Supplementary Information (SI) for Organic Chemistry Frontiers.

Supporting Information

Rhodaelectro-catalyzed C–H activations directed by pharmacophores: enabling modification of bioactive compounds

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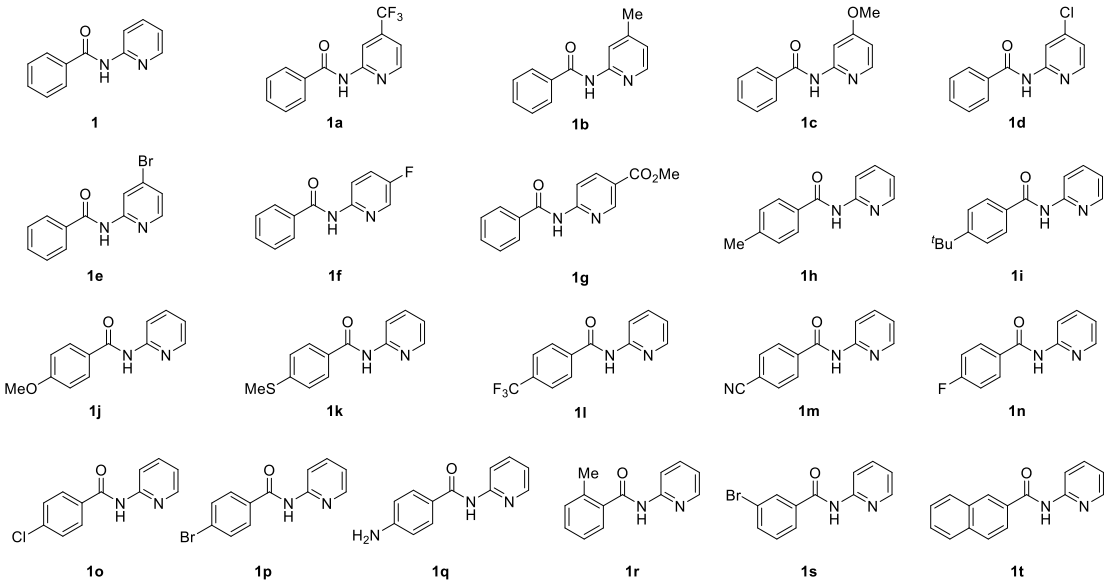
1. General Remarks

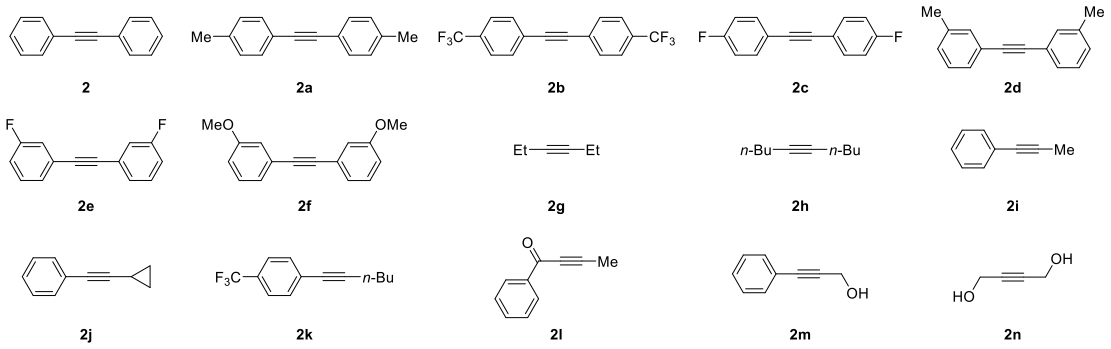
Unless otherwise noted, catalytic reactions were carried out in undivided electrochemical cells (10 mL) using pre-dried glassware. *N*-(pyridin-2-yl)benzamide **1**[1, 2, 9-14] and alkynes **2**[3-8] were prepared according to previously reported procedures. All reagents and solvents were purchased from commercial suppliers (Adamas-beta, Bidepharm, General Reagent) and used without further purification unless mentioned otherwise. Nickel foam (10 mm × 15 mm × 1.5 mm, 99.9%; obtained from Kunshan City Yushan town Wulife electronic material management department, China) and graphite felt electrodes (thickness 3.0 mm, Anhui Senrise Technologies, China) were connected using stainless steel adapters. The electrocatalytic reactions were conducted at constant current modes using a Mestek DP3005B as power supply. Thin-layer chromatography (TLC) was performed on 200 ± 50 μm glass-backed silica gel plates purchased from Shanghai Titan Technology Co., Ltd., China. Column chromatography was carried out on silica gel (200–300 mesh) purchased from Yantai Xinnuo Chemical Co., Ltd., China. NMR spectra were recorded on Bruker Avance NEO 600 instrument. Chemical shifts (δ) are given in ppm relative to the solvent residual peak, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, bs = broad singlet), and coupling constants (J) are in Hertz (Hz). All FT-IR spectra were recorded on a PerkinElmer L1600300 Spectrum TWO LiTa (UK). High revolution mass spectra (HRMS) were obtained on an Agilent 6545 Q-TOF. Melting point ranges were taken with a Melting Point Apparatus X-5 (Beijing Unitedvision Technology Co., Ltd.).

2. Synthesis of Substrates

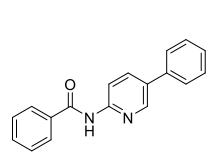
The amide **1q** was obtained from commercial sources. The amides **1**,[1] **1a-h**,[1] **1j-k,** [1] **1m**,[1] **1s-t**,[1] **1i**,[2] **1l**,[2] **1n-p**,[2] **1r**[2] were synthesized according to literature procedures. The characterization data were consistent with those reported.



The alkynes **2, 2g, 2h, 2i, 2m, 2n** were obtained from commercial sources. Alkynes **2a-2c**,[3] **2d**,[4] **2e**,[3] **2f**,[5] **2j**,[6] **2k**,[7] **2l**[8] were synthesized according to literature procedures. The characterization data were consistent with those reported.



The amide **BC-7** was obtained from commercial sources. The amides **BC-1**,[9] **BC-2**, [10] **BC-3**,[11] **BC-4**,[12] **BC-5**,[13] **BC-6**,[13] **BC-8**[14] were synthesized according to literature procedures. The characterization data were consistent with those reported.



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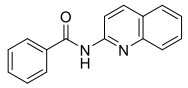

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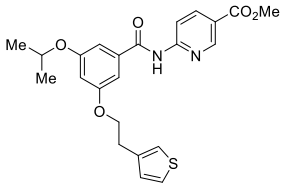

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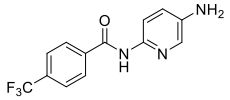

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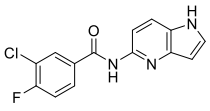

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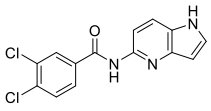

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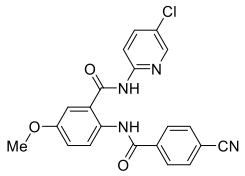

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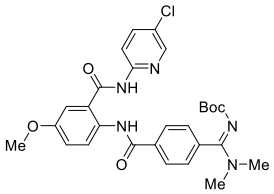
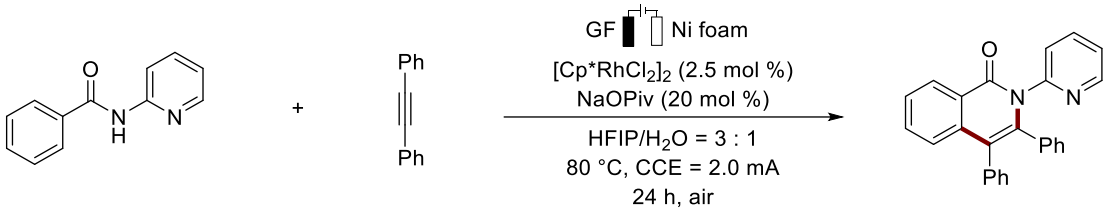


BC-8

3. Optimization of Reaction Conditions



1 **2** **3**

Entry	Variation from standard conditions	**3** [%]
1	None	90
2	16 h	82
3	CsF in place of NaOPiv	trace
4	HOPiv in place of NaOPiv	trace
5	GF(+) / Pt(-)	23
6	RVC(+) / Ni foam(-)	trace
7	RVC(+) / Pt(-)	trace
8	TFE / H_2O	trace
9	No electricity	NR
10	$[RuCl_2(\rho\text{-cymene})]_2$ in place of $[Cp^*RhCl_2]_2$	NR
11	$Pd(OAc)_2$ in place of $[Cp^*RhCl_2]_2$	NR

[a] Undivided cell, GF anode, Ni foam cathode, constant current electrolysis = 2.0 mA, **1** (0.40 mmol), **2** (0.60 mmol), NaOPiv (20 mol %), $[Cp^*RhCl_2]_2$ (2.5 mol %), solvent (4.0 mL), under air, 24 h; yields of isolated product.

4. General Procedure for Electrooxidative C–H Annulation

The electrocatalysis was carried out in an undivided cell with a graphite felt (GF) anode (10 mm × 15 mm × 3.0 mm) and a Nickel foam (Ni foam) cathode (10 mm × 15 mm × 1.5 mm). The cell was charged with *N*-(pyridin-2-yl)benzamide **1** (0.40 mmol), alkyne **2** (0.60 mmol, 1.50 equiv), NaOPiv (9.93 mg, 0.08 mmol, 20 mol %), $[Cp^*RhCl_2]_2$ (6.18 mg, 0.01 mmol, 2.5 mol %) and a HFIP/H_2O solvent mixture (3/1, 4.0 mL). Electrocatalysis was performed at 80 °C with a constant current of 2.0 mA maintained for 24 h. The electrodes were washed with dichloromethane (3 × 4.0 mL) in an ultrasonic bath. The combined mixtures were filtered and concentrated under reduced pressure at 50 °C. The residue was purified by chromatography on silica gel to afford the corresponding products **3**.

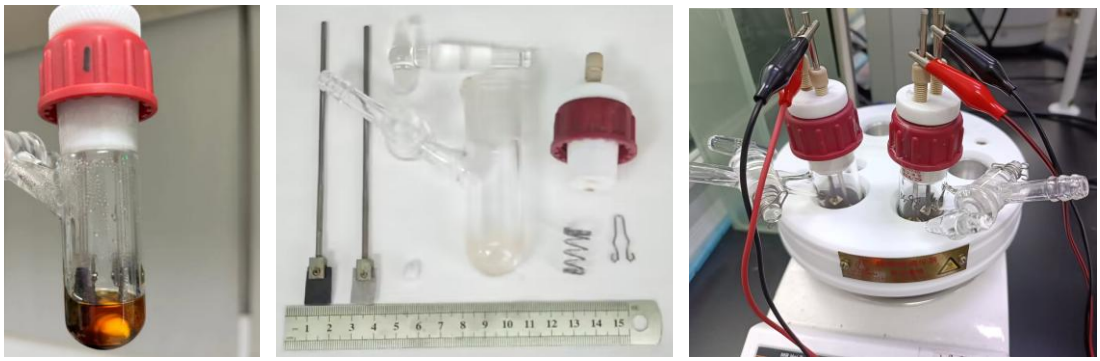
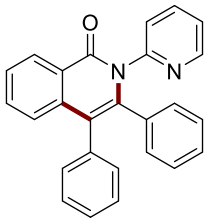


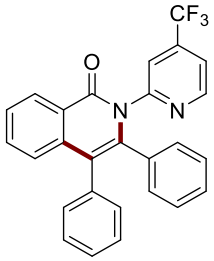
Figure SI-1. Setup diagram of the electrolysis.

Gram-scale: The electrocatalysis was carried out in an undivided cell under air with a GF anode (25 mm × 50 mm × 3.0 mm) and a Ni foam cathode (25 mm × 50 mm × 1.5 mm). The cell was charged with *N*-(pyridin-2-yl)benzamide **1** (793 mg, 4.0 mmol), alkyne **2** (1.07 g, 6.0 mmol, 1 .50 equiv), NaOPiv (99.3 mg, 0.80 mmol, 20 mol %), $[Cp^*RhCl_2]_2$ (61.8 mg, 0.10 mmol, 2.5 mol %) and HFIP/H_2O solvent mixture (3/1, 32 mL). Electrocatalysis was performed at 80 °C with a constant current of 8.0 mA maintained for 72 h. The electrodes were washed with dichloromethane (3 × 8.0 mL) in an ultrasonic bath. The combined mixtures were filtered and concentrated under reduced pressure at 50 °C. The residue was purified by chromatography on silica gel to afford product **3** (1.43 g, 95%).

5. Characterization Data of Products

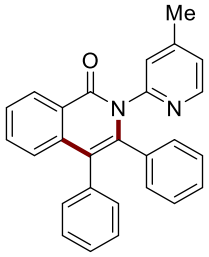


3,4-Diphenyl-2-(pyridin-2-yl)isoquinolin-1(2*H*)-one (3): The general procedure was followed using **1** (79.3 mg, 0.40 mmol) and **2** (107 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **3** (135 mg, 90%) as colorless solid. The NMR data is identical to that previously reported.[15] **M.p.** = 250–251 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.57 (d, J = 7.8 Hz, 1H), 8.40 (d, J = 6.0 Hz, 1H), 7.62–7.59 (m, 2H), 7.53 (t, J = 7.5 Hz, 1H), 7.27 (d, J = 8.1 Hz, 1H), 7.24–7.20 (m, 3H), 7.19 (d, J = 6.3 Hz, 1H), 7.17–7.13 (m, 2H), 7.09 (t, J = 6.0 Hz, 1H), 7.02–6.85 (m, 5H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 162.8 (C_q), 152.8 (C_q), 149.2 (CH), 140.2 (C_q), 137.9 (C_q), 137.7 (CH), 136.2 (C_q), 134.4 (C_q), 132.9 (CH), 131.7 (CH), 131.7 (CH), 128.3 (CH), 128.1 (CH), 128.1 (CH), 127.4 (CH), 127.4 (CH), 127.4 (CH), 127.2 (CH), 127.2 (CH), 127.1 (CH), 127.1 (CH), 125.8 (CH), 125.7 (C_q), 125.1 (CH), 123.0 (CH), 119.1 (C_q). **IR** (KBr): 3060, 1661, 1591, 1468, 1434, 1322, 1157, 997, 778, 754, 700 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 375 (100) $[M+H]^+$, 397 (4) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{26}H_{18}N_2O$ $[M+H]^+$ 375.1492, found 375.1492.

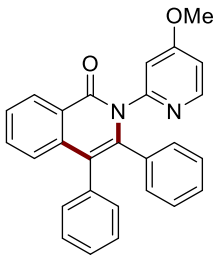


3,4-Diphenyl-2-(4-(trifluoromethyl)pyridin-2-yl)isoquinolin-1(2*H*)-one (4): The general procedure was followed using **1a** (107 mg, 0.40 mmol) and **2** (107 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 1:1) yielded **4** (168 mg, 95%) as yellow solid. **M.p.** = 230–231 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.57–8.55 (m, 2H), 7.62 (t, J = 7.8 Hz, 1H), 7.55 (t, J = 7.6 Hz, 1H), 7.46 (s, 1H),

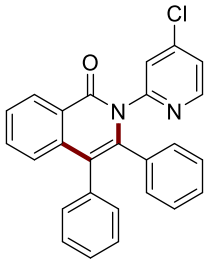
7.29 (d, J = 5.4 Hz, 1H), 7.27 (d, J = 8.2 Hz, 1 H), 7.25–7.22 (m, 2 H), 7.19 (d, J = 7 .2 Hz, 1 H), 7.18–7.14 (m, 2H), 6.97–6.89 (m, 5H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 162.7 (C_q), 154.0 (C_q), 150.2 (CH), 140.0 (q, $^2J_{C–F}$ = 34.5 Hz, C_q), 139.7 (C_q), 137.9 (C_q), 135.9 (C_q), 134.1 (C_q), 133.2 (CH), 131.7 (CH), 131.7 (CH), 128.3 (CH), 128.2 (CH), 128.2 (CH), 127.8 (CH), 127.5 (CH), 127.5 (CH), 127.4 (CH), 127.4 (CH), 127.2 (CH), 126.0 (CH), 125.5 (C_q), 122.3 (q, $^1J_{C–F}$ = 271.5 Hz, C_q), 121.4 (q, $^3J_{C–F}$ = 3.7 Hz, CH), 119.6 (CH), 119.6 (C_q), 118.7 (q, $^3J_{C–F}$ = 3.5 Hz, CH). **^{19}F NMR** (564 MHz, $CDCl_3$) δ = - 64.77 (s). **IR** (KBr): 3030, 1659, 1592, 1556, 1412, 1336, 1083, 994, 781, 699 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 443 (100) $[M+H]^+$, 465 (6) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{27}H_{17}F_3N_2O$ $[M+H]^+$ 443.1371, found 443.1366.



2-(4-Methylpyridin-2-yl)-3,4-diphenylisoquinolin-1(2*H*)-one (5): The general procedure was followed using **1b** (84.8 mg, 0.40 mmol) and **2** (107 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **5** (108 mg, 70%) as colorless solid. **M.p.** = 233–234 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.56 (dd, J = 8.0 Hz, 1.5Hz, 1 H), 8.23 (d, J = 5.4 Hz, 1 H), 7.58 (t, J = 7.8 Hz, 1 H), 7.52 (t, J = 7.2 Hz, 1 H), 7.25 (d, J = 8.4 Hz, 1 H), 7.23–7.20 (m, 2H), 7.18–7.12 (m, 3H), 7.11–7.01 (m, 2H), 6.96–6.87 (m, 5H), 2.24 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 162.8 (C_q), 152.8 (C_q), 149.1 (CH), 148.8 (C_q), 140.3 (C_q), 137.9 (C_q), 136.3 (C_q), 134.5 (C_q), 132.8 (CH), 131.7 (CH), 131.7 (CH), 128.2 (CH), 128.1 (CH), 128.1 (CH), 128.1 (CH), 127.4 (CH), 127.4 (CH), 127.1 (CH), 127.0 (CH), 126.9 (CH), 126.9 (CH), 125.7 (CH), 125.7 (CH), 125.7 (C_q), 124.1 (CH), 119.0 (C_q), 20.9 (CH_3). **IR** (KBr): 3054, 3022, 1656, 1605, 1479, 1442, 1331, 998, 785, 704 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 389 (100) $[M+H]^+$, 411(20) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{27}H_{20}N_2O$ $[M+H]^+$ 389.1650, found 389.1648.

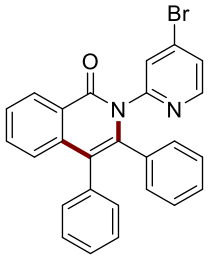


2-(4-Methoxypyridin-2-yl)-3,4-diphenylisoquinolin-1(2*H*)-one (6): The general procedure was followed using **1c** (91.2 mg, 0.40 mmol) and **2** (107 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **6** (114 mg, 71%) as colorless solid. **M.p.** = 252–253 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.56 (dd, J = 8.0, 1.5 Hz, 1H), 8.19 (d, J = 5.8 Hz, 1H), 7.58 (ddd, J = 8.3, 7.1, 1.5 Hz, 1H), 7.52 (ddd, J = 8.0, 7.1, 1.2 Hz, 1H), 7.24 (dd, J = 8.2, 1.2 Hz, 1H), 7.23–7.19 (m, 2H), 7.17 (d, J = 7.2 Hz, 1H), 7.15–7.12 (m, 2H), 7.11–6.88 (m, 5H), 6.71 (d, J = 2.3 Hz, 1H), 6.61 (dd, J = 5.8, 2.3 Hz, 1H), 3.72 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 167.0 (C_q), 162.6 (C_q), 154.2 (C_q), 149.8 (CH), 140.1 (C_q), 137.9 (C_q), 136.3 (C_q), 134.4 (C_q), 132.8 (CH), 131.7 (CH), 131.7 (CH), 128.3 (CH), 128.3 (CH), 128.1 (CH), 127.5 (CH), 127.5 (CH), 127.2 (CH), 127.2 (CH), 127.0 (CH), 127.0 (CH), 125.8 (CH), 125.8 (CH), 125.7 (C_q), 119.0 (C_q), 111.0 (CH), 109.9 (CH), 55.5 (CH_3). **IR** (KBr): 3062, 2975, 1651, 1590, 1445, 1335, 1273, 1029, 777, 699 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 405 (100) $[M+H]^+$, 427(13) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{27}H_{20}N_2O_2$ $[M+H]^+$ 405.1600, found 405.1598.

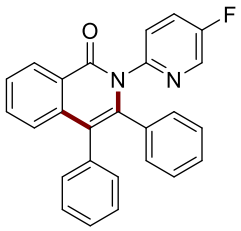


2-(4-Chloropyridin-2-yl)-3,4-diphenylisoquinolin-1(2*H*)-one (7): The general procedure was followed using **1d** (92.8 mg, 0.40 mmol) and **2** (107 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **7** (147 mg, 90%) as colorless solid. **M.p.** = 209–210 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.56 (dd, J = 8.2, 1.5 Hz, 1H), 8.27 (d, J = 5.4 Hz, 1H), 7.61 (ddd, J = 8.2, 7.1, 1.5 Hz, 1H), 7.55 (ddd,

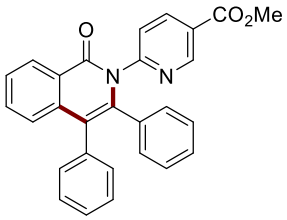
J = 8.2, 7.1, 1.5 Hz, 1H), 7.29 (d, J = 1.8 Hz, 1H), 7.27 (d, J = 7.1, 1.2 Hz, 1H), 7.25–7.22 (m, 2H), 7.20 (d, J = 7.1 Hz, 1H), 7.18–7.13 (m, 2H), 7.10 (dd, J = 5.4, 1.8 Hz, 1H), 7.04–6.90 (m, 5H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 162.7 (C_q), 153.8 (C_q), 149.6 (CH), 145.1 (C_q), 139.8 (C_q), 137.9 (C_q), 136.0 (C_q), 134.1 (C_q), 133.1 (CH), 131.7 (CH), 131.7 (CH), 128.3 (CH), 128.2 (CH), 128.2 (CH), 127.7 (CH), 127.4 (CH), 127.4 (CH), 127.3 (CH), 127.3 (CH), 127.2 (CH), 127.2 (CH), 125.9 (CH), 125.7 (CH), 125.5 (C_q), 123.5 (CH), 119.4 (C_q). **IR** (KBr): 3059, 1659, 1574, 1479, 1392, 1334, 829, 779, 725, 700 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 409 (100) $[M+H]^+$, 431(71) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{26}H_{17}{}^{35}ClN_2O$ $[M+H]^+$ 409.1103, found 409.1102.



2-(4-Bromopyridin-2-yl)-3,4-diphenylisoquinolin-1(2*H*)-one (8): The general procedure was followed using **1e** (111 mg, 0.40 mmol) and **2** (107 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **8** (133 mg, 74%) as yellowish solid. **M.p.** = 214–215 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.56 (dd, J = 7.8, 1.2 Hz, 1H), 8.19 (d, J = 5.3 Hz, 1H), 7.61 (ddd, J = 8.2, 7.1, 1.5 Hz, 1H), 7.54 (ddd, J = 8.2, 7.8, 1.2 Hz, 1H), 7.44 (s, 1H), 7.27 (d, J = 7.1, 1.5 Hz, 1H), 7.26–7.21 (m, 3H), 7.20 (d, J = 7.3 Hz, 1H), 7.18–7.13 (m, 2H), 7.05–6.90 (m, 5H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 162.7 (C_q), 153.5 (C_q), 149.5 (CH), 139.8 (C_q), 137.9 (C_q), 136.0 (C_q), 134.1 (C_q), 133.5 (C_q), 133.1 (CH), 131.7 (CH), 131.7 (CH), 128.6 (CH), 128.3 (CH), 128.2 (CH), 128.2 (CH), 127.7 (CH), 127.4 (CH), 127.4 (CH), 127.3 (CH), 127.3 (CH), 127.2 (CH), 127.2 (CH), 126.5 (CH), 125.9 (CH), 125.5 (C_q), 119.5 (C_q). **IR** (KBr): 3080, 1657, 1564, 1478, 1386, 1335, 1033, 780, 755, 699 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 453 (100) $[M+H]^+$, 475(78) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{26}H_{17}{}^{79}BrN_2O$ $[M+H]^+$ 453.0596, found 453.0597.

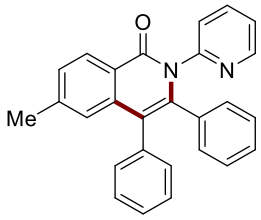


2-(5-Fluoropyridin-2-yl)-3,4-diphenylisoquinolin-1(2*H*)-one (9): The general procedure was followed using **1f** (86.4 mg, 0.40 mmol) and **2** (107 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **9** (95.1 mg, 61%) as colorless solid. **M.p.** = 161–162 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.54 (dd, J = 8.1, 1.2 Hz, 1H), 8.26 (d, J = 3.0 Hz, 1H), 7.64 (ddd, J = 8.3, 7.2, 1.2 Hz, 1H), 7.57 (ddd, J = 8.1, 7.2, 1.2 Hz, 1H), 7.33–7.28 (m, 2H), 7.25–7.17 (m, 3H), 7.16–7.09 (m, 3H), 7.00–6.87 (m, 5H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 163.5 (C_q), 158.6 (d, $^1J_{C–F}$ = 258.0 Hz, C_q), 148.3 (d, $^4J_{C–F}$ =3.4 Hz, C_q), 139.8 (C_q), 138.0 (C_q), 137.1 (d, $^2J_{C–F}$ = 26.0 Hz, CH), 135.8 (C_q), 134.0 (C_q), 133.4 (CH), 131.6 (CH), 131.6 (CH), 128.3 (CH), 128.2 (CH), 128.2 (CH), 127.9 (CH), 127.5 (CH), 127.5 (CH), 127.3 (CH), 127.3 (CH), 126.7 (CH), 126.1 (d, $^3J_{C–F}$ = 4.5 Hz, CH), 126.0 (CH), 125.4 (C_q), 125.3 (d, $^2J_{C–F}$ = 28.5 Hz, CH), 125.2 (CH), 120.2 (C_q). **^{19}F NMR** (564 MHz, $CDCl_3$) δ = - 127.43 (q, J = 3.2 Hz). **IR** (KBr): 3058, 1660, 1474, 1390, 1233, 1201, 1074, 780, 700, 549 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 393 (100) $[M+H]^+$, 415(85) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{26}H_{17}FN_2O$ $[M+H]^+$ 393.1400, found 393.1398.

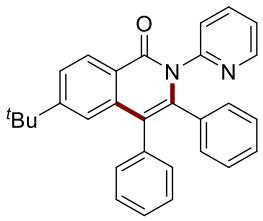


Methyl 6-(1-oxo-3,4-diphenylisoquinolin-2(1*H*)-yl)nicotinate (10): The general procedure was followed using **1g** (102 mg, 0.40 mmol) and **2** (107 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 1:1) yielded **10** (115 mg, 67%) as colorless solid. **M.p.** = 240–241 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.96 (d, J = 2.3 Hz, 1H), 8.54 (d, J = 8.0 Hz, 1H), 8.20 (dd, J = 8.2, 2.3 Hz, 1H), 7.60 (t, J = 7.7 Hz, 1H), 7.53 (t, J = 7.5 Hz, 1H), 7.33 (d, J = 8.2 Hz, 1H), 7.25 (d, J = 8.2 Hz, 1H), 7.22 (t,

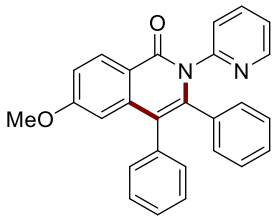
J = 7.3 Hz, 2H), 7.18 (d, *J* = 7.1 Hz, 1H), 7.13 (d, *J* = 7.4 Hz, 2H), 6.98–6.93 (m, 2H), 6.91–6.88 (m, 3H), 3.89 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 165.1 (C_q), 162.7 (C_q), 156.3 (C_q), 150.5 (CH), 139.6 (C_q), 138.8 (CH), 137.9 (C_q), 135.9 (C_q), 134.1 (C_q), 133.1 (CH), 131.7 (CH), 131.7 (CH), 128.2 (CH), 128.2 (CH), 128.2 (CH), 127.7 (CH), 127.4 (CH), 127.4 (CH), 127.2 (CH), 127.2 (CH), 127.2 (CH), 127.2 (CH), 125.9 (CH), 125.5 (C_q), 125.1 (C_q), 124.9 (CH), 119.5 (C_q), 52.6 (CH_3). **IR** (KBr): 3058, 1721, 1652, 1586, 1332, 1277, 1121, 1021, 776, 700 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 433 (36) $[M+H]^+$, 455 (100) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{28}H_{20}N_2O_3$ $[M+H]^+$ 433.1547, found 433.1547.



6-Methyl-3,4-diphenyl-2-(pyridin-2-yl)isoquinolin-1(2*H*)-one (11): The general procedure was followed using **1h** (84.9 mg, 0.40 mmol) and **2** (107 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **11** (146 mg, 94%) as yellowish solid. The NMR data is identical to that previously reported.[15] **M.p.** = 231–232 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.45 (d, *J* = 8.2 Hz, 1H), 8.38 (dd, *J* = 5.0, 1.8 Hz, 1H), 7.59 (ddd, *J* = 7.5, 7.2, 1.8 Hz, 1H), 7.34 (d, *J* = 8.2 Hz, 1H), 7.23–7.20 (m, 3H), 7.18 (d, *J* = 7.2 Hz, 1H), 7.14 (d, *J* = 7.3 Hz, 2H), 7.07 (dd, *J* = 7.5, 5.0 Hz, 1H), 7.02 (s, 1H), 7.01–6.83 (m, 5H), 2.38 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 162.8 (C_q), 152.9 (C_q), 149.2 (CH), 143.5 (C_q), 140.2 (C_q), 138.0 (C_q), 137.6 (CH), 136.3 (C_q), 134.6 (C_q), 131.8 (CH), 131.8 (CH), 128.7 (CH), 128.3 (CH), 128.1 (CH), 128.1 (CH), 127.4 (CH), 127.1 (CH), 127.1 (CH), 127.0 (CH), 127.0 (CH), 127.0 (CH), 125.5 (CH), 125.2 (CH), 123.4 (C_q), 123.0 (CH), 119.0 (C_q), 22.2 (CH_3). **IR** (KBr): 3058, 2918, 1655, 1616, 1589, 1471, 1325, 844, 760, 700 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 389 (100) $[M+H]^+$, 411 (1) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{27}H_{20}N_2O$ $[M+H]^+$ 389.1654, found 389.1648.

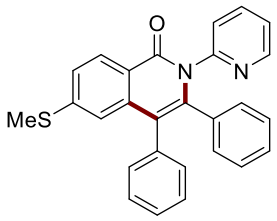


6-(Tert-butyl)-3,4-diphenyl-2-(pyridin-2-yl)isoquinolin-1(2*H*)-one (12): The general procedure was followed using **1i** (102 mg, 0.40 mmol) and **2** (107 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **12** (164 mg, 95%) as yellowish solid. **M.p.** = 260–261 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.48 (d, J = 8.5 Hz, 1H), 8.38 (d, J = 5.0 Hz, 1H), 7.60–7.57 (m, 2H), 7.25–7.20 (m, 4H), 7.18 (d, J = 6.7 Hz, 1H), 7.17–7.12 (m, 3H), 7.07 (dd, J = 7.5, 5.0 Hz, 1H), 7.03–6.88 (m, 4H), 1.25 (s, 9H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 162.7 (C_q), 156.4 (C_q), 153.0 (C_q), 149.2 (CH), 140.1 (C_q), 137.8 (C_q), 137.6 (CH), 136.3 (C_q), 134.7 (C_q), 131.8 (CH), 131.8 (CH), 128.0 (CH), 128.0 (CH), 128.0 (CH), 127.3 (CH), 127.2 (CH), 127.2 (CH), 127.0 (CH), 127.0 (CH), 127.0 (CH), 125.2 (CH), 125.1 (CH), 123.4 (C_q), 122.9 (CH), 121.9 (CH), 119.4 (C_q), 35.4 (C_q), 31.1 (CH_3). **IR** (KBr): 3055, 2965, 1658, 1606, 1588, 1467, 1433, 1324, 793, 705 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 431 (100) $[M+H]^+$, 453 (1) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{30}H_{26}N_2O$ $[M+H]^+$ 431.2124, found 431.2118.

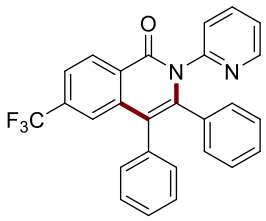


6-Methoxy-3,4-diphenyl-2-(pyridin-2-yl)isoquinolin-1(2*H*)-one (13): The general procedure was followed using **1j** (91.3 mg, 0.40 mmol) and **2** (107 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **14** (147 mg, 91%) as colorless solid. The NMR data is identical to that previously reported.[15] **M.p.** = 251–252 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.48 (d, J = 8.9 Hz, 1H), 8.37 (d, J = 4.8 Hz, 1H), 7.58 (ddd, J = 7.5, 7.4, 4.1 Hz, 1H), 7.23–7.18 (m, 3H), 7.18–7.11 (m, 3H), 7.09 (dd, J = 8 .9, 2.5 Hz, 1H), 7.06 (ddd, J = 7.5, 4.8, 1.0 Hz, 1H), 7.05–6.85 (m, 5H),

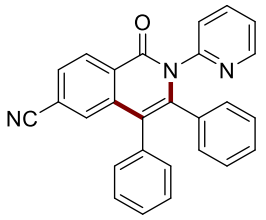
6.62 (d, J = 2.5 Hz, 1H), 3.73 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 163.2 (C_q), 162.4 (C_q), 152.9 (C_q), 149.1 (CH), 140.8 (C_q), 140.1 (C_q), 137.6 (CH), 136.3 (C_q), 134.6 (C_q), 131.7 (CH), 131.7 (CH), 130.5 (CH), 128.1 (CH), 128.1 (CH), 128.1 (CH), 127.4 (CH), 127.4 (CH), 127.2 (CH), 127.2 (CH), 127.1 (CH), 125.2 (CH), 122.9 (CH), 119.5 (C_q), 118.8 (C_q), 115.6 (CH), 107.8 (CH), 55.4 (CH_3). **IR** (KBr): 3058, 2969, 1658, 1590, 1482, 1327, 1221, 1028, 759, 700 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 405 (100) $[M+H]^+$, 427 (3) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{27}H_{20}N_2O_2$ $[M+H]^+$ 405.1602, found 405.1598.



6-(Methylthio)-3,4-diphenyl-2-(pyridin-2-yl)isoquinolin-1(2*H*)-one (14): The general procedure was followed using **1k** (97.7 mg, 0.40 mmol) and **2** (107 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **14** (114 mg, 68%) as yellow solid. **M.p.** = 277–278 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.42 (d, J = 8.5 Hz, 1H), 8.38 (ddd, J = 4.9, 1.9, 0.9 Hz, 1H), 7.59 (ddd, J = 7.5, 7.3, 1.9 Hz, 1H), 7.36 (d, J = 8.5, 1H), 7.22–7.19 (m, 3H), 7.17 (dd, J = 7.3, 1.1 Hz, 1H), 7.14–7.10 (m, 2H), 7.08 (ddd, J = 7.5, 4.9, 1.1 Hz, 1H), 7.08–6.95 (m, 2H), 6.95–6.88 (m, 4H), 2.37 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 162.5 (C_q), 152.8 (C_q), 149.2 (CH), 145.5 (C_q), 141.0 (C_q), 138.3 (C_q), 137.7 (CH), 135.9 (C_q), 134.4 (C_q), 131.7 (CH), 131.7 (CH), 128.6 (CH), 128.4 (CH), 128.2 (CH), 127.5 (CH), 127.2 (CH), 127.2 (CH), 127.2 (CH),127.2 (CH), 127.1 (CH), 125.1 (CH), 124.5 (CH), 123.0 (CH), 122.4 (C_q), 121.1 (CH), 118.5 (C_q), 14.8 (CH_3). **IR** (KBr): 2962, 2925, 1646, 1465, 1262, 1097, 1021, 800, 701 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 421 (100) $[M+H]^+$, 443 (4) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{27}H_{20}N_2OS$ $[M+H]^+$ 421.1373, found 421.1369.

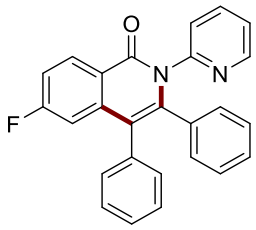


3,4-Diphenyl-2-(pyridin-2-yl)-6-(trifluoromethyl)isoquinolin-1(2*H*)-one (15): The general procedure was followed using **1l** (107 mg, 0.40 mmol) and **2** (107 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **15** (153 mg, 86%) as yellow solid. The NMR data is identical to that previously reported.[15] **M.p.** = 204–205 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.59 (d, J = 8.4 Hz, 1H), 8.33 (d, J = 3.7 Hz, 1H), 7.64 (d, J = 8.4 Hz, 1H), 7.53 (t, J = 8.1 Hz, 1H), 7.45 (s, 1H), 7.18–7.11 (m, 4H), 7.08–7.02 (m, 3H), 6.98–6.79 (m, 5H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 162.0 (C_q), 152.4 (C_q), 149.3 (CH), 141.9 (C_q), 138.1 (C_q), 137.9 (CH), 134.5 (C_q), 134.4 (q, $^2J_{C–F}$ = 32.3 Hz, C_q), 134.1 (C_q), 131.6 (CH), 131.6 (CH), 129.4 (CH), 128.4 (CH), 128.4 (CH), 127.9 (CH), 127.9 (CH), 127.8 (CH), 127.8 (CH), 127.5 (CH), 127.3 (CH), 124.9 (CH), 124.9 (CH), 124.7 (C_q), 123.8 (q, $^1J_{C–F}$ = 271.5 Hz, C_q), 123.3 (CH), 123.1 (q, $^3J_{C–F}$ = 4.2 Hz, CH), 118.8 (C_q). **^{19}F NMR** (564 MHz, $CDCl_3$) δ = -63.05 (s). **IR** (KBr): 2925, 1662, 1591, 1473, 1432, 1331, 1132, 1068, 908, 702 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 443 (100) $[M+H]^+$, 465 (5) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{27}H_{17}F_3N_2O$ $[M+H]^+$ 443.1370, found 443.1366.

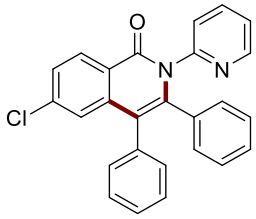


1-Oxo-3,4-diphenyl-2-(pyridin-2-yl)-1,2-dihydroisoquinoline-6-carbonitrile (16): The general procedure was followed using **1m** (89.5 mg, 0.40 mmol) and **2** (107 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **16** (93.8 mg, 59%) as colorless solid. **M.p.** = 241–242 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.67 (d, J = 8.2 Hz, 1H), 8.44 (dd, J = 4.9, 1.8 Hz, 1H), 7.74 (d, J = 8.2 Hz, 1H), 7.66 (t, J = 7.7 Hz, 1H), 7.62 (s, 1H), 7.31–7.26 (m, 3H), 7.23 (d, J = 7.9 Hz, 1H),

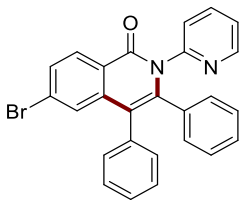
7.17–7.13 (m, 3H), 7.10–7.96 (m, 5H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 162.7 (C_q), 152.2 (C_q), 149.4 (CH), 142.4 (C_q), 138.2 (C_q), 137.9 (CH), 134.8 (C_q), 133.6 (C_q), 131.5 (CH), 131.5 (CH), 130.6 (CH), 129.4 (CH), 128.7 (CH), 128.6 (CH), 128.6 (CH), 128.1 (C_q), 127.9 (CH), 127.9 (CH), 127.7 (CH), 127.7 (CH), 127.4 (CH), 127.4 (CH), 124.8 (CH), 123.4 (CH), 118.4 (C_q), 118.1 (C_q), 116.3 (C_q). **IR** (KBr): 3054, 2233, 1665, 1589, 1467, 1326, 1215, 996, 761, 712 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 400 (100) $[M+H]^+$, 422 (2) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{27}H_{17}N_3O$ $[M+H]^+$ 400.1445, found 400.1444.



6-Fluoro-3,4-diphenyl-2-(pyridin-2-yl)isoquinolin-1(2*H*)-one (17): The general procedure was followed using **1n** (86.5 mg, 0.40 mmol) and **2** (107 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **17** (141 mg, 90%) as yellowish solid. The NMR data is identical to that previously reported.[15] **M.p.** = 207–208 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.56 (t, J = 7.2 Hz, 1H), 8.39 (d, J = 2.3 Hz, 1H), 7.60 (t, J = 7.9 Hz, 1H), 7.24–7.17 (m, 5H), 7.14–7.08 (m, 3H), 7.05–6.84 (m, 6H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 165.8 (d, $^1J_{C-F}$ = 252.4 Hz, C_q), 162.2 (C_q), 152.6 (C_q), 149.3 (CH), 141.6 (C_q), 140.5 (d, $^3J_{C-F}$ = 9.9 Hz, C_q), 137.8 (CH), 135.7 (C_q), 134.2 (C_q), 131.5 (d, $^3J_{C-F}$ = 9.0 Hz, CH), 131.5 (CH), 131.5 (CH), 128.3 (CH), 128.3 (CH), 127.6 (CH), 127.6 (CH), 127.6 (CH), 127.4 (CH), 127.4 (CH), 127.3 (CH), 125.0 (CH), 123.2 (CH), 122.3 (C_q), 118.6 (d, $^4J_{C-F}$ = 3.0 Hz, C_q), 115.6 (d, $^2J_{C-F}$ = 24.0 Hz, CH), 111.1 (d, $^2J_{C-F}$ = 24.0 Hz, CH). **^{19}F NMR** (564 MHz, $CDCl_3$) δ = -104.98 (q, J = 8.5). **IR** (KBr): 3058, 1666, 1614, 1472, 1324, 1183, 1138, 951, 761, 701 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 393 (100) $[M+H]^+$, 415 (2) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{26}H_{17}FN_2O$ $[M+H]^+$ 393.1399, found 393.1398.

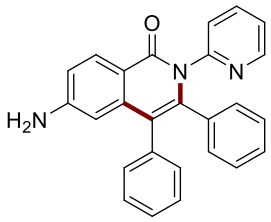


6-Chloro-3,4-diphenyl-2-(pyridin-2-yl)isoquinolin-1(2*H*)-one (18): The general procedure was followed using **1o** (93.1 mg, 0.40 mmol) and **2** (107 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **18** (144 mg, 88%) as colorless solid. **M.p.** = 243–244 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.48 (d, J = 8.6 Hz, 1H), 8.39 (ddd, J = 4.9, 1.9, 0.9 Hz, 1H), 7.60 (t, J = 7.7 Hz, 1H), 7.46 (d, J = 8.6, Hz, 1H), 7.25–7.21 (m, 3H), 7.21–7.17 (m, 2H), 7.12 (d, J = 6.6 Hz, 2H), 7.09 (dd, J = 7.5, 4.9 Hz, 1H), 7.04–6.83 (m, 5H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 162.2 (C_q), 152.5 (C_q), 149.3 (CH), 141.7 (C_q), 139.6 (C_q), 139.3 (C_q), 137.8 (CH), 135.5 (C_q), 134.1 (C_q), 131.6 (CH), 131.6 (CH), 130.1 (CH), 128.3 (CH), 128.3 (CH), 128.3 (CH), 127.6 (CH), 127.6 (CH), 127.6 (CH), 127.4 (CH), 127.4 (CH), 127.3 (CH), 125.2 (CH), 125.0 (CH), 124.0 (C_q), 123.2 (CH), 118.2 (C_q). **IR** (KBr): 3063, 1657, 1614, 1596, 1472, 1463, 1321, 883, 759, 706 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 409 (100) $[M+H]^+$, 431 (2) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{26}H_{17}{}^{35}ClN_2O$ $[M+H]^+$ 409.1105, found 409.1102.

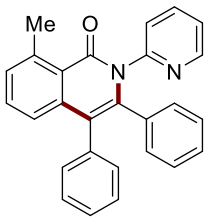


6-Bromo-3,4-diphenyl-2-(pyridin-2-yl)isoquinolin-1(2*H*)-one (19): The general procedure was followed using **1p** (111 mg, 0.40 mmol) and **2** (107 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 1:1) yielded **19** (163 mg, 90%) as yellowish solid. The NMR data is identical to that previously reported.[15] **M.p.** = 244–245 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.43–8.36 (m, 2H), 7.64–7.57 (m, 2H), 7.39 (d, J = 1.9 Hz, 1H), 7.25–7.21 (m, 2H), 7.21–7.17 (m, 2H), 7.11 (d, J = 7.4 Hz, 2H), 7.09 (ddd, J = 7.5, 4.8, 0.9 Hz, 1H), 7.04–6.80 (m, 5H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 162.3 (C_q), 152.5 (C_q), 149.3 (CH), 141.7 (C_q), 139.5 (C_q), 137.8 (CH),

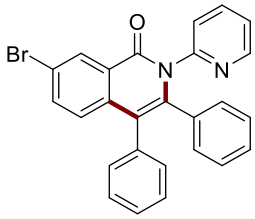
135.4 (C_q), 134.1 (C_q), 131.6 (CH), 131.6 (CH), 130.4 (CH), 130.1 (CH), 128.4 (C_q), 128.4 (CH), 128.4 (CH), 128.3 (CH), 127.6 (CH), 127.4 (CH), 127.4 (CH), 127.3 (CH), 127.3 (CH), 127.3 (CH), 125.0 (CH), 124.4 (C_q), 123.2 (CH), 118.1 (C_q). **IR** (KBr): 3060, 1658, 1590, 1472, 1433, 1320, 1148, 1069, 759, 704 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 453 (100) $[M+H]^+$, 475 (2) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{26}H_{17}{}^{79}BrN_2O$ $[M+H]^+$ 453.0601, found 453.0597.



6-Amino-3,4-diphenyl-2-(pyridin-2-yl)isoquinolin-1(2*H*)-one (20): The general procedure was followed using **1q** (42.7 mg, 0.20 mmol) and **2** (63.5 mg, 0.30 mmol). Purification by column chromatography (PE/EtOAc = 1:1) yielded **20** (34.2 mg, 44%) as colorless solid. **M.p.** = 305–306 °C. **^{1}H NMR** (600 MHz, DMSO-d_6) δ = 8.27 (d, J = 5.0 Hz, 1H), 8.0 (d, J = 8.7 Hz, 1H), 7.68 (t, J = 7.7 Hz, 1H), 7.34 (d, J = 7.8 Hz, 1H), 7.24–7.10 (m, 6H), 7.02–6.93 (m, 2H), 6.89–6.85 (m, 3H), 6.78 (dd, J = 8.7, 2.1 Hz, 1H), 6.12 (d, J = 2.1 Hz, 1H), 5.99 (s, 2H). **^{13}C NMR** (150 MHz, DMSO-d_6) δ = 161.5 (C_q), 153.3 (C_q), 152.9 (C_q), 148.7 (CH), 140.4 (C_q), 139.8 (C_q), 137.8 (CH), 136.7 (C_q), 134.6 (C_q), 131.6 (CH), 131.6 (CH), 129.3 (CH), 128.2 (CH), 128.2 (CH), 127.3 (CH), 127.3 (CH), 127.3 (CH), 127.0 (CH), 127.0 (CH), 127.0 (CH), 125.8 (CH), 123.1 (C_q), 117.4 (CH), 115.4 (CH), 114.2 (C_q), 106.1 (CH). **IR** (KBr): 3471, 2962, 1636, 1599, 1579, 1483, 1332, 1116, 758, 699 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 390 (100) $[M+H]^+$, 412 (2) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{26}H_{19}N_3O$ $[M+H]^+$ 390.1606, found 390.1602.

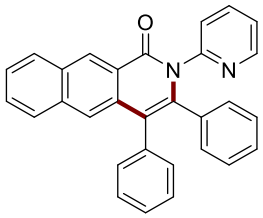


8-Methyl-3,4-diphenyl-2-(pyridin-2-yl)isoquinolin-1(2*H*)-one (21): The general procedure was followed using **1r** (84.9 mg, 0.40 mmol) and **2** (107 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 1:1) yielded **21** (148 mg, 95%) as yellowish solid. The NMR data is identical to that previously reported.[15] **M.p.** = 282–283 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.42 (d, J = 5.0 Hz, 1H), 7.58 (t, J = 7.8 Hz, 1H), 7.41 (t, J = 7.4 Hz, 1H), 7.28 (d, J = 7.4 Hz, 1H), 7.22–7.18 (m, 2H), 7.18–7.15 (m, 2H), 7.14–7.12 (m, 2H), 7.08–7.06 (m, 2H), 7.02–6.86 (m, 5H), 2.97 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 163.7 (C_q), 153.4 (C_q), 149.3 (CH), 142.6 (CH), 140.1 (C_q), 139.8 (C_q), 137.8 (CH), 137.0 (C_q), 134.5 (C_q), 132.0 (CH), 131.9 (C_q), 131.9 (CH), 131.9 (CH), 130.3 (CH), 128.1 (CH), 128.1 (CH), 127.4 (CH), 127.2 (CH), 127.2 (CH), 127.0 (CH), 127.0 (CH), 125.2 (CH), 124.2 (CH), 124.1 (C_q), 122.9 (CH), 119.1 (C_q), 24.4 (CH_3). **IR** (KBr): 2963, 1657, 1589, 1470, 1435, 1332, 1300, 1150, 997, 698 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 389 (100) $[M+H]^+$, 411 (1) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{27}H_{20}N_2O$ $[M+H]^+$ 389.1654, found 389.1648.

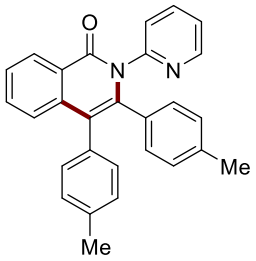


7-Bromo-3,4-diphenyl-2-(pyridin-2-yl)isoquinolin-1(2*H*)-one (22): The general procedure was followed using **1s** (111 mg, 0.40 mmol) and **2** (107 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **22** (152 mg, 84%) as yellowish solid. **M.p.** = 224–225 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.67 (s, 1H), 8.39 (d, J = 4.8 Hz, 1H), 7.66 (d, J = 8.7 Hz, 1H), 7.61 (t, J = 7.7 Hz, 1H), 7.23–7.17 (m, 4H), 7.14–7.08 (m, 4H), 7.03–6.86 (m, 5H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 161.6 (C_q), 152.5 (C_q), 149.3 (CH), 140.7 (C_q), 137.9 (CH), 136.7 (C_q), 136.0 (CH), 135.7

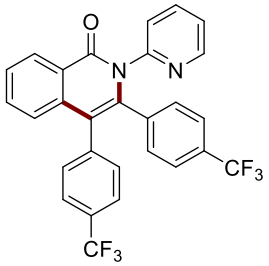
(C_q), 134.1 (C_q), 131.6 (CH), 131.6 (CH), 130.8 (CH), 128.3 (CH), 128.3 (CH), 128.3 (CH), 127.7 (CH), 127.6 (CH), 127.3 (CH), 127.3 (CH), 127.3 (CH), 127.3 (CH), 127.1 (C_q), 125.0 (CH), 123.2 (CH), 121.1 (C_q), 118.7 (C_q). **IR** (KBr): 3057, 1657, 1587, 1470, 1433, 1328, 835, 761, 699 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 453 (100) $[M+H]^+$, 475 (2) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{26}H_{17}{}^{79}BrN_2O$ $[M+H]^+$ 453.0599, found 453.0597.



3,4-Diphenyl-2-(pyridin-2-yl)benzo[g]isoquinolin-1(2*H*)-one (23): The general procedure was followed using **1t** (99.3 mg, 0.40 mmol) and **2** (107 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **23** (137 mg, 81%) as yellow solid. **M.p.** = 309–310 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 9.14 (s, 1H), 8.38 (d, J = 5.5 Hz, 1H), 8.07 (d, J = 7.8 Hz, 1H), 7.76 (d, J = 7.9 Hz, 1H), 7.67 (s, 1H), 7.59 (dd, J = 8.8, 6.8 Hz, 1H), 7.53–7.48 (m, 2H), 6.26–6.23 (m, 3H), 6.22–6.19 (m, 3H), 6.07 (t, J = 6.3 Hz, 1H), 6.04–5.94 (m, 2H), 5.90–5.87 (m, 3H) . **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 163.5 (C_q), 152.9 (C_q), 149.2 (CH), 139.0 (C_q), 137.8 (C_q), 137.8 (CH), 136.6 (C_q), 135.7 (C_q), 134.7 (C_q), 134.1 (C_q), 131.9 (CH), 131.9 (CH), 129.8 (CH), 129.5 (CH), 128.3 (CH), 128.3 (CH), 128.2 (CH), 128.2 (CH), 128.2 (CH), 127.4 (CH), 127.2 (CH), 127.2 (CH), 127.1 (CH), 127.1 (CH), 126.3 (CH), 125.3 (CH), 124.8 (CH), 124.1 (C_q), 123.0 (CH), 119.2 (C_q). **IR** (KBr): 3055, 1663, 1623, 1489, 1433, 1420, 1213, 890, 714, 699 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 425 (100) $[M+H]^+$, 447(1) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{30}H_{20}N_2O$ $[M+H]^+$ 425.1651, found 425.1648.

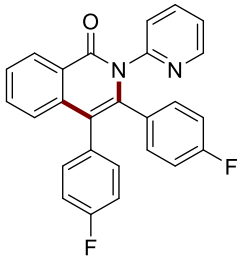


2-(Pyridin-2-yl)-3,4-di-p-tolylisoquinolin-1(2*H*)-one (24): The general procedure was followed using *t*-AmOH/HFIP/H_2O = 1/2/1 as solvent, **1** (79.3 mg, 0.40 mmol) and **2a** (124 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **24** (109 mg, 68%) as yellowish solid. **M.p.** = 242–243 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.54 (d, J = 8.0 Hz, 1H), 8.40 (dd, J = 4.9 Hz, 1H), 7.61–7.55 (m, 2H), 7.50 (t, J = 7.5 Hz, 1H), 7.25 (d, J = 8.0 Hz, 1H), 7.19 (d, J = 7.7 Hz, 1H), 7.09 (dd, J = 7.5, 4.9 Hz, 1H), 7.04–7.00 (m, 4H), 6.97–6.73 (m, 2H), 6.70 (d, J = 8.3 Hz, 2H), 2.29 (s, 3H), 2.08 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 162.9 (C_q), 153.0 (C_q), 149.1 (CH), 140.2 (C_q), 138.2 (C_q), 137.6 (CH), 137.0 (C_q), 137.0 (C_q), 136.5 (C_q), 133.2 (C_q), 132.7 (CH), 131.6 (CH), 131.6 (CH), 128.8 (CH), 128.2 (CH), 128.2 (CH), 127.9 (CH), 127.9 (CH), 126.9 (CH), 126.9 (CH), 126.9 (CH), 125.8 (CH), 125.6 (C_q), 125.1 (CH), 122.9 (CH), 119.0 (C_q), 21.3 (CH_3), 21.2 (CH_3). **IR** (KBr): 2922, 1663, 1587, 1466, 1434, 1325, 1146, 994, 760, 709 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 403 (100) $[M+H]^+$, 425(2) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{28}H_{22}N_2O$ $[M+H]^+$ 403.1810, found 403.1805.



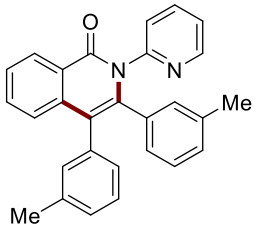
2-(Pyridin-2-yl)-3,4-bis(4-(trifluoromethyl)phenyl)isoquinolin-1(2*H*)-one (25): The general procedure was followed using **1** (79.3 mg, 0.40 mmol) and **2b** (189 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **25** (106 mg, 52%) as yellowish solid. **M.p.** = 260–261 °C. **^{1}H NMR** (600 MHz, $CDCl_3$)

δ = 8.57 (d, J = 7.5 Hz, 1H), 8.36 (d, J = 4.4 Hz, 1H), 7.67–7.62 (m, 2H), 7.58 (t, J = 7.6 Hz, 1H), 7.51 (d, J = 7.6 Hz, 2H), 7.29–7.25 (m, 3H), 7.20 (d, J = 7.8 Hz, 2H), 7.17–7.04 (m, 4H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 162.5 (C_q), 152.2 (C_q), 149.4 (CH), 139.7 (C_q), 139.0 (C_q), 138.0 (CH), 137.7 (C_q), 137.0 (C_q), 133.3 (CH), 132.1 (CH), 132.1 (CH), 129.9 (q, $^2J_{C–F}$ = 33.0 Hz, C_q), 129.7 (q, $^2J_{C–F}$ = 31.5 Hz, C_q), 128.6 (CH), 128.6 (CH), 127.9 (CH), 127.9 (CH), 125.8 (C_q), 125.5 (CH), 125.4 (q, $^3J_{C–F}$ = 4.0 Hz, CH), 125.4 (q, $^3J_{C–F}$ = 4.0 Hz, CH), 125.0 (CH), 124.4 (q, $^3J_{C–F}$ = 4.5 Hz, CH), 124.4 (q, $^3J_{C–F}$ = 4.5 Hz, CH), 124.1 (q, $^1J_{C–F}$ = 270.0 Hz, C_q), 123.6 (q, $^1J_{C–F}$ = 270.0 Hz, C_q), 123.5 (CH), 118.2 (C_q). **^{19}F NMR** (564 MHz, $CDCl_3$) δ = -62.64 (s), -62.99 (s). **IR** (KBr): 2935, 1667, 1608, 1464, 1434, 1322, 1123, 1067, 775, 703 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 511 (100) $[M+H]^+$, 533(2) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{28}H_{16}F_6N_2O$ $[M+H]^+$ 511.1241, found 511.1240.

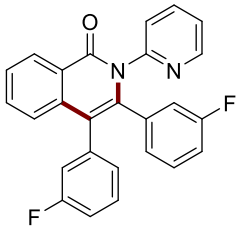


3,4-Bis(4-fluorophenyl)-2-(pyridin-2-yl)isoquinolin-1(2*H*)-one (26): The general procedure was followed using **1** (39.7 mg, 0.20 mmol) and **2c** (64.3 mg, 0.30 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **26** (72.5 mg, 88%) as yellowish solid. The NMR data is identical to that previously reported.[15] **M.p.** = 283–284 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.55 (d, J = 7.9 Hz, 1H), 8.40 (d, J = 5.3 Hz, 1H), 7.66–7.59 (m, 2H), 7.54 (t, J = 7.6 Hz, 1H), 7.22 (d, J = 8.0 Hz, 2H), 7.14–7.07 (m, 3H), 6.94 (t, J = 8.5 Hz, 4H), 6.62 (t, J = 8.5 Hz, 2H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 162.7 (C_q), 162.0 (d, $^1J_{C–F}$ = 246.0 Hz, C_q), 161.7 (d, $^1J_{C–F}$ = 252.0 Hz, C_q), 152.7 (C_q), 149.4 (CH), 139.5 (CH), 138.0 (CH), 137.9 (C_q), 137.7 (C_q), 133.3 (d, $^3J_{C–F}$ = 7.6 Hz, CH), 133.3 (d, $^3J_{C–F}$ = 7.6 Hz, CH), 133.0 (CH), 132.0 (d, $^4J_{C–F}$ = 3.4 Hz, C_q), 130.4 (d, $^4J_{C–F}$ = 3.5 Hz, C_q), 128.4 (CH), 127.3 (C_q), 125.7 (d, $^3J_{C–F}$ = 13.9 Hz, CH), 125.7 (d, $^3J_{C–F}$ = 13.9 Hz, CH), 125.6 (CH), 125.0 (CH), 123.2 (CH), 118.4 (C_q),

115.4 (d, $^2J_{C–F}$ = 21.4 Hz, CH), 115.4 (d, $^2J_{C–F}$ = 21.4 Hz, CH), 114.5 (d, $^2J_{C–F}$ = 21.8 Hz, CH), 114.5 (d, $^2J_{C–F}$ = 21.8 Hz, CH). **^{19}F NMR** (564 MHz, $CDCl_3$) δ = -112.90 (q, J = 7.0), -114.68 (q, J = 7.0). **IR** (KBr): 3052, 1661, 1616, 1508, 1467, 1434, 1325, 1158, 838, 712 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 411 (100) $[M+H]^+$, 433(2) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{26}H_{16}F_2N_2O$ $[M+H]^+$ 411.1307, found 411.1306.

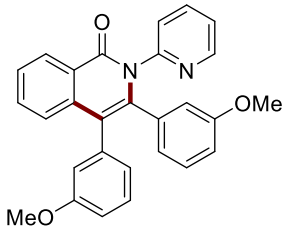


2-(Pyridin-2-yl)-3,4-di-*m*-tolylisoquinolin-1(2*H*)-one (27): The general procedure was followed using **1** (39.7 mg, 0.20 mmol) and **2d** (61.8 mg, 0.30 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **27** (79.8 mg, 99%) as brown solid. **M.p.** = 201–202 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.53 (d, J = 7.8 Hz, 1H), 8.38 (d, J = 4.6 Hz, 1H), 7.60–7.55 (m, 2H), 7.50 (t, J = 7.3 Hz, 1H), 7.25 (d, J = 7.9 Hz, 1H), 7.19 (d, J = 8.0 Hz, 1H), 7.10–7.05 (m, 2H), 6.98–6.94 (m, 2H), 6.92 (d, J = 7.3 Hz, 1H), 6.88–6.62 (m, 4H), 2.22 (s, 3H), 2.01 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 162.8 (C_q), 153.0 (C_q), 149.1 (CH), 140.2 (C_q), 138.1 (C_q), 137.6 (CH), 137.5 (C_q), 136.6 (C_q), 136.1 (C_q), 134.3 (C_q), 132.8 (CH), 132.4 (CH), 128.8 (CH), 128.2 (CH), 128.1 (CH), 128.1 (CH), 127.9 (CH), 127.7 (CH), 127.0 (CH), 126.9 (CH), 125.9 (CH), 125.9 (CH), 125.6 (C_q), 125.1 (CH), 123.0 (CH), 119.1 (C_q), 21.4 (CH_3), 21.1 (CH_3). **IR** (KBr): 2923, 2860, 1664, 1589, 1468, 1434, 1326, 997, 771, 704 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 403 (100) $[M+H]^+$, 425(2) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{28}H_{22}N_2O$ $[M+H]^+$ 403.1812, found 403.1805.



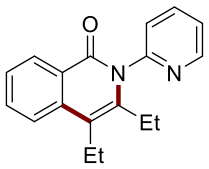
3,4-Bis(3-fluorophenyl)-2-(pyridin-2-yl)isoquinolin-1(2*H*)-one (28): The general

procedure was followed using **1** (79.3 mg, 0.40 mmol) and **2e** (129 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **28** (112 mg, 68%) as colorless solid. **M.p.** = 216–217 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.61 (d, J = 7.2 Hz, 1H), 8.46 (d, J = 4.8 Hz, 1H), 7.74–7.66 (m, 2H), 7.62 (t, J = 7.8 Hz, 1H), 7.33–7.27 (m, 3H), 7.20–7.17 (m, 1H), 7.03–6.91 (m, 4H), 6.90–6.63 (m, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 162.6 (d, $^1J_{C–F}$ = 246.0 Hz, C_q), 162.6 (C_q), 161.4 (d, $^1J_{C–F}$ = 246.0 Hz, C_q), 152.4 (C_q), 149.3 (CH), 138.9 (C_q), 138.1 (d, $^3J_{C–F}$ = 7.8 Hz, C_q), 137.9 (CH), 137.3 (C_q), 136.1 (d, $^3J_{C–F}$ = 8.1 Hz, C_q), 133.1 (CH), 129.9 (d, $^3J_{C–F}$ = 8.9 Hz, CH), 129.8 (d, $^3J_{C–F}$ = 8.1 Hz, CH), 129.0 (d, $^4J_{C–F}$ = 4.9 Hz, CH), 129.0 (d, $^2J_{C–F}$ = 21.0 Hz, CH), 128.4 (CH), 127.5 (CH), 127.5 (CH), 125.7 (C_q), 125.6 (CH), 125.0 (CH), 123.3 (CH), 118.5 (d, $^2J_{C–F}$ = 21.0 Hz, CH), 118.1 (C_q), 114.9 (d, $^2J_{C–F}$ = 21.0 Hz, CH), 114.5 (d, $^2J_{C–F}$ = 21.0 Hz, CH). **^{19}F NMR** (564 MHz, $CDCl_3$) δ = -113.51-(-)112.91 (m). **IR** (KBr): 3057, 1662, 1587, 1467, 1435, 1324, 1267, 1138, 760, 706 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 411 (100) $[M+H]^+$, 433 (2) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{26}H_{16}F_2N_2O$ $[M+H]^+$ 411.1308, found 411.1303.

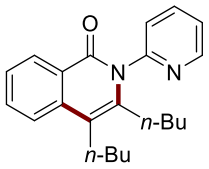


3,4-Bis(3-methoxyphenyl)-2-(pyridin-2-yl)isoquinolin-1(2*H*)-one (29): The general procedure was followed using *t*-AmOH/HFIP/H_2O = 1/2/1 as solvent, **1** (79.3 mg, 0.40 mmol) and **2f** (143 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **29** (122 mg, 70%) as colorless solid. **M.p.** = 167–168 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.54 (d, J = 7.9 Hz, 1H), 8.41 (d, J = 4.8 Hz, 1H), 7.63–7.58 (m, 2H), 7.52 (t, J = 7.5 Hz, 1H), 7.31 (t, J = 8.1 Hz, 1H), 7.22 (d, J = 7.9 Hz, 1H), 7.15 (d, J = 8.6 Hz, 1H), 7.11 (dd, J = 7.5, 4.9 Hz, 1H), 6.85–6.77 (m, 2H), 6.74 (d, J = 8.5 Hz, 2H), 6.67 (s, 1H), 6.57 (br, 1H), 6.46 (dd, J = 8.4, 2.5 Hz, 1H), 3.67 (d, J = 13.6 Hz, 3H), 3.53 (d, J = 8.9 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 162.7 (C_q), 159.3 (C_q), 158.4 (C_q), 152.9 (C_q), 149.1 (CH), 139.7 (C_q), 137.7 (C_q), 137.7 (CH),

137.5 (C_q), 135.5 (C_q), 132.8 (CH), 129.1 (CH), 129.0 (CH), 128.2 (CH), 127.1 (CH), 127.1 (CH), 125.8 (CH), 125.6 (C_q), 125.0 (CH), 124.2 (CH), 123.1 (CH), 118.8 (C_q), 117.1 (CH), 116.3 (CH), 114.0 (CH), 112.9 (CH), 55.2 (CH_3), 53.2 (CH_3). **IR** (KBr): 2966, 1658, 1595, 1468, 1328, 1284, 1226, 1035, 752, 713 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 435 (100) $[M+H]^+$, 457 (2) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{28}H_{22}N_2O_3$ $[M+H]^+$ 435.1707, found 435.1703.

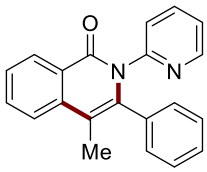


3,4-Diethyl-2-(pyridin-2-yl)isoquinolin-1(2*H*)-one (30): The general procedure was followed using **1** (39.7 mg, 0.20 mmol) and **2g** (24.6 mg, 0.30 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **30** (41.7 mg, 75%) as colorless solid. The NMR data is identical to that previously reported.[15] **M.p.** = 114–115 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.68 (d, *J* = 5.2 Hz, 1H), 8.44 (d, *J* = 8.0, 1H), 7.90 (td, *J* = 7.7, 2.0 Hz, 1H), 7.76–7.67 (m, 2H), 7.44 (ddd, *J* = 8.1, 6.7, 1.4 Hz, 1H), 7.42–7.39 (m, 2H), 2.81 (q, *J* = 7.5 Hz, 2H), 2.41 (q, *J* = 7.5 Hz, 2H), 1.27 (t, *J* = 7.5 Hz, 3H), 1.01 (t, *J* = 7.5 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 163.2 (C_q), 153.1 (C_q), 149.8 (CH), 140.3 (C_q), 138.3 (CH), 137.2 (C_q), 132.8 (CH), 128.6 (CH), 126.0 (CH), 125.6 (C_q), 124.8 (CH), 123.8 (CH), 122.9 (CH), 115.1 (C_q), 23.1 (CH_2), 20.4 (CH_2), 14.8 (CH_3), 13.9 (CH_3). **IR** (KBr): 3064, 2978, 1655, 1466, 1328, 1221, 995, 777, 702, 652 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 279 (100) $[M+H]^+$, 301 (3) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{18}H_{18}N_2O$ $[M+H]^+$ 279.1495, found 279.1492.

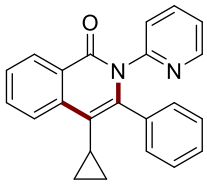


3,4-Dibutyl-2-(pyridin-2-yl)isoquinolin-1(2*H*)-one (31): The general procedure was followed using **1** (79.3 mg, 0.40 mmol) and **2h** (83.0 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **31** (77.6 mg, 58%) as reddish-

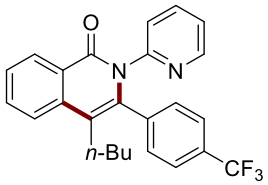
brown solid. **M.p.** = 67–68 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.69 (d, J = 7.3 Hz, 1H), 8.45 (d, J = 8.0 Hz, 1H), 7.90 (t, J = 7.8 Hz, 1H), 7.71–6.67 (m, 2H), 7.46–7.38 (m, 3H), 2.74 (t, J = 8.7 Hz, 2H), 2.35 (t, J = 8.5 Hz, 2H), 1.69–1.54 (m, 4H), 1.54–1.49 (m, 2H), 1.12–1.05 (m, 2H), 1.00 (t, J = 7.3 Hz, 3H), 0.68 (t, J = 7.3 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 163.3 (C_q), 153.2 (C_q), 149.8 (CH), 139.4 (C_q), 138.3 (CH), 137.5(C_q), 132.8 (CH), 128.5 (CH), 126.0 (CH), 125.5 (C_q), 125.0 (CH), 123.8 (CH), 123.0 (CH), 114.2 (C_q), 32.6 (CH_2), 31.2 (CH_2), 29.6 (CH_2), 27.2 (CH_2), 23.3 (CH_2), 22.8 (CH_2), 14.1 (CH_3), 13.4 (CH_3). **IR** (KBr): 2964, 1657, 1467, 1432, 1324, 1262, 1103, 1019, 800, 703 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 335 (100) $[M+H]^+$, 357 (3) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{22}H_{26}N_2O$ $[M+H]^+$ 335.2121, found 335.2118.



4-Methyl-3-phenyl-2-(pyridin-2-yl)isoquinolin-1(2*H*)-one (32): The general procedure was followed using **1** (39.7 mg, 0.20 mmol) and **2i** (34.9 mg, 0.30 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **32** (47.2 mg, 75%) as colorless solid. The NMR data is identical to that previously reported.[15] **M.p.** = 169–170 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.54 (d, J = 7.5 Hz, 1H), 8.37 (d, J = 4.8 Hz, 1H), 7.74 (d, J = 7.5 Hz, 2H), 7.59–7.54 (m, 2H), 7.25–7.08 (m, 6H), 7.06 (dd, J = 7.6, 4.8 Hz, 1H), 2.12 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 162.6 (C_q), 153.0 (C_q), 149.1 (CH), 139.2 (C_q), 137.9 (C_q), 137.5 (CH), 134.9 (C_q), 132.9 (CH), 128.5 (CH), 127.9 (CH), 127.8 (CH), 127.8 (CH), 126.9 (CH), 126.9 (CH), 126.9 (CH), 125.9 (C_q), 125.0 (CH), 123.6 (CH), 122.8 (CH), 110.7 (C_q), 14.7 (CH_3). **IR** (KBr): 3077, 2919, 1652, 1587, 1465, 1327, 1186, 996, 760, 699 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 313 (100) $[M+H]^+$, 335 (1) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{21}H_{16}N_2O$ $[M+H]^+$ 313.1339, found 313.1335.

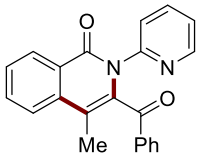


4-Cyclopropyl-3-phenyl-2-(pyridin-2-yl)isoquinolin-1(2*H*)-one (33): The general procedure was followed using **1** (39.7 mg, 0.20 mmol) and **2j** (42.7 mg, 0.30 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **33** (38.3 mg, 56%) as colorless solid. **M.p.** = 174–175 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.50 (d, J = 8.0 Hz, 1H), 8.40 (dd, J = 5.5, 1.9 Hz, 1H), 8.28 (d, J = 8.2 Hz, 1H), 7.76 (ddd, J = 8.0, 7.1, 1.1 Hz, 1H), 7.58 (td, J = 7.7, 1.9 Hz, 1H), 7.53 (t, J = 7.6 Hz, 1H), 7.21–7.11 (m, 5H), 7.10–7.07 (m, 2H), 1.75 (tt, J = 8.4, 5.6 Hz, 1H), 0.72–0.58 (m, 2H), 0.18–0.13 (m, 2H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 162.9 (C_q), 153.0 (C_q),149.1 (CH), 141.9 (C_q), 138.9 (C_q), 137.6 (CH), 135.3 (C_q), 132.6 (CH), 128.4 (CH), 127.7 (CH), 127.7 (CH), 127.5 (CH), 126.8 (CH), 126.8 (CH), 125.9 (C_q), 125.2 (CH), 124.9 (CH), 122.9 (CH), 122.9 (CH), 115.5 (C_q), 10.5 (CH), 9.0 (CH_2). **IR** (KBr): 2919, 2866, 1652, 1588, 1465, 1437, 1329, 996, 761, 699 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 339 (100) $[M+H]^+$, 361 (2) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{23}H_{18}N_2O$ $[M+H]^+$ 339.1492, found 339.1492.

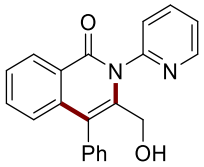


4-Butyl-2-(pyridin-2-yl)-3-(4-(trifluoromethyl)phenyl)isoquinolin-1(2*H*)-one (34): The general procedure was followed using **1** (39.7 mg, 0.20 mmol) and **2k** (67.9 mg, 0.30 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **34** (51.2 mg, 60%) as colorless solid. **M.p.** = 148–149 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.54 (d, J = 8.0 Hz, 1H), 8.35 (dd, J = 4.9, 1.9 Hz, 1H), 7.80–7.75 (m, 2H), 7.62–7.55 (m, 2H), 7.44 (d, J = 7.8 Hz, 2H), 7.39–7.26 (m, 2H), 7.16 (d, J = 7.9, 1H), 7.08 (ddd, J = 7.5, 4.9, 1.1 Hz, 1H), 2.44 (t, J = 8.2 Hz, 2H), 1.51 (p, J = 7.6 Hz, 2H), 1.24 (h, J = 7.4 Hz, 2H), 0.79 (t, J = 7.3 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 162.4 (C_q),

152.6 (C_q), 149.4 (CH), 138.5 (C_q), 137.8 (CH), 137.8 (C_q), 136.8 (C_q), 133.1 (CH), 130.2 (q, $^2J_{C–F}$ = 32.6 Hz, C_q), 129.0 (CH), 129.0 (CH), 128.9 (CH), 127.4 (CH), 127.2 (CH), 126.5 (C_q), 125.0 (CH), 124.7 (q, $^3J_{C–F}$ = 3.8 Hz, CH), 124.7 (q, $^3J_{C–F}$ = 3.8 Hz, CH), 123.9 (q, $^1J_{C–F}$ = 271.5 Hz, C_q), 123.2 (CH), 116.1 (C_q), 32.6 (CH_2), 28.0 (CH_2), 22.9 (CH_2), 13.8 (CH_3). **^{19}F NMR** (564 MHz, $CDCl_3$) δ = -62.81 (s). **IR** (KBr): 2964, 1657, 1467, 1432, 1324, 1262, 1103, 1019, 800, 703 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 423 (100) $[M+H]^+$, 445 (2) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{25}H_{21}F_3N_2O$ $[M+H]^+$ 423.1684, found 423.1679.

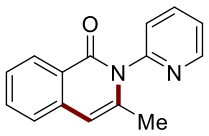


4-Benzoyl-3-methyl-2-(pyridin-2-yl)isoquinolin-1(2*H*)-one (35): The general procedure was followed using **1** (79.3 mg, 0.40 mmol) and **2l** (86.5 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **35** (106 mg, 78%) as yellowish solid. **M.p.** = 203–204 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.56 (dd, *J* = 8.1, 1.2 Hz, 1H), 8.18 (dd, *J* = 4.9, 1.9 Hz, 1H), 7.82–7.79 (m, 2H), 7.77 (d, *J* = 8.4 Hz, 2H), 7.66–7.61 (m, 2H), 7.54–7.49 (m, 2H), 7.37 (t, *J* = 7.8 Hz, 2H), 7.09 (dd, *J* = 7.4, 4.9 Hz, 1H), 2.2 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 192.0 (C_q), 161.6 (C_q), 151.5 (C_q), 148.3 (CH), 137.6 (C_q), 137.5 (CH), 137.0 (C_q), 136.3 (C_q), 133.6 (CH), 133.6 (CH), 133.3 (CH), 129.4 (CH), 128.8 (CH), 128.6 (CH), 128.6 (CH), 128.2 (CH), 126.6 (C_q), 124.5 (CH), 124.1 (CH), 123.1 (CH), 112.6 (C_q), 14.2 (CH_3). **IR** 3061, 3013, 1665, 1434, 1317, 1208, 777, 767, 722, 692 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 341 (100) $[M+H]^+$, 363 (4) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{22}H_{16}N_2O_2$ $[M+H]^+$ 341.1287, found 341.1285.

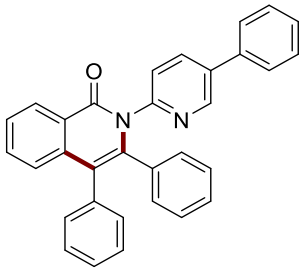


3-(Hydroxymethyl)-4-phenyl-2-(pyridin-2-yl)isoquinolin-1(2*H*)-one (36): The

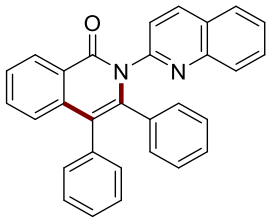
general procedure was followed using **1** (79.3 mg, 0.40 mmol) and **2m** (79.2 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 1:1) yielded **36** (35.0 mg, 27%) as colorless solid. **M.p.** = 239–240 °C. **^{1}H NMR** (600 MHz, DMSO-d_6) δ = 8.33–8.27 (m, 2H), 8.09 (d, J = 8.2 Hz, 1H), 7.87 (t, J = 7.6 Hz, 1H), 7.72 (t, J = 7.8 Hz, 1H), 7.62 (t, J = 7.7 Hz, 1H), 7.35 (d, J = 7.9 Hz, 1H), 7.25–7.17 (m, 6H), 4.92 (t, J = 4.9 Hz, 1H), 4.31 (s, 2H). **^{13}C NMR** (150 MHz, DMSO-d_6) δ = 161.5 (C_q), 152.4 (C_q), 148.7 (CH), 141.4 (C_q), 137.8 (CH), 136.8 (C_q), 133.3 (C_q), 133.0 (CH), 128.1 (CH), 127.4 (CH), 127.4 (CH), 127.4 (CH), 127.3 (CH), 127.3 (CH), 127.0 (CH), 125.4 (CH), 125.4 (C_q), 125.0 (CH), 123.2 (CH), 113.9 (C_q), 57.4 (CH_2). **IR** (KBr): 3408, 3053, 1644, 1589, 1471, 1434, 1341, 1026, 997, 773, 698 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 329 (36) $[M+H]^+$, 351 (100) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{21}H_{16}N_2O_2$ $[M+H]^+$ 329.1285, found 329.1285.



3-Methyl-2-(pyridin-2-yl)isoquinolin-1(*2H*)-one (37): The general procedure was followed using **1** (79.3 mg, 0.40 mmol) and **2o** (51.7 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **37** (65.0 mg, 69%) as colorless solid. The NMR data is identical to that previously reported.[16] **M.p.** = 118–119 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.67 (d, J = 4.8 Hz, 1H), 8.36 (d, J = 8.1 Hz, 1H), 7.90 (td, J = 7.7, 1.9 Hz, 1H), 7.63 (ddd, J = 8.3, 7.1, 1.4 Hz, 1H), 7.46 (d, J = 7.1 Hz, 1H), 7.43–7.38 (m, 3H), 6.42 (s, 1H), 2.01 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 163.7 (C_q), 152.5 (C_q), 150.0 (CH), 138.8 (C_q), 138.7 (CH), 137.5 (C_q), 132.9 (CH), 128.2 (CH), 126.3 (CH), 125.4 (CH), 124.9 (C_q), 124.3 (CH), 124.0 (CH), 106.0 (CH), 20.8 (CH_3). **IR** (KBr): 3052, 1667, 1586, 1496, 1436, 1309, 995, 821, 749, 694 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 237 (100) $[M+H]^+$, 259 (3) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{15}H_{12}N_2O$ $[M+H]^+$ 237.1023, found 237.1022.

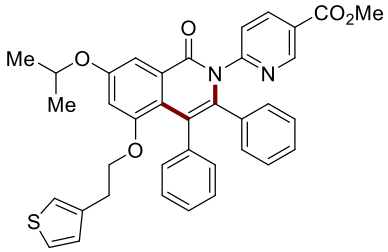


3,4-Diphenyl-2-(5-phenylpyridin-2-yl)isoquinolin-1(2*H*)-one (38): The general procedure was followed using **BC-1** (110 mg, 0.40 mmol) and **2** (107 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **38** (164 mg, 91%) as yellowish solid. **M.p.** = 274–275 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.61 (s, 1H), 8.59 (dd, J = 8.0, 1.5 Hz, 1H), 7.79 (dd, J = 8.1, 2.5 Hz, 1H), 7.61 (ddd, J = 8.4, 7.2, 1.5 Hz, 1H), 7.54 (ddd, J = 8.4, 8.0, 2.5 Hz, 1H), 7.49 (d, J = 7.1 Hz, 2H), 7.44 (t, J = 7.7 Hz, 2H), 7.38 (t, J = 7.3 Hz, 1H), 7.28 (dd, J = 8.4, 2.5 Hz, 2H), 7.23 (t, J = 7.4 Hz, 2H), 7.21–7.15 (m, 3H), 7.13–6.88 (m, 5H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 162.9 (C_q), 151.8 (C_q), 147.5 (CH), 140.2 (C_q), 138.0 (C_q), 137.0 (C_q), 136.2 (C_q), 136.0 (CH), 135.9 (C_q), 134.5 (C_q), 132.9 (CH), 131.8 (CH), 131.8 (CH), 129.2 (CH), 129.2 (CH), 128.4 (CH), 128.4 (CH), 128.3 (CH), 128.1 (CH), 128.1 (CH), 127.5 (CH), 127.3 (CH), 127.3 (CH), 127.3 (CH), 127.1 (CH), 127.1 (CH), 127.1 (CH), 127.1 (CH), 125.8 (CH), 125.7 (C_q), 124.8 (CH), 119.2 (C_q). **IR** (KBr): 3027, 1657, 1585, 1470, 1328, 1159, 1030, 784, 759, 700 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 451 (100) $[M+H]^+$, 473(1) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{32}H_{22}N_2O$ $[M+H]^+$ 451.1810, found 451.1805.



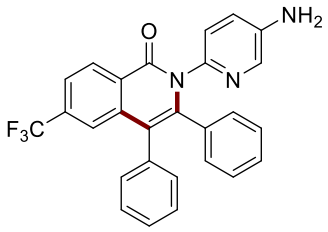
3,4-Diphenyl-2-(quinolin-2-yl)isoquinolin-1(2*H*)-one (39): The general procedure was followed using **BC-2** (99.3 mg, 0.40 mmol) and **2** (107 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **39** (142 mg, 84%) as colorless solid. **M.p.** = 251–252 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.58 (d, J = 7.9 Hz, 1H), 8.07 (d, J = 8.4 Hz, 1H), 7.91 (d, J = 8.5 Hz, 1H), 7.73 (d, J = 8.1 Hz, 1H),

7.65–7.58 (m, 2H), 7.54 (t, *J* = 7.6 Hz, 1H), 7.49 (t, *J* = 7.5 Hz, 1H), 7.38 (d, *J* = 8.4 Hz, 1H), 7.28 (d, *J* = 8.2 Hz, 1H), 7.23 (t, *J* = 7.5 Hz, 2H), 7.20–7.15 (m, 3H), 7.13–6.90 (m, 2H), 6.80 (t, *J* = 7.5 Hz, 2H), 6.77–6.72 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 163.0 (C_q), 152.3 (C_q), 147.2 (C_q), 140.2 (C_q), 138.0 (C_q), 137.9 (CH), 136.2 (C_q), 134.3 (C_q), 132.9 (CH), 131.8 (CH), 131.8 (CH), 129.8 (CH), 129.2 (CH), 128.2 (CH), 128.1 (CH), 128.1 (CH), 127.5 (CH), 127.4 (CH), 127.4 (CH), 127.3 (CH), 127.3 (CH), 127.1 (C_q), 127.1 (CH), 127.1 (CH), 127.1 (CH), 125.8 (CH), 125.8 (CH), 125.8 (C_q), 122.5 (CH), 119.4 (C_q). **IR** (KBr): 3057, 1665, 1586, 1492, 1330, 816, 762, 738, 701 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 425 (100) $[M+H]^+$, 447 (1) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{30}H_{20}N_2O$ $[M+H]^+$ 425.1653, found 425.1648.

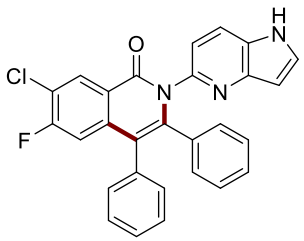


Methyl-6-(7-isopropoxy-1-oxo-3,4-diphenyl-5-(2-(thiophen-3-yl)ethoxy) isoquinolin-2(1*H*)-yl)nicotinate (40): The general procedure was followed using **BC-3** (88.2 mg, 0.20 mmol) and **2** (53.5 mg, 0.30 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **40** (48.0 mg, 39%) as colorless solid. **M.p.** = 190–191 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.97 (d, *J* = 2.3 Hz, 1H), 8.17 (dd, *J* = 8.3, 2.3 Hz, 1H), 7.64 (s, 1H), 7.27 (d, *J* = 3.8 Hz, 1H), 7.20 (dd, *J* = 4.9, 2.9 Hz, 1H), 7.07–7.06 (m, 2H), 7.03–6.99 (m, 3H), 6.92–6.88 (m, 2H), 6.87–6.83 (m, 3H), 6.80 (d, *J* = 2.9 Hz, 1H), 6.77 (d, *J* = 4.9 Hz, 1H), 6.67 (s, 1H), 4.76 (p, *J* = 6.1 Hz, 1H), 3.90 (s, 3H), 3.78 (t, *J* = 7.4 Hz, 2H), 2.19 (t, *J* = 7.4 Hz, 2H), 1.39 (d, *J* = 6.1 Hz, 6H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 165.2 (C_q), 162.0 (C_q), 158.0 (C_q), 157.0 (C_q), 156.6 (C_q), 150.5 (CH), 140.1 (C_q), 138.7 (CH), 138.2 (C_q), 137.3 (C_q), 134.3 (C_q), 131.0 (CH), 131.0 (CH), 128.3 (CH), 128.3 (CH), 127.3 (C_q),127.0 (CH), 127.0 (CH), 127.0 (CH), 126.8 (CH), 126.8 (CH), 126.8 (CH), 125.7 (CH), 125.5 (CH), 125.0 (C_q), 124.8 (CH), 121.8 (C_q), 121.3 (CH), 117.5 (C_q), 107.5 (CH), 102.5 (CH), 70.3 (CH), 68.5

(CH_2), 52.6 (CH_3), 29.0 (CH_2), 22.1 (CH_3). **IR** (KBr): 2976, 1736, 1650, 1593, 1491, 1371, 1281, 1117, 1057, 759, 700 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 617 (42) $[M+H]^+$, 639 (100) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{37}H_{32}N_2O_5S$ $[M+H]^+$ 617.2108, found 617.2105.

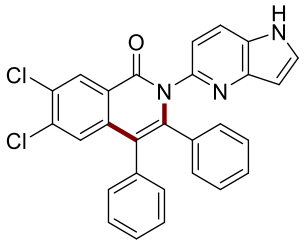


2-(5-Aminopyridin-2-yl)-3,4-diphenyl-6-(trifluoromethyl)isoquinolin-1(2*H*)-one (41): The general procedure was followed using **BC-4** (61.0 mg, 0.20 mmol) and **2** (53.5 mg, 0.30 mmol). Purification by column chromatography (PE/EtOAc = 1:1) yielded **41** (48.4 mg, 53%) as colorless solid. **M.p.** = 290–291 °C. **^{1}H NMR** (600 MHz, DMSO-d_6) δ = 8.55 (d, J = 8.4 Hz, 1H), 7.89 (d, J = 8.4 Hz, 1H), 7.59 (s, 1H), 7.33–7.20 (m, 5H), 7.17–7.05 (m, 2H), 7.02–6.90 (m, 5H), 6.79 (d, J = 8.4 Hz, 1H), 5.38 (s, 2H). **^{13}C NMR** (150 MHz, DMSO-d_6) δ = 161.0 (C_q), 144.3 (C_q), 143.4 (C_q), 140.1 (C_q), 137.7 (C_q), 135.1 (C_q), 134.0 (C_q), 132.5 (q, $^2J_{C–F}$ = 31.5 Hz, C_q), 131.3 (CH), 131.3 (CH), 129.3 (CH), 128.3 (CH), 128.3 (CH), 128.3 (CH), 127.5 (CH), 127.5 (CH), 127.4 (CH), 127.4 (CH), 126.8 (CH), 124.5 (CH), 124.5 (CH), 124.6 (C_q), 123.7 (q, $^1J_{C–F}$ = 271.5 Hz, C_q), 122.6 (q, $^3J_{C–F}$ = 3.5 Hz, CH), 121.7 (q, $^3J_{C–F}$ = 3.0 Hz, CH), 121.1 (CH), 116.8 (C_q). **IR** (KBr): 3022, 1662, 1486, 1316, 1282, 1170, 1067, 929, 794, 700 cm^{-1}. **^{19}F NMR** (564 MHz, DMSO-d_6) δ = -61.80 (s). **MS** (ESI) *m/z* (relative intensity): 458 (100) $[M+H]^+$, 480(50) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{27}H_{18}F_3N_3O$ $[M+H]^+$ 458.1487, found 458.1475.



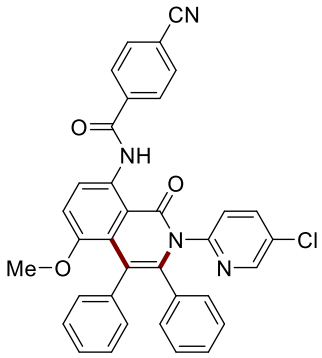
7-Chloro-6-fluoro-3,4-diphenyl-2-(1*H*-pyrrolo[3,2-b]pyridin-5-yl)isoquinolin-

1(2*H*)-one (42): The general procedure was followed using **BC-5** (116 mg, 0.40 mmol) and **2** (107 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 1:1) yielded **42** (167 mg, 90%) as yellow solid. **M.p.** = 316–317 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 9.40 (s, 1H), 8.63 (d, J = 7.5 Hz, 1H), 7.24–7.17 (m, 3H), 7.12 (d, J = 7.7 Hz, 1H), 7.09–7.00 (m, 5H), 6.88 (d, J = 7.7 Hz, 1H), 6.83–6.74 (m, 3H), 6.71 (d, J = 8.3 Hz, 1H), 6.32 (s, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 162.1 (C_q), 160.9 (d, $^1J_{C–F}$ = 255.0 Hz, C_q), 145.2 (C_q), 145.1 (C_q), 142.8 (CH), 138.9 (d, $^3J_{C–F}$ = 9.1 Hz, CH), 135.5 (C_q), 133.8 (C_q), 131.6 (C_q), 131.4 (d, $^2J_{C–F}$ = 24.0 Hz, C_q), 131.3 (C_q), 130.9 (CH), 130.9 (CH), 130.3 (C_q), 129.9 (CH), 128.5 (CH), 128.3 (CH), 127.6 (CH), 127.5 (CH), 127.4 (CH), 127.2 (CH), 127.0 (CH), 122.9 (d, $^4J_{C–F}$ = 2.1 Hz, C_q), 121.2 (d, $^2J_{C–F}$ = 19.5 Hz, C_q), 120.3 (CH), 118.4 (d, $^4J_{C–F}$ = 3.0 Hz, C_q), 116.3 (CH), 112.5 (d, $^2J_{C–F}$ = 23.3 Hz, CH), 102.5 (CH). **^{19}F NMR** (564 MHz, $CDCl_3$) δ = -107.8 (t, J = 9.6 Hz). **IR** (KBr): 3024, 1647, 1590, 1443, 1345, 1145, 1025, 874, 763, 699 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 466 (100) $[M+H]^+$, 324 (64), 301 (35), 279 (88), 149 (13). **HR-MS** (ESI) *m/z* calcd for $C_{28}H_{17}{}^{35}ClFN_3O$ $[M+H]^+$ 466.1124, found 466.1117.

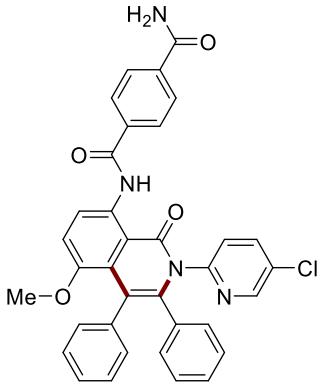


6,7-Dichloro-3,4-diphenyl-2-(1*H*-pyrrolo[3,2-*b*]pyridin-5-yl)isoquinolin-1(2*H*)-one (43): The general procedure was followed using **BC-6** (122 mg, 0.40 mmol) and **2** (107 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 1:1) yielded **43** (175 mg, 91%) as yellowish solid. **M.p.** = 348–349 °C. **^{1}H NMR** (600 MHz, DMSO-d_6) δ = 11.35 (s, 1H), 8.45 (s, 1H), 7.67 (d, J = 8.2 Hz, 1H), 7.60 (s, 1H), 7.28–7.24 (m, 3H), 7.21 (d, J = 7.1, 1H), 7.19 (s, 1H), 7.17–7.11 (m, 2H), 7.08 (d, J = 8.4 Hz, 1H), 7.02 (s, 1H), 6.88–6.86 (m, 1H), 6.82–6.80 (m, 2H), 6.45–6.42 (m, 1H). **^{13}C NMR** (150 MHz, DMSO-d_6) δ = 160.3 (C_q), 145.0 (C_q), 144.6 (C_q), 143.3 (C_q), 137.4 (CH), 136.1 (C_q), 135.0 (C_q), 133.7 (C_q), 131.4 (CH), 131.3 (C_q), 130.9 (C_q), 130.3 (CH), 130.1 (C_q), 129.6 (CH), 129.1 (CH), 128.3 (CH), 128.3 (CH), 127.5 (CH), 127.5 (CH),

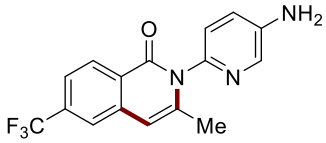
127.4 (CH), 127.2 (CH), 126.7 (C_q), 126.6 (CH), 124.8 (CH), 119.7 (C_q), 117.1 (CH), 115.9 (CH), 101.6 (CH). **IR** (KBr): 3020, 1645, 1561, 1458, 1342, 1126, 1030, 891, 720, 696 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 482 (100) $[M+H]^+$, 324 (18), 279 (34), 177 (15). **HR-MS** (ESI) *m/z* calcd for $C_{28}H_{17}{}^{35}Cl_2N_3O$ $[M+H]^+$ 482.0829, found 482.0821.



***N*-(2-(5-chloropyridin-2-yl)-5-methoxy-1-oxo-3,4-diphenyl-1,2-dihydroisoquinol-in-8-yl)-4-cyanobenzamide (44):** The general procedure was followed using **BC-7** (81.0 mg, 0.20 mmol) and **2** (53.5 mg, 0.30 mmol). Purification by column chromatography (PE/EtOAc = 1:1) yielded **44** (65.3 mg, 56%) as golden solid. **M.p.** = 268–269 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 13.85 (s, 1H), 9.03 (d, J = 9.1 Hz, 1H), 8.38 (d, J =2.7 Hz, 1H), 8.12 (d, J = 8.1 Hz, 2H), 7.73 (d, J =8.1 Hz, 2H), 7.56 (dd, J = 8.4, 2.6 Hz, 1H), 7.19 (d, J =9.1 Hz, 1H), 7.09–7.04 (m, 3H), 7.03–7.00 (m, 3H), 6.93–6.82 (m, 5H), 3.30 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 164.8 (C_q), 163.8 (C_q), 152.1 (C_q), 150.5 (C_q), 148.3 (CH), 140.3 (C_q), 139.7 (C_q), 139.4 (C_q), 137.8 (CH), 135.3 (C_q), 133.5 (C_q), 132.6 (C_q), 131.7 (CH), 131.7 (CH), 130.3 (C_q), 128.9 (C_q), 128.3 (CH), 128.3 (CH), 127.8 (CH), 127.8 (CH), 127.8 (CH), 127.8 (CH), 127.3 (CH), 127.3 (CH), 127.3 (CH), 127.3 (CH), 126.8 (CH), 125.8 (CH), 125.6 (CH), 119.3 (CH), 118.6 (CH), 118.4 (C_q), 117.8 (CH), 114.9 (C_q), 114.3 (C_q), 56.6 (CH_3). **IR** (KBr): 3392, 3022, 1655, 1486, 1316, 1281, 1170, 1067, 904, 794, 700 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 583 (100) $[M+H]^+$, 605 (8) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{35}H_{23}{}^{35}ClN_4O_3$ $[M+H]^+$ 583.1539, found 583.1531.

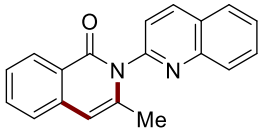


4-Carbamimidoyl-*N*-(2-(5-chloropyridin-2-yl)-5-methoxy-1-oxo-3,4-diphenyl-1,2-dihydroisoquinolin-8-yl)benzamide (45): The general procedure was followed using **BC-8** (150 mg, 0.27 mmol) and **2** (73.1 mg, 0.41 mmol). Purification by column chromatography (PE/EtOAc = 1:1) yielded **45** (31.6 mg, 20%) as brown solid. **M.p.** = 319–320 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 13.74 (s, 1H), 9.04 (d, J = 9.1 Hz, 1H), 8.37 (d, J =2.6 Hz, 1H), 8.09 (d, J = 8.1 Hz, 2H), 7.86 (d, J = 8.1 Hz, 2H), 7.55 (dd, J = 8.4, 2.6 Hz, 1H), 7.20 (d, J =9.1 Hz, 1H), 7.08 (d, J =8.4 Hz, 1H), 7.05 (d, J = 6.9 Hz, 2H), 7.03–7.00 (m, 3H), 6.94–6.84 (m, 5H), 6.18 (s, 1H), 5.73 (s, 1H), 3.29 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 168.6 (C_q), 164.8 (C_q), 164.8 (C_q), 151.9 (C_q), 150.7 (C_q), 148.3 (CH), 140.2 (C_q), 139.8 (C_q), 138.7 (C_q), 137.8 (CH), 135.9 (C_q), 135.7 (C_q), 133.6 (C_q), 131.7 (CH), 131.7 (CH), 130.4 (C_q), 128.9 (C_q), 128.0 (CH), 128.0 (CH), 127.9 (CH), 127.9 (CH), 127.9 (CH), 127.8 (CH), 127.8 (CH), 127.3 (CH), 127.3 (CH), 126.8 (CH), 126.8 (CH), 125.8 (CH), 125.7 (CH), 119.3 (CH), 118.5 (C_q), 118.0 (CH), 114.3 (C_q), 56.7 (CH_3). **IR** (KBr): 2955, 1654, 1611, 1490, 1459, 1383, 1316, 1272, 1134, 700 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 601 (62) $[M+H]^+$, 623 (100) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{35}H_{25}{}^{35}ClN_4O_4$ $[M+H]^+$ 601.1637, found 601.1637.

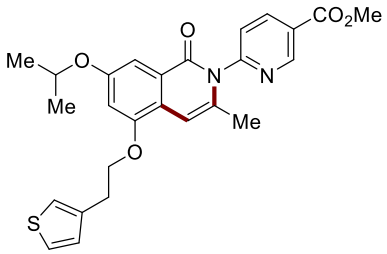


2-(5-Aminopyridin-2-yl)-3-methyl-6-(trifluoromethyl)isoquinolin-1(2*H*)-one (46): The general procedure was followed using **BC-4** (56.2 mg, 0.20 mmol) and **2o**

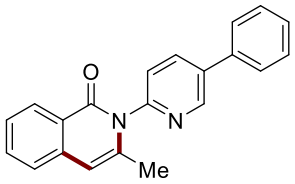
(25.9 mg, 0.30 mmol). Purification by column chromatography (PE/EtOAc = 1:1) yielded **46** (48.0 mg, 75%) as yellow solid. **M.p.** = 222–223 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.45 (d, J = 8.4 Hz, 1H), 8.03 (s, 1H), 7.72 (s, 1H), 7.59 (d, J = 8.4 Hz, 1H), 7.12–7.08 (m, 2H), 6.45 (s, 1H), 4.05 (s, 2H), 2.05 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 163.3 (C_q), 142.2 (C_q), 141.7 (C_q), 137.4 (C_q), 136.6 (CH), 134.3 (q, $^2J_{C–F}$ = 33.0 Hz, C_q), 129.3 (CH), 128.5 (C_q), 127.0 (C_q), 123.9 (q, $^1J_{C–F}$ = 272.2 Hz, C_q), 123.8 (CH), 123.7 (CH), 122.7 (q, $^3J_{C–F}$ = 4.4 Hz, CH), 122.1 (q,$^3J_{C–F}$ = 3.4 Hz, CH), 105.3 (CH), 21.0 (CH_3). **^{19}F NMR** (564 MHz, $CDCl_3$) δ = -63.07 (s). **IR** (KBr): 2957, 2925, 1670, 1570, 1484, 1320, 1114, 1073, 893, 699 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 320 (37) $[M+H]^+$, 342 (100) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{16}H_{12}F_3N_3O$ $[M+Na]^+$ 342.0825, found 342.0826.



3-Methyl-2-(quinolin-2-yl)isoquinolin-1(2*H*)-one (47): The general procedure was followed using **BC-2** (99.3 mg, 0.40 mmol) and **2o** (51.7 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc = 2:1) yielded **47** (104 mg, 91%) as colorless solid. **M.p.** = 165–166 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.38 (d, J = 8.0 Hz, 1H), 8.35 (d, J = 8.5 Hz, 1H), 8.11 (d, J = 8.4 Hz, 1H), 7.93 (dd, J = 8.2, 1.4 Hz, 1H), 7.77 (ddd, J = 8.4, 6.8, 1.4 Hz, 1H), 7.66–7.62 (m, 2H), 7.49 (d, J = 3.0 Hz, 1H), 7.48 (d, J = 2.6 Hz, 1H), 7.44 (t, J = 6.0 Hz, 1H), 6.47 (s, 1H), 2.07 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 163.8 (C_q), 151.9 (C_q), 147.6 (C_q), 138.9 (CH), 138.7 (C_q), 137.5 (C_q), 132.9 (CH), 130.2 (CH), 129.5 (CH), 128.1 (CH), 127.9 (C_q), 127.7 (CH), 127.7 (CH), 126.3 (CH), 125.5 (CH), 125.0 (C_q), 121.7 (CH), 106.2 (CH), 20.8 (CH_3). **IR** (KBr): 2923, 1663, 1628, 1430, 1377, 1238, 958, 810, 746, 695 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 287 (100) $[M+H]^+$, 309 (87) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{19}H_{14}N_2O$ $[M+H]^+$ 287.1180, found 287.1179.



Methyl-6-(7-isopropoxy-3-methyl-1-oxo-5-(2-(thiophen-3-yl)ethoxy)isoquinolin-2(1*H*)-yl)nicotinate (48): The general procedure was followed using **BC-3** (88.2 mg, 0.20 mmol) and **2o** (25.9 mg, 0.30 mmol). Purification by column chromatography (PE/EtOAc = 5:1) yielded **48** (26.0 mg, 27%) as yellow solid. **M.p.** = 101–102 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 9.27 (s, 1H), 8.49 (dd, *J* = 8.1, 2.4 Hz, 1H), 7.49 (d, *J* = 8.1 Hz, 1H), 7.34 (d, *J* = 2.3 Hz, 1H), 7.30 (dd, *J* = 4.9, 2.9 Hz, 1H), 7.12 (d, *J* = 3.0 Hz, 1H), 7.06 (d, *J* = 4.9 Hz, 1H), 6.71–6.68 (m, 2H), 4.69 (p, *J* = 6.0 Hz, 1H), 4.27 (t, *J* = 6.7 Hz, 2H), 4.00 (s, 3H), 3.23 (t, *J* = 6.7 Hz, 2H), 2.00 (s, 3H), 1.35 (d, *J* = 6.0 Hz, 6H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 165.2 (C_q), 163.0 (C_q), 157.2 (C_q), 156.1 (C_q), 154.7 (C_q), 151.2 (CH), 139.6 (CH), 138.5 (C_q), 134.8 (C_q), 128.5 (CH), 126.4 (C_q), 126.2 (C_q), 125.8 (CH), 124.2 (CH), 122.9 (C_q), 121.8 (CH), 106.0 (CH), 101.5 (CH), 100.6 (CH), 70.3 (CH), 68.8 (CH_2), 52.8 (CH_3), 30.3 (CH_2), 22.1 (CH_3), 22.1 (CH_3), 20.8 (CH_3). **IR** (KBr): 2923, 1728, 1663, 1607, 1566, 1379, 1280, 1117, 1024, 847, 782 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 479 (76) $[M+H]^+$, 501 (100) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{26}H_{26}N_2O_5S$ $[M+H]^+$ 479.1636, found 479.1635.

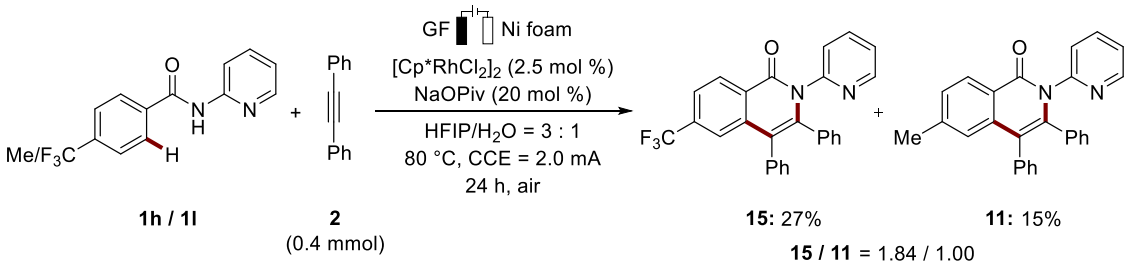


3-Methyl-2-(5-phenylpyridin-2-yl)isoquinolin-1(2*H*)-one (49): The general procedure was followed using **BC-1** (110 mg, 0.40 mmol) and **2o** (51.7 mg, 0.60 mmol). Purification by column chromatography (PE/EtOAc/DCM = 5:1:1) yielded **49** (76.0 mg, 61%) as colorless solid. **M.p.** = 171–172 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.88 (s, 1H), 8.39 (d, *J* = 8.0 Hz, 1H), 8.08 (dd, *J* = 8.1, 2.5 Hz, 1H), 7.66–

7.63 (m, 3H), 7.52 (t, J = 7.6 Hz, 2H), 7.49–7.42 (m, 4H), 6.45 (s, 1H), 2.09 (s, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 163.7 (C_q), 151.4 (C_q), 148.2 (CH), 138.8 (C_q), 137.5 (C_q), 137.1 (C_q), 137.0 (CH), 137.0 (C_q), 132.9 (CH), 129.3 (CH), 129.3 (CH), 128.6 (CH), 128.2 (CH), 127.4 (CH), 127.4 (CH), 126.3 (CH), 125.4 (CH), 124.9 (C_q), 124.0 (CH), 106.0 (CH), 20.9 (CH_3). **IR** (KBr): 3056, 2926, 1663, 1628, 1476, 1382, 1190, 804, 745, 693 cm^{-1}. **MS** (ESI) *m/z* (relative intensity): 313 (100) $[M+H]^+$, 335 (65) $[M+Na]^+$. **HR-MS** (ESI) *m/z* calcd for $C_{21}H_{16}N_2O$ $[M+H]^+$ 313.1339, found 313.1335.

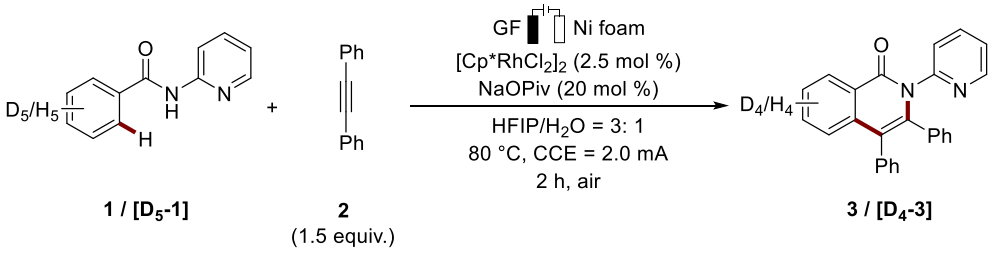
6. Mechanistic Studies

6.1 Competition Experiments



The electrocatalysis was carried out in an undivided cell with a GF anode (10 mm × 15 mm × 3.0 mm) and a Ni foam cathode (10 mm × 15 mm × 1.5 mm). The cell was charged with *N*-(pyridin-2-yl)benzamide **1h** (0.40 mmol), *N*-(pyridin-2-yl)benzamide **1l** (0.40 mmol), alkyne **2** (0.40 mmol, 1.0 equiv), NaOPiv (9.93 mg, 0.08 mmol, 20 mol %), $[Cp^*RhCl_2]_2$ (6.18 mg, 0.01 mmol, 2.5 mol %) and a HFIP/H_2O solvent mixture (3/1, 4.0 mL). Electrocatalysis was performed at 80 °C with a constant current of 2.0 mA maintained for 24 h. The electrodes were washed with dichloromethane (3 × 4.0 mL) in an ultrasonic bath. The combined mixtures were filtered and concentrated under reduced pressure at 50 °C. The residue was purified by column chromatography on silica gel (PE/EtOAc = 2:1) affording **15** (47.7 mg) and **11** (23.3 mg). Accordingly, the yields of **15** and **11** were calculated to be 27% and 15%, respectively, and the ratio between **15** and **11** was 1.84/1.00.

6.2 Kinetic Isotope Effect (KIE) Experiments



The model reaction using substrates **1** (0.40 mmol) or substrates [D_5]-**1** (0.40 mmol) were carried out to determine the KIE by comparison of the initial rates, after 20 minutes at a stable constant current of 2.0 mA. The conversions were determined by **^{1}H NMR** measurement using 1,3,5-trimethoxybenzene (0.10 mmol) as the internal standard.

Table SI-1

Time/min	20	40	60	80	100	120
3/%	4.10	6.21	8.63	10.84	13.58	16.84

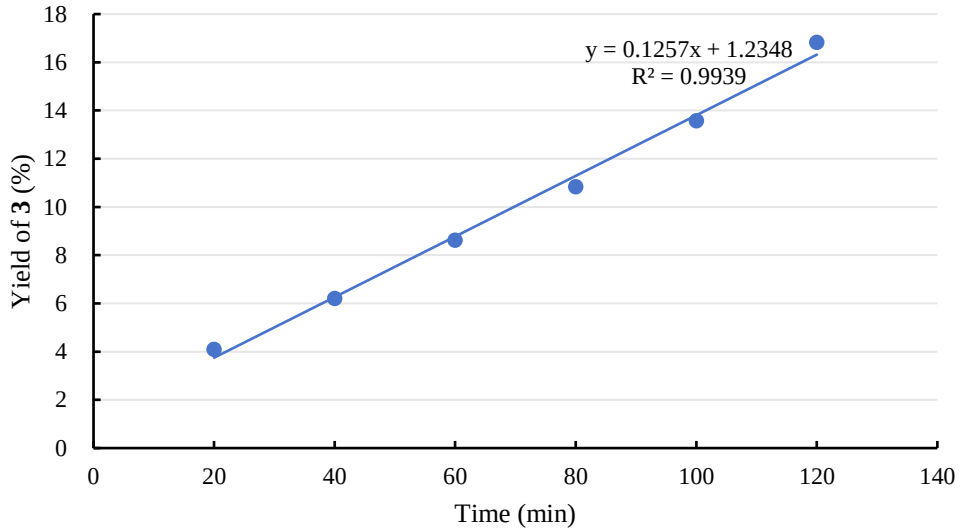


Figure SI-2. Linear function fit for the reaction rate of **3**.

Table SI-2

Time/min	20	40	60	80	100	120
[D_4]-**3**/%	3.58	5.58	7.37	10.00	12.31	14.63

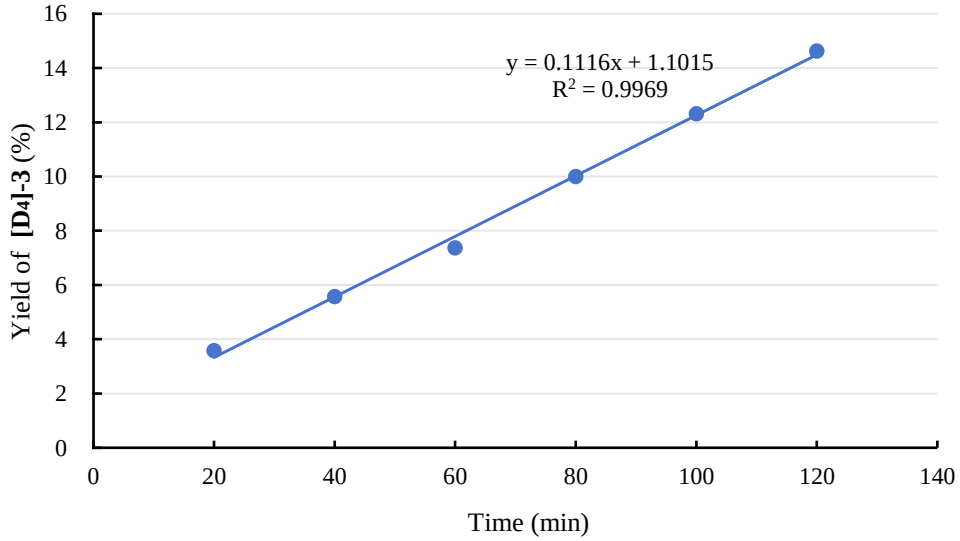
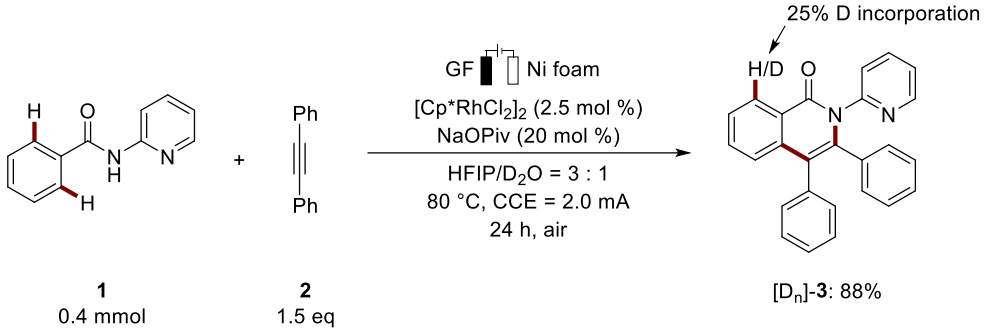


Figure SI-3. Linear function fit for the reaction rate of [D_4]-**3**.

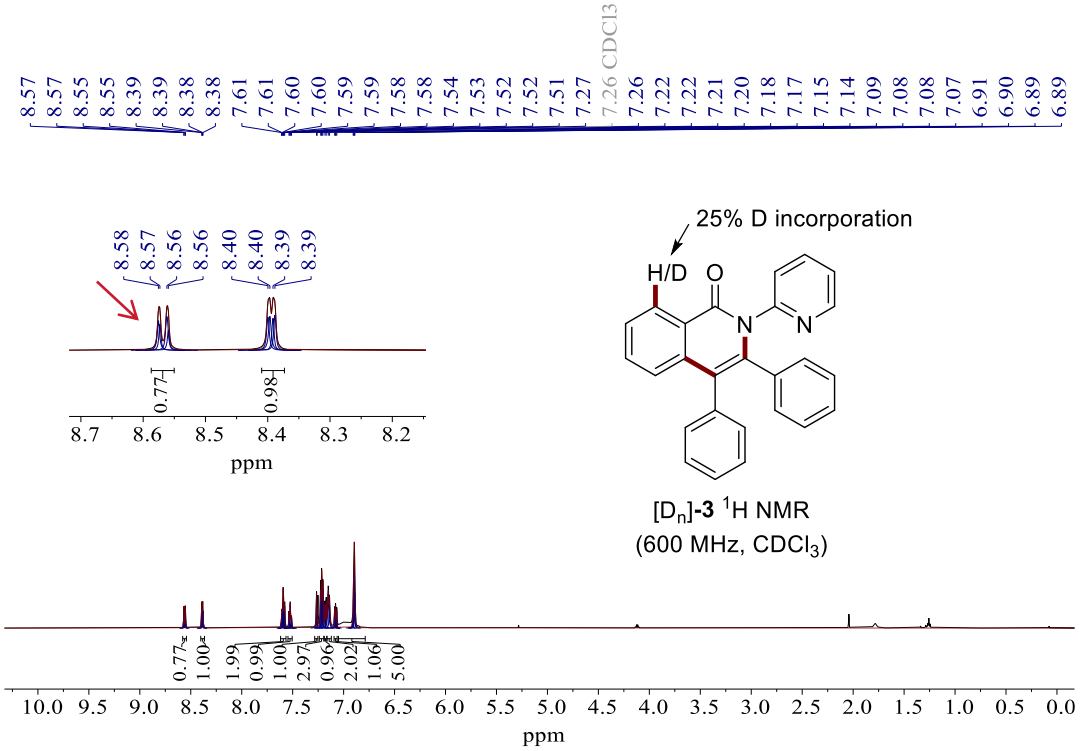
The intermolecular isotope effect value is determined to be 1.13.

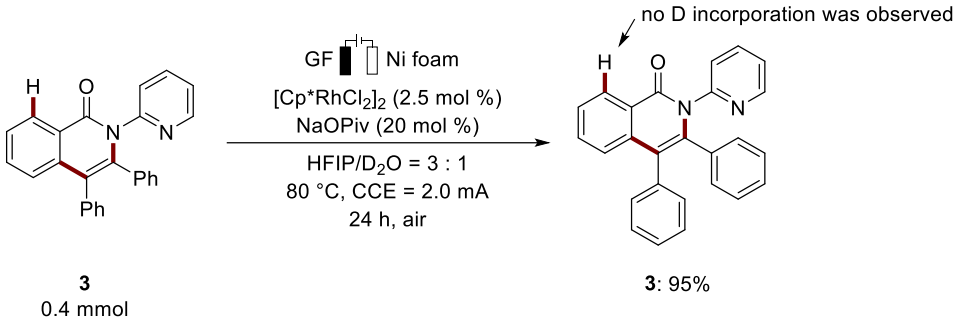
k_H/k_D = (0.1257)/(0.1116) = 1.13

6.3 H/D Exchange Experiments

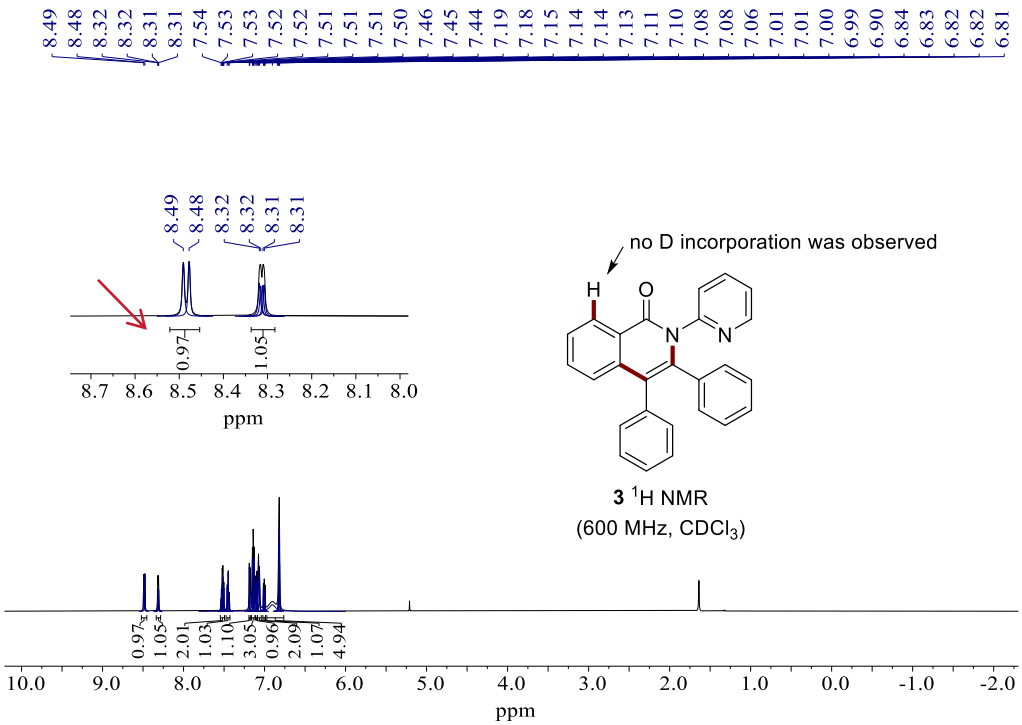


The electrocatalysis was carried out in an undivided cell with a GF anode (10 mm × 15 mm × 3.0 mm) and a Ni foam cathode (10 mm × 15 mm × 1.5 mm). The cell was charged with *N*-(pyridin-2-yl)benzamide **1** (0.40 mmol), alkyne **2** (0.60 mmol, 1.50 equiv.), NaOPiv (9.93 mg, 0.08 mmol, 20 mol %), $[Cp^*RhCl_2]_2$ (6.18 mg, 0.01 mmol, 2.5 mol %) and a HFIP/D_2O solvent mixture (3/1, 4.0 mL). Electrocatalysis was performed at 80 °C with a constant current of 2.0 mA maintained for 24 h. The electrodes were washed with dichloromethane (3 × 4.0 mL) in an ultrasonic bath. The combined mixtures were filtered and concentrated under reduced pressure at 50 °C. Purification by column chromatography (PE/EtOAc = 2/1) yielded $[D_n]$-**3** (132 mg, 88%) as a colorless solid.





The electrocatalysis was carried out in an undivided cell with a GF anode (10 mm × 15 mm × 3.0 mm) and a Ni foam cathode (10 mm × 15 mm × 1.5 mm). The cell was charged with 3,4-diphenyl-2-(pyridin-2-yl)isoquinolin-1(2*H*)-one **3** (0.40 mmol), NaOPiv (9.93 mg, 0.08 mmol, 20 mol %), $[Cp^*RhCl_2]_2$ (6.18 mg, 0.01 mmol, 2.5 mol %) and a HFIP/D_2O solvent mixture (3/1, 4.0 mL). Electrocatalysis was performed at 80 °C with a constant current of 2.0 mA maintained for 24 h. The electrodes were washed with dichloromethane (3 × 4.0 mL) in an ultrasonic bath. The combined mixtures were filtered and concentrated under reduced pressure at 50 °C. Purification by column chromatography (PE/EtOAc = 2/1) yielded **3** (142 mg, 95%) as a colorless solid.



7. DFT Calculations

All DFT calculations were performed with Gaussian 16, Revision A.03 package.[17] Geometry optimizations were conducted at the PBE0[18] level of theory in combination with Grimme's D3 dispersion corrections with a Becke-Johnson damping scheme (D3BJ)[19] in the gas phase. All atoms were described with a def2-SVP basis set.[20] The vibrational frequencies were computed at the same level of theory to identify each stationary point as either intermediate (zero imaginary frequencies) or transition states (one imaginary frequency) and further provide the thermal and nonthermal corrections at 353.15 K. The single-point energies were further evaluated with PBE0[18] functional in combination with a standalone version of Grimme's D4 dispersion corrections,[21] with a def2-TZVP basis set.[20] Solvent effects were taken into account using the polarizable continuum model (PCM)[22] for the mixed solvent system of HFIP and water in a 3:1 ratio. Since specific PCM solvent parameters for HFIP are not available in Gaussian 16, the parameters were defined according to literature values[23] (dielectric constant at 298 K (i.e. "Eps", ε) was set to 16.7 and square of refractive index (i.e. "EpsInf", n^2) was set to 1.625625). The reported energies are based on gas phase Gibbs free energies with def2-SVP basis set for which the electronic energies were corrected by PBE0-D4 with a def2-TZVP basis set including solvent effects.

Transition state **TS1** was verified by intrinsic reaction coordinate (IRC) calculations,[24] which was shown below.

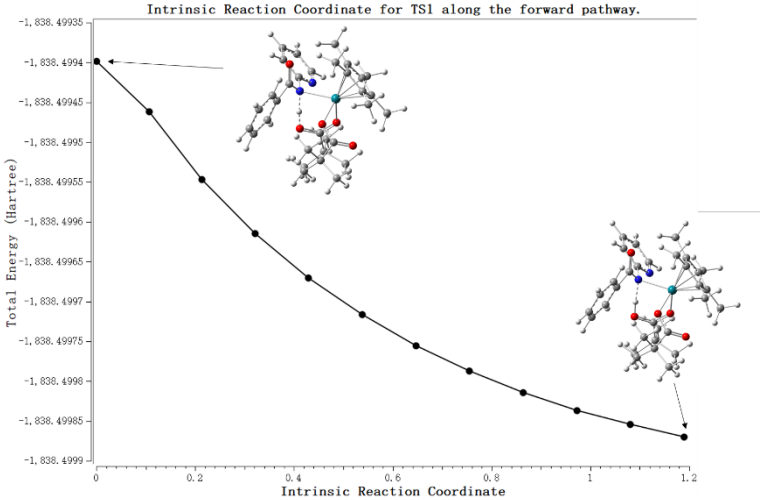


Figure SI-4. IRC results for the **TS1** along the forward pathway.

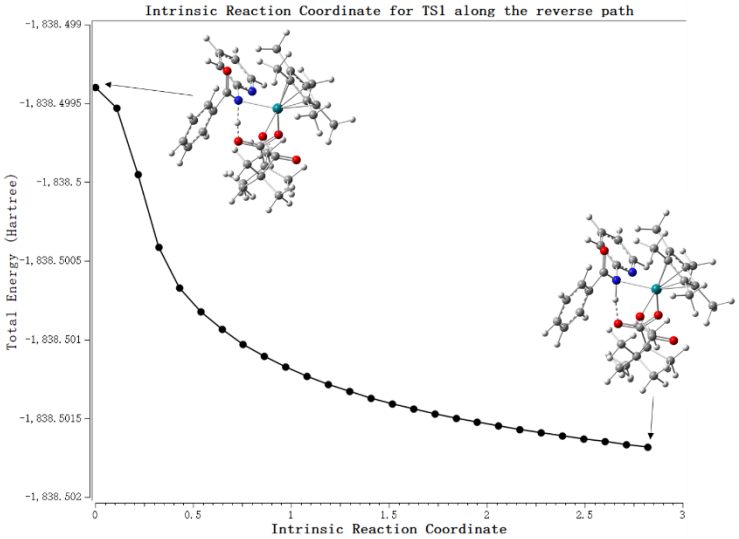


Figure SI-5. IRC results for the **TS1** along the reverse pathway.

Table SI-4. Calculated electronic energies at the PBE0-D4/def2-TZVP-PCM(HFIP/H_2O) level of theory and Gibbs free energies for all structures (all in Hartree).

Structure	Electronic Energy	Total Gibbs Free Energy
int1	-1192.810394	-1192.395495
int2	-1840.399753	-1839.801915
int3	-1840.388336	-1839.790421
TS1	-1840.384473	-1839.789244
int4	-1840.385178	-1839.787369
int5	-1493.583771	-1493.121073
TS2	-1493.572943	-1493.11289
int6	-1493.590422	-1493.126072
int7	-1685.828126	-1685.323785
TS3	-1685.810723	-1685.308037
int8	-1685.86699	-1685.359293
int9	-1685.88929	-1685.380095
TS4	-1685.849082	-1685.340004
int10	-1685.862965	-1685.353225
PivOH	-346.7829782	-346.6757592
benzamide	-647.5691104	-647.4190014
1,2-diphenylethyne	-539.0220241	-538.8751291

Cartesian Coordinates of the Optimized Structure

int1
Lowest frequency = 10.0983 cm^{-1}
Charge = 0, Multiplicity = 1

58

C	1.873514000	-1.969304000	-0.267154000
C	2.317194000	-0.986601000	-1.205366000
C	2.845826000	0.146697000	-0.460065000
C	2.693394000	-0.141544000	0.930629000
C	2.055776000	-1.437595000	1.060029000
C	1.201458000	-3.261101000	-0.569474000
C	2.273458000	-1.082714000	-2.690056000
C	3.425900000	1.374216000	-1.071415000
C	3.051595000	0.750006000	2.066242000
C	1.708516000	-2.136899000	2.327817000
C	-2.199435000	-0.753119000	-0.020845000
H	1.248623000	-3.502988000	-1.638652000
H	1.666678000	-4.083329000	-0.006120000
H	0.139583000	-3.187238000	-0.281760000
H	1.994671000	-0.118441000	-3.136983000
H	3.260957000	-1.368453000	-3.088742000
H	1.539798000	-1.828417000	-3.021690000
H	3.472662000	2.198303000	-0.347871000
H	4.448113000	1.183622000	-1.437245000
H	2.815860000	1.712951000	-1.920328000
H	4.012705000	0.439606000	2.507519000
H	3.141845000	1.794689000	1.743435000
H	2.285236000	0.711508000	2.852112000
H	0.807590000	-2.751821000	2.198646000
H	2.530723000	-2.795845000	2.653942000
H	1.509283000	-1.419929000	3.135457000

O	-0.974858000	-1.172761000	-0.027981000
C	-3.221519000	-1.912786000	-0.008978000
C	-4.632895000	-1.341766000	0.075455000
H	-5.375538000	-2.155829000	0.074451000
H	-4.763892000	-0.748824000	0.991958000
H	-4.838520000	-0.675515000	-0.773937000
C	-2.942593000	-2.810652000	1.199284000
H	-1.930949000	-3.238187000	1.148227000
H	-3.025079000	-2.244767000	2.140580000
H	-3.667960000	-3.639577000	1.238162000
C	-3.055226000	-2.715656000	-1.302884000
H	-3.776270000	-3.548735000	-1.334050000
H	-3.232186000	-2.081720000	-2.185890000
H	-2.040869000	-3.132479000	-1.382010000
O	-0.071581000	1.491699000	-1.088766000
C	-0.480550000	2.003997000	-0.005929000
C	-1.291696000	3.281601000	0.006702000
O	-0.099034000	1.457211000	1.073301000
C	-2.163224000	3.323839000	1.260333000
C	-2.149015000	3.354190000	-1.255414000
C	-0.271269000	4.431438000	0.026122000
H	-2.738398000	4.262786000	1.283565000
H	-2.858940000	2.473893000	1.261904000
H	-1.548915000	3.266344000	2.170075000
H	-1.524195000	3.316218000	-2.158964000
H	-2.845741000	2.505585000	-1.284351000
H	-2.722519000	4.294402000	-1.263555000
H	-0.798295000	5.398388000	0.033621000
H	0.364734000	4.381615000	0.923578000
H	0.376478000	4.401262000	-0.863695000

O	-2.570798000	0.408574000	-0.029594000
Rh	0.790392000	-0.133208000	-0.004828000

int2
Lowest frequency = 15.1394 cm^{-1}
Charge = 0, Multiplicity = 1

83

C	4.878563000	0.413648000	-0.984918000
C	6.020022000	0.166833000	-0.225058000
C	6.042122000	-0.891154000	0.686842000
C	4.924683000	-1.704714000	0.830076000
C	3.767657000	-1.438726000	0.089597000
C	2.616940000	-2.374698000	0.207941000
O	2.768488000	-3.556691000	0.445792000
H	4.925351000	-2.556508000	1.513361000
H	6.939317000	-1.084706000	1.279384000
H	6.902641000	0.799808000	-0.346100000
H	4.865448000	1.236014000	-1.703331000
C	0.331452000	-2.444171000	-0.641654000
C	0.417709000	-3.741148000	-1.190297000
C	-0.603456000	-4.188380000	-2.007182000
H	1.298253000	-4.343008000	-0.976914000
C	-1.745083000	-2.136891000	-1.627972000
C	-1.694198000	-3.355963000	-2.276886000
H	-0.536638000	-5.181376000	-2.458115000
H	-2.569731000	-1.438496000	-1.778053000
H	-2.492997000	-3.649140000	-2.958597000
N	-0.793315000	-1.720958000	-0.779373000
N	1.378107000	-1.807566000	-0.034060000
C	3.742954000	-0.378139000	-0.824090000

C	-3.538953000	-0.290436000	0.787536000
C	-2.876961000	-1.382444000	1.440727000
C	-1.951476000	-0.849632000	2.403894000
C	-2.106874000	0.586695000	2.396572000
C	-3.054125000	0.938788000	1.389677000
C	-4.583798000	-0.356072000	-0.272415000
C	-3.095100000	-2.834316000	1.194180000
C	-1.067110000	-1.627807000	3.316137000
C	-1.411585000	1.521367000	3.318926000
C	-3.462209000	2.318760000	1.014808000
C	-0.464263000	1.058598000	-2.056854000
H	-4.708972000	-1.375599000	-0.660327000
H	-5.559031000	-0.026620000	0.120158000
H	-4.318882000	0.302806000	-1.113237000
H	-2.145161000	-3.386000000	1.162053000
H	-3.699642000	-3.256780000	2.013045000
H	-3.624677000	-3.019910000	0.252115000
H	-0.126684000	-1.089648000	3.497634000
H	-1.552067000	-1.805189000	4.290780000
H	-0.808486000	-2.604246000	2.884515000
H	-1.929432000	1.517959000	4.292501000
H	-0.372919000	1.208340000	3.490130000
H	-1.399496000	2.541529000	2.920898000
H	-3.945791000	2.330362000	0.029918000
H	-4.167634000	2.732574000	1.753781000
H	-2.569514000	2.957047000	0.955839000
O	-1.514963000	0.886271000	-1.325207000
C	-0.696208000	2.050426000	-3.213011000
C	0.611881000	2.269839000	-3.965150000
H	0.455932000	2.961981000	-4.808135000

H	1.377988000	2.697330000	-3.301942000
H	1.007936000	1.321688000	-4.355590000
C	-1.203856000	3.371809000	-2.628907000
H	-2.162573000	3.224581000	-2.113032000
H	-0.496898000	3.775056000	-1.888784000
H	-1.341046000	4.116102000	-3.430246000
C	-1.751885000	1.452881000	-4.148784000
H	-1.946902000	2.132814000	-4.993937000
H	-1.416295000	0.487970000	-4.562121000
H	-2.697550000	1.287778000	-3.612103000
H	2.839609000	-0.171303000	-1.407257000
O	-0.344202000	2.724686000	0.692235000
C	0.572733000	1.951467000	0.932413000
C	1.950014000	2.520614000	1.321948000
O	0.481978000	0.658689000	0.880310000
C	2.817374000	1.501192000	2.052675000
C	1.732331000	3.743548000	2.214523000
C	2.601752000	2.964109000	0.005033000
H	3.789763000	1.948511000	2.313380000
H	2.336696000	1.170712000	2.987078000
H	3.009236000	0.612549000	1.442728000
H	1.059855000	4.460891000	1.725947000
H	1.283474000	3.459115000	3.180011000
H	2.694579000	4.236945000	2.424559000
H	3.630405000	3.316699000	0.182758000
H	2.633467000	2.138678000	-0.718056000
H	2.023260000	3.783381000	-0.447181000
O	0.618655000	0.505758000	-1.901828000
H	1.261386000	-0.784313000	0.061486000
Rh	-1.427668000	-0.112260000	0.466236000

int3
Lowest frequency = 22.8671 cm^{-1}
Charge = 0, Multiplicity = 1

83

C	3.296266000	2.453828000	2.163041000
C	4.065587000	3.334784000	1.406076000
C	3.543536000	3.890422000	0.236095000
C	2.252991000	3.570186000	-0.164837000
C	1.478259000	2.677816000	0.588716000
C	0.074673000	2.468749000	0.153536000
O	-0.466495000	3.240653000	-0.617989000
H	1.813944000	4.006482000	-1.063667000
H	4.147060000	4.577029000	-0.361804000
H	5.079396000	3.587822000	1.725761000
H	3.704526000	2.013878000	3.075435000
C	-1.956114000	1.573732000	1.175647000
C	-2.553396000	2.838668000	1.290295000
C	-3.836176000	2.909986000	1.818268000
H	-2.035017000	3.735697000	0.957723000
C	-3.793620000	0.544254000	2.075571000
C	-4.485009000	1.743633000	2.220520000
H	-4.326566000	3.881694000	1.915458000
H	-4.248223000	-0.404548000	2.383841000
H	-5.493205000	1.762369000	2.637870000
N	-2.571169000	0.464046000	1.563905000
N	-0.631173000	1.379191000	0.695788000
C	2.006618000	2.117712000	1.757496000
C	-1.276132000	-1.709940000	-2.308524000
C	-2.409893000	-0.976415000	-1.771442000

C	-2.231124000	0.396936000	-2.101122000
C	-0.988941000	0.540825000	-2.836140000
C	-0.429248000	-0.770212000	-2.995122000
C	-1.051782000	-3.174842000	-2.201561000
C	-3.518856000	-1.590200000	-0.991796000
C	-3.153006000	1.521663000	-1.795904000
C	-0.472037000	1.801303000	-3.435040000
C	0.811128000	-1.101291000	-3.743787000
C	-0.158736000	-1.518537000	1.810633000
H	-1.698916000	-3.614288000	-1.432535000
H	-1.267141000	-3.667784000	-3.163757000
H	-0.006246000	-3.359766000	-1.916605000
H	-4.201265000	-0.828308000	-0.596378000
H	-4.098335000	-2.282961000	-1.622252000
H	-3.109893000	-2.151829000	-0.138808000
H	-2.588368000	2.420500000	-1.514547000
H	-3.745535000	1.756403000	-2.695855000
H	-3.848654000	1.276770000	-0.983635000
H	-0.977539000	2.008470000	-4.393292000
H	-0.636328000	2.654844000	-2.763700000
H	0.606128000	1.730348000	-3.631110000
H	1.273269000	-2.013983000	-3.351220000
H	0.565871000	-1.241973000	-4.809801000
H	1.547088000	-0.289640000	-3.669354000
O	-0.633986000	-1.674270000	0.645274000
C	-0.211051000	-2.765622000	2.701793000
C	0.682081000	-2.570719000	3.923259000
H	0.617805000	-3.450110000	4.583340000
H	1.733235000	-2.438198000	3.627022000
H	0.383946000	-1.678805000	4.491054000

C	0.237389000	-3.985478000	1.895186000
H	-0.421265000	-4.146653000	1.031361000
H	1.256628000	-3.851703000	1.502632000
H	0.221397000	-4.886954000	2.528231000
C	-1.672512000	-2.929662000	3.139222000
H	-1.778045000	-3.810692000	3.792290000
H	-2.018544000	-2.044372000	3.694964000
H	-2.327959000	-3.063791000	2.265946000
H	1.425633000	1.411623000	2.351791000
O	1.784133000	-2.383935000	-1.106760000
C	2.182525000	-1.296925000	-0.709507000
C	3.654851000	-1.108026000	-0.295655000
O	1.456450000	-0.235590000	-0.567508000
C	4.169637000	0.250485000	-0.767586000
C	4.496311000	-2.230089000	-0.896544000
C	3.694408000	-1.190758000	1.235426000
H	5.215449000	0.394330000	-0.451527000
H	4.137425000	0.324056000	-1.866688000
H	3.565236000	1.067198000	-0.356948000
H	4.106858000	-3.213135000	-0.599928000
H	4.485412000	-2.189524000	-1.996704000
H	5.542062000	-2.142553000	-0.560812000
H	4.719106000	-1.015404000	1.601519000
H	3.025577000	-0.447897000	1.689336000
H	3.376585000	-2.187426000	1.579547000
O	0.293665000	-0.452774000	2.266824000
H	-0.111193000	0.690621000	1.358299000
Rh	-0.563487000	-0.311795000	-0.913030000

TS1
Lowest frequency = -678.9279 cm^{-1}
Charge = 0, Multiplicity = 1

83

C	-3.136865000	2.310565000	-2.463192000
C	-3.905521000	3.236070000	-1.760604000
C	-3.388727000	3.843745000	-0.614714000
C	-2.104404000	3.532419000	-0.185237000
C	-1.332167000	2.592327000	-0.879425000
C	0.079982000	2.404110000	-0.444841000
O	0.640745000	3.290812000	0.182432000
H	-1.668274000	4.017611000	0.689707000
H	-3.990121000	4.567365000	-0.059639000
H	-4.912350000	3.484488000	-2.104923000
H	-3.537684000	1.834270000	-3.360751000
C	2.072911000	1.311427000	-1.244770000
C	2.682591000	2.517477000	-1.642332000
C	3.981957000	2.474945000	-2.125396000
H	2.153562000	3.464212000	-1.552831000
C	3.954847000	0.118563000	-1.810616000
C	4.650085000	1.252989000	-2.214437000
H	4.473722000	3.401089000	-2.433725000
H	4.424093000	-0.871202000	-1.866667000
H	5.672992000	1.182013000	-2.587918000
N	2.713398000	0.147285000	-1.338111000
N	0.732210000	1.223690000	-0.815928000
C	-1.856705000	1.981275000	-2.022499000
C	1.078034000	-1.392643000	2.588167000
C	2.261894000	-0.758237000	2.029348000
C	2.098683000	0.650363000	2.142434000
C	0.805233000	0.913832000	2.744618000

C	0.207773000	-0.356349000	3.060839000
C	0.839732000	-2.856406000	2.686293000
C	3.415263000	-1.496944000	1.447936000
C	3.068955000	1.704647000	1.748274000
C	0.273817000	2.251665000	3.121038000
C	-1.090106000	-0.548507000	3.759130000
C	0.244523000	-1.723915000	-1.614896000
H	1.503428000	-3.406153000	2.007159000
H	1.026283000	-3.208025000	3.714384000
H	-0.197940000	-3.076446000	2.400302000
H	4.146597000	-0.812947000	1.002130000
H	3.920531000	-2.091250000	2.225821000
H	3.069329000	-2.179864000	0.658490000
H	2.550878000	2.545501000	1.266615000
H	3.577206000	2.082779000	2.650883000
H	3.832190000	1.323626000	1.058598000
H	0.674945000	2.561173000	4.100868000
H	0.550130000	3.010215000	2.376609000
H	-0.821866000	2.233349000	3.195621000
H	-1.530843000	-1.520193000	3.510665000
H	-0.930465000	-0.483981000	4.848431000
H	-1.809452000	0.231832000	3.476367000
O	0.591849000	-1.784164000	-0.417992000
C	0.263037000	-3.016831000	-2.422500000
C	-0.626808000	-2.887686000	-3.656488000
H	-0.582211000	-3.815511000	-4.247371000
H	-1.675145000	-2.711279000	-3.373701000
H	-0.305963000	-2.050871000	-4.291480000
C	-0.202633000	-4.172508000	-1.536313000
H	0.452600000	-4.285704000	-0.662348000

H	-1.220883000	-3.999456000	-1.157158000
H	-0.195830000	-5.112563000	-2.109389000
C	1.724663000	-3.226297000	-2.846415000
H	1.814663000	-4.150366000	-3.438696000
H	2.082645000	-2.384944000	-3.458957000
H	2.378352000	-3.311902000	-1.965700000
H	-1.267063000	1.254335000	-2.580448000
O	-1.877360000	-2.216383000	1.286481000
C	-2.243804000	-1.194547000	0.721027000
C	-3.695823000	-1.051007000	0.224142000
O	-1.500167000	-0.169302000	0.458706000
C	-4.229597000	0.336633000	0.576581000
C	-4.560843000	-2.131344000	0.865535000
C	-3.669767000	-1.239227000	-1.296985000
H	-5.258731000	0.458974000	0.202112000
H	-4.250000000	0.484388000	1.668607000
H	-3.602452000	1.122425000	0.139902000
H	-4.163510000	-3.132610000	0.650689000
H	-4.590381000	-2.018399000	1.959898000
H	-5.592874000	-2.067291000	0.485003000
H	-4.680918000	-1.112538000	-1.716599000
H	-3.000418000	-0.510283000	-1.772223000
H	-3.319891000	-2.250524000	-1.558443000
O	-0.080212000	-0.651695000	-2.211341000
H	0.187854000	0.284716000	-1.540901000
Rh	0.496309000	-0.191437000	0.947573000

int4
Lowest frequency = 12.5757 cm^{-1}
Charge = 0, Multiplicity = 1

83

C	3.057344000	-2.063422000	-2.701442000
C	3.849205000	-3.031603000	-2.087512000
C	3.355966000	-3.740044000	-0.990333000
C	2.071081000	-3.488232000	-0.523244000
C	1.276779000	-2.504454000	-1.124575000
C	-0.142444000	-2.379036000	-0.680037000
O	-0.696639000	-3.356269000	-0.192054000
H	1.651941000	-4.058485000	0.307653000
H	3.974649000	-4.498779000	-0.505429000
H	4.854631000	-3.235281000	-2.463770000
H	3.438292000	-1.510044000	-3.562801000
C	-2.126073000	-1.182674000	-1.285518000
C	-2.743967000	-2.309682000	-1.870703000
C	-4.050539000	-2.196792000	-2.317424000
H	-2.209870000	-3.254556000	-1.950005000
C	-4.031541000	0.070891000	-1.608553000
C	-4.728602000	-0.982626000	-2.187405000
H	-4.543000000	-3.062216000	-2.768541000
H	-4.508603000	1.051337000	-1.486618000
H	-5.758543000	-0.858043000	-2.525713000
N	-2.779987000	-0.024179000	-1.170846000
N	-0.782991000	-1.160527000	-0.887177000
C	1.779681000	-1.791748000	-2.216560000
C	-0.928596000	1.055248000	2.770478000
C	-2.138107000	0.467403000	2.213506000
C	-1.953934000	-0.940770000	2.143869000
C	-0.615967000	-1.245896000	2.617193000
C	-0.015163000	-0.008830000	3.050058000
C	-0.708936000	2.501297000	3.036599000

C	-3.338122000	1.247297000	1.807177000
C	-2.939262000	-1.956365000	1.690013000
C	-0.041282000	-2.606132000	2.798802000
C	1.327298000	0.122026000	3.674560000
C	-0.366721000	1.937761000	-1.404933000
H	-1.418700000	3.114837000	2.467403000
H	-0.845596000	2.719559000	4.108601000
H	0.306677000	2.781365000	2.725715000
H	-4.086757000	0.609354000	1.323940000
H	-3.798164000	1.724191000	2.687408000
H	-3.057460000	2.034986000	1.093264000
H	-2.450105000	-2.719072000	1.067495000
H	-3.376186000	-2.455111000	2.571099000
H	-3.753734000	-1.504723000	1.110509000
H	-0.326874000	-3.011645000	3.784074000
H	-0.400553000	-3.294435000	2.022417000
H	1.055831000	-2.579913000	2.749730000
H	1.730348000	1.131234000	3.534968000
H	1.251666000	-0.096970000	4.752707000
H	2.037546000	-0.591038000	3.234478000
O	-0.646117000	1.828173000	-0.206435000
C	-0.435640000	3.305336000	-2.063136000
C	0.473928000	3.359125000	-3.289560000
H	0.392726000	4.347432000	-3.766993000
H	1.526276000	3.198877000	-3.012232000
H	0.198518000	2.591755000	-4.025488000
C	-0.034772000	4.370663000	-1.042830000
H	-0.710262000	4.360105000	-0.176954000
H	0.982521000	4.194572000	-0.662789000
H	-0.071982000	5.367317000	-1.508254000

C	-1.901959000	3.490774000	-2.485361000
H	-2.028434000	4.472385000	-2.967738000
H	-2.211164000	2.710946000	-3.197405000
H	-2.569914000	3.442953000	-1.612517000
H	1.166487000	-1.036184000	-2.707392000
O	1.892567000	2.124109000	1.368069000
C	2.256304000	1.170427000	0.691731000
C	3.698004000	1.096962000	0.150466000
O	1.519558000	0.166129000	0.344903000
C	4.266957000	-0.299316000	0.401266000
C	4.555126000	2.151760000	0.842731000
C	3.635258000	1.382237000	-1.353862000
H	5.288904000	-0.376721000	-0.003677000
H	4.317621000	-0.514360000	1.481139000
H	3.644272000	-1.068706000	-0.070133000
H	4.135606000	3.156998000	0.700007000
H	4.608477000	1.970818000	1.926828000
H	5.580183000	2.132790000	0.439135000
H	4.640418000	1.312603000	-1.800245000
H	2.977818000	0.665470000	-1.862740000
H	3.252806000	2.398136000	-1.542090000
O	-0.056368000	0.944101000	-2.160967000
H	-0.216199000	0.040887000	-1.639382000
Rh	-0.444513000	0.062864000	0.955013000

int5
Lowest frequency = 23.556 cm^{-1}
Charge = 0, Multiplicity = 1

66

C	2.713511000	-0.034457000	-2.390395000
C	3.904574000	-0.747941000	-2.482023000

C	4.011840000	-2.007765000	-1.879044000
C	2.935402000	-2.551095000	-1.183688000
C	1.750569000	-1.823456000	-1.065499000
C	0.580273000	-2.393885000	-0.320904000
O	0.434976000	-3.604427000	-0.228158000
H	2.986074000	-3.540397000	-0.723500000
H	4.944298000	-2.571417000	-1.965643000
H	4.746950000	-0.341491000	-3.047365000
H	2.601772000	0.924734000	-2.901708000
C	-1.473238000	-1.696648000	0.725121000
C	-2.232161000	-2.824321000	0.337305000
C	-3.512878000	-2.968476000	0.844367000
H	-1.800522000	-3.557704000	-0.339703000
C	-3.191907000	-0.954343000	2.065081000
C	-4.025229000	-2.013705000	1.726326000
H	-4.118376000	-3.827388000	0.543414000
H	-3.537136000	-0.182192000	2.764956000
H	-5.031888000	-2.091582000	2.140385000
N	-1.960127000	-0.800648000	1.590161000
N	-0.218776000	-1.423957000	0.205842000
C	1.631850000	-0.564471000	-1.676521000
Rh	0.598319000	0.482777000	0.247596000
C	0.363625000	1.541753000	2.044852000
C	1.236069000	0.413792000	2.289542000
C	2.387524000	0.558069000	1.457729000
C	2.256047000	1.816875000	0.734448000
C	1.028290000	2.420446000	1.098996000
C	-0.925726000	1.865416000	2.707732000
C	0.955442000	-0.707622000	3.223928000
C	3.576466000	-0.336339000	1.425026000

C	3.286331000	2.400239000	-0.167481000
C	0.444661000	3.691369000	0.592953000
C	-1.661372000	0.799196000	-1.687602000
H	-1.263359000	1.047593000	3.351921000
H	-0.811683000	2.781118000	3.311644000
H	-1.702863000	2.038182000	1.949980000
H	1.446174000	-1.633373000	2.897030000
H	1.325719000	-0.457869000	4.231784000
H	-0.124286000	-0.896317000	3.274792000
H	4.026346000	-0.373145000	0.424098000
H	4.344207000	0.020153000	2.132040000
H	3.310842000	-1.363989000	1.704139000
H	3.941461000	3.070723000	0.413491000
H	3.913757000	1.623572000	-0.620283000
H	2.833209000	2.990526000	-0.974813000
H	-0.570254000	3.505716000	0.209930000
H	0.378878000	4.436707000	1.401535000
H	1.045772000	4.119205000	-0.219469000
O	-1.137915000	1.197532000	-0.581994000
C	-3.126062000	1.220332000	-1.908119000
C	-3.228681000	1.871617000	-3.288295000
H	-4.279231000	2.100039000	-3.528915000
H	-2.659362000	2.814254000	-3.327201000
H	-2.826024000	1.197751000	-4.057177000
C	-3.620140000	2.171687000	-0.823605000
H	-3.544036000	1.706546000	0.169457000
H	-3.032947000	3.102503000	-0.806667000
H	-4.674172000	2.436681000	-1.005023000
C	-3.948813000	-0.073939000	-1.880840000
H	-5.010867000	0.146342000	-2.075449000

H	-3.586717000	-0.774911000	-2.646130000
H	-3.876457000	-0.570174000	-0.901005000
O	-1.093355000	0.115919000	-2.533348000
H	0.605437000	-0.139310000	-1.862732000

TS2
Lowest frequency = -791.3996 cm^{-1}
Charge = 0, Multiplicity = 1

66

C	-2.571886000	-1.066979000	1.977964000
C	-3.616675000	-1.987492000	1.943441000
C	-3.627249000	-3.001183000	0.978343000
C	-2.583494000	-3.107575000	0.061452000
C	-1.550314000	-2.174442000	0.093660000
C	-0.397151000	-2.268109000	-0.854319000
O	-0.173171000	-3.291129000	-1.486523000
H	-2.546369000	-3.902354000	-0.687447000
H	-4.448998000	-3.721590000	0.957333000
H	-4.421125000	-1.931284000	2.681626000
H	-2.547077000	-0.304458000	2.761195000
C	1.575867000	-1.008447000	-1.460971000
C	2.389238000	-2.134007000	-1.734839000
C	3.673218000	-1.925208000	-2.210737000
H	1.991419000	-3.133590000	-1.576954000
C	3.249693000	0.411992000	-2.160858000
C	4.136568000	-0.625054000	-2.426755000
H	4.318303000	-2.784578000	-2.412408000
H	3.551181000	1.453720000	-2.332373000
H	5.142943000	-0.423942000	-2.797881000
N	2.016707000	0.232908000	-1.700442000
N	0.321249000	-1.104564000	-0.886076000

C	-1.530049000	-1.131999000	1.040189000
Rh	-0.618384000	0.538963000	-0.045651000
C	-0.467704000	2.370926000	-1.179548000
C	-1.207809000	1.405726000	-1.934177000
C	-2.366345000	1.025132000	-1.168173000
C	-2.378735000	1.835739000	0.037884000
C	-1.201733000	2.627256000	0.046349000
C	0.787522000	3.071209000	-1.562219000
C	-0.835122000	0.859082000	-3.266294000
C	-3.444790000	0.092130000	-1.599748000
C	-3.487015000	1.897253000	1.030107000
C	-0.753544000	3.575154000	1.103065000
C	1.479340000	-0.021211000	1.935754000
H	1.188841000	2.684404000	-2.504920000
H	0.600276000	4.152472000	-1.671348000
H	1.557855000	2.925681000	-0.791645000
H	-1.144629000	-0.189548000	-3.366506000
H	-1.329380000	1.440021000	-4.062157000
H	0.250785000	0.901720000	-3.411948000
H	-3.887842000	-0.430553000	-0.740806000
H	-4.248046000	0.637055000	-2.123219000
H	-3.055879000	-0.674390000	-2.282934000
H	-4.173749000	2.716296000	0.757697000
H	-4.065350000	0.966051000	1.051878000
H	-3.118197000	2.095899000	2.045216000
H	0.303877000	3.398965000	1.348352000
H	-0.854383000	4.616976000	0.757628000
H	-1.340819000	3.463407000	2.023721000
O	1.100197000	0.843586000	1.100071000
C	2.889263000	0.112336000	2.510300000

C	2.867045000	-0.242696000	3.996653000
H	3.889489000	-0.224167000	4.404817000
H	2.259955000	0.475994000	4.569316000
H	2.442647000	-1.244069000	4.150451000
C	3.431381000	1.521723000	2.292963000
H	3.447970000	1.774372000	1.223895000
H	2.813576000	2.272704000	2.808935000
H	4.456906000	1.593335000	2.687351000
C	3.745021000	-0.903173000	1.736691000
H	4.783879000	-0.868937000	2.101024000
H	3.360329000	-1.924093000	1.873156000
H	3.751254000	-0.679813000	0.659049000
O	0.782405000	-1.005331000	2.277247000
H	-0.370745000	-0.908955000	1.576416000

int6
Lowest frequency = 22.7074 cm^{-1}
Charge = 0, Multiplicity = 1

66

C	-2.530204000	2.070217000	-0.723266000
C	-3.139546000	3.237037000	-0.255020000
C	-2.869578000	3.716679000	1.029862000
C	-1.956174000	3.044672000	1.836847000
C	-1.340807000	1.886500000	1.358884000
C	-0.237632000	1.229276000	2.121035000
O	0.113870000	1.619371000	3.225753000
H	-1.682936000	3.401963000	2.833205000
H	-3.357058000	4.626752000	1.387672000
H	-3.832588000	3.781451000	-0.902758000
H	-2.756177000	1.719027000	-1.733746000
C	1.569731000	-0.320891000	1.639226000

C	2.369619000	0.028991000	2.756294000
C	3.624551000	-0.544857000	2.881809000
H	1.976827000	0.735554000	3.483475000
C	3.211160000	-1.758476000	0.883395000
C	4.077115000	-1.462203000	1.930273000
H	4.253132000	-0.276806000	3.735508000
H	3.507175000	-2.480838000	0.111075000
H	5.058009000	-1.935175000	2.001745000
N	2.009907000	-1.212629000	0.735454000
N	0.332789000	0.230973000	1.368550000
C	-1.638223000	1.357483000	0.089241000
Rh	-0.775524000	-0.431718000	-0.249152000
C	-0.619769000	-2.588790000	-0.928882000
C	-0.973694000	-2.563368000	0.429233000
C	-2.179911000	-1.752712000	0.569886000
C	-2.639725000	-1.418957000	-0.761370000
C	-1.632380000	-1.838140000	-1.671017000
C	0.591088000	-3.192592000	-1.549456000
C	-0.269692000	-3.199395000	1.574968000
C	-2.931712000	-1.539963000	1.839592000
C	-3.957252000	-0.812158000	-1.094131000
C	-1.628073000	-1.671438000	-3.151984000
C	1.435750000	1.359215000	-1.417756000
H	1.235959000	-3.655490000	-0.792848000
H	0.317303000	-3.960214000	-2.291459000
H	1.186367000	-2.420107000	-2.059831000
H	-0.106769000	-2.478051000	2.388290000
H	-0.880155000	-4.024399000	1.977807000
H	0.709109000	-3.595866000	1.283079000
H	-3.540332000	-0.626816000	1.790768000

H	-3.602852000	-2.389065000	2.052955000
H	-2.244249000	-1.431425000	2.689679000
H	-4.727176000	-1.601267000	-1.125605000
H	-4.264953000	-0.068761000	-0.347414000
H	-3.946606000	-0.320341000	-2.075670000
H	-0.619916000	-1.423659000	-3.513355000
H	-1.943871000	-2.602045000	-3.652928000
H	-2.307116000	-0.869113000	-3.470247000
O	0.784483000	0.328433000	-1.544775000
C	2.832133000	1.511500000	-1.988367000
C	2.856214000	2.725849000	-2.923936000
H	3.872082000	2.862437000	-3.324565000
H	2.171711000	2.588353000	-3.775405000
H	2.567097000	3.642963000	-2.391999000
C	3.216944000	0.238906000	-2.734920000
H	3.177793000	-0.630713000	-2.064215000
H	2.536743000	0.047323000	-3.577716000
H	4.239292000	0.335510000	-3.129605000
C	3.782208000	1.740349000	-0.801532000
H	4.811959000	1.845383000	-1.175763000
H	3.516094000	2.652804000	-0.250335000
H	3.756355000	0.893357000	-0.100010000
O	0.999475000	2.407946000	-0.771441000
H	0.103971000	2.213744000	-0.405722000

int7
Lowest frequency = 12.1210 cm^{-1}
Charge = 0, Multiplicity = 1

73

C	-2.167963000	-2.412399000	-0.492717000
C	-3.535105000	-2.683409000	-0.593516000

C	-4.479574000	-1.777493000	-0.104581000
C	-4.051795000	-0.584943000	0.471633000
C	-2.685576000	-0.319442000	0.570589000
C	-2.192414000	0.996842000	1.054128000
O	-2.953437000	1.861838000	1.469376000
H	-4.751167000	0.171344000	0.836932000
H	-5.546231000	-1.997372000	-0.191787000
H	-3.866762000	-3.611163000	-1.068948000
H	-1.447631000	-3.124383000	-0.903891000
C	-0.131181000	2.280235000	1.073782000
C	-0.709494000	3.469703000	1.588264000
C	0.087182000	4.593420000	1.735984000
H	-1.762560000	3.463564000	1.857056000
C	1.908473000	3.342881000	0.875610000
C	1.436426000	4.548105000	1.380926000
H	-0.350773000	5.511161000	2.138108000
H	2.962093000	3.252999000	0.577785000
H	2.095978000	5.410680000	1.489254000
N	1.165676000	2.252707000	0.719703000
N	-0.827485000	1.099998000	0.903130000
C	-1.731609000	-1.232938000	0.111760000
Rh	0.160051000	-0.658150000	0.464259000
C	2.275941000	-1.097042000	1.368956000
C	1.431326000	-0.589986000	2.367294000
C	0.256560000	-1.443381000	2.447754000
C	0.476112000	-2.567015000	1.573326000
C	1.655598000	-2.307216000	0.829795000
C	3.624984000	-0.575618000	1.019598000
C	1.683393000	0.570686000	3.262198000
C	-0.839414000	-1.304539000	3.448668000

C	-0.315734000	-3.826218000	1.566454000
C	2.302741000	-3.251858000	-0.123962000
H	3.634547000	0.522610000	1.012242000
H	4.369080000	-0.917913000	1.758761000
H	3.957771000	-0.917289000	0.031789000
H	0.786230000	1.193997000	3.379430000
H	1.965972000	0.206225000	4.264460000
H	2.490174000	1.209234000	2.885518000
H	-1.761043000	-1.789022000	3.099220000
H	-0.554668000	-1.759270000	4.412372000
H	-1.074422000	-0.247007000	3.631818000
H	0.071017000	-4.494181000	2.355229000
H	-1.379672000	-3.647118000	1.765119000
H	-0.233974000	-4.362224000	0.612198000
H	2.961946000	-2.726422000	-0.825841000
H	2.919905000	-3.986389000	0.421260000
H	1.559328000	-3.811140000	-0.709083000
C	0.975192000	-0.039004000	-1.565815000
C	-0.245477000	0.132268000	-1.713135000
C	2.347879000	-0.021106000	-1.994683000
C	-1.519830000	0.580813000	-2.189494000
C	3.155368000	1.094768000	-1.728306000
C	2.874258000	-1.085569000	-2.744282000
C	-1.923389000	1.900975000	-1.930025000
C	-2.375216000	-0.276327000	-2.899036000
C	4.466980000	1.133915000	-2.189209000
H	2.724942000	1.912533000	-1.152471000
C	4.190825000	-1.042203000	-3.194192000
H	2.235782000	-1.939198000	-2.978844000
C	-3.175592000	2.339736000	-2.343919000

H	-1.254844000	2.567920000	-1.384909000
C	-3.622989000	0.172527000	-3.313034000
H	-2.058551000	-1.299466000	-3.101489000
C	4.993381000	0.063875000	-2.913232000
H	5.086467000	2.009387000	-1.980011000
H	4.590710000	-1.875327000	-3.777125000
C	-4.030121000	1.476056000	-3.027461000
H	-3.489574000	3.360724000	-2.117519000
H	-4.289658000	-0.504902000	-3.851106000
H	6.025722000	0.096131000	-3.269178000
H	-5.019137000	1.819780000	-3.339588000

TS3
Lowest frequency = -260.3355 cm^{-1}
Charge = 0, Multiplicity = 1

73

C	2.213129000	1.421989000	-1.836028000
C	3.550445000	1.821376000	-1.877933000
C	4.388319000	1.604203000	-0.779879000
C	3.889013000	0.989976000	0.369575000
C	2.551971000	0.610368000	0.421023000
C	1.970879000	-0.052790000	1.624972000
O	2.689659000	-0.408245000	2.550800000
H	4.512597000	0.799142000	1.246412000
H	5.436045000	1.910515000	-0.826024000
H	3.946782000	2.291220000	-2.782108000
H	1.570450000	1.551116000	-2.709336000
C	-0.124622000	-1.012700000	2.357658000
C	0.439974000	-1.767653000	3.418224000
C	-0.384710000	-2.585431000	4.172289000
H	1.505122000	-1.681006000	3.615389000

C	-2.214844000	-1.866662000	2.847605000
C	-1.751801000	-2.651868000	3.895263000
H	0.045506000	-3.173830000	4.987407000
H	-3.281656000	-1.872885000	2.586359000
H	-2.431798000	-3.282459000	4.470434000
N	-1.441935000	-1.078131000	2.107207000
N	0.610289000	-0.203722000	1.513205000
C	1.702489000	0.828293000	-0.675857000
Rh	-0.250302000	0.954532000	0.001682000
C	-1.907295000	2.255869000	-0.740966000
C	-2.150371000	1.938305000	0.634026000
C	-1.032852000	2.452972000	1.390414000
C	-0.136639000	3.121061000	0.499299000
C	-0.676664000	2.984116000	-0.828958000
C	-2.831342000	1.978496000	-1.876758000
C	-3.396981000	1.358139000	1.202714000
C	-0.884899000	2.347940000	2.868877000
C	1.120482000	3.833762000	0.865287000
C	-0.155592000	3.649317000	-2.056230000
H	-3.426508000	1.072591000	-1.701988000
H	-3.528456000	2.821903000	-2.014448000
H	-2.284779000	1.837414000	-2.819016000
H	-3.171475000	0.704415000	2.054055000
H	-4.075647000	2.158921000	1.543683000
H	-3.935947000	0.760322000	0.455827000
H	0.170921000	2.319901000	3.168995000
H	-1.357050000	3.215549000	3.358883000
H	-1.366080000	1.437417000	3.248055000
H	0.951330000	4.919122000	0.963344000
H	1.518091000	3.470021000	1.822320000

H	1.903231000	3.680042000	0.108004000
H	-0.328395000	3.042527000	-2.956150000
H	-0.671584000	4.612854000	-2.207302000
H	0.919786000	3.855249000	-1.982800000
C	-0.639352000	-0.669141000	-1.200625000
C	0.641981000	-0.785360000	-1.236336000
C	-1.857795000	-1.256034000	-1.697923000
C	1.638623000	-1.850500000	-1.232761000
C	-2.927800000	-1.529272000	-0.829467000
C	-1.994147000	-1.548594000	-3.066016000
C	1.283665000	-3.040902000	-0.574710000
C	2.890438000	-1.763372000	-1.856732000
C	-4.101438000	-2.089917000	-1.321308000
H	-2.787864000	-1.300474000	0.228495000
C	-3.177265000	-2.098552000	-3.550591000
H	-1.163663000	-1.331650000	-3.741312000
C	2.157219000	-4.123574000	-0.559599000
H	0.319926000	-3.093851000	-0.064324000
C	3.758042000	-2.849313000	-1.839109000
H	3.181831000	-0.835737000	-2.350416000
C	-4.234959000	-2.370647000	-2.682617000
H	-4.923698000	-2.309763000	-0.635588000
H	-3.274158000	-2.318156000	-4.616697000
C	3.396102000	-4.031213000	-1.191519000
H	1.871879000	-5.040066000	-0.038066000
H	4.730454000	-2.770588000	-2.330742000
H	-5.162018000	-2.802860000	-3.066548000
H	4.086257000	-4.878040000	-1.171576000

int8

Lowest frequency = 22.0461 cm^{-1}
Charge = 0, Multiplicity = 1

73

C	1.131093000	3.094291000	-0.276111000
C	0.493418000	4.248217000	0.128838000
C	-0.389069000	4.220331000	1.226153000
C	-0.617644000	3.034204000	1.890362000
C	0.015190000	1.836271000	1.483861000
C	-0.176115000	0.615360000	2.352728000
O	0.048664000	0.670914000	3.550759000
H	-1.266046000	2.997023000	2.768354000
H	-0.874743000	5.140085000	1.561042000
H	0.685506000	5.188945000	-0.393169000
H	1.833795000	3.114729000	-1.112463000
C	-0.930356000	-1.660238000	2.085550000
C	-0.570538000	-2.070402000	3.393576000
C	-0.855863000	-3.366519000	3.787737000
H	-0.087310000	-1.356751000	4.056556000
C	-1.810930000	-3.748928000	1.649315000
C	-1.493582000	-4.243636000	2.906890000
H	-0.577200000	-3.695063000	4.792640000
H	-2.311819000	-4.391692000	0.913542000
H	-1.734672000	-5.270886000	3.184865000
N	-1.543032000	-2.508460000	1.248419000
N	-0.670642000	-0.394771000	1.599380000
C	0.932095000	1.860939000	0.397499000
Rh	-0.948187000	0.474601000	-0.288588000
C	-2.344449000	-0.568157000	-1.523955000
C	-3.153736000	0.160536000	-0.549217000
C	-2.922679000	1.534822000	-0.723451000

C	-1.955773000	1.687927000	-1.805635000
C	-1.663744000	0.403990000	-2.343132000
C	-2.468863000	-2.020672000	-1.814191000
C	-4.068851000	-0.483901000	0.430822000
C	-3.554597000	2.662721000	0.013634000
C	-1.524097000	2.995498000	-2.368035000
C	-0.866730000	0.113083000	-3.566165000
H	-2.479156000	-2.588473000	-0.876021000
H	-3.404055000	-2.211728000	-2.367985000
H	-1.630593000	-2.382472000	-2.422470000
H	-4.302043000	0.185332000	1.269385000
H	-5.017614000	-0.759392000	-0.059516000
H	-3.609953000	-1.396600000	0.832831000
H	-2.825650000	3.455090000	0.236401000
H	-4.362915000	3.114649000	-0.585648000
H	-3.988612000	2.329191000	0.965568000
H	-2.294780000	3.378038000	-3.058435000
H	-1.379764000	3.746527000	-1.580087000
H	-0.582779000	2.906866000	-2.925786000
H	-0.389212000	-0.873496000	-3.512184000
H	-1.519510000	0.128068000	-4.454791000
H	-0.072225000	0.856235000	-3.717637000
C	0.934869000	-0.217655000	-0.621323000
C	1.746678000	0.667823000	-0.008805000
C	1.284499000	-1.394611000	-1.413352000
C	3.187215000	0.605448000	0.297047000
C	0.746251000	-2.661639000	-1.141936000
C	2.156325000	-1.257480000	-2.509904000
C	3.905398000	-0.602052000	0.207090000
C	3.877867000	1.741287000	0.753726000

C	1.090548000	-3.759513000	-1.926965000
H	0.044972000	-2.765414000	-0.312548000
C	2.485817000	-2.353612000	-3.300209000
H	2.577484000	-0.273249000	-2.728488000
C	5.258098000	-0.655738000	0.519774000
H	3.390091000	-1.513312000	-0.095766000
C	5.233592000	1.684666000	1.067919000
H	3.344978000	2.685986000	0.876368000
C	1.957444000	-3.612544000	-3.009768000
H	0.670746000	-4.740935000	-1.691596000
H	3.163340000	-2.226022000	-4.148266000
C	5.935554000	0.488509000	0.944099000
H	5.788209000	-1.608271000	0.441880000
H	5.742292000	2.585841000	1.419275000
H	2.219228000	-4.474793000	-3.627742000
H	6.998842000	0.442455000	1.190874000

int9
Lowest frequency = 18.2975 cm^{-1}
Charge = 0, Multiplicity = 1

73

C	-2.281341000	-2.837903000	-0.547819000
C	-2.281816000	-4.183373000	-0.198902000
C	-1.585455000	-4.608437000	0.932849000
C	-0.904823000	-3.671415000	1.702422000
C	-0.861566000	-2.323418000	1.329447000
C	-0.194682000	-1.372012000	2.278918000
O	-0.463957000	-1.381617000	3.471062000
H	-0.402006000	-3.967303000	2.626161000
H	-1.594738000	-5.660475000	1.227296000
H	-2.840265000	-4.901630000	-0.804204000

H	-2.861168000	-2.501635000	-1.411133000
C	1.025196000	0.699257000	2.185418000
C	0.845695000	1.289548000	3.445325000
C	1.229943000	2.616892000	3.580411000
H	0.413440000	0.698278000	4.250638000
C	1.899976000	2.672000000	1.280516000
C	1.764974000	3.326973000	2.497415000
H	1.107368000	3.114864000	4.545785000
H	2.272337000	3.176201000	0.384660000
H	2.059268000	4.372522000	2.592528000
N	1.547598000	1.397885000	1.150846000
N	0.696526000	-0.528789000	1.697330000
C	-1.555803000	-1.881089000	0.181893000
Rh	1.303813000	-0.165995000	-0.237647000
C	2.626383000	0.119787000	-1.944984000
C	3.414630000	-0.511972000	-0.890966000
C	2.825275000	-1.756685000	-0.596408000
C	1.660843000	-1.922384000	-1.451253000
C	1.591324000	-0.783991000	-2.325583000
C	2.996247000	1.408138000	-2.600185000
C	4.618777000	0.098751000	-0.259583000
C	3.249757000	-2.747096000	0.432036000
C	0.890478000	-3.187114000	-1.602415000
C	0.608703000	-0.631363000	-3.436504000
H	3.143770000	2.212891000	-1.865140000
H	3.938677000	1.297262000	-3.161846000
H	2.226811000	1.743542000	-3.306933000
H	4.866761000	-0.390179000	0.691877000
H	5.497103000	0.013667000	-0.921284000
H	4.465516000	1.168204000	-0.053431000

H	2.381165000	-3.124156000	0.991165000
H	3.743931000	-3.612430000	-0.039583000
H	3.949896000	-2.308219000	1.154893000
H	1.471986000	-3.911213000	-2.198992000
H	0.666773000	-3.651898000	-0.633077000
H	-0.064817000	-3.018937000	-2.112429000
H	0.616111000	0.384093000	-3.853471000
H	0.846042000	-1.330114000	-4.255062000
H	-0.413322000	-0.844979000	-3.091686000
C	-0.636992000	0.397614000	-0.410586000
C	-1.679681000	-0.450135000	-0.225006000
C	-0.821989000	1.855662000	-0.552532000
C	-3.089809000	-0.000354000	-0.410153000
C	-1.470091000	2.572390000	0.468275000
C	-0.275078000	2.584795000	-1.618757000
C	-4.057331000	-0.302373000	0.560796000
C	-3.487986000	0.726527000	-1.540599000
C	-1.559215000	3.960296000	0.424900000
H	-1.893885000	2.021054000	1.310476000
C	-0.378666000	3.972075000	-1.672633000
H	0.234984000	2.045730000	-2.416823000
C	-5.371652000	0.133516000	0.418776000
H	-3.764216000	-0.878170000	1.442584000
C	-4.803940000	1.157348000	-1.686728000
H	-2.748890000	0.956049000	-2.310845000
C	-1.016314000	4.669545000	-0.646390000
H	-2.059106000	4.493318000	1.237543000
H	0.044919000	4.514326000	-2.522272000
C	-5.750902000	0.866953000	-0.705562000
H	-6.106398000	-0.101330000	1.193070000

H	-5.092498000	1.722741000	-2.576389000
H	-1.089367000	5.759121000	-0.681680000
H	-6.783407000	1.206143000	-0.819076000

TS4
Lowest frequency = -369.8507 cm^{-1}
Charge = 0, Multiplicity = 1

73

C	-2.604407000	-2.770006000	0.293120000
C	-2.622274000	-4.013484000	0.895659000
C	-1.749288000	-4.309152000	1.955381000
C	-0.878056000	-3.328323000	2.394458000
C	-0.825249000	-2.070469000	1.771669000
C	0.074768000	-1.077288000	2.369445000
O	0.513342000	-1.135939000	3.508091000
H	-0.208032000	-3.497023000	3.240491000
H	-1.766322000	-5.291624000	2.431789000
H	-3.320806000	-4.773782000	0.536300000
H	-3.290387000	-2.560049000	-0.529859000
C	1.231467000	1.019571000	1.871150000
C	1.368407000	1.671730000	3.093955000
C	2.231374000	2.761603000	3.131103000
H	0.836342000	1.301601000	3.968051000
C	2.706934000	2.458072000	0.798571000
C	2.902801000	3.171629000	1.974137000
H	2.383004000	3.299807000	4.069585000
H	3.202728000	2.731020000	-0.136466000
H	3.571708000	4.033115000	1.984127000
N	1.897328000	1.402177000	0.766451000
N	0.424082000	-0.044465000	1.505679000
C	-1.696172000	-1.755446000	0.689129000

Rh	1.284225000	-0.215311000	-0.421801000
C	2.269953000	-0.230984000	-2.335305000
C	3.184473000	-0.905025000	-1.406797000
C	2.537444000	-2.048923000	-0.915364000
C	1.210055000	-2.098248000	-1.513117000
C	1.096756000	-1.029836000	-2.463148000
C	2.625293000	0.972482000	-3.142972000
C	4.553178000	-0.419089000	-1.071439000
C	3.040734000	-3.040119000	0.076588000
C	0.273250000	-3.247536000	-1.377514000
C	-0.066921000	-0.804015000	-3.364359000
H	3.144922000	1.730003000	-2.538042000
H	3.296956000	0.704358000	-3.976416000
H	1.733528000	1.446039000	-3.576272000
H	4.945997000	-0.909545000	-0.170669000
H	5.256992000	-0.616435000	-1.897604000
H	4.566022000	0.666017000	-0.888922000
H	2.285434000	-3.239341000	0.852185000
H	3.271836000	-4.003414000	-0.408415000
H	3.952089000	-2.688125000	0.578169000
H	0.621009000	-4.087685000	-2.003107000
H	0.206231000	-3.606281000	-0.341539000
H	-0.740693000	-2.984082000	-1.699445000
H	-0.102458000	0.231506000	-3.730195000
H	-0.022306000	-1.468544000	-4.243362000
H	-1.012233000	-1.006108000	-2.839778000
C	-0.614274000	0.408912000	0.100623000
C	-1.732650000	-0.441729000	0.083796000
C	-0.845078000	1.880720000	0.049901000
C	-3.025604000	0.059105000	-0.438713000

C	-1.628024000	2.485990000	1.040957000
C	-0.296571000	2.685453000	-0.955620000
C	-4.220761000	-0.142261000	0.277168000
C	-3.109529000	0.775383000	-1.644945000
C	-1.861848000	3.858723000	1.023562000
H	-2.062121000	1.859951000	1.824386000
C	-0.549197000	4.052678000	-0.991142000
H	0.333273000	2.212351000	-1.712209000
C	-5.434283000	0.355606000	-0.185805000
H	-4.185686000	-0.686677000	1.223826000
C	-4.321249000	1.283106000	-2.105127000
H	-2.202115000	0.936693000	-2.228270000
C	-1.329531000	4.645043000	0.003230000
H	-2.471072000	4.316050000	1.806915000
H	-0.130322000	4.663510000	-1.794781000
C	-5.492984000	1.075660000	-1.379741000
H	-6.343031000	0.190606000	0.399016000
H	-4.349844000	1.840214000	-3.045084000
H	-1.519498000	5.720974000	-0.016498000
H	-6.445475000	1.470238000	-1.741435000

int10
Lowest frequency = 25.6714 cm^{-1}
Charge = 0, Multiplicity = 1

73

C	2.936295000	-2.367518000	-0.922121000
C	3.063349000	-3.515553000	-1.672211000
C	2.148395000	-3.824563000	-2.701459000
C	1.095924000	-2.963875000	-2.929503000
C	0.937292000	-1.793949000	-2.162110000

C	-0.216519000	-0.967965000	-2.444375000
O	-1.032109000	-1.133628000	-3.335414000
H	0.345634000	-3.161653000	-3.698101000
H	2.263883000	-4.735754000	-3.291488000
H	3.885120000	-4.203442000	-1.455183000
H	3.647788000	-2.170797000	-0.119538000
C	-1.489062000	0.990078000	-1.721339000
C	-1.814569000	1.674593000	-2.874467000
C	-2.920019000	2.526366000	-2.812752000
H	-1.236650000	1.523172000	-3.784393000
C	-3.212229000	1.926082000	-0.503994000
C	-3.619564000	2.659346000	-1.615059000
H	-3.229392000	3.084709000	-3.698446000
H	-3.726265000	1.990010000	0.457148000
H	-4.481347000	3.323992000	-1.537120000
N	-2.167815000	1.099322000	-0.574273000
N	-0.404112000	0.094877000	-1.521485000
C	1.876675000	-1.437654000	-1.145447000
Rh	-1.185249000	-0.349958000	0.529856000
C	-2.309939000	-0.678470000	2.297437000
C	-2.685352000	-1.770147000	1.402981000
C	-1.505827000	-2.491466000	1.131208000
C	-0.413623000	-1.891927000	1.891539000
C	-0.940731000	-0.841680000	2.698560000
C	-3.264883000	0.299315000	2.897183000
C	-4.056838000	-2.015504000	0.871550000
C	-1.335014000	-3.639860000	0.198071000
C	0.960688000	-2.462174000	1.979858000
C	-0.262699000	-0.120463000	3.813879000
H	-4.127245000	0.479546000	2.239744000

H	-3.661353000	-0.082435000	3.853572000
H	-2.778996000	1.264219000	3.102194000
H	-4.034365000	-2.686282000	0.001845000
H	-4.711156000	-2.474715000	1.632539000
H	-4.539455000	-1.080448000	0.547907000
H	-0.508595000	-3.457139000	-0.507919000
H	-1.094752000	-4.565808000	0.746339000
H	-2.242799000	-3.819794000	-0.392931000
H	1.020704000	-3.184051000	2.812194000
H	1.237035000	-2.991937000	1.059513000
H	1.717213000	-1.684291000	2.149820000
H	-0.441630000	0.964909000	3.781702000
H	-0.630676000	-0.481444000	4.790865000
H	0.823043000	-0.280636000	3.794051000
C	0.543061000	0.545502000	-0.505660000
C	1.741899000	-0.226676000	-0.409305000
C	0.681386000	2.046559000	-0.428418000
C	2.818617000	0.294387000	0.447540000
C	1.449213000	2.681419000	-1.411818000
C	0.091261000	2.822999000	0.569802000
C	4.163973000	0.296885000	0.034550000
C	2.524412000	0.866994000	1.697615000
C	1.612089000	4.064020000	-1.404215000
H	1.931096000	2.072711000	-2.181965000
C	0.260548000	4.205754000	0.587545000
H	-0.504820000	2.314220000	1.331871000
C	5.164682000	0.827472000	0.842407000
H	4.420053000	-0.101060000	-0.949790000
C	3.523824000	1.403018000	2.503925000
H	1.486854000	0.880293000	2.030695000

C	1.017762000	4.830334000	-0.401957000
H	2.212923000	4.545537000	-2.179592000
H	-0.199773000	4.799173000	1.381322000
C	4.852943000	1.381596000	2.084747000
H	6.199615000	0.822291000	0.490606000
H	3.260456000	1.839523000	3.470993000
H	1.149969000	5.915002000	-0.389707000
H	5.639925000	1.800462000	2.716245000

PivOH
Lowest frequency = 43.2569 cm^{-1}
Charge = 0, Multiplicity = 1

17

C	0.963879000	-0.799927000	1.255402000
C	0.571268000	-0.010252000	-0.000006000
H	0.678922000	-0.259430000	2.171313000
H	0.481292000	-1.787230000	1.272851000
H	2.054888000	-0.946234000	1.275514000
C	0.963755000	-0.800406000	-1.255144000
C	1.240103000	1.360029000	-0.000294000
H	0.678619000	-0.260311000	-2.171238000
H	2.054773000	-0.946629000	-1.275361000
H	0.481246000	-1.787755000	-1.272123000
H	2.334433000	1.243421000	-0.000255000
H	0.950378000	1.942682000	-0.886303000
H	0.950342000	1.943067000	0.885448000
C	-0.938687000	0.182024000	0.000076000
O	-1.513260000	1.239142000	-0.000004000
O	-1.601974000	-0.985371000	0.000000000
H	-2.544924000	-0.760556000	-0.000011000

benzamide
Lowest frequency = 35.6025 cm^{-1}
Charge = 0, Multiplicity = 1

25

C	3.587899000	-1.522661000	0.249139000
C	4.567125000	-0.573979000	-0.041319000
C	4.202418000	0.750668000	-0.283810000
C	2.863339000	1.123037000	-0.240481000
C	1.872449000	0.173300000	0.030788000
C	0.456563000	0.665776000	0.060783000
O	0.199420000	1.850011000	0.165267000
H	2.550158000	2.154578000	-0.412852000
H	4.968298000	1.497575000	-0.505155000
H	5.619204000	-0.867246000	-0.071840000
H	3.870301000	-2.557203000	0.456765000
C	-1.885356000	-0.185492000	-0.035317000
C	-2.557341000	1.032098000	0.154197000
C	-3.946012000	0.998996000	0.155303000
H	-1.986821000	1.948807000	0.286931000
C	-3.841765000	-1.355208000	-0.210041000
C	-4.614453000	-0.210959000	-0.028991000
H	-4.506553000	1.925954000	0.299901000
H	-4.319157000	-2.330212000	-0.360506000
H	-5.704224000	-0.268270000	-0.033981000
N	-2.513654000	-1.347371000	-0.213496000
N	-0.498407000	-0.309248000	-0.053760000
H	-0.206052000	-1.263615000	-0.227333000
C	2.245894000	-1.151810000	0.284969000
H	1.499357000	-1.906730000	0.545415000

1,2-diphenylethyne
Lowest frequency = 18.3058 cm^{-1}
Charge = 0, Multiplicity = 1

24

C	-0.608905000	-0.000014000	0.000006000
C	0.608908000	0.000000000	0.000246000
C	2.037116000	-0.000011000	0.000127000
C	2.751375000	0.856759000	0.856012000
C	2.751213000	-0.856771000	-0.855905000
C	4.142176000	0.853575000	0.852707000
H	2.199483000	1.523064000	1.521752000
C	4.142012000	-0.853595000	-0.852860000
H	2.199194000	-1.523060000	-1.521554000
C	4.841845000	-0.000014000	-0.000139000
H	4.685680000	1.524104000	1.522571000
H	4.685390000	-1.524119000	-1.522831000
H	5.934343000	-0.000017000	-0.000243000
C	-2.037117000	0.000016000	0.000009000
C	-2.751280000	0.856816000	-0.855926000
C	-2.751310000	-0.856801000	0.855904000
C	-4.142080000	0.853640000	-0.852772000
H	-2.199313000	1.523155000	-1.521569000
C	-4.142109000	-0.853617000	0.852708000
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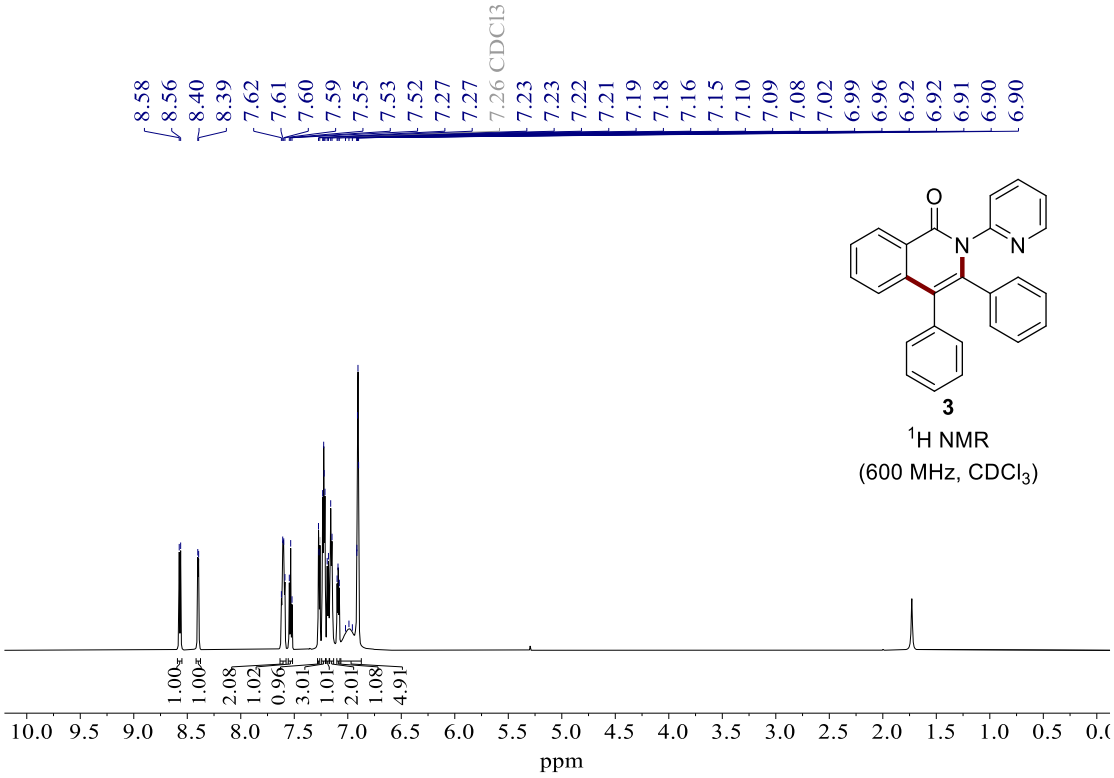
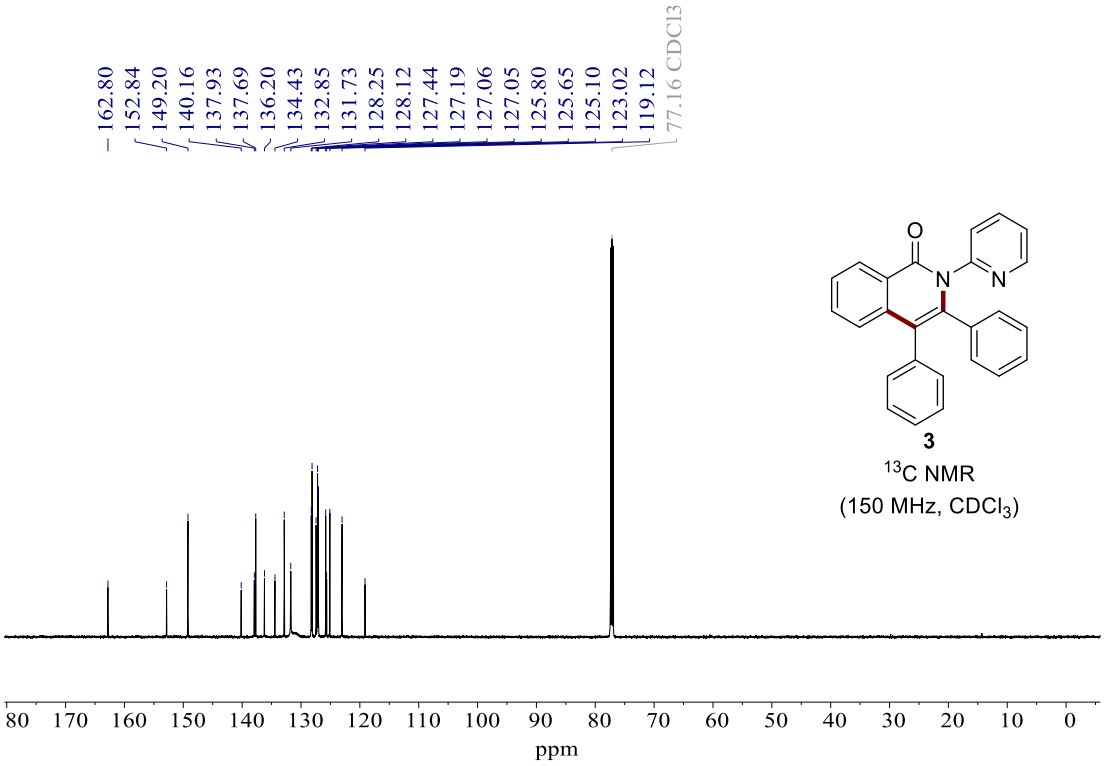
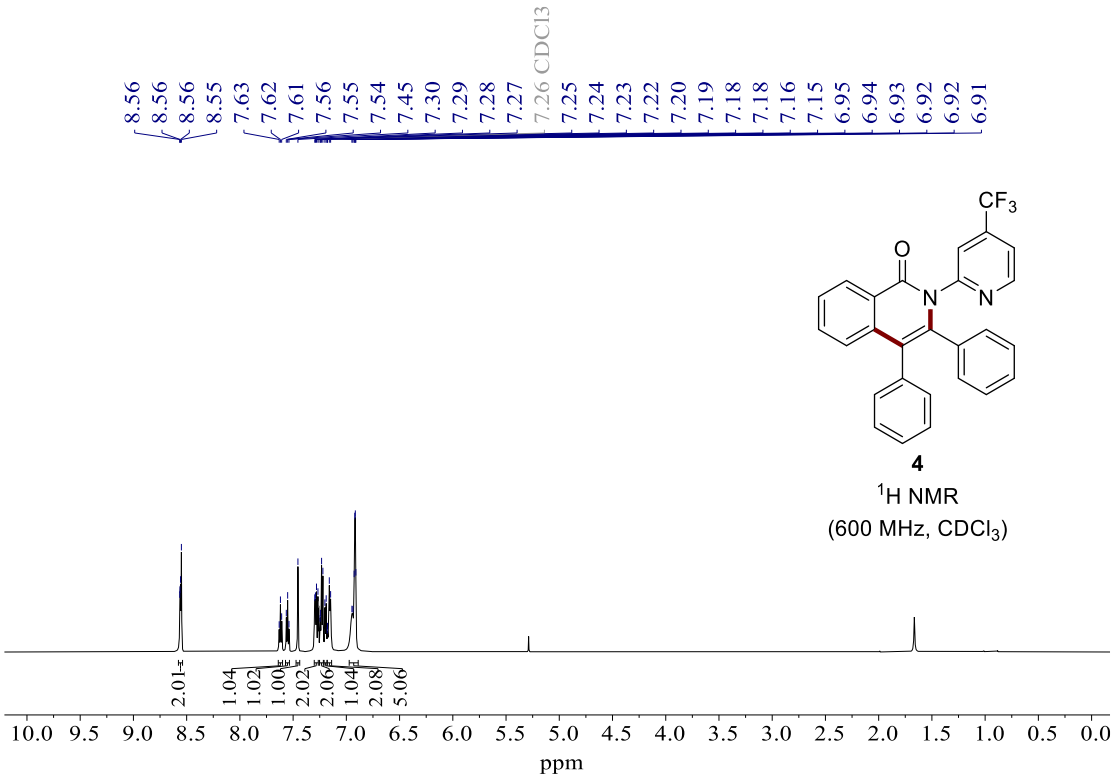
9. NMR Spectra



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CF3
O
N
N
4
1H NMR
(600 MHz, CDCl3)
2.01 1.04 1.02 1.00 2.02 2.06 1.04 2.08 5.06
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
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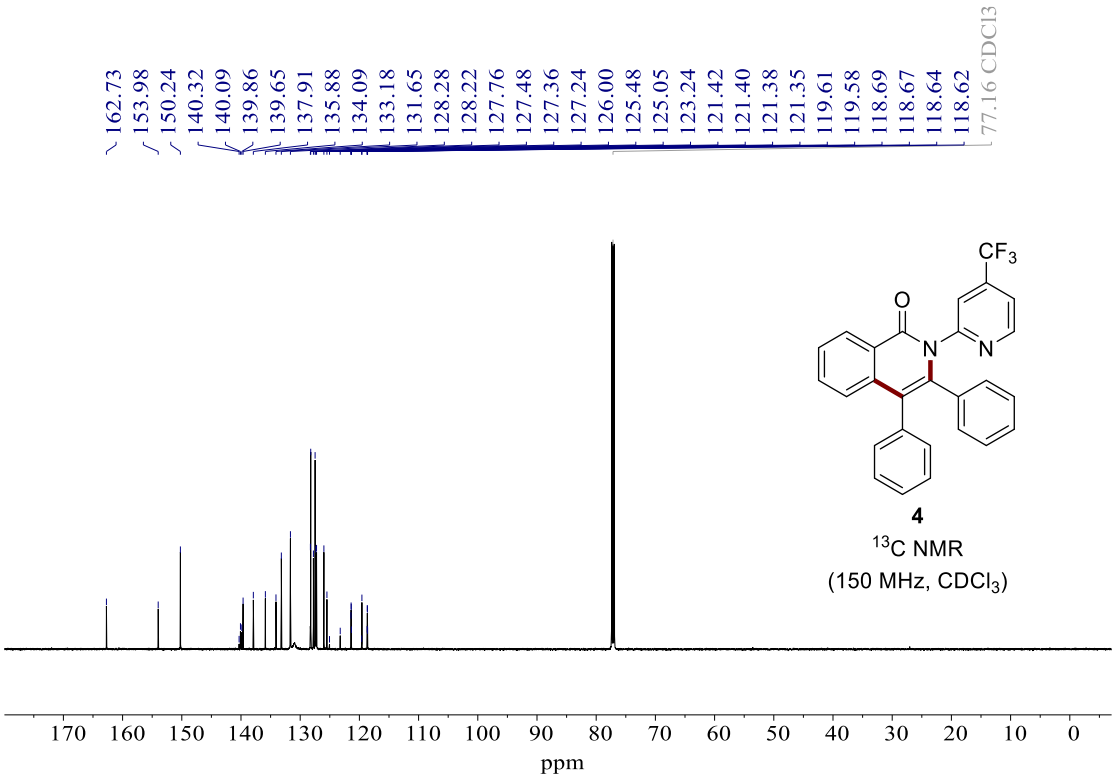
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CF3
O
N
N
4
13C NMR
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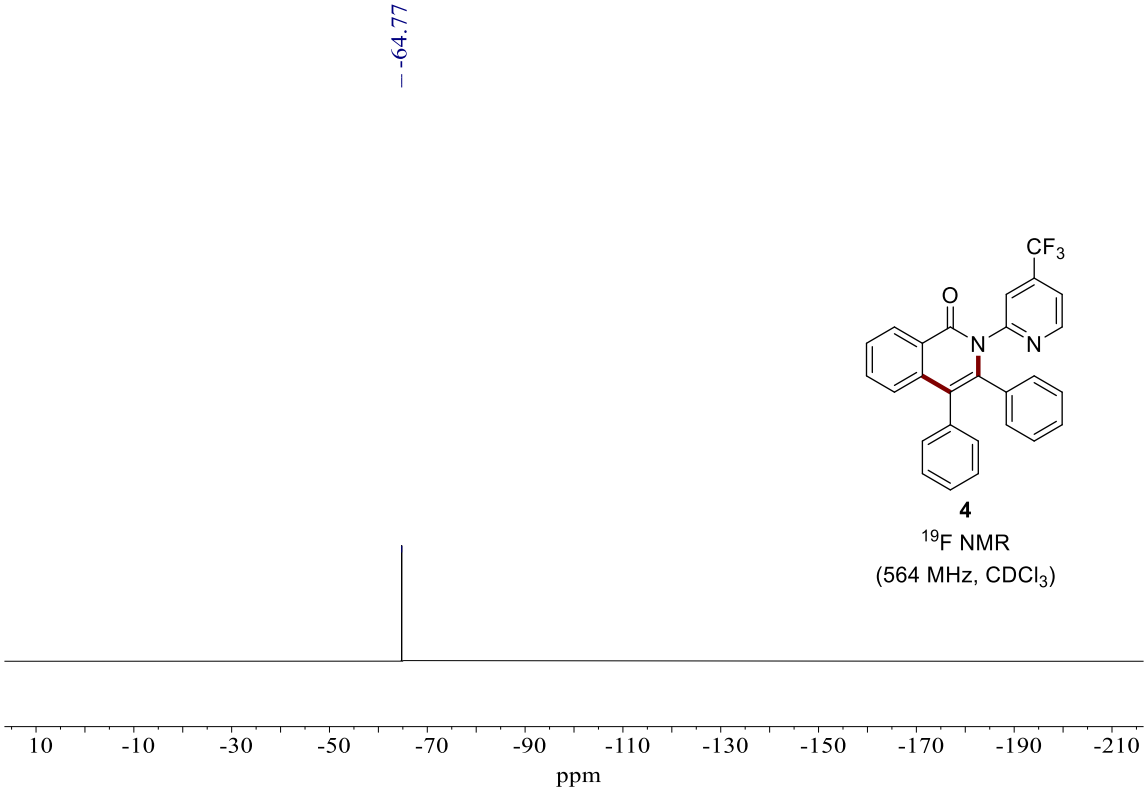
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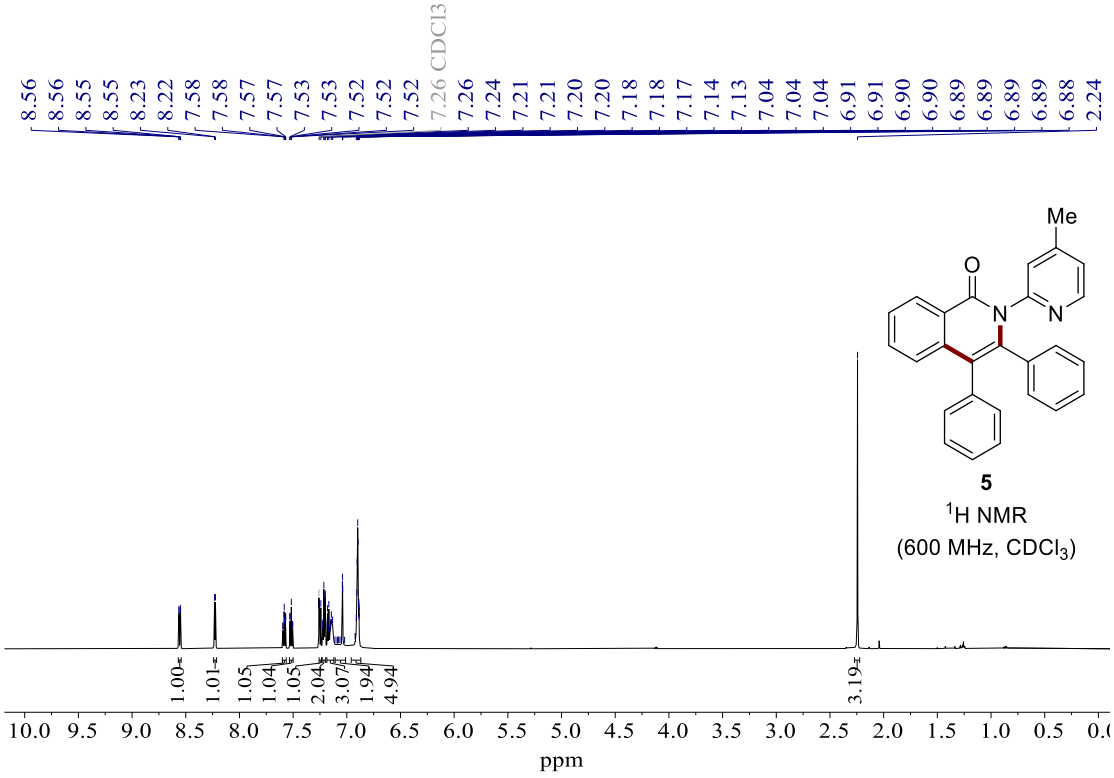
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7.52
7.52
7.26 CDCl3
7.26
7.24
7.21
7.21
7.20
7.20
7.18
7.18
7.17
7.14
7.13
7.04
7.04
7.04
6.91
6.91
6.90
6.90
6.89
6.89
6.89
6.89
6.88
2.24
Me
O
N
N
5
1H NMR
(600 MHz, CDCl3)
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1.01
1.05
1.04
1.05
2.04
3.07
1.94
4.94
3.19
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
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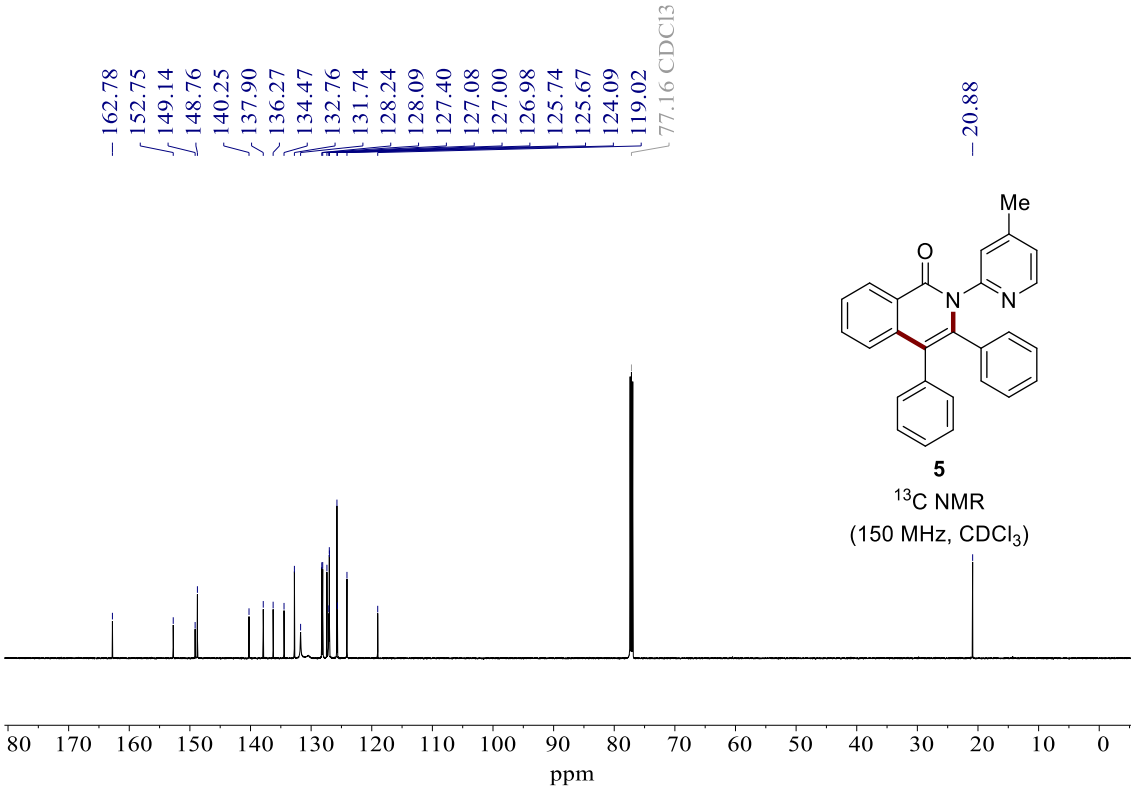
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127.08
127.00
126.98
125.74
125.67
124.09
119.02
77.16 CDCl3
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N
N
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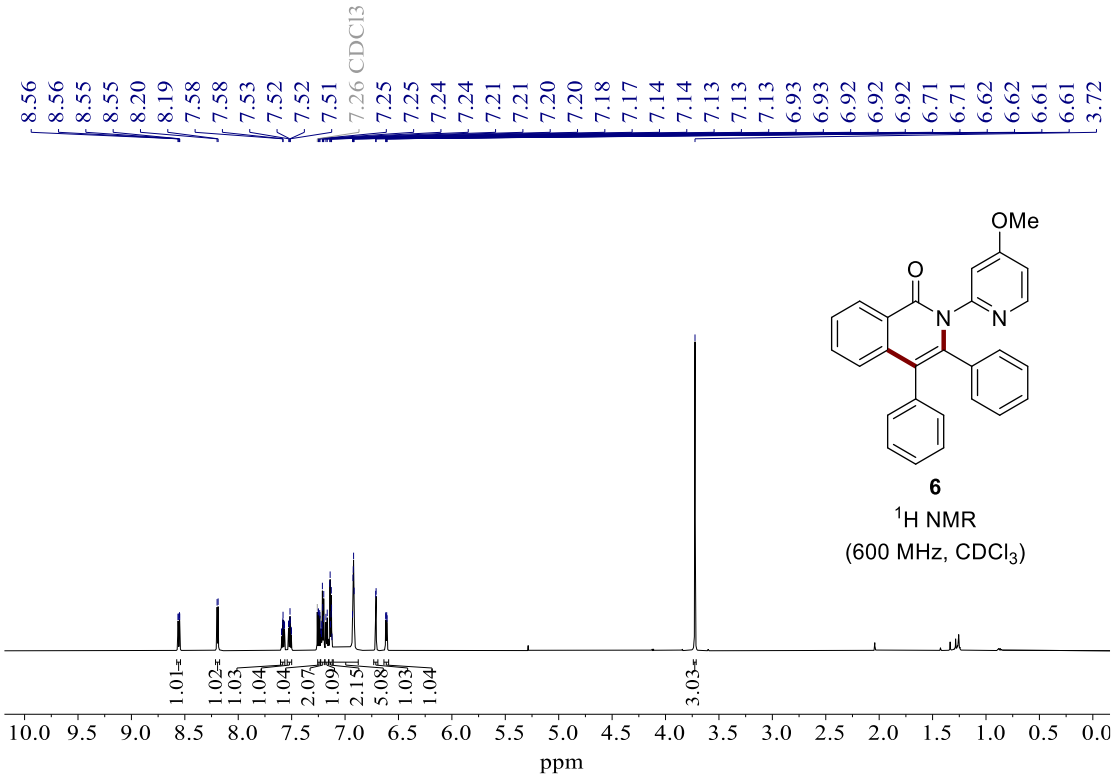
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7.25
7.25
7.24
7.24
7.21
7.21
7.20
7.20
7.18
7.17
7.14
7.14
7.13
7.13
7.13
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6.93
6.92
6.92
6.92
6.71
6.71
6.62
6.62
6.61
6.61
3.72
OMe
O
N
N
6
1H NMR
(600 MHz, CDCl3)
1.01
1.02
1.03
1.04
1.04
2.07
1.09
2.15
5.08
1.03
1.04
3.03
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
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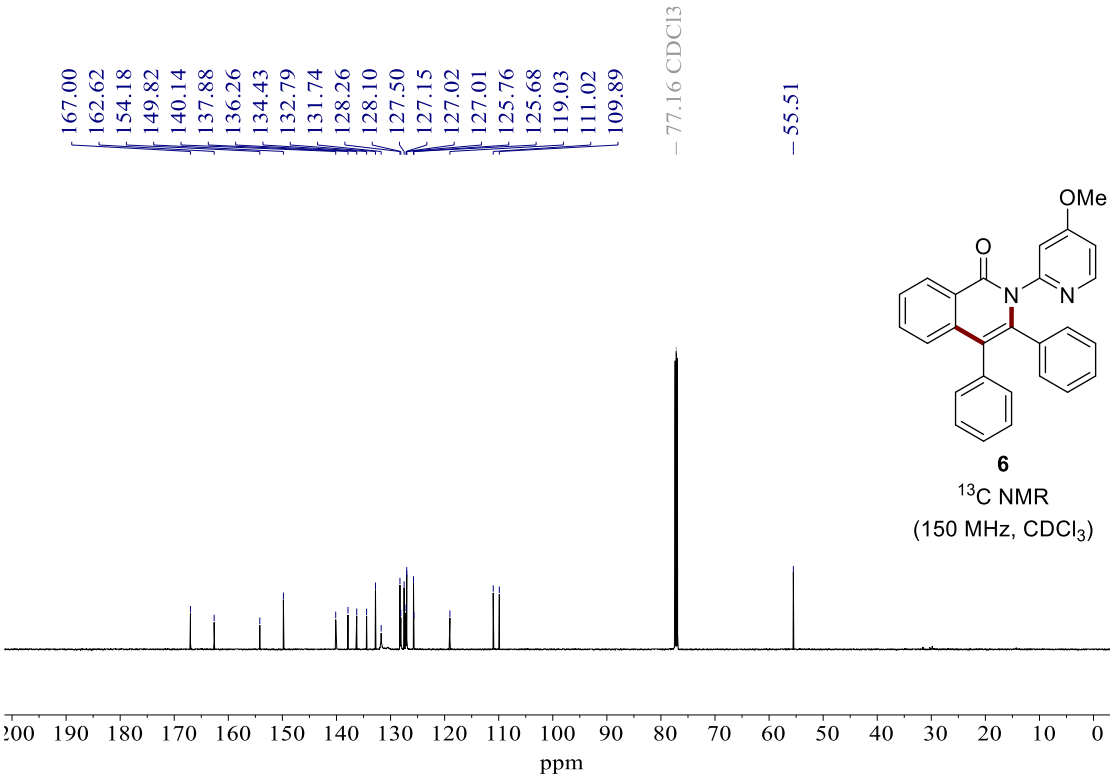
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125.68
119.03
111.02
109.89
77.16 CDCl3
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OMe
O
N
N
6
13C NMR
(150 MHz, CDCl3)
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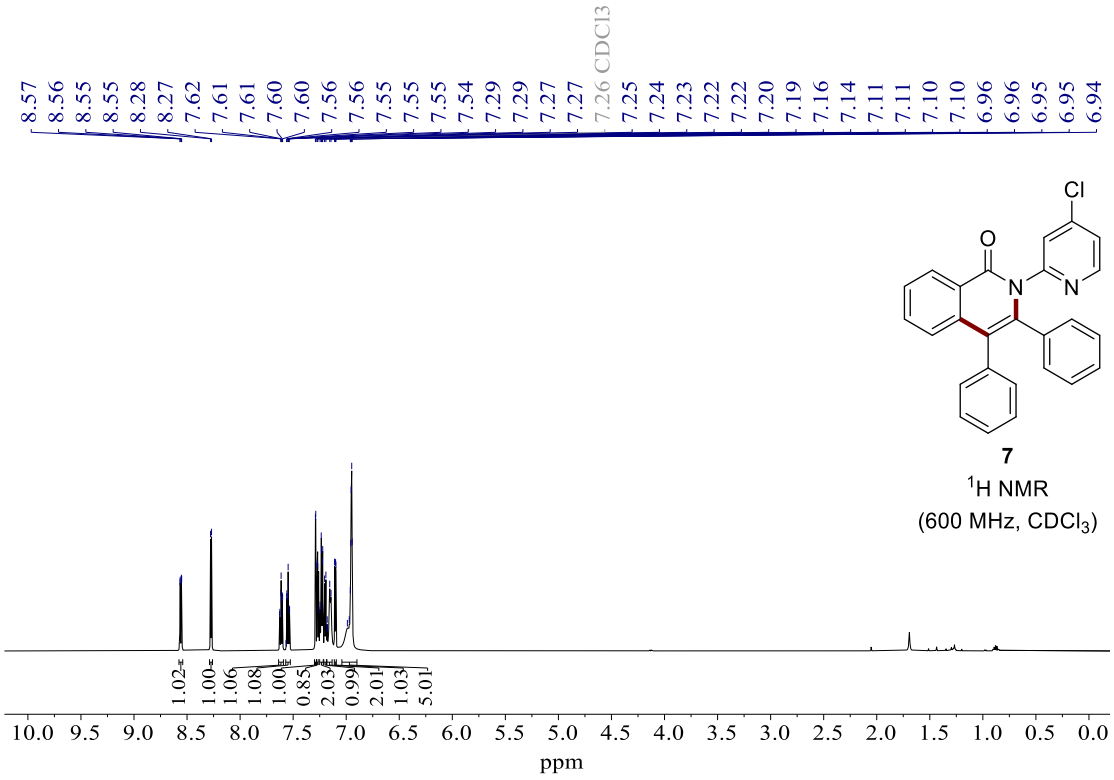
ppm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7.27
7.27
7.26 CDCl3
7.25
7.24
7.23
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7.19
7.16
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7.10
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6.96
6.95
6.95
6.94
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N
N
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(600 MHz, CDCl3)
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1.06
1.08
1.00
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0.99
2.01
1.03
5.01
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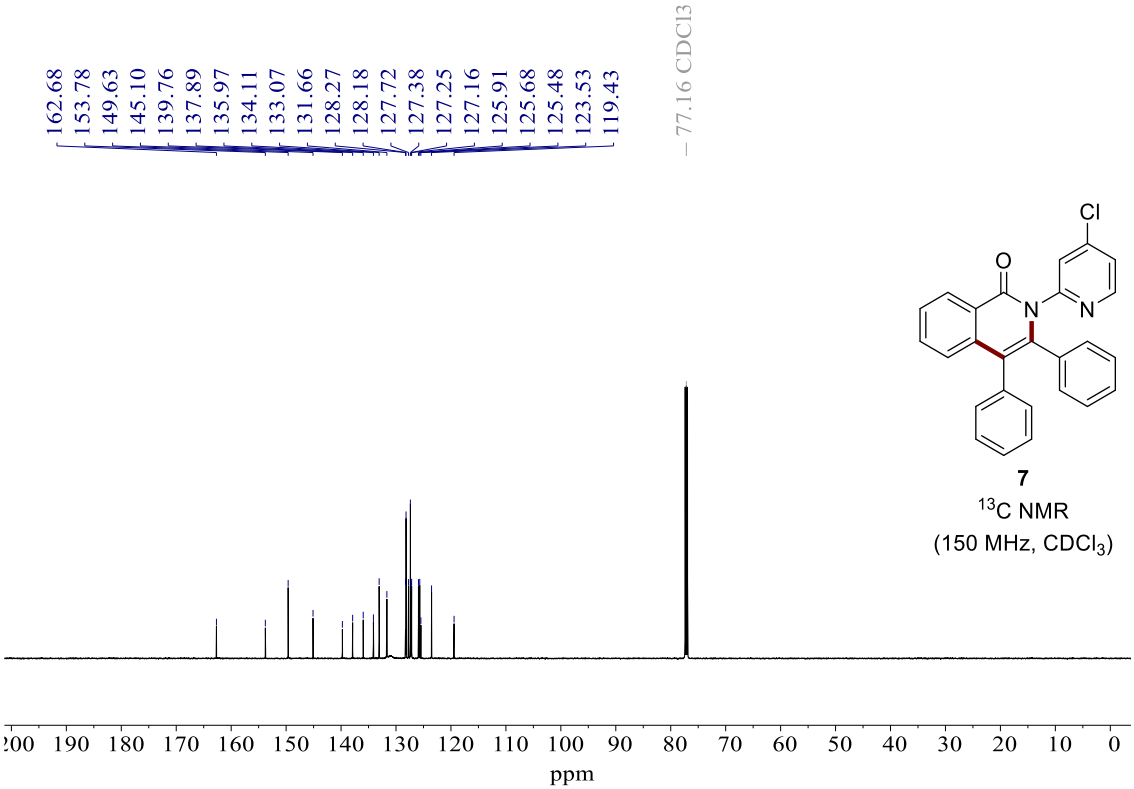
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125.68
125.48
123.53
119.43
77.16 CDCl3
Cl
O
N
N
7
13C NMR
(150 MHz, CDCl3)
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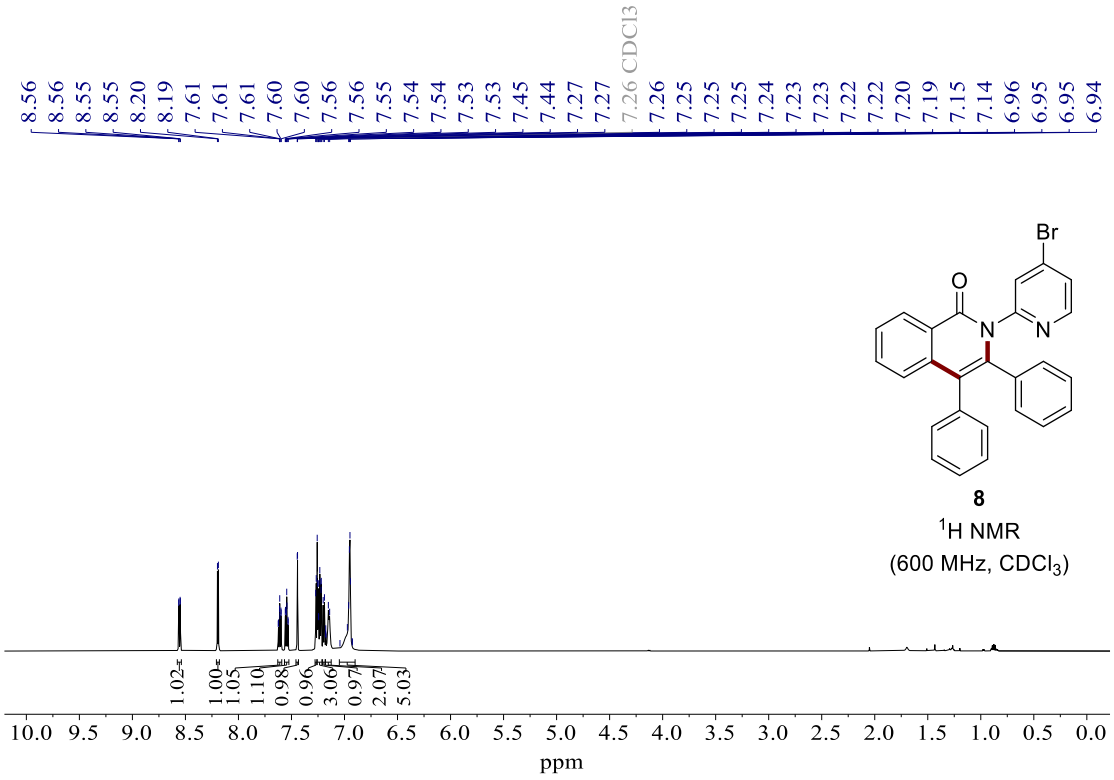
ppm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1.00
1.05
1.10
0.98
0.96
3.06
0.97
2.07
5.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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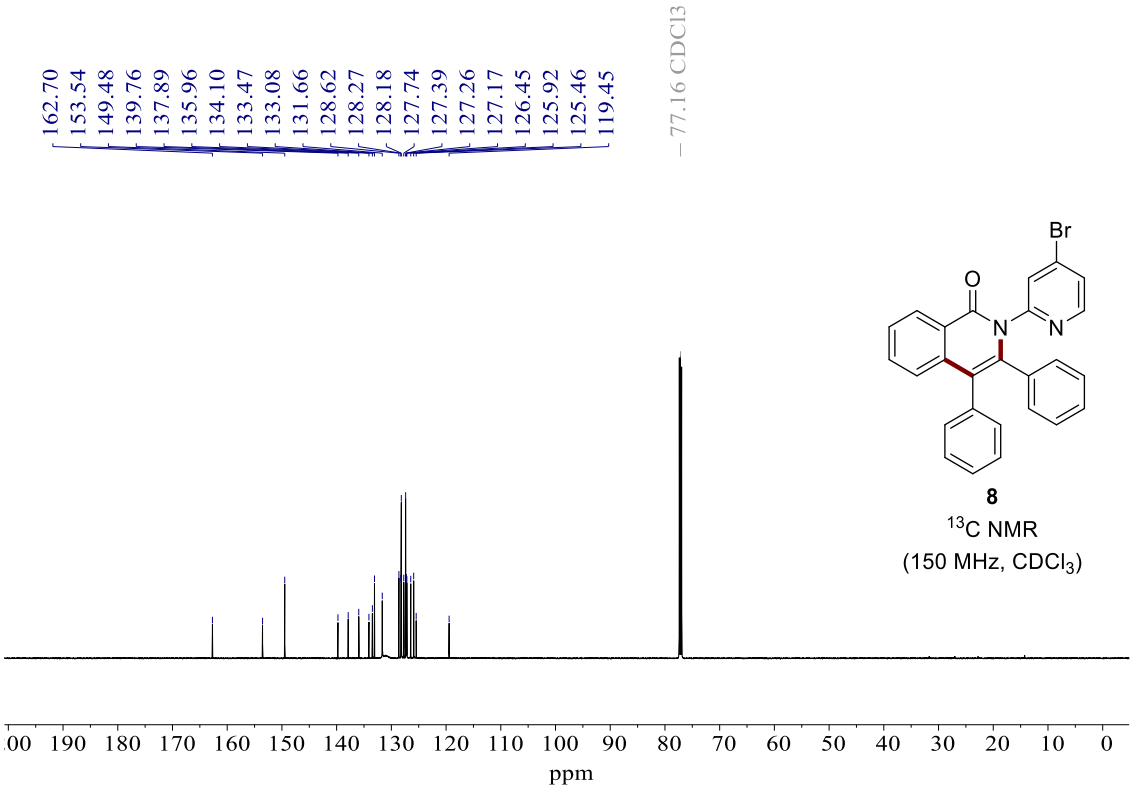
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N
N
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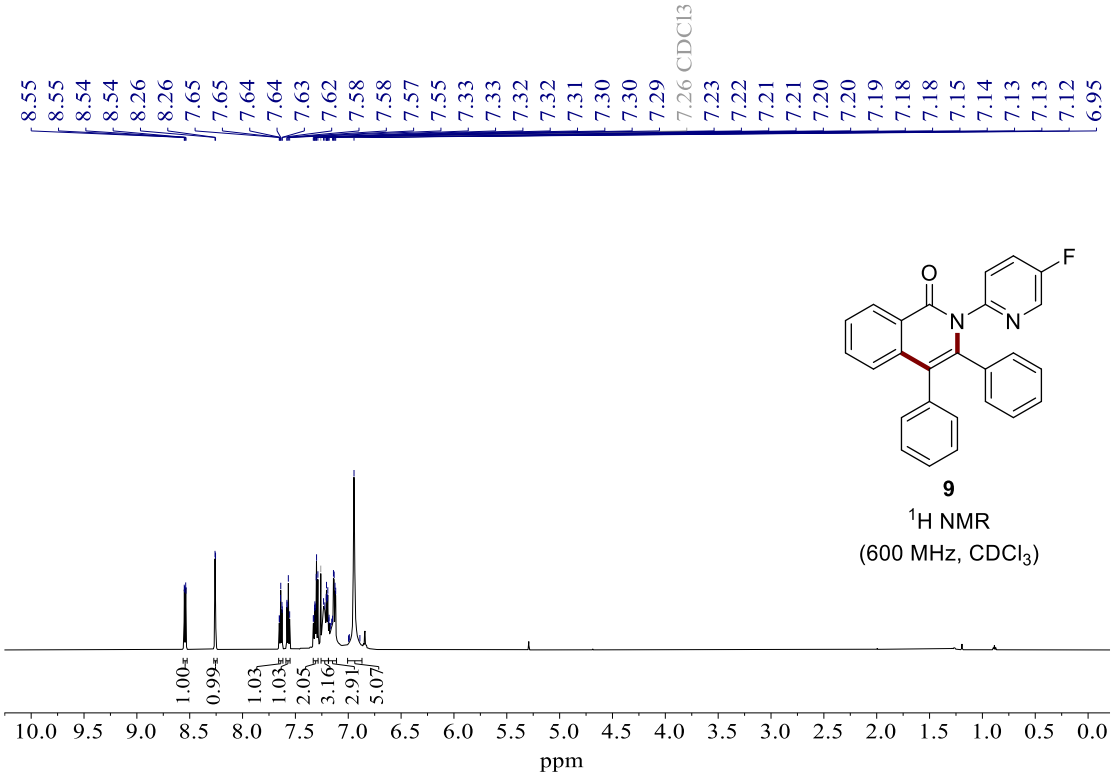
(150 MHz, CDCl3)
ppm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7.31
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7.30
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7.26 CDCl3
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N
N
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1.03
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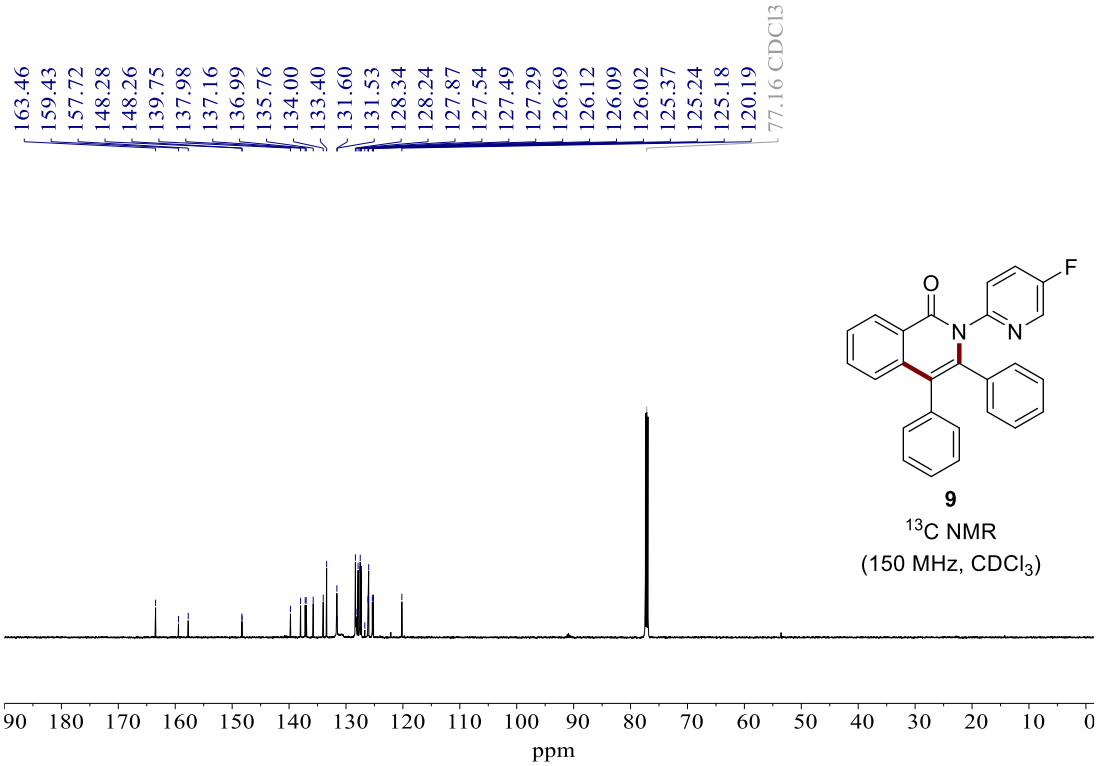
3.16
2.91
5.07
ppm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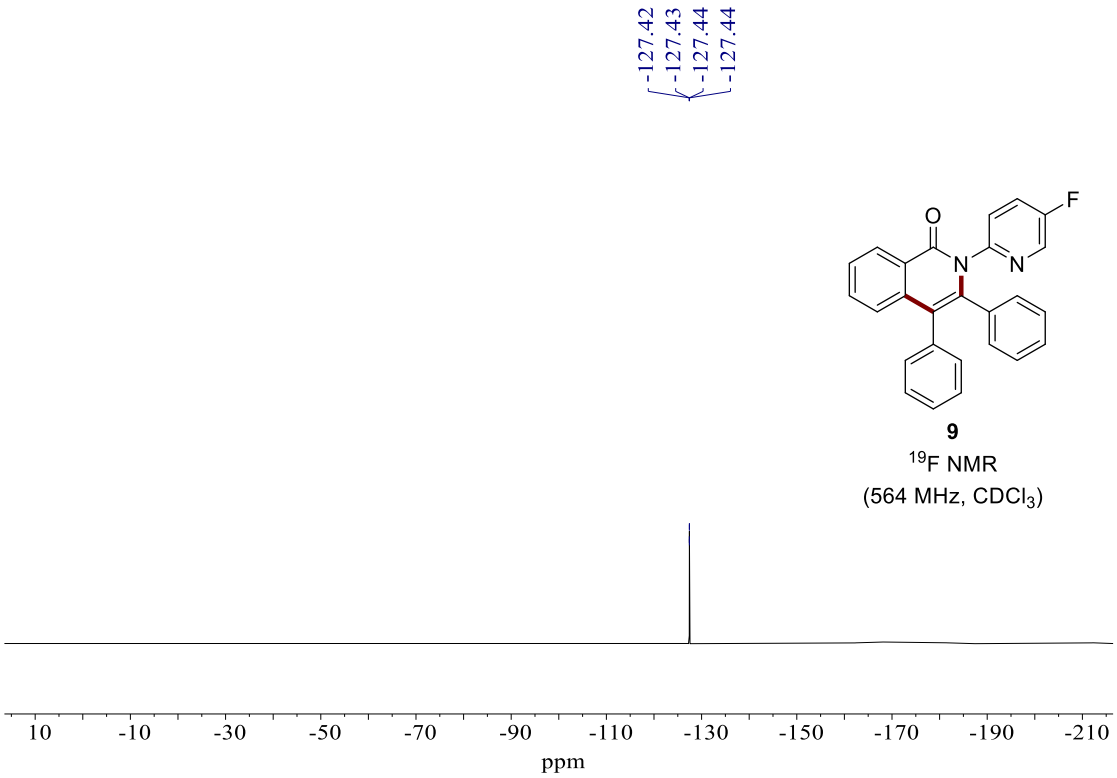
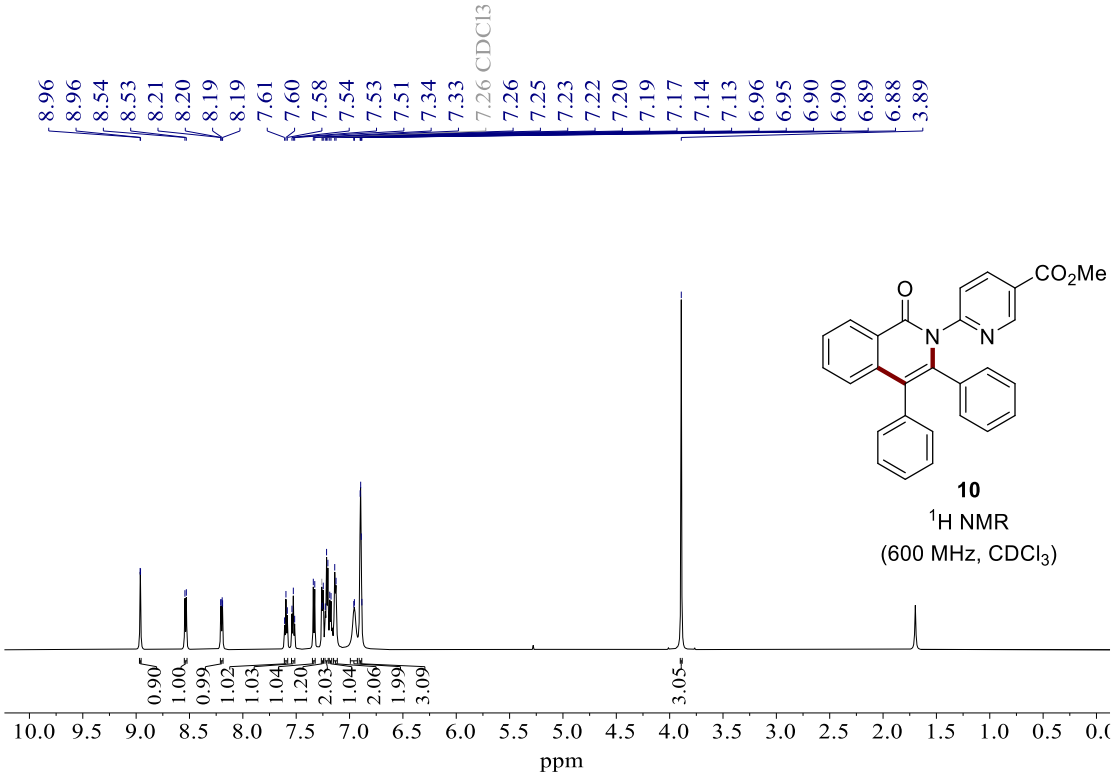
148.26
139.75
137.98
137.16
136.99
135.76
134.00
133.40
131.60
131.53
128.34
128.24
127.87
127.54
127.49
127.29
126.69
126.12
126.09
126.02
125.37
125.24
125.18
120.19
77.16 CDCl3
O
N
N
F
9
13C NMR
(150 MHz, CDCl3)
90 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm


-127.42
-127.43
-127.44
-127.44
O
N
N
F
9
19F NMR
(564 MHz, CDCl3)
10 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210
ppm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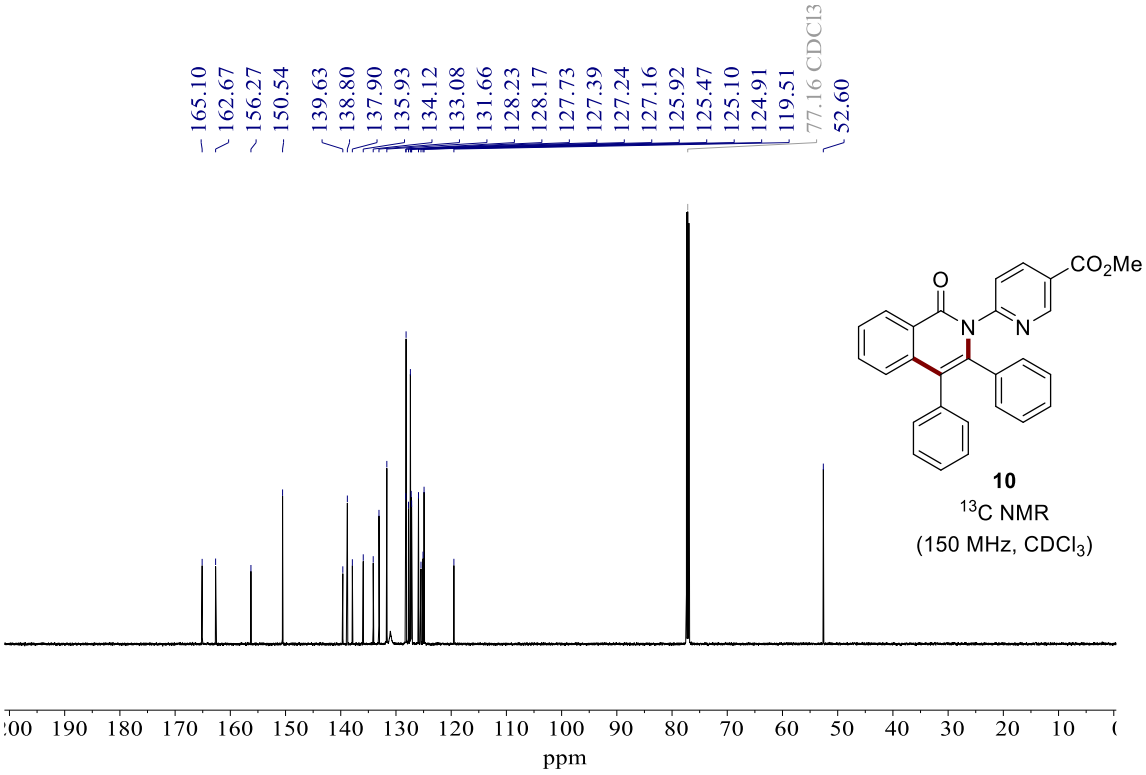
8.96
8.54
8.53
8.21
8.20
8.19
8.19
7.61
7.60
7.58
7.54
7.53
7.51
7.34
7.33
7.26 CDCl3
7.26
7.25
7.23
7.22
7.20
7.19
7.17
7.14
7.13
6.96
6.95
6.90
6.90
6.89
6.88
3.89
CO2Me
O
N
N
10
1H NMR
(600 MHz, CDCl3)
0.90
1.00
0.99
1.02
1.03
1.04
1.20
2.03
1.04
2.06
1.99
3.09
3.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
ppm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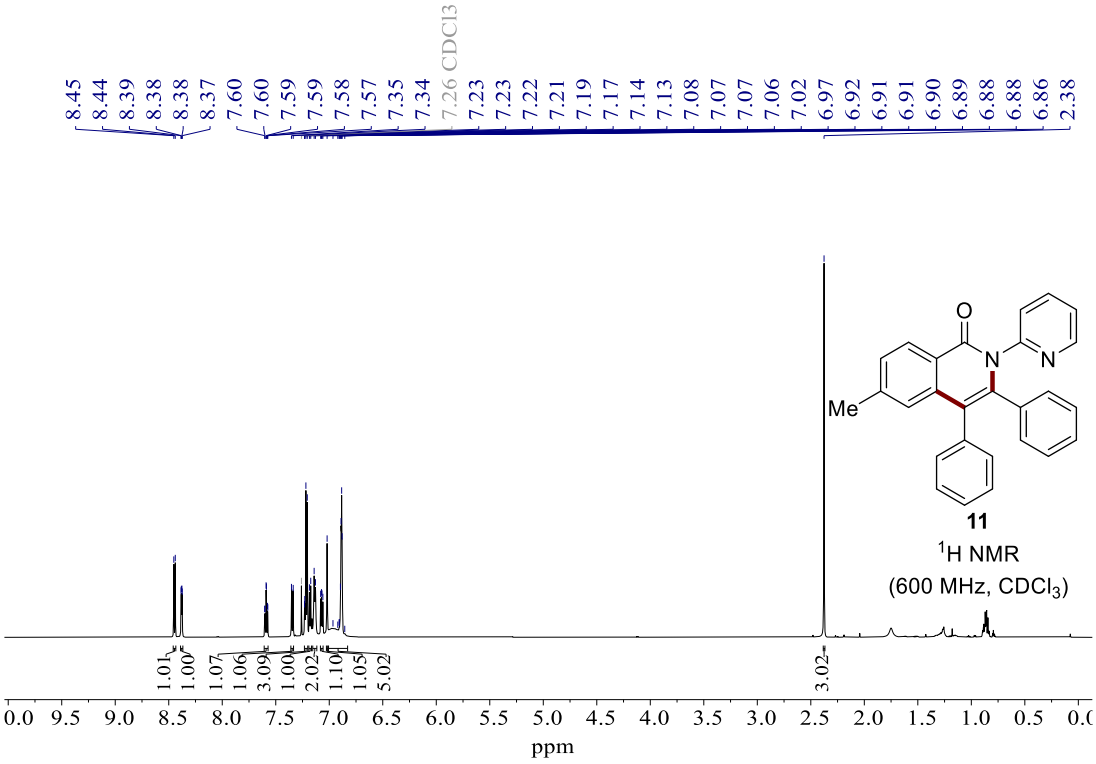
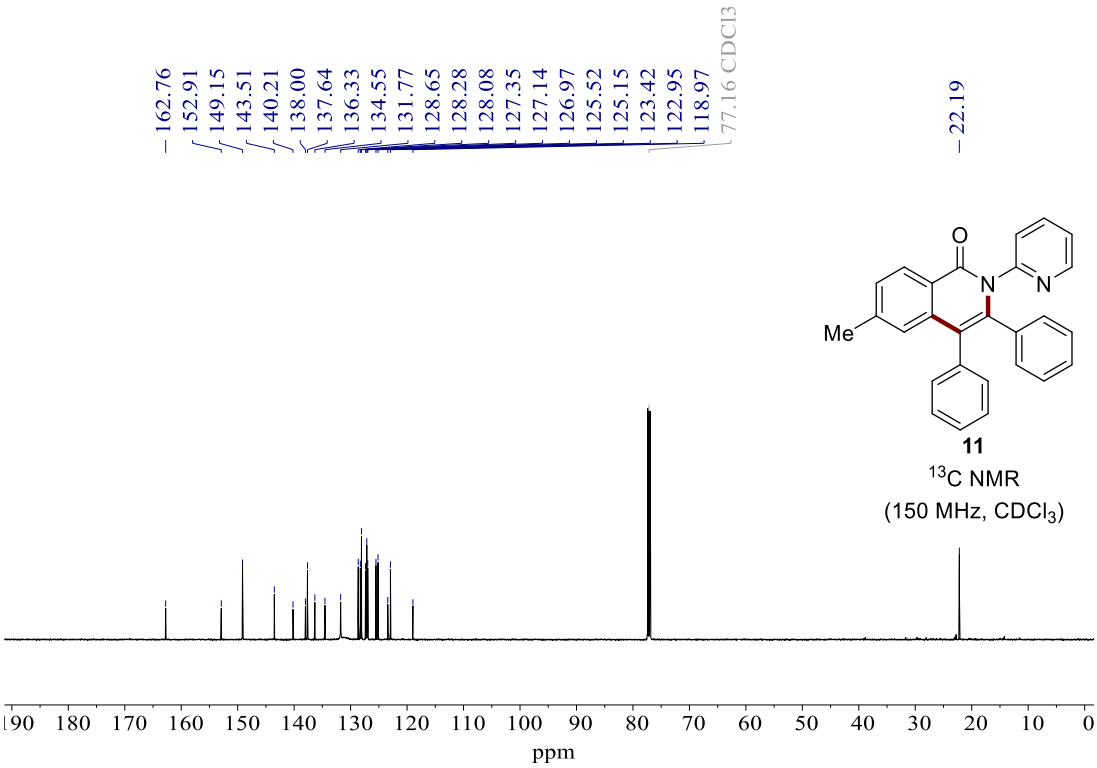
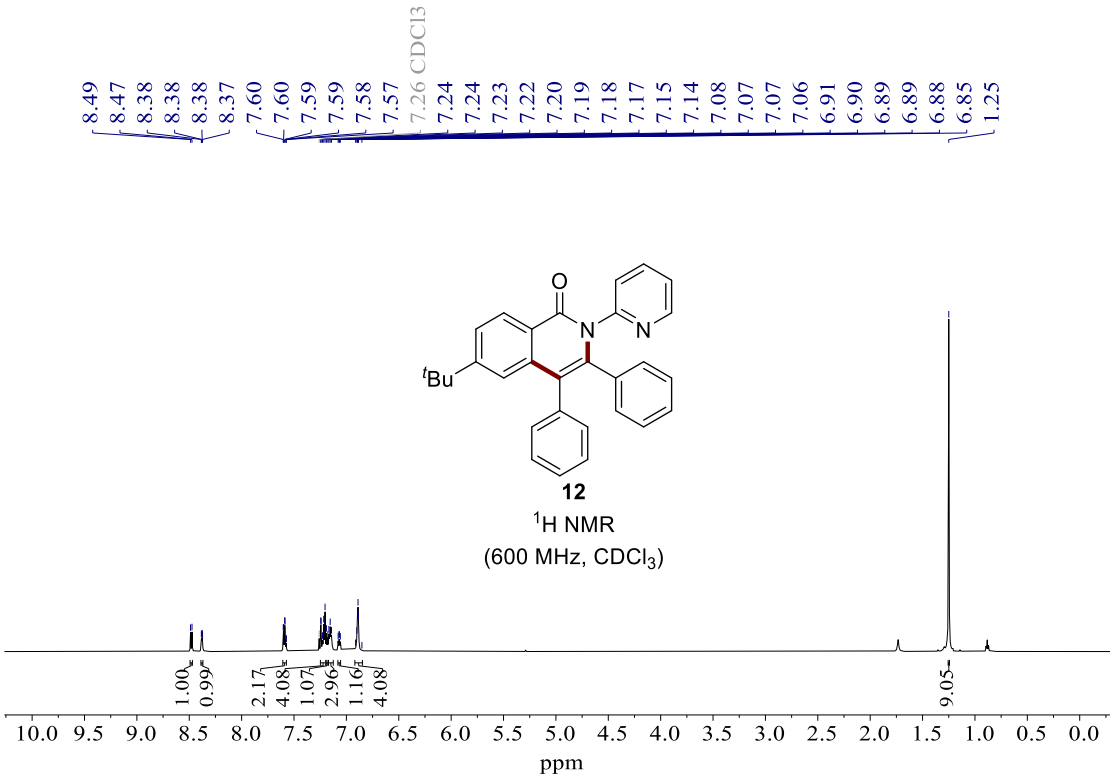
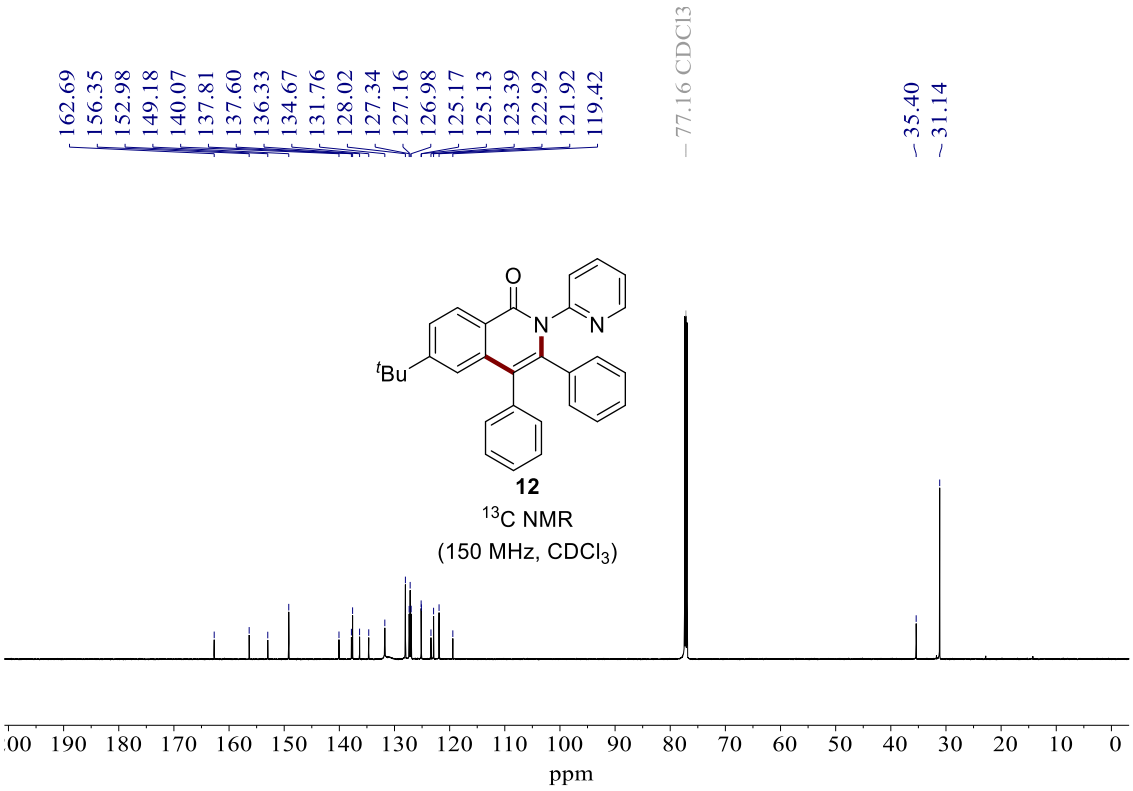
162.67
156.27
150.54
139.63
138.80
137.90
135.93
134.12
133.08
131.66
128.23
128.17
127.73
127.39
127.24
127.16
125.92
125.47
125.10
124.91
119.51
77.16 CDCl3
52.60
CO2Me
O
N
N
10
13C NMR
(150 MHz, CDCl3)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm


8.45 8.44 8.39 8.38 8.38 8.37 7.60 7.60 7.59 7.59 7.58 7.57 7.35 7.34 7.26 CDCl3 7.23 7.23 7.22 7.21 7.19 7.17 7.14 7.13 7.08 7.07 7.07 7.06 7.02 6.97 6.92 6.91 6.91 6.90 6.89 6.88 6.88 6.86 2.38
1.01 1.00 1.07 1.06 3.09 1.00 2.02 1.10 1.05 5.02 3.02
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
ppm
O
N
N
Me
11
1H NMR
(600 MHz, CDCl3)


162.76 152.91 149.15 143.51 140.21 138.00 137.64 136.33 134.55 131.77 128.65 128.28 128.08 127.35 127.14 126.97 125.52 125.15 123.42 122.95 118.97 77.16 CDCl3 22.19
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm
O
N
N
Me
11
13C NMR
(150 MHz, CDCl3)


8.49
8.47
8.38
8.38
8.38
8.37
7.60
7.60
7.59
7.59
7.58
7.57
7.26 CDCl3
7.24
7.24
7.23
7.22
7.20
7.19
7.18
7.17
7.15
7.14
7.08
7.07
7.07
7.06
6.91
6.90
6.89
6.89
6.88
6.85
1.25
O
N
N
tBu
12
1H NMR
(600 MHz, CDCl3)
1.00
0.99
2.17
4.08
1.07
2.96
1.16
4.08
9.05
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
ppm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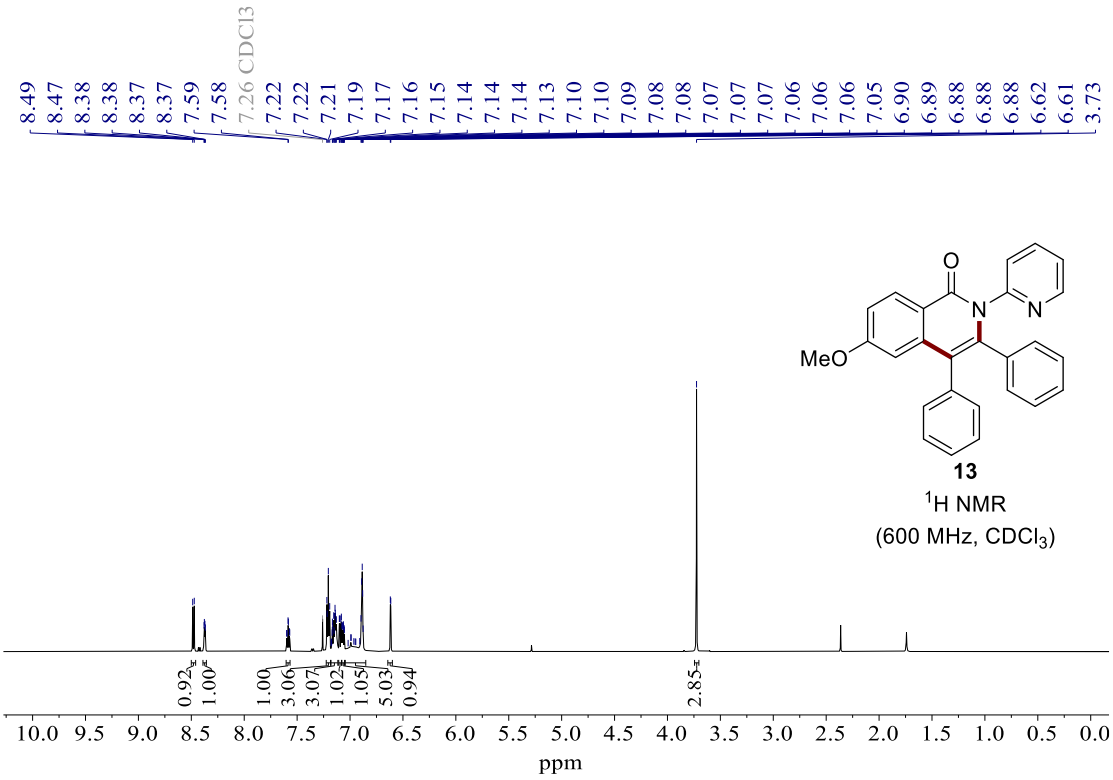
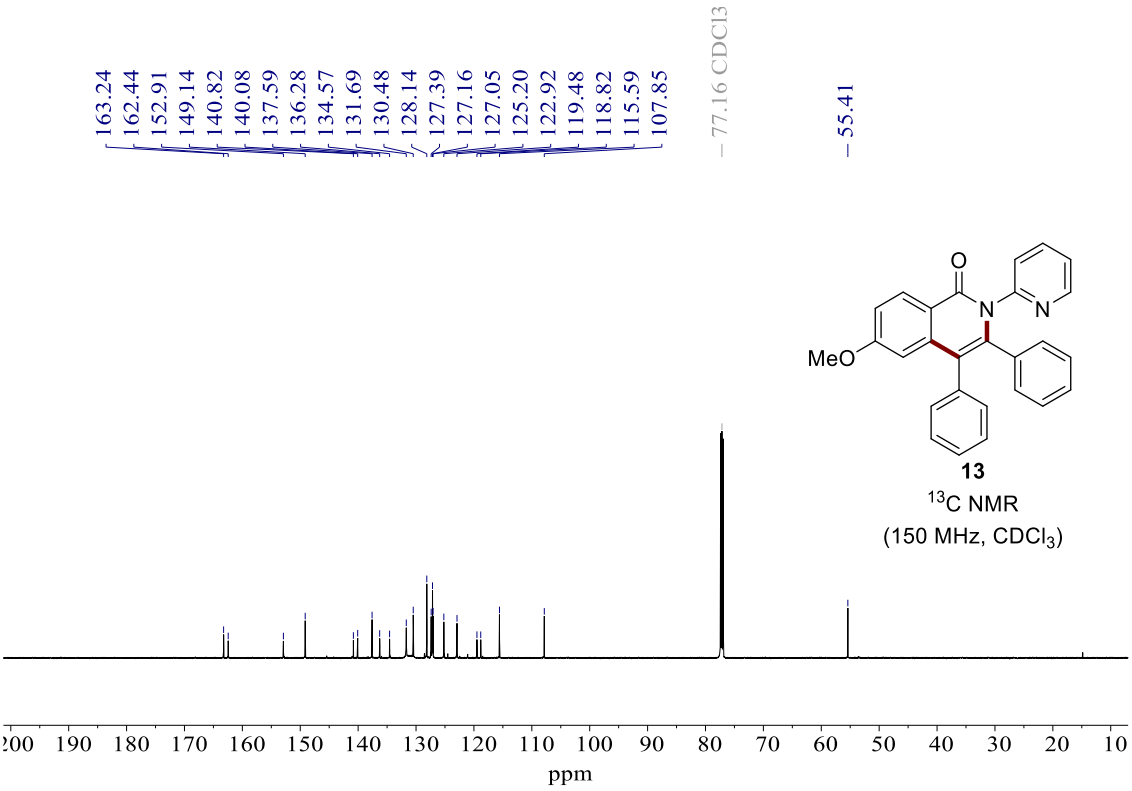
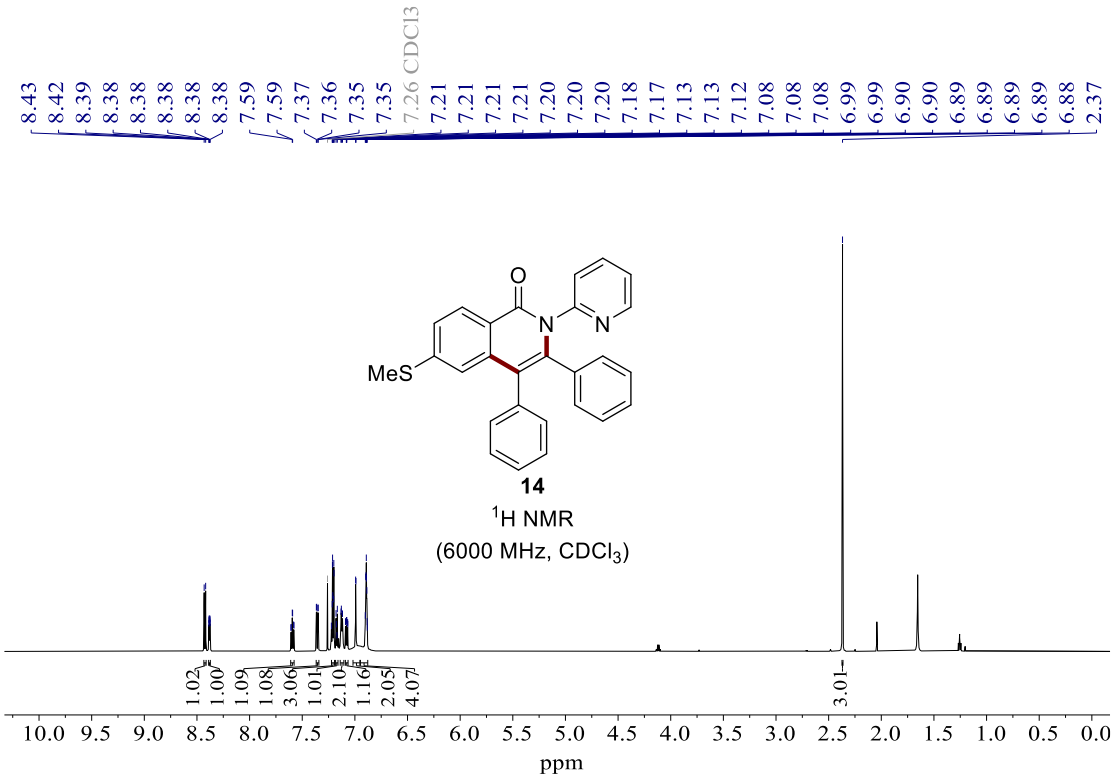
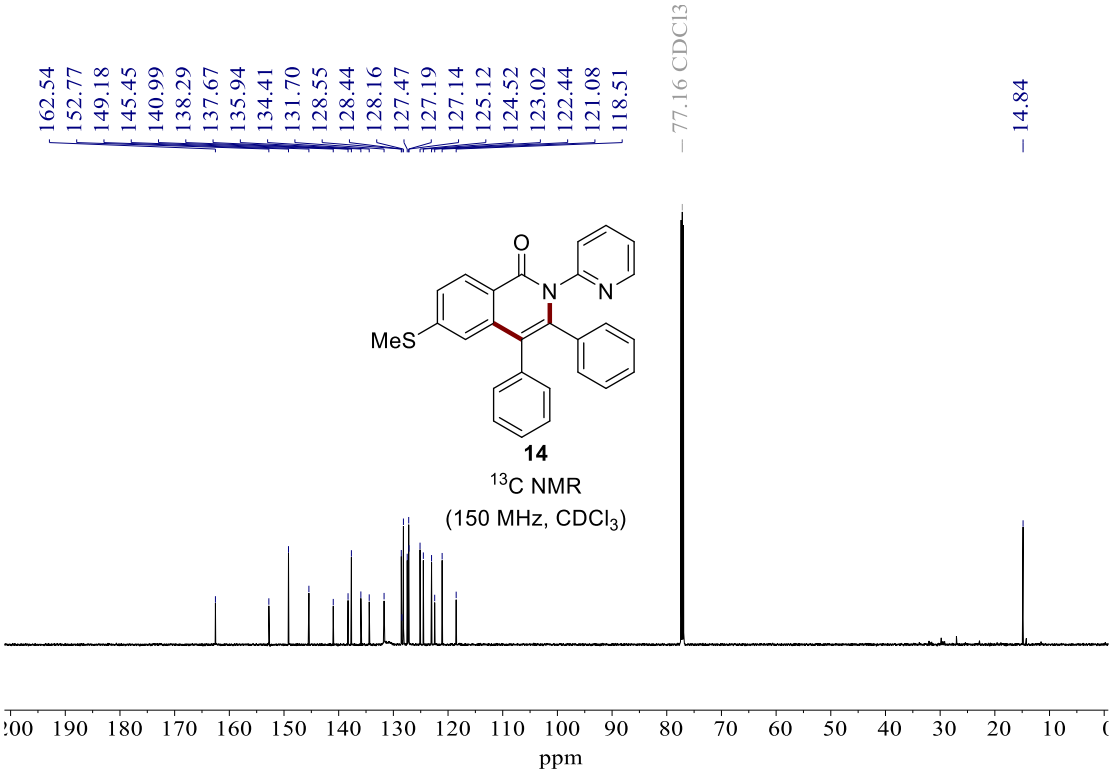
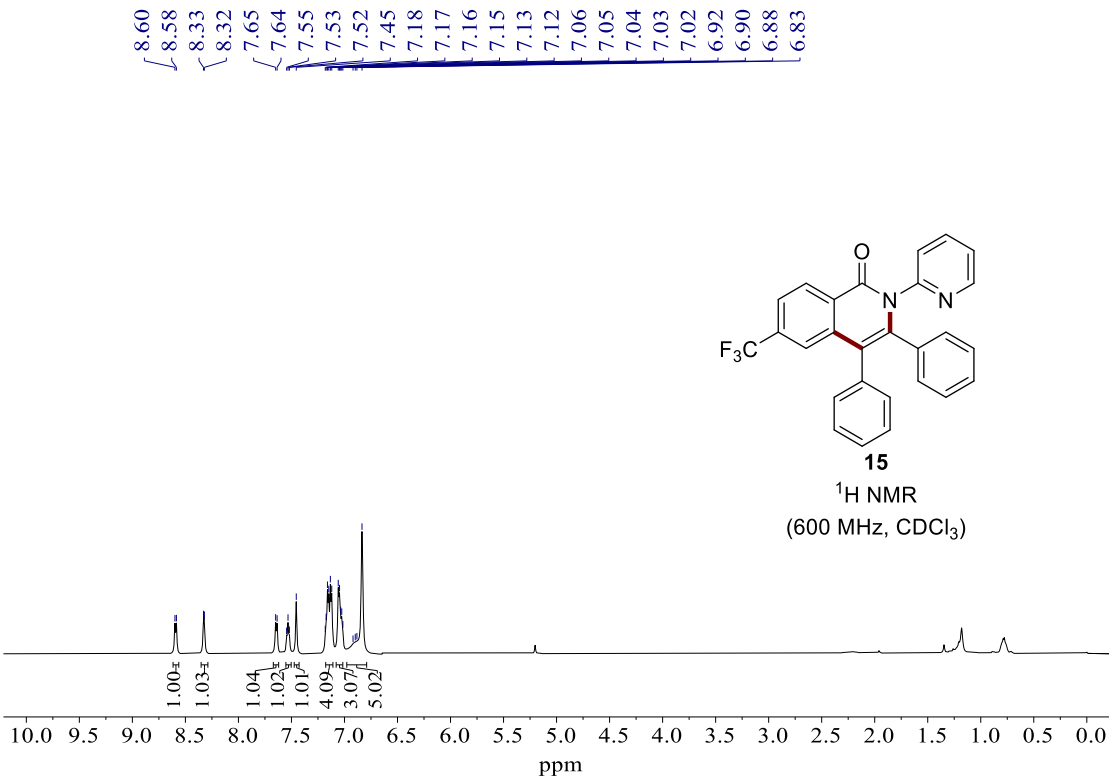
156.35
152.98
149.18
140.07
137.81
137.60
136.33
134.67
131.76
128.02
127.34
127.16
126.98
125.17
125.13
123.39
122.92
121.92
119.42
77.16 CDCl3
35.40
31.14
O
N
N
tBu
12
13C NMR
(150 MHz, CDCl3)
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm


8.49
8.47
8.38
8.38
8.37
8.37
7.59
7.58
7.26 CDCl3
7.22
7.22
7.21
7.19
7.17
7.16
7.15
7.14
7.14
7.14
7.13
7.10
7.10
7.09
7.08
7.08
7.07
7.07
7.07
7.06
7.06
7.06
7.05
6.90
6.89
6.88
6.88
6.88
6.62
6.61
3.73
O
N
N
MeO
13
1H NMR
(600 MHz, CDCl3)
0.92
1.00
1.00
3.06
3.07
1.02
1.05
5.03
0.94
2.85
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
ppm


163.24
162.44
152.91
149.14
140.82
140.08
137.59
136.28
134.57
131.69
130.48
128.14
127.39
127.16
127.05
125.20
122.92
119.48
118.82
115.59
107.85
77.16 CDCl3
55.41
O
N
N
MeO
13
13C NMR
(150 MHz, CDCl3)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm


8.43 8.42 8.39 8.38 8.38 8.38 8.38 8.38 7.59 7.59 7.37 7.36 7.35 7.35 7.26 CDCl3 7.21 7.21 7.21 7.21 7.20 7.20 7.20 7.18 7.17 7.13 7.13 7.12 7.08 7.08 7.08 6.99 6.99 6.90 6.90 6.89 6.89 6.89 6.89 6.88 2.37
O
N
N
MeS
14
1H NMR
(6000 MHz, CDCl3)
1.02 1.00 1.09 1.08 3.06 1.01 2.10 1.16 2.05 4.07 3.01
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
ppm


162.54 152.77 149.18 145.45 140.99 138.29 137.67 135.94 134.41 131.70 128.55 128.44 128.16 127.47 127.19 127.14 125.12 124.52 123.02 122.44 121.08 118.51 77.16 CDCl3 14.84
O
N
N
MeS
14
13C NMR
(150 MHz, CDCl3)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm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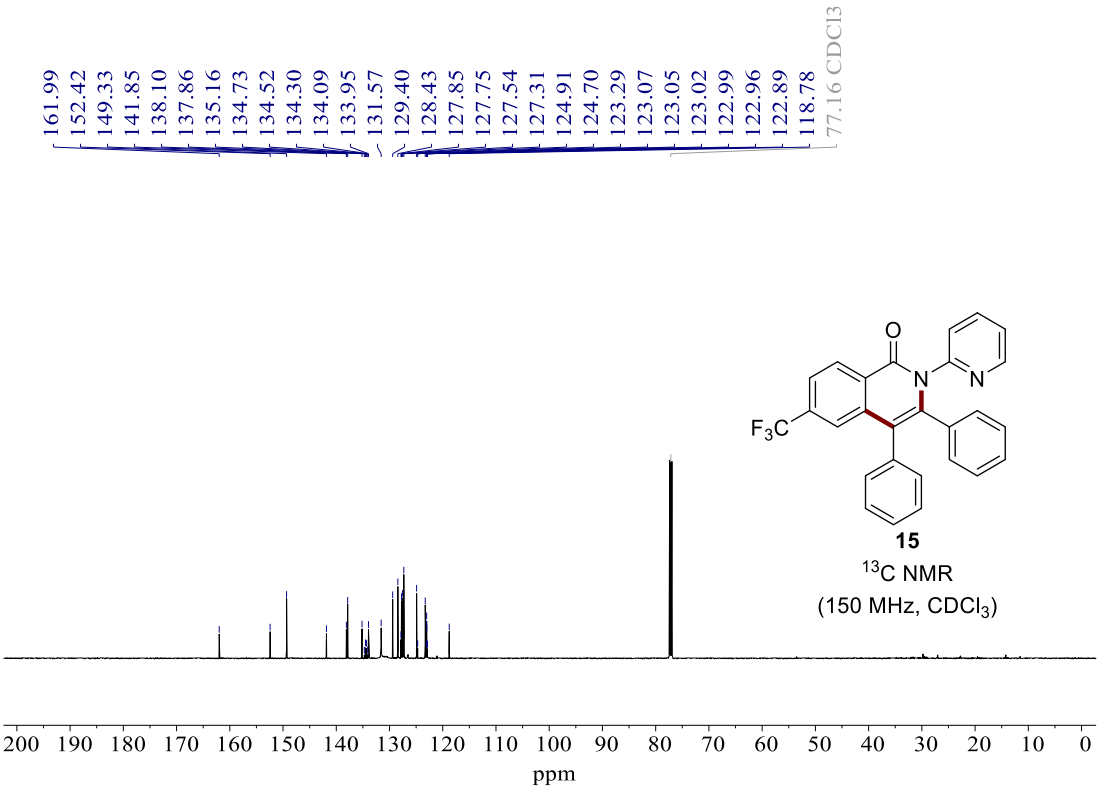
8.58
8.33
8.32
7.65
7.64
7.55
7.53
7.52
7.45
7.18
7.17
7.16
7.15
7.13
7.12
7.06
7.05
7.04
7.03
7.02
6.92
6.90
6.88
6.83
O
N
N
F3C
15
1H NMR
(600 MHz, CDCl3)
1.00
1.03
1.04
1.02
1.01
4.09
3.07
5.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm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152.42
149.33
141.85
138.10
137.86
135.16
134.73
134.52
134.30
134.09
133.95
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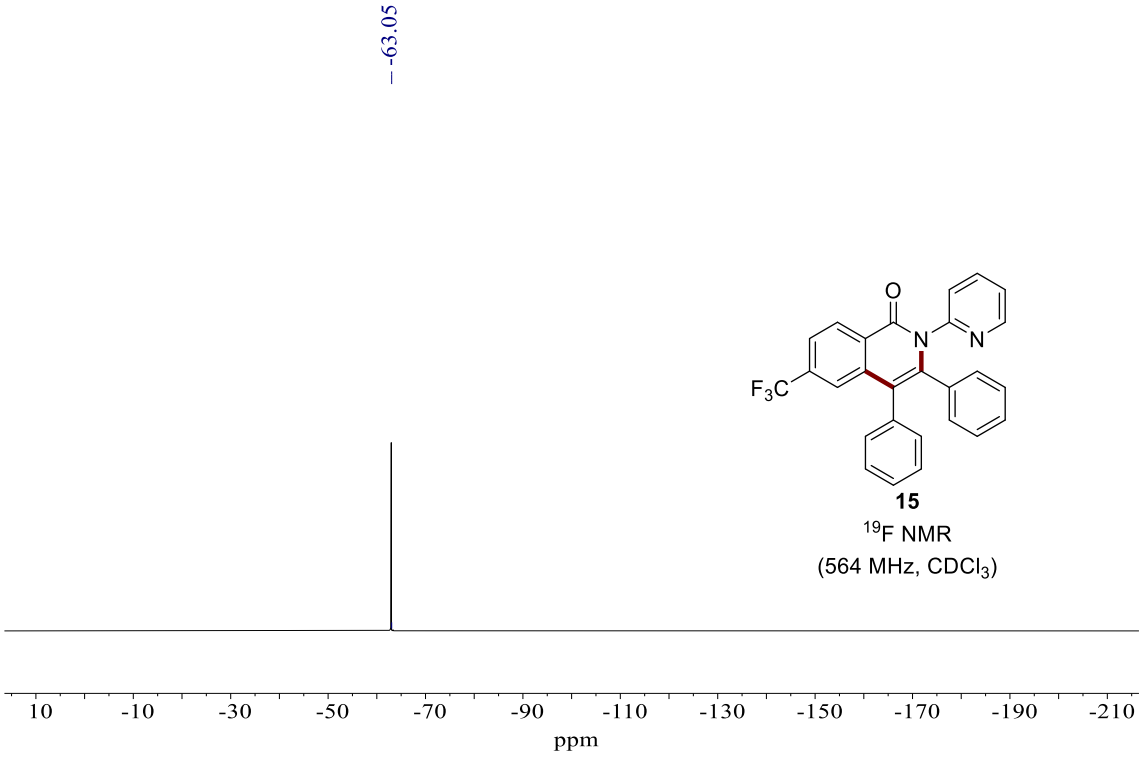
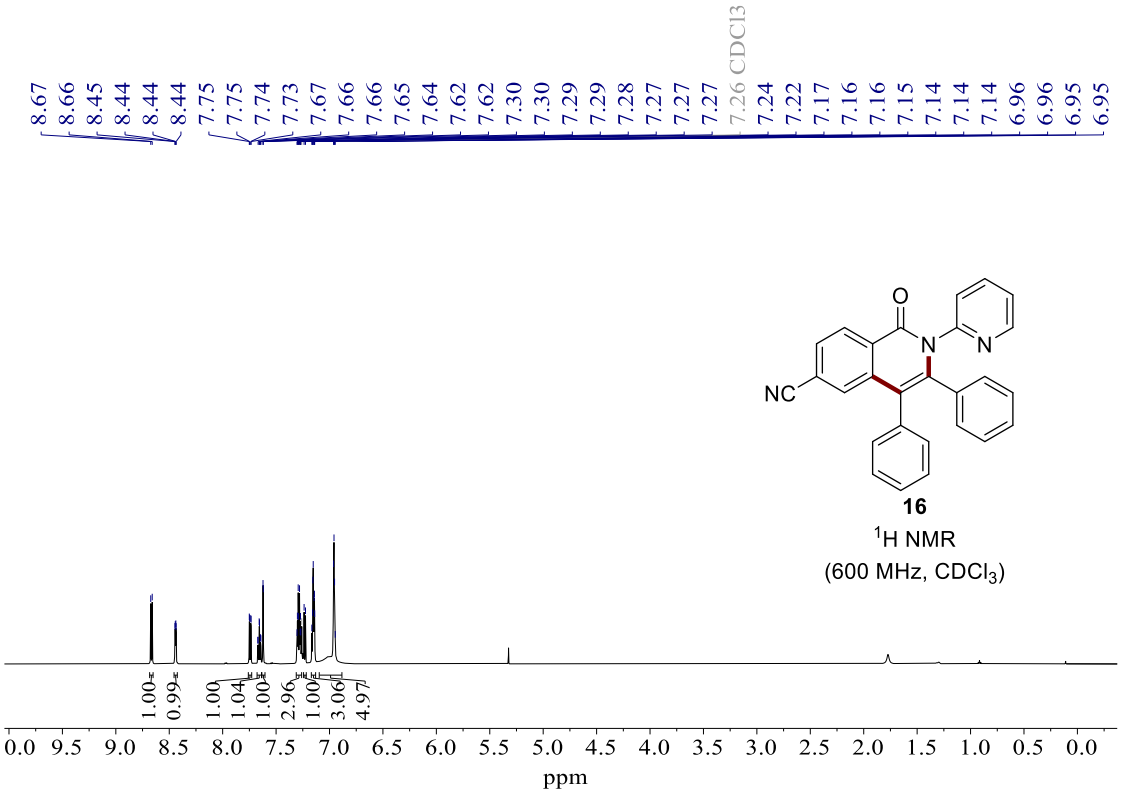
129.40
128.43
127.85
127.75
127.54
127.31
124.91
124.70
123.29
123.07
123.05
123.02
122.99
122.96
122.89
118.78
77.16 CDCl3
O
N
N
F3C
15
13C NMR
(150 MHz, CDCl3)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm


-63.05
O
N
N
F3C
15
19F NMR
(564 MHz, CDCl3)
10
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
ppm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8.66
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8.44
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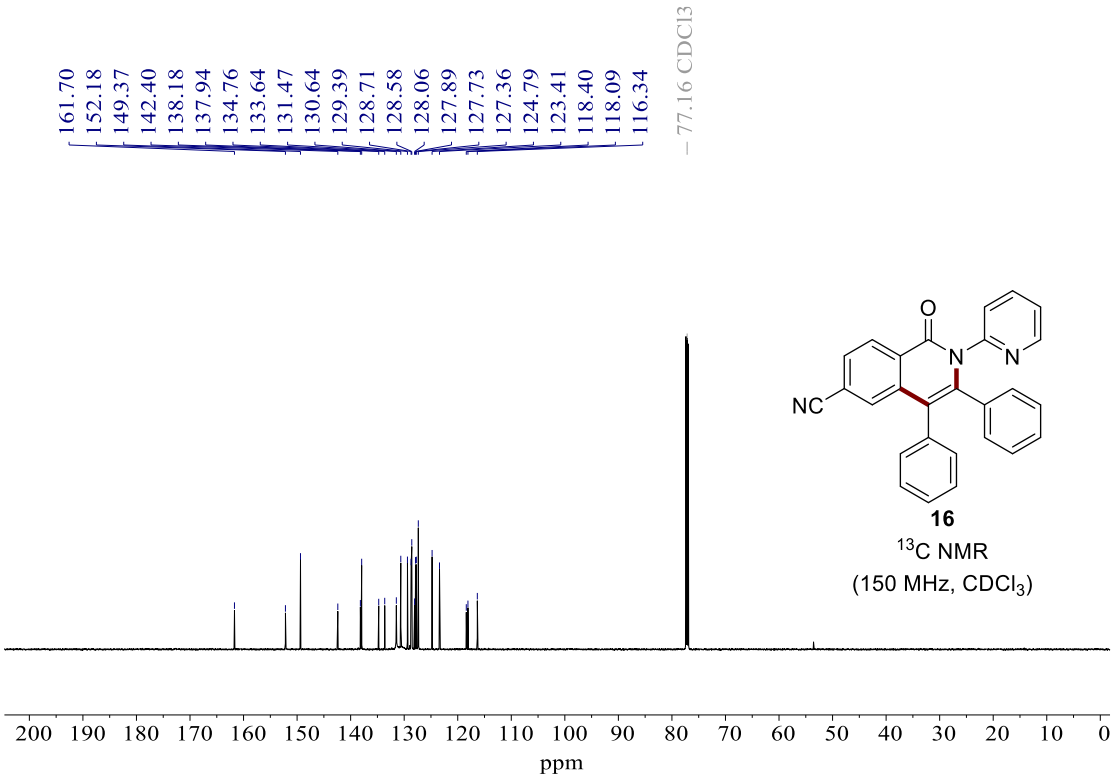
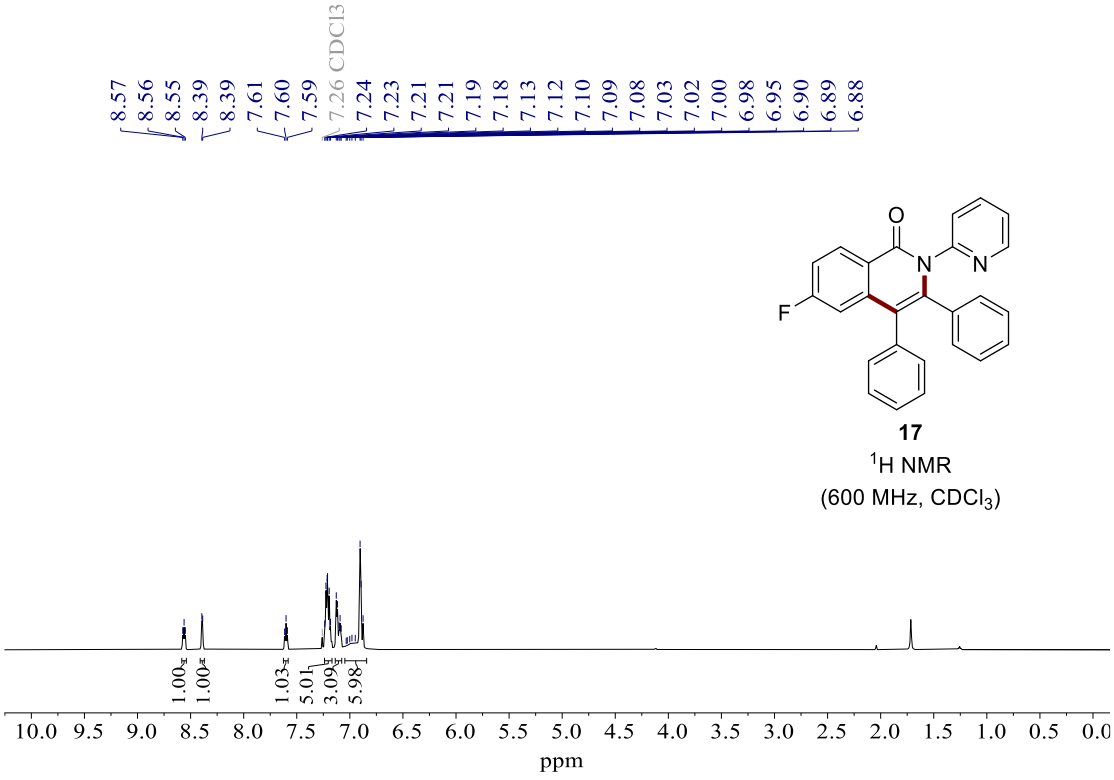
7.75
7.74
7.73
7.67
7.66
7.66
7.65
7.64
7.62
7.62
7.30
7.30
7.29
7.29
7.28
7.27
7.27
7.27
7.26 CDCl3
7.24
7.22
7.17
7.16
7.16
7.15
7.14
7.14
7.14
6.96
6.96
6.95
6.95
O
N
N
NC
16
1H NMR
(600 MHz, CDCl3)
1.00
0.99
1.00
1.04
1.00
2.96
1.00
3.06
4.97
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm



16

^{13}C NMR

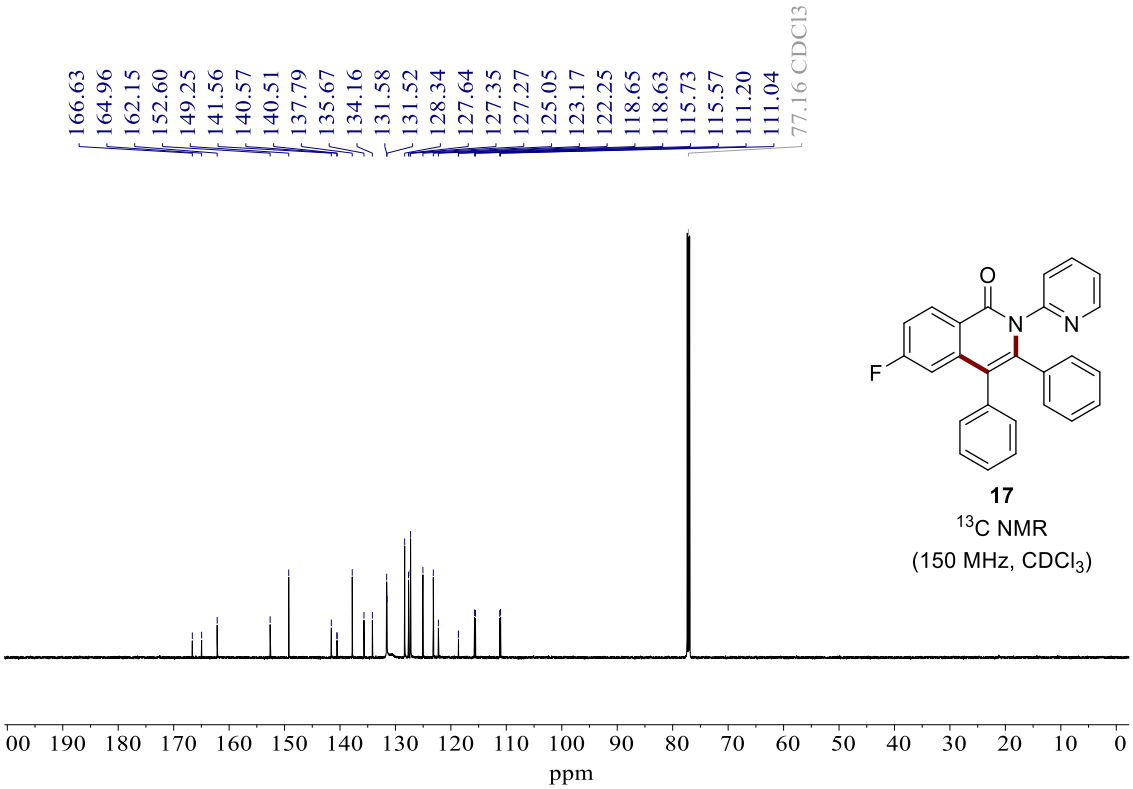
(150 MHz, $CDCl_3$)



17

^{1}H NMR

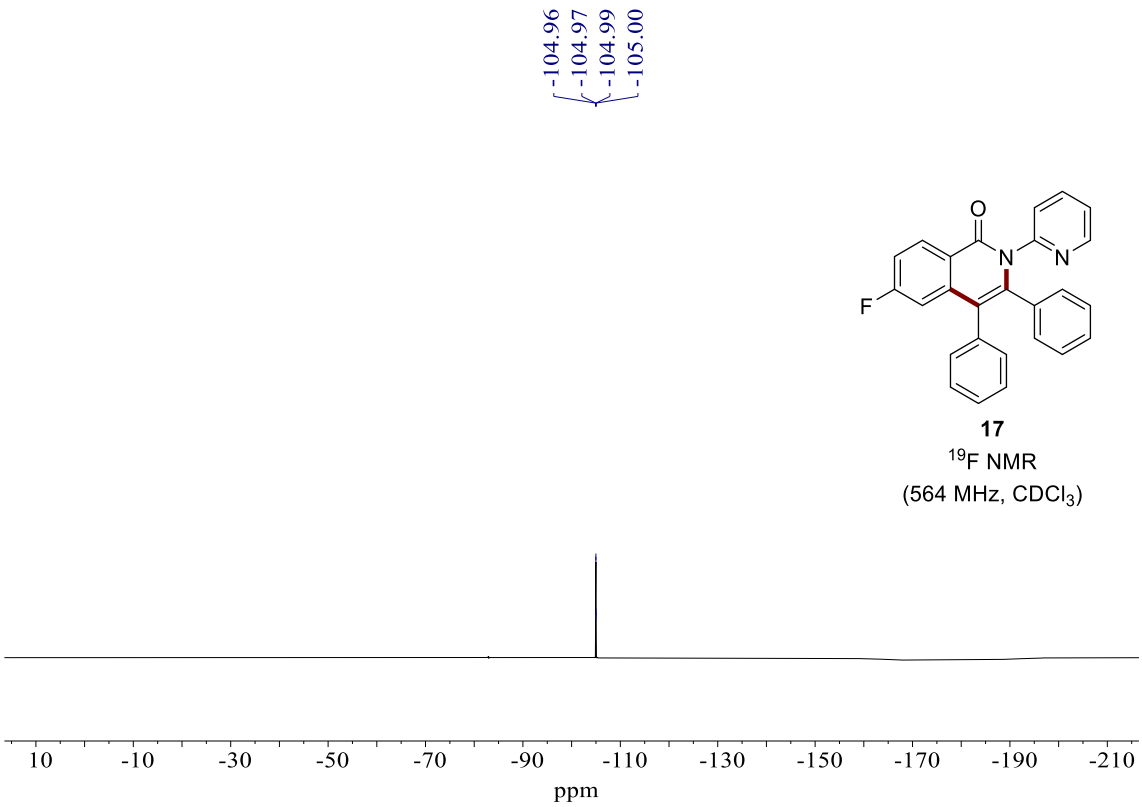
(600 MHz, $CDCl_3$)



17

^{13}C NMR

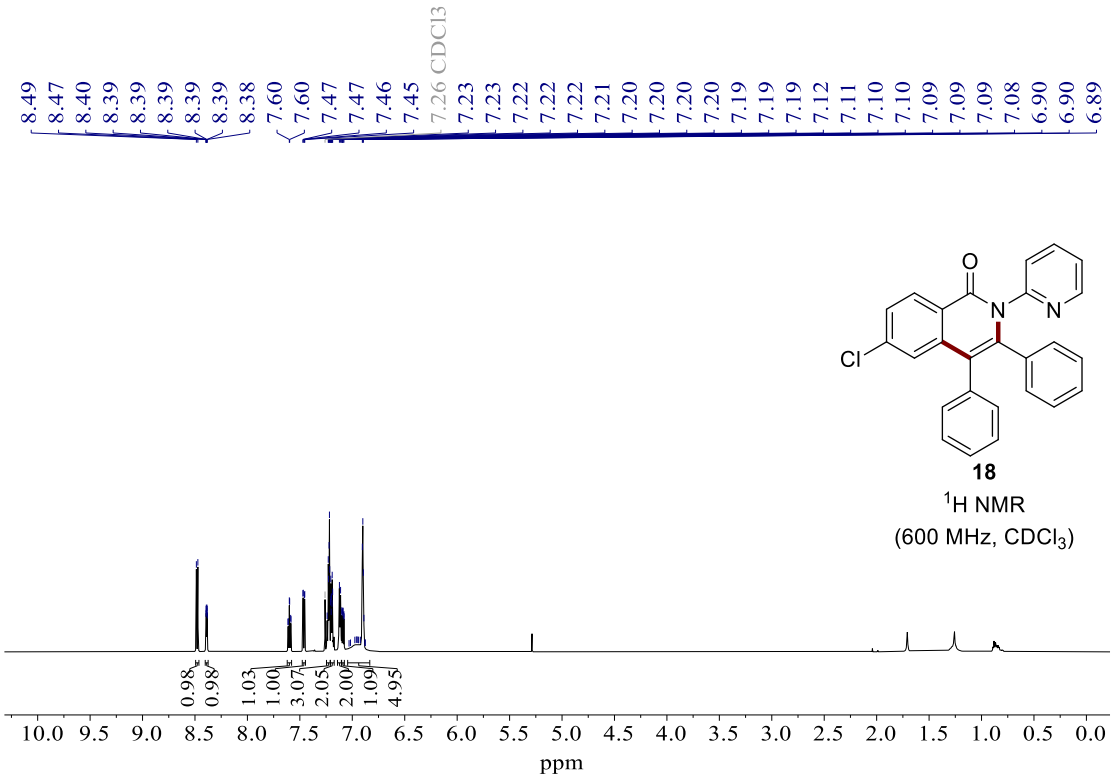
(150 MHz, $CDCl_3$)

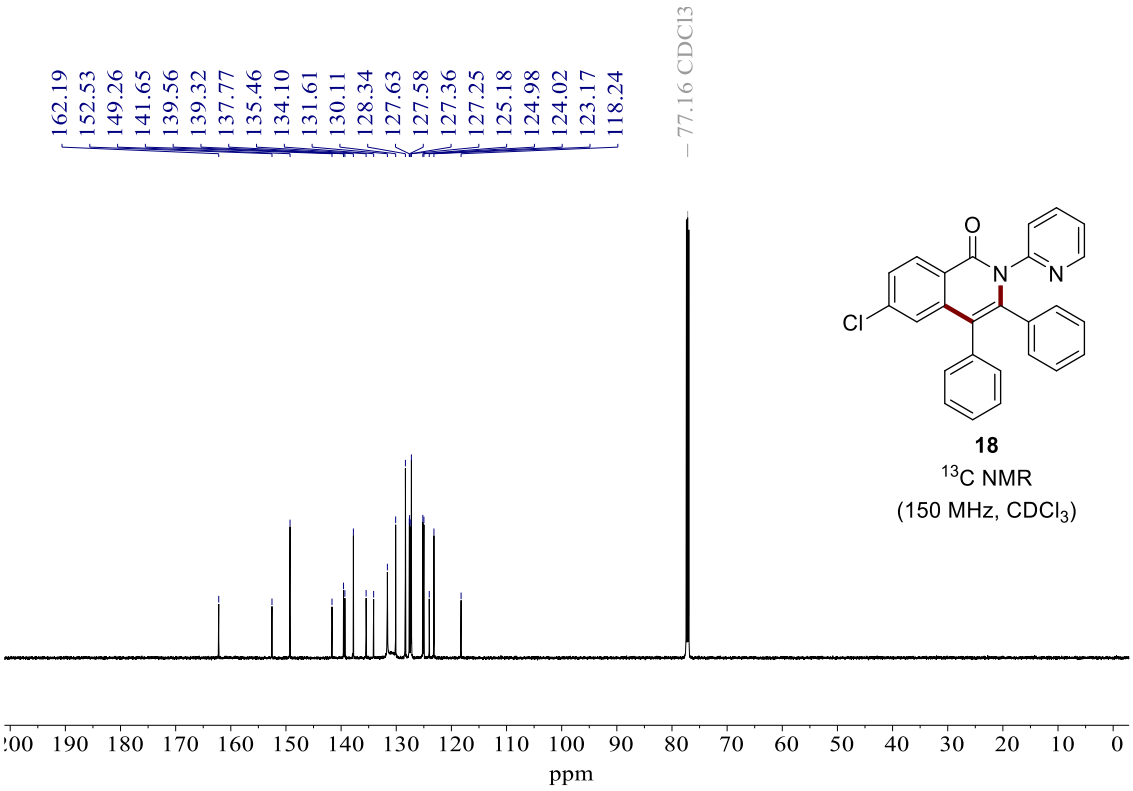


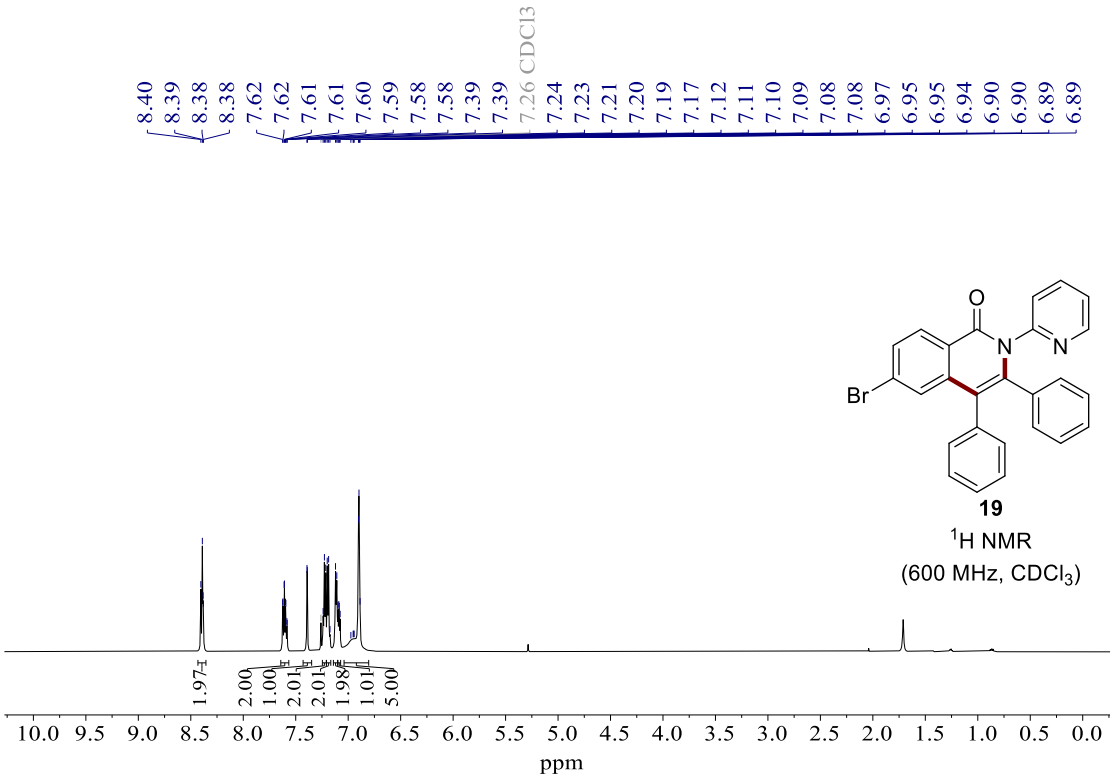
17

^{19}F NMR

(564 MHz, $CDCl_3$)


8.49 8.47 8.40 8.39 8.39 8.39 8.39 8.39 8.38 7.60 7.60 7.47 7.47 7.46 7.45 7.26 CDCl3 7.23 7.23 7.22 7.22 7.22 7.21 7.20 7.20 7.20 7.20 7.19 7.19 7.19 7.12 7.11 7.10 7.10 7.09 7.09 7.09 7.08 6.90 6.90 6.89
O
N
N
Cl
18
1H NMR
(600 MHz, CDCl3)
0.98 0.98 1.03 1.00 3.07 2.05 2.00 1.09 4.95
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
ppm


162.19 152.53 149.26 141.65 139.56 139.32 137.77 135.46 134.10 131.61 130.11 128.34 127.63 127.58 127.36 127.25 125.18 124.98 124.02 123.17 118.24
77.16 CDCl3
O
N
N
Cl
18
13C NMR
(150 MHz, CDCl3)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm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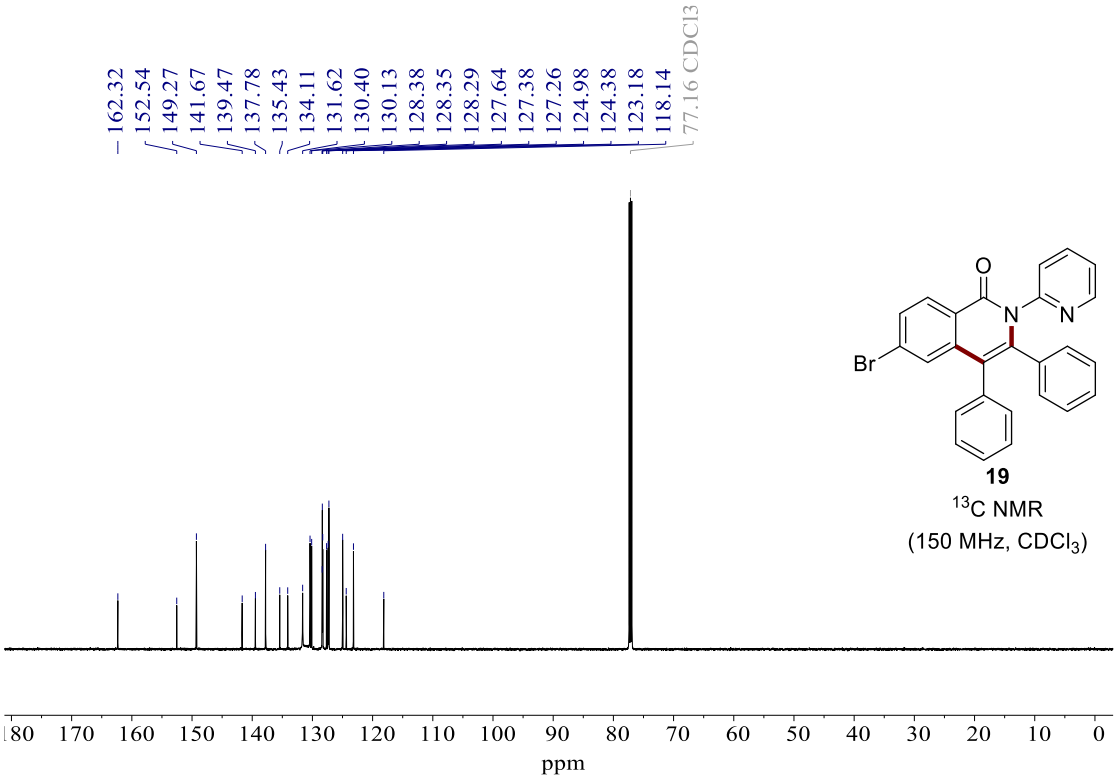
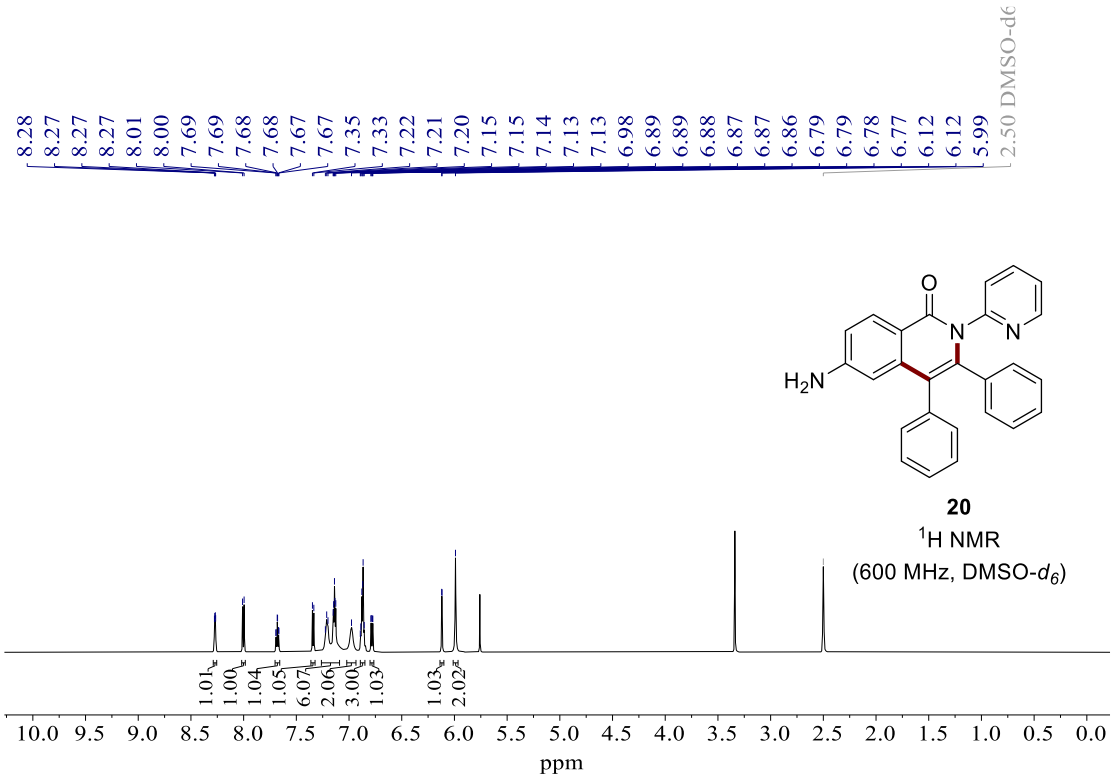
8.39
8.38
8.38
7.62
7.62
7.61
7.61
7.60
7.59
7.58
7.58
7.39
7.39
7.26 CDCl3
7.24
7.23
7.21
7.20
7.19
7.17
7.12
7.11
7.10
7.09
7.08
7.08
6.97
6.95
6.95
6.94
6.90
6.90
6.89
6.89
O
N
N
Br
19
1H NMR
(600 MHz, CDCl3)
1.97
2.00
1.00
2.01
2.01
1.98
1.01
5.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm


162.32
152.54
149.27
141.67
139.47
137.78
135.43
134.11
131.62
130.40
130.13
128.38
128.35
128.29
127.64
127.38
127.26
124.98
124.38
123.18
118.14
77.16 CDCl3
O
N
N
Br
19
13C NMR
(150 MHz, CDCl3)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm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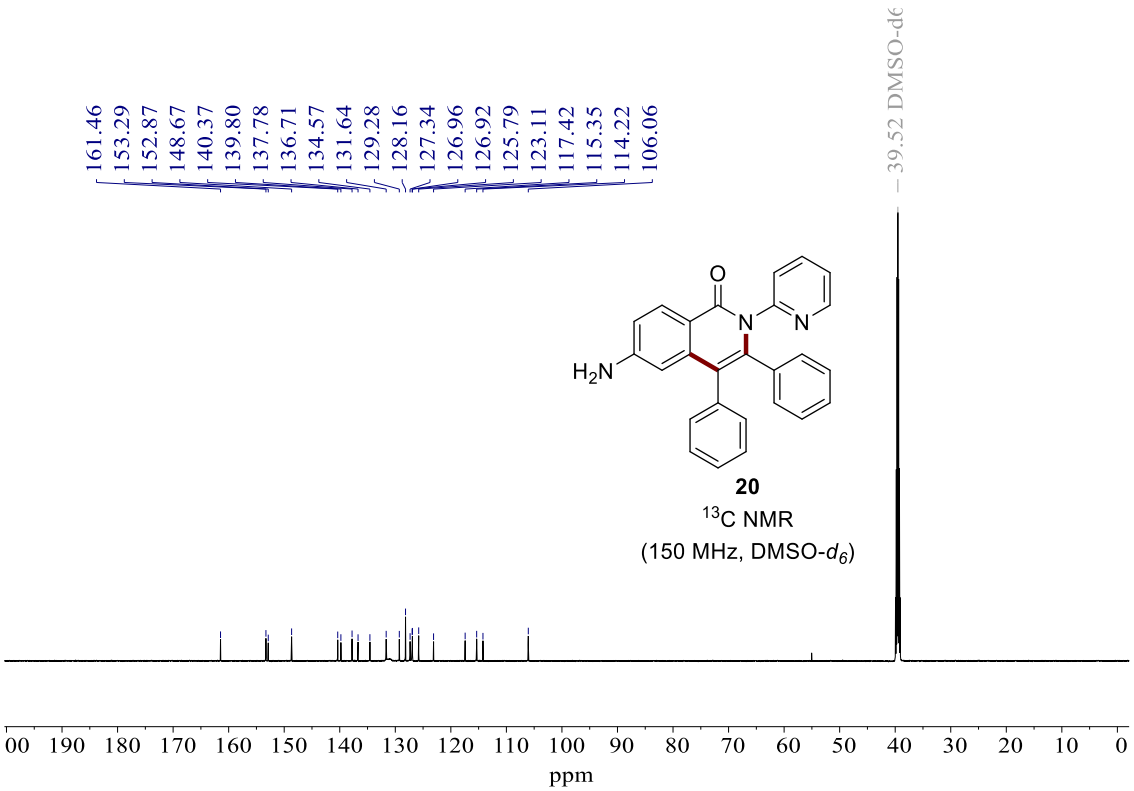
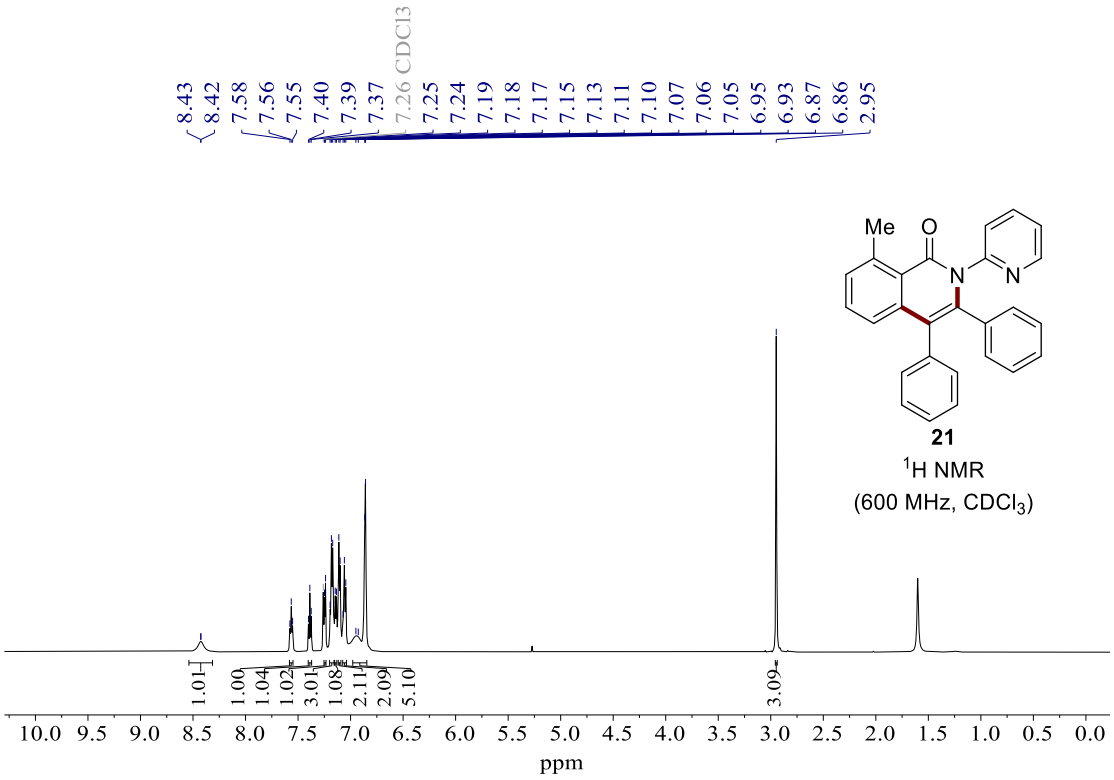
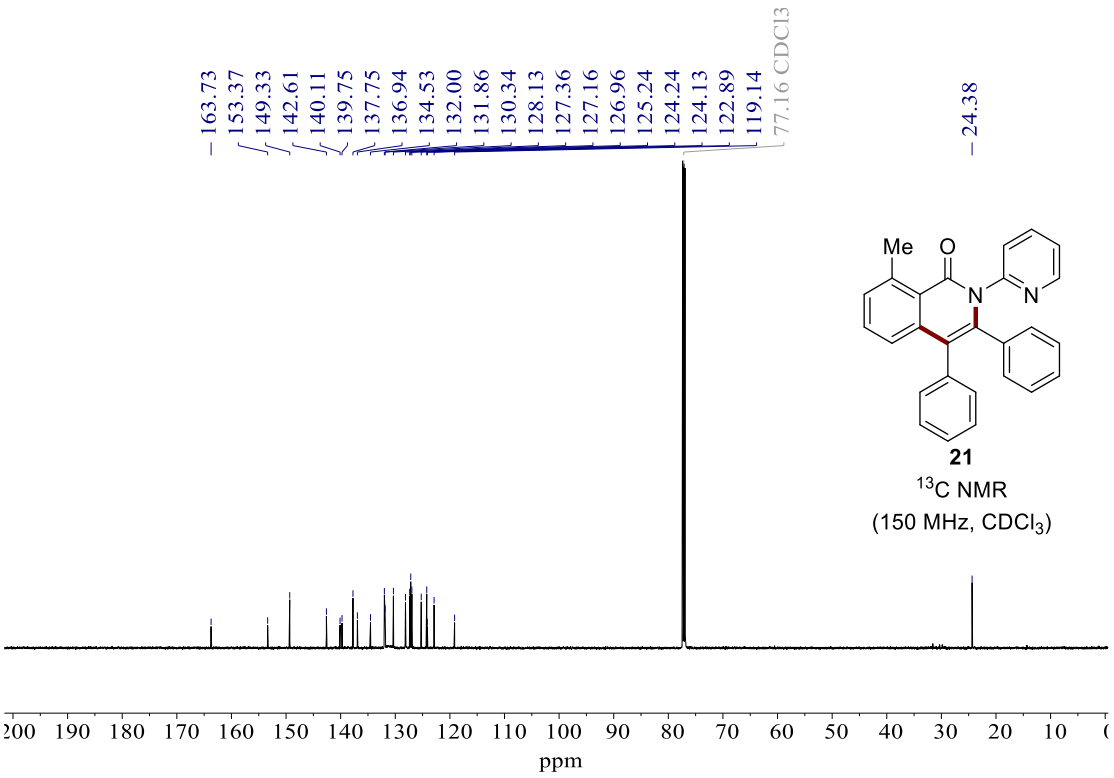
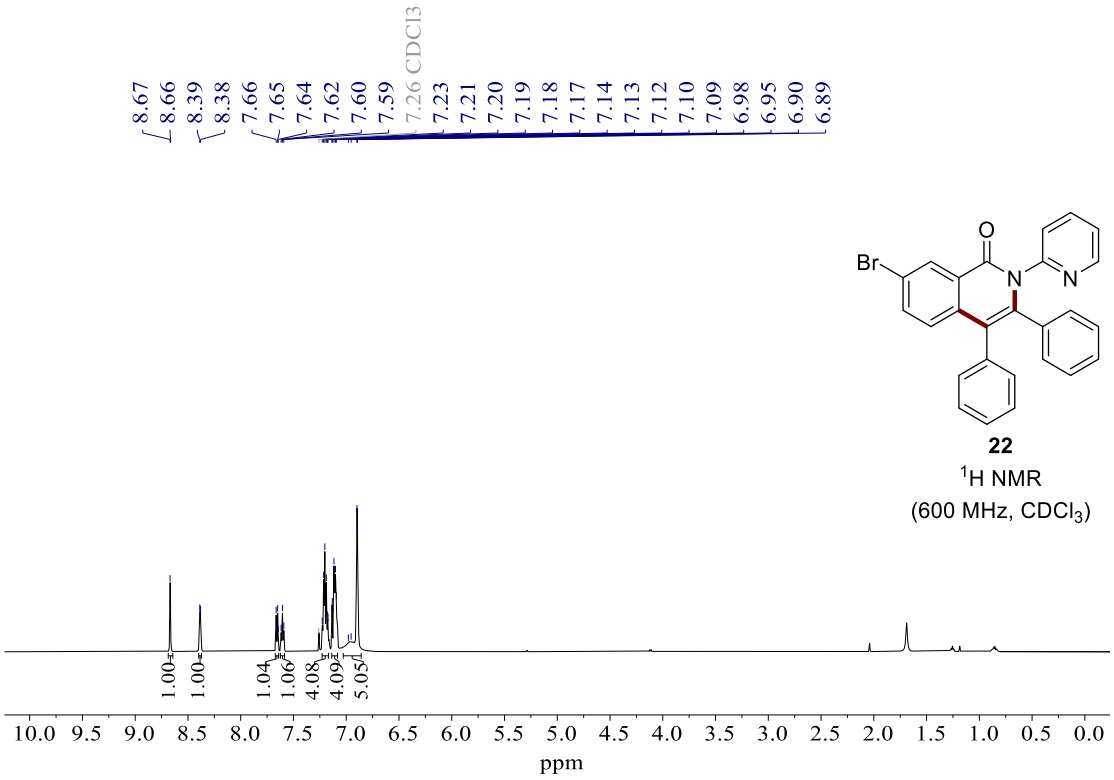
8.27
8.27
8.27
8.01
8.00
7.69
7.69
7.68
7.68
7.67
7.67
7.35
7.33
7.22
7.21
7.20
7.15
7.15
7.14
7.13
7.13
6.98
6.89
6.89
6.88
6.87
6.87
6.86
6.79
6.79
6.78
6.77
6.12
6.12
5.99
2.50 DMSO-d6
O
N
N
H2N
20
1H NMR
(600 MHz, DMSO-d6)
1.01
1.00
1.04
1.05
6.07
2.06
3.00
1.03
1.03
2.02
10.0 9.5 9.0 8.5 8.0 7.5 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
ppm


161.46
153.29
152.87
148.67
140.37
139.80
137.78
136.71
134.57
131.64
129.28
128.16
127.34
126.96
126.92
125.79
123.11
117.42
115.35
114.22
106.06
39.52 DMSO-d6
O
N
N
H2N
20
13C NMR
(150 MHz, DMSO-d6)
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm


8.43
8.42
7.58
7.56
7.55
7.40
7.39
7.37
7.26 CDCl3
7.25
7.24
7.19
7.18
7.17
7.15
7.13
7.11
7.10
7.07
7.06
7.05
6.95
6.93
6.87
6.86
2.95
Me
O
N
N
21
1H NMR
(600 MHz, CDCl3)
1.01
1.00
1.04
1.02
3.01
1.08
2.11
2.09
5.10
3.09
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
ppm

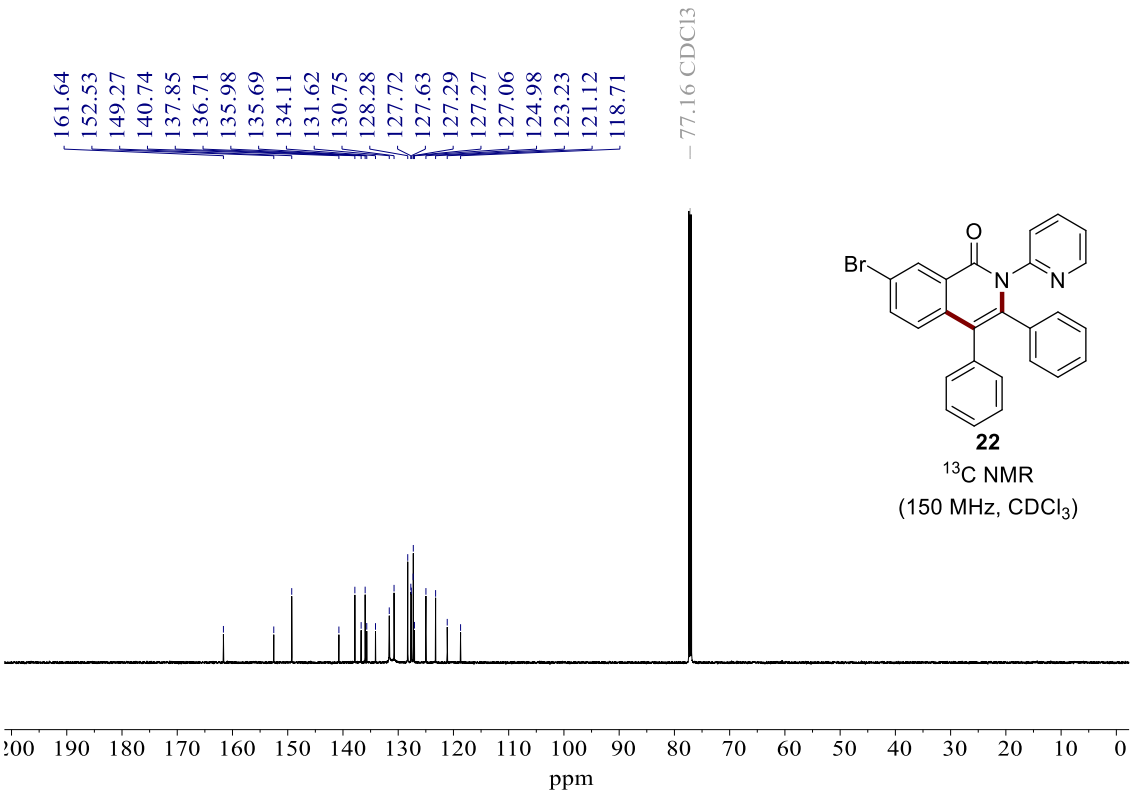

163.73
153.37
149.33
142.61
140.11
139.75
137.75
136.94
134.53
132.00
131.86
130.34
128.13
127.36
127.16
126.96
125.24
124.24
124.13
122.89
119.14
77.16 CDCl3
24.38
Me
O
N
N
21
13C NMR
(150 MHz, CDCl3)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm



22

^{1}H NMR

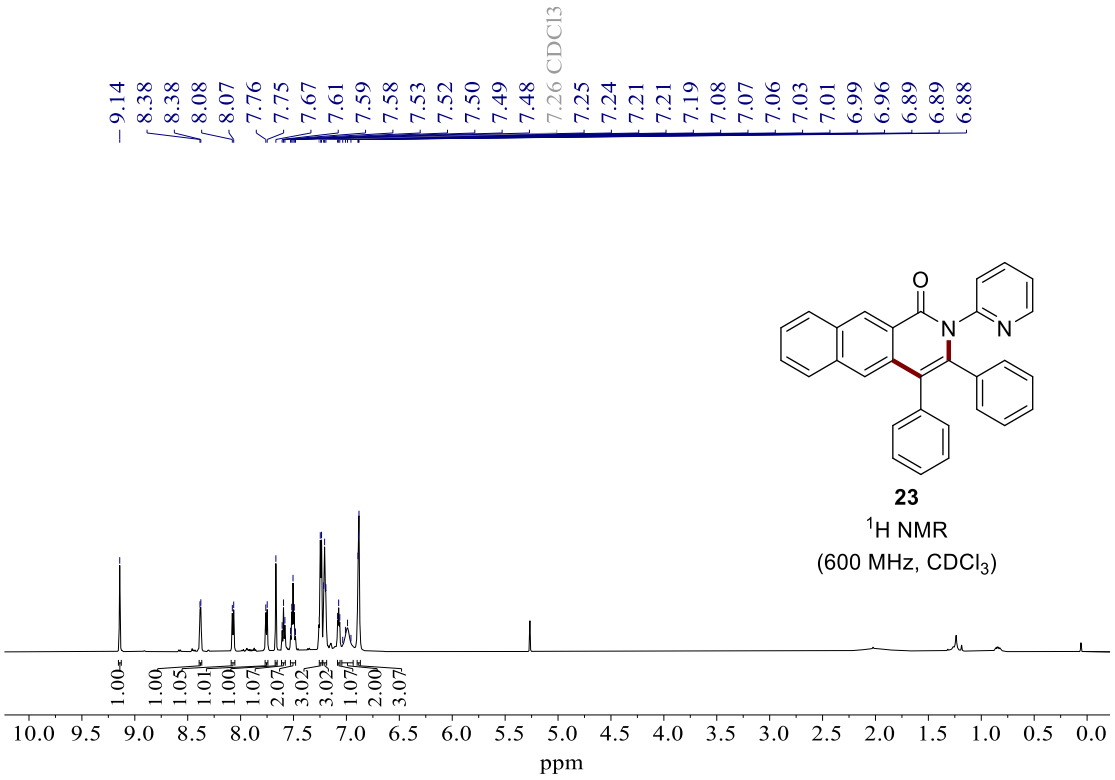
(600 MHz, $CDCl_3$)

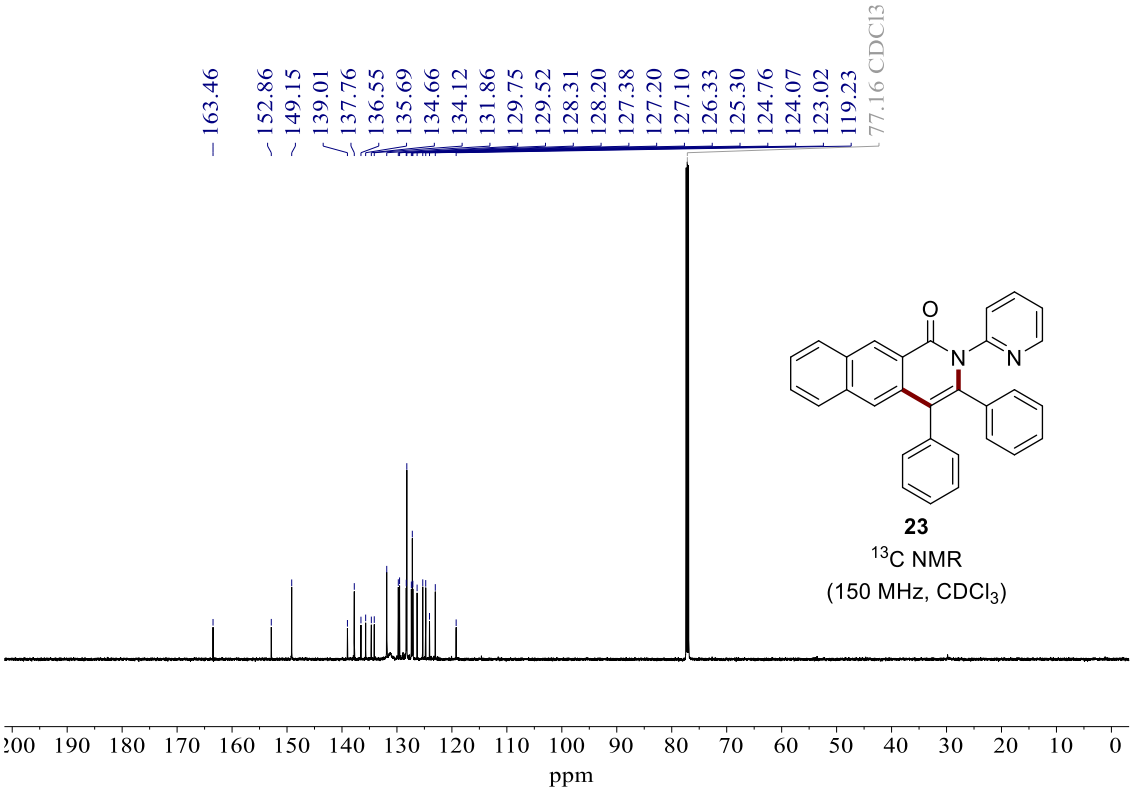


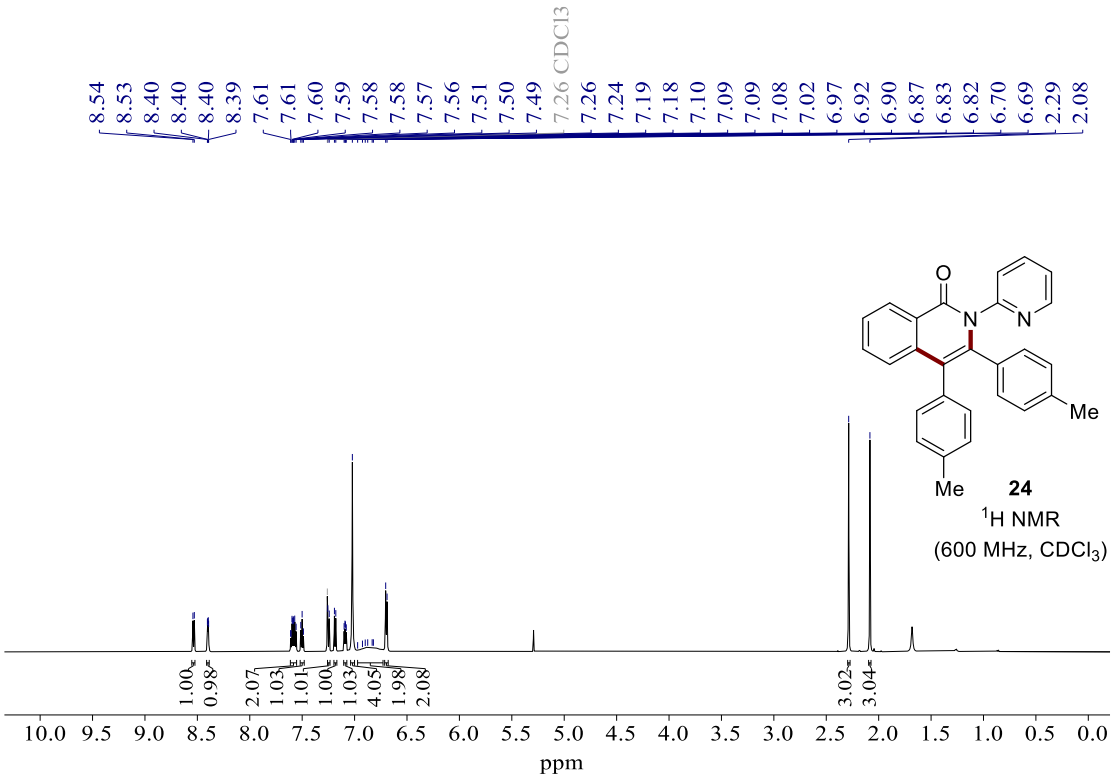
22

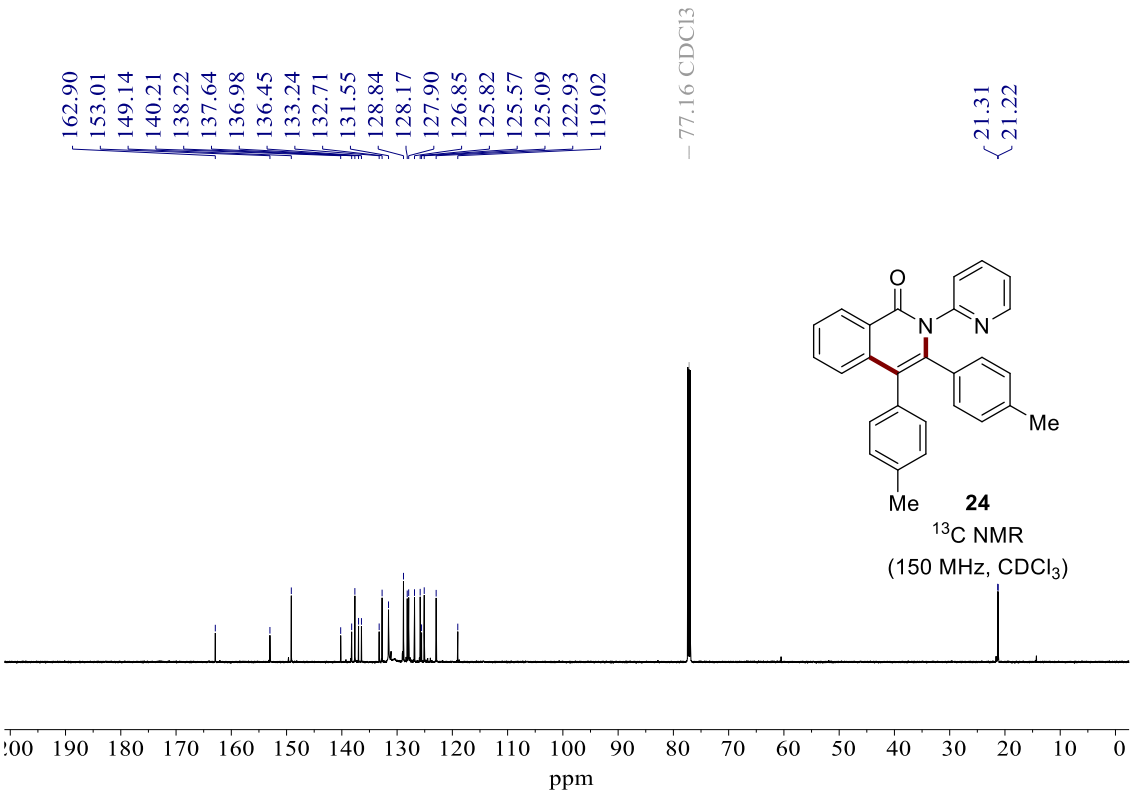
^{13}C NMR

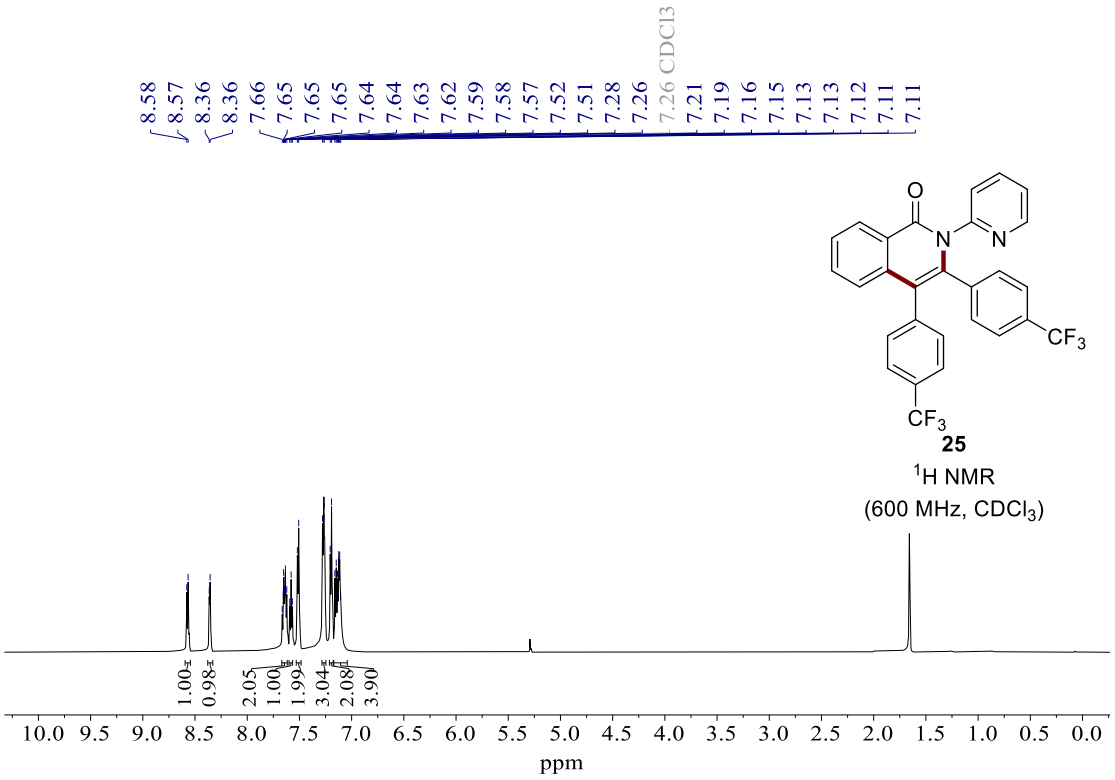
(150 MHz, $CDCl_3$)


9.14
8.38
8.38
8.08
8.07
7.76
7.75
7.67
7.61
7.59
7.58
7.53
7.52
7.50
7.49
7.48
7.26 CDCl3
7.25
7.24
7.21
7.21
7.19
7.08
7.07
7.06
7.03
7.01
6.99
6.96
6.89
6.89
6.88
O
N
N
23
1H NMR
(600 MHz, CDCl3)
1.00
1.00
1.05
1.01
1.00
1.07
2.07
3.02
3.02
1.07
2.00
3.07
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
ppm


163.46
152.86
149.15
139.01
137.76
136.55
135.69
134.66
134.12
131.86
129.75
129.52
128.31
128.20
127.38
127.20
127.10
126.33
125.30
124.76
124.07
123.02
119.23
77.16 CDCl3
O
N
N
23
13C NMR
(150 MHz, CDCl3)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm


8.54
8.53
8.40
8.40
8.40
8.39
7.61
7.61
7.60
7.59
7.58
7.58
7.57
7.56
7.51
7.50
7.49
7.26 CDCl3
7.26
7.24
7.19
7.18
7.10
7.09
7.09
7.08
7.02
6.97
6.92
6.90
6.87
6.83
6.82
6.70
6.69
2.29
2.08
O
N
N
Me
Me
24
1H NMR
(600 MHz, CDCl3)
1.00
0.98
2.07
1.03
1.01
1.00
1.03
4.05
1.98
2.08
3.02
3.04
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
ppm


162.90
153.01
149.14
140.21
138.22
137.64
136.98
136.45
133.24
132.71
131.55
128.84
128.17
127.90
126.85
125.82
125.57
125.09
122.93
119.02
77.16 CDCl3
21.31
21.22
O
N
N
Me
Me
24
13C NMR
(150 MHz, CDCl3)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm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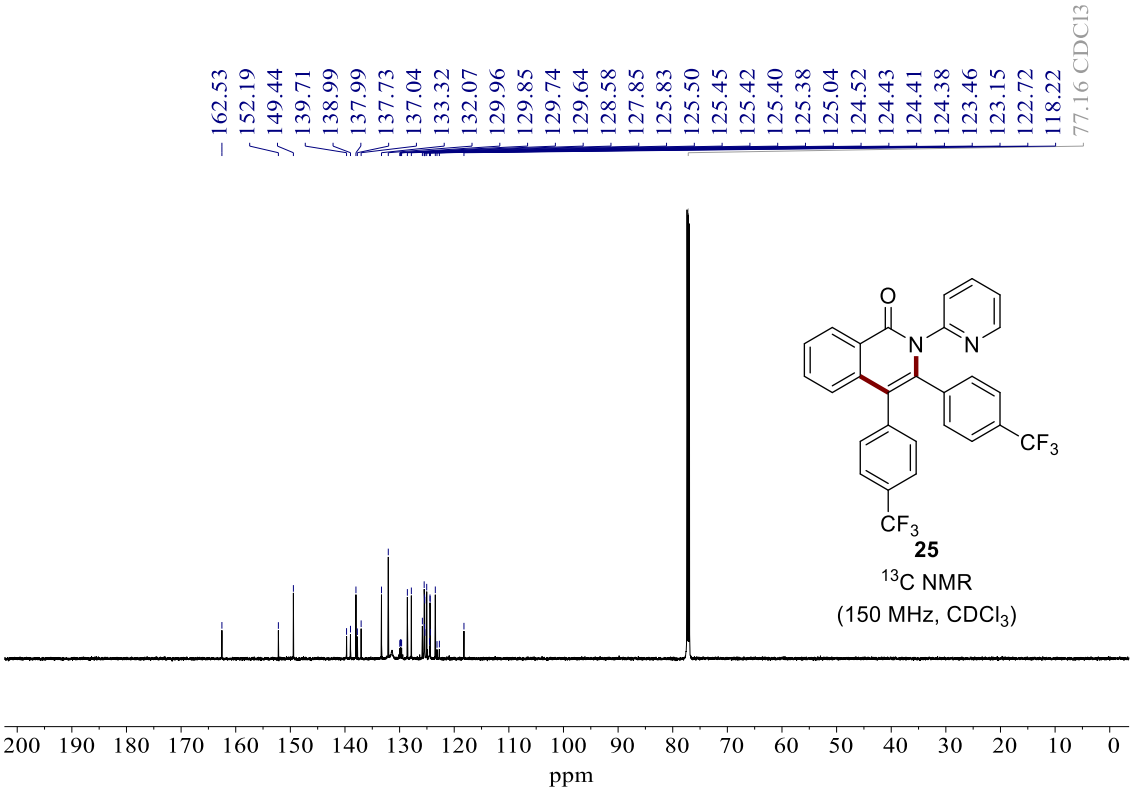
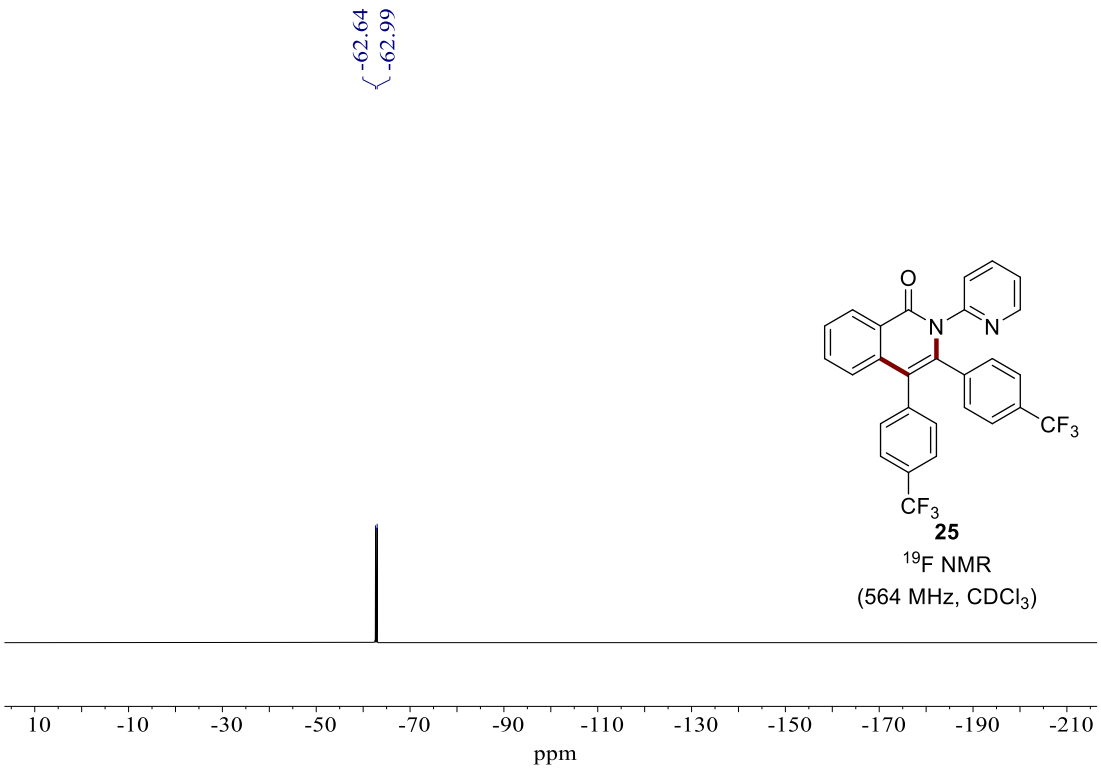
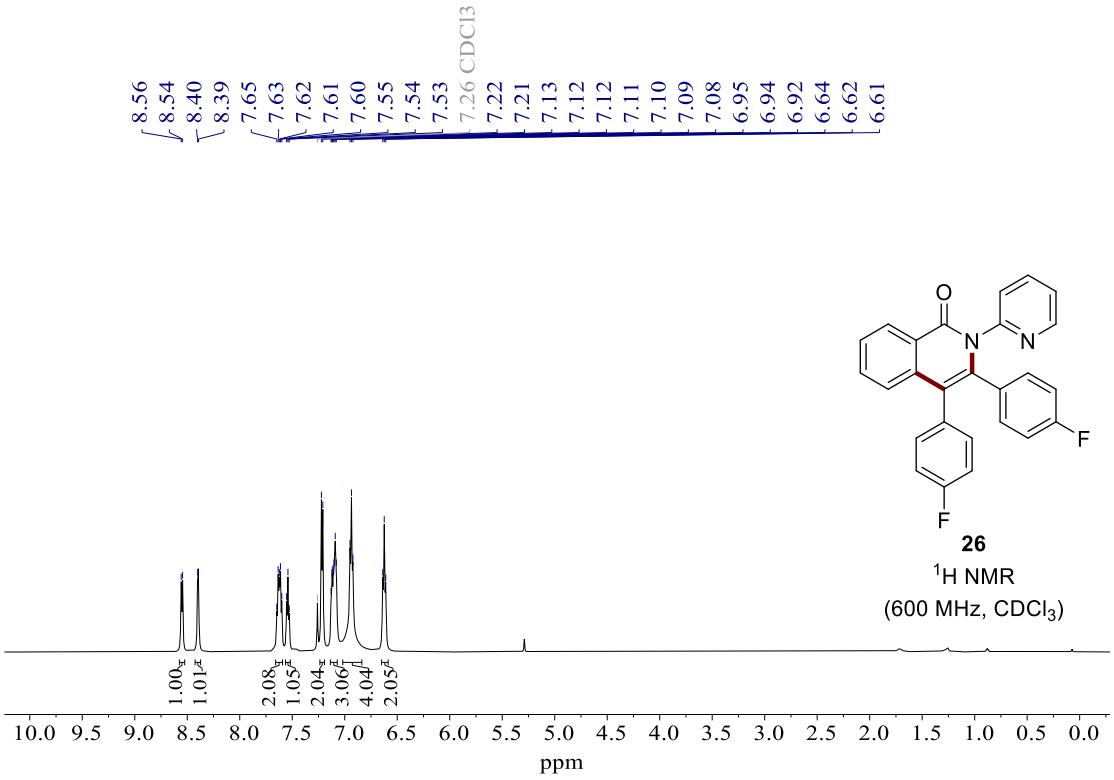
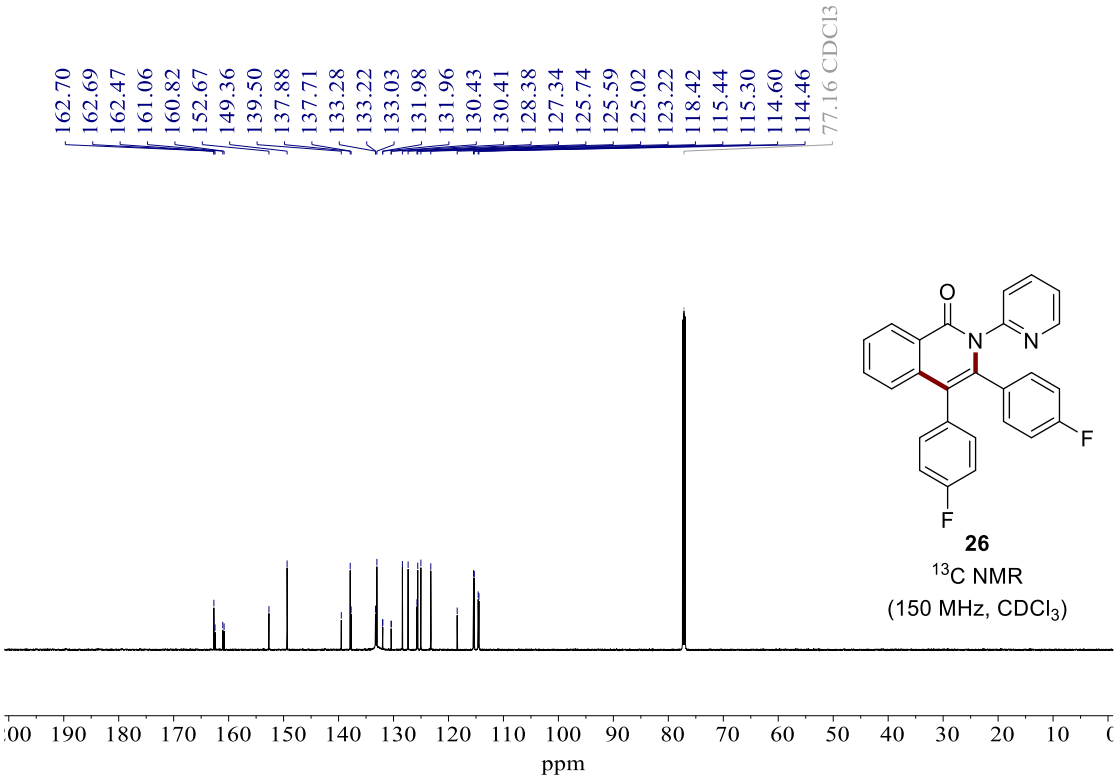
8.57
8.36
8.36
7.66
7.65
7.65
7.65
7.64
7.64
7.63
7.62
7.59
7.58
7.57
7.52
7.51
7.28
7.26
7.26 CDCl3
7.21
7.19
7.16
7.15
7.13
7.13
7.12
7.11
7.11
O
N
N
CF3
CF3
25
1H NMR
(600 MHz, CDCl3)
1.00
0.98
2.05
1.00
1.99
3.04
2.08
3.90
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm


162.53
152.19
149.44
139.71
138.99
137.99
137.73
137.04
133.32
132.07
129.96
129.85
129.74
129.64
128.58
127.85
125.83
125.50
125.45
125.42
125.40
125.38
125.04
124.52
124.43
124.41
124.38
123.46
123.15
122.72
118.22
77.16 CDCl3
O
N
N
CF3
CF3
25
13C NMR
(150 MHz, CDCl3)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm


-62.64
-62.99
O
N
N
CF3
CF3
25
19F NMR
(564 MHz, CDCl3)
10
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
ppm

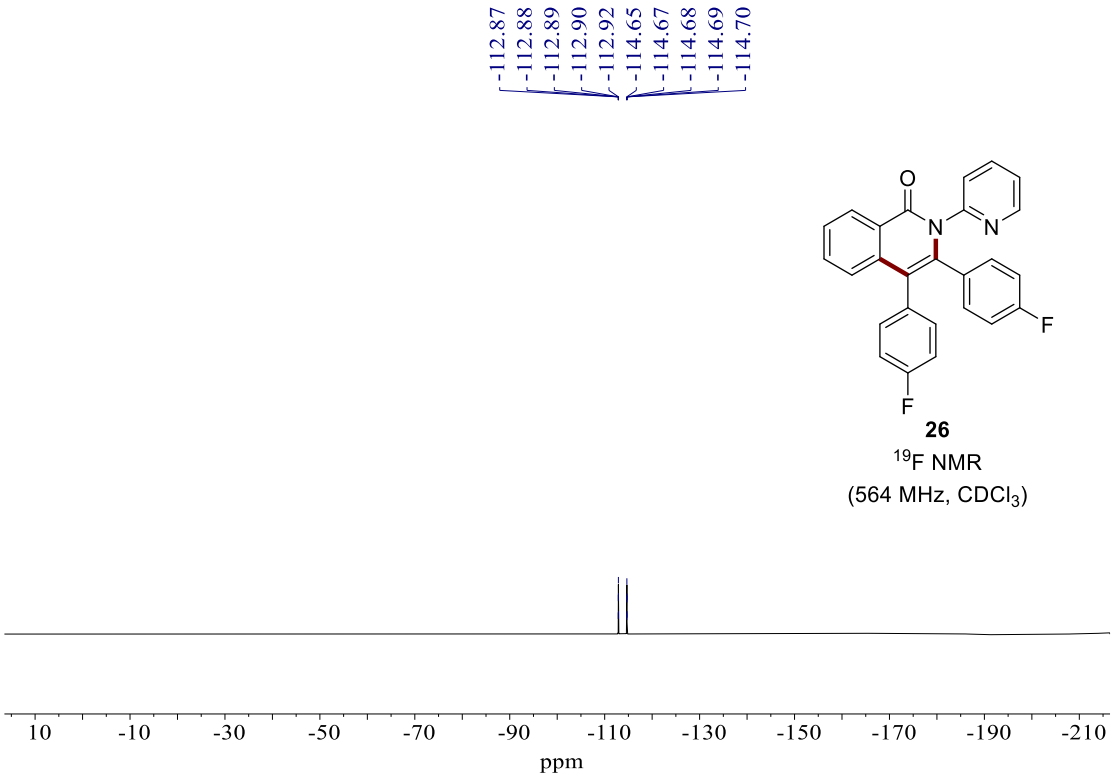

8.56
8.54
8.40
8.39
7.65
7.63
7.62
7.61
7.60
7.55
7.54
7.53
7.26 CDCl3
7.22
7.21
7.13
7.12
7.12
7.11
7.10
7.09
7.08
6.95
6.94
6.92
6.64
6.62
6.61
O
N
N
F
F
26
1H NMR
(600 MHz, CDCl3)
1.00
1.01
2.08
1.05
2.04
3.06
4.04
2.05
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm



26

^{13}C NMR

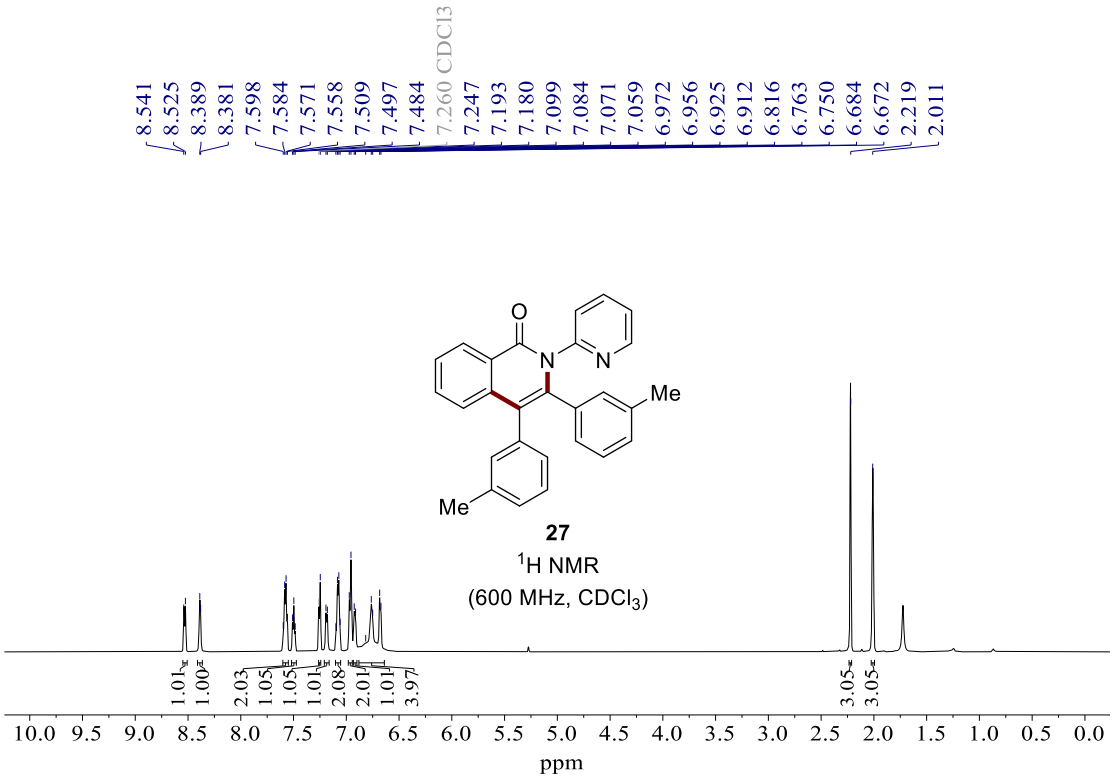
(150 MHz, $CDCl_3$)

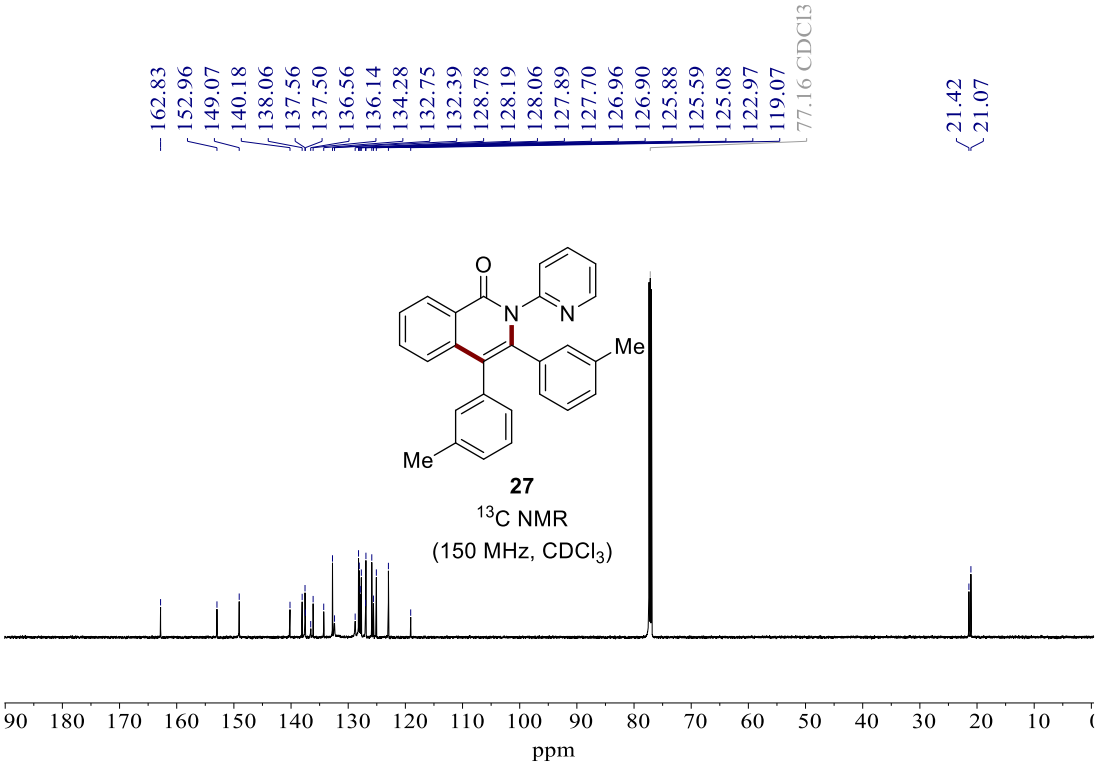


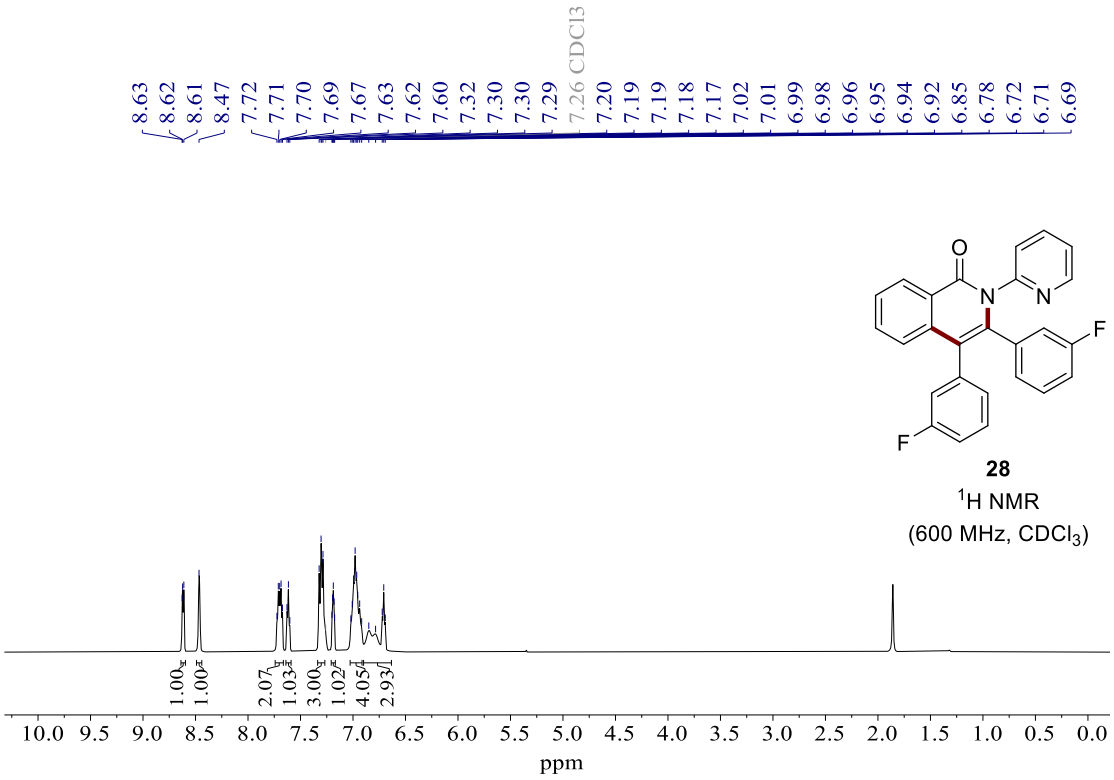
26

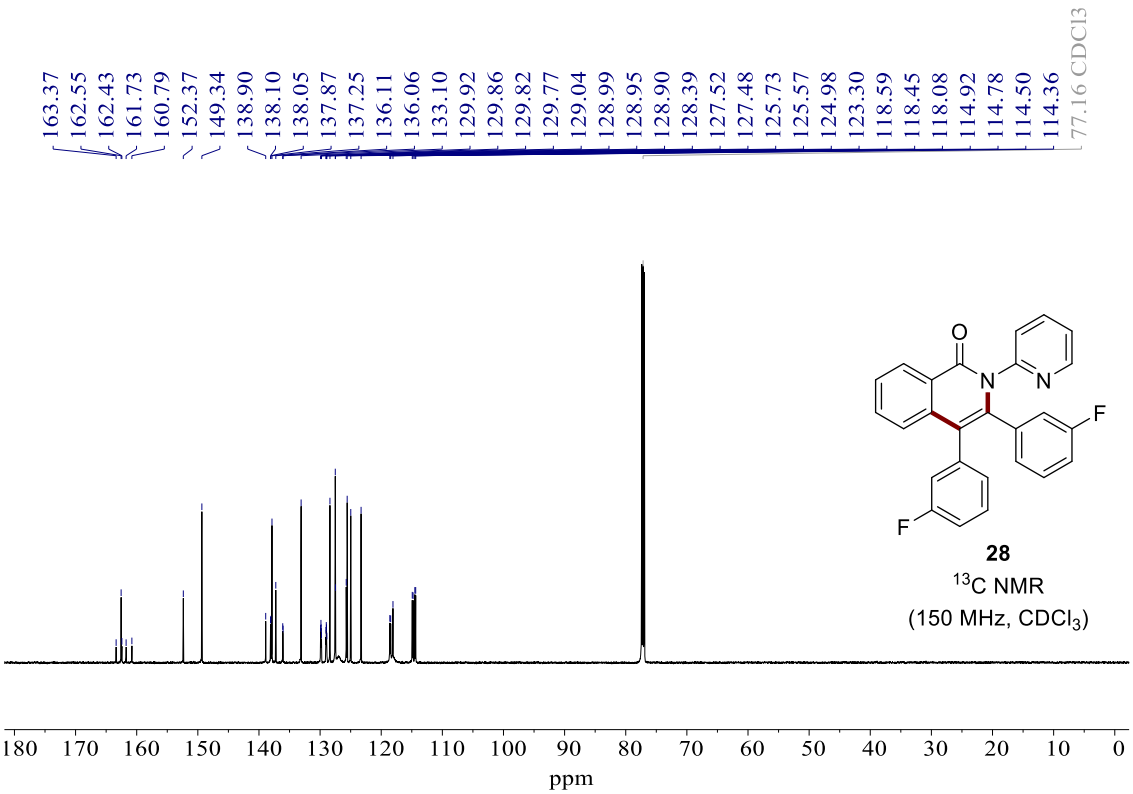
^{19}F NMR

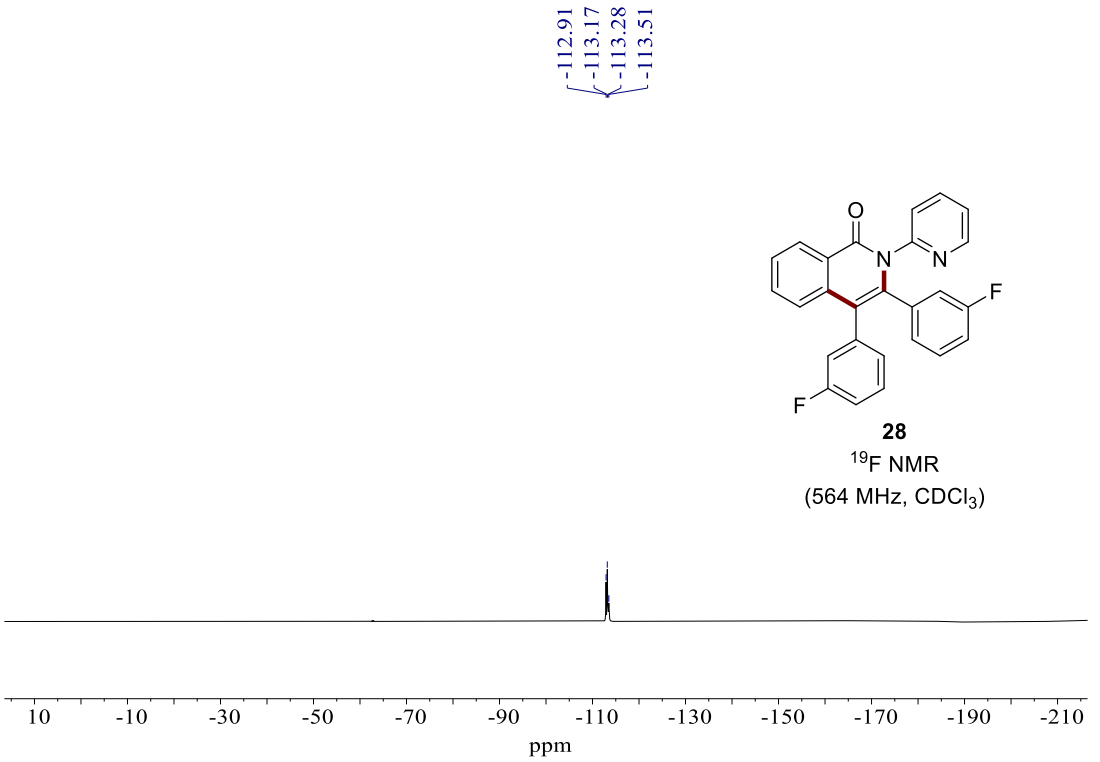
(564 MHz, $CDCl_3$)

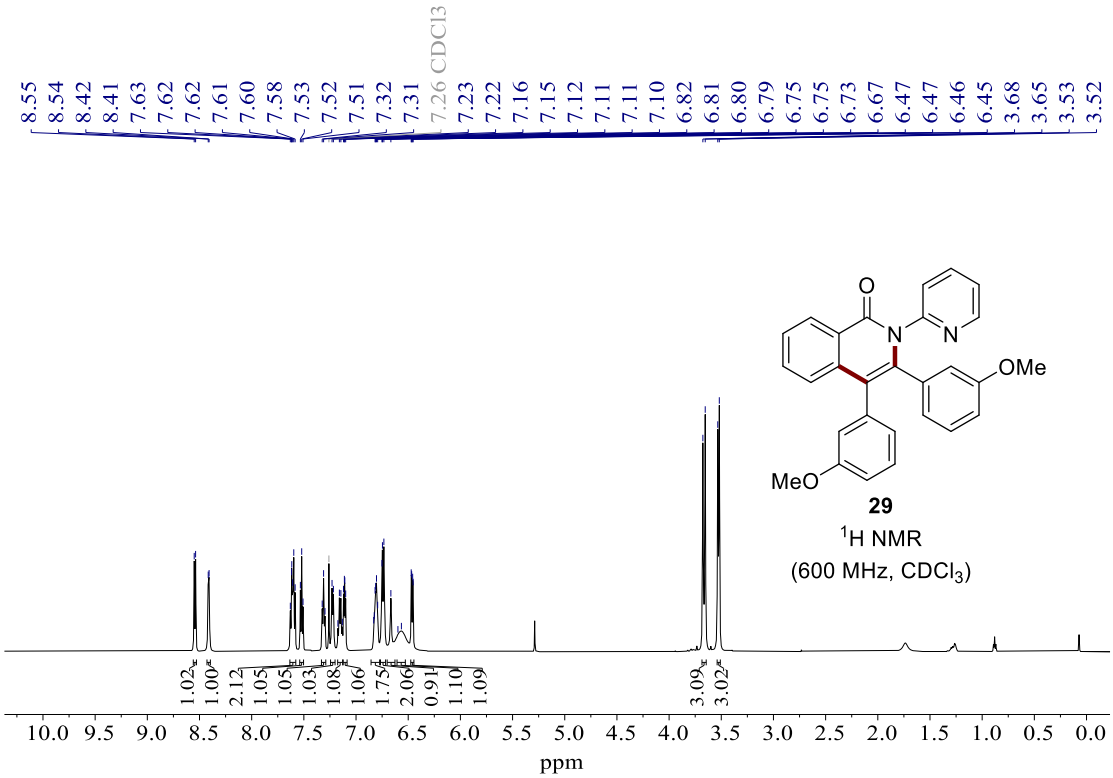

8.541
8.525
8.389
8.381
7.598
7.584
7.571
7.558
7.509
7.497
7.484
7.260 CDCl3
7.247
7.193
7.180
7.099
7.084
7.071
7.059
6.972
6.956
6.925
6.912
6.816
6.763
6.750
6.684
6.672
2.219
2.011
O
N
N
Me
Me
27
1H NMR
(600 MHz, CDCl3)
1.01
1.00
2.03
1.05
1.05
1.01
2.08
2.01
1.01
3.97
3.05
3.05
10.0 9.5 9.0 8.5 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
ppm

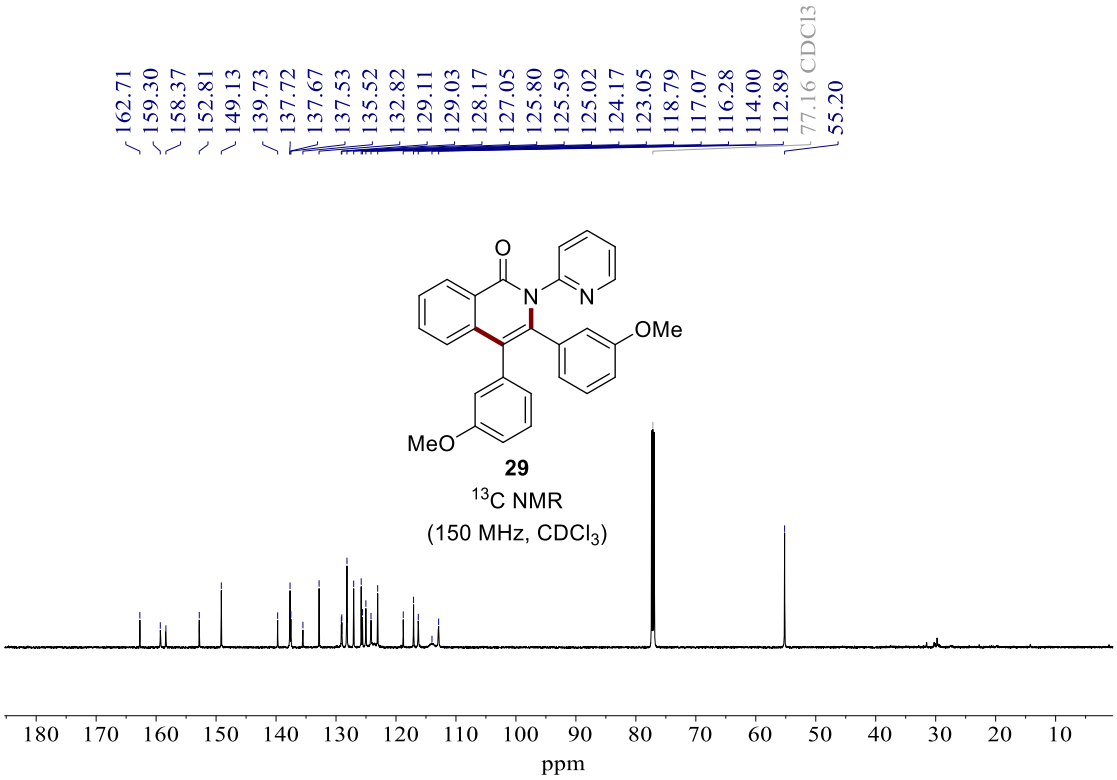

162.83
152.96
149.07
140.18
138.06
137.56
137.50
136.56
136.14
134.28
132.75
132.39
128.78
128.19
128.06
127.89
127.70
126.96
126.90
125.88
125.59
125.08
122.97
119.07
77.16 CDCl3
21.42
21.07
O
N
N
Me
Me
27
13C NMR
(150 MHz, CDCl3)
90 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm


8.63
8.62
8.61
8.47
7.72
7.71
7.70
7.69
7.67
7.63
7.62
7.60
7.32
7.30
7.30
7.29
7.26 CDCl3
7.20
7.19
7.19
7.18
7.17
7.02
7.01
6.99
6.98
6.96
6.95
6.94
6.92
6.85
6.78
6.72
6.71
6.69
O
N
N
F
F
28
1H NMR
(600 MHz, CDCl3)
1.00
1.00
2.07
1.03
3.00
1.02
4.05
2.93
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
ppm


163.37
162.55
162.43
161.73
160.79
152.37
149.34
138.90
138.10
138.05
137.87
137.25
136.11
136.06
133.10
129.92
129.86
129.82
129.77
129.04
128.99
128.95
128.90
128.39
127.52
127.48
125.73
125.57
124.98
123.30
118.59
118.45
118.08
114.92
114.78
114.50
114.36
77.16 CDCl3
O
N
N
F
F
28
13C NMR
(150 MHz, CDCl3)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm


-112.91
-113.17
-113.28
-113.51
O
N
N
F
F
28
19F NMR
(564 MHz, CDCl3)
10
-10
-30
-50
-70
-90
-110
-130
-150
-170
-190
-210
ppm


8.55
8.54
8.42
8.41
7.63
7.62
7.62
7.61
7.60
7.58
7.53
7.52
7.51
7.32
7.31
7.26 CDCl3
7.23
7.22
7.16
7.15
7.12
7.11
7.11
7.10
6.82
6.81
6.80
6.79
6.75
6.75
6.73
6.67
6.47
6.47
6.46
6.45
3.68
3.65
3.53
3.52
O
N
N
OMe
MeO
29
1H NMR
(600 MHz, CDCl3)
1.02
1.00
2.12
1.05
1.05
1.03
1.08
1.06
1.75
2.06
0.91
1.10
1.09
3.09
3.02
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
ppm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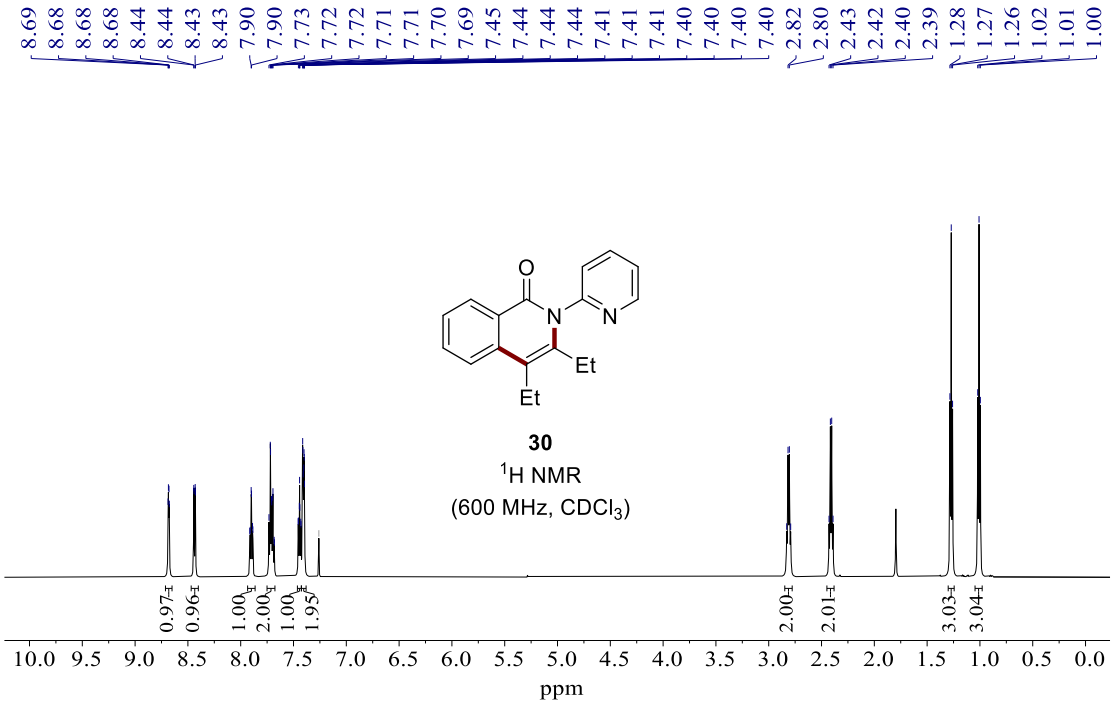
159.30
158.37
152.81
149.13
139.73
137.72
137.67
137.53
135.52
132.82
129.11
129.03
128.17
127.05
125.80
125.59
125.02
124.17
123.05
118.79
117.07
116.28
114.00
112.89
77.16 CDCl3
55.20
O
N
N
OMe
MeO
29
13C NMR
(150 MHz, CDCl3)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm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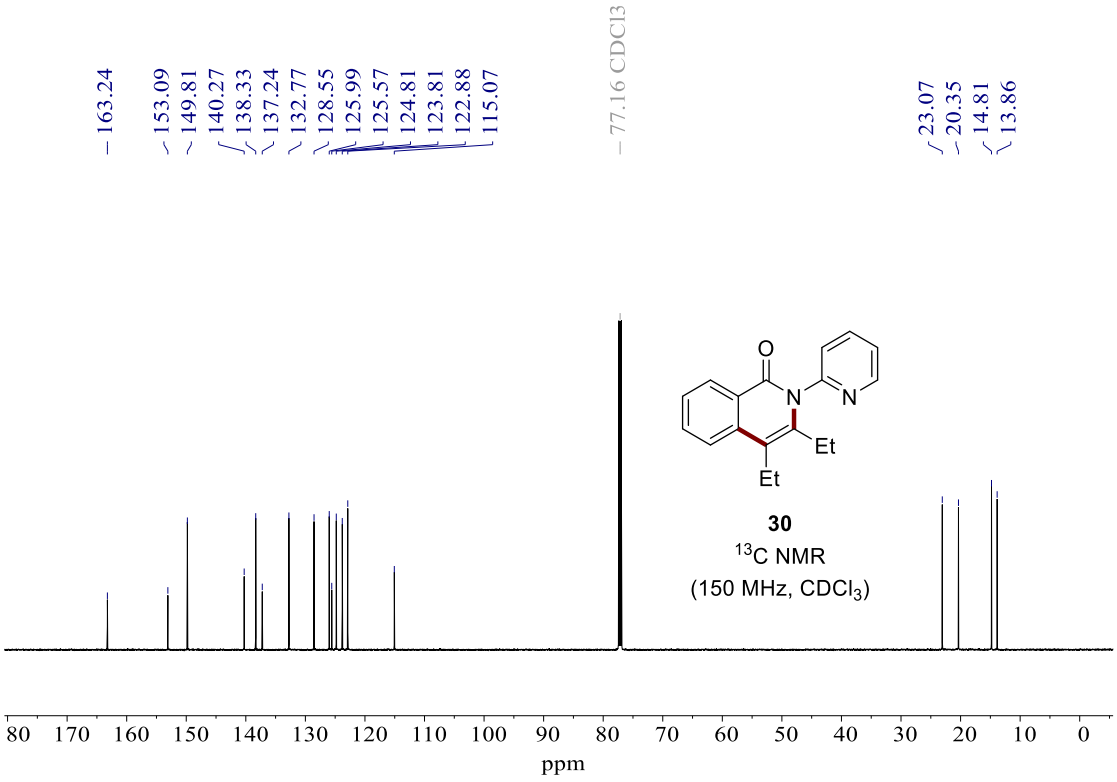
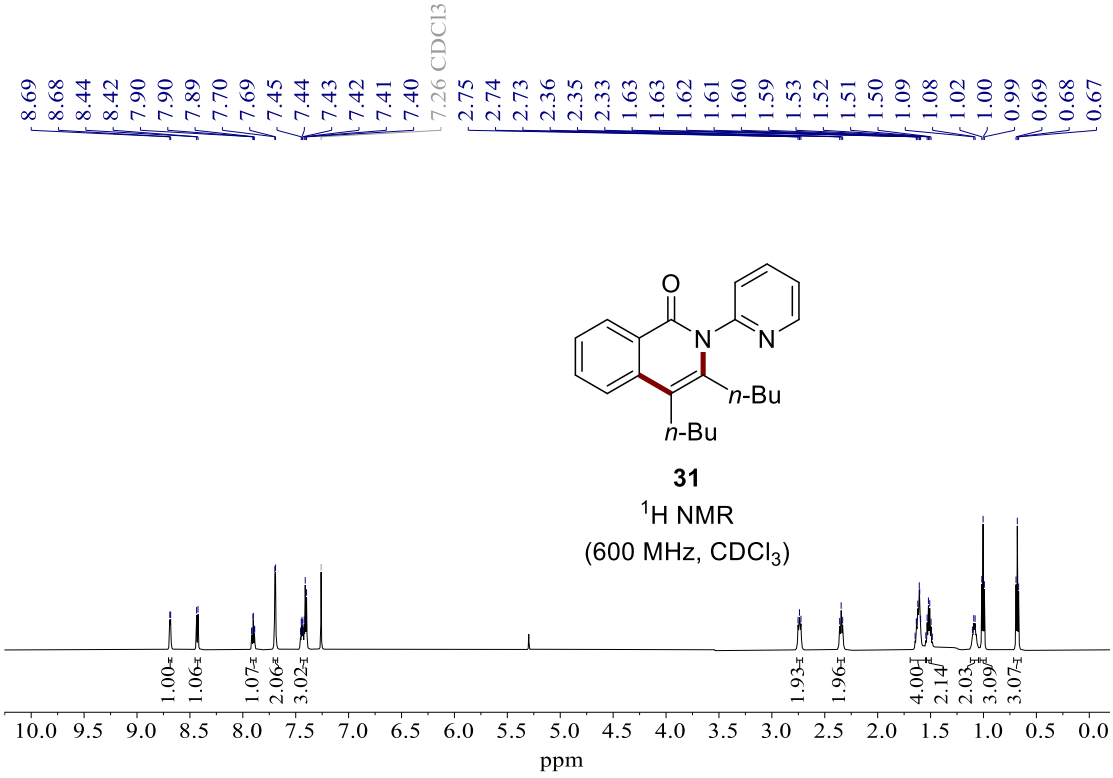
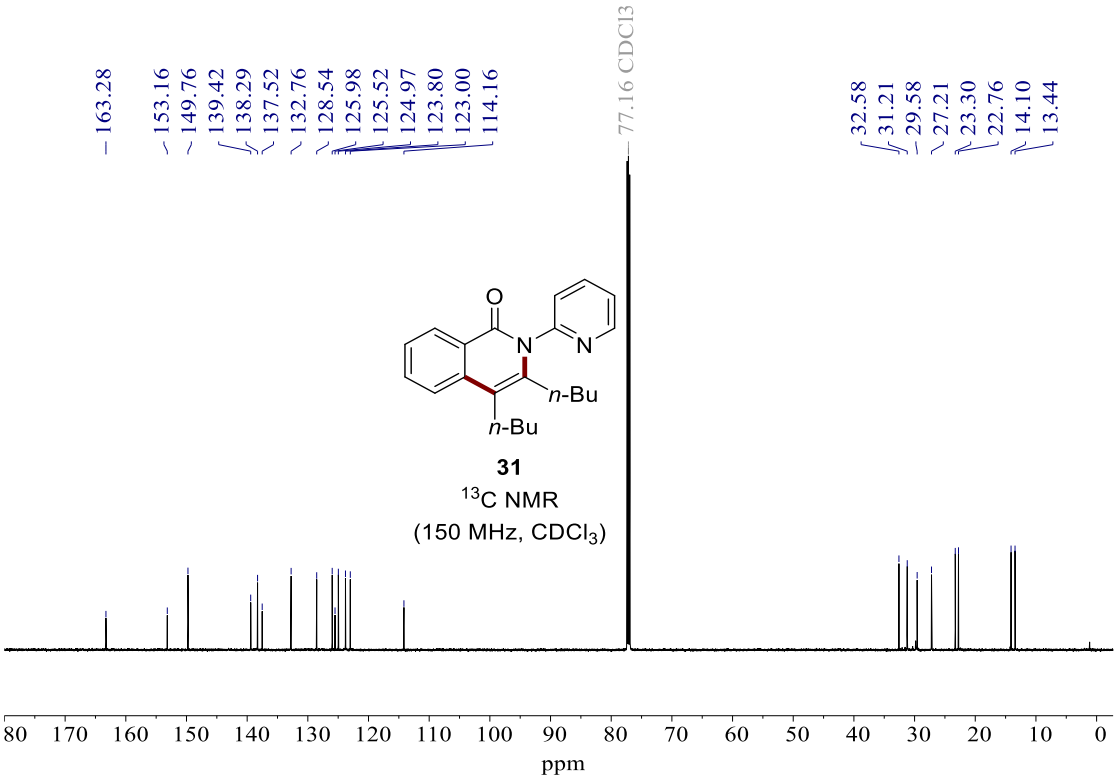
8.68
8.68
8.68
8.44
8.44
8.43
8.43
7.90
7.90
7.73
7.72
7.72
7.71
7.71
7.70
7.69
7.45
7.44
7.44
7.44
7.41
7.41
7.41
7.40
7.40
7.40
7.40
2.82
2.80
2.43
2.42
2.40
2.39
1.28
1.27
1.26
1.02
1.01
1.00
O
N
N
Et
Et
30
1H NMR
(600 MHz, CDCl3)
0.97
0.96
1.00
2.00
1.00
1.95
2.00
2.01
3.03
3.04
10.0 9.5 9.0 8.5 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
ppm


163.24
153.09
149.81
140.27
138.33
137.24
132.77
128.55
125.99
125.57
124.81
123.81
122.88
115.07
77.16 CDCl3
23.07
20.35
14.81
13.86
O
N
N
Et
Et
30
13C NMR
(150 MHz, CDCl3)
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm


8.69
8.68
8.44
8.42
7.90
7.90
7.89
7.70
7.69
7.45
7.44
7.43
7.42
7.41
7.40
7.26 CDCl3
2.75
2.74
2.73
2.36
2.35
2.33
1.63
1.63
1.62
1.61
1.60
1.59
1.53
1.52
1.51
1.50
1.09
1.08
1.02
1.00
0.99
0.69
0.68
0.67
O
N
N
n-Bu
n-Bu
31
1H NMR
(600 MHz, CDCl3)
1.00
1.06
1.07
2.06
3.02
1.93
1.96
4.00
2.14
2.03
3.09
3.07
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
ppm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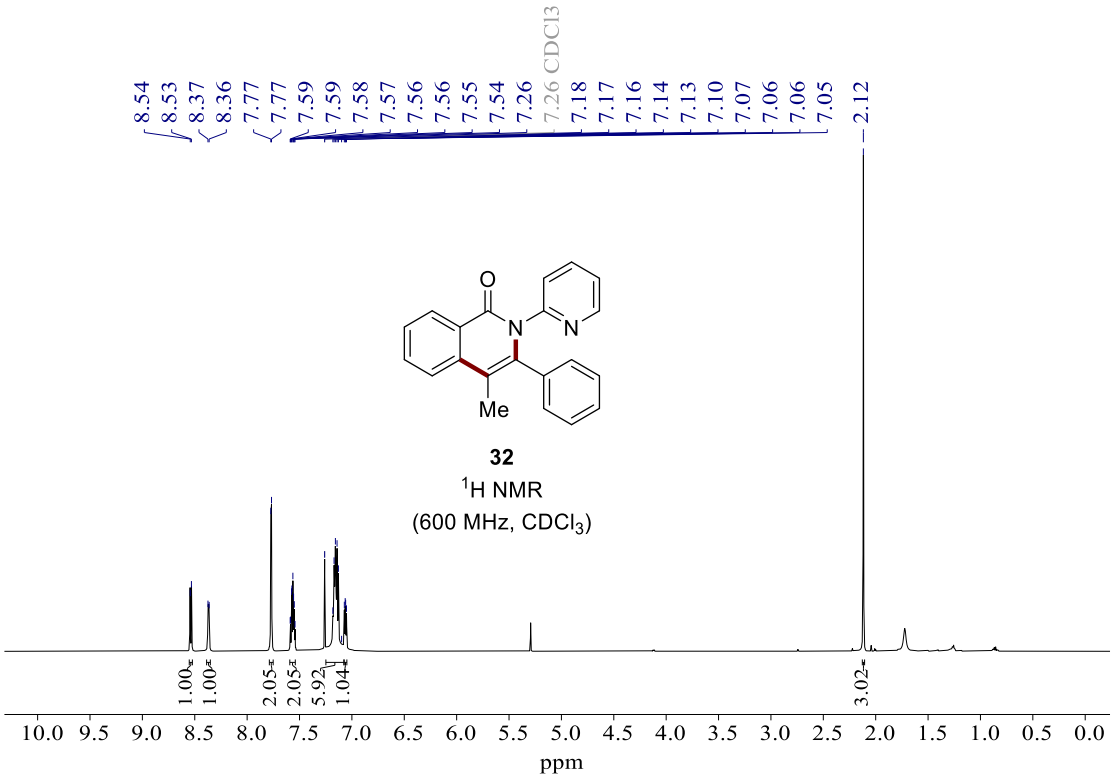
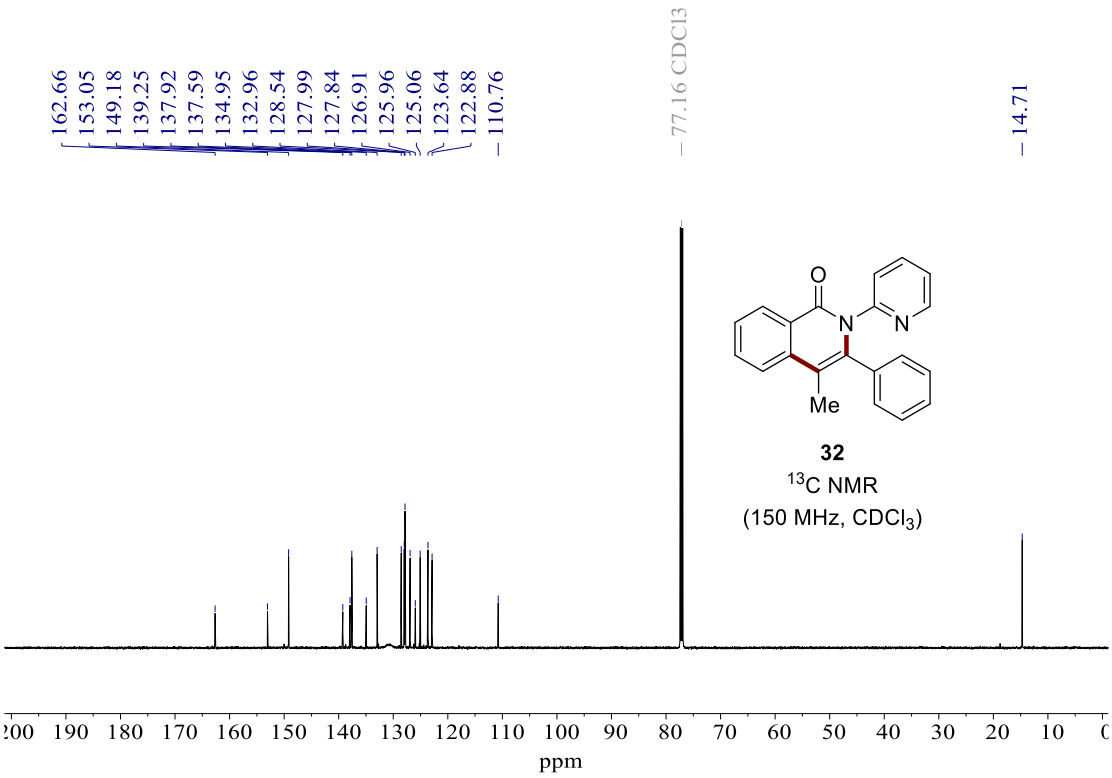
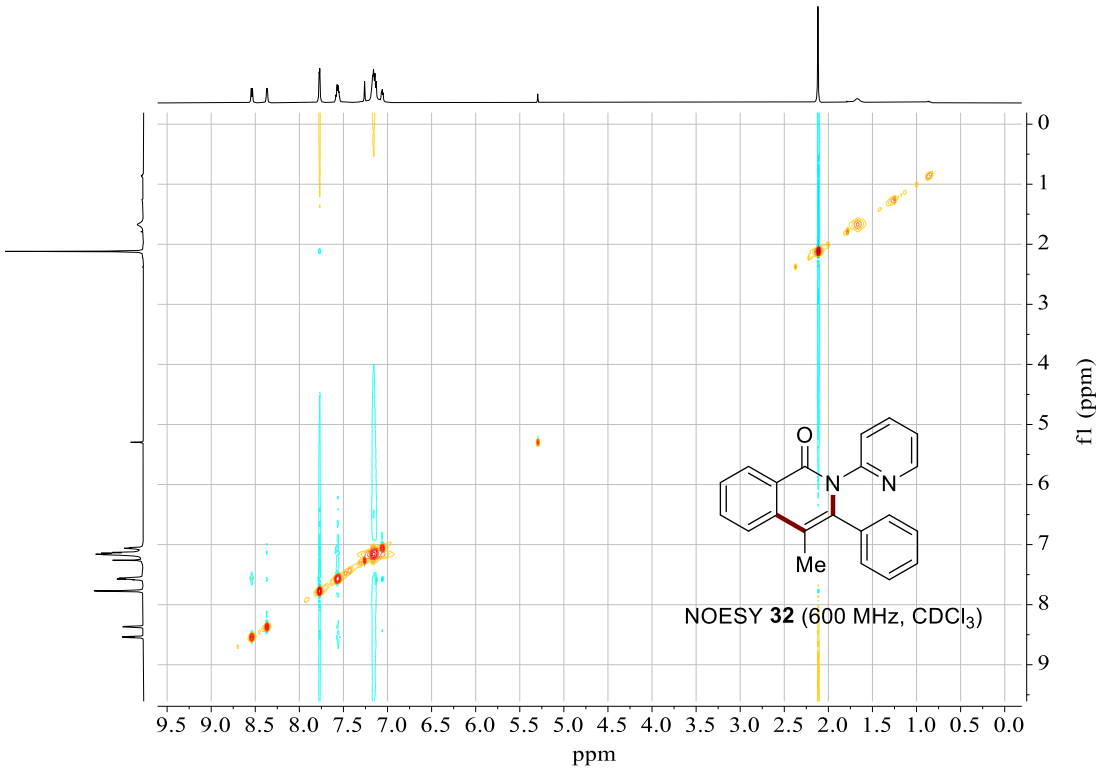
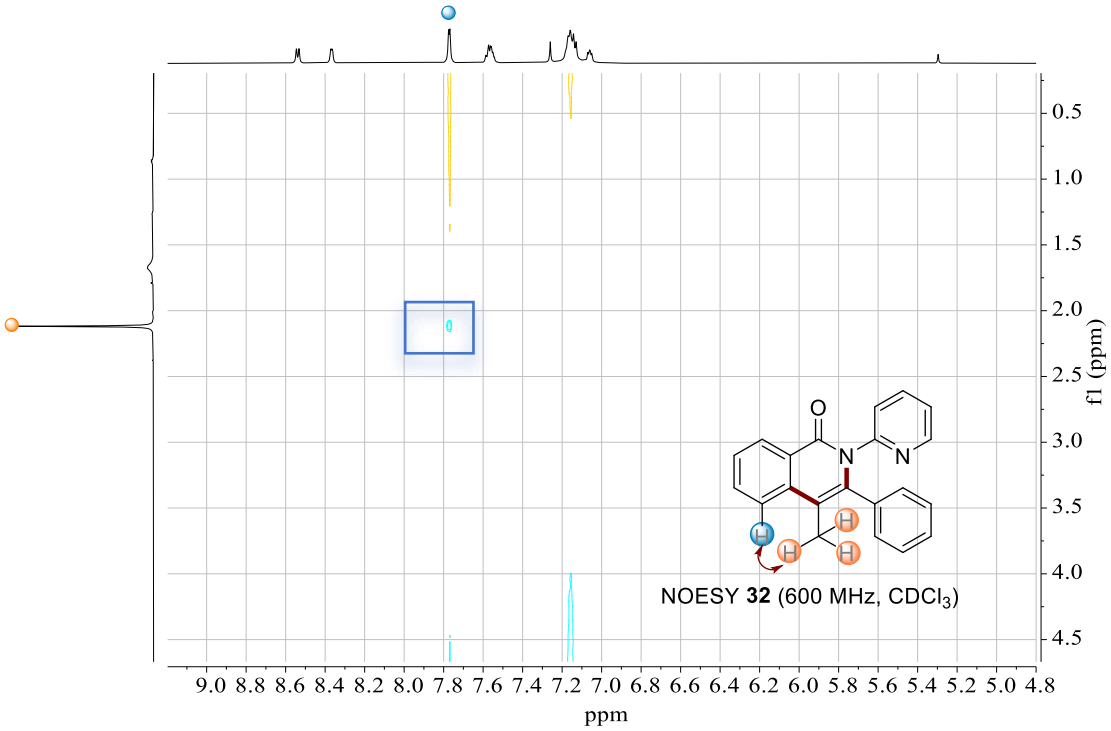
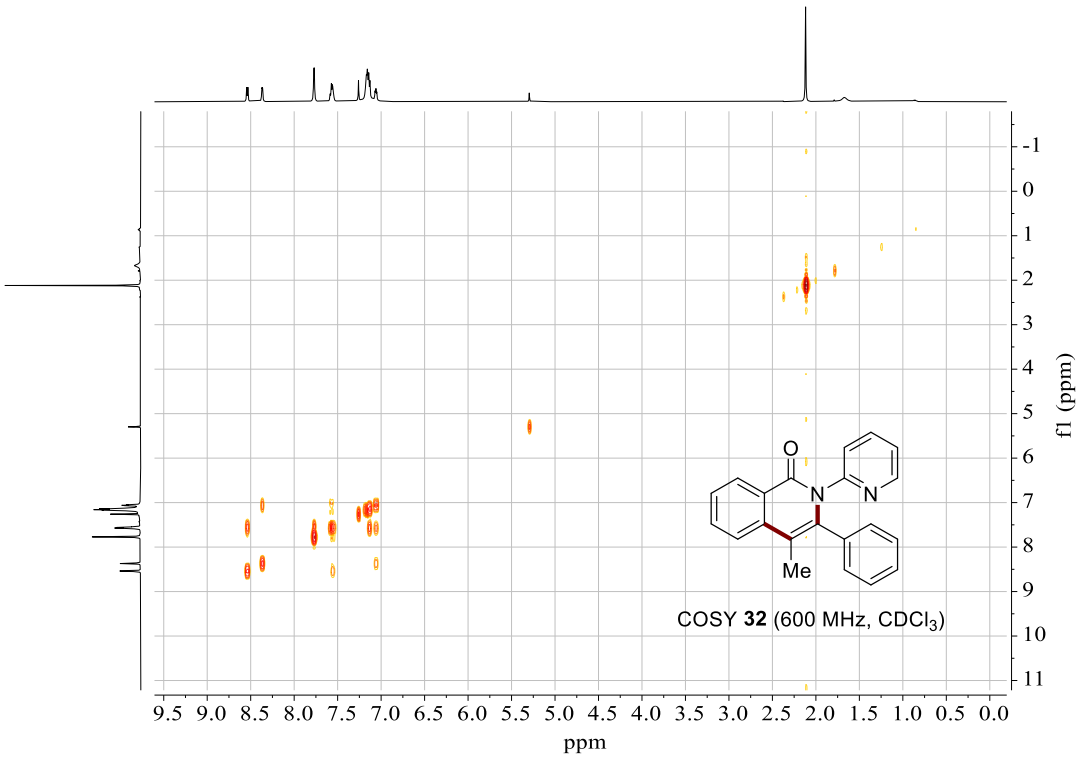
153.16
149.76
139.42
138.29
137.52
132.76
128.54
125.98
125.52
124.97
123.80
123.00
114.16
77.16 CDCl3
32.58
31.21
29.58
27.21
23.30
22.76
14.10
13.44
O
N
N
n-Bu
n-Bu
31
13C NMR
(150 MHz, CDCl3)
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

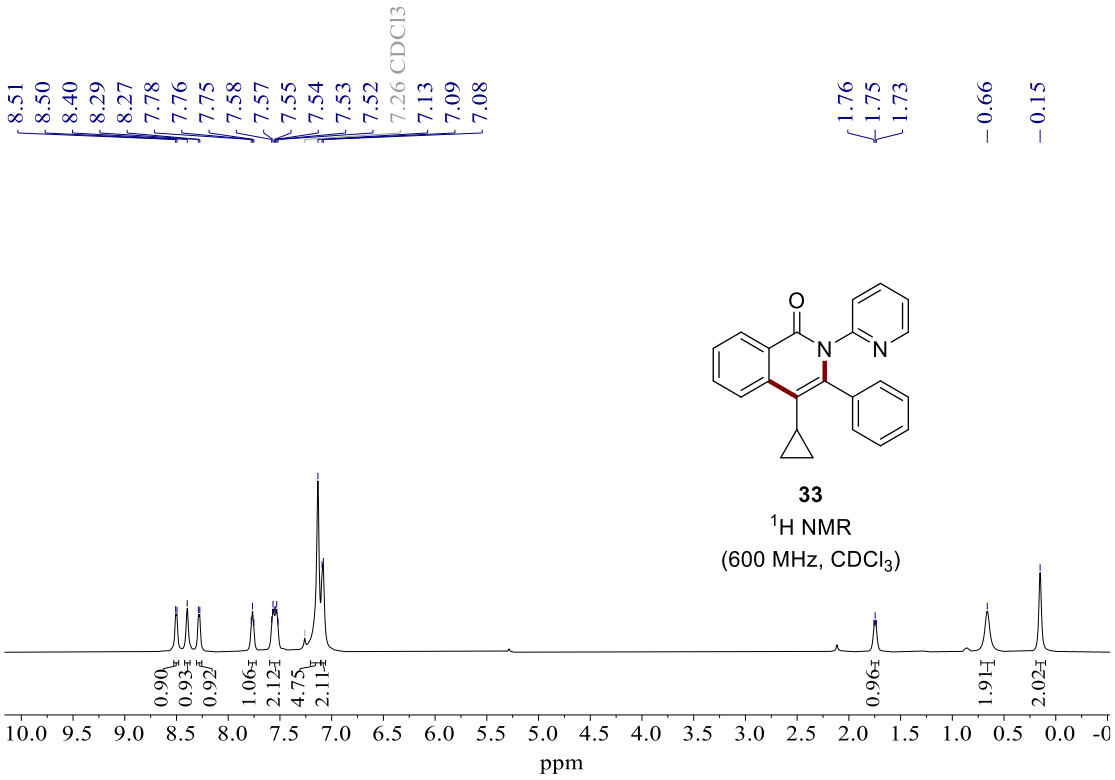

8.54
8.53
8.37
8.36
7.77
7.77
7.59
7.59
7.58
7.57
7.56
7.56
7.55
7.54
7.26
7.26 CDCl3
7.18
7.17
7.16
7.14
7.13
7.10
7.07
7.06
7.06
7.05
2.12
O
N
N
Me
32
1H NMR
(600 MHz, CDCl3)
1.00
1.00
2.05
2.05
5.92
1.04
3.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm

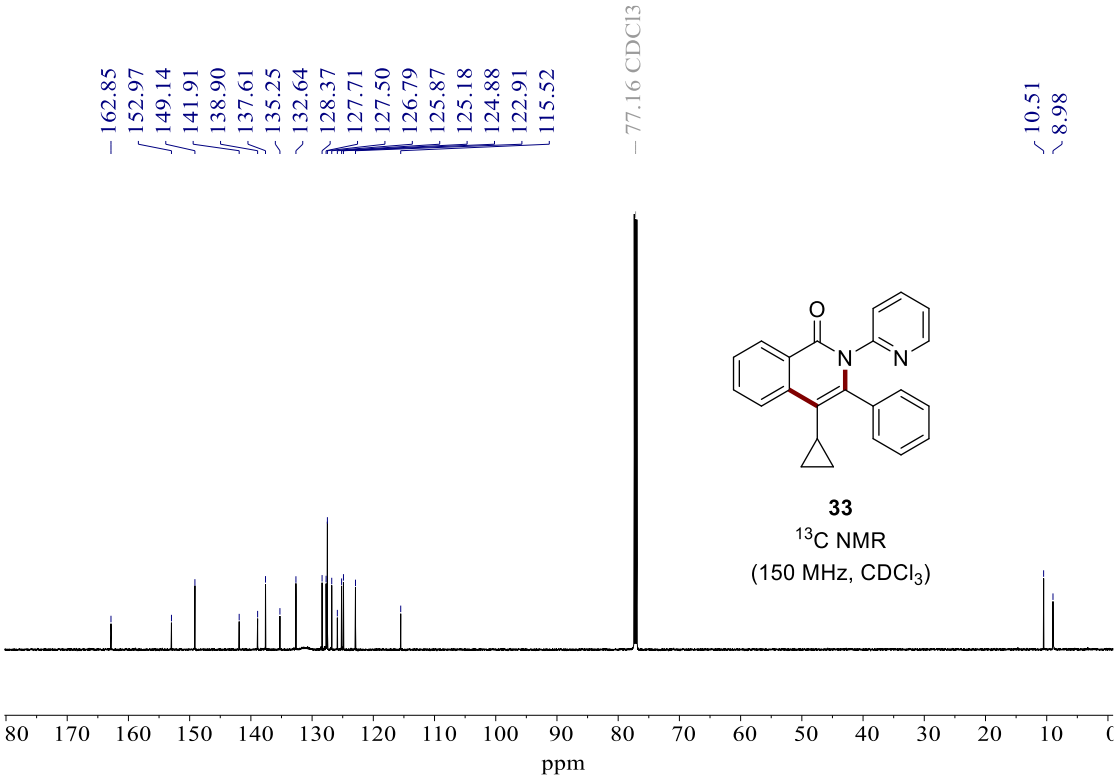

162.66
153.05
149.18
139.25
137.92
137.59
134.95
132.96
128.54
127.99
127.84
126.91
125.96
125.06
123.64
122.88
110.76
77.16 CDCl3
14.71
O
N
N
Me
32
13C NMR
(150 MHz, CDCl3)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm

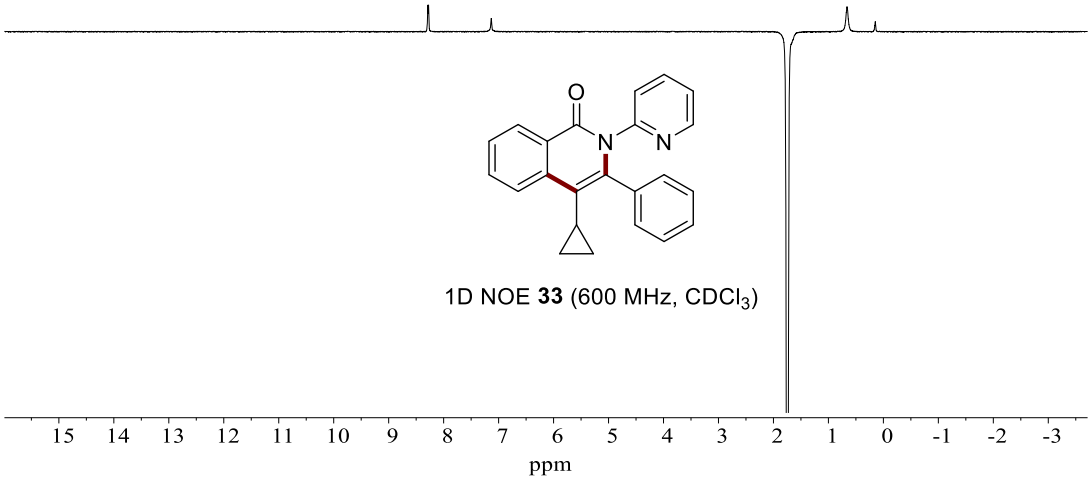

O
N
N
Me
NOESY 32 (600 MHz, CDCl3)
f1 (ppm)
0 1 2 3 4 5 6 7 8 9
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm

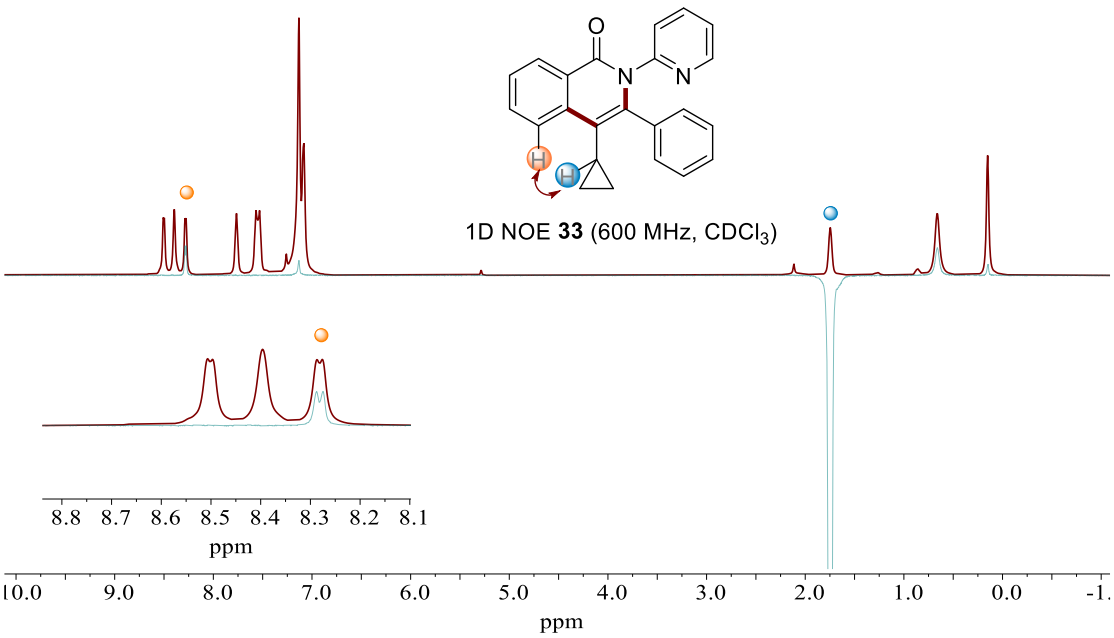

f1 (ppm)
ppm
NOESY 32 (600 MHz, CDCl3)

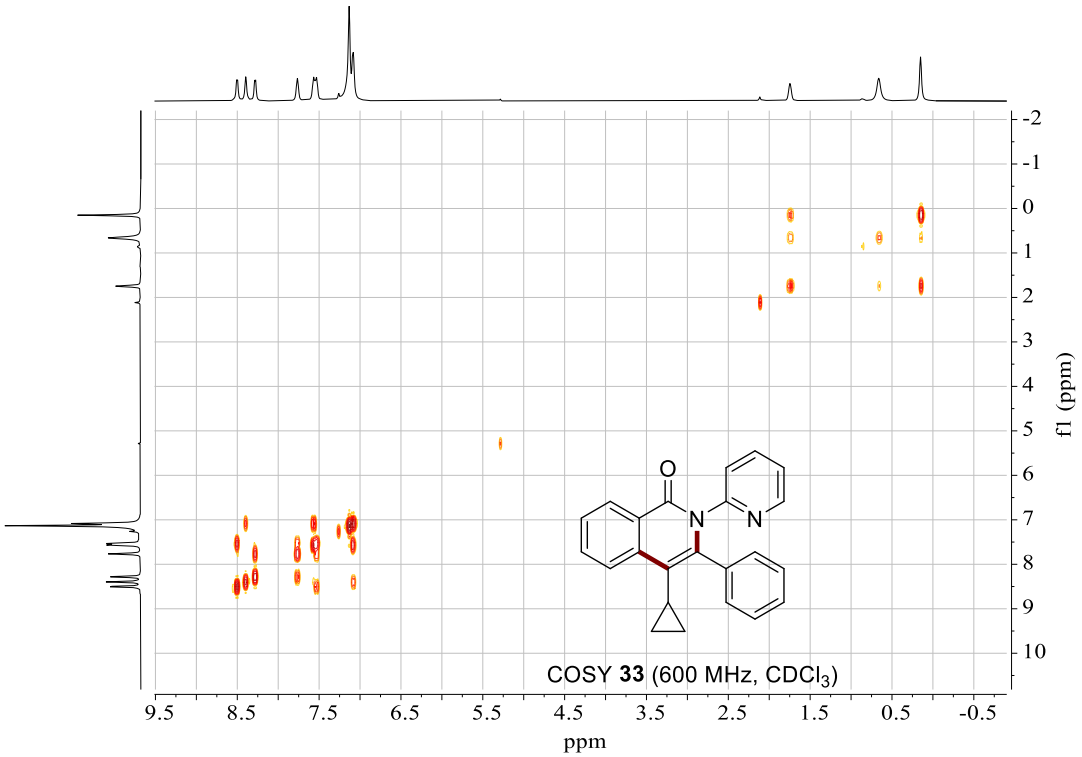

f1 (ppm)
ppm
Me
COSY 32 (600 MHz, CDCl3)

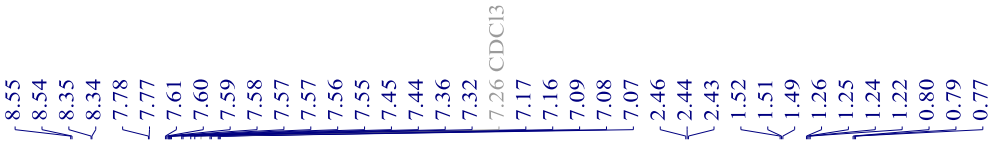

8.51
8.50
8.40
8.29
8.27
7.78
7.76
7.75
7.58
7.57
7.55
7.54
7.53
7.52
7.26 CDCl3
7.13
7.09
7.08
1.76
1.75
1.73
0.66
0.15
O
N
N
33
1H NMR
(600 MHz, CDCl3)
0.90
0.93
0.92
1.06
2.12
4.75
2.11
0.96
1.91
2.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
ppm

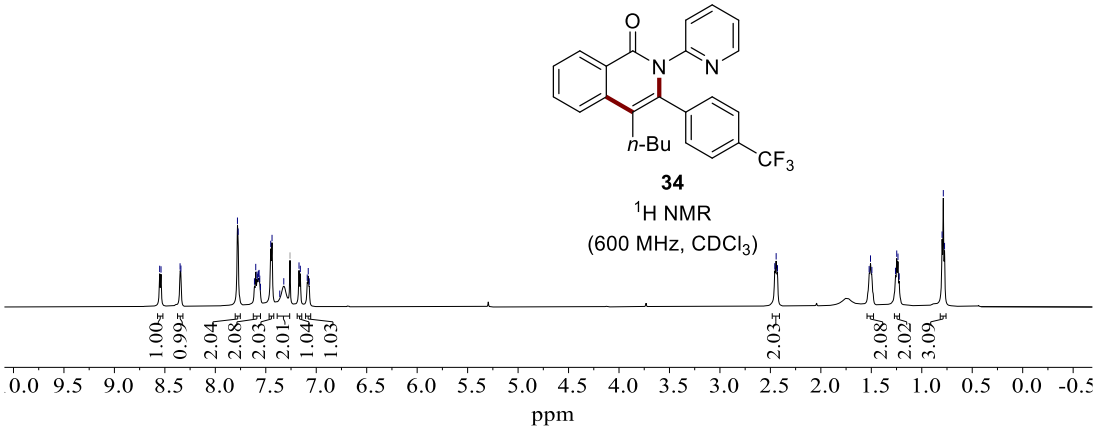

162.85
152.97
149.14
141.91
138.90
137.61
135.25
132.64
128.37
127.71
127.50
126.79
125.87
125.18
124.88
122.91
115.52
77.16 CDCl3
10.51
8.98
O
N
N
33
13C NMR
(150 MHz, CDCl3)
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

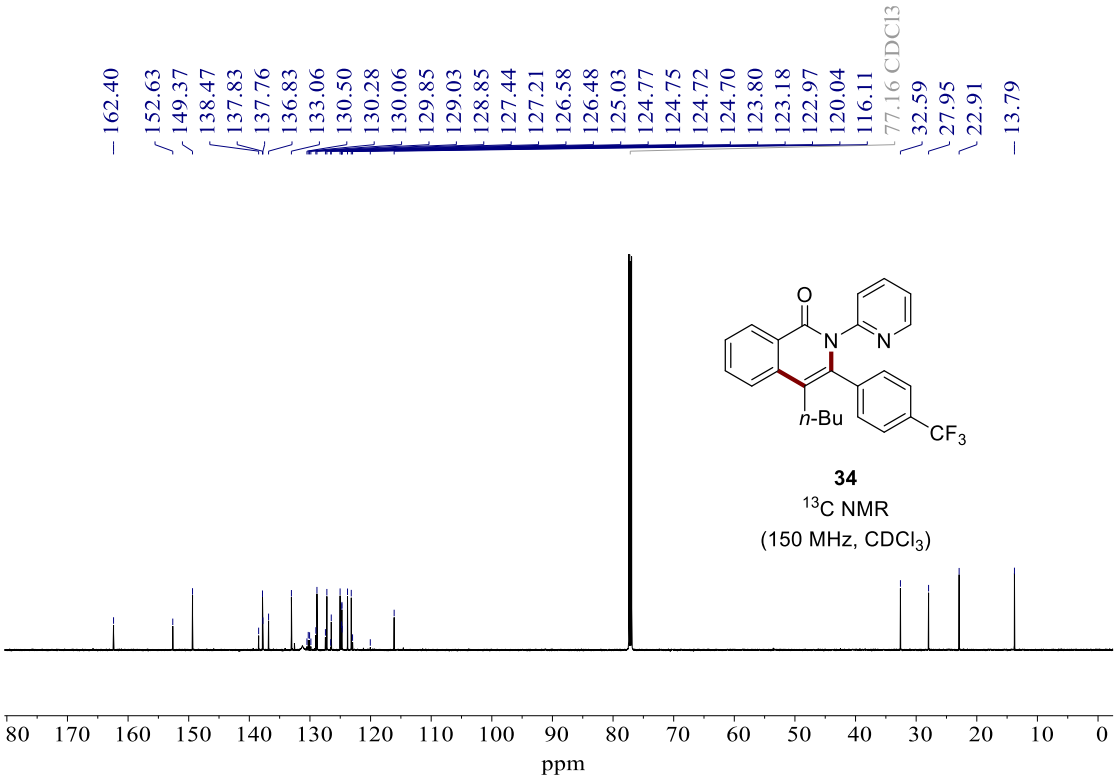

O
N
N
1D NOE 33 (600 MHz, CDCl3)
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
ppm


O
N
N
H
H
1D NOE 33 (600 MHz, CDCl3)
8.8 8.7 8.6 8.5 8.4 8.3 8.2 8.1
ppm
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.
ppm


COSY 33 (600 MHz, CDCl3)
f1 (ppm)
ppm


8.55
8.54
8.35
8.34
7.78
7.77
7.61
7.60
7.59
7.58
7.57
7.57
7.56
7.55
7.45
7.44
7.36
7.32
7.26 CDCl3
7.17
7.16
7.09
7.08
7.07
2.46
2.44
2.43
1.52
1.51
1.49
1.26
1.25
1.24
1.22
0.80
0.79
0.77

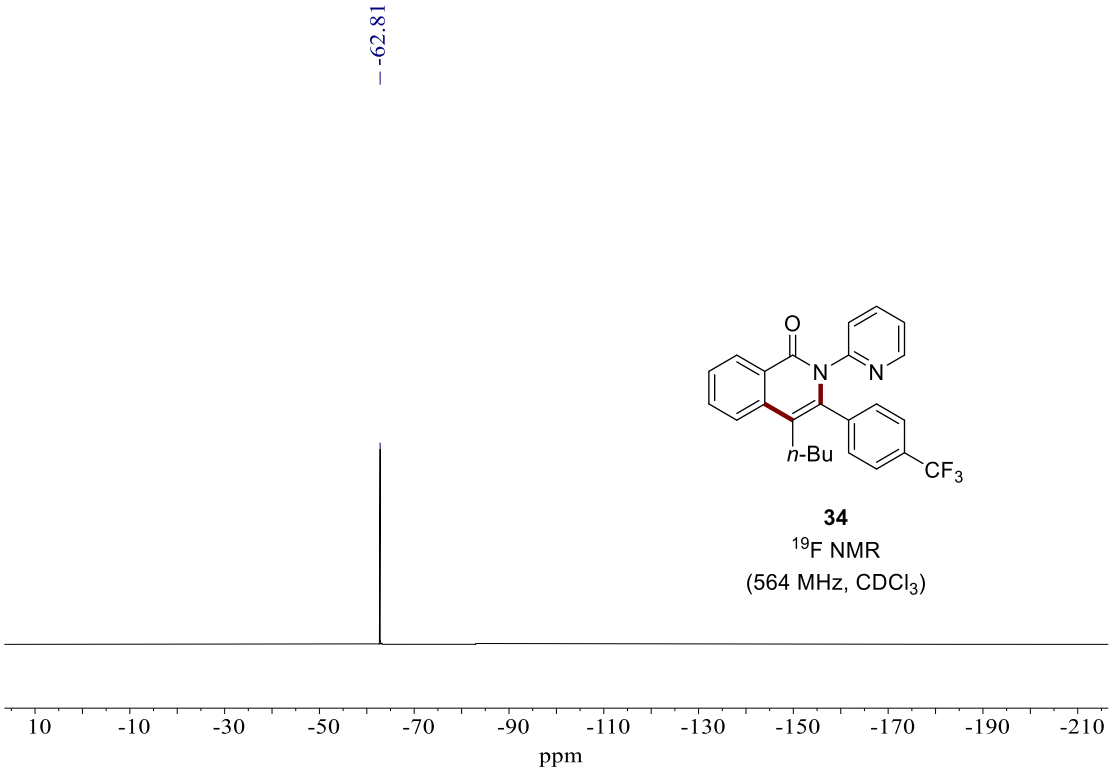

n-Bu
CF3
34
1H NMR
(600 MHz, CDCl3)
ppm



34

^{13}C NMR

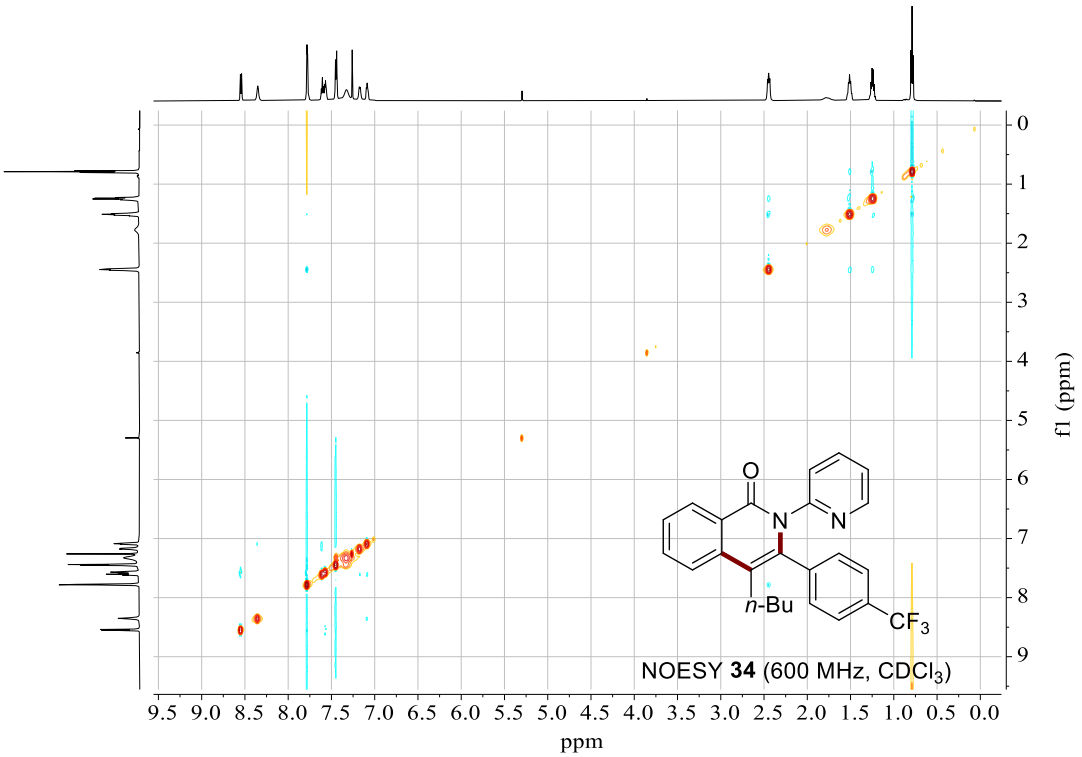
(150 MHz, $CDCl_3$)

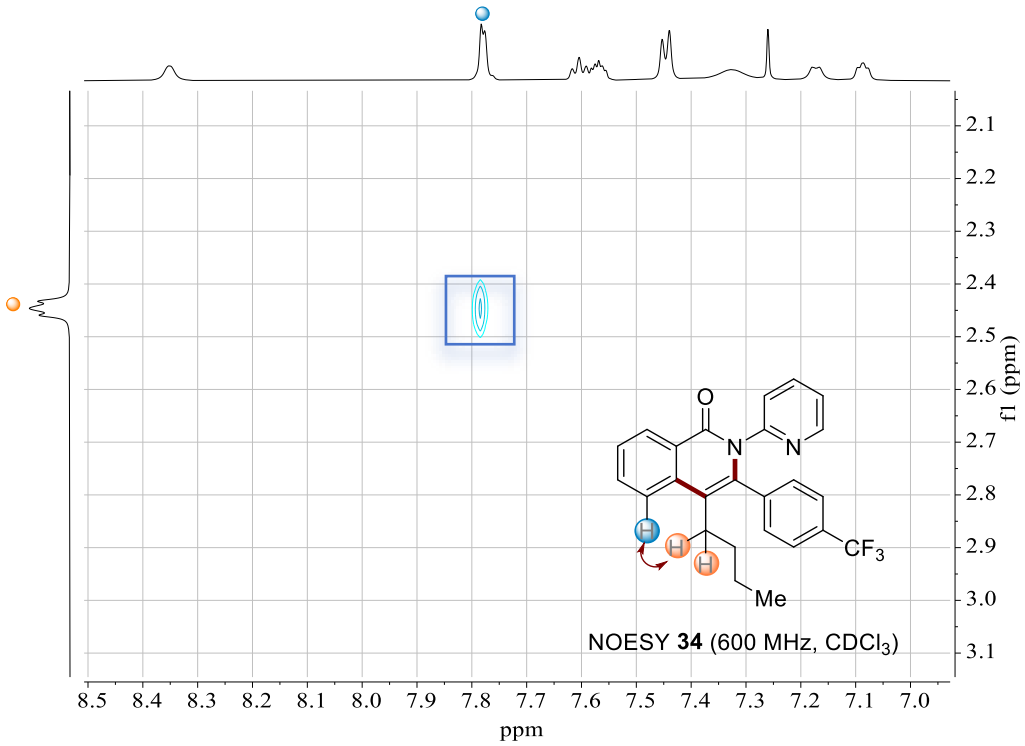


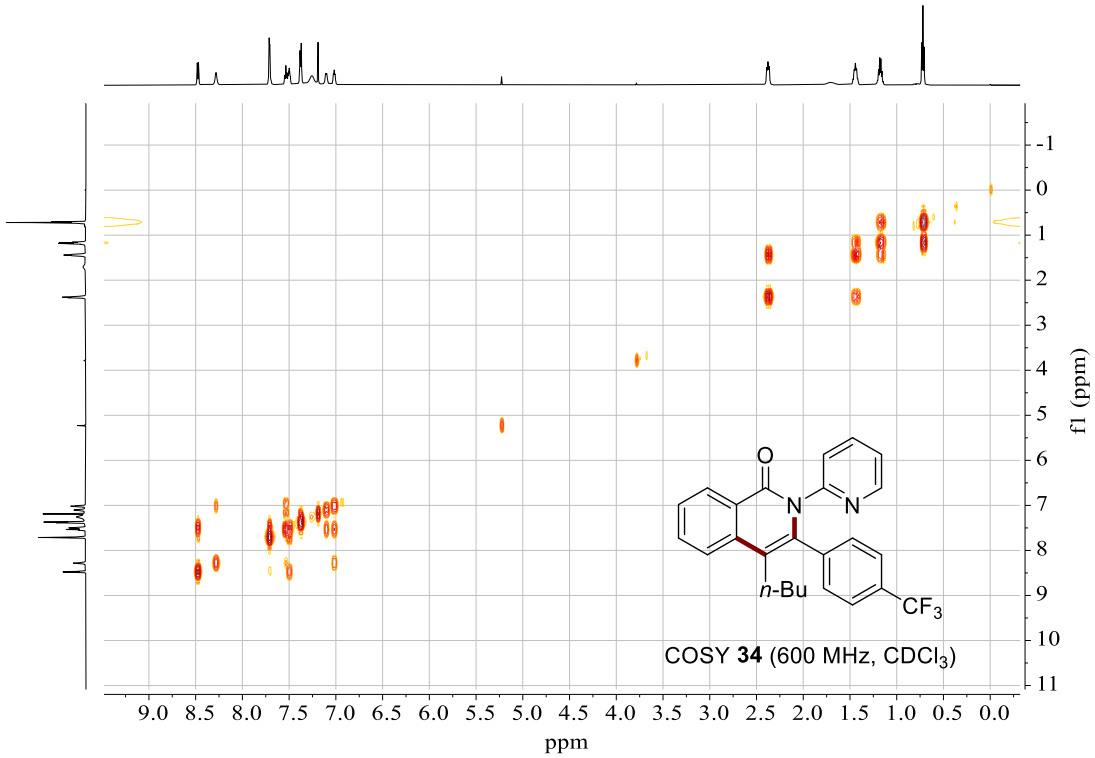
34

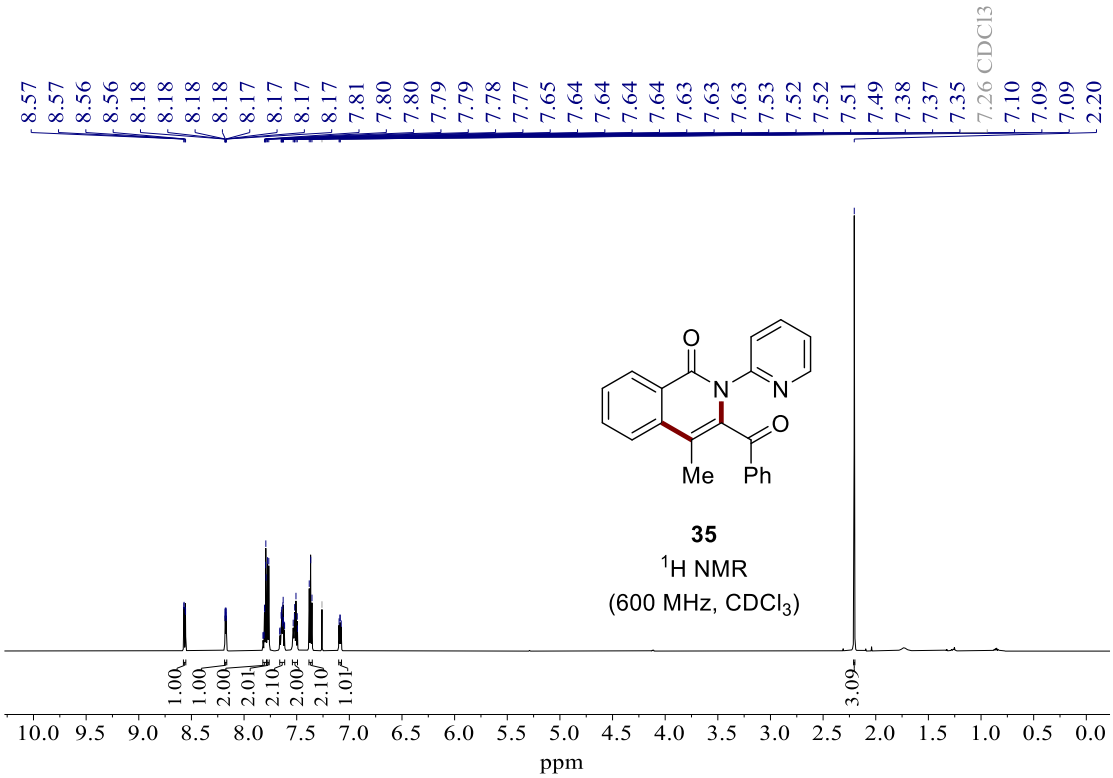
^{19}F NMR

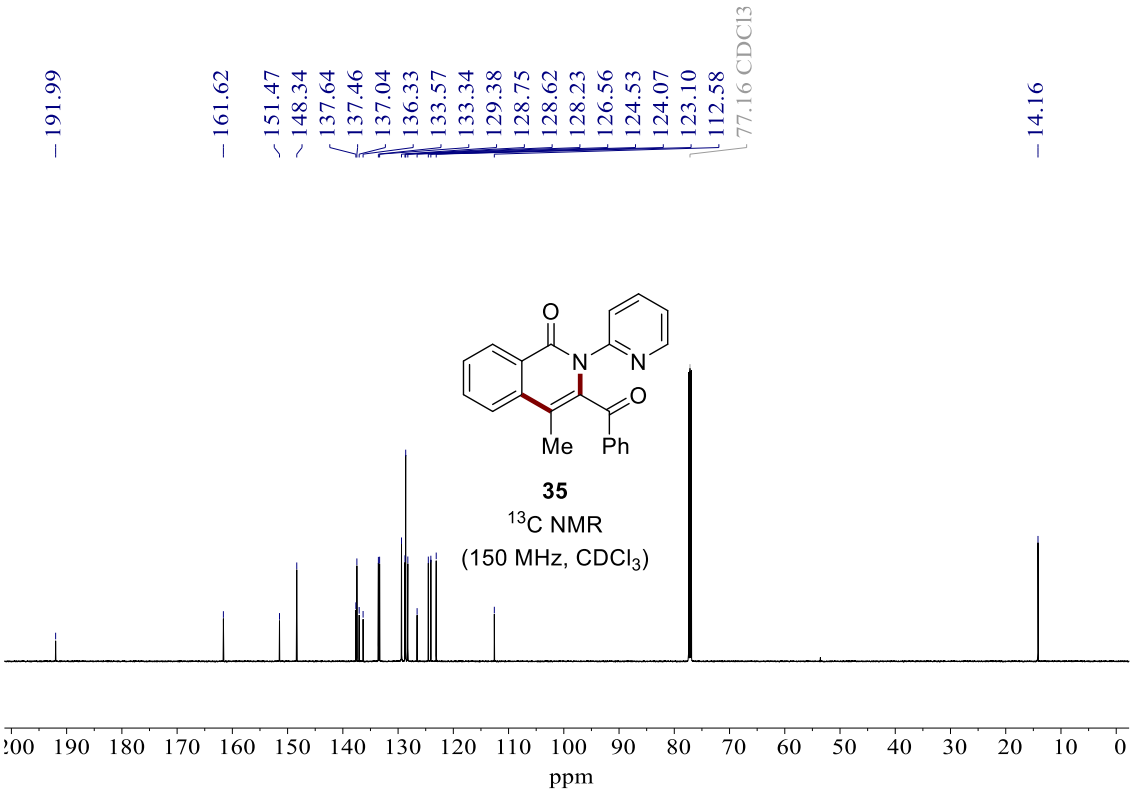
(564 MHz, $CDCl_3$)

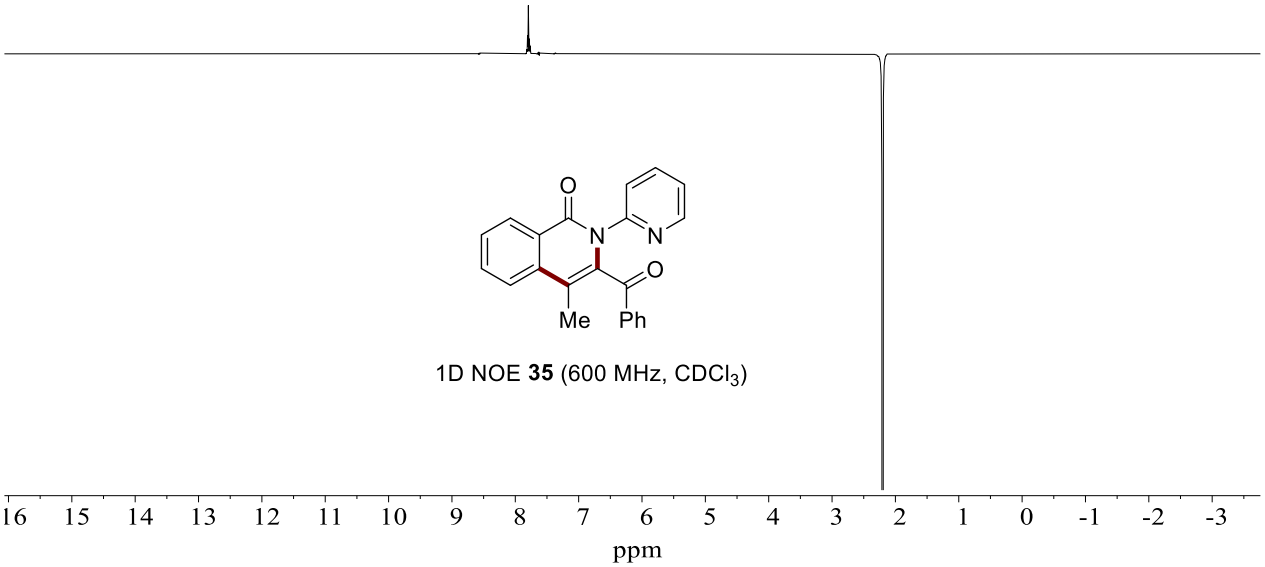

NOESY 34 (600 MHz, CDCl3)
n-Bu
CF3
f1 (ppm)
ppm

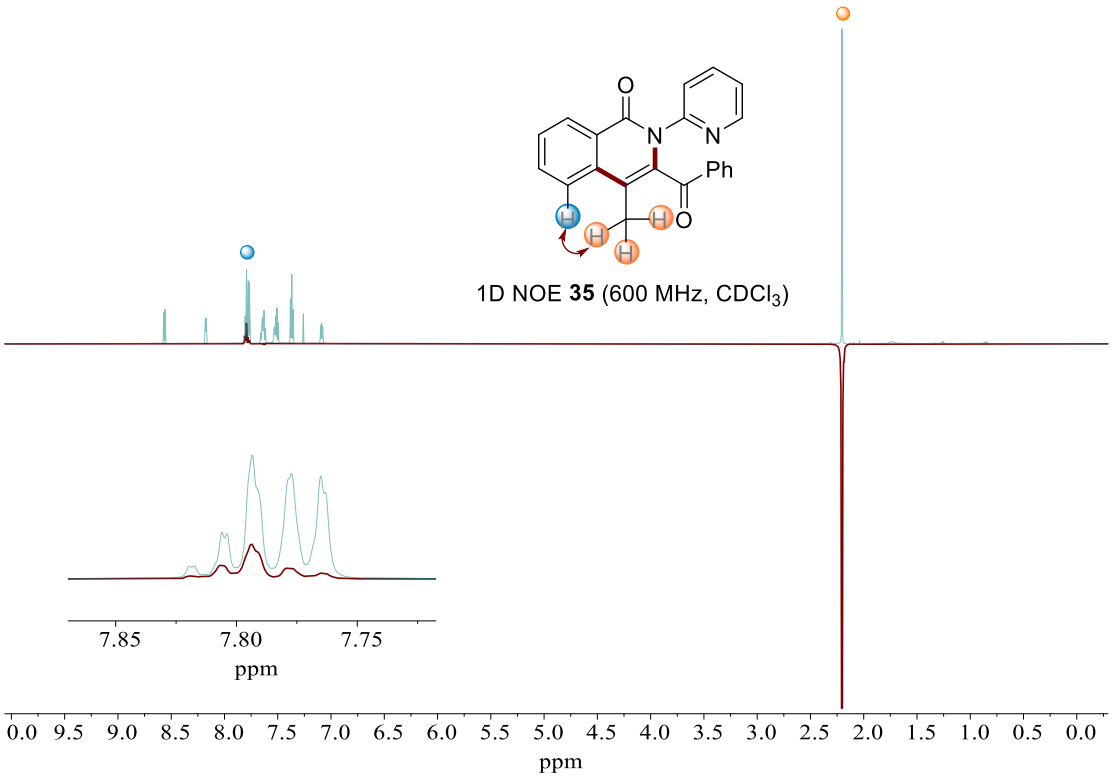

NOESY 34 (600 MHz, CDCl3)
Me
CF3
f1 (ppm)
ppm

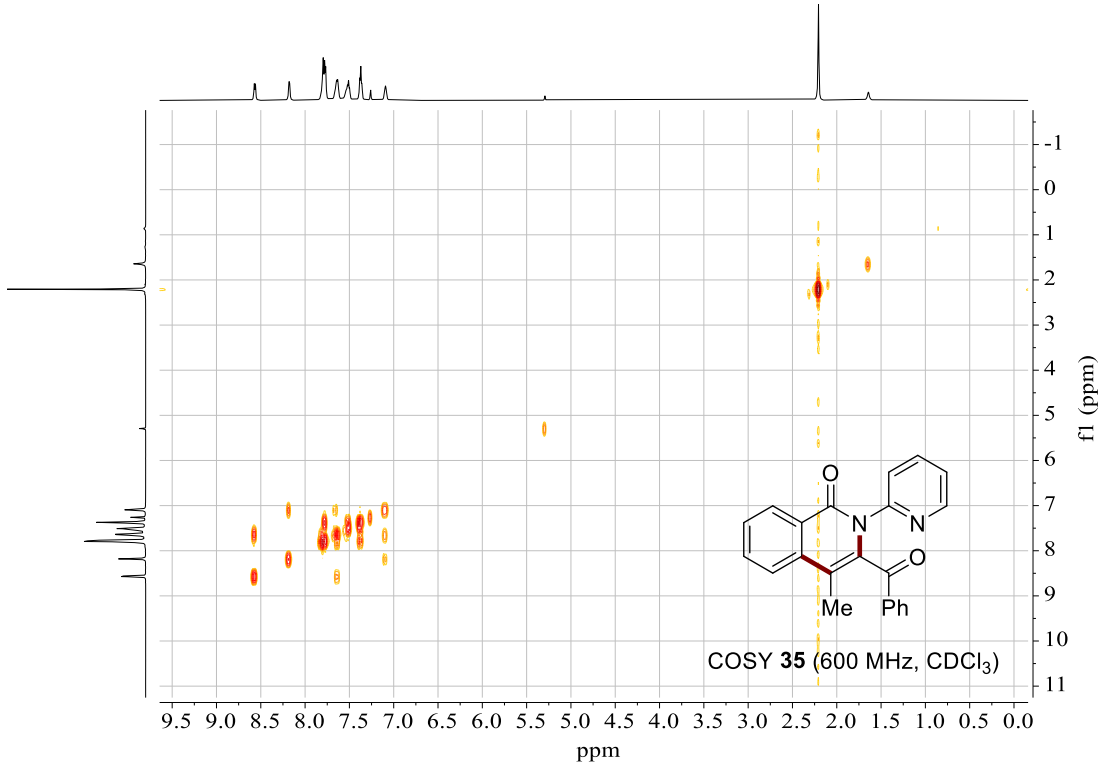

COSY **34** (600 MHz, $CDCl_3$)
f1 (ppm)
ppm

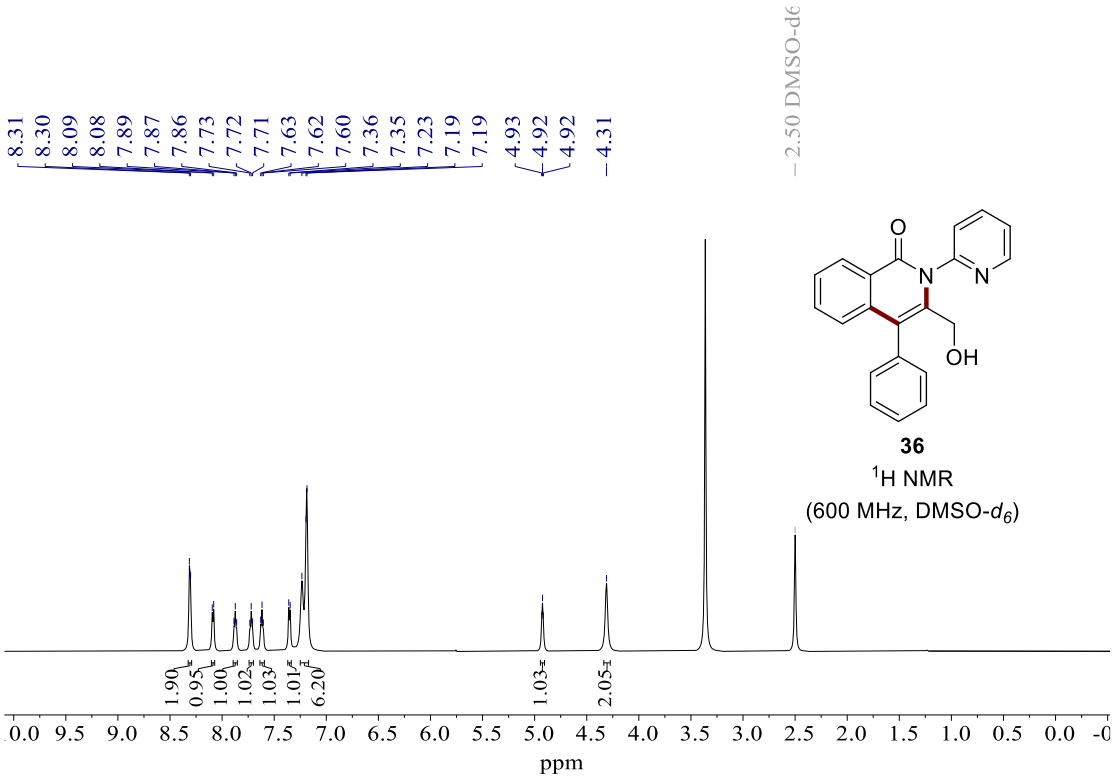

35
^{1}H NMR
(600 MHz, $CDCl_3$)
ppm


191.99
161.62
151.47
148.34
137.64
137.46
137.04
136.33
133.57
133.34
129.38
128.75
128.62
128.23
126.56
124.53
124.07
123.10
112.58
77.16 CDCl3
14.16
O
N
N
O
Me
Ph
35
13C NMR
(150 MHz, CDCl3)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm


O
N
N
O
Me
Ph
1D NOE 35 (600 MHz, CDCl3)
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
ppm


O
N
N
Ph
O
H
H
H
H
1D NOE 35 (600 MHz, CDCl3)
7.85
7.80
7.75
ppm
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
ppm

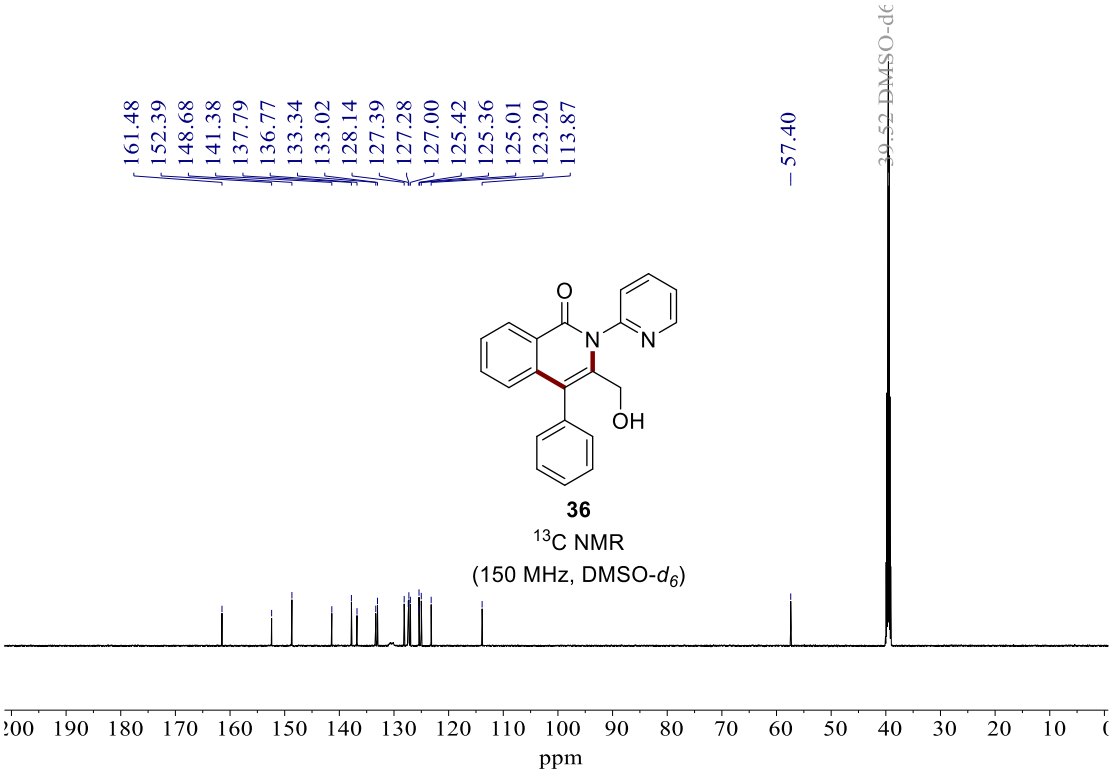

-1
0
1
2
3
4
5
6
7
8
9
10
11
f1 (ppm)
O
N
N
O
Me
Ph
COSY 35 (600 MHz, CDCl3)
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm



36

^{1}H NMR

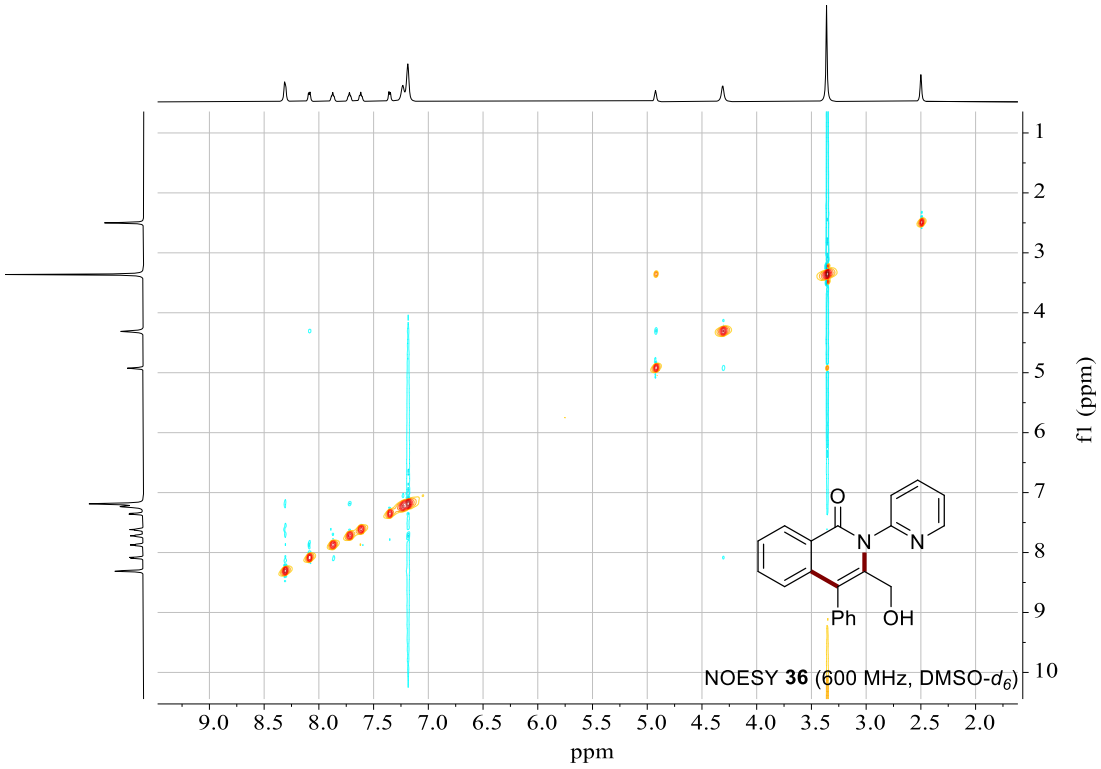
(600 MHz, DMSO-d_6)

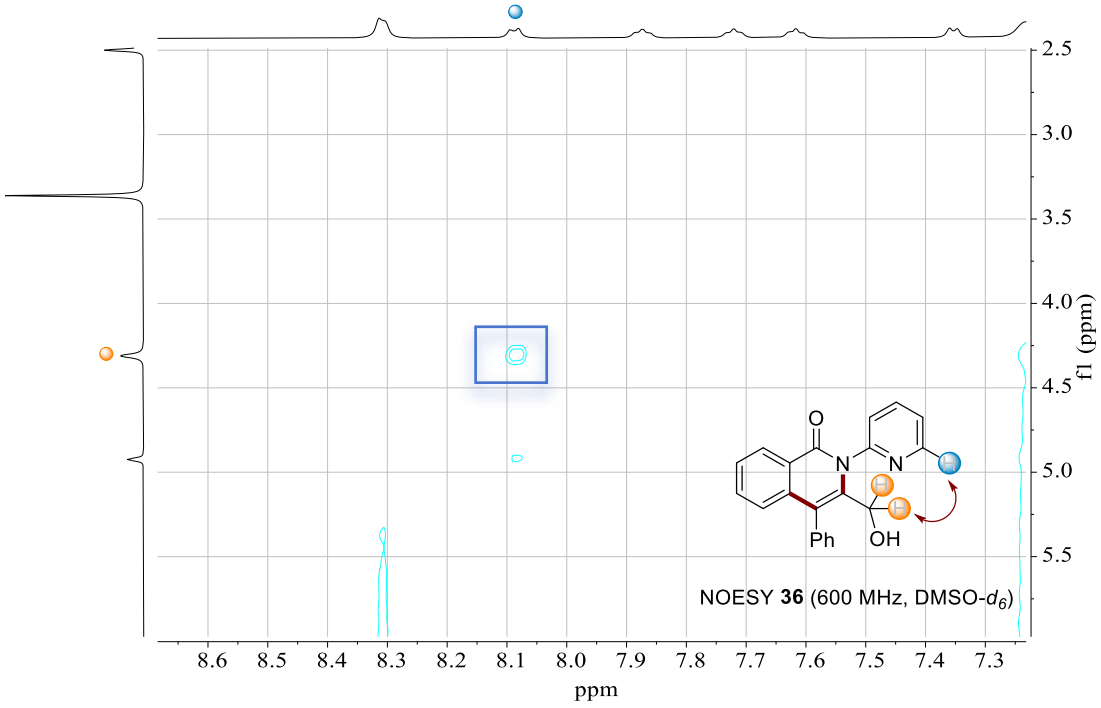


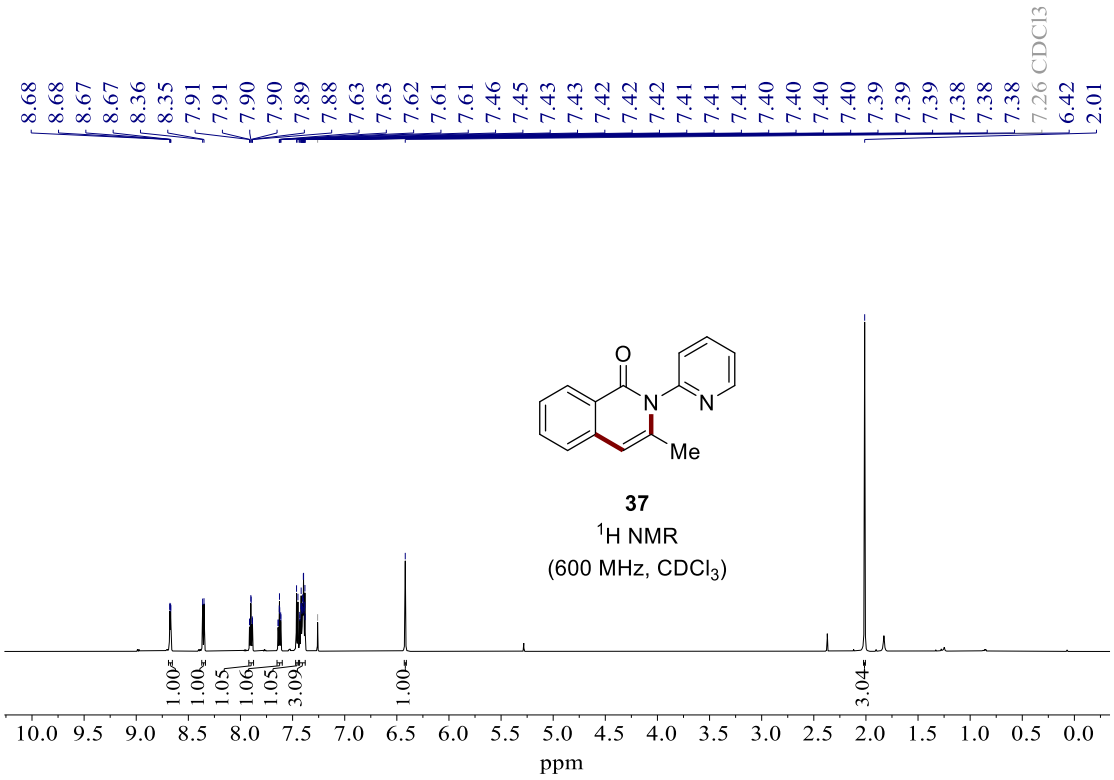
36

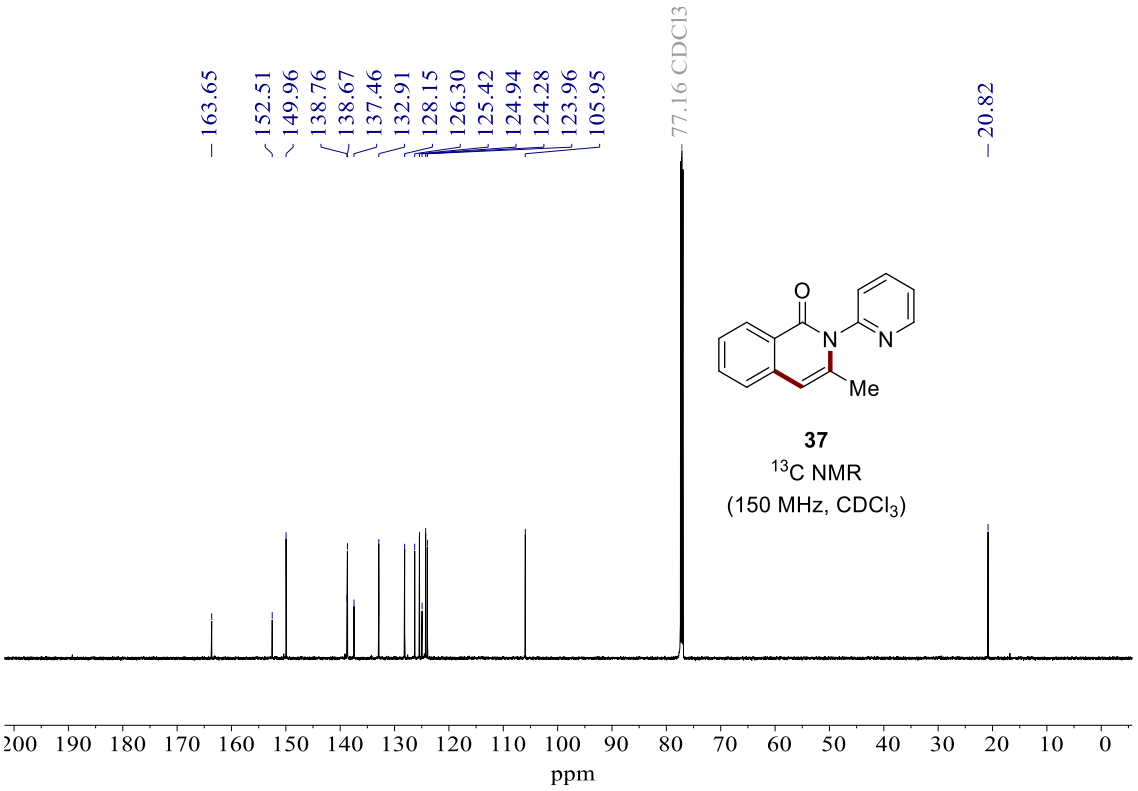
^{13}C NMR

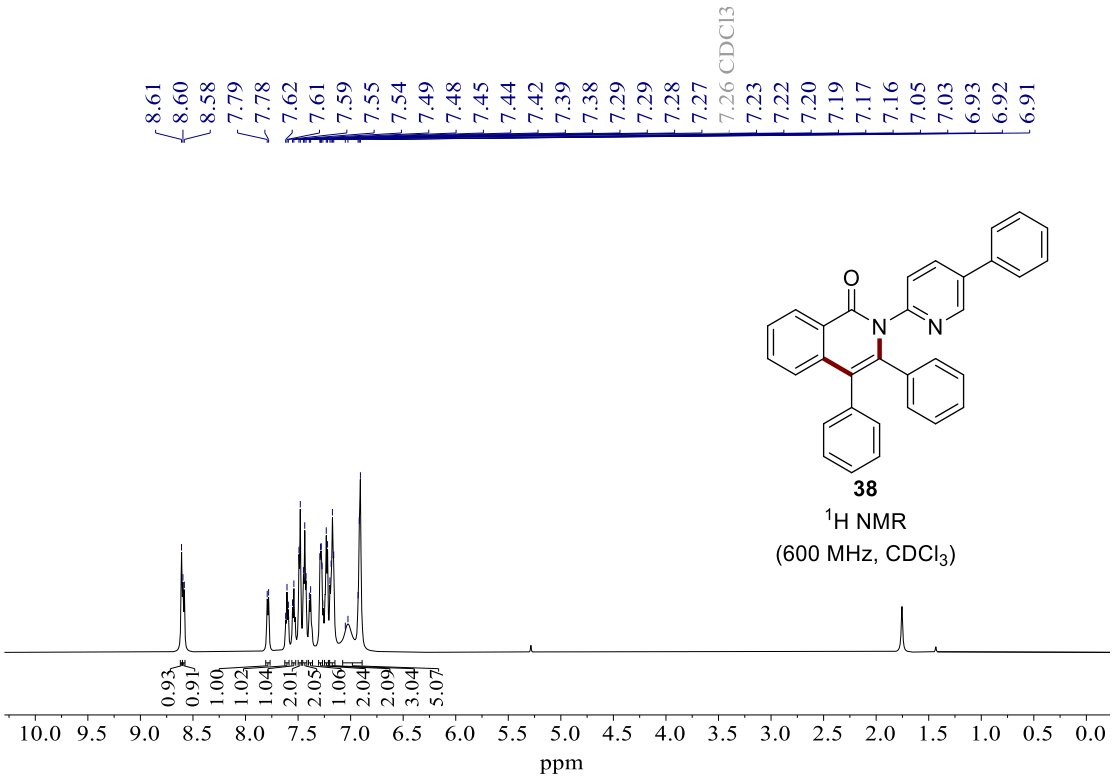
(150 MHz, DMSO-d_6)

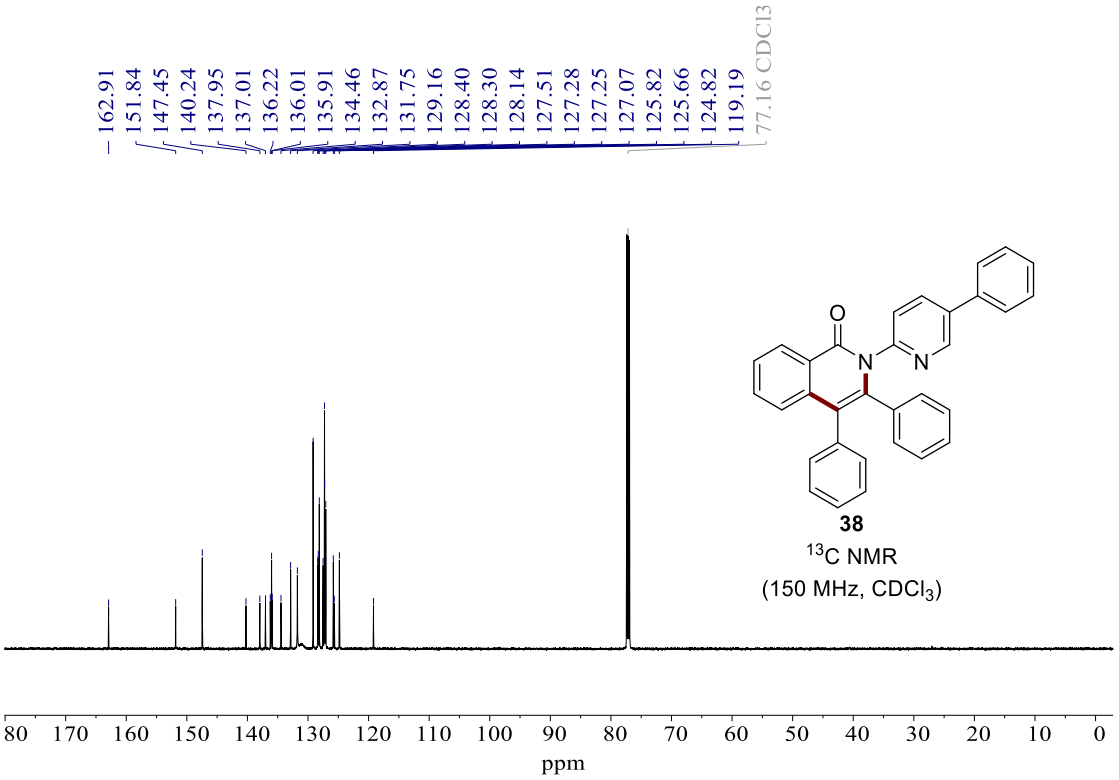

f1 (ppm)
ppm
NOESY 36 (600 MHz, DMSO-d_6)
O
N
N
Ph
OH

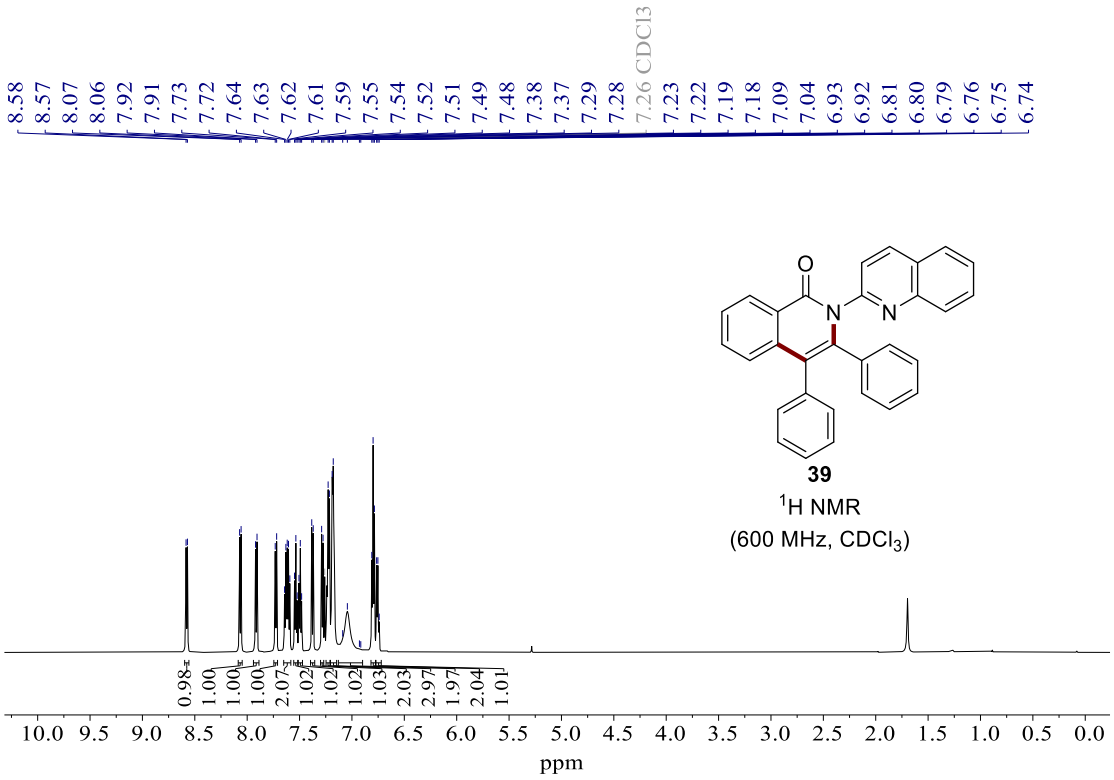

f1 (ppm)
ppm
NOESY 36 (600 MHz, DMSO-d_6)
O
N
N
Ph
OH

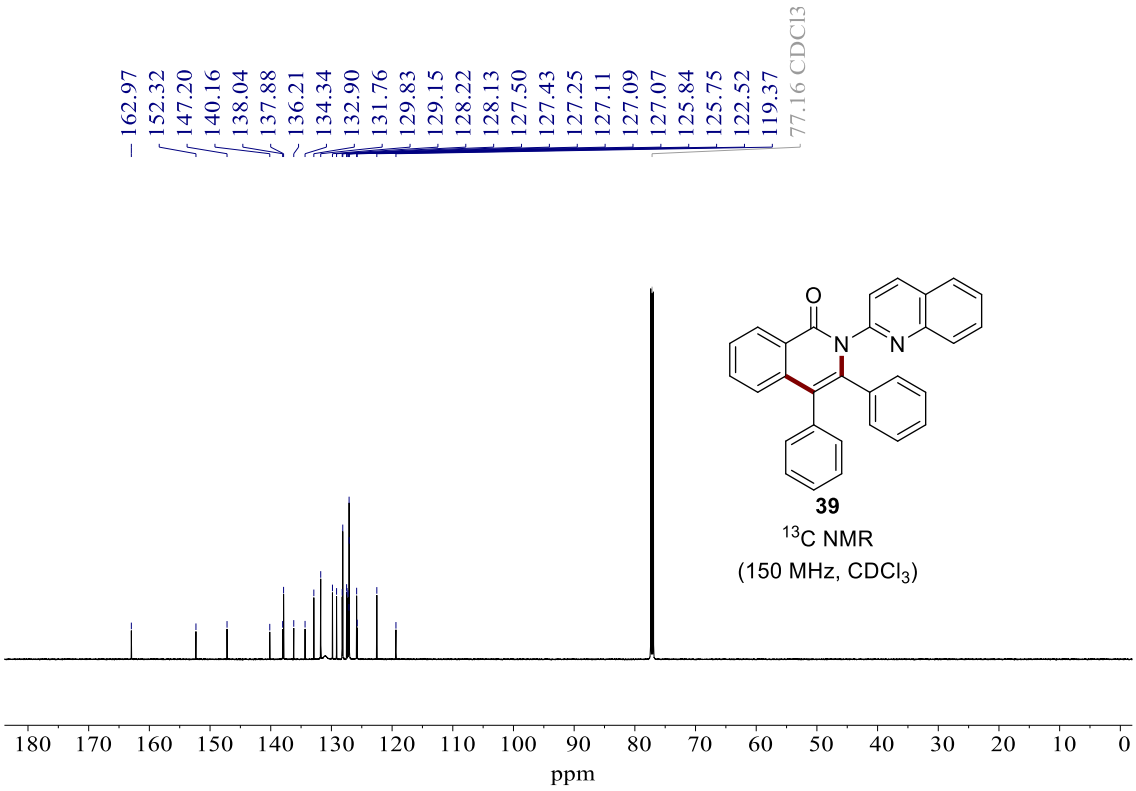

8.68 8.68 8.67 8.67 8.36 8.35 7.91 7.91 7.90 7.90 7.89 7.88 7.63 7.63 7.62 7.61 7.61 7.46 7.45 7.43 7.43 7.42 7.42 7.42 7.41 7.41 7.41 7.40 7.40 7.40 7.40 7.39 7.39 7.39 7.38 7.38 7.38 7.26 CDCl3 6.42 2.01
O
N
N
Me
37
1H NMR
(600 MHz, CDCl3)
1.00 1.00 1.05 1.06 1.05 3.09 1.00 3.04
10.0 9.5 9.0 8.5 8.0 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
ppm

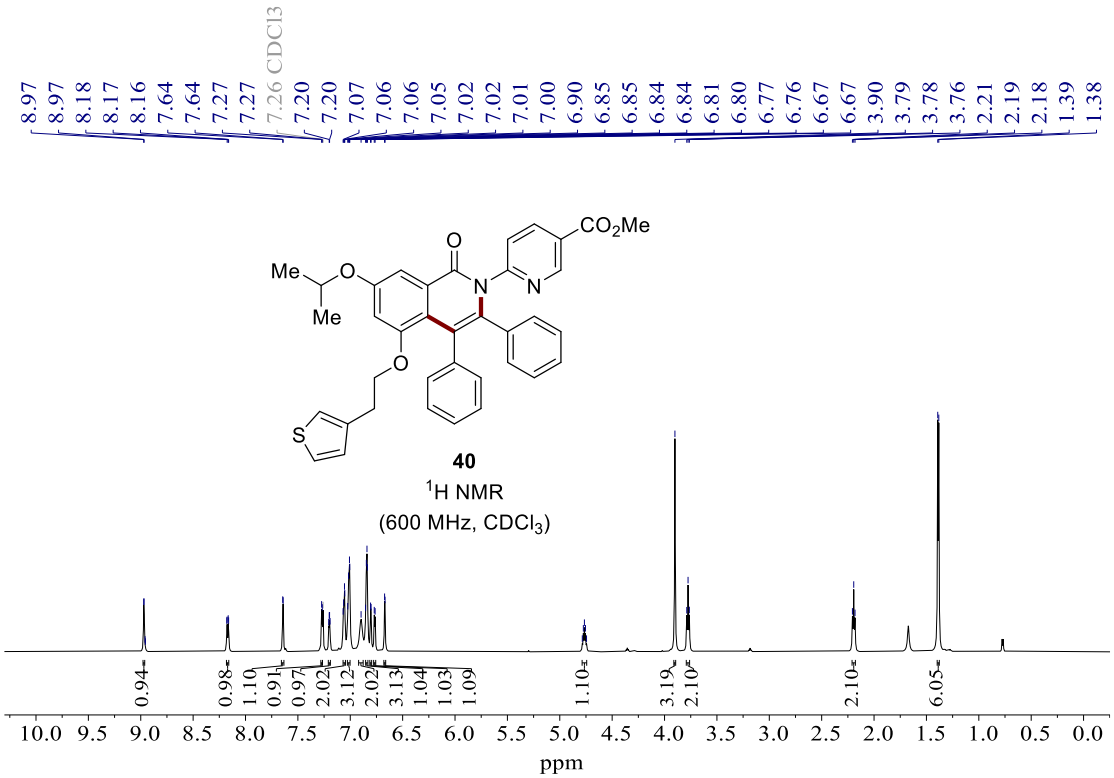

163.65 152.51 149.96 138.76 138.67 137.46 132.91 128.15 126.30 125.42 124.94 124.28 123.96 105.95 77.16 CDCl3 20.82
O
N
N
Me
37
13C NMR
(150 MHz, CDCl3)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

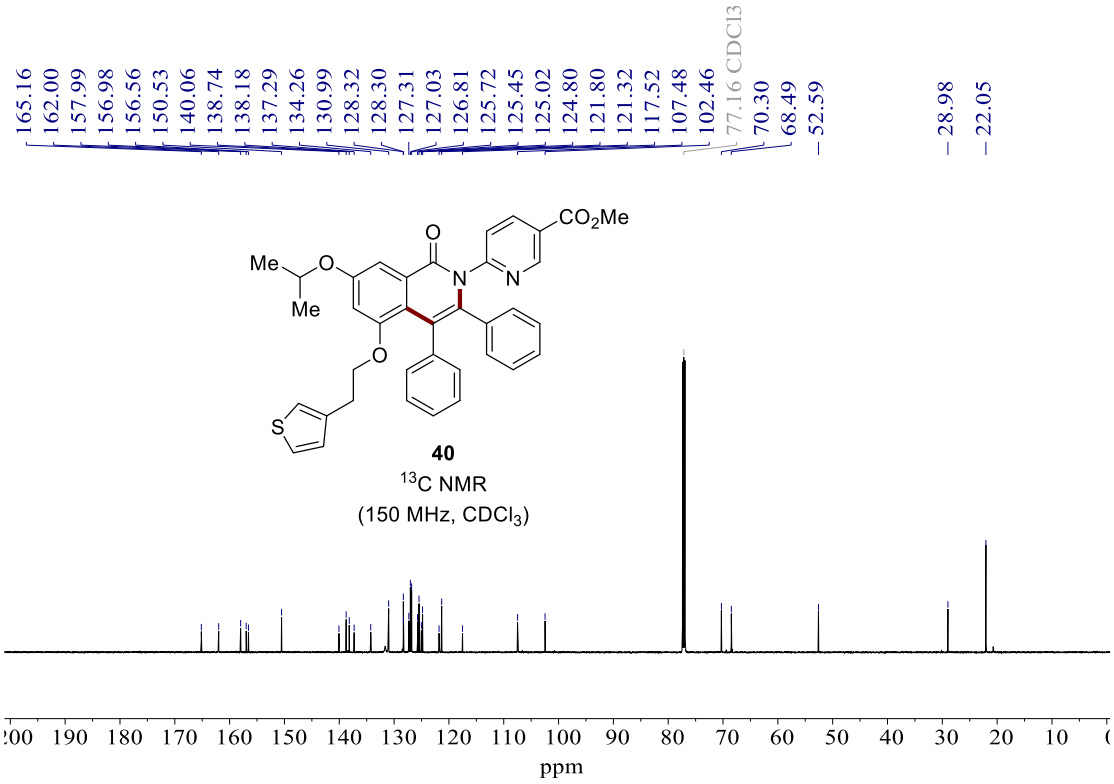

8.61
8.60
8.58
7.79
7.78
7.62
7.61
7.59
7.55
7.54
7.49
7.48
7.45
7.44
7.42
7.39
7.38
7.29
7.29
7.28
7.27
7.26 CDCl3
7.23
7.22
7.20
7.19
7.17
7.16
7.05
7.03
6.93
6.92
6.91
O
N
N
38
1H NMR
(600 MHz, CDCl3)
0.93
0.91
1.00
1.02
1.04
2.01
2.05
1.06
2.04
2.09
3.04
5.07
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm

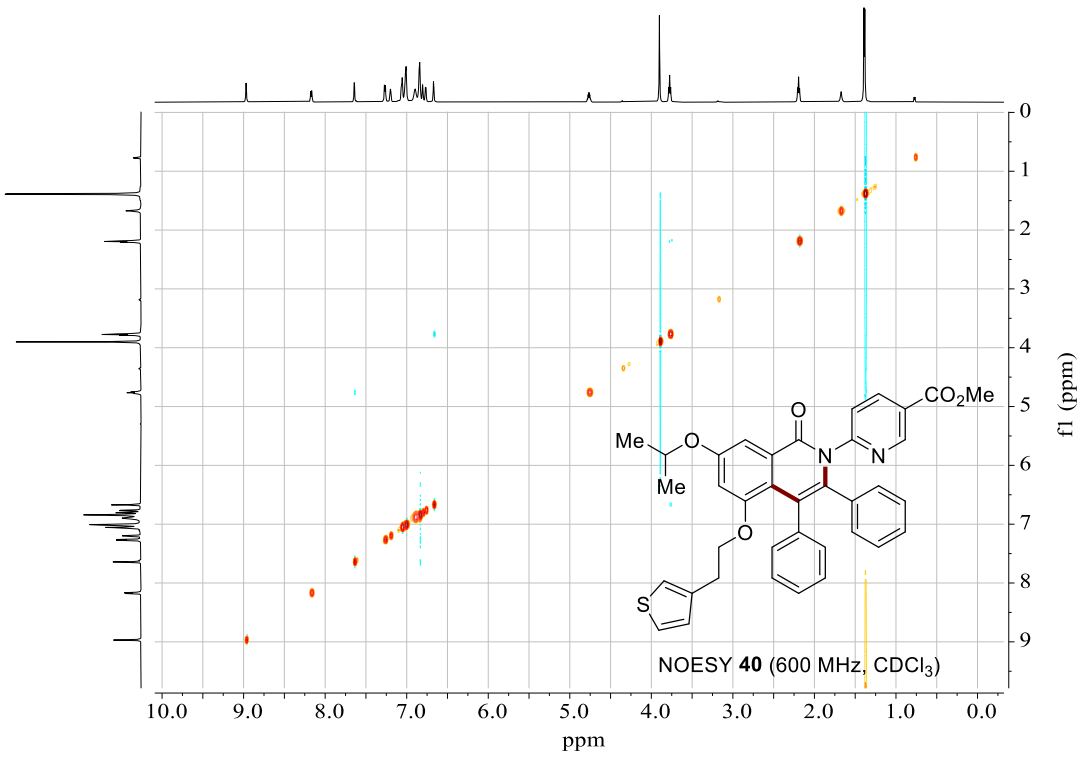

162.91
151.84
147.45
140.24
137.95
137.01
136.22
136.01
135.91
134.46
132.87
131.75
129.16
128.40
128.30
128.14
127.51
127.28
127.25
127.07
125.82
125.66
124.82
119.19
77.16 CDCl3
O
N
N
38
13C NMR
(150 MHz, CDCl3)
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

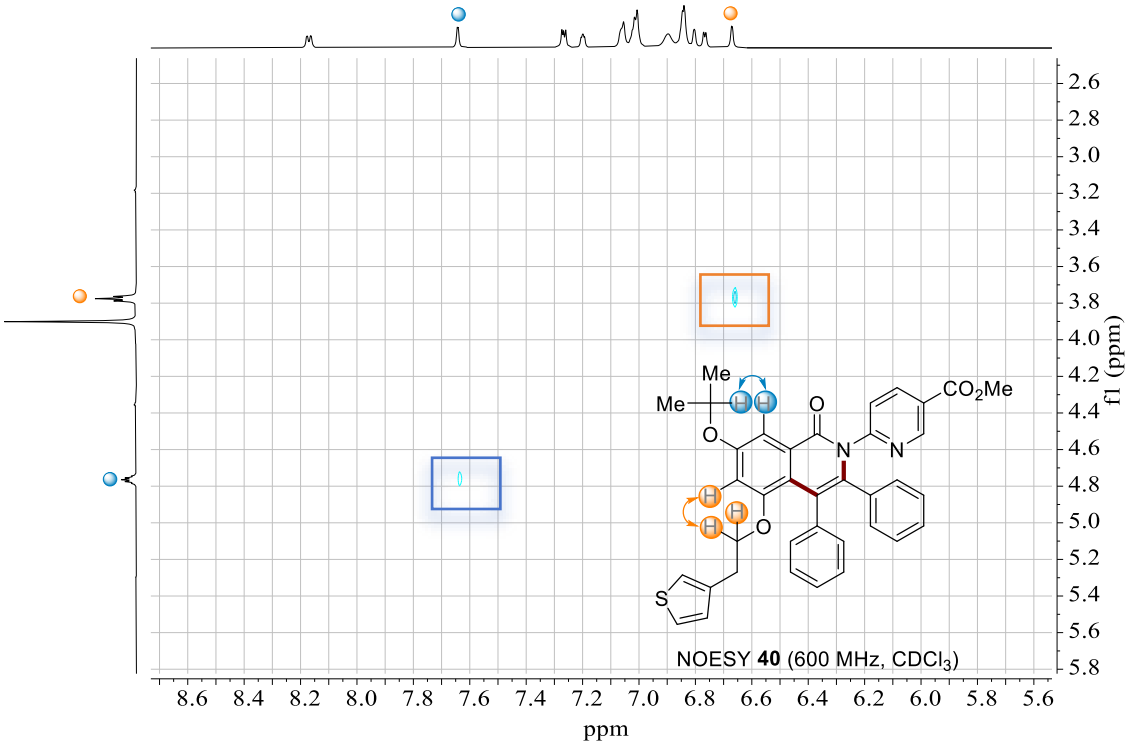

8.58
8.57
8.07
8.06
7.92
7.91
7.73
7.72
7.64
7.63
7.62
7.61
7.59
7.55
7.54
7.52
7.51
7.49
7.48
7.38
7.37
7.29
7.28
7.26 CDCl3
7.23
7.22
7.19
7.18
7.09
7.04
6.93
6.92
6.81
6.80
6.79
6.76
6.75
6.74
O
N
N
39
1H NMR
(600 MHz, CDCl3)
0.98
1.00
1.00
1.00
2.07
1.02
1.02
1.02
1.03
2.03
2.97
1.97
2.04
1.01
10.0 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
ppm

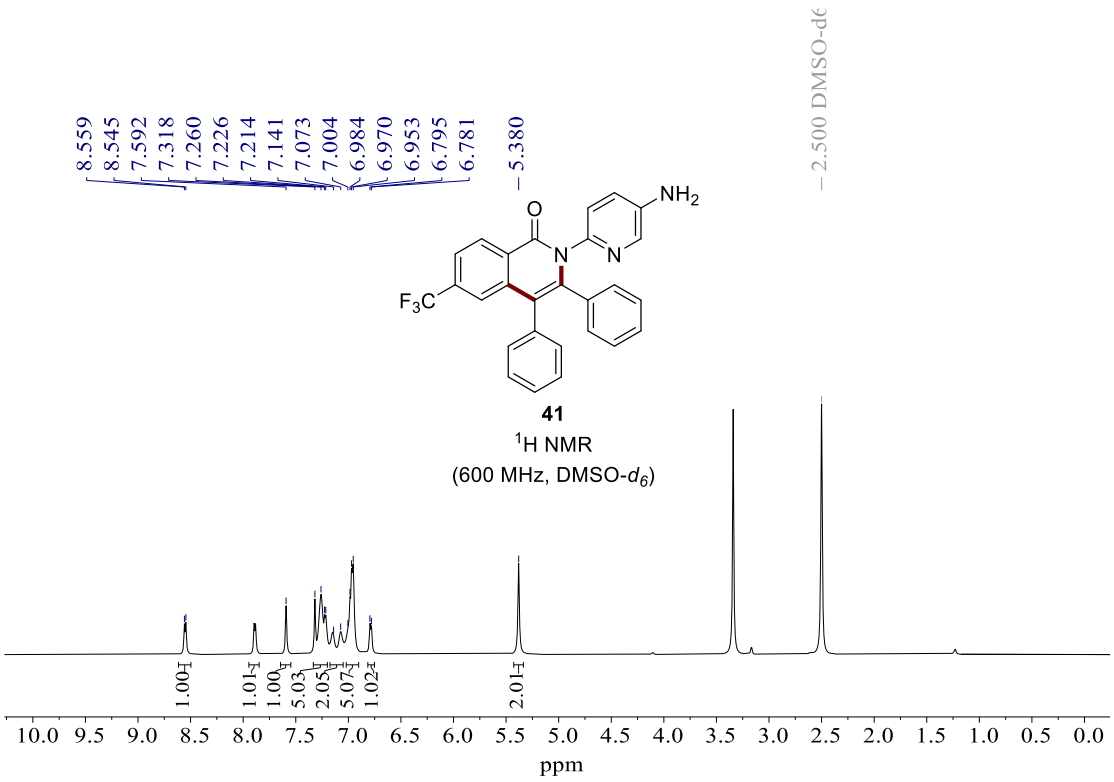

162.97
152.32
147.20
140.16
138.04
137.88
136.21
134.34
132.90
131.76
129.83
129.15
128.22
128.13
127.50
127.43
127.25
127.11
127.09
127.07
125.84
125.75
122.52
119.37
77.16 CDCl3
O
N
N
39
13C NMR
(150 MHz, CDCl3)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

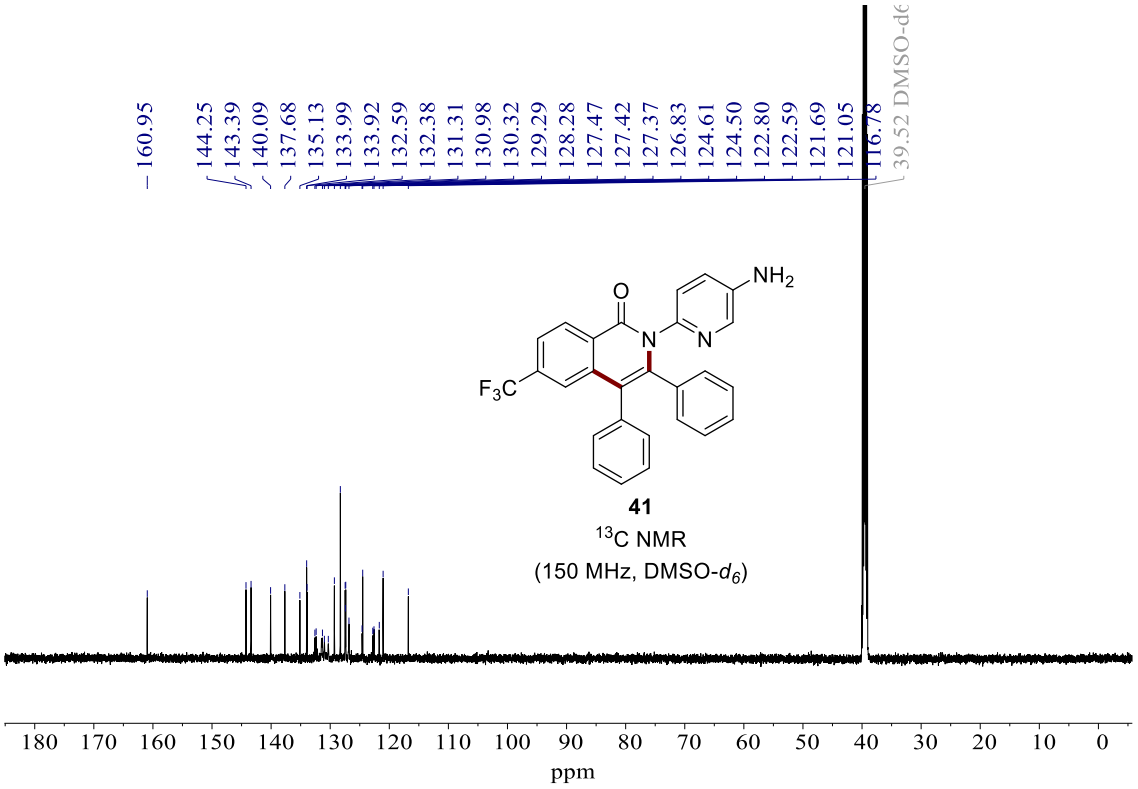

8.97 8.97 8.18 8.17 8.16 7.64 7.64 7.27 7.27 7.26 CDCl3 7.20 7.20 7.07 7.06 7.06 7.05 7.02 7.02 7.01 7.00 6.90 6.85 6.85 6.84 6.84 6.81 6.80 6.77 6.76 6.67 6.67 3.90 3.79 3.78 3.76 2.21 2.19 2.18 1.39 1.38
CO2Me
O
Me
O
N
N
Me
O
S
40
1H NMR
(600 MHz, CDCl3)
0.94 0.98 1.10 0.91 0.97 2.02 3.12 2.02 3.13 1.04 1.03 1.09 1.10 3.19 2.10 2.10 6.05
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
ppm

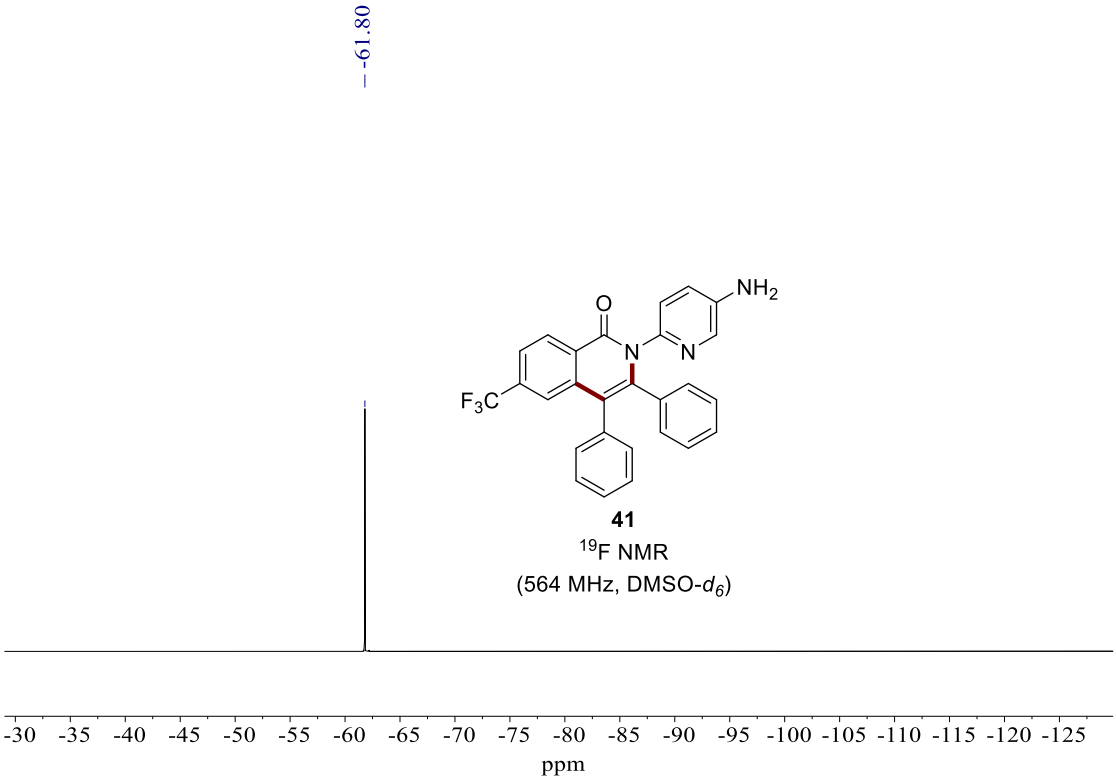

165.16 162.00 157.99 156.98 156.56 150.53 140.06 138.74 138.18 137.29 134.26 130.99 128.32 128.30 127.31 127.03 126.81 125.72 125.45 125.02 124.80 121.80 121.32 117.52 107.48 102.46 77.16 CDCl3 70.30 68.49 52.59 28.98 22.05
CO2Me
O
Me
O
N
N
Me
O
S
40
13C NMR
(150 MHz, CDCl3)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm

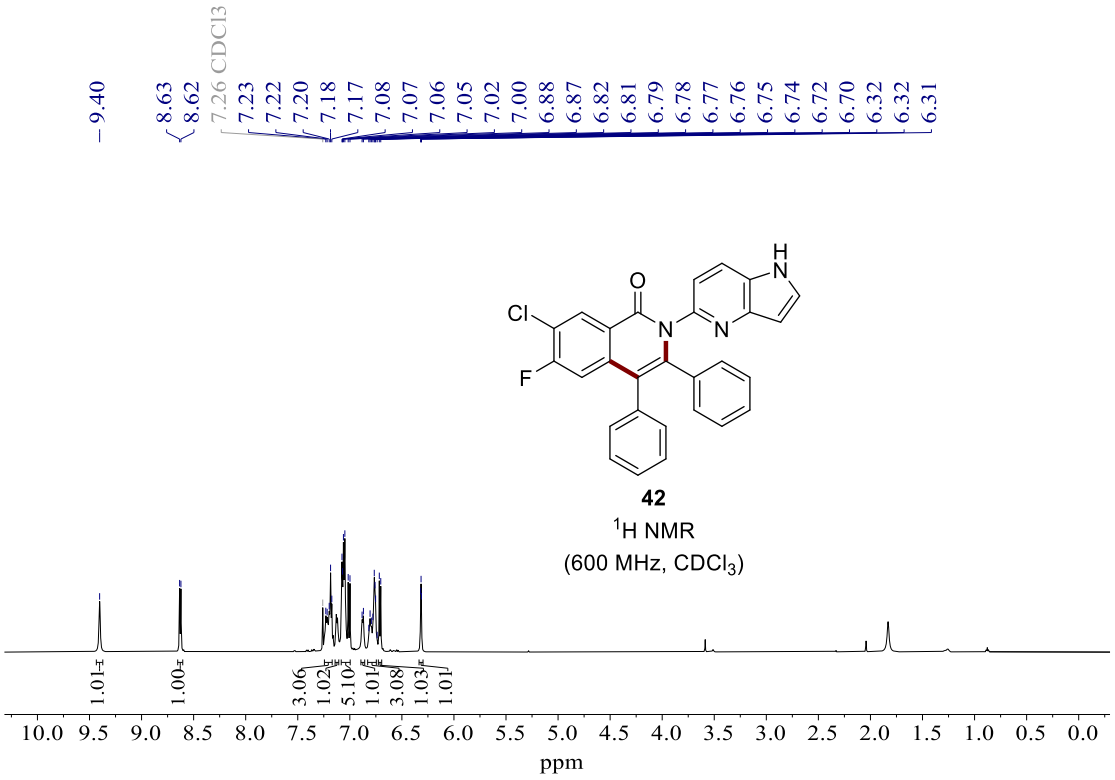

NOESY 40 (600 MHz, CDCl3)
ppm
f1 (ppm)
Me
Me
O
O
O
N
N
CO2Me
S

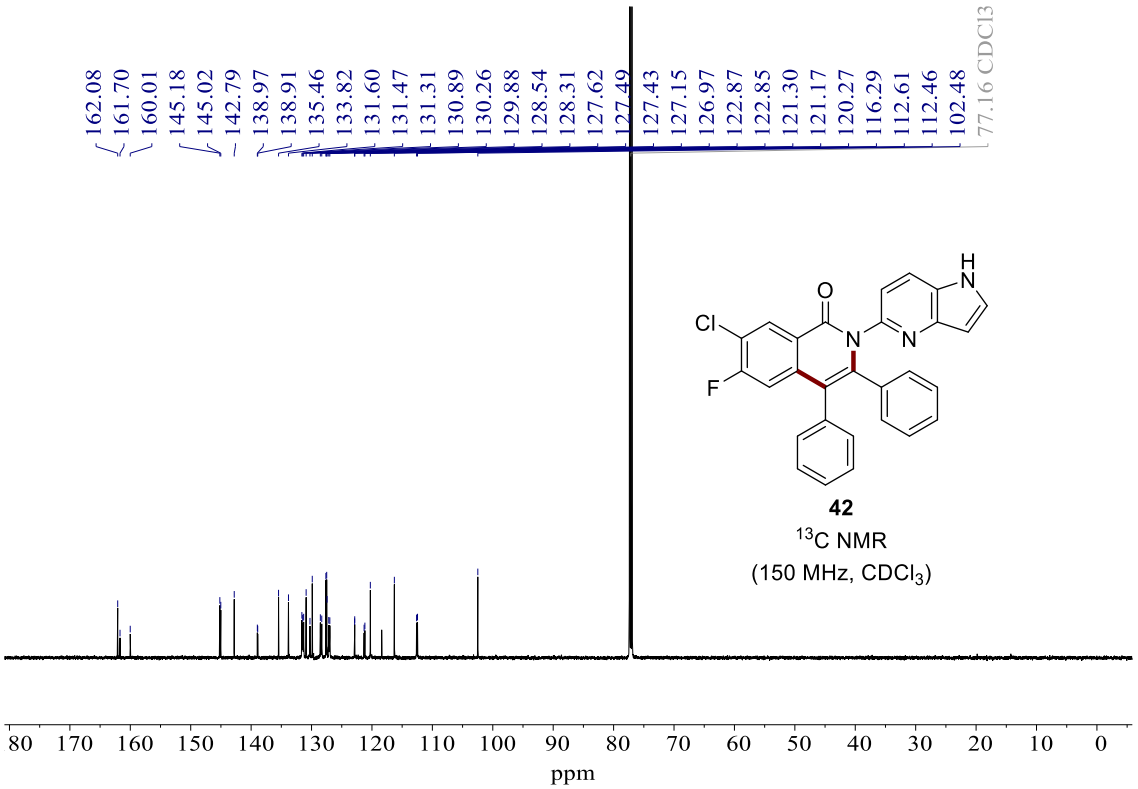

NOESY 40 (600 MHz, CDCl3)
ppm
f1 (ppm)
Me
Me
O
O
O
N
N
CO2Me
S

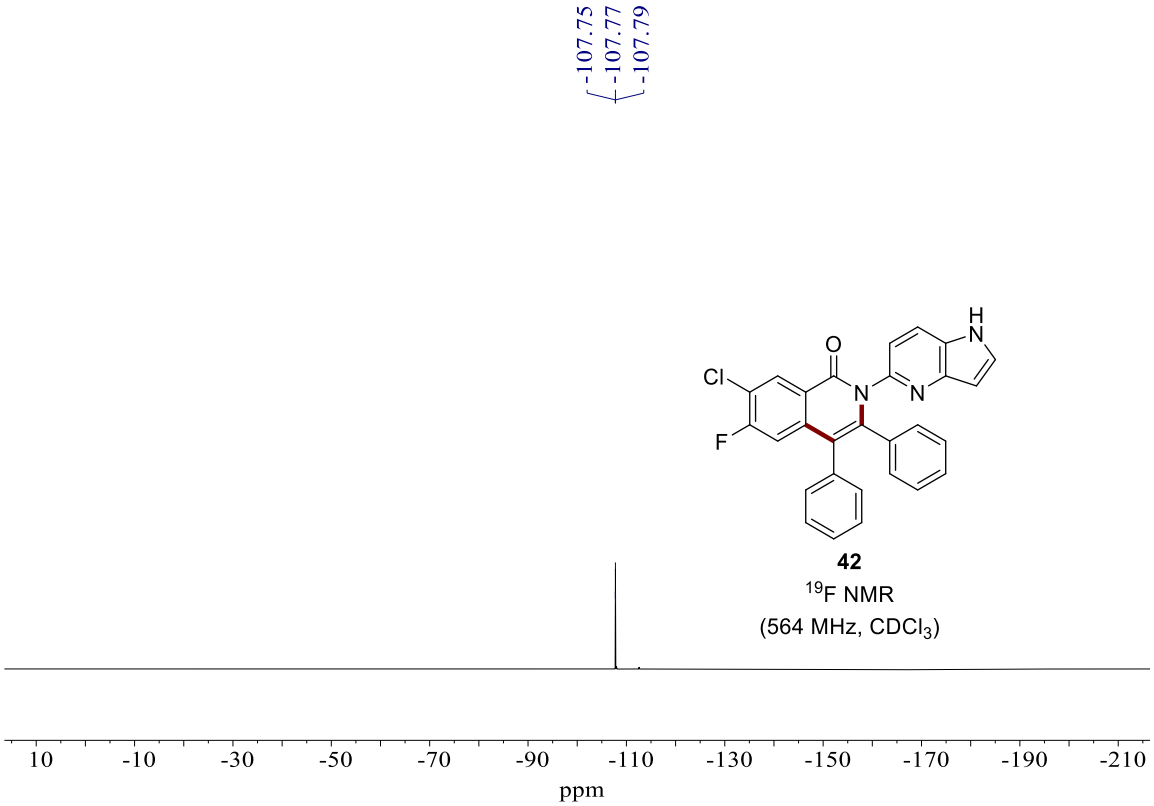

8.559
8.545
7.592
7.318
7.260
7.226
7.214
7.141
7.073
7.004
6.984
6.970
6.953
6.795
6.781
5.380
2.500 DMSO-d6
NH2
O
N
N
F3C
41
1H NMR
(600 MHz, DMSO-d6)
1.00
1.01
1.00
5.03
2.05
5.07
1.02
2.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm

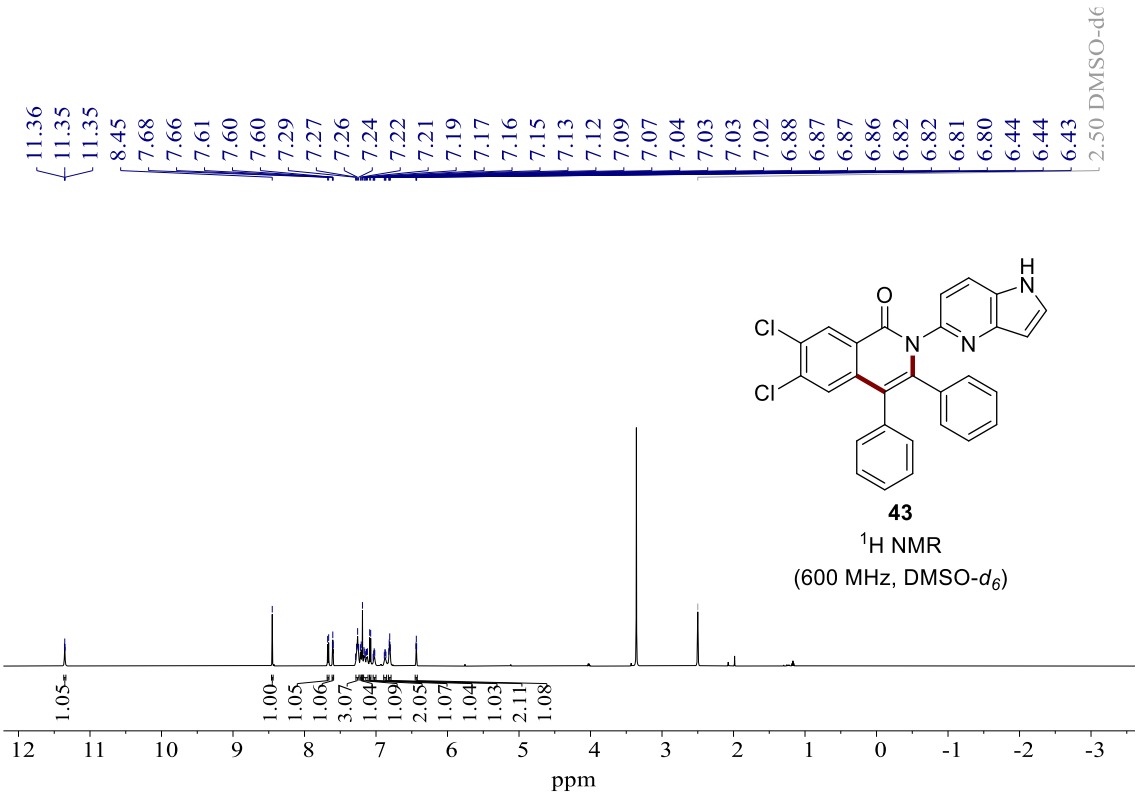

160.95
144.25
143.39
140.09
137.68
135.13
133.99
133.92
132.59
132.38
131.31
130.98
130.32
129.29
128.28
127.47
127.42
127.37
126.83
124.61
124.50
122.80
122.59
121.69
121.05
116.78
39.52 DMSO-d6
NH2
O
N
N
F3C
41
13C NMR
(150 MHz, DMSO-d6)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

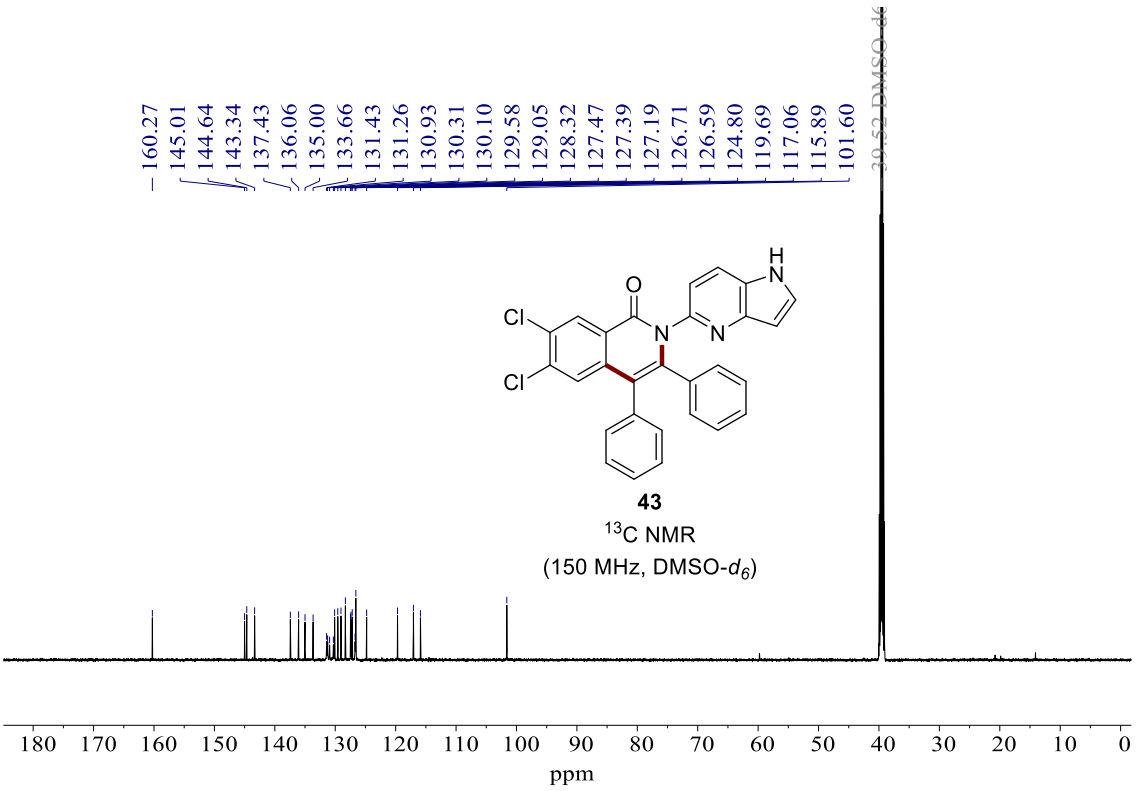

-61.80
O
N
N
NH2
F3C
41
19F NMR
(564 MHz, DMSO-d6)
-30 -35 -40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125
ppm

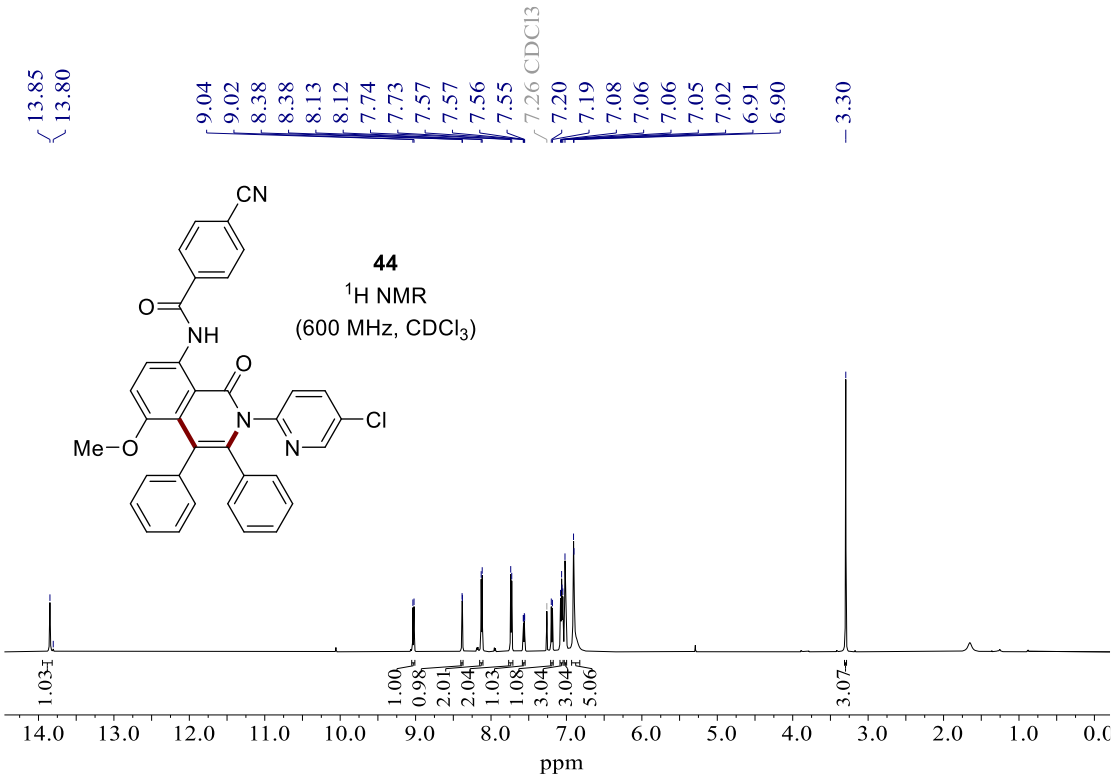

9.40
8.63
8.62
7.26 CDCl3
7.23
7.22
7.20
7.18
7.17
7.08
7.07
7.06
7.05
7.02
7.00
6.88
6.87
6.82
6.81
6.79
6.78
6.77
6.76
6.75
6.74
6.72
6.70
6.32
6.32
6.31
O
N
N
H
N
Cl
F
42
1H NMR
(600 MHz, CDCl3)
1.01
1.00
3.06
1.02
5.10
1.01
3.08
1.03
1.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm

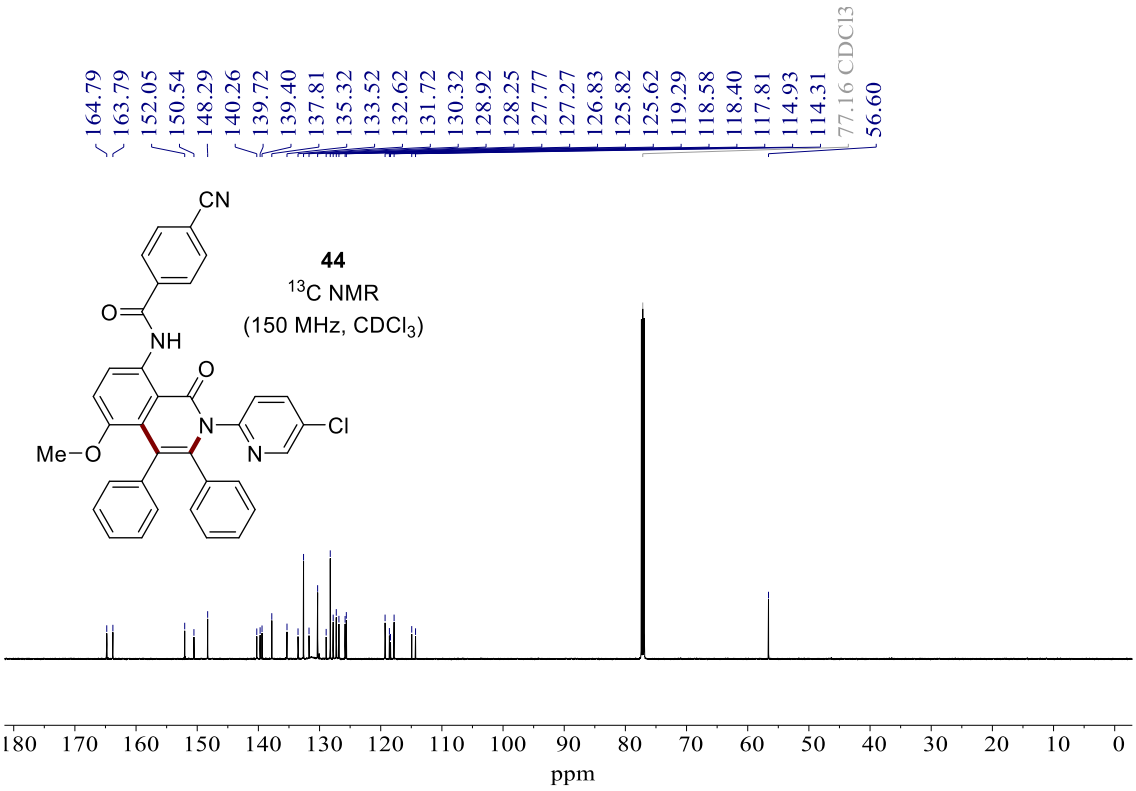

162.08
161.70
160.01
145.18
145.02
142.79
138.97
138.91
135.46
133.82
131.60
131.47
131.31
130.89
130.26
129.88
128.54
128.31
127.62
127.49
127.43
127.15
126.97
122.87
122.85
121.30
121.17
120.27
116.29
112.61
112.46
102.48
77.16 CDCl3
Cl
F
O
N
N
H
N
42
13C NMR
(150 MHz, CDCl3)
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

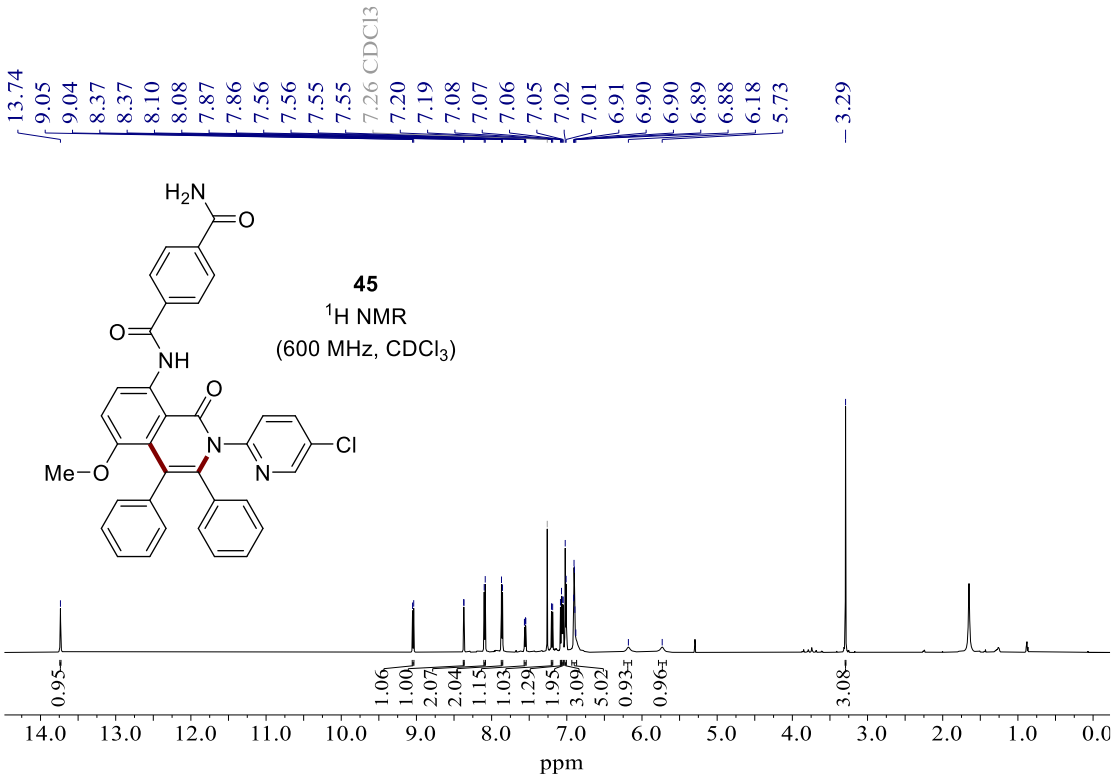

-107.75
-107.77
-107.79
Cl
F
O
N
N
H
N
42
19F NMR
(564 MHz, CDCl3)
10 -10 -30 -50 -70 -90 -110 -130 -150 -170 -190 -210
ppm

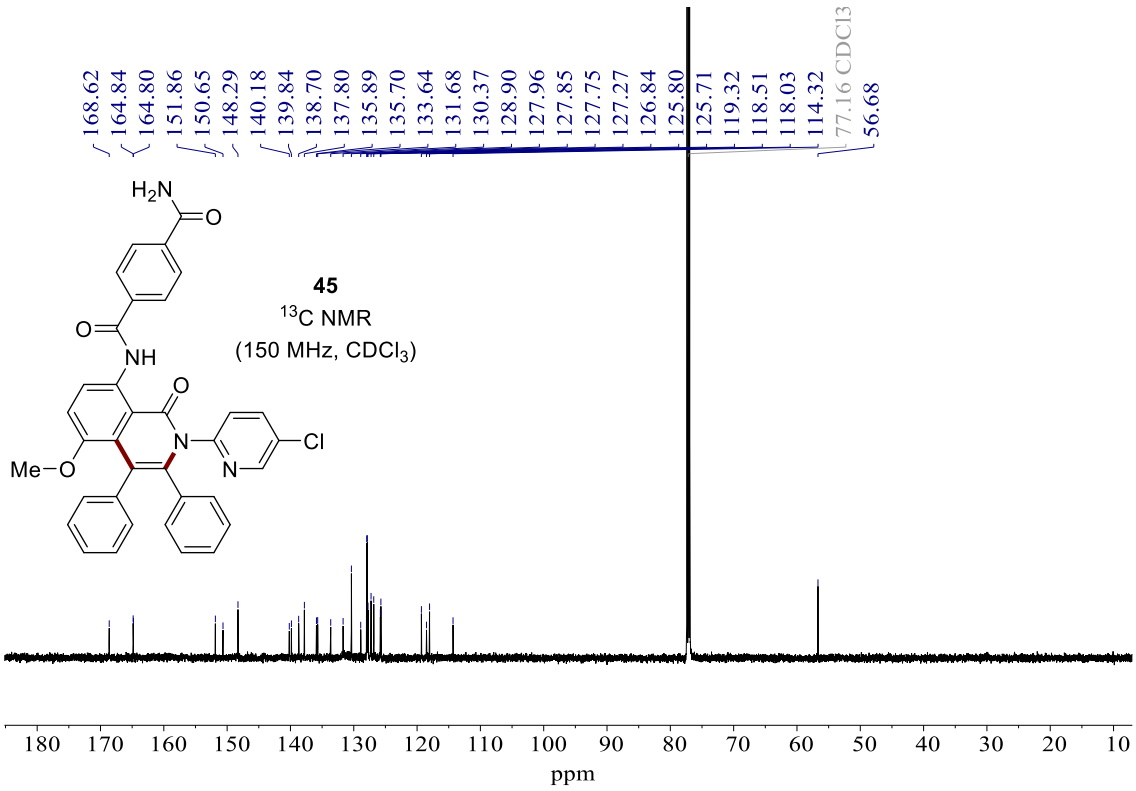

11.36
11.35
11.35
8.45
7.68
7.66
7.61
7.60
7.60
7.29
7.27
7.26
7.24
7.22
7.21
7.19
7.17
7.16
7.15
7.13
7.12
7.09
7.07
7.04
7.03
7.03
7.02
6.88
6.87
6.87
6.86
6.82
6.82
6.81
6.80
6.44
6.44
6.43
2.50 DMSO-d6
Cl
Cl
O
N
N
H
N
43
1H NMR
(600 MHz, DMSO-d6)
1.05
1.00
1.05
1.06
3.07
1.04
1.09
2.05
1.07
1.04
1.03
2.11
1.08
12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
ppm

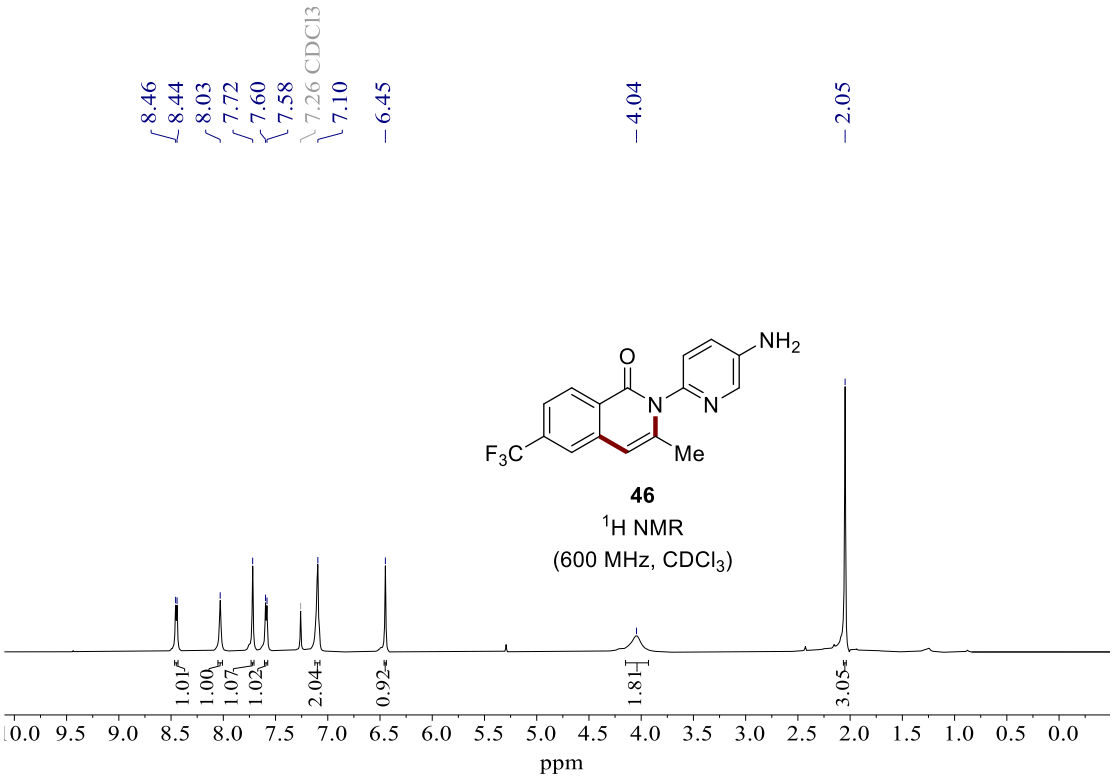

160.27
145.01
144.64
143.34
137.43
136.06
135.00
133.66
131.43
131.26
130.93
130.31
130.10
129.58
129.05
128.32
127.47
127.39
127.19
126.71
126.59
124.80
119.69
117.06
115.89
101.60
39.52 DMSO-d6
Cl
Cl
O
N
N
H
N
43
13C NMR
(150 MHz, DMSO-d6)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm

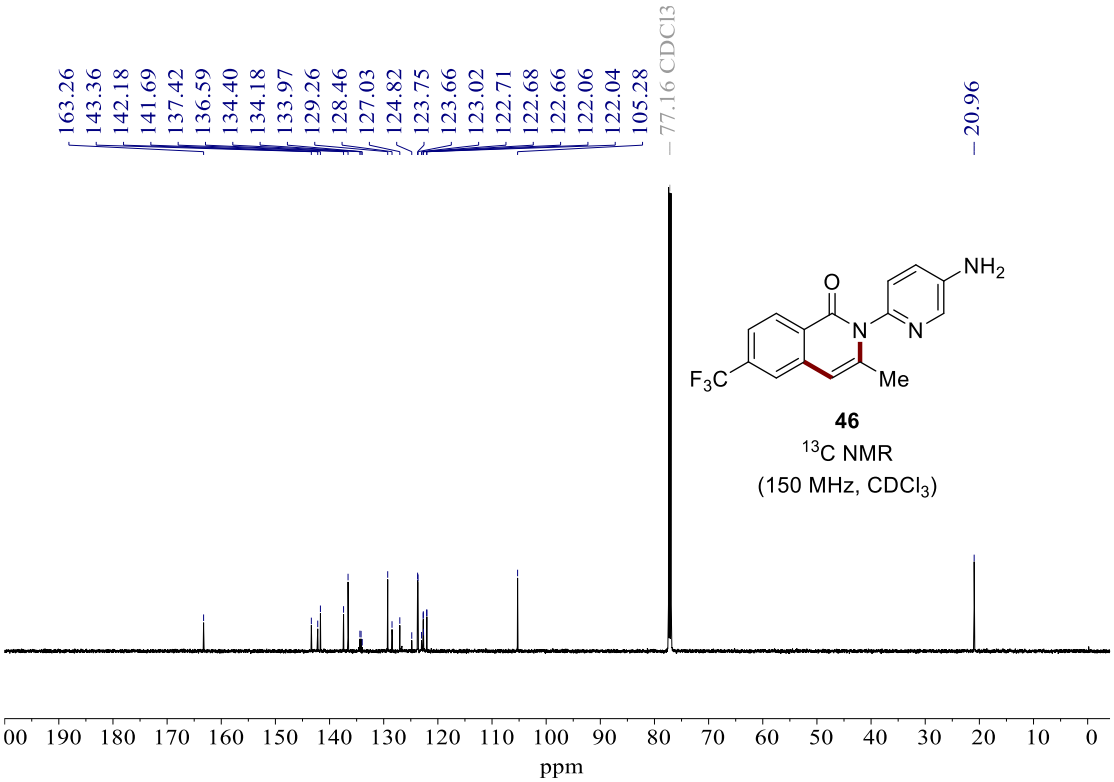

13.85
13.80
9.04
9.02
8.38
8.38
8.13
8.12
7.74
7.73
7.57
7.57
7.56
7.55
7.26 CDCl3
7.20
7.19
7.08
7.06
7.06
7.05
7.02
6.91
6.90
3.30
CN
O
NH
O
N
Cl
Me−O
N
44
1H NMR
(600 MHz, CDCl3)
1.03
1.00
0.98
2.01
2.04
1.03
1.08
3.04
3.04
5.06
3.07
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm

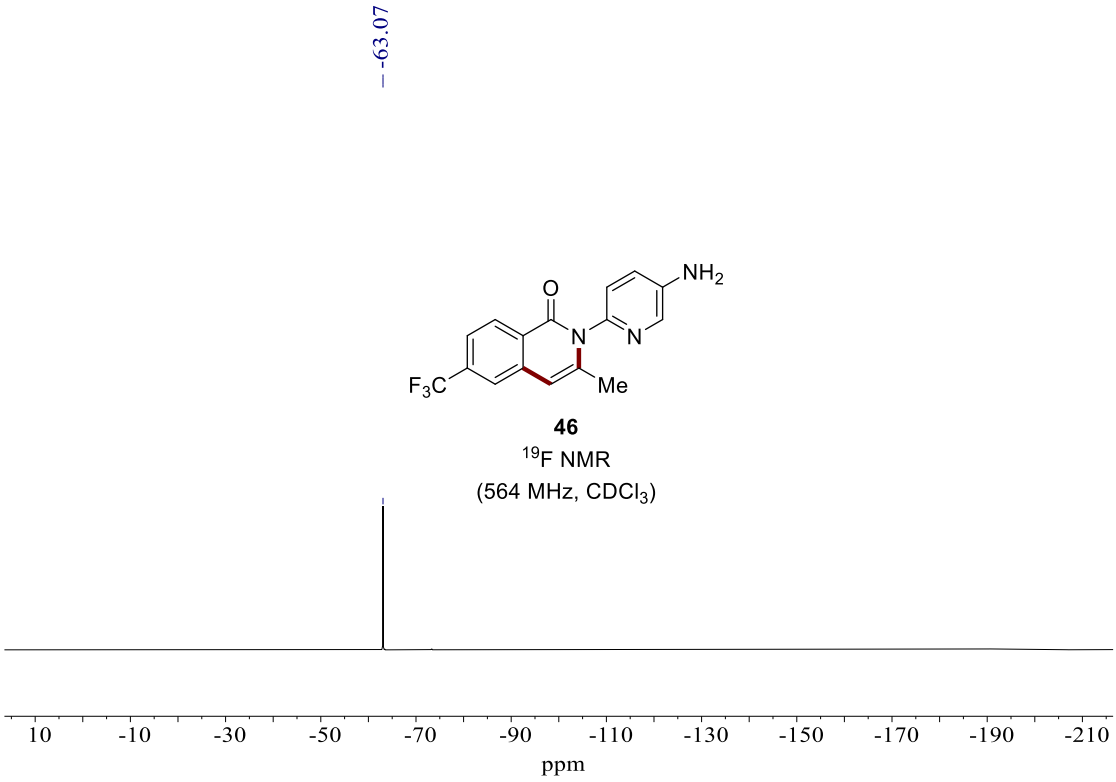

164.79
163.79
152.05
150.54
148.29
140.26
139.72
139.40
137.81
135.32
133.52
132.62
131.72
130.32
128.92
128.25
127.77
127.27
126.83
125.82
125.62
119.29
118.58
118.40
117.81
114.93
114.31
77.16 CDCl3
56.60
CN
O
NH
O
N
Cl
Me−O
N
44
13C NMR
(150 MHz, CDCl3)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


13.74
9.05
9.04
8.37
8.37
8.10
8.08
7.87
7.86
7.56
7.56
7.55
7.55
7.26 CDCl3
7.20
7.19
7.08
7.07
7.06
7.05
7.02
7.01
6.91
6.90
6.90
6.89
6.88
6.18
5.73
3.29
H2N
O
O
NH
O
N
Cl
Me−O
N
45
1H NMR
(600 MHz, CDCl3)
0.95
1.06
1.00
2.07
2.04
1.15
1.03
1.29
1.95
3.09
5.02
0.93
0.96
3.08
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm


168.62
164.84
164.80
151.86
150.65
148.29
140.18
139.84
138.70
137.80
135.89
135.70
133.64
131.68
130.37
128.90
127.96
127.85
127.75
127.27
126.84
125.80
125.71
119.32
118.51
118.03
114.32
77.16 CDCl3
56.68
H2N
O
O
NH
O
N
Cl
Me−O
N
45
13C NMR
(150 MHz, CDCl3)
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


8.46
8.44
8.03
7.72
7.60
7.58
7.26 CDCl3
7.10
6.45
4.04
2.05
NH2
O
N
N
F3C
Me
46
1H NMR
(600 MHz, CDCl3)
1.01
1.00
1.07
1.02
2.04
0.92
1.81
3.05
ppm

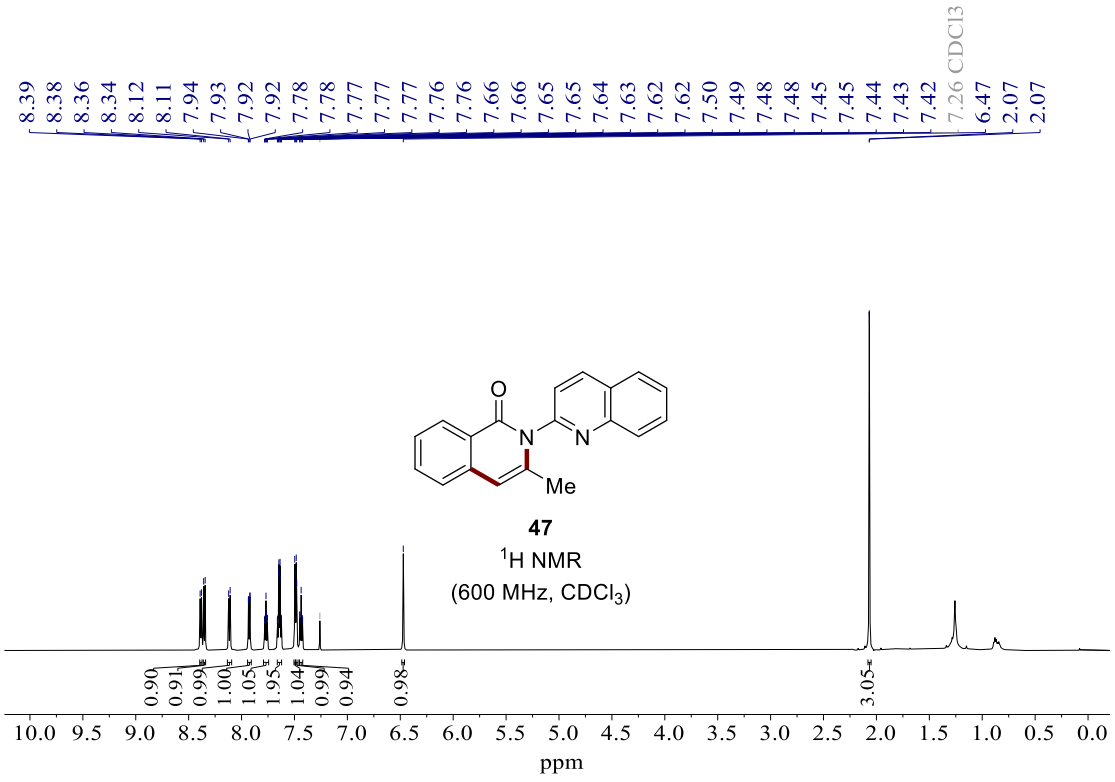

163.26
143.36
142.18
141.69
137.42
136.59
134.40
134.18
133.97
129.26
128.46
127.03
124.82
123.75
123.66
123.02
122.71
122.68
122.66
122.06
122.04
105.28
77.16 CDCl3
20.96
NH2
O
N
N
F3C
Me
46
13C NMR
(150 MHz, CDCl3)
ppm



46

^{19}F NMR

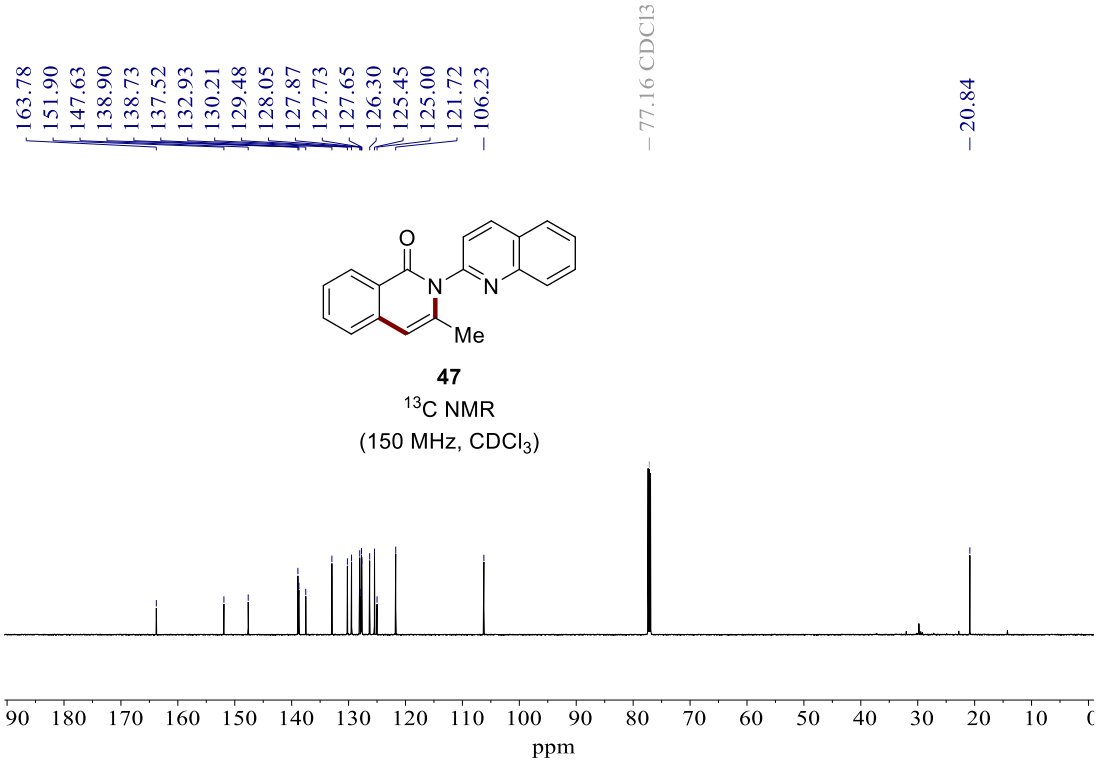
(564 MHz, $CDCl_3$)

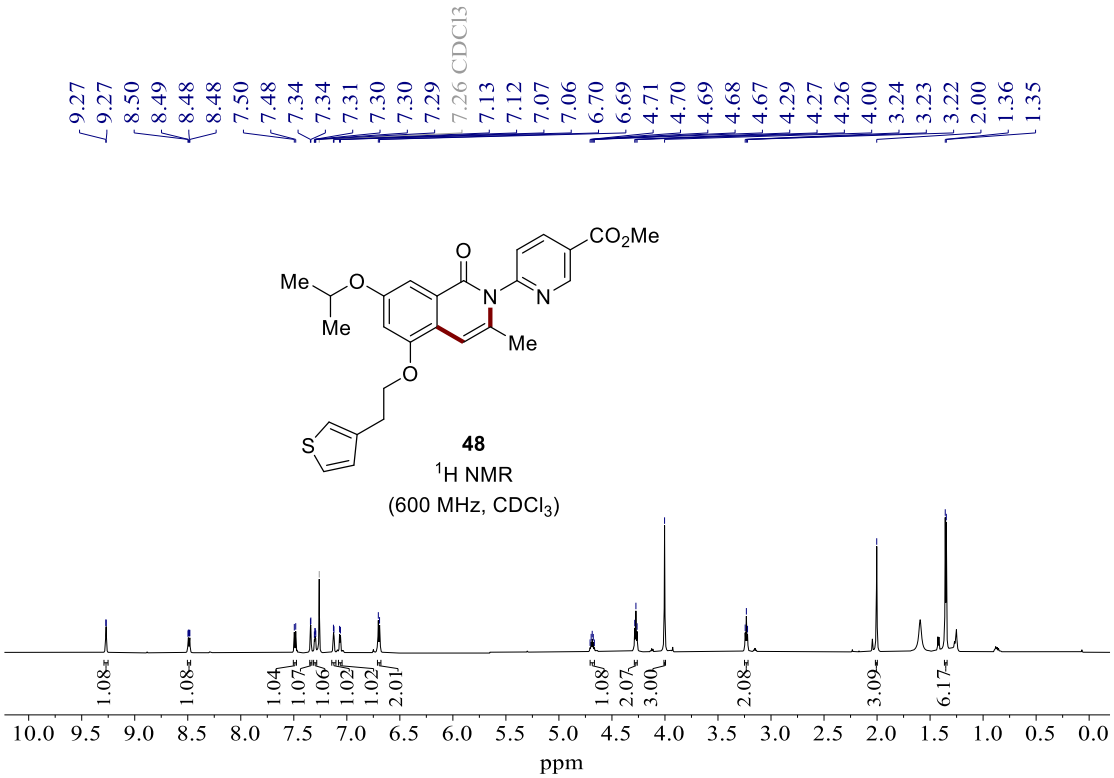


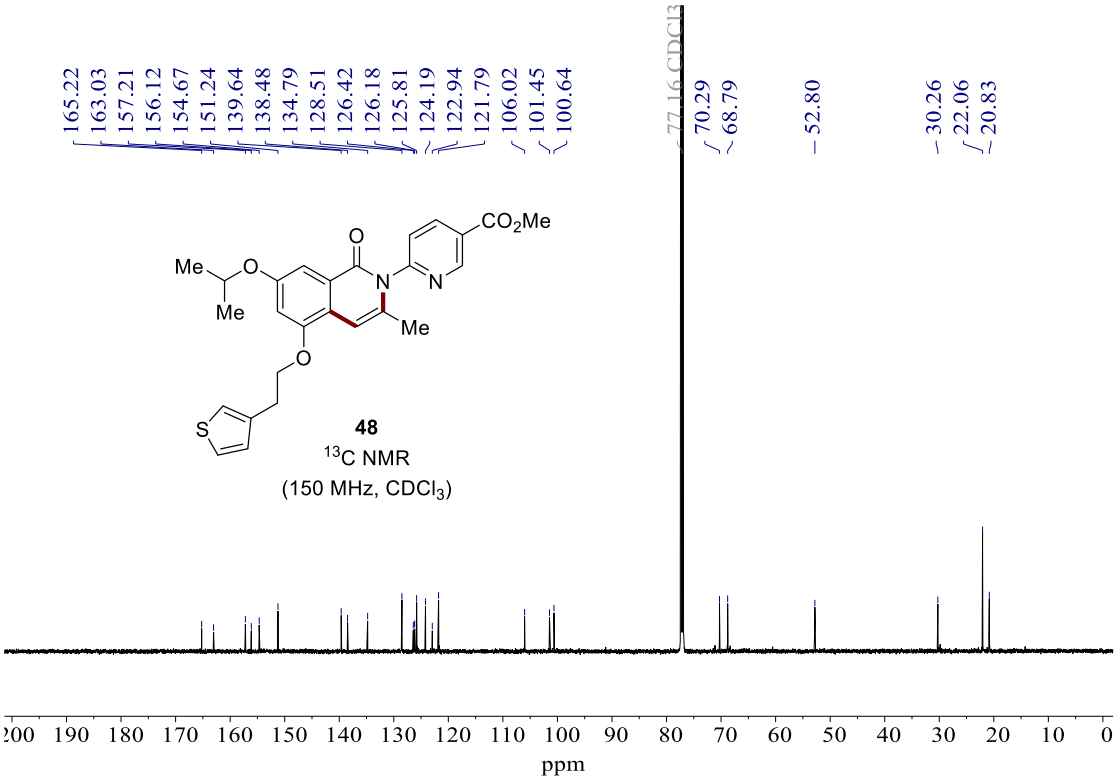
47

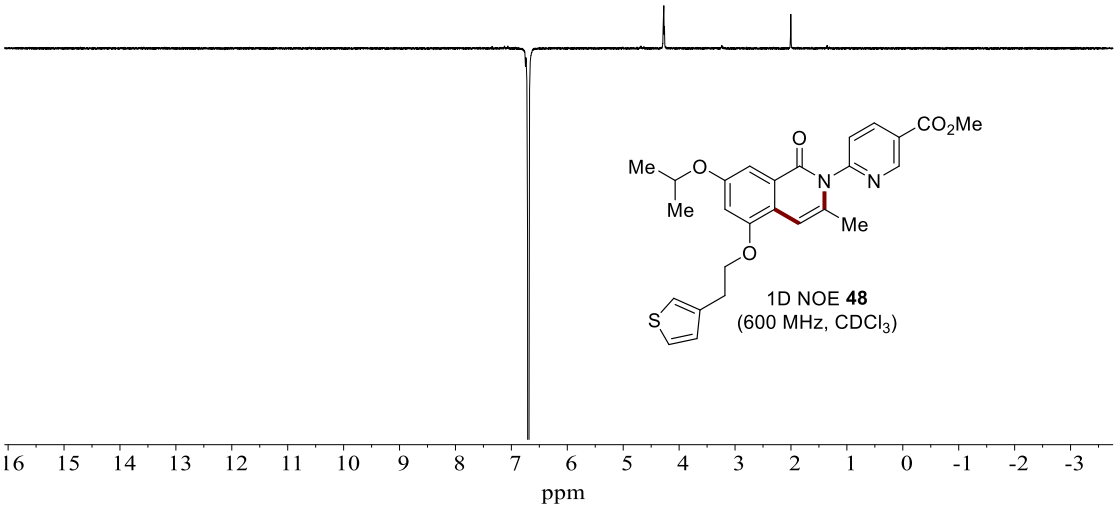
^{1}H NMR

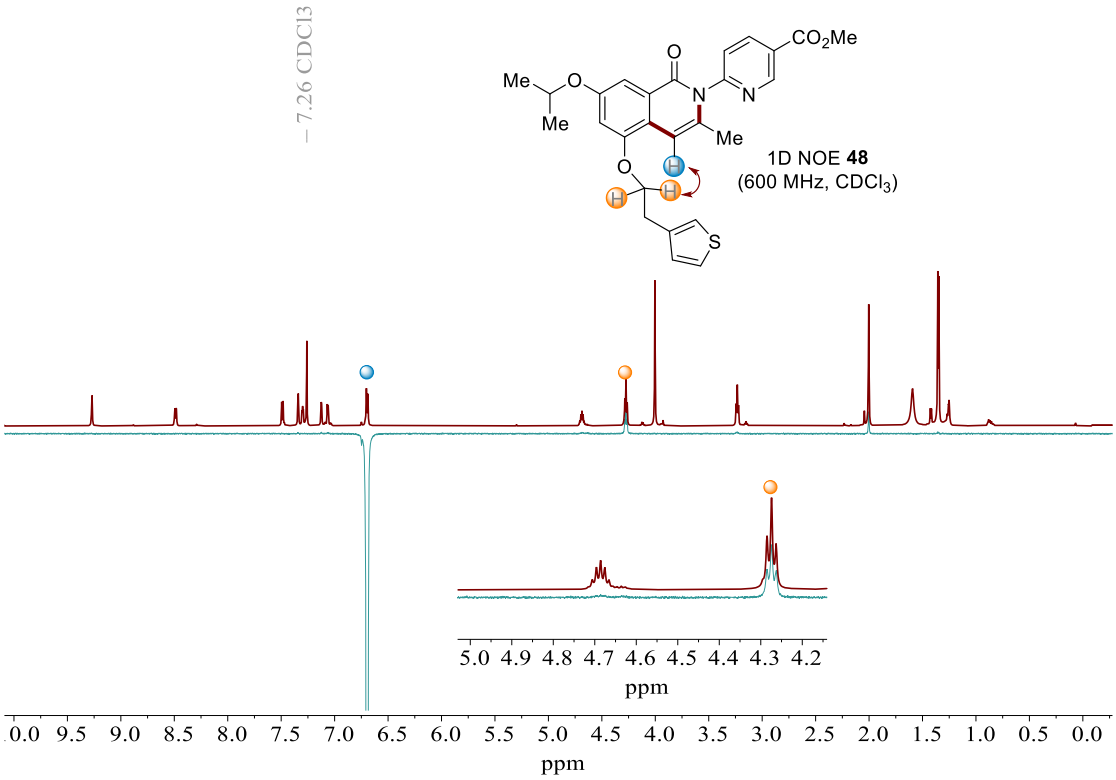
(600 MHz, $CDCl_3$)

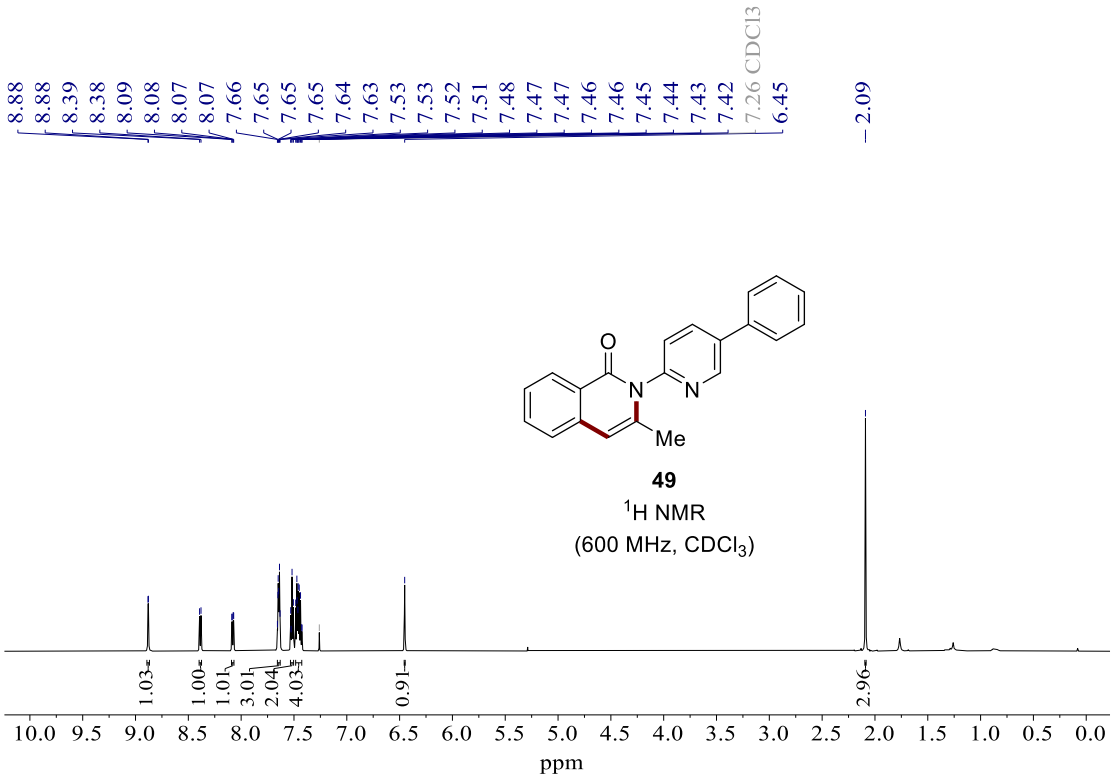

163.78
151.90
147.63
138.90
138.73
137.52
132.93
130.21
129.48
128.05
127.87
127.73
127.65
126.30
125.45
125.00
121.72
106.23
77.16 CDCl3
20.84
O
N
N
Me
47
13C NMR
(150 MHz, CDCl3)
90 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
ppm

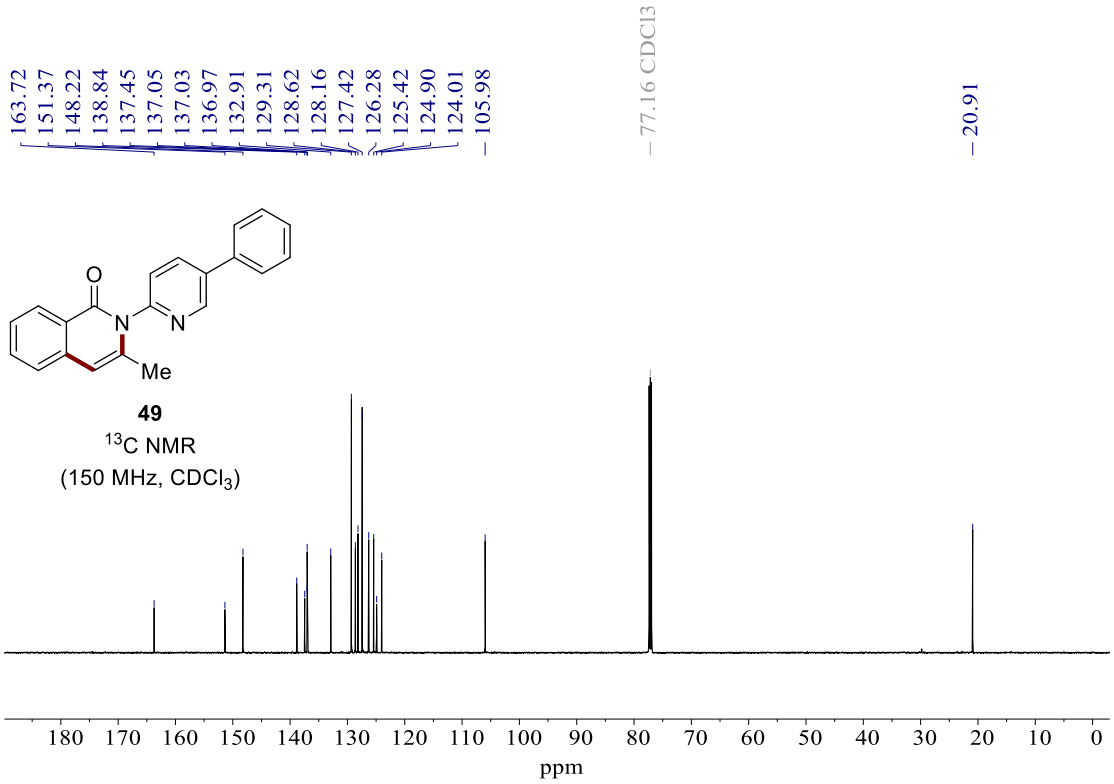

9.27
9.27
8.50
8.49
8.48
8.48
7.50
7.48
7.34
7.34
7.31
7.30
7.30
7.29
7.26 CDCl3
7.13
7.12
7.07
7.06
6.70
6.69
4.71
4.70
4.69
4.68
4.67
4.29
4.27
4.26
4.00
3.24
3.23
3.22
2.00
1.36
1.35
CO2Me
O
Me
O
Me
N
N
Me
O
S
48
1H NMR
(600 MHz, CDCl3)
1.08
1.08
1.04
1.07
1.06
1.02
1.02
2.01
1.08
2.07
3.00
2.08
3.09
6.17
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
ppm


165.22
163.03
157.21
156.12
154.67
151.24
139.64
138.48
134.79
128.51
126.42
126.18
125.81
124.19
122.94
121.79
106.02
101.45
100.64
77.16 CDCl3
70.29
68.79
52.80
30.26
22.06
20.83
CO2Me
O
N
N
Me
O
Me
Me
O
S
48
13C NMR
(150 MHz, CDCl3)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm


CO2Me
O
N
N
Me
O
Me
Me
O
S
1D NOE 48
(600 MHz, CDCl3)
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
ppm


7.26 CDCl3
CO2Me
Me
O
Me
N
N
Me
O
S
1D NOE 48
(600 MHz, CDCl3)
5.0 4.9 4.8 4.7 4.6 4.5 4.4 4.3 4.2
ppm
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
ppm


8.88
8.88
8.39
8.38
8.09
8.08
8.07
8.07
7.66
7.65
7.65
7.65
7.64
7.63
7.53
7.53
7.52
7.51
7.48
7.47
7.47
7.46
7.46
7.45
7.44
7.43
7.42
7.26 CDCl3
6.45
2.09
O
N
N
Me
49
1H NMR
(600 MHz, CDCl3)
1.03
1.00
1.01
3.01
2.04
4.03
0.91
2.96
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
ppm


163.72
151.37
148.22
138.84
137.45
137.05
137.03
136.97
132.91
129.31
128.62
128.16
127.42
126.28
125.42
124.90
124.01
105.98
77.16 CDCl3
20.91
O
N
N
Me
49
13C NMR
(150 MHz, CDCl3)
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
ppm