

Supplementary Materials for

Efficient iron catalyzed ligand free access to diversely substituted acridines and acridinium ions

Authors: Susanta Mandal, Karan Chhetri, Samuzal Bhuyan and Biswajit Gopal Roy*

Affiliations:

Department of Chemistry, Sikkim University, 6th Mile, Tadong, Gangtok, Sikkim-737102, India.

*Correspondence to: bgroy@cus.ac.in

Table of Content

General Experimental details	S2
General Experimental Procedures	S2-S3
Optimization Table	S3-S4
Figure S1	S5
Characterization Data of New Compounds (¹ H NMR, ¹³ C NMR, LC-MS)	S6-S120
Crystallographic Information	S21-S22
¹ H NMR and ¹³ C NMR of new compounds	S23-S64

General experimental details:

All commercially available compounds were purchased from Sigma-aldrich and Alfa Aesar. Methanol was dried by using magnesium turning and other alcohols were used as received from the company. NMR spectra were recorded on BRUKER AVANCE III 400 (400 MHz for ^1H ; 100 MHz for ^{13}C) spectrometer. The chemical shifts are given in parts per million (ppm) relative to CDCl_3 (7.28 ppm for ^1H and 77.00 for ^{13}C) and $\text{DMSO}-d_6$ (2.49 for ^1H and 40.09 for ^{13}C). High resolution mass spectra were recorded on Agilent Technologies, Accurate Mass Q-TOF LC/MS G65208. Single crystal data were recorded on Single Crystal Diffractometer, Agilent Technologies-8D-91-45-400. High performance liquid chromatography was performed on Agilent HPLC system 1200 Infinity Series, reverse phase analytical column eluted with a mixture of water and methanol. Normal column chromatography was performed on silica gel (60-120 mesh) purchased from SRL and eluted with petroleum ether and ethyl acetate mixture.

General Experimental procedures:

Typical one pot procedure for synthesis of 1,8-dimethoxyacridines:

An oven dried 10 mL microwave tube was charged with 1,3-cyclohexanedione (0.4 mmol, 2 equiv), aldehyde (0.2 mmol, 1equiv), NH_4OAc (0.3 mmol, 1.5 equiv) and MeOH (5 mL). The mouth of the tube was closed with a MW tube cap and kept under microwave radiation at 100 °C for 30 min with vigorous stirring. After that the tube was cooled, FeCl_3 (5 equiv) was added to the mixture and kept under microwave radiation for 40 min with stirring. After the reaction mixture reached to room temperature, the solvent was evaporated and the dried mixture was extracted with DCM (3 x 20 mL). The combined DCM extracts were washed with deionized water and brine solution. The organic layer was passed over anhydrous sodium sulfate and the solvent was evaporated under reduced pressure to obtain the crude product which was further purified using column chromatography with 10-20% ethyl acetate in petroleum ether.

Typical stepwise method for synthesis of 1,8-dimethoxyacridines:

Construction of hexahydro-1,8-acridinediones: In a round bottom flask, 1,3-cyclohexanedione (4 mmol, 2 equiv), aldehyde (2 mmol, 1 equiv) and NH_4OAc (231 mg, 3 mmol, 1.5 equiv) were dissolved in water (50 mL). The mixture was stirred for 6 h in reflux condition to obtain the hexahydroacridine-1,8-diones as precipitate. The precipitate was then filtered through Whatman filter paper and dried over P_2O_5 in a desiccator for next step.

Aromatization to 1,8-dimethoxyacridines: To a methanolic solution (30 mL) of hexahydroacridine-1,8-dione (0.5 mmol, 1equiv), FeCl_3 (81 mg, 0.5 mmol, 1 equiv) was added and refluxed under a constant pressure of O_2 (approx. 1 atm) for 24 h. The solvent was then evaporated under reduced pressure and the residue was extracted with DCM (3 x 20 mL). The combined DCM extract was washed with brine and passed through anhydrous sodium sulphate and finally concentrated under reduced pressure to obtain the solid crude product, which was purified using column chromatography with 7-14% ethyl acetate in petroleum ether as eluent.

General procedure for synthesis of 1,8-dimethoxy-(10-phenyl/methyl)acridinium chlorides:

One pot procedure for synthesis of 1,8-dimethoxy-(10-aryl)acridinium chlorides:

An oven dried 10 mL microwave tube was charged with 1,3-cyclohexanedione (2 mmol), aldehyde (1 mmol), Aniline (1 mmol) NH_4Cl (20 mol%) and MeOH (4 mL). The mouth of the tube was closed with a MW tube cap and kept under microwave radiation at 100 °C for 30 min with vigorous stirring. After that the tube was cooled, FeCl_3 (9 equiv.) was added to the mixture and kept under microwave radiation for 30-120 min with stirring. The reaction was cooled to room temperature and methanol was evaporated completely under reduced pressure to obtain a crude residue. The residue was extracted with CHCl_3 (3 x 20 mL) and the combined extract was washed with brine solution (2 x 15 mL), passed over anhydrous Na_2SO_4 and concentrated *in vacuo* to obtain a bright red solid. The crude was then purified by column chromatography using silica gel (60-120 mesh) and methanol:chloroform (~10:90) as eluent to yield acridinium chlorides as red solid.

One pot procedure for synthesis of 1,8-dimethoxy-10-(methyl)acridin-10-ium chloride:

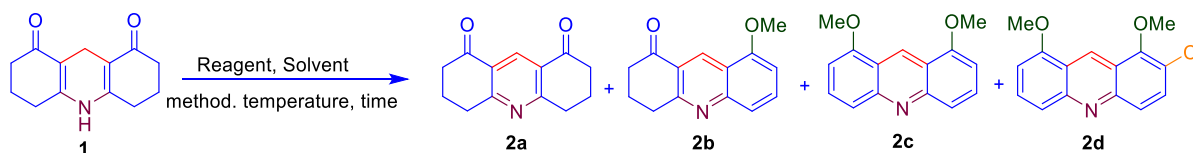
An oven dried 10 mL microwave tube was charged with 1,3-cyclohexanedione (2 mmol), aldehyde (1 mmol), Methyl amine hydrochloride ($\text{MeNH}_2\cdot\text{HCl}$) (1.5 mmol), Sodium acetate (NaOAc) (1.5 mmol) and MeOH (4 mL). The mouth of the tube was closed with a MW tube cap and kept under microwave radiation at 100 °C for 30 min with vigorous stirring. After that the tube was cooled, FeCl_3 (9 equiv.) was added to the mixture and kept under microwave radiation for 30-120 min with stirring. The reaction was cooled to room temperature and methanol was evaporated completely under reduced pressure to obtain a crude residue. The residue was extracted with CHCl_3 (3 x 20 mL) and the combined extract was washed with brine solution (2 x 15 mL), passed over anhydrous Na_2SO_4 and concentrated *in vacuo* to obtain a bright red solid. The crude was then purified by column chromatography using silica gel (60-120 mesh) and methanol:chloroform (~10:90) as eluent to yield acridinium chlorides as red solid.

Stepwise Procedure:

Construction of 10-phenyl/methyl-1,8-acridinediones: Aldehyde (1 equiv, 0.5 mmol), cyclohexane-1,3-dione (2 equiv, 1 mmol), aniline (1 equiv, 0.5 mmol) and ammonium chloride (20 mol%) was dissolved in methanolic water (1:9). The solution was then refluxed for 6-10 h in an oil bath. In most cases 10-aryl-1,8-hexahydroacridinediones appeared as a precipitate, which was then filtered to obtain the pure product. In few cases, where no well-formed precipitate was obtained, the methanol was evaporated under reduced pressure, and the aqueous solution was extracted with ethyl acetate (3 x 10 mL). The combined extract was passed through anhydrous sodium sulfate and finally concentrated under reduced pressure to obtain the solid crude product, which was purified using column chromatography with 50-80% ethyl acetate in petroleum ether as eluent.

Aromatization to 1,8-dimethoxy-10-(phenyl/methyl)acridin-10-ium chloride: To a methanolic solution of *N*-alkyl/aryl-1,8-hexahydroacridine (0.52 mmol) in a 10 mL of microwave tube 8-10 equivalent of ferric chloride (FeCl_3) was added and the closed microwave vessel was irradiated at 100 °C for 30-120 min with constant stirring. The reaction was cooled to room temperature and methanol was evaporated completely under reduced pressure to obtain a crude residue. The residue was extracted with CHCl_3 (3 x 20 mL) and the combined extract was washed with brine solution (2 x 15 mL), passed over anhydrous Na_2SO_4 and concentrated *in vacuo* to obtain a bright red solid. The crude was then purified by column chromatography using silica gel (60-120 mesh) and methanol:chloroform (~10:90) as eluent to yield acridinium chlorides as red solid.

Table S1. Catalyst Screening and Reaction Optimization Data for Dehydrogenation of hexahydroacridine-1,8-dione.



Sl. No.	Reagent and condition				Time	Yield (%)			
	Reagents (equiv.)	Solvent	Method	Temp.(°C)		2a	2b	2c	2d
1	CuBr ₂ (5 equiv.)	MeOH	MW	100	40 min	40	16	8	0
2	Cu(OAc) ₂ .H ₂ O (5 equiv.)	MeOH	MW	100	40 min	16	0	0	0
3	Fe(ClO ₄) ₃ .H ₂ O (5 equiv.)	MeOH	MW	100	40 min	30	25	10	0
4	Pd(OAc) ₂ (5 equiv.)	MeOH	MW	100	40 min	20	50	9	0
5	FeCl ₃ (5 equiv.)	THF	MW	100	40 min	83	0	0	0
6	FeCl ₃ (5 equiv.)	CH ₃ CN	MW	100	40 min	88	0	0	0
7	FeCl ₃ (5 equiv.)	CH ₂ Cl ₂	MW	100	40 min	75	0	0	0
8	FeCl ₃ (5 equiv.)	CHCl ₃	MW	100	40 min	78	0	0	0
9	FeCl ₃ (5 equiv.)	MeOH	MW	100	30 min	10	24	38	0
10	FeCl ₃ (5 equiv.)	MeOH	MW	100	50 min	0	13	67	0
11	FeCl ₃ (7 equiv.)	MeOH	MW	100	40 min	0	4	62	7
12	FeCl ₃ (6 equiv.)	MeOH	MW	100	40 min	0	7	66	5
13	FeCl ₃ (5 equiv.)	MeOH	MW	100	40 min	0	12	73	0
14	FeCl ₃ (4 equiv.)	MeOH	MW	100	40 min	3	29	48	0
15	FeCl ₃ (3 equiv.)	MeOH	MW	100	40 min	9	43	26	0
16	FeCl ₃ (2 equiv.)	MeOH	MW	100	40 min	21	42	8	0
17	FeCl ₃ (1 equiv.)	MeOH	MW	100	40 min	38	13	0	0
18	FeCl ₃ (0.5 equiv.)	MeOH	MW	100	40 min	31	5	0	0
19	TEMPO (5 equiv)	MeOH	MW	100	2 h	90	0	0	0
20	FeCl ₃ (1 equiv.), O ₂ (1 atm)	MeOH	Conventional	Reflux	36 h	0	36	32	0
21	FeCl ₃ (1 equiv.), O ₂ (1 atm)	MeOH	Conventional	Reflux	50 h	0	35	29	0
22	FeCl ₃ (0.5 equiv.), air (1 atm)	MeOH	Conventional	Reflux	24 h	10	46	11	0
23	FeCl ₃ (0.5 equiv.), O ₂ (1 atm)	MeOH	Conventional	Reflux	24 h	2	40	25	0
24	FeCl ₃ (0.5 equiv), Ar (1 atm)	MeOH	Conventional	Reflux	24 h	42	0	0	0
25	FeCl ₃ (0.4 equiv), O ₂ (1 atm)	MeOH	Conventional	Reflux	24 h	10	46	18	0
26	FeCl ₃ (0.2 equiv), O ₂ (1 atm)	MeOH	Conventional	Reflux	24 h	21	40	5	0
27	FeCl ₃ (1 equiv), O ₂ (1 atm), TEMPO (3 equiv)	MeOH	Conventional	Reflux	24 h	0	18	63	0
28	FeCl ₃ (0.5 equiv), O ₂ (1 atm), TEMPO (3 equiv)	MeOH	Conventional	Reflux	24 h	0	25	44	0
29	FeCl ₃ (0.3 equiv), O ₂ (1 atm), TEMPO (3 equiv)	MeOH	Conventional	Reflux	24 h	0	33	35	0
30	FeCl ₃ (0.2 equiv), O ₂ (1 atm), TEMPO (3 equiv)	MeOH	Conventional	Reflux	24 h	5	38	24	0
31	TEMPO (5 equiv)	MeOH	Conventional	Reflux	24 h	86	0	0	0
32	FeCl ₃ (0.5 equiv), O ₂ (1 atm), 0.3 mL AcOH	MeOH	Conventional	Reflux	24 h	0	30	23	0
33	FeCl ₃ (0.5 equiv), O ₂ (1 atm), 0.3 mL TFA	MeOH	Conventional	Reflux	24 h	0	20	29	0

34	FeCl ₃ (0.5 equiv), O ₂ (1 atm), 0.3 mL AcOH, K ₂ S ₂ O ₈ (3 equiv)	MeOH	Conventional	Reflux	24 h	0	30	25	0
35	FeCl ₃ (0.5 equiv), O ₂ (1 atm), 0.3 mL AcOH, KI (3 equiv)	MeOH	Conventional	Reflux	24 h	0	29	21	0

Reaction Condition: Substrate (0.5 mmol), 1 atm. O₂, Solvent (5 mL for MW heating condition and 30 mL for normal reflux condition). Yield was determined either by chromatic separation using HPLC or through isolation of pure product using normal phase column chromatography. THF = tetrahydrofuran, MW = microwave, TEMPO = (2,2,6,6-tetramethyl piperidin-1-yl) oxyl, TFA = trifluoro acetic acid.

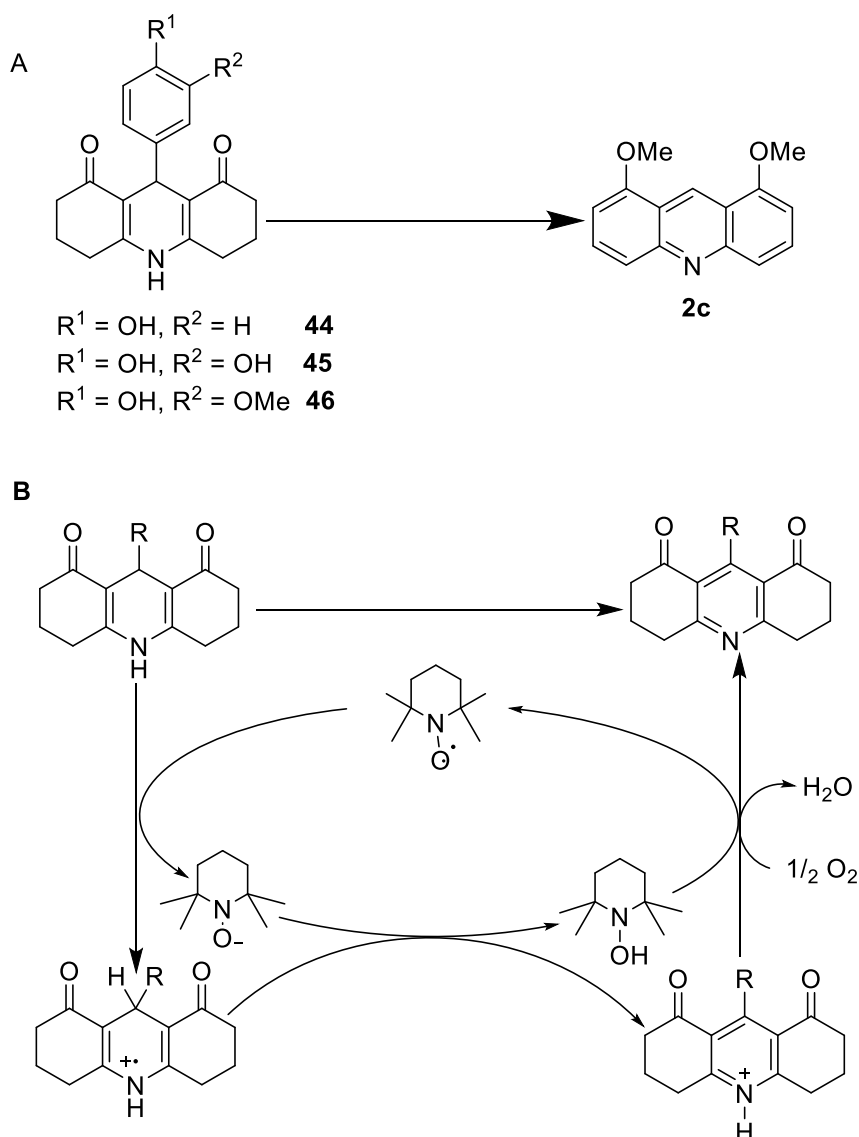
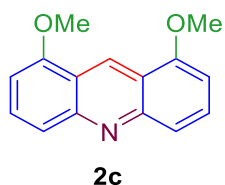
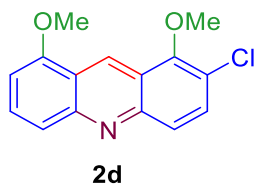


Fig. S1. A. Fate of 9-phenol substituted hexahydroacridine-1,8-diones in presence of FeCl₃ catalyzed oxidative aromatization. B. Mechanism of acceleration of aromatization of middle ring of hexahydroacridinedione by TEMPO.

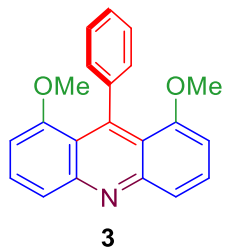
Characterization Data of New Compounds:



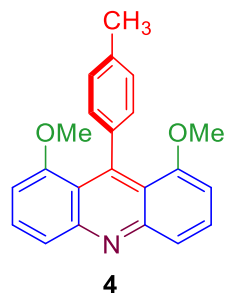
1,8-dimethoxyacridine (2c): ^1H NMR (CDCl_3 , 400 MHz): δ 9.62 (s, 1H), 7.81 (d, J = 8.9 Hz, 2H), 7.70 (t like, J = 7.6, 8.6 Hz, 2H), 6.79 (d, J = 7.5 Hz, 2H), 4.10 (s, 6H); ^{13}C NMR (CDCl_3 , 100 MHz): δ 155.8, 149.7, 130.7, 126.9, 121.2, 119.6, 101.6, 55.8; HRMS: m/z (ESI) calculated for ($\text{C}_{15}\text{H}_{14}\text{NO}_2$) $[\text{M}+\text{H}]^+$: 240.1019, measured: 240.1024.



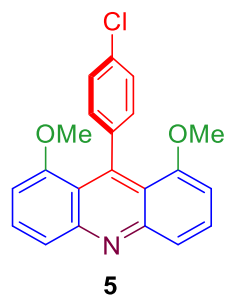
2-chloro-1,8-dimethoxyacridine (2d): ^1H NMR (CDCl_3 , 400 MHz): 9.63 (s, 1H), 7.95 (d, J = 8.8 Hz, 1H), 7.82 (d, J = 8.5 Hz, 1H), 7.74 (t, J = 8.3 Hz, 1H), 6.83 (d, J = 7.6 Hz, 1H), 6.70 (d, J = 8.2 Hz, 1H), 4.10 (s, 3H), 4.09 (s, 3H); ^{13}C NMR (CDCl_3 , 100 MHz): 155.6, 155.0, 149.8, 145.2, 131.1, 129.7, 127.7, 124.2, 122.0, 120.4, 119.8, 102.3, 101.4, 55.9, 55.8; HRMS: m/z (ESI) calculated for ($\text{C}_{15}\text{H}_{13}\text{ClNO}_2$) $[\text{M}+\text{H}]^+$: 274.0629, measured: 274.0635.



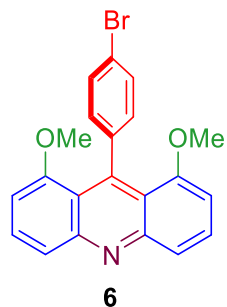
1,8-dimethoxy-9-phenylacridine (3): ^1H NMR (400 MHz, CDCl_3) δ 7.85 (d, J = 8.7 Hz, 2H), 7.66 (t, J = 8.4 Hz, 2H), 7.38-7.33 (m, 3H), 7.25 (d, J = 7.9 Hz, 2H), 6.66 (d, J = 7.4 Hz, 2H), 3.40 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 157.5, 149.6, 144.3, 130.4, 127.4, 125.4, 125.4, 121.8, 118.9, 104.2, 55.7; HRMS: m/z (ESI) calculated for ($\text{C}_{21}\text{H}_{17}\text{NO}_2\text{Na}$) $[\text{M}+\text{Na}]^+$: 338.1151, measured: 338.1153.



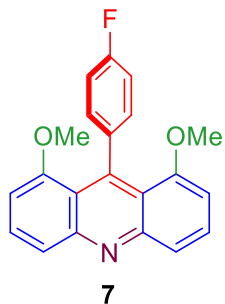
1,8-dimethoxy-9-p-tolylacridine (4): ^1H NMR (400 MHz, CDCl_3) δ 7.85 (d, J = 8.8 Hz, 2H), 7.65 (t, J = 8.4 Hz, 2H), 7.18 (d, J = 8.0 Hz, 2H), 7.13 (d, J = 8.0 Hz, 2H), 6.66 (d, J = 7.4 Hz, 2H), 3.42 (s, 6H), 2.48 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 157.7, 149.7, 141.2, 134.5, 130.2, 127.3, 127.3, 122.0, 119.2, 104.3, 55.7, 21.3; HRMS: m/z (ESI) calculated for $(\text{C}_{22}\text{H}_{20}\text{NO}_2)$ $[\text{M}+\text{H}]^+$: 330.1489, measured: 330.1493.



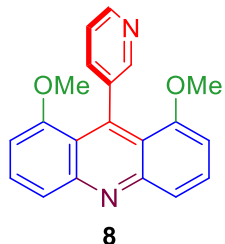
9-(4-chlorophenyl)-1,8-dimethoxyacridine (5): ^1H NMR (400 MHz, CDCl_3): δ 7.83 (d, J = 8.6 Hz, 2H), 7.64 (t, J = 8.5 Hz, 2H), 7.34 (d, J = 8.3 Hz, 2H), 7.17 (d, J = 8.3 Hz, 2H), 6.65 (d, J = 7.6 Hz, 2H), 3.43 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 157.2, 149.5, 142.8, 131.1, 130.5, 128.8, 125.9, 121.8, 118.7, 104.1, 55.5; HRMS: m/z (ESI) calculated for $(\text{C}_{21}\text{H}_{16}\text{ClNO}_2\text{Na})$ $[\text{M}+\text{Na}]^+$: 372.0762, measured: 372.0758.



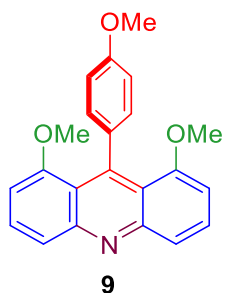
9-(4-bromophenyl)-1,8-dimethoxyacridine (6): ^1H NMR (400 MHz, CDCl_3): δ 7.89 (d, J = 8.7 Hz, 2H), 7.68 (t, J = 8.1 Hz, 2H), 7.50 (d, J = 8.3 Hz, 3H), 7.11 (d, J = 8.3 Hz, 2H), 6.67 (d, J = 7.6 Hz, 2H), 3.44 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 157.1, 149.5, 143.4, 130.5, 129.2, 128.8, 121.8, 119.1, 118.6, 104.1, 55.6; HRMS: m/z (ESI) calculated for $(\text{C}_{21}\text{H}_{17}\text{BrNO}_2)$ $[\text{M}+\text{H}]^+$: 394.0443, 396.0422 measured: 394.0440, 396.0423



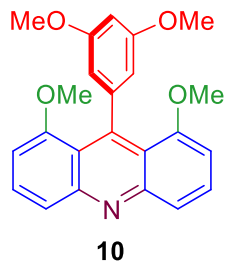
9-(4-fluorophenyl)-1,8-dimethoxyacridine (7): ^1H NMR (400 MHz, CDCl_3): δ 7.85 (d, J = 8.5 Hz, 2H), 7.66 (t, J = 8.4 Hz, 2H), 7.21-7.17 (m, 3H), 7.06 (t, J = 8.8 Hz, 2H), 6.66 (d, J = 7.5 Hz, 2H), 3.45 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 162.5, 160.1, 157.3, 149.6, 140.1, 130.4, 128.8, 121.9, 118.9, 112.7, 112.5, 104.1, 55.6; HRMS: m/z (ESI) calculated for $(\text{C}_{21}\text{H}_{17}\text{FNO}_2)$ $[\text{M}+\text{H}]^+$: 334.1238, measured: 334.1243.



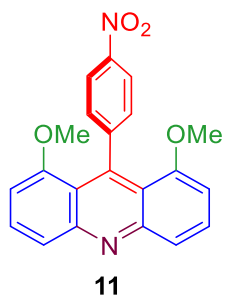
1,8-dimethoxy-9-(pyridine-3-yl)acridine (8): ^1H NMR (400 MHz, CDCl_3): δ 8.63 (d, J = 4.8 Hz, 1H), 7.86 (d, J = 8.7 Hz, 2H), 7.72 (t, J = 7.7 Hz, 1H), 7.65 (t, J = 7.8 Hz, 2H), 7.38 (d, J = 7.8 Hz, 1H), 7.29 (t, J = 8.4 Hz, 1H), 6.67 (d, J = 7.5 Hz, 2H), 3.42 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 162.5, 156.7, 149.8, 146.7, 143.6, 133.5, 130.4, 123.6, 122.0, 120.6, 118.2, 104.0, 56.0; HRMS: m/z for $(\text{C}_{20}\text{H}_{17}\text{N}_2\text{O}_2)$ (ESI) calculated $[\text{M}+\text{H}]^+$: 317.1285, measured: 317.1290.



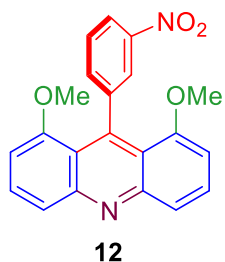
1,8-dimethoxy-9-(4-methoxyphenyl)acridine (9): ^1H NMR (400 MHz, CDCl_3): δ 7.88 (d, J = 6.7 Hz, 2H), 7.66 (t, J = 8.0 Hz, 2H), 7.16 (d, J = 8.6 Hz, 2H), 6.95 (d, J = 8.5 Hz, 2H), 6.68 (d, J = 7.4 Hz, 2H), 3.94 (s, 3H), 3.46 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 158.0, 151.9, 139.3, 133.9, 132.2, 128.6, 128.0, 119.1, 114.1, 111.7, 105.0, 56.0, 55.4; HRMS: m/z (ESI) calculated for $(\text{C}_{22}\text{H}_{19}\text{NNaO}_3)$ $[\text{M}+\text{Na}]^+$: 368.1257, measured: 368.1260.



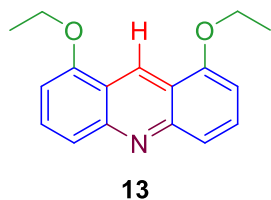
9-(3,5-dimethoxyphenyl)-1,8-dimethoxyacridine (10): ^1H NMR (400 MHz, CDCl_3): δ 7.84 (d, J = 8.6 Hz, 2H), 7.65 (t, J = 8.5 Hz, 2H), 6.68 (d, J = 7.5 Hz, 2H), 6.52 (t, J = 2.2 Hz, 1H), 6.46 (d, J = 2.2 Hz, 2H), 3.82 (s, 6H), 3.50 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 159.0, 157.5, 149.5, 146.2, 130.5, 121.6, 118.7, 106.8, 106.5, 104.2, 98.3, 55.9, 55.5; HRMS: m/z (ESI) calculated for ($\text{C}_{23}\text{H}_{22}\text{NO}_4$) $[\text{M}+\text{H}]^+$: 376.1543, measured: 376.1545.



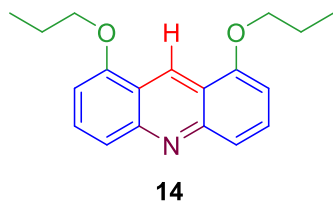
1,8-dimethoxy-9-(4-nitrophenyl)acridine (11): ^1H NMR (400 MHz, CDCl_3): δ 8.28 (d, J = 8.5 Hz, 2H), 7.86 (d, J = 8.7 Hz, 2H), 7.69 (t, J = 8.2 Hz, 2H), 7.45 (d, J = 8.5 Hz, 2H), 6.68 (d, J = 7.6 Hz, 2H), 3.40 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 156.5, 152.3, 149.6, 145.9, 143.3, 130.6, 128.5, 122.2, 121.1, 118.0, 104.1, 55.4; HRMS: m/z (ESI) calculated for ($\text{C}_{21}\text{H}_{17}\text{N}_2\text{O}_4$) $[\text{M}+\text{H}]^+$: 361.1183, measured: 361.1185.



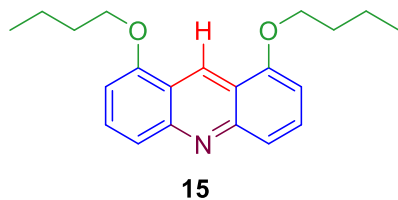
1,8-dimethoxy-9-(3-nitrophenyl)acridine (12): ^1H NMR (400 MHz, CDCl_3): δ 8.27 (d, J = 10.2 Hz, 1H), 8.17 (t, J = 1.8 Hz, 1H), 7.88 (d, J = 9.5 Hz, 2H), 7.68 (dd, J = 8.6, 7.7 Hz, 2H), 7.63 (d, J = 6.3 Hz, 1H), 7.54 (t, J = 7.9 Hz, 1H), 6.68 (d, J = 7.5 Hz, 2H), 3.40 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 156.7, 149.9, 146.4, 133.8, 130.5, 126.5, 122.6, 120.6, 118.4, 104.3, 55.7; HRMS: m/z (ESI) calculated for ($\text{C}_{21}\text{H}_{17}\text{N}_2\text{O}_4$) $[\text{M}+\text{H}]^+$: 361.1183, measured: 361.1180.



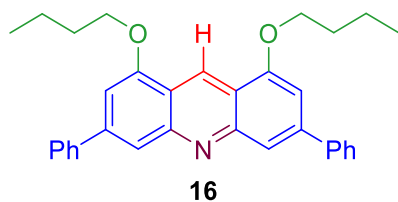
1,8-diethoxyacridine (13): ^1H NMR (400 MHz, CDCl_3): δ 9.65 (s, 1H), 7.82 (d, J = 8.8 Hz, 2H), 7.69 (t, J = 8.6 Hz, 2H), 6.77 (d, J = 7.5 Hz, 2H), 4.31 (q, J = 7.0 Hz, 4H), 1.65 (t, J = 7.0 Hz, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 155.1, 149.4, 130.9, 127.3, 120.7, 119.7, 102.4, 64.1, 14.7; HRMS: m/z (ESI) calculated for ($\text{C}_{17}\text{H}_{17}\text{NNaO}_2$) $[\text{M}+\text{Na}]^+$: 290.1151, measured: 290.1155.



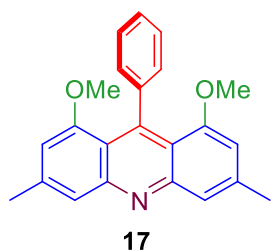
1,8-dipropoxyacridine (14): ^1H NMR (400 MHz, CDCl_3): δ 9.66 (s, 1H), 7.80 (d, J = 8.8 Hz, 2H), 7.67 (t, J = 8.7 Hz, 2H), 6.76 (d, J = 7.5 Hz, 2H), 4.19 (t, J = 6.4 Hz, 4H), 2.00-2.09 (m, 4H), 1.21 (t, J = 7.4 Hz, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 155.2, 149.7, 130.7, 127.0, 120.9, 119.8, 102.3, 69.9, 22.6, 10.7; HRMS: m/z (ESI) calculated for ($\text{C}_{19}\text{H}_{22}\text{NO}_2$) $[\text{M}+\text{H}]^+$: 296.1645, measured: 296.1641.



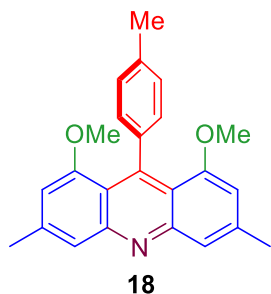
1,8-dibutoxyacridine (15): ^1H NMR (400 MHz, CDCl_3): δ 9.68 (s, 1H), 7.83 (d, J = 8.8 Hz, 2H), 7.69 (t, J = 8.6 Hz, 2H), 6.78 (d, J = 7.5 Hz, 2H), 4.25 (t, J = 6.2 Hz, 4H), 1.97-2.04 (m, 4H), 1.65-1.75 (m, 4H), 1.10 (t, J = 7.4 Hz, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 155.3, 149.3, 131.1, 127.5, 120.5, 119.8, 102.4, 68.3, 31.3, 19.6, 14.0; HRMS: m/z (ESI) calculated for ($\text{C}_{21}\text{H}_{26}\text{NO}_2$) $[\text{M}+\text{H}]^+$: 324.1958, measured: 324.1964.



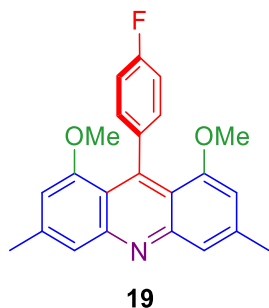
1,8-dibutoxy-3,6-diphenylacridine (16): ^1H NMR (400 MHz, CDCl_3) δ 9.61 (s, 1H), 8.04 (s, 2H), 7.85 (d, $J = 7.4$ Hz, 4H), 7.54 (t, $J = 7.4$ Hz, 4H), 7.44 (t, $J = 7.2$ Hz, 2H), 7.05 (s, 2H), 4.34 (t, $J = 6.2$ Hz, 4H), 2.08-2.02 (m, 4H), 1.78-1.69 (m, 4H), 1.13 (t, $J = 7.4$ Hz, 6H). ^{13}C NMR (100 MHz, CDCl_3) δ 155.8, 150.5, 143.7, 141.3, 129.1, 128.2, 127.7, 127.5, 119.2, 118.8, 102.9, 68.5, 31.5, 19.8, 14.2. HRMS: m/z (ESI) calculated for ($\text{C}_{33}\text{H}_{34}\text{NO}_2$) $[\text{M}+\text{H}]^+$: 476.2584, measured: 476.2586



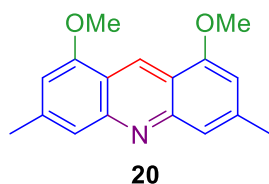
1,8-dimethoxy-3,6-dimethyl-9-phenylacridine (17): ^1H NMR (400 MHz, CDCl_3): δ 7.68 (s, 2H), 7.37-7.31 (m, 3H), 7.22 (d, $J = 9.1$ Hz, 2H), 6.46 (s, 2H), 3.38 (s, 6H), 2.54 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 157.2, 149.4, 144.2, 141.2, 127.3, 125.7, 125.3, 120.0, 116.9, 106.5, 55.1, 22.4; HRMS: m/z (ESI) calculated for ($\text{C}_{23}\text{H}_{22}\text{NO}_2$) $[\text{M}+\text{H}]^+$: 344.1645, measured: 344.1644.



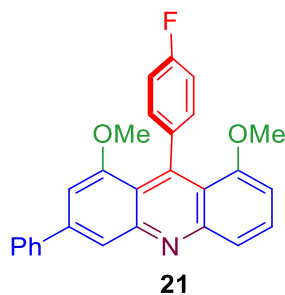
1,8-dimethoxy-3,6-dimethyl-9-p-tolylacridine (18): ^1H NMR (400 MHz, CDCl_3): δ 7.60 (s, 2H), 7.17 (d, $J = 8.0$ Hz, 2H), 7.10 (d, $J = 8.0$ Hz, 2H), 6.45 (s, 2H), 3.39 (s, 6H), 2.52 (s, 6H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 157.5, 150.0, 141.3, 141.0, 127.4, 126.5, 127.4, 120.4, 117.3, 106.8, 55.8, 22.5, 21.5; HRMS: m/z (ESI) calculated for ($\text{C}_{24}\text{H}_{24}\text{NO}_2$) $[\text{M}+\text{H}]^+$: 358.1802, measured: 358.1805.



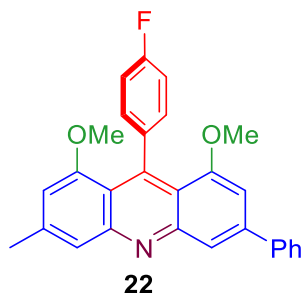
9-(4-fluorophenyl)-1,8-dimethoxy-3,6-dimethylacridine (19): ^1H NMR (400 MHz, CDCl_3): δ 7.61 (s, 2H), 7.18-7.14 (m, 2H), 7.07- 7.03 (m, 2H), 6.46 (s, 2H), 3.42 (s, 6H), 2.54 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 162.7, 160.3, 157.2, 149.9, 141.2, 140.3, 128.9, 120.4, 117.1, 112.8, 112.6, 106.7, 55.7, 22.5; HRMS: m/z (ESI) calculated for $(\text{C}_{23}\text{H}_{20}\text{FNNaO}_2)$ $[\text{M}+\text{Na}]^+$: 384.1370, measured: 384.1372.



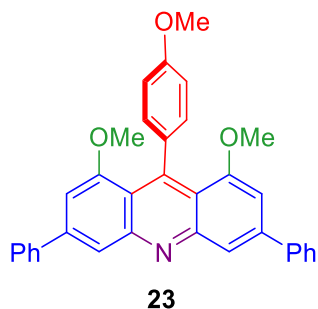
1,8-dimethoxy-3,6-methylacridine (20): ^1H NMR (400 MHz, CDCl_3): δ 9.49 (s, 1H), 7.62 (s, 2H), 6.61 (s, 2H), 4.08 (s, 6H), 2.59 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 155.4, 149.6, 141.5, 126.6, 119.4, 117.6, 104.1, 55.7, 23.0; HRMS: m/z (ESI) calculated for $(\text{C}_{17}\text{H}_{18}\text{NO}_2)$ $[\text{M}+\text{H}]^+$: 268.1332, measured: 268.1329.



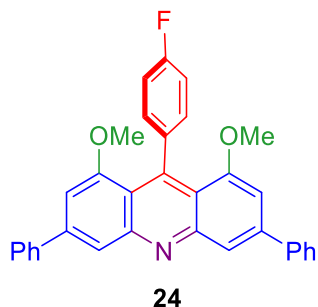
9-(4-fluorophenyl)-1,8-dimethoxy-3-phenylacridine (21): ^1H NMR (400 MHz, CDCl_3): δ 8.09 (s, 1H), 7.83 (t, J = 8.2 Hz, 3H), 7.66 (t, J = 8.2 Hz, 1 H), 7.53 (t, J = 7.5 Hz, 2H), 7.45-7.42 (m, 1H), 7.24-7.21 (m, 2H), 7.09 (t, J = 8.8 Hz, 2H), 6.94 (s, 1H), 6.67 (d, J = 7.4 Hz 1H), 3.53 (s, 3H), 3.46 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3): δ 162.7, 160.3, 157.8, 157.6, 150.4, 150.2, 145.6, 142.8, 140.5, 140.2, 130.6, 129.1, 128.3, 127.5, 122.2, 119.7, 119.1, 118.3, 112.9, 112.7, 104.3, 55.8, 55.8; HRMS: m/z (ESI) calculated for $(\text{C}_{27}\text{H}_{20}\text{FNNaO}_2)$ $[\text{M}+\text{Na}]^+$: 432.1370, measured: 432.1373.



9-(4-fluorophenyl)-1,8-dimethoxy-3-methyl-6-phenylacridine (22): ^1H NMR (400 MHz, CDCl_3): δ 8.06 (s, 1H), 7.82 (d, J = 7.5 Hz, 2H), 7.63 (s, 1H), 7.53 (t, J = 6.6 Hz, 2 H), 7.44 (t, J = 7.2 Hz, 1H), 7.23-7.19 (m, 2H), 7.08 (t, J = 8.8 Hz, 2H), 6.90 (s, 1H), 6.49 (s, 1H), 3.52 (s, 3H), 3.45 (s, 3H), 2.56 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3): δ 162.7, 160.3, 157.9, 157.1, 150.6, 150.2, 141.3, 140.5, 140.1, 139.5, 129.1, 128.3, 127.5, 120.7, 119.5, 117.9, 117.5, 114.3, 112.9, 112.7, 106.9, 104.0, 77.5, 77.2, 76.9, 55.8, 55.7, 22.9; HRMS: m/z (ESI) calculated for ($\text{C}_{28}\text{H}_{23}\text{FNO}_2$) $[\text{M}+\text{H}]^+$: 424.1707, measured: 424.1705.

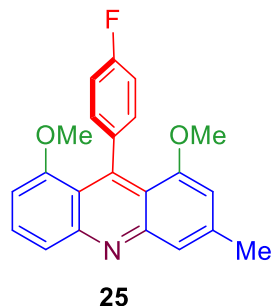


1,8-dimethoxy-9-(4-methoxyphenyl)-3,6-diphenylacridine (23): ^1H NMR (400 MHz, CDCl_3): δ 8.09 (s, 1H), 7.84 (d, J = 8.3 Hz, 4H), 7.53 (t, J = 7.6 Hz, 4H), 7.44 (t, J = 7.3 Hz, 2H), 7.22 (d, J = 8.3 Hz, 2H), 6.98-6.94 (d, 4H), 6.95 (s, 2H), 3.96 (s, 3H), 3.55 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 158.2, 158.0, 150.7, 142.8, 140.6, 136.7, 129.1, 128.7, 128.3, 127.5, 119.6, 118.7, 111.6, 104.4, 56.1, 55.6; HRMS: m/z (ESI) calculated for ($\text{C}_{34}\text{H}_{28}\text{NO}_3$) $[\text{M}+\text{H}]^+$: 498.2064, measured: 498.2069.

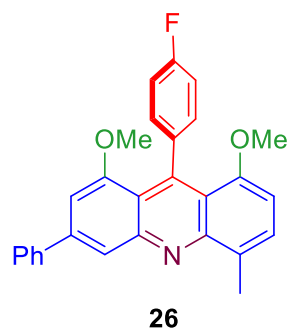


9-(4-fluorophenyl)-1,8-dimethoxy-3,6-diphenylacridine (24): ^1H NMR (400 MHz, CDCl_3): δ 8.12 (s, 1H), 7.84 (d, J = 7.6 Hz, 4H), 7.53 (t, J = 7.6 Hz, 4H), 7.44 (t, J = 7.3 Hz, 2H), 7.28-7.24 (m, 2H), 7.11 (t, J = 8.8 Hz, 2H), 6.94 (s, 2H), 3.54 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3): δ 162.8, 160.4, 157.9, 150.4, 143.2,

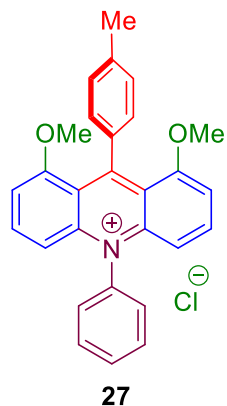
140.4, 140.0, 129.2, 128.4, 127.5, 119.4, 118.3, 113.0, 112.8, 104.4, 55.9; HRMS: m/z (ESI) calculated for (C₃₃H₂₅FNO₂) [M+H]⁺: 486.1864, measured: 486.1869.



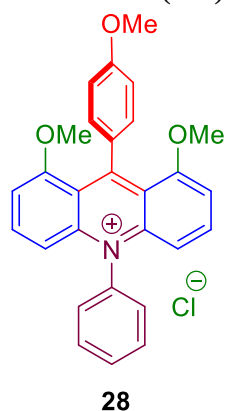
9-(4-fluorophenyl)-1,8-dimethoxy-3-methylacridine (25): ¹H NMR (400 MHz, CDCl₃): δ 7.81 (d, J = 8.6 Hz, 1H), 7.65-7.61 (m, 2H), 7.20-7.17 (m, 2H), 7.06 (t, J = 8.8 Hz, 2H), 6.64 (d, J = 7.5 Hz, 1H), 6.49 (s, 1H), 3.44 (s, 6H), 2.55 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 162.7, 160.3, 157.5, 157.1, 150.1, 145.5, 141.0, 140.3, 130.3, 129.0, 122.1, 120.8, 118.7, 117.6, 112.6, 112.6, 106.9, 104.0, 55.7, 22.5; HRMS: m/z (ESI) calculated for (C₂₂H₁₉FNO₂) [M+H]⁺: 348.1394, measured: 348.1400.



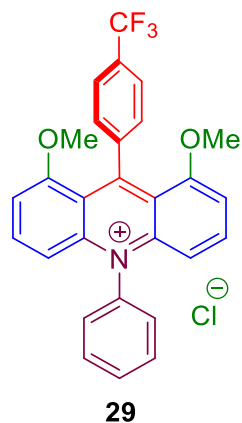
9-(4-fluorophenyl)-1,8-dimethoxy-5-methyl-3-phenylacridine (26): ¹H NMR (400 MHz, CDCl₃): δ 8.13 (s, 1H), 7.85 (d, J = 7.7 Hz, 2H), 7.55-7.50 (m, 3H), 7.44 (t, J = 7.1 Hz, 1H), 7.23-7.21 (m, 2H), 7.08 (t, J = 8.8 Hz, 2H), 6.93 (s, 1H), 6.59 (d, J = 7.7 Hz, 1H), 3.53 (s, 3H), 3.42 (s, 3H), 2.87 (s, 3H); ¹³C NMR (100 MHz, CDCl₃): δ 162.5, 160.1, 157.5, 155.7, 149.3, 144.9, 142.1, 140.5, 139.3, 129.3, 129.0, 128.0, 127.3, 123.5, 120.3, 118.9, 117.8, 115.9, 114.1, 112.7, 112.5, 104.1, 55.7, 22.7; HRMS: m/z (ESI) calculated for (C₂₈H₂₃FNO₂)⁺ [M+H]⁺: 424.1707, measured: 424.1711.



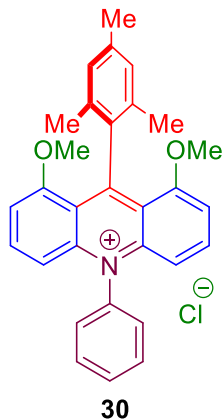
1,8-dimethoxy-10-phenyl-9-(p-tolyl)acridin-10-ium chloride (27): ^1H NMR (400 MHz, CDCl_3) δ 8.07–7.95 (m, 2H), 7.93–7.79 (m, 3H), 7.55–7.45 (m, 2H), 7.31–7.23 (m, 3H), 7.13 (d, J = 7.0 Hz, 2H), 7.04 (d, J = 6.8 Hz, 2H), 6.86 (d, J = 8.4 Hz, 2H), 3.52 (s, 6H), 2.49 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 164.1, 160.3, 142.6, 140.6, 138.2, 138.1, 137.0, 131.8, 131.7, 127.7, 127.5, 125.6, 119.1, 110.6, 107.2, 56.9, 21.4; HRMS: m/z : (ESI) calculated for $(\text{C}_{28}\text{H}_{24}\text{NO}_2)^+$ ($[\text{M}^+]$) 406.1802, found 406.1805.



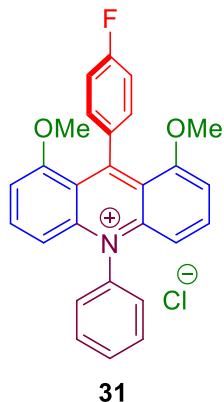
1,8-dimethoxy-9-(4-methoxyphenyl)-10-phenylacridin-10-ium chloride (28): ^1H NMR (400 MHz, CDCl_3) δ 8.02 (t, J = 8.8 Hz, 2H), 7.91–7.83 (m, 3H), 7.52 (d, J = 7.2 Hz, 2H), 7.19 (d, J = 8.8 Hz, 2H), 7.07–7.02 (m, 4H), 6.88 (d, J = 9.2 Hz, 2H), 3.94 (s, 3H), 3.58 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 160.3, 159.1, 142.6, 140.5, 138.2, 133.4, 131.9, 131.7, 127.7, 127.1, 119.3, 112.6, 110.6, 107.2, 57.0, 55.5; HRMS: m/z : (ESI) calculated for $(\text{C}_{28}\text{H}_{24}\text{NO}_3)^+$ ($[\text{M}^+]$) 422.1751, found 422.1757.



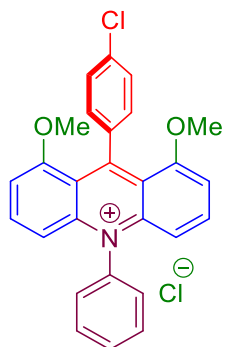
1,8-dimethoxy-10-phenyl-9-(4-(trifluoromethyl)phenyl)acridin-10-ium chloride (29): ^1H NMR (400 MHz, CDCl_3) δ 8.05 (t, J = 7.6 Hz, 2H), 7.93–7.83 (m, 3H), 7.77 (d, J = 6.4 Hz, 2H), 7.60 (d, J = 6.0 Hz, 2H), 7.54–7.48 (m, 2H), 7.07 (d, J = 7.2 Hz, 2H), 6.92 (d, J = 8.4 Hz, 2H), 3.50 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 160.8, 159.6, 145.2, 142.8, 140.8, 138.2, 131.84, 131.77, 127.8, 126.4, 123.9, 123.8, 118.7, 111.1, 107.3, 56.9; HRMS: m/z : (ESI) calculated for $(\text{C}_{28}\text{H}_{21}\text{F}_3\text{NO}_2)^+$ ($[\text{M}^+]$) 460.1519, found 460.1515.



9-mesityl-1,8-dimethoxy-10-phenylacridin-10-ium chloride (30): ^1H NMR (400 MHz, CDCl_3) δ 8.15 (t, J = 8.4 Hz, 2H), 7.90–7.80 (m, 3H), 7.50 (d, J = 7.2 Hz, 2H), 7.23 (d, J = 8.0 Hz, 2H), 6.92 (s, 2H), 6.89 (d, J = 8.8 Hz, 2H), 3.58 (s, 6H), 2.40 (s, 3H), 1.77 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 164.6, 160.3, 142.5, 141.2, 138.2, 138.0, 136.7, 131.8, 131.7, 131.6, 127.8, 127.2, 118.5, 110.9, 107.6, 57.6, 21.2, 20.5; HRMS: m/z : (ESI) calculated for $(\text{C}_{30}\text{H}_{28}\text{NO}_2)^+$ ($[\text{M}^+]$) 434.2115, found 434.2118.

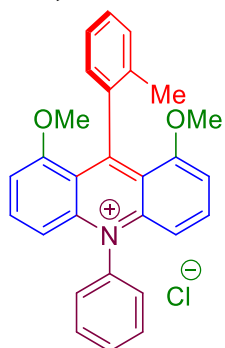


9-(4-fluorophenyl)-1,8-dimethoxy-10-phenylacridin-10-ium chloride (31): ^1H NMR (400 MHz, CDCl_3) δ 8.04 (t, J = 8.0 Hz, 2H), 7.90–7.84 (m, 3H), 7.62 (d, J = 6.4 Hz, 2H), 7.37–7.31 (m, 2H), 7.22 (t, J = 8.0 Hz, 2H), 7.07 (d, J = 8.0 Hz, 2H), 6.93 (d, J = 8.8 Hz, 2H), 3.59 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 160.0, 142.7, 140.5, 131.8, 131.7, 127.8, 127.7, 127.6, 119.2, 114.2, 114.0, 113.3, 111.0, 107.1, 56.9; HRMS: m/z : (ESI) calculated for $(\text{C}_{27}\text{H}_{21}\text{FNO}_2)^+$ ($[\text{M}^+]$) 410.1551, found 410.1558.



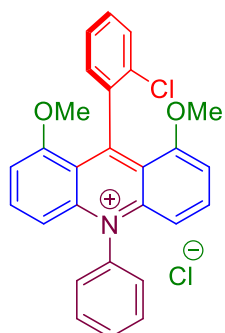
32

9-(4-chlorophenyl)-1,8-dimethoxy-10-phenylacridin-10-ium chloride (32): ^1H NMR (400 MHz, CDCl_3) δ 8.01 (t, J = 8.8 Hz, 2H), 7.87–7.80 (m, 3H), 7.52 (d, J = 7.2 Hz, 2H), 7.45 (d, J = 8.4 Hz, 2H), 7.24 (d, J = 8.4 Hz, 2H), 7.06 (d, J = 8.0 Hz, 2H), 6.87 (d, J = 8.8 Hz, 2H), 3.54 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 161.6, 159.8, 142.6, 140.7, 139.6, 138.1, 133.1, 131.8, 131.7, 127.6, 127.19, 127.17, 118.8, 110.8, 107.3, 56.9; HRMS: m/z : (ESI) calculated for $(\text{C}_{27}\text{H}_{21}\text{ClNO}_2)^+$ ($[\text{M}^+]$) 426.1255, found 426.1258.



33

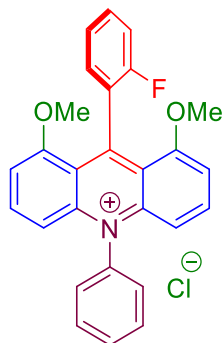
1,8-dimethoxy-10-phenyl-9-(o-tolyl)acridin-10-ium chloride (33): ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 8.09 (t, J = 8.4 Hz, 2H), 7.96–7.86 (m, 3H), 7.83 (d, J = 8.0 Hz, 1H), 7.71 (d, J = 6.8 Hz, 1H), 7.37 (d, J = 4.1 Hz, 2H), 7.26 (dt, J = 8.4, 4.2 Hz, 1H), 7.21 (d, J = 8.0 Hz, 2H), 6.90 (d, J = 7.6 Hz, 1H), 6.85 (d, J = 8.8 Hz, 2H), 3.47 (s, 6H), 2.09 (s, 3H); ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) δ 162.5, 159.8, 143.1, 142.1, 140.3, 139.2, 134.4, 131.9, 131.8, 131.7, 128.4, 128.2, 128.2, 127.6, 125.2, 124.7, 119.2, 111.3, 107.4, 57.5, 20.5; HRMS: m/z : (ESI) calculated for $(\text{C}_{28}\text{H}_{24}\text{NO}_2)^+$ ($[\text{M}^+]$) 406.1802, found 406.1806.



34

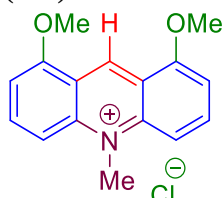
9-(2-chlorophenyl)-1,8-dimethoxy-10-phenylacridin-10-ium chloride (34): ^1H NMR (400 MHz, CDCl_3) δ 8.08 (t, J = 8.4 Hz, 2H), 7.95–7.85 (m, 3H), 7.73 (d, J = 7.2 Hz, 1H), 7.57–7.49 (m, 2H), 7.47–7.41 (m, 2H), 7.23 (d, J = 6.4 Hz, 1H), 7.12 (d, J = 8.0 Hz, 2H), 6.95 (d, J = 8.8 Hz, 2H), 3.61 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 161.6, 159.8, 142.6, 140.7, 139.6, 138.1, 133.1, 131.8, 131.7, 127.6, 127.2, 127.2,

118.8, 110.8, 107.3, 56.9; HRMS: m/z : (ESI) calculated for $(C_{27}H_{21}ClNO_2)^+$ ($[M^+]$) 426.1255, found 426.1260.



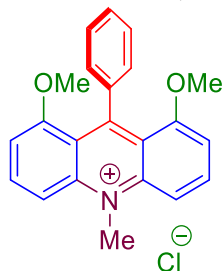
35

9-(2-fluorophenyl)-1,8-dimethoxy-10-phenylacridin-10-ium chloride (35): 1H NMR (400 MHz, $CDCl_3$) δ 8.07 (t, $J = 8.4$ Hz, 2H), 7.93–7.90 (m, 1H), 7.88 (m, 2H), 7.76 (d, $J = 7.2$ Hz, 1H), 7.54–7.44 (m, 2H), 7.31–7.27 (m, 2H), 7.26–7.22 (m, 2H), 7.13 (d, $J = 8.0$ Hz, 2H), 6.94 (d, $J = 8.8$ Hz, 2H), 3.62 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 157.3, 156.9, 142.7, 140.7, 138.2, 132.2, 131.8, 131.5, 129.7, 129.6, 129.3, 129.1, 128.2, 127.6, 127.3, 123.7, 119.4, 113.7, 113.4, 110.9, 107.3, 57.2; HRMS: m/z : (ESI) calculated for $(C_{27}H_{21}FNO_2)^+$ ($[M^+]$) 410.1551, found 410.1556.



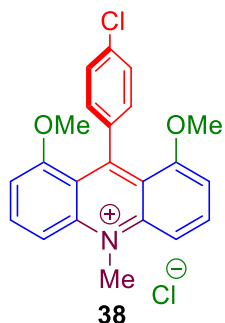
36

1,8-dimethoxy-10-methylacridin-10-ium chloride (36): 1H NMR (400 MHz, $DMSO-d_6$) δ 9.85 (s, 1H), 8.31 (t, $J = 8.0$ Hz, 2H), 8.12 (d, $J = 7.6$ Hz, 2H), 7.34 (d, $J = 6.4$ Hz, 2H), 4.62 (s, 3H), 4.16 (s, 6H); ^{13}C NMR (100 MHz, $DMSO-d_6$) δ 157.4, 142.0, 141.4, 138.0, 118.8, 110.3, 105.9, 58.0; HRMS: m/z : (ESI) calculated for $(C_{16}H_{16}NO_2)^+$ ($[M^+]$) 254.1176, found 254.1180.

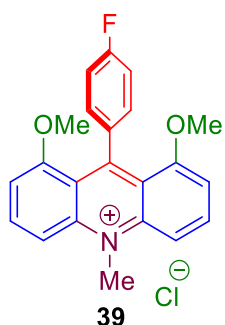


37

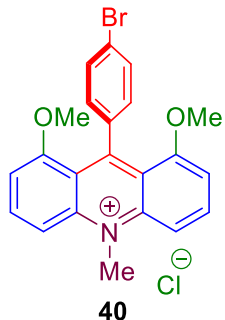
1,8-dimethoxy-10-methyl-9-phenylacridin-10-ium chloride (37): 1H NMR (400 MHz, $CDCl_3$) δ 8.33–8.22 (m, 4H), 7.45–7.43 (m, 3H), 7.17–7.15 (m, 2H), 6.97 (dd, $J = 6.4, 2.8$ Hz, 2H), 5.01 (s, 3H), 3.47 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.0, 160.0, 142.3, 141.4, 140.6, 127.1, 126.8, 125.6, 119.0, 110.3, 106.7, 56.5, 42.0; HRMS: m/z : (ESI) calculated for $(C_{22}H_{20}NO_2)^+$ ($[M^+]$) 330.1489, found 330.1478.



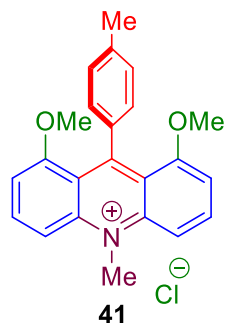
9-(4-chlorophenyl)-1,8-dimethoxy-10-methylacridin-10-ium chloride (38): ^1H NMR (400 MHz, CDCl_3) δ 8.30–8.24 (m, 4H), 7.45 (d, $J = 8.4$ Hz, 2H), 7.13 (d, $J = 8.4$ Hz, 2H), 6.99 (d, $J = 7.2$ Hz, 2H), 5.02 (s, 3H), 3.53 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.8, 142.5, 140.9, 140.2, 133.1, 127.4, 127.2, 119.1, 110.8, 106.9, 56.7, 42.4; HRMS: m/z : (ESI) calculated for $(\text{C}_{22}\text{H}_{19}\text{ClNO}_2)^+$ ($[\text{M}^+]$) 364.1099, found 364.1096.



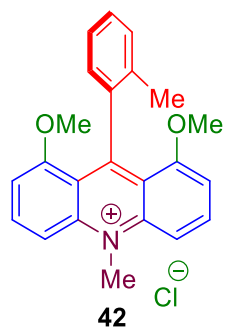
9-(4-fluorophenyl)-1,8-dimethoxy-10-methylacridin-10-ium chloride (39): ^1H NMR (400 MHz, CDCl_3) δ 8.30–8.25 (m, 4H), 7.19–7.13 (m, 4H), 7.01–6.90 (m, 2H), 5.02 (s, 3H), 3.53 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.9, 142.5, 140.9, 137.5, 130.1, 127.8, 127.7, 119.4, 114.3, 114.0, 110.7, 106.9, 56.7, 42.3; HRMS: m/z (ESI) calculated for $(\text{C}_{22}\text{H}_{19}\text{FNO}_2)^+$ ($[\text{M}^+]$) 348.1394, found 348.1390.



9-(4-bromophenyl)-1,8-dimethoxy-10-methylacridin-10-ium chloride (40): ^1H NMR (400 MHz, CDCl_3) δ 8.29–8.23 (m, 4H), 7.57 (d, $J = 8.4$ Hz, 2H), 7.05 (d, $J = 8.4$ Hz, 2H), 6.99 (dd, $J = 6.8$ s, 1.6 Hz, 2H), 5.00 (s, 3H), 3.51 (s, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ 159.6, 159.2, 142.3, 141.0, 140.4, 129.9, 127.6, 120.8, 118.9, 110.5, 107.0, 56.7, 42.4; HRMS: m/z : (ESI) calculated for $(\text{C}_{22}\text{H}_{19}\text{BrNO}_2)^+$ ($[\text{M}^+]$) 408.0594, 410.0574, found 408.0598, 410.0577.

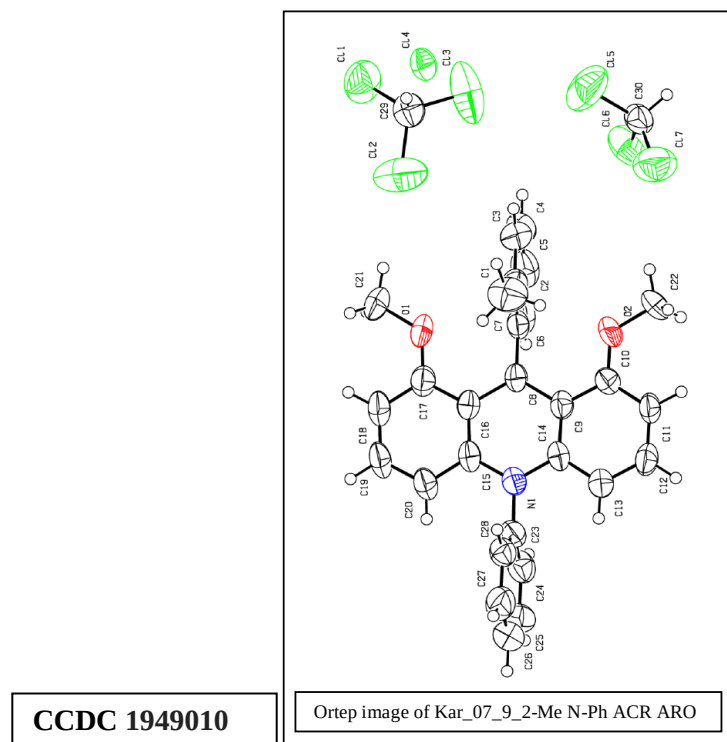


1,8-dimethoxy-10-methyl-9-(p-tolyl)acridin-10-ium chloride (41): ^1H NMR (400 MHz, CDCl_3) δ 8.26–8.20 (m, 4H), 7.24 (d, J = 8.0 Hz, 2H), 7.02 (d, J = 8.0 Hz, 2H), 6.97 (d, J = 6.8 Hz, 2H), 4.95 (s, 3H), 3.48 (s, 6H), 2.48 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 161.7, 160.1, 142.3, 140.6, 138.5, 136.7, 127.4, 125.7, 119.2, 110.1, 106.7, 56.5, 41.9, 21.4; HRMS: m/z : (ESI) calculated for $(\text{C}_{23}\text{H}_{22}\text{NO}_2)^+$ ($[\text{M}^+]$) 344.1645, found 344.1650.



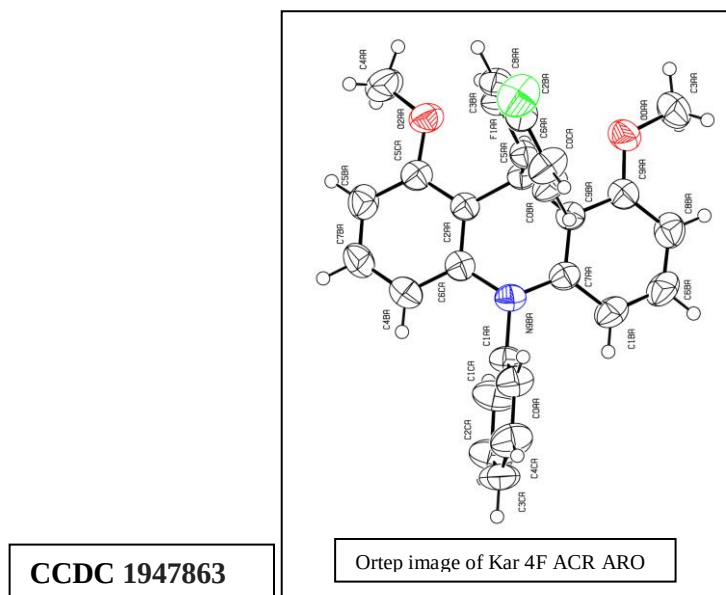
1,8-dimethoxy-10-methyl-9-(o-tolyl)acridin-10-ium chloride (42): ^1H NMR (400 MHz, CDCl_3) δ 8.30–8.26 (m, 4H), 7.34–7.26 (m, 3H), 7.20 (t, J = 7.2 Hz, 1H), 7.04–6.98 (m, 2H), 6.73 (d, J = 7.6 Hz, 1H), 5.01 (s, 3H), 3.49 (s, 6H), 2.00 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ 161.5, 160.0, 142.4, 141.5, 140.6, 134.0, 128.0, 127.5, 124.9, 124.3, 119.0, 110.3, 106.7, 56.7, 41.8, 20.4; HRMS: m/z : (ESI) calculated for $(\text{C}_{23}\text{H}_{22}\text{NO}_2)^+$ ($[\text{M}^+]$) 344.1645, found 344.1640.

Fig. S2: (a) Crystallographic Information of 1,8-dimethoxy-10-phenyl-9-(o-tolyl)acridin-10-ium chloride (33)



Identification code	kar_07
Empirical formula	C ₃₀ H ₂₆ Cl ₇ NO ₂
Formula weight	680.67
Temperature (K)	100
Crystal system	Monoclinic
Space group	P2 ₁
<i>a</i> (Å)	10.1043(8)
<i>b</i> (Å)	12.8257(9)
<i>c</i> (Å)	12.9176(9)
α (°)	90
β (°)	104.397(8)
γ (°)	90
Volume (Å ³)	1621.5(2)
<i>Z</i>	2
ρ_{calc} (g/cm ³)	1.394
μ (mm ⁻¹)	0.640
<i>F</i> (000)	696.0
Crystal size (mm ³)	0.025 × 0.023 × 0.020
Radiation	MoK α (λ = 0.71073)
2 θ range for data collection (°)	6.802 to 50.05
Index ranges	-11 ≤ <i>h</i> ≤ 12, -15 ≤ <i>k</i> ≤ 14, -9 ≤ <i>l</i> ≤ 15
Reflections collected	5391
Data/restraints/parameters	4527/1/317
Goodness-of-fit on <i>F</i> ²	1.047
Final <i>R</i> indexes [<i>I</i> > 2 σ (<i>I</i>)]	<i>R</i> ₁ = 0.0895, <i>wR</i> ₂ = 0.2241
Final <i>R</i> indexes [all data]	<i>R</i> ₁ = 0.1070, <i>wR</i> ₂ = 0.2535
Largest diff. peak/hole (e Å ⁻³)	0.39/-0.43

Fig. S2: (b) Crystallographic Information of 9-(4-fluorophenyl)-1,8-dimethoxy-10-phenyl-9,10-dihydroacridine



Identification code	kar 4F ACR ARO
Empirical formula	C ₂₇ H ₂₂ FNO ₂
Formula weight	411.48
Temperature/K	100
Crystal system	triclinic
Space group	P-1
a/Å	8.2718(8)
b/Å	10.4182(9)
c/Å	13.1630(11)
α (°)	113.112(8)
β (°)	93.907(7)
γ (°)	91.575(8)
Volume (Å ³)	1039.07(17)
Z	2
ρ_{calc} (g/cm ³)	1.3151
μ /mm ⁻¹	0.716
F(000)	433.4
Crystal size (mm ³)	N/A $\times$ N/A $\times$ N/A
Radiation	Cu K α (λ = 1.54184)
2 θ range for data collection(°)	7.32 to 143.44
Index ranges	-10 $\leq$ h $\leq$ 8, -12 $\leq$ k $\leq$ 8, -14 $\leq$ l $\leq$ 16
Reflections collected	6200
Independent reflections	3863 [R int = 0.0883, R sigma = 0.0787]
Data/restraints/parameters	3863/0/282
Goodness-of-fit on F ²	1.073
Final R indexes [I $\geq$ 2 σ (I)]	R 1 = 0.0926, wR 2 = 0.2442
Final R indexes [all data]	R 1 = 0.1112, wR 2 = 0.2934
Largest diff. peak/hole (e Å ⁻³)	0.34/-0.37

¹H and ¹³C NMR Spectra of Acridines.

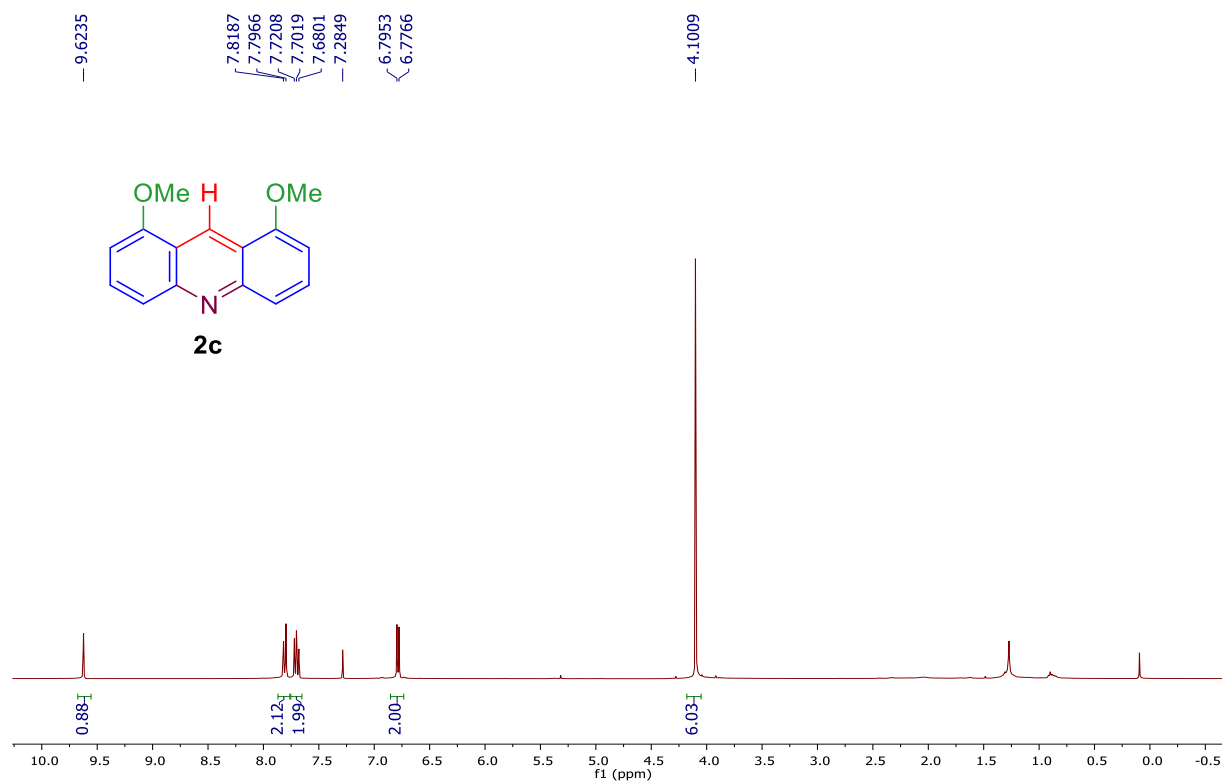


Figure S3. ¹H NMR spectrum of 1,8-dimethoxyacridine (2c).

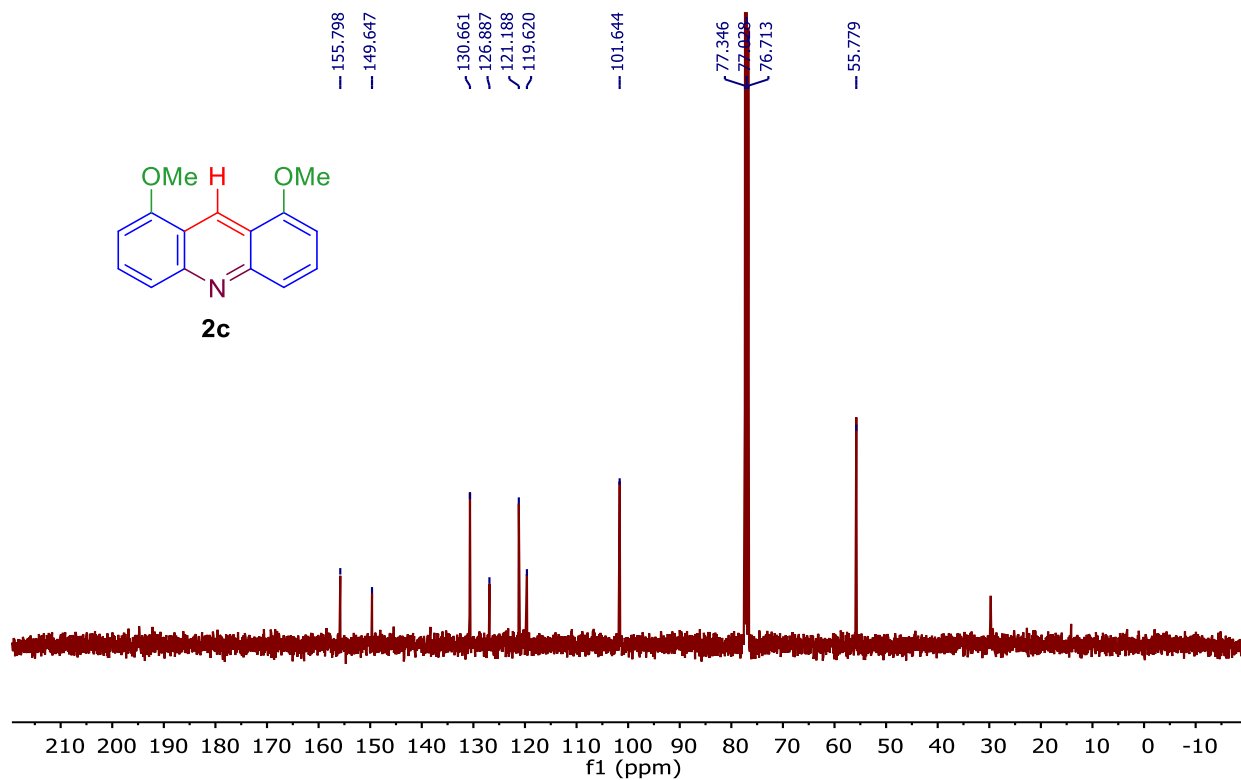


Figure S4. ¹³C NMR spectrum of 1,8-dimethoxyacridine (2c).

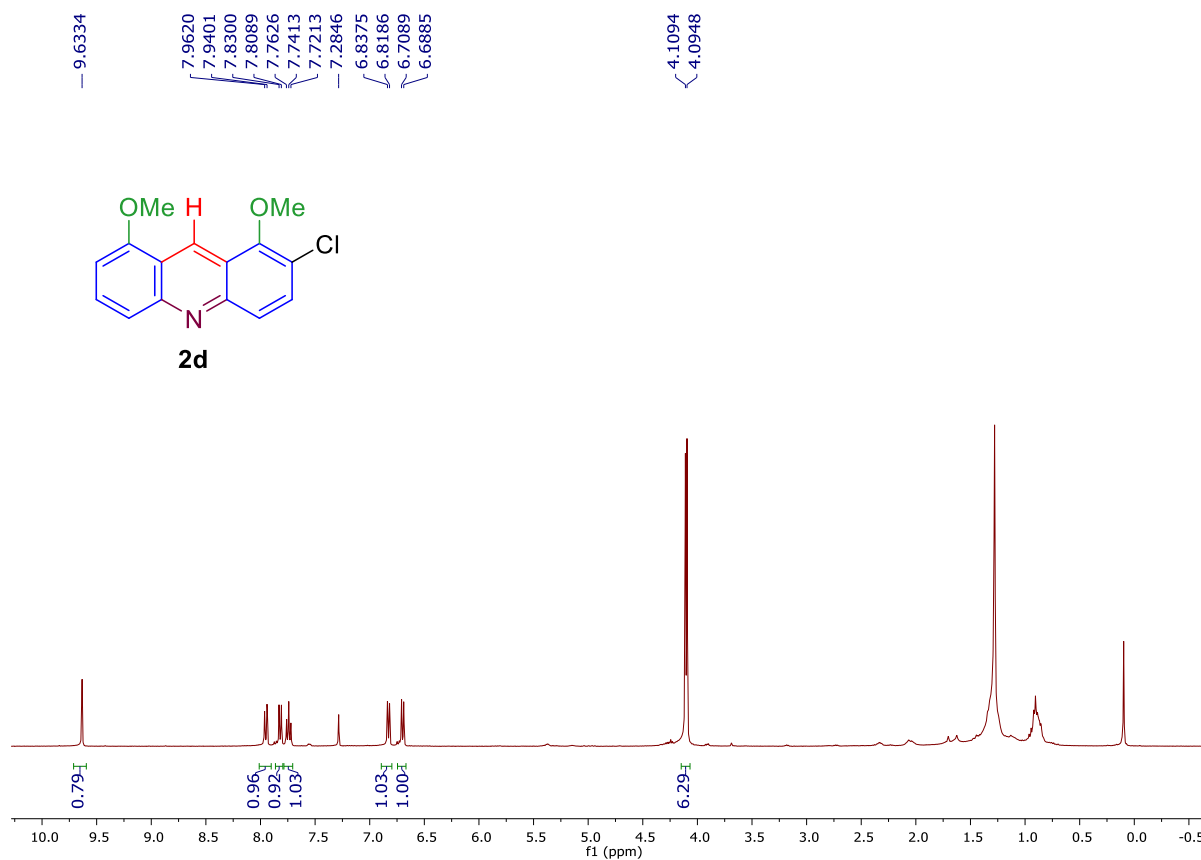


Figure S5. ¹H NMR spectrum of 2-chloro-1,8-dimethoxyacridine (2d).

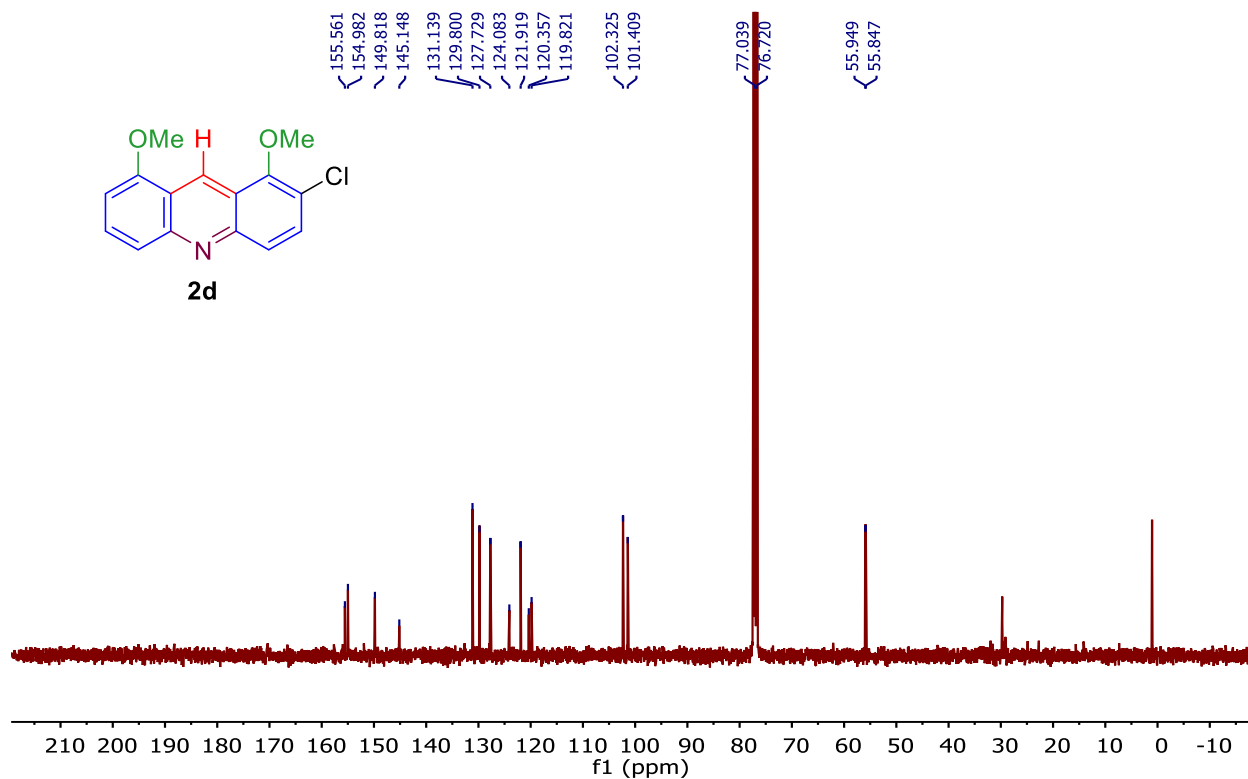


Figure S6. ¹³C NMR spectrum of 2-chloro-1,8-dimethoxyacridine (2d).

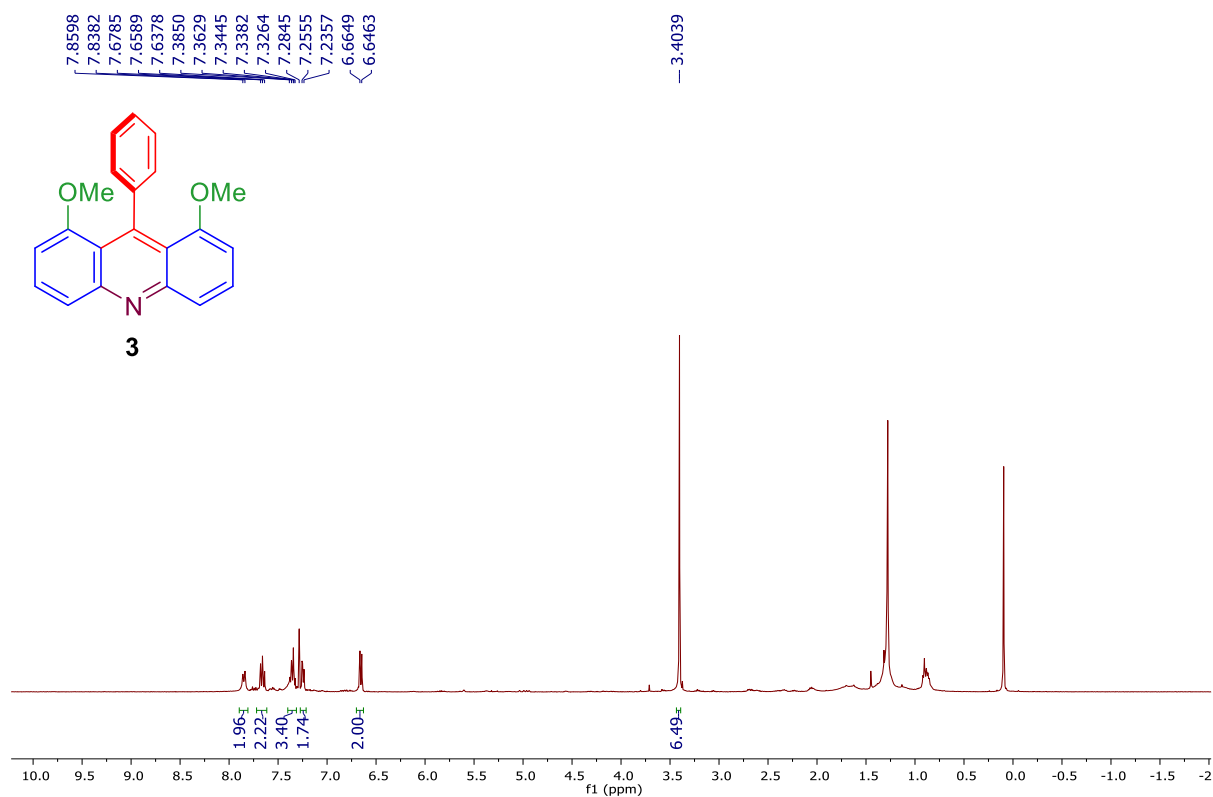


Figure S7. ^1H NMR spectrum of 1,8-dimethoxy-9-phenylacridine (3).

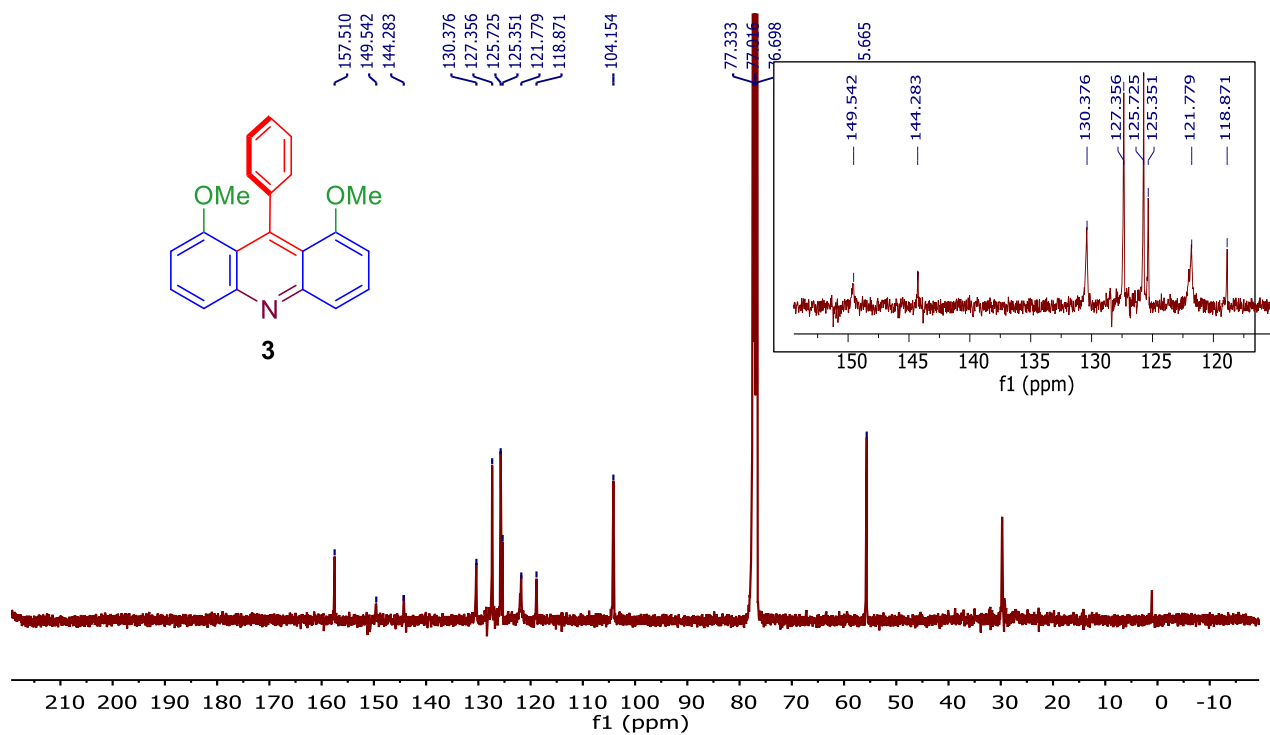


Figure S8. ^{13}C NMR spectrum of 1,8-dimethoxy-9-phenylacridine (3).

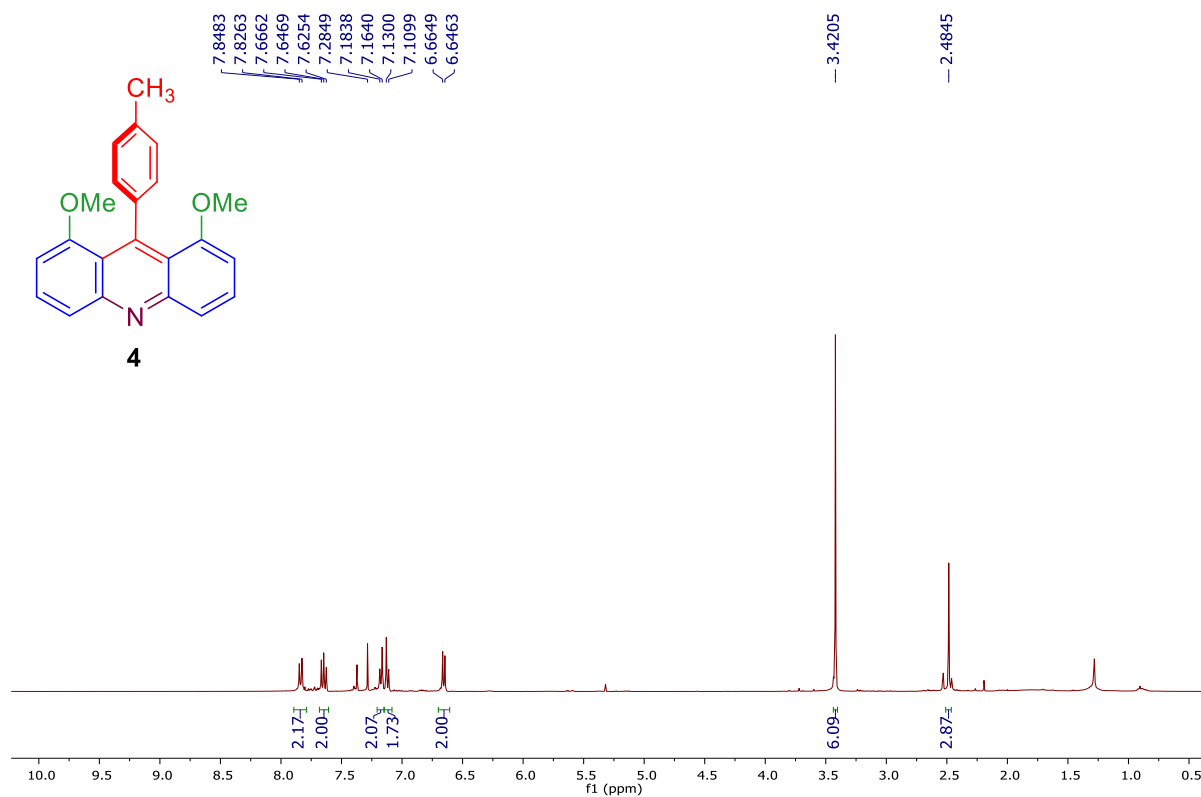


Figure S9. ¹H NMR spectrum of 1,8-dimethoxy-9-p-tolylacridine (4).

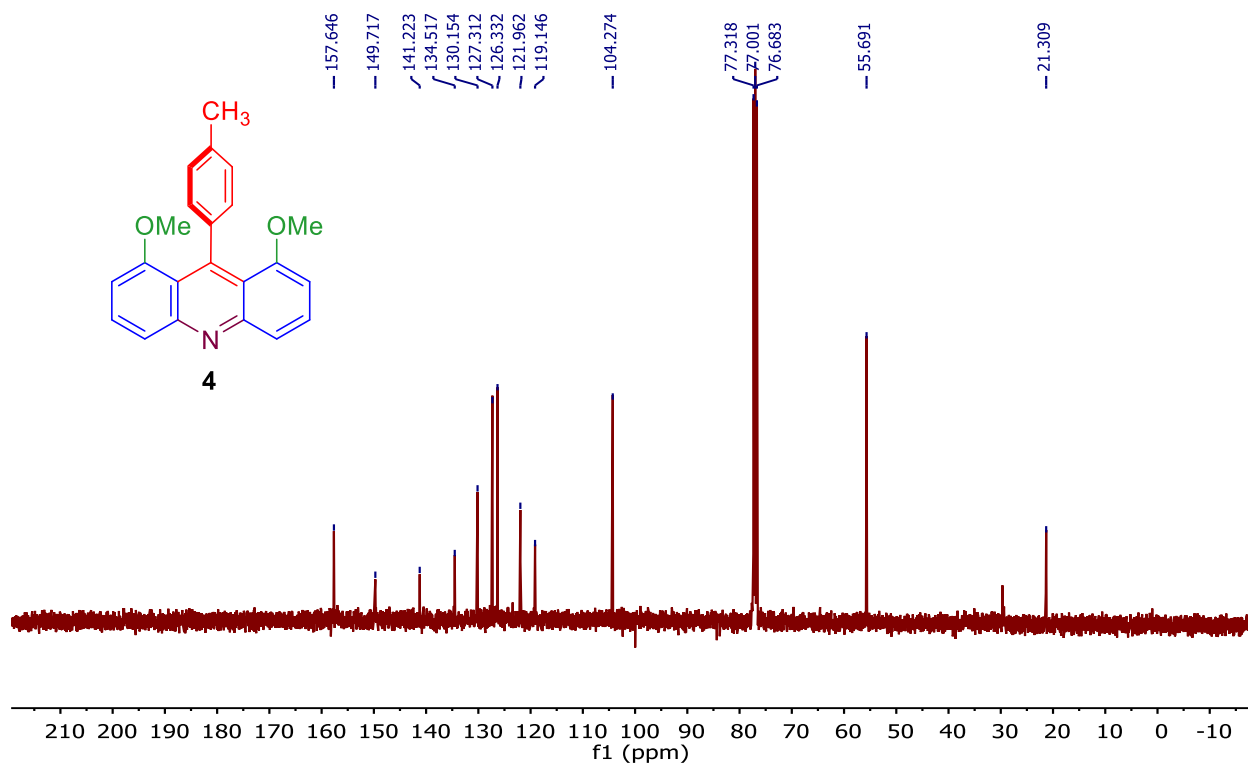


Figure S10. ¹³C NMR spectrum of 1,8-dimethoxy-9-p-tolylacridine (4).

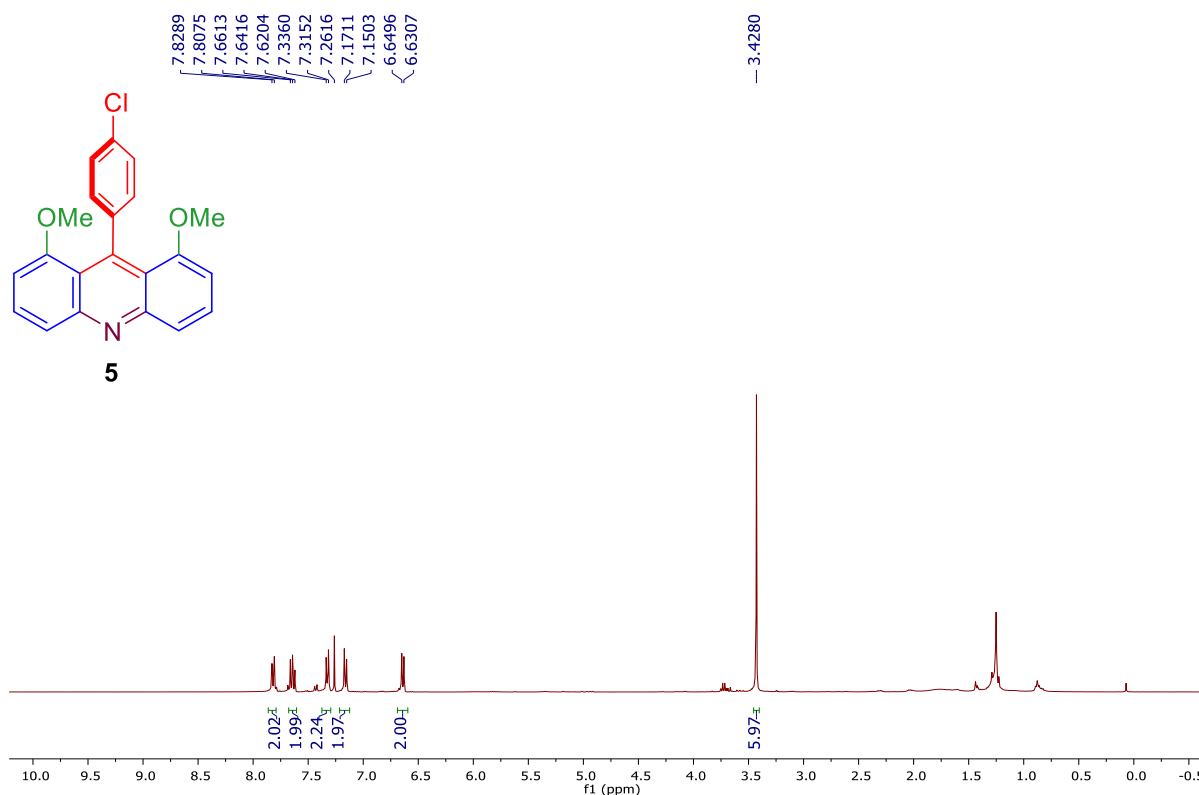


Figure S11. ¹H NMR spectrum of 9-(4-chlorophenyl)-1,8-dimethoxyacridine (5).

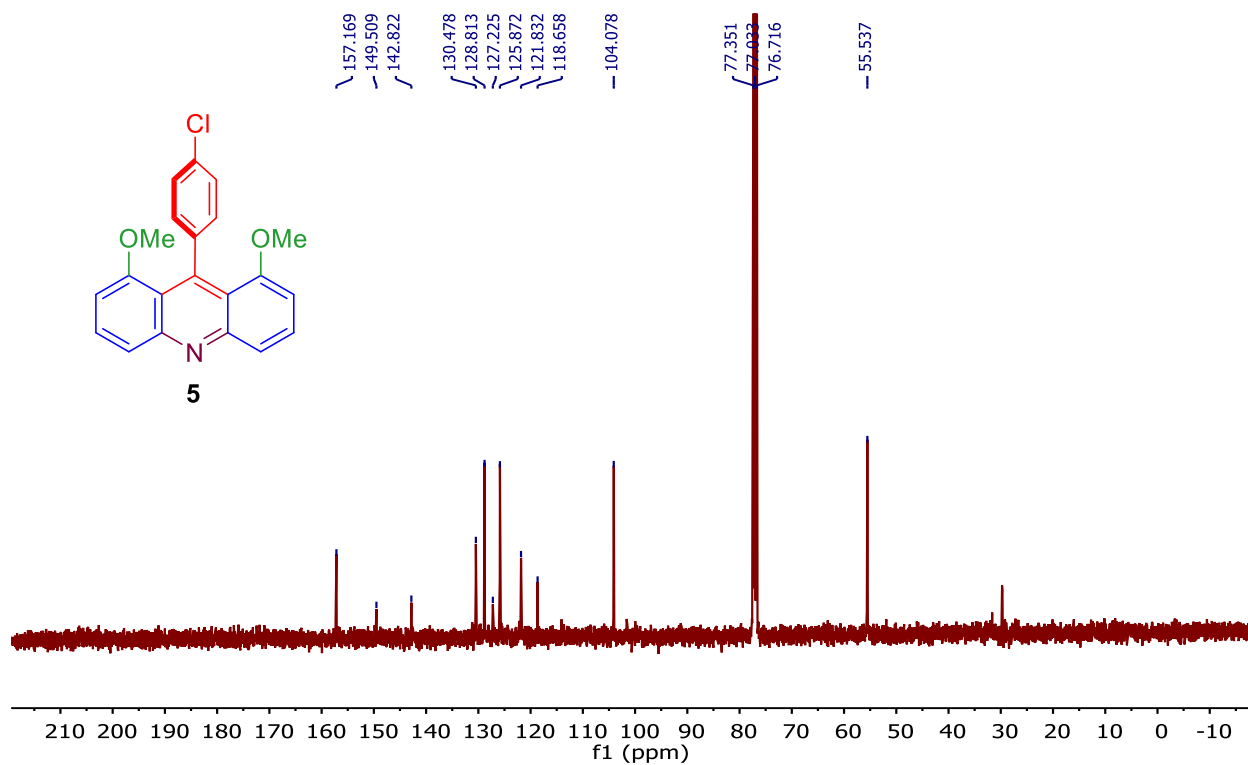


Figure S12. ¹³C NMR spectrum of 9-(4-chlorophenyl)-1,8-dimethoxyacridine (5).

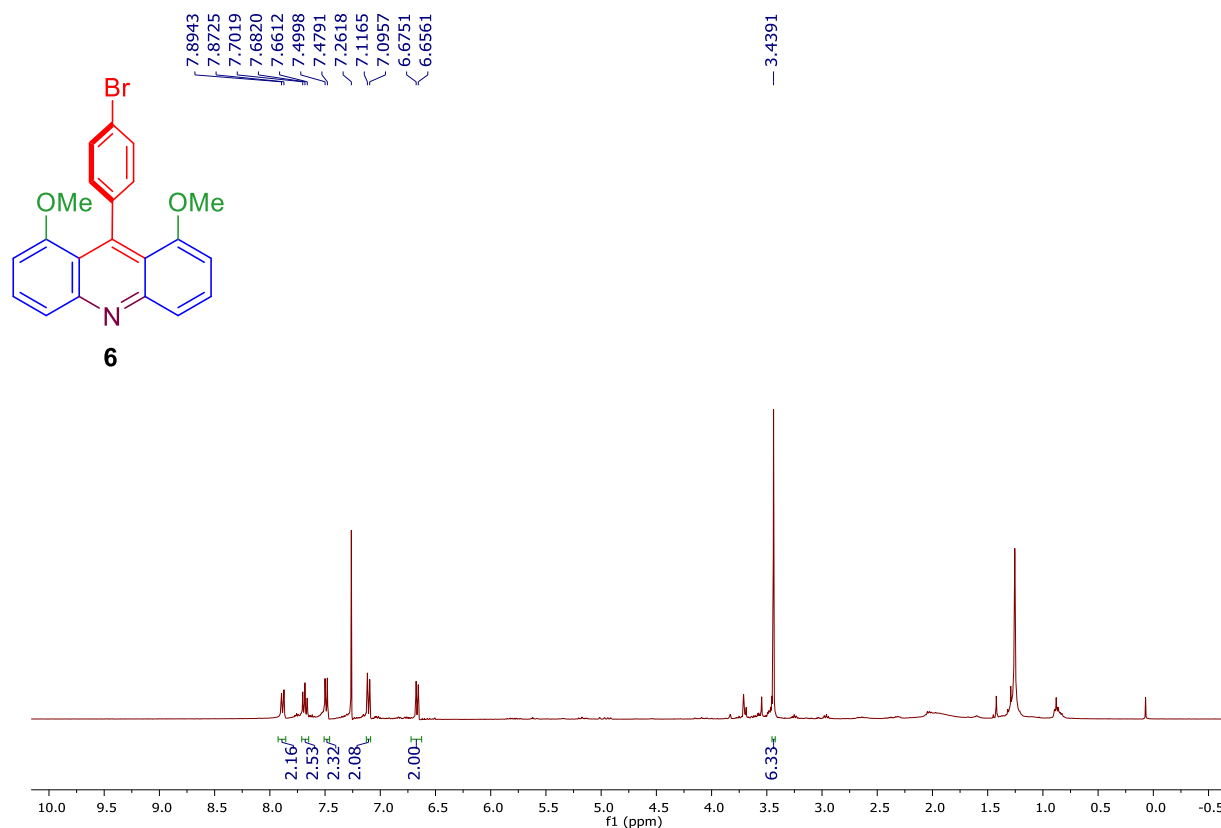


Figure S13. ^1H NMR spectrum of 9-(4-bromophenyl)-1,8-dimethoxyacridine (6).

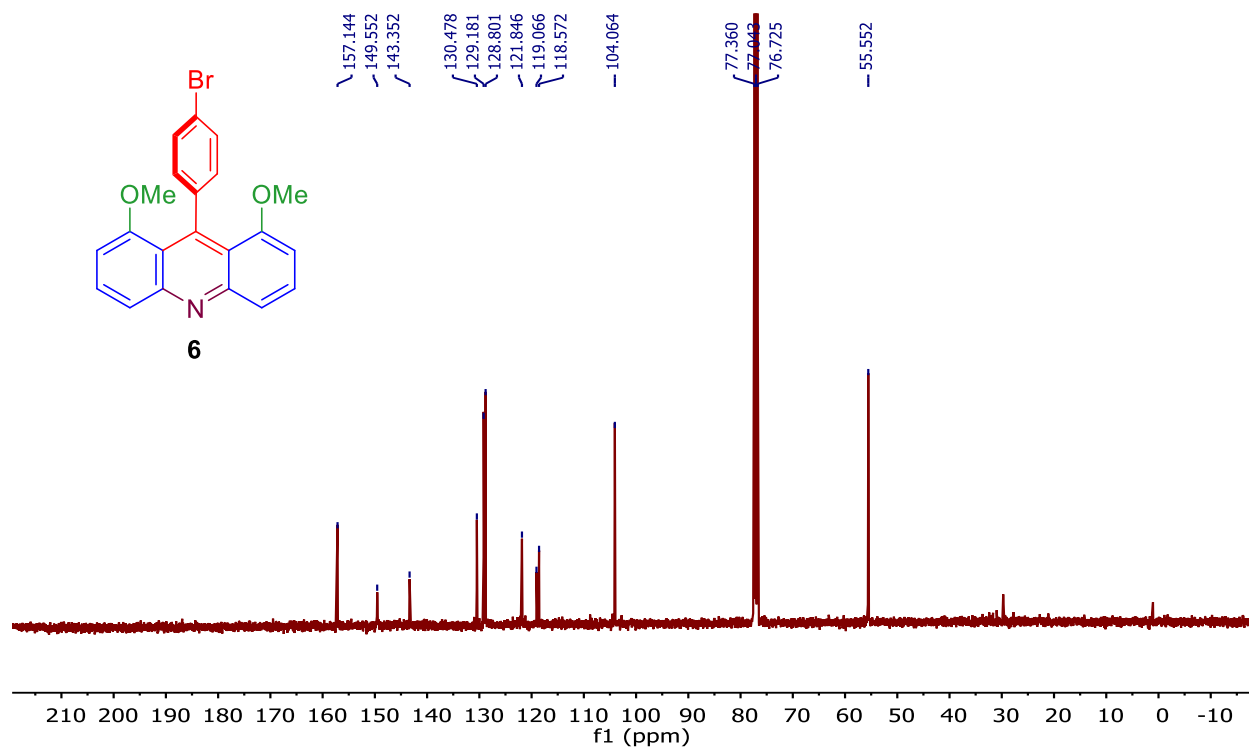


Figure S14. ^{13}C NMR spectrum of 9-(4-bromophenyl)-1,8-dimethoxyacridine (6).

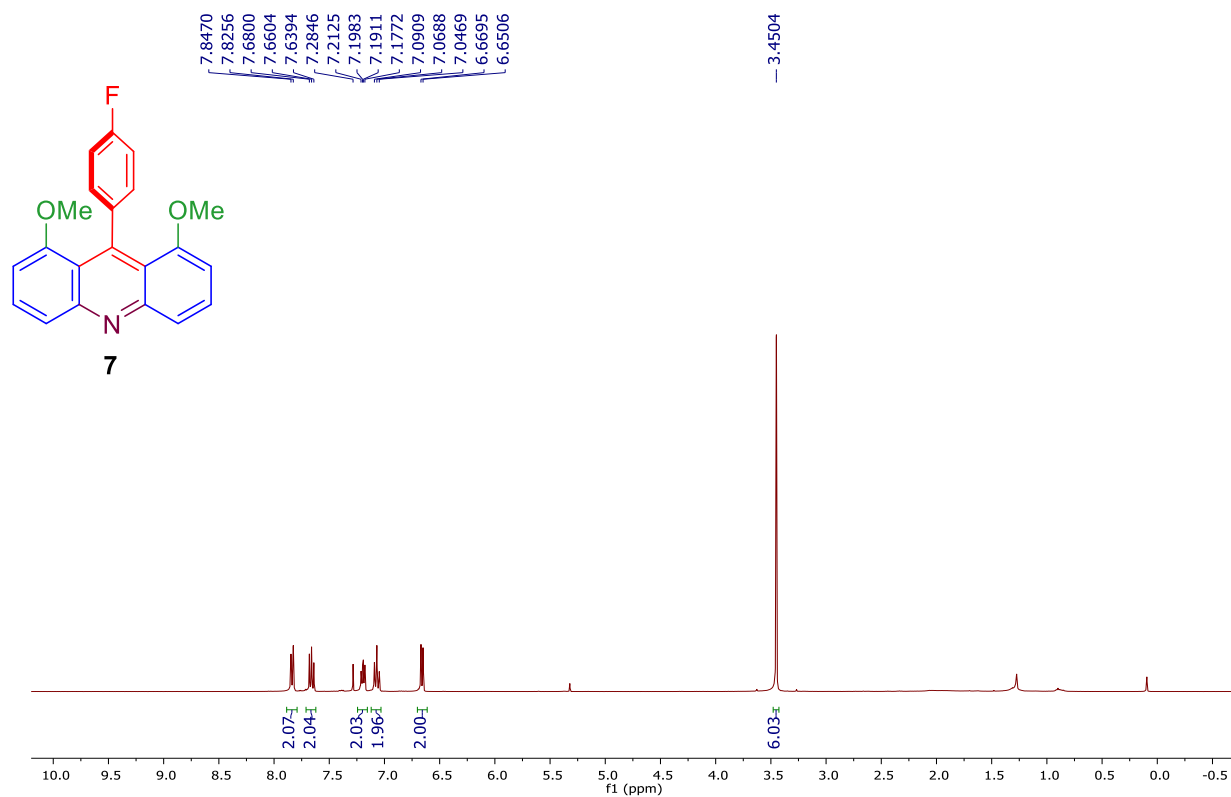


Figure S15. ^1H NMR spectrum of 9-(4-fluorophenyl)-1,8-dimethoxyacridine (7).

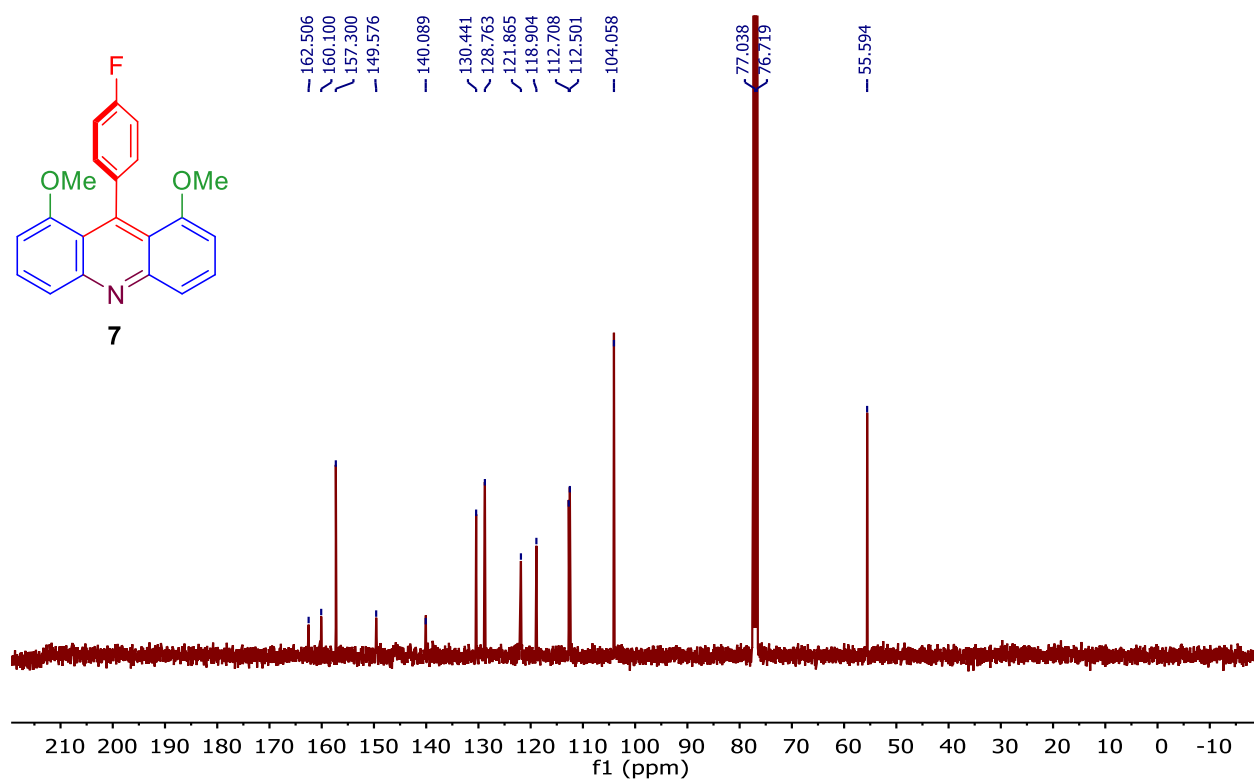


Figure S16. ^{13}C NMR spectrum of 9-(4-fluorophenyl)-1,8-dimethoxyacridine (7).

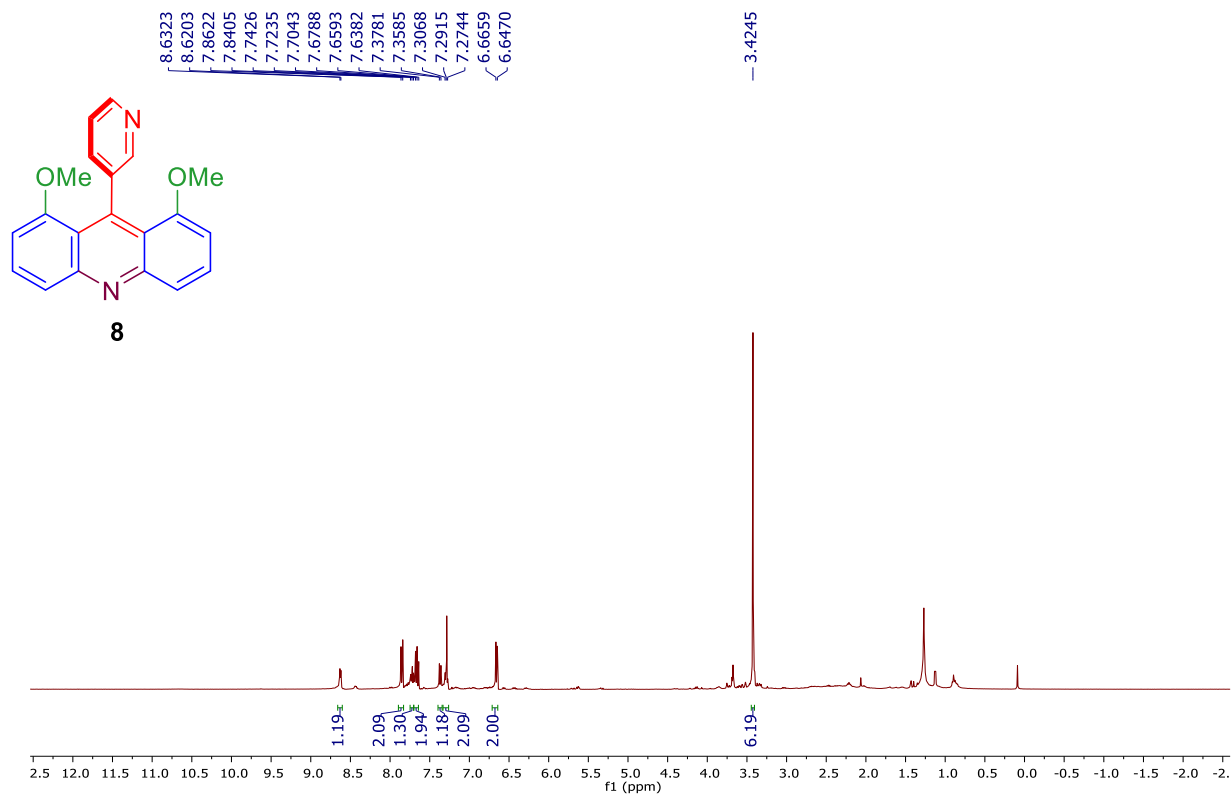


Figure S17. ^1H NMR spectrum of 1,8-dimethoxy-9-(pyridine-3-yl)acridine (8)

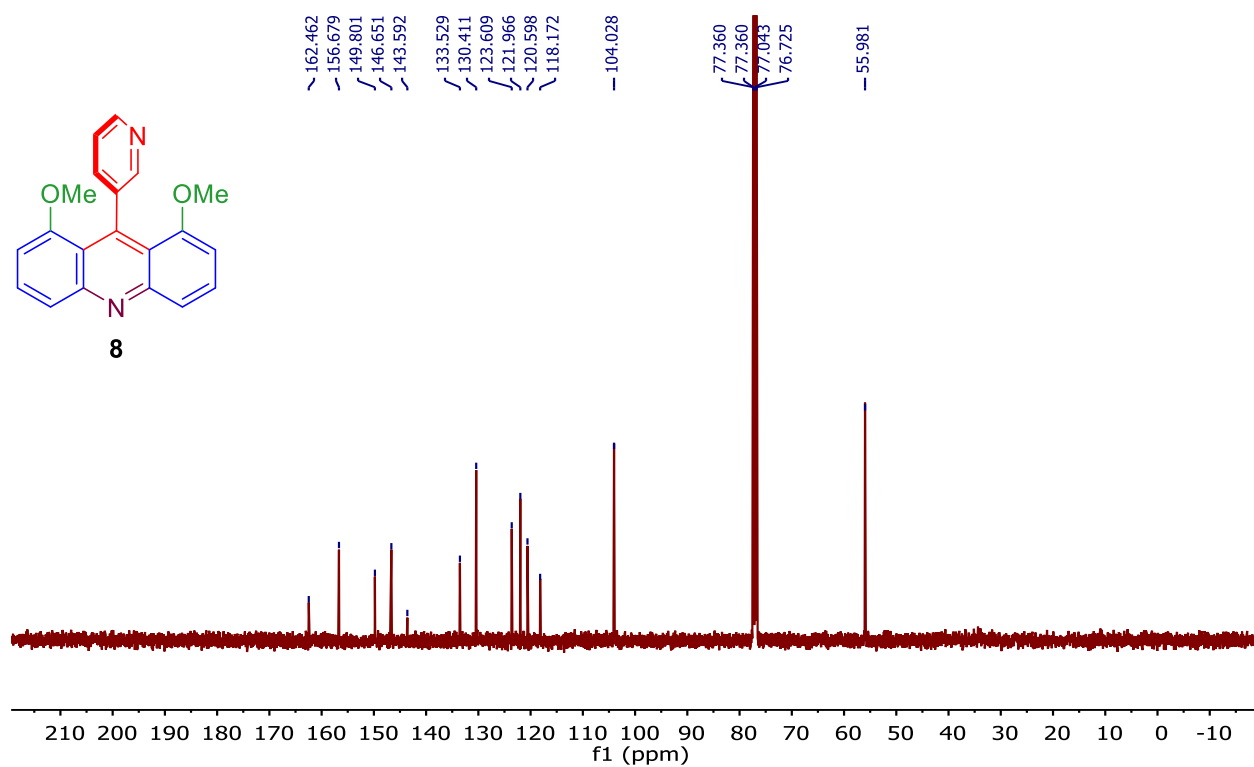


Figure S18. ^{13}C NMR spectrum of 1,8-dimethoxy-9-(pyridine-3-yl)acridine (8)

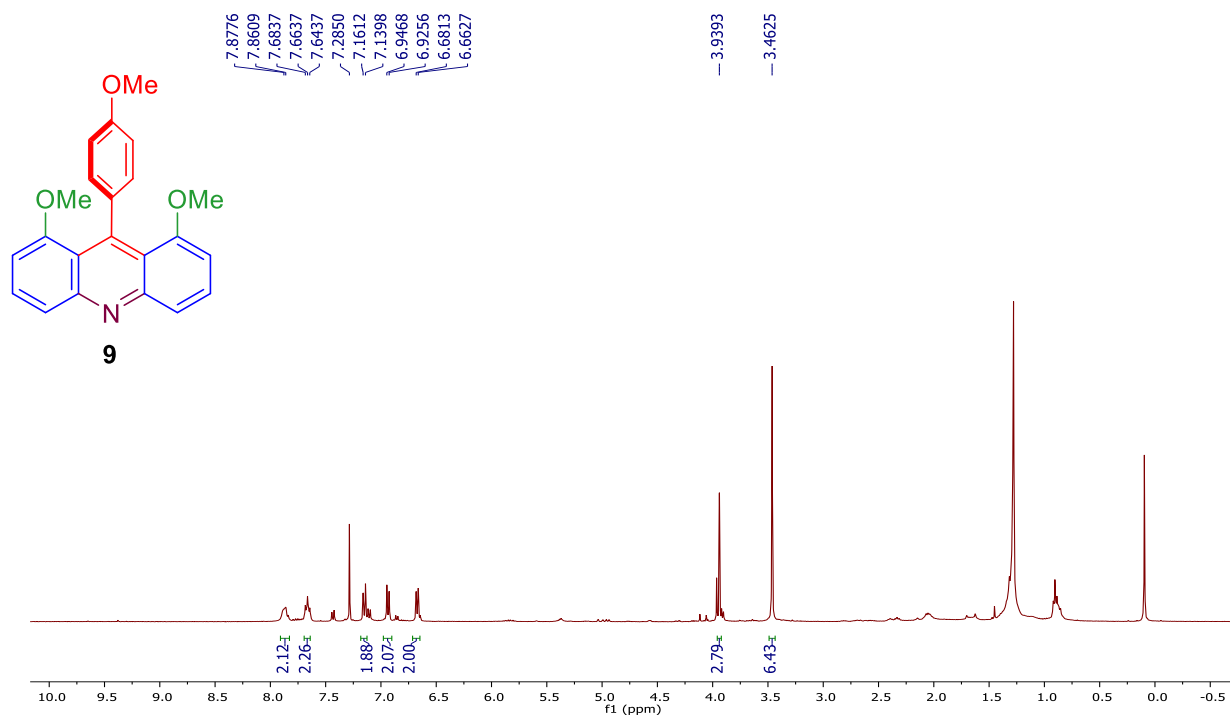


Figure S19. ¹H NMR spectrum of 1,8-dimethoxy-9-(4-methoxyphenyl)acridine (9).

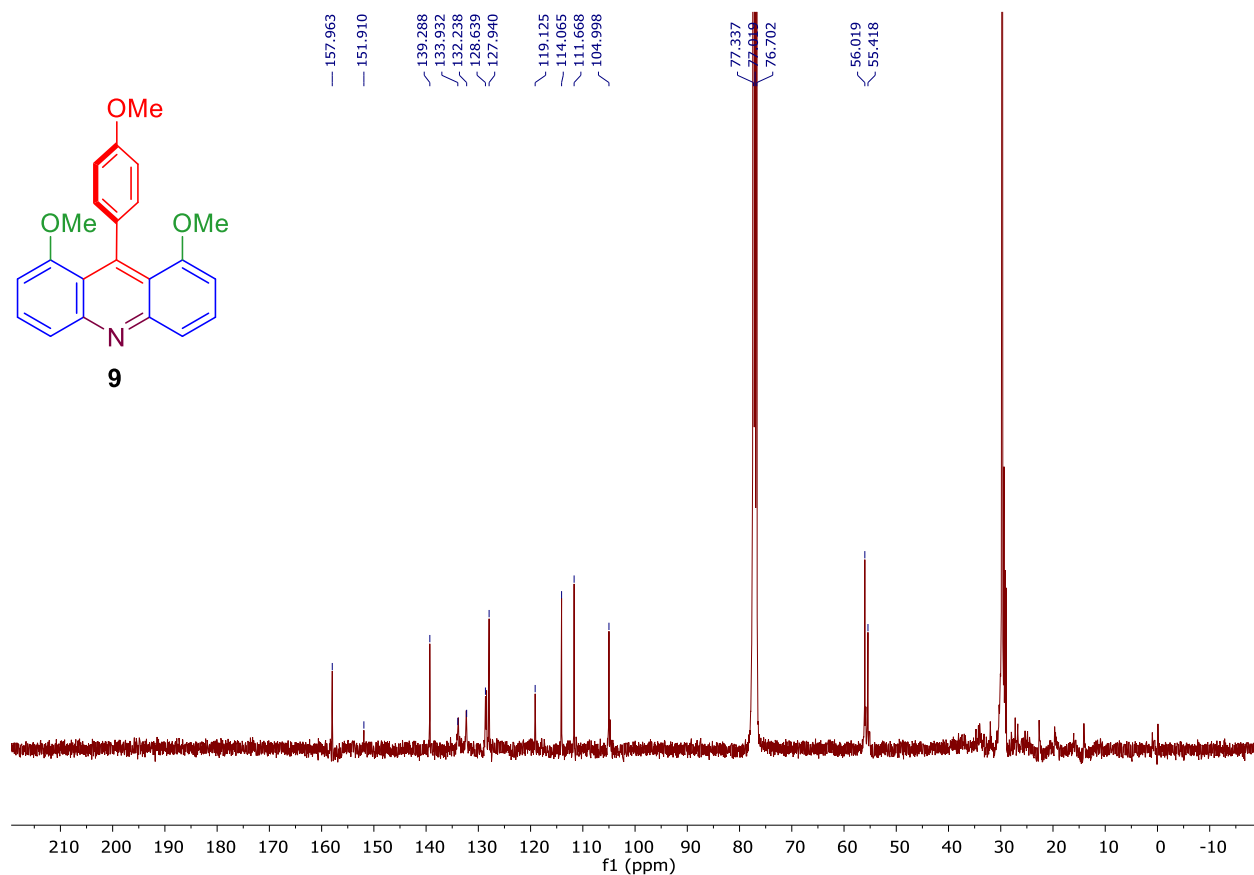


Figure S20. ¹³C NMR spectrum of 1,8-dimethoxy-9-(4-methoxyphenyl)acridine (9).

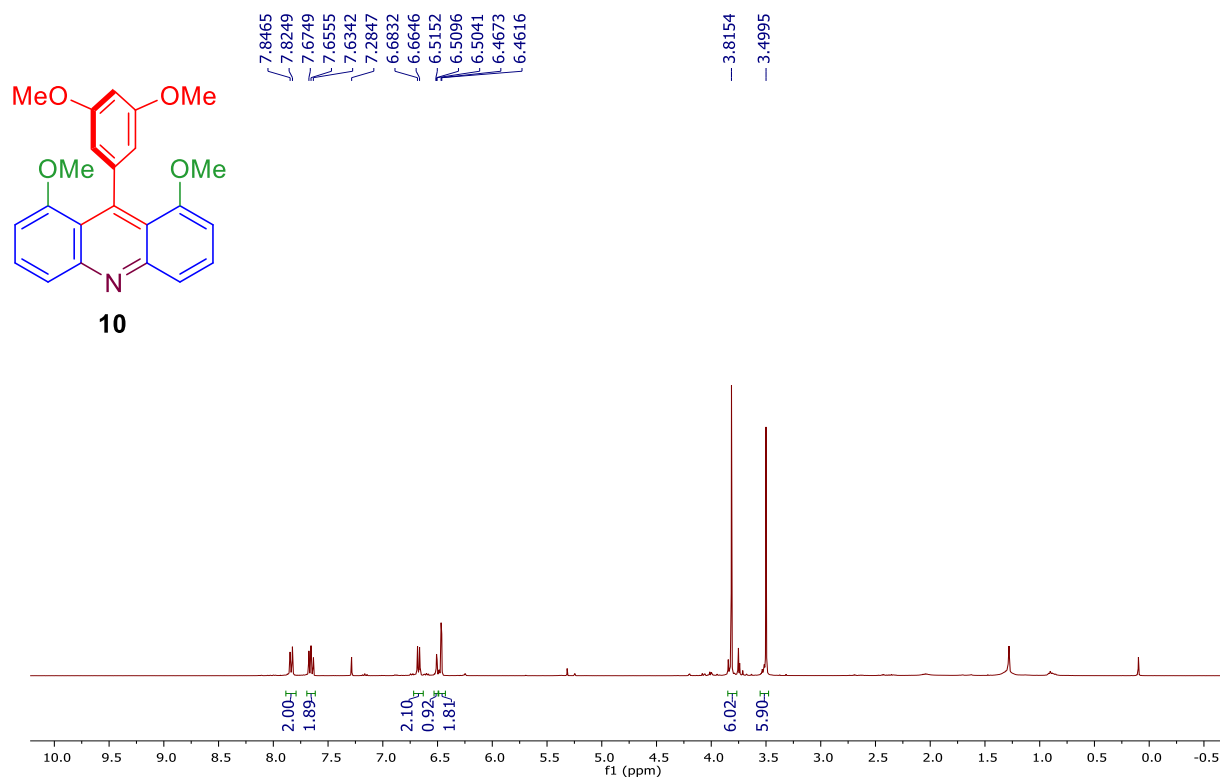


Figure S21. ^1H NMR spectrum of 9-(3,5-dimethoxyphenyl)-1,8-dimethoxyacridine (10).

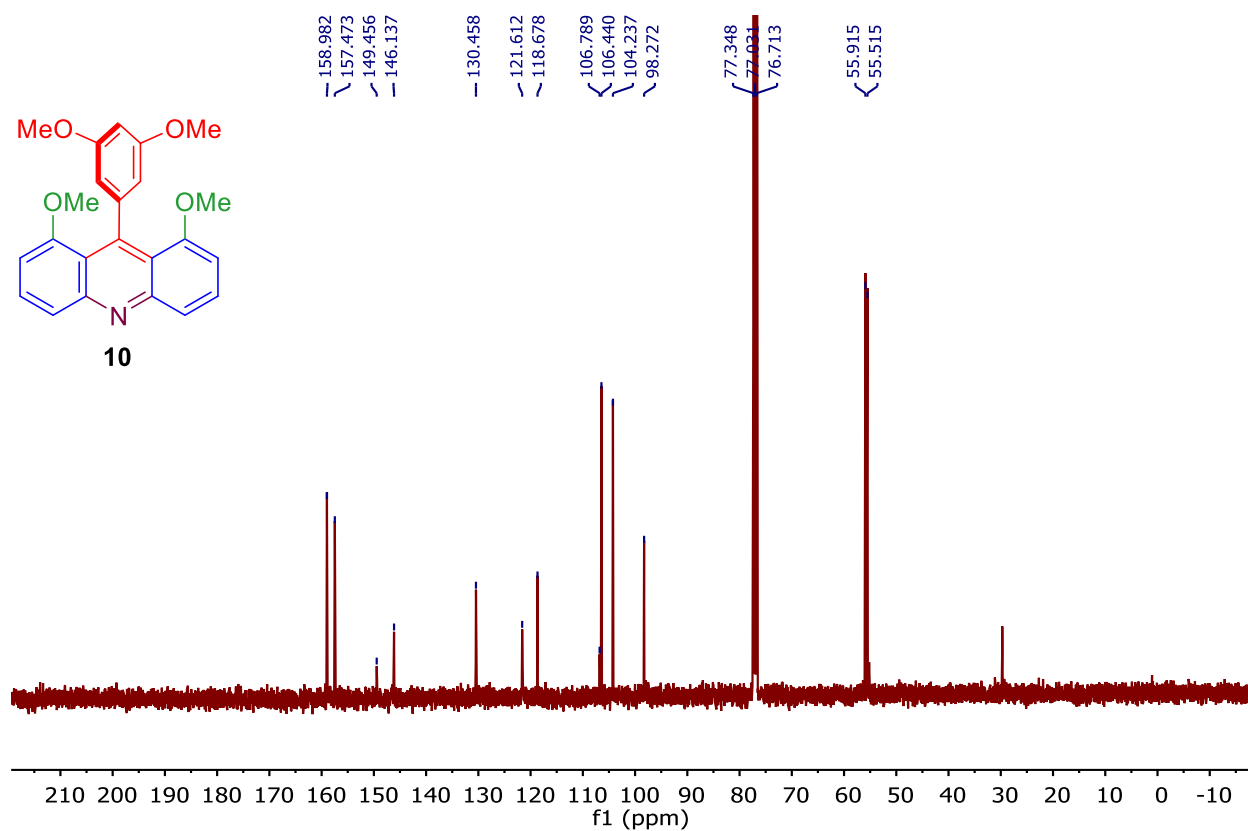


Figure S22. ^{13}C NMR spectrum of 9-(3,5-dimethoxyphenyl)-1,8-dimethoxyacridine (10).

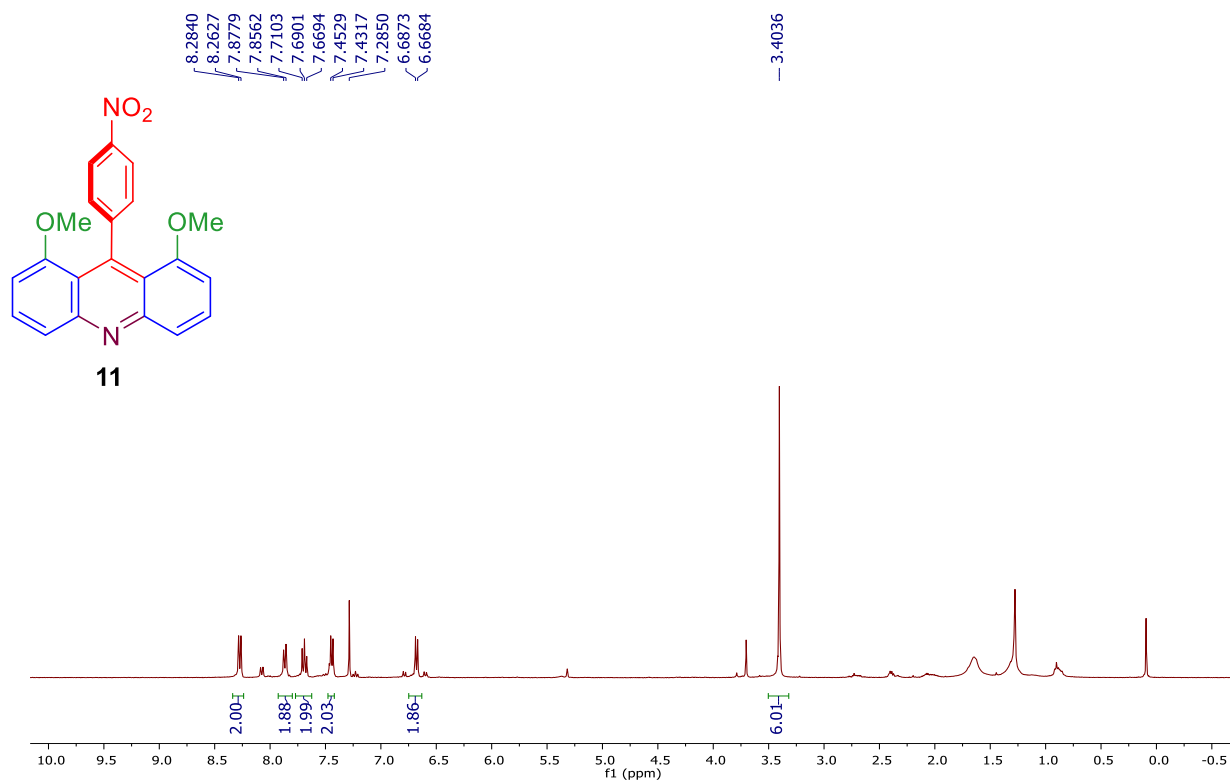


Figure S23. ¹H NMR spectrum of 1,8-dimethoxy-9-(4-nitrophenyl)acridine (11).

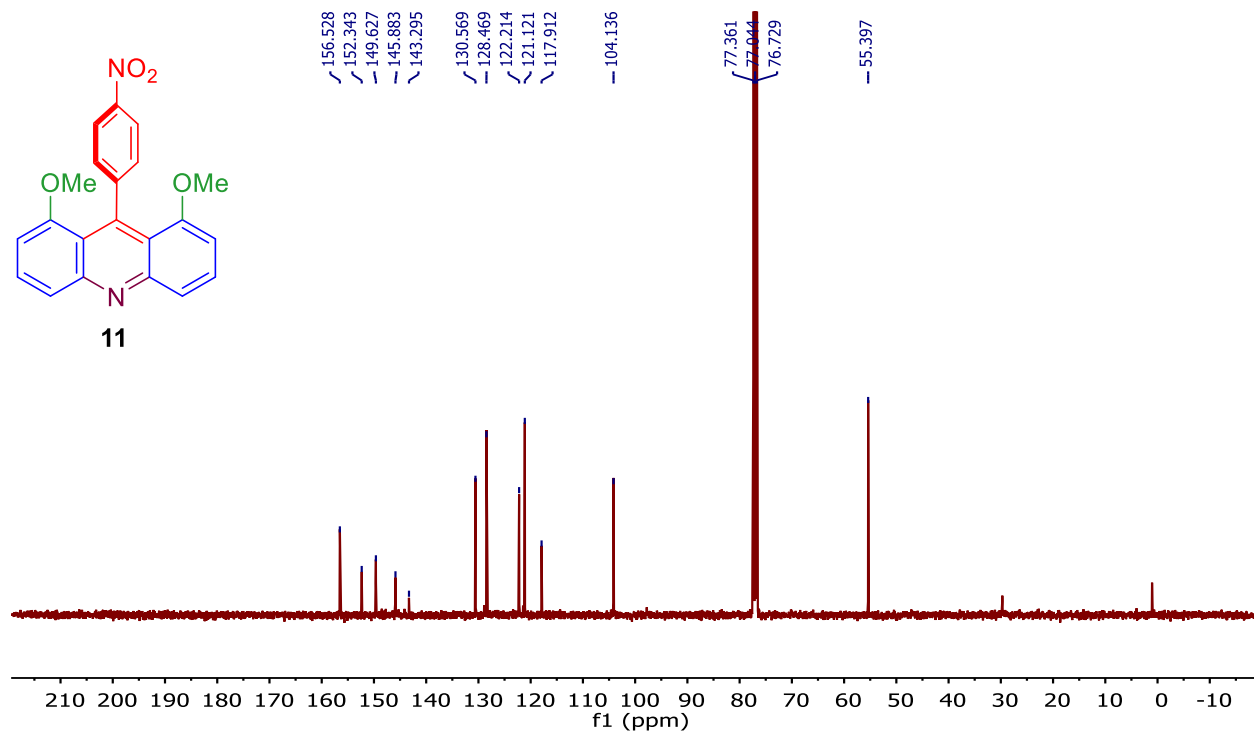


Figure S24. ¹³C NMR spectrum of 1,8-dimethoxy-9-(4-nitrophenyl)acridine (11).

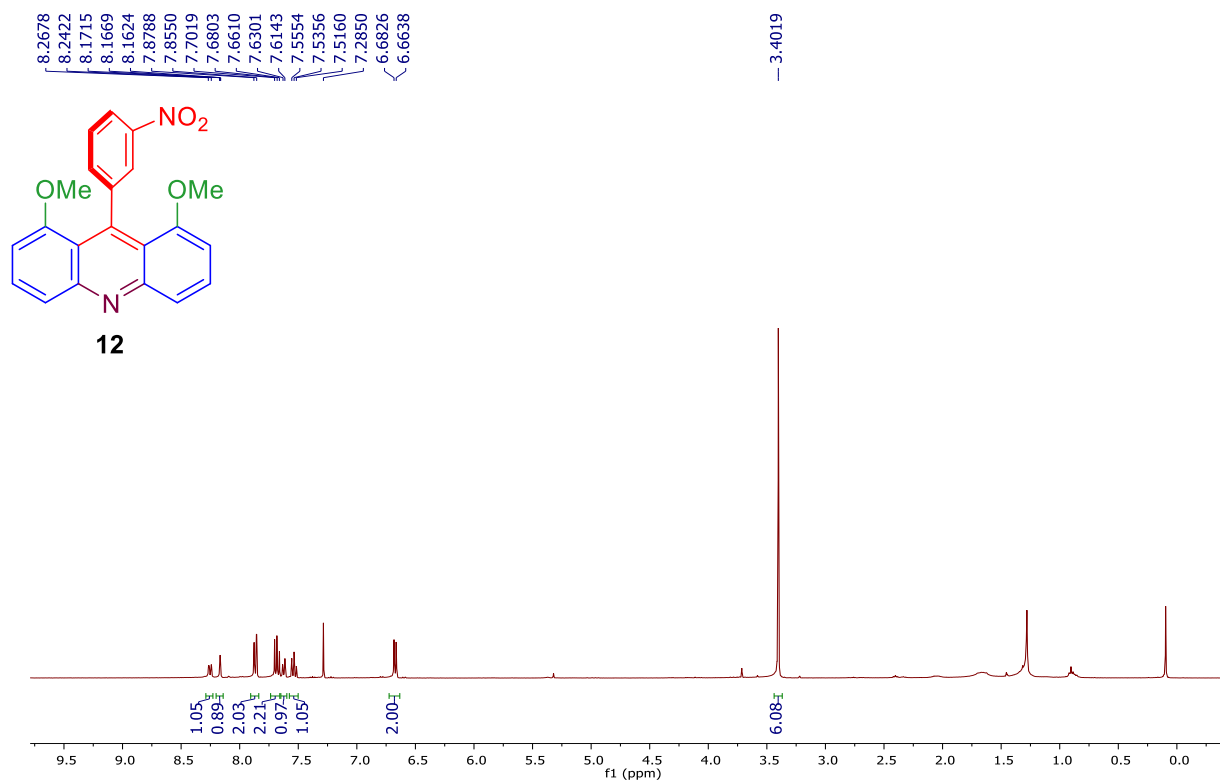


Figure S25. ¹H NMR spectrum of 1,8-dimethoxy-9-(3-nitrophenyl)acridine (12).

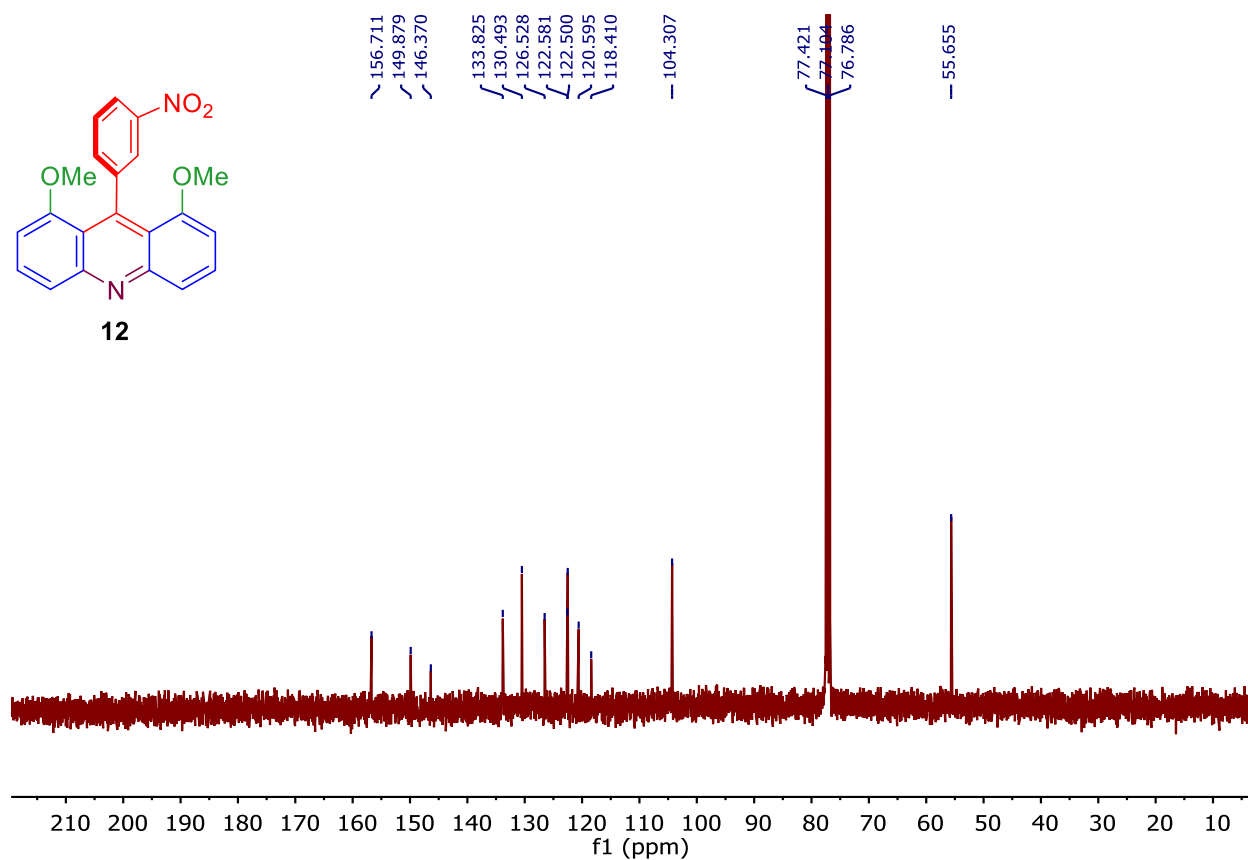


Figure S26. ¹³C NMR spectrum of 1,8-dimethoxy-9-(3-nitrophenyl)acridine (12).

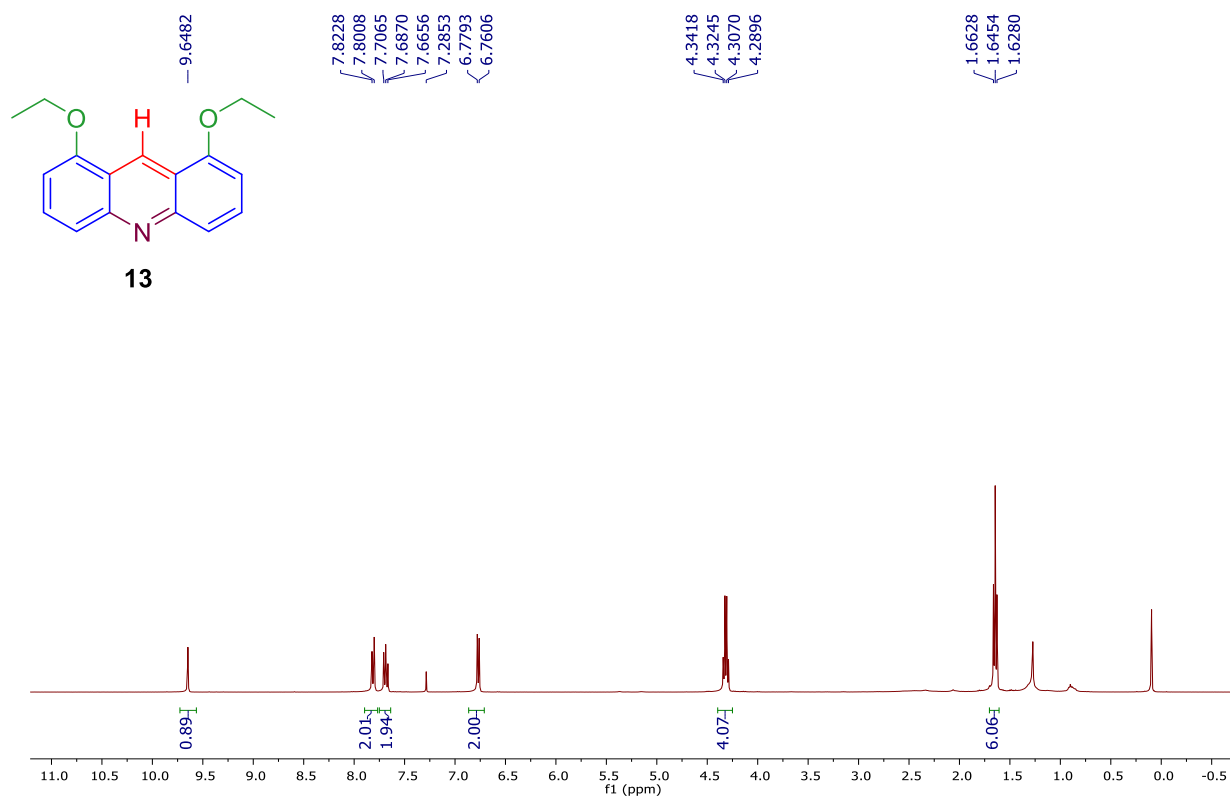


Figure S27. ^1H NMR spectrum of 1,8-diethoxyacridine (13).

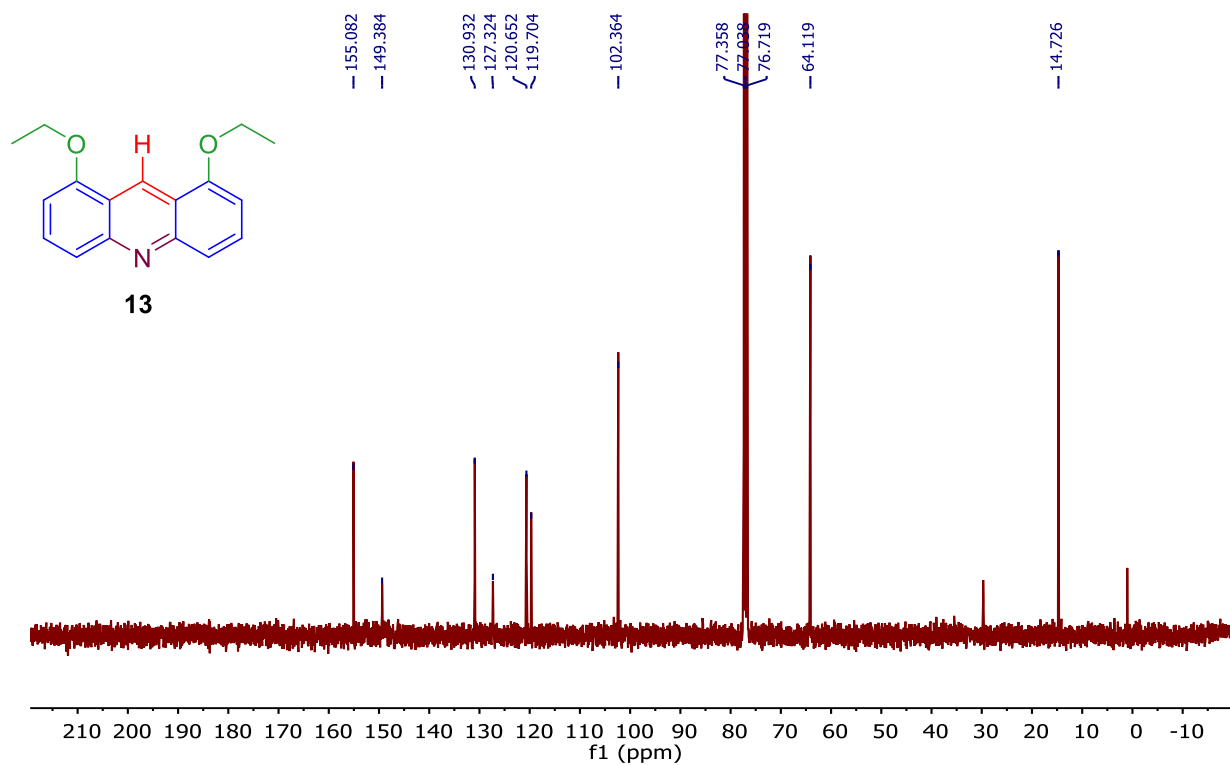


Figure S28. ^{13}C NMR spectrum of 1,8-diethoxyacridine (13).

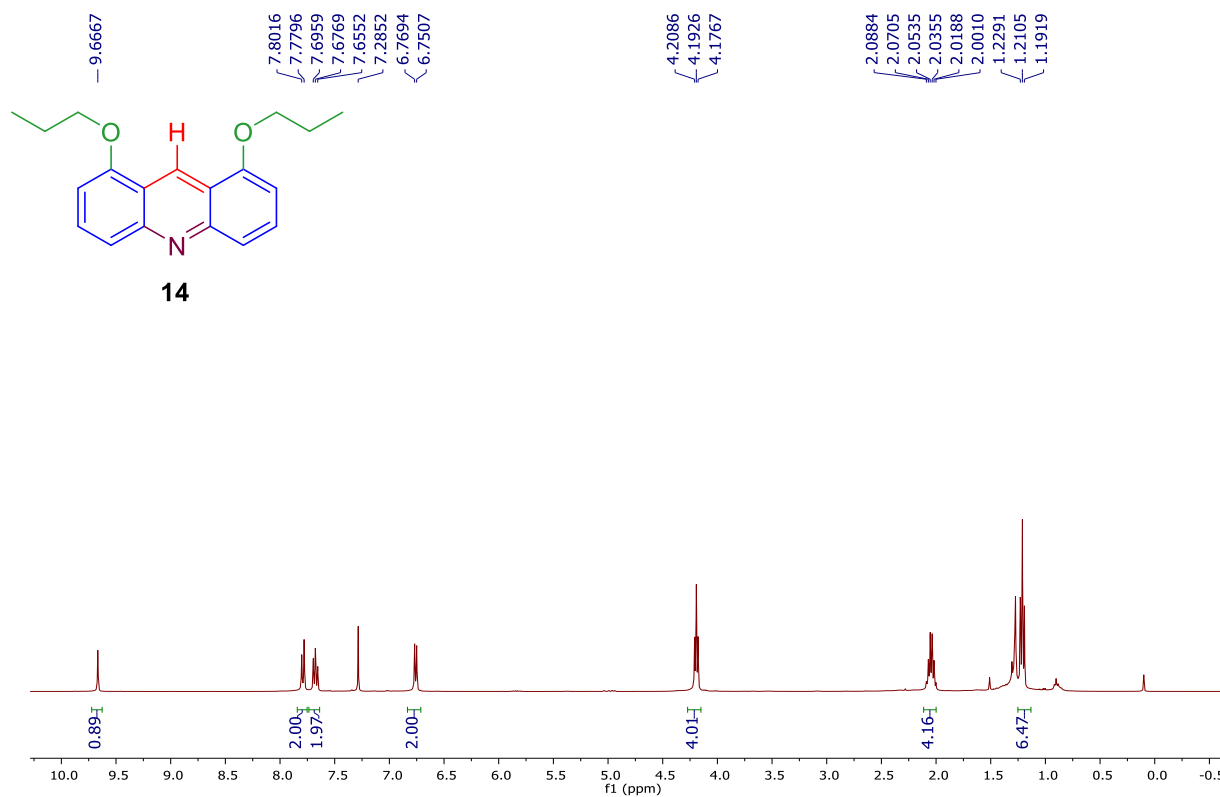


Figure S29. ^1H NMR spectrum of 1,8-dipropoxyacridine (14).

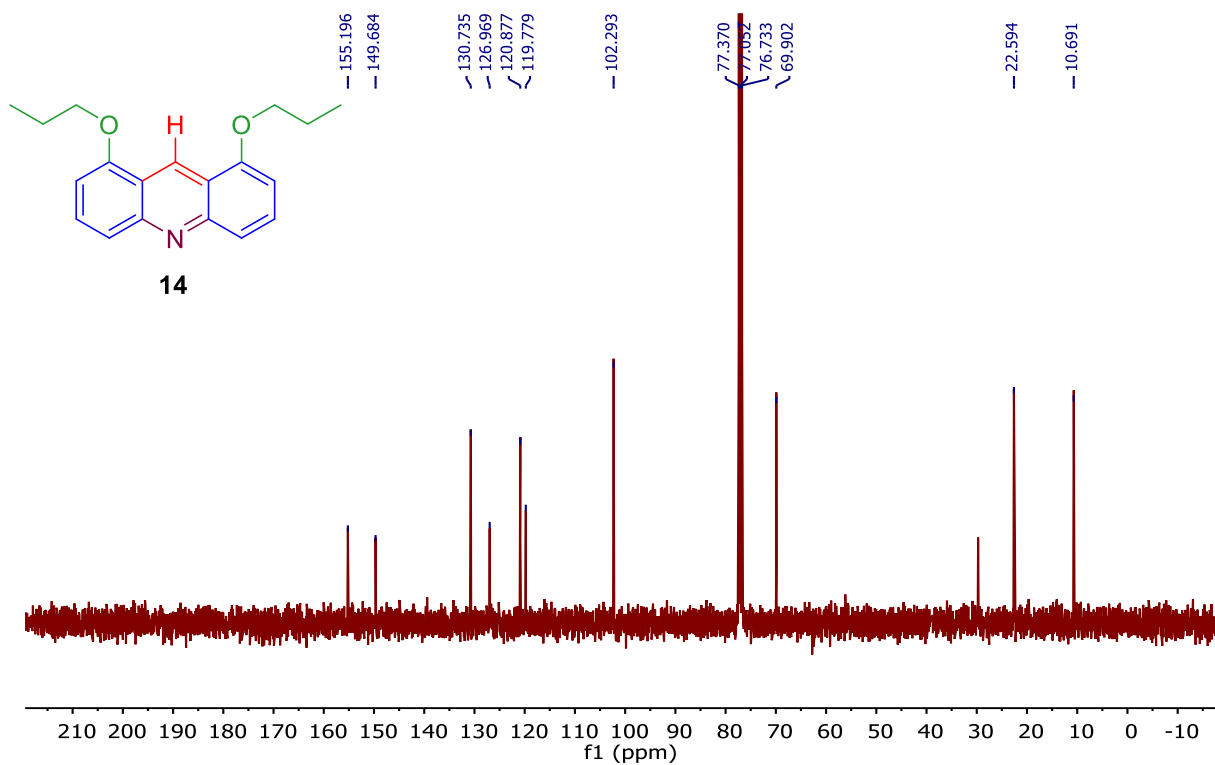


Figure S30. ^{13}C NMR spectrum of 1,8-dipropoxyacridine (14).

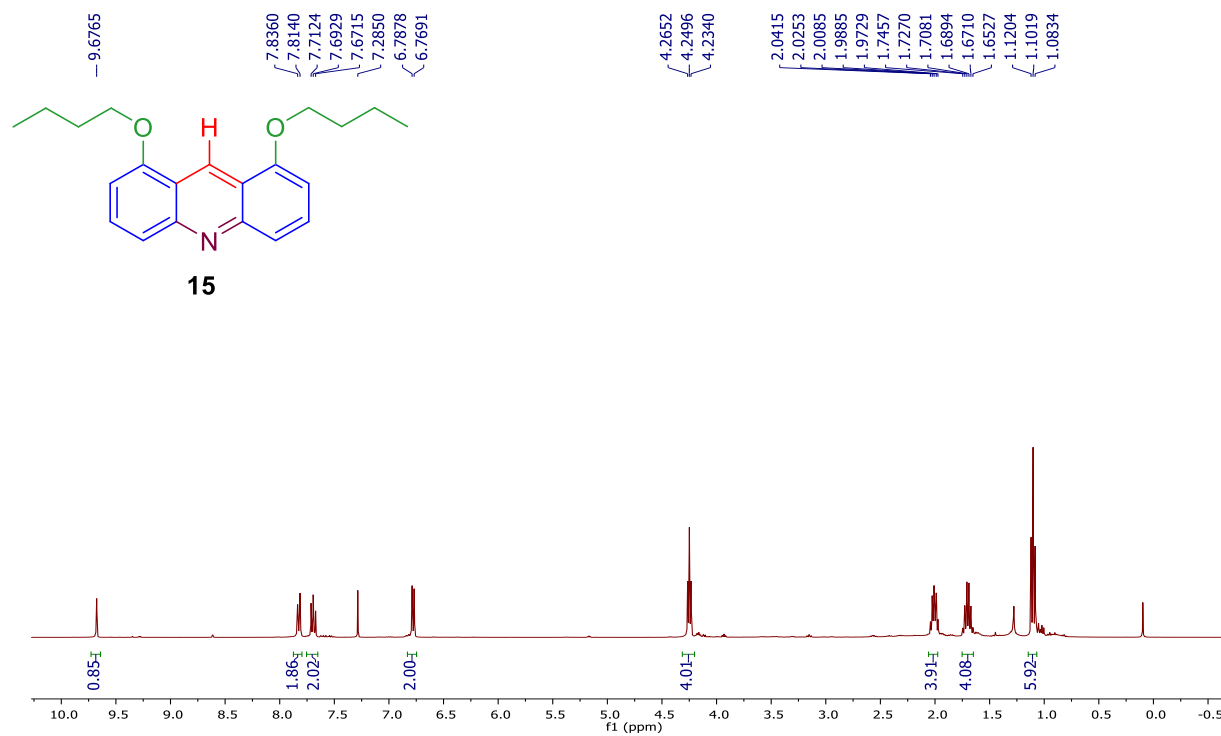


Figure S31. ^1H NMR spectrum of 1,8-dibutoxyacridine (15).

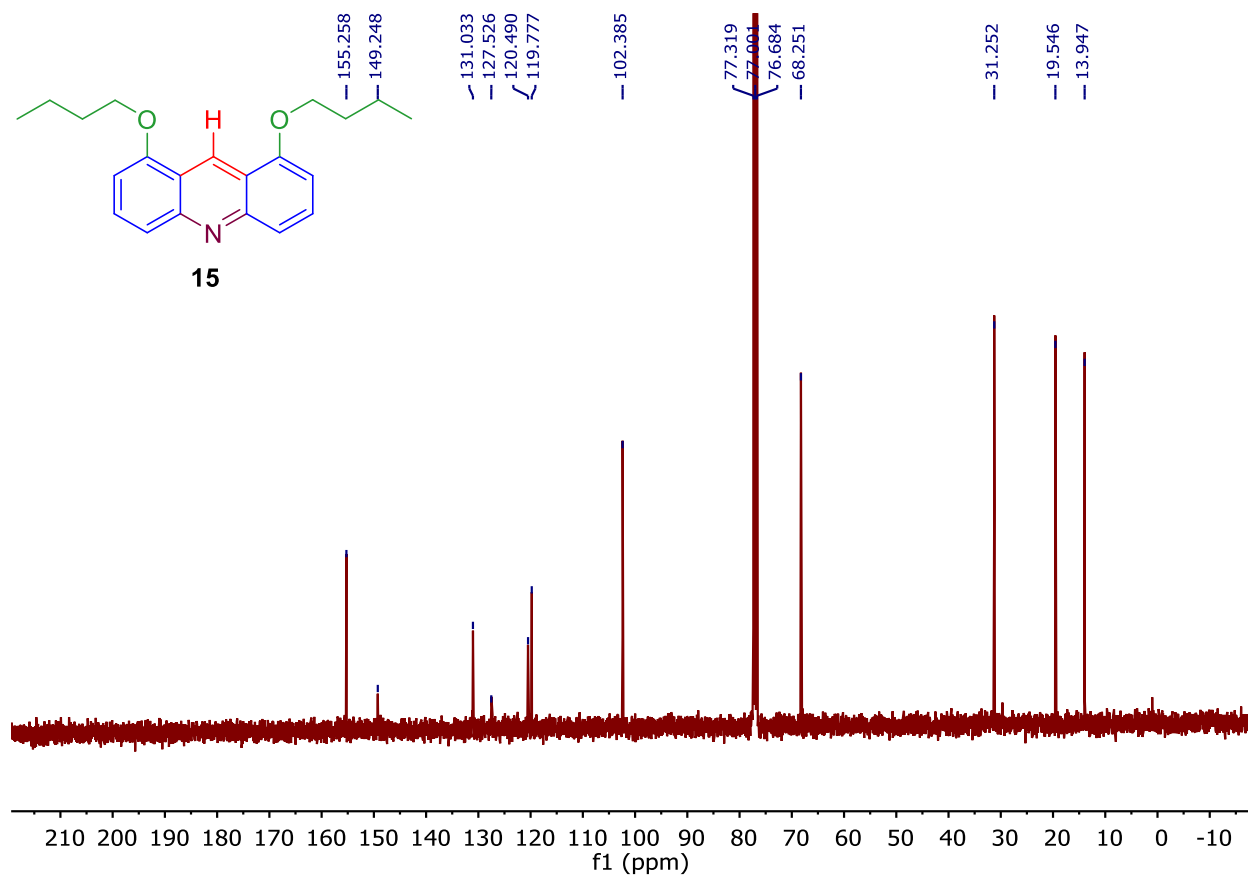


Figure S32. ^{13}C NMR spectrum of 1,8-dibutoxyacridine (15).

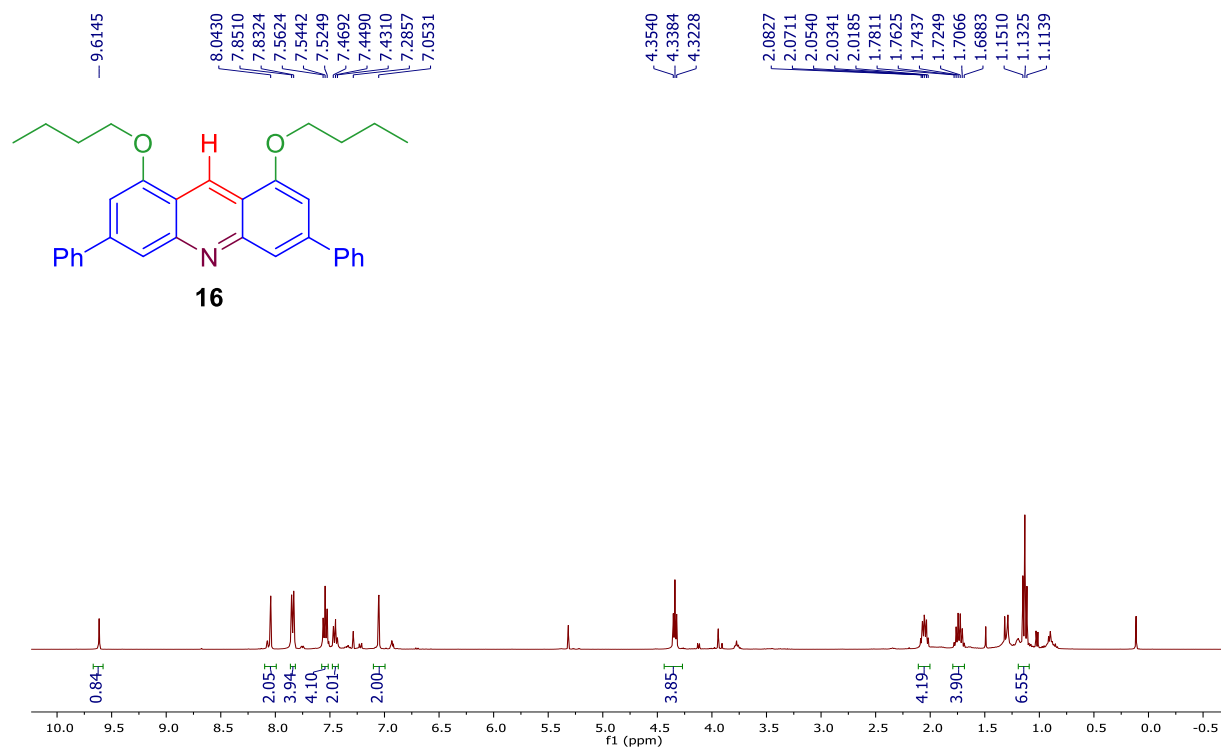


Figure S33. ^1H NMR spectrum of 1,8-dibutoxy-3,6-diphenylacridine (16).

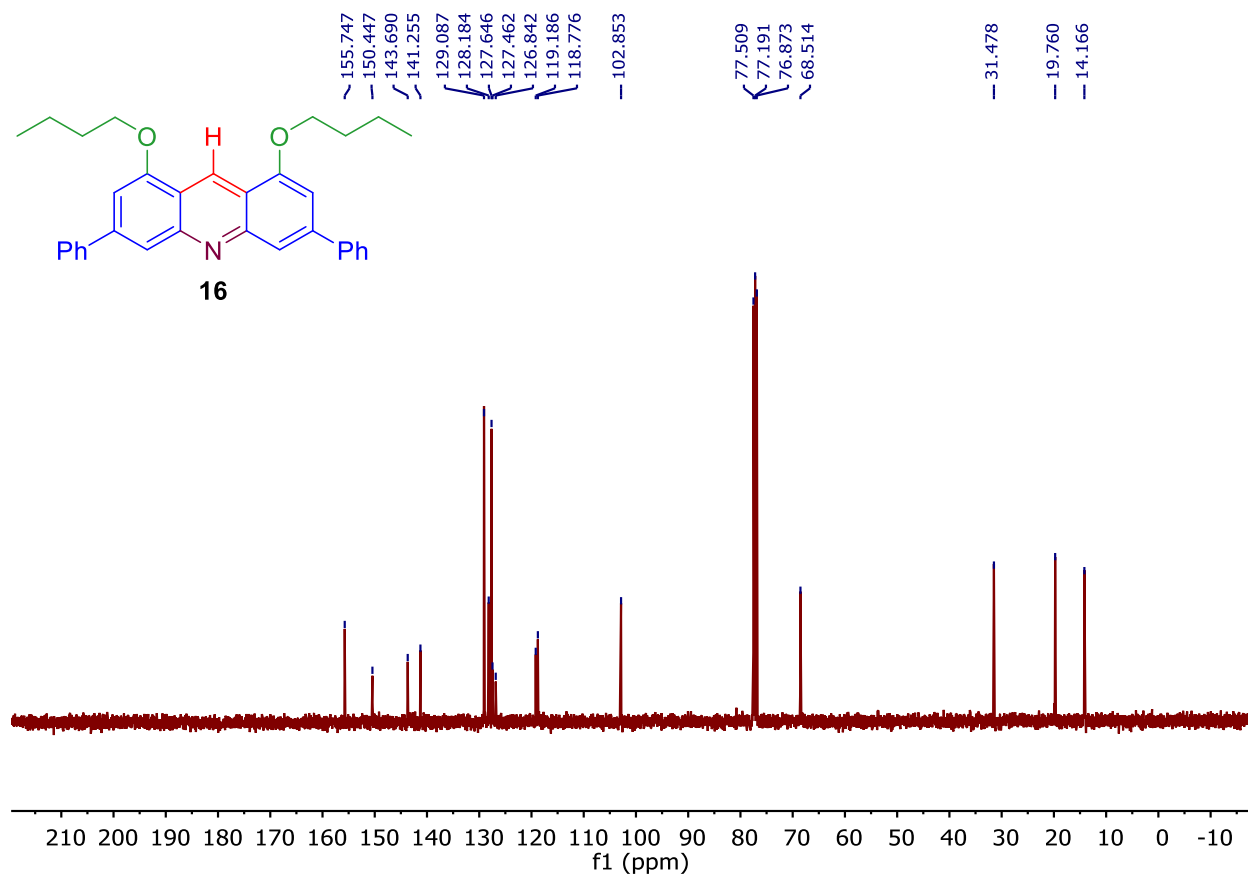


Figure S34. ^{13}C NMR spectrum of 1,8-dibutoxy-3,6-diphenylacridine (16).

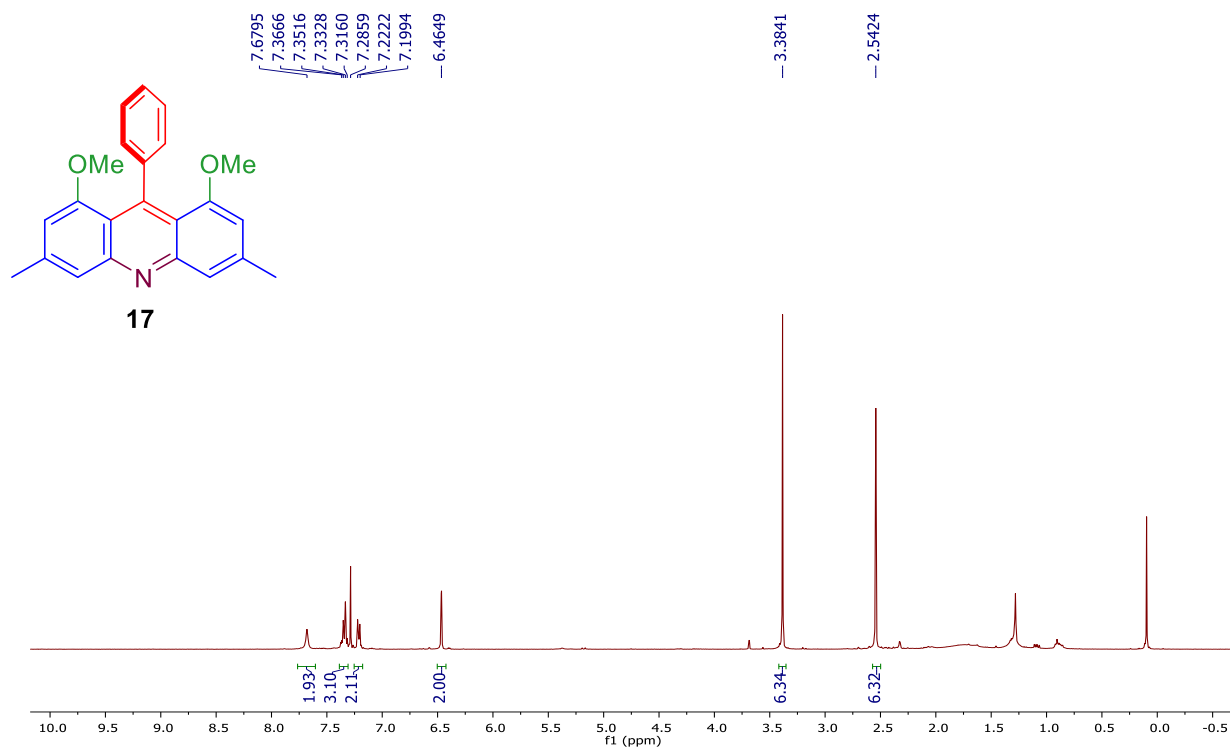


Figure S35. ^1H NMR spectrum of 1,8-dimethoxy-3,6-dimethyl-9-phenylacridine (17).

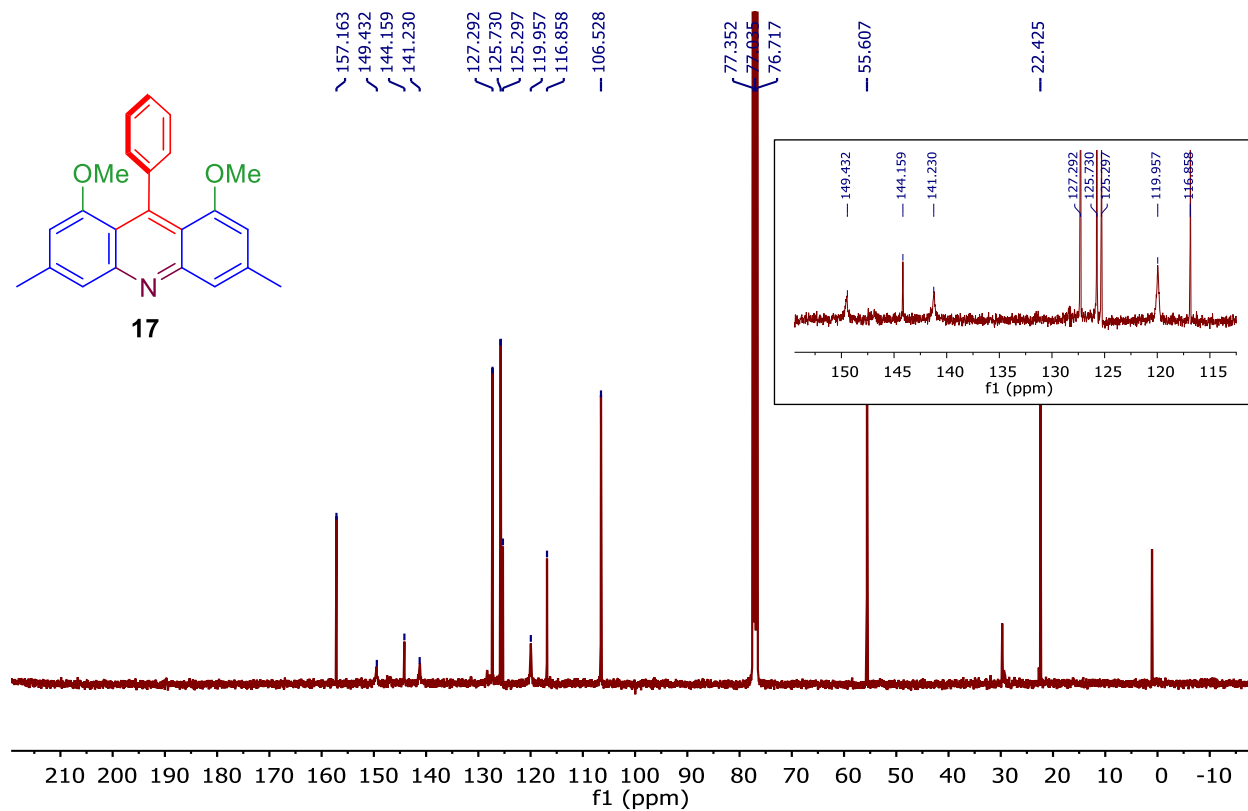


Figure S36. ^{13}C NMR spectrum of 1,8-dimethoxy-3,6-dimethyl-9-phenylacridine (17).

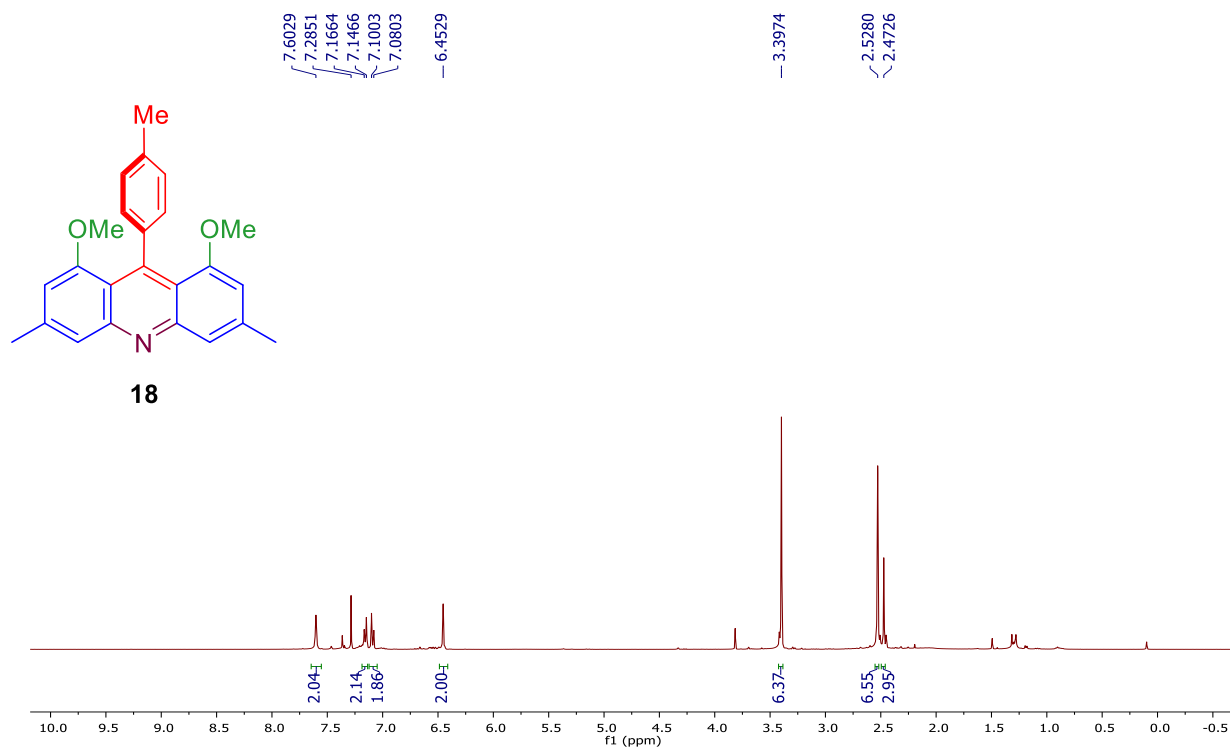


Figure S37. ¹H NMR spectrum of 1,8-dimethoxy-3,6-dimethyl-9-p-tolylacridine (18).

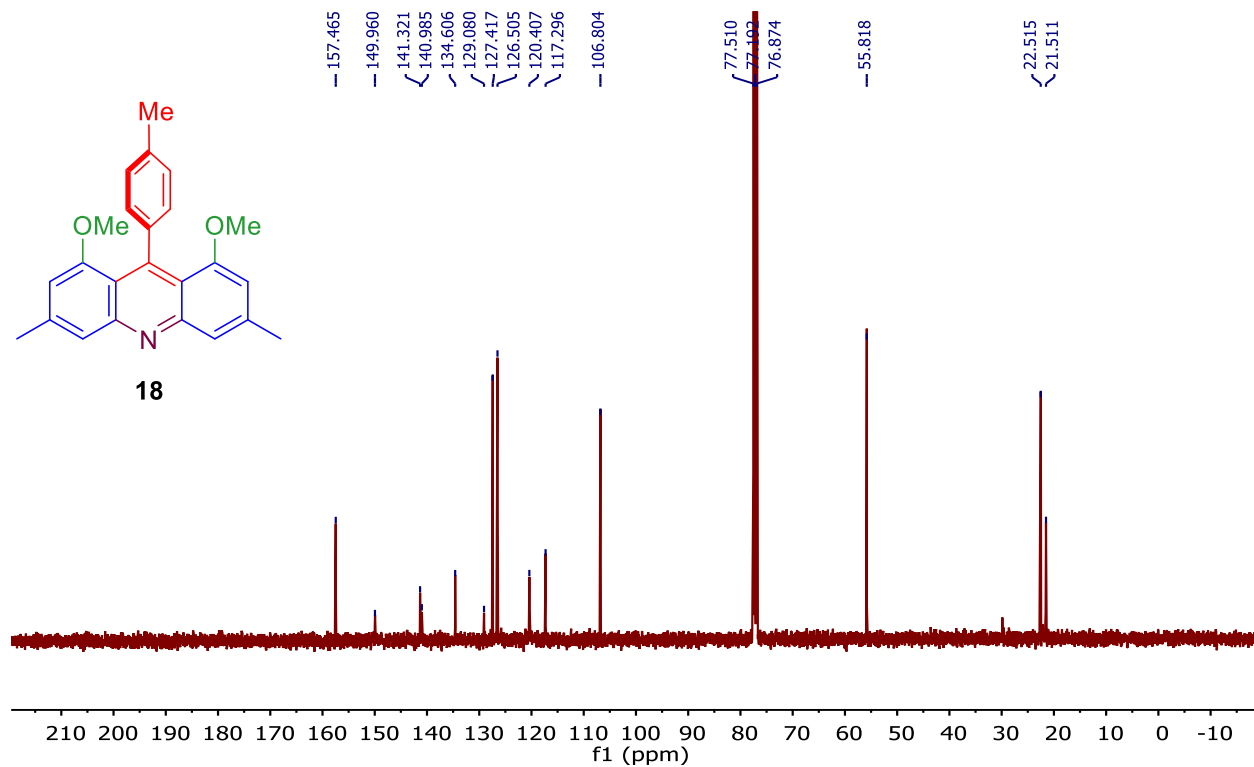


Figure S38. ¹³C NMR spectrum of 1,8-dimethoxy-3,6-dimethyl-9-p-tolylacridine (18).

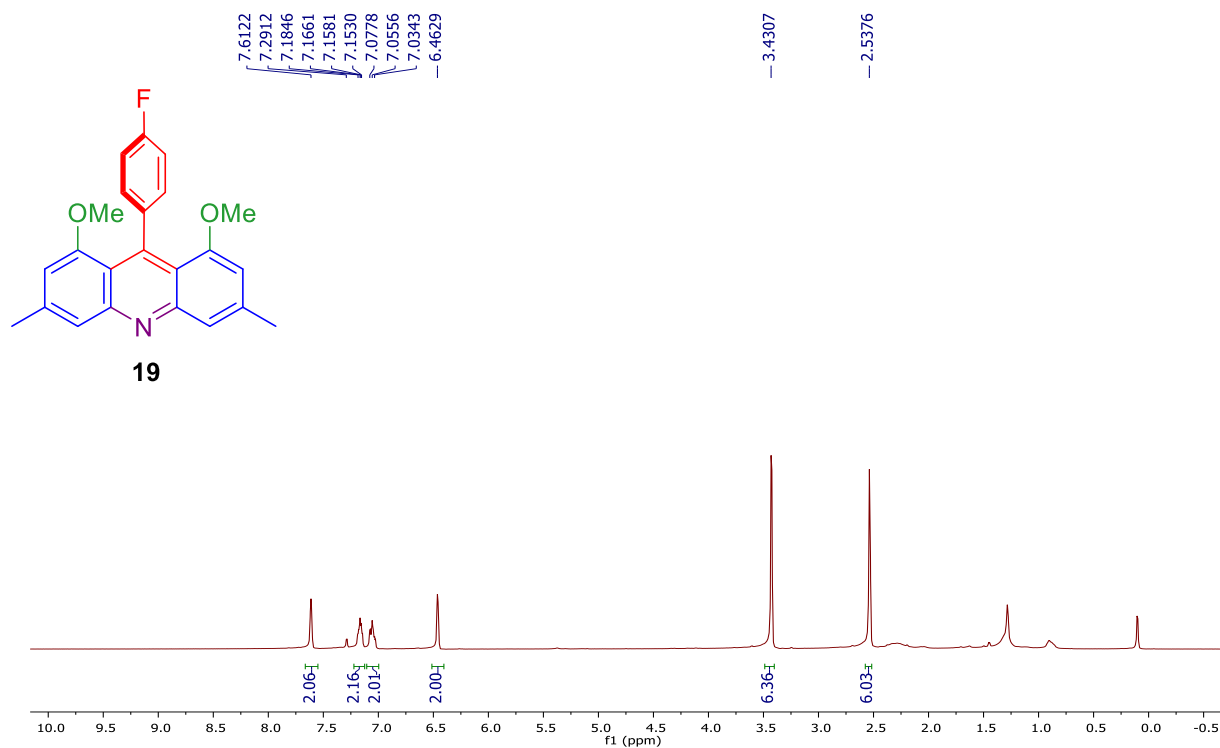


Figure S39. ^1H NMR spectrum of 9-(4-fluorophenyl)-1,8-dimethoxy-3,6-dimethylacridine (19).

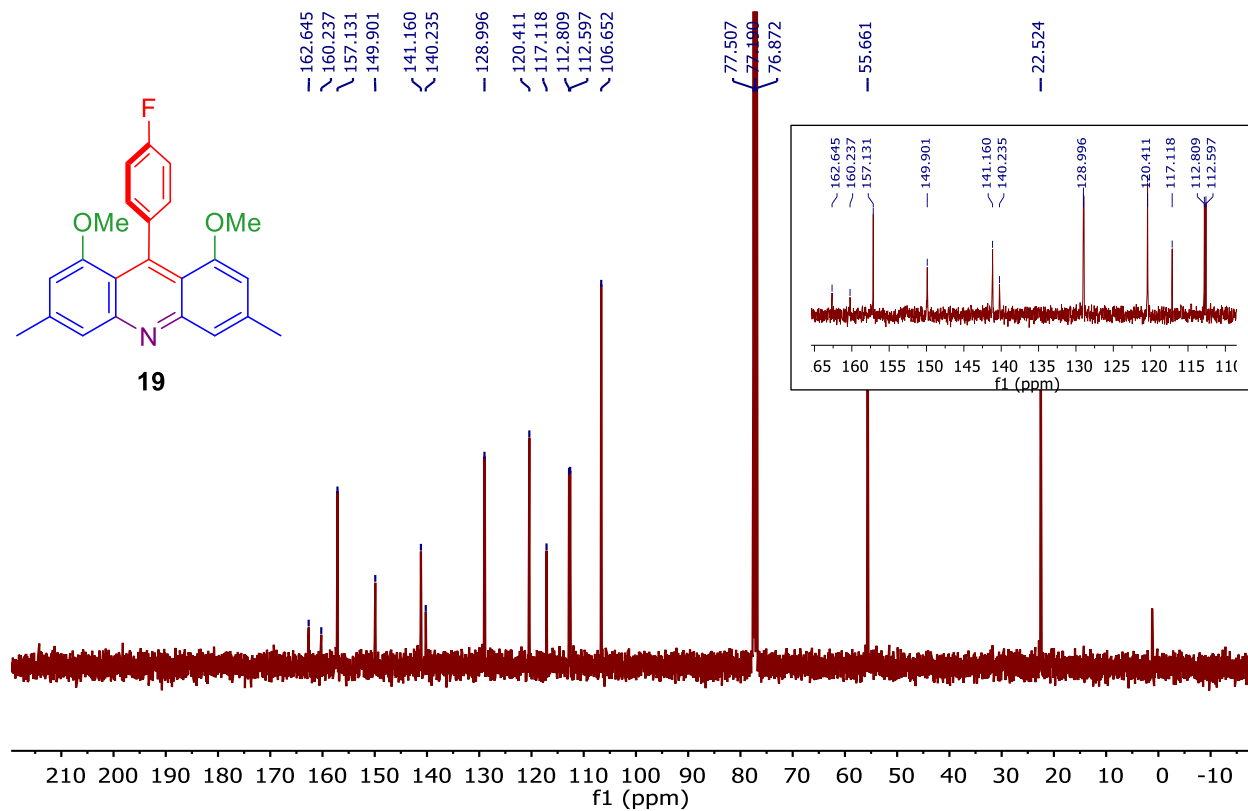


Figure S40. ^{13}C NMR spectrum of 9-(4-fluorophenyl)-1,8-dimethoxy-3,6-dimethylacridine (19).

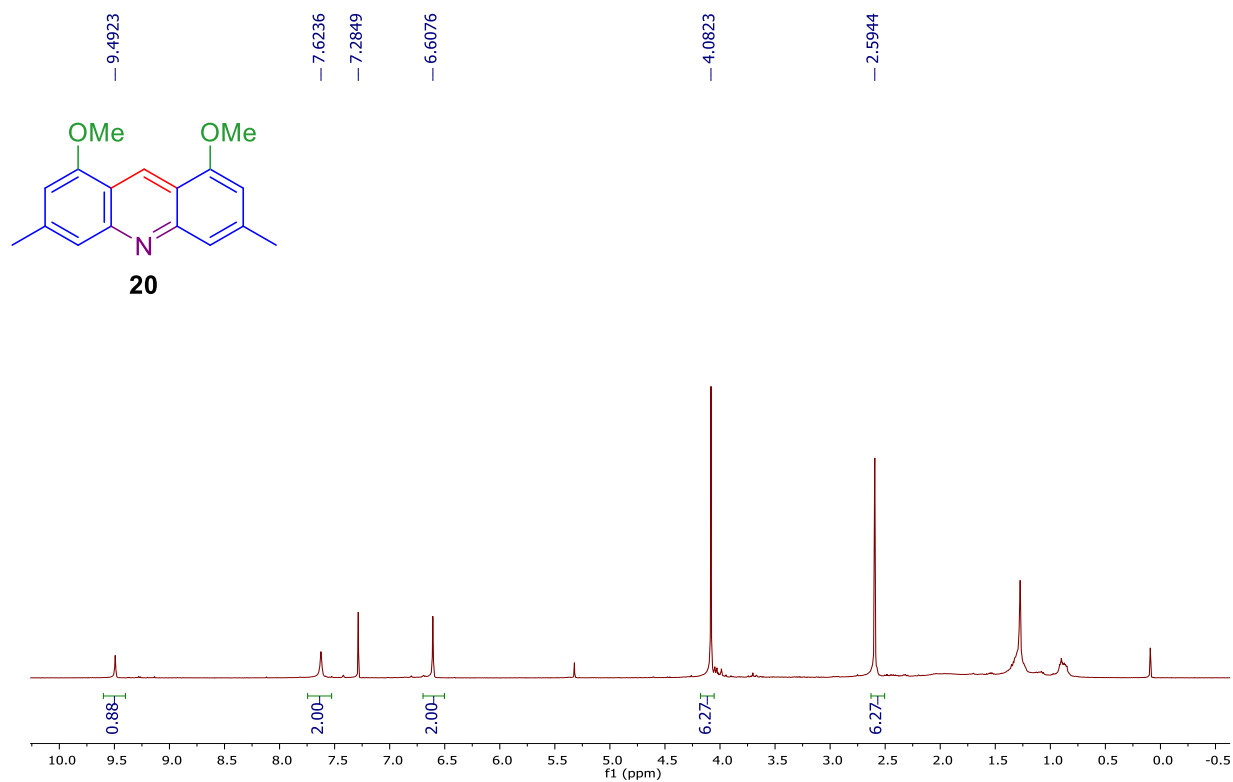


Figure S41. ^1H NMR spectrum of 1,8-dimethoxy-3,6-dimethylacridine (20).

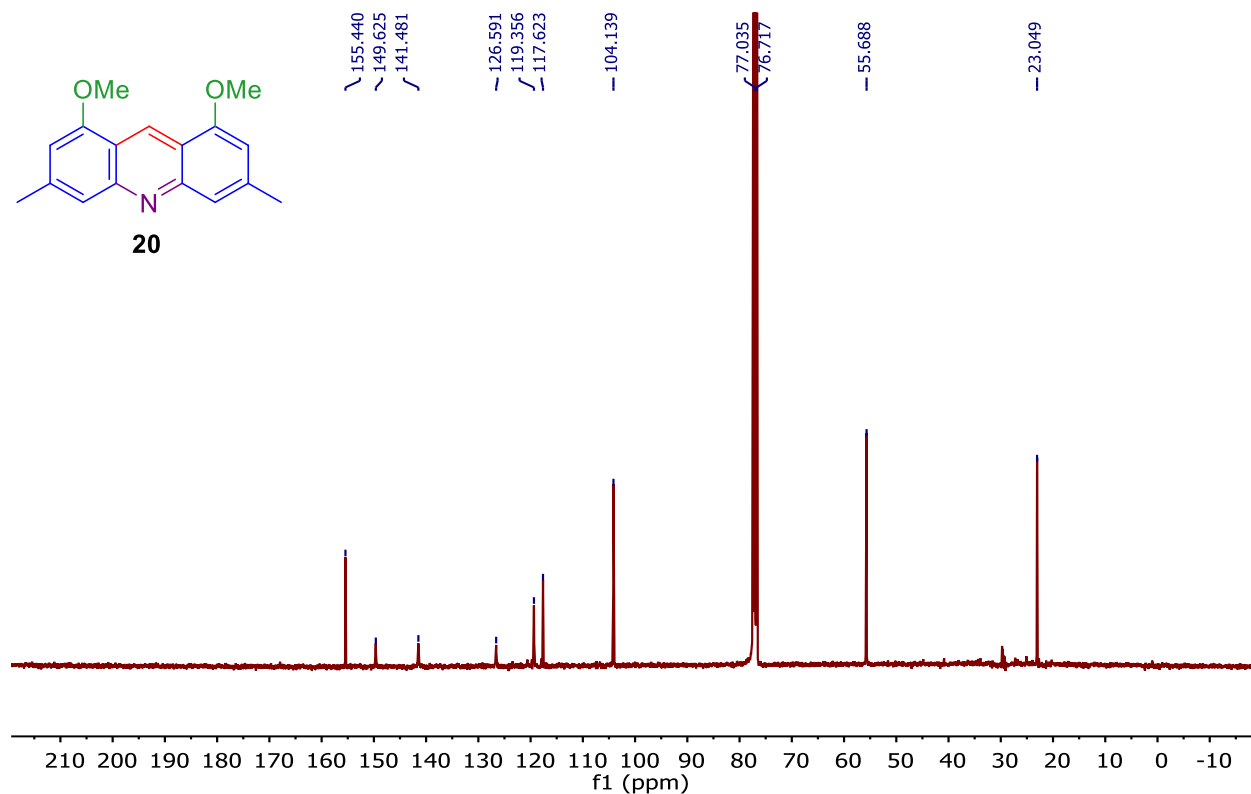


Figure S42. ^{13}C NMR spectrum of 1,8-dimethoxy-3,6-dimethylacridine (20).

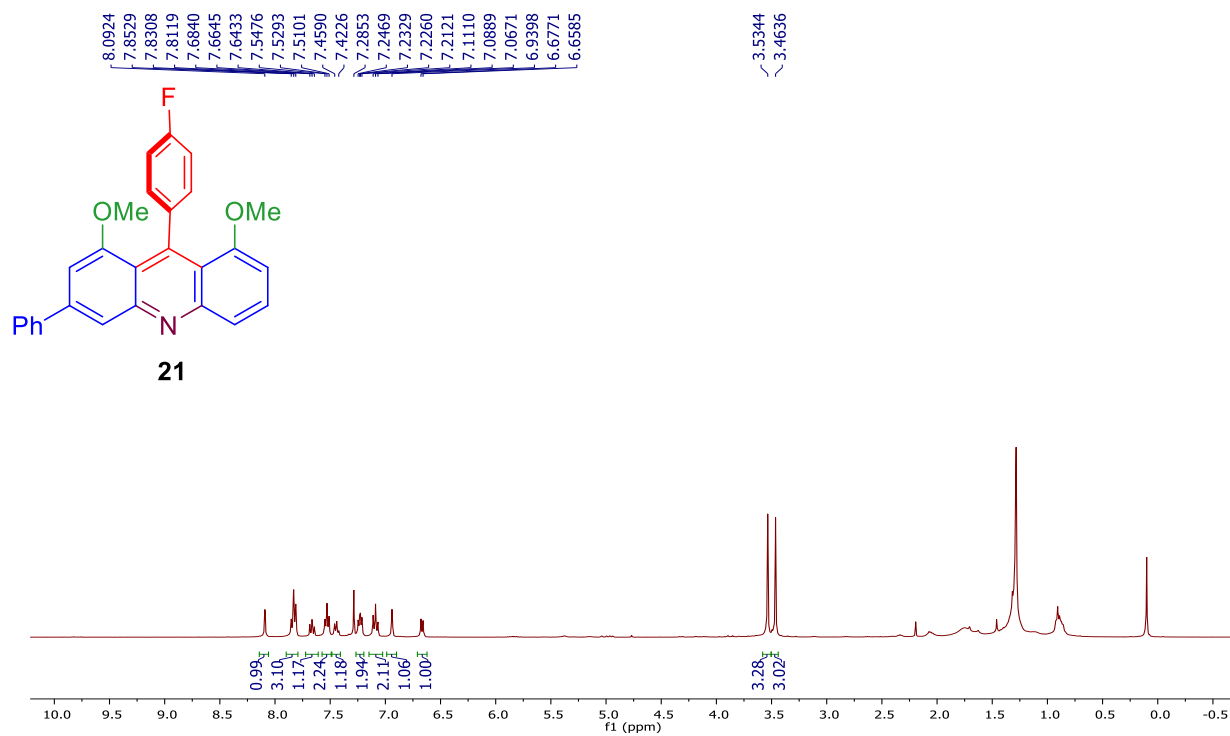


Figure S43. ¹H NMR spectrum of 9-(4-fluorophenyl)-1,8-dimethoxy-3-phenylacridine (21).

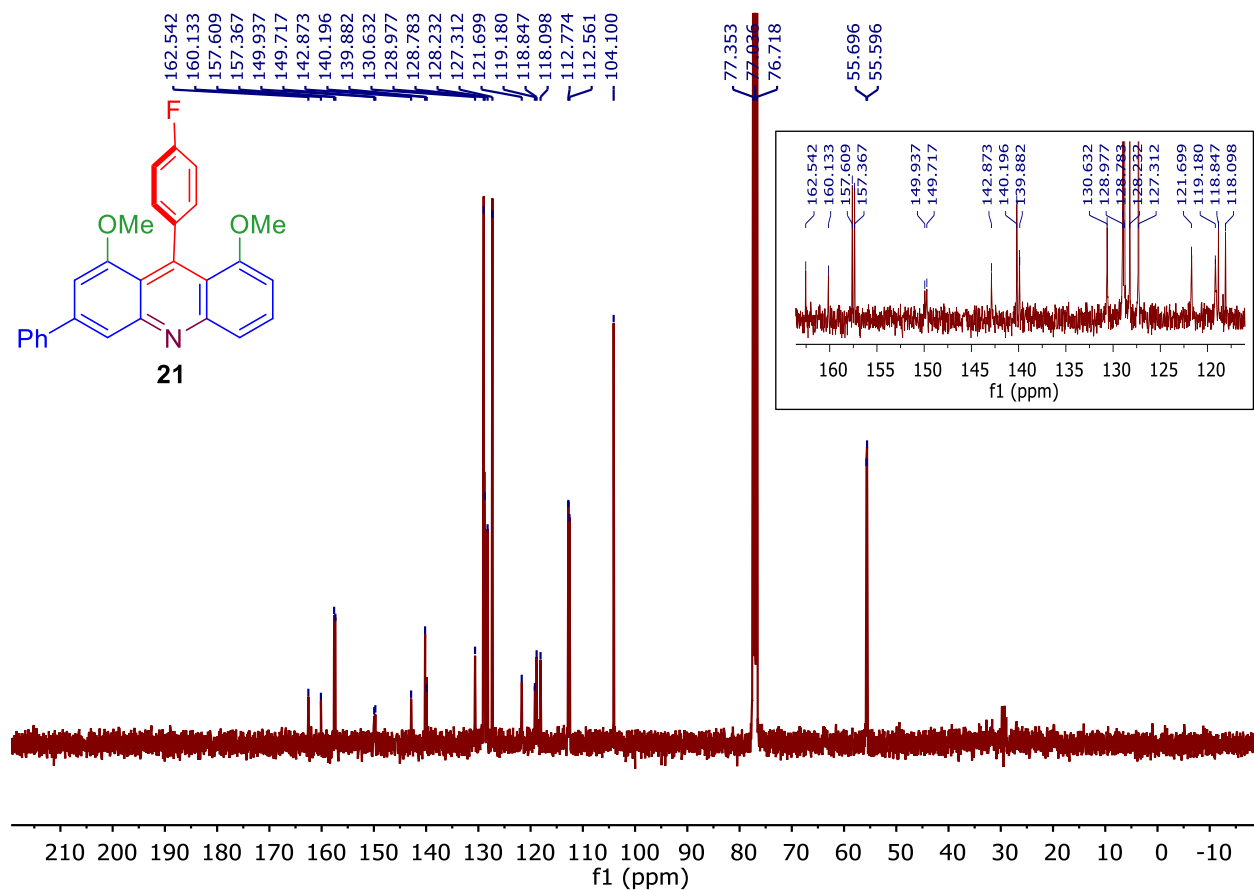


Figure S44. ¹³C NMR spectrum of 9-(4-fluorophenyl)-1,8-dimethoxy-3-phenylacridine (21).

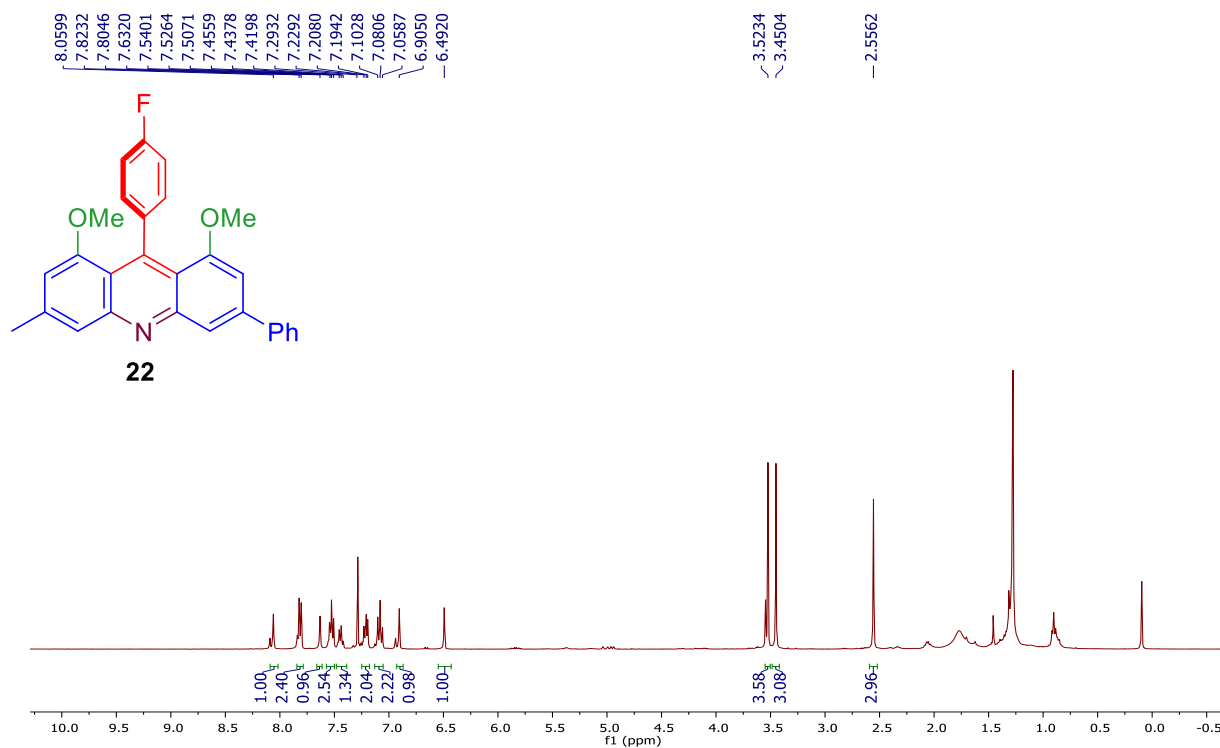


Figure S45. ^1H NMR spectrum of 9-(4-fluorophenyl)-1,8-dimethoxy-3-methyl-6-phenylacridine (22).

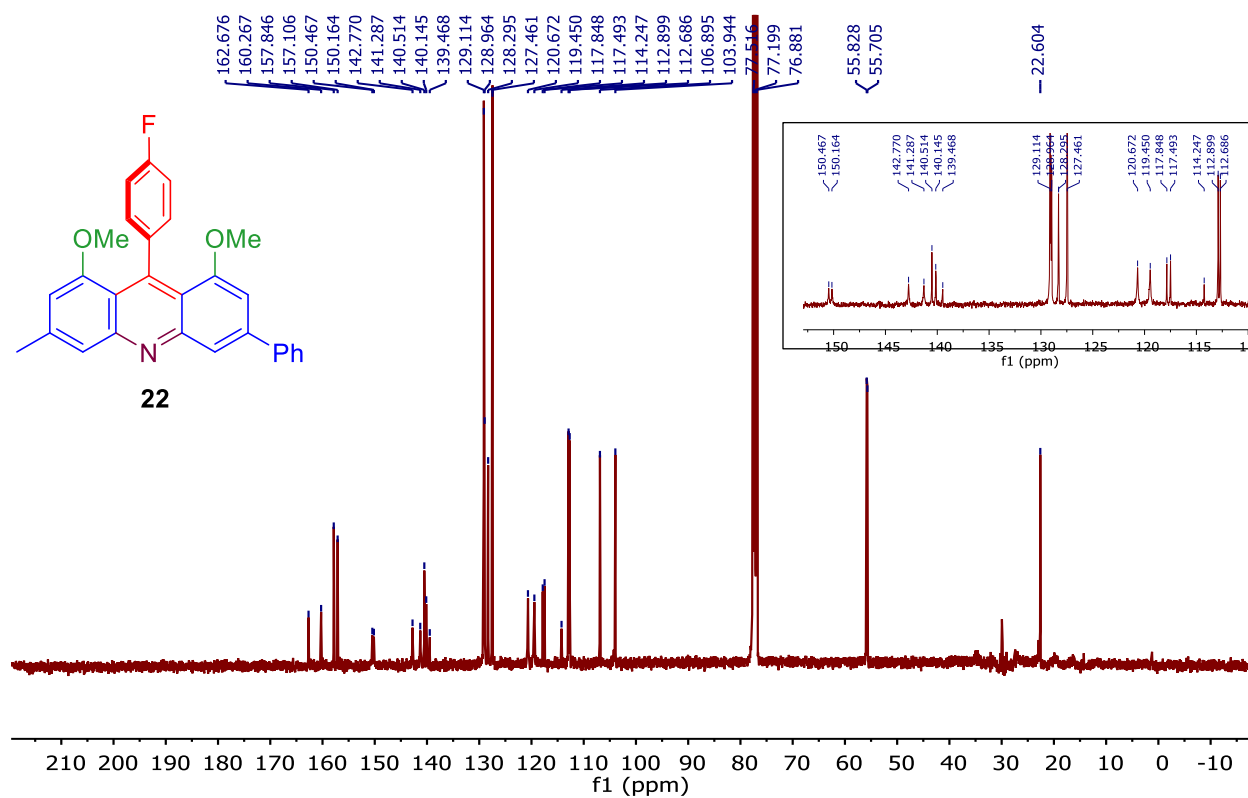


Figure S46. ^{13}C NMR spectrum of 9-(4-fluorophenyl)-1,8-dimethoxy-3-methyl-6-phenylacridine (22).

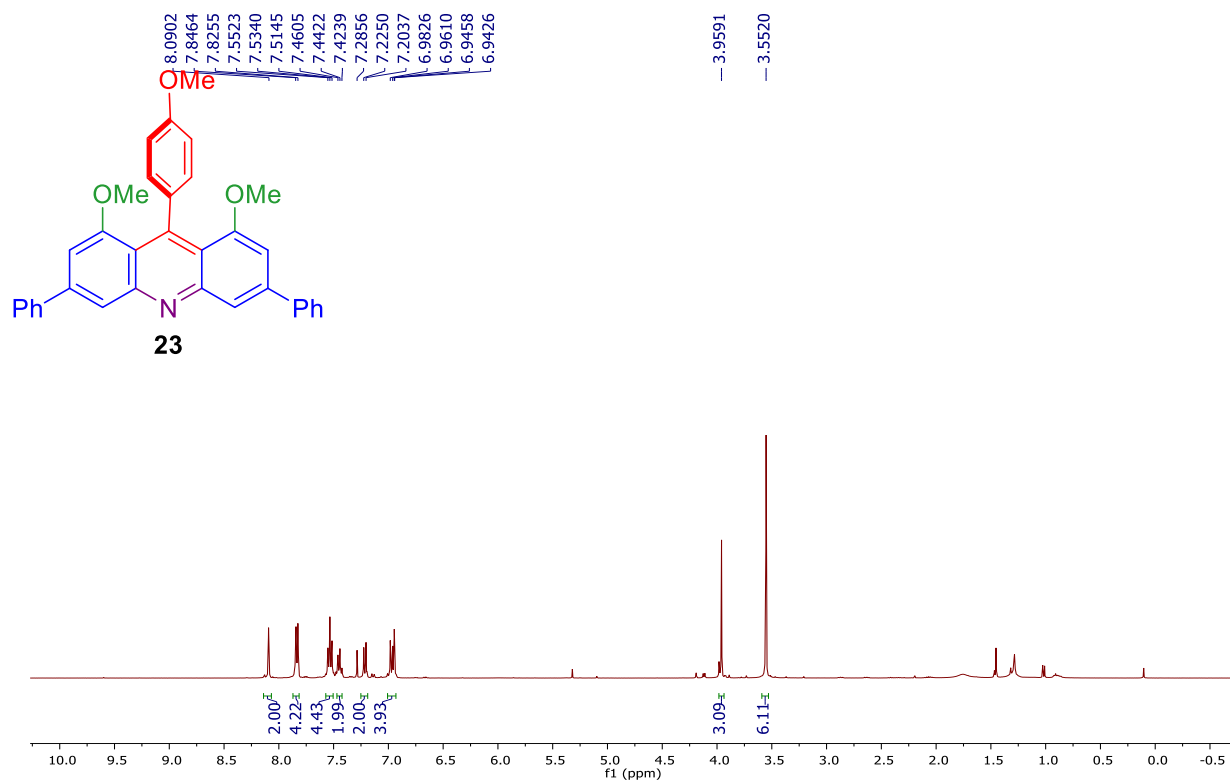


Figure S47. ¹H NMR spectrum of 1,8-dimethoxy-9-(4-methoxyphenyl)-3,6-diphenylacridine (23).

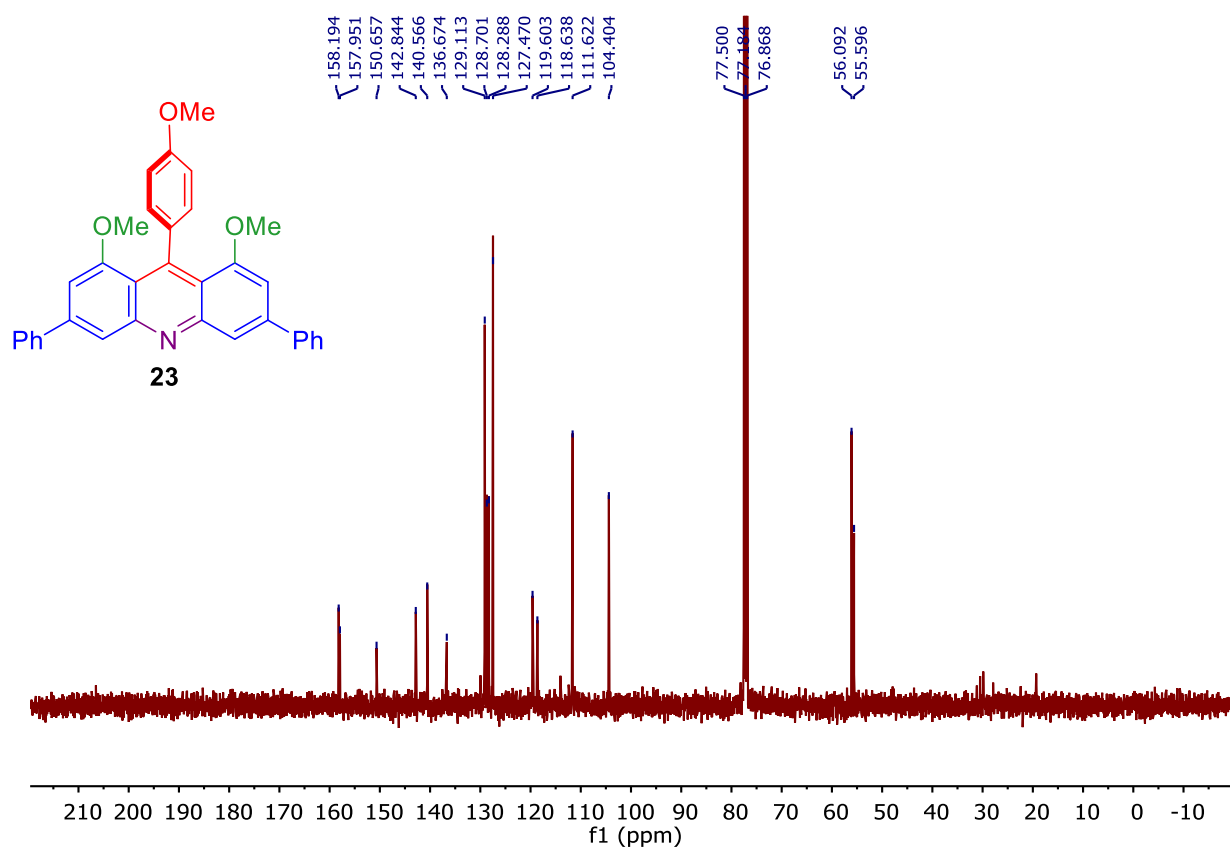


Figure S48. ¹³C NMR spectrum of 1,8-dimethoxy-9-(4-methoxyphenyl)-3,6-diphenylacridine (23).

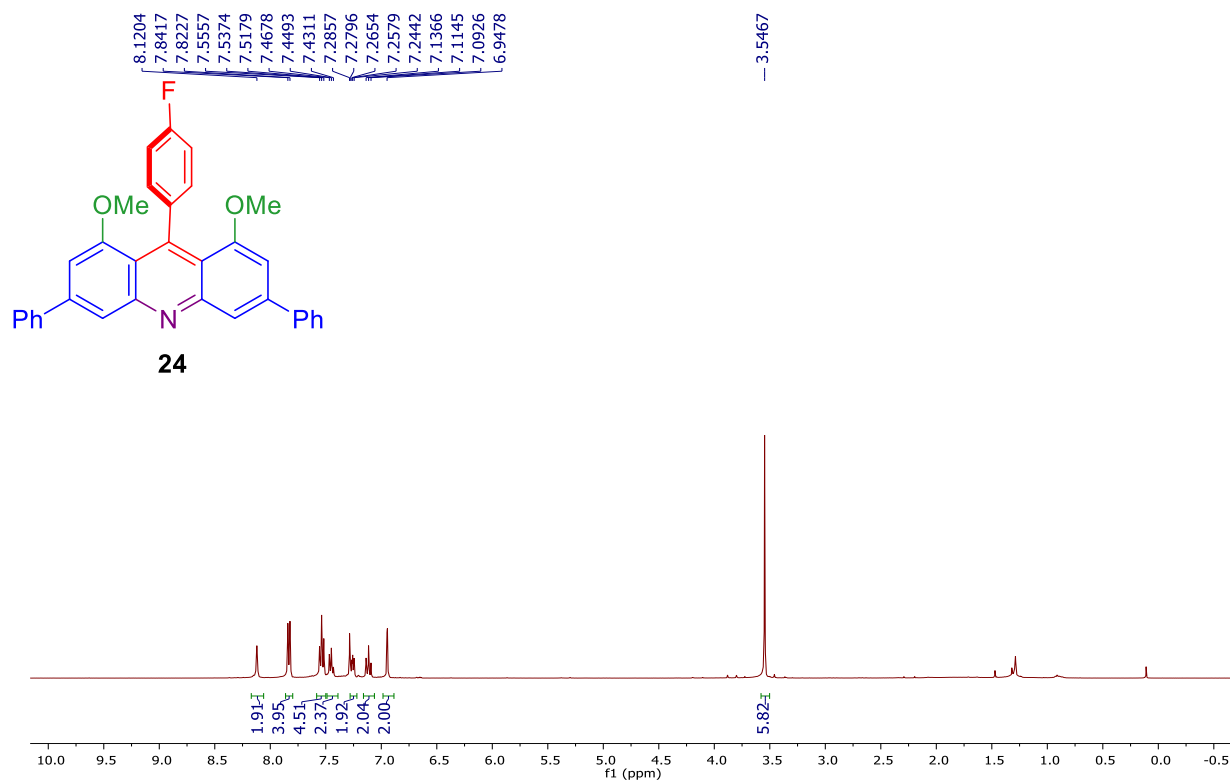


Figure S49. ^1H NMR spectrum of 9-(4-fluorophenyl)-1,8-dimethoxy-3,6-diphenylacridine (24).

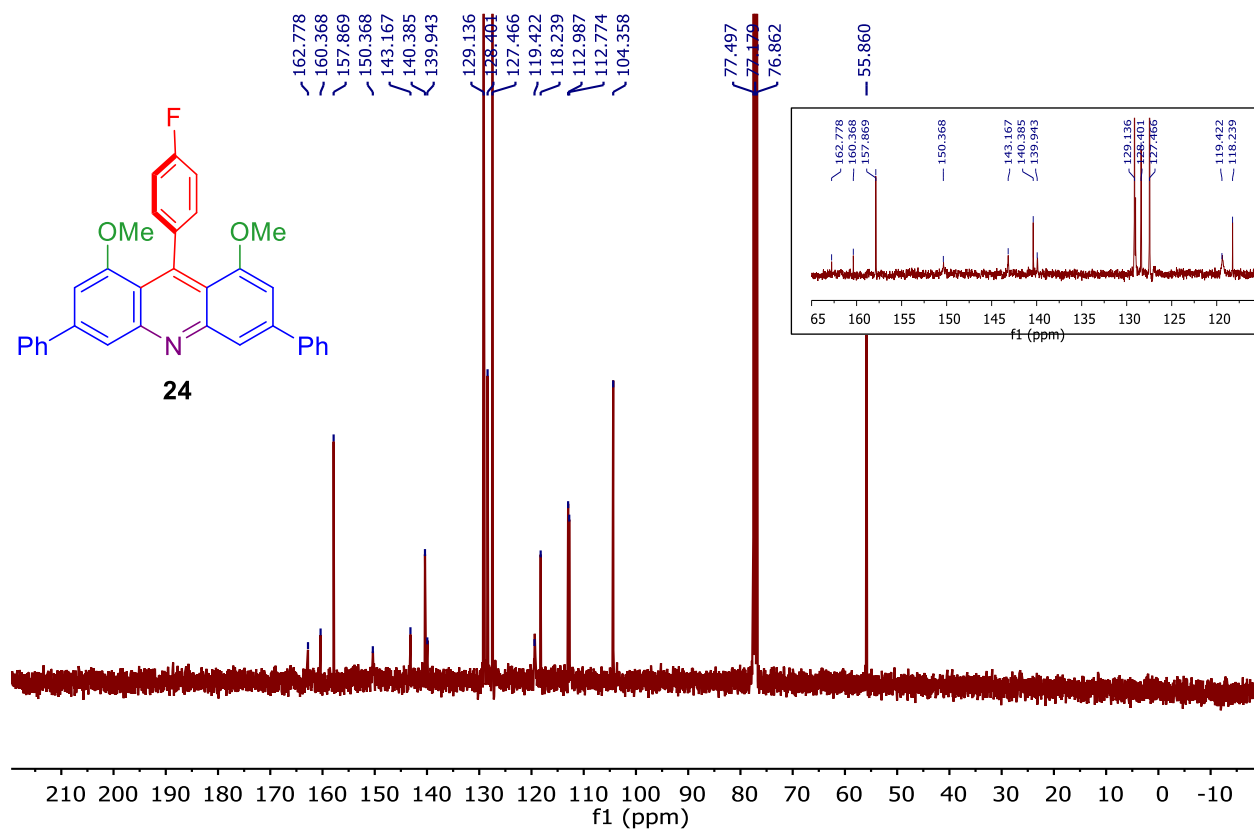


Figure S50. ^{13}C NMR spectrum of 9-(4-fluorophenyl)-1,8-dimethoxy-3,6-diphenylacridine (24).

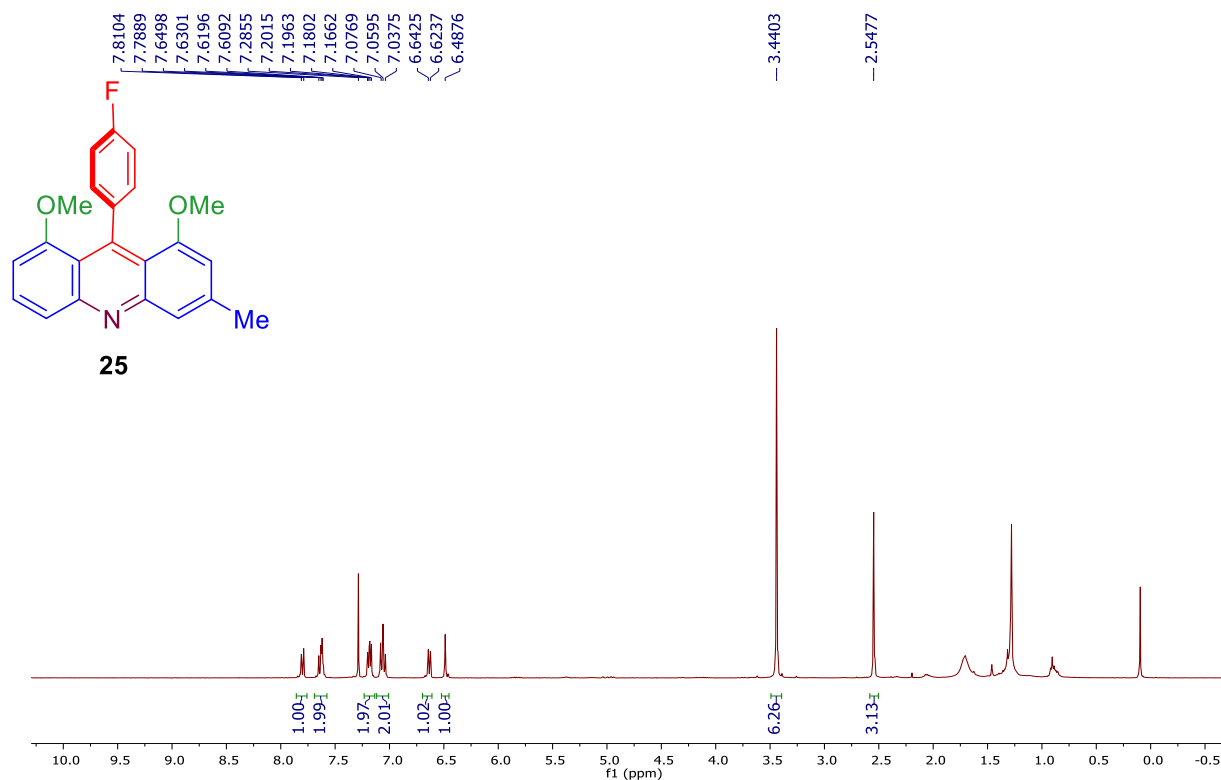


Figure S51. ¹H NMR spectrum of 9-(4-fluorophenyl)-1,8-dimethoxy-3-methylacridine (25).

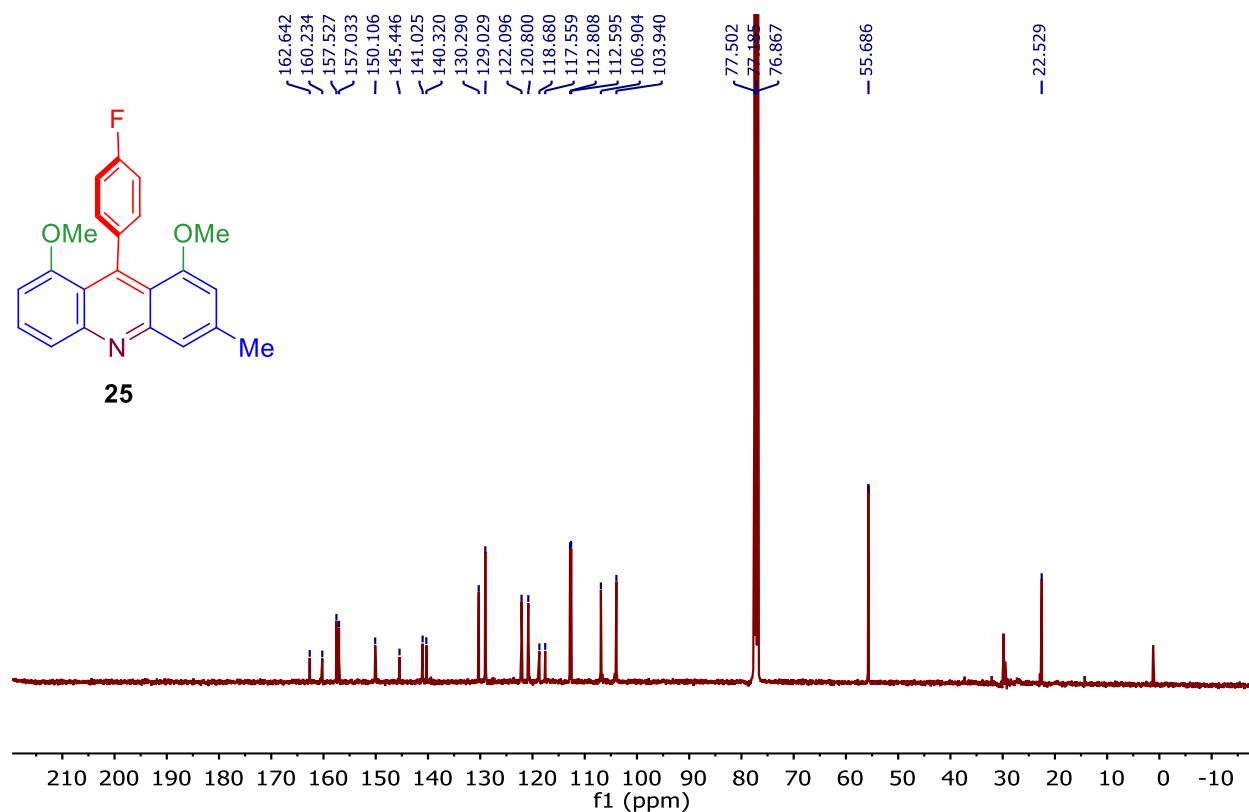


Figure S52. ¹³C NMR spectrum of 9-(4-fluorophenyl)-1,8-dimethoxy-3-methylacridine (25)

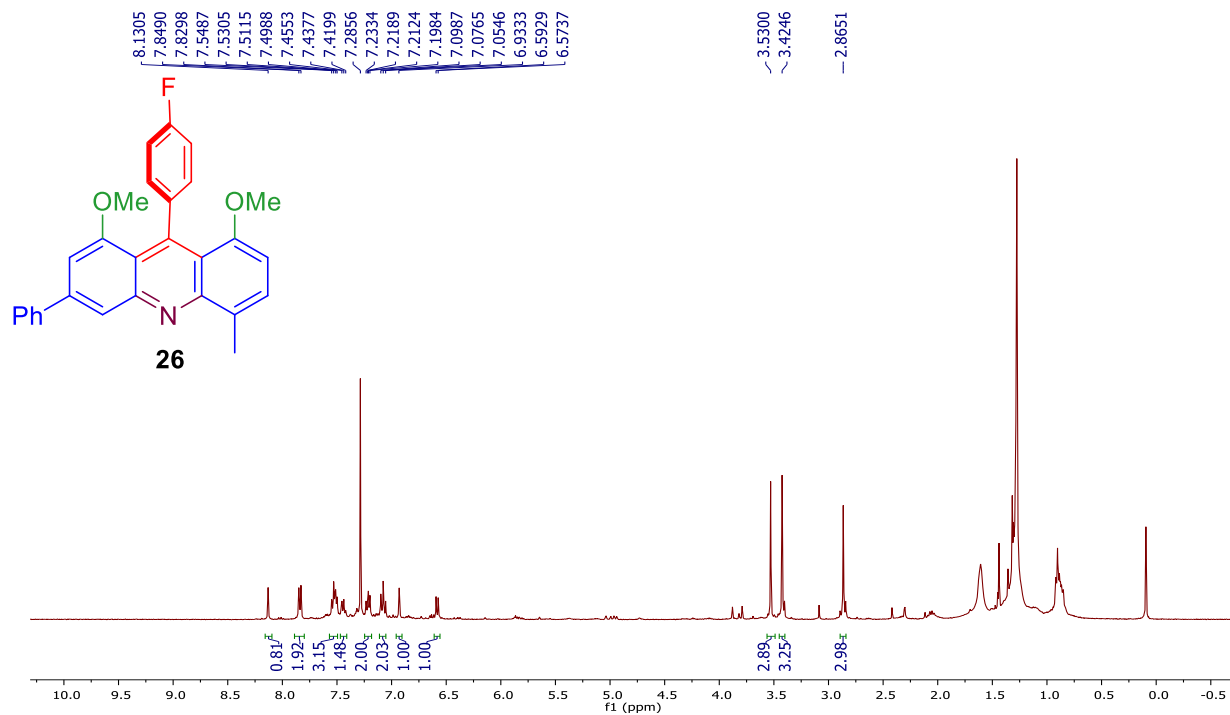


Figure S53. ¹H NMR spectrum of 9-(4-fluorophenyl)-1,8-dimethoxy-5-methyl-3-phenylacridine (26).

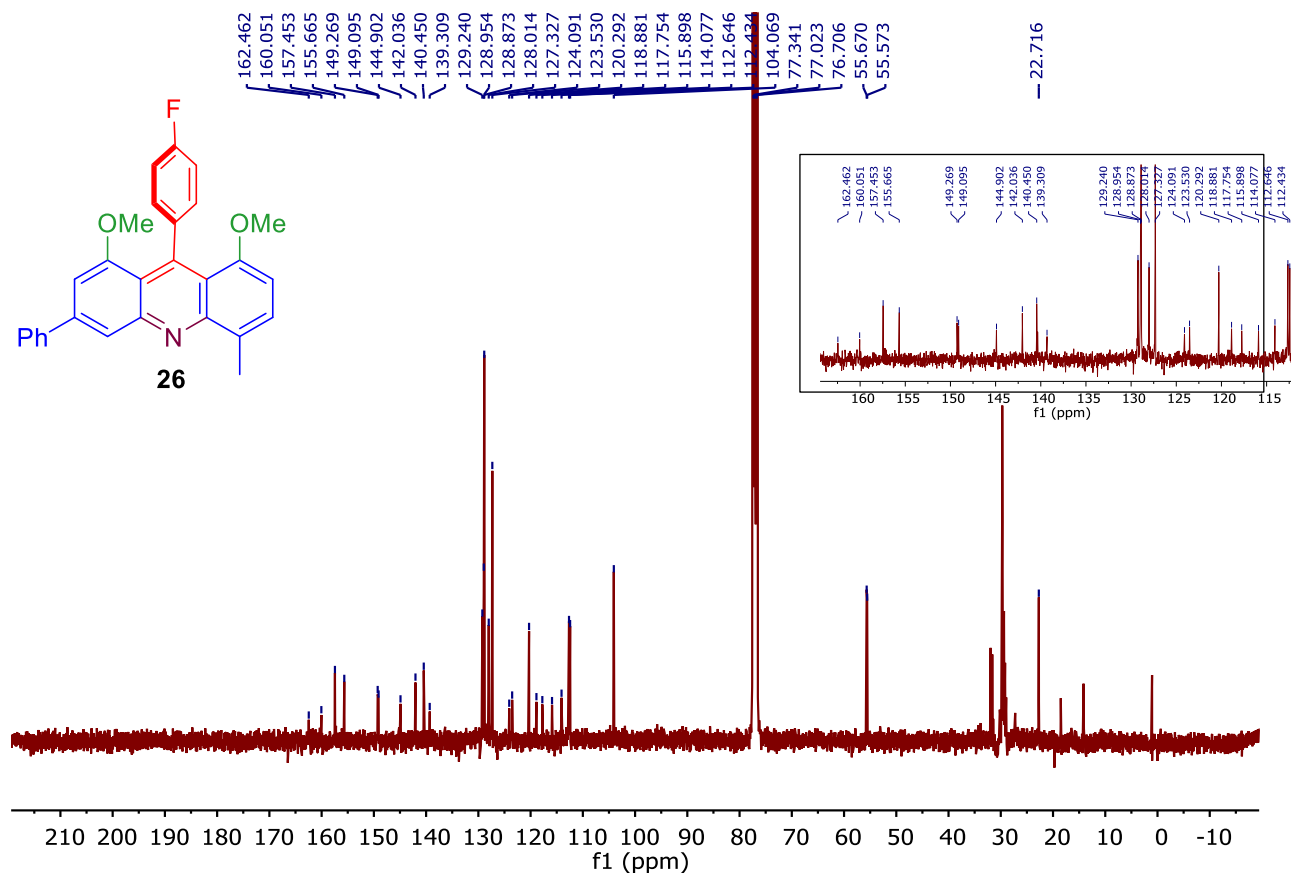


Figure S54. ¹³C NMR spectrum of 9-(4-fluorophenyl)-1,8-dimethoxy-5-methyl-3-phenylacridine (26).

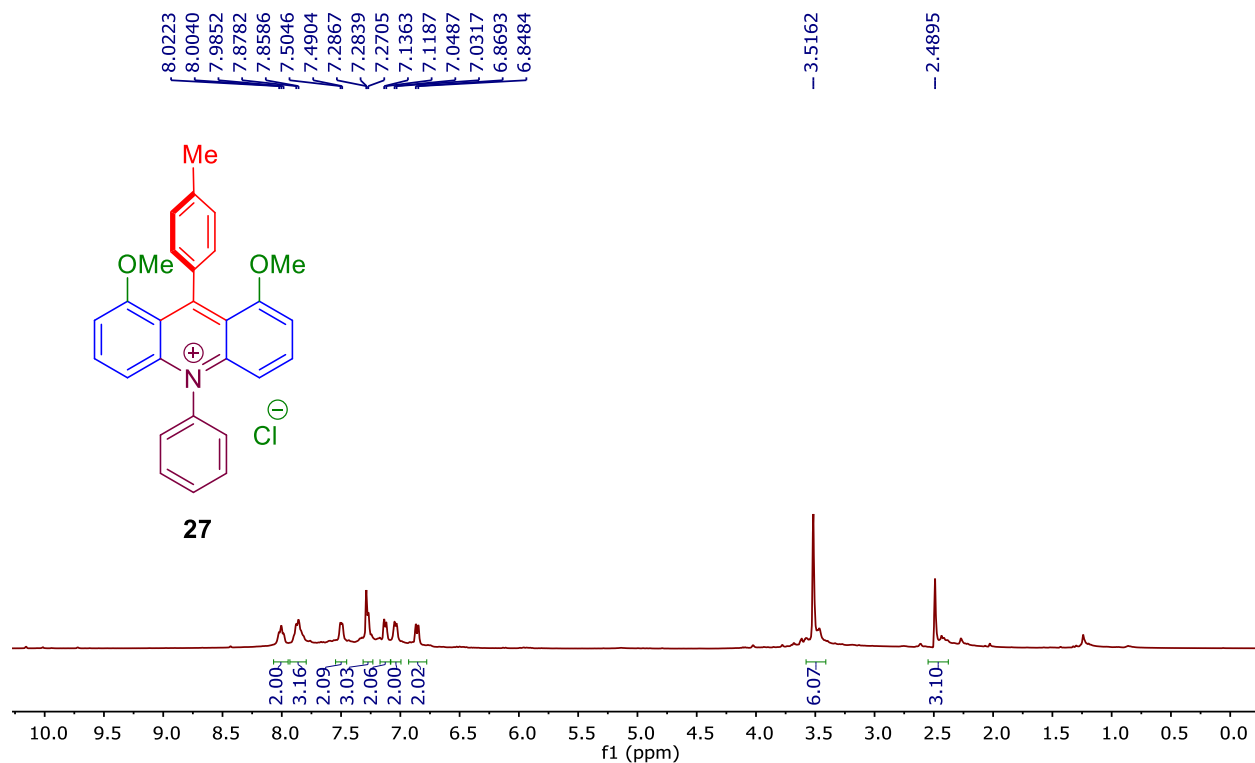


Figure S55. ¹H NMR (CDCl₃, 400MHz) spectrum of 1,8-dimethoxy-10-phenyl-9-(p-tolyl)acridin-10-ium chloride (27)

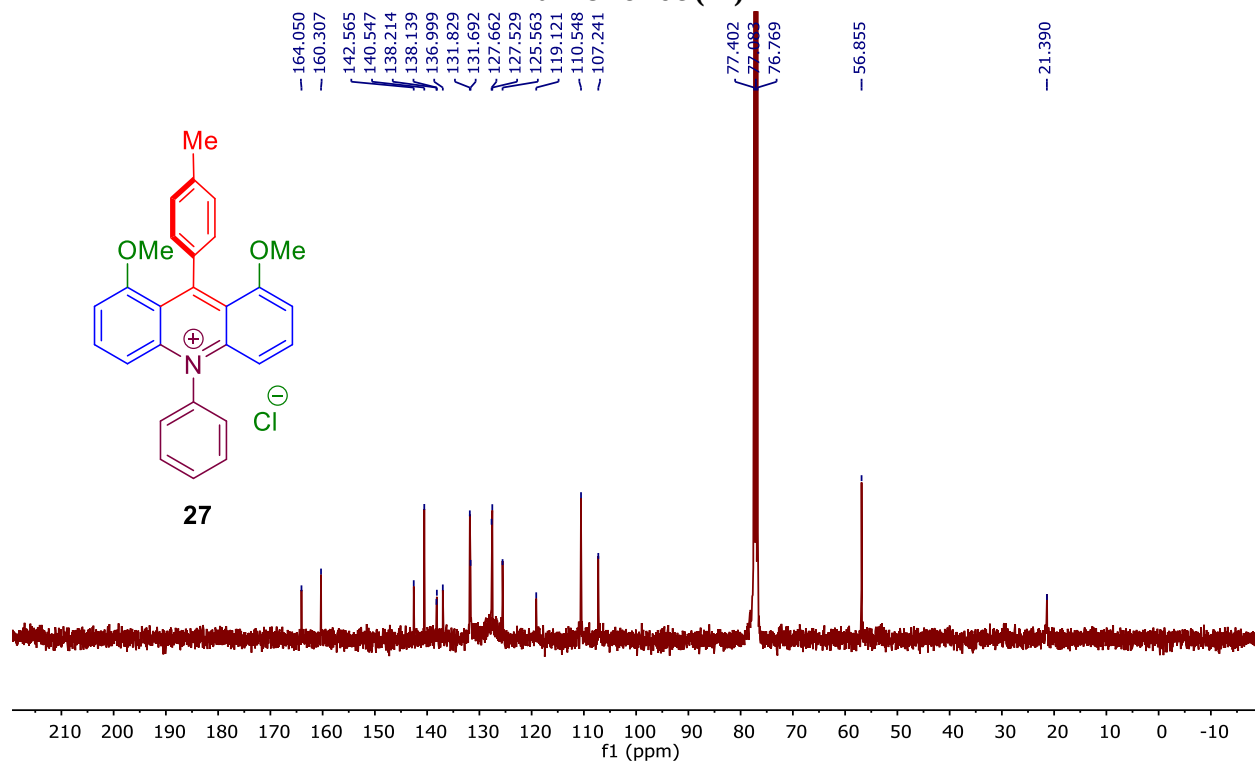


Figure S56. ¹³C NMR (CDCl₃, 100MHz) spectrum of 1,8-dimethoxy-10-phenyl-9-(p-tolyl)acridin-10-ium chloride (27)

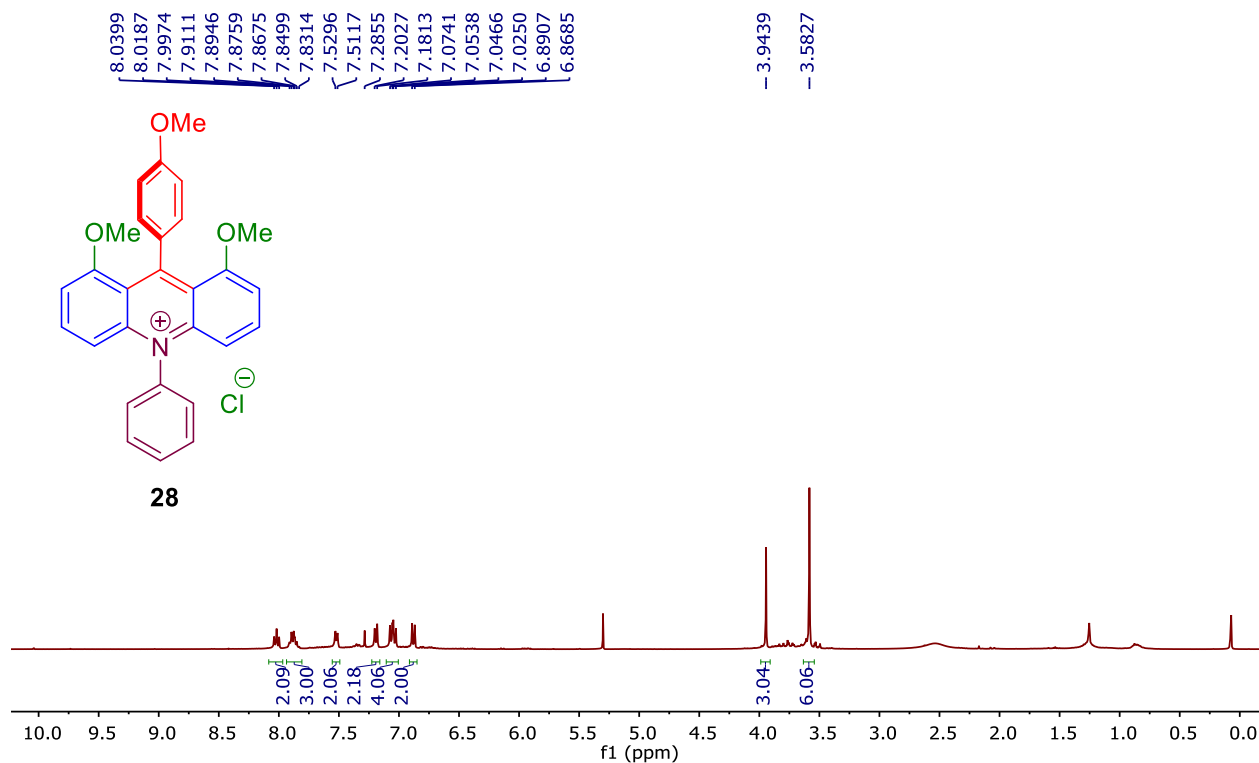


Figure S57. ¹H NMR (CDCl₃, 400MHz) spectrum of 1,8-dimethoxy-9-(4-methoxyphenyl)-10-phenylacridin-10-ium chloride (28)

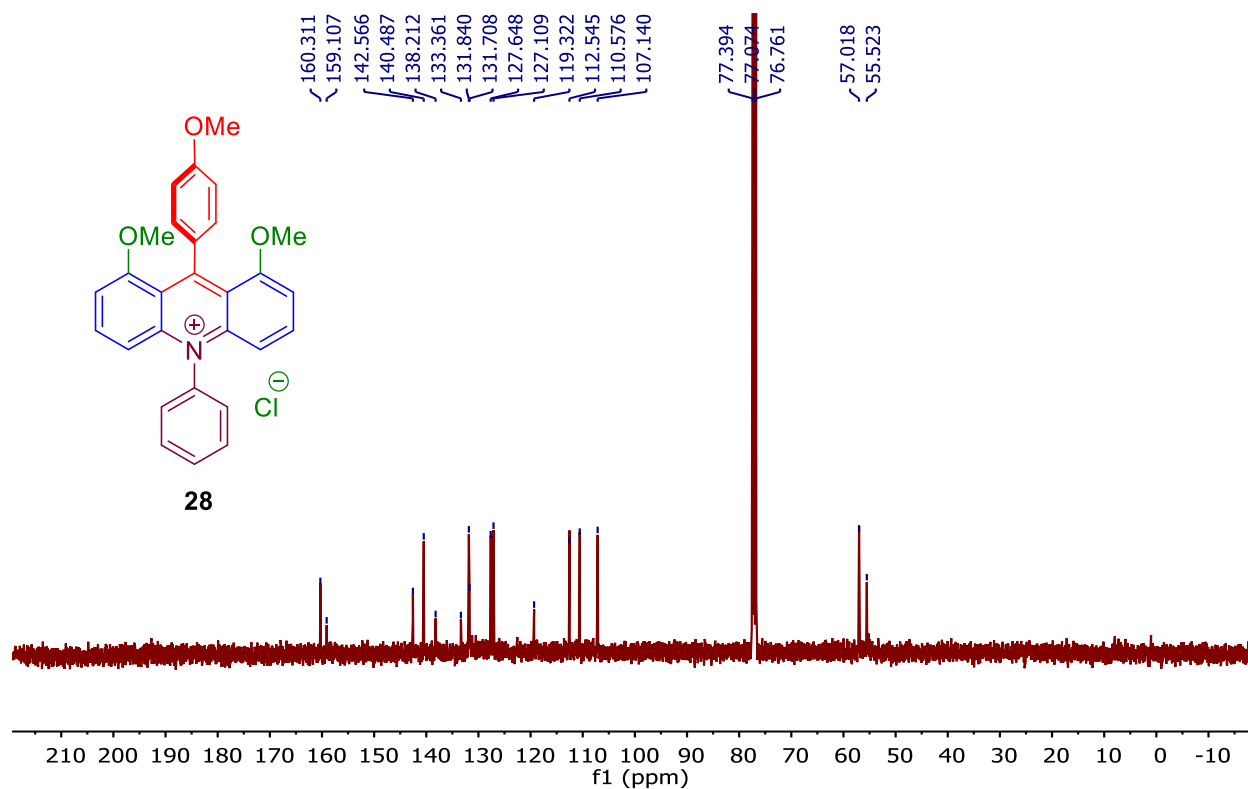


Figure S58. ¹³C NMR (CDCl₃, 100MHz) spectrum of 1,8-dimethoxy-9-(4-methoxyphenyl)-10-phenylacridin-10-ium chloride (28)

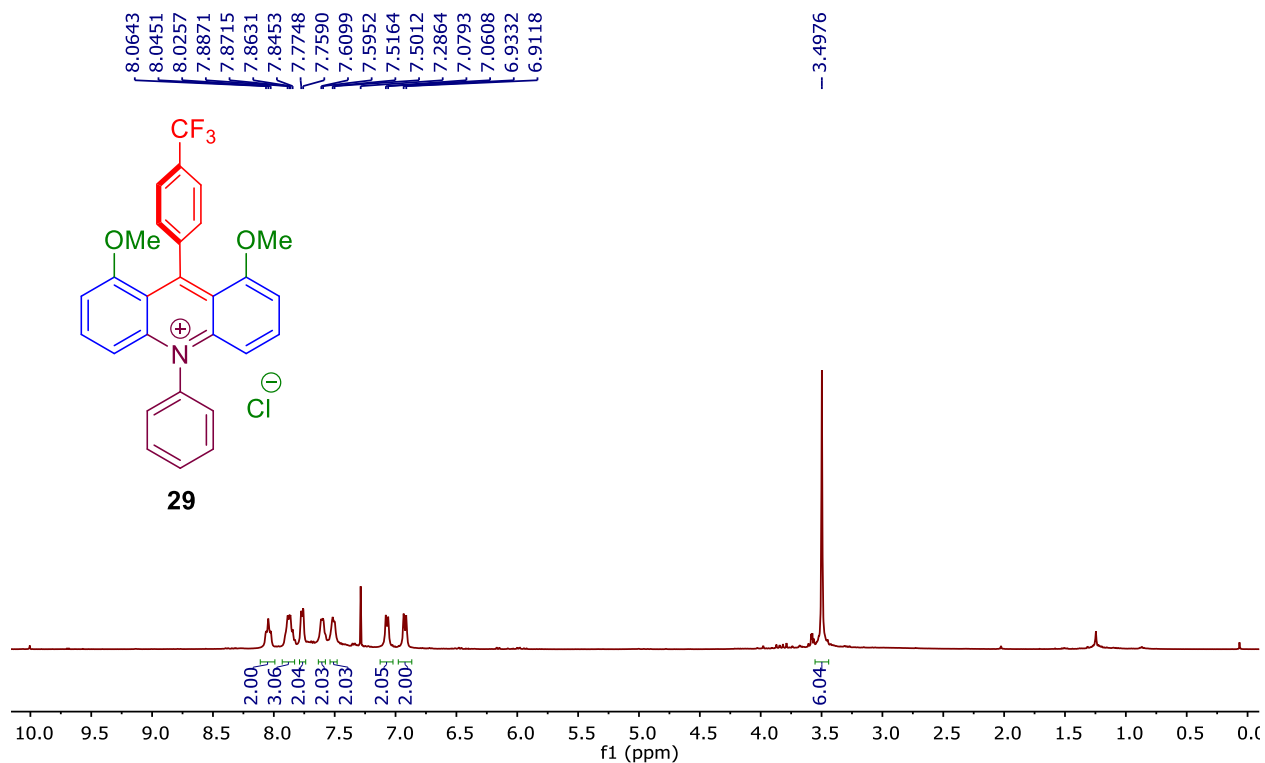


Figure S59. ¹H NMR (CDCl₃, 400MHz) spectrum of 1,8-dimethoxy-10-phenyl-9-(4-(trifluoromethyl)phenyl)acridin-10-ium chloride (29)

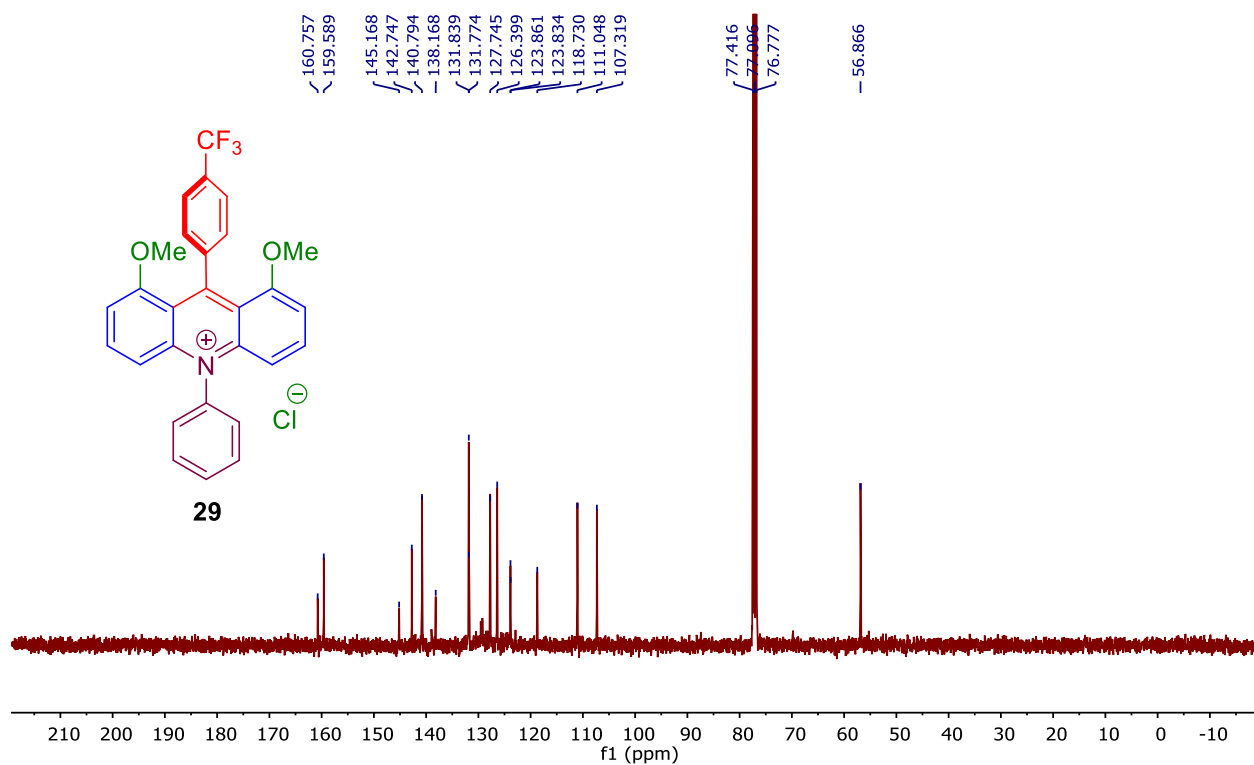


Figure S60. ¹³C NMR (CDCl₃, 100MHz) spectrum of 1,8-dimethoxy-10-phenyl-9-(4-(trifluoromethyl)phenyl)acridin-10-ium chloride (29)

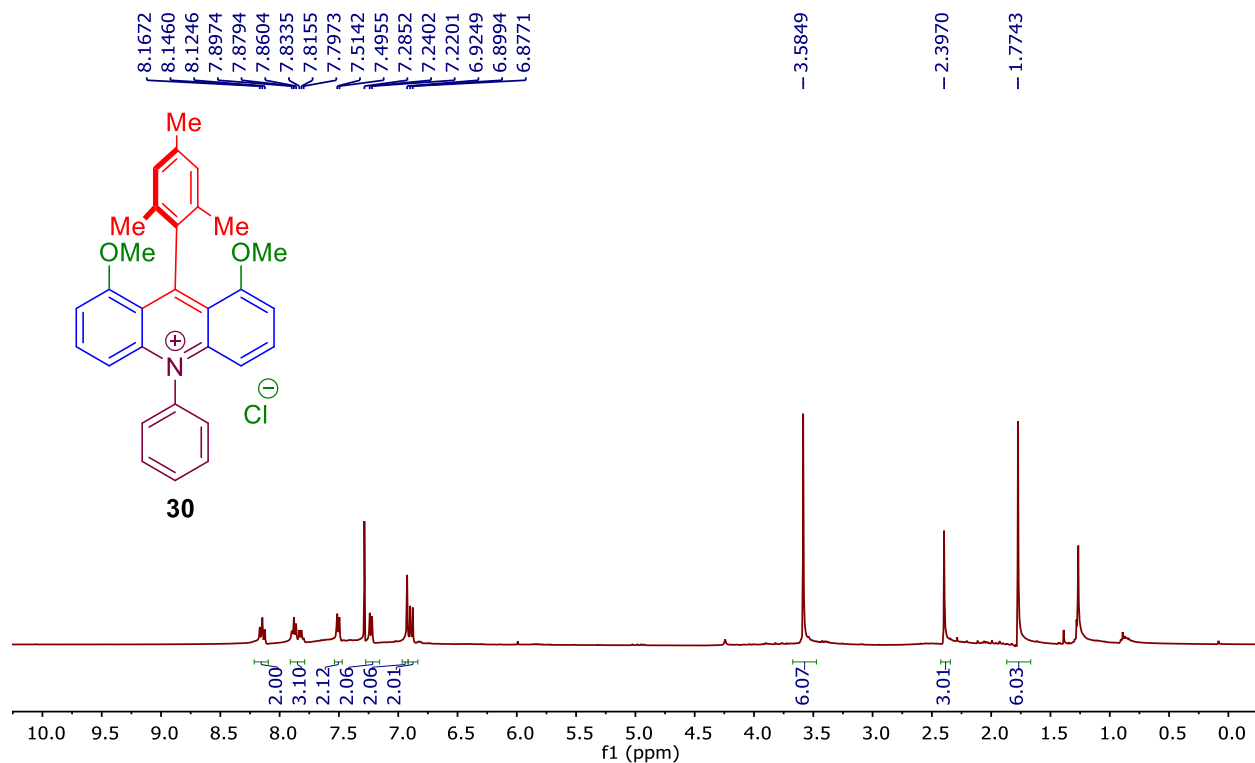


Figure S61. ¹H NMR (CDCl₃, 400MHz) spectrum of 9-mesityl-1,8-dimethoxy-10-phenylacridin-10-ium chloride(30)

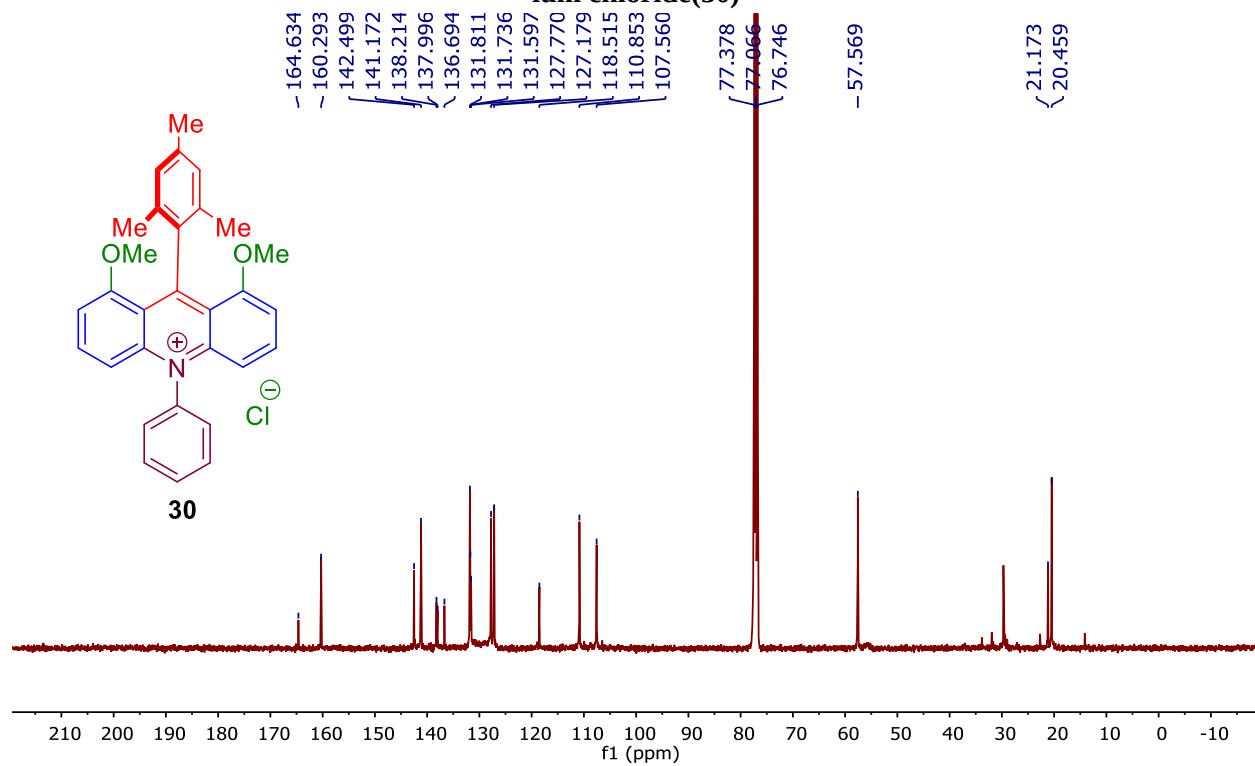


Figure S62. ¹³C NMR (CDCl₃, 100MHz) spectrum of 9-mesityl-1,8-dimethoxy-10-phenylacridin-10-ium chloride (30)

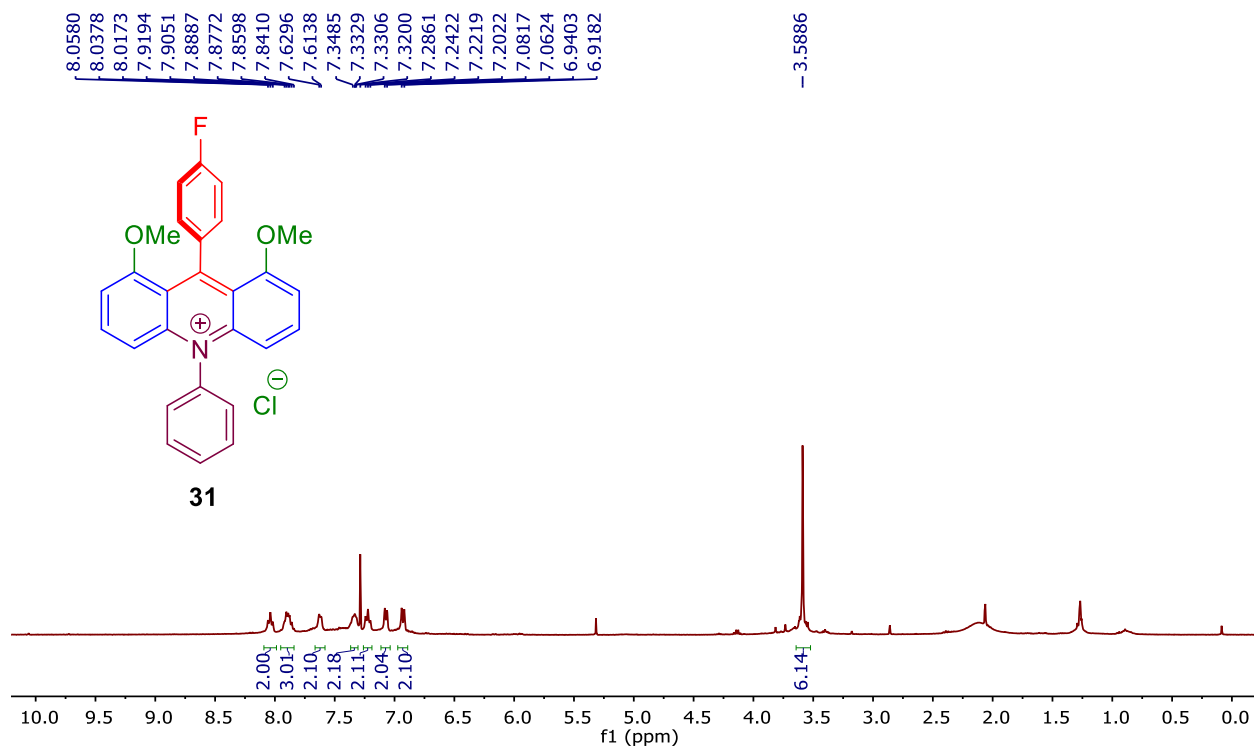


Figure S63. ¹H NMR (CDCl₃, 400MHz) spectrum of 9-(4-fluorophenyl)-1,8-dimethoxy-10-phenylacridin-10-ium chloride (31)

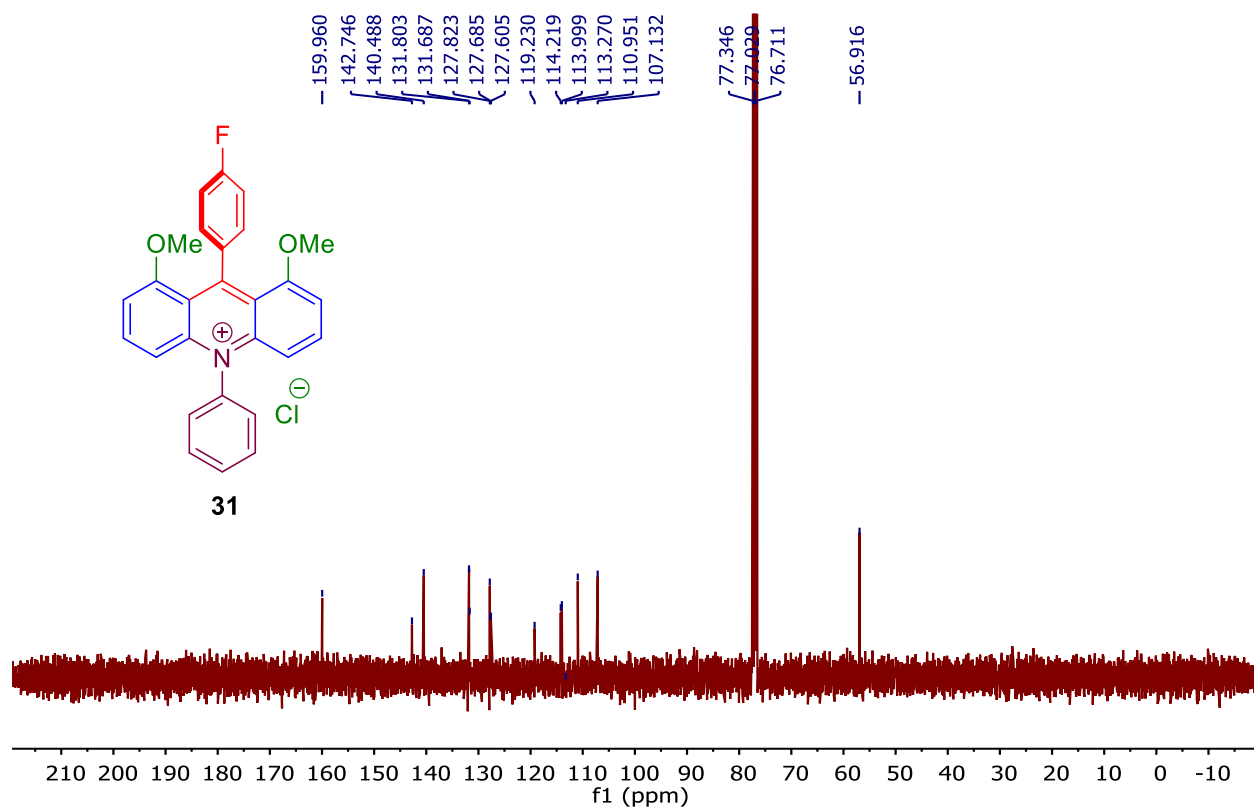


Figure S64. ¹³C NMR (CDCl₃, 100MHz) spectrum of 9-(4-fluorophenyl)-1,8-dimethoxy-10-phenylacridin-10-ium chloride (31)

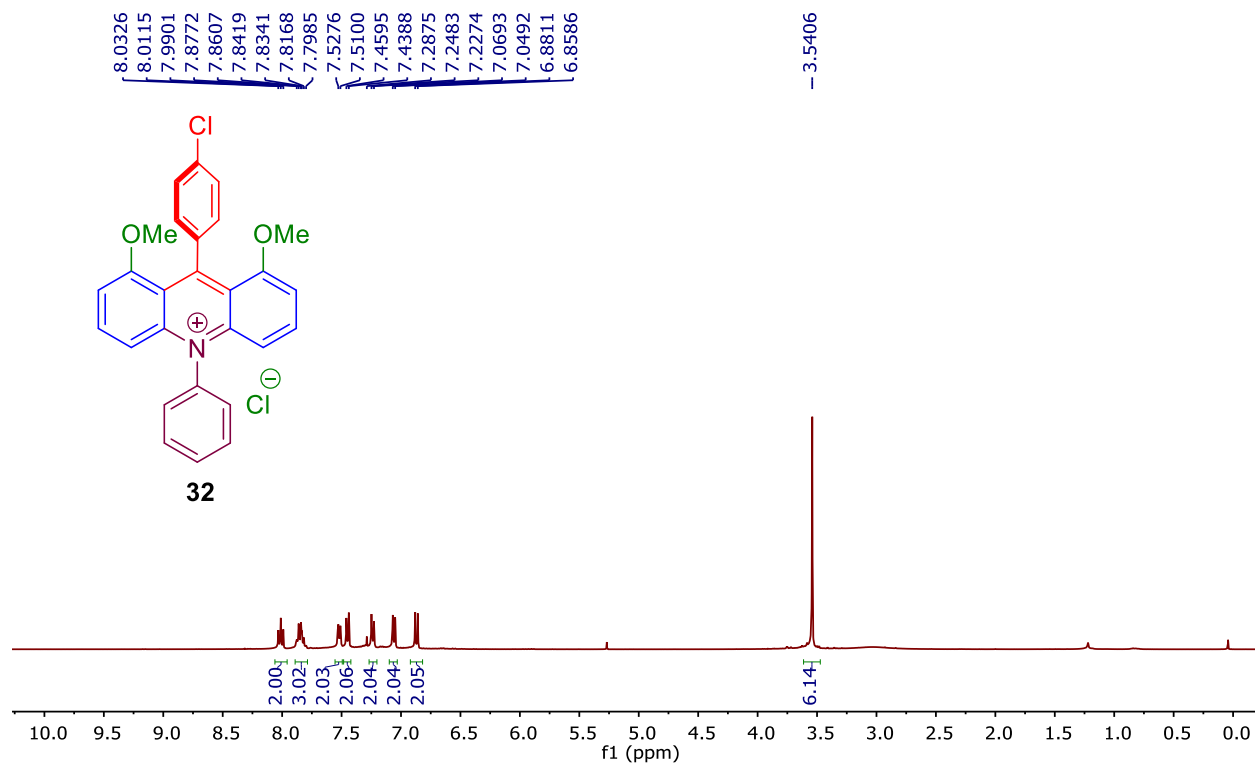


Figure S65. ¹H NMR (CDCl₃, 400MHz) spectrum of 9-(4-chlorophenyl)-1,8-dimethoxy-10-phenylacridin-10-ium chloride (32)

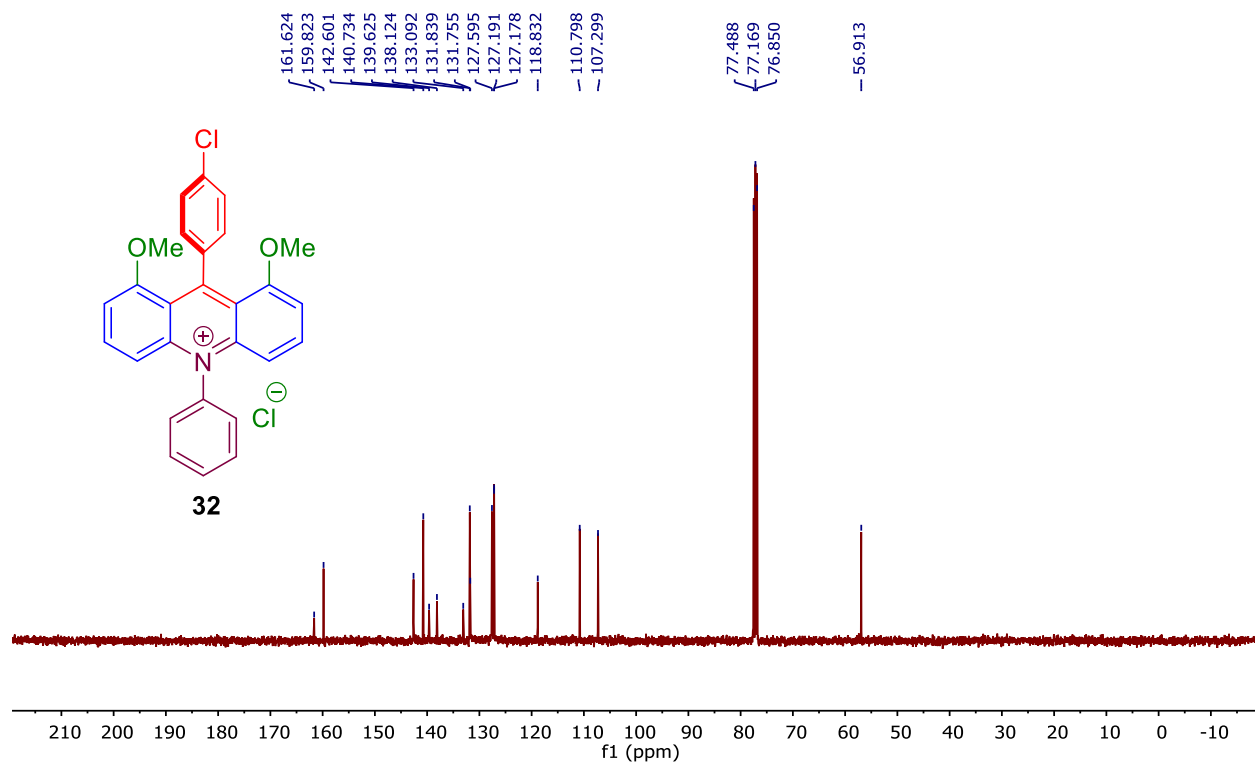


Figure S66. ¹³C NMR (CDCl₃, 100MHz) spectrum of 9-(4-chlorophenyl)-1,8-dimethoxy-10-phenylacridin-10-ium chloride (32)

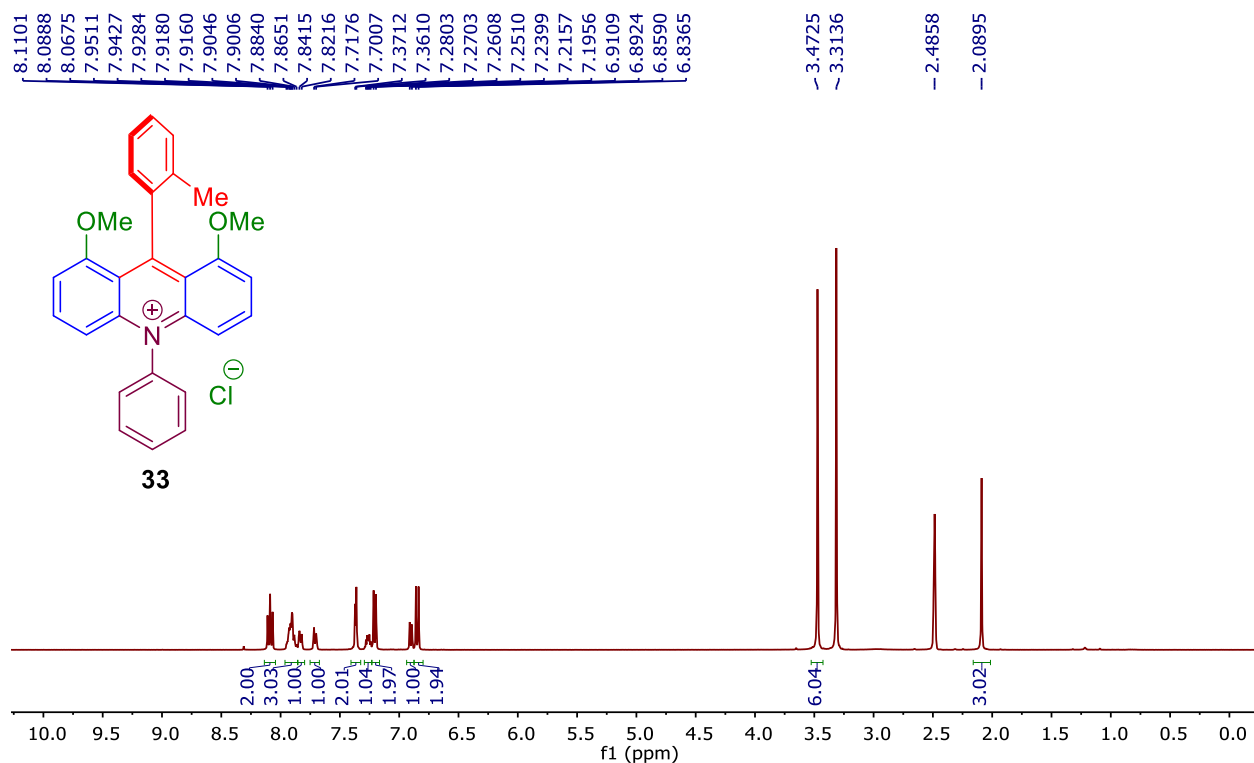


Figure S67. ¹H NMR (DMSO-*d*₆, 400MHz) spectrum of 1,8-dimethoxy-10-phenyl-9-(*o*-tolyl)acridin-10-ium chloride (33)

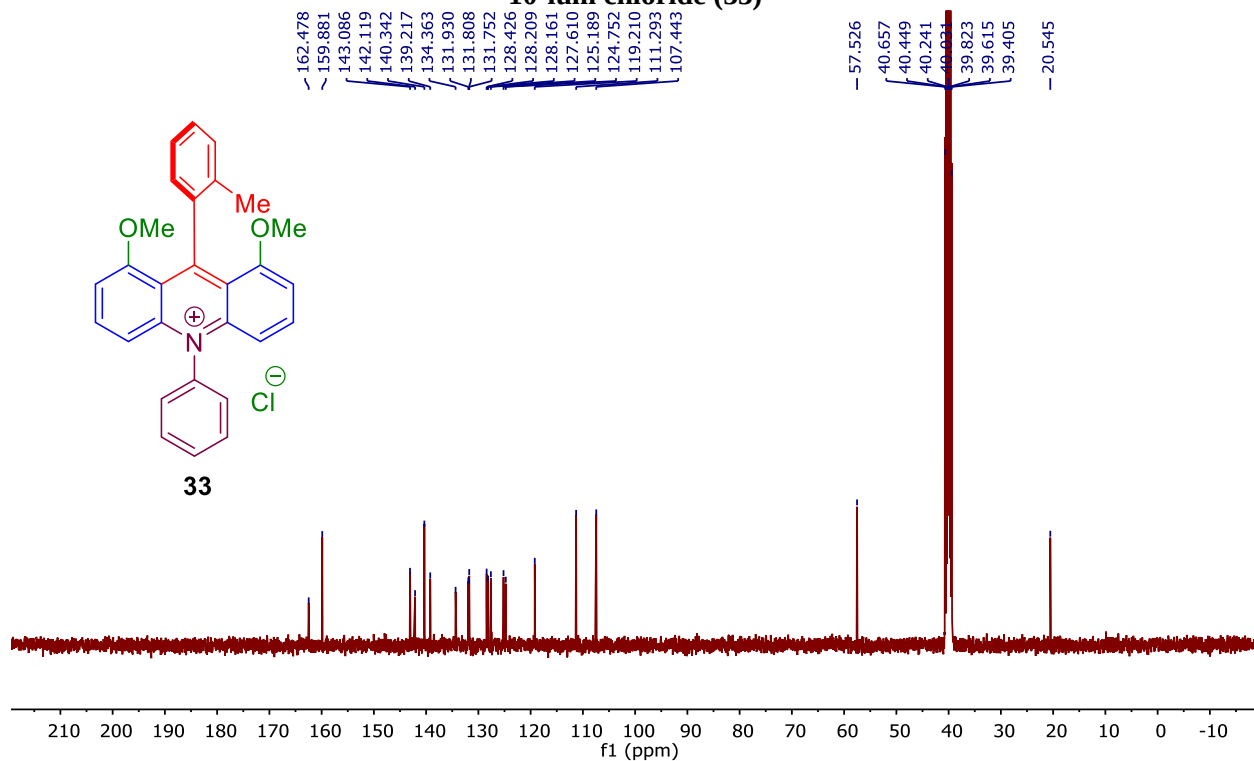


Figure S68. ¹³C NMR (DMSO-*d*₆, 100MHz) spectrum of 1,8-dimethoxy-10-phenyl-9-(*o*-tolyl)acridin-10-ium chloride (33)

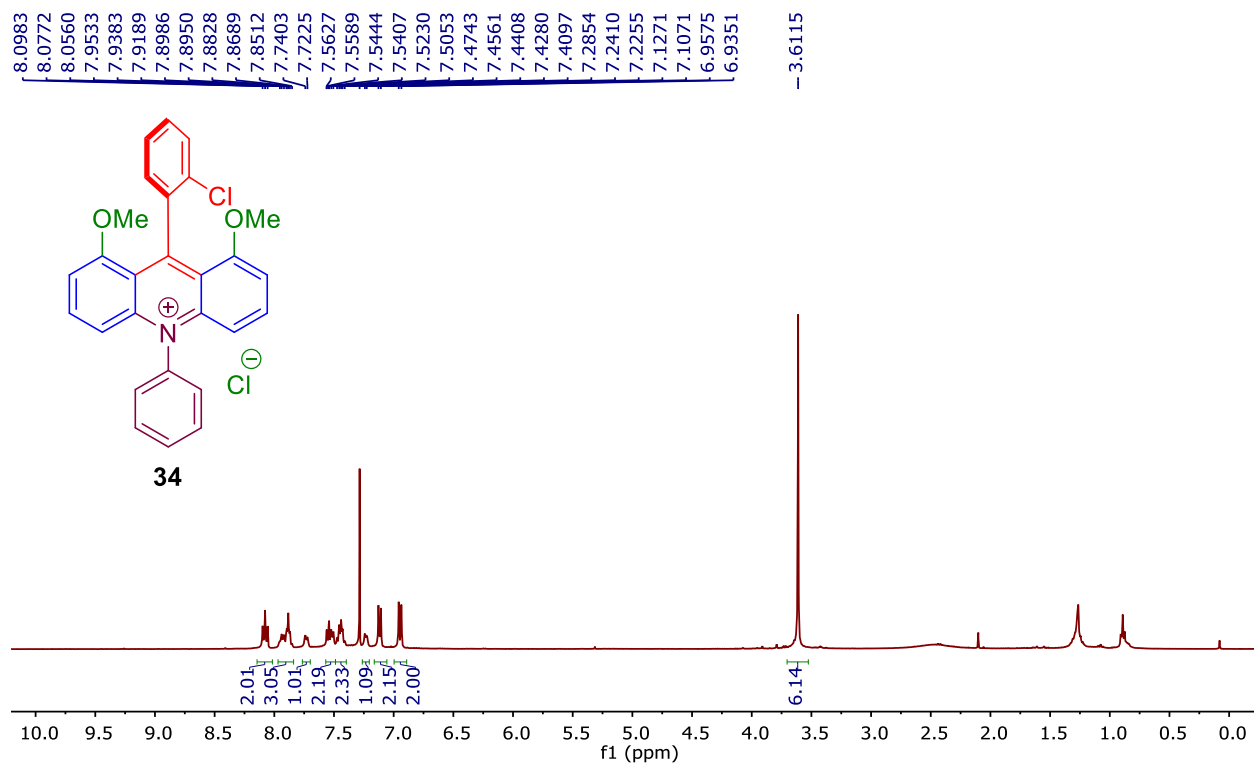


Figure S69. ¹H NMR (CDCl₃, 400MHz) spectrum of 9-(2-chlorophenyl)-1,8-dimethoxy-10-phenylacridin-10-ium chloride (34)

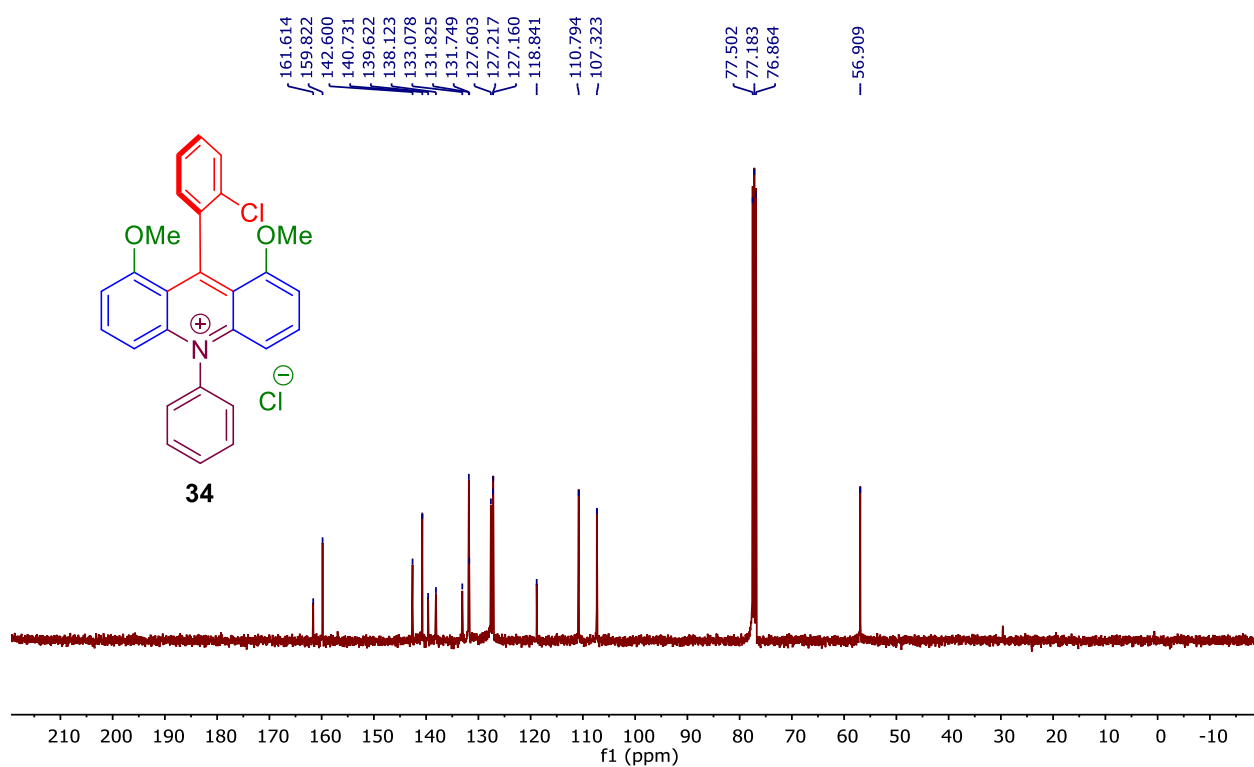


Figure S70. ¹³C NMR (CDCl₃, 100MHz) spectrum of 9-(2-chlorophenyl)-1,8-dimethoxy-10-phenylacridin-10-ium chloride (34)

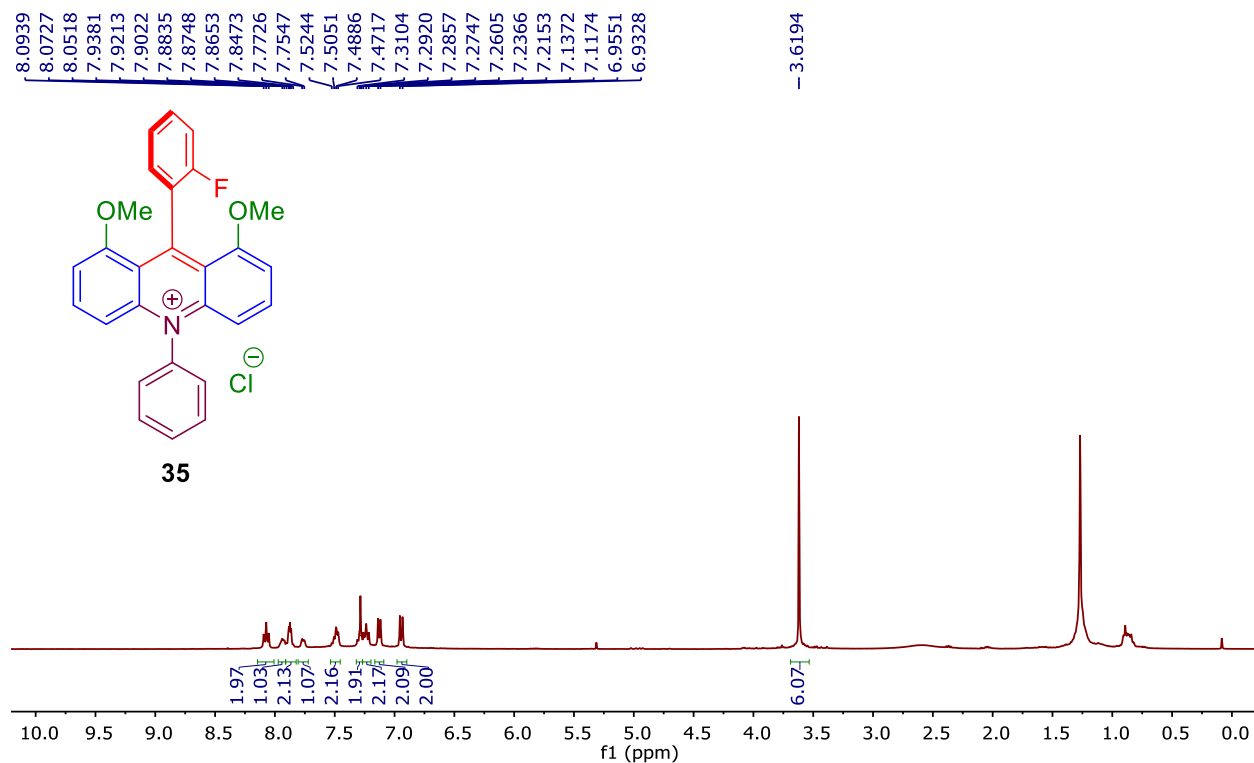


Figure S71. ¹H NMR (CDCl₃, 400MHz) spectrum of 9-(2-fluorophenyl)-1,8-dimethoxy-10-phenylacridin-10-ium chloride (35)

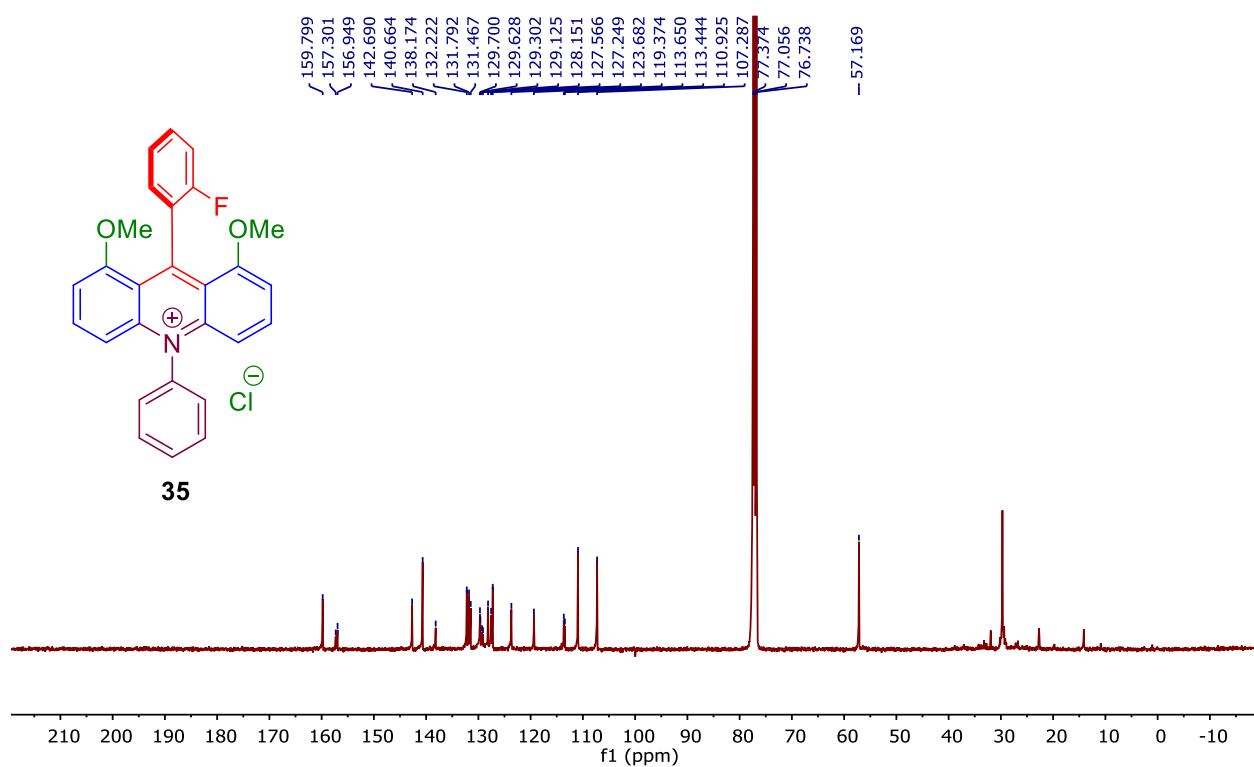


Figure S72. ¹³C NMR (CDCl₃, 100MHz) spectrum of 9-(2-fluorophenyl)-1,8-dimethoxy-10-phenylacridin-10-ium chloride (35)

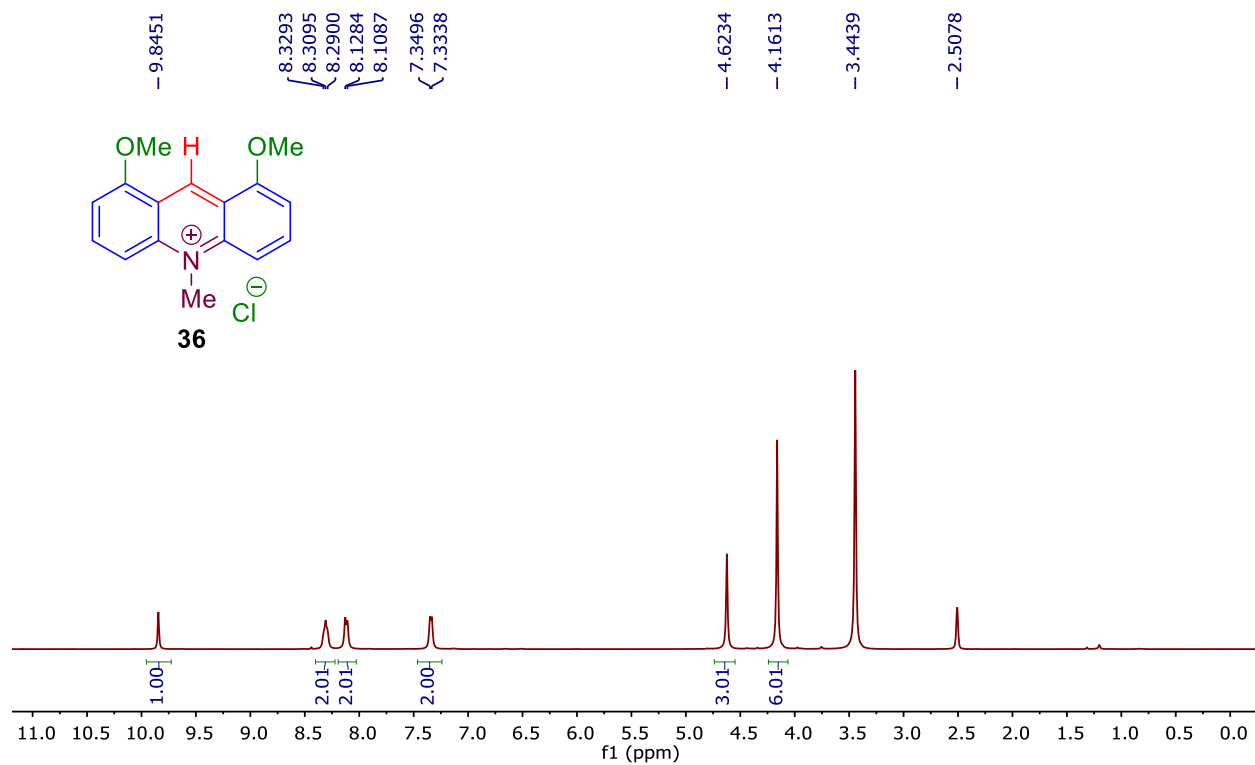


Figure S73. ¹H NMR (DMSO-*d*₆, 400MHz) spectrum of 1,8-dimethoxy-10-methylacridin-10-ium chloride (36)

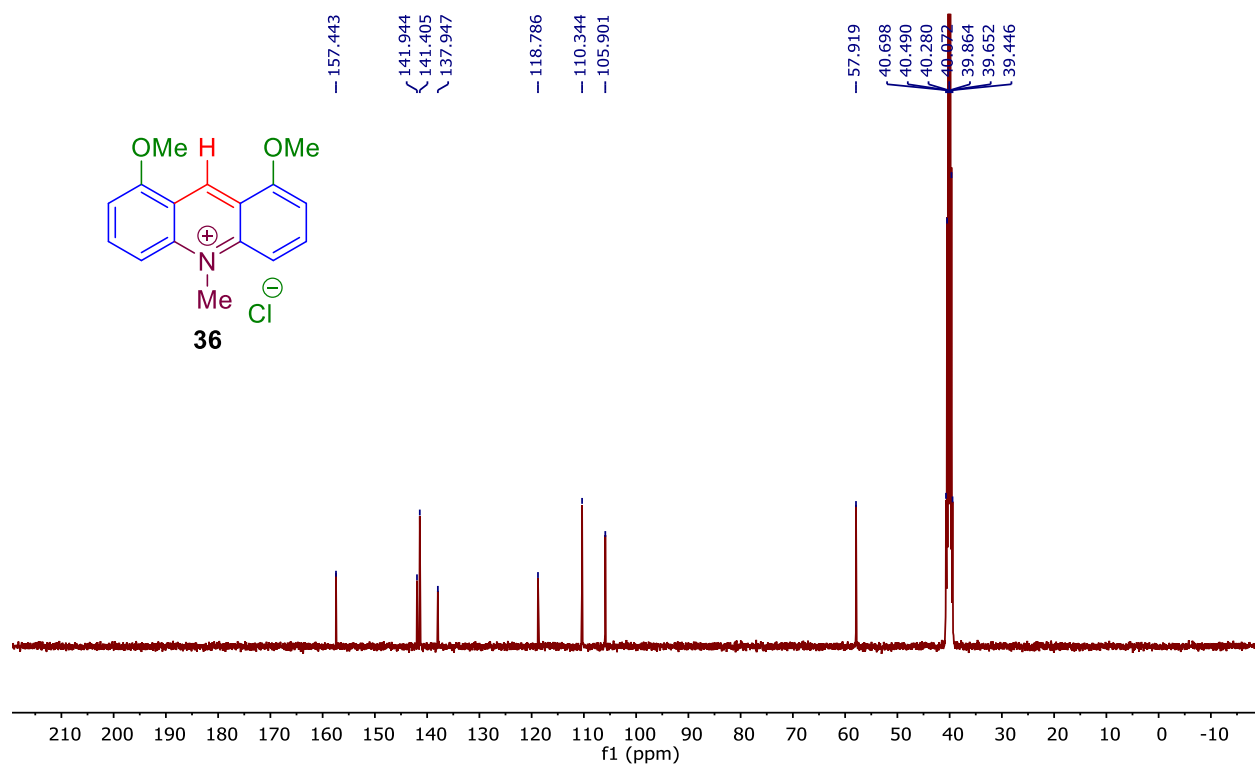


Figure S74. ¹³C NMR (DMSO-*d*₆, 100MHz) spectrum of 1,8-dimethoxy-10-methylacridin-10-ium chloride (36)

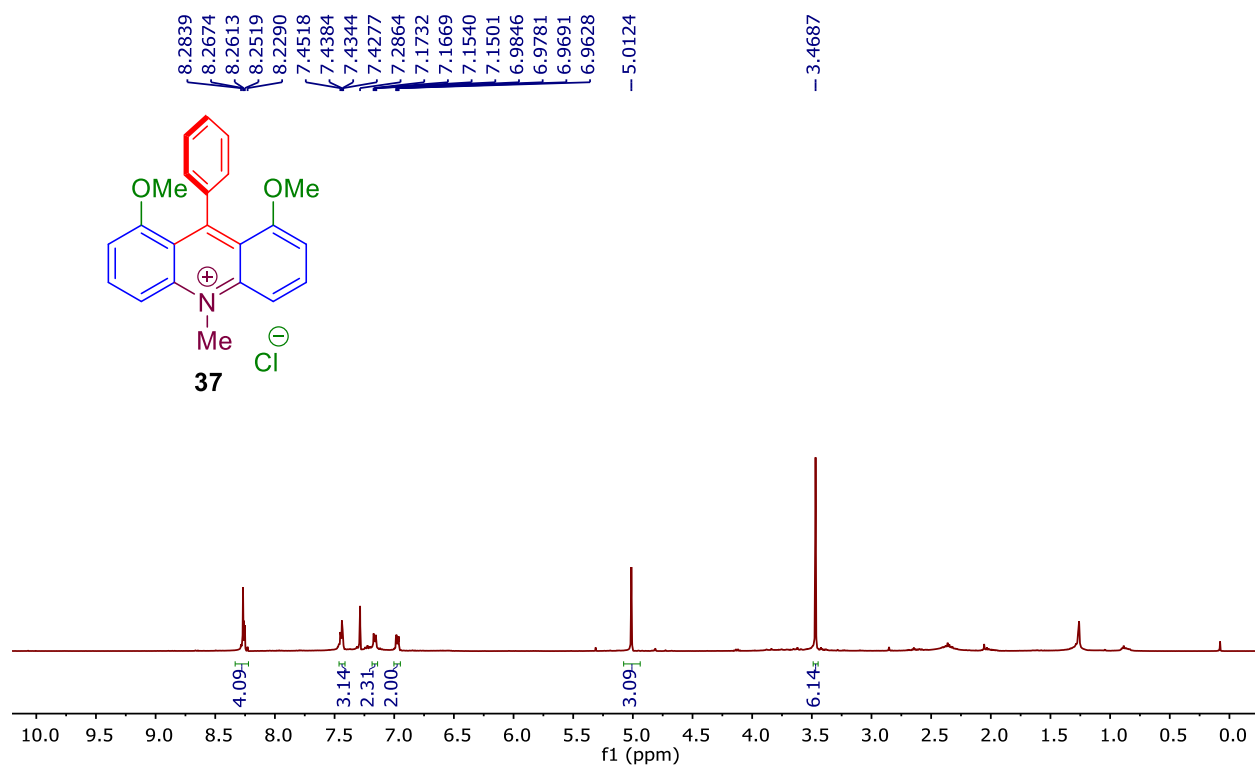


Figure S75. ¹H NMR (CDCl₃, 400MHz) spectrum of 1,8-dimethoxy-10-methyl-9-phenylacridin-10-ium chloride (37)

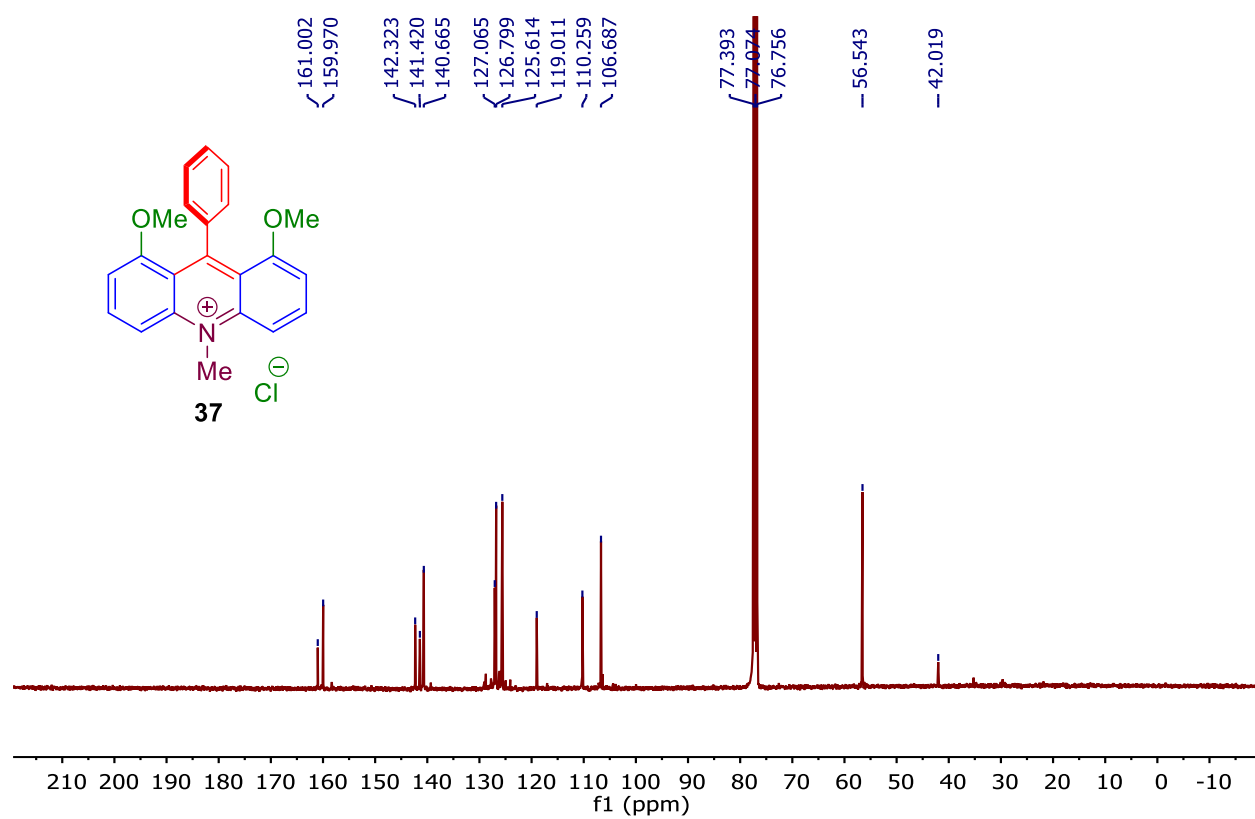


Figure S76. ¹³C NMR (CDCl₃, 100MHz) spectrum of 1,8-dimethoxy-10-methyl-9-phenylacridin-10-ium chloride (37)

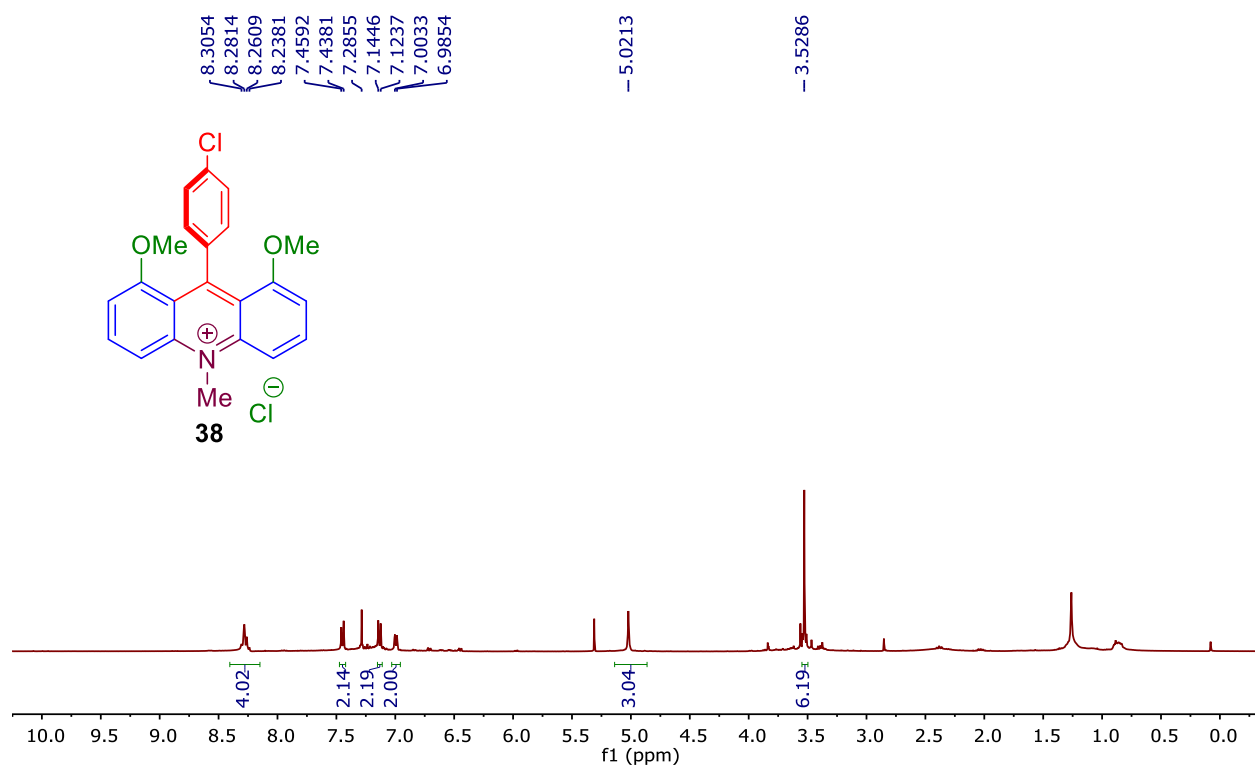


Figure S77. ¹H NMR (CDCl₃, 400MHz) spectrum of 9-(4-chlorophenyl)-1,8-dimethoxy-10-methylacridin-10-ium chloride (38)

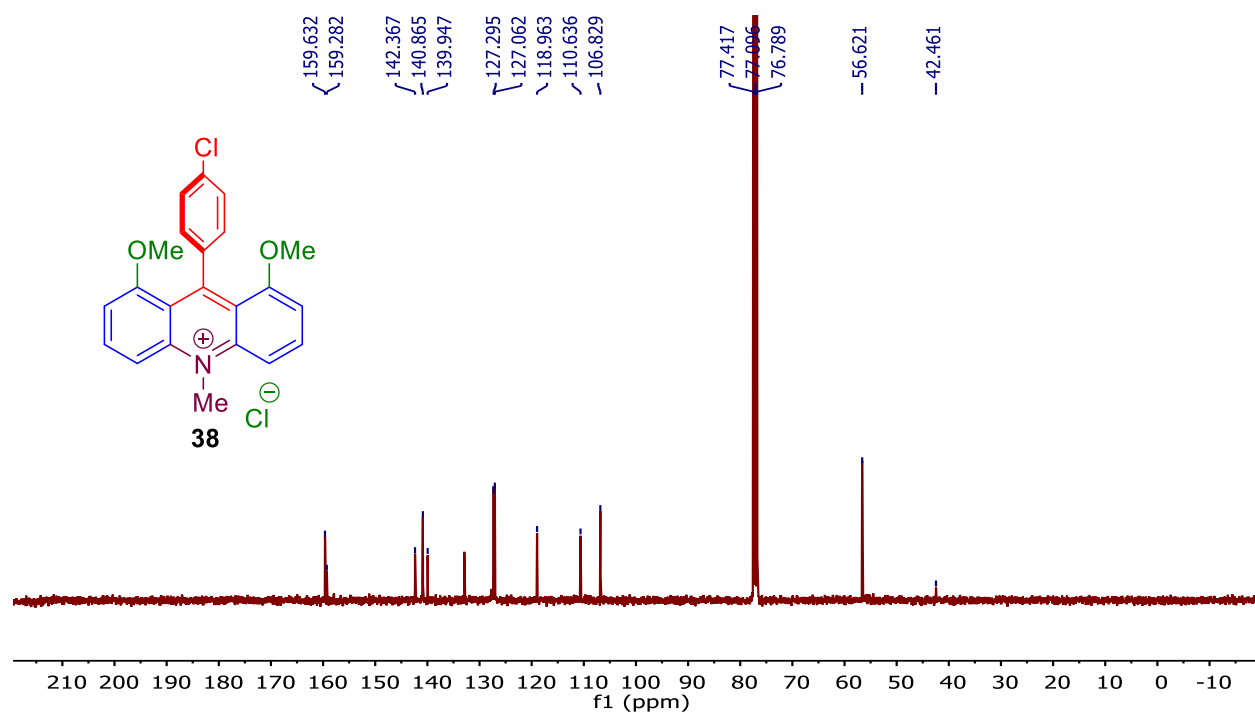


Figure S78. ¹³C NMR (CDCl₃, 100MHz) spectrum of 9-(4-chlorophenyl)-1,8-dimethoxy-10-methylacridin-10-ium chloride (38)

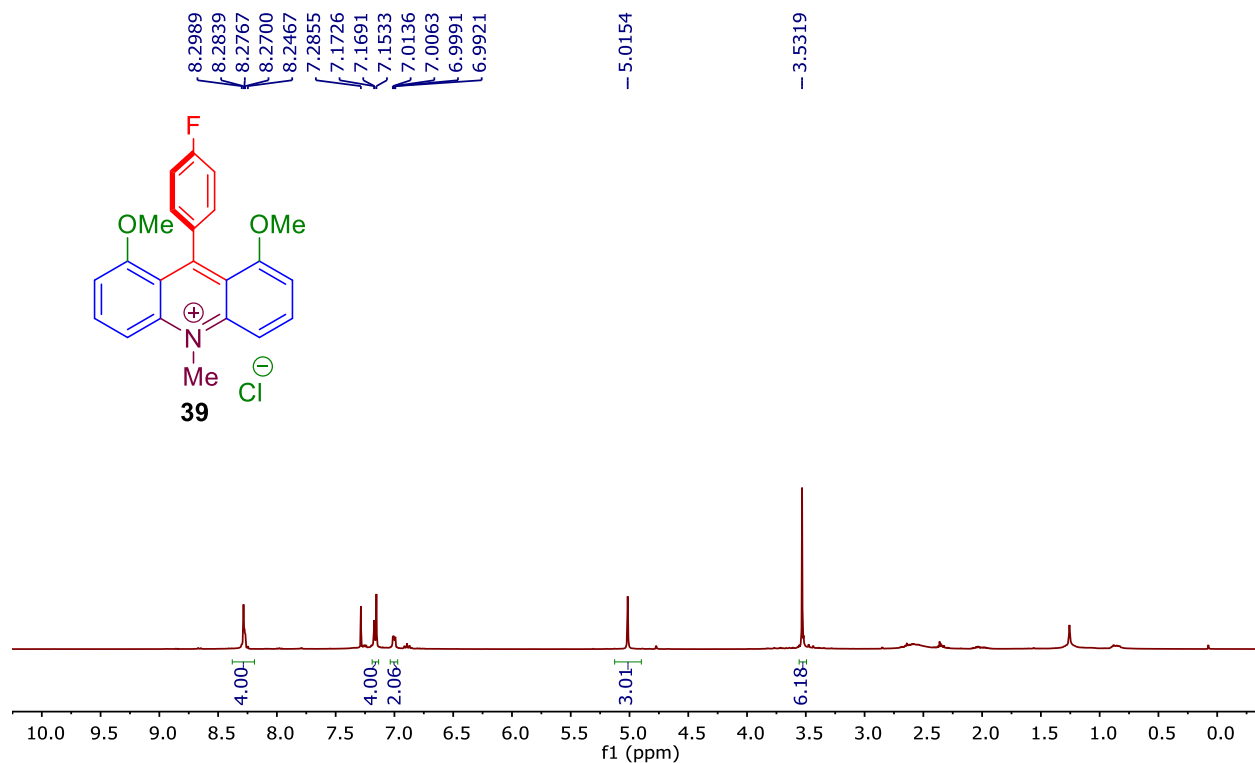


Figure S79. ¹H NMR (CDCl₃, 400MHz) spectrum of 9-(4-fluorophenyl)-1,8-dimethoxy-10-methylacridin-10-ium chloride (39)

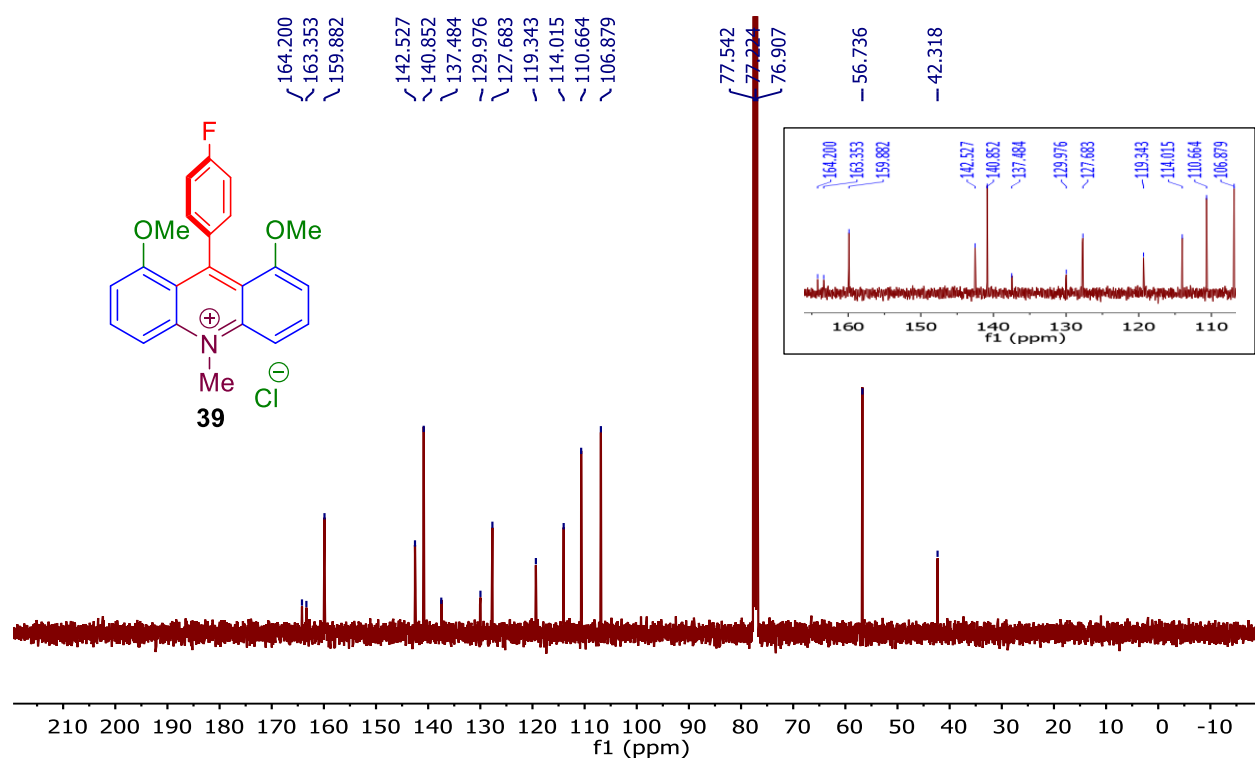


Figure S80. ¹³C NMR (CDCl₃, 100MHz) spectrum of 9-(4-fluorophenyl)-1,8-dimethoxy-10-methylacridin-10-ium chloride (39)

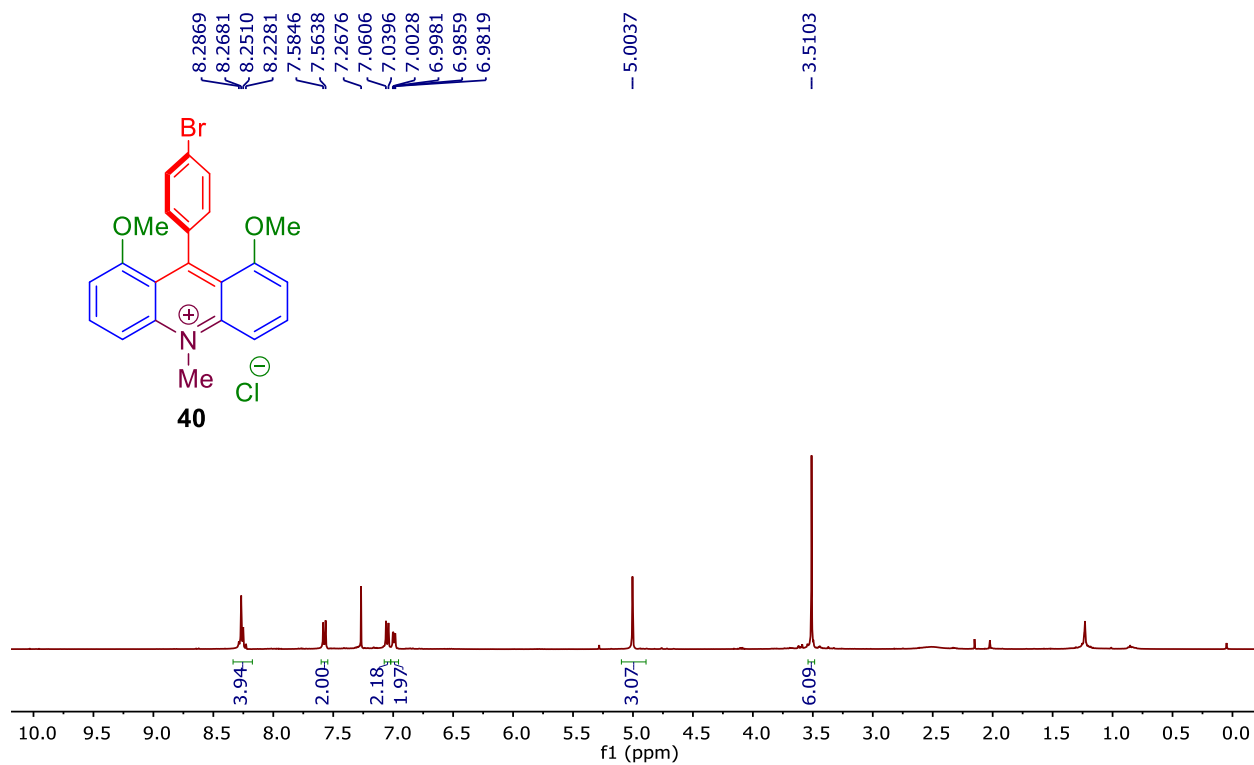


Figure S81. ¹H NMR (CDCl₃, 400MHz) spectrum of 9-(4-bromophenyl)-1,8-dimethoxy-10-methylacridin-10-ium chloride (40)

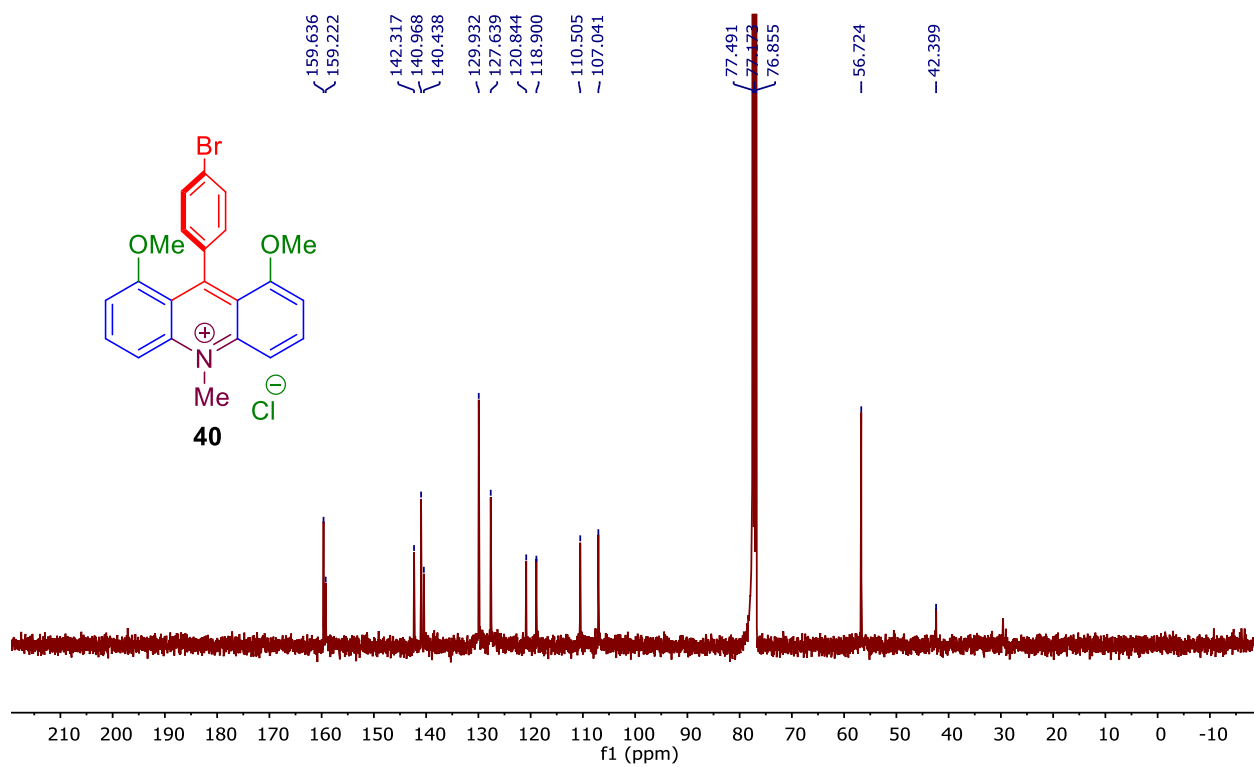


Figure S82. ¹³C NMR (CDCl₃, 100MHz) spectrum of 9-(4-bromophenyl)-1,8-dimethoxy-10-methylacridin-10-ium chloride (40)

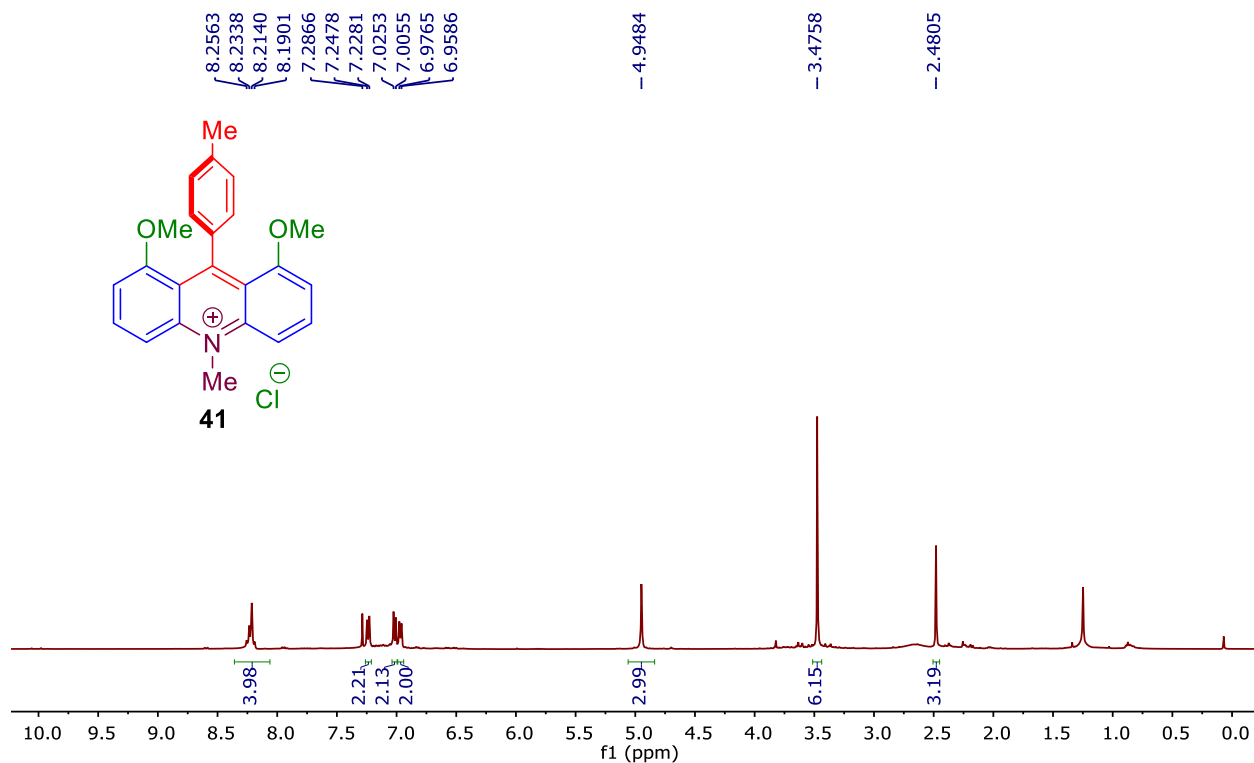


Figure S83. ¹H NMR (CDCl₃, 400MHz) spectrum of 1,8-dimethoxy-10-methyl-9-(p-tolyl)acridin-10-ium chloride (41)

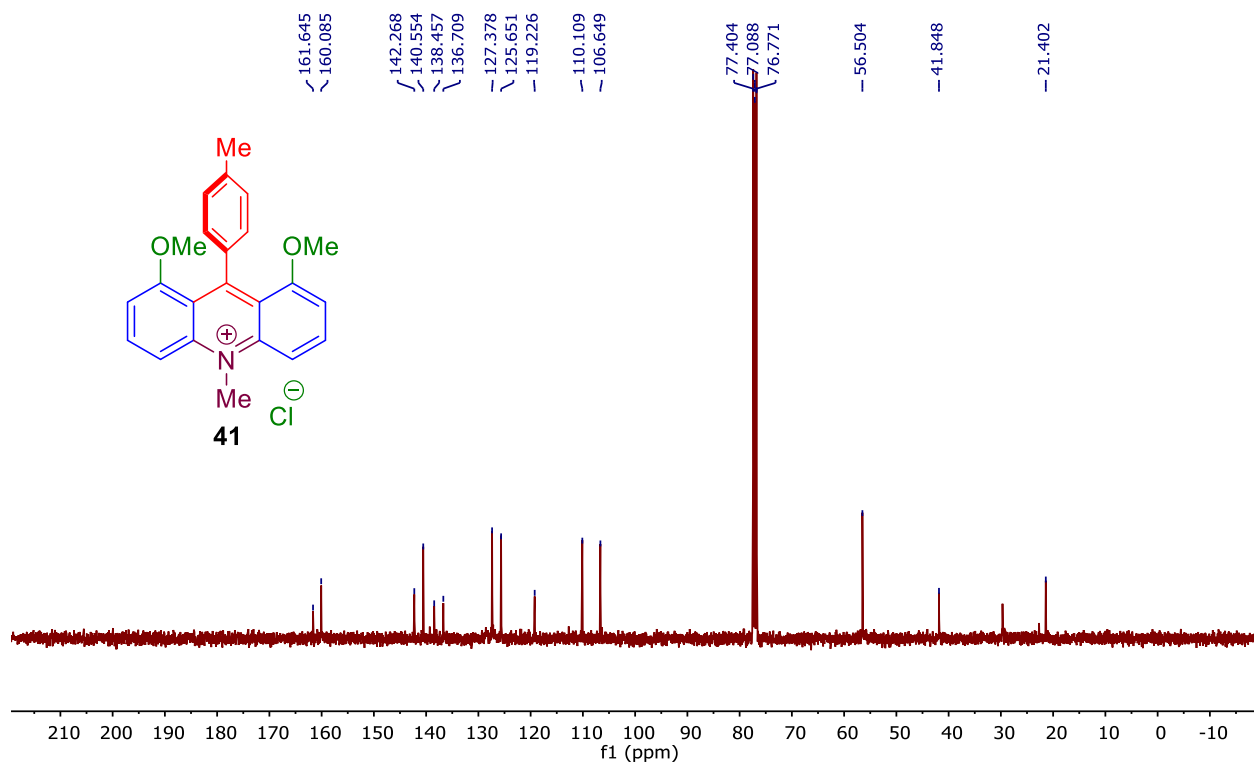


Figure S84. ¹³C NMR (CDCl₃, 100MHz) spectrum of 1,8-dimethoxy-10-methyl-9-(p-tolyl)acridin-10-ium chloride (41)

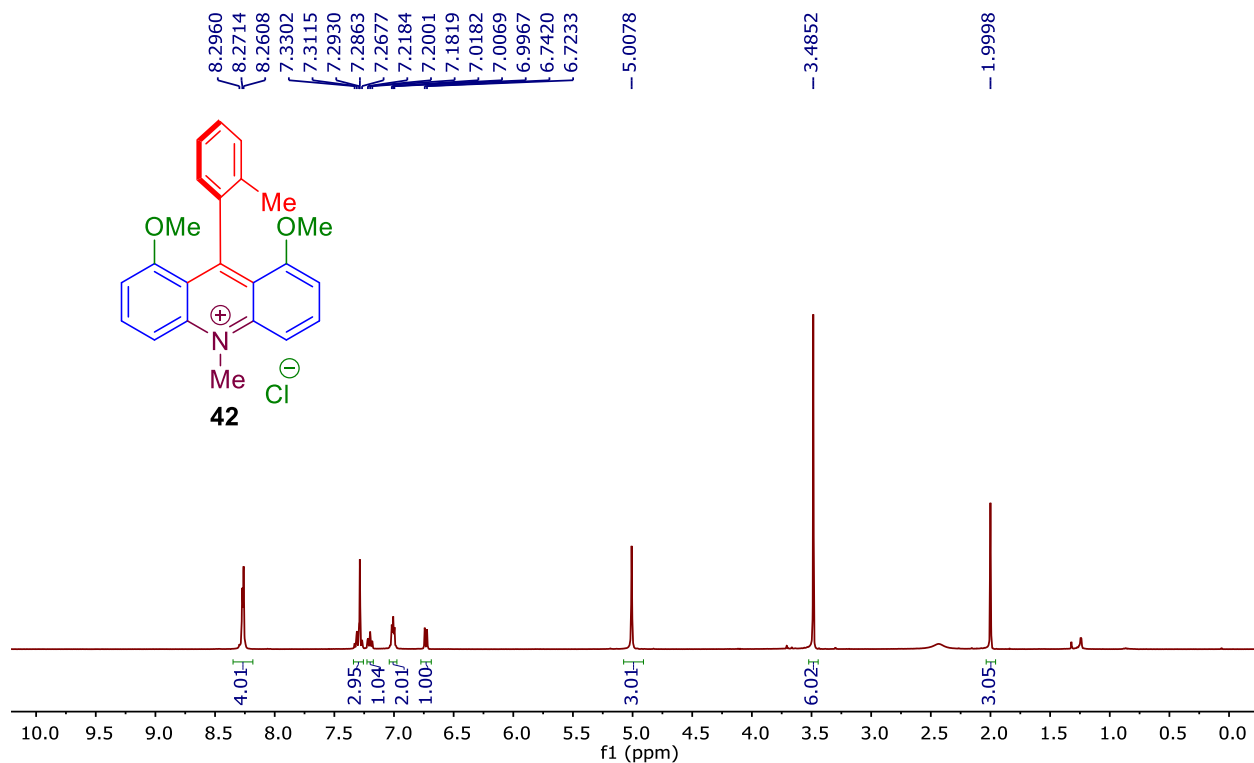


Figure S85. ¹H NMR (CDCl₃, 400MHz) spectrum of 1,8-dimethoxy-10-methyl-9-(o-tolyl)acridin-10-ium chloride (42)

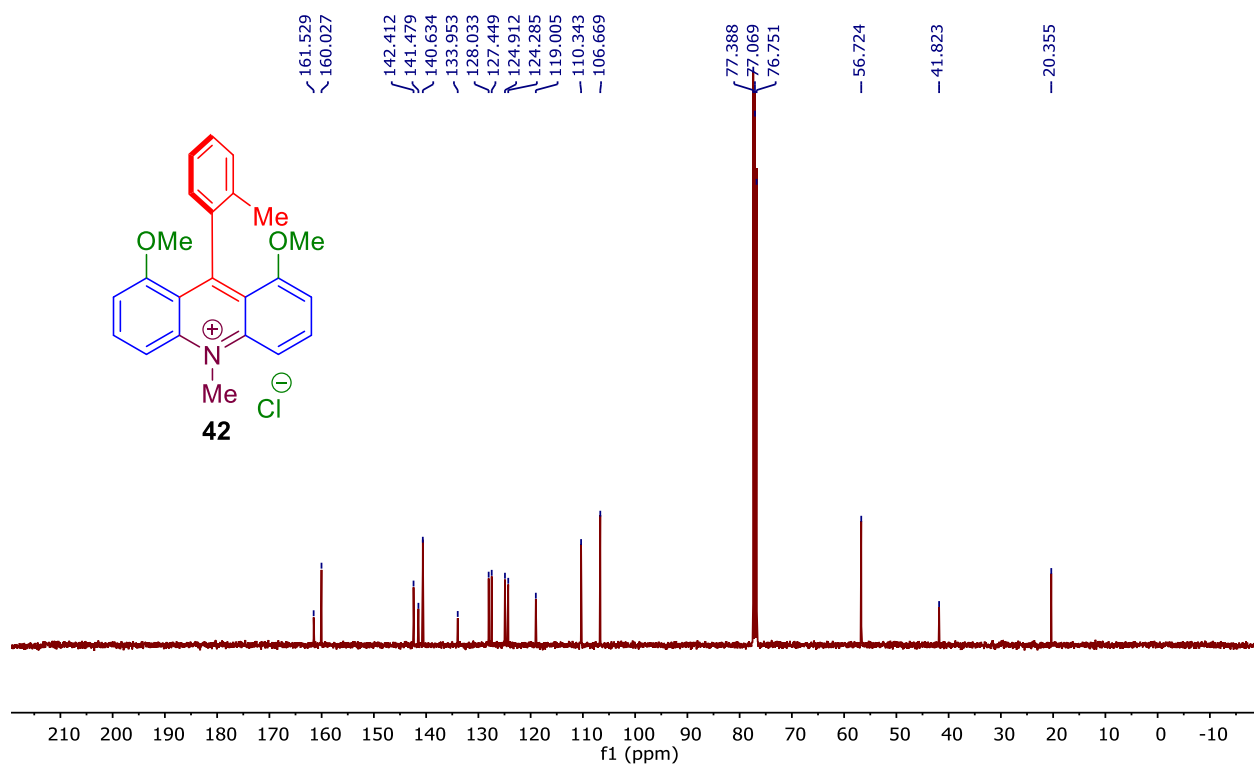


Figure S86. ¹³C NMR (CDCl₃, 100MHz) spectrum of 1,8-dimethoxy-10-methyl-9-(o-tolyl)acridin-10-ium chloride (42)