Supporting Information

Rh-catalyzed [3+3]-annulation of quinolines with cyclopropenones: access to functionalized 2-quinolones

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General Information. Quinolines, $AgSbF_6$ (99%), $AgNTf_2$ (97%), Ag_2O (99%), AgOAc (≥99.9%), $AgBF_4$ (98%), Ag_2CO_3 (99%), Cu_2O ((≥99.9%), $Cu(OAc)_2$ (98%) and *m*-CPBA (≥77%) of Aldrich used as received. $[RhCp^*Cl_2]_2$ (98%) of BLD Pharma used as received. Quinoline N-oxides[1] and cyclopropenones[2] were prepared according to the reported procedure. SRL silica gel G/GF 254 plates were used for analytical TLC and SRL silica gel (100-200 mesh) was used for column chromatography while compound spots were visualized using UV lamp (254 nm) and iodine. NMR (^1H, ^{13}C, ^{19}F and NOESY) spectra were recorded with Bruker Ascend 400, 500 and 600 MHz spectrometers using $CDCl_3$ as solvent and TMS as an internal standard. Chemical shifts (δ) and spin-spin coupling constant (*J*) are reported in ppm and in Hz, respectively, and other data are reported as mentioned: s = singlet, d = doublet, t = triplet, m = multiplet. HRMS was recorded with a quadrupole time-of-flight electrospray ionization (ESI) mass spectrometer (Agilent6546). Perkin Elmer FT-IR spectrometer was used to record IR spectra. Melting points were determined using a Büchi B-540 apparatus and are uncorrected. Single crystal X-ray data was collected on a Bruker SMART APEX equipped with a CCD area detector using Mo/Kα radiation and the structure was solved by direct method using SHELXL-19 (Göttingen, Germany).

Sample Preparation for Crystal Growth

The compounds **3aa** and **6** were separately dissolved in a minimum volume of acetonitrile and kept at room temperature for slow evaporation for 2 days. The crystals were subjected to *X*-ray diffraction.

Crystal Data and Structure Refinement for 3aa

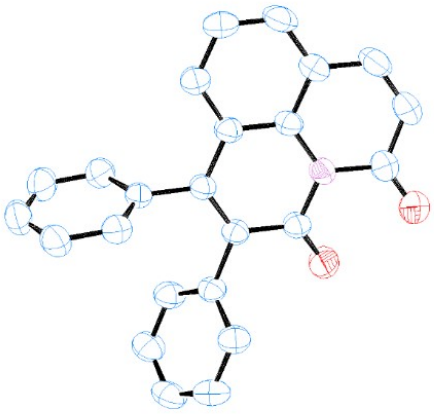


Figure S1. ORTEP diagram of **3aa** with 50% ellipsoid (CCDC 2382651). H-Atoms are omitted for clarity.

Identification code	**3aa**
Empirical formula	'C24 H15 N O2'
Formula weight	349.37
Crystal habit, color	Needle, colorless
Crystal size, mm^3	0.25 x 0.21 x 0.19
Temperature, *T*/K	297 K
Wavelength, λ/Å	0.71073
Crystal system	'Monoclinic'
Space group	' P 21/n'
Unit cell dimensions	a = 9.3265 (7) Å b = 16.1716 (11) Å c = 11.8420 (8) Å α = 90 β = 92.342 (2) γ = 90
Volume, *V*/$Å^3$	1784.6 (2)
Z	4
Calculated density, g cm^{-3}	1.300
Absorption coefficient, μ/mm^{-1}	0.083
F(000)	728.0
θ range for data collection	2.52 to 25.08°
Limiting indices	$-11 \leq h \leq 11$, $-19 \leq k \leq 19$, $-14 \leq l \leq 14$
Reflection collected / unique	3162/2251
Completeness to θ	99.7%
Absorption correction	None
Max. and min. transmission	0.984 and 0.979
Refinement method	SHELXL-2019/1 (Sheldrick, 2019)
Data / restraints / parameters	3162/0/245
Goodness–of–fit on F^2	1.089
Final *R* indices [*I*>2sigma(*I*)]	R1 = 0.0589, wR2 = 0.1293
R indices (all data)	R1 = 0.0913, wR2 = 0.1553

Crystal Data and Structure Refinement for 6

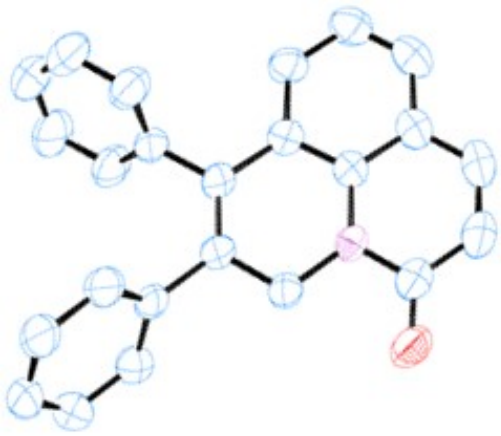
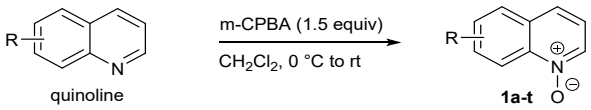


Figure S2. ORTEP diagram of **6** with 50% ellipsoid (CCDC 2382652). H-Atoms are omitted for clarity.

Identification code	**6**
Empirical formula	'C24 H17 N O'
Formula weight	335.38
Crystal habit, color	Block, Colorless
Crystal size, mm^3	0.27 x 0.24 x 0.20
Temperature, *T*/K	295 K
Wavelength, λ/Å	0.71073
Crystal system	'Orthorhombic'
Space group	'P b c a'
Unit cell dimensions	a = 6.9180 (7) Å b = 16.8553 (17) Å c = 29.099 (3) Å α = 90 β = 90 γ = 90
Volume, *V*/$Å^3$	3393.1 (6)
Z	8
Calculated density, g cm^{-3}	1.313
Absorption coefficient, μ/mm^{-1}	0.080
F(000)	1408.0

θ range for data collection	2.52 to 26.39°
Limiting indices	$-8 \le h \le 8$, $-21 \le k \le 21$, $-36 \le l \le 36$
Reflection collected / unique	3429/2109
Completeness to θ	98.3%
Absorption correction	None
Max. and min. transmission	0.984 and 0.979
Refinement method	SHELXL-2019/1 (Sheldrick, 2019)
Data / restraints / parameters	3429/0/244
Goodness–of–fit on F^2	1.110
Final R indices [I>2sigma(I)]	R1 = 0.0591, wR2 = 0.0999
R indices (all data)	R1 = 0.1169, wR2 = 0.1247

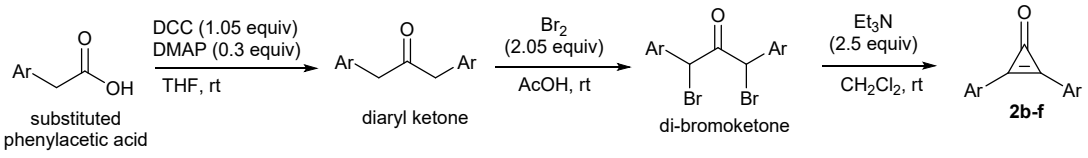
Synthesis of Quinoline *N*-Oxides[1]



To a stirred solution of quinoline (1 mmol) in CH_2Cl_2 (3 mL), *m*-CPBA (1.5 mmol, 259 mg) was added portion-wise at 0 °C and the reaction mixture was allowed to stir overnight at room temperature under air. The reaction mixture was quenched with a saturated aqueous solution of $NaHCO_3$ (10 mL) and extracted with CH_2Cl_2 (3 x 15 mL). Drying (Na_2SO_4) and evaporation of the solvent gave a residue that was purified on silica gel column chromatography to afford desired *N*-oxides **1**.

Quinoline *N*-oxides **1g**, **1j** and **1r-t** are new, whose characterization data are provided. For known quinoline *N*-oxides, ^{1}H NMR data are given to show the purity.

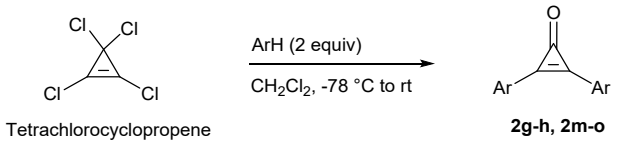
Synthesis of Cyclopropenones[2]



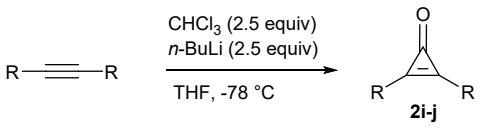
Synthesis of Cyclopropenones 2b-f. Substituted phenylacetic acid (5 mmol) was added to a stirred solution of DCC (5.3 mmol, 1.1 g) and DMAP (1.5 mmol, 183 mg) in THF (10 mL) and

the reaction was allowed to stir for 90 minutes at room temperature. The resultant mixture was passed through a short pad of celite. Evaporation of the solvent gave a residue that was purified by column chromatography to afford diaryl ketone.

Next, the above diaryl ketone (1 mmol) was dissolved in acetic acid (2 mL) and a solution of bromine (2.05 mmol, 106 µL) in acetic acid (1 mL) was added drop wise over a period of 10 minutes and the stirring was continued for 3 h. The reaction mixture was then poured into an ice-cold water, and filtered to get a solid of dibromoketone, which was dissolved in CH_2Cl_2 (5 mL) and stirred at room temperature. A solution of triethylamine (2.5 mmol, 360 µL) in CH_2Cl_2 (5 mL) was added and the stirring was continued for an additional 1 hour. The reaction mixture was then diluted with CH_2Cl_2 (5 mL), washed with 1 N HCl (2 X 5 mL), brine (5 mL) and dried (Na_2SO_4). Evaporation of the solvent gave a residue that was purified on silica gel column chromatography using hexane/ethyl acetate as an eluent to afford cyclopropenones **2b-f**.

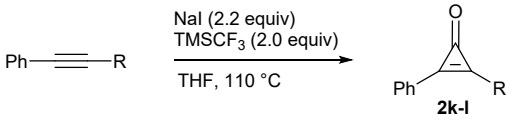


Synthesis of Cyclopropenones 2g-h and 2m-o. To a suspension of tetrachlorocyclopropene (1 mmol, 123 µL) and $AlCl_3$ (1.05 mmol, 140 mg) in CH_2Cl_2 (5 mL) at -78 °C, a solution of substituted benzene (2 mmol) in CH_2Cl_2 (1 mL) was added dropwise over a period of 10 minutes. The resultant mixture was stirred for an additional 15 minutes at the same temperature, then allowed to stir at room temperature for 12 h. After completion (monitored by TLC analysis), water (5 mL) was added and the stirring was continued for an additional 5 minutes. The resultant mixture was extracted using CH_2Cl_2 (2 x 10 mL) and dried (Na_2SO_4). Evaporation of the solvent gave a residue that was purified on silica gel column chromatography using hexane/ethyl acetate as eluent to give cyclopropenones **2g-h** and **2m-o**.



Synthesis of Cyclopropenones 2i-j. To a stirred solution of alkyne (5 mmol) and chloroform (12.5 mmol, 1 mL)) in THF (10 mL), *n*-BuLi (12.5 mmol, 6.5 mL of 2M solution in cyclohexane) was added dropwise over a period of 10 minutes at -78 °C under nitrogen atmosphere. The resultant mixture was stirred at -78 °C for an additional 4 h. Then, conc. HCl

(5 mL) was added dropwise over a period of 10 minutes and the resultant mixture was allowed to stir at room temperature for 10 minutes. The reaction mixture was then quenched with water (10 mL) and extracted using CH_2Cl_2 (3 x 20 mL). Drying (Na_2SO_4) and evaporation of the solvent gave a residue that was purified on silica gel column chromatography using ethyl acetate and methanol as eluent to afford cyclopropenones **2i-j**.



2k-l

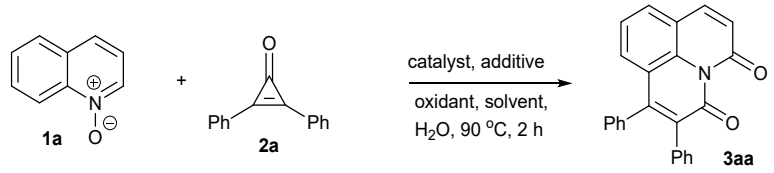
Synthesis of Cyclopropenones 2k-l. Alkyne (5 mmol), trifluoromethyltrimethylsilane (10 mmol, 1.5 mL) and NaI (11 mmol, 1.6 g) were stirred in THF (15 mL) at 110 °C for 2 h under nitrogen atmosphere. The reaction mixture was then cooled to room temperature and water (10 mL) was added. The resultant mixture was extracted with CH_2Cl_2 (3 x 20 mL) and dried (Na_2SO_4). Evaporation of the solvent gave a residue that was purified on silica gel column chromatography using hexane/ethyl acetate as an eluent to give cyclopropenones **2k-l**.

The commercial cyclopropenone **2a** was used as received whereas cyclopropenone **2c** and **2o** are new whose characterization data are provided. For other known cyclopropenones, ^{1}H NMR data are given to show the purity.

Procedure for the Rh-Catalyzed Annulation of Quinoline *N*-oxides with Cyclopropenones. In a pressure tube, quinoline *N*-oxide **1** (0.2 mmol), cyclopropenone **2** (0.24 mmol), $[RhCp^*Cl_2]_2$ (0.01 mmol, 6 mg), $AgBF_4$ (0.04 mmol, 8 mg), Ag_2O (0.2 mmol, 46 mg), H_2O (50 µL) and $(CH_2Cl)_2$ (1 mL) were stirred for 2 h at 90 °C under argon atmosphere. Upon completion, the reaction mixture was passed through a short pad of celite using CH_2Cl_2 (20 mL). Evaporation of the solvent gave a residue that was purified on silica gel column chromatography using hexane/ethyl acetate as an eluent to afford the annulated product **3**.

Scale-up Synthesis of 3aa. In a pressure tube, quinoline *N*-oxide **1** (3.44 mmol, 500 mg), cyclopropenone **2** (4.1 mmol, 850 mg), $[RhCp^*Cl_2]_2$ (0.17 mmol, 106 mg), $AgBF_4$ (1.7 mmol, 134.5 mg), Ag_2O (3.4 mmol, 797 mg), H_2O (250 µL) and $(CH_2Cl)_2$ (5 mL) were subjected to the above-described reaction conditions and purification to furnish **3aa** in 61% yield (734 mg).

Table S1. Optimization of Reaction Conditions[a]



entry	catalyst	additive	oxidant	solvent	yield (%)[b]
1	$[RhCp^*Cl_2]_2$	$AgSbF_6$	Ag_2O	$(CH_2Cl)_2$	62
2	$[RhCp^*Cl_2]_2$	$AgNTf_2$	Ag_2O	$(CH_2Cl)_2$	57
3	$[RhCp^*Cl_2]_2$	$AgBF_4$	Ag_2O	TFE	26
4	$[RhCp^*Cl_2]_2$	$AgBF_4$	Ag_2O	MeOH	trace
5	$[RhCp^*Cl_2]_2$	$AgBF_4$	Ag_2O	toluene	55
6	$[RhCp^*Cl_2]_2$	$AgBF_4$	Ag_2O	CH_3CN	42
7	$[RhCp^*Cl_2]_2$	$AgBF_4$	Ag_2O	THF	48
8	$[RhCp^*Cl_2]_2$	$AgBF_4$	Ag_2O	DMF	38
9[c]	$[RhCp^*Cl_2]_2$	$AgBF_4$	Ag_2O	H_2O	n.d.
10[d]	$[RhCp^*Cl_2]_2$	$AgBF_4$	Ag_2O	$(CH_2Cl)_2$	trace
11[e]	$[RhCp^*Cl_2]_2$	$AgBF_4$	Ag_2O	$(CH_2Cl)_2$	65
12	$[RhCp^*Cl_2]_2$	-	-	$(CH_2Cl)_2$	n.d.
13[f]	$[RhCp^*Cl_2]_2$	$AgBF_4$	Ag_2O	$(CH_2Cl)_2$	44
14[g]	$[RhCp^*Cl_2]_2$	$AgBF_4$	Ag_2O	$(CH_2Cl)_2$	66
15[h]	$[RhCp^*Cl_2]_2$	$AgBF_4$	Ag_2O	$(CH_2Cl)_2$	58
16[i]	$[RhCp^*Cl_2]_2$	$AgBF_4$	Ag_2O	$(CH_2Cl)_2$	54
17[j]	$[RhCp^*Cl_2]_2$	$AgBF_4$	Ag_2O	$(CH_2Cl)_2$	70
18[k]	$[RhCp^*Cl_2]_2$	$AgBF_4$	Ag_2O	$(CH_2Cl)_2$	69
19[l]	$[RhCp^*Cl_2]_2$	$AgBF_4$	Ag_2O	$(CH_2Cl)_2$	64

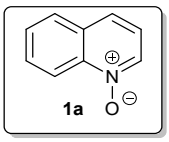
[a]Reaction conditions: **1a** (0.2 mmol), **2a** (0.24 mmol), catalyst (5 mol %), additive (20 mol %), oxidant (0.2 mmol), solvent (1 mL), H_2O (50 µL, 14 equiv), 90 °C, argon atmosphere, 2 h. [b]Isolated yield. [c] only H_2O (1 mL). [d]At 50 °C. [e]At 120 °C. [f]Oxidant (0.1 mmol, 0.5 equiv). [g]Oxidant (0.4 mmol, 2 equiv). [h]$[RhCp^*Cl_2]_2$ (2.5 mol %). [i]$[RhCp^*Cl_2]_2$ (2.5 mol %) stirred for additional 12 h. [j]$[RhCp^*Cl_2]_2$ (4 mol %). [k]H_2O (36 µL, 10 equiv). [l]H_2O (72 µL, 20 equiv). n.d. = not detected.

Post-synthetic Transformations

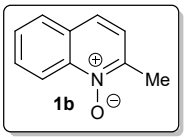
Synthesis of 6. To an ice-cold solution of 1,2-diphenyl-3H,5H-pyrido[3,2,1-ij]quinoline-3,5-dione **3aa** (0.1 mmol, 35 mg) in THF (1 mL), $BH_3{\cdot}SMe_2$ (0.25 mmol, 25 µL) was added and the resultant mixture was allowed stir at room temperature for 6 h under nitrogen atmosphere. Evaporation of solvent gave a residue that was purified on silica gel column chromatography using hexane/ethyl acetate as an eluent to afford 1,2-dihydroquinoline derivative **6** in 68% (23 mg) yield.

Synthesis of 7. In a pressure tube, a mixture having **3ka** (0.1 mmol, 43 mg), $PhB(OH)_2$ (0.2 mmol, 25 mg), Na_2CO_3 (0.2 mmol, 21 mg), toluene (1 mL), ethanol (1 mL) and water (100 µL) was degassed with argon for 10 minutes. Then, $Pd(PPh_3)_4$ (2 mol %, 2.5 mg) was added and the mixture was allowed to stir at 100 °C for 8 h. After completion (monitored by TLC), the resultant solution was diluted with ethyl acetate (20 mL) and washed with water (5 mL). Drying (Na_2SO_4) and evaporation of the solvent gave a residue, which was purified on silica gel column chromatography using hexane/ethyl acetate as an eluent to afford **7** in 74% (31.5 mg) yield.

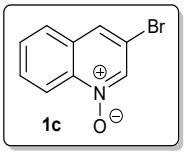
Characterization Data of Quinoline *N*-oxides



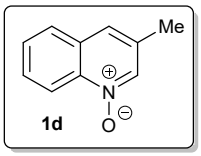
Quinoline 1-oxide 1a.[1d] Brown solid; yield 87% (126 mg); ^1H NMR (400 MHz, $CDCl_3$) δ 8.76 (d, J = 8.8 Hz, 1H), 8.55 (d, J = 6.0 Hz, 1H), 7.89 (d, J = 8.4 Hz, 1H), 7.79-7.75 (m, 2H), 7.67-7.63 (m, 1H), 732-7.28 (m, 1H).



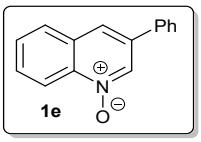
2-Methylquinoline 1-oxide 1b.[1d] Brown solid; yield 84% (133.5 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.79 (d, *J* = 8.8 Hz, 1H), 7.84 (d, *J* = 8.4 Hz, 1H), 7.77-7.73 (m, 1H), 7.66 (d, *J* = 8.4 Hz, 1H), 7.61-7.57 (m, 1H), 7.32 (d, *J* = 8.8 Hz, 1H).



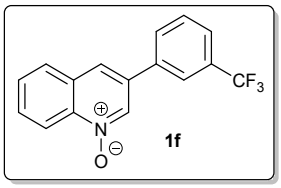
3-Bromoquinoline 1-oxide 1c.[1c] Brown solid; yield 81% (182 mg);^{1}H NMR (400 MHz, $CDCl_3$) δ 8.68 (d, *J* = 8.8 Hz, 1H), 8.63 (d, *J* = 1.5 Hz, 1H), 7.90 (s, 1H), 7.80-7.74 (m, 2H), 7.69-7.65 (m, 1H).



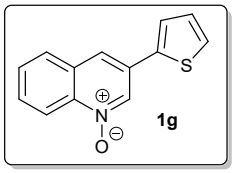
3-Methylquinoline 1-oxide 1d.[1d] Brown solid; yield 86% (137 mg);^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, *J* = 8.8 Hz, 1H), 8.43 (s, 1H), 7.78 (d, *J* = 8.0 Hz, 1H), 7.71-7.67 (m, 1H), 7.62-7.58 (m, 1H), 7.53 (s, 1H), 2.45 (s, 3H).



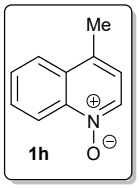
3-Phenylquinoline 1-oxide 1e.[1c] Brown solid; yield 82% (181 mg);^{1}H NMR (500 MHz, $CDCl_3$) δ 8.79 (d, *J* = 1.0 Hz, 1H), 8.69 (d, *J* = 8.5 Hz, 1H), 7.86-7.85 (m, 2H), 7.71 (t, *J* = 7.0 Hz, 1H), 7.62-7.58 (m, 3H), 7.47 (t, *J* = 7.0 Hz, 2H), 7.41-7.38 (m, 1H).



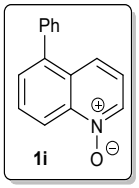
3-(3-Trifluoromethyl)phenyl)quinoline 1-oxide 1f.[1d] Brown solid; yield 78% (225.5 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.85 (d, *J* = 1.5 Hz, 1H), 8.77 (d, *J* = 8.4 Hz, 1H), 7.96-7.92 (m, 3H), 7.85-7.77 (m, 2H), 7.74-7.64 (m, 3H). δ 8.69 (d, *J* = 8.5 Hz, 1H), 8.43 (s, 1H), 7.78 (d, *J* = 8.0 Hz, 1H), 7.71-7.67 (m, 1H), 7.62-7.59 (m, 1H), 7.54 (s, 1H), 2.46 (s, 3H).



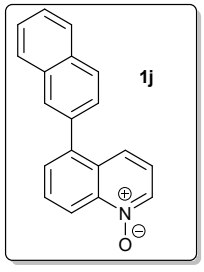
3-(Thiophen-3-yl)quinoline 1-oxide 1g. Analytical TLC on silica gel, 3:2 hexane/ethyl acetate R_f = 0.42; brown solid; mp 89-90 ˚C; yield 82% (186 mg); ^{1}H NMR (500 MHz, CDCl3) δ 8.86 (s, 1H), 8.72 (d, *J* = 8.5 Hz, 1H), 7.89 (d, *J* = 8.0 Hz, 2H), 7.74 (t, *J* = 7.5 Hz 1H), 7.66-7.62 (m, 2H), 7.50-7.48 (m, 1H), 7.45 (d, *J* = 5.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 140.3, 137.0, 134.7, 130.4, 130.1, 129.8, 129.3, 128.3, 127.7, 125.7, 122.6, 122.5, 119.8; FT-IR (neat) 3379, 1684, 1580, 1497, 1397, 1341, 1210, 1138, 1086, 957, 781 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{13}H_{10}NOS$: 228.0478, found 228.0479.



4-Methylquinoline 1-oxide 1h.[1d] Brown solid; yield 85% (123 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.82 (d, *J* = 8.8 Hz, 1H), 8.45 (d, *J* = 6.4 Hz, 1H), 7.99 (d, *J* = 8.4 Hz, 1H), 7.80-7.76 (m, 1H), 7.70-7.66 (m, 1H), 7.13 (d, *J* = 6.0 Hz, 1H), 2.67 (s, 3H).

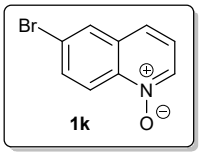


5-Phenylquinoline 1-oxide 1i.[1d] Brown solid; yield 80% (177 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.83 (d, *J* = 8.8 Hz, 1H), 8.56 (d, *J* = 5.6 Hz, 1H), 7.82-7.77 (m, 2H), 7.61-7.59 (m, 1H), 7.54-7.43 (m, 5H), 7.26-7.22 (m, 1H).

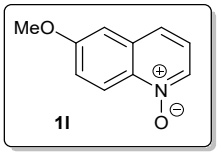


5-(Naphthalen-2-yl)quinoline 1-oxide 1j. Analytical TLC on silica gel; 3:2 hexane/ethyl acetate R_f = 0.30; brown solid; mp:179-180 ˚C; yield 86% (233 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.86 (d, *J* = 8.8 Hz, 1H), 8.57-8.56 (m, 1H), 7.99-7.89 (m, 4H), 7.85-7.80 (m, 2H), 7.70-7.68 (m, 1H), 7.59-7.54 (m, 3H), 7.24-7.21 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 142.3, 141.2, 136.2, 135.5, 133.3, 132.9, 130.0, 129.9, 129.5, 129.1, 128.3, 128.2, 127.9, 127.9, 126.9, 126.8, 124.9, 120.8, 119.4; FT-IR (neat) 3057, 2924, 1719, 1627, 1443,

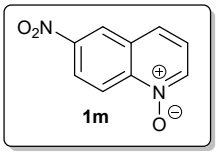
1252, 1148, 947, 700 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{19}H_{14}NO$: 272.1071, found 272.1075.



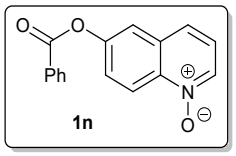
6-Bromoquinoline 1-oxide 1k.[1a] Brown solid; yield 84% (187 mg); ^1H NMR (400 MHz, $CDCl_3$) δ 8.64 (d, *J* = 9.2 Hz, 1H), 8.53-8.51 (m, 1H), 8.05 (d, *J* = 2.0 Hz, 1H), 7.84-7.81 (m, 1H), 7.66 (d, *J* = 8.8 Hz, 1H), 7.34-7.31 (m, 1H).



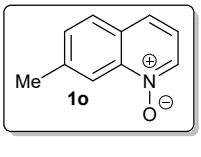
6-Methoxyquinoline 1-oxide 1l.[1d] Brown solid; yield 79% (183 mg); ^1H NMR (400 MHz, $CDCl_3$) δ 8.65 (d, *J* = 9.6 Hz, 1H), 8.40-8.39 (m, 1H), 7.65 (d, *J* = 8.4 Hz, 1H), 7.40-7.37 (m, 1H), 7.27-7.23 (m, 1H), 7.11 (d, *J* = 2.4 Hz, 1H), 3.94 (s, 3H).



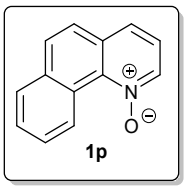
6-Nitroquinoline 1-oxide 1m.[1d] Yellow solid; yield 75% (142 mg); ^1H NMR (400 MHz, $CDCl_3$) δ 8.94 (d, *J* = 9.6 Hz, 1H), 8.84 (d, *J* = 2.4 Hz, 1H), 8.68 (d, *J* = 6.0 Hz, 1H), 8.52-8.49 (m, 1H), 7.94 (d, *J* = 8.4 Hz, 1H), 7.51-7.48 (m, 1H).



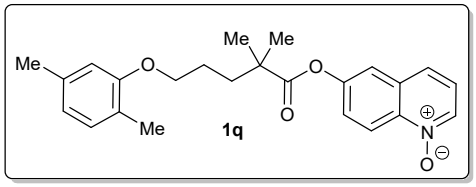
6-(Benzoyloxy)quinoline 1-oxide 1n.[1d] Brown solid; yield 81% (215 mg); ^1H NMR (400 MHz, $CDCl_3$) δ 8.84 (d, *J* = 9.6 Hz, 1H), 8.54 (d, *J* = 6.0 Hz, 1H), 8.25-8.22 (m, 2H), 7.80 (d, *J* = 2.4 Hz, 1H), 7.74 (d, *J* = 8.4 Hz, 1H), 7.70-7.62 (m, 2H), 7.57 (t, *J* = 7.6 Hz, 2H), 7.35-7.32 (m, 1H).



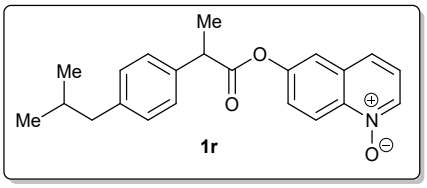
7-Methylquinoline 1-oxide 1o.[1d] Brown solid; yield 84% (122 mg); ^1H NMR (400 MHz, $CDCl_3$) δ 8.56 (s, 1H), 8.52 (d, *J* = 6.0 Hz, 1H), 7.78 (d, *J* = 8.4 Hz, 1H), 7.72 (d, *J* = 8.4 Hz, 1H), 7.49-7.47(m, 1H), 7.26-7.21 (m, 1H), 2.60 (s, 3H).



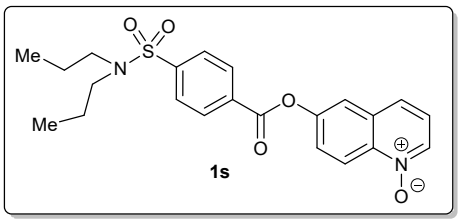
Benzo[h]quinoline 1-oxide 1p.[1b] Brown solid; yield 83% (162 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.86-10.83 (m, 1H), 8.68-8.66 (m, 1H), 7.94-7.92 (m, 1H), 7.87 (d, *J* = 8.8 Hz, 1H), 7.81-7.77 m, 3H), 7.67-7.64 (m, 1H), 7.43-7.39 (m, 1H).



6-(5-(2,5-Dimethylphenoxy)-2,2-dimethyl-pentanoyl)oxy)quinoline 1-oxide 1q.[1d] Brown sticky liquid; yield 76% (299 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.77 (d, *J* = 9.2 Hz, 1H), 8.51-8.49 (m, 1H), 7.66 (d, *J* = 8.8 Hz, 1H), 7.55 (d, *J* = 2.4 Hz, 1H), 7.44-7.41 (m, 1H), 7.32-7.28 (m, 1H), 7.01 (d, *J* = 7.2 Hz, 1H), 6.68 (d, *J* = 7.6 Hz, 1H), 6.63 (s, 1H), 4.03 (t, *J* = 5.6 Hz, 2H), 2.30 (s, 3H), 2.17 (s, 3H), 1.95-1.88 (m, 4H), 1.42 (s, 6H).

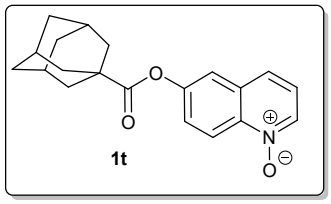


6-(2-(4-Isobutylphenyl)propanoyl)oxy)quinoline 1-oxide 1r. Analytical TLC on silica gel; 3:2 hexane/ethyl acetate R_f = 0.35; brown liquid; yield 83% (289 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.73 (d, *J* = 9.6 Hz, 1H), 8.49-8.47 (m, 1H), 7.65 (d, *J* = 8.4 Hz, 1H), 7.56 (d, *J* = 2.4 Hz, 1H), 7.40-7.37 (m, 1H), 7.33-7.26 (m, 3H), 7.18 (d, *J* = 8.4 Hz, 2H), 4.02 (q, *J* = 7.2 Hz, 1H), 2.49 (d, *J* = 7.2 Hz, 2H), 1.91-1.84 (m, 1H), 1.65 (d, *J* = 7.2 Hz, 3H), 0.92 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 172.9, 150.6, 141.2, 139.5, 136.8, 135.4, 131.2, 129.7, 125.7, 125.5, 121.8, 121.7, 118.9, 45.416, 45.1, 30.2, 22.4, 18.5; FT-IR (neat) 3401, 2954, 1455, 1571, 1369, 1196, 1143, 1069, 851, 789 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{22}H_{24}NO_3$: 350.1751, found 350.1756.



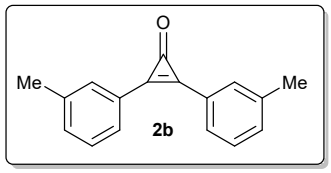
6-((4-(*N*,*N*-Di(prop-1-en-1-yl)sulfamoyl)benzoyl)-oxy)quinoline 1-oxide 1s. Analytical TLC on silica gel; 7:3 hexane/ethyl acetate R_f = 0.25;

brown liquid; yield 78% (325 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.85 (d, *J* = 9.5 Hz, 1H), 8.57 (d, *J* = 6.0 Hz, 1H), 8.36 (d, *J* = 8.5 Hz, 2H), 7.99 (d, *J* = 8.0 Hz, 2H), 7.82 (d, *J* = 2.0 Hz, 1H), 7.77 (d, *J* = 8.5 Hz, 1H), 7.65-7.63 (m, 1H), 7.38-7.35 (m, 1H), 3.16 (t, *J* = 7.5 Hz, 4H), 1.51-1.54 (m, 4H), 0.91 (t, *J* = 7.5 Hz, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.5, 150.4, 145.5, 139.7, 135.8, 132.1, 131.3, 131.0, 127.4, 125.9, 125.4, 122.1, 122.1, 119.2, 50.0, 22.0, 11.2; FT-IR (neat) 3400, 2964, 1741, 1340, 1258, 1193, 1154, 1063, 993, 730 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{22}H_{25}N_2O_5S$: 429.1479, found 429.1479.

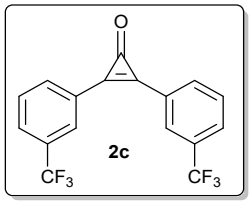


6-((Adamantane-1-carbonyl)oxy)quinoline 1-oxide 1t. Brown liquid; yield 81% (261 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.77 (d, *J* = 9.5 Hz, 1H), 8.50 (d, *J* = 6.0 Hz, 1H), 7.69 (d, *J* = 8.5 Hz, 1H), 7.61 (d, *J* = 2.0 Hz, 1H), 7.47-7.49 (m, 1H), 7.32-7.29 (m, 1H), 2.12-2.09 (m, 9H), 1.82-1.76 (m, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 175.8, 151.0, 139.5, 135.4, 131.3, 125.8, 125.6, 121.9, 121.7, 119.0, 41.3, 38.8, 36.5, 27.9; FT-IR (neat) 3401, 2905, 1746, 1571, 1453, 1368, 1211, 1179, 1194, 1039, 793 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{20}H_{22}NO_3$: 324.1594, found 324.1599.

Characterization Data of Cyclopropenones

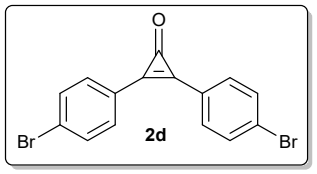


2,3-Di-*m*-tolylcycloprop-2-en-1-one 2b.[2d] Colorless solid; yield 68% (159 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80-7.77 (m, 4H), 7.49 (t, *J* = 7.6 Hz, 2H), 7.41 (d, *J* = 7.6 Hz, 2H), 2.46 (s, 6H).

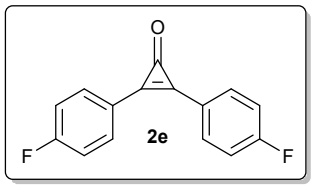


2,3-Bis(3-(trifluoromethyl)phenyl)cycloprop-2-en-1-one 2c. Analytical TLC on silica gel; 3:1 hexane/ethyl acetate R_f = 0.30; colorless solid; mp 148-147; yield 56% (191.5 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.22 (s, 2H), 8.16 (d, *J* = 7.5 Hz, 2H), 7.90 (d, *J* = 7.5 Hz, 2H), 7.79 (t, *J* = 7.5 Hz, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 154.6, 149.1, 134.3, 132.8

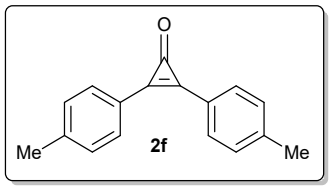
(q, $J_{C\text{-}F}$ = 33.0 Hz), 130.4, 129.7 (q, $J_{C\text{-}F}$ = 3.6 Hz), 128.3 (q, $J_{C\text{-}F}$ = 3.6 Hz), 126.6 (q, $J_{C\text{-}F}$ = 271.1 Hz), 124.4; ^{19}F NMR (470 MHz, $CDCl_3$) δ -63.04; FT-IR (neat) 1838, 1634, 1605, 1423, 1310, 1267, 1131, 1066, 806, 694 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{17}H_9F_6O$: 343.0552, found 343.0556



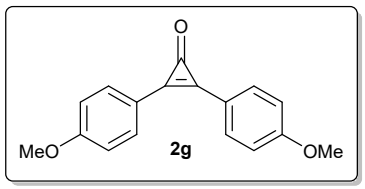
2,3-Bis(4-bromophenyl)cycloprop-2-en-1-one 2d.[2d] Colorless solid; yield 65% (237 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.4 Hz, 4H), 7.74 (d, *J* = 8.4 Hz, 4H).



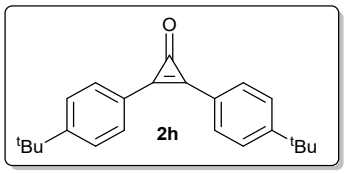
2,3-Bis(4-fluorophenyl)cycloprop-2-en-1-one 2e.[2c] Colorless solid; yield 71% (340 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99-7.96 (m, 4H), 7.30 (t, *J* = 8.4 Hz, 4H).



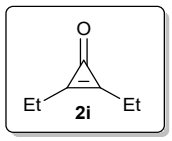
2,3-Di-*p*-tolylcycloprop-2-en-1-one 2f.[2c] Colorless solid; yield 73% (170 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.8 Hz, 4H), 7.38 (d, *J* = 8.8 Hz, 4H), 2.46 (s, 6H).



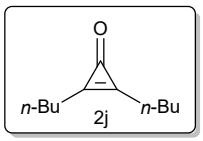
2,3-Bis(4-methoxyphenyl)cycloprop-2-en-1-one 2g.[2b] Colorless solid; yield 78% (207 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 5.6 Hz, 4H), 7.06 (d, *J* = 6.0 Hz, 4H), 3.90 (s, 6H).



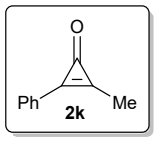
2,3-Bis(4-(*tert*-butyl)phenyl)cycloprop-2-en-1-one 2h.[2c] Colorless solid; yield 72% (229 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 8.4 Hz, 4H), 7.60 (d, *J* = 8.4 Hz, 4H), 1.37 (s, 18H).



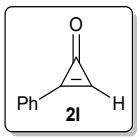
2,3-Diethylcycloprop-2-en-1-one 2i.[2d] Brown liquid; yield 58% (319 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.66 (q, *J* = 7.6 Hz, 4H), 1.32 (t, *J* = 7.5 Hz, 6H).



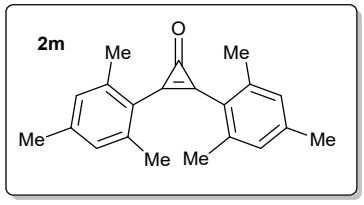
2,3-Dibutylcycloprop-2-en-1-one 2j.[2d] Brown liquid; yield 53% (439 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.62 (t, *J* = 7.2 Hz, 4H), 1.71-1.64 (m, 4H), 1.47-1.38 (m, 4H), 0.97 (*t*, *J* = 7.2 Hz, 6H).



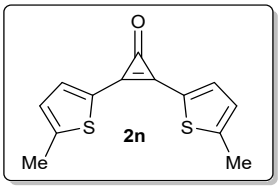
2-Methyl-3-phenylcycloprop-2-en-1-one 2k.[2d] Brown solid; yield 61% (439 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79-7.77 (m, 2H), 7.56-7.50 (m, 3H), 2.49 (s, 3H).



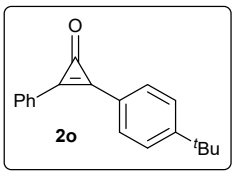
2-Phenylcycloprop-2-en-1-one 2l.[2d] Brown liquid; yield 56% (363.5 mg) ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (s, 1H), 7.87-7.85 (m, 2H), 7.64-7.60 (m, 1H), 7.57-7.53 (m, 2H).



2,3-Dimesitylcycloprop-2-en-1-one 2m.[2a] Colorless solid; yield 83% (241 mg) ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.95 (s, 4H), 2.34 (s, 6H), 2.31 (s, 12H).

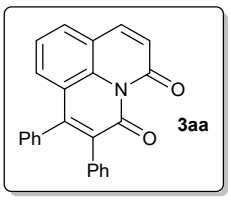


2,3-Bis(5-methylthiophen-2-yl)cycloprop-2-en-1-one 2n.[2e] Brown solid; yield 74% (182 mg) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 3.6 Hz, 2H), 6.92-6.91 (m, 2H), 2.61 (s, 7H).

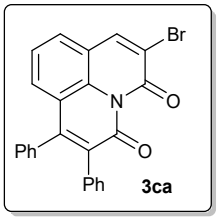


2-(4-(*tert*-Butyl)phenyl)-3-phenylcycloprop-2-en-1-one 2o. Analytical TLC on silica gel; 7:3 hexane/ethyl acetate R_f = 0.4; thick liquid; yield 68% (180 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.99 (d, *J* = 7.0 Hz, 2H), 7.95 (d, *J* = 8.0 Hz, 2H), 7.61-7.57 (m, 5H), 1.37 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.1, 156.4, 147.7, 146.5, 132.8, 131.7, 131.6, 129.4, 126.5, 123.9, 121.0, 35.4, 31.1; FT-IR (neat) 3460, 2959, 1848, 1616, 1450, 1343, 840, 769, 690 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{19}H_{19}O$: 263.1430, found 263.1429.

Characterization Data of 3

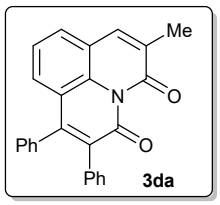


1,2-Diphenyl-3H,5H-pyrido[3,2,1-ij]quinoline-3,5-dione 3aa. Analytical TLC on silica gel; 3:2 hexane/ethyl acetate R_f = 0.3; colorless solid; mp 247-248 °C; yield 73% (51 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 (d, *J* = 10.0 Hz, 1H), 7.67 (d, *J* = 7.5 Hz, 1H), 7.44 (d, *J* = 8.0 Hz, 1H), 7.32-7.29 (m, 4H), 7.18-7.12 (m, 7H), 6.79 (d, *J* = 10.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.9, 161.8, 148.2, 139.9, 135.3, 134.9, 134.4, 134.3, 131.1, 130.9, 130.6, 129.9, 128.3, 128.2, 127.6, 127.5, 124.4, 123.8, 121.1, 119.5; FT-IR (neat) 2924, 1719, 1627, 1443, 1252, 1148, 947, 700 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{24}H_{16}NO_2$: 350.1176, found 350.1171.

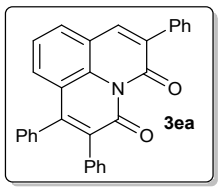


6-Bromo-1,2-diphenyl-3H,5H-pyrido[3,2,1-ij]quinoline-3,5-dione 3ca. Analytical TLC on silica gel; 7:3 hexane/ethyl acetate R_f = 0.4; brown solid; mp 255-256 °C;

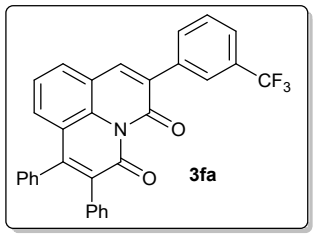
yield 71% (62 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.20 (s, 1H), 7.64 (d, *J* = 7.5 Hz, 1H), 7.46 (d, *J* = 8.0 Hz, 1H), 7.34-7.2 (m, 4H), 7.16-7.11 (m, 7H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.3, 157.4, 148.3, 141.4, 135.1, 134.3, 134.2, 134.1, 131.3, 130.8, 129.9, 129.8, 128.3, 127.72, 127.70, 124.2, 121.2, 119.4, 119.2; FT-IR (neat) 2923, 1725, 1616, 1448, 1234, 1616, 960, 699 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{24}H_{15}NO_2Br$: 428.0281, found 428.0272.



6-Methyl-1,2-diphenyl-3H,5H-pyrido[3,2,1-ij]quinoline-3,5-dione 3da. Analytical TLC on silica gel; 7:3 hexane/ethyl acetate R_f = 0.4; brown solid; mp 230-231 °C; yield 74% (54 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60-7.58 (m, 2H), 7.35-7.34 (m, 1H), 7.29-7.26 (m, 4H), 7.11-7.11 (m, 7H), 2.33 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.8, 162.0, 148.2, 136.4, 135.5, 134.5, 134.2, 134.1, 132.9, 130.9, 129.9, 129.8, 129.7, 123.7, 120.7, 119.4, 17.698; FT-IR (neat) 2923, 1715, 1459, 1442, 1150, 765 752, 702 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{25}H_{18}NO_2$: 364.1332, found 364.1333.

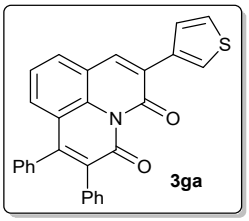


1,2,6-Triphenyl-3H,5H-pyrido[3,2,1-ij]quinoline-3,5-dione 3ea. Analytical TLC on silica gel; 7:3 hexane/ethyl acetate R_f = 0.4; brown solid; mp 258-259 °C; yield 69% (59 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (s, 1H), 7.78-7.76 (m, 2H), 7.71-7.70 m, 1H), 7.48 (t, *J* = 7.0 Hz, 2H), 7.43-7.40 (m, 2H), 7.32-7.29 (m, 4H), 7.17-7.13 (m, 7H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.9, 161.6, 148.1, 137.0, 135.4, 134.9, 134.5, 134.4, 131.0, 130.6, 130.5, 129.9, 129.1, 128.9, 128.5, 128.3, 128.2, 127.6, 127.5, 123.8, 120.7, 119.4; FT-IR (neat) 2922, 1721, 1664, 1444, 1275, 1153, 753, 698 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{30}H_{20}NO_2$: 426.1489, found 426.1490.

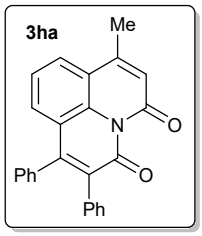


1,2-Diphenyl-6-(3-(trifluoromethyl)phenyl)-3H,5H-pyrido-[3,2,1-ij]quinoline-3,5-dione 3fa. Analytical TLC on silica gel; 7:3 hexane/ethyl acetate R_f = 0.35;

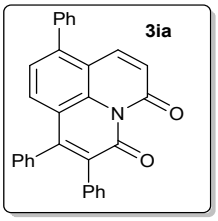
brown solid; mp 262-263 °C; yield 62% (61 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.01 (d, J = 10.0 Hz, 2H), 7.91 (s, 1H), 7.75 (d, J = 7.0 Hz, 1H), 7.68 (d, J = 7.5 Hz, 1H), 7.60 (t, J = 8.0 Hz, 1H), 7.46 (d, J = 7.5 Hz, 1H), 7.35-7.30 (m, 4H), 7.19-7.14 (m, 7H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.8, 161.2, 148.2, 137.9, 136.1, 135.2, 134.5, 134.4, 134.3, 133.4, 132.6, 131.1 ($J_{C\text{-}F}$ = 32.0 Hz), 131.0, 130.97, 130.95 129.9, 128.954, 128.3, 128.3, 127.6, 125.9 ($J_{C\text{-}F}$ = 3.8 Hz), 125.5 ($J_{C\text{-}F}$ = 4.0 Hz), 125.2 ($J_{C\text{-}F}$ = 270.7 Hz), 124.0, 120.8, 119.1; ^{19}F NMR (470 MHz, $CDCl_3$) δ -62.50; FT-IR (neat) 3059, 2922, 1720, 1663, 1442, 1332, 1217, 1153, 1124, 1075, 750, 697 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{31}H_{19}F_3NO_2$: 494.1362, found 494.1356.



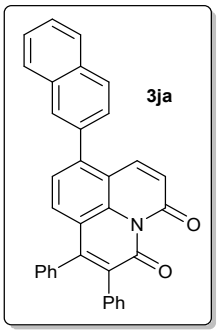
1,2-Diphenyl-6-(thiophen-3-yl)-3H,5H-pyrido[3,2,1-ij]quinoline-3,5-dione 3ga. Analytical TLC on silica gel, 7:3 hexane/ethyl acetate R_f = 0.42; brown solid; mp 244-245 °C; yield 64% (56 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32-8.31 (m, 1H), 8.00 (s, 1H), 7.72-7.70 (m, 1H), 7.61-7.59 (m, 1H), 7.41-7.39 (m, 2H), 7.33-7.29 (m, 4H), 7.18-7.13 (m, 7H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.0, 161.2, 148.1, 135.4, 134.8, 134.7, 134.5, 134.4, 133.8, 131.0, 130.5, 130.3, 129.9, 129.0, 128.3, 128.2, 127.6, 127.5, 126.8, 126.6, 125.4, 123.8, 120.6, 119.3; FT-IR (neat) 2924, 1719, 1661, 1444, 1149, 699 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{28}H_{18}NO_2S$: 432.1053, found 432.1050.



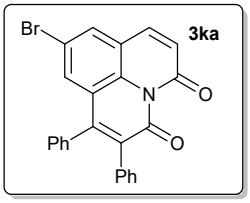
7-Methyl-1,2-diphenyl-3H,5H-pyrido[3,2,1-ij]quinoline-3,5-dione 3ha. Analytical TLC on silica gel; 3:2 hexane/ethyl acetate R_f = 0.32; brown solid; mp 230-231 °C; yield 73% (52.5 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, J = 7.5 Hz, 1H), 7.43 (d, J = 8.0 Hz, 1H), 7.33-7.29 (m, 4H), 7.16-7.11 (m, 7H), 6.67 (s, 1H), 2.53 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.7, 161.6, 148.2, 147.7, 135.5, 134.8, 134.3, 134.2, 131.0, 130.9, 129.9, 128.3, 128.2, 127.6, 127.5, 127.1, 123.5, 123.4, 121.2, 120.6, 19.417; FT-IR (neat) 3057, 2923, 1720, 1664, 1443, 1256, 1205, 1146, 744, 710 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{25}H_{18}NO_2$: 364.1332, found 364.1338.



1,2,8-Triphenyl-3H,5H-pyrido[3,2,1-ij]quinoline-3,5-dione 3ia. Analytical TLC on silica gel; 3:2 hexane/ethyl acetate R_f = 0.3; brown solid; mp 210-211 °C; yield 67% (56 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 10.0 Hz, 1H), 7.54-7.48 (m, 3H), 7.46 (d, *J* = 8.0 Hz, 1H), 7.40-7.37 (m, 2H), 7.34-7.28 (m, 4H), 7.17-7.14 (m, 7H), 6.714 (d, *J* = 10.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.1, 161.7, 148.1, 144.1, 138.4, 138.0, 135.6, 135.4, 134.3, 134.0, 130.9, 130.6, 130.0, 129.9, 128.8, 128.6, 128.3, 128.3, 127.6, 127.5, 125.4, 123.8, 120.2, 117.3; FT-IR (neat) 3057, 1727, 1667, 1442, 1275, 1147, 763, 697 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{30}H_{20}NO_2$: 426.1489, found 426.1491.

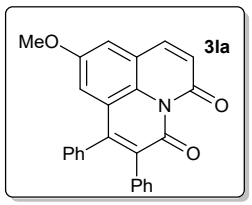


8-(Naphthalen-2-yl)-1,2-diphenyl-3H,5H-pyrido[3,2,1-ij]quinoline-3,5-dione 3ja. Analytical TLC on silica gel; 7:3 hexane/ethyl acetate R_f = 0.33; brown solid; mp 231-232 °C; yield 65% (61.5 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.4 Hz, 1H), 7.95-7.91 (m, 2H), 7.86-7.83 (m, 2H), 7.61-7.56 (m, 2H), 7.51-7.47 (m, 2H), 7.37-7.31 (m, 4H), 7.19-7.16 (m, 7H), 6.72 (d, *J* = 10.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.1, 161.7, 148.2, 144.1, 138.1, 135.8, 135.6, 135.4, 134.3, 134.0, 133.1, 133.0, 130.9, 130.6, 129.9, 129.3, 128.5, 128.3, 128.3, 127.9, 127.6, 127.5, 127.1, 127.0, 125.6, 123.9, 120.3, 117.4.; FT-IR (neat) 5034, 2924, 1724, 16649, 1570, 1441, 1275, 1148, 763, 750, 702 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{34}H_{22}NO_2$: 476.1645, found 476.1648.

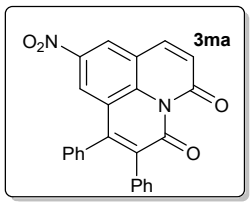


9-Bromo-1,2-diphenyl-3H,5H-pyrido[3,2,1-ij]quinoline-3,5-dione 3ka. Analytical TLC on silica gel; 3:2 hexane/ethyl acetate R_f = 0.30; brown solid; mp 251-252 °C; yield 77% (66 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.78 (d, *J* = 2.5 Hz, 1H), 7.66 (d, *J* = 10.0

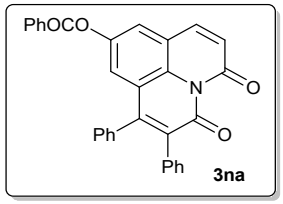
Hz, 1H), 7.49 (d, J = 2.5 Hz, 1H), 7.32-7.31 (m, 3H), 7.18-7.15 (m, 3H), 7.12-7.10 (m, 4H), 6.81 (d, J = 10.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.3, 161.2, 147.1, 138.7, 135.5, 134.6, 133.9, 133.8, 132.9, 132.6, 130.7, 129.7, 128.6, 128.5, 127.7, 127.6, 125.6, 122.9, 121.0, 116.9; FT-IR (neat) 3060, 1723, 1565, 1444, 1252, 1153, 1113, 741, 699 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{24}H_{15}NO_2Br$: 428.0281, found 428.0283.



9-Methoxy-1,2-diphenyl-3H,5H-pyrido[3,2,1-ij]quinoline-3,5-dione 3la. Analytical TLC on silica gel; 3:2 hexane/ethyl acetate R_f = 0.28; brown solid; mp 245-246 °C; yield 72% (54 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.67 (d, J = 9.5 Hz, 1H), 7.31-7.28 (m, 3H), 7.17-7.10 (m, 8H), 6.96 (d, J = 2.5 Hz, 1H), 6.79 (d, J = 9.5 Hz, 1H), 3.7 (s, 3H).; ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.7, 161.7, 155.5, 147.8, 139.5, 135.3, 135.0, 134.4, 130.9, 129.8, 129.4, 128.3, 128.3, 127.5, 127.5, 125.1, 122.5, 120.5, 117.0, 114.7, 55.872; FT-IR (neat) 3060, 2922, 1715, 1590, 1461, 1349, 1291, 1148, 1054, 764, 750, 702 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{25}H_{18}NO_3$: 380.1281, found 380.1286.

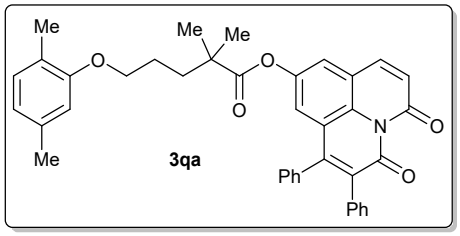


9-Nitro-1,2-diphenyl-3H,5H-pyrido[3,2,1-ij]quinoline-3,5-dione 3ma. Analytical TLC on silica gel; 1:1 hexane/ethyl acetate R_f = 0.27; brown solid; mp 275-276 °C; yield 48% (38 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (d, J = 2.4 Hz, 1H), 8.27 (d, J = 2.4 Hz, 1H), 7.83 (d, J = 9.6 Hz, 1H), 7.37-7.35 (m, 3H), 7.20-7.19 (m, 3H), 7.15-7.12 (m, 4H), 6.918 (d, J = 10.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.9, 160.6, 147.3, 143.4, 138.9, 138.3, 136.2, 134.0, 133.4, 130.7, 129.7, 129.1, 128.9, 128.1, 127.8, 126.4, 125.0, 124.6, 122.0, 119.8; FT-IR (neat) 6063, 2929, 1733, 1527, 1447, 1334, 747, 700 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{24}H_{15}N_2O_4$: 395.1026, found 395.1032.

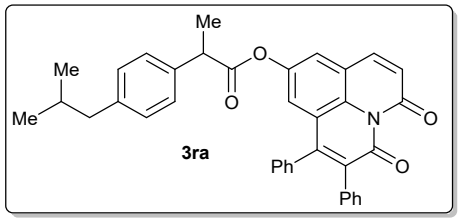


3,5-Dioxo-1,2-diphenyl-3H,5H-pyrido[3,2,1-ij]quinolin-9-yl benzoate 3na. Analytical TLC on silica gel; 3:2 hexane/ethyl acetate R_f = 0.37; brown solid;

mp 212-213 °C; yield 67% (64 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.15 (d, *J* = 8.5 Hz, 2H), 7.72 (d, *J* = 10.0 Hz, 1H), 7.66 (t, *J* = 7.5 Hz, 1H), 7.57 (d, *J* = 2.5 Hz, 1H), 7.51 (t, *J* = 8.0 Hz, 2H), 7.31-7.30 (m, 3H), 7.25-7.4 (m, 1H), 7.17-7.14 (m, 7H), 6.84 (d, *J* = 10.0 Hz, 1H).; ^{13}C NMR (125 MHz, $CDCl_3$) 165.1, 161.5, 147.5, 146.6, 139.3, 135.3, 134.9, 134.2, 134.1, 132.7, 130.8, 130.4, 129.8, 128.8, 128.5, 128.4, 127.7, 127.6, 125.4, 123.7, 123.5, 122.4, 120.53; FT-IR (neat) 3060, 2925, 1726, 1592, 1449, 1248, 1147, 1061, 750, 702 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{31}H_{20}NO_4$: 470.1387, found 470.1389.

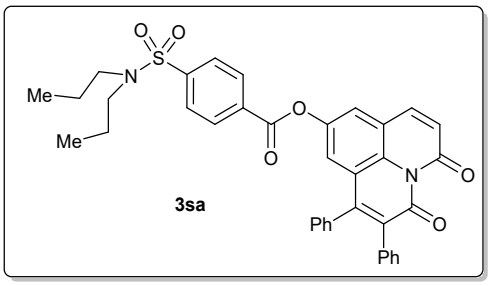


3,5-Dioxo-1,2-diphenyl-3H,5H-pyrido[3,2,1-ij]quinolin-9-yl 5-(2,5-dimethylphenoxy)-2,2-dimethylpentanoate 3qa. Analytical TLC on silica gel; 7:3 hexane/ethyl acetate R_f = 0.35; brown sticky liquid; yield 61% (72 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.62 (d, *J* = 10.0 Hz, 1H), 7.33 (d, *J* = 2.5 Hz, 1H), 7.25-7.20 (m, 3H), 7.16-7.14 (m, 3H), 7.13-7.10 (m, 4H), 7.07 (d, *J* = 2.5 Hz, 1H), 7.00 (d, *J* = 7.0 Hz, 1H), 6.80 (d, *J* = 9.5 Hz, 1H), 6.68 (d, *J* = 7.5 Hz, 1H), 6.59 (s, 1H), 3.91 (t, *J* = 6.0 Hz, 2H), 2.30 (s, 3H), 2.12 (s, 3H), 1.87-1.83 (m, 2H), 1.80-1.76 (m, 2H), 1.32 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 176.4, 161.5, 156.9, 147.5, 146.7, 139.2, 136.6, 135.1, 134.8, 132.5, 130.8, 130.5, 129.8, 128.44, 128.40, 127.7, 127.6, 125.2, 123.6, 123.4, 123.3, 122.3, 120.9, 120.4, 112.0, 67.6, 42.6, 37.2, 25.3, 25.1, 21.5, 15.9; FT-IR (neat) 3059, 2925, 1727, 1667, 1450, 1251, 1149, 1105, 705 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{39}H_{36}NO_5$: 598.2588, found 598.2584.

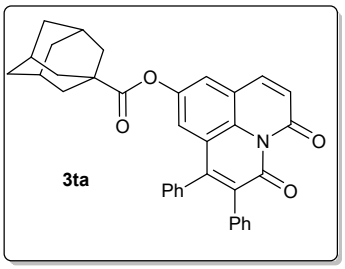


3,5-Dioxo-1,2-diphenyl-3H,5H-pyrido[3,2,1-ij]quinolin-9-yl 2-(4-isobutylphenyl)propanoate 3ra. Analytical TLC on silica gel; 7:3 hexane/ethyl acetate R_f = 0.38; brown sticky liquid; yield 64% (70.5 mg); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.63 (d, *J* = 9.6 Hz, 1H), 7.31-7.29 (m, 4H), 7.21 (d, *J* = 7.8 Hz, 2H), 7.16-7.14 (m, 3H), 7.12-7.09 (m, 6H), 7.04 (d, *J* = 2.4 Hz, 1H), 6.79 (d, *J* = 10.2 Hz, 1H), 3.90-3.86 (m, 1H), 2.46 (d, *J* = 7.2 Hz, 2H), 1.88-1.81 (m, 1H), 1.55 (d, *J* = 7.2 Hz, 3H), 0.91 (d, *J* = 6.6 Hz, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 173.2, 161.4, 147.4, 146.5, 141.1, 139.2, 136.9, 135.1, 134.9,

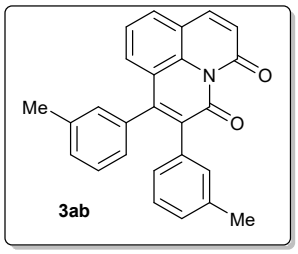
134.1, 132.6, 130.8, 129.8, 129.7, 128.4, 127.7, 127.6, 127.2, 125.2, 123.4, 123.1, 122.2, 120.3, 45.2, 45.1, 30.3, 22.5, 18.6; FT-IR (neat) 3056, 2954, 1755, 1727, 1455, 1443, 1286, 1250,1145, 765, 750, 702 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{37}H_{32}NO_4$: 554.2326, found 554.2320.



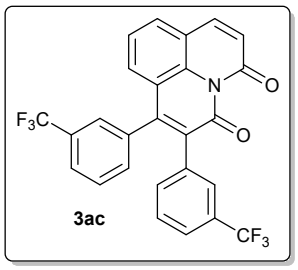
3,5-dioxo-1,2-diphenyl-3H,5H-pyrido[3,2,1-ij]quinolin-9-yl 4-(*N*,*N*-dipropylsulfamoyl)benzoate 3sa. Analytical TLC on silica gel; 7:3 hexane/ethyl acetate R_f = 0.33; brown sticky liquid; yield 58% (74 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 8.4 Hz, 2H), 7.93 (d, *J* = 8.4 Hz, 2H), 7.72 (d, *J* = 9.6 Hz, 1H), 7.58 (d, *J* = 2.8 Hz, 1H), 7.30-7.27 (m, 3H), 7.25 (d, *J* = 2.8 Hz, 1H), 7.18-7.12 (m, 7H), 6.85 (d, *J* = 9.6 Hz, 1H), 3.13-3.09 (m, 4H), 1.58-1.50 (m, 5H), 0.89 (t, *J* = 7.6 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.8, 161.4, 161.4, 147.4, 146.2, 145.6, 139.1, 135.5, 134.9, 134.0, 132.9, 132.0, 131.0, 130.8, 129.8, 128.5, 128.5, 127.7, 127.6, 127.3, 125.5, 123.4, 123.2, 122.5, 120.6, 50.0, 22.0, 11.2. FT-IR (neat) 3057, 9965, 2931, 1725, 1452, 1342, 1251, 1153, 1071, 992, 751, 701 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{37}H_{33}N_2O_6S$: 633.2054, found 633.2055.



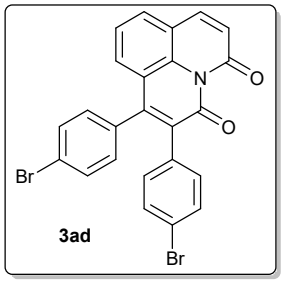
3,5-Dioxo-1,2-diphenyl-3H,5H-pyrido[3,2,1-ij]quinolin-9-yl adamantane-1-carboxylate 3ta. Analytical TLC on silica gel, 7:3 hexane/ethyl acetate R_f = 0.40; brown sticky liquid; yield 65% (66 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, *J* = 9.6 Hz, 1H), 7.39 (d, *J* = 2.4 Hz, 1H), 7.32-7.28 (m, 3H), 7.17-7.10 (m, 7H), 7.07 (d, *J* = 2.8 Hz, 1H), 6.81 (d, *J* = 9.6 Hz, 1H), 2.06 (s, 3H), 2.00 (d, *J* = 2.4 Hz, 6H), 1.78-1.70 (m, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 176.1, 161.5, 161.5, 147.5, 146.8, 139.2, 135.1, 134.9, 134.2, 132.5, 130.8, 129.9, 128.4, 127.6, 127.6, 125.2, 123.4, 122.2, 120.3, 41.2, 38.7, 36.4, 27.9; FT-IR (neat) 2907, 2853, 1726, 1449, 1207, 1180, 1048, 703 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{35}H_{30}NO_4$: 528.2169, found 528.2169.



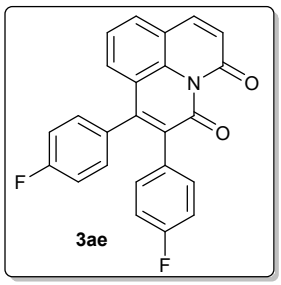
1,2-Di-*m*-tolyl-3H,5H-pyrido[3,2,1-ij]quinoline-3,5-dione 3ab. Analytical TLC on silica gel; 3:2 hexane/ethyl acetate R_f = 0.33; brown solid; mp 223-224 °C; yield 68% (52 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.73 (d, *J* = 9.5 Hz, 1H), 7.66 (d, *J* = 7.5 Hz, 1H), 7.44-7.43 (m, 1H), 7.31(t, *J* = 7.5 Hz, 1H), 7.19 (t, *J* = 7.5 Hz, 1H), 7.09 (d, *J* = 7.5 Hz, 1H), 7.05 (t, *J* = 7.5 Hz, 1H), 7.00 (s, 1H), 6.96-6.89 (m, 4H), 6.79 (d, *J* = 10.0 Hz, 1H), 2.28 (s, 3H), 2.21 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.93, 161.90, 148.2, 139.9, 137.8, 136.9, 135.3, 134.8, 134.4, 134.2, 131.5, 131.1, 130.5, 130.4, 128.9, 128.2, 128.1, 127.9, 127.4, 126.9, 124.4, 123.7, 121.2, 119.4, 21.5, 21.4; FT-IR (neat) 3054, 2922, 1718, 1665, 1258, 1137, 837, 774, 703 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{26}H_{20}NO_2$: 378.1489, found 378.1496.



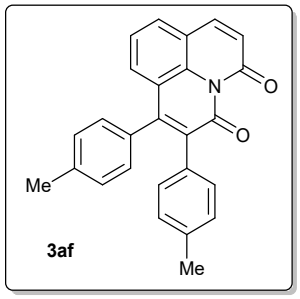
1,2-Bis(3-(trifluoromethyl)phenyl)-3H,5H-pyrido[3,2,1-ij]quinoline-3,5-dione 3ac. Analytical TLC on silica gel; 3:2 hexane/ethyl acetate R_f = 0.3; colourless solid; mp 240-241 °C; yield 67% (68 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.77-7.73 (m, 2H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.48 (t, *J* = 7.8 Hz, 1H), 7.44 (d, *J* = 7.5 Hz, 1H), 7.40-7.37 (m, 4H), 7.35-7.31 (m, 2H), 7.30 (s, 1H), 6.82 (d, *J* = 9.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.5, 161.0, 147.5, 140.0, 135.7, 135.0, 134.6, 134.2, 133.6, 133.0, 131.5, 131.1 (J_{C-F} = 33.0 Hz), 130.7, 130.1 (J_{C-F} = 32.0 Hz), 129.2, 128.3, 127.8 (J_{C-F} = 3.8 Hz), 126.7 (J_{C-F} = 3.6 Hz), 125.4 (J_{C-F} = 3.8 Hz), 124.6 (J_{C-F} = 3.6 Hz), 124.6, 124.3, 122.7 (J_{C-F} = 270.6 Hz), 122.5 (J_{C-F} = 270.5 Hz), 120.1, 119.7; ^{19}F NMR (470 MHz, $CDCl_3$) δ -63.00, -63.05; FT-IR (neat) 3064, 1723, 1666, 1433, 1331, 1123, 1075, 834, 707 cm^{-1}; HRMS (ESI) *m/z* $[M+Na]^+$ calcd for $C_{26}H_{13}F_6NO_2Na$: 508.0743, found 508.0739.



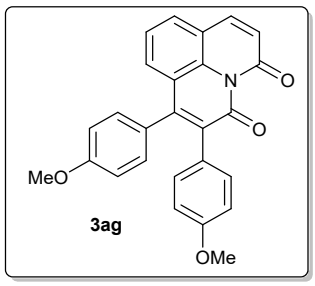
1,2-Bis(4-bromophenyl)-3H,5H-pyrido[3,2,1-ij]quinoline-3,5-dione 3ad. Analytical TLC on silica gel, 3:2 hexane/ethyl acetate R_f = 0.32; dark brown solid; mp 272-273°C; yield 76% (76.5 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 9.6 Hz, 1H), 7.70 (dd, *J* = 1.6, 7.3 Hz, 1H), 7.49-7.47 (m, 2H), 7.39-7.32 (m, 4H), 7.02-6.99 (m, 4H), 6.79 (d, *J* = 9.6 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.6, 161.2, 147.2, 139.9, 134.9, 133.9, 133.4, 132.9, 132.5, 131.9, 131.4, 131.1, 131.1, 130.8, 124.5, 124.0, 122.9, 122.2, 120.5, 119.6; FT-IR (neat) 3062, 2924, 1717, 1567, 1486, 1252, 1148, 1071, 1011, 802, 776 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{24}H_{14}Br_2NO_2$: 505.9386, found 505.9394.



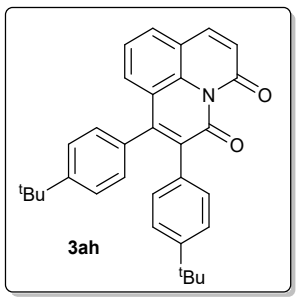
1,2-Bis(4-fluorophenyl)-3H,5H-pyrido[3,2,1-ij]quinoline-3,5-dione 3ae. Analytical TLC on silica gel; 3:2 hexane/ethyl acetate R_f = 0.29; dark brown solid; mp 255-256 °C; yield 71% (54 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 9.6 Hz, 1H), 7.70-7.67 (m, 1H), 7.42-7.39 (m, 1H), 7.35 (t, *J* = 7.2 Hz, 1H), 7.12-7.07 (m, 4H), 7.05 (t, *J* = 8.8 Hz, 2H), 6.91 (t, *J* = 8.4 Hz, 2H), 6.80 (d, *J* = 10.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.5 (d, J_{C-F} = 247.7 Hz), 163.1 (d, J_{C-F} = 246.1 Hz), 161.6, 161.5, 147.5, 139.9, 134.9, 133.8, 132.7 (d, J_{C-F} = 8.1 Hz), 131.7 (d, J_{C-F} = 8.1 Hz), 131.1 (d, J_{C-F} = 3.6 Hz), 130.9, 130.8, 130.1 (J_{C-F} = 3.7 Hz), 124.5, 123.9, 120.9, 119.6, 115.8 (d, J_{C-F} = 21.7 Hz), 114.9, (d, J_{C-F} = 21.3 Hz); ^{19}F NMR (470 MHz, $CDCl_3$) δ -112.31, -113.85; FT-IR (neat) 3069, 1721, 1600, 1507, 1224, 1155, 838, 816 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{24}H_{14}FNO_2$: 386.0987, found 386.0974.



1,2-Di-p-tolyl-3H,5H-pyrido[3,2,1-ij]quinoline-3,5-dione 3af. Analytical TLC on silica gel; 3:2 hexane/ethyl acetate R_f= 0.32; brown solid; mp 268-269 °C; yield 75% (55.5 mg); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 9.6 Hz, 1H), 7.64 (dd, *J* = 1.5, 7.5 Hz, 1H), 7.44 (dd, *J* = 1.5, 8.0 Hz, 1H), 7.30 (d, *J* = 7.6 Hz, 1H), 7.12 (d, J = 8.0 Hz, 2H), 7.04-6.97 (m, 7H), 6.78 (d, *J* = 9.6 Hz, 1H), 2.34 (s, 3H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.0, 161.9, 147.9, 139.8, 137.9, 137.1, 134.8, 134.3, 132.5, 131.4, 131.1, 130.8, 130.4, 129.8, 129.0, 128.3, 124.4, 123.7, 121.4, 119.4, 21.44, 21.41; FT-IR (neat) 3025, 2920, 1720, 1569, 1252, 1147, 1113, 838, 798, 748 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{26}H_{20}NO_2$: 378.1489, found 378.1492.

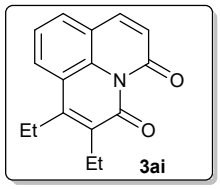


1,2-Bis(4-methoxyphenyl)-3H,5H-pyrido[3,2,1-ij]quinoline-3,5-dione 3ag. Yield: trace; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{26}H_{20}NO_4$: 410.1387, found 410.1396.

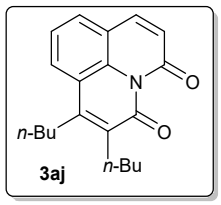


1,2-Bis(4-(*tert*-butyl)phenyl)-3H,5H-pyrido[3,2,1-ij]quinoline-3,5-dione 3ah. Analytical TLC on silica gel; 7:3 hexane/ethyl acetate R_f = 0.35; brown solid; mp 265-266 °C; yield 70% (63 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.73 (d, *J* = 9.5 Hz, 1H), 7.65 (d, *J* = 7.5 Hz, 1H), 7.55 (d, *J* = 8.0 Hz, 1H), 7.32-7.27 (m, 3H), 7.15 (d, *J* = 8.5 Hz, 2H), 7.04 (t, *J* = 8.0 Hz, 4H), 6.78 (d, *J* = 9.5 Hz, 1H), 1.28 (s, 9H), 1.22 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.9, 151.2, 150.1, 148.2, 139.9, 134.9, 134.4, 132.5, 131.4, 131.1, 130.6, 130.4,

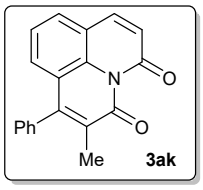
129.7, 125.0, 124.4, 124.3, 123.7, 121.3, 119.4, 34.7, 34.5, 31.34, 31.33; FT-IR (neat) 2959, 1722, 1567, 1457, 1254, 1152, 1115, 837, 812, 752 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{32}H_{32}NO_2$: 462.2428, found 462.2435.



1,2-Diethyl-3H,5H-pyrido[3,2,1-ij]quinoline-3,5-dione 3ai. Analytical TLC on silica gel; 7:3 hexane/ethyl acetate R_f = 0.4; sticky brown liquid; yield 61% (31 mg); ^1H NMR (600 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.4 Hz, 1H), 7.66 (d, *J* = 9.6 Hz, 1H), 7.61 (d, *J* = 7.2 Hz, 1H), 7.44 (t, *J* = 7.8 Hz, 1H), 6.73 (d, *J* = 9.6 Hz, 1H), 2.95-2.91 (m, 2H), 2.81-2.77 (m, 2H), 1.32 (t, *J* = 7.8 Hz, 3H), 1.24 (t, *J* = 7.8 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.1, 147.1, 139.9, 135.2, 134.5, 129.8, 127.3, 124.3, 123.9, 120.0, 119.7, 22.134, 21.1, 14.4, 13.8.; FT-IR (neat) 2970, 1715, 1456, 1234, 1124, 839, 751 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{16}H_{16}NO_2$: 254.1176, found 254.1171.

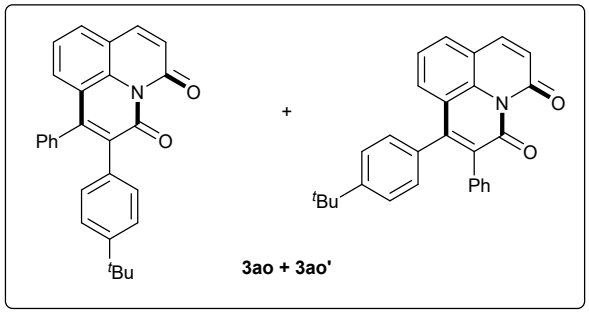


1,2-Dibutyl-3H,5H-pyrido[3,2,1-ij]quinoline-3,5-dione 3aj. Analytical TLC on silica gel; 7:3 hexane/ethyl acetate R_f = 0.4; brown liquid; yield 56% (34 mg); ^1H NMR (500 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.0 Hz, 1H), 7.66 (d, *J* = 10.0 Hz, 1H), 7.60 (d, *J* = 7.5 Hz, 1H), 7.43 (t, *J* = 8.0 Hz, 1H), 6.72 (d, *J* = 9.5 Hz, 1H), 2.88 (t, *J* = 8.0 Hz, 2H), 2.75 (t, *J* = 8.0 Hz, 2H), 1.59-1.45 (m, 8 H), 1.03 (t, *J* = 7.5 Hz, 3H), 0.97 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.2, 162.1, 146.0, 139.8, 134.4, 134.3, 129.7, 127.4, 124.2, 123.8, 120.3, 119.6, 32.1, 31.4, 28.8, 27.7, 23.3, 23.3, 14.1, 14.0; FT-IR (neat) 2957, 2928, 2862, 1717, 1662, 1568, 1251, 1125, 838, 751 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{20}H_{24}NO_2$: 310.1802, found 310.1805.



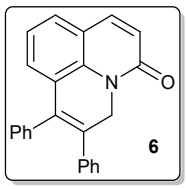
2-Methyl-1-phenyl-3H,5H-pyrido[3,2,1-ij]quinoline-3,5-dione 3ak. Analytical TLC on silica gel; 3:2 hexane/ethyl acetate R_f = 0.35; brown solid; mp 245-246 °C; yield 69% (39.5 mg); ^1H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 9.6 Hz, 1H), 7.61-7.60 (m,

1H), 7.56-7.49 (m, 3H), 7.26-7.21 (m, 4H), 6.78 (d, J = 9.6 Hz, 1H), 2.06 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.8, 162.0, 147.2, 140.0, 135.9, 134.1, 130.7, 130.3, 129.9, 129.0, 128.8, 128.6, 124.3, 123.8, 121.3, 119.4, 15.2; DEPT-135 (125 MHz, $CDCl_3$) 140.0 (upward), 130.3 (upward), 129.9 (upward), 129.0 (upward), 128.7 (upward), 128.6 (upward), 124.3 (upward), 123.8 (upward), 15.2 (upward); FT-IR (neat) 3063, 1720, 1632, 1569, 1351, 1253, 1129, 761 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{19}H_{14}NO_2$: 288.1019, found 288.1019.



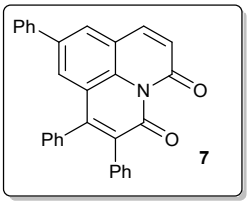
3ao + 3ao'

2-(4-(*tert*-Butyl)phenyl)-1-phenyl-3H,5H-pyrido[3,2,1-ij]quinoline-3,5-dioneb (3ao) and 1-(4-(*tert*-Butyl)phenyl)-2-phenyl-3H, 5H-pyrido[3,2,1-ij]quinoline-3,5-dione (3ao'). Analytical TLC on silica gel; 3:2 hexane/ethyl acetate R_f= 0.4; thick brown liquid; yield 69% (58 mg); 1:1 mixture of regioisomers; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.73 (d, J = 9.5 Hz, 2H), 7.66-7.63 (m, 2H), 7.50 (d, J = 8.0 Hz, 1H), 7.43 (d, J = 7.0 Hz, 1H), 7.32-7.26 (m, 7H), 7.17-7.12 (m, 9H), 7.07-7.02 (m, 4H), 6.78 (d, J = 9.5 Hz, 2H), 1.29 (s, 9H), 1.23 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.0, 161.9, 161.87, 161.86, 151.3, 150.3, 148.3, 147.7, 140.0, 139.9, 135.5, 135.0, 134.9, 134.5, 134.4, 134.3, 132.2, 131.2, 131.1, 131.0, 130.7, 130.6, 130.5, 130.0, 129.6, 128.2, 128.1, 127.5, 127.4, 125.1, 124.5, 124.45, 124.44, 123.7, 121.3, 121.2, 119.5, 119.4, 34.7, 34.5, 31.4, 31.3; FT-IR (neat) 3063, 2960, 1723, 1454, 1254, 1150, 947, 837, 701 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{28}H_{24}NO_2$: 406.1802, found 406.1790.



6,7-Diphenyl-3H,5H-pyrido[3,2,1-ij]quinolin-3-one 6. Analytical TLC on silica gel; 9:1 hexane/ethyl acetate R_f= 0.35; colorless solid; mp 203-204 °C; yield 68% (23 mg); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.75 (d, J = 9.5 Hz, 1H), 7.38 (d, J = 8.0 Hz, 1H), 7.29-7.26 (m, 2H), 7.25-7.22 (m, 1H), 7.17-7.09 (m, 7H), 7.01 (t, J = 7.5 Hz, 1H), 6.94 (d, J = 7.5 Hz, 1H), 6.78 (d, J = 9.5 Hz, 1H), 5.21 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.7, 139.1, 138.4, 136.8, 135.5, 132.2, 132.0, 130.7, 128.5, 128.5, 128.2, 127.6, 127.4, 127.3, 124.8, 122.2,

121.2, 119.7, 49.0; FT-IR (neat) 3056, 2924, 1644, 1582, 1466, 830, 749, 696 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{24}H_{18}NO$: 336.1383, found 336.1384.



1,2,9-Triphenyl-3H,5H-pyrido[3,2,1-ij]quinoline-3,5-dione 7. Analytical TLC on silica gel; 7:3 hexane/ethyl acetate R_f = 0.35; brown solid; mp 245-246 °C; yield 74% (31.5 mg); ^1H NMR (500 MHz, $CDCl_3$) δ 7.86 (d, *J* = 2.0 Hz, 1H), 7.80 (d, *J* = 10.0 Hz, 1H), 7.64 (d, *J* = 2.0 Hz, 1H), 7.437 (dt, *J* = 7.5, 15.0 Hz, 4H), 7.46-7.40 (m, 1H), 7.37-7.34 (m, 3H), 7.32-7.29 (m, 7H), 6.83 (d, *J* = 10.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.7, 161.7, 148.2, 139.9, 139.0, 137.0, 135.2, 134.8, 134.3, 134.1, 130.9, 129.9, 129.4, 129.2, 129.0, 128.4, 128.4, 128.1, 127.63, 127.60, 127.1, 124.8, 121.6, 119.9; FT-IR (neat) 3055, 2923, 2853, 1723, 1454, 1259, 1154, 757, 699 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{30}H_{20}NO_2$: 426.1489, found 426.1472.

Mechanistic Investigation

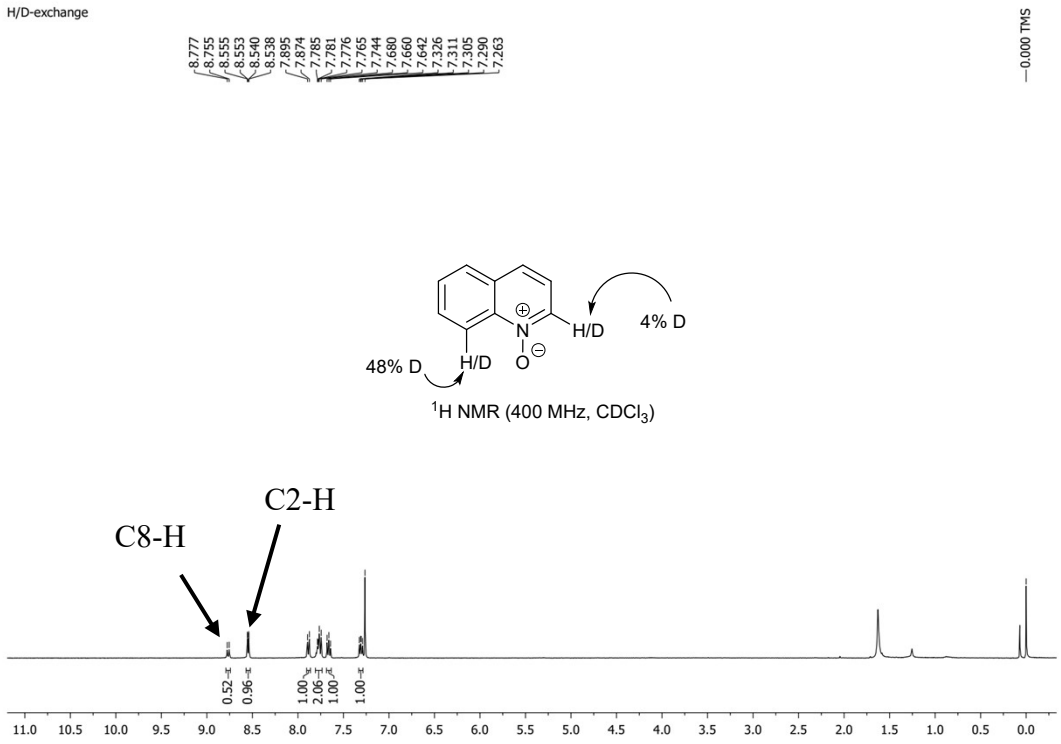
Radical Scavenger Experiment (Scheme 4a). In a pressure tube, quinoline *N*-oxide **1a** (0.2 mmol, 29 mg), diphenylcyclopropenone **2a** (0.24 mmol, 49.5 mg), $[RhCp^*Cl_2]_2$ (0.01 mmol, 6 mg), $AgBF_4$ (0.04 mmol, 8 mg), Ag_2O (0.2 mmol, 46 mg), TEMPO or BHT (1 or 2 equiv), H_2O (50 μL) and $(CH_2Cl)_2$ (1 mL) were stirred for 2 h at 90 °C under argon atmosphere. The reaction mixture was cooled to room temperature and passed through celite pad using CH_2Cl_2 (20 mL). Evaporation of the solvent gave a residue that was purified according to general procedure to isolate **3aa**.

Radical scavenger	Equiv	Yield **3aa**
TEMPO	1	65 (45 mg)
	2	60 (42 mg)

Radical scavenger	Equiv	Yield **3aa**
BHT	1	68 (47.5 mg)
	2	66 (46 mg)

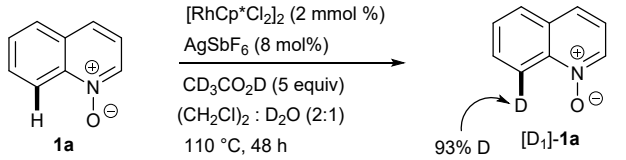
H/D Exchange Experiment of 1a with D_2O in Absence of 2a (Scheme 4b). In a pressure tube, quinoline *N*-oxide **1a** (0.2 mmol, 29 mg), $[RhCp^*Cl_2]_2$ (0.01 mmol, 6 mg), $AgBF_4$ (0.04 mmol, 8 mg), Ag_2O (0.2 mmol, 46 mg), H_2O (50 μL), $(CH_2Cl)_2$ (1 mL) and D_2O (6 mmol, 110 μL) were

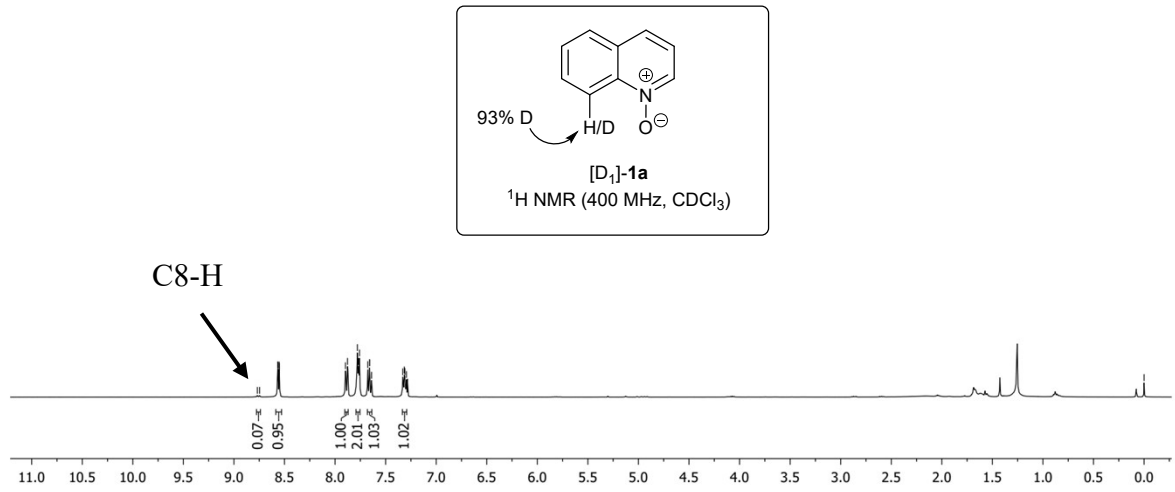
stirred for 2 h at 90 °C under argon atmosphere. The reaction mixture was cooled to room temperature and passed through short celite pad using CH_2Cl_2 (20 mL). Evaporation of the solvent gave a residue that was purified according to general procedure and the starting material was recovered (86%, 25 mg). Deuterium incorporation of the recovered starting material was found to be 48% at C8 position while 4% at C2 position confirmed by using ^{1}H NMR.



Preparation of Quinoline *N*-oxide-8-d$_1$ [D$_1$]-1a.[1c] In a pressure tube, quinoline *N*-oxide **1a** (1 mmol, 145 mg), $[RhCp^*Cl_2]_2$ (0.02 mmol, 12 mg), $AgSbF_6$ (0.08 mmol, 28 mg), PivOH (0.1 mmol, 11 mg), CD_3CO_2D (5 mmol, 305 µL), D_2O (0.5 mL) and $(CH_2Cl)_2$ (1 mL) were stirred at 110 °C for 48 h. The reaction mixture was cooled to room temperature and passed through

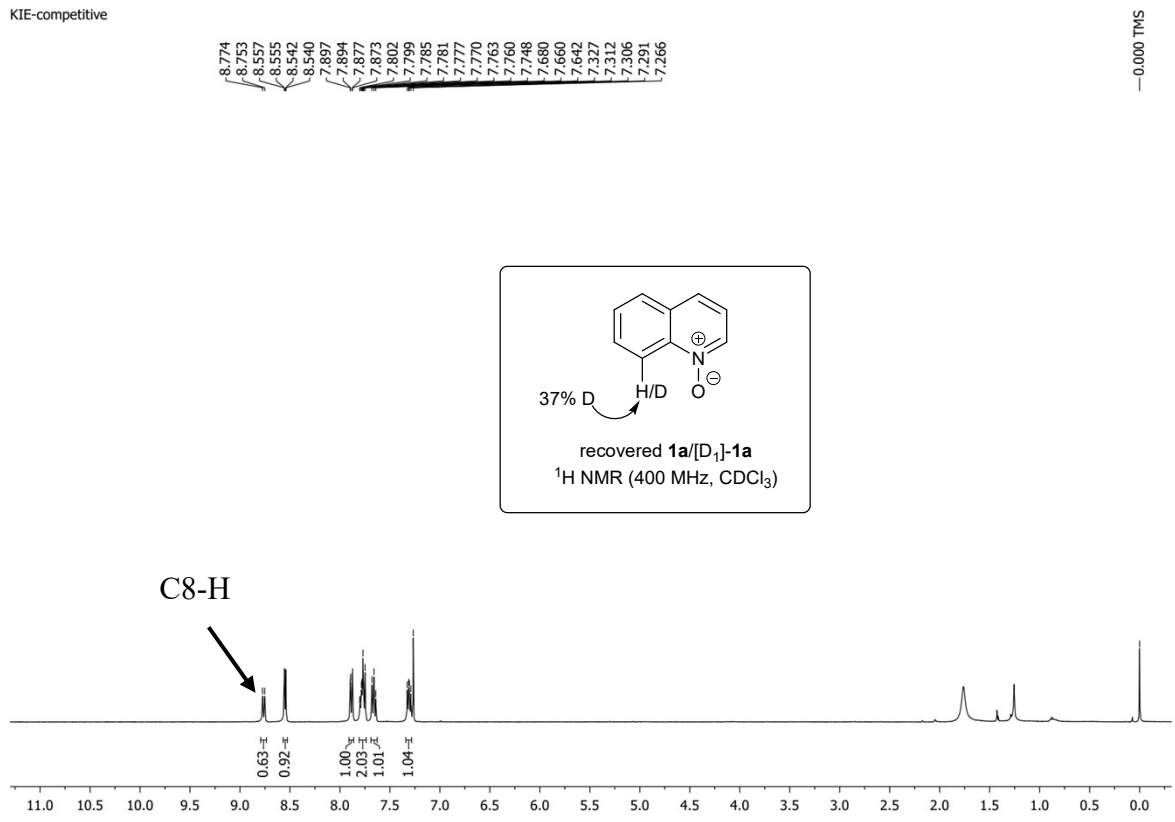
a short celite pad using CH_2Cl_2 (20 mL). Evaporation of the solvent gave a residue that was purified according to general procedure to afford [D_1]-**1a** in 84% yield (123 mg). The deuterium incorporation at C8 position of the recovered starting material was found 93% using ^{1}H NMR.





Kinetic Isotope Effect Experiments (Scheme 4c)

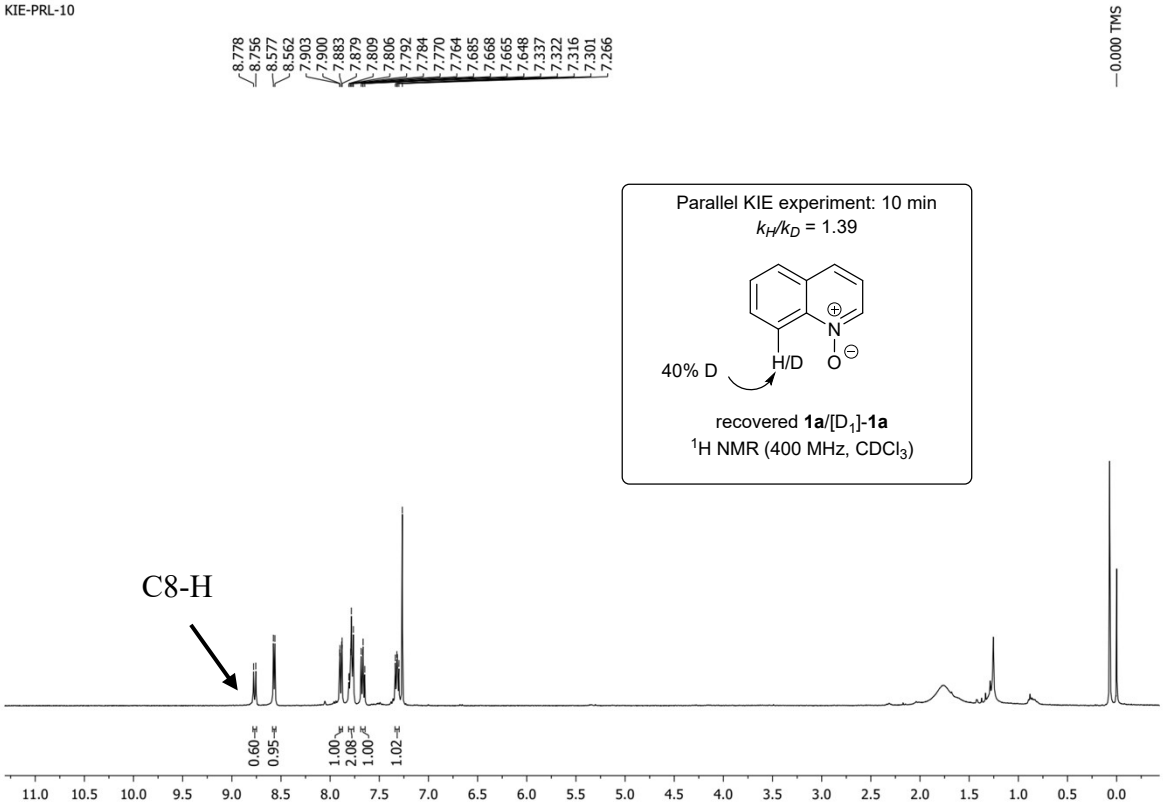
Competitive Kinetic Isotope Experiment. In a pressure tube, *N*-oxide **1a** (0.2 mmol, 29 mg), diphenylcyclopropenone **2a** (0.24 mmol, 49.5 mg), [$RhCp^*Cl_2$]$_2$ (0.01 mmol, 6 mg), $AgBF_4$ (0.04 mmol, 8 mg), Ag_2O (0.2 mmol, 46 mg), H_2O (50 µL) and $(CH_2Cl)_2$ (1 mL) were stirred for 10 minutes at 90 °C under argon atmosphere. The quinoline *N*-oxide **1a**/[D_1]-**1a** was recovered in 73% (22.5 mg) yield by using the general procedure as described. The KIE value was found as k_H/k_D =1.58 based on ^{1}H NMR analysis of recovered **1a**/[D_1]-**1a**.



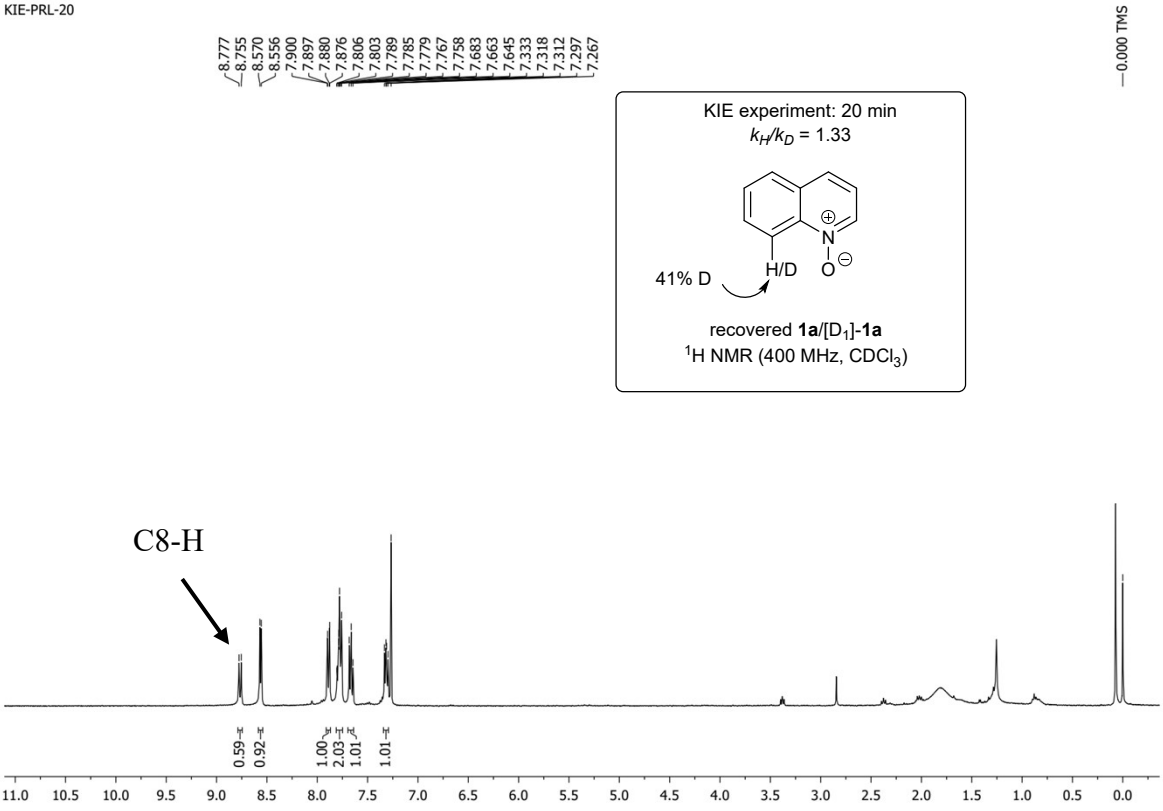
Parallel Kinetic Isotope Experiments. Quinoline *N*-oxide **1a** (0.2 mmol, 29 mg) and quinoline 1-oxide-8-d_1 [D_1]-**1a** (0.2 mmol, 32 mg) were reacted with diphenylcyclopropenone **2a** (0.24 mmol, 49.5 mg) under standard conditions for 10 minutes (set 1), 20 minutes (set 2) and 30 minutes (set 3). Then, the reaction mixtures were mixed and purified according to described general procedure. The recovered *N*-oxide **1a**/[D_1]-**1a** was examined using 400 MHz ^{1}H NMR analysis.

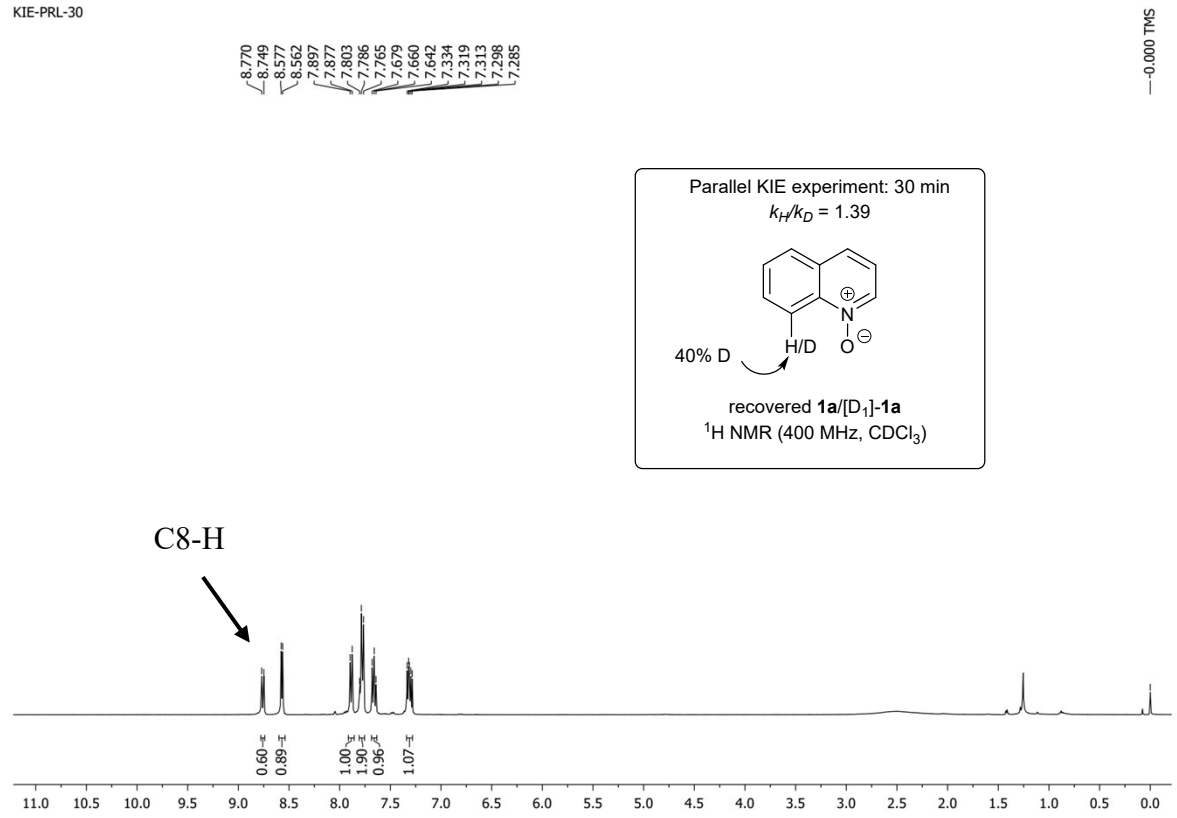
time (minutes)	k_H/k_D	yield **1a**/[D_1]-**1a**
10	1.39	79%
20	1.33	65%
30	1.39	57%

KIE-PRL-10



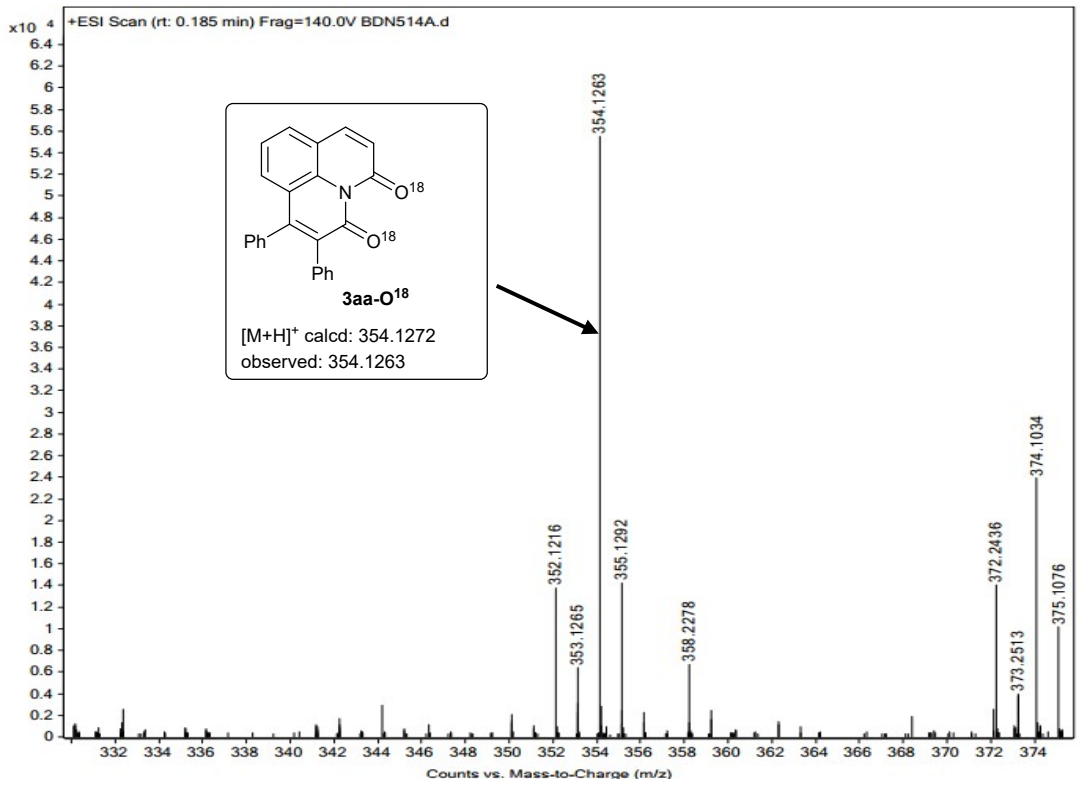
KIE-PRL-20





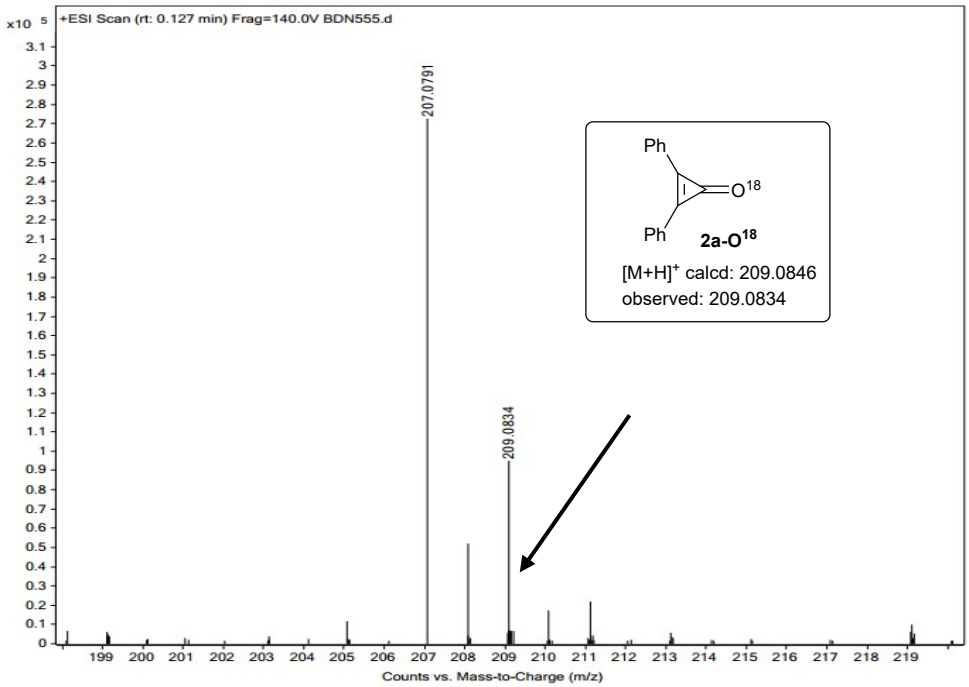
Control Experiments (Scheme 4d)

i) Reaction of 1a and 2a in presence of $H_2{}^{18}O$. In a pressure tube, quinoline *N*-oxide **1a** (0.2 mmol, 29 mg), diphenylcyclopropenone **2a** (0.24 mmol, 49.5 mg), $[RhCp^*Cl_2]_2$ (0.01 mmol, 6 mg), $AgBF_4$ (0.04 mmol, 8 mg), Ag_2O (0.2 mmol, 46 mg), $(CH_2Cl)_2$ (1 mL) and $H_2{}^{18}O$ (50 µL) were stirred for 2 h at 90 °C under argon atmosphere. The reaction mixture was cooled to room temperature and passed through celite pad using CH_2Cl_2 (20 mL). Evaporation of the solvent gave a residue that was purified according to general procedure to isolate **3aa-^{18}O** in 71% yield (49.5 mg). (ESI) *m/z* $[M+H]^+$ calcd for $[C_{24}H_{16}N^{18}O_2]^+$ (**3aa-^{18}O**): 354.1272, found 354.1263.

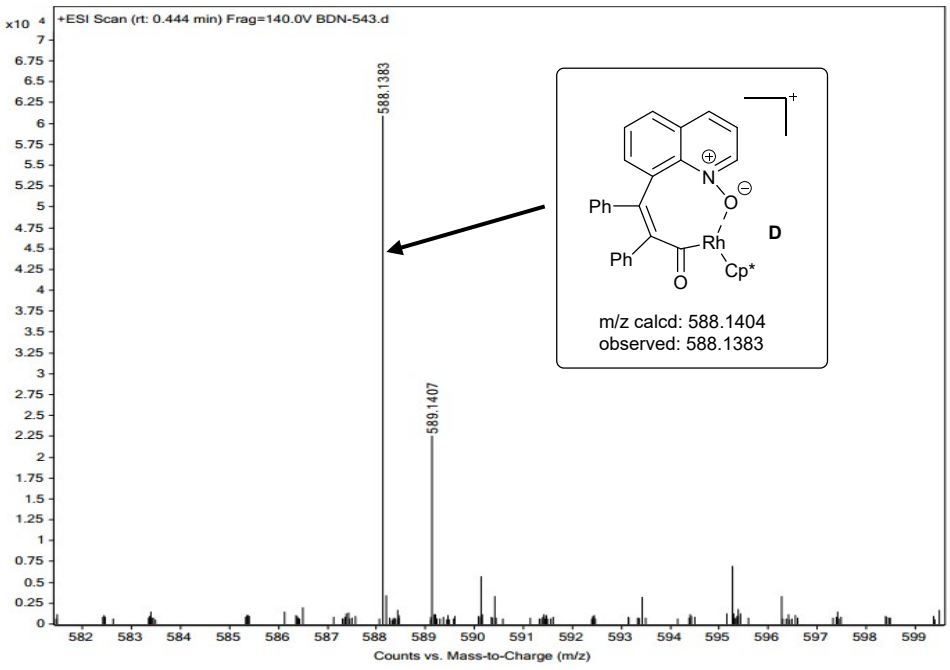


ii) Reaction of 2a with 4. In a pressure tube, 2-quinolone **4** (0.2 mmol, 29 mg), diphenylcyclopropenone **2a** (0.24 mmol, 49.5 mg), $[RhCp^*Cl_2]_2$ (0.01 mmol, 6 mg), $AgBF_4$ (0.04 mmol, 8 mg), Ag_2O (0.2 mmol, 46 mg), H_2O (50 µL) and $(CH_2Cl)_2$ (1 mL) were stirred for 2 h at 90 °C under argon atmosphere. The reaction mixture was cooled to room temperature and HRMS analysis confirmed no **3aa** was formed.

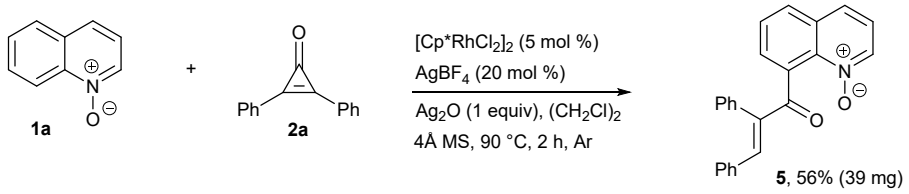
iii) Reaction of 2a in with $H_2{}^{18}O$ in Absence of 1a. In a pressure tube, diphenylcyclopropenone **2a** (0.1 mmol, 21 mg), $[RhCp^*Cl_2]_2$ (0.05 mmol, 3 mg), $AgBF_4$ (0.02 mmol, 4 mg), Ag_2O (0.1 mmol, 23 mg), $(CH_2Cl)_2$ (0.5 mL) and $H_2{}^{18}O$ (25 µL) were stirred for 30 minutes at 90 °C under argon atmosphere. The reaction mixture was cooled to room temperature and HRMS analysis of the crude reaction mixture: (ESI) *m/z* $[M+H]^+$ calcd for $[C_{15}H_{11}{}^{18}O]^+$ (**2a-^{18}O**): 209.0846, found 209.0834.



Detection of Intermediate D (Scheme 4e). In a pressure tube, quinoline *N*-oxide **1a** (0.1 mmol, 14.5 mg), diphenylcyclopropenone **2a** (0.12 mmol, 25 mg), $[RhCp^*Cl_2]_2$ (0.005 mmol 3 mg), $AgBF_4$ (0.02 mmol, 4 mg), Ag_2O (0.1 mmol, 23 mg), H_2O (25 µL) and $(CH_2Cl)_2$ (0.5 mL) were stirred for 30 minutes at 90 °C under argon atmosphere. HRMS analysis of the crude reaction mixture: (ESI) *m/z* calcd for $[C_{34}H_{31}NO_2Rh]^+$ (intermediate **D**): 588.1404, found 588.1383.



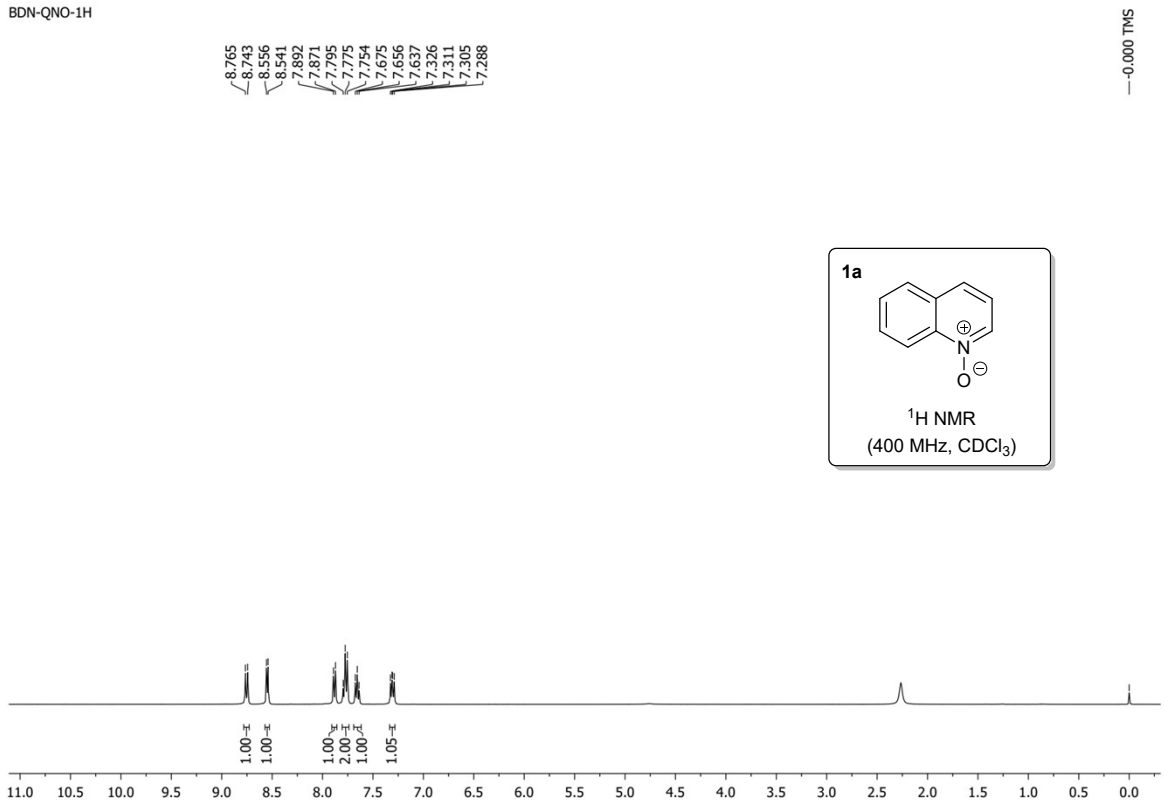
Reaction without H_2O. In a pressure tube, quinoline *N*-oxide **1a** (0.2 mmol, 29 mg), diphenylcyclopropenone **2a** (0.24 mmol, 49.5 mg), $[RhCp^*Cl_2]_2$ (0.01 mmol, 6 mg), $AgBF_4$ (0.04 mmol, 8 mg), Ag_2O (0.2 mmol, 46 mg), $(CH_2Cl)_2$ (2 mL) and 4Å molecular sieves (300 mg) were stirred for 2 h at 90 °C under argon atmosphere. The reaction mixture was cooled to room temperature and passed through celite pad using CH_2Cl_2 (20 mL). Evaporation of the solvent gave a residue that was purified according to general procedure to isolate **5** in 56% (39 mg) yield. Analytical TLC on silica gel; 3:7 hexane/ethyl acetate R_f = 0.25; thick liquid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.43 (d, *J* = 6.0 Hz, 1H), 7.92 (t, *J* = 4.5 Hz 1H), 7.78 (d, *J* = 8.5 Hz, 1H), 7.71-7.70 (m, 2H), 7.44 (d, *J* = 7.0 Hz, 2H), 7.35-7.31 (m, 3H), 7.30-7.27 (m, 1H), 7.14-7.11 (m, 1H), 7.08 (t, *J* = 7.5 Hz, 2H), 6.96-6.93 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 194.7, 142.9, 140.3, 139.1, 136.3, 135.4, 135.0, 134.6, 131.1, 130.6, 130.3, 130.1, 129.0, 128.8, 128.6, 128.4, 128.1, 127.7, 126.0, 121.9; FT-IR (neat) 3060, 1657, 1500, 1312, 1232, 1087, 825, 764 cm^{-1}; HRMS (ESI) *m/z* $[M+H]^+$ calcd for $C_{24}H_{18}NO_2$: 352.1332, found 352.1332.

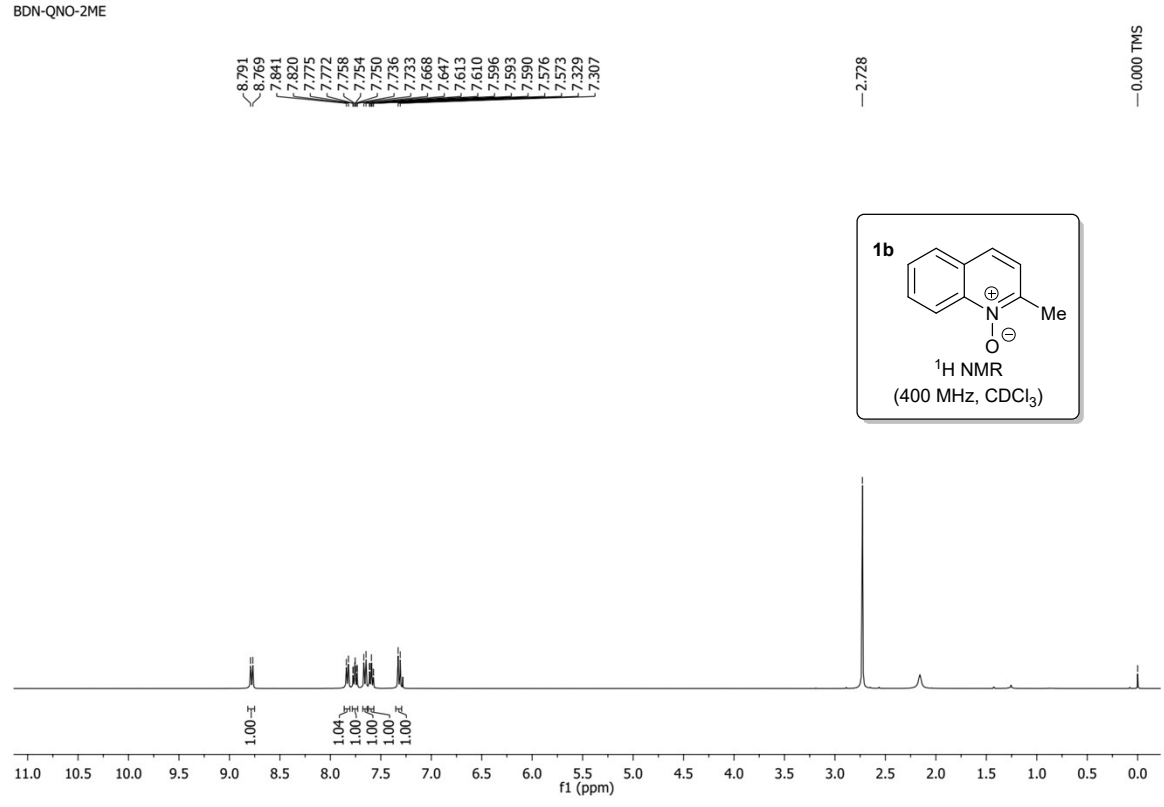


References

1. (a) H. Hwang, J. Kim, J. Jeong and S. Chang, *J. Am. Chem. Soc*., 2014, **136**, 10770; (b) A. K. Dhiman, S. S. Gupta, R. Sharma, R. Kumar and U. Sharma, *J. Org. Chem.*, 2019, **84**, 12871; (c) S. Mandal, P. Karjee, S. Saha and T. Punniyamurthy, *Chem. Commun.*, 2023, **59**, 2823; (d) S. Mandal, T. Paul, P. Karjee, M. Barman and T. Punniyamurthy, *Org. Lett.*, 2023, **25**, 7805.
2. (a) A. Poloukhtine and V. V. Popik, *J. Org. Chem*., 2003, **68**, 7833; (b) G. Kuzmanich, M. N. Gard and M. A. Garcia-Garibay, *J. Am. Chem. Soc.*, 2009, **131**, 11606; (c) C. M. Vanos and T. H. Lambert, *Angew. Chem. Int. Ed.*, 2011, **50**, 12222; (d) R. Li, B. Li, H. Zhang, C.-W. Ju, Y. Qin, X.-S. Xue and D. Zhao, *Nat. Chem.*, 2021, **13**, 1006; (e) Y.-B. Zhang, B.-S. Li, G.-J. Xu, W. Sun and M. Sun, *Org. Lett.*, 2023, **25**, 3922.

NMR (^{1}H, ^{13}C and ^{19}F) Spectra





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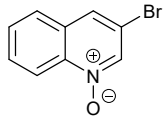
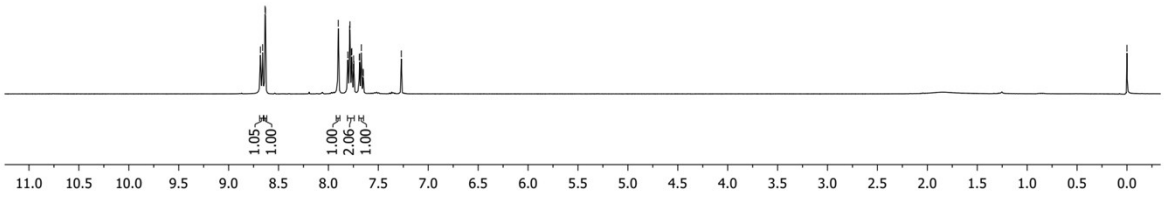
1c



^{1}H NMR
(400 MHz, $CDCl_3$)



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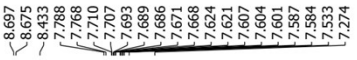
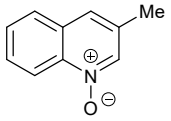
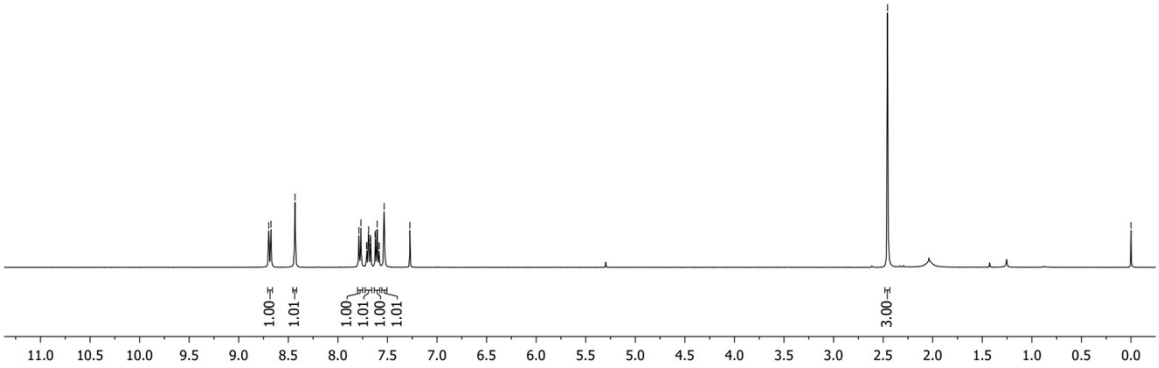


1d



^{1}H NMR
(400 MHz, $CDCl_3$)



BDN-QNO-3Ph

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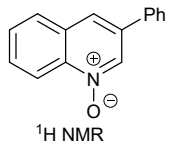
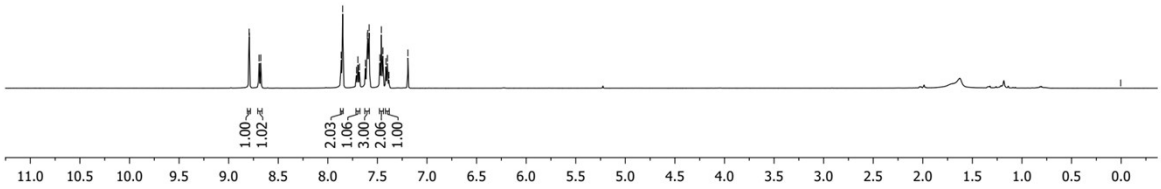
1e



^{1}H NMR
(500 MHz, $CDCl_3$)



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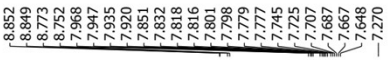

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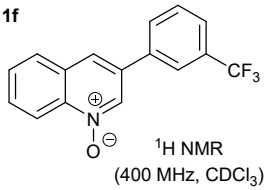
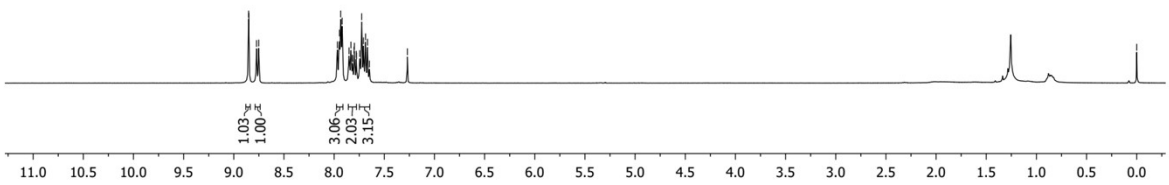
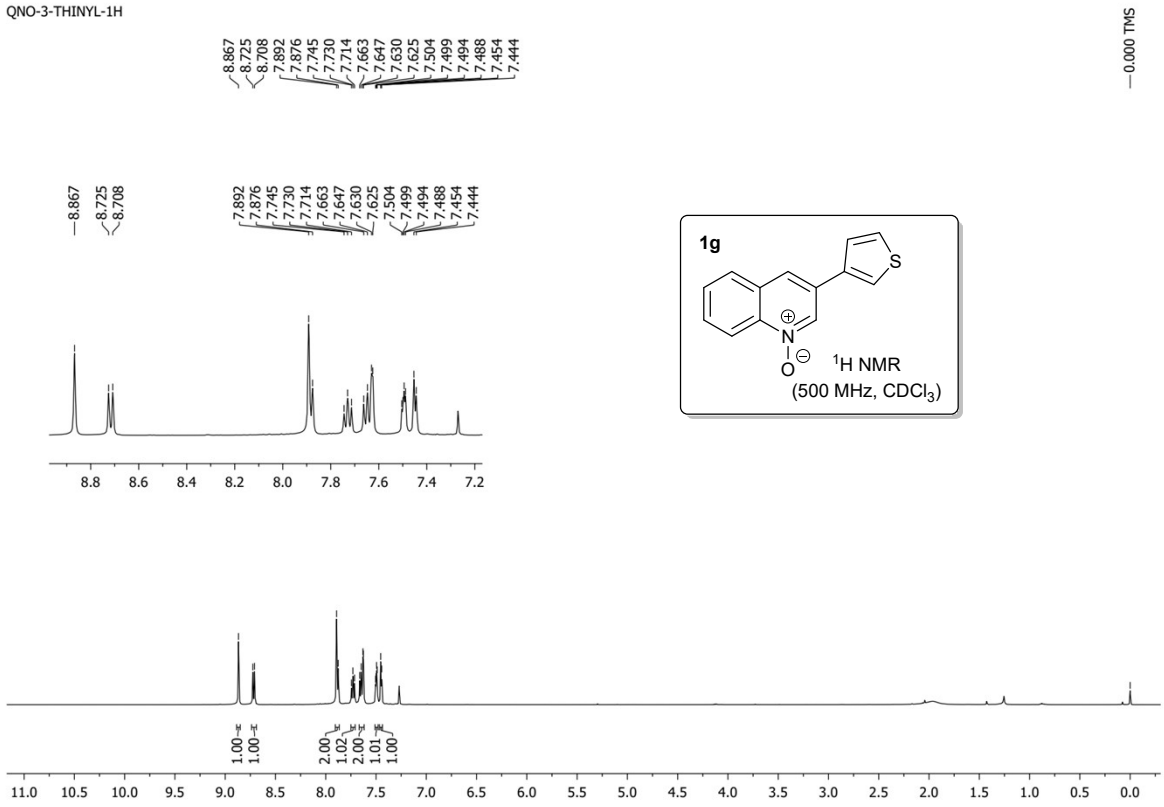
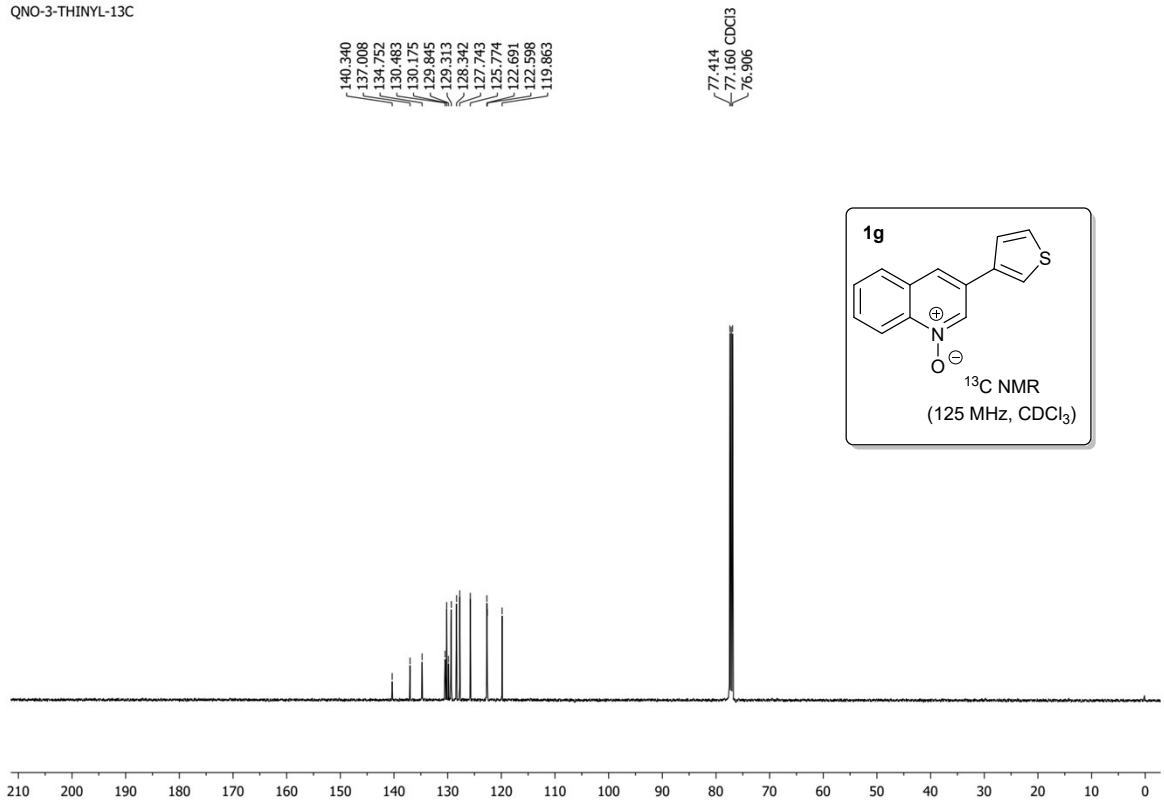
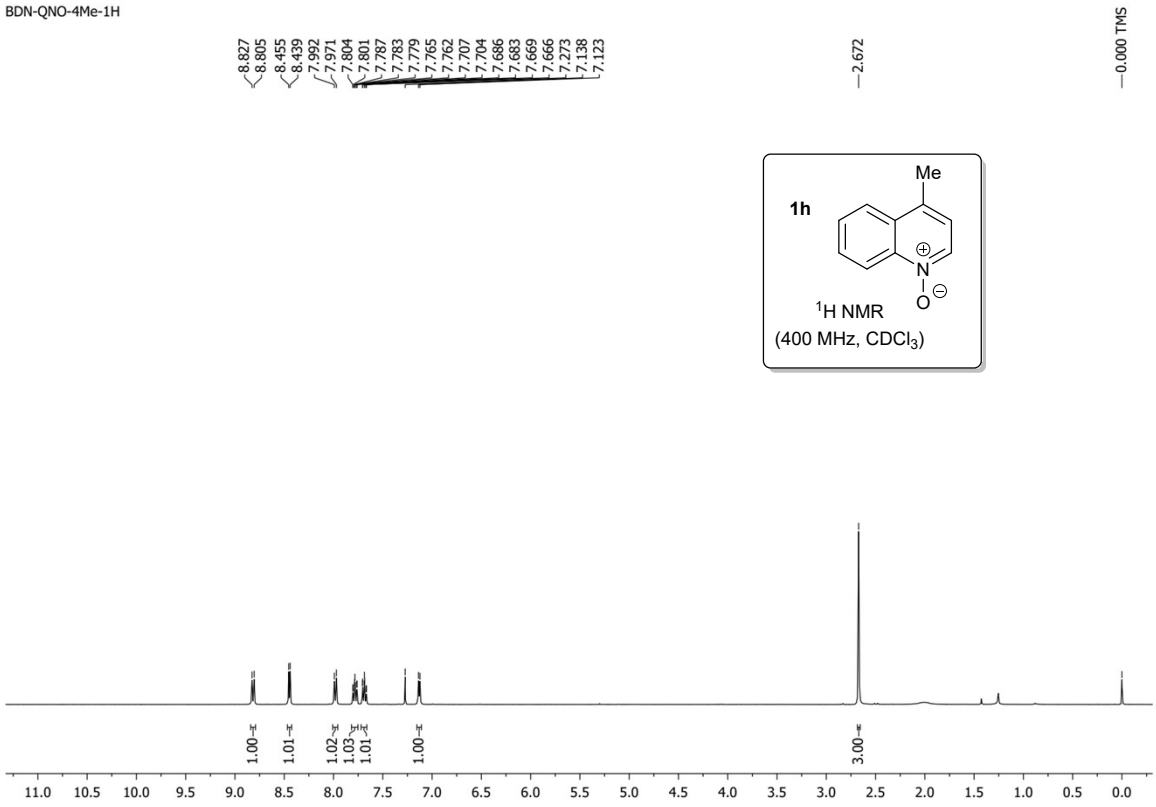


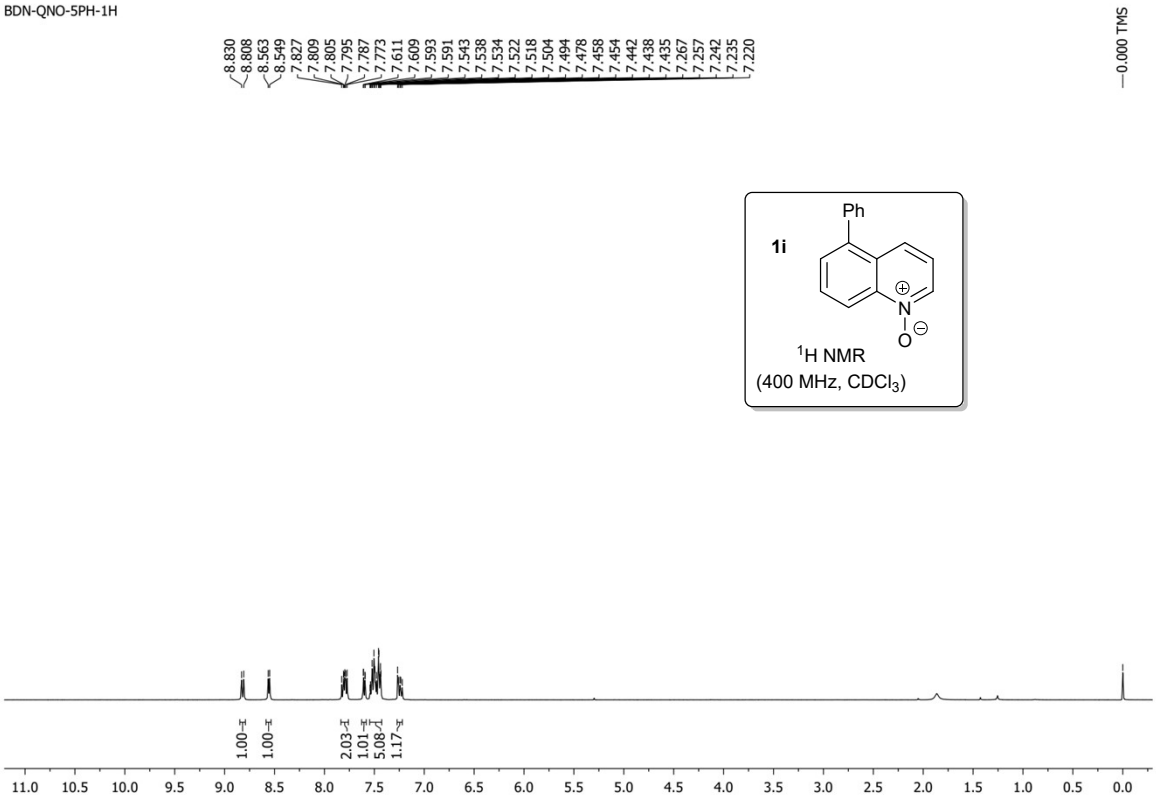
^{1}H NMR
(400 MHz, $CDCl_3$)

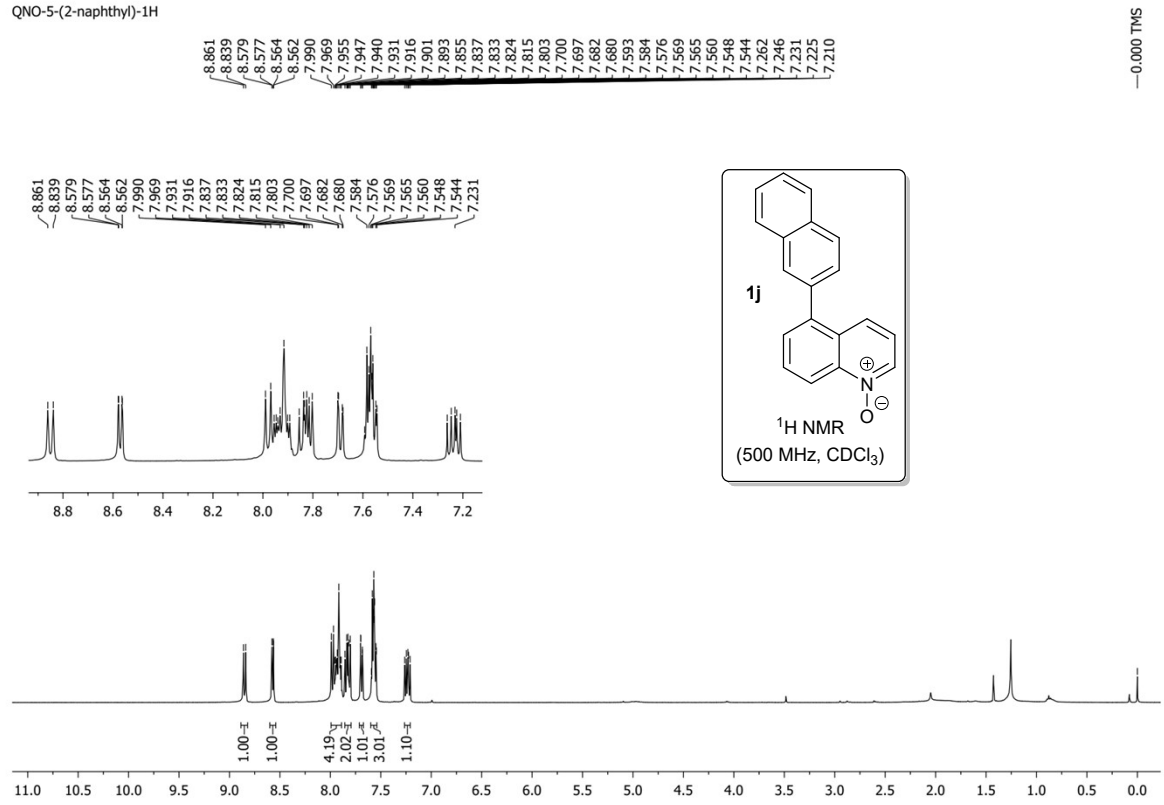


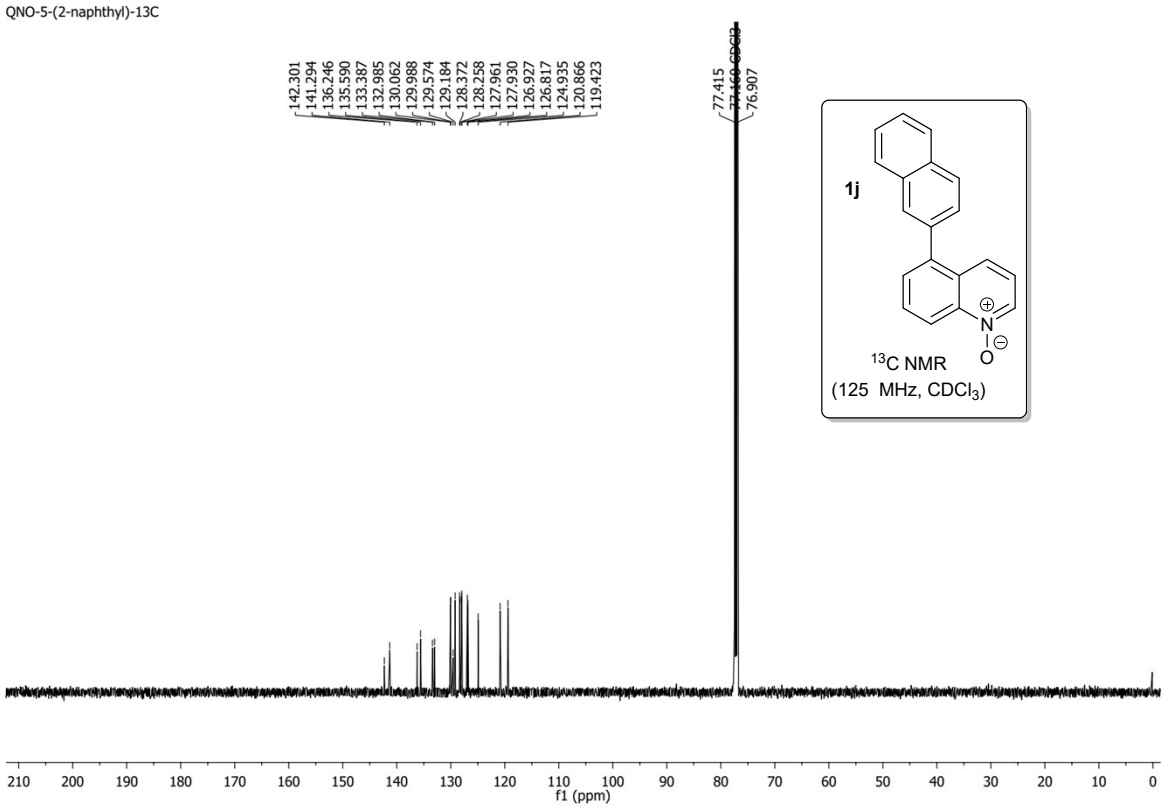

QNO-3-THINYL-1H
8.867
8.725
8.708
7.892
7.876
7.745
7.730
7.714
7.663
7.647
7.630
7.625
7.504
7.499
7.494
7.488
7.454
7.444
0.000 TMS
1g
S
N
O
1H NMR
(500 MHz, CDCl3)
1.00
1.00
2.00
1.02
2.00
1.01
1.00


QNO-3-THINYL-13C
140.340
137.008
134.752
130.483
130.175
129.845
129.313
128.342
127.743
125.774
122.691
122.598
119.863
77.414
77.160 CDCl3
76.906
1g
S
N
O
13C NMR
(125 MHz, CDCl3)

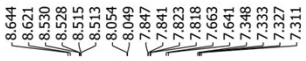

BDN-QNO-4Me-1H
8.827
8.805
8.455
8.439
7.992
7.971
7.804
7.801
7.787
7.783
7.779
7.765
7.762
7.707
7.704
7.686
7.683
7.669
7.666
7.273
7.138
7.123
2.672
0.000 TMS
1h
Me
N
O
^{1}H NMR
(400 MHz, $CDCl_3$)
1.00
1.01
1.02
1.03
1.01
1.00
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

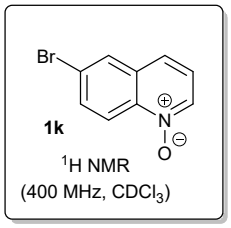

BDN-QNO-5PH-1H
8.830
8.808
8.563
8.549
7.827
7.809
7.805
7.795
7.787
7.773
7.611
7.609
7.593
7.591
7.543
7.538
7.534
7.522
7.518
7.504
7.494
7.478
7.458
7.454
7.442
7.438
7.435
7.267
7.257
7.242
7.235
7.220
0.000 TMS
1i
Ph
N
O
^{1}H NMR
(400 MHz, $CDCl_3$)
1.00
1.00
2.03
1.01
5.08
1.17
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

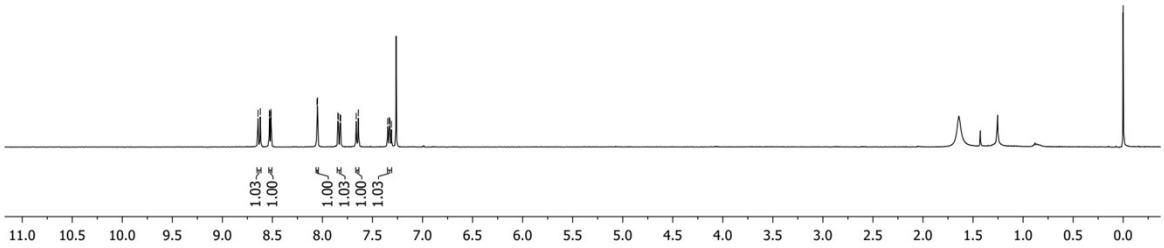

QNO-5-(2-naphthyl)-1H
8.861
8.839
8.579
8.577
8.564
8.562
7.990
7.969
7.955
7.947
7.940
7.931
7.916
7.901
7.893
7.855
7.837
7.833
7.824
7.815
7.803
7.700
7.697
7.682
7.680
7.593
7.584
7.576
7.569
7.565
7.560
7.548
7.544
7.262
7.246
7.231
7.225
7.210
0.000 TMS
1j
^{1}H NMR
(500 MHz, $CDCl_3$)
1.00
1.00
4.19
2.02
1.01
3.01
1.10


QNO-5-(2-naphthyl)-13C
142.301
141.294
136.246
135.590
133.387
132.985
130.062
129.988
129.574
129.184
128.372
128.258
127.961
127.930
126.927
126.817
124.935
120.866
119.423
77.415
77.160
76.907
1j
^{13}C NMR
(125 MHz, $CDCl_3$)
f1 (ppm)

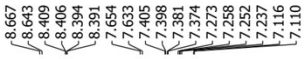
BDN-QNO-6BR-1H

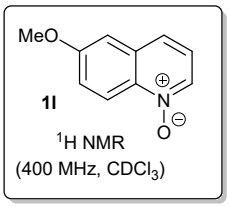


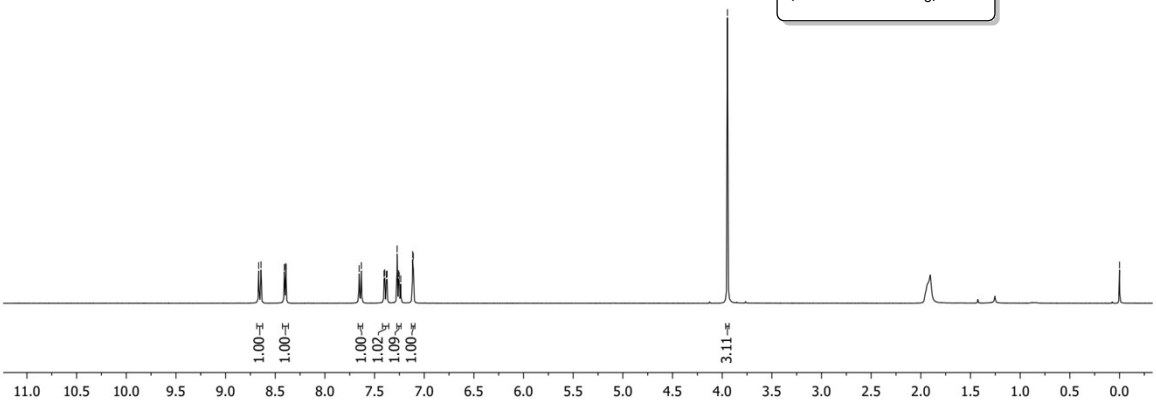




BDN-QNO-6-OME-1H



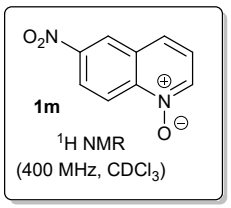




BDN-QNO-6NO2-1H

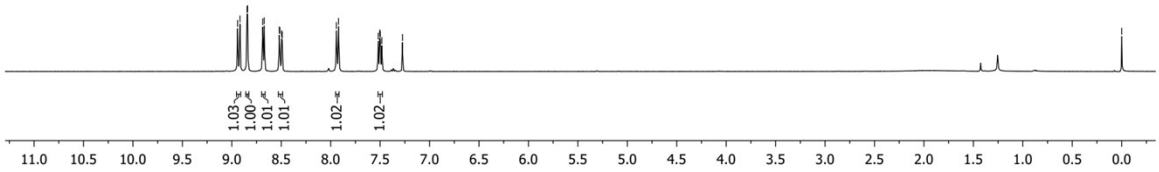
8.941
8.918
8.846
8.840
8.687
8.672
8.520
8.514
8.496
8.490
7.942
7.921
7.519
7.504
7.498
7.483
7.274

0.000 TMS



1m

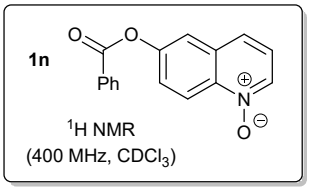
^{1}H NMR
(400 MHz, $CDCl_3$)



BDN-QNO-6-CO2Ph

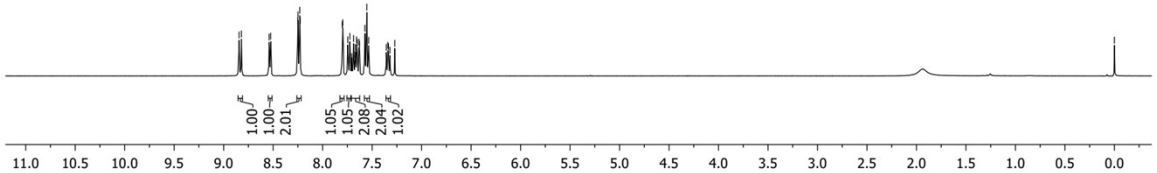
8.844
8.821
8.540
8.525
8.252
8.249
8.231
8.228
7.802
7.796
7.746
7.725
7.709
7.706
7.703
7.688
7.672
7.669
7.666
7.657
7.651
7.633
7.627
7.573
7.554
7.535
7.356
7.341
7.335
7.320
7.271

0.000 TMS

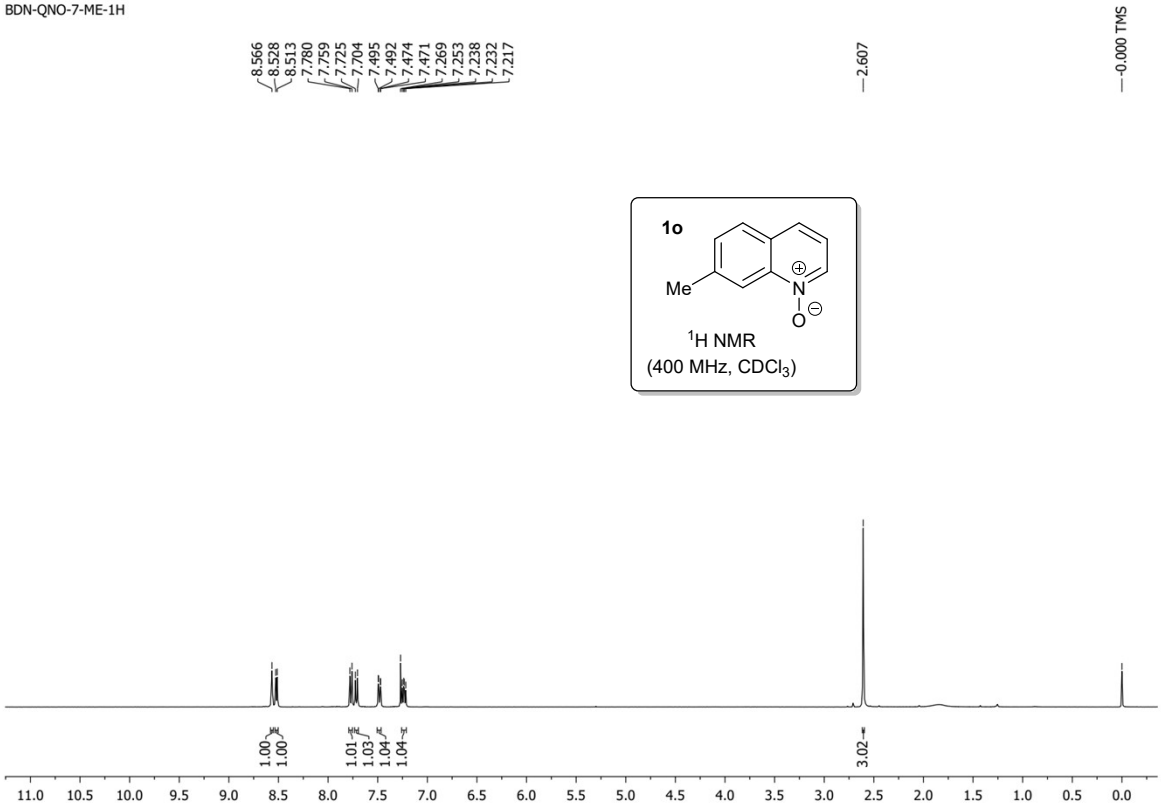


1n

^{1}H NMR
(400 MHz, $CDCl_3$)



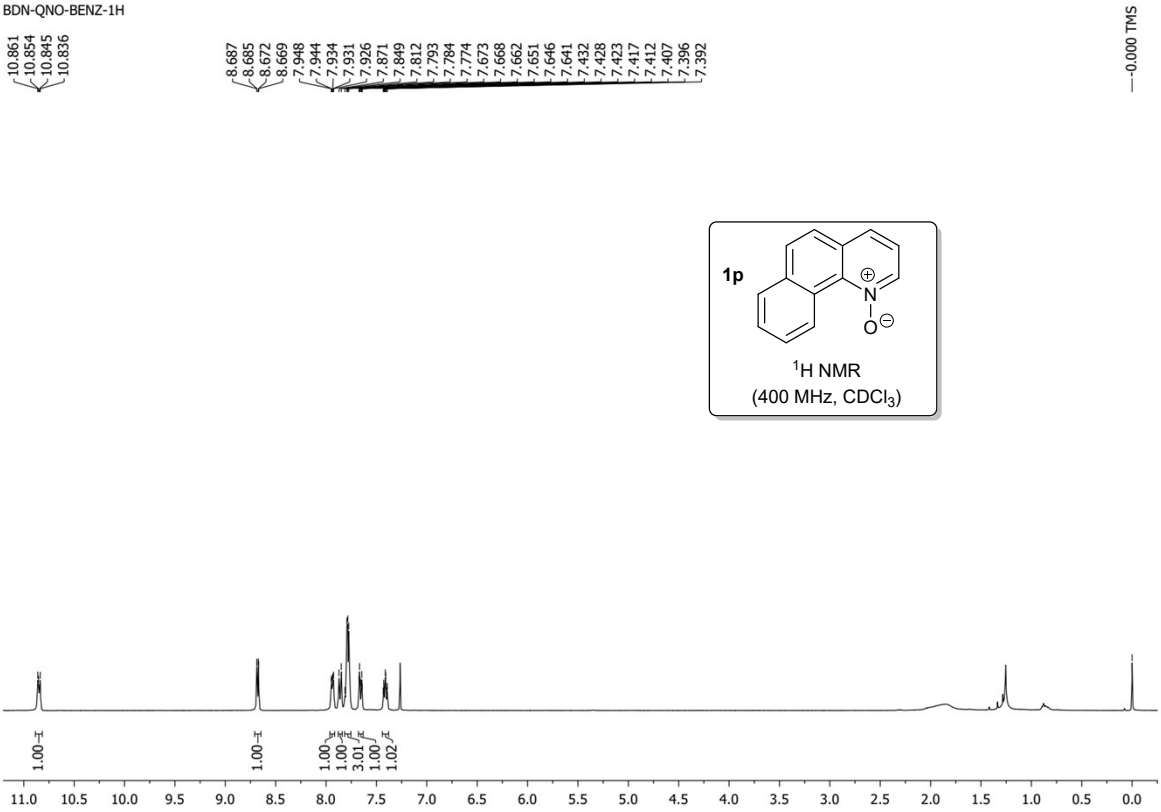
BDN-QNO-7-ME-1H



1o

^{1}H NMR
(400 MHz, $CDCl_3$)

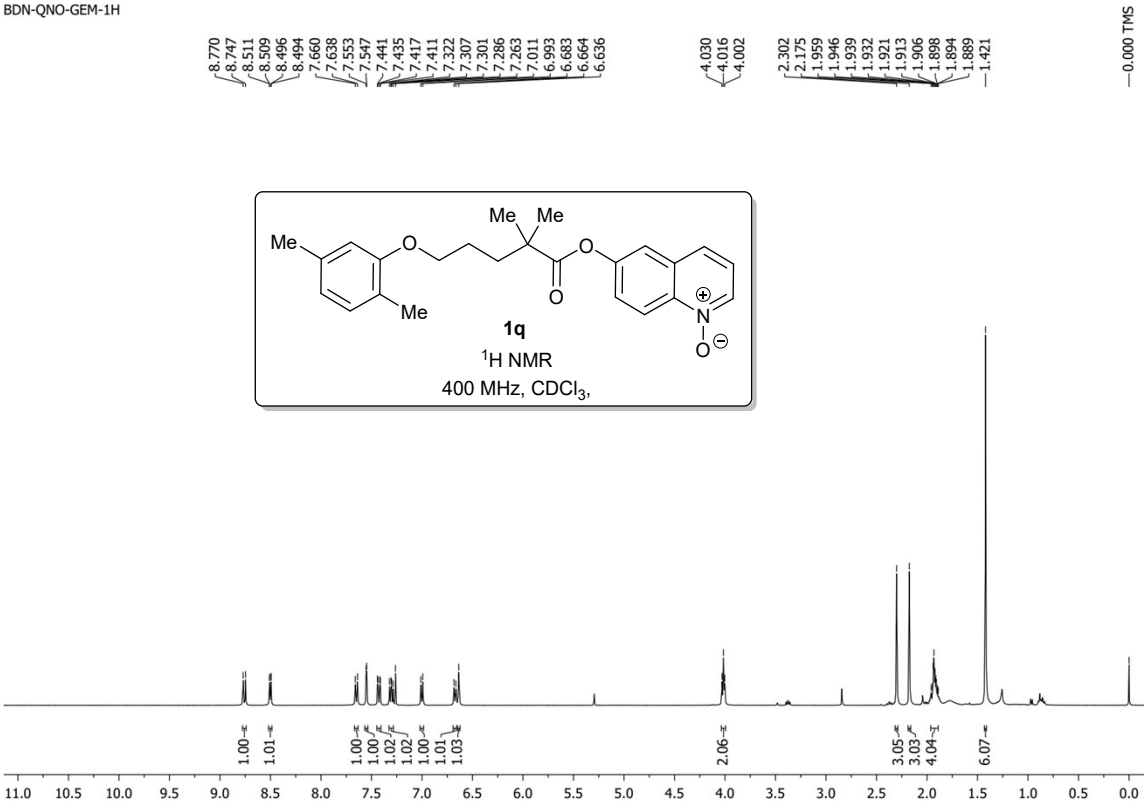
BDN-QNO-BENZ-1H



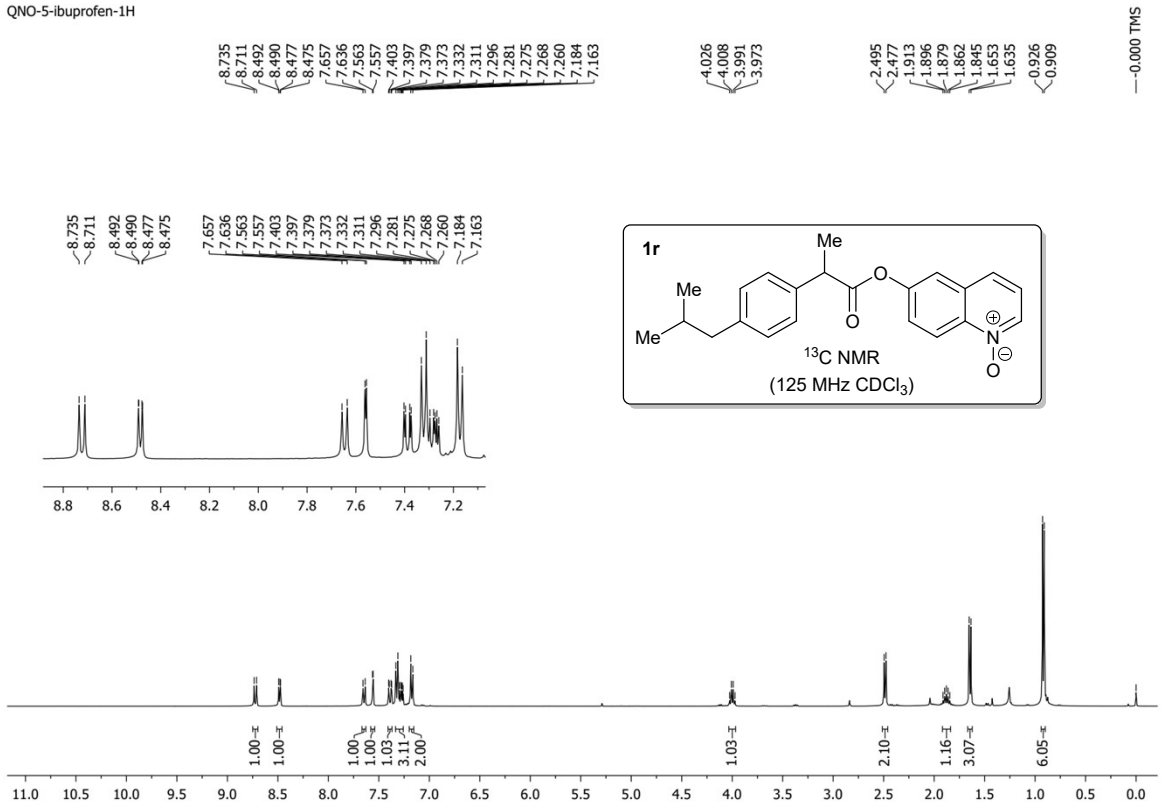
1p

^{1}H NMR
(400 MHz, $CDCl_3$)

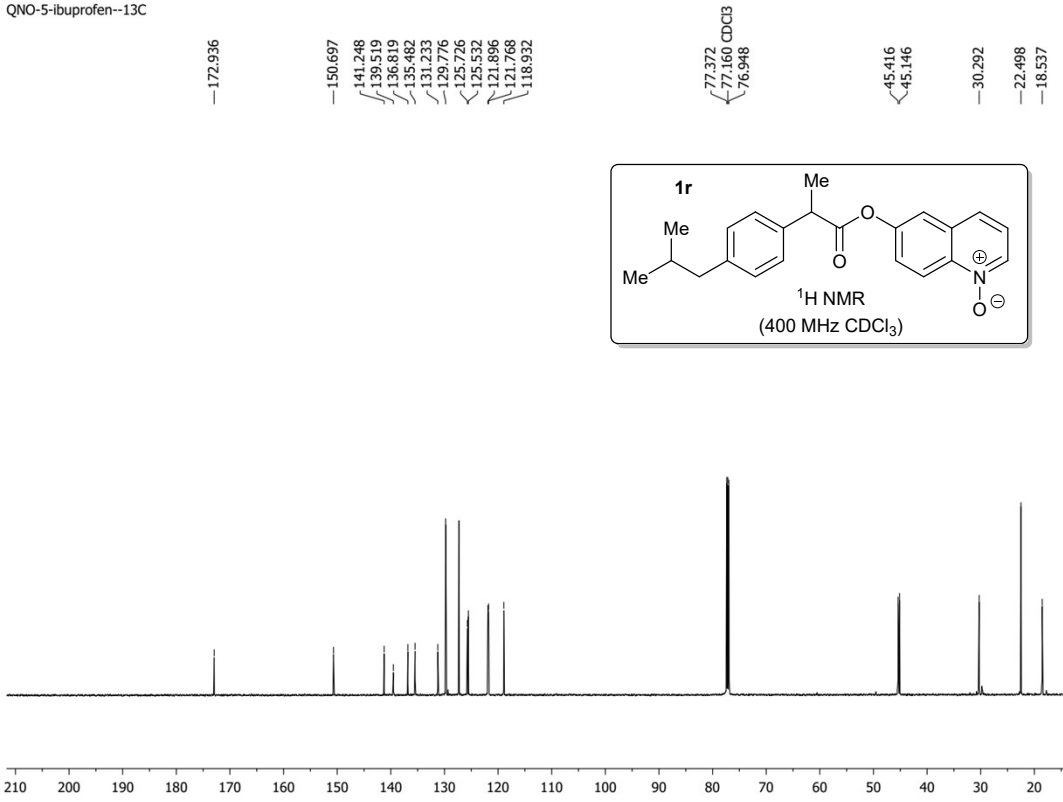
BDN-QNO-GEM-1H



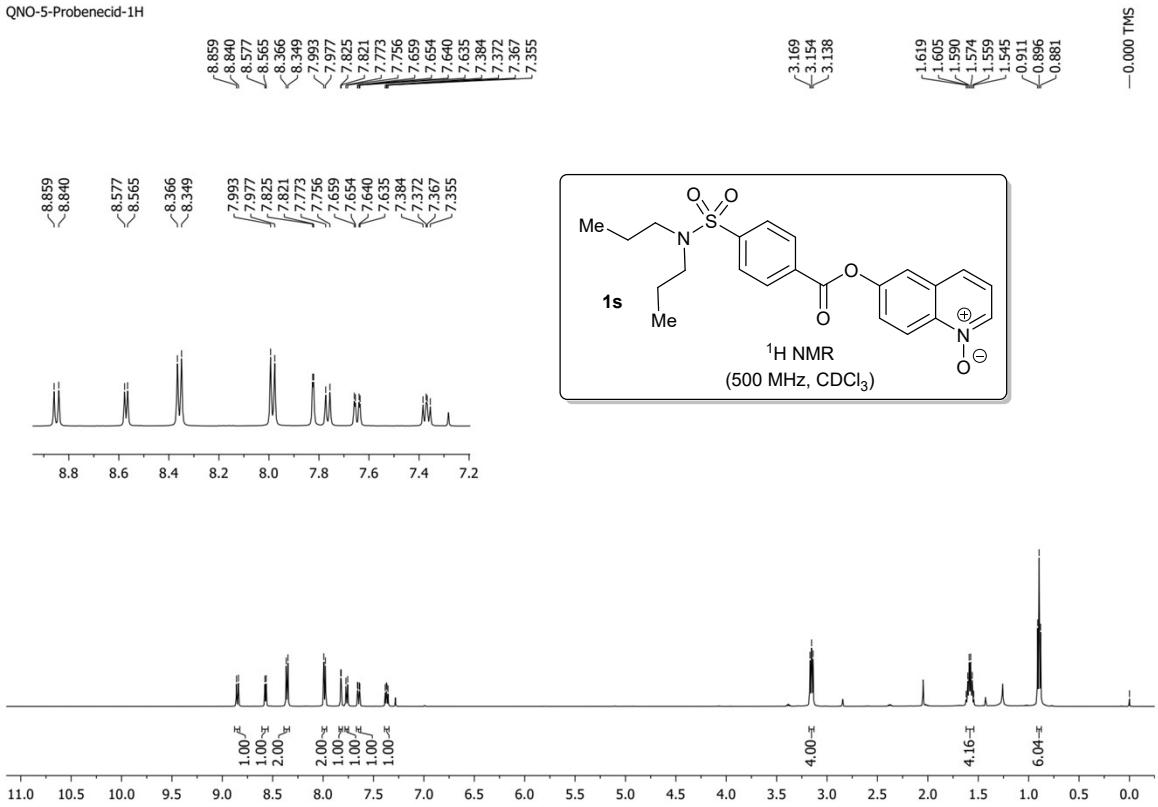
QNO-5-ibuprofen-1H

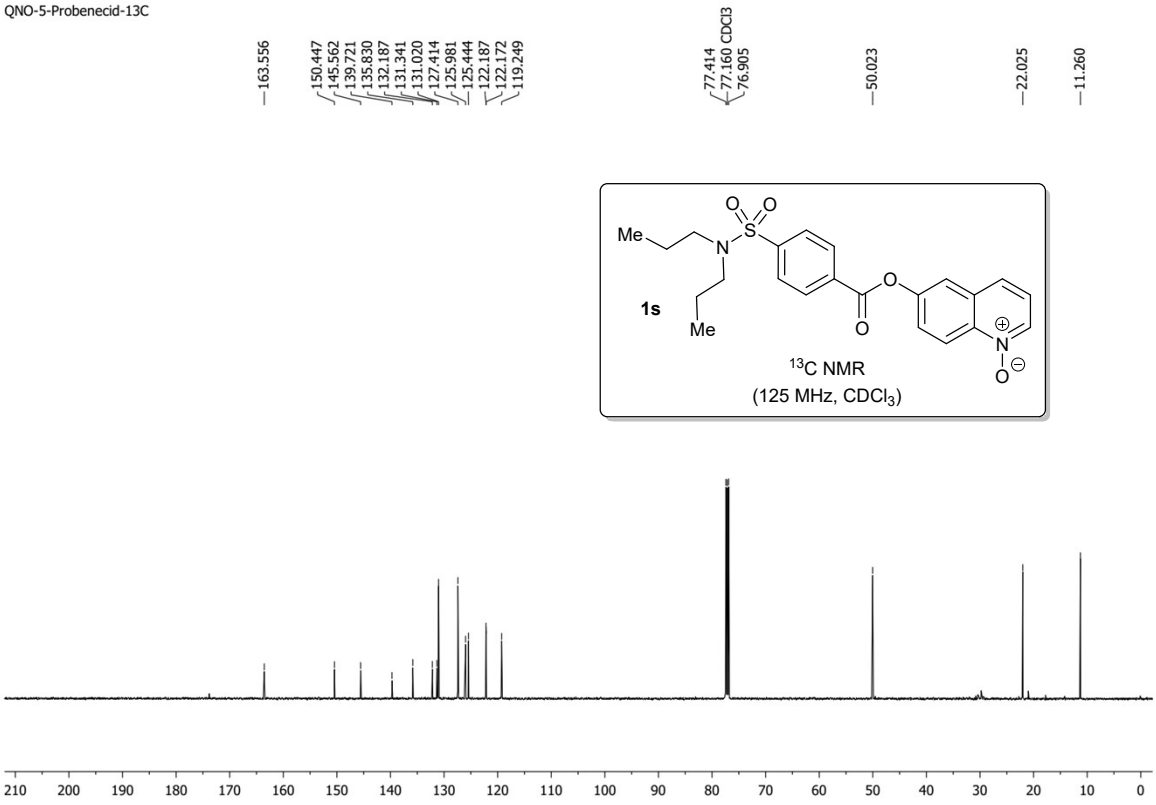


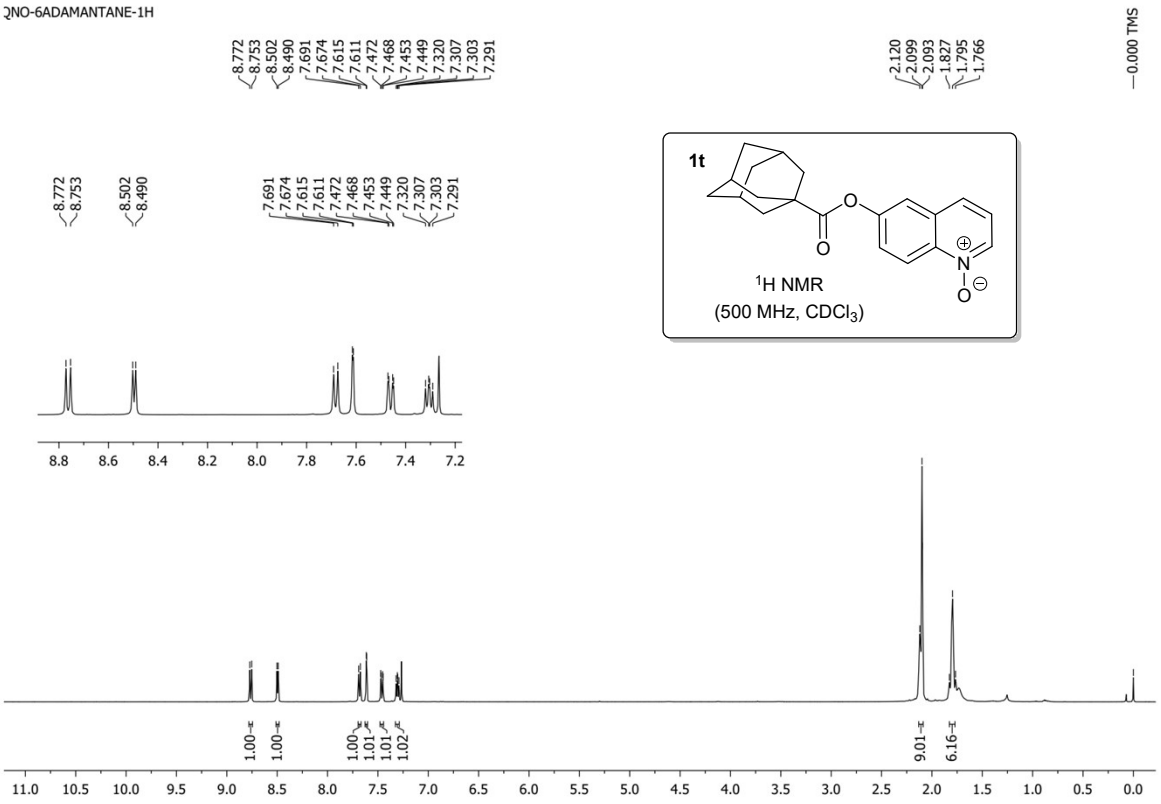
QNO-5-ibuprofen--13C

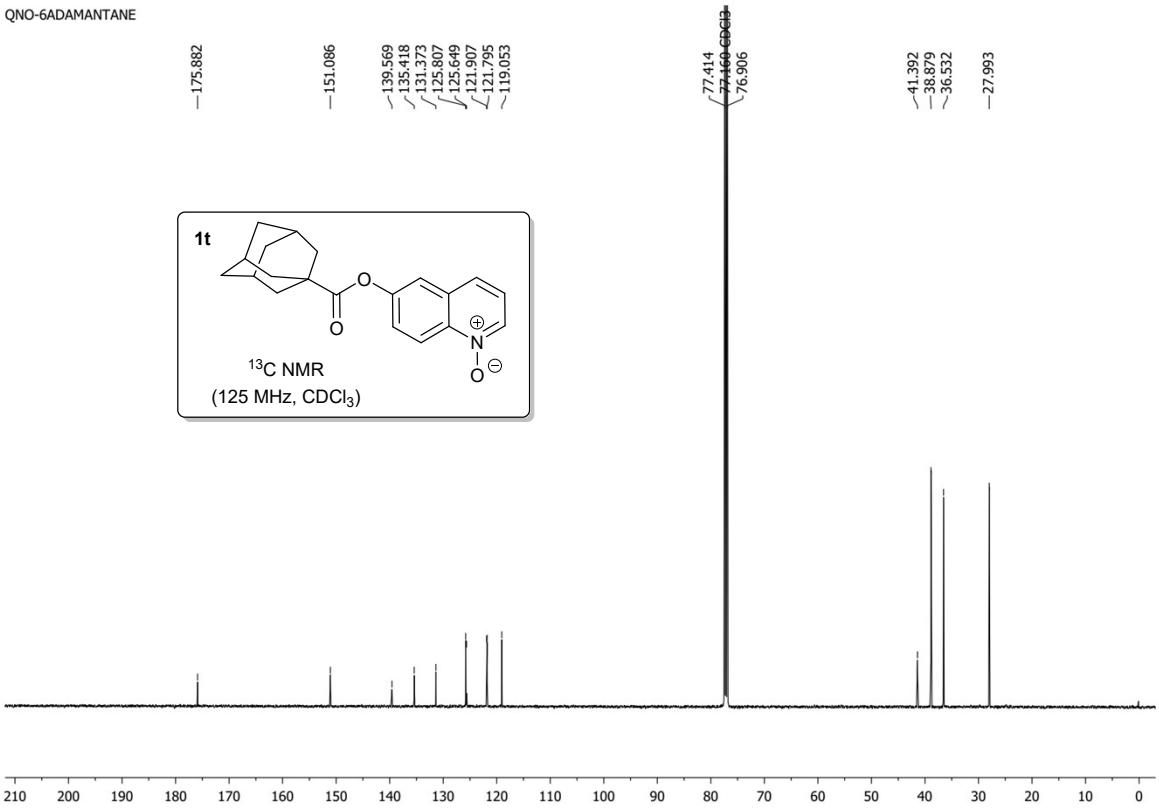


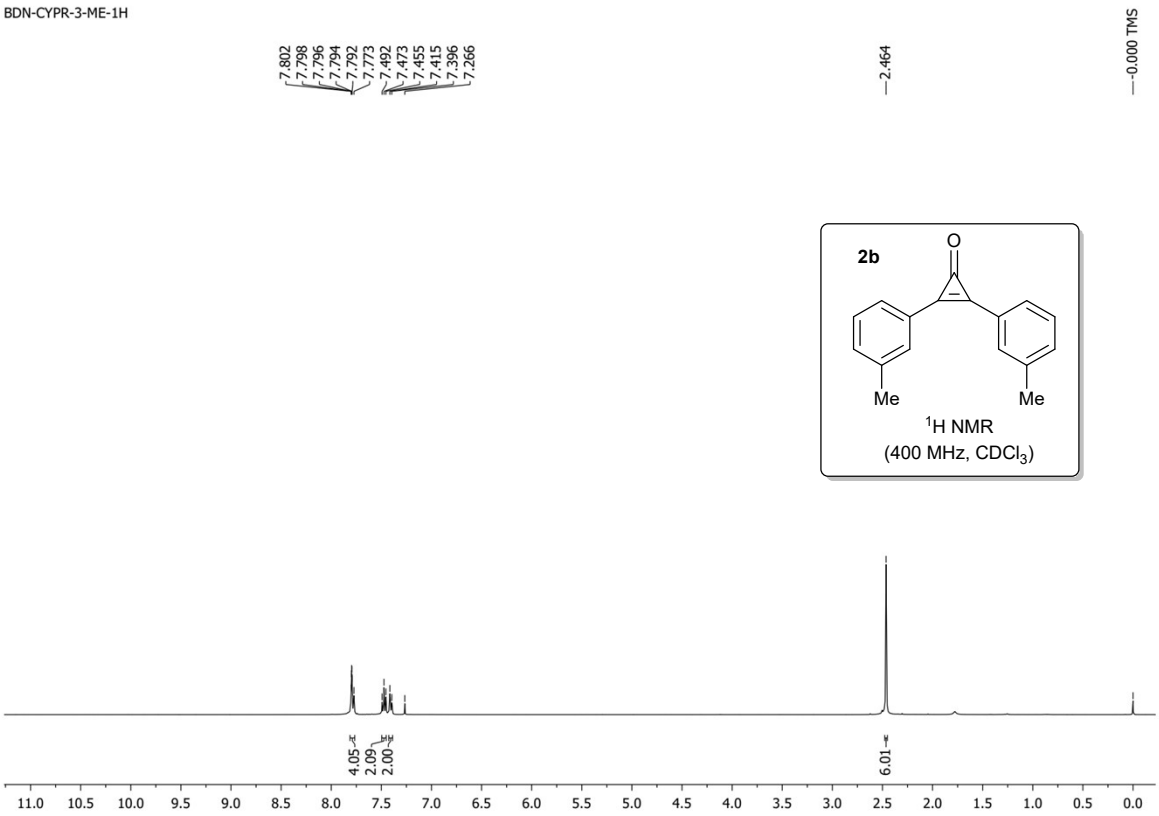
QNO-5-Probenecid-1H

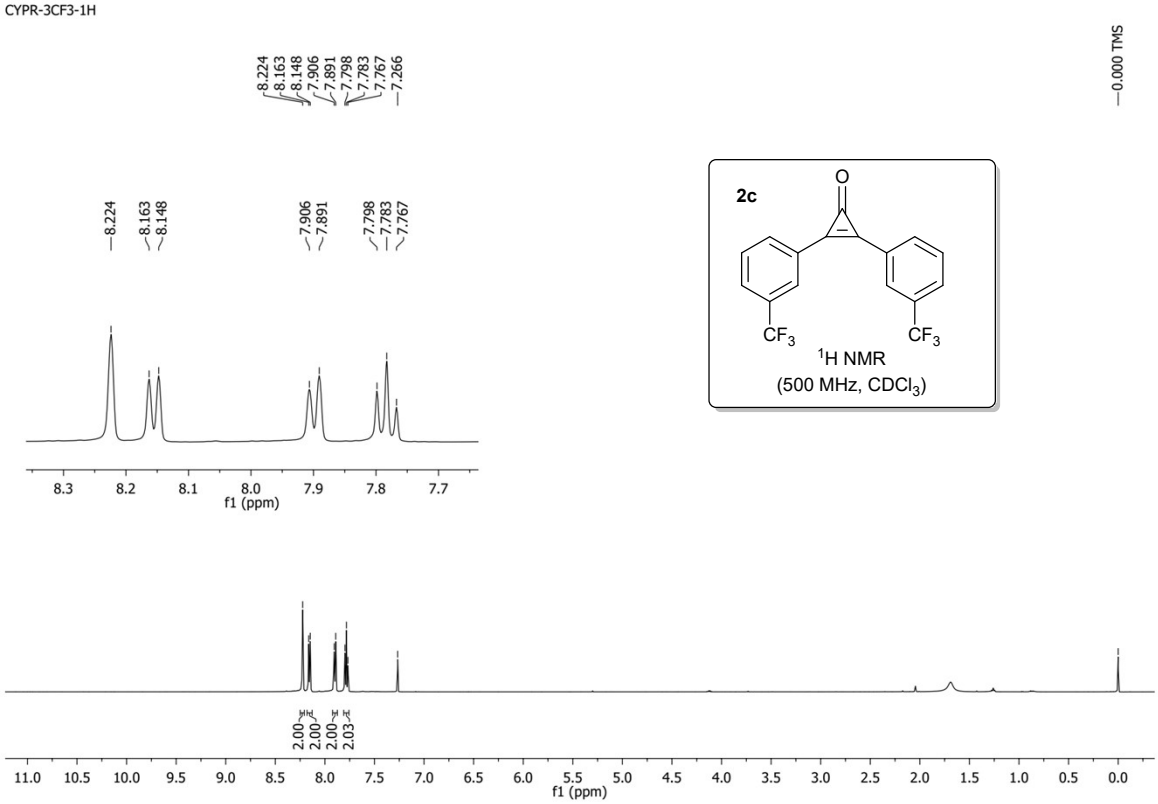


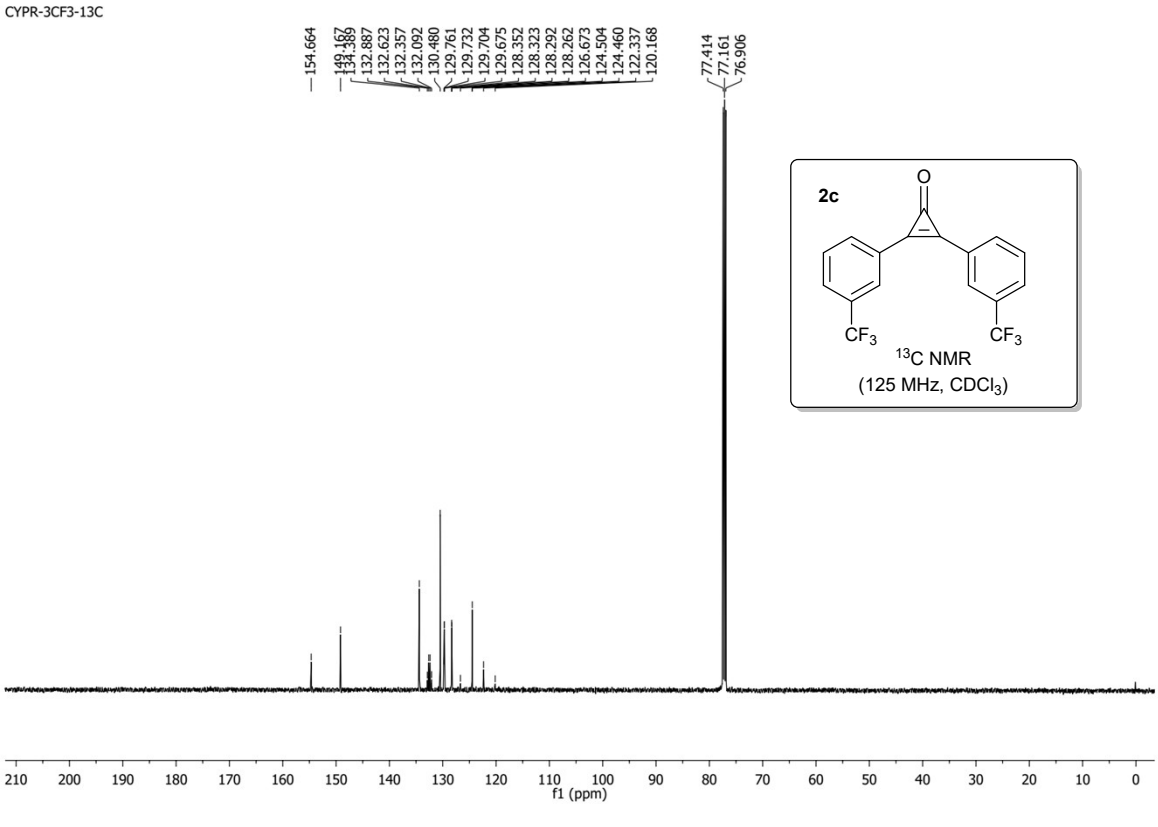

QNO-5-Probenecid-13C
163.556
150.447
145.562
139.721
135.830
132.187
131.341
131.020
127.414
125.981
125.444
122.187
122.172
119.249
77.414
77.160 CDCl3
76.905
50.023
22.025
11.260
1s
Me
Me
13C NMR
(125 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


QNO-6ADAMANTANE-1H
8.772
8.753
8.502
8.490
7.691
7.674
7.615
7.611
7.472
7.468
7.453
7.449
7.320
7.307
7.303
7.291
2.120
2.099
2.093
1.827
1.795
1.766
0.000 TMS
1t
1H NMR
(500 MHz, CDCl3)
8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2
1.00
1.00
1.00
1.01
1.01
1.02
9.01
6.16
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

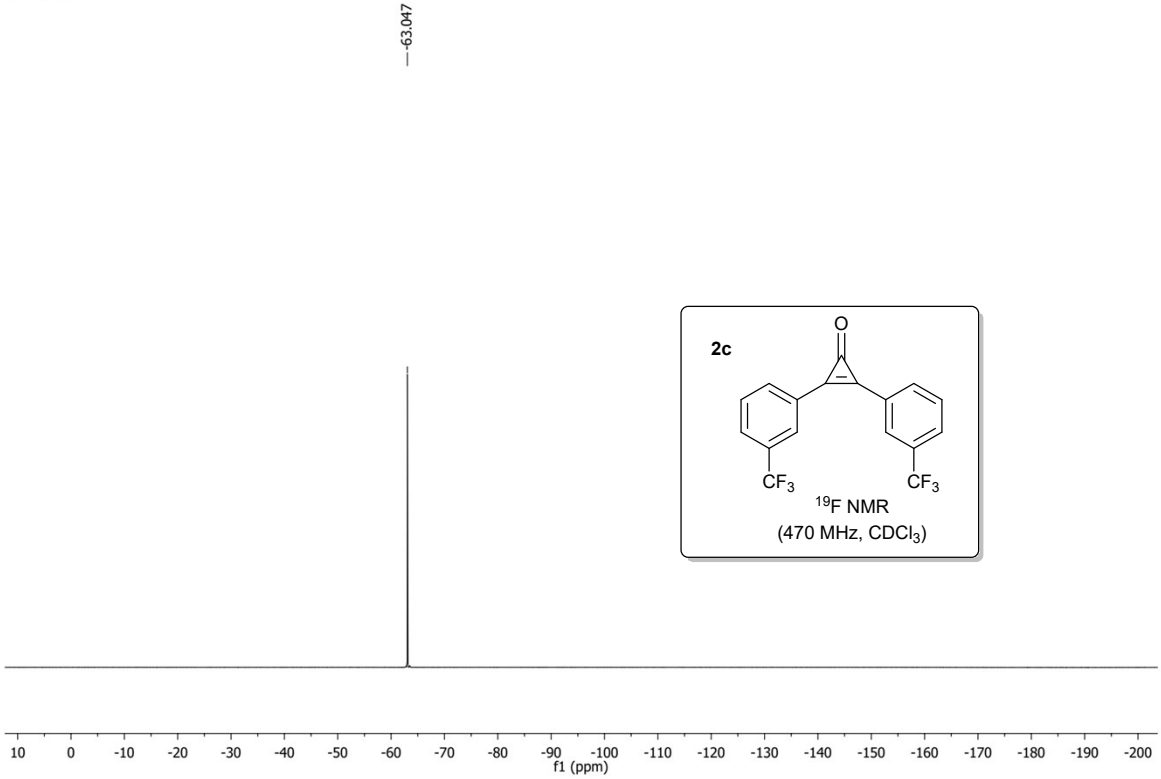

QNO-6ADAMANTANE
175.882
151.086
139.569
135.418
131.373
125.807
125.649
121.907
121.795
119.053
77.414
77.160 CDCl3
76.906
41.392
38.879
36.532
27.993
1t
O
O
N
O
13C NMR
(125 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


BDN-CYPR-3-ME-1H
7.802
7.798
7.796
7.794
7.792
7.773
7.492
7.473
7.455
7.415
7.396
7.266
2.464
0.000 TMS
2b
O
Me
Me
1H NMR
(400 MHz, CDCl3)
4.05
2.09
2.00
6.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0


CYPR-3CF3-1H
8.224
8.163
8.148
7.906
7.891
7.798
7.783
7.767
7.266
0.000 TMS
2c
O
CF3
CF3
1H NMR
(500 MHz, CDCl3)
f1 (ppm)


CYPR-3CF3-13C
154.664
149.167
134.386
132.887
132.623
132.357
132.092
130.480
129.761
129.732
129.704
129.675
128.352
128.323
128.292
128.262
126.673
124.504
124.460
122.337
120.168
77.414
77.161
76.906
2c
O
CF3
CF3
13C NMR
(125 MHz, CDCl3)
f1 (ppm)

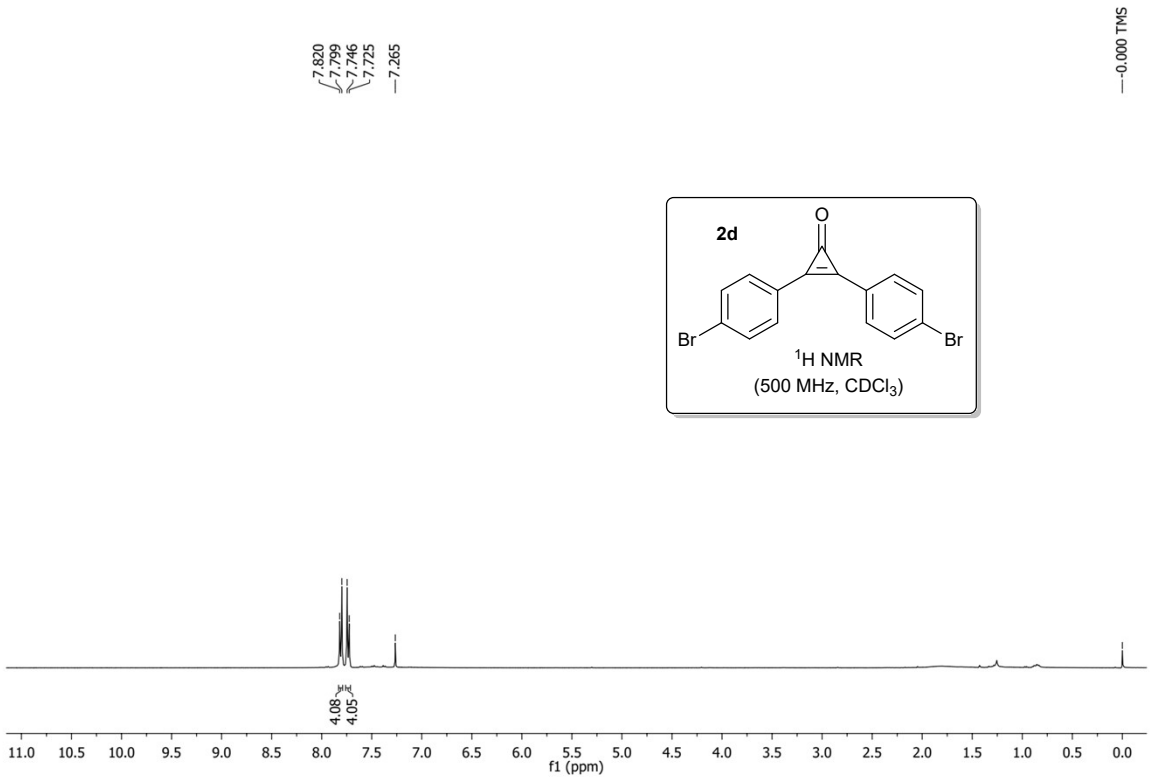
CYPR-3CF3-19F



2c

^{19}F NMR
(470 MHz, $CDCl_3$)

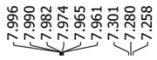
BDN-CYPR-4BR-1H.1.fid

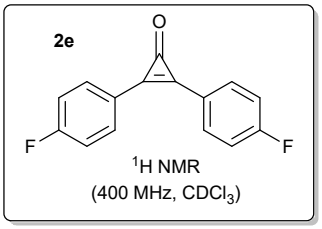


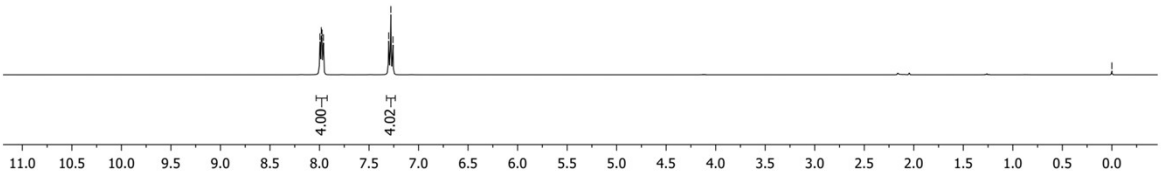
2d

^{1}H NMR
(500 MHz, $CDCl_3$)

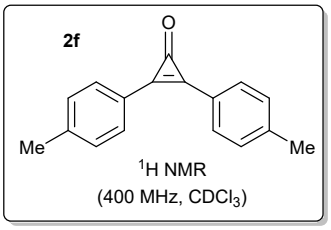
BDN-CYPR-4F-1H

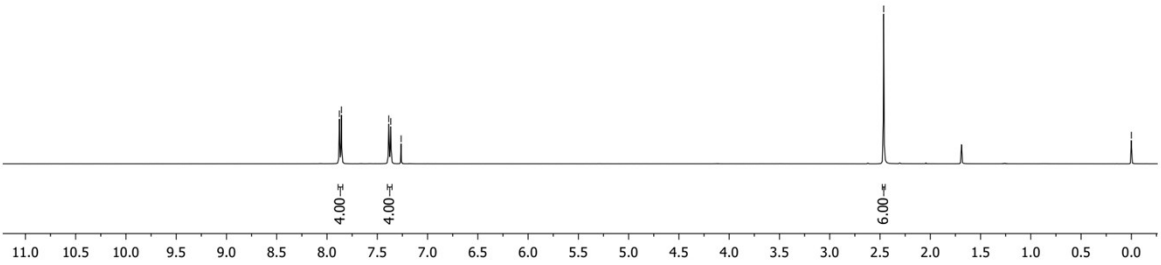




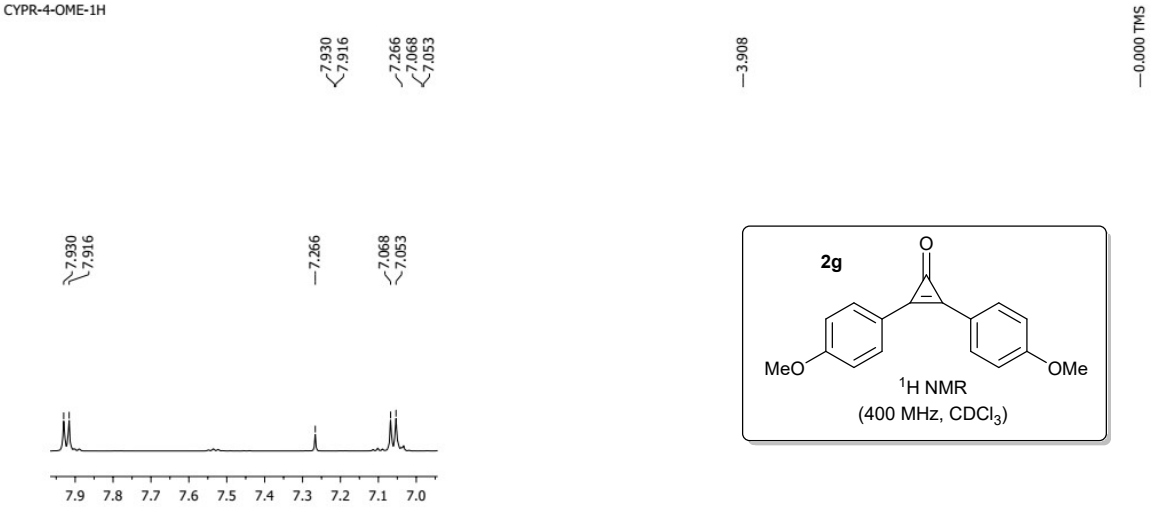


BDN-CYPR4ME-1H





CYPR-4-OME-1H



2g

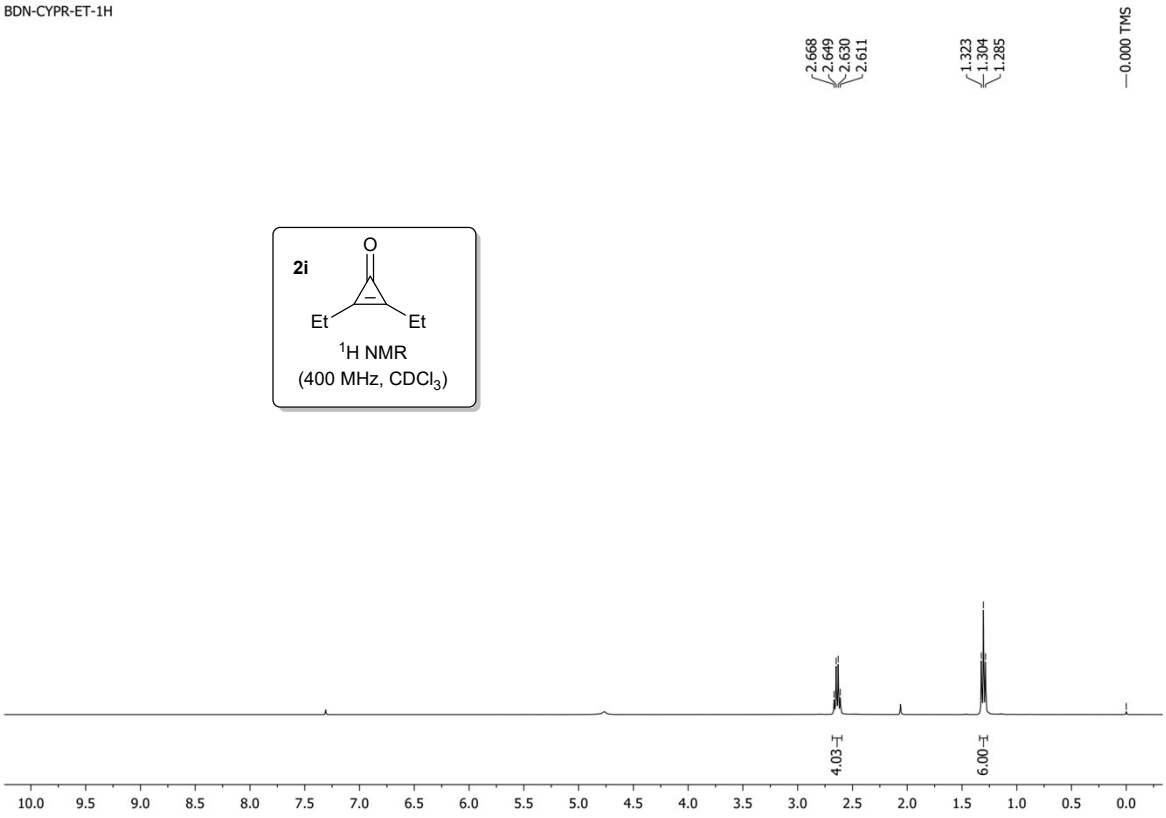
^{1}H NMR
(400 MHz, $CDCl_3$)

BDN-CYPR-4-tBu-1H

2h

^{1}H NMR
(400 MHz, $CDCl_3$)

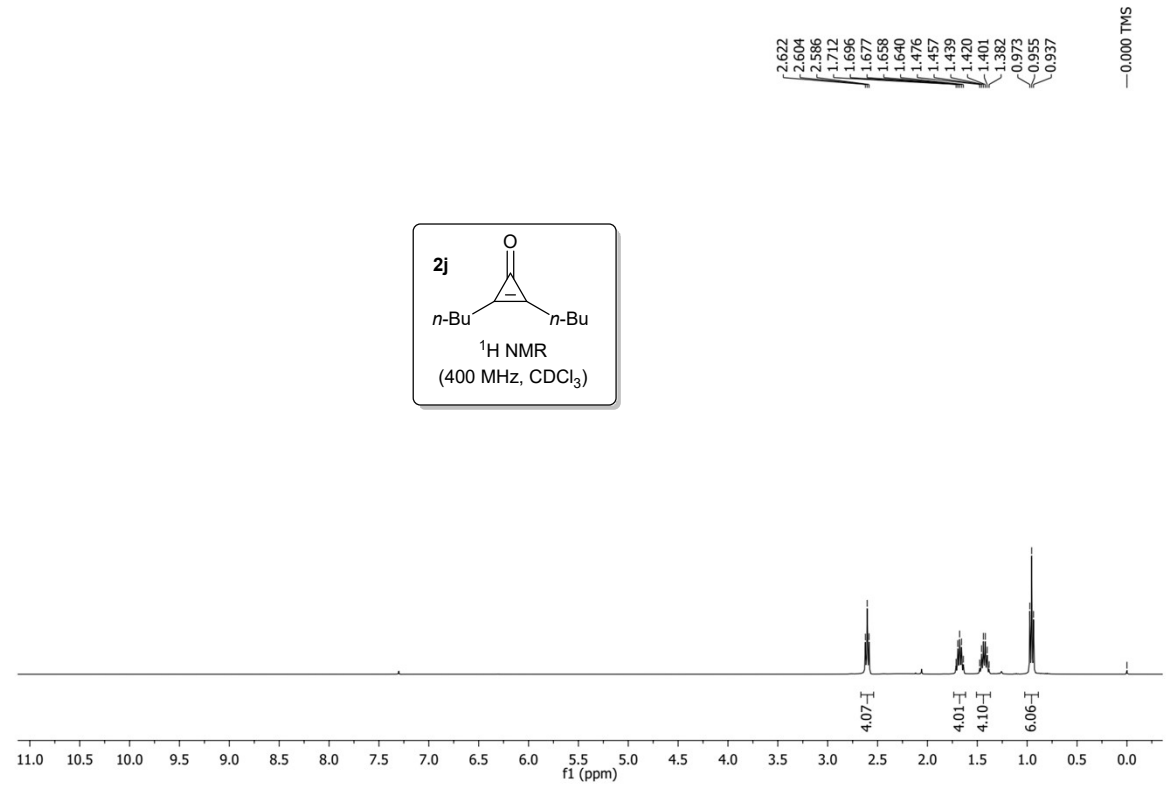
BDN-CYPR-ET-1H



2i

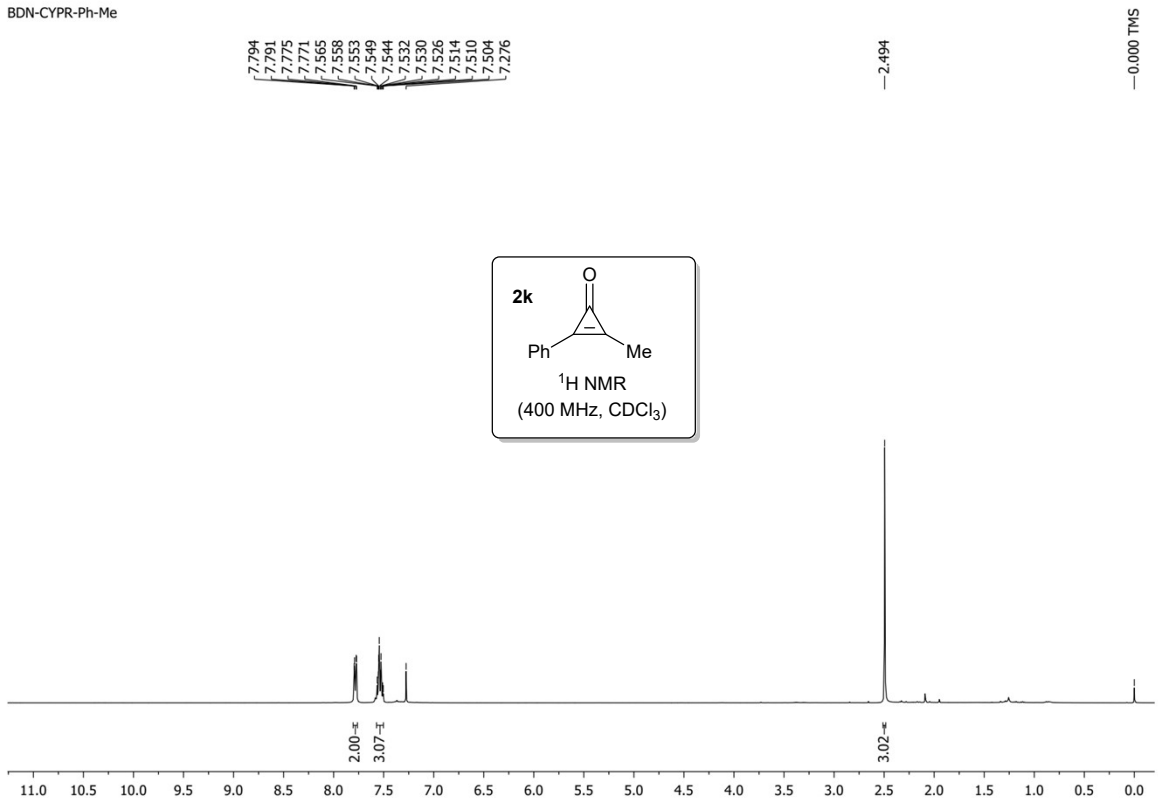
^{1}H NMR
(400 MHz, $CDCl_3$)

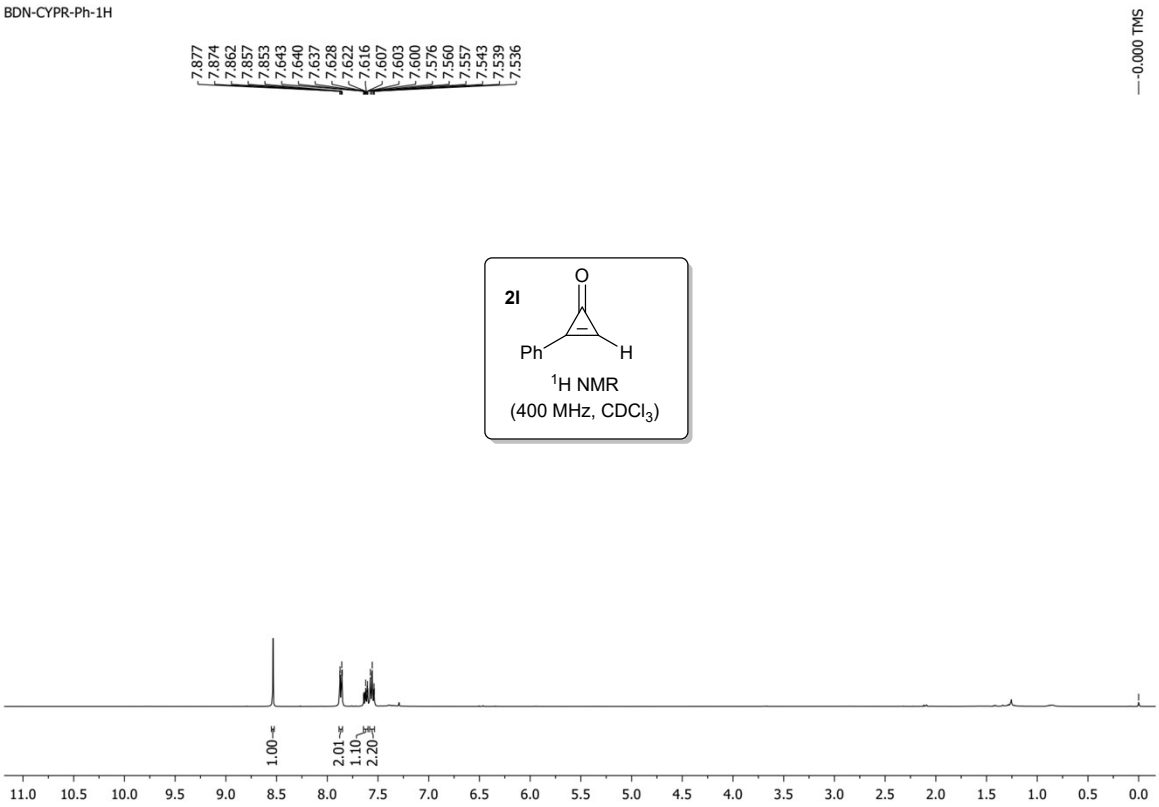
BDN-CYPR-n-Bn-1H



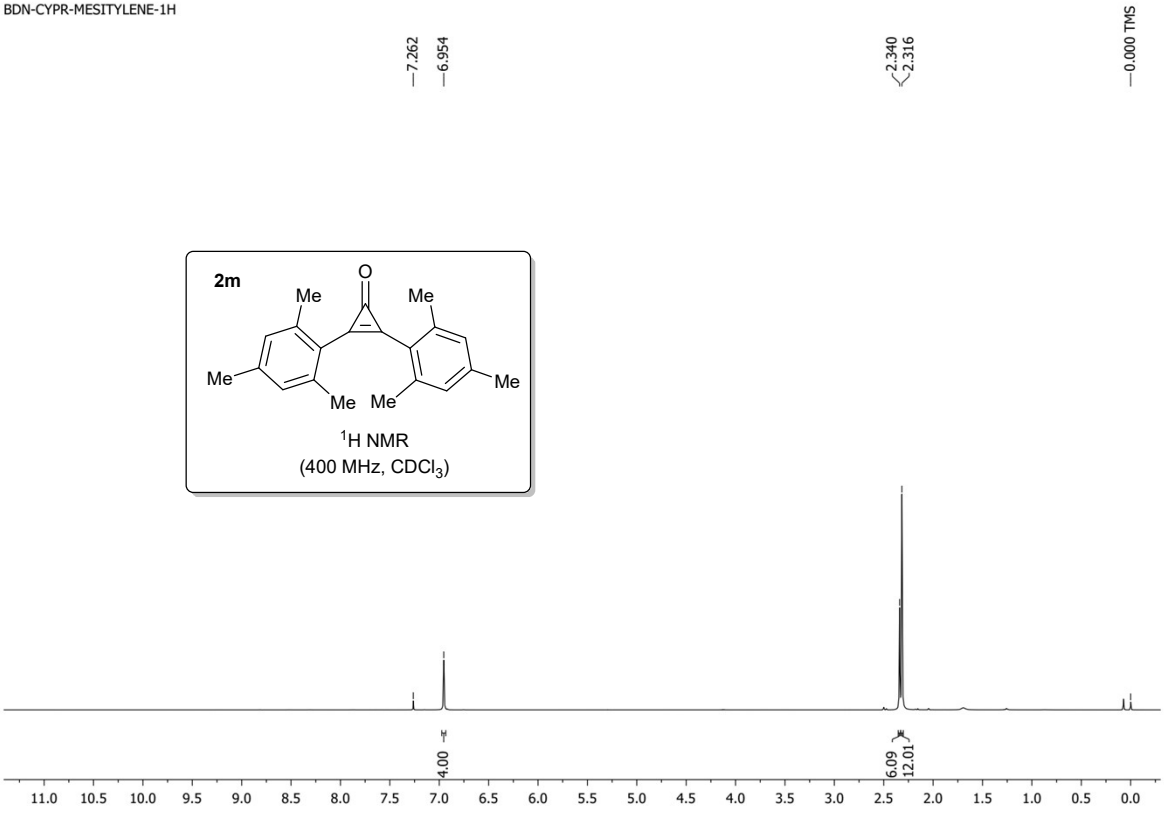
2j

^{1}H NMR
(400 MHz, $CDCl_3$)

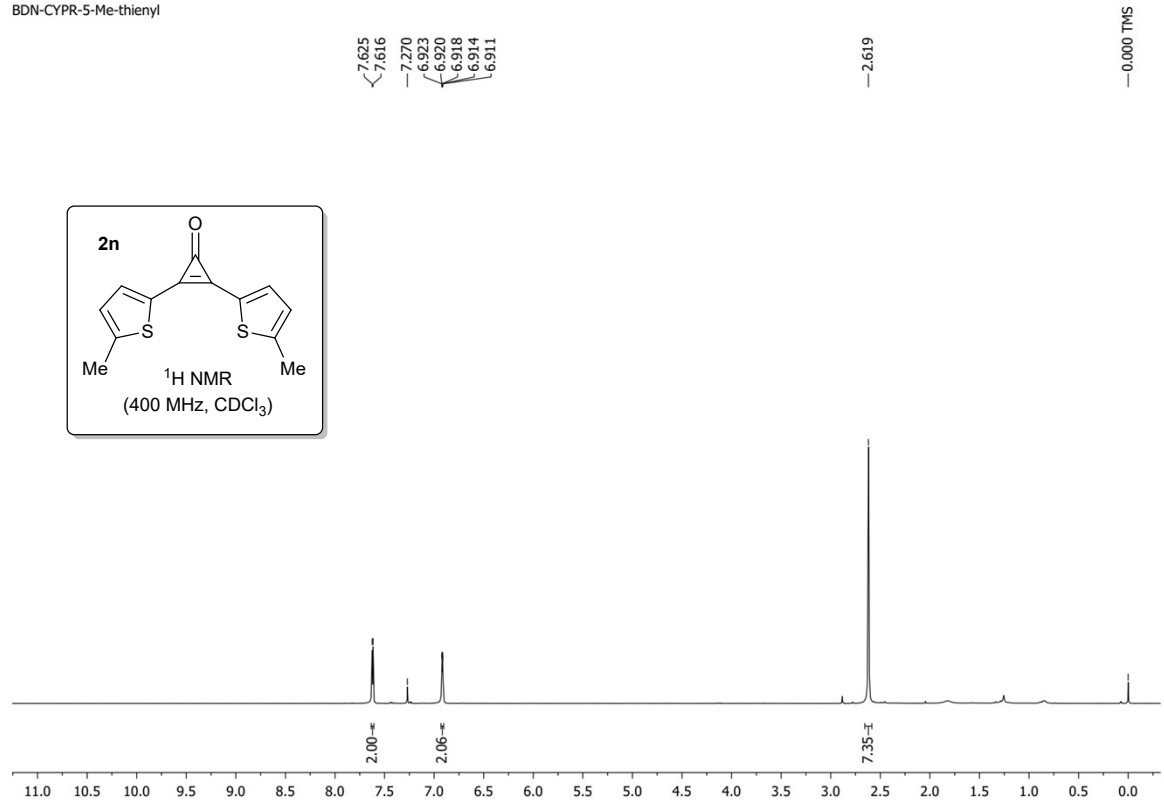

BDN-CYPR-Ph-Me
7.794
7.791
7.775
7.771
7.565
7.558
7.553
7.549
7.544
7.532
7.530
7.526
7.514
7.510
7.504
7.276
2.494
0.000 TMS
2k
O
Ph
Me
1H NMR
(400 MHz, CDCl3)
2.00
3.07
3.02
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0


BDN-CYPR-Ph-1H
7.877
7.874
7.862
7.857
7.853
7.643
7.640
7.637
7.628
7.622
7.616
7.607
7.603
7.600
7.576
7.560
7.557
7.543
7.539
7.536
0.000 TMS
2l
O
Ph
H
1H NMR
(400 MHz, CDCl3)
1.00
2.01
1.10
2.20
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

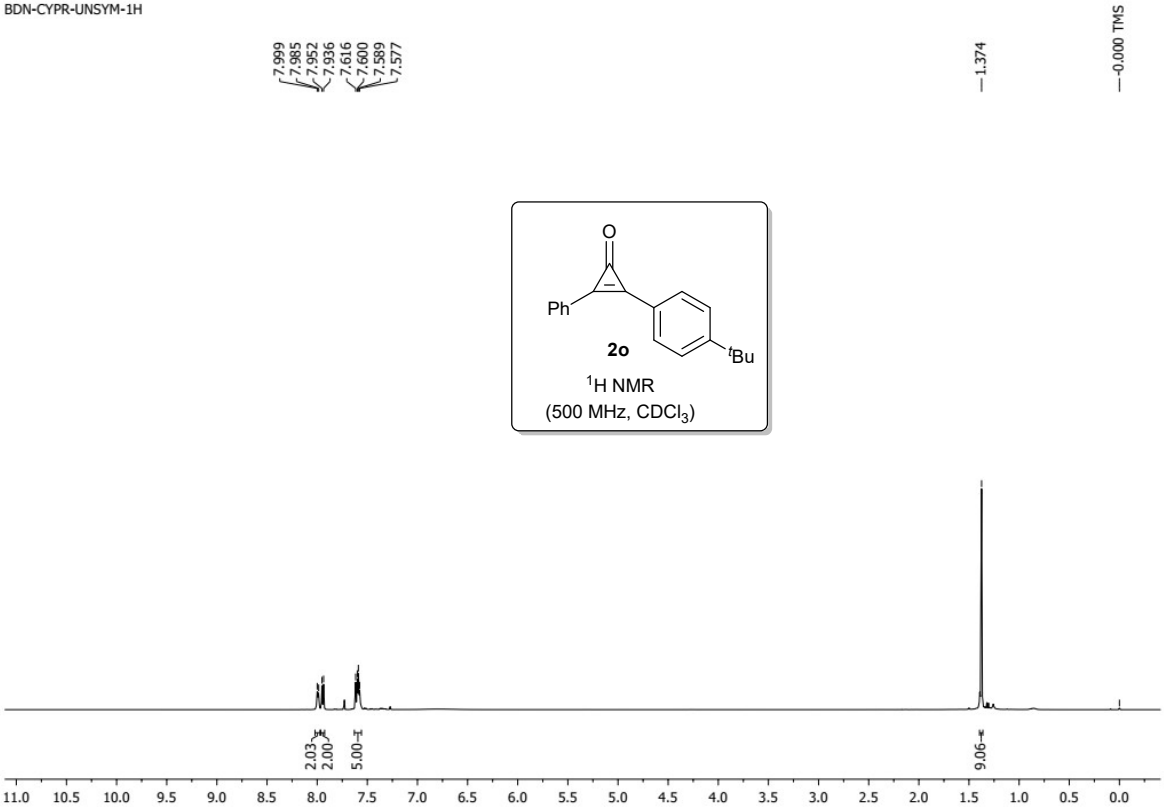
BDN-CYPR-MESITYLENE-1H



BDN-CYPR-5-Me-thienyl



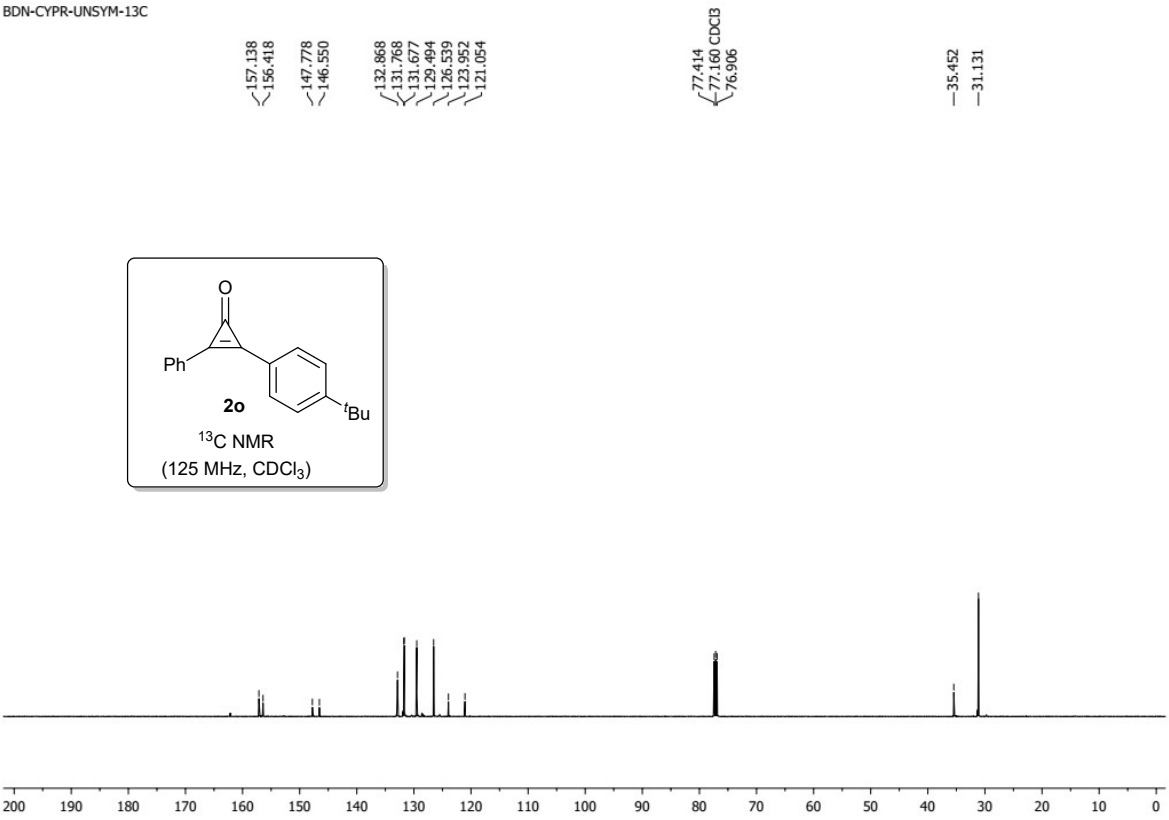
BDN-CYPR-UNSYM-1H



2o

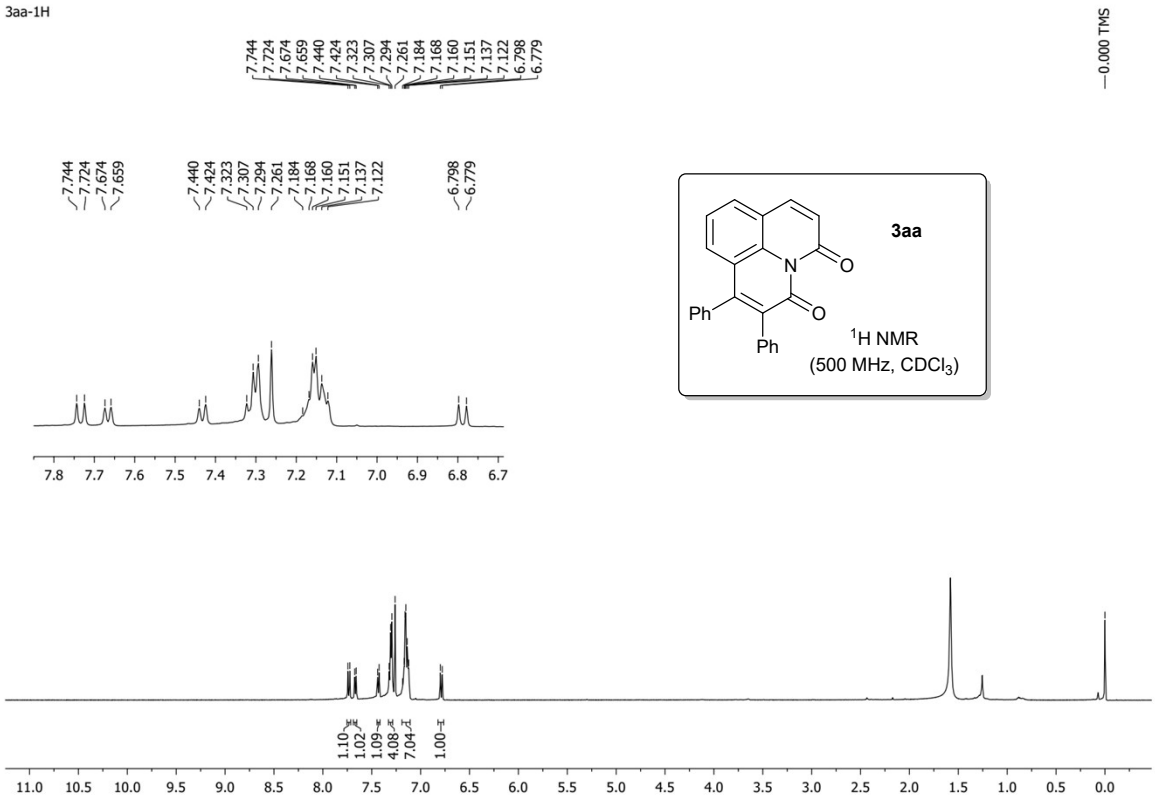
^{1}H NMR
(500 MHz, $CDCl_3$)

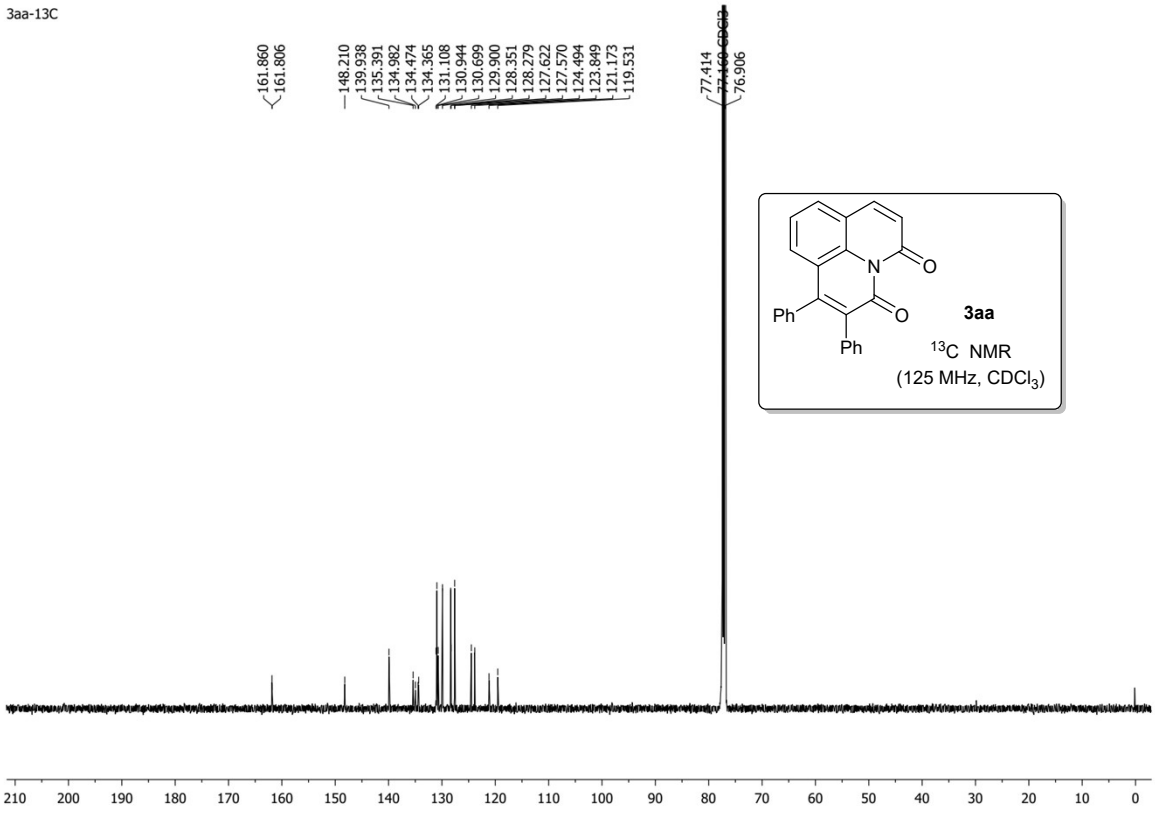
BDN-CYPR-UNSYM-13C

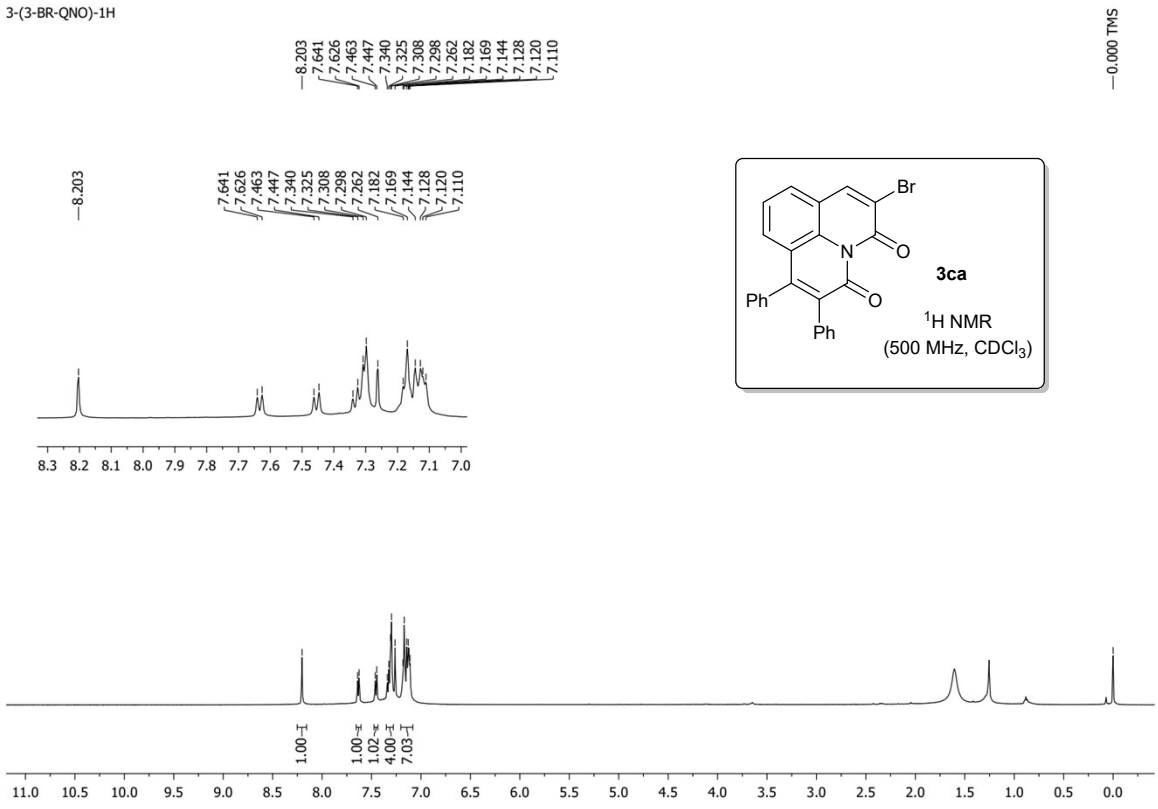


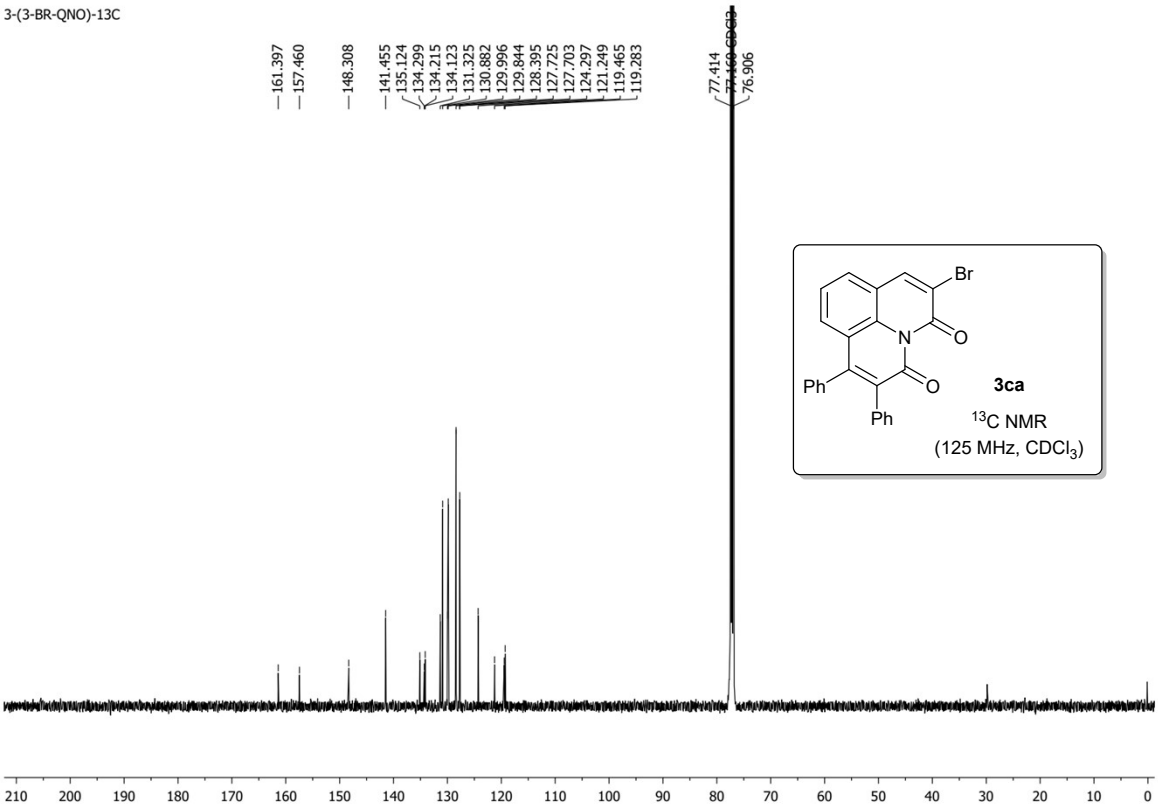
2o

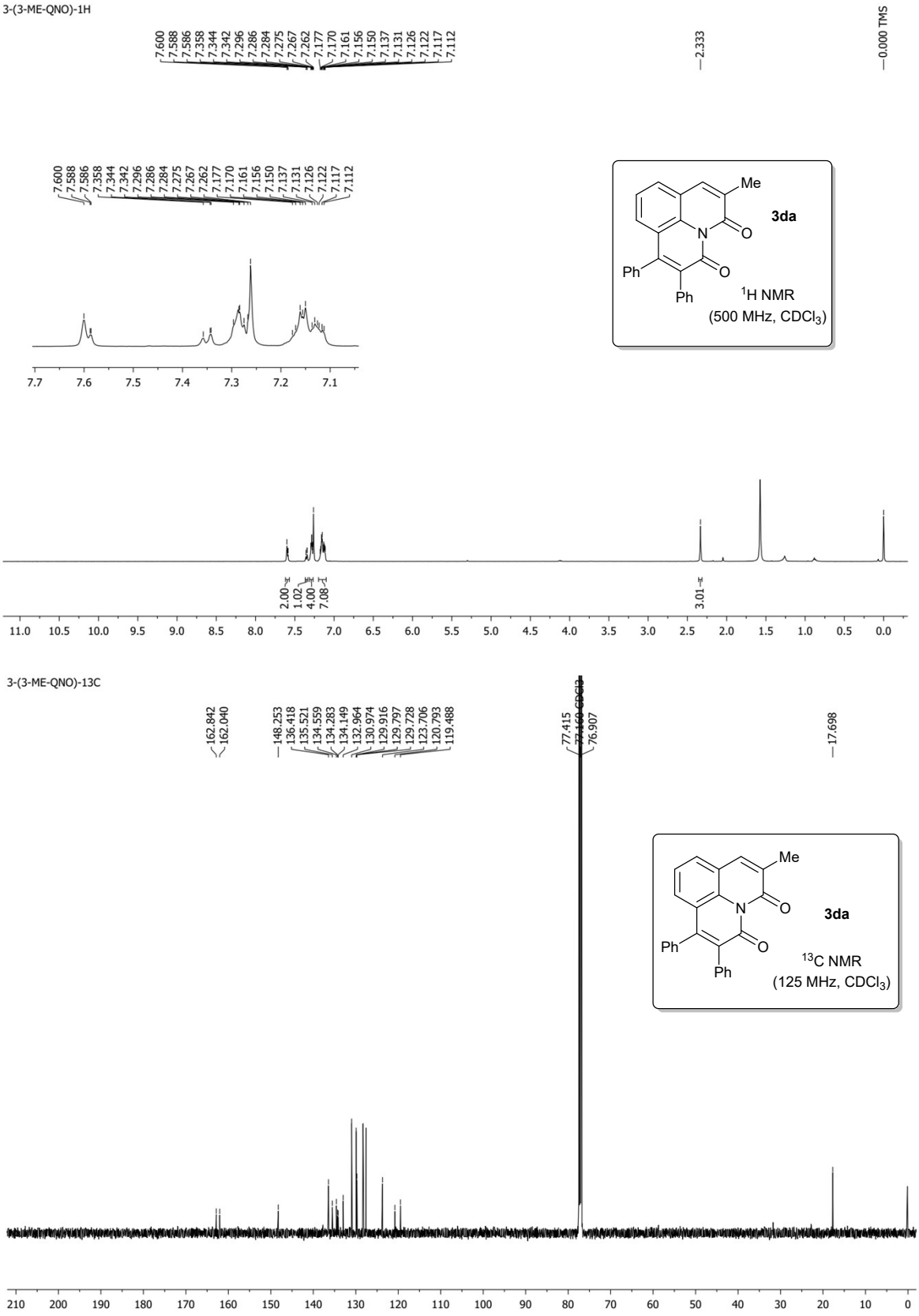
^{13}C NMR
(125 MHz, $CDCl_3$)

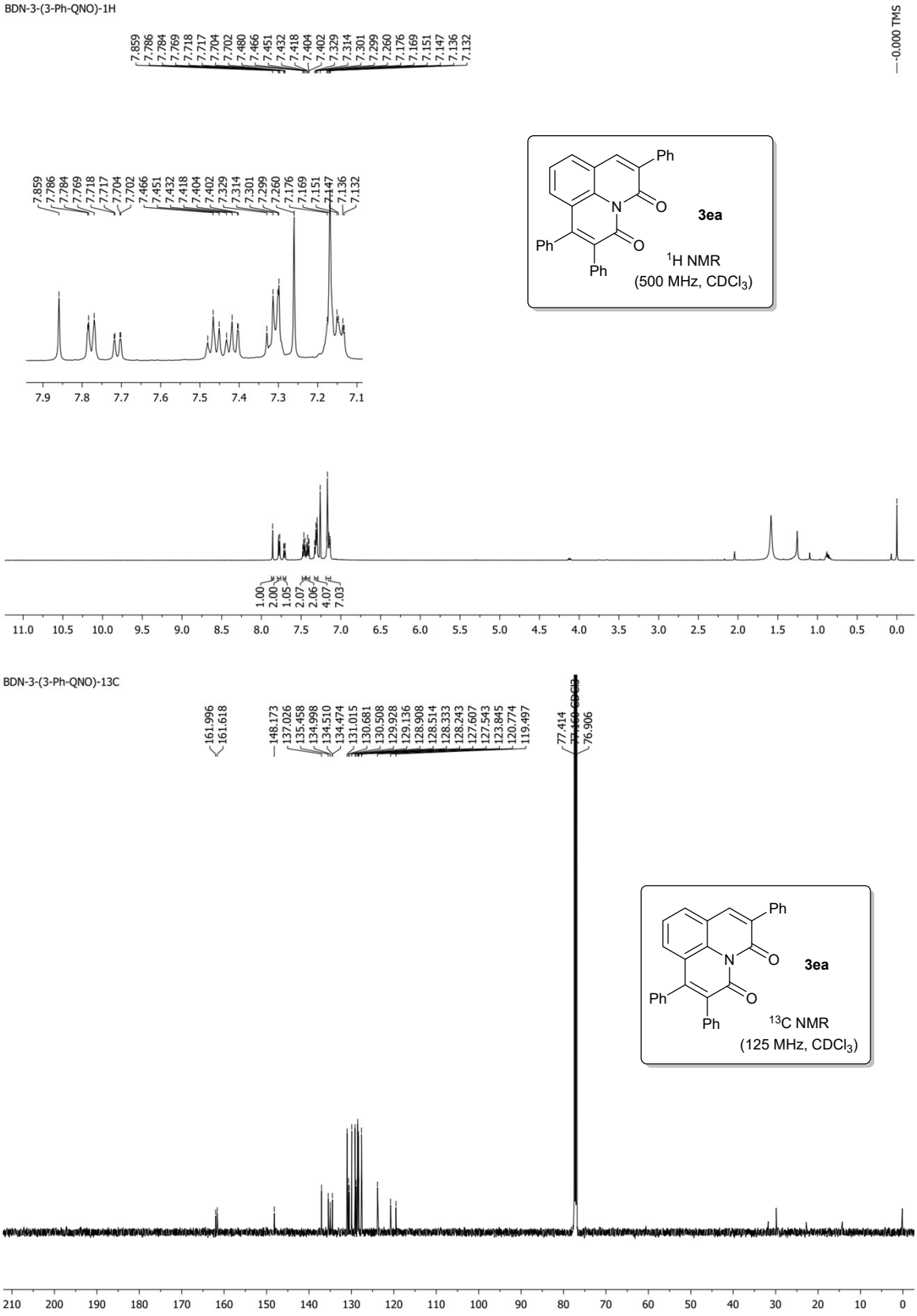

3aa-1H
7.744
7.724
7.674
7.659
7.440
7.424
7.323
7.307
7.294
7.261
7.184
7.168
7.160
7.151
7.137
7.122
6.798
6.779
0.000 TMS
3aa
Ph
Ph
^{1}H NMR
(500 MHz, $CDCl_3$)
1.10
1.02
1.09
4.08
7.04
1.00

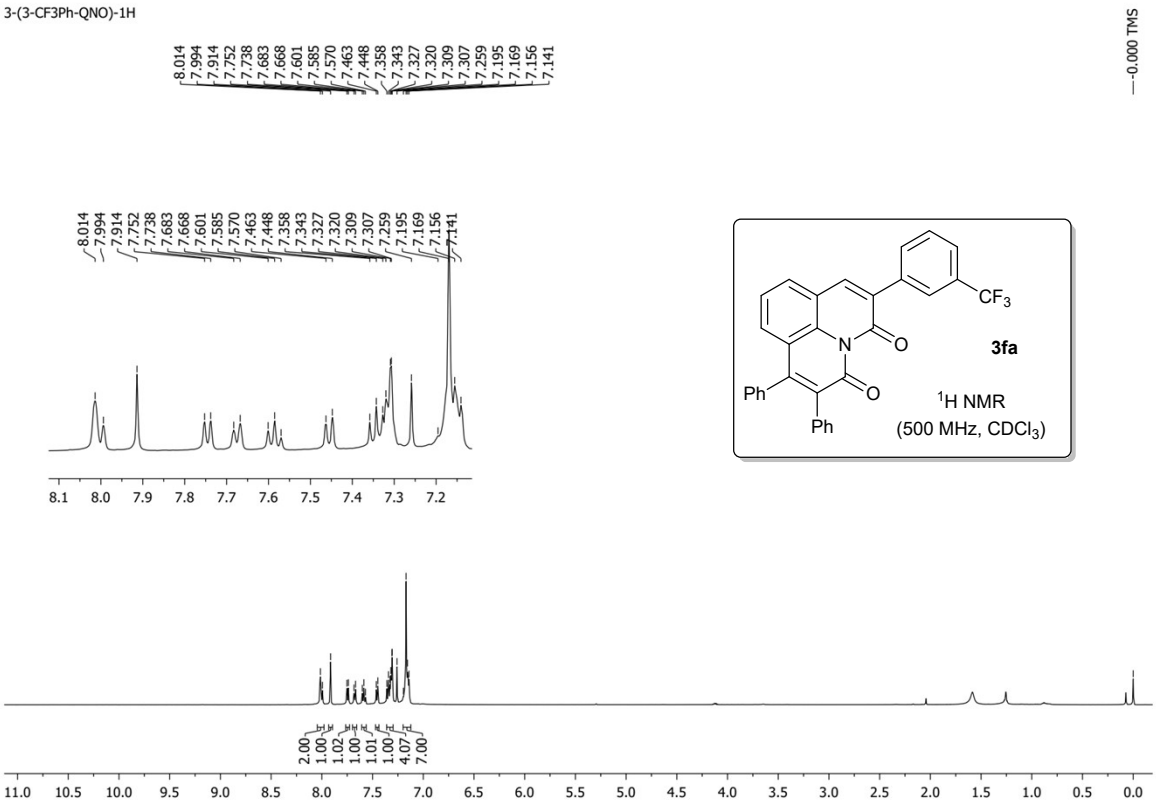

3aa-13C
161.860
161.806
148.210
139.938
135.391
134.982
134.474
134.365
131.108
130.944
130.699
129.900
128.351
128.279
127.622
127.570
124.494
123.849
121.173
119.531
77.414
76.906
3aa
Ph
Ph
^{13}C NMR
(125 MHz, $CDCl_3$)

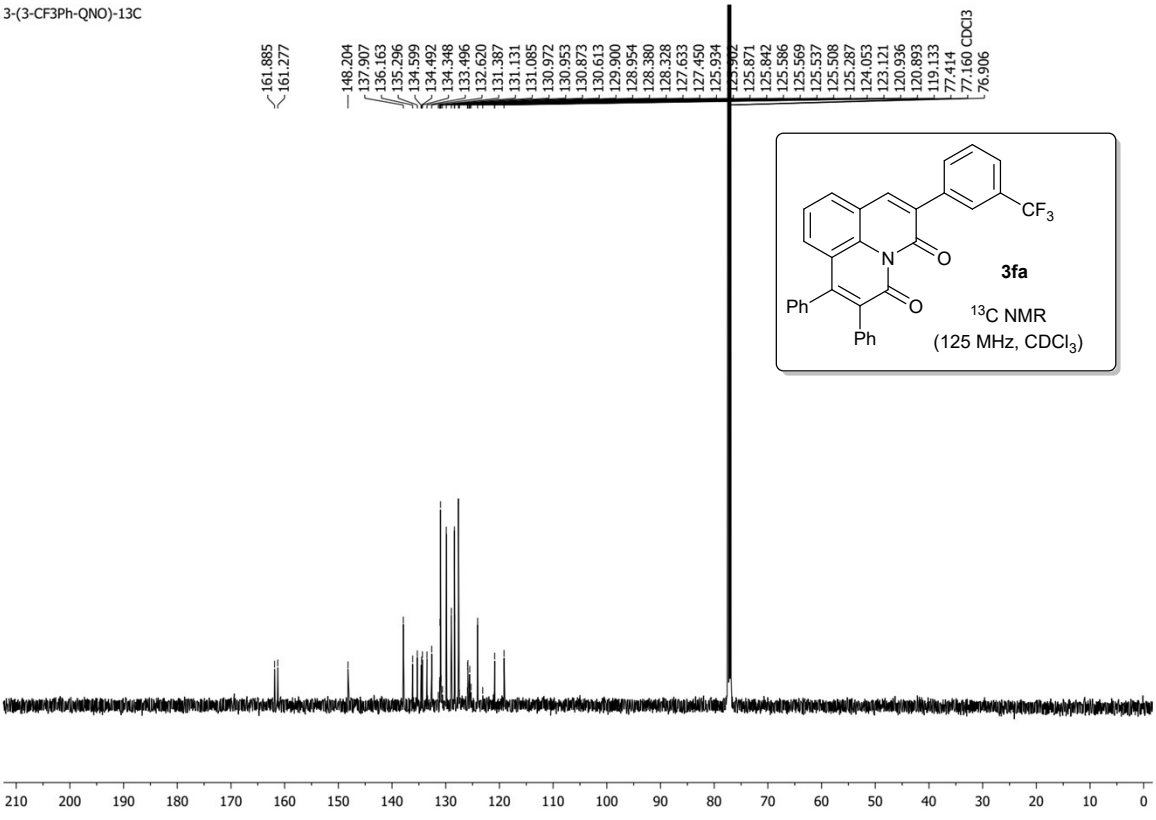

3-(3-BR-QNO)-1H
8.203
7.641
7.626
7.463
7.447
7.340
7.325
7.308
7.298
7.262
7.182
7.169
7.144
7.128
7.120
7.110
0.000 TMS
1.00
1.00
1.02
4.00
7.03
3ca
^{1}H NMR
(500 MHz, $CDCl_3$)

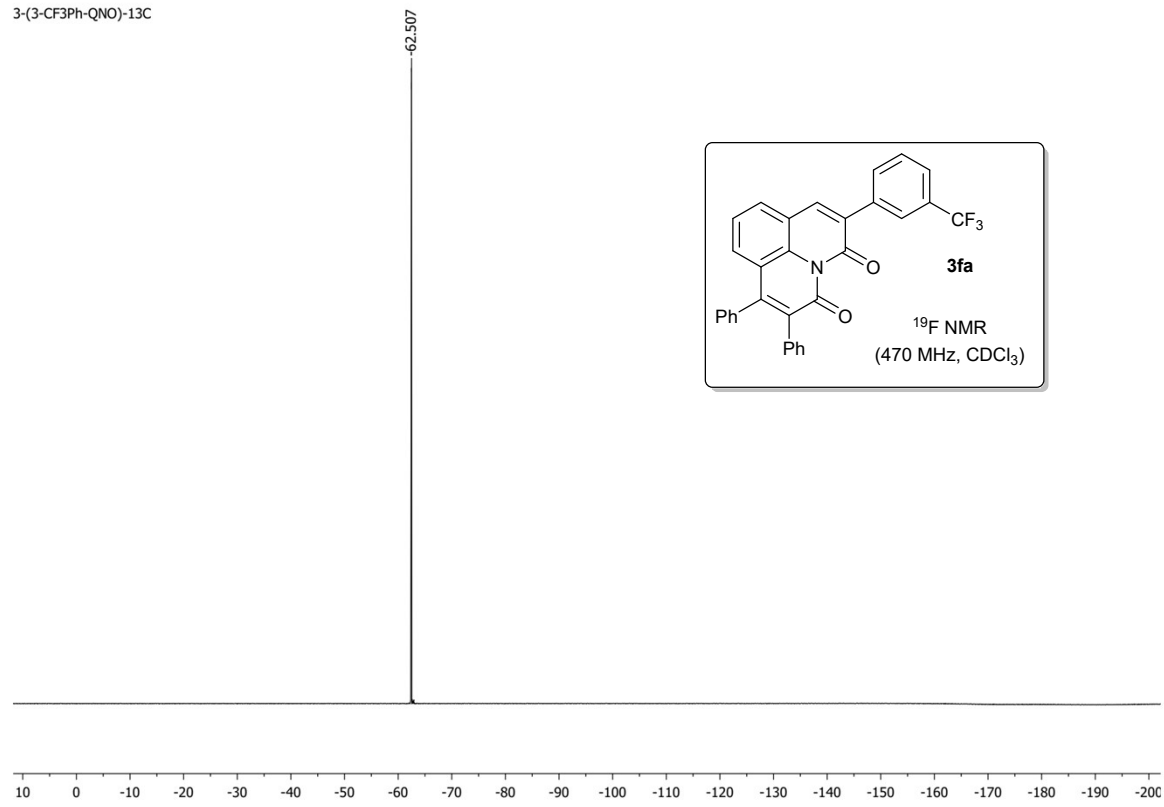

3-(3-BR-QNO)-13C
161.397
157.460
148.308
141.455
135.124
134.299
134.215
134.123
131.325
130.882
129.996
129.844
128.395
127.725
127.703
124.297
121.249
119.465
119.283
77.414
76.906
3ca
^{13}C NMR
(125 MHz, $CDCl_3$)

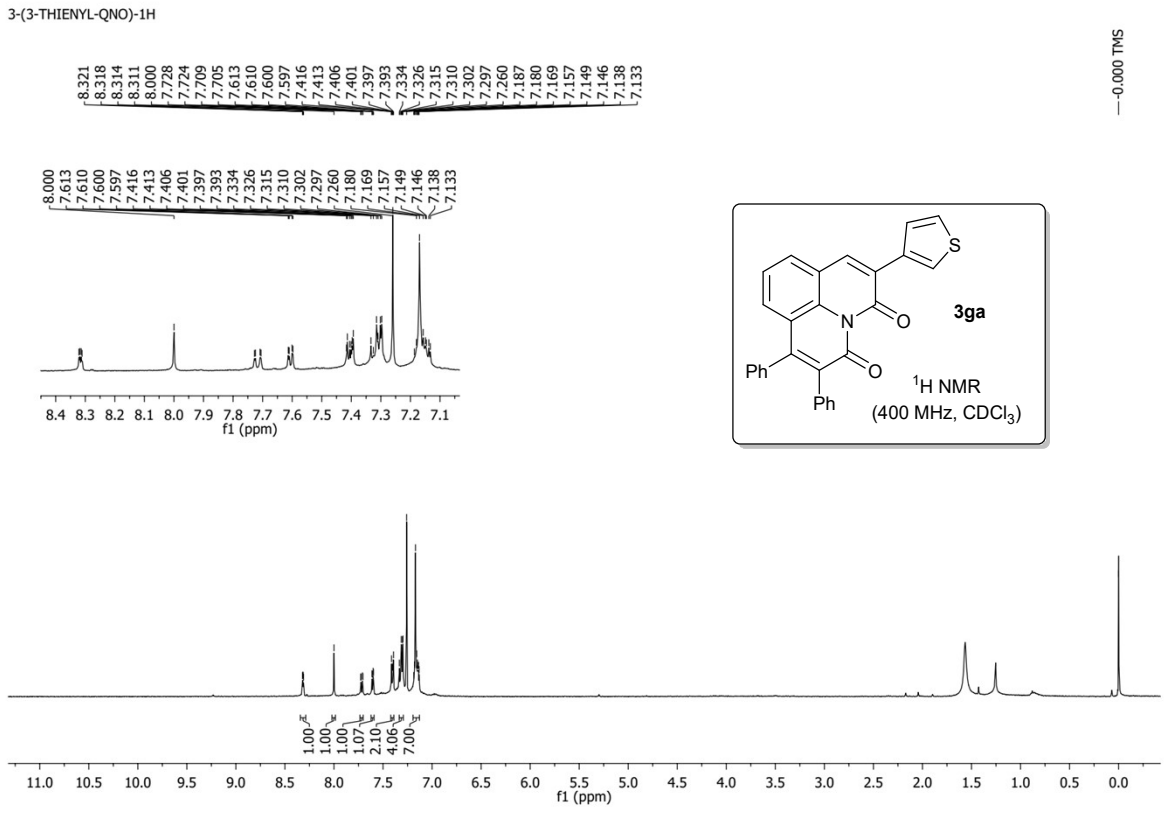

3-(3-ME-QNO)-1H
7.600
7.588
7.586
7.358
7.344
7.342
7.296
7.286
7.284
7.275
7.267
7.262
7.177
7.170
7.161
7.156
7.150
7.137
7.131
7.126
7.122
7.117
7.112
2.333
0.000 TMS
Me
3da
N
O
O
Ph
Ph
1H NMR
(500 MHz, CDCl3)
2.00
1.02
4.00
7.08
3.01
3-(3-ME-QNO)-13C
162.842
162.040
148.253
136.418
135.521
134.559
134.283
134.149
132.964
130.974
129.916
129.797
129.728
123.706
120.793
119.488
77.415
77.160 CDCl3
76.907
17.698
13C NMR
(125 MHz, CDCl3)

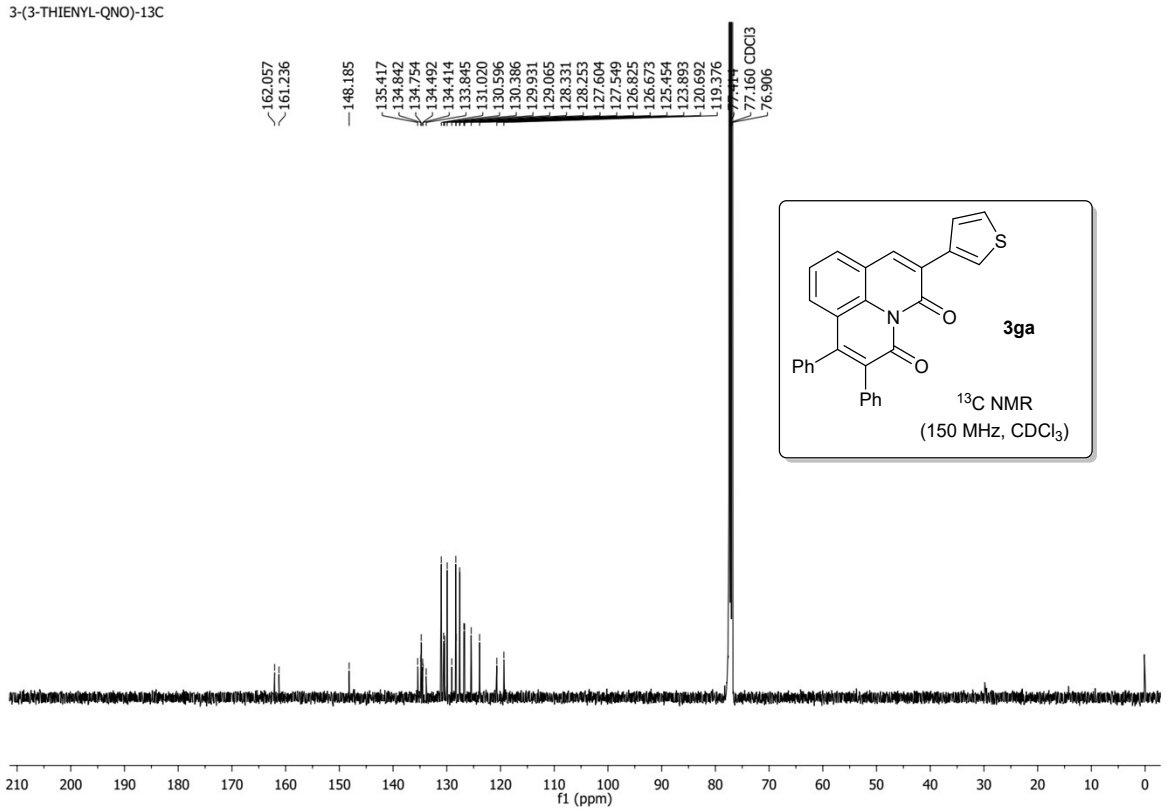

BDN-3-(3-Ph-QNO)-1H
—0.000 TMS
7.859
7.786
7.784
7.769
7.718
7.717
7.704
7.702
7.480
7.466
7.451
7.432
7.418
7.404
7.402
7.329
7.314
7.301
7.299
7.260
7.176
7.169
7.151
7.147
7.136
7.132
Ph
N
O
O
Ph
Ph
3ea
1H NMR
(500 MHz, CDCl3)
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
1.00
2.00
1.05
2.07
2.06
4.07
7.03
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
BDN-3-(3-Ph-QNO)-13C
161.996
161.618
148.173
137.026
135.458
134.998
134.510
134.474
131.015
130.681
130.508
129.928
129.136
128.908
128.514
128.333
128.243
127.607
127.543
123.845
120.774
119.497
77.414
76.906
Ph
N
O
O
Ph
Ph
3ea
13C NMR
(125 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

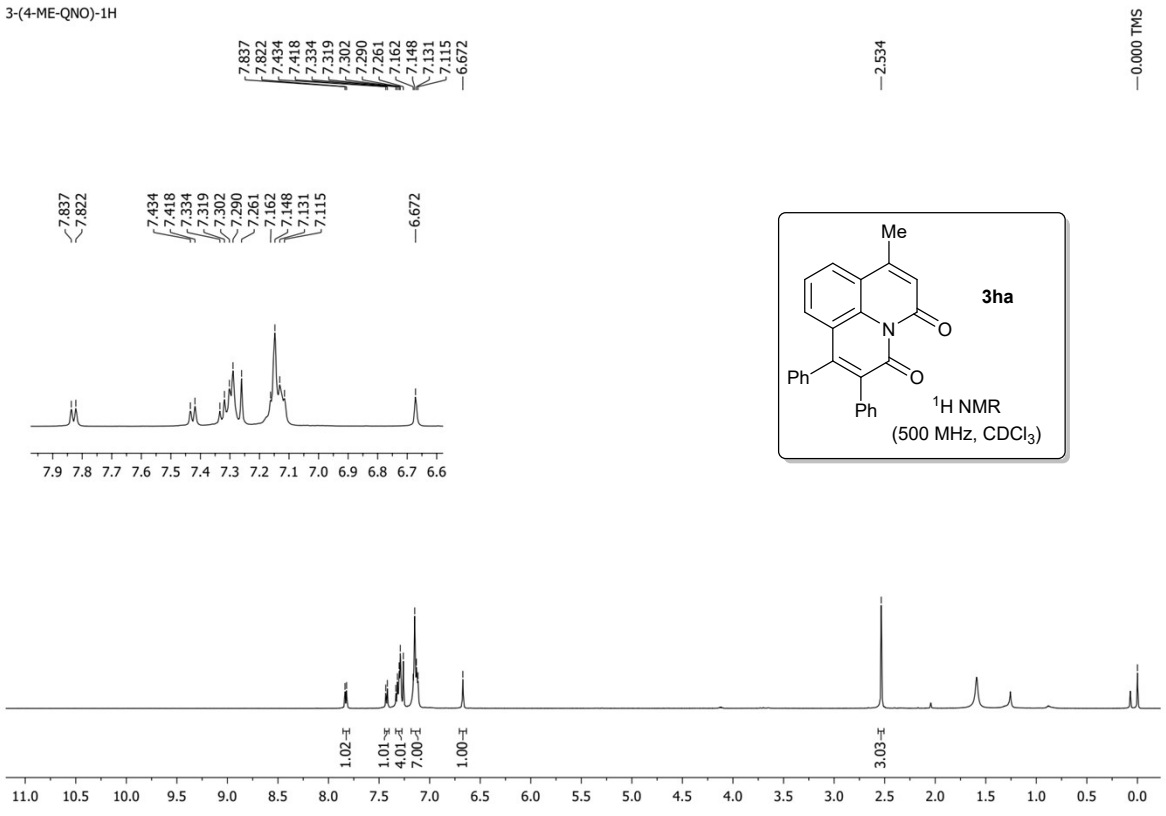

3-(3-CF3Ph-QNO)-1H
8.014
7.994
7.914
7.752
7.738
7.683
7.668
7.601
7.585
7.570
7.463
7.448
7.358
7.343
7.327
7.320
7.309
7.307
7.259
7.195
7.169
7.156
7.141
0.000 TMS
CF3
N
O
O
Ph
Ph
3fa
1H NMR
(500 MHz, CDCl3)
2.00
1.00
1.02
1.00
1.01
1.00
4.07
7.00

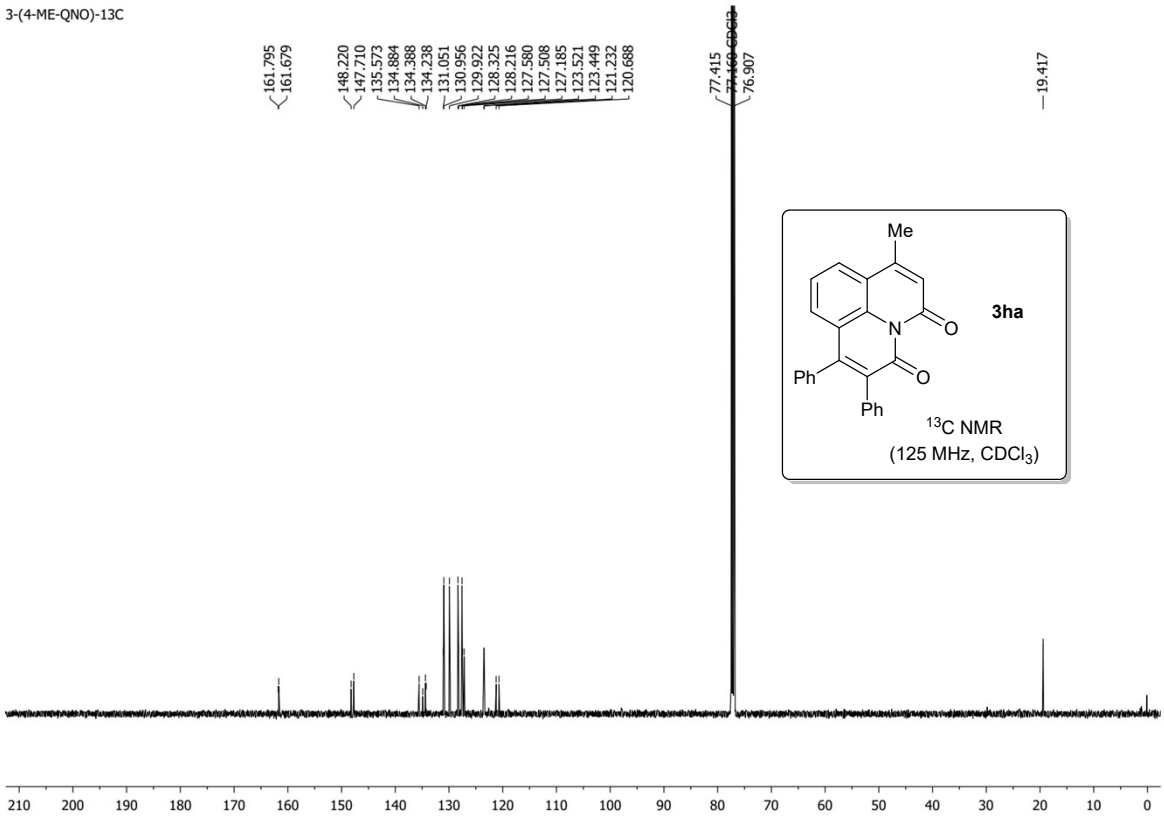

3-(3-CF3Ph-QNO)-13C
161.885
161.277
148.204
137.907
136.163
135.296
134.599
134.492
134.348
133.496
132.620
131.387
131.131
131.085
130.972
130.953
130.873
130.613
129.900
128.954
128.380
128.328
127.633
127.450
125.934
125.902
125.871
125.842
125.586
125.569
125.537
125.508
125.287
124.053
123.121
120.936
120.893
119.133
77.414
77.160 CDCl3
76.906
CF3
N
O
O
Ph
Ph
3fa
13C NMR
(125 MHz, CDCl3)

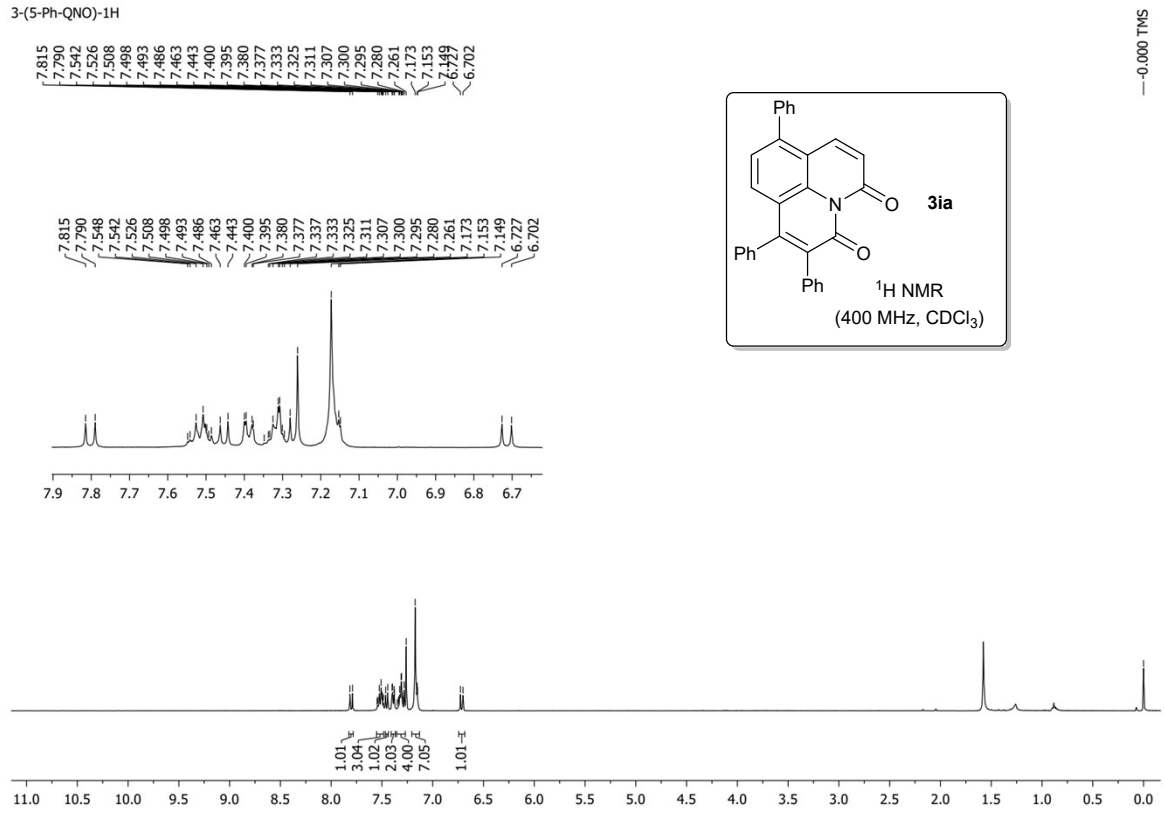

3-(3-CF3Ph-QNO)-13C
-62.507
CF3
N
O
O
Ph
Ph
3fa
19F NMR
(470 MHz, CDCl3)
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200

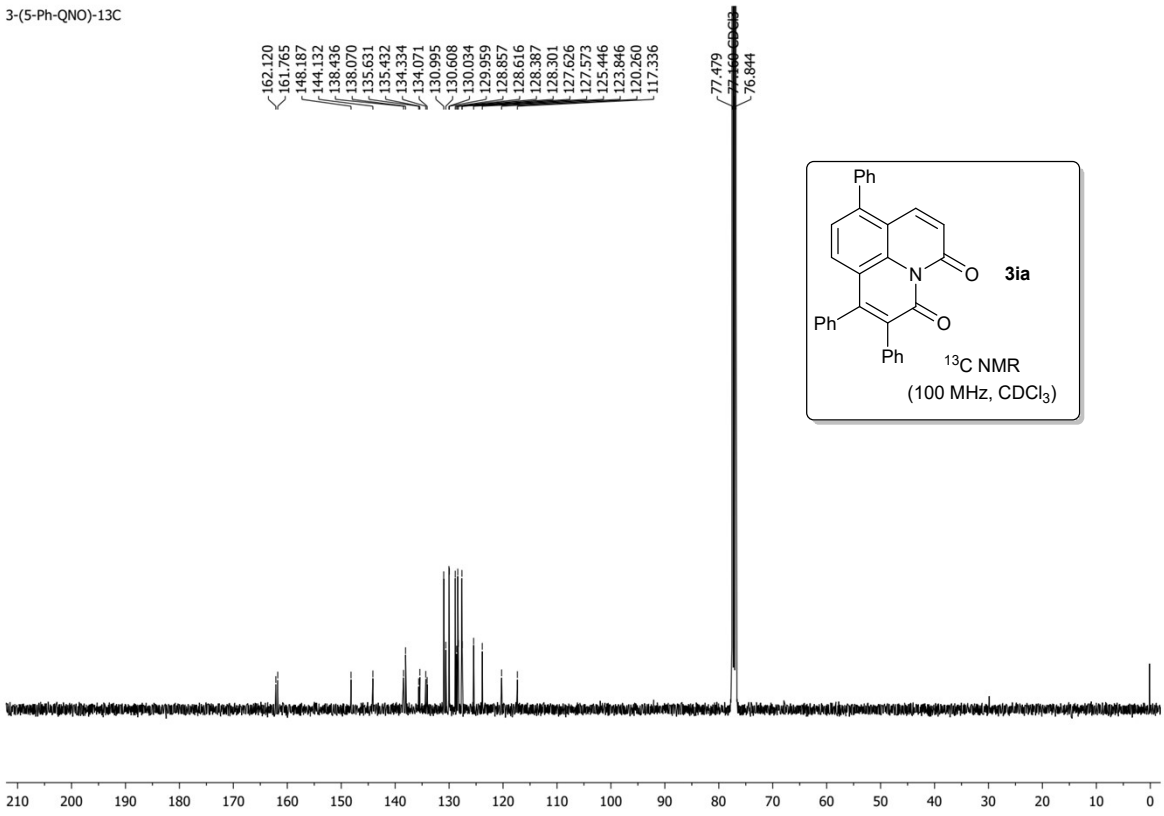

3-(3-THIENYL-QNO)-1H
8.321 8.318 8.314 8.311 8.000 7.728 7.724 7.709 7.705 7.613 7.610 7.600 7.597 7.416 7.413 7.406 7.401 7.397 7.393 7.334 7.326 7.315 7.310 7.302 7.297 7.260 7.187 7.180 7.169 7.157 7.149 7.146 7.138 7.133
0.000 TMS
8.000 7.613 7.610 7.600 7.597 7.416 7.413 7.406 7.401 7.397 7.393 7.334 7.326 7.315 7.310 7.302 7.297 7.260 7.180 7.169 7.157 7.149 7.146 7.138 7.133
8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1
f1 (ppm)
S
N
O
O
Ph
Ph
3ga
1H NMR
(400 MHz, CDCl3)
1.00 1.00 1.00 1.07 2.10 4.06 7.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

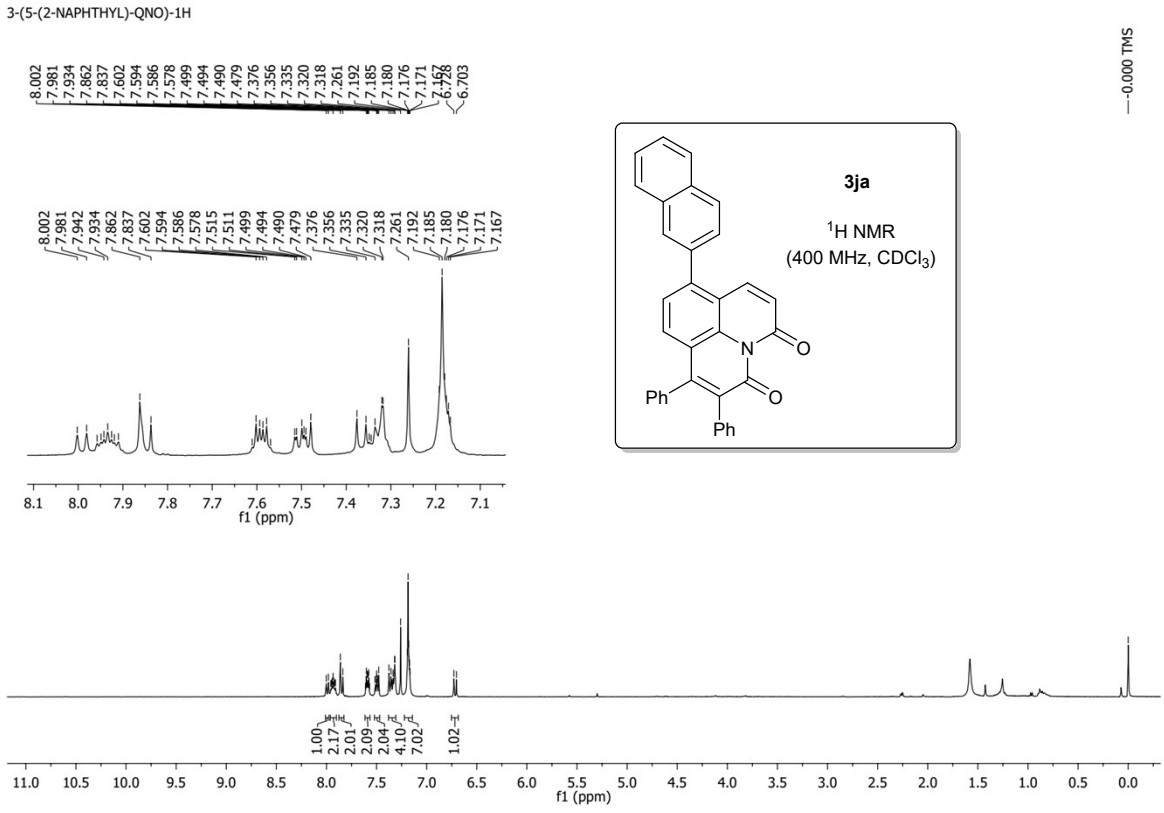

3-(3-THIENYL-QNO)-13C
162.057
161.236
148.185
135.417
134.842
134.754
134.492
134.414
133.845
131.020
130.596
130.386
129.931
129.065
128.331
128.253
127.604
127.549
126.825
126.673
125.454
123.893
120.692
119.376
77.414
77.160 CDCl3
76.906
S
N
O
O
Ph
Ph
3ga
13C NMR
(150 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

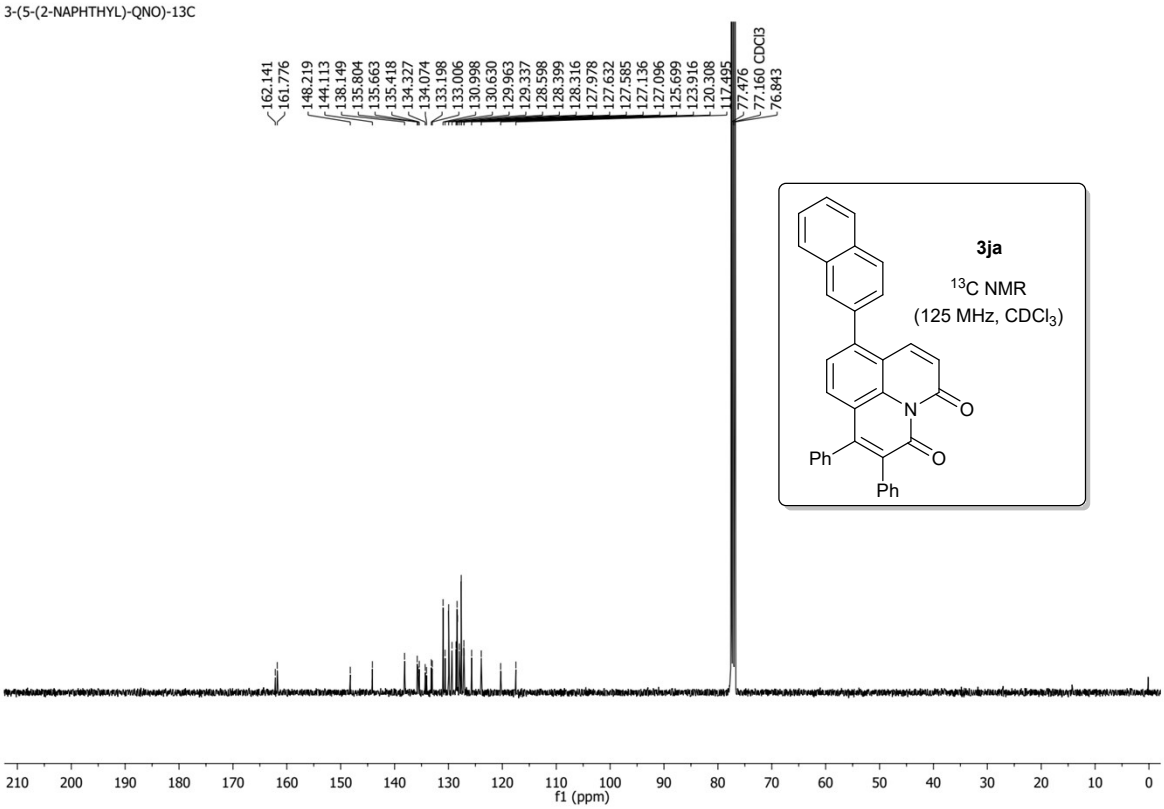

3-(4-ME-QNO)-1H
7.837
7.822
7.434
7.418
7.334
7.319
7.302
7.290
7.261
7.162
7.148
7.131
7.115
6.672
2.534
0.000 TMS
Me
N
O
O
Ph
Ph
3ha
1H NMR
(500 MHz, CDCl3)
7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6
1.02
1.01
4.01
7.00
1.00
3.03
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

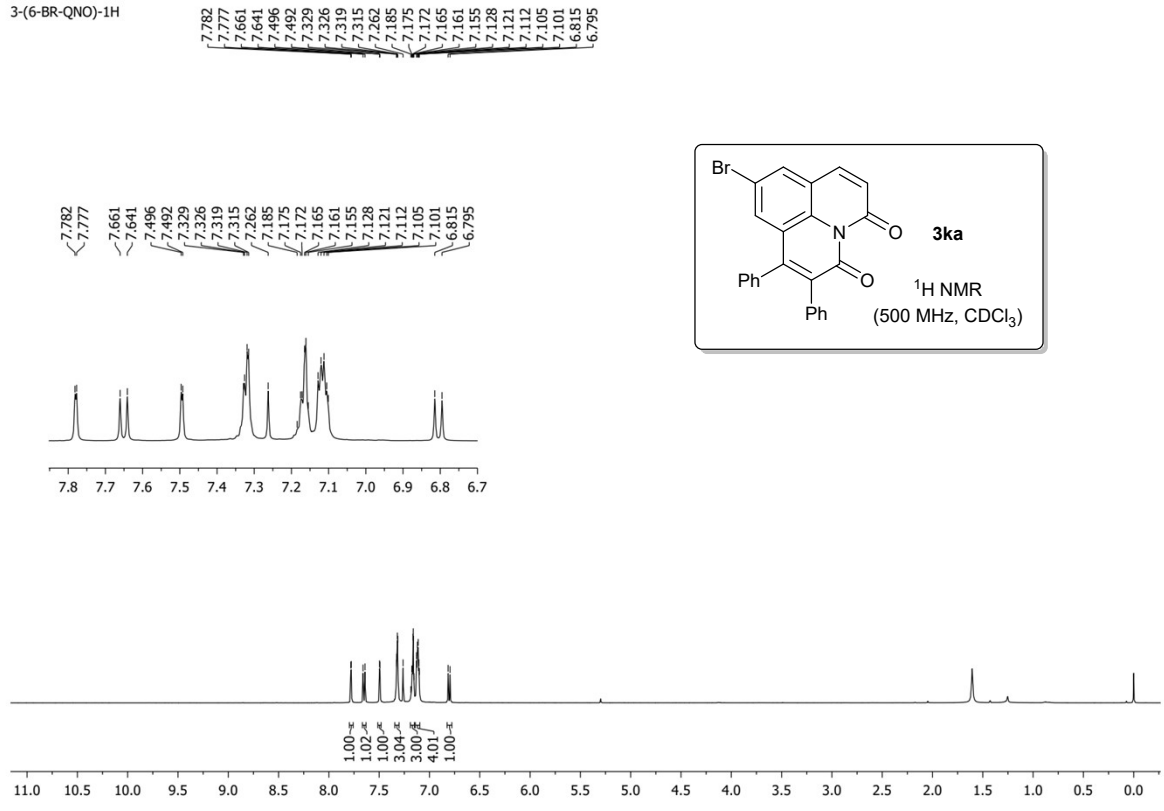

3-(4-ME-QNO)-13C
161.795
161.679
148.220
147.710
135.573
134.884
134.388
134.238
131.051
130.956
129.922
128.325
128.216
127.580
127.508
127.185
123.521
123.449
121.232
120.688
77.415
77.160 CDCl3
76.907
19.417
Me
N
O
O
Ph
Ph
3ha
13C NMR
(125 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

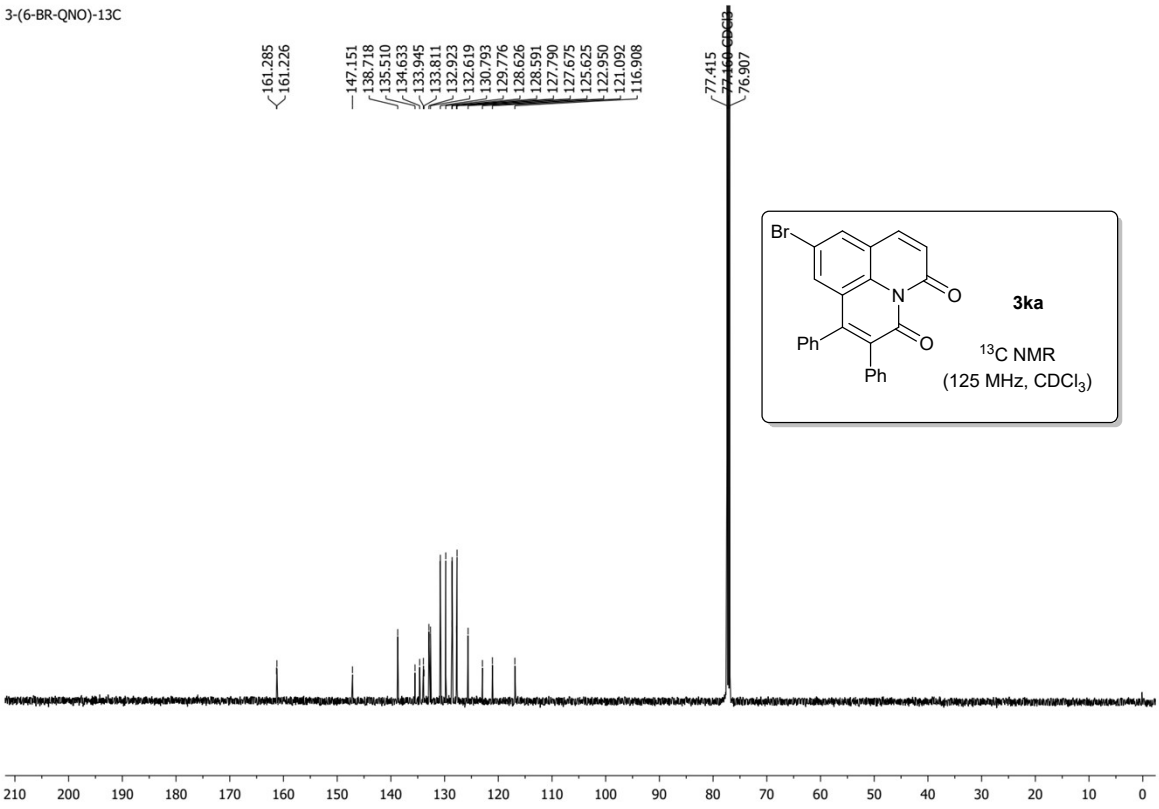

3-(5-Ph-QNO)-1H
7.815
7.790
7.542
7.526
7.508
7.498
7.493
7.486
7.463
7.443
7.400
7.395
7.380
7.377
7.333
7.325
7.311
7.307
7.300
7.295
7.280
7.261
7.173
7.153
7.149
6.727
6.702
0.000 TMS
Ph
N
O
O
Ph
Ph
3ia
1H NMR
(400 MHz, CDCl3)
1.01
3.04
1.02
2.03
4.00
7.05
1.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7

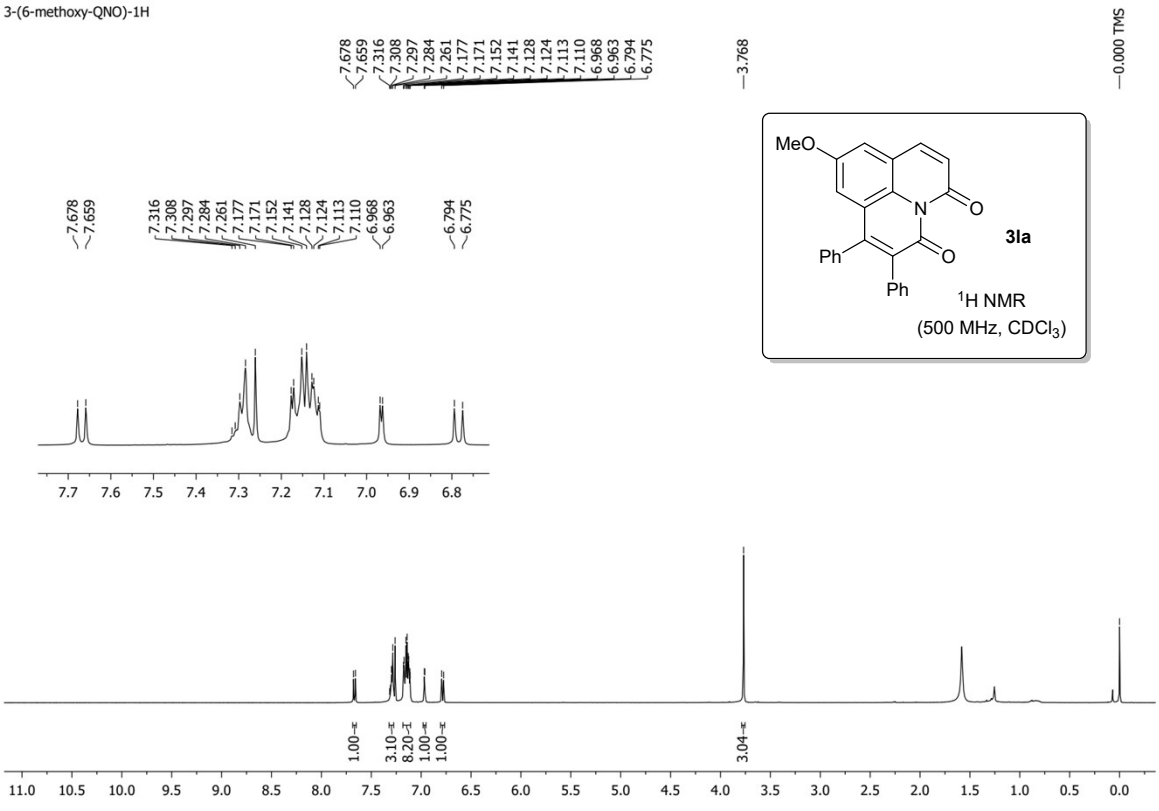

3-(5-Ph-QNO)-13C
162.120
161.765
148.187
144.132
138.436
138.070
135.631
135.432
134.334
134.071
130.995
130.608
130.034
129.959
128.857
128.616
128.387
128.301
127.626
127.573
125.446
123.846
120.260
117.336
77.479
76.844
Ph
N
O
Ph
O
Ph
3ia
13C NMR
(100 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

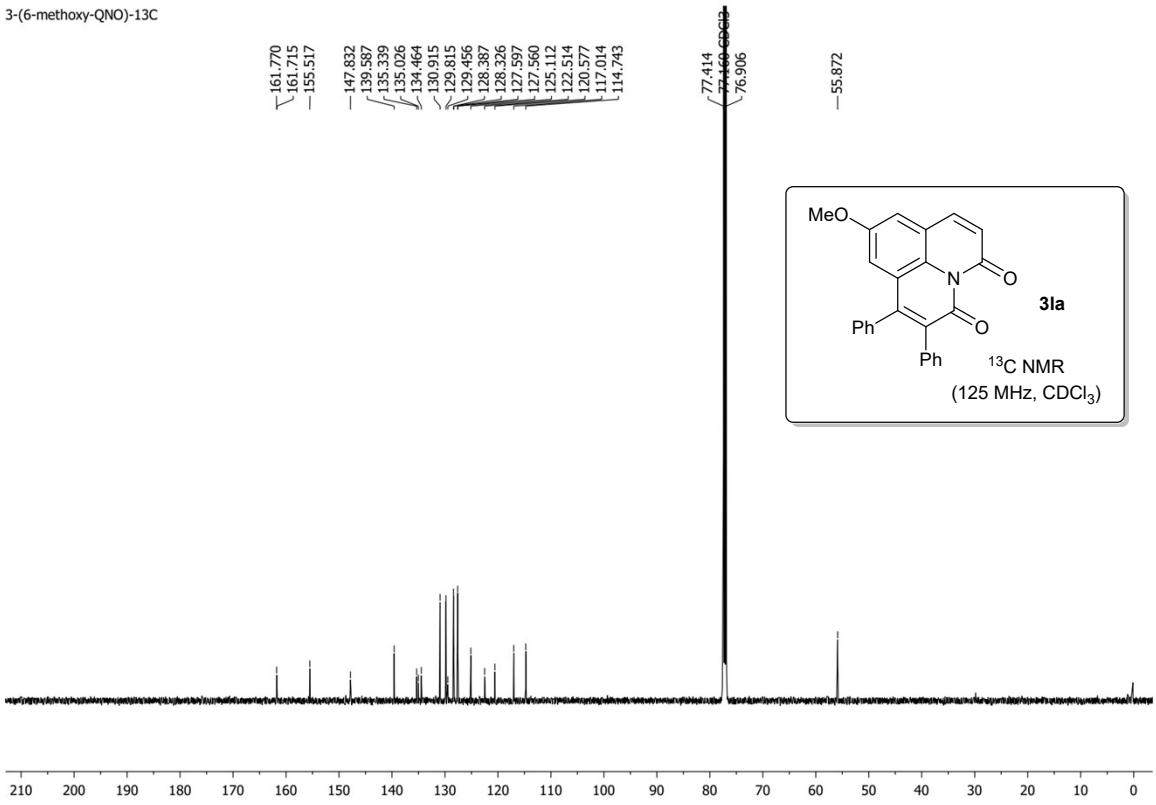

3-(5-(2-NAPHTHYL)-QNO)-1H
8.002
7.981
7.934
7.862
7.837
7.602
7.594
7.586
7.578
7.499
7.494
7.490
7.479
7.376
7.356
7.335
7.320
7.318
7.261
7.192
7.185
7.180
7.176
7.171
7.167
6.728
6.703
0.000 TMS
3ja
1H NMR
(400 MHz, CDCl3)
N
O
Ph
O
Ph
8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1
f1 (ppm)
1.00
2.17
2.01
2.09
2.04
4.10
7.02
1.02
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

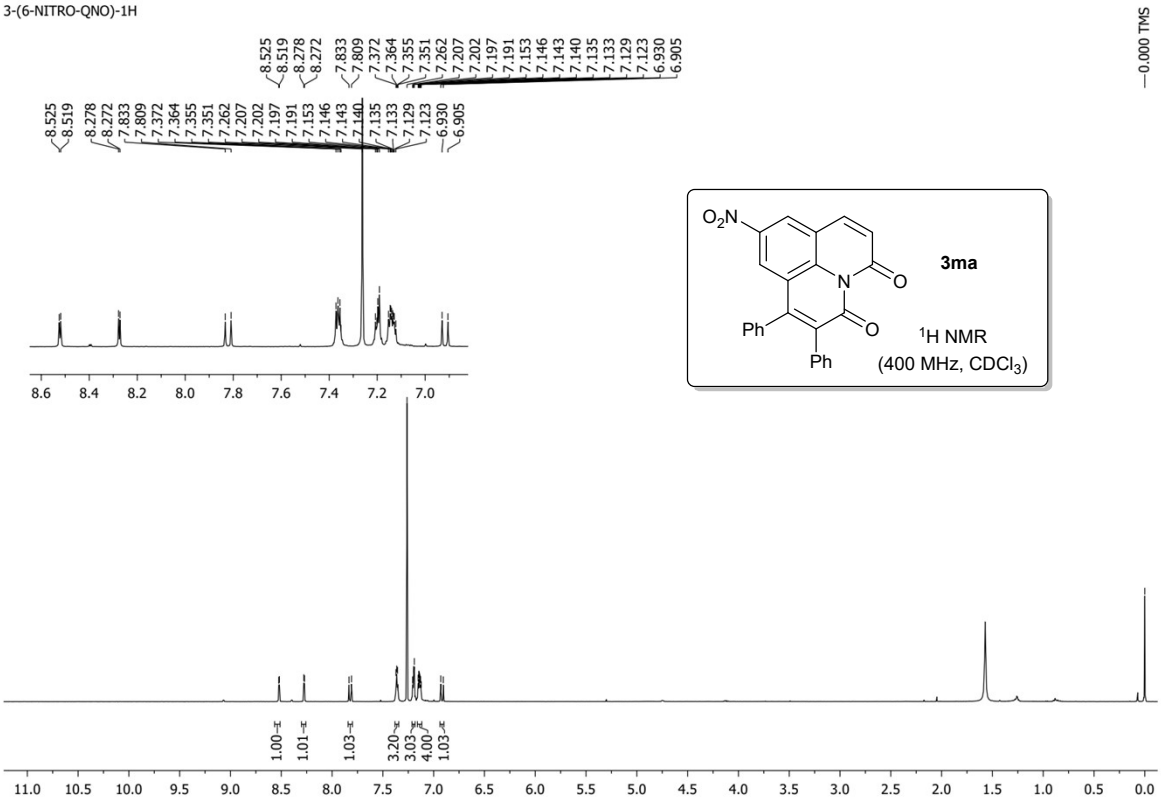

3-(5-(2-NAPHTHYL)-QNO)-13C
162.141
161.776
148.219
144.113
138.149
135.804
135.663
135.418
134.327
134.074
133.198
133.006
130.998
130.630
129.963
129.337
128.598
128.399
128.316
127.978
127.632
127.585
127.136
127.096
125.699
123.916
120.308
117.495
77.476
77.160 CDCl3
76.843
3ja
13C NMR
(125 MHz, CDCl3)
N
O
O
Ph
Ph
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

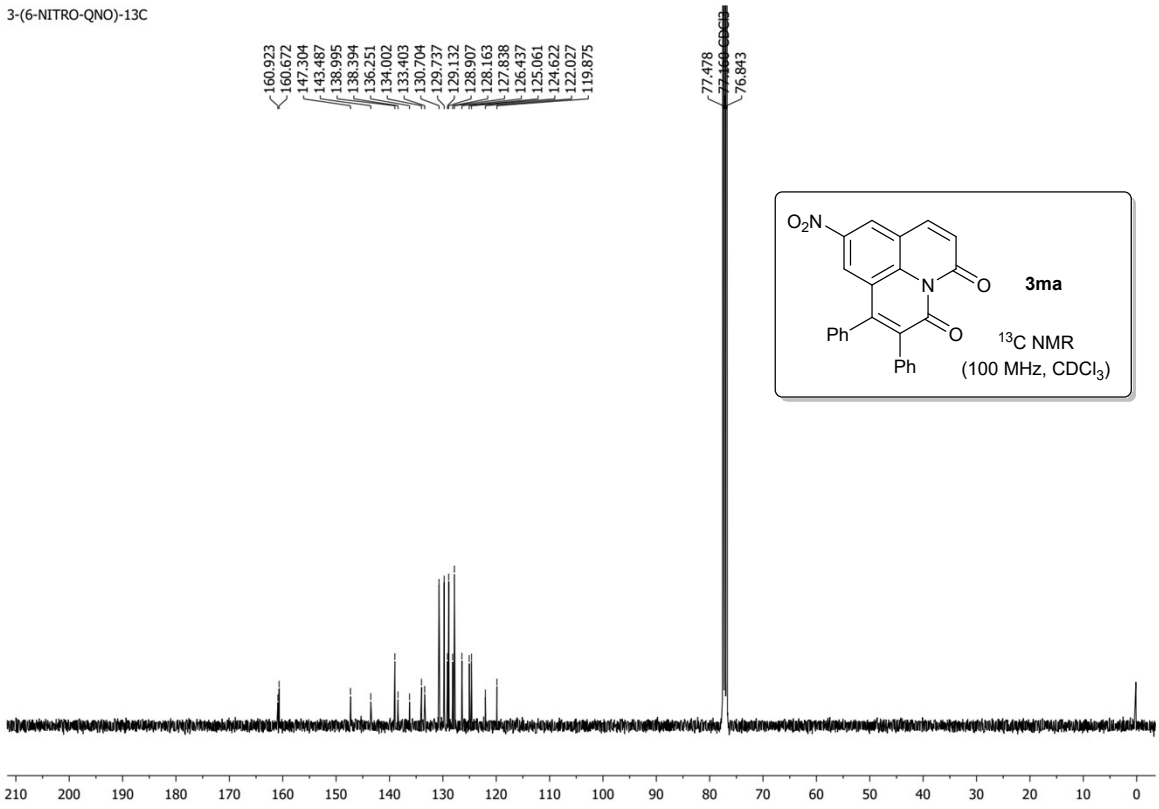

3-(6-BR-QNO)-1H
7.782
7.777
7.661
7.641
7.496
7.492
7.329
7.326
7.319
7.315
7.262
7.185
7.175
7.172
7.165
7.161
7.155
7.128
7.121
7.112
7.105
7.101
6.815
6.795
Br
N
O
O
Ph
Ph
3ka
1H NMR
(500 MHz, CDCl3)
7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7
1.00
1.02
1.00
3.04
3.00
4.01
1.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

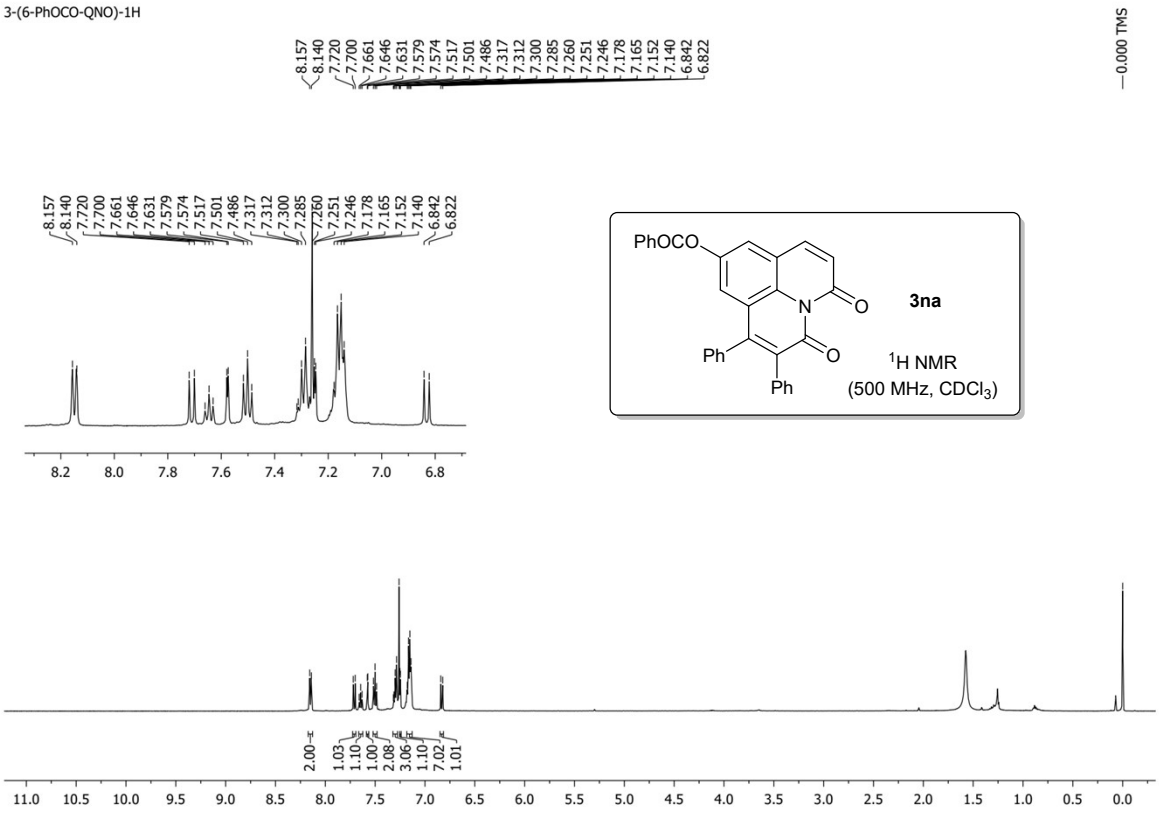

3-(6-BR-QNO)-13C
161.285
161.226
147.151
138.718
135.510
134.633
133.945
133.811
132.923
132.619
130.793
129.776
128.626
128.591
127.790
127.675
125.625
122.950
121.092
116.908
77.415
77.160 CDCl3
76.907
Br
N
O
O
Ph
Ph
3ka
13C NMR
(125 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

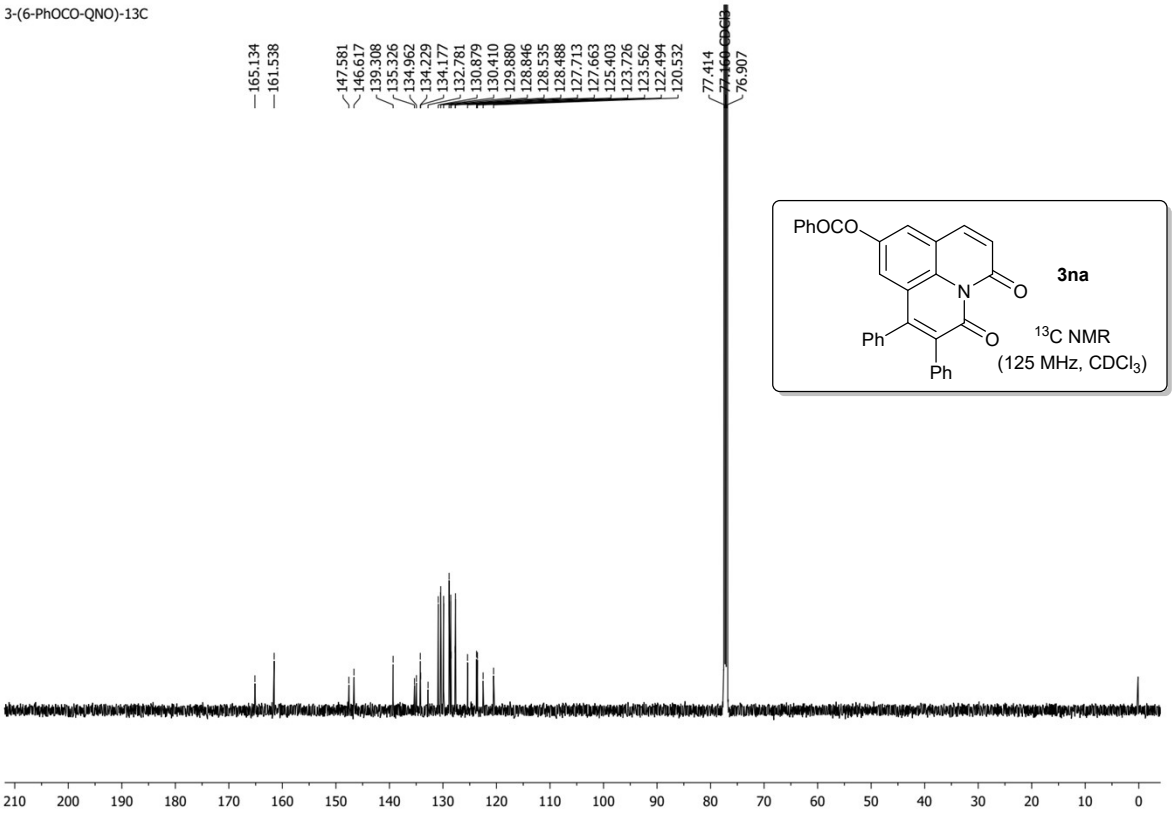

3-(6-methoxy-QNO)-1H
7.678
7.659
7.316
7.308
7.297
7.284
7.261
7.177
7.171
7.152
7.141
7.128
7.124
7.113
7.110
6.968
6.963
6.794
6.775
3.768
0.000 TMS
MeO
N
O
O
Ph
Ph
3la
1H NMR
(500 MHz, CDCl3)
7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8
1.00
3.10
8.20
1.00
1.00
3.04
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

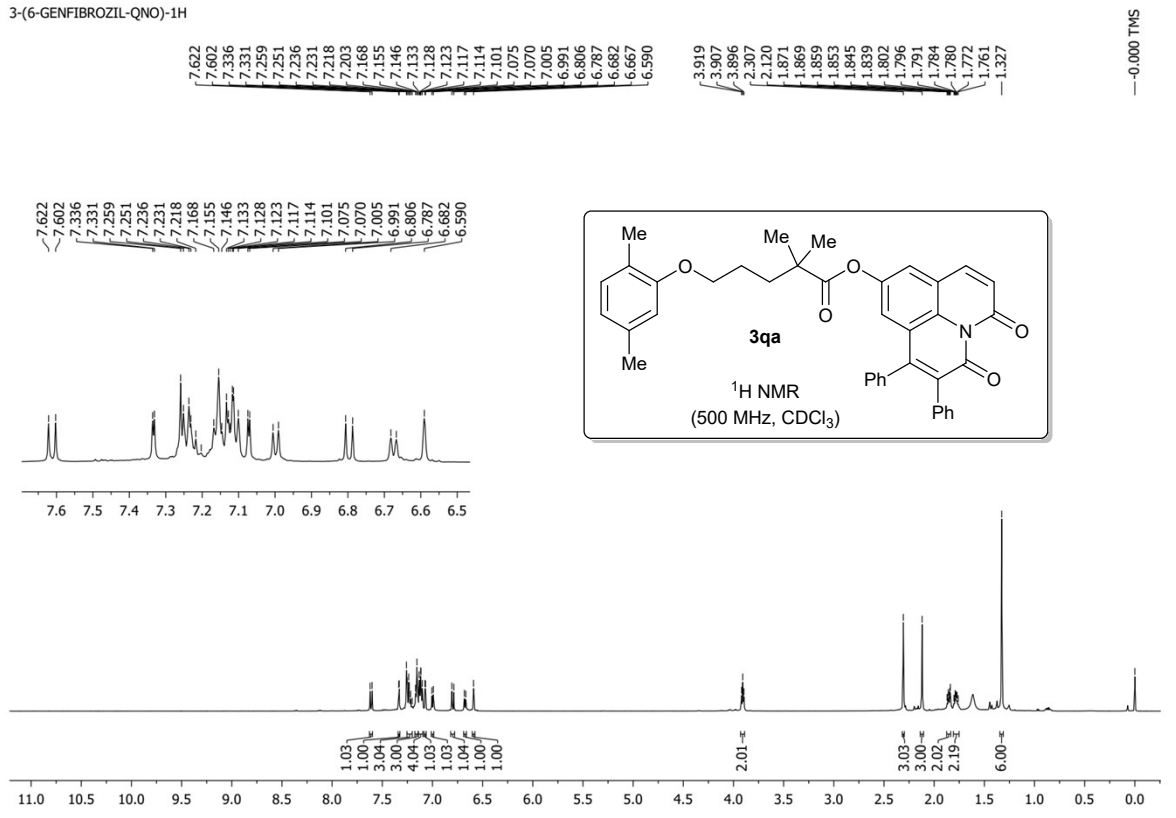

3-(6-methoxy-QNO)-13C
161.770
161.715
155.517
147.832
139.587
135.339
135.026
134.464
130.915
129.815
129.456
128.387
128.326
127.597
127.560
125.112
122.514
120.577
117.014
114.743
77.414
77.160 CDCl3
76.906
55.872
MeO
N
O
O
Ph
Ph
3la
13C NMR
(125 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

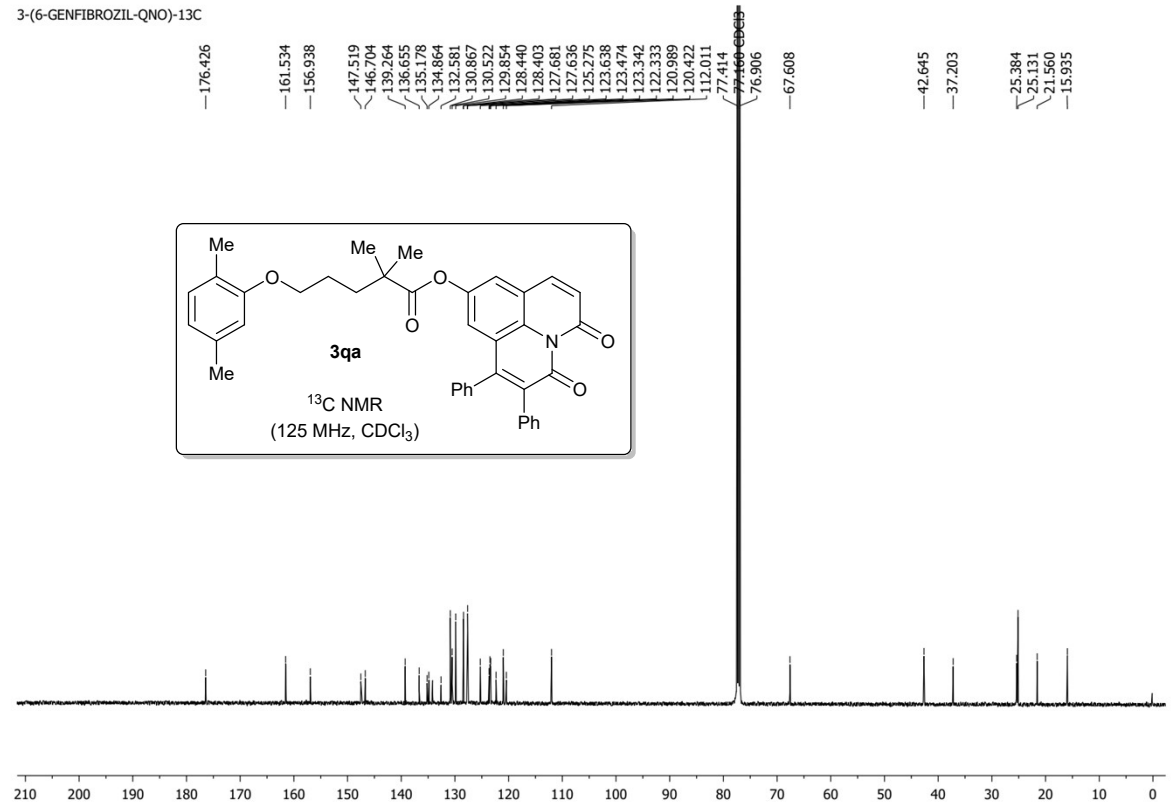

3-(6-NITRO-QNO)-1H
0.000 TMS
8.525
8.519
8.278
8.272
7.833
7.809
7.372
7.364
7.355
7.351
7.262
7.207
7.202
7.197
7.191
7.153
7.146
7.143
7.140
7.135
7.133
7.129
7.123
6.930
6.905
O2N
N
O
O
Ph
Ph
3ma
1H NMR
(400 MHz, CDCl3)
8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0
1.00
1.01
1.03
3.20
3.03
4.00
1.03
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

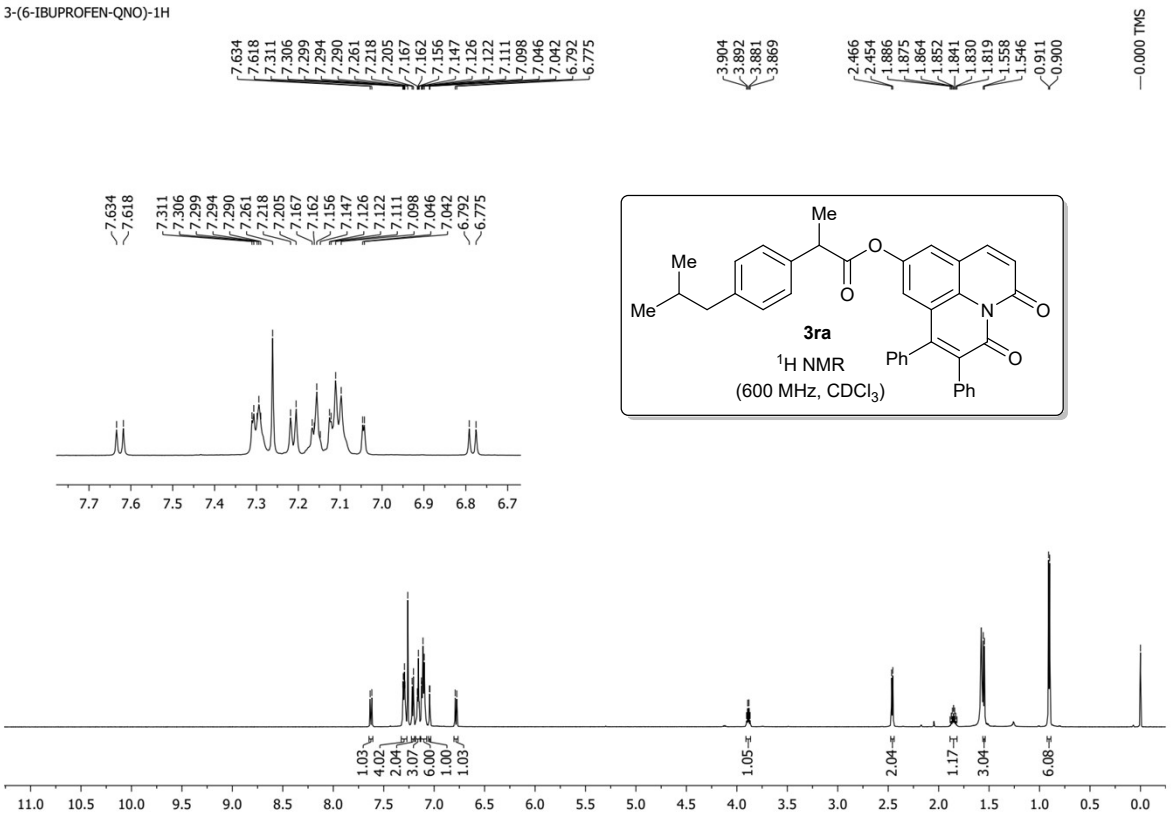

3-(6-NITRO-QNO)-13C
160.923
160.672
147.304
143.487
138.995
138.394
136.251
134.002
133.403
130.704
129.737
129.132
128.907
128.163
127.838
126.437
125.061
124.622
122.027
119.875
77.478
76.843
O2N
N
O
Ph
Ph
3ma
13C NMR
(100 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

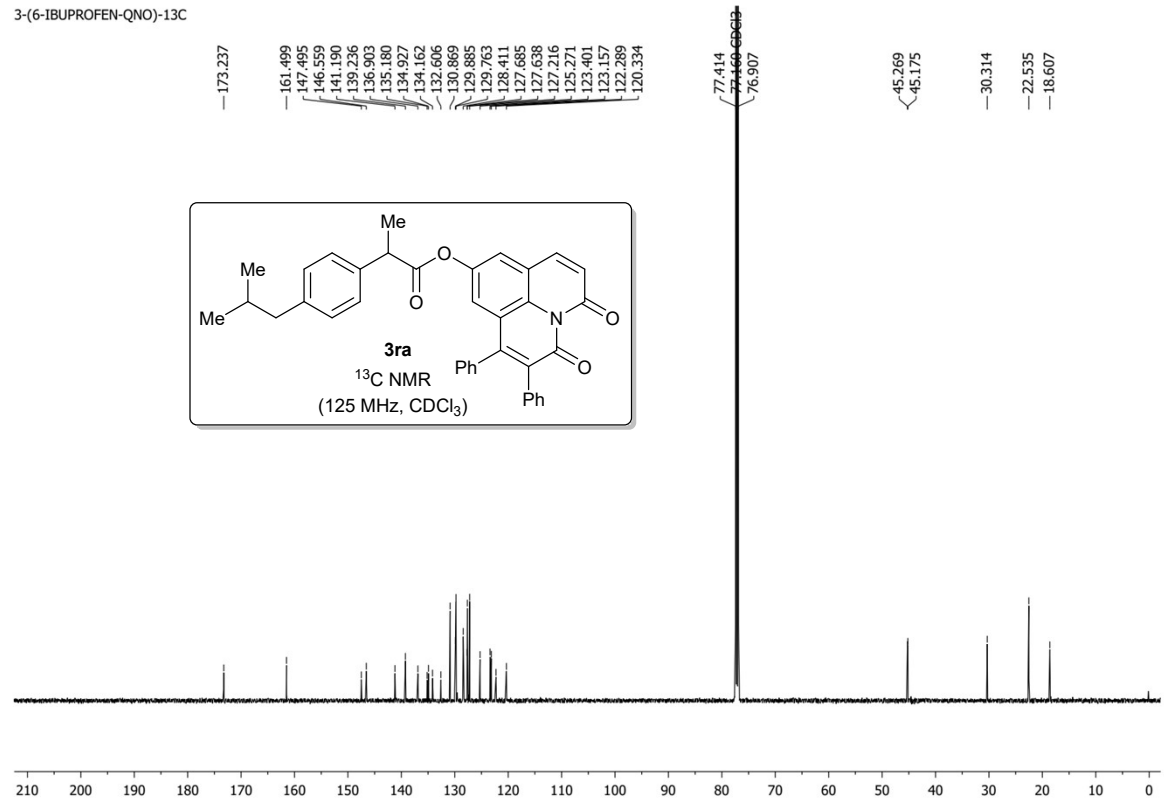

3-(6-PhOCO-QNO)-1H
8.157
8.140
7.720
7.700
7.661
7.646
7.631
7.579
7.574
7.517
7.501
7.486
7.317
7.312
7.300
7.285
7.260
7.251
7.246
7.178
7.165
7.152
7.140
6.842
6.822
0.000 TMS
PhOCO
N
O
Ph
Ph
3na
1H NMR
(500 MHz, CDCl3)
8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8
2.00
1.03
1.10
1.00
2.08
3.06
1.10
7.02
1.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

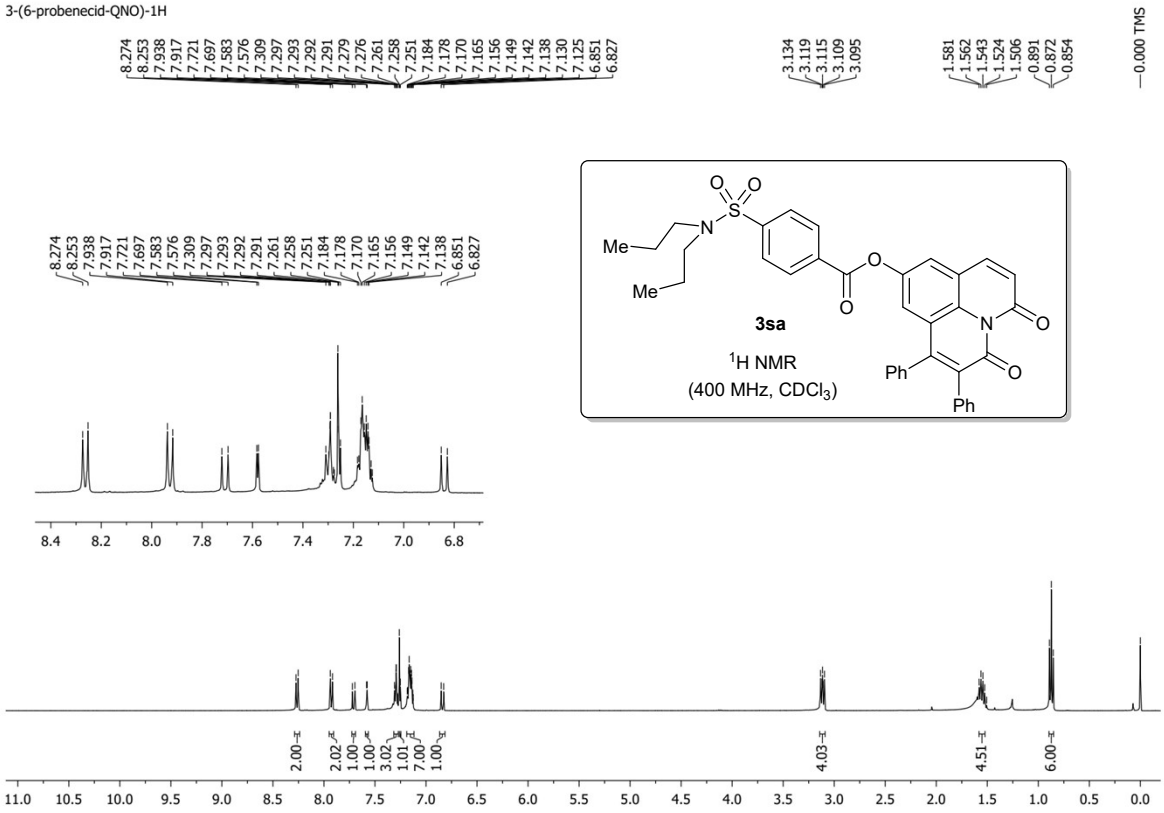

3-(6-PhOCO-QNO)-13C
PhOCO
3na
Ph
Ph
^{13}C NMR
(125 MHz, CDCl$_3$)

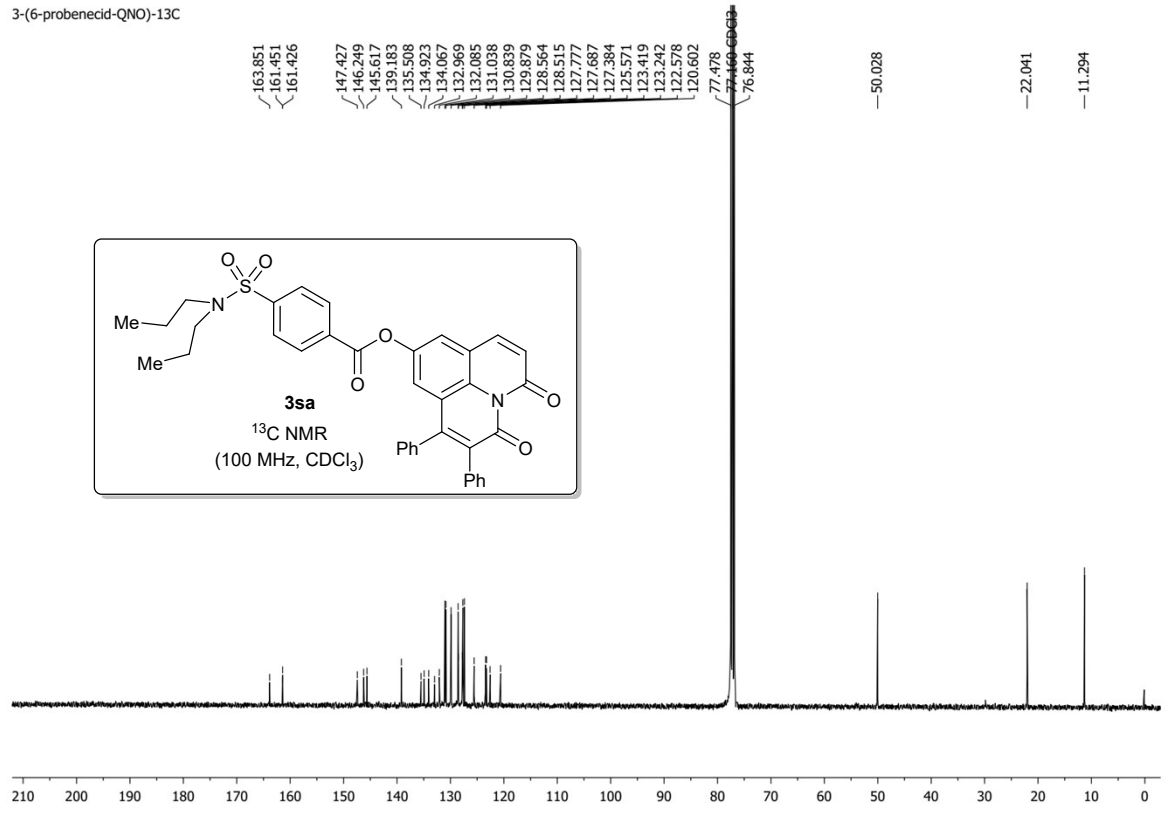

3-(6-GENFIBROZIL-QNO)-1H
Me
Me
Me
Me
3qa
Ph
Ph
^{1}H NMR
(500 MHz, CDCl$_3$)

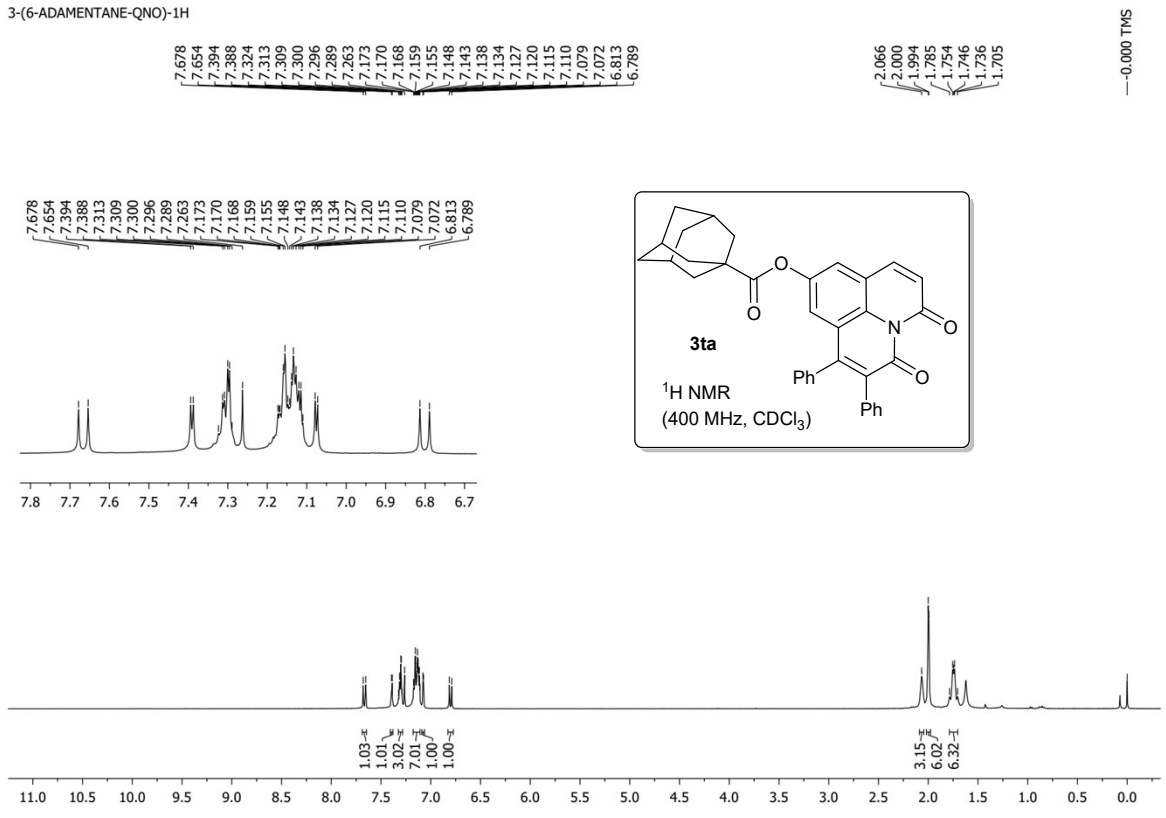

3-(6-GENFIBROZIL-QNO)-13C
176.426
161.534
156.938
147.519
146.704
139.264
136.655
135.178
134.864
132.581
130.867
130.522
129.854
128.440
128.403
127.681
127.636
125.275
123.638
123.474
123.342
122.333
120.989
120.422
112.011
77.414
77.160 CDCl3
76.906
67.608
42.645
37.203
25.384
25.131
21.560
15.935
Me
Me
Me
Me
O
O
O
O
N
O
Ph
Ph
3qa
13C NMR
(125 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

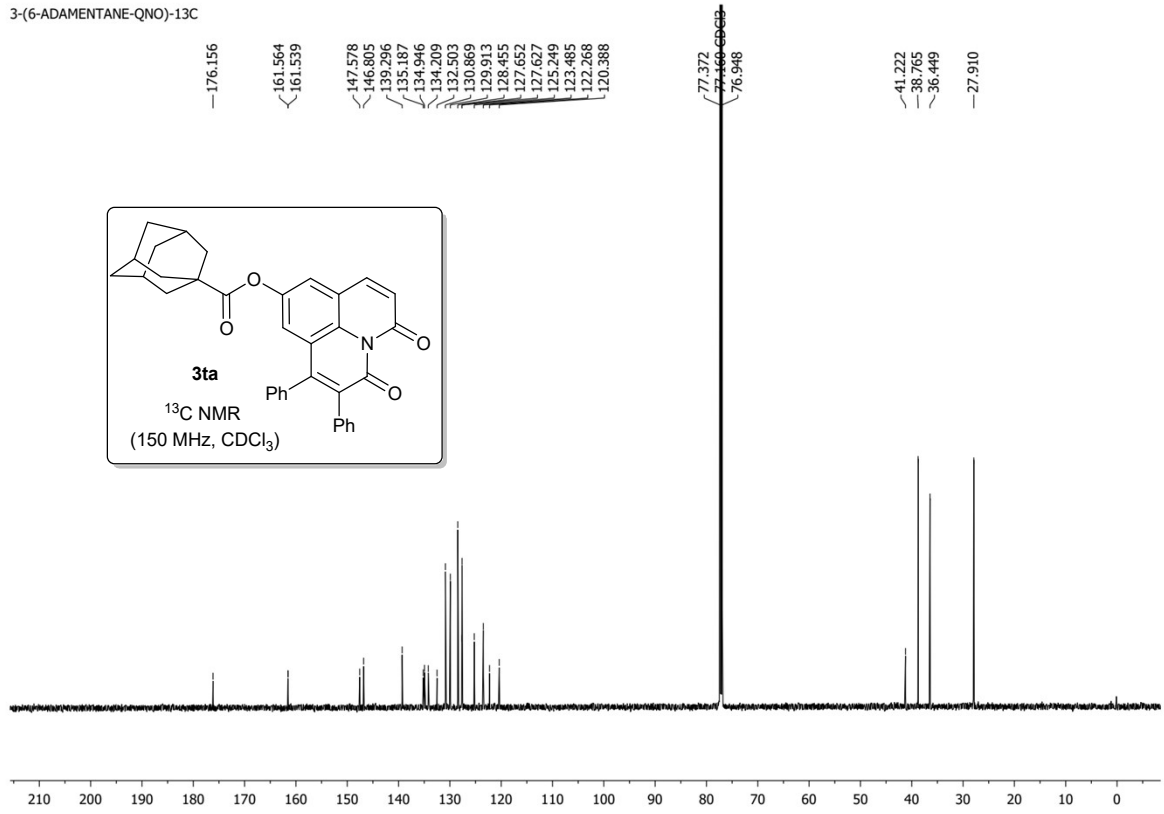

3-(6-IBUPROFEN-QNO)-1H
7.634
7.618
7.311
7.306
7.299
7.294
7.290
7.261
7.218
7.205
7.167
7.162
7.156
7.147
7.126
7.122
7.111
7.098
7.046
7.042
6.792
6.775
3.904
3.892
3.881
3.869
2.466
2.454
1.886
1.875
1.864
1.852
1.841
1.830
1.819
1.558
1.546
0.911
0.900
0.000 TMS
Me
Me
Me
O
O
N
O
Ph
Ph
O
3ra
1H NMR
(600 MHz, CDCl3)
7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7
1.03
4.02
2.04
3.07
6.00
1.00
1.03
1.05
2.04
1.17
3.04
6.08
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

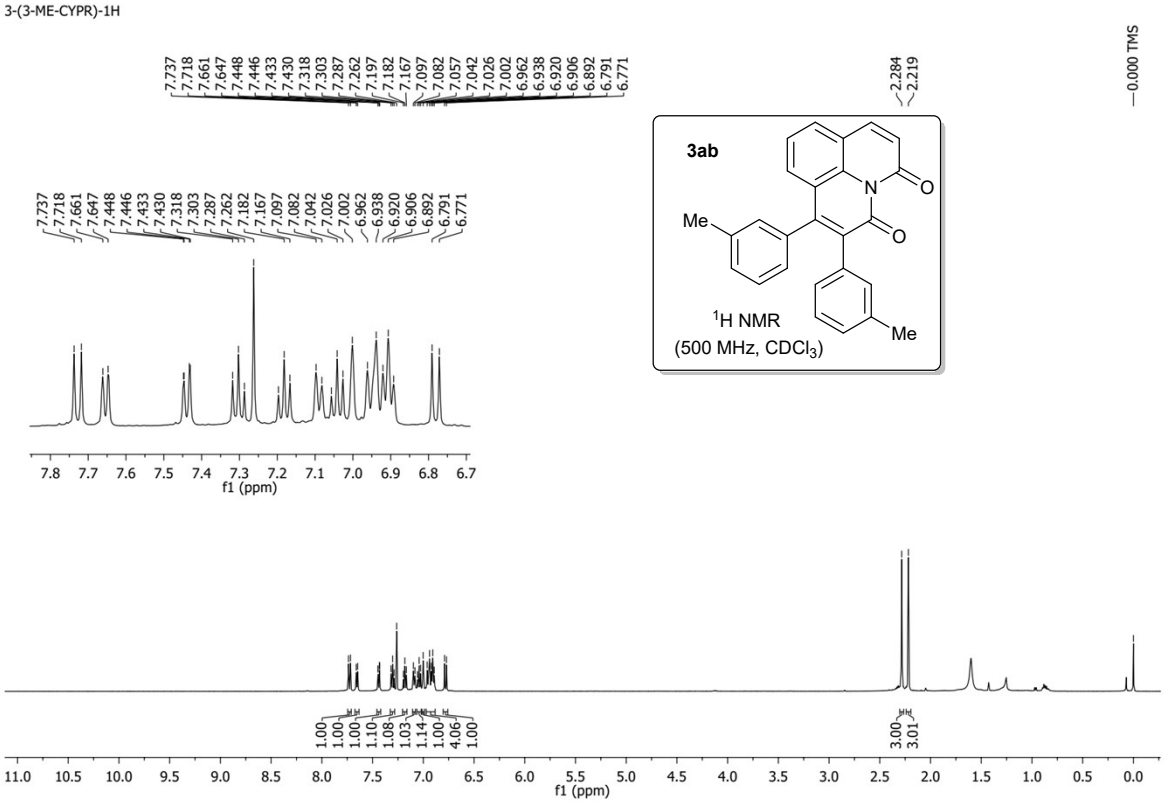

3-(6-IBUPROFEN-QNO)-13C
173.237
161.499
147.495
146.559
141.190
139.236
136.903
135.180
134.927
134.162
132.606
130.869
129.885
129.763
128.411
127.685
127.638
127.216
125.271
123.401
123.157
122.289
120.334
77.414
77.160 CDCl3
76.907
45.269
45.175
30.314
22.535
18.607
Me
Me
Me
O
O
N
O
O
Ph
Ph
3ra
13C NMR
(125 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

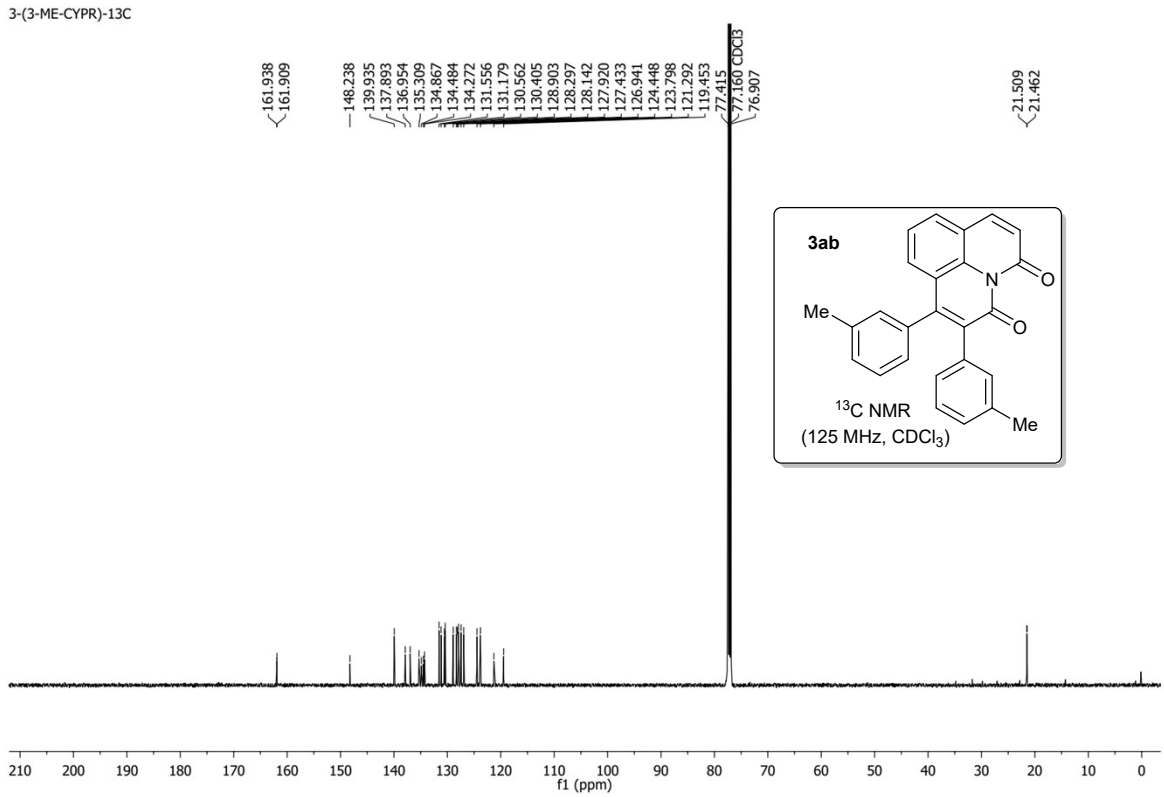

3-(6-probenecid-QNO)-1H
8.274
8.253
7.938
7.917
7.721
7.697
7.583
7.576
7.309
7.297
7.293
7.292
7.291
7.279
7.276
7.261
7.258
7.251
7.184
7.178
7.170
7.165
7.156
7.149
7.142
7.138
7.130
7.125
6.851
6.827
3.134
3.119
3.115
3.109
3.095
1.581
1.562
1.543
1.524
1.506
0.891
0.872
0.854
0.000 TMS
Me
Me
N
S
O
O
O
O
O
N
O
Ph
Ph
O
3sa
1H NMR
(400 MHz, CDCl3)
8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8
2.00
2.02
1.00
1.00
3.02
1.01
7.00
1.00
4.03
4.51
6.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

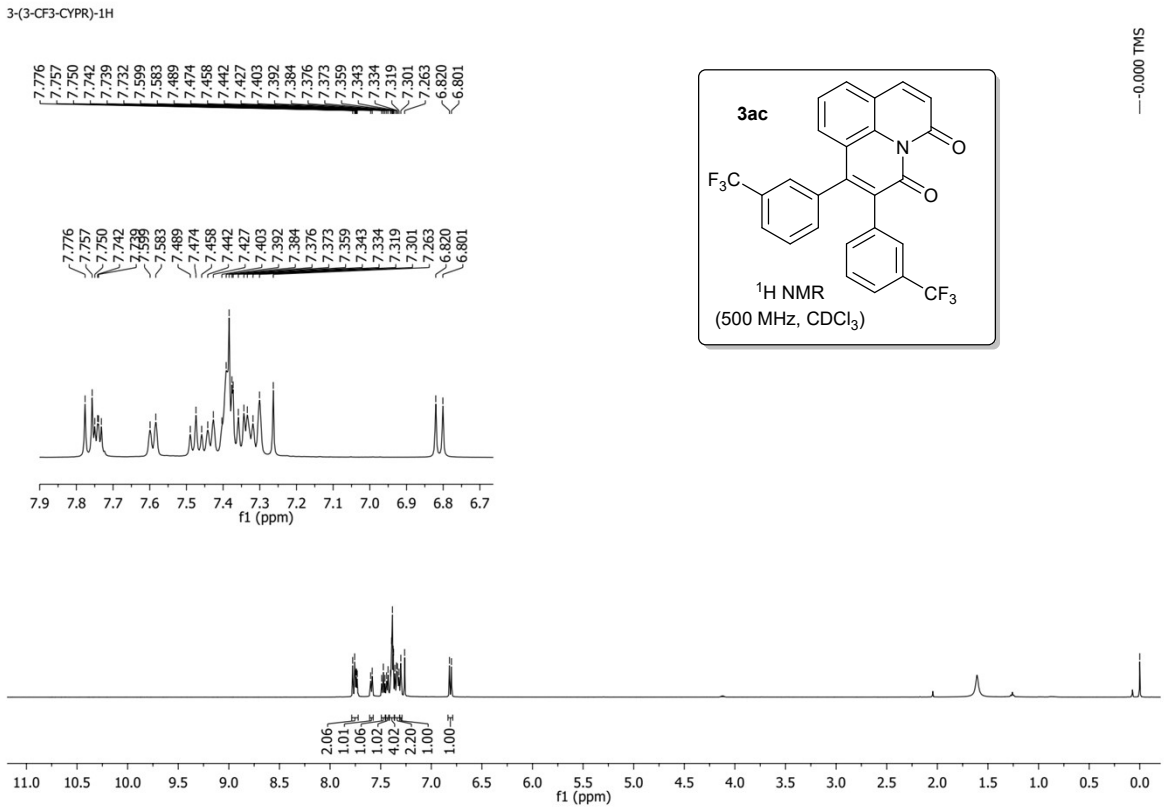

3-(6-probenecid-QNO)-13C
163.851
161.451
161.426
147.427
146.249
145.617
139.183
135.508
134.923
134.067
132.969
132.085
131.038
130.839
129.879
128.564
128.515
127.777
127.687
127.384
125.571
123.419
123.242
122.578
120.602
77.478
77.160 CDCl3
76.844
50.028
22.041
11.294
Me
Me
3sa
13C NMR
(100 MHz, CDCl3)
Ph
Ph


3-(6-ADAMENTANE-QNO)-1H
7.678
7.654
7.394
7.388
7.324
7.313
7.309
7.300
7.296
7.289
7.263
7.173
7.170
7.168
7.159
7.155
7.148
7.143
7.138
7.134
7.127
7.120
7.115
7.110
7.079
7.072
6.813
6.789
2.066
2.000
1.994
1.785
1.754
1.746
1.736
1.705
0.000 TMS
3ta
1H NMR
(400 MHz, CDCl3)
Ph
Ph
1.03
1.01
3.02
7.01
1.00
3.15
6.02
6.32

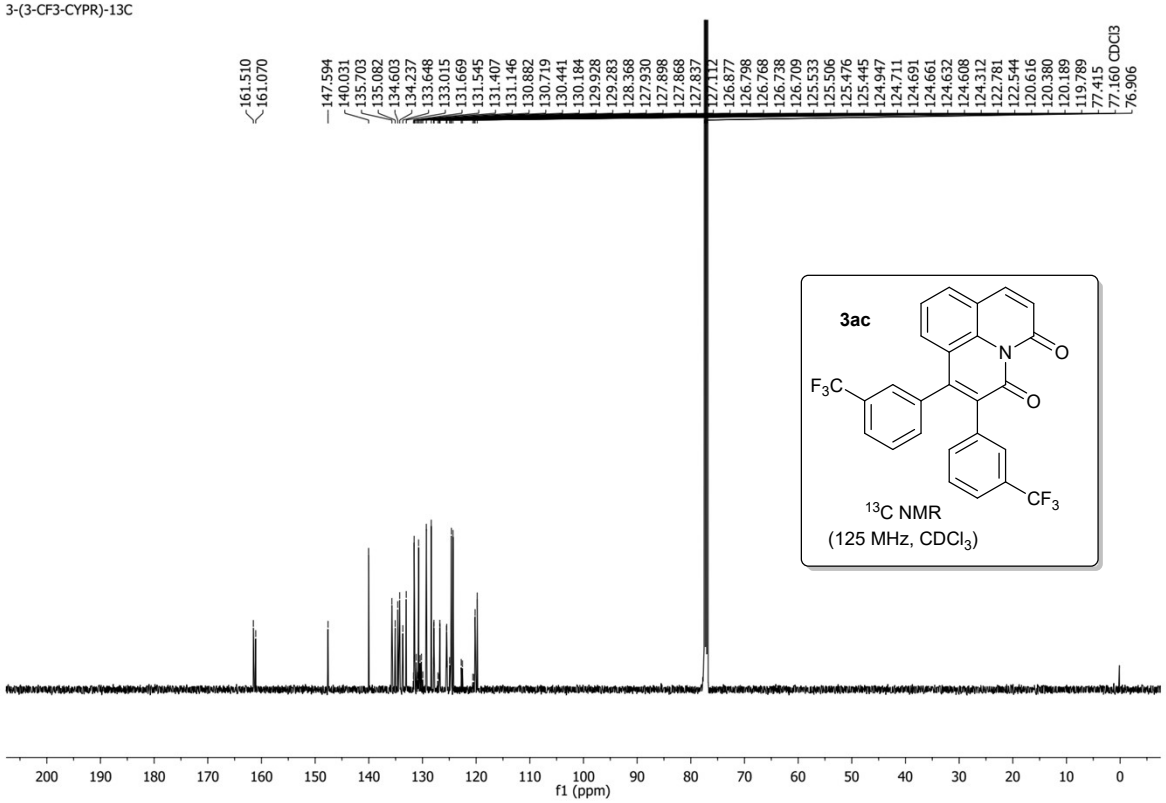

3-(6-ADAMENTANE-QNO)-13C
176.156
161.564
161.539
147.578
146.805
139.296
135.187
134.946
134.209
132.503
130.869
129.913
128.455
127.652
127.627
125.249
123.485
122.268
120.388
77.372
77.160 CDCl3
76.948
41.222
38.765
36.449
27.910
3ta
13C NMR
(150 MHz, CDCl3)
Ph
Ph
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0


3-(3-ME-CYPR)-1H
7.737
7.718
7.661
7.647
7.448
7.446
7.433
7.430
7.318
7.303
7.287
7.262
7.197
7.182
7.167
7.097
7.082
7.057
7.042
7.026
7.002
6.962
6.938
6.920
6.906
6.892
6.791
6.771
2.284
2.219
0.000 TMS
3ab
Me
Me
1H NMR
(500 MHz, CDCl3)
7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7
f1 (ppm)
1.00
1.00
1.00
1.10
1.08
1.03
1.14
1.00
4.06
1.00
3.00
3.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

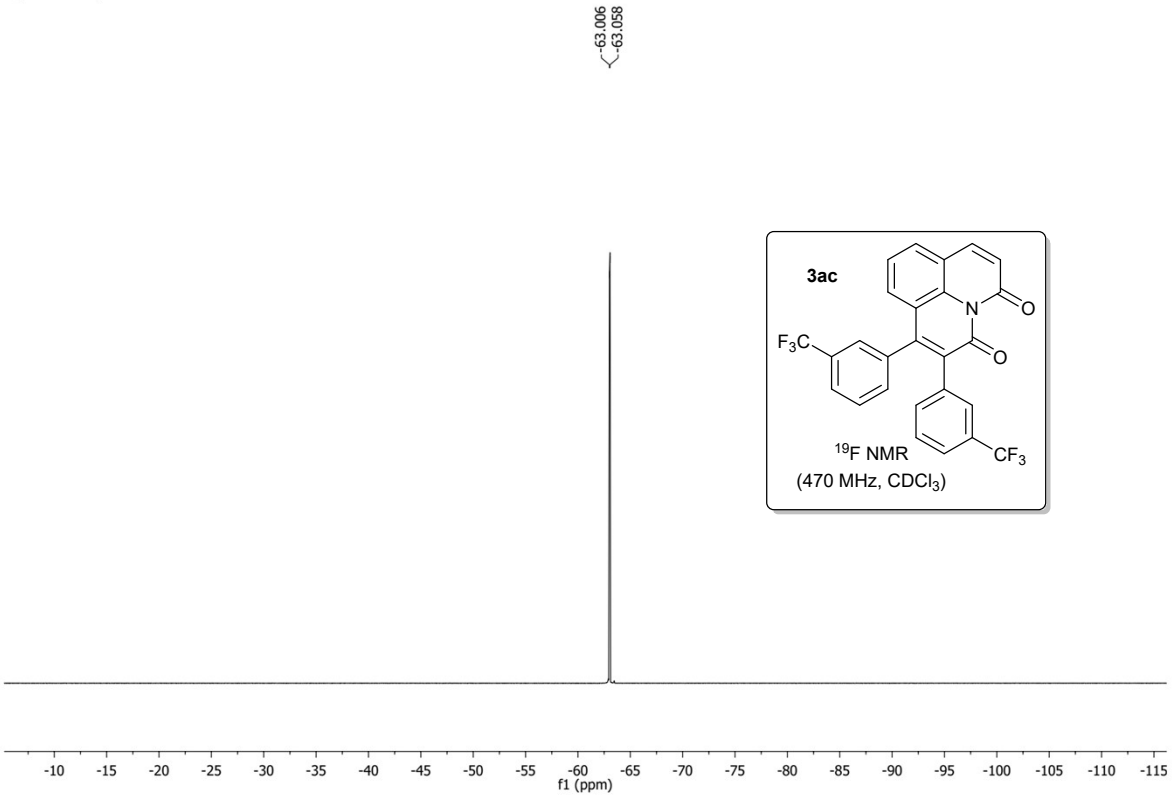

3-(3-ME-CYPR)-13C
161.938
161.909
148.238
139.935
137.893
136.954
135.309
134.867
134.484
134.272
131.556
131.179
130.562
130.405
128.903
128.297
128.142
127.920
127.433
126.941
124.448
123.798
121.292
119.453
77.415
77.160 CDCl3
76.907
21.509
21.462
3ab
Me
N
O
O
Me
13C NMR
(125 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


3-(3-CF3-CYPR)-1H
7.776
7.757
7.750
7.742
7.739
7.732
7.599
7.583
7.489
7.474
7.458
7.442
7.427
7.403
7.392
7.384
7.376
7.373
7.359
7.343
7.334
7.319
7.301
7.263
6.820
6.801
0.000 TMS
3ac
F3C
N
O
O
CF3
1H NMR
(500 MHz, CDCl3)
7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7
f1 (ppm)
2.06
1.01
1.06
1.02
4.02
2.20
1.00
1.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

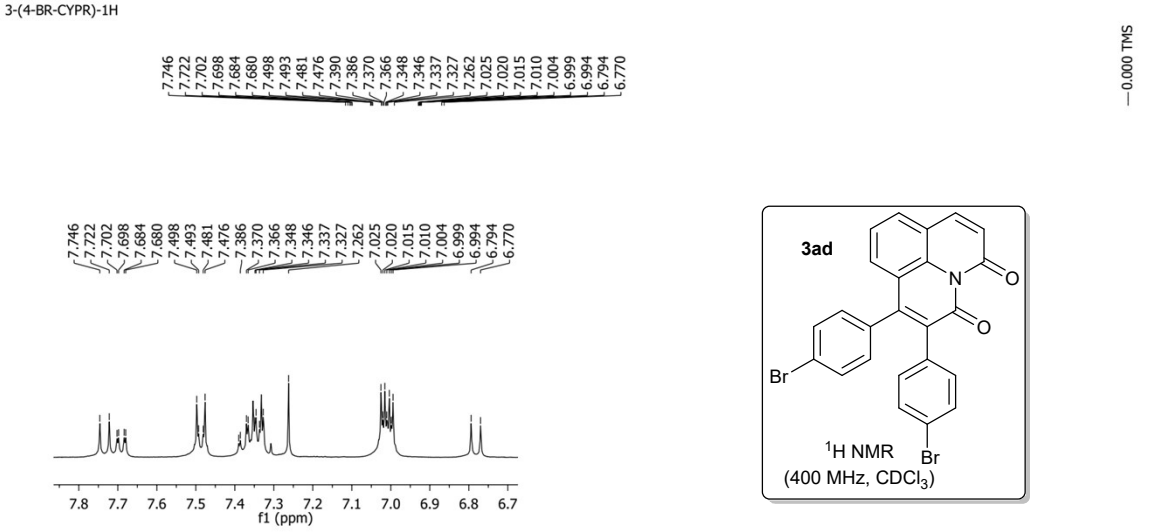
3-(3-CF3-CYPR)-13C

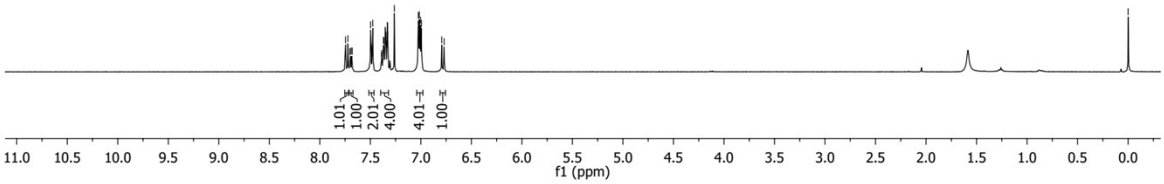


3-(3-CF3-CYPR)-19F

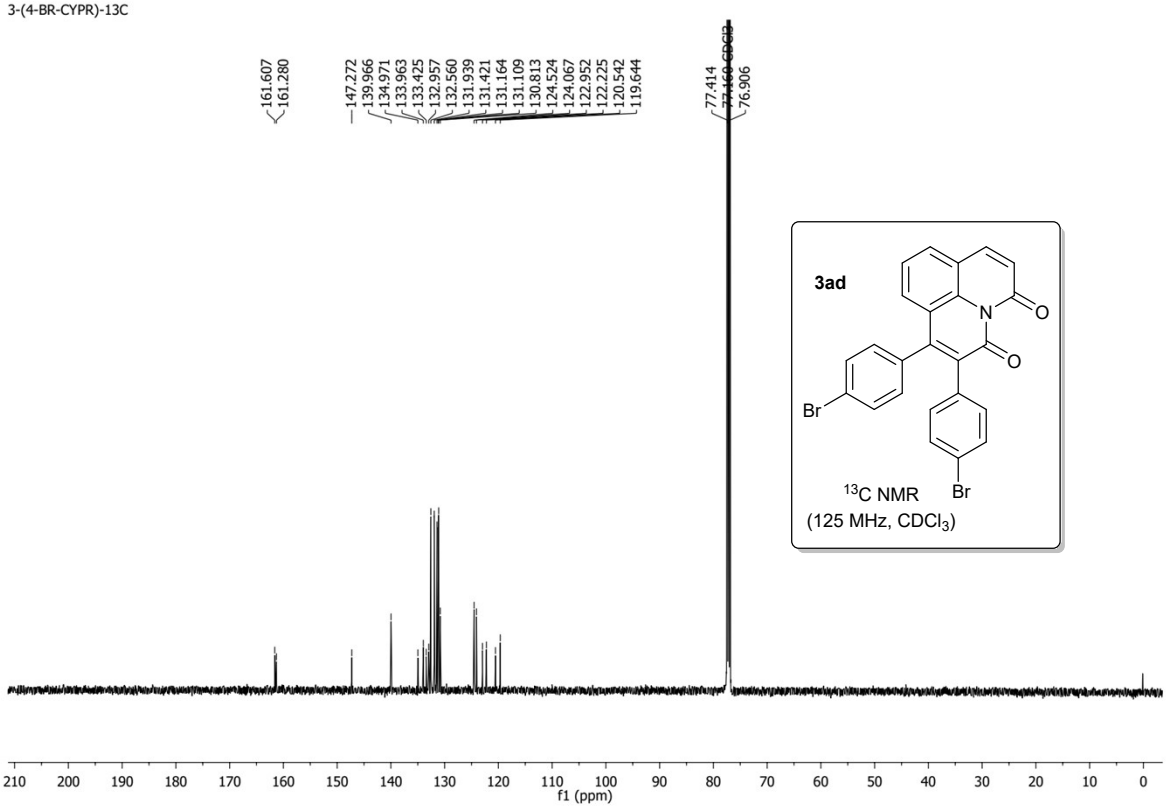


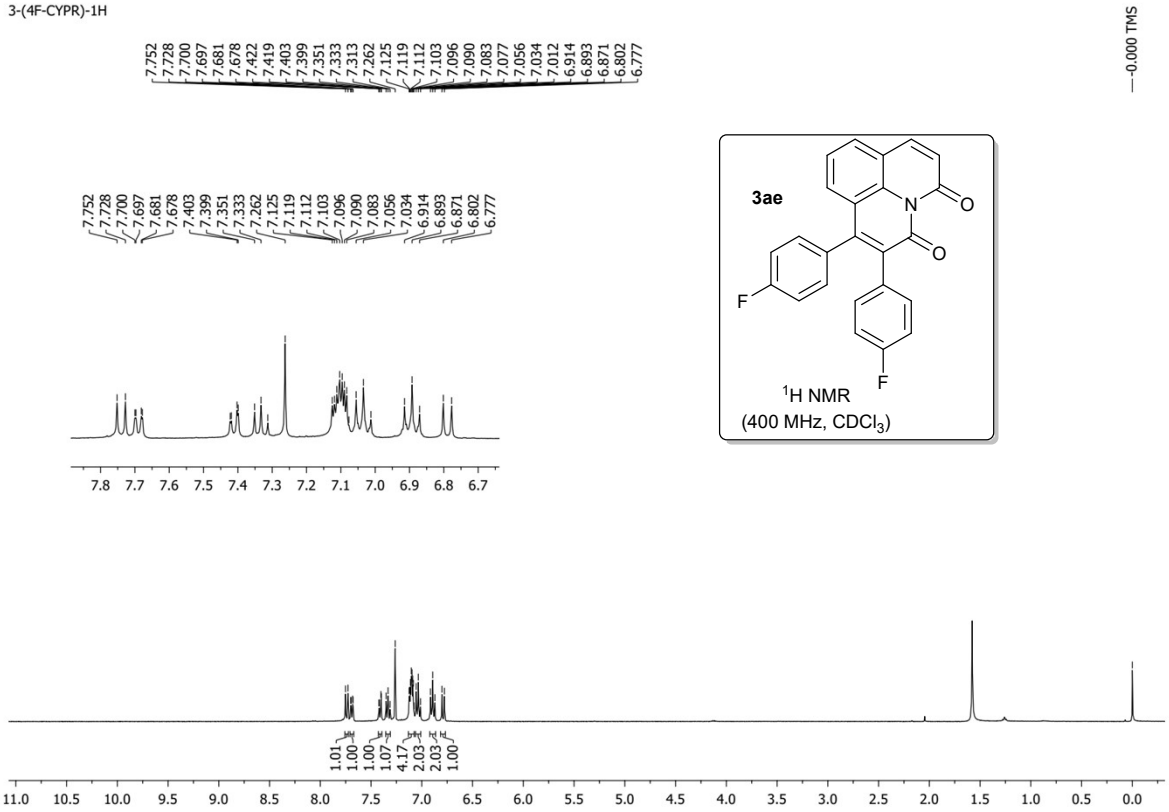
3-(4-BR-CYPR)-1H

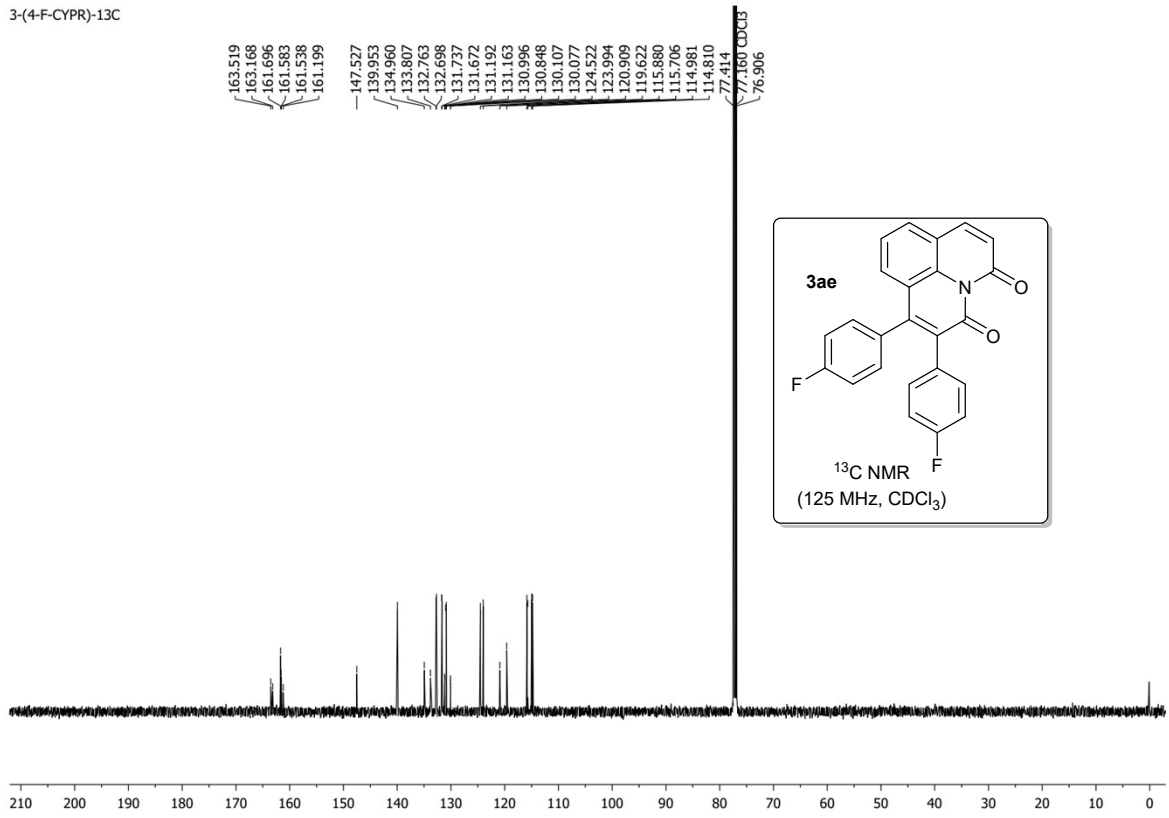




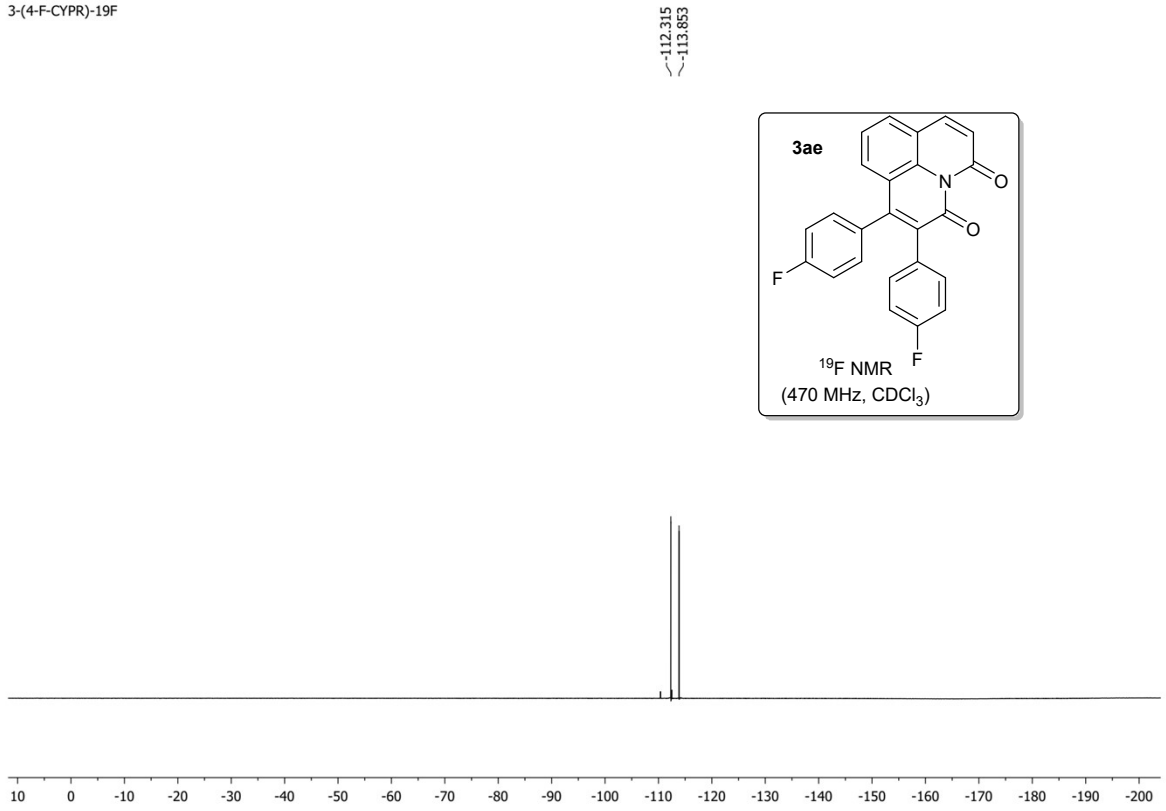
3-(4-BR-CYPR)-13C



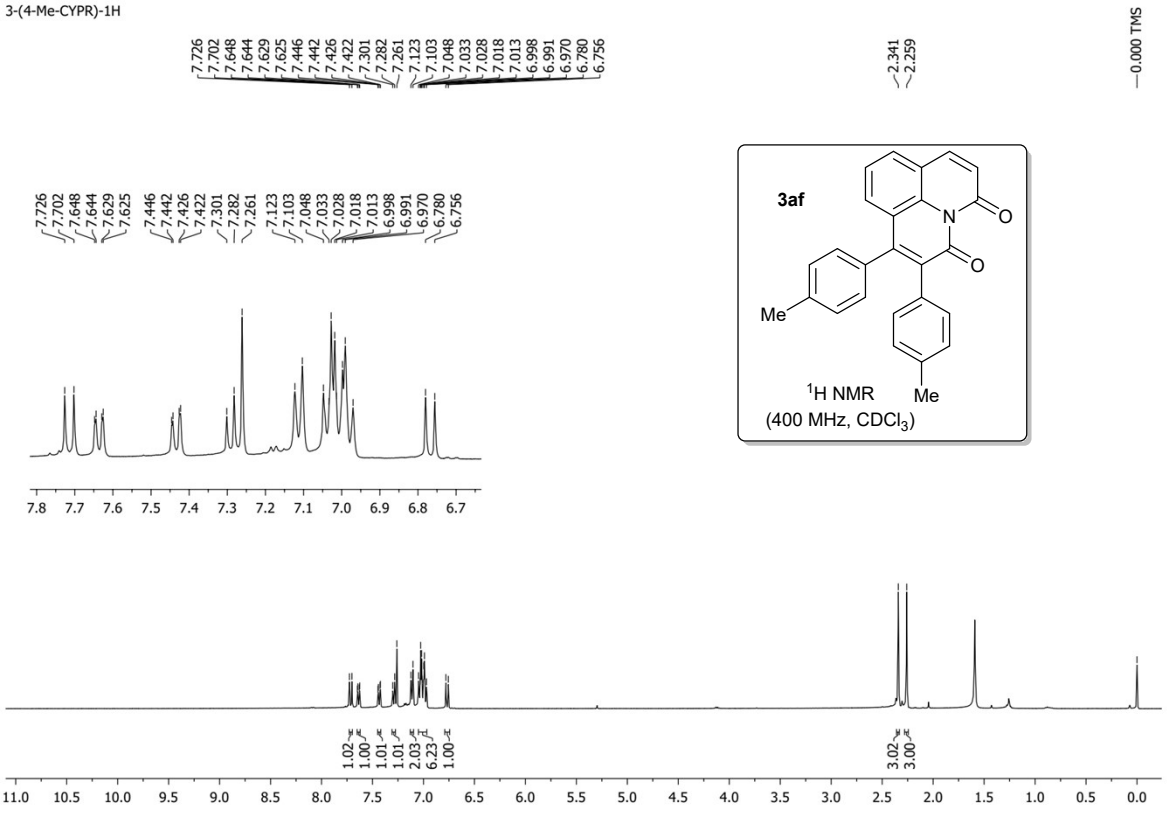

3-(4F-CYPR)-1H
7.752
7.728
7.700
7.697
7.681
7.678
7.422
7.419
7.403
7.399
7.351
7.333
7.313
7.262
7.125
7.119
7.112
7.103
7.096
7.090
7.083
7.077
7.056
7.034
7.012
6.914
6.893
6.871
6.802
6.777
0.000 TMS
3ae
N
O
O
F
F
1H NMR
(400 MHz, CDCl3)
1.01
1.00
1.00
1.07
4.17
2.03
2.03
1.00

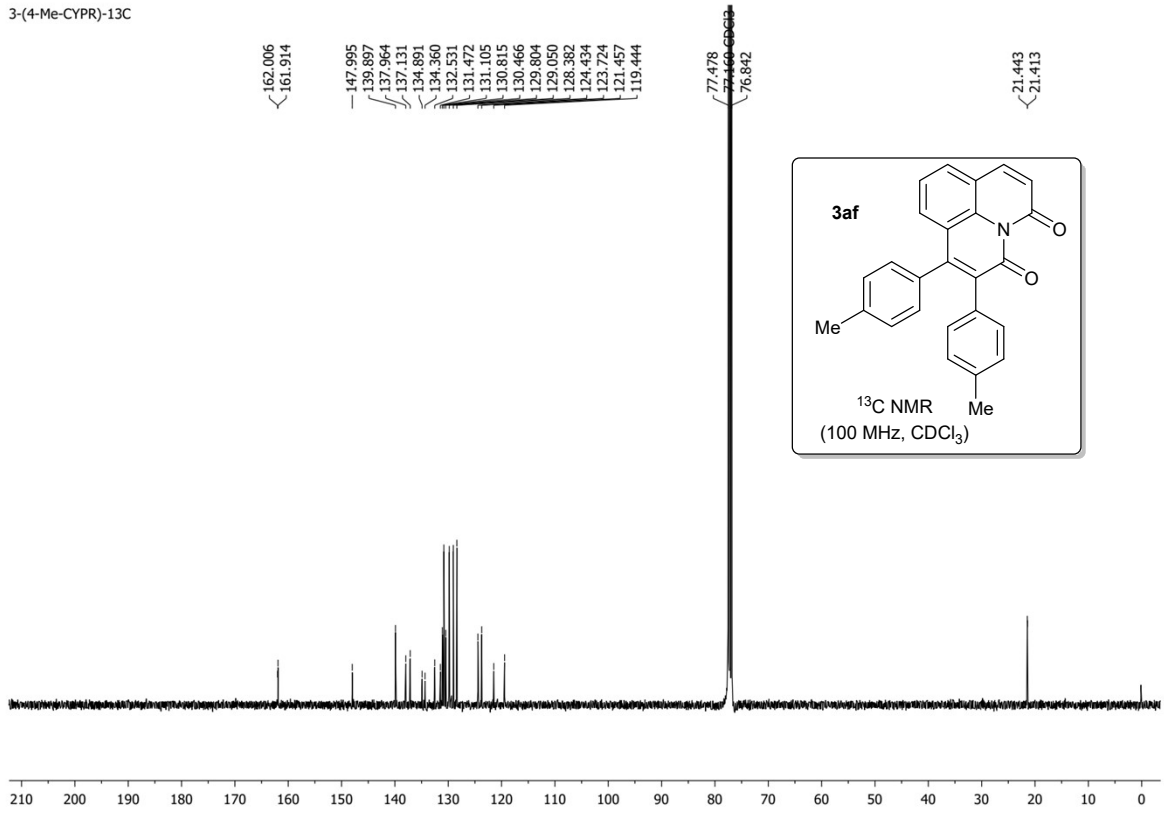

3-(4-F-CYPR)-13C
163.519
163.168
161.696
161.583
161.538
161.199
147.527
139.953
134.960
133.807
132.763
132.698
131.737
131.672
131.192
131.163
130.996
130.848
130.107
130.077
124.522
123.994
120.909
119.622
115.880
115.706
114.981
114.810
77.414
77.160 CDCl3
76.906
3ae
N
O
O
F
F
13C NMR
(125 MHz, CDCl3)

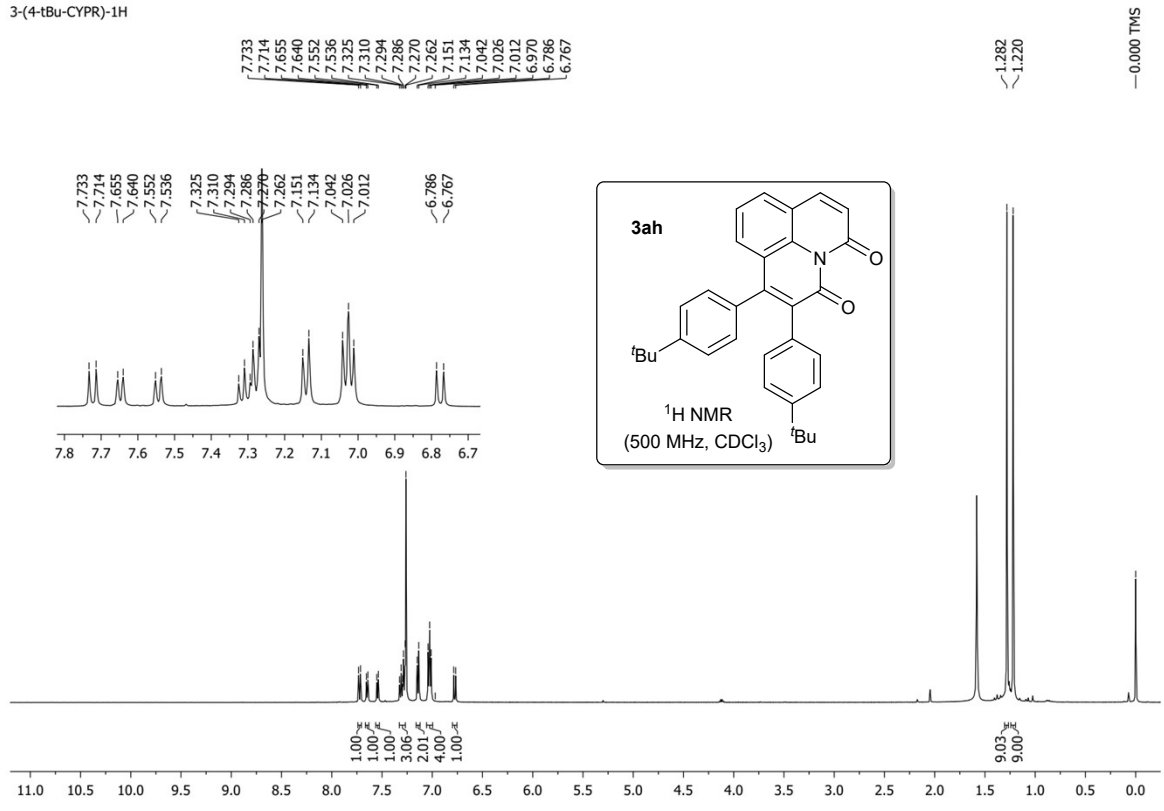
3-(4-F-CYPR)-19F

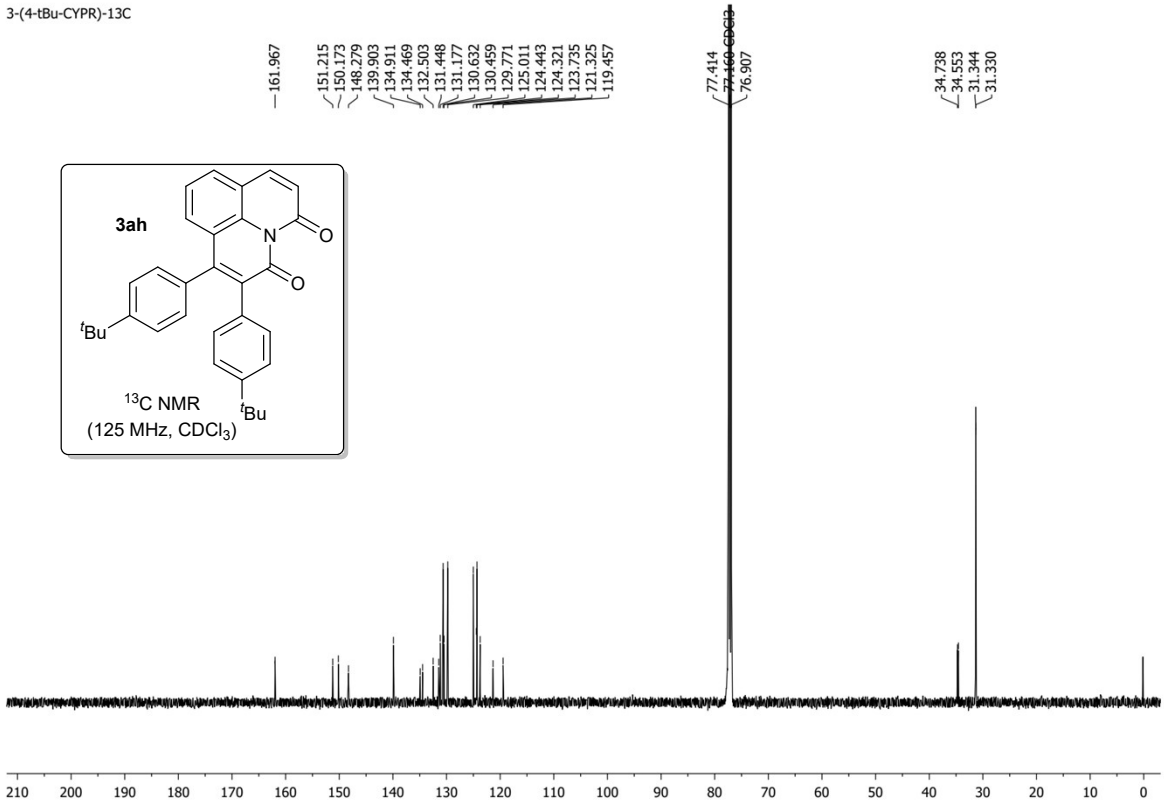


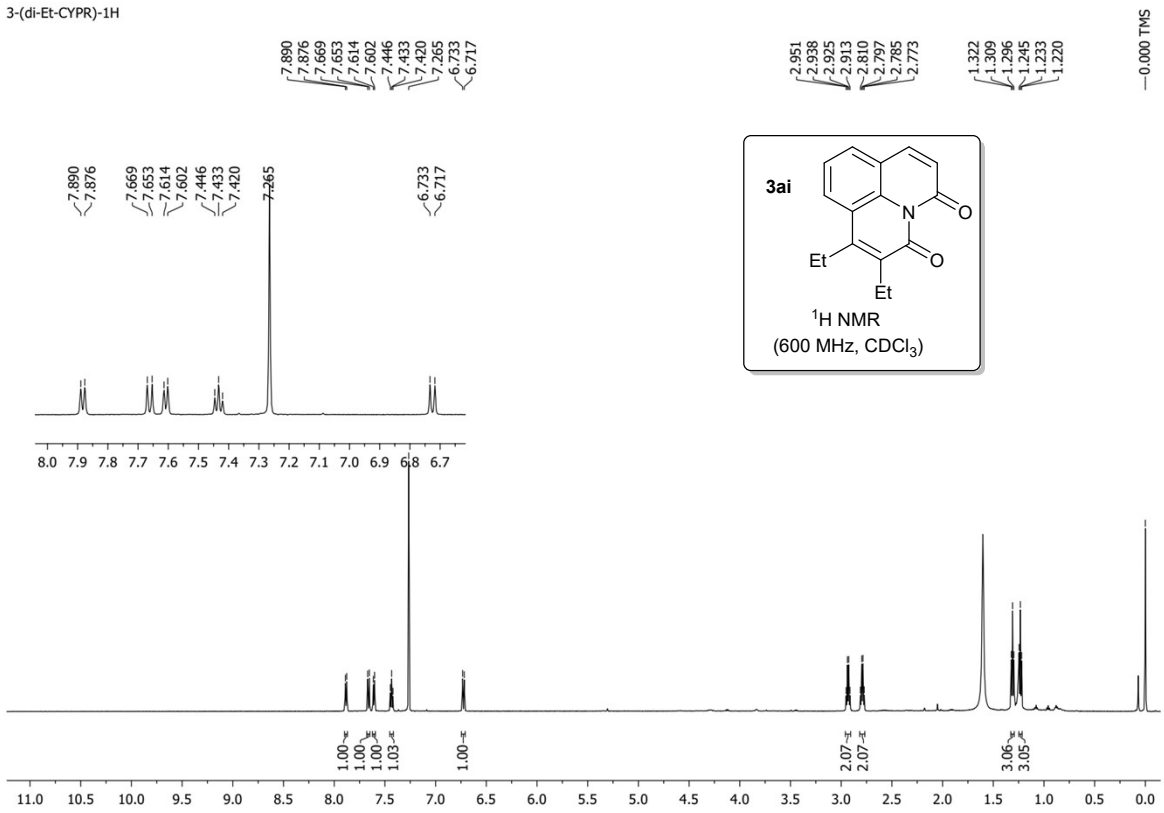
3-(4-Me-CYPR)-1H

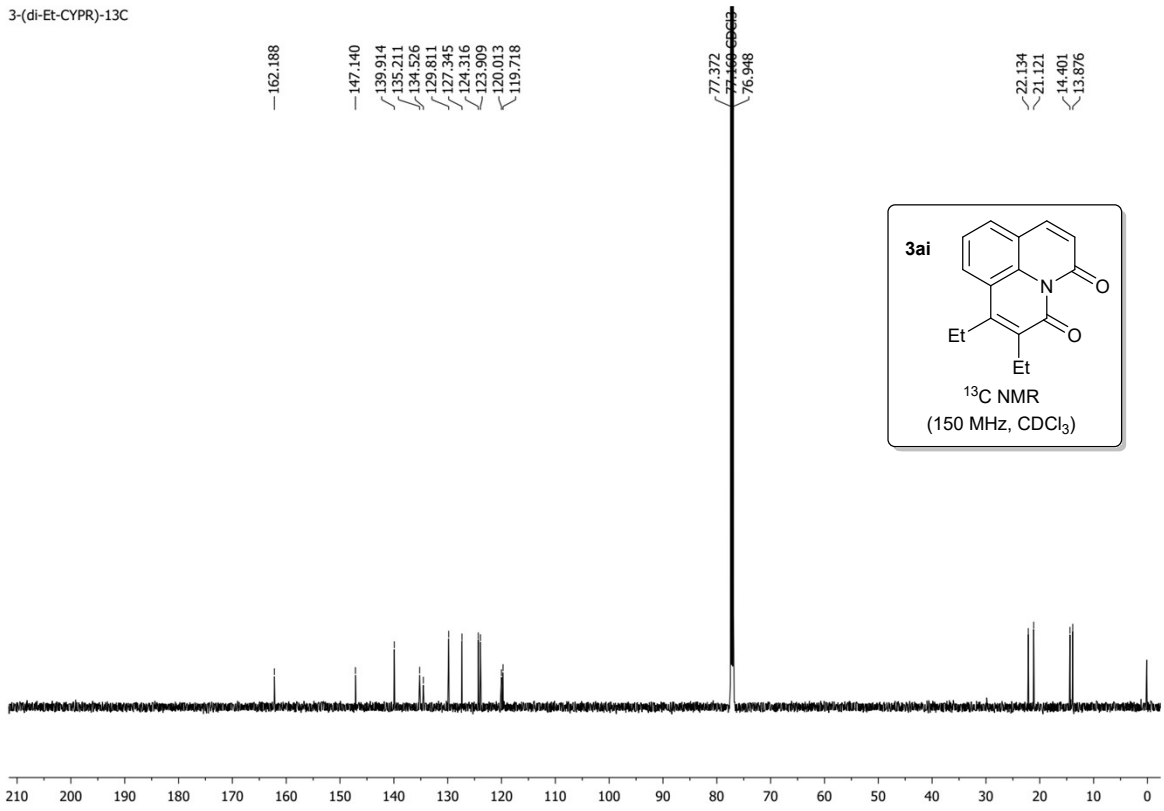


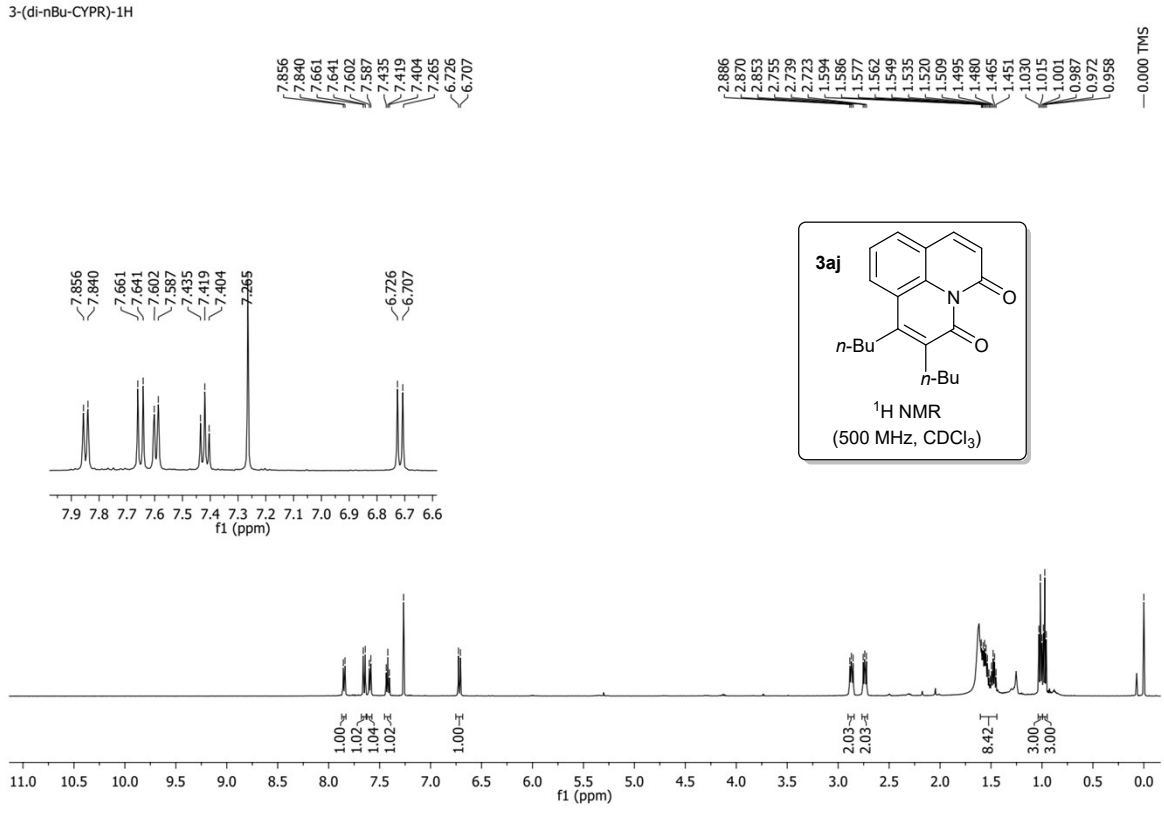

3-(4-Me-CYPR)-13C
162.006
161.914
147.995
139.897
137.964
137.131
134.891
134.360
132.531
131.472
131.105
130.815
130.466
129.804
129.050
128.382
124.434
123.724
121.457
119.444
77.478
77.160
76.842
21.443
21.413
3af
Me
Me
^{13}C NMR
(100 MHz, $CDCl_3$)

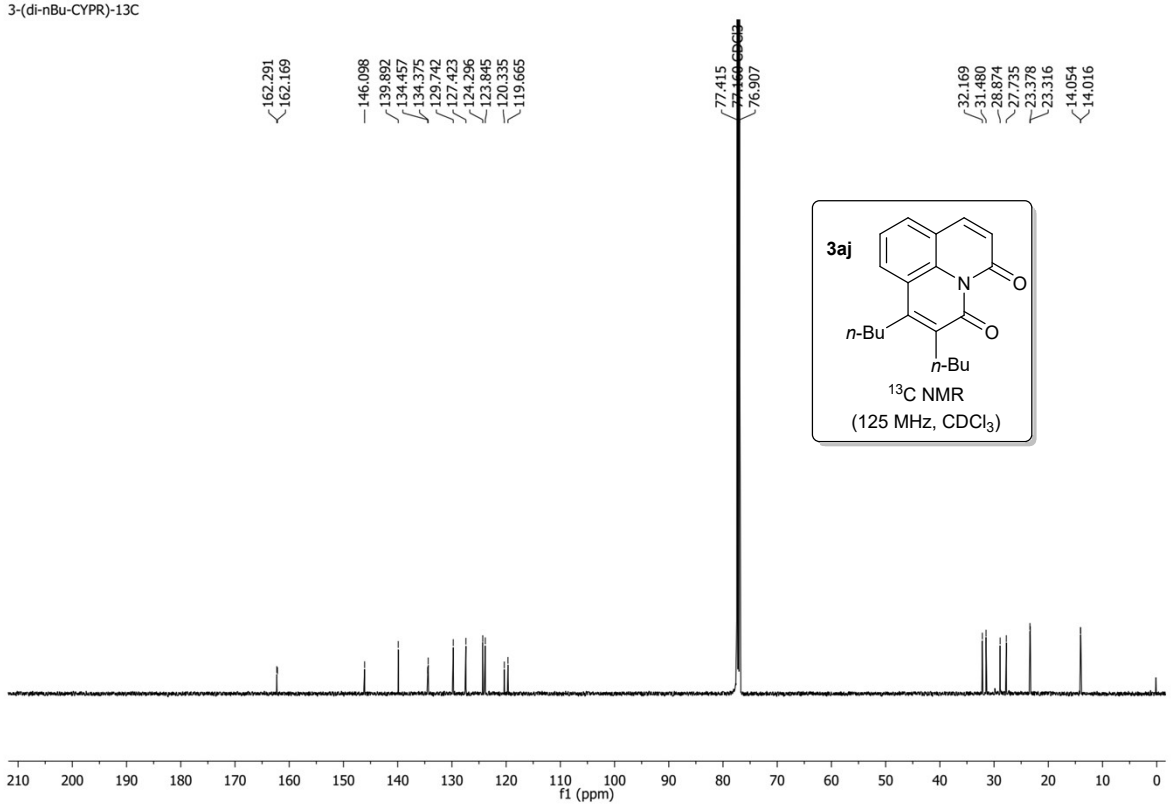

3-(4-tBu-CYPR)-1H
7.733
7.714
7.655
7.640
7.552
7.536
7.325
7.310
7.294
7.286
7.270
7.262
7.151
7.134
7.042
7.026
7.012
6.970
6.786
6.767
1.282
1.220
0.000 TMS
3ah
^{t}Bu
^{t}Bu
^{1}H NMR
(500 MHz, $CDCl_3$)
1.00
1.00
1.00
3.06
2.01
4.00
1.00
9.03
9.00

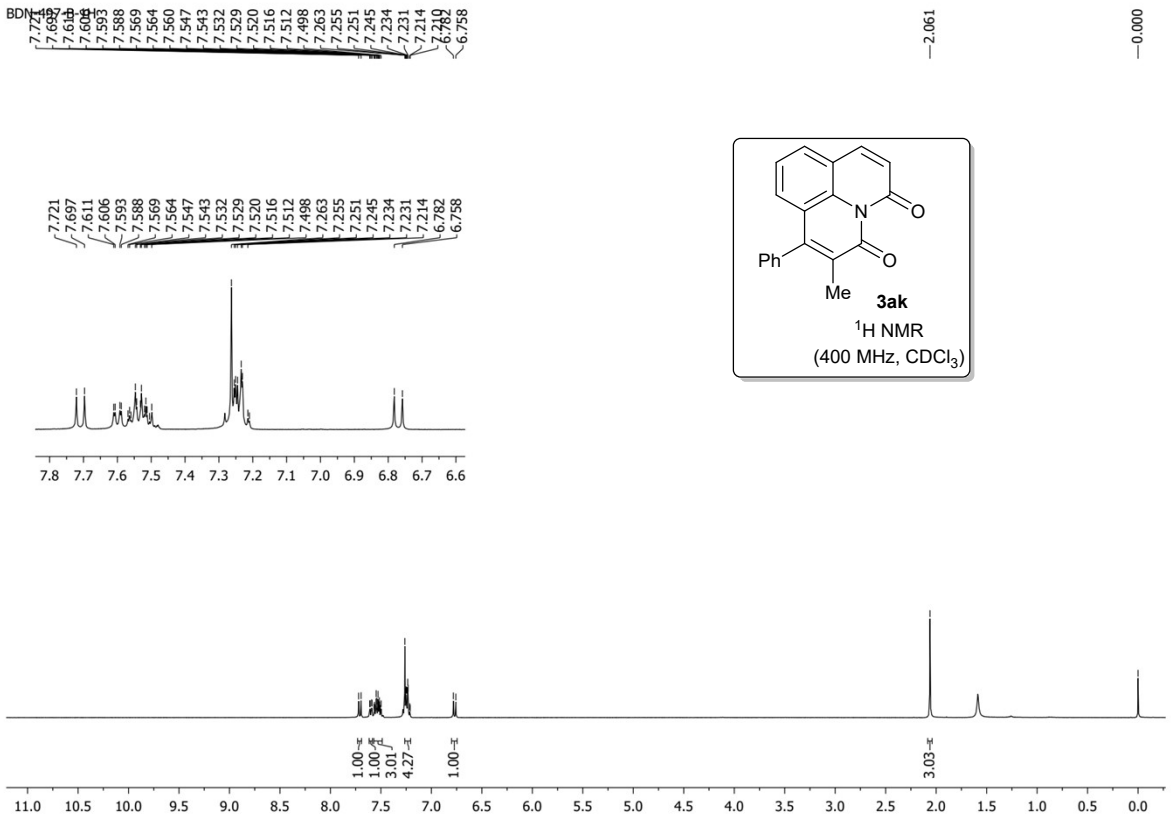

3-(4-tBu-CYPR)-13C
161.967
151.215
150.173
148.279
139.903
134.911
134.469
132.503
131.448
131.177
130.632
130.459
129.771
125.011
124.443
124.321
123.735
121.325
119.457
77.414
77.160 CDCl3
76.907
34.738
34.553
31.344
31.330
3ah
tBu
tBu
13C NMR
(125 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

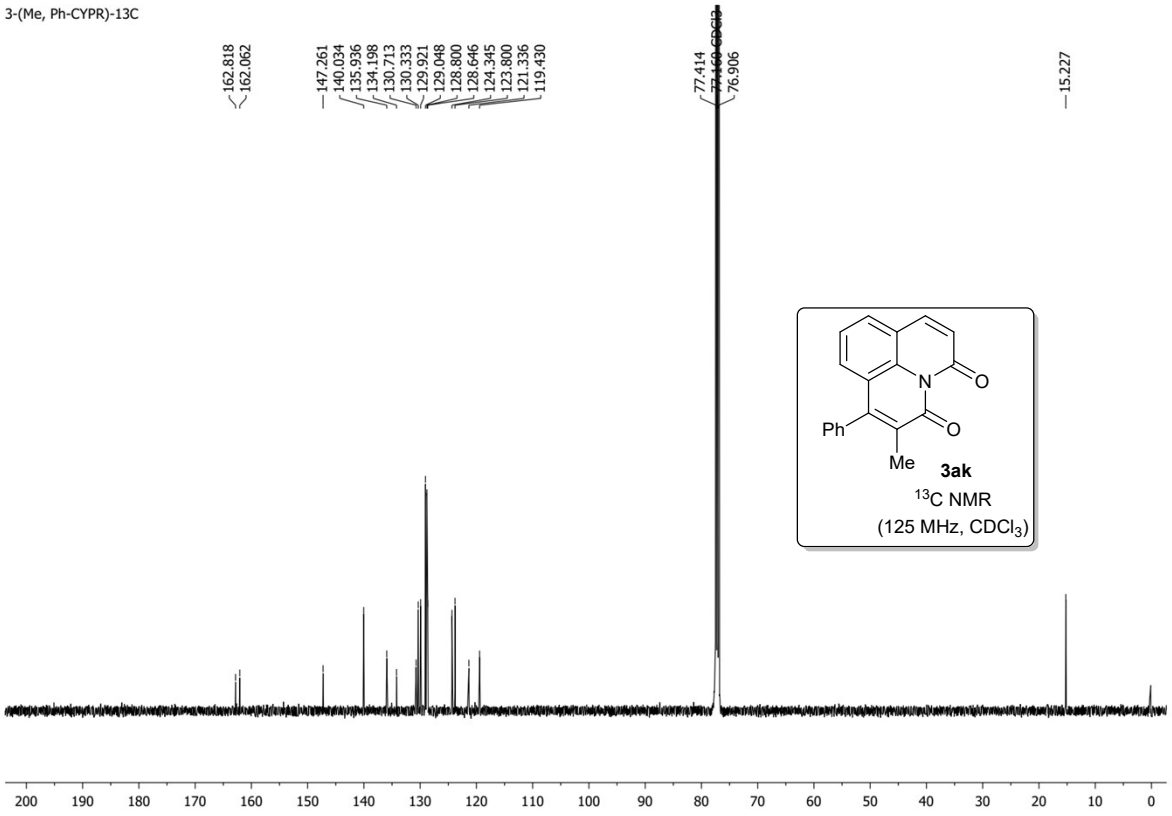

3-(di-Et-CYPR)-1H
7.890
7.876
7.669
7.653
7.614
7.602
7.446
7.433
7.420
7.265
6.733
6.717
2.951
2.938
2.925
2.913
2.810
2.797
2.785
2.773
1.322
1.309
1.296
1.245
1.233
1.220
0.000 TMS
3ai
Et
Et
1H NMR
(600 MHz, CDCl3)
8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7
1.00
1.00
1.00
1.03
1.00
2.07
2.07
3.06
3.05
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

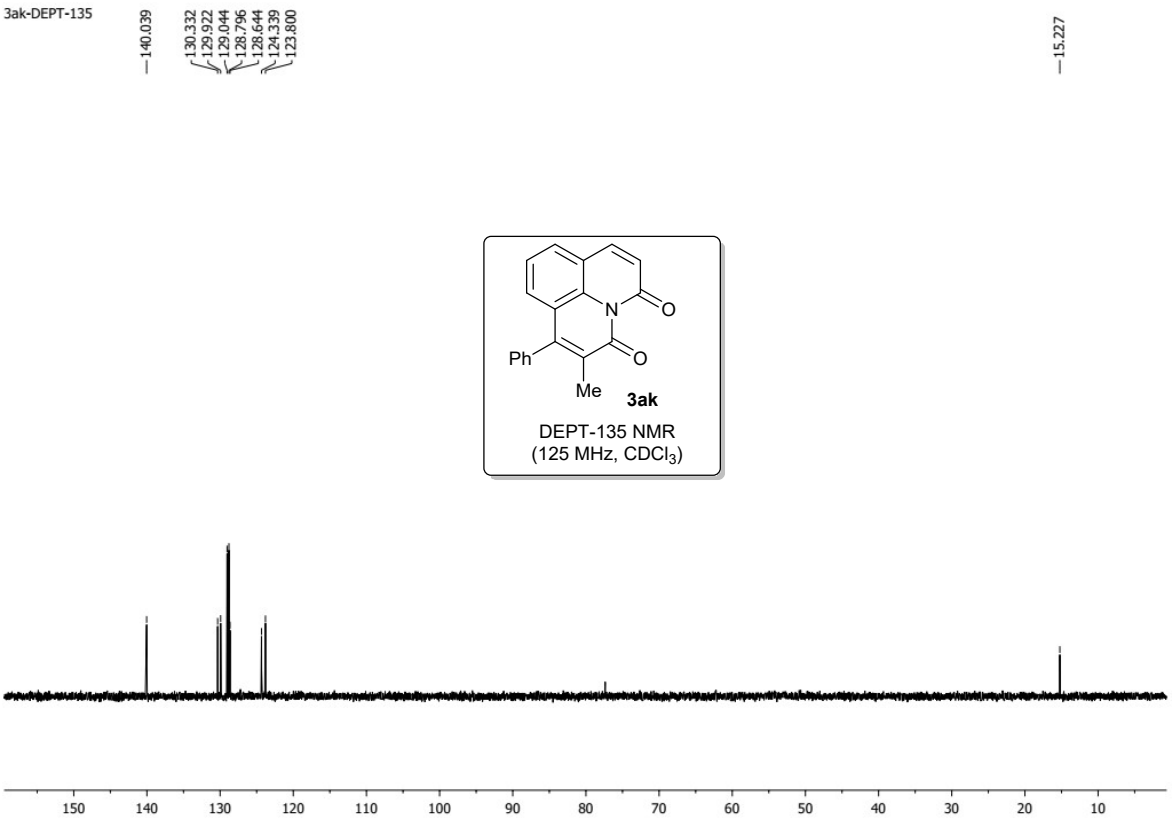

3-(di-Et-CYPR)-13C
162.188
147.140
139.914
135.211
134.526
129.811
127.345
124.316
123.909
120.013
119.718
77.372
77.160 CDCl3
76.948
22.134
21.121
14.401
13.876
3ai
Et
Et
13C NMR
(150 MHz, CDCl3)

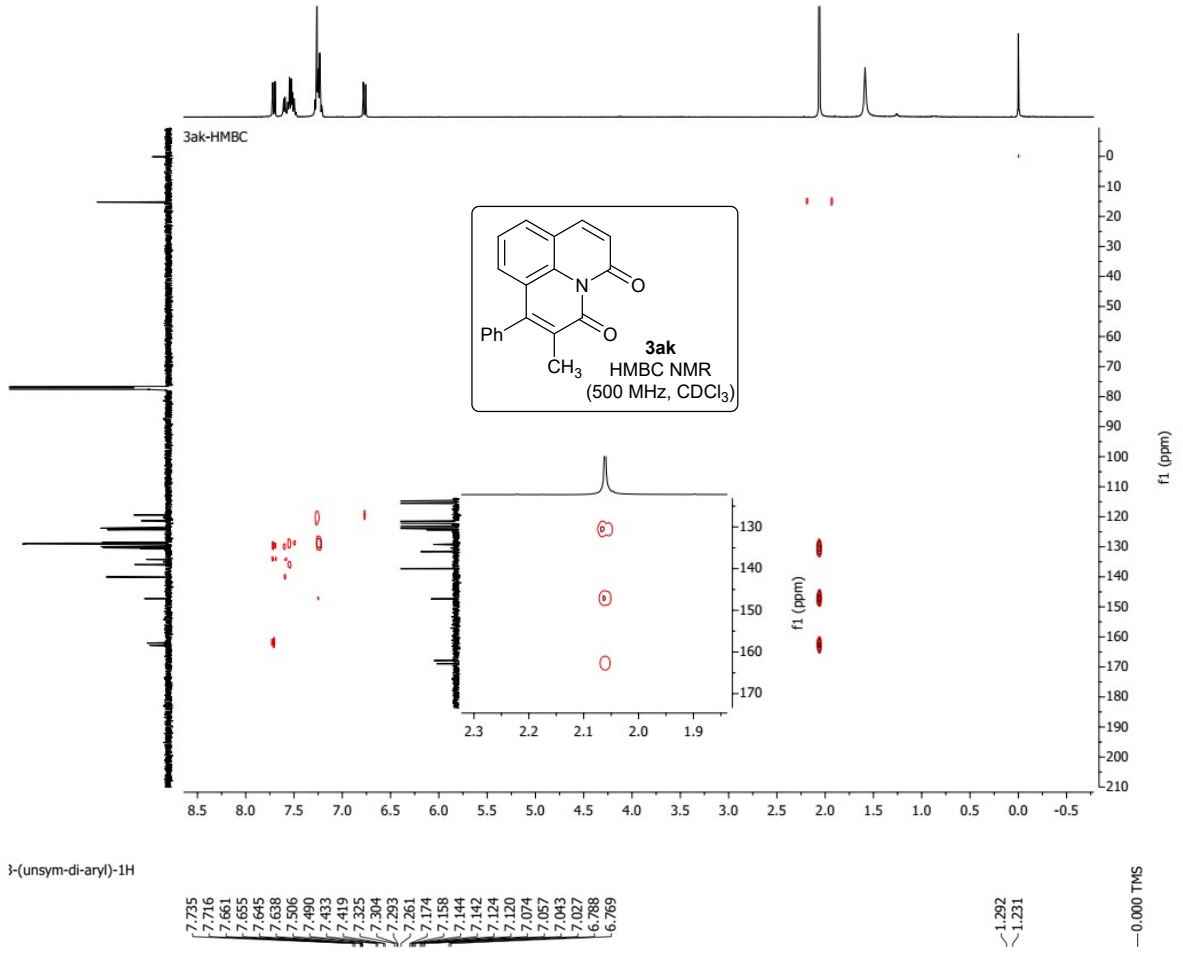

3-(di-nBu-CYPR)-1H
7.856
7.840
7.661
7.641
7.602
7.587
7.435
7.419
7.404
7.265
6.726
6.707
2.886
2.870
2.853
2.755
2.739
2.723
1.594
1.586
1.577
1.562
1.549
1.535
1.520
1.509
1.495
1.480
1.465
1.451
1.030
1.015
1.001
0.987
0.972
0.958
0.000 TMS
3aj
n-Bu
n-Bu
1H NMR
(500 MHz, CDCl3)
f1 (ppm)
1.00
1.02
1.04
1.02
1.00
2.03
2.03
8.42
3.00
3.00


3-(di-nBu-CYPR)-13C
162.291
162.169
146.098
139.892
134.457
134.375
129.742
127.423
124.296
123.845
120.335
119.665
77.415
77.160 CDCl3
76.907
32.169
31.480
28.874
27.735
23.378
23.316
14.054
14.016
3aj
n-Bu
n-Bu
13C NMR
(125 MHz, CDCl3)
f1 (ppm)

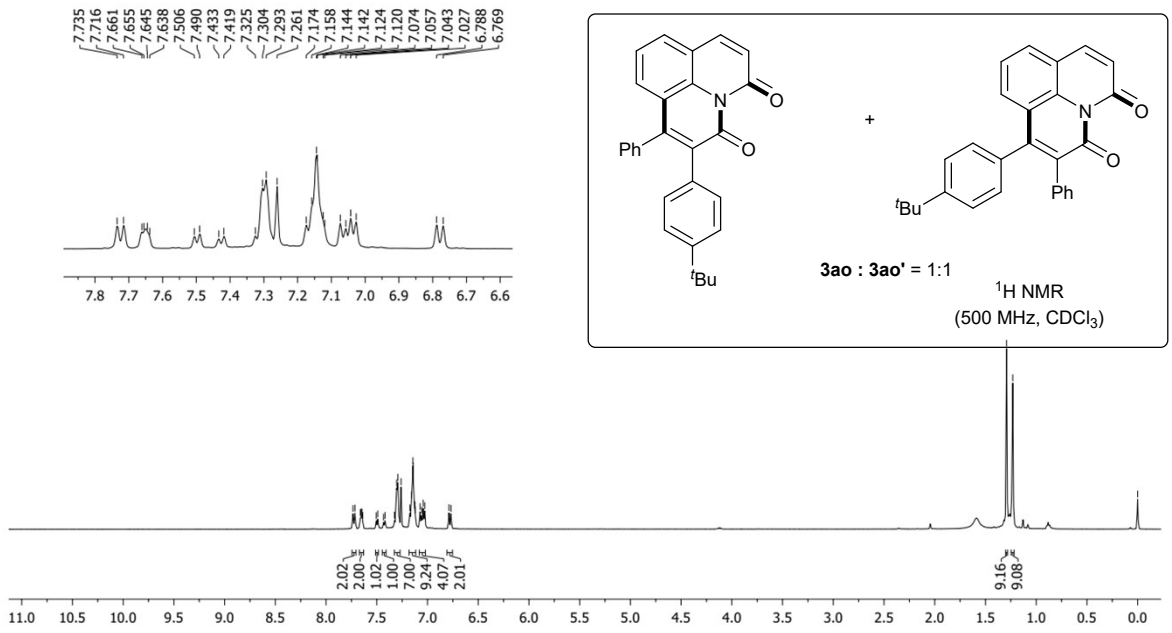

7.721
7.697
7.611
7.606
7.593
7.588
7.569
7.564
7.560
7.547
7.543
7.532
7.529
7.520
7.516
7.512
7.498
7.263
7.255
7.251
7.245
7.234
7.231
7.214
6.782
6.758
2.061
0.000
Ph
Me
3ak
1H NMR
(400 MHz, CDCl3)
1.00
1.00
3.01
4.27
1.00
3.03

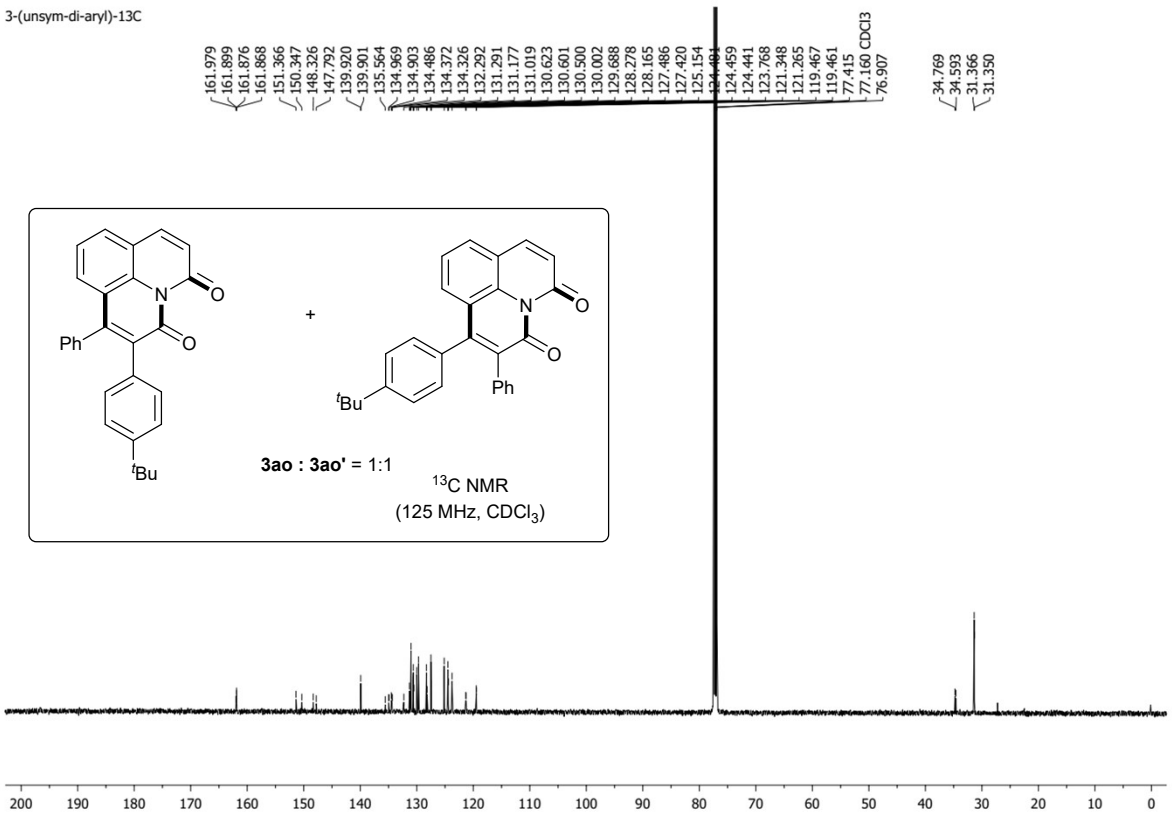

3-(Me, Ph-CYPR)-13C
162.818
162.062
147.261
140.034
135.936
134.198
130.713
130.333
129.921
129.048
128.800
128.646
124.345
123.800
121.336
119.430
77.414
76.906
15.227
Ph
Me
3ak
^{13}C NMR
(125 MHz, $CDCl_3$)

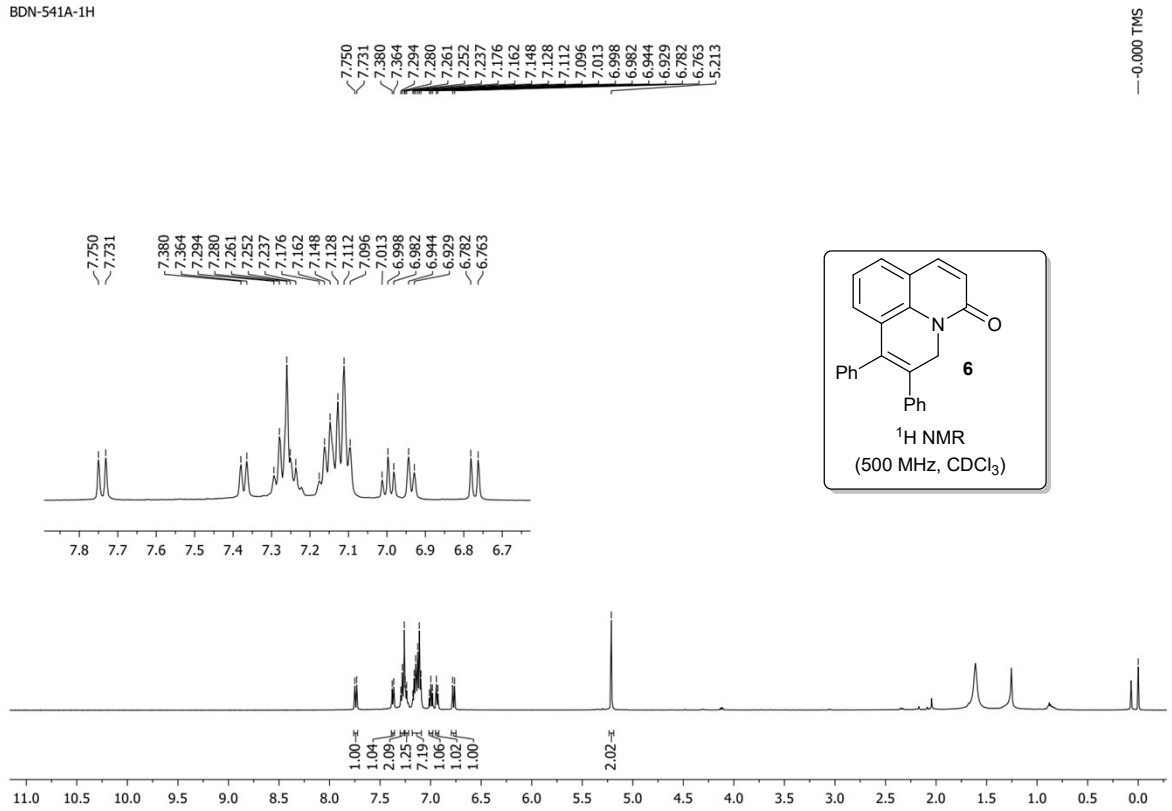

3ak-DEPT-135
140.039
130.332
129.922
129.044
128.796
128.644
124.339
123.800
15.227
Ph
Me
3ak
DEPT-135 NMR
(125 MHz, $CDCl_3$)

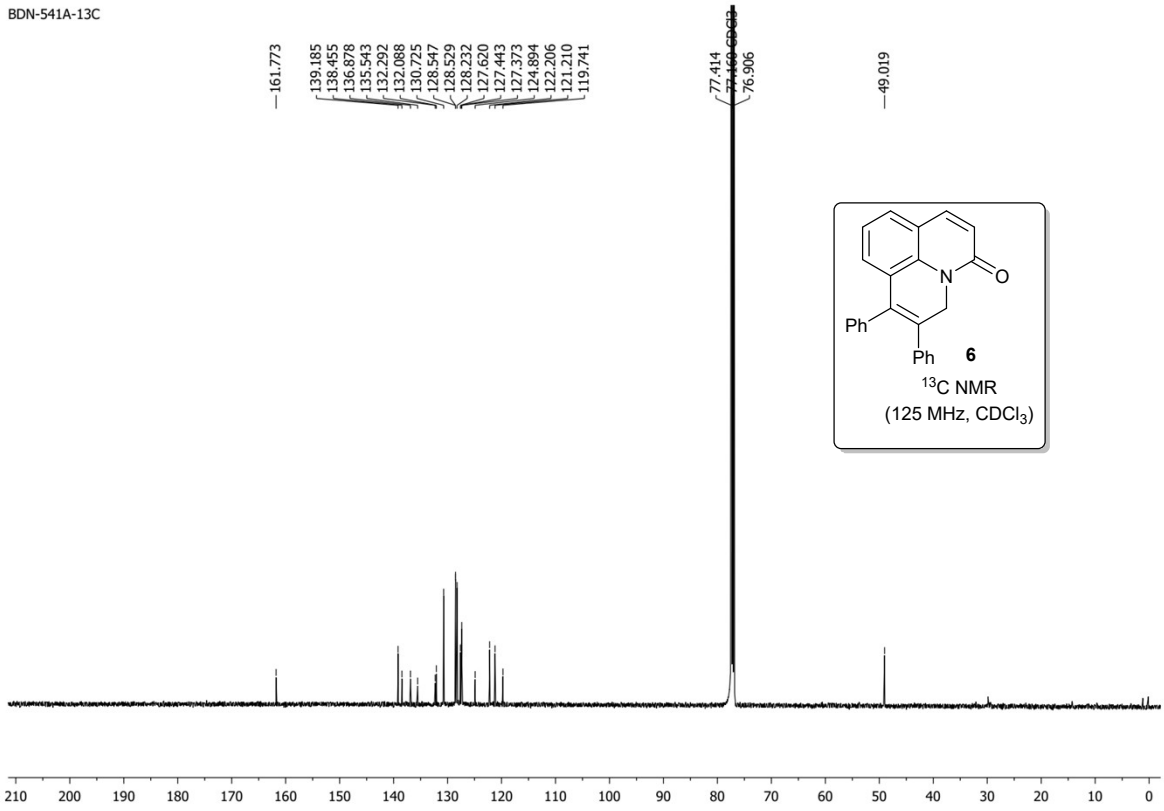

3ak-HMBC
Ph
CH3
3ak
HMBC NMR
(500 MHz, CDCl3)
f1 (ppm)
f1 (ppm)

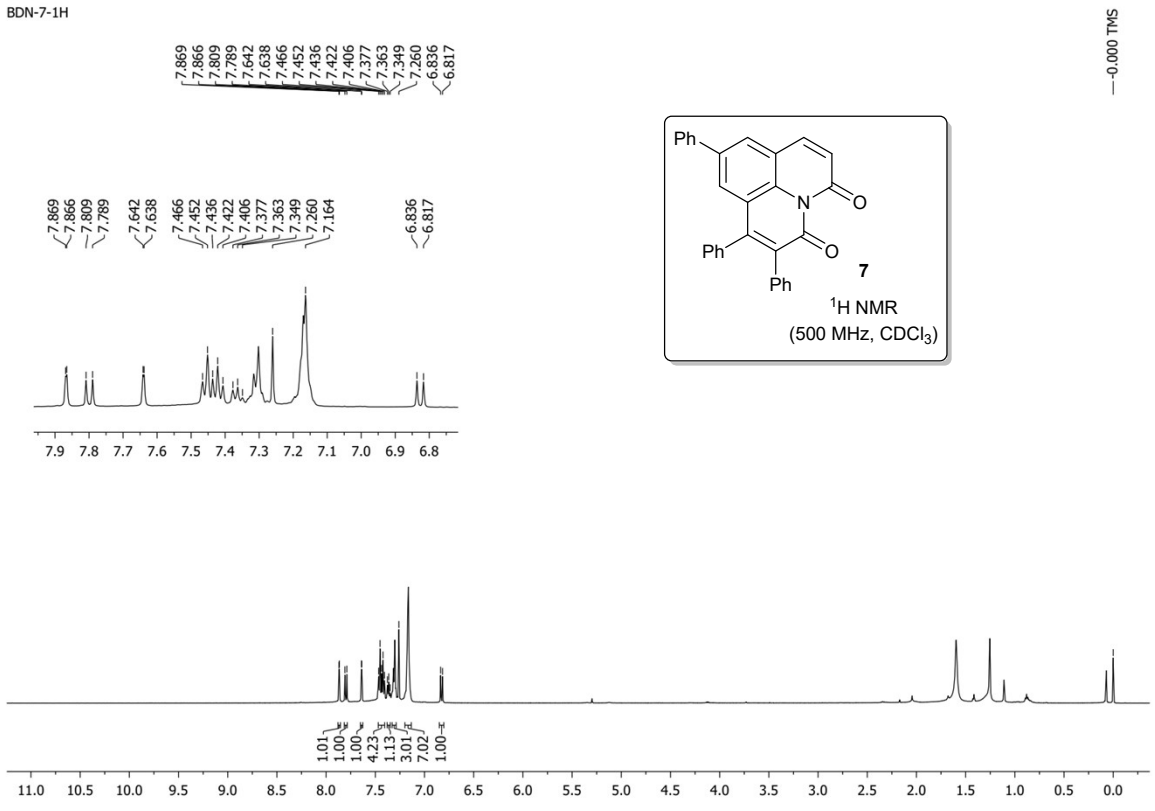
3-(unsym-di-aryl)-1H
7.735
7.716
7.661
7.655
7.645
7.638
7.506
7.490
7.433
7.419
7.325
7.304
7.293
7.261
7.174
7.158
7.144
7.142
7.124
7.120
7.074
7.057
7.043
7.027
6.788
6.769
1.292
1.231
0.000 TMS

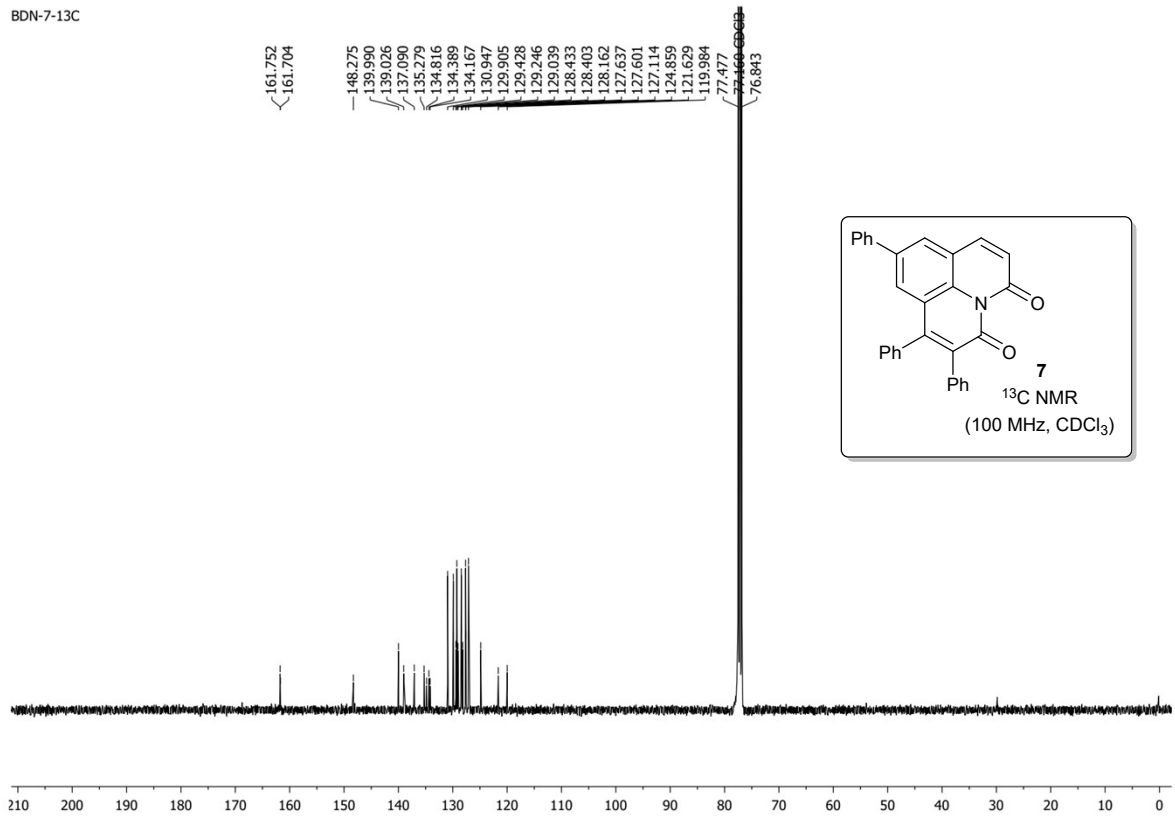

Ph
tBu
+
tBu
Ph
3ao : 3ao' = 1:1
1H NMR
(500 MHz, CDCl3)
2.02
2.00
1.02
1.00
7.00
9.24
4.07
2.01
9.16
9.08

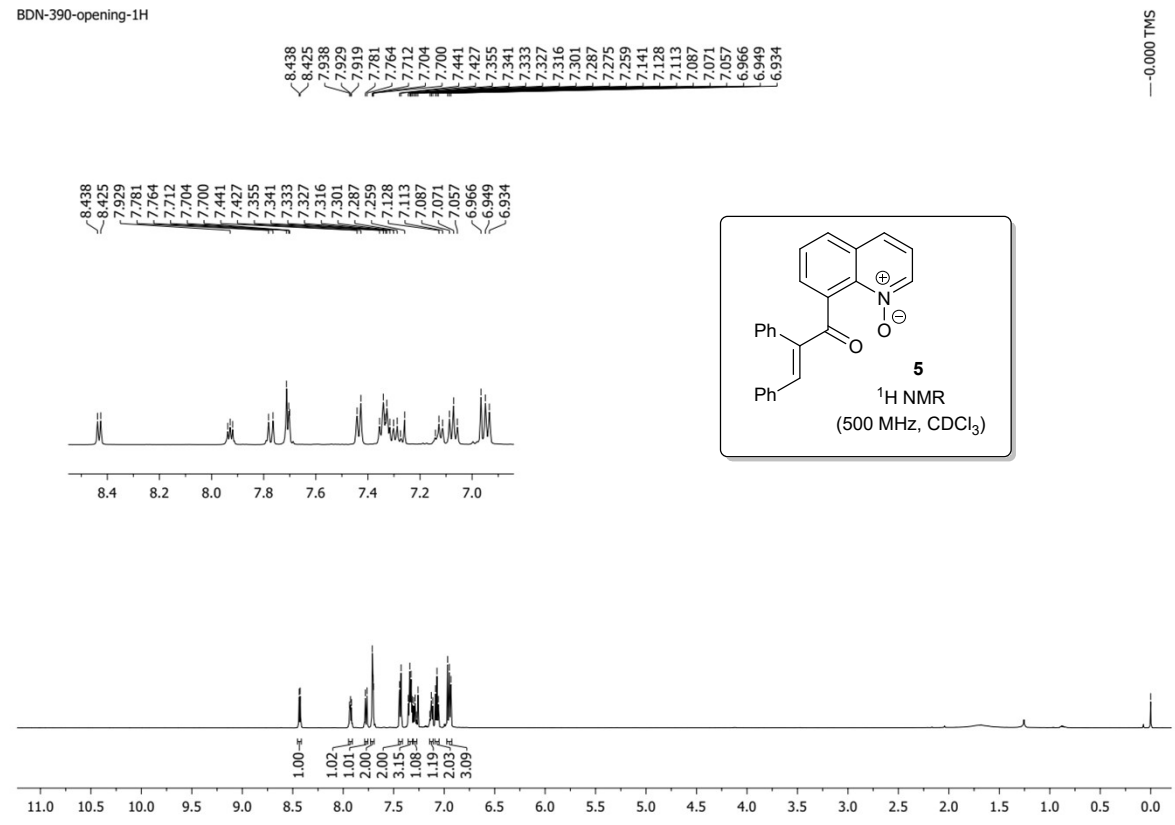

3-(unsym-di-aryl)-13C
161.979
161.899
161.876
161.868
151.366
150.347
148.326
147.792
139.920
139.901
135.564
134.969
134.903
134.486
134.372
134.326
132.292
131.291
131.177
131.019
130.623
130.601
130.500
130.002
129.688
128.278
128.165
127.486
127.420
125.154
124.481
124.459
124.441
123.768
121.348
121.265
119.467
119.461
77.415
77.160 CDCl3
76.907
34.769
34.593
31.366
31.350
Ph
tBu
tBu
Ph
3ao : 3ao' = 1:1
13C NMR
(125 MHz, CDCl3)
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

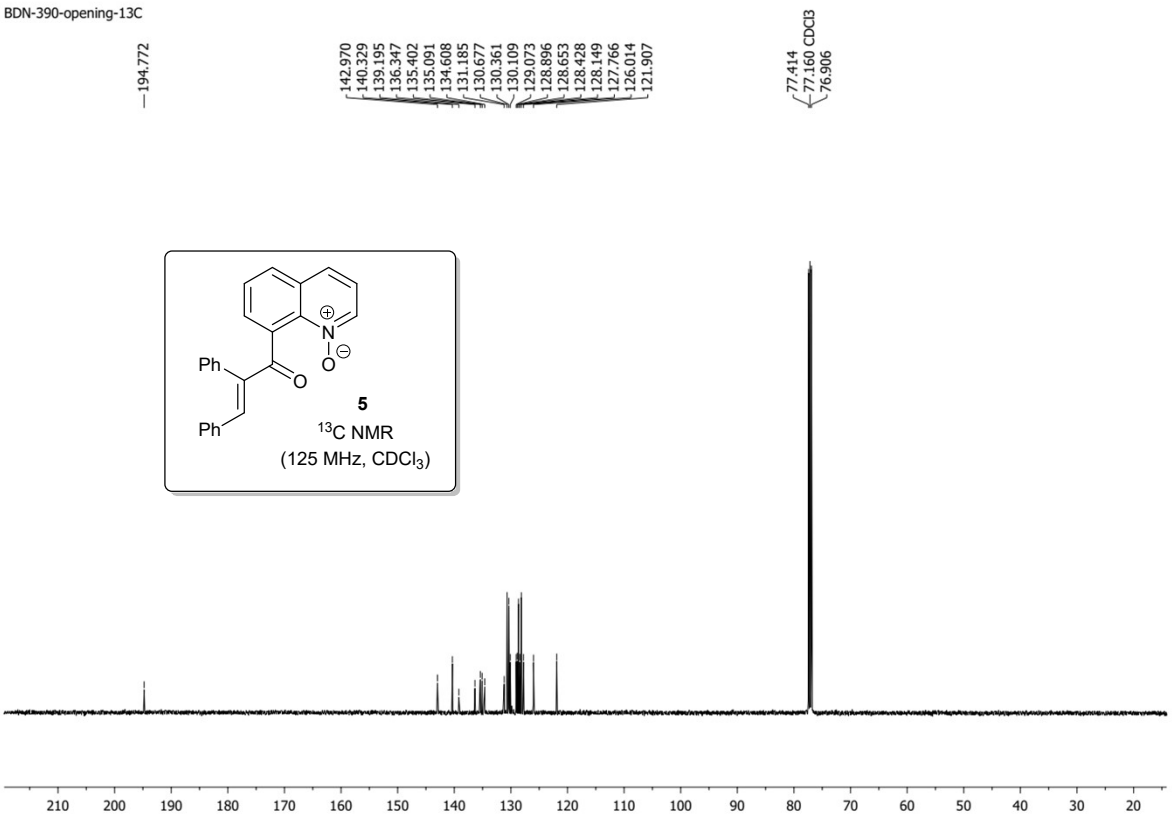

BDN-541A-1H
7.750
7.731
7.380
7.364
7.294
7.280
7.261
7.252
7.237
7.176
7.162
7.148
7.128
7.112
7.096
7.013
6.998
6.982
6.944
6.929
6.782
6.763
5.213
0.000 TMS
7.750
7.731
7.380
7.364
7.294
7.280
7.261
7.252
7.237
7.176
7.162
7.148
7.128
7.112
7.096
7.013
6.998
6.982
6.944
6.929
6.782
6.763
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
Ph
Ph
6
1H NMR
(500 MHz, CDCl3)
1.00
1.04
2.09
1.25
7.19
1.06
1.02
1.00
2.02
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0


BDN-541A-13C
161.773
139.185
138.455
136.878
135.543
132.292
132.088
130.725
128.547
128.529
128.232
127.620
127.443
127.373
124.894
122.206
121.210
119.741
77.414
77.160 CDCl3
76.906
49.019
N
O
Ph
Ph
6
13C NMR
(125 MHz, CDCl3)


BDN-7-1H
0.000 TMS
7.869
7.866
7.809
7.789
7.642
7.638
7.466
7.452
7.436
7.422
7.406
7.377
7.363
7.349
7.260
6.836
6.817
7.164
Ph
Ph
Ph
N
O
O
7
1H NMR
(500 MHz, CDCl3)
1.01
1.00
1.00
4.23
1.13
3.01
7.02
1.00


BDN-7-13C
161.752
161.704
148.275
139.990
139.026
137.090
135.279
134.816
134.389
134.167
130.947
129.905
129.428
129.246
129.039
128.433
128.403
128.162
127.637
127.601
127.114
124.859
121.629
119.984
77.477
76.843
Ph
N
O
Ph
O
Ph
7
13C NMR
(100 MHz, CDCl3)


BDN-390-opening-1H
8.438
8.425
7.938
7.929
7.919
7.781
7.764
7.712
7.704
7.700
7.441
7.427
7.355
7.341
7.333
7.327
7.316
7.301
7.287
7.275
7.259
7.141
7.128
7.113
7.087
7.071
7.057
6.966
6.949
6.934
0.000 TMS
Ph
N
O
O
Ph
5
1H NMR
(500 MHz, CDCl3)
1.00
1.02
1.01
2.00
2.00
3.15
1.08
1.19
2.03
3.09


BDN-390-opening-13C
194.772
142.970
140.329
139.195
136.347
135.402
135.091
134.608
131.185
130.677
130.361
130.109
129.073
128.896
128.653
128.428
128.149
127.766
126.014
121.907
77.414
77.160 CDCl3
76.906
Ph
Ph
O
N
O
5
13C NMR
(125 MHz, CDCl3)
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20