Supporting Information

Transition-Metal-Free Insertion Reactions of Alkynes into C-N σ-Bond of Imides: Synthesis of Substituted Enamides or Chromones

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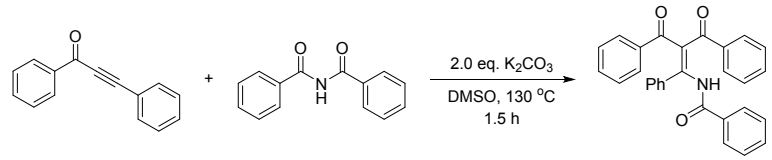
1. General Methods

All reactions were carried out under N_2 protection. Anhydrous DMSO, DMF and DMAc were prepared by distillation from CaH_2. Unless noted, all commercial reagents were used without further purification. Reactions were monitored by thin layer chromatography. Preparation of ynone were using reported method. Purification of reaction products was carried out by flash chromatography on silica gel (300~400 mesh). ^1H NMR spectra were recorded at 400 MHz, ^{13}C NMR spectra were recorded at 100 MHz, and in $CDCl_3$ (containing 0.03% TMS) solutions. ^1H 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. IR spectra was recorded on a Thermo-Scientific NICOLET iS50 FT-IR spectrometer. High-resolution mass spectra were performed on a mass spectrometer with a TOF (for EI or ESI) or FT-ICR (for MALDI) analyzer. Single crystal X-ray diffraction data was collected in Bruker SMARTAPEX diffractiometers.

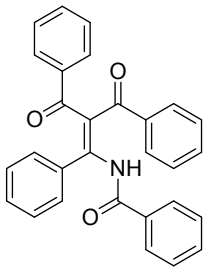
2. Preparation of product 3 and 5

General Procedure for the preparation of 3



1a 1.0 eq. **2a** 2.0 eq. **3a**

Under N_2 atmosphere, in a dried Schlenk tube ynone **1a** (0.20 mmol, 41.2 mg), K_2CO_3 (0.40 mmol, 55.2 mg), and imide **2a** (0.40 mmol, 90.1 mg) and DMSO (3 mL) were added, and mixture was stirred at 130 °C. After the reaction was complete as monitored by thin-layer chromatography, the reaction mixture was then quenched by water, and the mixture were extracted with ethyl acetate (15 mL × 3). The combined organic layer was washed with water (15 mL× 2), brine (15 mL), and dried over with anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure, Purification by chromatography on silica gel (petroleum ether / ethyl acetate = 10/1) afforded desired compound **3a**.



***N*-(2-benzoyl-3-oxo-1,3-diphenylprop-1-en-1-yl)benzamide (3a)**

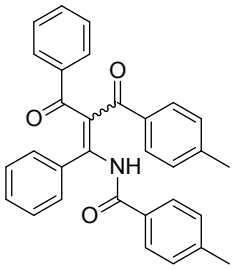
Yellow solid. 80% yield (69 mg), mp 165-168 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.16-7.27 (m, 7H), 7.28-7.38 (m, 4H), 7.46-7.53 (m, 2H), 7.54-7.61 (m, 3H), 7.64 (d, *J* = 7.2 Hz, 2H), 8.05 (d, *J* = 7.6 Hz, 2H), 13.22 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 121.21, 128.03, 128.06, 128.31, 128.34, 128.36, 128.67, 129.16, 129.30, 129.72, 131.90, 132.95, 133.26, 133.42, 134.04, 139.12, 140.22, 156.60, 165.45, 195.81, 196.71.

IR (neat): 3307, 3060, 1663, 1596, 1557, 1473, 1265, 1237, 735, 693 cm^{-1}.

HRMS (ESI) calcd for $C_{29}H_{21}NNaO_3$ $[M+Na]^+$: 454.1414, found 454.1423.



***N*-(2-benzoyl-3-oxo-1-phenyl-3-(p-tolyl)prop-1-en-1-yl)-4-methylbenzamide (3b)**

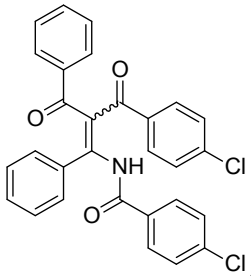
Pale yellow solid. 64% yield (59 mg), mp 168-171 °C.

^{1}H NMR (400 MHz, $CDCl_3$) Obtained as 1: 1 isomer. Isomer 1: δ 2.26 (s, 3H), 7.04 (d, *J* = 8.0 Hz, 2H), 7.14-7.25 (m, 5H), 7.26-7.36 (m, 5H), 7.52-7.58 (m, 2H), 7.64 (d, *J* = 7.6 Hz, 2H), 7.89-7.99 (m, 2H), 13.15 (s, 1H); Isomer 2: δ2.41 (s, 3H),6.99 (d, *J* = 7.6 Hz, 2H), 7.50 (d, *J* = 8.0 Hz, 2H), 13.24 (s, 1H); other peaks are overlapped with the other isomer.

^{13}C NMR (100 MHz, $CDCl_3$) δ 21.19, 21.27, 21.30, 121.02, 121.15, 127.92, 128.02, 128.25, 128.30, 128.33, 128.56, 128.68, 129.01, 129.08, 129.29, 129.48, 129.54, 129.80, 130.66, 131.76, 132.85, 134.16, 134.20, 136.65, 137.51, 139.16, 140.34, 142.66, 143.85, 144.01, 144.05, 156.25, 156.51, 165.36, 195.38, 195.93, 196.28, 196.60.

IR (neat):3318, 3058, 1663, 1604, 1560, 1491, 1268, 1180, 745, 696 cm^{-1}

HRMS (ESI) calcd for $C_{31}H_{25}NNaO_3$ $[M+Na]^+$: 482.1727, found 482.1744.



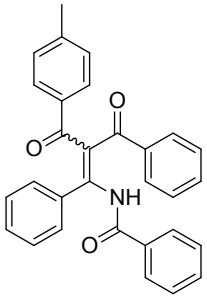
***N*-(2-benzoyl-3-(4-chlorophenyl)-3-oxo-1-phenylprop-1-en-1-yl)-4-chlorobenzamide (3c)**

Yellow solid, 78% yield (78 mg), mp 94-97 °C.

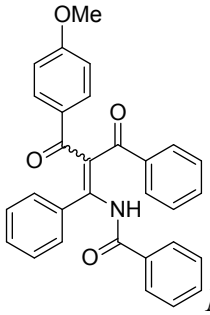
^{1}H NMR (400 MHz, $CDCl_3$) Obtained as 1 : 1 isomer. Isomer 1: δ 7.15-7.31 (m, 9H), 7.32-7.40 (m, 1H), 7.46-7.58 (m, 5H), 7.63 (d, *J* = 7.6 Hz, 1H), 7.98 (d, *J* = 8.0 Hz, 2H), 13.10 (s, 1H); Isomer 2: δ 13.24 (s, 1H); other peaks are overlapped with the other isomer.

^{13}C NMR (100 MHz, $CDCl_3$) δ 120.98, 121.26, 128.05, 128.12, 128.18, 128.48, 128.52, 128.63, 128.72, 128.77, 129.31, 129.52, 129.65, 129.70, 129.72, 129.97, 130.01, 130.61, 131.77, 132.18, 133.26, 133.73, 133.76, 137.35, 138.33, 138.42, 138.86, 139.48, 139.88, 140.00, 156.57, 156.64, 164.42, 194.43, 195.34, 195.60, 196.59.

IR (neat):3303, 3061, 1666, 1591, 1474, 1266, 1241, 1091, 1007, 845, 695 cm^{-1}
HRMS (ESI) calcd for $C_{29}H_{19}Cl_2NNaO_3$ $[M+Na]^+$: 522.0634, found 522.0645.



***N*-(2-benzoyl-3-oxo-1-phenyl-3-(*p*-tolyl)prop-1-en-1-yl)benzamide (3d)**
Yellow solid. 67% yield (60 mg), mp 161-163 °C.
^1H NMR (400 MHz, $CDCl_3$) Obtained as 1 : 1 isomer. Isomer 1: δ 2.27 (s, 3H), 7.05 (d, *J* = 7.6 Hz, 2H), 7.16-7.28 (m, 5H), 7.28-7.38 (m, 3H), 7.46-7.68 (m, 7H), 8.00-8.11 (m, 2H), 13.16 (s, 1H); Isomer 2: δ 7.00 (d, *J* = 8.0 Hz, 2H), 13.26 (s, 1H); other peaks are overlapped with the other isomer.
^{13}C NMR (100 MHz, $CDCl_3$) δ 21.23, 21.30, 121.34, 121.47, 127.98, 128.09, 128.31, 128.35, 128.41, 128.61, 128.74, 129.06, 129.14, 129.32, 129.51, 129.64, 131.88, 132.93, 133.20, 133.50, 134.09, 134.13, 136.62, 137.45, 139.13, 140.28, 142.81, 143.94, 156.00, 156.28, 165.45, 195.29, 195.84, 196.35, 196.69.
IR (neat):3303, 3060, 1664, 1603, 1559, 1475, 1269, 1240, 1179, 1011, 695 cm^{-1}
HRMS (ESI) calcd for $C_{30}H_{23}NNaO_3$ $[M+Na]^+$: 468.1570, found 468.1577.

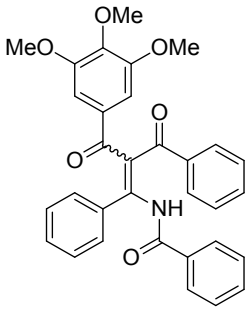


***N*-(2-benzoyl-3-(4-methoxyphenyl)-3-oxo-1-phenylprop-1-en-1-yl)benzamide (3e)**
Yellow solid. Yield 67% (62 mg), mp 72-76 °C.
^1H NMR (400 MHz, $CDCl_3$) Obtained as 1.5 : 1 isomer. Major isomer: δ 3.77 (s, 3H), 6.68 (d, *J* = 8.8 Hz, 2H), 7.17-7.29 (m, 5H), 7.29-7.38 (m, 3H), 7.46-7.55 (m, 2H), 7.55-7.62 (m, 2H), 7.63-7.70 (m, 3H), 7.99-8.09 (m, 2H), 13.21 (s, 1H); minor isomer: δ 6.75 (d, *J* = 8.4 Hz, 2H), 12.92 (s, 1 H); other peaks are overlapped with the other isomer.
^{13}C NMR (100 MHz, $CDCl_3$) δ 55.21, 113.58, 113.63, 121.50, 122.05, 127.99, 128.09, 128.22, 128.28, 128.40, 128.58, 128.83, 129.12, 129.31, 129.63, 131.02, 131.78,

131.88, 132.17, 132.50, 132.96, 133.08, 133.16, 133.53, 133.57, 134.16, 134.27, 139.10, 140.26, 154.99, 155.75, 163.12, 163.59, 165.47, 194.07, 194.93, 195.78, 196.64.

IR (neat):3316, 3062, 1663, 1572, 1596, 1476, 1313, 1254, 1171, 1025, 696 cm^{-1}

HRMS (ESI) calcd for $C_{30}H_{23}NNaO_4$ $[M+Na]^+$: 484.1519, found 484.1527.



***N*-(2-benzoyl-3-oxo-1-phenyl-3-(3,4,5-trimethoxyphenyl)prop-1-en-1-yl)benzamide (3f)**

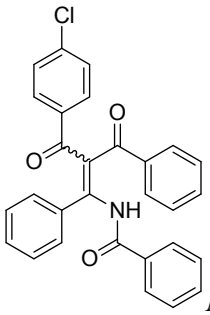
Orange solid. Yield 58% (60 mg), mp 214-218 °C.

^1H NMR (400 MHz, $CDCl_3$) Obtained as 1.5 : 1 isomer. Major isomer: δ 3.64 (s, 6H), 3.79 (s, 3H), 6.88 (s, 2H), 7.18-7.40 (m, 8H), 7.46-7.56 (m, 2H), 7.56-7.64 (m, 2H), 7.72 (d, *J* = 7.6 Hz, 1H), 8.05 (d, *J* = 7.6 Hz, 2H), 13.00 (s, 1H); Minor isomer: δ 3.78 (s, 6H), 3.82 (s, 3H), 6.92 (s, 2H), 8.02 (d, *J* = 8.0 Hz, 2H), 12.95 (s, 1H); other peaks are overlapped with the other isomer.

^{13}C NMR (100 MHz, $CDCl_3$) δ 55.75, 56.14, 60.72, 105.83, 107.00, 121.29, 121.48, 128.08, 128.16, 128.29, 128.43, 128.47, 128.61, 128.74, 129.19, 129.42, 129.77, 129.87, 132.06, 133.13, 133.27, 133.40, 133.48, 134.10, 134.19, 134.29, 134.98, 138.79, 140.16, 141.42, 142.54, 152.89, 153.04, 155.90, 156.05, 165.44, 165.51, 194.58, 195.20, 195.87, 196.60.

IR (neat):3313, 3062, 2938, 1663, 1580, 1464, 1413, 1329, 1240, 1124, 696 cm^{-1}

HRMS (ESI) calcd for $C_{32}H_{27}NNaO_6$ $[M+Na]^+$: 544.1731, found 544.1739.



***N*-(2-benzoyl-3-(4-chlorophenyl)-3-oxo-1-phenylprop-1-en-1-yl)benzamide (3g)**

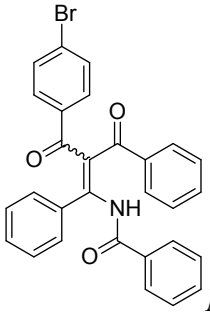
Light yellow solid. Yield 63% (59 mg), mp 149-152 °C.

^{1}H NMR (400 MHz, $CDCl_3$) Obtained as 1 : 1 isomer. Isomer 1: δ 7.12-7.40 (m, 10H), 7.46-7.68 (m, 7H), 8.03 (d, *J* = 8.0 Hz, 2H), 12.97 (s, 1H); Isomer 2: δ 13.13 (s, 1H); other peaks are overlapped with the other isomer.

^{13}C NMR (100 MHz, $CDCl_3$) δ 120.85, 121.17, 128.04, 128.11, 128.16, 128.29, 128.31, 128.44, 128.48, 128.65, 128.67, 128.73, 129.20, 129.32, 129.64, 129.91, 129.95, 130.62, 132.06, 133.17, 133.34, 133.96, 134.00, 137.44, 138.27, 138.42, 138.93, 139.37, 140.09, 156.56, 156.70, 165.43, 194.60, 195.19, 195.77, 196.45.

IR (neat):3311, 3060, 1664, 1585, 1559, 1475, 1267, 1238, 1089, 1009, 694 cm^{-1}

HRMS (ESI) calcd for $C_{29}H_{20}ClNNaO_3$ $[M+Na]^+$: 488.1024, found 488.1036.



***N*-(2-benzoyl-3-(4-bromophenyl)-3-oxo-1-phenylprop-1-en-1-yl)benzamide (3h)**

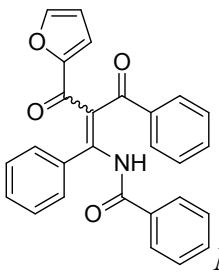
Bright yellow solid. Yield 76% (78 mg), mp 84-87 °C.

^{1}H NMR (400 MHz, $CDCl_3$) Obtained as 1 : 1 isomer. Isomer 1: δ 7.14-7.39 (m, 10H), 7.43-7.65 (m, 7H), 8.02 (d, *J* = 8.0 Hz, 2H), 12.87 (s, 1H); Isomer 2: δ 13.03 (s, 1H); other peaks are overlapped with the other isomer.

^{13}C NMR (100 MHz, $CDCl_3$) δ 120.93, 121.28, 126.78, 128.02, 128.08, 128.13, 128.23, 128.25, 128.40, 128.44, 128.64, 128.74, 129.15, 129.29, 129.72, 129.90, 129.94, 130.69, 131.60, 131.68, 132.05, 133.14, 133.29, 133.93, 133.99, 137.76, 138.76, 138.83, 139.98, 156.30, 156.46, 165.42, 194.79, 195.23, 195.76, 196.33.

IR (neat): 3302, 3062, 1664, 1582, 1559, 1267, 1238, 1069, 1008, 694 cm^{-1}

HRMS (ESI) calcd for $C_{29}H_{20}BrNNaO_3$ $[M+Na]^+$: 532.0519, found 532.0530.



***N*-(2-benzoyl-3-(furan-2-yl)-3-oxo-1-phenylprop-1-en-1-yl)benzamide (3i)**

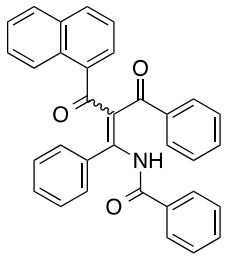
Yellow solid. Yield 73% (62 mg), mp 191-192 °C.

^{1}H NMR (400 MHz, $CDCl_3$) Obtained as 3.5 : 1 isomer. Major isomer: δ 6.39 (d, *J* = 2 Hz, 1H), 7.11 (d, *J* = 3.2 Hz, 1H), 7.13-7.44 (m, 9H), 7.47-7.54 (m, 2H), 7.55-7.75 (m, 3H), 8.00-8.12 (m, 2H), 13.80 (s, 1H); Minor isomer: δ 6.27 (s, 1H), 6.84 (d, *J* = 3.2 Hz, 1H), 13.27 (s, 1H); other peaks are overlapped with the other isomer.

^{13}C NMR (100 MHz, $CDCl_3$) δ 112.58, 112.68, 118.41, 118.80, 119.94, 127.86, 127.94, 128.02, 128.37, 128.42, 128.47, 128.62, 129.16, 129.26, 129.38, 129.77, 131.96, 133.18, 133.22, 133.29, 133.40, 133.44, 133.69, 133.77, 139.10, 140.23, 146.62, 147.10, 152.21, 154.17, 157.06, 157.52, 165.19, 165.40, 180.01, 182.63, 195.65, 196.24.

IR (neat):3305, 3060, 1660, 1556, 1462, 1288, 1228, 1041, 1022, 763, 696 cm^{-1}

HRMS (ESI) calcd for $C_{27}H_{19}NNaO_4$ $[M+Na]^+$: 444.1206, found 444.1218.



***N*-(2-(1-naphthoyl)-3-oxo-1,3-diphenylprop-1-en-1-yl)benzamide (3j)**

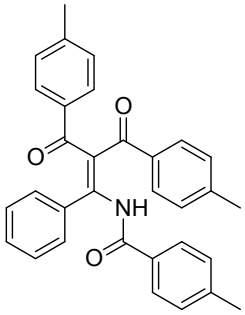
Yellow solid. Yield 66% (64 mg), mp 166-168^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) Obtained as 4 : 1 isomer.Major isomer: δ 6.92-7.80 (m, 19H), 8.13 (d, *J* = 8.0 Hz, 3H), 13.87 (s, 1H). Minor isomer: δ 7.96 (d, *J* = 7.2 Hz, 1H), 8.03 (d, *J* = 7.6 Hz, 2H), 8.45 (d, *J* = 8.4 Hz, 1H), 13.01 (s, 1H); other peaks are overlapped with the other isomer.

^{13}C NMR (100 MHz, $CDCl_3$) δ 122.01, 123.41, 123.97, 124.11, 125.34, 125.47, 125.87, 126.44, 127.26, 127.81, 127.92, 128.00, 128.04, 128.25, 128.27, 128.36, 128.45, 128.87, 129.12, 129.18, 129.74, 129.84, 130.30, 130.46, 131.01, 131.57, 132.52, 133.22, 133.32, 133.36, 133.52, 133.55, 133.67, 133.92, 134.25, 136.99, 138.09, 138.90, 140.35, 157.08, 158.22, 165.41, 165.49, 195.26, 196.55, 197.40, 198.11.

IR (neat):3303, 3058, 2926, 1663, 1597, 1557, 1491, 1246, 977, 793, 693 cm^{-1}

HRMS (ESI) calcd for $C_{33}H_{23}NNaO_3$ $[M+Na]^+$: 504.1570, found 504.1579.



4-methyl-*N*-(2-(4-methylbenzoyl)-3-oxo-1-phenyl-3-(*p*-tolyl)prop-1-en-1-yl)benzamide (3k)

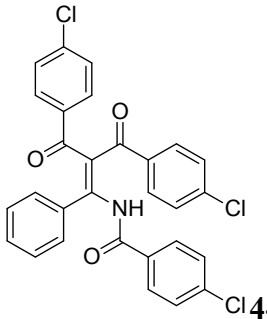
Pale yellow solid. Yield 62% (59 mg), mp 97-99 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.26 (s, 6H), 2.41 (s, 3H), 7.00 (d, *J* = 7.6 Hz, 2H), 7.04 (d, *J* = 8.0 Hz, 2H), 7.14-7.35 (m, 7H),7.51 (d, *J* = 7.6 Hz, 2H), 7.56 (d, *J* = 8.0 Hz, 2H), 7.94 (d, *J* = 7.6 Hz, 2H), 13.17 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 21.20, 21.29, 121.30, 127.88, 128.34, 128.36, 128.63, 129.00, 129.08, 129.46, 129.50, 129.78, 130.74, 134.25, 136.65, 137.55, 142.64, 143.83, 143.95, 155.88, 165.37, 195.42, 196.24.

IR (neat):3312, 3028, 2921, 1663, 1603, 1559, 1267, 1180, 1010, 821, 744 cm^{-1}

HRMS (ESI) calcd for $C_{32}H_{27}NNaO_3$ $[M+Na]^+$: 496.1883, found 496.1884.



4-chloro-*N*-(2-(4-chlorobenzoyl)-3-(4-chlorophenyl)-3-oxo-1-phenylprop-1-en-1-yl) benzamide (3l)

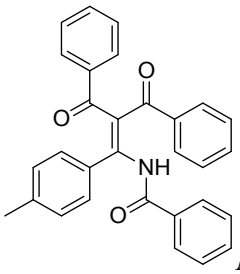
Pale yellow solid. Yield 80% (86 mg), mp 176-178 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.14-7.31 (m, 9H), 7.44-7.54 (m, 4H), 7.57 (d, *J* = 8.4 Hz, 2H), 7.96 (d, *J* = 8.0 Hz, 2H), 12.97 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 120.91, 128.26, 128.70, 128.82, 128.89, 129.55, 129.63, 129.68, 130.20, 130.61, 131.66, 133.68, 137.13, 138.14, 138.61, 139.73, 139.97, 156.55, 164.40, 194.38, 195.05.

IR (neat):3315, 3063, 1664, 1586, 1476, 1265, 1091, 1007, 845, 751, 698 cm^{-1}

HRMS (ESI) calcd for $C_{29}H_{18}Cl_3NNaO_3$ $[M+Na]^+$: 556.0244, found 556.0255.



***N*-(2-benzoyl-3-oxo-3-phenyl-1-(*p*-tolyl)prop-1-en-1-yl)benzamide (3m)**

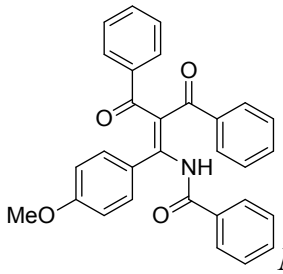
Yellow solid. Yield 69% (61 mg), mp 177-179 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ2.24 (s, 3H), 7.01 (d, *J* = 7.6 Hz, 2H), 7.14-7.27 (m, 6H), 7.27-7.35 (m, 2H), 7.46-7.52 (m, 2H), 7.53-7.60 (m, 3H), 7.64 (d, *J* = 7.2 Hz, 2H), 8.05 (d, *J* = 7.6 Hz, 2H), 13.12 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 21.11, 121.21, 128.04, 128.28, 128.62, 128.81, 129.11, 129.29, 131.13, 131.80, 132.84, 133.18, 133.47, 139.17, 139.95, 140.26, 156.83, 165.49, 195.92, 196.62.

IR (neat):3313. 3059, 1664, 1596, 1577, 1473, 1269, 1238, 1011, 735, 692 cm^{-1}

HRMS (ESI) calcd for $C_{30}H_{23}NNaO_3$ $[M+Na]^+$: 468.1570, found 468.1577.



***N*-(2-benzoyl-1-(4-methoxyphenyl)-3-oxo-3-phenylprop-1-en-1-yl)benzamide(3n)**

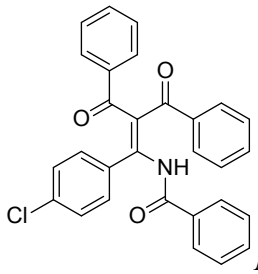
Bright yellow solid. Yield 41% (38 mg), mp 207-210 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.72 (s, 3H), 6.72 (d, *J* = 7.6 Hz, 2H), 7.16-7.29 (m, 6H), 7.30-7.39 (m, 2H), 7.50-7.53 (m, 2H), 7.54-7.63 (m, 3H), 7.65 (d, *J* = 7.2 Hz, 2H), 8.05 (d, *J* = 7.6 Hz, 2H), 12.98 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 55.01, 113.56, 121.37, 126.32, 128.11, 128.30, 128.38, 129.16, 129.30, 130.58, 131.81, 132.90, 133.22, 133.60, 139.19, 140.28, 156.33, 161.01, 165.69, 196.09, 196.66.

IR (neat):3318, 3063, 1663, 1597, 1560, 1509, 1252, 1176, 1025, 736, 692 cm^{-1}

HRMS (ESI) calcd for $C_{30}H_{23}NNaO_4$ $[M+Na]^+$: 484.1519, found 484.1528.



***N*-(2-benzoyl-1-(4-chlorophenyl)-3-oxo-3-phenylprop-1-en-1-yl)benzamide (3o)**

Yellow solid. Yield 58% (54 mg), mp 181-183 °C.

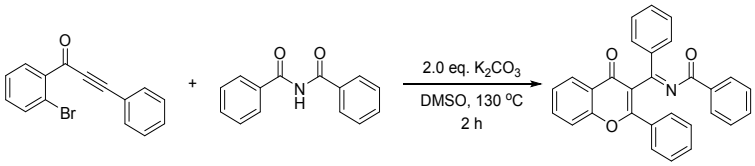
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.11-7.29 (m, 8H), 7.29-7.40 (m, 2H), 7.45-7.67 (m, 7H), 8.05 (d, *J* = 7.6 Hz, 2H), 13.34 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 121.24, 128.10, 128.29, 128.34, 128.39, 128.52, 129.23, 130.03, 132.10, 132.40, 133.19, 133.24, 133.41, 135.82, 139.01, 140.09, 155.56, 165.50, 195.52, 196.65.

IR (neat):3303, 3061, 1663, 1596, 1576, 1556, 1487, 1266, 1239, 1013, 702 cm^{-1}

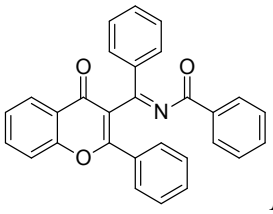
HRMS (ESI) calcd for $C_{29}H_{20}ClNNaO_3$ $[M+Na]^+$: 488.1024, found 488.1034.

General Procedure for the preparation of 5



4a 1.0 eq. **2a** 2.0 eq. **5a**

Under N_2 atmosphere, in a dried Schlenk tube ynone **4a** (0.20 mmol, 57.0 mg) and DMSO (3 mL) were added, and K_2CO_3 (0.40 mmol, 55.2 mg), and imide **2a** (0.40 mmol, 90.1 mg) were added subsequently, and mixture was stirred at 130 °C. After the reaction was complete as monitored by thin-layer chromatography, the reaction mixture was then quenched by water, and the mixture were extracted with ethyl acetate (15 mL × 3). The combined organic layer was washed with water (15 mL× 2), brine (15 mL), and dried over with anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure, Purification by chromatography on silica gel (petroleum ether / ethyl acetate = 10/1) afforded desired compound **5a**.



***N*-((4-oxo-2-phenyl-4*H*-chromen-3-yl)(phenyl)methyl-ene)benzamide (5a)**

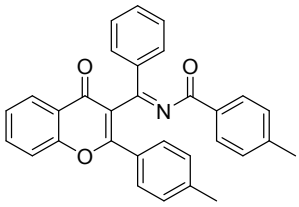
Light yellow solid. Yield 75% (64 mg), mp 79-81 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.20-7.28 (m, 3H), 7.28-7.48 (m, 8H), 7.52 (d, *J* = 8.4Hz, 1H), 7.63-7.76 (m, 3H), 7.83-7.96 (m, 4H), 8.13 (d, *J* = 7.6 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 118.21, 118.68, 122.92, 125.68, 126.52, 128.28, 128.67, 128.74, 128.83, 128.94, 129.82, 131.54, 132.22, 132.37, 132.95, 133.10, 134.40, 137.02, 156.40, 162.86, 163.53, 175.64, 180.02.

IR (neat):3062, 2925, 1662, 1644, 1617, 1464, 1375, 1239, 1049, 761, 689 cm^{-1}

HRMS (ESI) calcd for $C_{29}H_{19}NNaO_3$ $[M+Na]^+$: 452.1257, found 452.1265.



4-methyl-*N*-((4-oxo-2-(*p*-tolyl)-4*H*-chromen-3-yl)(phenyl)methylene)benzamide (5b)

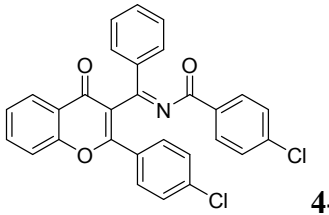
Pale yellow solid. Yield 66% (60 mg), mp 224-226 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ2.29 (s, 3H), 2.36 (s, 3H), 7.04 (d, *J* = 8.0 Hz, 2H), 7.10 (d, *J* = 8.0 Hz, 2H), 7.32-7.41 (m, 3H), 7.42-7.53 (m, 2H), 7.58 (d, *J* = 7.6 Hz, 2H), 7.64-7.71 (m, 1H), 7.76 (d, *J* = 8.0 Hz, 2H), 7.92 (d, *J* = 7.2Hz, 2H),8.12 (d, *J* = 7.6 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 21.20, 21.46, 118.17, 118.31, 122.97, 125.53, 126.51, 128.60, 128.85, 128.94, 129.45, 129.55, 129.88, 130.46, 132.12, 134.26, 137.16, 142.08, 143.54, 156.40, 162.89, 163.37, 175.76, 179.97.

IR (neat):3062, 2922, 1663, 1644, 1616, 1464, 1372, 1239, 1174, 1050, 761 cm^{-1}

HRMS (ESI) calcd for $C_{31}H_{23}NNaO_3$ $[M+Na]^+$: 480.1570, found 480.1579.



4-chloro-*N*-((2-(4-chlorophenyl)-4-oxo-4*H*-chromen-3-yl)(phenyl)methylene)benzamide (5c)

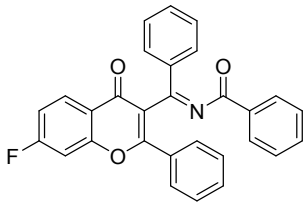
Pale white solid. Yield 85% (85 mg), mp 181-182 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ7.24 (d, *J* = 8.4 Hz, 2H), 7.29-7.43 (m, 5H), 7.43-7.49 (m, 1H), 7.52 (d, *J* = 8.4 Hz, 1H), 7.65 (d, *J* = 8.4 Hz, 2H), 7.68-7.75 (m, 1H), 7.80-7.90 (m, 4H), 8.12 (d, *J* = 8.0Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 118.20, 118.63, 122.82, 125.92, 126.55, 128.68, 128.93, 128.99, 129.14, 130.01, 130.70, 131.22, 131.50, 132.63, 134.63, 136.61, 138.13, 139.55, 156.31, 161.71, 163.77, 175.38, 179.09.

IR (neat):3066, 1664, 1617, 1592, 1465, 1375, 1245, 1091, 1050, 1013, 760 cm^{-1}

HRMS (ESI) calcd for $C_{29}H_{17}Cl_2NNaO_3$ $[M+Na]^+$: 520.0478, found 520.0490.



***N*-((7-fluoro-4-oxo-2-phenyl-4*H*-chromen-3-yl)(phenyl)methylene)benzamide (5d)**

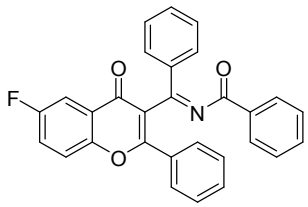
Yellow solid. Yield 67% (60 mg), mp 133-136 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ7.05-7.15 (m, 1H), 7.16-7.27 (m, *3*H), 7.27-7.40 (m, 5H), 7.40-7.49 (m, 2H), 7.67 (d, *J* = 7.6 Hz, 2H), 7.79-7.94 (m, 4H), 8.14 (dd, J_1 = 8.4 Hz, J_2 = 6.4 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 104.86 (d, *J* = 25.4 Hz), 114.46 (d, *J* = 22.8 Hz), 118.75, 119.72, 128.29, 128.60, 128.78, 128.87, 128.90, 129.12 (d, *J* = 10.6 Hz), 129.78, 131.69, 131.96, 132.33, 133.01, 136.87, 157.37 (d, *J* = 13.4 Hz), 163.03, 163.24, 166.31 (d, *J* = 256.0 Hz), 174.73, 179.97.

IR (neat):3064, 2928, 1652, 1618, 1440, 1372, 1240, 1155, 1048, 766, 692 cm^{-1}

HRMS (ESI) calcd for $C_{29}H_{19}FNO_3$ $[M+H]^+$: 448.1343, found 448.1344.



***N*-((6-fluoro-4-oxo-2-phenyl-4*H*-chromen-3-yl)(phenyl)methylene)benzamide (5e)**

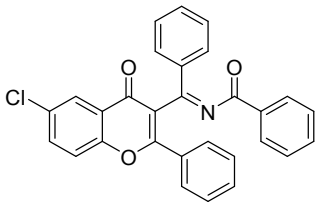
Pale white solid. Yield 75% (67mg), mp 182-184 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21-7.29 (m, 2H), 7.29-7.40 (m, *5*H), 7.40-7.49 (m, 3H), 7.53 (dd,J_1 = 9.2 Hz, J_2 = 4.0 Hz, 1H), 7.70 (d, *J* = 7.6 Hz, 2H), 7.76 (dd, J_1 = 8.0 Hz, J_2 = 3.2 Hz, 1H), 7.88 (d, *J* = 8.0 Hz, 4H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 111.32 (d, *J* = 24.0 Hz), 118.01, 120.40 (d, *J* = 8.2 Hz), 122.60 (d, *J* = 25.6 Hz), 124.11 (d, *J* = 7.5 Hz), 128.32, 128.68, 128.79, 128.87, 128.92, 129.80, 131.70, 132.12, 132.33, 133.05, 136.87, 152.61, 160.05 (d, *J* = 247.4 Hz), 163.14, 163.28, 174.90, 180.01.

IR (neat):3061, 2927, 1663, 1644, 1624, 1478, 1449, 1367, 1239, 1048, 689 cm^{-1}

HRMS (ESI) calcd for $C_{29}H_{19}FNO_3$ $[M+H]^+$: 448.1343, found 448.1347.



***N*-((6-chloro-4-oxo-2-phenyl-4*H*-chromen-3-yl)(phenyl)methylene)benzamide (5f)**

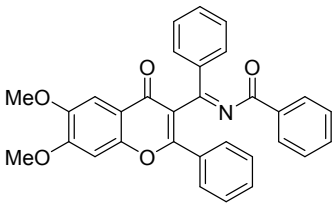
Pale white solid. Yield 62% (57 mg), mp 185-188 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21-7.28 (m, 2H), 7.29-7.39 (m, 5H), 7.41-7.51 (m, 3H), 7.64 (dd,J_1 = 9.2 Hz, J_2 = 2.4 Hz, 1H), 7.70 (d, *J* = 7.6 Hz, 2H), 7.82-7.92 (m, 4H), 8.08 (d, *J* = 2.0 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 118.61, 119.99, 123.87, 125.90, 128.34, 128.70, 128.81, 128.89, 128.92, 129.84, 131.77, 132.05, 132.36, 133.02, 133.10, 134.64, 136.81, 154.73, 163.13, 174.50, 180.02.

IR (neat):3064, 1648, 1611, 1559, 1447, 1432, 1359, 1237, 1048, 767, 723, 687 cm^{-1}

HRMS (ESI) calcd for $C_{29}H_{18}ClNNaO_3$ $[M+Na]^+$: 486.0867, found 486.0876.



***N*-((6,7-dimethoxy-4-oxo-2-phenyl-4*H*-chromen-3-yl)(phenyl)methylene)benzamide (5g)**

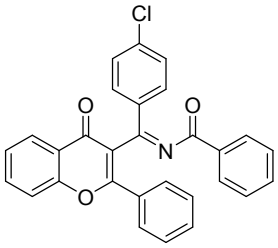
Yellow solid. Yield 56% (55 mg), mp 214-216 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.92 (s, 3H), 3.98 (s, 3H), 6.94 (s, 1H), 7.20-7.27 (m, 2H), 7.28-7.39 (m, 5H), 7.40-7.48 (m, 3H), 7.67 (d, *J* = 7.6 Hz, 2H), 7.89 (d, *J* = 7.2 Hz, 4H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 56.20, 56.36, 99.68, 104.91, 116.23, 118.12, 128.23, 128.51, 128.63, 128.75, 128.90, 129.76, 131.23, 132.10, 132.45, 132.84, 133.15, 137.15, 148.15, 152.47, 155.13, 162.03, 163.84, 174.69, 179.93.

IR (neat):3061, 1619, 1427, 1363, 1237, 1173, 1050, 720, 690 cm^{-1}

HRMS (ESI) calcd for $C_{31}H_{23}NNaO_5$ $[M+Na]^+$: 512.1468, found 512.1478.



***N*-((4-chlorophenyl)(4-oxo-2-phenyl-4*H*-chromen-3-yl)methylene)benzamide (5h)**

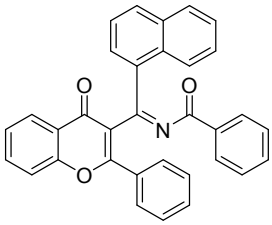
Light yellow solid. Yield 73% (68 mg), mp 190-193 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22-7.40 (m, 8H), 7.41-7.47 (m, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.62-7.73 (m, 3H), 7.84 (d, *J* = 8.4 Hz, 2H), 7.87 (d, *J* = 8.0 Hz, 2H),8.10 (d, *J* = 7.6 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 118.17, 118.20, 122.79, 125.76, 126.42, 128.29, 128.57, 128.80, 129.13, 129.76, 130.20, 131.70, 132.16, 132.92, 133.04, 134.50, 135.52, 138.50, 156.34, 162.54, 162.99, 175.50, 179.83.

IR (neat):3063, 1663, 1644, 1618, 1587, 1464, 1375, 1239, 1050, 761 cm^{-1}

HRMS (ESI) calcd for $C_{29}H_{18}ClNNaO_3$ $[M+Na]^+$: 486.0867, found 486.0874.



***N*-(naphthalen-1-yl(4-oxo-2-phenyl-4*H*-chromen-3-yl)methylene)benzamide (5i)**

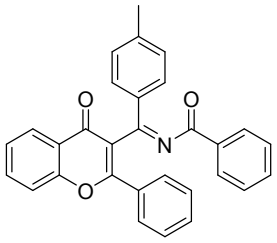
Light yellow solid. Yield 33% (32 mg), mp 185-188 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.07-7.15 (m, 3H), 7.21-7.28 (m, 1H), 7.34-7.52 (m, 7H), 7.55 (d, *J* = 7.2 Hz, 1H), 7.66-7.81 (m, 5H), 8.06 (d, *J* = 7.6 Hz, 2H), 8.16 (d, *J* = 8.0 Hz, 1H), 8.85 (d, *J* = 8.4 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 118.26, 121.40, 123.12, 124.44, 125.73, 126.17, 126.36, 126.74, 127.61, 128.29, 128.46, 128.59, 128.74, 130.15, 130.22, 130.97, 131.13, 132.21, 132.49, 132.94, 133.60, 133.94, 134.40, 135.09, 156.34, 164.15, 164.50, 175.19, 179.59.

IR (neat):3061, 2925, 1660, 1617, 1464, 1376, 1256, 1230, 1047, 1020, 763 cm^{-1}

HRMS (ESI) calcd for $C_{33}H_{21}NNaO_3$ $[M+Na]^+$: 502.1414, found 502.1425.



***N*-((4-oxo-2-phenyl-4*H*-chromen-3-yl)(*p*-tolyl)methylene)benzamide (5j)**

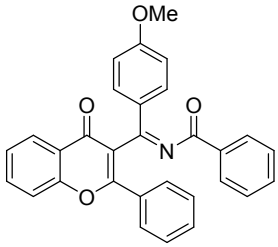
Yellow solid. Yield 80 % (71mg), mp 191-194 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.34 (s, 3H), 7.16 (d, *J* = 7.6 Hz, 2H), 7.20-7.39 (m, 6H), 7.39-7.46 (m, 1H), 7.49 (d, *J* = 8.4 Hz, 1H), 7.62-7.74 (m, 3H), 7.81 (d, *J* = 7.6 Hz, 2H), 7.86 (d, *J* = 7.6 Hz, 2H), 8.12 (d, *J* = 7.6 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 21.24, 118.15, 118.78, 122.88, 125.59, 126.44, 128.21, 128.60, 128.67, 128.96, 129.61, 129.73, 131.44, 132.36, 132.80, 133.16, 134.33, 142.97, 156.35, 162.53, 163.33, 175.70, 179.96.

IR (neat):3061, 1659, 1644, 1617, 1600, 1464, 1374, 1237, 1051, 1021, 764 cm^{-1}

HRMS (ESI) calcd for $C_{30}H_{21}NNaO_3$ $[M+Na]^+$: 466.1414, found 466.1428.



***N*-((4-methoxyphenyl)(4-oxo-2-phenyl-4*H*-chromen-3-yl)methylene)benzamide (5k)**

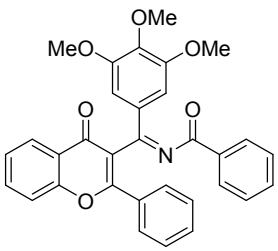
Orange solid. Yield 86 % (79mg), mp 167-170 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ3.79 (s, 3H), 6.86 (d, *J* = 8.8 Hz, 2H), 7.18-7.38 (m, 6H), 7.39-7.45 (m, 1H), 7.49 (d, *J* = 8.4 Hz, 1H), 7.60-7.74 (m, 3H), 7.79-7.95 (m, 4H), 8.12 (d, *J* = 8.0 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 55.22, 114.14, 118.13, 118.73, 122.84, 125.56, 126.40, 128.17, 128.56, 128.65, 129.64, 129.69, 130.96, 131.42, 132.36, 132.73, 133.32, 134.31, 156.31, 162.38, 162.72, 163.12, 175.65, 179.92.

IR (neat):3063, 2930, 1654, 1596, 1464, 1375, 1239, 1174, 1163, 1051, 1021 cm^{-1}

HRMS (ESI) calcd for $C_{30}H_{21}NNaO_4$ $[M+Na]^+$: 482.1363, found 482.1370.



***N*-((4-oxo-2-phenyl-4*H*-chromen-3-yl)(3,4,5-trimethoxyphenyl)methylene)benzamide (5l)**

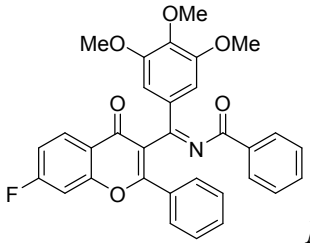
Yellow solid. Yield 95% (98 mg), mp 191-193 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.80 (s, 6H), 3.89 (s, 3H). 7.17 (s, 2H), 7.25-7.34 (m, 4H), 7.34-7.48 (m, 3H), 7.53 (d, *J* = 8.4 Hz, 1H), 7.66-7.75 (m, 3H), 7.85 (d, *J* = 7.6 Hz, 2H), 8.13 (d, *J* = 8.0 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 56.14, 60.72, 106.41, 118.18, 118.43, 122.74, 125.67, 126.43, 128.21, 128.53, 128.78, 129.68, 131.58, 132.21, 132.31, 132.88, 132.97, 134.41, 142.03, 153.45, 156.30, 162.65, 162.81, 175.58, 179.80.

IR (neat):3063, 2937, 1654, 1617, 1578, 1464, 1375, 1261, 1126, 1050, 763 cm^{-1}

HRMS (ESI) calcd for $C_{32}H_{25}NNaO_6$ $[M+Na]^+$: 542.1574, found 542.1581.



***N*-((7-fluoro-4-oxo-2-phenyl-4*H*-chromen-3-yl)(3,4,5-trimethoxyphenyl)methylene)benzamide (5m)**

Light yellow solid. Yield 78% (84 mg), mp 183-186 °C.

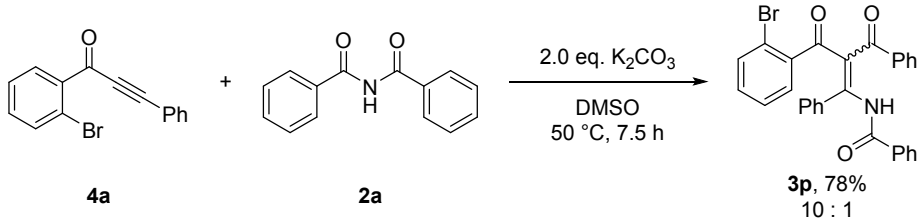
^{1}H NMR (400 MHz, $CDCl_3$) δ 3.81 (s, 6H), 3.89 (s, 3H), 7.12 (dd, J_1 = 8.8 Hz, J_2 = 2.0 Hz, 1H), 7.16 (s, 2H), 7.21 (dd, J_1 = 8.8 Hz, J_2 = 2.0 Hz, 1H), 7.24-7.34 (m, 4H), 7.34-7.40 (m, 1H), 7.42-7.48 (m, 1H), 7.69 (d, *J* = 7.6 Hz, 2H), 7.84 (d, *J* = 7.6 Hz, 2H), 8.14 (dd, J_1 = 8.4 Hz, J_2 = 6.0 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 56.17, 60.72, 104.86 (d, *J* = 25.4 Hz), 106.45, 114.48 (d, *J* = 22.8 Hz), 118.51, 119.58, 128.23, 128.49, 128.84, 129.08 (d, *J* = 10.6 Hz), 129.68, 131.75, 131.93, 132.05, 132.93, 132.95, 142.18, 153.49, 157.30 (d, *J* = 13.4 Hz), 162.52, 162.86, 166.29 (d, *J* = 255.9 Hz), 174.70, 179.79.

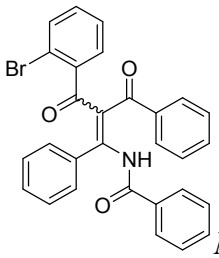
IR (neat):3063, 2938, 1663, 1617, 1578, 1439, 1370, 1255, 1126, 1047, 726 cm^{-1}

HRMS (ESI) calcd for $C_{32}H_{24}FNNaO_6$ $[M+Na]^+$: 560.1480, found 560.1485.

3. Control Experiment



Under N_2 atmosphere, in a dried Schlenk tube ynone **4a** (0.20 mmol, 57.0 mg), K_2CO_3 (0.40 mmol, 55.2 mg), and imide **2a** (0.40 mmol, 90.1 mg) and DMSO (3 mL) were added, and mixture was stirred at 50 °C. After the reaction was complete as monitored by thin-layer chromatography, the reaction mixture was then quenched by water, and the mixture were extracted with ethyl acetate (15 mL × 3). The combined organic layer was washed with water (15 mL× 2), brine (15 mL), and dried over with anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure, Purification by chromatography on silica gel (petroleum ether / ethyl acetate = 10/1) afforded desired compound **3p** in 78% yield (79 mg).



***N*-(2-benzoyl-3-(2-bromophenyl)-3-oxo-1-phenylprop-1-en-1-yl)benzamide (3p)**

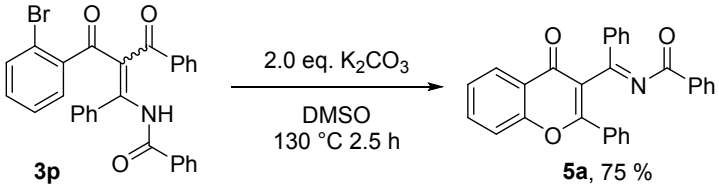
Yellow solid. Yield 78% (79 mg), mp 136-138 °C.

^{1}H NMR (400 MHz, $CDCl_3$) Obtained as 10 : 1 isomer. Major isomer: δ 7.02-7.11 (m, 1H), 7.12-7.27 (m, 6H), 7.27-7.34 (m, 3H), 7.34-7.41 (m, 1H), 7.45-7.82 (m, 5H), 8.12 (d, *J* = 7.2 Hz, 2H), 13.79 (s, 1H); minor isomer: δ 8.02 (d, *J* = 7.2 Hz, 2H), 13.05 (s, 1H); other peaks are overlapped with the other isomer.

^{13}C NMR (100 MHz, $CDCl_3$) δ 119.02, 120.55, 126.77, 128.08, 128.12, 128.29, 128.30, 128.50, 128.52, 128.91, 129.22, 129.97, 130.96, 132.86, 133.12, 133.19, 133.50, 133.82, 138.96, 141.34, 159.21, 165.52, 195.06, 195.84.

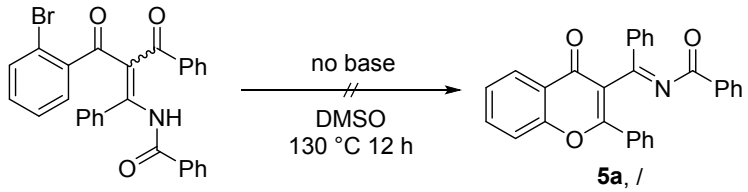
IR (neat):3063, 1701, 1597, 1581, 1559, 1491, 1244, 1008, 764, 695 cm^{-1}

HRMS (ESI) calcd for $C_{29}H_{20}BrNNaO_3$ $[M+Na]^+$: 532.0519, found 532.0528.



Under N_2 atmosphere, in a dried Schlenk intermediate **3p** (0.156 mmol, 79.0 mg),

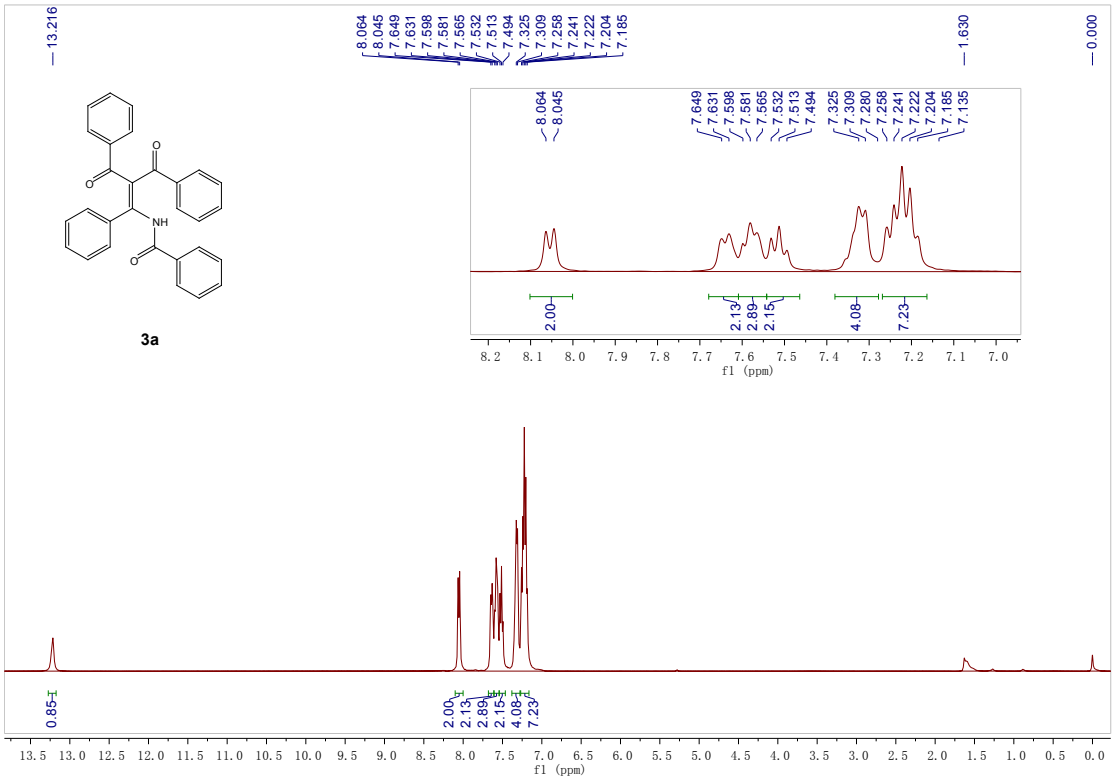
K_2CO_3 (0.312 mmol, 42.5 mg)and DMSO (2.5 mL) were added, and mixture was stirred at 130 °C. After the reaction was complete as monitored by thin-layer chromatography, the reaction mixture was then quenched by water, and the mixture were extracted with ethyl acetate (15 mL × 3). The combined organic layer was washed with water (15 mL× 2), brine (15 mL), and dried over with anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure, Purification by chromatography on silica gel (petroleum ether / ethyl acetate = 5/1) afforded compound **5a** in 75% yield (50.2 mg).

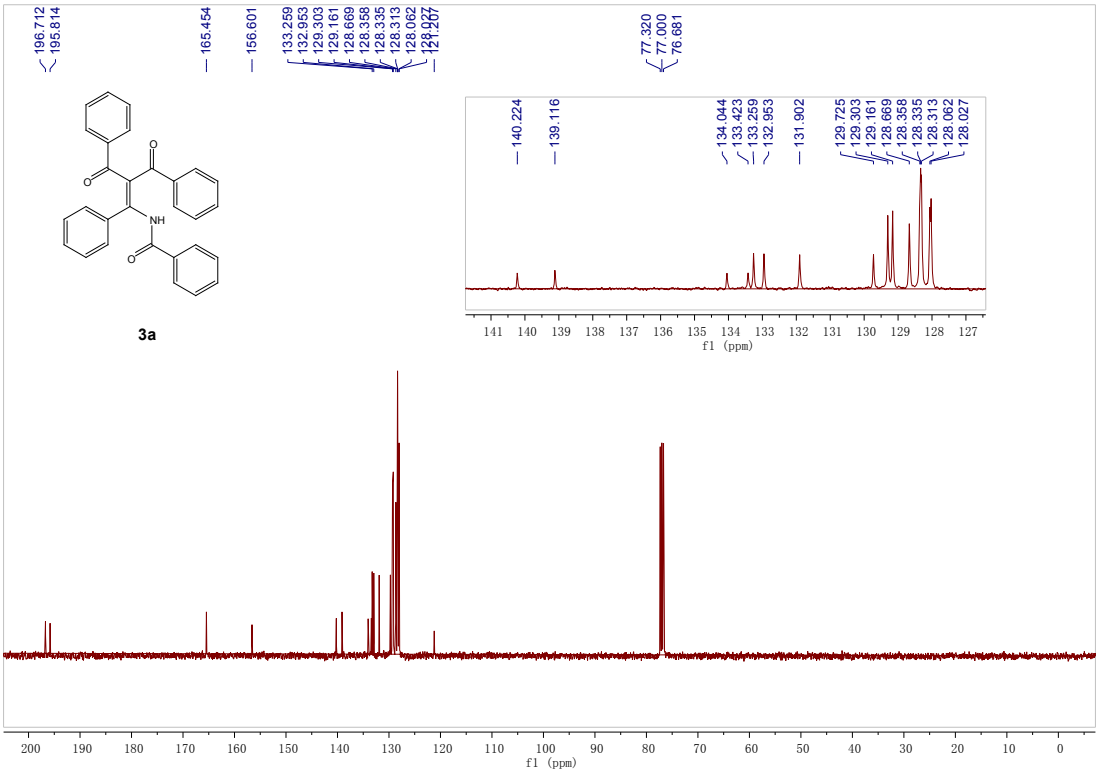


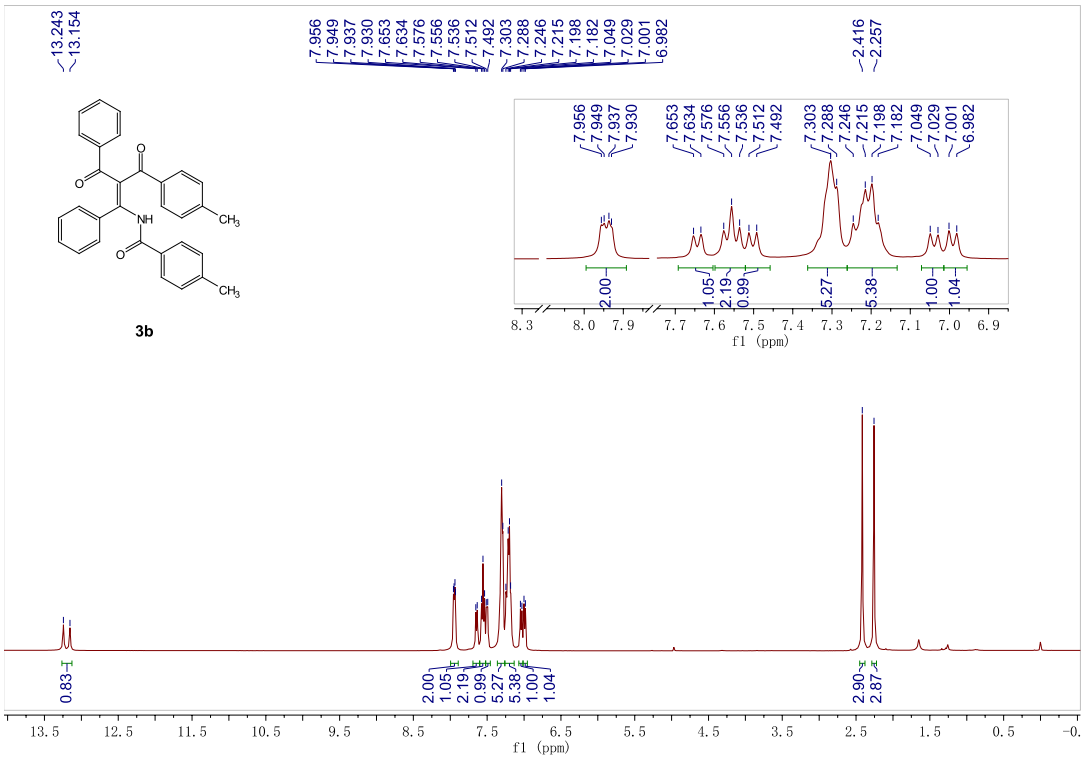
3p **5a**, /
(85 % recovery of **3p**)

Under N_2 atmosphere, in a dried Schlenk tube intermediate **3p** (0.11 mmol, 59.0 mg) and DMSO (1.5 mL) were added, and mixture was stirred at 130 °C. After 12 h the reaction mixture was quenched by water, and the mixture were extracted with ethyl acetate (15 mL × 3). The combined organic layer was washed with water (15 mL× 2), brine (15 mL), and dried over with anhydrous Na_2SO_4, filtered, and concentrated under reduced pressure, Purification by chromatography on silica gel (petroleum ether / ethyl acetate = 10/1) recovered 85% compound **3o** (50.2 mg).

4. Copies of Spectra of New Products



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7.303
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7.246
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7.198
7.182
7.049
7.029
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2.416
2.257
3b
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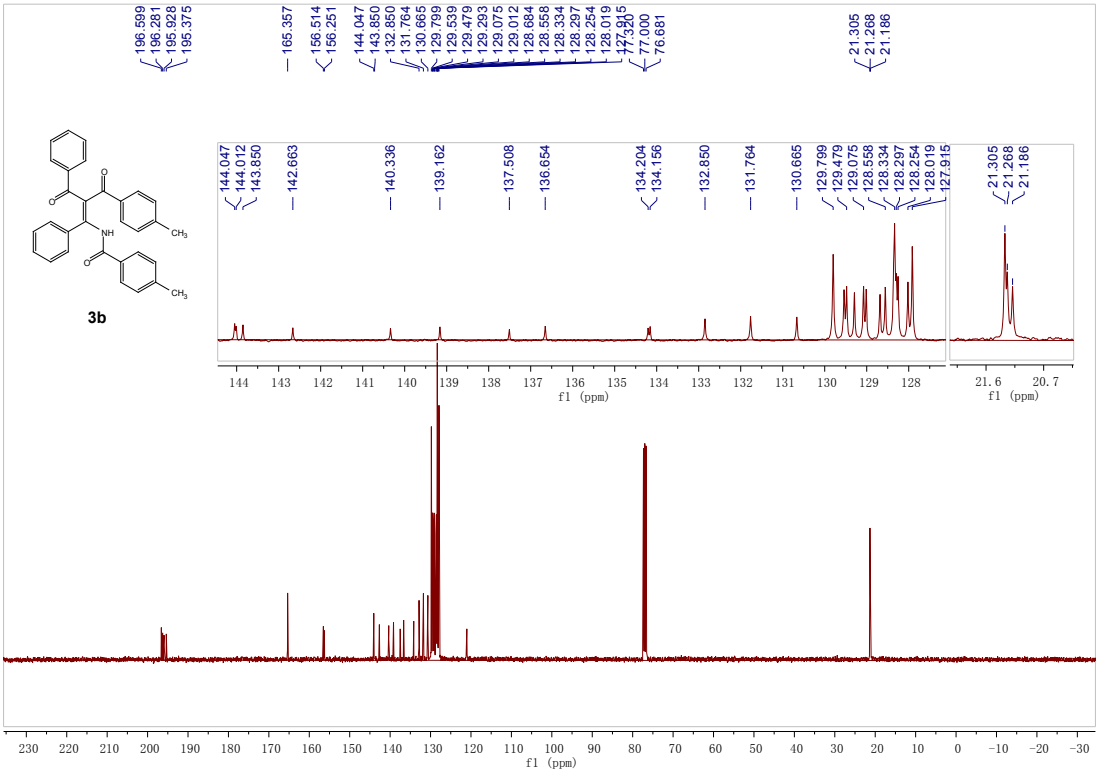
f1 (ppm)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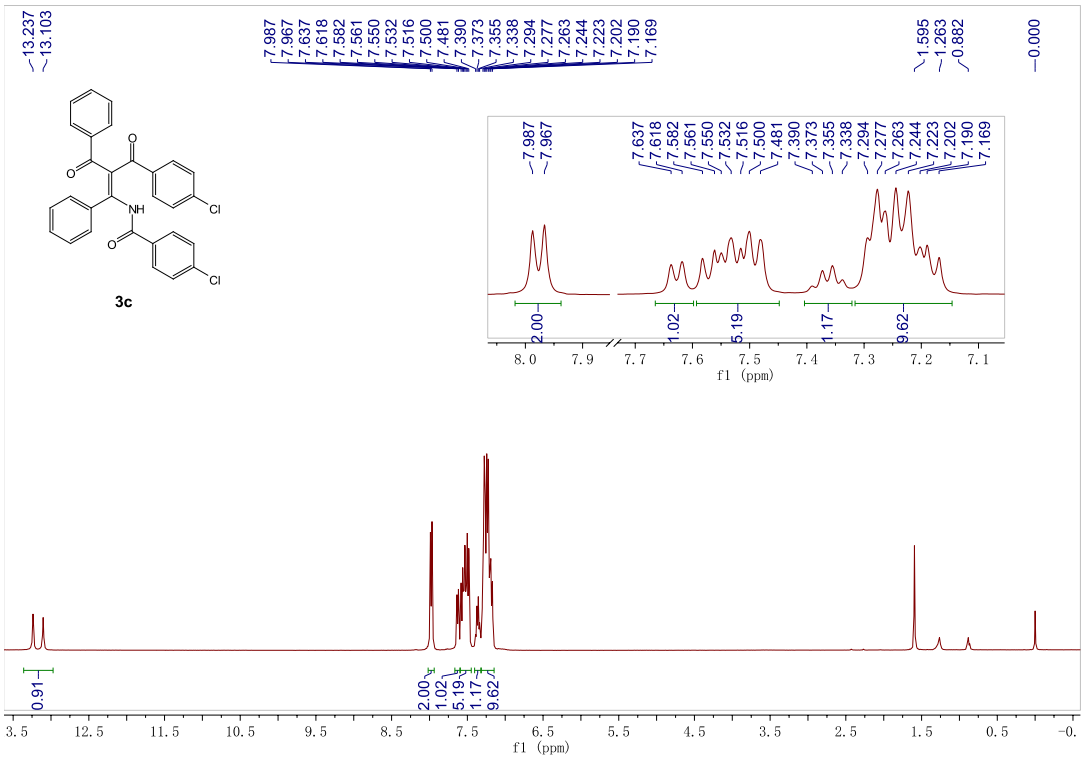
3b
f1 (ppm)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7.481
7.390
7.373
7.355
7.338
7.294
7.277
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7.202
7.190
7.169
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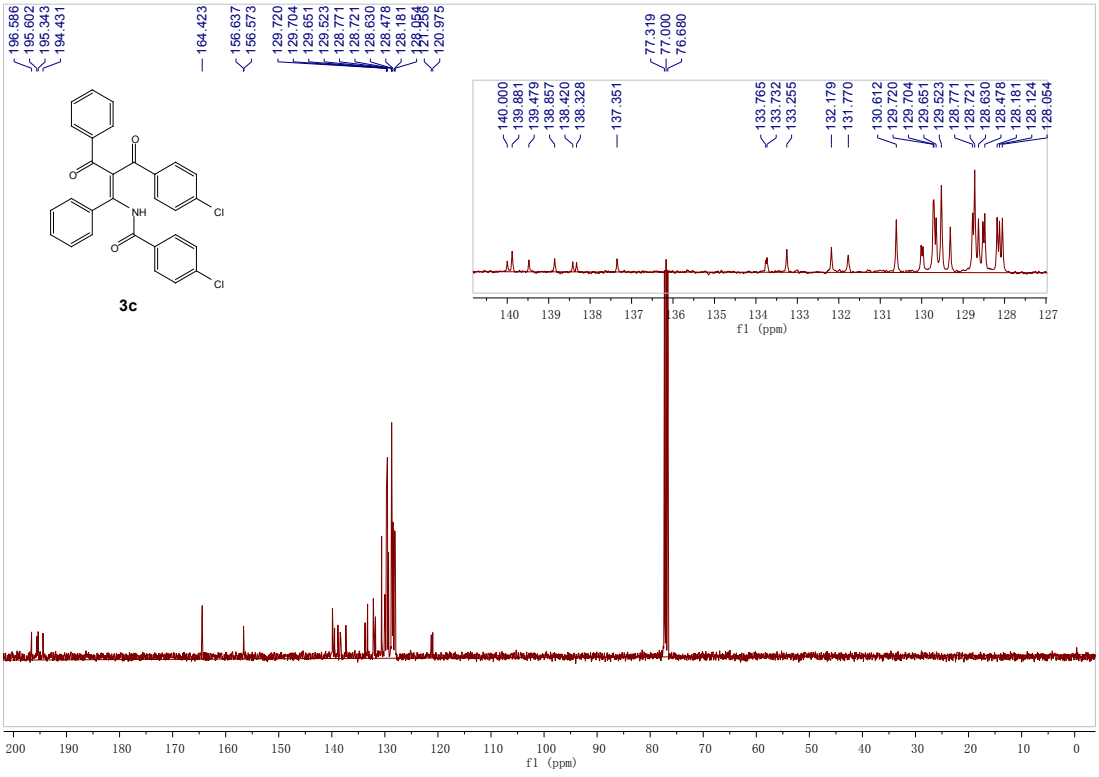
0.000
3c
f1 (ppm)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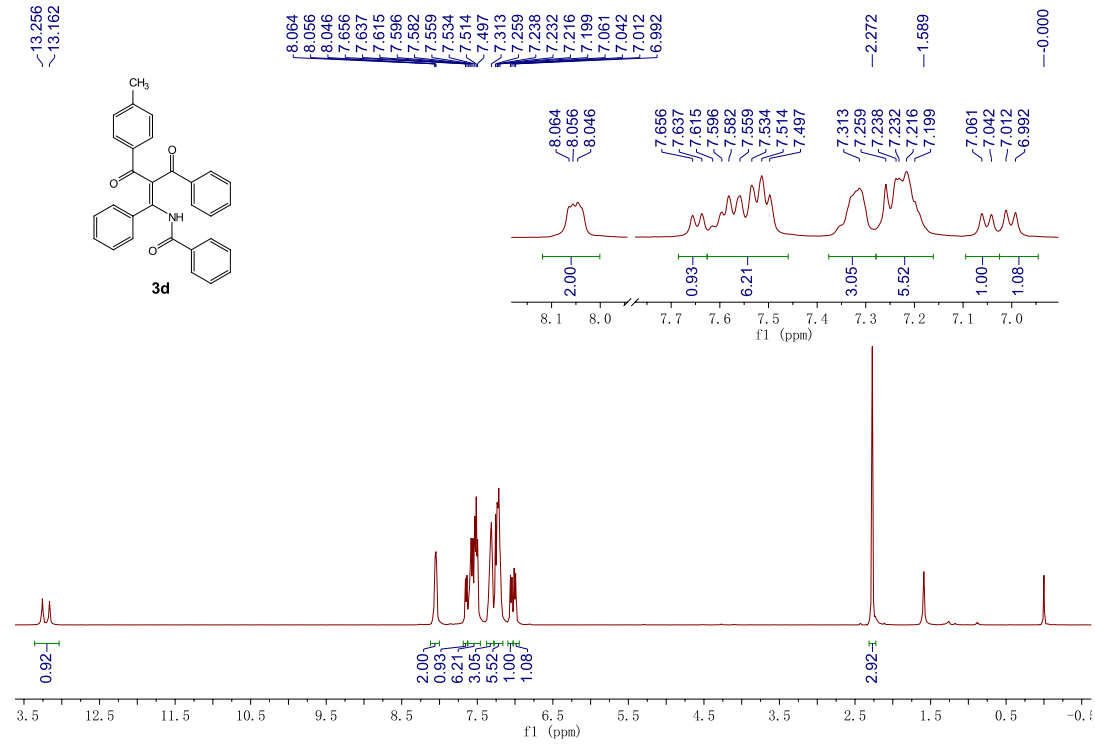
f1 (ppm)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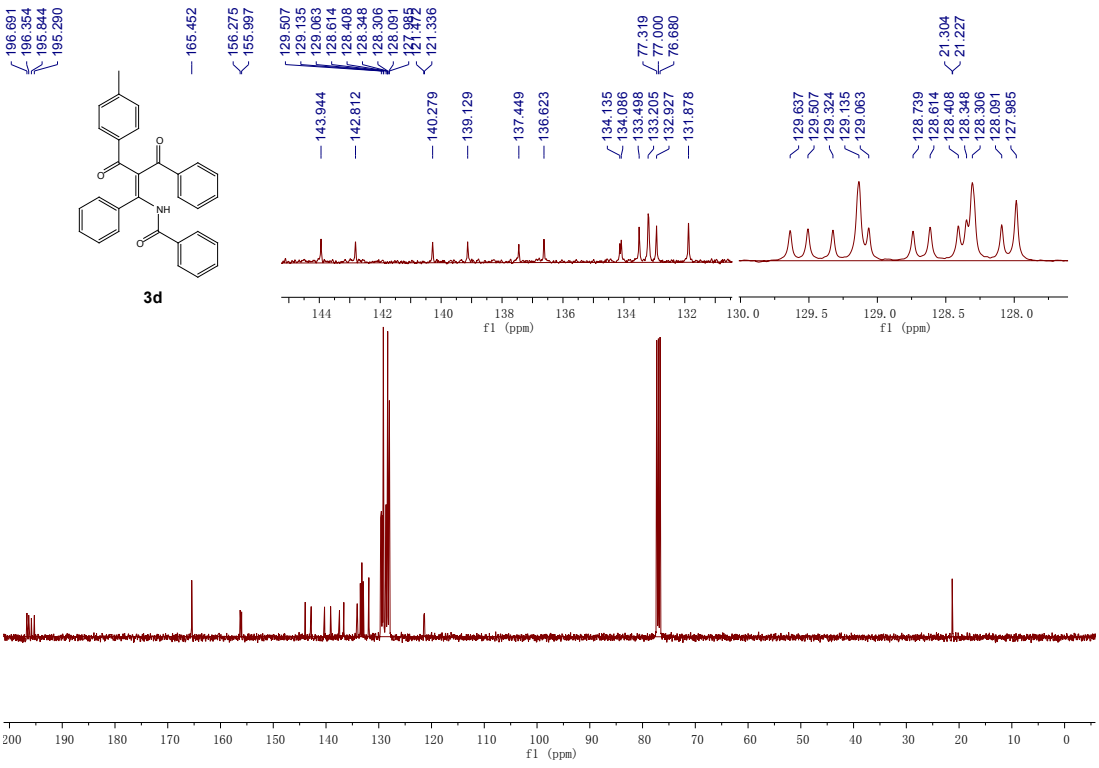
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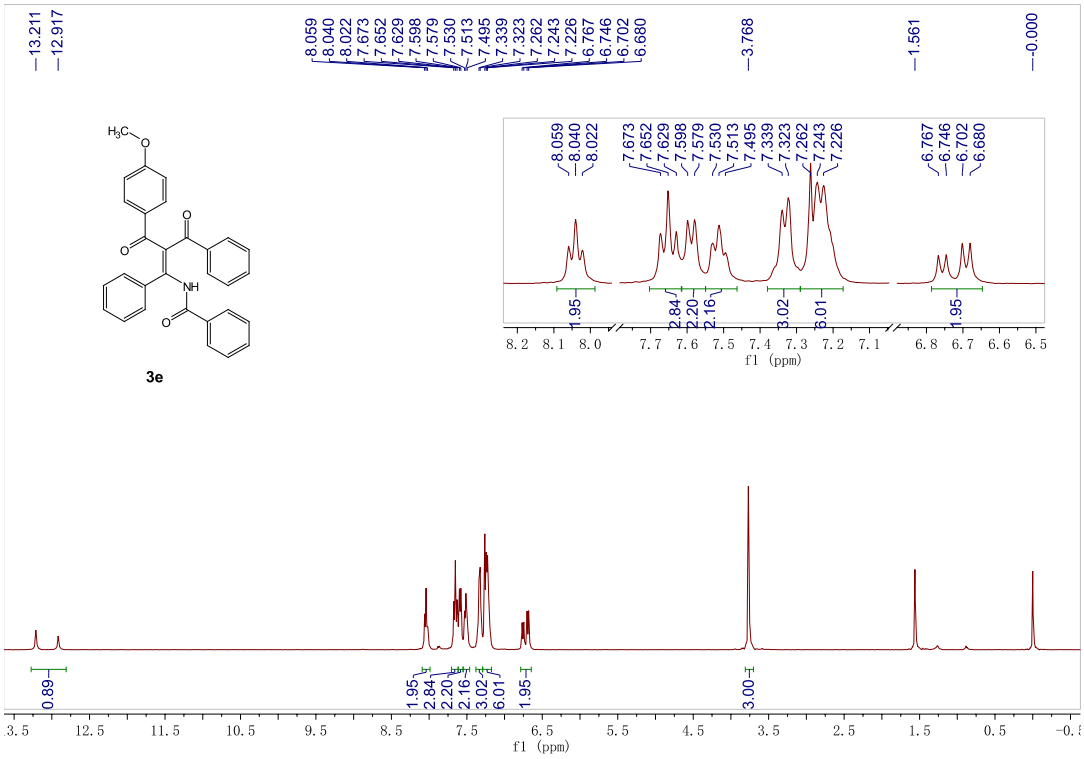
f1 (ppm)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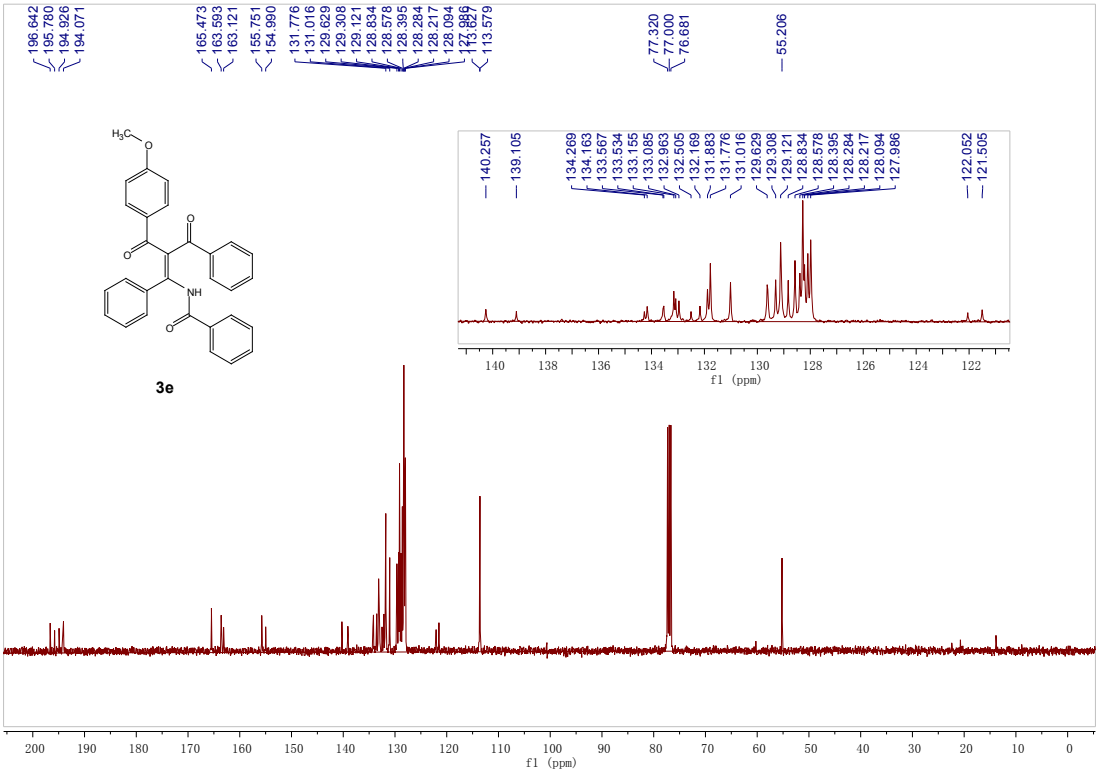
f1 (ppm)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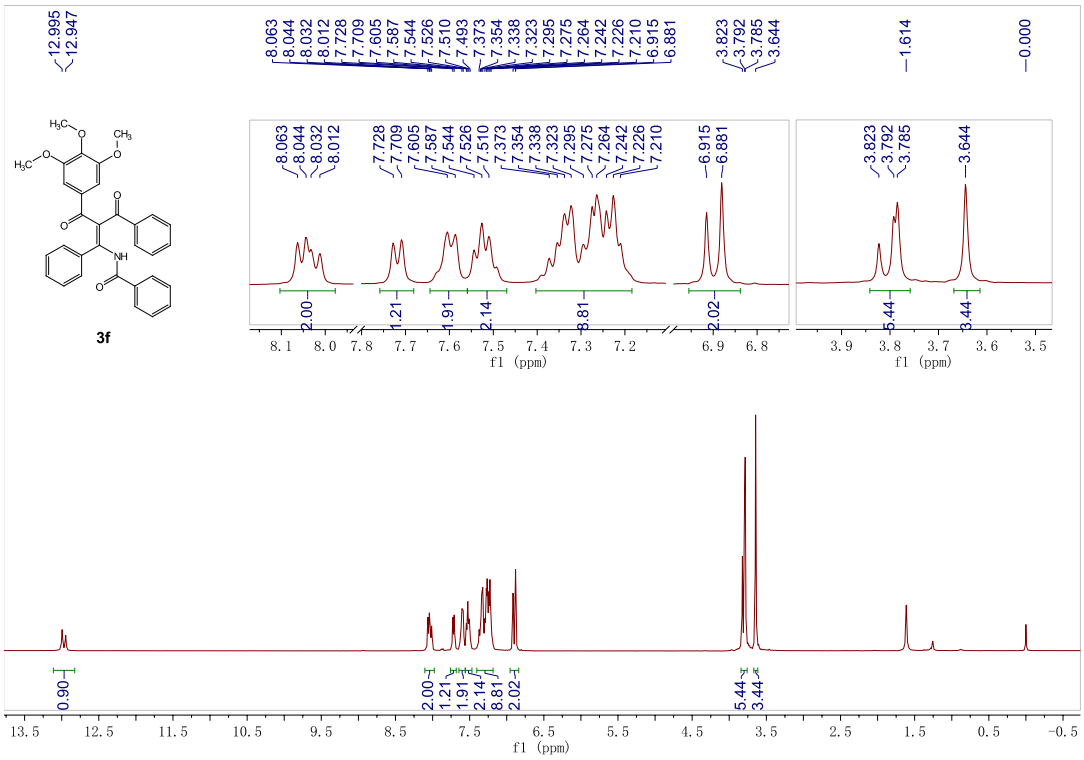
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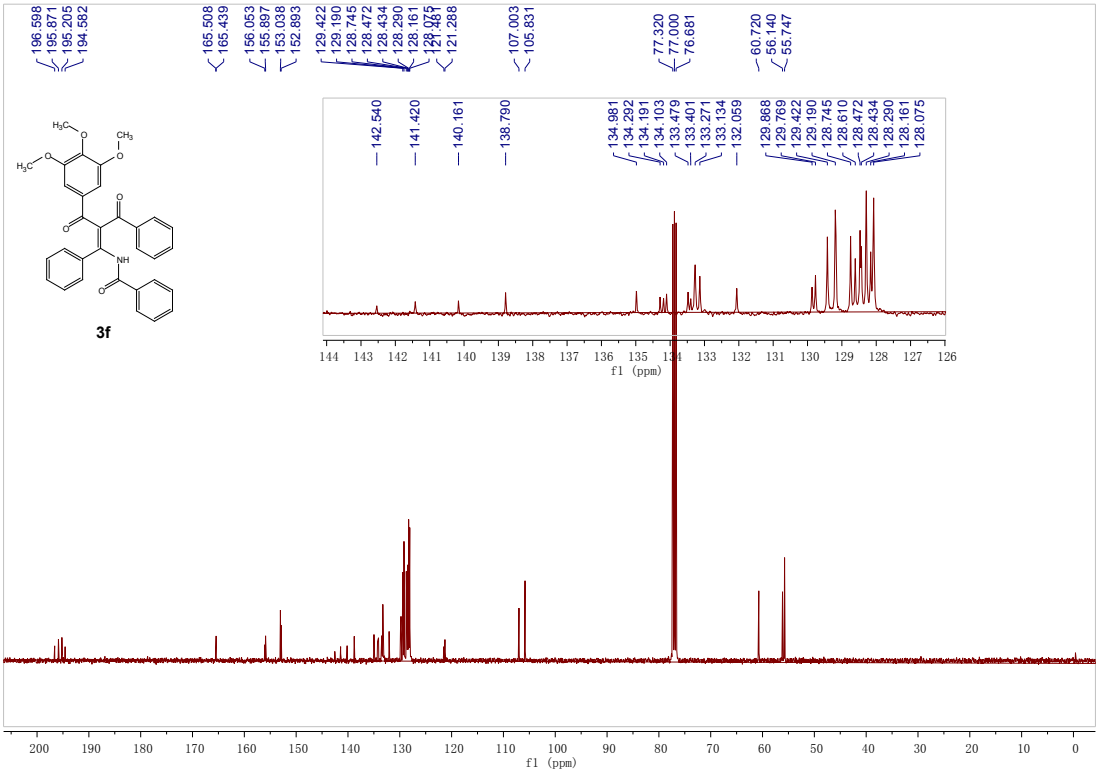
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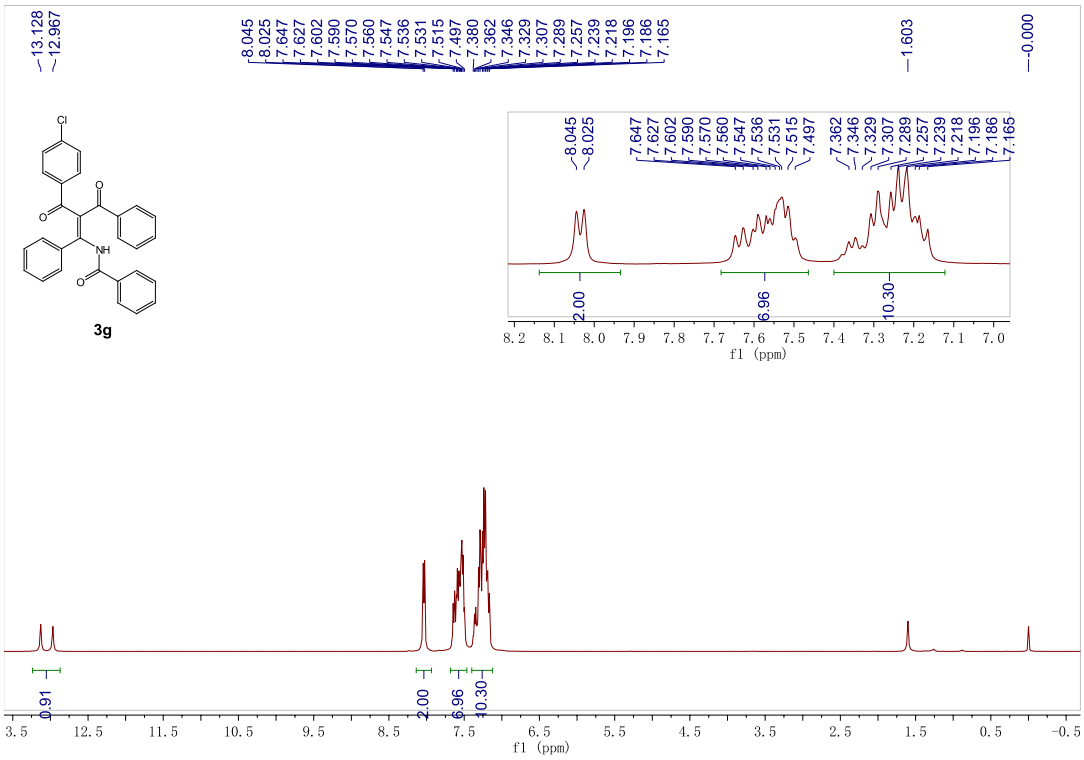
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O
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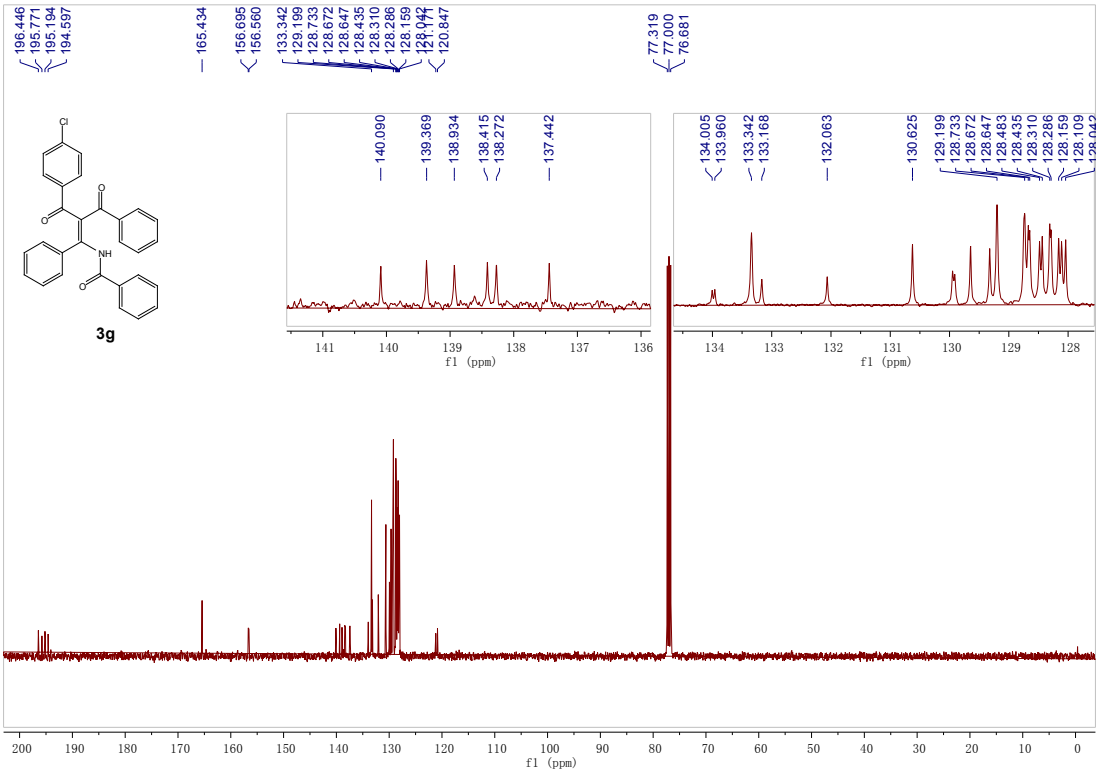
f1 (ppm)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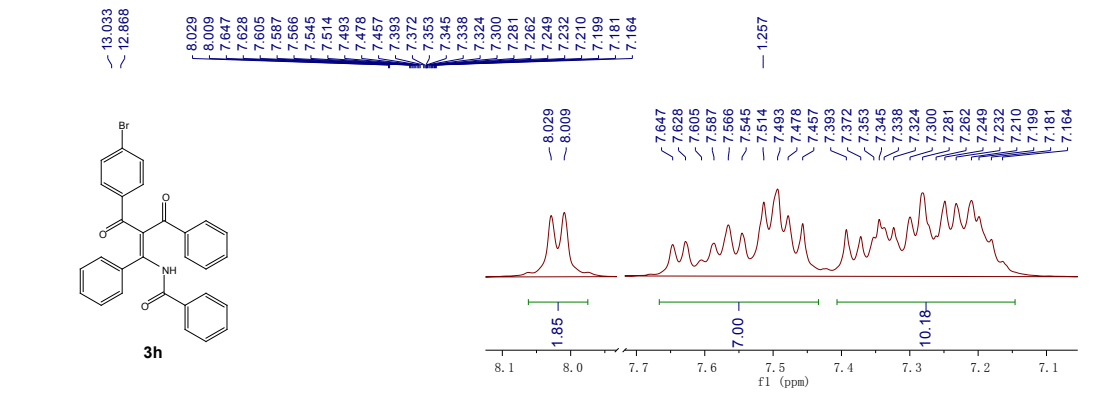
3g
f1 (ppm)
f1 (ppm)
f1 (ppm)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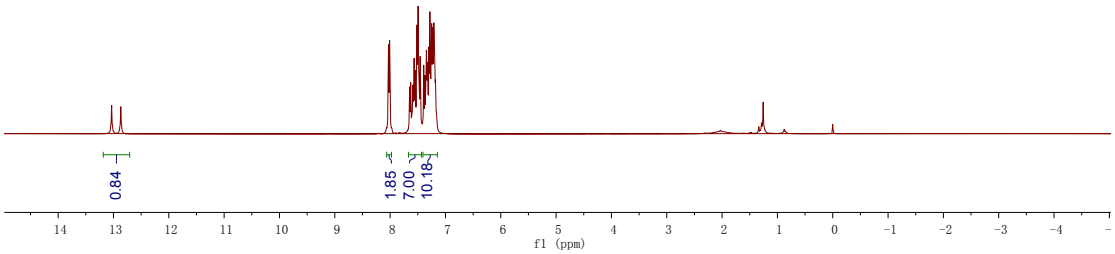
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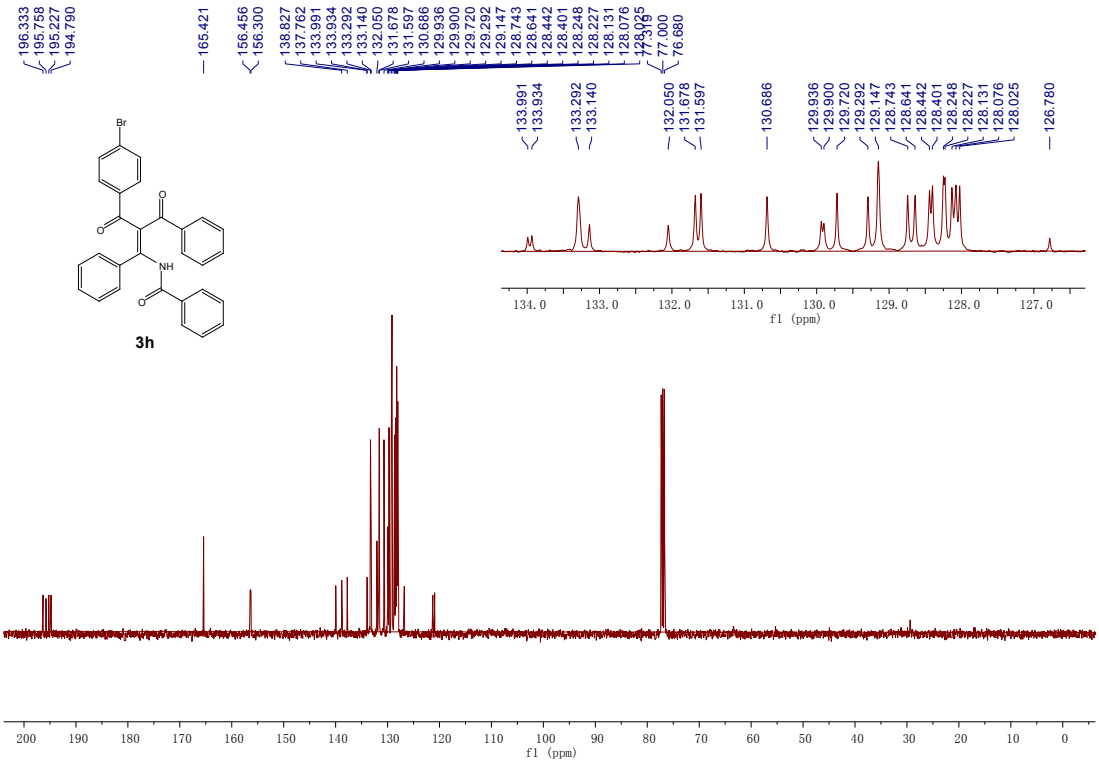
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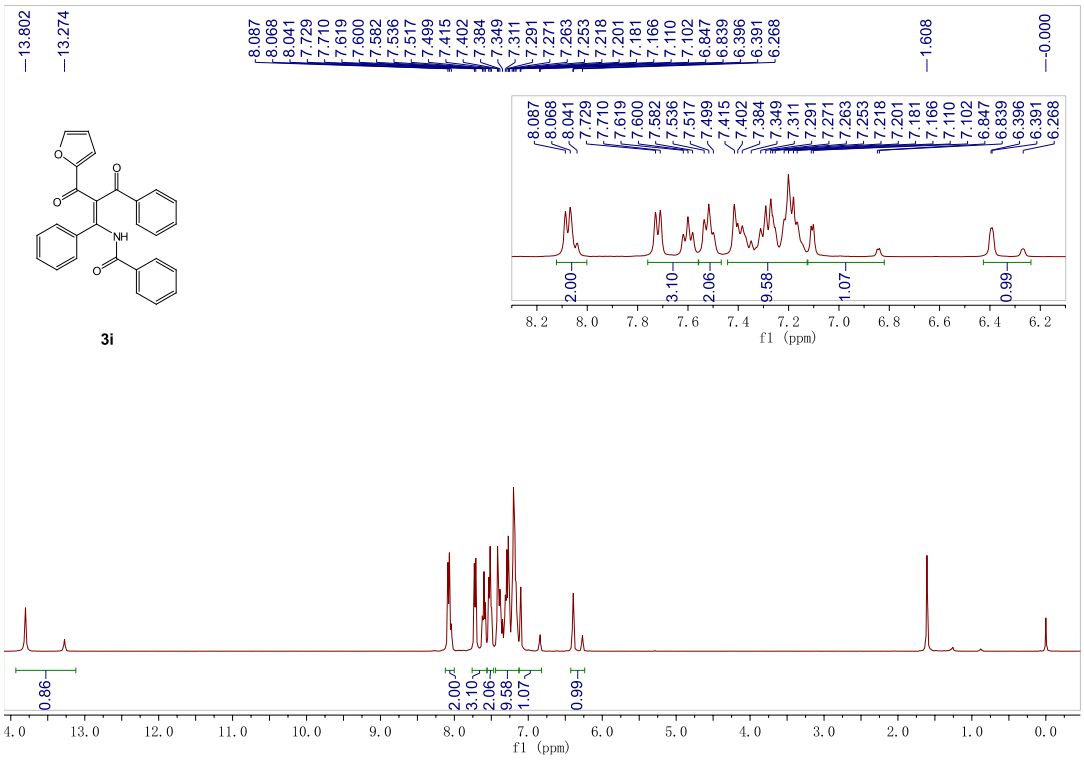
f1 (ppm)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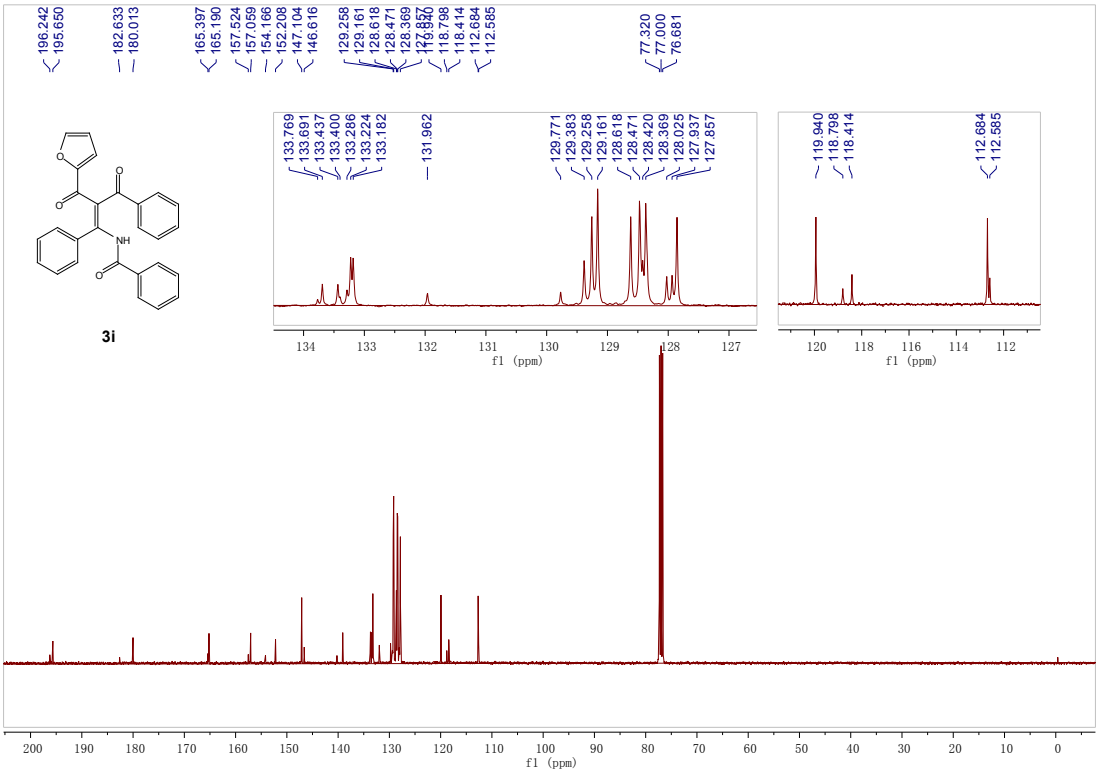
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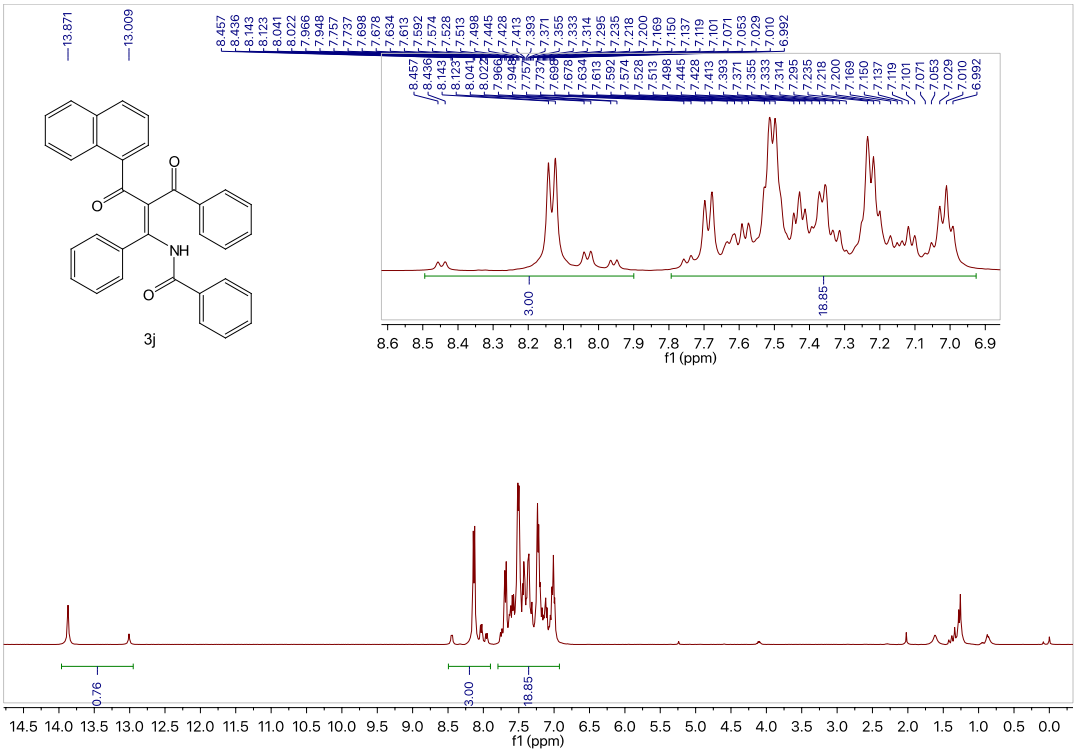
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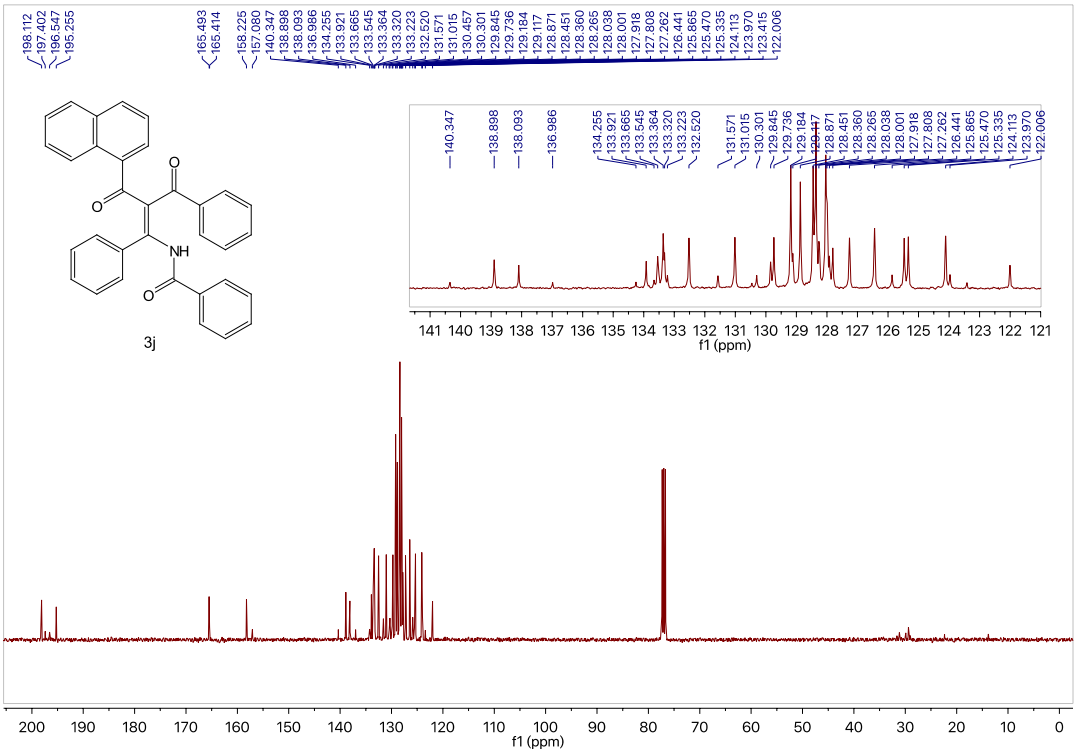
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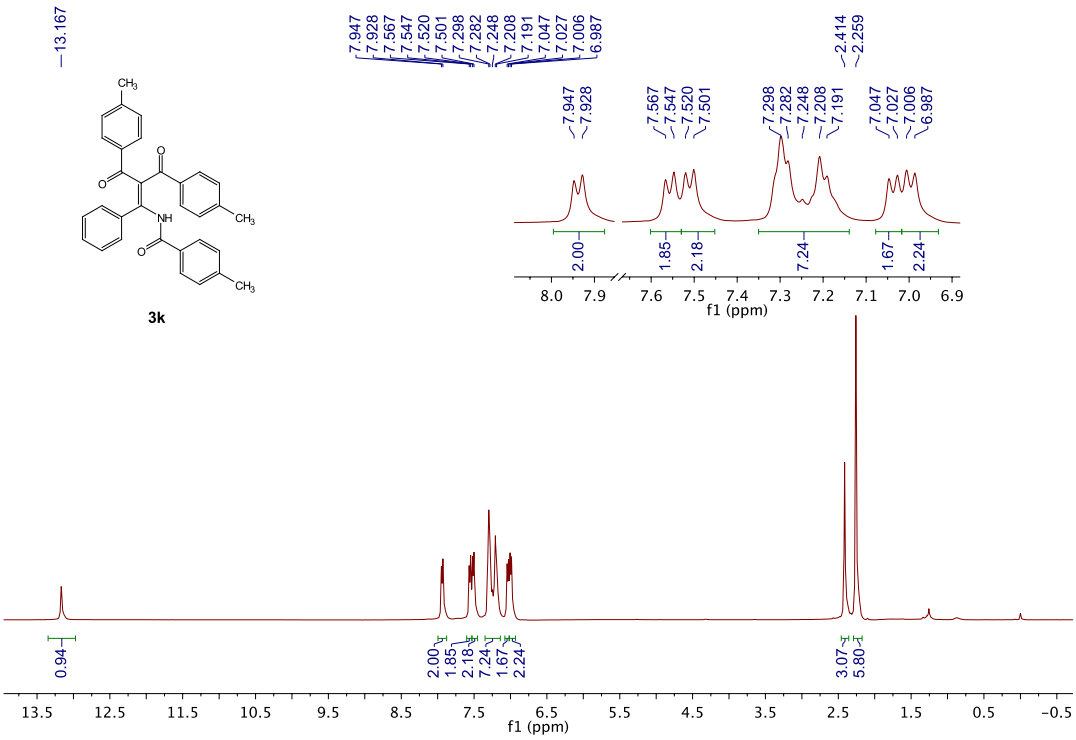
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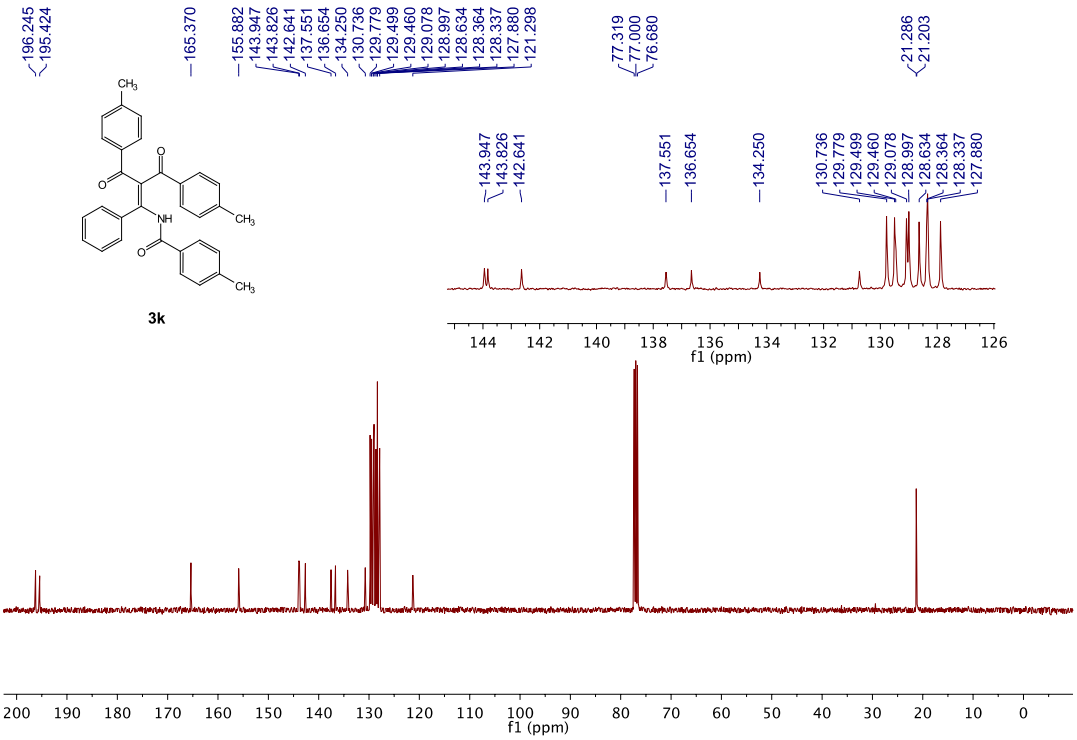
7.208
7.191
7.047
7.027
7.006
6.987
2.414
2.259
3k
2.00
1.85
2.18
7.24
1.67
2.24
0.94
3.07
5.80
f1 (ppm)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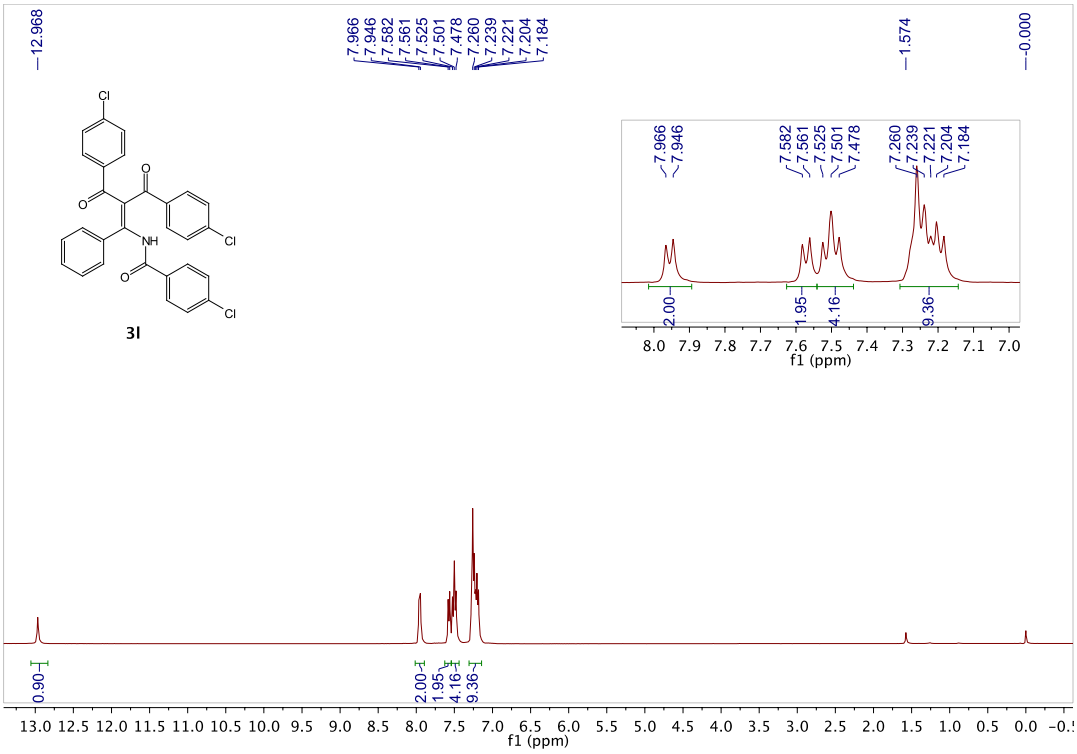
195.424
165.370
155.882
143.947
143.826
142.641
137.551
136.654
134.250
130.736
129.779
129.499
129.460
129.078
128.997
128.634
128.364
128.337
127.880
121.298
77.319
77.000
76.680
21.286
21.203
3k
f1 (ppm)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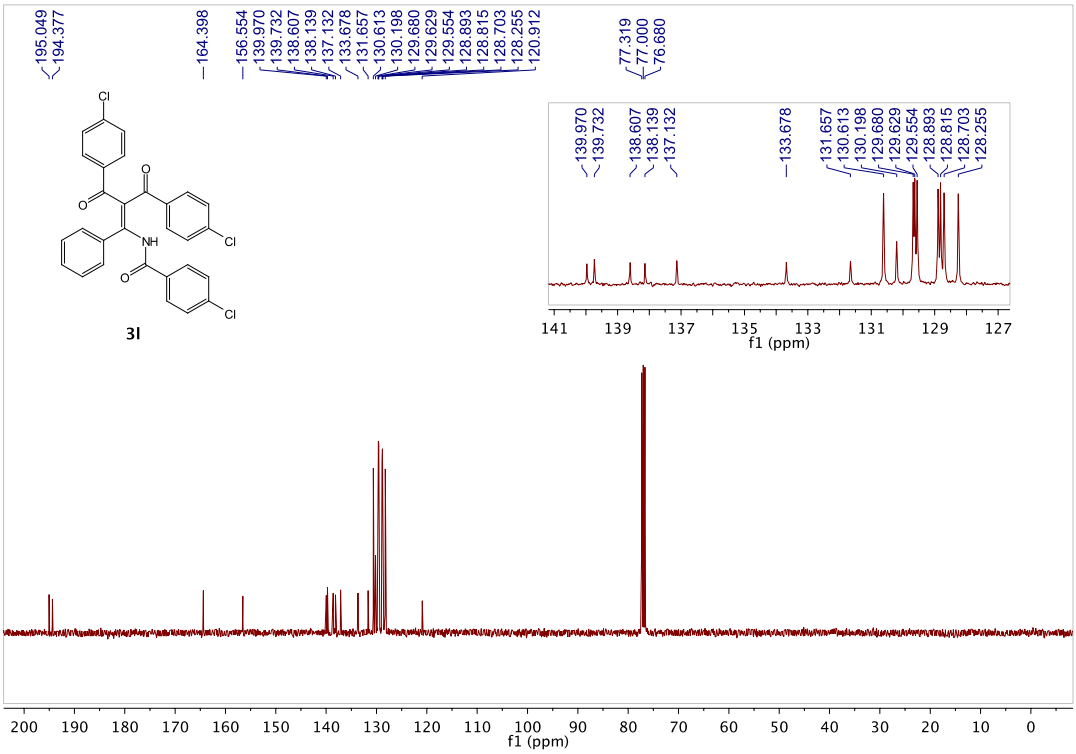
7.966
7.946
7.582
7.561
7.525
7.501
7.478
7.260
7.239
7.221
7.204
7.184
1.574
0.000
3l
2.00
1.95
4.16
9.36
0.90
f1 (ppm)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194.377
164.398
156.554
139.970
139.732
138.607
138.139
137.132
133.678
131.657
130.613
130.198
129.680
129.629
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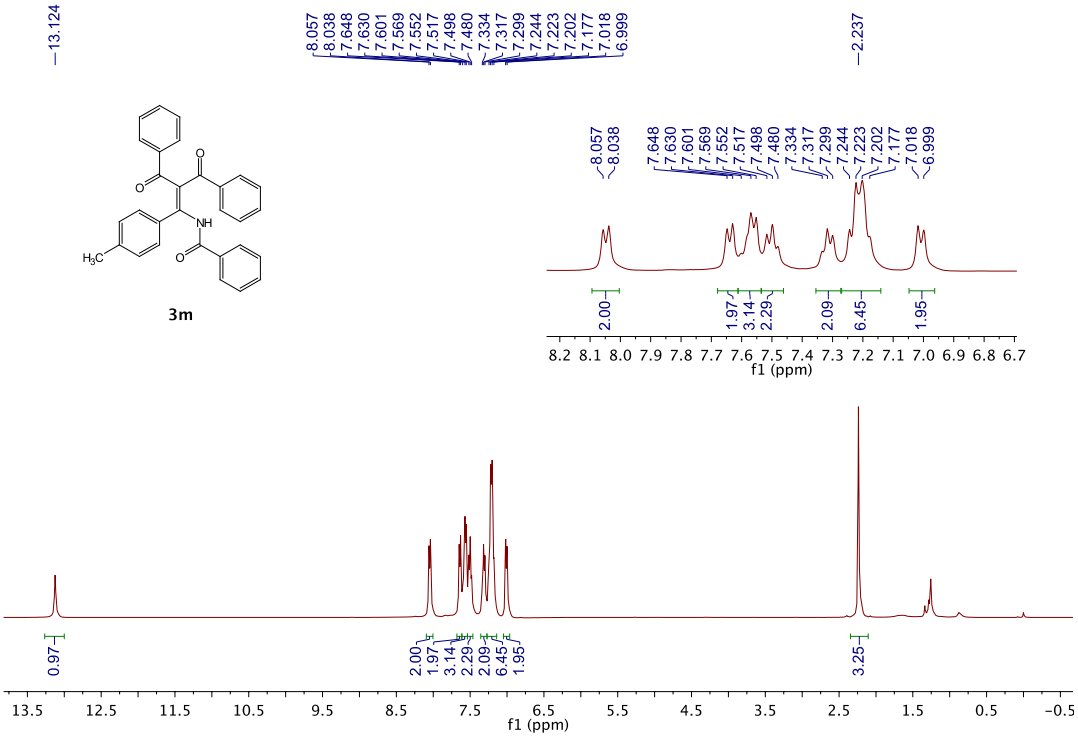
128.815
128.703
128.255
120.912
77.319
77.000
76.680
3l
f1 (ppm)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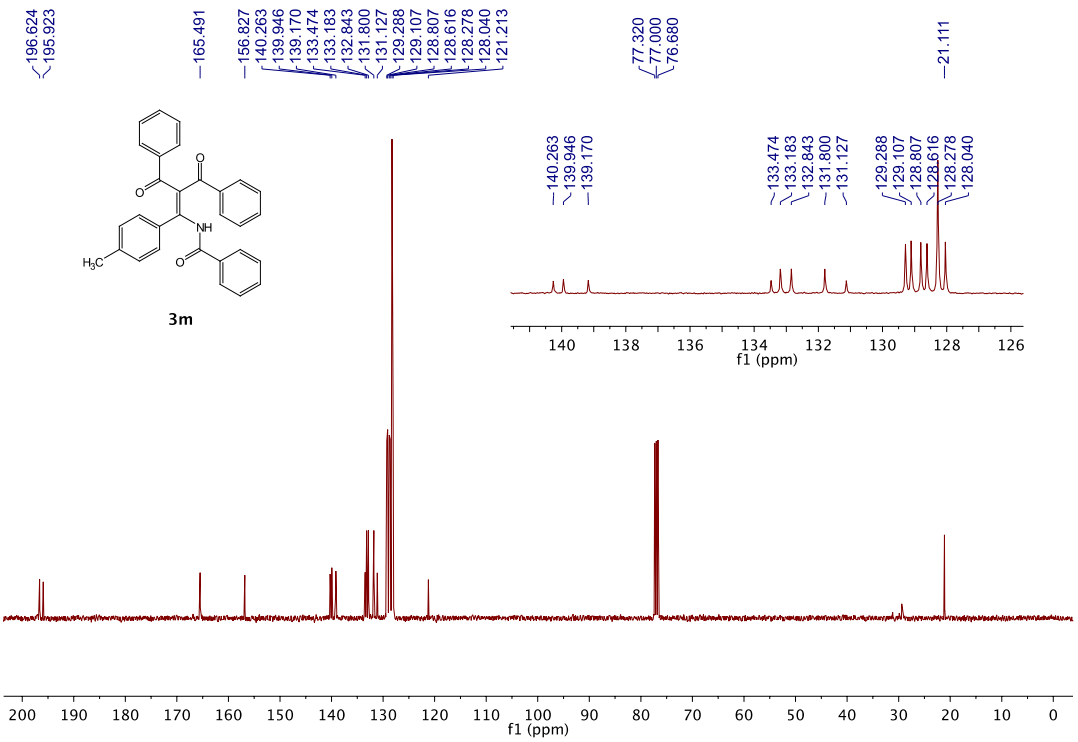
8.057
8.038
7.648
7.630
7.601
7.569
7.552
7.517
7.498
7.480
7.334
7.317
7.299
7.244
7.223
7.202
7.177
7.018
6.999
2.237
3m
2.00
1.97
3.14
2.29
2.09
6.45
1.95
0.97
3.25
f1 (ppm)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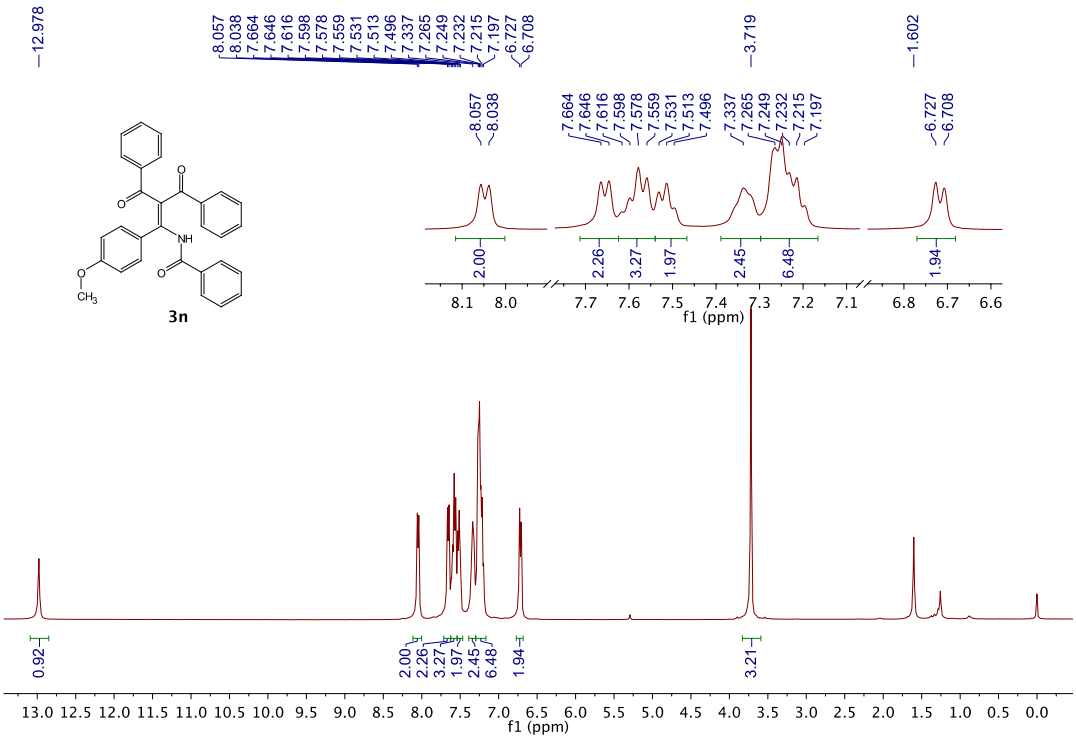
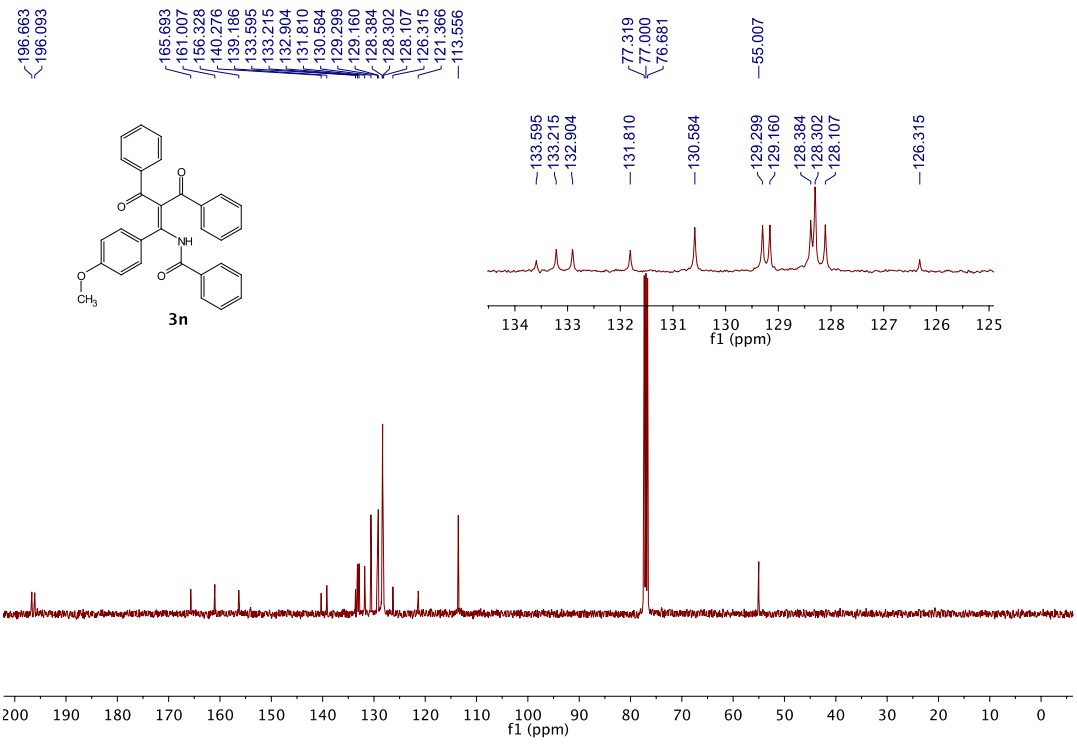
165.491
156.827
140.263
139.946
139.170
133.474
133.183
132.843
131.800
131.127
129.288
129.107
128.807
128.616
128.278
128.040
121.213
77.320
77.000
76.680
21.111
3m
f1 (ppm)


12.978
8.057
8.038
7.664
7.646
7.616
7.598
7.578
7.559
7.531
7.513
7.496
7.337
7.265
7.249
7.232
7.215
7.197
6.727
6.708
3.719
1.602
3n
f1 (ppm)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196.093
165.693
161.007
156.328
140.276
139.186
133.595
133.215
132.904
131.810
130.584
129.299
129.160
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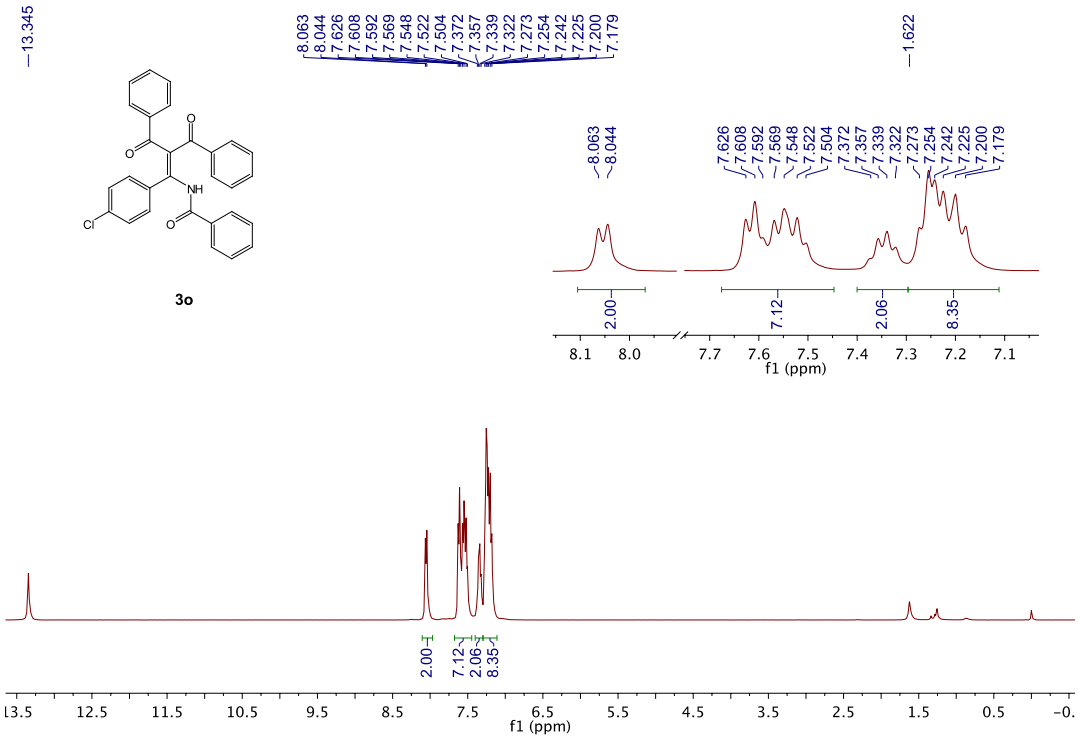
77.000
76.681
55.007
3n
f1 (ppm)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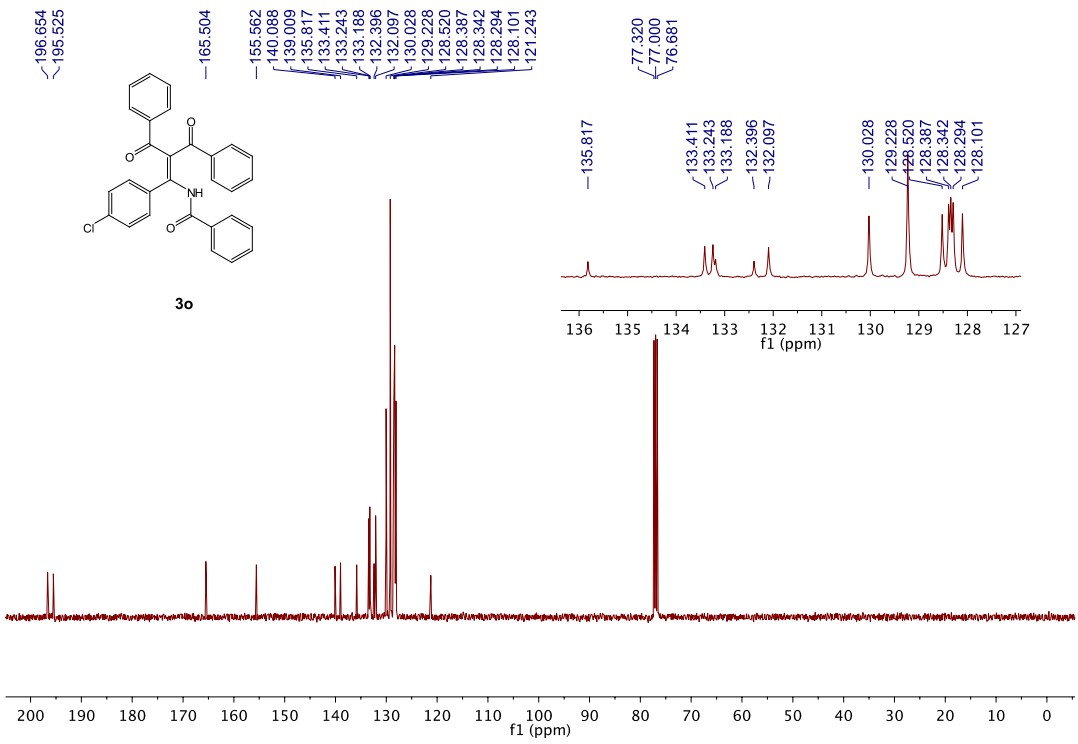
8.063
8.044
7.626
7.608
7.592
7.569
7.548
7.522
7.504
7.372
7.357
7.339
7.322
7.273
7.254
7.242
7.225
7.200
7.179
1.622
O
O
NH
O
Cl
3o
2.00
7.12
2.06
8.35
f1 (ppm)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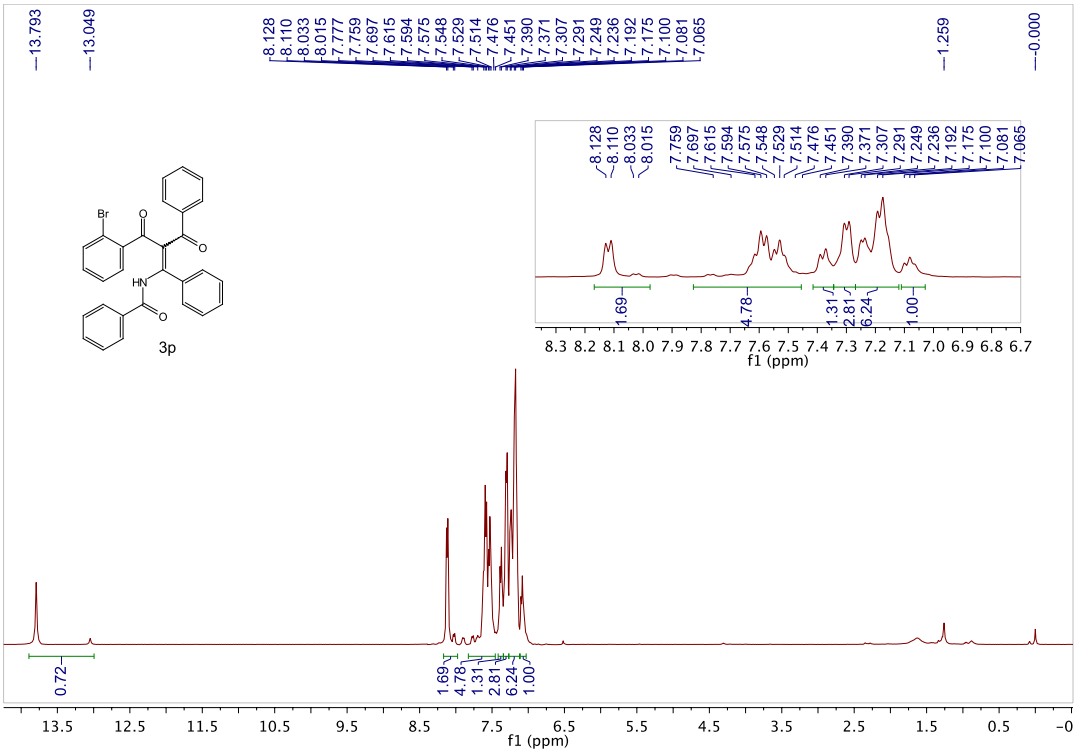
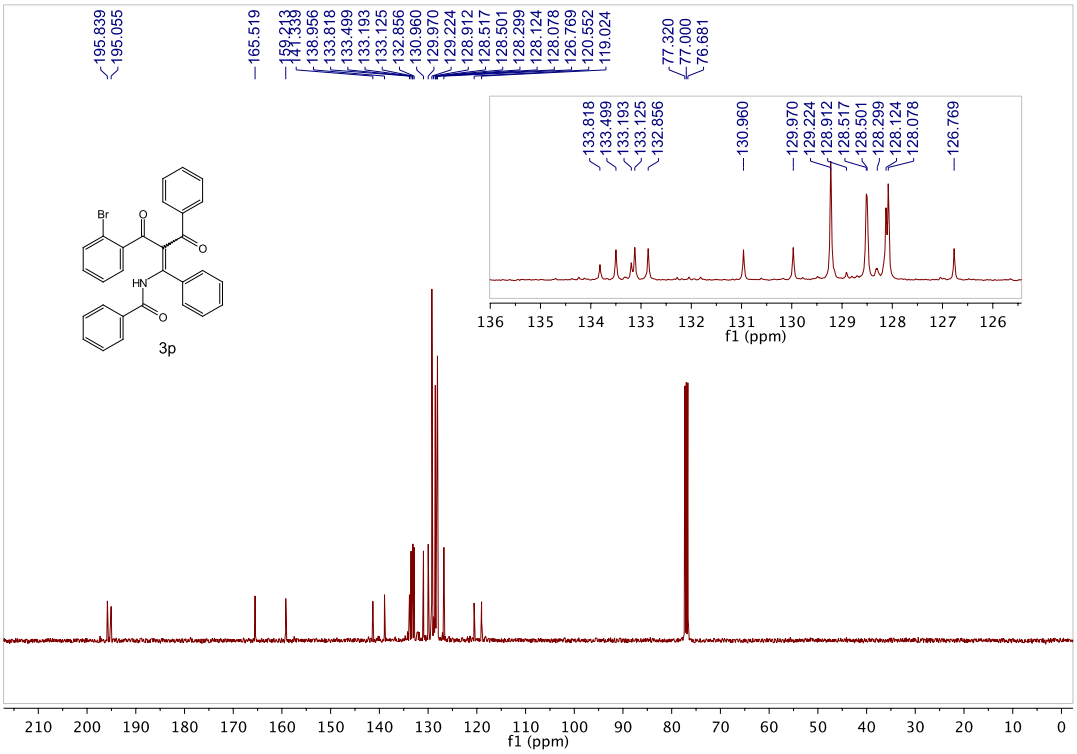
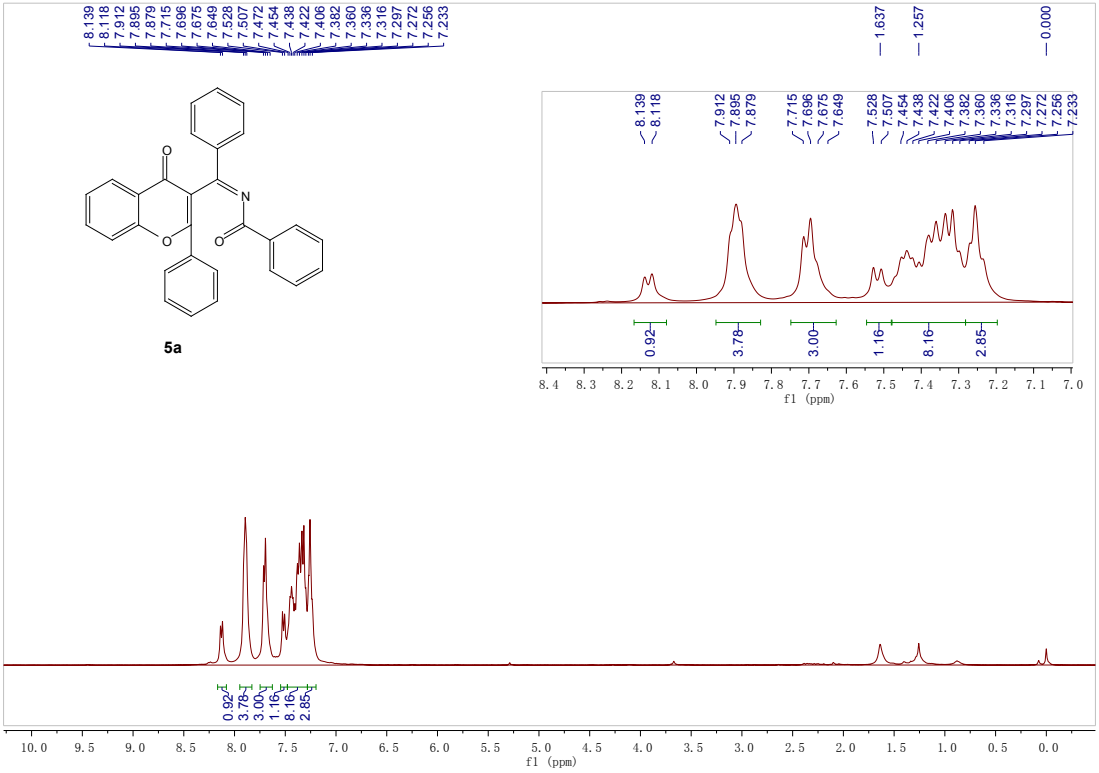
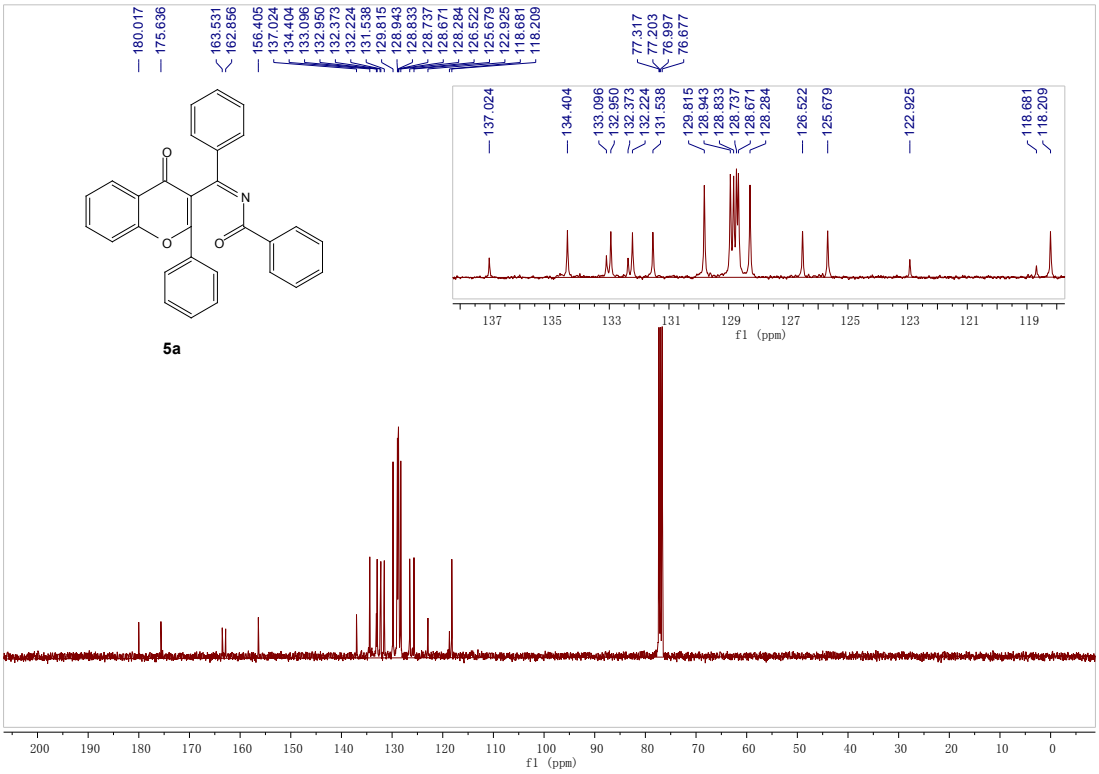
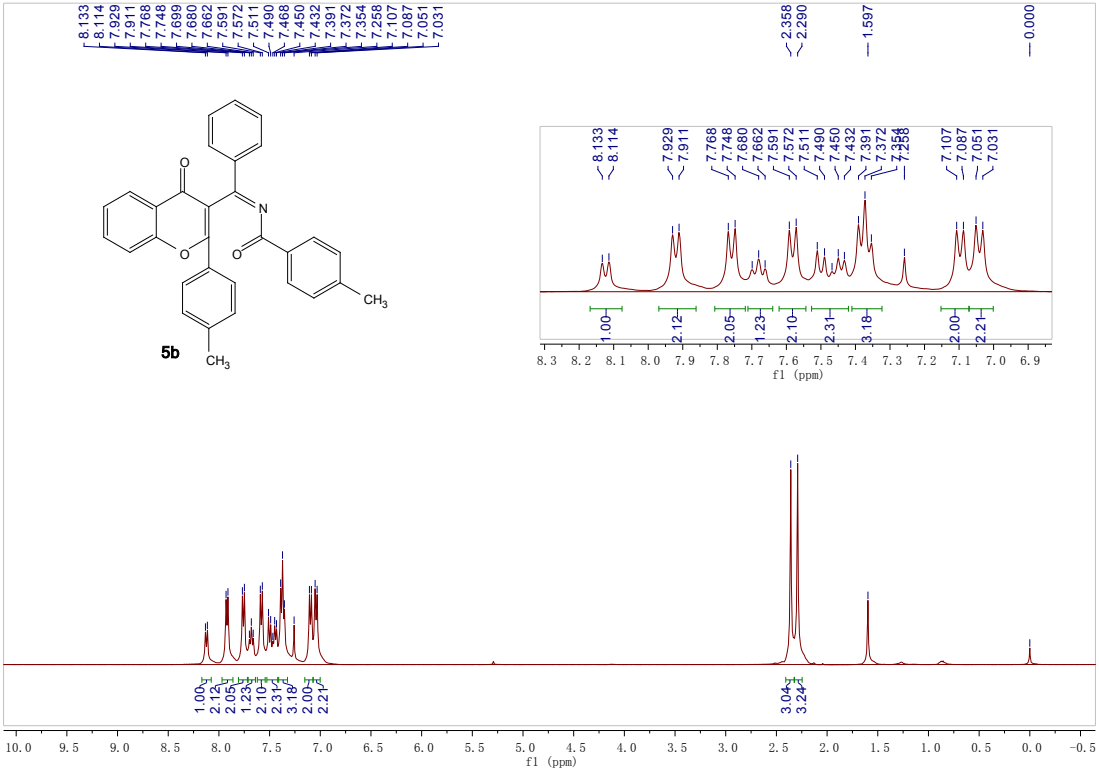
195.525
165.504
155.562
140.088
139.009
135.817
133.411
133.243
133.188
132.396
132.097
130.028
129.228
128.520
128.387
128.342
128.294
128.101
121.243
77.320
77.000
76.681
O
O
NH
O
Cl
3o
f1 (ppm)

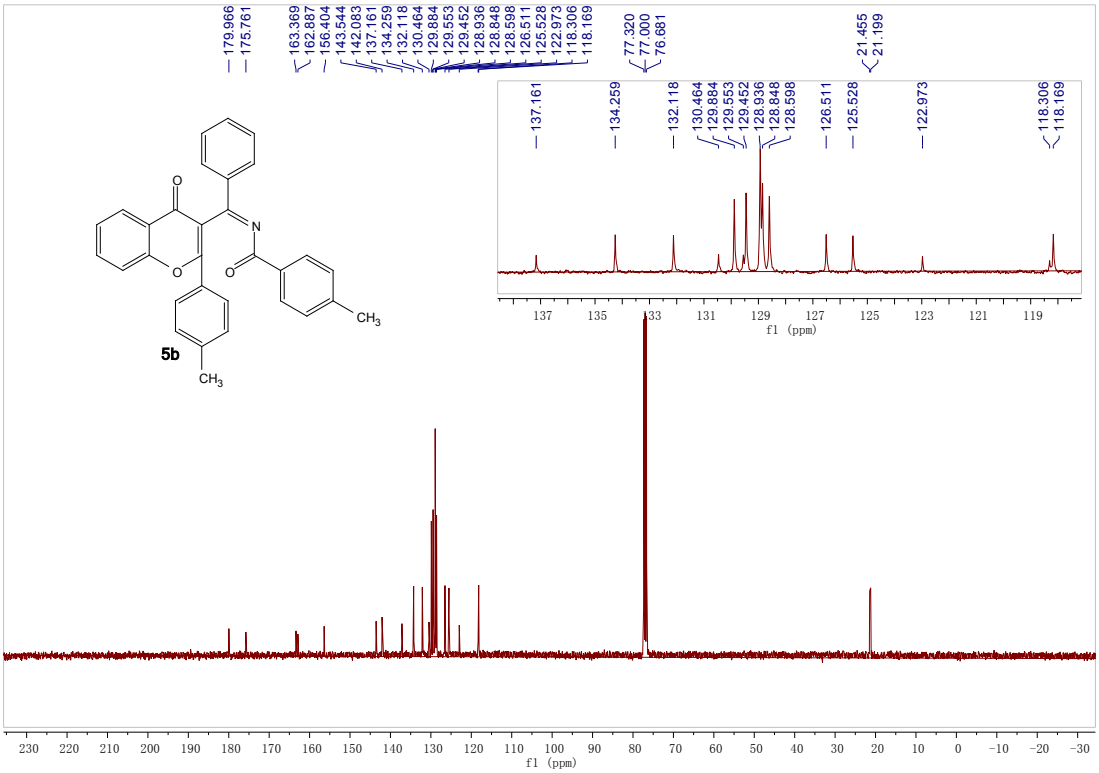

13.793
13.049
8.128
8.110
8.033
8.015
7.777
7.759
7.697
7.615
7.594
7.575
7.548
7.529
7.514
7.476
7.451
7.390
7.371
7.307
7.291
7.249
7.236
7.192
7.175
7.100
7.081
7.065
1.259
0.000
Br
O
O
HN
O
3p
1.69
4.78
1.31
2.81
6.24
1.00
0.72
f1 (ppm)

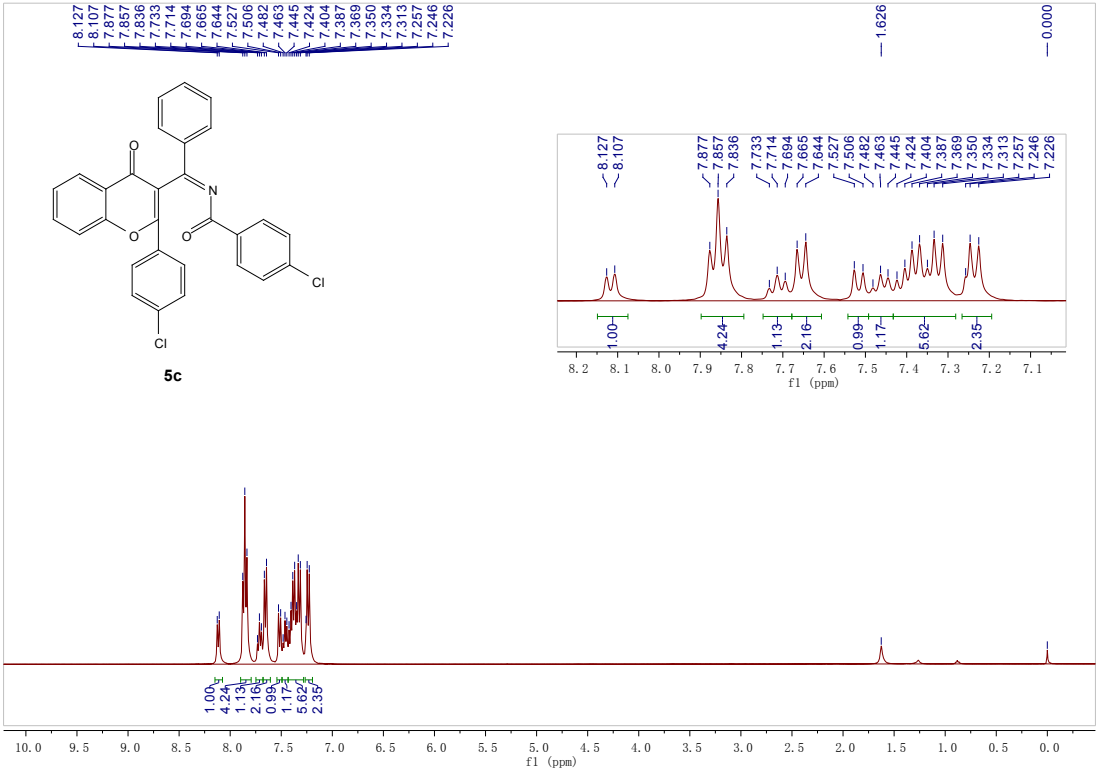

195.839
195.055
165.519
158.213
141.339
138.956
133.818
133.499
133.193
133.125
132.856
130.960
129.970
129.224
128.912
128.517
128.501
128.299
128.124
128.078
126.769
120.552
119.024
77.320
77.000
76.681
Br
O
O
HN
O
3p
f1 (ppm)

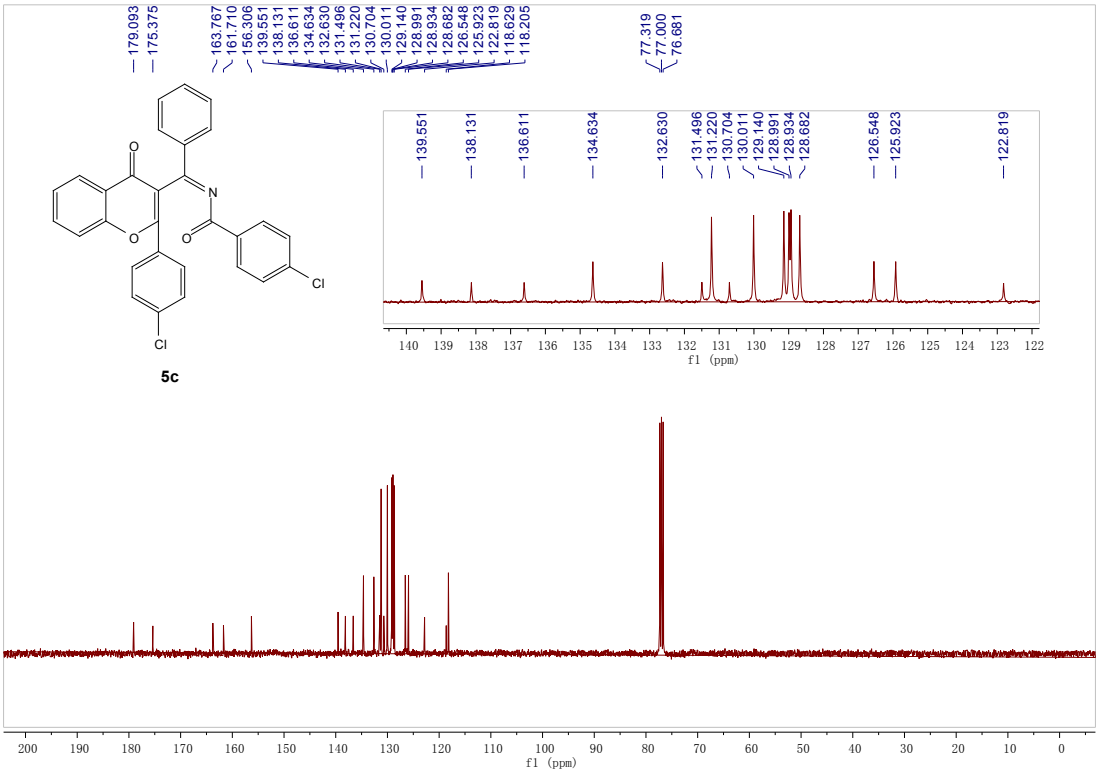

8.139
8.118
7.912
7.895
7.879
7.715
7.696
7.675
7.649
7.528
7.507
7.472
7.454
7.438
7.422
7.406
7.382
7.360
7.336
7.316
7.297
7.272
7.256
7.233
1.637
1.257
0.000
5a
0.92
3.78
3.00
1.16
8.16
2.85
f1 (ppm)


180.017
175.636
163.531
162.856
156.405
137.024
134.404
133.096
132.950
132.373
132.224
131.538
129.815
128.943
128.833
128.737
128.671
128.284
126.522
125.679
122.925
118.681
118.209
77.317
77.203
76.997
76.677
5a
f1 (ppm)


5b
f1 (ppm)


5b
f1 (ppm)


8.127
8.107
7.877
7.857
7.836
7.733
7.714
7.694
7.665
7.644
7.527
7.506
7.482
7.463
7.445
7.424
7.404
7.387
7.369
7.350
7.334
7.313
7.257
7.246
7.226
1.626
0.000
O
N
O
O
Cl
Cl
5c
1.00
4.24
1.13
2.16
0.99
1.17
5.62
2.35
f1 (ppm)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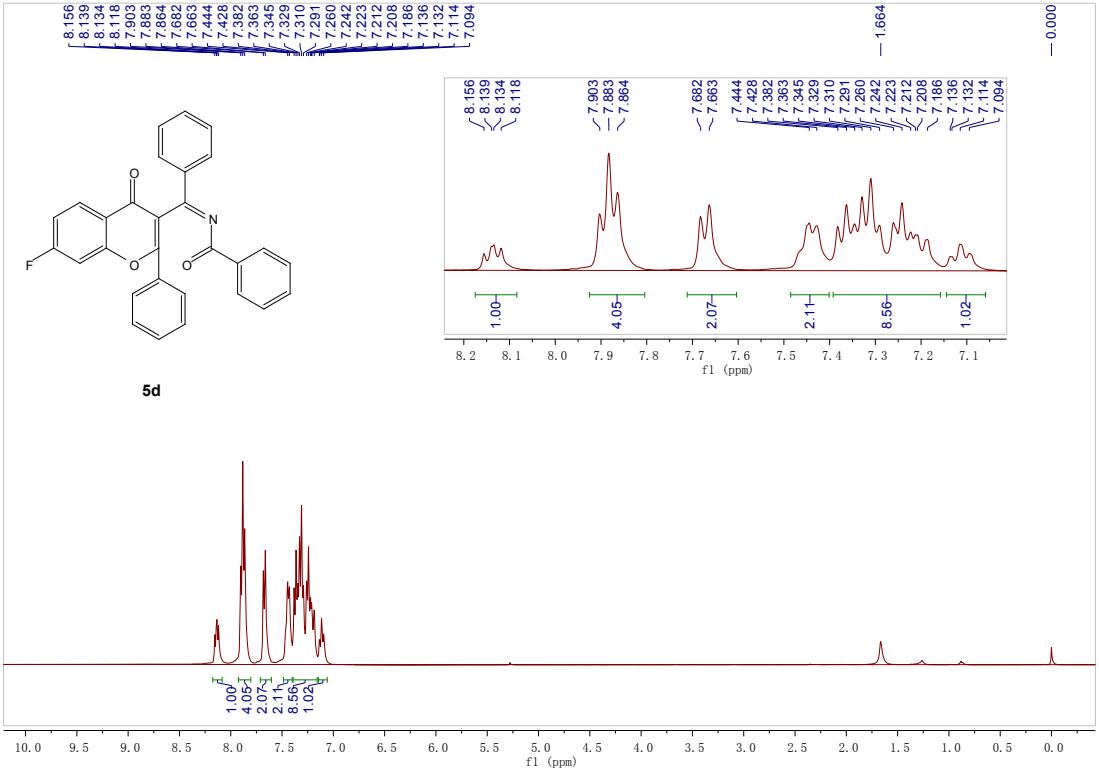
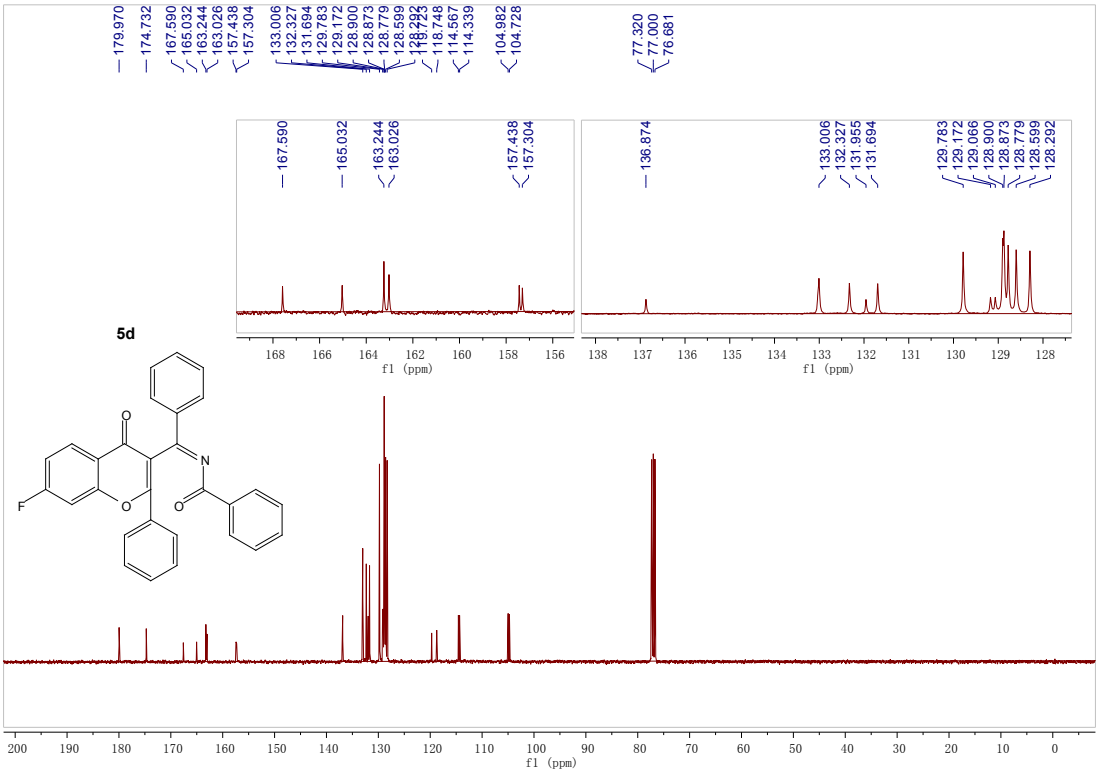
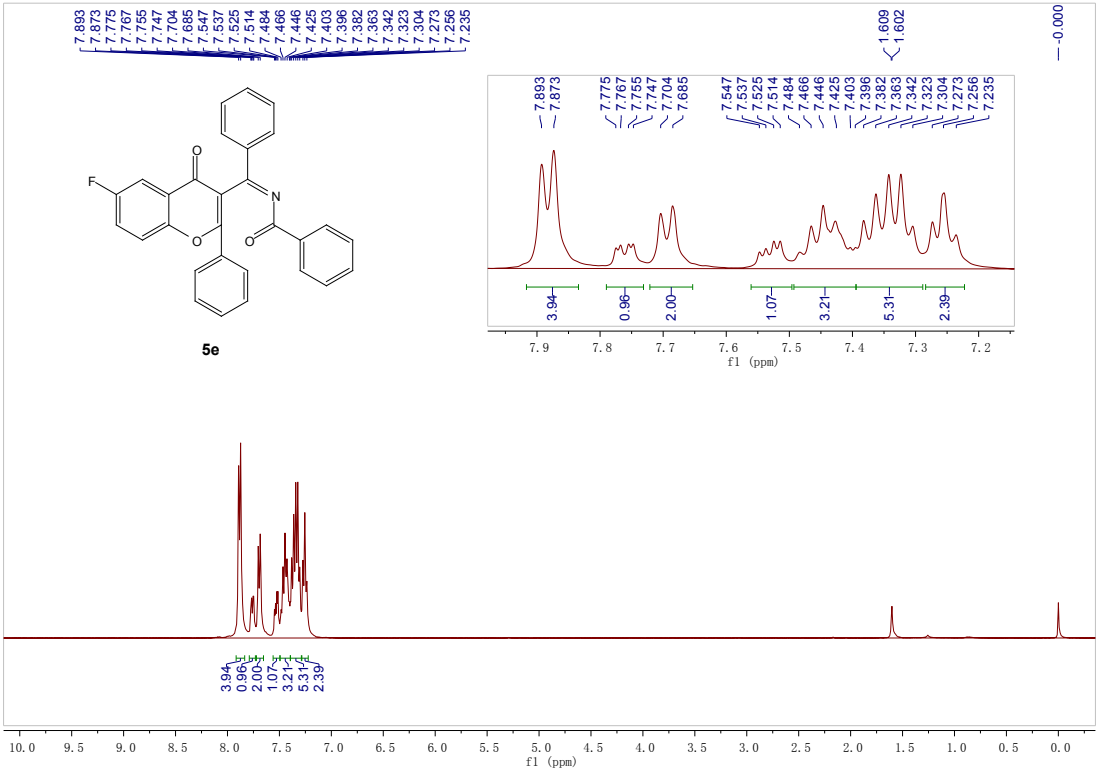
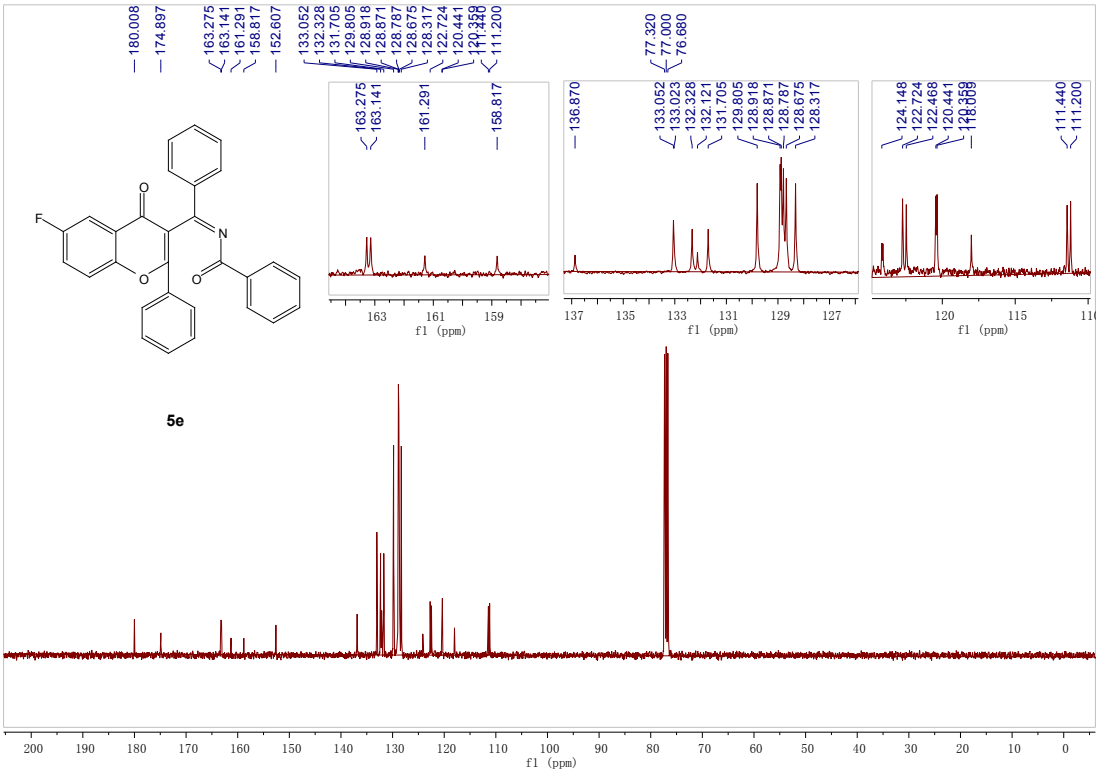
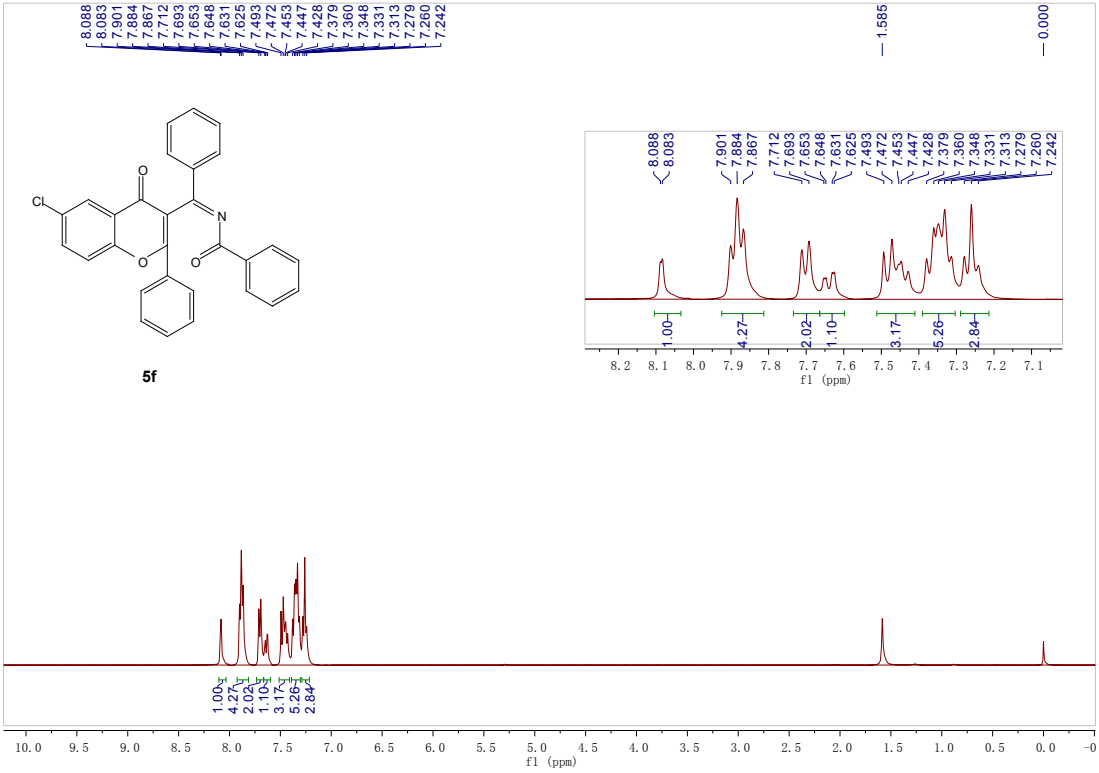
175.375
163.767
161.710
158.306
139.551
138.131
136.611
134.634
132.630
131.496
131.220
130.704
130.011
129.140
128.991
128.934
128.682
126.548
125.923
122.819
118.629
118.205
77.319
77.000
76.681
O
N
O
O
Cl
Cl
5c
f1 (ppm)


5d
f1 (ppm)


5d
f1 (ppm)


5e
f1 (ppm)


5e
f1 (ppm)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8.083
7.901
7.884
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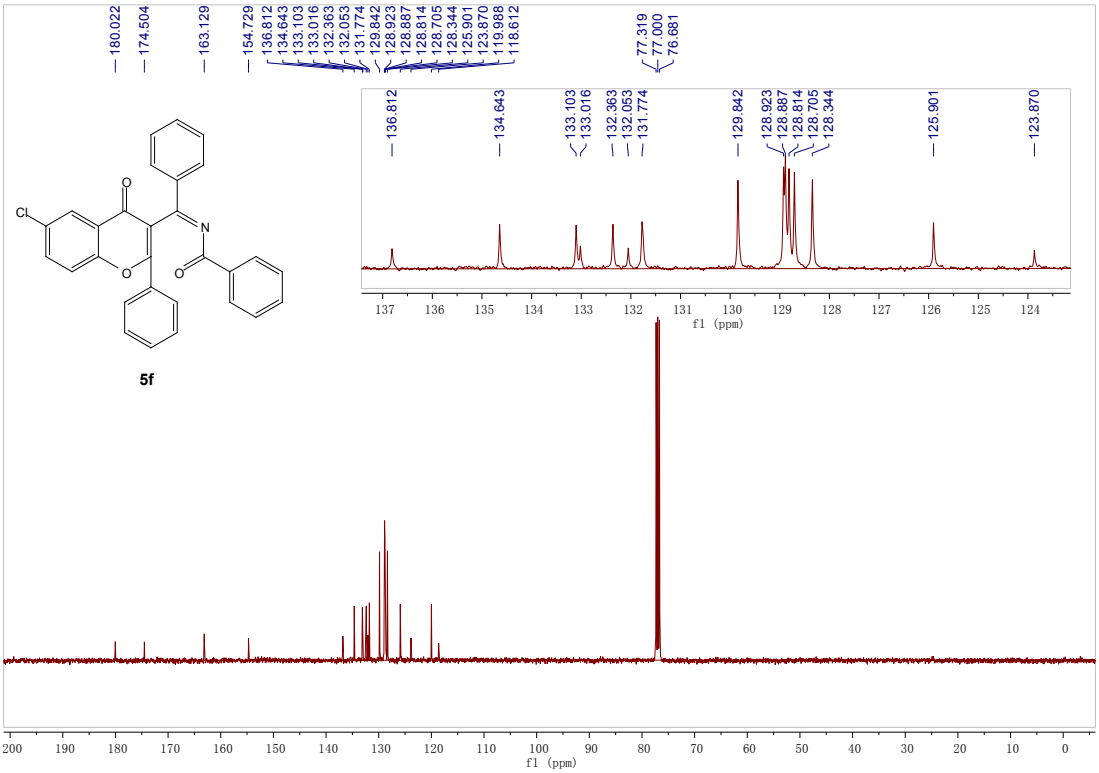
7.693
7.653
7.648
7.631
7.625
7.493
7.472
7.453
7.447
7.428
7.379
7.360
7.348
7.331
7.313
7.279
7.260
7.242
1.585
0.000
Cl
O
N
O
O
5f
1.00
4.27
2.02
1.10
3.17
5.26
2.84
f1 (ppm)


180.022
174.504
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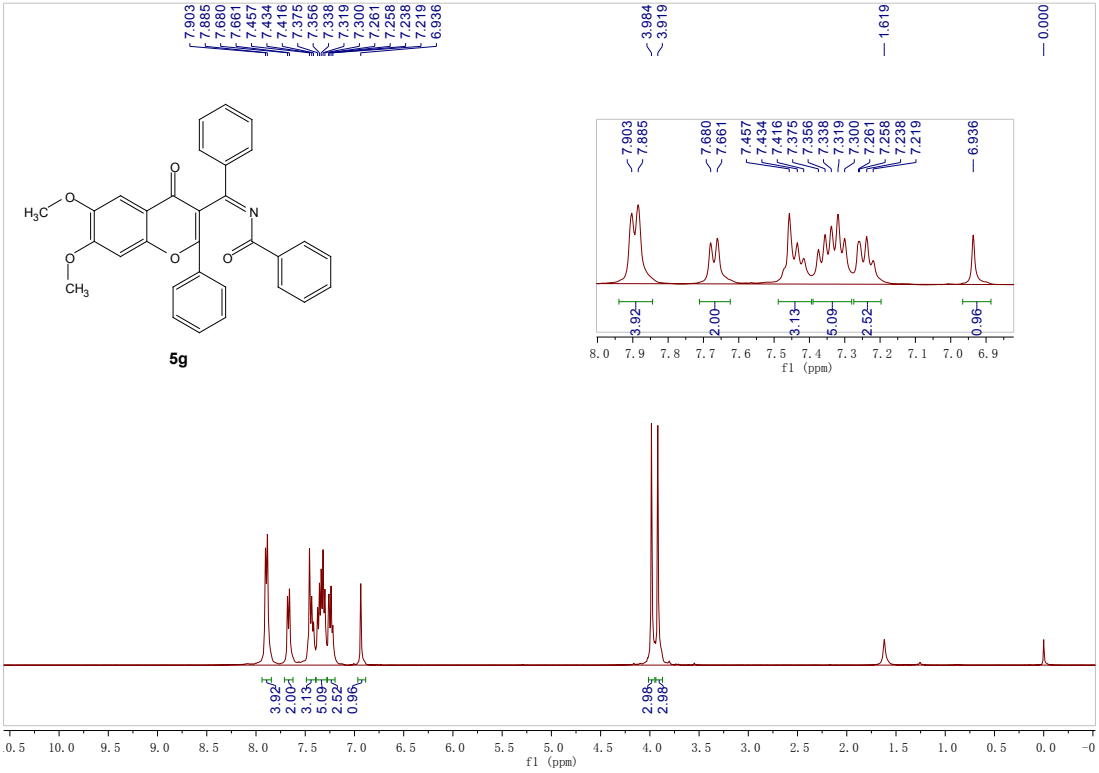
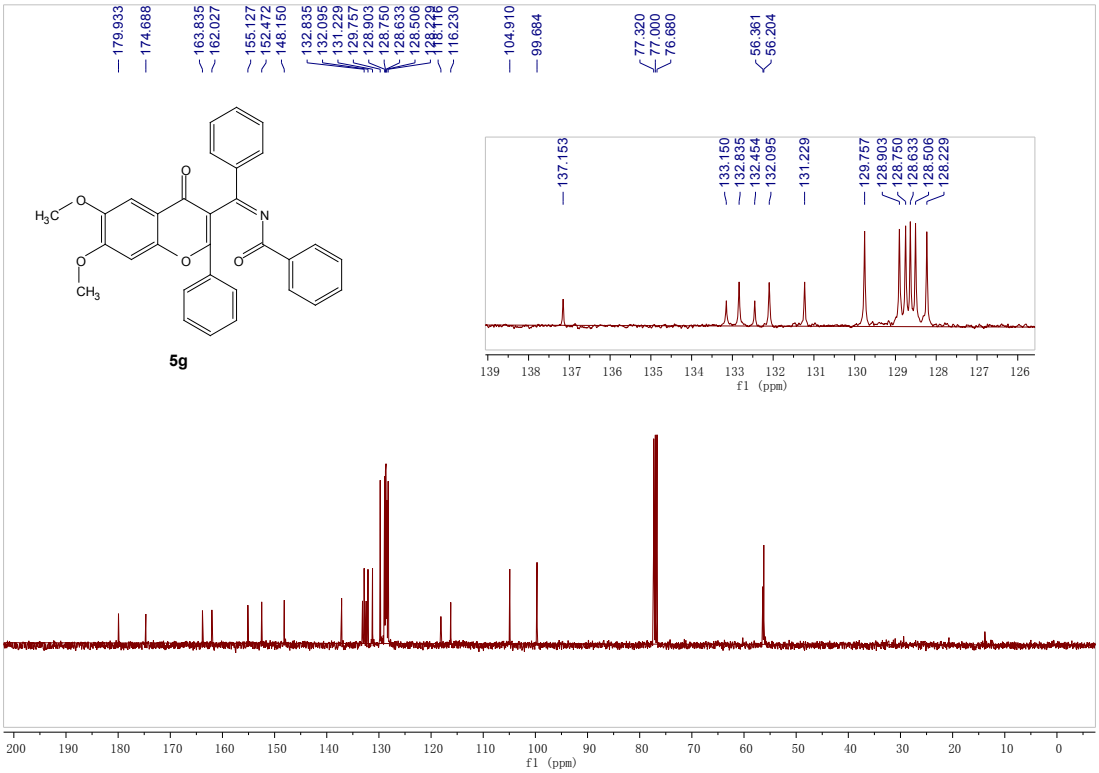
154.729
136.812
134.643
133.103
133.016
132.363
132.053
131.774
129.842
128.923
128.887
128.814
128.705
128.344
125.901
123.870
119.988
118.612
77.319
77.000
76.681
Cl
O
N
O
O
5f
f1 (ppm)


7.903
7.885
7.680
7.661
7.457
7.434
7.416
7.375
7.356
7.338
7.319
7.300
7.261
7.258
7.238
7.219
6.936
3.984
3.919
1.619
0.000
5g
3.92
2.00
3.13
5.09
2.52
0.96
2.98
2.98
f1 (ppm)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162.027
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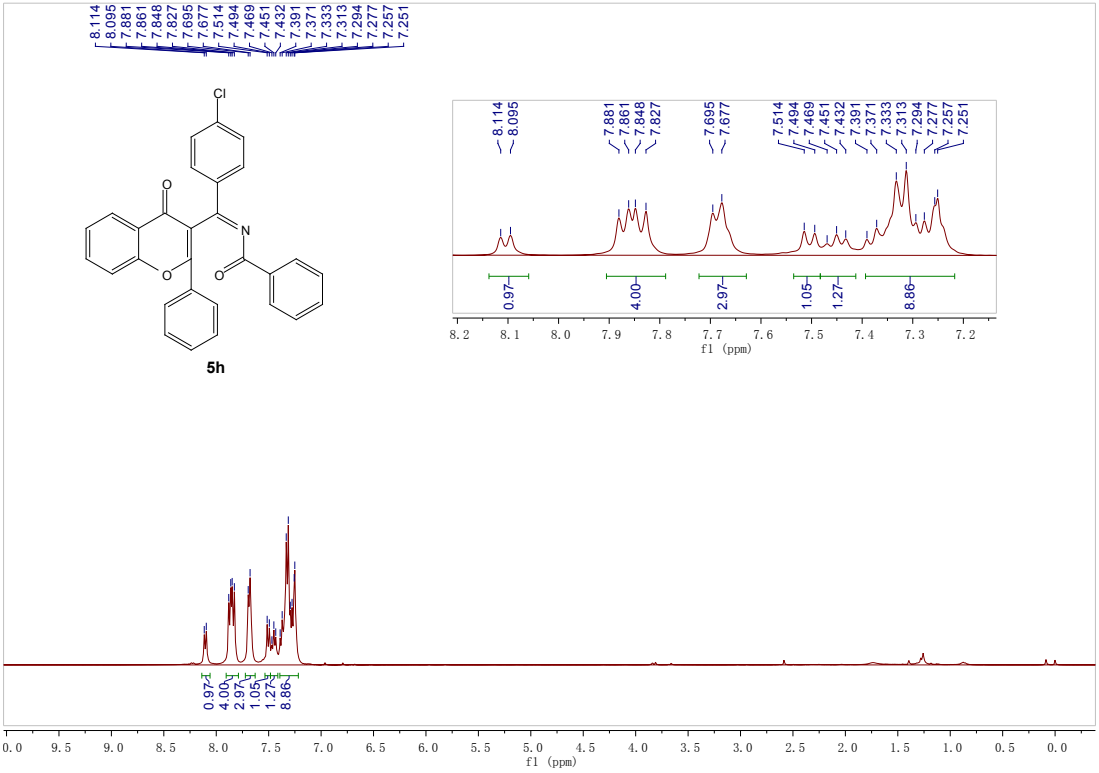
152.472
148.150
132.835
132.095
131.229
129.757
128.903
128.750
128.633
128.506
116.230
104.910
99.684
77.320
77.000
76.680
56.361
56.204
137.153
133.150
132.835
132.454
132.095
131.229
129.757
128.903
128.750
128.633
128.506
128.229
5g
f1 (ppm)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8.095
7.881
7.861
7.848
7.827
7.695
7.677
7.514
7.494
7.469
7.451
7.432
7.391
7.371
7.333
7.313
7.294
7.277
7.257
7.251
Cl
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N
O
O
5h
0.97
4.00
2.97
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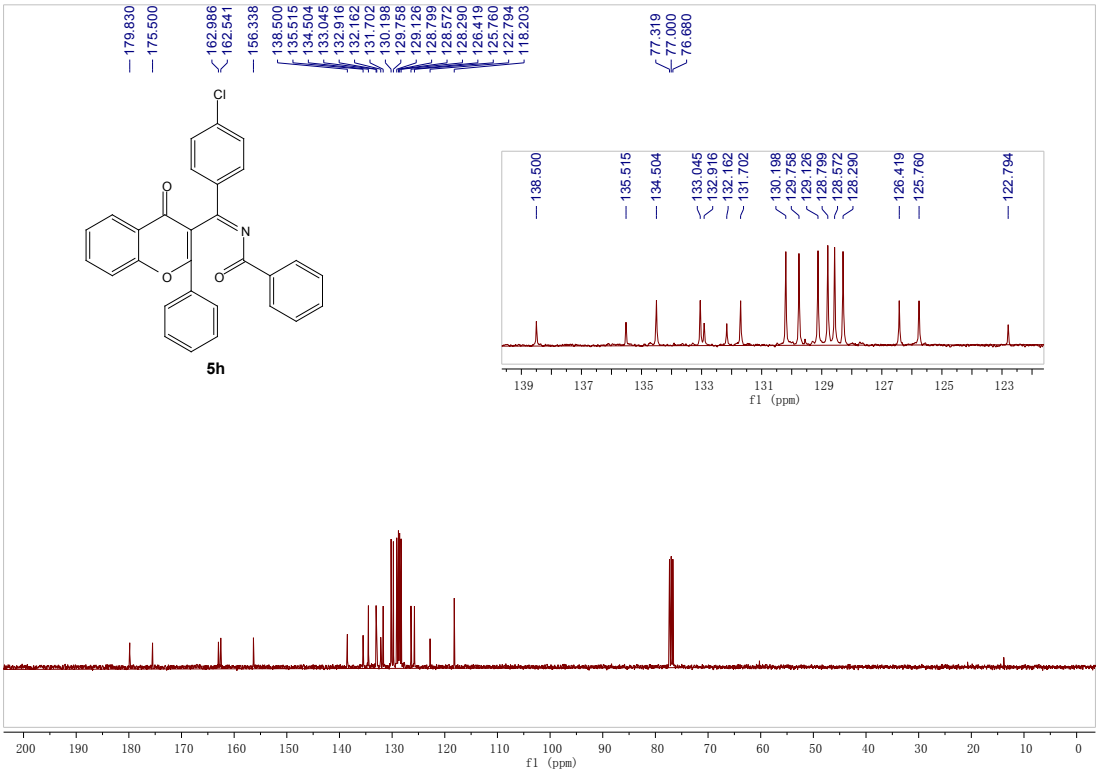
1.27
8.86
f1 (ppm)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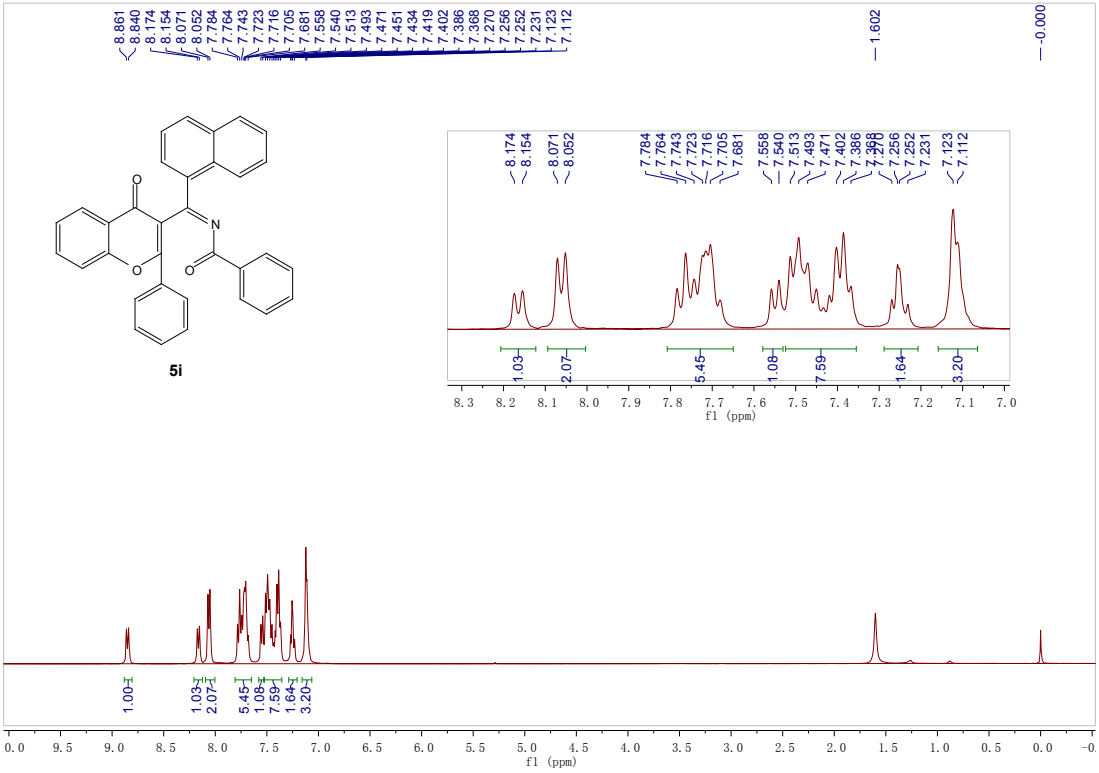
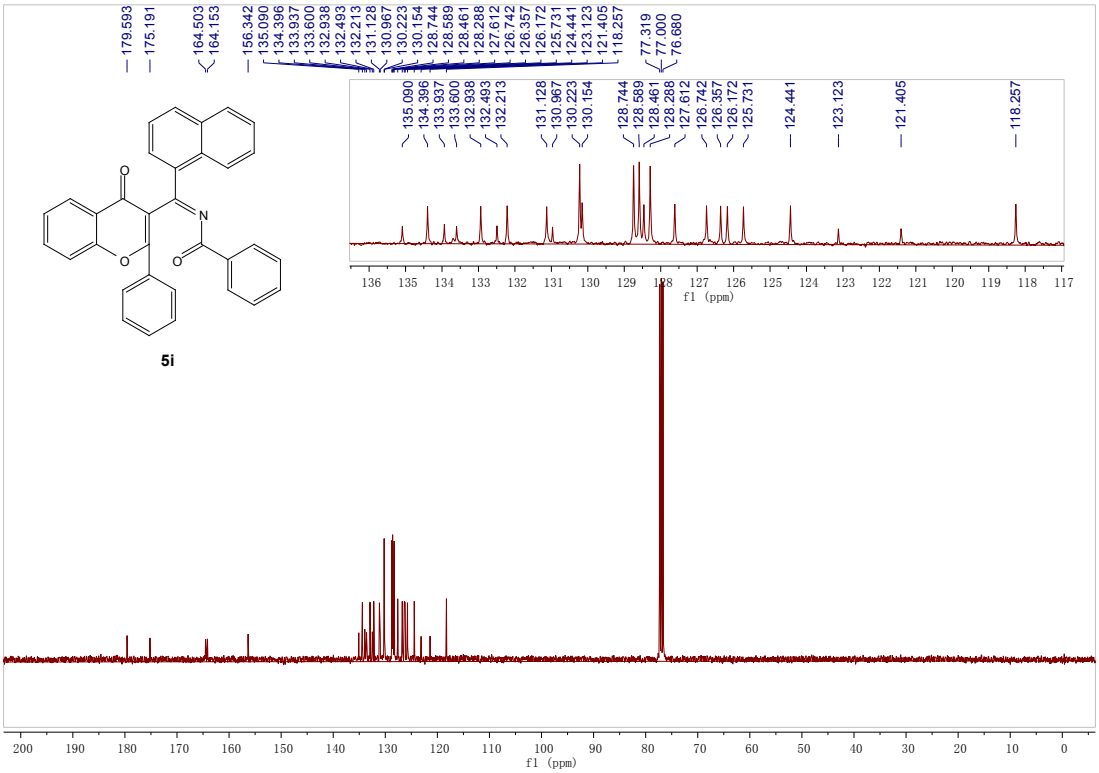
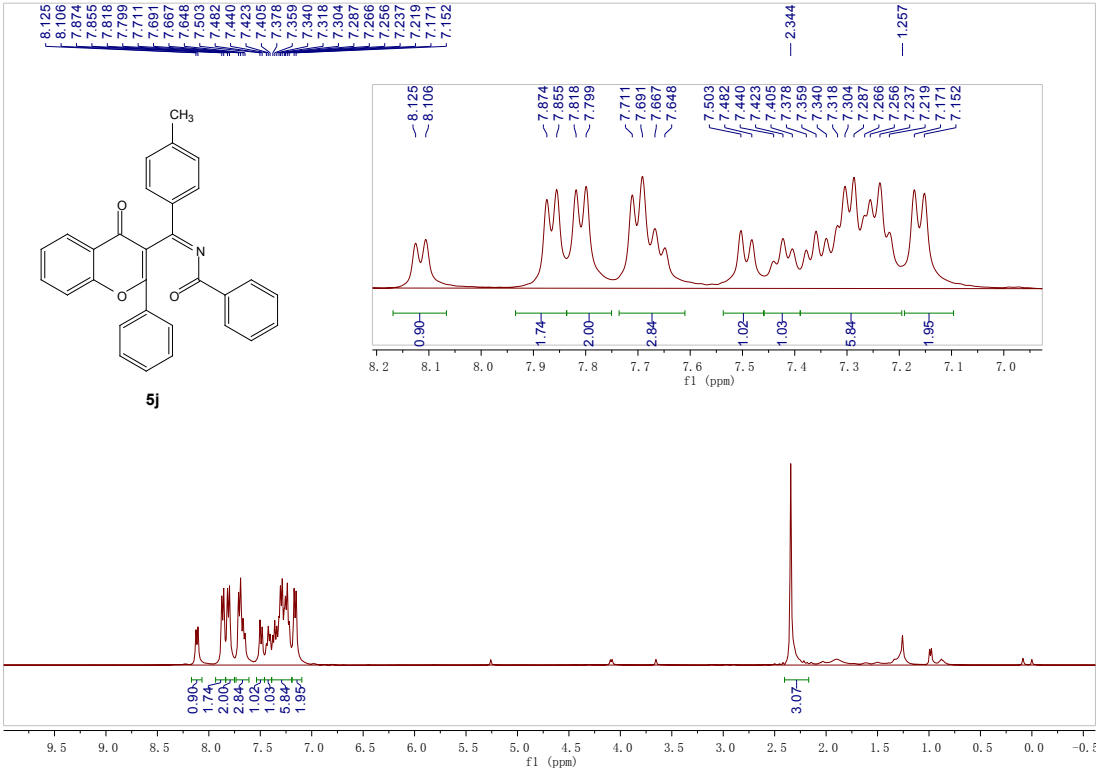
162.541
156.338
138.500
135.515
134.504
133.045
132.916
132.162
131.702
130.198
129.758
129.126
128.799
128.572
128.290
126.419
125.760
122.794
118.203
77.319
77.000
76.680
Cl
O
N
O
O
5h
f1 (ppm)


5i
f1 (ppm)


5i
f1 (ppm)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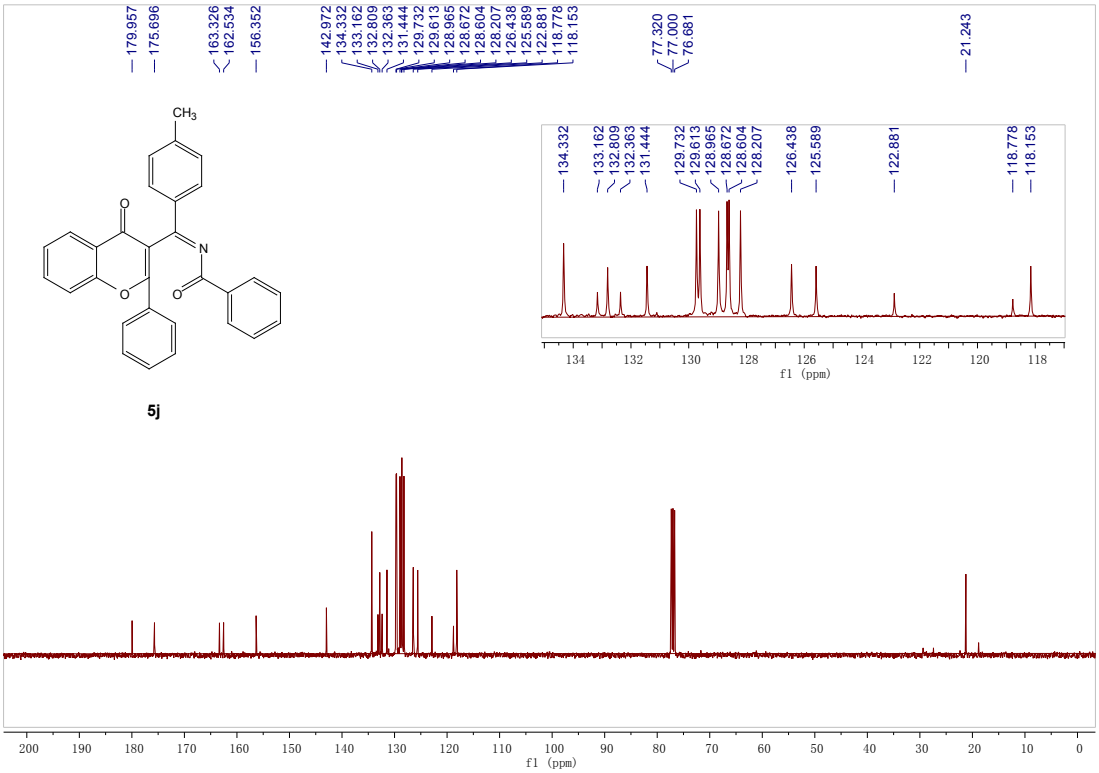
8.106
7.874
7.855
7.818
7.799
7.711
7.691
7.667
7.648
7.503
7.482
7.440
7.423
7.405
7.378
7.359
7.340
7.318
7.304
7.287
7.266
7.256
7.237
7.219
7.171
7.152
2.344
1.257
CH3
O
N
O
O
5j
0.90
1.74
2.00
2.84
1.02
1.03
5.84
1.95
3.07
f1 (ppm)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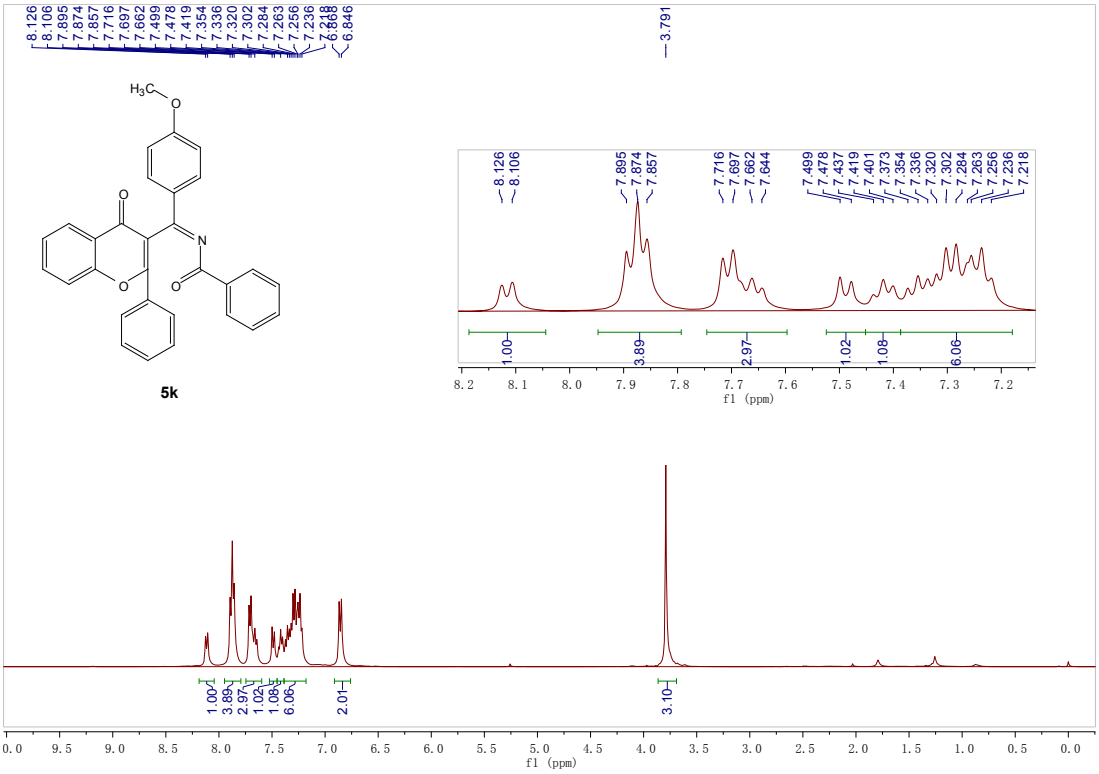
134.332
133.162
132.809
132.363
131.444
129.732
129.613
128.965
128.672
128.604
128.207
126.438
125.589
122.881
118.778
118.153
77.320
77.000
76.681
21.243
CH3
O
N
O
O
5j
f1 (ppm)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8.106
7.895
7.874
7.857
7.716
7.697
7.662
7.499
7.478
7.419
7.354
7.336
7.320
7.302
7.284
7.263
7.256
7.236
6.868
6.846
3.791
H3C
O
O
N
O
O
5k
8.126
8.106
7.895
7.874
7.857
7.716
7.697
7.682
7.644
7.499
7.478
7.437
7.419
7.401
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7.354
7.336
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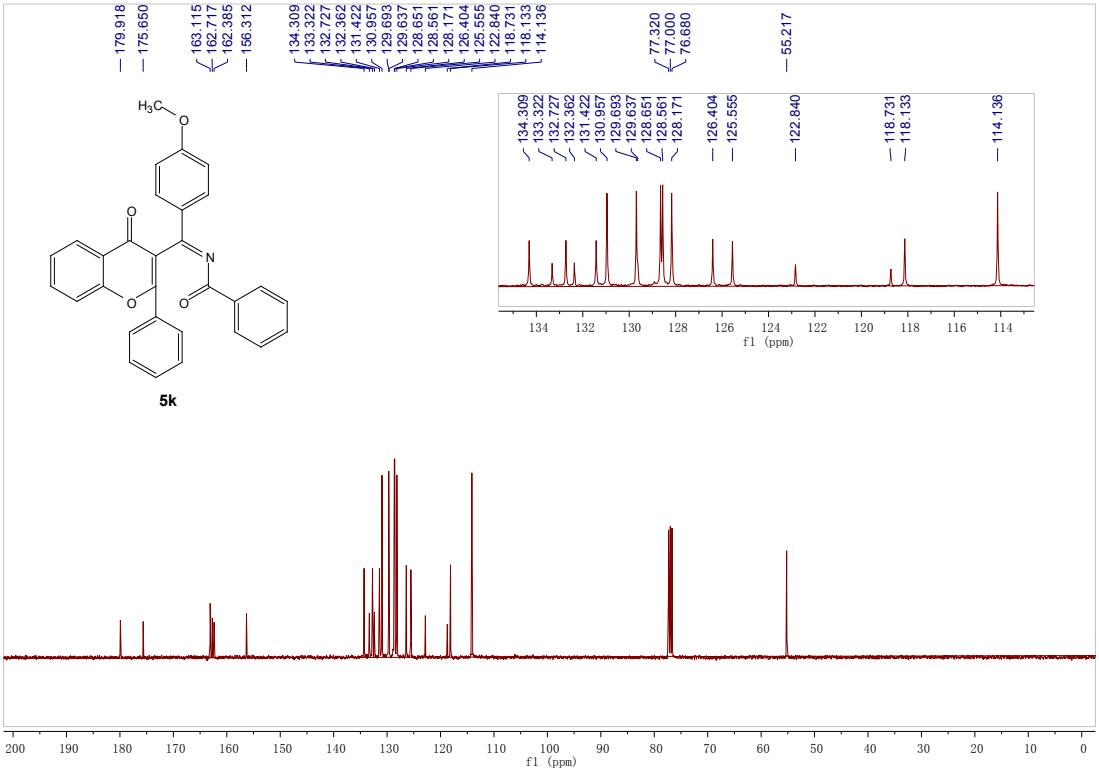
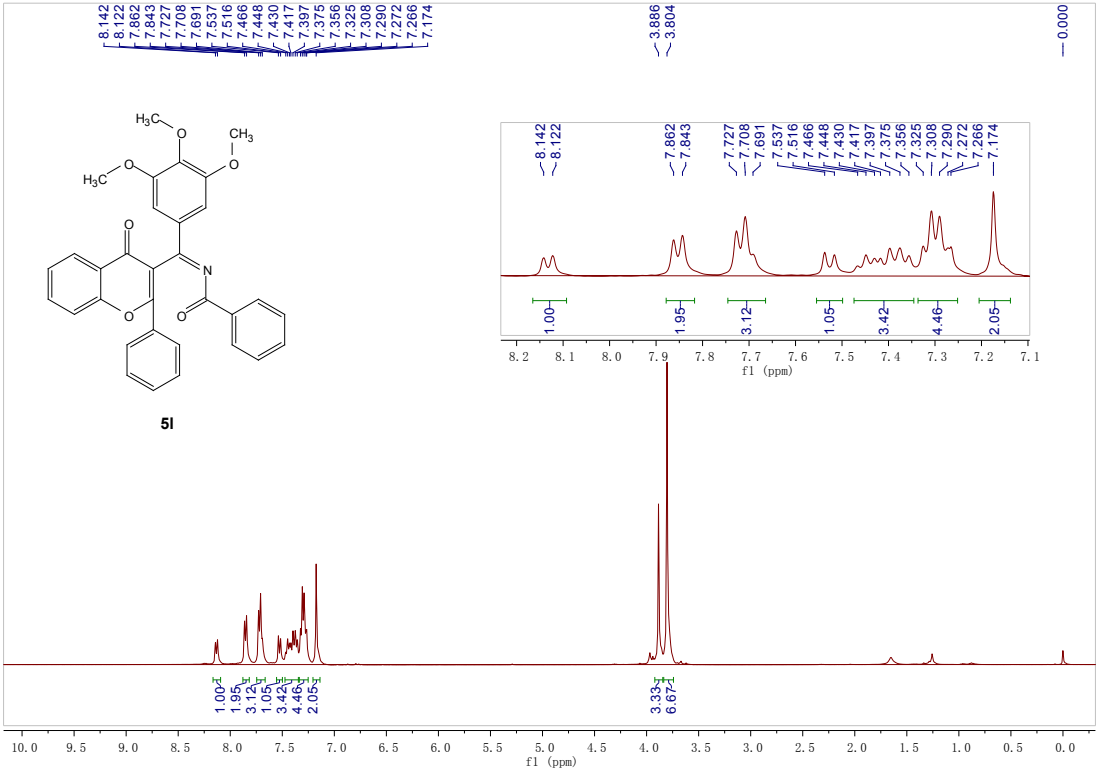
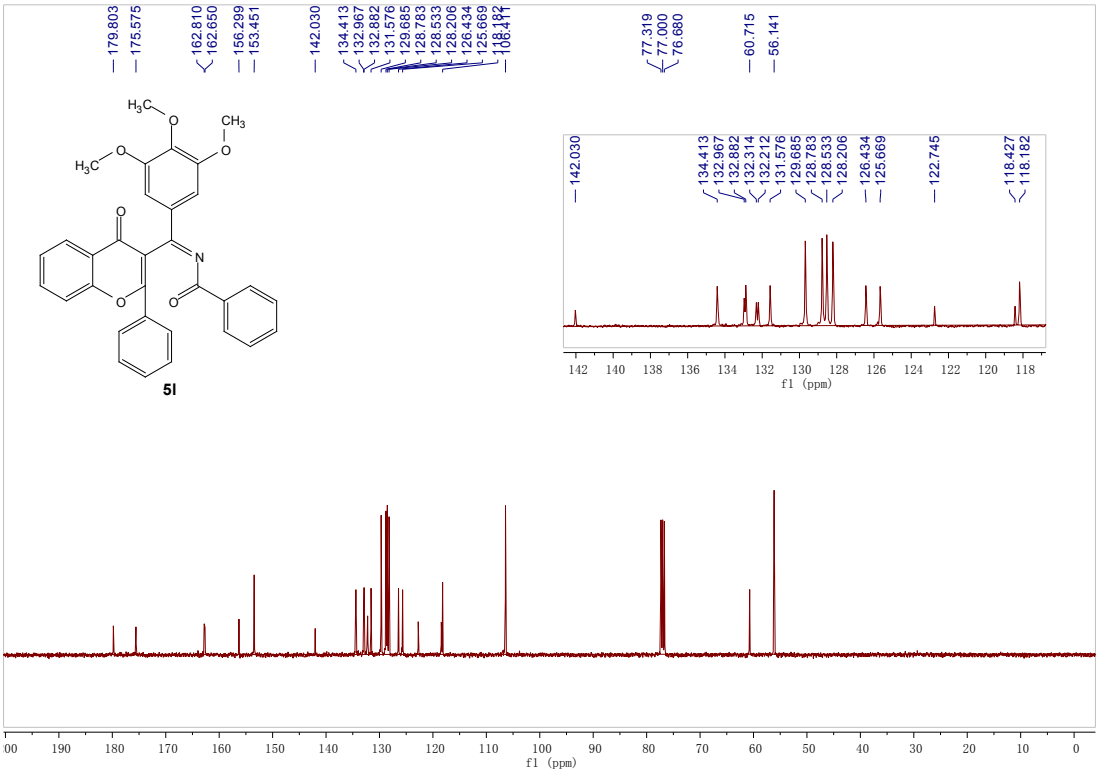
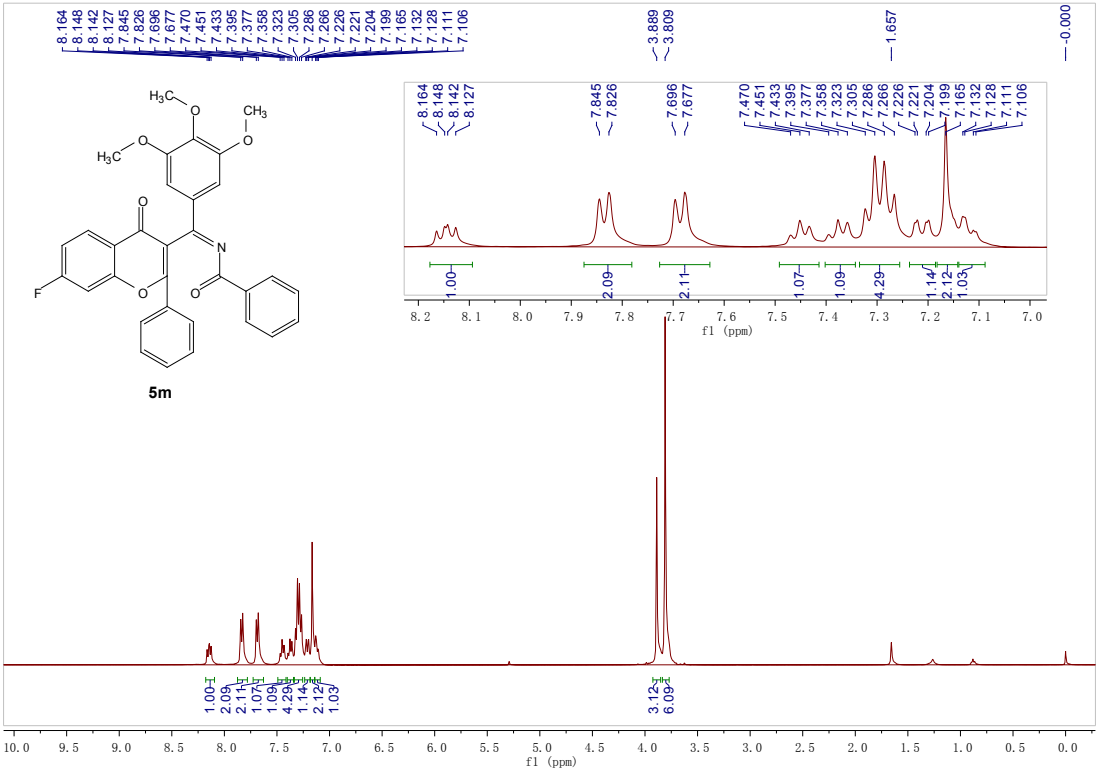
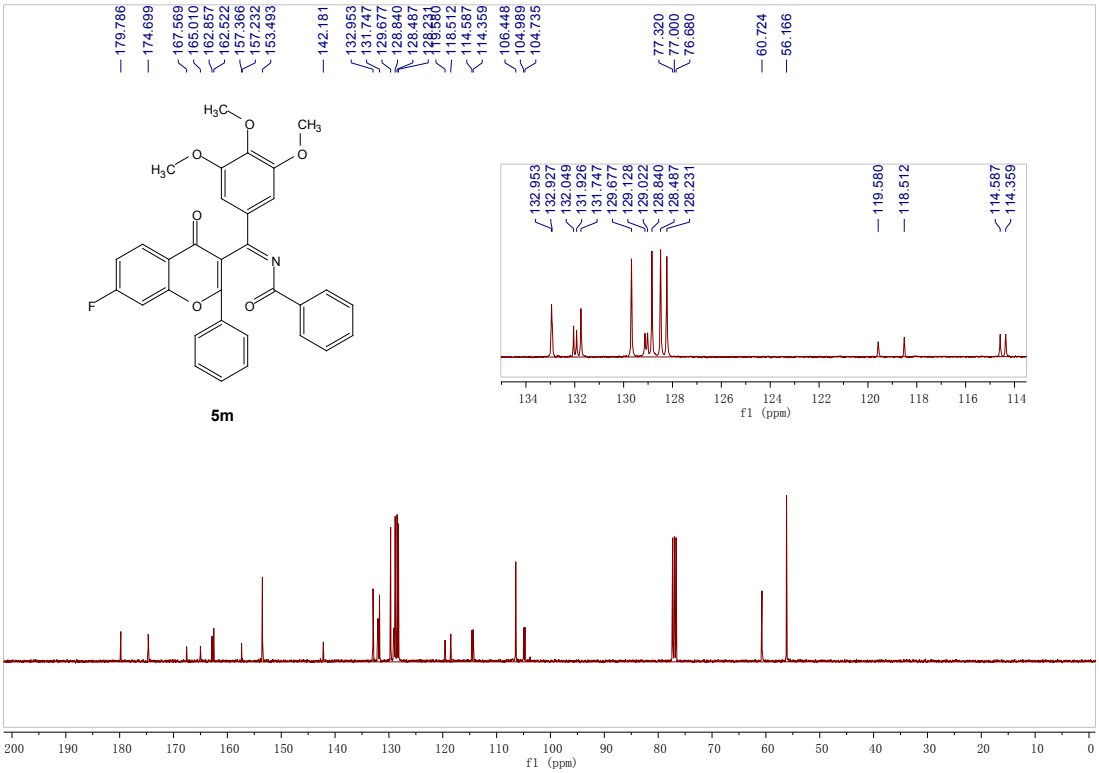
7.263
7.256
7.236
7.218
1.00
3.89
2.97
1.02
1.08
6.06
8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2
f1 (ppm)
1.00
3.89
2.97
1.02
1.08
6.06
2.01
3.10
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


179.918
175.650
163.115
162.717
162.385
156.312
134.309
133.322
132.727
132.362
131.422
130.957
129.693
129.637
128.651
128.561
128.171
126.404
125.555
122.840
118.731
118.133
114.136
77.320
77.000
76.680
55.217
H3C
O
O
N
O
O
5k
134.309
133.322
132.727
132.362
131.422
130.957
129.693
129.637
128.651
128.561
128.171
126.404
125.555
122.840
118.731
118.133
114.136
134 132 130 128 126 124 122 120 118 116 114
f1 (ppm)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.142
8.122
7.862
7.843
7.727
7.708
7.691
7.537
7.516
7.466
7.448
7.430
7.417
7.397
7.375
7.356
7.325
7.308
7.290
7.272
7.266
7.174
3.886
3.804
0.000
5l
1.00
1.95
3.12
1.05
3.42
4.46
2.05
3.33
6.67
f1 (ppm)

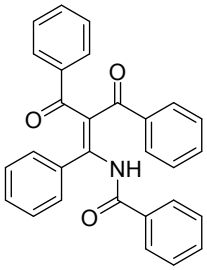

179.803
175.575
162.810
162.650
156.299
153.451
142.030
134.413
132.967
132.882
131.576
129.685
128.783
128.533
128.206
126.434
125.669
118.427
118.182
77.319
77.000
76.680
60.715
56.141
5l
f1 (ppm)


8.164
8.148
8.142
8.127
7.845
7.826
7.696
7.677
7.470
7.451
7.433
7.395
7.377
7.358
7.323
7.305
7.286
7.266
7.226
7.221
7.204
7.199
7.165
7.132
7.128
7.111
7.106
3.889
3.809
1.657
-0.000
5m
f1 (ppm)


179.786
174.699
167.569
165.010
162.857
162.522
157.366
157.232
153.493
142.181
132.953
131.747
129.677
128.840
128.487
128.231
118.512
114.587
114.359
106.448
104.989
104.735
77.320
77.000
76.680
60.724
56.166
119.580
118.512
114.587
114.359
5m
f1 (ppm)

6. X-ray Crystallography of Compounds 3a and 5e

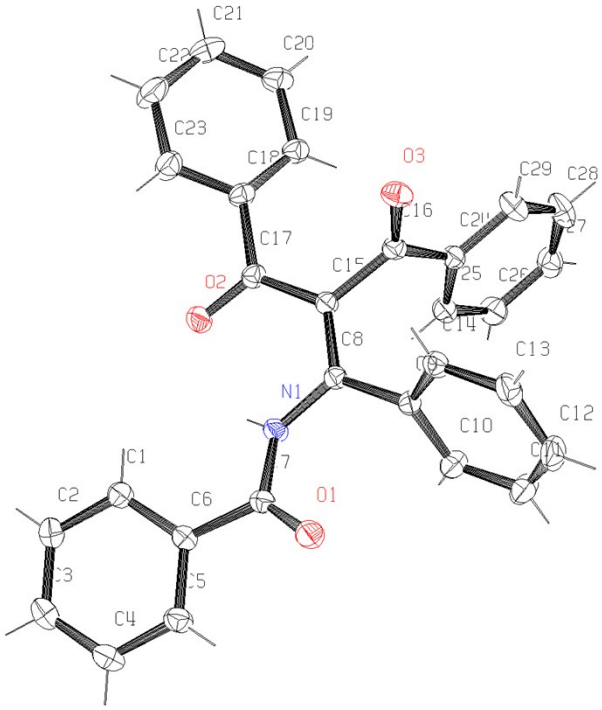
***N*-(2-benzoyl-3-oxo-1,3-diphenylprop-1-en-1-yl)benzamide (3a, CCDC 1557390)**
(Ortep ellipsoids are depicted at the 50% level)

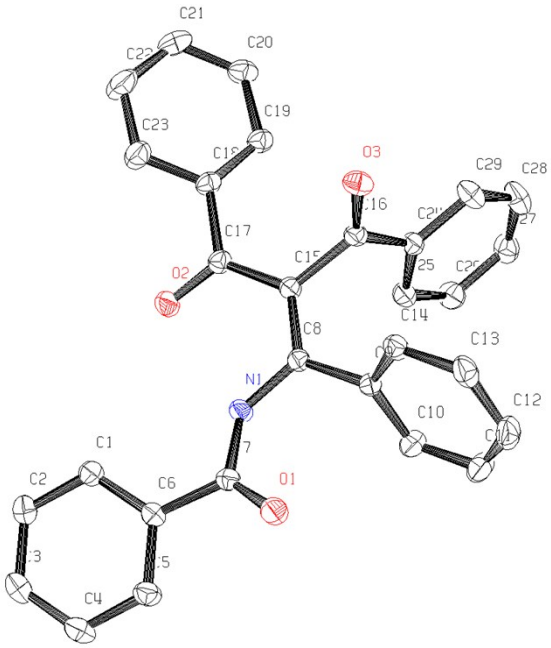


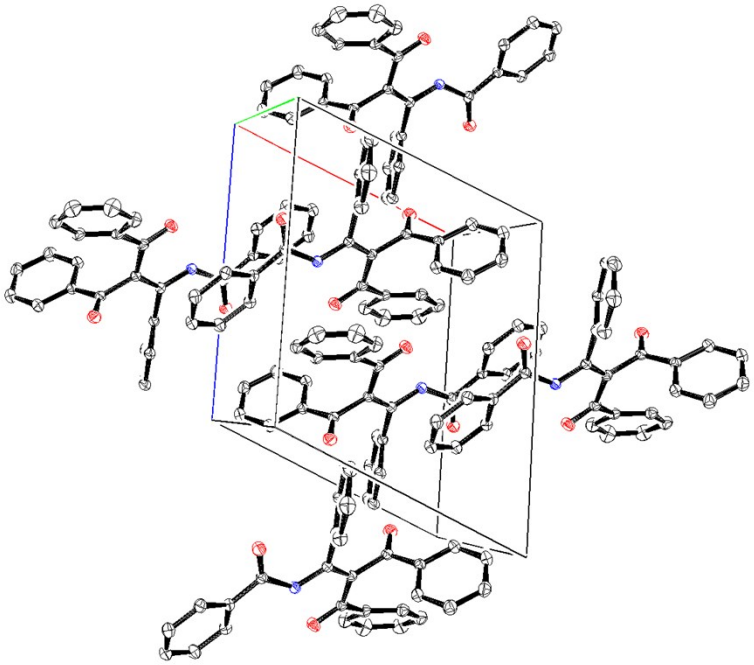
3a

Crystal data and structure refinement for **3a**

Identification code	**3a**
Empirical formula	$C_{29}H_{21}NO_3$
Formula weight	431.47
Temperature	130 K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P -1
Unit cell dimensions	a = 9.7087(8) Åα= 78.551(2)°. b = 10.8041(9) Åβ= 66.3730(10)°. c = 11.9237(10) Åγ = 74.2780(10)°
Volume	1097.26(16) $Å^3$
Z	2
Density (calculated)	1.306 Mg/m^3
Absorption coefficient	0.085 mm^{-1}
F(000)	452
Crystal size	0.28 x 0.25 x 0.2 mm^3
Theta range for data collection	1.874 to 30.656°
Index ranges	-13<=h<=13, -14<=k<=15, -17<=l<=16
Reflections collected	11232
Independent reflections	6688 [R(int) = 0.0135]
Completeness to theta = 26.000°	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7461 and 0.6835
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6688 / 0 / 298
Goodness-of-fit on F^2	1.038
Final R indices [I>2sigma(I)]	R1 = 0.0452, wR2 = 0.1157
R indices (all data)	R1 = 0.0575, wR2 = 0.1247
Extinction coefficient	n/a
Largest diff. peak and hole	0.370 and -0.315 $e.Å^{-3}$

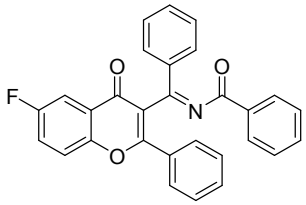

C21
C20
C22
C19
C23
O3
C29
C28
C16
C17
O2
C8
C13
N1
C10
C12
C1
C2
C6
O1
C3
C5
C4


C21
C20
C22
C19
C23
O3
C29
C28
C16
C17
C15
O2
C14
C8
C13
N1
C10
C12
C1
C2
C6
O1
C4



***N*-((6-fluoro-4-oxo-2-phenyl-4H-chromen-3-yl)(phenyl)methylene)benzamide (5e, CCDC 1557391)**

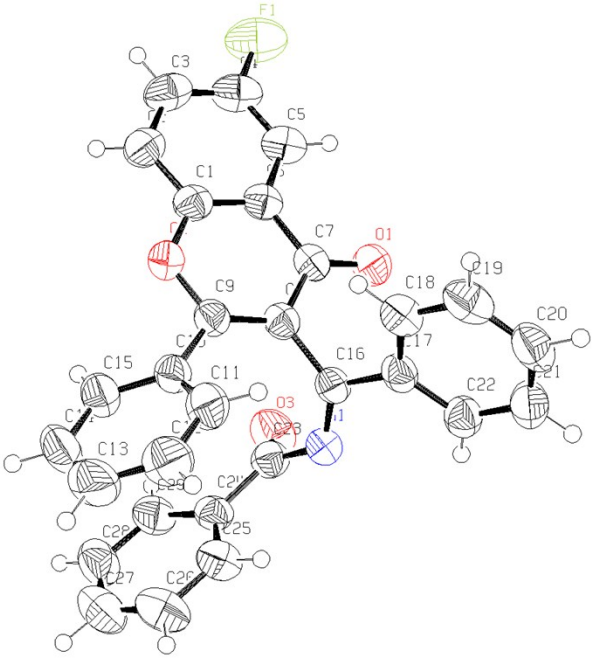
(Ortep ellipsoids are depicted at the 50% level)

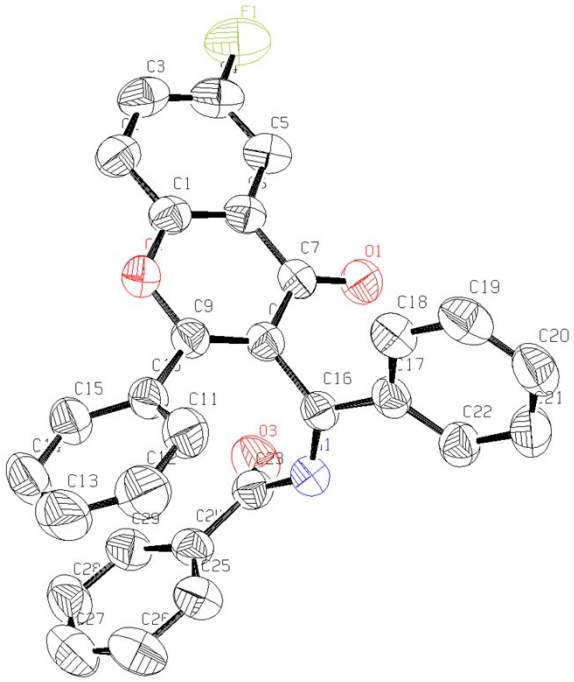


5e

Crystal data and structure refinement for **5e**

Identification code	**5e**
Empirical formula	$C_{29}H_{18}FNO_3$
Formula weight	447.44
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 2/n
Unit cell dimensions	a = 7.5691(10) Å α = 90° b = 11.0082(13) Åβ= 93.532(3)° c = 26.381(3) Å γ = 90°
Volume	2193.9(5) $Å^3$
Z	4
Density (calculated)	1.355 Mg/m^3
Absorption coefficient	0.094 mm^{-1}
F(000)	928
Crystal size	0.200 x 0.170 x 0.130 mm^3
Theta range for data collection	1.547 to 25.500°
Index ranges	-6<=h<=9, -13<=k<=13, -31<=l<=29
Reflections collected	12409
Independent reflections	4089 [R(int) = 0.0410]
Completeness to theta = 26.000°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.6373
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4089 / 0 / 307
Goodness-of-fit on F^2	1.023
Final R indices [I>2sigma(I)]	R1 = 0.0526, wR2 = 0.1198
R indices (all data)	R1 = 0.0787, wR2 = 0.1332
Extinction coefficient	n/a
Largest diff. peak and hole	0.183 and -0.133 e.$Å^{-3}$


F1
C3
C5
C1
C7
O1
C9
C18
C19
C20
C17
C15
C11
C16
C21
C22
O3
C13
C25
C27
C26


F1
C3
C5
C1
C7
O1
C9
C18
C19
C20
C17
C16
C15
C11
C21
C22
O3
N1
C13
C25
C27