

Supporting information

Nickel-Catalyzed Cross-Electrophile Coupling of Aryl Bromides and Primary Alkyl Bromides with Spiro-bidentate-pyox Ligand

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Table of Contents

I. Experimental Section	1
General.....	1
The Procedure for Cross-Electrophile Coupling product 3	1
Characterization data of compound 3	2
Radical Clock Experiment	6
II. Spectral Data for Compounds 3	7

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I. Experimental Section

General

All reagents were purchased from commercial suppliers and used without purification. All reactions were monitored by TLC. Chromatography refers to open column chromatography on silica gel (200-300 mesh). Melting points were uncorrected values. ¹H NMR spectra were recorded at 500 MHz and ¹³C NMR spectra were recorded at 126 MHz by using a Bruker Avance 500M spectrometer. Mass spectra were performed on an Ultima Global spectrometer with an ESI source.

General procedure for the cross electrophile coupling product 3

Details of Optimization and Control Experiments 3

A typical procedure for optimization and control reactions: To a dried vial equipped with a magnetic stir bar was added metal catalyst (x mmol) and additive (if applicable) in glove box. The vial was moved out of the glove box, ligand and solvent were added via syringe. The reaction mixture was stirred for one hour at room temperature. Aryl bromide (0.40 mmol), alkyl bromide (0.20 mmol) and reductant (0.60 mmol) were added sequentially. The reaction mixture was allowed to stir under argon atmosphere at heated. After the reaction finished, it was directly loaded onto a silica column without work-up. Through flash column chromatography (SiO₂: ethyl acetate in petroleum) to provide the cross coupling product.

The Procedure for Cross-Electrophile Coupling product 3

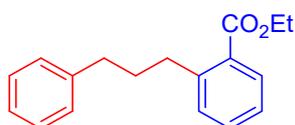
To a dried vial equipped with a magnetic stir bar was added NiBr₂ (6.6 mg, 0.03 mmol) and lithium bromide (17.4 mg, 0.20 mmol) in glove box. The vial was moved out of the glove box, **L1d** (9.60 mg, 0.03 mmol) and DMPU (1 mL) were added via syringe. The reaction mixture was stirred for one hour at room temperature. Aryl bromide (0.40 mmol), alkyl bromide (0.20 mmol) and manganese powder (33 mg, 0.60 mmol) were added sequentially. The reaction mixture was allowed to stir under argon atmosphere at 80 °C. After the reaction finished, it was directly loaded onto a silica column without work-up. Through flash column chromatography (SiO₂: ethyl acetate in petroleum) to provide the cross coupling product.



Ethyl 4-(3-phenylpropyl)benzoate **3a**

The compound was reported previously in *Angew. Chem. Int. Ed*, **2018**, 57, 11339-11343. The title compound was isolated as a colorless oil in 91% yield.

¹H NMR (500 MHz, Chloroform-d) δ 8.02 (d, J = 8.2 Hz, 2H), 7.34 (t, J = 7.5 Hz, 2H), 7.30 (d, J = 7.8 Hz, 2H), 7.27 – 7.21 (m, 3H), 4.42 (q, J = 7.1 Hz, 2H), 2.75 (t, J = 7.7 Hz, 2H), 2.70 (t, J = 7.7 Hz, 2H), 2.07 – 1.98 (m, 2H), 1.44 (t, J = 7.1 Hz, 3H). ¹³C NMR (126 MHz, Chloroform-d) δ 166.82, 147.83, 142.06, 129.78, 128.55, 128.49, 128.29, 125.99, 60.90, 35.54, 35.46, 32.73, 14.48. HRMS (ESI-TOF⁺) [M+H]⁺ m/z calcd for C₁₈H₂₀O₂H⁺ 269.1542, found 269.1544.

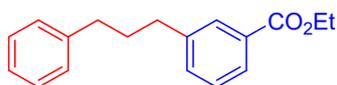


Ethyl 2-(3-phenylpropyl)benzoate **3b**

The compound was reported previously in *Nature Chemistry*, **2016**, 8, 1126-1130.

The title compound was isolated as a colorless oil in 76% yield.

¹H NMR (500 MHz, Chloroform-d) δ 7.89 (dd, J = 7.7, 1.5 Hz, 1H), 7.44 (td, J = 7.5, 1.5 Hz, 1H), 7.34 – 7.25 (m, 5H), 7.25 – 7.19 (m, 3H), 4.37 (q, J = 7.1 Hz, 2H), 3.06 – 3.01 (m, 2H), 2.73 (t, J = 7.8 Hz, 2H), 2.01 – 1.94 (m, 2H), 1.41 (t, J = 7.1 Hz, 3H). ¹³C NMR (126 MHz, Chloroform-d) δ 168.03, 144.00, 142.50, 131.85, 131.00, 130.72, 130.16, 128.57, 128.41, 125.96, 125.85, 60.95, 36.07, 34.30, 33.53, 14.46. HRMS (ESI-TOF⁺) [M+H]⁺ m/z calcd for C₁₈H₂₀O₂H⁺ 269.1542, found 269.1542.

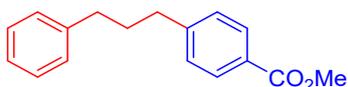


Ethyl 3-(3-phenylpropyl)benzoate **3c**

The compound was reported previously in *Nature Chemistry*, **2009**, 1, 494-499.

The title compound was isolated as a colorless oil in 52% yield.

¹H NMR (500 MHz, Chloroform-d) δ 7.91 – 7.86 (m, 2H), 7.40 – 7.33 (m, 2H), 7.30 (dd, J = 8.7, 6.5 Hz, 2H), 7.20 (dd, J = 7.7, 5.6 Hz, 3H), 4.39 (q, J = 7.2 Hz, 2H), 2.69 (dt, J = 21.3, 7.7 Hz, 4H), 2.03 – 1.95 (m, 2H), 1.41 (t, J = 7.1 Hz, 3H). ¹³C NMR (126 MHz, Chloroform-d) δ 166.95, 142.67, 142.15, 133.12, 130.67, 129.63, 128.57, 128.48, 128.43, 127.20, 125.96, 61.04, 35.51, 35.33, 32.98, 14.49. HRMS (ESI-TOF⁺) [M+H]⁺ m/z calcd for C₁₈H₂₀O₂H⁺ 269.1542, found 269.1545.

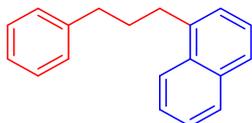


Methyl 4-(3-phenylpropyl)benzoate **3d**

The compound was reported previously in *ACS Catalysis*, **2020**, 10, 12642-12656

The title compound was isolated as a colorless oil in 89% yield.

^1H NMR (500 MHz, Chloroform-*d*) δ 8.00 (d, J = 8.0 Hz, 2H), 7.33 (t, J = 7.5 Hz, 2H), 7.30 – 7.27 (m, 2H), 7.26 – 7.20 (m, 3H), 3.94 (s, 3H), 2.74 (t, J = 7.7 Hz, 2H), 2.69 (t, J = 7.7 Hz, 2H), 2.05 – 1.98 (m, 2H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 167.30, 147.97, 142.04, 129.82, 128.60, 128.55, 128.50, 127.93, 126.00, 52.10, 35.54, 35.47, 32.72. HRMS (ESI-TOF $^+$) $[\text{M}+\text{Na}]^+$ m/z calcd for $\text{C}_{17}\text{H}_{18}\text{O}_2\text{Na}^+$ 277.1204, found 277.1215.



1-(3-Phenylpropyl)naphthalene **3e**

The compound was reported previously in *Organic Letters*, **2018**, 20, 5644-5647.

The title compound was isolated as a colorless oil in 59% yield.

^1H NMR (500 MHz, Chloroform-*d*) δ 8.04 – 7.99 (m, 1H), 7.94 – 7.87 (m, 1H), 7.77 (d, J = 8.1 Hz, 1H), 7.53 (tt, J = 7.1, 5.1 Hz, 2H), 7.45 (dd, J = 8.2, 7.0 Hz, 1H), 7.40 – 7.33 (m, 3H), 7.30 – 7.23 (m, 3H), 3.20 – 3.13 (m, 2H), 2.82 (t, J = 7.7 Hz, 2H), 2.20 – 2.12 (m, 2H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 142.32, 138.54, 134.03, 132.01, 128.89, 128.62, 128.47, 126.70, 126.05, 125.95, 125.83, 125.65, 125.53, 123.93, 36.02, 32.68, 32.39. HRMS (ESI-TOF $^+$) $[\text{M}+\text{Na}]^+$ m/z calcd for $\text{C}_{19}\text{H}_{18}\text{Na}^+$ 269.1306, found 269.1299.

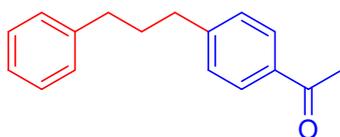


4-(3-Phenylpropyl)benzaldehyde **3f**

The compound was reported previously in *ACS Catalysis*, **2020**, 10, 12642-12656.

The title compound was isolated as a colorless oil in 67% yield.

^1H NMR (500 MHz, Chloroform-*d*) δ 9.98 (s, 1H), 7.81 (d, J = 7.8 Hz, 2H), 7.35 (d, J = 7.8 Hz, 2H), 7.30 (t, J = 7.5 Hz, 2H), 7.23 – 7.17 (m, 3H), 2.74 (t, J = 7.8 Hz, 2H), 2.67 (t, J = 7.7 Hz, 2H), 2.00 (tt, J = 9.1, 6.8 Hz, 2H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 192.12, 149.94, 141.89, 134.66, 130.07, 129.24, 128.53, 126.06, 35.73, 35.48, 32.64. HRMS (ESI-TOF $^+$) $[\text{M}+\text{H}]^+$ m/z calcd for $\text{C}_{16}\text{H}_{16}\text{OH}^+$ 225.1279, found 225.1277.

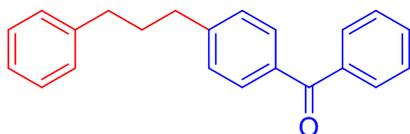


1-(4-(3-Phenylpropyl)phenyl)ethan-1-one **3g**

The compound was reported previously in *J. Am. Chem. Soc.* **2016**, 138, 5016–5019.

The title compound was isolated as a colorless oil in 69% yield.

^1H NMR (500 MHz, Chloroform-*d*) δ 7.90 (d, J = 7.9 Hz, 2H), 7.29 (dq, J = 10.4, 6.0, 4.4 Hz, 4H), 7.20 (dd, J = 10.8, 7.4 Hz, 3H), 2.72 (t, J = 7.8 Hz, 2H), 2.67 (t, J = 7.7 Hz, 2H), 2.60 (s, 3H), 1.99 (tt, J = 8.8, 6.9 Hz, 2H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 197.99, 148.28, 141.99, 135.20, 128.77, 128.65, 128.54, 128.50, 126.01, 35.52, 35.47, 32.67, 26.67. HRMS (ESI-TOF $^+$) $[\text{M}+\text{H}]^+$ m/z calcd for $\text{C}_{17}\text{H}_{18}\text{OH}^+$ 239.1436, found 239.1434.

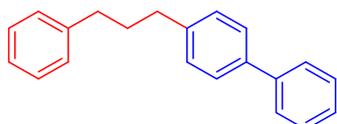


Phenyl(4-(3-phenylpropyl)phenyl)methanone **3h**

The compound was reported previously in *Organic Letters*, 2020, 22, 2350-2353.

The title compound was isolated as a colorless oil in 56% yield.

¹H NMR (500 MHz, Chloroform-*d*) δ 7.62 – 7.56 (m, 2H), 7.52 (dd, $J = 8.4, 2.1$ Hz, 2H), 7.43 (dd, $J = 8.5, 6.8$ Hz, 2H), 7.37 – 7.24 (m, 6H), 7.23 – 7.18 (m, 3H), 2.70 (td, $J = 7.7, 4.2$ Hz, 4H), 2.01 (tdd, $J = 9.3, 6.9, 4.1$ Hz, 2H). ¹³C NMR (126 MHz, Chloroform-*d*) δ 142.39, 141.56, 141.26, 138.85, 129.00, 128.85, 128.60, 128.46, 127.19, 127.13, 125.91, 35.60, 35.19, 33.05. HRMS (ESI-TOF⁺) [M+H]⁺ m/z calcd for C₂₂H₂₀OH⁺ 301.1592, found 301.1570.

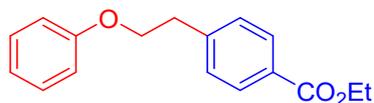


4-(3-Phenylpropyl)-1,1'-biphenyl **3i**

The compound was reported previously in *Organic Letters*, 2020, 22, 2350-2353.

The title compound was isolated as a colorless oil in 69% yield.

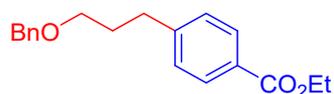
¹H NMR (500 MHz, Chloroform-*d*) δ 7.59 (dt, $J = 8.4, 1.9$ Hz, 2H), 7.55 – 7.50 (m, 2H), 7.43 (dd, $J = 8.5, 6.8$ Hz, 2H), 7.37 – 7.24 (m, 6H), 7.23 – 7.18 (m, 3H), 2.70 (td, $J = 7.7, 4.2$ Hz, 4H), 2.05 – 1.96 (m, 2H). ¹³C NMR (126 MHz, Chloroform-*d*) δ 142.39, 141.56, 141.26, 138.85, 129.00, 128.85, 128.60, 128.46, 127.19, 127.13, 125.91, 35.60, 35.19, 33.05. HRMS (ESI-TOF⁺) [M+H]⁺ m/z calcd for C₂₁H₂₀H⁺ 273.1643, found 273.1652; [M+Na]⁺ m/z calcd for C₂₁H₂₀Na⁺ 295.1463, found 295.1479.



Ethyl 4-(2-phenoxyethyl)benzoate **3j**

The title compound was isolated as a colorless oil in 65% yield.

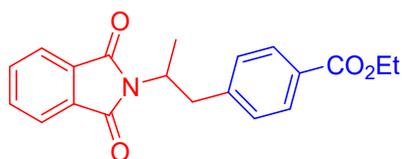
¹H NMR (500 MHz, Chloroform-*d*) δ 7.97 (d, $J = 8.1$ Hz, 2H), 7.33 (d, $J = 8.0$ Hz, 2H), 7.26 – 7.21 (m, 2H), 6.91 (t, $J = 7.3$ Hz, 1H), 6.88 – 6.83 (m, 2H), 4.34 (q, $J = 7.1$ Hz, 2H), 4.17 (t, $J = 6.8$ Hz, 2H), 3.12 (t, $J = 6.8$ Hz, 2H), 1.36 (t, $J = 7.1$ Hz, 3H). ¹³C NMR (126 MHz, Chloroform-*d*) δ 166.66, 158.75, 143.86, 129.85, 129.59, 129.10, 128.94, 121.01, 114.68, 68.08, 60.97, 35.90, 14.46. HRMS (ESI-TOF⁺) [M+H]⁺ m/z calcd for C₁₇H₁₈O₃H⁺ 271.1334, found 271.1339.



Ethyl 4-(3-(benzyloxy)propyl)benzoate **3k**

The title compound was isolated as a colorless oil in 71% yield.

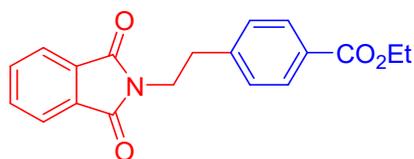
¹H NMR (500 MHz, Chloroform-*d*) δ 7.96 (d, $J = 8.3$ Hz, 2H), 7.35 (d, $J = 5.9$ Hz, 4H), 7.30 (td, $J = 5.9, 3.4$ Hz, 1H), 7.24 (d, $J = 8.1$ Hz, 2H), 4.51 (s, 2H), 4.37 (q, $J = 7.1$ Hz, 2H), 3.48 (t, $J = 6.3$ Hz, 2H), 2.81 – 2.75 (m, 2H), 1.99 – 1.91 (m, 2H), 1.39 (t, $J = 7.1$ Hz, 3H). ¹³C NMR (126 MHz, Chloroform-*d*) δ 166.81, 147.57, 138.58, 129.78, 128.61, 128.52, 128.29, 127.81, 127.73, 73.11, 69.32, 60.90, 32.56, 31.19, 14.49. HRMS (ESI-TOF⁺) [M+Na]⁺ m/z calcd for C₁₉H₂₂O₃Na⁺ 321.1467, found 321.1454.



Ethyl 4-(2-(1,3-dioxoisindolin-2-yl)propyl)benzoate **3l**

The title compound was isolated as a colorless oil in 61% yield.

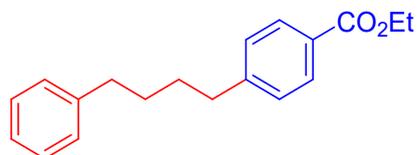
¹H NMR (500 MHz, Chloroform-*d*) δ 7.87 (dd, *J* = 8.2, 2.5 Hz, 2H), 7.78 – 7.70 (m, 2H), 7.65 (td, *J* = 5.0, 2.8 Hz, 2H), 7.24 (dd, *J* = 8.2, 2.2 Hz, 2H), 4.67 (tdd, *J* = 11.7, 6.9, 3.5 Hz, 1H), 4.31 (qd, *J* = 7.0, 2.8 Hz, 2H), 3.42 (ddd, *J* = 13.1, 9.8, 2.1 Hz, 1H), 3.13 (ddd, *J* = 13.9, 6.4, 2.3 Hz, 1H), 1.54 (dd, *J* = 7.0, 2.2 Hz, 3H), 1.34 (td, *J* = 7.1, 3.3 Hz, 3H). ¹³C NMR (126 MHz, Chloroform-*d*) δ 168.40, 166.62, 143.81, 134.00, 131.82, 129.86, 129.00, 128.93, 123.22, 60.95, 48.40, 39.92, 18.63, 14.42. HRMS (ESI-TOF⁺) [*M*+Na]⁺ *m/z* calcd for C₂₀H₁₉NO₄Na⁺ 360.1212, found 360.1211.



Ethyl 4-(2-(1,3-dioxoisindolin-2-yl)ethyl)benzoate **3m**

The title compound was isolated as a white solid in 62% yield.

¹H NMR (500 MHz, Chloroform-*d*) δ 7.94 (d, *J* = 8.0 Hz, 2H), 7.81 (dt, *J* = 7.5, 3.7 Hz, 2H), 7.70 (dd, *J* = 5.4, 3.0 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 4.34 (q, *J* = 7.1 Hz, 2H), 3.94 (dd, *J* = 8.4, 6.7 Hz, 2H), 3.05 (t, *J* = 7.6 Hz, 2H), 1.37 (t, *J* = 7.1 Hz, 3H). ¹³C NMR (126 MHz, Chloroform-*d*) δ 168.21, 166.60, 143.36, 134.12, 132.08, 129.97, 129.11, 128.97, 123.41, 60.99, 38.93, 34.65, 14.44. Melting Point: 115-116 °C. HRMS (ESI-TOF⁺) [*M*+Na]⁺ *m/z* calcd for C₁₉H₁₇NO₄Na⁺ 346.1055, found 346.1049.

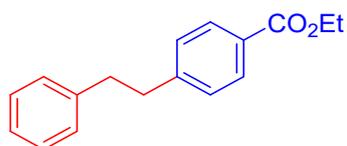


Ethyl 4-(4-phenylbutyl)benzoate **3n**

The compound was reported previously in *Org. Biomol. Chem.* **2016**, 14, 3314-3321.

The title compound was isolated as a colorless oil in 94% yield.

¹H NMR (500 MHz, Chloroform-*d*) δ 7.97 (d, *J* = 8.1 Hz, 2H), 7.29 (t, *J* = 7.5 Hz, 2H), 7.24 (d, *J* = 7.9 Hz, 2H), 7.21 – 7.15 (m, 3H), 4.38 (q, *J* = 7.1 Hz, 2H), 2.70 (t, *J* = 7.0 Hz, 2H), 2.65 (t, *J* = 7.0 Hz, 2H), 1.69 (dt, *J* = 7.2, 3.4 Hz, 4H), 1.40 (t, *J* = 7.1 Hz, 3H). ¹³C NMR (126 MHz, Chloroform-*d*) δ 166.82, 148.09, 142.47, 129.74, 128.51, 128.42, 128.21, 125.85, 60.88, 35.94, 35.86, 31.09, 30.81, 14.48. HRMS (ESI-TOF⁺) [*M*+H]⁺ *m/z* calcd for C₁₉H₂₂O₂H⁺ 283.1698, found 283.1694.



Ethyl 4-phenethylbenzoate **3o**

The compound was reported previously in *Organic Letters*, **2010**, 12, 1692-1695.

The title compound was isolated as a colorless oil in 83% yield.

^1H NMR (500 MHz, Chloroform- d) δ 8.03 (d, J = 8.2 Hz, 2H), 7.39 – 7.32 (m, 2H), 7.29 (t, J = 7.9 Hz, 3H), 7.25 – 7.20 (m, 2H), 4.44 (q, J = 7.1 Hz, 2H), 3.10 – 2.96 (m, 4H), 1.47 (t, J = 7.1 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform- d) δ 166.68, 147.05, 141.17, 129.66, 128.50, 128.46, 128.40, 128.30, 126.08, 60.81, 37.88, 37.49, 14.36. HRMS (ESI-TOF $^+$) $[\text{M}+\text{H}]^+$ m/z calcd for $\text{C}_{17}\text{H}_{18}\text{O}_2\text{H}^+$ 255.1385, found 255.1377.

Radical Clock Experiment

To a dried vial equipped with a magnetic stir bar was added NiBr_2 (6.6 mg, 0.03 mmol) and lithium bromide (17.4 mg, 0.20 mmol) in glove box. The vial was moved out of the glove box, **L1d** (9.60 mg, 0.03 mmol) and DMPU (1 mL) were added via syringe. The reaction mixture was stirred for one hour at room temperature. Then **1a** (0.40 mmol), cyclopropylmethyl bromide (0.20 mmol) and manganese powder (33 mg, 0.60 mmol) were added sequentially. The reaction mixture was allowed to stir under argon atmosphere at 80 $^\circ\text{C}$. After the reaction finished, it was directly loaded onto a silica column without work-up. Through flash column chromatography (SiO_2 : ethyl acetate in petroleum) to provide the ring-opened products **3qb-3qd** in 51% yield, the ratio of the **3qb**: **3qd**: **3qe** is about 2:0.4: 2.4. The ratio of the products was determined by ^1H NMR (500 MHz) analysis (Figure S1).

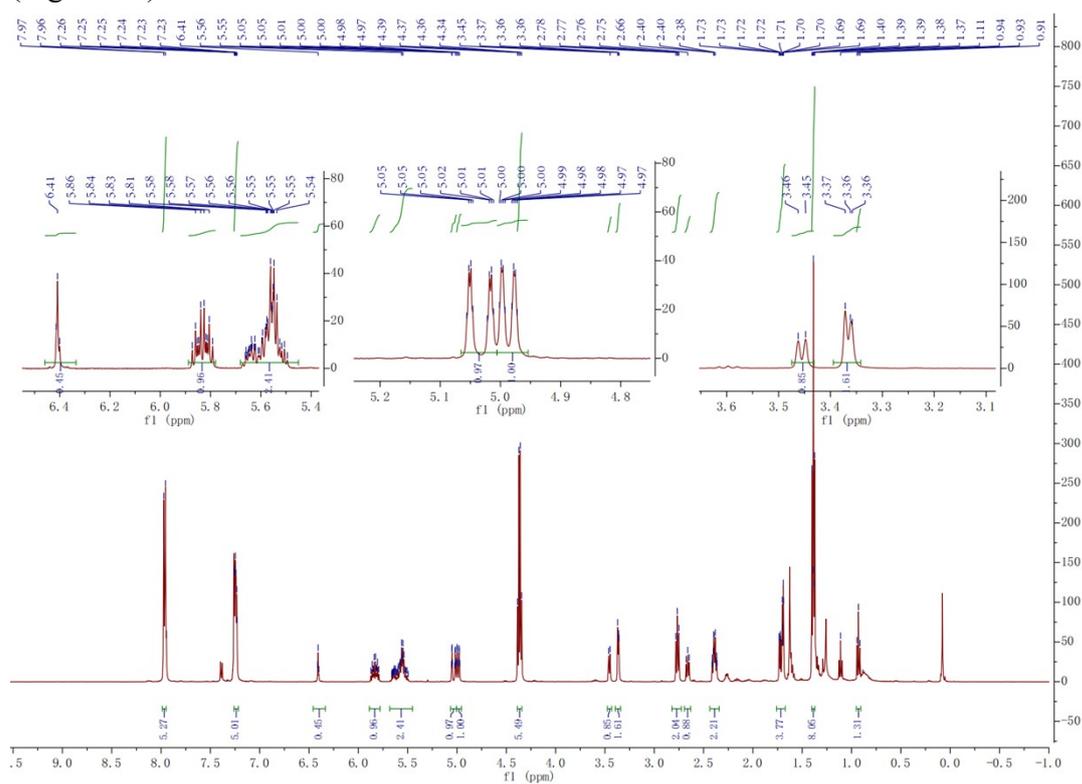
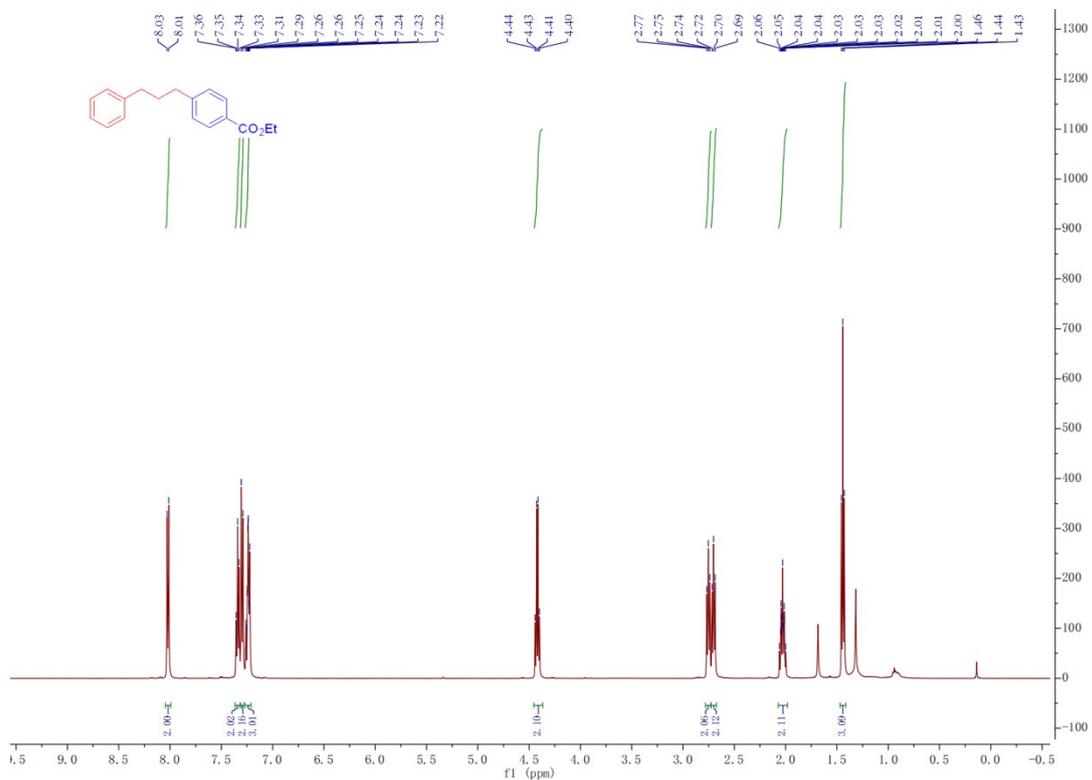


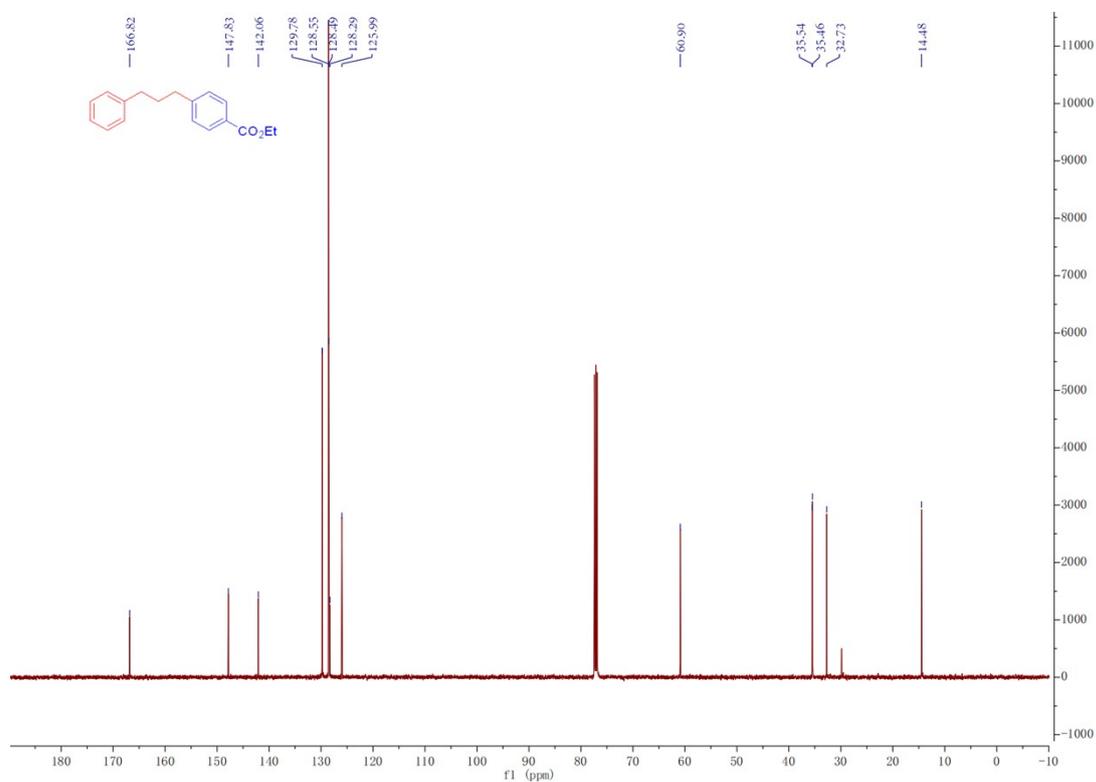
Figure S1. ^1H NMR (500 MHz, CDCl_3) spectrum of a reaction mixture obtained from radical clock experiment

II. Spectral Data for Compounds 3

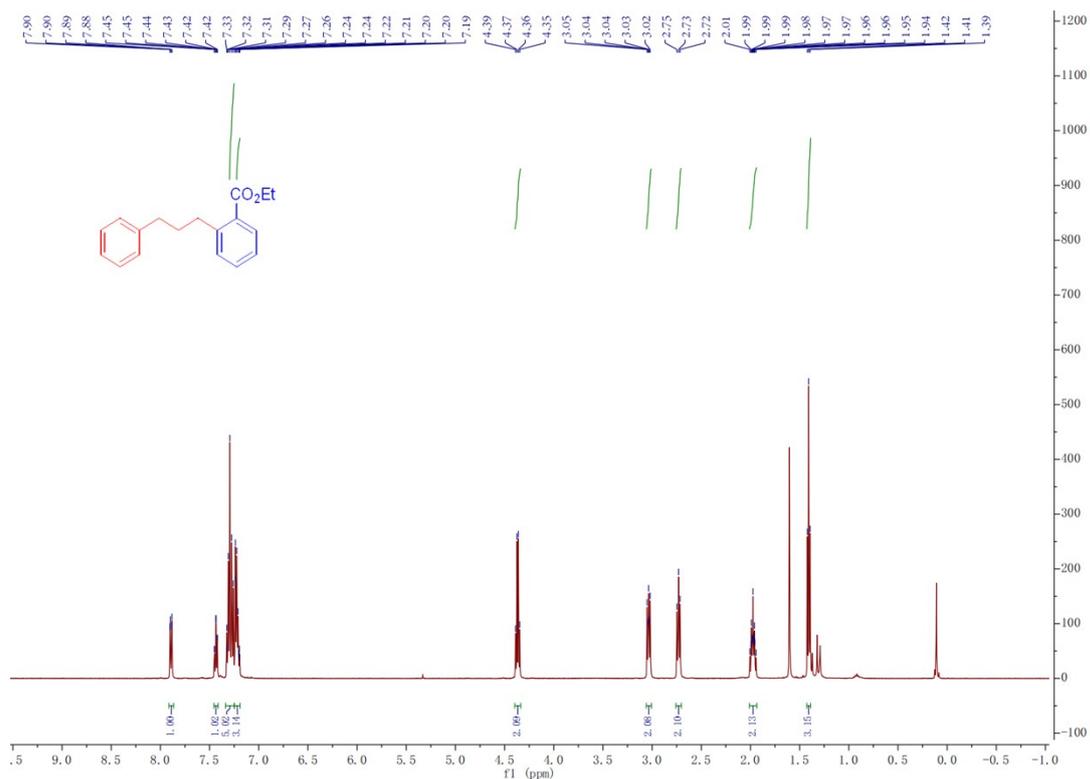
¹H NMR spectra of ethyl 4-(3-phenylpropyl)benzoate 3a



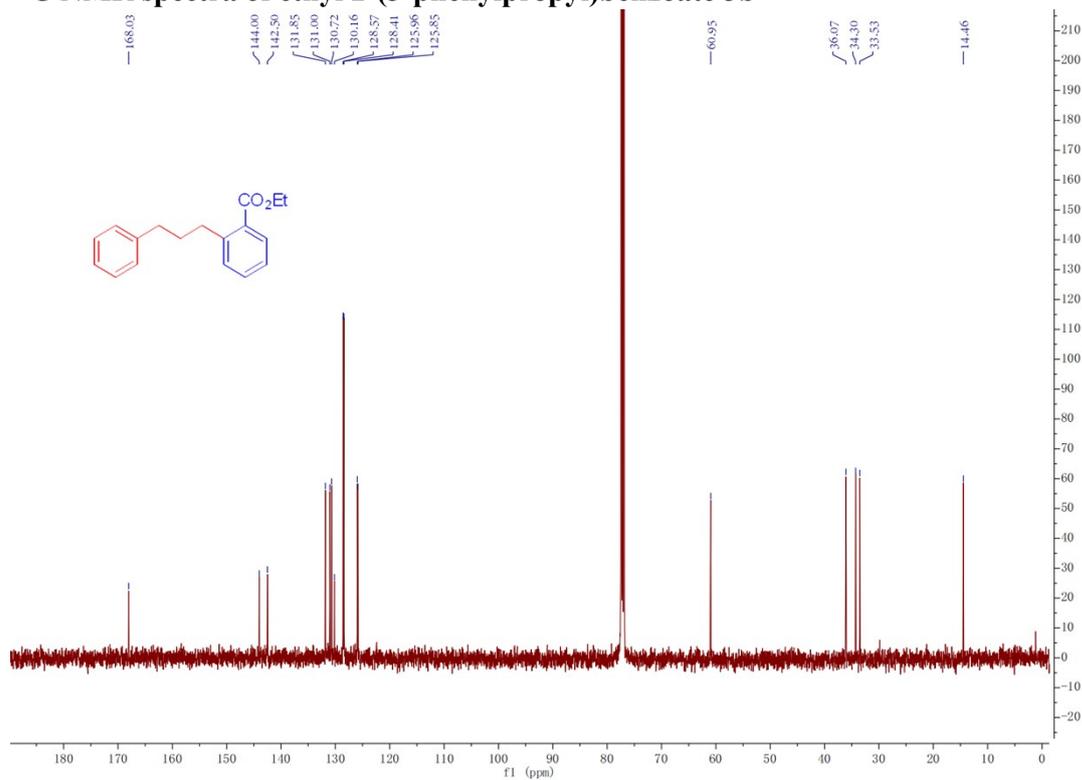
¹³C NMR spectra of ethyl 4-(3-phenylpropyl)benzoate 3a



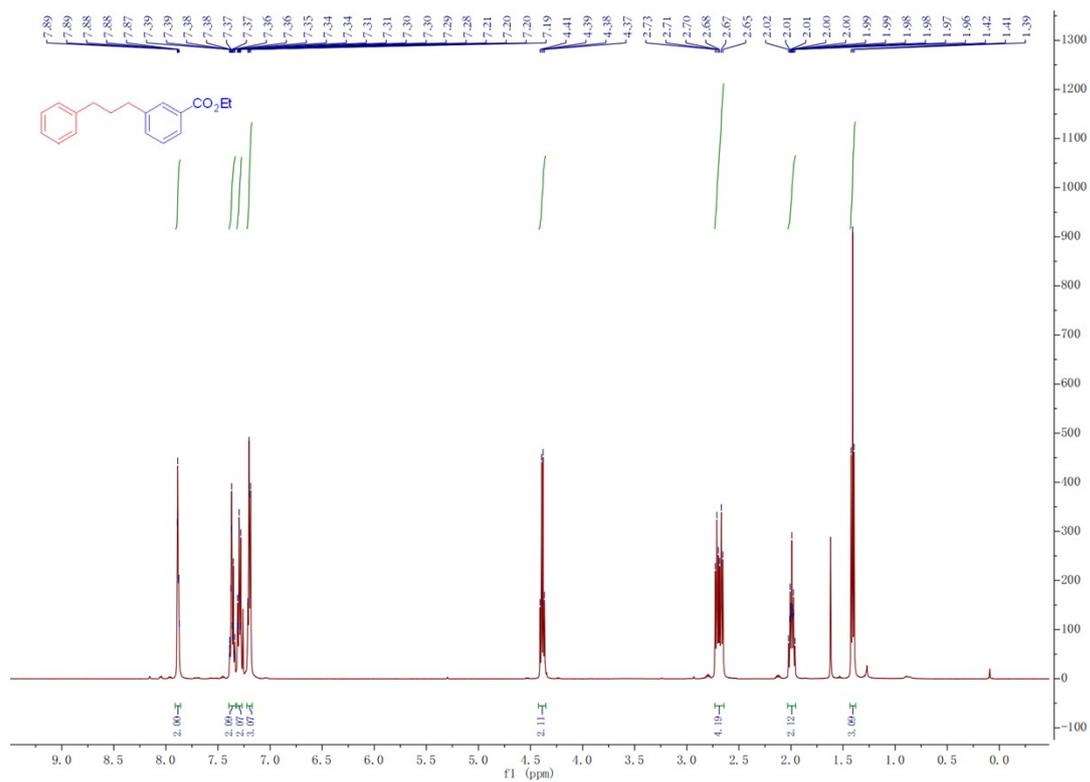
¹H NMR spectra of ethyl 2-(3-phenylpropyl)benzoate 3b



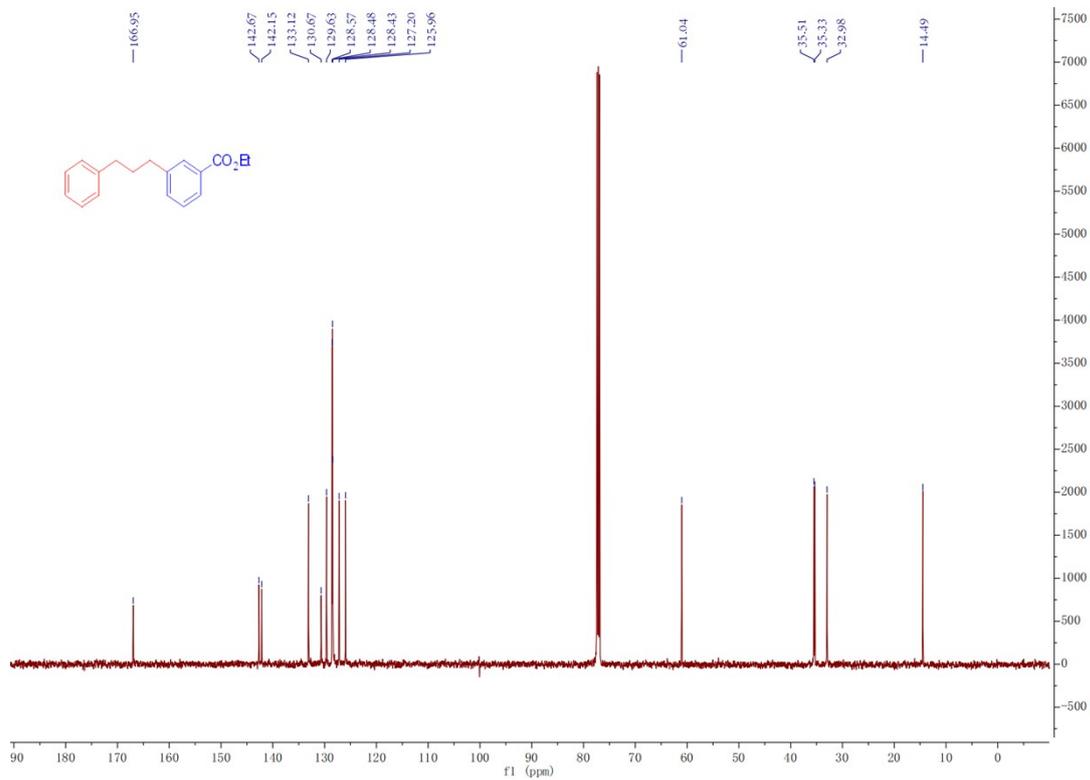
¹³C NMR spectra of ethyl 2-(3-phenylpropyl)benzoate 3b



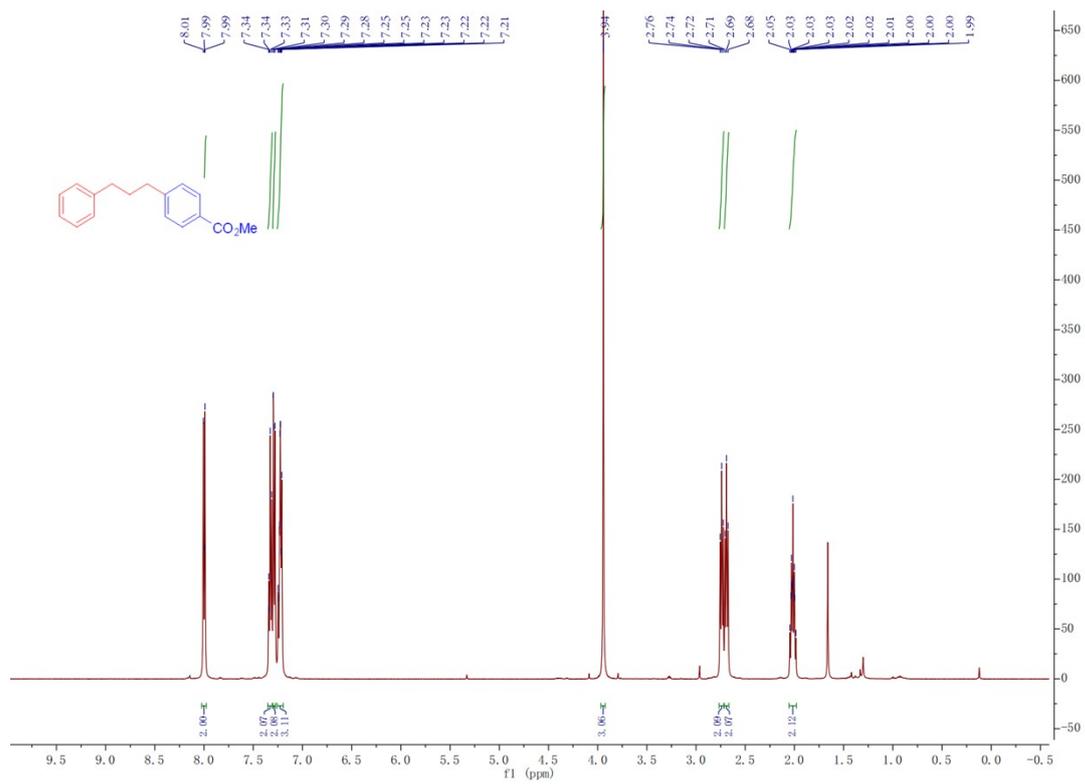
¹H NMR spectra of ethyl 3-(3-phenylpropyl)benzoate 3c



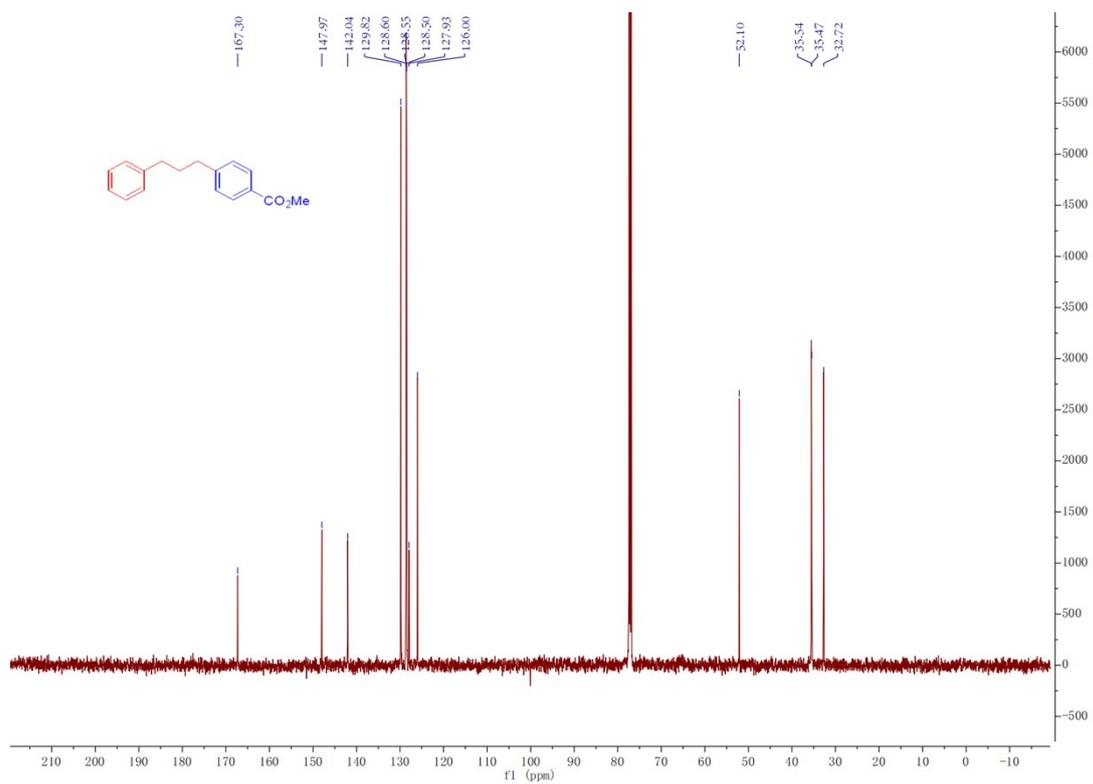
¹³C NMR spectra of ethyl 3-(3-phenylpropyl)benzoate 3c



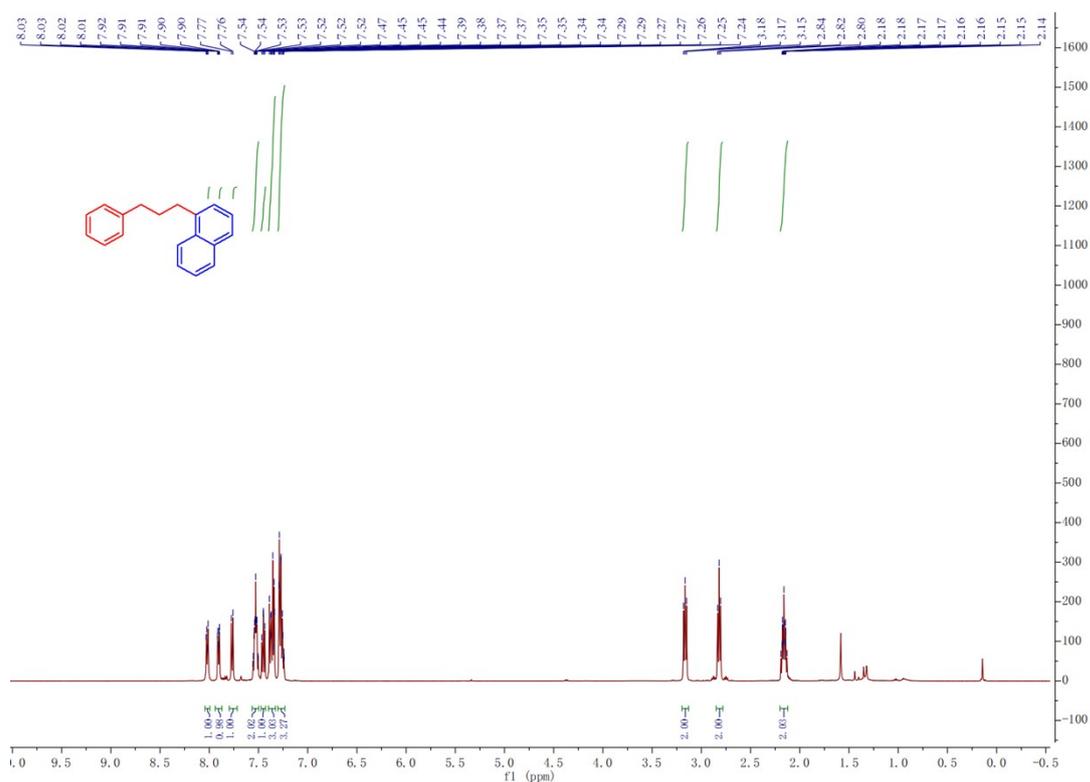
¹H NMR spectra of methyl 4-(3-phenylpropyl)benzoate 3d



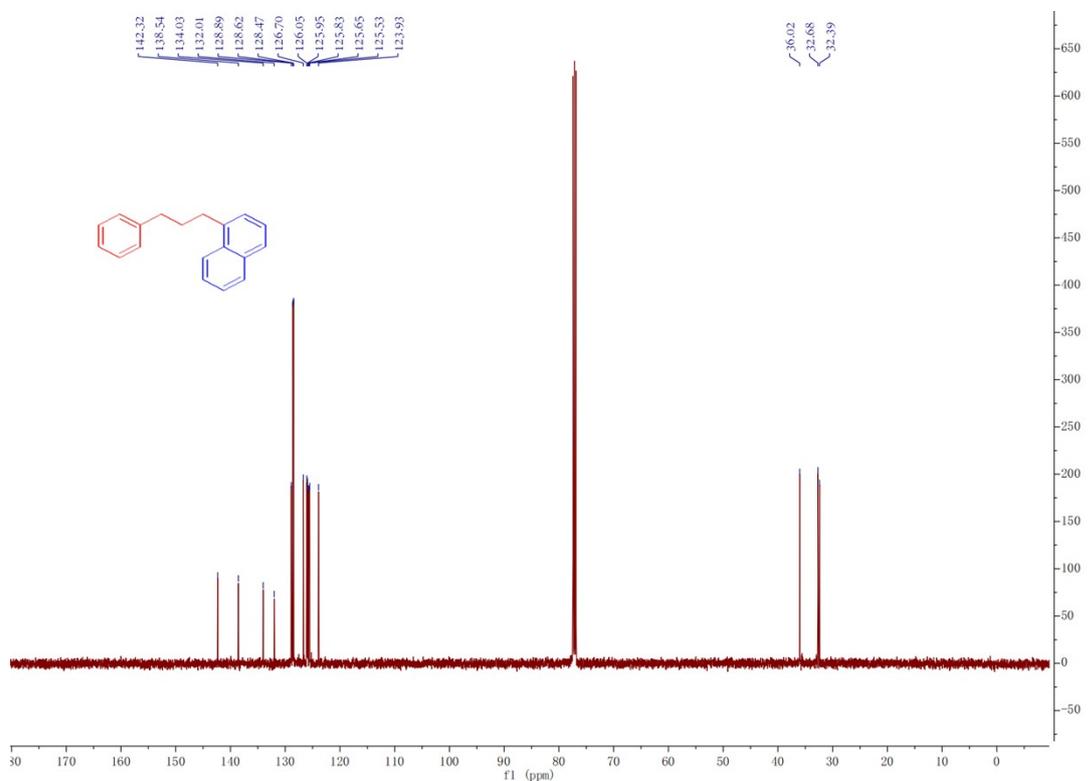
¹³C NMR spectra of methyl 4-(3-phenylpropyl)benzoate 3d



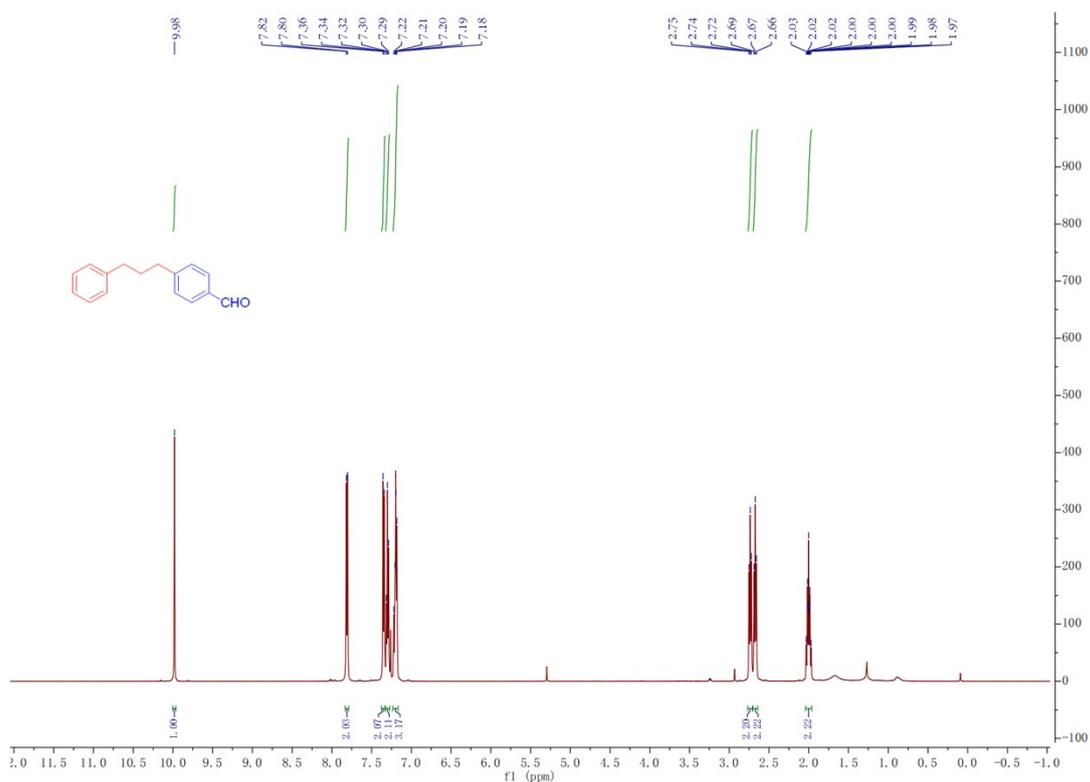
¹H NMR spectra of 1-(3-phenylpropyl)naphthalene 3e



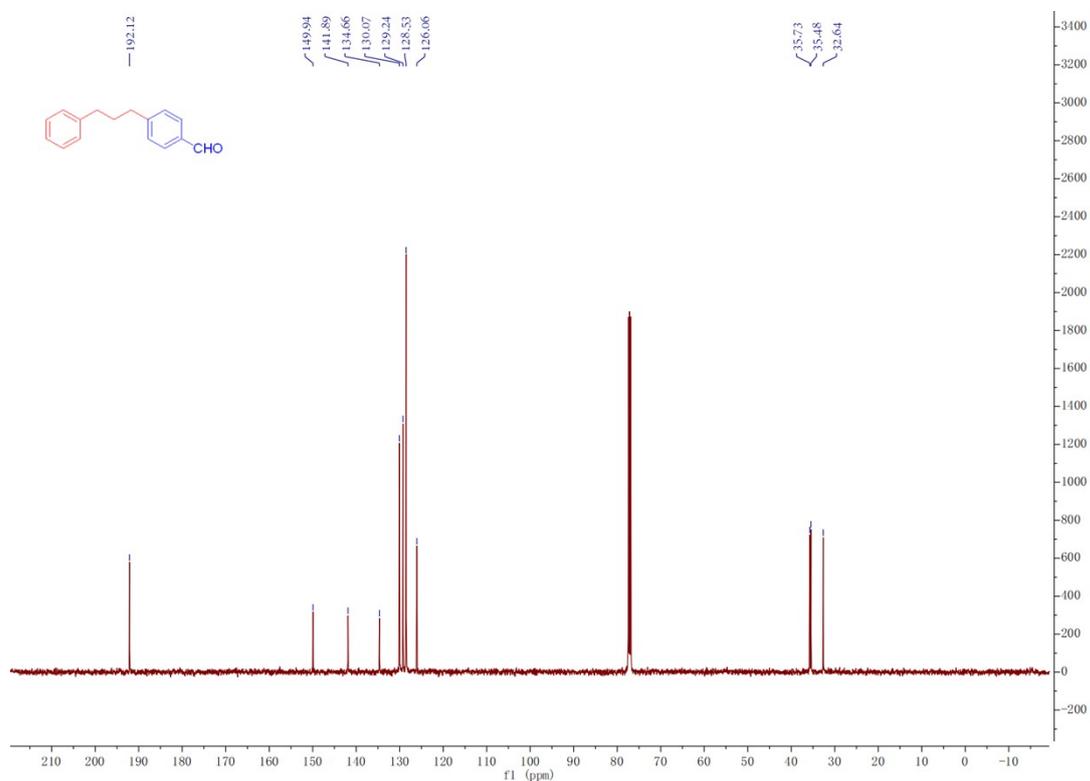
¹³C NMR spectra of 1-(3-phenylpropyl)naphthalene 3e



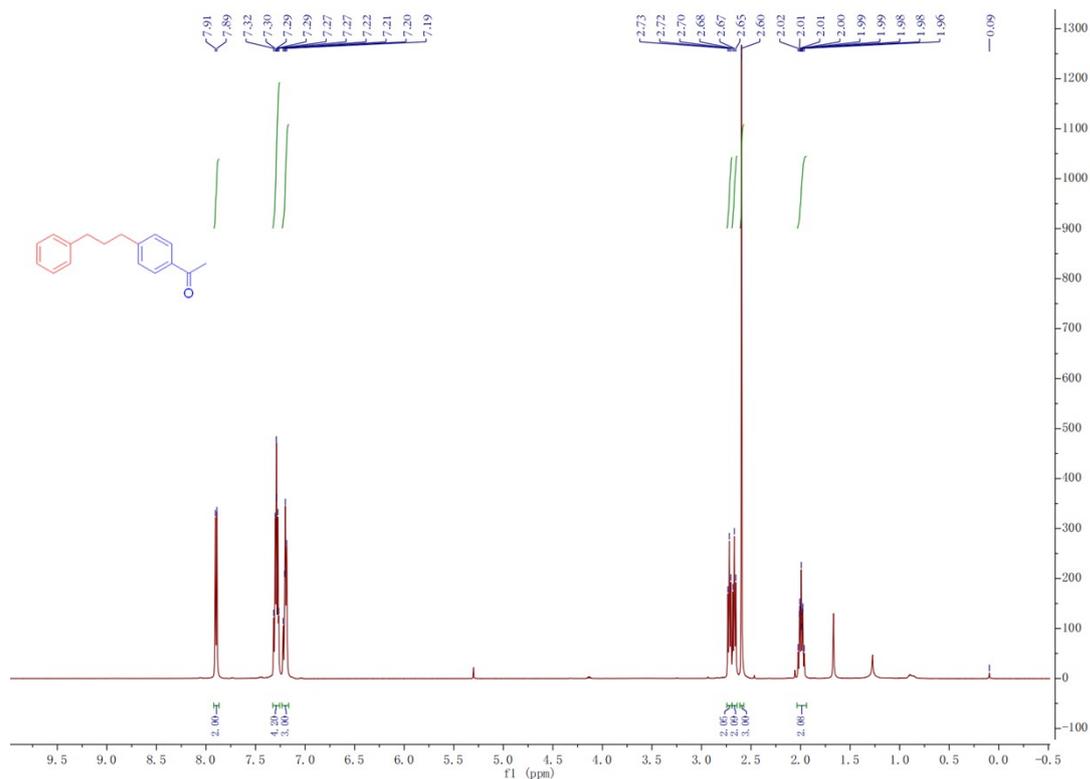
¹H NMR spectra of 4-(3-phenylpropyl)benzaldehyde 3f



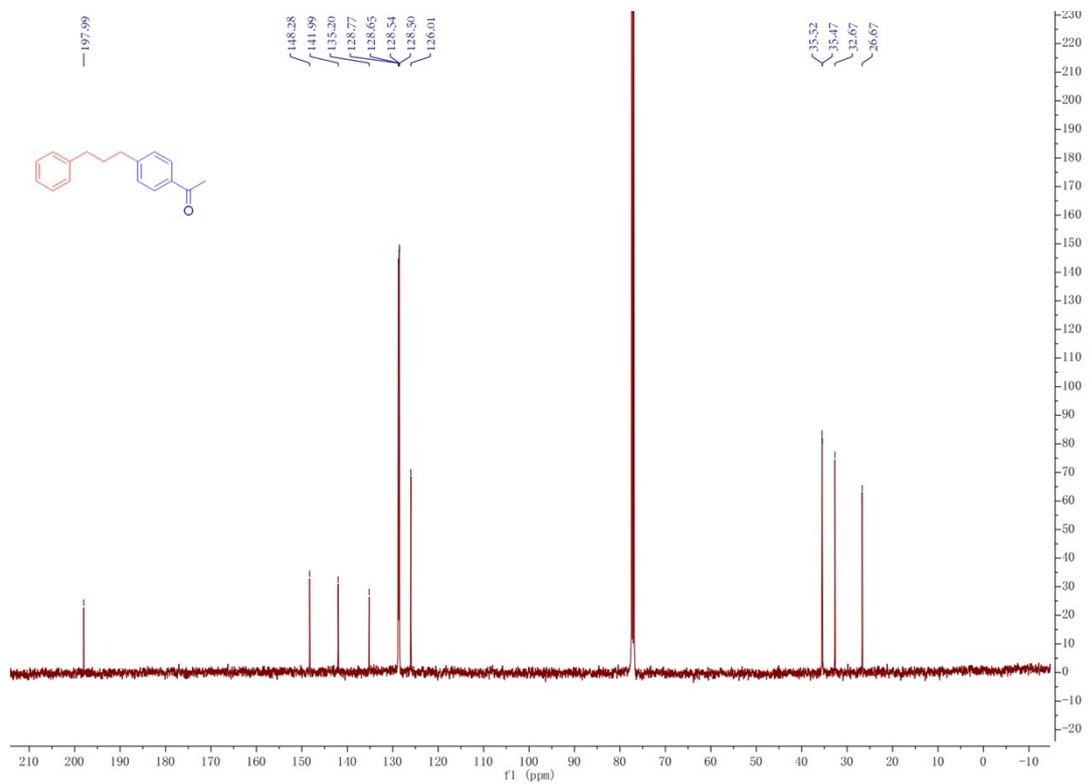
¹³C NMR spectra of 4-(3-phenylpropyl)benzaldehyde 3f



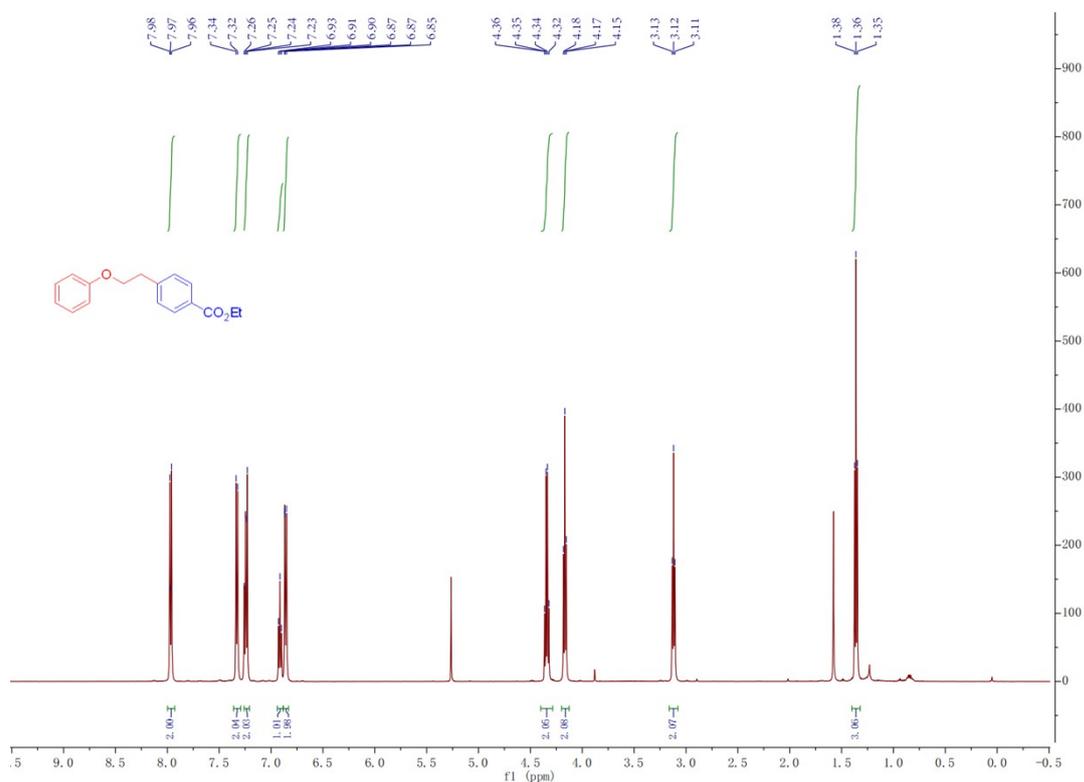
¹H NMR spectra of 1-(4-(3-phenylpropyl)phenyl)ethan-1-one 3g



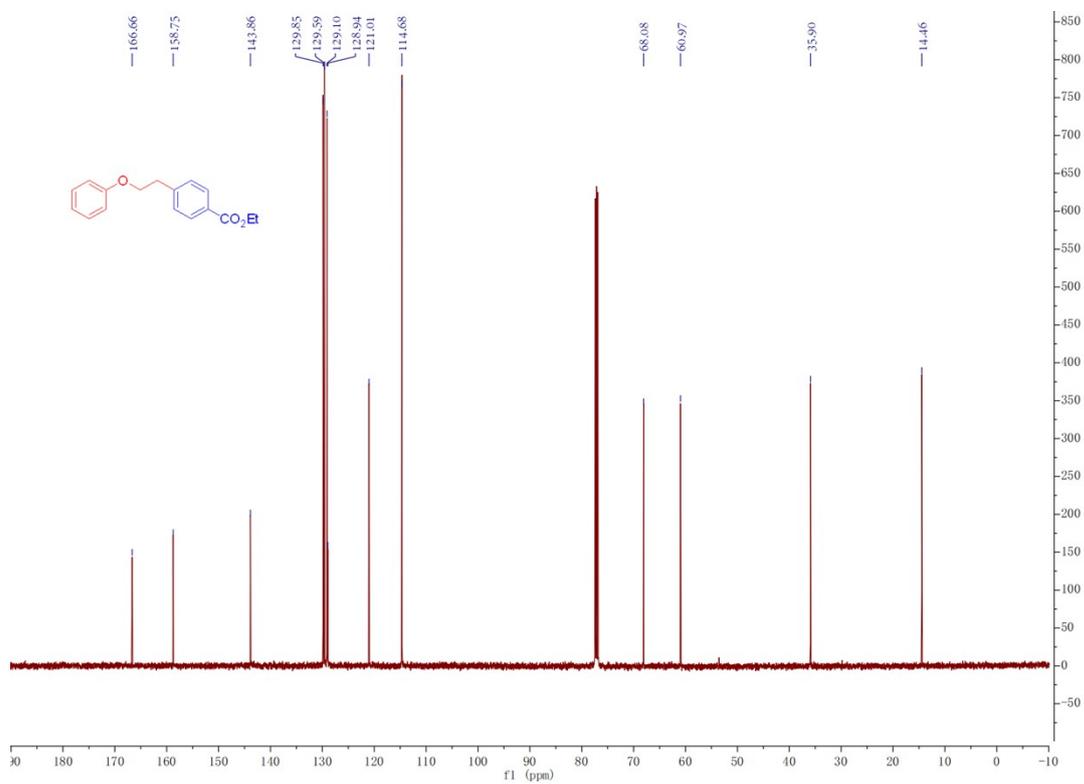
¹³C NMR spectra of 1-(4-(3-phenylpropyl)phenyl)ethan-1-one 3g



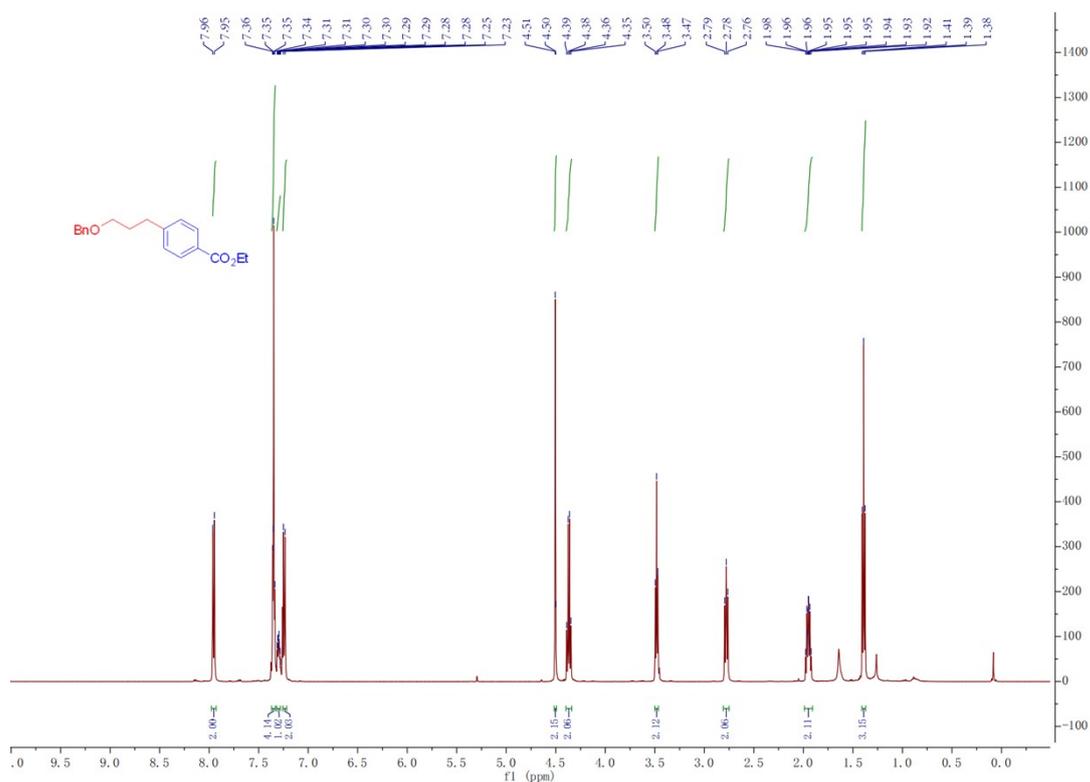
¹H NMR spectra of ethyl 4-(2-phenoxyethyl)benzoate 3j



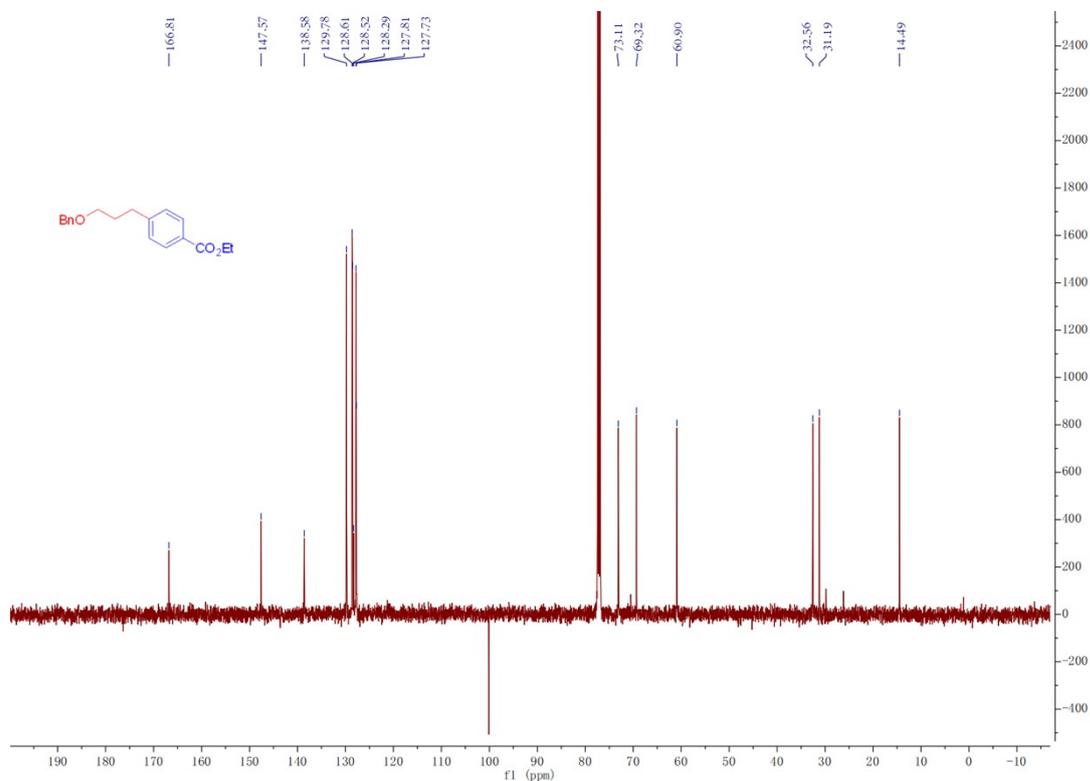
¹³C NMR spectra of ethyl 4-(2-phenoxyethyl)benzoate 3j



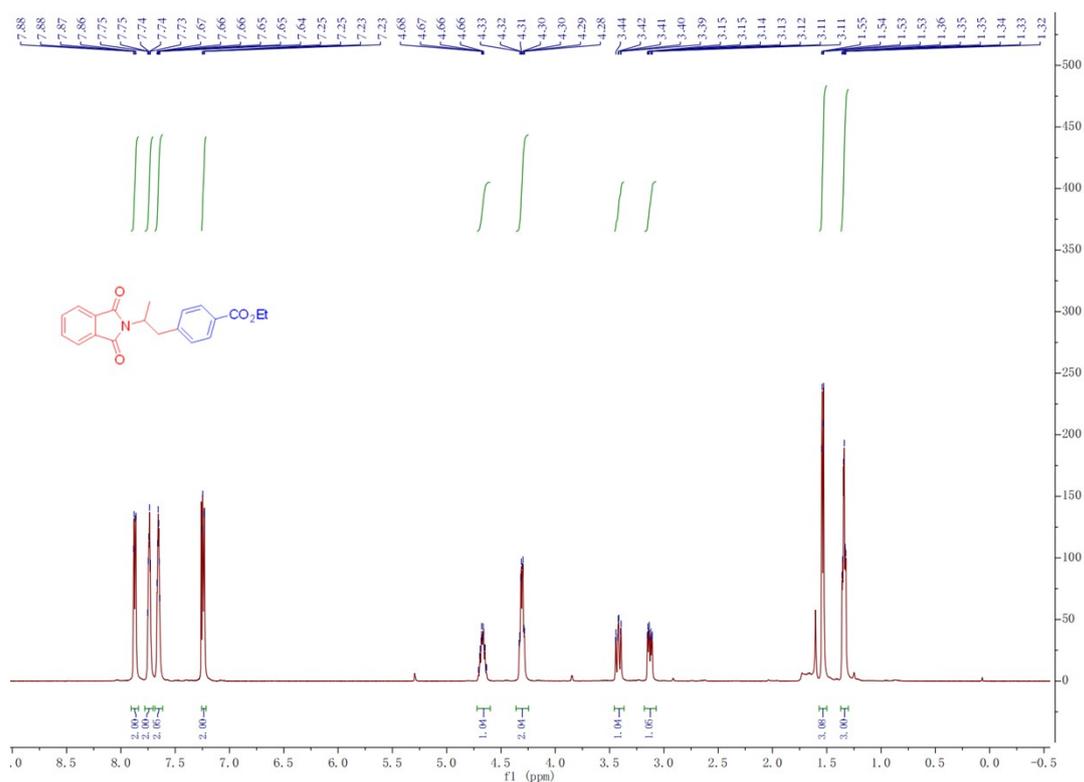
¹H NMR spectra of ethyl 4-(3-(benzyloxy)propyl)benzoate 3k



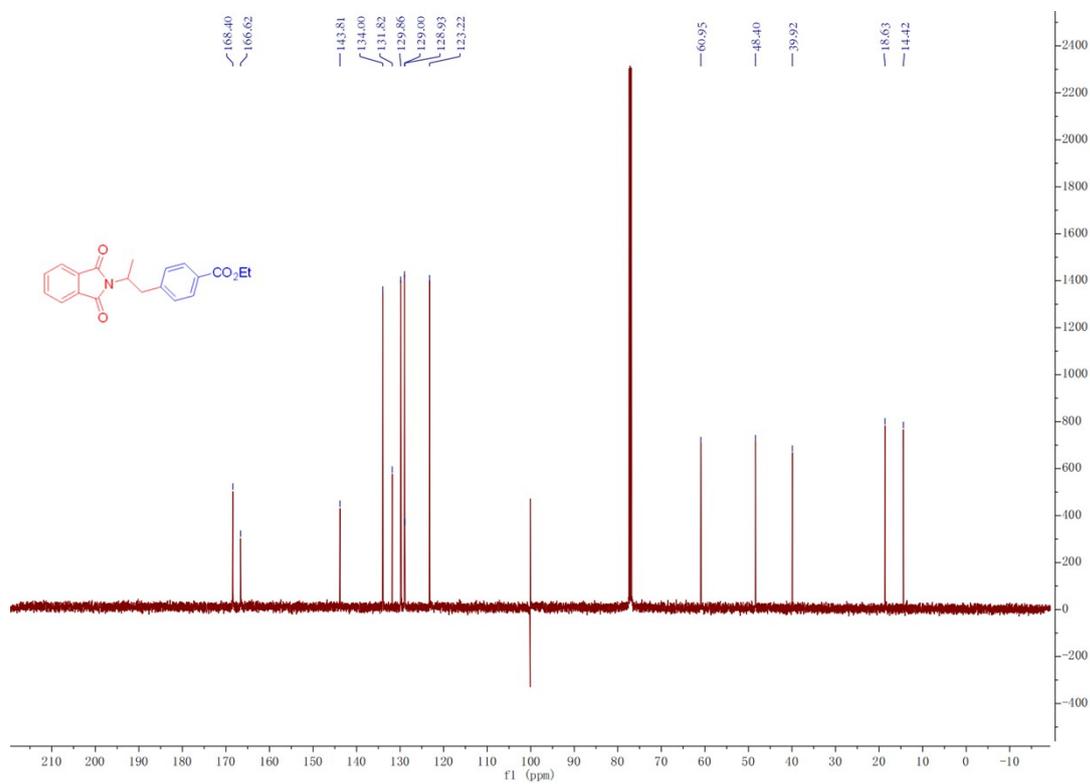
¹³C NMR spectra of ethyl 4-(3-(benzyloxy)propyl)benzoate 3k



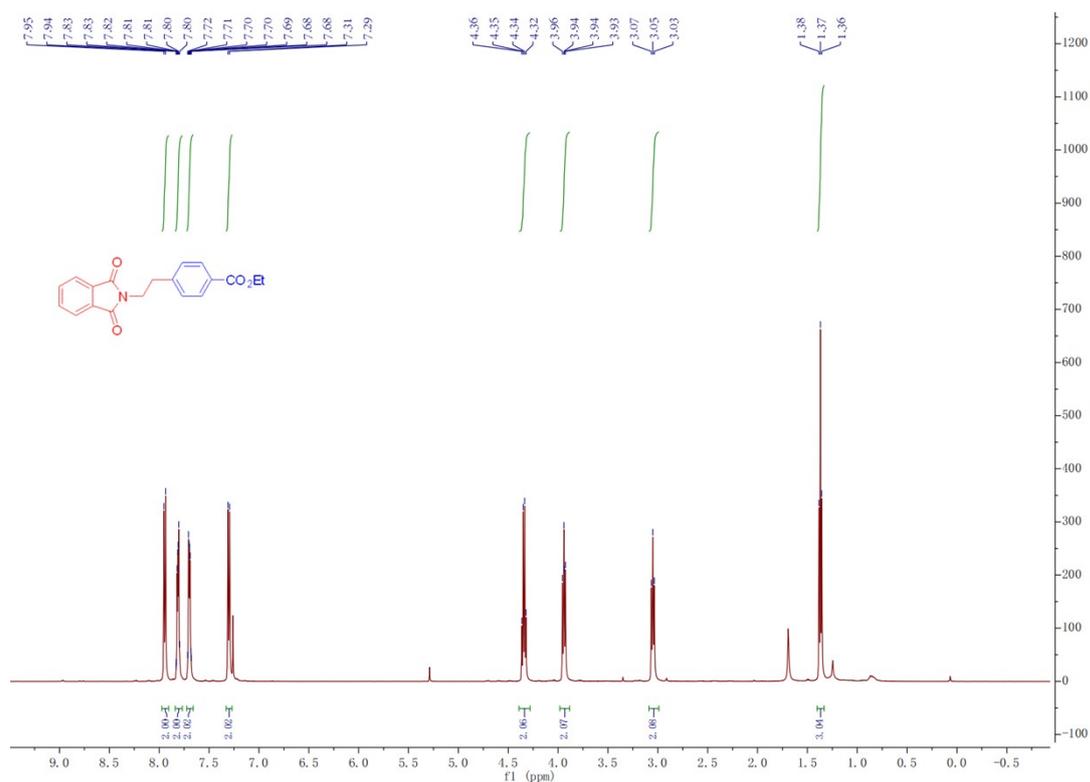
¹H NMR spectra of ethyl 4-(2-(1,3-dioxisoindolin-2-yl)propyl)benzoate 3l



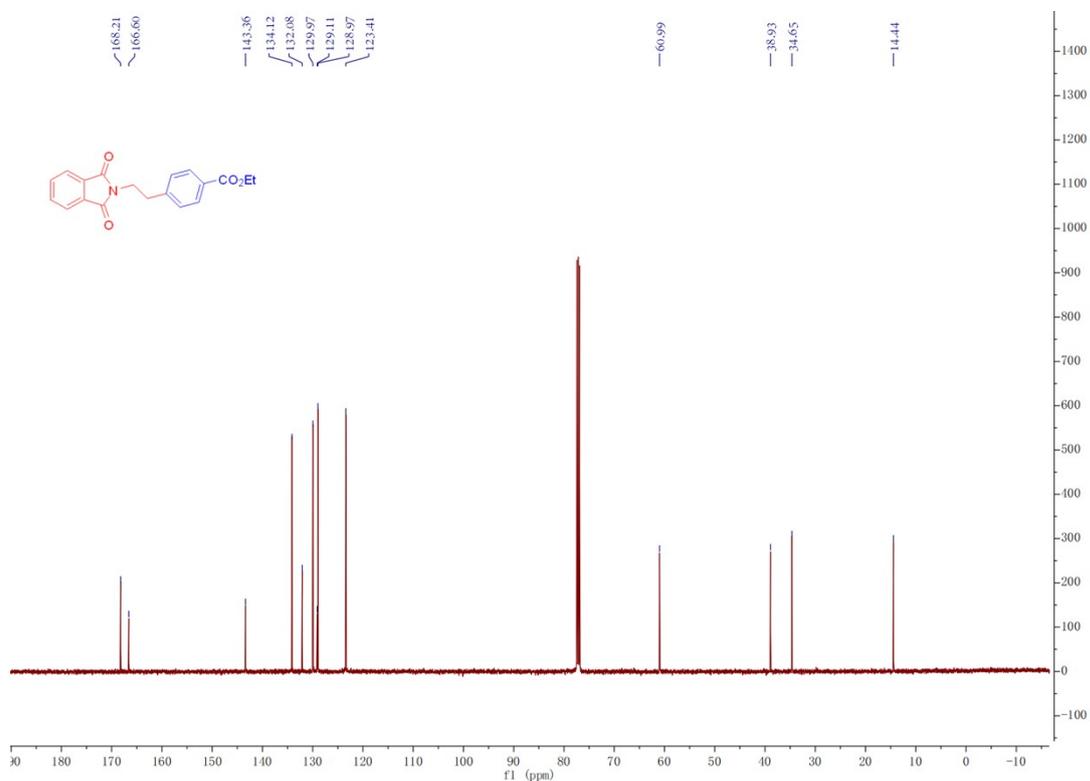
¹³C NMR spectra of ethyl 4-(2-(1,3-dioxisoindolin-2-yl)propyl)benzoate 3l



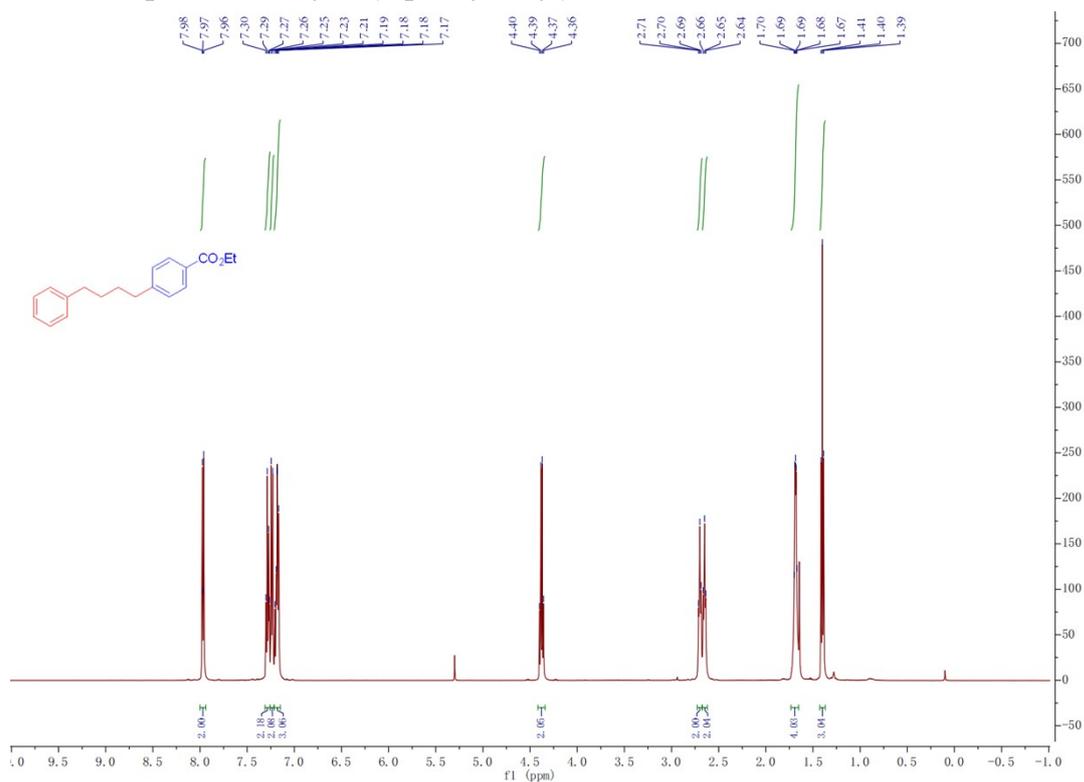
¹H NMR spectra of ethyl 4-(2-(1,3-dioxisoindolin-2-yl)ethyl)benzoate 3m



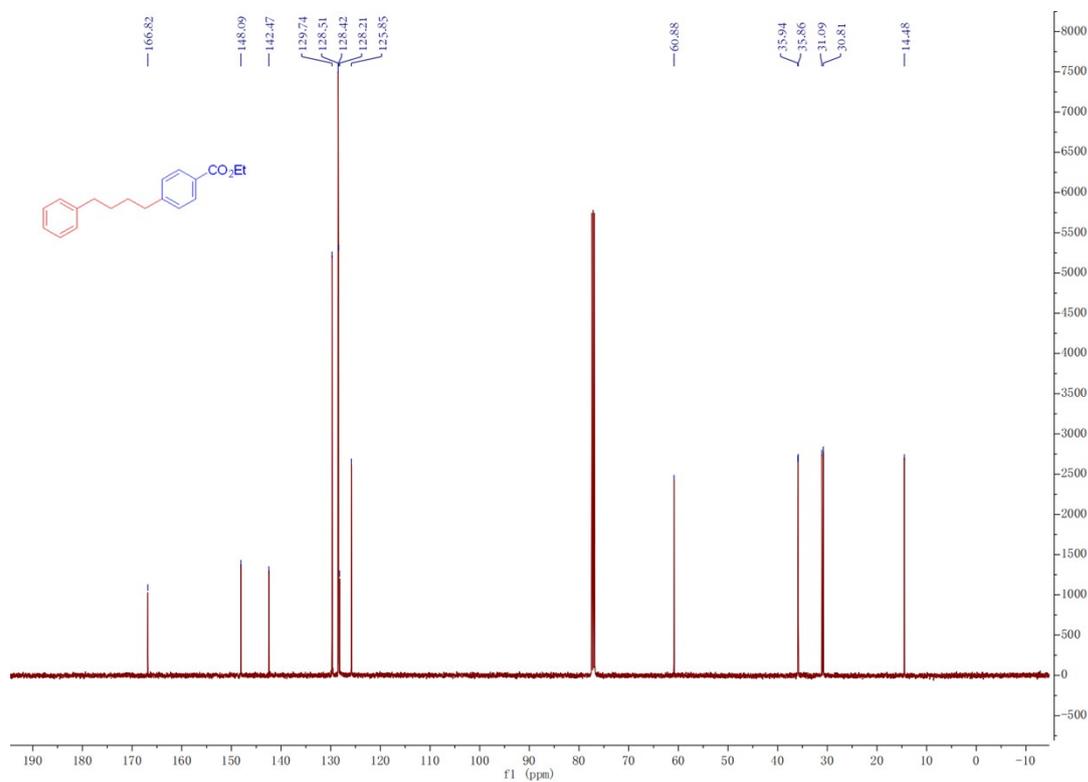
¹³C NMR spectra of ethyl 4-(2-(1,3-dioxisoindolin-2-yl)ethyl)benzoate 3m



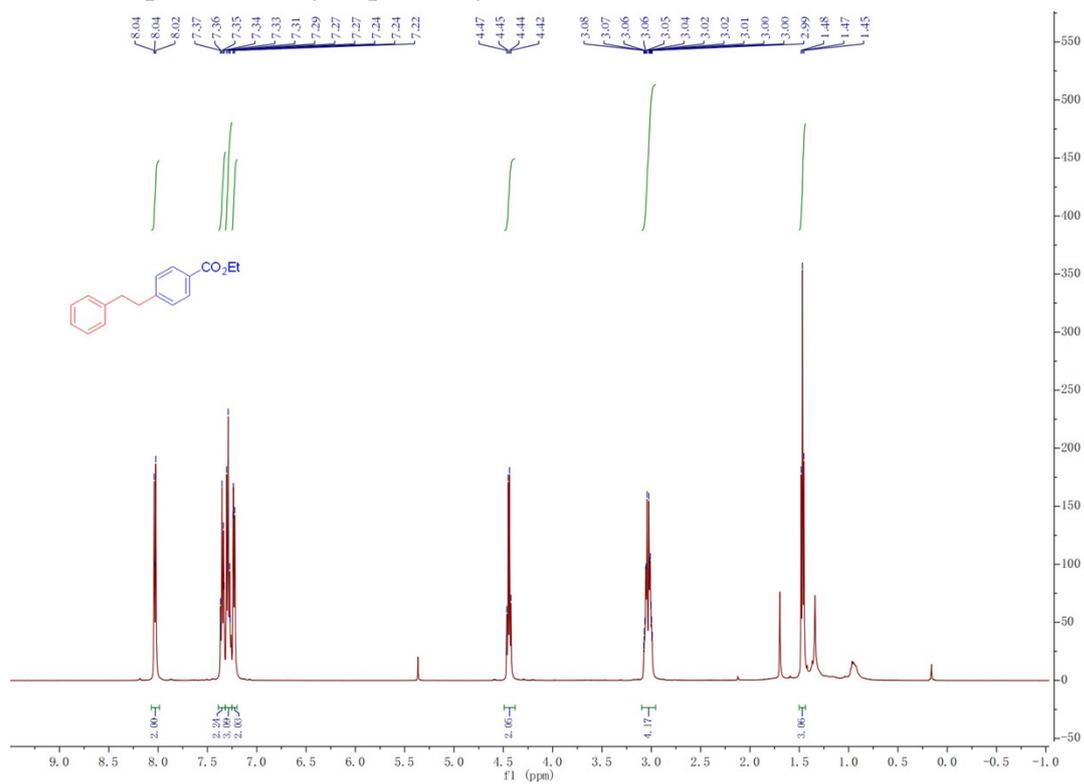
¹H NMR spectra of ethyl 4-(4-phenylbutyl)benzoate 3n



¹³C NMR spectra of ethyl 4-(4-phenylbutyl)benzoate 3n



¹H NMR spectra of ethyl 4-phenethylbenzoate 3o



¹³C NMR spectra of ethyl 4-phenethylbenzoate 3o

