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Electronic Supporting Information

Electrochemical C(sp^3)-C(sp^3) Cross Dehydrogenative Coupling: Enabling Access to 9-Substituted Fluorescent Acridanes

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Table of contents

General Information……... S2

Preparation of starting materials……..... S3 – S5
Representative Bioactive Acridines, 3-coumaranone and 3-isochromanone…… S5
Additional optimizations of reaction condition, Table S1 and Table S2……... S6 – S7
Experimental procedure for electrolysis…….……...…….. S8
Large scale synthetic reaction…..……..……...…… S9
Product transformation……. S9
Unsuccessful Results……...…… S10
Characterization of products……..……..... S11 – S25
Mechanistic study: Radical scavenging and control potential experiments……. S26
Cyclic voltammetry experiments…….. S27
Kinetic isotope effect experiments…… S27 – S28
Fate of 9,10-dihydroacridine and *N*-protected 9,10-dihydroacridine in standard electrochemical conditions …… S28
Comparison with non-electrochemical methods…….. S29
Fluorescence decay curves……. S30
Photophysical Study: Absorption and Fluorescence spectroscopic studies…….. S30 – S35
Theoretical calculations……. S35 – S86
References…… S87
^{1}H and ^{13}C NMR spectra of compounds……... S88 –S134

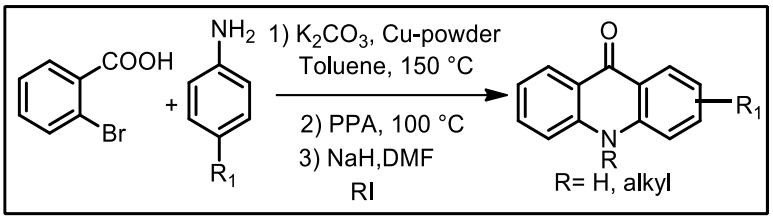
General Information:

All reactions were carried out in oven-dried reaction vessels under a nitrogen atmosphere unless otherwise mentioned. TLC analysis was performed on silica gel TLC plates. Column chromatography was done using 230−400 mesh silica gel by applying pressure through an air pump. ^{1}H and ^{13}C NMR spectra were recorded on 400 and 600 MHz spectrometers and are reported as chemical shifts (δ) in parts per million (ppm), and multiplicities are abbreviated as s = singlet, d = doublet, t = triplet, q = quartet, qu = quintet, m = multiplet, app = apparent, comp = complex. Internal standards or residual solvent signals were used as reference. HRMS (m/z) was recorded using ESI (Q-Tof, positive ion) and EI (magnetic sector, positive ion) mode. Melting points were determined in a capillary melting point apparatus and are uncorrected. Single-crystal X-ray diffraction data were collectedon either Bruker APEX II diffractometer with a graphite monochromator using Mo Kα radiation or Bruker D8 Venture with a microfocus optics using CuKα radiation. The CIF fileswere submitted to CCDC (**2238292-2238293**) and can be obtained at https://summary.ccdc.cam.ac.uk/structure-summary-form.The electrochemical reactions were studied on the ElectraSyn 2.0 pro. Graphite, Platinum and other electrodes were supplied by IKA. All cyclic voltametric experiments were carried out in K-Lyte 1.2 potentiostat. The fluorescence studies were performed using PTI QM-400 Fluorimeter. Absorption spectra were measured on a Cary 60 UV-Vis Spectrophotometer. Relative quantum yields were determined by using literature method taking quinine sulfate solution in 0.5 M H_2SO_4 as the standard. Luminescence lifetime measurements were carried out by using time–correlated single photon counting set up from Horiba Jobin-Yvon. The luminescence decay data were collected on a Hamamatsu MCP photomultiplier (R3809) and were analyzed by using IBH DAS6 software. Single crystals of **3aa** and **3bb** were obtained taking 10 mg of the sample in 5 mL round bottom flasks using EtOH/$CHCl_3$ mixture applying solvent evaporation method.

Preparation of starting materials:

Preparation of *N*-alkyl acridones:

These compounds were synthesized according to the known literature procedure with slight modifications. [1], [2]

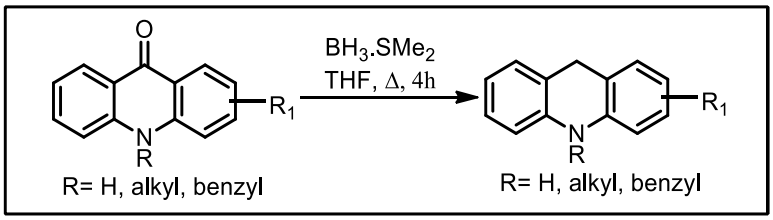


A round-bottomed flask equipped with a magnetic stirrer and reflux condenser was charged with 2-bromobenzoic acid derivatives (5 mmol), potassium carbonate (5.75 mmol), copper (0.9 mmol) and aniline derivatives (7 mmol) in anhydrous toluene. The mixture was heated to reflux (160 °C oil bath) and stirred for further 3 hours. The solvent was evaporated under reduced pressure, and the residue was dissolved in hot water (90 mL) and filtered through Celite. The Celite was washed with water (30 mL), and the filtrate was acidified with concentrated HCl to pH 6. A solid precipitated, which was isolated by filtration and washed with water. The solid was crystallized from $CHCl_3$ to give 2-(phenylamino)benzoic acid derivatives.

A mixture of 2-(phenylamino)benzoic acid derivatives (4.7 mmol) and polyphosphoric acid (3.9 mL) was heated to 110 °C for 3 h. The solution was poured onto ice (120 mL), and the precipitate was filtered and washed with water. The precipitate was dissolved in hot EtOH, filtered, and evaporated to afford acridone derivatives.

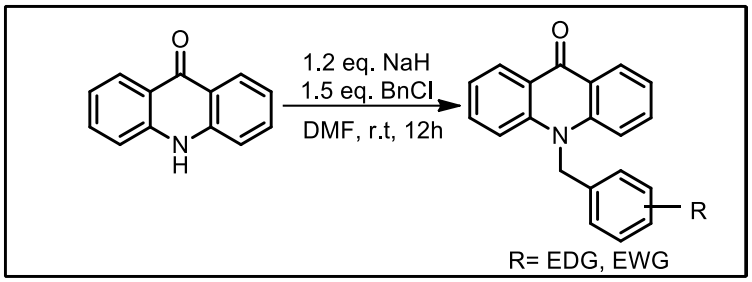
Acridone derivatives (5 mmol) was dissolved in dimethylformamide (8 mL) and cooled to 0 °C. Sodium hydride (12.5 mmol, 2.5 equiv.) was then added in portions while stirring. This was then heated to 60 °C and stirred for 30 mins at which point alkyl iodide (2.5 equiv.) was added and stirred at 60 °C for 18 h. Upon completion, the reaction was cooled to ambient temperature and quenched with water. The solid was filtered via suction filtration and dissolved in chloroform then washed with a brine solution. The organic fractions were combined and dried over MgSO4 with the volatiles being removed in vacuo to give the crude product.

9,10-Dihydroacridines:



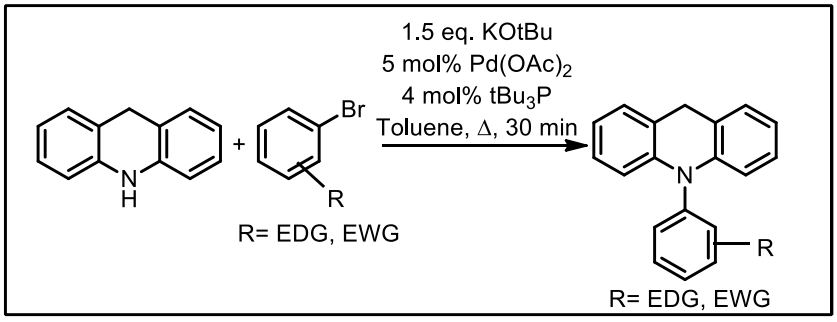
To a slurry of acridone (5.0 mmol) in THF (20 mL) was $BH_3.SMe_2$ solution (1 mL,10.0 mmol) added dropwise and the mixture was refluxed for 4 hours under Ar-atmosphere. On completion (checked by TLC) the mixture was cooled to 0-5 °C and brine (100 mL) was cautiously added followed by 2M aq. NaOH (5 mL). The organic layer was separated, and the aqueous layer was extracted with Et_2O (1 × 20 mL). The collected organic layers were washed with conc. aq. $NaHCO_3$ (1 × 10 mL), dried over $NaSO_4$ and evaporated. The crude product was subjected to column chromatography on silica with DCM to afford crude products.

N-Benzylacridone derivatives:



A two-necked round bottom flusk equipped with a magnetic stirrer was evacuated and refilled with argon, then charged with NaH (60% in mineral oil; 6.0 mmol) and DMF (8 mL). The slurry was cooled to 0-5 °C and acridone derivatives (5 mmol) were added portion-wise. After an additional 1h at room temperature, benzyl chloride (8 mmol) in DMF (5 mL) was added dropwise and the mixture was stirred overnight. Then H_2O (25 mL) was added and the product was extracted with EtOAc (3 × 25 mL). The collected organic phases were dried over NaSO4, filtered, and evaporated to give the crude product. Column chromatography on silica with DCM-EtOAc (95:5) gave N-benzylacridine-9(10H)-one derivatives.

***N*-Phenylacridane derivatives:**



These compounds were synthesized according to the known literature procedure.[1] A Schlenk-tube equipped with a magnetic stirrer and a reflux condenser was evacuated and refilled with argon. Then 9,10-dihydroacridine (1.812 g, 10.0 mmol), bromobenzene (1.16 mL, 11.0 mmol), Pd(OAc)2 (0.112 g, 0.5 mmol), tris(tert-butyl)phosphine (0.081 g, 0.4 mmol) and toluene (12 mL) were added followed by potassium tert-butoxide (1.683 g, 15.0 mmol). The reaction mixture was stirred under reflux (130°Coil bath) for 30 minutes and then allowed to cool to room temperature. The reaction mixture was filtered through a celite bed and washed with DCM (100 mL) and the collected filtrates were evaporated to give the crude product. Column chromatography on silica) with hexanes-DCM (90:10) gave *N*-phenylacridanes.

***N*-(Benzyloxycarbonyl)acridane** and ***N*-(tert-butyloxycarbonyl)acridane** were synthesized according to the known literature procedure.[1]

Preparation of 10-methylacridine-*d*$_2$ (10-methylacridine-d_2 (1a-d_2) was prepared according to the literature procedure): [3] Taking 10-methyl-9,10-dihydroacridine (0.170 g, 0.87 mmol) in DMSO-d_6 (5.0 mL) along with NaH (0.10 g, 4.2 mmol) under an inert atmosphere. The reaction mixture was stirred for ~ 2 hours at 50 ^{0}C and then quenched with D_2O (5.0 mL). The crude product

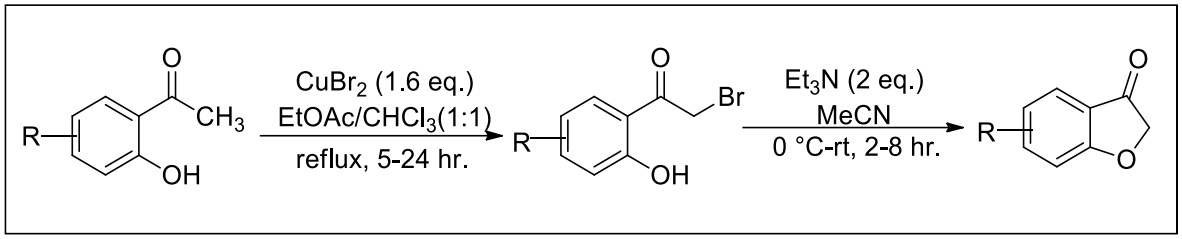
was filtered and washed thoroughly with distilled H_2O. 1H NMR of the product confirmed the formation of 10-methylacridine -d_2 (99% D).

10-methylacridine -d_2 (1a-d_2):

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.34 – 7.22 (comp, 4H), 7.05 – 6.93 (comp, 4H), 3.44 (s, 3H).; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 143.6, 127.5, 126.8, 124.1, 120.5, 111.8, 33.0, 32.4 (qu, *J* = 18.9 Hz).

Preparation of 3-Coumaranone Derivatives:

3-Coumaranone Derivatives were synthesized from literature procedure with slight modifications. [4], [5]



To a solution of o-Acetyl phenol (1eq.) in $CHCl_3$ was added $CuBr_2$(1.6 eq.) dissolved in ethyl acetate, the reaction was kept at reflux until the starting material was consumed. White CuBr was removed by filtration and washed with EtOAc. The solvent was concentrated under vacuum and the residue was purified by flash chromatography on silica gel to give the desired 2-Bromo-1-(2-hydroxyacetophenone)**.** 2-Bromo-1-(2-hydroxyacetophenone(1eq.) was dissolved in MeCN, then cooled to 0°C, and Et_3N (2eq.) was slowly added. The solution was quenched with water and extracted with DCM. The combined organic phase was dried over Na_2SO_4 and concentrated. The residue was purified by flash chromatography on silica gel to afford the 3-Coumaranone Derivatives.

Figure S1. Representative Bioactive Acridines, 3-coumaranone and 3-isochromanone

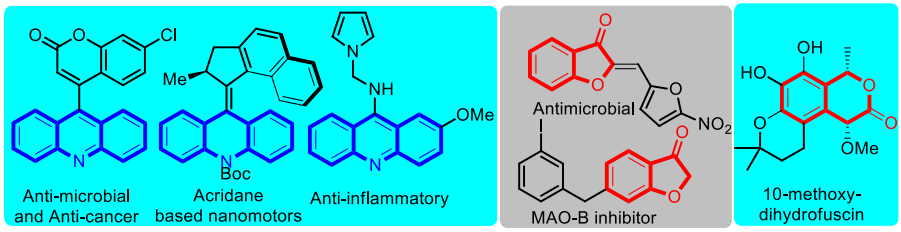
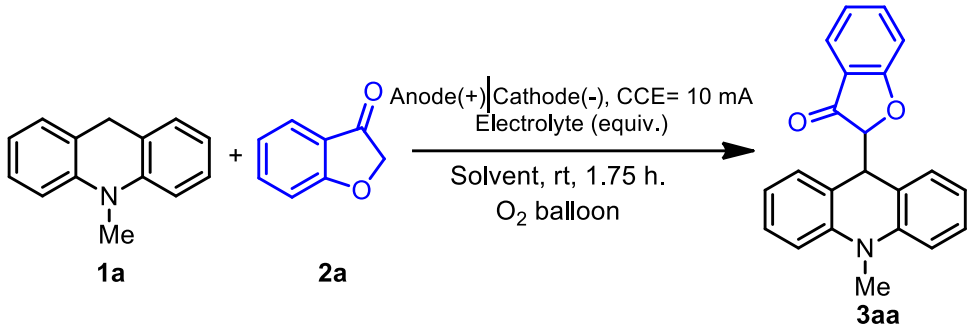


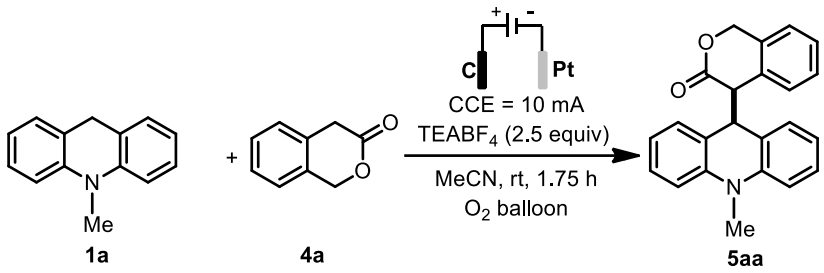
Table S1: Additional optimization of reaction conditions: [a]



Entry	Anode-Cathode	Electrolyte (equiv.)	Solvent	Yield[b] of **3aa** (%)
1	C-Pt	$TEABF_4$ (2.0)	MeOH	69
2	C-Pt	$TEABF_4$ (3.0)	MeOH	69
3	C-Pt	$TBABF_4$ (2.0)	MeOH	51
4	C-Pt	$TBAPF_6$ (2.0)	MeOH	42
5	C-Pt	TBAB (2.0)	MeOH	46
7	C-Pt	$LiClO_4$ (2.0)	MeOH	63
8[c]	C-Pt	$TEABF_4$ (2.5)	MeOH	nr
9[d]	C-Pt	$TEABF_4$ (2.5)	MeOH	35
10	C-Pt	$TEABF_4$ (2.5)	MeCN	60
11	C-Pt	$TEABF_4$ (2.5)	MeCN/MeOH (1:2)	46
12	C-Pt	$TEABF_4$ (2.5)	$CHCl_3$	nr
13	C-Pt	$TEABF_4$ (2.5)	^{t}AmOH	nr
14	C-Pt	$TEABF_4$ (2.5)	Dry THF	42
15[e]	C-Pt	$TEABF_4$ (2.5)	MeOH	50
16[f]	C-Pt	$TEABF_4$ (2.5)	MeOH	65
17[g]	C-Pt	$TEABF_4$ (2.5)	MeOH	39
18[h]	C-Pt	$TEABF_4$ (2.5)	MeOH	78

[a]Reaction conditions: Unless otherwise mentioned, all reactions were performed with **1a** (0.2 mmol, 1.0 equiv), **2a** (0.26 mmol, 1.3 equiv), in 2 mL solvent (0.1 M), constant current = 10 mA, undivided cell, at rt (30 °C) under O_2 balloon for 1.75 h. [b]Isolated yield. [c] MsOH(1 equiv.) as additive. [d] K_2CO_3 (1equiv.) as additive. [e] Platinum plated ceramic electrode as cathode. [f] air. [g] Under N_2 atmosphere. [h] 40 ^{0}C instead of rt. "nr": no reaction. CCE= constant current electrolysis:

Table S2: Additional optimization Scheme 3:[a]



1a 4a 5aa

Entry	1a:4a (Equivalent ratio)	Solvent	Yield[b] of 5**aa** (%)
1	1:1.3	MeOH	60
2	1:1.5	MeCN	72
3	1.5:1	MeCN	76

[a]Reaction conditions: Unless otherwise mentioned, all reactions were performed with **1** (1.5 equiv), **2** (0.2 mmol, 1.0 equiv), $TEABF_4$ (2.5 equiv), solvent (2 mL), carbon rod anode, platinum plate cathode, constant current = 10 mA, rt (30 °C), O_2 balloon, 1.75 h. [b]Isolated yield.

Experimental procedures and characterization data of products:

General information for Electrolysis

The ElectraSyn 2.0 package (IKA) was used to execute Electrochemical reactions in constant current mode. The reactions were carried out in a 5 or 20 mL vial with a stir bar and a graphite-SK-50 (5.0 x 0.8 x 0.2 cm) working electrode (anode) and a platinum-plated (5.0 x 0.8 x 0.2 cm) counter-electrode (cathode) separated by 0.6 cm. (Figure S1)

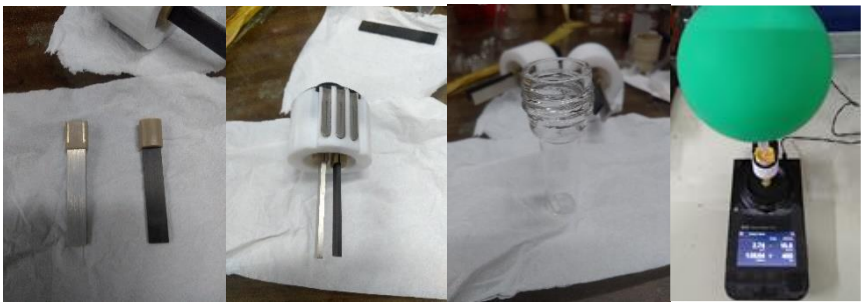
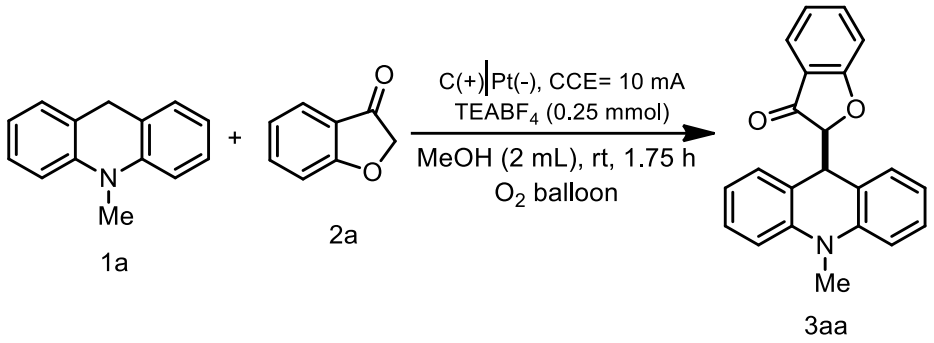


Figure S2. Experimental electrochemical set-up with ElectraSyn 2.0

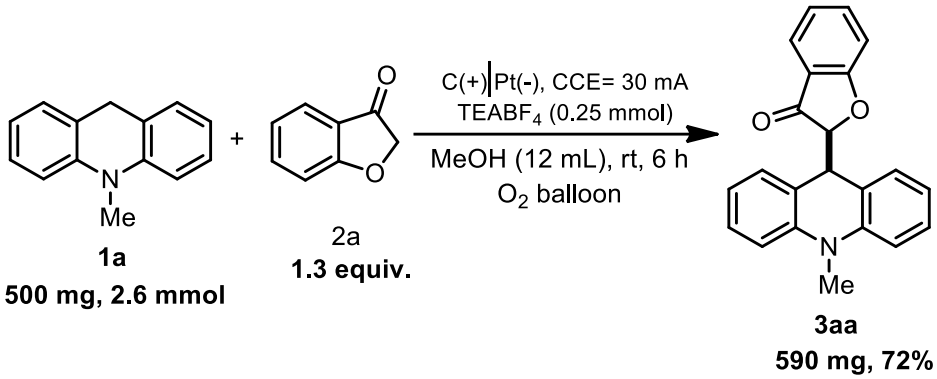
General Procedure for Electrochemical C(sp^3)/C(sp^3) Cross Dehydrogenative Coupling Reaction: (0.2 mmol Scale):



1a 2a 3aa

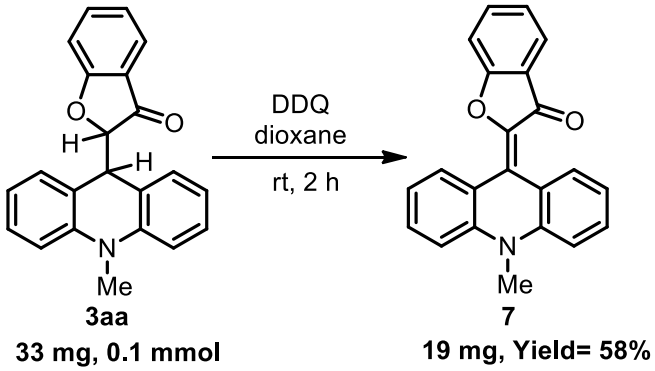
A 5 mL oven-dried electrasyn vial was charged with 10-methyl-9,10-dihydroacridine **1a** (39 mg, 0.2 mmol), 3-coumaranone **2a** (35 mg, 0.26 mmol), $TEABF_4$ (0.5 mmol, 2.5 equiv,) and MeOH (2.0 mL). The vial was equipped with a graphite rod as the anode (immersed surface area 1.2 x 0.5 cm^2) and a platinum plate as the cathode (immersed surface area 1.2 x 0.5 cm^2), the distance between the electrodes was 0.6 cm. The resulting mixture was stirred and electrolyzed at a constant current of 10 mA at ambient temperature for 1.75 h. with an O_2-balloon. After completion of the reaction indicated by TLC the volatiles were evaporated in vacuum and the crude product was directly purified by column chromatography using ethyl acetate / petroleum ether (5%) to afford product **3aa** (54.9 mg; yield = 84%; Rf = 0.2).

Large Scale Synthesis of 3aa at 2.6 mmol:



A 20 mL oven-dried electrasyn vial was charged with10-methyl-9,10-dihydroacridine**1a** (500 mg, 2.6 mmol), 3-coumaranone **2a** (442 mg, 3.3 mmol), $TEABF_4$ (6.5 mmol, 2.5 equiv,) and MeOH (12 mL). The vial was equipped with a graphite rod as the anode (immersed surface area 1.2 x 0.5 cm^2) and platinum a plate as the cathode (immersed surface area 1.2 x 0.5 cm^2), the distance between the electrodes was 0.6 cm.The resulting mixture was stirred and electrolyzed at a constant current of 30 mA at ambient temperature for 6 h. with O_2-balloon. After completion of the reaction indicated by TLC the volatiles was evaporated in vacuum and the crude product was directly purified by column chromatography using ethyl acetate / petroleum ether (5%) to afford product **3aa** (590 mg; yield = 72%; Rf = 0.2).

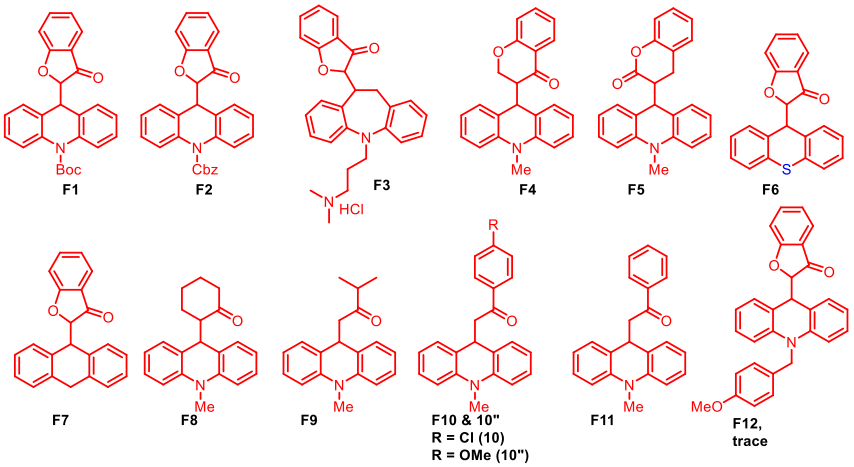
Product Transformation:



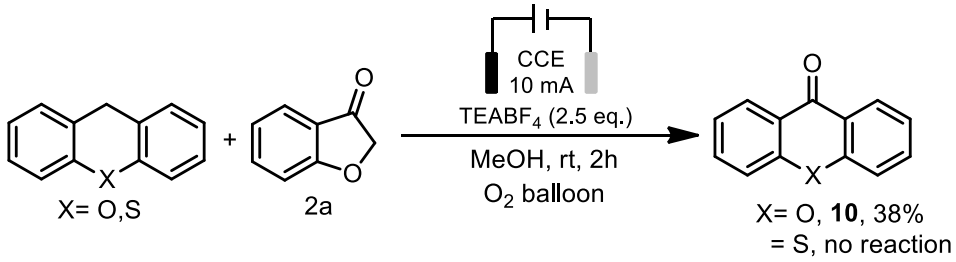
A 5 mL oven-dried sample vial was charged with **3aa** (33 mg, 0.1 mmol), DDQ (45 mg, 0.2 mmol), and Dioxane (2 mL). The mixture was stirred for 2 h. After completion of the reaction indicated by TLC the volatiles were evaporated in vacuum and the crude product was directly purified by column chromatography using ethyl acetate / petroleum ether (10%) to afford product **4aa** (19 mg; yield = 58%; Rf = 0.1).

Red solid; $\mathbf{R_f}$ 0.10 (pet ether/ethyl acetate = 10:1); **eluent composition** petroleum ether/ethyl acetate = 10:1; **mp**128-130 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.44 (dd, *J* = 8.0, 1.2 Hz, 2H), 7.81 (app d, *J* = 7.6 Hz, 1H), 7.56-7.53 (comp, 3H), 7.31 – 7.25 (comp, 5H), 7.17 – 7.14 (m, 1H), 3.74 (s, 1H).; **^{13}C NMR**(100 MHz, $CDCl_3$) δ 162.9, 141.4, 139.5, 134.5, 131.2 (X 2), 130.7 (X 2), 127.8, 124.2 (X 2), 123.8, 122.5, 120.7 (X 2), 119.3, 113.0 (X 3), 112.3 (X 2), 34.6. **HRMS** (ESI, m/z) calcd for $C_{22}H_{15}NO_2$ $[M + H]^+$ 326.1181, found 326.1179.

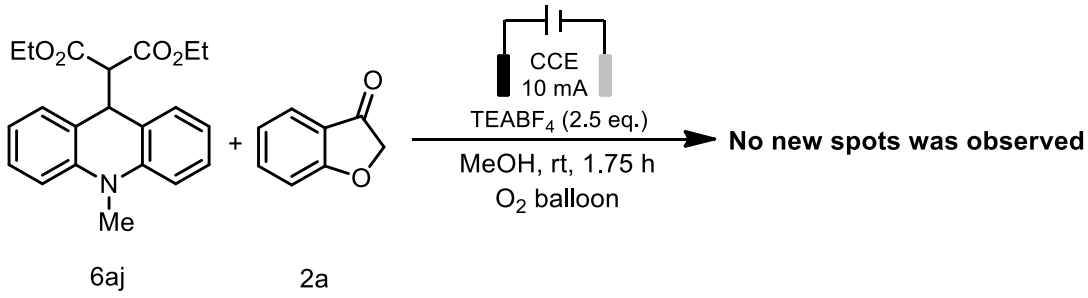
Table S3. Unsuccessful Substrates:



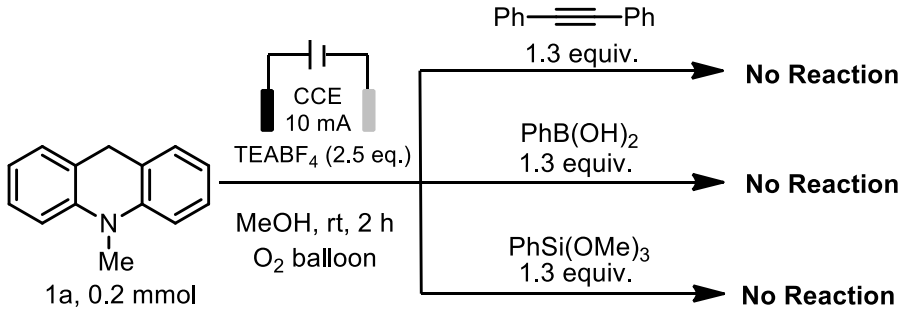
Reactivity of 9*H*-Xanthene and 9*H*-Thioxanthene:



Reactivity of tertiary C-H:

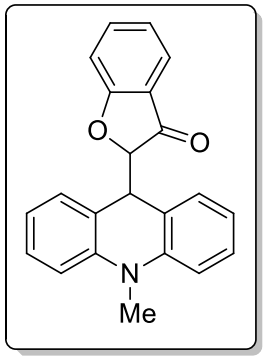


Reactivity of Acridane with others coupling agents:



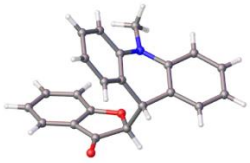
Characterization Data for the products:

2-(10-methyl-9,10-dihydroacridin-9-yl)benzofuran-3(2H)-one (3aa):



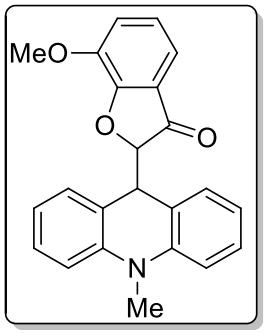
Yield 84% (54.9 mg); Brown solid; $\mathbf{R_f}$ 0.20 (pet ether/ethyl acetate = 20:1); **eluent composition** petroleum ether/ethyl acetate = 20:1; **mp**126-128 ºC (crystallization from hot EtOH/$CHCl_3$ mixture);**^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.50 (dd, *J* =7.6, 0.4, 1H), 7.45 – 7.40 (m, 1H), 7.31 – 7.27 (comp, 2H), 7.13 – 7.08 (comp, 2H), 7.02 – 6.96 (comp, 2H), 6.91 (t, *J* = 7.6 Hz, 1H), 6.87 (app d, *J* = 8.4 Hz, 1H), 6.83 (app d, *J* =8.0 Hz, 1H), 6.77 (app td, *J* = 7.6, 1.2 Hz, 1H), 4.64 (app d, *J* = 4.0 Hz, 1H), 4.61 (app d, *J* = 4.0 Hz, 1H), 3.44 (s, 3H).; **^{13}CNMR**(100 MHz, $CDCl_3$) δ 200.0, 172.8, 143.4, 143.2, 137.5, 129.1, 128.9, 128.1, 127.9, 123.8, 121.8, 121.7, 121.4, 120.6, 120.2, 119.6, 112.8, 112.4, 112.2, 89.8, 46.0, 33.2.; **HRMS** (ESI, m/z) calcd for $C_{22}H_{17}NO_2$ $[M + H]^+$328.1338, found 328.1331.

Figure S3.X-ray crystal structure of **3aa** (ellipsoid contour at 50% probability level) (**CCDC-2238292**)



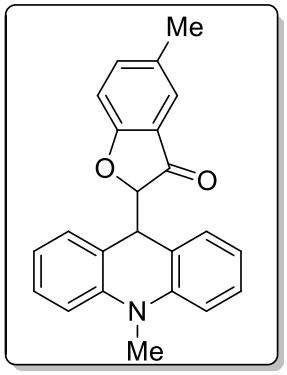
Empirical formula	**$C_{22}H_{17}NO_2$**
Formula weight	**327.36**
Temperature/K	**100**
Crystal system	**monoclinic**
Space group	**$P2_1/n$**
a/Å	**8.549(3)**
b/Å	**9.093(2)**
c/Å	**20.815(5)**
α/°	**90**
β/°	**96.522(10)**
γ/°	**90**
Volume/Å^3	**1607.6(7)**
Z	**4**
ρ_{calc}g/cm^3	**1.353**
μ/mm^{-1}	**0.689**
F(000)	**688.0**
Crystal size/mm^3	**0.2 × 0.2 × 0.2**
Radiation	**Cu Kα (λ = 1.54184)**
2Θ range for data collection/°	**8.552 to 145.336**
Index ranges	**$-10 \le h \le 10$, $-11 \le k \le 10$, $-25 \le l \le 25$**
Reflections collected	**23659**
Independent reflections	**3123 [R_{int} = 0.0566, R_{sigma} = 0.0339]**
Data/restraints/parameters	**3123/0/227**
Goodness-of-fit on F^2	**1.100**
Final R indexes [I>=2σ (I)]	**R_1 = 0.0503, wR_2 = 0.1158**
Final R indexes [all data]	**R_1 = 0.0543, wR_2 = 0.1186**
Largest diff. peak/hole / e Å^{-3}	**0.31/-0.27**

7-methoxy-2-(10-methyl-9,10-dihydroacridin-9-yl)benzofuran-3(2H)-one (3ab):



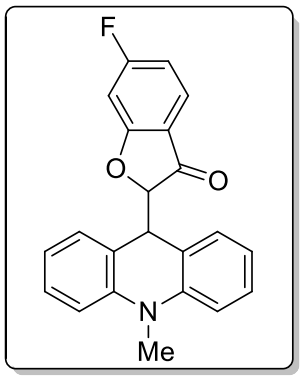
Yield 70% (50 mg); Colorless solid; **R_f** 0.3 (pet ether/ethyl acetate = 10:1); **eluent composition** petroleum ether/ethyl acetate = 20:1; **mp** 143-145°C; **^{1}H NMR** (400 MHz, $CDCl_3$) 7.29 (app td, *J* = 6.9, 1.5 Hz, 1H), 7.26 – 7.23 (m, 1H), 7.11 – 7.09 (m, 1H), 7.08 – 7.05 (comp, 2H), 6.97 – 6.91 (comp, 3H), 6.84-6.80 (comp, 2H), 6.74 (app td, *J* = 7.4, 1.0 Hz, 1H), 4.69 – 4.67 (m, 1H), 4.65 (app d, *J* = 3.6 Hz, 1H), 3.84 (s, 3H), 3.41 (s, 3H).; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 200.1, 146.2, 143.5, 143.2, 128.9, 128.8, 128.0, 127.9, 123.1, 121.9 (x 2), 121.8, 120.5, 120.1, 119.2, 119.0, 115.2, 112.5, 112.3, 90.6, 56.4, 46.2, 33.3.; **HRMS** (ESI, m/z) calcd for $C_{23}H_{20}NO_3[M + H]^+$ 358.1443, found 358.1441.

5-methyl-2-(10-methyl-9,10-dihydroacridin-9-yl)benzofuran-3(2H)-one (3ac):



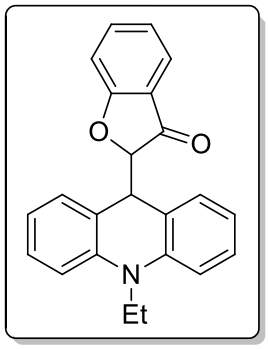
Yield 68% (46 mg); Red solid; **R_f** 0.2 (pet ether/ethyl acetate = 20:1); **eluent composition** petroleum ether/ethyl acetate = 20:1; **mp** 113-115°C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.31 – 7.27 (comp, 3H), 7.24 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.14 – 7.08 (comp, 2H), 7.01 – 6.95 (comp, 2H), 6.84 (d, *J* = 8.0 Hz, 1H), 6.79 – 6.75 (comp, 2H), 4.62 (app d, *J* =3.6 Hz, 1H), 4.59 (app d, *J* = 4.0 Hz, 1H), 3.43 (s, 3H), 2.25 (s, 3H).; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 200.0, 171.3, 143.4, 143.2, 138.9, 131.0 , 129.1, 128.9, 128.0, 127.9, 123.2, 122.0, 121.5, 120.6, 120.2, 119.8, 112.43, 112.39, 112.2, 90.0, 46.0, 33.3, 20.5.;**HRMS** (ESI, m/z) calcd for $C_{23}H_{19}NNaO_2[M + Na]^+$ 364.1313, found 364.1311.

7-fluoro-2-(10-methyl-9,10-dihydroacridin-9-yl)benzofuran-3(2H)-one (3ad):



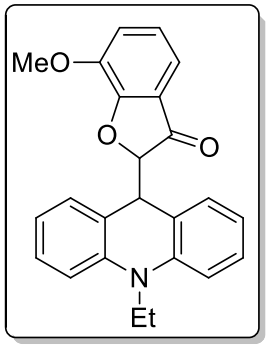
Yield 71% (49.0 mg); Orange Jelly; **R_f** 0.3 (pet ether/ethyl acetate = 20:1); **eluent composition** petroleum ether/ethyl acetate = 20:1;**^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.48 (dd, *J* = 8.5, 5.8 Hz, 1H), 7.32 –7.27 (comp, 2H), 7.14 – 7.10 (m, 1H), 7.07 (dd, *J* = 7.5, 1.6 Hz, 1H), 7.01 (dd, *J* = 7.2, 0.8 Hz, 1H), 6.98 – 6.95 (m, 1H), 6.84 (app d, *J* = 8.0 Hz, 1H), 6.76 (app td, *J* = 7.6, 1.2 Hz, 1H), 6.63 (app td, *J* = 8.4, 2.0 Hz, 1H), 6.52 (dd, *J* = 9.2, 2.0 Hz, 1H), 4.67 – 4.64 (comp, 2H), 3.43 (s, 3H).**^{13}C NMR** (100 MHz, $CDCl_3$) δ 198.0, 174.3 (d, $^2J_{C-F}$ = 15.0 Hz), 169.0 (d, $^1J_{C-F}$ = 256.0 Hz), 143.3, (d, $^2J_{C-F}$ = 16 Hz), 129.2, 128.9, 128.2 (d, $^3J_{C-F}$ = 10 Hz), 125.7 (d, $^3J_{C-F}$ = 13 Hz), 121.7, 120.8, 120.4, 119.2, 118.5, 112.6, 112.4, 110.6, 110.3, 100.3, 100.1, 91.4, 46.1, 33.4.; **^{19}F NMR** (376 MHz, $CDCl_3$) δ_F -97.4 (s, 1F); **HRMS** (ESI, m/z) calcd for $C_{22}H_{16}FNO_2$ $[M + H]^+$ 346.1243, found 346.1230.

2-(10-ethyl-9,10-dihydroacridin-9-yl)benzofuran-3(2H)-one (3ba):



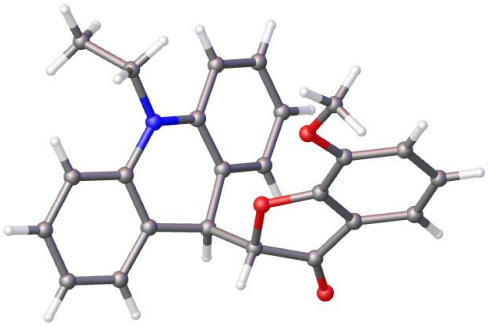
Yield 52% (36 mg); Red solid; **R_f** 0.2 (pet ether/ethyl acetate = 20:1); **eluent composition** petroleum ether/ethyl acetate = 20:1; **mp** 134-136°C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.48 – 7.46 (m, 1H), 7.42 –7.37 (m, 1H), 7.31 – 7.26 (comp, 2H), 7.06 – 7.00 (comp, 3H), 6.97 (app td, J = 7.6, 1.2 Hz, 1H), 6.90 – 6.80 (comp, 3H), 6.66 (app td, *J* = 7.6, 0.8 Hz, 1H), 4.72 (d, *J* = 3.2 Hz, 1H), 4.55 (d, *J* = 3.6 Hz, 1H), 4.09 – 3.98 (m, 2H), 1.41 (t, *J* = 7.0 Hz, 3H).; **^{13}C NMR** (100 MHz, $CDCl_3$)) δ 200.1, 173.0, 141.8, 141.7, 137.5, 129.3, 129.0, 128.1, 127.9, 123.7, 121.8, 121.6, 121.4, 120.5, 119.9, 118.5, 112.8, 112.4, 112.3, 91.3, 45.7, 40.3, 11.9.; **HRMS** (ESI, m/z) calcd for $C_{23}H_{19}NO_2$ $[M + H]^+$ 342.1494, found 342.1492.

2-(10-ethyl-9,10-dihydroacridin-9-yl)-7-methoxybenzofuran-3(2H)-one (3bb):



Yield 68% (50 mg); Yellow solid; **R_f** 0.3 (pet ether/ethyl acetate = 10:1); **eluent composition** petroleum ether/ethyl acetate = 20:1;**mp** 146-148°C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.30 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.26 – 7.21 (m, 1H), 7.08 – 7.03 (comp, 3H), 6.99 (app d, *J* = 8.4 Hz, 1H), 6.94 – 6.89 (m, 2H), 6.86 (app d, *J* = 8.0 Hz, 1H), 6.80 (app t, *J* = 7.8 Hz 1H), 6.78 (app td, *J* = 7.6, 0.8 Hz, 1H), 4.74 (d, *J* = 3.2 Hz, 1H), 4.60 (d, *J* = 3.2 Hz, 1H), 4.07 – 3.93 (m, 2H), 3.82 (s, 3H), 1.41 (t, *J* = 7.1 Hz, 3H).; **^{13}C NMR** (100 MHz, $CDCl_3$)) δ 200.1, 163.2, 146.1, 142.0, 141.6, 129.2, 128.9, 128.1, 127.9, 123.2, 121.8, 121.4, 120.4, 119.8, 119.0, 118.2, 115.1, 112.5, 112.2, 91.7, 56.4, 45.9, 40.5, 11.8.; **HRMS** (ESI, m/z) calcd for $C_{24}H_{21}NO_3$ $[M + H]^+$ 372.1600, found 372.1598.

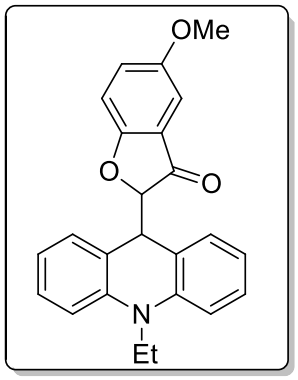
Figure S4.X-ray crystal structure of **3bb** (ellipsoid contour at 50% probability level) (**CCDC-2238293**)



Empirical formula	**$C_{24}H_{21}NO_3$**
Formula weight	**371.42**
Temperature/K	**100.0**
Crystal system	**monoclinic**
Space group	**$P2_1/n$**
a/Å	**13.5269(9)**
b/Å	**9.3422(6)**
c/Å	**15.1324(10)**
α/°	**90**
β/°	**105.484(2)**
γ/°	**90**

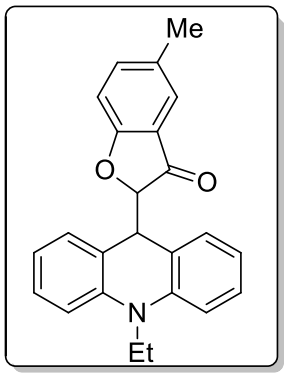
Volume/Å^3	**1842.9(2)**
Z	**4**
ρ_{calc}g/cm^3	**1.339**
μ/mm^{-1}	**0.707**
F(000)	**784.0**
Crystal size/mm^3	**0.35 × 0.25 × 0.2**
Radiation	**Cu Kα (λ = 1.54178)**
2Θ range for data collection/°	**7.796 to 130.198**
Index ranges	**-15 ≤ h ≤ 15, -9 ≤ k ≤ 10, -17 ≤ l ≤ 17**
Reflections collected	**27657**
Independent reflections	**3095 [R_{int} = 0.0655, R_{sigma} = 0.0386]**
Data/restraints/parameters	**3095/0/115**
Goodness-of-fit on F^2	**1.039**
Final R indexes [I>=2σ (I)]	**R_1 = 0.0736, wR_2 = 0.1861**
Final R indexes [all data]	**R_1 = 0.0746, wR_2 = 0.1869**
Largest diff. peak/hole / e Å^{-3}	**0.56/-0.60**

2-(10-ethyl-9,10-dihydroacridin-9-yl)-5-methoxybenzofuran-3(2H)-one (3bc):



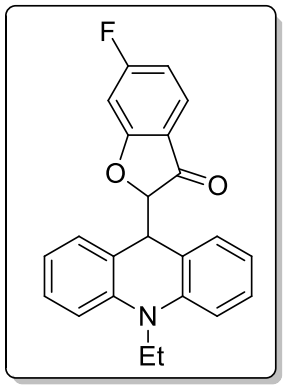
Yield 66% (49 mg); Red solid; **R_f** 0.3 (pet ether/ethyl acetate = 20:1); **eluent composition** petroleum ether/ethyl acetate = 20:1;**mp** 126-128^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.31 – 7.27 (comp, 2H), 7.08 – 7.01 (comp, 4H), 6.97 (app td, *J* = 7.6, 0.8 Hz, 1H), 6.88 – 6.86 (comp, 2H), 6.75 (app d, *J* = 9.2 Hz, 1H), 6.69 (app td, *J* = 7.6, 0.8 Hz, 1H), 4.71 (d, *J* = 3.2 Hz, 1H), 4.57 (d, *J* = 3.2 Hz, 1H), 4.09 – 4.00 (m, 2H), 3.71 (s, 3H), 1.40 (t, *J* = 7.1 Hz, 3H).; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 200.3, 168.4, 154.5, 141.8, 141.7, 129.3, 129.0, 128.1, 127.9, 127.6, 121.7, 121.6, 120.4, 119.9, 118.6, 113.7, 112.4, 112.3, 103.5, 92.2, 55.8, 45.7, 40.3, 11.8.; **HRMS** (ESI, m/z) calcd for $C_{24}H_{21}NO_3$ $[M + H]^+$ 372.1600, found 372.1603.

5-ethyl-2-(10-methyl-9,10-dihydroacridin-9-yl)benzofuran-3(2H)-one (3bd):



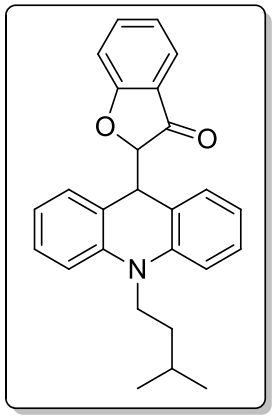
Yield 50% (35 mg); Red solid; **R_f** 0.3 (pet ether/ethyl acetate = 20:1); **eluent composition** petroleum ether/ethyl acetate = 20:1; **mp** 135-137^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.31 – 7.29 (m, 1H), 7.27 – 7.25 (comp, 2H), 7.21 (dd, *J*= 8.4, 2.0, 1H), 7.08 – 7.03 (comp, 3H), 6.98 – 6.94 (m, 1H), 6.87 (d, *J* = 8.4 Hz, 1H), 6.72 (d, *J* = 9.2 Hz, 1H), 6.71 – 6.67 (m, 1H), 4.70 (d, *J* = 3.2 Hz, 1H), 4.55 (d, *J* = 3.2 Hz, 1H), 4.09 – 3.99 (comp, 2H), 2.24 (s, 3H), 1.41 (t, *J* = 7.0 Hz, 3H).; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 200.1, 171.5, 141.8, 141.7, 138.9 (x 2), 130.9, 129.3, 129.0, 128.1, 127.9, 123.1, 121.8, 120.4, 119.9, 118.7, 112.41, 112.35, 112.3, 91.6, 45.6, 40.3, 20.5, 11.9.; **HRMS** (ESI, m/z) calcd for $C_{24}H_{21}NO_2[M + H]^+$356.1651, found 356.1646.

2-(10-ethyl-9,10-dihydroacridin-9-yl)-7-fluorobenzofuran-3(2H)-one (3be):



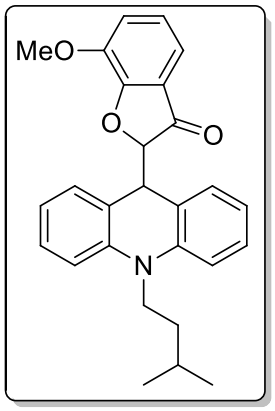
Yield 56% (40 mg); Red Jelly; **R_f** 0.2 (pet ether/ethyl acetate = 20:1); **eluent composition** petroleum ether/ethyl acetate = 20:1; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.46 (dd, *J* = 8.5, 5.8 Hz, 1H), 7.32 – 7.28 (comp, 2H), 7.10 – 7.05 (m, 1H), 7.03 (app dd, *J* = 7.6, 2.0 Hz, 2H), 6.98 (app td, *J* = 7.6, 0.8 Hz, 1H), 6.88 (app d, *J* = 8.0 Hz, 1H), 6.68 (app td, *J* = 7.6, 1.2 Hz, 1H), 6.61 (app td, *J* = 8.4, 2.0 Hz, 1H), 6.48 (dd, *J* = 9.2, 2.0 Hz, 1H), 4.72 (d, *J* = 3.2 Hz, 1H), 4.62 (d, *J* = 3.2 Hz, 1H), 4.07 – 4.01 (m, 2H), 1.41 (t, *J* = 7.2 Hz, 3H).; **^{13}C NMR** (100 MHz, $CDCl_3$) 13C NMR (101 MHz, Chloroform-d) δ 198.0 , 174.3 (d, $^2J_{C–F}$ = 14.8 Hz), 168.9 (d, $^1J_{C–F}$ = 257.7 Hz), 141.7 (d, $^2J_{C–F}$ = 17.4 Hz), 129.3, 128.9, 128.1 (d, $^3J_{C–F}$ = 11.0 Hz), 125.6 (d, $^3J_{C–F}$ = 12.3 Hz), 121.4, 120.5, 119.9, 118.5, 118.1, 112.5, 112.3, 110.4, 110.2, 100.1, 99.9, 92.7, 45.6, 40.3, 11.8.; **^{19}F NMR** (376 MHz, $CDCl_3$) δ_F -97.4 (s, 1F); **HRMS** (ESI, m/z) calcd for $C_{23}H_{18}FNO_2$ $[M + H]^+$ 360.1400, found 360.1385.

2-(10-isopentyl-9,10-dihydroacridin-9-yl)benzofuran-3(2H)-one (3ca):



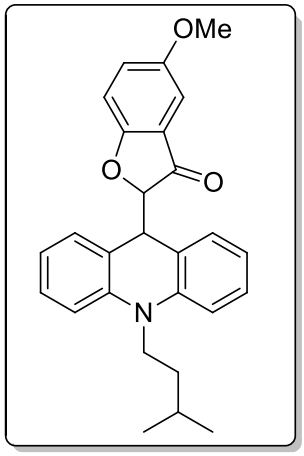
Yield 59% (45 mg); Red Jelly; **R_f** 0.4 (pet ether/ethyl acetate = 20:1); **eluent composition** petroleum ether/ethyl acetate = 20:1; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.49 – 7.46 (m, 1H), 7.42 – 7.38 (m, 1H), 7.32 – 7.25 (comp, 2H), 7.08 – 7.03 (comp, 2H), 7.00 – 6.94 (comp, 2H), 6.91 – 6.87 (m, 1H), 6.84 – 6.82 (comp, 2H), 6.68 (app td, *J* = 7.6, 1.2 Hz, 1H), 4.72 (d, *J* = 3.2 Hz, 1H), 4.56 (d, *J* = 3.2 Hz, 1H), 3.97 – 3.92 (comp, 2H), 1.87 – 1.78 (m, 1H), 1.76 – 1.70 (m, 2H), 1.08 (d, *J* = 1.6 Hz, 3H), 1.07 (d, *J* = 1.6 Hz, 3H).; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 200.1, 172.9, 142.0, 141.8, 137.5, 129.3, 129.0, 128.1, 127.9, 123.7, 121.8, 121.6, 121.4, 120.4, 119.9, 118.4, 112.8, 112.4, 112.3, 91.3, 45.7, 44.4, 34.5, 26.8, 22.6 (x 2).;**HRMS** (ESI, m/z) calcd for $C_{26}H_{25}NO_2$ $[M + H]^+$ 384.1964, found 384.1966.

2-(10-isopentyl-9,10-dihydroacridin-9-yl)-7-methoxybenzofuran-3(2H)-one (3cb):



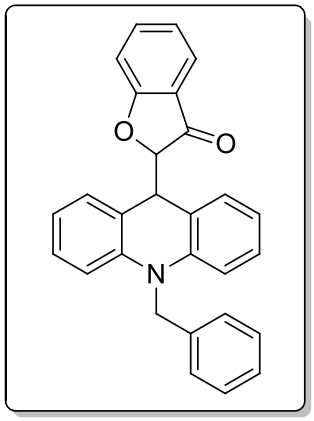
Yield 56% (46 mg); Red solid; **R_f** 0.4 (pet ether/ethyl acetate = 20:1); **eluent composition** petroleum ether/ethyl acetate = 20:1;**mp** 118-120^{o}C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.29 (dd, *J* = 7.5, 1.3 Hz, 1H), 7.25 – 7.21 (m, 1H), 7.09 – 7.02 (m, 3H), 6.97 – 6.88 (m, 3H), 6.85 – 6.77 (m, 2H), 6.68 (app td, *J* =7.5, 0.8 Hz, 1H), 4.73 (d, *J* = 3.2 Hz, 1H), 4.60 (d, *J* = 3.2 Hz, 1H), 3.99 – 3.86 (m, 2H), 3.83 (s, 3H), 1.85 – 1.70 (comp, 3H), 1.09 (d, *J* = 1.2 Hz, 3H), 1.07 (d, *J* = 1.2 Hz, 3H).; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 200.1, 163.1, 146.1, 142.2, 141.8, 129.1, 128.9, 128.1, 127.9, 123.2, 121.8, 121.2, 120.3, 119.8, 118.9, 118.2, 115.1, 112.4, 112.2, 91.6, 56.3, 45.9, 45.0, 34.3, 26.9, 22.6 (x 2).; **HRMS** (ESI, m/z) calcd for $C_{27}H_{27}NO_3$ $[M + H]^+$414.2069, found 414.2063.

2-(10-isopentyl-9,10-dihydroacridin-9-yl)-5-methoxybenzofuran-3(2H)-one (3cc):



Yield 54% (45 mg); Red solid; **R_f** 0.4 (pet ether/ethyl acetate = 20:1); **eluent composition** petroleum ether/ethyl acetate = 20:1;**mp** 123-125°C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.31 – 7.24 (comp, 3H), 7.08 – 7.06 (m, 1H), 7.05 – 7.02 (comp, 2H), 6.99 – 6.94 (comp, 2H), 6.87 (app d, *J* = 2.8 Hz, 1H), 6.84 (app d, *J* = 8.4 Hz, 1H), 6.75 (app d, *J* = 9.2 Hz, 1H), 6.68 (app td, *J* = 7.6, 0.8 Hz, 1H), 4.71 (d, *J* = 3.2 Hz, 1H), 4.56 (d, *J* = 3.2 Hz, 1H), 3.96 – 3.91 (m, 2H), 3.72 (s, 3H), 1.77 – 1.69 (comp, 3H), 1.08 (d, *J* = 1.6 Hz, 3H), 1.06 (d, *J* = 1.6 Hz, 3H).; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 200.3, 168.4, 154.5, 142.0, 141.8, 129.2, 129.0, 128.1, 127.9, 127.6, 121.7, 121.6, 120.4, 119.9, 118.5, 113.7, 112.4, 112.3, 103.5, 92.2, 55.8, 45.7, 44.4, 34.5, 26.7, 22.6 (x 2).;**HRMS** (ESI, m/z) calcd for $C_{27}H_{27}NO_3$ $[M + H]^+$414.2069, found 414.2067.

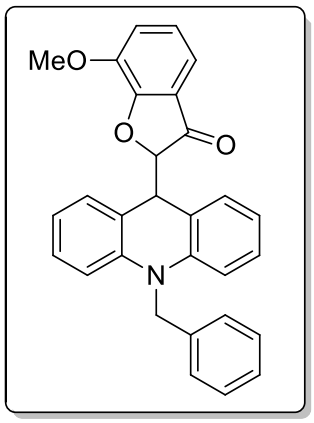
2-(10-benzyl-9,10-dihydroacridin-9-yl)benzofuran-3(2H)-one (3da):



Yield 58% (47 mg); colourless solid; **R_f** 0.3 (pet ether/ethyl acetate = 10:1); **eluent composition** petroleum ether/ethyl acetate = 20:1;**mp** 98-100°C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.47 (dd, *J*= 8.0 Hz, 0.8 Hz, 1H), 7.44 - 7.39 (m, 1H), 7.36 – 7.28 (comp, 4H), 7.21 (app d, *J* = 7.2 Hz, 2H), 7.16 – 7.14 (m, 1H), 7.08 (dd, *J* = 7.6, 1.2 Hz, 1H), 6.97 (dd, *J* = 7.4, 0.9 Hz, 1H), 6.95 – 6.91 (m, 1H), 6.86 – 6.90 (comp, 2H), 6.76 (app d, *J* = 8.4 Hz, 1H), 6.69 (app td, *J* = 7.2, 0.8 Hz, 1H), 6.61 (app d, *J* = 8.0 Hz, 1H), 5.25 – 5.11 (comp, 2H), 4.82 (d, *J*= 2.8 Hz, 1H), 4.65 (d, *J*= 3.2 Hz, 1H).;

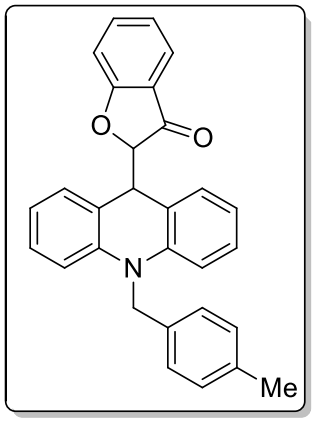
^{13}C NMR (100 MHz, $CDCl_3$) δ 200.1, 173.0, 142.6, 142.3, 137.6, 137.2, 129.0, 128.8 (X 2), 128.7, 128.2, 128.0, 126.9, 126.0 (x 2), 123.8, 121.8, 121.4, 121.0, 120.4, 118.6, 113.5, 113.3, 112.8, 108.4, 91.4, 51.4, 45.5.; **HRMS** (ESI, m/z) calcd for $C_{28}H_{21}NKO_2$ $[M + K]^+$ 442.1209, found 442.1242.

2-(10-benzyl-9,10-dihydroacridin-9-yl)-7-methoxybenzofuran-3(2H)-one (3db):



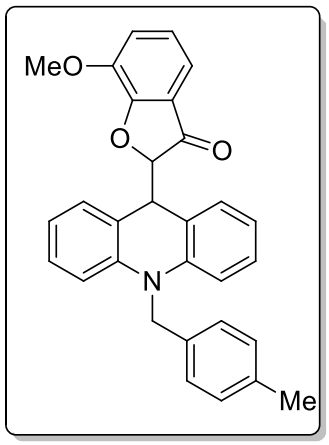
Yield 72% (62 mg); pink solid; **R_f** 0.3 (pet ether/ethyl acetate = 10:1); **eluent composition** petroleum ether/ethyl acetate = 10:1;**mp** 172-174°C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.35 – 7.28 (comp, 4H), 7.21 (app d, *J* = 6.8 Hz, 2H), 7.11 – 7.07 (comp, 2H), 7.05 (dd, *J* = 7.6, 1.2 Hz, 1H), 6.95 – 6.90 (comp, 3H), 6.83 – 6.79 (m, 1H), 6.73 – 6.67 (comp, 2H), 6.60 (d, *J* = 8.4 Hz, 1H), 5.23 – 5.06 (comp, 2H), 4.83 (d, *J* = 3.2 Hz, 1H), 4.68 (d, *J* = 2.8 Hz, 1H), 3.89 (s, 3H).; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 200.1, 163.1, 146.1, 142.9, 142.4, 137.5, 128.84, 128.79 (x 2), 128.5, 128.1, 128.0, 126.9, 126.0 (x 2), 123.2, 121.9, 121.8, 120.9, 120.4, 118.8, 118.5, 115.0, 113.7, 113.3, 91.7, 56.4, 52.0, 45.7.;**HRMS** (ESI, m/z) calcd for $C_{29}H_{23}NNaO_3$ $[M + Na]^+$456.1576, found 456.1577.

2-(10-(4-methylbenzyl)-9,10-dihydroacridin-9-yl)benzofuran-3(2H)-one (3ea):



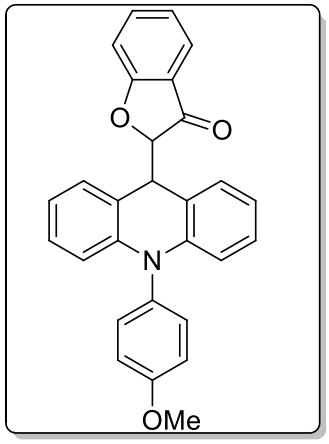
Yield 44% (37 mg); Red solid; **R_f** 0.2 (pet ether/ethyl acetate = 20:1); **eluent composition** petroleum ether/ethyl acetate = 20:1;**mp** 60-65°C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.48 – 7.46 (m, 1H), 7.44 – 7.39 (m, 1H), 7.34 (dd, *J* = 7.5, 1.4 Hz, 1H), 7.15 – 7.06 (comp, 6H), 6.97 (dd, *J* = 7.6, 1.2 Hz 1H), 6.94 – 6.86 (comp, 3H), 6.77 (app d, *J* = 8.4 Hz, 1H), 6.68 (app td, *J* = 7.6, 1.2 Hz, 1H), 6.63 (app d, *J* = 8.4 Hz, 1H), 5.22 – 5.07 (comp, 2H), 4.82 (d, *J* = 3.2, 1H), 4.64 (d, *J* = 3.2 Hz, 1H), 2.34 (s, 3H).; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 200.1, 173.0, 142.6, 142.4, 137.6, 136.5, 134.0, 129.5 (X 2), 129.0, 128.6, 128.2, 128.0, 125.9 (X 2), 123.8, 121.84, 121.81 121.4, 120.9, 120.4, 118.6, 113.5, 113.3, 112.8, 91.4, 51.2, 45.5, 21.1. **HRMS** (ESI, m/z) calcd for $C_{29}H_{23}NNaO_2$ $[M + Na]^+$ 440.1626, found 440.1661.

7-methoxy-2-(10-(4-methylbenzyl)-9,10-dihydroacridin-9-yl)benzofuran-3(2H)-one (3eb):



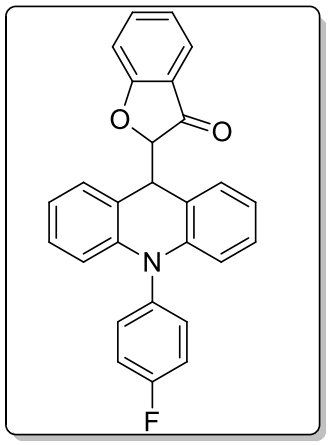
Yield 55% (49 mg); Red solid; **R_f** 0.2 (pet ether/ethyl acetate = 10:1); **eluent composition** petroleum ether/ethyl acetate = 10:1;**mp** 83-85°C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.34 (dd, *J* = 7.4, 1.4 Hz, 1H), 7.13(app d, *J* = 8.0 Hz, 2H), 7.12 – 7.07 (comp, 4H), 7.05 (dd, *J* = 8.0, 1.2 Hz, 1H), 6.94 – 6.90 (comp, 3H), 6.81 (app t, *J* = 7.6 Hz, 1H), 6.75 – 6.73 (m, 1H), 6.69 (app td, *J* = 7.6, 0.8 Hz, 1H), 6.63 – 6.61 (m, 1H), 5.23 – 5.06 (comp, 2H), 4.83 (d, *J* =3.2 Hz, 1H), 4.68 (d, *J* = 2.8 Hz, 1H), 3.89 (s, 3H), 2.34 (s, 3H).; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 200.1, 163.1, 146.1, 142.9, 142.5, 136.4, 134.3, 129.5 (x 2), 128.8, 128.5, 128.1, 128.0, 125.9 (x 2), 123.2, 121.8, 121.7, 120.8, 120.3, 118.8, 118.5, 115.0, 113.7, 113.4, 91.7, 56.4, 51.7, 45.7, 21.0.;**HRMS** (ESI, m/z) calcd for $C_{30}H_{25}NNaO_3$ $[M + Na]^+$ 470.1732, found 470.1742.

2-(10-(4-methoxyphenyl)-9,10-dihydroacridin-9-yl)benzofuran-3(2H)-one (3fa):



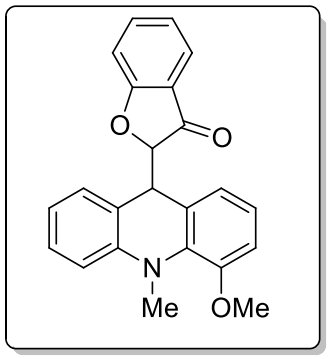
Yield 41% (34 mg); White solid; **R_f** 0.3 (pet ether/ethyl acetate = 20:1); **eluent composition** petroleum ether/ethyl acetate = 20:1;**mp** 150-152°C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.48 (dd, *J* = 4.4, 0.4 Hz, 1H), 7.42 – 7.38 (m, 1H), 7.36 (dd, *J* = 7.2, 1.2 Hz, 1H), 7.34 – 7.30 (comp, 2H), 7.17 – 7.14 (comp, 2H), 7.08 – 7.02 (comp, 2H), 6.95 – 6.86 (comp, 3H), 6.81 (app td, *J* = 8.4 Hz, 1.6 Hz, 1H), 6.62 (td, *J* = 7.6, 1.2 Hz, 1H), 6.36 (dd, *J* = 8.4, 0.8 Hz, 1H), 6.22 (dd, *J* = 8.4, 0.8 Hz, 1H), 4.92 (d, *J* = 2.8 Hz, 1H), 4.69 (d, *J* = 2.4 Hz, 1H), 3.92 (s, 3H).; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 200.2, 173.1, 159.2, 143.3, 143.0, 137.6, 133.3, 132.0 (X 2), 128.9, 128.5, 127.7, 127.6, 123.8, 121.9, 121.4, 120.8, 120.2, 120.1, 116.4, 115.9 (X 2), 114.3, 114.0, 112.7, 92.2, 55.5, 45.2.; **HRMS** (ESI, m/z) calcd for $C_{28}H_{21}NO_3Na$ $[M + Na]^+$ 442.1419, found 442.1419.

2-(10-(4-fluorophenyl)-9,10-dihydroacridin-9-yl)benzofuran-3(2H)-one (3ga):



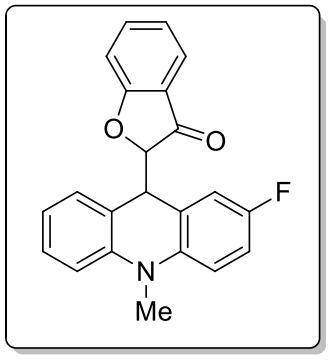
Yield 60% (49 mg); Red solid; **R_f** 0.3 (pet ether/ethyl acetate = 20:1); **eluent composition** petroleum ether/ethyl acetate = 20:1;**mp** 150-152ºC; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.48 (dd, *J* = 8.1, 0.9 Hz, 1H), 7.43 – 7.35 (comp, 5H), 7.36 – 7.30 (m, 1H), 7.09 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.07 – 7.03 (m, 1H), 6.96 – 6.92 (m, 1H), 6.91 – 6.87 (comp, 2H), 6.85 – 6.81 (m, 1H), 6.67 – 6.63 (m, 1H), 6.31 (dd, *J* = 8.4, 0.8 Hz, 1H), 6.18 (dd, *J* = 8.3, 0.9 Hz, 1H), 4.92 (d, *J* = 2.8 Hz, 1H), 4.69 (d, *J* = 2.8 Hz, 1H).; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 200.1, 173.0, 162.1 (d, $^1J_{C–F}$ = 246.9 Hz), 142.8 (d, $^2J_{C–F}$ = 30.3 Hz), 137.6 (d, $^4J_{C–F}$ = 3.0 Hz), 136.6, 132.8 (d, $^3J_{C–F}$ = 8.4 Hz), 129.0, 128.7, 127.8, 127.6 (x 2), 123.8, 121.9, 121.5, 121.1 (x 2), 120.5, 120.2, 117.9, 117.6, 116.6, 114.1, 113.8, 112.6, 92.1, 45.1.; **HRMS** (ESI, m/z) calcd for $C_{27}H_{18}FNNaO_2$ $[M + Na]^+$ 430.1219, found 430.1242.

2-(4-methoxy-10-methyl-9,10-dihydroacridin-9-yl)benzofuran-3(2H)-one (3ha):



Combined Yield 77% (55 mg, dr 1.1:1); Red Jelly; **R_f** 0.1 (pet ether/ethyl acetate = 20:1); **eluent composition** petroleum ether/ethyl acetate = 20:1; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.50 – 7.46 (comp, 2H), 7.39 – 7.44 (comp, 2H), 7.25 – 7.23 (m, 1H), 7.09 (app d, *J* = 7.6 Hz, 1H), 7.04 – 7.00 (comp, 2H), 7.00 – 6.93 (comp, 4H), 6.92 – 6.90 (comp, 2H), 6.89 – 6.87 (comp, 2H), 6.86 – 6.83 (comp, 2H), 6.76 – 6.72 (m, 1H), 6.69 – 6.65 (m, 3H), 4.65 – 4.63 (comp, 3H), 4.58 (d, *J* = 3.2 Hz, 1H), 3.88 (s, 3H), 3.77 (s, 3H), 3.62 (s, 3H), 3.60 (s, 3H).; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 200.0, 199.8, 173.0, 172.9, 150.4, 150.3, 147.0, 146.8, 137.6 (x 2), 134.0, 128.4, 127.9, 127.8, 127.7 (x 2), 124.7, 124.4, 123.9 (x 2), 122.5, 122.0, 121.9, 121.8, 121.6, 121.4 (x 2), 121.3, 121.2, 120.8, 120.6, 116.1, 116.0, 113.0, 112.9, 111.61, 111.56, 90.1, 90.0, 55.9, 55.86, 45.8, 45.7, 41.0, 40.9.; **HRMS** (ESI, m/z) calcd for $C_{23}H_{20}NO_3$ $[M + H]^+$ 358.1443, found 358.1429.

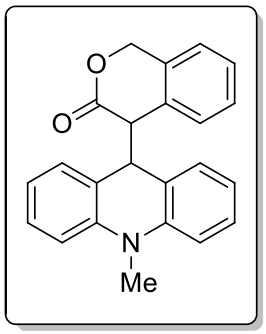
2-(2-bromo-10-methyl-9,10-dihydroacridin-9-yl)benzofuran-3(2H)-one (3ia):



Combined Yield 72% (50 mg, dr 1.1:1); Red solid; **R_f** 0.15 (pet ether/ethyl acetate = 20:1); **eluent composition** petroleum ether/ethyl acetate = 20:1;**mp** 116-118ºC; **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.7 Hz, 1H), 7.50 – 7.48 (m, 1H), 7.47 – 7.42 (comp, 2H), 7.31 – 7.27 (comp, 2H), 7.14 – 7.11 (m, 1H), 7.07 (dd, *J* = 7.5, 1.3 Hz, 1H), 7.03 (dd, *J* = 8.4, 3.0 Hz, 1H), 7.01 – 6.98 (comp, 2H), 6.96 – 6.94 (comp, 2H), 6.94 – 6.91 (m, 1H), 6.89 – 6.88 (comp, 2H), 6.87 – 6.85 (m, 1H), 6.84 – 6.81 (comp, 3H), 6.78 – 6.74 (comp, 2H), 4.85 – 4.63 (comp, 3H), 4.56 (d, *J* = 4.5 Hz, 1H), 3.411 (s, 3H), 3.406 (s, 3H).; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 199.7, 199.6, 172.73, 172.71, 158.5 (d, $^1J_{C–F}$ = 112.8 Hz), 156.2 (d, $^1J_{C–F}$ = 112.8 Hz), 143.3, 143.2, 139.9, 139.7 (d, $^4J_{C–F}$ = 2.8 Hz), 137.7, 137.6, 129.04, 129.0, 128.3, 128.1, 123.9, 123.8, 123.2 (d, $^3J_{C–F}$ = 26.3 Hz), 121.7, 121.6 (x 2), 121.2 (d, $^3J_{C–F}$ = 30.0 Hz), 120.9, 120.7, 120.3, 118.8, 115.7, 115.4, 115.2, 114.5 (d, $^2J_{C–F}$ = 48.7 Hz), 114.3 (d, $^2J_{C–F}$ =

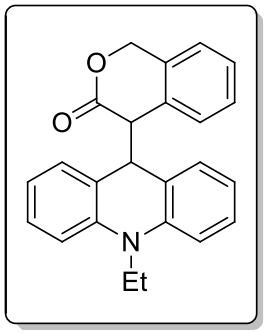
48.7 Hz), 113.2 (d, $^2J_{C-F}$ = 30.0 Hz), 113.1 (d, $^2J_{C-F}$ = 26.2 Hz), 112.84, 112.82, 112.4, 112.2, 89.2, 89.1, 46.0 (x 2), 33.5 (x 2). **^{19}F NMR** (376 MHz, $CDCl_3$) δ_F -124.5 (s, 1F), -124.7 (s, 1F); **HRMS** (ESI, m/z) calcd for $C_{22}H_{16}FNO_2$ $[M + H]^+$ 346.1243, found 346.1246.

4-(10-methyl-9,10-dihydroacridin-9-yl)isochroman-3-one (5aa):



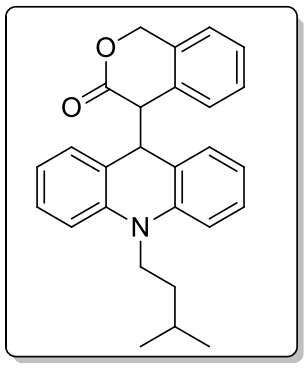
Yield 76% (52 mg); White solid; **R_f**0.20 (pet ether/ethyl acetate = 5:1); **eluent composition** petroleum ether/ethyl acetate = 5:1;**mp**156-158^{o}C**^{1}H NMR** (400 MHz, $CDCl_3$) δ7.33 (dd, *J* =7.2 Hz, 1.2 Hz,1H), 7.29-7.25 (m, 1H), 7.24-7.21 (comp, 2H), 7.12 (app td, *J* = 7.6, 0.8 Hz, 1H), 7.06-7.02 (m, 1H), 6.99-6.92 (comp, 2H), 6.87 (app d, *J* = 7.6 Hz,1H), 6.69 (app d, *J* = 8.0 Hz, 1H), 6.61 (app d, *J* = 8.0 Hz, 1H), 6.60 (app d, *J* = 7.6 Hz, 1H), 4.84 (d, *J* = 4.8 Hz, 1H),4.72 (d, *J* = 14.4 Hz, 1*H*), 3.81 (d, *J* = 4.8 Hz, 1*H*), 3.67 (d, *J* = 14.3 Hz, 1*H*), 2.70 (s, 3H).; **^{13}CNMR**(100 MHz, $CDCl_3$) δ172.0, 143.3 (x 2), 131.2, 130.8, 129.0, 128.8, 128.7, 128.6, 128.3, 127.4, 126.9, 123.1 (x 2), 121.6, 121.2, 121.1, 112.5, 112.0, 70.0, 55.2, 49.0, 32.8; **HRMS** (ESI, m/z) calcd for $C_{23}H_{19}NNaO_2$$[M + Na]^+$364.1313, found 364.1315.

4-(10-ethyl-9,10-dihydroacridin-9-yl)isochroman-3-one (5ba):



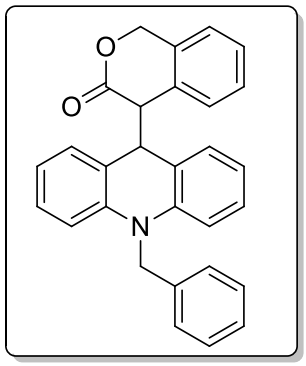
Yield 64% (45 mg); White solid; **R_f** 0.25 (pet ether/ethyl acetate = 10:1); **eluent composition** petroleum ether/ethyl acetate = 10:1; **mp** 133-135 ^{o}C**^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.34 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.29 – 7.21 (comp, 3H), 7.11 (app td, *J* = 0.8, 7.2 Hz, 1H), 7.03 (app td, *J* = 7.6, 1.2 Hz, 1H), 6.96 – 6.94 (m, 1H), 6.93 – 6.91 (m, 1H), 6.84 (app d, *J* = 7.6 Hz, 1H), 6.74 (app d, *J* = 8.4 Hz, 1H), 6.65 (app d, *J* = 8.0 Hz, 1H), 5.94 (d, *J* = 8.0 Hz, 1H), 4.86 (d, *J* = 4.4 Hz, 1H), 4.68 (d, *J* = 14.4 Hz, 1H), 3.75 (d, *J* = 4.8 Hz, 1H), 3.54 (d, *J* = 14.0 Hz, 1H), 3.20 – 3.08 (m, 2H), 1.12 (t, *J* = 7.1 Hz, 3H). ; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 171.8, 141.7, 141.6, 131.2, 130.2, 129.1, 128.7, 128.64, 128.58, 128.2, 127.2, 126.6, 122.8, 122.1, 120.9, 120.7, 120.4, 112.1, 111.6, 69.8, 55.7, 48.7, 40.4, 11.6.;**HRMS** (ESI, m/z) calcd for $C_{24}H_{21}NO_2$ $[M + H]^+$ 356.1651, found 356.1645.

4-(10-isopentyl-9,10-dihydroacridin-9-yl)isochroman-3-one (5ca):



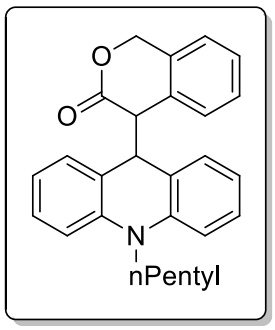
Yield 59% (40 mg); Brown solid; **R_f** 0.30 (pet ether/ethyl acetate = 10:1); **eluent composition** petroleum ether/ethyl acetate = 10:1; **mp** 156-158 ^{o}C;**^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.32 (dd, *J* = 7.4, 1.4 Hz, 1H), 7.28 – 7.21 (comp, 3H), 7.13 (app td, *J* = 7.6, 1.2 Hz, 1H), 7.02 (app td, *J* = 7.6, 0.8 Hz, 1H), 6.96 (app d, *J* = 7.6 Hz, 1H), 6.94 – 6.90 (m, 1H), 6.86 (app d, *J* = 7.6 Hz, 1H), 6.70 (app d, *J* = 8.2 Hz, 1H), 6.60 (app d, *J* = 8.3 Hz, 1H), 5.94 (app d, *J* = 7.6 Hz, 1H), 4.88 (d, *J* = 4.4 Hz, 1H), 4.69 (d, *J* = 14.4 Hz, 1H), 3.75 (d, *J* = 4.8 Hz, 1H), 3.56 (d, *J* = 14.4 Hz, 1H), 3.11 – 3.00 (m, 2H), 1.66 – 1.61 (m, 1H), 1.43 – 1.36 (m, 2H), 0.97 (d, *J* = 2.4 Hz, 3H), 0.95 (d, *J* = 2.8 Hz, 3H).; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 171.8, 141.8, 141.7, 131.2, 130.3, 129.1, 128.8, 128.7, 128.6, 128.2, 127.2, 126.7, 122.9, 122.0, 120.8, 120.7, 120.4, 112.1, 111.6, 69.8, 55.8, 48.7, 44.7, 34.0, 26.7, 22.5.; **HRMS** (ESI, m/z) calcd for $C_{27}H_{27}NNaO_2$ $[M + Na]^+$ 420.1939, found 420.1941.

4-(10-benzyl-9,10-dihydroacridin-9-yl)isochroman-3-one (5da):



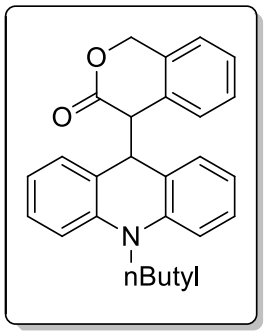
Yield 46% (38 mg); Colorless solid; **R_f** 0.30 (pet ether/ethyl acetate = 10:1); **eluent composition** petroleum ether/ethyl acetate = 10:1; **mp** 138-140 °C;**^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.39 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.32 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.24 – 7.18 (comp, 4H), 7.16 – 7.13 (comp, 2H), 7.08 – 7.05 (m, 1H), 7.04 – 7.00 (m, 1H), 6.96 (dd, *J* = 7.4, 1 Hz, 2H), 6.92 (app d, *J* = 8.8 Hz, 2H), 6.48 – 6.46 (m, 1H), 6.38 – 6.36 (m, 1H), 6.01 (app d, *J* = 7.6 Hz, 1H), 4.98 (d, *J* = 4.8 Hz, 1H), 4.71 (d, *J* = 14.4 Hz, 1H), 4.16 (AB q, *J* = 16.8 Hz, 2H), 3.85 (d, *J* = 4.4 Hz, 1H), 3.51 (d, *J* = 14.4 Hz, 1H).; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 171.8, 142.9, 142.3, 136.6, 131.3, 130.3, 128.8, 128.73 (x 3), 128.70, 128.5, 128.3, 127.4, 126.9, 126.7, 125.7 (x 2), 123.0, 122.8, 121.5, 121.4, 121.0, 113.4, 112.9, 69.8, 55.8, 50.9, 48.7.; **HRMS** (ESI, m/z) calcd for $C_{29}H_{23}NO_2$ $[M + H]^+$ 418.1807, found 418.1806.

4-(10-pentyl-9,10-dihydroacridin-9-yl)isochroman-3-one (5ja):



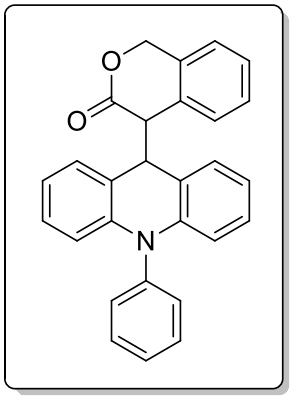
Yield 38% (30 mg); Brown solid; **R_f** 0.20 (pet ether/ethyl acetate = 10:1); **eluent composition** petroleum ether/ethyl acetate = 10:1; **mp** 156-158 °C;**^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.32 (dd, *J* = 7.4, 1.4 Hz, 1H), 7.27 – 7.20 (comp, 3H), 7.11 (app td, *J* = 7.6, 0.8 Hz, 1H), 7.02 (app td, *J* = 7.6, 0.8 Hz, 1H), 6.95 – 6.89 (comp, 2H), 6.85 (app d, *J* = 7.2 Hz, 1H), 6.68 (app d, *J* = 8.4 Hz, 1H), 6.59 (app d, *J* = 8.4 Hz, 1H), 5.92 (d, J = 7.6 Hz, 1H), 4.88 (d, *J* = 4.8 Hz, 1H), 4.68 (d, *J* = 14.4 Hz, 1H), 3.73 (d, *J* = 4.8 Hz, 1H), 3.54 (d, *J* = 14.4 Hz, 1H), 3.06 – 2.92 (m, 2H), 1.56 – 1.47 (m, 2H), 1.39 – 1.25 (comp, 4H), 0.92 (t, *J* = 7.2 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 172.1, 142.0, 141.9, 131.3, 130.3, 129.2, 128.9, 128.8, 128.7, 128.3, 127.4, 126.8, 123.0, 122.1, 121.0, 120.8, 120.4, 112.3, 111.8, 69.9, 55.9, 48.8, 46.3, 29.2, 25.4, 22.6, 14.3; **HRMS** (ESI, m/z) calcd for $C_{27}H_{27}NNaO_2$ $[M + Na]^+$ 420.1939, found 420.1925.

4-(10-butyl-9,10-dihydroacridin-9-yl)isochroman-3-one (5ka):



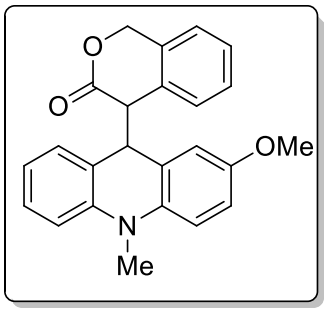
Yield 40% (31 mg); White solid; **R_f** 0.1 (pet ether/ethyl acetate = 20:1); **eluent composition** petroleum ether/ethyl acetate = 10:1; **mp** 122-124 °C**^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.33 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.28 – 7.21 (comp, 3H), 7.12 (app td, *J* = 7.6, 1.2 Hz, 1H), 7.03 (app td, *J* = 7.2, 1.2 Hz, 1H), 6.96 – 6.90 (comp, 2H), 6.85 (app d, *J* = 7.6 Hz, 1H), 6.70 (app d, *J* = 8.4 Hz, 1H), 6.60 (app d, *J* = 8.4 Hz, 1H), 5.94 (d, *J* = 7.6 Hz, 1H), 4.88 (d, *J* = 4.8 Hz, 1H), 4.69 (d, *J* =14.4 Hz, 1H), 3.75 (d, *J* = 4.8 Hz, 1H), 3.56 (d, *J* = 14.4 Hz, 1H), 3.08 – 2.94 (m, 2H), 1.53 – 1.46 (m, 2H), 1.34 (comp, 2H), 0.96 (t, *J* = 7.3 Hz, 3H). ; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 171.9, 141.8, 141.7, 131.1, 130.2, 129.1, 128.7, 128.63, 128.57, 128.2, 127.2, 126.6, 122.8, 121.9, 120.9, 120.7, 120.3, 112.1, 111.6, 69.8, 55.7, 48.6, 45.9, 27.6, 20.1, 13.8.; **HRMS** (ESI, m/z) calcd for $C_{26}H_{25}NNaO_2$ $[M + Na]^+$406.1783, found 406.1763.

4-(10-phenyl-9,10-dihydroacridin-9-yl)isochroman-3-one (5la):



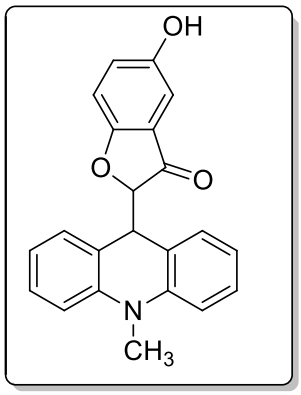
Yield 40% (32 mg) Colorless solid; **R_f** 0.30 (pet ether/ethyl acetate = 10:1); **eluent composition** petroleum ether/ethyl acetate = 10:1; **mp** 160-162 °C ;**^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.47 – 7.43 (comp, 2H), 7.42 – 7.37 (comp, 3H), 7.30 (app td, *J* = 7.6, 0.8 Hz, 1H), 7.06 – 6.96 (comp, 5H), 6.93 (app td, *J* = 7.6, 1.2 Hz, 1H), 6.52 – 6.50 (comp, 2H), 6.04 – 6.00 (comp, 2H), 5.93 – 5.90 (m, 1H), 5.17 (d, *J* = 4.4 Hz, 1H), 4.70 (d, *J* = 14.0 Hz, 1H), 3.94 (d, *J* = 4.4 Hz, 1H), 3.56 (d, *J* = 14.4 Hz, 1H).; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 172.0, 142.7, 139.6, 131.7, 130.7 (x 3), 130.6 (x 3), 129.2, 129.0, 128.7, 128.23, 128.20, 127.8, 127.4, 127.2, 123.6, 121.3, 121.2, 119.8, 118.5, 113.9, 113.5, 69.9, 56.5, 48.3.; **HRMS** (ESI, m/z) calcd for $C_{28}H_{21}NNaO_2$[M + Na]$^+$426.1470, found 426.1469.

4-(2-methoxy-10-methyl-9,10-dihydroacridin-9-yl)isochroman-3-one (5ma):



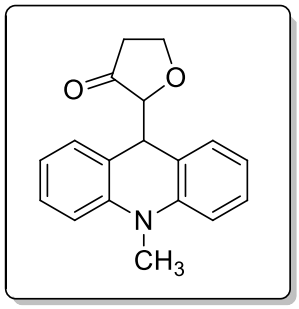
Yield 54% (40 mg, dr 1:1) White solid; **R_f** 0.20 (pet ether/ethyl acetate = 10:1); **eluent composition** petroleum ether/ethyl acetate = 10:1; **mp** 150-152 °C ;**^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.28 – 7.24 (comp, 3H), 7.21 (d, *J* = 7.2 Hz, 1H), 7.15-7.10 (comp, 2H), 7.01 – 6.96 (comp, 3H), 6.92 – 6.81 (comp, 6H), 6.77 (d, *J* = 2.8 Hz, 1H), 6.66 (d, *J* = 8.1 Hz, 1H), 6.62 (d, *J* = 8.8 Hz, 1H), 6.56 (d, *J* = 8.9 Hz, 1H), 6.12 (d, *J* = 7.6 Hz, 1H), 6.08 (d, *J* = 7.6 Hz, 1H), 4.82 (d, *J* = 4.7 Hz, 1H), 4.79 (d, *J* = 6.2 Hz, 1H), 4.76 (d, *J* = 2.9 Hz, 1H), 4.72 (d, *J* = 14.4 Hz, 1H), 3.86-3.80 (comp, 6H), 3.77 (s, 3H), 3.64 (d, *J* = 14.3 Hz, 1H), 2.71 (s, 3H), 2.65 (s, 3H).; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 171.9, 171.7, 154.5, 154.3, 143.4, 137.4, 131.1, 130.8, 130.5, 128.7 (x 3), 128.5, 128.4, 128.1, 127.2 (x 3), 126.8, 126.7, 123.9, 123.0, 122.9, 122.4, 122.1, 120.6, 120.51, 120.46 (x 2), 114.8, 114.1, 113.4 (x 2), 113.3, 113.1, 112.8, 112.1, 111.5, 69.9 (x 2), 55.9, 55.8, 54.8 (x 2), 49.2, 49.1, 32.71, 32.68.; **HRMS** (ESI, m/z) calcd for $C_{24}H_{21}NNaO_3$ [M + Na]$^+$394.1419, found 394.1423.

5-hydroxy-2-(10-methyl-9,10-dihydroacridin-9-yl)benzofuran-3(2H)-one (6aa):



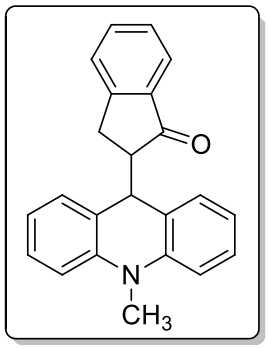
Yield 58% (40 mg); Green solid; **R_f** 0.3 (pet ether/ethyl acetate = 5:1); **eluent composition** petroleum ether/ethyl acetate = 5:1; **mp**140-142 °C**^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.35 – 7.29 (m, 2H), 7.17 – 7.12 (m, 2H), 7.04 – 7.01 (m, 1H), 6.93 (d, *J* = 8.0 Hz, 1H), 6.86 (app td, *J* = 7.6, 0.8 Hz, 1H), 6.68 – 6.63 (comp, 2H), 6.57 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.03 (d, *J* = 2.4 Hz, 1H), 4.80 (d, *J* = 4.4 Hz, 1H), 3.80 (d, *J* = 4.4 Hz, 1H), 3.18 (s, 3H).; **^{13}C NMR** (100 MHz, $CDCl_3$)) δ 176.0, 151.6, 147.6, 143.0, 142.6, 128.9 (X 2), 128.8 (X 2), 128.3, 128.1, 125.8, 122.7, 121.0, 120.6 (X 2), 120.5, 115.1, 112.8, 112.6 (X 2), 112.3, 110.2 (X 2), 53.3, 45.8, 33.1.; **HRMS** (ESI, m/z) calcd for $C_{27}H_{17}NNaO_3$ [M + Na]$^+$ 366.1106, found 366.1129.

2-(10-methyl-9,10-dihydroacridin-9-yl)dihydrofuran-3(2H)-one (6ab):



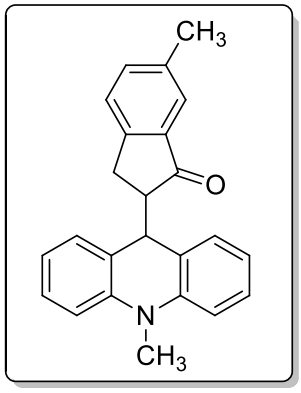
Yield 41% (25 mg); Yellow solid; **R_f** 0.20 (pet ether/ethyl acetate = 20:1); **eluent composition** petroleum ether/ethyl acetate = 20:1; **mp** 96-98 °C **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.28 – 7.22 (comp, 3H), 7.15 (dd, *J* = 7.6, 1.3 Hz, 1H), 7.01 – 6.97 (m, 1H), 6.94 – 6.91 (comp, 3H), 4.62 (d, *J* = 4.4 Hz, 1H), 4.05 (app t, *J* = 8.8 Hz, 1H), 3.89 (d, *J* = 17.0 Hz, 1H), 3.70 (app t, *J* = 9.2 Hz, 1H), 3.47 (d, *J* = 17.0 Hz, 1H), 3.39 (s, 1H), 2.69 (m, 1H).; **^{13}C NMR** (100 MHz, $CDCl_3$)) δ 214.6, 143.5, 142.7 , 128.9, 128.1, 127.9, 127.6, 125.2, 122.7, 121.1, 121.0, 112.3, 112.2, 71.3, 68.8, 55.6, 41.3, 33.0.; **HRMS** (ESI, m/z) calcd for $C_{18}H_{17}NO_2$ $[M + H]^+$ 280.1338, found 280.1339.

2-(10-methyl-9,10-dihydroacridin-9-yl)-2,3-dihydro-1H-inden-1-one (6ac):



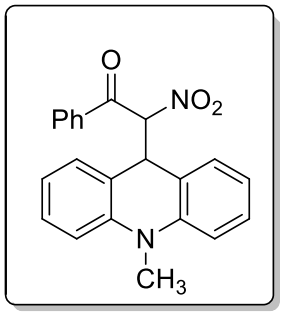
Yield 40% (26 mg); White solid; **R_f** 0.2 (pet ether/ethyl acetate = 20:1); **eluent composition** petroleum ether/ethyl acetate = 20:1; **mp**160-165 °C **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.70 (app d, *J* = 7.6 Hz, 1H), 7.44 (app td, *J* = 7.2, 0.8 Hz, 1H), 7.33 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.28 – 7.23 (comp, 3H), 7.15 – 7.08 (comp, 2H), 7.00 (app td, *J* = 7.2, 0.8 Hz, 1H), 6.94 (app d, *J* = 8.0 Hz, 1H), 6.85 (app d, *J* = 8.0 Hz, 1H), 6.76 (app td, *J* = 7.6, 0.8 Hz, 1H), 4.93 (d, *J* = 3.6 Hz, 1H), 3.40 (s, 3H), 2.99 – 2.96 (m, 1H), 2.92 – 2.89 (m, 2H).; **^{13}C NMR** (100 MHz, $CDCl_3$) δ 206.4, 154.2, 143.4, 142.9, 136.8, 134.4, 129.6, 128.5, 127.4, 127.3, 127.0, 126.2, 126.0, 123.7, 122.9, 121.0, 120.7, 112.13, 112.10, 58.0, 42.8, 33.0, 28.5.; **HRMS** (ESI, m/z) calcd for $C_{23}H_{19}NNaO$ $[M + Na]^+$ 348.1364, found 348.1362.

6-methyl-2-(10-methyl-9,10-dihydroacridin-9-yl)-2,3-dihydro-1H-inden-1-one (6ad):



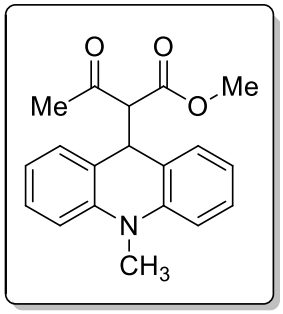
Yield 35% (24 mg); White solid; **R_f** 0.2 (pet ether/ethyl acetate = 20:1); **eluent composition** petroleum ether/ethyl acetate = 20:1; **mp**130-132 °C **^{1}H NMR** (400 MHz, $CDCl_3$) 1H NMR (400 MHz, Chloroform-d) δ 7.50 (app s, 1H), 7.32 (dd, *J* = 7.4, 1 Hz, 1H), 7.25 – 7.22 (comp, 2H), 7.14 – 7.08 (comp, 3H), 6.99 (app td, *J* = 7.6, 0.8 Hz, 1H), 6.93 (app d, *J* = 8.4 Hz, 1H), 6.84 (app d, *J* = 8.0 Hz, 1H), 6.78 – 6.74 (m, 1H), 4.92 (d, *J* = 3.6 Hz, 1H), 3.40 (s, 3H), 2.98 – 2.94 (m, 1H), 2.84 (t, *J* = 6.4 Hz, 2H), 2.34 (s, 3H).; **^{13}C NMR** (100 MHz, $CDCl_3$)δ 206.5, 151.6, 143.4, 142.9, 137.0, 136.9, 135.7, 129.6, 128.5, 127.4, 127.2, 126.1, 125.9, 123.7, 123.0, 121.0, 120.7, 112.1 (x 2), 58.3, 42.7, 33.0, 28.1, 21.0.; **HRMS** (ESI, m/z) calcd for $C_{24}H_{21}NNaO$ $[M + Na]^+$ 362.1521, found 362.1537.

2-(10-methyl-9,10-dihydroacridin-9-yl)-2-nitro-1-phenylethanone (6ae):



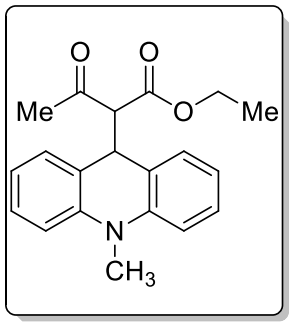
Yield 56% (40 mg); Yellow solid; **R_f** 0.15 (pet ether/ethyl acetate = 20:1); **eluent composition** petroleum ether/ethyl acetate = 20:1; **mp**132-134 ºC **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.64 (d, *J* =1.2 Hz, 1H), 7.62 (d, *J* =1.2 Hz, 1H), 7.50 – 7.46 (m, 1H), 7.37 – 7.33 (m, 1H), 7.34 – 7.28 (comp, 3H), 7.20 (dd, *J* =7.6 Hz, 1.2 Hz, 1H), 7.08 – 7.00 (comp, 3H), 6.84 (d, *J* = 8.0 Hz, 1H), 6.77 (app td, *J* = 7.6, 0.8 Hz, 1H), 6.25 (d, *J* = 10.0 Hz, 1H), 5.29 (d, J = 10 Hz, 1H), 3.46 (s, 3H).; **^{13}C NMR** (100 MHz, $CDCl_3$)) δ 188.0, 143.5, 143.0, 135.0, 134.2, 129.9, 128.9, 128.6 (x 2), 128.6 (x 3), 128.4, 121.8, 121.4 (x 2), 119.4, 112.6, 112.5, 88.0, 45.8, 33.1.; **HRMS** (ESI, m/z) calcd for $C_{22}H_{18}N_2O_3$ $[M]^+$ 358.1317, found 358.1313.

Methyl 2-(10-methyl-9,10-dihydroacridin-9-yl)-3-oxobutanoate (6af):



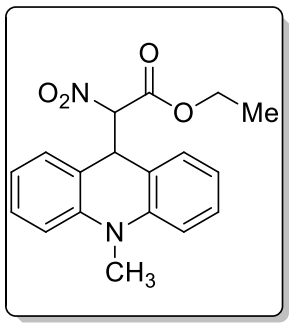
Yield 71% (44 mg); White solid; **R_f** 0.2 (pet ether/ethyl acetate = 20:1); **eluent composition** petroleum ether/ethyl acetate = 20:1; **mp**126-128 ºC **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.29 – 7.19 (comp, 4H), 6.98 – 6.91 (comp, 4H), 4.79 (d, *J* = 10.4 Hz, 1H), 3.89 (d, J = 10.4 Hz, 1H), 3.52 (s, 3H), 3.45 (s, 3H), 1.79 (s, 3H).; **^{13}C NMR** (100 MHz, $CDCl_3$)) δ 202.2, 167.9, 143.0 129.0, 128.6, 127.7, 127.6, 123.7, 123.3, 121.0, 120.9, 112.3 (X 3), 62.1, 52.2, 44.1, 33.1, 31.5.; **HRMS** (ESI, m/z) calcd for $C_{19}H_{19}NNaO_3$ $[M + Na]^+$ 332.1263, found 332.1284.

Ethyl 2-(10-methyl-9,10-dihydroacridin-9-yl)-3-oxobutanoate (6ag):



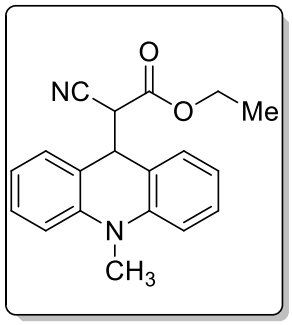
Yield 46% (30 mg); White solid; **R_f** 0.25 (pet ether/ethyl acetate = 10:1); **eluent composition** petroleum ether/ethyl acetate = 10:1; **mp**116-118 ºC **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.29 (dd, *J* = 7.4, 1.4 Hz, 1H), 7.25 – 7.20 (comp, 3H), 6.98 – 6.91 (comp, 4H), 4.79 (d, *J* = 10.4 Hz, 1H), 4.00 - 3.92 (m, 2H), 3.86 (d, *J* = 10.4 Hz, 1H), 3.45 (s, 3H), 1.81 (s, 3H), 1.07 (q, *J* = 7.2 Hz, 3H).; **^{13}C NMR** (100 MHz, $CDCl_3$)) δ 202.2, 167.5, 143.1, 143.0, 129.0, 128.7, 127.6, 127.6, 123.8, 123.5, 121.0, 120.9, 112.3, 112.2, 62.3, 61.2, 44.0, 33.1, 31.3, 13.9.; **HRMS** (ESI, m/z) calcd for $C_{20}H_{21}N_2NaO_3$ $[M + Na]^+$ 346.1419, found 346.1429.

Ethyl 2-(10-methyl-9,10-dihydroacridin-9-yl)-2-nitroacetate (6ah):



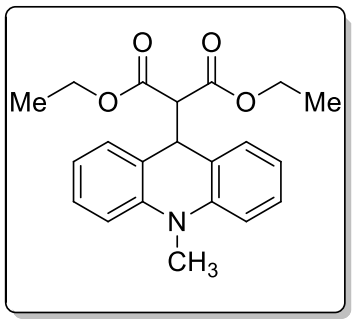
Yield 69% (45 mg); Colourless solid; **R_f** 0.1 (pet ether/ethyl acetate = 20:1); **eluent composition** petroleum ether/ethyl acetate = 20:1; **mp**128-130 ºC **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.33 – 7.28 (comp, 4H), 7.02 – 6.96 (comp, 4H), 5.16 – 5.04 (comp, 2H), 4.11 – 3.94 (m, 2H), 3.47 (s, 3H), 1.07 (t, J = 7.1 Hz, 3H).; **^{13}C NMR** (100 MHz, $CDCl_3$)) δ 163.0, 143.3, 142.7, 129.1, 128.8, 128.7 (x 2), 121.6, 121.2, 120.7, 119.4, 112.6 (x 2), 88.8, 62.8, 45.6, 33.2, 13.6.; **HRMS** (ESI, m/z) calcd for $C_{18}H_{18}N_2KO_2$ $[M + K]^+$ 365.0904, found 365.0930.

Ethyl 2-cyano-2-(10-methyl-9,10-dihydroacridin-9-yl)acetate (6ai):



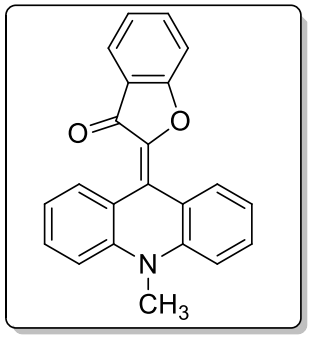
Yield 65% (40 mg); Yellow solid; **R_f** 0.10 (pet ether/ethyl acetate = 10:1); **eluent composition** petroleum ether/ethyl acetate = 10:1; **mp** 68-70 °C **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.39 – 7.28 (comp, 3H), 7.18 (dd, *J* = 7.2, 1.2 Hz, 1H), 7.06 – 6.94 (comp, 4H), 4.66 (d, *J* = 8.8 Hz, 1H), 4.12 – 4.00 (m, 2H), 3.54 (d, *J* = 8.8 Hz, 1H), 3.45 (s, 3H), 1.14 (t, *J* = 7.2 Hz, 3H).; **^{13}C NMR** (100 MHz, $CDCl_3$)) δ 164.9, 142.7, 142.5, 128.9, 128.7 (x 2), 128.3, 121.2, 121.15, 121.07, 121.0, 115.6, 112.8, 112.7, 62.6, 45.5, 43.7, 33.2, 13.8.; **HRMS** (ESI, m/z) calcd for $C_{19}H_{18}N_2O_2$ $[M + H]^+$ 307.1447, found 307.1450.

Diethyl 2-(10-methyl-9,10-dihydroacridin-9-yl)malonate (6aj):



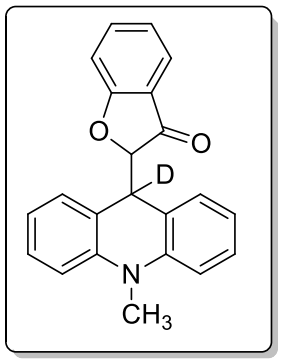
Yield 63% (44 mg); Brown solid; **R_f** 0.30 (pet ether/ethyl acetate = 10:1); **eluent composition** petroleum ether/ethyl acetate = 10:1; **mp** 70-72 °C **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.28 (dd, *J* = 7.4, 1.5 Hz, 2H), 7.26 – 7.21 (comp, 2H), 6.98 – 6.90 (comp, 4H), 4.77 (d, *J* = 10.6 Hz, 1H), 4.04 – 3.89 (comp, 4H), 3.58 (d, *J* = 10.6 Hz, 1H), 3.44 (s, 3H), 1.06 (t, *J* = 7.1 Hz, 6H).; **^{13}C NMR** (100 MHz, $CDCl_3$)) δ 167.7, 143.1, 128.8, 127.8 123.7, 120.8, 112.3, 61.3, 56.0, 44.2, 33.2, 14.0,; **HRMS** (ESI, m/z) calcd for $C_{21}H_{23}NNaO_4$ $[M + Na]^+$ 376.1525, found 376.1537.

2-(10-methylacridin-9(10H)-ylidene)benzofuran-3(2H)-one (7):



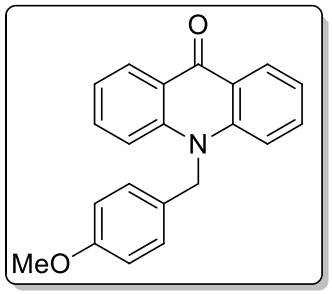
Yield 58% (38 mg); Red solid; **R_f** 0.10 (pet ether/ethyl acetate = 10:1); **eluent composition** petroleum ether/ethyl acetate = 10:1; **mp** 128-130 °C, **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.43 (dd, *J* = 8.0, 1.2 Hz, 2H), 7.81 (d, *J* = 7.6 Hz, 1H), 7.56 – 7.53 (comp, 3H), 7.31 – 7.25 (comp, 5H), 7.17 – 7.14 (m, 1H), 3.74 (s, 3H).; **^{13}C NMR** (100 MHz, $CDCl_3$)) δ 163.3, 141.5, 139.9, 134.7 (X 2), 130.8 (X 2), 130.7 (X 2), 124.1 (X 2), 123.9 , 122.5 (X 2), 120.4 (X 2), 112.8 (X 3), 112.4 (X 2) , 34.4.; **HRMS** (ESI, m/z) calcd for $C_{22}H_{15}NO_2$ $[M + H]^+$ 326.1181, found 326.1179.

3aa-d_1:



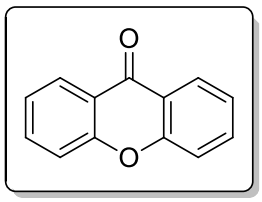
Yield 61% (40 mg); Yellow solid; **R_f** 0.30 (pet ether/ethyl acetate = 10:1); **eluent composition** petroleum ether/ethyl acetate = 10:1; **mp** 133-135 °C **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.51 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.45 – 7.40 (m, 1H), 7.31 – 7.25 (comp, 2H), 7.13 – 7.08 (comp, 2H), 7.03 – 6.95 (comp, 2H), 6.93 – 6.89 (m, 1H), 6.85 (dd, *J* = 13.3, 8.2 Hz, 2H), 6.76 (app td, *J* = 7.4, 1.0 Hz, 1H), 4.61 (s, 1H), 3.44 (s, 3H).; **^{13}C NMR** (100 MHz, $CDCl_3$)) δ 200.0, 172.8, 143.4, 143.2, 137.5, 129.0, 128.9, 128.1, 127.9, 123.8, 121.8, 121.7, 121.4, 120.6, 120.2, 119.5, 112.8, 112.4, 112.3, 89.7, 50.0 – 45.3 (m), 33.2.; **HRMS** (ESI, m/z) calcd for $C_{22}H_{16}DNO_2$ $[M + H]^+$ 329.1416, found 329.1393.

10-(4-methoxybenzyl)acridin-9(10*H*)-one (9):



Yield 50% (30 mg); Brown solid; **R_f** 0.20 (pet ether/ethyl acetate = 5:1); **eluent composition** petroleum ether/ethyl acetate = 5:1; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.60 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.66 – 7.62 (comp, 2H), 7.38 (d, *J* = 8.7 Hz, 1H), 7.32 – 7.28 (comp, 2H), 7.13 (d, *J* = 8.7 Hz, 2H), 6.89 – 6.87 (comp, 2H), 5.55 (s, 2H), 3.78 (s, 3H).; **^{13}C NMR** (100 MHz, $CDCl_3$)) δ 178.3, 159.2, 142.6 (X 2), 134.0 (X 2), 127.8 (X 2), 127.2, 126.8 (X 2), 122.6 (X 2), 121.6 (X 2), 115.2 (X 2), 114.6 (X 2), 55.3, 50.3; **HRMS** (ESI, m/z) calcd for $C_{21}H_{17}NO_2$ $[M + H]^+$ 316.1338, found 316.1334.

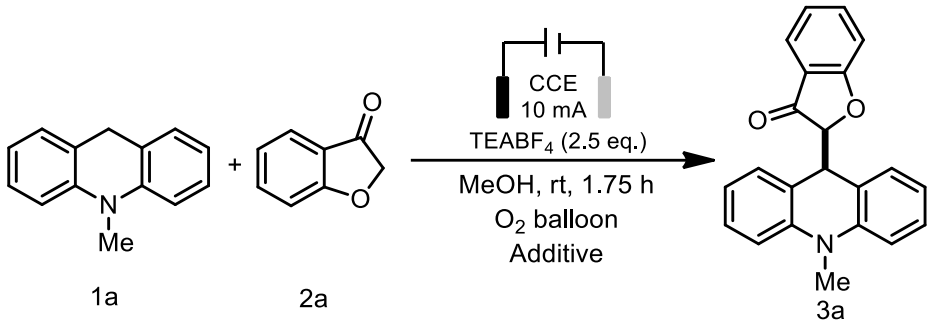
9*H*-xanthen-9-oneone (10):



Yield 31% (12 mg); White solid; **R_f** 0.30 (pet ether/ethyl acetate = 5:1); **eluent composition** petroleum ether/ethyl acetate = 5:1; **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.35 (dd, *J* = 8.0, 1.7 Hz, 2H), 7.74 (ddd, *J* = 8.7, 7.1, 1.7 Hz, 2H), 7.51 (d, *J* = 8.4 Hz, 2H), 7.42 – 7.36 (comp, 2H).

Mechanistic studies:

Radical scavenging experiments:

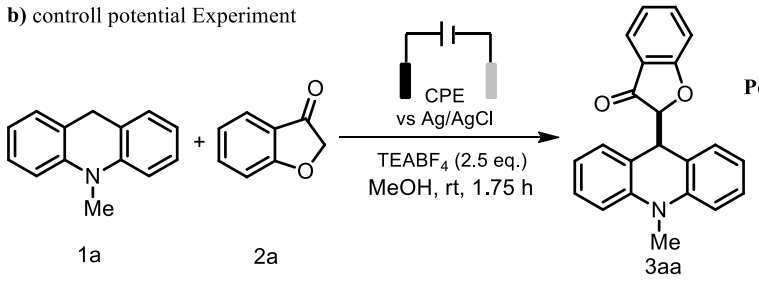


Exp. No	Additive	Equiv.	Yield of 3a
1	-	-	84%
2	TEMPO	2.0	82%
3	BHT	2.0	82%

A 5 mL oven-dried electrasyn vial was charged with10-methyl-9,10-dihydroacridine**1a** (39 mg, 0.2 mmol), 3-coumaranone**2a** (35 mg, 0.26 mmol), $TEABF_4$ (0.5 mmol, 2.5 equiv,), radical scavengers (2 equiv.) and MeOH (2.0 mL). The vial was equipped with a graphite rod as anode (immersed surface area 1.2 x 0.5 cm^2) and platinum plate as the cathode (immersed surface area 1.2 x 0.5 cm^2), the distance between the electrodes was 0.6 cm.The resulting mixture was stirred and electrolyzed at a constant current of 10 mA at ambient temperature for 1.75 h. with O_2-balloon.After completion of the reaction indicated by TLC the volatiles was evaporated in vacuum and the crude product was directly purified by column chromatography using ethyl acetate / petroleum ether (5%) to afford product **3aa.**

Control potential experiment:

b) controll potential Experiment



Potential (V)	Condition	Yield (%)
0.8	inert	nr
1.2	inert	trace
1.2	O_2	30
3.0	inert	55
3.0	O_2	70

A 5 mL oven-dried electrasyn vial was charged with 10-methyl-9,10-dihydroacridine **1a** (39 mg, 0.2 mmol), 3-coumaranone **2a** (35 mg, 0.26 mmol), $TEABF_4$ (0.5 mmol, 2.5 equiv,) and MeOH (2.0 mL). The vial was equipped with a graphite rod as anode, platinum plate as the cathode and Ag/AgCl as reference electrode. The resulting mixture was stirred and electrolyzed at a constant potential at room temperature for 1.75 h. After completion of the reaction indicated by TLC the volatiles was evaporated in vacuum and the crude product was directly purified by column chromatography using ethyl acetate / petroleum ether (5%) to afford product **3aa.**

Cyclic voltammetry experiments:

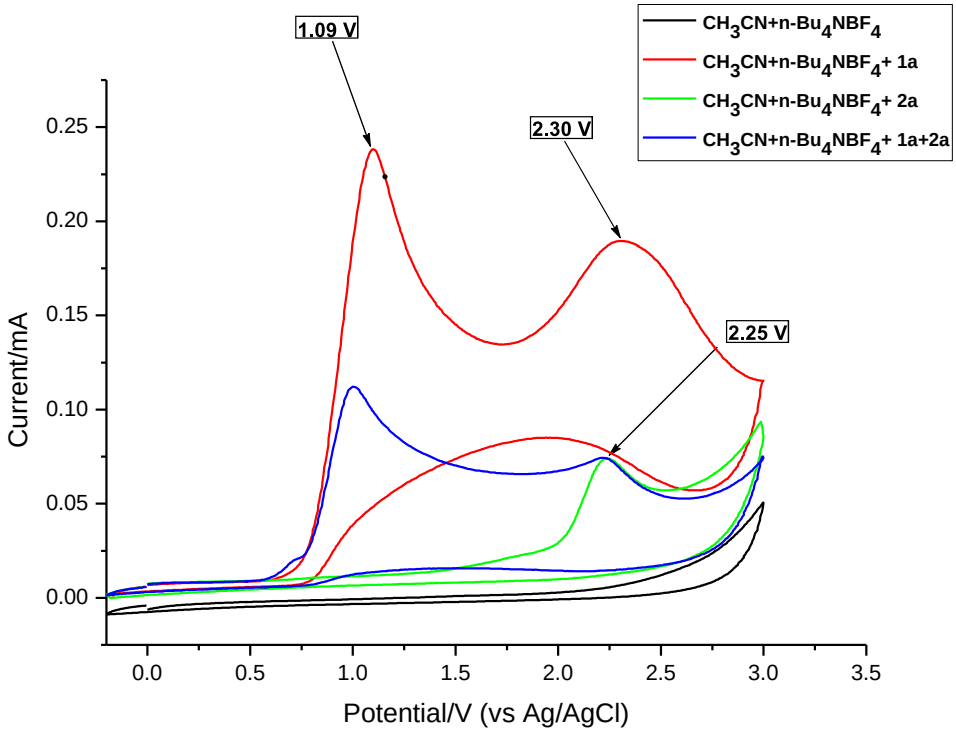
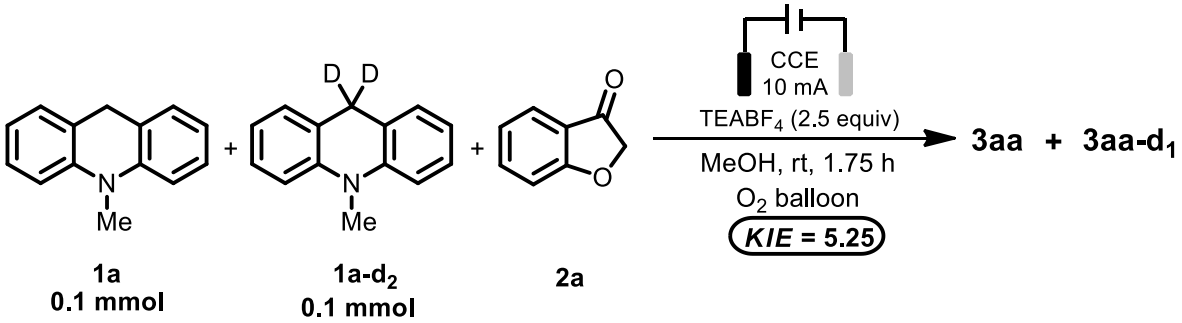


Figure S5. Cyclic Voltammogram recorded with K-Lite 1.2 work workstation at room temperature in MeCN with 0.04 M $TBABF_4$ and 1a (20 mM), 2a (20 mM), 1a+2a (20 mM). A glassy-carbon disk was used as a working electrode. Pt-disk and Ag/AgCl was used as counter and reference electrode, respectively. Sweeprate was 50 mV/s.

Kinetic isotope effect experiment:

Kinetic isotope experiments (KIE) were performed between acridine (1a) and acridine-d2 (1a-d2) to check whether the C–H abstraction step of the reaction is involved in the rate–determining step (rds) of the reaction or not. Intermolecular competitive experiment suggested a high kH/kD value of 5.25 from 1H NMR spectroscopy. This result indicated that the C–H cleavage step might be involved in the rate-determining step of the reaction.

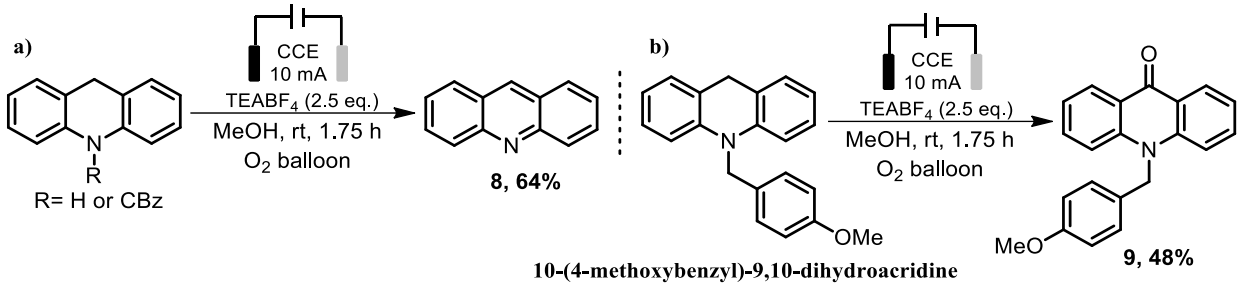
Procedure for competitive experiment between 1a and 1a-d_2:



A 5 mL oven-dried electrasyn vial was charged with 10-methyl-9,10-dihydroacridine **1a** (39 mg, 0.2 mmol), 3-coumaranone **2a** (35 mg, 0.26 mmol), $TEABF_4$ (0.5 mmol, 2.5 equiv,) and MeOH (2.0 mL). The vial was equipped with graphite rod as anode (immersed surface area 1.2 x 0.5 cm^2)

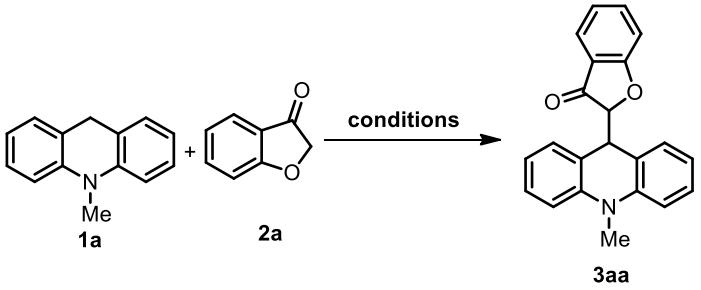
and platinum plate as the cathode (immersed surface area 1.2 x 0.5 cm^2), the distance between the electrodes was 0.6 cm. The resulting mixture was stirred and electrolyzed at a constant current of 10 mA at ambient temperature for 15 min. with O_2-balloon. Then reaction mixture was concentrated in vacuum and the crude product was directly purified by column chromatography using ethyl acetate/petroleum ether (5%) as eluent to afford recovered starting material and product. The ratio of **3aa** and **3aa**-d_1 was determined by 1H NMR spectroscopy. Primary kinetic isotopic effect (KIE) was found be $k_H/k_D \approx 0.84/0.16 \approx 5.3$. 1H NMR spectroscopy of recovered starting material showed that the ratio of **1a:1a**-d_2 = 25:75.

Fate of 9,10-dihydroacridine and N-protected 9,10-dihydroacridine in standard electrochemical conditions:



The above reactions **a** and **b** were performed in similar way. A 5 mL oven-dried electrasyn vial was charged with 0.2 mmol of starting materials, $TEABF_4$ (0.5 mmol, 2.5 equiv,) and MeOH (2.0 mL). The vial was equipped with graphite rod as anode and platinum plate as the cathode. The resulting mixture was stirred and electrolyzed at a constant current of 10 mA at ambient temperature for 1.75 h. with O_2-balloon. After completion of the reaction indicated by TLC the volatiles were evaporated in vacuum and the crude product was directly purified by column chromatography using ethyl acetate / petroleum ether (5%) to afford product **8** and **9**.

Table S4: Comparison with non-electrochemical methods



Entry	Conditions	Yield of 3aa
1	1a (0.2 mmol, 1 equiv), 2a (0.26 mmol, 1.3 equiv), Eosin Y (10 mol%), MeOH (2 mL), blue LED (455 nm), rt, 12 h	trace
2	1a (0.2 mmol, 1 equiv), 2a (0.26 mmol, 1.3 equiv), O_2 balloon, MeOH (2 mL), blue LED (455 nm), rt, 12 h	trace
3	1a (0.2 mmol, 1 equiv), 2a (0.26 mmol, 1.3 equiv), DDQ (2 equiv), MeOH (2 mL), rt, 24 h	23%
4	1a (0.2 mmol, 1 equiv), 2a (0.26 mmol, 1.3 equiv), TBHP (2 equiv), MeOH (2 mL), rt, 24 h	43%
5	Optimized electrochemical condition	84%

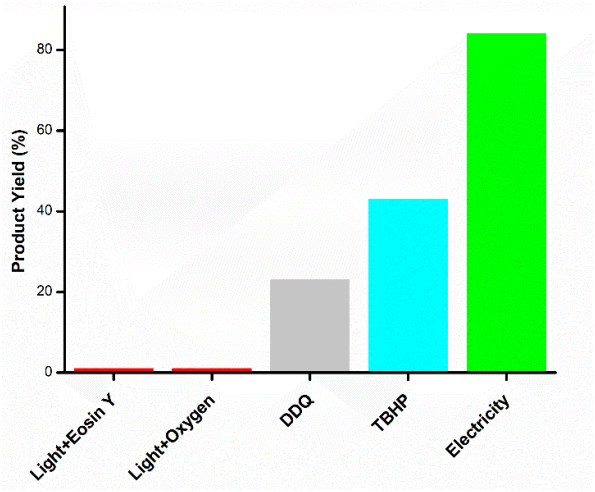


Figure S6. Effect of common oxidants on the product yield.

Fluorescence lifetime of compounds 3aa, 5ba, 3ae, 6af and 3db in Acetonitrile.

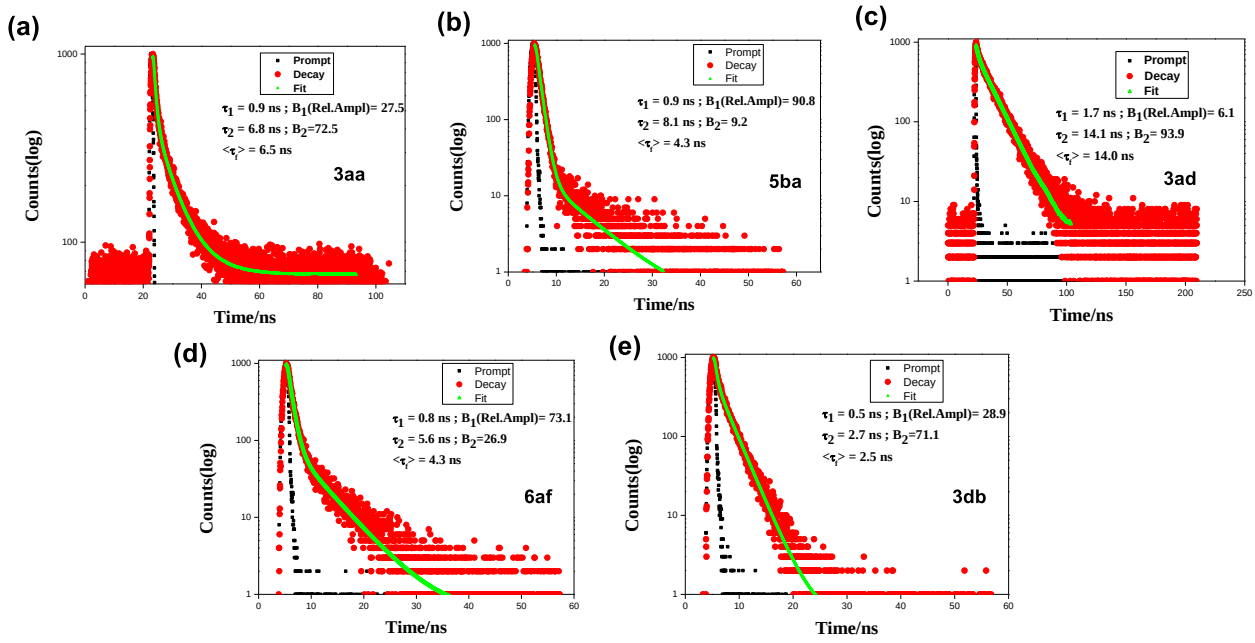


Figure S7. Fluorescence decay curves of compounds (a) 3aa, (b) 5ba, (c) 3ad, (d) 6af and (e) 3db in acetonitrile at room temperature. Green line denotes the curve of best fit by a biexponential function.

Table S5. Fluorescence lifetime of compounds 3aa, 5ba, 3ad, 6af and 3db in Acetonitrile.

Compound	τ_1/ns	τ_2/ns	$<\tau_f$/ns$>$ [a]	χ^2
3aa	0.9	6.8	6.5	1.11
5ba	0.9	8.1	4.3	1.01
3ad	1.7	14.1	14.0	1.17
6af	0.8	5.6	4.3	0.96
3db	0.5	2.7	2.5	0.92

[a]The area-weighted mean fluorescence lifetime was calculated as follows: $<\tau_f>=\Sigma(A_n\tau_n^2)/\Sigma(A_n\tau_n)$ where A_n is the coefficient of exponential function of the n-th component. [6]

Table S6. Absorption, emission and Relative quantum yield data of 9- Substituted Fluorescent Acridines (Acetonitrile)

Entry	Compound Name	Absorption (nm)	Emission (nm)	Stokes shift (nm)	Relative Quantum Yield (Φ_f)
1	**1a**	284	382	98	0.22
2	**1b**	292	410	118	0.09
3	**3aa**	287	490	203	0.55
4	**5ba**	293	411	118	0.46
5	**3ad**	288	485	197	0.09
6	**6af**	280	484	204	0.33
7	**1d**	289	384	95	0.03
8	**3db**	287	495	208	0.06

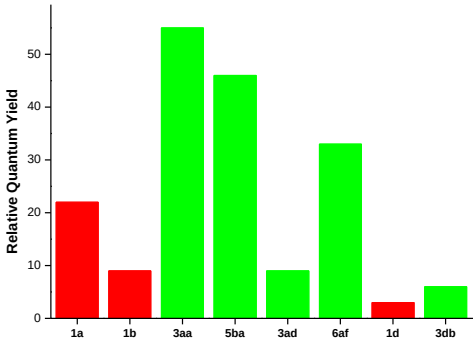


Figure S8. Relative Quantum Yield Comparison

Fluorescence studies:

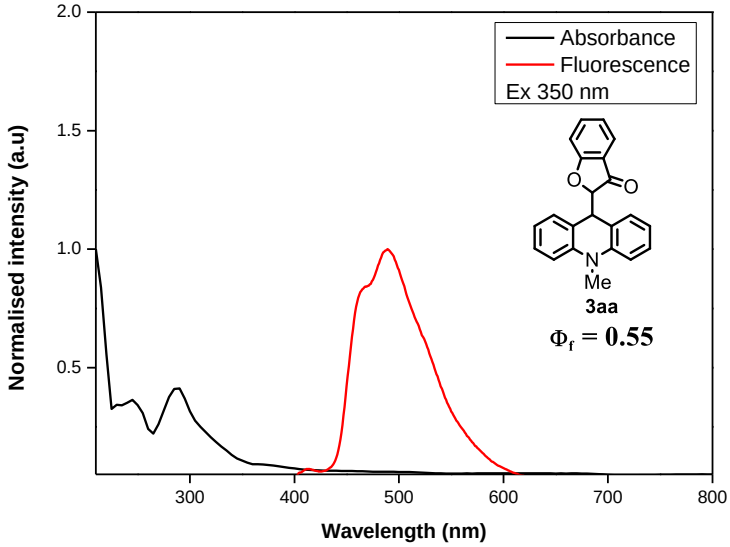


Figure S9. Absorption (black, left) and fluorescence (red, right) spectra of compound 3aa (50 μM) in Acetonitrile.

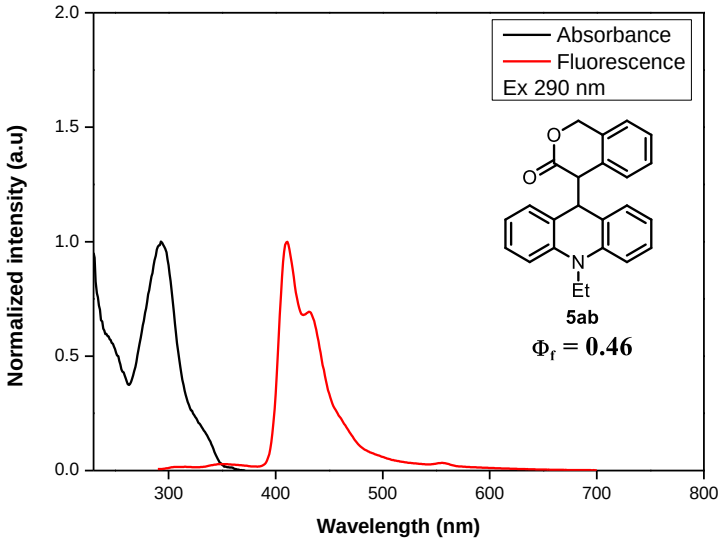


Figure S10. Absorption (black, left) and fluorescence (red, right) spectra of compound 5ba (50 μM) in Acetonitrile.

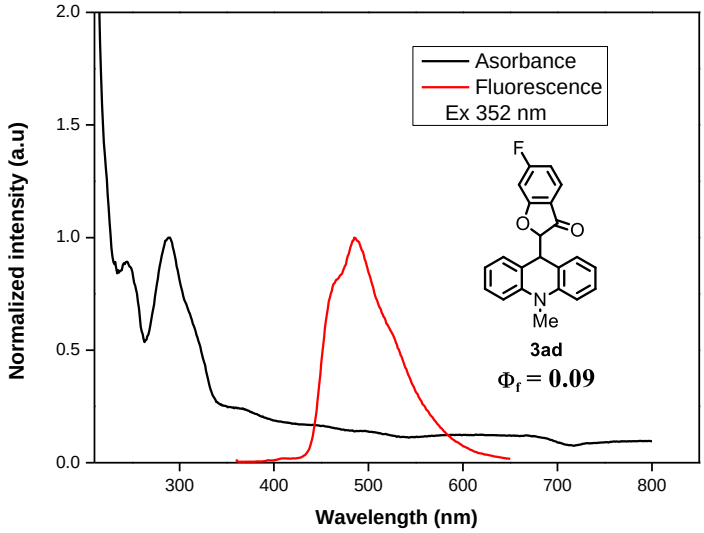


Figure S11. Absorption (black, left) and fluorescence (red, right) spectra of compound 3ad (50 μM) in Acetonitrile.

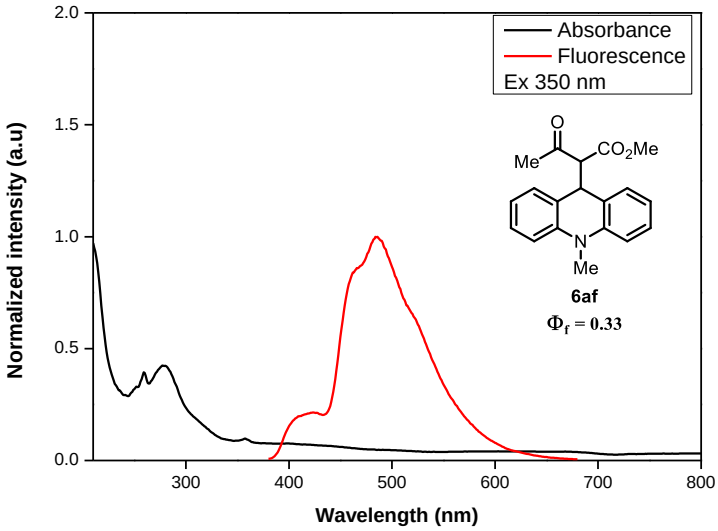


Figure S12. Absorption (black, left) and fluorescence (red, right) spectra of compound 6af (50 μM) in Acetonitrile.

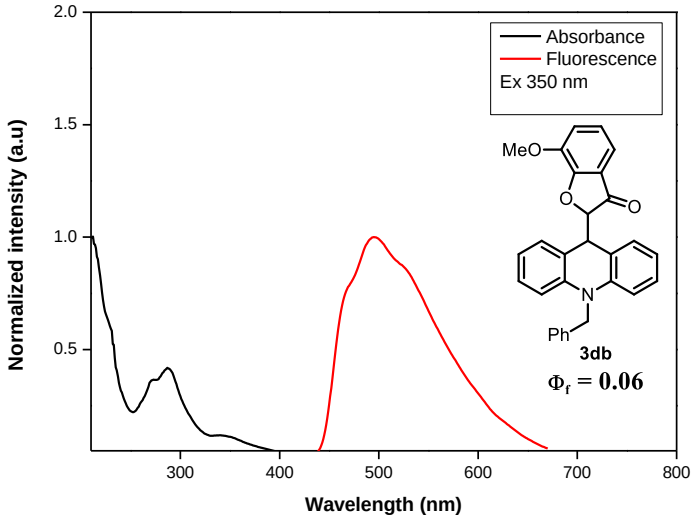


Figure S13. Absorption (black, left) and fluorescence (red, right) spectra of compound 3db (50 μM) in Acetonitrile.

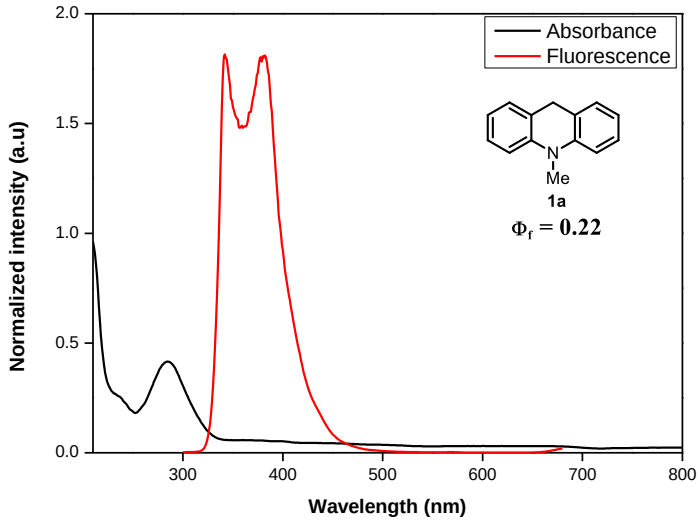


Figure S14. Absorption (black, left) and fluorescence (red, right) spectra of compound 1a (50 μM) in Acetonitrile.

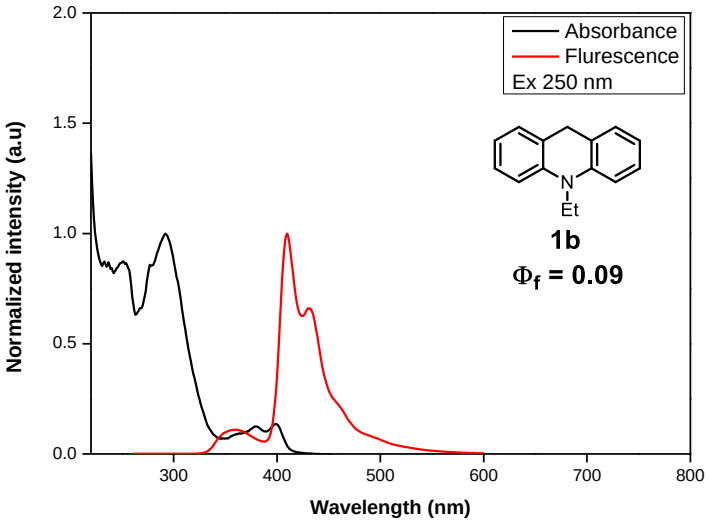


Figure S15. Absorption (black, left) and fluorescence (red, right) spectra of compound 1b (50 μM) in Acetonitrile.

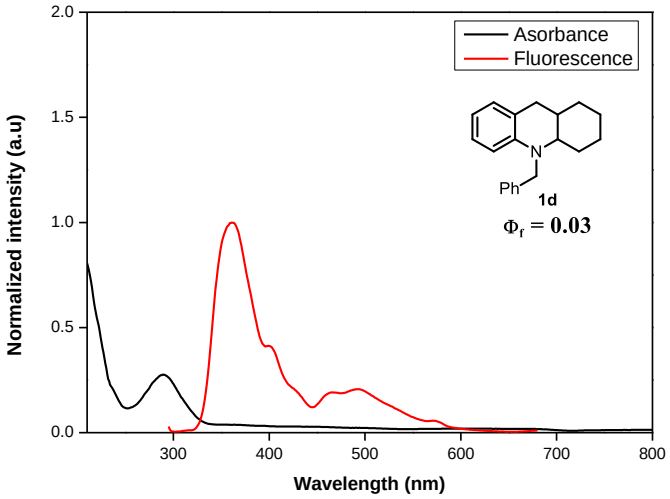


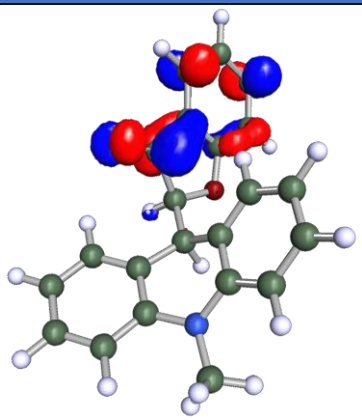
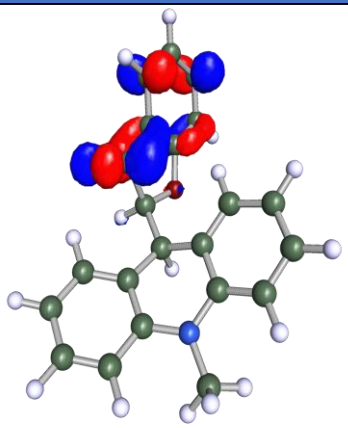
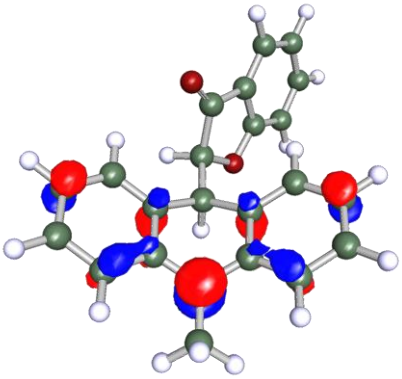
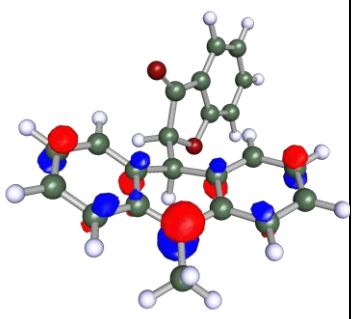
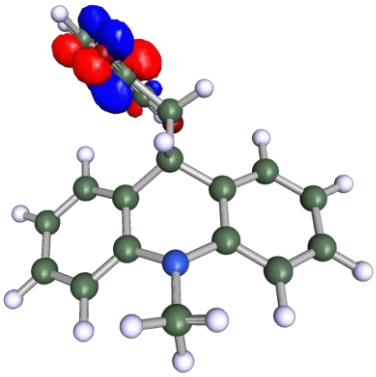
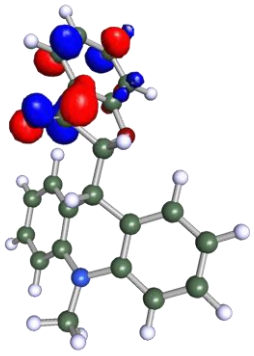
Figure S16. Absorption (black, left) and fluorescence (red, right) spectra of compound 1d (50 μM) in Acetonitrile.

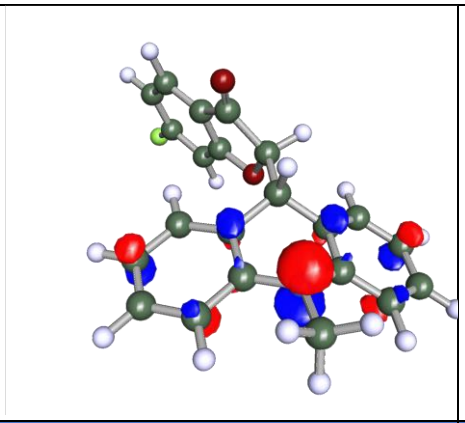
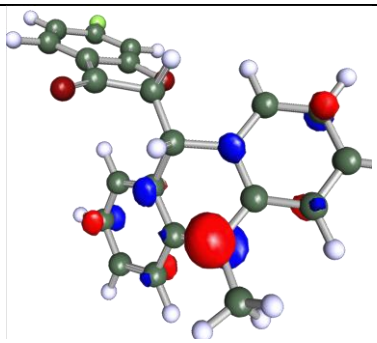
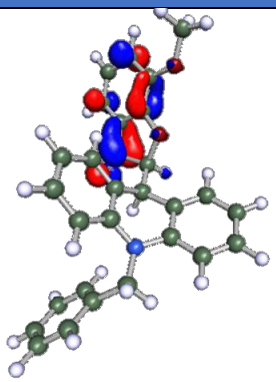
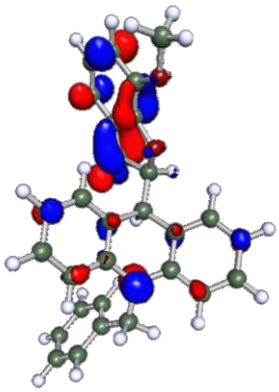
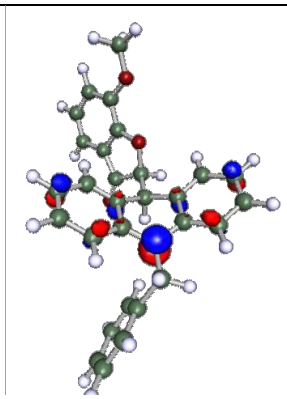
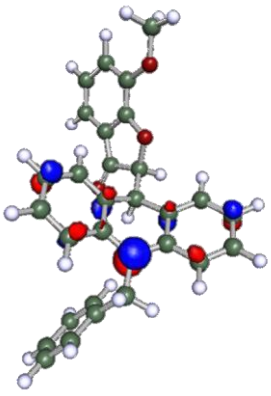
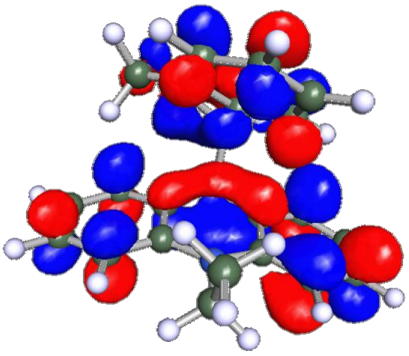
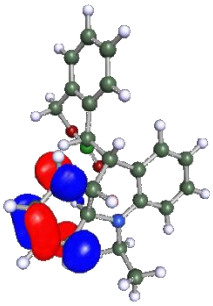
Table S7. Theoretical Calculations:

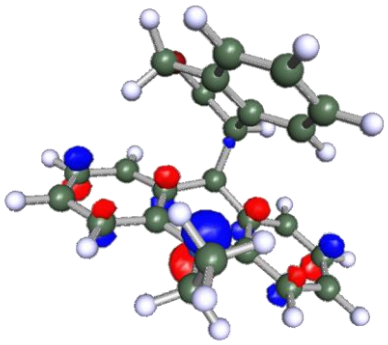
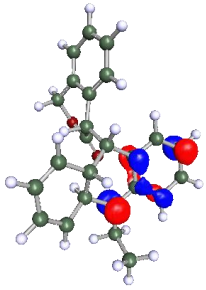
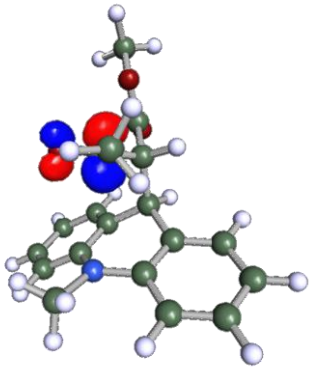
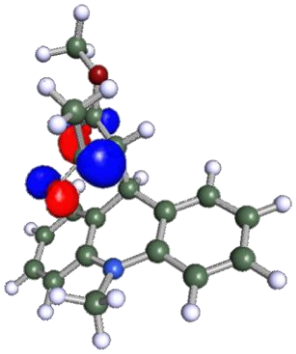
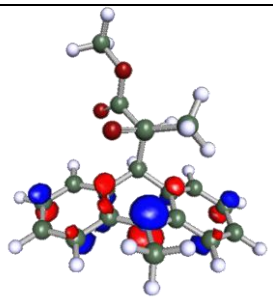
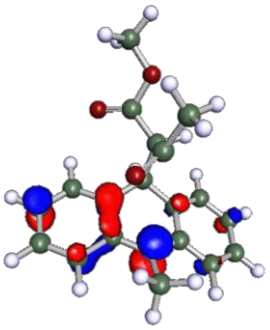
The geometrical optimization was carried out at the B3LYP/def2-SVP level of theory implemented on Turbomole (TmoleX2023) in gas phase. Convergence at a local minimum structure in the ground state and excited state was confirmed.

Energy level	3aa		5ba		3ad		6af		3bd	
	Ground State Energy (ev)	Excited State Energy (ev)	Ground State Energy (ev)	Excited State Energy (ev)	Ground State Energy (ev)	Excited State Energy (ev)	Ground State Energy (ev)	Excited State Energy (ev)	Ground State Energy (ev)	Excited State Energy (ev)
LUMO+1	-0.2966	-0.4217	-0.5360	-0.6748	-0.5714	-0.6911	-0.3945	-0.3428	-0.4027	-0.3646
LUMO	-1.8063	-2.2729	-0.7969	-1.8804	-1.8332	-2.2885	-0.5199	-1.8699	-1.6081	-2.0999
HOMO	-5.3013	-4.9660	-5.279	-4.4912	-5.3701	-5.0695	-5.2380	-4.7342	-5.3349	-4.99522
HOMO-1	-6.340	-6.4137	-6.604	-6.0354	-6.6422	-6.6205	-6.4028	-6.0926	-6.0382	-6.2749
E_{gap} (HOMO-LUMO)	**3.495**	**2.6931**	**4.4815**	**2.611**	**3.5369**	**2.7809**	**4.71807**	**2.864**	**3.72686**	**2.89526**

Frontier molecular orbital of acridanes both in ground state and in excited state (HOMO and LUMO) by DFT (Turbomole):

	Ground state	Energy (ev)	Excited State	Energy (ev)
3aa				
LUMO		-1.8063		-2.272
HOMO		-5.3013		-4.966
3ad				
LUMO		-1.8332		-2.2884

HOMO		-5.37015		-5.0695
3db				
LUMO		-1.6081		-2.0999
HOMO		-5.336		-4.9952
5ba				
LUMO		-0.7969		-1.8804

HOMO		-5.2784		-4.4912
6af				
LUMO		-0.5199		-1.8699
HOMO		-5.2380		-4.7342

Cartesian coordinates and Cartesian gradients and Energy for the compounds 3aa, 5ba, 3ad, 6af and 3bd

The geometrical optimization was carried out at the B3LYP/def2-SVP level of theory implemented on Turbomole (TmoleX2023) in gas phase. Convergence at a local minimum structure in the ground state and excited state was confirmed.

For the compound **3aa**, ground state: Cartesian coordinates and Cartesian gradients and Energy:

No Imaginary frequency was observed.

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ATOM	CARTESIAN COORDINATES		
1 c	-1.60378069257824	-5.34581088805835	0.37905920980765
2 c	-2.19899346854222	-2.83151624166591	0.91899614740490
3 c	-4.76543002741024	-2.13707061076930	1.22074959380156
4 c	-6.65325437372587	-4.00110187669224	1.09938410647897
5 c	-6.00455267666260	-6.52069613327820	0.64529166985805
6 c	-3.48836465235207	-7.19780930109847	0.25106654390711
7 n	-5.32792632054956	0.44334849064124	1.58142829267982
8 c	-3.80041599286873	2.21190079235408	0.29653543949494
9 c	-1.20058517584691	1.64844093964885	-0.00423484328659
10 c	-0.30613156674216	-0.71120311243540	1.37519091562327
11 c	2.47130958667892	-1.48013335727657	1.11652652330752
12 o	4.06836726021131	0.33811536105652	2.38643968597362
13 c	6.14171685054488	0.75373713749526	0.95199533722826
14 c	6.08315432355456	-0.48434019598647	-1.39058724185523
15 c	3.68736449649918	-1.89125673899706	-1.51637800657958
16 o	2.84826692373192	-3.19354205306531	-3.20094636300607
17 c	8.06862091588729	-0.22441424762969	-3.12092771465343

18 c	10.11993063662903	1.28462690135293	-2.44740238167056
19 c	10.15769178330246	2.51390249884296	-0.08272792802334
20 c	8.18295365378623	2.27815542807574	1.65417231564694
21 c	0.32283188253056	3.32320746343127	-1.35859927715048
22 c	-0.65996608516485	5.56111681984329	-2.37086973504030
23 c	-3.20890356492153	6.13194316373441	-2.02397276321284
24 c	-4.78219012598007	4.46361326241188	-0.71384615082824
25 c	-7.84782705314570	1.16899361197491	2.36975851302887
26 h	0.35036726671392	-5.88885529203412	0.01683424737535
27 h	-8.63943081150243	-3.49535118862378	1.31040524935777
28 h	-7.49473958062508	-7.94935736654822	0.55670483509447
29 h	-2.97986382855333	-9.15650504306158	-0.15846996165657
30 h	-0.49156788447685	-0.24668475403968	3.41491039059102
31 h	2.71404063752392	-3.28223461483656	2.14499846732804
32 h	7.97940650708131	-1.19702056290639	-4.94090936559865
33 h	11.70866769239859	1.52217266209770	-3.74397750035387
34 h	11.78345886337061	3.69059138669661	0.41093101747151
35 h	8.20905692786204	3.23750108843004	3.47998356399544
36 h	2.32607158925893	2.92334870707759	-1.61646362638260
37 h	0.57486206840257	6.85094950204140	-3.40733947993508
38 h	-4.00281195815256	7.87412199486996	-2.80091855390891
39 h	-6.78507458955440	4.90770330357673	-0.52479910730126
40 h	-8.50431846472718	-0.11861474377726	3.86151280803399
41 h	-7.79981198017448	3.08741902520299	3.16393971138601
42 h	-9.25219899171090	1.13860878192388	0.81655541556806

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ATOM		CARTESIAN GRADIENTS	
1 c	0.00002970249289	0.00008765915247	0.00013166614721
2 c	-0.00000242379511	0.00000138287909	-0.00004964437489
3 c	-0.00004767157195	0.00003569438316	0.00014993225203
4 c	0.00000679472702	-0.00001098558109	-0.00005665363699
5 c	-0.00001500987834	-0.00000681040153	0.00000139031438
6 c	0.00000754958523	-0.00001714933710	-0.00013859805957
7 n	0.00005404809174	-0.00007163540134	-0.00001357865462
8 c	-0.00007639689045	0.00004483339417	0.00005041087508
9 c	0.00000143824153	-0.00006741908218	-0.00002814330462
10 c	-0.00000493377014	-0.00001493746279	0.00007869476780
11 c	0.00002655776351	-0.00003958230120	0.00003591190088
12 o	0.00006745262284	-0.00008098640747	0.00002548232196
13 c	-0.00014646228341	0.00020594420404	-0.00011630715256
14 c	-0.00003204463487	0.00005704369421	-0.00001186279610
15 c	0.00004395249284	-0.00004472383551	0.00001362980508
16 o	-0.00002733224213	-0.00000395959008	-0.00002244779902
17 c	0.00002877023522	-0.00011431978225	0.00005469821913
18 c	-0.00000551529514	0.00001406889570	-0.00001250396683
19 c	0.00003830389146	-0.00005009022775	0.00003473335263
20 c	0.00001648474498	-0.00009503354199	0.00005607176269
21 c	0.00001204403449	0.00001339035519	-0.00001991159094
22 c	-0.00001185993360	0.00000262663078	-0.00001378058182
23 c	0.00000191333457	0.00001810126856	-0.00001016634771
24 c	0.00003695607035	0.00004240333600	-0.00003408632655
25 c	0.00000294566224	0.00000343249284	0.00003690443501

26 h	-0.00001184426338	-0.00002705134508	-0.00008911789021
27 h	-0.00001191285119	0.00001243961526	-0.00009820982491
28 h	-0.00000170796259	-0.00002719759433	0.00010888548277
29 h	0.00000623581325	-0.00001373547071	0.00002127391738
30 h	-0.00002274676094	-0.00000626796379	0.00004076710975
31 h	-0.00001527343238	0.00001676807968	0.00001647842626
32 h	-0.00001844610935	0.00002831297105	-0.00003722775134
33 h	0.00001201859116	-0.00000894564650	-0.00001679157024
34 h	0.00001945395553	-0.00000799030351	0.00001734111285
35 h	-0.00003525501549	0.00006819339514	-0.00001784877595
36 h	-0.00004666020107	-0.00000858316577	-0.00005680515082
37 h	0.00002120617630	0.00003086615621	0.00003819496430
38 h	-0.00000223566346	0.00001564886274	-0.00000495654929
39 h	-0.00000384689444	-0.00001405646734	-0.00003356446774
40 h	-0.00000183670116	0.00000347346221	0.00000509475836
41 h	0.00000483772821	0.00000084463288	0.00000804511890
42 h	-0.00000974709811	-0.00000033267653	-0.00000367074043

****

norm of actual CARTESIAN gradient: 5.54849E-04

norm of actual INTERNAL gradient: 9.94736E-04

ENERGY =   -1052.3883116500 a.u.; # of cycle =   11

Approximate Hessian read from $hessapprox data section

Hessian updated according to BFGS formula

Number of zero Hessian eigenvalues: 0

| total energy = -1052.38831294818 |

: kinetic energy = 1041.66449400756 :

: potential energy = -2094.05280695574 :

: virial theorem = 1.98981001707 :

: wavefunction norm = 0.99999999990 :

.....

HOMO-LUMO Separation

HOMO : -0.19481786 H = -5.30127 eV

LUMO : -0.06638186 H = -1.80634 eV

HOMO-LUMO gap: 0.12843600 H = +3.49492 eV

For the compound **3aa**, excited state: Cartesian coordinates and Cartesian gradients and Energy

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ATOM	CARTESIAN COORDINATES		
1 c	-1.51831762129636	-5.35964637378737	0.59583467276804
2 c	-2.15349640586273	-2.83078292016033	0.97759231272851
3 c	-4.76688443322855	-2.18029081078678	1.08762287253674
4 c	-6.65504342522592	-4.08009844237381	1.00402344918141
5 c	-5.95688194809080	-6.58630035686239	0.70667924839440
6 c	-3.39202636144413	-7.21966498700240	0.46256044069427

7 n	-5.43507832324533	0.36655887904075	1.13756351724183
8 c	-3.76524659775634	2.21970406790919	0.24663854539310
9 c	-1.12572584725772	1.68533651749527	0.20055015797397
10 c	-0.26180935568331	-0.73811305841844	1.46278248937113
11 c	2.53936797666235	-1.50325669814311	1.29201216932060
12 o	4.06236677231051	0.44094270117491	2.38176593907529
13 c	6.14060678591381	0.80690435349315	0.81589362391220
14 c	5.94224323913396	-0.64911997096323	-1.44113838206038
15 c	3.67381399187815	-2.08049613505248	-1.36047818048458
16 o	2.67276992662641	-3.62611458018556	-2.85424202279864
17 c	7.91623201170837	-0.41204900843918	-3.26952037015086
18 c	9.93582542993079	1.20606864068903	-2.75557769109384
19 c	10.07778123235998	2.61207126866895	-0.50849559104466
20 c	8.11232712196859	2.40929405492130	1.33601580758252
21 c	0.49085668867688	3.51762331670432	-0.79371015051280
22 c	-0.45862763735172	5.80093354422523	-1.72592590685516
23 c	-3.05451319425998	6.32586244191226	-1.64997040666703
24 c	-4.70989178619483	4.55173843180945	-0.66024582813451
25 c	-8.01791420710370	1.08250975790709	1.81091636864340
26 h	0.44845993330770	-5.86095371777714	0.28338836996860
27 h	-8.65287686763483	-3.59138905591527	1.07388044509825
28 h	-7.40899516797994	-8.04903490857517	0.60412650757728
29 h	-2.84475241896336	-9.18437278431039	0.14651687436419
30 h	-0.53832452698557	-0.30126758297546	3.50686504593796
31 h	2.74682706720419	-3.20276058737263	2.50264372230231
32 h	7.82541552645827	-1.50243751117330	-5.01840390280288

33 h	11.46205187129043	1.38082876759470	-4.14162814438519
34 h	11.68682423415016	3.85392527034517	-0.15419098798832
35 h	8.16775169991962	3.47362709855007	3.10358802563077
36 h	2.51179513679156	3.17356891414076	-0.85262311896622
37 h	0.85096296601597	7.18463216508554	-2.51861545792084
38 h	-3.78457988496690	8.11016712536790	-2.38618226173973
39 h	-6.72984823046023	4.94590687437356	-0.66282247428846
40 h	-8.74174676264043	-0.22573591705808	3.24272546785838
41 h	-8.01097679582115	2.98863348174372	2.61717008967647
42 h	-9.28072181285369	1.04704773417984	0.15441471466202

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ATOM CARTESIAN GRADIENTS

1 c	-0.00000791031313	-0.00001380607122	0.00000038698132
2 c	-0.00000026512476	0.00000046314386	0.00000119788551
3 c	-0.00000550314892	0.00000946527246	0.00000323406855
4 c	-0.00000557915465	0.00000155659360	0.00000371163269
5 c	0.00000145796369	-0.00000241471758	0.00000971066836
6 c	-0.00001817594788	0.00000342247513	0.00000617341806
7 n	-0.00000363038352	-0.00000780780722	0.00000039333680
8 c	-0.00000037834581	0.00000690589077	-0.00000030562044
9 c	-0.00000653842603	0.00000311113836	-0.00000100468323
10 c	-0.00000752663264	0.00000034488706	0.00000477704731
11 c	0.00000465833786	-0.00000497129984	0.00000175183155
12 o	-0.00000609539925	0.00000171592465	-0.00001109046381
13 c	0.00000175028540	0.00000220621512	-0.00000676247167
14 c	-0.00000421841737	-0.00001141607221	-0.00000178567804

15 c	-0.00000180767570	0.00001743549399	0.00001704175327
16 o	-0.00000740558324	-0.00001394616710	-0.00001102350489
17 c	0.00000209383441	-0.00000463665772	-0.00000377959142
18 c	-0.00000618674209	-0.00000552470868	-0.00000590233555
19 c	-0.00000609305213	0.00000231541056	-0.00001016401069
20 c	-0.00000732725604	-0.00000397042367	-0.00000337465422
21 c	-0.00000146972712	-0.00000405184890	0.00000235192201
22 c	-0.00000633349029	0.00000448413945	0.00000212454717
23 c	0.00000406809324	0.00000201714919	0.00000088833343
24 c	-0.00000127901896	-0.00000251833800	0.00000343591887
25 c	-0.00000445453346	0.00000443679006	0.00000797810872
26 h	0.00000101874555	0.00001188217560	0.00000476400099
27 h	-0.00000228849253	0.00000054136529	0.00000225363690
28 h	-0.00000671477976	0.00000349630090	0.00000325143949
29 h	-0.00000495374452	-0.00000004458320	0.00000738519440
30 h	0.00000605550831	0.00000057195220	-0.00000141741405
31 h	-0.00000556871427	-0.00000530565482	-0.00000480166797
32 h	-0.00001198613388	-0.00000317153369	-0.00000509336954
33 h	-0.00000149738468	-0.00000866188610	-0.00000410335102
34 h	-0.00000433046925	-0.00000132638386	-0.00001172714525
35 h	0.00000175437588	-0.00000354155560	-0.00000716549275
36 h	-0.00000336819962	-0.00000138430044	-0.00000130556158
37 h	-0.00000152476298	0.00000082960412	0.00000354237928
38 h	-0.00000209969713	0.00000022876237	-0.00000020803392
39 h	-0.00000124051294	0.00000523499466	0.00000867583719
40 h	-0.00000078615064	0.00000525331724	0.00000466379076

41 h 0.00000115644063 0.00000362778152 0.00000597509922

42 h -0.00000068318667 0.00000412755754 0.00000574190307

****

norm of actual CARTESIAN gradient: 6.62762E-05

norm of actual INTERNAL gradient: 1.35457E-04

ENERGY = -1052.2940897822 a.u.; # of cycle = 22

Approximate Hessian read from $hessapprox data section

Hessian updated according to BFGS formula

Number of zero Hessian eigenvalues: 0

| total energy = -1052.37399251638 |

: kinetic energy = 1041.46833992165 :

: potential energy = -2093.84233243803 :

: virial theorem = 1.98963709416 :

: wavefunction norm = 0.99999999990 :

HOMO-LUMO Separation

HOMO : -0.18249804 H = -4.96603 eV

LUMO : -0.08352970 H = -2.27296 eV

HOMO-LUMO gap: 0.09896834 H = +2.69307 eV

SUMMARY OF EXCITATION ENERGIES AND DIPOLE OSCILLATOR STRENGTHS (velocity/length):

1- 5 singlet a excitation

Exc.	energy (Eh)	energy (eV)	energy (cm-1)	energy (nm)	Osc.(vel)	Osc.(len)
1 a	0.079903	2.17427	17536.640	570.235	0.00282	0.00315
2 a	0.114850	3.12522	25206.630	396.721	0.00087	0.00069
3 a	0.135543	3.68831	29748.241	336.154	0.00426	0.00432
4 a	0.137963	3.75417	30279.411	330.257	0.01117	0.01050
5 a	0.144566	3.93385	31728.664	315.172	0.00564	0.00659

For the compound **5ba,** ground state: Cartesian coordinates and Cartesian gradients and Energy

: ***No Imaginary frequency was observed.***

**********##########

ATOM	CARTESIAN COORDINATES		
1 c	-2.75200422403436	5.74779553821674	0.68851386578108
2 c	-2.08557815271751	3.20834061213644	1.01897877863347
3 c	-3.55196759332194	1.28763514485986	-0.13491541941671
4 c	-5.54040757720596	2.04647604372689	-1.75309284358101
5 c	-6.13273907239671	4.59141844685664	-2.09510230228996
6 c	-4.77116854114924	6.47377044164561	-0.84256658286884
7 n	-3.03995883933271	-1.27482252114484	0.36562360412616
8 c	-1.34405630192924	-1.96275835842943	2.29573814395926
9 c	0.14839283361707	-0.09827463170768	3.51127730094258

10 c	0.28702966620361	2.54559571368055	2.45119483853227
11 c	2.73212041521926	3.03121544656101	0.75135648403068
12 c	5.08167123600776	2.80843151925168	2.41816046298862
13 o	6.58221915890113	0.76690284990906	2.14942527300341
14 c	5.89444939325037	-1.34496752763813	0.60107141147062
15 c	4.47867271153990	-0.60858129343290	-1.75310990294175
16 c	2.91972685810936	1.53535369602404	-1.67494714507343
17 c	1.64723542078498	2.28464897349747	-3.88010509446318
18 c	1.87149562868371	0.88271900196779	-6.10465430639890
19 c	3.39906940710144	-1.27524494276481	-6.16074338628885
20 c	4.71469548221264	-2.00246165982711	-3.99199246385103
21 o	5.61192100471848	4.39538335123850	3.96215942159052
22 c	1.58208905501784	-0.74783552335875	5.64103501530847
23 c	1.72195052370352	-3.23031694613513	6.52000150344817
24 c	0.40393147976746	-5.10340380442921	5.20985354829948
25 c	-1.10699297762198	-4.48910181287056	3.13832396054120
26 c	-4.51794235052981	-3.23603120031614	-0.90422829022781
27 c	-3.28563985332742	-4.24815642784769	-3.31523785692805
28 h	-1.61964245111519	7.19108820483073	1.64477042377626
29 h	-6.65651643673850	0.65750289287446	-2.77906965817733
30 h	-7.69193267520701	5.09392031356376	-3.35444451723898
31 h	-5.25253015696062	8.46743540255909	-1.07683283745274
32 h	0.52629410222114	3.88935512388662	4.02235552073444
33 h	2.62832464116157	5.05492805722248	0.28548816227520
34 h	7.68621150991072	-2.28496333672539	0.12371715513975
35 h	4.77835596802590	-2.66834354589223	1.76632935182833
36 h	0.47891245542164	3.98675896753640	-3.85081211227809
37 h	0.87055911650584	1.49026208950024	-7.80670381621609

38 h	3.59803859284115	-2.36519731562717	-7.90435401908931
39 h	5.95966671120237	-3.65309159492438	-4.04364698448829
40 h	2.64521316720403	0.74071877392022	6.60189666926143
41 h	2.86496751018162	-3.69391152818064	8.17494740946636
42 h	0.52150094884164	-7.07719041066905	5.81018926339329
43 h	-2.10708787220513	-6.01753775887806	2.19386136637695
44 h	-4.86534070618836	-4.78018651271198	0.43549126583608
45 h	-6.40595067270353	-2.48661954619225	-1.31786898234355
46 h	-1.42451739219501	-5.08776100578857	-2.91285322718597
47 h	-4.48606573456154	-5.71252421316116	-4.18506830969824
48 h	-2.99667541690789	-2.72837318681373	-4.70664647381471

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ATOM CARTESIAN GRADIENTS

1 c	0.00001289749683	-0.00000022915741	-0.00002761168419
2 c	0.00001751047699	0.00002381070766	-0.00000736204487
3 c	0.00001763941617	0.00000217061524	0.00000478472290
4 c	0.00000959062016	-0.00001064019832	-0.00001817570069
5 c	-0.00001121719188	-0.00000419714749	0.00001970831527
6 c	-0.00000744425322	0.00000410447341	0.00000293976165
7 n	-0.00001232224875	0.00000113951995	0.00001839530986
8 c	0.00000441279111	0.00000683125395	-0.00000375345544
9 c	-0.00000922654640	-0.00000495450593	-0.00002996085060
10 c	0.00000699046328	-0.00005368225831	0.00003537907519
11 c	-0.00000425094162	0.00000118953938	-0.00002030397936
12 c	0.00001859754059	0.00006582470673	-0.00007424793316
13 o	-0.00003990440095	-0.00004808138809	0.00004689917000
14 c	0.00003150254266	-0.00001222963179	-0.00002244048935
15 c	-0.00001032580717	0.00000832591027	0.00000532327631

16 c	0.00003369848375	-0.00000196162699	0.00000377574640
17 c	-0.00000866830015	0.00000568450177	-0.00000792432578
18 c	-0.00000507022801	0.00001028179701	0.00000214931145
19 c	0.00000359403604	-0.00001727294483	0.00000657658202
20 c	-0.00000798324398	-0.00001862899564	-0.00000627935664
21 o	-0.00000129853754	-0.00003123655557	-0.00000780547046
22 c	-0.00000618354486	0.00000260043698	-0.00000168995352
23 c	0.00000510663175	0.00000433913305	-0.00000156703559
24 c	-0.00000446250685	-0.00000223247938	0.00000568940663
25 c	-0.00000333661122	0.00000374542581	-0.00000725221734
26 c	0.00002323398390	0.00000332063266	-0.00001376651738
27 c	-0.00001478748226	0.00001869632409	0.00001596387204
28 h	-0.00000704712449	0.00000125197562	0.00000981542328
29 h	-0.00000292356990	-0.00001208161677	0.00000902029366
30 h	0.00000081702080	-0.00000136379221	-0.00000354810852
31 h	0.00000855950646	0.00000346626214	-0.00001325459441
32 h	0.00000877134976	0.00000231837721	-0.00001394160539
33 h	-0.00000965887322	0.00001141225885	-0.00000366579377
34 h	-0.00000257821016	-0.00000347661759	-0.00001174318509
35 h	0.00000217432139	-0.00000294957567	-0.00000472898416
36 h	-0.00000612975250	-0.00000555297337	0.00000340949126
37 h	-0.00000348661423	-0.00000486535011	-0.00000203758195
38 h	-0.00000404658090	-0.00000385504806	-0.00000388064897
39 h	0.00001119960991	0.00000002384513	-0.00001168395391
40 h	0.00000783294389	0.00000007714019	-0.00000367420024
41 h	0.00000105931903	0.00000362646941	0.00000026133546
42 h	0.00000449027027	-0.00000173032627	-0.00000634417822
43 h	-0.00000883994536	0.00000169603777	0.00000172935895

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 44 h     -0.00000765471599     0.00000020599702     0.00000186038369
 45 h     -0.00001276973084     0.00000486789078     0.00001338895687
 46 h     -0.00000166352027    -0.00000016767199    -0.00000452702380
 47 h     -0.00000469301819    -0.00000249369376    -0.00000262886195
 48 h     -0.00000119564675    -0.00001068859998    -0.00000820240225
 ***************************************************************************

 norm of actual CARTESIAN gradient:  1.88358E-04
 norm of actual INTERNAL  gradient:  2.90630E-04

 ENERGY =   -1130.9163698790 a.u.; # of cycle =   14

 Approximate Hessian read from $hessapprox data section

 Hessian updated according to BFGS formula
 Number of zero Hessian eigenvalues:   0
            | total energy      =  -1130.91637019225  |
             ----------------------------------------
            :  kinetic energy    =   1119.13019024968  :
            :  potential energy  =  -2250.04656044193  :
            :  virial theorem    =      1.98957820379  :
            :  wavefunction norm =      1.00000000000  :
             ........................................
HOMO-LUMO Separation
 HOMO        :   -0.19397948 H =     -5.27845 eV
 LUMO        :   -0.02928582 H =     -0.79691 eV
 HOMO-LUMO gap:    0.16469367 H =     +4.48155 eV
```

For the compound **5ba** excited state: Cartesian coordinates and Cartesian gradients and Energy

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ATOM	CARTESIAN COORDINATES		
1 c	9.49296445774426	1.75749546544861	1.95031154262732
2 c	6.93133343143266	1.26302163030218	2.35053970659197
3 c	5.33851611035980	0.55721063241525	0.33731623590168
4 c	6.39803360647435	0.33527498965710	-2.07911285060051
5 c	8.96949802084407	0.81283646979133	-2.47792169434729
6 c	10.52563011836265	1.52774723776726	-0.47062132016408
7 c	2.59241350157566	0.01658364095126	1.05308348915784
8 c	0.70955744002266	-0.56717451670765	-1.13587266352815
9 c	-1.00754176032691	-2.86459038249601	-0.60967164251666
10 c	0.42230629618742	-5.14440993353174	0.32175066520210
11 c	-0.96933580705736	-7.09194201262358	1.44699610434003
12 c	-3.52866324381547	-6.75007364289715	2.09603707602589
13 c	-4.80677649606689	-4.44895638966055	1.77086569912044
14 c	-3.20425939947560	-2.16049138262220	1.17049665111870
15 n	-4.65809043526980	0.02675689168238	0.03054375406549
16 c	-3.55485843088597	1.75973729054029	-1.46253682601305
17 c	-0.87030409399340	1.63009130226049	-2.04842262701128
18 c	0.18332605968757	3.52774741079940	-3.51808020960465
19 c	-1.24901659228769	5.54517869496122	-4.46728928933762
20 c	-3.85648063914988	5.66851738531428	-3.95617086083812
21 c	-4.98964649306874	3.83277221094208	-2.49951839558866
22 c	-7.29420511348228	0.35023847822998	0.85841947658115
23 c	-9.22111581986396	-0.80824568315715	-0.96117161241592
24 c	1.67014714209289	1.99210082957096	2.94863427243633

25	o	3.30671353886357	2.63141690749611	4.79047911600242
26	c	5.71814775095977	1.40091860141478	4.91187988719766
27	o	-0.39192544403974	2.96921445275128	2.92056190280738
28	h	10.68815068315333	2.32055460575233	3.54078505535411
29	h	5.24448735317400	-0.24013984468929	-3.68835748625971
30	h	9.75469176154773	0.61985008393204	-4.37902168848506
31	h	12.53085497323251	1.90800914900796	-0.78636345296703
32	h	2.62844317900229	-1.80417603269269	2.12659709912390
33	h	1.88595401642723	-1.13240058097552	-2.74918262632323
34	h	-1.94036743315913	-3.30186564735189	-2.44453994691178
35	h	2.26562636072165	-5.52345454847334	-0.53583034606294
36	h	-0.07115082822503	-8.92011051037144	1.80381644312883
37	h	-4.56685054427685	-8.32827186368505	2.93934891969182
38	h	-6.58629057886477	-4.19598664525568	2.78075065738923
39	h	-2.40164618407510	-1.30249520690446	2.90528599160711
40	h	2.20014722478589	3.44306097634472	-3.94140364925908
41	h	-0.34515173108682	7.00317888138575	-5.61420819487087
42	h	-4.99082794764575	7.21607618571372	-4.71593080956692
43	h	-7.00875566791361	3.95787880631210	-2.14892851423007
44	h	-7.65356849544061	2.37130015530908	1.16233111679555
45	h	-7.44148766622978	-0.54955290086234	2.71436020482297
46	h	-9.16766491789134	0.10528371042756	-2.83019683990181
47	h	-11.13569638591476	-0.57180786857797	-0.17893735638684
48	h	-8.84316418316052	-2.83438633039053	-1.20326099470192
49	h	6.84906932672515	2.50292297352292	6.25938588205574
50	h	5.44882997929054	-0.51244412607785	5.71197494874772

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ATOM CARTESIAN GRADIENTS

1 c	0.00000002057023	-0.00000013335943	0.00000120686477
2 c	0.00000081059403	-0.00000087456407	-0.00000477808790
3 c	0.00000864591463	-0.00002139979794	0.00000277479626
4 c	-0.00000396896648	0.00000035275323	-0.00000118461360
5 c	0.00000391584518	0.00000043585726	-0.00000010274450
6 c	-0.00000144521644	-0.00000071137890	-0.00000359773763
7 c	-0.00000407480650	-0.00000247396685	-0.00000785771041
8 c	0.00000225476511	0.00001106346231	0.00001575825853
9 c	0.00000577906985	-0.00001056858818	-0.00000556957474
10 c	-0.00001202879350	-0.00002244823546	0.00000051604756
11 c	0.00001945846120	0.00000902128960	-0.00001430543851
12 c	-0.00000396885700	-0.00000414183043	0.00000294034595
13 c	0.00000722635247	-0.00000624529020	-0.00001148956035
14 c	-0.00000368246591	-0.00000189372151	0.00001390063915
15 n	0.00000995621413	-0.00000122956631	-0.00000343926063
16 c	-0.00000573354139	-0.00000424545279	0.00000867798160
17 c	0.00000494644535	-0.00001054223717	-0.00001934032964
18 c	-0.00000247677055	-0.00000363642566	0.00000096768894
19 c	0.00000114111535	-0.00000351176102	-0.00000280925938
20 c	0.00000045207770	-0.00000583141376	-0.00000182864457
21 c	0.00000338817757	0.00000289854421	0.00000071878421
22 c	-0.00000980363944	0.00000214086827	0.00000399950884
23 c	0.00000206633329	-0.00000863997058	-0.00000385644615
24 c	-0.00000195110955	-0.00000471147558	-0.00000458011365
25 o	0.00000036524298	0.00000053160420	0.00000076513813
26 c	0.00000675825422	0.00000169435295	0.00000004515895
27 o	0.00000823353714	-0.00000669166890	0.00000017005656
28 h	0.00000314171621	-0.00001089657479	-0.00000171115252

29 h	0.00000021672377	0.00000295363844	-0.00000227847767
30 h	0.00000217291940	-0.00000593711282	-0.00000073181872
31 h	-0.00000099088529	0.00000406041075	-0.00000320163229
32 h	0.00000476994192	-0.00000105383573	0.00000181354774
33 h	0.00000124472448	-0.00000147267247	-0.00000222921103
34 h	-0.00000006971349	-0.00000236176772	-0.00000060437100
35 h	-0.00000241135958	-0.00000060202665	-0.00000596437714
36 h	0.00000016997549	-0.00000346215566	-0.00000354732372
37 h	0.00000745937805	-0.00000181688009	0.00000581456975
38 h	0.00000225309811	-0.00000402657512	-0.00000022445778
39 h	0.00000311701097	-0.00000408283572	-0.00000402285720
40 h	0.00000052324303	-0.00000059389422	0.00000010598277
41 h	-0.00000017360757	-0.00000342432645	0.00000012527344
42 h	0.00000202060451	0.00000044392215	0.00000718017677
43 h	0.00000237068827	-0.00000607082487	-0.00000583396736
44 h	0.00000117770259	-0.00000988089486	0.00000229985158
45 h	0.00000459978565	-0.00000439776814	-0.00000025601773
46 h	0.00000222409005	-0.00000183287026	0.00000074057374
47 h	0.00000290683746	-0.00000015877393	0.00000337093151
48 h	0.00000290704162	0.00000009524423	-0.00000267084935
49 h	0.00000106204357	-0.00000370769254	-0.00000107879646
50 h	0.00000245414674	-0.00000297569957	-0.00000371206859

****

norm of actual CARTESIAN gradient: 7.18638E-05

norm of actual INTERNAL gradient: 1.02934E-04

ENERGY = -1131.9587345589 a.u.; # of cycle = 31

Approximate Hessian read from $hessapprox data section

Hessian updated according to BFGS formula

Number of zero Hessian eigenvalues: 0

HOMO-LUMO Separation

HOMO : -0.16505037 H = -4.49125 eV

LUMO : -0.06910573 H = -1.88046 eV

HOMO-LUMO gap: 0.09594464 H = +2.61079 eV

SUMMARY OF EXCITATION ENERGIES AND DIPOLE OSCILLATOR STRENGTHS (velocity/length):

Exc.	energy (Eh)	energy (eV)	energy (cm-1)	energy (nm)	Osc.(vel)	Osc.(len)
1 a	0.071059	1.93361	15595.634	641.205	0.00021	0.00029
2 a	0.122489	3.33310	26883.287	371.978	0.00173	0.00161
3 a	0.124343	3.38356	27290.218	366.432	0.00074	0.00070
4 a	0.134490	3.65967	29517.249	338.785	0.00286	0.00264
5 a	0.143924	3.91638	31587.765	316.578	0.09356	0.09322

For the compound **3ad,** ground state: Cartesian coordinates and Cartesian gradients and Energy

: ***No Imaginary frequency was observed.***

****

ATOM	CARTESIAN COORDINATES		
1 c	0.26067620200857	-3.68228238654757	-0.32240853928306
2 c	-1.34533431327600	-1.61064171593493	-0.62614377333982
3 c	-3.99336002567330	-1.99804437168212	-0.53765732828220
4 c	-4.94959626158292	-4.45667405010828	-0.22543582637482
5 c	-3.30279303502371	-6.50570358971644	0.02215831240997
6 c	-0.69525983076538	-6.12775298609004	-0.00322195919852
7 n	-5.59033160160526	0.12847939982181	-0.72940963449294
8 c	-4.73676148748877	2.39712834415979	0.37235581628893
9 c	-2.11253740988143	2.90966313298847	0.31562180349422
10 c	-0.52155805355404	1.07709711763030	-1.23167177183712
11 c	2.29461202724496	1.67131409201432	-1.24979967623032
12 o	3.53301392120473	1.32048044851520	1.15634801693706
13 c	5.80260622984914	0.23080098610893	0.74166138776891
14 c	6.21323079378107	-0.46498812796810	-1.78801647888744
15 c	3.94032967192099	0.26009390450230	-3.21093373898954
16 o	3.41254287976191	-0.03394931466539	-5.41704674004559
17 c	8.46194461690786	-1.65795666114138	-2.51325474822234
18 c	10.29883418897861	-2.11583509683566	-0.68699135537863
19 c	9.82901594485447	-1.38067037482290	1.82380940412111
20 c	7.60703793040486	-0.20958521112253	2.61583916427927
21 f	11.61995169171293	-1.82755806849094	3.54611001818375
22 c	-1.19358452228708	5.05700975552654	1.54644435945920

23 c	-2.83324328485086	6.75952526978335	2.73426175538626
24 c	-5.42739466820803	6.29366954239678	2.70465764462752
25 c	-6.38184169467181	4.11659345546158	1.55370609275606
26 c	-8.27146967510763	-0.23457925612742	-1.15206376833810
27 h	2.30300033751076	-3.42232129731898	-0.37222775141024
28 h	-6.98168966460080	-4.78402976139162	-0.13423336006193
29 h	-4.07929693647154	-8.40477180037278	0.26524445873535
30 h	0.60034872043132	-7.72132034437294	0.20615415551560
31 h	-1.05829232150718	1.38568923187239	-3.23963654459720
32 h	2.49570015333095	3.69352118168610	-1.73870375125026
33 h	8.74987210790695	-2.20234295409592	-4.48424744566067
34 h	12.09501294828950	-3.02385345936864	-1.13667505900025
35 h	7.31702649062326	0.31966386713604	4.58580238010995
36 h	0.83508941422424	5.42469573325634	1.59149474998641
37 h	-2.07829108504291	8.43756764628877	3.67091878310982
38 h	-6.73210408399826	7.60846518755333	3.61996125664811
39 h	-8.40769611741286	3.74757010978611	1.62375945850783
40 h	-8.55435243626020	-1.72179579530307	-2.57366840416342
41 h	-9.09709100832112	1.51862766577282	-1.89877714032627
42 h	-9.32596675335558	-0.77099944878811	0.57591577704109

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ATOM CARTESIAN GRADIENTS

1 c	-0.00000960640627	0.00000513203771	0.00000155908308
2 c	-0.00000981855061	0.00000064751849	0.00000925961945
3 c	0.00001237532223	0.00000298417509	-0.00001653404521
4 c	-0.00000615899719	0.00000705821951	-0.00000973913635
5 c	-0.00001222379831	-0.00000265756774	-0.00000429617525
6 c	-0.00000569259992	-0.00000924099919	-0.00001518137772

7 n	-0.00000938029982	-0.00000029235866	-0.00001278964925
8 c	0.00001413004427	-0.00000732885265	0.00003252880163
9 c	-0.00000281264027	-0.00000629522250	0.00001017152558
10 c	-0.00001139709854	-0.00000049288681	-0.00001282125071
11 c	0.00000977444263	-0.00002042640079	-0.00004539468825
12 o	0.00003286682570	0.00001056879370	0.00000426345791
13 c	-0.00001441075813	-0.00000798537417	0.00000193082155
14 c	-0.00000823681502	-0.00001639589406	0.00000200997819
15 c	0.00003596179597	0.00003033987637	0.00001146918284
16 o	-0.00001695095484	-0.00005988256847	0.00000945348839
17 c	-0.00000220337482	-0.00003931135804	0.00000482496662
18 c	-0.00000353823204	-0.00002999578928	0.00000723027804
19 c	-0.00001738035431	-0.00004635021695	0.00000646259831
20 c	0.00001703690587	0.00002259013593	-0.00000451814265
21 f	0.00000907790462	-0.00000075080333	0.00000115518810
22 c	0.00000670312984	-0.00000434255859	-0.00000430736170
23 c	0.00001843050681	-0.00000594978582	0.00000798914623
24 c	0.00000792101741	-0.00001276427952	0.00001865058674
25 c	0.00000826614072	0.00001309632882	0.00000013116211
26 c	0.00001446967015	0.00000963444642	0.00000874863726
27 h	-0.00000910339521	-0.00001843266332	-0.00000064464733
28 h	-0.00000669194928	0.00000641795124	-0.00001408124044
29 h	-0.00001317079128	0.00000517421671	0.00000017377641
30 h	-0.00001114495376	-0.00000401866874	-0.00002504443688
31 h	0.00001424616887	-0.00000164063322	0.00000773925021
32 h	-0.00000478529319	-0.00001461062588	0.00001373849497
33 h	-0.00000134095950	-0.00002060565379	0.00000806985987
34 h	-0.00001530651099	-0.00003676334187	-0.00000035321563

35 h	-0.00000433372503	-0.00003053491862	-0.00000060416443
36 h	0.00000059515804	-0.00001764140627	0.00002867153362
37 h	0.00001344562333	-0.00000722986315	0.00000138851062
38 h	0.00001462041684	-0.00000230160772	0.00000721679004
39 h	0.00001348167612	-0.00000669264614	0.00002157341643
40 h	-0.00000102665828	0.00001379116935	-0.00000355568685
41 h	0.00000464213905	0.00000899076304	0.00000176362810
42 h	0.00000020817755	0.00000711759296	-0.00000643076633

****

norm of actual CARTESIAN gradient: 1.73025E-04

norm of actual INTERNAL gradient: 4.37857E-04

ENERGY =   -1151.5196908270 a.u.; # of cycle =   17

Approximate Hessian read from $hessapprox data section

Hessian updated according to BFGS formula

Number of zero Hessian eigenvalues: 0

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 ----------------------------------------
| total energy     = -1151.51969188143  |
 ----------------------------------------
: kinetic energy   =  1140.37897385328  :
: potential energy = -2291.89866573471  :
: virial theorem   =     1.99032520407  :
```

: wavefunction norm = 1.00000000000 :

HOMO-LUMO Separation

HOMO : -0.19734914 H = -5.37015 eV

LUMO : -0.06736950 H = -1.83322 eV

HOMO-LUMO gap: 0.12997964 H = +3.53693 eV

For the compound **3ad**, Excited State : Cartesian coordinates and Cartesian gradients and Energy

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ATOM	CARTESIAN COORDINATES		
1 c	0.29081029190775	-3.66715334457911	-0.53672143959168
2 c	-1.30868436638709	-1.57543976152157	-0.60375148446418
3 c	-3.96699931683994	-2.01325146594082	-0.44532352018588
4 c	-4.94194467930421	-4.50325262382101	-0.28071947101106
5 c	-3.29757582672369	-6.53871589698236	-0.21076967976872
6 c	-0.68191628062205	-6.11681192412263	-0.32728300834129
7 n	-5.60537240130492	0.05272522625501	-0.37118597566428
8 c	-4.75237754842487	2.41599903127672	0.45025267678807
9 c	-2.12093695600475	2.95038128052880	0.32010832660724
10 c	-0.43941617983357	1.11058038837669	-1.08446327715902
11 c	2.38396577787963	1.70187994782931	-1.03939527339850
12 o	3.54911317642040	1.25684246534803	1.34659429365532
13 c	5.88711327104025	0.16955482403958	0.86756930694229
14 c	6.17131870942332	-0.49160957410592	-1.73628488938559
15 c	3.95481906553625	0.25244104572635	-3.05230772563383

16 o	3.15165432296470	-0.01987409152098	-5.26108930865744
17 c	8.45758362434463	-1.73917190242602	-2.47576885348557
18 c	10.31918732135292	-2.19526668728251	-0.64957077244795
19 c	9.94509058869124	-1.47377734950309	1.85240402826732
20 c	7.68392924226024	-0.26968753324401	2.68360417931366
21 f	11.77268169755916	-1.91606543079835	3.59780994975974
22 c	-1.26787509932744	5.20545688719634	1.38708108872874
23 c	-2.95247925519167	6.93198021514629	2.47062090931895
24 c	-5.55329430002046	6.43460682194464	2.50073563261181
25 c	-6.45978827149912	4.18488468329677	1.50179189197189
26 c	-8.30105280805705	-0.32111761205561	-0.85367842813942
27 h	2.31967418137687	-3.39767368995336	-0.68376972015629
28 h	-6.96721548842230	-4.83692671020075	-0.12964582144132
29 h	-4.04311855297227	-8.45595195687086	-0.04930174795671
30 h	0.62160459673594	-7.71534585128970	-0.27146527013491
31 h	-0.87266588692619	1.38254921508766	-3.13130763418700
32 h	2.56406672359077	3.73775087406727	-1.50840075567802
33 h	8.73855243914140	-2.29231775248072	-4.44131975927816
34 h	12.09958243131032	-3.11499299435872	-1.14985063269070
35 h	7.42015526201669	0.25112476831055	4.65906658689744
36 h	0.74717933777308	5.61505079662365	1.39602256464976
37 h	-2.22662571473901	8.67680451046571	3.30066774536655
38 h	-6.86742947253310	7.78477536918974	3.34204605895630
39 h	-8.47335312609098	3.77343976150678	1.61464952213884
40 h	-8.54442973599126	-1.81465943268403	-2.26556119055432
41 h	-9.10667329662326	1.42741599440216	-1.61418566040906
42 h	-9.32685749748601	-0.84718052088046	0.88209653784279

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ATOM		CARTESIAN GRADIENTS	
1 c	0.00000246145337	0.00000260808614	-0.00002071427653
2 c	-0.00000341898541	-0.00001073124866	0.00004398518230
3 c	-0.00000115423348	0.00000243163064	-0.00003680113504
4 c	-0.00000963158238	0.00000689400334	-0.00001721620262
5 c	-0.00000120570156	0.00000267274870	-0.00000080229272
6 c	-0.00001249244502	-0.00000636767808	0.00000303004920
7 n	0.00000139079075	0.00000243529575	-0.00000063117157
8 c	0.00000912042998	0.00002525314952	-0.00003814410879
9 c	0.00000789952210	0.00000057361974	0.00000002737172
10 c	0.00001590773878	0.00000024439520	-0.00000244920697
11 c	0.00001604188823	-0.00004204963423	-0.00002380972298
12 o	-0.00000121647433	-0.00001558389438	0.00002268467190
13 c	0.00001645042715	-0.00001774980839	-0.00000018259105
14 c	0.00000325847262	-0.00001406140076	0.00001022930809
15 c	-0.00000334026369	0.00000577232317	0.00000068490549
16 o	0.00000678310361	-0.00001447152970	0.00000598821131
17 c	0.00000171513902	-0.00001592667530	0.00000596923760
18 c	-0.00000372412719	-0.00002400393263	0.00000364330253
19 c	0.00000585812960	-0.00002633360222	0.00000330844077
20 c	-0.00000770809548	-0.00001945369548	0.00000989901044
21 f	-0.00000037408294	-0.00001616142661	0.00000211520220
22 c	0.00001715570329	0.00000168750934	0.00001655517031
23 c	0.00000491934594	-0.00001217322569	0.00001099406882
24 c	0.00001691309217	-0.00000854102871	0.00001492626616
25 c	0.00000266942913	-0.00001214406740	0.00000970068799
26 c	-0.00001006554761	0.00000878147344	0.00000253778584
27 h	0.00000118355877	-0.00000383975719	0.00001039489655

28 h	-0.00000696374950	0.00000910974788	0.00000141965285
29 h	-0.00000927099246	-0.00000079665069	-0.00001104432002
30 h	-0.00000955428027	-0.00000830039989	-0.00002880429175
31 h	-0.00000964492949	-0.00000790345375	0.00000382289723
32 h	-0.00000326910375	-0.00001251485147	0.00001156762153
33 h	0.00000465742839	-0.00000131846271	-0.00000128577851
34 h	-0.00001333892295	-0.00004791865491	0.00001064647940
35 h	0.00000874740080	-0.00000984706898	0.00000307810012
36 h	0.00000801602937	-0.00000916667789	-0.00000114989786
37 h	0.00001371265292	-0.00001132468361	0.00002015914624
38 h	0.00001146438668	0.00000372116662	0.00000111204263
39 h	0.00000649977547	-0.00000154535081	0.00000063861793
40 h	0.00000533665677	0.00000414755408	-0.00000661095544
41 h	0.00000851192761	0.00001037216102	0.00000489570858
42 h	-0.00000163051958	0.00000227155671	-0.00000637466928

****

norm of actual CARTESIAN gradient: 1.48504E-04

norm of actual INTERNAL gradient: 2.32210E-04

ENERGY =   -1151.4223245090 a.u.; # of cycle =   17

Approximate Hessian read from $hessapprox data section

Hessian updated according to BFGS formula

Number of zero Hessian eigenvalues: 0

| total energy = -1151.50601902373 |

: kinetic energy = 1140.13015218496 :

: potential energy = -2291.63617120869 :

: virial theorem = 1.99012087940 :

: wavefunction norm = 1.00000000000 :

HOMO-LUMO Separation

HOMO : -0.18630132 H = -5.06952 eV

LUMO : -0.08410306 H = -2.28856 eV

HOMO-LUMO gap: 0.10219826 H = +2.78096 eV

SUMMARY OF EXCITATION ENERGIES AND DIPOLE OSCILLATOR STRENGTHS (velocity/length):

| Exc. | energy (Eh) | energy (eV) | energy (cm-1) | energy (nm) | Osc.(vel) | Osc.(len) |

| 1 a | 0.083693 | 2.27741 | 18368.567 | 544.408 | 0.00330 | 0.00307 |

| 2 a | 0.122327 | 3.32870 | 26847.775 | 372.470 | 0.00088 | 0.00068 |

| 3 a | 0.139406 | 3.79343 | 30596.077 | 326.839 | 0.00067 | 0.00057 |

| 4 a | 0.142132 | 3.86761 | 31194.347 | 320.571 | 0.00274 | 0.00285 |

| 5 a | 0.143783 | 3.91254 | 31556.732 | 316.890 | 0.00550 | 0.00577 |

For the compound **6af**, ground state : Cartesian coordinates and Cartesian gradients and Energy

: ***No Imaginary frequency was observed.***

ATOM	CARTESIAN COORDINATES		
1 c	1.84453150829968	4.57552922126266	-1.99730646580209
2 c	0.26558855572869	2.63192733456430	-1.14866906168663
3 c	-1.62164978459954	3.17685337536320	0.66061694770401
4 c	-1.83547821004398	5.64707082452772	1.62023095035063
5 c	-0.20881859006384	7.54657833729932	0.78022735724043
6 c	1.62650361795003	7.02766073356186	-1.04348355339494
7 n	-3.28173423427096	1.22965904683489	1.41631373168762
8 c	-3.86952447880835	-0.67550474909000	-0.33489930342318
9 c	-2.05890467385835	-1.30252669640283	-2.19997137549323
10 c	0.52197087787239	-0.06462332579596	-2.08335364179867
11 c	2.42388394537509	-1.73878145603059	-0.51679356149739
12 c	5.16819352452151	-1.16202077231305	-1.19572766806825
13 o	5.87885699909609	0.18737089023455	-2.88993664687173
14 o	6.74704664902535	-2.48499272494948	0.28833753041667
15 c	9.39078378994560	-2.13211038656488	-0.13860211881781
16 c	2.04184797343988	-1.60069597527316	2.36668284458984
17 o	2.77224105987471	0.21477926148404	3.54823576733111
18 c	0.75597676612387	-3.83446501529635	3.60461981416071
19 c	-2.65069942823511	-3.12233073373098	-4.02188210147713
20 c	-4.96979914397646	-4.38857814752155	-4.00447760790771
21 c	-6.73250518874725	-3.80273355985211	-2.12854898039170
22 c	-6.20644527284020	-1.95460394681240	-0.31837241163060
23 c	-4.86602732879157	1.58749527171529	3.62120886690806
24 h	3.30046818851603	4.12303717322880	-3.38661163431738
25 h	-3.29596789658782	6.11422219327581	2.99618672117976

26 h	-0.40635105908972	9.45574934807758	1.54587145418616
27 h	2.88908653297555	8.51798905554396	-1.71334127492785
28 h	1.33842859799561	-0.02659047478335	-3.99370196351214
29 h	2.11805675317823	-3.71022086173168	-1.12528467120677
30 h	9.91466185538451	-0.13756853707677	0.12723640211927
31 h	9.91020067645605	-2.70378460574247	-2.07016724218370
32 h	10.36333465731530	-3.32240885214397	1.25259678008548
33 h	-1.00705769577521	-4.33272932105314	2.61433703611574
34 h	0.37930546806585	-3.41745228679709	5.60262419491180
35 h	2.01887603789758	-5.49021371060422	3.47296452163358
36 h	-1.24403194054132	-3.57171529050986	-5.47043877255857
37 h	-5.39247815487467	-5.81376675227117	-5.43714316054106
38 h	-8.56118841490270	-4.76375972962410	-2.08483242340531
39 h	-7.64507143703973	-1.48074883486244	1.07772963675961
40 h	-3.77775560622869	2.55428423281604	5.10164220843269
41 h	-6.59293209975864	2.70540810587069	3.23486990066780
42 h	-5.44542339599951	-0.26068765882576	4.37101297443117

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ATOM CARTESIAN GRADIENTS

1 c	-0.00001040577753	0.00000101579697	-0.00000439380256
2 c	-0.00000303747282	0.00000163308408	0.00002035631468
3 c	0.00001039125840	-0.00000587768576	0.00002355746481
4 c	0.00000259528798	-0.00000279157153	0.00000616406216
5 c	0.00000141372145	0.00000171684418	0.00001469812488
6 c	-0.00001778416000	0.00000595046548	-0.00001948437278
7 n	-0.00000245131292	0.00000681906446	-0.00000111798893
8 c	0.00000904702730	-0.00004049458851	0.00002446583103
9 c	-0.00000763653916	0.00004294823884	-0.00002018047802

10 c	-0.00001348842488	0.00001139199879	-0.00002178443188
11 c	0.00003450768353	-0.00000298996690	0.00002554027035
12 c	-0.00000674839863	-0.00003557181912	0.00000838457351
13 o	0.00001225188147	0.00003197687199	-0.00000147421399
14 o	-0.00001730886095	0.00002579409187	-0.00001870498227
15 c	-0.00000425496127	0.00001530672399	0.00001337382788
16 c	0.00000796078619	0.00000030989391	-0.00003972666230
17 o	-0.00001556388270	0.00000352683592	0.00002051890973
18 c	0.00002856263701	0.00000148639024	0.00000292623671
19 c	0.00000339092606	0.00000943103860	-0.00000045360082
20 c	0.00000437626854	-0.00000181895538	0.00000906720329
21 c	0.00000221170991	-0.00000336119770	0.00000303889827
22 c	0.00000893793238	0.00000985692218	0.00001234685916
23 c	0.00000440518181	-0.00000712031174	0.00000837512024
24 h	0.00000121245079	0.00000397960661	-0.00000009898519
25 h	-0.00000273270645	0.00000412801264	-0.00000215895126
26 h	0.00001438171574	-0.00000214961181	0.00002043013134
27 h	-0.00001466113985	0.00001090661841	-0.00000624615895
28 h	0.00000339229447	-0.00000441928668	0.00000248950561
29 h	0.00000032230756	0.00001357726937	0.00000026207093
30 h	0.00000042283261	0.00000575579423	-0.00001461106767
31 h	0.00000862046617	-0.00000242259472	-0.00000165345244
32 h	0.00000274617538	0.00001149740044	-0.00000392008971
33 h	0.00000548348789	0.00000747312851	-0.00000251645587
34 h	0.00000620746757	-0.00000422019686	-0.00000182224278
35 h	-0.00000635046583	-0.00000458387536	-0.00000425516620
36 h	0.00000185591925	-0.00000138410842	0.00000607942106
37 h	0.00001249511560	-0.00001934918329	0.00002118404074

38 h	-0.00000276797326	0.00001117221084	-0.00000528324818
39 h	-0.00000522839002	0.00001048499597	-0.00000872265689
40 h	0.00000377749179	-0.00000266013095	0.00000285904862
41 h	0.00000212138106	-0.00000189272710	0.00001110215301
42 h	0.00000911667330	0.00000081837481	0.00000475596221

****

norm of actual CARTESIAN gradient: 1.46202E-04

norm of actual INTERNAL gradient: 4.05506E-04

ENERGY = -1014.5651095250 a.u.; # of cycle = 75

Approximate Hessian read from $hessapprox data section

Hessian updated according to BFGS formula

Number of zero Hessian eigenvalues: 0

```
 ----------------------------------------
| total energy     = -1014.56510970676 |
 ----------------------------------------
: kinetic energy   =  1004.38502383314 :
: potential energy =  -2018.95013353990 :
: virial theorem   =     1.98996605957 :
: wavefunction norm =     1.00000000000 :
 ........................................
```

HOMO-LUMO Separation

HOMO : -0.19249348 H = -5.23802 eV

LUMO : -0.01910772 H = -0.51995 eV

HOMO-LUMO gap: 0.17338577 H = +4.71807 eV

For the compound **6af**, Excited State: Cartesian coordinates and Cartesian gradients and Energy

****

ATOM	CARTESIAN COORDINATES		
1 c	1.90594005872317	4.55455304733418	-1.65340664772712
2 c	0.14325644334920	2.69313411101622	-1.05482403124737
3 c	-1.94547448929844	3.38046193692489	0.52726283820442
4 c	-2.09874336097465	5.85119485499014	1.56778773788764
5 c	-0.30232548174650	7.64287136554052	0.95052507353697
6 c	1.69754818038096	7.00051720114850	-0.68063461995047
7 n	-3.82415806438470	1.65984536841666	0.99771005382349
8 c	-4.20052913730959	-0.41529832413518	-0.62237259079219
9 c	-2.21404056962008	-1.19851957843533	-2.22101609004770
10 c	0.37256094181178	0.00042727917443	-2.00721181589842
11 c	2.15723850630910	-1.77592721658968	-0.44841622255324
12 c	4.92569253038398	-1.28610626785414	-0.99259053078111
13 o	5.91095903724679	0.69558530754376	-1.63055576387059
14 o	6.32558568223904	-3.37873797981573	-0.49918295834724
15 c	8.99346111048772	-3.07827884458283	-0.60832505827848
16 c	1.60171280691290	-1.66507978760995	2.44681975458281
17 o	1.02140987684109	0.47252581807994	3.45386881611538
18 c	2.80634936559582	-3.71921922991723	4.03157344130796

19 c	-2.67114570016486	-3.18519603337904	-3.90141455225414
20 c	-5.01860885464079	-4.38774744400728	-4.01224894456115
21 c	-6.97020348641491	-3.60617640570917	-2.40884356507242
22 c	-6.57000607048959	-1.62985710005541	-0.71993678614431
23 c	-5.36062257026567	1.90689953551691	3.27889612732099
24 h	3.53036151921052	4.03039370257349	-2.80020569848683
25 h	-3.67919934051662	6.36894312093958	2.78039909097570
26 h	-0.45443191043858	9.55611682171376	1.70994815667313
27 h	3.11778235971879	8.41635424841255	-1.17107992424198
28 h	1.17409227447028	0.10880318854795	-3.92704366021188
29 h	1.80223579499069	-3.72381655767506	-1.10262499282944
30 h	9.64465793732239	-1.64709921923446	0.75529437452930
31 h	9.60621567580007	-2.48537387292121	-2.50815681681320
32 h	9.80854224679264	-4.92799878573313	-0.13846569945225
33 h	2.71481777541775	-5.59381147034925	3.12098654063333
34 h	1.80688551961276	-3.81413082210846	5.85815039697717
35 h	4.83410932968295	-3.38050087471911	4.48321625919450
36 h	-1.14010367990446	-3.81055873533416	-5.13914106327713
37 h	-5.32577578282366	-5.93165726374877	-5.34806459243808
38 h	-8.81749663874593	-4.52472861776070	-2.48501957956104
39 h	-8.11802775207504	-1.00063328923065	0.48452827533811
40 h	-4.17287904333668	2.67496098864809	4.79018424479036
41 h	-7.02406217671608	3.12614176170494	2.97657449689247
42 h	-5.99358086342977	0.02672406268087	3.86705652605260

****

ATOM CARTESIAN GRADIENTS

1 c	-0.00001421973345	-0.00002376672178	-0.00000380490944
2 c	0.00000480428587	0.00000721800214	-0.00001749538483

3 c	-0.00001841603840	-0.00002687306014	0.00000948858001
4 c	-0.00000328864960	0.00000838315310	0.00000181492463
5 c	-0.00000283127894	-0.00000439099690	0.00000903179649
6 c	-0.00000135836169	0.00001250210444	-0.00000131137537
7 n	-0.00000136821064	0.00001099293169	0.00000601248912
8 c	0.00000590570444	-0.00000834994339	-0.00002318478084
9 c	-0.00000206793276	-0.00001127010213	0.00000915810195
10 c	-0.00001136298825	0.00001507973600	0.00000140970843
11 c	0.00001121516307	0.00000325377269	0.00000536613195
12 c	0.00000623598637	0.00000413822739	0.00000651092974
13 o	-0.00001157044430	-0.00000150421607	-0.00000020463037
14 o	-0.00001392647948	0.00000447603513	-0.00000495619158
15 c	0.00000077276969	0.00000193410462	-0.00000705441882
16 c	-0.00000434766601	0.00000313520008	0.00000187121187
17 o	0.00000401225449	-0.00000526795927	0.00000334248837
18 c	0.00001398538216	0.00000870729703	0.00000437529611
19 c	-0.00000995406709	-0.00000352960547	0.00000283228824
20 c	-0.00000274801909	-0.00000571868269	-0.00000059496281
21 c	-0.00000084399123	0.00000031283488	0.00000496337463
22 c	0.00000403693086	0.00001382814452	0.00000597025092
23 c	-0.00001434684496	-0.00000175393272	0.00000117994143
24 h	0.00000356684263	0.00001286507070	0.00000940381375
25 h	-0.00000291351760	0.00000094076045	0.00000193826561
26 h	-0.00000966326122	-0.00000039773895	0.00000002658735
27 h	-0.00000331056649	-0.00000282258359	0.00000012582867
28 h	0.00000476257490	-0.00000306944817	0.00000723968840
29 h	-0.00000444695152	-0.00000429420100	0.00000190738953
30 h	-0.00000962428384	0.00000289391193	-0.00000615342009

31 h	-0.00000390542745	0.00000234432761	-0.00000201664756
32 h	-0.00000168288820	0.00000262252449	-0.00000255812452
33 h	-0.00000242209945	-0.00000529393917	0.00000048763804
34 h	-0.00000805080635	-0.00000131262247	-0.00000777203069
35 h	-0.00000453525290	-0.00000347617123	-0.00000940862190
36 h	-0.00000657589108	0.00000465149920	-0.00000623449653
37 h	-0.00000487993354	0.00000302418291	-0.00000278445384
38 h	-0.00000239194428	-0.00000259790526	0.00000289689141
39 h	-0.00000425069413	-0.00000291179825	0.00001112820784
40 h	-0.00000666395956	-0.00000637168220	0.00000686277913
41 h	-0.00000262116945	-0.00000223632816	0.00000046423842
42 h	0.00000188231938	-0.00000843330695	0.00000573040287

****

norm of actual CARTESIAN gradient: 8.54368E-05

norm of actual INTERNAL gradient: 1.32141E-04

ENERGY = -1014.4546245576 a.u.; # of cycle = 32

Approximate Hessian read from $hessapprox data section

Hessian updated according to BFGS formula

Number of zero Hessian eigenvalues: 0

```
 ----------------------------------------
| total energy     =  -1014.53091746416  |
 ----------------------------------------
: kinetic energy   =   1004.20103409037  :
```

: potential energy = -2018.73195155453 :

: virial theorem = 1.98981806942 :

: wavefunction norm = 1.00000000000 :

HOMO-LUMO Separation

HOMO : -0.17397827 H = -4.73419 eV

LUMO : -0.06871949 H = -1.86995 eV

HOMO-LUMO gap: 0.10525877 H = +2.86424 eV

SUMMARY OF EXCITATION ENERGIES AND DIPOLE OSCILLATOR STRENGTHS (velocity/length):

Exc.	energy (Eh)	energy (eV)	energy (cm-1)	energy (nm)	Osc.(vel)	Osc.(len)
1 a	0.076290	2.07597	16743.806	597.236	0.00307	0.00276
2 a	0.116103	3.15933	25481.751	392.438	0.00188	0.00178
3 a	0.136640	3.71815	29988.906	333.457	0.03107	0.02564
4 a	0.138022	3.75577	30292.350	330.116	0.00924	0.00769
5 a	0.146167	3.97740	32079.865	311.722	0.00796	0.00744

For the compound **3bd,** ground state: Cartesian coordinates and Cartesian gradients and Energy

: ***No Imaginary frequency was observed.***

****

ATOM CARTESIAN COORDINATES

1 c 0.90333677437769 2.98302744356195 1.21869220332808

2 c	-0.36559316062527	0.78299739031835	0.50118181838294
3 c	-2.77854246142722	0.27759455621114	1.53775795011013
4 c	-3.89034647805524	2.02557512775381	3.19610827229154
5 c	-2.60468307407666	4.23559066955884	3.85199629240538
6 c	-0.20031974554959	4.71464319772043	2.88402162850816
7 n	-3.96481010313344	-2.03182646330509	0.88372559597672
8 c	-2.36103693589087	-4.15844960370140	0.66188005644445
9 c	0.06010633678281	-3.77196997636096	-0.40555369008138
10 c	0.54704103248268	-1.13264394505805	-1.43813806004347
11 c	3.15057141494400	-0.76047774632413	-2.60823598040097
12 o	5.20937439931153	-0.82766028287734	-0.82742777687182
13 c	6.84954197370165	1.03287941115754	-1.45512239449191
14 c	6.03936756971029	2.59938060267558	-3.41903623760176
15 c	3.53731972112675	1.66004380140584	-4.19685521433111
16 o	2.07852719111109	2.46091812972772	-5.76626571151607
17 c	7.49534925334295	4.65219212547667	-4.25965560358967
18 c	9.80109788043830	5.06503761686842	-3.07619108035480
19 c	10.63407021352961	3.48113881110686	-1.09366717352844
20 c	9.18870289785757	1.43757815602295	-0.23543756618910
21 o	9.81422288773367	-0.17285289708061	1.64487881977725
22 c	12.12207260729999	0.17765944870503	2.93226914710720
23 c	1.76426526686001	-5.78577628516402	-0.51388135337995
24 c	1.07806219261858	-8.19879920561095	0.32282656979330
25 c	-1.33293106633152	-8.58901829000831	1.31405149161923
26 c	-3.03758143124403	-6.58145892967151	1.51494142659353
27 c	-6.64704444485317	-2.38436764444971	1.38763703691870
28 c	-8.37312763857138	-0.51241834494703	0.05287108708401
29 c	-7.85859305106939	0.32341220601926	-2.40909442014189

30 c	-9.53451675597328	1.93472704866152	-3.66047870544536
31 c	-11.75848435727516	2.72833270832872	-2.47241902340682
32 c	-12.28996066335516	1.90346341877208	-0.02026702588353
33 c	-10.60303806922057	0.30037061258409	1.23183251859884
34 h	2.77016837047694	3.39720432168328	0.45522233913211
35 h	-5.75733041100045	1.67244872823641	3.98864322061442
36 h	-3.49480134525617	5.57849976752329	5.14530789117102
37 h	0.81469498932005	6.43766403591073	3.39850433223493
38 h	-0.72877105009866	-0.90305733369908	-3.09223149466502
39 h	3.45964109946749	-2.33490904896280	-3.94850962251833
40 h	6.81135160637765	5.85328982077092	-5.79191491824356
41 h	11.01078511076343	6.63133798627389	-3.66580786384868
42 h	12.45669723485510	3.87587580601850	-0.21451311690978
43 h	13.76040827749350	0.00569576423146	1.64741970686644
44 h	12.23012297613150	-1.31839497858958	4.36667628558954
45 h	12.20384936546494	2.03602067521692	3.88274258985336
46 h	3.66612260961281	-5.48099542674161	-1.25138012866694
47 h	2.42869113382945	-9.75612207876460	0.20465852822845
48 h	-1.89184663703551	-10.46013306477434	1.98894118979870
49 h	-4.87378511116131	-6.91161648854674	2.38958896423089
50 h	-7.14013161469181	-4.28340345302435	0.70172679616071
51 h	-7.06765257124668	-2.38406179079976	3.43901233445785
52 h	-6.12029869622938	-0.28525717641913	-3.34268089685884
53 h	-9.09745327844104	2.57578689922643	-5.57551878779050
54 h	-13.06790098818387	3.99074827360331	-3.45232466104262
55 h	-14.01900103439175	2.51863425019107	0.92954918649454
56 h	-11.02598021330777	-0.32409835670241	3.15852723295352

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ATOM		CARTESIAN GRADIENTS	
1 c	-0.00000844175592	-0.00001574690693	0.00000167592159
2 c	-0.00002191478754	0.00001500688217	-0.00000962866443
3 c	-0.00000965224833	0.00000805843285	-0.00005058059335
4 c	-0.00000156105159	0.00000756674417	0.00001046283191
5 c	-0.00001085960548	-0.00000613031034	-0.00001936876188
6 c	0.00002966863430	-0.00002612001296	0.00003623117895
7 n	-0.00000168493092	0.00000835677650	0.00003754936132
8 c	0.00003208309044	0.00002663157287	0.00002543036133
9 c	0.00004032888523	0.00000074692570	0.00003399029313
10 c	-0.00002773986110	0.00001270178345	-0.00003758606946
11 c	-0.00001207779638	-0.00002813394745	-0.00005350830856
12 o	-0.00000334042929	0.00000238433009	0.00000768338222
13 c	0.00001459358378	0.00000091801937	-0.00001257051398
14 c	-0.00001367421222	-0.00000363704968	-0.00002196238912
15 c	-0.00014433484804	0.00010506918089	-0.00000964998860
16 o	0.00014116958059	-0.00009345517157	0.00008299842903
17 c	0.00000048500368	-0.00000326471058	0.00000962999334
18 c	-0.00000774533876	0.00000246172679	0.00001128664758
19 c	-0.00000937514266	0.00000983494517	-0.00000038215545
20 c	0.00000348354498	0.00001564082397	-0.00004030330779
21 o	-0.00000619382851	-0.00000328110074	0.00002257853970
22 c	-0.00000493325921	0.00000672056022	0.00000976037002
23 c	-0.00002392772806	-0.00002236650528	-0.00001014407968
24 c	-0.00000656887198	0.00000416095798	0.00000795509673
25 c	-0.00001829357655	0.00001667871676	-0.00000675252171
26 c	-0.00001774764098	0.00000644249649	-0.00002107397717
27 c	-0.00002615704029	-0.00003884072727	-0.00003609040855

28 c	-0.00003492814178	0.00000497952452	0.00002344540542
29 c	-0.00002311831150	-0.00000840986758	-0.00001807763073
30 c	0.00000536529661	-0.00003375435481	-0.00000379985355
31 c	0.00000883836606	0.00003016452587	0.00003697477030
32 c	0.00000348704796	0.00000787628530	-0.00001771551333
33 c	0.00000568054837	-0.00002477497654	-0.00001880101575
34 h	0.00002764703352	-0.00000960295301	0.00000942169702
35 h	0.00000069025394	-0.00000082345101	-0.00001674683886
36 h	0.00003029987194	-0.00002656933275	0.00004381840769
37 h	-0.00003343515353	0.00003874404896	-0.00006554780172
38 h	-0.00000985602259	0.00001432877316	-0.00001045229364
39 h	-0.00000319889637	-0.00001766459193	-0.00001636549731
40 h	0.00001147046134	-0.00001854173923	-0.00002504751446
41 h	-0.00001895624397	0.00001234447085	0.00001350351188
42 h	-0.00000100509053	-0.00000979304111	-0.00001685674361
43 h	0.00000226848127	0.00000332997268	-0.00000222610495
44 h	-0.00000118649086	-0.00000166802553	-0.00000093032962
45 h	-0.00000631280862	0.00000295760374	-0.00000416734274
46 h	0.00001215520436	0.00000414801288	0.00004169540042
47 h	-0.00002076017001	-0.00001406761857	-0.00003852150287
48 h	0.00000581947574	0.00000773020764	0.00001812968916
49 h	-0.00000800636226	0.00001812529360	0.00000396393050
50 h	0.00000459920066	-0.00002138734754	0.00000656614599
51 h	-0.00000020894871	0.00000986199469	0.00000060114282
52 h	0.00002233220836	0.00004293903104	0.00002308191771
53 h	-0.00002075050197	-0.00001364963630	-0.00001139481230
54 h	0.00000104990428	0.00000416027549	-0.00000344614624
55 h	-0.00001844517234	-0.00003322464975	-0.00001353260876

56 h 0.00003708385485 0.00006915730633 0.00002322577020

****

norm of actual CARTESIAN gradient: 3.71815E-04

norm of actual INTERNAL gradient: 1.09590E-03

ENERGY = -1397.5010685940 a.u.; # of cycle = 18

Approximate Hessian read from $hessapprox data section

Hessian updated according to BFGS formula

Number of zero Hessian eigenvalues: 0

total energy = -1397.50106874115 |

: kinetic energy = 1383.33204973229 :

: potential energy = -2780.83311847345 :

: virial theorem = 1.98986117483 :

: wavefunction norm = 0.99999999990 :

.....

HOMO-LUMO Separation

HOMO : -0.19605636 H = -5.33497 eV

LUMO : -0.05909701 H = -1.60811 eV

HOMO-LUMO gap: 0.13695935 H = +3.72686 eV

For the compound **3db,** excited state: Cartesian coordinates and Cartesian gradients and Energy

****

ATOM CARTESIAN COORDINATES

1 c	0.87707409386944	2.96140463500044	1.26781852702738
2 c	-0.33818785312003	0.70358427143613	0.67302794761082
3 c	-2.75179087449879	0.22818271133522	1.78327572284145
4 c	-3.91861864910169	2.05146752739641	3.36388429928279
5 c	-2.65764548016303	4.27375003329448	3.92200080818259
6 c	-0.25356927560985	4.71875094177837	2.88879566029564
7 n	-3.91969263699598	-2.09488662329961	1.35009522591608
8 c	-2.44927798118060	-4.22343653527798	0.75937677892130
9 c	-0.05200822089036	-3.83294190671000	-0.39125684643220
10 c	0.59641437273396	-1.18778446044242	-1.25818800604511
11 c	3.21173943895513	-0.81518740131424	-2.41461167845292
12 o	5.20817884610081	-0.80731789307663	-0.61382626787839
13 c	6.86910317586630	1.10671543442903	-1.33421457838564
14 c	5.84849781431875	2.63400848139909	-3.31216160409708
15 c	3.44427714237315	1.64978401107957	-3.99109181169696
16 o	1.70943356902432	2.33617937023217	-5.45305831053655
17 c	7.29104496800247	4.75212817143626	-4.16073656162278
18 c	9.63414467135959	5.19133254598921	-3.06178533156848
19 c	10.62753351764520	3.64541795119068	-1.12873376539797
20 c	9.19509570836086	1.54493375422764	-0.23316623122614
21 o	9.95717076016504	-0.05348829913212	1.67005755485935
22 c	12.32341746134694	0.35378127474443	2.78444643454065
23 c	1.51107118814143	-5.92533776408164	-0.75022208225750
24 c	0.72132296757303	-8.35458510912140	-0.06839949488305

25 c	-1.67097424081677	-8.73594957225841	0.99888860279596
26 c	-3.25279184405349	-6.68569821880180	1.42400629141221
27 c	-6.66988196889045	-2.35028154205541	1.73391707285197
28 c	-8.24364618513925	-0.52939146741926	0.16532716097524
29 c	-7.62161491859384	0.01026998611616	-2.35415492094981
30 c	-9.16420418209830	1.59180430999759	-3.79923418640201
31 c	-11.35502222757973	2.63323515452727	-2.75000732748083
32 c	-11.99315260508081	2.09284575636398	-0.24487910273355
33 c	-10.43909330729220	0.52557720939609	1.20753181758492
34 h	2.70586801341529	3.38276420938805	0.43822036221753
35 h	-5.76963542544100	1.70027320304775	4.18710432543791
36 h	-3.53213255227132	5.66412944228658	5.17102261808606
37 h	0.74856883820070	6.46740178022173	3.33276394768214
38 h	-0.63318432548293	-0.80268446540636	-2.93128847438066
39 h	3.50031397055031	-2.40559504643747	-3.75460737699223
40 h	6.55391967429889	5.96515748139751	-5.65770035751908
41 h	10.77231103228209	6.79216366601551	-3.71234435323091
42 h	12.48027572784776	4.06467849543564	-0.33795505104647
43 h	13.89289101834223	0.19310839189669	1.40994262163697
44 h	12.56620113311083	-1.11494159237182	4.23646039640081
45 h	12.46286097146755	2.22736725827021	3.70617601571615
46 h	3.38770674128597	-5.65199755788139	-1.54724741437800
47 h	1.98918315135980	-9.95728768758702	-0.35962603145980
48 h	-2.28392774681180	-10.62917457736354	1.54508318868033
49 h	-5.05989595629431	-6.99582878770771	2.35921230521462
50 h	-7.17702426874063	-4.28415558591759	1.19960321929978
51 h	-7.11757203078905	-2.14790739174652	3.75759823256490
52 h	-5.91551608458011	-0.78730774158091	-3.20274797558500

53 h	-8.64433355775068	2.01238080191236	-5.75258921439808
54 h	-12.55871946382570	3.87100325945639	-3.88309109365370
55 h	-13.69845629006894	2.90428788679280	0.59129115078790
56 h	-10.94404981551056	0.12329781943939	3.17258116679106

****

ATOM CARTESIAN GRADIENTS

1 c	0.00001174313700	-0.00001318477271	0.00002212659271
2 c	-0.00002101740306	0.00003394009492	-0.00002898313974
3 c	-0.00005330769561	-0.00001810839274	-0.00003330868944
4 c	0.00001288140909	0.00003114885079	0.00002274527785
5 c	-0.00001431684465	-0.00000718241365	-0.00000012589642
6 c	0.00000050214264	-0.00000039014806	0.00000467710879
7 n	-0.00000330421170	0.00004317768265	-0.00002772713126
8 c	0.00005063850757	-0.00004795408862	0.00001793673763
9 c	-0.00001867774363	-0.00000415809238	-0.00002093079142
10 c	0.00004406792936	-0.00004683932188	0.00002080102301
11 c	-0.00003340925061	0.00010219065454	-0.00006328956107
12 o	0.00001793821195	-0.00005105513600	-0.00000102656043
13 c	-0.00000479738943	0.00002656283494	0.00002694393867
14 c	-0.00002805874514	0.00002403793974	0.00002962261763
15 c	0.00002301965277	-0.00003685160755	-0.00001834150424
16 o	0.00001242288824	0.00001185073244	0.00001659743058
17 c	0.00000129738298	0.00000198565394	0.00000464176928
18 c	-0.00000057608749	-0.00000463285371	-0.00000058404699
19 c	0.00001961937708	-0.00001431913059	-0.00002531314428
20 c	-0.00003229218395	0.00004524071077	0.00003988833319
21 o	0.00005515758664	-0.00007557588167	-0.00007441530520
22 c	-0.00003786228080	0.00004444529469	0.00004482103886

23 c	-0.00000432419969	-0.00002890906821	-0.00000145249971
24 c	-0.00001031069650	0.00000555374286	-0.00000012497716
25 c	0.00000781012930	-0.00000195527393	-0.00000575326673
26 c	-0.00000351239065	0.00001005666508	0.00000300973920
27 c	-0.00000089512616	-0.00000915382909	0.00001912071205
28 c	-0.00000608713301	-0.00002343095042	-0.00002472216866
29 c	0.00000957784281	0.00002032331652	0.00001171289684
30 c	-0.00001939668330	-0.00001852868595	-0.00000879685304
31 c	0.00002656807103	0.00003321732498	0.00001281412373
32 c	-0.00001846421768	-0.00003001411131	-0.00000766750218
33 c	-0.00000011687063	0.00000594161323	0.00000416106888
34 h	-0.00000099121599	-0.00000274943465	0.00000621573445
35 h	0.00000860412545	-0.00001125510759	0.00000575657945
36 h	0.00000148812264	0.00000201108689	-0.00000098007432
37 h	-0.00000967367804	0.00000657014370	-0.00001083103466
38 h	-0.00001246707370	0.00000725174009	0.00002989416976
39 h	-0.00001205600321	0.00000655404455	0.00000676588906
40 h	-0.00000643355400	0.00000711950674	0.00000848652822
41 h	0.00000227567512	-0.00000107626771	0.00000121664645
42 h	0.00000304213839	-0.00000603029462	-0.00000407158487
43 h	0.00000186804905	-0.00001363182137	0.00000727612638
44 h	-0.00000271807476	0.00000381215000	0.00000717194171
45 h	0.00000347238382	0.00000702167656	-0.00001202318248
46 h	-0.00000123449911	0.00000119505928	0.00002099123387
47 h	0.00000142494343	-0.00000103005288	0.00000077846000
48 h	-0.00000304819980	-0.00000255792726	-0.00001529268694
49 h	-0.00000607869531	0.00000404402754	-0.00000921384961
50 h	0.00000309500643	-0.00000310497031	-0.00000459312248

51 h	-0.00000307062628	-0.00000211373153	-0.00000610808303
52 h	0.00000629870896	0.00000751386106	0.00000263340573
53 h	-0.00000070490215	-0.00000176598882	-0.00000183833699
54 h	-0.00000065513223	0.00000061185769	0.00000023697461
55 h	-0.00000375703230	-0.00000372528444	-0.00000334298472
56 h	0.00000134541223	0.00000525211575	-0.00000018628269

****

norm of actual CARTESIAN gradient: 2.90985E-04

norm of actual INTERNAL gradient: 5.43275E-04

ENERGY = -1397.3987945012 a.u.; # of cycle = 17

Approximate Hessian read from $hessapprox data section

Hessian updated according to BFGS formula

Number of zero Hessian eigenvalues: 0

total energy = -1397.48605798372 |

: kinetic energy = 1383.10626423579 :

: potential energy = -2780.59232221950 :

: virial theorem = 1.98971024171 :

: wavefunction norm = 1.00000000000 :

.....

HOMO-LUMO Separation

HOMO : -0.18357077 H = -4.99522 eV

LUMO : -0.07717207 H = -2.09996 eV

HOMO-LUMO gap: 0.10639869 H = +2.89526 eV

SUMMARY OF EXCITATION ENERGIES AND DIPOLE OSCILLATOR STRENGTHS (velocity/length):

Exc.	energy (Eh)	energy (eV)	energy (cm-1)	energy (nm)	Osc.(vel)	Osc.(len)
1 a	0.087265	2.37459	19152.386	522.128	0.00322	0.00287
2 a	0.122237	3.32624	26827.959	372.745	0.00387	0.00343
3 a	0.135470	3.68634	29732.299	336.335	0.05561	0.05526
4 a	0.139703	3.80152	30661.297	326.144	0.00921	0.00898
5 a	0.142010	3.86428	31167.512	320.847	0.00148	0.00164

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9) (a) M. de M. Silva, T. S.Macedo, H. M. P. Teixeira, D. R. M. Moreira, M. B. P. Soares, A. L. da C. Pereira, V.de L. Serafim, F. J. B. Mendonça-Júnior, M. do Carmo A. de Lima, R. O. de Moura, E. F. da Silva-Júnior, J. X. de Araújo-Júnior, M. D. de A. Dantas, O. O. de E.Nascimento, T. M. S.Maciel, T. M. de Aquino, I. M. Figueiredo, J. C. C. Santos, *J. Photochem. Photobiol. B Biol.* 2018, **189**, 165-175. (b) M. Gensicka-Kowalewska, G.Cholewiński, and K. Dzierzbicka, *RSC Adv.* 2017, **7**, 15776-15804. (c) K. K. K. Leung, and B. H.Shilton, *Biochemistry* 2015, **54**, 7438-7448. (d) X.-Y. Liu, Y.-Y. Ma, W.Zhang, B.Song, L.Ding, M.-K. Fung, and J.Fan, *Chem. - Eur. J.* 2018, **24**, 11755-11762. (e) A. A. Kulago, E. M. Mes, M.Klok, A. Meetsma, A. M. Brouwer, and B. L. Feringa, *J. Org. Chem.* 2010, **75**, 666-679.
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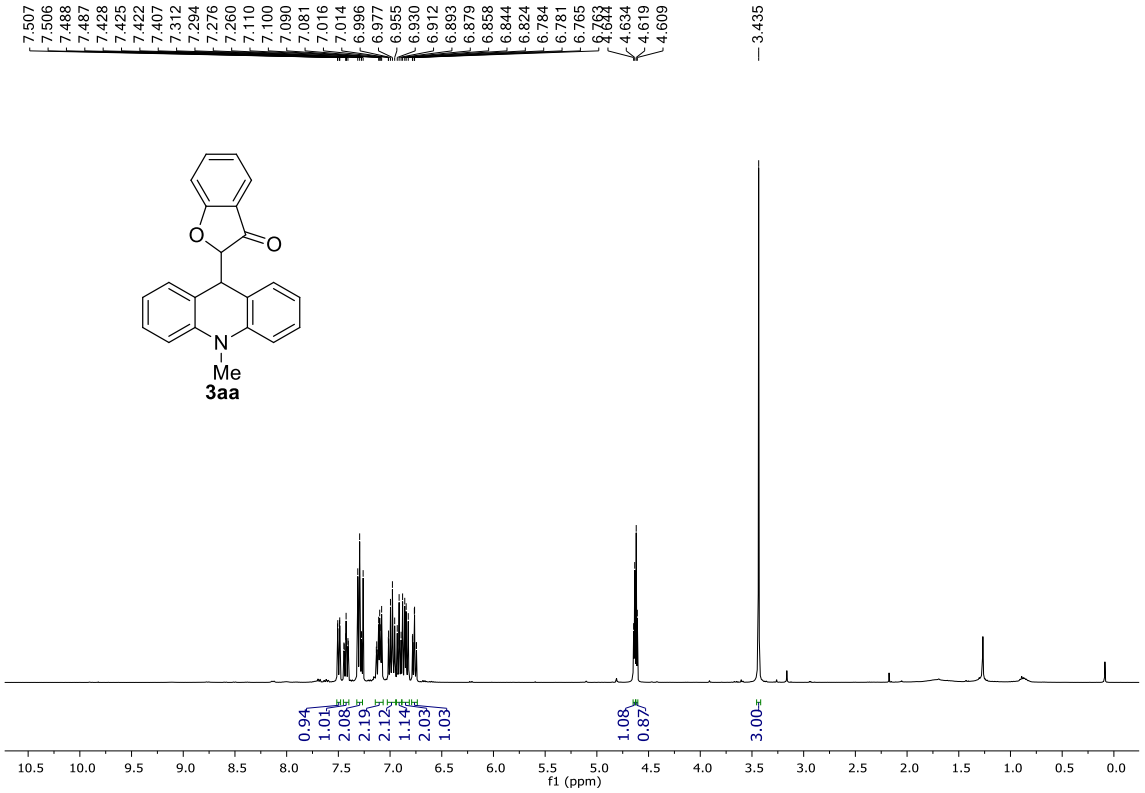
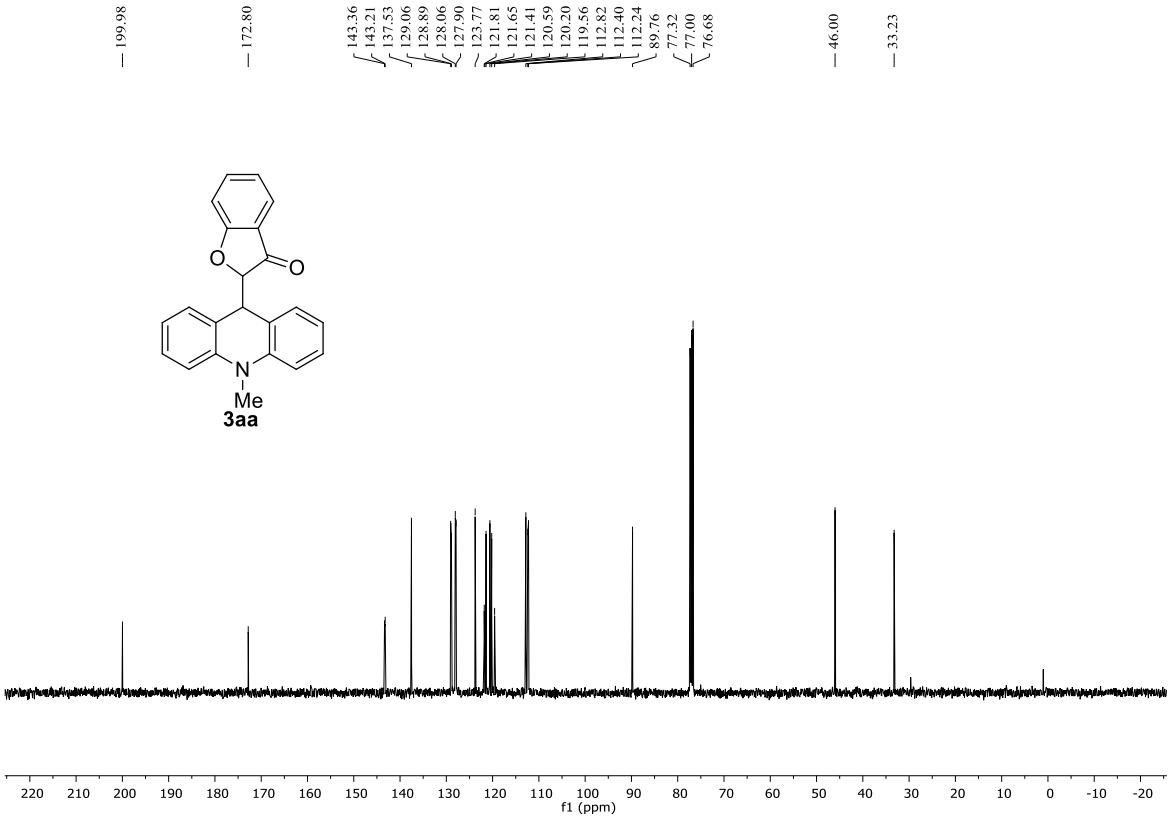
^{1}H and ^{13}C NMR spectra of compounds:

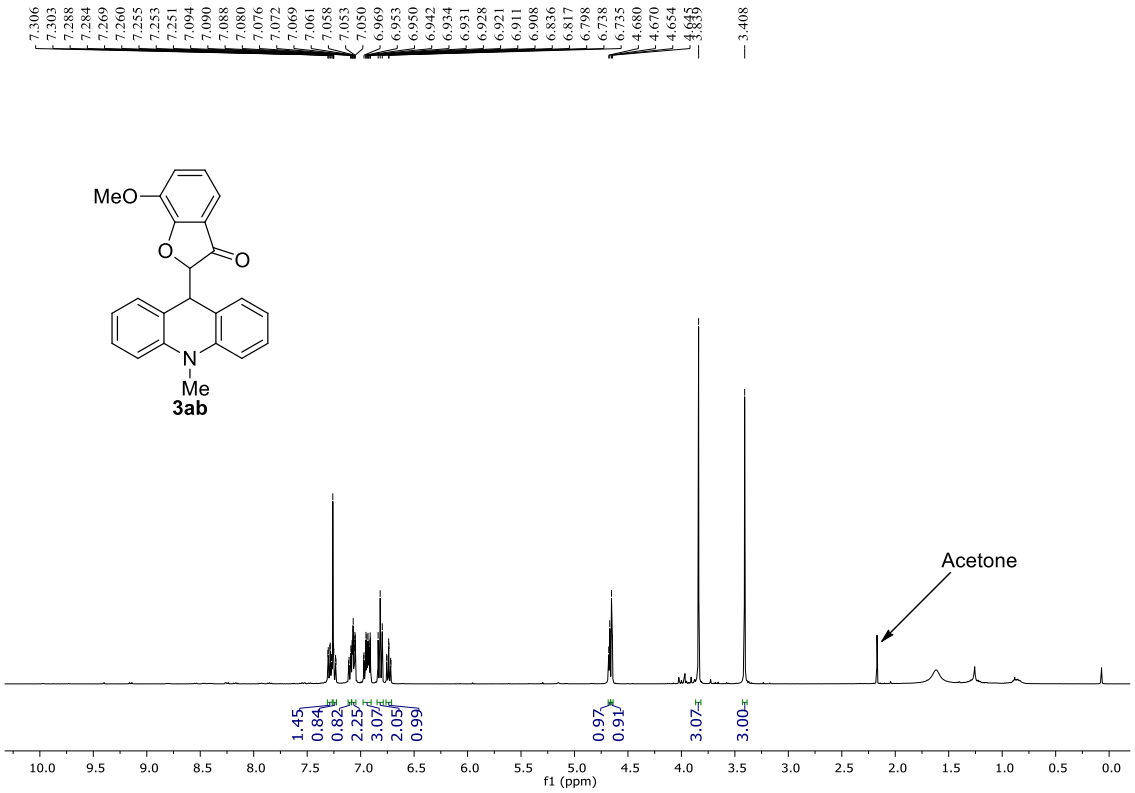
^{1}H NMR of **3aa** (400 MHz, $CDCl_3$):



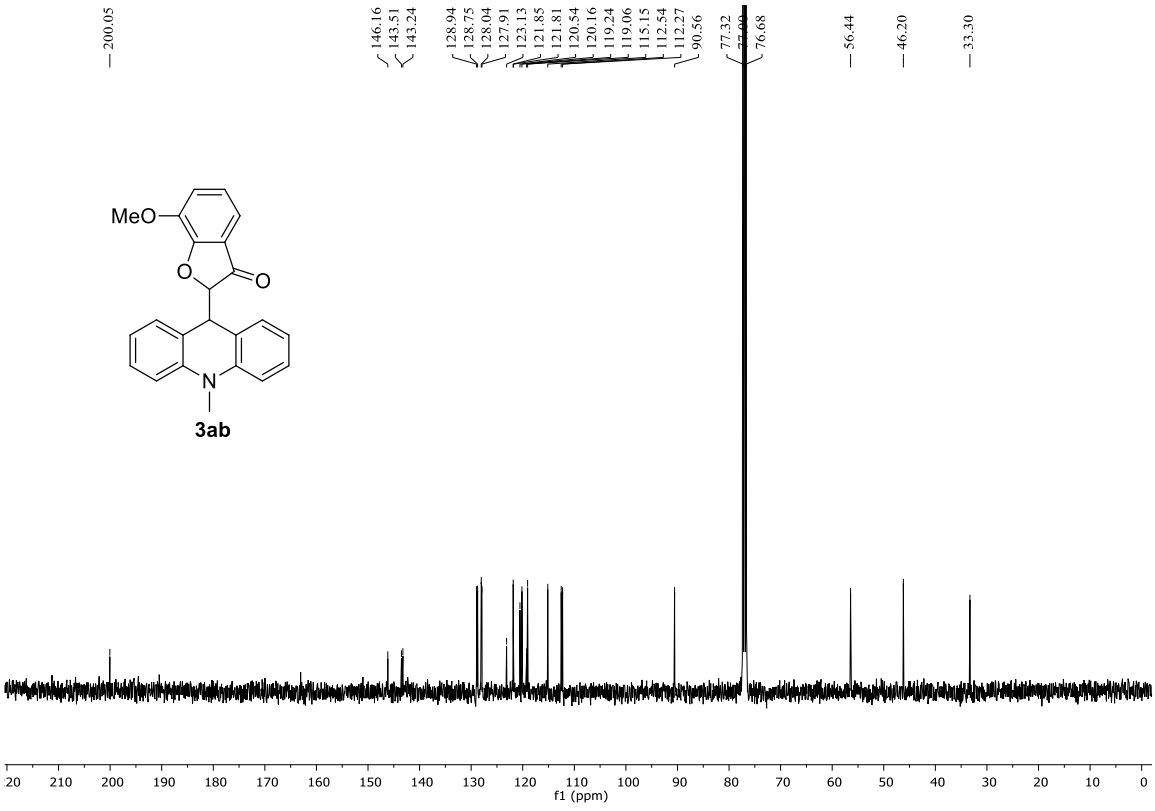
^{13}C {^{1}H} NMR of **3aa** (100 MHz, $CDCl_3$):



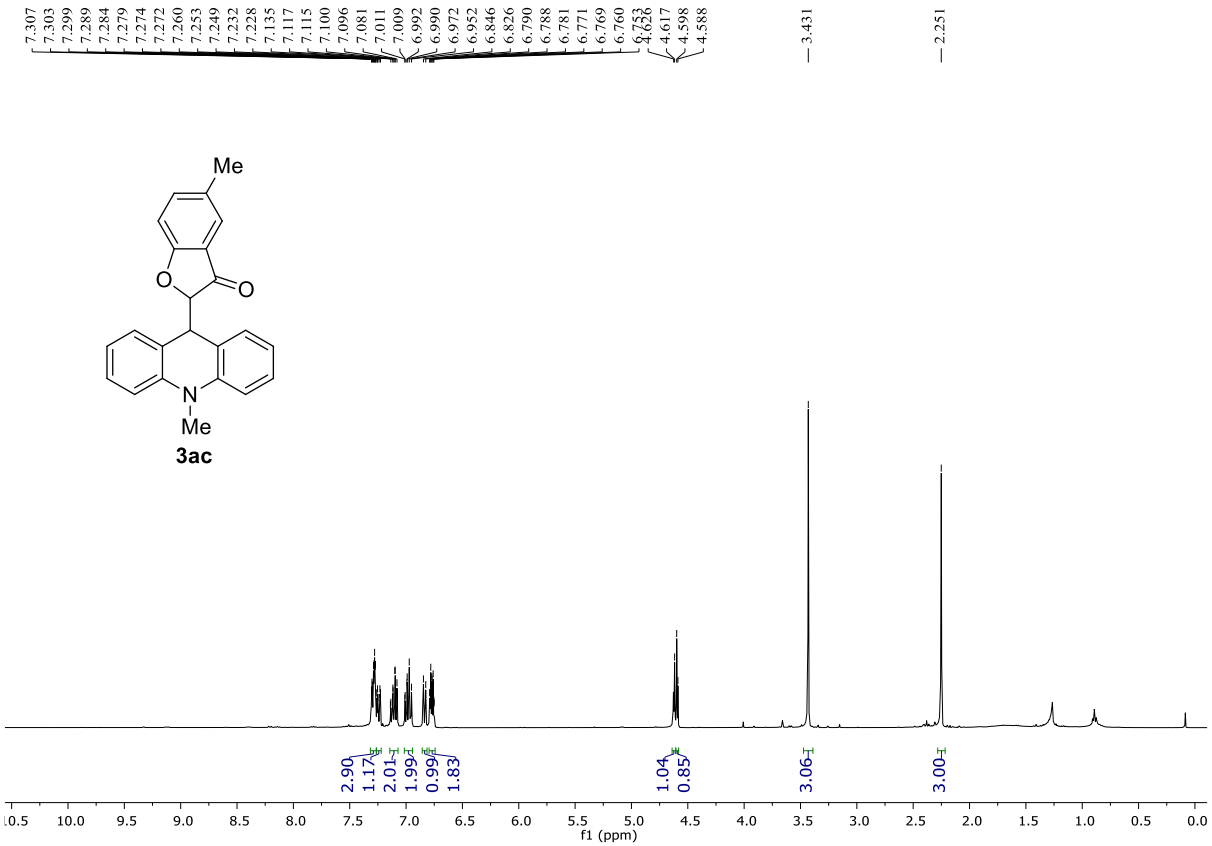
^{1}H NMR of **3ab** (400 MHz, $CDCl_3$):



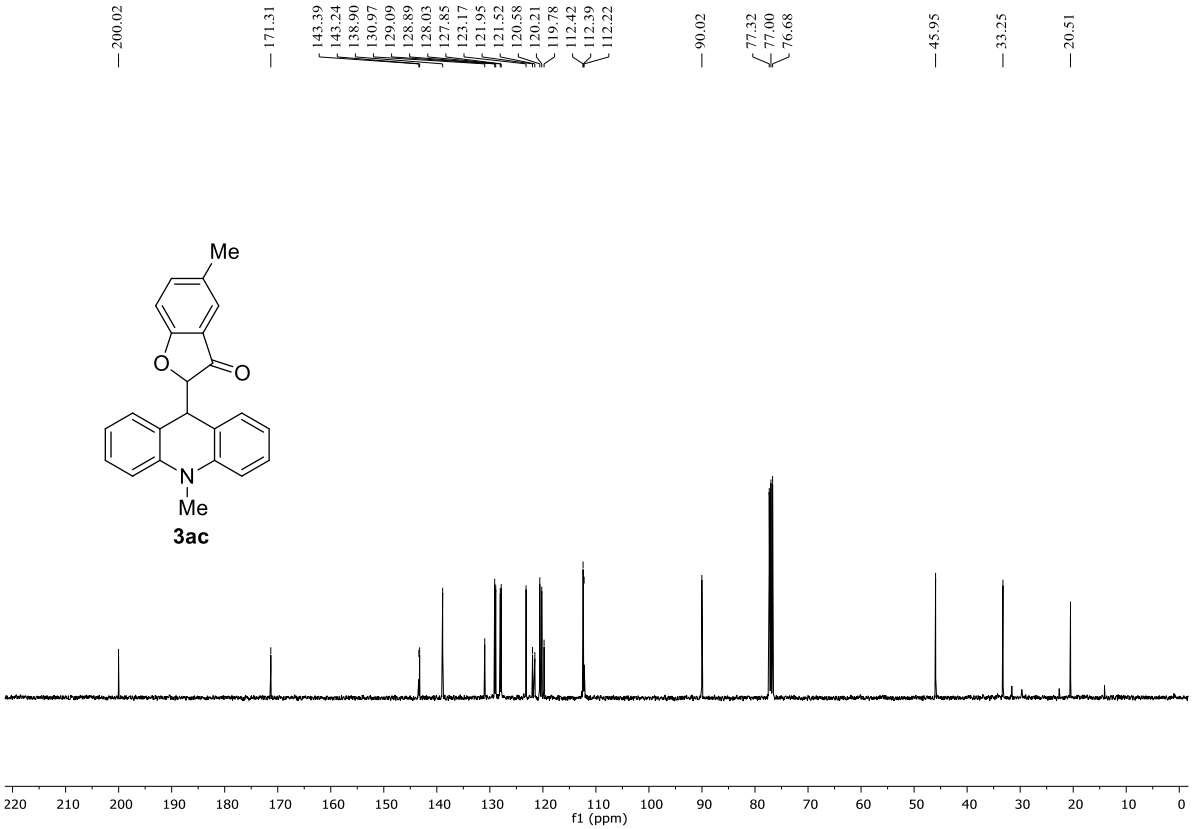
^{13}C {^{1}H} NMR of **3ab** (100 MHz, $CDCl_3$):



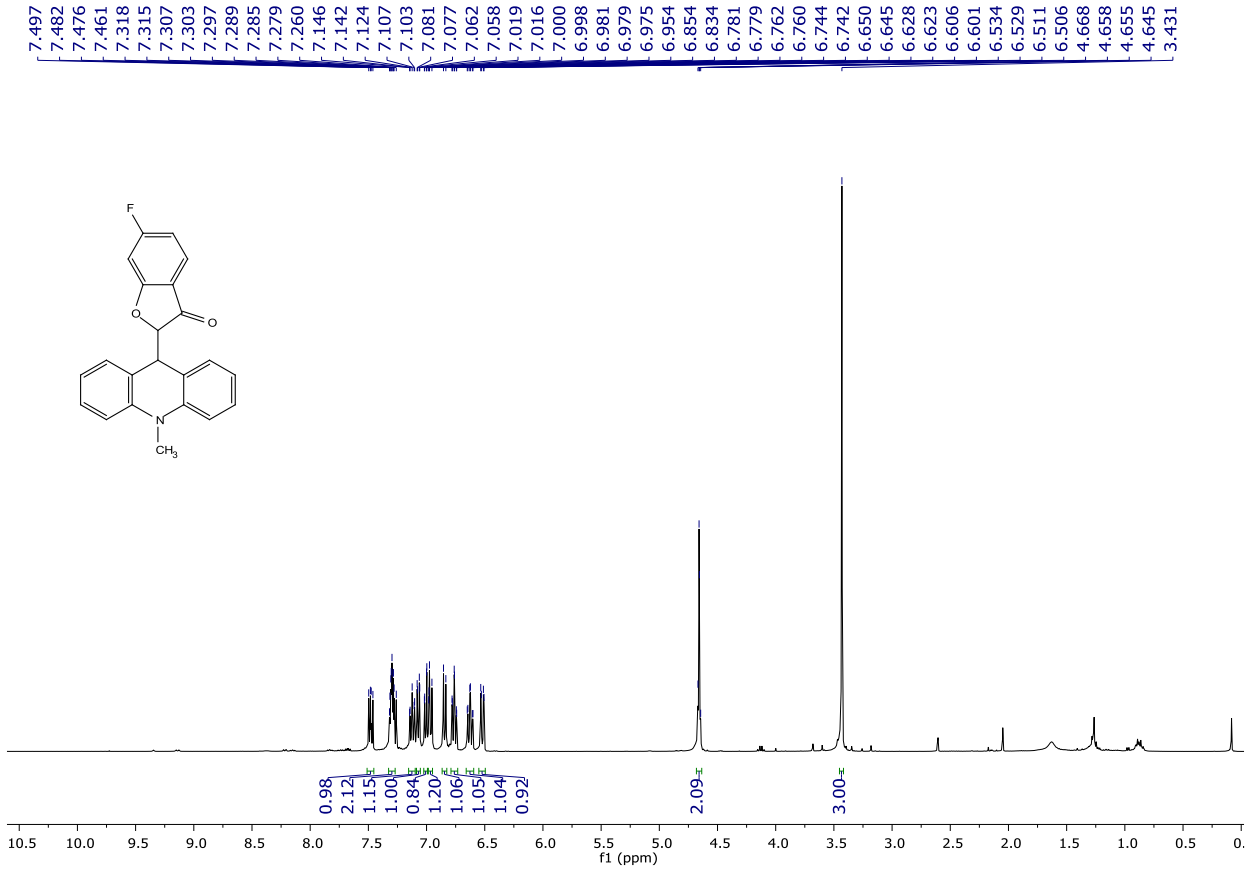
^{1}H NMR of **3ac** (400 MHz, $CDCl_3$):



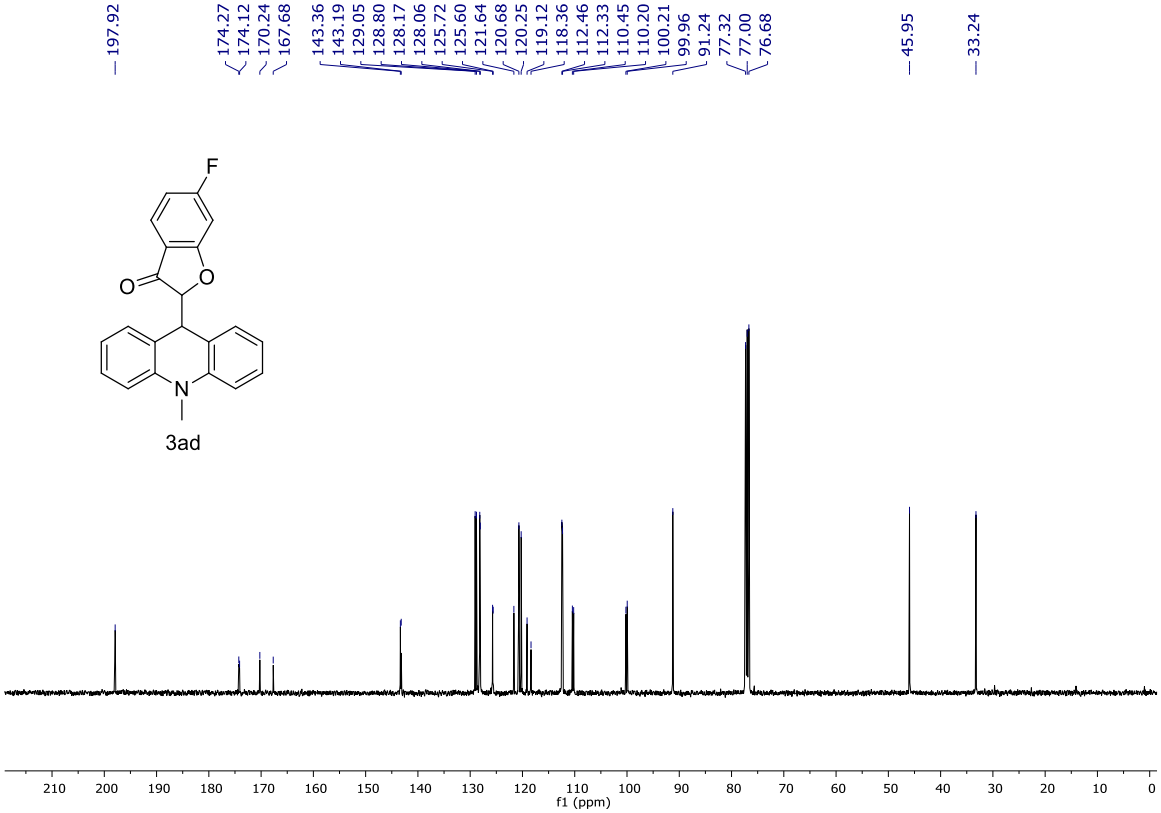
^{13}C {^{1}H} NMR of **3ac** (100 MHz, $CDCl_3$):



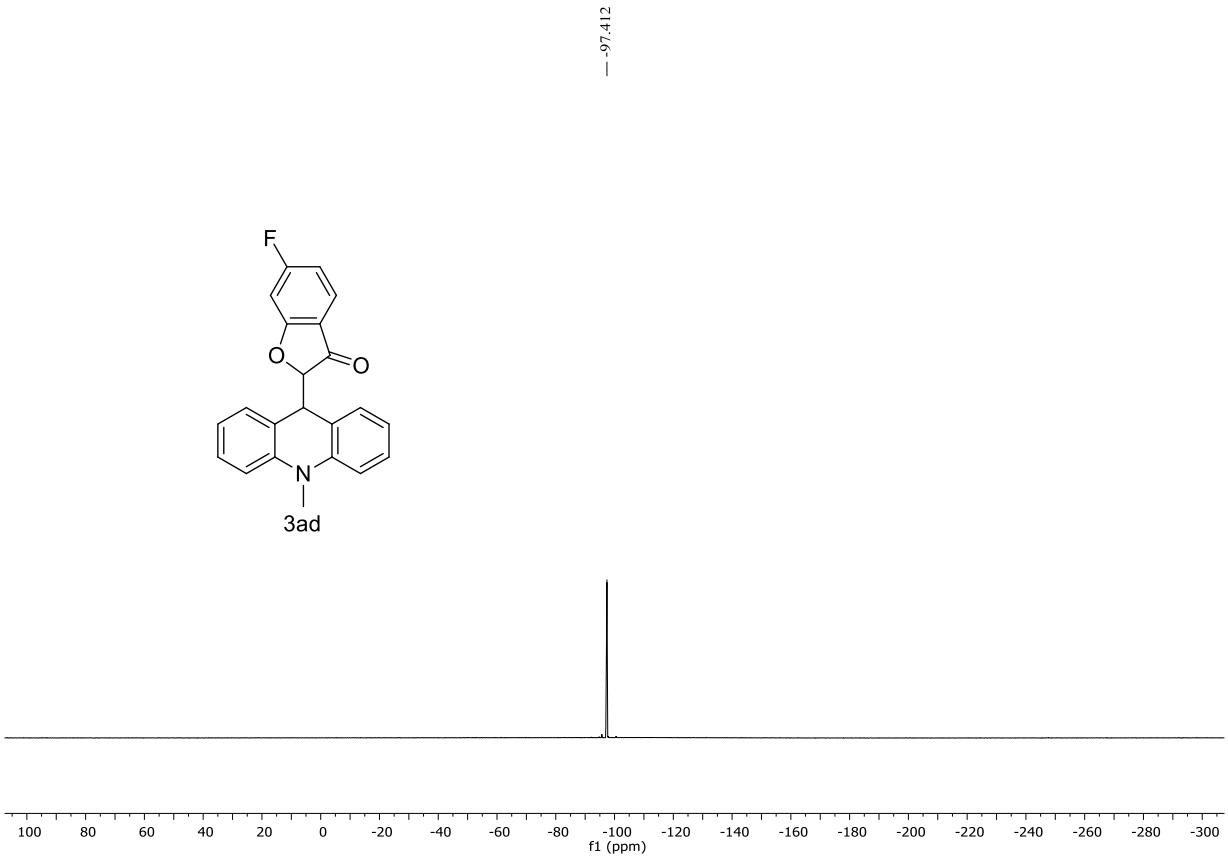
^{1}H NMR of **3ad** (400 MHz, $CDCl_3$):



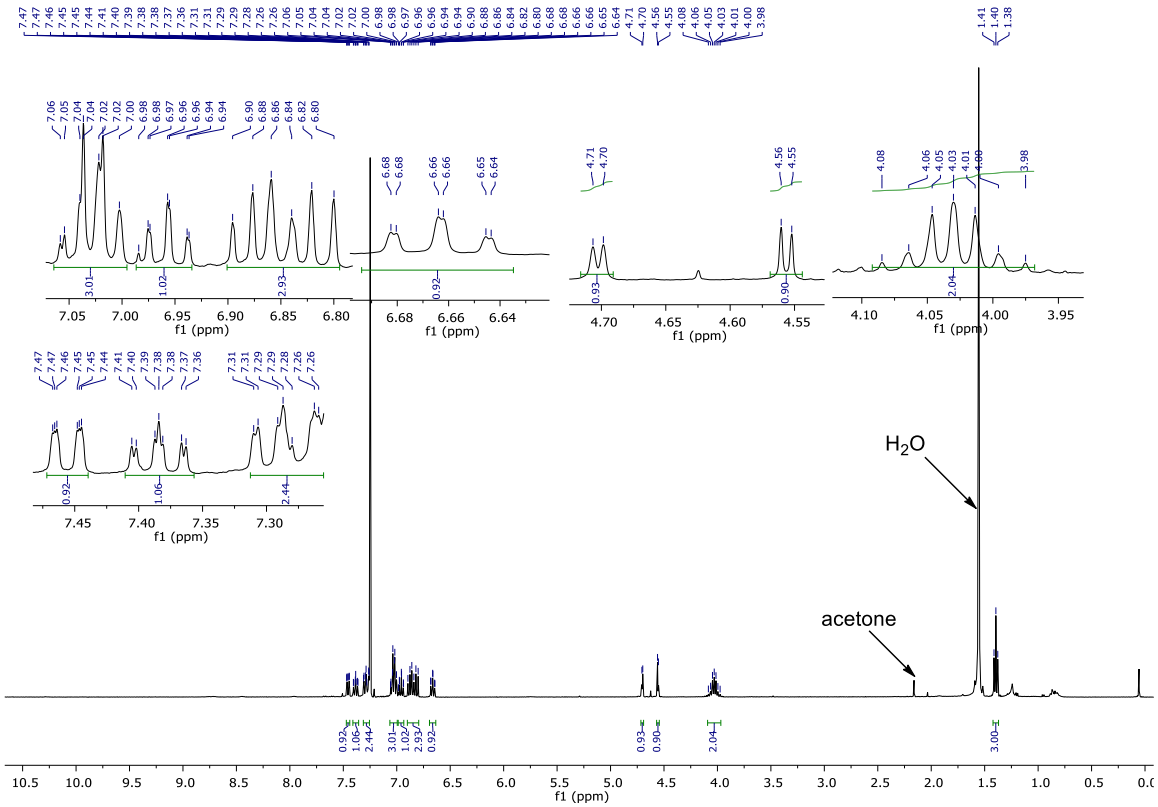
^{13}C {^{1}H} NMR of **3ad** (100 MHz, $CDCl_3$):



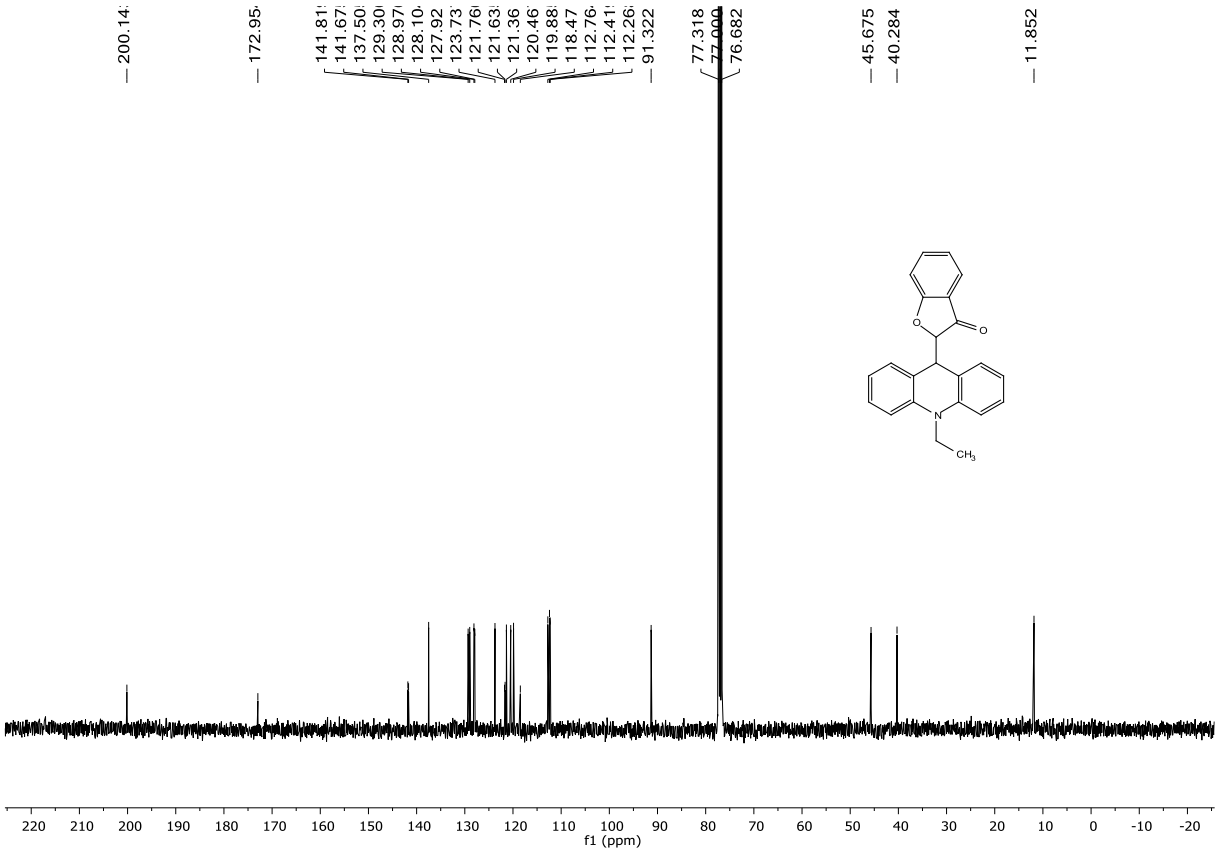
^{19}F NMR of **3ad** (376 MHz, $CDCl_3$):



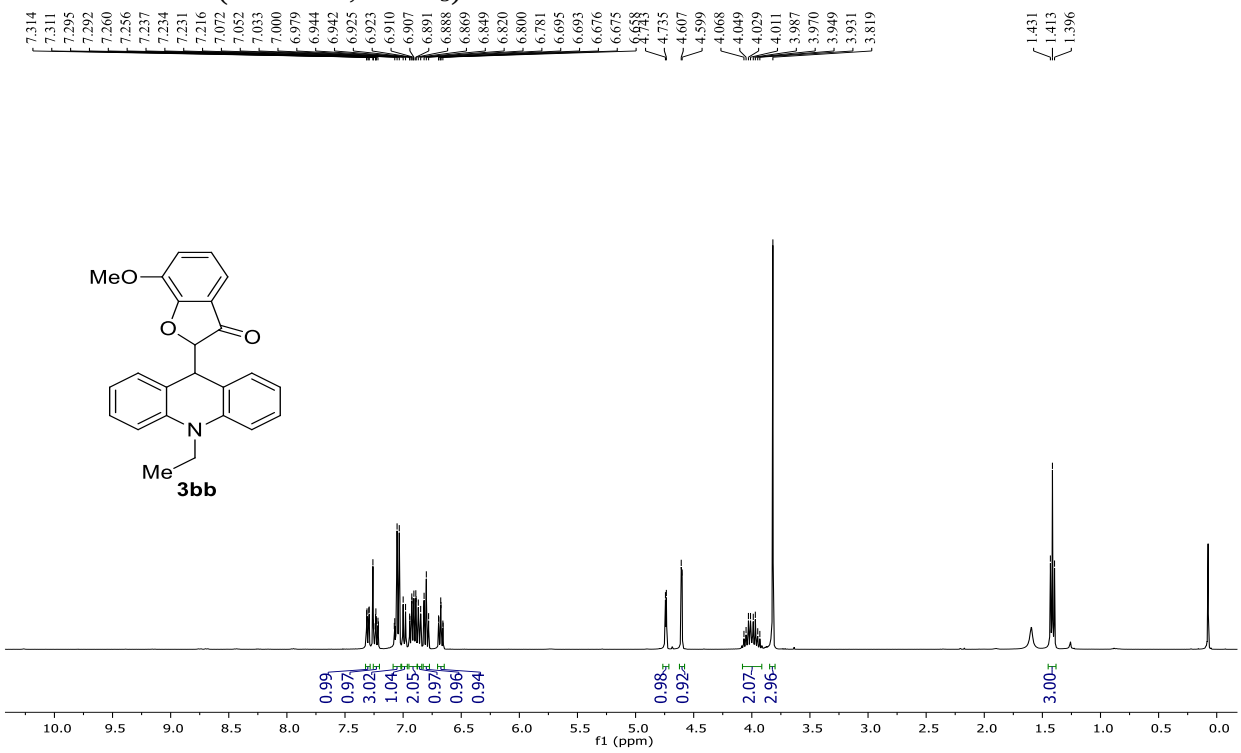
^{1}H NMR of **3ba** (400 MHz, $CDCl_3$):



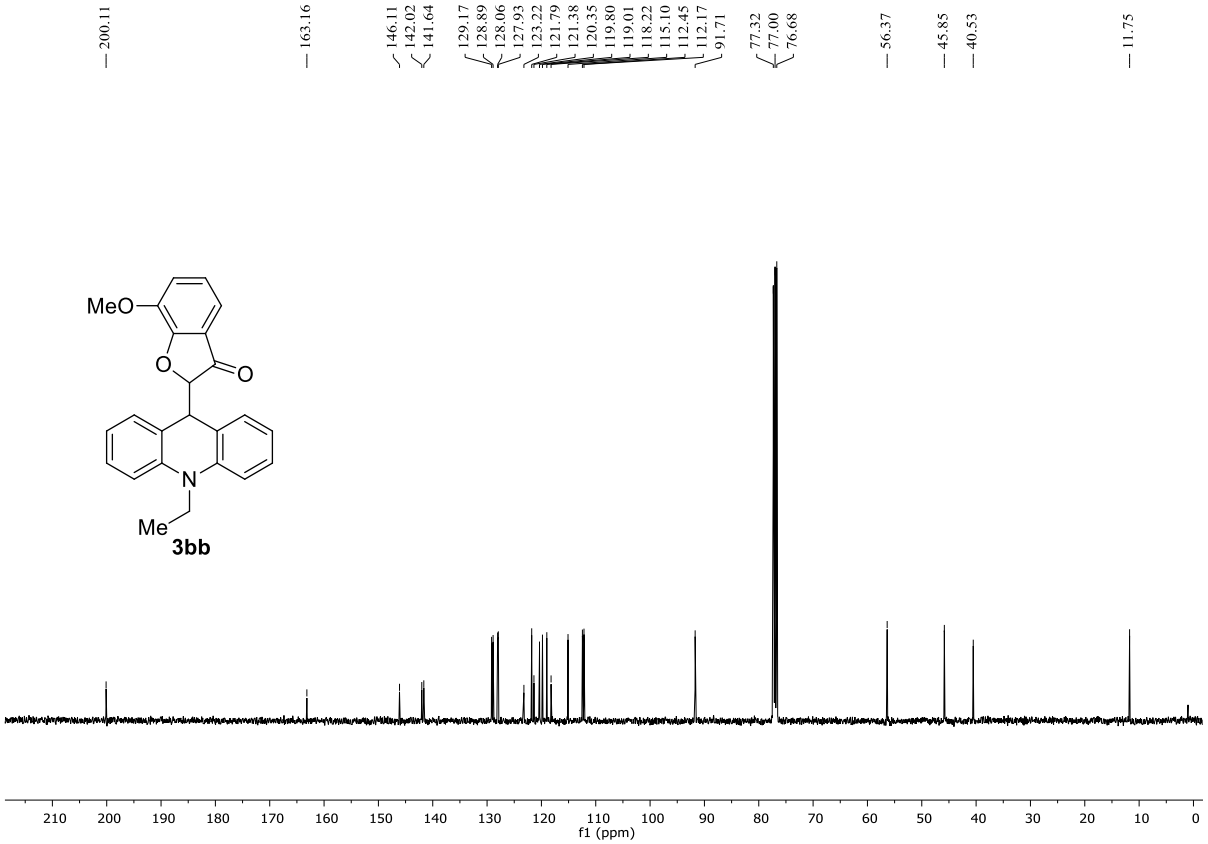
^{13}C {^{1}H} NMR of **3ba** (100 MHz, $CDCl_3$):



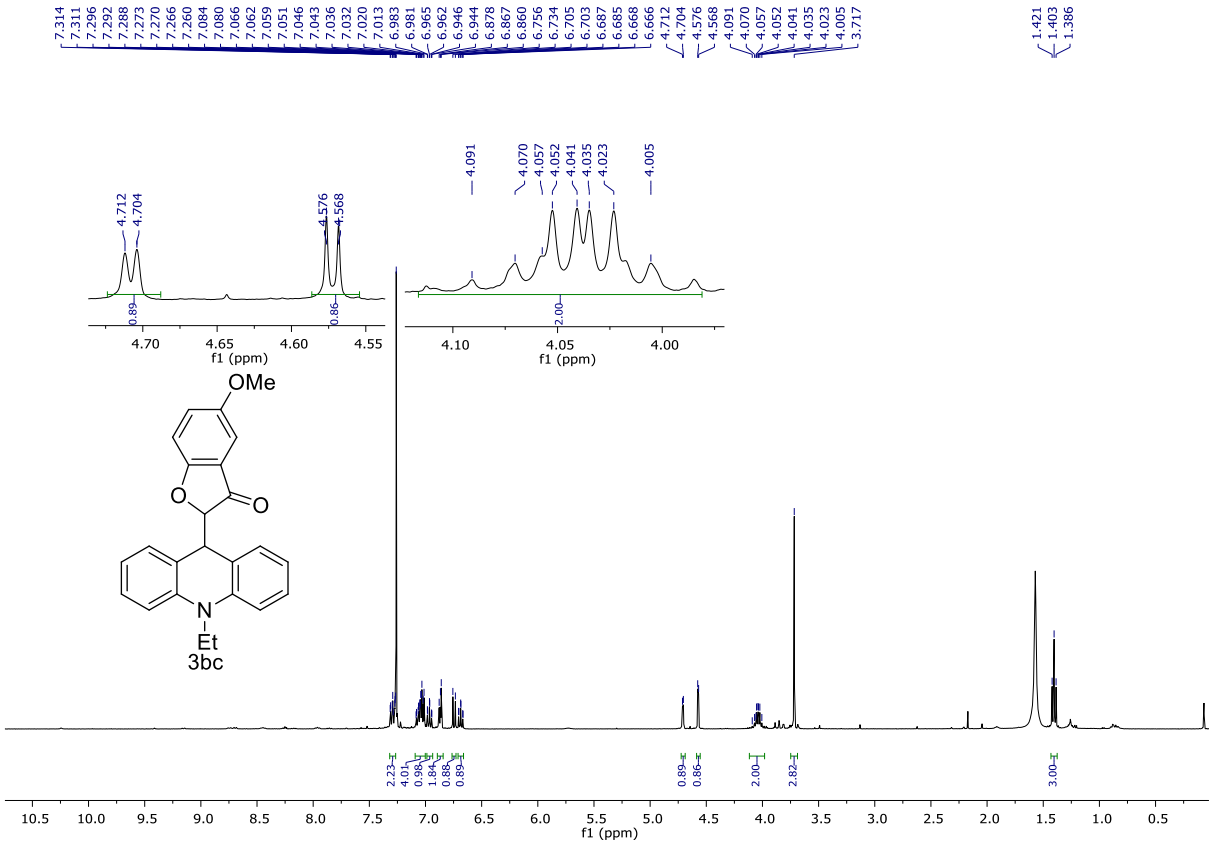
^{1}H NMR of **3bb** (400 MHz, $CDCl_3$):



^{13}C {^{1}H} NMR of **3bb** (100 MHz, $CDCl_3$):



^{1}H NMR of **3bc** (400 MHz, $CDCl_3$):



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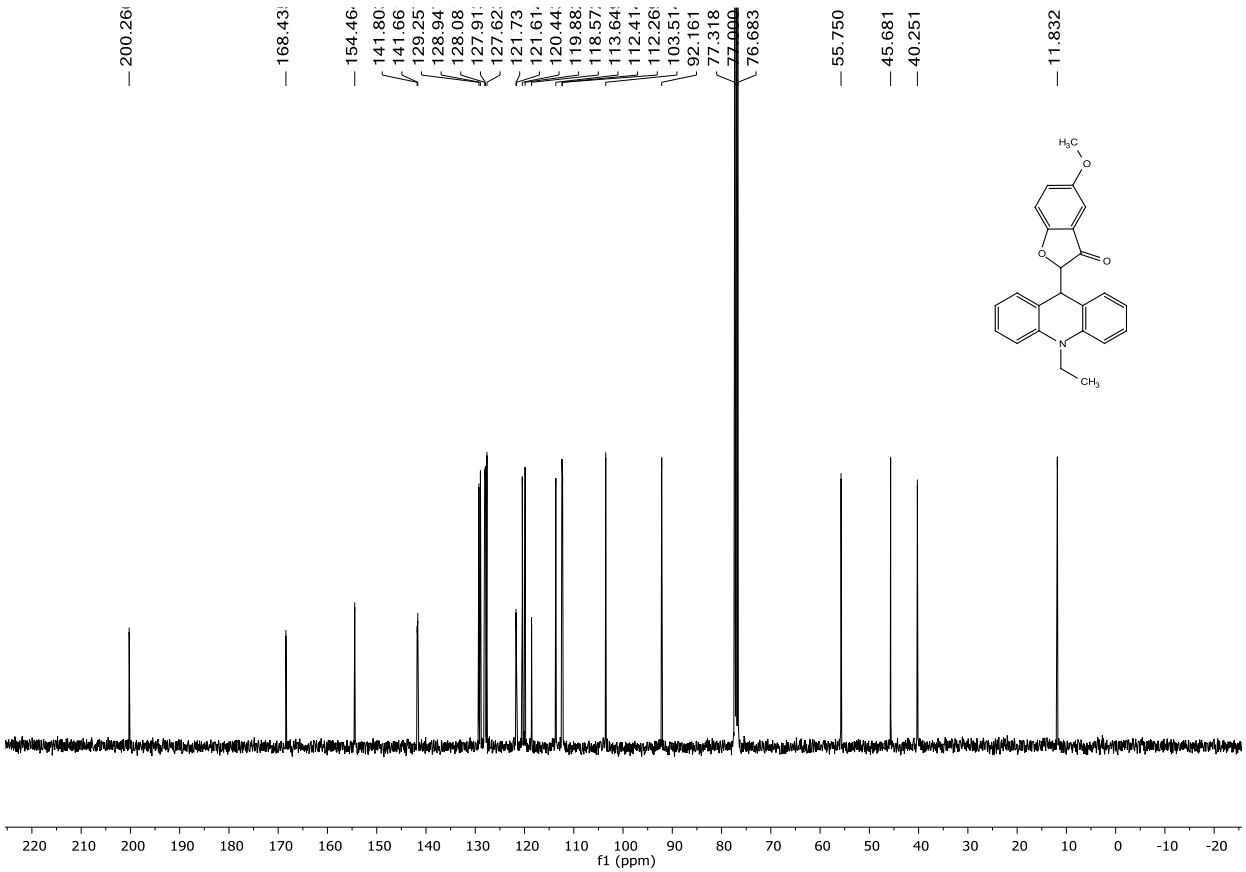
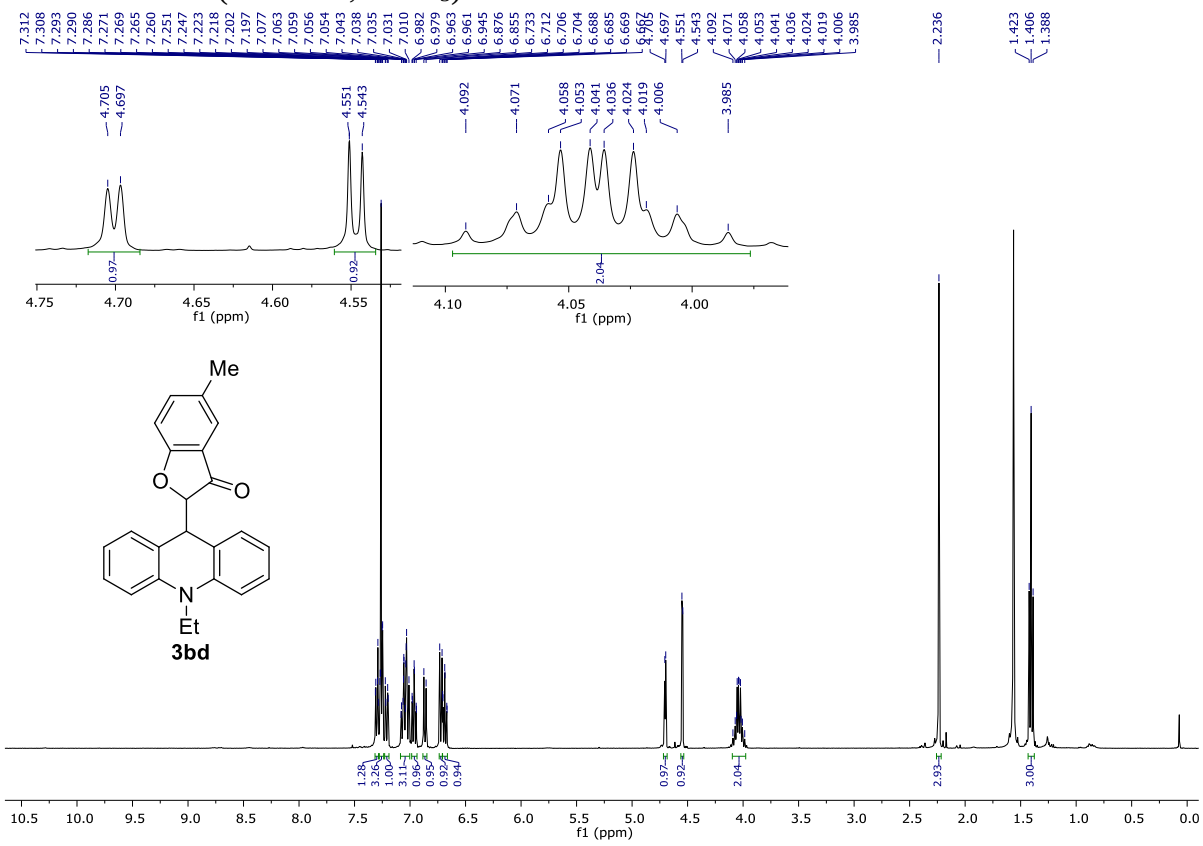
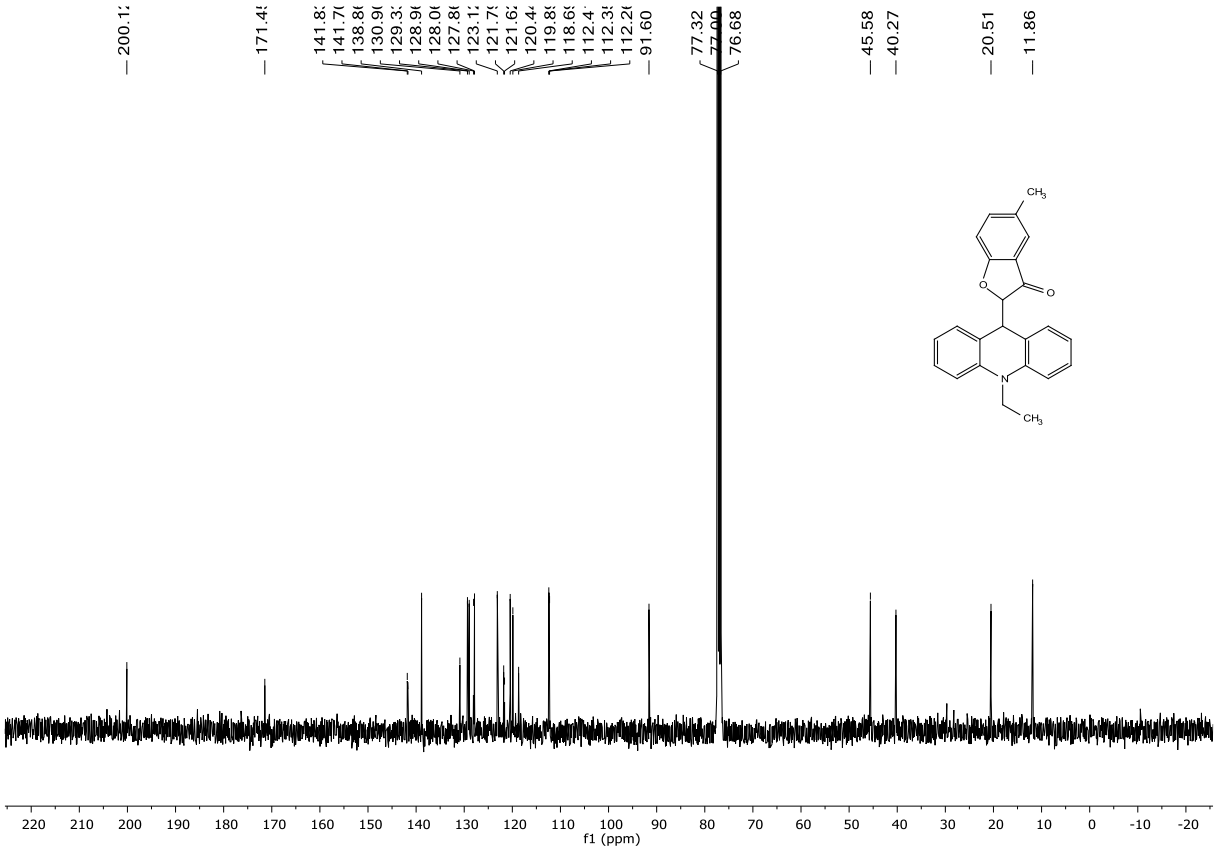


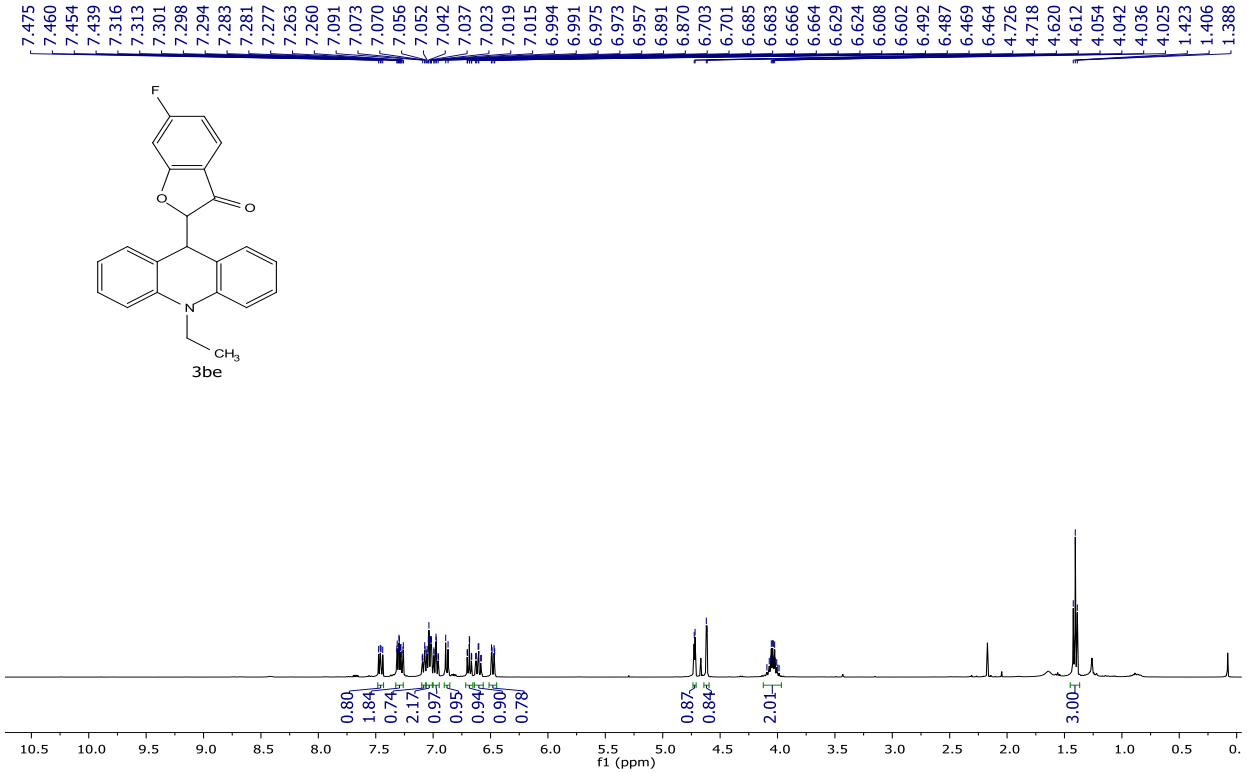
^{1}H NMR of **3bd** (400 MHz, $CDCl_3$):



^{13}C {^{1}H} NMR of **3bd** (100 MHz, $CDCl_3$):



^{1}H NMR of **3be** (400 MHz, $CDCl_3$):



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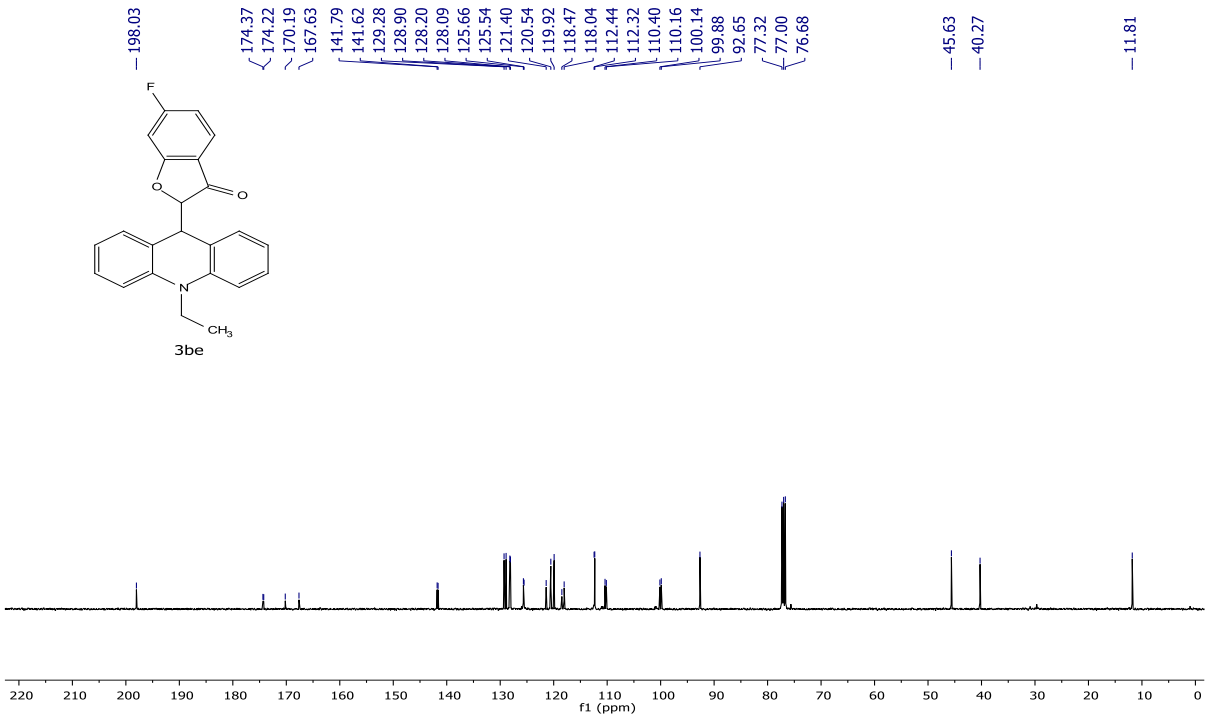
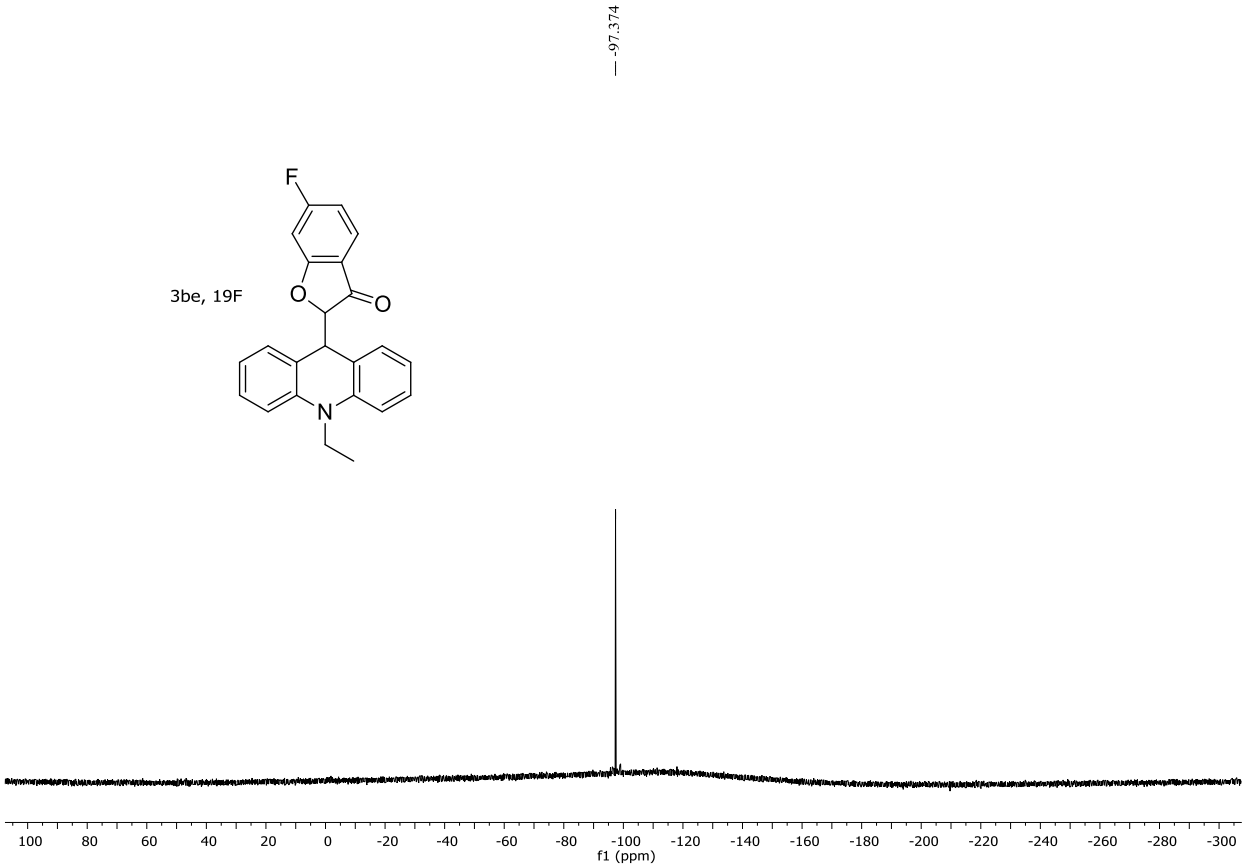


^{19}F NMR of **3be** (376 MHz, $CDCl_3$):



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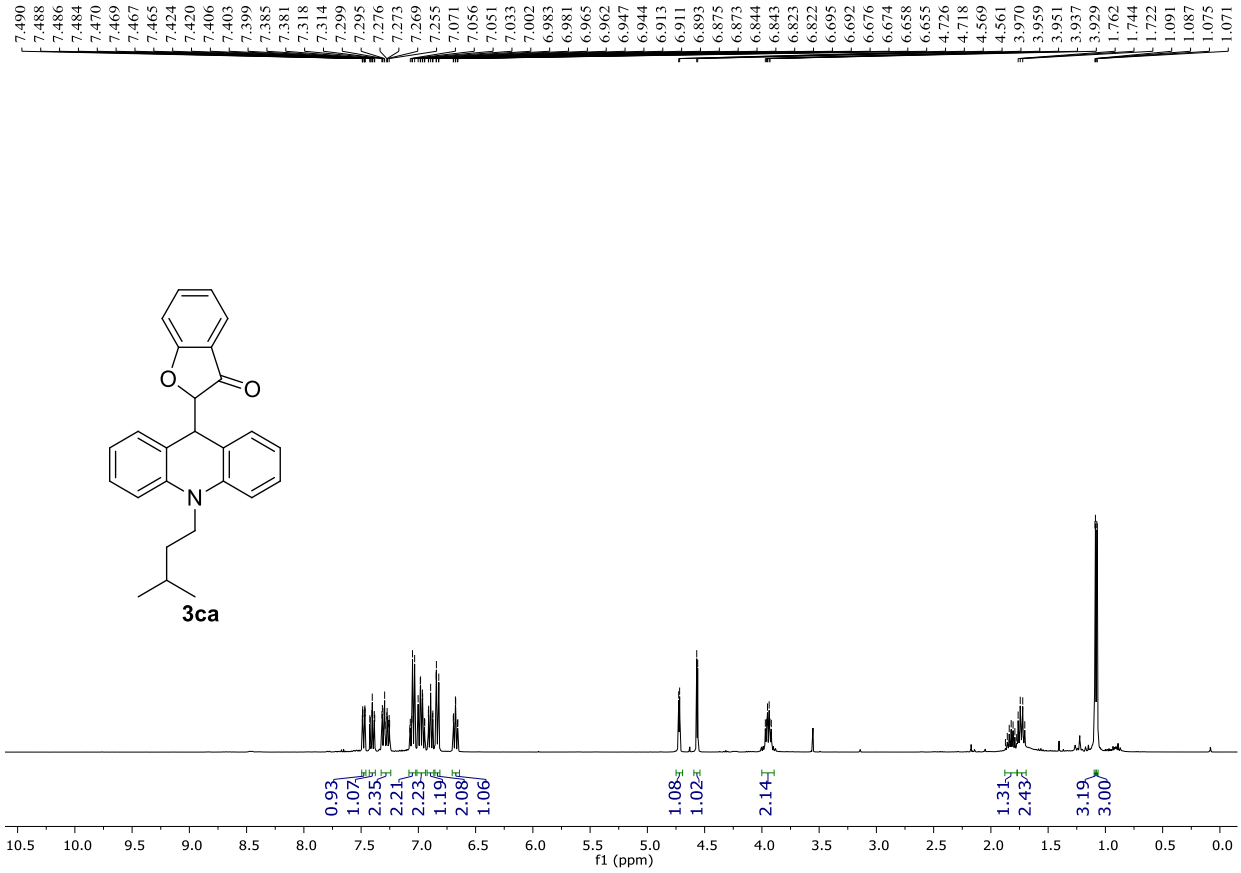

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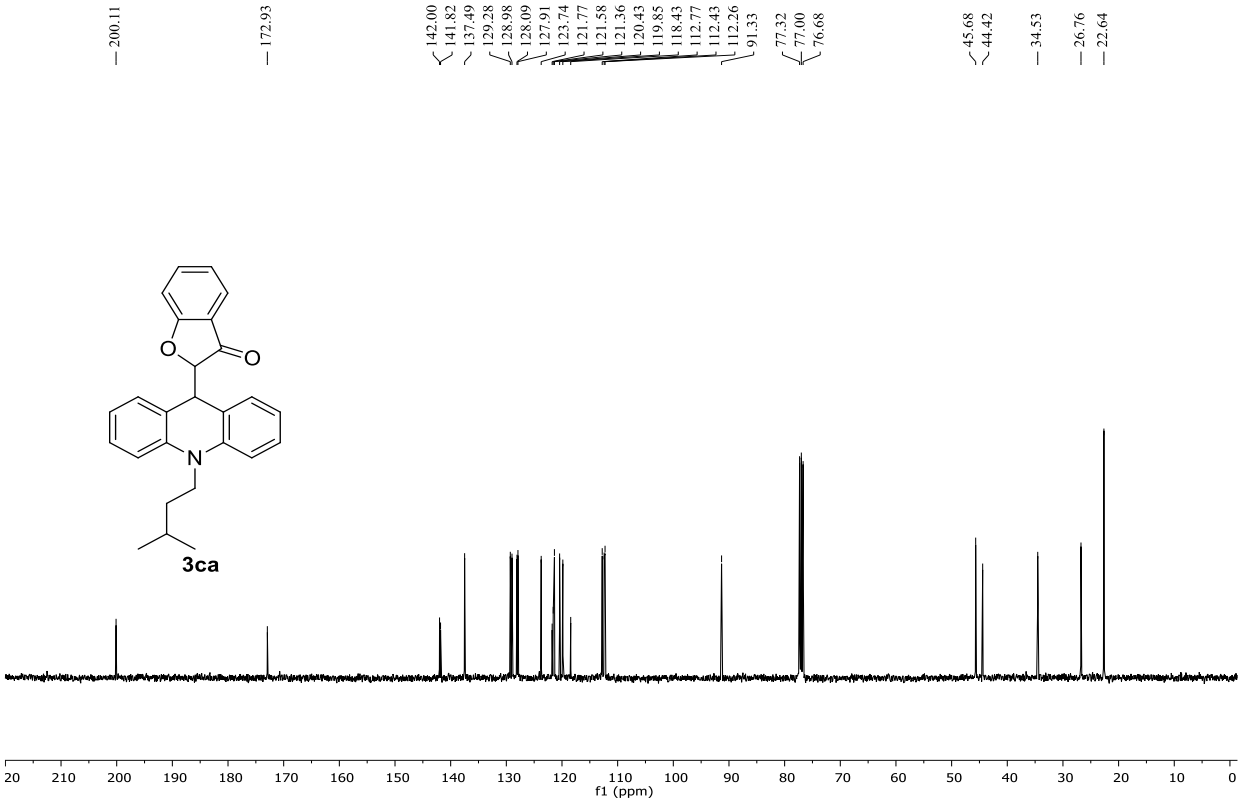
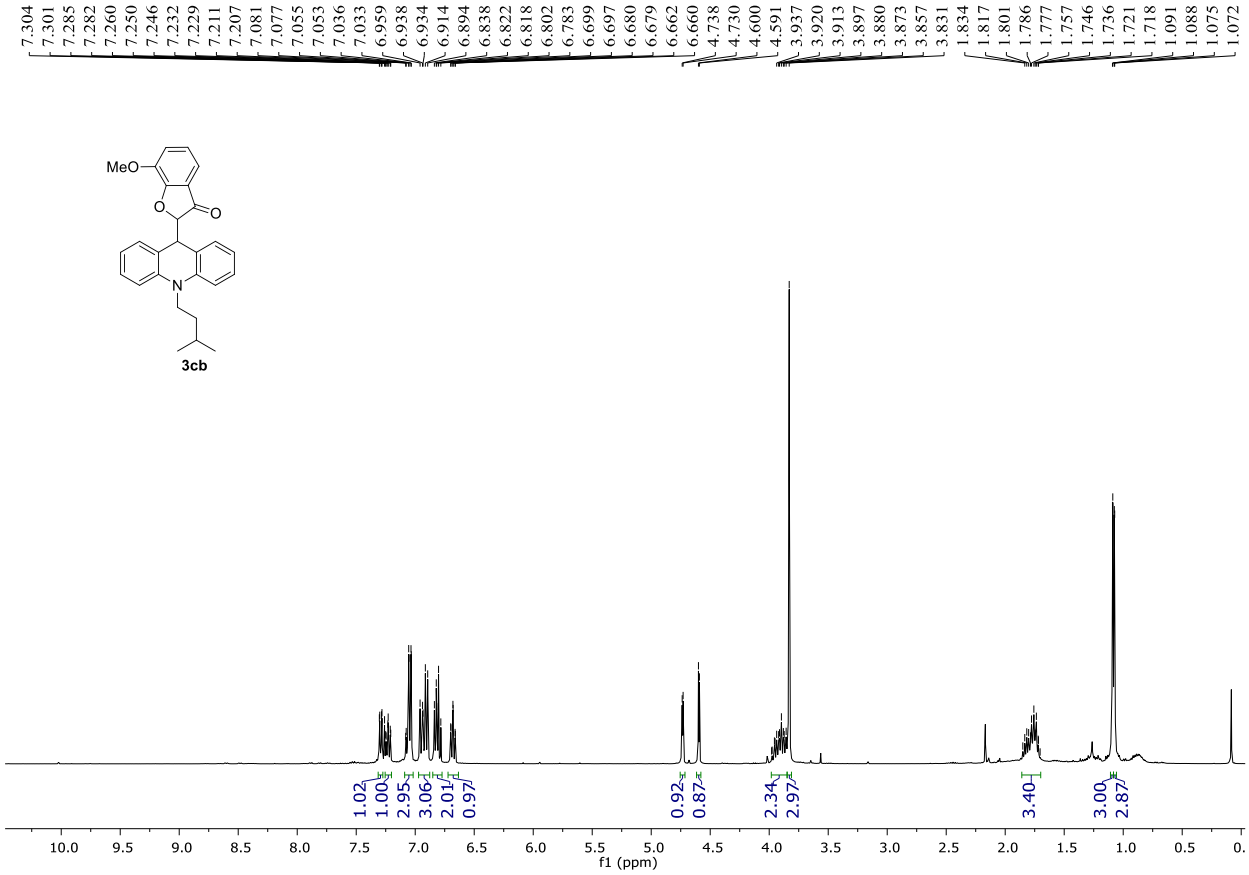
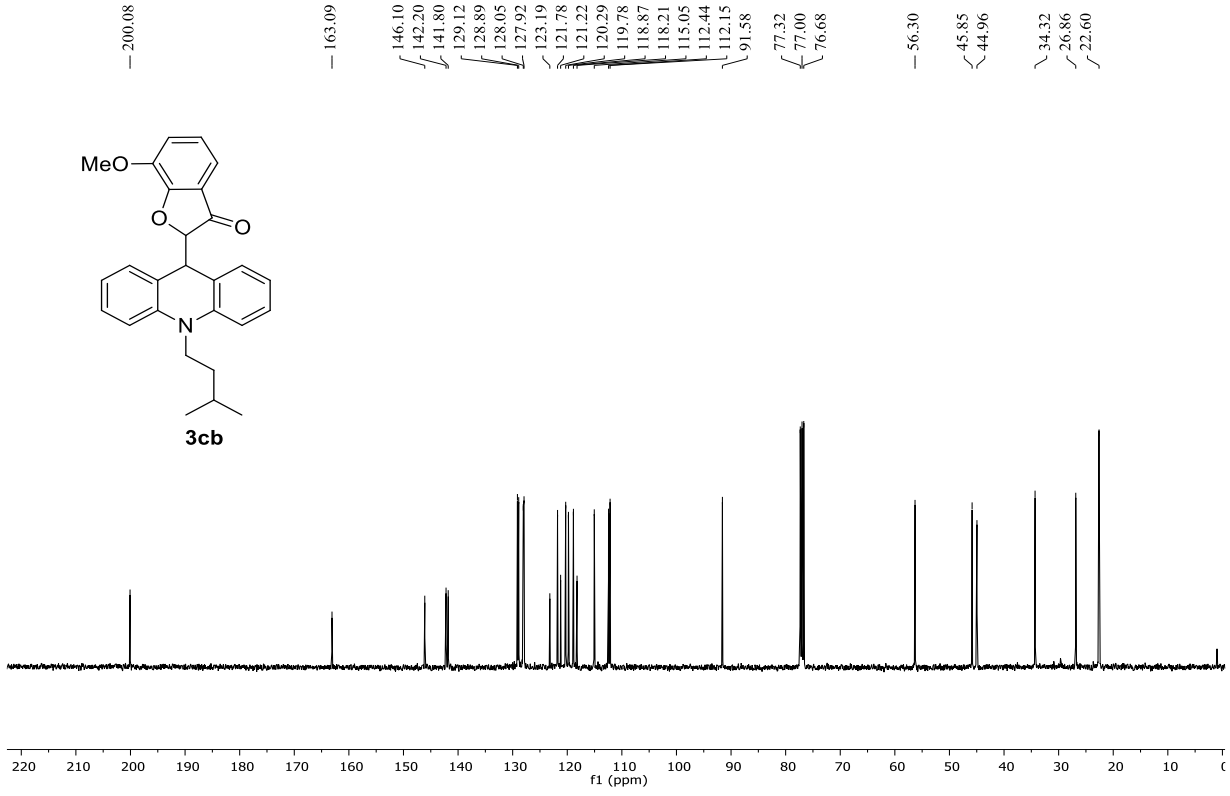


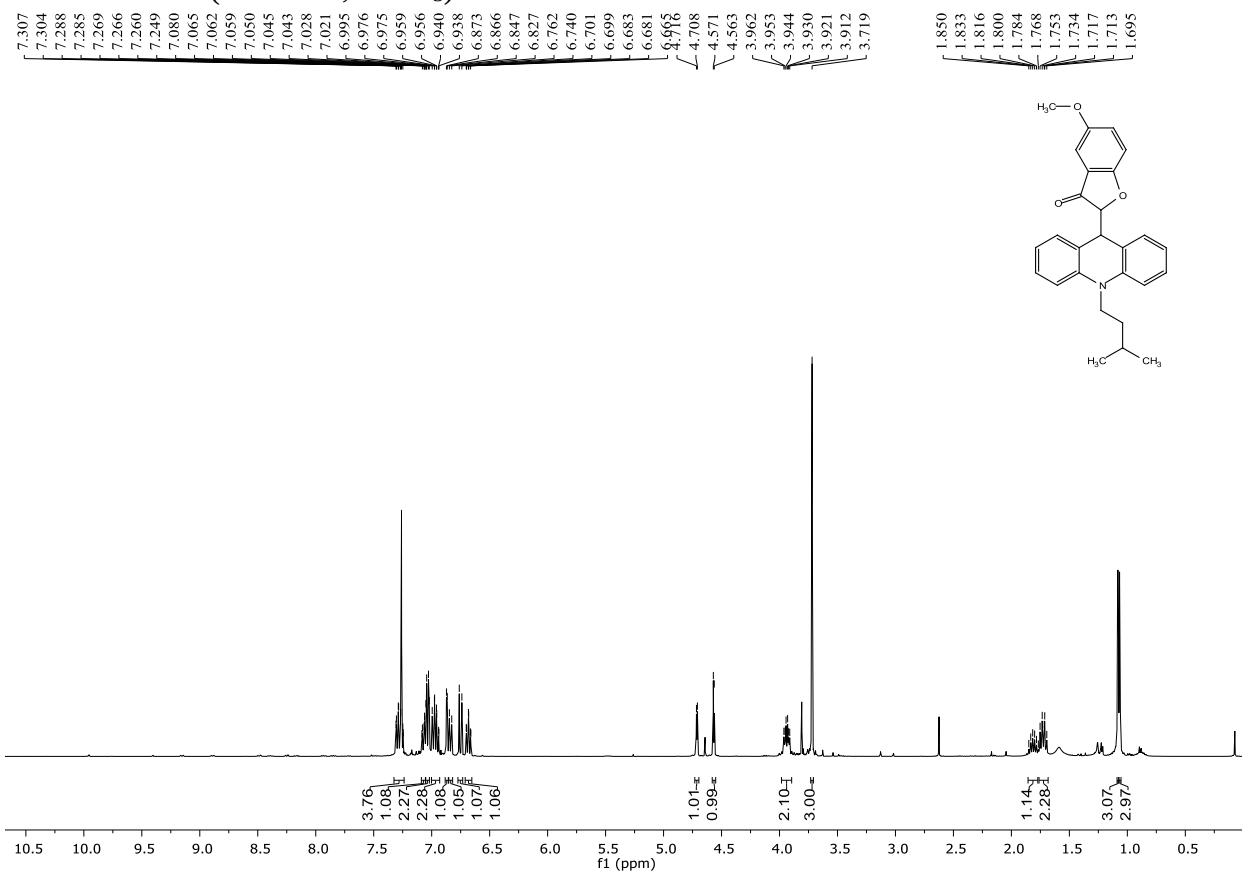
^{1}H NMR of **3cb** (400 MHz, $CDCl_3$):



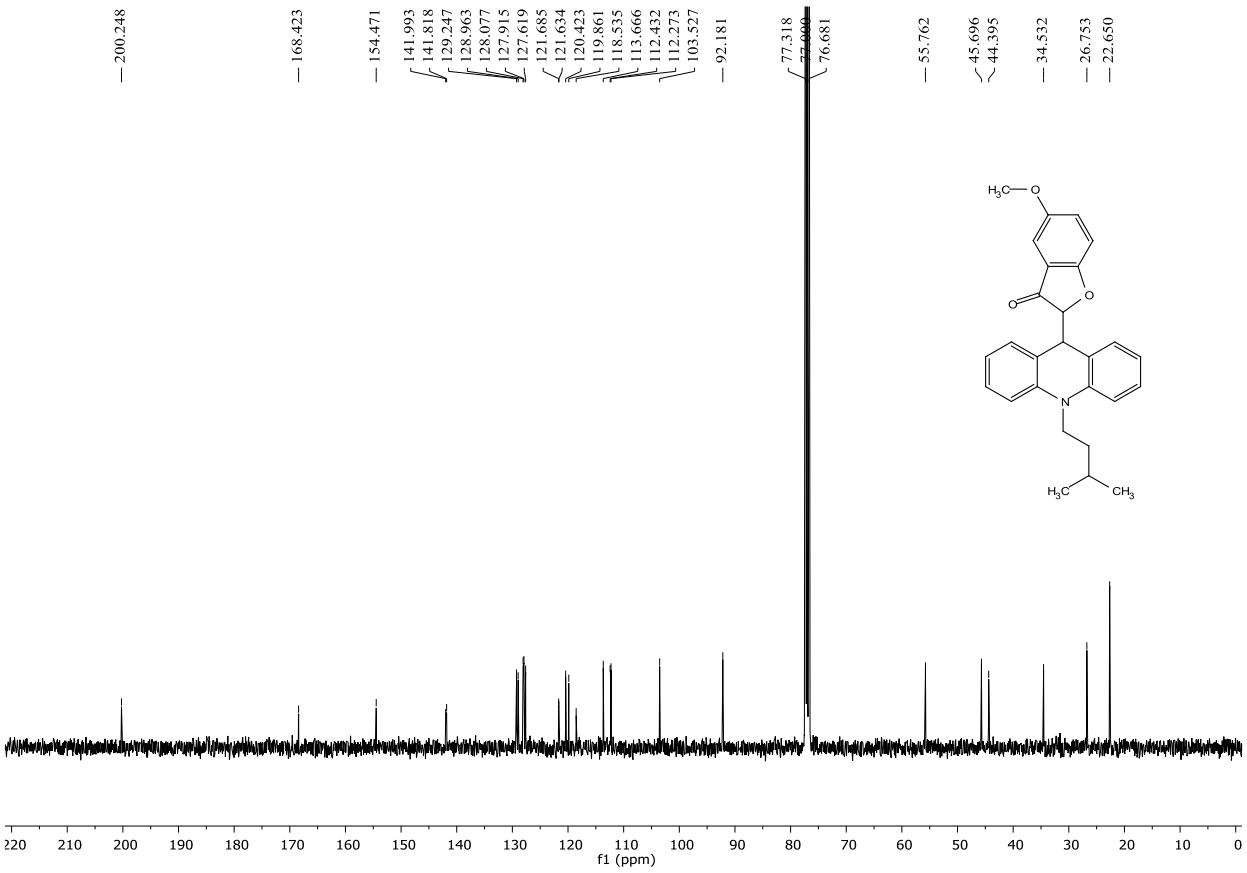
^{13}C {^{1}H} NMR of **3cb** (100 MHz, $CDCl_3$):



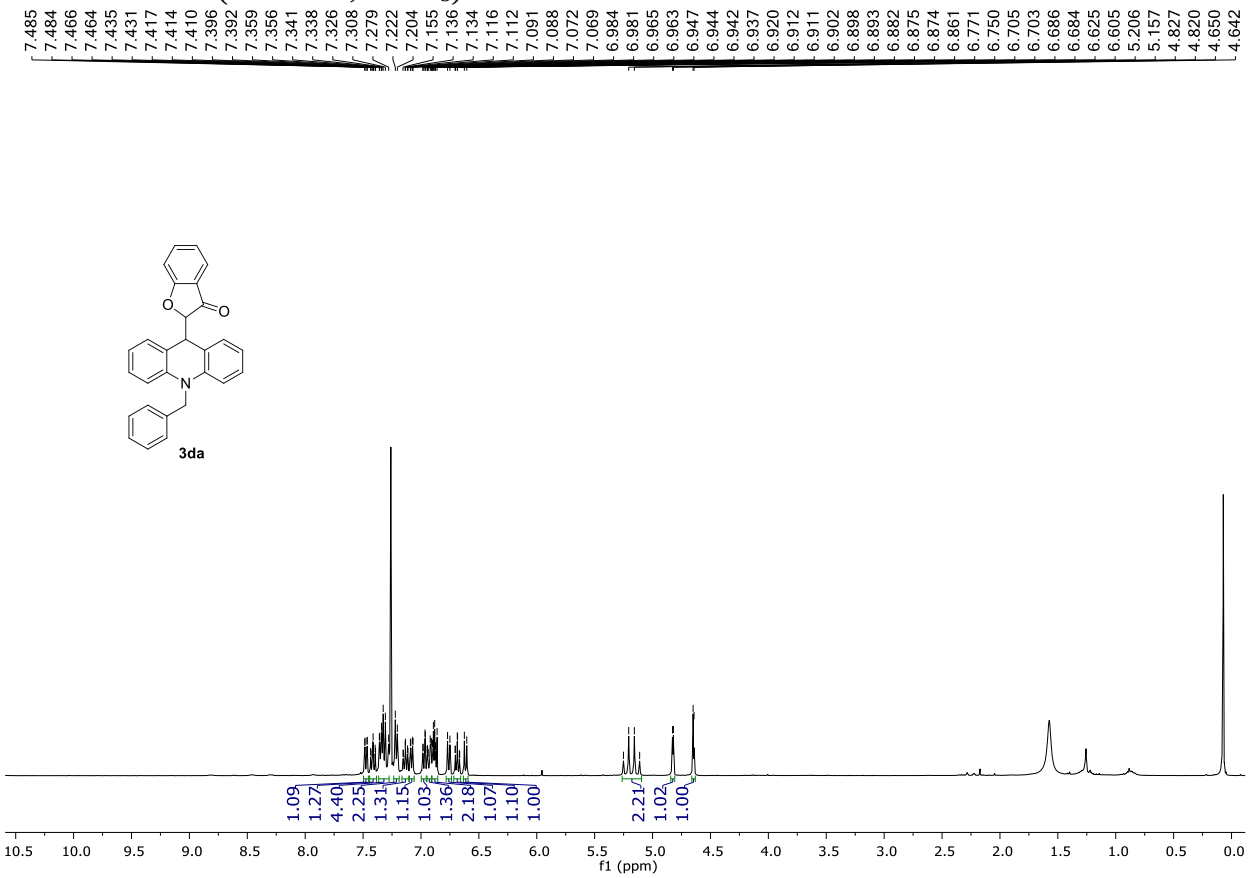
^{1}H NMR of **3cc** (400 MHz, $CDCl_3$):



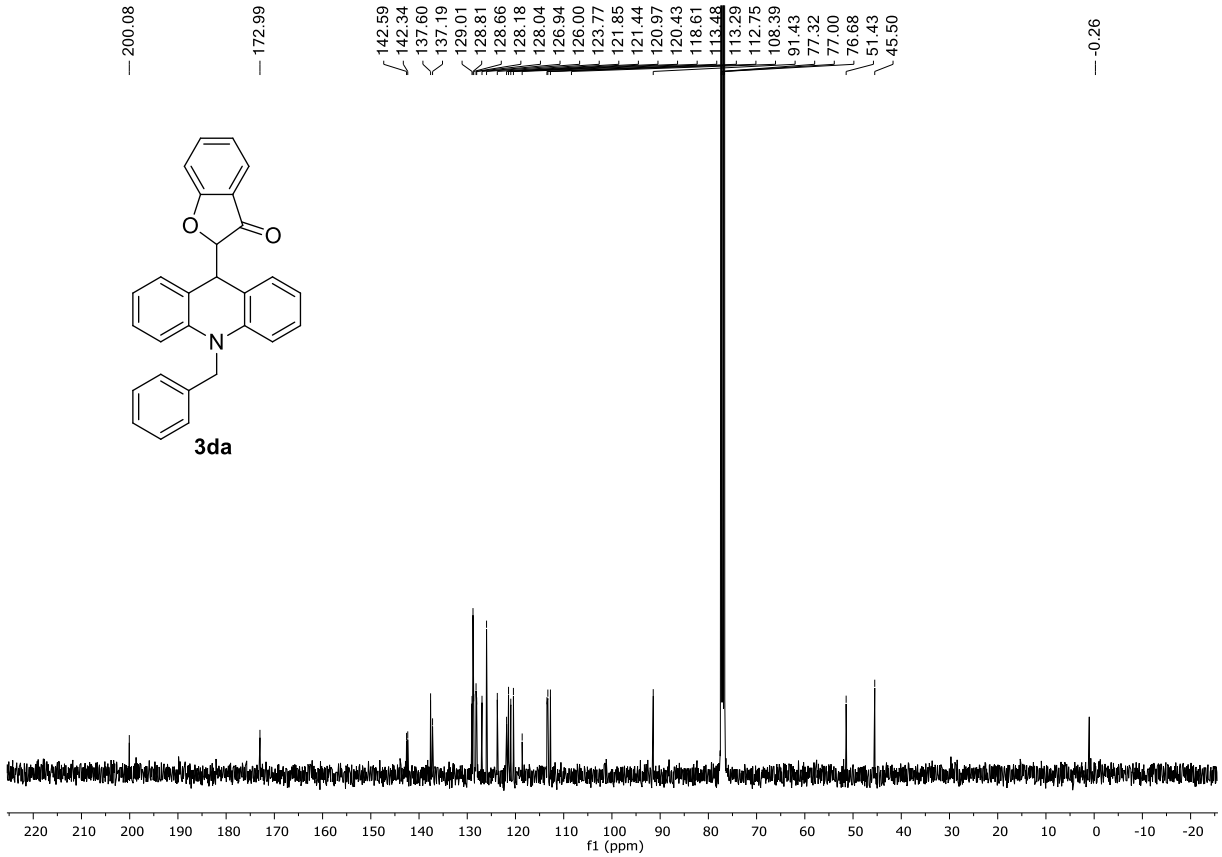
^{13}C {^{1}H} NMR of **3cc** (100 MHz, $CDCl_3$):



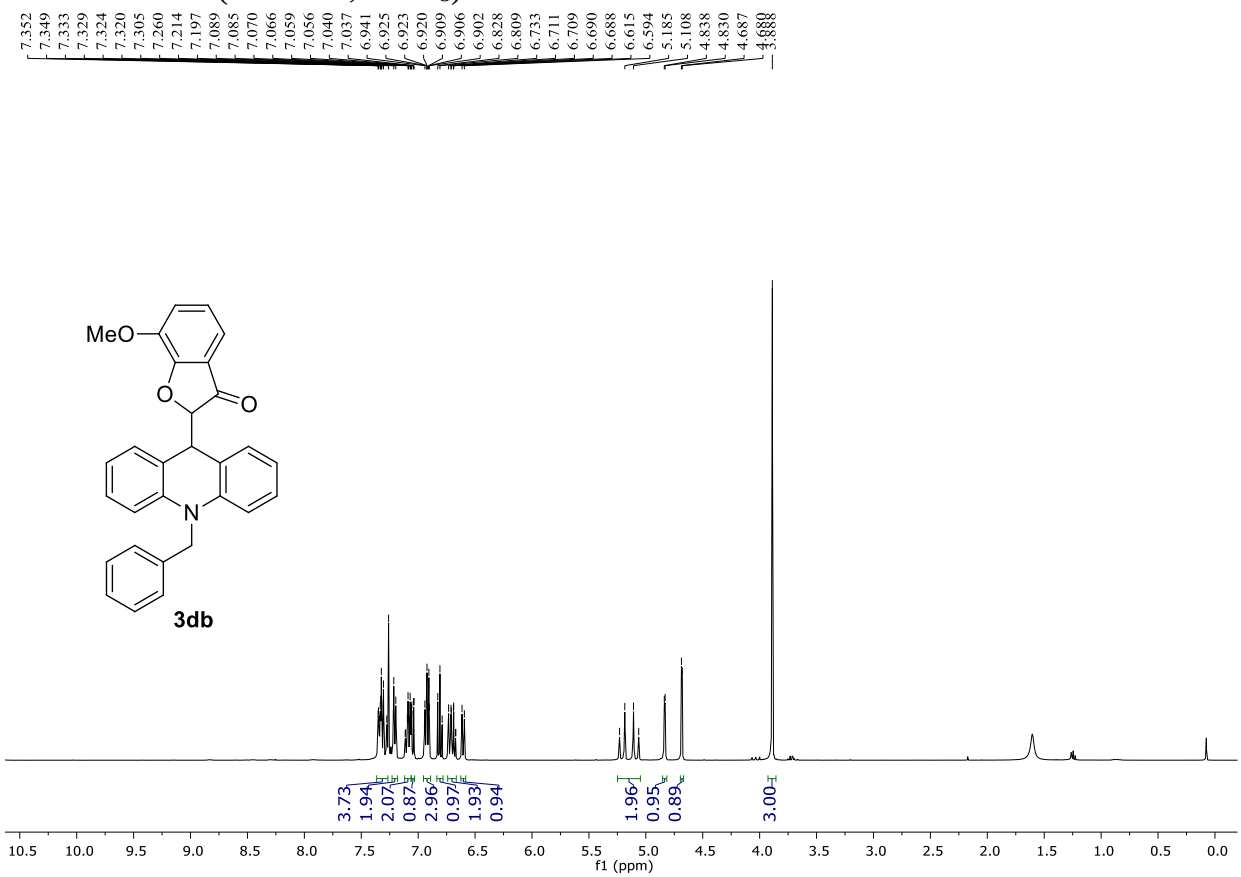
^{1}H NMR of **3da** (400 MHz, $CDCl_3$):



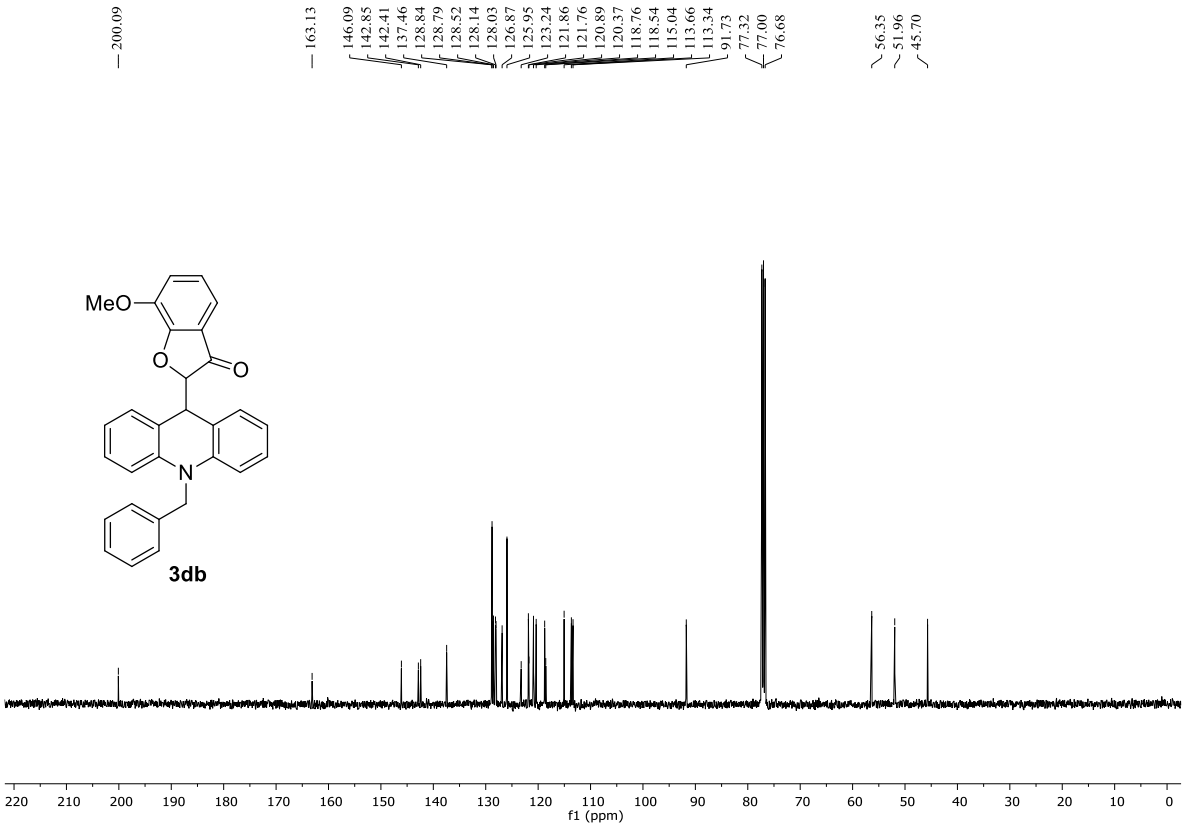
^{13}C {^{1}H} NMR of **3da** (100 MHz, $CDCl_3$):



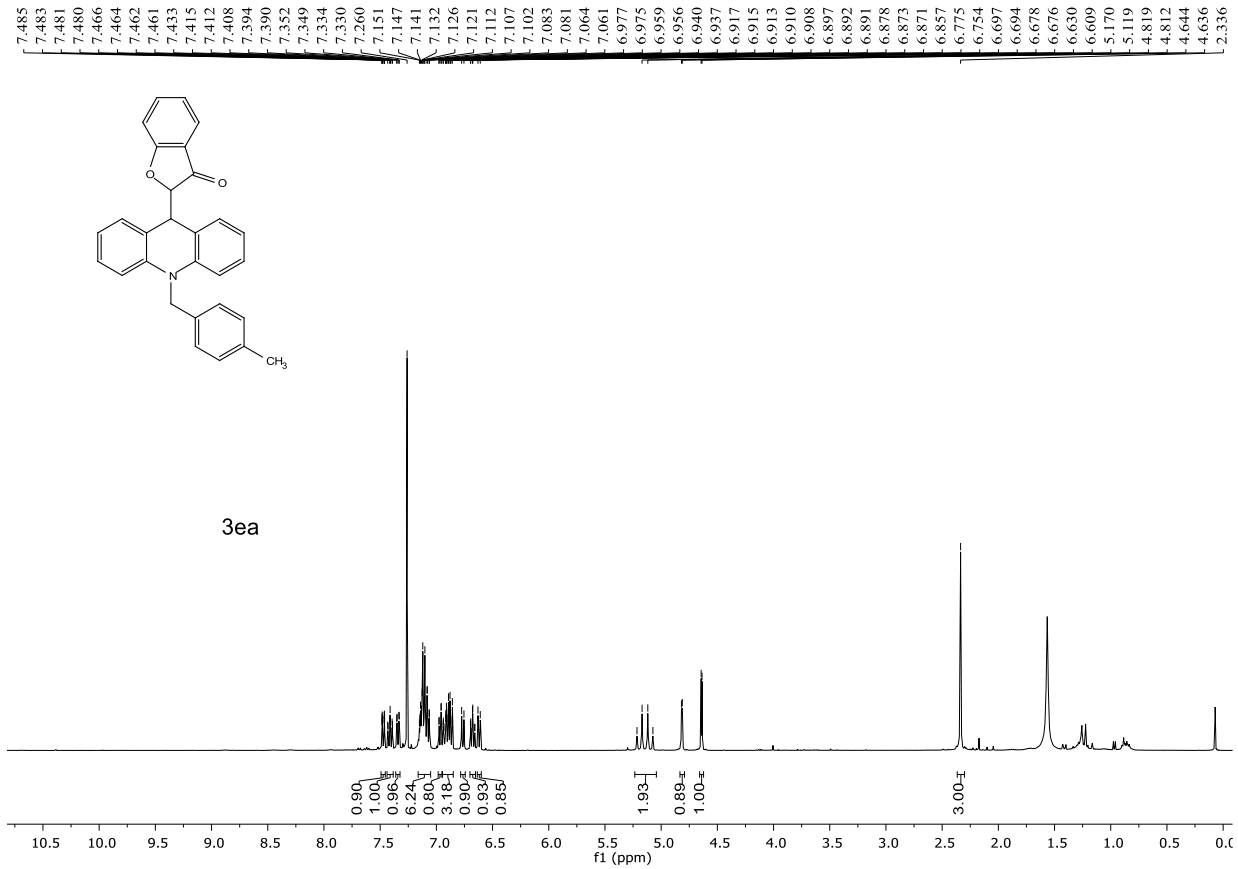
^{1}H NMR of **3db** (400 MHz, $CDCl_3$):



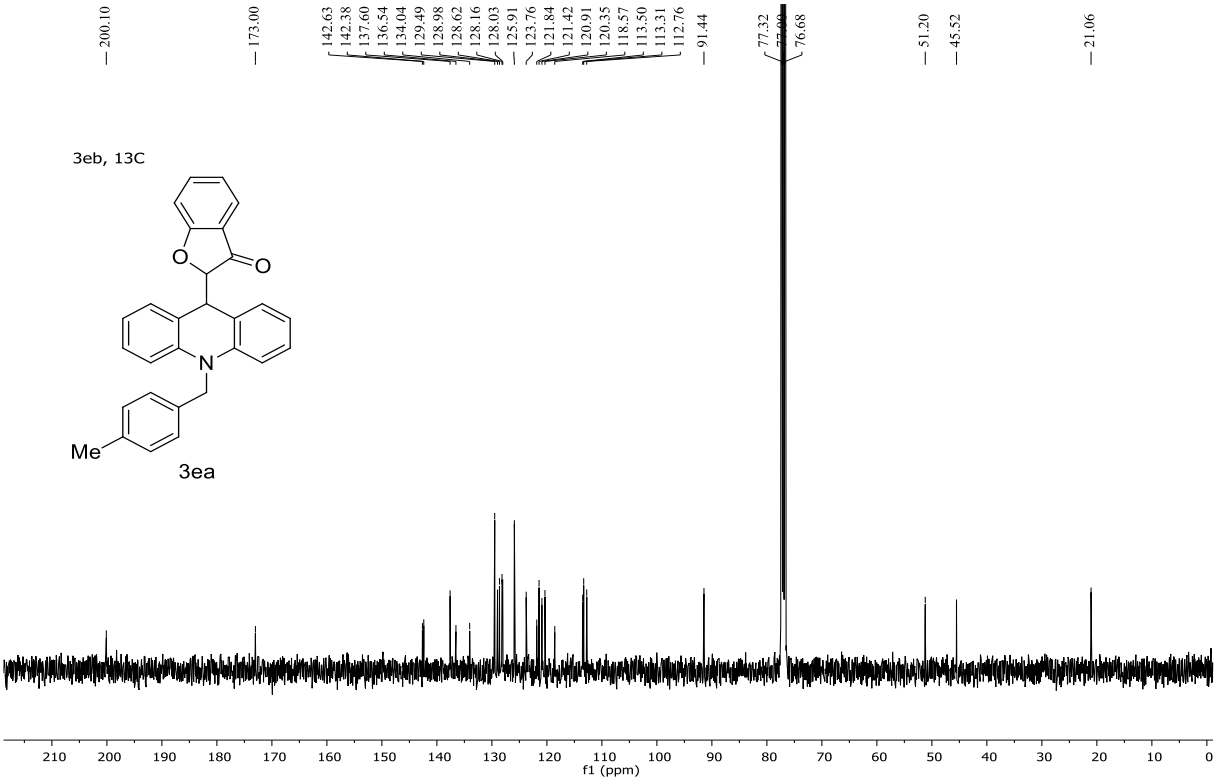
^{13}C {^{1}H} NMR of **3db** (100 MHz, $CDCl_3$):



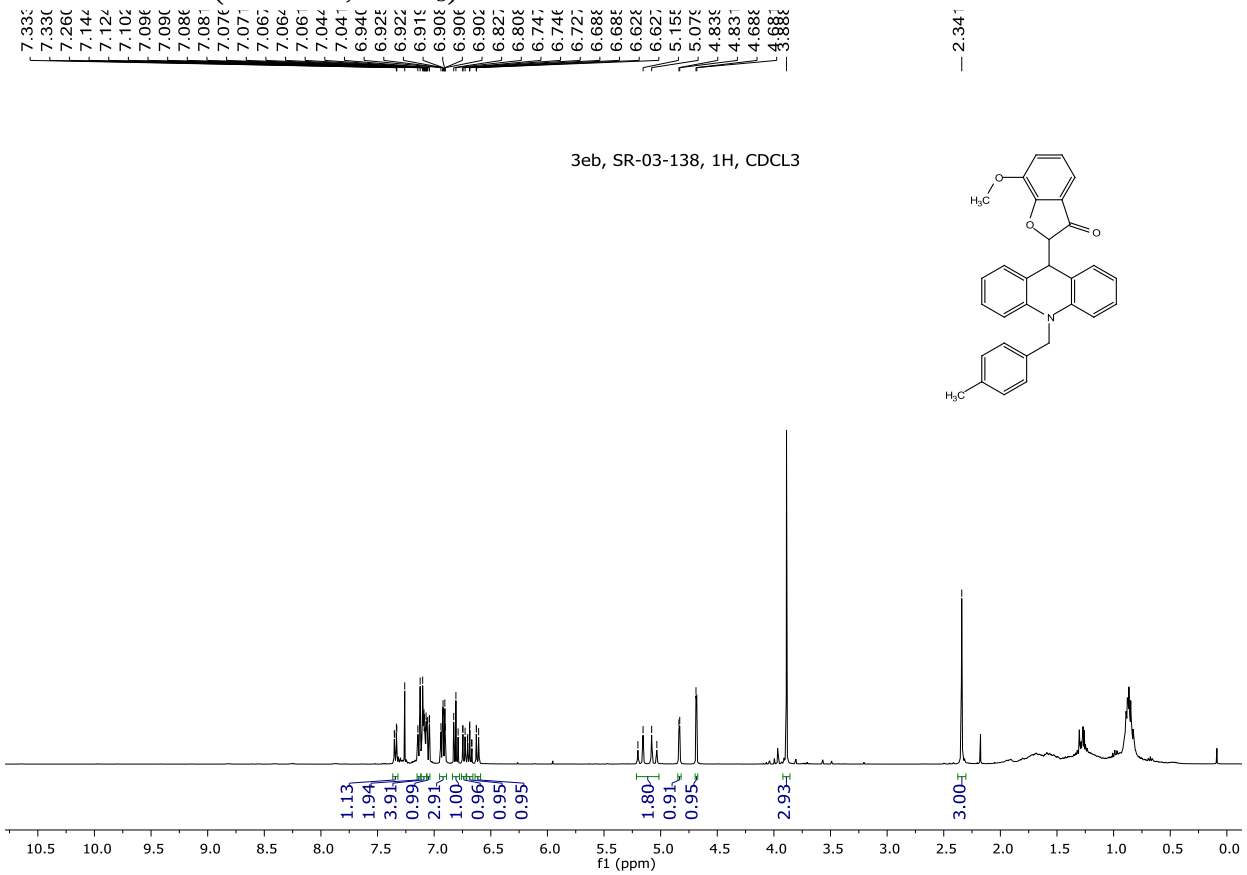
^{1}H NMR of **3ea** (400 MHz, $CDCl_3$):



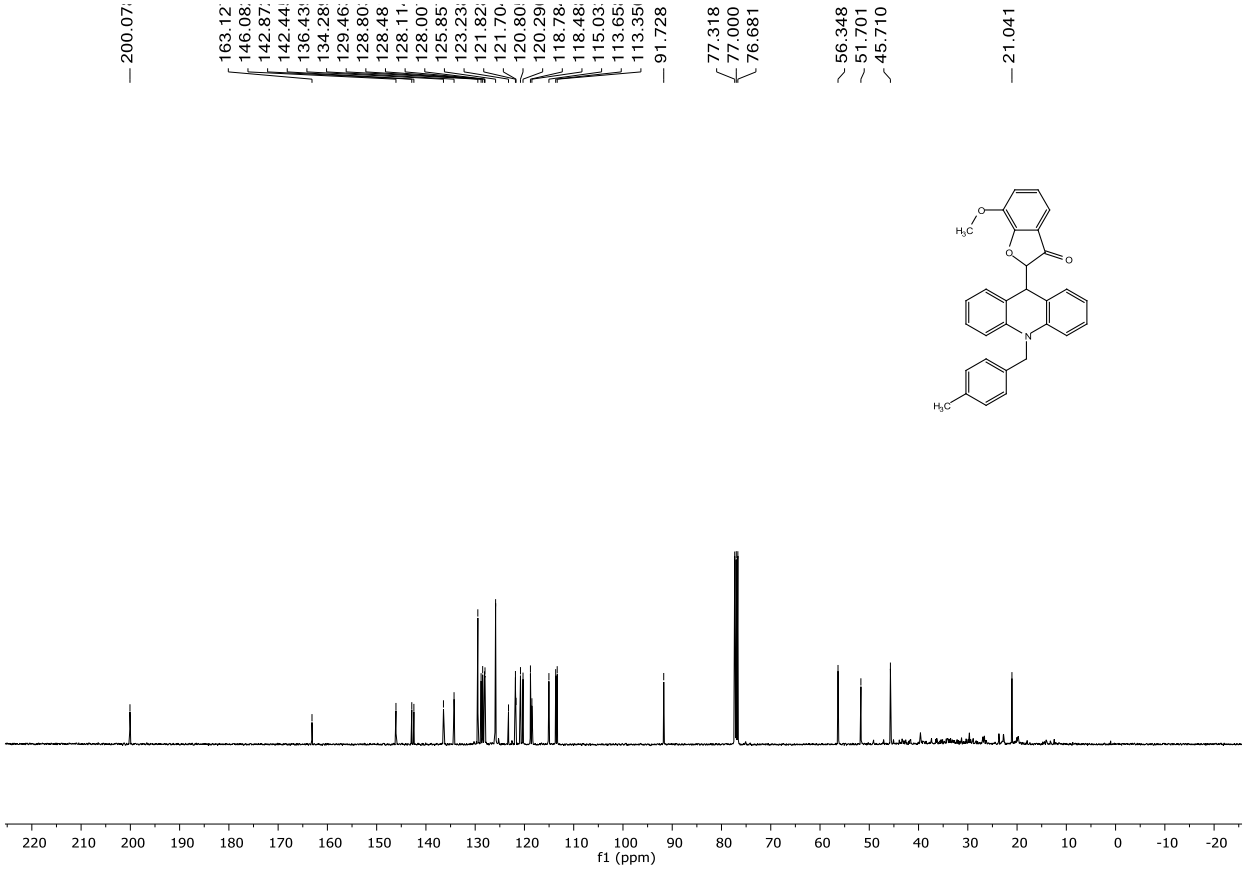
^{13}C {^{1}H} NMR of **3ea** (100 MHz, $CDCl_3$):



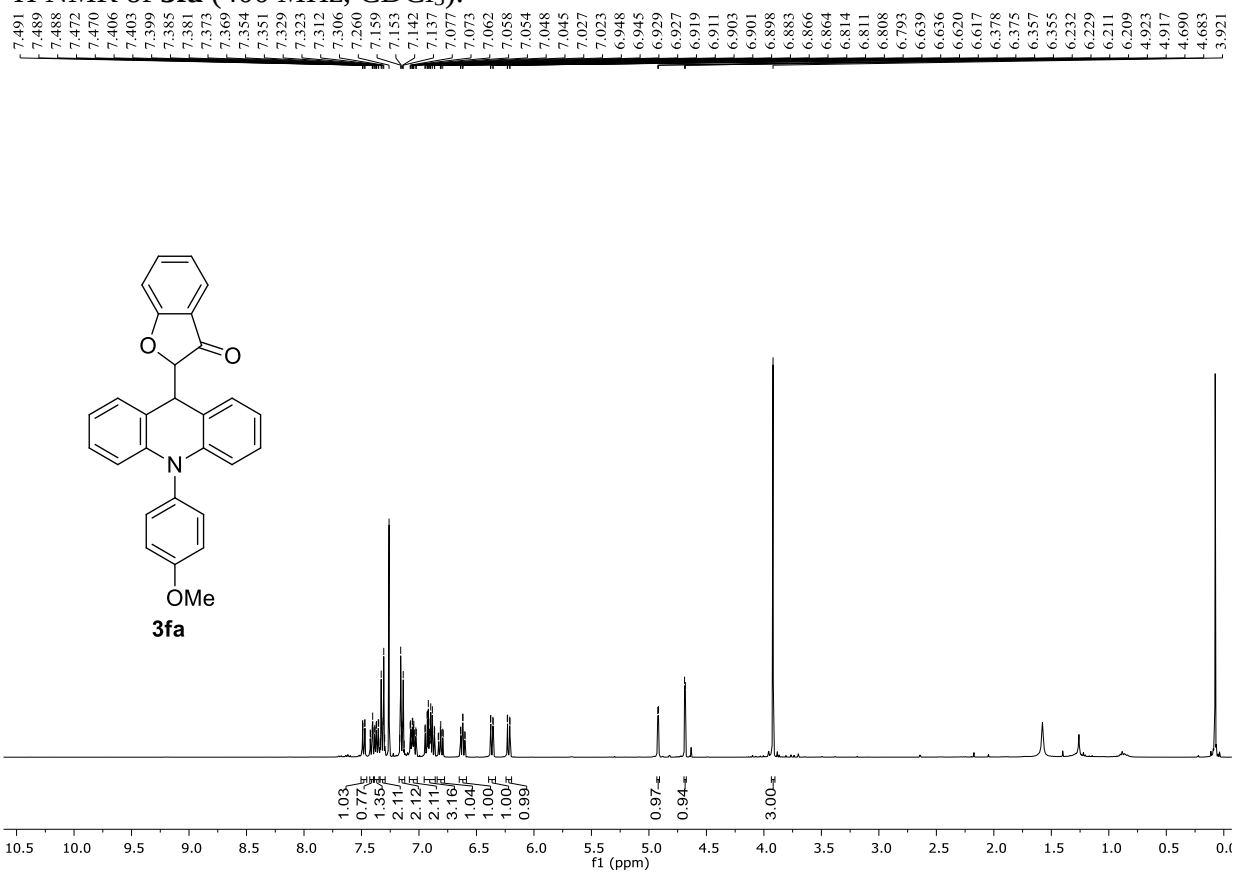
^{1}H NMR of **3eb** (400 MHz, $CDCl_3$):



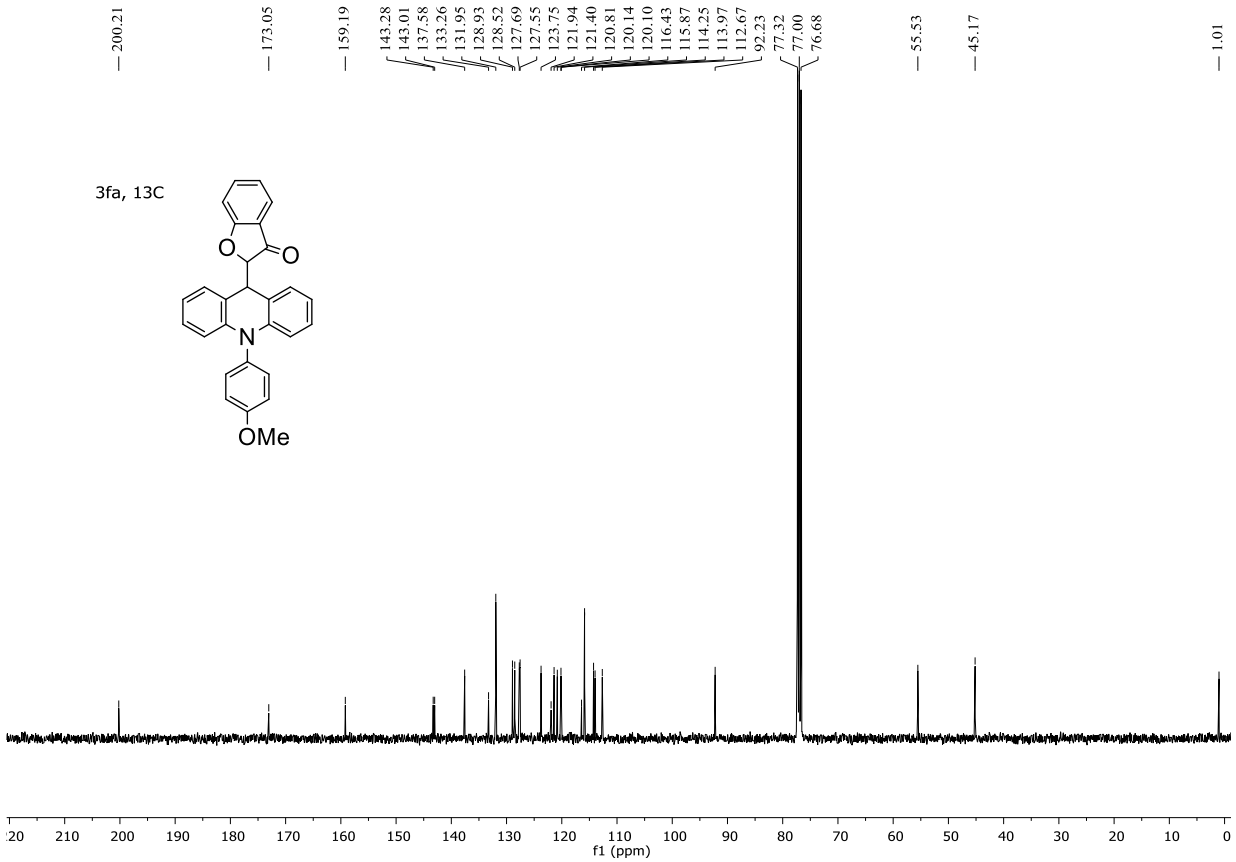
^{13}C {^{1}H} NMR of **3eb** (100 MHz, $CDCl_3$):



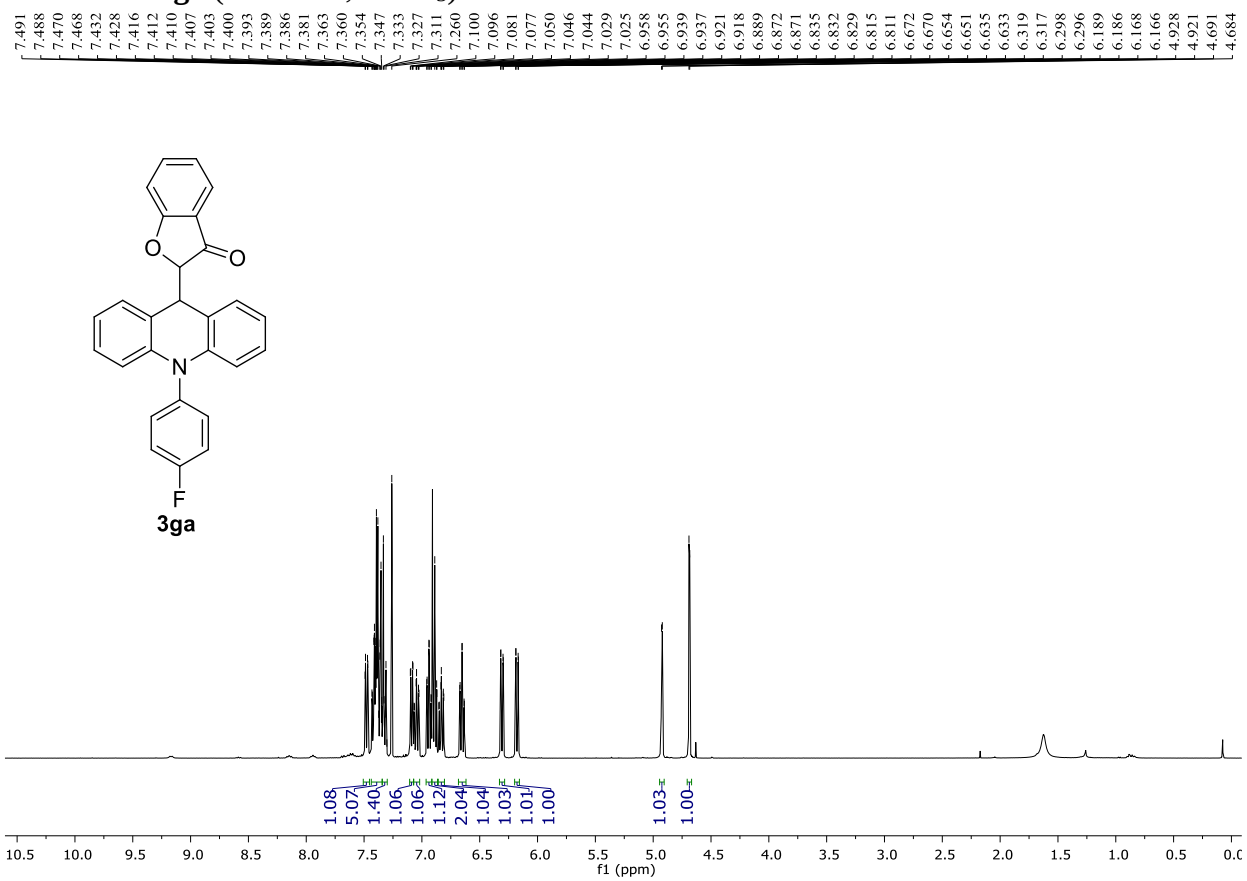
^{1}H NMR of **3fa** (400 MHz, $CDCl_3$):



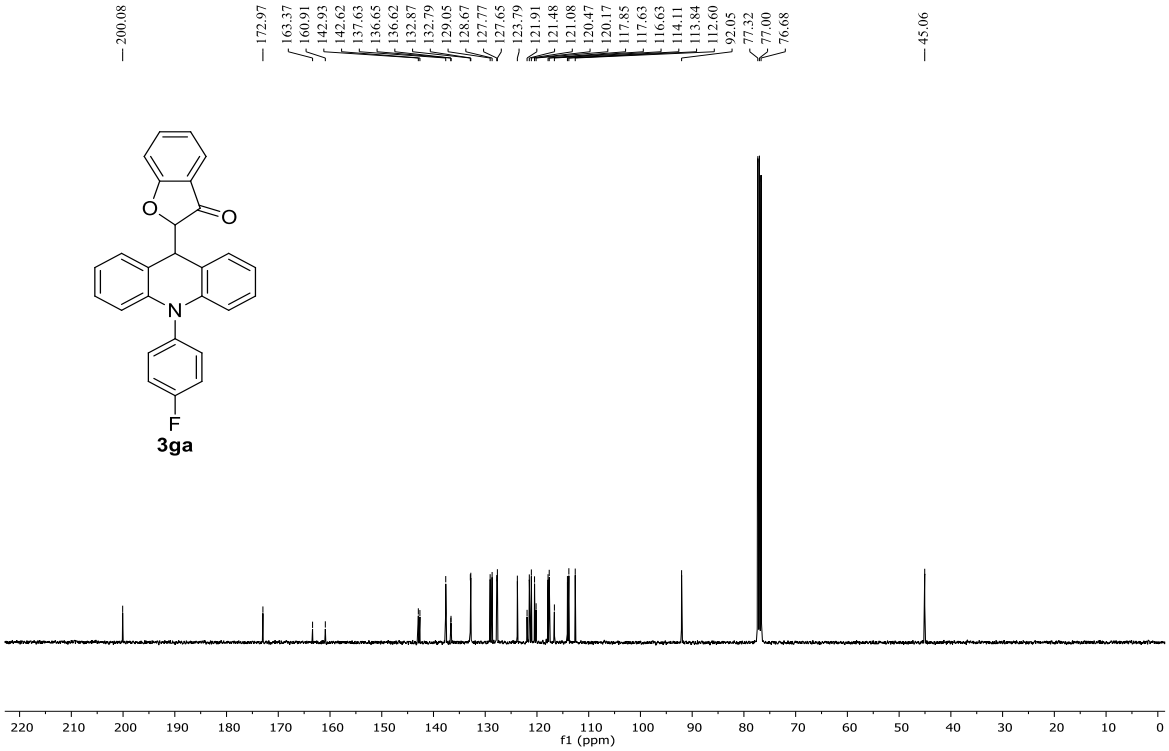
^{13}C {^{1}H} NMR of **3fa** (100 MHz, $CDCl_3$):



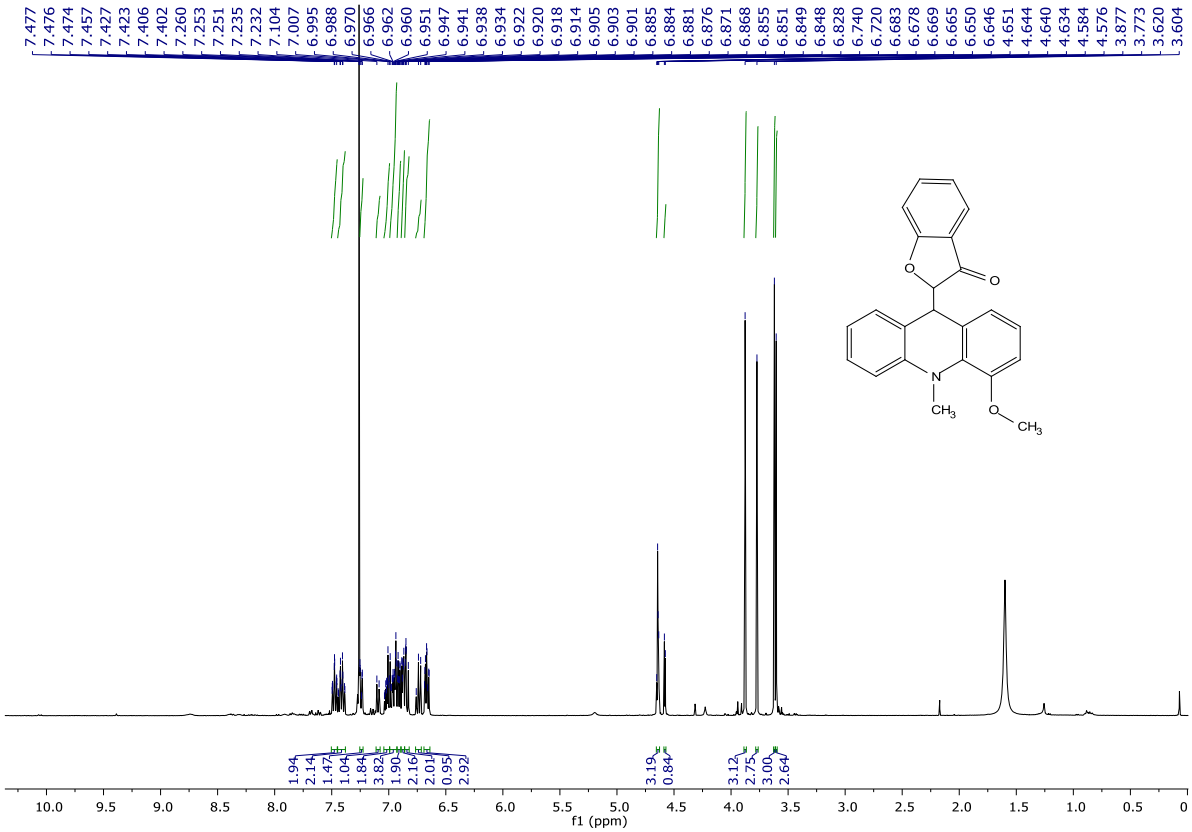
^{1}H NMR of **3ga** (400 MHz, $CDCl_3$):



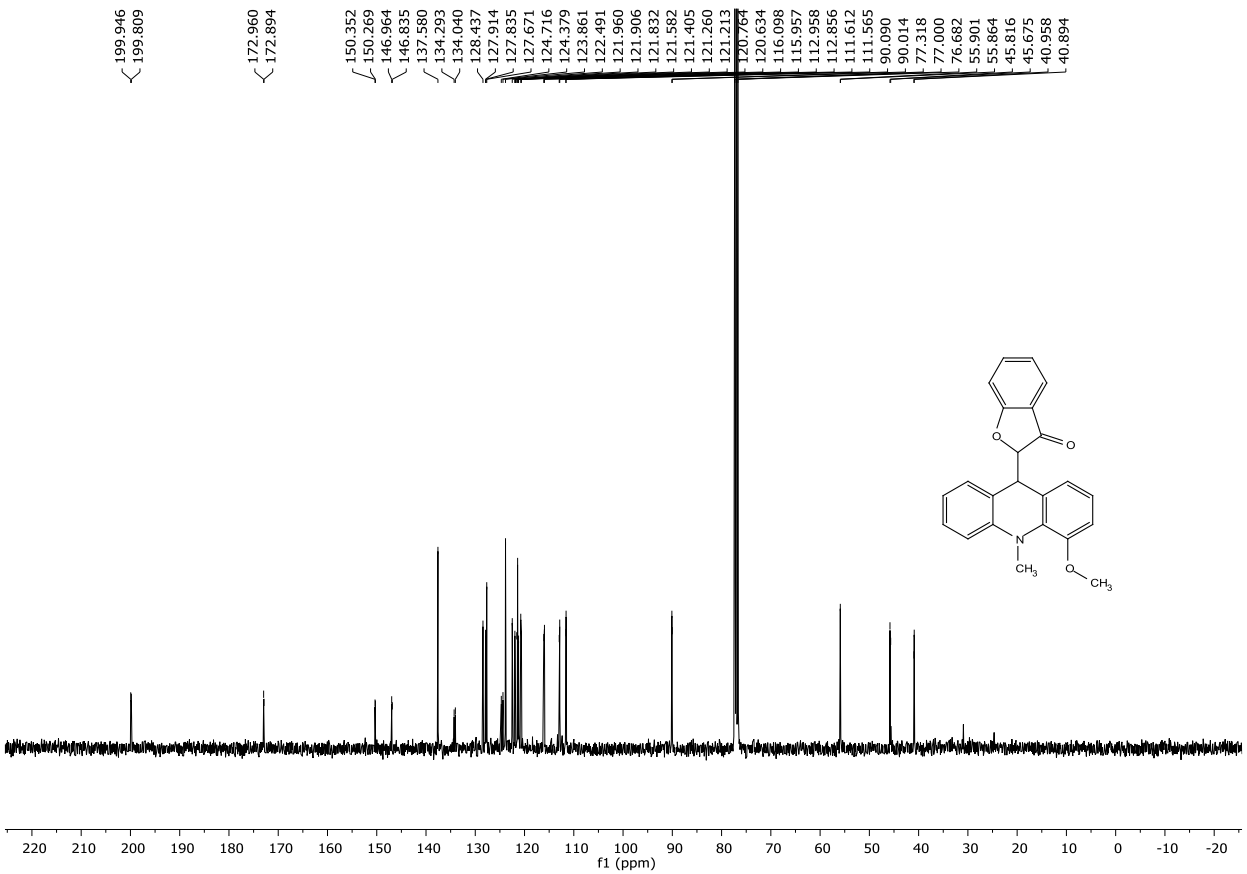
^{13}C {^{1}H} NMR of **3ga** (100 MHz, $CDCl_3$):



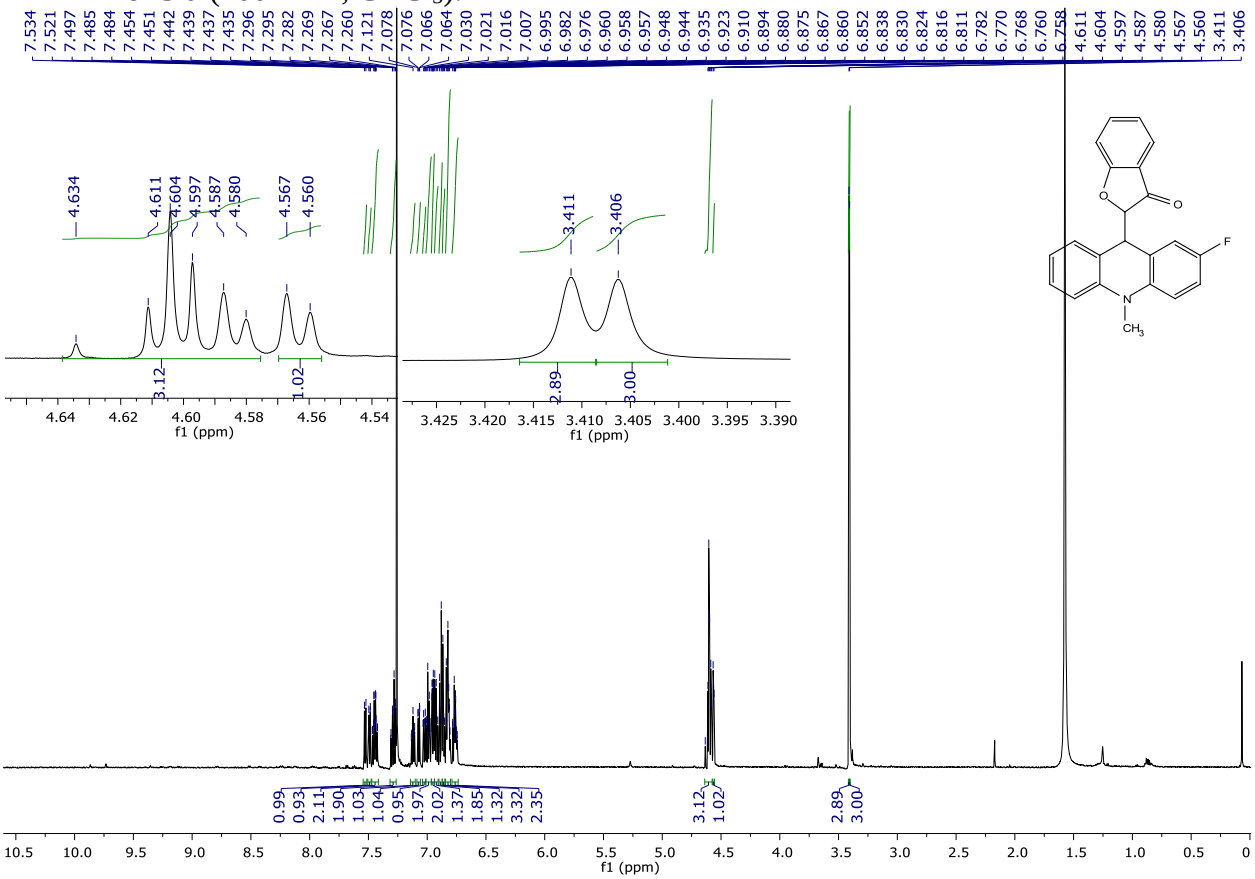
^{1}H NMR of **3ha** (400 MHz, $CDCl_3$):



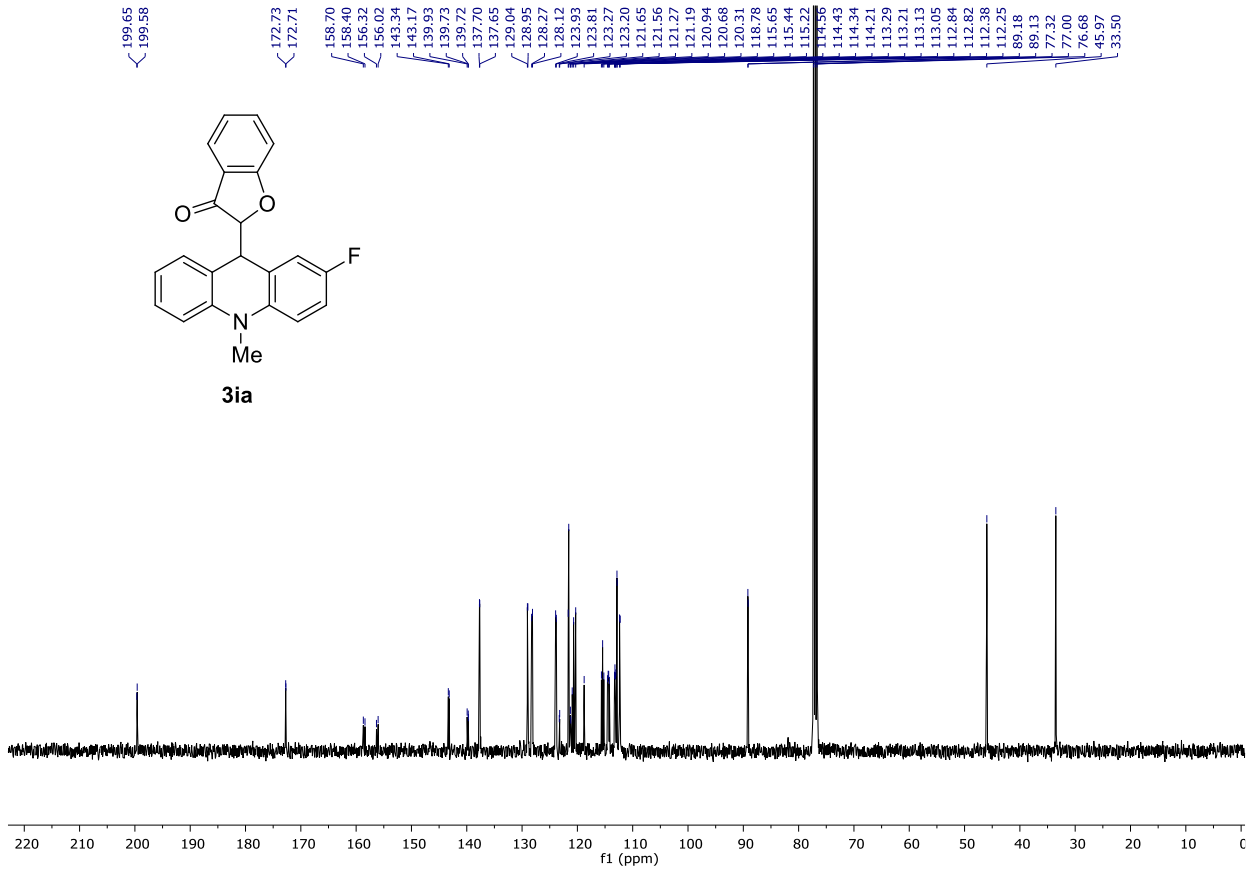
^{13}C {^{1}H} NMR of **3ha** (100 MHz, $CDCl_3$):



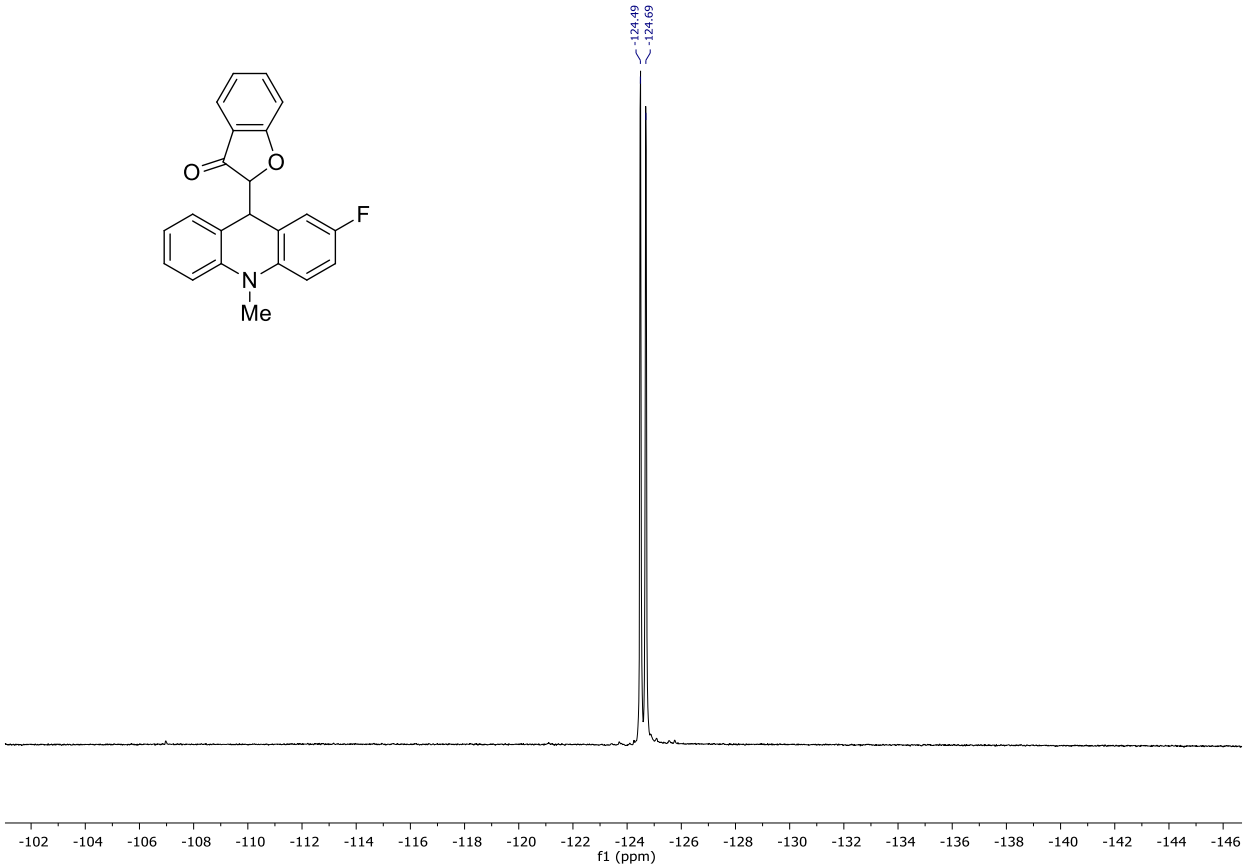
^{1}H NMR of **3ia** (400 MHz, $CDCl_3$):



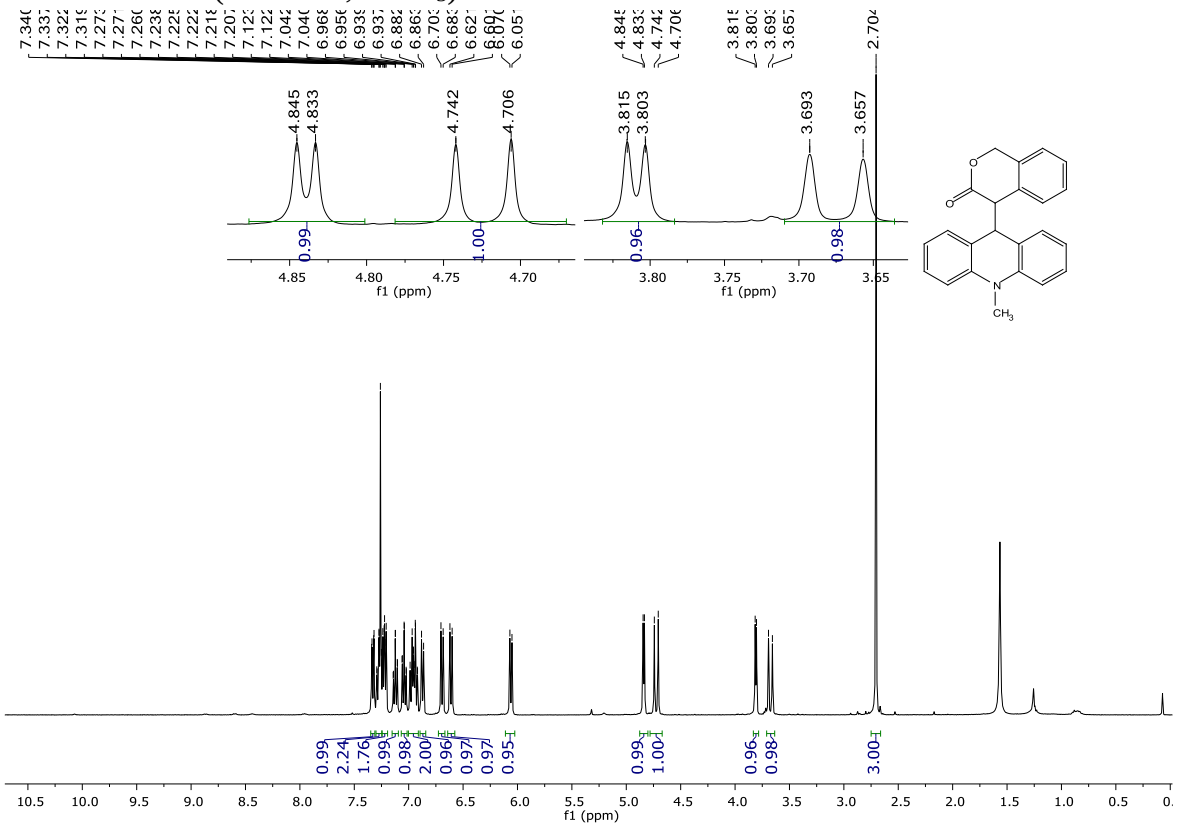
^{13}C {^{1}H} NMR of **3ia** (100 MHz, $CDCl_3$):



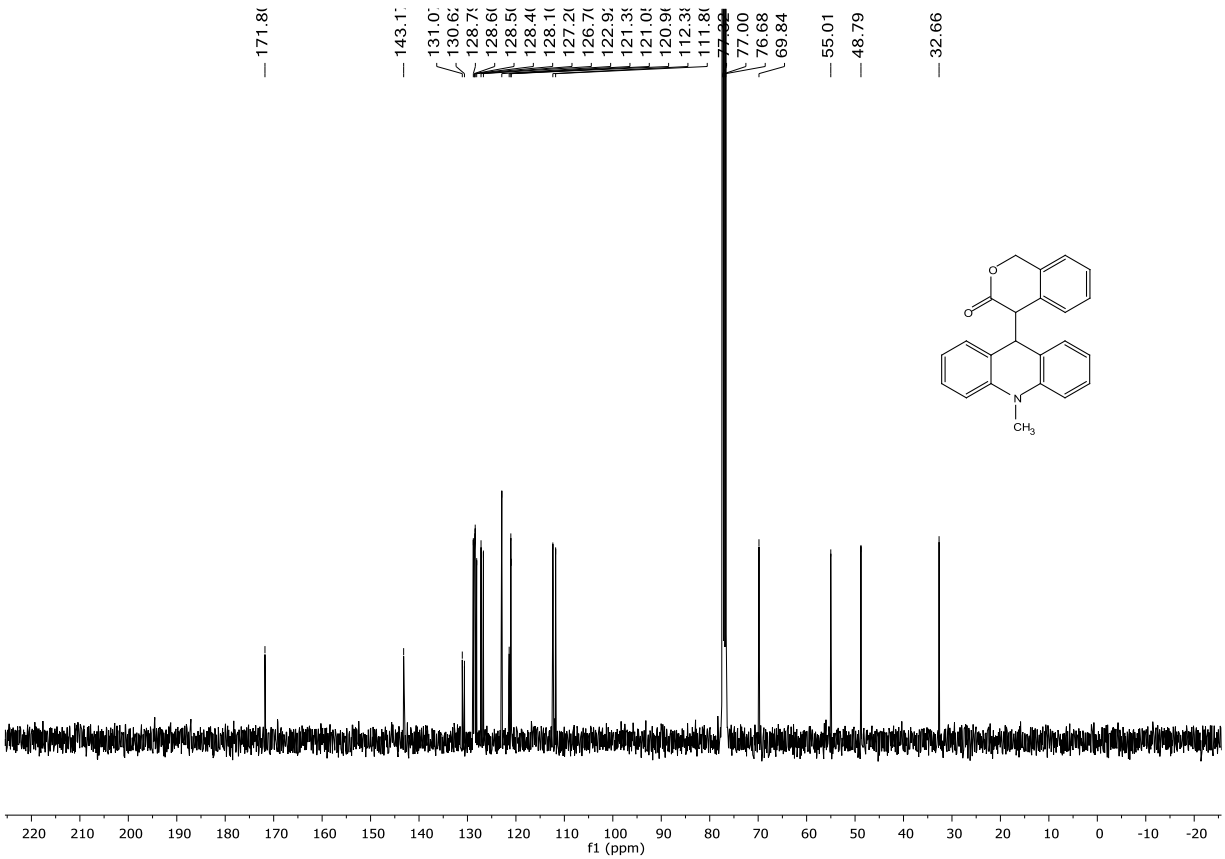
^{19}F NMR of **3ia** (376 MHz, $CDCl_3$):



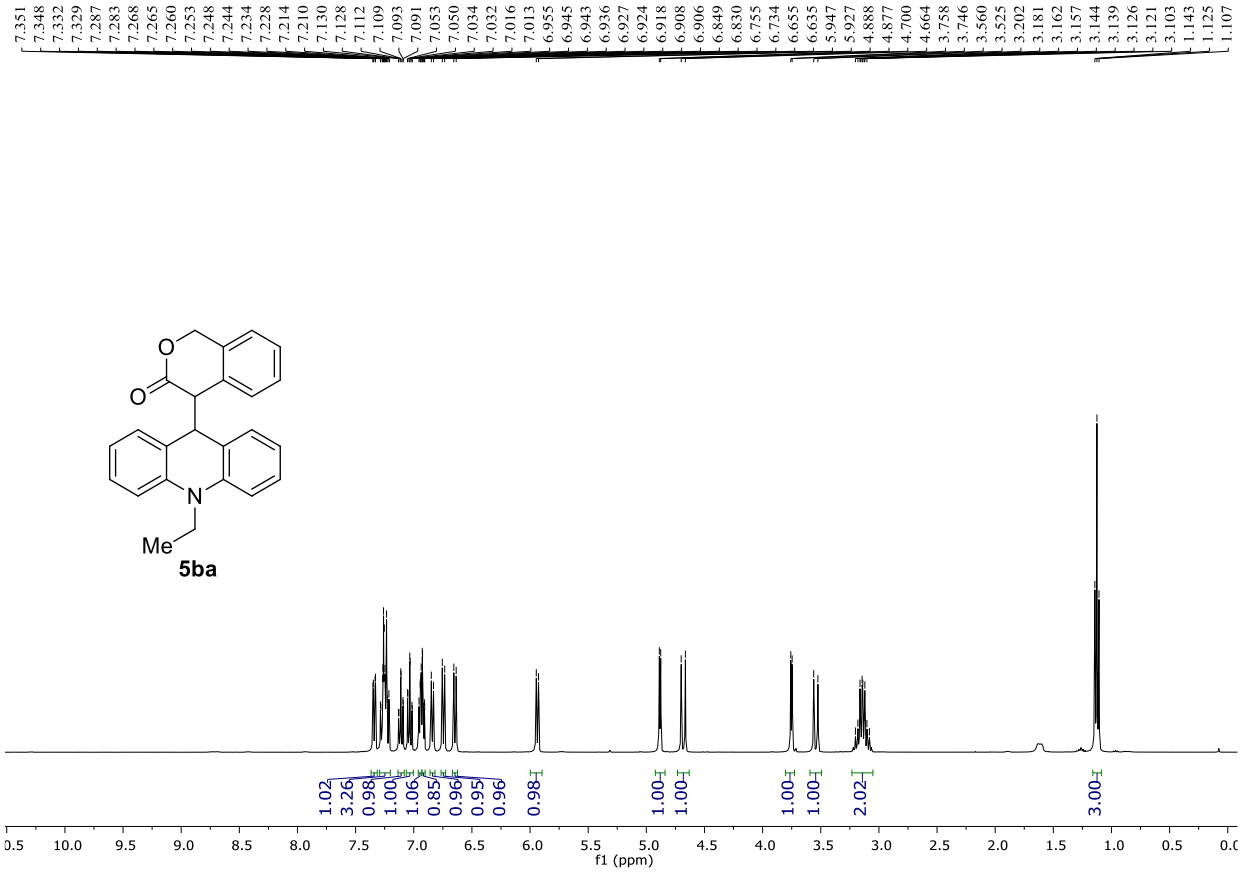
^{1}H NMR of **5aa** (400 MHz, $CDCl_3$):



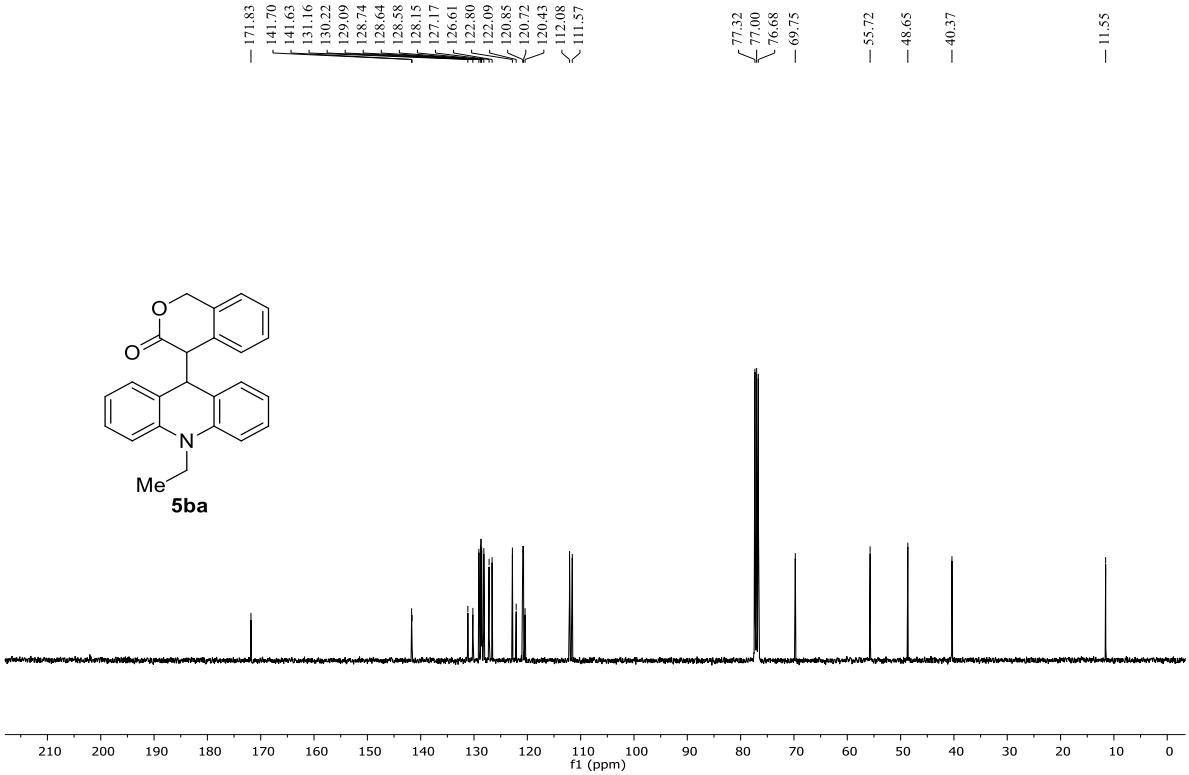
^{13}C {^{1}H} NMR of **5aa** (100 MHz, $CDCl_3$):



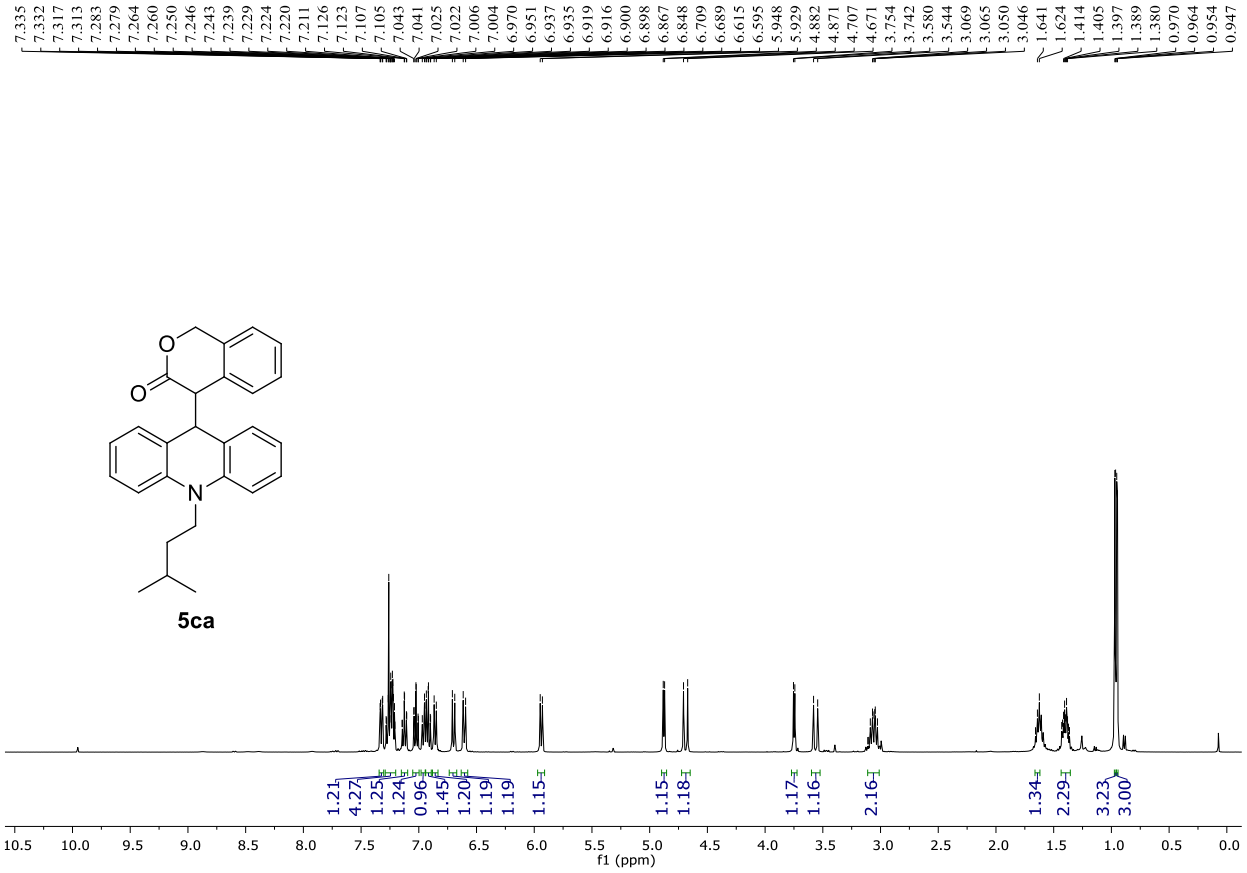
^{1}H NMR of **5ba** (400 MHz, $CDCl_3$):



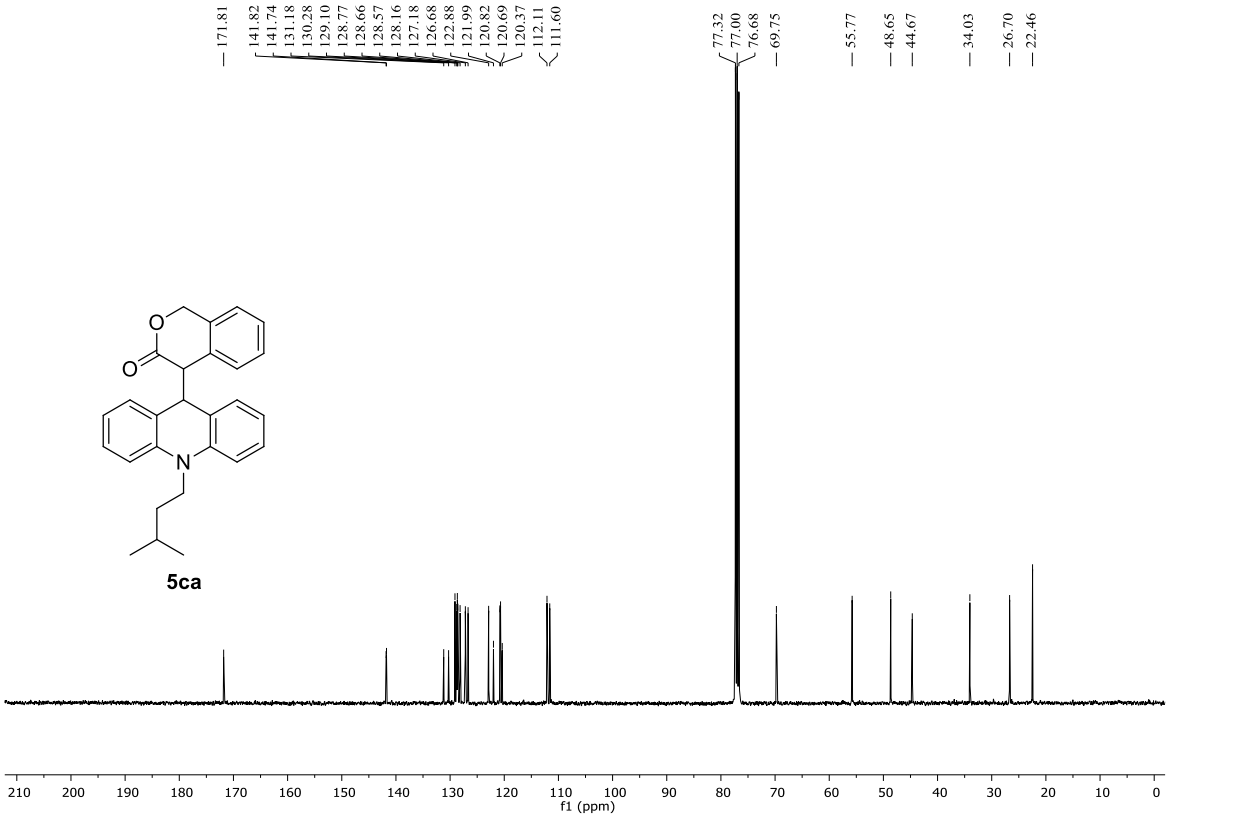
^{13}C {^{1}H} NMR of **5ba** (100 MHz, $CDCl_3$):



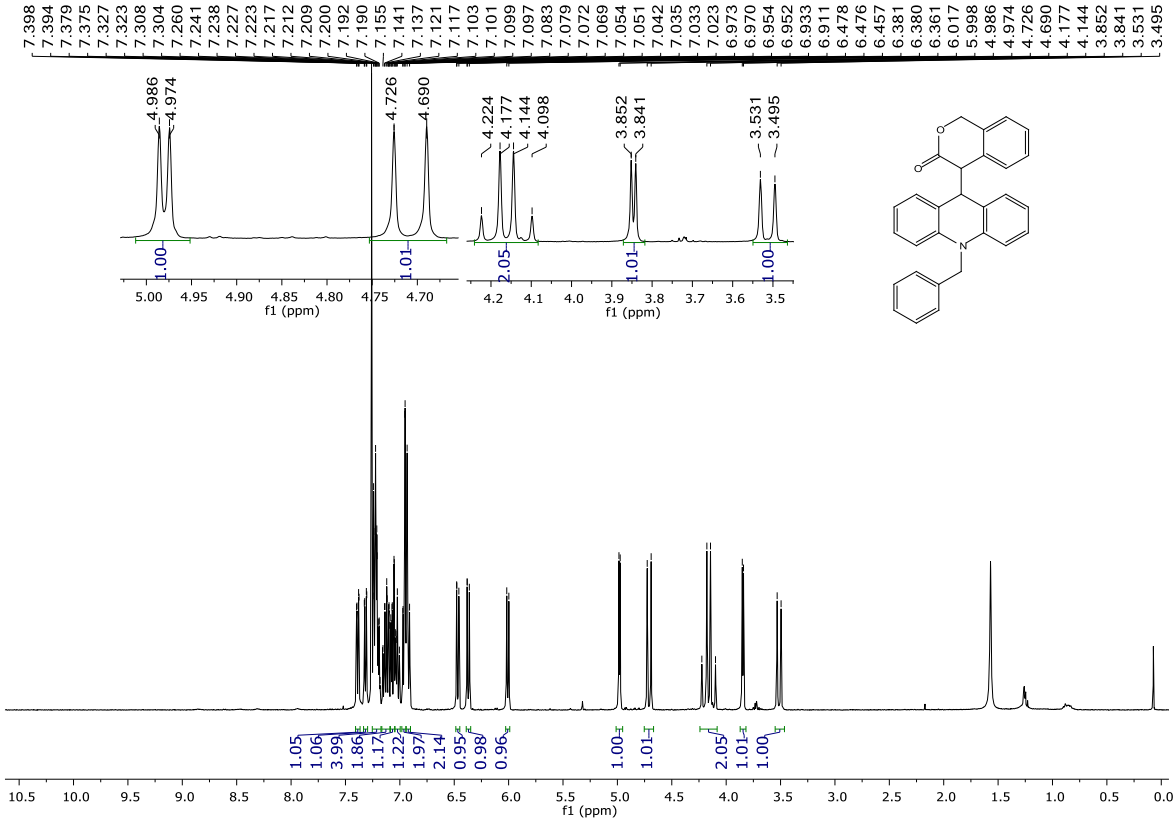
^{1}H NMR of **5ca** (400 MHz, $CDCl_3$):



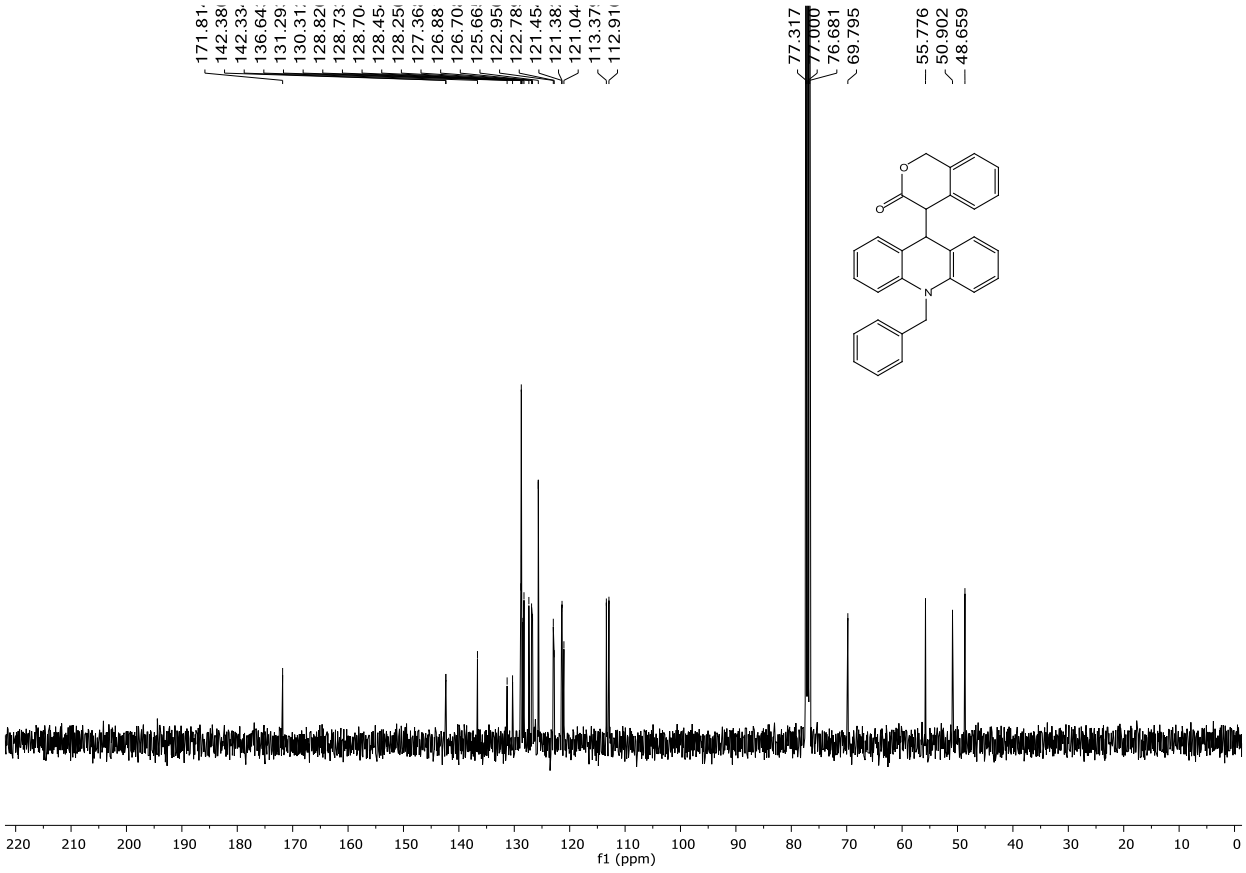
^{13}C {^{1}H} NMR of **5ca** (100 MHz, $CDCl_3$):



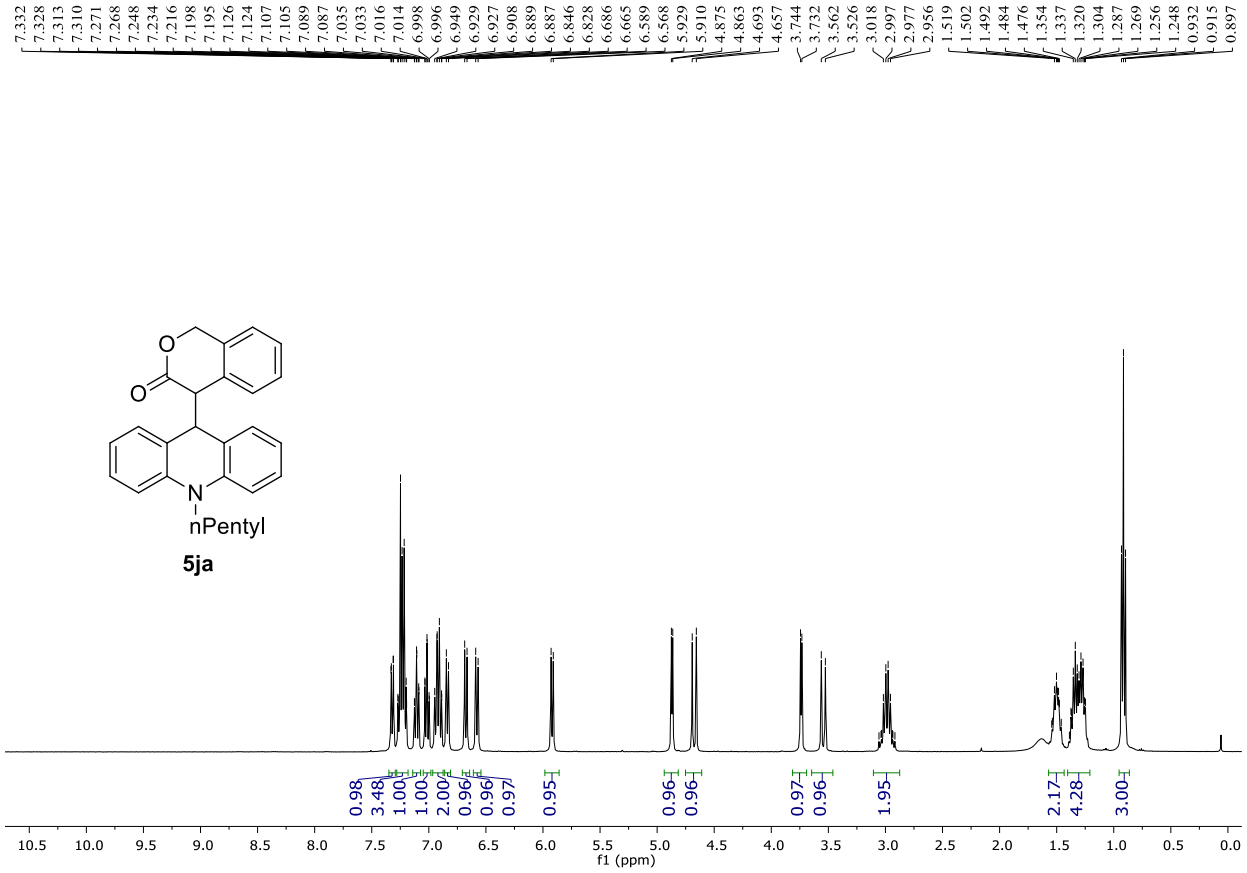
^{1}H NMR of **5da** (400 MHz, $CDCl_3$):



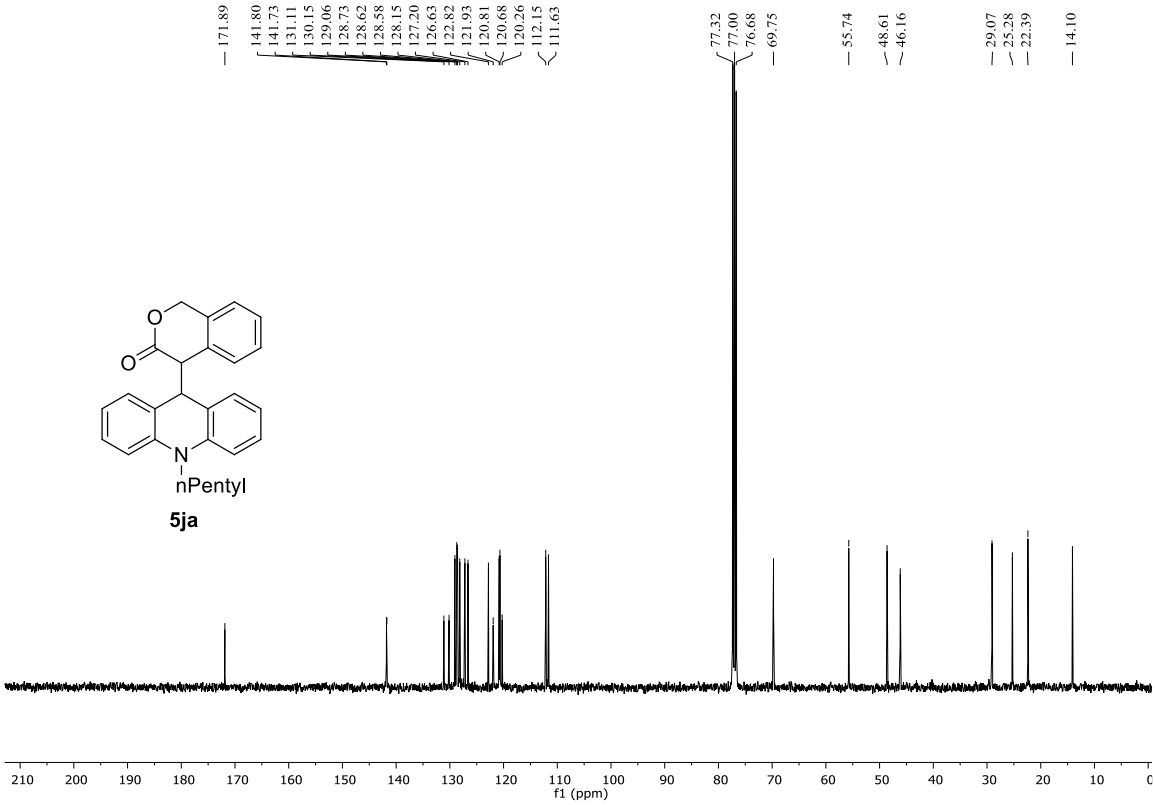
^{13}C {^{1}H} NMR of **5da** (100 MHz, $CDCl_3$):



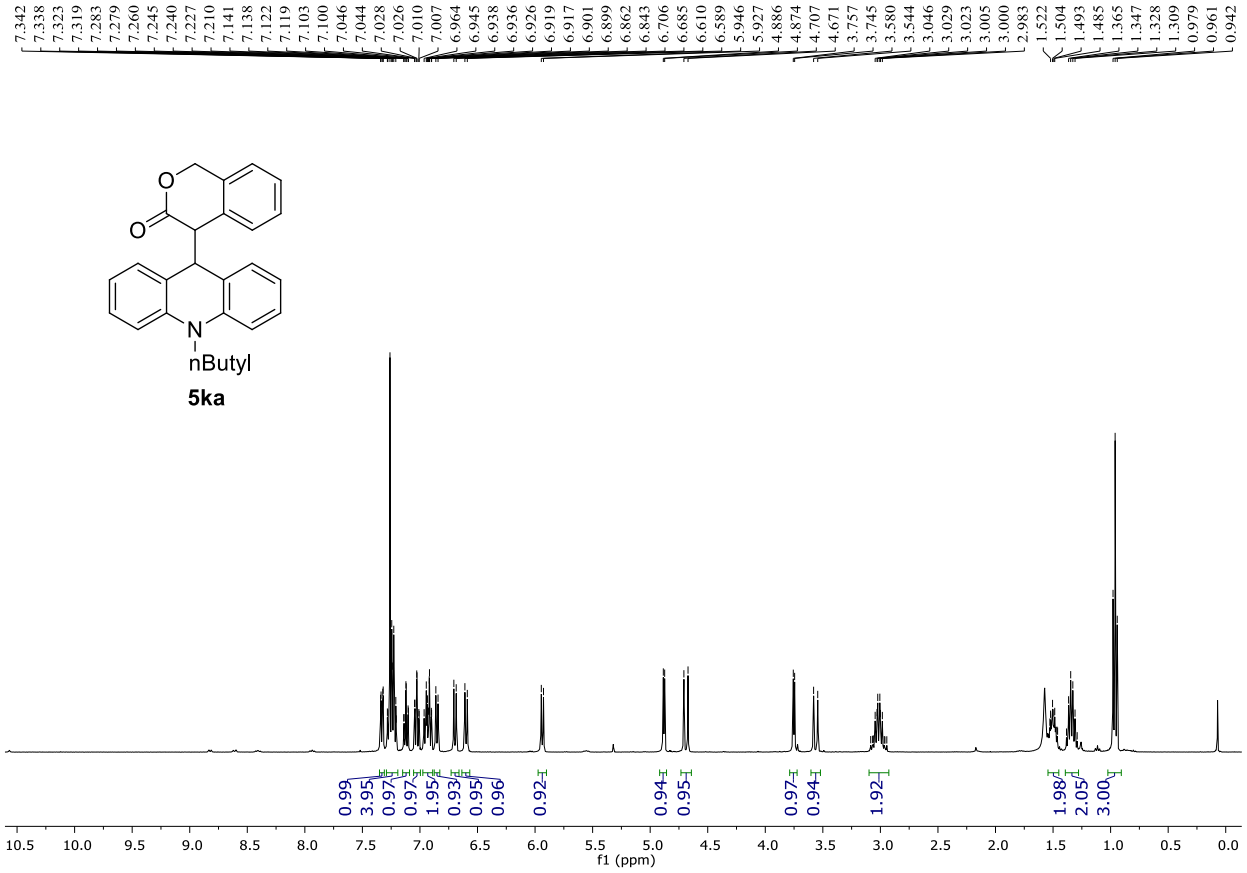
^{1}H NMR of **5ja** (400 MHz, $CDCl_3$):



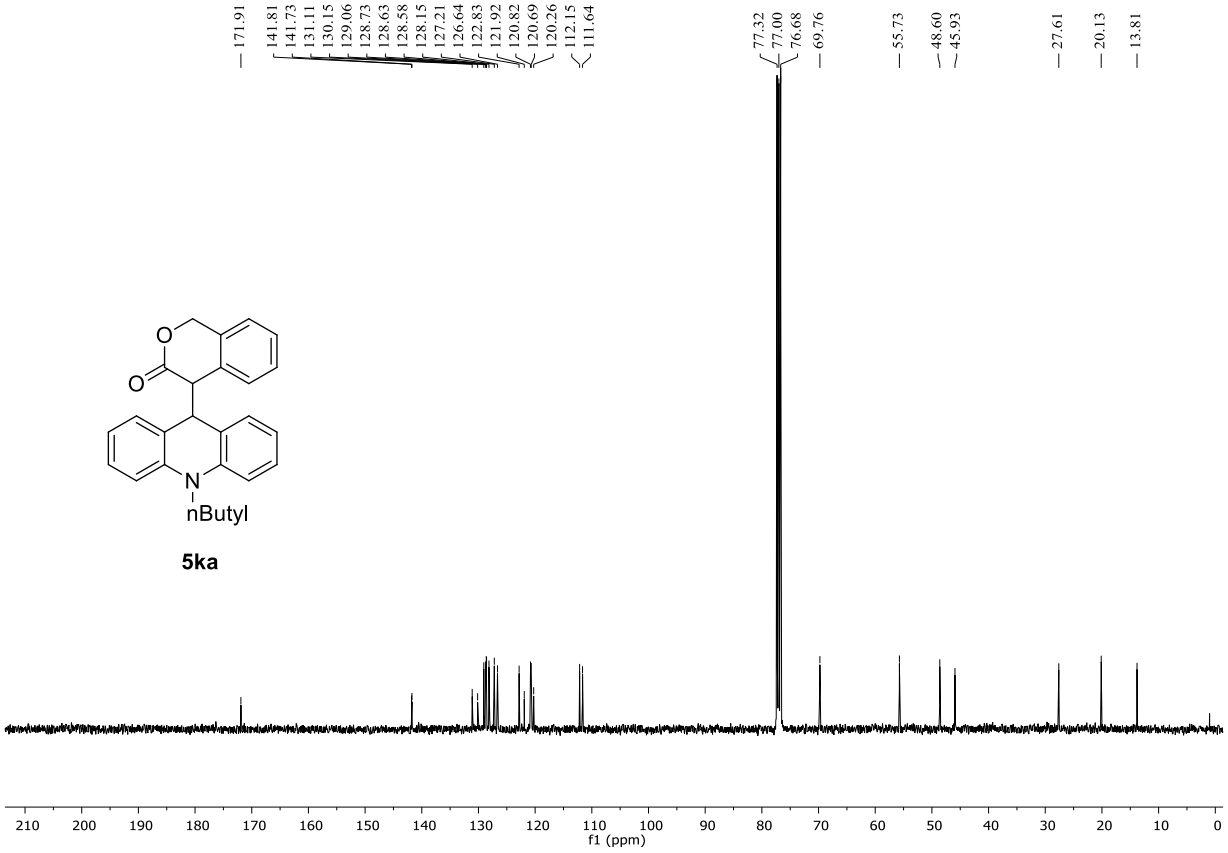
^{13}C {^{1}H} NMR of **5ja** (100 MHz, $CDCl_3$):



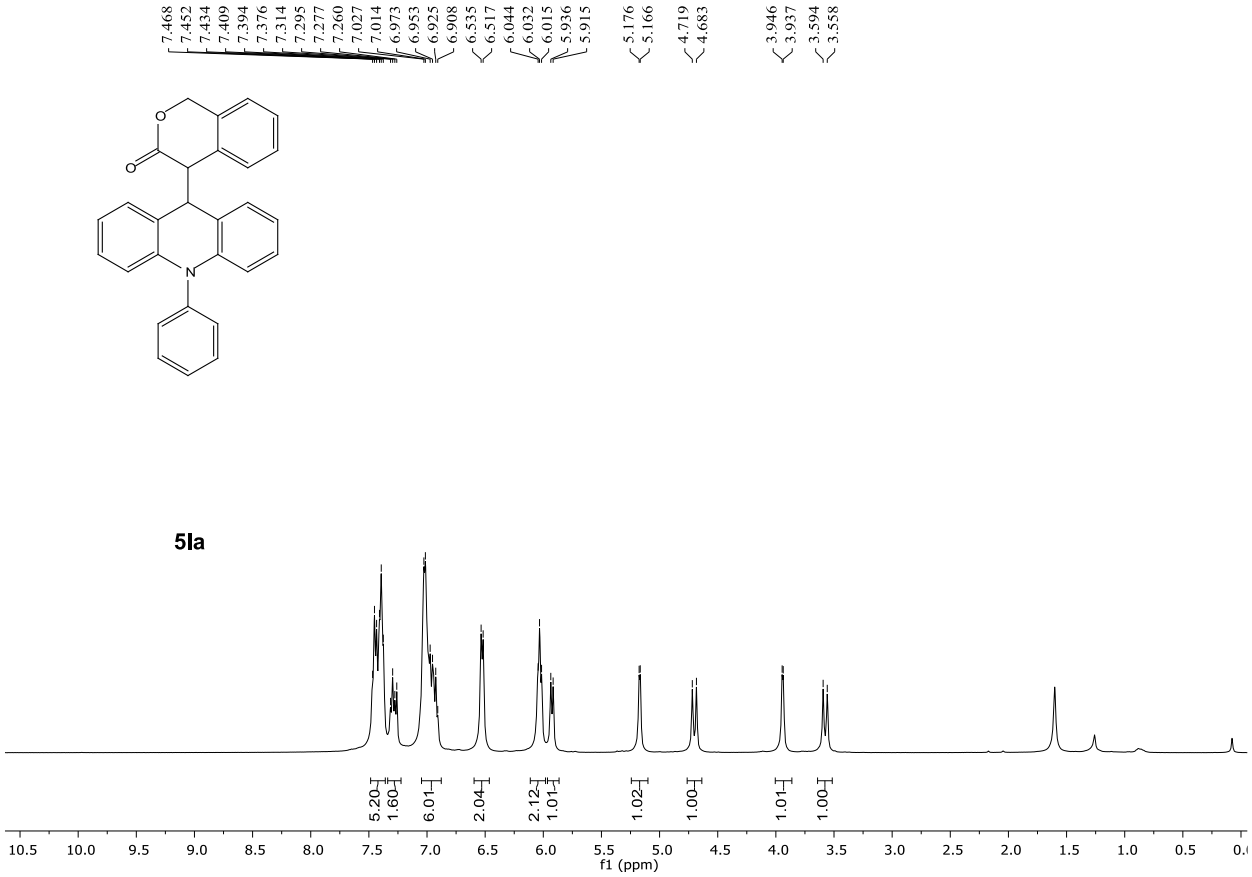
^{1}H NMR of **5ka** (400 MHz, $CDCl_3$):



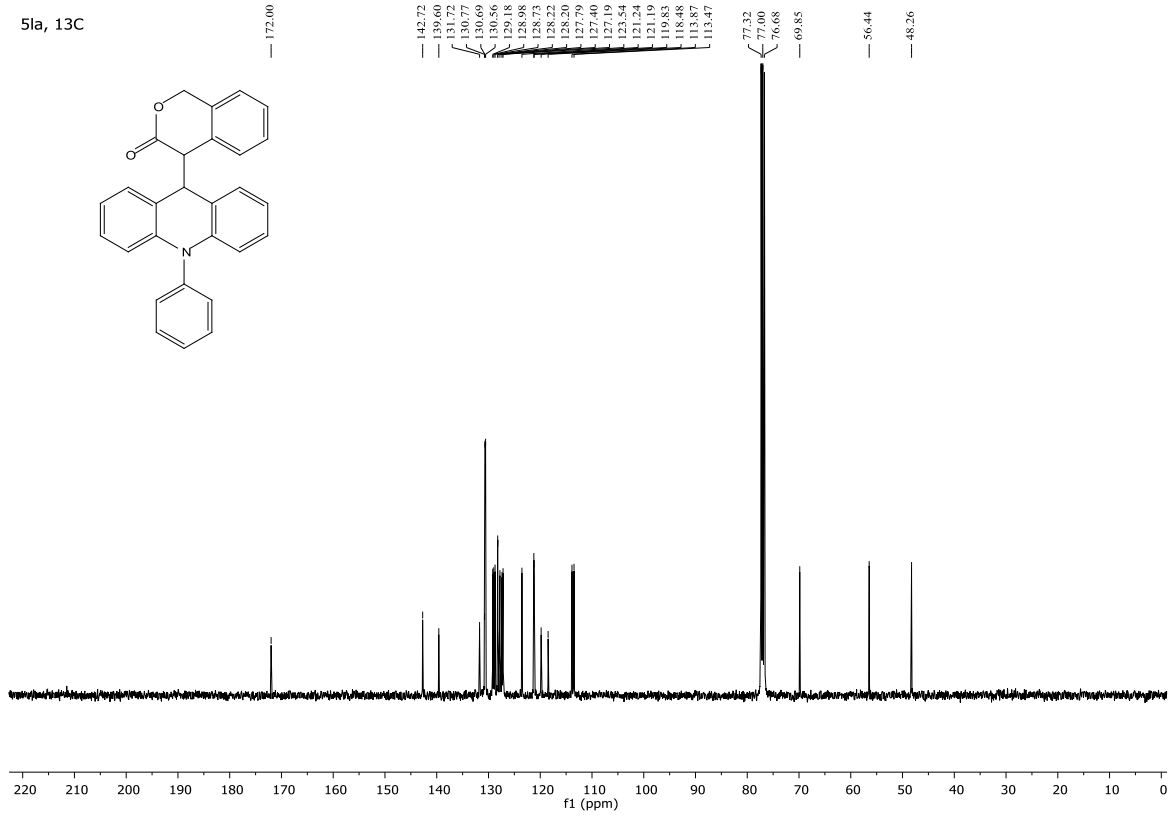
^{13}C {^{1}H} NMR of **5ka** (100 MHz, $CDCl_3$):



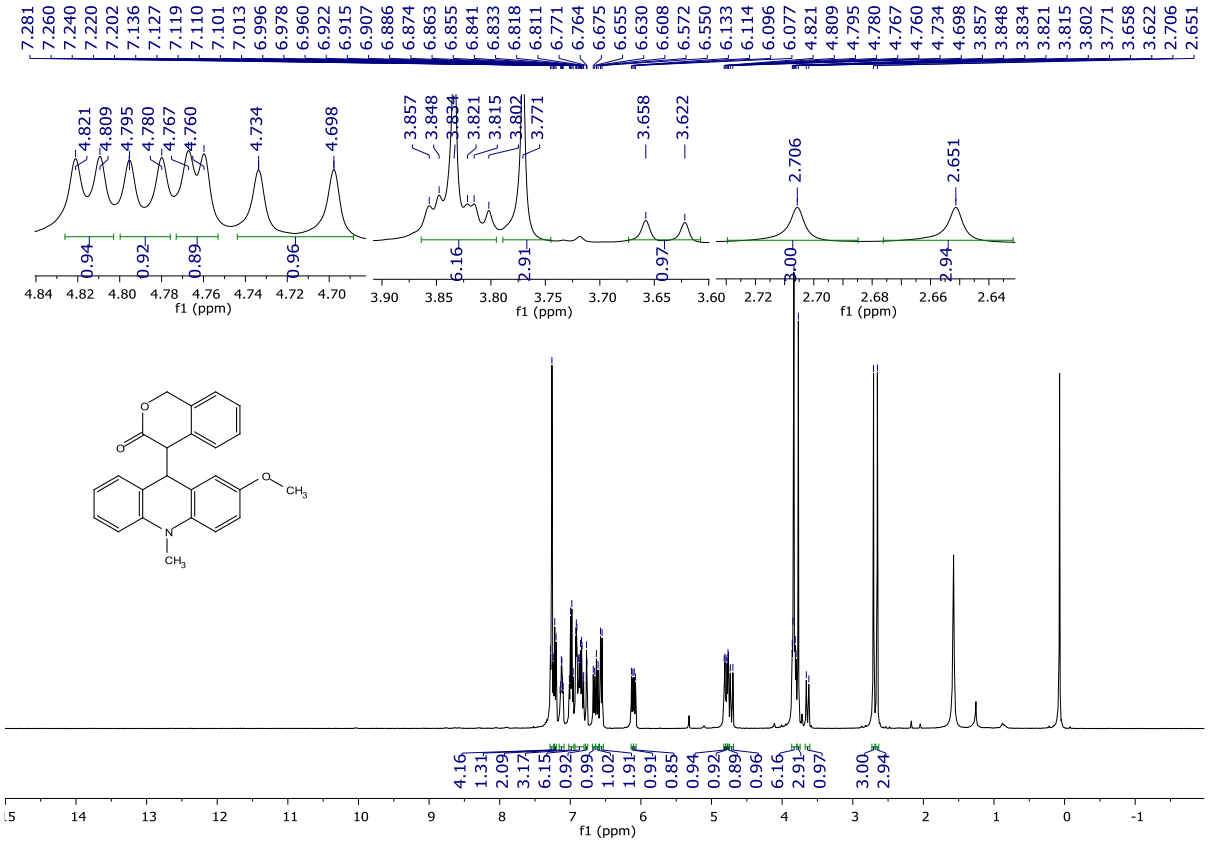
^{1}H NMR of **5la** (400 MHz, $CDCl_3$):



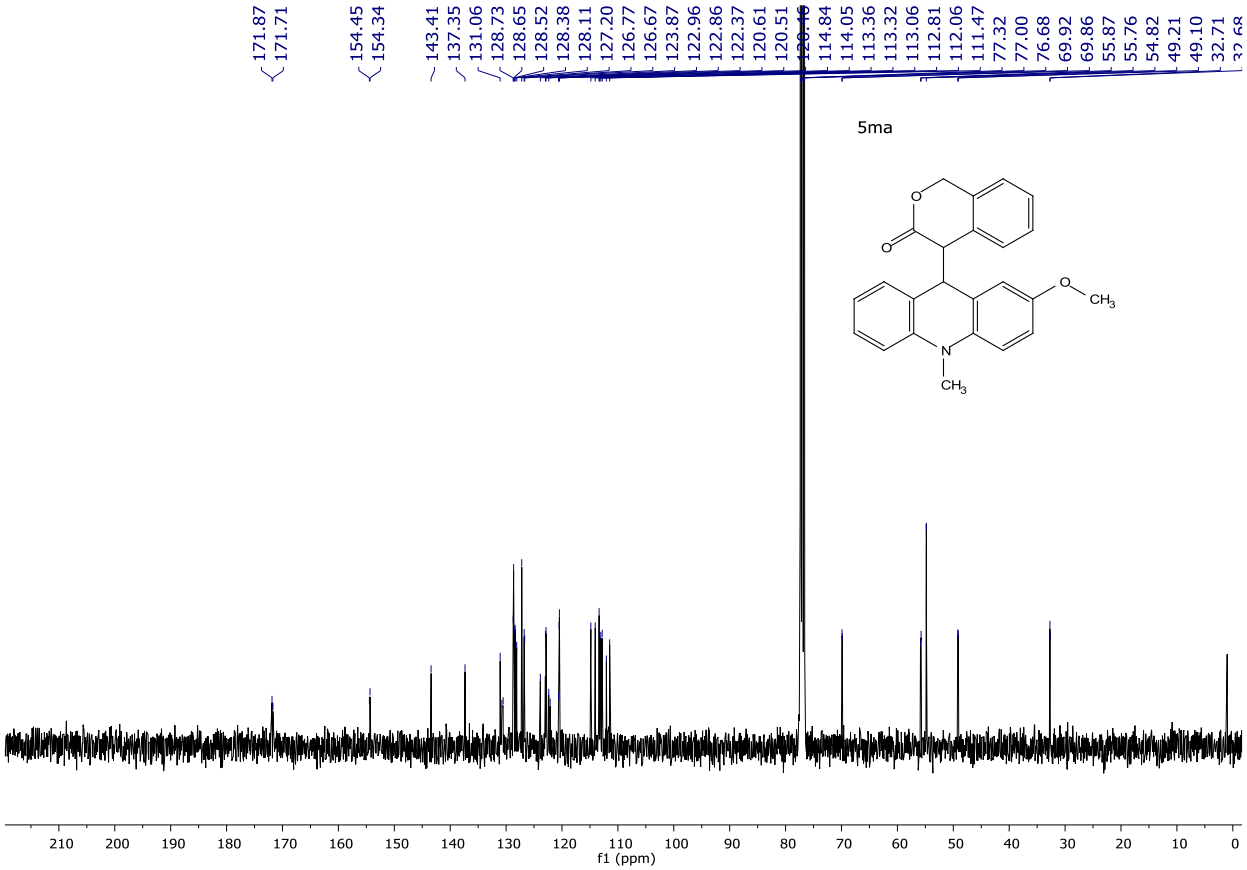
^{13}C {^{1}H} NMR of **5la** (100 MHz, $CDCl_3$):



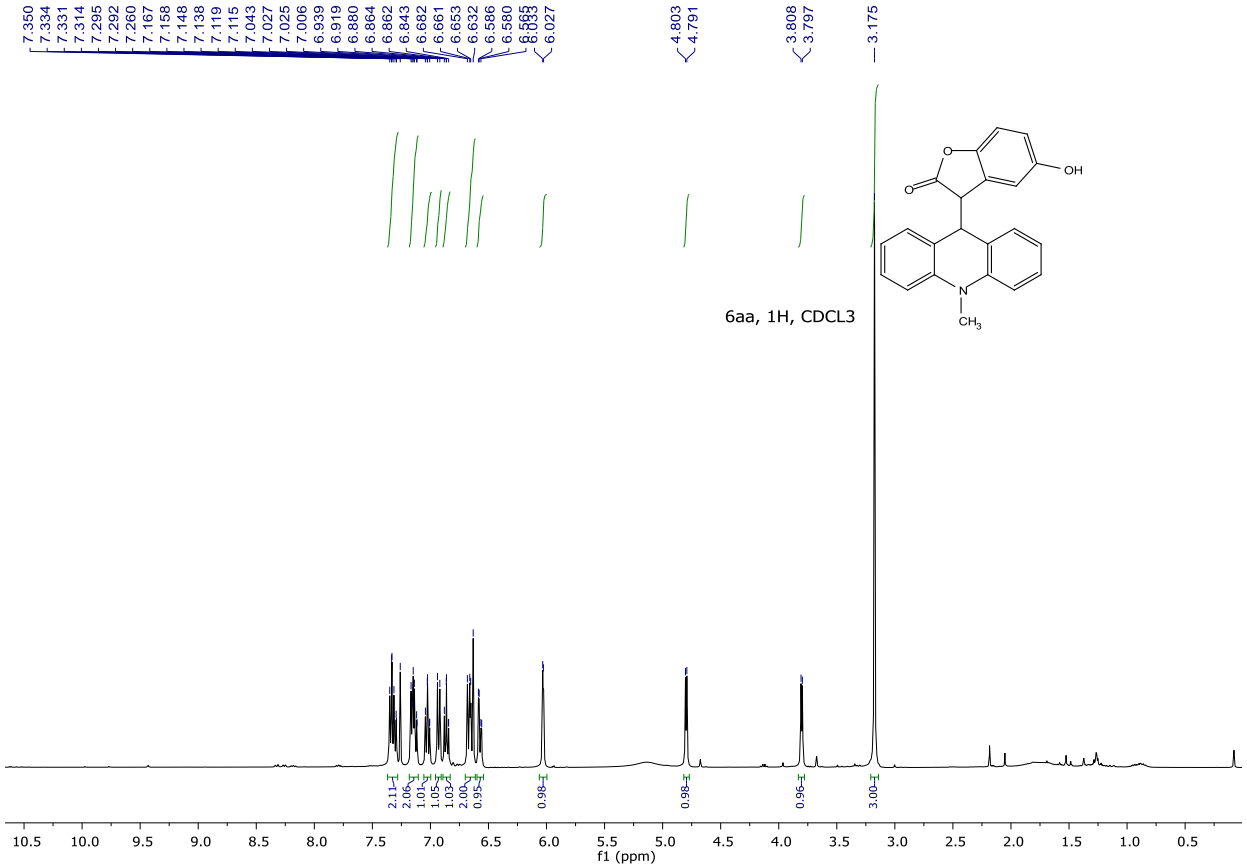
^{1}H NMR of **5ma** (400 MHz, $CDCl_3$):



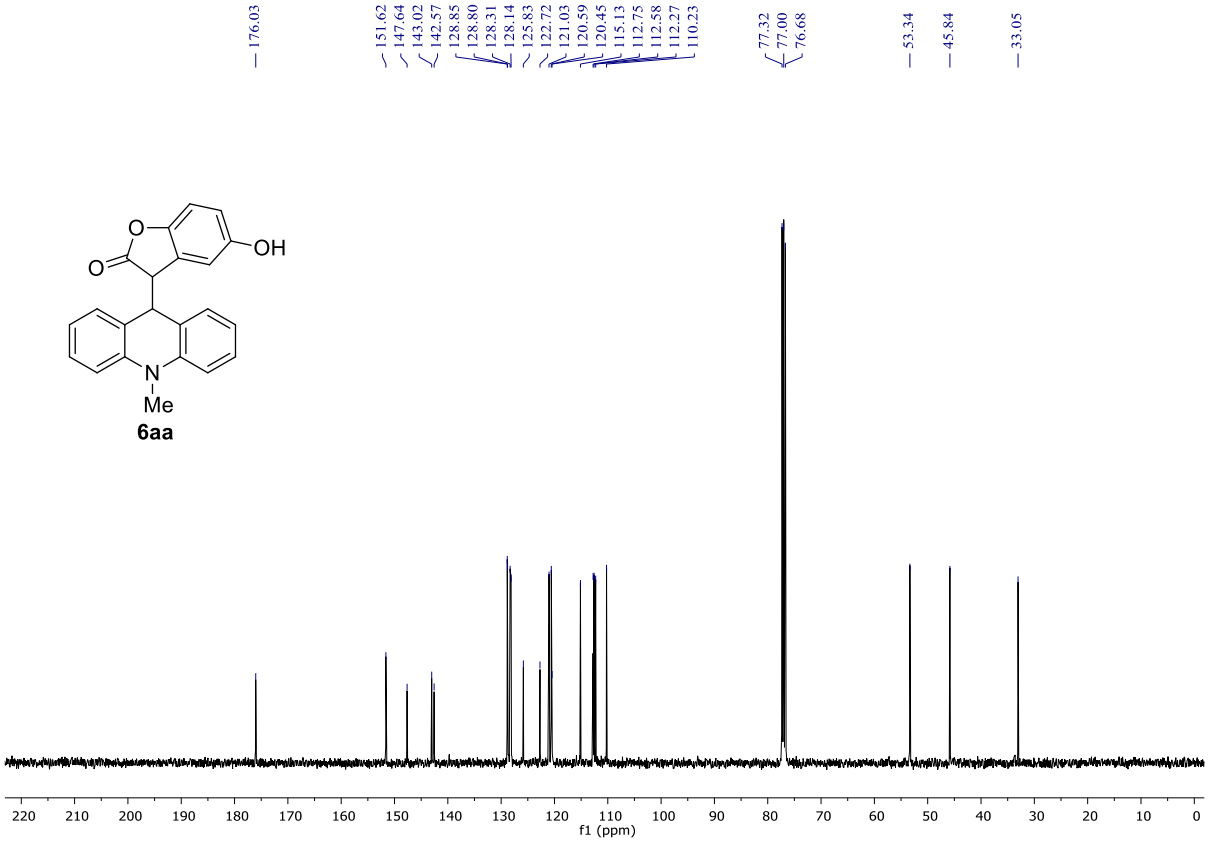
^{13}C {^{1}H} NMR of **5ma** (100 MHz, $CDCl_3$):



^{1}H NMR of **6aa** (400 MHz, $CDCl_3$):

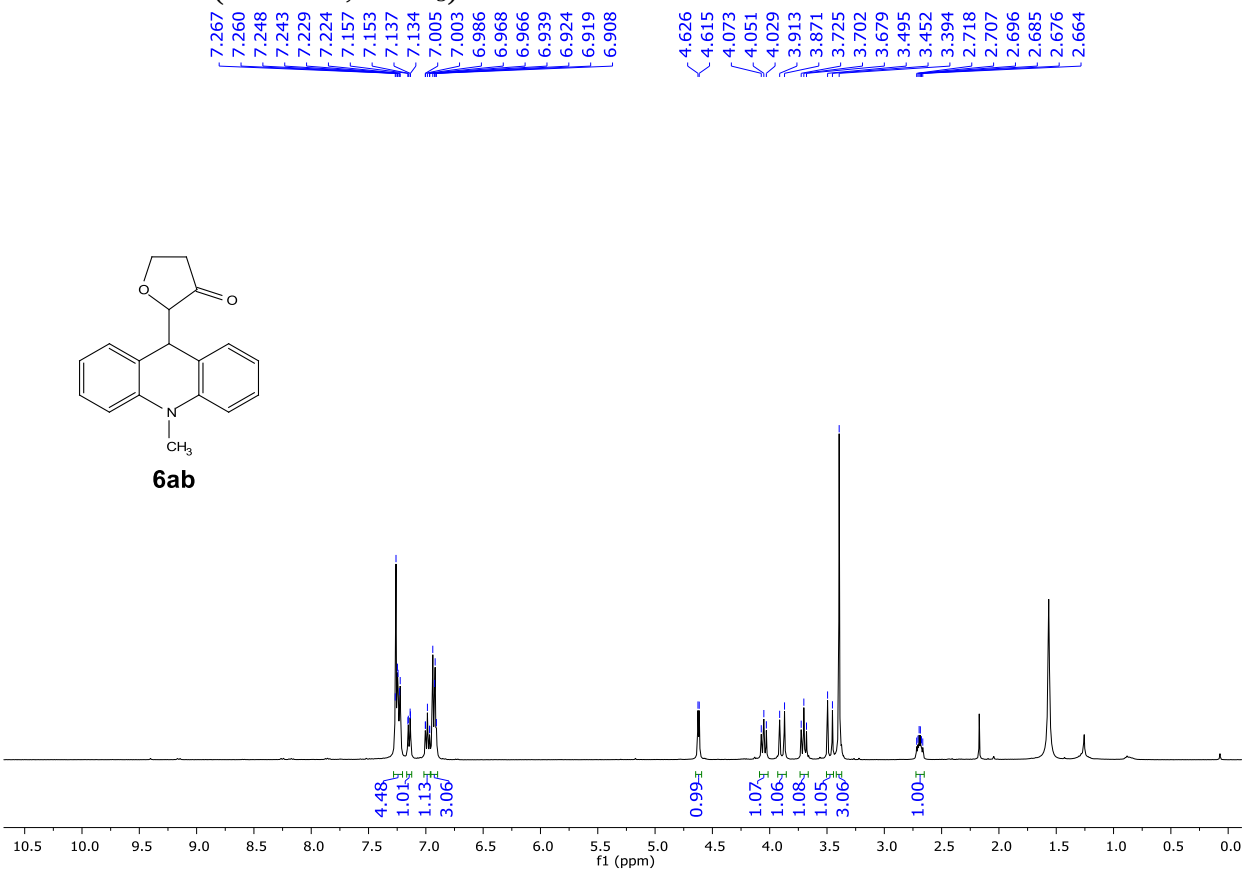


^{13}C {^{1}H} NMR of **6aa** (100 MHz, $CDCl_3$):

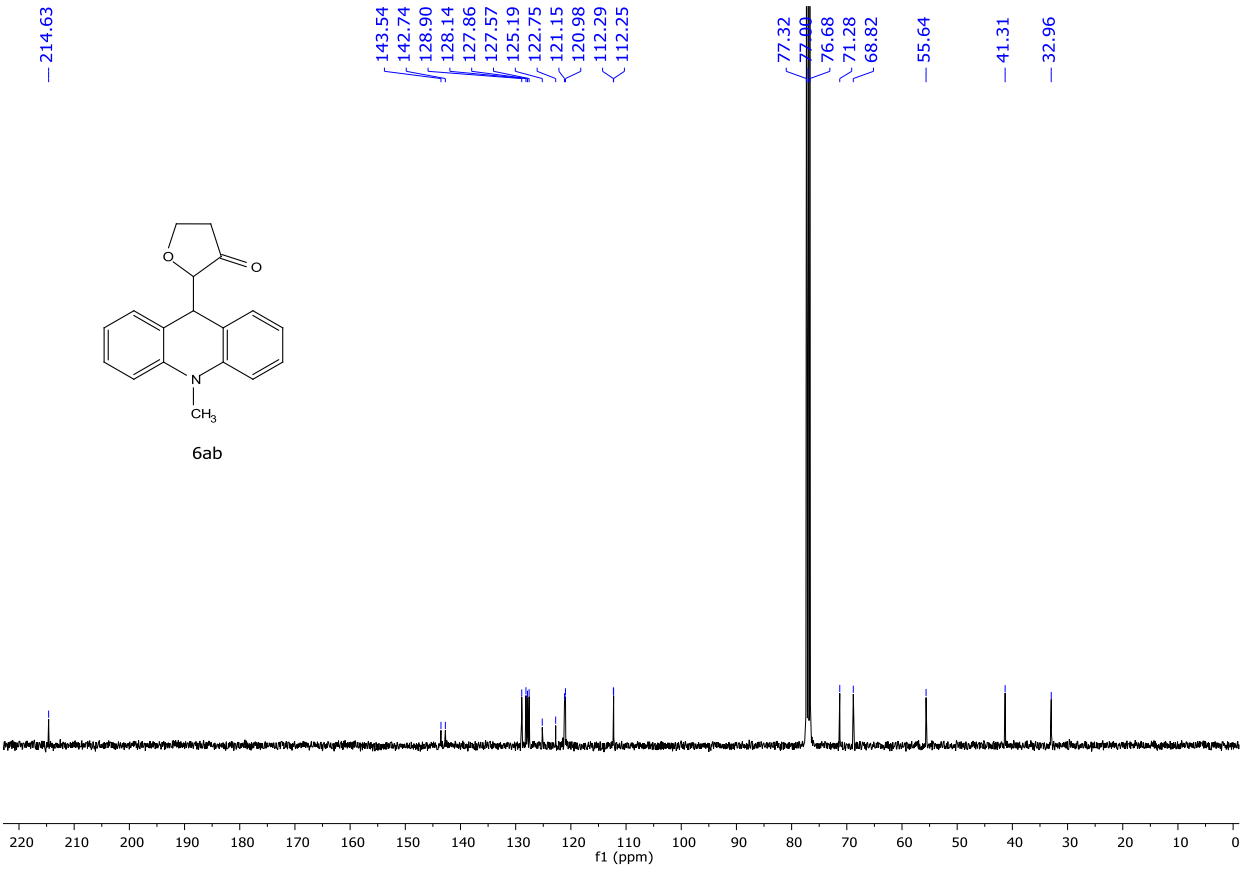


6aa

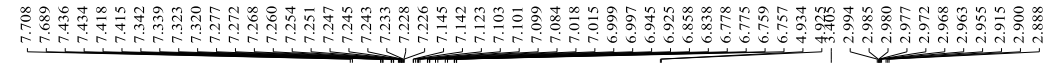
^{1}H NMR of **6ab** (400 MHz, $CDCl_3$):

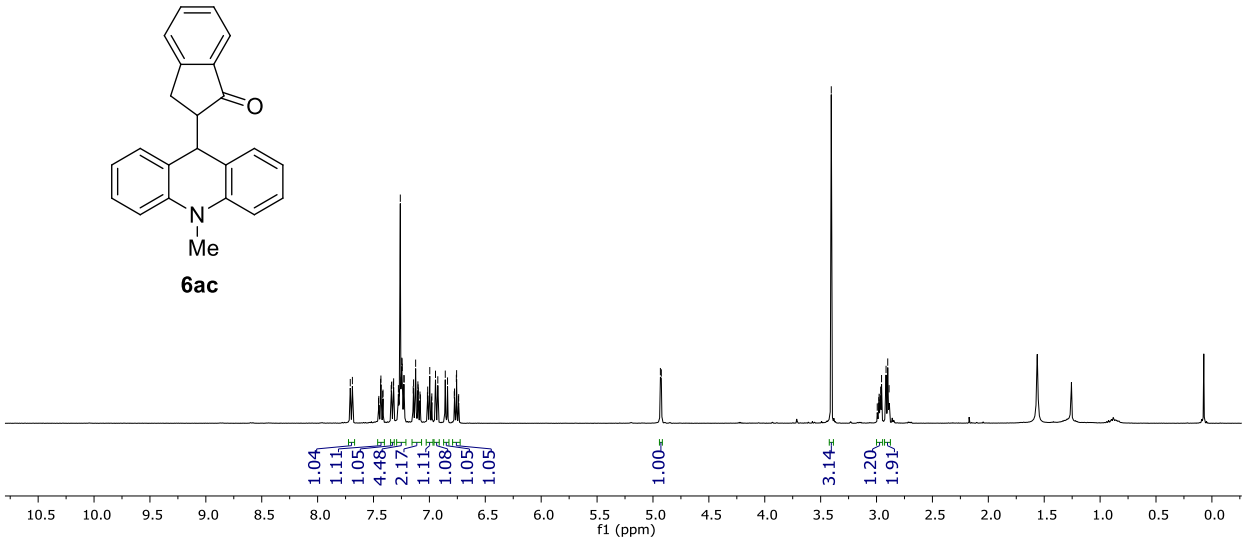


^{13}C {^{1}H} NMR of **6ab** (100 MHz, $CDCl_3$):

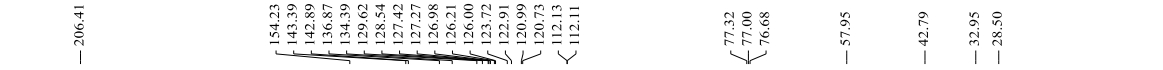


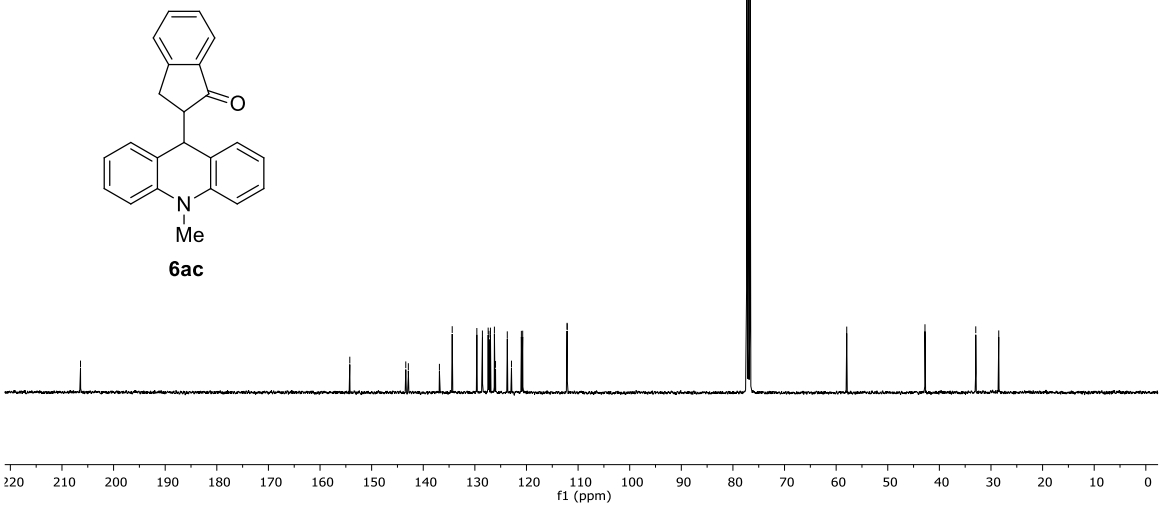
^{1}H NMR of **6ac** (400 MHz, $CDCl_3$):



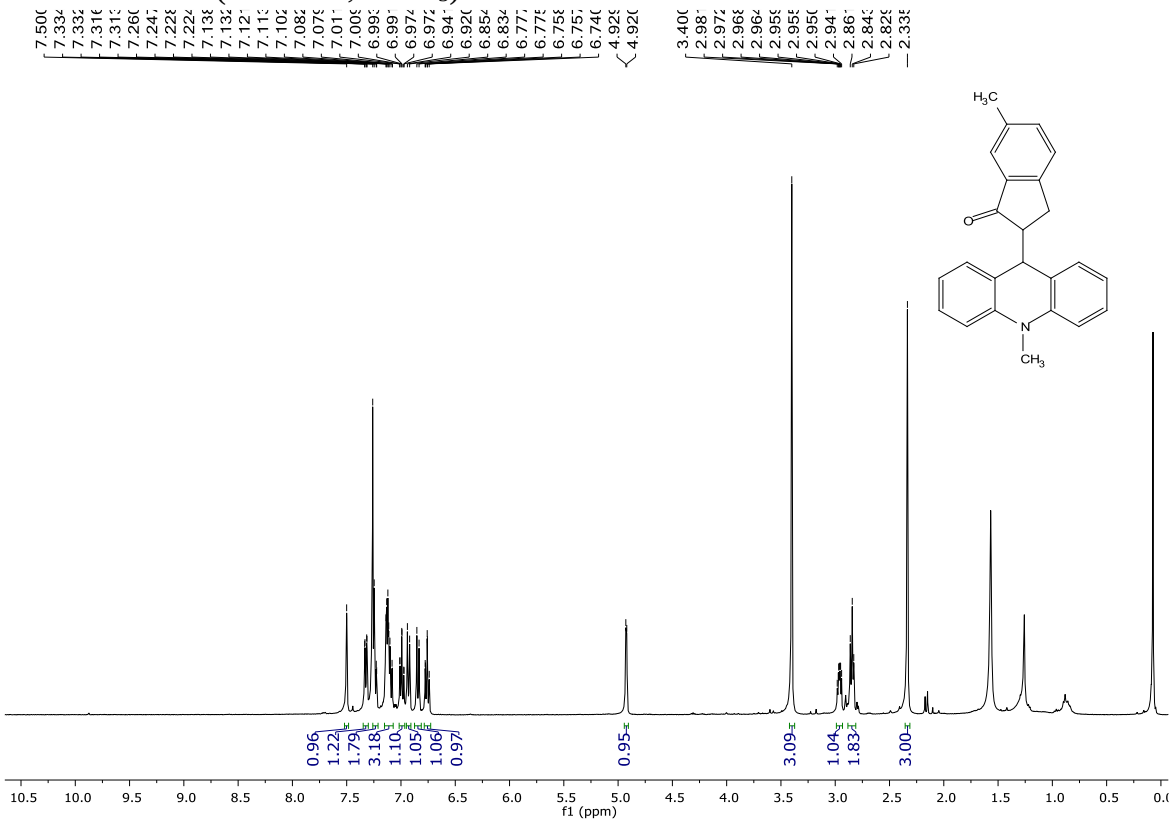


^{13}C {^{1}H} NMR of **6ac** (100 MHz, $CDCl_3$):

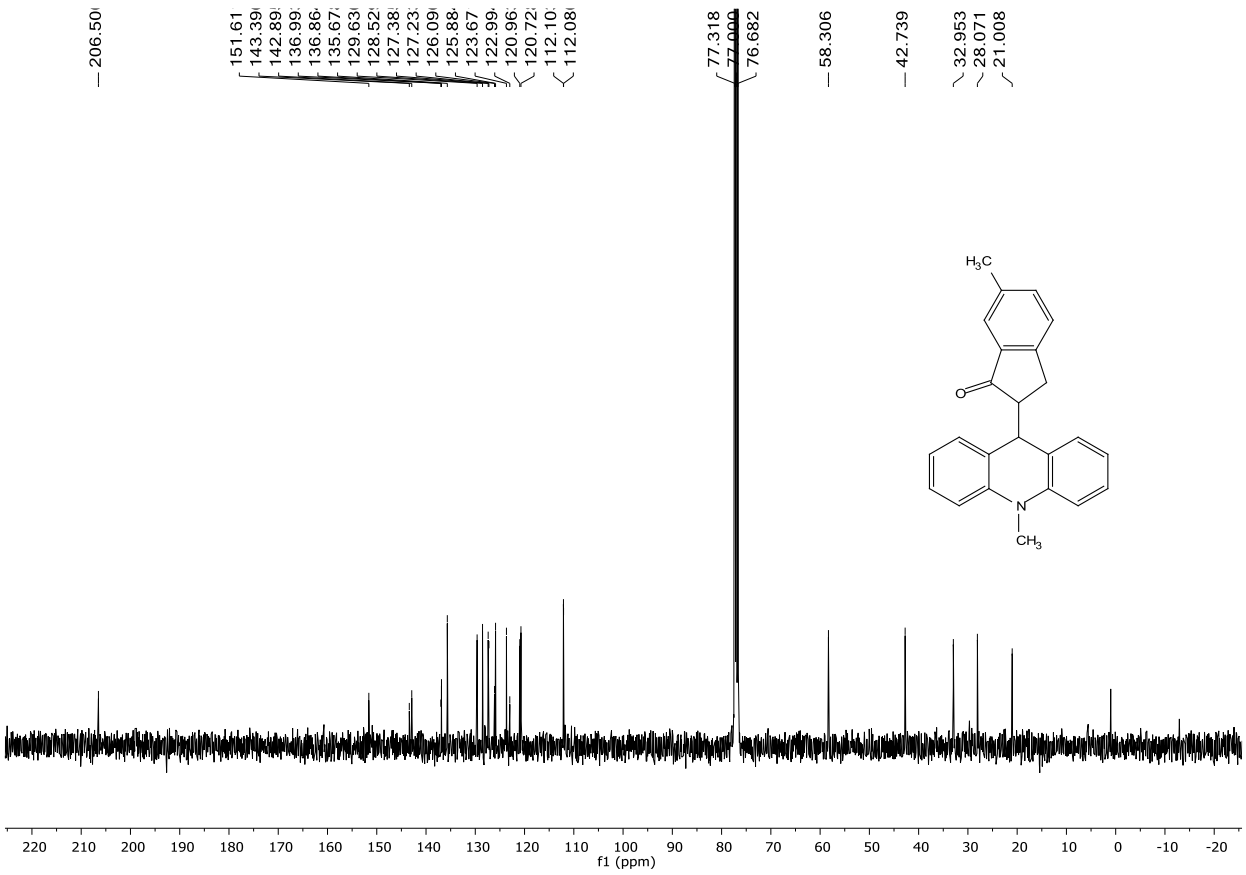




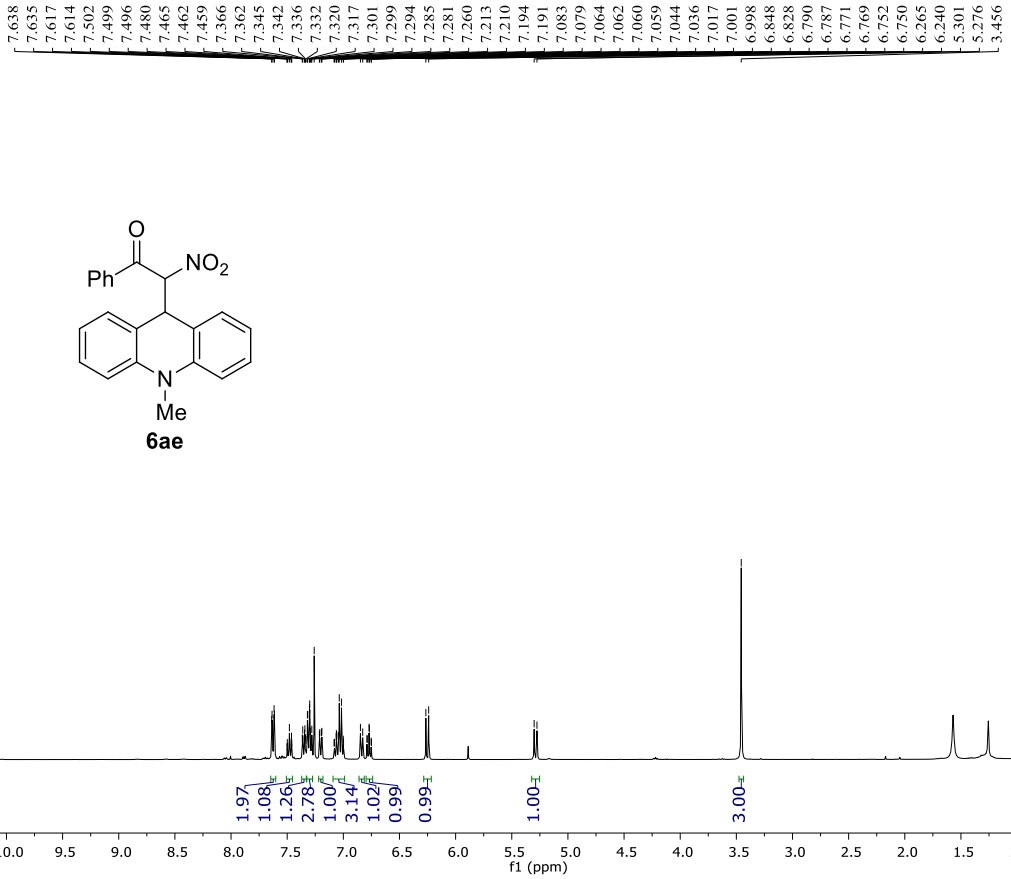
^{1}H NMR of **6ad** (400 MHz, $CDCl_3$):



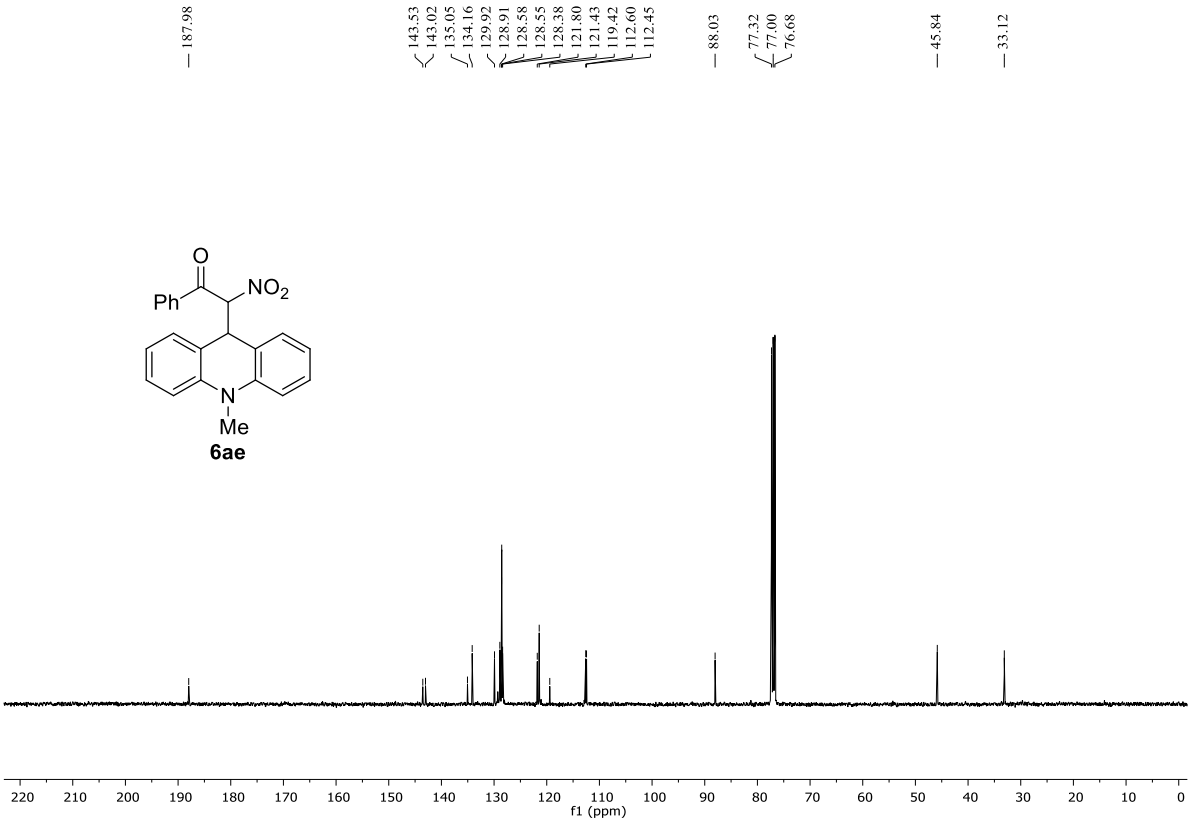
^{13}C {^{1}H} NMR of **6ad** (100 MHz, $CDCl_3$):



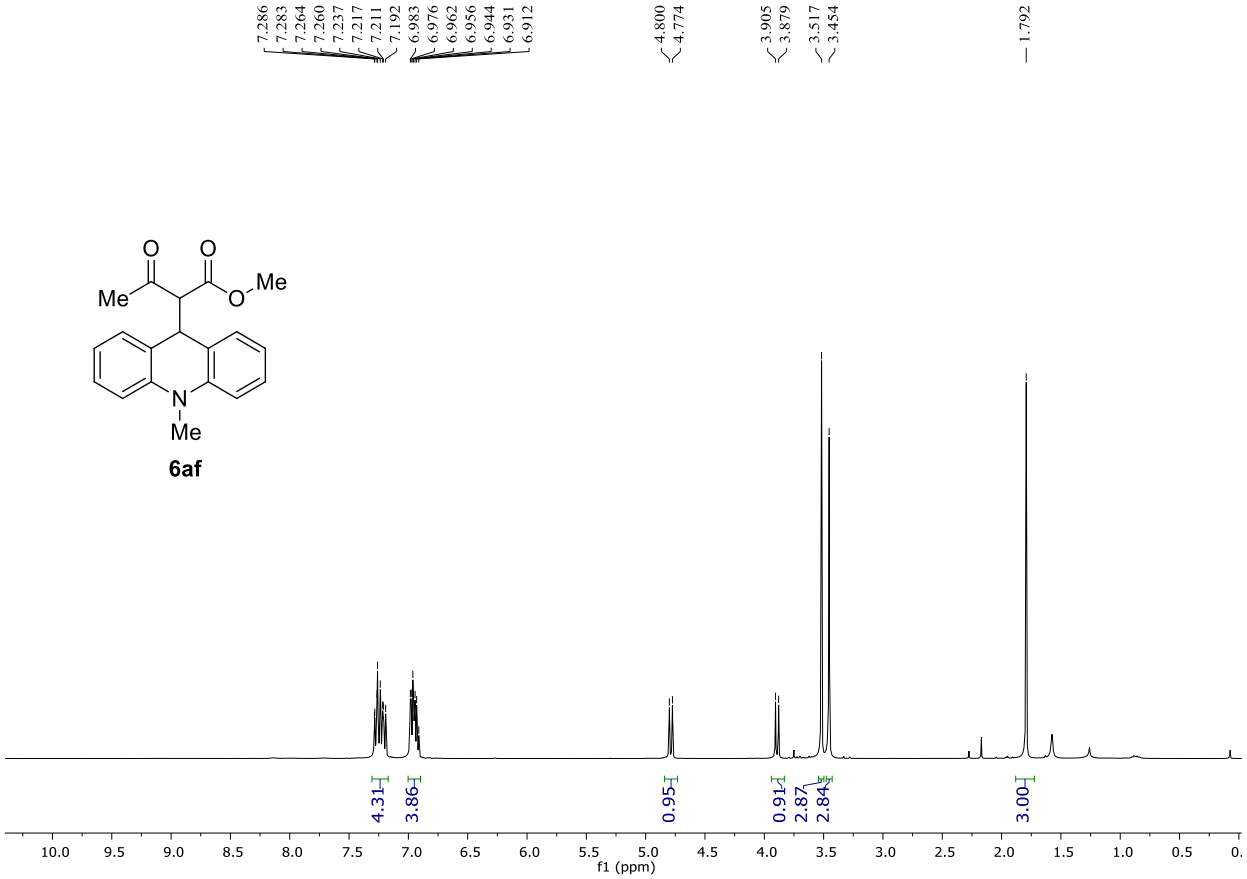
^{1}H NMR of **6ae** (400 MHz, $CDCl_3$):



^{13}C {^{1}H} NMR of **6ae** (100 MHz, $CDCl_3$):

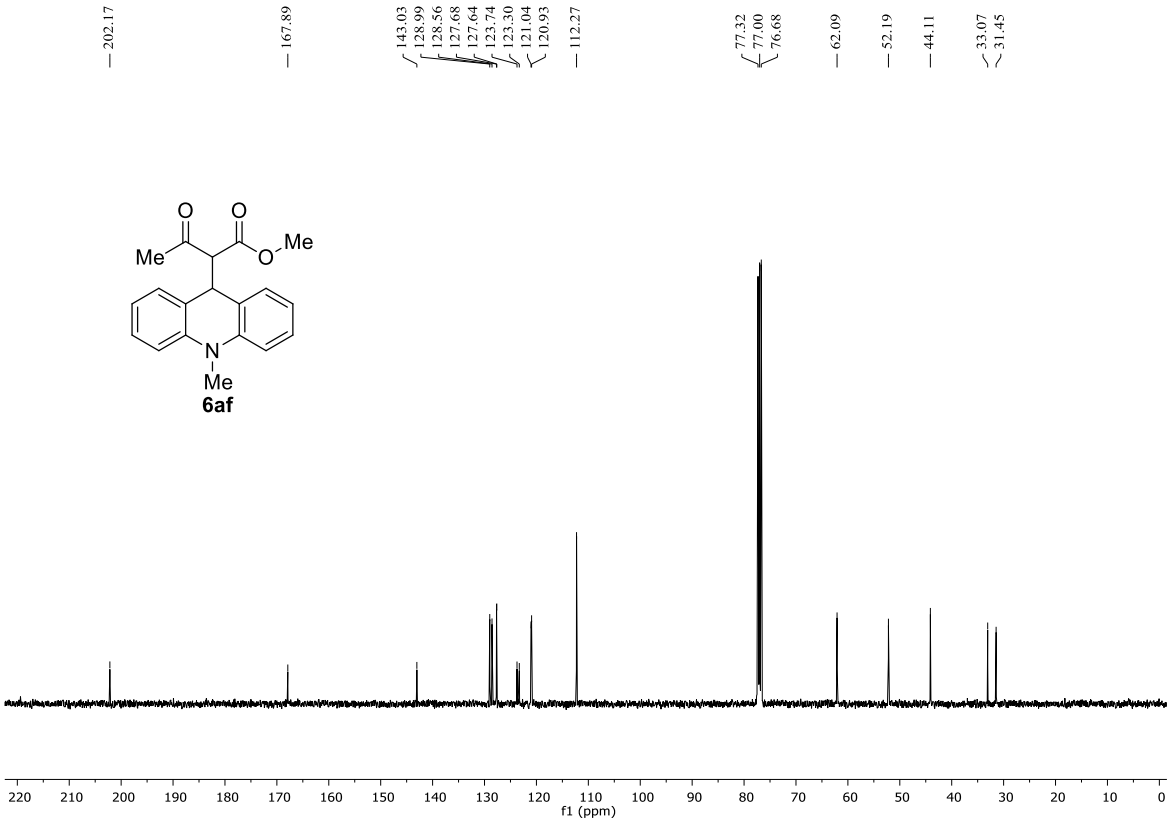


^{1}H NMR of **6af** (400 MHz, $CDCl_3$):



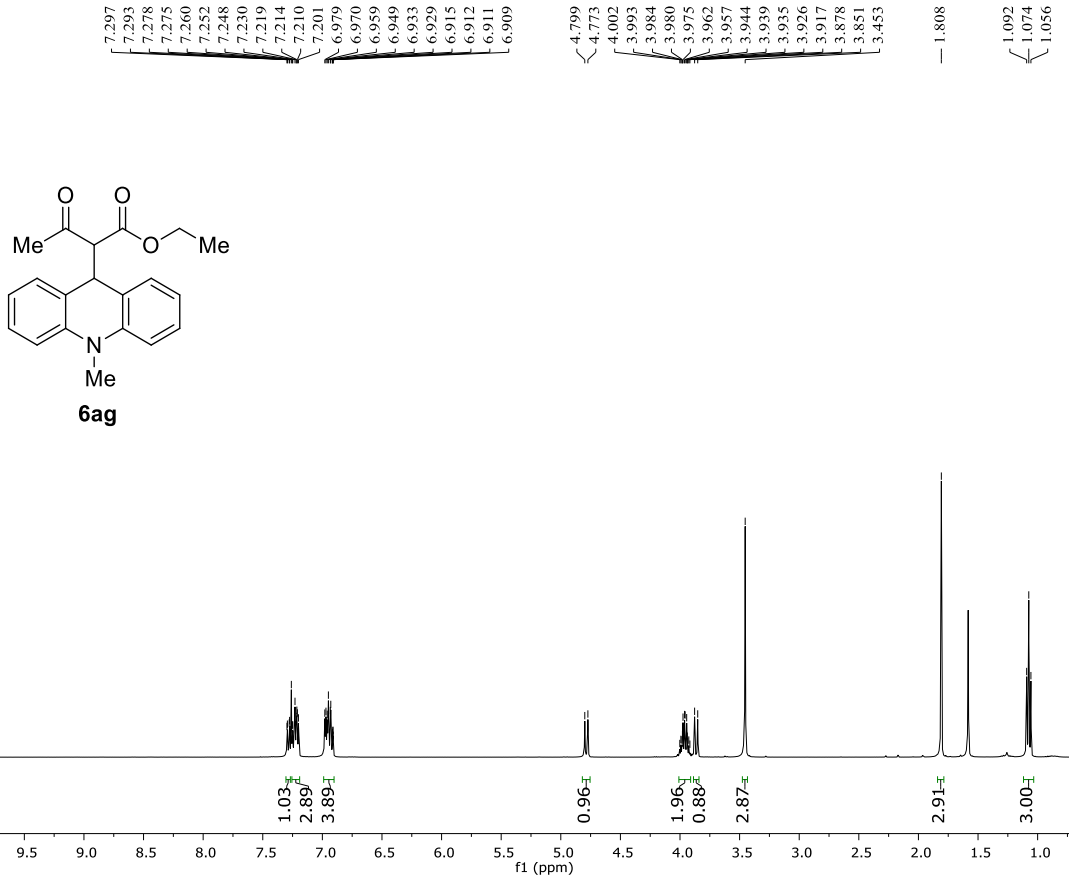
6af

^{13}C {^{1}H} NMR of **6af** (100 MHz, $CDCl_3$):



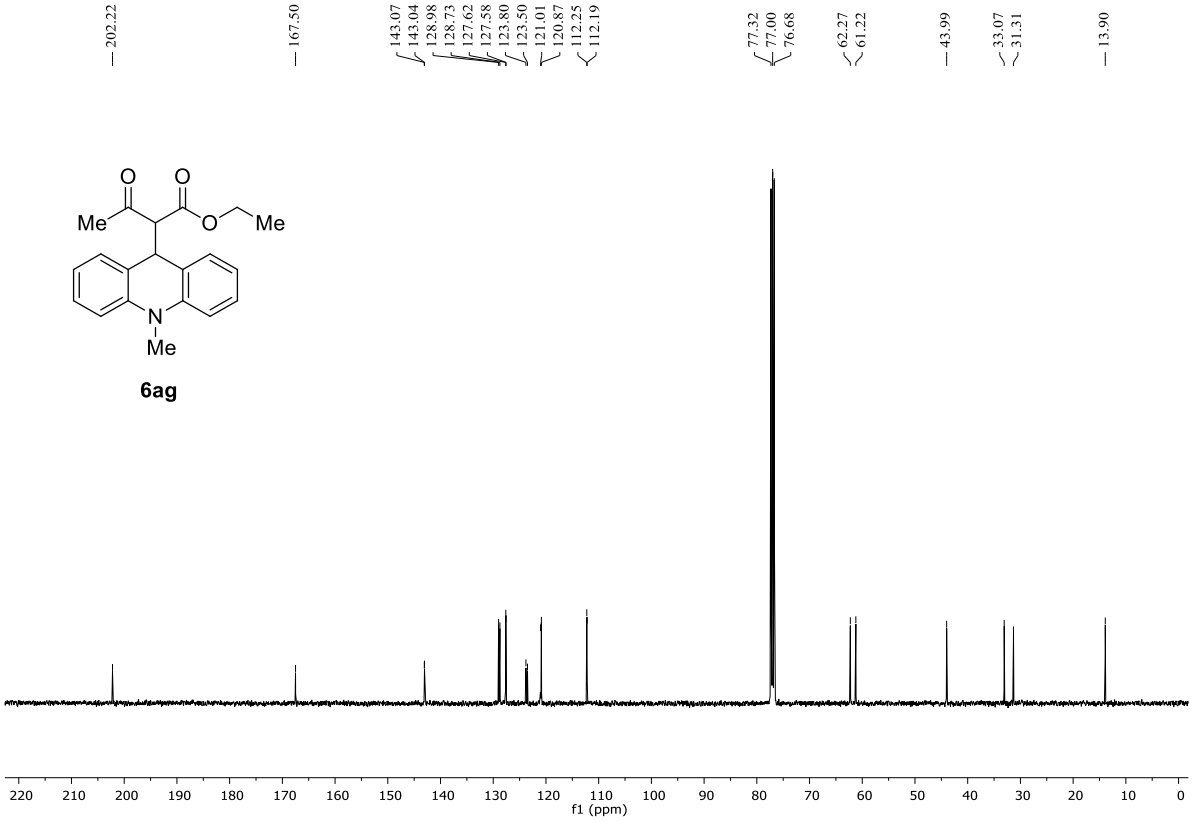
6af

^{1}H NMR of **6ag** (400 MHz, $CDCl_3$):



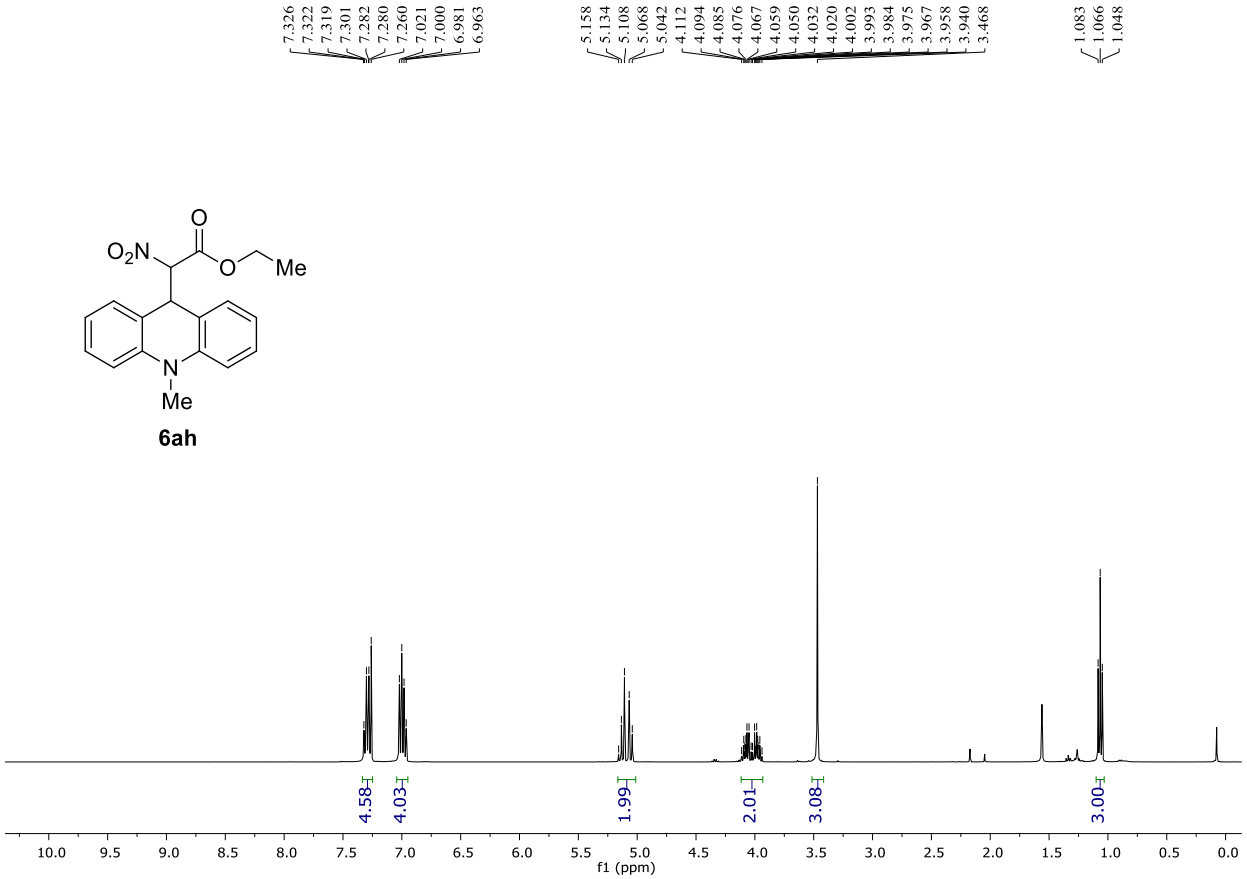
6ag

^{13}C {^{1}H} NMR of **6ag** (100 MHz, $CDCl_3$):

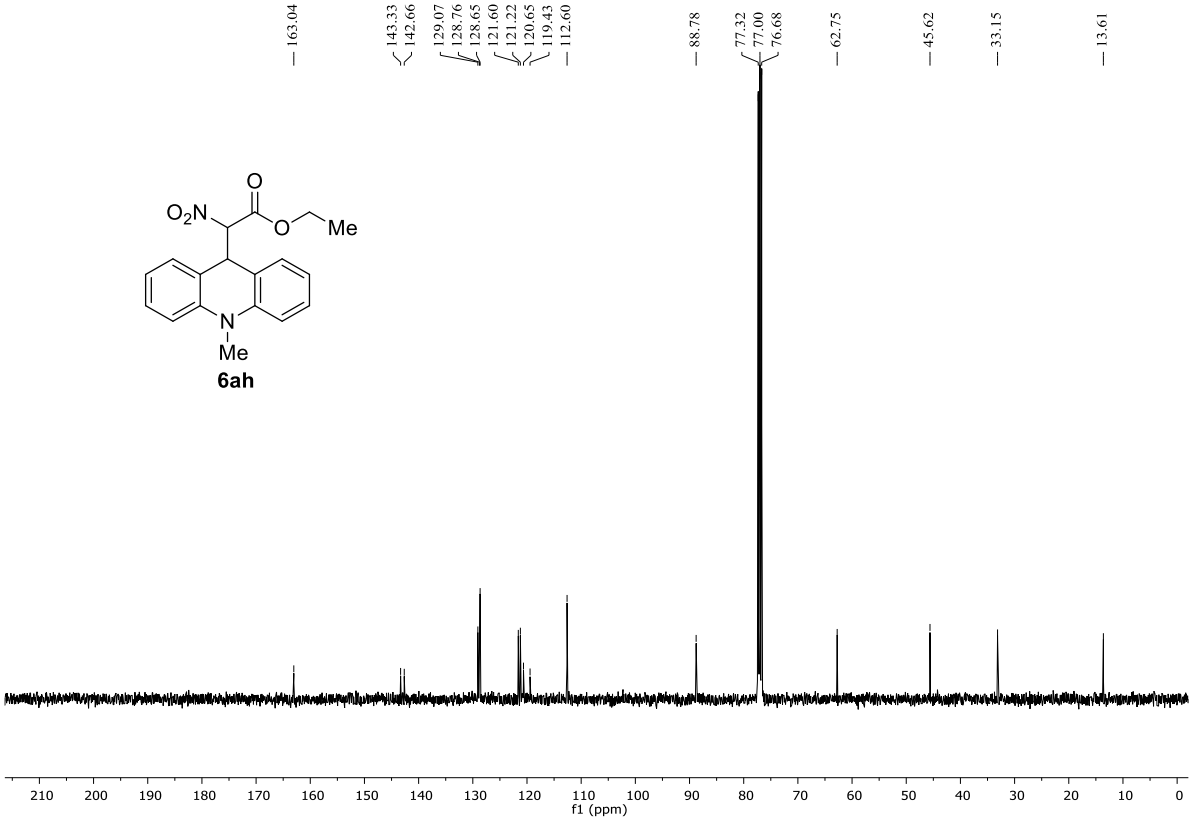


6ag

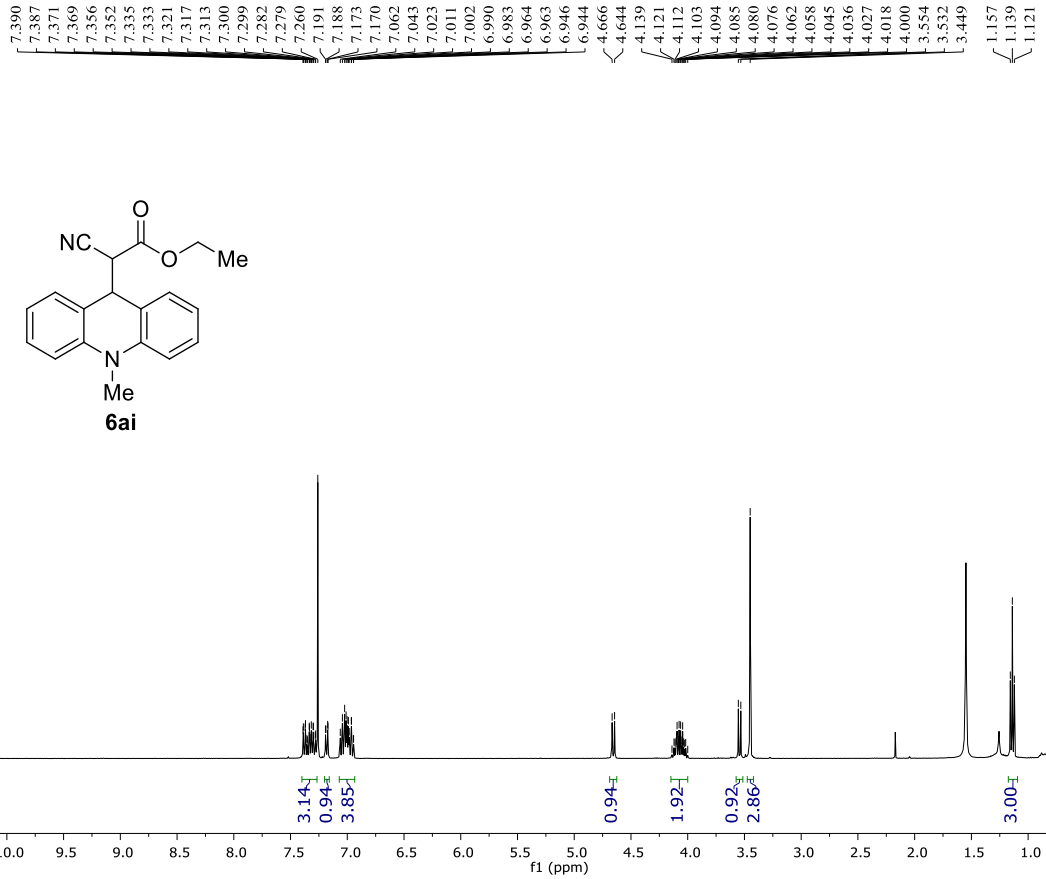
^{1}H NMR of **6ah** (400 MHz, $CDCl_3$):



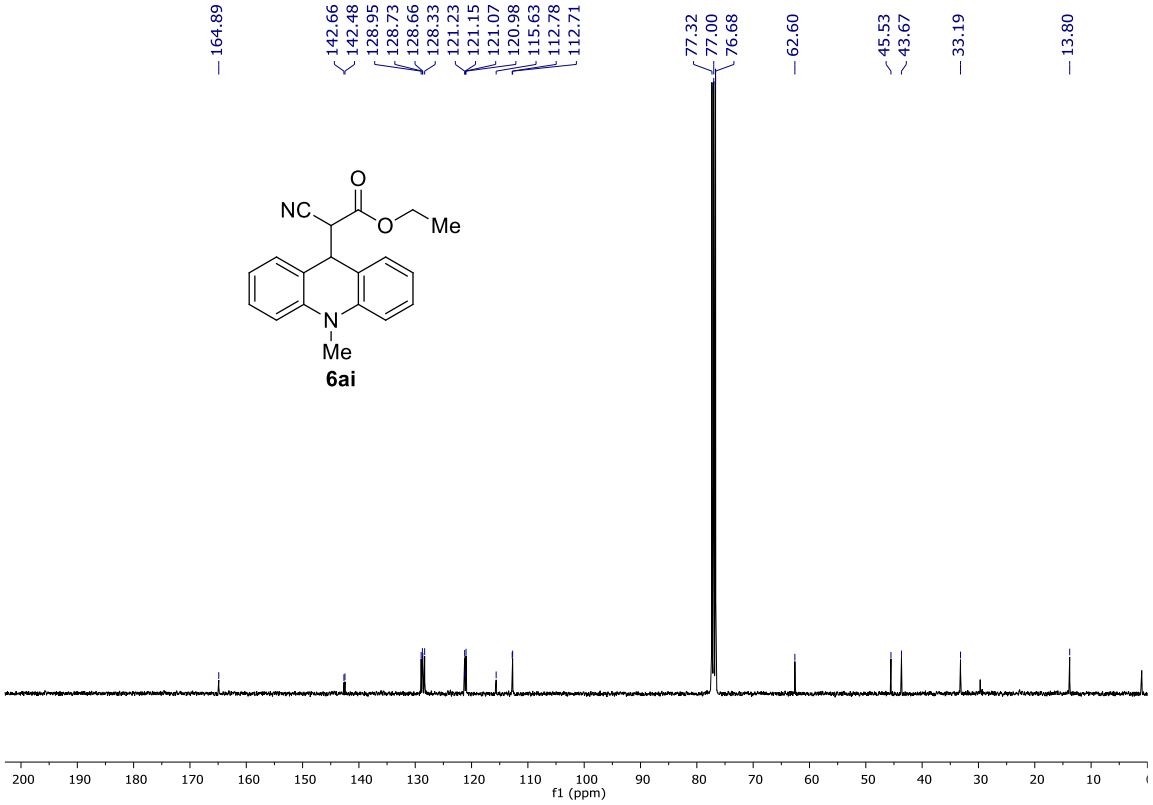
^{13}C {^{1}H} NMR of **6ah** (100 MHz, $CDCl_3$):



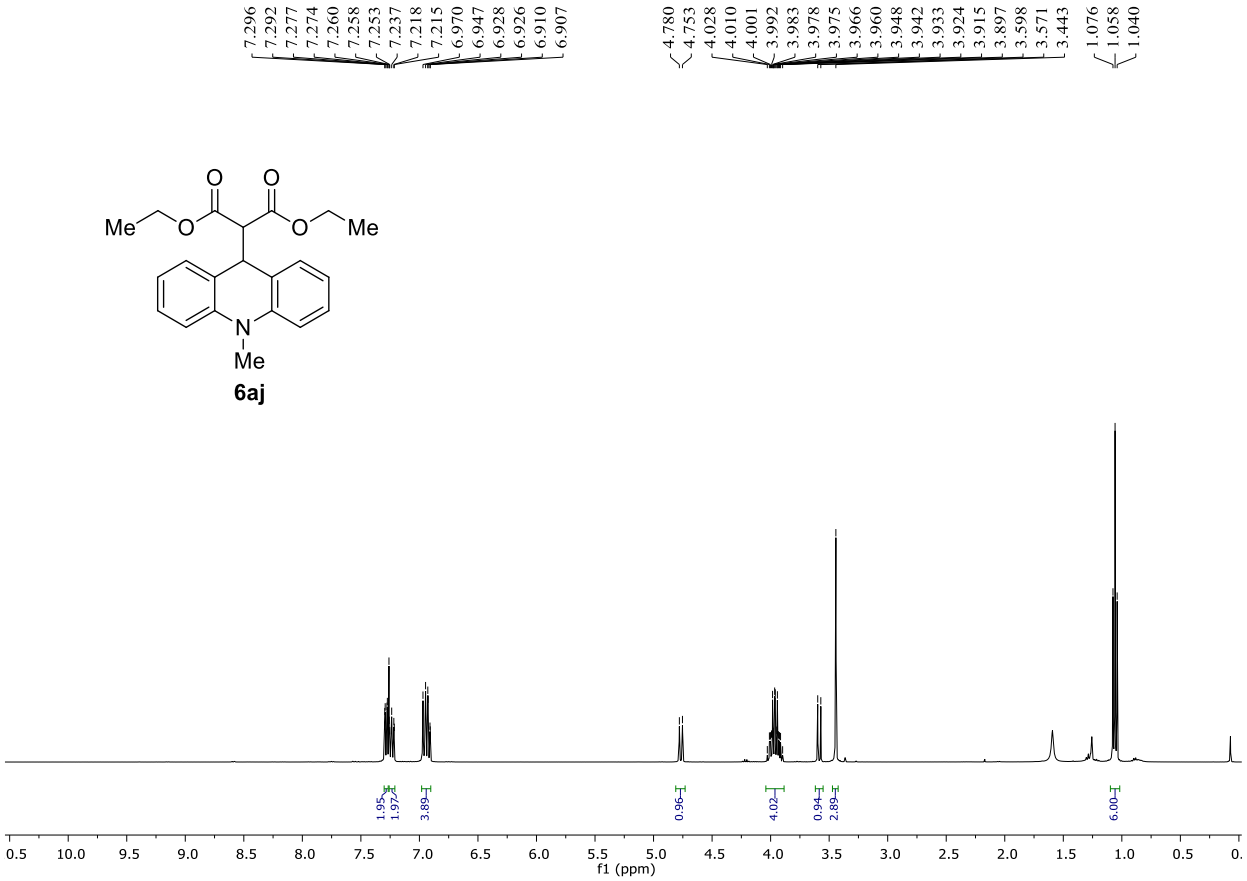
^{1}H NMR of **6ai** (400 MHz, $CDCl_3$):



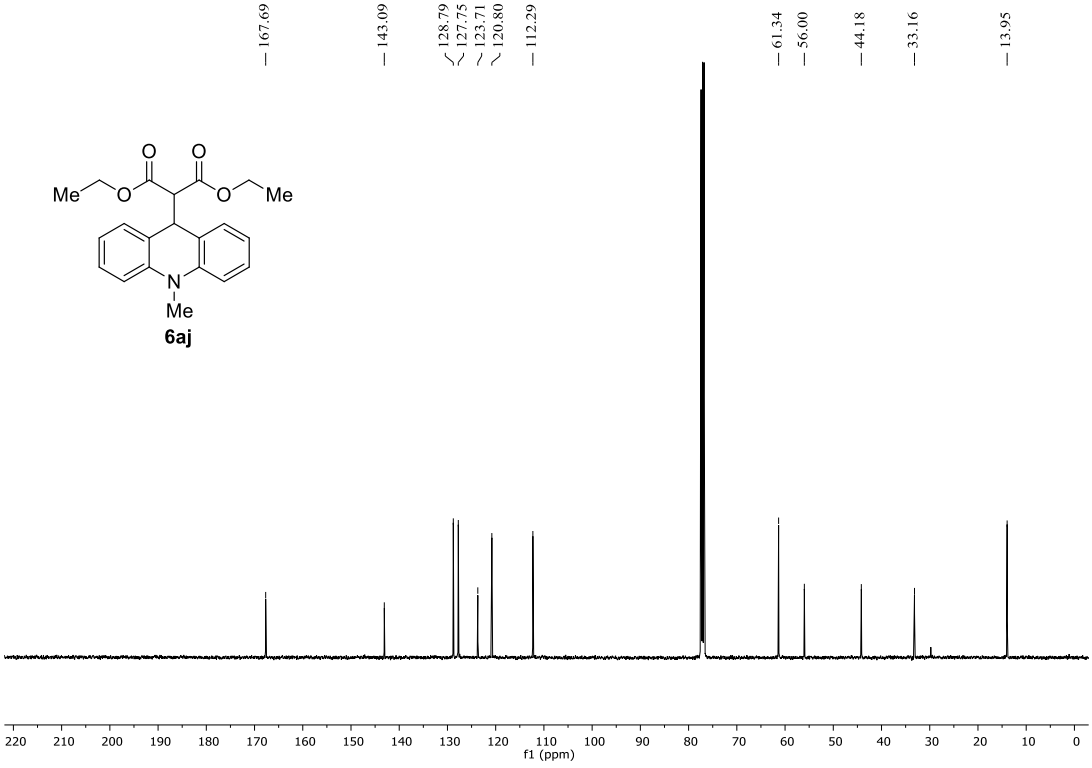
^{13}C {^{1}H} NMR of **6ai** (100 MHz, $CDCl_3$):



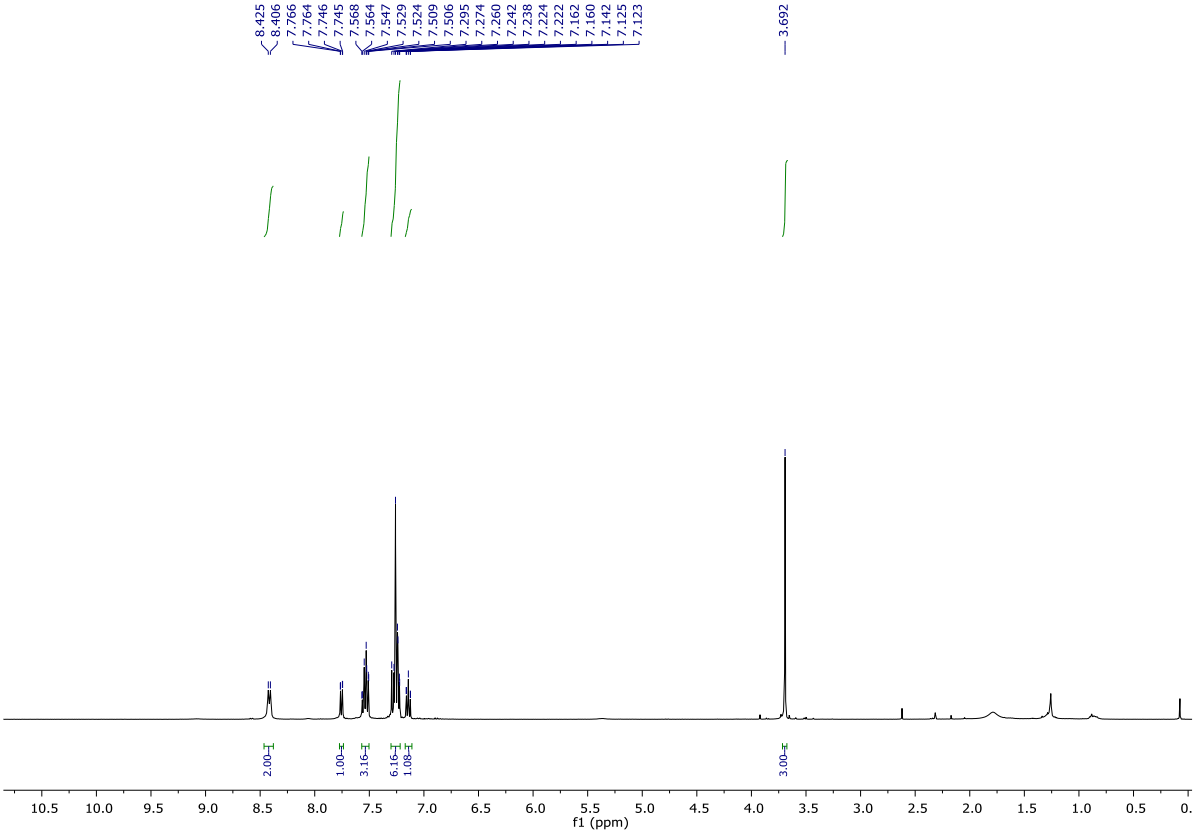
^{1}H NMR of **6aj** (400 MHz, $CDCl_3$):



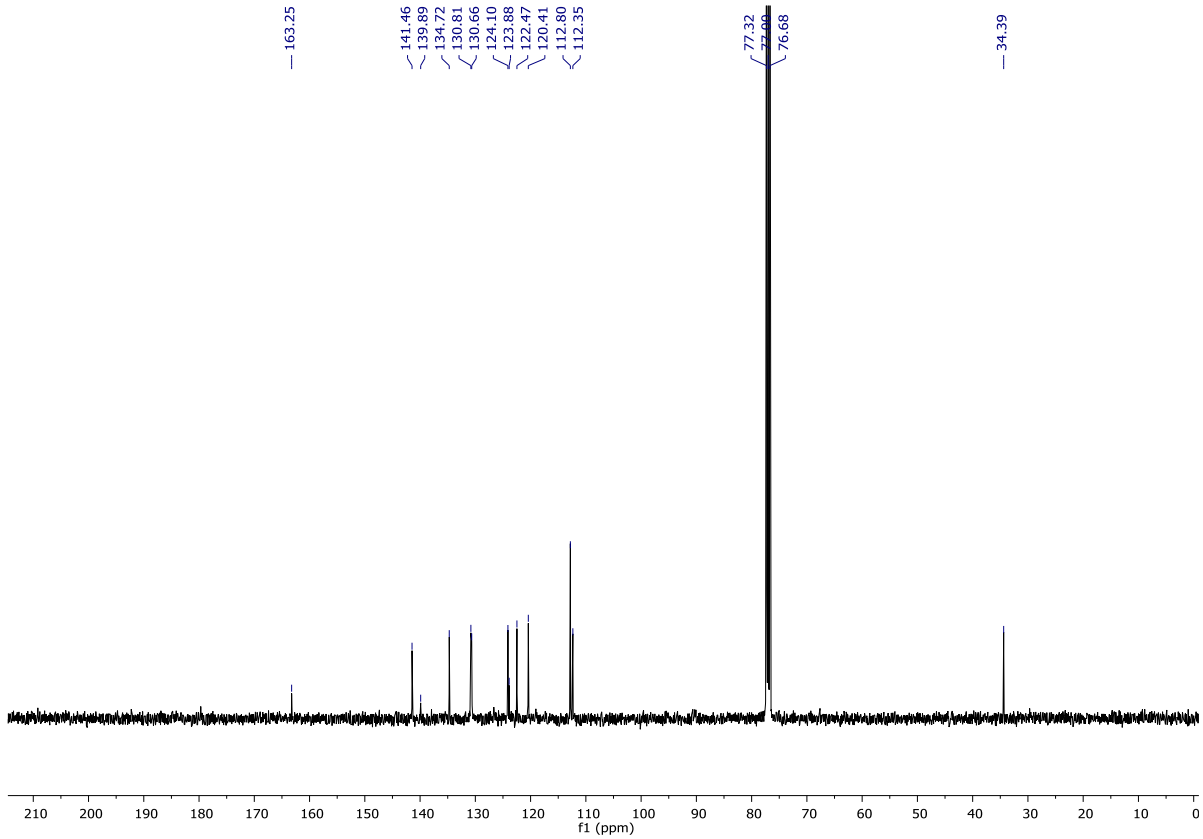
^{13}C {^{1}H} NMR of **6aj** (100 MHz, $CDCl_3$):



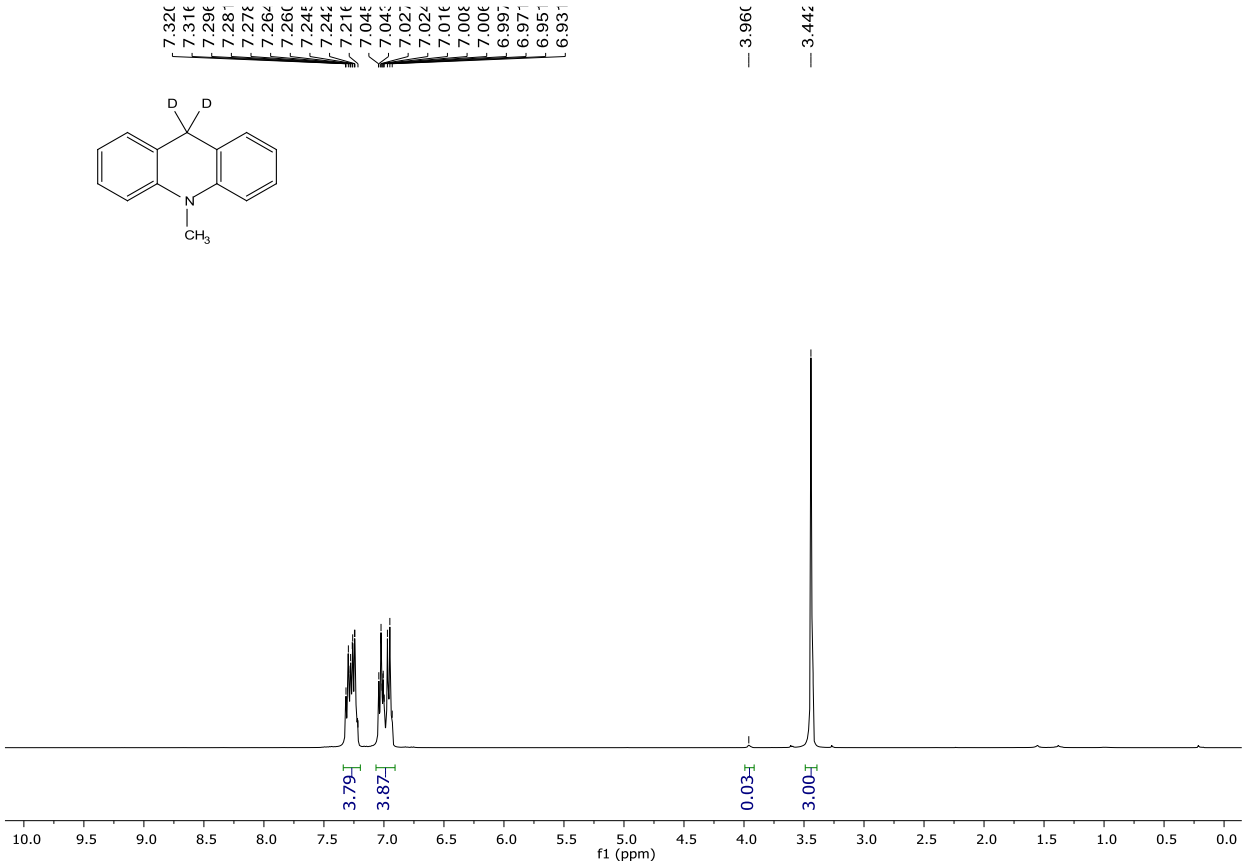
^{1}H NMR of **7** (400 MHz, $CDCl_3$):



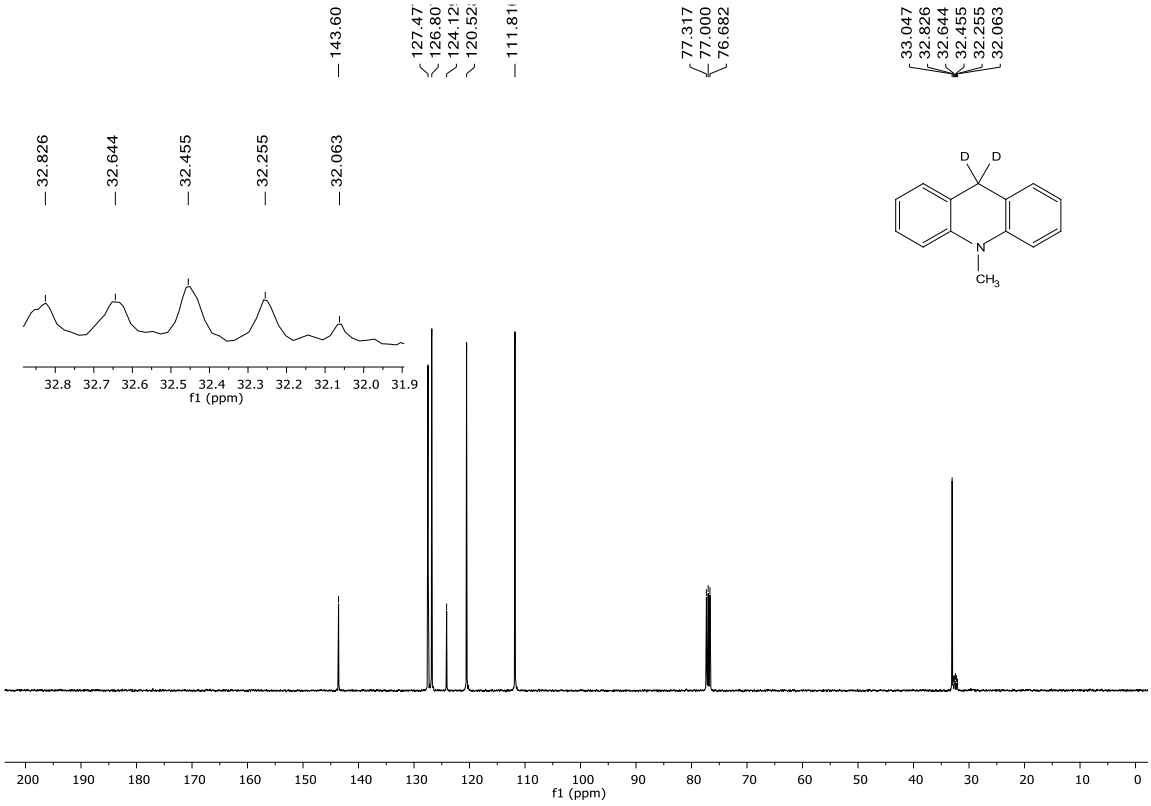
^{13}C {^{1}H} NMR of **7** (100 MHz, $CDCl_3$):



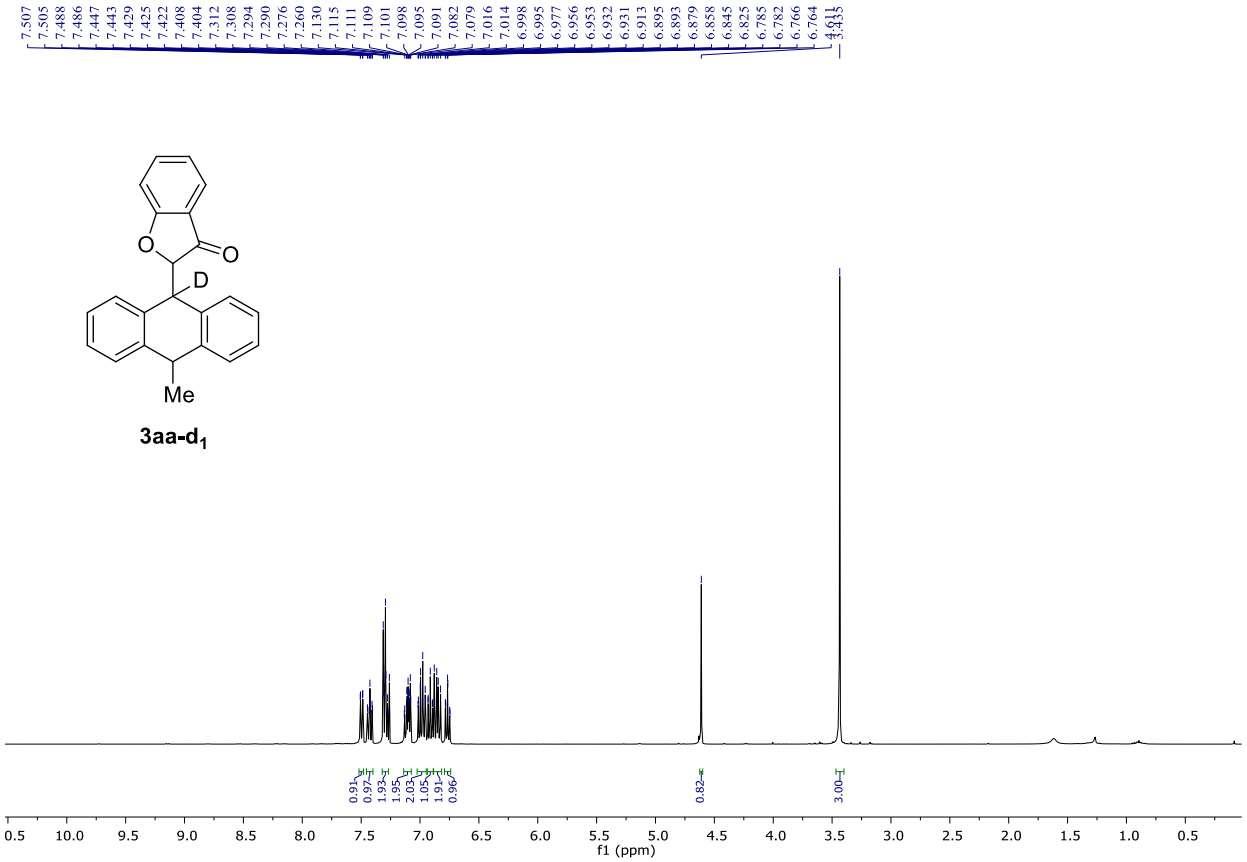
^{1}H NMR of **1a-*d*$_2$** (400 MHz, $CDCl_3$):



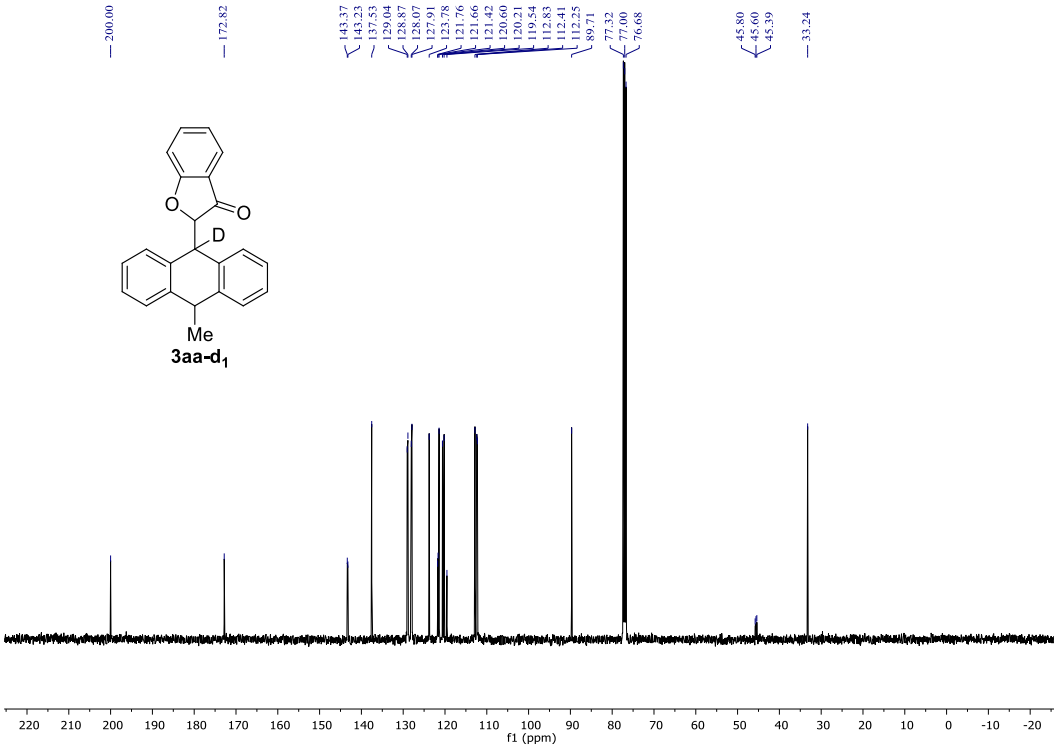
^{13}C {^{1}H} NMR of **1a-*d*$_2$** (100 MHz, $CDCl_3$):



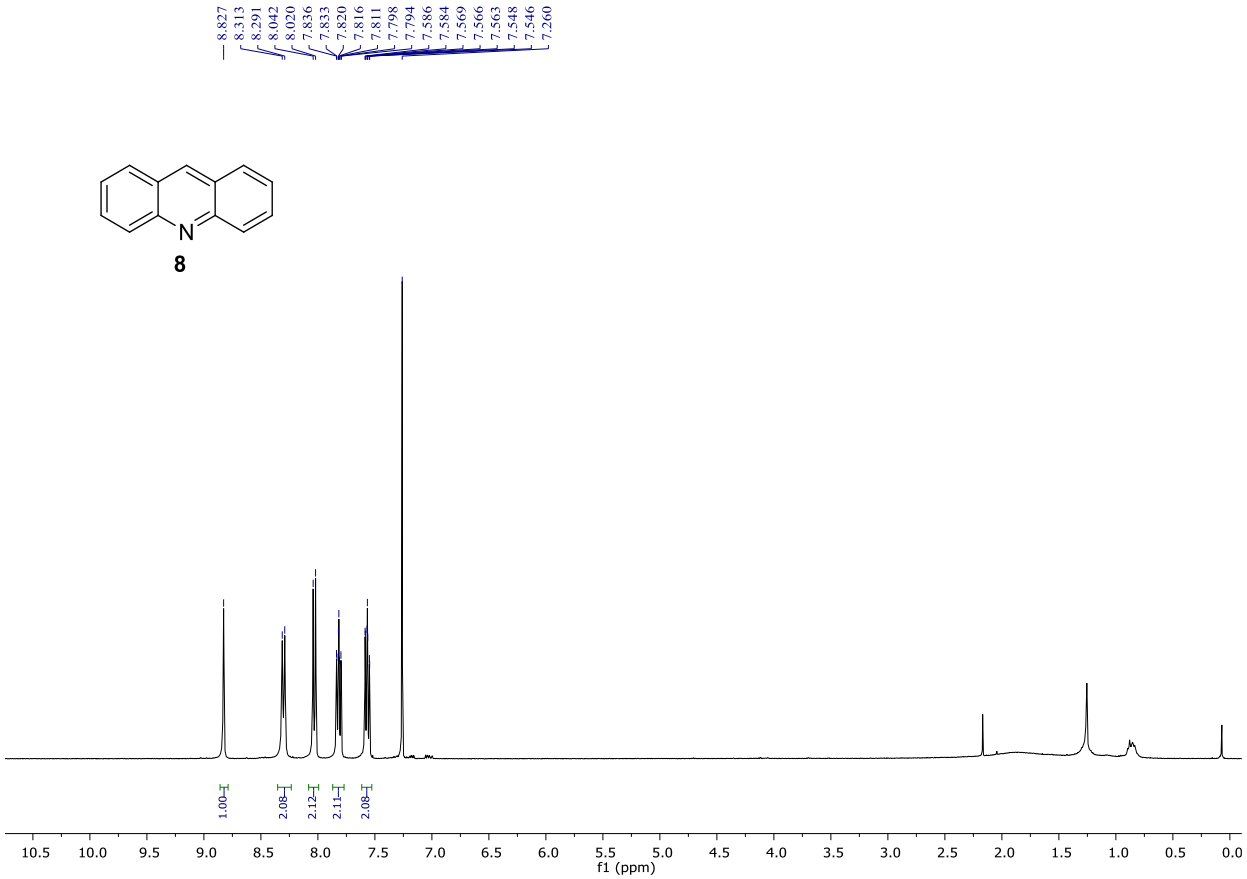
^{1}H NMR of **3aa-d$_1$** (400 MHz, $CDCl_3$):



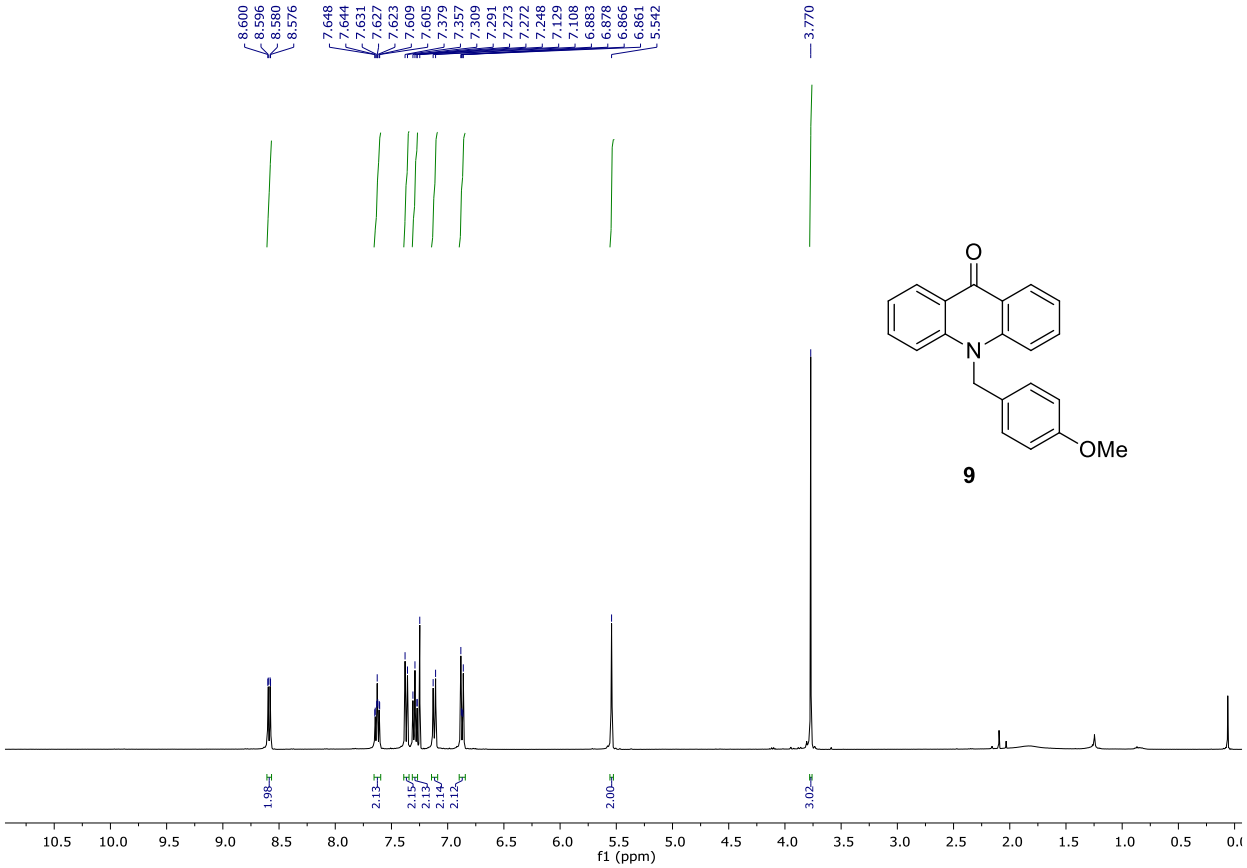
^{13}C {^{1}H} NMR of **3aa-d$_1$** (100 MHz, $CDCl_3$):



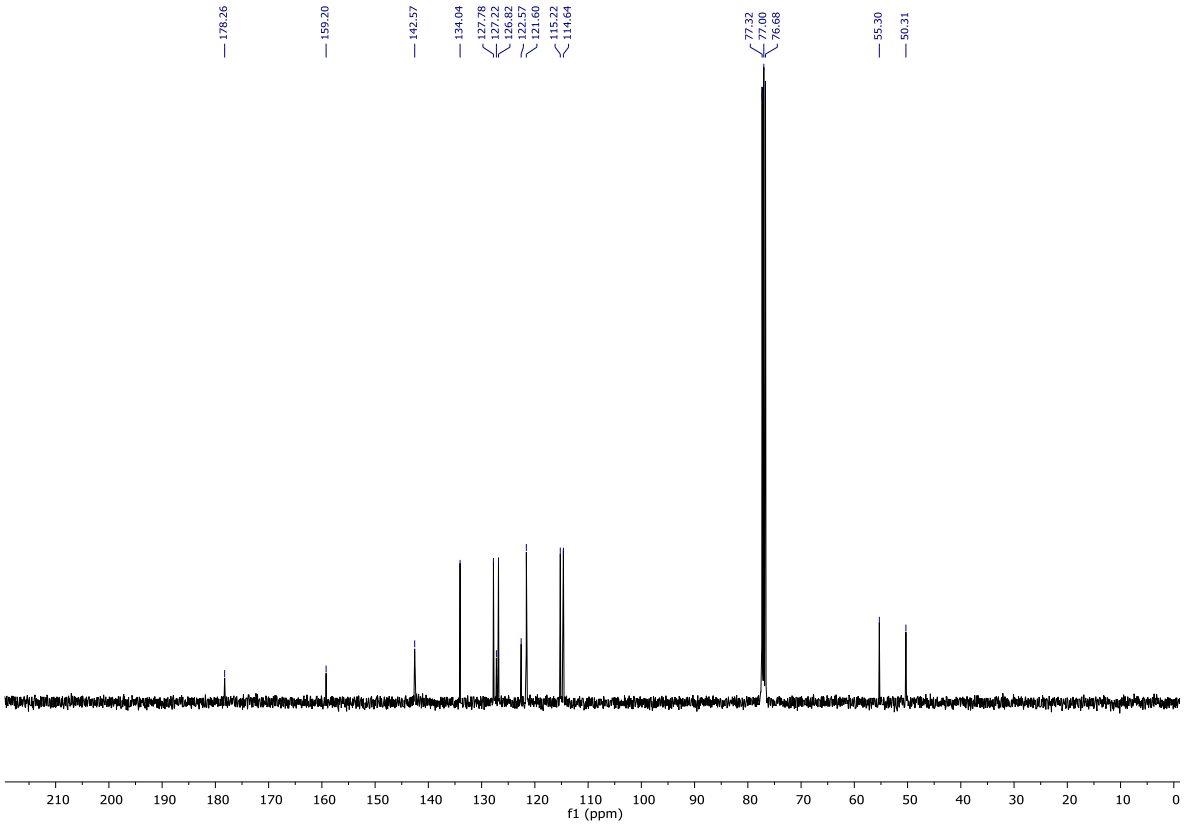
^{1}H NMR of **8** (400 MHz, $CDCl_3$):



^{1}H NMR of **9** (400 MHz, $CDCl_3$):



^{13}C {^{1}H} NMR of **9** (100 MHz, $CDCl_3$):



^{1}H NMR of **10** (400 MHz, $CDCl_3$):