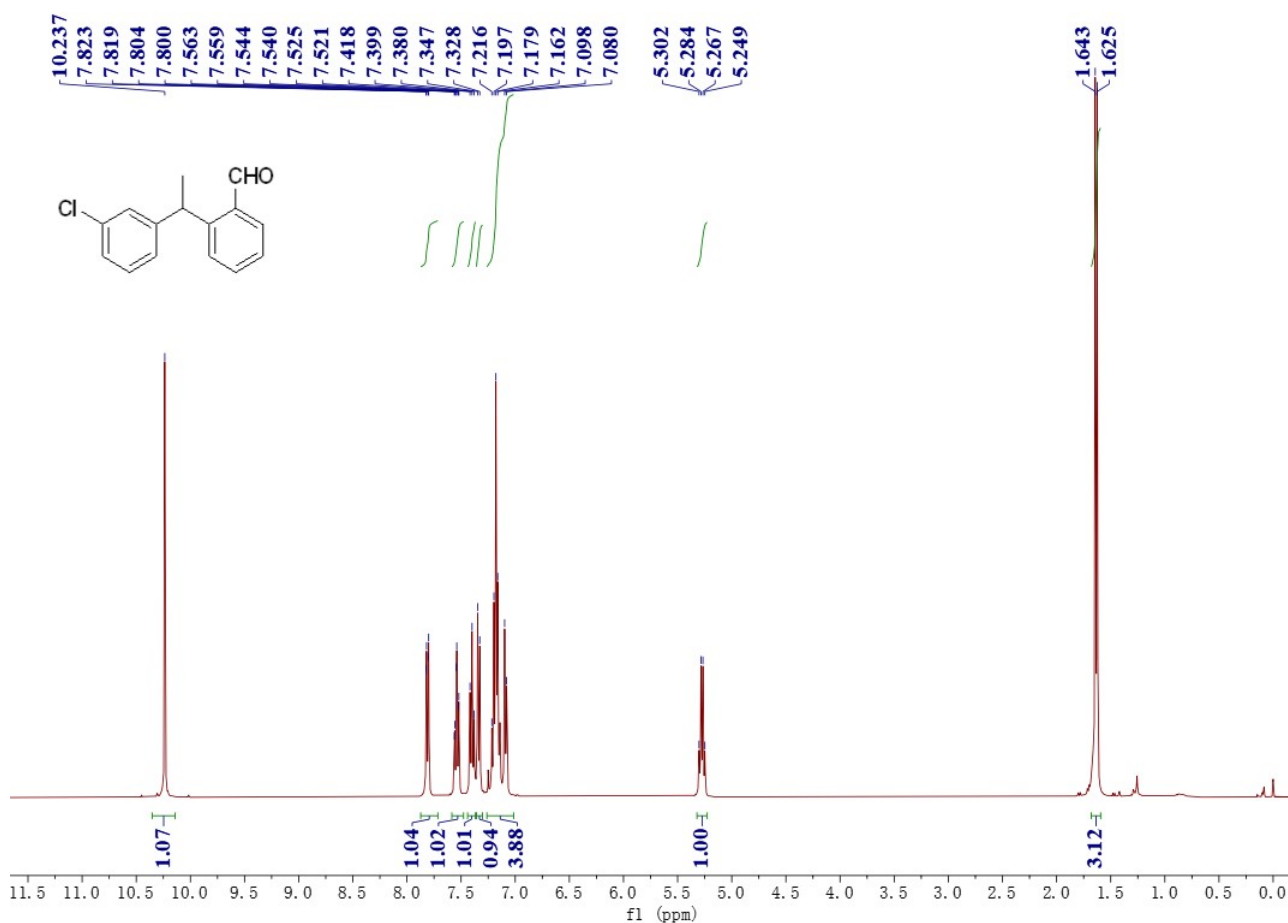


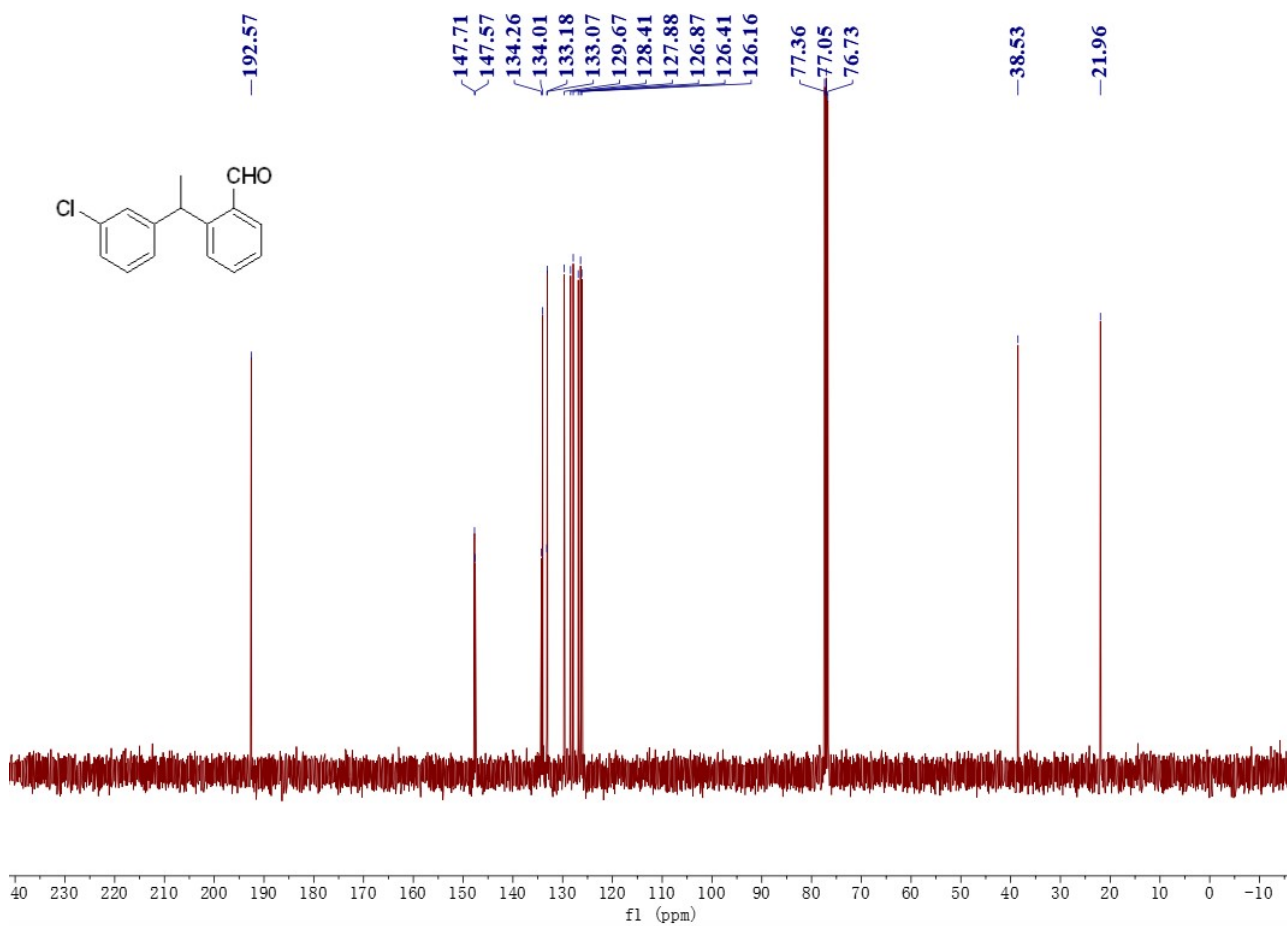


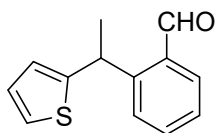


2-(1-(3-chlorophenyl)ethyl)benzaldehyde (2g)

A colorless oil. 44.1 mg, 90% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 10.24 (s, 1H), 7.81 (dd, $J = 7.6, 1.6$ Hz, 1H), 7.54 (td, $J = 7.6, 1.6$ Hz, 1H), 7.40 (t, $J = 7.6$ Hz, 1H), 7.34 (d, $J = 7.8$ Hz, 1H), 7.22-7.08 (m, 4H), 5.28 (q, $J = 7.2$ Hz, 1H), 1.63 (d, $J = 7.2$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 192.6, 147.7, 147.6, 134.3, 134.0, 133.2, 133.1, 129.7, 128.4, 127.9, 126.9, 126.4, 126.2, 38.5, 22.0. IR (acetone) ν 3076, 2970, 2735, 1690, 1596, 1474, 1409, 1080, 824, 695 cm^{-1} . HRMS (EI) calcd. for $\text{C}_{15}\text{H}_{13}\text{ClO}$ (M^+): 244.0649, Found: 244.0648.

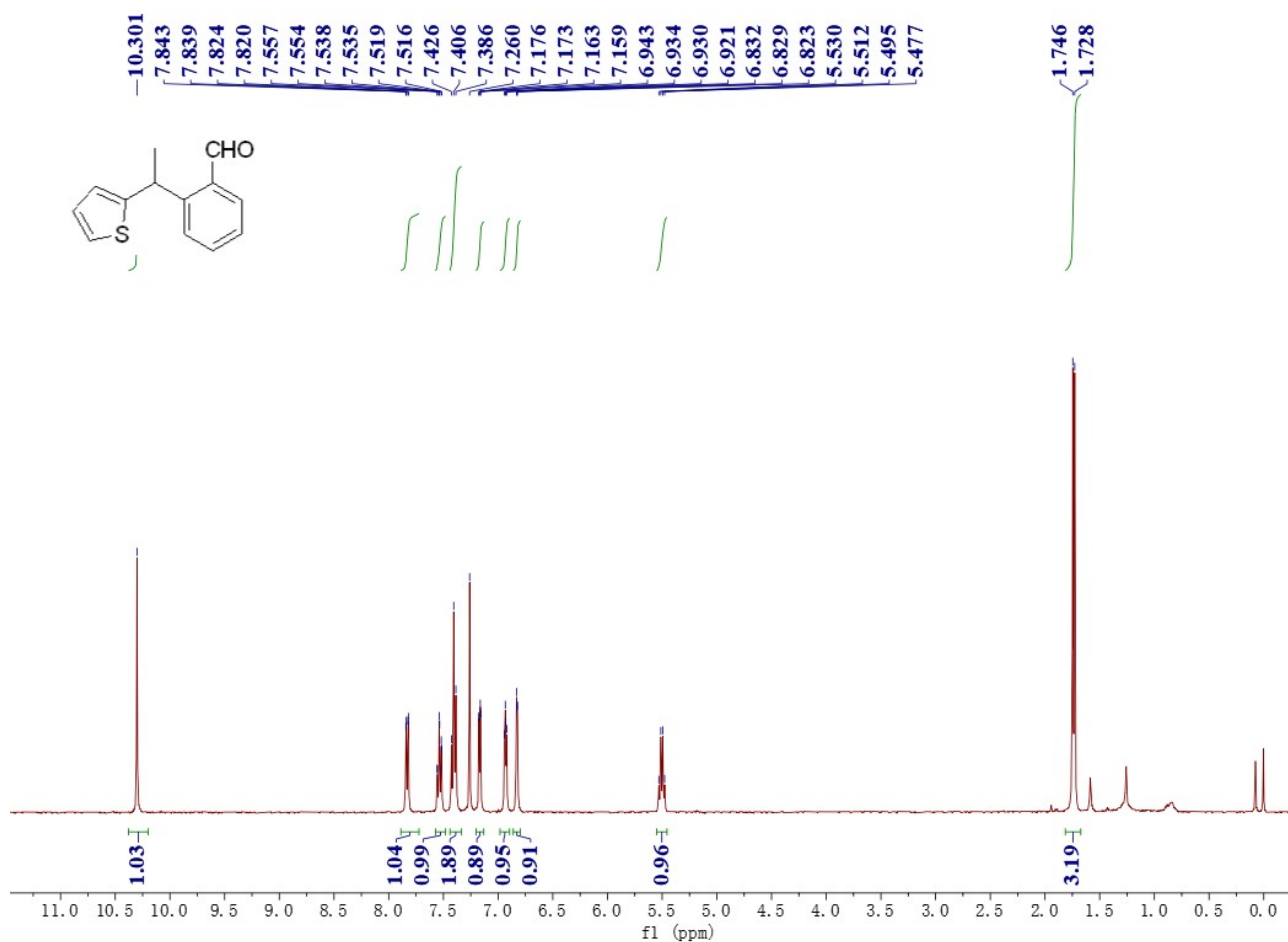


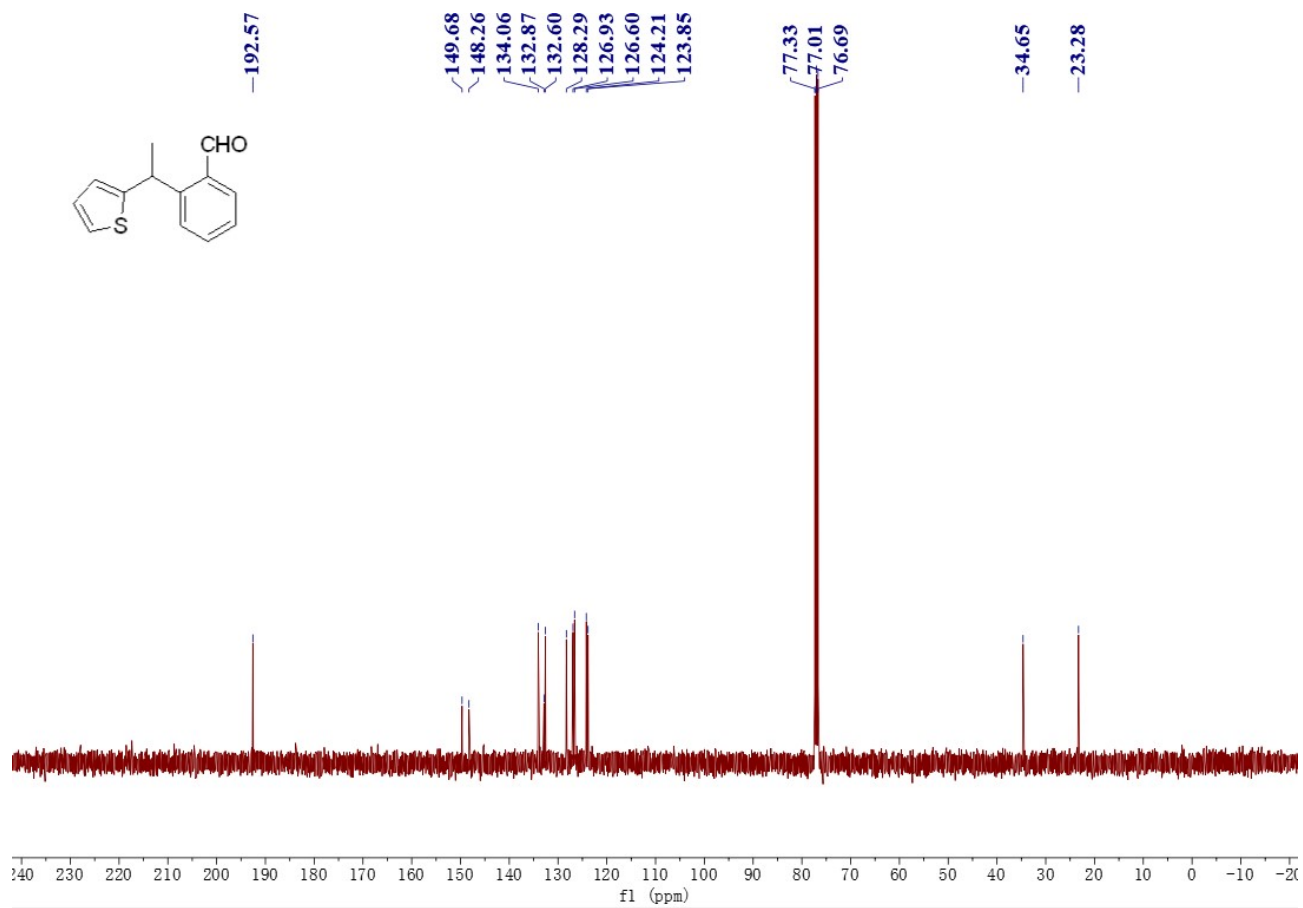
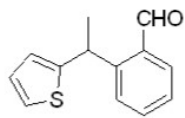


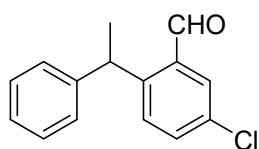


2-(1-(thiophen-2-yl)ethyl)benzaldehyde (2h)

A colorless oil. 35.9 mg, 83% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 10.30 (s, 1H), 7.83 (dd, $J = 7.6, 1.6$ Hz, 1H), 7.54 (td, $J = 7.6, 1.6$ Hz, 1H), 7.41 (t, $J = 8.0$ Hz, 2H), 7.17 (dd, $J = 5.2, 1.2$ Hz, 1H), 6.93 (dd, $J = 5.2, 3.6$ Hz, 1H), 6.83-6.82 (m, 1H), 5.50 (q, $J = 7.2$ Hz, 1H), 1.74 (d, $J = 7.2$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 192.6, 149.7, 148.3, 134.1, 132.9, 132.6, 128.3, 126.9, 126.6, 124.2, 123.9, 34.6, 23.3. IR (acetone) ν 3061, 2969, 2865, 1691, 1598, 1485, 1450, 1023, 851, 697 cm^{-1} . HRMS (EI) calcd. for $\text{C}_{13}\text{H}_{12}\text{SO}$ (M^+): 216.0603, Found: 216.0604.

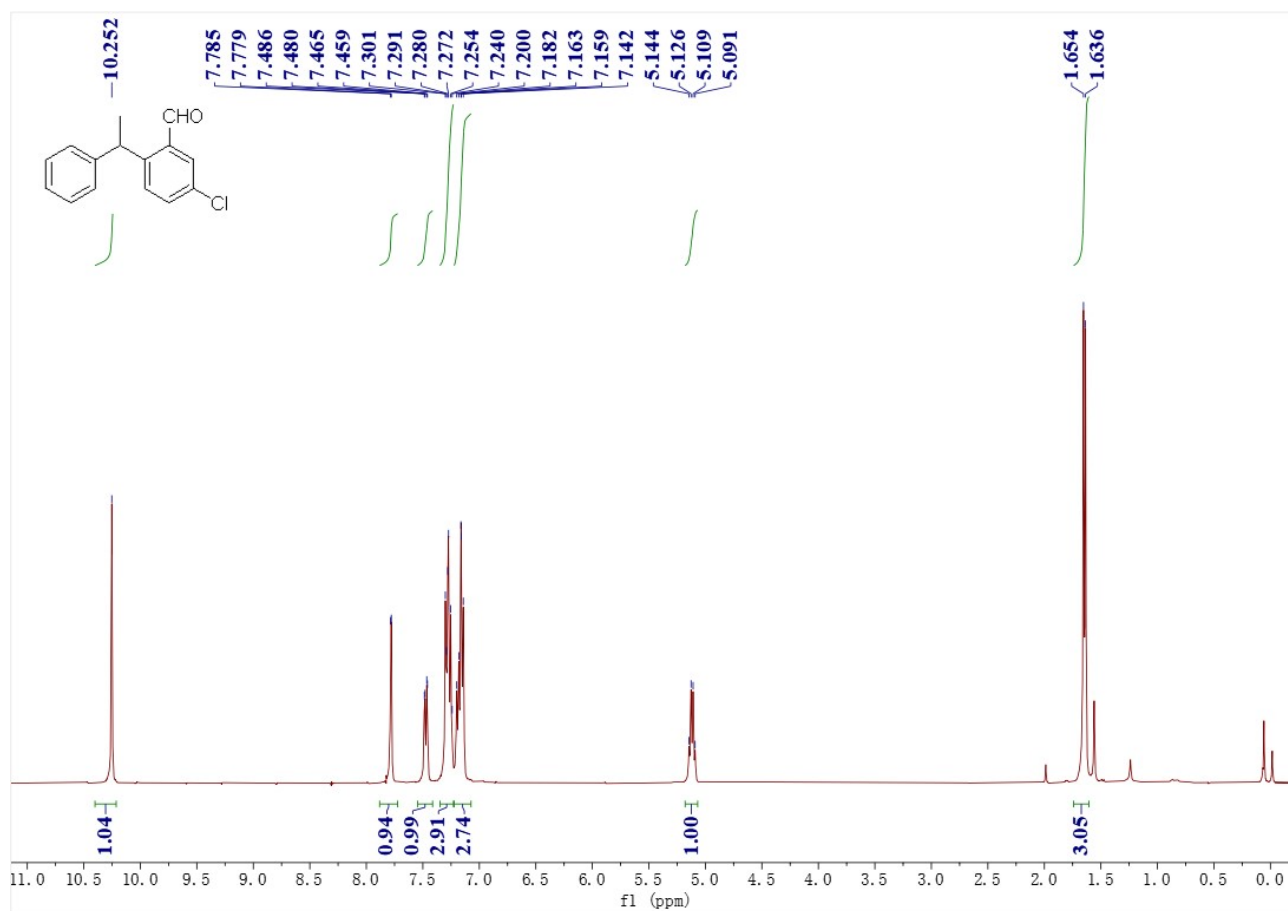


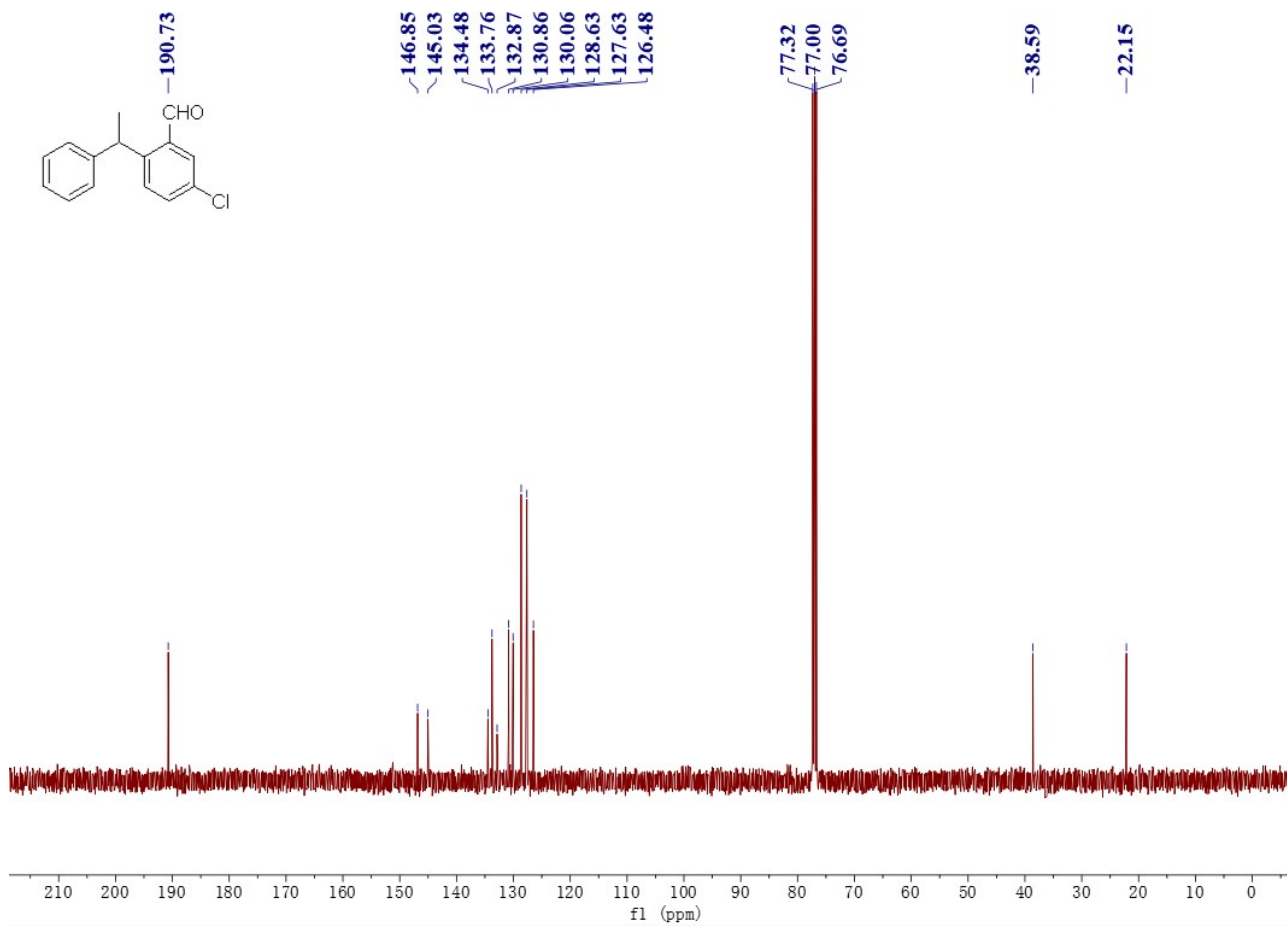
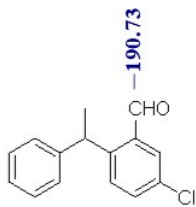


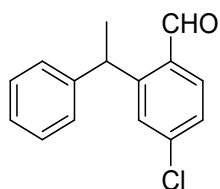


5-chloro-2-(1-phenylethyl)benzaldehyde (2i)

A colorless oil. 45.4 mg, 93% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 10.25 (s, 1H), 7.78 (d, $J = 2.4$ Hz, 1H), 7.47 (dd, $J = 8.4, 2.5$ Hz, 1H), 7.30-7.24 (m, 3H), 7.20-7.14 (m, 3H), 5.12 (q, $J = 7.2$ Hz, 1H), 1.64 (d, $J = 7.2$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 190.7, 146.9, 145.0, 134.5, 133.8, 132.9, 130.9, 130.1, 128.6, 127.6, 126.5, 38.6, 22.2. IR (acetone) ν 3061, 2971, 2863, 1688, 1594, 1479, 1451, 1027, 832, 699 cm^{-1} . HRMS (EI) calcd. for $\text{C}_{15}\text{H}_{13}\text{ClO}$ (M^+): 244.0649, Found: 244.0656.

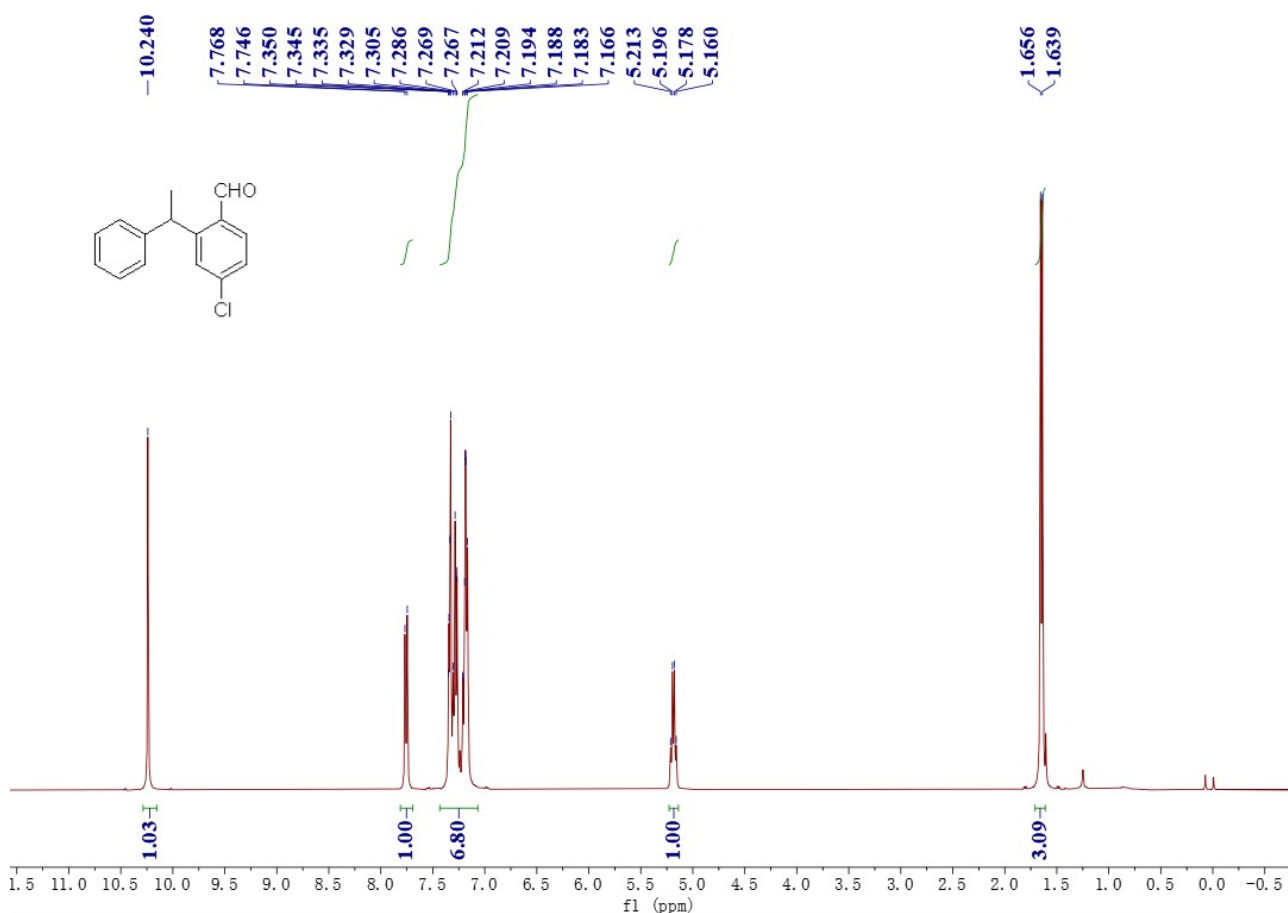


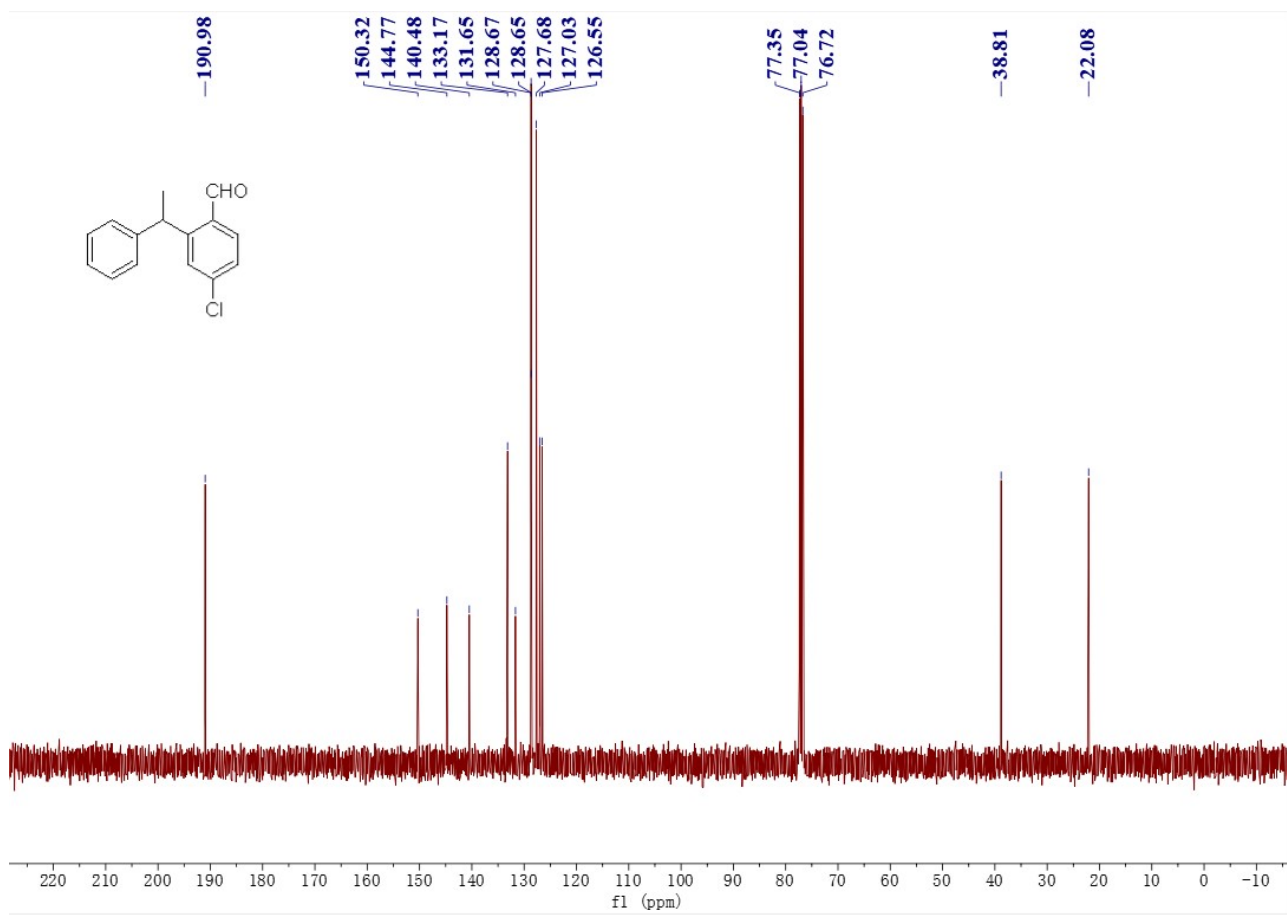


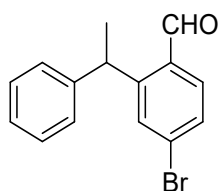


4-chloro-2-(1-phenylethyl)benzaldehyde (2j)

A colorless oil. 44.4 mg, 91% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 10.24 (s, 1H), 7.76 (d, $J=8.8$ Hz, 1H), 7.35-7.17 (m, 7H), 5.19 (q, $J=7.2$ Hz, 1H), 1.65 (d, $J=7.2$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 191.0, 150.3, 144.8, 140.5, 133.2, 131.7, 128.7, 128.6, 127.7, 127.0, 126.5, 38.8, 22.1. IR (acetone) ν 3060, 2970, 2873, 1687, 1587, 1479, 1450, 1027, 832, 698 cm^{-1} . HRMS (EI) calcd. for $\text{C}_{15}\text{H}_{13}\text{ClO}$ (M^+): 244.0649, Found: 244.0669.

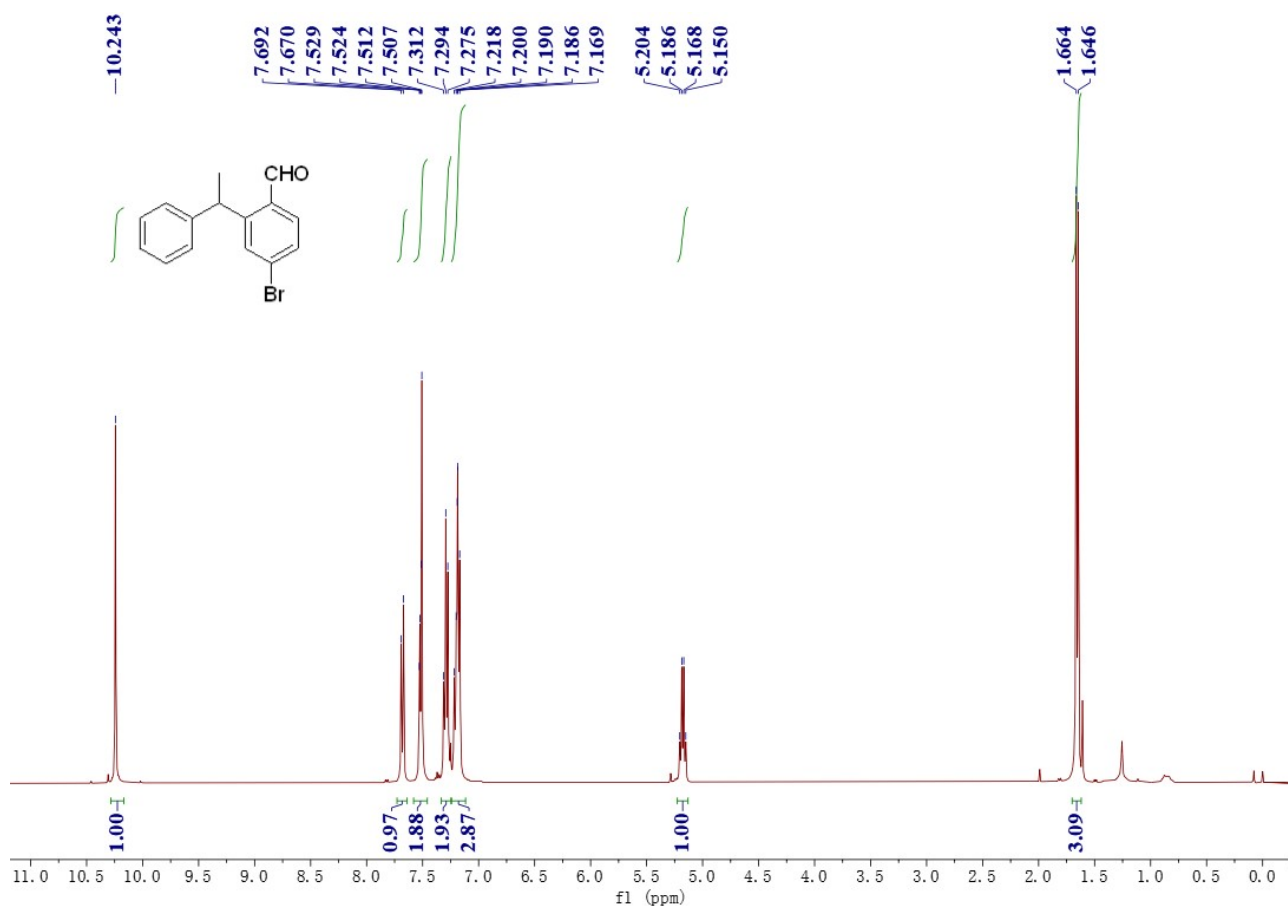


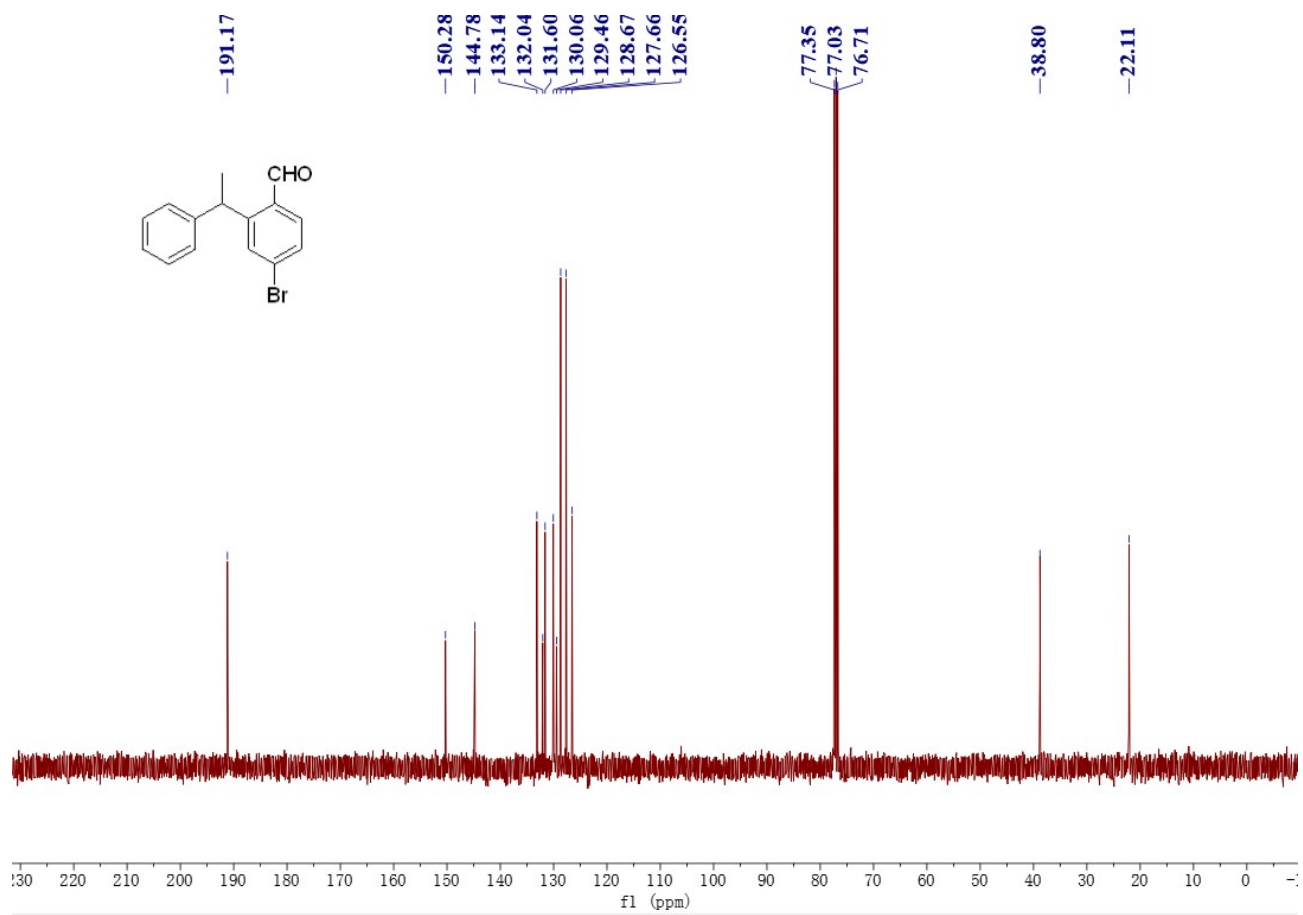


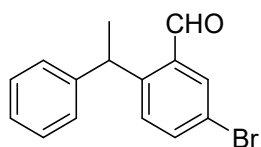


4-bromo-2-(1-phenylethyl)benzaldehyde (2k)

A colorless oil. 53.6 mg, 93% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 10.24 (s, 1H), 7.68 (d, $J = 8.8$ Hz, 1H), 7.53-7.51 (m, 2H), 7.29 (t, $J = 7.2$ Hz, 2H), 7.20-7.17 (m, 3H), 5.18 (q, $J = 7.2$ Hz, 1H), 1.66 (d, $J = 7.2$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 191.2, 150.3, 144.8, 133.1, 132.0, 131.6, 130.1, 129.5, 128.7, 127.7, 126.6, 38.8, 22.1. IR (acetone) ν 3063, 2970, 2870, 1689, 1583, 1473, 1450, 1028, 854, 699 cm^{-1} . HRMS (EI) calcd. for $\text{C}_{15}\text{H}_{13}\text{BrO}$ (M^+): 288.0144, Found: 288.0148.

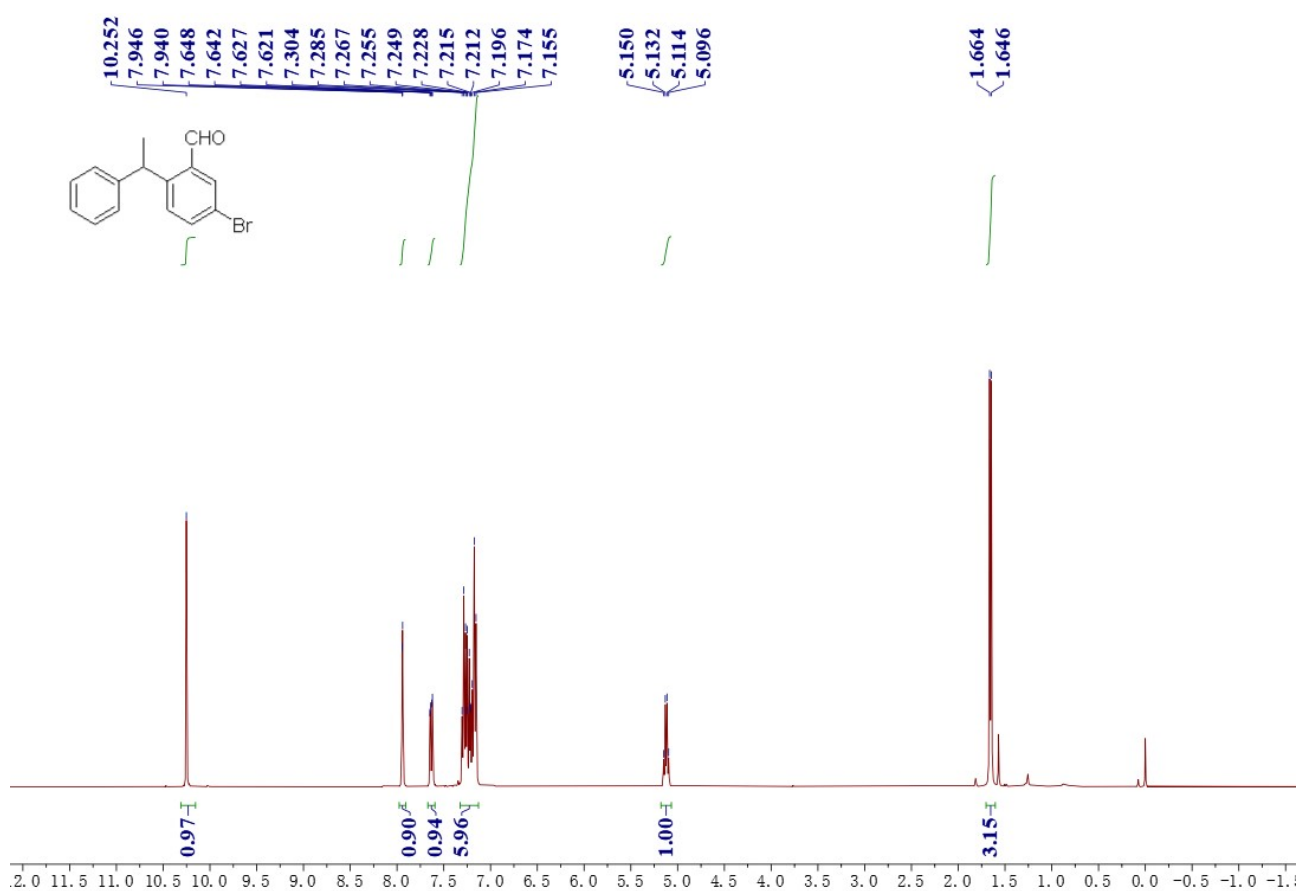


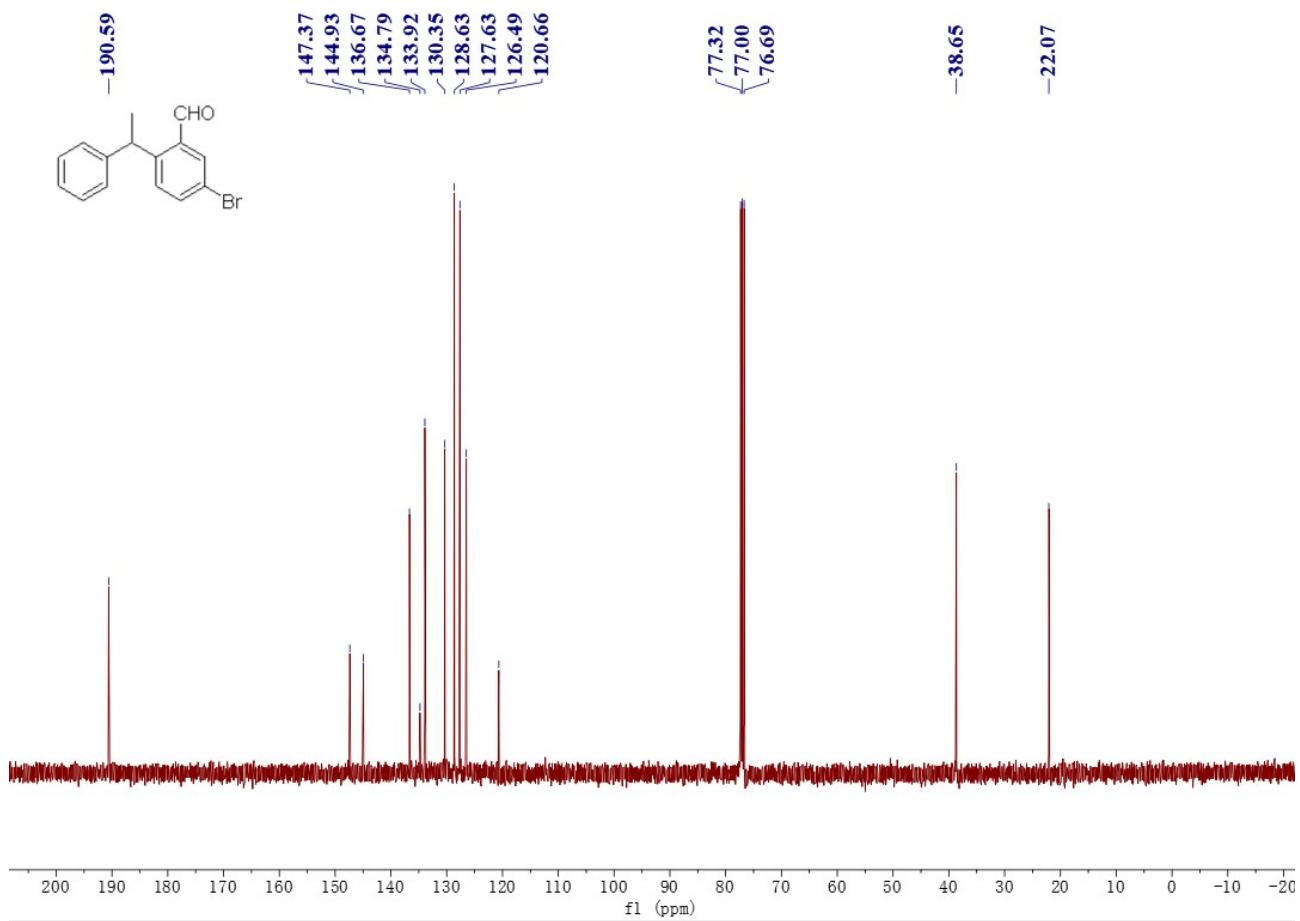


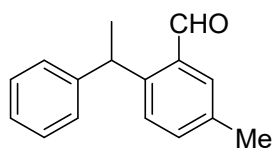


5-bromo-2-(1-phenylethyl)benzaldehyde (2I)

A colorless oil. 34.6 mg, 60% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 10.25 (s, 1H), 7.94 (d, $J = 2.2$ Hz, 1H), 7.63 (dd, $J = 8.4, 2.2$ Hz, 1H), 7.30-7.16 (m, 6H), 5.12 (q, $J = 7.2$ Hz, 1H), 1.66 (d, $J = 7.2$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 190.6, 147.4, 144.9, 136.7, 134.8, 133.9, 130.3, 128.6, 127.6, 126.5, 120.7, 38.7, 22.1. IR (acetone) ν 3060, 2970, 2873, 1689, 1587, 1479, 1450, 1027, 877, 697 cm^{-1} . HRMS (EI) calcd. for $\text{C}_{15}\text{H}_{13}\text{BrO}$ (M^+): 288.0144, Found: 288.0146.

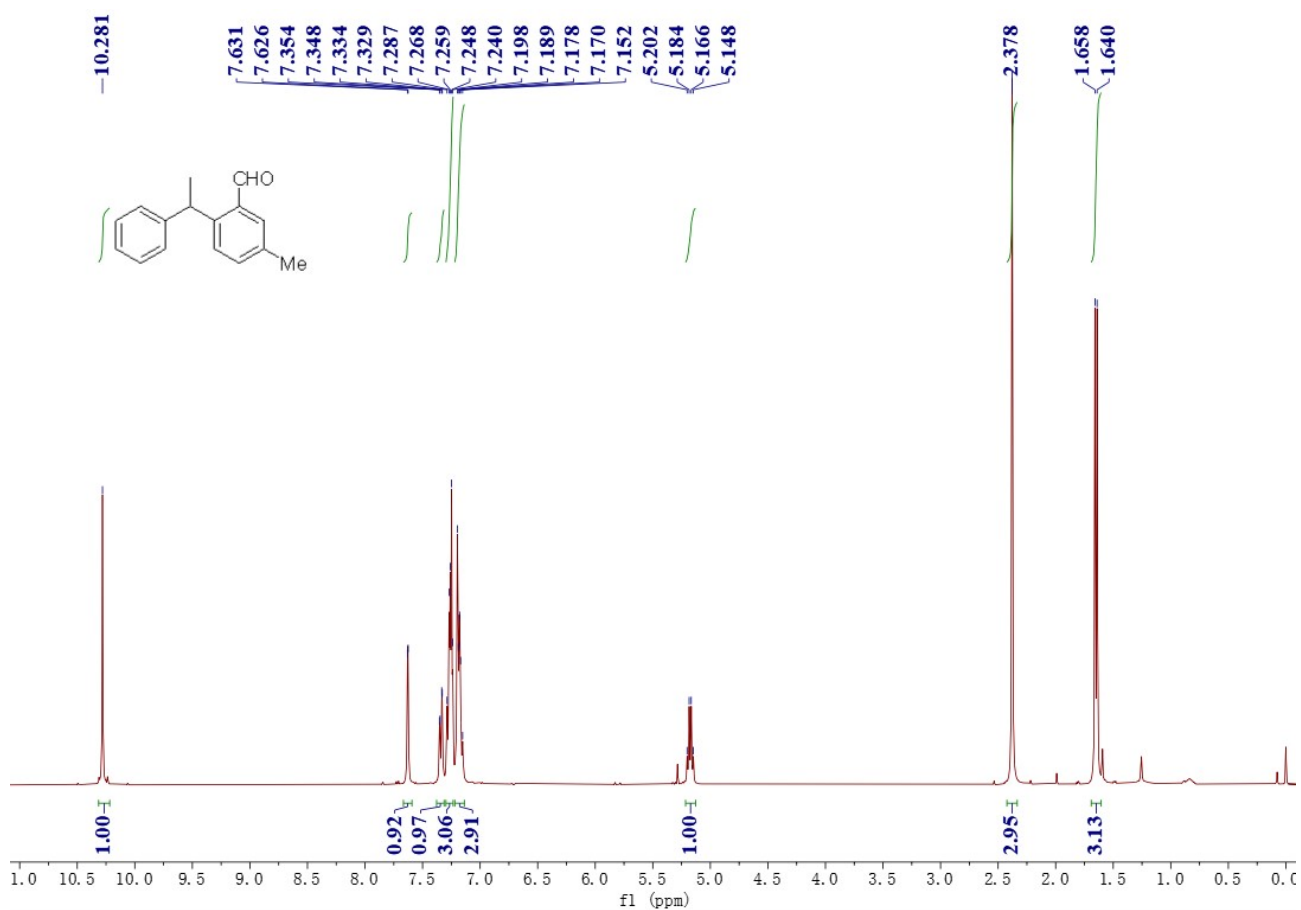


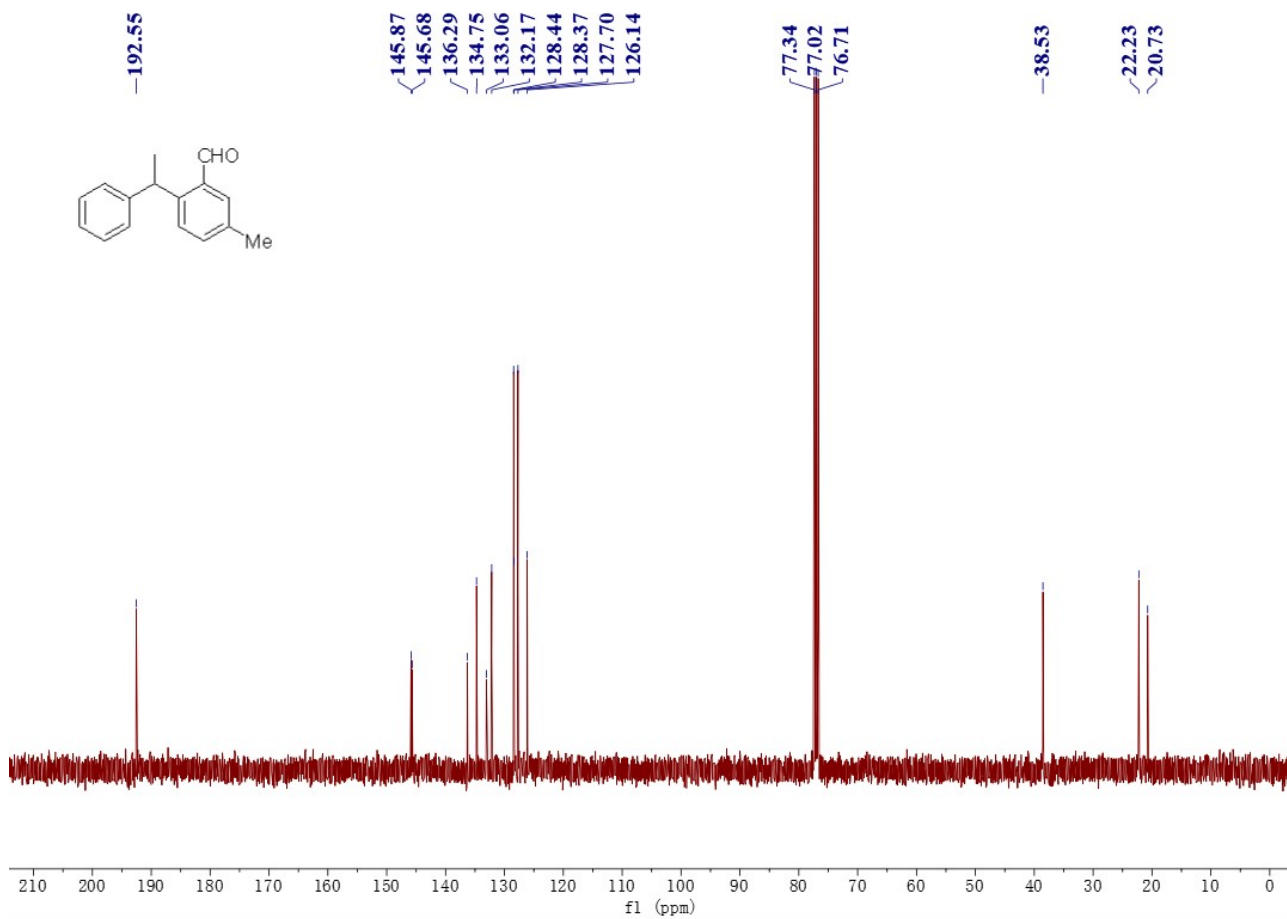


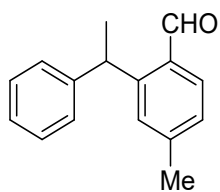


5-methyl-2-(1-phenylethyl)benzaldehyde (2m)

This is a known compound and its spectroscopic data are consistent with those in the previous literature.¹² CAS number: 1979200-43-5. A colorless oil. 25.6 mg, 57% yield. ¹H NMR (CDCl₃, TMS, 400 MHz) δ 10.28 (s, 1H), 7.63 (d, *J* = 2.2 Hz, 1H), 7.34 (dd, *J* = 8.0, 2.2 Hz, 1H), 7.29-7.24 (m, 3H), 7.20-7.15 (m, 3H), 5.17 (q, *J* = 7.2 Hz, 1H), 2.38 (s, 3H), 1.65 (d, *J* = 7.2 Hz, 3H). ¹³C NMR (CDCl₃, TMS, 100 MHz) δ 192.6, 145.9, 145.7, 136.3, 134.7, 133.1, 132.2, 128.4, 128.4, 127.7, 126.1, 38.5, 22.2, 20.7.

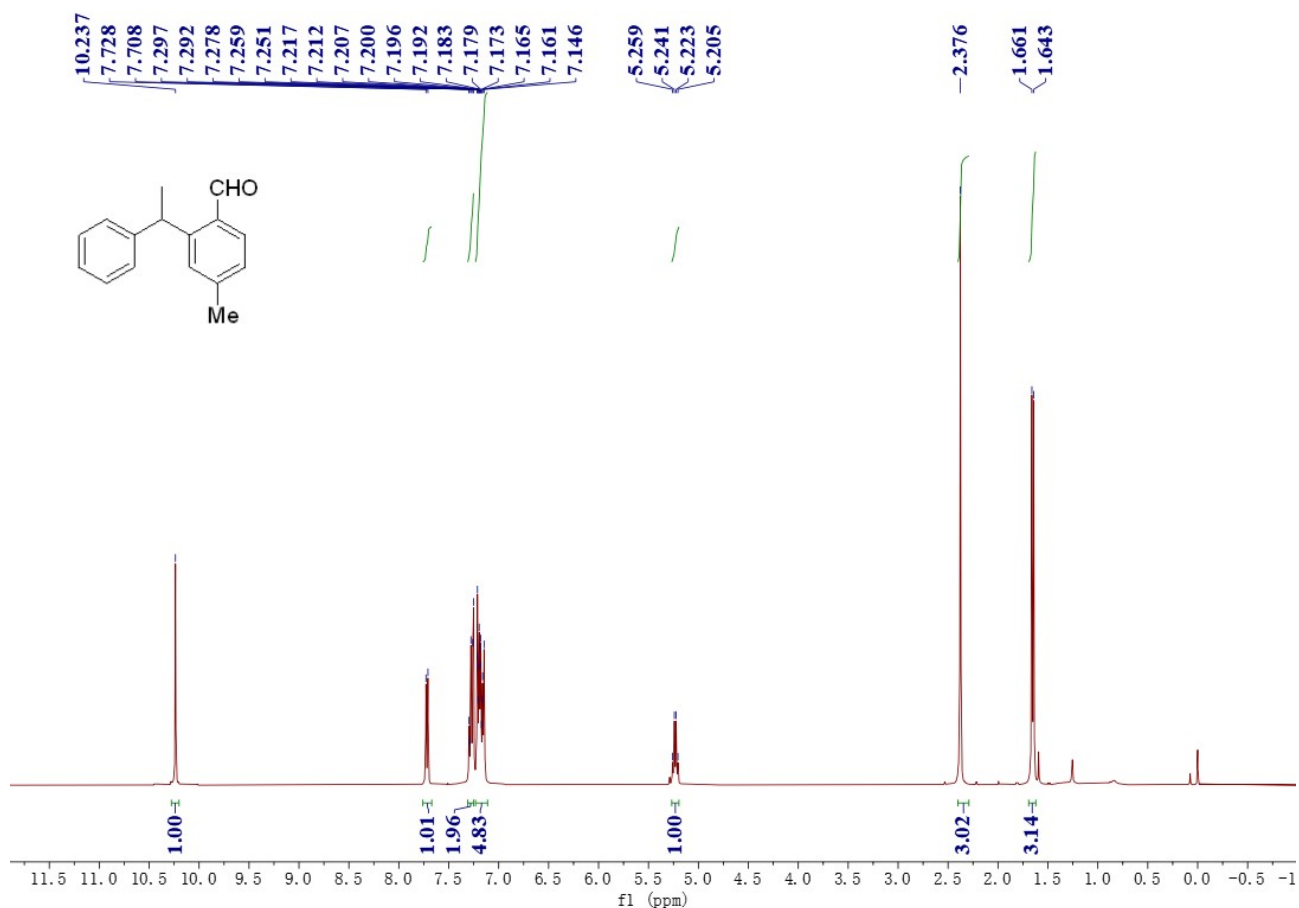


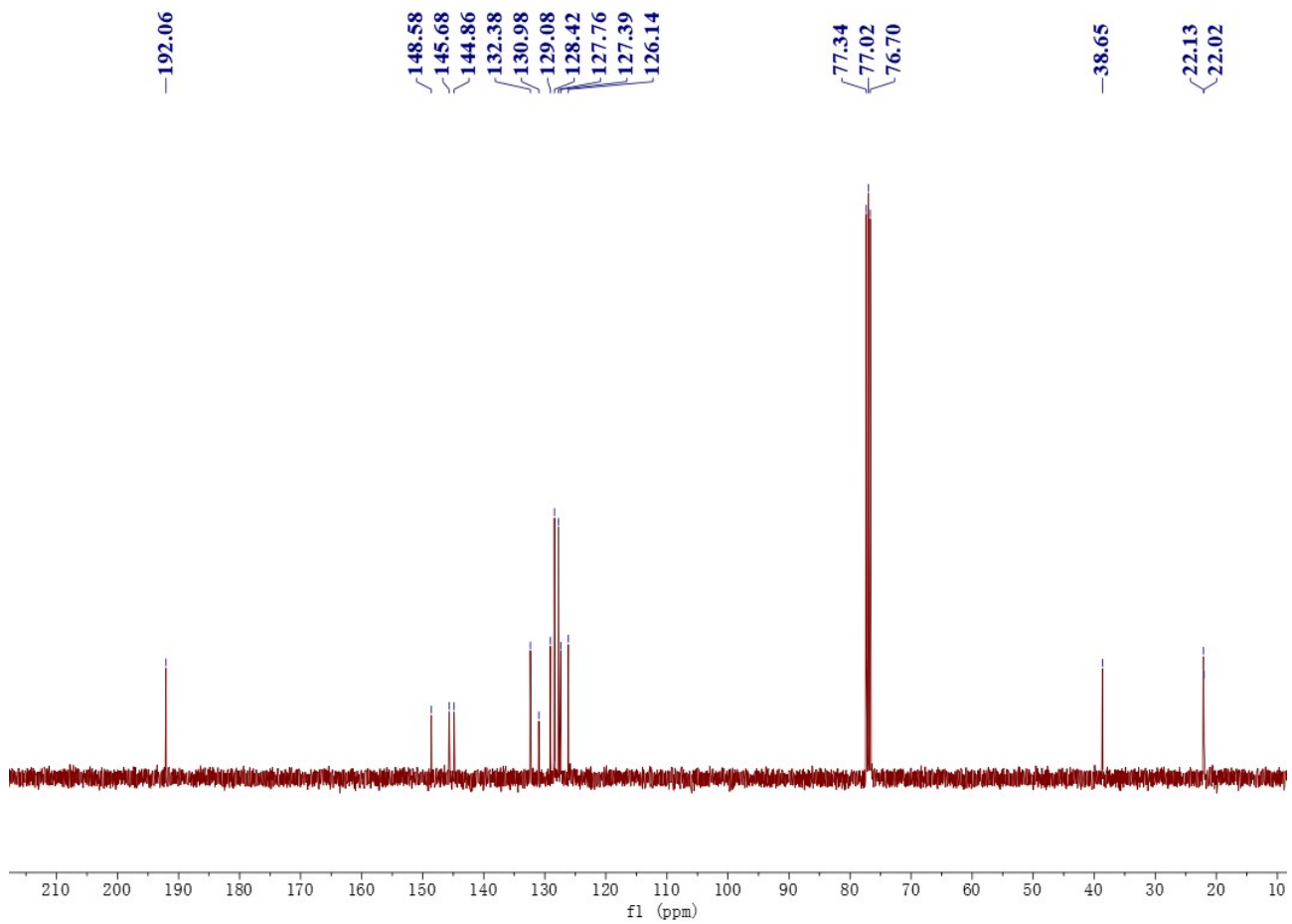


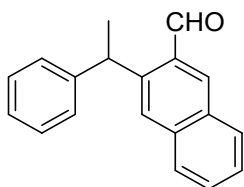


4-(2-bromophenyl)-1-phenylbutan-1-one (2n)

A colorless oil. 40.4 mg, 90% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 10.24 (s, 1H), 7.72 (d, $J = 7.8$ Hz, 1H), 7.30-7.25 (m, 2H), 7.22-7.15 (m, 5H), 5.23 (q, $J = 7.2$ Hz, 1H), 2.38 (s, 3H), 1.65 (d, $J = 7.2$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 192.1, 148.6, 145.7, 144.9, 132.4, 131.0, 129.1, 128.4, 127.8, 127.4, 126.1, 38.7, 22.1, 22.0. IR (acetone) ν 3055, 2970, 2877, 1692, 1627, 1494, 1451, 1179, 891, 698 cm^{-1} . HRMS (EI) calcd. for $\text{C}_{16}\text{H}_{16}\text{O}$ (M^+): 224.1196, Found: 224.1198.

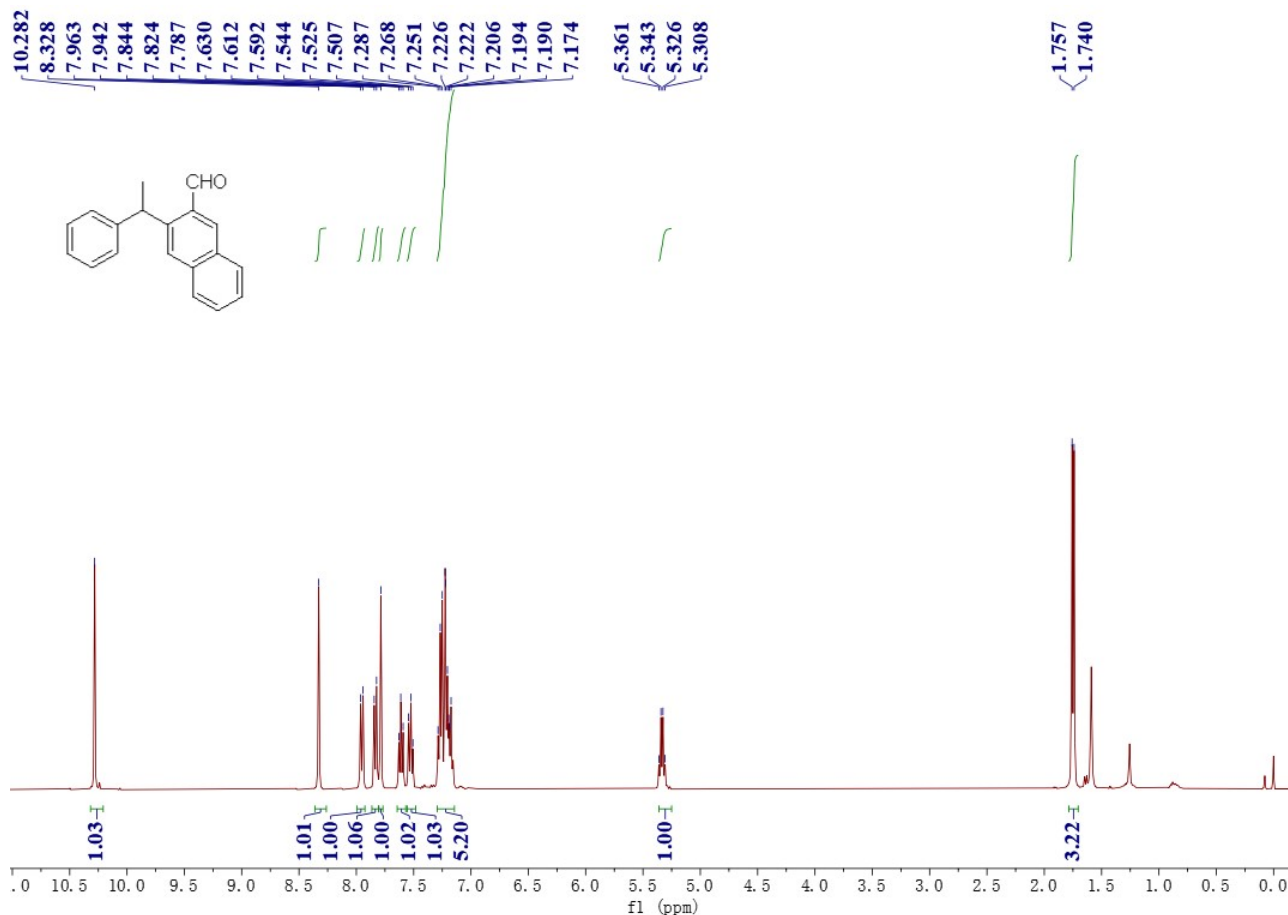


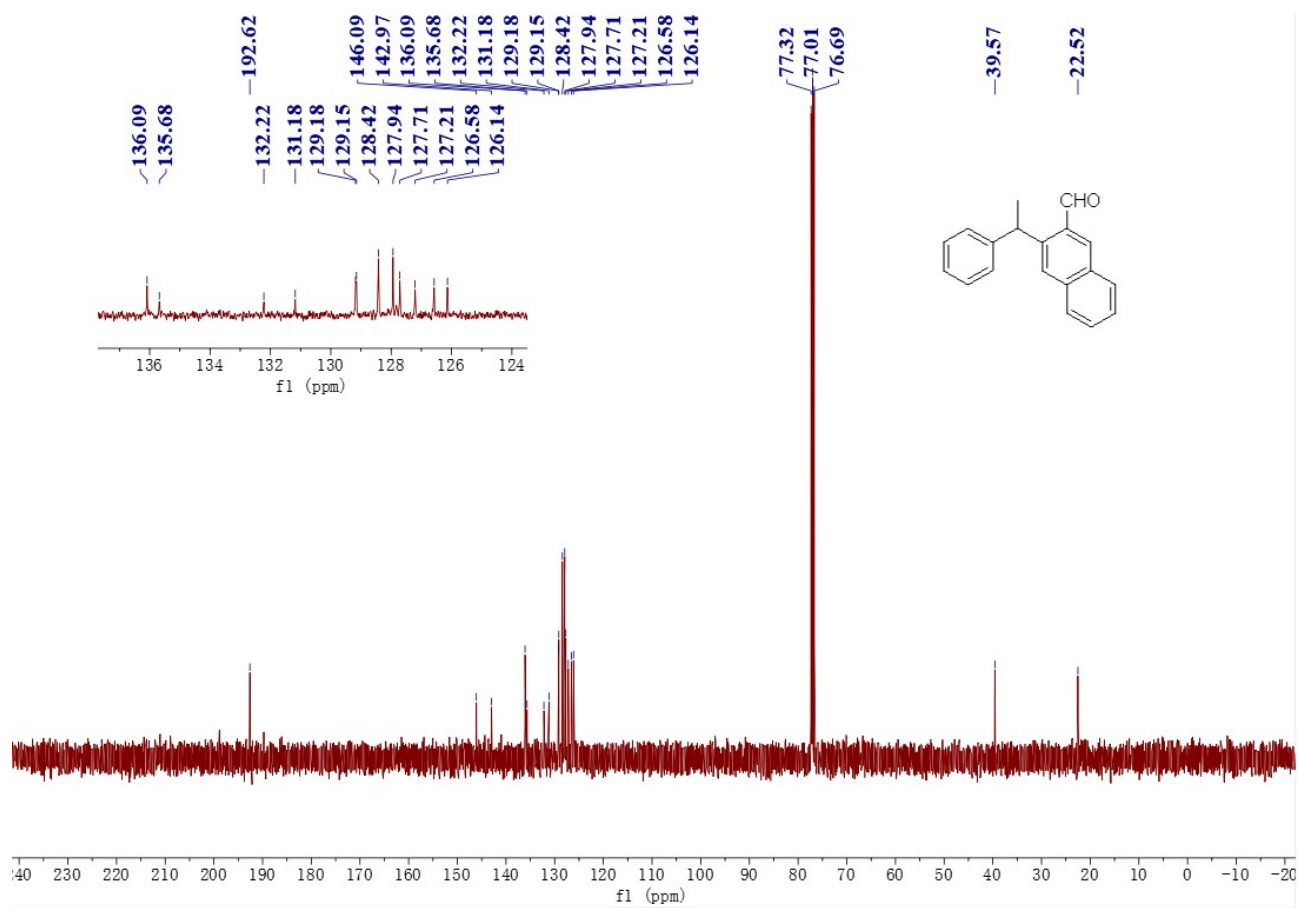


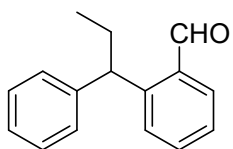


3-(1-phenylethyl)-2-naphthaldehyde (2o)

A white solid. 36.4 mg, 70% yield. M.P.: 72-74 °C. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 10.28 (s, 1H), 8.33 (s, 1H), 7.95 (d, $J = 8.2$ Hz, 1H), 7.83 (d, $J = 8.2$ Hz, 1H), 7.79 (s, 1H), 7.61 (d, $J = 7.2$ Hz, 1H), 7.53 (t, $J = 7.6$ Hz, 1H), 7.29-7.17 (m, 5H), 5.33 (q, $J = 7.2$ Hz, 1H), 1.75 (d, $J = 7.2$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 192.6, 146.1, 143.0, 136.1, 135.7, 132.2, 131.2, 129.2, 129.1, 128.4, 127.9, 127.7, 127.2, 126.6, 126.1, 39.6, 22.5. IR (acetone) ν 3053, 2968, 2876, 1692, 1626, 1493, 1450, 1174, 894, 700 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{19}\text{H}_{16}\text{ONa}$ ($\text{M}+\text{Na}$) $^+$: 283.1093, Found: 283.1088.

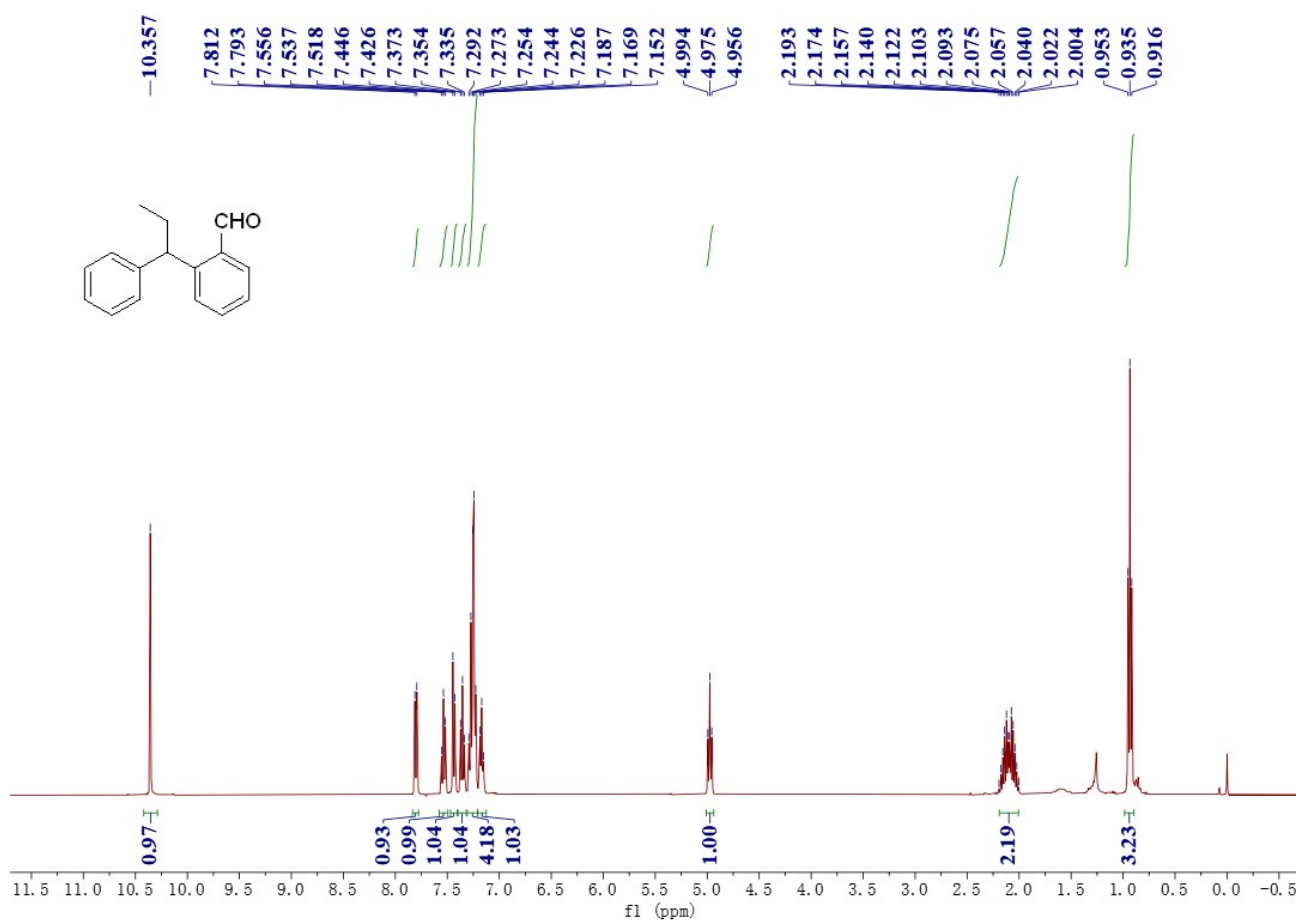


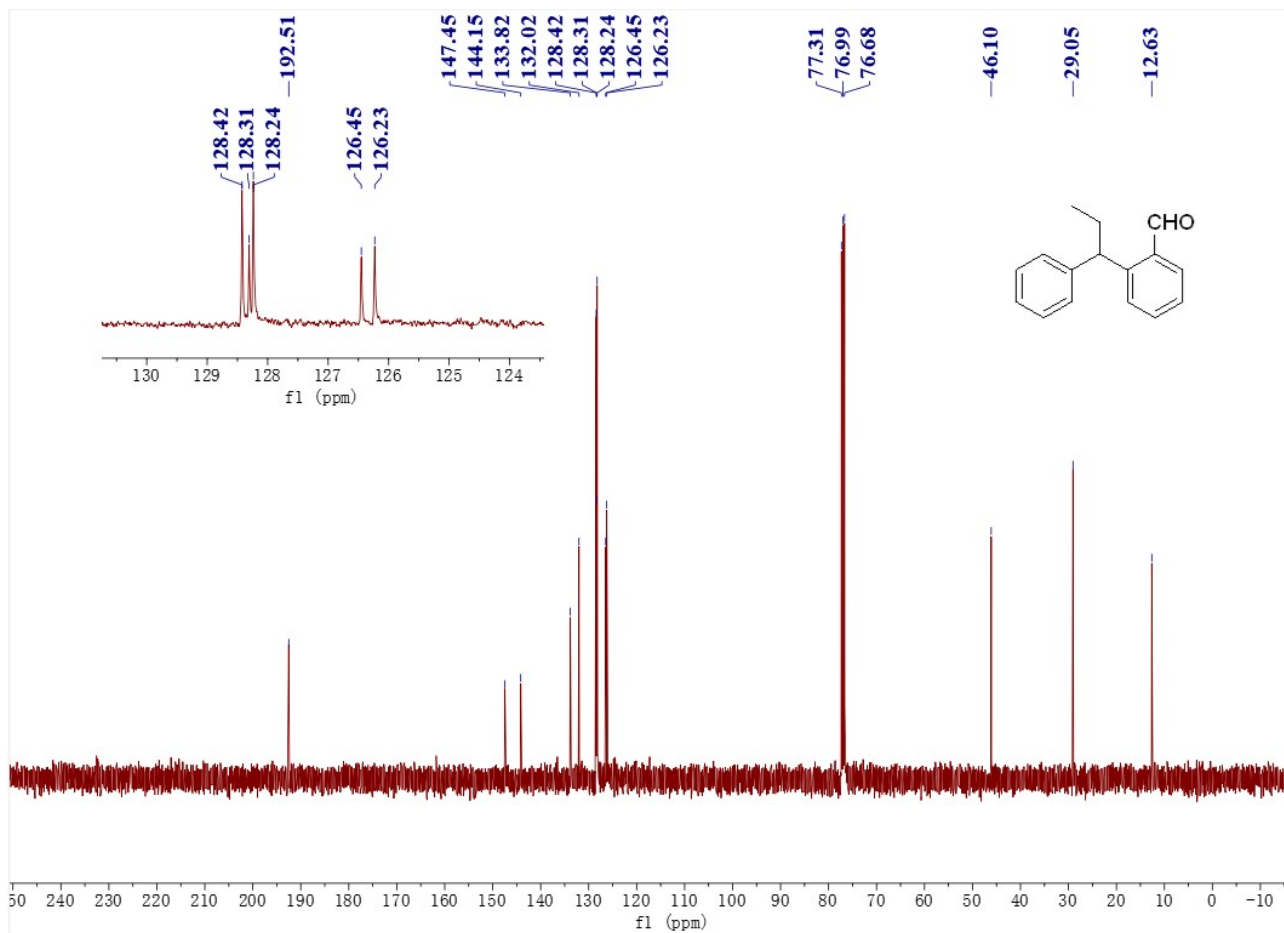


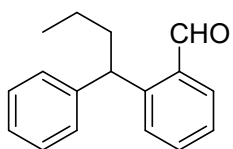


2-(1-phenylpropyl)benzaldehyde (2p)

A colorless oil. 26.9 mg, 60% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 10.36 (s, 1H), 7.80 (d, $J = 7.8$ Hz, 1H), 7.54 (t, $J = 7.6$ Hz, 1H), 7.44 (d, $J = 7.8$ Hz, 1H), 7.35 (t, $J = 7.6$ Hz, 1H), 7.29-7.23 (m, 4H), 7.17 (t, $J = 7.0$ Hz, 1H), 4.98 (t, $J = 7.6$ Hz, 1H), 2.19-2.00 (m, 2H), 0.93 (t, $J = 7.2$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 192.5, 147.5, 144.2, 133.8, 132.0, 128.4, 128.3, 128.2, 126.5, 126.2, 77.3, 29.1, 12.6. IR (acetone) ν 3027, 2957, 2931, 1690, 1573, 1494, 1408, 1285, 700, 660 cm^{-1} . HRMS (EI) calcd. for $\text{C}_{16}\text{H}_{16}\text{O}$ (M^+): 224.1196, Found: 224.1201.

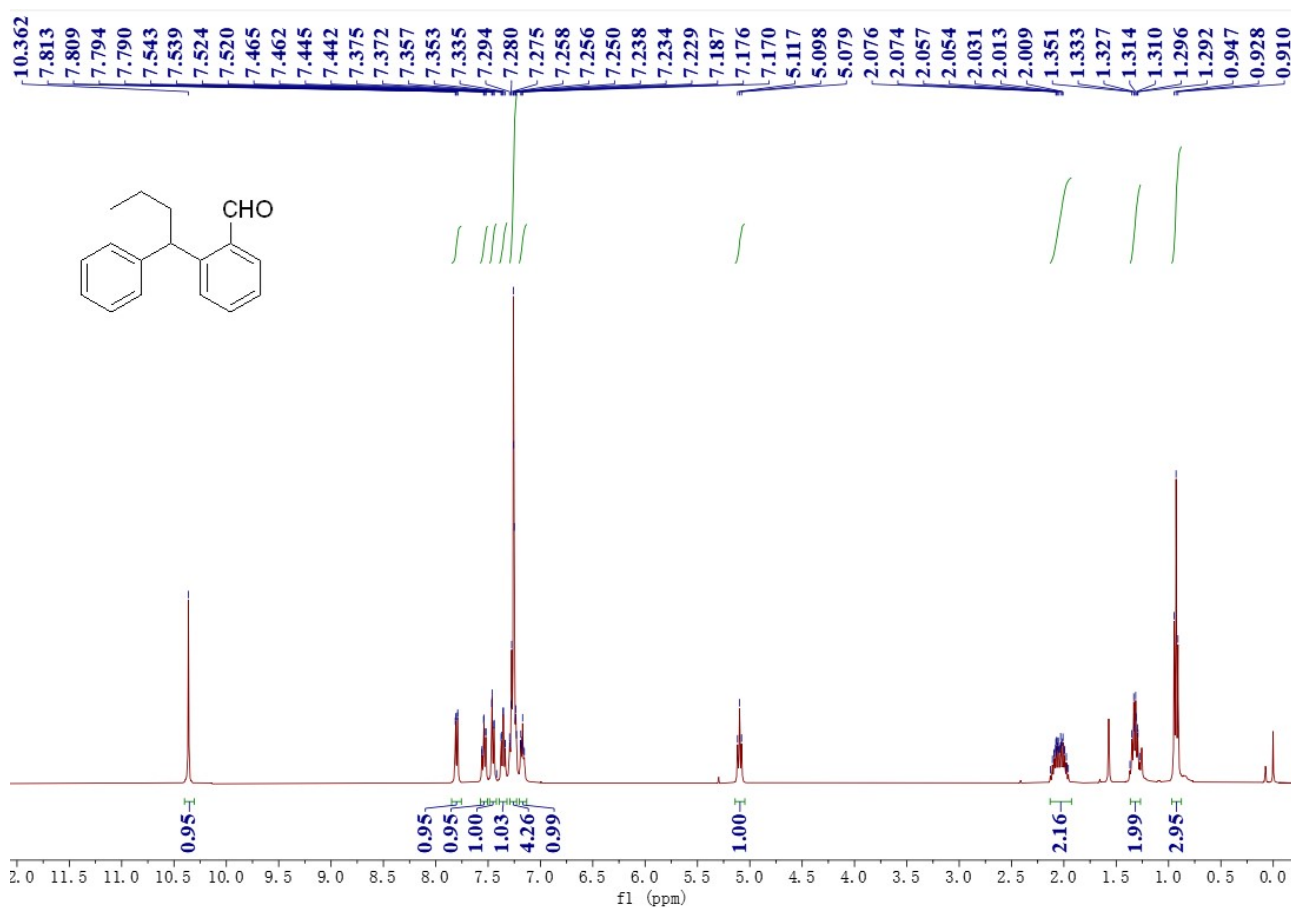


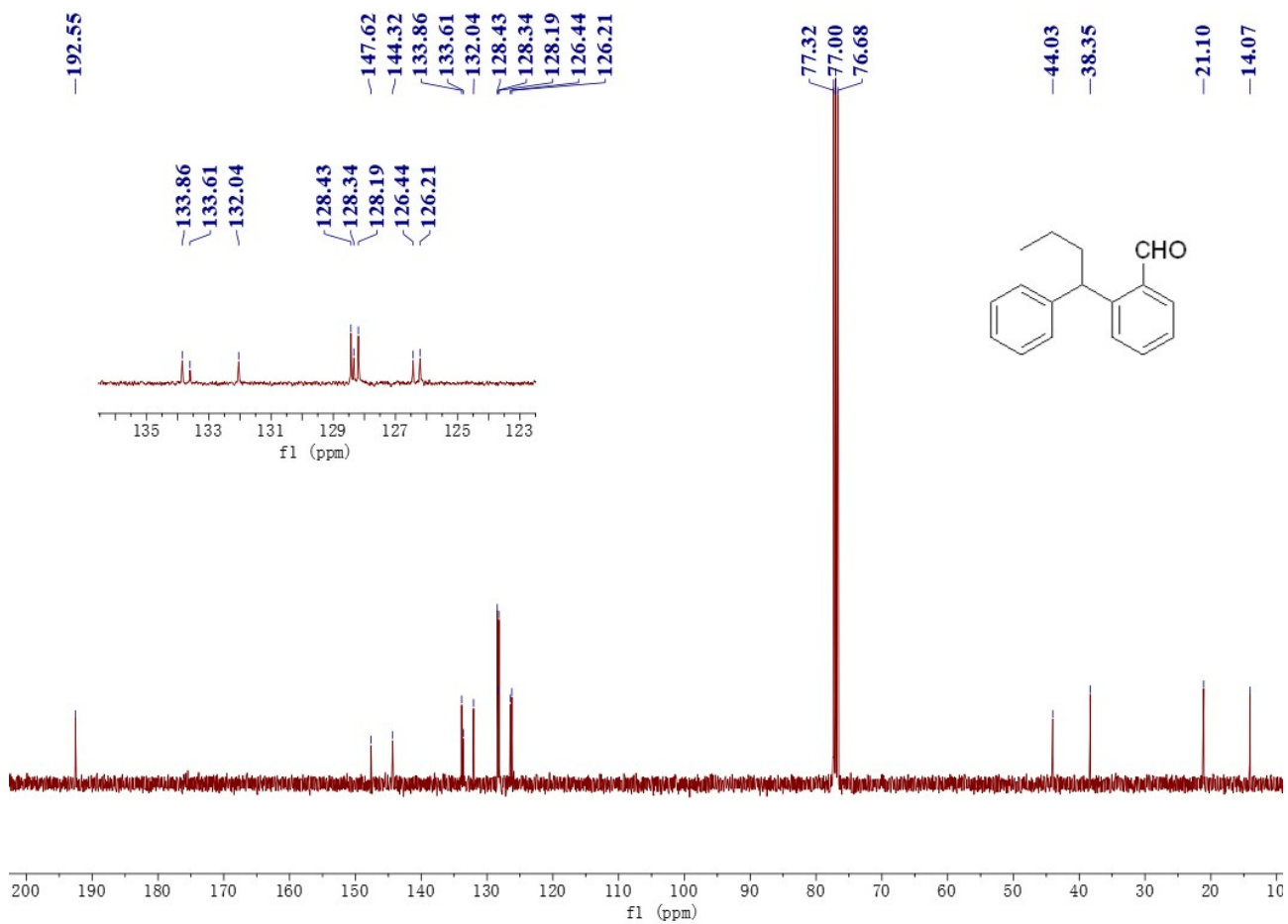


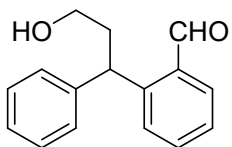


2-(1-phenylbutyl)benzaldehyde (2q)

A colorless oil. 11.9 mg, 25% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 10.36 (s, 1H), 7.80 (dd, $J = 7.6, 1.6$ Hz, 1H), 7.54 (td, $J = 7.6, 1.6$ Hz, 1H), 7.45 (dd, $J = 8.0, 1.4$ Hz, 1H), 7.36 (td, $J = 7.6, 1.4$ Hz, 1H), 7.29-7.23 (m, 4H), 7.19-7.15 (m, 1H), 5.10 (t, $J = 7.6$ Hz, 1H), 2.08-2.00 (m, 2H), 1.37-1.28 (m, 2H), 0.93 (t, $J = 7.6$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 192.5, 147.6, 144.3, 133.9, 133.6, 132.0, 128.4, 128.3, 128.2, 126.4, 126.2, 44.0, 38.4, 21.1, 14.1. IR (acetone) ν 3028, 2957, 2931, 2870, 1627, 1494, 1452, 1203, 756, 660 cm^{-1} . HRMS (EI) calcd. for $\text{C}_{17}\text{H}_{18}\text{O}$ (M^+): 238.1352, Found: 238.1354.

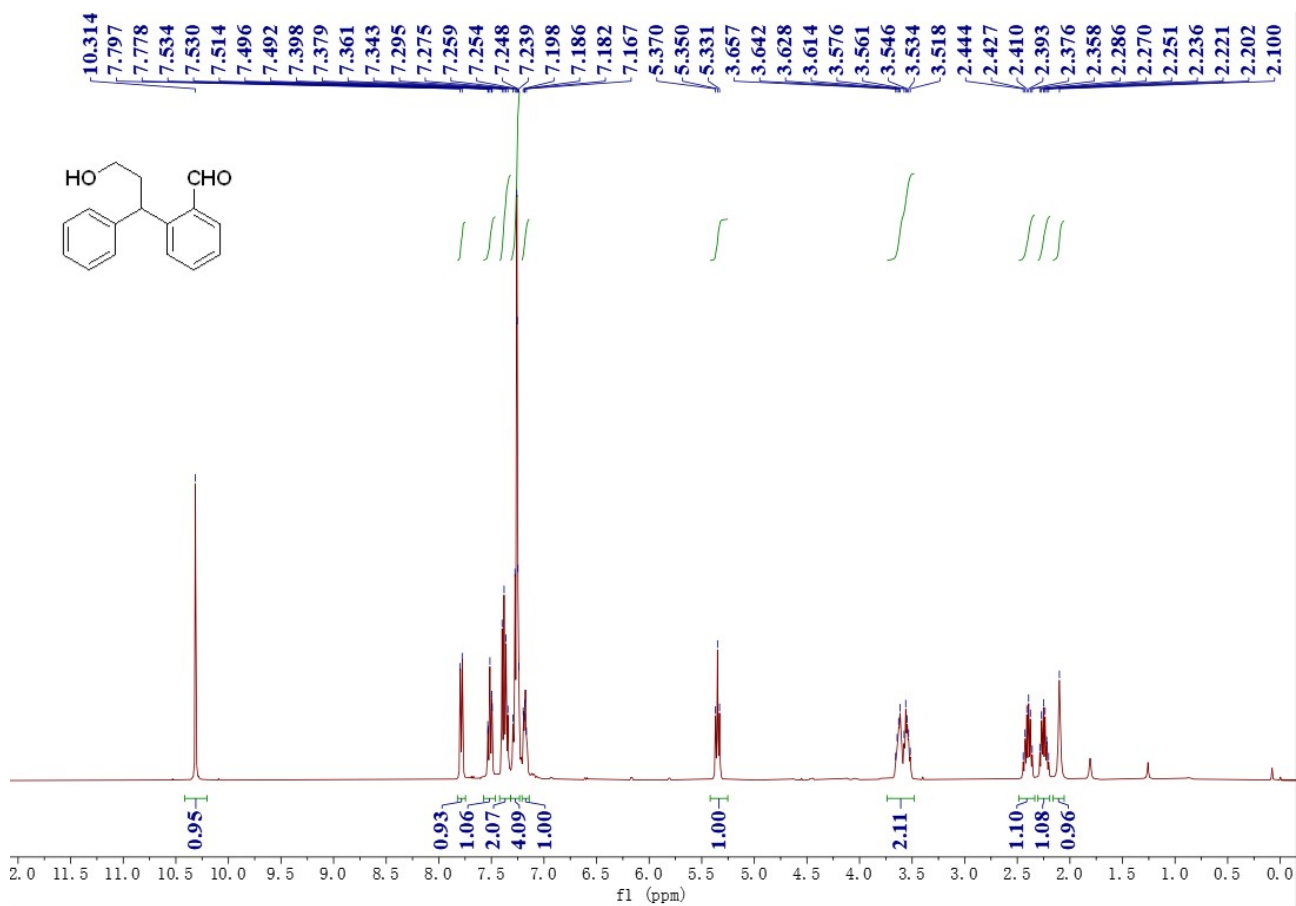


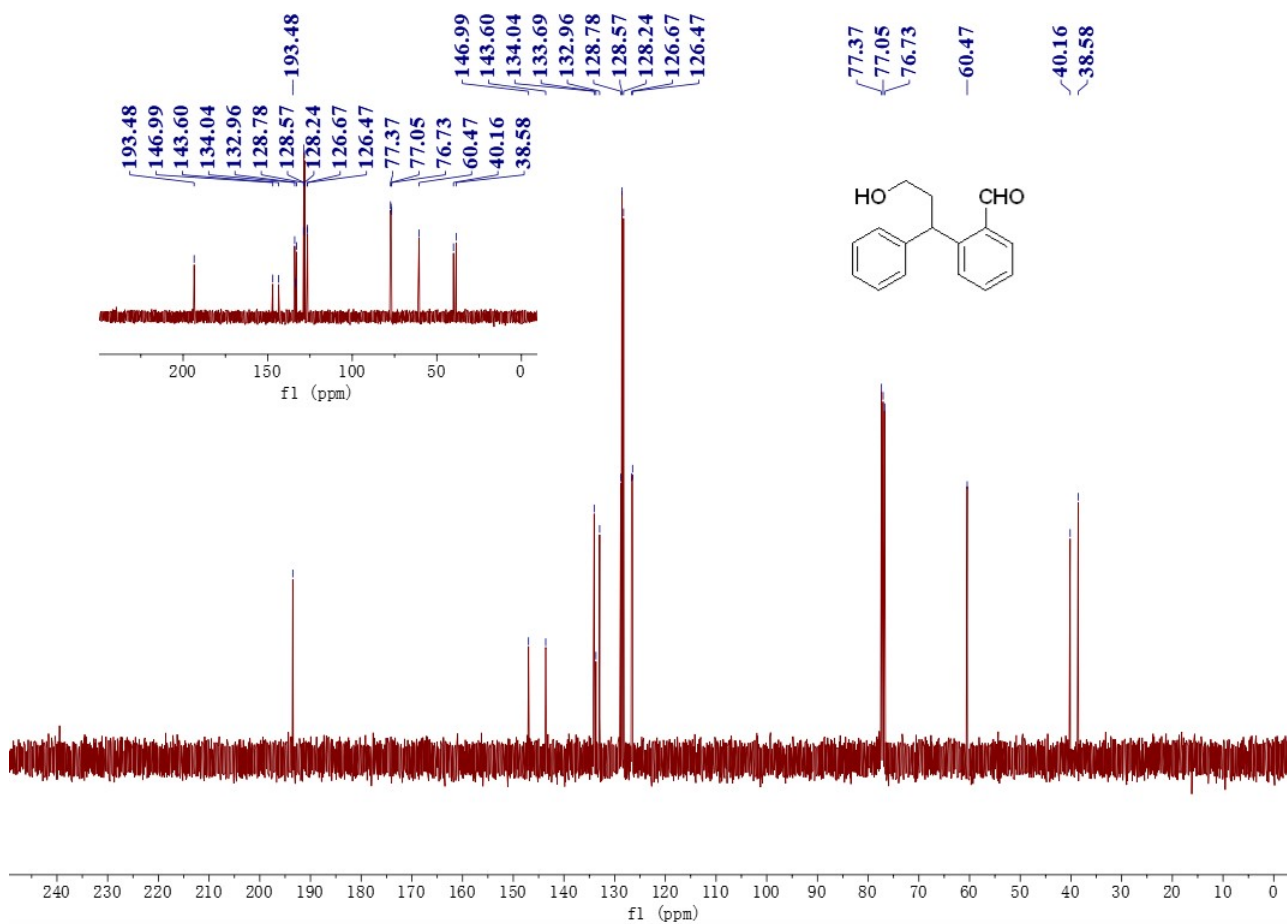


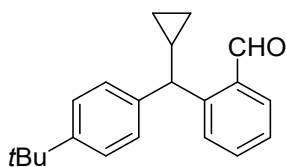


2-(3-hydroxy-1-phenylpropyl)benzaldehyde (2r)

A colorless oil. 28.8 mg, 60% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 10.31 (s, 1H), 7.79 (d, J = 7.6 Hz, 1H), 7.53-7.49 (m, 1H), 7.40-7.34 (m, 2H), 7.30-7.24 (m, 4H), 7.21-7.17 (m, 1H), 5.35 (t, J = 7.6 Hz, 1H), 3.66-3.52 (m, 2H), 2.44-2.36 (m, 1H), 2.29-2.20 (m, 1H), 2.10 (s, 1H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 193.5, 147.0, 143.6, 134.0, 133.7, 133.0, 128.8, 128.6, 128.2, 126.7, 126.5, 60.5, 40.2, 38.6. IR (acetone) ν 3389, 3026, 2936, 2875, 1626, 1494, 1451, 1206, 758, 700 cm^{-1} . HRMS (EI) calcd. for $\text{C}_{16}\text{H}_{14}\text{O}$ ($\text{M}-\text{H}_2\text{O}$) $^+$: 222.1039, Found: 222.1039.

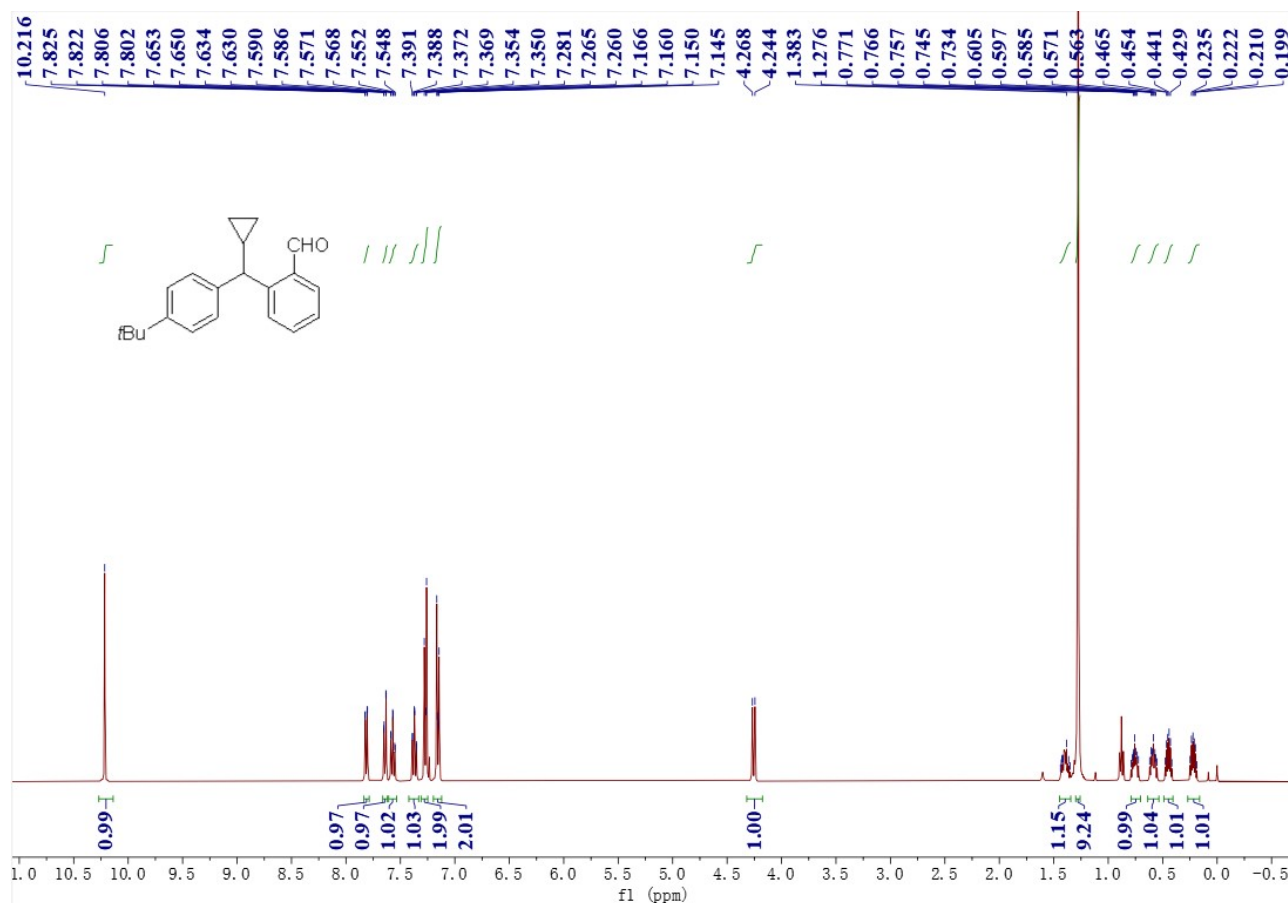


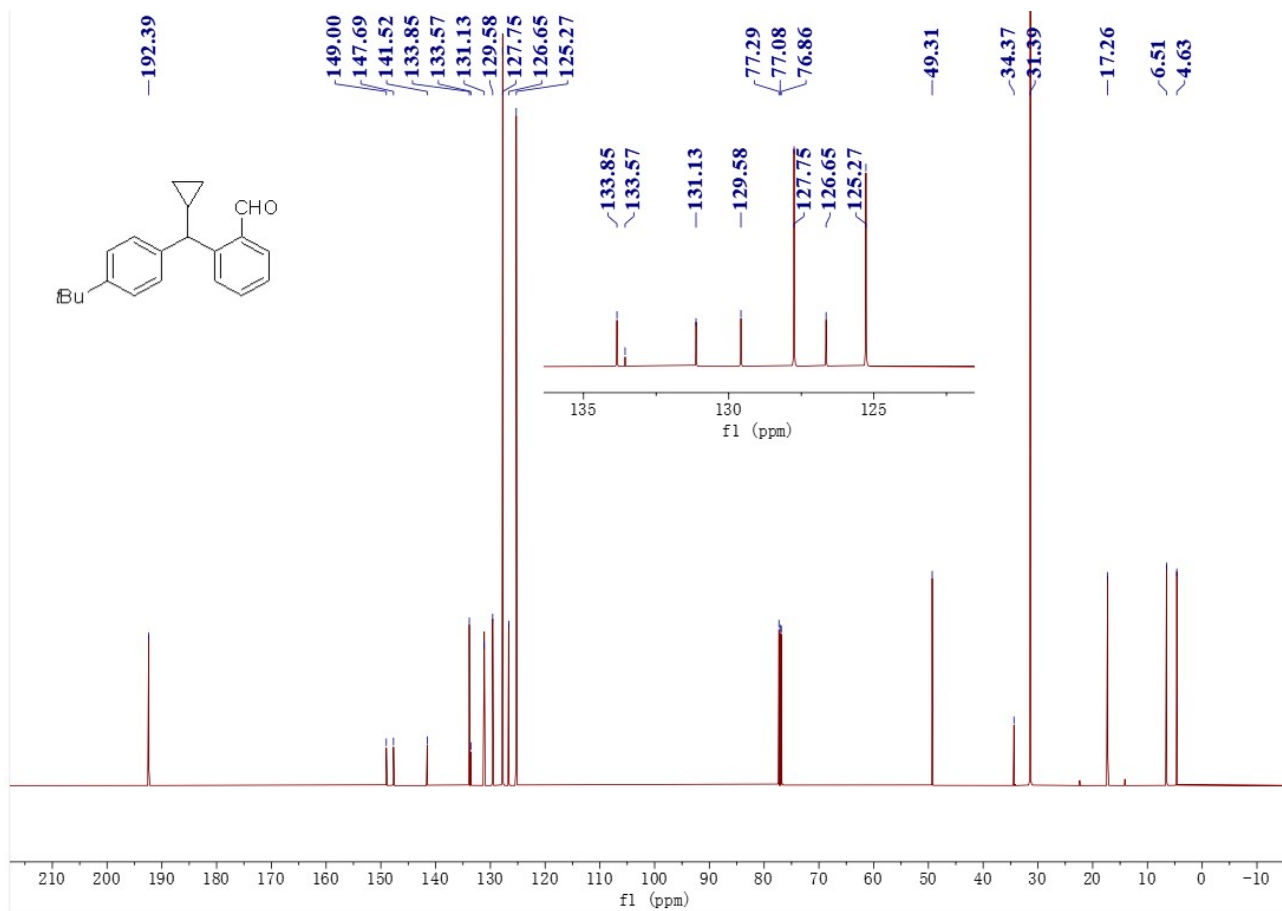


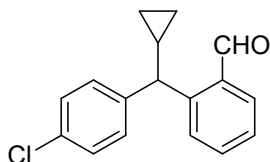


2-((4-(tert-butyl)phenyl)(cyclopropyl)methyl)benzaldehyde (2s)

A colorless oil. 53.8 mg, 92% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 10.22 (s, 1H), 7.81 (dd, $J = 7.8, 1.6$ Hz, 1H), 7.64 (dd, $J = 8.0, 1.4$ Hz, 1H), 7.57 (td, $J = 7.6, 1.6$ Hz, 1H), 7.37 (td, $J = 7.6, 1.4$ Hz, 1H), 7.28-7.26 (m, 2H), 7.17-7.15 (m, 2H), 4.26 (d, $J = 9.4$ Hz, 1H), 1.38-1.28 (m, 1H), 1.28 (s, 9H), 0.79-0.70 (m, 1H), 0.62-0.56 (m, 1H), 0.48-0.42 (m, 1H), 0.25-0.20 (m, 1H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 192.4, 149.0, 147.7, 141.5, 133.8, 133.6, 131.1, 129.6, 127.7, 126.6, 125.3, 49.3, 34.4, 31.4, 17.3, 6.5, 4.6. IR (acetone) ν 3001, 2961, 2866, 1693, 1461, 1409, 1201, 1019, 755, 659 cm^{-1} . HRMS (EI) calcd. for $\text{C}_{21}\text{H}_{24}\text{O}$ (M^+): 292.1822, Found: 292.1831.

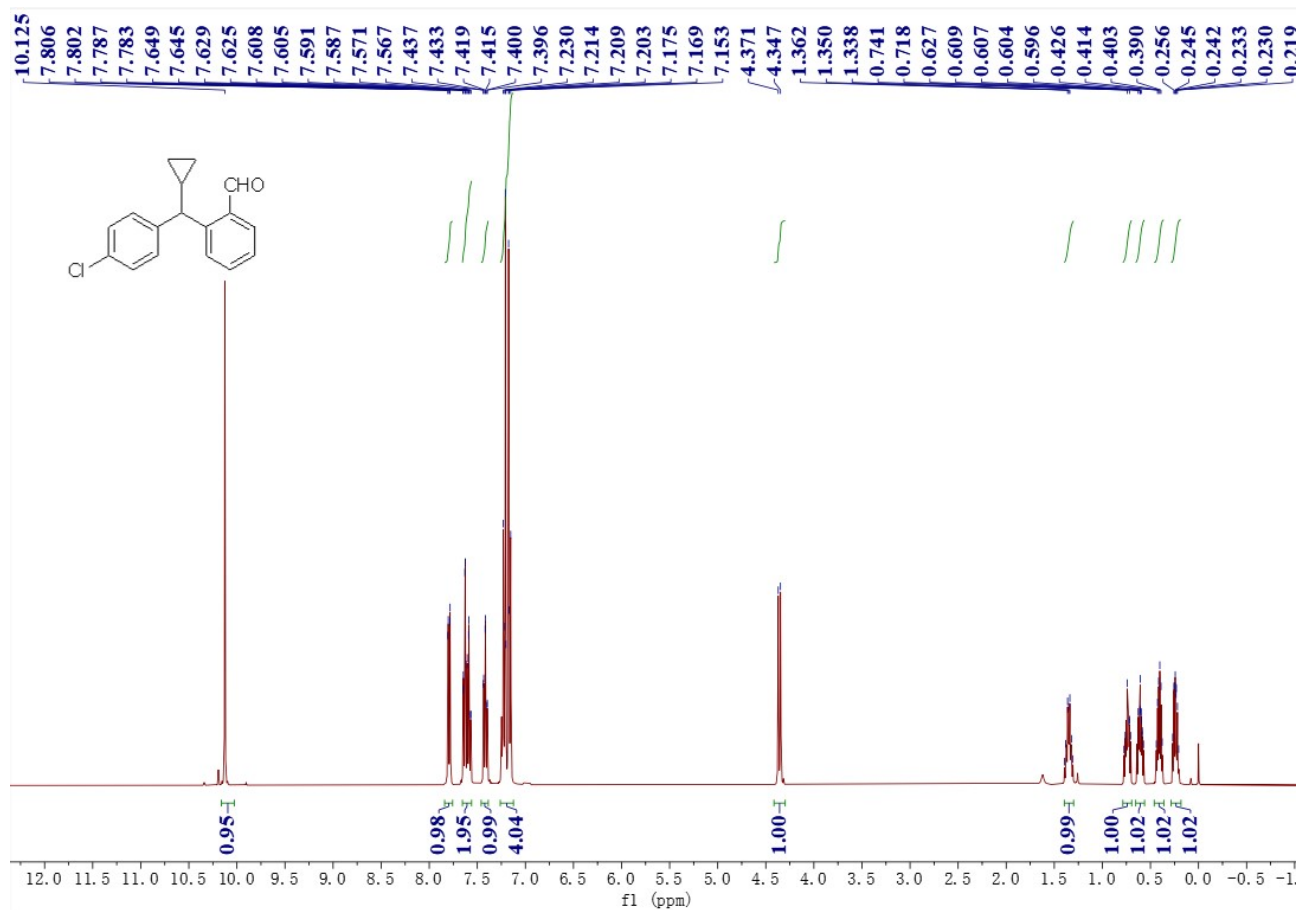


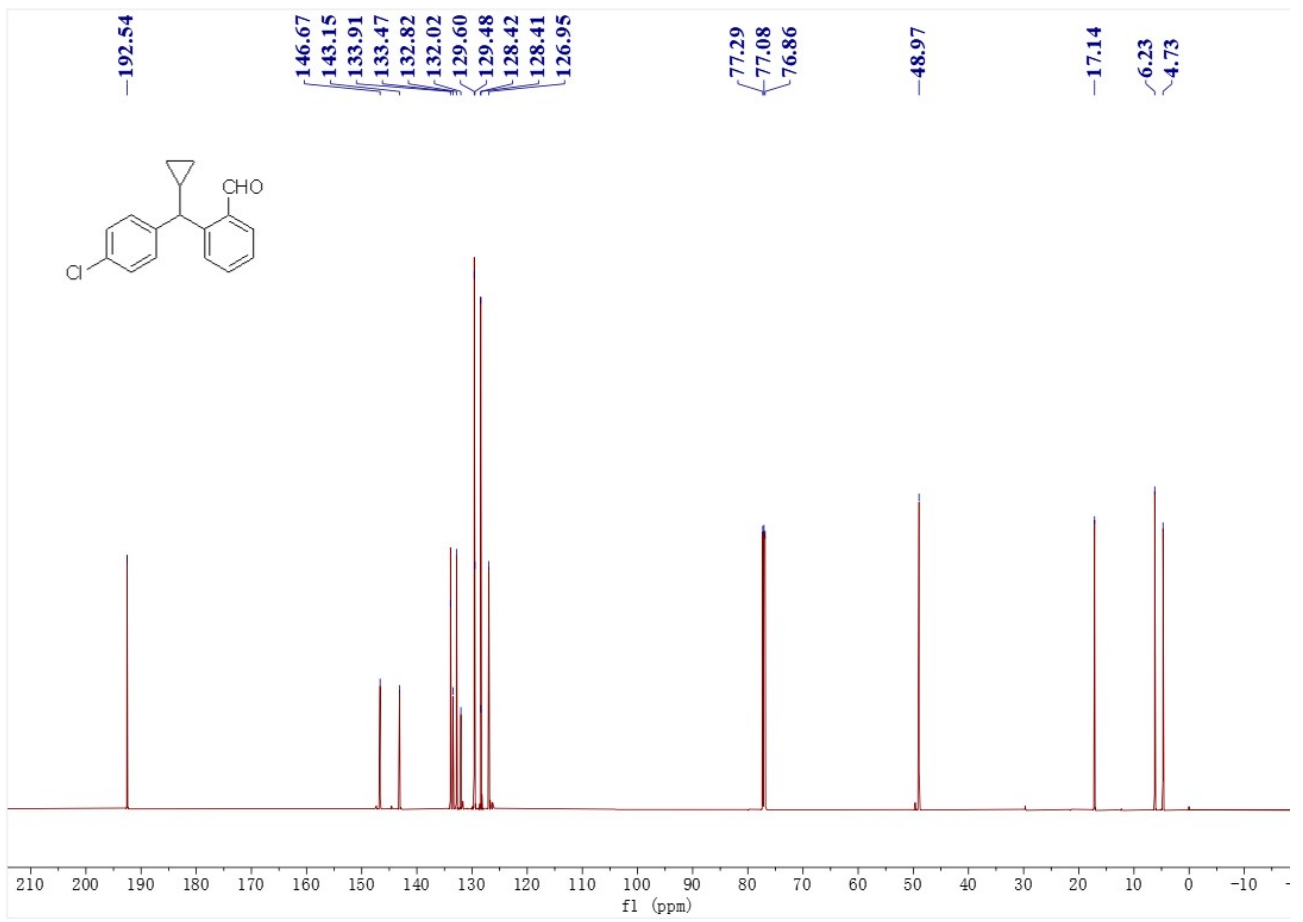


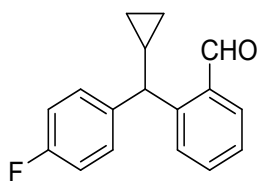


2-((4-chlorophenyl)(cyclopropyl)methyl)benzaldehyde (2t)

A colorless oil. 51.4 mg, 95% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 10.13 (s, 1H), 7.81-7.78 (m, 1H), 7.65-7.57 (m, 2H), 7.42 (td, $J = 7.4, 1.4$ Hz, 1H), 7.23-7.15 (m, 4H), 4.36 (d, $J = 9.4$ Hz, 1H), 1.36-1.34 (m, 1H), 0.74-0.63 (m, 1H), 0.61-0.60 (m, 1H), 0.43-0.39 (m, 1H), 0.26-0.22 (m, 1H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 192.5, 146.7, 143.2, 133.9, 133.5, 132.8, 132.0, 129.6, 129.5, 128.42, 128.41, 126.9, 49.0, 17.1, 6.2, 4.7. IR (acetone) ν 3073, 3001, 2857, 2740, 1692, 1573, 1450, 1020, 870, 657 cm^{-1} HRMS (EI) calcd. for $\text{C}_{17}\text{H}_{15}\text{ClO}$ (M^+): 270.0806, Found: 270.0801.

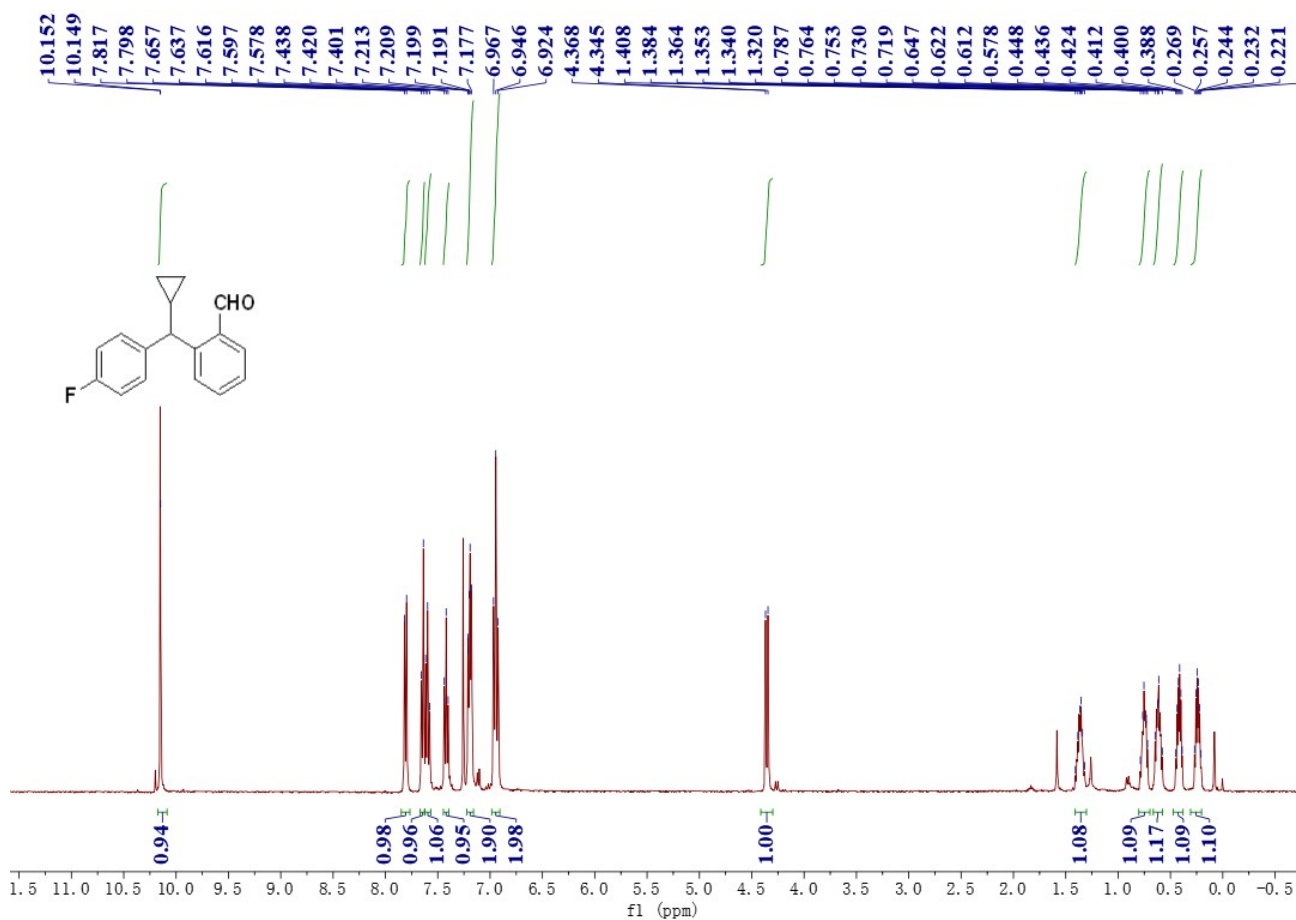


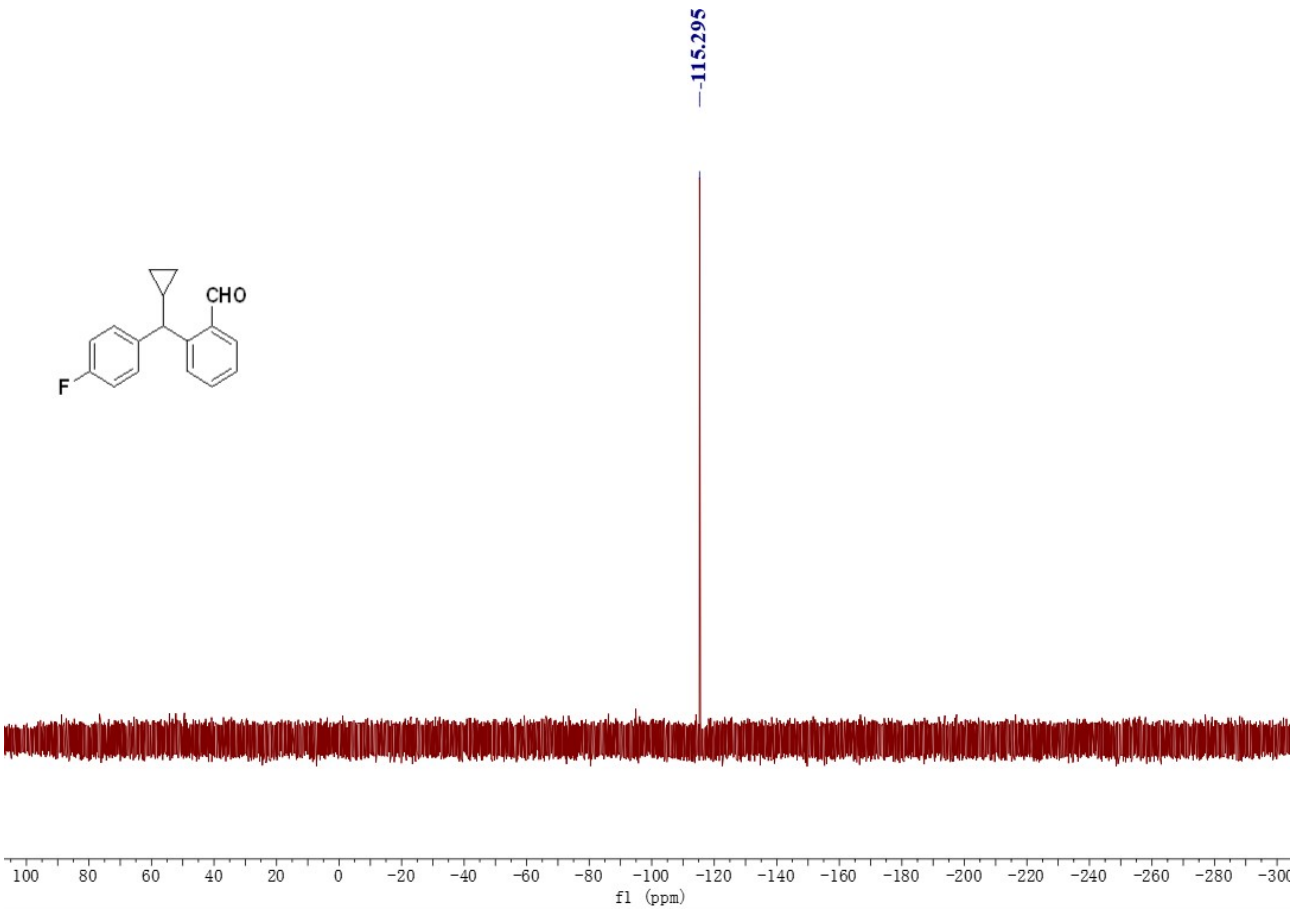
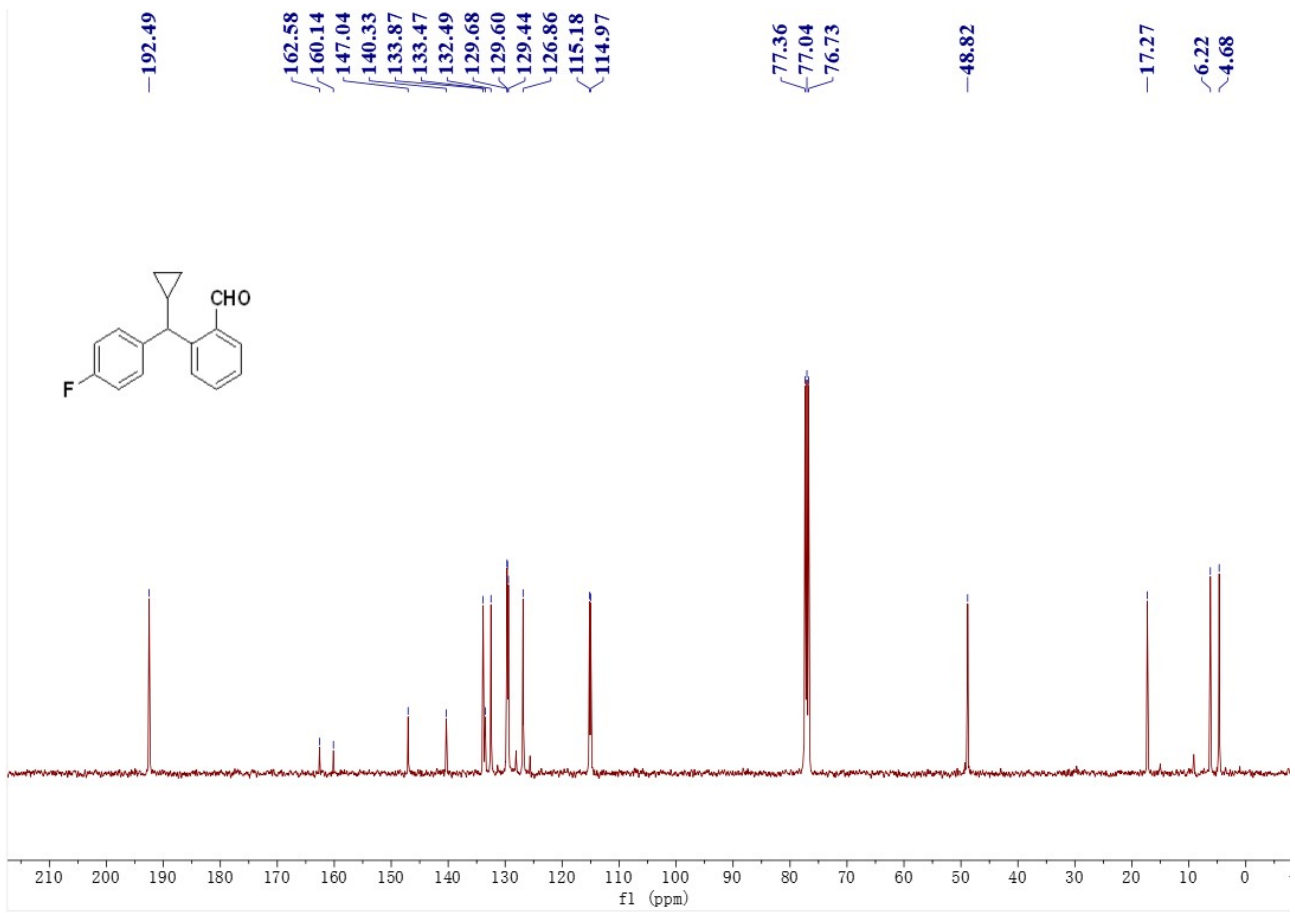


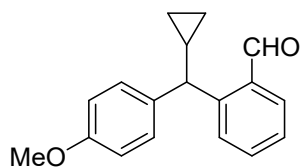


2-(cyclopropyl(4-fluorophenyl)methyl)benzaldehyde (2u)

A colorless oil. 38.7 mg, 76% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 10.15 (s, 1H), 7.81 (d, $J = 7.6$ Hz, 1H), 7.65 (d, $J = 7.6$ Hz, 1H), 7.60 (t, $J = 7.6$ Hz, 1H), 7.42 (t, $J = 7.6$ Hz, 1H), 7.21-7.18 (m, 2H), 6.95 (t, $J = 8.8$ Hz, 1H), 4.36 (d, $J = 9.4$ Hz, 1H), 1.41-1.32 (m, 1H), 0.79-0.72 (m, 1H), 0.65-0.58 (m, 1H), 0.45-0.39 (m, 1H), 0.27-0.21 (m, 1H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 192.5, 161.4 (d, $J = 246.4$ Hz), 147.0, 140.3, 133.9, 133.5, 132.5, 129.6 (d, $J = 8$ Hz), 129.4, 126.9, 115.1 (d, $J = 21$ Hz), 48.8, 17.3, 6.2, 4.7. ^{19}F NMR (376 MHz, CDCl_3) δ -115.3. IR (acetone) ν 3063, 3001, 2860, 1690, 1597, 1572, 1450, 1408, 1019, 871, 699 cm^{-1} HRMS (EI) calcd. for $\text{C}_{17}\text{H}_{15}\text{FO}$ (M^+): 254.1101, Found: 254.1105.

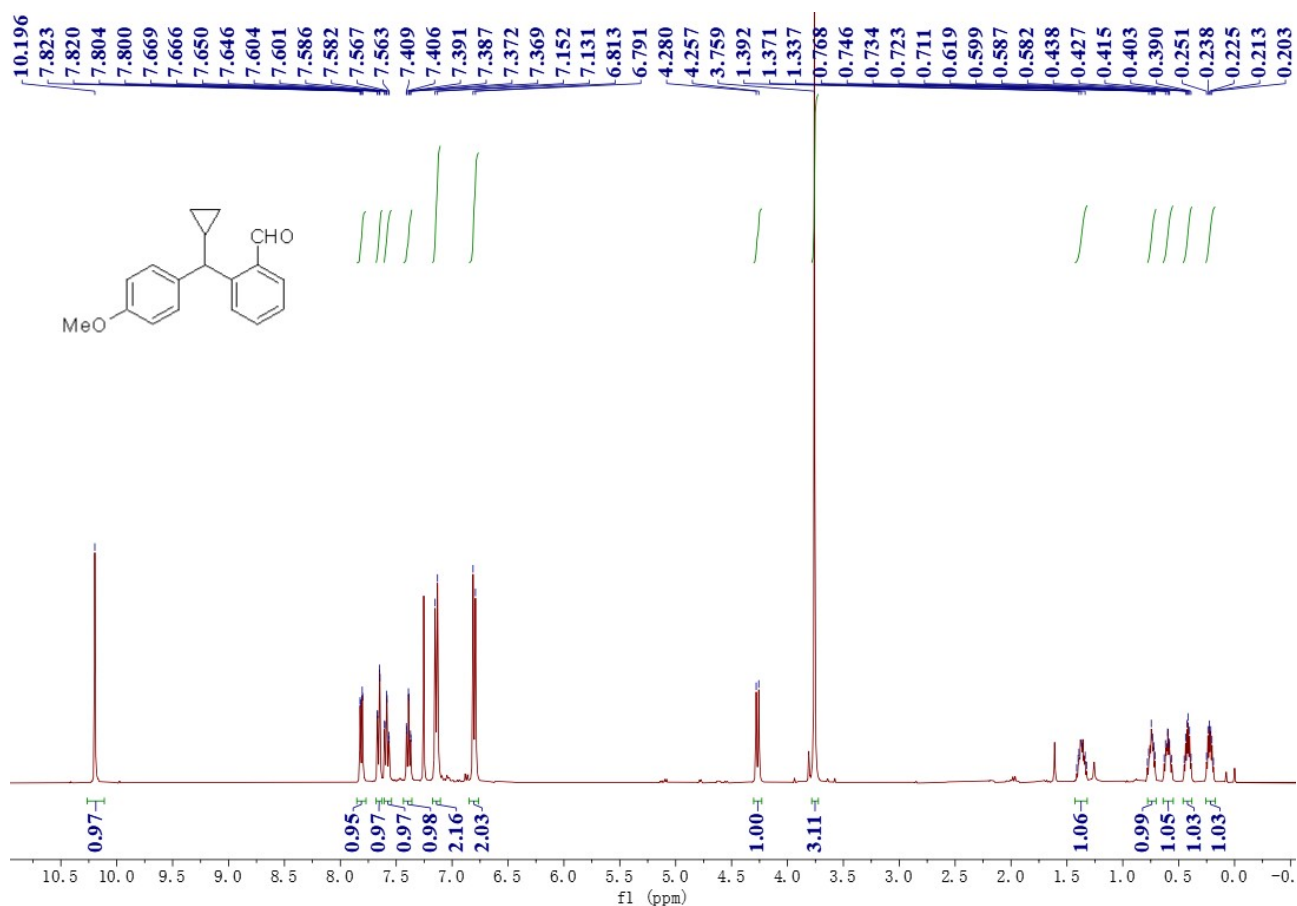


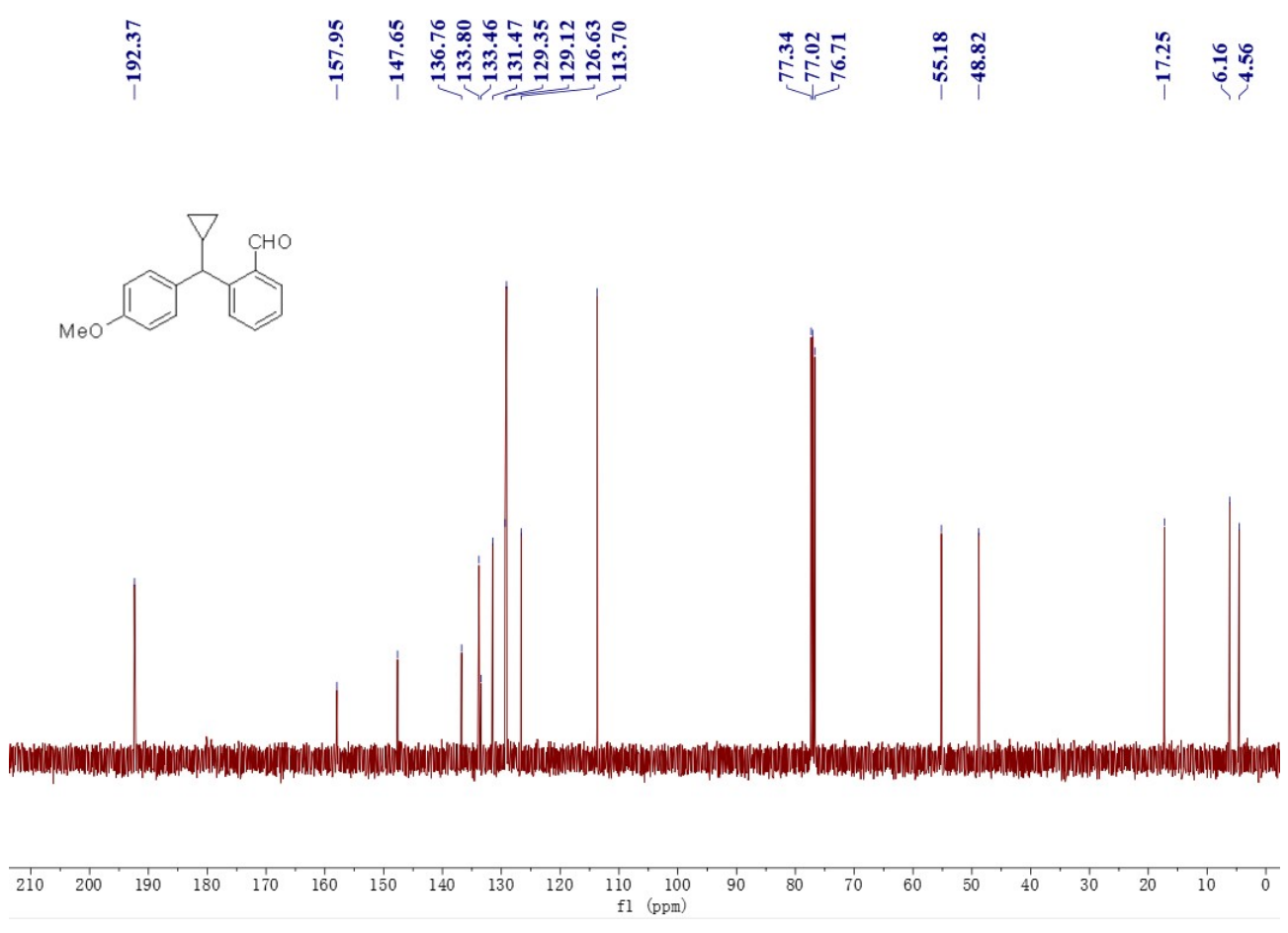
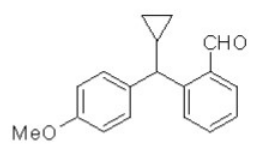


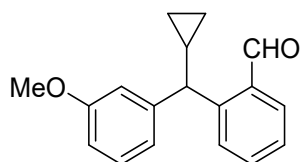


2-(cyclopropyl(4-methoxyphenyl)methyl)benzaldehyde (2v)

A colorless oil. 43.6 mg, 82% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 10.20 (s, 1H), 7.81 (dd, $J = 7.6, 1.6$ Hz, 1H), 7.66 (dd, $J = 7.6, 1.4$ Hz, 1H), 7.58 (td, $J = 7.6, 1.6$ Hz, 1H), 7.39 (td, $J = 7.4, 1.4$ Hz, 1H), 7.14 (d, $J = 8.6$ Hz, 2H), 6.80 (d, $J = 8.6$ Hz, 2H), 4.27 (d, $J = 9.2$ Hz, 1H), 3.76 (s, 3H), 1.41-1.32 (m, 1H), 0.78-0.71 (m, 1H), 0.63-0.56 (m, 1H), 0.45-0.39 (m, 1H), 0.25-0.19 (m, 1H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 192.4, 157.9, 147.6, 136.8, 133.8, 133.5, 131.5, 129.4, 129.1, 126.6, 113.7, 55.2, 48.8, 17.2, 6.2, 4.6. IR (acetone) ν 3002, 2955, 2835, 1693, 1491, 1463, 1248, 1035, 758, 700 cm^{-1} . HRMS (EI) calcd. for $\text{C}_{18}\text{H}_{18}\text{O}_2$ (M^+): 266.1301, Found: 266.1303.

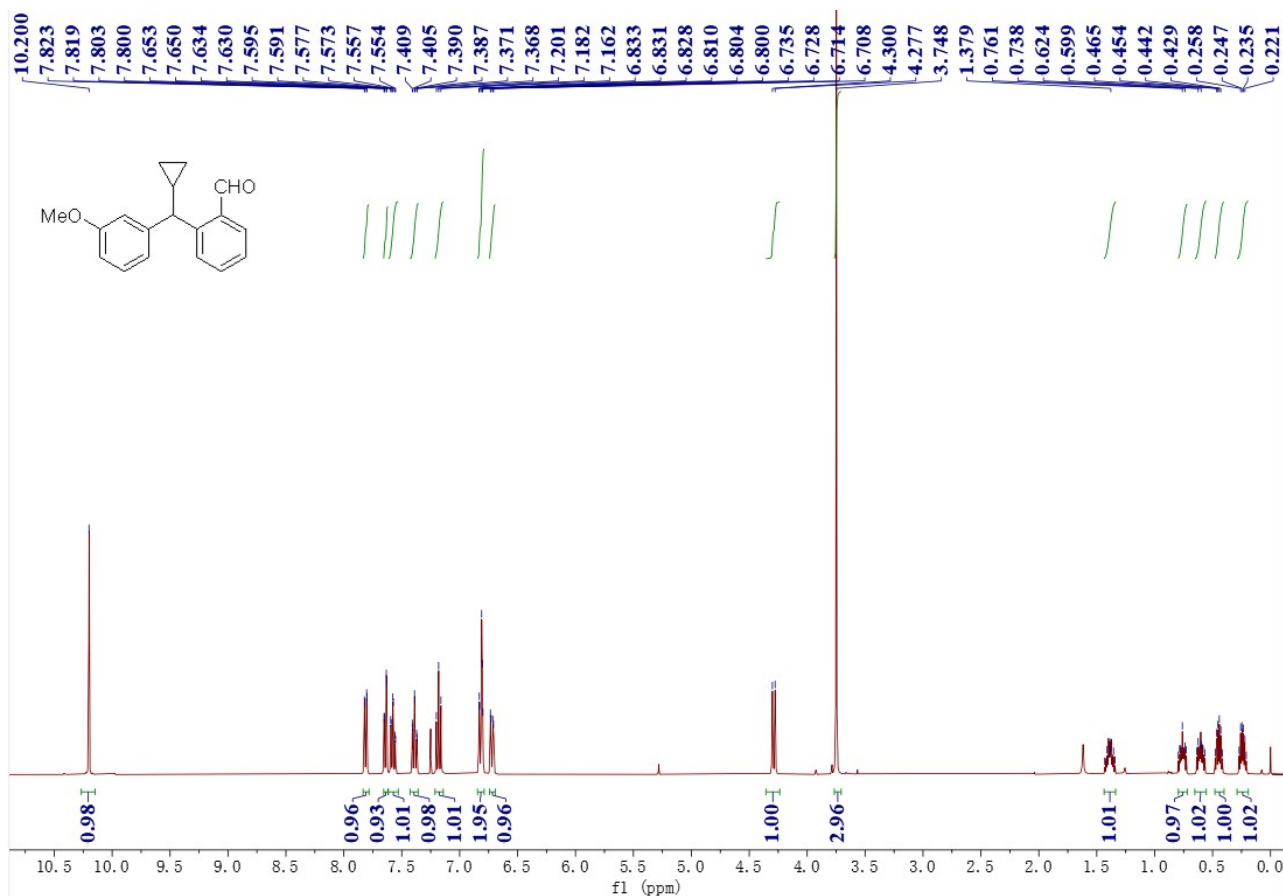


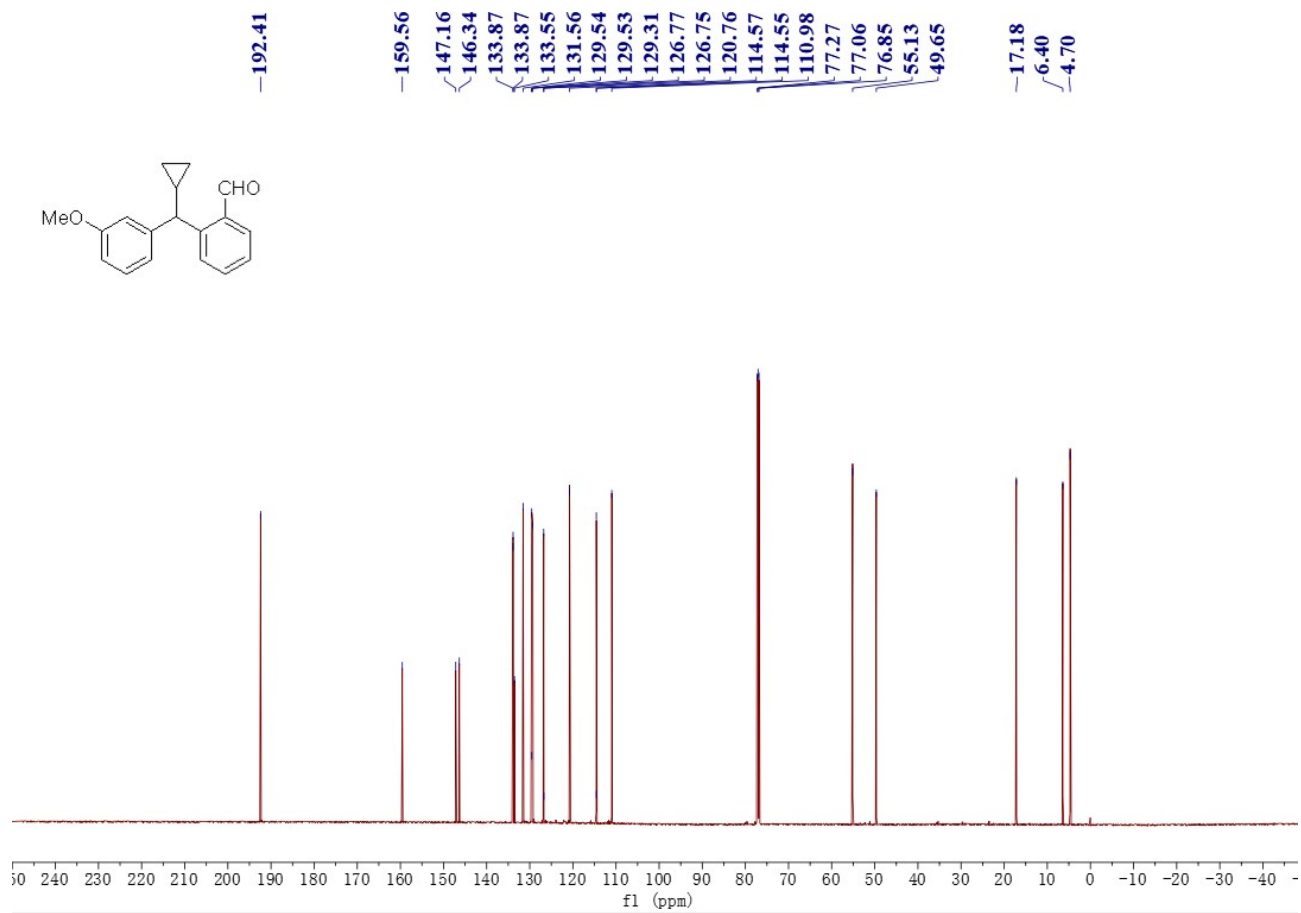
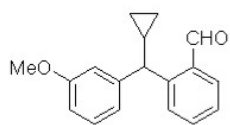


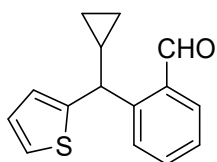


2-(cyclopropyl(3-methoxyphenyl)methyl)benzaldehyde (2w)

A colorless oil. 31.9 mg, 60% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 10.20 (s, 1H), 7.81 (dd, $J = 7.8, 1.6$ Hz, 1H), 7.64 (dd, $J = 7.8, 1.4$ Hz, 1H), 7.57 (td, $J = 7.6, 1.6$ Hz, 1H), 7.39 (td, $J = 7.6, 1.4$ Hz, 1H), 7.18 (t, $J = 8.0$ Hz, 1H), 6.83-6.80 (m, 2H), 6.72 (dd, $J = 8.2, 2.6$ Hz, 1H), 4.29 (d, $J = 9.4$ Hz, 1H), 3.75 (s, 3H), 1.43-1.34 (m, 1H), 0.80-0.73 (m, 1H), 0.64-0.57 (m, 1H), 0.48-0.42 (m, 1H), 0.27-0.21 (m, 1H). ^{13}C NMR (CDCl_3 , TMS, 150 MHz) δ 192.4, 159.6, 147.2, 146.3, 134.0, 133.9, 133.5, 131.6, 129.54, 129.53, 129.3, 126.8, 126.7, 120.8, 114.6, 114.5, 111.0, 55.1, 49.7, 17.2, 6.4, 4.7. IR (acetone) ν 3071, 2955, 2835, 1693, 1490, 1463, 1179, 1109, 758, 700 cm^{-1} . HRMS (EI) calcd. for $\text{C}_{18}\text{H}_{18}\text{O}_2$ (M^+): 266.1301, Found: 266.1298.

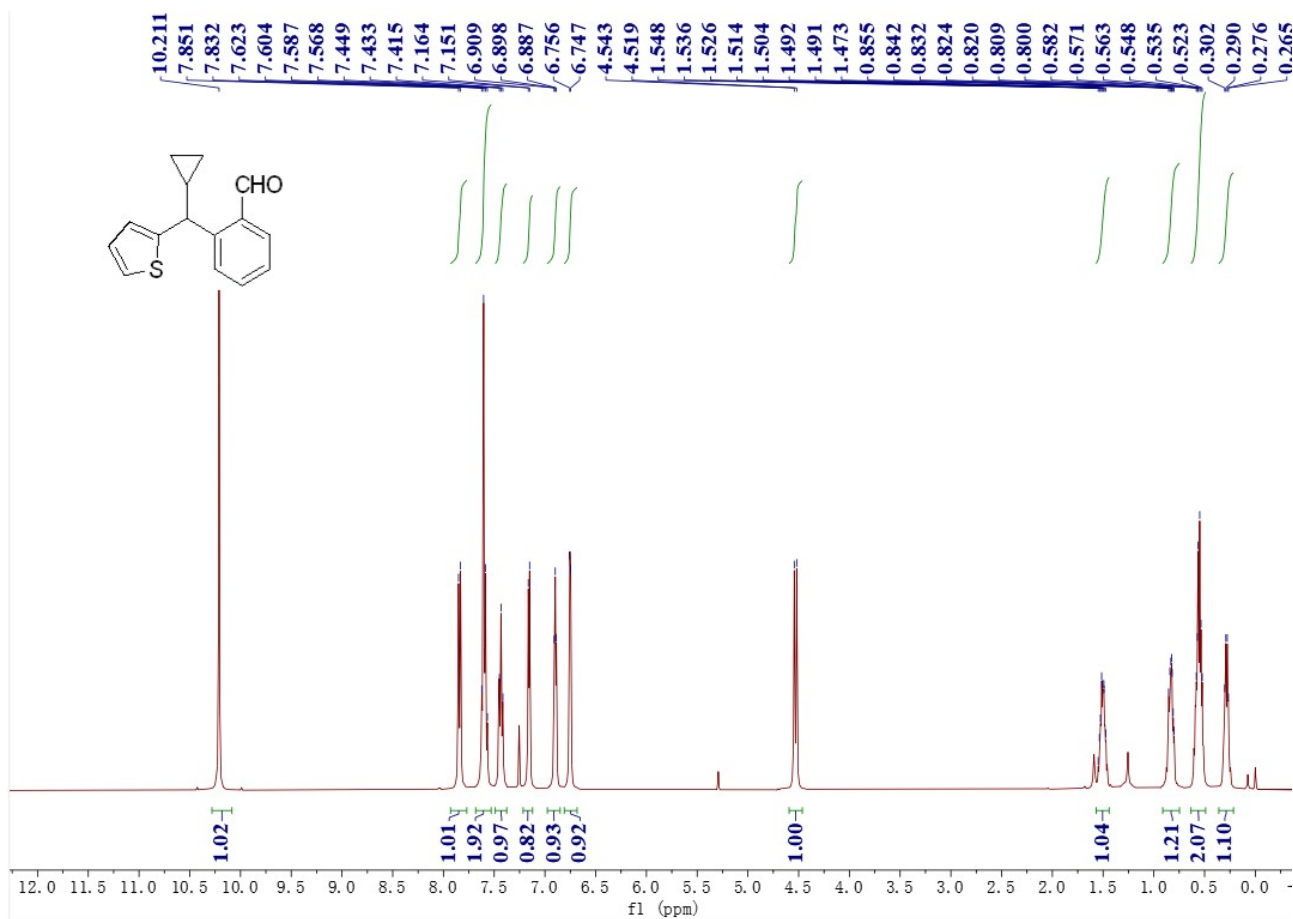


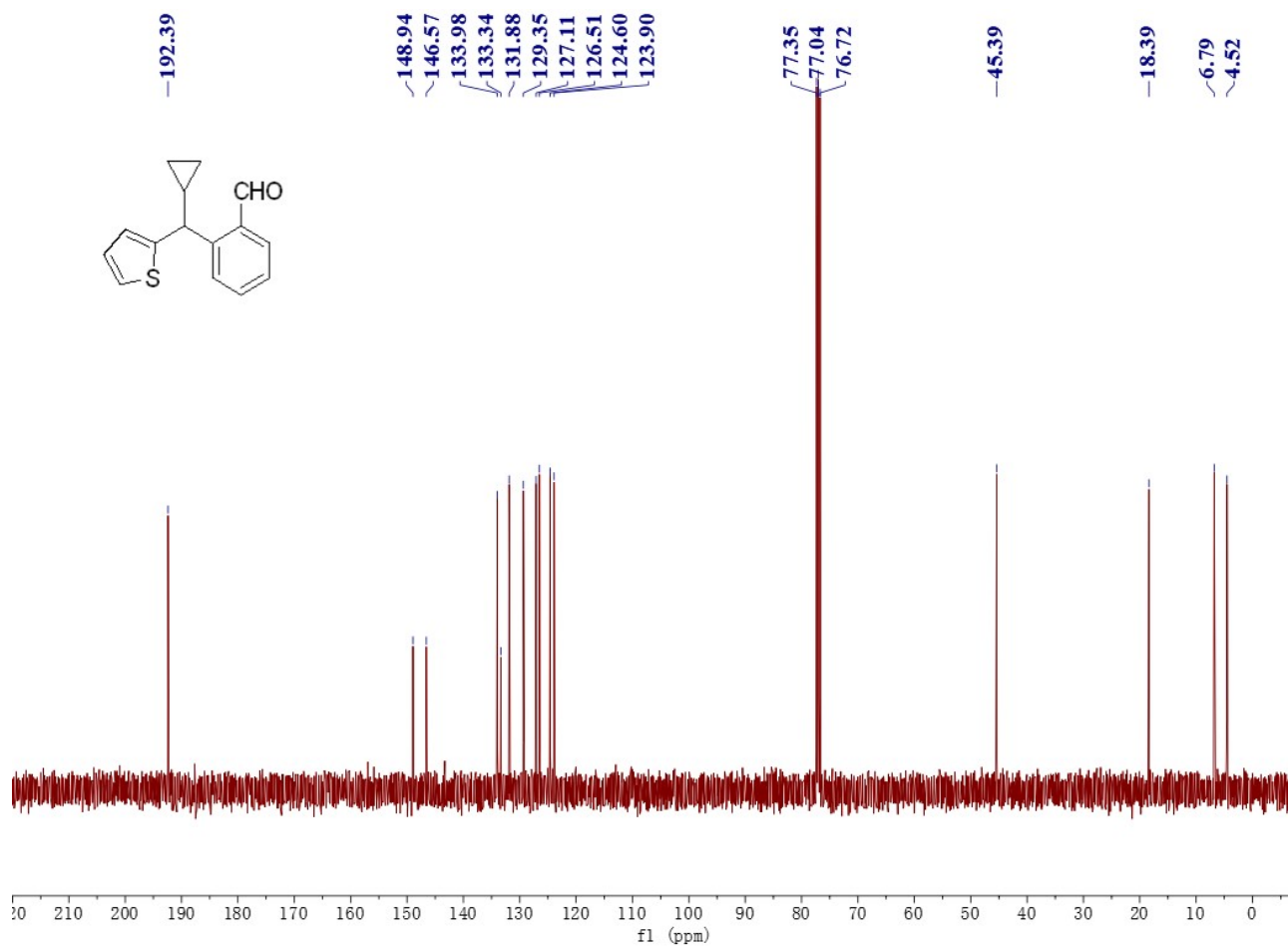


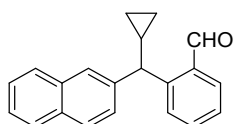


2-(cyclopropyl(thiophen-2-yl)methyl)benzaldehyde (2x)

A colorless oil. 41.2 mg, 85% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 10.21 (s, 1H), 7.84 (d, $J = 7.8$ Hz, 1H), 7.62-7.57 (m, 2H), 7.43 (t, $J = 6.8$ Hz, 1H), 7.16 (d, $J = 5.2$ Hz, 1H), 6.90 (t, $J = 4.4$ Hz, 1H), 6.75 (d, $J = 3.8$ Hz, 1H), 4.53 (d, $J = 9.6$ Hz, 1H), 1.55-1.47 (m, H), 0.86-0.80 (m, 1H), 0.58-0.52 (m, 2H), 0.30-0.27 (m, 1H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 192.4, 148.9, 146.6, 134.0, 133.3, 131.9, 129.4, 127.1, 126.5, 124.6, 123.9, 45.4, 18.4, 6.8, 4.5. IR (acetone) ν 3074, 3001, 2857, 1692, 1450, 1293, 1183, 1020, 750, 696 cm^{-1} . HRMS (EI) calcd. for $\text{C}_{15}\text{H}_{14}\text{OS}$ (M^+): 242.0760, Found: 242.0763.

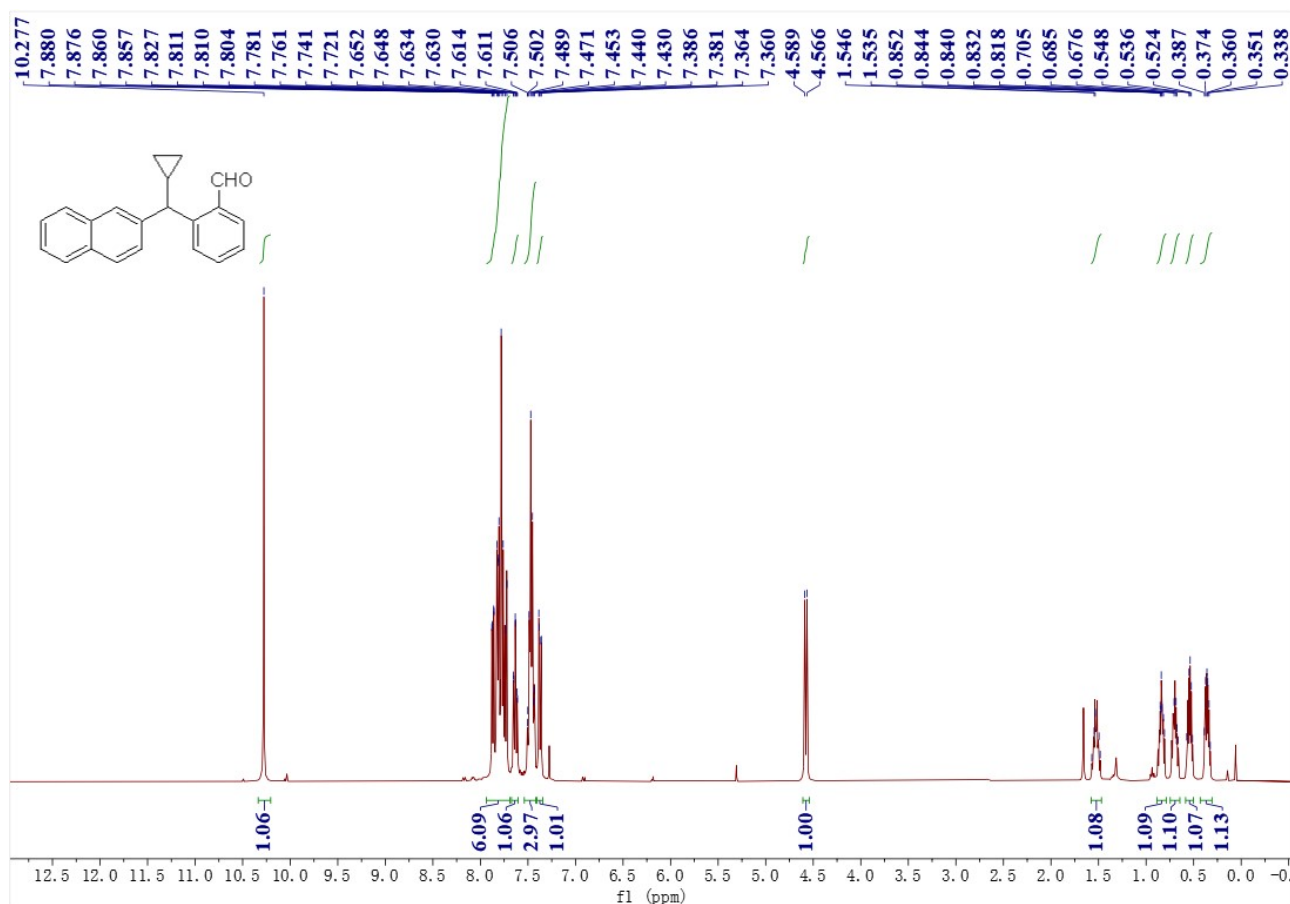


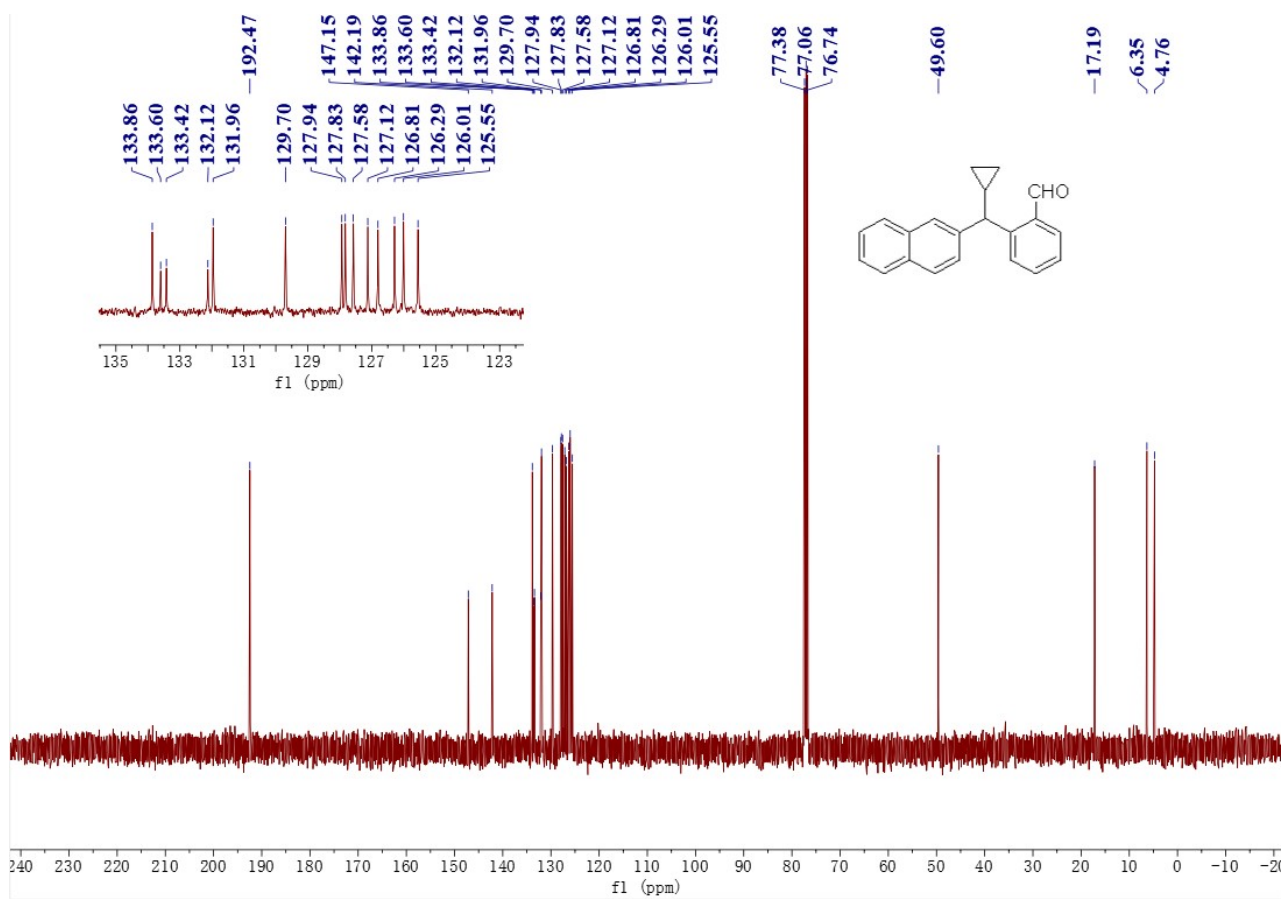


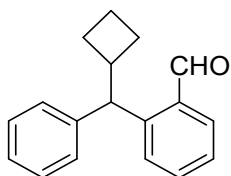


2-(cyclopropyl(naphthalen-2-yl)methyl)benzaldehyde (2y)

A colorless oil. 40.1 mg, 70% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 10.28 (s, 1H), 7.88-7.72 (m, 6H), 7.63 (td, $J = 7.6, 1.6$ Hz, 1H), 7.51-7.43 (m, 3H), 7.37 (dd, $J = 8.6, 1.8$ Hz, 1H), 4.58 (d, $J = 9.4$ Hz, 1H), 1.57-1.48 (m, 1H), 0.85-0.81 (m, 1H), 0.71-0.66 (m, 1H), 0.57-0.51 (m, 1H), 0.39-0.33 (m, 1H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 192.5, 147.1, 142.2, 133.9, 133.6, 133.4, 132.1, 132.0, 129.7, 127.9, 127.8, 127.6, 127.1, 126.8, 126.3, 126.0, 125.6, 49.6, 17.2, 6.3, 4.8. IR (acetone) ν 3057, 3001, 2855, 1691, 1507, 1291, 1201, 1019, 750, 661 cm^{-1} . HRMS (EI) calcd. for $\text{C}_{21}\text{H}_{18}\text{O}$ (M^+): 286.1352, Found: 286.1345.

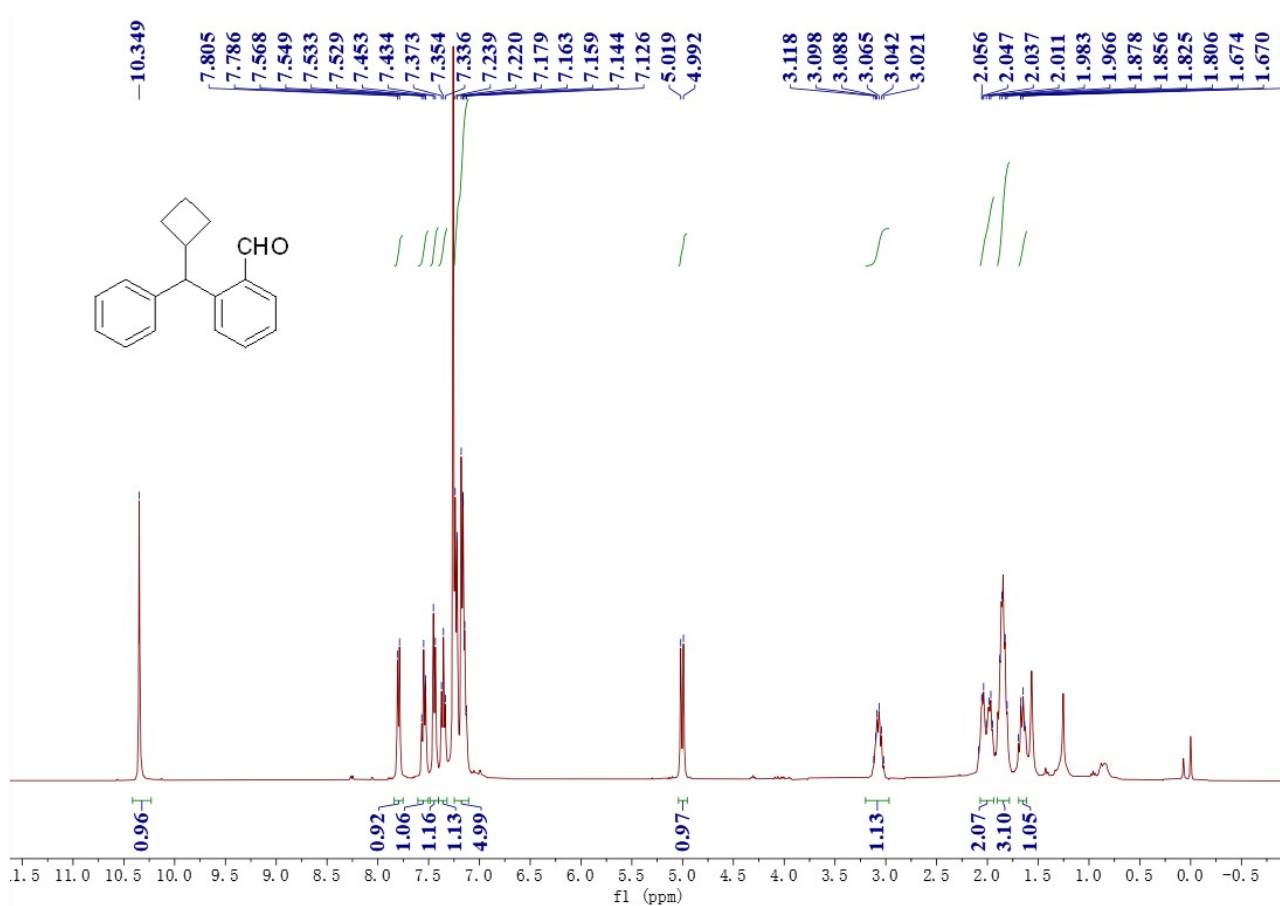


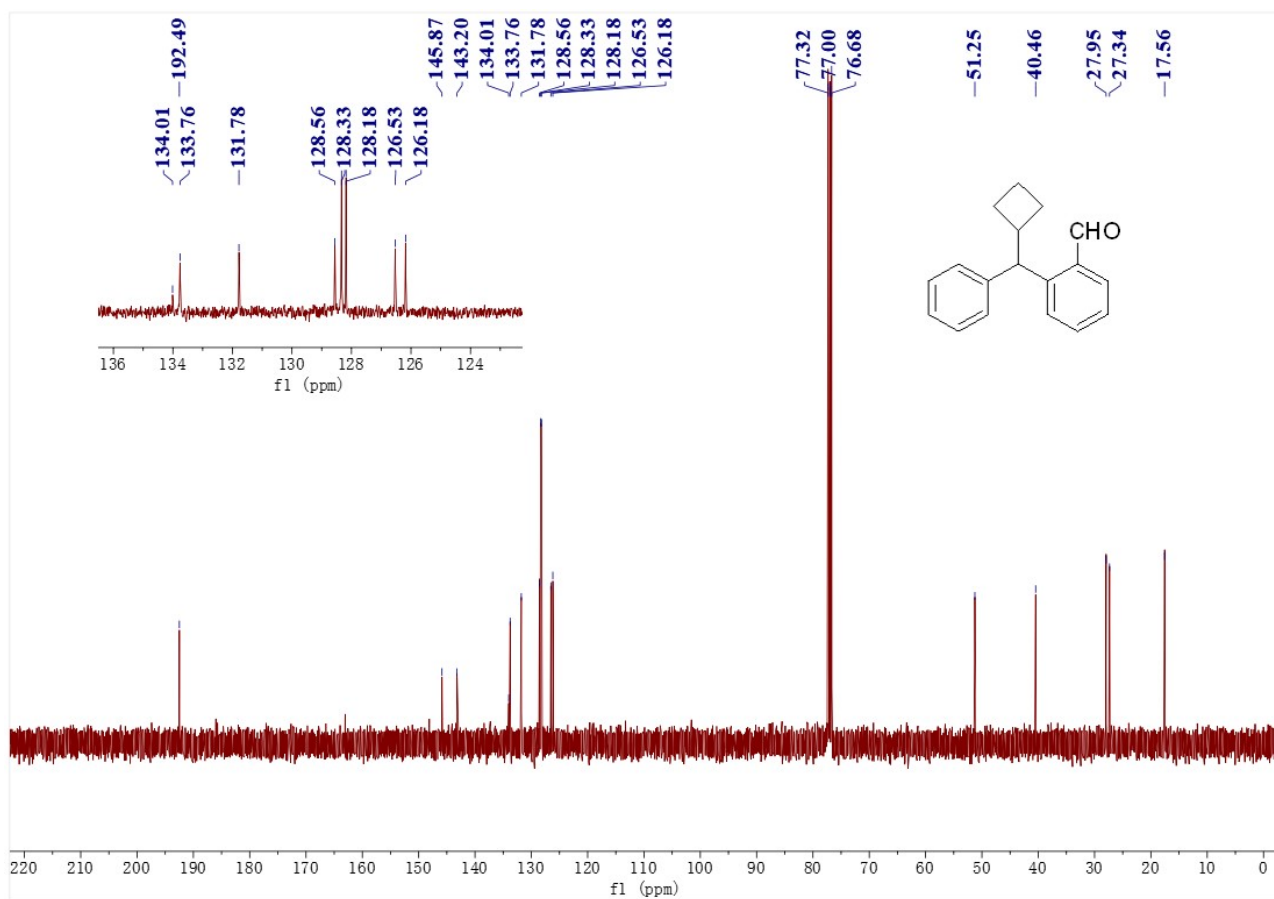


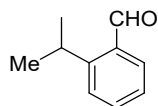


2-(cyclobutyl(phenyl)methyl)benzaldehyde (2z)

A colorless oil. 29.5 mg, 59% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 10.35 (s, 1H), 7.80 (d, $J = 7.8$ Hz, 1H), 7.55 (t, $J = 7.8$ Hz, 1H), 7.44 (d, $J = 7.8$ Hz, 1H), 7.35 (t, $J = 7.6$ Hz, 1H), 7.24-7.13 (m, 5H), 5.01 (d, $J = 10.8$ Hz, 1H), 3.12-3.02 (m, 1H), 2.09-1.95 (m, 2H), 1.89-1.81 (m, 3H), 1.69-1.63 (m, 1H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 192.5, 145.9, 143.2, 134.0, 133.8, 131.8, 128.6, 128.3, 128.2, 126.5, 126.2, 51.3, 40.5, 27.9, 27.3, 17.6. IR (acetone) ν 3063, 3026, 2856, 1690, 1494, 1290, 1206, 1030, 754, 667 cm^{-1} . HRMS (EI) calcd. for $\text{C}_{18}\text{H}_{18}\text{O}$ (M^+): 250.1352, Found: 250.1353.

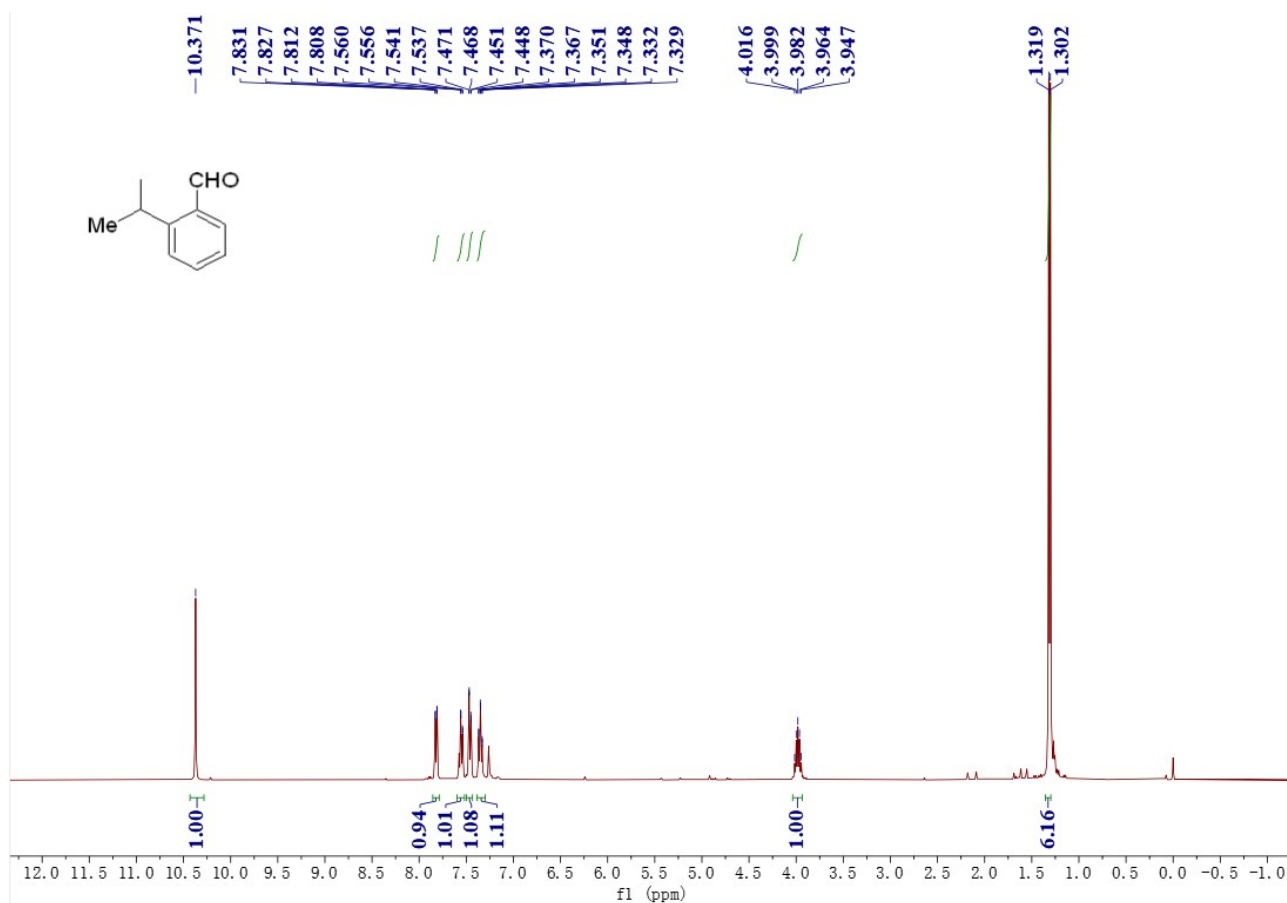


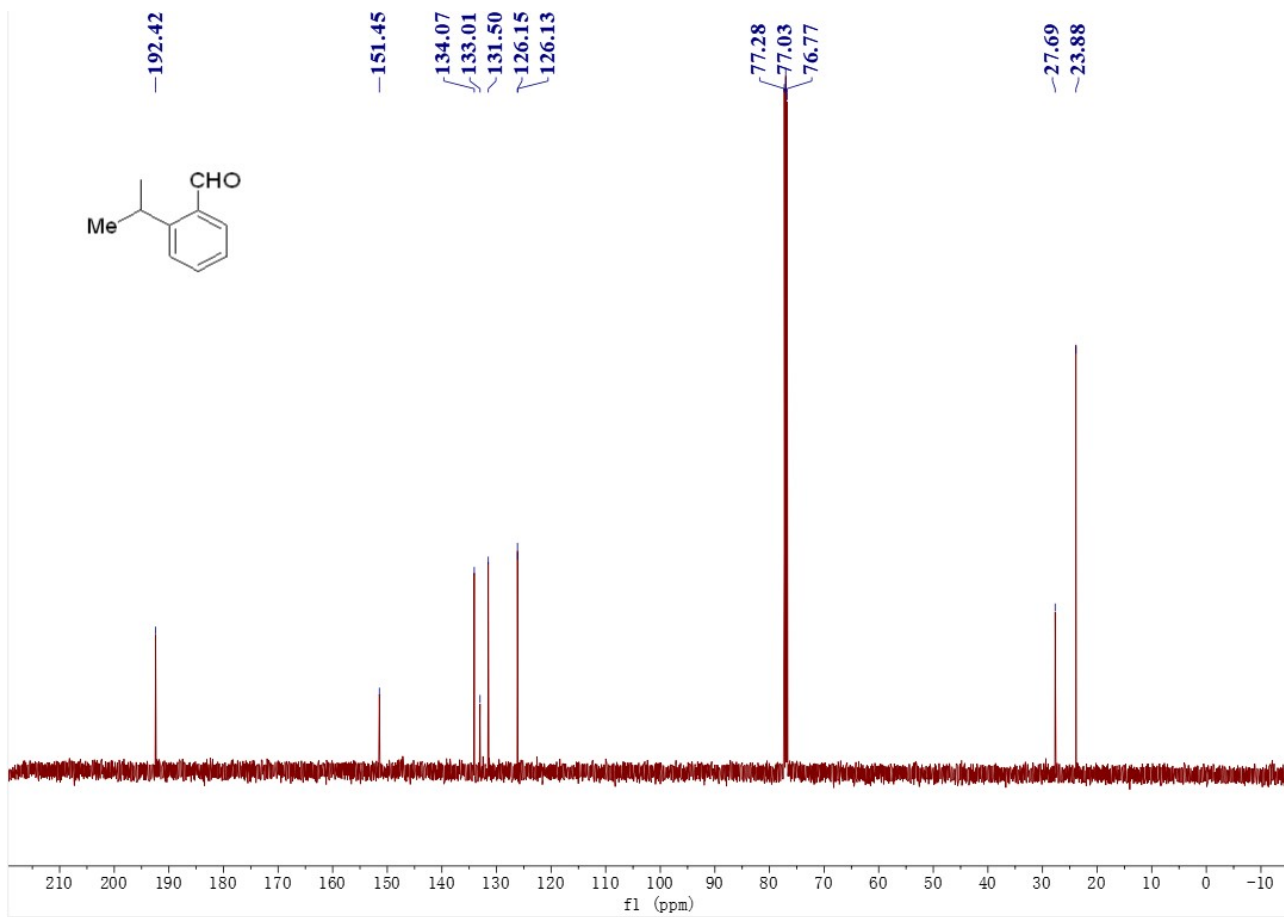


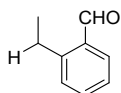


2-isopropylbenzaldehyde (2aa)

This is a known compound and its spectroscopic data are consistent with those in the previous literature.¹³ CAS number: 6502-22-3. A colorless oil. 10.1 mg, 34% yield. ¹H NMR (CDCl₃, TMS, 400 MHz) δ 10.37 (s, 1H), 7.82 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.56 (td, *J* = 7.6, 1.6 Hz, 1H), 7.46 (d, *J* = 7.8 Hz, 1H), 7.35 (t, *J* = 7.6 Hz, 1H), 4.02-3.95 (m, 1H), 1.31 (d, *J* = 6.8 Hz, 6H). ¹³C NMR (CDCl₃, TMS, 100 MHz) δ 192.4, 151.4, 134.1, 133.0, 131.5, 126.2, 126.1, 27.7, 23.9.

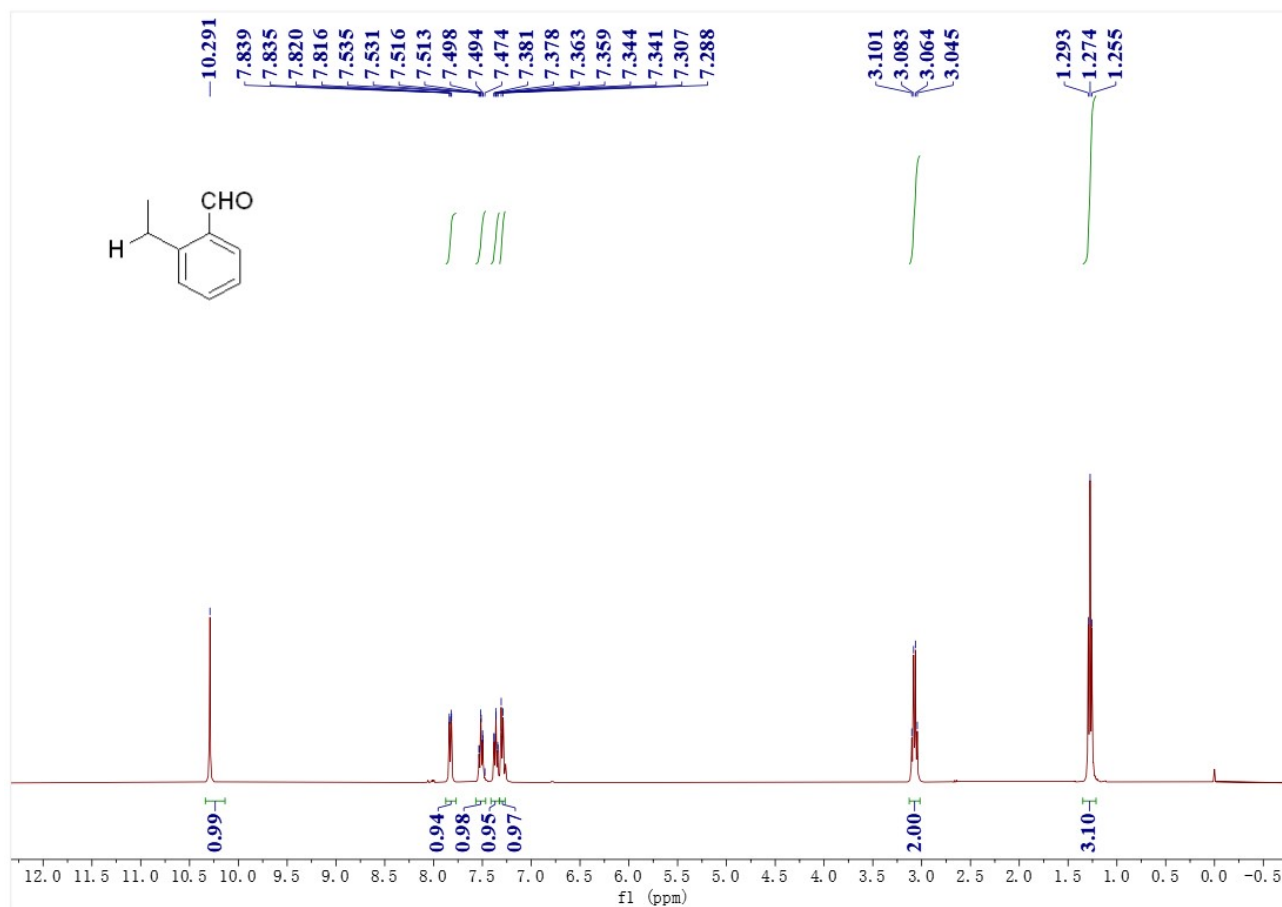


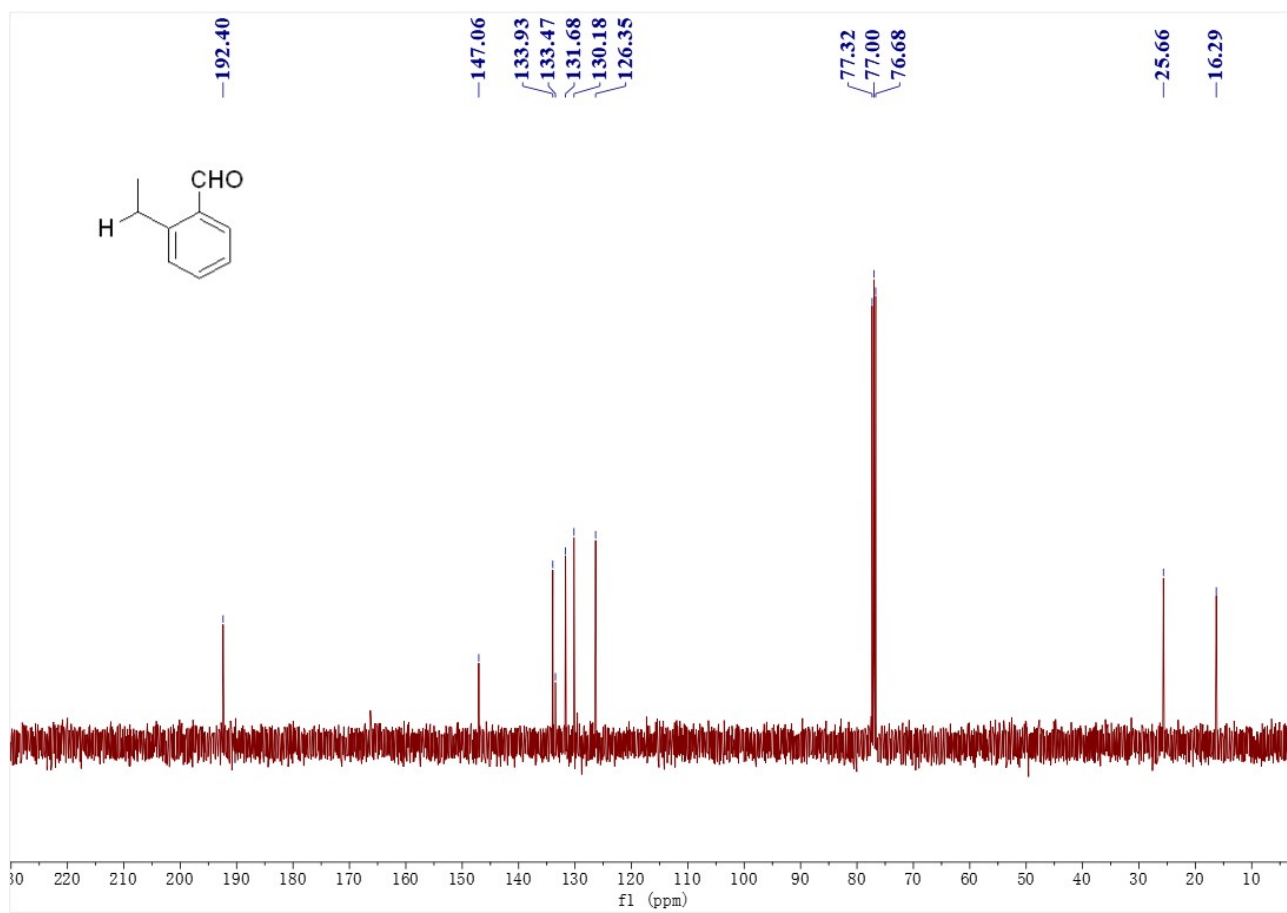


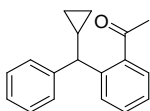


2-ethylbenzaldehyde (2ab)

This is a known compound and its spectroscopic data are consistent with those in the previous literature.¹⁴ CAS number: 22927-13-5. A colorless oil. 6.5 mg, 24% yield. ¹H NMR (CDCl₃, TMS, 400 MHz) δ 10.29 (s, 1H), 7.83 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.54-7.48 (m, 1H), 7.48-7.34 (m, 1H), 7.30 (d, *J* = 7.6 Hz, 1H), 3.07 (q, *J* = 7.6 Hz, 2H), 1.27 (t, *J* = 7.6 Hz, 3H). ¹³C NMR (CDCl₃, TMS, 100 MHz) δ 192.4, 147.1, 133.9, 133.5, 131.7, 130.2, 126.3, 25.7, 16.3.

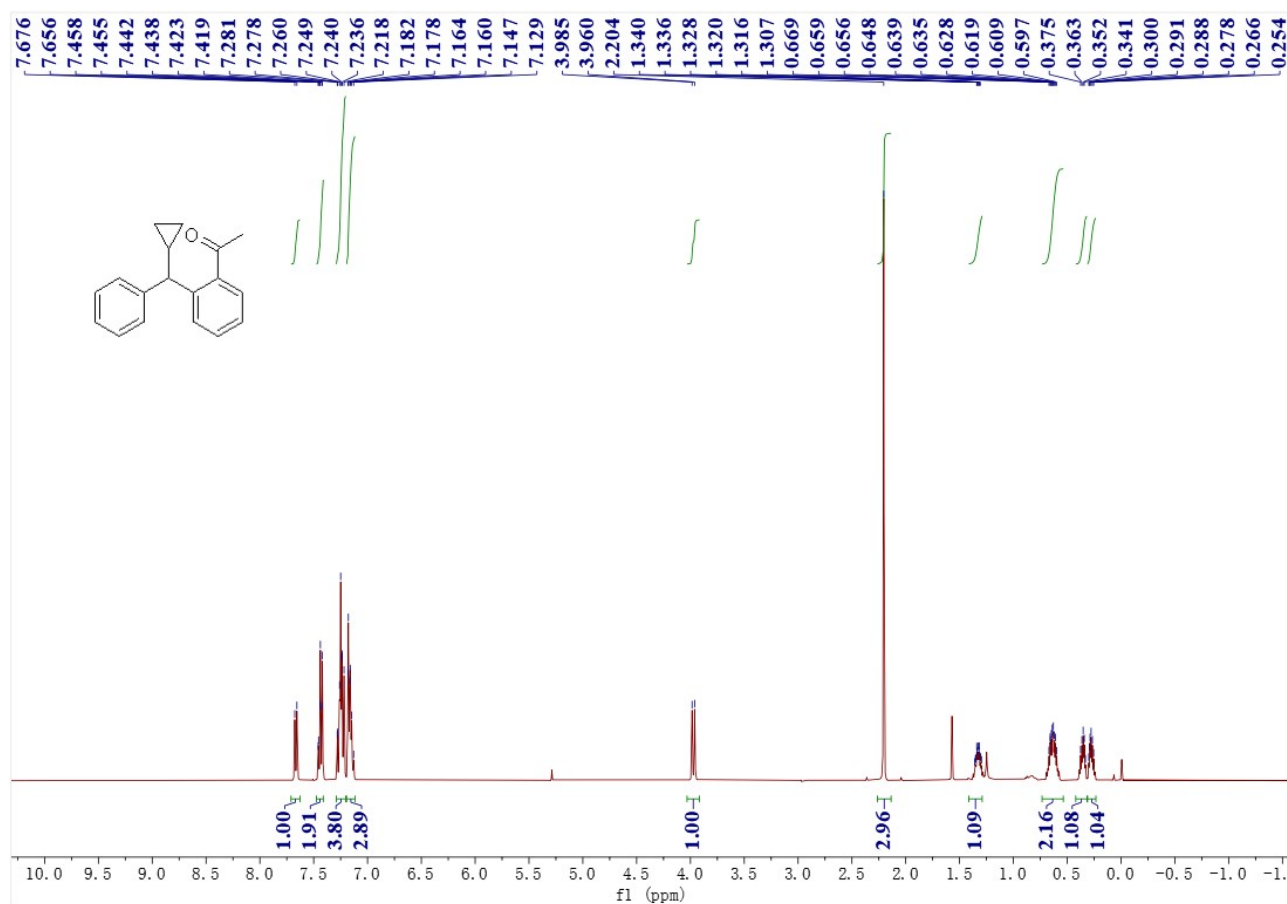


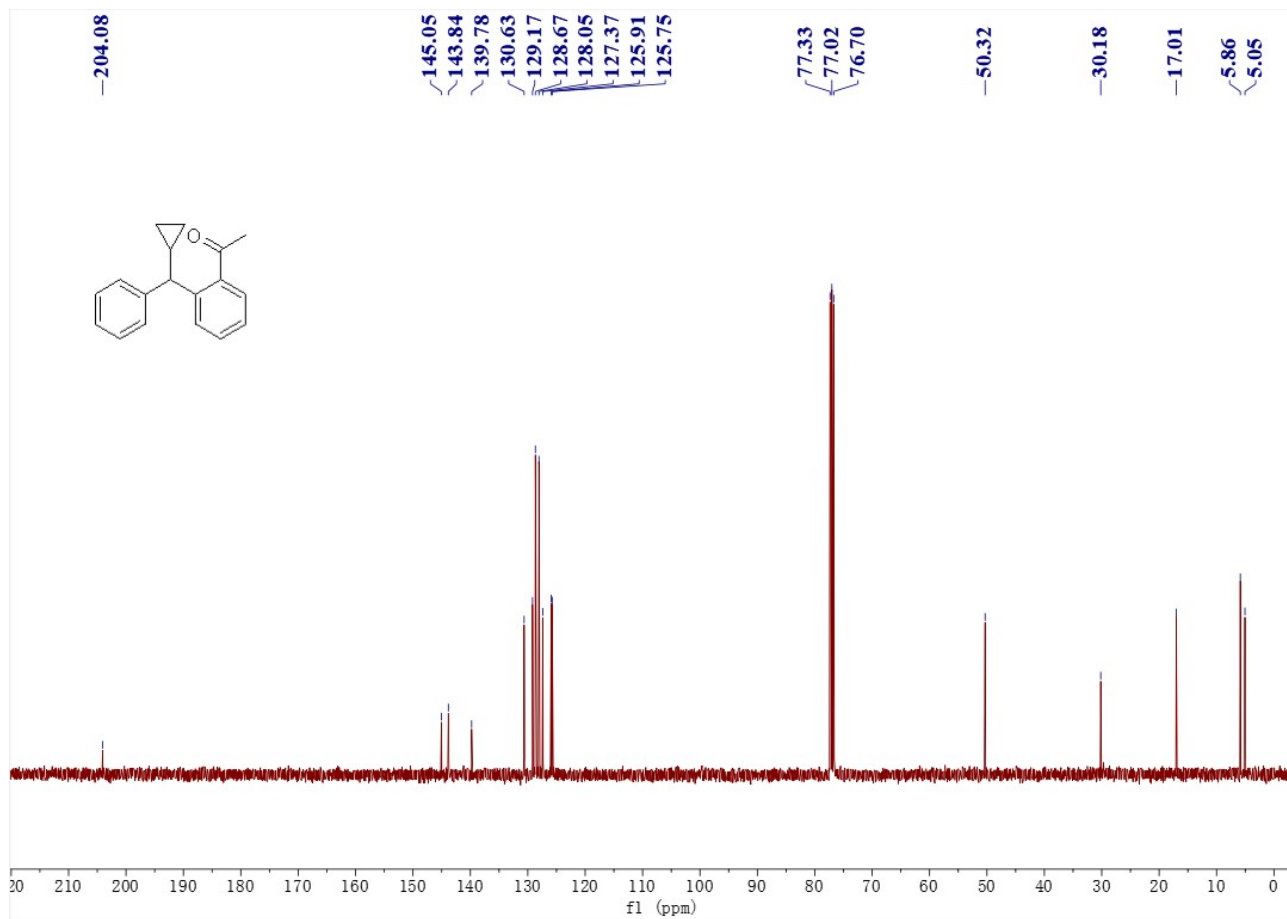


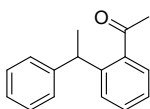


1-(2-(cyclopropyl(phenyl)methyl)phenyl)ethan-1-one (2ac)

A colorless oil. 30.0 mg, 60% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.67 (d, $J = 8.0$ Hz, 1H), 7.46-7.42 (m, 2H), 7.28-7.22 (m, 4H), 7.18-7.13 (m, 3H), 3.97 (d, $J = 9.8$ Hz, 1H), 2.20 (s, 3H), 1.36-1.20 (m, 1H), 0.70-0.60 (m, 2H), 0.38-0.33 (m, 1H), 0.30-0.25 (m, 1H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 204.1, 145.1, 143.8, 139.8, 130.6, 129.2, 128.7, 128.1, 127.4, 125.9, 125.7, 50.3, 30.2, 17.0, 5.9, 5.1. IR (acetone) ν 3063, 3025, 2857, 1692, 1492, 1252, 1072, 1019, 738, 700 cm^{-1} . HRMS (EI) calcd. for $\text{C}_{18}\text{H}_{18}\text{O}$ (M^+): 250.1352, Found: 250.1353.

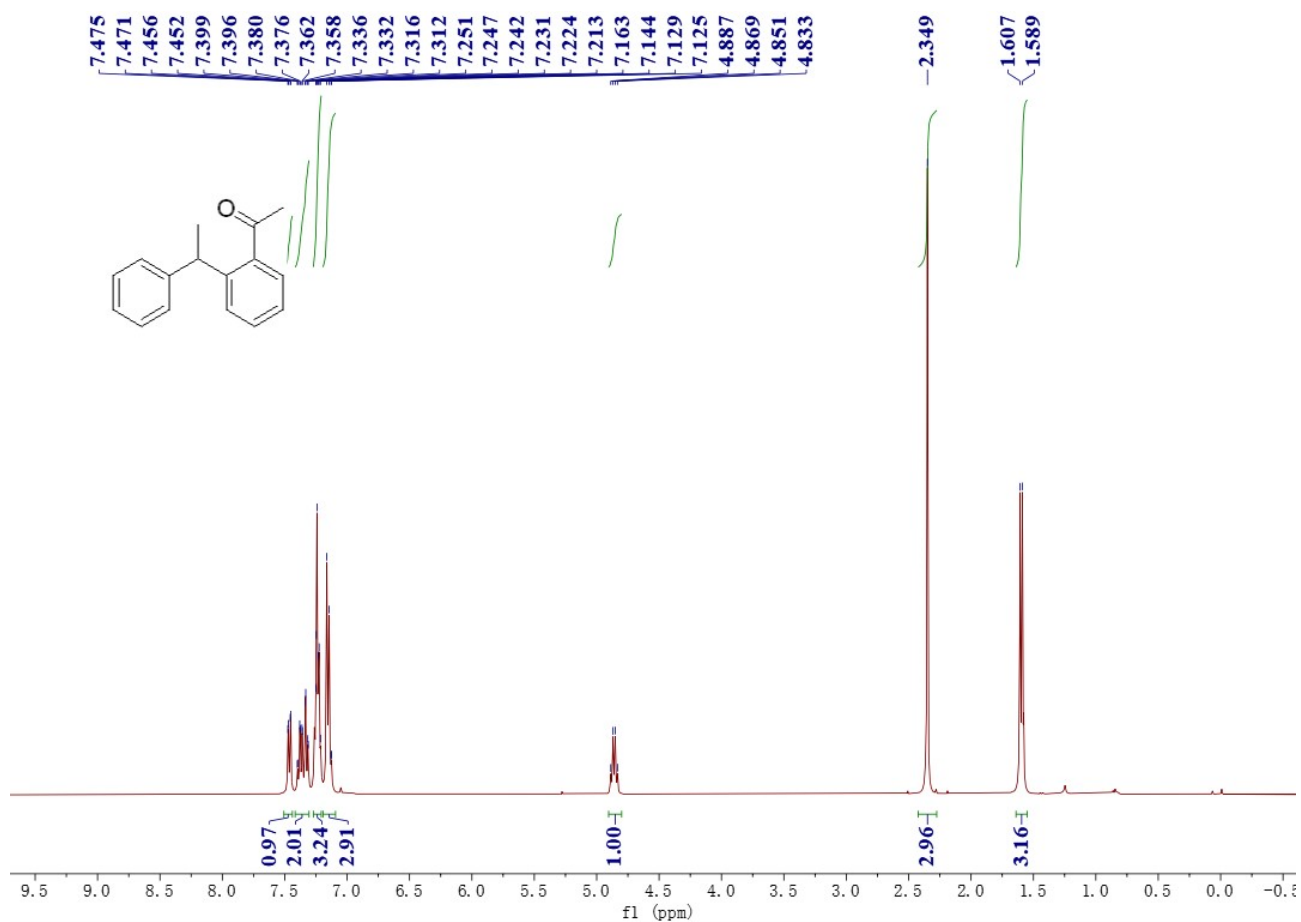


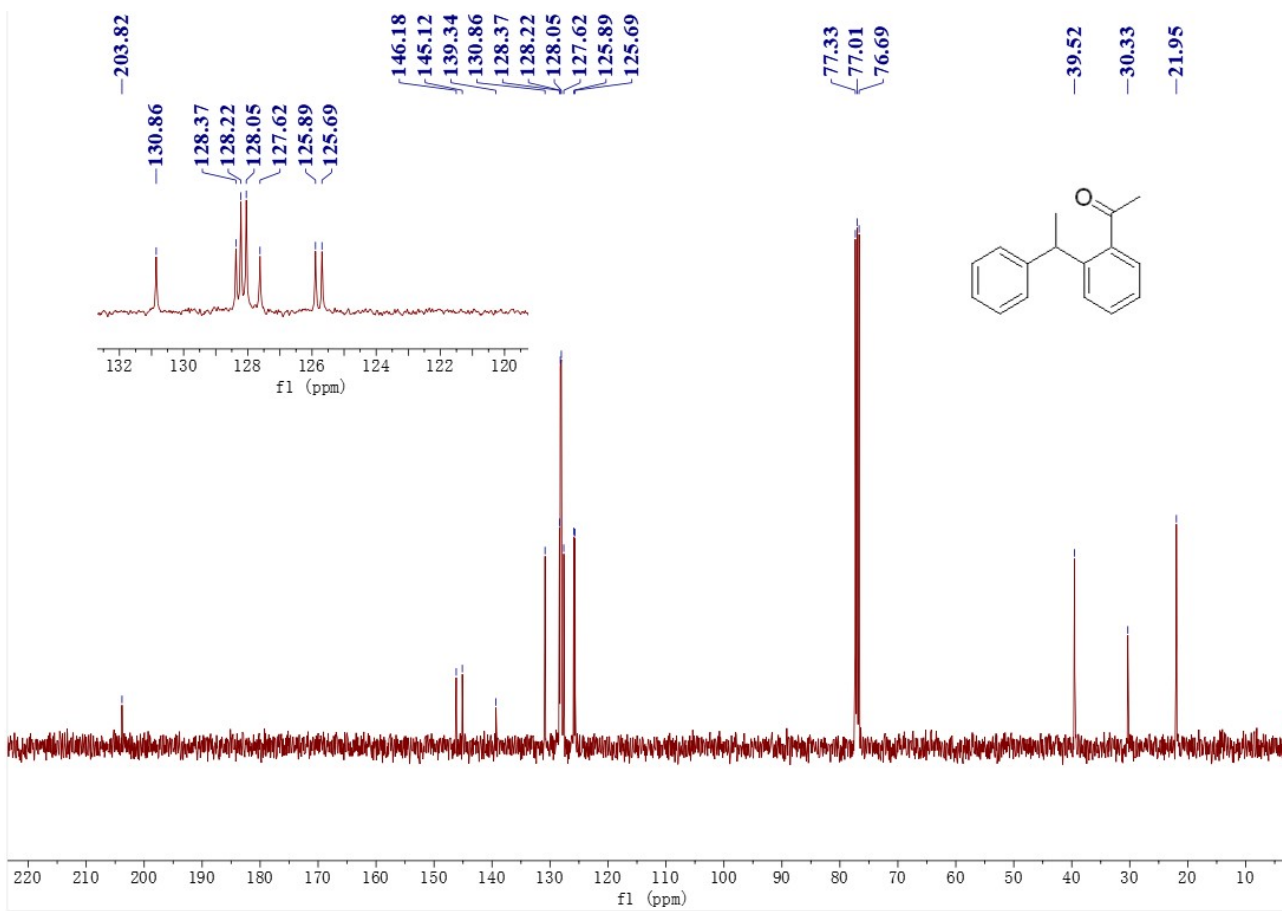


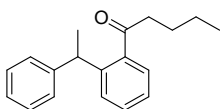


1-(2-(1-phenylethyl)phenyl)ethan-1-one (2ad)

This is a known compound and its spectroscopic data are consistent with those in the previous literature.¹⁵ CAS number: 161467-47-6. A colorless oil. 36.3 mg, 81% yield. ¹H NMR (CDCl₃, TMS, 400 MHz) δ 7.46 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.40-7.31 (m, 2H), 7.25-7.21 (m, 3H), 7.16-7.13 (m, 3H), 4.86 (q, *J* = 7.2 Hz, 1H), 2.35 (s, 3H), 1.60 (d, *J* = 7.2 Hz, 3H). ¹³C NMR (CDCl₃, TMS, 100 MHz) δ 203.8, 146.2, 145.1, 139.3, 130.9, 128.4, 128.2, 128.0, 127.6, 125.9, 125.7, 39.5, 30.3, 22.0.

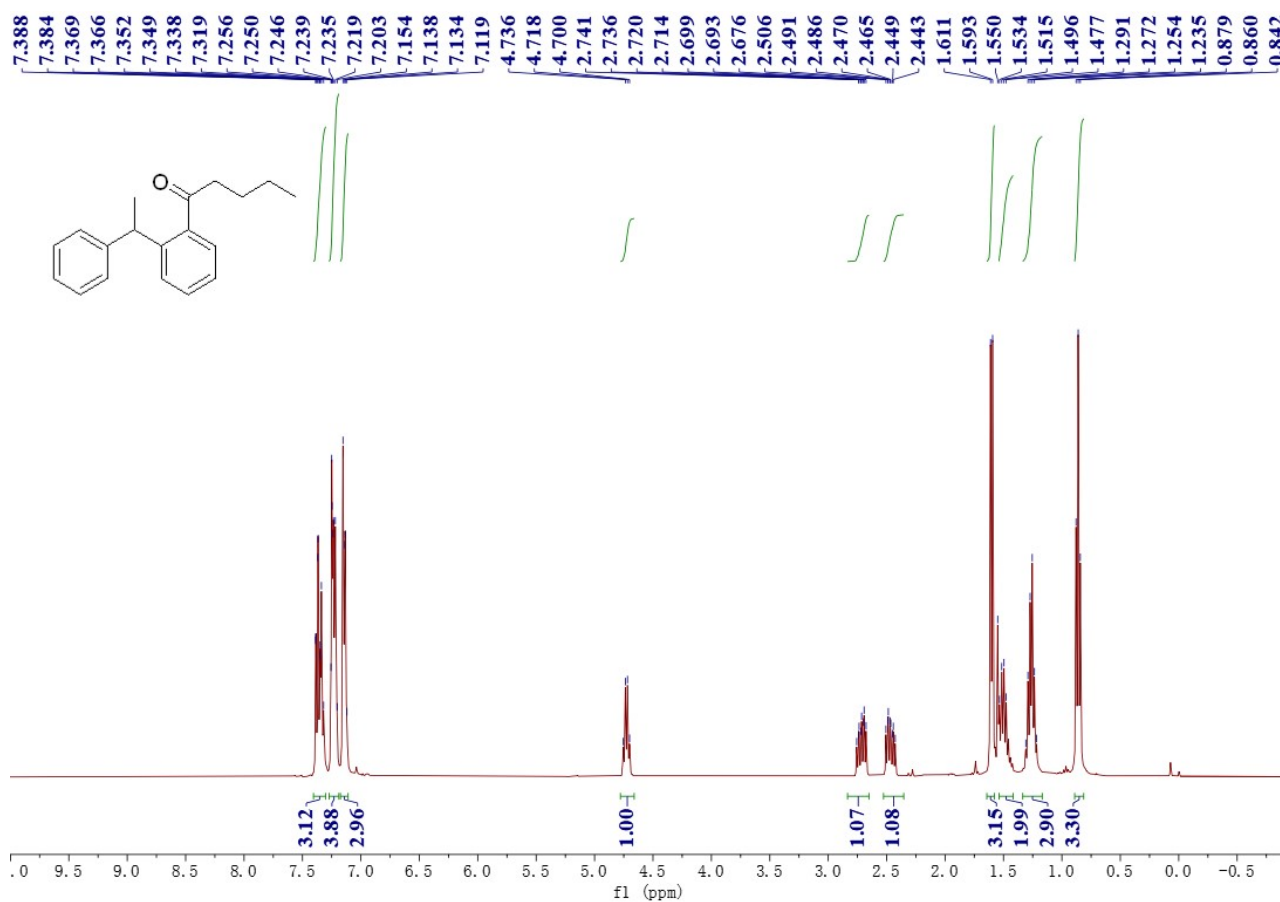


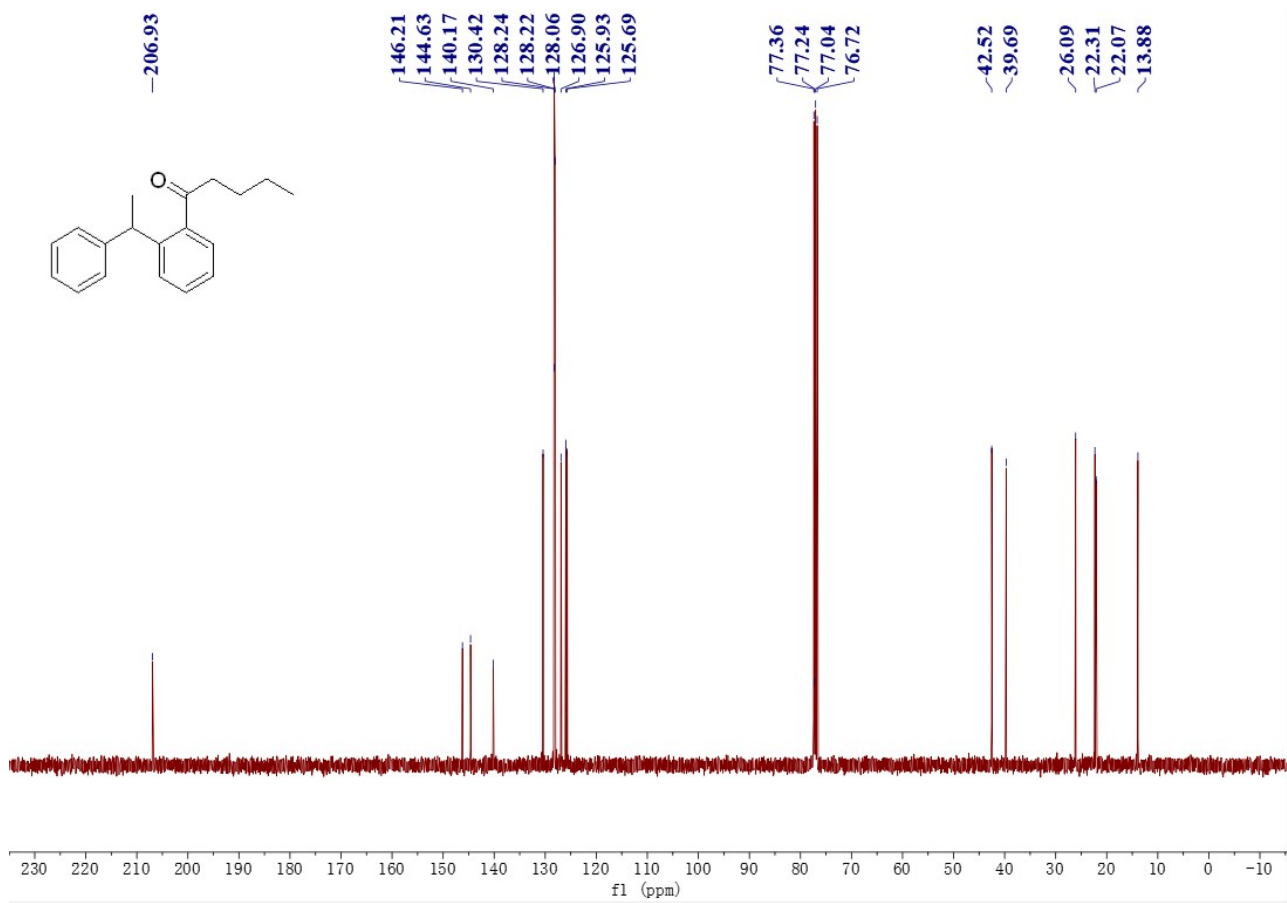


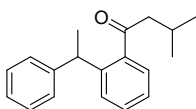


1-(2-(1-phenylethyl)phenyl)pentan-1-one (2ae)

This is a known compound and its spectroscopic data are consistent with those in the previous literature.¹⁶ CAS number: 854660-28-9. A colorless oil. 42.1 mg, 79% yield. ¹H NMR (CDCl₃, TMS, 400 MHz) δ 7.39-7.32 (m, 3H), 7.26-7.20 (m, 4H), 7.15-7.12 (m, 3H), 4.73 (q, *J* = 7.2 Hz, 1H), 2.76-2.68 (m, 1H), 2.51-2.43 (m, 1H), 1.60 (d, *J* = 7.2 Hz, 3H), 1.55-1.48 (m, 2H), 1.31-1.22 (m, 3H), 0.86 (t, *J* = 7.4 Hz, 3H). ¹³C NMR (CDCl₃, TMS, 100 MHz) δ 206.9, 146.2, 144.6, 140.2, 130.4, 128.2, 128.2, 128.1, 126.9, 125.9, 125.7, 77.4, 42.5, 39.7, 26.1, 22.3, 22.1, 13.9.

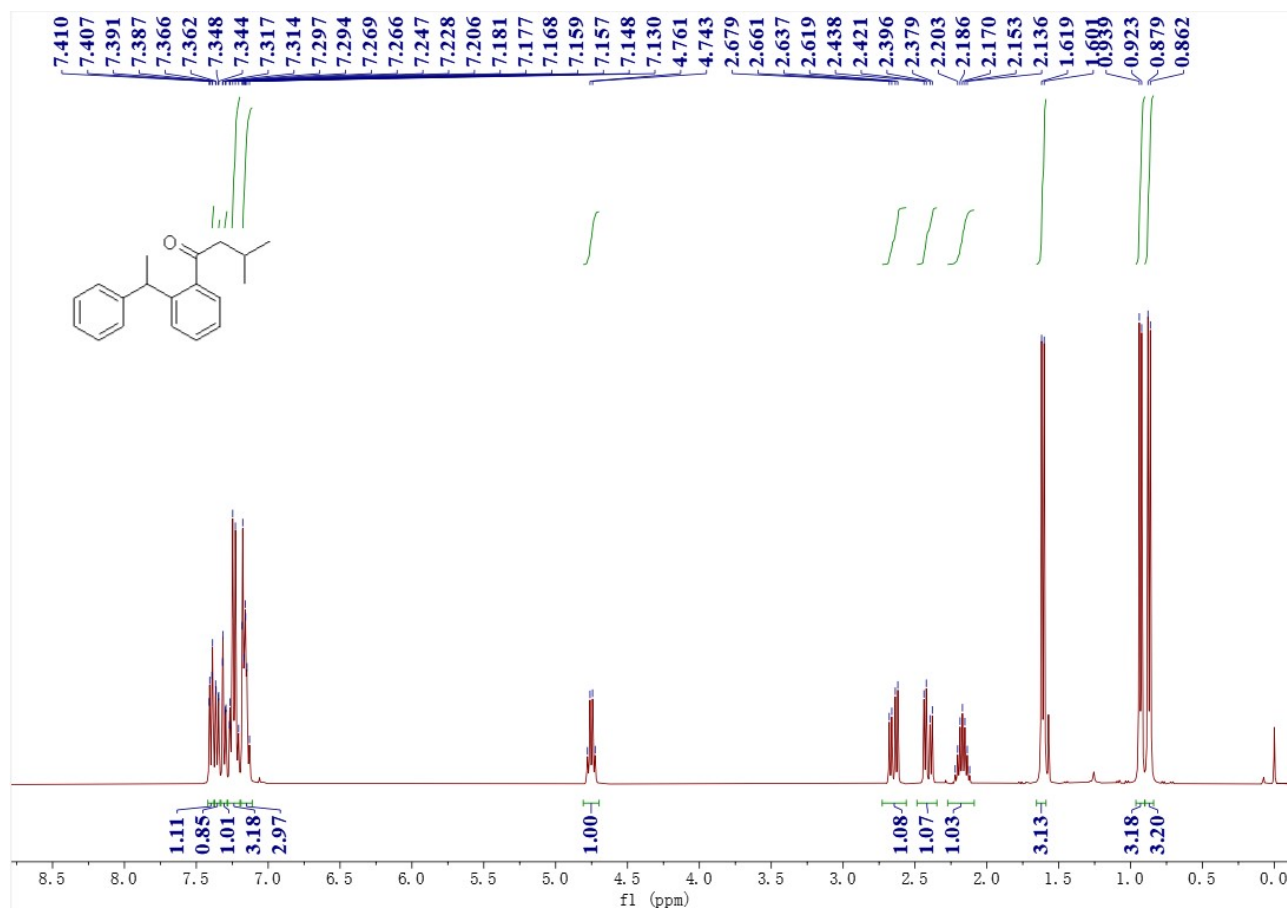


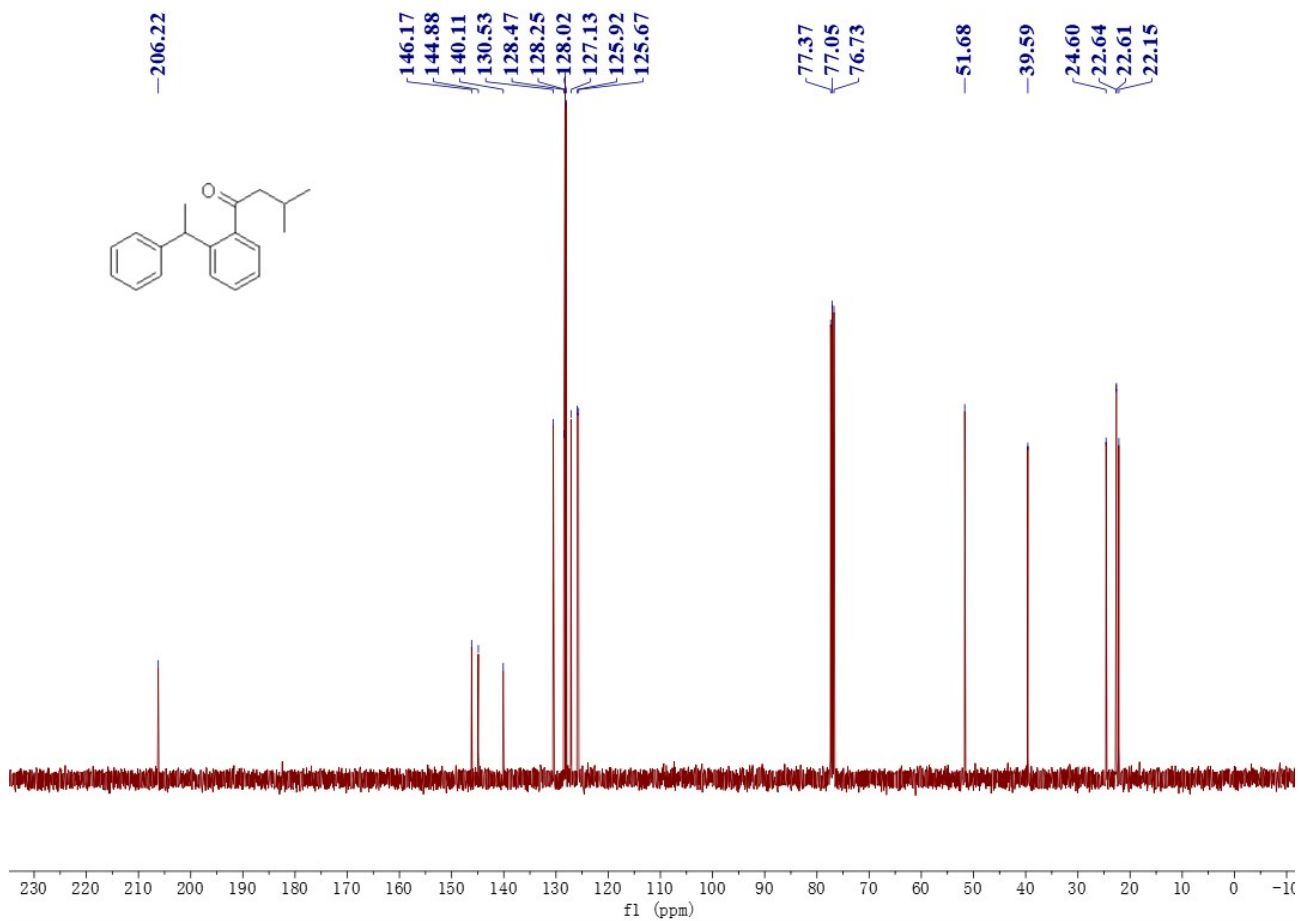


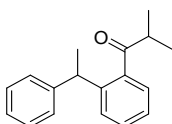


3-methyl-1-(2-(1-phenylethyl)phenyl)butan-1-one (2af)

A colorless oil. 39.9 mg, 75% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.40 (dd, $J = 7.8, 1.6$ Hz, 1H), 7.35 (dd, $J = 7.2, 1.4$ Hz, 1H), 7.31 (dd, $J = 8.0, 1.4$ Hz, 1H), 7.27-7.21 (m, 3H), 7.18-7.13 (m, 3H), 4.75 (q, $J = 7.2$ Hz, 1H), 2.65 (dd, $J = 16.8, 7.2$ Hz, 1H), 2.41 (dd, $J = 16.8, 6.6$ Hz, 1H), 2.20-2.12 (m, 1H), 1.61 (d, $J = 7.2$ Hz, 3H), 0.93 (d, $J = 6.8$ Hz, 3H), 0.87 (d, $J = 6.6$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 206.2, 146.2, 144.9, 140.1, 130.5, 128.5, 128.3, 128.0, 127.1, 125.9, 125.7, 51.7, 39.6, 24.6, 22.64, 22.61, 22.1. IR (acetone) ν 30631 2954, 2869, 1685, 1493, 1260, 1057, 1011, 998, 754 cm^{-1} . HRMS (EI) calcd. for $\text{C}_{19}\text{H}_{22}\text{O}$ (M^+): 266.1665, Found: 266.1668.

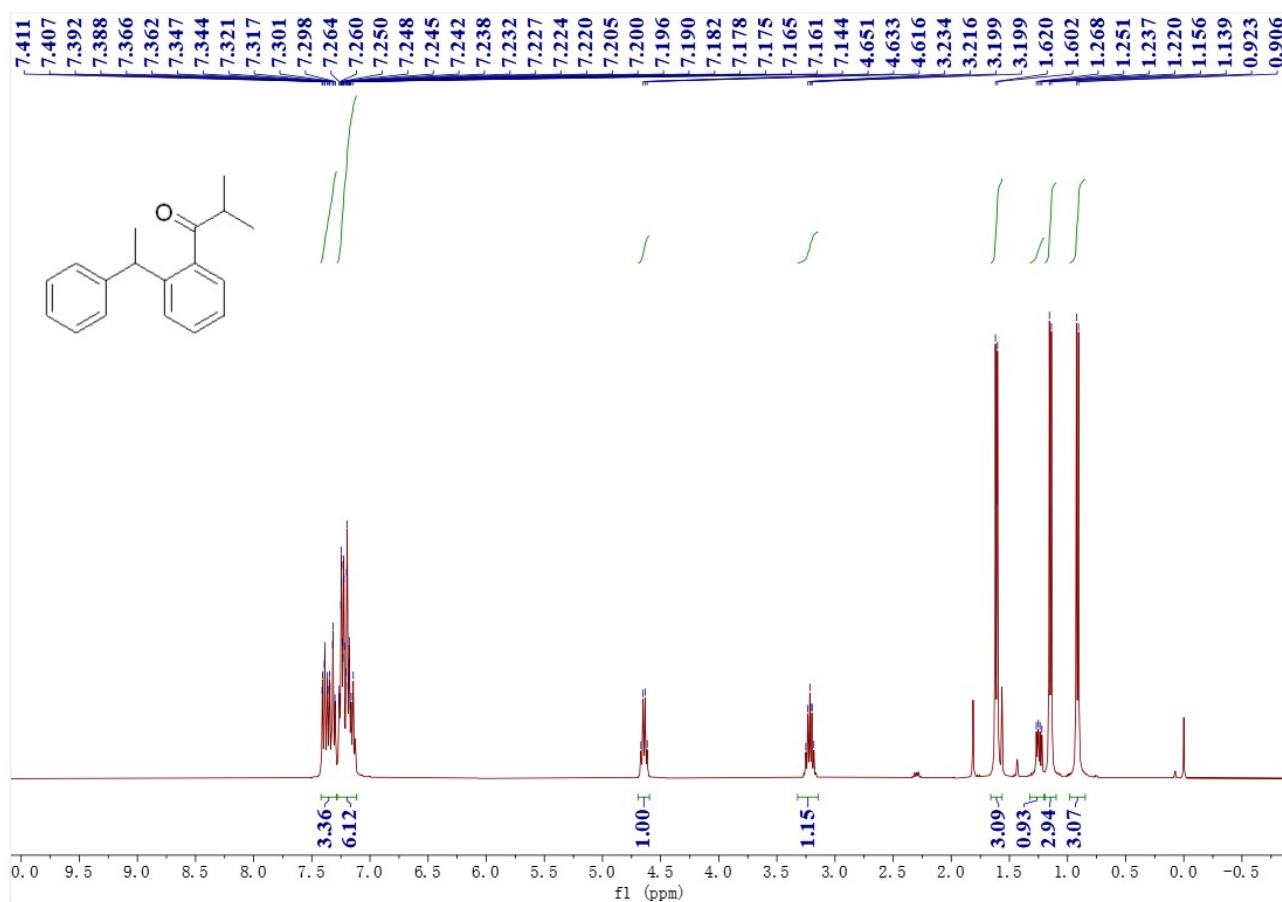


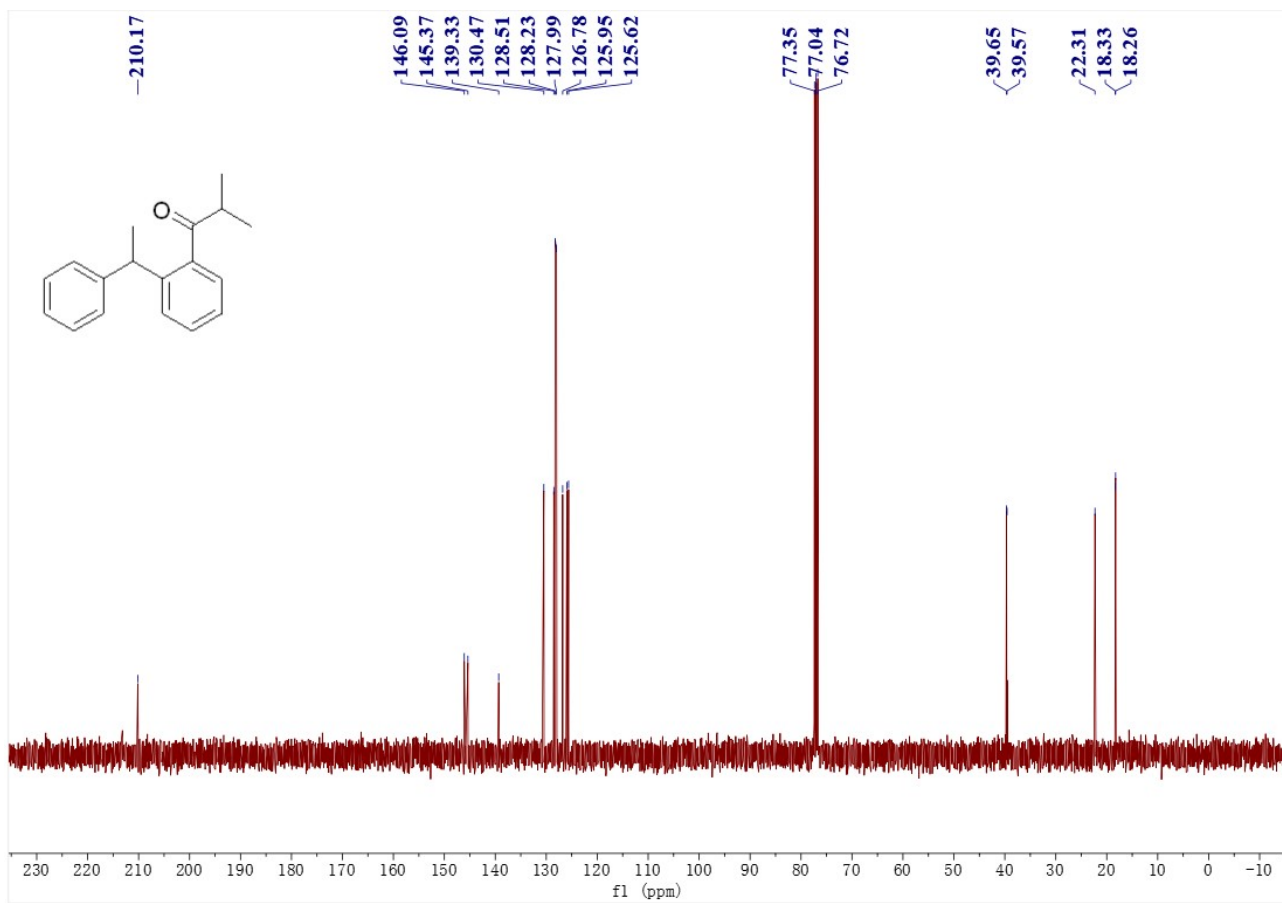


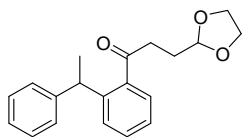


2-methyl-1-(2-(1-phenylethyl)phenyl)propan-1-one (2ag)

This is a known compound and its spectroscopic data are consistent with those in the previous literature.¹⁷ CAS number: 1620210-43-6. A colorless oil. 36.3 mg, 72% yield. ¹H NMR (CDCl₃, TMS, 400 MHz) δ 7.41-7.30 (m, 3H), 7.25-7.14 (m, 6H), 4.64 (q, *J* = 7.2 Hz, 1H), 3.25-3.18 (m, 1H), 1.61 (d, *J* = 7.2 Hz, 3H), 1.27-1.22 (m, 1H), 1.15 (d, *J* = 6.8 Hz, 3H), 0.91 (d, *J* = 7.2 Hz, 3H). ¹³C NMR (CDCl₃, TMS, 100 MHz) δ 210.2, 146.1, 145.4, 139.3, 130.5, 128.5, 128.2, 128.0, 126.8, 126.0, 125.6, 39.7, 39.6, 22.3, 18.3, 18.3.

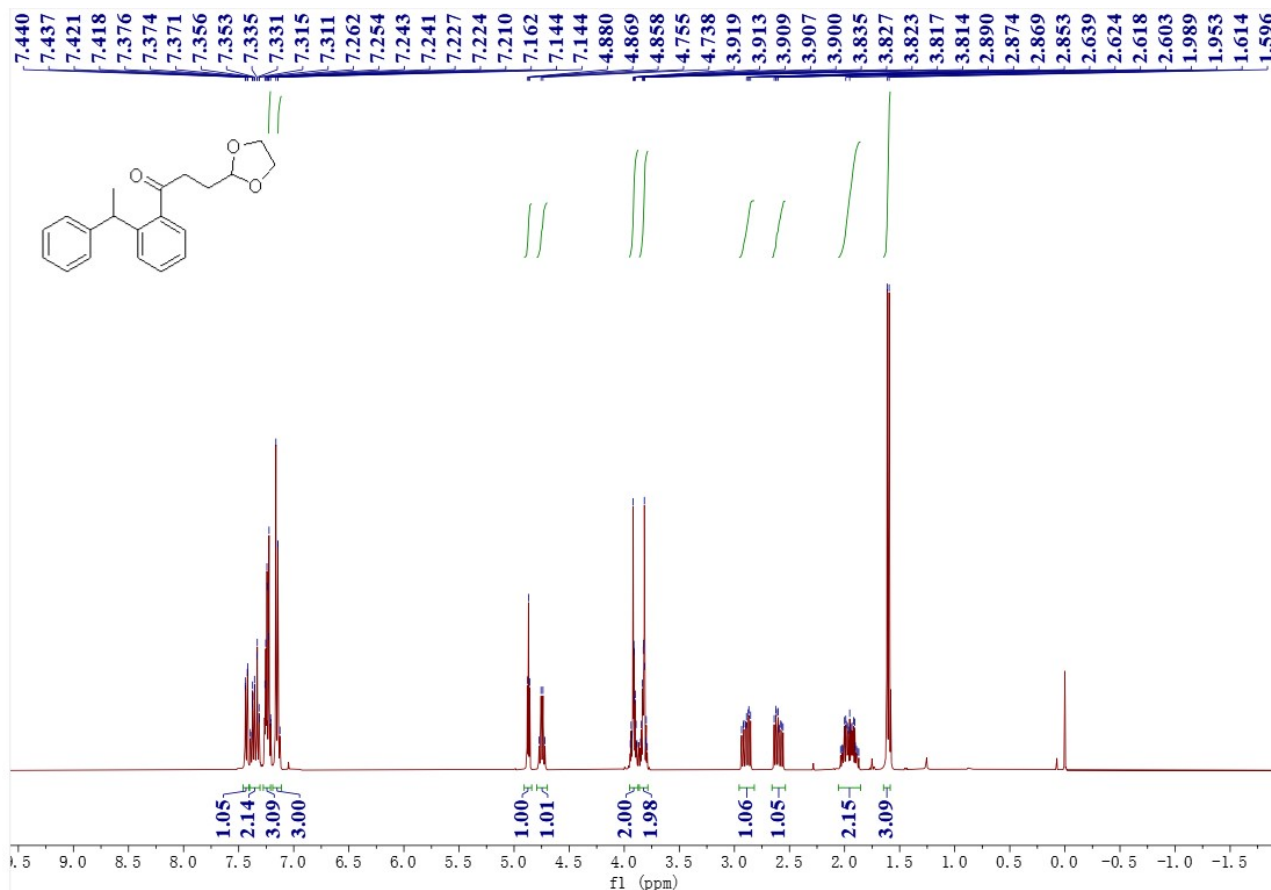


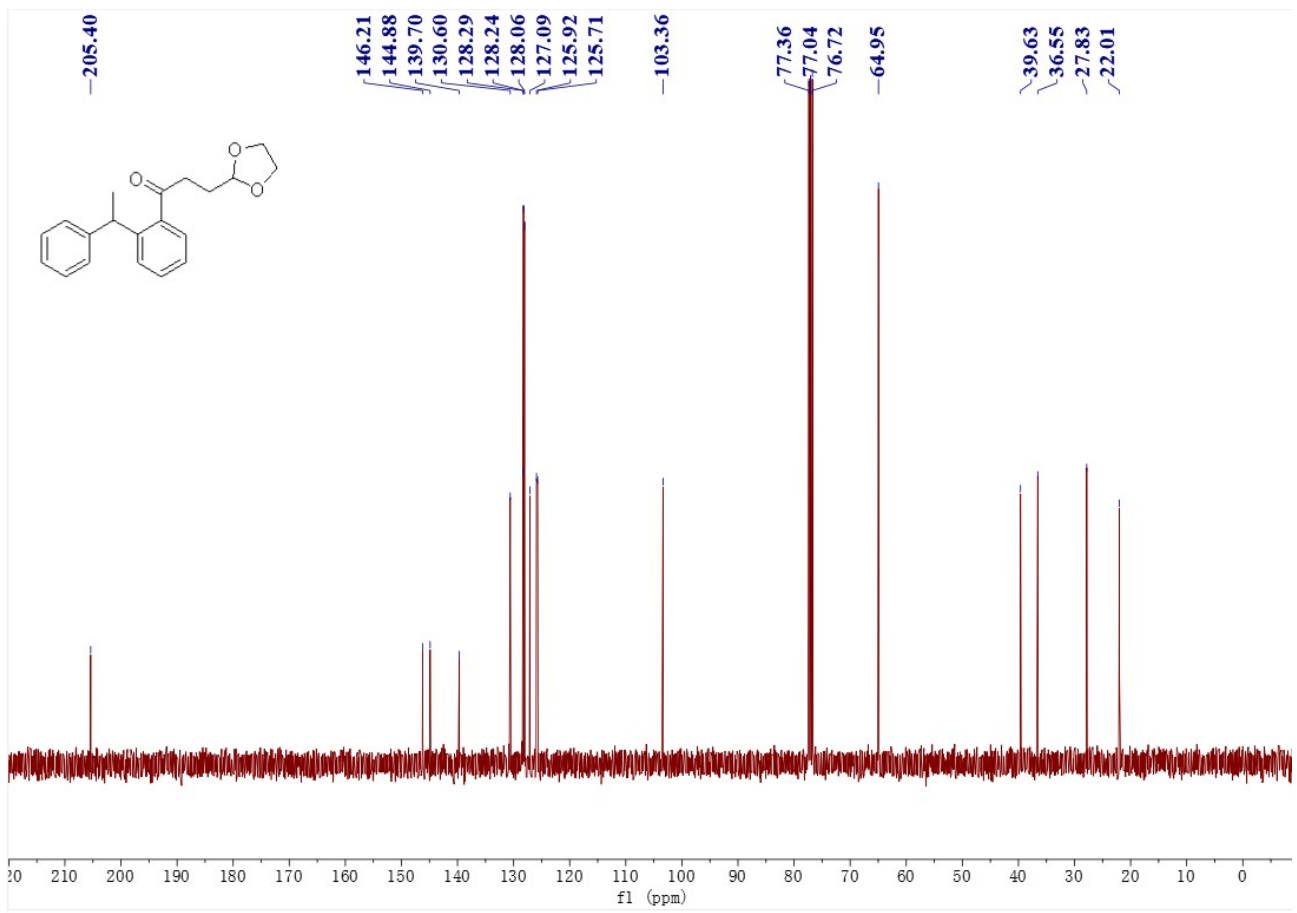


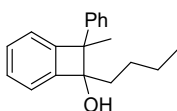


2-methyl-1-(2-(1-phenylethyl)phenyl)propan-1-one (2ah)

A colorless oil. 43.5 mg, 70% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.43 (dd, $J = 7.8, 1.4$ Hz, 1H), 7.40-7.31 (m, 2H), 7.26-7.21 (m, 3H), 7.16-7.13 (m, 3H), 4.87 (t, $J = 4.4$ Hz, 1H), 4.75 (q, $J = 7.2$ Hz, 1H), 3.92-3.89 (m, 2H), 3.85-3.79 (m, 2H), 2.89-2.85 (m, 1H), 2.64-2.60 (m, 1H), 2.04-1.87 (m, 2H), 1.60 (d, $J = 7.2$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 205.4, 146.2, 144.9, 139.7, 130.6, 128.3, 128.2, 128.1, 127.1, 125.9, 125.7, 103.4, 65.0, 39.6, 36.6, 27.8, 22.0. IR (acetone) ν 3060, 3025, 2966, 1690, 1493, 1408, 1139, 1026, 785, 701 cm^{-1} . HRMS (EI) calcd. for $\text{C}_{20}\text{H}_{22}\text{O}_3$ (M^+): 310.1563, Found: 310.1568.



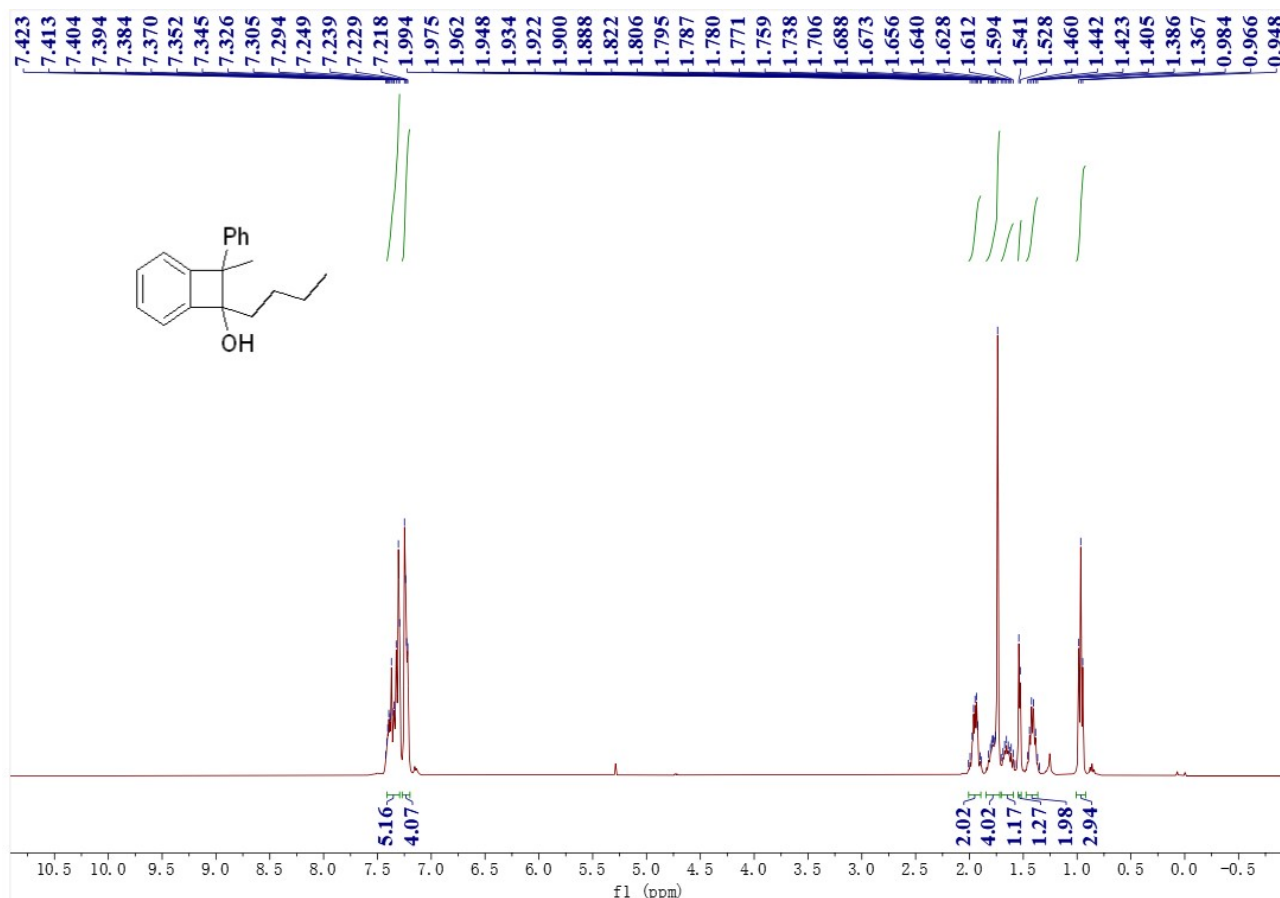


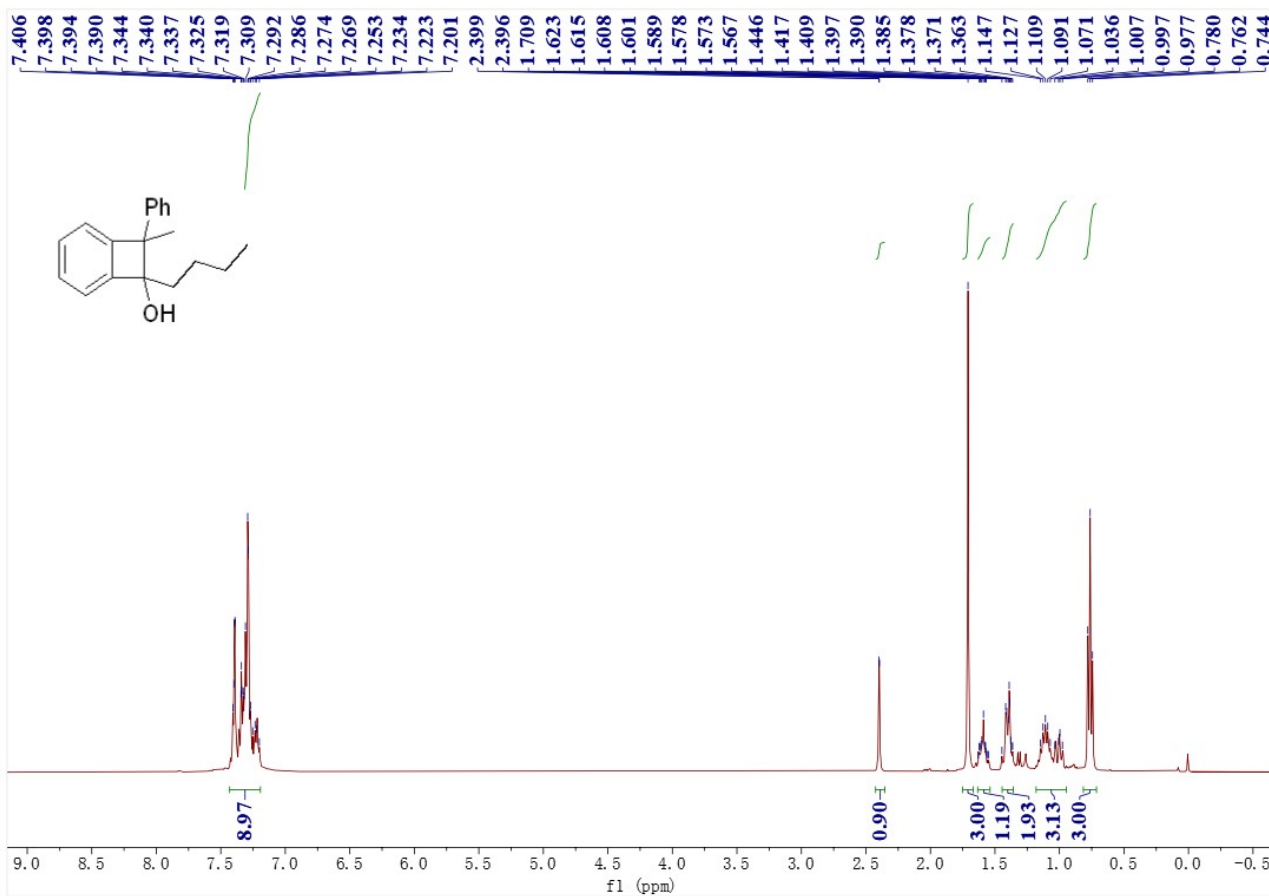
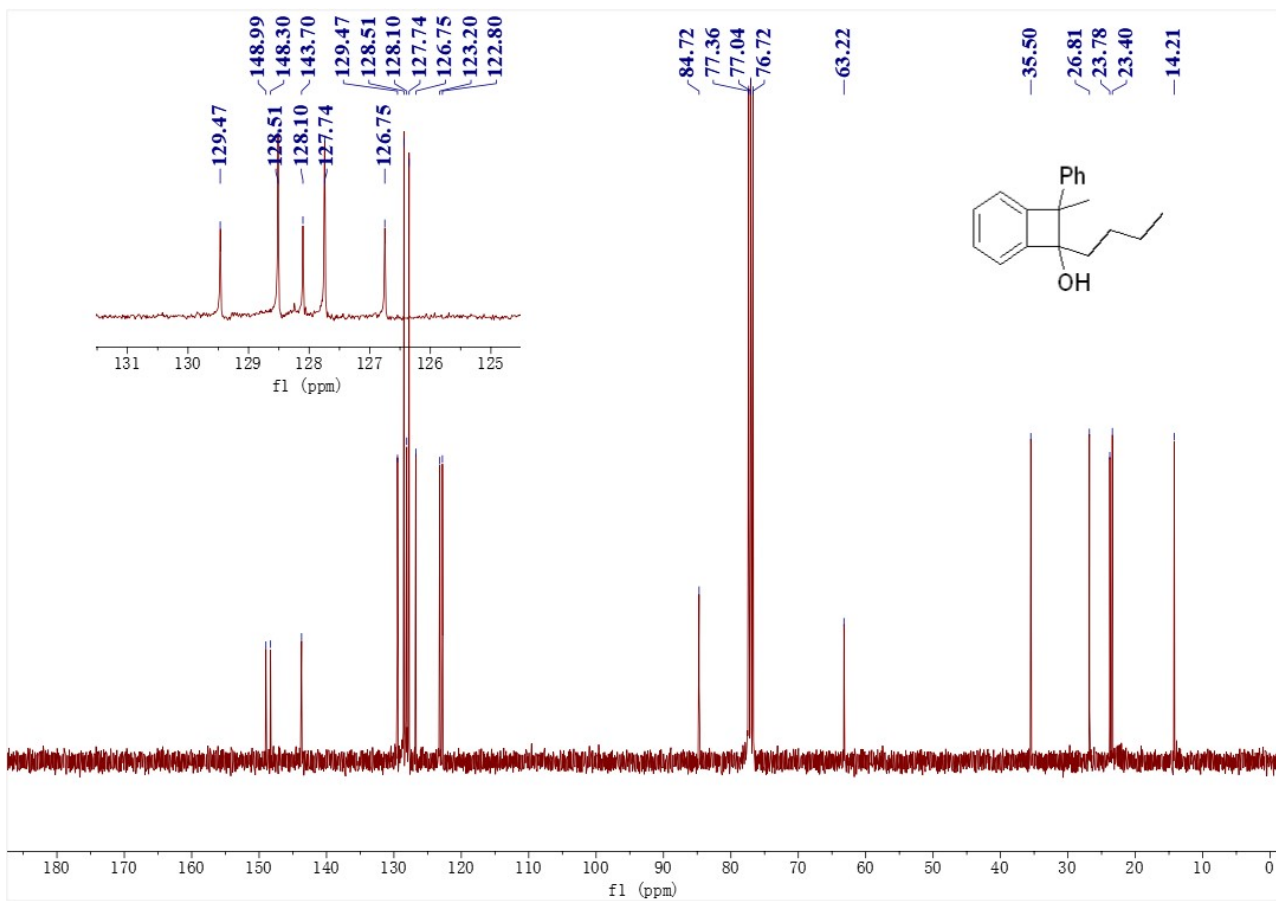


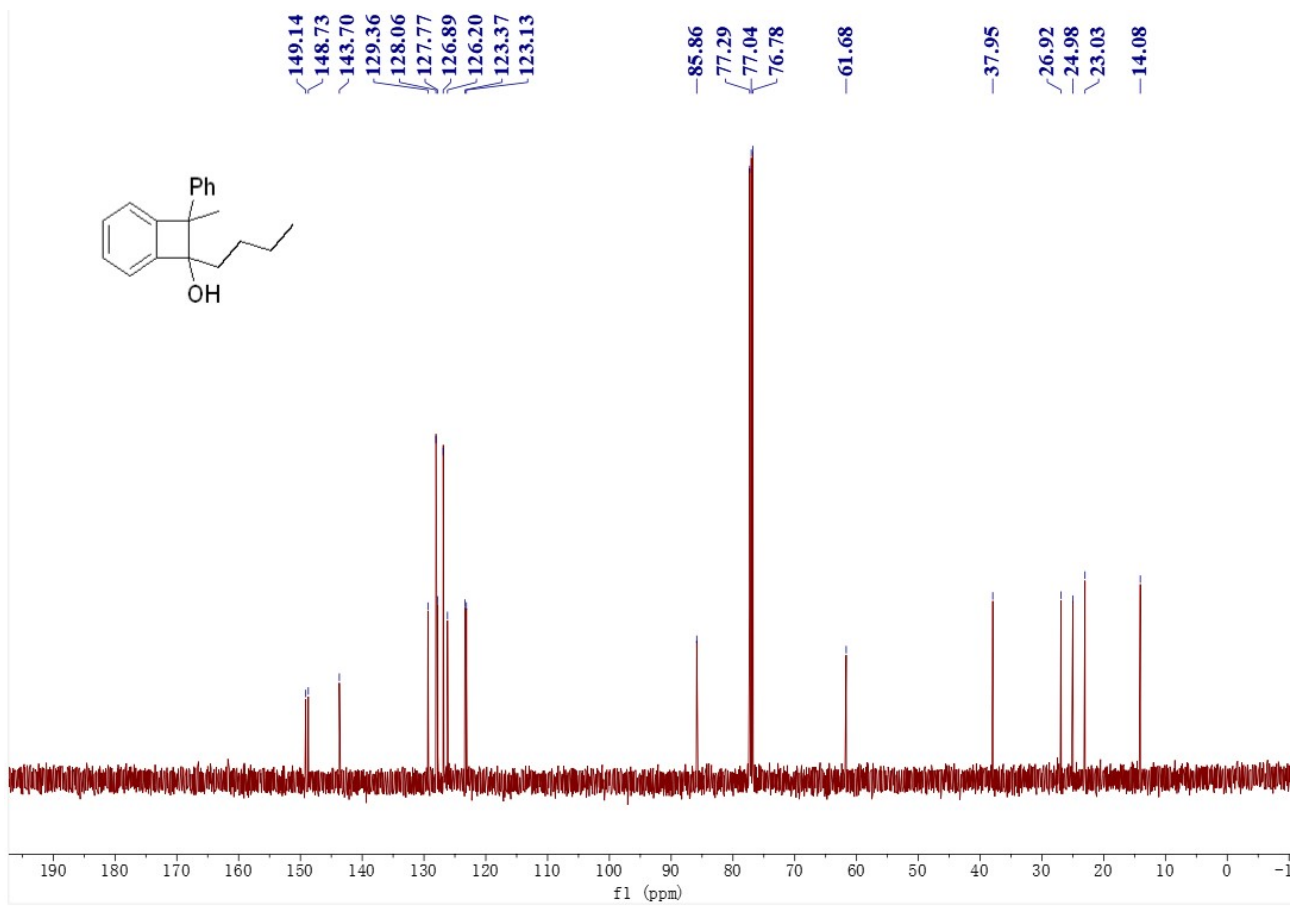
7-butyl-8-methyl-8-phenylbicyclo[4.2.0]octa-1,3,5-trien-7-ol (3 and 3')

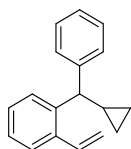
A colorless oil. 27.6 mg, 51% yield, *d.r.* = 3 : 2. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.43-7.27 (m, 5H), 7.26-7.20 (m, 4H), 2.03-1.88 (m, 2H), 1.84-1.67 (m, 4H), 1.73-1.57 (m, 1H), 1.57-1.51 (m, 1H), 1.47-1.34 (m, 2H), 0.97 (t, $J = 7.4$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 125 MHz) δ 149.0, 148.3, 143.7, 129.5, 128.5, 128.1, 127.7, 126.8, 123.2, 122.8, 84.7, 63.2, 35.5, 26.8, 23.8, 23.4, 14.2. IR (acetone) ν 3465, 3027, 2957, 2871, 1489, 1447, 1397, 1092, 934, 698 cm^{-1} . HRMS (EI) calcd. for $\text{C}_{19}\text{H}_{22}\text{O}$ (M^+): 266.1665, Found: 266.1666.

^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.48-7.15 (m, 9H), 2.40 (s, 1H), 1.71 (s, 3H), 1.65-1.53 (m, 1H), 1.47-1.34 (m, 2H), 1.20-0.92 (m, 3H), 0.76 (t, $J = 7.3$ Hz, 3H). ^{13}C NMR (125 MHz, CDCl_3) δ 149.1, 148.7, 143.7, 129.4, 128.1, 127.8, 126.9, 126.2, 123.4, 123.1, 85.9, 61.7, 38.0, 26.9, 25.0, 23.0, 14.1. IR (acetone) ν 3464, 3026, 2930, 2871, 1487, 1446, 1395, 1092, 934, 700 cm^{-1} . HRMS (FI) calcd. for $\text{C}_{19}\text{H}_{22}\text{O}$ (M^+): 266.1665, Found: 266.1670.



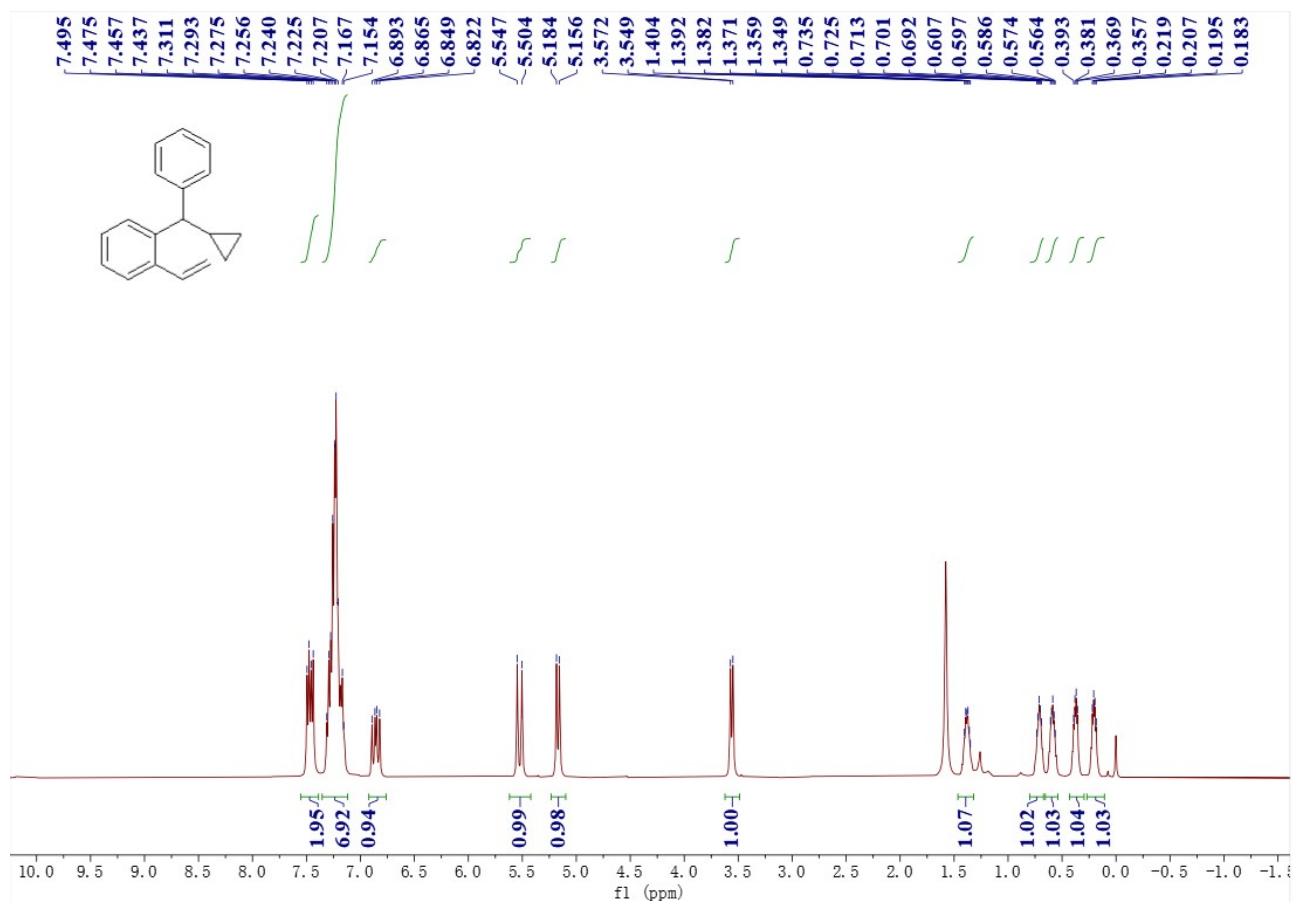


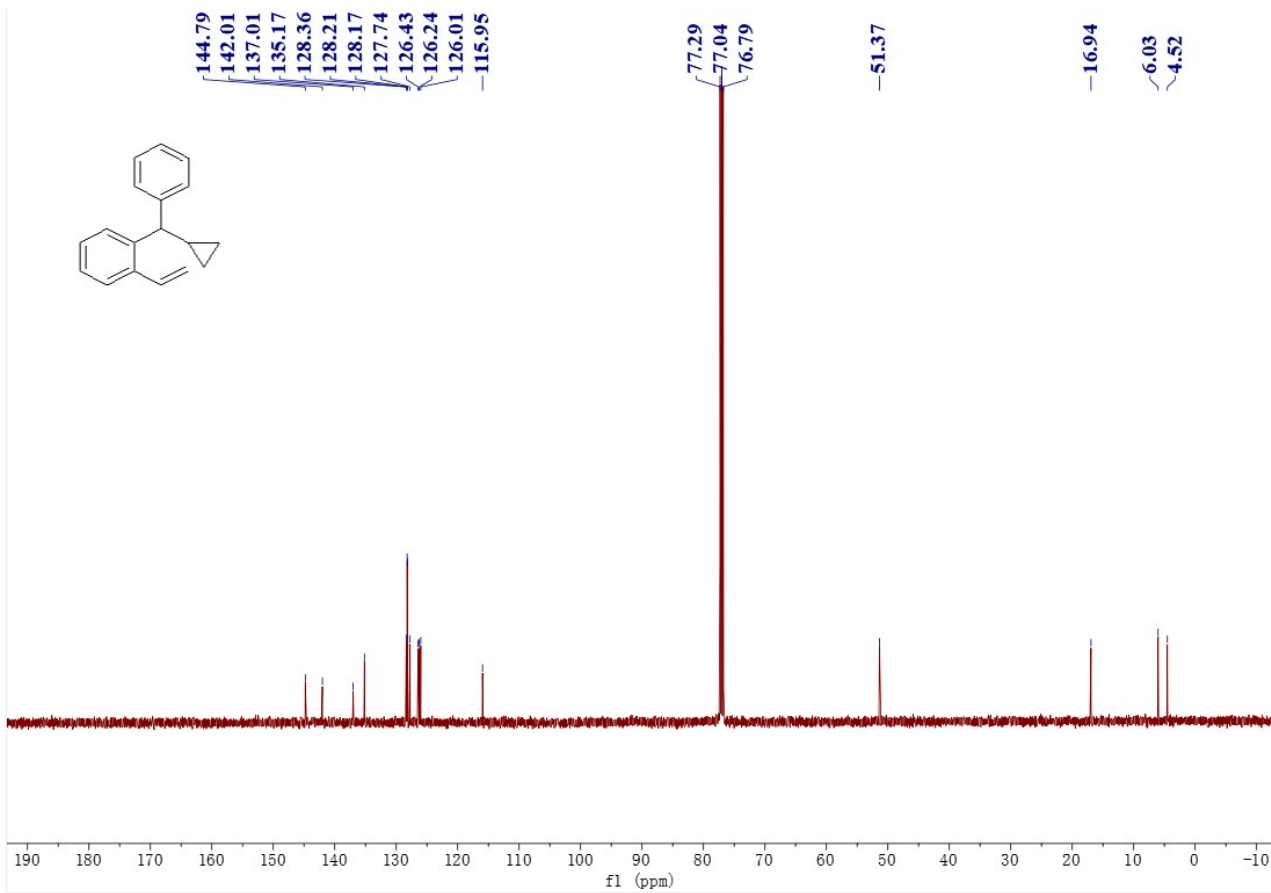


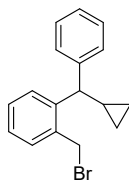


1-(cyclopropyl(phenyl)methyl)-2-vinylbenzene (4)

A colorless oil. 42.2 mg, 90% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.50-7.44 (m, 2H), 7.31-7.15 (m, 7H), 6.86 (dd, $J = 17.4, 11.2$ Hz, 1H), 5.53 (d, $J = 17.4$ Hz, 1H), 5.17 (d, $J = 11.2$ Hz, 1H), 3.56 (d, $J = 9.2$ Hz, 1H), 1.40-1.35 (m, 1H), 0.74-0.69 (m, 1H), 0.61-0.56 (m, 1H), 0.39-0.36 (m, 1H), 0.22-0.18 (m, 1H). ^{13}C NMR (CDCl_3 , TMS, 125 MHz) δ 144.8, 142.0, 137.0, 135.2, 128.4, 128.2, 128.2, 127.7, 126.4, 126.2, 126.0, 115.9, 51.4, 16.9, 6.0, 4.5. IR (acetone) ν 3061, 3024, 3001, 1493, 1480, 1450, 1019, 989, 749, 699 cm^{-1} . HRMS (EI) calcd. for $\text{C}_{18}\text{H}_{18}$ (M^+): 234.1403, Found: 234.1405.

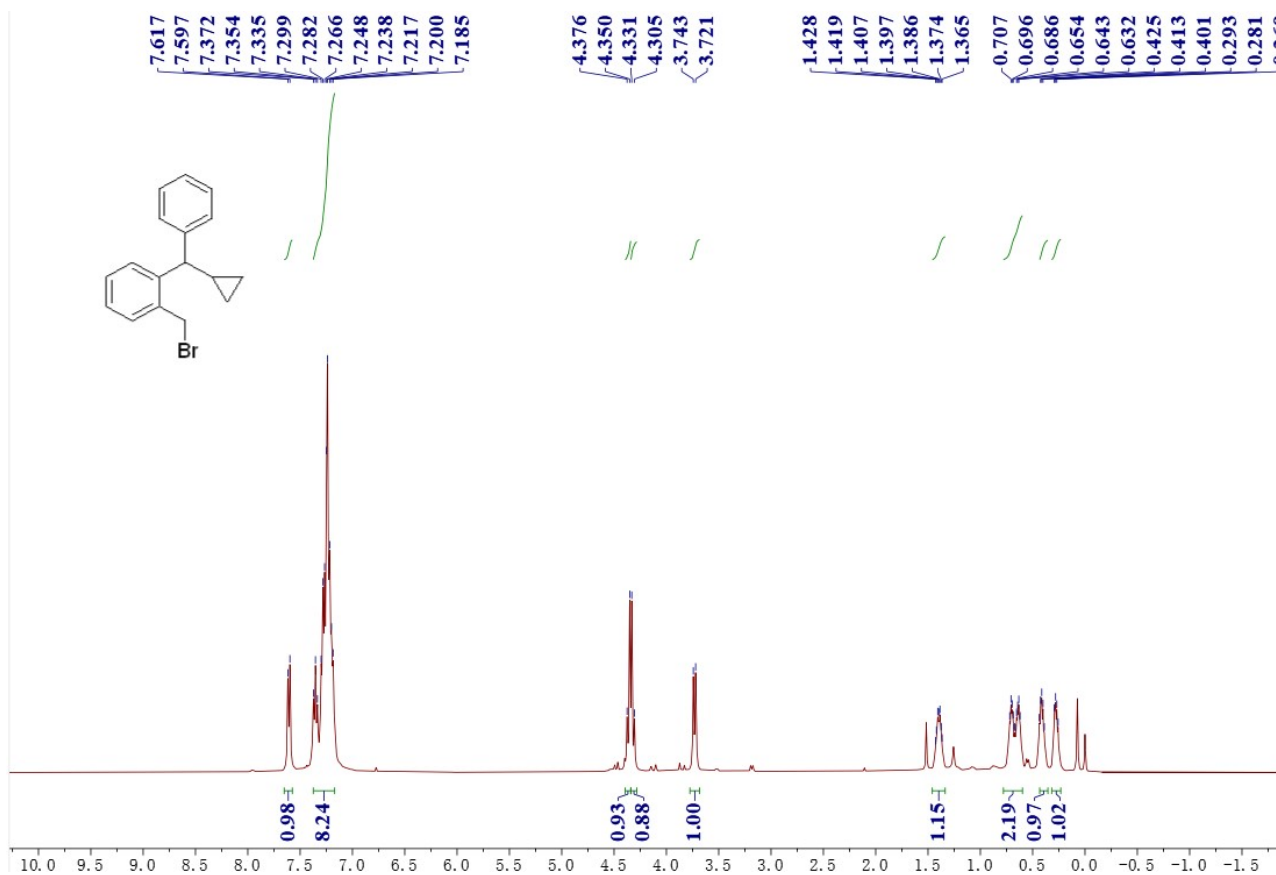


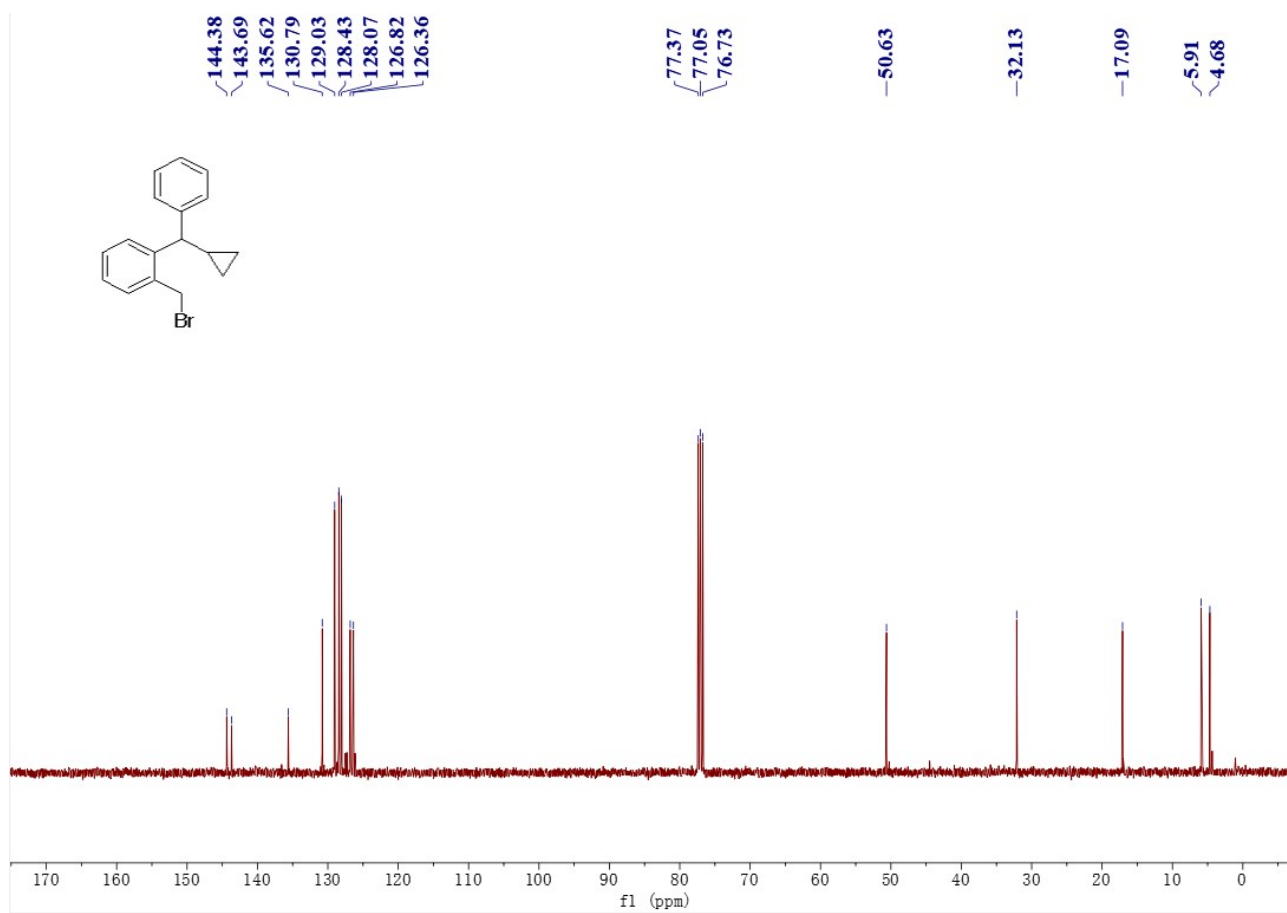


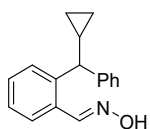


1-(bromomethyl)-2-(cyclopropyl(phenyl)methyl)benzene (5)

A colorless oil. 18.7 mg, 31% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 7.61 (d, $J = 7.8$ Hz, 1H), 7.37-7.19 (m, 8H), 4.36 (d, $J = 10.2$ Hz, 1H), 4.32 (d, $J = 10.2$ Hz, 1H), 3.73 (d, $J = 8.8$ Hz, 1H), 1.43-1.37 (m, 1H), 0.72-0.62 (m, 2H), 0.44-0.39 (m, 1H), 0.29-0.26 (m, 1H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 144.4, 143.7, 135.6, 130.8, 129.0, 128.4, 128.1, 126.8, 126.4, 50.6, 32.1, 17.1, 5.9, 4.7. IR (acetone) ν 3061, 3025, 3001, 1493, 1450, 1428, 1074, 1020, 767, 699 cm^{-1} . HRMS (FI) calcd. for $\text{C}_{17}\text{H}_{17}\text{Br}$ (M^+): 300.0508, Found: 300.0504.

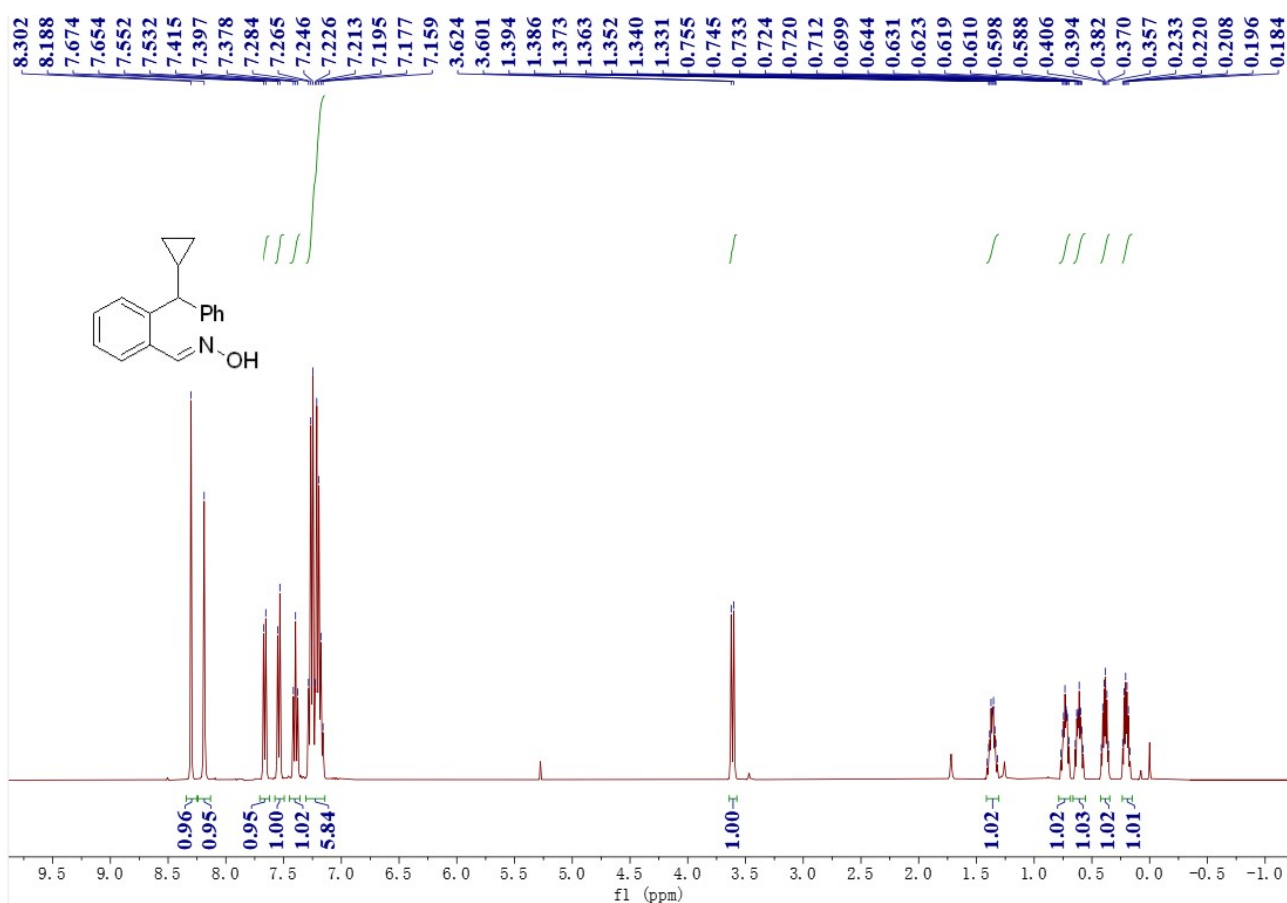


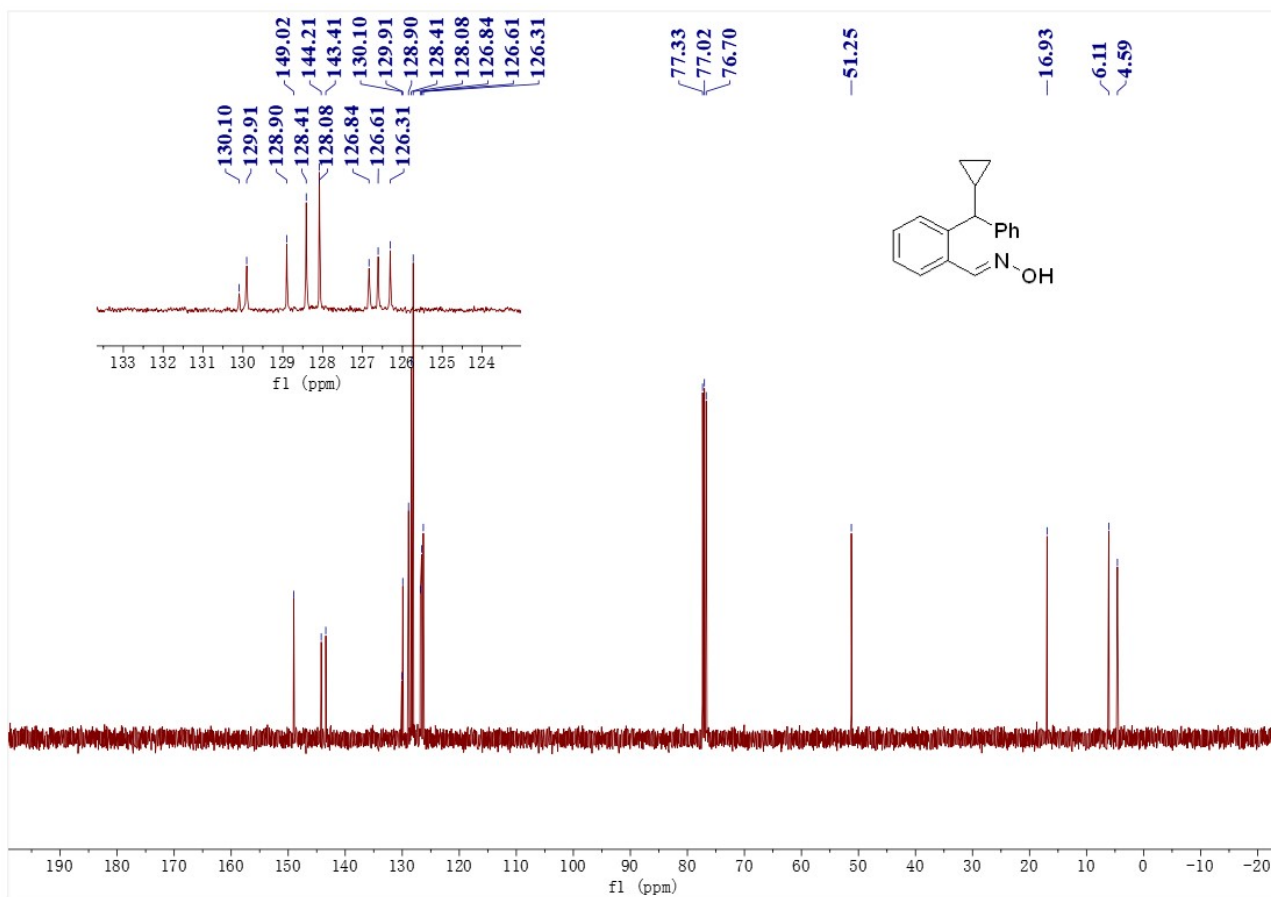


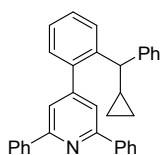


(E)-2-(cyclopropyl(phenyl)methyl)benzaldehyde oxime (6)

A colorless oil. 30.2 mg, 60% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 8.30 (s, 1H), 8.19 (s, 1H), 7.66 (d, $J = 7.8$ Hz, 1H), 7.54 (d, $J = 7.8$ Hz, 1H), 7.40 (t, $J = 7.2$ Hz, 1H), 7.28-7.16 (m, 6H), 3.61 (d, $J = 9.2$ Hz, 1H), 1.41-1.32 (m, 1H), 0.77-0.70 (m, 1H), 0.63-0.58 (m, 1H), 0.41-0.36 (m, 1H), 0.23-0.17 (m, 1H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 149.0, 144.2, 143.4, 130.1, 129.9, 128.9, 128.4, 128.1, 126.8, 126.6, 126.3, 51.2, 16.9, 6.1, 4.6. IR (acetone) ν 3329, 3062, 3001, 2886, 1746, 1493, 1450, 1048, 1020, 755, 700 cm^{-1} . HRMS (FI) calcd. for $\text{C}_{17}\text{H}_{17}\text{ON}$ (M^+): 251.1305, Found: 251.1308.

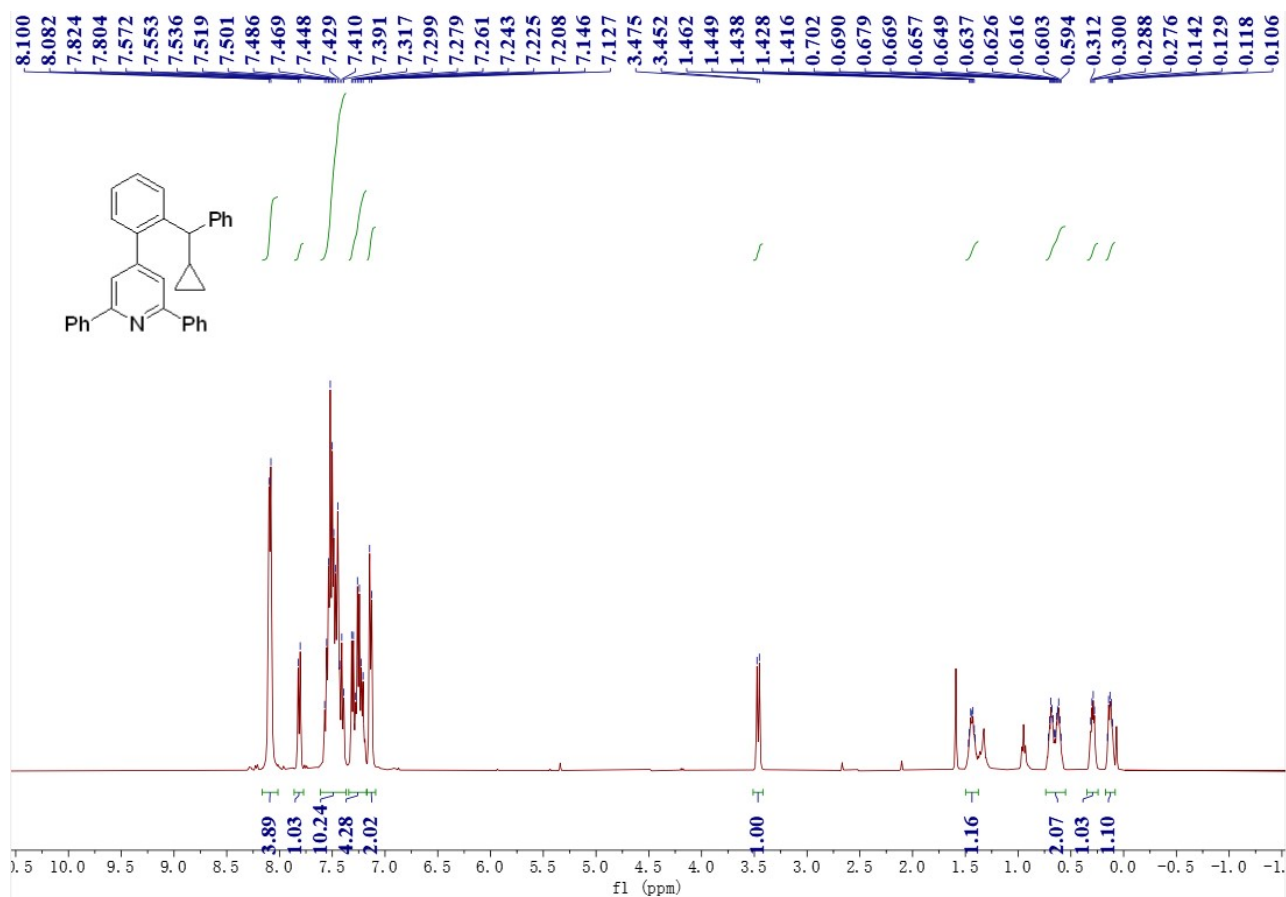


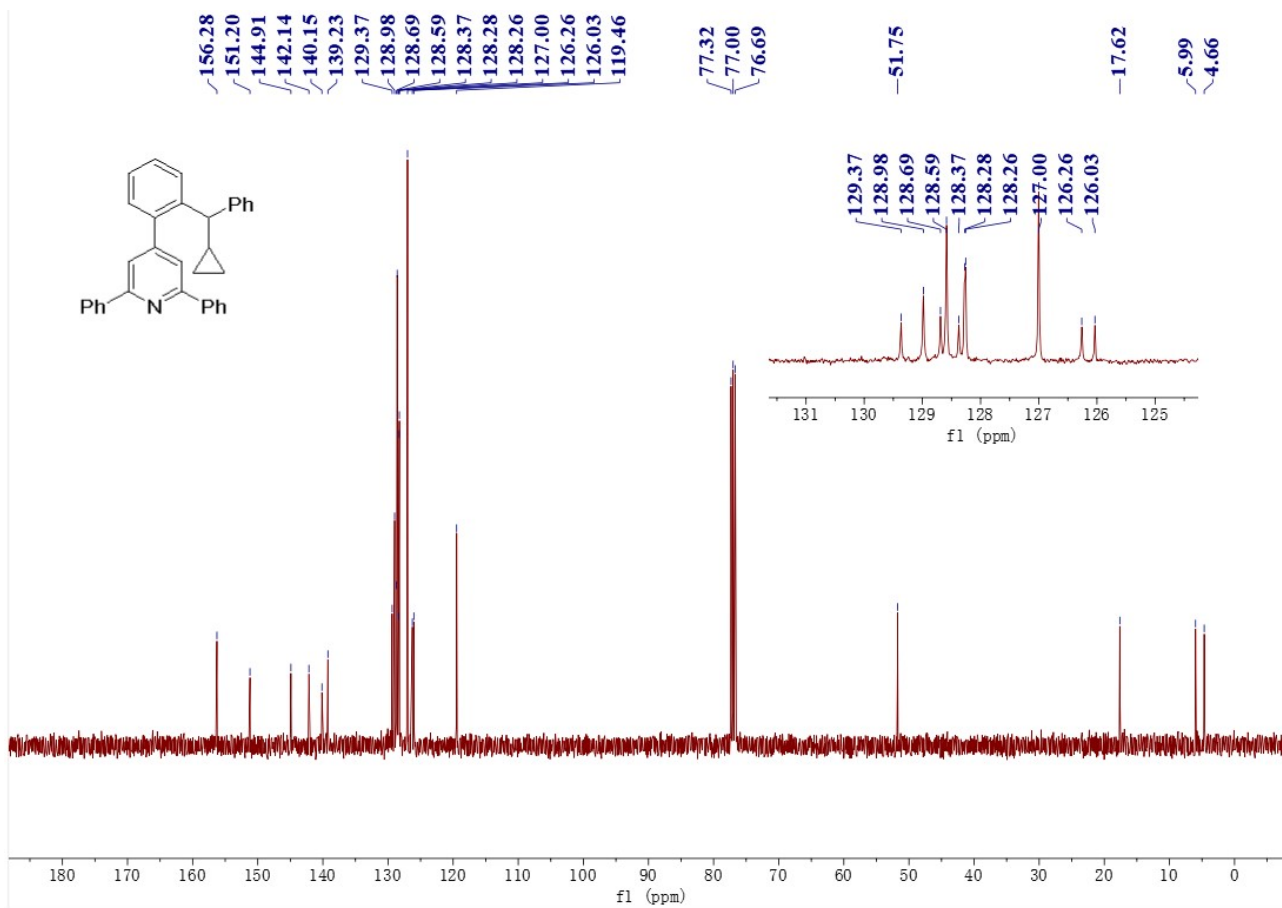


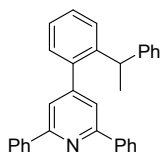


4-(2-(cyclopropyl(phenyl)methyl)phenyl)-2,6-diphenylpyridine (7)

A colorless oil. 30.1 mg, 35% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 8.09 (d, $J = 7.4$ Hz, 4H), 7.81 (d, $J = 8.0$ Hz, 1H), 7.57-7.39 (m, 10H), 7.32-7.21 (m, 4H), 7.14 (d, $J = 7.6$ Hz, 2H), 3.46 (d, $J = 9.2$ Hz, 1H), 1.47-1.41 (m, 1H), 0.71-0.59 (m, 2H), 0.31-0.28 (m, 1H), 0.15-0.11 (m, 1H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 156.3, 151.2, 144.9, 142.1, 140.1, 139.2, 129.4, 129.0, 128.7, 128.6, 128.4, 128.28, 128.26, 127.0, 126.3, 126.0, 119.5, 51.7, 17.6, 6.0, 4.7. IR (acetone) ν 3062, 3025, 2928, 1690, 1594, 1450, 1069, 1027, 777, 696 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{33}\text{H}_{28}\text{N}$ (M^+): 438.2216, Found: 438.2210.

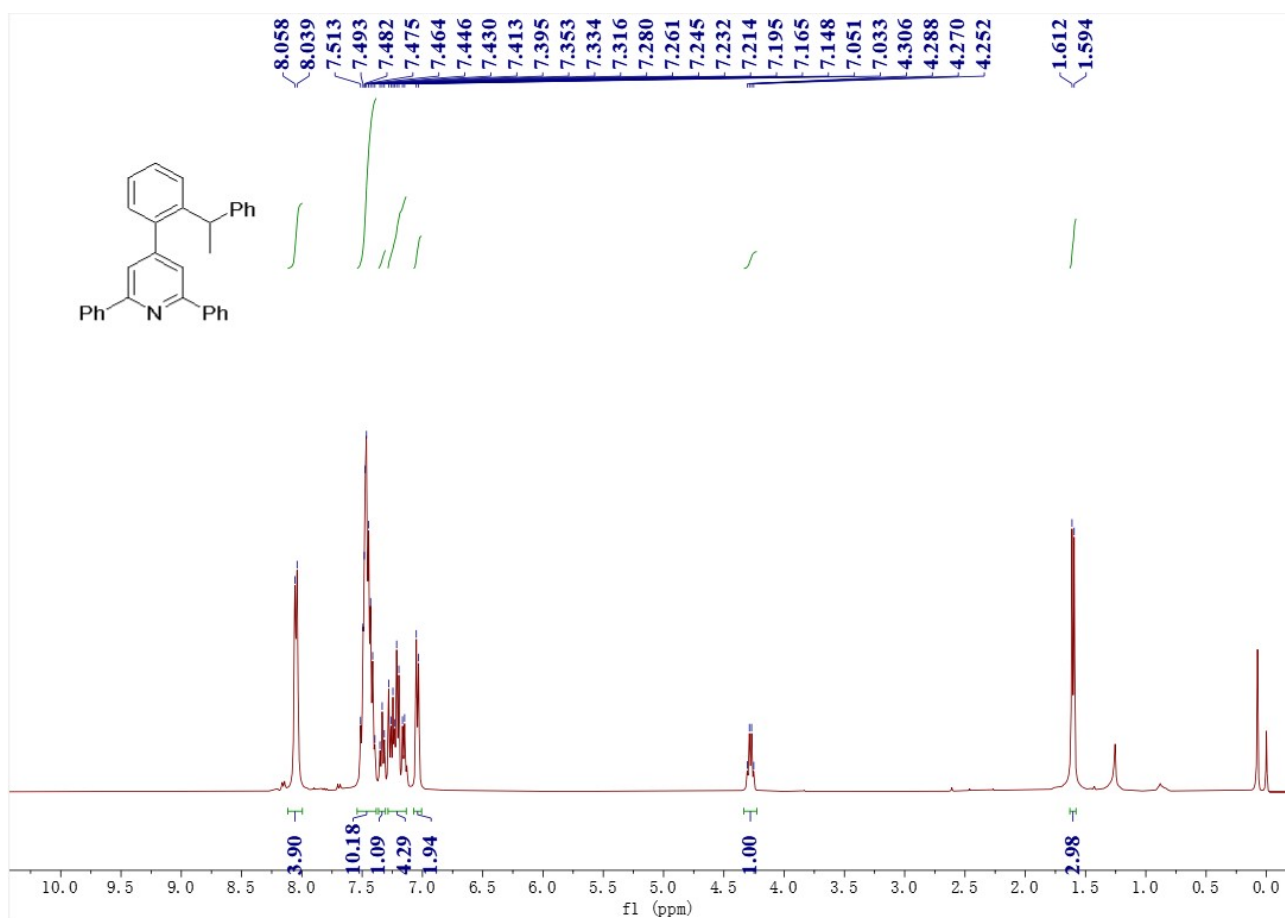


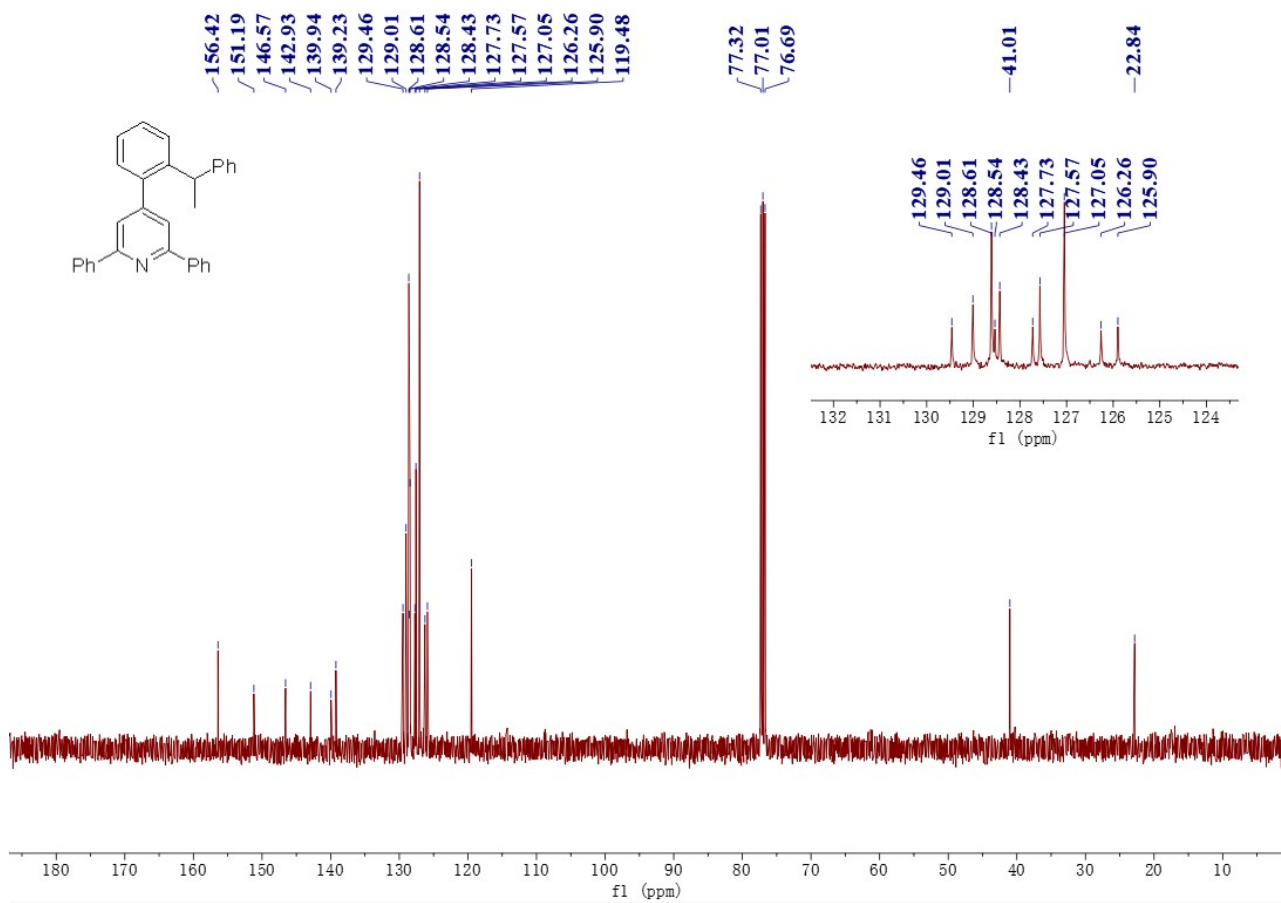


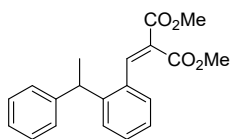


2,6-diphenyl-4-(2-(1-phenylethyl)phenyl)pyridine (8)

A colorless oil. 31.3 mg, 38% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 8.05 (d, $J = 7.4$ Hz, 4H), 7.51-7.40 (m, 10H), 7.33 (t, $J = 7.4$ Hz, 1H), 7.28-7.15 (m, 4H), 7.04 (d, $J = 7.4$ Hz, 2H), 4.28 (q, $J = 7.2$ Hz, 1H), 1.60 (d, $J = 7.2$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 156.4, 151.2, 146.6, 142.9, 139.9, 139.2, 129.5, 129.0, 128.6, 128.5, 128.4, 127.7, 127.6, 127.0, 126.3, 125.9, 119.5, 41.0, 22.8. IR (acetone) ν 3061, 3026, 2927, 1689, 1540, 1449, 1125, 1027, 760, 668 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{31}\text{H}_{26}\text{N}$ (M^+): 412.2060, Found: 412.2052.

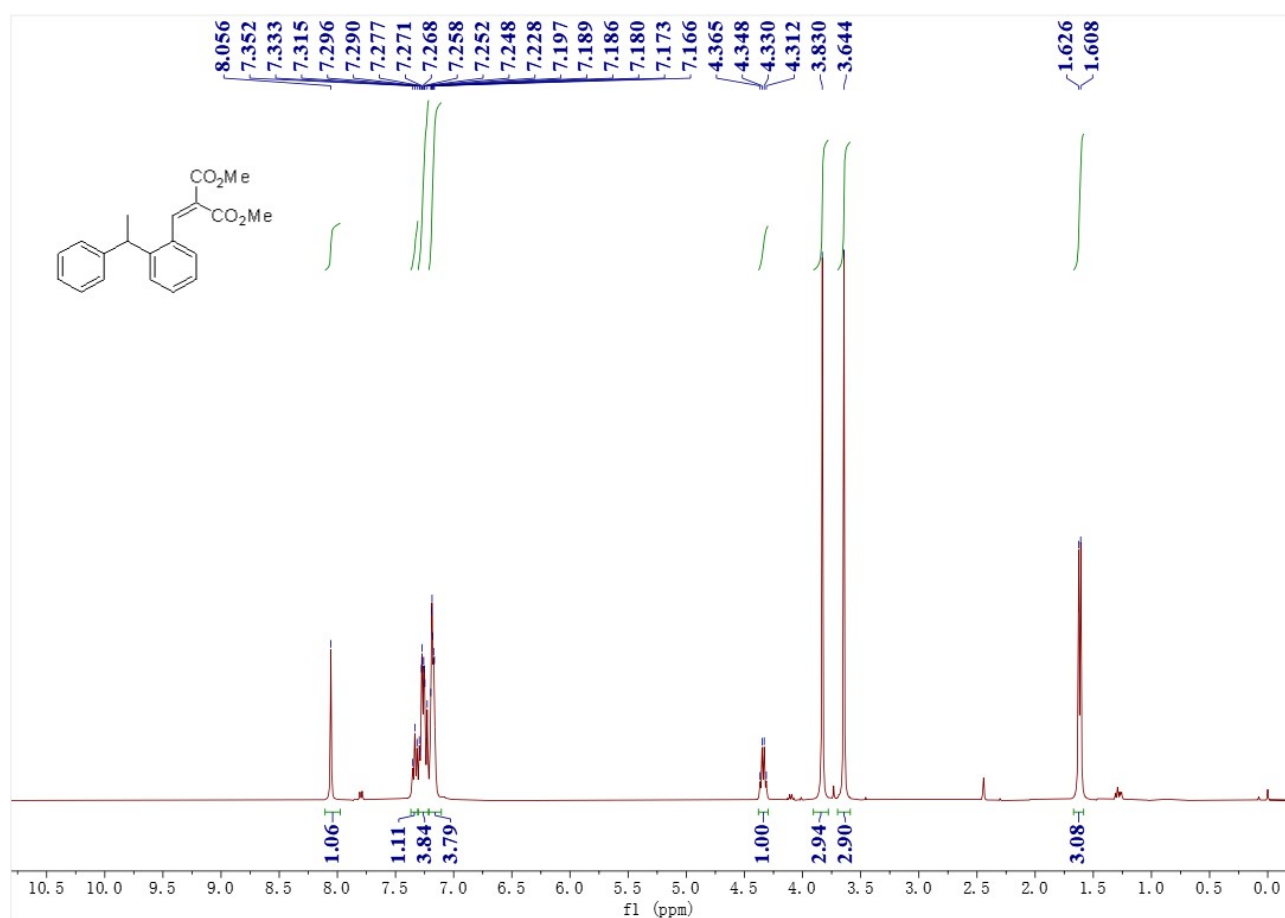


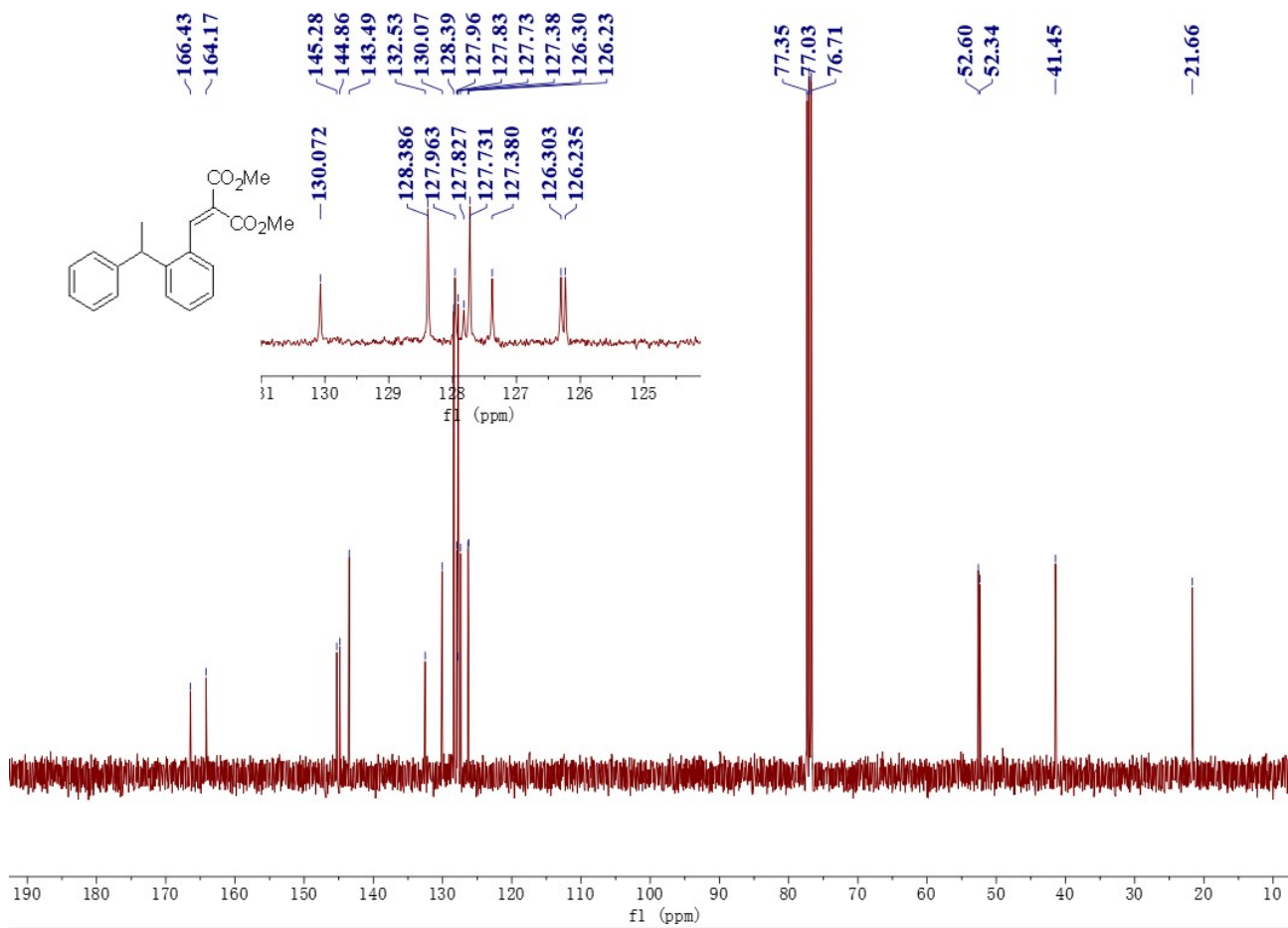




Dimethyl 2-(2-(1-phenylethyl)benzylidene)malonate (9)

A colorless oil. 54.5 mg, 84% yield. ^1H NMR (CDCl_3 , TMS, 400 MHz) δ 8.06 (s, 1H), 7.33 (t, $J = 7.0$ Hz, 1H), 7.30-7.23 (m, 4H), 7.20-7.17 (m, 4H), 4.34 (q, $J = 7.2$ Hz, 1H), 3.83 (s, 3H), 3.64 (s, 3H), 1.62 (d, $J = 7.2$ Hz, 3H). ^{13}C NMR (CDCl_3 , TMS, 100 MHz) δ 166.4, 164.2, 145.3, 144.9, 143.5, 132.5, 130.1, 128.4, 128.0, 127.8, 127.7, 127.4, 126.3, 126.2, 52.6, 52.3, 41.5, 21.7. IR (acetone) ν 3025, 2952, 1726, 1627, 1435, 1363, 1211, 1178, 816, 699 cm^{-1} . HRMS (ESI) calcd. for $\text{C}_{20}\text{H}_{20}\text{O}_4\text{Na}$ ($\text{M}+\text{Na}$) $^+$: 347.1253, Found: 347.1248.





8. Computational details

All quantum mechanical calculations have been performed with Gaussian 16. The geometries of all species have been optimized at M06/def2svp level. The subsequent frequency calculations on the stationary points were carried out at the same level of theory to ascertain the nature of the stationary points as minima on the respective potential energy surfaces. The conformational space of flexible systems has first been searched manually and checked by xtb 6.0 program.¹⁸ Thermochemical corrections to 298.15 K have been calculated for all minima from unscaled vibrational frequencies obtained at this same level. The thermochemical corrections have been combined with single-point energies calculated at the SMD/M06/def2tzvpp//M06/def2svp level to yield free energy G_{298} at 298.15 K. The solvent effect was estimated by the IEFPCM method with radii and nonelectrostatic terms for SMD salvation model in acetonitrile ($\epsilon = 35.688$).

	E_{tot}	H_{298}	G_{298}
1a	-732.338744	-732.338744	-732.104125
Int-1a	-732.263832	-731.970064	-732.033133
Ts-1a	-732.242619	-731.954231	-732.014331
Int-2a	-732.302194	-732.008444	-732.070964
Int-3a	-732.310752	-732.014776	-732.073992
Ts-2a	-732.306983	-732.016095	-732.073266
Ts-3a	-732.293235	-731.999234	-732.057507
2a	-732.368948	-732.072449	-732.131522
3a	-732.336894	-732.040463	-732.099048
1b	-654.989248	-654.728352	-654.7849
Int-1b	-654.907313	-654.650127	-654.707531
Ts-1b	-654.889165	-654.636564	-654.691715
Int-2b	-654.939631	-654.681757	-654.7403
Int-3b	-654.960637	-654.700351	-654.756498
Ts-2b	-654.947388	-654.691995	-654.744907
Ts-3b	-654.933922	-654.675422	-654.728953
2b	-655.011335	-654.750471	-654.806058
3b	-654.977768	-654.716674	-654.770762
1ae	-812.176189	-811.797548	-811.866363
Int-1ae	-812.095129	-811.720512	-811.791202
Ts-1ae	-812.079921	-811.709825	-811.778621
Int-2ae	-812.127374	-811.751853	-811.823366

Int-3ae	-812.147986	-811.770428	-811.839520
Int-2ae'	-812.127120	-811.751467	-811.823698
Int-3ae'	-812.149408	-811.77166	-811.840823
Ts-2ae	-812.140132	-811.766959	-811.834335
Ts-3ae	-812.123888	-811.748006	-811.813468
Ts-3ae'	-812.123368	-811.813846	-811.854388
Ts-4	-812.107609	-811.733128	-811.801746
Ts-5	-812.086964	-811.712161	-811.778749
2ae	-812.202019	-811.823613	-811.893181
3	-812.165864	-811.787379	-811.852386
3'	-812.164283	-811.786353	-811.854980

1a

```

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6535\H,0,-4.020988,0.530039,-2.108992\H,0,-4.70583,-1.408251,-0.688018
\C,0,0.133193,2.226098,0.257531\C,0,-0.646641,3.427361,0.524259\C,0,0.
874793,3.459959,0.484952\H,0,1.365907,3.94665,-0.368272\H,0,1.407937,3
.598201,1.435108\H,0,-1.140421,3.534259,1.498922\H,0,-1.195018,3.90053
8,-0.300498\C,0,-0.709142,-1.424915,1.677207\H,0,-1.29759,-1.540881,2.
61318\O,0,-0.245357,-2.669149,1.214375\H,0,0.122083,-0.73143,1.9098\H,
0,0.441231,-2.982618,1.812748\Version=ES64L-G16RevA.03\State=1-A\HF=-
732.3387442\RMSD=8.285e-09\Dipole=0.2534951,0.5277172,0.7099081\Quadru
pole=1.6223833,-0.1952131,-1.4271702,-1.1478394,3.6668724,-1.974771\PG
=C01 [X(C17H16O1)]\@

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Int-1a

1\1\GINC-B2146\SP\UM06\def2TZVPP\C17H16O1(3)\ROOT\23-Mar-2023\0\#p sc
rf=(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\int1\0,3\C,0,1.63
131,-1.11589,-0.679459\C,0,1.477484,0.22947,-0.254409\C,0,2.656938,0.9
76685,0.003963\C,0,3.911269,0.411311,-0.153183\C,0,4.041285,-0.916706,
-0.573161\C,0,2.892136,-1.670541,-0.832491\H,0,0.740735,-1.721875,-0.8
68362\H,0,2.553615,2.018049,0.330721\H,0,4.804656,1.009209,0.051727\H,
0,5.032895,-1.361284,-0.697896\H,0,2.985446,-2.710376,-1.160239\C,0,0.
191981,0.828304,-0.098449\C,0,-1.076766,0.095243,-0.345259\C,0,-1.6009
26,-0.813209,0.593508\C,0,-1.802857,0.357396,-1.516031\C,0,-2.814134,-
1.451131,0.323698\C,0,-3.011982,-0.282737,-1.769941\H,0,-1.389472,1.06
436,-2.243741\C,0,-3.521076,-1.193186,-0.846143\H,0,-3.203996,-2.16776
4,1.055312\H,0,-3.557039,-0.072464,-2.694849\H,0,-4.470175,-1.701754,-
1.038149\C,0,0.04554,2.201129,0.349229\C,0,-0.811787,2.818483,1.379645
\C,0,-0.825273,3.322387,-0.041273\H,0,-1.706442,3.108624,-0.66278\H,0,
-0.362703,4.297334,-0.246924\H,0,-0.34556,3.448247,2.149455\H,0,-1.679
122,2.243758,1.737258\C,0,-0.849543,-1.173133,1.841704\H,0,-1.571914,-
1.272124,2.680338\O,0,-0.168809,-2.382183,1.611307\H,0,-0.153933,-0.35
1913,2.108044\H,0,0.47189,-2.515812,2.31794\Version=ES64L-G16RevA.03\
State=3-A\HF=-732.2638318\S2=2.034883\S2-1=0.\S2A=2.000639\RMSD=7.871e
-09\Dipole=-0.3548634,0.4988659,0.6905083\Quadrupole=1.754865,-1.84562
71,0.0907621,-0.357858,2.9141383,-1.3654654\PG=C01 [X(C17H16O1)]\@

Ts-1a

1\1\GINC-B2117\SP\UM06\def2TZVPP\C17H16O1(3)\ROOT\23-Mar-2023\0\#p sc
rf=(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\ts1\0,3\C,0,1.679
107,-1.32788,0.826344\C,0,1.488127,-0.219213,-0.029244\C,0,2.640253,0.
337931,-0.625369\C,0,3.903421,-0.193838,-0.394912\C,0,4.065578,-1.2931
22,0.447097\C,0,2.943025,-1.852734,1.058862\H,0,0.813467,-1.755708,1.3

4059\H,0,2.541112,1.183717,-1.310248\H,0,4.773186,0.253065,-0.885778\H
,0,5.060689,-1.70852,0.629532\H,0,3.056332,-2.703751,1.737228\C,0,0.16
1263,0.349151,-0.22837\C,0,-1.027909,-0.484686,-0.24158\C,0,-2.306124,
0.057948,0.078063\C,0,-0.982934,-1.830845,-0.671224\C,0,-3.45413,-0.71
8037,-0.062086\C,0,-2.135486,-2.592521,-0.793035\H,0,-0.020528,-2.2645
94,-0.958279\C,0,-3.383068,-2.040238,-0.495179\H,0,-4.422594,-0.274247
,0.193669\H,0,-2.063697,-3.626021,-1.144888\H,0,-4.29323,-2.637866,-0.
596801\C,0,-0.037906,1.794394,-0.392129\C,0,0.427545,2.760861,-1.42547
9\C,0,0.798374,2.94391,0.01968\H,0,1.835558,2.750842,0.3251\H,0,0.3234
55,3.764312,0.576325\H,0,-0.313173,3.443617,-1.863425\H,0,1.201154,2.4
52124,-2.140418\C,0,-2.378221,1.440367,0.603592\H,0,-3.315887,1.974206
,0.352814\O,0,-2.025648,1.498468,1.941112\H,0,-1.378124,1.950281,-0.05
1605\H,0,-1.998038,2.422116,2.217105\\Version=ES64L-G16RevA.03\State=3
-A\HF=-732.2426193\S2=2.031326\S2-1=0.\S2A=2.000625\RMSD=7.900e-09\Dip
ole=-0.1566856,0.8148417,-0.2220208\Quadrupole=3.6447767,5.0736961,-8.
7184728,-3.7114693,-0.7023492,1.0740496\PG=C01 [X(C17H16O1)]\@

Int-2a

1\1\GINC-B2173\SP\RM06\def2TZVPP\C17H16O1\ROOT\23-Mar-2023\0\#\p scrf=
(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\\int3\\0,1\C,0,1.54550
1,-0.522853,-1.255962\C,0,1.257197,0.365071,-0.210623\C,0,2.319545,0.8
07108,0.590507\C,0,3.61849,0.356289,0.375916\C,0,3.886185,-0.540929,-0
.656232\C,0,2.843534,-0.973821,-1.475022\H,0,0.729898,-0.856062,-1.906
14\H,0,2.11102,1.492554,1.419213\H,0,4.429469,0.707996,1.021288\H,0,4.
907455,-0.892291,-0.831341\H,0,3.046296,-1.66041,-2.302796\C,0,-0.1266
91,0.855595,0.005389\C,0,-1.176686,-0.025512,0.117112\C,0,-0.995624,-1
.488475,0.297439\C,0,-2.577644,0.367097,-0.005496\C,0,-1.997273,-2.369
404,-0.282021\C,0,-3.534293,-0.516543,-0.383987\H,0,-2.868445,1.408224
,0.136807\C,0,-3.220212,-1.903131,-0.623709\H,0,-1.764155,-3.437802,-0
.360716\H,0,-4.562156,-0.169154,-0.527065\H,0,-3.984651,-2.57516,-1.02

3195\C,0,-0.203254,2.348599,-0.00294\C,0,-1.171902,3.186717,0.788485\C,0,-1.251386,3.18275,-0.699905\H,0,-2.077154,2.661685,-1.191666\H,0,-0.901013,4.067289,-1.240649\H,0,-0.776032,4.076794,1.287316\H,0,-1.940965,2.664965,1.36616\C,0,-0.061317,-2.080271,1.087432\H,0,0.794821,2.793689,-0.078029\H,0,-0.028717,-3.177753,1.136648\O,0,0.818618,-1.419504,1.850622\H,0,1.410372,-2.038252,2.290902\\Version=ES64L-G16RevA.03\State=1-A\HF=-732.3107516\RMSD=7.442e-09\Dipole=0.7250124,-0.7213111,0.6476335\Quadrupole=-1.026256,5.8711189,-4.8448629,-3.8217098,4.6550977,-1.5022602\PG=C01 [X(C17H16O1)]\@

Int-3a

1\1\GINC-B2173\SP\RM06\def2TZVPP\C17H16O1\ROOT\23-Mar-2023\0\#\#p scrf=(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\\int3\\0,1\C,0,1.545501,-0.522853,-1.255962\C,0,1.257197,0.365071,-0.210623\C,0,2.319545,0.807108,0.590507\C,0,3.61849,0.356289,0.375916\C,0,3.886185,-0.540929,-0.656232\C,0,2.843534,-0.973821,-1.475022\H,0,0.729898,-0.856062,-1.90614\H,0,2.11102,1.492554,1.419213\H,0,4.429469,0.707996,1.021288\H,0,4.907455,-0.892291,-0.831341\H,0,3.046296,-1.66041,-2.302796\C,0,-0.126691,0.855595,0.005389\C,0,-1.176686,-0.025512,0.117112\C,0,-0.995624,-1.488475,0.297439\C,0,-2.577644,0.367097,-0.005496\C,0,-1.997273,-2.369404,-0.282021\C,0,-3.534293,-0.516543,-0.383987\H,0,-2.868445,1.408224,0.136807\C,0,-3.220212,-1.903131,-0.623709\H,0,-1.764155,-3.437802,-0.360716\H,0,-4.562156,-0.169154,-0.527065\H,0,-3.984651,-2.57516,-1.023195\C,0,-0.203254,2.348599,-0.00294\C,0,-1.171902,3.186717,0.788485\C,0,-1.251386,3.18275,-0.699905\H,0,-2.077154,2.661685,-1.191666\H,0,-0.901013,4.067289,-1.240649\H,0,-0.776032,4.076794,1.287316\H,0,-1.940965,2.664965,1.36616\C,0,-0.061317,-2.080271,1.087432\H,0,0.794821,2.793689,-0.078029\H,0,-0.028717,-3.177753,1.136648\O,0,0.818618,-1.419504,1.850622\H,0,1.410372,-2.038252,2.290902\\Version=ES64L-G16RevA.03\State=1-A\HF=-732.3107516\RMSD=7.442e-09\Dipole=0.7250124,-0.7213111,0.6476335\Quadrupole=-1.026256,5.8711189,-4.8448629,-3.8217098,4.6550977,

-1.5022602\PG=C01 [X(C17H16O1)]\@

Ts-2a

1\1\GINC-B2153\SP\RM06\def2TZVPP\C17H16O1\ROOT\23-Mar-2023\0\#\#p scrf=(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\ts2\0,1\C,0,1.840419,-1.232778,0.747509\C,0,1.548131,0.007253,0.14539\C,0,2.626059,0.723727,-0.403285\C,0,3.923117,0.217112,-0.368165\C,0,4.186324,-1.01904,0.21538\C,0,3.132238,-1.741873,0.775425\H,0,1.028686,-1.797032,1.220148\H,0,2.444401,1.690709,-0.879449\H,0,4.73896,0.798031,-0.809505\H,0,5.205762,-1.414425,0.241982\H,0,3.322707,-2.707671,1.253573\C,0,0.167852,0.538196,0.173234\C,0,-0.924625,-0.352742,-0.108531\C,0,-2.225685,-0.14799,0.488527\C,0,-0.795082,-1.506775,-0.935004\C,0,-3.335353,-0.962488,0.115834\C,0,-1.883984,-2.268832,-1.282212\H,0,0.185907,-1.729421,-1.3654\C,0,-3.179461,-1.99015,-0.772209\H,0,-4.309206,-0.760445,0.576254\H,0,-1.753573,-3.095783,-1.987202\H,0,-4.031035,-2.606753,-1.070783\C,0,0.026921,1.995618,-0.188231\C,0,-1.205861,2.5936,-0.784319\C,0,-0.004584,2.393918,-1.646127\H,0,-0.029665,1.570111,-2.369515\H,0,0.573264,3.266679,-1.969169\H,0,-1.460774,3.613417,-0.480376\H,0,-2.076926,1.954064,-0.958286\C,0,-2.29149,0.596809,1.675879\H,0,0.600285,2.675904,0.458634\H,0,-0.431541,0.932958,1.530602\H,0,-3.188487,0.517213,2.313932\O,0,-1.306049,1.253883,2.15\Version=ES64L-G16RevA.03\State=1-A\HF=-732.306983\RMSD=6.346e-09\Dipole=-1.2279223,-0.3269,-0.1528412\Quadrupole=5.611882,0.5511522,-6.1630342,2.3814376,-3.5064287,-0.6692986\PG=C01 [X(C17H16O1)]\@

Ts-3a

1\1\GINC-B2135\SP\RM06\def2TZVPP\C17H16O1\ROOT\29-Mar-2023\0\#\#p def2tzvpp m06 scrf=(iefpcm,smd,solvent=Acetonitrile)\ts3\0,1\C,0,1.269061,-1.220736,-0.892119\C,0,1.233879,0.080501,-0.352183\C,0,2.466124,0.66695,-0.003465\C,0,3.666516,-0.017897,-0.16652\C,0,3.679993,-1.310445,-

0.686161\C,0,2.469362,-1.90269,-1.047361\H,0,0.33363,-1.69514,-1.20771
3\H,0,2.477013,1.676894,0.420514\H,0,4.605384,0.466884,0.120076\H,0,4.
62325,-1.848074,-0.817748\H,0,2.460296,-2.910758,-1.47376\C,0,-0.01946
8,0.839276,-0.189802\C,0,-1.293924,0.168315,-0.286932\C,0,-1.368876,-0
.787133,0.747879\C,0,-2.332213,0.240421,-1.235442\C,0,-2.241419,-1.888
934,0.669722\C,0,-3.259389,-0.788426,-1.25216\H,0,-2.346587,1.024019,-
2.000199\C,0,-3.189278,-1.865801,-0.336754\H,0,-2.209375,-2.692827,1.4
11264\H,0,-4.039193,-0.798669,-2.020025\H,0,-3.919835,-2.676572,-0.415
039\C,0,0.080147,2.308763,-0.411232\C,0,0.000524,3.275972,0.750756\C,0
, -1.108725,3.207129,-0.239786\H,0,-2.049421,2.746794,0.080685\H,0,-1.2
3168,4.0339,-0.94572\H,0,0.669372,4.142622,0.741738\H,0,-0.175955,2.85
727,1.747701\C,0,-0.446361,-0.384443,1.750135\H,0,-0.503436,0.623785,2
.169044\O,0,0.269031,-1.297863,2.411471\H,0,0.715418,-0.901337,3.16965
9\H,0,0.803148,2.609173,-1.183697\\Version=ES64L-G16RevA.03\State=1-A\
HF=-732.2932348\RMSD=4.962e-09\Dipole=-0.3163795,0.7017269,1.2441033\Q
uadrupole=-3.080414,-0.4476268,3.5280408,2.6507993,4.7016802,0.3587966
\PG=C01 [X(C17H16O1)]\@

2a

1\1\GINC-B2153\SP\RM06\def2TZVPP\C17H16O1\ROOT\23-Mar-2023\0\#\#p scrf=
(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\\2b\\0,1\C,0,1.929907,
-0.882082,1.189316\C,0,1.569318,0.169622,0.336226\C,0,2.53295,0.666437
, -0.544547\C,0,3.818775,0.123824,-0.575131\C,0,4.161538,-0.922766,0.27
4462\C,0,3.208717,-1.425642,1.161214\H,0,1.18228,-1.277303,1.887606\H,
0,2.277939,1.488432,-1.219672\H,0,4.559278,0.52774,-1.272157\H,0,5.169
958,-1.345909,0.250537\H,0,3.46767,-2.244734,1.838843\C,0,0.155162,0.7
1085,0.416391\C,0,-0.857574,-0.307457,-0.070809\C,0,-2.120522,-0.48669
8,0.542123\C,0,-0.56053,-1.09672,-1.186256\C,0,-3.019482,-1.431953,0.0
26187\C,0,-1.468454,-2.021254,-1.696737\H,0,0.420635,-0.98802,-1.66034
6\C,0,-2.709732,-2.195663,-1.089916\H,0,-3.986423,-1.558631,0.526611\H

, 0, -1.198018, -2.615261, -2.574667\H, 0, -3.424725, -2.924085, -1.48119\C, 0, -0.005282, 2.068548, -0.252419\C, 0, -1.320072, 2.600642, -0.7172\C, 0, -0.268041, 2.241041, -1.71902\H, 0, -0.435624, 1.342054, -2.323582\H, 0, 0.25518, 3.043437, -2.249517\H, 0, -1.538916, 3.65702, -0.536903\H, 0, -2.197786, 1.948319, -0.654421\C, 0, -2.595961, 0.247211, 1.738228\H, 0, 0.667073, 2.815104, 0.190814\H, 0, -0.057794, 0.884849, 1.48352\H, 0, -3.611138, -0.105463, 2.074286\O, 0, -2.031736, 1.125602, 2.340948\\Version=ES64L-G16RevA.03\State=1-A\HF=-732.3689482\RMSD=3.954e-09\Dipole=-0.3939918, -1.0252717, -1.0721315\Quadrupole=5.6349364, -0.2730597, -5.3618767, 5.434219, 0.1236291, -3.3179892\PG=C01 [X(C17H16O1)]\\@

3a

1\1\GINC-B2131\SP\RM06\def2TZVPP\C17H16O1\ROOT\03-Apr-2023\0\#\#p scrf=(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\\int1\\0,1\C, 0, -1.557372, -0.931742, 1.100714\C, 0, -1.374192, -0.022223, 0.057576\C, 0, -2.495843, 0.354472, -0.695357\C, 0, -3.75751, -0.161246, -0.4158\C, 0, -3.925839, -1.062348, 0.634559\C, 0, -2.821639, -1.443273, 1.390853\H, 0, -0.694621, -1.25198, 1.69266\H, 0, -2.382152, 1.075082, -1.515609\H, 0, -4.617129, 0.145748, -1.019104\H, 0, -4.91654, -1.46692, 0.860513\H, 0, -2.941419, -2.15181, 2.215848\C, 0, -0.024842, 0.553739, -0.287861\C, 0, 1.193967, -0.101296, 0.343825\C, 0, 1.698347, -0.556781, -0.867083\C, 0, 1.865203, -0.307062, 1.542462\C, 0, 2.887376, -1.2621, -0.966079\C, 0, 3.070255, -1.01521, 1.458903\H, 0, 1.489296, 0.041899, 2.510269\C, 0, 3.568093, -1.482688, 0.236538\H, 0, 3.282264, -1.633933, -1.915606\H, 0, 3.639308, -1.215244, 2.372095\H, 0, 4.512553, -2.035468, 0.228189\C, 0, -0.045437, 2.069306, -0.213721\C, 0, 1.20571, 2.865738, -0.009265\C, 0, 0.188975, 2.766737, 1.08664\H, 0, 0.434978, 2.142677, 1.953617\H, 0, -0.416417, 3.6452, 1.328568\H, 0, 1.303697, 3.816056, -0.542639\H, 0, 2.148731, 2.322502, 0.119203\C, 0, 0.559702, 0.003219, -1.676791\H, 0, 0.848676, 0.848066, -2.341565\O, 0, -0.161394, -0.975238, -2.347649\H, 0, -1.014536, -0.611389, -2.613731\H, 0, -0.795265, 2.527959, -0.872194\\Version=ES64L-G16RevA.03\State=1-A\HF=-

732.3368942\RMSD=4.450e-09\Dipole=-0.2844837,0.7514912,0.0332811\Quadrupole=4.0238943,-4.7762762,0.752382,-2.300155,3.5517738,-5.8658127\PG=C01 [X(C17H16O1)]\@

1b

1\1\GINC-A01R04N01\SP\RM06\def2TZVPP\C15H14O1\ACJSGGHI7X\05-May-2023\0
\#p scrf=(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\1\0,1\C,0,
-1.563191,-0.201725,-1.028959\C,0,-1.605906,0.096395,0.341459\C,0,-2.8
63015,0.202892,0.956159\C,0,-4.033076,0.040411,0.223467\C,0,-3.974713,
-0.236553,-1.142175\C,0,-2.734836,-0.358291,-1.764196\H,0,-0.592274,-0
.305299,-1.524952\H,0,-2.922044,0.392809,2.032262\H,0,-5.001964,0.1194
11,0.725419\H,0,-2.676921,-0.58161,-2.833509\C,0,-0.35013,0.300287,1.1
01624\C,0,0.879062,-0.367681,0.582937\C,0,1.905377,0.365824,-0.037376\
C,0,0.999147,-1.755751,0.698038\C,0,3.032135,-0.307777,-0.513981\C,0,2
.129354,-2.417923,0.228556\H,0,0.183184,-2.316967,1.16681\C,0,3.148061
, -1.688536,-0.37906\H,0,3.815634,0.273807,-1.005043\H,0,2.211253,-3.50
3665,0.333031\H,0,4.038697,-2.198601,-0.758042\C,0,-0.288351,1.047223,
2.214908\C,0,1.785616,1.856063,-0.203679\H,0,1.854172,2.339714,0.79454
8\O,0,2.778159,2.324458,-1.07005\H,0,2.711947,3.282128,-1.121518\H,0,-
1.15974,1.578214,2.610639\H,0,0.652342,1.152536,2.765113\H,0,0.762999,
2.090501,-0.573327\H,0,-4.895758,-0.367784,-1.717369\Version=ES64L-G1
6RevC.01\State=1-A\HF=-654.989248\RMSD=6.427e-09\Dipole=-0.5342839,0.6
870356,0.2145184\Quadrupole=-0.8489455,3.2000785,-2.3511331,1.2323526,
-0.0945339,1.5543305\PG=C01 [X(C15H14O1)]\@

Int-1b

1\1\GINC-A01R04N04\SP\UM06\def2TZVPP\C15H14O1(3)\ACJSGGHI7X\05-May-202
3\0\#p scrf=(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\int1\0,
3\C,0,-1.931397,0.809392,0.75165\C,0,-1.666058,-0.264481,-0.136019\C,0
, -2.78179,-1.000069,-0.609468\C,0,-4.077077,-0.661908,-0.249135\C,0,-4
.313628,0.411088,0.613246\C,0,-3.229121,1.135674,1.11482\H,0,-1.095208

,1.36917,1.179724\H,0,-2.607751,-1.846147,-1.283507\H,0,-4.91683,-1.24
2314,-0.64306\H,0,-3.400849,1.963124,1.809894\C,0,-0.328499,-0.657192,
-0.504821\C,0,0.826643,0.234196,-0.351616\C,0,2.098985,-0.234331,0.064
811\C,0,0.70119,1.59801,-0.686386\C,0,3.168884,0.654938,0.144423\C,0,1
.778938,2.470527,-0.611876\H,0,-0.266058,1.963522,-1.044605\C,0,3.0196
71,1.998865,-0.191083\H,0,4.131459,0.273069,0.49137\H,0,1.649544,3.519
94,-0.892356\H,0,3.875805,2.67643,-0.123558\C,0,-0.135098,-1.948791,-1
.174702\C,0,2.302949,-1.669592,0.460611\H,0,2.226906,-2.304095,-0.4509
02\O,0,3.538414,-1.830486,1.094836\H,0,3.66914,-2.765482,1.276009\H,0,
-0.172042,-2.900107,-0.628219\H,0,-0.131245,-2.014754,-2.271707\H,0,1.
45748,-1.980436,1.113572\H,0,-5.335217,0.674022,0.901919\\Version=ES64
L-G16RevC.01\State=3-A\HF=-654.9073129\S2=2.036553\S2-1=0.\S2A=2.00081
7\RMSD=9.073e-09\Dipole=-0.3971991,-0.8788425,-0.1409607\Quadrupole=-1
.7417965,7.5025552,-5.7607587,-3.3337276,0.1571418,0.964926\PG=C01 [X(
C15H14O1)]\@

Int-1b

1\1\GINC-A01R04N04\SP\UM06\def2TZVPP\C15H14O1(3)\ACJSGGHI7X\05-May-202
3\0\#p scrf=(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\int1\0,
3\C,0,-1.931397,0.809392,0.75165\C,0,-1.666058,-0.264481,-0.136019\C,0
, -2.78179,-1.000069,-0.609468\C,0,-4.077077,-0.661908,-0.249135\C,0,-4
.313628,0.411088,0.613246\C,0,-3.229121,1.135674,1.11482\H,0,-1.095208
,1.36917,1.179724\H,0,-2.607751,-1.846147,-1.283507\H,0,-4.91683,-1.24
2314,-0.64306\H,0,-3.400849,1.963124,1.809894\C,0,-0.328499,-0.657192,
-0.504821\C,0,0.826643,0.234196,-0.351616\C,0,2.098985,-0.234331,0.064
811\C,0,0.70119,1.59801,-0.686386\C,0,3.168884,0.654938,0.144423\C,0,1
.778938,2.470527,-0.611876\H,0,-0.266058,1.963522,-1.044605\C,0,3.0196
71,1.998865,-0.191083\H,0,4.131459,0.273069,0.49137\H,0,1.649544,3.519
94,-0.892356\H,0,3.875805,2.67643,-0.123558\C,0,-0.135098,-1.948791,-1
.174702\C,0,2.302949,-1.669592,0.460611\H,0,2.226906,-2.304095,-0.4509

02\O,0,3.538414,-1.830486,1.094836\H,0,3.66914,-2.765482,1.276009\H,0,
-0.172042,-2.900107,-0.628219\H,0,-0.131245,-2.014754,-2.271707\H,0,1.
45748,-1.980436,1.113572\H,0,-5.335217,0.674022,0.901919\\Version=ES64
L-G16RevC.01\State=3-A\HF=-654.9073129\S2=2.036553\S2-1=0.\S2A=2.00081
7\RMSD=9.073e-09\Dipole=-0.3971991,-0.8788425,-0.1409607\Quadrupole=-1
.7417965,7.5025552,-5.7607587,-3.3337276,0.1571418,0.964926\PG=C01 [X(
C15H14O1)]\@

Ts-1b

1\1\GINC-A01R04N04\SP\UM06\def2TZVPP\C15H14O1(3)\ACJSGGHI7X\05-May-202
3\0\#p scrf=(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\ts1\0,3
\C,0,-2.04536,0.818862,0.738121\C,0,-1.661448,-0.278469,-0.071017\C,0,
-2.700306,-1.052261,-0.641188\C,0,-4.03519,-0.730379,-0.441652\C,0,-4.
388435,0.364019,0.349736\C,0,-3.381825,1.129726,0.942383\H,0,-1.273029
,1.40877,1.240238\H,0,-2.437651,-1.907663,-1.271756\H,0,-4.813602,-1.3
39762,-0.910809\H,0,-3.64574,1.975943,1.584013\C,0,-0.276989,-0.647953
, -0.26942\C,0,0.820185,0.298938,-0.167044\C,0,2.12684,-0.153587,0.1765
49\C,0,0.673518,1.662078,-0.511522\C,0,3.215013,0.716885,0.120677\C,0,
1.760441,2.522018,-0.54033\H,0,-0.31014,2.028199,-0.81939\C,0,3.039837
,2.05183,-0.229746\H,0,4.205316,0.328496,0.373949\H,0,1.615521,3.56633
1,-0.83232\H,0,3.899012,2.728037,-0.261499\C,0,0.061537,-2.033871,-0.6
68164\C,0,2.291297,-1.555405,0.611508\O,0,3.568746,-2.036384,0.436965\
H,0,3.664298,-2.865411,0.916682\H,0,0.263857,-2.206355,-1.739099\H,0,1
.369743,-2.123443,-0.097198\H,0,-0.5143,-2.847921,-0.205953\H,0,1.8730
07,-1.742131,1.622619\H,0,-5.440965,0.613383,0.51145\\Version=ES64L-G1
6RevC.01\State=3-A\HF=-654.8891648\S2=2.03225\S2-1=0.\S2A=2.000655\RMS
D=6.286e-09\Dipole=-0.0472013,-0.7399848,0.5260634\Quadrupole=-0.51815
19,5.863523,-5.3453712,-3.3552396,3.8909293,-1.4023043\PG=C01 [X(C15H1
4O1)]\@

Ts-1b

1\1\GINC-A01R04N04\SP\UM06\def2TZVPP\C15H14O1(3)\ACJSGGHI7X\05-May-2023\0\#\#p scrf=(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\ts1\0,3\C,0,-2.04536,0.818862,0.738121\C,0,-1.661448,-0.278469,-0.071017\C,0,-2.700306,-1.052261,-0.641188\C,0,-4.03519,-0.730379,-0.441652\C,0,-4.388435,0.364019,0.349736\C,0,-3.381825,1.129726,0.942383\H,0,-1.273029,1.40877,1.240238\H,0,-2.437651,-1.907663,-1.271756\H,0,-4.813602,-1.339762,-0.910809\H,0,-3.64574,1.975943,1.584013\C,0,-0.276989,-0.647953,-0.26942\C,0,0.820185,0.298938,-0.167044\C,0,2.12684,-0.153587,0.176549\C,0,0.673518,1.662078,-0.511522\C,0,3.215013,0.716885,0.120677\C,0,1.760441,2.522018,-0.54033\H,0,-0.31014,2.028199,-0.81939\C,0,3.039837,2.05183,-0.229746\H,0,4.205316,0.328496,0.373949\H,0,1.615521,3.566331,-0.83232\H,0,3.899012,2.728037,-0.261499\C,0,0.061537,-2.033871,-0.668164\C,0,2.291297,-1.555405,0.611508\O,0,3.568746,-2.036384,0.436965\H,0,3.664298,-2.865411,0.916682\H,0,0.263857,-2.206355,-1.739099\H,0,1.369743,-2.123443,-0.097198\H,0,-0.5143,-2.847921,-0.205953\H,0,1.873007,-1.742131,1.622619\H,0,-5.440965,0.613383,0.51145\Version=ES64L-G16RevC.01\State=3-A\HF=-654.8891648\S2=2.03225\S2-1=0.\S2A=2.000655\RMSD=6.286e-09\Dipole=-0.0472013,-0.7399848,0.5260634\Quadrupole=-0.5181519,5.863523,-5.3453712,-3.3552396,3.8909293,-1.4023043\PG=C01 [X(C15H14O1)]\@

Int-2b

1\1\GINC-A01R04N01\SP\UM06\def2TZVPP\C15H14O1(3)\ACJSGGHI7X\05-May-2023\0\#\#p scrf=(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\int1\0,3\C,0,-1.427792,0.415763,-1.047064\C,0,-1.462583,-0.477854,0.05781\C,0,-2.733952,-0.741812,0.63362\C,0,-3.884983,-0.144204,0.142417\C,0,-3.823109,0.733851,-0.942731\C,0,-2.584337,1.003817,-1.532698\H,0,-0.46766,0.623208,-1.5296\H,0,-2.811228,-1.421258,1.487246\H,0,-4.848821,-0.364619,0.611523\H,0,-2.524644,1.680846,-2.390322\C,0,-0.271912,-1.087788

,0.56264\C,0,1.064272,-0.702707,0.054369\C,0,1.609155,0.602306,0.29436
3\C,0,1.835415,-1.636339,-0.63336\C,0,2.906634,0.895879,-0.204734\C,0,
3.111442,-1.330135,-1.116355\H,0,1.414267,-2.633846,-0.80478\C,0,3.637
564,-0.053406,-0.897506\H,0,3.321689,1.88981,-0.017985\H,0,3.687985,-2
.083832,-1.659758\H,0,4.635438,0.198111,-1.269585\C,0,-0.34459,-2.1550
44,1.607448\C,0,0.891115,1.566473,1.024879\H,0,-0.102056,1.366305,1.44
0722\O,0,1.446261,2.775371,1.252002\H,0,0.823909,3.334742,1.727488\H,0
, -1.066949,-2.949674,1.347034\H,0,0.63741,-2.624187,1.765343\H,0,-0.66
9807,-1.752228,2.586808\H,0,-4.733655,1.200857,-1.32874\\Version=ES64L
-G16RevC.01\State=3-A\HF=-654.9396309\S2=2.054035\S2-1=0.\S2A=2.001816
\RMSD=8.144e-09\Dipole=-0.7203345,0.3437949,0.8125015\Quadrupole=-2.48
43459,3.6415651,-1.1572192,-2.1535501,-3.5624668,1.3680499\PG=C01 [X(C
15H14O1)]\@

Int-3b

1\1\GINC-A01R04N04\SP\RM06\def2TZVPP\C15H14O1\ACJSGGHI7X\05-May-2023\
\#p scrf=(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\\int1\\0,1\C
,0,-2.132394,0.182339,1.153341\C,0,-1.6615,-0.366392,-0.049503\C,0,-2.
588176,-0.575644,-1.081971\C,0,-3.927953,-0.2335,-0.925701\C,0,-4.3777
84,0.314125,0.274575\C,0,-3.473345,0.519759,1.314238\H,0,-1.424223,0.3
38893,1.974203\H,0,-2.24497,-0.994913,-2.034104\H,0,-4.627901,-0.39276
9,-1.751525\H,0,-3.815955,0.942056,2.263756\C,0,-0.237313,-0.758365,-0
.199234\C,0,0.7759,0.160915,-0.042519\C,0,2.218717,-0.168084,0.014258\
C,0,0.476402,1.58733,-0.03888\C,0,3.183383,0.866135,-0.318417\C,0,1.43
0177,2.529001,-0.235224\H,0,-0.5699,1.894811,0.029551\C,0,2.810491,2.1
61228,-0.427224\H,0,4.231247,0.571898,-0.417627\H,0,1.144293,3.583803,
-0.289391\H,0,3.551975,2.935828,-0.643046\C,0,-0.024501,-2.199732,-0.5
43923\C,0,2.683553,-1.359867,0.479055\H,0,2.016057,-2.129512,0.877383\
O,0,4.004153,-1.62462,0.540954\H,0,4.146114,-2.493731,0.928139\H,0,-0.
839587,-2.566591,-1.188712\H,0,0.936059,-2.368237,-1.059292\H,0,-0.038

512,-2.858396,0.346349\H,0,-5.431856,0.578345,0.39947\\Version=ES64L-G
16RevC.01\State=1-A\HF=-654.9606367\RMSD=5.994e-09\Dipole=0.17014,-1.3
572807,0.4558334\Quadrupole=1.1224865,3.4406814,-4.5631679,-8.4372924,
3.2479443,-1.5211806\PG=C01 [X(C15H14O1)]\\@

Ts-2b

1\1\GINC-A01R02N08\SP\RM06\def2TZVPP\C15H14O1\ACJSGGHI7X\05-May-2023\
\#p scrf=(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\\ts2\\0,1\C,
0,1.718359,-0.725825,0.921834\C,0,1.486605,0.20706,-0.109579\C,0,2.605
956,0.638582,-0.843326\C,0,3.880658,0.143041,-0.579789\C,0,4.081882,-0
.79588,0.427745\C,0,2.987949,-1.225199,1.180457\H,0,0.87771,-1.046332,
1.546984\H,0,2.483101,1.372288,-1.644527\H,0,4.728237,0.497188,-1.1746
93\H,0,3.129566,-1.947162,1.99064\C,0,0.133839,0.752748,-0.335743\C,0,
-1.006819,-0.115142,-0.254527\C,0,-2.297949,0.41428,0.129727\C,0,-0.95
6683,-1.520046,-0.489185\C,0,-3.467741,-0.400245,0.067117\C,0,-2.10074
3,-2.277747,-0.544166\H,0,0.009453,-1.974647,-0.726393\C,0,-3.380736,-
1.716958,-0.288188\H,0,-4.430927,0.046399,0.339151\H,0,-2.02664,-3.334
808,-0.818328\H,0,-4.275449,-2.341517,-0.350566\C,0,0.026085,1.935331,
-1.286406\C,0,-2.316508,1.574074,0.918118\H,0,-3.228515,1.824531,1.486
475\O,0,-1.284936,2.292824,1.144048\H,0,-0.43299,1.685925,0.741689\H,0
,0.578597,2.823055,-0.931591\H,0,0.436714,1.670444,-2.278192\H,0,-1.01
8047,2.236331,-1.45203\H,0,5.083746,-1.182736,0.634476\\Version=ES64L-
G16RevC.01\State=1-A\HF=-654.9473878\RMSD=7.318e-09\Dipole=-1.2612361,
-0.3635929,-0.0409423\Quadrupole=6.6608312,-2.1245686,-4.5362625,-0.40
7443,-2.9125702,-2.336493\PG=C01 [X(C15H14O1)]\\@

Ts-3b

1\1\GINC-A02R04N06\SP\RM06\def2TZVPP\C15H14O1\ACJSGGHI7X\05-May-2023\
\#p scrf=(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\\ts3\\0,1\C,
0,-1.762079,-0.846679,-0.805827\C,0,-1.520117,0.113588,0.200944\C,0,-2

.6451,0.714766,0.803981\C,0,-3.936649,0.356624,0.435204\C,0,-4.151392,
-0.608083,-0.548303\C,0,-3.053373,-1.206906,-1.16735\H,0,-0.907853,-1.
302955,-1.318011\H,0,-2.505423,1.467351,1.5847\H,0,-4.78984,0.834995,0
.925999\H,0,-3.207549,-1.956075,-1.949952\C,0,-0.15427,0.491828,0.5413
96\C,0,0.943765,-0.410542,0.267613\C,0,2.003963,0.323977,-0.308472\C,0
,1.127444,-1.778341,0.545096\C,0,3.330619,-0.155438,-0.281344\C,0,2.41
4553,-2.285433,0.471332\H,0,0.299331,-2.39571,0.909282\C,0,3.511912,-1
.469478,0.104382\H,0,4.166512,0.467166,-0.614216\H,0,2.600926,-3.32679
3,0.751633\H,0,4.516972,-1.902421,0.102337\C,0,0.04214,1.575383,1.5698
69\C,0,1.436128,1.476259,-0.903442\O,0,2.11493,2.632137,-0.943313\H,0,
1.721413,3.232661,-1.588152\H,0,-0.405204,1.281988,2.541279\H,0,1.1082
57,1.772835,1.752463\H,0,-0.431324,2.532077,1.283656\H,0,0.558056,1.37
5776,-1.548726\H,0,-5.168969,-0.887128,-0.836258\\Version=ES64L-G16Rev
C.01\State=1-A\HF=-654.9339223\RMSD=2.105e-09\Dipole=-0.0606505,0.8405
196,-0.8086397\Quadrupole=-1.6572914,3.8564963,-2.1992049,0.2143846,-2
.2348861,-3.3663866\PG=C01 [X(C15H14O1)]\@

2b

1\1\GINC-A01R04N01\SP\RM06\def2TZVPP\C15H14O1\ACJSGGHI7X\05-May-2023\
\#p scrf=(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\\int1\\0,1\C
,0,1.83884,-0.152038,-1.294389\C,0,1.588615,-0.505919,0.038213\C,0,2.6
2515,-0.370698,0.963906\C,0,3.876103,0.108255,0.570009\C,0,4.109827,0.
456867,-0.755613\C,0,3.082727,0.32358,-1.690822\H,0,1.031479,-0.250054
, -2.030143\H,0,2.466405,-0.639925,2.012189\H,0,4.674492,0.206761,1.311
547\H,0,3.255137,0.59159,-2.73735\C,0,0.206139,-1.007459,0.404814\C,0,
-0.847613,0.080027,0.25321\C,0,-2.159115,-0.183654,-0.194083\C,0,-0.53
6987,1.388649,0.640058\C,0,-3.102443,0.853064,-0.262808\C,0,-1.482002,
2.406722,0.577959\H,0,0.476387,1.613024,0.989815\C,0,-2.773494,2.14332
6,0.11924\H,0,-4.103133,0.599203,-0.624962\H,0,-1.205638,3.419194,0.88
7051\H,0,-3.515807,2.944251,0.063895\C,0,0.106863,-1.618264,1.798054\C

,0,-2.624693,-1.530863,-0.600054\O,0,-3.743601,-1.772887,-0.980414\H,0
,0.264779,-0.855834,2.579603\H,0,-0.896382,-2.042402,1.962554\H,0,0.84
6317,-2.422138,1.943495\H,0,-1.866857,-2.354094,-0.532445\H,0,-0.01651
6,-1.806522,-0.324826\H,0,5.090633,0.830467,-1.063273\\Version=ES64L-G
16RevC.01\State=1-A\HF=-655.0113348\RMSD=7.388e-09\Dipole=1.3000127,0.
6665061,0.6590625\Quadrupole=-6.6292011,3.3934851,3.235716,-6.1009573,
-2.5350801,-1.8525623\PG=C01 [X(C15H14O1)]\@

3b

1\1\GINC-A01R08N05\SP\RM06\def2TZVPP\C15H14O1\ACJSGGHI7X\05-May-2023\
\#p scrf=(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\\3-3\\0,1\C,
0,-1.476874,-1.047987,-0.673833\C,0,-1.389201,0.084933,0.149364\C,0,-2
.57948,0.615516,0.65914\C,0,-3.812469,0.039471,0.355234\C,0,-3.882088,
-1.08118,-0.466481\C,0,-2.7053,-1.623521,-0.980878\H,0,-0.558295,-1.49
1155,-1.075335\H,0,-2.553502,1.493135,1.310868\H,0,-4.727657,0.472456,
0.770337\H,0,-2.744153,-2.507869,-1.62399\C,0,-0.039324,0.708216,0.419
28\C,0,1.135755,-0.255448,0.494511\C,0,1.822352,0.32278,-0.565229\C,0,
1.637236,-1.337682,1.201591\C,0,3.07985,-0.107261,-0.961635\C,0,2.9029
44,-1.788148,0.807368\H,0,1.097378,-1.816611,2.024322\C,0,3.609386,-1.
184001,-0.240977\H,0,3.636957,0.351752,-1.783207\H,0,3.360993,-2.63196
5,1.333014\H,0,4.598767,-1.572057,-0.502357\C,0,0.706272,1.279692,-0.8
88111\O,0,1.058016,2.622915,-0.915063\H,0,0.297977,3.13599,-1.211371\H
,0,0.148046,0.981325,-1.801221\C,0,-0.027837,1.730505,1.539879\H,0,-0.
664396,2.599917,1.303234\H,0,-0.386234,1.289755,2.484863\H,0,0.991744,
2.111274,1.698654\H,0,-4.849085,-1.534572,-0.702639\\Version=ES64L-G16
RevC.01\State=1-A\HF=-654.9777681\RMSD=5.248e-09\Dipole=-0.6020119,0.0
146908,-0.203206\Quadrupole=0.7468128,0.3364833,-1.0832961,-5.5915777,
-0.8709648,-0.5463649\PG=C01 [X(C15H14O1)]\@

1ae

1\1\GINC-A06R04N08\SP\RM06\def2TZVPP\C19H22O1\ACJSGGHI7X\20-Apr-2023\
\\#p scrf=(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\\1\\0,1\C,0,
1.835182,0.306781,-0.90498\C,0,1.840681,0.655518,0.455081\C,0,3.067367
,0.621689,1.136517\C,0,4.235391,0.228577,0.493318\C,0,4.208632,-0.1363
36,-0.852137\C,0,3.00344,-0.092337,-1.548385\H,0,0.895612,0.345024,-1.
465867\H,0,3.109458,0.931355,2.185096\H,0,5.17975,0.217409,1.045522\H,
0,2.970679,-0.366769,-2.606889\C,0,0.582801,1.034856,1.145141\C,0,-0.5
24713,1.584796,0.308103\C,0,-1.761994,0.932087,0.138445\C,0,-0.308849,
2.816211,-0.322838\C,0,-2.743248,1.543872,-0.648217\C,0,-1.29476,3.416
104,-1.097837\H,0,0.660963,3.30843,-0.189357\C,0,-2.519099,2.773961,-1
.258422\H,0,-3.699569,1.031577,-0.770996\H,0,-1.106308,4.383069,-1.573
113\H,0,-3.306636,3.231237,-1.864796\C,0,0.431243,0.928275,2.474981\C,
0,-2.0339,-0.439294,0.72022\O,0,-3.409253,-0.716638,0.588338\H,0,-3.59
1006,-1.544243,1.043913\H,0,-0.493034,1.257457,2.960096\H,0,5.128212,-
0.442881,-1.358812\C,0,-1.189371,-1.506763,0.030015\H,0,-1.362375,-1.4
22411,-1.059981\H,0,-0.120539,-1.280876,0.198217\H,0,1.211275,0.512611
,3.120083\C,0,-1.475721,-2.921239,0.507812\H,0,-2.466653,-3.246173,0.1
32597\H,0,-1.545561,-2.924744,1.6143\C,0,-0.423866,-3.93407,0.07542\H,
0,0.536839,-3.683697,0.564347\H,0,-0.703952,-4.930679,0.461072\C,0,-0.
22247,-4.003611,-1.427424\H,0,0.455218,-4.824561,-1.708845\H,0,-1.1794
95,-4.167832,-1.953146\H,0,0.215328,-3.07249,-1.824904\H,0,-1.754663,-
0.432185,1.795874\\Version=ES64L-G16RevC.01\State=1-A\HF=-812.1761886\
RMSD=2.532e-09\Dipole=0.5582958,-0.7465115,0.3859963\Quadrupole=-0.296
0604,-1.1493477,1.4454081,3.0067173,-0.183406,-2.9030182\PG=C01 [X(C19
H22O1)]\\@

Int-1ae

1\1\GINC-A06R04N08\SP\UM06\def2TZVPP\C19H22O1 (3) \ACJSGGHI7X\20-Apr-202
3\0\\#p scrf=(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\\int1\\0,
3\C,0,2.427092,0.022444,-0.971995\C,0,2.093337,-0.118586,0.399362\C,0,

2.979438,-0.878293,1.204052\C,0,4.139486,-1.428607,0.681126\C,0,4.4543
51,-1.263011,-0.669713\C,0,3.583789,-0.540536,-1.489827\H,0,1.745161,0
.561527,-1.636061\H,0,2.740068,-1.018069,2.264065\H,0,4.809271,-1.9976
3,1.332934\H,0,3.808625,-0.423286,-2.554268\C,0,0.874159,0.411215,0.95
9505\C,0,0.104913,1.47175,0.291966\C,0,-1.312213,1.481581,0.219447\C,0
,0.803335,2.568882,-0.252184\C,0,-1.959745,2.559939,-0.383732\C,0,0.14
3453,3.6362,-0.846267\H,0,1.894429,2.587267,-0.169118\C,0,-1.247009,3.
632283,-0.914362\H,0,-3.050345,2.542947,-0.431797\H,0,0.717738,4.47782
, -1.244483\H,0,-1.781486,4.466603,-1.377969\C,0,0.44624,-0.070077,2.27
8145\C,0,-2.133033,0.315531,0.714378\O,0,-3.496701,0.665862,0.677454\H
,0,-3.997638,-0.041049,1.095444\H,0,0.697984,0.487398,3.190667\H,0,5.3
66265,-1.703014,-1.083118\C,0,-1.874838,-0.943036,-0.11275\H,0,-2.1704
58,-0.712956,-1.153622\H,0,-0.787784,-1.153263,-0.138206\H,0,0.035839,
-1.079498,2.41875\C,0,-2.61377,-2.167472,0.403316\H,0,-3.705714,-2.028
046,0.269093\H,0,-2.446658,-2.252859,1.496102\C,0,-2.202967,-3.470278,
-0.268491\H,0,-1.127363,-3.648585,-0.077811\H,0,-2.733902,-4.307782,0.
218433\C,0,-2.469322,-3.499115,-1.762297\H,0,-2.246131,-4.486187,-2.19
6178\H,0,-3.526868,-3.271603,-1.982912\H,0,-1.856203,-2.761045,-2.3048
28\H,0,-1.831394,0.10953,1.767183\\Version=ES64L-G16RevC.01\State=3-A\
HF=-812.0951292\S2=2.035738\S2-1=0.\S2A=2.000772\RMSD=8.593e-09\Dipole
=0.120643,-0.9373114,0.4547608\Quadrupole=1.3771684,-2.2635031,0.88633
47,3.2906246,-2.6115138,-4.8141817\PG=C01 [X(C19H22O1)]\@

Ts-1ae

1\1\GINC-A01R08N02\SP\UM06\def2TZVPP\C19H22O1(3)\ACJSGGHI7X\20-Apr-202
3\0\#p scrf=(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\ts1\0,3
\C,0,2.643654,-0.233877,-1.011667\C,0,2.177579,-0.390072,0.316593\C,0,
2.958933,-1.191293,1.182851\C,0,4.146869,-1.769257,0.758616\C,0,4.5928
38,-1.589346,-0.552007\C,0,3.826575,-0.82363,-1.433514\H,0,2.040033,0.
332875,-1.726619\H,0,2.624331,-1.334281,2.215353\H,0,4.73622,-2.368724

,1.459129\H,0,4.152503,-0.694792,-2.470166\C,0,0.926857,0.178209,0.772
654\C,0,0.326029,1.356935,0.17069\C,0,-1.082182,1.559669,0.23363\C,0,1
.107371,2.390647,-0.395061\C,0,-1.645915,2.751955,-0.219013\C,0,0.5311
94,3.56313,-0.858794\H,0,2.195688,2.282429,-0.414335\C,0,-0.850873,3.7
51823,-0.771052\H,0,-2.729197,2.87844,-0.137099\H,0,1.16765,4.350852,-
1.272771\H,0,-1.305508,4.679656,-1.130095\C,0,0.231502,-0.426766,1.932
256\C,0,-1.939289,0.46469,0.754685\O,0,-3.093504,0.957769,1.336446\H,0
,-3.690484,0.22181,1.513982\H,0,-1.121801,-0.05385,1.604373\H,0,5.5260
33,-2.050653,-0.88743\C,0,-2.175158,-0.67757,-0.215448\H,0,-2.731014,-
0.277722,-1.08739\H,0,-1.193001,-1.010082,-0.602804\H,0,0.227489,-1.52
474,1.998719\C,0,-2.907352,-1.864356,0.394985\H,0,-3.955297,-1.584208,
0.633047\H,0,-2.4302,-2.119877,1.360906\C,0,-2.935914,-3.098661,-0.495
864\H,0,-1.896038,-3.428801,-0.680244\H,0,-3.416472,-3.925942,0.055941
\C,0,-3.649576,-2.886516,-1.818254\H,0,-3.727415,-3.822861,-2.392144\H
,0,-4.675142,-2.508476,-1.662308\H,0,-3.126039,-2.157731,-2.45852\H,0,
0.376827,0.060252,2.91118\\Version=ES64L-G16RevC.01\State=3-A\HF=-812.
0799214\S2=2.03387\S2-1=0.\S2A=2.000727\RMSD=2.313e-09\Dipole=-0.45281
, -0.9657201, -0.074947\Quadrupole=4.5229354, -2.505937, -2.0169984, 2.6331
815, -1.9224132, -5.4399683\PG=C01 [X(C19H22O1)]\@

Int-2ae

1\1\GINC-A06R04N08\SP\UM06\def2TZVPP\C19H22O1(3)\ACJSGGHI7X\20-Apr-202
3\0\#p scrf=(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\int2\0,
3\C,0,1.167451,1.934498,-0.9726\C,0,1.255512,1.336154,0.313385\C,0,2.5
39269,1.294768,0.920138\C,0,3.652067,1.82484,0.284033\C,0,3.538772,2.4
10444,-0.979439\C,0,2.286469,2.456953,-1.600265\H,0,0.193661,1.973886,
-1.471163\H,0,2.655395,0.849714,1.912709\H,0,4.626418,1.784408,0.78070
7\H,0,2.186146,2.908609,-2.591955\C,0,0.108127,0.767224,0.946714\C,0,-
1.255132,0.951297,0.393012\C,0,-2.034409,-0.118906,-0.164739\C,0,-1.83
525,2.211737,0.536327\C,0,-3.393747,0.164135,-0.486999\C,0,-3.159951,2

.470475,0.179639\H,0,-1.218514,3.012902,0.960078\C,0,-3.938254,1.42428
2,-0.322038\H,0,-4.00255,-0.642085,-0.901453\H,0,-3.57924,3.472685,0.3
03788\H,0,-4.982816,1.599334,-0.59747\C,0,0.217057,0.063894,2.261288\C
,0,-1.53962,-1.424883,-0.426967\O,0,-2.474204,-2.350647,-0.780221\H,0,
-2.031845,-3.148753,-1.090745\H,0,-0.721743,-0.455102,2.510187\H,0,4.4
19195,2.826987,-1.47685\C,0,-0.129519,-1.899172,-0.48479\H,0,0.058724,
-2.262386,-1.519041\H,0,0.56949,-1.060321,-0.347128\H,0,1.036898,-0.67
8263,2.282282\C,0,0.208408,-3.015329,0.507731\H,0,-0.386343,-3.923344,
0.280713\H,0,-0.113528,-2.700076,1.516511\C,0,1.686339,-3.376453,0.528
074\H,0,2.269513,-2.477969,0.811332\H,0,1.86252,-4.112102,1.332935\C,0
,2.20785,-3.926928,-0.786775\H,0,3.25263,-4.263303,-0.70059\H,0,1.6100
3,-4.7929,-1.121752\H,0,2.179401,-3.174834,-1.592359\H,0,0.421554,0.77
3909,3.086663\\Version=ES64L-G16RevC.01\State=3-A\HF=-812.127374\S2=2.
05823\S2-1=0.\S2A=2.002117\RMSD=4.784e-09\Dipole=0.8206807,-1.1920668,
0.023684\Quadrupole=-3.9737212,4.4967179,-0.5229968,0.1286613,2.451882
5,1.0547201\PG=C01 [X(C19H22O1)]\@

Int-3ae

1\1\GINC-A06R05N04\SP\RM06\def2TZVPP\C19H22O1\ACJSGGHI7X\20-Apr-2023\0
\#p scrf=(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\\int3\\0,1\C
,0,-2.408007,0.799282,-1.060288\C,0,-2.113884,0.466493,0.271806\C,0,-3
.107654,0.690289,1.236652\C,0,-4.350918,1.205512,0.881794\C,0,-4.62740
6,1.524369,-0.446427\C,0,-3.648429,1.319562,-1.416836\H,0,-1.636135,0.
64726,-1.823153\H,0,-2.910501,0.433229,2.282789\H,0,-5.114068,1.356491
,1.651294\H,0,-3.850022,1.573874,-2.461826\C,0,-0.772104,-0.049794,0.6
35641\C,0,-0.251069,-1.174242,0.038784\C,0,1.153067,-1.622048,0.170275
\C,0,-1.122671,-2.119772,-0.648247\C,0,1.391576,-3.05677,0.220126\C,0,
-0.790696,-3.429472,-0.758834\H,0,-2.116746,-1.787889,-0.959355\C,0,0.
459888,-3.92435,-0.239986\H,0,2.370355,-3.410187,0.553231\H,0,-1.50378
6,-4.132559,-1.200267\H,0,0.661727,-4.999424,-0.250289\C,0,-0.080231,0
.707372,1.725048\C,0,2.235193,-0.791025,0.050562\O,0,3.469177,-1.33870

2,0.186253\H,0,4.141118,-0.673013,0.002844\H,0,-0.77187,0.878611,2.568
004\H,0,0.800012,0.167751,2.107169\H,0,-5.602906,1.934062,-0.723893\C,
0,2.241483,0.638458,-0.379619\H,0,2.730304,0.661432,-1.376659\H,0,1.21
0473,0.990167,-0.541136\H,0,0.247954,1.715894,1.408381\C,0,2.994356,1.
587033,0.554758\H,0,4.071463,1.320101,0.578368\H,0,2.636643,1.445023,1.
.589327\C,0,2.870793,3.052337,0.163341\H,0,1.805945,3.349664,0.217813\
H,0,3.388224,3.665713,0.922041\C,0,3.421959,3.37465,-1.213522\H,0,3.40
5165,4.456966,-1.413865\H,0,4.468951,3.038021,-1.313593\H,0,2.842792,2.
.891121,-2.017422\\Version=ES64L-G16RevC.01\State=1-A\HF=-812.1479859\
RMSD=4.589e-09\Dipole=0.9958096,1.4627865,-0.0895557\Quadrupole=9.2577
205,-6.9633844,-2.2943361,3.03555,-0.2975995,0.6968731\PG=C01 [X(C19H2
201)]\@

Int-2ae'

1\1\GINC-A04R05N04\SP\UM06\def2TZVPP\C19H22O1(3)\ACJSGGHI7X\27-Apr-202
3\0\#p scrf=(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\int2\0,
3\C,0,2.33025,-0.434324,-1.195487\C,0,2.42199,-0.394246,0.221255\C,0,3
.414855,-1.208844,0.826597\C,0,4.258923,-2.001313,0.063125\C,0,4.14907
6,-2.023184,-1.329647\C,0,3.174995,-1.233281,-1.948741\H,0,1.568103,0.
173926,-1.693136\H,0,3.525669,-1.206924,1.914875\H,0,5.018488,-2.61347
9,0.559551\H,0,3.07533,-1.245689,-3.038641\C,0,1.539569,0.412833,0.999
992\C,0,0.618848,1.377163,0.351722\C,0,-0.795593,1.151159,0.231933\C,0
,1.154897,2.580524,-0.103916\C,0,-1.577851,2.199792,-0.334108\C,0,0.36
6306,3.587815,-0.663765\H,0,2.237468,2.724847,-0.008995\C,0,-1.012416,
3.38485,-0.767596\H,0,-2.65637,2.060089,-0.452625\H,0,0.823031,4.51801
4,-1.012508\H,0,-1.652234,4.158763,-1.202206\C,0,1.550268,0.361301,2.4
9261\C,0,-1.420359,-0.057177,0.626808\O,0,-0.632438,-1.108639,0.969496
\H,0,-1.1856,-1.83638,1.277102\H,0,0.686633,0.90068,2.911267\H,0,4.816
446,-2.650258,-1.927807\C,0,-2.881651,-0.339138,0.544809\H,0,-3.150719
, -0.999604,1.394952\H,0,-3.471999,0.580481,0.698857\H,0,1.514816,-0.67

6873,2.867963\C,0,-3.292889,-1.002775,-0.773056\H,0,-2.704249,-1.932514,-0.902674\H,0,-2.985461,-0.34195,-1.603696\C,0,-4.778541,-1.312502,-0.876781\H,0,-5.352103,-0.371751,-0.769963\H,0,-4.994162,-1.674005,-1.897757\C,0,-5.27144,-2.331902,0.134354\H,0,-6.327454,-2.594225,-0.033572\H,0,-4.687278,-3.266845,0.073583\H,0,-5.195821,-1.963335,1.171012\H,0,2.461544,0.825635,2.917814\\Version=ES64L-G16RevC.01\State=3-A\HF=-812.1271199\S2=2.059817\S2-1=0.\S2A=2.002239\RMSD=5.315e-09\Dipole=-1.4630714,-0.7559608,0.5279495\Quadrupole=3.0018264,-1.9995978,-1.0022286,0.8572898,0.6700958,-3.1270448\PG=C01 [X(C19H22O1)]\@

Int-3ae'

1\1\GINC-A03R06N05\SP\RM06\def2TZVPP\C19H22O1\ACJSGGHI7X\27-Apr-2023\0\\#p scrf=(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\\int3\\0,1\C,0,-3.050875,-0.51685,1.248196\C,0,-2.774998,-0.463552,-0.127279\C,0,-3.858652,-0.528625,-1.016043\C,0,-5.166523,-0.623,-0.549941\C,0,-5.422739,-0.669244,0.819161\C,0,-4.357723,-0.617131,1.716511\H,0,-2.213076,-0.488031,1.953084\H,0,-3.672483,-0.480504,-2.094226\H,0,-5.99514,-0.657292,-1.263811\H,0,-4.545664,-0.66237,2.793602\C,0,-1.377208,-0.388322,-0.615516\C,0,-0.536257,0.626827,-0.22562\C,0,0.918575,0.646611,-0.505259\C,0,-1.063062,1.849183,0.364831\C,0,1.526075,1.949827,-0.732749\C,0,-0.384413,3.020901,0.298861\H,0,-2.080662,1.838929,0.764526\C,0,0.906148,3.087076,-0.337819\H,0,2.525903,2.008126,-1.173921\H,0,-0.843081,3.937862,0.680887\H,0,1.389302,4.057485,-0.484332\C,0,-0.978639,-1.453549,-1.582319\C,0,1.725938,-0.445352,-0.331575\O,0,1.203756,-1.614758,0.106405\H,0,1.916816,-2.243638,0.265661\H,0,-1.811692,-1.689481,-2.264476\H,0,-0.104116,-1.157904,-2.183766\H,0,-6.450254,-0.748549,1.185943\C,0,3.214961,-0.447844,-0.483872\H,0,3.511326,-1.428354,-0.907357\H,0,3.542654,0.299648,-1.224406\H,0,-0.711746,-2.394077,-1.068222\C,0,3.940453,-0.204775,0.840544\H,0,3.610258,-0.959568,1.582365\H,0,3.604546,0.768642,1.240648\C,0,5.457224,-0.228783,0.72842\H,0,5.777692,0.546

971,0.006994\H,0,5.887694,0.076043,1.698497\C,0,6.028719,-1.575372,0.3
2297\H,0,7.129509,-1.572344,0.340956\H,0,5.69209,-2.37333,1.007928\H,0
,5.728051,-1.868367,-0.696829\\Version=ES64L-G16RevC.01\State=1-A\HF=-
812.1494082\RMSD=4.896e-09\Dipole=1.6405847,-0.9598534,-0.0137092\Quad
rupole=9.0694208,-4.6950634,-4.3743575,-3.3635694,-1.0406927,0.5107026
\PG=C01 [X(C19H22O1)]\@

Ts-2ae

1\1\GINC-A06R05N04\SP\RM06\def2TZVPP\C19H22O1\ACJSGGHI7X\20-Apr-2023\0
\#p scrf=(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\ts2\0,1\C,
0,-2.575512,-0.441713,1.248822\C,0,-2.526379,-0.444149,-0.160838\C,0,-
3.68333,-0.872872,-0.836637\C,0,-4.831902,-1.248368,-0.143953\C,0,-4.8
6483,-1.214186,1.247081\C,0,-3.722511,-0.809414,1.93939\H,0,-1.67747,-
0.162037,1.810706\H,0,-3.6944,-0.908455,-1.929322\H,0,-5.715157,-1.570
79,-0.704188\H,0,-3.721269,-0.795634,3.033808\C,0,-1.282475,-0.090977,
-0.869756\C,0,-0.469907,0.995386,-0.397039\C,0,0.962097,1.007204,-0.62
8446\C,0,-1.000046,2.092954,0.340746\C,0,1.714268,2.183848,-0.327316\C
,0,-0.240416,3.197729,0.635\H,0,-2.066466,2.086655,0.583595\C,0,1.1289
75,3.264207,0.274032\H,0,2.780384,2.216015,-0.569954\H,0,-0.711016,4.0
57725,1.121743\H,0,1.710363,4.165358,0.485395\C,0,-1.245508,-0.369691,
-2.364283\C,0,1.615594,-0.241307,-0.785281\O,0,0.945777,-1.328802,-0.9
34188\H,0,-0.116927,-1.057905,-0.739072\H,0,-2.070991,0.157735,-2.8774
8\H,0,-0.313224,-0.012107,-2.824293\H,0,-5.767089,-1.510765,1.789444\C
,0,3.083841,-0.436932,-0.58404\H,0,3.382645,-1.298001,-1.204722\H,0,3.
655337,0.436275,-0.940085\H,0,-1.346638,-1.443038,-2.604319\C,0,3.4119
63,-0.712339,0.884315\H,0,2.823842,-1.590915,1.211116\H,0,3.057067,0.1
38682,1.493748\C,0,4.891379,-0.95189,1.145743\H,0,5.464164,-0.055003,0
.840813\H,0,5.042538,-1.040216,2.236167\C,0,5.452992,-2.181582,0.45598
1\H,0,6.497399,-2.369479,0.749266\H,0,4.869597,-3.082532,0.712452\H,0,
5.441348,-2.086624,-0.642451\\Version=ES64L-G16RevC.01\State=1-A\HF=-8

12.1401318\RMSD=5.090e-09\Dipole=1.6191664,0.7558516,0.1218337\Quadrupole=4.4951744,-3.3204001,-1.1747744,1.7214986,-0.0475373,1.3803387\PG=C01 [X(C19H22O1)]\@

Ts-3ae

1\1\GINC-A06R04N08\SP\RM06\def2TZVPP\C19H22O1\ACJSGGHI7X\20-Apr-2023\0
\#p scrf=(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\ts3\0,1\C,
0,-1.281701,-1.516472,-0.947028\C,0,-1.011159,-1.273428,0.420154\C,0,-
2.081091,-1.459098,1.324589\C,0,-3.3364,-1.865992,0.887743\C,0,-3.5742
81,-2.110083,-0.464311\C,0,-2.533082,-1.935388,-1.377924\H,0,-0.485566
, -1.359011,-1.682927\H,0,-1.924215,-1.283079,2.392196\H,0,-4.142324,-1
.999522,1.616122\H,0,-2.703959,-2.117514,-2.443472\C,0,0.282293,-0.771
056,0.850416\C,0,1.44946,-0.876857,0.004102\C,0,2.187704,0.328248,0.03
8322\C,0,1.983508,-1.980383,-0.691665\C,0,3.56457,0.352975,-0.267801\C
,0,3.304338,-1.917331,-1.103474\H,0,1.40742,-2.905161,-0.802982\C,0,4.
102994,-0.776434,-0.854234\H,0,4.159703,1.258371,-0.114786\H,0,3.76114
4,-2.788941,-1.582703\H,0,5.154134,-0.784306,-1.158034\C,0,0.494041,-0
.537583,2.326029\C,0,1.331662,1.417584,0.37759\O,0,1.853715,2.363743,1
.176699\H,0,1.308924,3.163217,1.152256\H,0,0.336508,-1.475933,2.89633\
H,0,1.518149,-0.199871,2.539805\H,0,-4.562994,-2.430478,-0.804664\C,0,
0.125134,1.827106,-0.404539\H,0,0.448442,2.656271,-1.077135\H,0,-0.180
301,1.003214,-1.067501\H,0,-0.195362,0.207523,2.765408\C,0,-1.070082,2
.290963,0.425275\H,0,-0.853272,3.266278,0.91079\H,0,-1.230062,1.568088
,1.244104\C,0,-2.351869,2.416718,-0.385345\H,0,-2.618794,1.414334,-0.7
72719\H,0,-3.173987,2.699325,0.295763\C,0,-2.270292,3.412244,-1.527766
\H,0,-3.243669,3.538309,-2.026663\H,0,-1.95209,4.407917,-1.170773\H,0,
-1.55205,3.09663,-2.302807\\Version=ES64L-G16RevC.01\State=1-A\HF=-812
.1238881\RMSD=6.713e-09\Dipole=-0.2676375,1.6008299,-0.1584702\Quadrupole=-2.2848997,4.4126323,-2.1277326,0.9249189,-2.4212397,3.0707421\PG=C01 [X(C19H22O1)]\@

Ts-3ae'

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1\1\GINC-B2146\SP\RM06\def2TZVPP\C19H22O1\ROOT\25-Jul-2023\0\#\#p scrf=
(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\ts3\0,1\C,0,-1.12197
3,-2.136535,0.904223\C,0,0.056355,-1.403647,0.643071\C,0,1.061947,-2.0
7602,-0.096658\C,0,0.870409,-3.363657,-0.582081\C,0,-0.319499,-4.05335
1,-0.340613\C,0,-1.30601,-3.426689,0.416762\H,0,-1.9236,-1.67634,1.490
738\H,0,2.030593,-1.58691,-0.250681\H,0,1.679675,-3.849757,-1.137201\H
,0,-2.242411,-3.95022,0.63451\C,0,0.2336,-0.056505,1.19172\C,0,1.33169
6,0.767659,0.770923\C,0,1.341811,0.912895,-0.63415\C,0,2.397391,1.3176
73,1.514411\C,0,2.52497,1.228805,-1.330595\C,0,3.522656,1.739415,0.827
764\H,0,2.38387,1.311236,2.609581\C,0,3.608313,1.652449,-0.581834\H,0,
2.555441,1.233965,-2.42572\H,0,4.388061,2.107742,1.387451\H,0,4.528202
,1.968751,-1.082199\C,0,-0.514152,0.295472,2.44098\C,0,0.029848,0.6954
76,-1.165788\H,0,-1.559584,0.590143,2.219359\H,0,-0.575226,-0.539875,3
.161599\H,0,-0.464608,-5.068093,-0.72062\C,0,-1.143366,1.572886,-0.886
41\H,0,-0.941334,2.15229,0.028311\H,0,-1.186267,2.314854,-1.716989\H,0
,-0.057621,1.163141,2.944086\C,0,-2.485865,0.856104,-0.827274\H,0,-2.4
6586,0.113395,-0.008053\H,0,-2.61114,0.271347,-1.754571\C,0,-3.665559,
1.799013,-0.643758\H,0,-3.649361,2.562407,-1.445605\H,0,-4.601692,1.23
3228,-0.79553\C,0,-3.705576,2.478148,0.713323\H,0,-3.735493,1.732559,1
.527523\H,0,-2.823056,3.116509,0.88798\H,0,-4.593284,3.120255,0.824735
\O,0,-0.125596,-0.048537,-2.262376\H,0,0.567477,-0.729884,-2.283787\Ver
sion=ES64L-G16RevA.03\State=1-A\HF=-812.1233682\RMSD=5.544e-09\Dipol
e=0.0870087,0.8088174,-0.3915484\Quadrupole=3.5397944,-4.4041144,0.864
32,0.4886119,-3.8842012,2.7806762\PG=C01 [X(C19H22O1)]\#@
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Ts-4

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1\1\GINC-A01R03N03\SP\UM06\def2TZVPP\C19H22O1(3)\ACJSGGHI7X\27-Apr-202
3\0\#\#p scrf=(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\ts2\0,3
\C,0,-0.820594,-1.544977,-1.014996\C,0,-0.711134,-1.479339,0.401151\C,
```

0,-1.8555,-1.858813,1.153401\C,0,-3.024706,-2.266167,0.529563\C,0,-3.1
07678,-2.319161,-0.864793\C,0,-1.993617,-1.956901,-1.628148\H,0,0.0390
37,-1.25672,-1.628648\H,0,-1.816207,-1.831067,2.246181\H,0,-3.888362,-
2.551752,1.137966\H,0,-2.045321,-1.995155,-2.720599\C,0,0.476163,-1.00
489,1.038718\C,0,1.673668,-0.672541,0.231968\C,0,2.001083,0.672972,-0.
052276\C,0,2.484201,-1.695719,-0.274463\C,0,3.13308,0.941579,-0.831199
\C,0,3.609968,-1.407979,-1.04203\H,0,2.212379,-2.736002,-0.06249\C,0,3
.936828,-0.08409,-1.322389\H,0,3.374511,1.987004,-1.051486\H,0,4.23134
2,-2.222855,-1.425364\H,0,4.81762,0.151141,-1.926953\C,0,0.564329,-0.8
55656,2.522978\C,0,1.131924,1.780372,0.397661\O,0,1.270264,2.119635,1.
718733\H,0,0.596397,2.770099,1.950256\H,0,1.474018,-0.309881,2.809522\
H,0,-4.031943,-2.641984,-1.352157\C,0,-0.107955,2.18439,-0.327419\H,0,
-0.049869,3.24081,-0.672711\H,0,-0.16872,1.580641,-1.252622\H,0,-0.296
536,-0.303358,2.942071\C,0,-1.401318,1.998605,0.479592\H,0,-1.503175,2
.814043,1.226077\H,0,-1.332389,1.059515,1.056787\C,0,-2.655774,1.95681
2,-0.379511\H,0,-2.590674,1.076694,-1.049041\H,0,-3.526909,1.763839,0.
272437\C,0,-2.89385,3.215518,-1.193035\H,0,-3.853497,3.17731,-1.731865
\H,0,-2.913464,4.111524,-0.5476\H,0,-2.1067,3.375014,-1.948689\H,0,0.5
81641,-1.840037,3.030419\\Version=ES64L-G16RevC.01\State=3-A\HF=-812.1
076093\S2=2.036706\S2-1=0.\S2A=2.000714\RMSD=5.879e-09\Dipole=-0.61584
04,0.344268,0.0236101\Quadrupole=-1.1321345,0.6673362,0.4647983,-1.948
6437,-5.1509569,0.8596968\PG=C01 [X(C19H22O1)]\@

Ts-5

1\1\GINC-A04R05N04\SP\RM06\def2TZVPP\C19H22O1\ACJSGGHI7X\27-Apr-2023\0
\#p scrf=(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\\ts4\\0,1\C,
0,3.139286,-0.651178,-1.188069\C,0,2.366791,-0.747871,-0.019405\C,0,2.
975107,-1.303695,1.117305\C,0,4.300442,-1.727802,1.094906\C,0,5.054316
, -1.612855,-0.071896\C,0,4.465917,-1.073803,-1.214245\H,0,2.677126,-0.
243793,-2.094125\H,0,2.391411,-1.387867,2.04106\H,0,4.751936,-2.14654,

1.999732\H,0,5.043474,-0.989223,-2.140127\C,0,0.936731,-0.35138,0.0105
95\C,0,0.522126,0.96433,-0.175444\C,0,-0.879674,1.413433,-0.095099\C,0
,1.494894,1.999774,-0.45623\C,0,-1.0622,2.824556,0.132054\C,0,1.206377
,3.329659,-0.430267\H,0,2.51826,1.687986,-0.672894\C,0,-0.101863,3.770
794,-0.100079\H,0,-2.073163,3.16356,0.392193\H,0,1.994104,4.058147,-0.
646405\H,0,-0.343306,4.836101,-0.055714\C,0,-0.020863,-1.45925,0.26044
5\C,0,-1.979918,0.710776,0.498374\O,0,-2.099385,0.781524,1.825021\H,0,
-2.96884,0.462506,2.118879\H,0,0.480745,-2.348644,0.672366\H,0,-0.8118
67,-1.144763,0.969317\H,0,6.096366,-1.945262,-0.091612\C,0,-2.875972,-
0.198464,-0.25875\H,0,-3.591306,0.434561,-0.826226\H,0,-2.255299,-0.64
6495,-1.063961\H,0,-0.561714,-1.798614,-0.651166\C,0,-3.630942,-1.2649
4,0.520995\H,0,-4.361837,-0.787724,1.208208\H,0,-2.920517,-1.820743,1.
160955\C,0,-4.37799,-2.25008,-0.368117\H,0,-3.64258,-2.772188,-1.00923
7\H,0,-4.822927,-3.033455,0.269957\C,0,-5.458239,-1.618357,-1.226417\H
,0,-6.032083,-2.378934,-1.777552\H,0,-6.17527,-1.047482,-0.610904\H,0,
-5.043601,-0.92522,-1.976845\\Version=ES64L-G16RevC.01\State=1-A\HF=-8
12.0869639\RMSD=6.283e-09\Dipole=-3.2111566,-1.0589904,0.5560642\Quadr
upole=13.3669958,-9.1047513,-4.2622445,0.4944209,-5.8718353,-1.5180145
\PG=C01 [X(C19H22O1)]\@

2ae

1\1\GINC-A06R03N06\SP\RM06\def2TZVPP\C19H22O1\ACJSGGHI7X\20-Apr-2023\0
\#p scrf=(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\2\0,1\C,0,
-2.498644,-1.027074,1.176125\C,0,-2.55757,-0.686141,-0.182326\C,0,-3.8
13316,-0.62546,-0.790725\C,0,-4.975014,-0.892271,-0.063591\C,0,-4.9001
2,-1.226346,1.284292\C,0,-3.651704,-1.294009,1.90411\H,0,-1.518673,-1.
078893,1.665931\H,0,-3.897381,-0.367301,-1.850441\H,0,-5.947998,-0.838
724,-0.561392\H,0,-3.578549,-1.560262,2.962877\C,0,-1.260111,-0.408608
, -0.914384\C,0,-0.571191,0.834773,-0.372209\C,0,0.824982,0.942602,-0.1
64893\C,0,-1.366981,1.951612,-0.088471\C,0,1.348792,2.144862,0.341527\

C,0,-0.828802,3.143491,0.379893\H,0,-2.449428,1.87299,-0.237023\C,0,0.542122,3.242674,0.602549\H,0,2.423975,2.232669,0.51637\H,0,-1.48466,3.995988,0.579251\H,0,0.981159,4.170694,0.978619\C,0,-1.399401,-0.291364,-2.427117\C,0,1.769916,-0.175372,-0.480023\O,0,1.491561,-1.045928,-1.28047\H,0,-0.601036,-1.27047,-0.723523\H,0,-1.993473,0.594061,-2.712661\H,0,-0.403439,-0.19469,-2.883065\H,0,-5.810722,-1.4368,1.852614\C,0,3.107791,-0.200322,0.230255\H,0,3.692245,0.671213,-0.122196\H,0,2.949303,-0.015467,1.310687\H,0,-1.882752,-1.1845,-2.855115\C,0,3.883055,-1.48406,0.004399\H,0,4.082246,-1.598738,-1.076613\H,0,3.237596,-2.340166,0.266864\C,0,5.185914,-1.554937,0.786875\H,0,4.968096,-1.482931,1.870097\H,0,5.629293,-2.556034,0.642986\C,0,6.201567,-0.495493,0.398036\H,0,7.162733,-0.641612,0.91514\H,0,6.403373,-0.518038,-0.687007\H,0,5.857888,0.523091,0.645429\\Version=ES64L-G16RevC.01\State=1-A\HF=-812.2020188\RMSD=8.616e-09\Dipole=0.3679855,1.0830318,0.8277685\Quadrupole=6.1165976,-2.3361761,-3.7804215,1.7250045,3.8880326,-1.6041\PG=C01 [X(C19H22O1)]\@

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1\1\GINC-A04R06N02\SP\RM06\def2TZVPP\C19H22O1\ACJSGGHI7X\20-Apr-2023\0\\#p scrf=(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\\3\\0,1\C,0,1.757269,1.608839,1.09782\C,0,0.633799,1.279898,0.326305\C,0,0.657578,1.629717,-1.031283\C,0,1.76034,2.264344,-1.598218\C,0,2.872402,2.570996,-0.817956\C,0,2.863887,2.240385,0.535036\H,0,1.775007,1.369475,2.165408\H,0,-0.210212,1.399577,-1.658837\H,0,1.746327,2.525361,-2.660686\H,0,3.725545,2.482709,1.164365\C,0,-0.555968,0.557582,0.922658\C,0,-1.840736,0.618921,0.112771\C,0,-1.956609,-0.754655,-0.034305\C,0,-2.785773,1.498083,-0.396762\C,0,-3.031782,-1.351555,-0.674966\C,0,-3.87413,0.912416,-1.054689\H,0,-2.703696,2.585349,-0.298435\C,0,-3.996628,-0.476921,-1.187759\H,0,-3.136698,-2.435443,-0.780601\H,0,-4.656176,1.552687,-1.47498\H,0,-4.870889,-0.882118,-1.706712\C,0,-0.782606,0.891676,2.3

88788\C,0,-0.656222,-1.058666,0.668819\O,0,-0.860986,-1.824206,1.8224\
H,0,-0.00395,-2.013041,2.223217\H,0,-0.849364,1.982468,2.53673\H,0,-1.
712099,0.4288,2.749812\H,0,3.738421,3.071944,-1.259998\C,0,0.426728,-1
.661611,-0.209063\H,0,0.037869,-2.61662,-0.610449\H,0,0.58724,-1.00588
3,-1.083225\H,0,0.032555,0.511326,3.027958\C,0,1.747833,-1.887493,0.52
0673\H,0,1.690044,-2.81869,1.120177\H,0,1.916888,-1.064029,1.241278\C,
0,2.951003,-1.971204,-0.407012\H,0,3.05451,-1.003446,-0.935045\H,0,3.8
68151,-2.079355,0.199162\C,0,2.865369,-3.105174,-1.411446\H,0,3.778318
, -3.179072,-2.022628\H,0,2.725968,-4.076593,-0.905417\H,0,2.019606,-2.
975223,-2.106772\\Version=ES64L-G16RevC.01\State=1-A\HF=-812.165864\RM
SD=4.086e-09\Dipole=0.795331,0.0094218,-0.0918741\Quadrupole=1.0741753
, -1.0659844,-0.008191,-1.4738655,6.1898066,-0.517029\PG=C01 [X(C19H22O
1)]\@

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1\1\GINC-B2157\SP\RM06\def2TZVPP\C19H22O1\ROOT\24-Jul-2023\0\#\#p scrf=
(iefpcm,smd,solvent=Acetonitrile) M06 def2tzvpp\\3\\0,1\C,0,1.287301,-
2.207865,-0.018985\C,0,1.489476,-0.845473,0.235979\C,0,2.797433,-0.358
968,0.229708\C,0,3.877062,-1.208541,-0.014673\C,0,3.662701,-2.559932,-
0.263273\C,0,2.359015,-3.056566,-0.268436\H,0,0.26654,-2.604561,-0.040
808\H,0,2.979883,0.70473,0.411541\H,0,4.894186,-0.805081,-0.012907\H,0
,2.176581,-4.115919,-0.472752\C,0,0.305535,0.038613,0.556564\C,0,0.534
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601452,1.096341\C,0,-0.623698,2.978075,-1.10812\C,0,0.913669,3.872066,
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,0,-1.322367,3.140209,-1.93584\H,0,1.399373,4.748155,1.009026\H,0,-0.1
35669,5.071154,-0.880563\C,0,-0.306407,-0.371951,1.89279\C,0,-0.704081
,0.254266,-0.679432\H,0,0.442026,-0.22254,2.689466\H,0,-1.187341,0.238
946,2.149701\H,0,4.507814,-3.2269,-0.457494\C,0,-2.179914,-0.04255,-0.
464922\H,0,-2.516569,0.457897,0.4597\H,0,-2.73882,0.464235,-1.281112\H

,0,-0.596163,-1.434658,1.915059\C,0,-2.541681,-1.51867,-0.461119\H,0,-
1.956524,-2.041929,0.319715\H,0,-2.21572,-1.961954,-1.417797\C,0,-4.02
1826,-1.788412,-0.23125\H,0,-4.614547,-1.261838,-1.004155\H,0,-4.21779
, -2.863497,-0.391658\C,0,-4.508494,-1.389705,1.150929\H,0,-5.555952,-1
.685846,1.317919\H,0,-3.900181,-1.869315,1.938169\H,0,-4.453269,-0.300
708,1.315376\O,0,-0.215838,-0.398065,-1.824313\H,0,-0.6657,-0.026234,-
2.592383\\Version=ES64L-G16RevA.03\State=1-A\HF=-812.1642831\RMSD=4.58
5e-09\Dipole=-0.8670917,0.4403069,-0.0278347\Quadrupole=0.1276343,2.14
34009,-2.2710352,1.0554737,4.8442982,-0.8001218\PG=C01 [X(C19H22O1)]\\
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