Supplementary Information

Rh(III)-Catalyzed C−H Activation of (Hetero)Arenes with Cyclobutenones via C-C bond Cleavage

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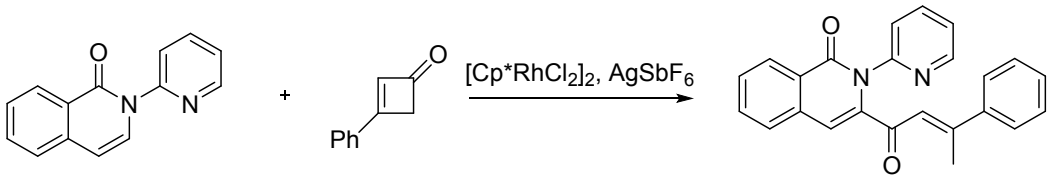
1. General Information

All the reactions were carried out under argon atmosphere using standard Schlenk technique or in a argon-filled glove box. The ^{1}H NMR spectra were recorded on a 400 MHz or 600 MHz NMR spectrometer. The ^{13}C NMR spectra were recorded at 100 MHz or 150 MHz. The ^{19}F NMR spectra were recorded at 376 or 565 MHz. The residual solvent signals were used as references and the chemical shifts were converted to the TMS scale. HRMS data were obtained using a TOF mode. The conversion of starting materials was monitored by thin layer chromatography (TLC), and components were visualized under UV light (254 and 365 nm). Column chromatography was performed on silica gel 300-400 mesh. Unless otherwise noted, all other compounds have been reported in the literature or are commercially available. Commercial reagents were used without further purification. The substrates N-pyridinylisoquinolones [1], N-pyrimidylindoles [2] and cyclobutenones [3] were prepared according to the literature reports.

2. Optimization Studies

Table S1 Optimization studies for the synthesis of 5aa.[a]



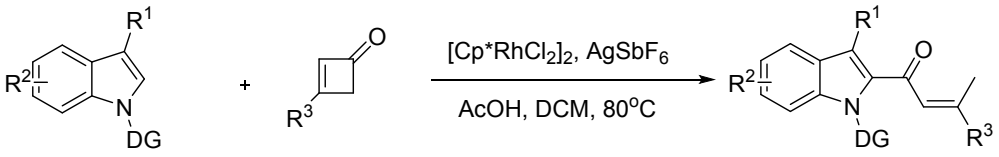
4a **2a** **5aa**

Entry	Additive	Solvent	T (°C)	Yield (%)[b]
1	CsOAc	TFE	100	10%
2	AcOH	TFE	100	61%
3	PivOH	TFE	100	70%
4	$B(OH)_3$	TFE	100	85%
5	$Zn(OTf)_2$	TFE	100	N.R
6	K_2CO_3	TFE	100	N.R
7	--	TFE	100	79%
8	$B(OH)_3$	Dioxane	100	29%
9	$B(OH)_3$	PhCl	100	18%
10	$B(OH)_3$	DCE	100	32%
11	$B(OH)_3$	TFE	80	64%

12[c]	$B(OH)_3$	TFE	100	N.R

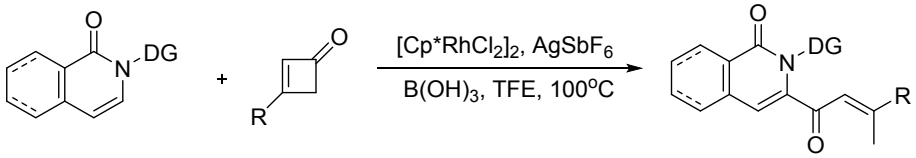
[a]Reaction Conditions: **4a** (0.2 mmol), **2a** (0.4 mmol), $[Cp^*RhCl_2]_2$ (4 mol %), $AgSbF_6$ (16 mol %), additive (0.4 mmol), solvent (2.0 mL) under Argon for 20 h. [b]Isolated yield. [c]No rhodium or $AgSbF_6$ was used.

3. General Procedure



1 **2** **3**

General Procedure A: A mixture of 3-methyl-1-(pyrimidin-2-yl)-1H-indole **1** (0.2 mmol), 3-phenylcyclobut-2-en-1-one **2** (0.4 mmol), $[Cp^*RhCl_2]_2$ (0.008 mmol, 4.0 mol %)**,** $AgSbF_6$ (0.032 mmol, 16.0 mol %), HOAc (0.2 mmol, 1.0 equiv) and DCM (2.0 mL) were charged into a pressure tube under argon. The reaction mixture was stirred at 80 ºC for 20 h. After the reaction was complete (20 h), The reaction mixture was filtered through a pad of celite eluting with ethyl acetate, concentrated, and purified by silica gel chromatography (PE : EA = 10:1) to give the indicated product **3.**

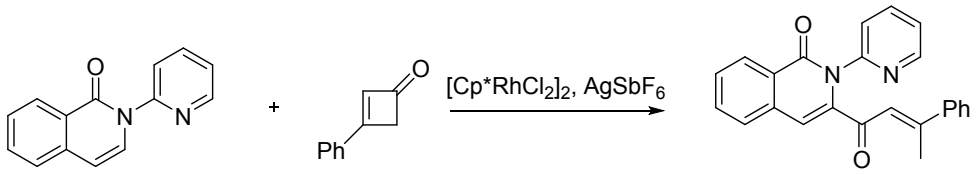


4 **2** **5**

General Procedure B: A mixture of *N*-pyridylisoquinolone **4** (0.2 mmol), 3-phenylcyclobut-2-en-1-one **2** (0.4 mmol), $[Cp^*RhCl_2]_2$ (0.008 mmol, 4.0 mol %)**,** $AgSbF_6$ (0.032 mmol, 16.0 mol %), $B(OH)_3$ (0.4 mmol, 2.0 equiv) and TFE (2.0 mL) were charged into a pressure tube under argon. The reaction mixture was stirred at 100 ºC for 20 h. The reaction mixture was filtered through a pad of celite eluting with ethyl acetate, concentrated, and purified by silica gel chromatography (PE : EA = 3:1) to give the indicated product **5.**

4. Derivatization

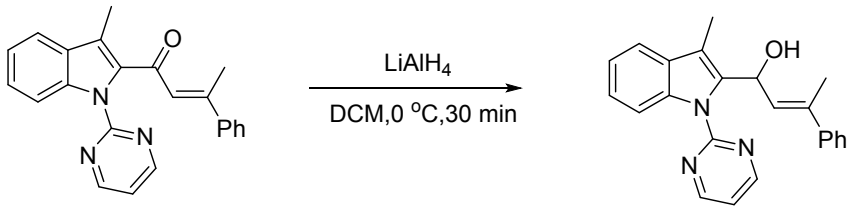
4.1 Scale-Up Synthesis of 5aa.



4a **2a** **5aa**

A mixture of N-pyridylisoquinolone **4a** (666.0 mg, 3.0 mmol), 3-phenylcyclobut-2-en-1-one **2a** (864.0 mg, 6.0 mmol), $[Cp^*RhCl_2]_2$ (74.2 mg, 0.12 mmol, 4.0 mol %), $AgSbF_6$ (164.6 mg, 0.48 mmol, 16.0 mol %), $B(OH)_3$ (360.0 mg, 6.0 mmol, 2.0 equiv) and TFE (30 mL) were charged into a pressure tube under argon. The reaction mixture was stirred at 100 ºC for 20 h. After the solvent was removed under reduced pressure, the residue was purified by silica gel chromatography (PE:EA = 3:1) to give the indicated product **5aa** as a yellow solid. (613 mg, 56% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.39 (d, *J* = 7.9 Hz, 1H), 8.36 (d, *J* = 4.7 Hz, 1H), 7.82 – 7.76 (m, 2H), 7.68 – 7.63 (m, 1H), 7.59 – 7.51 (m, 2H), 7.43 – 7.38 (m, 2H), 7.34 – 7.29 (m, 3H), 7.21 – 7.15 (m, 1H), 7.07 (s, 1H), 6.76 (s, 1H), 2.36 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 187.2, 162.2, 156.7, 152.1, 148.4, 142.2, 141.8, 137.4, 135.1, 133.3, 129.6, 129.2, 128.6, 128.6, 127.5, 127.2, 126.5, 124.0, 122.8, 122.7, 111.5, 18.6. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{24}H_{19}N_2O_2^+$ 367.1441, Found: 367.1440.

4.2 Reduction of 3aa

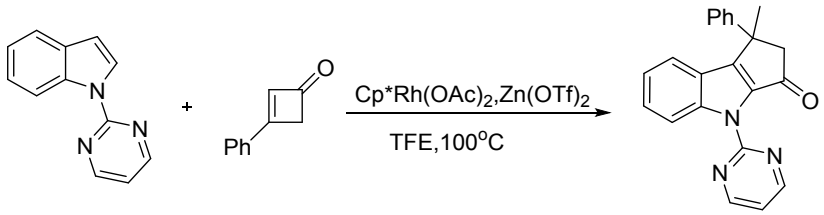


3aa **8**

To a solution of **3aa** (70.0 mg, 0.2 mmol) in anhydrous dichloromethane (2 mL) was added $LiAlH_4$ (0.06 mmol, 1.0 M THF solution, 0.3 equiv) at 0 °C. After stirring for 0.5 h at the same temperature, the reaction was quenched with H_2O and extracted with dichloromethane. The organic layer was washed with brine and then dried over anhydrous Na_2SO_4. The solvent was evaporated in vacuo and the residue was purified by chromatography on silica gel (petroleum ether/ethyl acetate = 3:1) to afford **8** (52

mg, 73% yield) as yellow oil.[1]H NMR (400 MHz, CD_2Cl_2) δ 8.72 (d, *J* = 4.9 Hz, 2H), 8.34 – 8.27 (m, 1H), 7.54 – 7.46 (m, 1H), 7.25 – 7.12 (m, 2H), 7.12 – 7.04 (m, 4H), 7.00 – 6.94 (m, 2H), 6.51 (d, *J* = 10.0 Hz, 1H), 5.84 – 5.72 (m, 2H), 2.39 (s, 3H), 1.81 – 1.76 (m, 3H). [13]C NMR (100 MHz, CD_2Cl_2) δ 158.2, 157.9, 143.2, 137.1, 136.5, 136.3, 130.3, 130.2, 128.0, 126.9, 125.6, 124.2, 122.0, 119.0, 116.8, 115.6, 114.3, 63.6, 15.9, 9.2. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{23}H_{22}N_3O^+$ 356.1757, Found: 356.1757.

4.3 The cyclization reaction

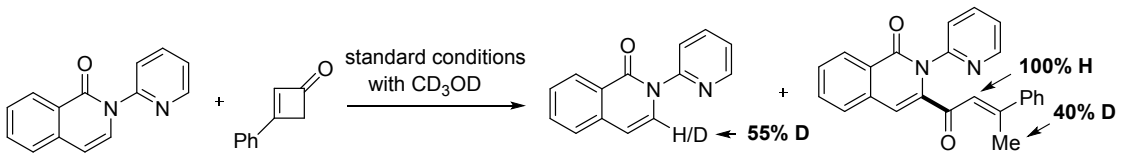


9 **2a** **10**

A mixture of *N*-pyrimidinylindole **6a** (39.0 mg, 0.2 mmol), 3-phenylcyclobut-2-en-1-one **2a** (57.0 mg, 0.4 mmol), $Cp^*Rh(OAc)_2$ (6.0 mg, 0.016 mmol, 8.0 mol %)**,** $Zn(OTf)_2$ (145.2 mg, 0.4 mmol, 2.0 equiv) and TFE (2.0 mL) were charged into a pressure tube under argon. The reaction mixture was stirred at 100 ºC for 20 h. After the solvent was removed under reduced pressure, the residue was purified by silica gel chromatography (PE:EA = 3:1) to give the indicated product **10** as a White solid (37 mg, 54% yield, m.p. 149 – 151 °C). [1]H NMR (600 MHz, $CDCl_3$) δ 8.85 (d, *J* = 4.8 Hz, 2H), 8.57 (d, *J* = 8.6 Hz, 1H), 7.52 – 7.47 (m, 1H), 7.47 – 7.43 (m, 1H), 7.40 – 7.37 (m, 2H), 7.33 – 7.28 (m, 2H), 7.25 – 7.20 (m, 3H), 3.32 (d, J = 17.8 Hz, 1H), 3.24 (d, J = 17.8 Hz, 1H), 1.98 (s, 3H). [13]C NMR (150 MHz, $CDCl_3$) δ 190.5, 158.5, 157.3, 156.8, 146.0, 143.9, 137.7, 128.6, 128.4, 126.6, 126.1, 123.7, 122.9, 122.3, 117.7, 116.1, 60.7, 42.1, 27.6. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{22}H_{18}N_3O^+$ 340.1444, Found: 340.1444.

5. Mechanism Studies.

5.1 H/D exchange experiments:

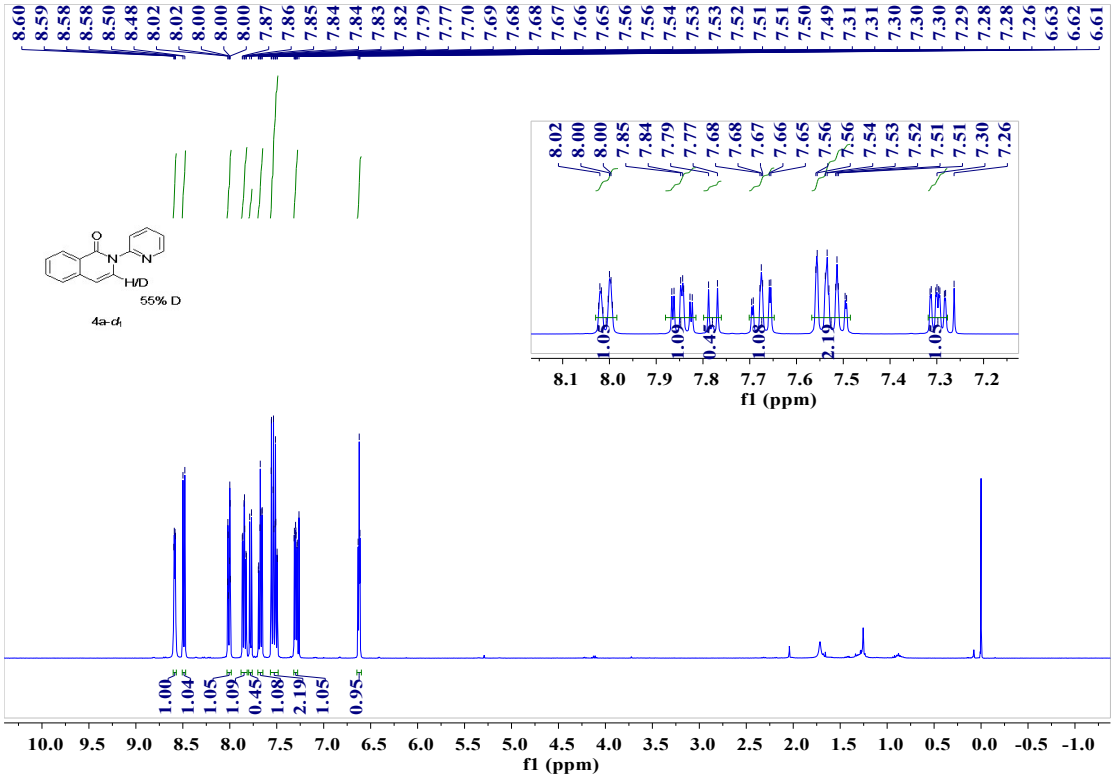


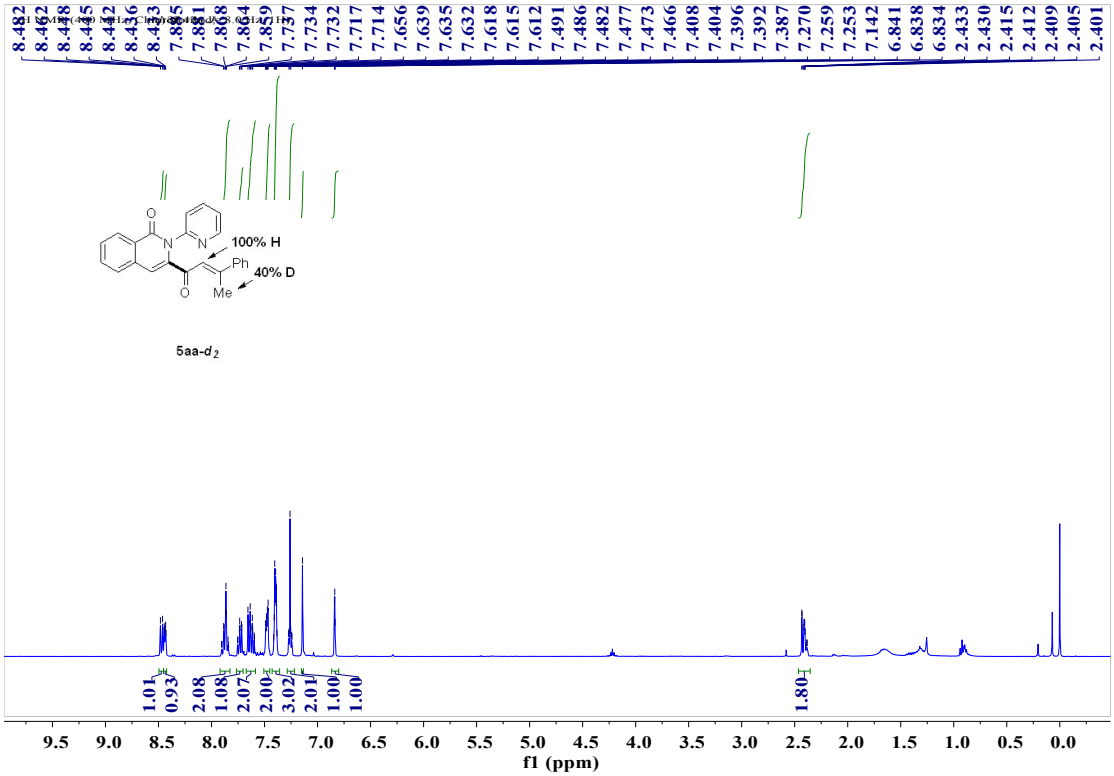
4a **2a** **4a-*d*$_1$** **5aa-*d*$_2$**

A mixture of **4a** (44.4 mg, 0.2 mmol, 1.0 equiv), **2a** (57.6 mg, 0.4 mmol, 2.0 equiv), $[Cp^*RhCl_2]_2$ (5.0 mg, 0.008 mmol, 4.0 mol %), $AgSbF_6$ (11.6mg, 0.032mmol, 16.0 mol %), $B(OH)_3$ (24.7 mg, 0.4 mmol, 2.0 equiv) and CD_3OD (10.0 equiv) were added into a tube. DCE (2.0 mL) was added and the mixture was stirred at 100 °C for 12 h. Then it was evaporated under reduced pressure and the residue was absorbed onto small amounts of silica. The product **5aa-*d*$_2$** and the recovered **4a-*d*$_1$** were obtained by flash column chromatography on silica gel (eluent: PE/EA = 3:1).

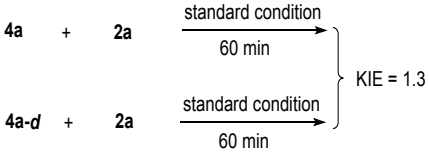
4a-*d*$_1$. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62-8.56 (m, 1H), 8.49 (d, *J* = 8.0 Hz, 1H), 8.03-7.97 (m, 1H), 7.88 – 7.81 (m, 1H), 7.8.-7.75 (m, 0.45H), 7.70-7.64 (m, 1H), 7.58 – 7.48 (m, 2H), 7.32-7.67 (m, 1H), 6.65-6.59 (m, 1H).

5aa-*d*$_2$. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (d, *J* = 8.0, Hz 1H), 8.45-8.41 (m, 1H), 7.92 – 7.80 (m, 2H), 7.77-7.68 (m, 1H), 7.68 – 7.58 (m, 2H), 7.52 – 7.45 (m, 2H), 7.43-7.35 (m, 3H), 7.28 – 7.23 (m, 1H), 7.14 (s, 1H), 6.86-6.82 (m, 1H), 2.41-6-2.36(m, 1.8H).



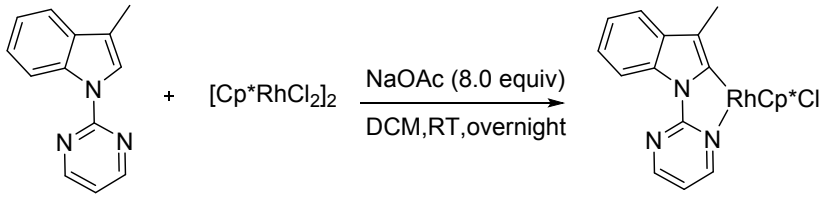


5.2. KIE experiments:



Two tubes each was charged with **4a** (22.2 mg, 0.1 mmol, 0.5 equiv) or **4a-*d*** (22.2 mg, 0.1 mmol, 0.5 equiv). To each tube was added **2a** (28.8 mg, 0.2 mmol, 1.0 equiv), $[Cp^*RhCl_2]_2$ (2.5 mg, 0.004 mmol, 2.0 mol %), $AgSbF_6$ (5.5 mg, 0.016 mmol, 8.0 mol %) and TFE (1.0 mL) was added and the mixture was stirred side-by-side in a pre-heated oil bath at 100 °C for 60 minutes. The reaction mixture was filtered through a pad of celite eluting with ethyl acetate, concentrated, After the solvent was removed under reduced pressure, the residue was purified by silica gel chromatography using PE/EA (3:1) to afford the product. The KIE value was determined to be k_H/k_D = 1.3 on the basis of ^{1}H NMR analysis using dibromomethane as internal standard.

5.3. Procedure for the synthesis of cyclometalated Rh(III) complex 11.



1a **11**

$[Cp^*RhCl_2]_2$ (61.8 mg, 0.1 mmol), *N*-Pyrimidinylindole **1a** (42.0 mg, 0.2 mmol), and sodium acetate (65.6 mg, 8.0 equiv) in DCM (2.0 mL) were added to a schlenk tube under Argon protected. Then, the mixture was stirred at room temperature for overnight. The solution was filtered through Celite and evaporated to dryness. The product was crystallized from DCM/hexane to give **11** (23.0 mg, 48% yield) as orange crystals. ^{1}H NMR (400 MHz, CD_2Cl_2) δ 8.72 – 8.65 (m, 2H), 8.41 (d, *J* = 8.0, 1H), 7.38 (d, *J* = 7.7, 1H), 7.25 – 7.19 (m, 1H), 7.13 – 7.07 (m, 1H), 7.02 – 6.97 (m, 1H), 2.50 (s, 3H), 1.73 (s, 9H). ^{13}C NMR (150 MHz, CD_2Cl_2) δ 159.6, 159.2 (d, *J* = 38.6 Hz), 158.8, 136.8, 135.8, 122.2, 121.7, 120.3, 119.5, 116.0, 114.4, 113.2, 96.8 (d, *J* = 6.6 Hz), 11.7, 9.3.HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{23}H_{25}N_3Rh^+$ ([M-Cl]) 446.1098, Found: 446.1098.

6. X-Ray Crystallographic Data

Crystal structure details for Product 3ga (CCDC: 1977120).

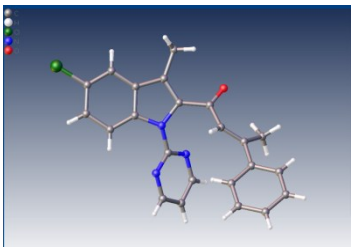
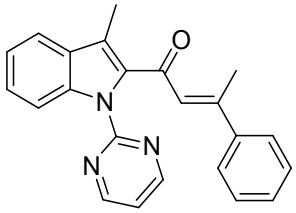


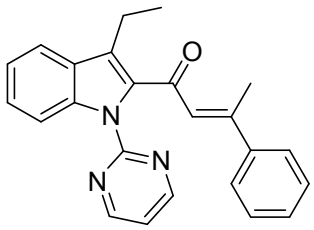
Table 1 Crystal data and structure refinement for 3ga.

Identification code	**3ga**
Empirical formula	$C_{23}H_{18}ClN_3O$
Formula weight	387.87
Temperature/K	292.90(10)
Crystal system	orthorhombic
Space group	Pbca
a/Å	18.3148(3)
b/Å	7.58000(10)
c/Å	27.7096(5)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3846.82(11)
Z	8
ρ_{calc}g/cm^3	1.3393
μ/mm^{-1}	1.901
F(000)	1623.4
Crystal size/mm^3	0.9 × 0.3 × 0.08
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	9.66 to 142.86
Index ranges	$-22 \le h \le 21$, $-9 \le k \le 8$, $-33 \le l \le 33$
Reflections collected	9900
Independent reflections	3667 [R_{int} = 0.0477, R_{sigma} = 0.0378]
Data/restraints/parameters	3667/0/255
Goodness-of-fit on F^2	1.036
Final R indexes [I>=2σ (I)]	R_1 = 0.0869, wR_2 = 0.2393
Final R indexes [all data]	R_1 = 0.0920, wR_2 = 0.2446
Largest diff. peak/hole / e Å^{-3}	0.54/-0.55

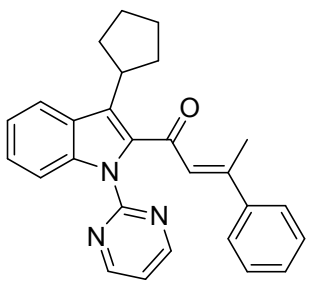
7. Analytical Data for All Products.



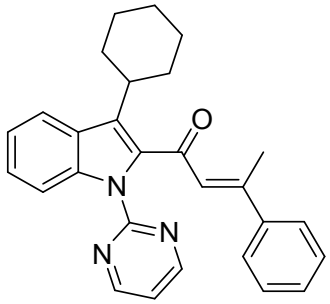
(*E*)-1-(3-methyl-1-(pyrimidin-2-yl)-1H-indol-2-yl)-3-phenylbut-2-en-1-one (3aa). Yellow oil (58 mg, 82% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.70 (d, *J* = 4.8 Hz, 2H), 8.48 – 8.43 (m, 1H), 7.70 – 7.64 (m, 1H), 7.39 – 7.33 (m, 1H), 7.34 – 7.27 (m, 6H), 7.05 (t, *J* = 4.8 Hz, 1H), 6.64 (q, *J* = 1.3 Hz, 1H), 2.54 (s, 3H), 2.53 (d, *J* = 1.3 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 187.1, 157.9, 157.9, 151.7, 142.4, 137.2, 136.4, 130.2, 128.9, 128.5, 126.5, 126.5, 126.2, 122.5, 122.0, 120.5, 116.7, 114.5, 18.3, 9.6. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{23}H_{19}N_3NaO^+$ 376.1420, Found: 376.1421.



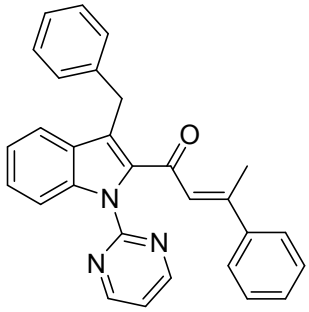
(*E*)-1-(3-ethyl-1-(pyrimidin-2-yl)-1H-indol-2-yl)-3-phenylbut-2-en-1-one (3ba). Yellow oil (62 mg, 85% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.69 (d, *J* = 4.8 Hz, 2H), 8.50 (d, *J* = 8.4 Hz, 1H), 7.71 (d, *J* = 7.8 Hz, 1H), 7.45 – 7.41 (m, 1H), 7.32 – 7.26 (m, 6H), 7.04 (t, *J* = 4.8 Hz, 1H), 6.62 (q, *J* = 1.2 Hz,1H), 3.01 (q, *J* = 7.6 Hz, 2H), 2.53 (d, *J* = 1.2 Hz, 3H), 1.38 (t, *J* = 1.2 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 187.2, 157.9, 151.6, 142.4, 137.2, 135.8, 129.3, 128.9, 128.5, 128.0, 126.4, 126.3, 126.2, 122.5, 120.5, 116.7, 114.7, 18.2, 17.8, 15.6. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{24}H_{22}N_3O^+$ 368.1757, Found: 368.1751.



(*E*)-1-(3-cyclopentyl-1-(pyrimidin-2-yl)-1H-indol-2-yl)-3-phenylbut-2-en-1-one (3ca). Yellow oil (63 mg, 78% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (d, *J* = 4.8 Hz, 2H), 8.48 (d, *J* = 8.4 Hz, 1H), 7.70 (d, *J* = 7.9 Hz, 1H), 7.36 – 7.28 (m, 1H), 7.24 – 7.14 (m, 6H), 6.94 (t, *J* = 4.8 Hz, 1H), 6.53 (q, *J* = 1.3 Hz, 1H), 3.60 (p, *J* = 9.3 Hz, 1H), 2.42 (d, *J* = 1.2 Hz, 3H), 2.06 – 1.96 (m, 4H), 1.94 – 1.83 (m, 2H), 1.76 – 1.65 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 188.0, 157.8, 157.7, 151.5, 142.4, 137.4, 136.1, 128.9, 128.5, 128.3, 128.0, 126.9, 126.2, 125.7, 122.07, 121.9, 116.6, 115.0, 36.5, 33.0, 26.8, 18.2. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{27}H_{26}N_3O^+$ 408.2070, Found:408.2070.

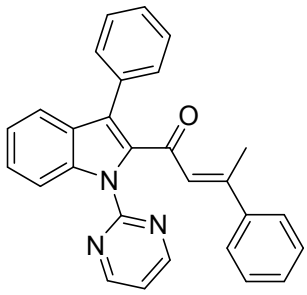


(*E*)-1-(3-cyclohexyl-1-(pyrimidin-2-yl)-1H-indol-2-yl)-3-phenylbut-2-en-1-one (3da).Yellow oil (51 mg, 60% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (d, *J* = 4.8 Hz, 2H), 8.47 (d, *J* = 8.4 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.34 – 7.28 (m, 1H), 7.25 – 7.15 (m, 6H), 6.95 (t, *J* = 4.8 Hz, 1H), 6.54 (q, *J* = 1.3 Hz, 1H), 3.17 (tt, *J* = 12.2, 3.7 Hz, 1H), 2.42 (d, *J* = 1.3 Hz, 3H), 2.02 – 1.89 (m, 2H), 1.88 – 1.76 (m, 4H), 1.76 – 1.68 (m, 1H), 1.43 – 1.22 (m, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 188.2, 157.8, 157.7, 151.4, 142.4, 137.2, 135.3, 129.5, 128.9, 128.5, 127.1, 126.2, 125.6, 122.4, 122.0, 116.6, 114.8, 36.3, 32.6, 27.0, 26.3, 18.2. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{28}H_{27}N_3NaO^+$:444.2046, Found: 444.2044.

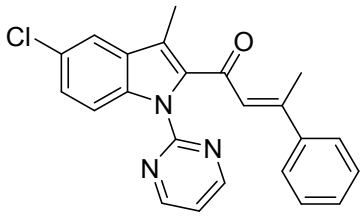


(*E*)-1-(3-benzyl-1-(pyrimidin-2-yl)-1H-indol-2-yl)-3-phenylbut-2-en-1-one (3ea).

Yellow solid (76 mg, 88% yield, m.p. 130 – 132 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.70 (d, *J* = 4.8 Hz, 2H), 8.48 (d, *J* = 8.4 Hz, 1H), 7.57 (d, *J* = 7.9 Hz, 1H), 7.43 – 7.32 (m, 3H), 7.31 – 7.12 (m, 9H), 7.06 (t, *J* = 4.9 Hz, 1H), 6.63 (d, *J* = 1.5 Hz, 1H), 4.35 (s, 2H), 2.49 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 187.0, 157.9, 157.8, 152.2, 142.2, 140.0, 137.1, 137.1, 129.5, 128.9, 128.6, 128.4, 126.3, 126.2, 126.1, 123.5, 122.7, 121.0, 116.9, 114.6, 30.3, 18.2. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{29}H_{24}N_3O^+$ 430.1914, Found: 430.1897.

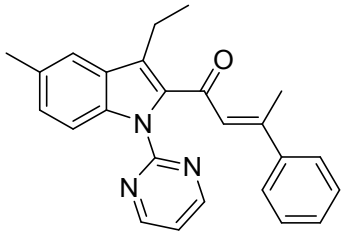


(*E*)-3-phenyl-1-(3-phenyl-1-(pyrimidin-2-yl)-1H-indol-2-yl)but-2-en-1-one (3fa). Brown oil (18 mg, 21% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, *J* = 4.8 Hz, 2H), 8.28 – 8.19 (m, 1H), 7.57 – 7.53 (m, 1H), 7.53 – 7.49 (m, 2H), 7.44 – 7.37 (m, 2H), 7.36 – 7.30 (m, 2H), 7.22 – 7.11 (m, 4H), 7.08 (t, *J* = 4.8 Hz, 1H), 6.93 – 6.88 (m, 2H), 6.49 (q, *J* = 1.2 Hz, 1H), 2.40 (d, *J* = 1.2 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 186.5, 158.1, 157.8, 153.0, 142.4, 137.2, 136.4, 133.2, 130.5, 128.8, 128.5, 128.2, 127.8, 126.4, 126.3, 126.3, 125.5, 122.8, 121.3, 117.6, 113.8, 18.4. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{28}H_{22}N_3O^+$ 416.1757, Found: 416.1750.

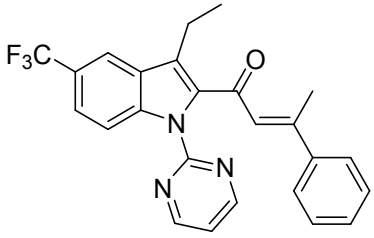


(*E*)-1-(5-chloro-3-methyl-1-(pyrimidin-2-yl)-1H-indol-2-yl)-3-phenylbut-2-en-1-one (3ga). White solid (78 mg, 93% yield, m.p. 138 – 140 °C). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.69 (d, *J* = 4.7 Hz, 2H), 8.41 (d, *J* = 8.9 Hz, 1H), 7.64 – 7.60 (m, 1H), 7.36 (dt, *J* = 9.0, 1.8 Hz, 1H), 7.33-7.29 (m, 5H), 7.09-7.06 (m, 1H), 6.62 (s, 1H), 2.54 (s,

3H), 2.48 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 186.9, 158.0, 157.6, 152.3, 142.3, 137.4, 135.3, 129.0, 128.5, 128.1, 126.4, 126.3, 126.2, 120.5, 119.9, 117.0, 115.9, 110.8, 18.3, 9.4. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{23}H_{18}ClN_3NaO^+$ 410.1031, Found: 410.1018.

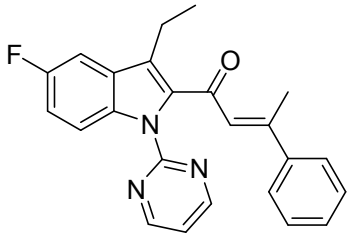


(*E*)-1-(3-ethyl-5-methyl-1-(pyrimidin-2-yl)-1H-indol-2-yl)-3-phenylbut-2-en-1-one (3ha). Yellow oil (63 mg, 82% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (d, *J* = 4.8 Hz, 2H), 8.30 (d, *J* = 8.5 Hz, 1H), 7.40 (s, 1H), 7.24 – 7.14 (m, 6H), 6.93 (t, *J* = 4.8 Hz, 1H), 6.52 (q, *J* = 1.3 Hz, 1H), 2.89 (q, *J* = 7.5 Hz, 2H), 2.43 (d, *J* = 1.3 Hz, 3H), 2.42 (s, 3H), 1.29 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 187.2, 157.9, 157.8, 151.2, 142.5, 135.9, 135.5, 132.0, 129.5, 128.8, 128.4, 127.9, 127.8, 126.6, 126.2, 120.2, 116.5, 114.5, 21.5, 18.2, 17.8, 15.6. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{25}H_{24}N_3O^+$ 382.1914, Found: 382.1898.

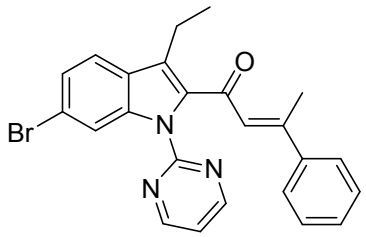


(*E*)-1-(3-ethyl-1-(pyrimidin-2-yl)-5-(trifluoromethyl)-1H-indol-2-yl)-3-phenylbut-2-en-1-one (3ia). Yellow oil (71 mg, 82% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.72 (d, *J* = 4.8 Hz, 2H), 8.59 (d, *J* = 8.8 Hz, 1H), 7.97 (s, 1H), 7.66 – 7.62 (m, 1H), 7.35 – 7.28 (m, 5H), 7.11 (t, *J* = 4.8 Hz, 1H), 6.63 (q, *J* = 1.4 Hz, 1H), 3.00 (q, *J* = 7.6 Hz, 2H), 2.55 (d, *J* = 1.4 Hz, 3H), 1.38 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 186.8, 158.1, 157.5, 152.7, 142.2, 138.3, 137.2, 129.1, 128.9, 128.5, 127.1, 126.3, 124.9 (q, *J* = 270.0 Hz), 124.8 (q, *J* = 32.0 Hz), 122.7 (q, *J* = 3.7 Hz), 117.88 (q, *J* = 4.4 Hz), 117.87, , 117.3, 115.2, 18.4, 17.7, 15.6. ^{19}F NMR (376 MHz, $CDCl_3$) δ -60.9 (S, 3F).

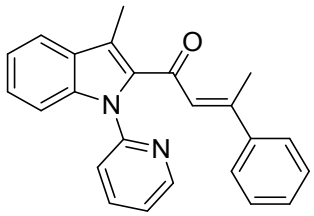
HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{25}H_{20}F_3N_3NaO^+$ 458.1451, Found: 458.1435.



(*E*)-1-(3-ethyl-5-fluoro-1-(pyrimidin-2-yl)-1H-indol-2-yl)-3-phenylbut-2-en-1-one (3ja). Yellow solid (69 mg, 89% yield, m.p. 115 – 117 °C). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.60 (d, *J* = 4.7 Hz, 2H), 8.41 (dd, *J* = 9.0, 4.5 Hz, 1H), 7.28 – 7.16 (m, 6H), 7.10 – 7.04 (m, 1H), 7.00-6.96 (m, 1H), 6.53 (s, 1H), 2.85 (q, *J* = 7.5 Hz, 2H), 2.46 (s, 3H), 1.27 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 187.0, 159.2 (d, *J* = 239.8 Hz), 157.9, 157.6, 152.0, 142.3, 137.1, 133.3, 130.1 (d, *J* = 9.1 Hz), 129.0, 128.5, 127.0 (d, *J* = 4.5 Hz), 126.3, 126.2, 116.8, 116.1 (d, *J* = 8.7 Hz) 114.1 (d, *J* = 25.1 Hz), 105.5 (d, *J* = 24.0 Hz)., 18.3, 17.8, 15.4. ^{19}F NMR (376 MHz, $CDCl_3$) δ -120.71 – -120.83 (m, 1F). HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{24}H_{21}FN_3O^+$ 386.1663, Found: 386.1659.

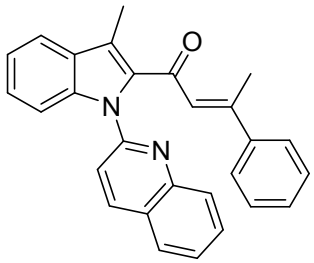


(*E*)-1-(6-bromo-3-ethyl-1-(pyrimidin-2-yl)-1H-indol-2-yl)-3-phenylbut-2-en-1-one(3ka). Yellow oil (56 mg, 63% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 – 8.64 (m, 1H), 8.63 (d, *J* = 4.8 Hz, 2H), 7.48 (d, *J* = 8.4 Hz, 1H), 7.36 – 7.31 (m, 1H), 7.25 – 7.19 (m, 5H), 7.01 (t, *J* = 4.8 Hz, 1H), 6.53 (q, *J* = 1.3 Hz, 1H), 2.88 (q, *J* = 7.6 Hz, 2H), 2.45 (d, *J* = 1.3 Hz, 3H), 1.27 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 186.8, 158.0, 157.5, 152.1, 142.3, 137.6, 136.1, 129.0, 128.5, 128.1, 127.3, 126.2, 126.1, 125.8, 121.6, 119.9, 117.9, 117.1, 18.3, 17.7, 15.5. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{24}H_{20}BrN_3NaO$+ 468.0682, Found: 468.0671.



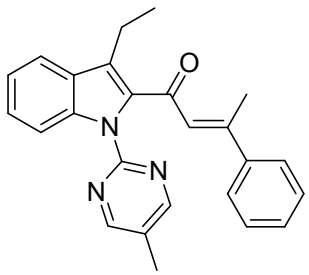
(*E*)-1-(3-methyl-1-(pyridin-2-yl)-1H-indol-2-yl)-3-phenylbut-2-en-1-one (3la).

Yellow oil (51 mg, 71% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (d, *J* = 4.4 Hz, 1H), 7.84 – 7.77 (m, 1H), 7.71 (d, *J* = 7.9 Hz, 1H), 7.58 (d, *J* = 8.4 Hz, 1H), 7.38 – 7.28 (m, 5H), 7.27 – 7.18 (m, 4H), 6.69 (s, 1H), 2.64 (s, 3H), 2.47 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 186.2, 152.8, 152.2, 149.2, 142.3, 138.3, 138.2, 136.5, 129.0, 128.9, 128.5, 126.5, 126.3, 126.2, 121.9, 121.7, 121.5, 121.0, 120.6, 111.4, 18.4, 10.5. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{24}H_{21}N_2O^+$ 353.1648, Found: 353.1647.

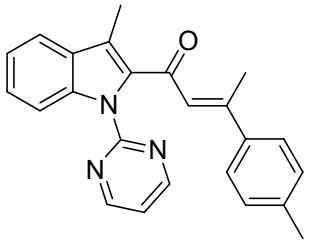


(*E*)-1-(3-methyl-1-(quinolin-2-yl)-1H-indol-2-yl)-3-phenylbut-2-en-1-one(3ma).

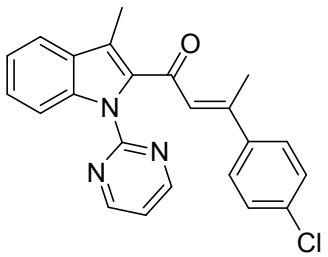
Yellow oil (69 mg, 85% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 8.6 Hz, 1H), 8.02 (d, *J* = 8.4 Hz, 1H), 7.76 – 7.72 (m, 1H), 7.69 – 7.63 (m, 3H), 7.50 – 7.43 (m, 1H), 7.37 (d, *J* = 8.6 Hz, 1H), 7.32 – 7.26 (m, 1H), 7.19 – 7.10 (m, 2H), 7.09 – 7.03 (m, 2H), 6.98 – 6.92 (m, 2H), 6.60 (q, *J* = 1.3 Hz, 1H), 2.60 (s, 3H), 2.37 (d, *J* = 1.3 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 186.1, 153.0, 151.2, 147.0, 142.2, 138.5, 138.1, 136.4, 130.5, 129.1, 128.9, 128.7, 128.5, 128.3, 127.6, 126.7, 126.7, 126.7, 126.1, 122.5, 121.7, 121.1, 119.4, 111.7, 18.5, 10.5. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{28}H_{23}N_2O^+$ 403.1805, Found: 403.1797.



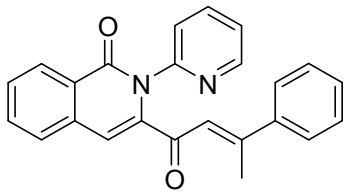
(*E*)-1-(3-ethyl-1-(5-methylpyrimidin-2-yl)-1H-indol-2-yl)-3-phenylbut-2-en-1-one (3na). Yellow solid (53 mg, 70% yield, m.p. 103 – 105 °C). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.45 (s, 2H), 8.30 (d, *J* = 8.4 Hz, 1H), 7.63 (d, *J* = 7.8 Hz, 1H), 7.36 – 7.31 (m, 1H), 7.26 – 7.17 (m, 7H), 6.57 (s, 1H), 2.94 (q, *J* = 7.5 Hz, 1H), 2.44 (s, 3H), 2.21 (s, 3H), 1.30 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 187.1, 157.9, 156.1, 151.6, 142.4, 137.3, 135.8, 129.0, 128.9, 128.5, 127.7, 127.2, 126.3, 126.3, 126.2, 122.2, 120.5, 114.2, 18.3, 18.0, 15.6, 15.1. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{25}H_{24}N_3O^+$ 382.1914, Found: 382.1898.



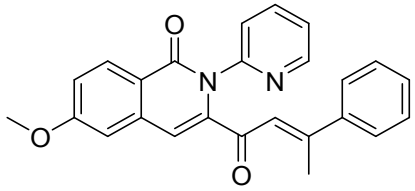
(*E*)-1-(3-methyl-1-(pyrimidin-2-yl)-1H-indol-2-yl)-3-(p-tolyl)but-2-en-1-one (3ab). Yellow oil (44 mg, 59% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, *J* = 4.8 Hz, 2H), 8.45 (d, *J* = 8.4 Hz, 1H), 7.67 (d, *J* = 7.8 Hz, 1H), 7.46 – 7.39 (m, 1H), 7.33-7.27 (m, 1H), 7.24 – 7.18 (m, 2H), 7.11 (d, *J* = 8.2 Hz, 2H), 7.07 – 7.02 (m, 1H), 6.65 (q, *J* = 1.3 Hz, 1H), 2.54 (s, 3H), 2.52 (d, *J* = 1.3 Hz, 3H), 2.33 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 187.1, 158.0, 157.9, 151.7, 139.4, 139.1, 137.1, 136.5, 130.2, 129.2, 126.4, 126.2, 125.7, 122.5, 121.8, 120.5, 116.7, 114.4, 21.2, 18.2, 9.6. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{24}H_{22}N_3O^+$ 368.1757, Found:368.1751.



(*E*)-3-(4-chlorophenyl)-1-(3-methyl-1-(pyrimidin-2-yl)-1H-indol-2-yl)but-2-en-1-one (3ac). Yellow oil (54 mg, 70% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.61 (d, *J* = 4.8 Hz, 2H), 8.38 (d, *J* = 8.4 Hz, 1H), 7.60 (d, *J* = 7.8 Hz, 1H), 7.40 – 7.33 (m, 1H), 7.26 – 7.11 (m, 5H), 6.97 (t, *J* = 4.8 Hz, 1H), 6.53 (q, *J* = 1.3 Hz, 1H), 2.46 (s, 3H), 2.41 (d, *J* = 1.3 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 186.8, 158.0, 157.9, 150.0, 140.8, 137.2, 136.2, 134.9, 130.1, 128.7, 127.5, 126.7, 126.6, 122.6, 122.2, 120.5, 116.8, 114.5, 18.1, 9.6. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{23}H_{19}ClN_3O^+$ 388.1211, Found: 388.1206.

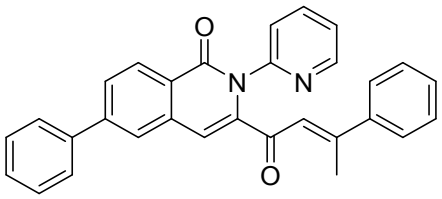


(*E*)-3-(3-phenylbut-2-enoyl)-2-(pyridin-2-yl)isoquinolin-1(2H)-one (5aa). Yellow solid (60 mg, 83% yield, m.p. 126 – 128 °C). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.39 (d, *J* = 7.9 Hz, 1H), 8.36 (d, *J* = 4.7 Hz, 1H), 7.82 – 7.76 (m, 2H), 7.68 – 7.63 (m, 1H), 7.59 – 7.51 (m, 2H), 7.43 – 7.38 (m, 2H), 7.34 – 7.29 (m, 3H), 7.21 – 7.15 (m, 1H), 7.07 (s, 1H), 6.76 (s, 1H), 2.36 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 187.2, 162.2, 156.7, 152.1, 148.4, 142.2, 141.8, 137.4, 135.1, 133.3, 129.6, 129.2, 128.6, 128.6, 127.5, 127.2, 126.5, 124.0, 122.8, 122.7, 111.5, 18.6. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{24}H_{19}N_2O_2^+$ 367.1441, Found: 367.1440.

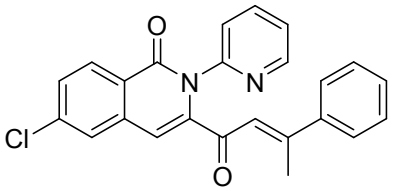


(*E*)-6-methoxy-3-(3-phenylbut-2-enoyl)-2-(pyridin-2-yl)isoquinolin-1(2H)-one (3ba). Yellow oil (44 mg, 55% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, *J* = 4.9

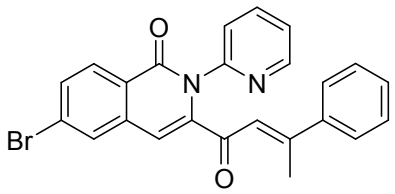
Hz, 1H), 8.30 (d, *J* = 8.9 Hz, 1H), 7.85 – 7.70 (m, 2H), 7.42 – 7.36(m, 2H), 7.35 – 7.29 (m, 3H), 7.18 – 7.13 (m, 1H), 7.08 (dd, *J* = 8.9, 2.5 Hz, 1H), 6.99 (s, 1H), 6.93 (d, *J* = 2.5 Hz, 1H), 6.73 (q, *J* = 1.3 Hz, 1H), 3.86 (s, 3H), 2.35 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 187.3, 163.5, 161.8, 156.5, 152.1, 148.3, 142.8, 141.8, 137.3, 137.3, 130.7, 129.5, 128.6, 126.4, 124.0, 122.8, 122.7, 120.7, 118.1, 111.2, 108.8, 55.7, 18.6. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{25}H_{21}N_2O_3^+$ 397.1547, Found: 397.1547.



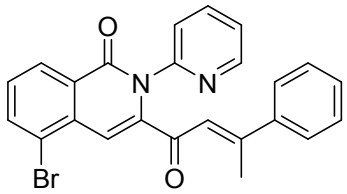
(*E*)-6-phenyl-3-(3-phenylbut-2-enoyl)-2-(pyridin-2-yl)isoquinolin-1(2H)-one (5ca). Yellow oil (46 mg, 53% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45 (d, *J* = 8.7 Hz, 1H), 8.39 – 8.35 (m, 1H), 7.84 –7.74 (m, 4H), 7.66 – 7.58 (m, 2H), 7.48 – 7.29 (m, 8H), 7.22 – 7.16 (m, 1H), 7.13 (s, 1H), 6.78 (q, *J* = 1.3 Hz, 1H), 2.37 (d, *J* = 1.3 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.2, 162.1, 156.7, 152.1, 148.4, 146.1, 142.6, 141.8, 139.6, 137.4, 135.6, 129.6, 129.2, 129.1, 128.6, 128.5, 128.2, 127.5, 126.5, 125.9, 125.6, 124.0, 122.8, 122.8, 111.6, 18.7. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{30}H_{23}N_2O_2^+$ 443.1754, Found: 443.1752.



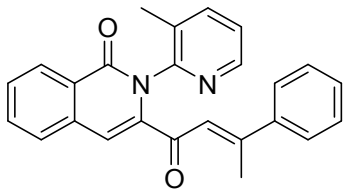
(*E*)-6-chloro-3-(3-phenylbut-2-enoyl)-2-(pyridin-2-yl)isoquinolin-1(2H)-one (5da). Yellow oil (34 mg, 42% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44 (d, *J* = 4.9 Hz, 1H), 8.40 (d, *J* = 8.5 Hz, 1H), 7.94 – 7.81 (m, 2H), 7.63 (d, *J* = 2.0 Hz, 1H), 7.54 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.49 – 7.44 (m, 2H), 7.42 – 7.37 (m, 3H), 7.29 – 7.24 (m, 1H), 7.02 (s, 1H), 6.79 (q, *J* = 1.3 Hz, 1H), 2.43 (d, *J* = 1.3 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 185.9, 160.5, 156.3, 150.7, 147.4, 142.4, 140.7, 138.8, 136.5, 135.5, 129.3, 128.6, 128.4, 127.6, 125.7, 125.4, 124.3, 122.8, 122.0, 121.4, 108.7, 17.6. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{24}H_{18}ClN_2O_2^+$ 401.1051, Found: 401.1051.



(*E*)-6-bromo-3-(3-phenylbut-2-enoyl)-2-(pyridin-2-yl)isoquinolin-1(2H)-one (5ea). Yellow oil (33 mg, 37% yield). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.35 (d, *J* = 4.7 Hz, 1H), 8.23 (d, *J* = 8.6 Hz, 1H), 7.83 – 7.73 (m, 2H), 7.72 (d, *J* = 1.8 Hz, 1H), 7.61 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.41 – 7.27(m, 5H), 7.21 – 7.16 (m, 1H), 6.93 (s, 1H), 6.71 (d, *J* = 1.4 Hz, 1H), 2.35 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 186.9, 161.7, 157.3, 151.7, 148.3, 143.4, 141.7, 137.5, 136.7, 132.2, 130.3, 129.9, 129.7, 128.7, 128.5, 126.5, 125.7, 123.9, 123.0, 122.5, 109.6, 18.7. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{24}H_{18}BrN_2O_2^+$ 445.0546, Found: 445.0546.

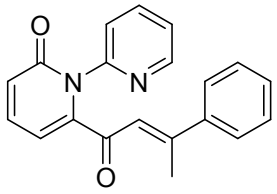


(*E*)-5-bromo-3-(3-phenylbut-2-enoyl)-2-(pyridin-2-yl)isoquinolin-1(2H)-one(5fa). Green solid (28 mg, 32% yield, m.p. 65 – 67 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 (d, *J* = 3.8 Hz, 1H), 8.37 – 8.35 (m, 1H), 7.89 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.85-7.79 (m, 1H), 7.79 - 7.73 (m, 1H), 7.44 – 7.31 (m, 6H) , 7.24 – 7.17 (m, 2H), 6.79 (q, *J* = 1.1 Hz, 1H), 2.38 (d, *J* = 1.1 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 187.0, 161.5, 157.6, 151.7, 148.4, 143.1, 141.8, 137.6, 137.1, 134.8, 129.7, 129.5, 128.7, 128.7, 128.1, 126.5, 123.8, 123.0, 122.5, 122.3, 109.3, 18.8. HRMS (ESI-TOF) m/z: $[M + Na]^+$ Calcd for $C_{24}H_{17}BrN_2NaO_2^+$ 467.0366, Found: 467.0363.

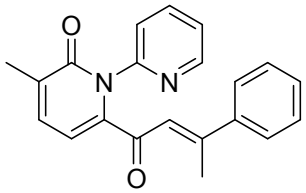


(*E*)-2-(3-methylpyridin-2-yl)-3-(3-phenylbut-2-enoyl)isoquinolin-1(2H)-one(5ga). Yellow solid (45 mg, 59% yield, m.p. 119 – 121 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (d, *J* = 7.9 Hz, 1H), 8.27 – 8.22 (m, 1H), 7.75 – 7.56 (m, 5H), 7.52 – 7.35 (m, 5H), 7.13 (s, 1H), 6.84 (s, 1H), 2.44 (s, 3H), 2.35 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ

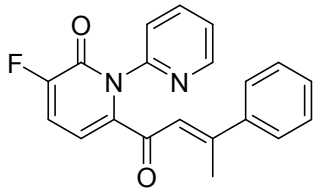
187.3, 162.3, 156.6, 149.8, 148.5, 142.2, 141.8, 138.1, 135.1, 133.2, 132.5, 129.5, 129.1, 128.6, 128.6, 127.5, 127.2, 126.4, 123.3, 122.9, 111.3, 18.6, 18.1. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{25}H_{21}N_2O_2^+$ 381.1598, Found: 381.1599.



(*E*)-6-(3-phenylbut-2-enoyl)-2H-[1,2'-bipyridin]-2-one (5ha). Yellow solid (35 mg, 55% yield), m.p. 88 – 90 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38 – 8.34 (m, 1H), 7.82-7.75 (m, 1H), 7.72 – 7.67 (m, 1H), 7.41 – 7.28 (m, 6H), 7.23 – 7.16 (m, 1H), 6.69 (dd, *J* = 9.2, 1.2 Hz, 1H), 6.62-6.57 (m, 2H), 2.33 (d, *J* = 1.2 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 186.8, 162.0, 157.6, 151.3, 148.6, 147.5, 141.6, 138.9, 137.5, 129.7, 128.6, 126.4, 124.7, 123.7, 123.4, 122.5, 108.7, 18.7. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{20}H_{17}N_2O_2^+$ 317.1285, Found: 317.1285.

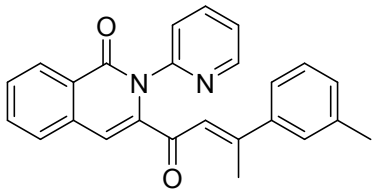


(*E*)-3-methyl-6-(3-phenylbut-2-enoyl)-2H-[1,2'-bipyridin]-2-one (5ia). Gray solid (43 mg, 65% yield, m.p. 157 – 159 °C) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 – 8.33 (m, 1H), 7.81 – 7.73 (m, 1H), 7.70 – 7.64 (m, 1.0 Hz, 1H), 7.37 – 7.26 (m, 5H),, 7.26 – 7.15 (m, 2H), 6.64 – 6.58 (m, 2H), 2.31 (d, *J* = 1.3 Hz, 3H), 2.15 (d, *J* = 1.2 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 186.6, 162.5, 156.9, 151.9, 148.5, 145.0, 141.7, 137.3, 135.6, 134.7, 129.6, 128.6, 126.4, 123.9, 123.1, 122.6, 109.5, 18.6, 17.7. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{19}N_2O_2^+$ 331.1441, Found: 331.1439.

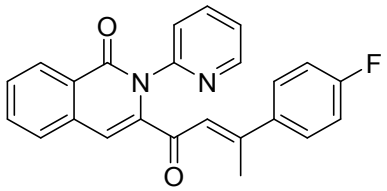


(*E*)-3-fluoro-6-(3-phenylbut-2-enoyl)-2H-[1,2'-bipyridin]-2-one (5ja). Green solid (56 mg, 83% yield, m.p. 123 – 125 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 – 8.40 (m, 1H), 7.92 – 7.84 (m, 1H), 7.80 – 7.73 (d, *J* = 8.0 Hz, 1H), 7.44 – 7.34 (m, 5H), 7.33 –

7.27 (m, 1H), 7.18 (t, J = 8.0 Hz, 1H), 6.71 – 6.65 (m, 2H), 2.39 (d, J = 1.2 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 185.6, 157.9, 155.9 (d, J = 26.4 Hz), 153.8 (d, J = 258.5 Hz), 150.6, 148.6, 143.0 (d, J = 5.9 Hz), 141.5, 137.9, 129.8, 128.7, 126.4, 123.7, 123.6, 122.2, 118.8 (d, J = 17.6 Hz), 107.8 (d, J = 6.1 Hz), 18.7. ^{19}F NMR (376 MHz, $CDCl_3$) δ -123.15 – -123.28. (m, 1F). HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{20}H_{16}FN_2O_2^+$ 335.1190, Found: 335.1190.

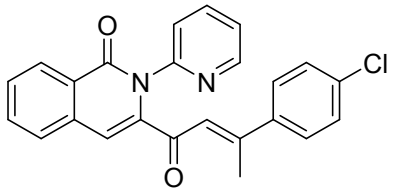


(*E*)-2-(pyridin-2-yl)-3-(3-(m-tolyl)but-2-enoyl)isoquinolin-1(2H)-one.(5ab).Yellow oil (40 mg, 53% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (d, J = 8.0 Hz, 1H), 8.38 – 8.35 (m, 1H), 7.85 – 7.75 (m, 2H), 7.70 – 7.62 (m, 1H), 7.60 – 7.50 (m, 2H), 7.25 – 7.11 (m, 5H), 7.06 (s, 1H), 6.76 (q, J = 1.3 Hz, 1H), 2.35 (d, J = 1.3 Hz, 3H), 2.32 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 187.2, 162.2, 157.1, 152.2, 148.4, 142.2, 141.9, 138.3, 137.4, 135.2, 133.3, 130.3, 129.1, 128.6, 128.5, 127.5, 127.2, 127.1, 124.0, 123.6, 122.8, 122.6, 111.39, 21.5, 18.7. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{25}H_{21}N_2O_2^+$ 381.1598, Found: 381.1598.

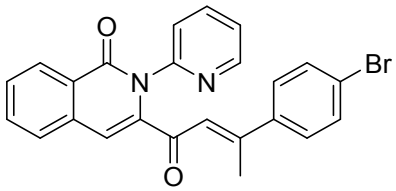


(*E*)-3-(3-(4-fluorophenyl)but-2-enoyl)-2-(pyridin-2-yl)isoquinolin-1(2H)-one (5ac). Yellow solid (37 mg, 48% yield, m.p 124 – 126 °C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (d, J = 8.0 Hz, 1H), 8.37 – 8.33 (m, 1H), 7.84 – 7.74 (m, 2H), 7.6 – 7.61 (m, 1H), 7.59 – 7.50 (m, 2H), 7.41 – 7.34 (m, 2H), 7.20 – 7.14 (m, 1H), 7.05 (s, 1H), 7.03 – 6.95 (m, 2H), 6.71 (q, J = 1.2 Hz, 1H), 2.33 (d, J = 1.2 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 187.0, 163.5 (d, J = 249.8 Hz), 162.1, 155.3, 152.1, 148.4, 142.1,137.8 (d, J = 4.1 Hz), 137.4, 135.1, 133.3, 129.2, 128.6, 128.3 (d, J = 8.7 Hz), 127.5, 127.2, 124.0, 122.8, 122.6, 115.6 (d, J = 21.2 Hz), 111.4, 18.6. ^{19}F NMR (376 MHz, $CDCl_3$) δ -111.28 – -

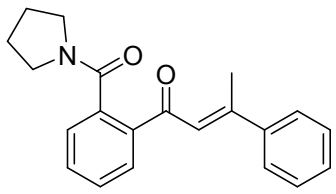
111.41 (m, 1F). HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{24}H_{18}FN_2O_2^+$ 385.1347, Found: 385.1347.



(*E*)-3-(3-(4-chlorophenyl)but-2-enoyl)-2-(pyridin-2-yl)isoquinolin-1(2H)-one (5ad). Yellow oil (47 mg, 58% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.40 (d, *J* = 8.0 Hz, 1H), 8.36 (d, *J* = 4.9 Hz, 1H), 7.85 – 7.75 (m, 2H), 7.70 – 7.63 (m, 1H), 7.60 – 7.51 (m, 2H), 7.37 – 7.25 (m, 4H), 7.23 – 7.14 (m, 1H), 7.05 (s, 1H), 6.72 (q, *J* = 1.3 Hz, 1H), 2.32 (d, *J* = 1.3 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 186.0, 161.1, 154.0, 151.0, 147.3, 141.0, 140.0, 136.4, 134.5, 134.0, 132.3, 128.2, 127.8, 127.6, 126.7, 126.5, 126.1, 122.9, 121.9, 121.8, 110.5, 17.4. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{24}H_{18}ClN_2O_2^+$ 401.1051, Found: 401.1027.

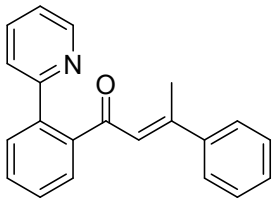


(*E*)-3-(3-(4-bromophenyl)but-2-enoyl)-2-(pyridin-2-yl)isoquinolin-1(2H)-one (5ae). Yellow oil (54 mg, 61% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.39 (d, *J* = 8.1 Hz, 1H), 8.36 (d, *J* = 4.8 Hz, 1H), 7.87 - 7.75 (m, 2H), 7.70 – 7.62 (m, 1H), 7.60 – 7.51 (m, 2H), 7.47 – 7.41 (m, 2H), 7.30 – 7.23 (m, 2H), 7.22 – 7.14 (m, 1H), 7.05 (s, 1H), 6.72 (d, *J* = 1.5 Hz, 1H), 2.31 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 187.0, 162.1, 155.0, 152.0, 148.3, 142.0, 140.6, 137.4, 135.0, 133.4, 131.8, 129.3, 128.6, 128.0, 127.6, 127.2, 124.0, 123.8, 123.0, 122.8, 111.5, 18.4. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{24}H_{18}BrN_2O_2^+$ 445.0546, Found: 445.0548.



(*E*)-3-phenyl-1-(2-(pyrrolidine-1-carbonyl)phenyl)but-2-en-1-one (6). Yellow oil (35 mg, 55% yield),^{1}H NMR (600 MHz, $CDCl_3$) δ 7.78-7.75 (m, 1H), 7.59 – 7.56 (m, 2H), 7.55-7.51

(m, 1H), 7.48-7.43 (m, 1H), 7.42 – 7.35 (m, 4H), 7.01 (q, J = 1.3 Hz, 1H), 3.60 (t, J = 6.9 Hz, 2H), 3.15 (t, J = 6.6 Hz, 2H), 2.57 (d, J = 1.3 Hz, 3H), 1.96 – 1.80 (m, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 193.07, 169.78, 155.44, 142.28, 138.22, 137.89, 131.68, 129.33, 128.92, 128.64, 127.08, 126.58, 123.43, 48.66, 45.75, 25.93, 24.58, 18.78. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{22}NO_2^+$ 320.1645, Found: 320.1645.



(*E*)-3-phenyl-1-(2-(pyridin-2-yl)phenyl)but-2-en-1-one (7). Yellow solid (32 mg, 53% yield), m.p. (67 – 69 °C). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.57 (d, J = 4.8 Hz, 1H), 7.68-7.63 (m, 1H), 7.62 – 7.57 (m, 2H), 7.54 – 7.37 (m, 3H), 7.27 – 7.10 (m, 4H), 7.10 – 7.01 (m, 2H), 6.31 (s, 1H), 2.41 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 196.19, 158.09, 152.98, 149.37, 142.42, 142.26, 139.31, 136.42, 130.41, 129.52, 128.88, 128.72, 128.50, 128.30, 126.26, 126.03, 123.65, 122.33, 18.38. HRMS (ESI-TOF) m/z: $[M + H]^+$ Calcd for $C_{21}H_{18}NO^+$, 300.1383, Found: 300.1382.

8. References

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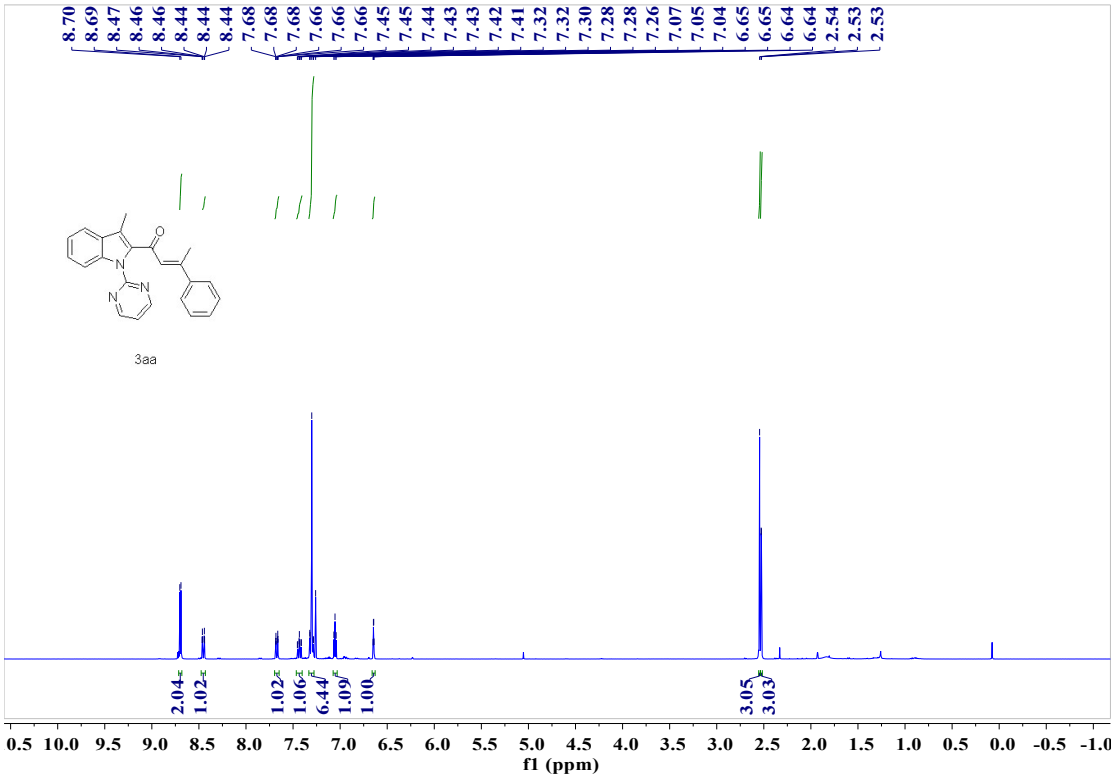
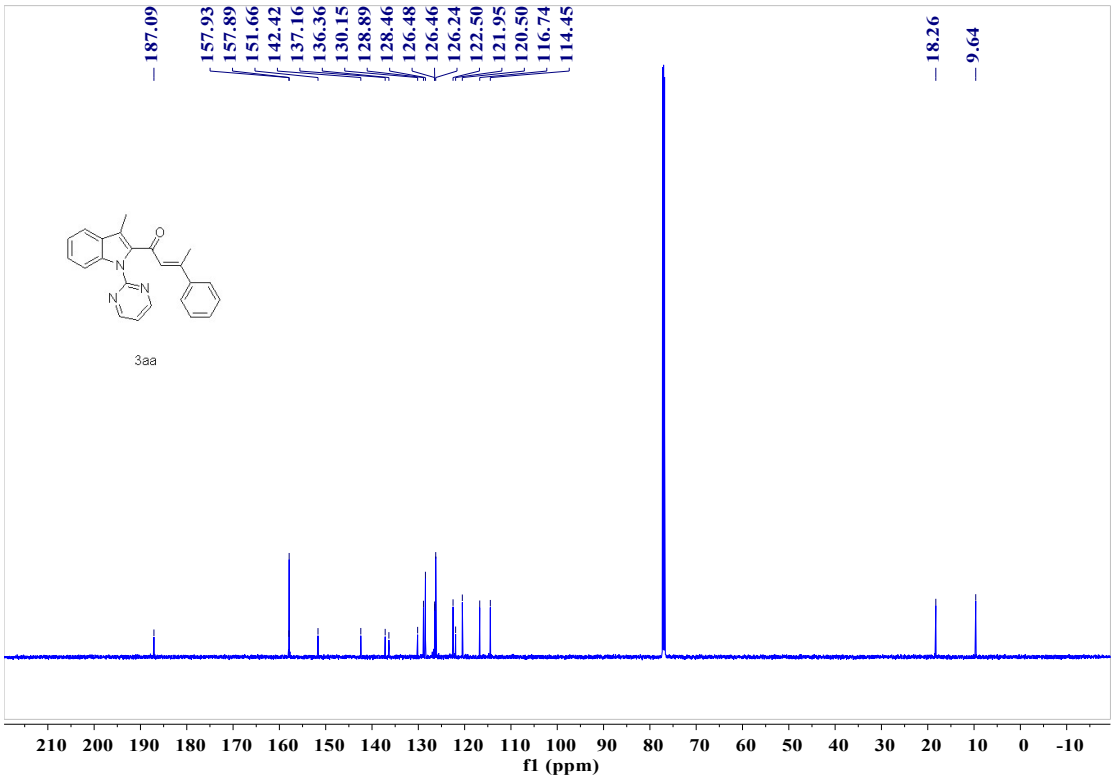
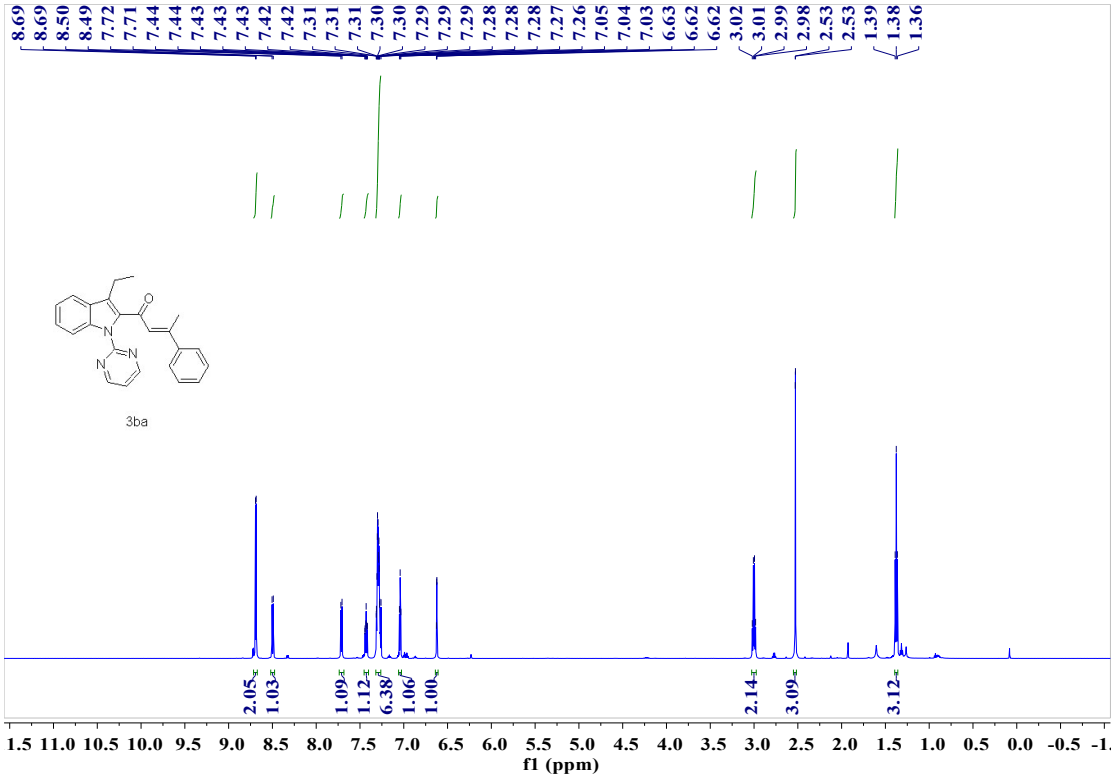
(2) Leitch, J. A.; Heron, C. J.; McKnight, J.; Kociok-Köhn, G.; Bhonoahd, Y.; Frost, C. G. Ruthenium catalyzed remote C4-selective C-H functionalisation of carbazoles via σ-activation. *Chem. Commun.* **2017**, *53*, 13039-13042.

(3) Qin, Q.; Luo, X.; Wei, J.; Zhu, Y.; Wen, X.; Song, S.; Jiao, N. Acetonitrile Activation: An Effective Two-Carbon Unit for Cyclization. *Angew. Chem. Int. Ed.* **2019***, 131,* 4420–4424.

9. NMR Spectra



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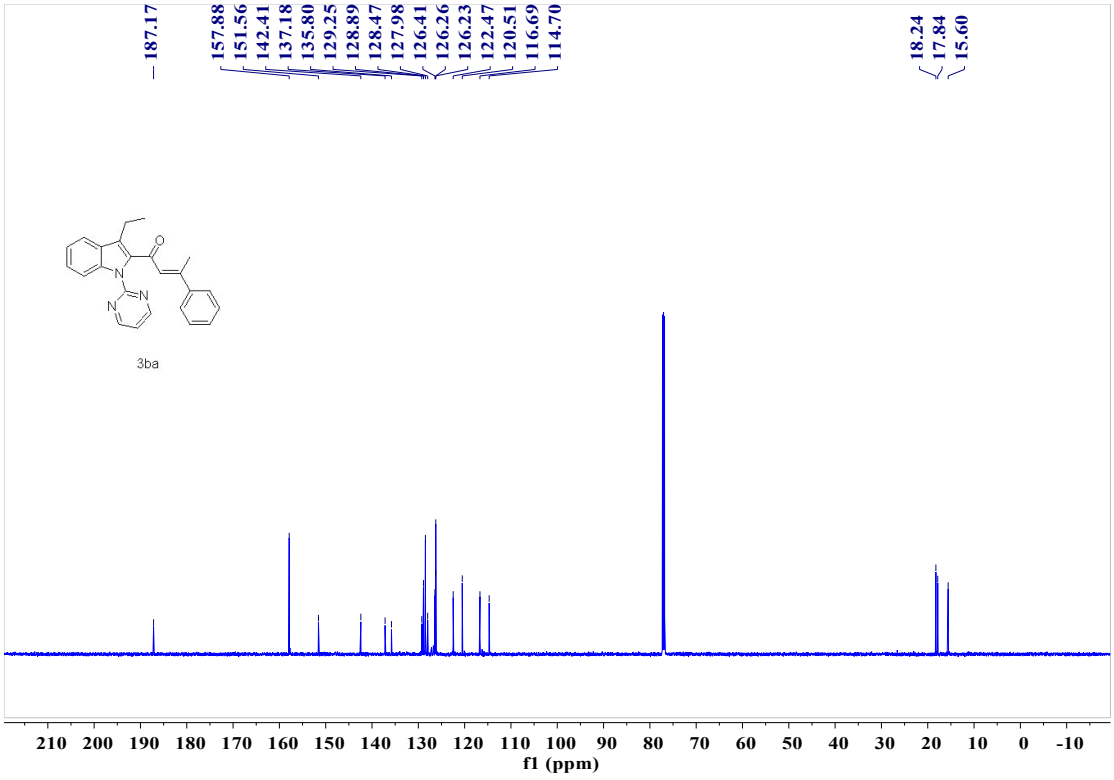
f1 (ppm)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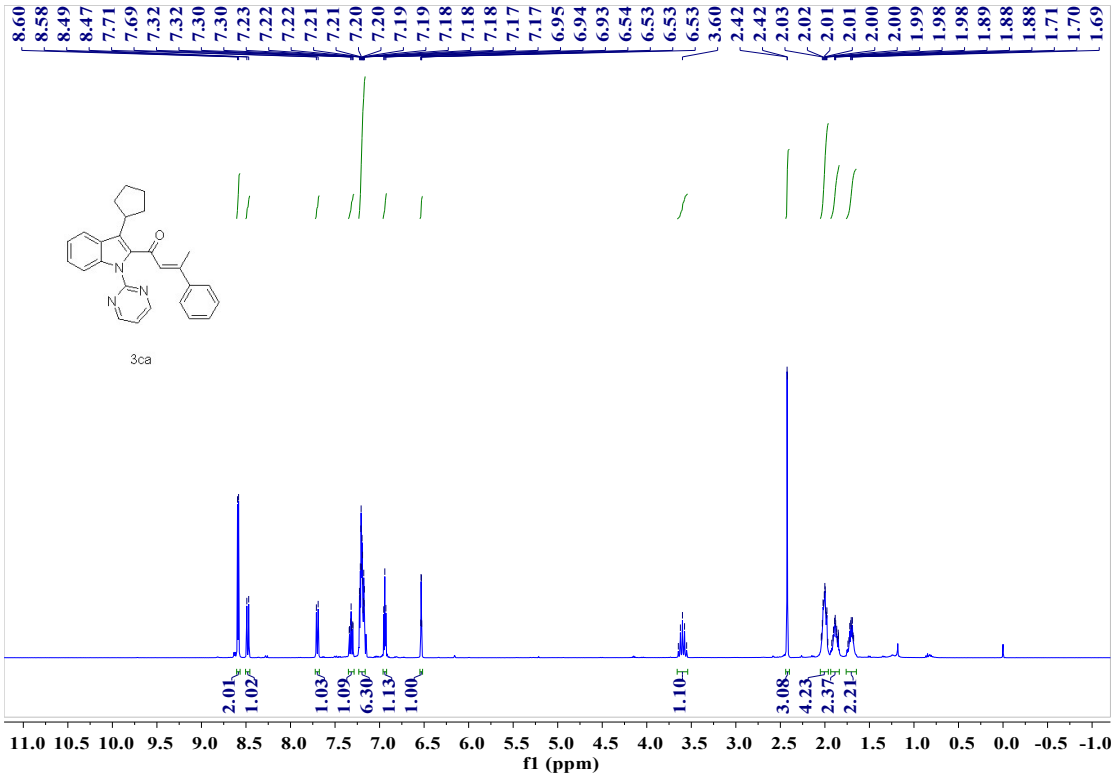
18.24 17.84 15.60
3ba
f1 (ppm)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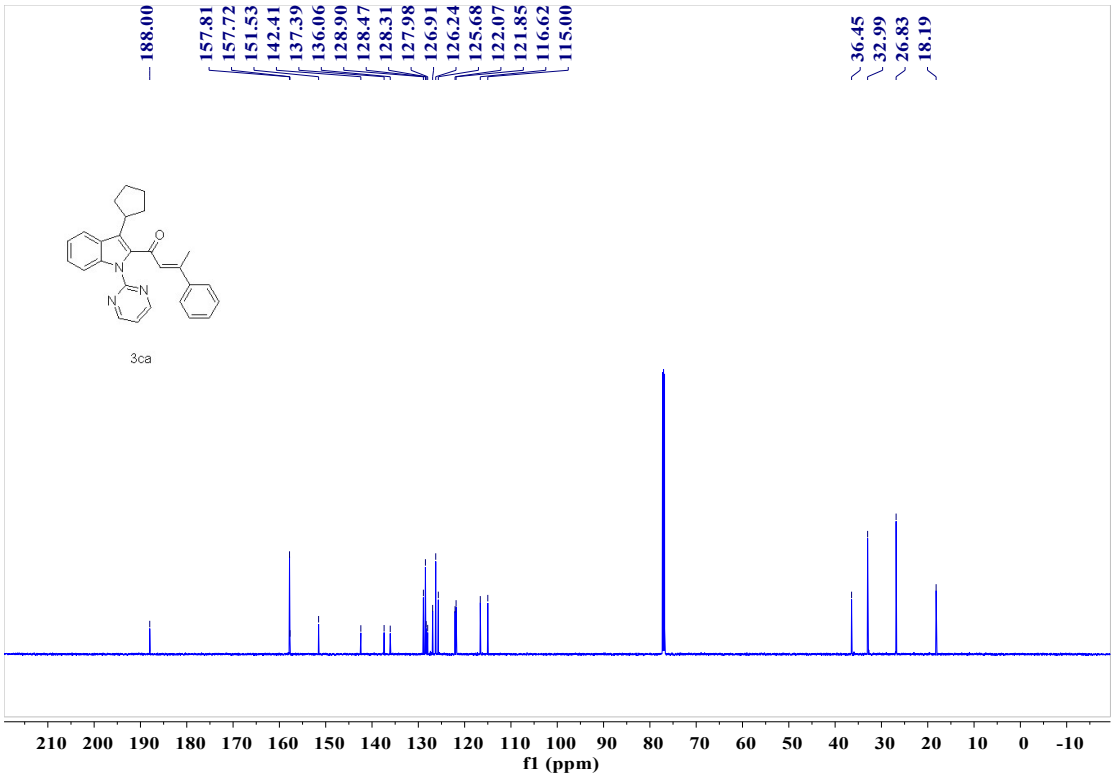
3ca
2.01 1.02 1.03 1.09 6.30 1.13 1.00 1.10 3.08 4.23 2.37 2.21
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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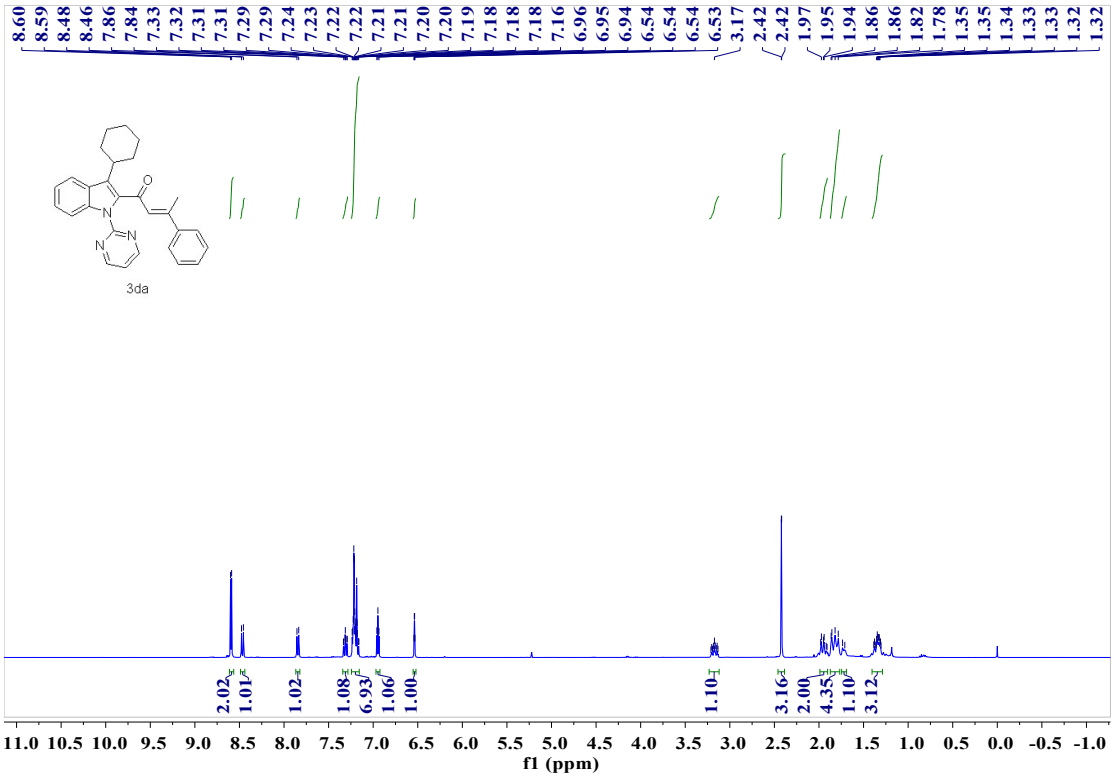
f1 (ppm)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3da
2.02 1.01 1.02 1.08 6.93 1.06 1.00 1.10 3.16 2.00 4.35 1.10 3.12
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
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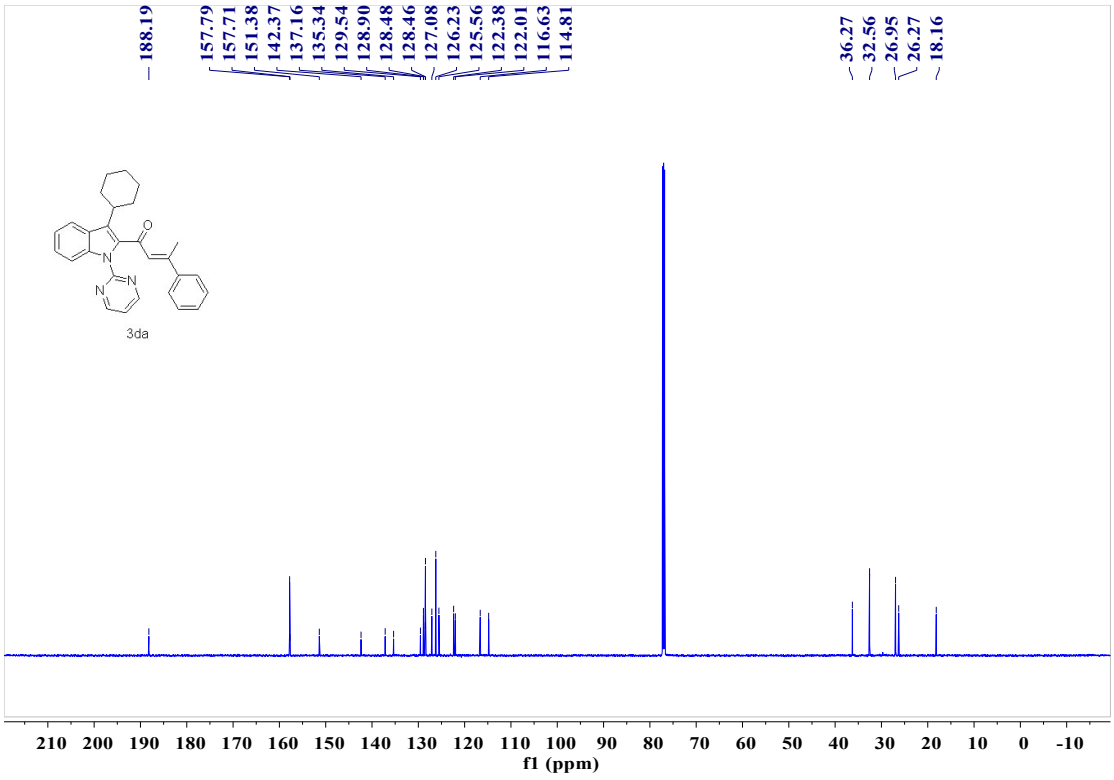
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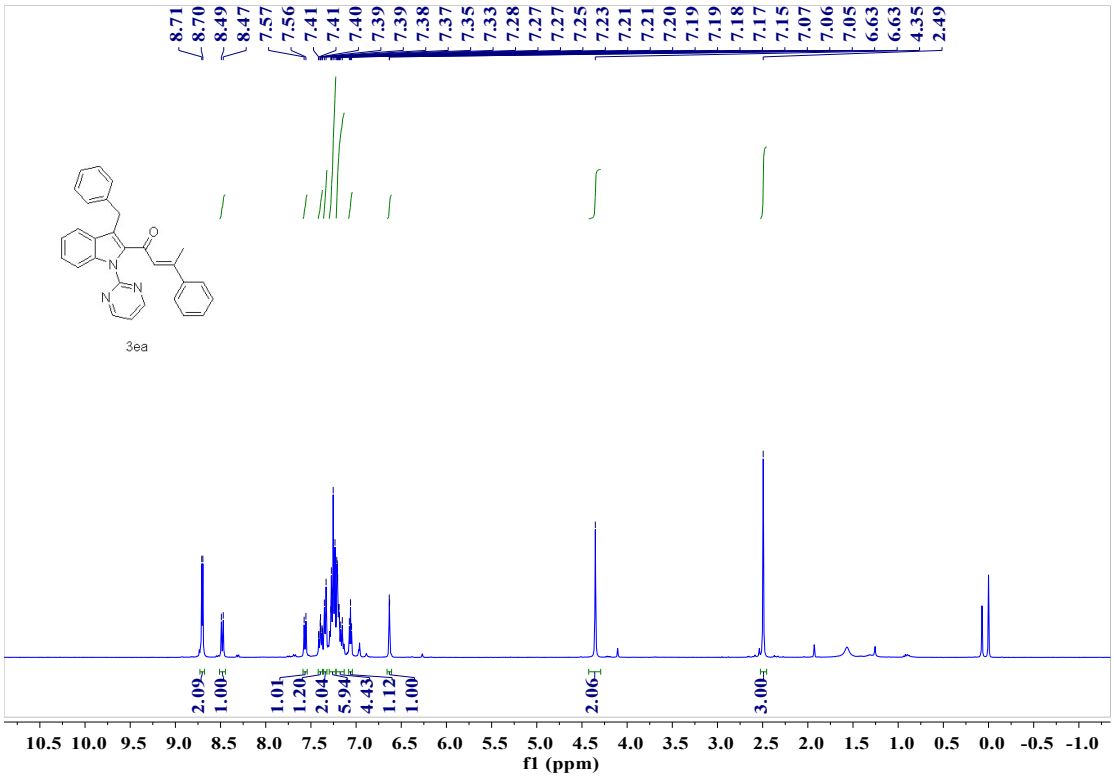
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7.28
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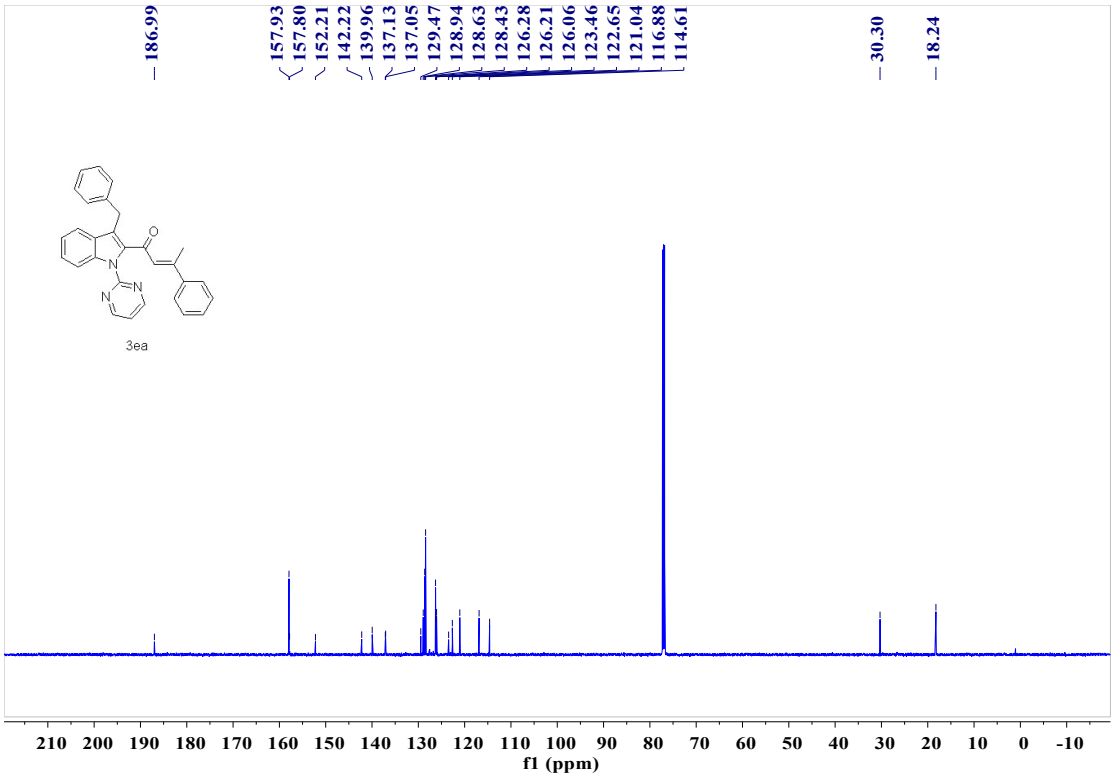
7.19
7.18
7.17
7.15
7.07
7.06
7.05
6.63
6.63
4.35
2.49
3ea
2.09
1.00
1.01
1.20
2.04
5.94
4.43
1.12
1.00
2.06
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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137.13
137.05
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123.46
122.65
121.04
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30.30
18.24
3ea
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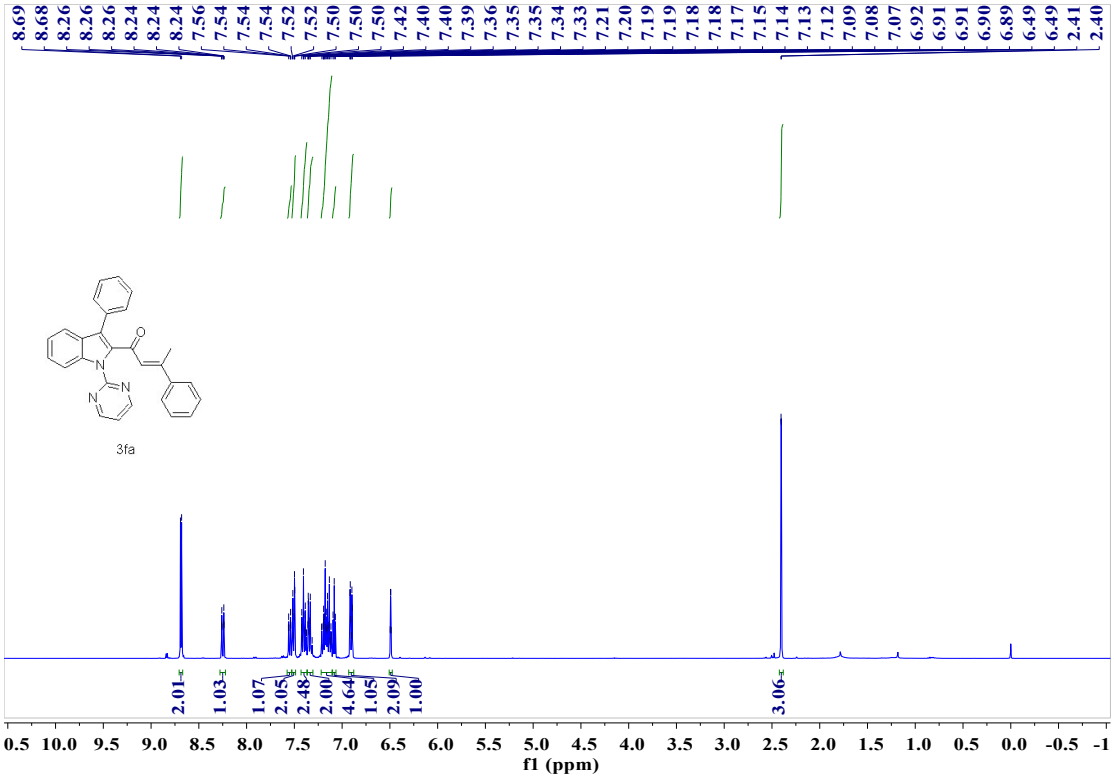
f1 (ppm)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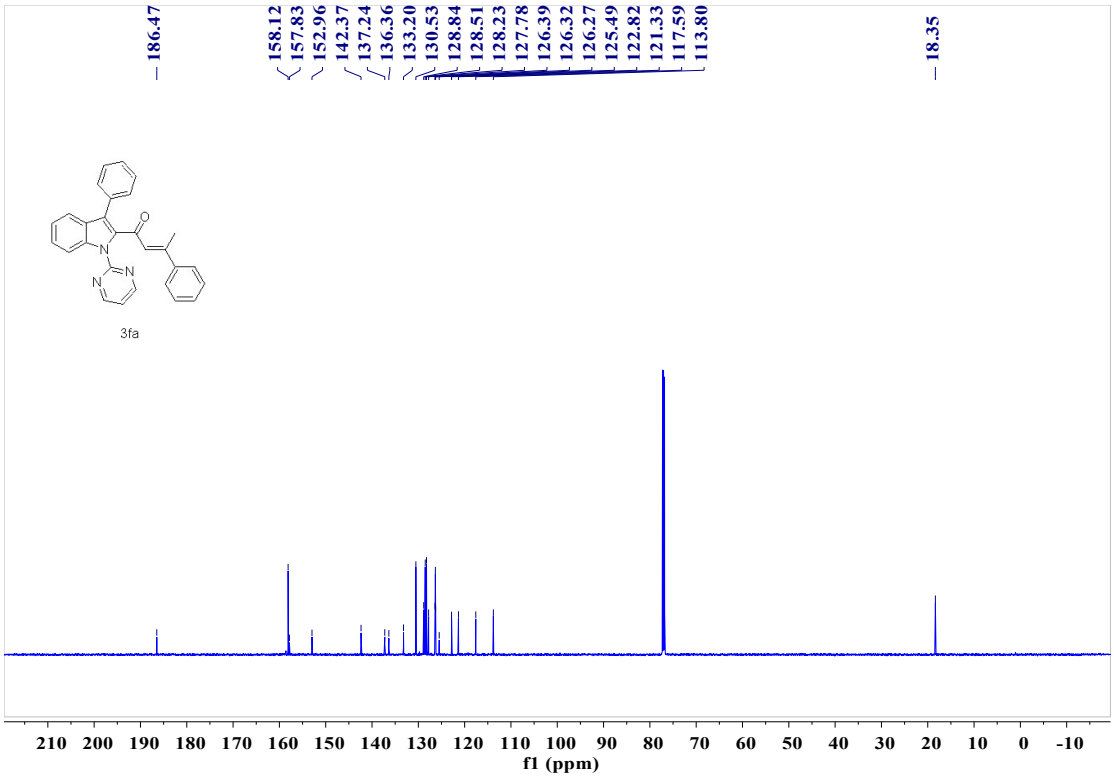
3fa
2.01 1.03 1.07 2.05 2.48 2.00 4.64 1.05 2.09 1.00 3.06
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)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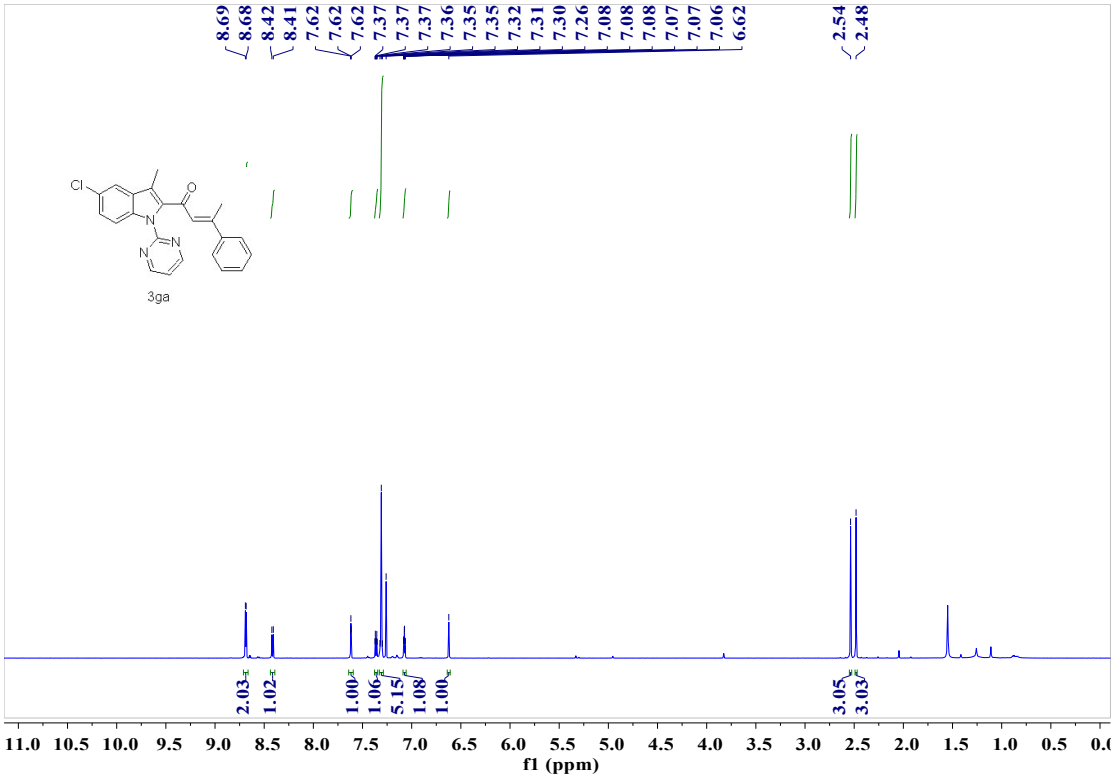
f1 (ppm)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7.08
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N
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1.00
1.06
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1.08
1.00
3.05
3.03
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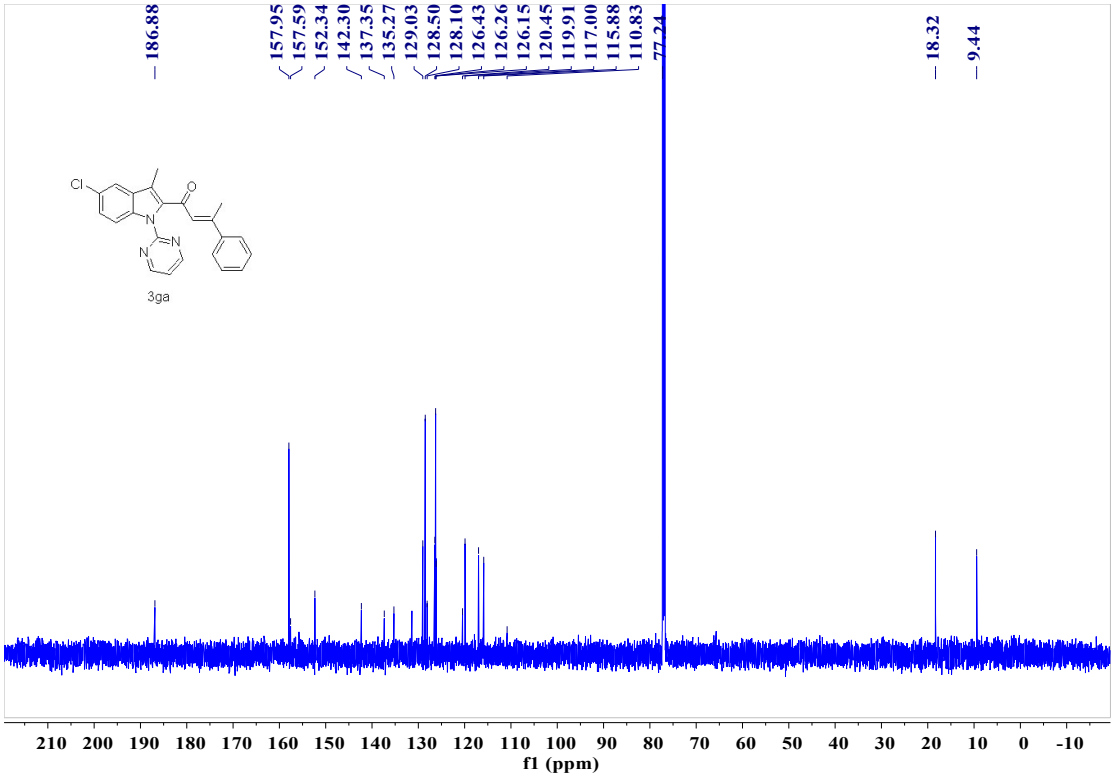
f1 (ppm)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126.15
120.45
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117.00
115.88
110.83
77.24
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Cl
O
N
N
3ga
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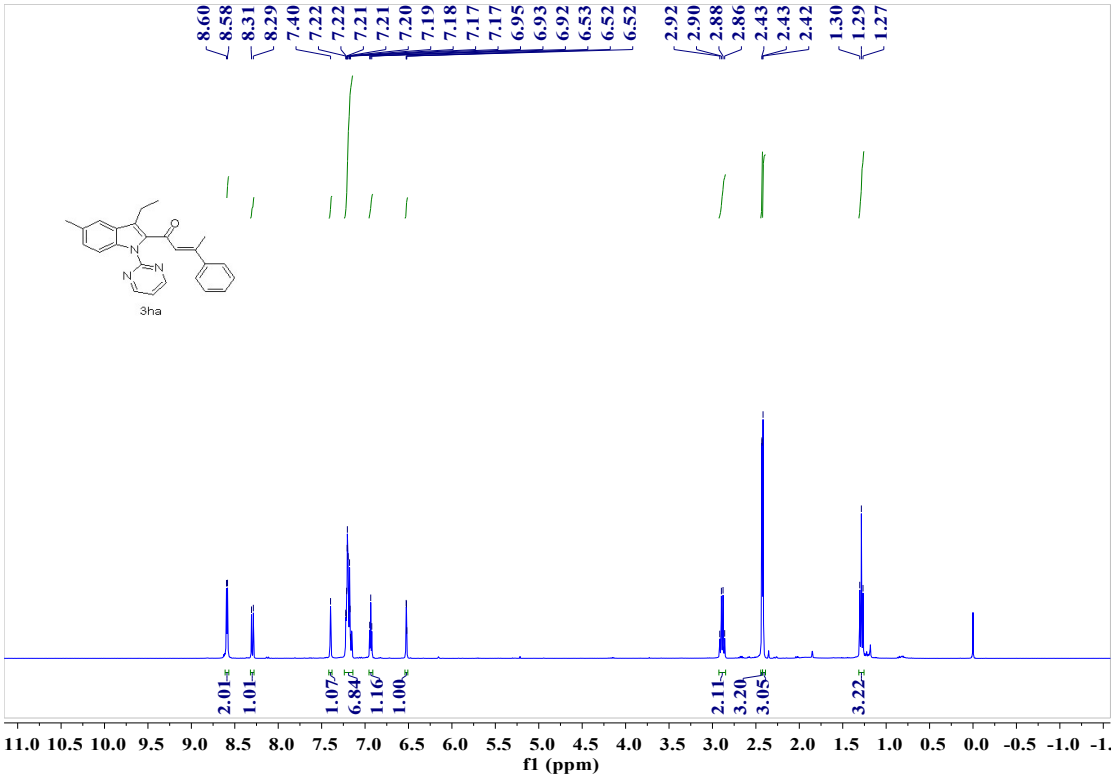
f1 (ppm)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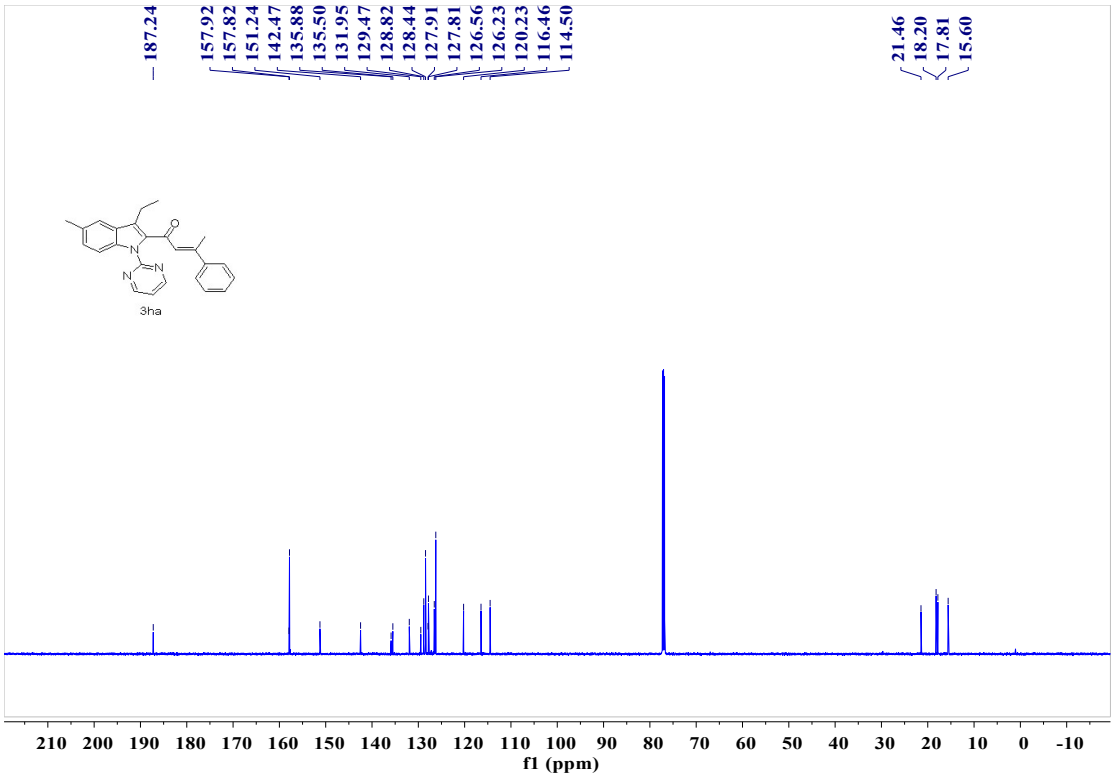
7.17
7.17
6.95
6.93
6.92
6.53
6.52
6.52
2.92
2.90
2.88
2.86
2.43
2.43
2.42
1.30
1.29
1.27
3ha
2.01
1.01
1.07
6.84
1.16
1.00
2.11
3.20
3.05
3.22
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.
f1 (ppm)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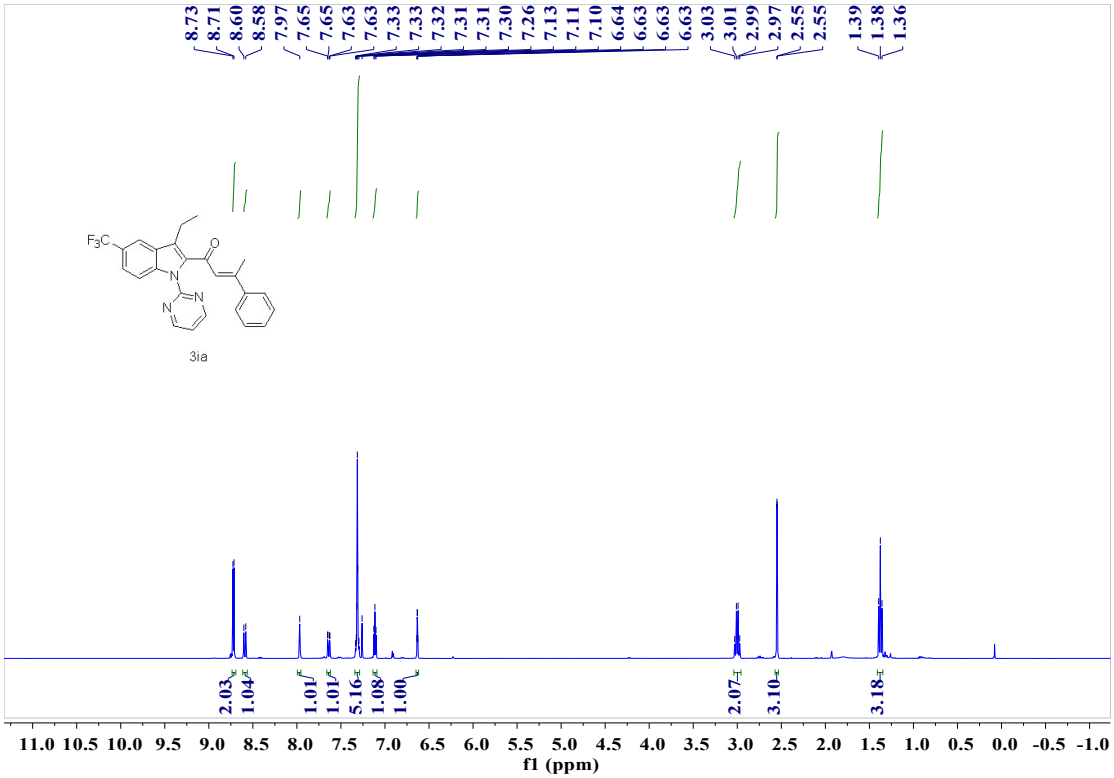
126.23
120.23
116.46
114.50
21.46
18.20
17.81
15.60
3ha
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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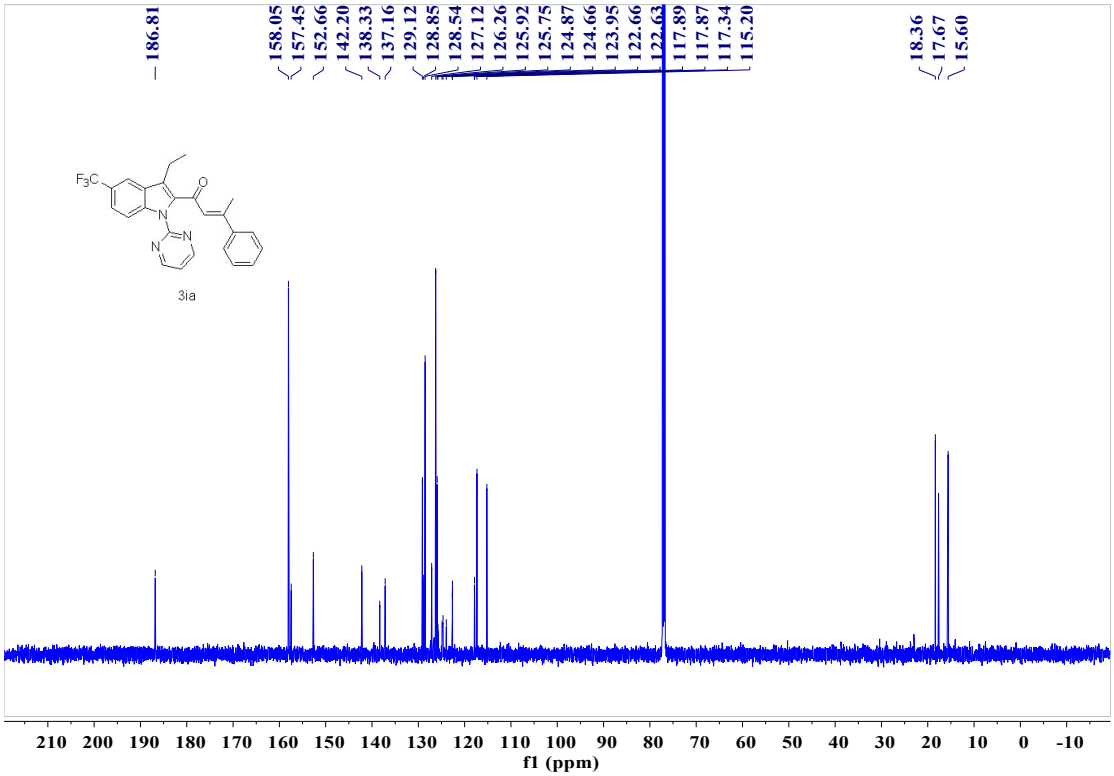
6.63
6.63
3.03
3.01
2.99
2.97
2.55
2.55
1.39
1.38
1.36
F3C
O
N
N
N
3ia
2.03
1.04
1.01
1.01
5.16
1.08
1.00
2.07
3.10
3.18
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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18.36
17.67
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O
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N
N
3ia
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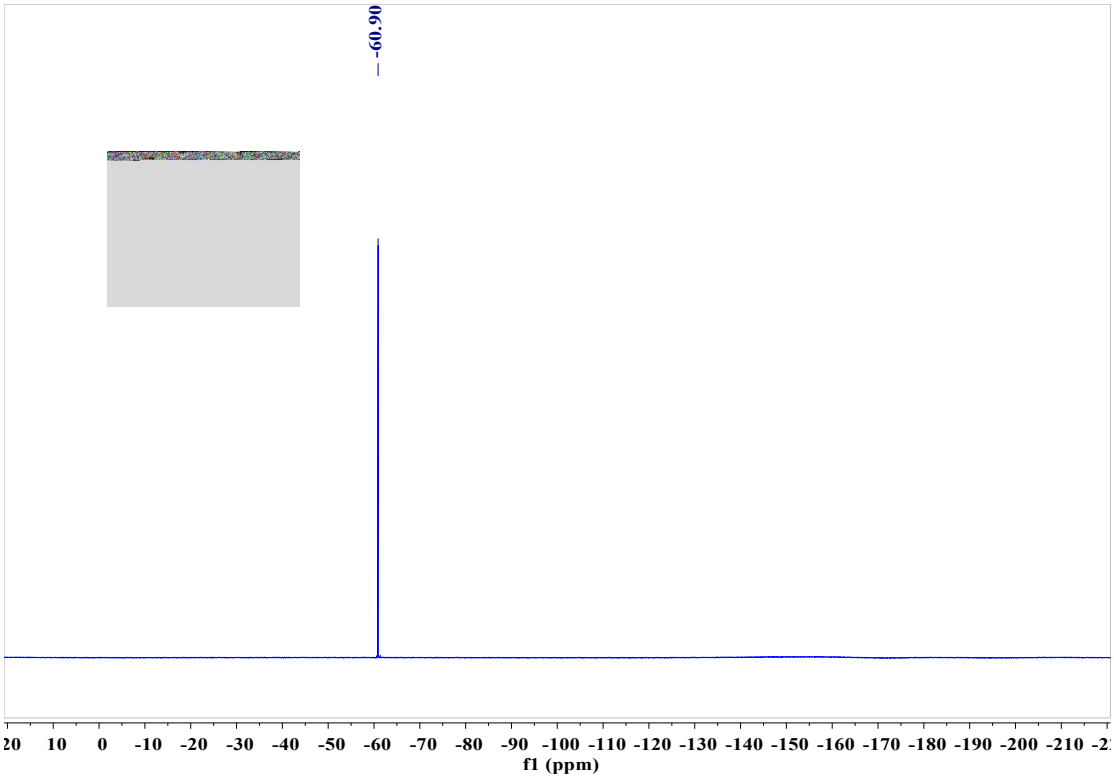
f1 (ppm)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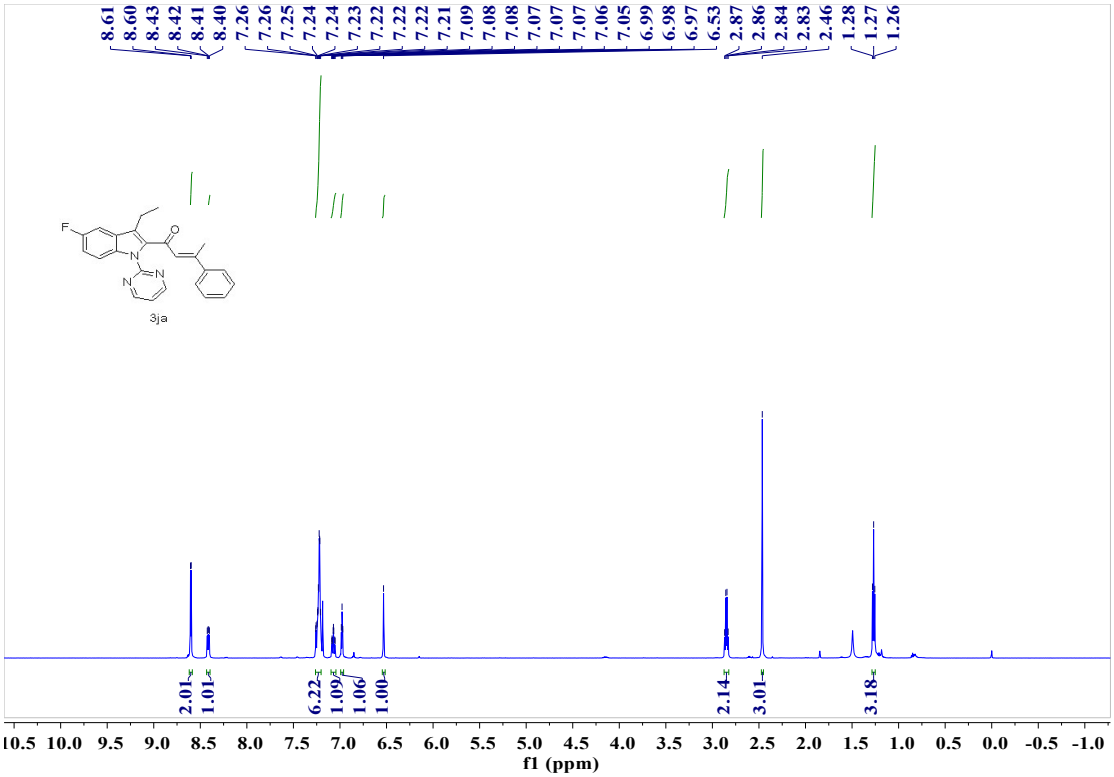
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7.08
7.08
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7.07
7.07
7.06
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1.27
1.26
F
O
N
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6.22
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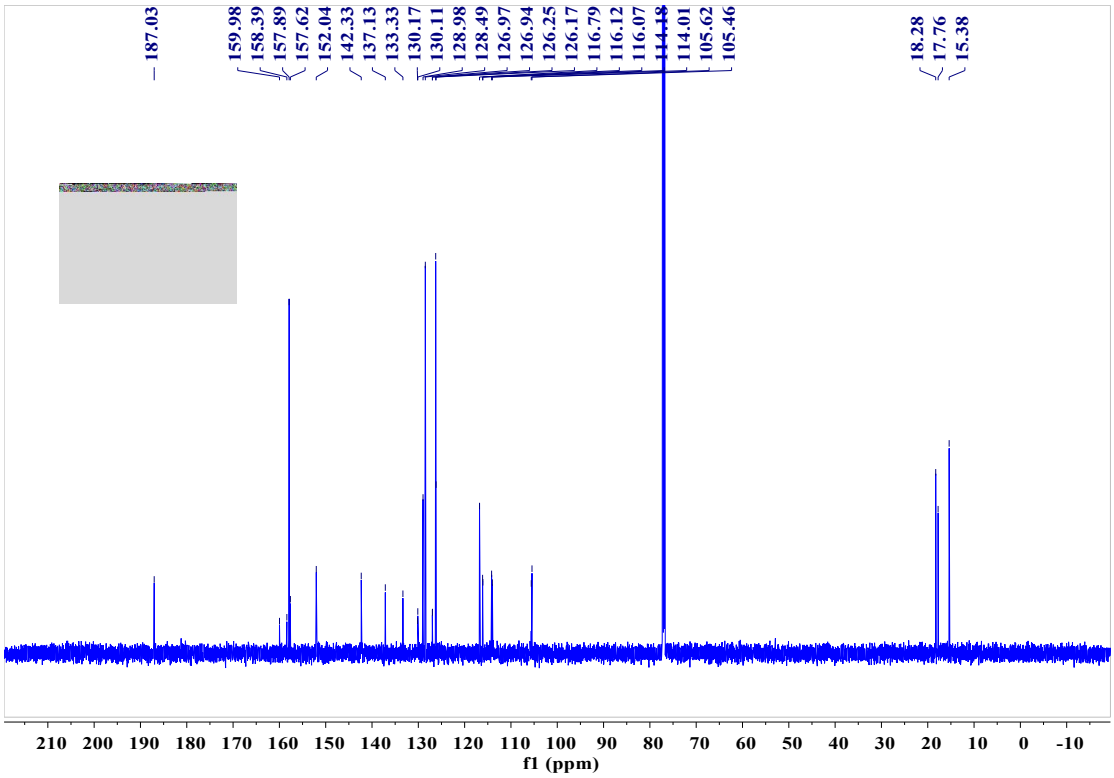
1.06
1.00
2.14
3.01
3.18
f1 (ppm)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126.97
126.94
126.25
126.17
116.79
116.12
116.07
114.18
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18.28
17.76
15.38
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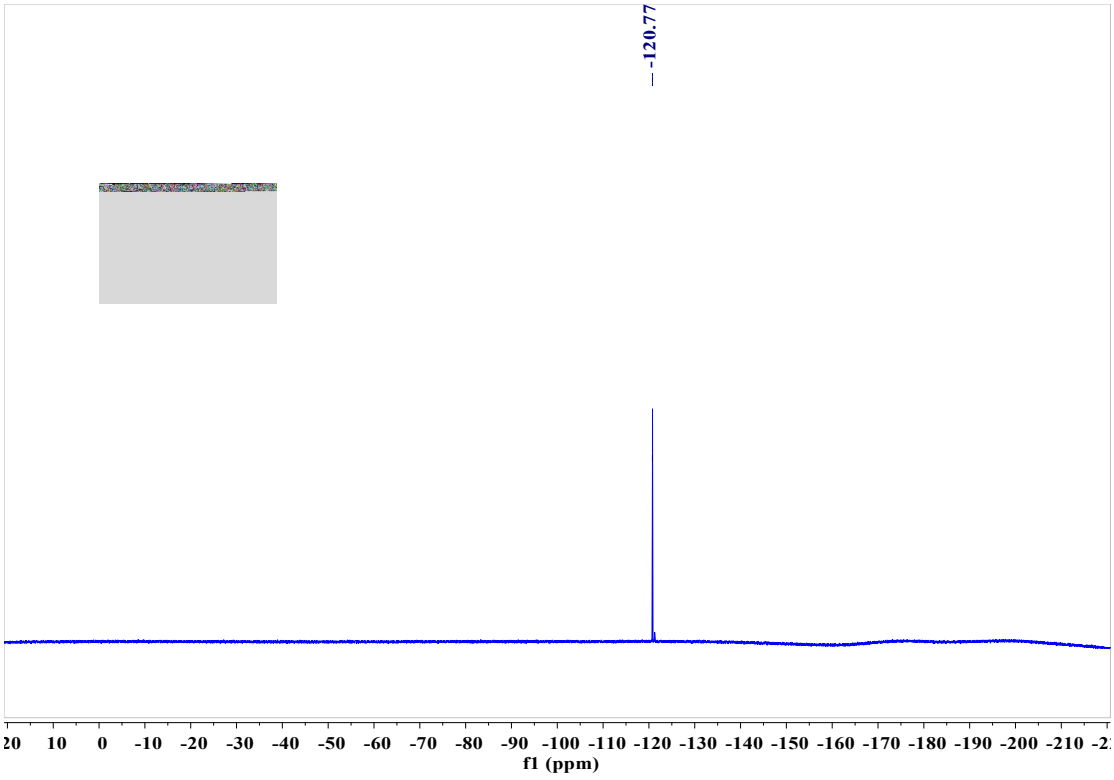
f1 (ppm)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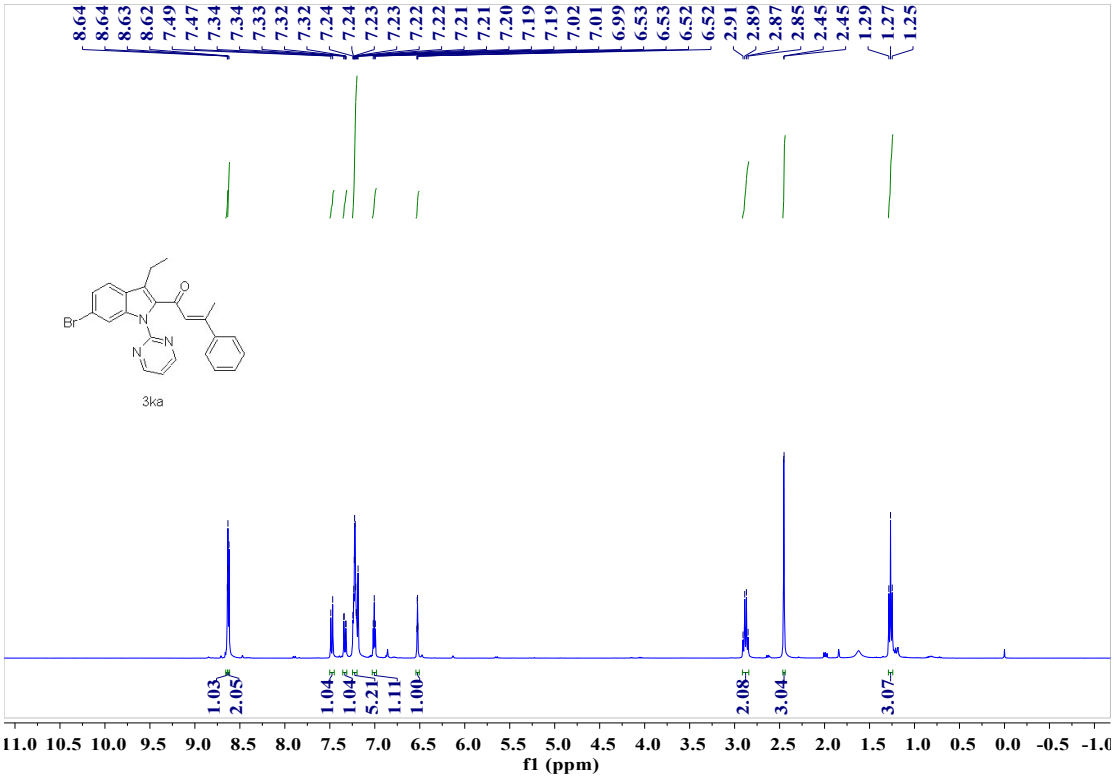
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Br
N
N
O
3ka
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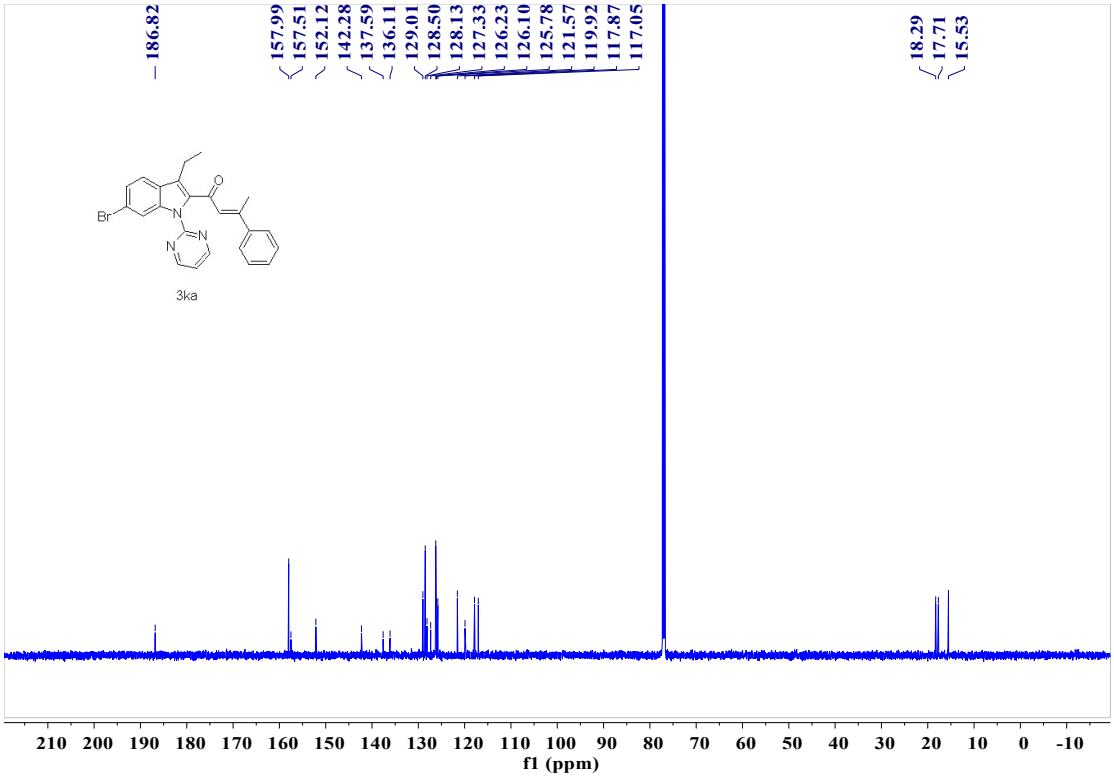
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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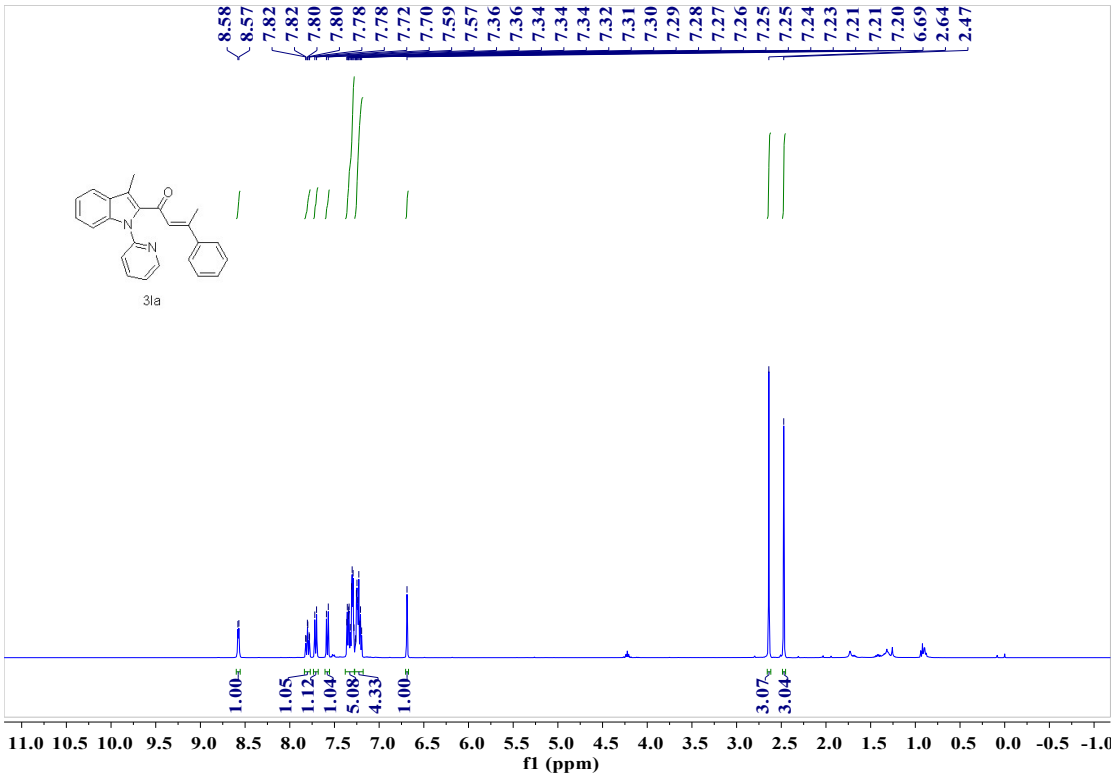
18.29 17.71 15.53
Br
N
N
O
3ka
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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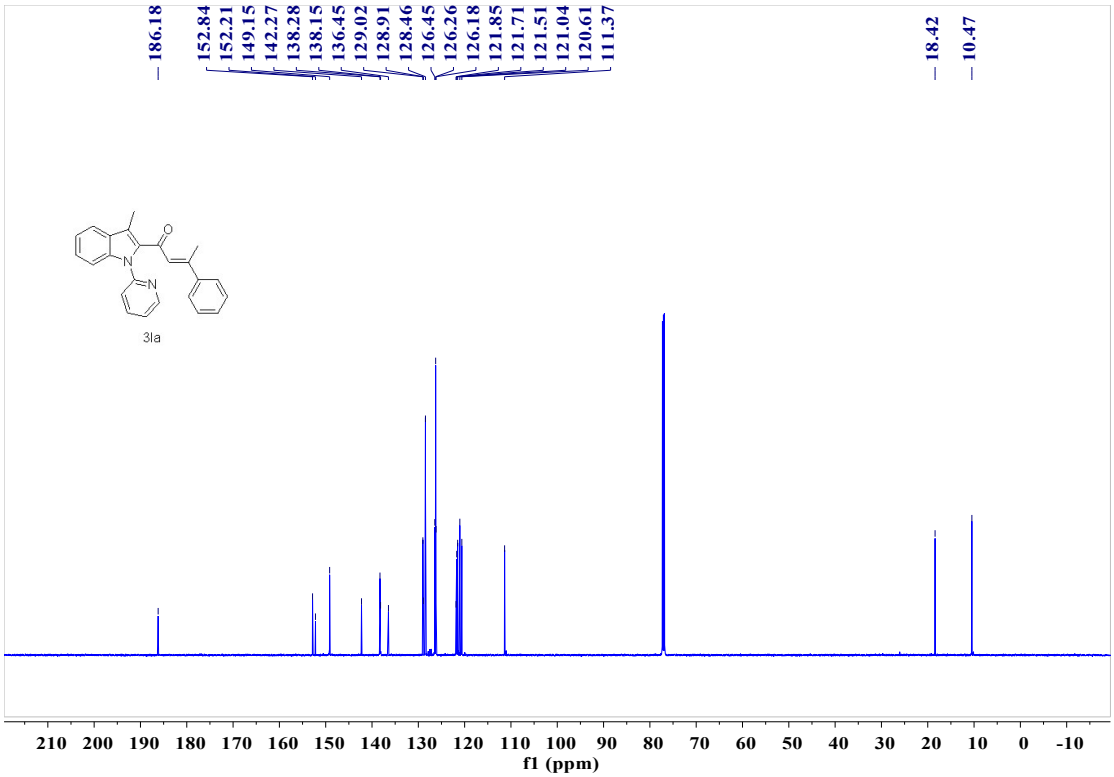
1.05
1.12
1.04
5.08
4.33
1.00
3.07
3.04
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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121.71
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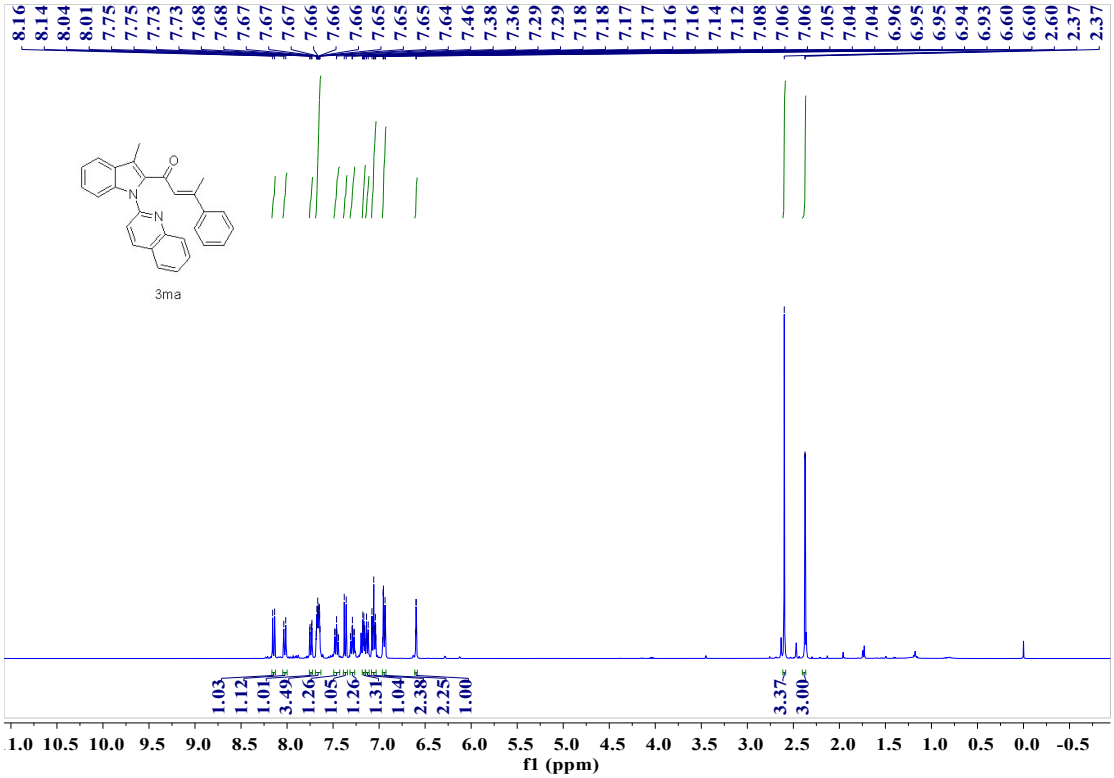
f1 (ppm)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1.03 1.12 1.01 3.49 1.26 1.05 1.26 1.31 1.04 2.38 2.25 1.00
3.37 3.00
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
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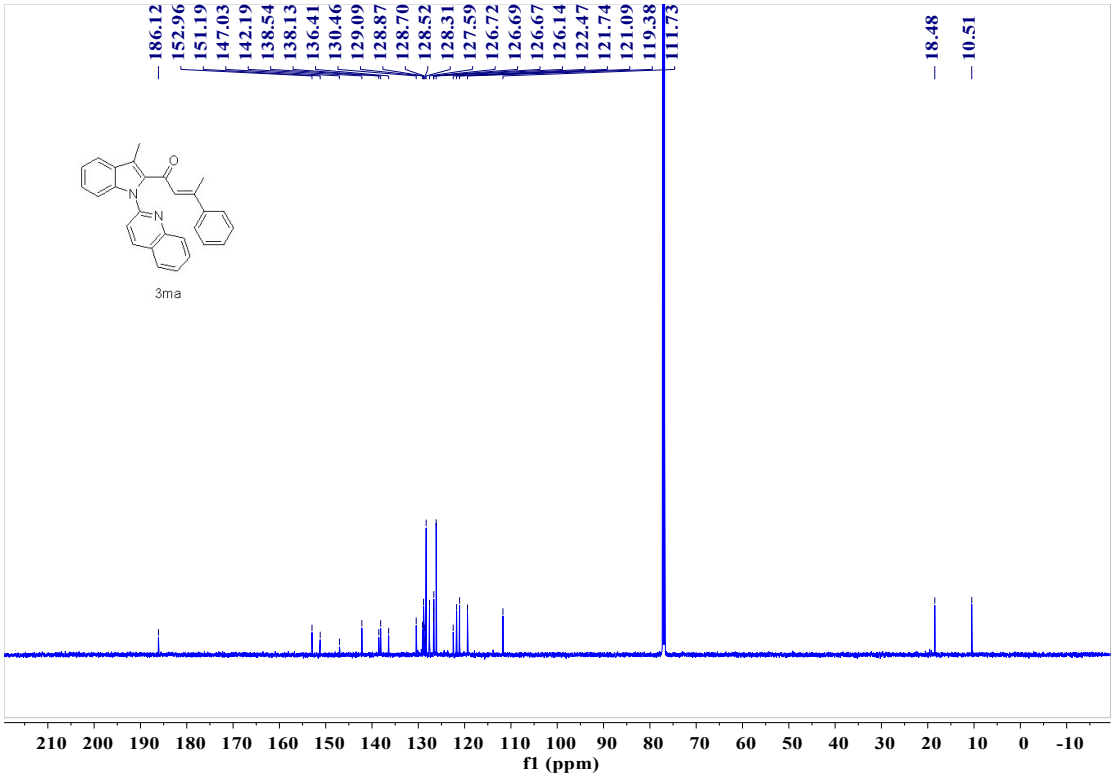
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18.48 10.51
3ma
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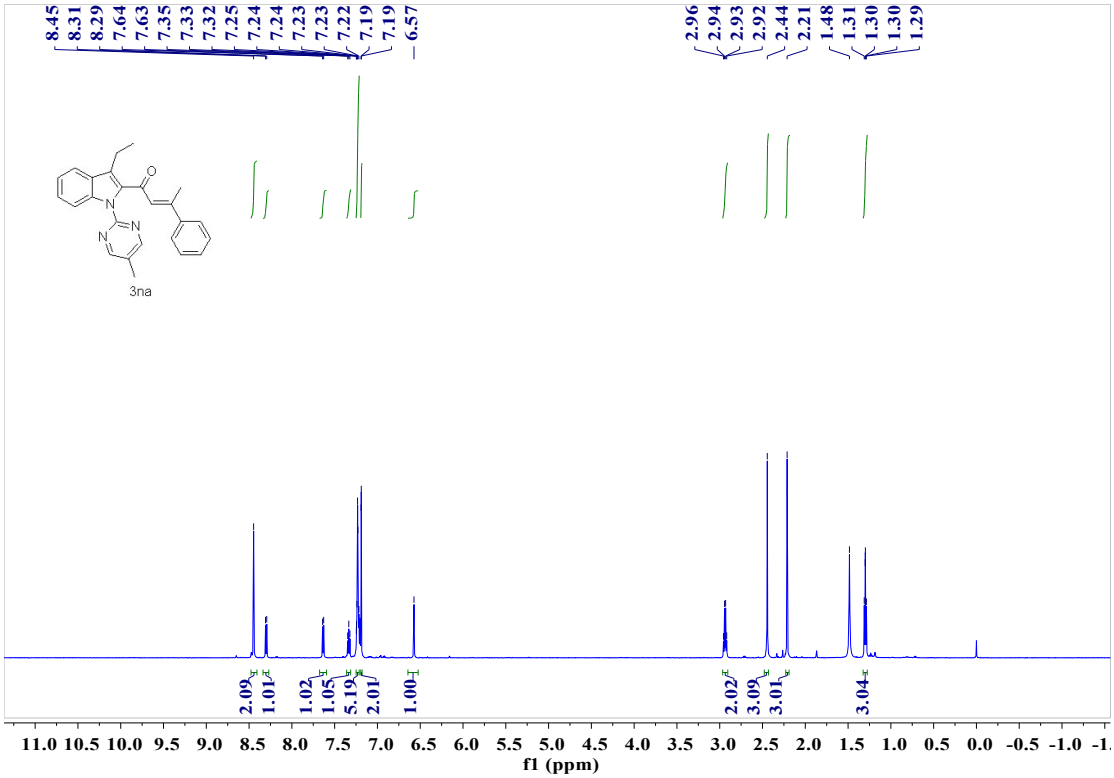
f1 (ppm)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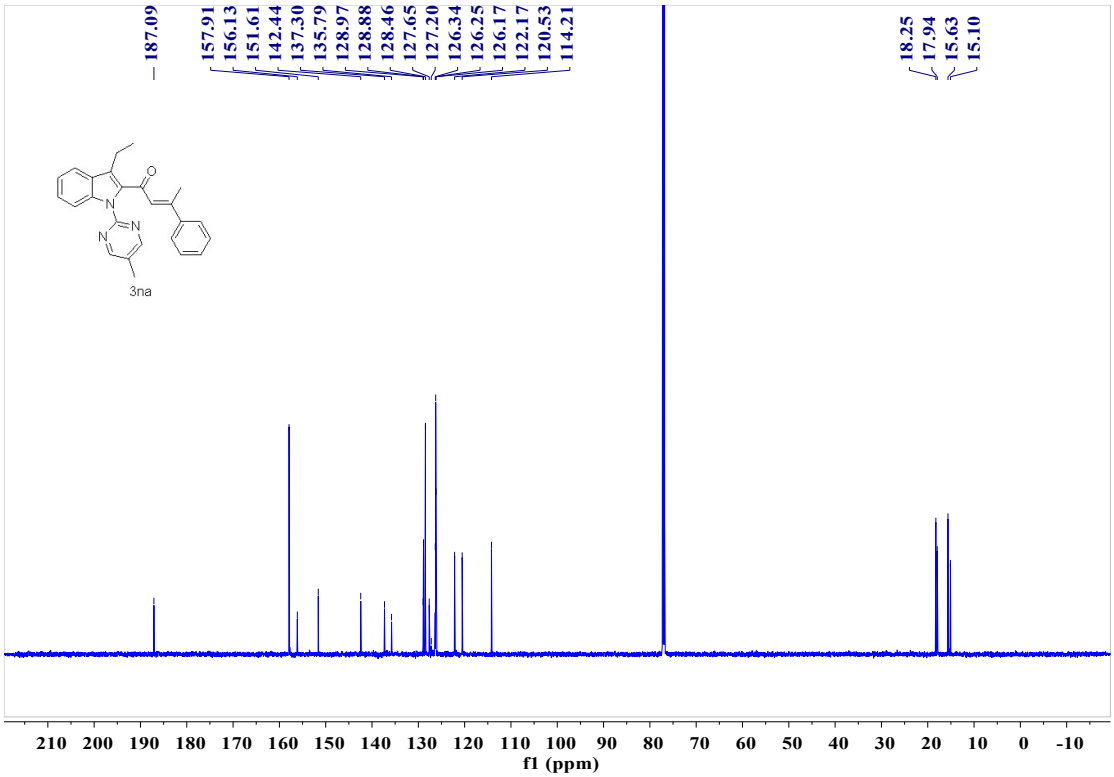
7.23
7.22
7.19
7.19
6.57
2.96
2.94
2.93
2.92
2.44
2.21
1.48
1.31
1.30
1.30
1.29
3na
2.09
1.01
1.02
1.05
5.19
2.01
1.00
2.02
3.09
3.01
3.04
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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126.34
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122.17
120.53
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15.63
15.10
3na
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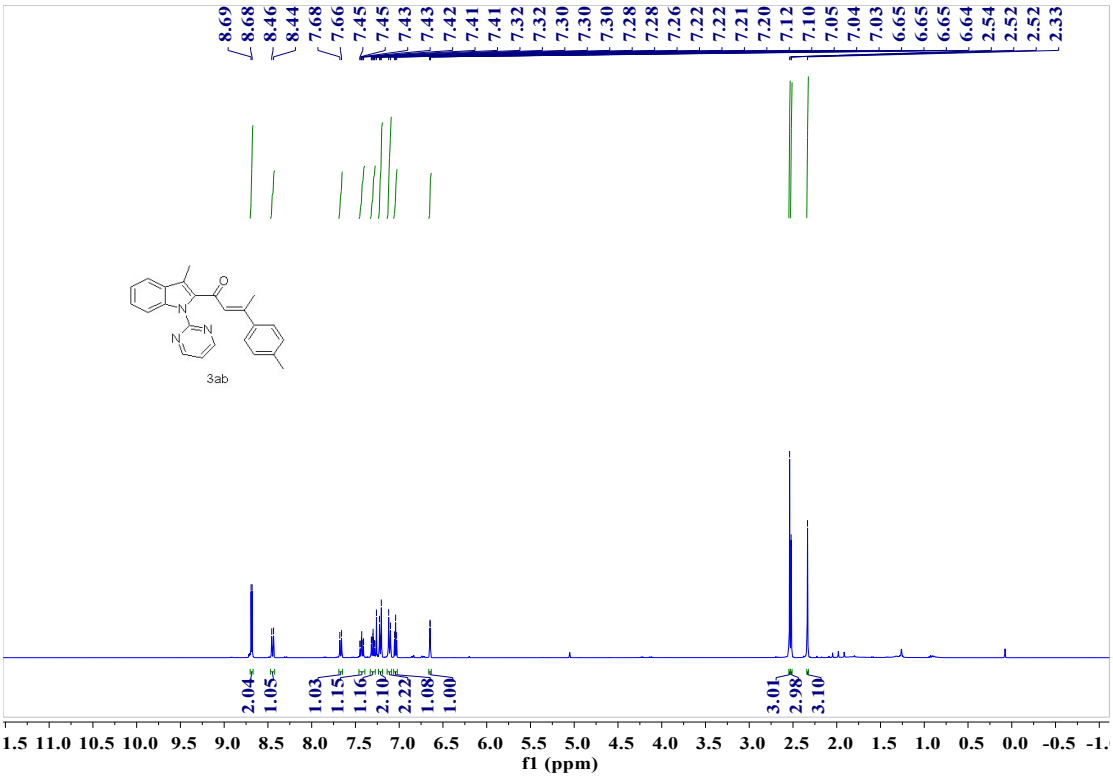
f1 (ppm)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7.41
7.32
7.32
7.30
7.30
7.30
7.28
7.28
7.26
7.22
7.22
7.21
7.20
7.12
7.10
7.05
7.04
7.03
6.65
6.65
6.64
2.54
2.52
2.52
2.33
3ab
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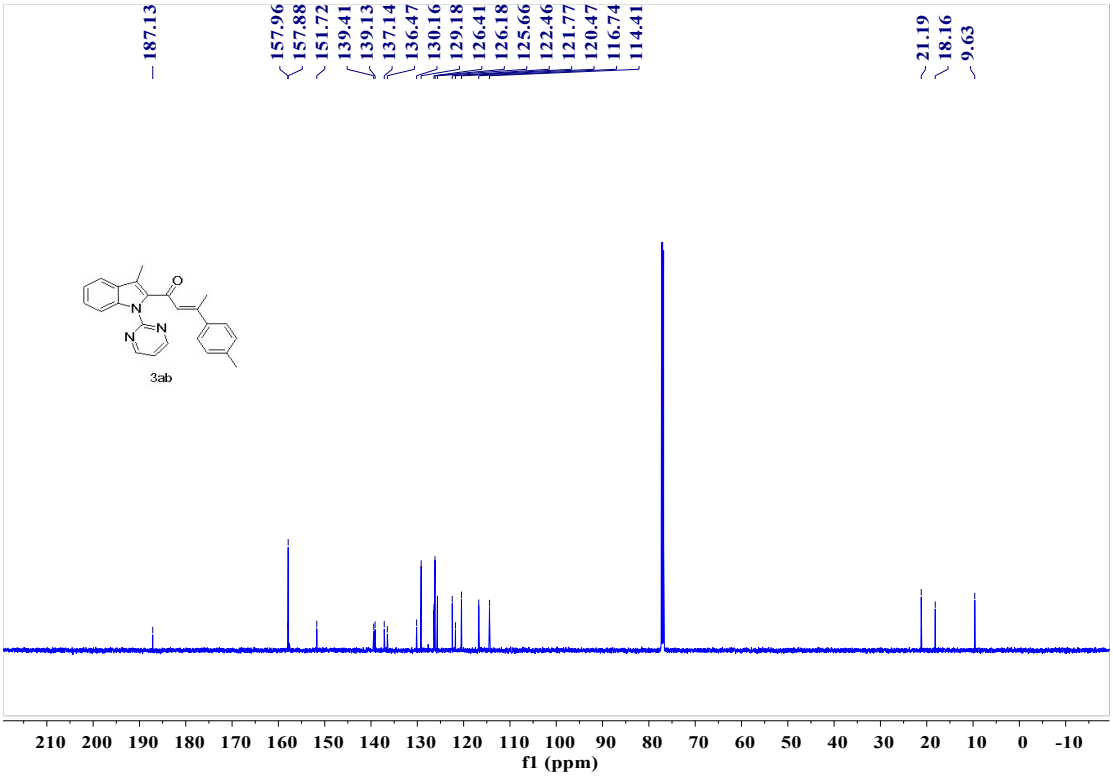
1.05
1.03
1.15
1.16
2.10
2.22
1.08
1.00
3.01
2.98
3.10
1.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)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126.41
126.18
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122.46
121.77
120.47
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18.16
9.63
3ab
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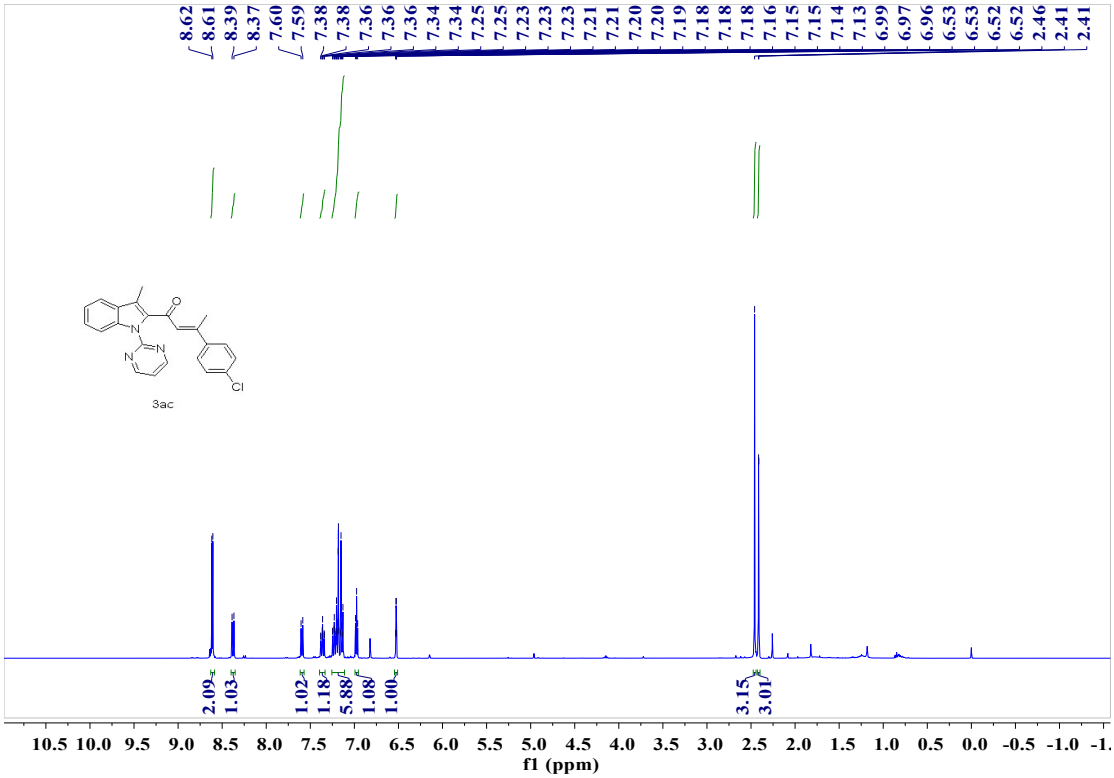
f1 (ppm)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7.18
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7.14
7.13
6.99
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6.96
6.53
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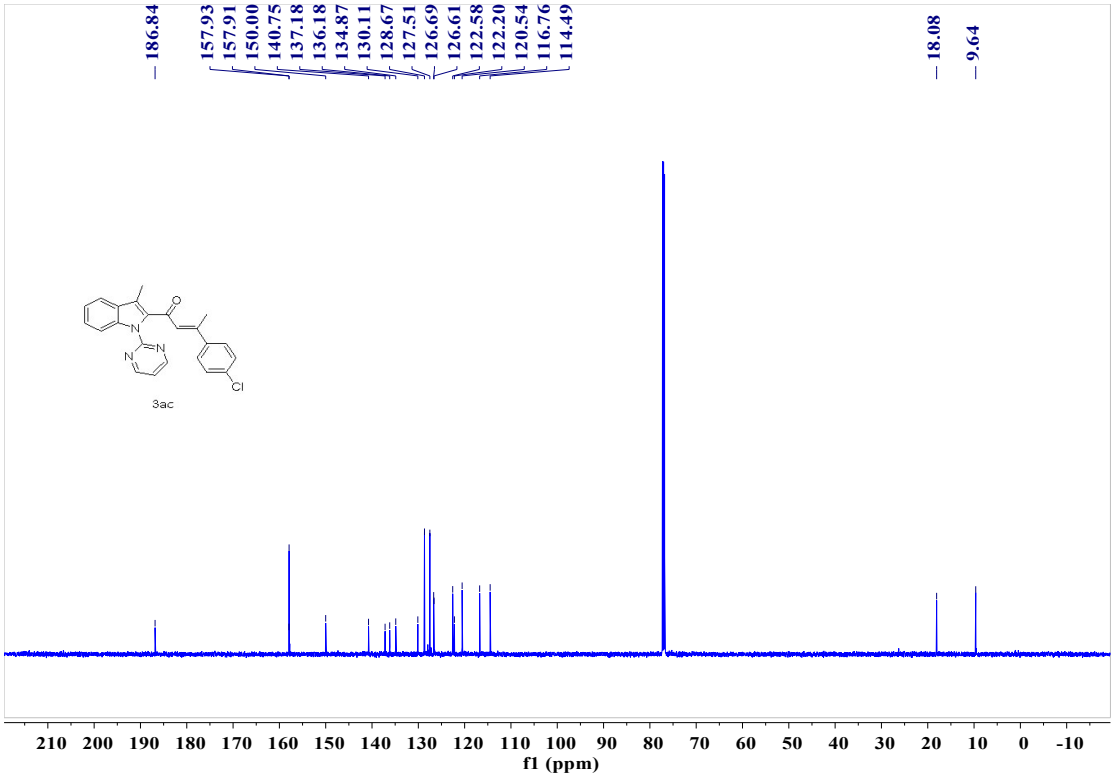
6.52
6.52
2.46
2.41
2.41
3ac
Cl
N
N
O
2.09
1.03
1.02
1.18
5.88
1.08
1.00
3.15
3.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.
f1 (ppm)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134.87
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127.51
126.69
126.61
122.58
122.20
120.54
116.76
114.49
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9.64
3ac
Cl
N
N
O
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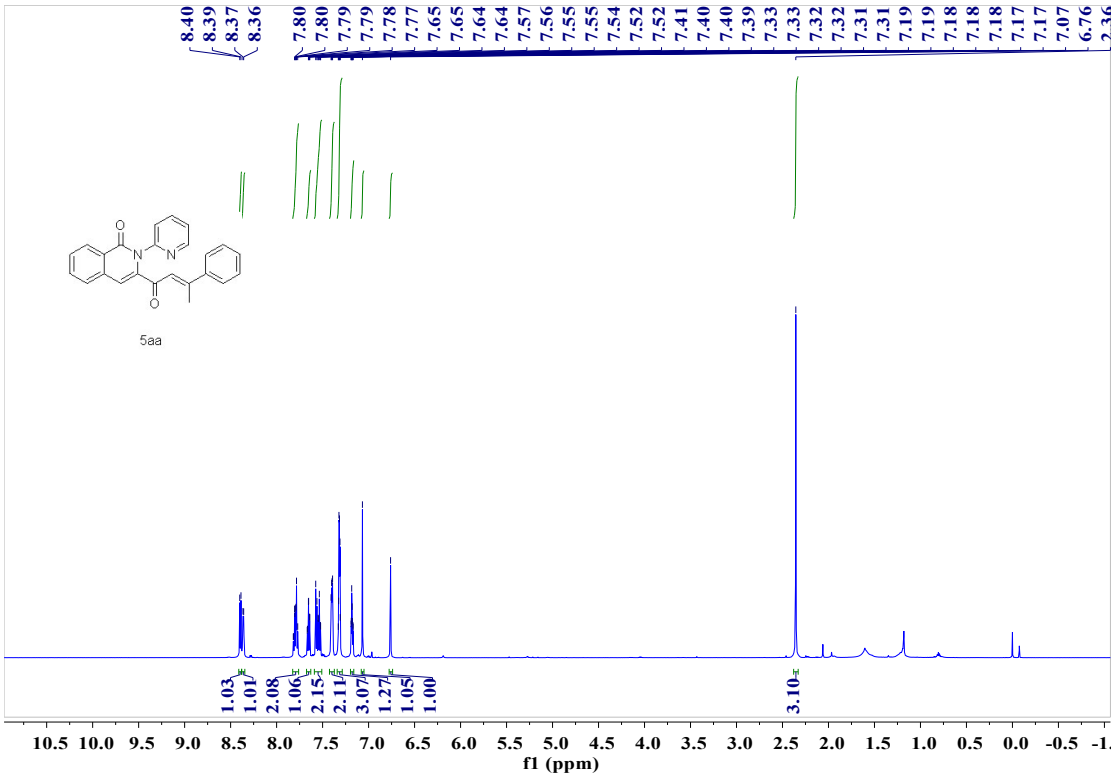
f1 (ppm)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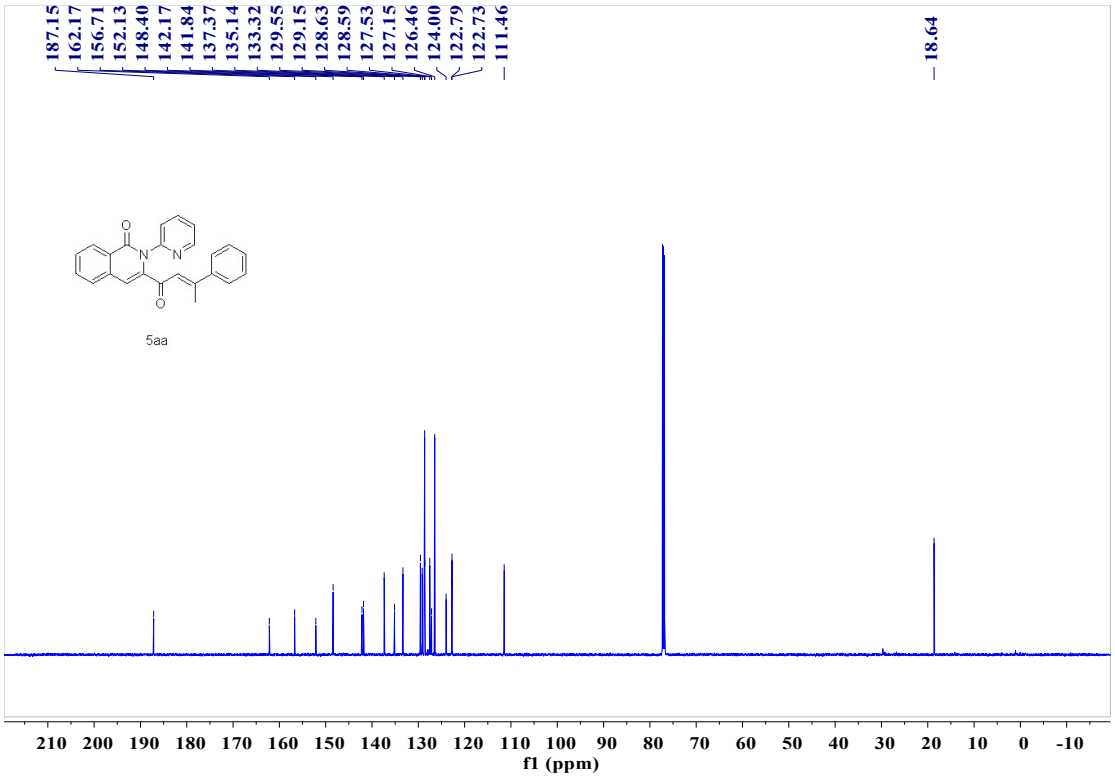
5aa
1.03 1.01 2.08 1.06 2.15 2.11 3.07 1.27 1.05 1.00 3.10
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


187.15 162.17 156.71 152.13 148.40 142.17 141.84 137.37 135.14 133.32 129.55 129.15 128.63 128.59 127.53 127.15 126.46 124.00 122.79 122.73 111.46 18.64
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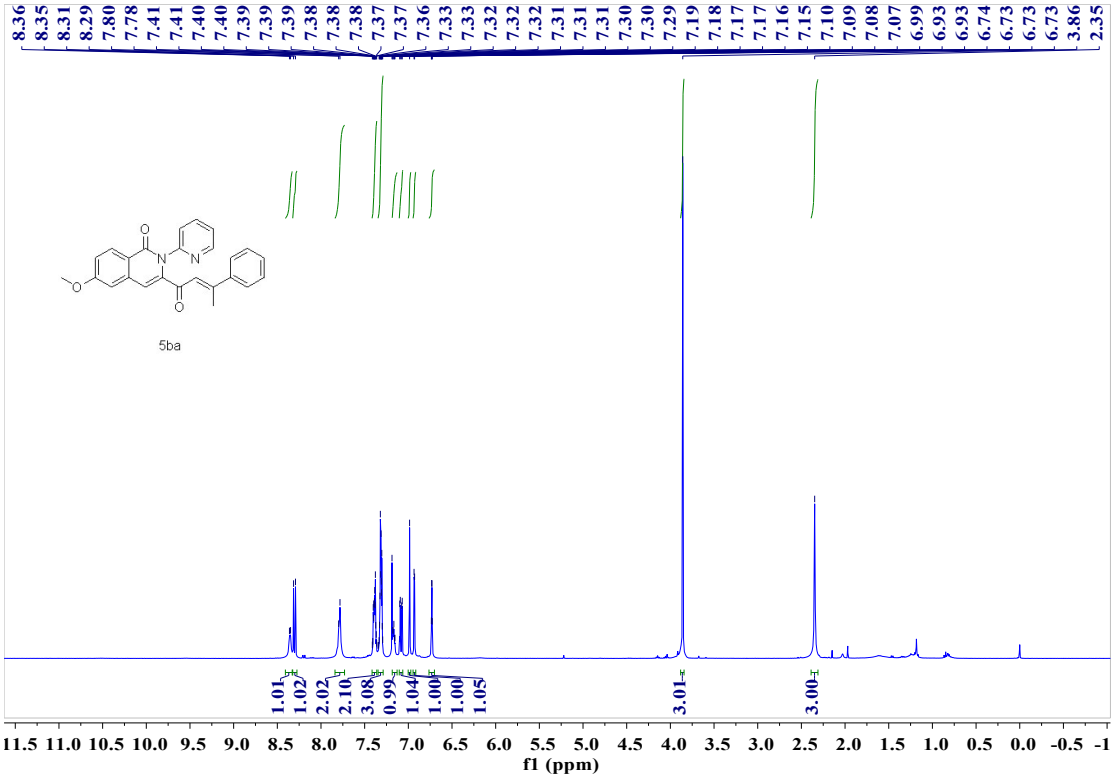
f1 (ppm)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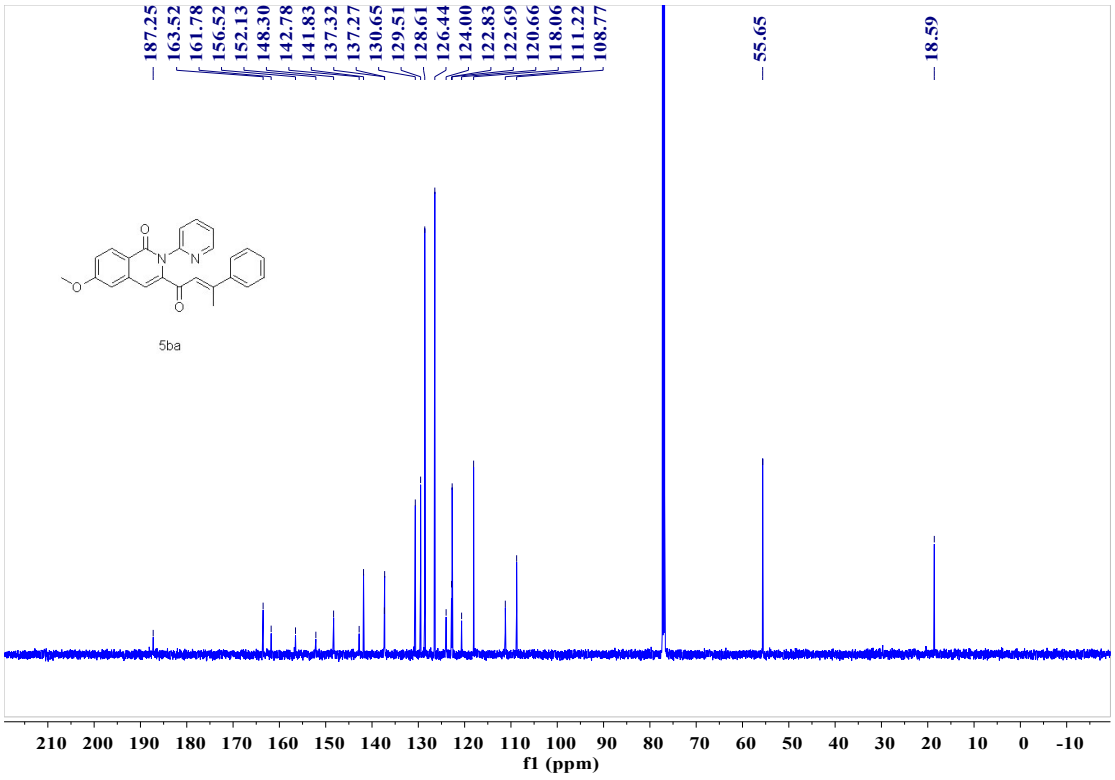
5ba
1.01 1.02 2.02 2.10 3.08 0.99 1.04 1.00 1.00 1.05 3.01 3.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)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55.65
18.59
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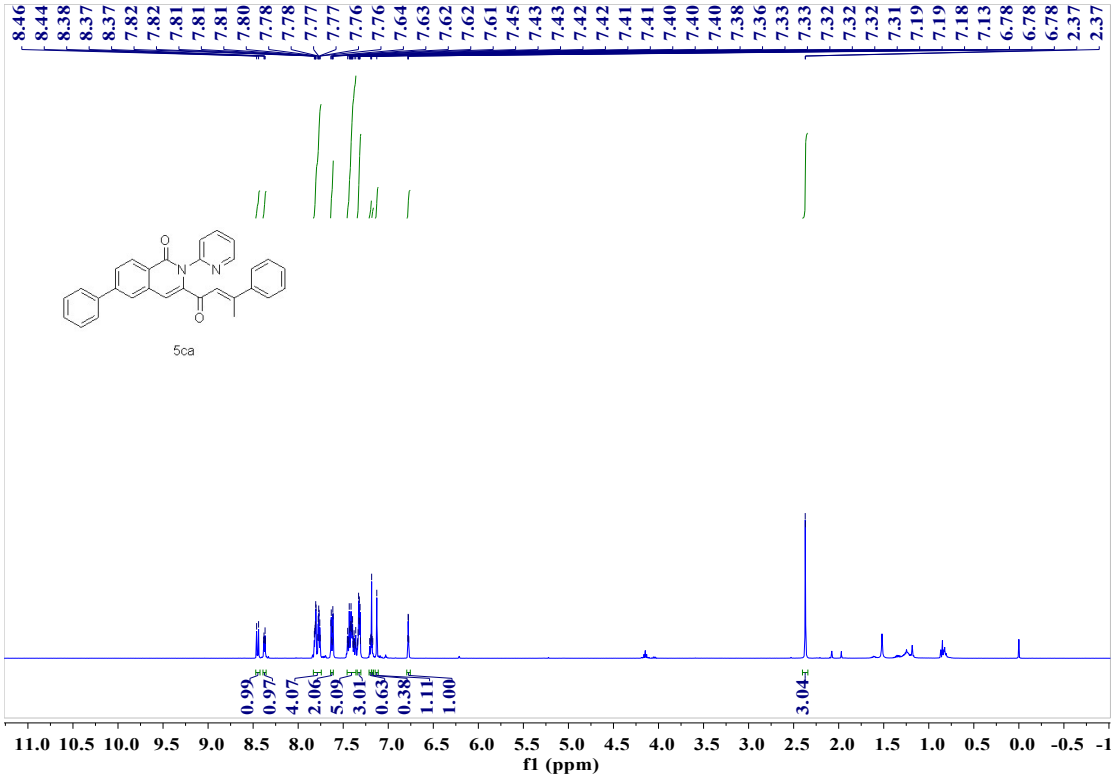
f1 (ppm)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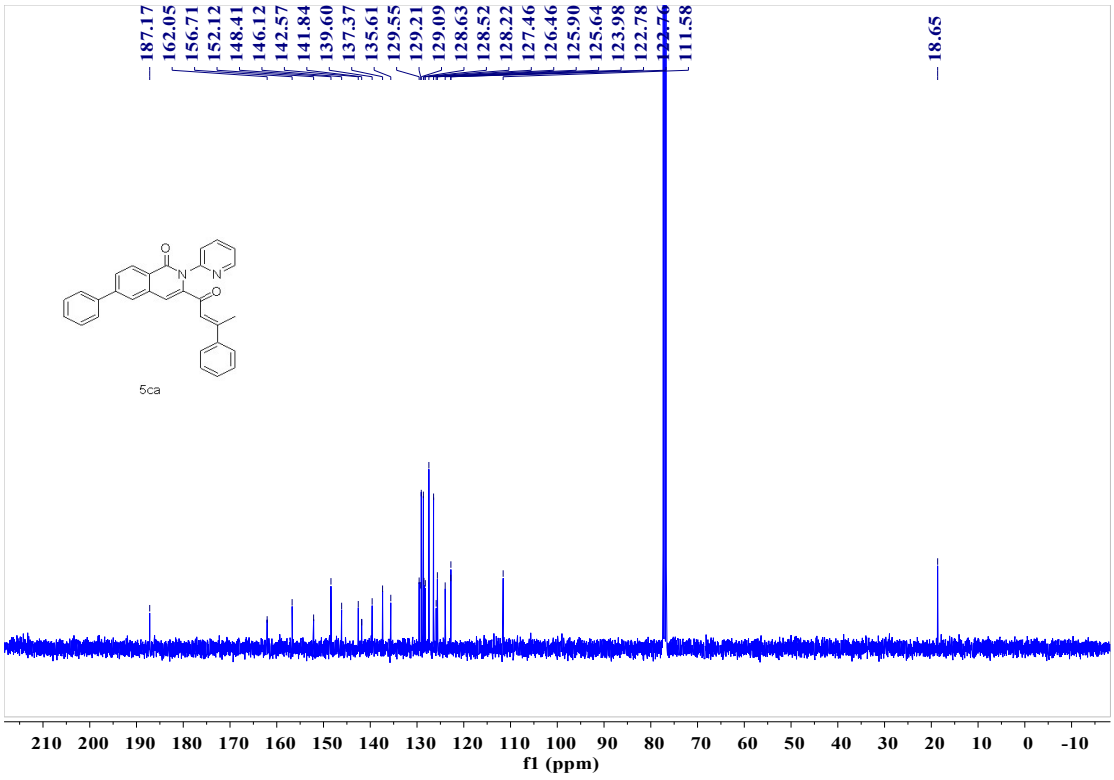
5ca
0.99 0.97 4.07 2.06 5.09 3.01 0.63 0.38 1.11 1.00 3.04
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)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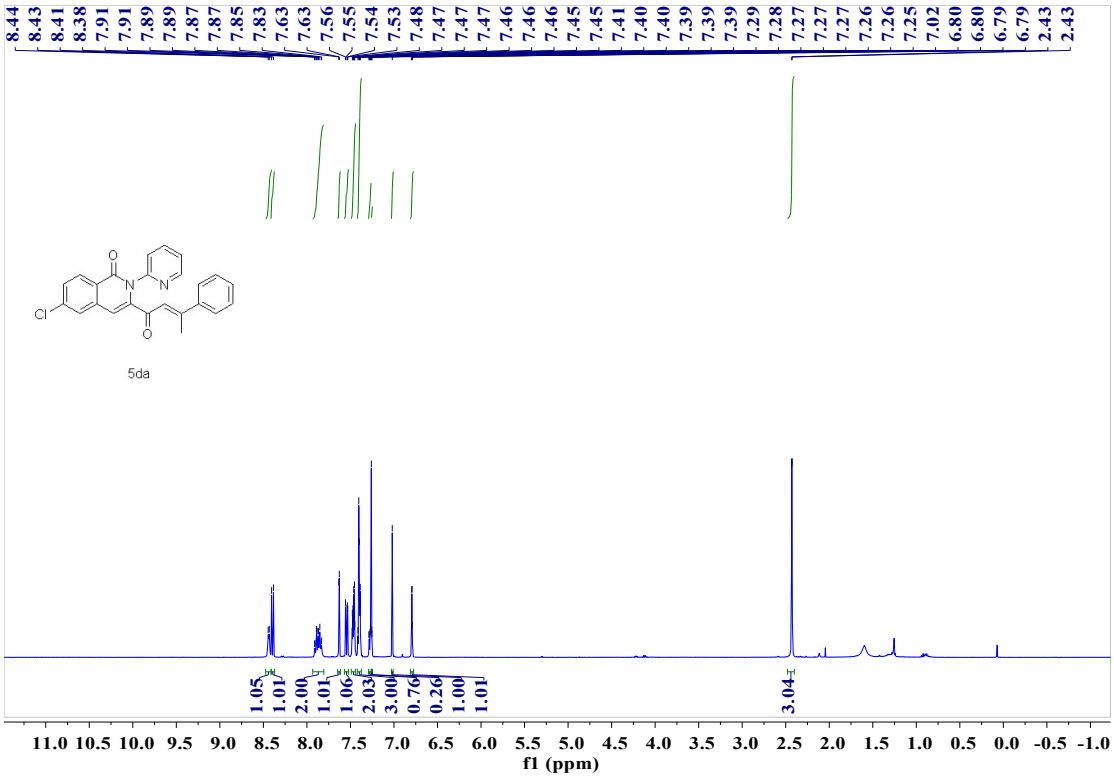
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Cl
O
N
N
O
5da
1.05 1.01 2.00 1.01 1.06 2.03 3.00 0.76 0.26 1.00 1.01 3.04
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
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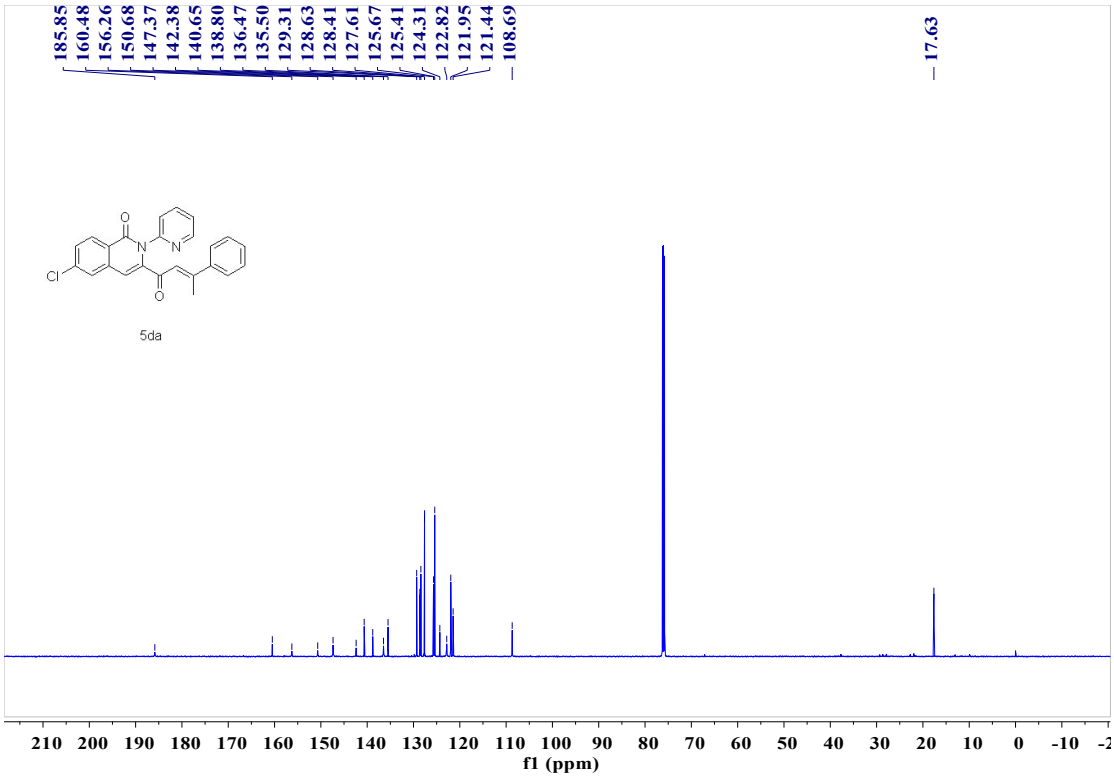
185.85 160.48 156.26 150.68 147.37 142.38 140.65 138.80 136.47 135.50 129.31 128.63 128.41 127.61 125.67 125.41 124.31 122.82 121.95 121.44 108.69
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N
O
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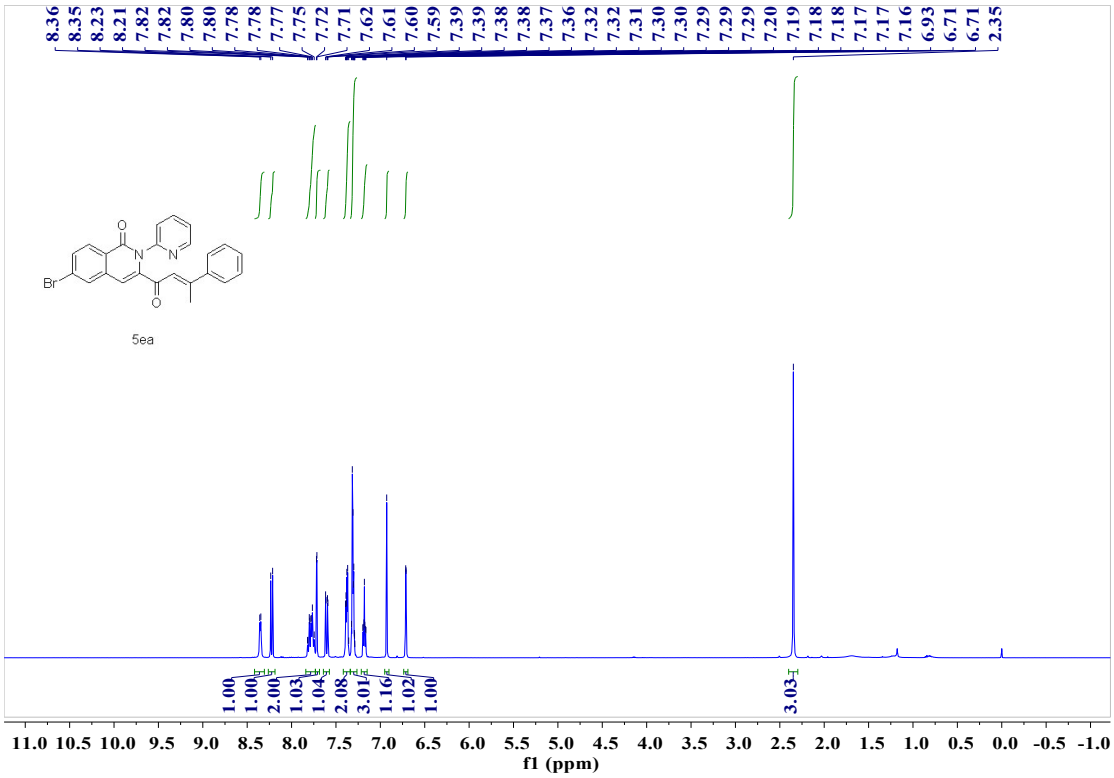
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Br
5ea
1.00 1.00 2.00 1.03 1.04 2.08 3.01 1.16 1.02 1.00
3.03
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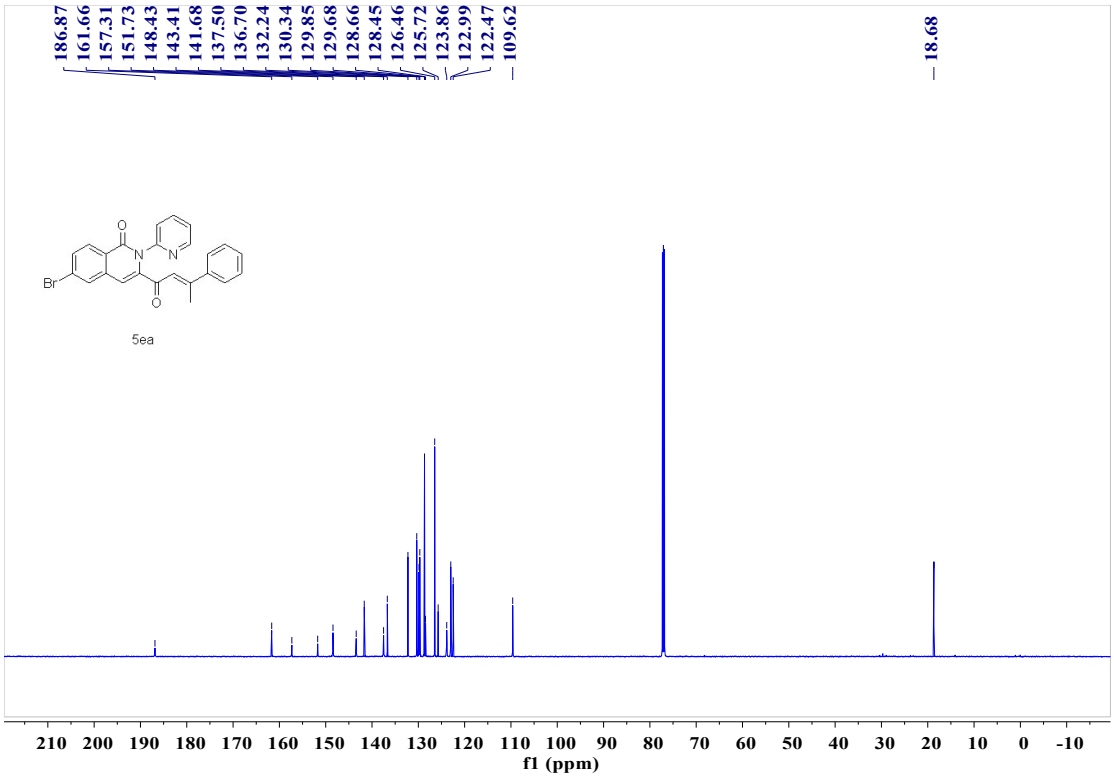
f1 (ppm)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18.68
Br
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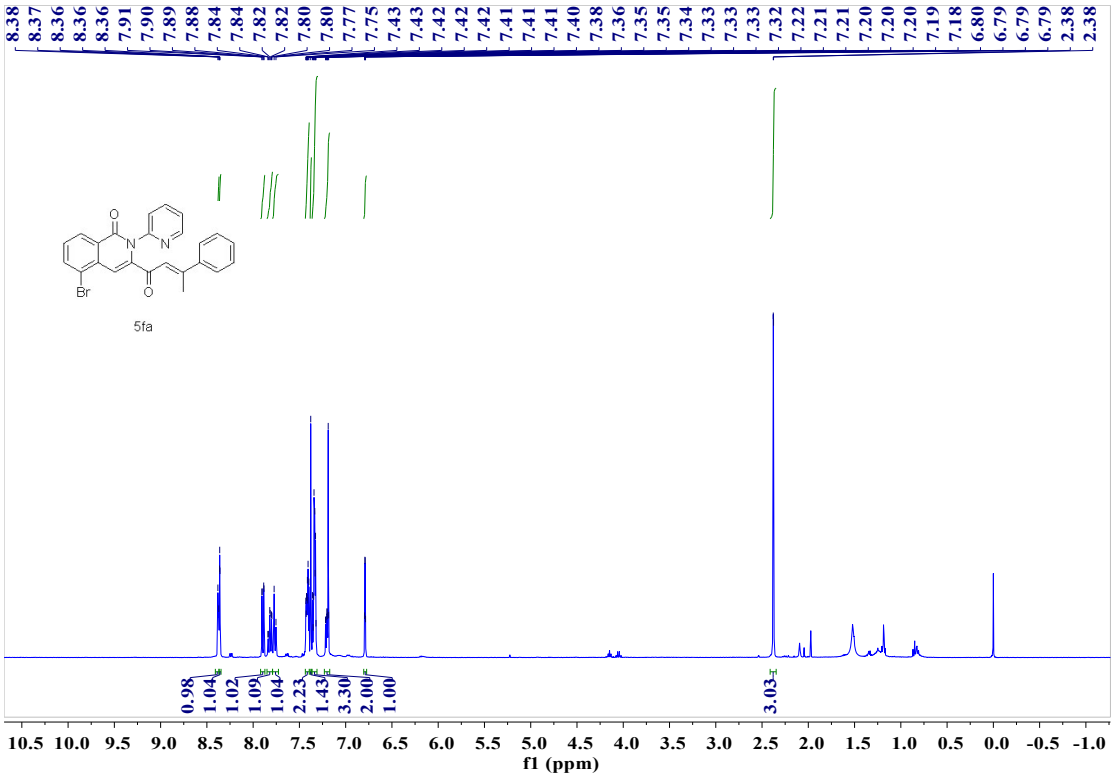
f1 (ppm)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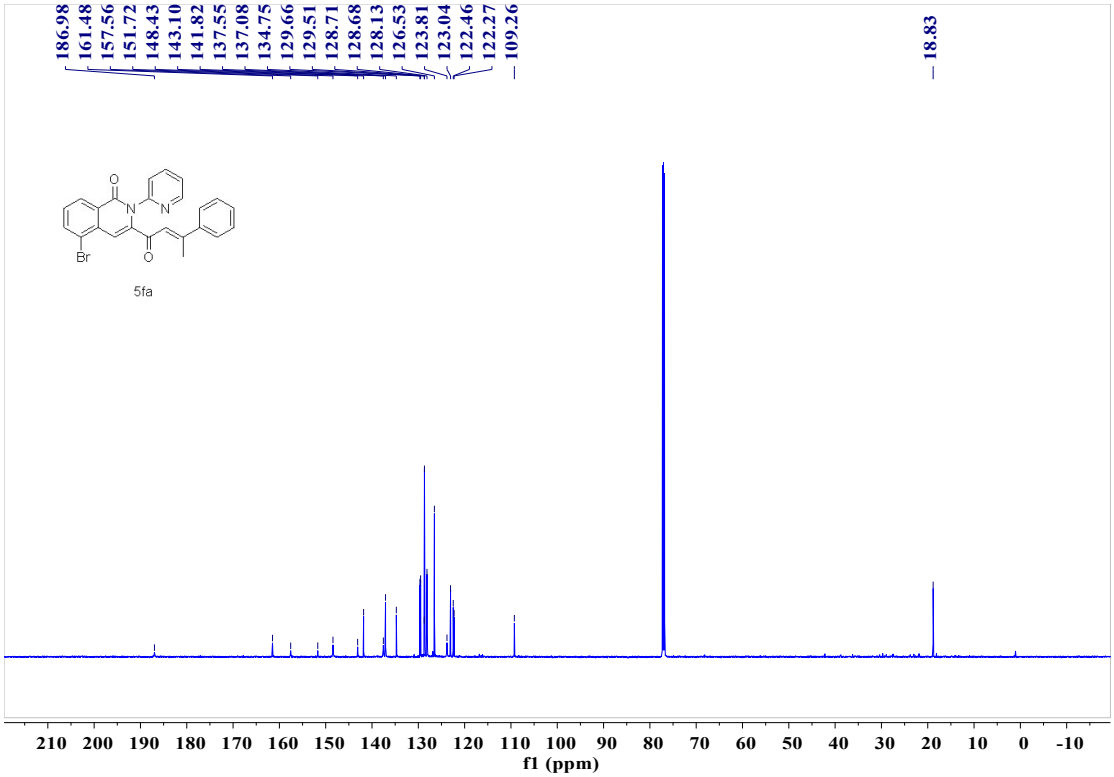
O
N
N
Br
O
5fa
0.98 1.04 1.02 1.09 1.04 2.23 1.43 3.30 2.00 1.00
3.03
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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18.83
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N
Br
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5fa
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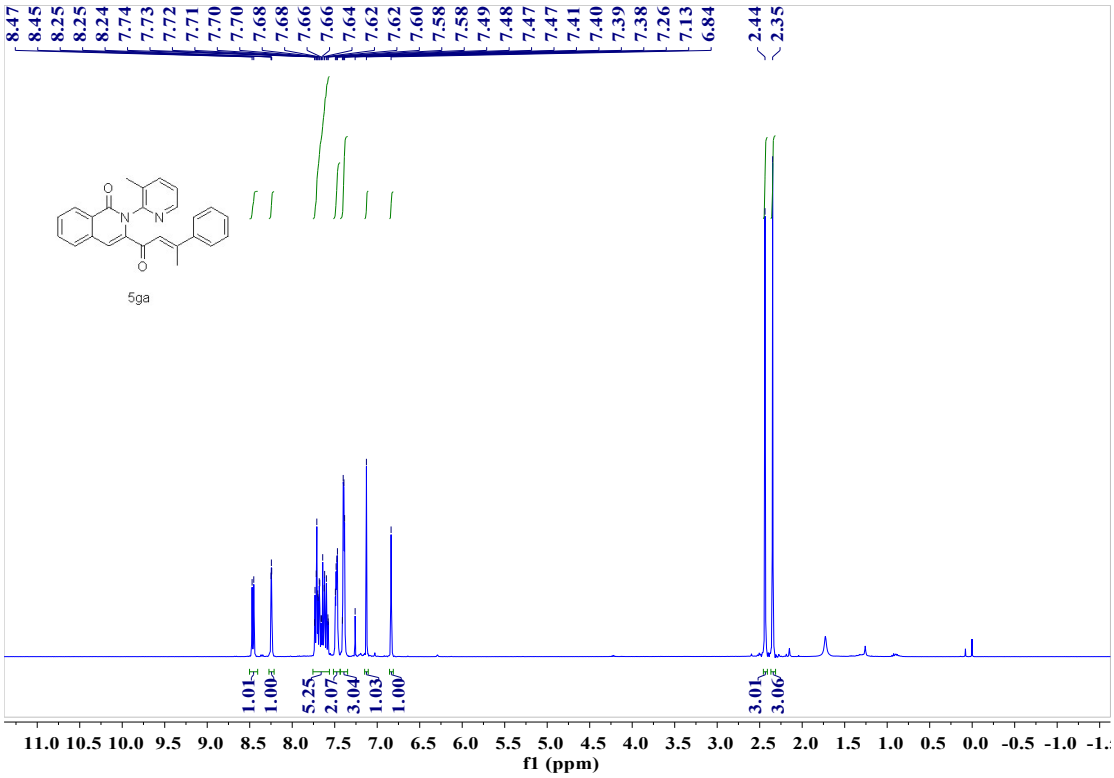
f1 (ppm)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3.01
3.06
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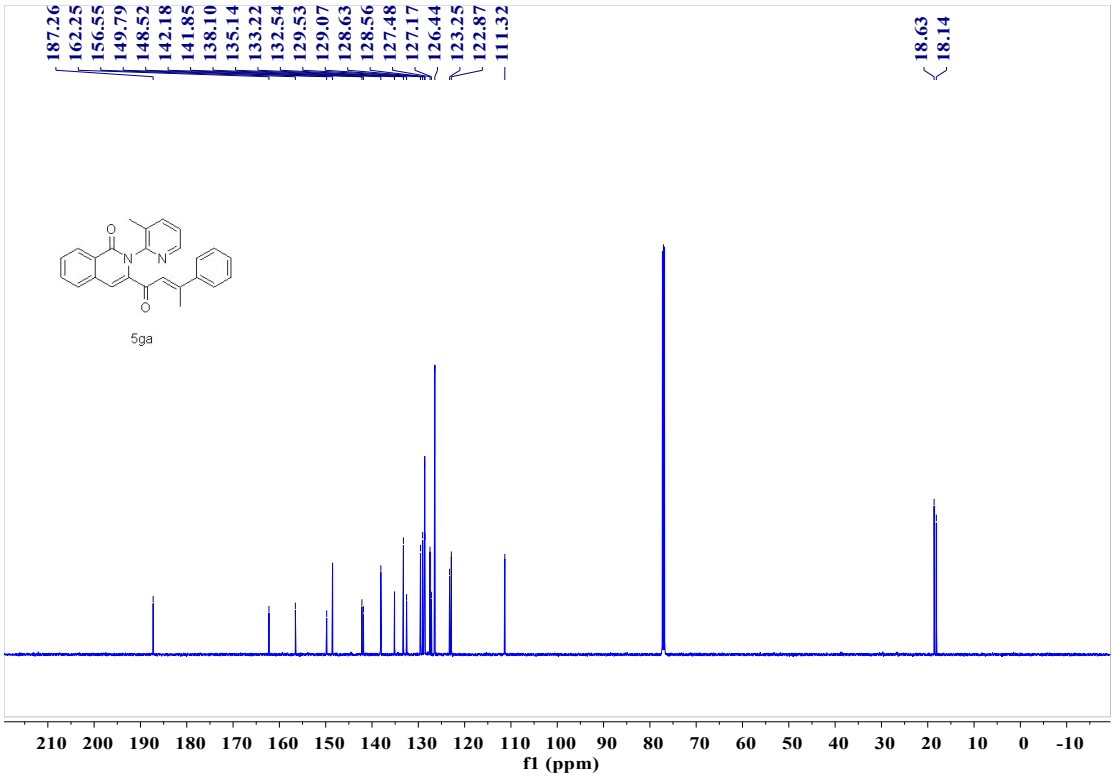
f1 (ppm)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128.63
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127.48
127.17
126.44
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18.63
18.14
5ga
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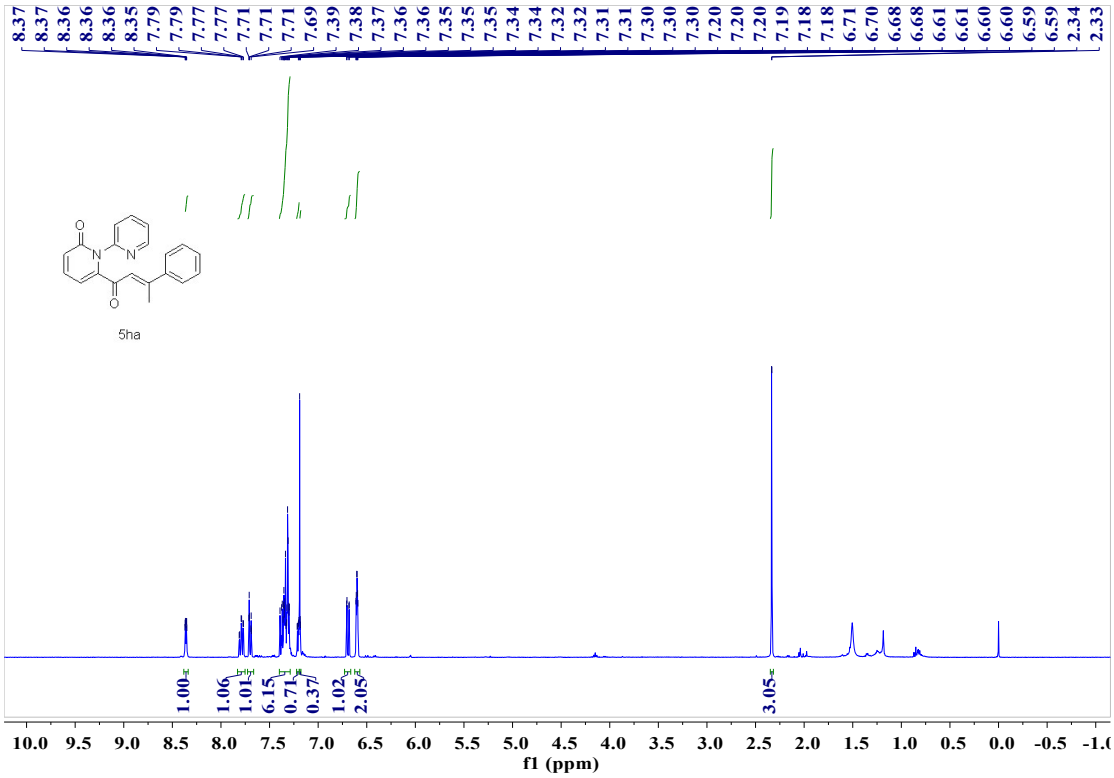
f1 (ppm)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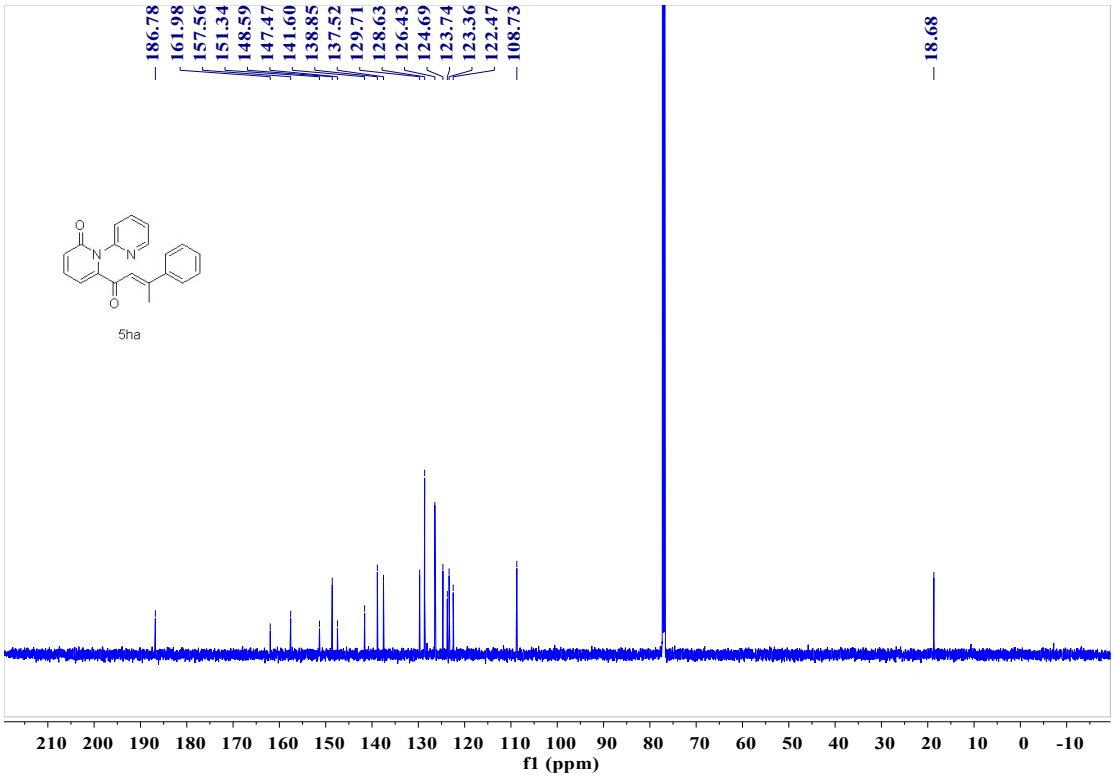
5ha
1.00 1.06 1.01 6.15 0.71 0.37 1.02 2.05 3.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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18.68
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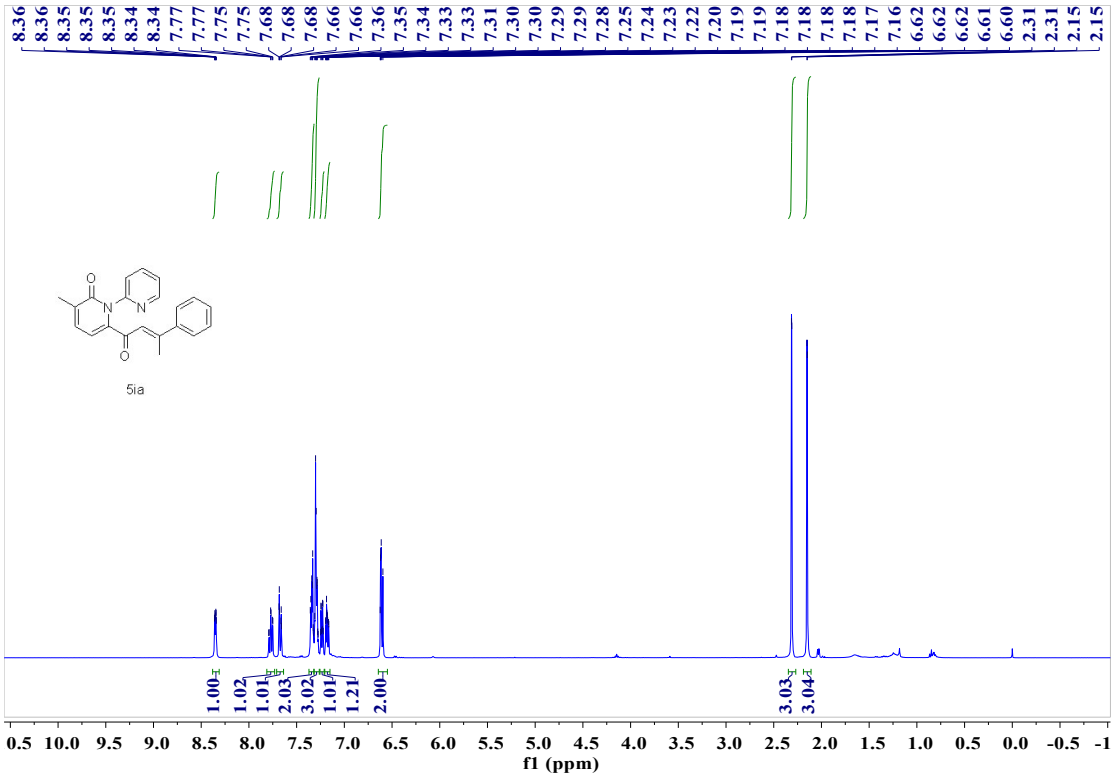
f1 (ppm)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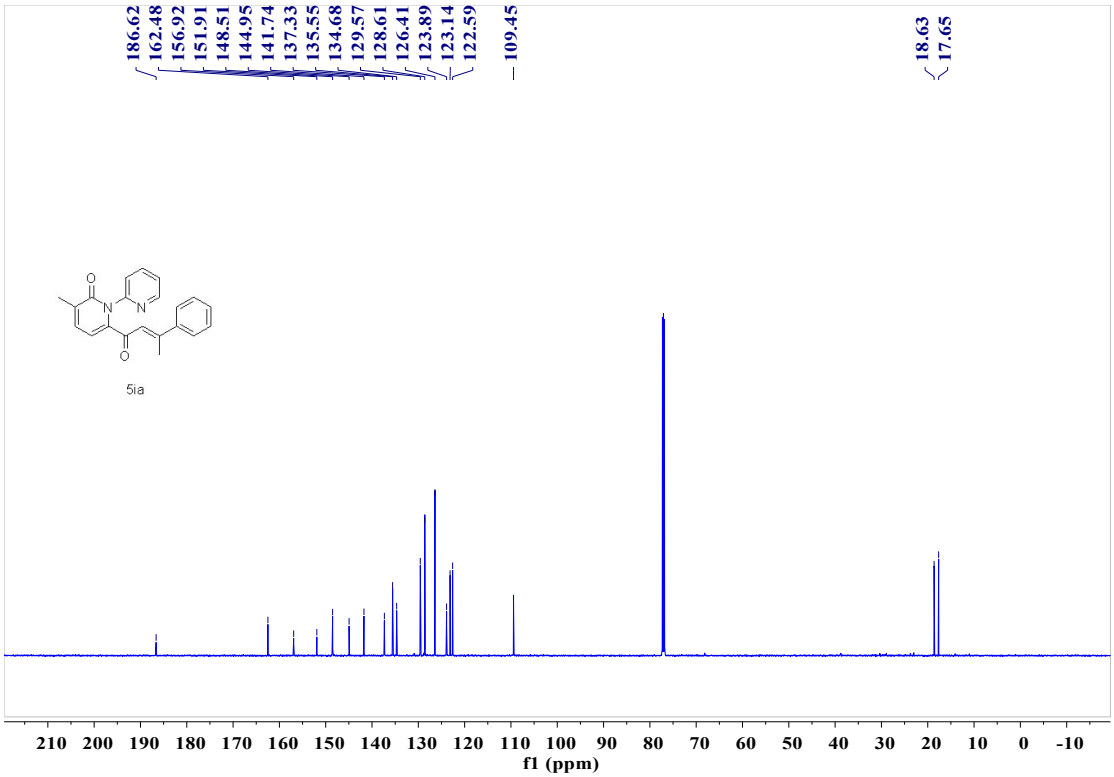
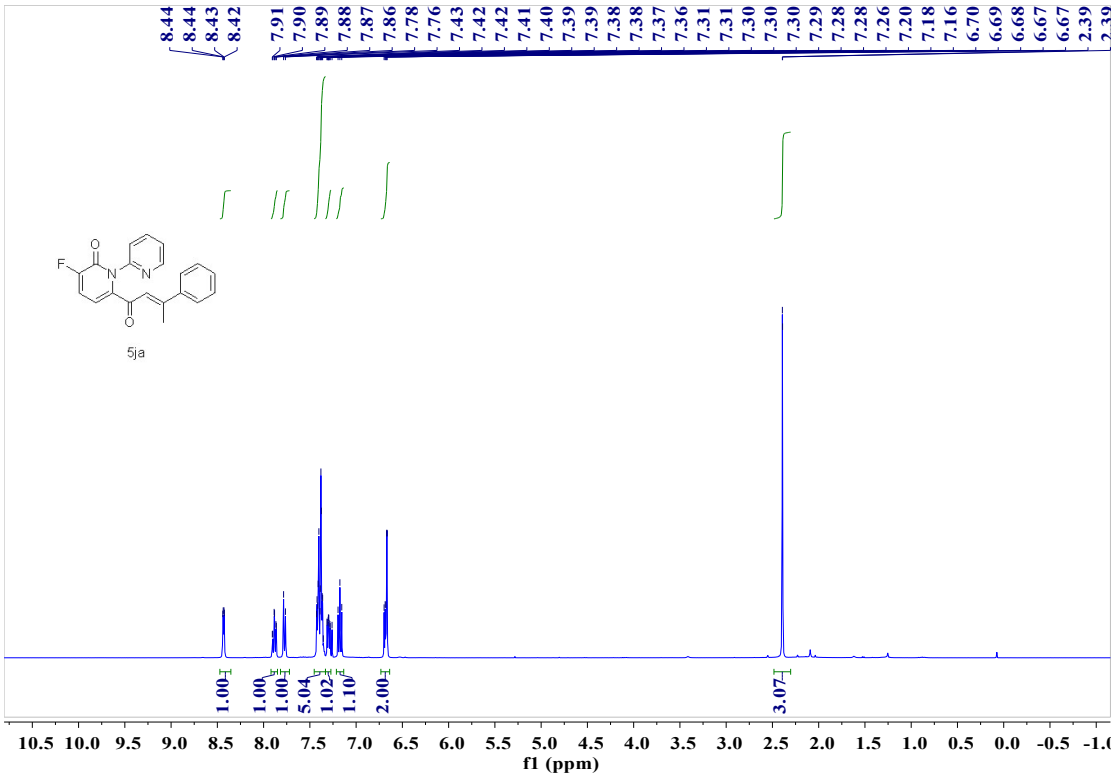
5ia
1.00 1.02 1.01 2.03 3.02 1.01 1.21 2.00 3.03 3.04
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)


186.62 162.48 156.92 151.91 148.51 144.95 141.74 137.33 135.55 134.68 129.57 128.61 126.41 123.89 123.14 122.59 109.45 18.63 17.65
5ia
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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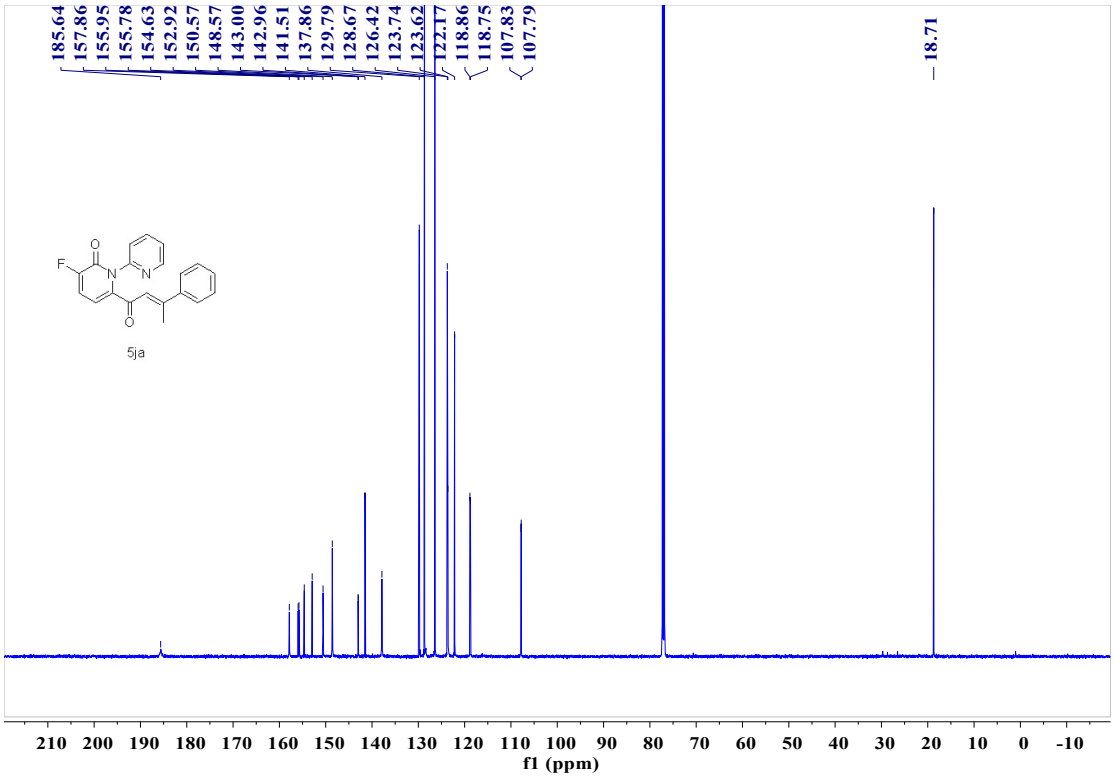
F
O
N
N
O
5ja
1.00 1.00 1.00 5.04 1.02 1.10 2.00 3.07
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


185.64 157.86 155.95 155.78 154.63 152.92 150.57 148.57 143.00 142.96 141.51 137.86 129.79 128.67 126.42 123.74 123.62 122.17 118.86 118.75 107.83 107.79
18.71
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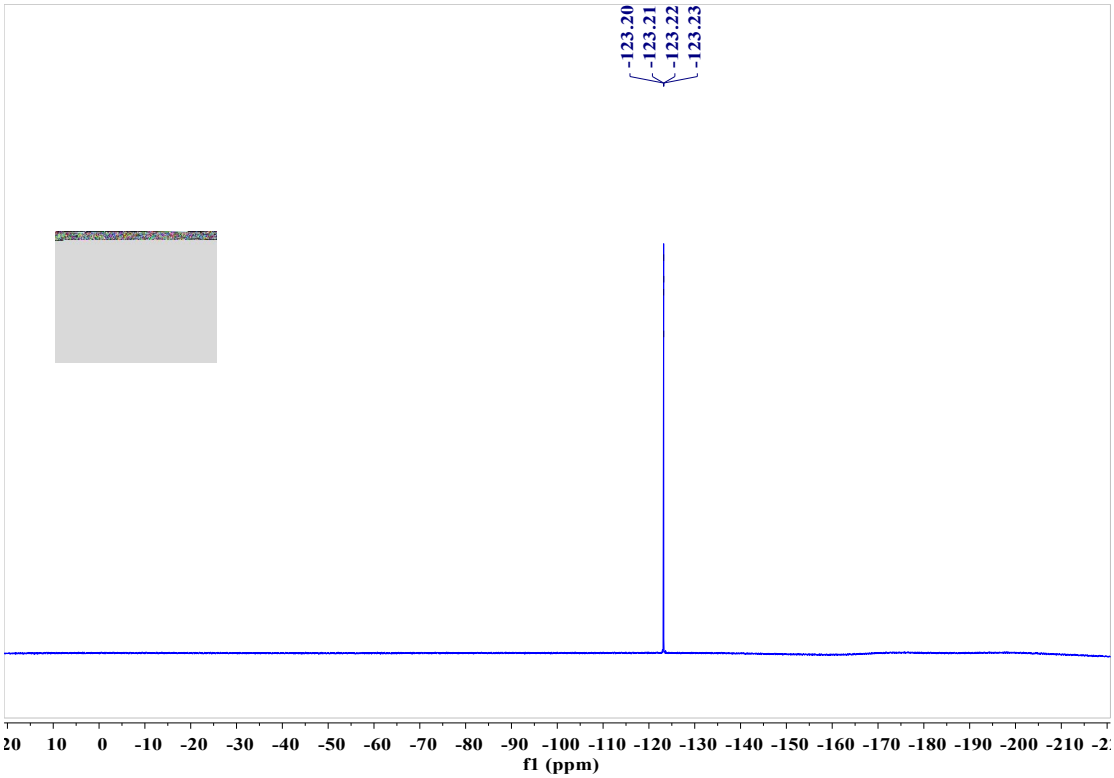
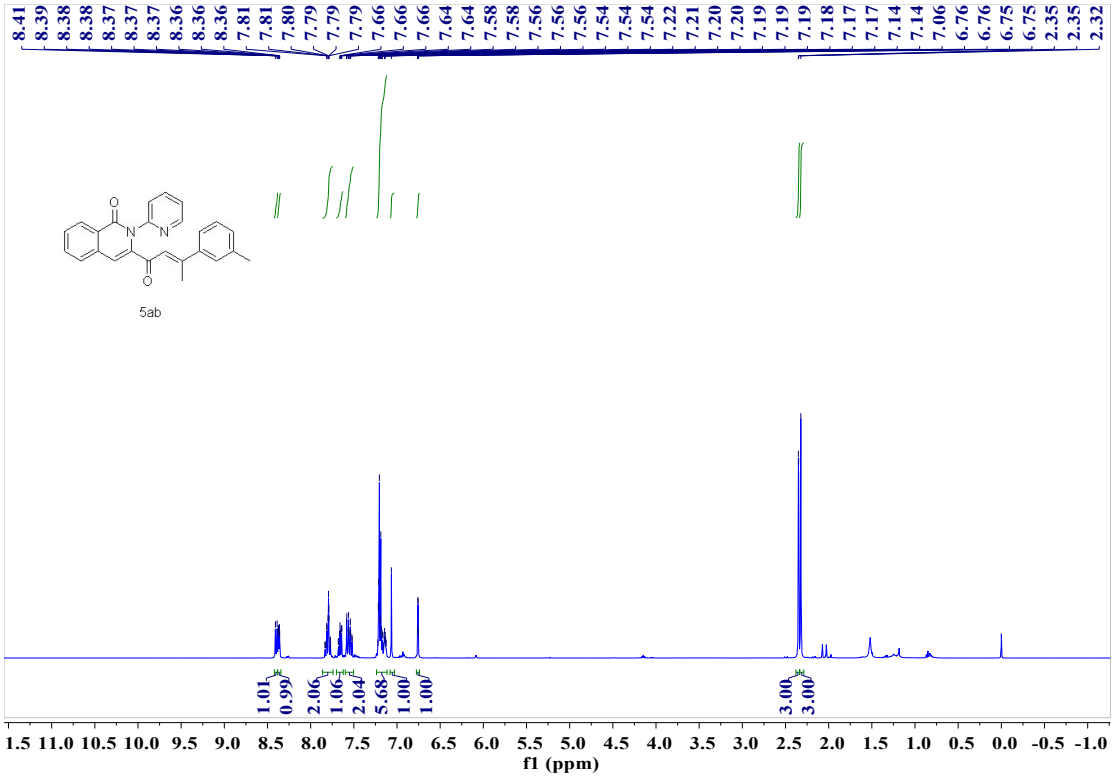
O
N
N
O
5ja
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-123.20
-123.21
-123.22
-123.23
f1 (ppm)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1.01
0.99
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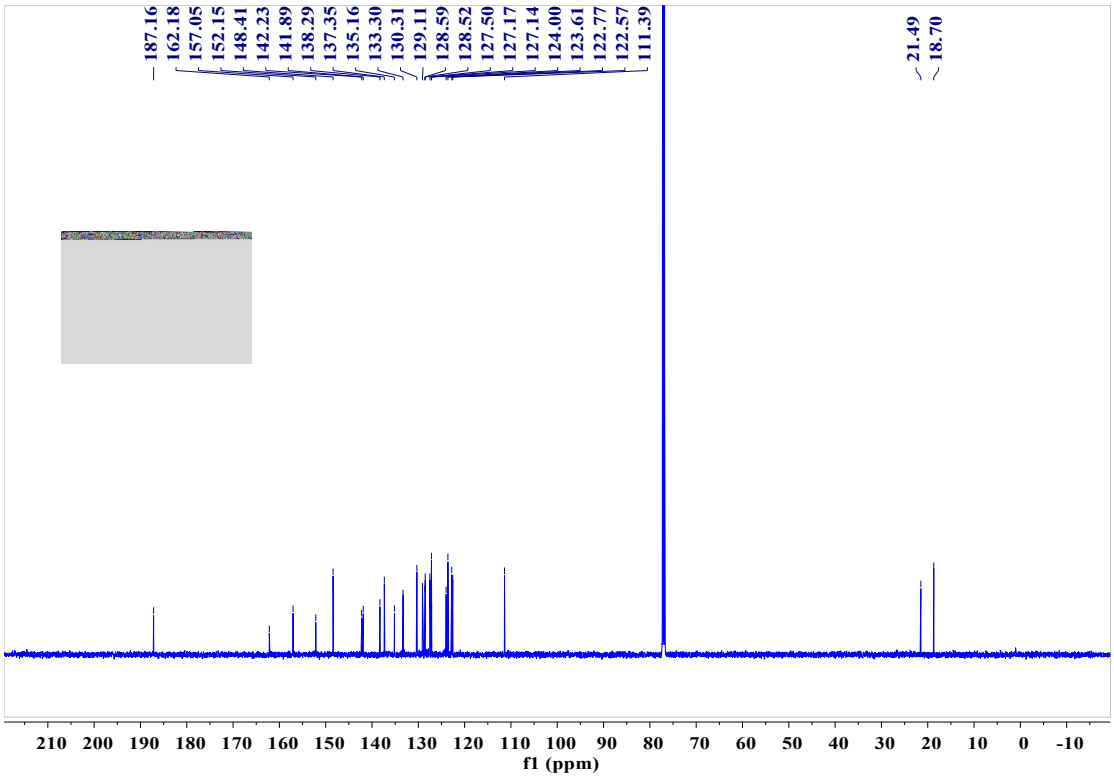
1.06
2.04
5.68
1.00
1.00
3.00
3.00
f1 (ppm)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157.05
152.15
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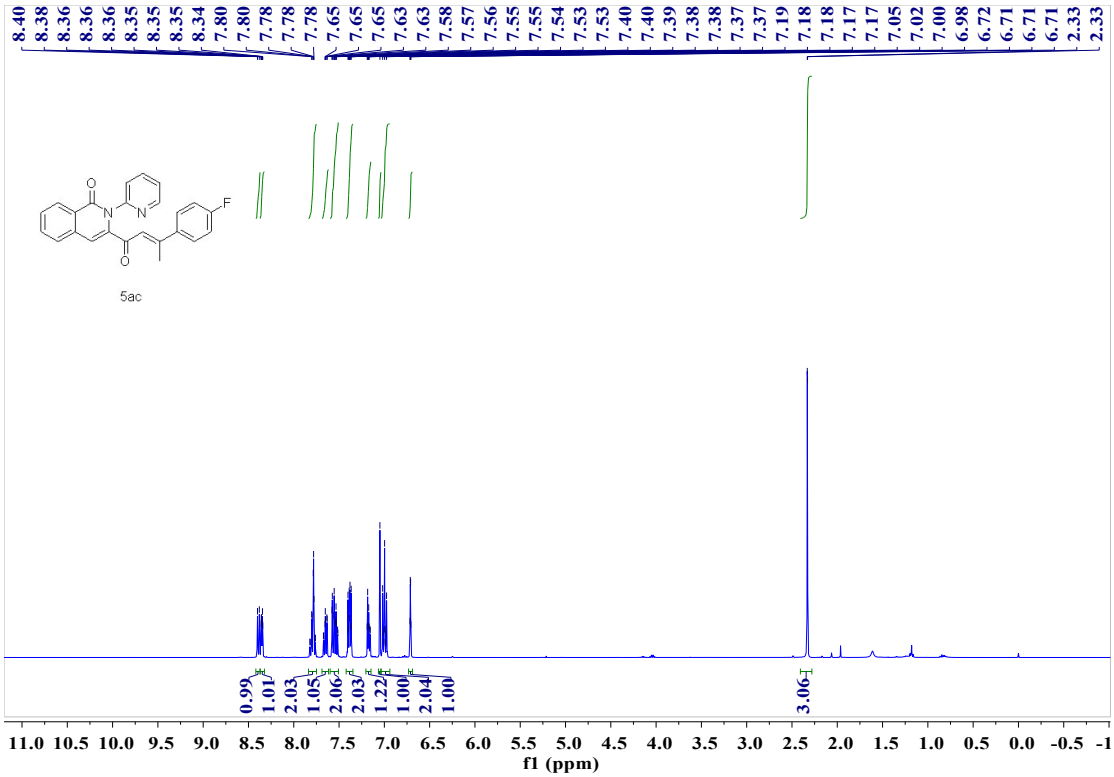
142.23
141.89
138.29
137.35
135.16
133.30
130.31
129.11
128.59
128.52
127.50
127.17
127.14
124.00
123.61
122.77
122.57
111.39
21.49
18.70
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.78
7.65
7.65
7.65
7.63
7.63
7.58
7.57
7.56
7.55
7.55
7.54
7.53
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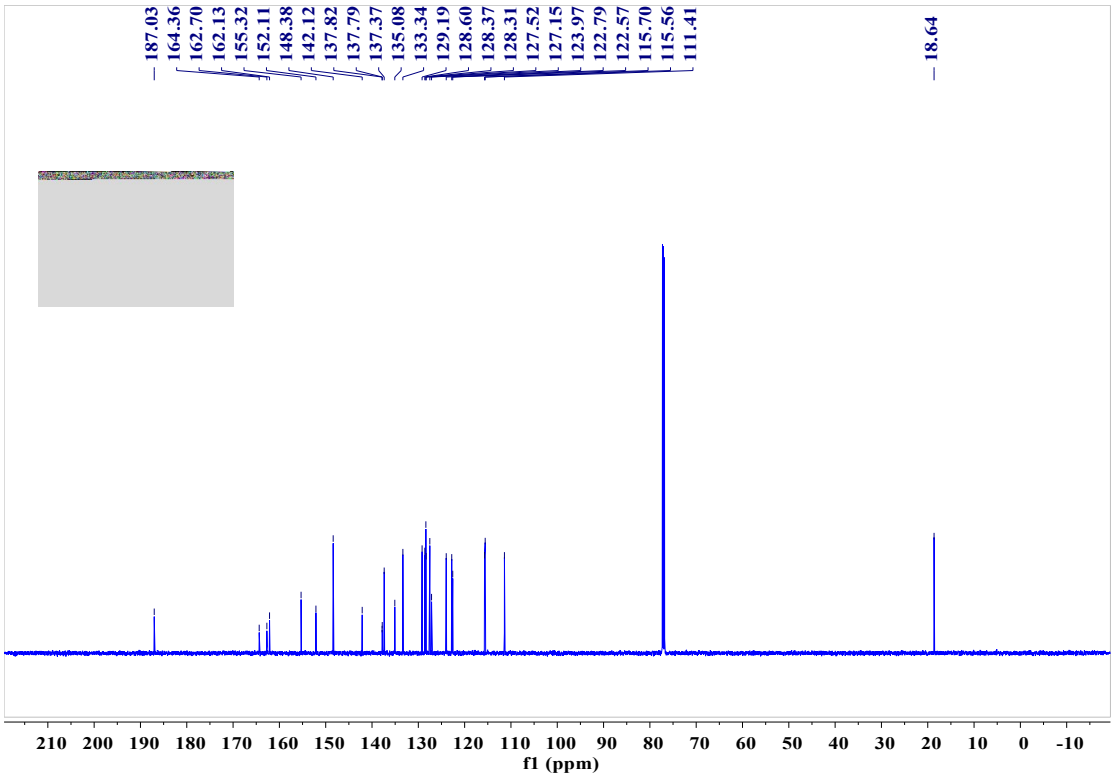
7.37
7.19
7.18
7.18
7.17
7.17
7.05
7.02
7.00
6.98
6.72
6.71
6.71
6.71
2.33
2.33
O
N
N
F
O
5ac
0.99
1.01
2.03
1.05
2.06
2.03
1.22
1.00
2.04
1.00
3.06
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)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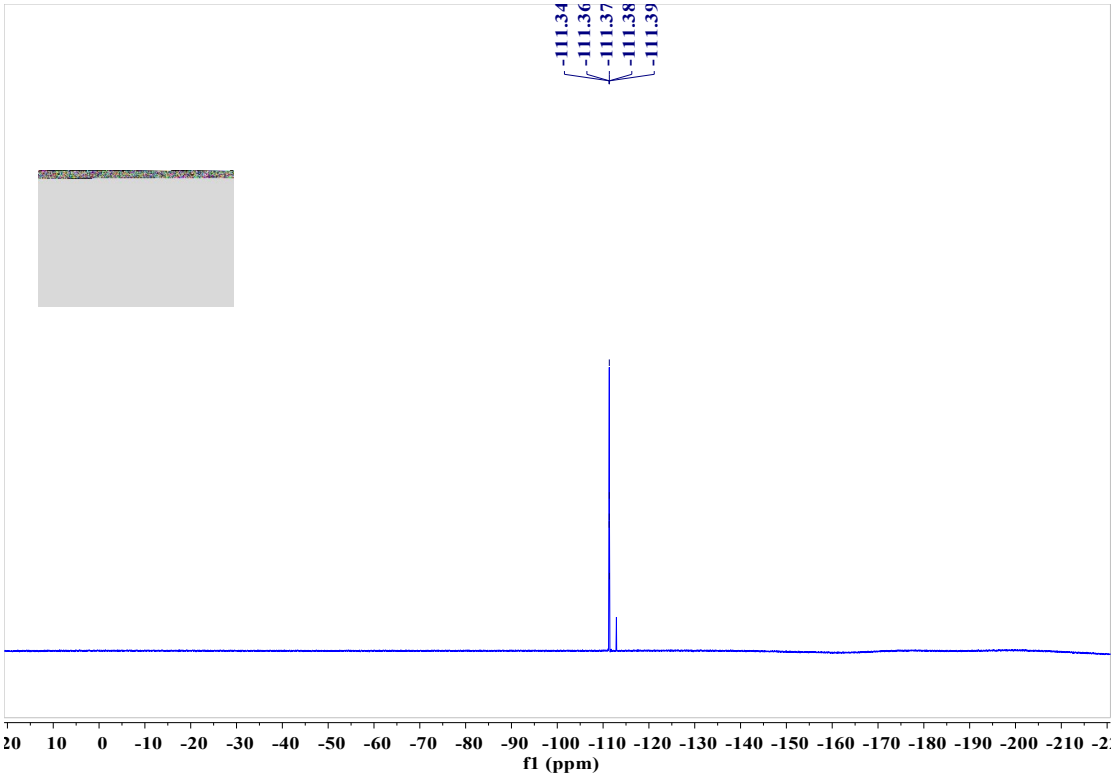
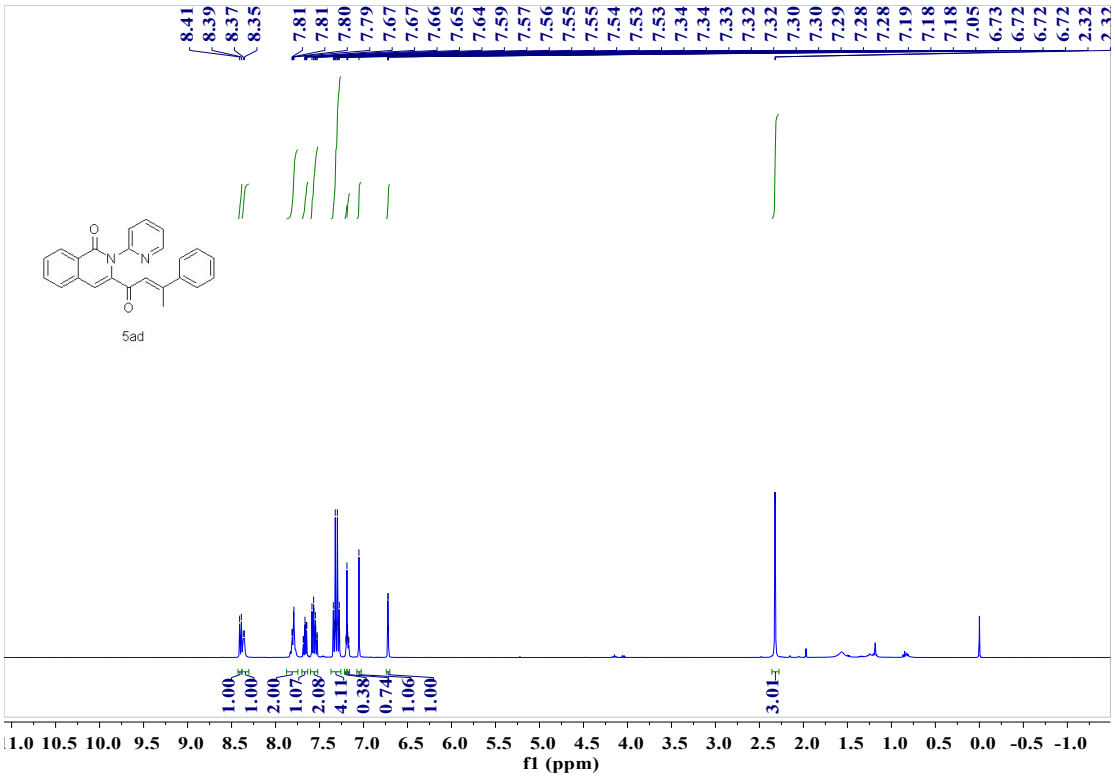
164.36
162.70
162.13
155.32
152.11
148.38
142.12
137.82
137.79
137.37
135.08
133.34
129.19
128.60
128.37
128.31
127.52
127.15
123.97
122.79
122.57
115.70
115.56
111.41
18.64
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-111.34
-111.36
-111.37
-111.38
-111.39
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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8.35
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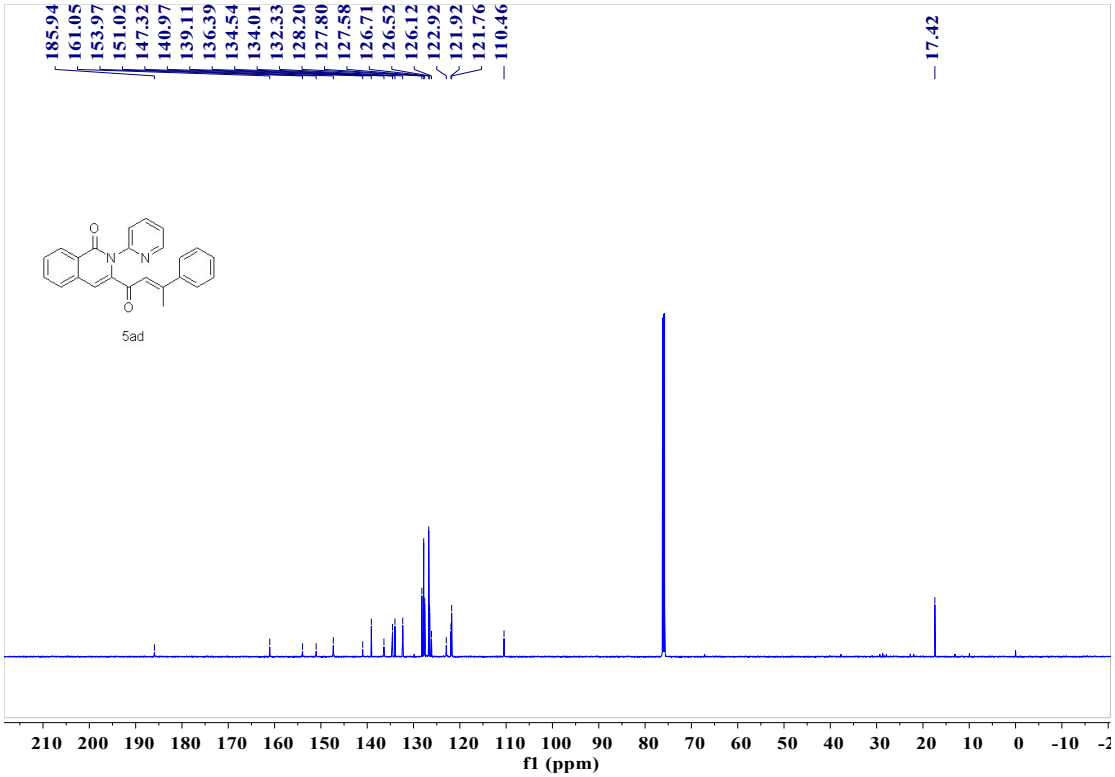
7.81
7.80
7.79
7.67
7.67
7.66
7.65
7.64
7.59
7.57
7.56
7.55
7.55
7.54
7.53
7.53
7.34
7.34
7.33
7.32
7.32
7.30
7.30
7.29
7.28
7.28
7.19
7.18
7.18
7.05
6.73
6.72
6.72
6.72
2.32
5ad
1.00
1.00
2.00
1.07
2.08
4.11
0.38
0.74
1.06
1.00
3.01
f1 (ppm)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161.05
153.97
151.02
147.32
140.97
139.11
136.39
134.54
134.01
132.33
128.20
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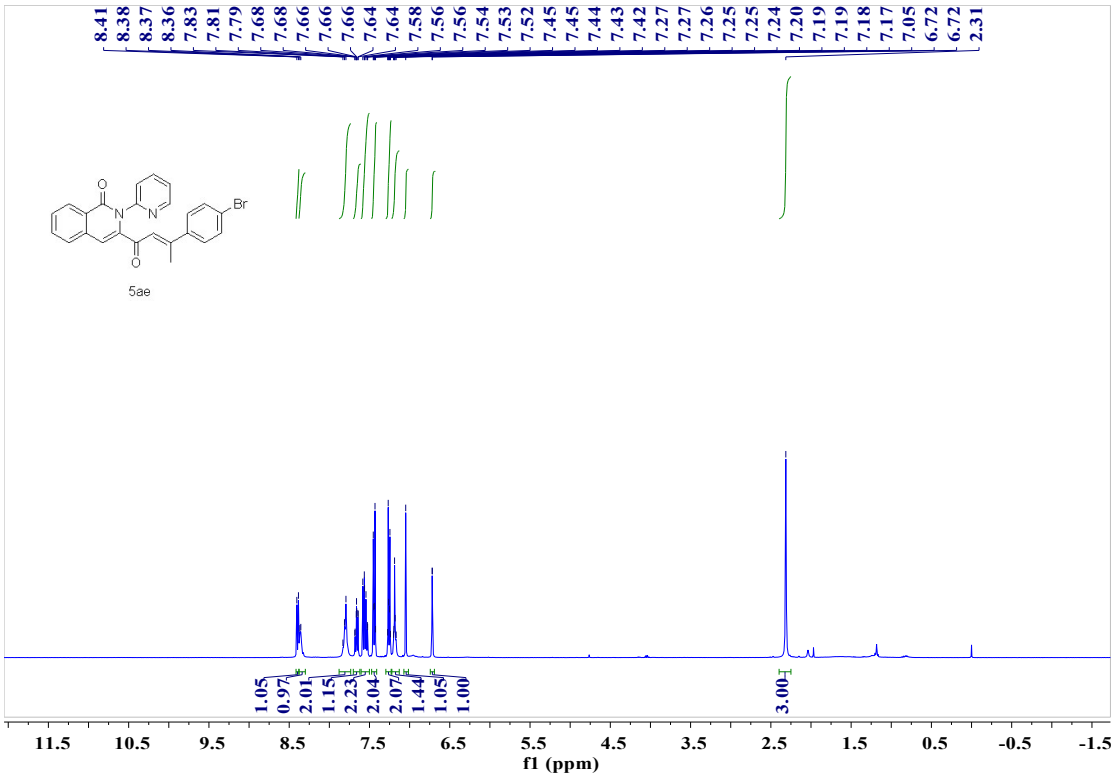
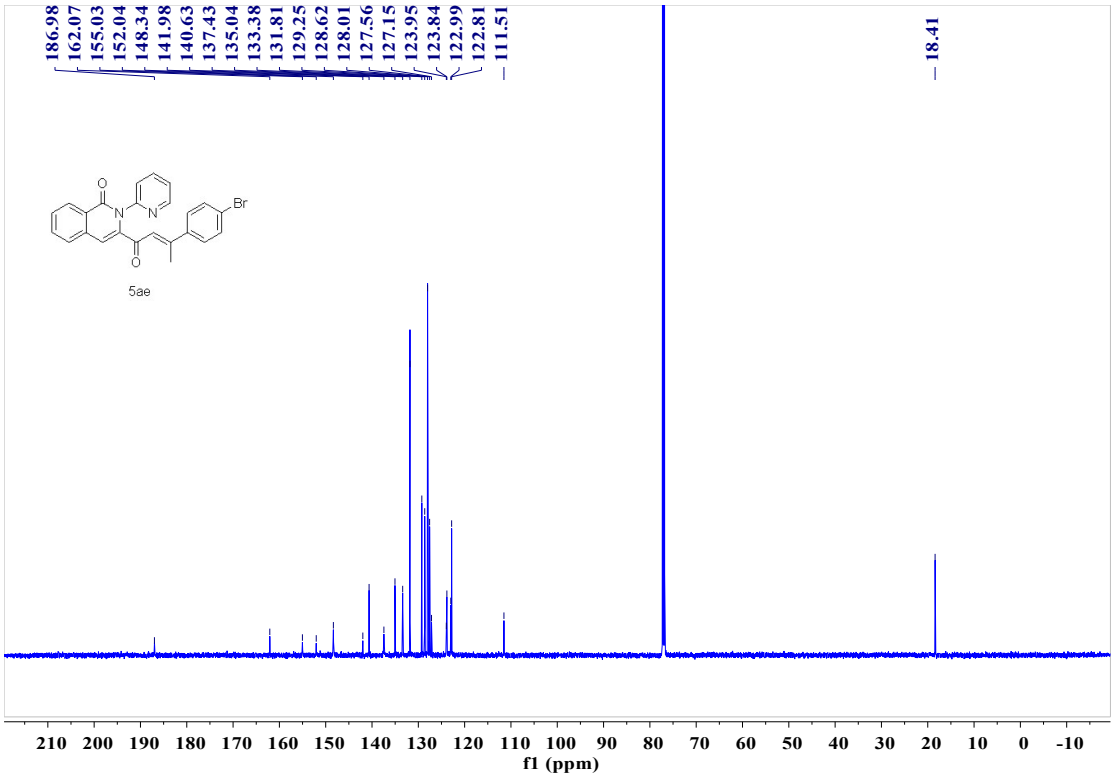
121.76
110.46
17.42
5ad
f1 (ppm)


8.41 8.38 8.37 8.36 7.83 7.81 7.79 7.68 7.68 7.66 7.66 7.66 7.64 7.64 7.58 7.56 7.56 7.54 7.53 7.52 7.45 7.45 7.44 7.43 7.42 7.27 7.27 7.26 7.25 7.25 7.24 7.20 7.19 7.19 7.18 7.17 7.05 6.72 6.72 2.31
Br
5ae
1.05 0.97 2.01 1.15 2.23 2.04 2.07 1.44 1.05 1.00
3.00
11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0.5 -1.5
f1 (ppm)


186.98 162.07 155.03 152.04 148.34 141.98 140.63 137.43 135.04 133.38 131.81 129.25 128.62 128.01 127.56 127.15 123.95 123.84 122.99 122.81 111.51
18.41
Br
5ae
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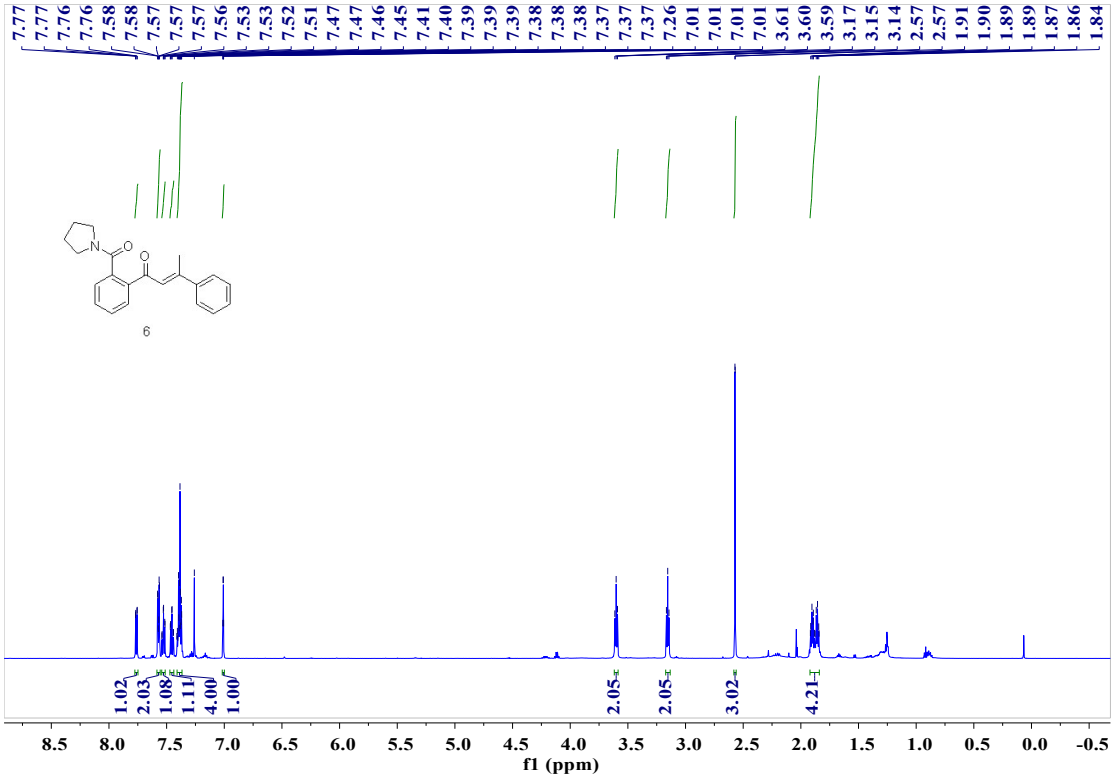
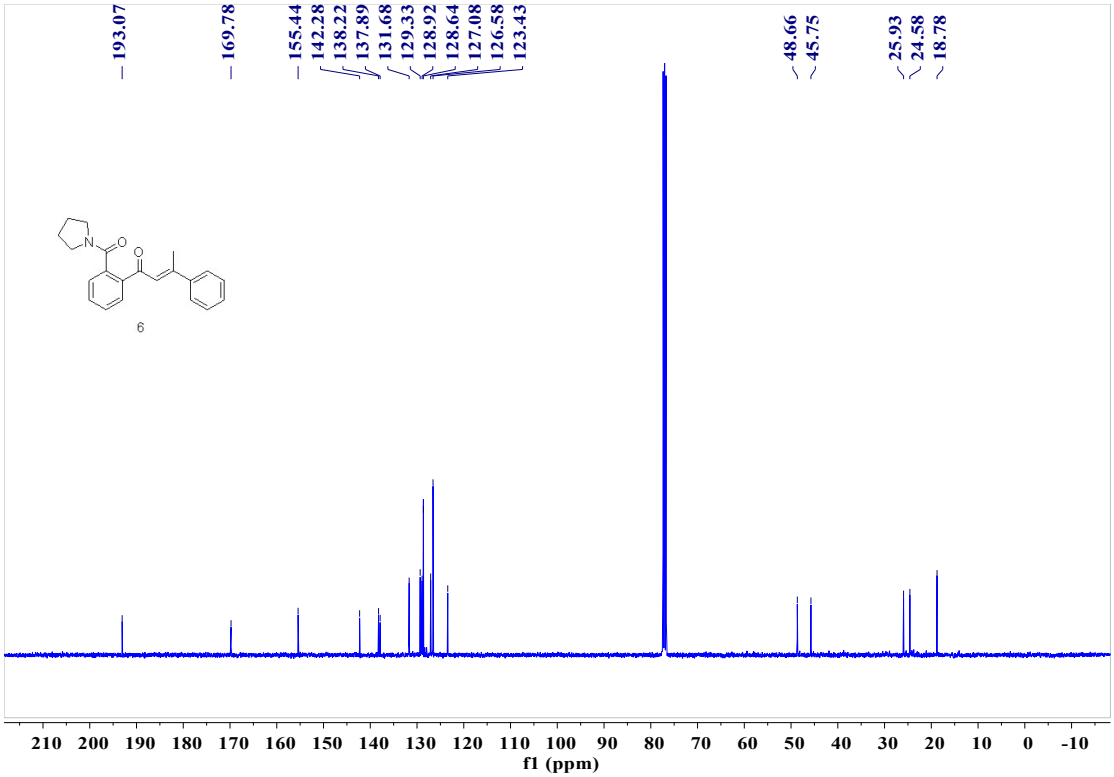
f1 (ppm)


7.77 7.77 7.76 7.76 7.58 7.58 7.57 7.57 7.57 7.56 7.53 7.53 7.52 7.51 7.47 7.47 7.46 7.45 7.41 7.40 7.39 7.39 7.39 7.38 7.38 7.38 7.37 7.37 7.37 7.26 7.01 7.01 7.01 7.01 3.61 3.60 3.59 3.17 3.15 3.14 2.57 2.57 1.91 1.90 1.89 1.89 1.87 1.86 1.84
6
1.02 2.03 1.08 1.11 4.00 1.00 2.05 2.05 3.02 4.21
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 -0.5
f1 (ppm)


193.07 169.78 155.44 142.28 138.22 137.89 131.68 129.33 128.92 128.64 127.08 126.58 123.43 48.66 45.75 25.93 24.58 18.78
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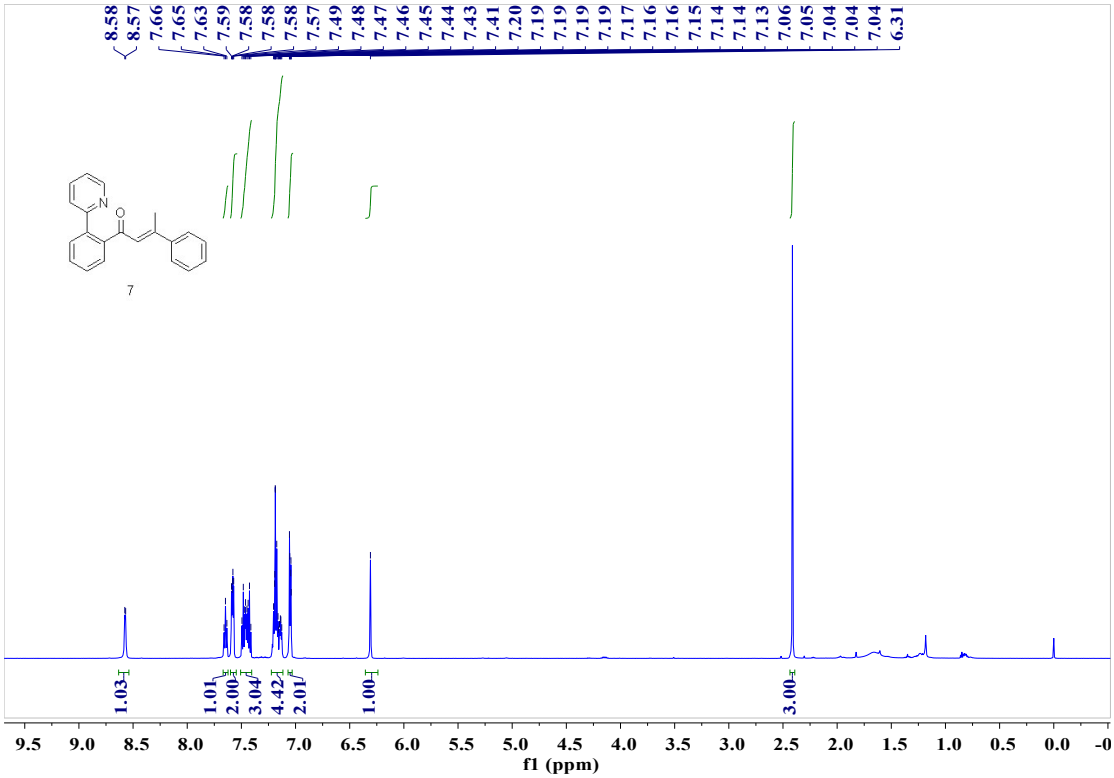
f1 (ppm)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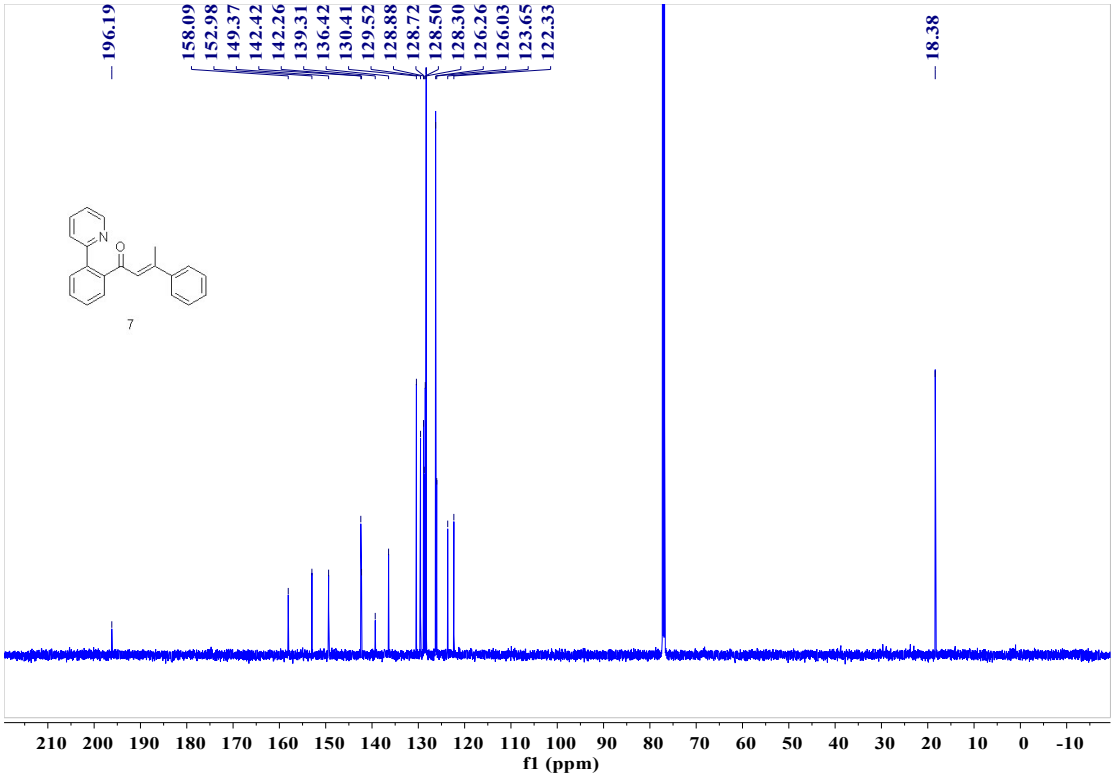
7.47
7.46
7.45
7.44
7.43
7.41
7.20
7.19
7.19
7.19
7.19
7.17
7.16
7.16
7.15
7.14
7.14
7.13
7.06
7.05
7.04
7.04
7.04
6.31
1.03
1.01
2.00
3.04
4.42
2.01
1.00
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)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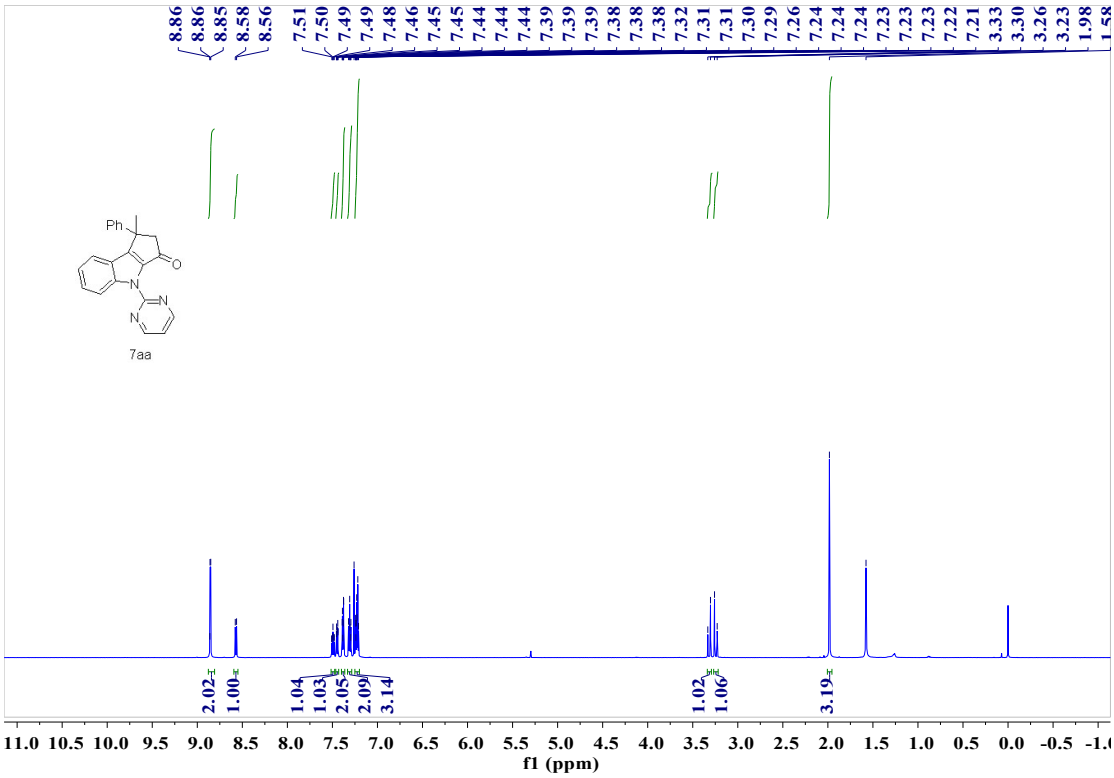
142.26
139.31
136.42
130.41
129.52
128.88
128.72
128.50
128.30
126.26
126.03
123.65
122.33
18.38
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.48
7.46
7.45
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7.44
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7.38
7.38
7.32
7.31
7.31
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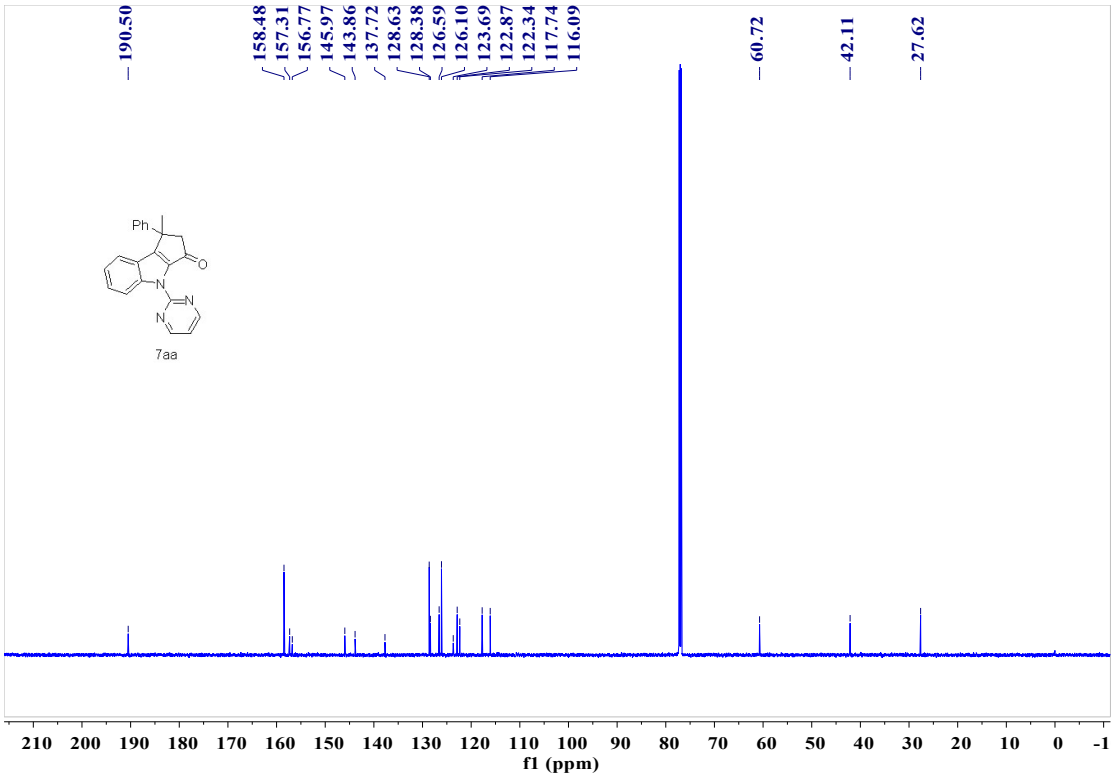
7.24
7.24
7.24
7.23
7.23
7.23
7.22
7.21
3.33
3.30
3.26
3.23
1.98
Ph
O
N
N
N
7aa
2.02
1.00
1.04
1.03
2.05
2.09
3.14
1.02
1.06
3.19
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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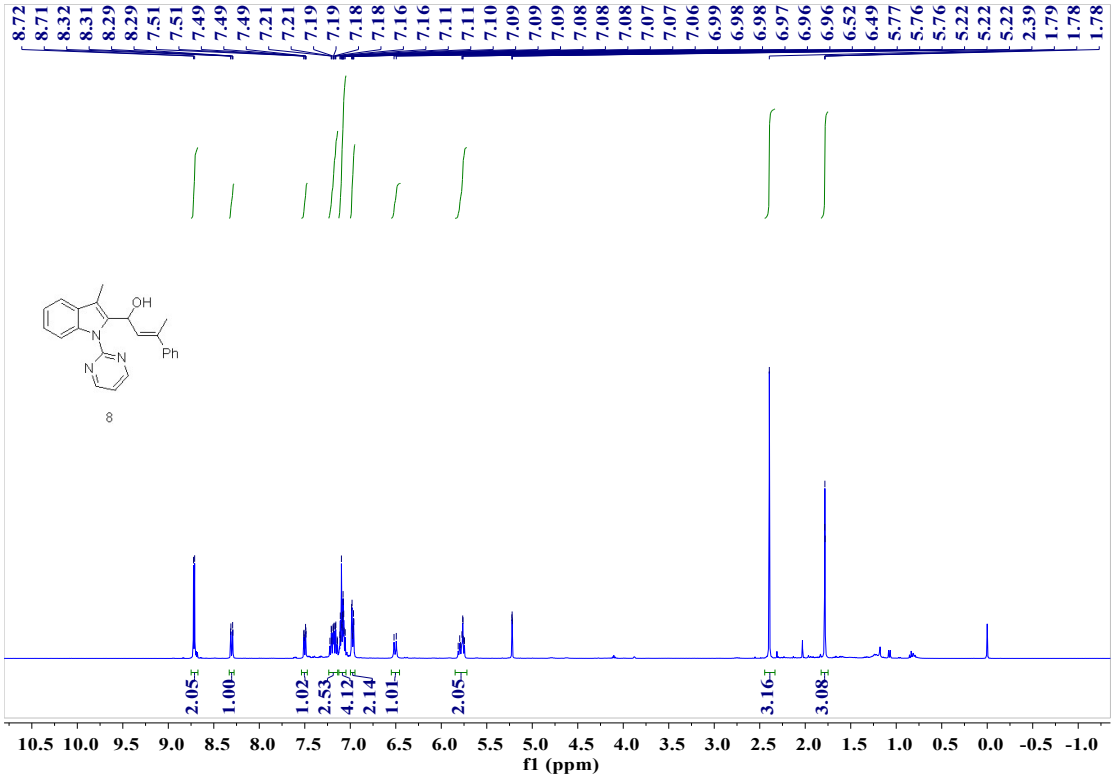
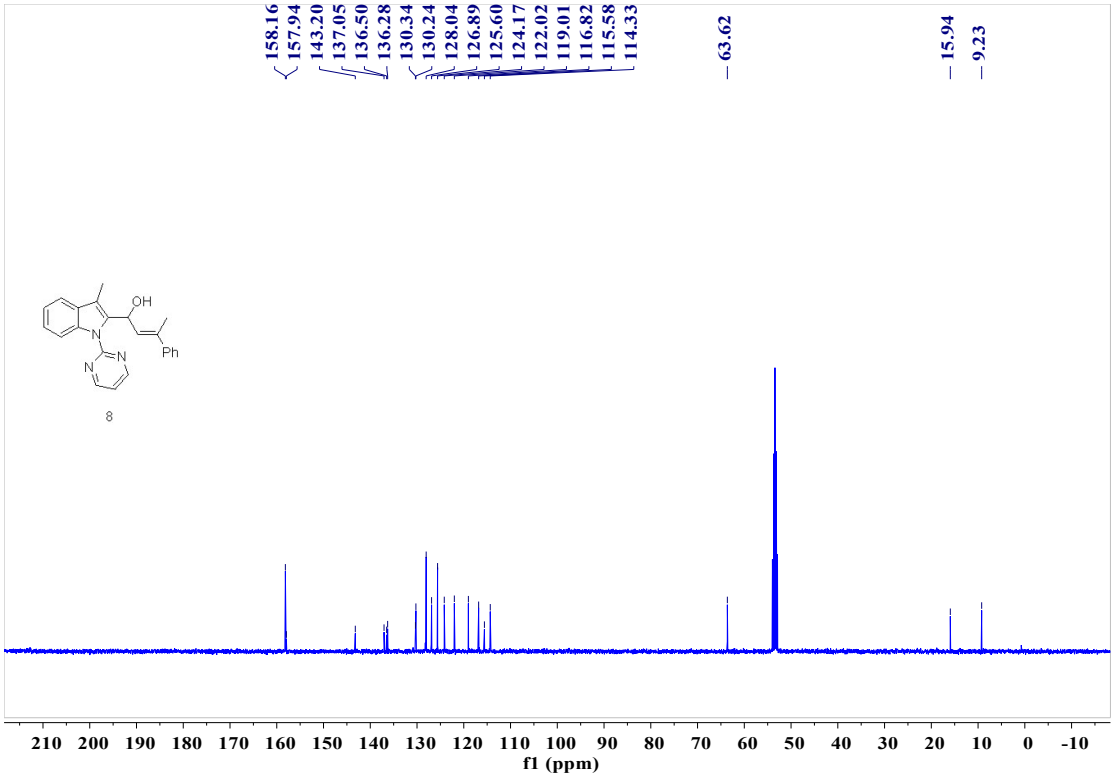
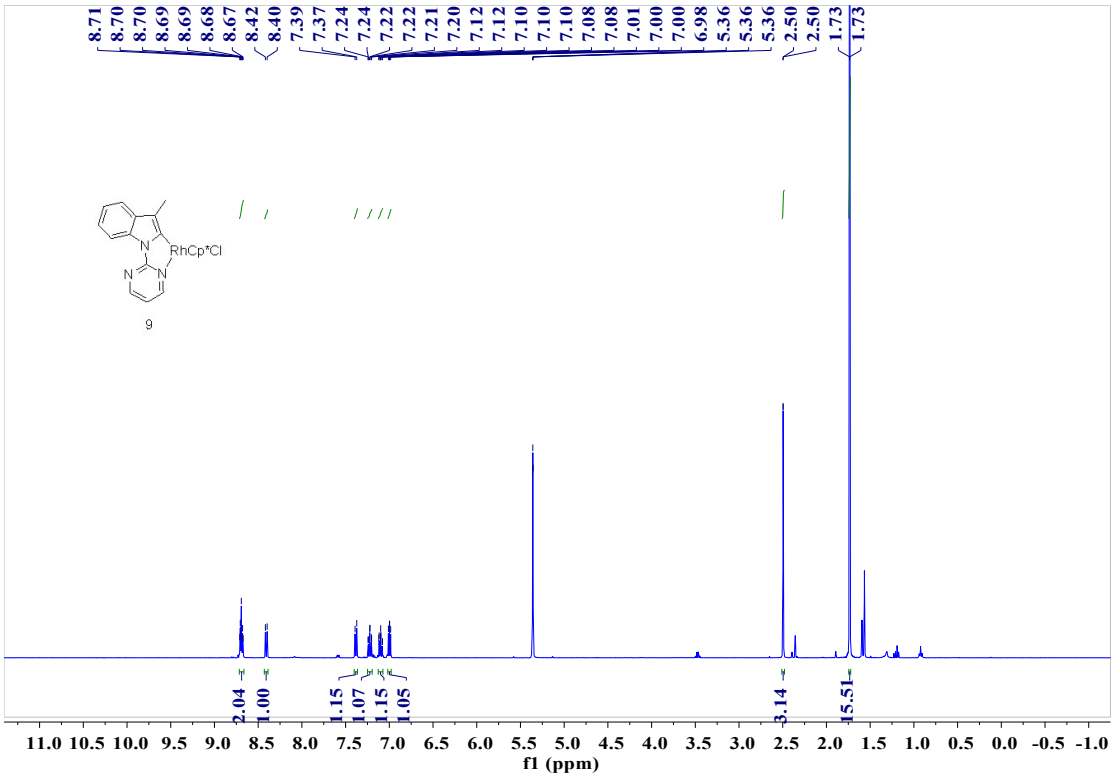
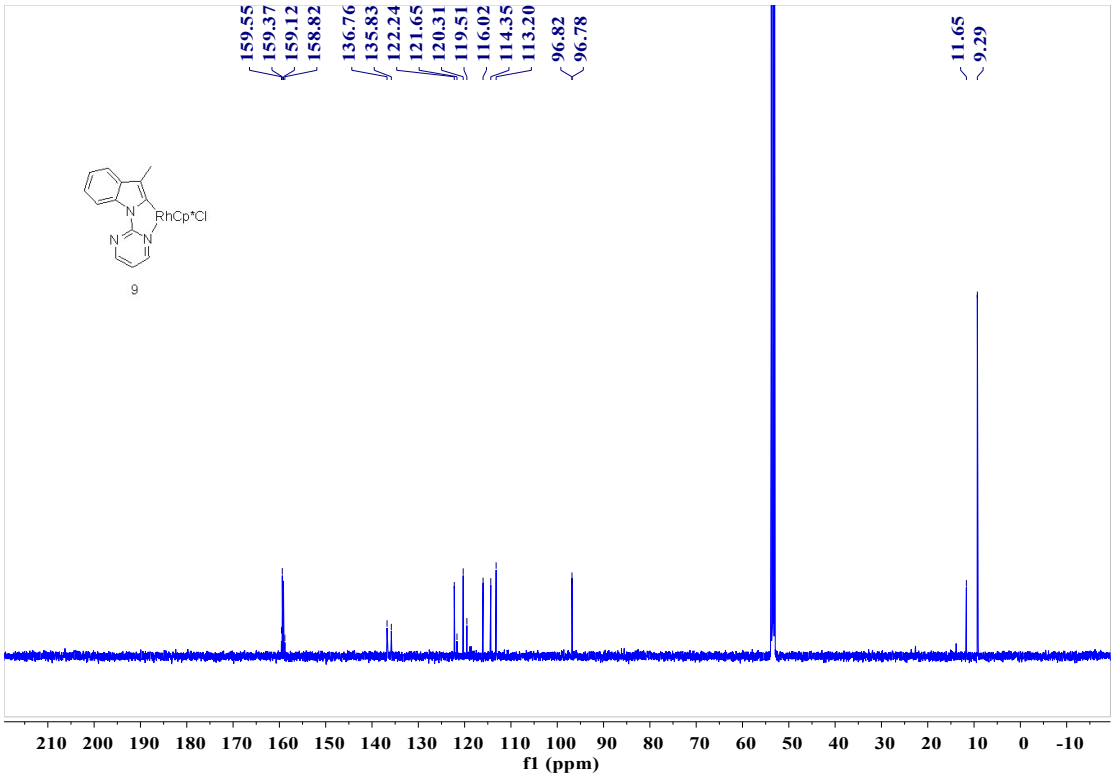
156.77
145.97
143.86
137.72
128.63
128.38
126.59
126.10
123.69
122.87
122.34
117.74
116.09
60.72
42.11
27.62
Ph
O
N
N
N
7aa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.72 8.71 8.32 8.31 8.29 8.29 7.51 7.51 7.49 7.49 7.49 7.21 7.21 7.19 7.19 7.18 7.18 7.16 7.16 7.11 7.11 7.10 7.09 7.09 7.09 7.08 7.08 7.08 7.07 7.07 7.06 6.99 6.98 6.98 6.97 6.96 6.96 6.52 6.49 5.77 5.76 5.76 5.22 5.22 5.22 2.39 1.79 1.78 1.78
OH
Ph
N
N
8
2.05 1.00 1.02 2.53 4.12 2.14 1.01 2.05 3.16 3.08
10.5 10.0 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 -0.5 -1.0
f1 (ppm)


158.16 157.94 143.20 137.05 136.50 136.28 130.34 130.24 128.04 126.89 125.60 124.17 122.02 119.01 116.82 115.58 114.33
63.62
15.94
9.23
OH
Ph
N
N
8
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.71 8.70 8.70 8.69 8.69 8.68 8.67 8.42 8.40 7.39 7.37 7.24 7.24 7.22 7.22 7.21 7.20 7.12 7.12 7.10 7.10 7.10 7.08 7.08 7.01 7.00 7.00 6.98 5.36 5.36 5.36 2.50 2.50 1.73 1.73
RhCp*Cl
9
2.04 1.00 1.15 1.07 1.15 1.05 3.14 15.51
11.0 10.5 10.0 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 -0.5 -1.0
f1 (ppm)


159.55 159.37 159.12 158.82 136.76 135.83 122.24 121.65 120.31 119.51 116.02 114.35 113.20 96.82 96.78 11.65 9.29
RhCp*Cl
9
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)