Supplementary Information

Stereoselective Synthesis of 1,3,5-Trienes from Alkynones and Allyl Carbonyl Compounds Through C-C σ-Bond Cleavage under Transition-Metal-Free Conditions

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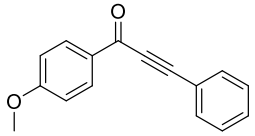
1. General information

Unless otherwise stated, all experiments were carried out under the atmosphere of nitrogen gas. Visualization of spots on TLC plate was accomplished with UV light (254 nm). All commercial reagents were used without further purification. Reactions were monitored by thin layer chromatography. Purification of reaction products was carried out by flash chromatography on silica gel (200~300 mesh). NMR spectra were recorded on Bruker AV-500 or Brucker AV-600 NMR spectrometer. ^{1}H NMR spectra was recorded with tetramethylsilane (δ = 0.00 ppm) as internal reference; ^{13}C NMR spectra was recorded with $CDCl_3$ (δ = 77.00 ppm) as internal reference. The following abbreviations (or combinations thereof) were used to explain multiplicities: s = singlet, d = doublet, m = multiplet. High-resolution mass spectra were performed on a mass spectrometer with a TOF (for EI or ESI) or FTICR (for MALDI) analyzer. Single crystal X-ray diffraction data was collected in Bruker SMARTAPEX diffractiometers.

2. Synthesis of substrates

2.1 Synthesis of Acetyenic Ketones 1

All the substrates **1** are known compounds and have been prepared according to methods reported in the previous literature.



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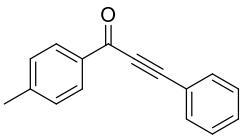

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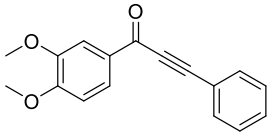

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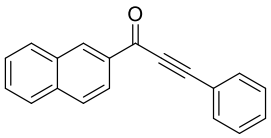

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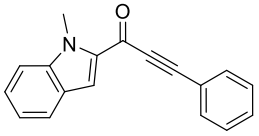

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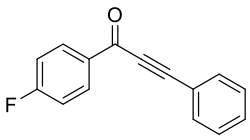

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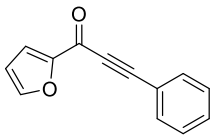

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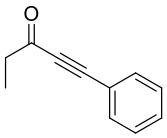

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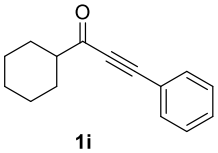

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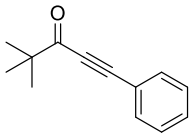

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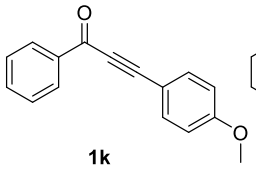

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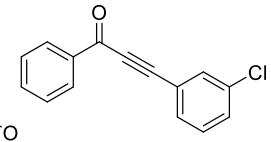

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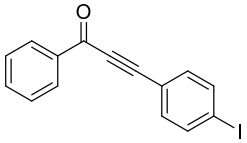

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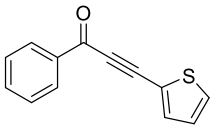

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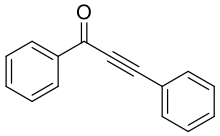

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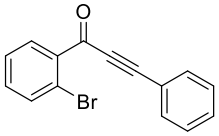
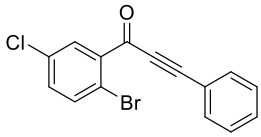


4a



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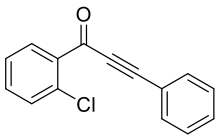

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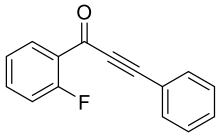
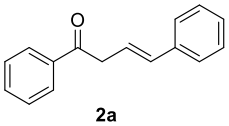


4d

1a - 1d, **1g**, **1k, 4b**[1]; **1f**, **1l**, **1o**[2]; **1e**[3]; **1i - 1j**[4]; **1h**[5]; **1m**[6]; **1n**[7]; **4a, 4c, 4d**[8]

2.2 Synthesis of allyl ketones 2

All the substrates **2** are known compounds and have been prepared according to methods reported in the previous literature.



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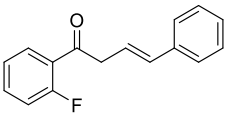

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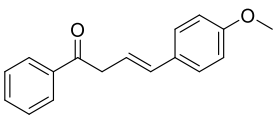

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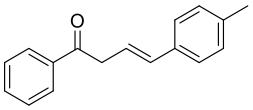

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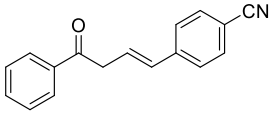

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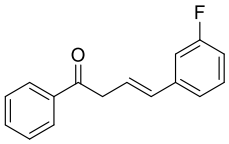

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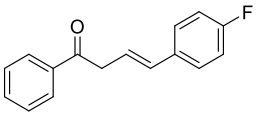

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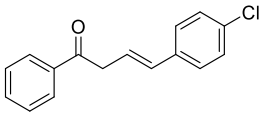

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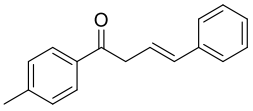

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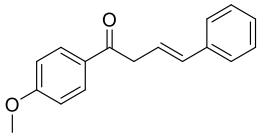

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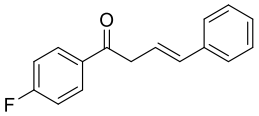

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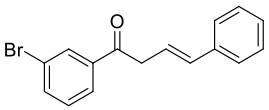

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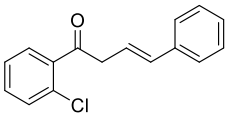
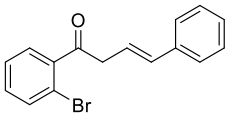


2y

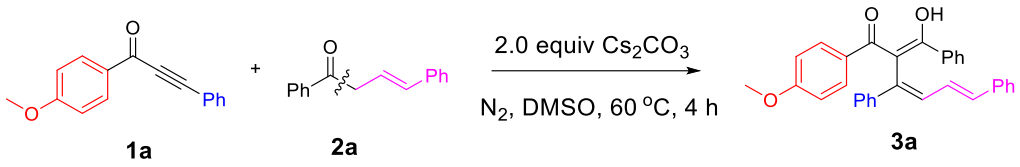


2z

2a, **2s**, **2t**[9]; **2v**, **2w**, **2r**[10]; **2o**, **2x**[11]; **2b**, **2y**, **2z**, **2u**, **2p**, **2q**[12]

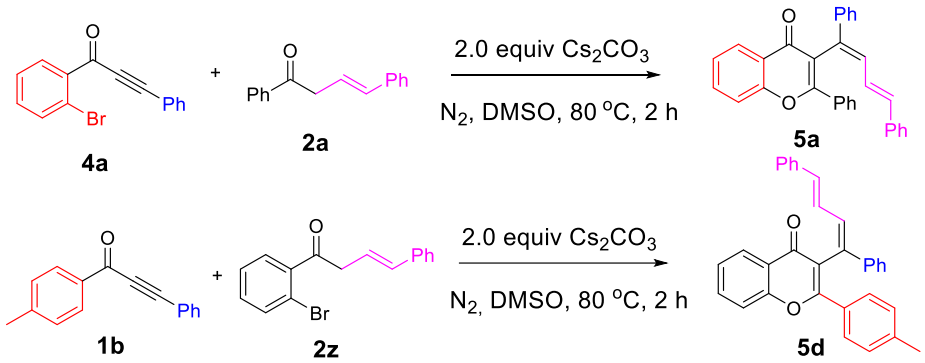
4. Experimental Section

4.1 General procedure for the synthesis of trienes 3



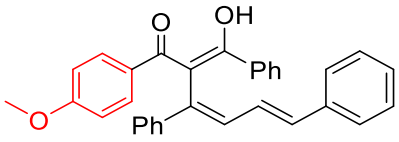
In an oven-dried Schlenk tube was charged with a stir bar, alkynones **1a** (0.30 mmol, 1.0 equiv.), (*E*)- allyl ketones **2a** (0.36 mmol, 1.2 equiv.), Cs_2CO_3 (0.6 mmol, 2.0 equiv.) and DMSO (3.0 mL). The mixture was stirred at 60 °C for 4 hours. Upon completion of the reaction, the reaction mixture was cooled down to room temperature and then quenched by water. The aqueous layer was extracted with ethyl acetate (10 mL × 3). The combined organic layers were washed with brine, dried with anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The pure products **3a** were isolated by column chromatography on silica gel (eluted with PE/EA, 12:1).

4.2 General procedure for the synthesis of chromones 5

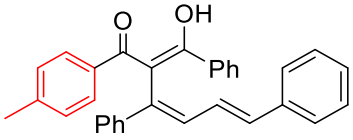


In an oven-dried Schlenk tube was charged with a stir bar, alkynones **4a** or **1b** (0.30 mmol, 1.0 equiv.), (*E*)- allyl ketones **2a** or **2z** (0.36 mmol, 1.2 equiv.), Cs_2CO_3 (0.6 mmol, 2.0 equiv.) and DMSO (3.0 mL). The mixture was stirred at 80 °C for 2 hours. Upon completion of the reaction, the reaction mixture was cooled down to room temperature and then quenched by water. The aqueous layer was extracted with ethyl acetate (10 mL × 3). The combined organic layers were washed with brine, dried with anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. The pure products **5a** or **5d** were isolated by column chromatography on silica gel (eluted with PE/EA, 10:1).

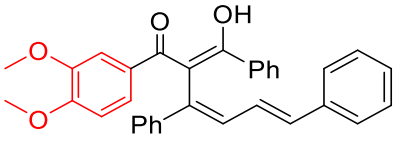
4.3 Characterization data of products



(2*Z*,3*Z*,5*E*)-2-(hydroxy(phenyl)methylene)-1-(4-methoxyphenyl)-3,6-diphenylhexa-3,5-dien-1-one (**3a**). Following the general procedure, the crude product was purified by column chromatography (PE/EA = 12:1, v/v) to provide the title compound as a yellow solid (111.4 mg, 81% yield). m.p. 148 - 150 ºC. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 18.23 (s, 1H), 7.64 - 7.61 (m, 2H), 7.46 - 7.43 (m, 2H), 7.40 - 7.37 (m, 2H), 7.32 - 7.29 (m, 4H), 7.25 - 7.16 (m, 4H), 7.15 - 7.10 (m, 3H), 6.99 - 6.93 (m, 1H), 6.68 - 6.65 (m, 3H), 6.49 (d, *J* = 20.0 Hz, 1H), 3.70 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 189.89, 189.24, 161.71, 141.44, 137.29, 137.21, 136.95, 134.72, 131.28, 130.24, 130.02, 129.29, 128.61, 128.36, 127.78, 127.59, 127.31, 126.49, 126.46, 126.42, 113.09, 108.99, 55.17. **HRMS** (ESI) calcd for $C_{32}H_{27}O_3$ [M + H] $^{+}$: 459.1955, found: 459.1955.

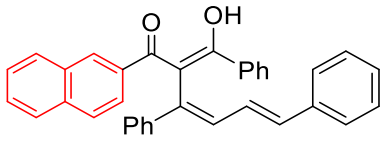


(2*Z*,3*Z*,5*E*)-2-(hydroxy(phenyl)methylene)-3,6-diphenyl-1-(p-tolyl)hexa-3,5-dien-1-one (**3b**). Following the general procedure, the crude product was purified by column chromatography (PE/EA = 20:1, v/v) to provide the title compound as a yellow solid (108.9 mg, 82% yield). m.p. 166 - 168 ºC. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 18.09 (s, 1H), 7.48 - 7.45 (m, 4H), 7.37 - 7.34 (m, 2H), 7.32 - 7.28 (m, 4H),7.24 - 7.08 (m, 7H), 6.98 - 6.92 (m, 3H), 6.64 (d, *J* = 15.0 Hz, 1H), 6.48 (d, *J* =20.0 Hz, 1H), 2.22 (s, 3H).**^{13}C NMR** (125 MHz, $CDCl_3$) δ 190.29, 189.96, 141.48, 141.17, 137.24, 136.79, 134.71, 134.15, 131.28, 130.40, 128.62, 128.46, 128.43, 128.31, 127.78, 127.73, 127.62, 127.39, 127.27, 126.49, 126.44, 109.35, 21.43. **HRMS** (ESI) calcd for $C_{32}H_{27}O_2$ [M + H] $^{+}$: 443.2006, found: 443.1997.

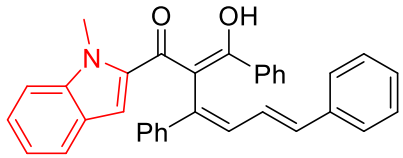


(2*Z*,3*Z*,5*E*)-1-(3,4-dimethoxyphenyl)-2-(hydroxy(phenyl)methylene)-3,6-diphenylhexa-3,5-dien-1-one (**3c**). Following the general procedure, the crude product was purified by column chromatography (PE/EA = 10:1, v/v) to provide the title compound as a yellow solid (96.7 mg, 66% yield). m.p. 183 - 185 ºC. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 18.02 (s, 1H), 7.48 - 7.46 (m, 2H), 7.42 - 7.40 (m, 2H), 7.34 - 7.29 (m, 5H), 7.24 - 7.10 (m, 8H), 7.01 - 6.94 (m, 1H), 6.71 (d, *J* = 20.0 Hz, 1H), 6.64 (d, *J* = 10.0 Hz, 1H), 6.50 (d, *J* = 20.0 Hz, 1H), 3.79 (s, 3H), 3.57 (s, 3H). **^{13}C NMR** (125 MHz,

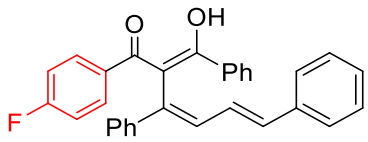
$CDCl_3$) 189.84, 189.15, 151.25, 147.86, 141.17, 137.14, 137.09, 136.90, 134.81, 131.20, 130.33, 129.48, 128.63, 128.44, 127.85, 127.63, 127.40, 127.37, 126.49, 126.32, 126.29, 121.90, 110.97, 109.96, 108.94, 55.75, 55.51. **HRMS** (ESI) calcd for $C_{33}H_{28}O_4Na$ $[M + Na]^+$: 511.1880, found: 511.1880.



(2*Z*,3*Z*,5*E*)-2-(hydroxy(phenyl)methylene)-1-(naphthalen-2-yl)-3,6-diphenylhexa-3,5-dien-1-one (**3d**). Following the general procedure, the crude product was purified by column chromatography (PE/EA = 15:1, v/v) to provide the title compound as a yellow solid (97.6 mg, 68% yield). m.p. 182 - 184 ºC. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 18.02 (s, 1H), 8.02 (d, *J* = 10.0 Hz, 1 H), 7.68 - 7.63 (m, 4H), 7.37 - 7.34 (m, 1H), 7.31 - 7.25 (m, 4H), 7.21 - 7.17 (m, 3H), 7.16 - 7.11 (m, 5 H), 7.00 - 6.97 (m, 2H), 6.95 - 6.93 (m, 1H), 6.90 - 6.87 (m, 1H), 6.40 (d, *J* = 15.0 Hz, 1H), 6.32 (d, *J* = 20.0 Hz, 1H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ193.38, 188.95, 141.68, 137.05, 136.54, 134.50, 134.38, 133.16, 131.10, 131.07, 129.85, 129.57, 128.45, 128.03, 128.01, 127.85, 127.66, 126.95, 126.50, 126.40, 126.36, 125.73, 125.50, 124.96, 123.94, 111.63. **HRMS** (ESI) calcd for $C_{35}H_{27}O_2$ $[M + H]^+$: 479.2006, found: 479.2006

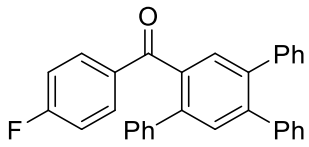


(2*Z*,3*Z*,5*E*)-2-(hydroxy(phenyl)methylene)-1-(1-methyl-1H-indol-2-yl)-3,6-diphenylhexa-3,5-dien-1-one (**3e**). Following the general procedure, the crude product was purified by column chromatography (PE/EA = 15:1, v/v) to provide the title compound as a yellow solid (80.9 mg, 68% yield). m.p. 122 - 124 ºC. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 18.02 (s, 1H), 7.53 - 7.50 (m, 2H), 7.48 - 7.44 (m, 2H), 7.43 - 7.41 (m, 1H), 7.34 - 7.27 (m, 4H), 7.24 - 7.09 (m, 9H), 7.07 - 7.01 (m, 1H), 7.01 - 6.97 (m, 1H), 6.94 (s, 1H), 6.78 (d, *J* = 20.0 Hz, 1H), 6.54 (d, *J* = 20.0 Hz, 1H), 3.87 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 185.62, 185.42, 141.31, 139.29, 137.06, 136.65, 136.37, 134.96, 134.27, 131.45, 130.41, 128.61, 128.47, 127.80, 127.73, 127.40, 127.38, 126.44, 126.23, 126.12, 124.63, 122.35, 120.03, 110.22, 109.88, 32.13. **HRMS** (ESI) calcd for $C_{34}H_{27}NO_2Na$ $[M + Na]^+$:504.1934, found: 504.1932.

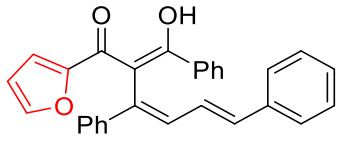


(2*Z*,3*Z*,5*E*)-1-(4-fluorophenyl)-2-(hydroxy(phenyl)methylene)-3,6-diphenylhexa-3,5-dien-1-one (**3f**). Following the general procedure, the crude product was purified by column chromatography (PE/EA = 30:1, v/v) to provide the title compound as a

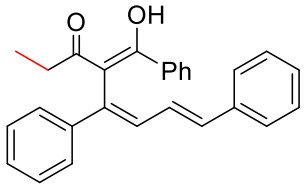
yellow solid (60.3 mg, 45% yield). m.p. 105 - 107 ºC. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 18.03 (s, 1H), 7.56 - 7.53 (m, 2H), 7.50 - 7.49 (m, 2H), 7.35 - 7.34 (m, 2H), 7.32 - 7.31 (m, 4H), 7.25 - 7.21 (m, 2H), 7.19 - 7.10 (m, 5H), 6.95 - 6.90 (m, 1H), 6.84 - 6.80 (m, 2H), 6.64 (d, *J* = 15.0 Hz, 1H), 6.49 (d, *J* = 20.0 Hz, 1H).**^{13}C NMR** (125 MHz, $CDCl_3$) δ 190.13, 189.29, 164.01 (d, *J* = 250.0 Hz), 141.31, 137.09, 136.86, 136.49, 135.15, 133.25 (d, *J* = 3.75 Hz), 131.44, 130.75, 130.08 (d, *J* = 8.75 Hz), 128.73, 128.51, 128.00, 127.78, 127.51, 126.55, 126.47, 126.12, 114.93 (d, *J* = 21.3 Hz), 109.45. **HRMS** (ESI) calcd for $C_{31}H_{23}FO_2Na$ [M + Na] $^+$: 469.1574, found: 469.1577



(4-fluorophenyl)(4'-phenyl-[1,1':2',1''-terphenyl]-3'-yl)methanone (**3f'**) Following the general procedure, the crude product was purified by column chromatography (PE/EA = 50:1, v/v) to provide the title compound as a white solid (47.6 mg, 37% yield). m.p. 162 - 164 ºC. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.77 - 7.76 (m, 2H), 7.58 (s, 1H), 7.53 (s, 1H), 7.44 - 7.41 (m, 1H), 7.34 - 7.29 (m, 4H), 7.24 - 7.18 (m, 10H), 6.96 - 6.93 (m, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 198.24, 162.08 (d, *J* = 246.3 Hz), 141.45, 140.45, 140.07, 139.64, 139.38, 138.11, 137.32, 136.54 (d, *J* = 3.75 Hz), 132.98, 132.34, 131.42(d, *J* = 8.75 Hz), 131.17, 130.04, 129.85, 128.98, 128.38, 128.21, 128.19, 127.54, 127.05, 115.12(d, *J* = 21.3 Hz). **HRMS** (ESI) calcd for $C_{31}H_{22}FO$ [M + H] $^+$: 429.1649, found: 429.1649

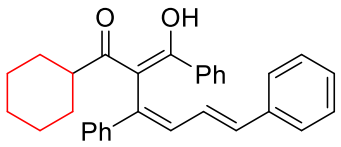


(2*Z*,3*Z*,5*E*)-1-(furan-2-yl)-2-(hydroxy(phenyl)methylene)-3,6-diphenylhexa-3,5-dien-1-one (**3g**). Following the general procedure, the crude product was purified by column chromatography (PE/EA = 20:1, v/v) to provide the title compound as a yellow solid (79.1 mg, 63% yield). m.p. 104 - 106 ºC. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 18.14 (s,1H), 7.50 - 7.45 (m, 5H), 7.34 - 7.10 (m, 12H), 6.99 - 6.93 (m, 2H), 6.65 - 6.58 (m, 1H), 6.31 - 6.29 (m, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 187.40, 177.67, 149.08, 146.43, 140.60, 136.98, 136.57, 135.40, 135.38, 132.28, 130.41, 128.65, 128.62, 127.96, 127.66, 127.56, 127.51, 126.60, 126.12, 125.99, 120.13, 112.36, 107.40. **HRMS** (ESI) calcd for $C_{29}H_{22}O_3Na$ [M + Na] $^+$: 441.1461, found: 441.1461.

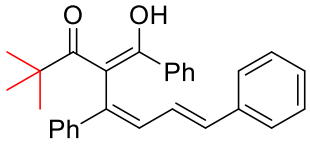


(4*Z*,5*Z*,7*E*)-4-(hydroxy(phenyl)methylene)-5,8-diphenylocta-5,7-dien-3-one (**3h**).

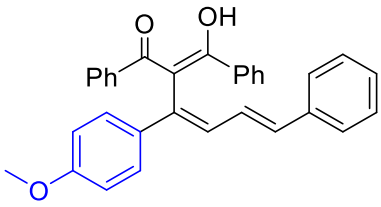
Following the general procedure, the crude product was purified by column chromatography (PE/EA = 50:1, v/v) to provide the title compound as a yellow oil (54.8 mg, 48% yield). **^{1}H NMR** (500 MHz, $CDCl_3$) δ 17.56 (s, 1H),7.56 - 7.54 (m, 2H), 7.48 - 7.45 (m 2H), 7.36 - 7.28 (m, 6H), 7.24 - 7.20 (m, 3H),7.16 - 7.12 (m, 2H), 6.90 - 6.87 (m, 2H), 6.66 - 6.59 (m, 1H), 2.45 - 2.39 (m, 1H) 2.28 - 2.23 (m, 1H), 1.03 - 1.00 (m, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 202.11, 182.34, 140.90, 137.04, 136.00, 135.90, 135.15, 131.36, 130.55, 128.71, 128.66, 127.94, 127.78, 127.75, 127.67, 126.55, 126.06, 126.01, 109.18, 30.83, 8.85. **HRMS** (ESI) calcd for $C_{27}H_{25}O_2$ $[M + H]^+$: 381.1849, found: 381.1846.



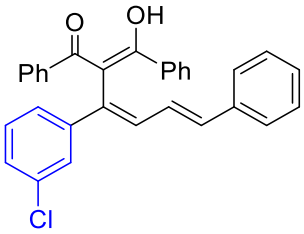
(2*Z*,3*Z*,5*E*)-1-cyclohexyl-2-(hydroxy(phenyl)methylene)-3,6-diphenylhexa-3,5-dien-1-one(3i). Following the general procedure, the crude product was purified by column chromatography (PE/EA = 50:1, v/v) to provide the title compound as a yellow solid (88.7 mg, 68% yield). m.p. 163 - 165 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 17.99 (s, 1H), 7.53 - 7.50 (m, 2H), 7.48 - 7.46 (m, 2H), 7.34 - 7.28 (m, 6H), 7.23 - 7.19 (m, 3H), 7.14 - 7.11 (m, 2H), 6.92 - 6.84 (m, 2H), 6.60 (d, J = 20.0 Hz, 1H), 2.46 - 2.41 (m, 1H), 1.69 - 1.61 (m, 2H), 1.57 - 1.39 (m, 5H), 1.15 - 1.09 (m, 1H), 1.05 - 1.00 (m, 1H), 0.90 - 0.84 (m, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 202.43, 186.29, 141.47, 137.14, 136.61, 136.19, 134.75, 131.25, 130.47, 128.65, 128.61, 127.83, 127.67, 127.61, 126.50, 126.24, 126.21, 108.63, 44.59, 29.55, 28.94, 25.66, 25.56, 25.42. **HRMS** (ESI) calcd for $C_{31}H_{31}O_2$ $[M + H]^+$: 435.2319, found: 435.2316.



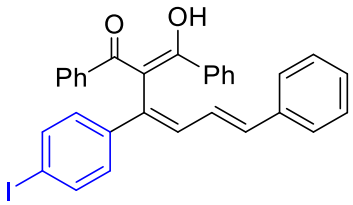
(4*Z*,5*Z*,7*E*)-4-(hydroxy(phenyl)methylene)-2,2-dimethyl-5,8-diphenylocta-5,7-dien-3-one (**3j**). Following the general procedure, the crude product was purified by column chromatography (PE/EA = 60:1, v/v) to provide the title compound as a yellow solid (46.6 mg, 38% yield). m.p. 142 - 144 °C. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 18.58 (s, 1H), 7.48 - 7.44 (m, 2H), 7.40 - 7.36 (m, 2H), 7.35 - 7.27 (m, 6H), 7.26 - 7.20 (m, 2H), 7.18 - 7.14 (m, 1H), 7.09 - 7.03 (m, 2H), 6.98 - 6.91 (m, 1H), 6.84 - 6.79 (m, 1H), 6.60 - 6.55 (m, 1H), 1.12 (s, 9H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 203.63, 189.58, 142.04, 137.56, 137.20, 136.27, 134.72, 132.01, 129.58, 128.72, 128.52, 127.93, 127.47, 127.34, 127.05, 126.92, 126.56, 126.45, 108.13, 43.06, 28.57. **HRMS** (ESI) calcd for $C_{29}H_{29}O_2$ $[M + H]^+$: 409.2162, found: 409.2159.



(2*Z*,3*Z*,5*E*)-2-(hydroxy(phenyl)methylene)-3-(4-methoxyphenyl)-1,6-diphenylhexa-3,5-dien-1-one (**3k**). Following the general procedure, the crude product was purified by column chromatography (PE/EA = 20:1, v/v) to provide the title compound as a yellow solid (89.4 mg, 65% yield). m.p. 172 - 174 ºC. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 18.01 (s, 1H), 7.53 - 7.50 (m, 4H), 7.32 - 7.27 (m, 6H),7.26 - 7.21 (m, 3H), 7.17 - 7.13(m,4H), 6.96 - 6.90 (m, 1H), 6.72 - 6.69 (m, 2H), 6.54 (d, *J* = 15.0 Hz, 1H), 6.44 (d, *J* = 20.0 Hz, 1H), 3.75 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 190.15, 158.97, 137.33, 137.04, 136.11, 134.09, 133.82, 130.60, 129.67, 128.59, 127.65, 127.59, 127.43, 126.47, 126.37, 113.76, 109.58, 55.18. **HRMS** (ESI) calcd for $C_{32}H_{26}O_3Na$ [M + Na] $^{+}$: 481.1774, found: 481.1775.

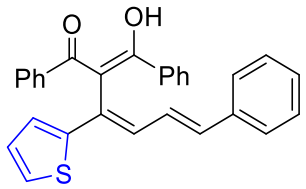


(2*Z*,3*Z*,5*E*)-3-(3-chlorophenyl)-2-(hydroxy(phenyl)methylene)-1,6-diphenylhexa-3,5-dien-1-one (**3l**). Following the general procedure, the crude product was purified by column chromatography (PE/EA = 15:1, v/v) to provide the title compound as a yellow solid (105.6 mg, 76% yield). m.p. 172 - 174 ºC. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 18.00 (s, 1H), 7.49 - 7.46 (m, 4H), 7.33 - 7.30 (m, 5H), 7.28 - 7.21 (m, 4H), 7.19 - 7.15 (m, 4H), 7.10 - 7.05 (m, 2H), 6.94 - 6.89 (m, 1H), 6.61 (d, *J* = 15.0 Hz, 1H), 6.49 (d, *J* = 20.0 Hz, 1H).**^{13}C NMR** (125 MHz, $CDCl_3$) δ 190.38, 143.45, 136.90, 136.82, 135.79, 135.17, 134.33, 132.33, 130.75, 129.51, 128.66, 128.07, 127.77, 127.38, 127.18, 126.59, 126.29, 125.88, 124.57, 109.05..**HRMS** (ESI) calcd for $C_{31}H_{23}ClO_2Na$ [M + Na] $^{+}$: 485.1279, found: 485.1279

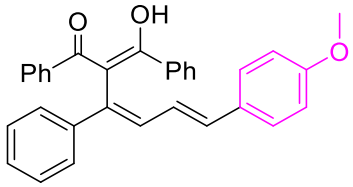


(2*Z*,3*Z*,5*E*)-2-(hydroxy(phenyl)methylene)-3-(4-iodophenyl)-1,6-diphenylhexa-3,5-dien-1-one (**3m**). Following the general procedure, the crude product was purified by column chromatography (PE/EA = 10:1, v/v) to provide the title compound as a yellow solid (99.8 mg, 60% yield). m.p. 157 - 159 ºC. **^{1}H NMR** (500 MHz, $CDCl_3$) δ

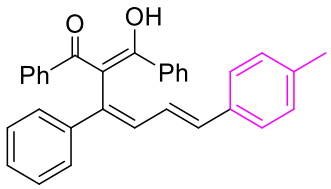
18.01 (s, 1H), 7.49 - 7.46 (m, 6H), 7.32 - 7.31 (m, 4H), 7.27 - 7.22 (m, 3H), 7.17 - 7.14 (m, 4H), 7.09 - 7.07 (m, 2H), 6.94 - 6.89 (m, 1H), 6.61 (d, *J* = 20.0 Hz, 1H), 6.49 (d, *J* = 20,0 Hz, 1H).**^{13}C NMR** (125 MHz, $CDCl_3$) δ 190.31, 141.04, 137.41, 136.96, 136.84, 135.55, 135.50, 131.86, 130.79, 128.67, 128.06, 128.03, 127.79, 127.39, 126.57, 125.99, 108.92, 92.91. **HRMS** (ESI) calcd for $C_{31}H_{24}IO_2$ $[M + H]^+$: 555.0812, found: 555.1744.



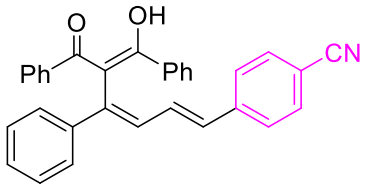
(2*Z*,3*E*,5*E*)-2-(hydroxy(phenyl)methylene)-1,6-diphenyl-3-(thiophen-2-yl)hexa-3,5-dien-1-one (**3n**). Following the general procedure, the crude product was purified by column chromatography (PE/EA = 15:1, v/v) to provide the title compound as a yellow solid (87.3 mg, 67% yield). m.p. 110 - 112 ºC. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 18.06 (s, 1H), 7.59 - 7.56 (m, 4H), 7.32 - 7.30 (m, 3H), 7.29 - 7.25 (m, 2H), 7.24 - 7.17 (m, 6H), 7.04 - 7.02 (m, 1H), 6.95 - 6.93 (m, 1H), 6.92 - 6.86 (m, 1H) 6.82 - 6.79 (m, 1H), 6.59 (d *J* = 20.0 Hz, 1H), 6.49 (d *J* = 10.0 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 190.18, 147.61, 137.11, 136.90, 134.76, 130.90, 130.77, 130.46, 128.66, 127.87, 127.77, 127.63, 127.43, 126.50, 125.43, 125.17, 124.98, 109.13. **HRMS** (ESI) calcd for $C_{29}H_{22}O_2SNa$ $[M + Na]^+$: 457.1233, found: 457.1233



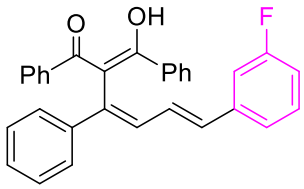
(2*Z*,3*Z*,5*E*)-2-(hydroxy(phenyl)methylene)-6-(4-methoxyphenyl)-1,3-diphenylhexa-3,5-dien-1-one (**3o**). Following the general procedure, the crude product was purified by column chromatography (PE/EA = 15:1, v/v) to provide the title compound as a yellow solid (72.9 mg, 53% yield). m.p. 165 - 167 ºC. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 18.00 (s, 1H), 7.52 - 7.49 (m, 4H) 7.34 - 7.31 (m, 2H), 7.27 - 7.20 (m, 4H), 7.17 - 7.12 (m, 6H), 7.10 - 7.06 (m, 1H), 6.86 - 6.84 (m, 2H), 6.82 - 6.78 (m, 1H), 6.60 (d, *J* = 15.0 Hz, 1H), 6.42 (d, *J* = 20.0 Hz, 1H), 3.81 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 190.29, 159.46, 141.59, 137.07, 135.30, 134.43, 131.61, 130.56, 130.02, 128.28, 127.78, 127.65, 127.46, 127.05, 126.37, 124.38, 114.09, 109.65, 55.31. **HRMS** (ESI) calcd for $C_{32}H_{27}O_3$ $[M + H]^+$: 459.1955, found: 459.1955



(2*Z*,3*Z*,5*E*)-2-(hydroxy(phenyl)methylene)-1,3-diphenyl-6-(p-tolyl)hexa-3,5-dien-1-one (**3p**). Following the general procedure, the crude product was purified by column chromatography (PE/EA = 30:1, v/v) to provide the title compound as a yellow solid (71.7 mg, 54% yield). m.p. 166 - 168 ºC. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 18.00 (s, 1H), 7.51 - 7.48 (m, 4H), 7.34 - 7.32 (m, 2H), 7.25 - 7.20 (m, 4H), 7.17 - 7.15 (m, 3H), 7.14 - 7.08 (m, 6H), 6.92 - 6.86 (m, 1H), 6.61 (d, *J* = 15,0 Hz, 1H), 6.44 (d, *J* = 20,0 Hz, 1H), 2.34 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 190.30, 141.54, 137.85, 137.05, 135.93, 134.81, 134.40, 131.51, 130.56, 129.35, 128.29, 127.65, 127.46, 127.15, 126.43, 125.39, 109.62, 21.28. **HRMS** (ESI) calcd for $C_{32}H_{27}O_2$ [M + H] $^+$: 443.2006, found: 443.2006.

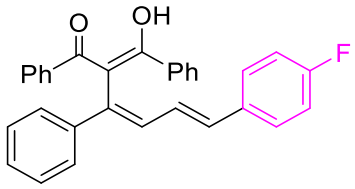


4-((1*E*,3*Z*,5*Z*)-5-benzoyl-6-hydroxy-4,6-diphenylhexa-1,3,5-trien-1-yl)benzonitrile (**3q**). Following the general procedure, the crude product was purified by column chromatography (PE/EA = 10:1, v/v) to provide the title compound as a yellow solid (28.6 mg, 21% yield). m.p. 190 - 192 ºC. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 18.00 (s, 1H), 7.49 - 7.46 (m, 4H), 7.34 - 7.29 (m, 5H), 7.27 - 7.20 (m, 4H), 7.18 - 7.14 (m, 4H), 7.10 - 7.05 (m, 2H), 6.94 - 6.88 (m, 1H), 6.61 (d, *J* = 15.0 Hz, 1H), 6.49 (d, *J* = 20.0 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 190.30, 141.57, 141.17, 139.55, 136.82, 132.39, 132.21, 130.75, 130.26, 129.65, 128.42, 127.85, 127.74, 127.43, 126.72, 126.68, 119.00, 110.50, 109.36. **HRMS** (ESI) calcd for $C_{32}H_{24}NO_2$ [M + H] $^+$: 454.1802, found: 454.1802.

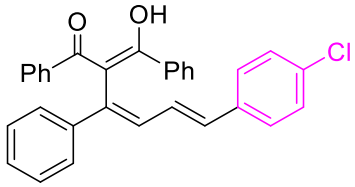


(2*Z*,3*Z*,5*E*)-6-(3-fluorophenyl)-2-(hydroxy(phenyl)methylene)-1,3-diphenylhexa-3,5-dien-1-one (**3r**). Following the general procedure, the crude product was purified by column chromatography (PE/EA = 20:1, v/v) to provide the title compound as a yellow solid (111.2 mg, 83% yield). m.p. 135 - 137 ºC. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 18.02 (s, 1H), 7.51 - 7.49 (m, 4H), 7.36 - 7.33 (m, 2H), 7.27 - 7.21 (m, 3H) 7.19 - 7.09 (m, 7H), 7.08 - 7.05 (m, 1H), 6.70 - 6.95 (m, 1H), 6.93 - 6.88 (m, 2H), 6.60 - 6.56 (m, 1H), 6.40 (d, *J* = 20.0 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 190.33, 163.12 (d, *J* =

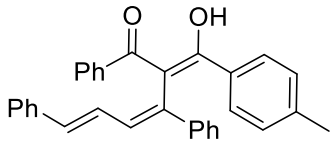
243.8 Hz), 141.44, 139.58 (d, J = 7.5 Hz), 137.78, 137.02, 133.34, 133.32, 130.78, 130.68, 130.06 (d, J = 7.5 Hz), 128.39, 127.74, 127.50, 126.63, 122.28 (d, J = 2.5 Hz), 114.56 (d, J = 21.3 Hz) 112.85 (d, J = 21.3 Hz), 109.51. **HRMS** (ESI) calcd for $C_{31}H_{24}FO_2$ [M + H] $^+$: 447.1755, found: 447.1755



(2*Z*,3*Z*,5*E*)-6-(4-fluorophenyl)-2-(hydroxy(phenyl)methylene)-1,3-diphenylhexa-3,5-dien-1-one (**3s**). Following the general procedure, the crude product was purified by column chromatography (PE/EA = 20:1, v/v) to provide the title compound as a yellow solid (91.1 mg, 68% yield). m.p. 175 - 177 ºC. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 18.01 (s, 1H), 7.51 - 7.48 (m, 4H), 7.35 - 7.32 (m, 2H), 7.28 - 7.21 (m, 4H), 7.18 - 7.08 (m, 7H), 7.02 - 6.97 (m, 2H), 6.87 - 6.81 (m, 1H), 6.58 (d, J = 15.0 Hz, 1H), 6.40 (d, J = 20.0 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 190.34, 162.43 (J = 246.3 Hz), 141.50, 137.05, 136.72, 133.44, 131.12, 130.68, 128.39, 128.02 (J = 7.50 Hz), 127.73, 127.51, 127.37, 126.54, 126.10 (J = 2.50 Hz), 115.67 (d, J = 22.5 Hz), 109.59. **HRMS** (ESI) calcd for $C_{31}H_{23}FO_2Na$ [M + Na] $^+$: 469.1574, found: 469.1575

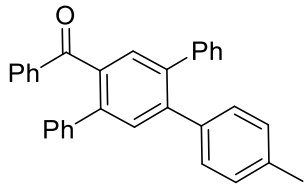


(2*Z*,3*Z*,5*E*)-6-(4-chlorophenyl)-2-(hydroxy(phenyl)methylene)-1,3-diphenylhexa-3,5-dien-1-one (**3t**). Following the general procedure, the crude product was purified by column chromatography (PE/EA = 15:1, v/v) to provide the title compound as a yellow solid (70.8 mg, 51% yield). m.p. 198 - 200 ºC. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 18.01 (s, 1H), 7.50 - 7.47 (m, 4H), 7.35 - 7.32 (m, 2H), 7.28 - 7.26 (m, 2H), 7.25 - 7.20 (m, 4H), 7.18 - 7.08 (m, 7H), 6.93 - 6.86 (m, 1H), 6.58 (d, J = 15.0 Hz, 1H), 6.38 (d, J = 20.0 Hz,1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 190.29, 141.41, 137.27, 136.96, 135.64, 133.31, 133.20, 130.91, 130.64, 128.79, 128.34, 127.69, 127.57, 127.51, 127.44, 127.42, 126.80, 126.54, 109.50. HRMS (ESI) calcd for $C_{31}H_{23}ClO_2Na$ [M + Na] $^+$: 485.1279, found: 485.1279.

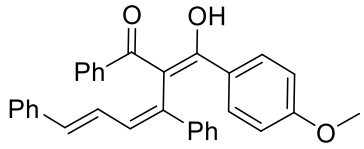


(2*Z*,3*Z*,5*E*)-2-(hydroxy(p-tolyl)methylene)-1,3,6-triphenylhexa-3,5-dien-1-one (**3u**) Following the general procedure, the crude product was purified by column

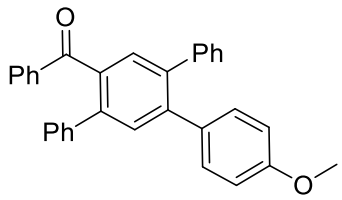
chromatography (PE/EA = 30:1, v/v) to provide the title compound as a yellow solid (42.5 mg, 32% yield). m.p. 169 - 171 ºC. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 18.12 (s, 1H), 7.47 - 7.45 (m, 4H), 7.36 - 7.35 (m, 2H), 7.31 - 7.30 (m, 4H), 7.22 - 7.10 (m, 7H), 6.98 - 6.92 (m, 3H), 6.64 (d, *J* = 15.0 Hz, 1H), 6.48 (d, *J* = 20.0 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 190.29, 189.95, 141.47, 141.17, 137.24, 136.79, 134.70, 134.14, 131.27, 130.40, 128.62, 128.43, 128.31, 127.78, 127.72, 127.62, 127.39, 127.26, 126.49, 126.43, 109.34, 21.43. **HRMS** (ESI) calcd for $C_{32}H_{27}O_2$ [M + H] $^+$: 443.2006, found: 443.2006.



(4''-methyl-4'-phenyl-[1,1':2',1''-terphenyl]-3'-yl)(phenyl)methanone (**3u'**). Following the general procedure, the crude product was purified by column chromatography (PE/EA = 45:1, v/v) to provide the title compound as a white solid (29.3 mg, 23% yield). m.p. 168 - 170 ºC. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.71 - 7.70 (m, 2H), 7.56 - 7.55 (m, 2H), 7.36 - 7.35 (m, 2H), 7.25 - 7.18 (m, 13H), 7.13 - 7.11 (m, 2H), 2.34 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 197.89, 143.83, 142.27, 140.59, 140.26, 140.17, 139.77, 139.19, 138.16, 134.80, 132.47, 130.94, 130.25, 129.83, 129.79, 128.93, 128.91, 128.30, 128.03, 127.99, 127.38, 126.99, 126.84, 77.25, 77.00, 76.75, 21.64. **HRMS** (ESI) calcd for $C_{32}H_{24}ONa$ [M + Na] $^+$: 447.1719, found: 447.1846.

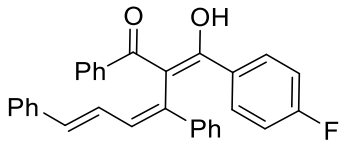


(2*Z*,3*Z*,5*E*)-2-(hydroxy(4-methoxyphenyl)methylene)-1,3,6-triphenylhexa-3,5-dien-1-one (**3v**). Following the general procedure, the crude product was purified by column chromatography (PE/EA = 15:1, v/v) to provide the title compound as a yellow solid (41.3 mg, 30% yield). m.p. 126 - 128 ºC. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 18.23 (s, 1H), 7.63-7.60 (m, 2H), 7.45-7.43 (m, 2H), 7.39-7.37 (m, 2H), 7.32-7.30 (m, 4H), 7.22-7.10 (m, 7H), 6.99-6.92 (m, 1H), 6.67-6.64 (m, 3H), 6.49 (d *J* = 20.0 Hz, 1H). **^{13}C NMR** (125 MHz, CDCl3) δ 189.89, 189.23, 161.70, 141.43, 137.28, 137.20, 136.94, 134.72, 131.27, 130.24, 130.02, 129.28, 128.61, 128.36, 127.77, 127.59, 127.31, 127.30, 126.48, 126.46, 126.41, 113.09, 108.98, 55.17. **HRMS** (ESI) calcd for $C_{32}H_{27}O_3$ [M + H] $^+$: 459.1955, found: 459.1946.

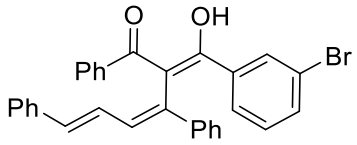


(4''-methoxy-4'-phenyl-[1,1':2',1''-terphenyl]-3'-yl)(phenyl)methanone (**3v'**).

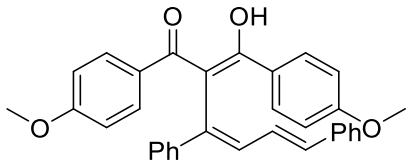
Following the general procedure, the crude product was purified by column chromatography (PE/EA = 40:1, v/v) to provide the title compound as a white solid (42.3 mg, 32% yield). m.p. 158 - 160 ºC. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.79 - 7.77 (m, 2H), 7.56 - 7.55 (m, 2H), 7.38 - 7.36 (m, 2H), 7.23 - 7.22 (m, 8H), 7.21 - 7.20 (m, 5H), 6.81 - 6.79 (m, 2H), 3.80 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 196.91, 163.47, 142.18, 140.67, 140.34, 140.02, 139.83, 139.26, 138.33, 132.49, 132.46, 130.86, 130.36, 129.89, 129.84, 128.93, 128.36, 128.08, 128.04, 127.45, 127.01, 126.88, 113.51, 55.44. **HRMS** (ESI) calcd for $C_{32}H_{24}O_2$ [M + H] $^+$: 441.1849, found: 441.1846.



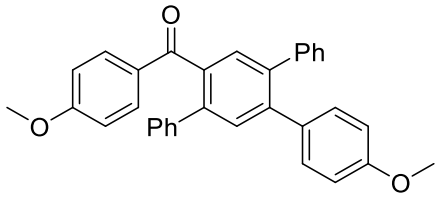
(2*Z*,3*Z*,5*E*)-2-((4-fluorophenyl)(hydroxy)methylene)-1,3,6-triphenylhexa-3,5-dien-1-one (**3w**). Following the general procedure, the crude product was purified by column chromatography (PE/EA = 30:1, v/v) to provide the title compound as a yellow solid (116.5 mg, 87% yield). m.p. 112 - 114 ºC. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 17.99 (s, 1H), 7.56 - 7.52 (m, 2H), 7.51 - 7.48 (m, 2H), 7.35 - 7.33 (m, 2H), 7.31 - 7.28 (m, 4H), 7.24 - 7.20 (m, 2H), 7.19 - 7.16 (m, 2H), 7.15 - 7.09 (m, 3H), 6.95 - 6.89 (m, 1H), 6.83 - 6.80 (m, 2H), 6.64 (d, *J* = 18.0 Hz, 1H), 6.49 (d, *J* = 18.0 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 190.11, 189.25, 164.02 (d, *J* = 249.0 Hz), 141.32, 136.90, 136.90, 136.51, 135.15, 133.28 (*J* = 3.0 Hz), 131.45, 130.71, 130.07 (d, *J* = 9.0 Hz), 128.71, 128.50, 127.98, 127.76, 127.51, 126.55, 126.47, 126.15, 114.90 (d, *J* = 22.5 Hz), 109.47. **HRMS** (ESI) calcd for $C_{31}H_{24}FO_2$ [M + H] $^+$: 447.1755, found: 447.1759.



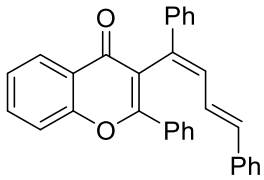
(2Z,3Z,5E)-2-((3-bromophenyl)(hydroxy)methylene)-1,3,6-triphenylhexa-3,5-dien-1-one (**3x**). Following the general procedure, the crude product was purified by column chromatography (PE/EA = 10:1:1, v/v) to provide the title compound as a yellow solid (129.4 mg, 85% yield). m.p. 136 - 138 ºC. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 17.85 (s, 1H), 7.64 (s, 1H), 7.54 - 7.53 (m, 2H), 7.39 - 7.38 (m, 1H), 7.33 - 7.31 (m, 7H), 7.24 - 7.23 (m, 2H), 7.19 - 7.12 (m, 5H), 7.00 - 6.97 (m, 1H), 6.92 - 6.87 (m, 1H), 6.64 (d, *J* = 18.0 Hz, 1H), 6.50 (d, *J* = 18.0 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 190.22, 188.61, 141.25, 138.92, 137.05, 136.63, 136.08, 135.25, 133.35, 131.54, 130.89, 130.56, 129.18, 128.67, 128.46, 127.94, 127.76, 127.56, 127.48, 126.53, 126.44, 126.01, 125.97, 121.72, 109.70. **HRMS** (ESI) calcd for $C_{31}H_{24}BrO_2$ [M + H] $^+$:501.1826, found: 501.1830.



(2Z,3Z,5E)-2-(hydroxy(4-methoxyphenyl)methylene)-1-(4-methoxyphenyl)-3,6-diphenylhexa-3,5-dien-1-one (**3y**). Following the general procedure, the crude product was purified by column chromatography (PE/EA = 20:1:1, v/v) to provide the title compound as a yellow solid (71.7 mg, 49% yield). m.p. 168 - 170 ºC. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 18.40 (s, 1H), 7.56 - 7.54 (m, 4H), 7.42 - 7.40 (m, 2H), 7.30 - 7.29 (m, 4H), 7.20 - 7.17 (m,3H), 7.13 - 7.10 (m, 1H), 6.98 - 6.93 (m, 1H), 6.71 (d, *J* = 15.0 Hz, 1H), 6.65 - 6.63 (m, 4H), 6.51 (d, *J* = 20.0 Hz, 1H), 3.69 (s, 6H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 188.93, 161.42, 141.41, 137.27, 137.25, 134.68, 131.25, 129.79, 129.61, 128.58, 128.40, 127.72, 127.34, 126.51, 126.49, 126.43, 113.01, 108.52, 77.26, 77.00, 76.75, 55.13. HRMS (ESI) calcd for $C_{33}H_{29}O_4$ $[M + H]^+$:489.2060, found: 489.2062.

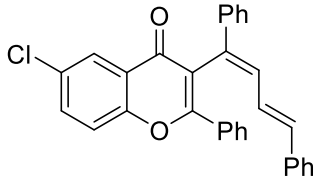


(4''-methoxy-4'-phenyl-[1,1':2',1''-terphenyl]-3'-yl)(4-methoxyphenyl)methanone (**3y'**) Following the general procedure, the crude product was purified by column chromatography (PE/EA = 15:1:1, v/v) to provide the title compound as a white solid (22.0 mg, 16% yield). m.p. 190 - 192 ºC. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.78 - 7.77 (m, 2H), 7.53 - 7.52 (m, 2H), 7.37 - 7.14 (m, 2H), 7.25 - 7.19 (m, 8H), 7.15 - 7.14 (m, 2H), 6.80 - 6.78 (m, 4H), 3.80 (s, 3H), 3.79 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 196.91, 163.39, 158.70, 141.76, 140.53, 140.02, 139.89, 139.08, 137.91, 132.94, 132.44, 132.32, 130.91, 130.38, 129.82, 128.88, 128.30, 128.05, 127.37, 126.76, 113.53, 113.45, 55.40, 55.19. HRMS (ESI) calcd for $C_{33}H_{27}O_3$ $[M + H]^+$: 471.1955, found: 471.1957



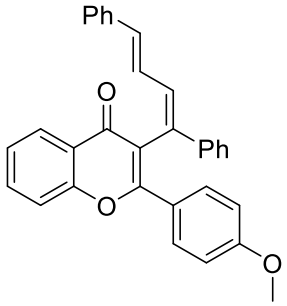
3-((1*Z*,3*E*)-1,4-diphenylbuta-1,3-dien-1-yl)-2-phenyl-4H-chromen-4-one (**5a**) Following the general procedure, the crude product was purified by column chromatography (PE/EA = 10:1:1, v/v) to provide the title compound as a yellow solid (58.3 mg, 46% yield) m.p. 174 - 176 ºC. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.30 - 8.28 (m, 1H), 7.76 - 7.73 (m, 1H), 7.69 - 7.67 (m, 2H), 7.60 (d, *J* = 12.0 Hz, 1H), 7.47 - 7.42 (m, 3H), 7.35 - 7.31 (m, 1H), 7.30 - 7.18 (m, 9H), 7.18 - 7.14 (m, 1H), 6.96 (d,

J = 12.0 1H), 6.73 - 6.67 (m, 1H), 6.64-6.61 (d, *J* = 18.0 Hz, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 177.02, 162.54, 156.25, 140.12, 137.21, 135.19, 133.78, 133.63, 133.02, 131.04, 130.53, 128.51, 128.43, 128.20, 128.18, 127.65, 127.44, 126.55, 125.92, 125.90, 125.18, 123.19, 120.42, 118.03. HRMS (ESI) calcd for $C_{31}H_{22}O_2Na$ $[M + Na]^+$: 449.1512, found: 449.1513.



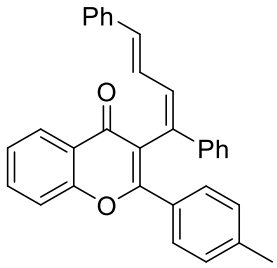
6-chloro-3-((1*Z*,3*E*)-1,4-diphenylbuta-1,3-dien-1-yl)-2-phenyl-4H-chromen-4-one (5b)

Following the general procedure, the crude product was purified by column chromatography (PE/EA = 10:1:1, v/v) to provide the title compound as a yellow solid (71.3 mg, 52% yield) m.p. 195 - 197 ºC. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.25 - 8.23 (m, 1H), 7.67 - 7.65 (m, 3H), 7.56 - 7.54 (m, 1H), 7.41 - 7.39 (m, 2H), 7.34 - 7.31 (m, 1H), 7.30 - 7.16 (m, 10H), 6.96 (d, *J* = 15.0 Hz, 1H), 6.70 - 6.61 (m, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 175.89, 162.78, 154.56, 139.89, 137.11, 135.48, 134.00, 133.15, 132.65, 131.22, 131.13, 130.75, 128.54, 128.45, 128.26, 128.17, 127.76, 127.52, 126.56, 125.88, 125.84, 125.69, 124.09, 120.46, 119.82. HRMS (ESI) calcd for $C_{31}H_{21}ClO_2Na$ $[M + Na]^+$: 483.1122, found: 483.1130.

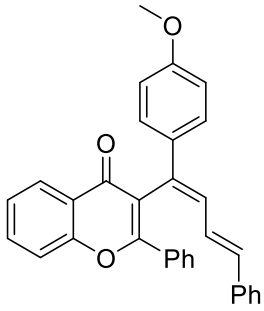


3-((1*Z*,3*E*)-1,4-diphenylbuta-1,3-dien-1-yl)-2-(4-methoxyphenyl)-4H-chromen-4-one (5c)

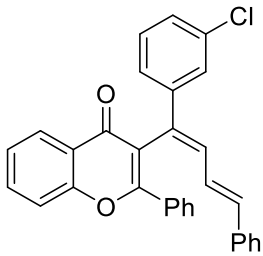
Following the general procedure, the crude product was purified by column chromatography (PE/EA = 10:1:1, v/v) to provide the title compound as a yellow solid (56.3 mg, 41% yield) m.p. 82 - 84 ºC. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.28 - 8.26 (m, 1H), 7.75 - 7.70 (m, 3H), 7.60 - 7.58 (m, 1H), 7.47 - 7.42 (m, 3H), 7.29 - 7.24 (m, 4H), 7.24 - 7.20 (m, 3H), 7.18 - 7.14 (m, 1H), 7.01 (d, *J* = 15.0 Hz, 1H), 6.81 - 6.78 (m, 2H), 6.74 - 6.68 (m, 1H), 6.66 (d, *J* = 15.0 Hz, 1H), 3.75 (s, 3H). **^{13}C NMR (125 MHz, $CDCl_3$)** δ 177.00, 162.18, 161.29, 156.15, 140.02, 137.25, 135.14, 134.01, 133.63, 130.86, 129.99, 128.54, 128.41, 127.61, 127.45, 126.56, 126.51, 126.00, 125.88, 125.21, 125.03, 123.10, 119.38, 117.91, 113.68, 55.23. HRMS (ESI) calcd for $C_{32}H_{24}O_3Na$ [M + Na] +: 479.1618, found: 479.1628.



3-((1*Z*,3*E*)-1,4-diphenylbuta-1,3-dien-1-yl)-2-(p-tolyl)-4H-chromen-4-one (**5d**)
Following the general procedure, the crude product was purified by column chromatography (PE/EA = 10:1:1, v/v) to provide the title compound as a yellow solid (83.1 mg, 63% yield) m.p. 182 - 184 ºC. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.29-8.27 (m, 1H), 7.74 - 7.70 (m, 1H), 7.62 - 7.57 (m, 3H), 7.46 - 7.42 (m, 3H), 7.28 - 7.19 (m, 7H), 7.17 - 7.13 (m, 1H), 7.09 - 7.07 (m, 2H), 6.98 (d, *J* = 12.0 Hz, 1H), 6.73 - 6.68 (m, 1H), 6.64 (d, *J* = 18.0 Hz, 1H), 2.28 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 177.04, 162.56, 156.21, 140.93, 140.05, 137.25, 135.10, 133.84, 133.68, 130.86, 130.12, 128.95, 128.50, 128.40, 128.12, 127.59, 127.41, 126.53, 126.49, 125.98, 125.88, 125.07, 123.13, 119.94, 117.98, 21.40. HRMS (ESI) calcd for $C_{32}H_{24}O_2Na$ $[M + Na]^+$:463.1669, found: 463.1671.

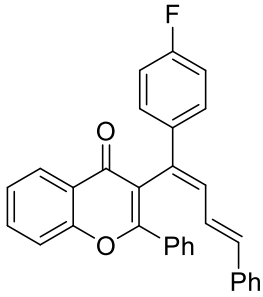


3-((1*Z*,3*E*)-1-(4-methoxyphenyl)-4-phenylbuta-1,3-dien-1-yl)-2-phenyl-4H-chromen-4-one (**5e**)
Following the general procedure, the crude product was purified by column chromatography (PE/EA = 10:1:1, v/v) to provide the title compound as a yellow solid (65.2 mg, 48% yield) m.p. 234 - 236 ºC. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.30 - 8.27 (m, 1H), 7.76 - 7.72(m, 1H), 7.70 - 7.68 (m, 2H), 7.60 (d, *J* = 15.0 Hz, 1H), 7.46 - 7.43 (m, 1H), 7.39 - 7.36 (m, 2H), 7.35 - 7.27 (m, 3H), 7.25 - 7.19 (m, 4H), 7.16 - 7.14 (m, 1H), 6.88 (d, *J* = 15.0 Hz, 1H), 6.82 - 6.79 (m, 2H), 6.71 - 6.64 (m, 1H), 6.58 (d, *J* = 20.0 Hz, 1H), 3.77 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 177.06, 162.38, 159.15, 156.25, 137.38, 134.23, 133.75, 133.22, 133.05, 132.74, 130.52, 129.22, 128.40, 128.20, 128.15, 127.44, 127.09, 126.56, 126.44, 126.06, 125.15, 123.20, 120.47, 118.02, 114.01, 55.22. HRMS (ESI) calcd for $C_{32}H_{24}O_3Na$ $[M + Na]^+$: 479.1618, found: 479.1625.



3-((1*Z*,3*E*)-1-(3-chlorophenyl)-4-phenylbuta-1,3-dien-1-yl)-2-phenyl-4H-chromen-4-one (**5f**)

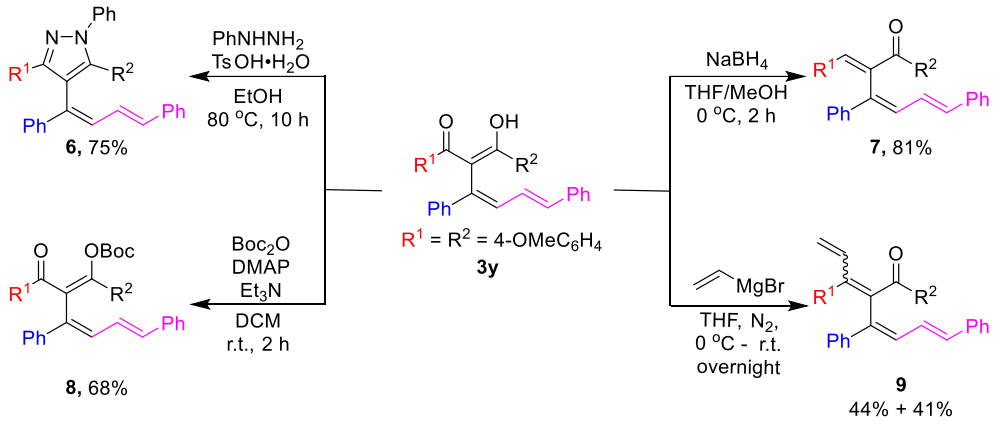
Following the general procedure, the crude product was purified by column chromatography (PE/EA = 10:1:1, v/v) to provide the title compound as a yellow solid (90.3 mg, 65% yield) m.p. 145 - 147 ºC. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.25 - 8.23 (m, 1H), 7.70 - 7.65 (m, 3H), 7.57 - 7.54 (m, 1H), 7.41 - 7.39 (m, 1H), 7.33 - 7.31 (m, 1H), 7.30 - 7.16 (m, 10 H), 6.96 (d, *J* = 15,0 Hz, 1H), 6.70 - 6.62 (m, 2H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 175.89, 162.78, 154.56, 139.89, 137.11, 135.48, 134.00, 133.15, 132.65, 131.22, 131.13, 130.75, 128.54, 128.45, 128.26, 128.17, 127.76, 127.52, 126.56, 125.88, 125.84, 125.69, 124.09, 120.46, 119.82, 77.25, 77.00, 76.75. HRMS (ESI) calcd for $C_{31}H_{21}ClO_2Na$ $[M + Na]^+$: 483.1122, found: 483.1136.



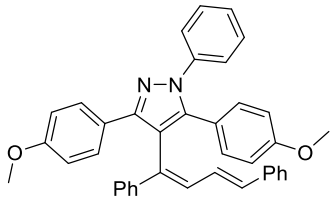
3-((1*Z*,3*E*)-1-(4-fluorophenyl)-4-phenylbuta-1,3-dien-1-yl)-2-phenyl-4H-chromen-4-one (**5g**)

Following the general procedure, the crude product was purified by column chromatography (PE/EA = 10:1:1, v/v) to provide the title compound as a yellow solid (84.5 mg, 63% yield) m.p. 184 - 186 ºC. **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.30 - 8.27 (m, 1H), 7.78 - 7.73 (m, 1H), 7.67 - 7.64(m, 2H), 7.66 (d, *J* = 15.0 Hz, 1H), 7.49 - 7.45 (m, 1H), 7.40 - 7.33 (m, 3H), 7.31 - 7.21 (m, 6H), 7.19 - 7.15 (m, 1H), 6.96 - 6.92 (m, 2H), 6.90 (d, *J* = 15.0 Hz, 1H), 6.72 - 6.65 (m, 1H), 6.63 (d, *J* = 20.0 Hz, 1H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 176.96, 162.69, 162.22 (*J* = 246.3 Hz), 156.22, 137.09, 136.34 (*J* = 5.00 Hz), 135.31, 133.89, 132.89, 132.48, 131.00, 130.65, 128.44, 128.25, 128.12, 127.48 (*J* = 8.75 Hz), 127.45, 126.56, 126.52, 125.75, 125.28, 123.12, 120.25, 118.06, 115.43 (*J* = 22.5 Hz). HRMS (ESI) calcd for $C_{31}H_{21}FO_2Na$ $[M + Na]^+$: 467.1418, found: 467.1429.

4.4 Further transformations of 3y



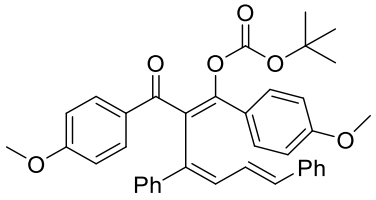
Procedure for preparation of **6**[13]: To an oven-dried 10 mL sealed tube charged with a PTFE-coated magnetic stirring bar, **3y** (0.2 mmol, 1.0 equiv., 97.7 mg), *p*-toluenesulfonic acid monohydrate (0.6 mmol, 30 mol%, 11.4 mg), and phenylhydrazine (2.0 mmol, 10.0 equiv., 216.3 mg) are diluted in 2 mL ethanol and stirred at 80 °C. Upon the completion of reaction monitored by TLC, the reaction was quenched with water, and the aqueous layer was extracted with ethyl acetate (3x10 mL). The combined organic layers were washed with brine (10 mL), dried over $MgSO_4$, and concentrated under reduced pressure the pure product was isolated by column chromatography on silica gel (PE: EA = 15: 1, v: v) as white solid. (83.6 mg, 75%).



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.76 - 7.74 (m, 2H), 7.43 - 7.40 (m, 4H), 7.33 - 7.30 (m, 2H), 7.25 - 7.18 (m, 7H), 7.14 - 7.12 (m, 2H), 7.00 - 6.96 (m, 3H), 6.86 - 6.81 (m, 1H), 6.77 - 6.75 (m, 2H), 6.62 - 6.6.57 (m, 3H), 3.68 (s, 3H), 3.61 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 159.24, 159.16, 150.37, 142.19, 140.89, 140.10, 137.37, 134.06, 130.87, 130.63, 128.71, 128.43, 128.33, 128.29, 127.47, 127.26, 127.22, 126.80, 126.47, 126.36, 125.79, 124.78, 122.45, 116.66, 113.65, 113.63, 55.02, 54.94. m.p. 74 - 76 °C HRMS (ESI) calcd for $C_{39}H_{33}N_2O_2$ $[M + H]^+$: 561.2537, found: 561.2542

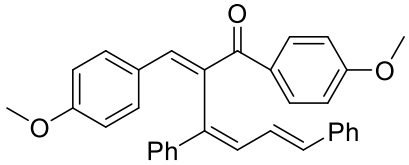
Procedure for preparation of **8**[14]: To an oven-dried 10 mL sealed tube charged with a PTFE-coated magnetic stirring bar, **3y** (0.2 mmol, 1.0 equiv., 97.7 mg), DMAP (0.02 mmol, 10 mol%, 2.4 mg) and Et_3N (0.22 mmol, 1.1 equiv., 22.3 mg) are diluted in 2 mL DCM. Boc_2O (0.3 mmol, 1.5 equiv., 65.5 mg) was added to the reaction vessel, and the reaction was stirred for 2 h at room temperature. Upon the completion of reaction monitored by TLC, the solution was transferred to a separatory funnel, and $NaHSO_4$ (0.5 M, 10 mL) was added. The layers were separated, and the aqueous layer was extracted with CH_2Cl_2 (3x10 mL). The combined organic layers were washed with

brine (10 mL), dried over $MgSO_4$, and concentrated under reduced pressure, the pure product was isolated by column chromatography on silica gel (PE: EA = 12: 1, v: v) as yellow solid. (80.6 mg, 68%)



^{1}H NMR (500 MHz, $CDCl_3$) δ 7.99 - 7.97 M, 2H), 7.55 - 7.53 (m, 2H), 7.46 - 7.44 (m, 2H), 7.29 - 7.23 (m, 6H), 7.20 - 7.17 (m, 3H), 6.86 - 6.85 (m, 2H), 6.69 - 6.63 (m, 3H), 6.54 (d, *J* = 20.0 Hz, 1H), 3.79 (s, 3H), 3.66 (s, 3H), 1.34 (s, 9H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 192.96, 163.12, 160.40, 151.46, 150.29, 139.88, 137.33, 137.12, 135.23, 131.46, 131.19, 130.64, 129.13, 128.43, 128.41, 127.64, 127.54, 126.93, 126.75, 126.58, 126.56, 125.72, 113.56, 113.44, 83.65, 55.33, 55.06, 27.42. m.p. 69 - 71 ºC HRMS (ESI) calcd for $C_{38}H_{36}O_6Na$ $[M + Na]^+$: 611.2404, found: 611.2408

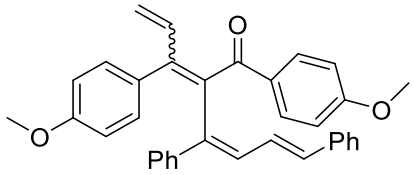
Procedure for preparation of **7**[15]: To an oven-dried 10 mL Schlenk tube charged with a PTFE-coated magnetic stirring bar, **3y** (0.2 mmol, 1.0 equiv., 97.7 mg) are diluted in dry THF and methanol (THF: MeOH=1:1, v: v) at 0 °C. $NaBH_4$ (0.6 mmol, 3.0 equiv., 22.7 mg) was added to the reaction vessel, and the reaction was stirred for 2 h at room temperature under N_2 atmosphere. Upon the completion of reaction monitored by TLC, and the reaction was quenched with water, and the aqueous layer was extracted with ethyl acetate (3x10 mL). The combined organic layers were washed with brine (10 mL), dried over $MgSO_4$, and concentrated under reduced pressure, the pure product was isolated by column chromatography on silica gel (PE: EA = 9: 1, v: v) as white solid. (76.6 mg, 81%)



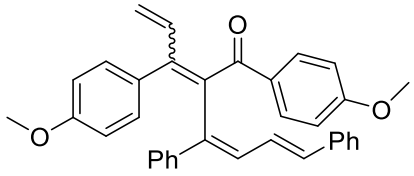
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.89 - 7.87 (m, 2H), 7.54 - 7.50 (m, 5H), 7.28 - 7.12 (m, 8H), 6.99 - 6.90 (m, 4H), 6.73 - 6.67 (m, 3H), 3.81 (s, 3H), 3.67 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 195.57, 162.62, 160.56, 142.62, 139.14, 138.04, 137.32, 135.40, 134.94, 131.87, 131.76, 131.01, 129.81, 128.60, 128.41, 127.60, 127.56, 127.21, 126.49, 126.47, 126.15, 113.94, 113.41, 55.34, 55.09. m.p. 71 - 73 ºC HRMS (ESI) calcd for $C_{33}H_{29}O_3$ $[M + H]^+$:473.2111, found: 473.2116

Procedure for preparation of **9**[16]: To an oven-dried 10 mL sealed tube charged with a PTFE-coated magnetic stirring bar, **3y** (0.2 mmol, 1.0 equiv., 97.7 mg) are diluted in 2 mL dry THF at 0 °C. Vinylmagnesium bromide solution (0.1 M in THF, 8 mL, 0.8 mmol) was added dropwise and the reaction mixture was slowly allowed to reach room temperature overnight. Upon the completion of reaction monitored by TLC, the reaction

was quenched with Sat. NH_4Cl-solution (10 mL), and the aqueous layer was extracted with ethyl acetate (3x10 mL). The combined organic layers were washed with brine (10 mL), dried over $MgSO_4$, and concentrated under reduced pressure, the pure product was isolated by column chromatography on silica gel (PE: EA = 15: 1, v: v) as white soild. (**9** (isomer 1): 44.0 mg, 44%, **9** (isomer 2): 40.4 mg, 41%).

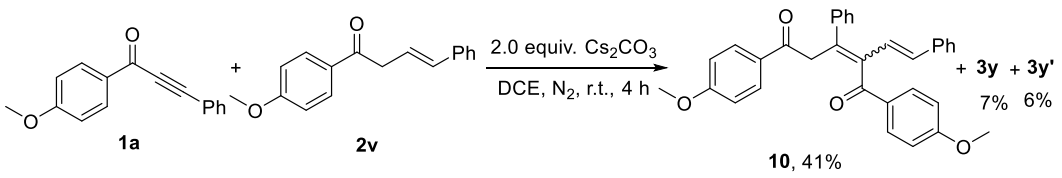


9 (isomer 1) **^{1}H NMR** (500 MHz, $CDCl_3$) δ 8.00 - 7.98 (m, 2H), 7.35 - 7.32 (m, 2H), 7.29 - 7.21 (m, 5H), 7.19 - 7.10 (m, 6H), 6.89 - 6.78 (m, 3H), 6.64-6.62 (m, 2H), 6.48 - 6.39 (m, 2H), 5.30 (dd, *J* = 10.7, 1.5 Hz, 1H), 5.16 (dd, *J* = 17.1, 1.5 Hz, 1H), 3.82 (s, 3H), 3.66 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 196.13, 163.45, 159.08, 147.04, 141.02, 140.33, 137.94, 137.38, 136.99, 134.56, 131.99, 131.05, 130.77, 130.30, 130.08, 128.53, 127.96, 127.64, 127.44, 127.15, 126.96, 126.53, 121.35, 113.64, 113.03, 55.41, 55.07. m.p.82 - 84 ºC HRMS (ESI) calcd for $C_{35}H_{31}O_3$ [M + H]$^+$:499.2268, found: 499.2273



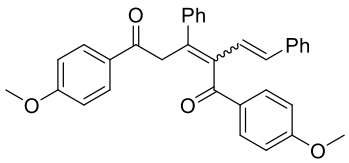
9 (isomer 2) **^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.71 - 6.69 (m, 2H), 7.50 - 7.48 (m, 2H), 7.37 - 7.35 (m, 2H), 7.30 - 7.26 (m, 4H), 7.25 - 7.20 (m, 5H), 6.91 - 6.83 (m, 2H), 6.80 - 6.73 (m, 3H), 6.66 - 6.64 (m, 2H), 5.36 (dd, *J* = 10.7, 1.4 Hz, 1H), 5.21 (dd, *J* = 17.2, 1.5 Hz, 1H), 3.73 (s, 3H), 3.72 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 195.77, 162.71, 159.33, 145.57, 140.12, 138.94, 137.88, 137.54, 137.29, 135.30, 132.14, 131.72, 131.69, 130.33, 130.09, 128.62, 128.35, 127.78, 127.61, 127.24, 127.12, 126.51, 122.14, 113.50, 113.04, 55.25, 55.11. m.p.81 - 83 ºC HRMS (ESI) calcd for $C_{35}H_{31}O_3$. [M + H] $^+$:499.2268, found: 499.2269

4.5 Synthesis of 10



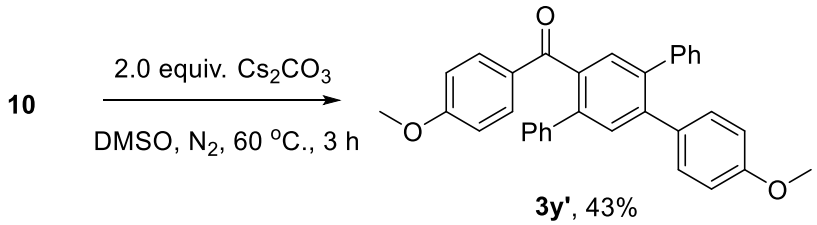
To an oven-dried 10 mL Schlenk tube charged with a PTFE-coated magnetic stirring bar, **1a** (0.3 mmol, 1.0 equiv., 70.9 mg), **2v** (0.36 mmol, 1.2 equiv., 90.8 mg) and Cs_2CO_3 (0.6 mmol, 2.0 equiv., 195.5 mg) are diluted in dry DCE and the reaction was stirred for 4 h at room temperature under N_2 atmosphere. Upon the completion of

reaction monitored by TLC, and the reaction was quenched with water, and the aqueous layer was extracted with ethyl acetate (3x10 mL). The combined organic layers were washed with brine (10 mL), dried over $MgSO_4$, and concentrated under reduced pressure, the pure product was isolated by column chromatography on silica gel (PE: EA = 8: 1, v: v) as yellow solid. (60.5 mg, 41%)



^{1}H NMR (600 MHz, $CDCl_3$) Obtained as 1.5: 1 isomer. major isomer: δ 8.11 - 8.09 (m, 3H), 7.75 - 7.73 (m, 2H), 7.43 - 7.37 (m, 4H), 6.94 - 6.92 (m, 3H), 6.83 - 6.80 (m, 3H), 6.27 (d, *J* = 18 Hz, 1H) 4.05 (s, 2H), 3.85 (s, 3H), 3.80 (s, 3H); miner isomer δ 8.06 - 8.04 (m, 2H), 6.99 - 6.96 (m, 3H), 6.48 (d, *J* = 18 Hz, 1H), 4.40 (s, 2H), 3.90 (s,3H), 3.79 (s, 3H); other peaks are overlapped with the other isomer. **^{13}C NMR (150 MHz, $CDCl_3$)** δ 198.00, 197.59, 195.28, 194.69, 164.20, 163.85, 163.55, 163.35, 141.63, 140.08, 139.79, 139.64, 136.93, 136.00, 134.21, 133.64, 132.51, 132.45, 132.30, 130.68, 130.35, 129.91, 129.74, 129.59, 129.50, 129.34, 128.44, 128.23, 128.12, 128.00, 127.93, 127.74, 127.71, 127.37, 126.66, 126.48, 125.30, 123.88, 113.95, 113.60, 113.51, 55.55, 55.48, 55.39, 55.32, 45.27, 44.04. m.p. 185 - 187 ºC HRMS (ESI) calcd for $C_{33}H_{28}O_4Na$ $[M + Na]^+$: 511.1880, found: 511.1875.

4.6 Synthesis of 3y'



3y', 43%

To an oven-dried 10 mL Schlenk tube charged with a PTFE-coated magnetic stirring bar, **10** (0.1 mmol, 1.0 equiv., 48.9 mg) and Cs_2CO_3 (0.2 mmol, 2.0 equiv., 65.2 mg) are diluted in dry DMSO and the reaction was stirred for 3 h at 60 °C under N_2 atmosphere. Upon the completion of reaction monitored by TLC, and the reaction was quenched with water, and the aqueous layer was extracted with ethyl acetate (3x10 mL). The combined organic layers were washed with brine (10 mL), dried over $MgSO_4$, and concentrated under reduced pressure, the pure product was isolated by column chromatography on silica gel (PE: EA = 15: 1, v: v) as **3y'**. (20.2 mg, 43%)

5. References

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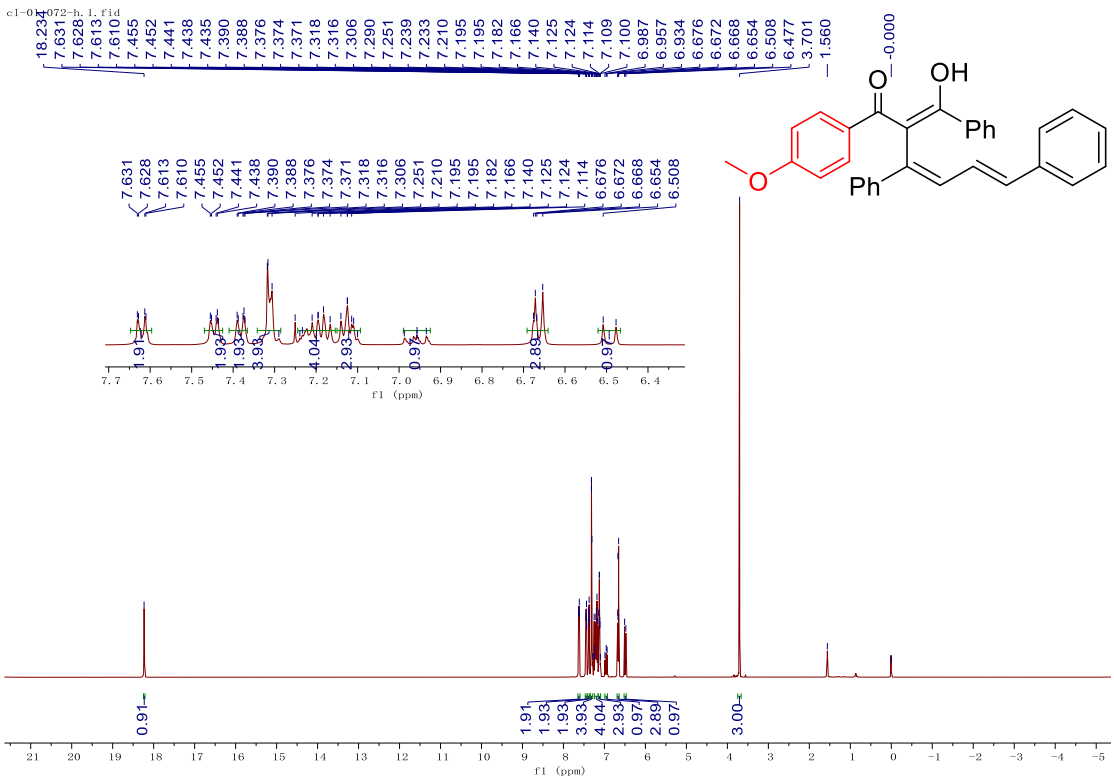
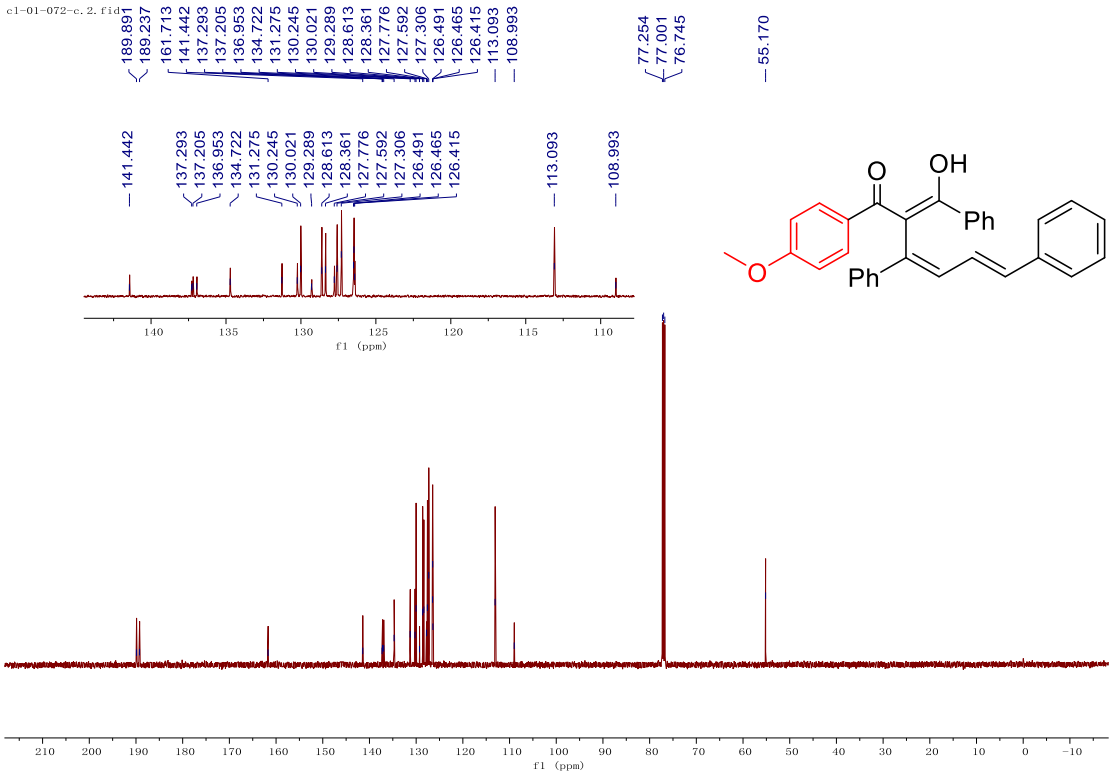
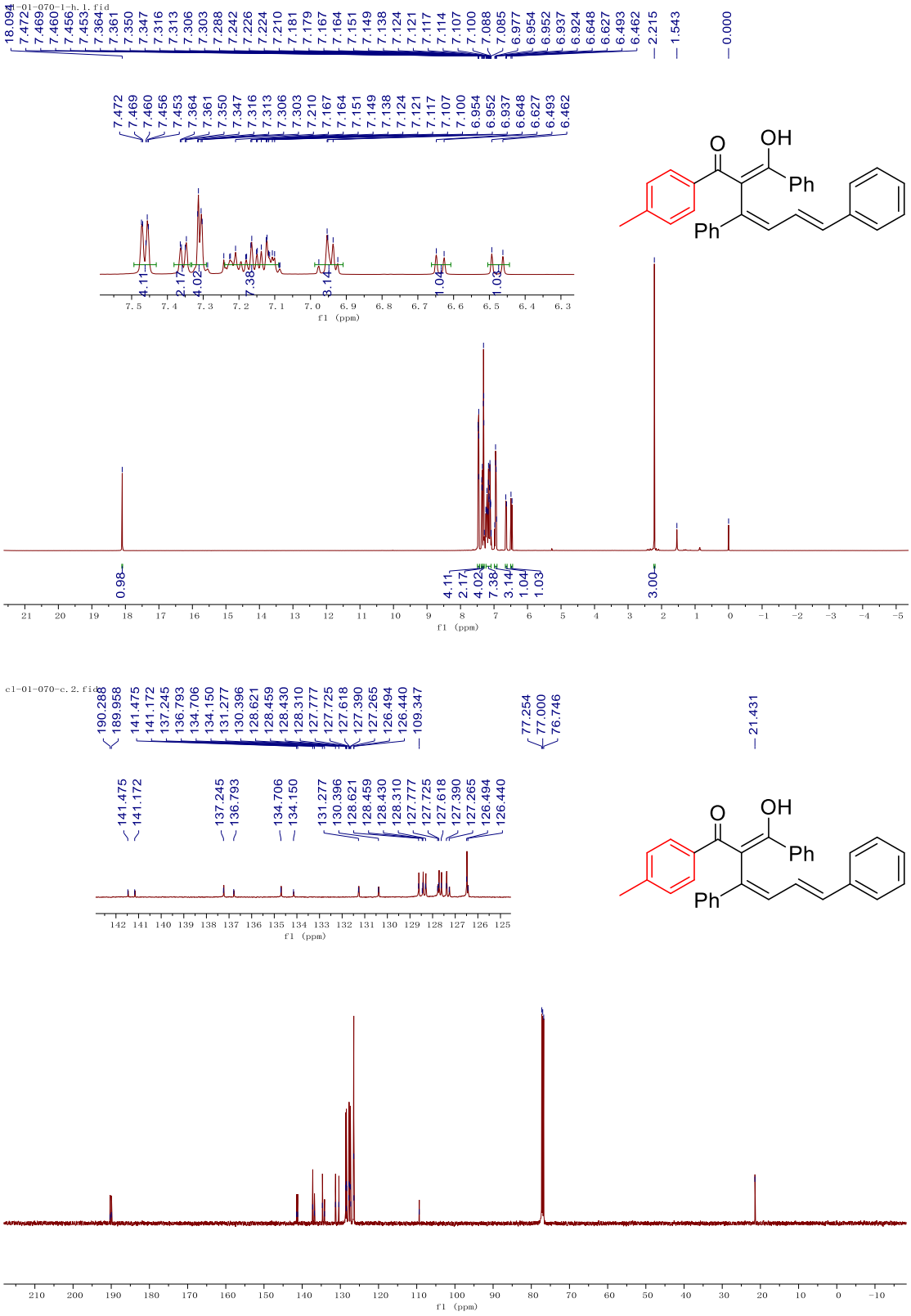
6. Copies of NMR spectra



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4.02
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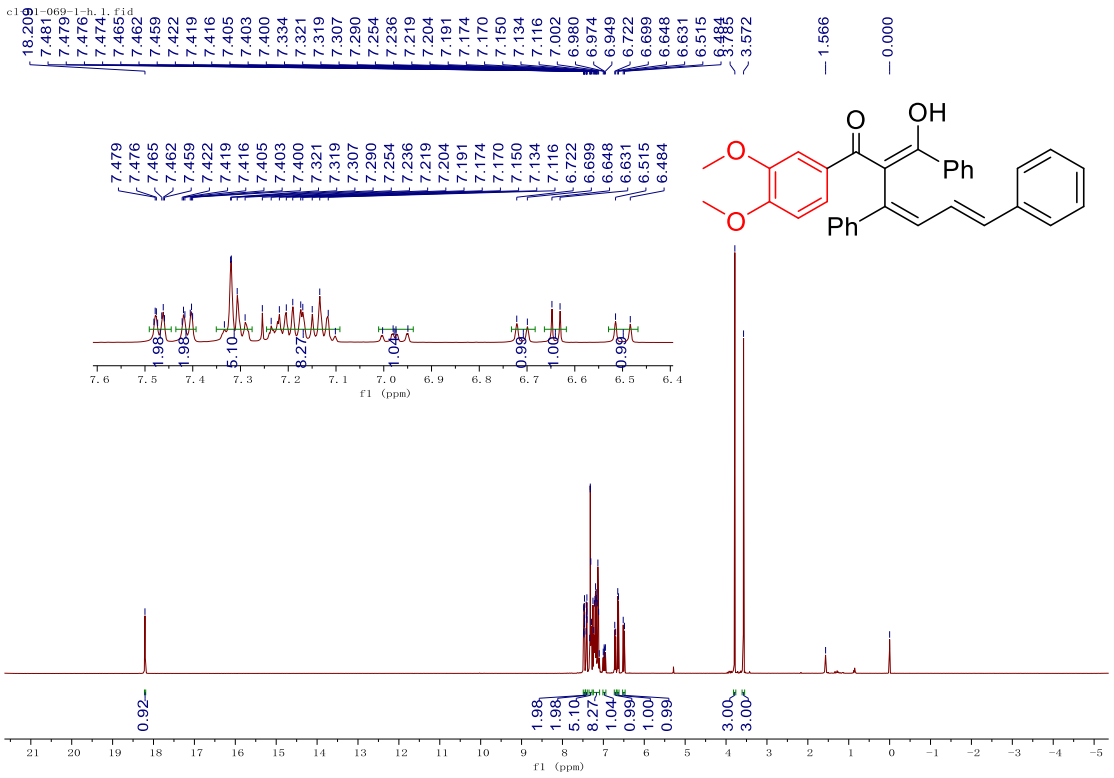
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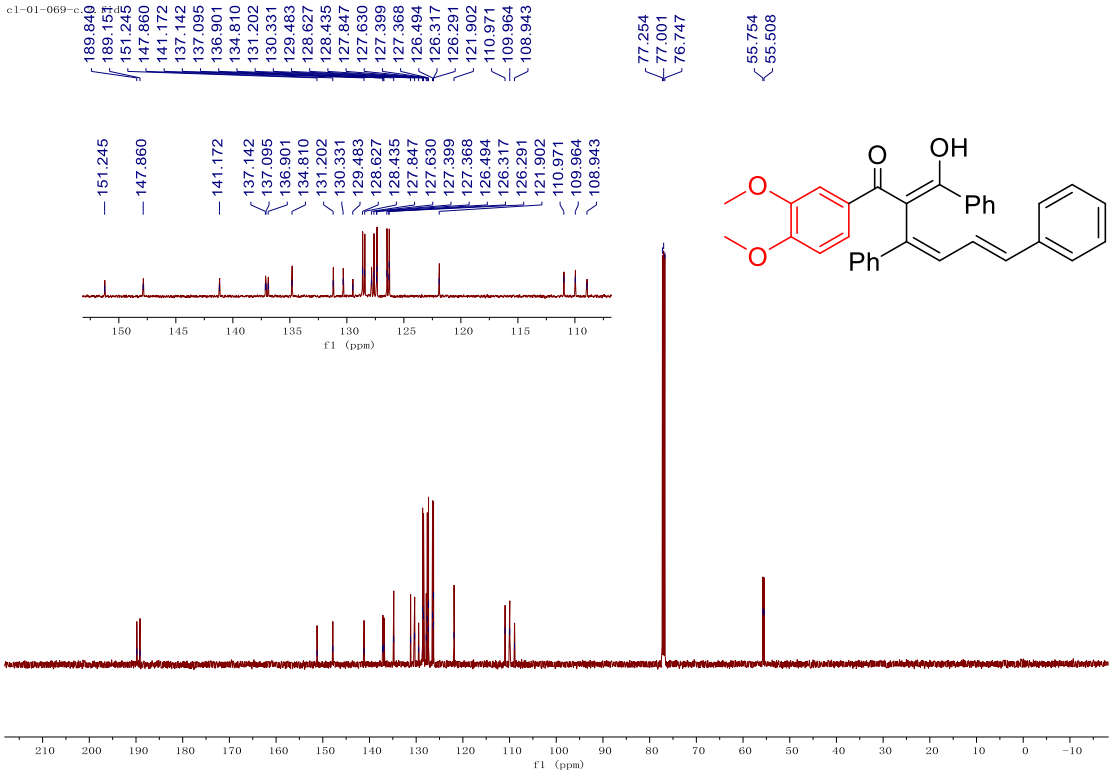
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O
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Ph
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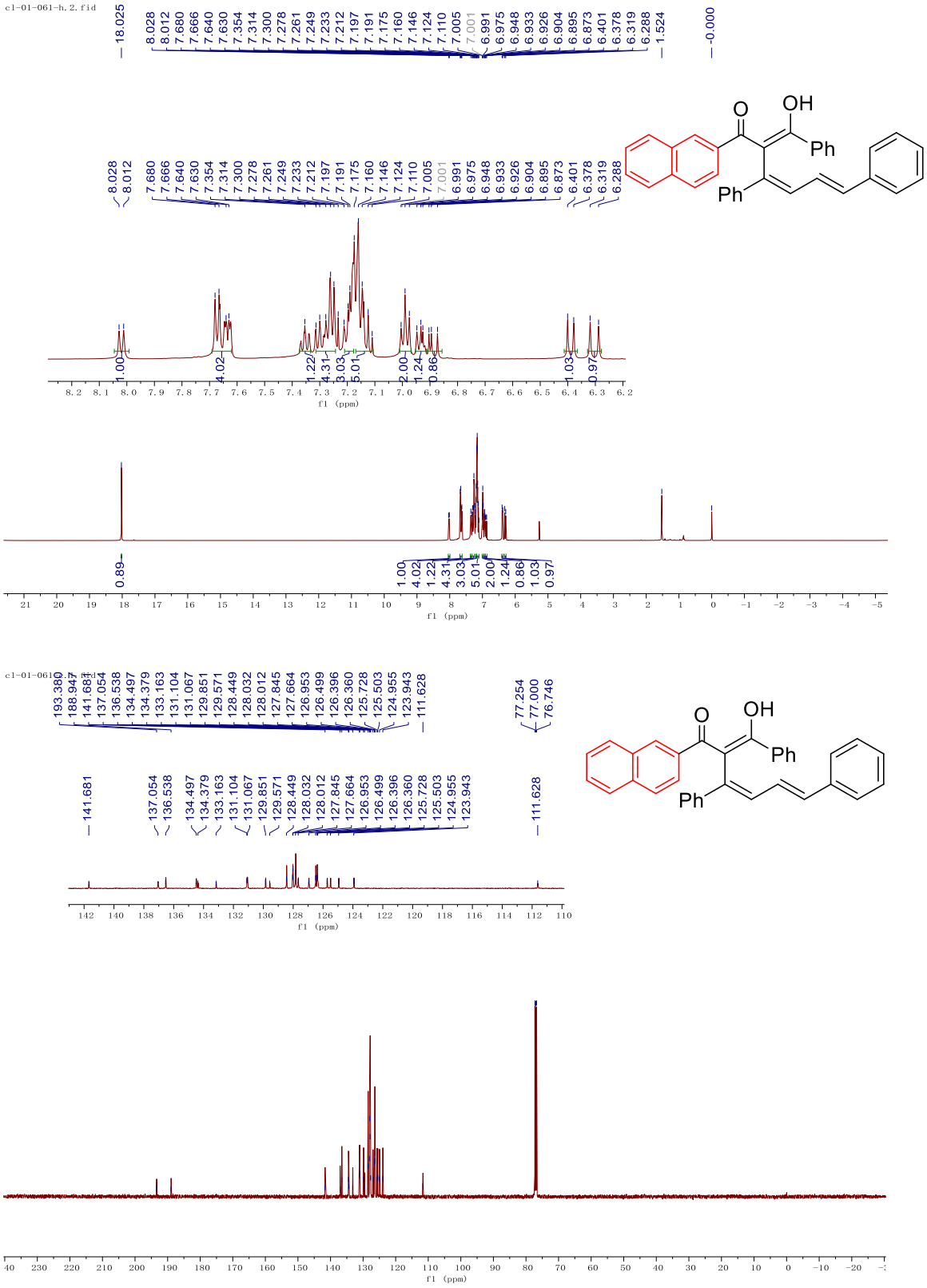
f1 (ppm)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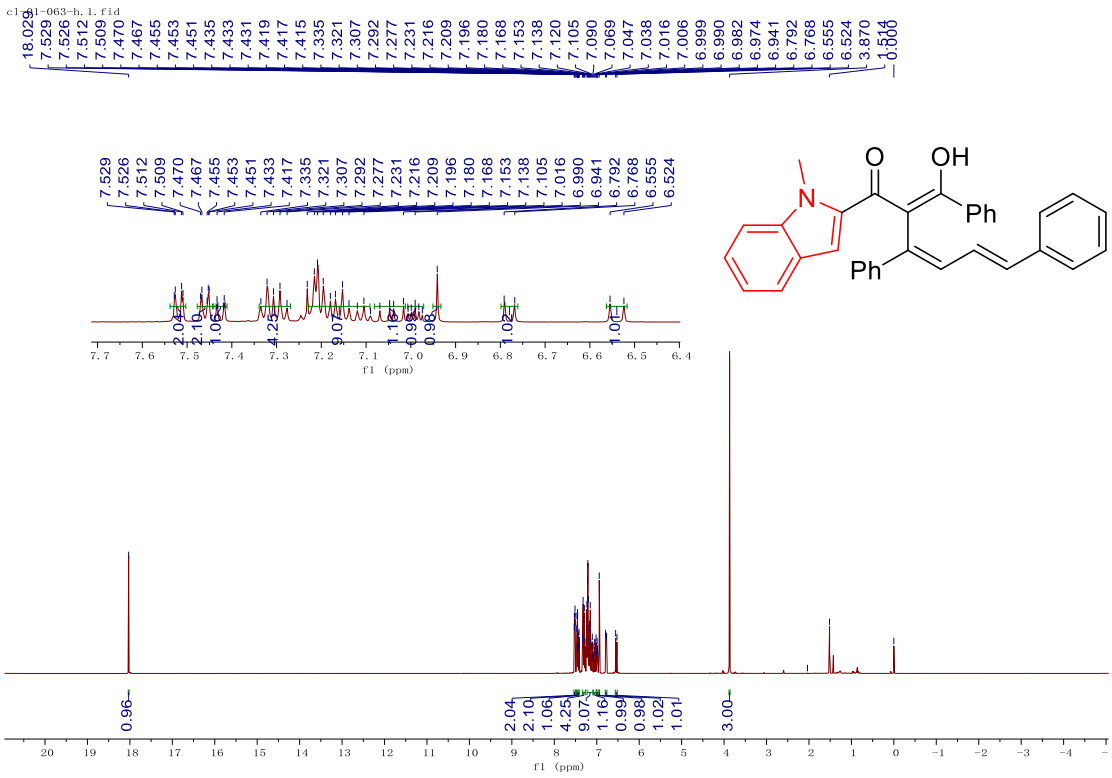
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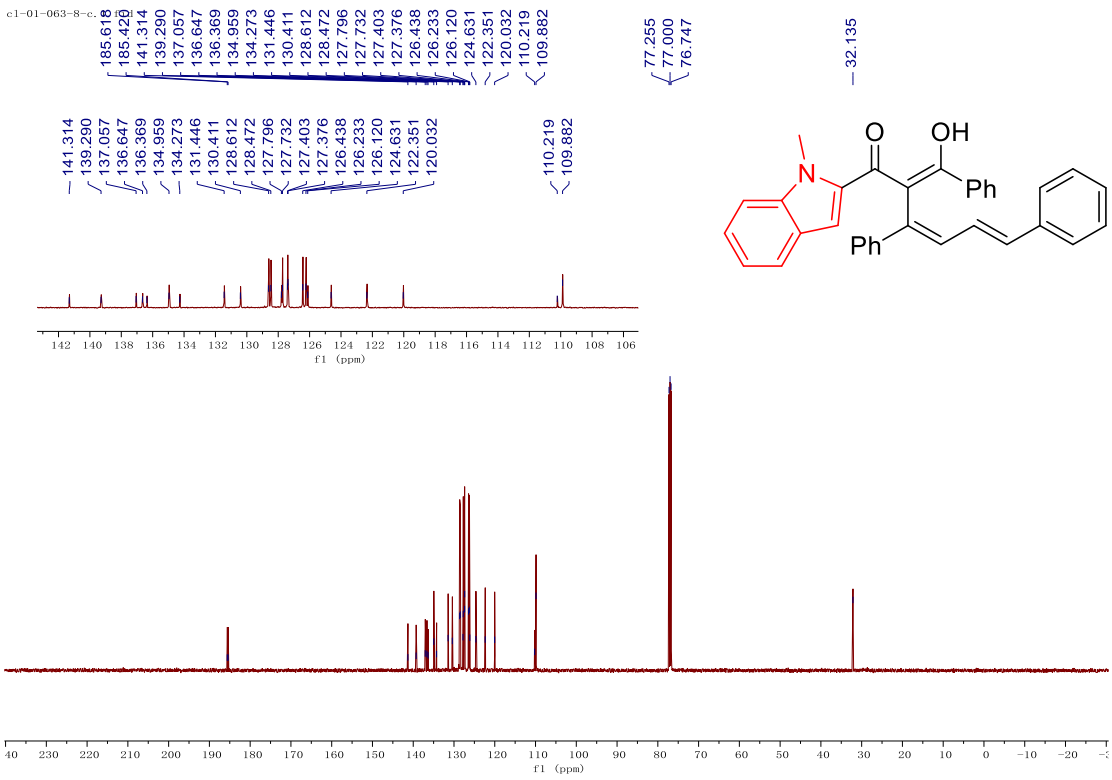
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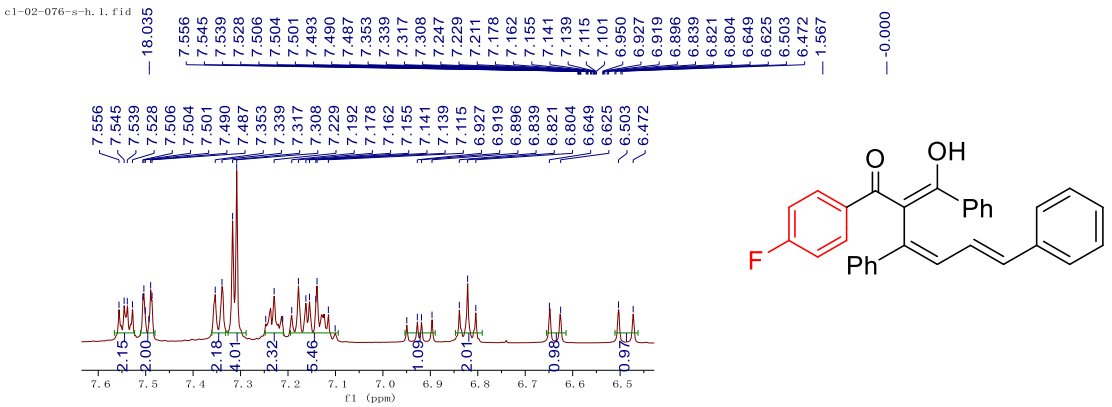
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2.00
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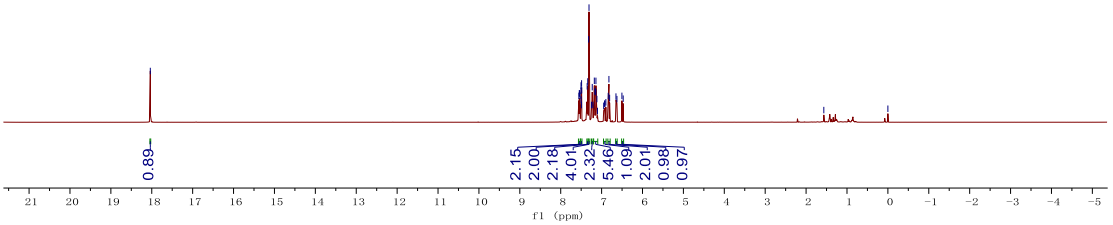
OH
Ph
F
Ph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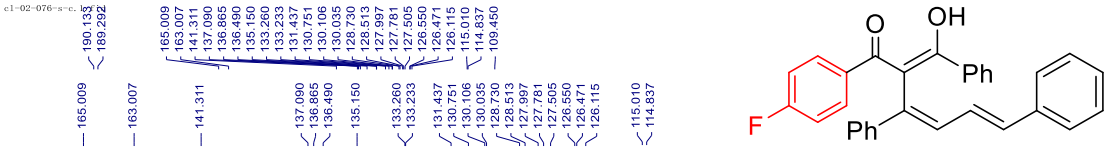
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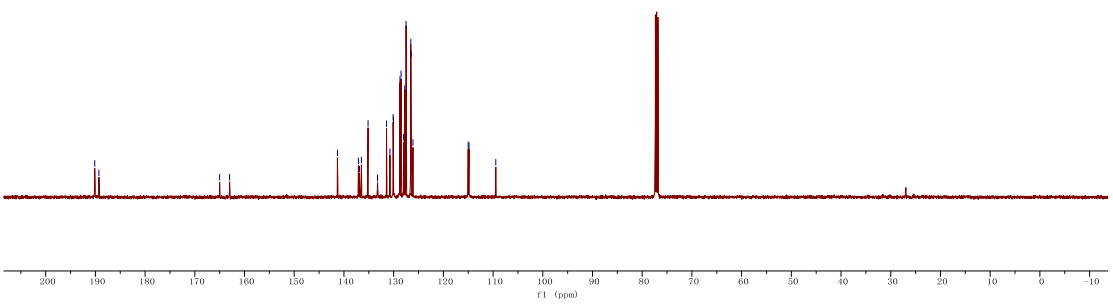
Ph
F
Ph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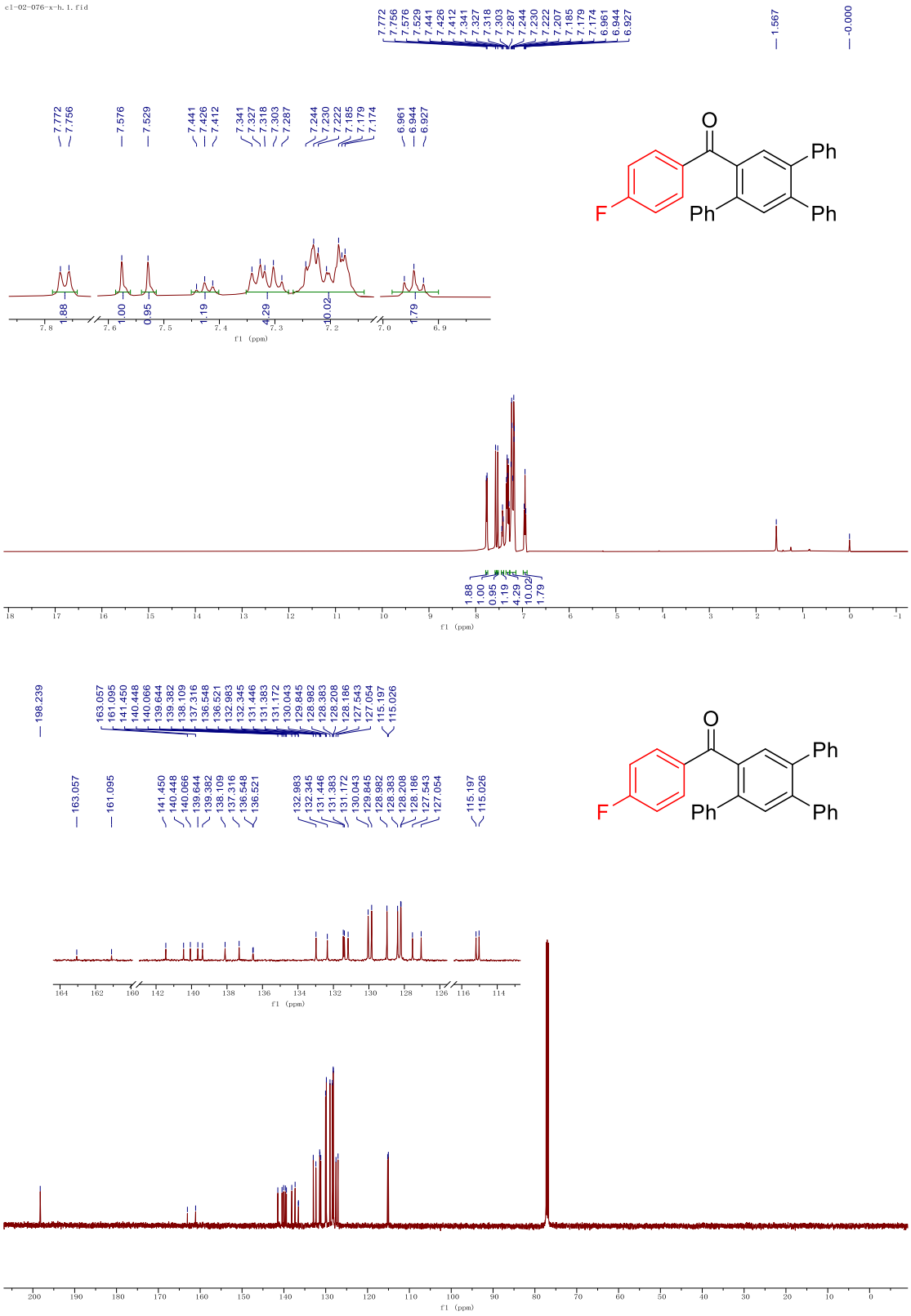
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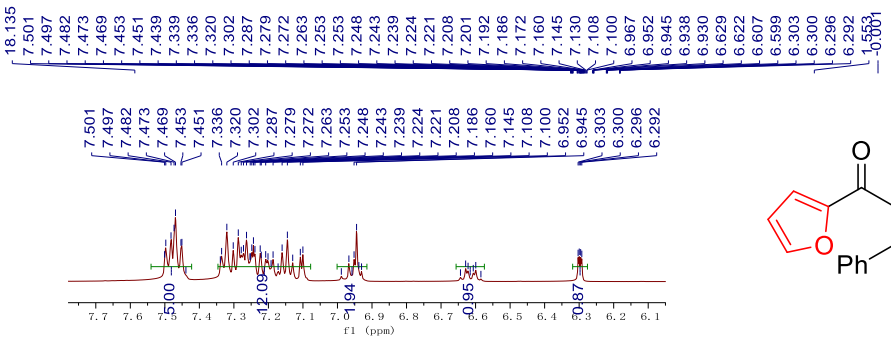
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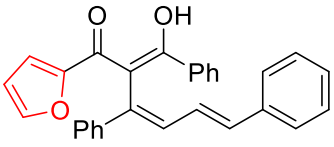
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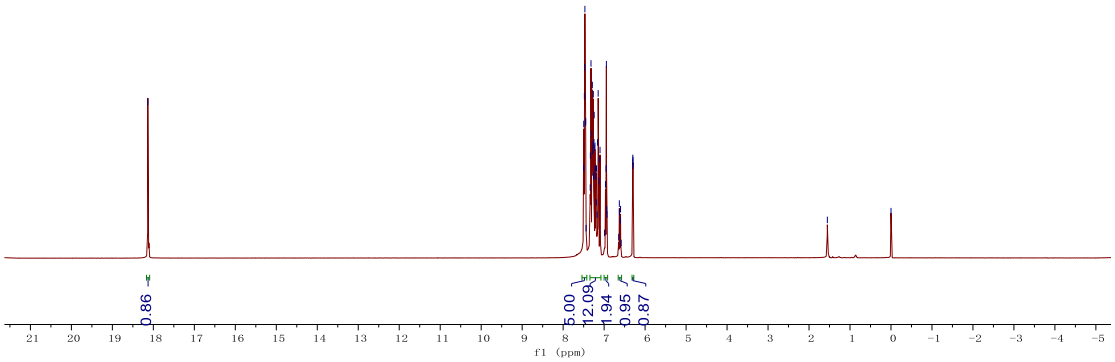
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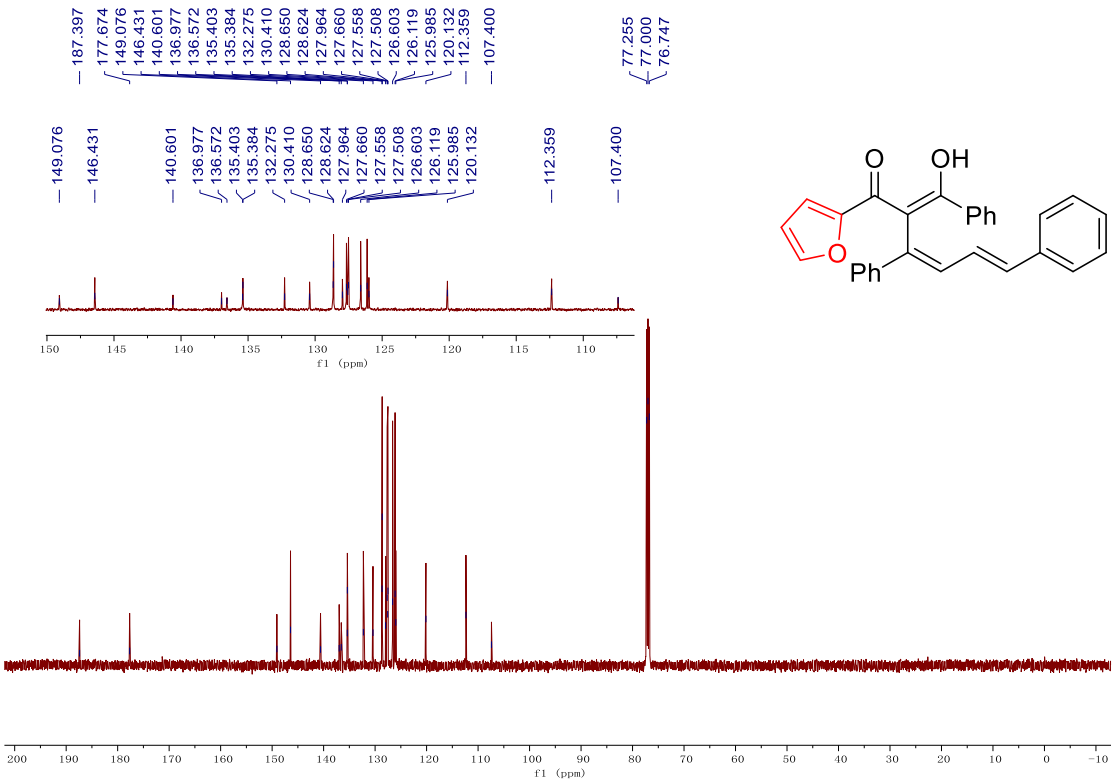
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f1 (ppm)

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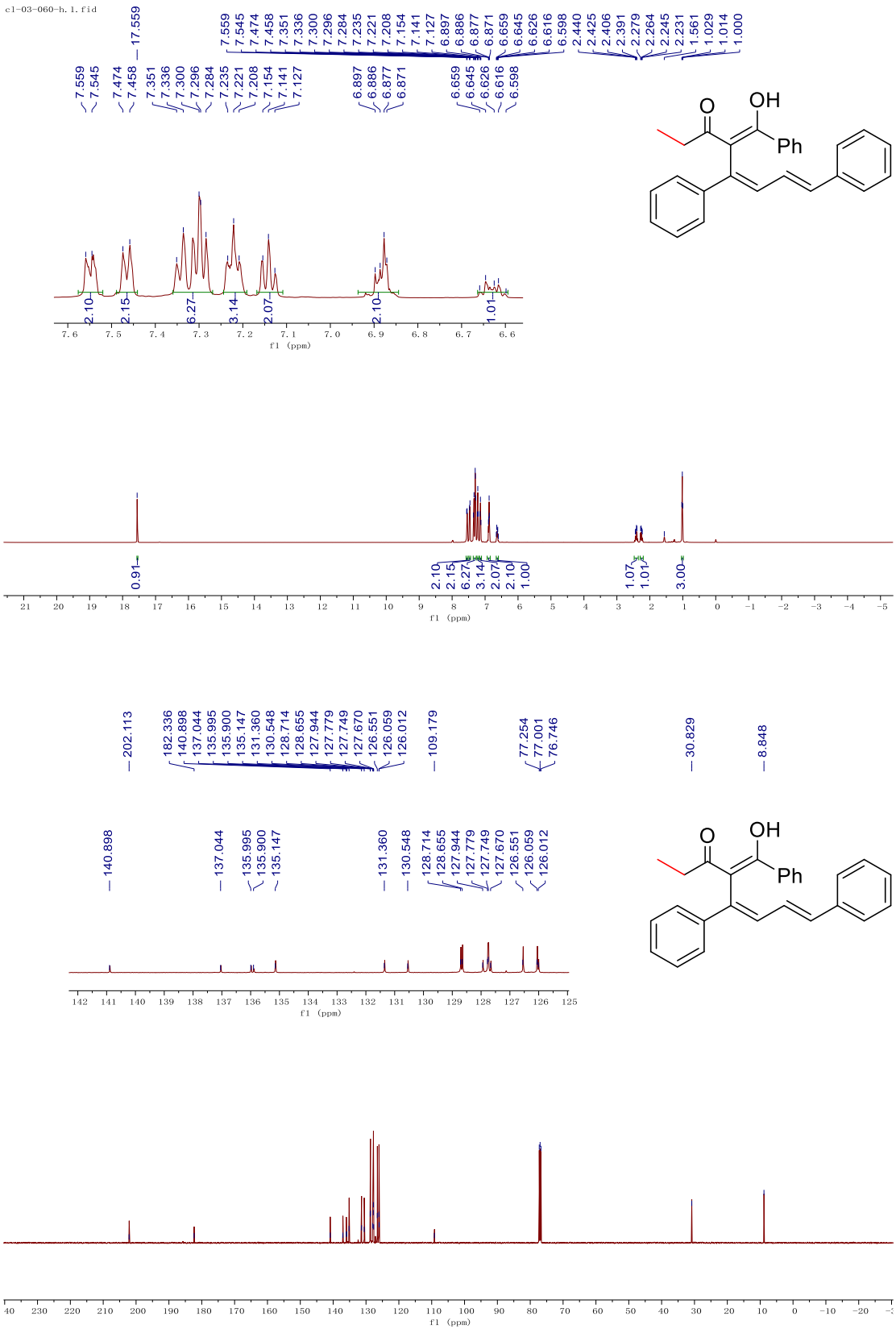
Ph
O
Ph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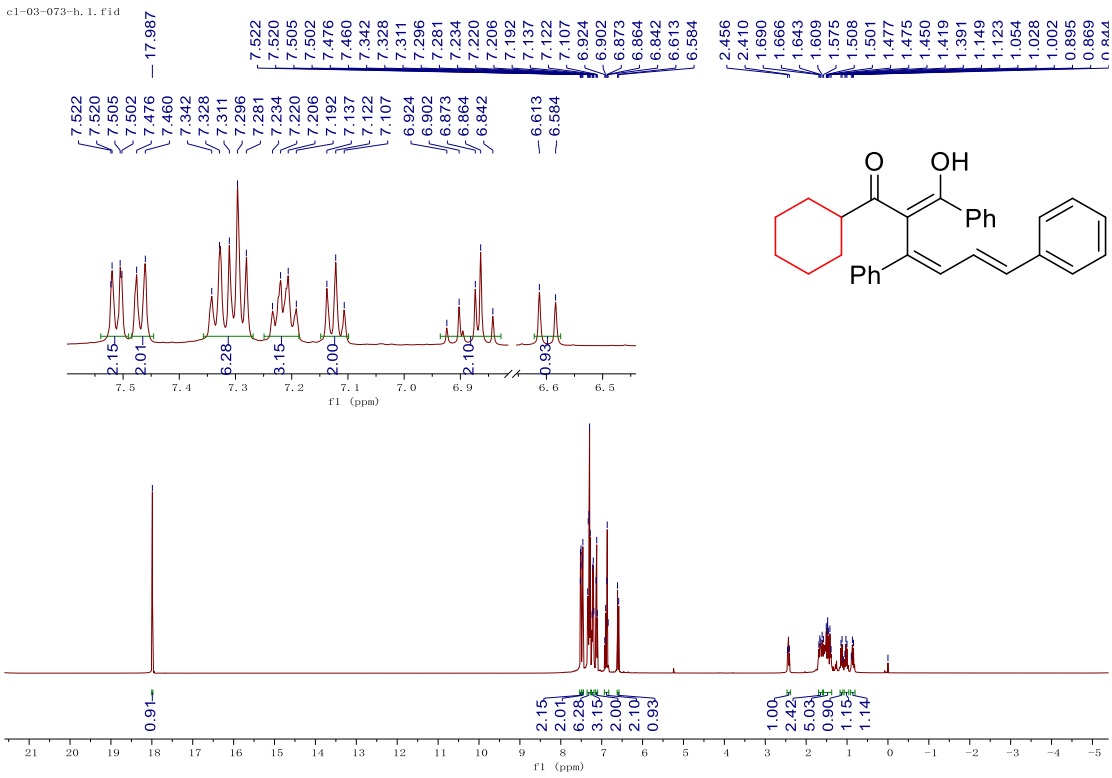
f1 (ppm)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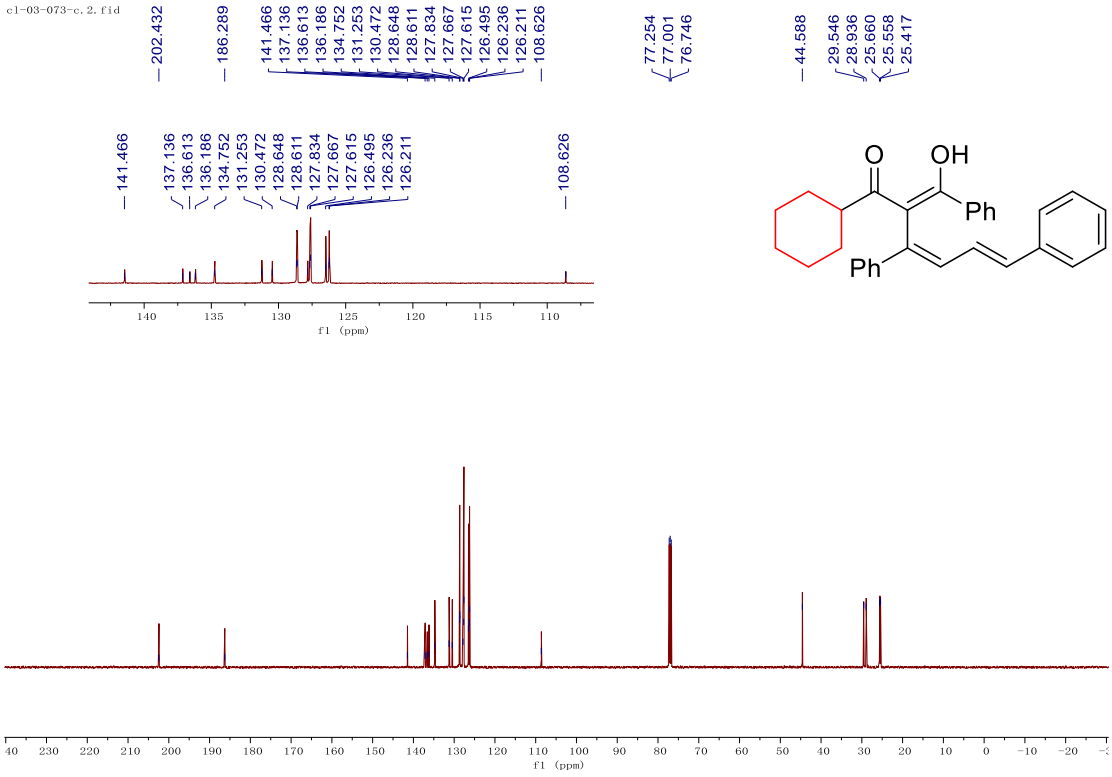
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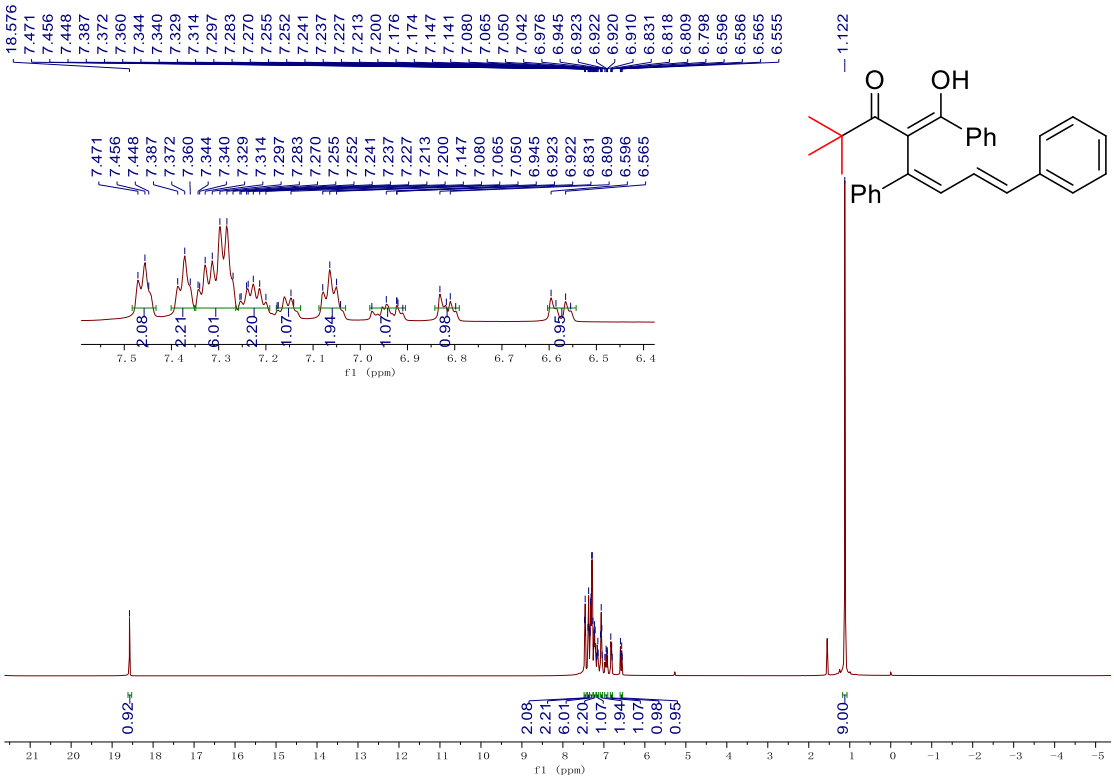
f1 (ppm)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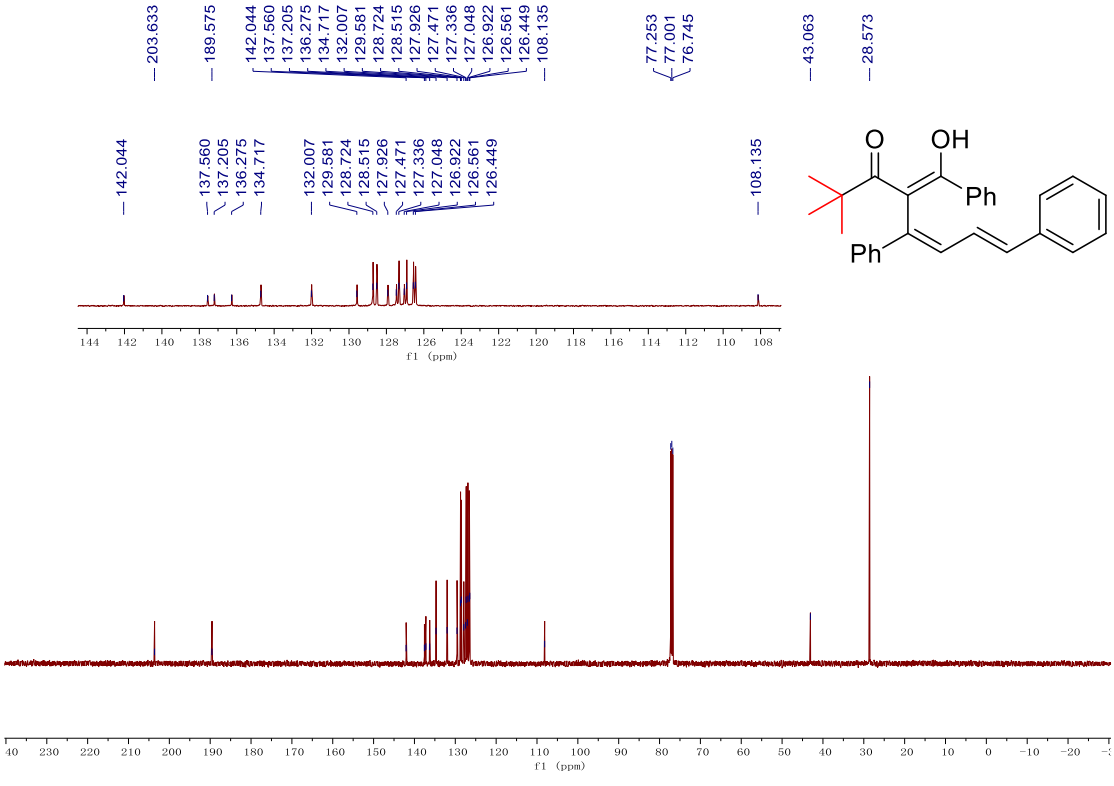
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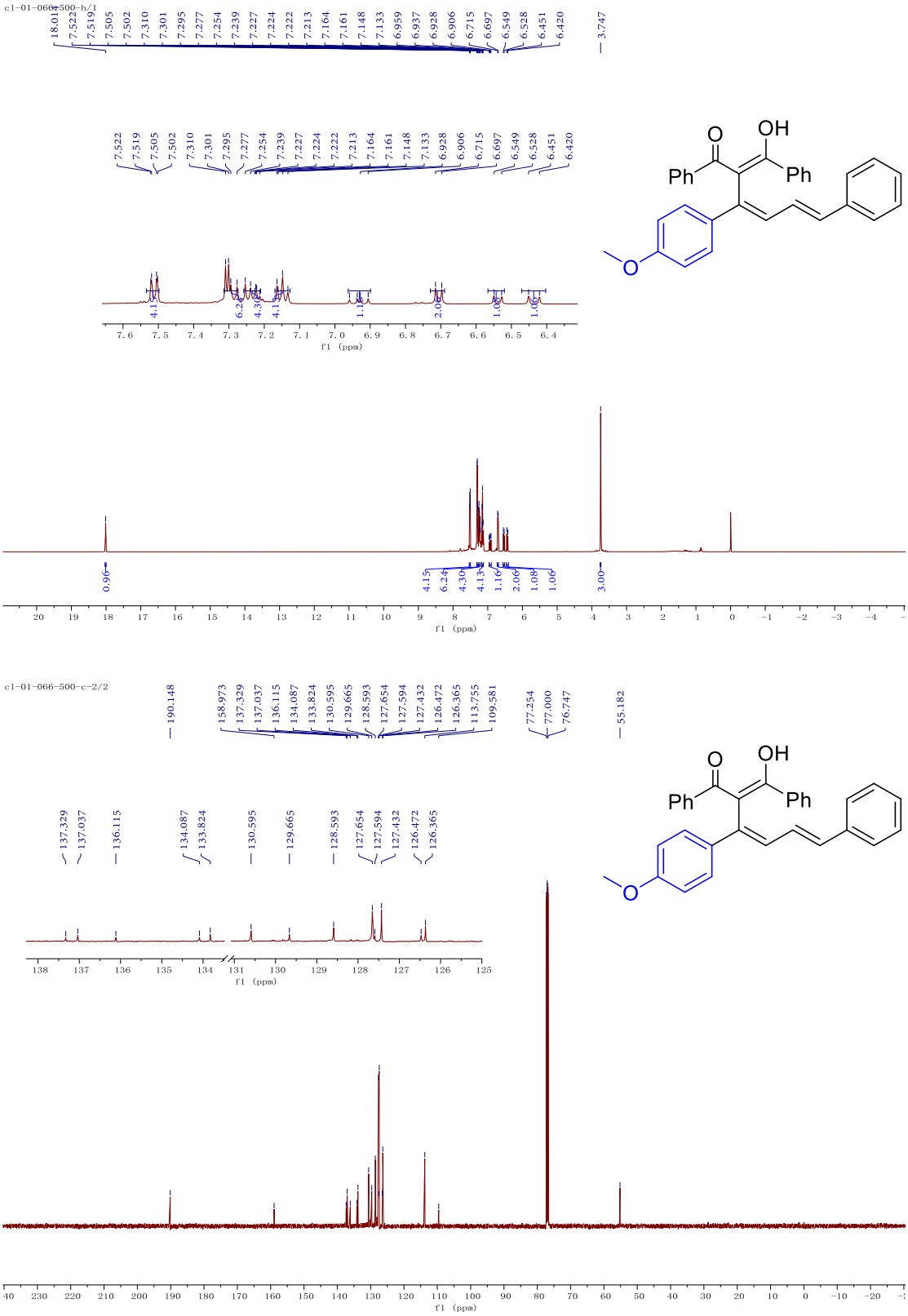
f1 (ppm)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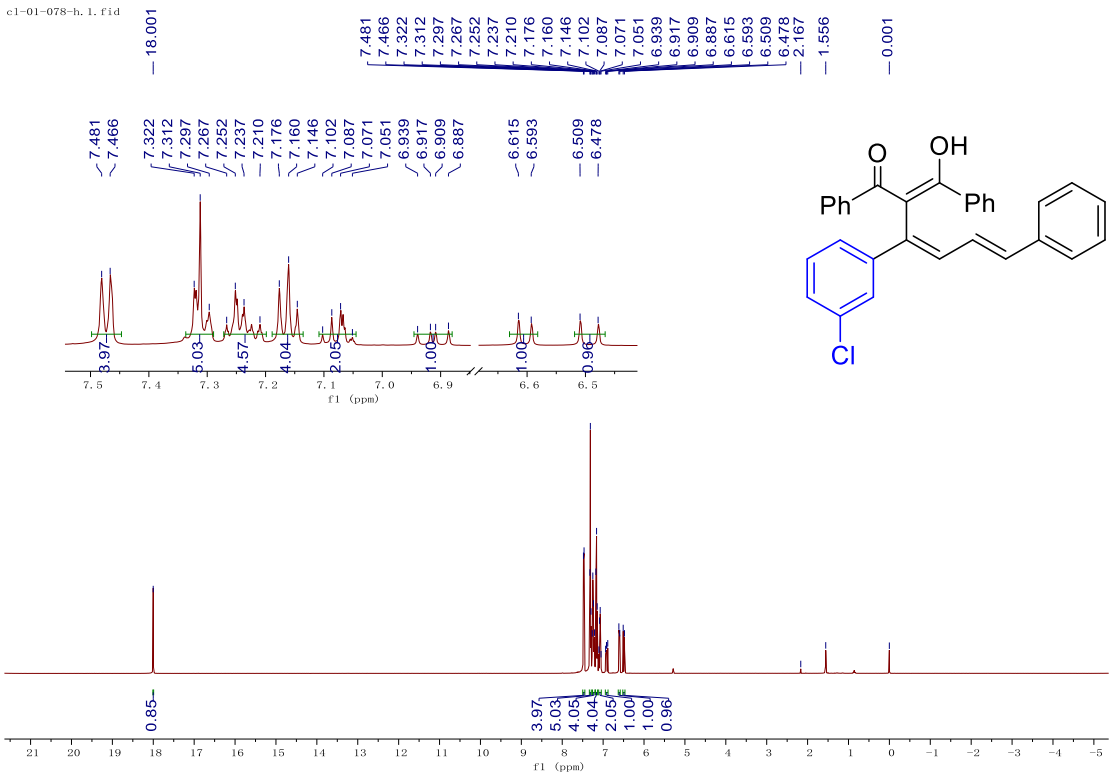
6.697
6.549
6.528
6.451
6.420
3.747
O
OH
Ph
Ph
O
f1 (ppm)
0.96
4.15
6.24
4.30
4.13
1.16
2.06
1.08
1.06
3.00

c1-01-066-500-c-2/2
190.148
158.973
137.329
137.037
136.115
134.087
133.824
130.595
129.665
128.593
127.654
127.594
127.432
126.472
126.365
113.755
109.581
77.254
77.000
76.747
55.182
O
OH
Ph
Ph
O
f1 (ppm)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7.481
7.466
7.322
7.312
7.297
7.267
7.252
7.237
7.210
7.176
7.160
7.146
7.102
7.087
7.071
7.051
6.939
6.917
6.909
6.887
6.615
6.593
6.509
6.478
2.167
1.556
0.001
O
OH
Ph
Ph
Cl
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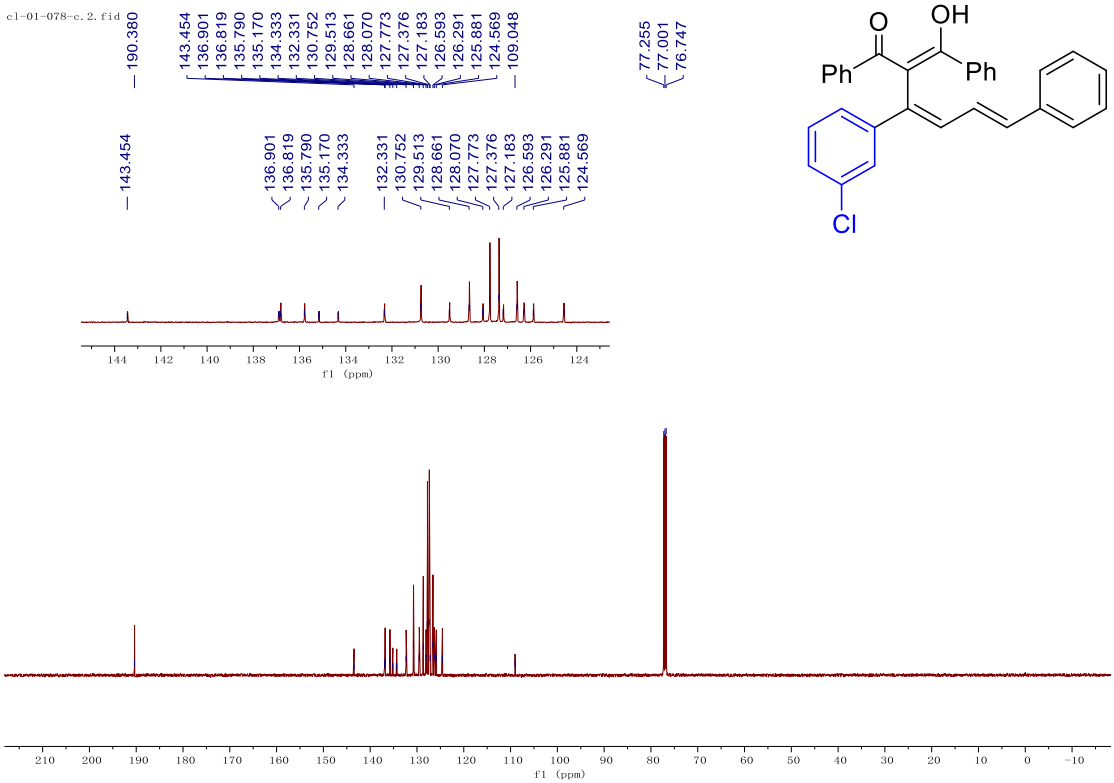
3.97
5.03
4.05
4.04
2.05
1.00
1.00
0.96
f1 (ppm)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136.819
135.790
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134.333
132.331
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129.513
128.661
128.070
127.773
127.376
127.183
126.593
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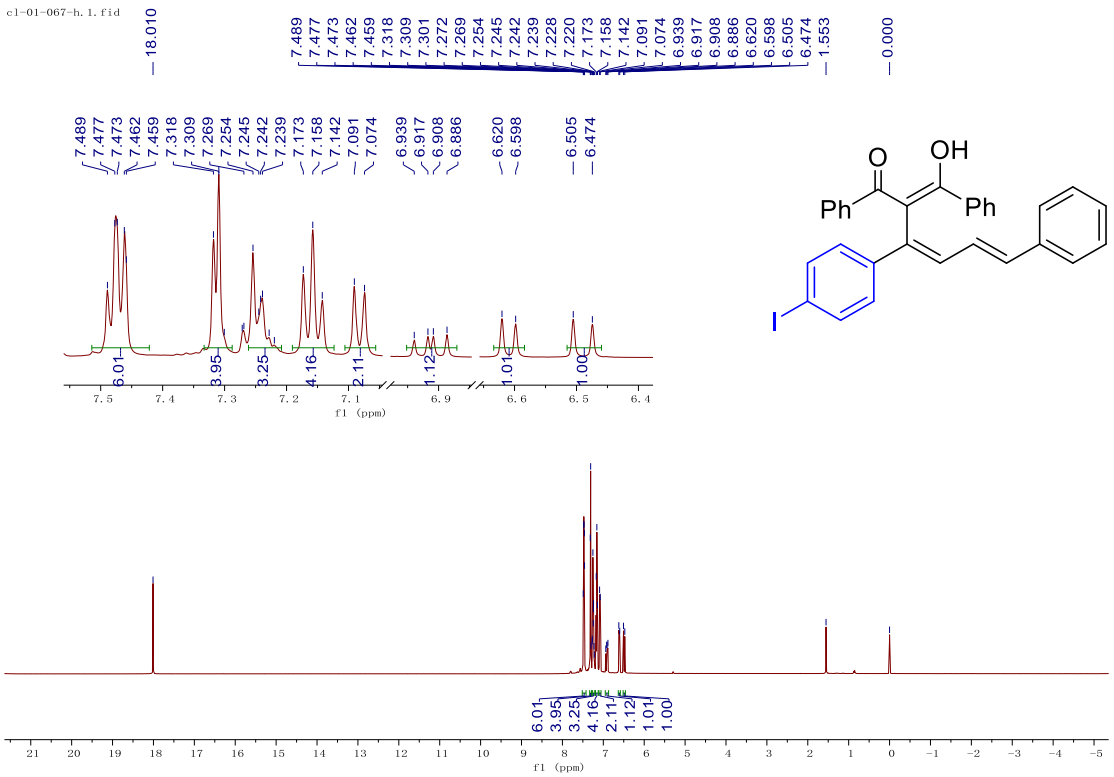
124.569
109.048
77.255
77.001
76.747
O
OH
Ph
Ph
Cl
f1 (ppm)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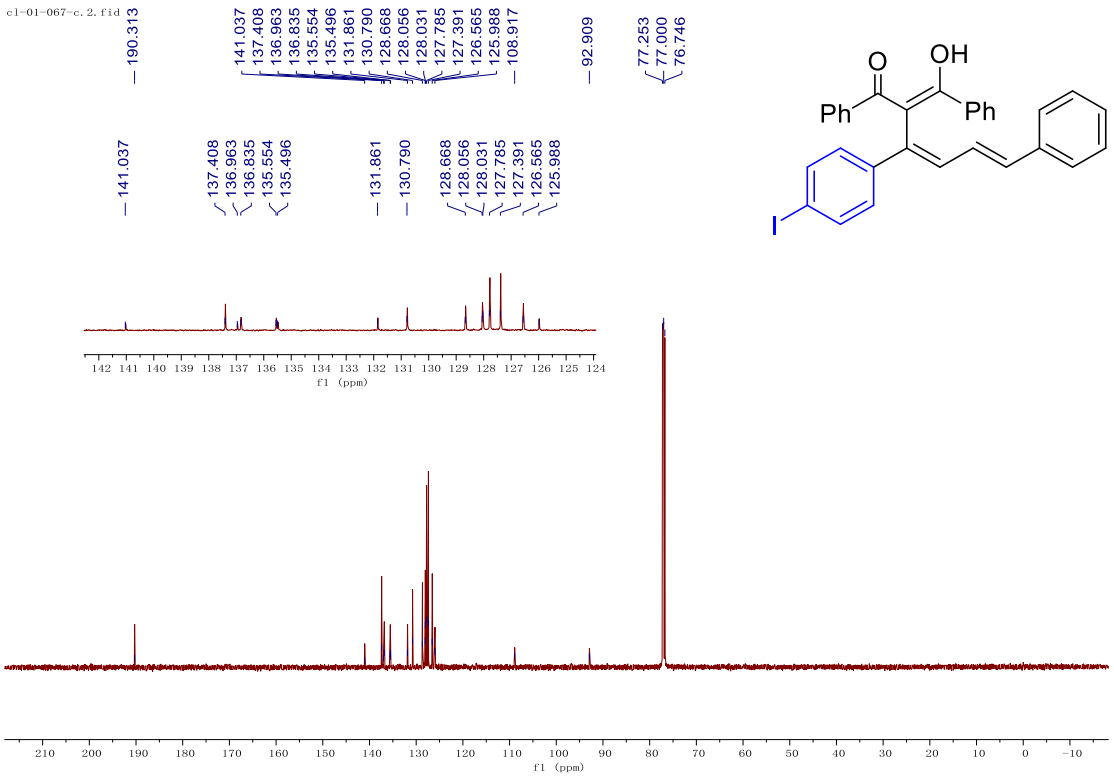
7.477
7.473
7.462
7.459
7.318
7.309
7.301
7.272
7.269
7.254
7.245
7.242
7.239
7.228
7.220
7.173
7.158
7.142
7.091
7.074
6.939
6.917
6.908
6.886
6.620
6.598
6.505
6.474
1.553
0.000
6.01
3.95
3.25
4.16
2.11
1.12
1.01
1.00
f1 (ppm)
O
OH
Ph
Ph
I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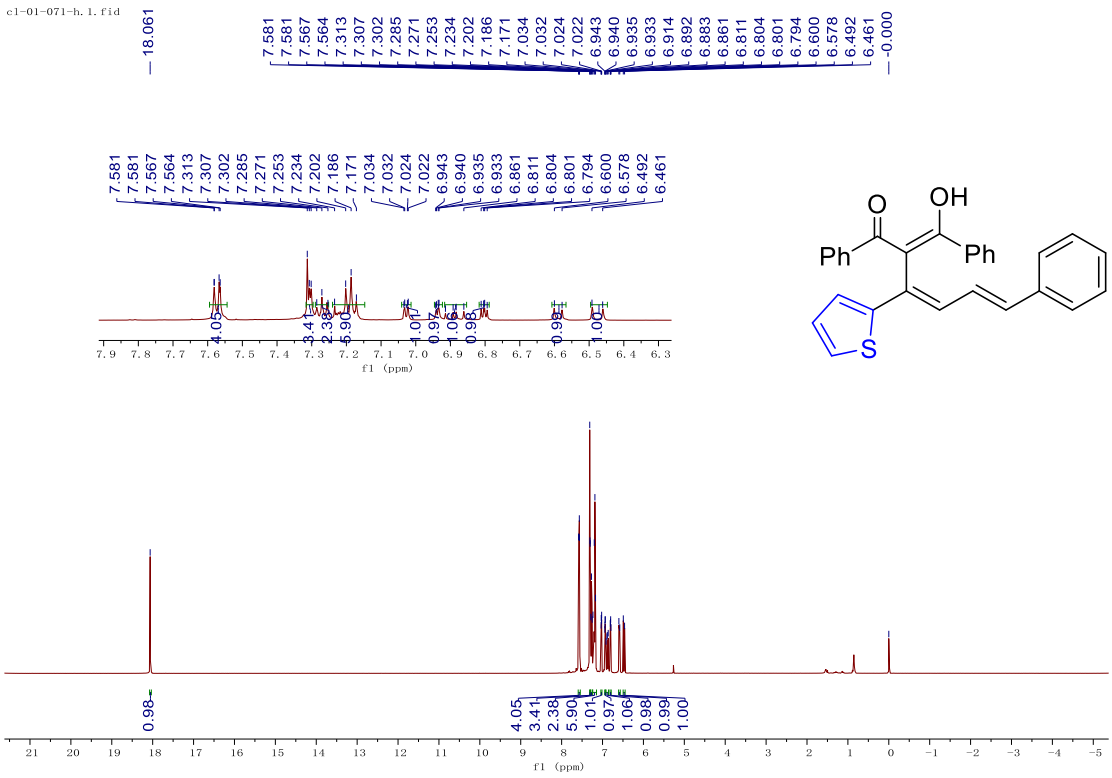
135.496
131.861
130.790
128.668
128.056
128.031
127.785
127.391
126.565
125.988
108.917
92.909
77.253
77.000
76.746
f1 (ppm)
O
OH
Ph
Ph
I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7.581
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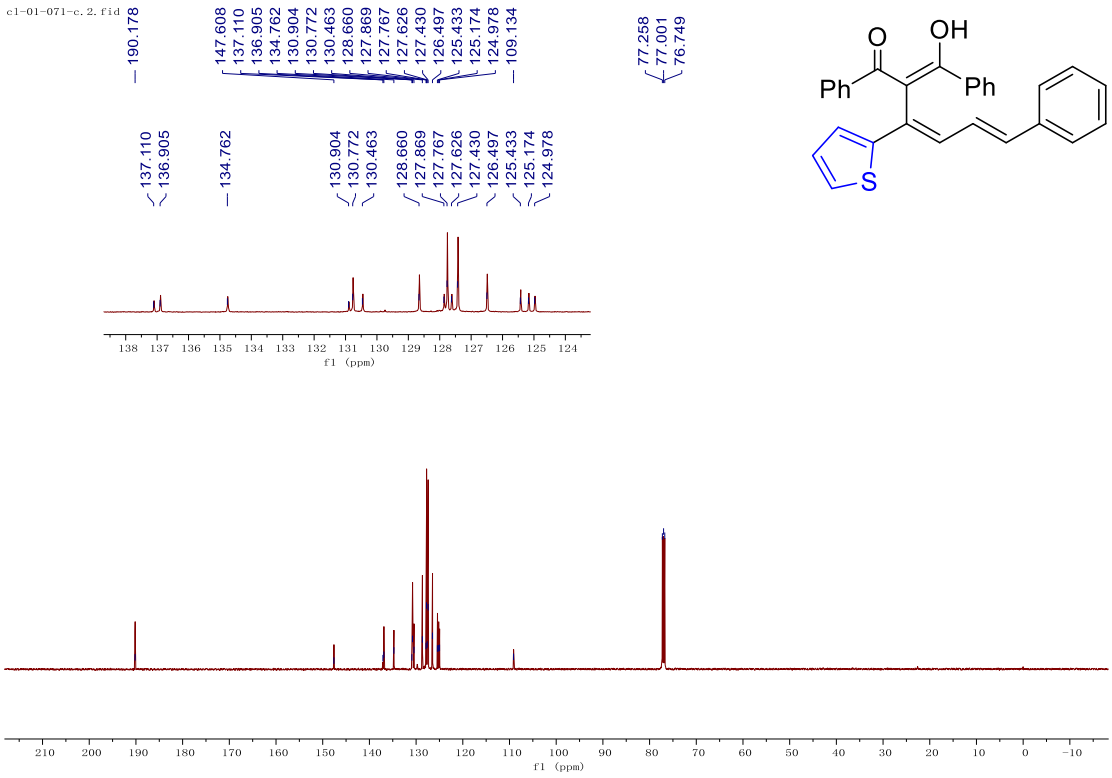
7.307
7.302
7.285
7.271
7.253
7.234
7.202
7.186
7.171
7.034
7.032
7.024
7.022
6.943
6.940
6.935
6.933
6.861
6.811
6.804
6.801
6.794
6.600
6.578
6.492
6.461
-0.000
4.05
3.41
2.38
5.90
1.01
0.97
1.06
0.98
0.99
1.00
f1 (ppm)
O
OH
Ph
Ph
S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137.110
136.905
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130.463
128.660
127.869
127.767
127.626
127.430
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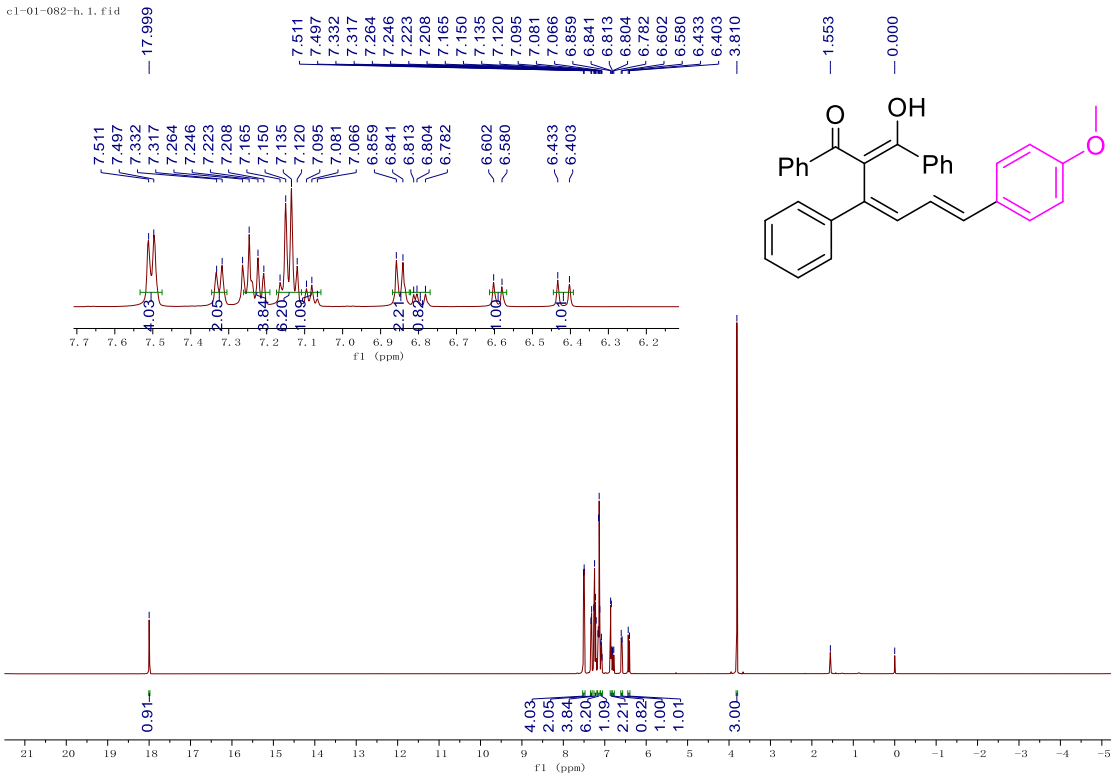
125.433
125.174
124.978
109.134
77.258
77.001
76.749
f1 (ppm)
O
OH
Ph
Ph
S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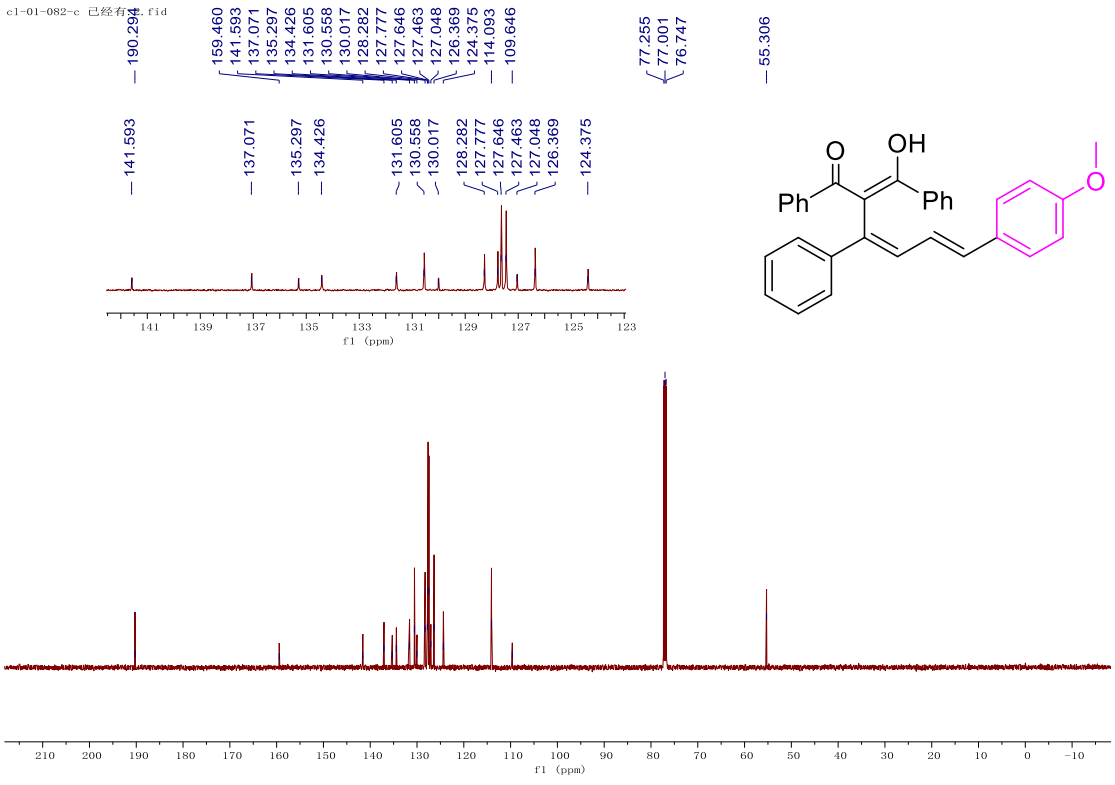
7.497
7.332
7.317
7.264
7.246
7.223
7.208
7.165
7.150
7.135
7.120
7.095
7.081
7.066
6.859
6.841
6.813
6.804
6.782
6.602
6.580
6.433
6.403
3.810
1.553
0.000
O
OH
Ph
Ph
O
4.03
2.05
3.84
6.20
1.09
2.21
0.82
1.00
1.01
3.00
0.91
f1 (ppm)


c1-01-082-c 已经有4.fid
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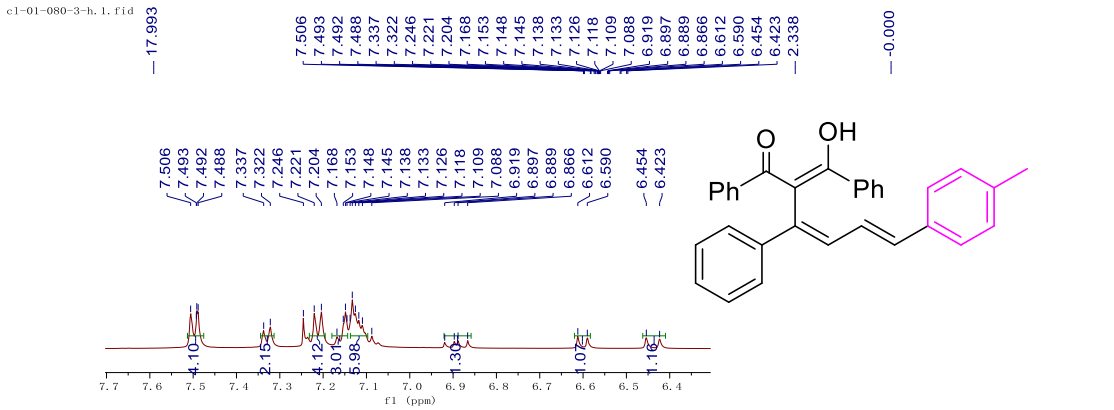
159.460
141.593
137.071
135.297
134.426
131.605
130.558
130.017
128.282
127.777
127.646
127.463
127.048
126.369
124.375
114.093
109.646
77.255
77.001
76.747
55.306
O
OH
Ph
Ph
O
f1 (ppm)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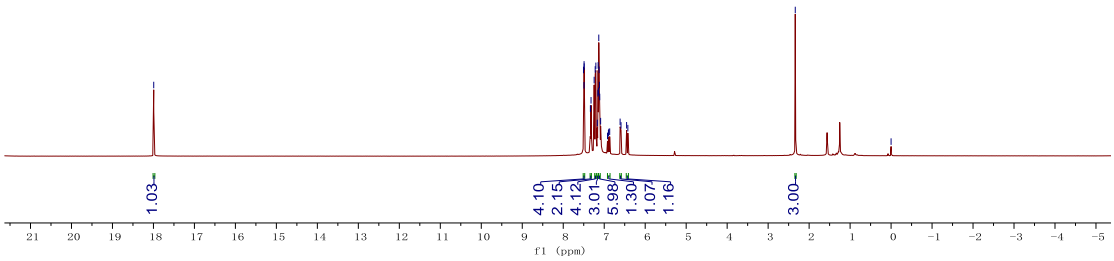
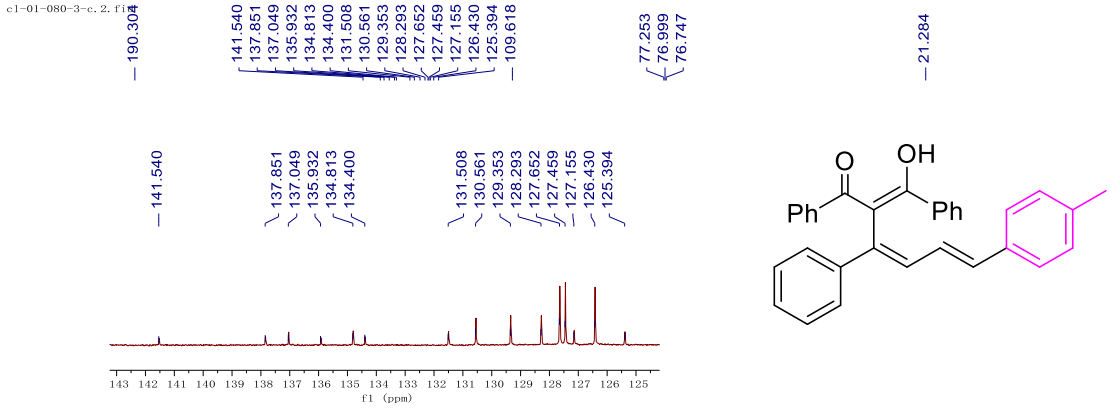
7.493
7.492
7.488
7.337
7.322
7.246
7.221
7.204
7.168
7.153
7.148
7.145
7.138
7.133
7.126
7.118
7.109
7.088
6.919
6.897
6.889
6.866
6.612
6.590
6.454
6.423
2.338
-0.000
O
OH
Ph
Ph
4.10
2.15
4.12
3.01
5.98
1.30
1.07
1.16
f1 (ppm)


1.03
4.10
2.15
4.12
3.01
5.98
1.30
1.07
1.16
3.00
f1 (ppm)


c1-01-080-3-c.2.fid
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137.049
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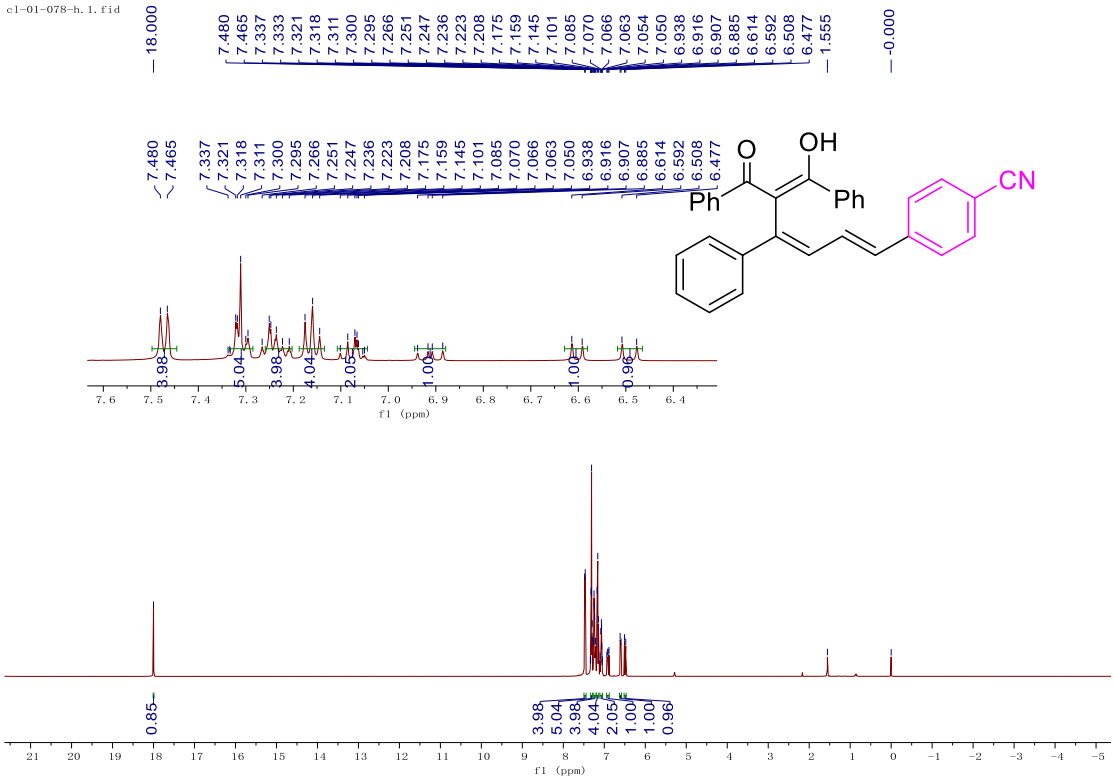
134.400
131.508
130.561
129.353
128.293
127.652
127.459
127.155
126.430
125.394
109.618
77.253
76.999
76.747
21.284
O
OH
Ph
Ph
f1 (ppm)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7.465
7.337
7.321
7.318
7.311
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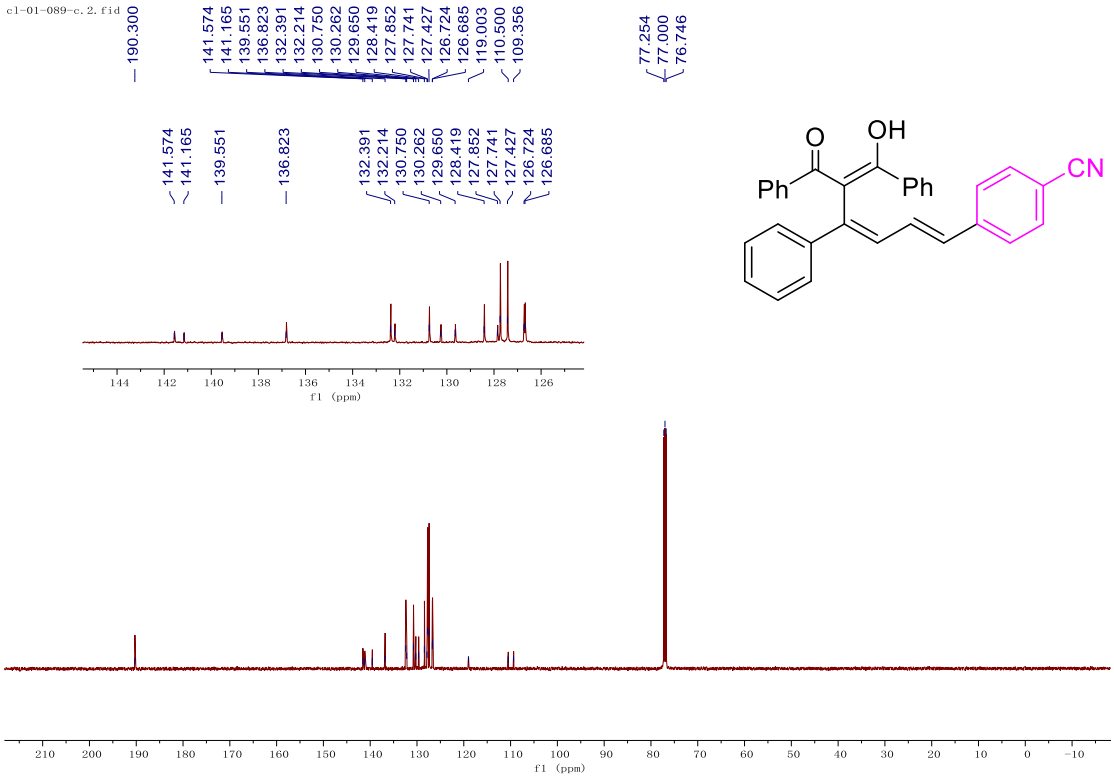
7.266
7.251
7.247
7.236
7.223
7.208
7.175
7.159
7.145
7.101
7.085
7.070
7.066
7.063
7.050
6.938
6.916
6.907
6.885
6.614
6.592
6.508
6.477
1.555
-0.000
O
OH
Ph
Ph
CN
3.98
5.04
3.98
4.04
2.05
1.00
1.00
0.96
f1 (ppm)
0.85
3.98
5.04
3.98
4.04
2.05
1.00
1.00
0.96
f1 (ppm)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139.551
136.823
132.391
132.214
130.750
130.262
129.650
128.419
127.852
127.741
127.427
126.724
126.685
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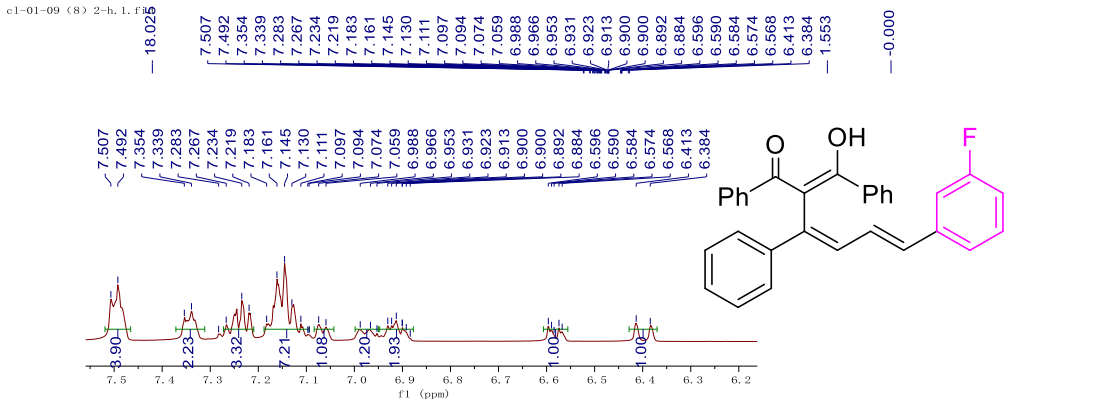
109.356
77.254
77.000
76.746
O
OH
Ph
Ph
CN
f1 (ppm)
f1 (ppm)


c1-01-09 (8) 2-h.1.fid
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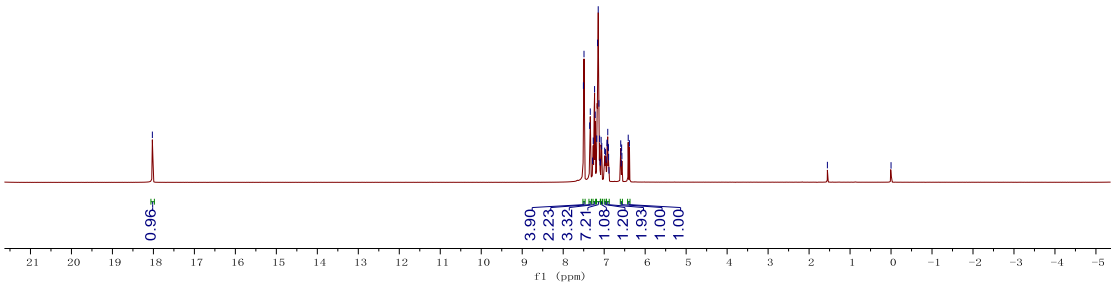
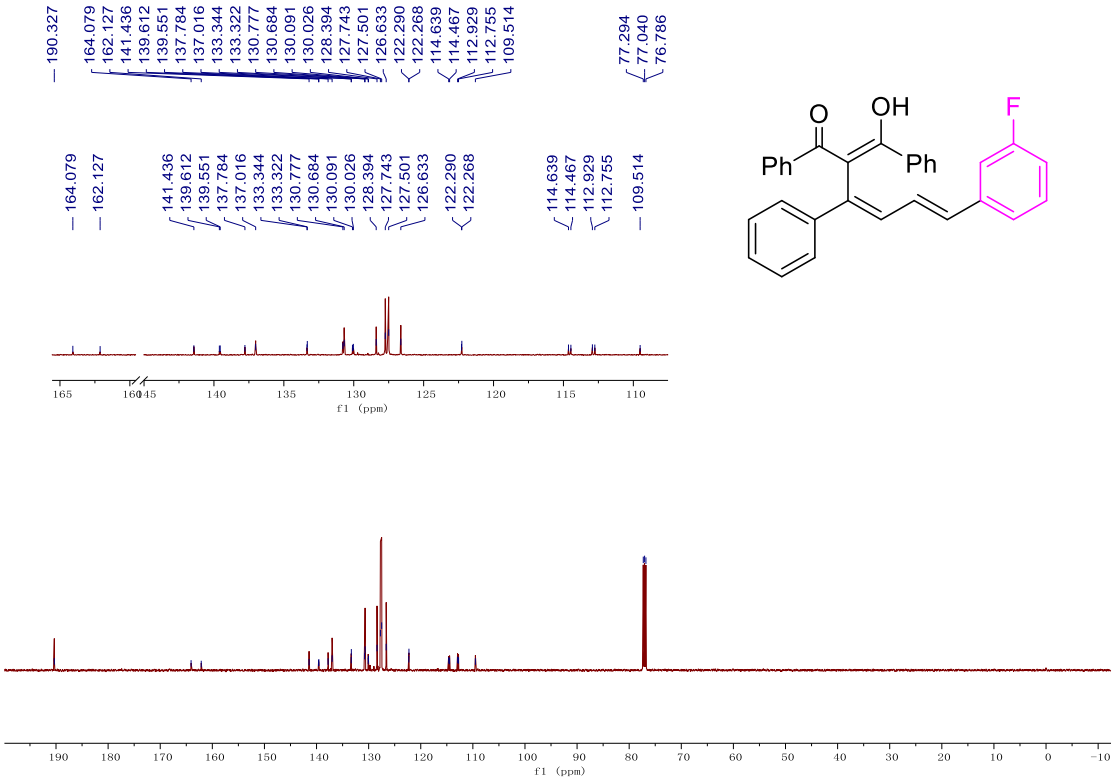
7.283
7.267
7.234
7.219
7.183
7.161
7.145
7.130
7.111
7.097
7.094
7.074
7.059
6.988
6.966
6.953
6.931
6.923
6.913
6.900
6.900
6.892
6.884
6.596
6.590
6.584
6.574
6.568
6.413
6.384
1.553
-0.000
O
OH
F
Ph
Ph
3.90
2.23
3.32
7.21
1.08
1.20
1.93
1.00
1.00
f1 (ppm)


0.96
3.90
2.23
3.32
7.21
1.08
1.20
1.93
1.00
1.00
f1 (ppm)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139.551
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137.016
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133.322
130.777
130.684
130.091
130.026
128.394
127.743
127.501
126.633
122.290
122.268
114.639
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112.755
109.514
77.294
77.040
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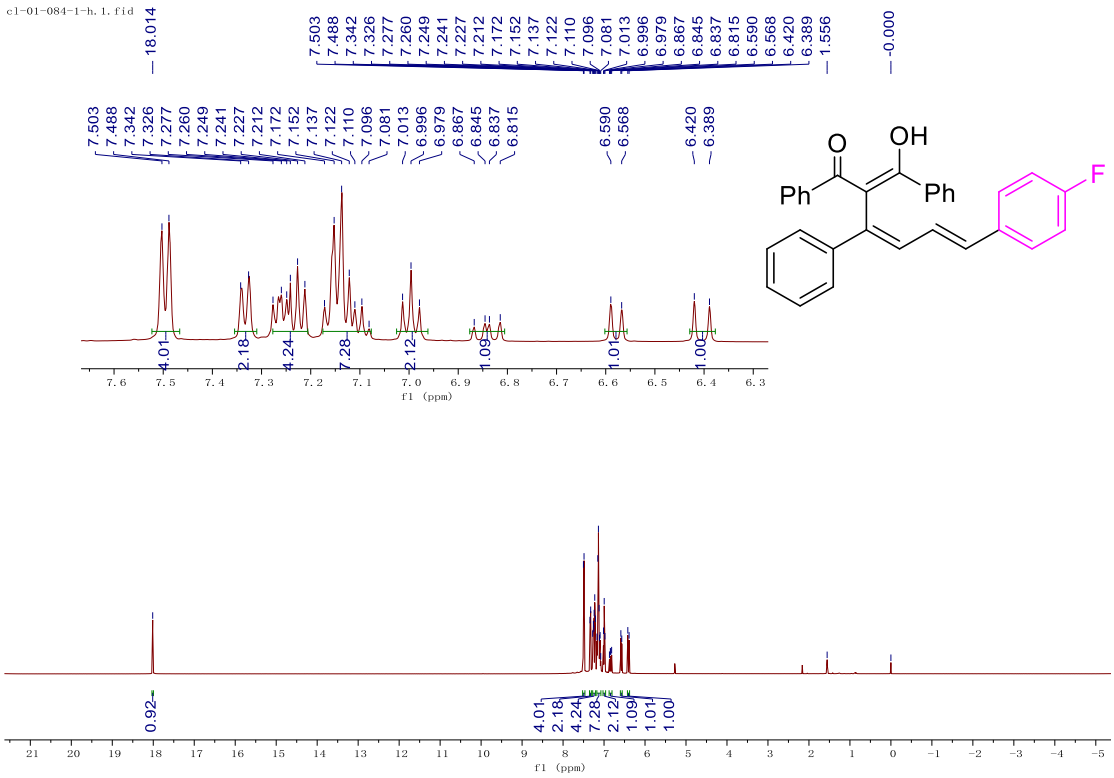
O
OH
F
Ph
Ph
f1 (ppm)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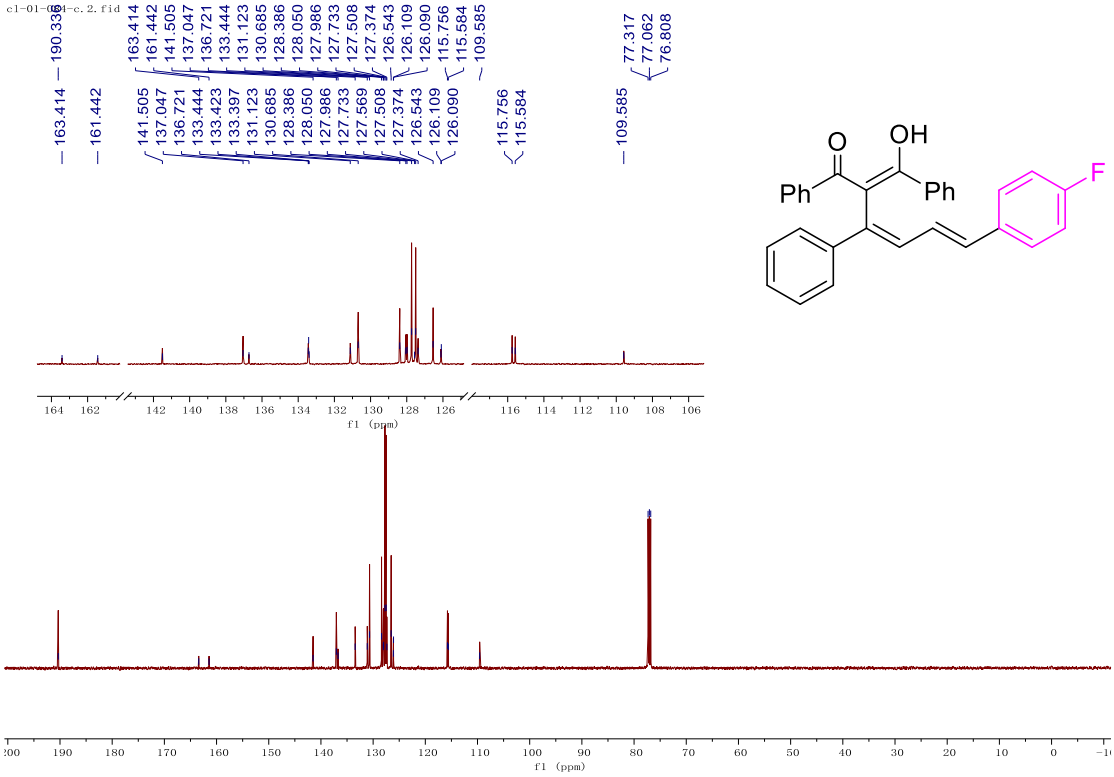
7.260
7.249
7.241
7.227
7.212
7.172
7.152
7.137
7.122
7.110
7.096
7.081
7.013
6.996
6.979
6.867
6.845
6.837
6.815
6.590
6.568
6.420
6.389
1.556
-0.000
4.01
2.18
4.24
7.28
2.12
1.09
1.01
1.00
f1 (ppm)
O
OH
Ph
Ph
F
0.92
4.01
2.18
4.24
7.28
2.12
1.09
1.01
1.00
f1 (ppm)


cl-01-084-c.2.fid
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133.423
133.397
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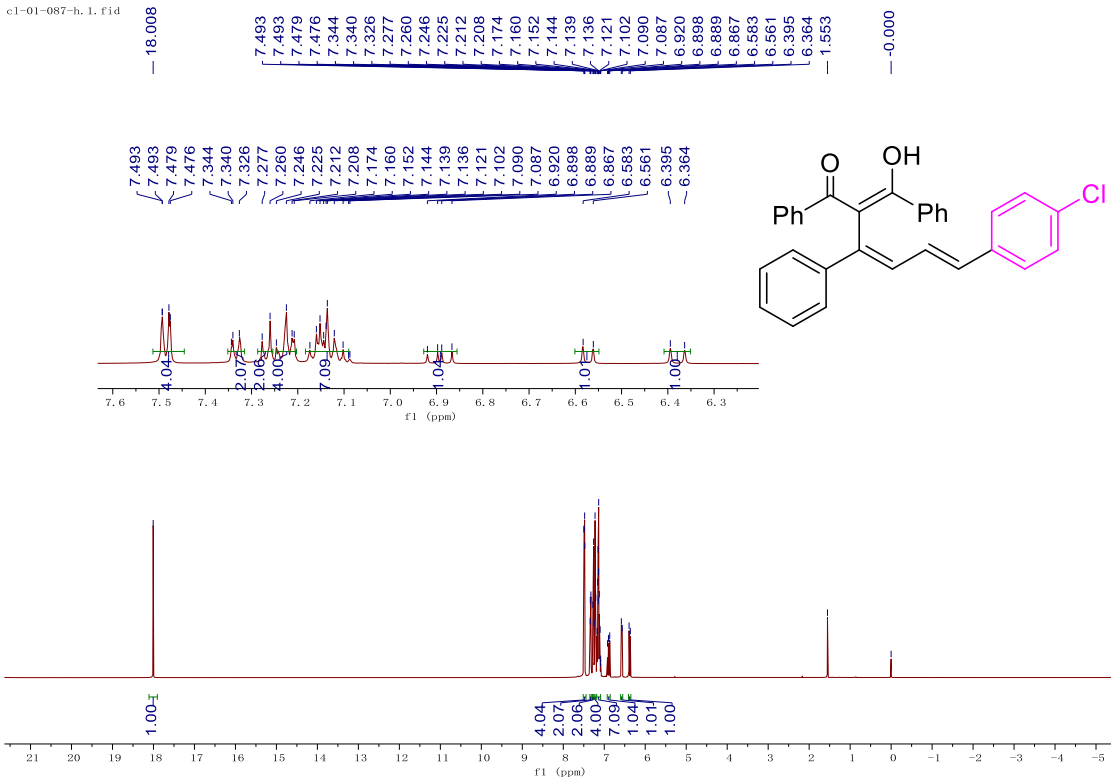
130.685
128.386
128.050
127.986
127.733
127.569
127.508
127.374
126.543
126.109
126.090
115.756
115.584
109.585
77.317
77.062
76.808
f1 (ppm)
O
OH
Ph
Ph
F
f1 (ppm)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7.493
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7.476
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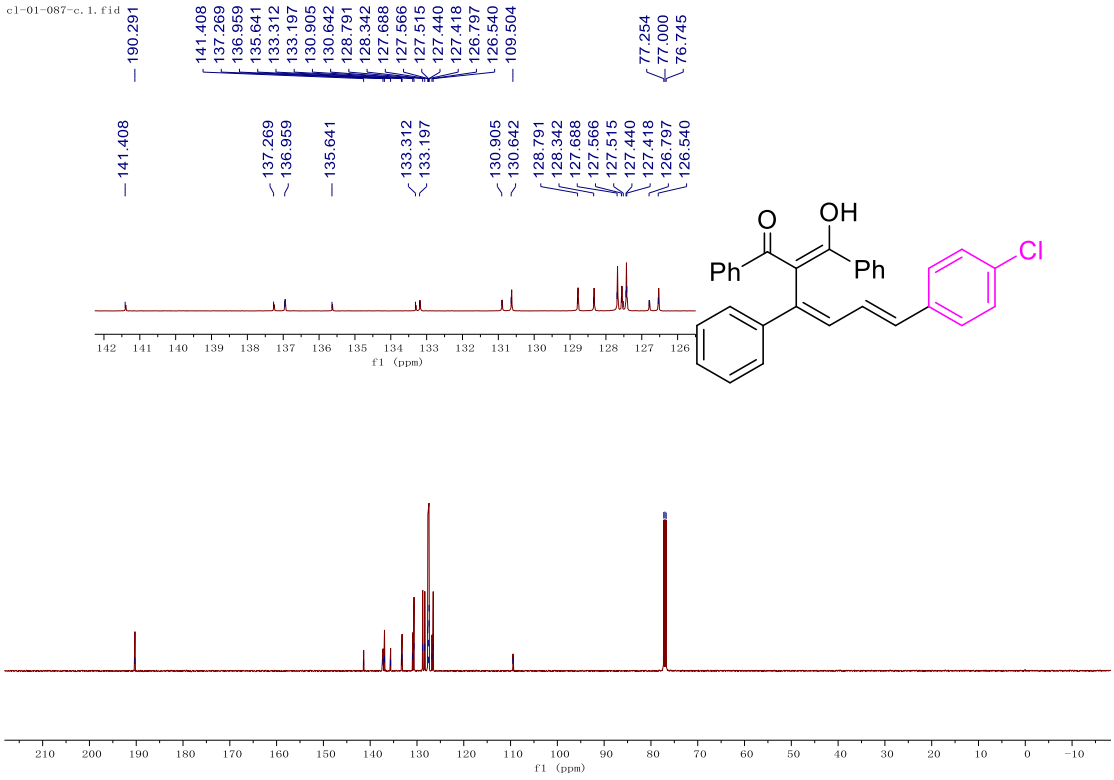
7.260
7.246
7.225
7.212
7.208
7.174
7.160
7.152
7.144
7.139
7.136
7.121
7.102
7.090
7.087
6.920
6.898
6.889
6.867
6.583
6.561
6.395
6.364
1.553
-0.000
4.04
2.07
2.06
4.00
7.09
1.04
1.01
1.00
f1 (ppm)
O
OH
Ph
Ph
Cl

1.00
4.04
2.07
2.06
4.00
7.09
1.04
1.01
1.00
f1 (ppm)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127.566
127.515
127.440
127.418
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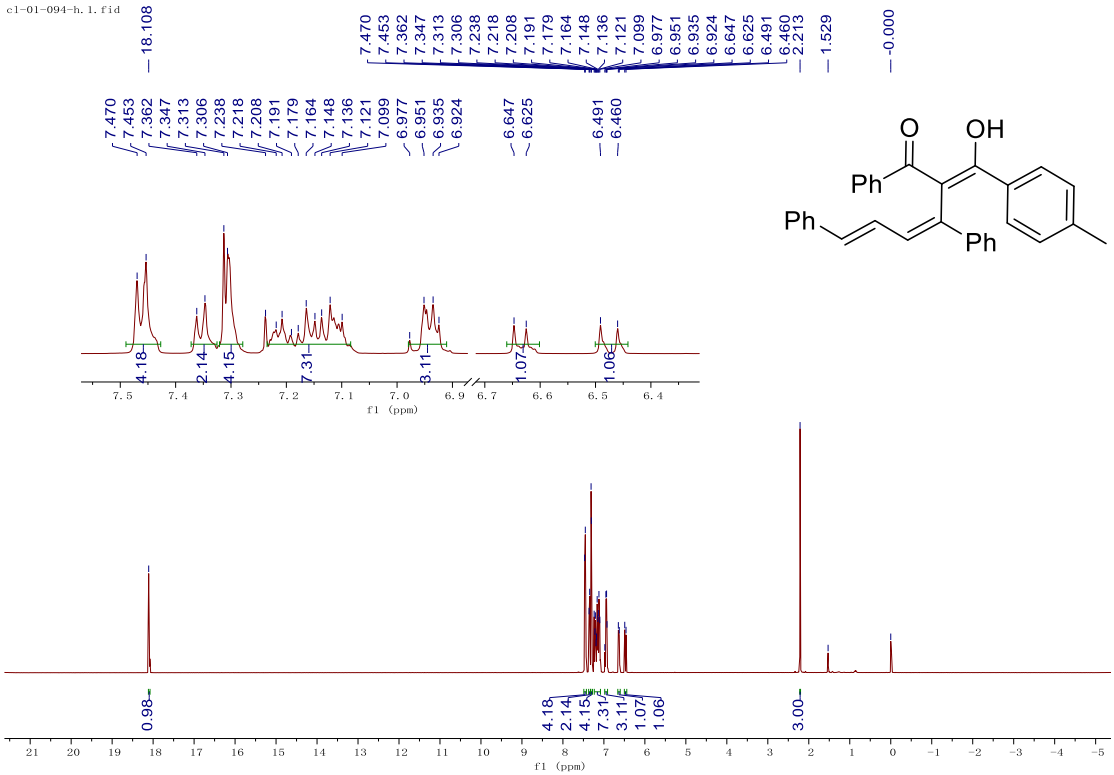
109.504
77.254
77.000
76.745
f1 (ppm)
O
OH
Ph
Ph
Cl

f1 (ppm)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7.208
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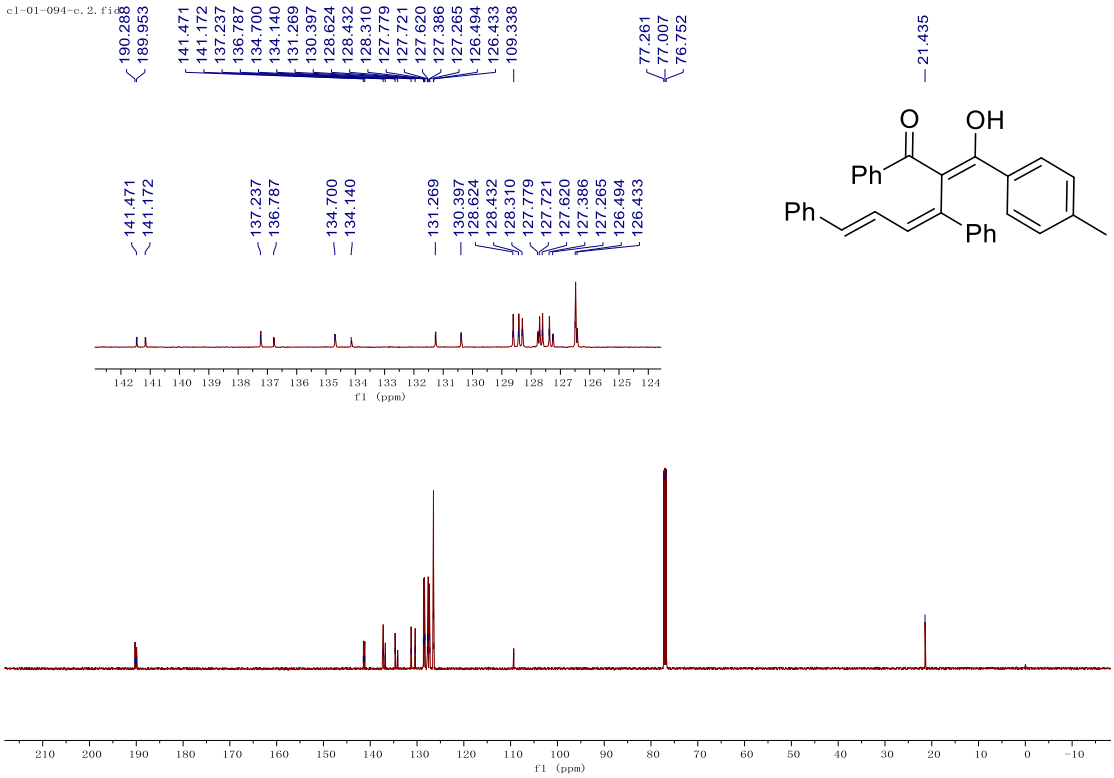
7.179
7.164
7.148
7.136
7.121
7.099
6.977
6.951
6.935
6.924
6.647
6.625
6.491
6.460
2.213
1.529
-0.000
4.18
2.14
4.15
7.31
3.11
1.07
1.06
f1 (ppm)
O
OH
Ph
Ph
Ph

0.98
4.18
2.14
4.15
7.31
3.11
1.07
1.06
3.00
f1 (ppm)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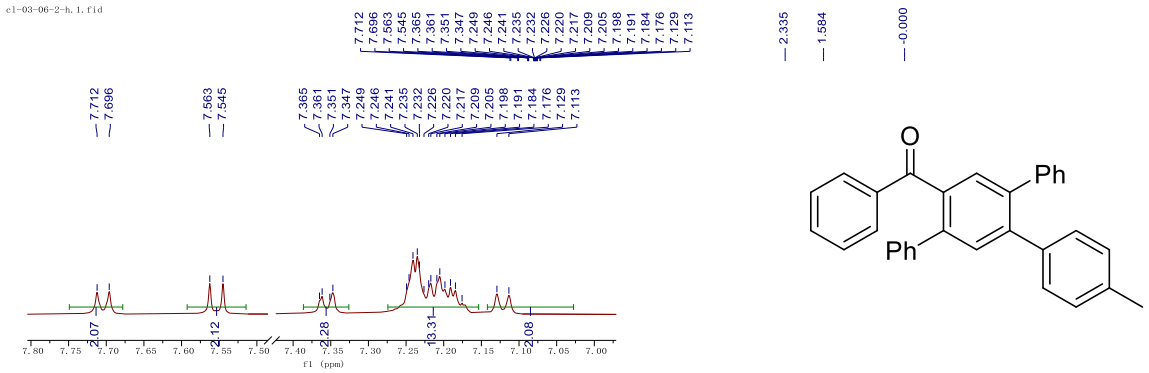
141.471
141.172
137.237
136.787
134.700
134.140
131.269
130.397
128.624
128.432
128.310
127.779
127.721
127.620
127.386
127.265
126.494
126.433
109.338
77.261
77.007
76.752
21.435
f1 (ppm)
O
OH
Ph
Ph
Ph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7.545
7.365
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7.351
7.347
7.249
7.246
7.241
7.235
7.232
7.226
7.220
7.217
7.209
7.205
7.198
7.191
7.184
7.176
7.129
7.113
2.335
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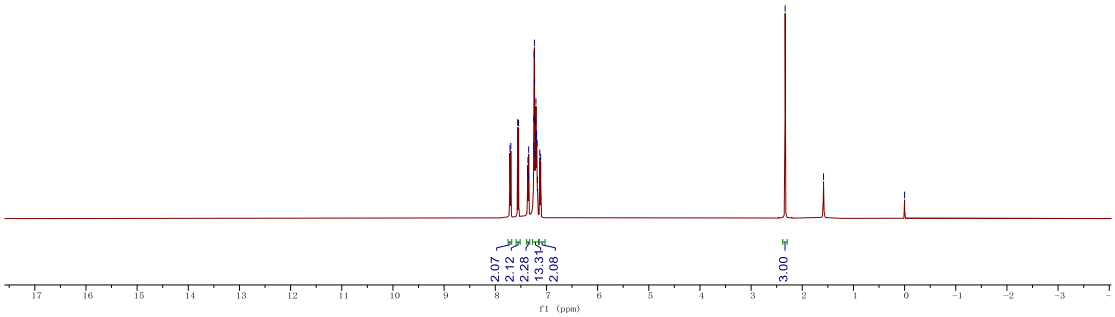
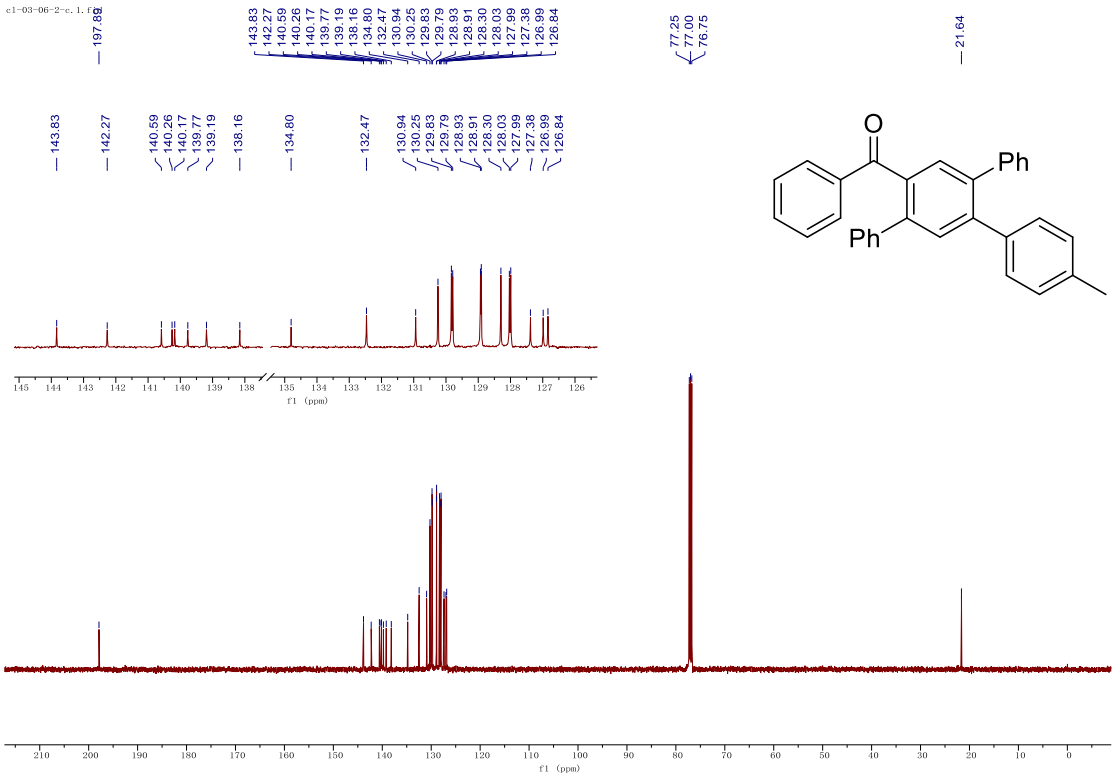
-0.000
O
Ph
Ph
2.07
2.12
2.28
13.31
2.08
f1 (ppm)


2.07
2.12
2.28
13.31
2.08
3.00
f1 (ppm)


c1-03-06-2-c.1.fid
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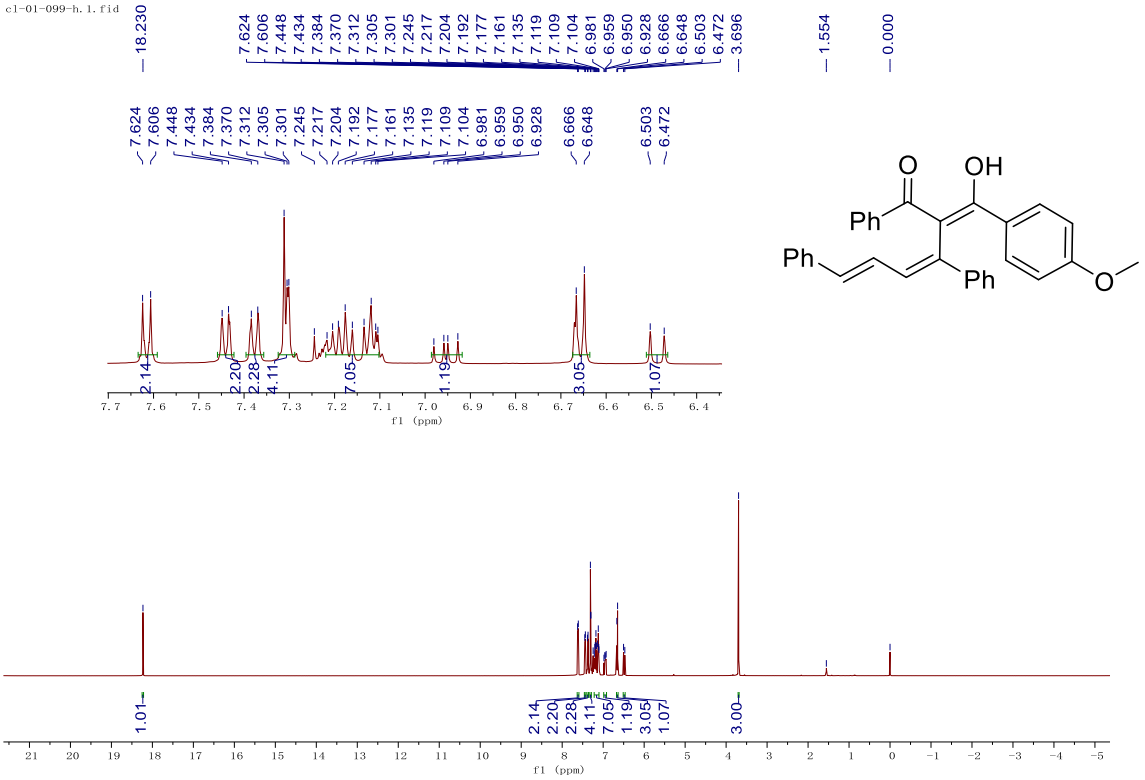
142.27
140.59
140.26
140.17
139.77
139.19
138.16
134.80
132.47
130.94
130.25
129.83
129.79
128.93
128.91
128.30
128.03
127.99
127.38
126.99
126.84
77.25
77.00
76.75
21.64
O
Ph
Ph
f1 (ppm)


c1-01-099-h.1.fid
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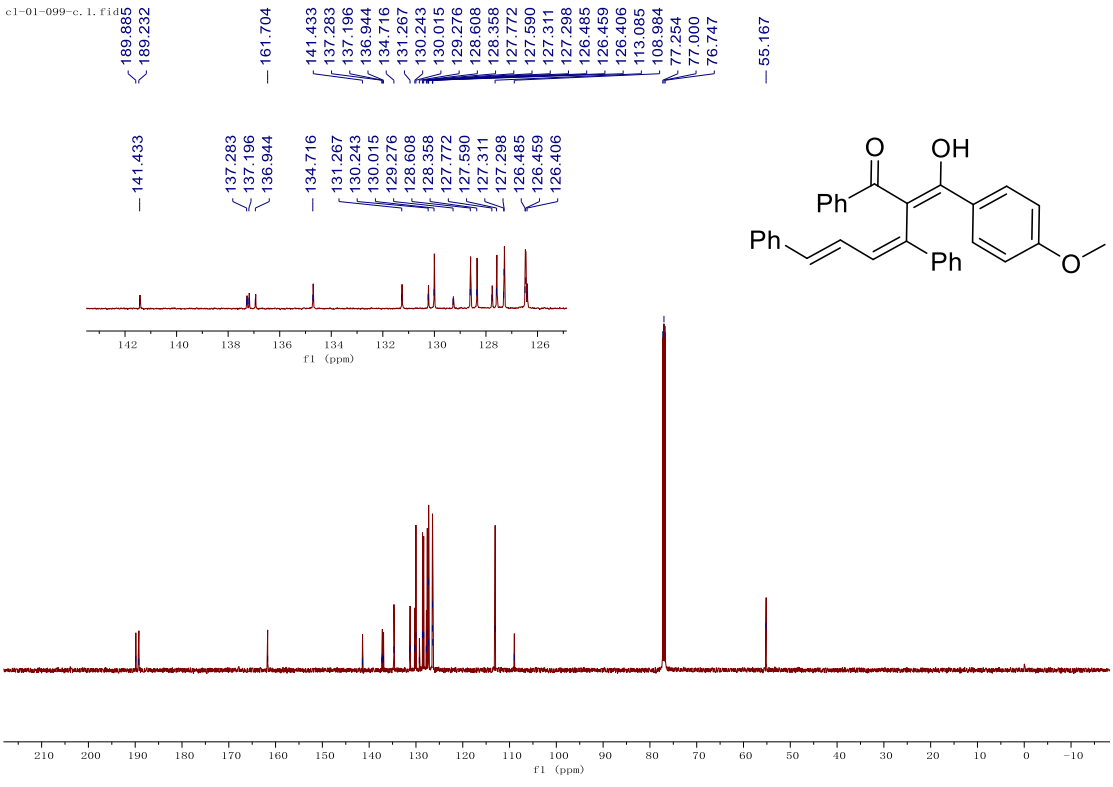
7.624
7.606
7.448
7.434
7.384
7.370
7.312
7.305
7.301
7.245
7.217
7.204
7.192
7.177
7.161
7.135
7.119
7.109
7.104
6.981
6.959
6.950
6.928
6.666
6.648
6.503
6.472
3.696
1.554
0.000
2.14
2.20
2.28
4.11
7.05
1.19
3.05
1.07
f1 (ppm)
O
OH
Ph
Ph
Ph
O
1.01
2.14
2.20
2.28
4.11
7.05
1.19
3.05
1.07
3.00
f1 (ppm)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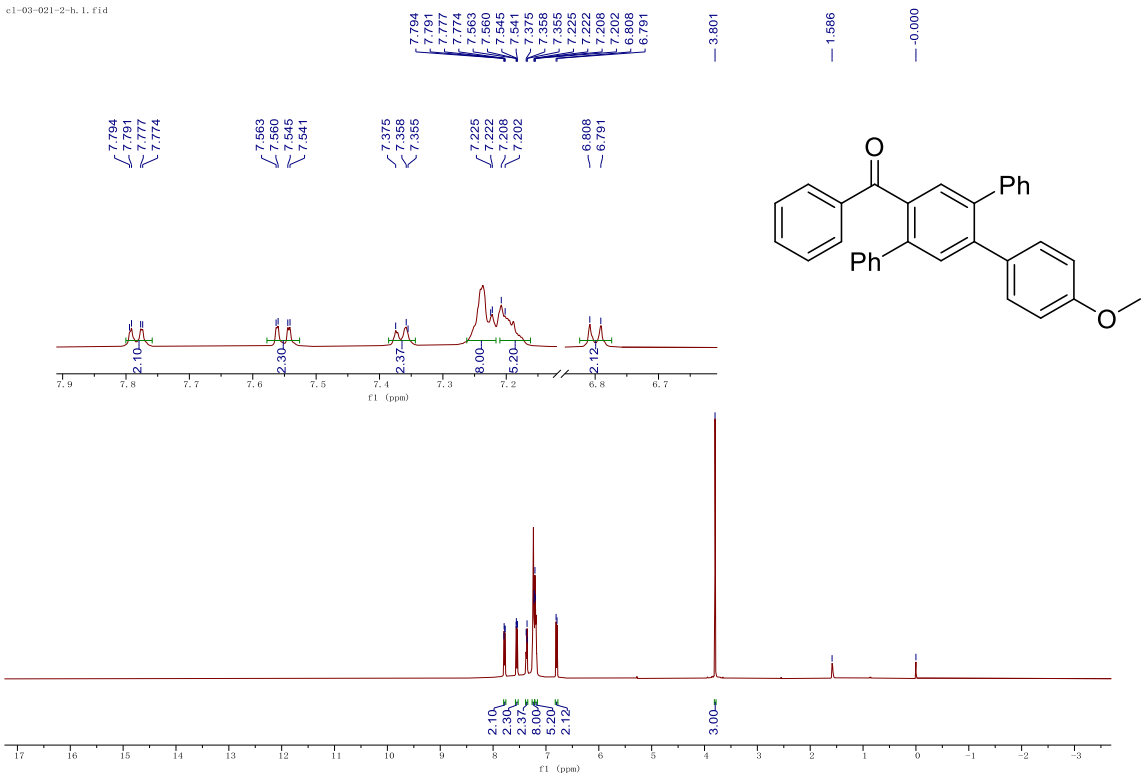
189.232
161.704
141.433
137.283
137.196
136.944
134.716
131.267
130.243
130.015
129.276
128.608
128.358
127.772
127.590
127.311
127.298
126.485
126.459
126.406
113.085
108.984
77.254
77.000
76.747
55.167
f1 (ppm)
O
OH
Ph
Ph
Ph
O
f1 (ppm)


c1-03-021-2-h.1.fid
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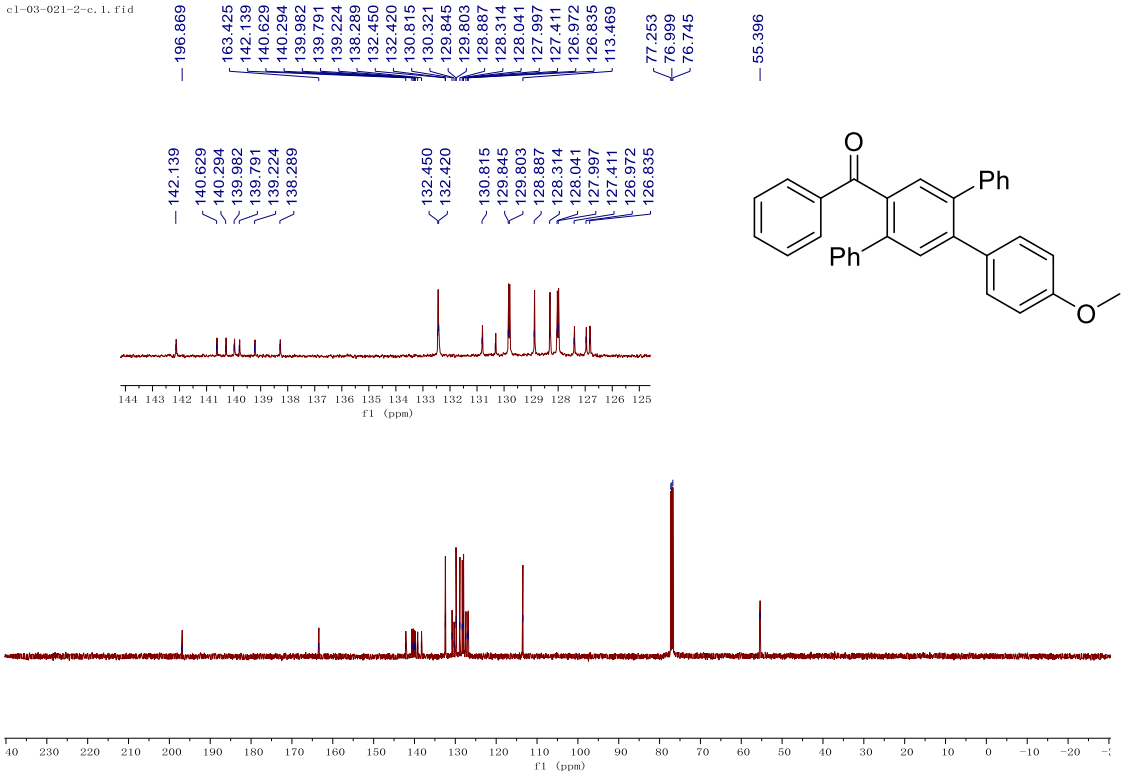
7.791
7.777
7.774
7.563
7.560
7.545
7.541
7.375
7.358
7.355
7.225
7.222
7.208
7.202
6.808
6.791
3.801
1.586
-0.000
O
Ph
Ph
O
2.10
2.30
2.37
8.00
5.20
2.12
3.00
f1 (ppm)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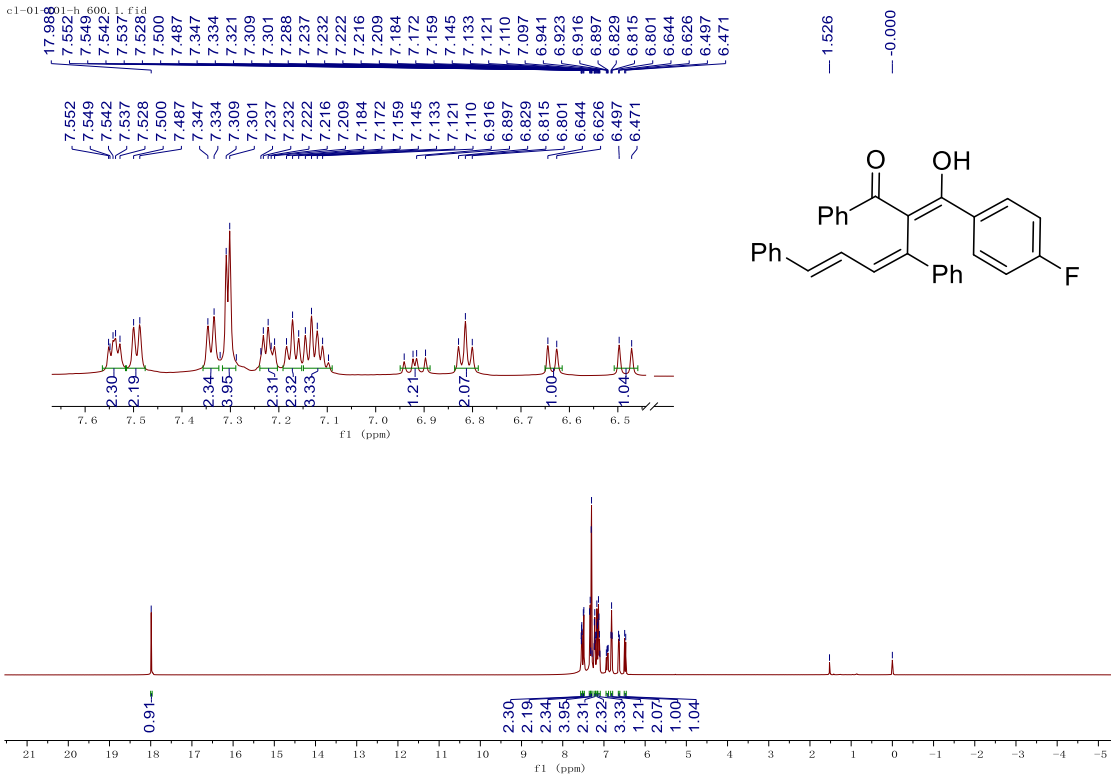
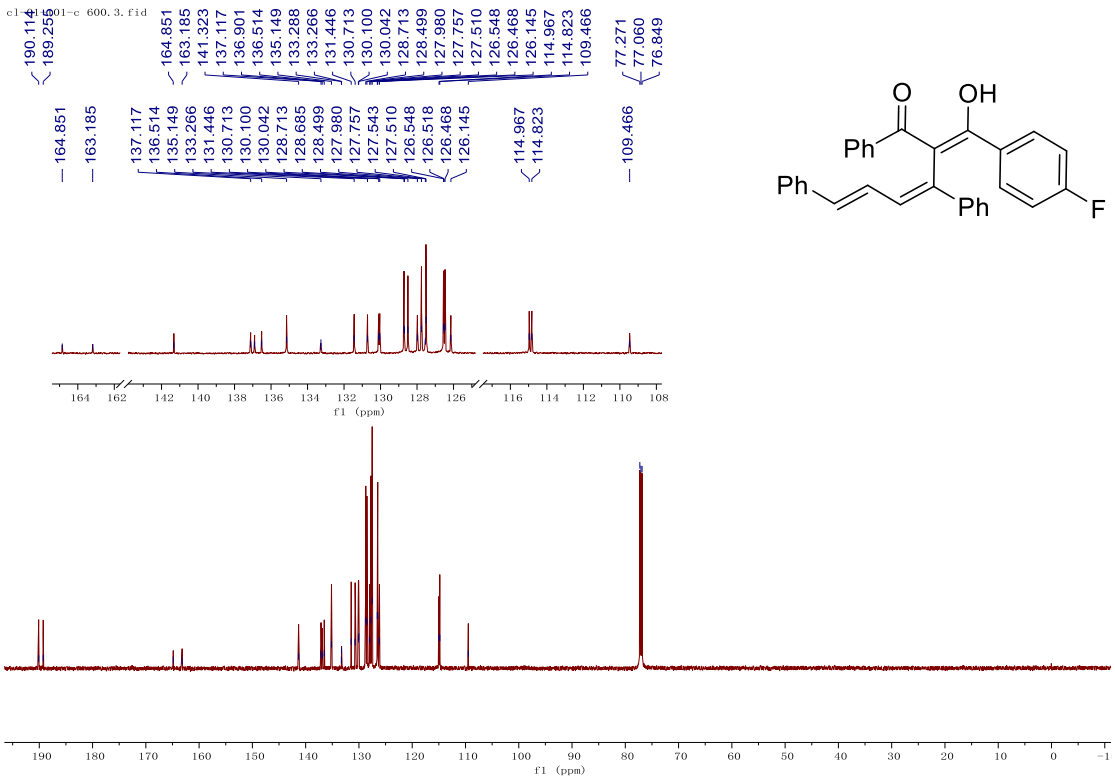
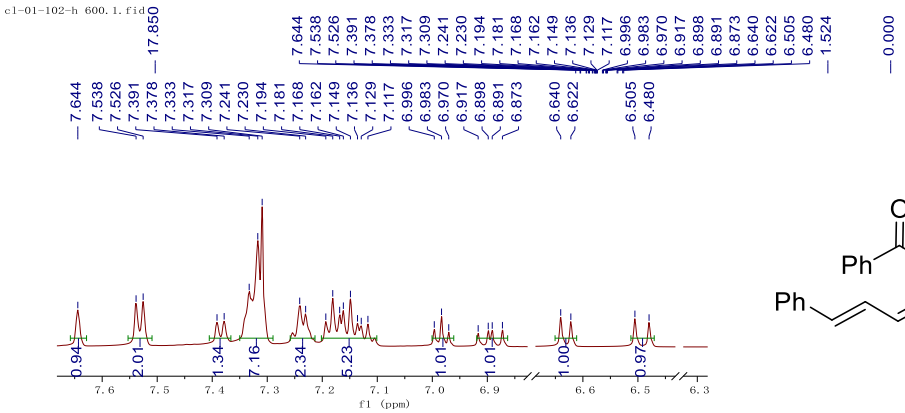
163.425
142.139
140.629
140.294
139.982
139.791
139.224
138.289
132.450
132.420
130.815
130.321
129.845
129.803
128.887
128.314
128.041
127.997
127.411
126.972
126.835
113.469
77.253
76.999
76.745
55.396
O
Ph
Ph
O
f1 (ppm)


O
OH
Ph
Ph
Ph
F
f1 (ppm)


O
OH
Ph
Ph
Ph
F
f1 (ppm)


c1-01-102-h 600.1.fid
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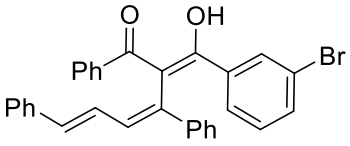
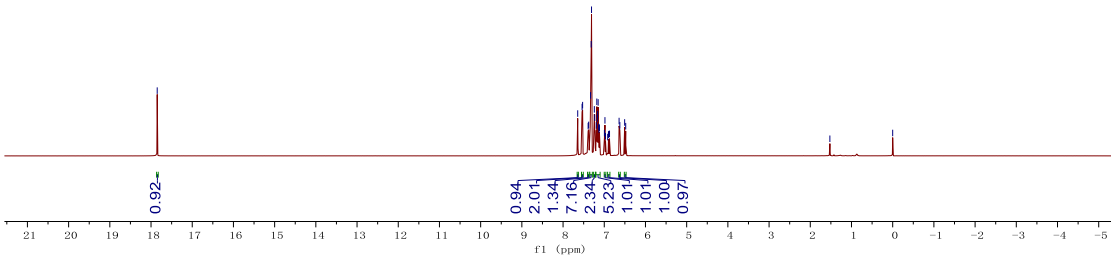
7.538
7.526
7.391
7.378
7.333
7.317
7.309
7.241
7.230
7.194
7.181
7.168
7.162
7.149
7.136
7.129
7.117
6.996
6.983
6.970
6.917
6.898
6.891
6.873
6.640
6.622
6.505
6.480
1.524
0.000
0.94
2.01
1.34
7.16
2.34
5.23
1.01
1.01
1.00
0.97
f1 (ppm)


O
OH
Ph
Br
Ph
Ph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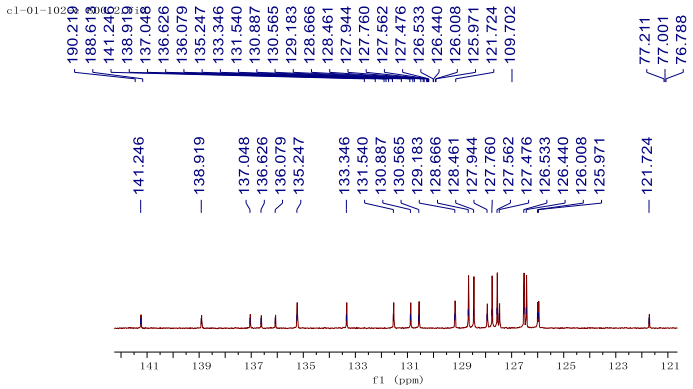
0.94
2.01
1.34
7.16
2.34
5.23
1.01
1.01
1.00
0.97
f1 (ppm)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188.613
141.246
138.919
137.048
136.626
136.079
135.247
133.346
131.540
130.887
130.565
129.183
128.666
128.461
127.944
127.760
127.562
127.476
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126.008
125.971
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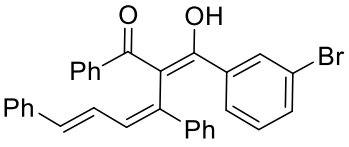
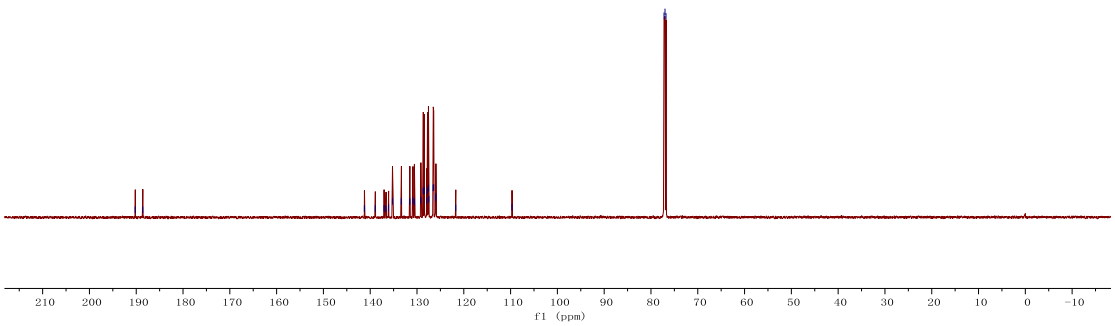
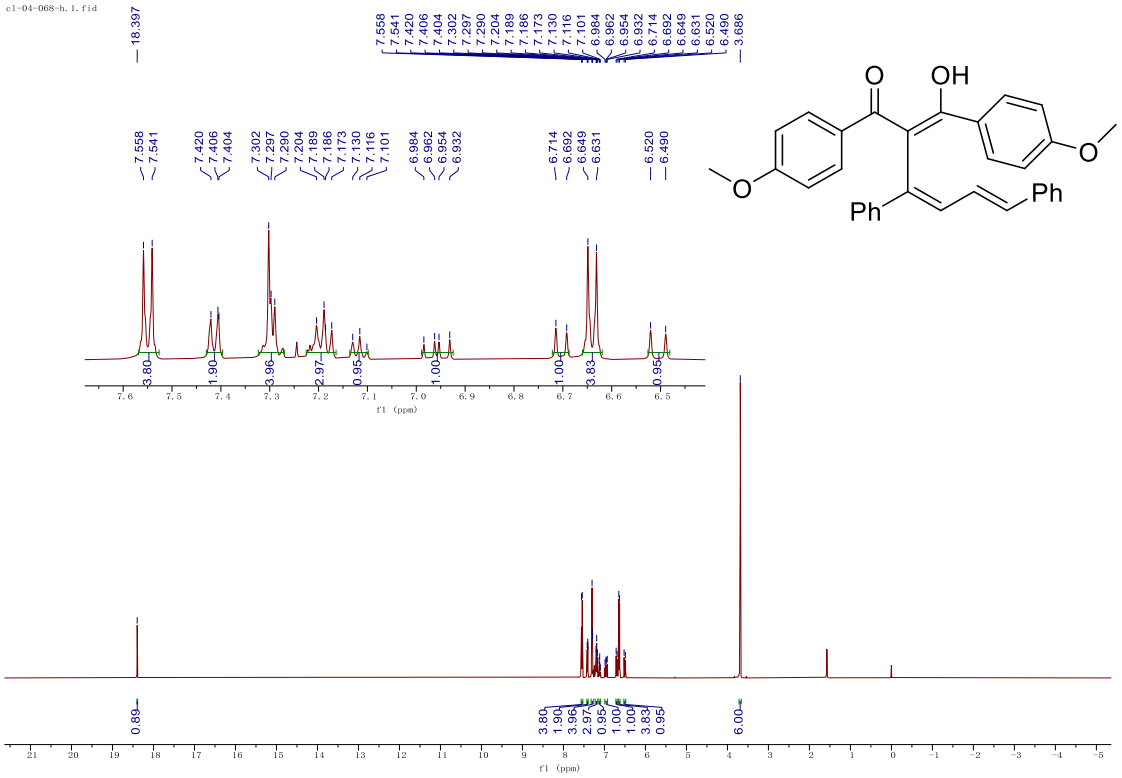
109.702
77.211
77.001
76.788
f1 (ppm)


O
OH
Ph
Br
Ph
Ph


f1 (ppm)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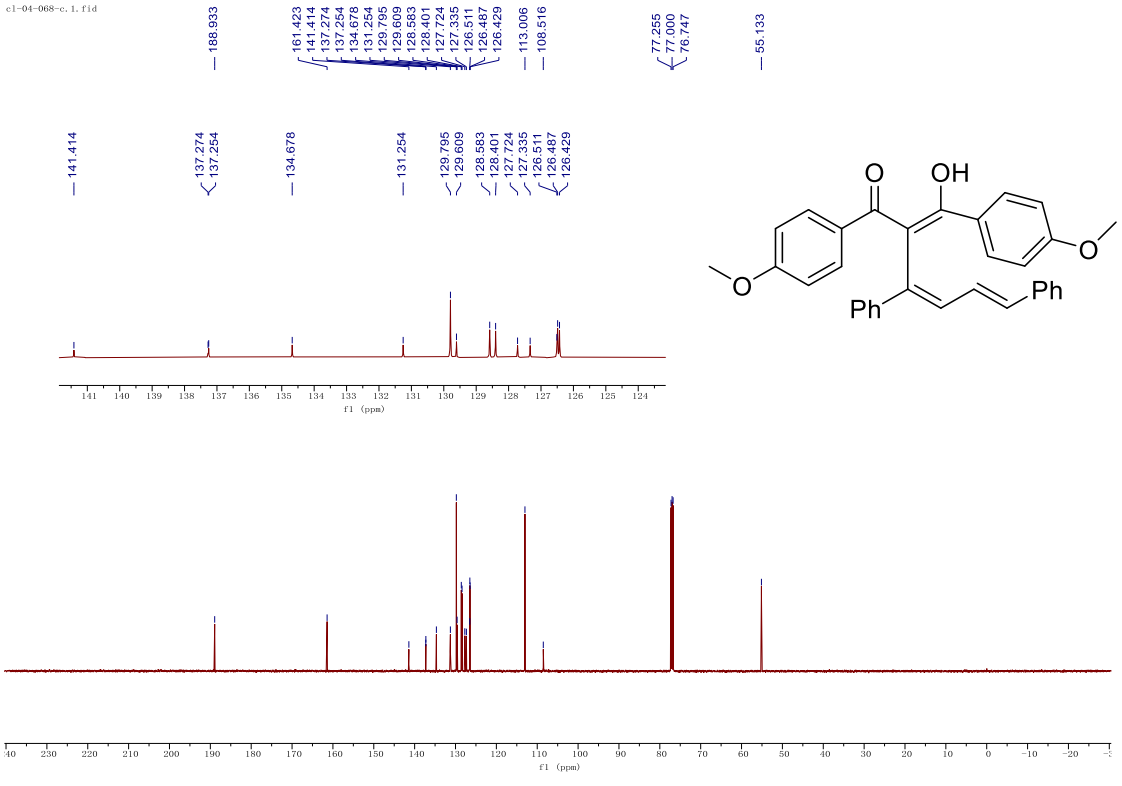
7.406
7.404
7.302
7.297
7.290
7.204
7.189
7.186
7.173
7.130
7.116
7.101
6.984
6.962
6.954
6.932
6.714
6.692
6.649
6.631
6.520
6.490
3.686
O
OH
O
Ph
Ph
3.80
1.90
3.96
2.97
0.95
1.00
1.00
3.83
0.95
6.00
0.89
f1 (ppm)


c1-04-068-c.1.fid
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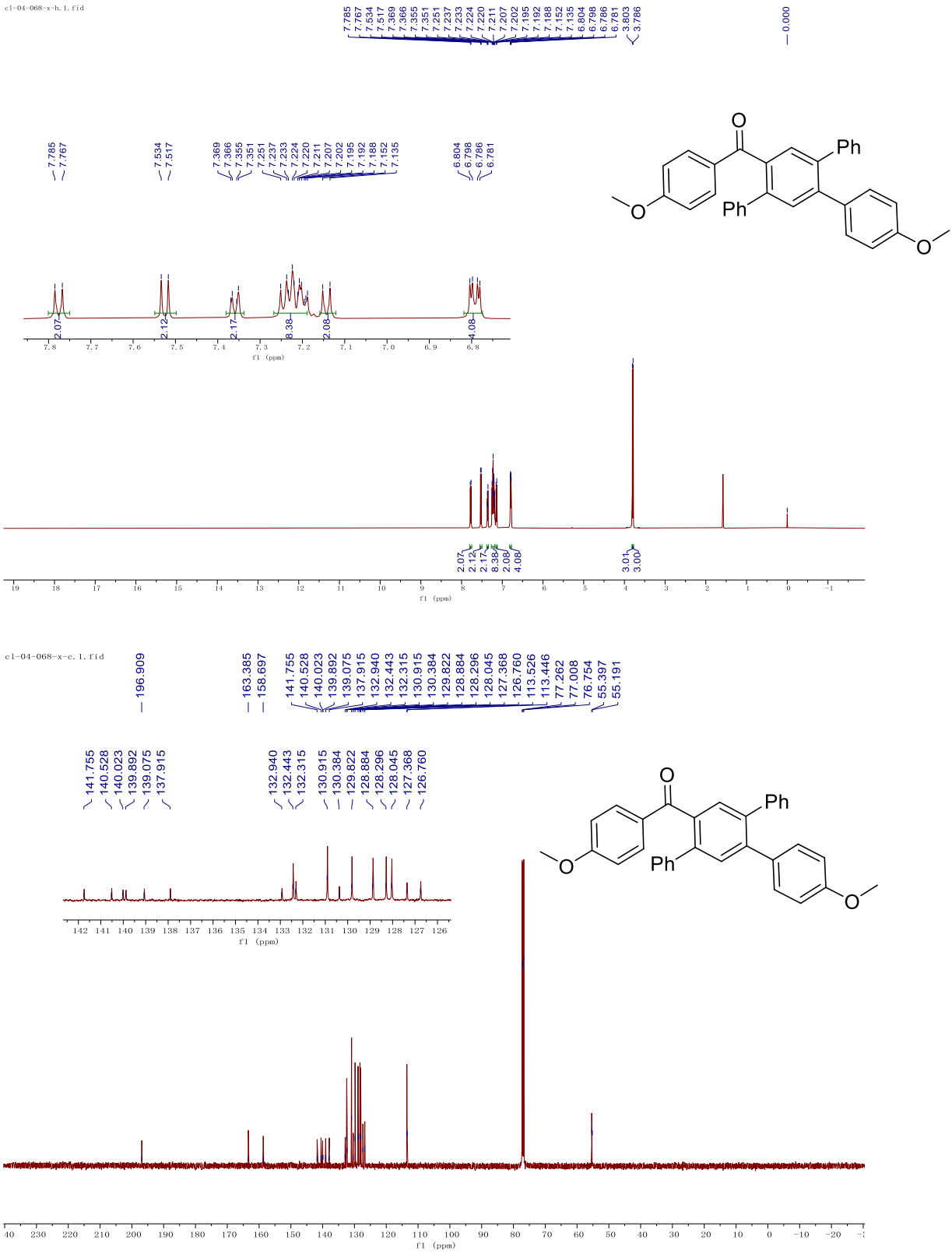
161.423
141.414
137.274
137.254
134.678
131.254
129.795
129.609
128.583
128.401
127.724
127.335
126.511
126.487
126.429
113.006
108.516
77.255
77.000
76.747
55.133
O
OH
O
Ph
Ph
f1 (ppm)


c1-04-068-x-h.1.fid
7.785
7.767
7.534
7.517
7.369
7.366
7.355
7.351
7.251
7.237
7.233
7.224
7.220
7.211
7.207
7.202
7.195
7.192
7.188
7.152
7.135
6.804
6.798
6.786
6.781
3.803
3.786
0.000
O
Ph
Ph
O
O
2.07
2.12
2.17
8.38
2.08
4.08
3.01
3.00
f1 (ppm)
c1-04-068-x-c.1.fid
196.909
163.385
158.697
141.755
140.528
140.023
139.892
139.075
137.915
132.940
132.443
132.315
130.915
130.384
129.822
128.884
128.296
128.045
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126.760
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113.446
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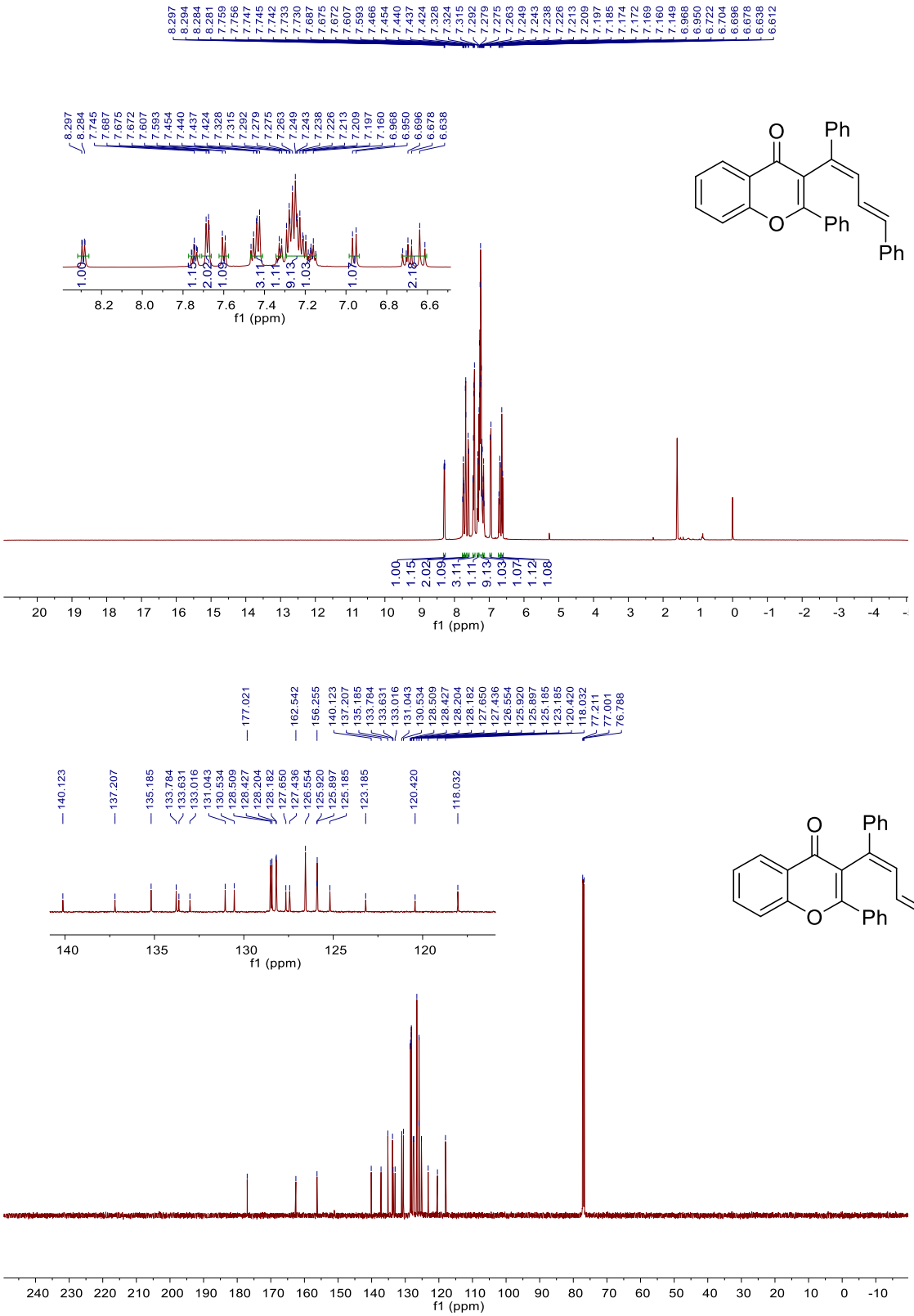
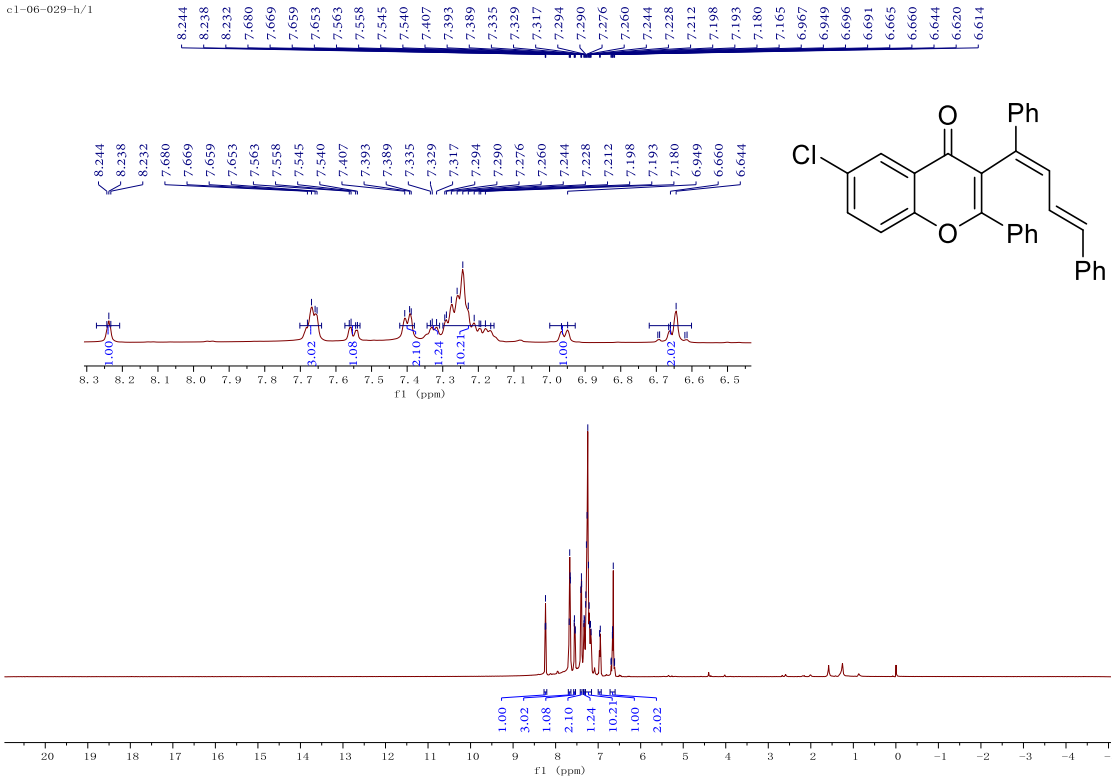
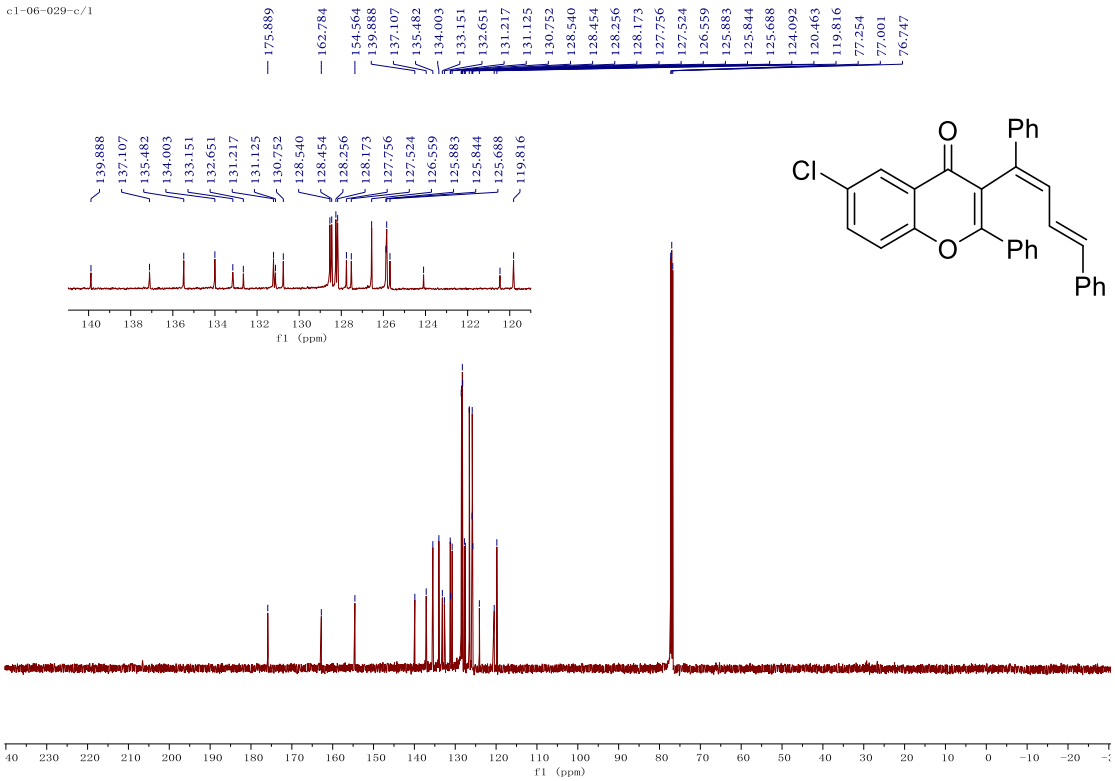
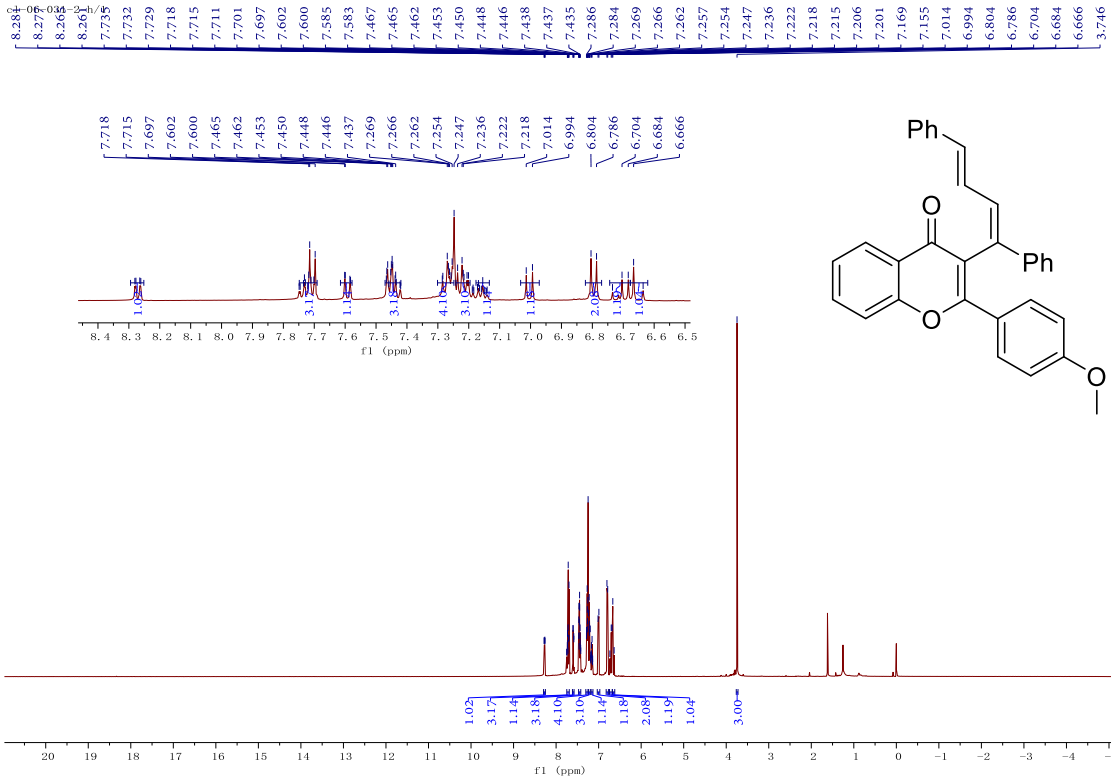
77.008
76.754
55.397
55.191
f1 (ppm)

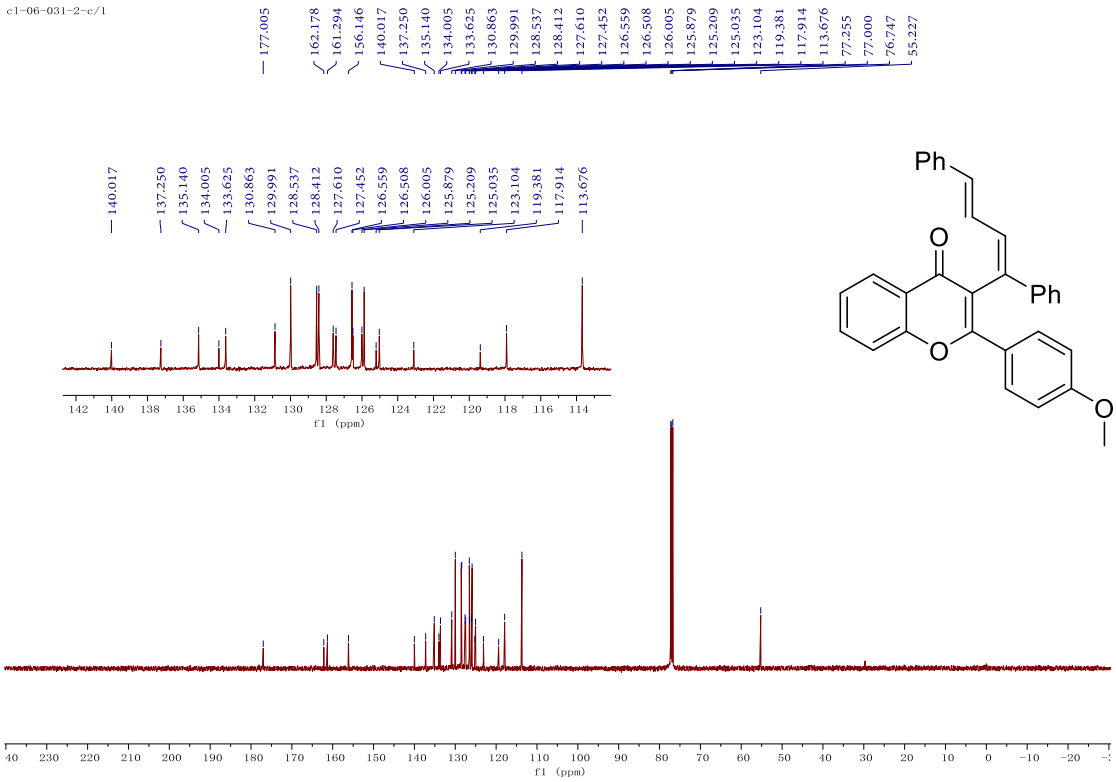

8.297
8.284
7.745
7.687
7.675
7.672
7.607
7.593
7.454
7.440
7.437
7.424
7.328
7.315
7.292
7.279
7.275
7.263
7.249
7.243
7.238
7.226
7.213
7.209
7.197
6.968
6.950
6.696
6.678
6.638
1.00
1.15
2.02
1.09
3.11
1.11
9.13
1.03
1.07
2.18
f1 (ppm)
O
Ph
O
Ph
Ph
1.00
1.15
2.02
1.09
3.11
1.11
9.13
1.03
1.07
1.12
1.08
f1 (ppm)

177.021
162.542
156.255
140.123
137.207
135.185
133.784
133.631
133.016
131.043
130.534
128.509
128.427
128.204
128.182
127.650
127.436
126.554
125.920
125.897
125.185
123.185
120.420
118.032
77.211
77.001
76.788
f1 (ppm)
O
Ph
O
Ph
Ph
f1 (ppm)


c1-06-029-h/1
8.244 8.238 8.232 7.680 7.669 7.659 7.653 7.563 7.558 7.545 7.540 7.407 7.393 7.389 7.335 7.329 7.317 7.294 7.290 7.276 7.260 7.244 7.228 7.212 7.198 7.193 7.180 7.165 6.967 6.949 6.696 6.691 6.665 6.660 6.644 6.620 6.614
Cl
O
Ph
O
Ph
Ph
1.00 3.02 1.08 2.10 1.24 10.21 1.00 2.02
f1 (ppm)


c1-06-029-c/1
175.889 162.784 154.564 139.888 137.107 135.482 134.003 133.151 132.651 131.217 131.125 130.752 128.540 128.454 128.256 128.173 127.756 127.524 126.559 125.883 125.844 125.688 124.092 120.463 119.816 77.254 77.001 76.747
Cl
O
Ph
O
Ph
Ph
f1 (ppm)


8.281 8.277 8.265 8.261 7.735 7.732 7.729 7.718 7.715 7.711 7.701 7.697 7.602 7.600 7.585 7.583 7.467 7.465 7.462 7.453 7.450 7.448 7.446 7.438 7.437 7.435 7.286 7.284 7.269 7.266 7.262 7.257 7.254 7.247 7.236 7.222 7.218 7.215 7.206 7.201 7.169 7.155 7.014 6.994 6.804 6.786 6.704 6.684 6.666 3.746
7.718 7.715 7.697 7.602 7.600 7.465 7.462 7.453 7.450 7.448 7.446 7.437 7.269 7.266 7.262 7.254 7.247 7.236 7.222 7.218 7.014 6.994 6.804 6.786 6.704 6.684 6.666
1.02 3.17 1.14 3.18 4.10 3.10 1.14 1.18 2.08 1.19 1.04 3.00
f1 (ppm)
Ph
O
Ph
O
O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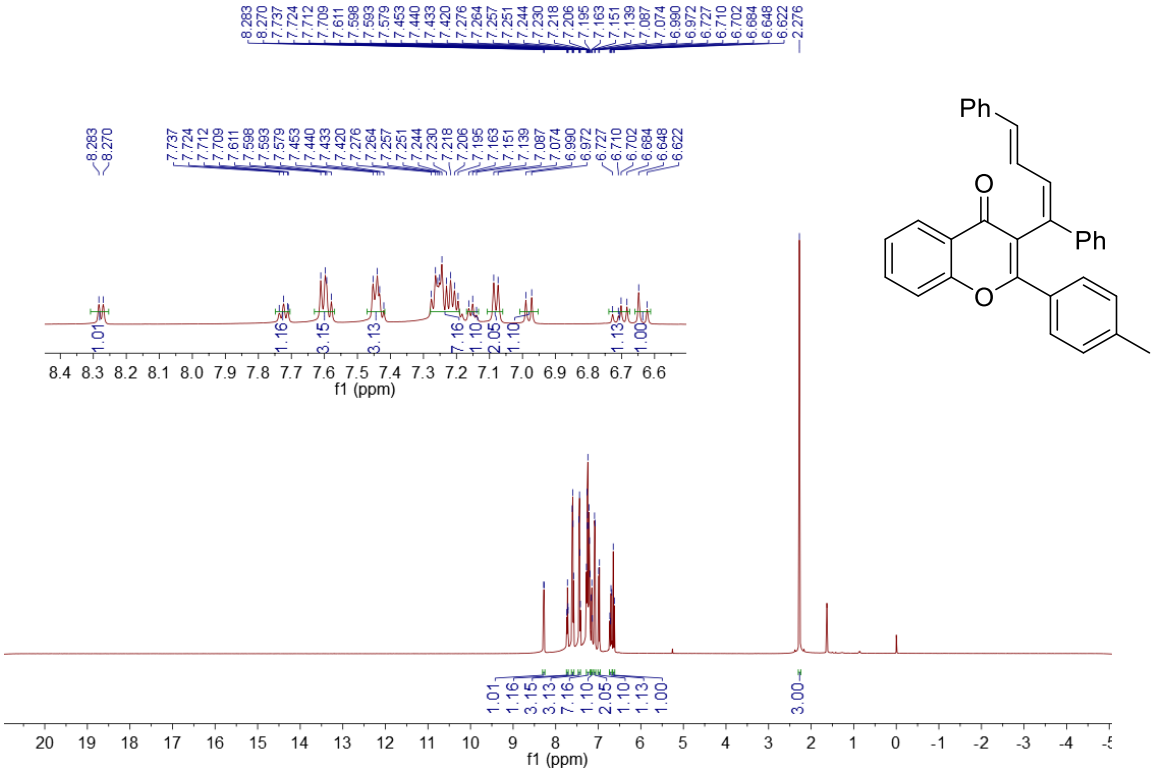
177.005 162.178 161.294 156.146 140.017 137.250 135.140 134.005 133.625 130.863 129.991 128.537 128.412 127.610 127.452 126.559 126.508 126.005 125.879 125.209 125.035 123.104 119.381 117.914 113.676 77.255 77.000 76.747 55.227
f1 (ppm)
Ph
O
Ph
O
O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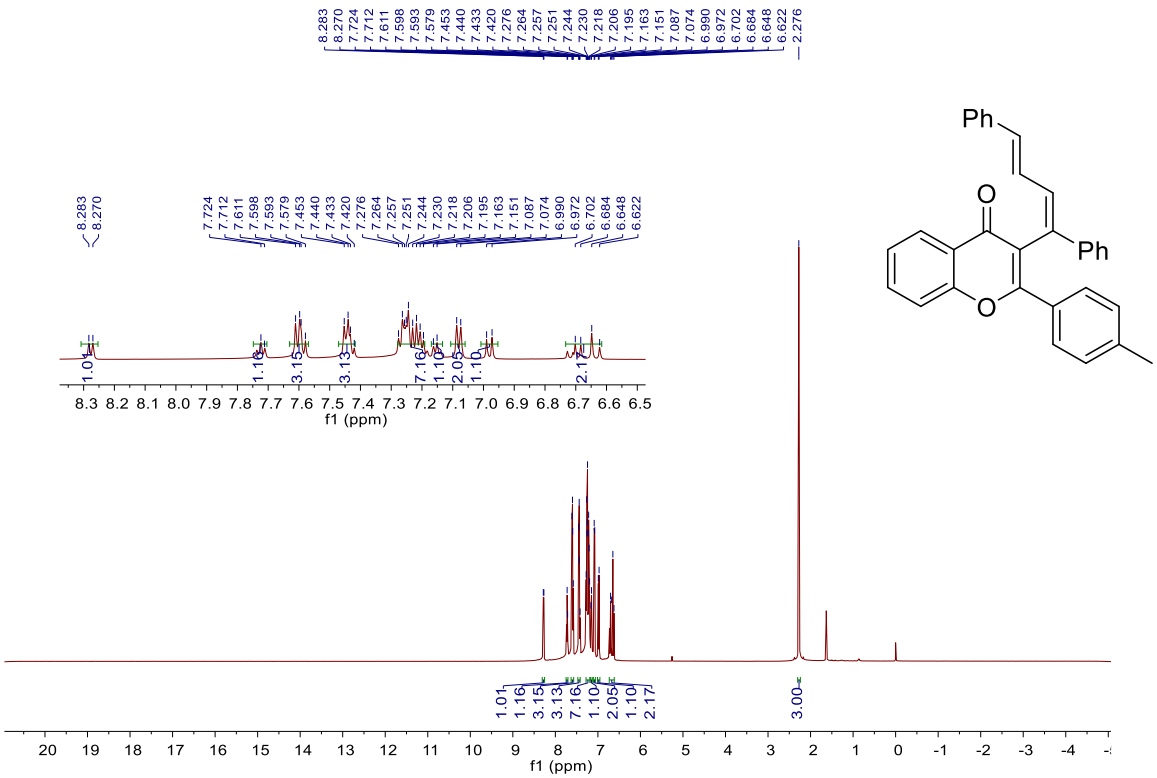
8.270
7.737
7.724
7.712
7.709
7.611
7.598
7.593
7.579
7.453
7.440
7.433
7.420
7.276
7.264
7.257
7.251
7.244
7.230
7.218
7.206
7.195
7.163
7.151
7.139
7.087
7.074
6.990
6.972
6.727
6.710
6.702
6.684
6.648
6.622
2.276
1.01
1.16
3.15
3.13
7.16
1.10
2.05
1.10
1.13
1.00
3.00
f1 (ppm)
Ph
O
Ph
O


8.283
8.270
7.724
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7.440
7.433
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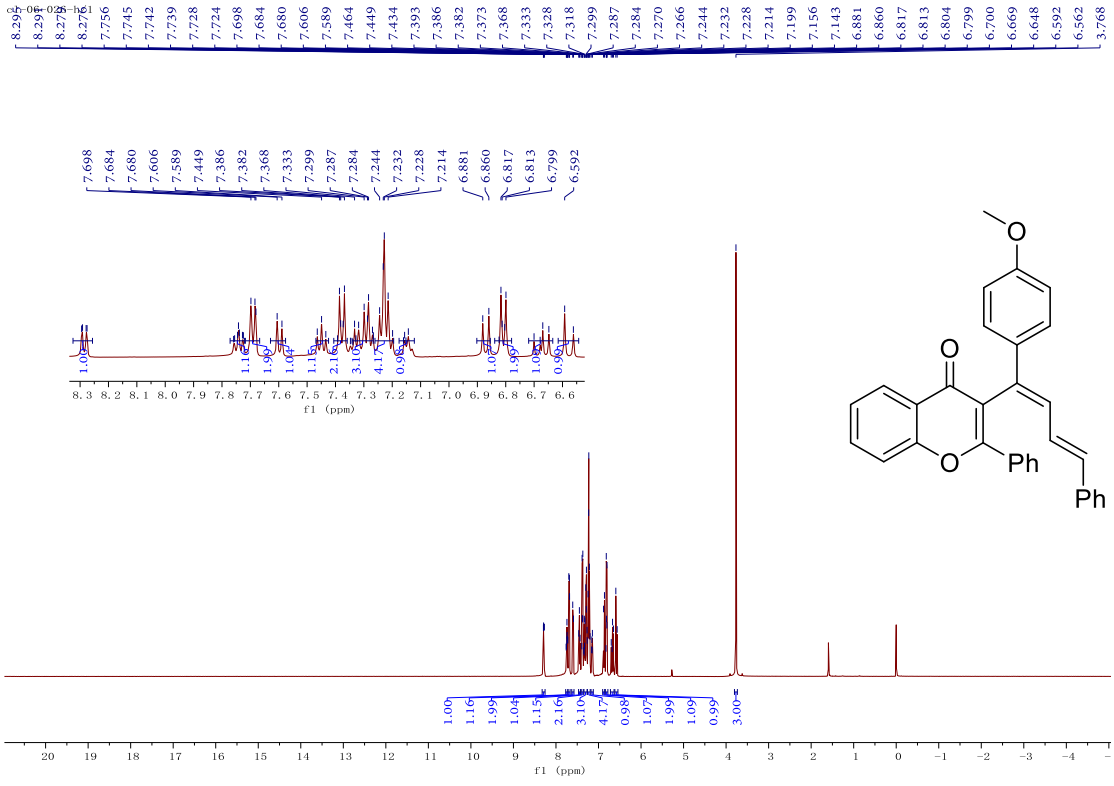
7.276
7.264
7.257
7.251
7.244
7.230
7.218
7.206
7.195
7.163
7.151
7.087
7.074
6.990
6.972
6.702
6.684
6.648
6.622
2.276
1.01
1.16
3.15
3.13
7.16
1.10
2.05
1.10
2.17
3.00
f1 (ppm)
Ph
O
Ph
O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7.728
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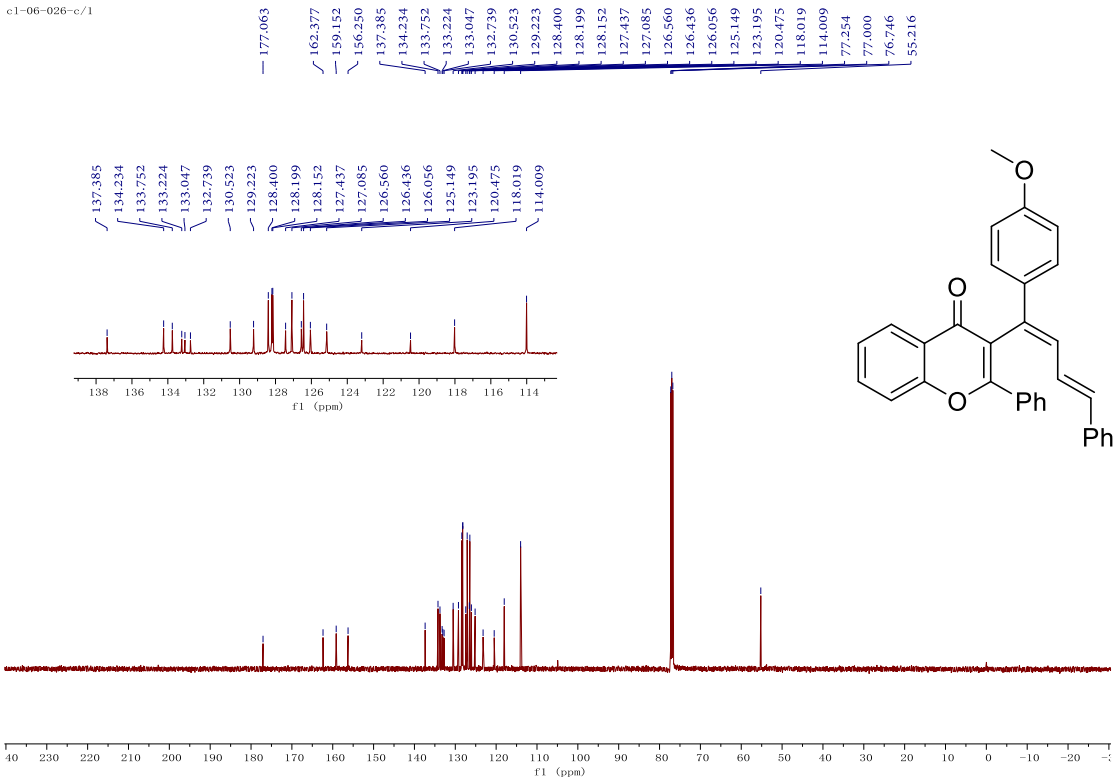
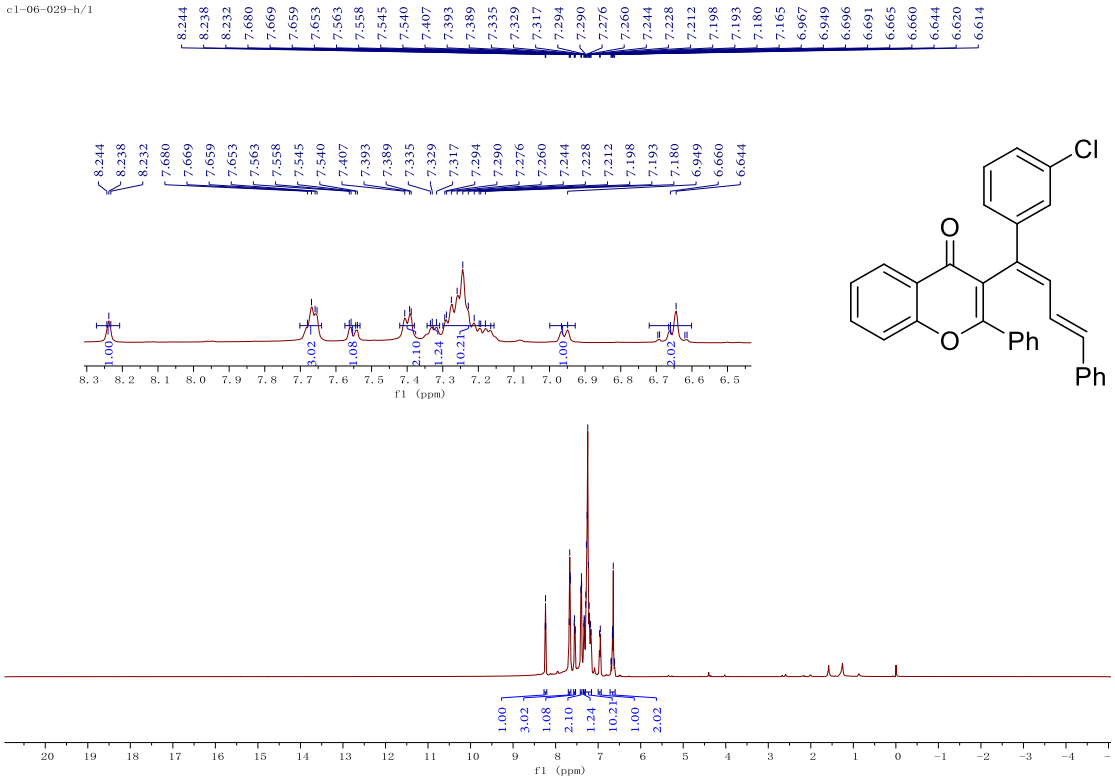
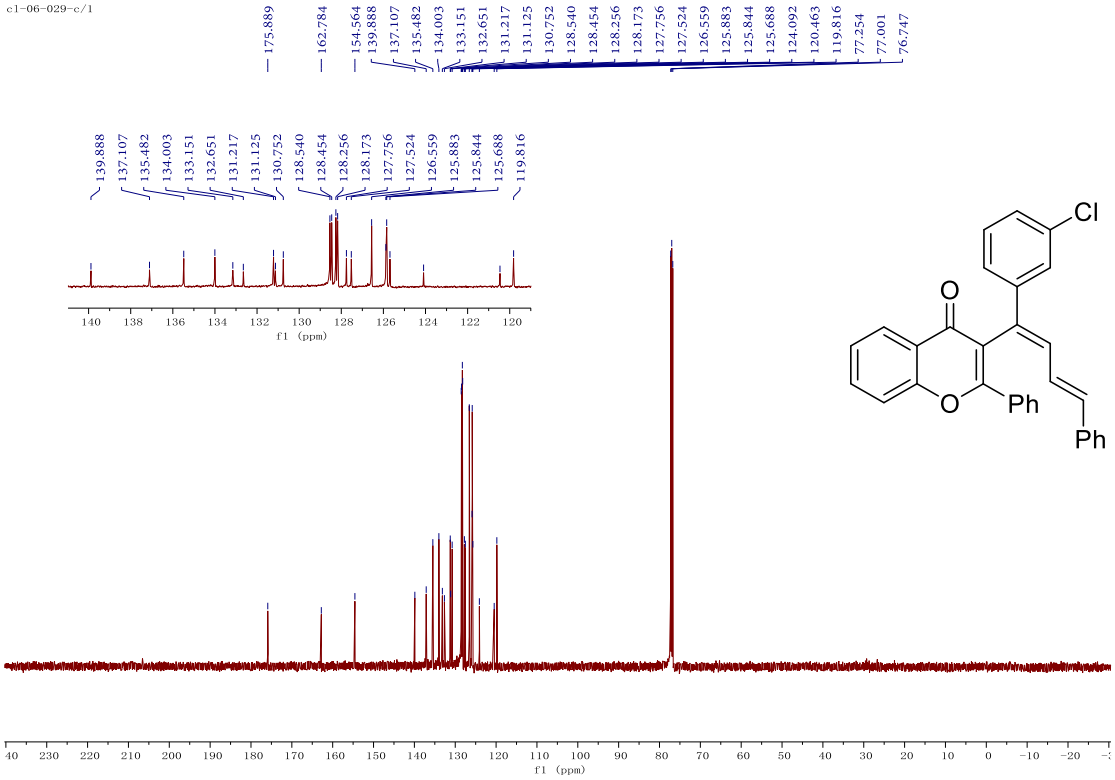
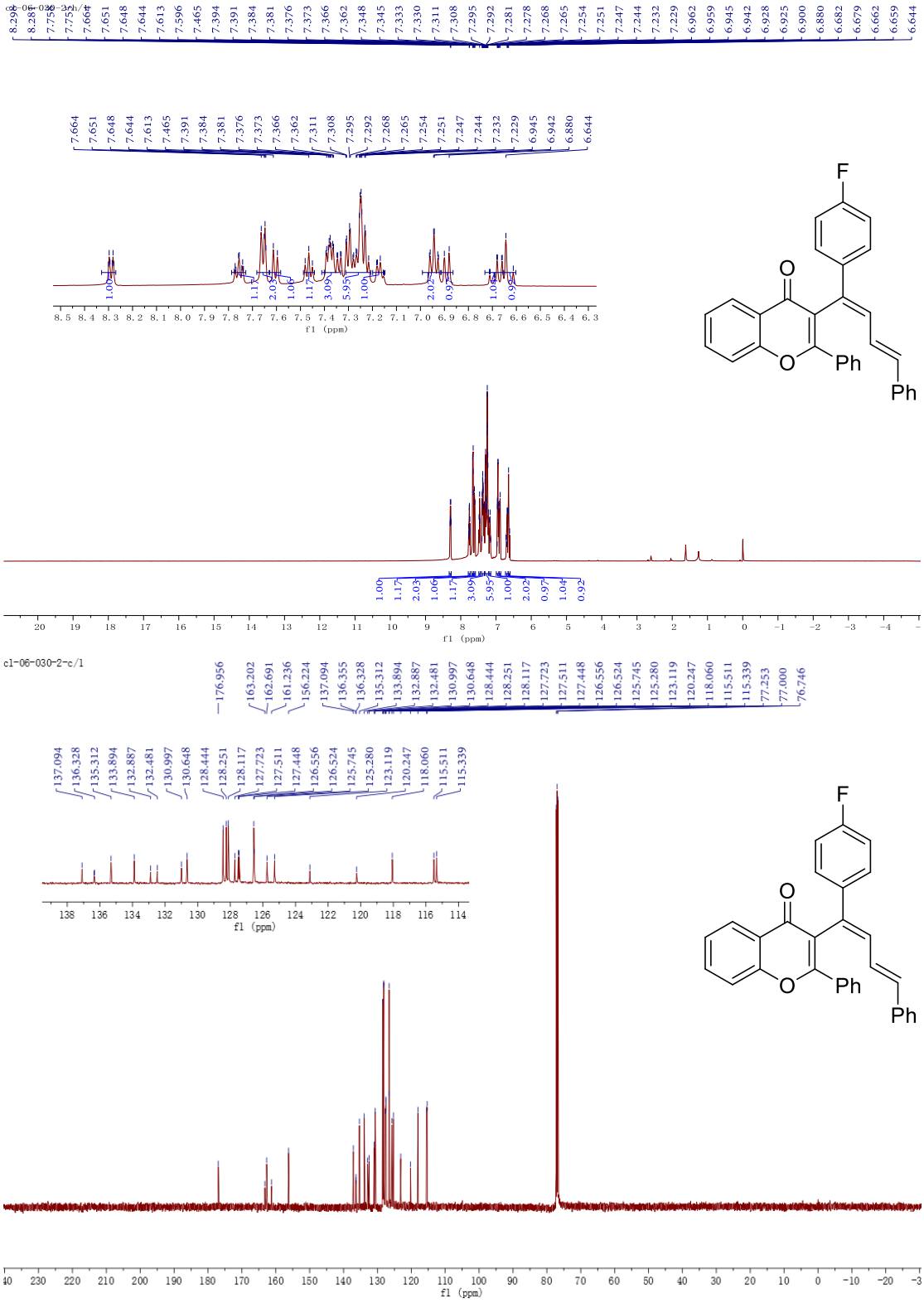
7.680
7.606
7.589
7.464
7.449
7.434
7.393
7.386
7.382
7.373
7.368
7.333
7.328
7.318
7.299
7.287
7.284
7.270
7.266
7.244
7.232
7.228
7.214
7.199
7.156
7.143
6.881
6.860
6.817
6.813
6.804
6.799
6.700
6.669
6.648
6.592
6.562
3.768
f1 (ppm)
O
O
Ph
Ph


177.063
162.377
159.152
156.250
137.385
134.234
133.752
133.224
133.047
132.739
130.523
129.223
128.400
128.199
128.152
127.437
127.085
126.560
126.436
126.056
125.149
123.195
120.475
118.019
114.009
77.254
77.000
76.746
55.216
f1 (ppm)
O
O
Ph
Ph


c1-06-029-h/1
8.244 8.238 8.232 7.680 7.669 7.659 7.653 7.563 7.558 7.545 7.540 7.407 7.393 7.389 7.335 7.329 7.317 7.294 7.290 7.276 7.260 7.244 7.228 7.212 7.198 7.193 7.180 7.165 6.967 6.949 6.696 6.691 6.665 6.660 6.644 6.620 6.614
1.00 3.02 1.08 2.10 1.24 10.21 1.00 2.02
f1 (ppm)
Cl
O
O
Ph
Ph


c1-06-029-c/1
175.889 162.784 154.564 139.888 137.107 135.482 134.003 133.151 132.651 131.217 131.125 130.752 128.540 128.454 128.256 128.173 127.756 127.524 126.559 125.883 125.844 125.688 124.092 120.463 119.816 77.254 77.001 76.747
f1 (ppm)
Cl
O
O
Ph
Ph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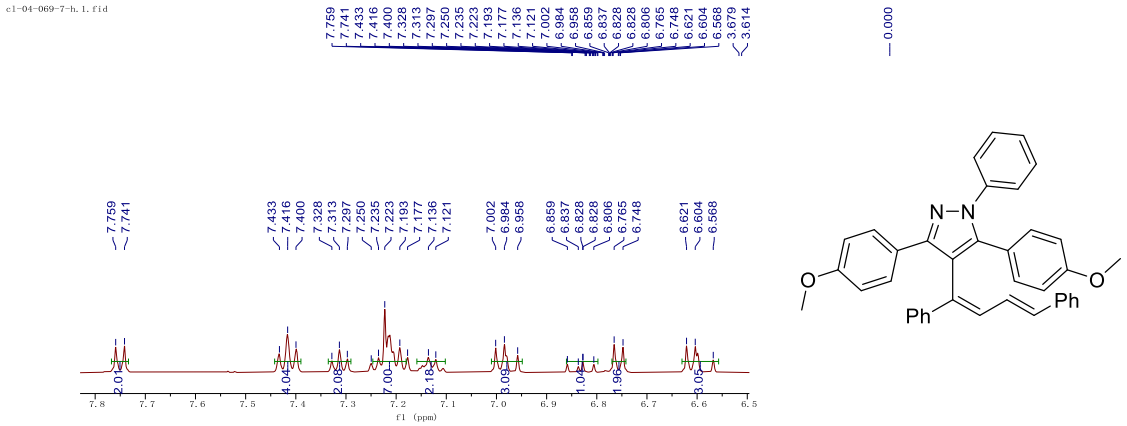
O
Ph
Ph
f1 (ppm)
F
O
O
Ph
Ph
f1 (ppm)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7.235
7.223
7.193
7.177
7.136
7.121
7.002
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6.958
6.859
6.837
6.828
6.828
6.806
6.765
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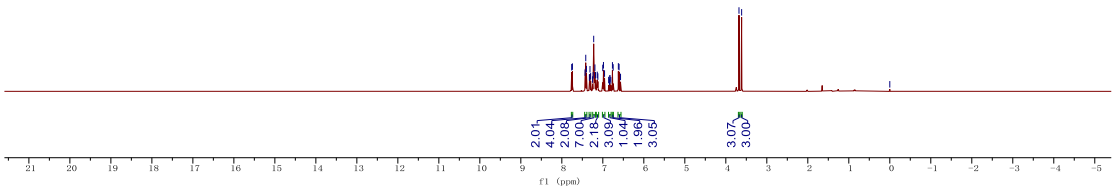
6.621
6.604
6.568
3.679
3.614
0.000
N–N
O
O
Ph
Ph
f1 (ppm)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1.04
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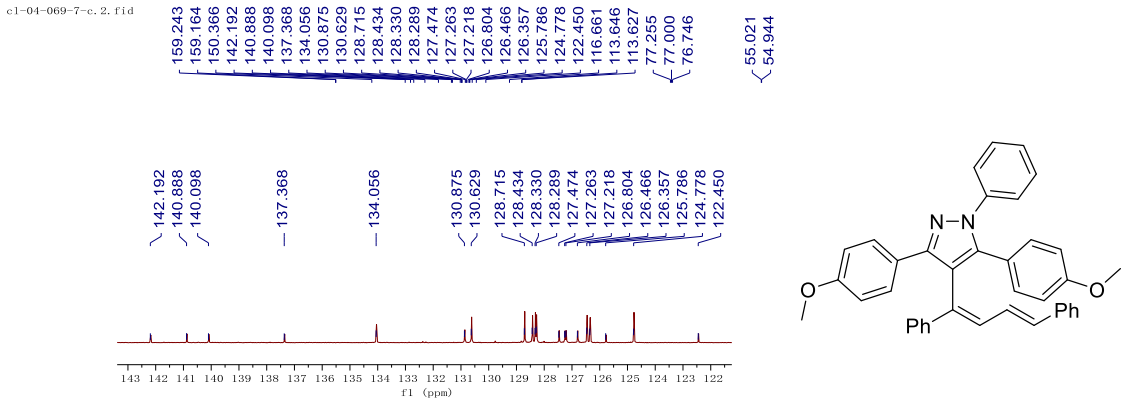
3.07
3.00
f1 (ppm)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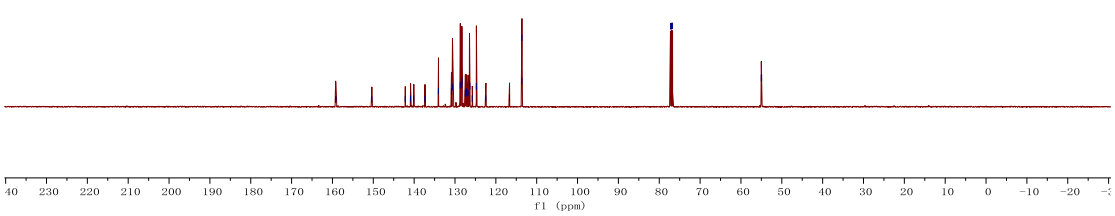
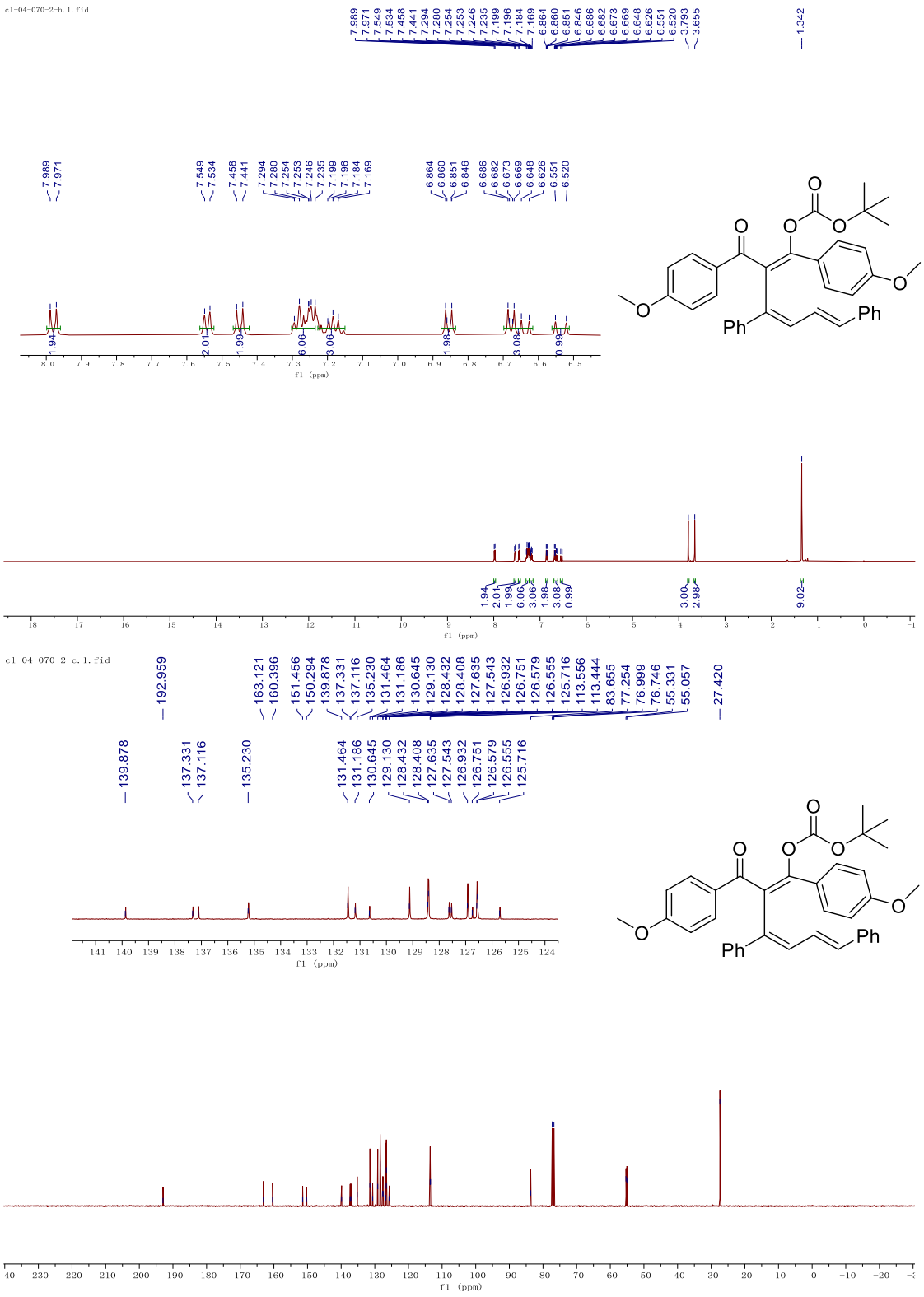
128.289
127.474
127.263
127.218
126.804
126.466
126.357
125.786
124.778
122.450
116.661
113.646
113.627
77.255
77.000
76.746
55.021
54.944
N–N
O
O
Ph
Ph
f1 (ppm)


f1 (ppm)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7.534
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7.441
7.294
7.280
7.254
7.253
7.246
7.235
7.199
7.196
7.184
7.169
6.864
6.860
6.851
6.846
6.686
6.682
6.673
6.669
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6.626
6.551
6.520
3.793
3.655
1.342
1.94
2.01
1.99
6.06
3.06
1.98
3.08
0.99
3.00
2.98
9.02
f1 (ppm)
O
O
O
O
O
Ph
Ph
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160.396
151.456
150.294
139.878
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137.116
135.230
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131.186
130.645
129.130
128.432
128.408
127.635
127.543
126.932
126.751
126.579
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125.716
113.556
113.444
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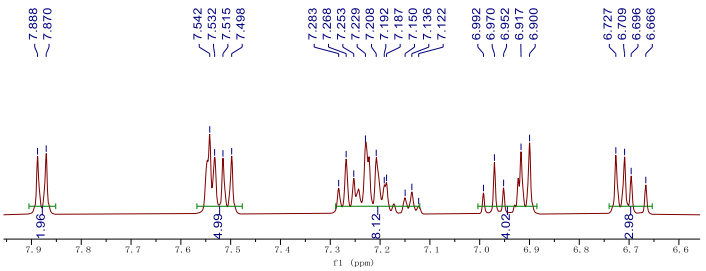

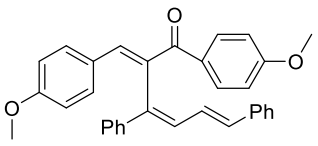

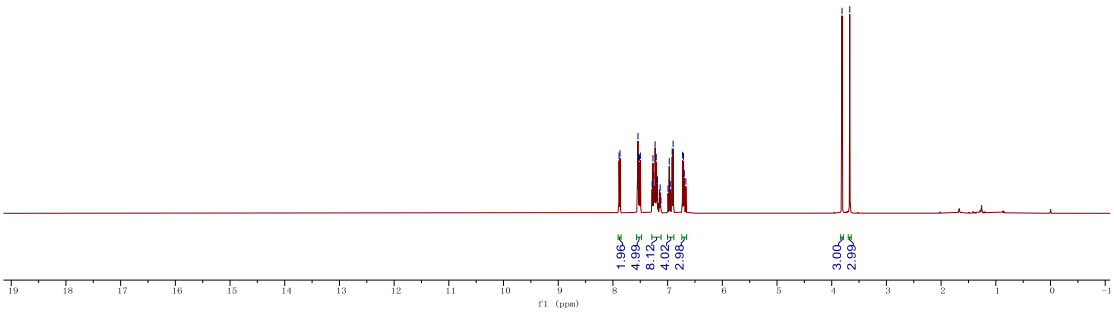

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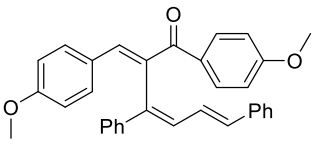
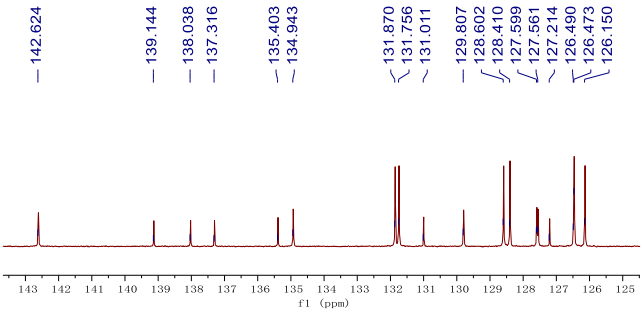
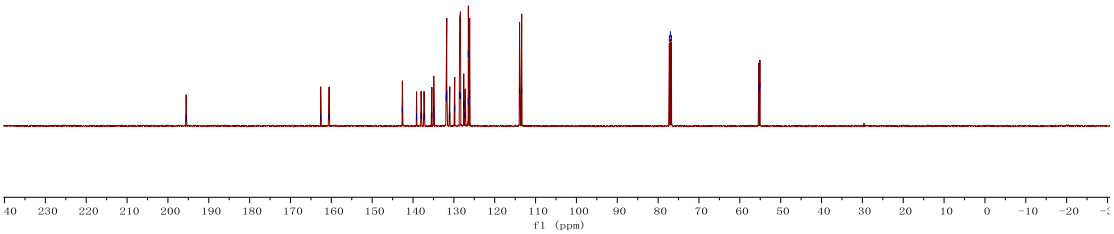
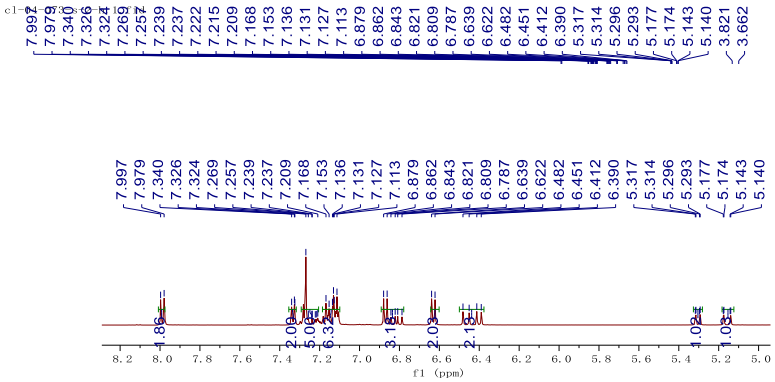
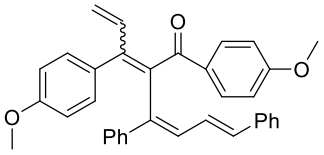


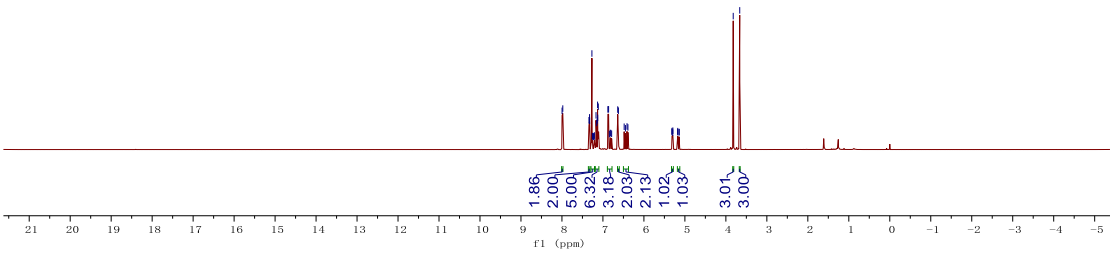


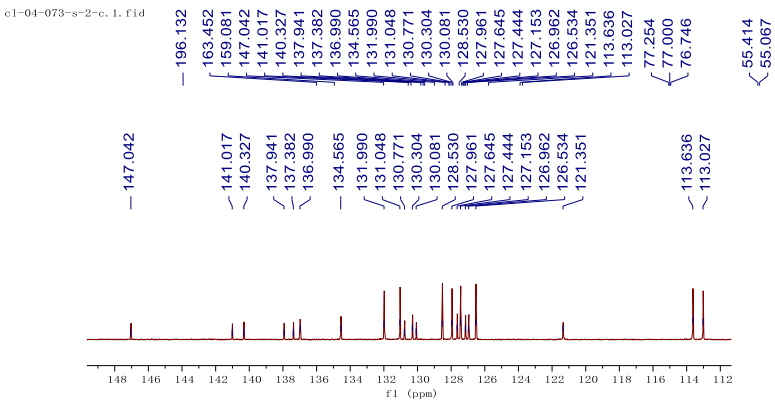


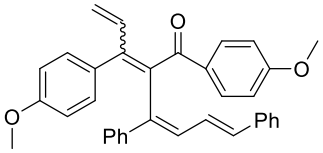




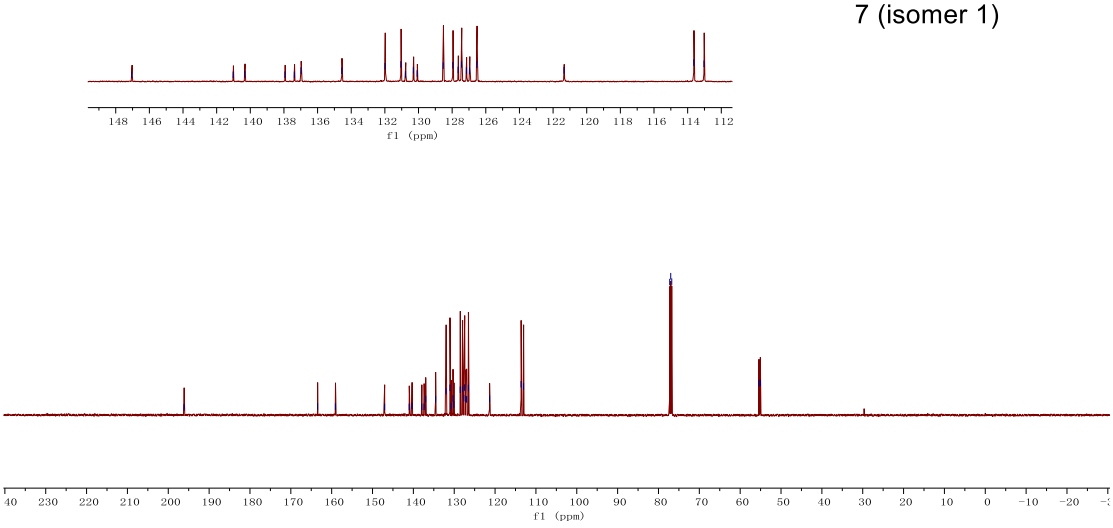
7 (isomer 1)

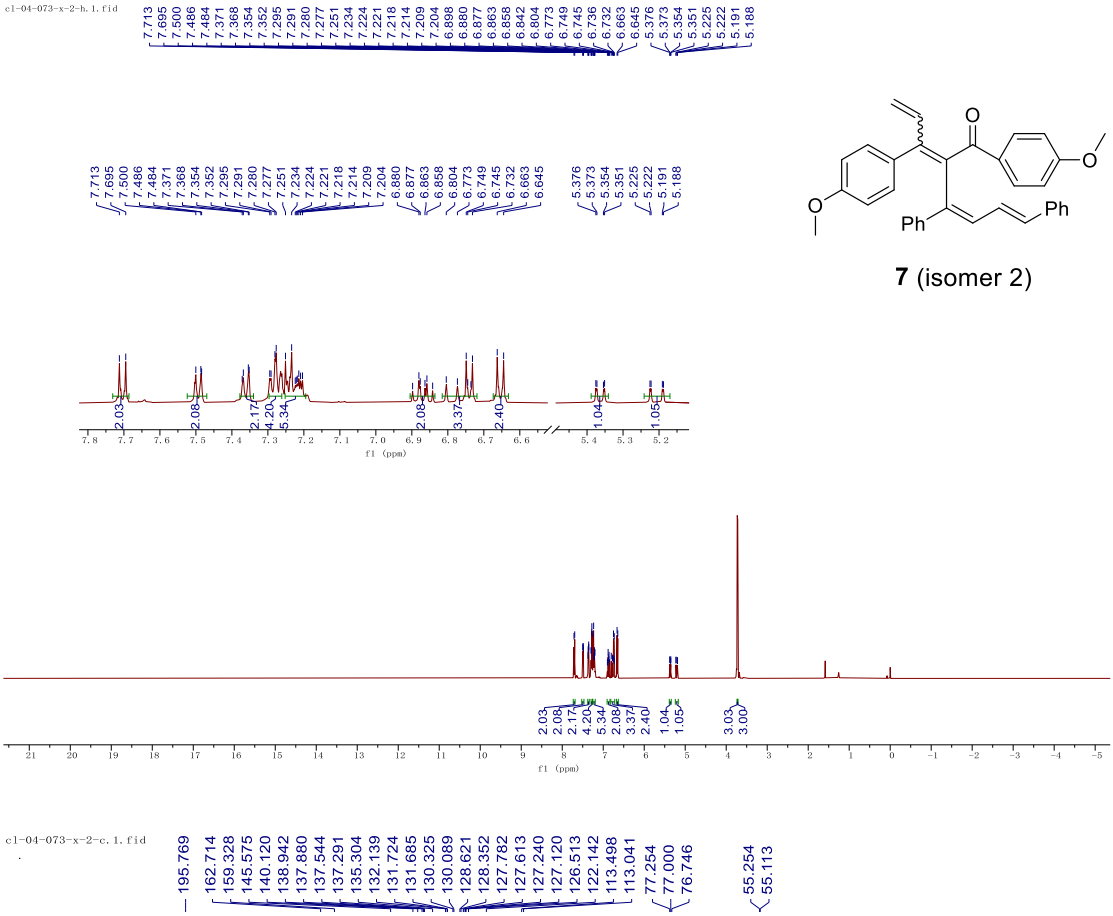






7 (isomer 1)




c1-04-073-x-2-h.1.fid
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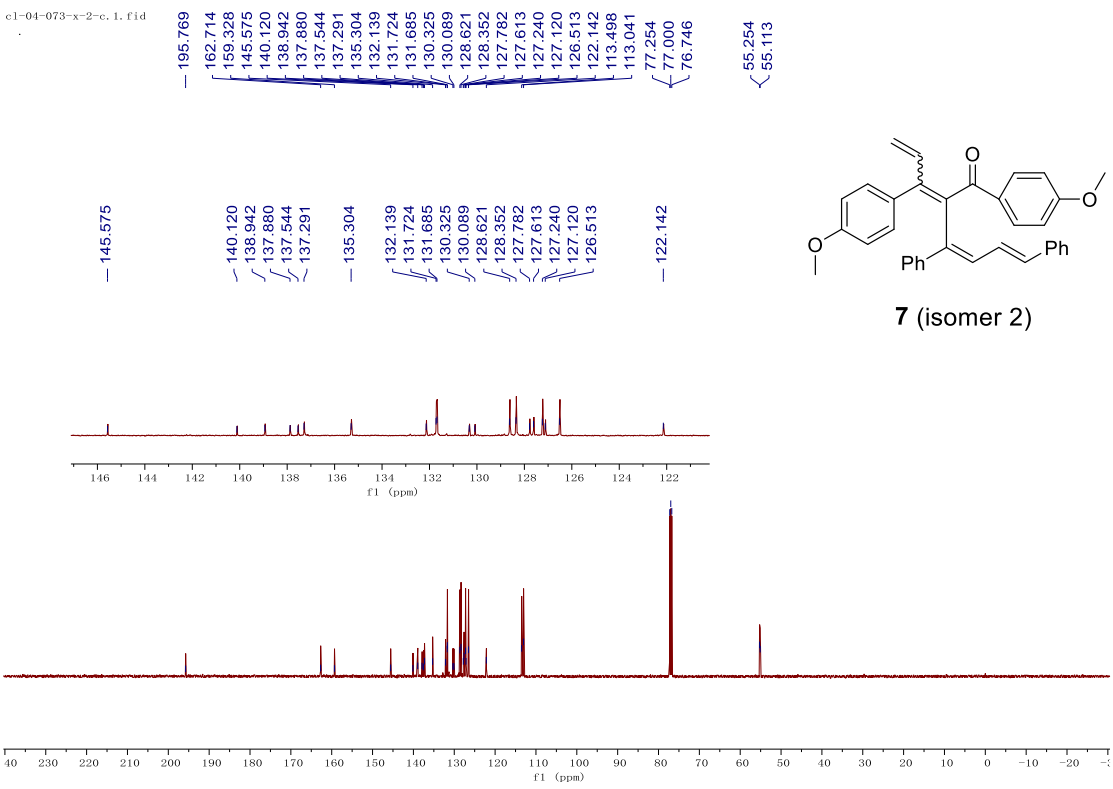
7.368
7.354
7.352
7.295
7.291
7.280
7.277
7.251
7.234
7.224
7.221
7.218
7.214
7.209
7.204
6.880
6.877
6.863
6.858
6.804
6.773
6.749
6.745
6.732
6.663
6.645
5.376
5.373
5.354
5.351
5.225
5.222
5.191
5.188
O
O
Ph
Ph
2.03
2.08
2.17
4.20
5.34
2.08
3.37
2.40
1.04
1.05
f1 (ppm)
7 (isomer 2)

2.03
2.08
2.17
4.20
5.34
2.08
3.37
2.40
1.04
1.05
3.03
3.00
f1 (ppm)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145.575
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138.942
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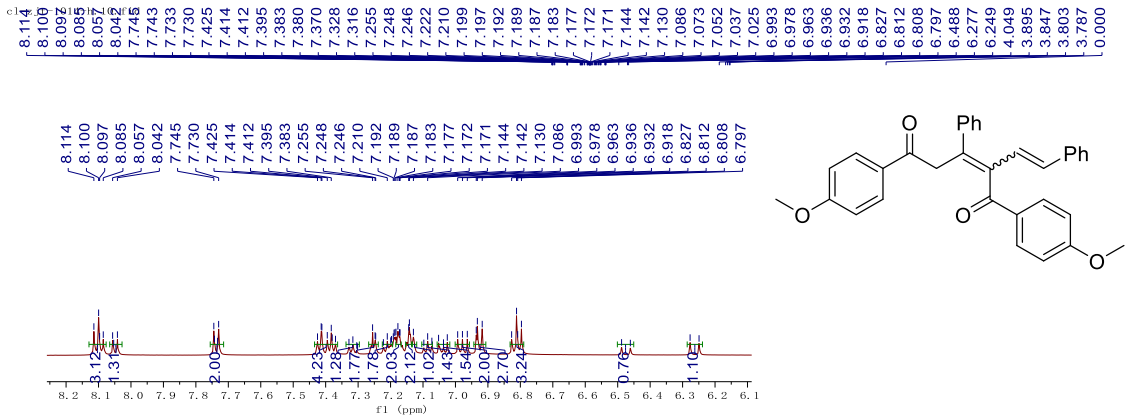
137.544
137.291
135.304
132.139
131.724
131.685
130.325
130.089
128.621
128.352
127.782
127.613
127.240
127.120
126.513
122.142
113.498
113.041
77.254
77.000
76.746
55.254
55.113
O
O
Ph
Ph
f1 (ppm)
7 (isomer 2)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7.255
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7.246
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7.192
7.189
7.187
7.183
7.177
7.172
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7.130
7.086
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6.978
6.963
6.936
6.932
6.918
6.827
6.812
6.808
6.797
O
Ph
Ph
O
O
3.12
1.31
2.00
4.23
1.28
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2.03
2.12
1.02
1.43
1.54
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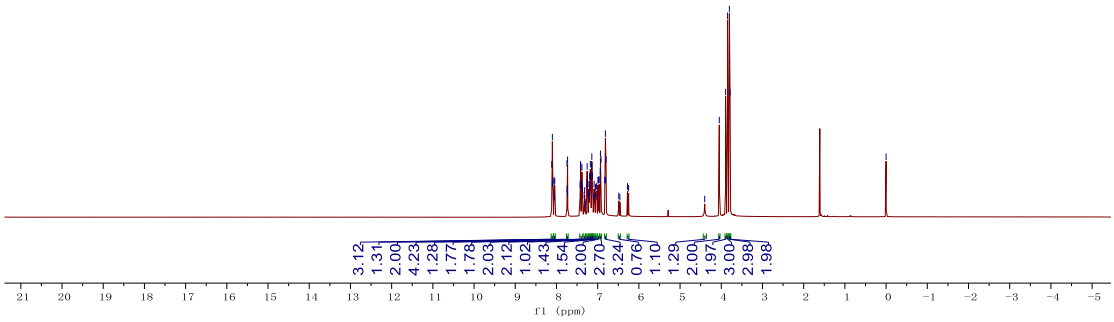
2.70
3.24
0.76
1.10
f1 (ppm)


3.12
1.31
2.00
4.23
1.28
1.77
2.03
2.12
1.02
1.43
1.54
2.00
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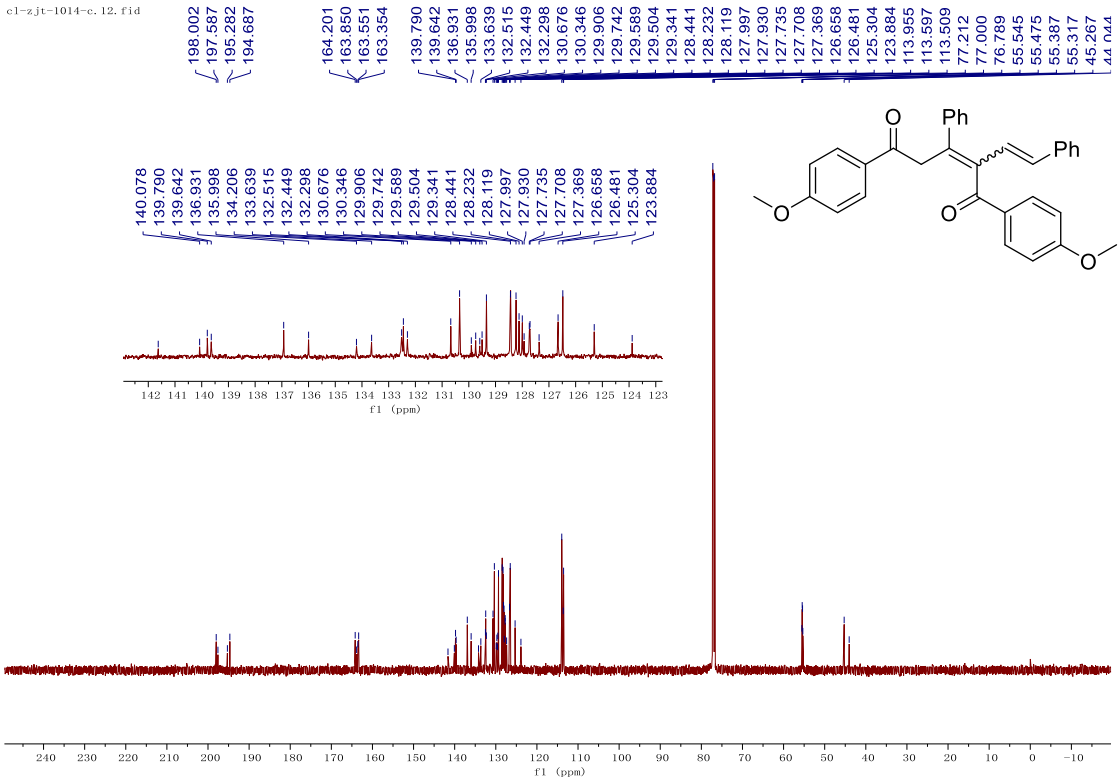
3.24
0.76
1.10
1.29
2.00
1.97
3.00
2.98
1.98
f1 (ppm)


c1-zjt-1014-c.12.fid
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132.515
132.449
132.298
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130.346
129.906
129.742
129.589
129.504
129.341
128.441
128.232
128.119
127.997
127.930
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139.642
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135.998
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132.515
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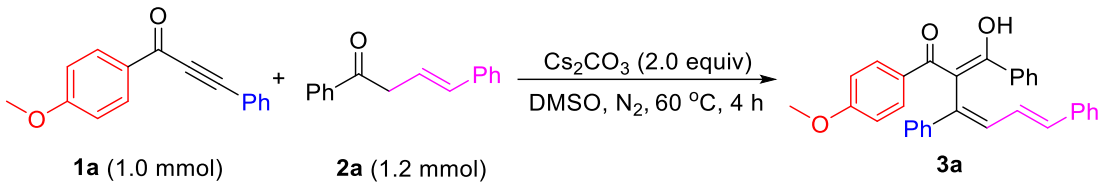
129.589
129.504
129.341
128.441
128.232
128.119
127.997
127.930
127.735
127.708
127.369
126.658
126.481
125.304
123.884
O
Ph
Ph
O
O
f1 (ppm)

7. 1.0 mmol scale reactions for the preparation of 3a



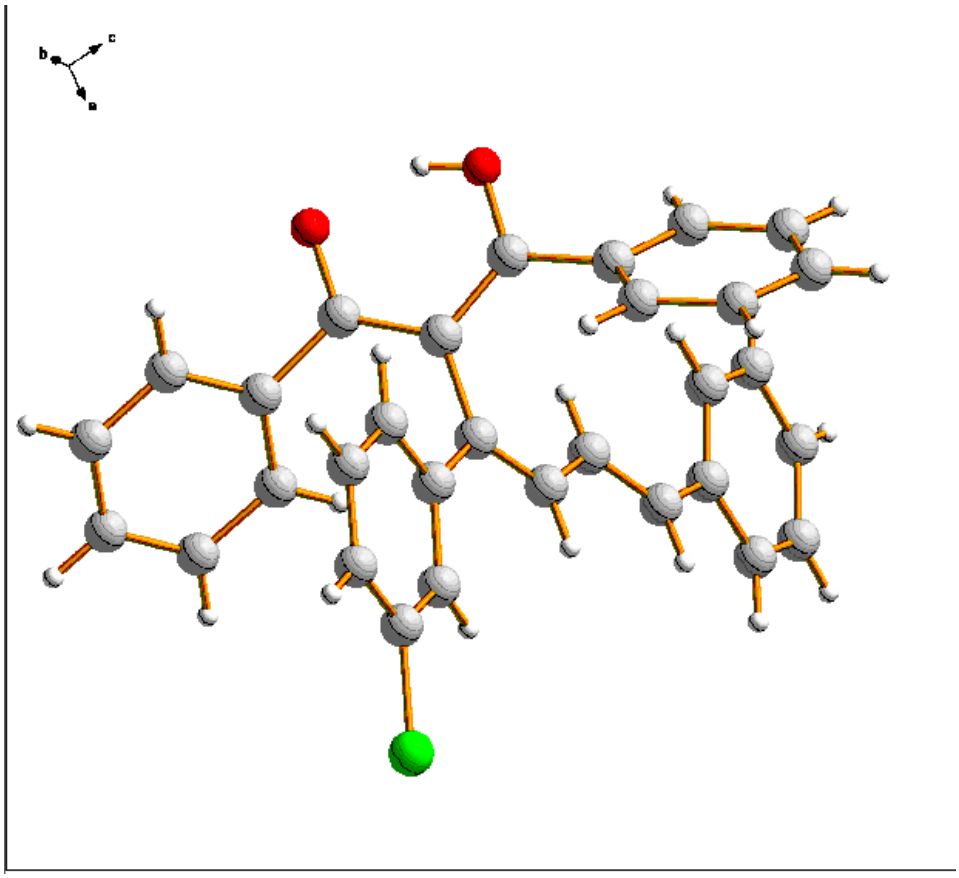
1a (1.0 mmol) **2a** (1.2 mmol) **3a**

In a schlenk tube 1-(4-methoxyphenyl)-3-phenylprop-2-yn-1-one **1a** (1.0 mmol, 236.3 mg), (*E*)-1,4-diphenylbut-3-en-1-one **2a** (1.2 mmol, 266.7 mg), Cs_2CO_3 (2.0 mmol, 651.6 mg) and DMSO (10.0 mL) were stirred at 60 °C. After the reaction was completed as monitored by thin-layer chromatography, the reaction mixture was then quenched by water, and the water layers were extracted with ethyl acetate (10 mL × 3). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure. Purification by chromatography on silica gel (petroleum ether/ethyl acetate = 12:1) afforded desired compound **3a** (yellow solid, 343.92 mg, 75%).

8. X-Ray Crystal Structure of 3l (CCDC: 2156724)

(2*Z*,3*Z*,5*E*)-3-(3-chlorophenyl)-2-(hydroxy(phenyl)methylene)-1,6-diphenylhexa-3,5-dien-1-one (3l).

Sample preparation for crystal growth: Compound **3l** (50 mg) was dissolved in the mixed solvent of dichloromethane/petroleum ether = 3 ml/6 ml in a 50 mL round-bottom flask. The yellow single crystal of **3l** was obtained by slowly evaporating mixed solvent at room temperature under air.



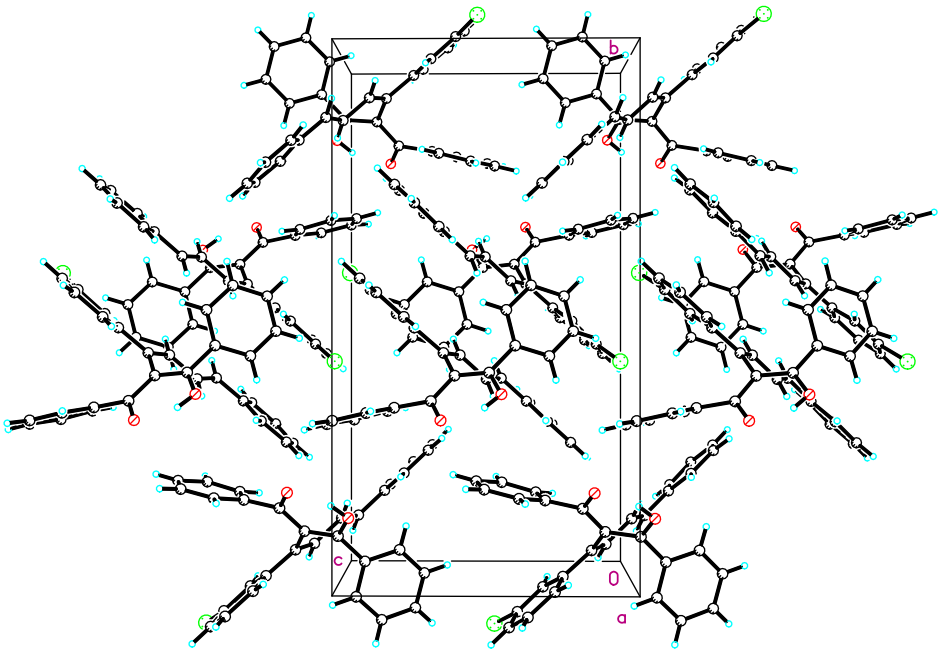


Table 1. Crystal data and structure refinement for **3l**

Identification code	**3l**
Empirical formula	$C_{31}H_{23}ClO_2$
Formula weight	462.94
Temperature	213(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 21/c
Unit cell dimensions	a = 10.4144(4) Å α = 90°. b = 20.4948(8) Å β = 91.1890(10)°. c = 11.3123(5) Å γ = 90°.
Volume	2413.99(17) $Å^3$
Z	4
Density (calculated)	1.274 Mg/m^3
Absorption coefficient	0.185 mm^{-1}
F(000)	968
Crystal size	0.20 x 0.15 x 0.100 mm^3
Theta range for data collection	2.682 to 25.998°.
Index ranges	-12<=h<=12, -25<=k<=25, -13<=l<=13
Reflections collected	32059
Independent reflections	4709 [R(int) = 0.0339]
Completeness to theta = 25.242°	99.5 %
Absorption correction	Semi-empirical from equivalents

Max. and min. transmission	0.7456 and 0.6806
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4709 / 0 / 309
Goodness-of-fit on F^2	1.036
Final R indices [I>2sigma(I)]	R1 = 0.0373, wR2 = 0.0896
R indices (all data)	R1 = 0.0469, wR2 = 0.0973
Extinction coefficient	0.013(2)
Largest diff. peak and hole	0.204 and -0.224 e.Å^{-3}

8. X-Ray Crystal Structure of 3y' (CCDC: 2119670)

(4''-methoxy-4'-phenyl-[1,1':2',1''-terphenyl]-3'-yl)(4-methoxyphenyl)methanone (3y')

Sample preparation for crystal growth: Compound **3y'** (50 mg) was dissolved in the mixed solvent of dichloromethane/petroleum ether = 3 ml/6 ml in a 50 mL round-bottom flask. The white single crystal of **3y'** was obtained by slowly evaporating mixed solvent at room temperature under air.

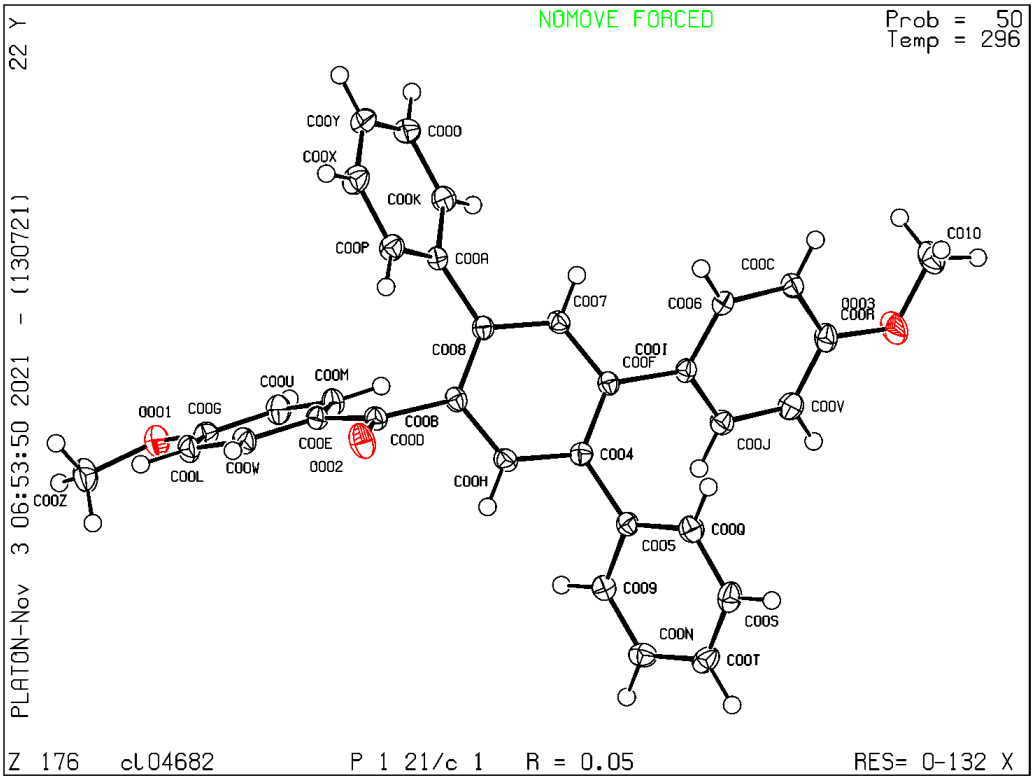


Table 2. Crystal data and structure refinement for **3y'**.

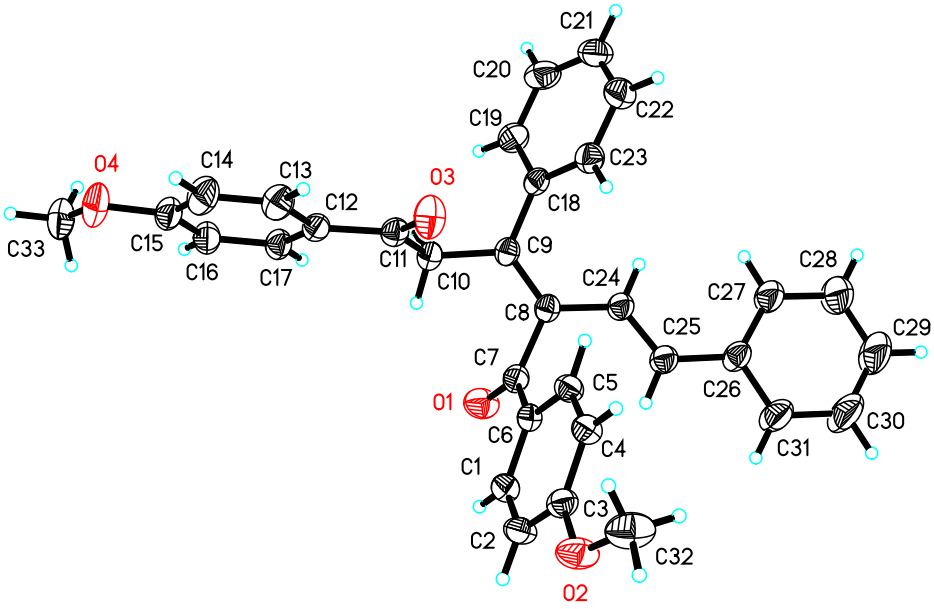
Identification code	**3y'**

Empirical formula	$C_{33}H_{26}O_3$	
Formula weight	470.54	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Space group	P 21/c	
Unit cell dimensions	a = 14.2205(8) Å b = 9.9027(6) Å c = 17.0375(12) Å	α= 90°. β= 93.389(2)°. γ = 90°
Volume	2395.1(3) $Å^3$	
Z	4	
Density (calculated)	1.305 Mg/m^3	
Absorption coefficient	0.082 mm^{-1}	
F(000)	992.0	
Index ranges	-19<=h<=19, -13<=k<=13, -23<=l<=23	
Completeness to theta = 29.975°	99.7 %	
Max. and min. transmission	0.746 and 0.698	
R indices (all data)	R1 = 0.0475, wR2 = 0.1341	

9. X-Ray Crystal Structure of 10 (CCDC: 2122766)

1,5-bis(4-methoxyphenyl)-3-phenyl-2-styrylpent-2-ene-1,5-dione (10)

Sample preparation for crystal growth: Compound **10**' (50 mg) was dissolved in the mixed solvent of dichloromethane/petroleum ether = 3 ml/6 ml in a 50 mL round-bottom flask. The yellow single crystal of **10** was obtained by slowly evaporating mixed solvent at room temperature under air.



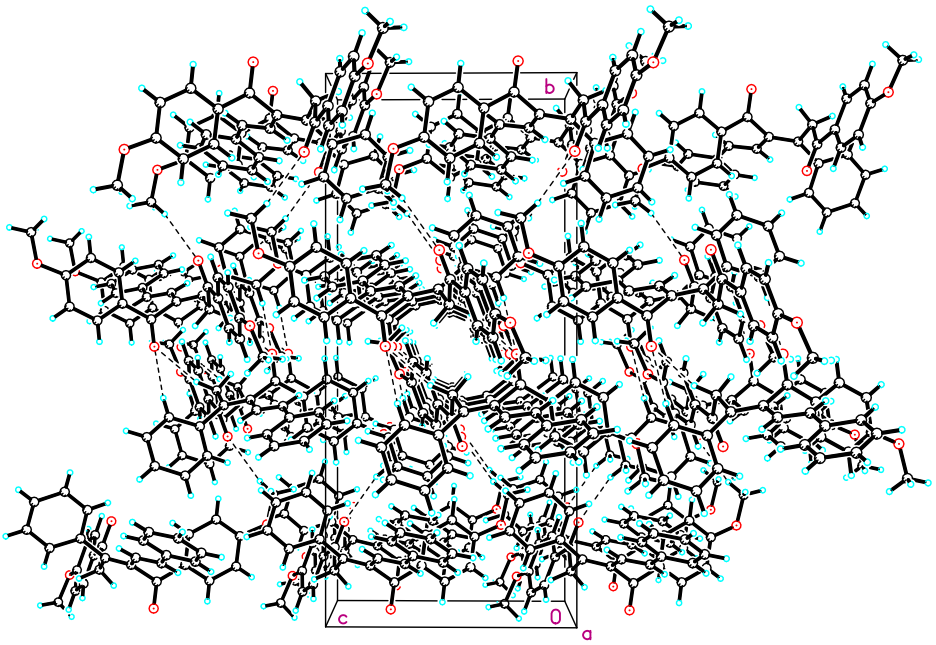


Table 3. Crystal data and structure refinement for **10**

Identification code	**10**
Empirical formula	$C_{33}H_{28}O_4$
Formula weight	488.55

Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 21/c
Unit cell dimensions	a = 11.0647(3) Å α = 90° b = 23.0493(8) Å β = 92.0670(10)° c = 10.4440(3) Å γ = 90°
Volume	2661.84(14) $Å^3$
Z	4
Density (calculated)	1.219 Mg/m^3
Absorption coefficient	0.079 mm^{-1}
F(000)	1032
Crystal size	0.200 x 0.150 x 0.120 mm^3
Theta range for data collection	2.553 to 25.999°.
Index ranges	-12<=h<=13, -28<=k<=28, -12<=l<=12
Reflections collected	27068
Independent reflections	5218 [R(int) = 0.0668]
Completeness to theta = 25.242°	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.5367
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5218 / 0 / 337
Goodness-of-fit on F^2	1.025
Final R indices [I>2sigma(I)]	R1 = 0.0474, wR2 = 0.1142
R indices (all data)	R1 = 0.0728, wR2 = 0.1331
Extinction coefficient	0.018(3)
Largest diff. peak and hole	0.135 and -0.190 $e.Å^{-3}$