Electronic Supplementary Information

Indolizino[3,2-*c*]quinolines as Imaging Probes Differentiating Dense-Core, Diffuse, and Coronal Plaques of Amyloid-β

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Figure S1. Excitation and emission spectra of 51 **YIQ** compounds

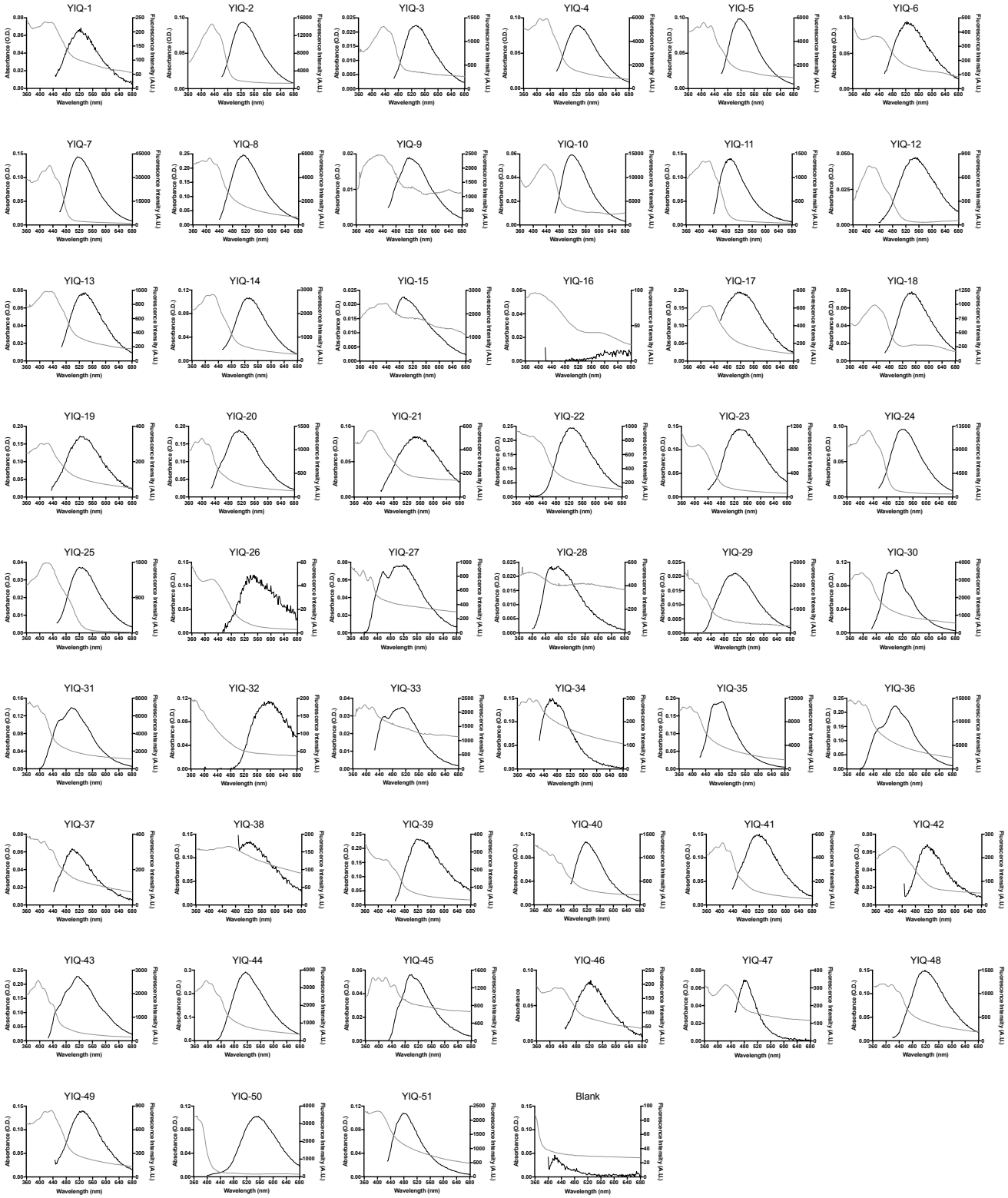


Fig. S1 Excitation and emission spectra of 51 **YIQ** compounds are measured by plate reader.

Figure S2. Densitometry of monomers bands in figure 2

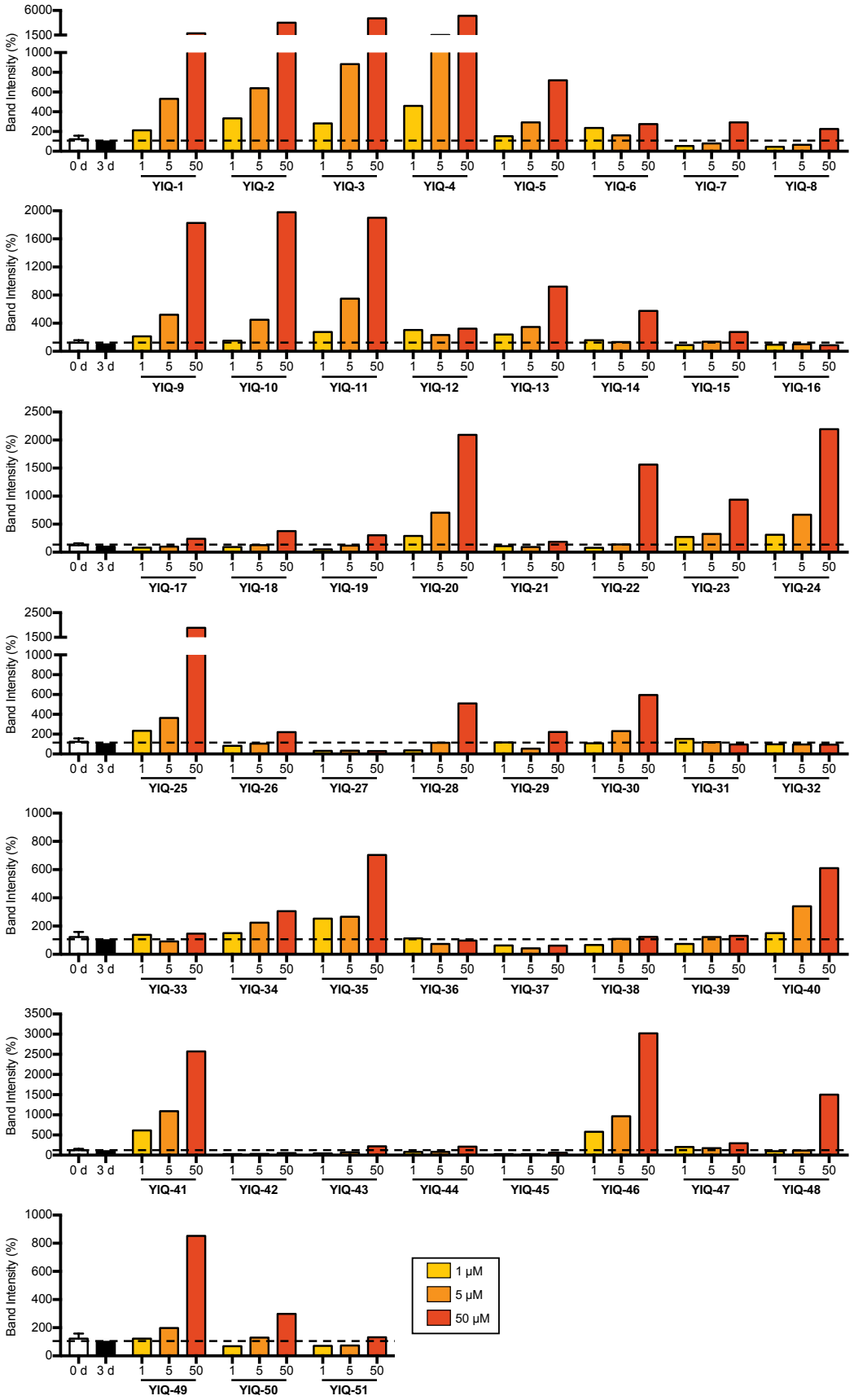


Fig. S2 Densitometry of monomers bands in figure 2. Band area was measured by ImageJ software and normalized to the 3-day aggregates (black, 100%).

Figure S3. Densitometry of aggregates bands in figure 2

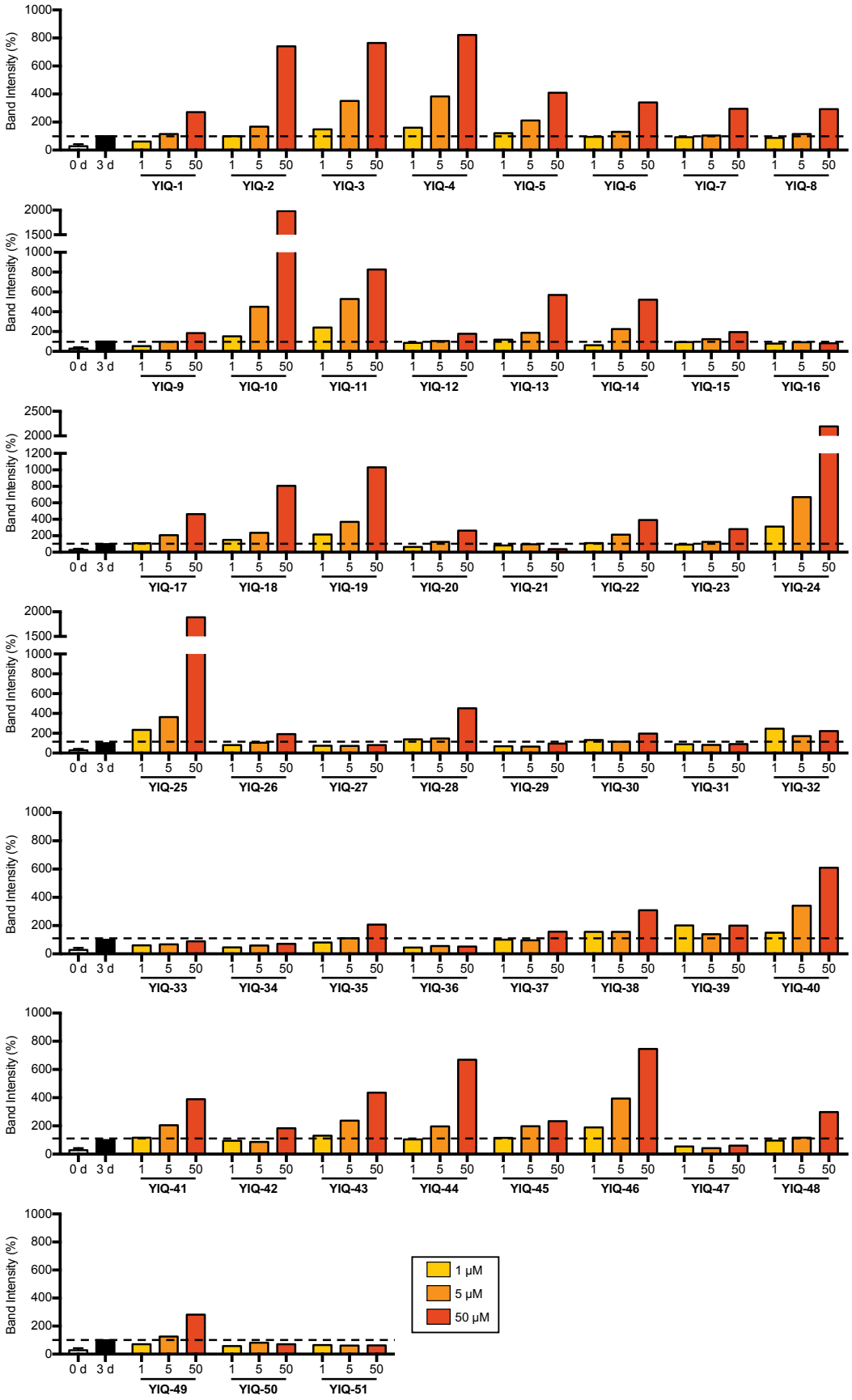


Fig. S3 Densitometry of aggregates bands in figure 2. Band area was measured by ImageJ software and normalized to the 3-day aggregates (black, 100%).

Figure S4. Fluorescence scanned whole gel image displayed in figure 2

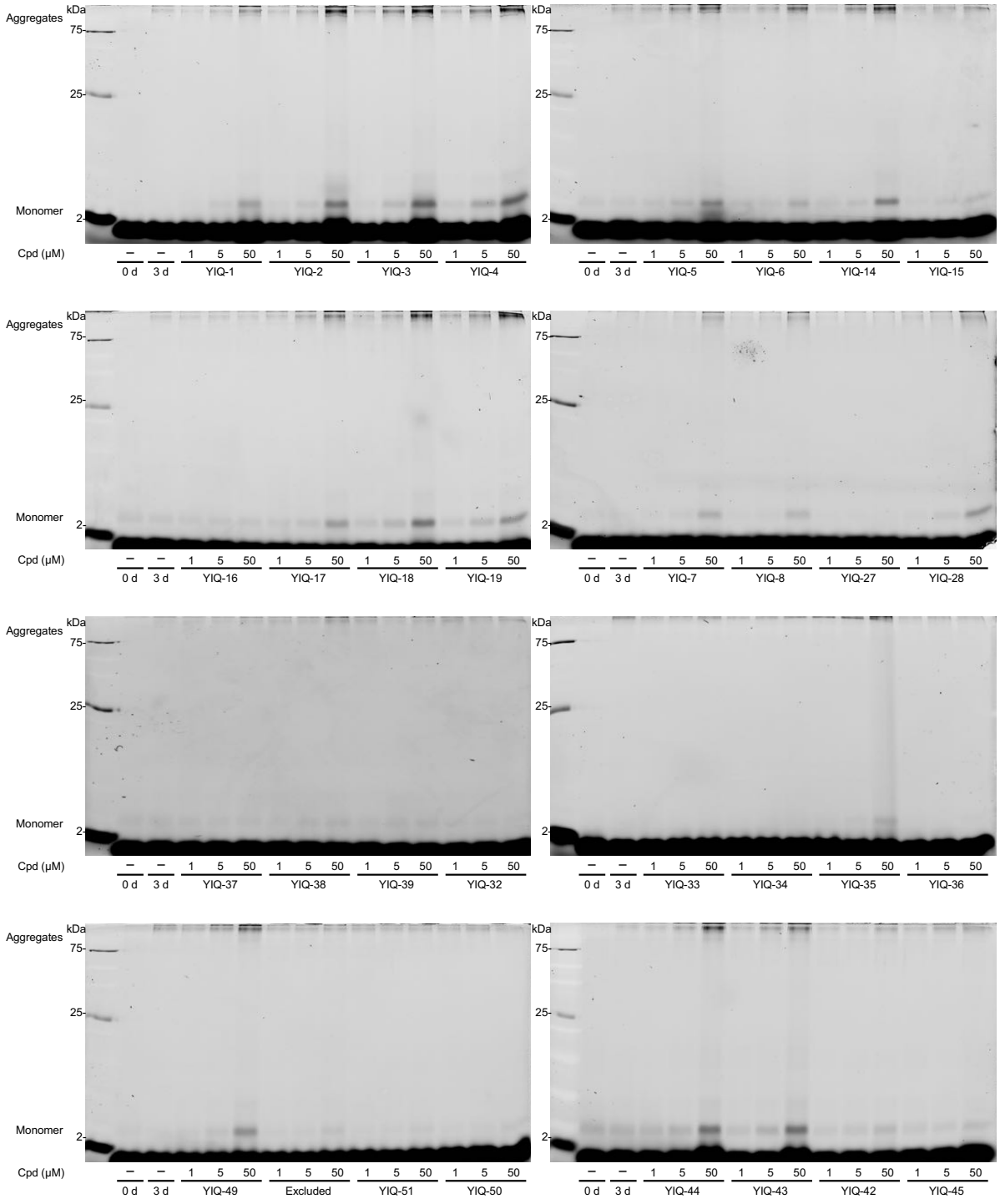


Figure S4. Fluorescence scanned whole gel image displayed in figure 2 (Continue)

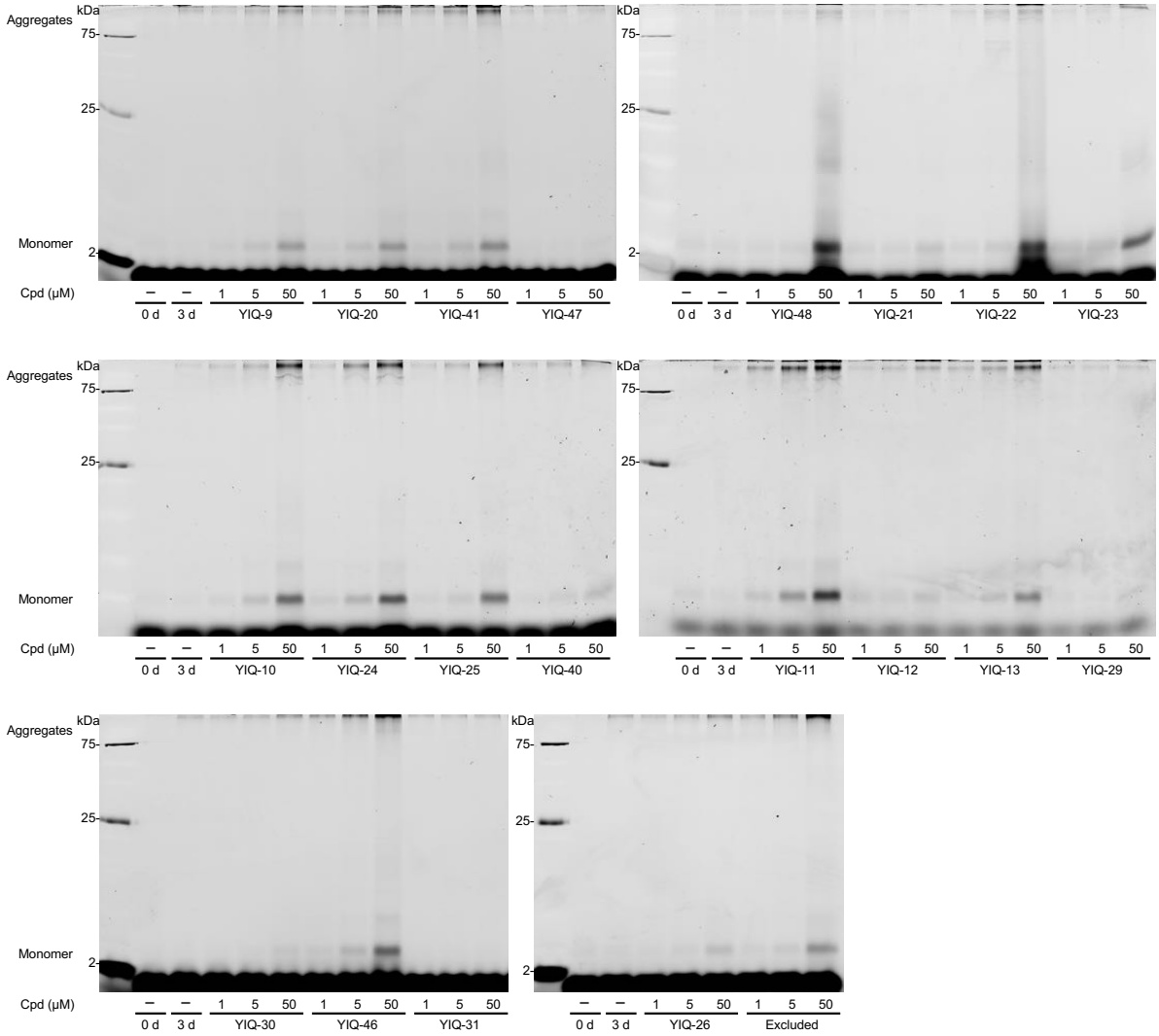


Fig. S4 Whole gel image displayed in figure 2. Two samples were excluded.

Figure S5. Silver-stained whole gel image displayed in figure 2

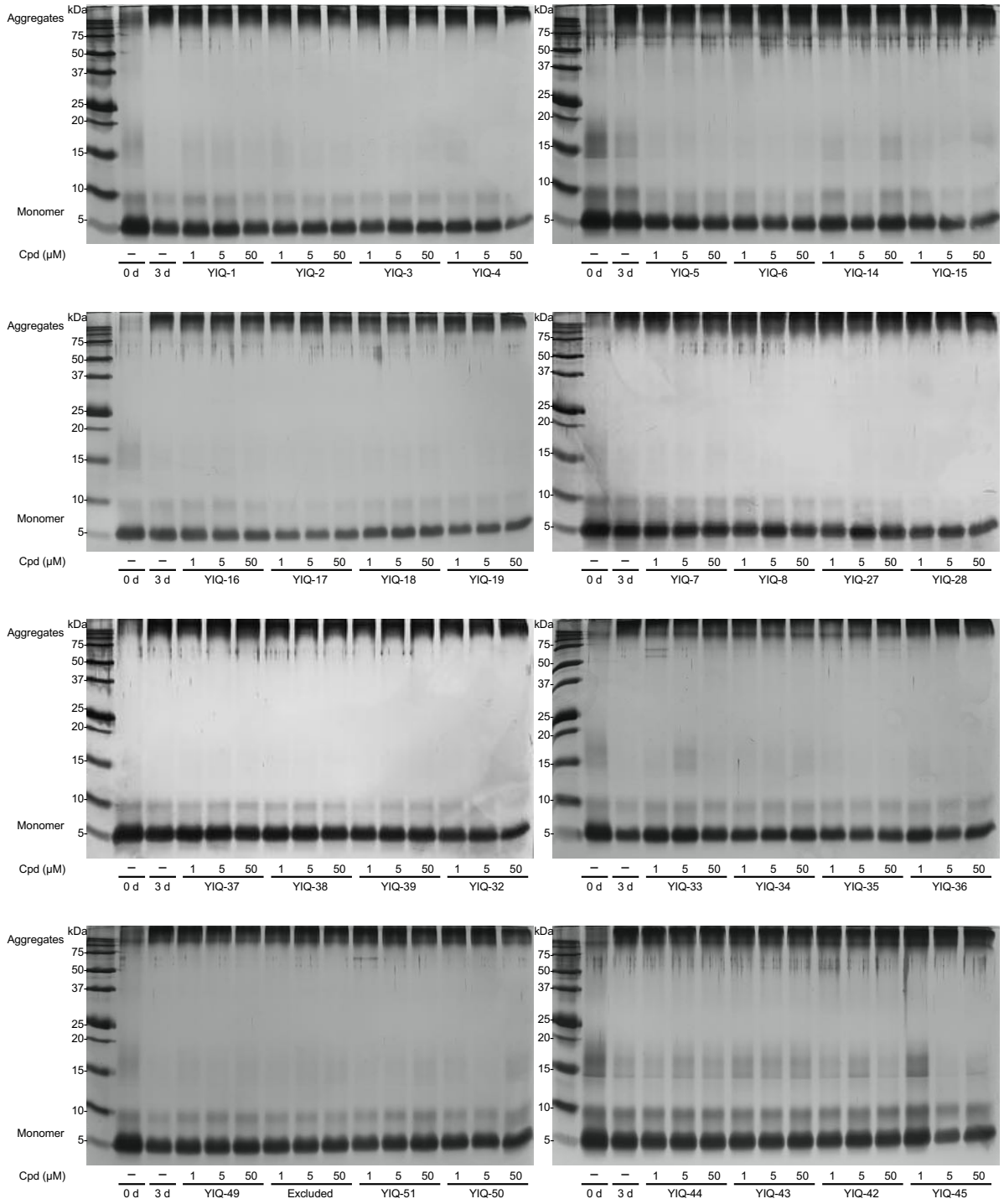


Figure S5. Silver-stained whole gel image displayed in figure 2 (continue)

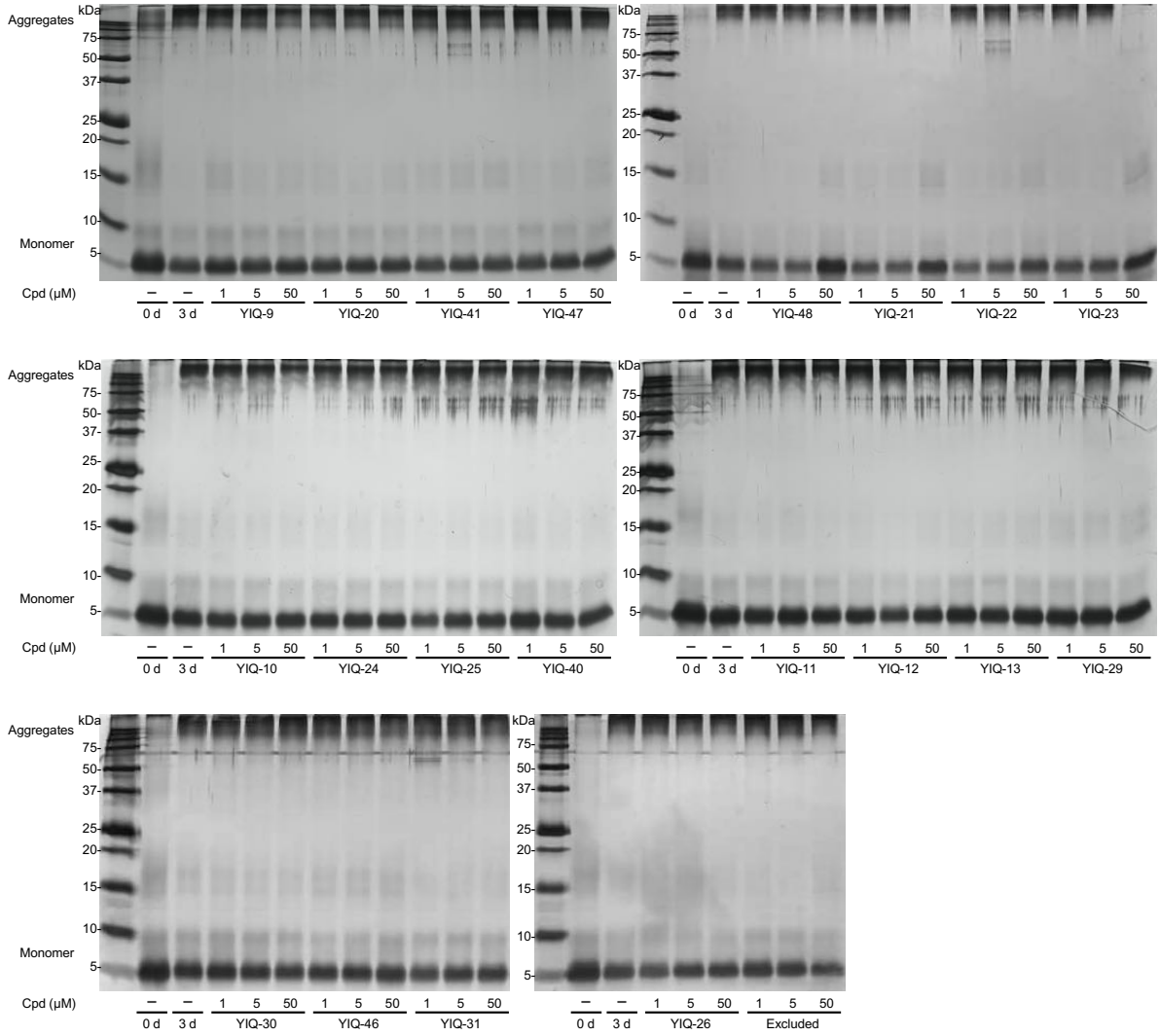


Fig. S5 Silver staining image of the gels displayed in figure 2 and S4. Two samples were excluded.

Figure S6. MTT assay of 32 **YIQ** compounds.

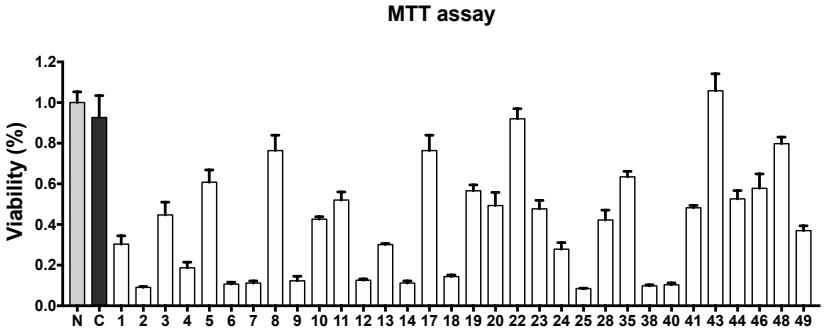


Fig. S6 MTT assay of 32 YIQ compounds selected for further experiments.

Figure S7. Wild-type mice brain staining with 32 **YIQ** compounds.

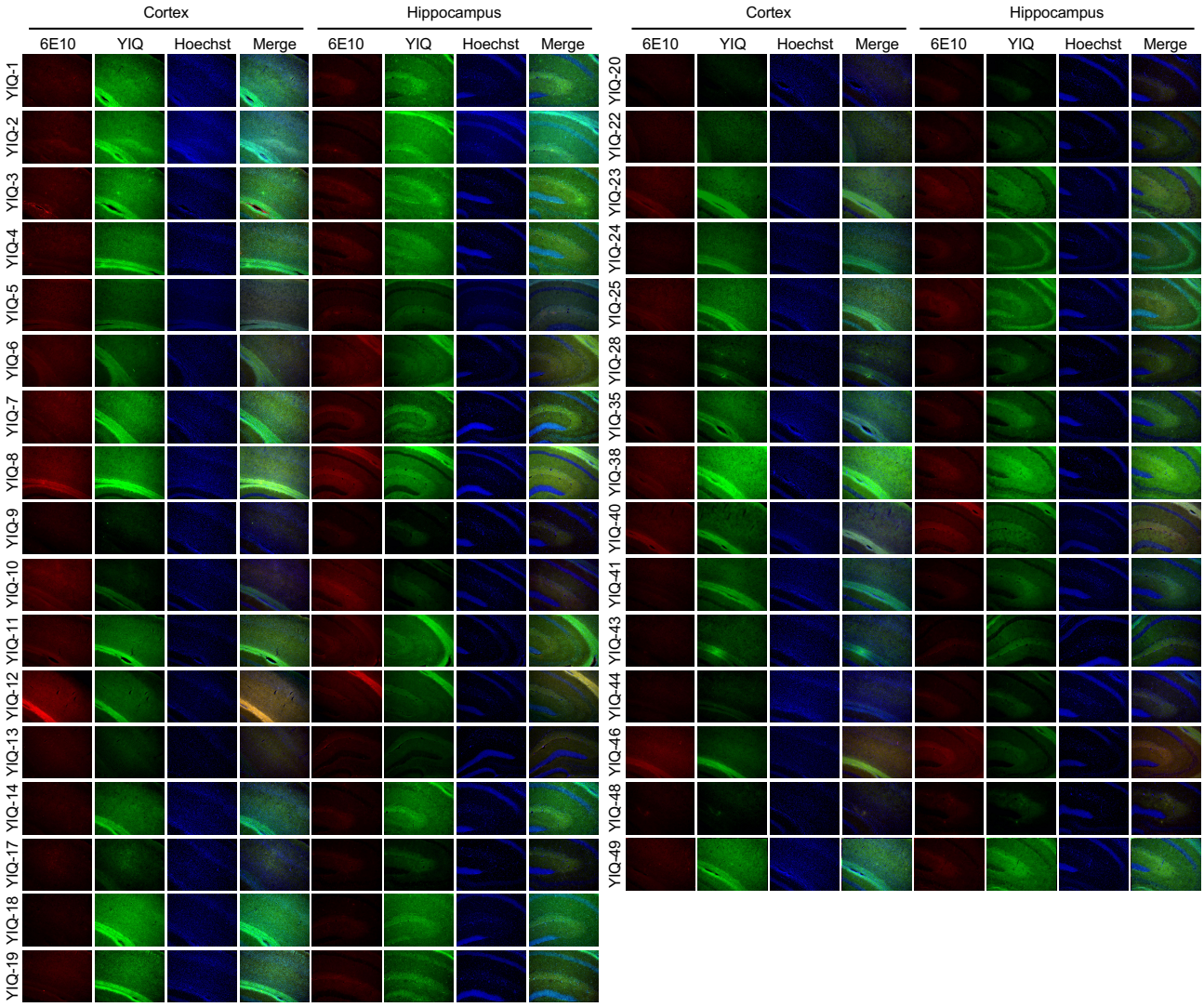


Fig. S7 Fluorescence microscope images of wild-type mice brain stained with selected YIQ derivatives (green), 6E10 (red), and Hoechst 33342 (blue).

Figure S8. Co-staining of **YIQ** compounds and 4G8 antibody.

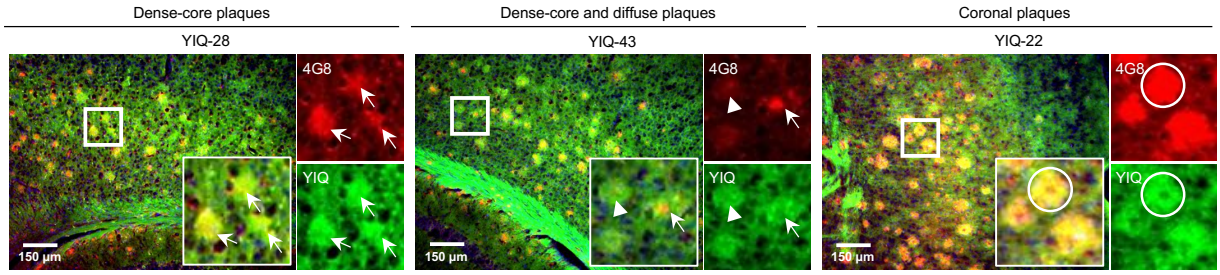


Fig. S8 Fluorescence microscope images of 5XFAD mice brain stained with selected YIQ derivatives (green), 4G8 (red), and Hoechst 33342 (blue). Dense core plaques (arrow), diffuse plaques (arrowhead) and coronal plaques (circle) are indicated on the brain images. All images were enlarged to a same sized scale.

Figure S9. Silver-stained whole gel image displayed in figure 6

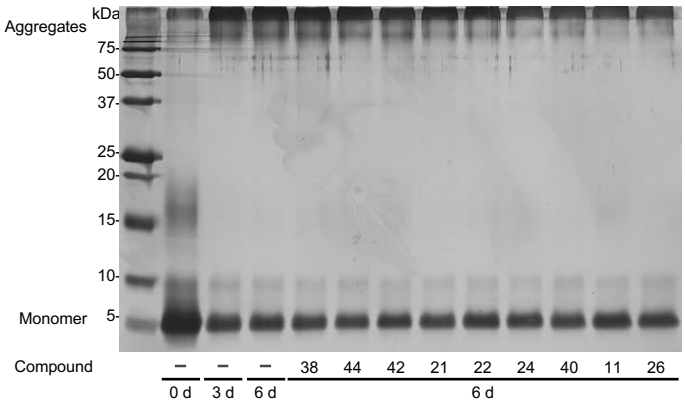


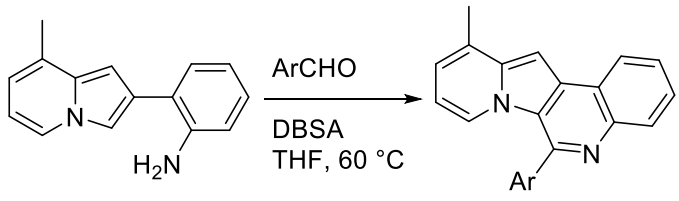
Fig. S9 Whole gel image displayed in figure 6, B).

Experimental Section

General Methods

Unless specified, all reagents and starting materials were purchased from commercial sources and used as received without purification. “Concentrated” refers to the removal of volatile solvents via distillation using a rotary evaporator. “Dried” refers to pouring onto, or passing through, anhydrous magnesium sulfate followed by filtration. Flash chromatography was performed using silica gel (230−400 mesh) with hexanes, ethyl acetate, and dichloromethane as eluent. All reactions were monitored by thin-layer chromatography on 0.25 mm silica plates (F-254) visualizing with UV light. Melting points were measured using a capillary melting point apparatus. ^{1}H and ^{13}C NMR spectra were recorded on 400 MHz NMR spectrometer and were described as chemical shifts, multiplicity (s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet), coupling constant in hertz (Hz), and number of protons. HRMS were measured with electrospray ionization (ESI) and Q-TOF mass analyzer.

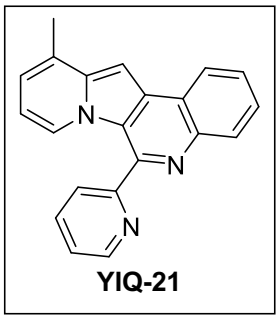
Representative Procedure for the Synthesis of YIQ-21



To a solution of 2-(8-methylindolizin-2-yl)aniline (50 mg, 0.22 mmol) in THF (1.5 mL) were added aldehyde (0.27 mmol, 1.2 equiv) and DBSA (0.04 mmol, 0.2 equiv) at rt. After being stirred at 60 °C for 16 h, the reaction mixture was concentrated under reduced pressure, diluted with ethyl acetate (2 mL), and washed with aq. $NaHCO_3$

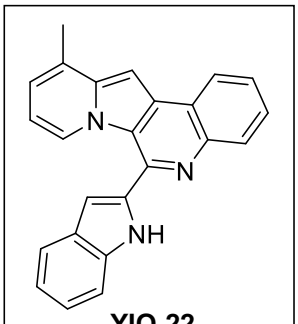
solution (2 mL). The water layer was extracted with ethyl acetate (2 mL) one more time. The organic layer was dried over $MgSO_4$, filtered, and concentrated *in vacuo* to give the residue, which was purified by column chromatography (hexane:ethyl acetate:dichloromathane = 10:1:2) to afford **YIQ-21**.

11-Methyl-6-(pyridin-2-yl)indolizino[3,2-*c*]quinoline (YIQ-21). Yellow solid, mp: 188.3- 189.7 °C (47.3 mg, 68 %); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.83 (d, *J* = 4.8 Hz, 1H), 8.43 (d, *J* = 8.0 Hz, 1H), 8.25 (d, *J* = 7.6 Hz, 1H), 8.05 – 7.98 (m, 2H), 7.95 (d, *J* = 7.2 Hz, 1H), 7.72 – 7.62 (m, 2H), 7.52 – 7.49 (m, 1H), 7.29 (s, 1H), 6.88 (d, *J* = 6.8 Hz, 1H), 6.43 (t, *J* = 6.8 Hz, 1H), 2.60 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 149.3, 147.1, 143.0, 140.2, 137.8, 129.7, 128.0, 127.5, 126.1, 125.8, 125.2, 124.1, 123.7, 123.0, 122.5, 121.6, 118.8, 118.7, 109.8, 90.9, 18.8; **HRMS** (ESI-QTOF) *m/z* $[M+Na]^+$ calcd for $C_{21}H_{15}N_3Na$ 332.1158, found 332.1155.



YIQ-21

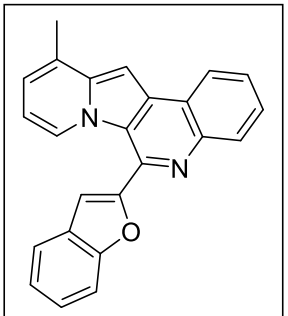
6-(1*H*-indol-2-yl)-11-methylindolizino[3,2-*c*]quinoline (YIQ-22). Yellow solid, mp: 205.4- 205.7 °C (38.3 mg, 49 %); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.80 (s, 1H), 8.81 (d, *J* = 7.2 Hz, 1H), 8.29 (d, *J* = 7.6 Hz, 1H), 8.12 (d, *J* = 8.0 Hz, 1H), 7.72 (d, *J* = 7.6 Hz, 1H), 7.58 – 7.48 (m, 3H), 7.28 (t, *J* = 7.6 Hz, 1H), 7.20 – 7.16 (m, 2H), 7.02 (s, 1H), 6.88 (d, *J* = 6.4 Hz, 1H), 6.46 (d, *J* = 6.8 Hz, 1H), 2.58 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 142.7, 140.4, 140.1, 136.8, 136.4, 134.9, 131.9, 129.0, 128.0, 127.5, 125.7, 125.1, 123.4, 123.3, 122.5, 122.4, 121.9, 121.3, 120.3, 111.6, 109.8, 104.6, 90.7, 18.7; **HRMS** (ESI-QTOF) *m/z* $[M+H]^+$ calcd for $C_{24}H_{18}N_3$



YIQ-22

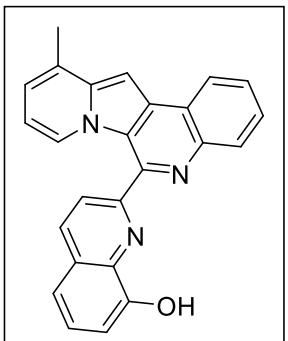
348.1495, found 348.1499.

6-(Benzofuran-2-yl)-11-methylindolizino[3,2-*c*]quinoline (YIQ-23). Yellow solid, mp: 179.1-179.9 °C (31.3mg, 40 %); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.43 (d, *J* = 8.0 Hz, 1H), 8.29 (d, *J* = 8.4 Hz, 1H), 8.06 (d, *J* = 7.2 Hz, 1H), 7.78 (d, *J* = 7.2 Hz, 1H), 7.74 – 7.63 (m, 3H), 7.45 – 7.36 (m, 3H), 7.30 (s, 1H), 6.92 (d, *J* = 6.4 Hz, 1H), 6.50 (t, *J* = 7.2 Hz, 1H), 2.63 (s, 3H); **^{13}C NMR** (100 MHz, CDCl3) δ 155.1, 153.6, 142.9, 140.2, 138.0, 131.8, 129.8, 128.6, 128.0, 127.6, 126.4, 125.3, 125.0, 123.5, 123.5, 122.9, 122.6, 121.9, 111.8, 110.3, 108.0, 104.4, 90.8, 18.7; **HRMS** (ESI-QTOF) *m/z* $[M+H]^+$ calcd for $C_{24}H_{17}N_2O$ 349.1335, found 349.1331.

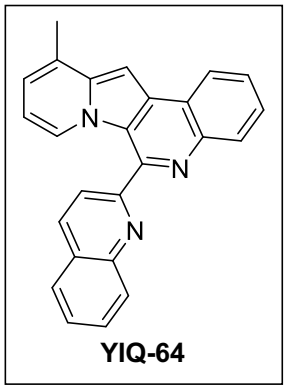


YIQ-23

2-(11-Methylindolizino[3,2-*c*]quinolin-6-yl)quinolin-8-ol (YIQ-26). Yellow solid, mp: 277.3-277.6 °C (34.6mg, 41 %); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.84 – 8.39 (m, 2H), 8.31 (s, 1H), 8.25 (d, *J* = 8.8 Hz, 2H), 8.10 (d, *J* = 7.2 Hz, 1H), 7.70 – 7.63 (m, 2H), 7.55 (t, *J* = 8.0 Hz, 1H), 7.45 (d, *J* = 8.0 Hz, 1H), 7.31 (s, 1H), 7.59 – 7.24 (m, 1H), 6.87 (d, *J* = 6.0 Hz, 1H), 6.38 (t, *J* = 6.8 Hz, 1H), 2.62 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 155.4, 152.7, 146.5, 142.6, 140.0, 137.4, 136.9, 133.9, 131.9, 129.3, 128.5, 128.3, 127.8, 127.4, 126.1, 125.7, 123.3, 123.2, 122.5, 121.3, 117.9, 110.9, 109.6, 90.7, 18.7; **HRMS** (ESI-QTOF) *m/z* $[M+H]^+$ calcd for $C_{25}H_{18}N_3O$ 376.1444, found 376.1443.



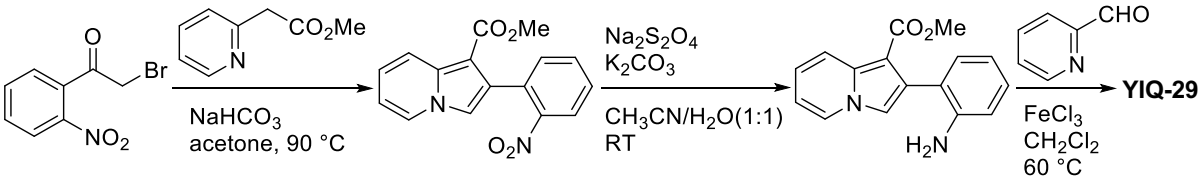
YIQ-26



YIQ-64

11-Methyl-6-(quinolin-2-yl)indolizino[3,2-*c*]quinoline (YIQ-64). Yellow solid, mp: 247.4- 248.1 °C (24.3mg, 30 %); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.45 (t, *J* = 7.0 Hz, 2H), 8.28 – 8.17 (m, 4H), 7.98 (d, *J* = 8.0 Hz, 1H), 7.81 (t, *J* = 7.6 Hz, 1H), 7.72 – 7.64 (m, 3H), 7.33 (s, 1H), 6.87 (d, *J* = 7.2 Hz, 1H), 6.36 (d, *J* = 6.8 Hz, 1H), 2.61 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 158.3, 147.4, 147.3, 143.1, 140.3, 138.8, 137.8, 132.4, 130.2, 129.8, 128.1, 128.0, 127.9, 127.5, 127.5, 126.3, 126.2, 123.7, 123.1, 122.8, 122.6, 121.9, 109.7, 90.9, 18.9; **HRMS** (ESI-QTOF) *m/z* $[M+Na]^+$ calcd for $C_{25}H_{17}N_3Na$ 382.1315, found 382.1315.

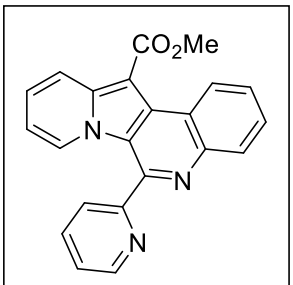
Synthesis of YIQ-29



To a solution of 2-bromo-1-(2-nitrophenyl)ethan-1-one (500 mg, 2.23 mmol) in acetone (6.0 mL) were added methyl 2-(pyridin-2-yl)acetate (447.81 μL, 1.5 equiv) and $NaHCO_3$ (374.98 mg, 2.0 equiv) at rt. After being stirred at 90 °C for 16 h, the reaction mixture was concentrated under reduced pressure, diluted with dichloromethane (5 mL), and washed with water (5 mL). The water layer was extracted with dichloromethane (5 mL) one more time. The organic layer was dried over $MgSO_4$, filtered, and concentrated *in vacuo* to give the residue, which was purified by column

chromatography (hexane:ethyl acetate:dichloromathane = 10:1:2) to afford methyl 2-(2-nitrophenyl)indolizine-1-carboxylate (512.2 mg, 77.5 %). To a solution of methyl 2-(2-nitrophenyl)indolizine-1-carboxylate (512 mg, 1.73 mmol) in acetonitrile/H_2O (1:1) solution (10 mL) were added sodium dithionite (1504.4 mg, 5.0 equiv) and K_2CO_3 (1194.20 mg, 5.0 equiv) at rt. After being stirred at rt for 0.5 h, the reaction mixture was concentrated under reduced pressure, diluted with dichloromethane (5 mL), and washed with water (5 mL). The water layer was extracted with dichloromethane (5 mL) one more time. The organic layer was dried over $MgSO_4$, filtered, and concentrated *in vacuo* to give the residue to afford methyl 2-(2-aminophenyl)indolizine-1-carboxylate (437.3 mg, 94.9 %). To a solution of methyl 2-(2-aminophenyl)indolizine-1-carboxylate (30 mg, 0.113 mmol) in anhydrous dichloromethane (1 mL) were added pyridine-2-carboxaldehyde (12.92 μL, 1.2 equiv) and $FeCl_3$ (3.45 mg, 0.3 equiv) at rt. After being stirred at 60 °C for 16 h, the reaction mixture was diluted with dichloromethane (1 mL), and washed with water (2 mL). The water layer was extracted with dichloromethane (1 mL) one more time. The organic layer was dried over $MgSO_4$, filtered, and concentrated *in vacuo* to give the residue, which was purified by column chromatography (hexane:ethyl acetate:dichloromathane = 1:1:1) to afford **YIQ-29**.

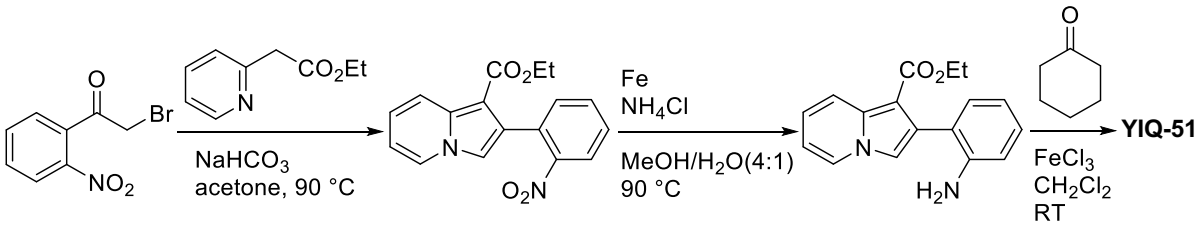
Methyl 6-(pyridin-2-yl)indolizino[3,2-*c*]quinoline-12-carboxylate (YIQ-29). Yellow solid, mp: 199.8-200.3 °C (21.4 mg, 54 %); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.70 (d, *J* = 7.5 Hz, 1H), 8.80 (s, 1H), 8.47 (d, *J* = 8.4 Hz, 1H), 8.25 (d, *J* = 7.3 Hz, 1H), 8.07-7.95 (m, 3H), 7.78-7.72 (m, 1H), 7.71-7.64 (m, 1H), 7.52 (s, 1H), 7.39-7.31 (m, 1H), 6.66 (s, 1H), 4.11 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 165.8, 158.0, 149.3, 146.4, 144.4, 141.5, 137.9, 131.6, 129.7, 128.3, 128.1, 127.6, 127.5,



YIQ-29

126.2, 125.0, 124.2, 122.6, 122.0, 120.4, 111.8, 99.3, 51.4; **HRMS** (ESI-QTOF) *m/z* $[M+H]^+$ calcd for $C_{22}H_{16}N_3O_2$, 354.1237, found 354.1240.

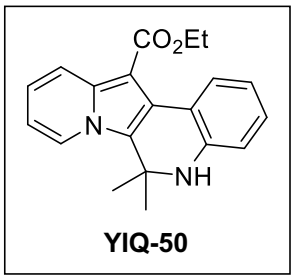
Representative Procedure for the Synthesis of YIQ-51



To a solution of 2-bromo-1-(2-nitrophenyl)ethan-1-one (500 mg, 2.23 mmol) in acetone (7.5 mL) were added ethyl 2-(pyridin-2-yl)acetate (509.78 μL, 1.5 equiv) and $NaHCO_3$ (374.98 mg, 2.0 equiv) at rt. After being stirred at 90 °C for 16 h, the reaction mixture was concentrated under reduced pressure, diluted with dichloromethane (5 mL), and washed with water (5 mL). The water layer was extracted with dichloromethane (5 mL) one more time. The organic layer was dried over $MgSO_4$, filtered, and concentrated *in vacuo* to give the residue, which was triturated using diethyl ether to afford ethyl 2-(2-nitrophenyl)indolizine-1-carboxylate. To a solution of ethyl 2-(2-nitrophenyl)indolizine-1-carboxylate (100 mg, 1.13 mmol) in methanol/H_2O (4:1) solution (4 mL) were added iron powder (179.98 mg, 10.0 equiv) and NH_4Cl (258.57 mg, 15.0 equiv) at rt. After being stirred at 90 °C for 16 h, the reaction mixture was filtered through a pad of Celite and washed with dichloromethane (10 mL). The filtrate was concentrated under reduced pressure, diluted with dichloromethane (10 mL), and washed with water (5 mL). The organic layer was dried over $MgSO_4$, filtered, and concentrated *in vacuo* to give the residue, which was purified by column chromatography (hexane:ethyl acetate:dichloromathane = 25:1:2) to afford ethyl 2-(2-aminophenyl)indolizine-1-

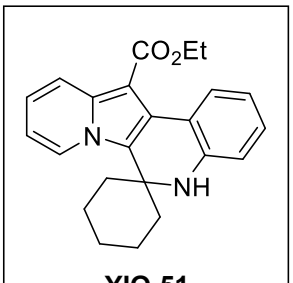
carboxylate. To a solution of ethyl 2-(2-aminophenyl)indolizine-1-carboxylate (50 mg, 0.18 mmol) in anhydrous dichloromethane (1 mL) were added cyclohexanone (46.63 μL, 2.5 equiv) and $FeCl_3$ (1.84 mg, 0.1 equiv) at rt. After being stirred at rt for 2.5 h, the reaction mixture was diluted with dichloromethane (1 mL), and washed with water (2 mL). The water layer was extracted with dichloromethane (1 mL) one more time. The organic layer was dried over $MgSO_4$, filtered, and concentrated *in vacuo* to give the residue, which was purified by column chromatography (hexane:ethyl acetate:dichloromathane = 30:1:2) to afford **YIQ-51**.

Ethyl 6,6-dimethyl-5,6-dihydroindolizino[3,2-*c*]quinoline-12-carboxylate (YIQ-50). Yellow solid, mp: 122.3-123.0 °C (44.5 mg, 78 %); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.26 (m, 2H), 8.04 (s, 1H), 7.09-7.01 (m, 1H), 7.00-6.97 (m, 1H), 6.80 (s, 1H), 6.68 (s, 1H), 6.62 (d, *J* = 5.8 Hz, 1H), 4.44 (s, 2H), 1.70 (s, 6H), 1.45 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 165.6, 141.8, 137.5, 127.9, 127.7, 126.5, 123.5, 120.8, 120.6, 118.4, 117.6, 114.1, 112.3, 99.7, 59.9, 53.1, 28.3, 14.5; **HRMS** (ESI-QTOF) *m/z* $[M+H]^+$ calcd for $C_{20}H_{21}N_2O_2$ 321.1598, found 321.1602.



YIQ-50

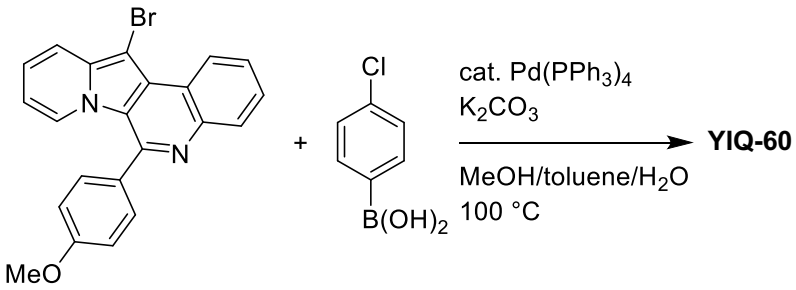
Ethyl 5'*H*-spiro[cyclohexane-1,6'-indolizino[3,2-*c*]quinoline]-12'-carboxylate (YIQ-51). Orange solid, mp: 71.8-72.3 °C (44.2 mg, 69 %); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.25-8.15 (m, 3H), 7.04 (t, *J* = 7.2 Hz, 1H), 6.95 (dd, *J* = 8.4, 7.1 Hz, 1H), 6.77 (t, *J* = 7.3 Hz, 1H), 6.65 (d, *J* = 7.1 Hz, 2H), 4.45 (t, *J* = 6.8 Hz, 2H), 2.32-2.20 (m, 2H), 2.06 (d, *J* = 12.8 Hz, 2H), 1.86 (d, *J* = 12.4 Hz, 1H), 1.77 (d, *J*



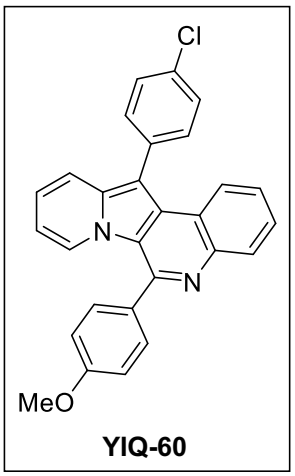
YIQ-51

= 11.9 Hz, 2H), 1.65 (t, *J* = 13.2 Hz, 3H), 1.44 (t, *J* = 6.9 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 165.7, 141.3, 137.8, 127.9, 127.7, 126.7, 124.1, 121.8, 120.7, 120.6, 118.1, 117.8, 114.1, 112.1, 99.8, 59.9, 54.8, 32.9, 25.0, 20.8, 14.5; **HRMS** (ESI-QTOF) *m/z* $[M+Na]^+$ calcd for $C_{23}H_{24}N_2O_2Na$ 383.1730, found 383.1756.

Synthesis of YIQ-60



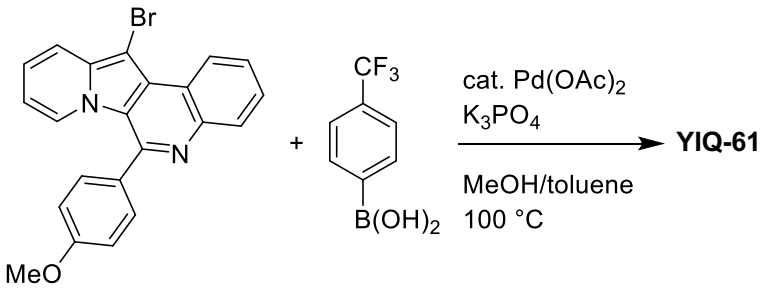
12-(4-Chlorophenyl)-6-(4-methoxyphenyl)indolizino[3,2-*c*]quinoline (YIQ-60).



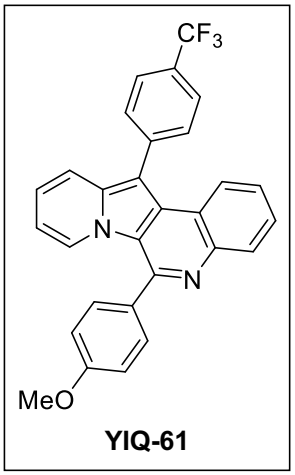
YIQ-60

Yellow solid, mp: 204.3-205.1 °C (21.2 mg 66 %); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.24 (d, *J* = 7.9 Hz, 1H), 8.05 (d, *J* = 8.0 Hz, 1H), 7.95 (d, *J* = 6.9 Hz, 1H), 7.63 (d, *J* = 7.5 Hz, 3H), 7.56 (s, 4H), 7.43 (d, *J* = 8.0 Hz, 1H), 7.37 (t, *J* = 7.3 Hz, 1H), 7.16 (d, *J* = 7.9 Hz, 2H), 7.02 (t, *J* = 8.0 Hz, 1H), 6.47 (t, *J* = 6.3 Hz, 1H), 3.95 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 160.3, 148.5, 143.6, 136.8, 133.6, 133.4, 132.6, 132.1, 130.0, 129.7, 129.2, 127.9, 127.3, 126.7, 125.2, 123.8, 123.7, 122.5, 120.7, 117.4, 114.8, 110.2, 108.0; **HRMS** (ESI-QTOF) *m/z* $[M+H]^+$ calcd for $C_{28}H_{20}ClN_2O$, 435.1259, found 435.1263.

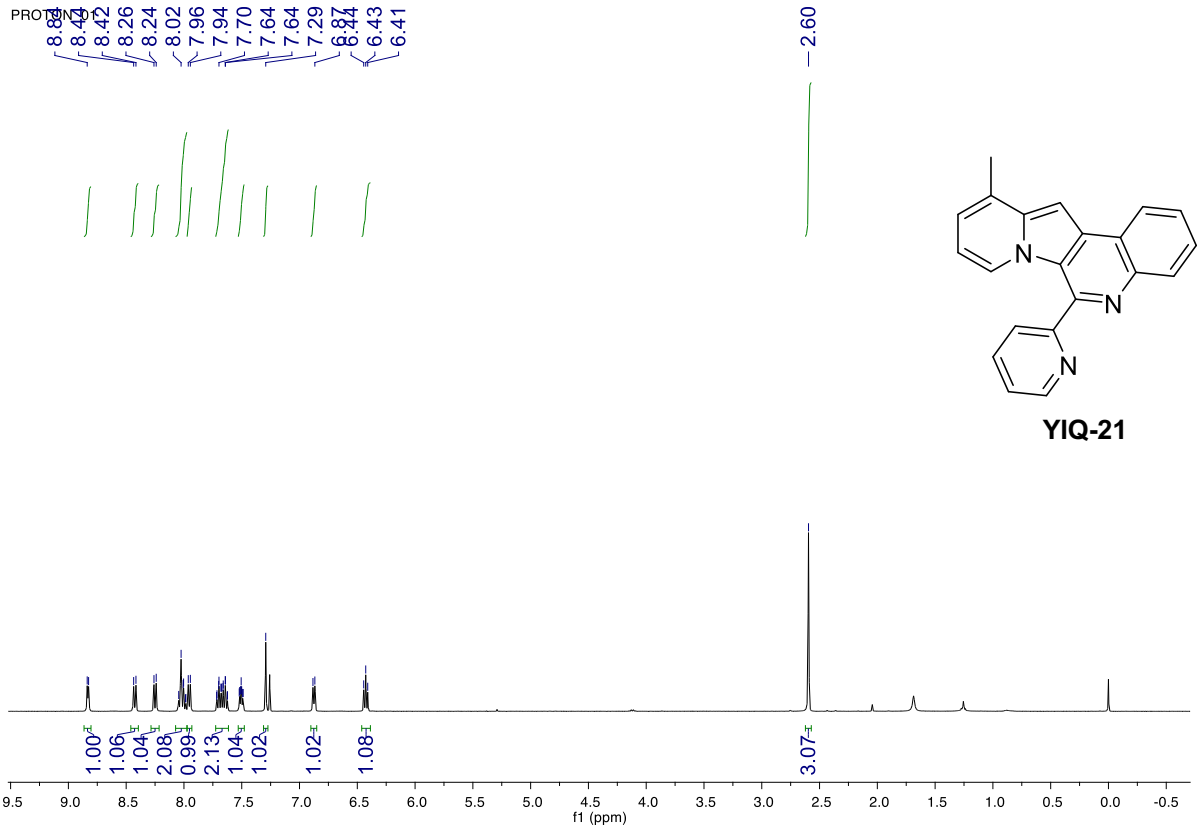
Synthesis of YIQ-61



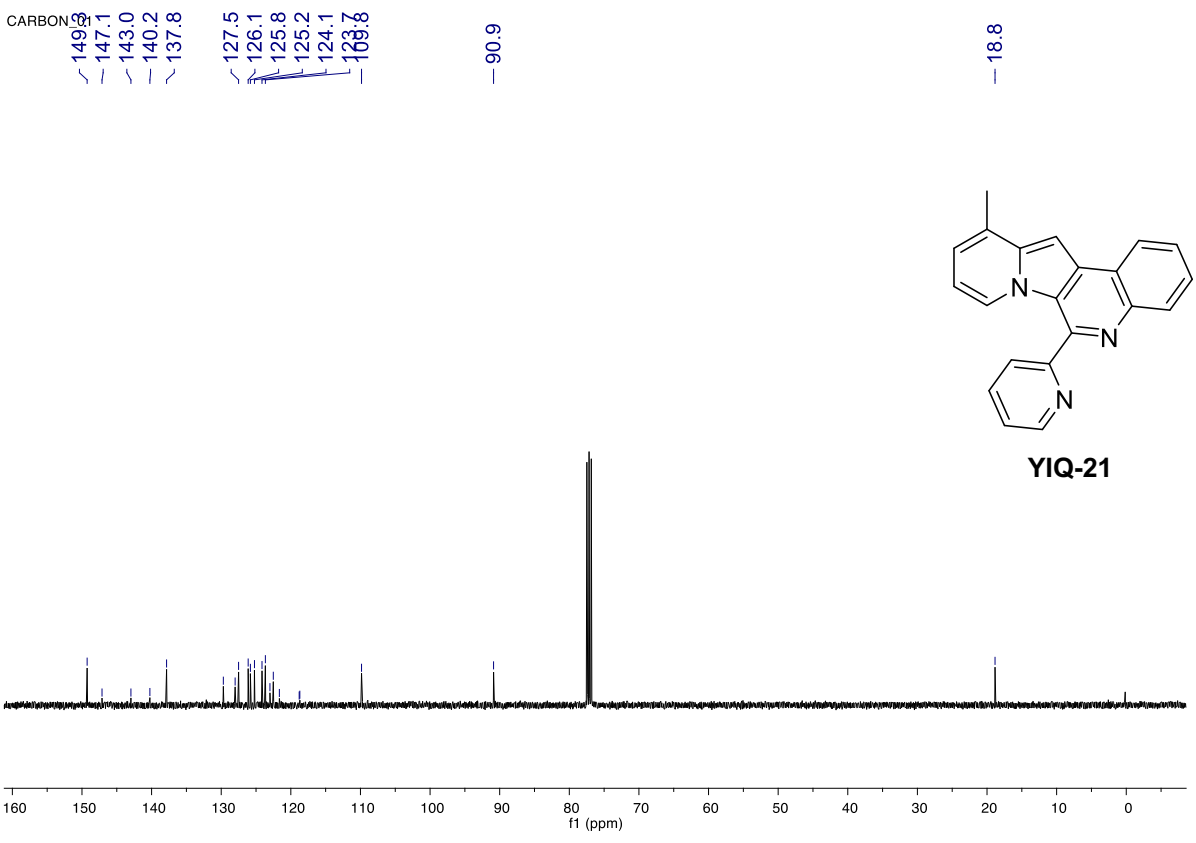
6-(4-Methoxyphenyl)-12-(4-(trifluoromethyl)phenyl)indolizino[3,2-*c*]quinoline



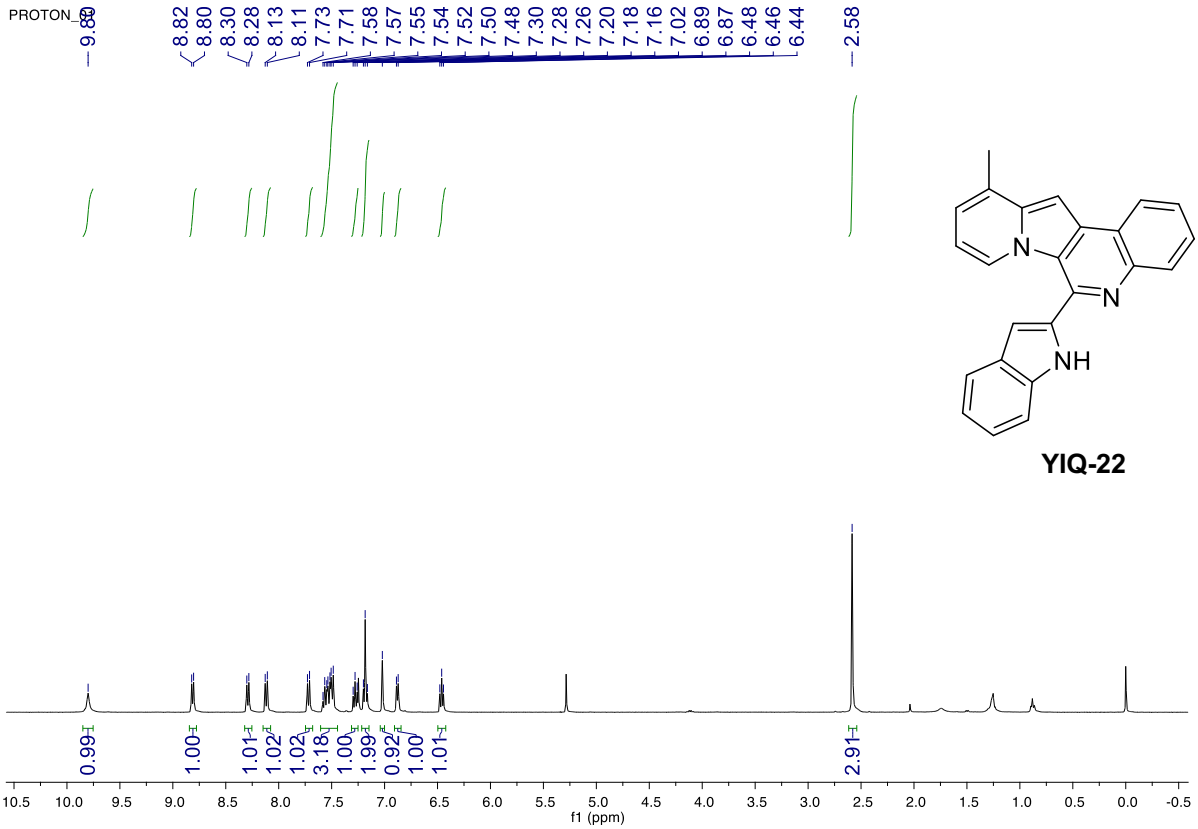
(YIQ-62). Yellow solid, mp: 220.4-221.2 °C (15.3 mg, 44.0%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.26 (d, *J* = 7.5 Hz, 1H), 8.02 (d, *J* = 7.7 Hz, 1H), 7.97 (d, *J* = 7.4 Hz, 1H), 7.85 (d, *J* = 7.6 Hz, 2H), 7.77 (d, *J* = 6.9 Hz, 2H), 7.64 (d, *J* = 6.1 Hz, 3H), 7.45 (d, *J* = 8.7 Hz, 1H), 7.37 (t, *J* = 7.1 Hz, 1H), 7.16 (d, *J* = 8.0 Hz, 2H), 7.05 (t, *J* = 8.0 Hz, 1H), 6.50 (t, *J* = 6.6 Hz, 1H), 3.96 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 160.4, 148.5, 143.6, 139.2, 136.9, 131.9, 131.6, 130.0, 129.7, 127.9, 127.5, 126.8, 125.9, 125.8, 125.3, 124.1, 123.8, 122.3, 120.9, 117.3, 115.5, 114.8, 110.4, 107.9, 94.45; **HRMS** (ESI-QTOF) *m/z* $[M+H]^+$ calcd for $C_{29}H_{20}F_3N_2O$, 469.1522, found 469.1525.


PROTON-01
8.83
8.42
8.42
8.26
8.24
8.02
7.96
7.94
7.70
7.64
7.64
7.29
6.44
6.43
6.41
2.60
1.00
1.06
1.04
2.08
0.99
2.13
1.04
1.02
1.02
1.08
3.07
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

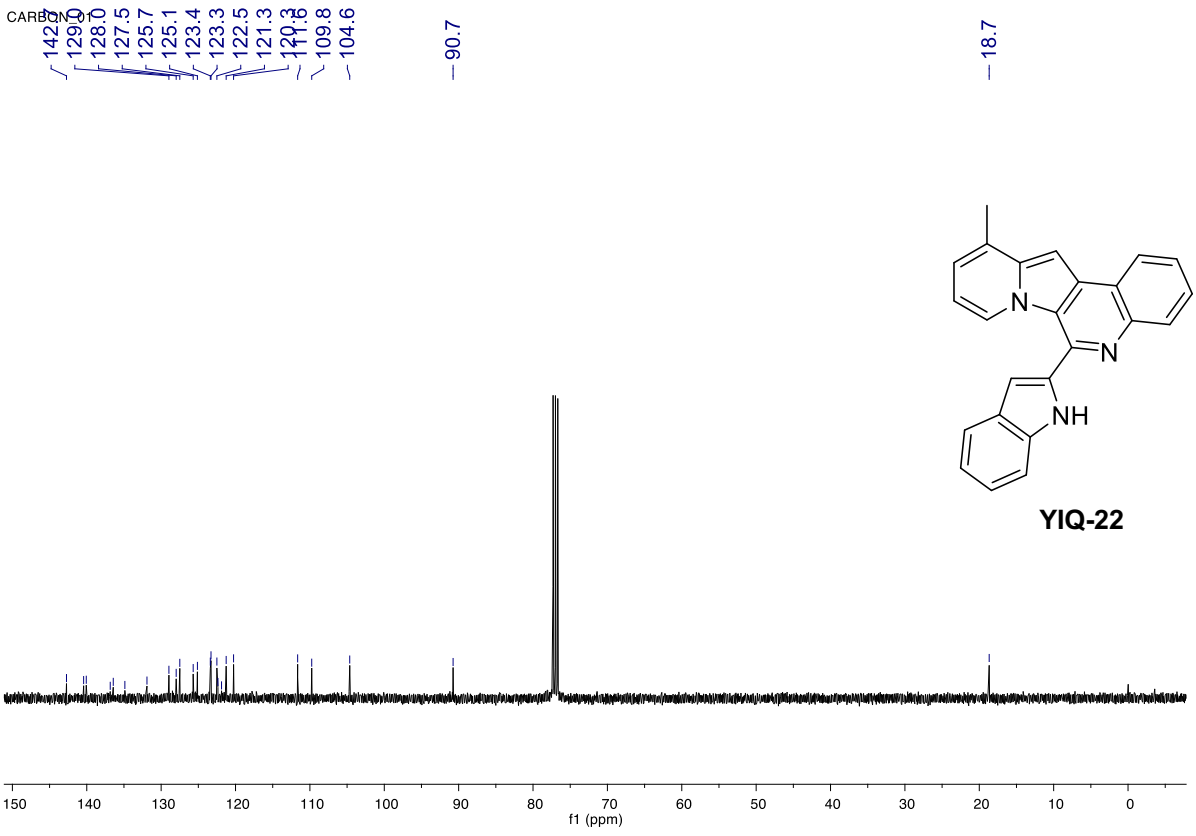
YIQ-21


CARBON-01
149.3
147.1
143.0
140.2
137.8
127.5
126.1
125.8
125.2
124.1
123.7
109.8
90.9
18.8
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

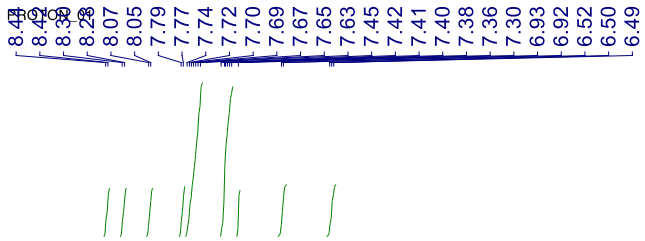
YIQ-21

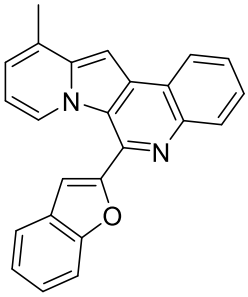

PROTON_01
9.80
8.82
8.80
8.30
8.28
8.13
8.11
7.73
7.71
7.58
7.57
7.55
7.54
7.52
7.50
7.48
7.30
7.28
7.26
7.20
7.18
7.16
7.02
6.89
6.87
6.48
6.46
6.44
2.58
0.99
1.00
1.01
1.02
1.02
3.18
1.00
1.99
0.92
1.00
1.01
2.91
f1 (ppm)

YIQ-22

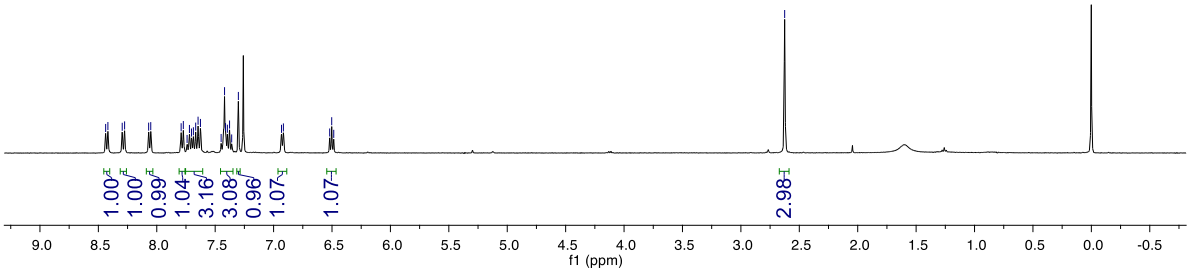

CARBON_01
142.0
129.0
128.0
127.5
125.7
125.1
123.4
123.3
122.5
121.3
120.3
111.6
109.8
104.6
90.7
18.7
f1 (ppm)

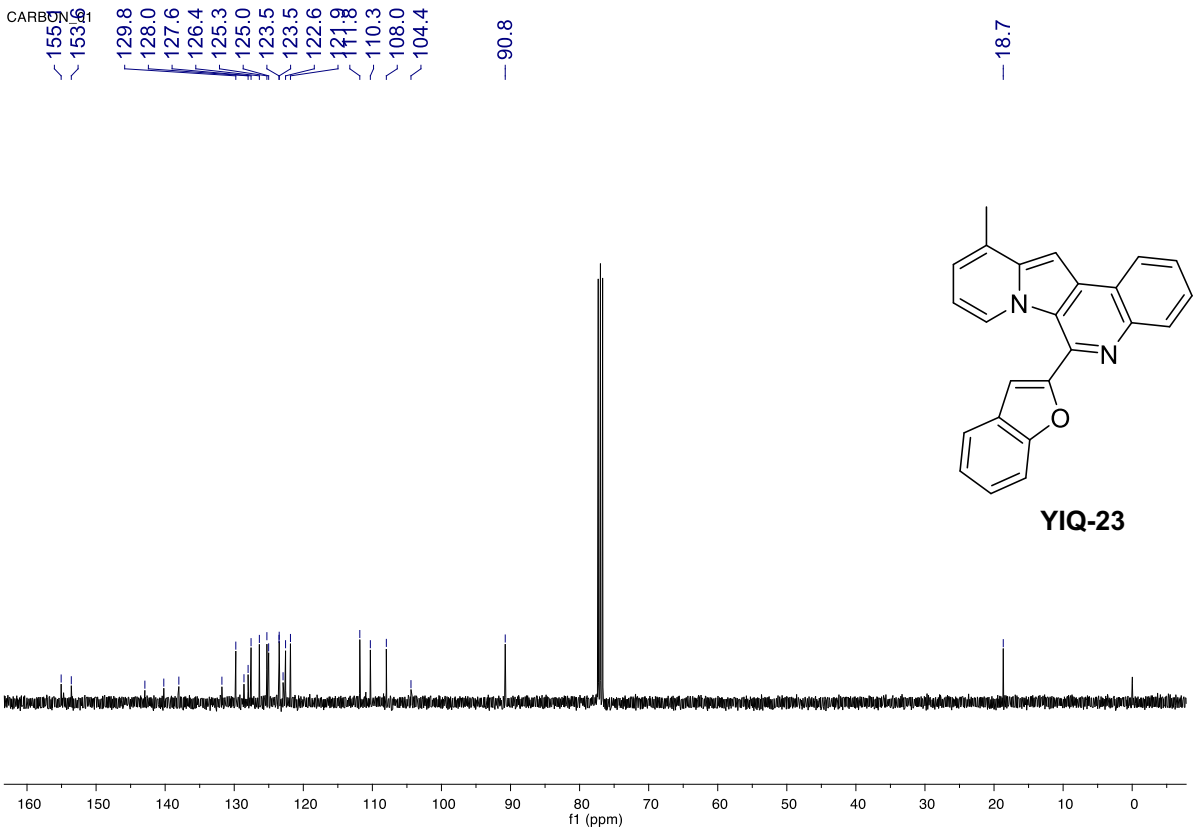
YIQ-22


8.44
8.42
8.39
8.28
8.07
8.05
7.79
7.77
7.74
7.72
7.70
7.69
7.67
7.65
7.63
7.45
7.42
7.41
7.40
7.38
7.36
7.30
6.93
6.92
6.52
6.50
6.49
2.63

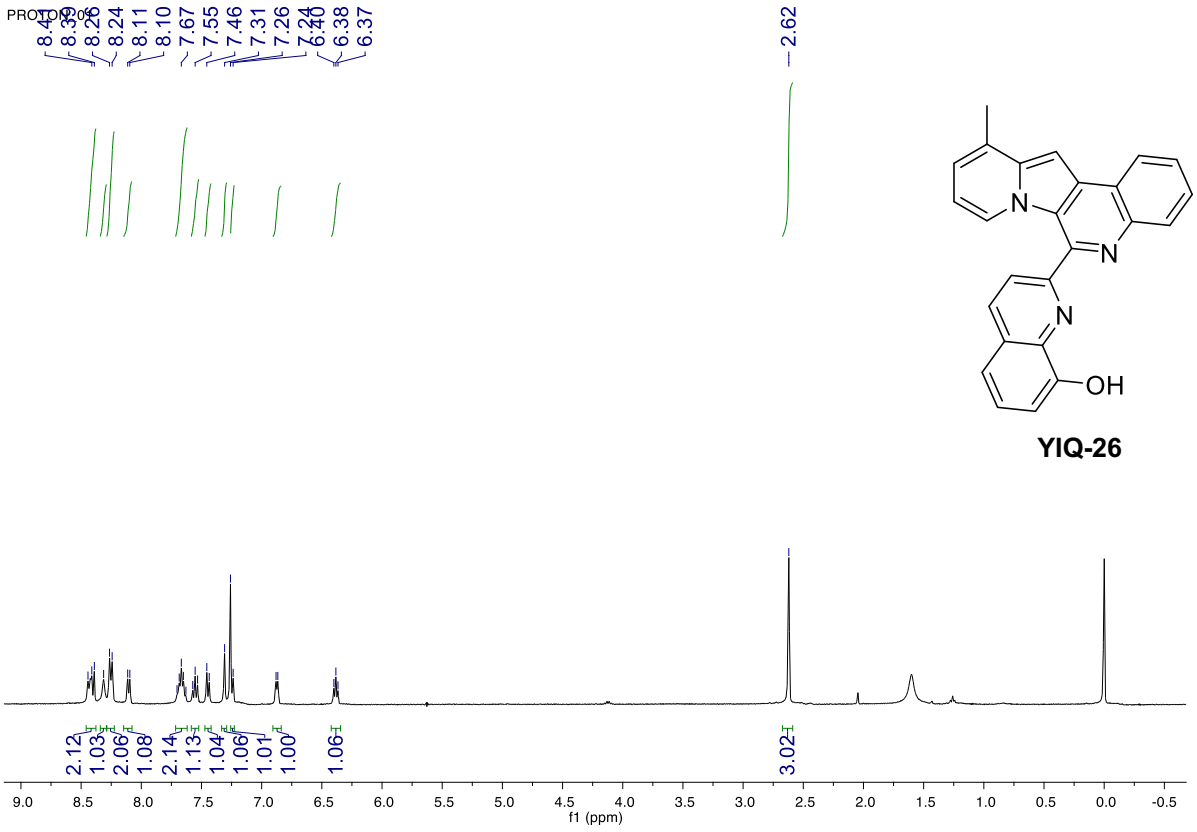


YIQ-23

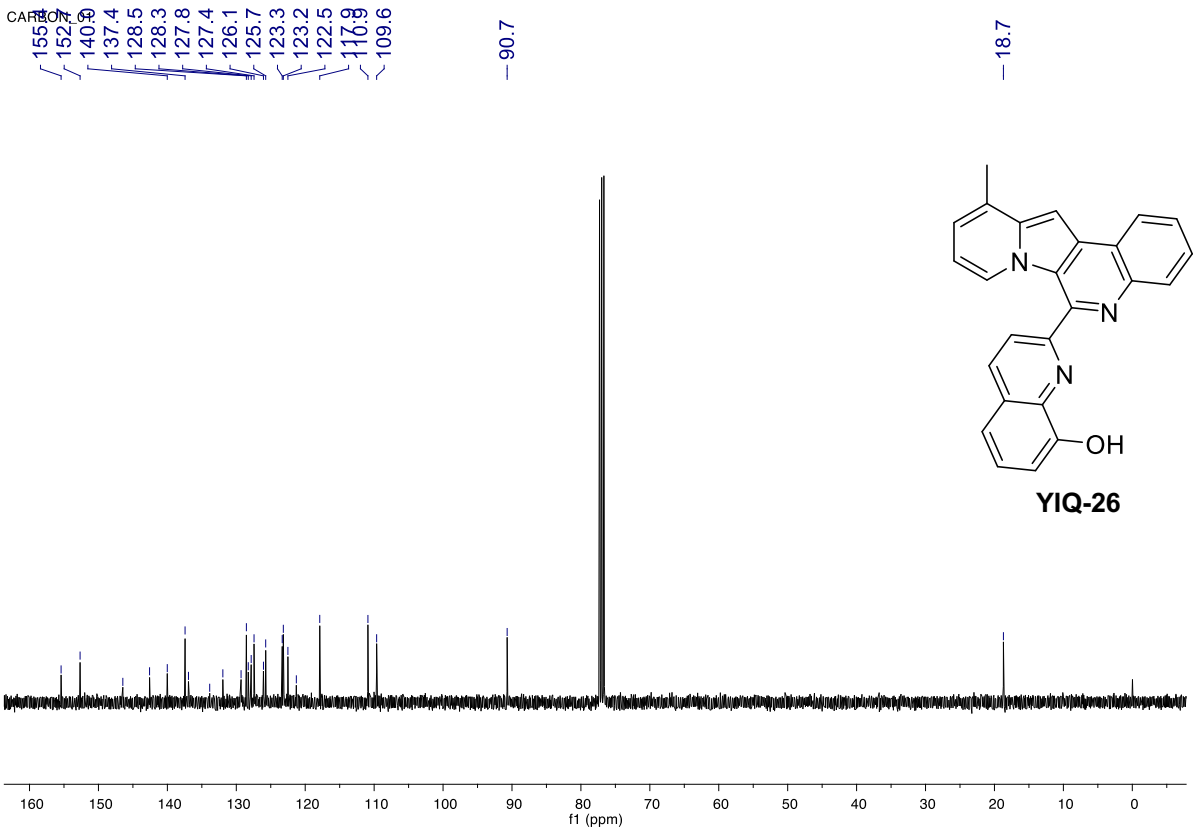

1.00
1.00
0.99
1.04
3.16
3.08
0.96
1.07
1.07
2.98
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


CARBON_01
155.6
153.6
129.8
128.0
127.6
126.4
125.3
125.0
123.5
123.5
122.6
111.9
111.8
110.3
108.0
104.4
90.8
18.7
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

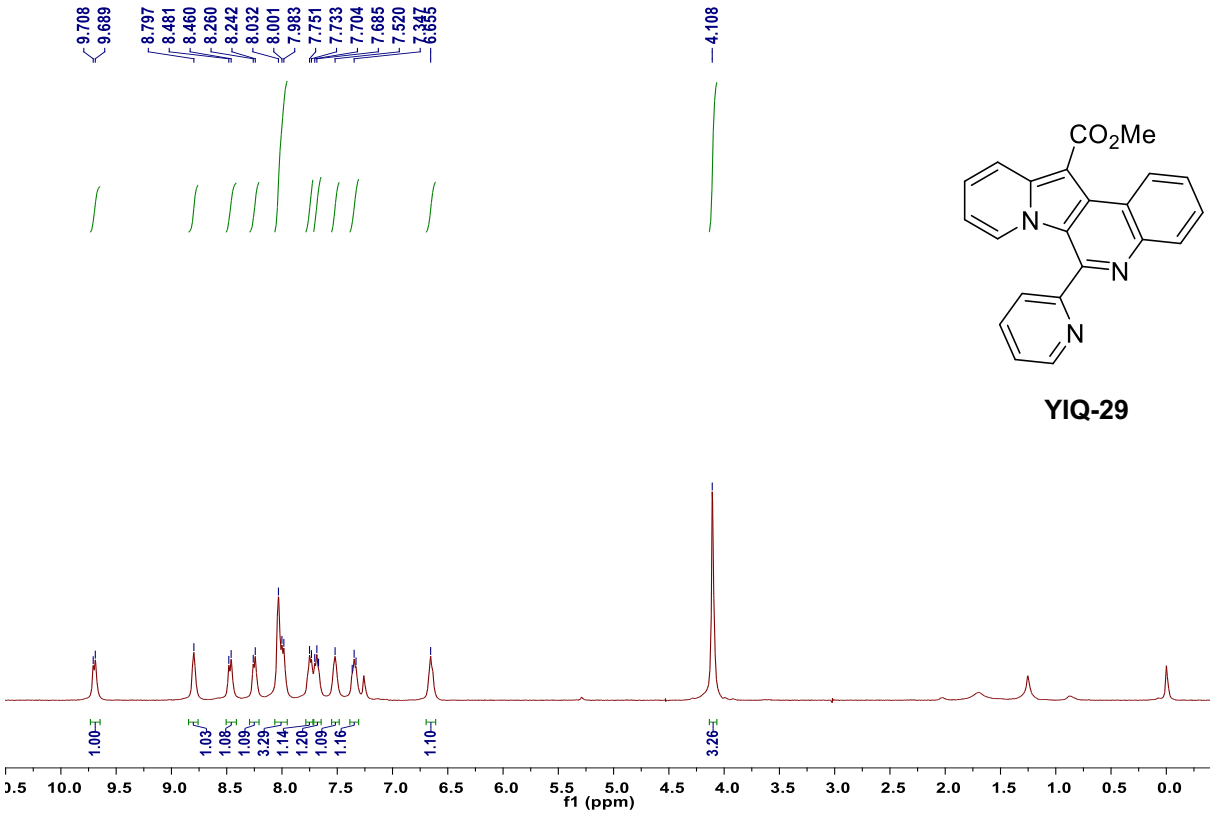
YIQ-23


PROTON_01
8.41
8.39
8.26
8.24
8.11
8.10
7.67
7.55
7.46
7.31
7.26
7.24
6.40
6.38
6.37
2.62
N
N
N
OH
2.12
1.03
2.06
1.08
2.14
1.13
1.04
1.06
1.01
1.00
1.06
3.02
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

YIQ-26

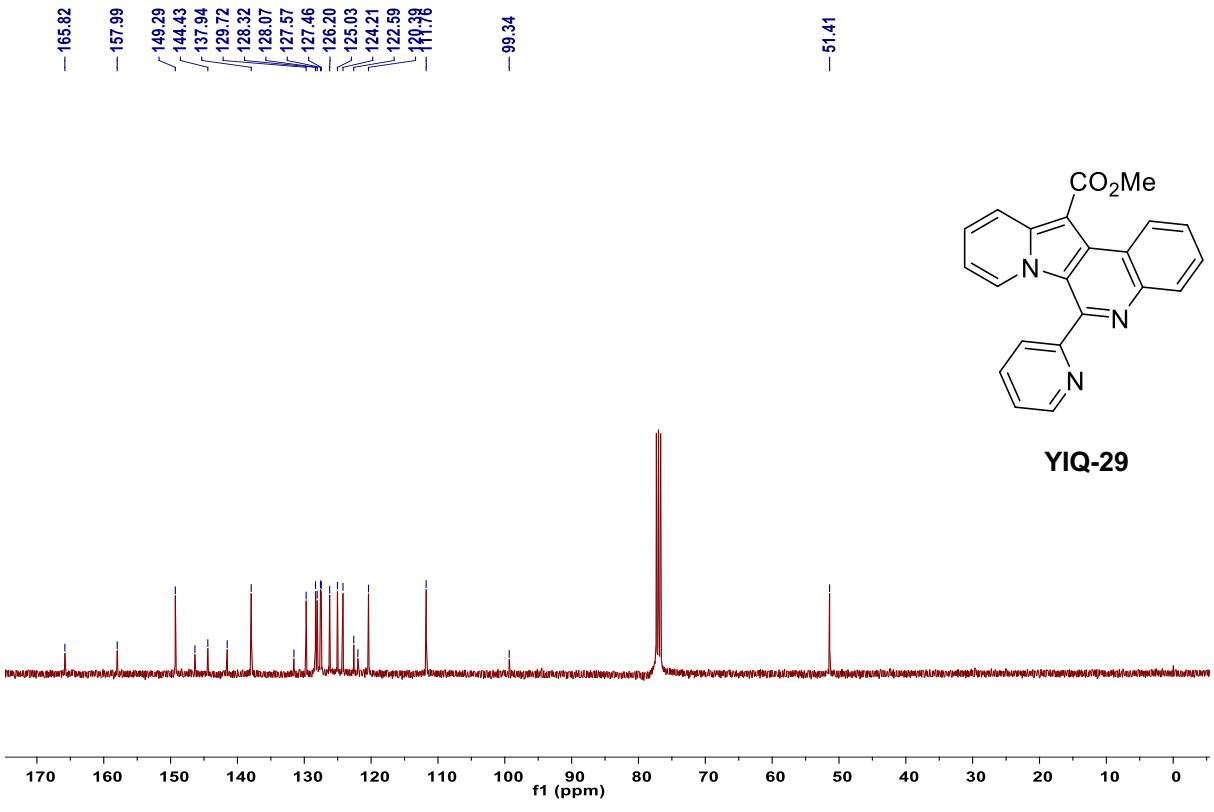

CARBON_01
155.7
152.6
140.6
137.4
128.5
128.3
127.8
127.4
126.1
125.7
123.3
123.2
122.5
117.9
110.9
109.6
90.7
18.7
N
N
N
OH
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

YIQ-26


9.708
9.689
8.797
8.481
8.460
8.260
8.242
8.032
8.001
7.983
7.751
7.733
7.704
7.685
7.520
4.108
1.00
1.03
1.08
1.09
3.29
1.14
1.20
1.09
1.16
1.10
3.26
f1 (ppm)

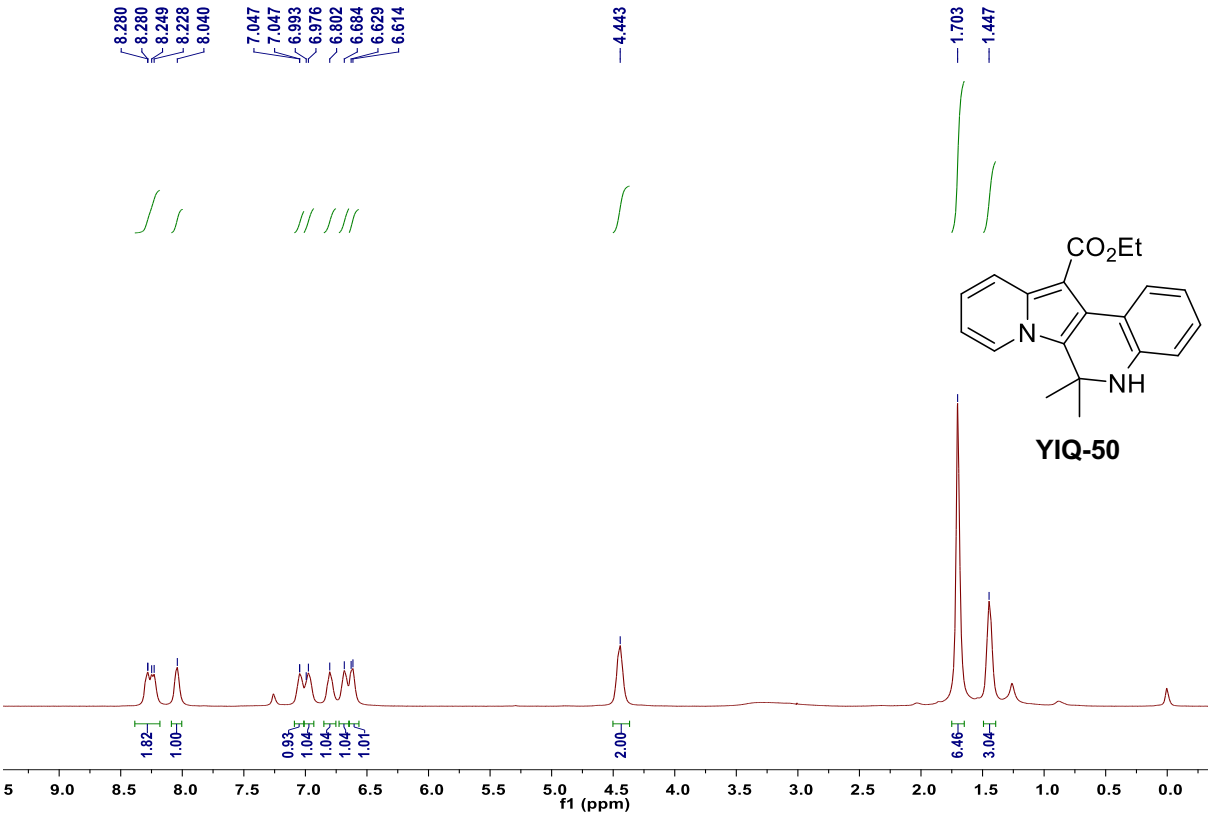
CO2Me
N
N
N

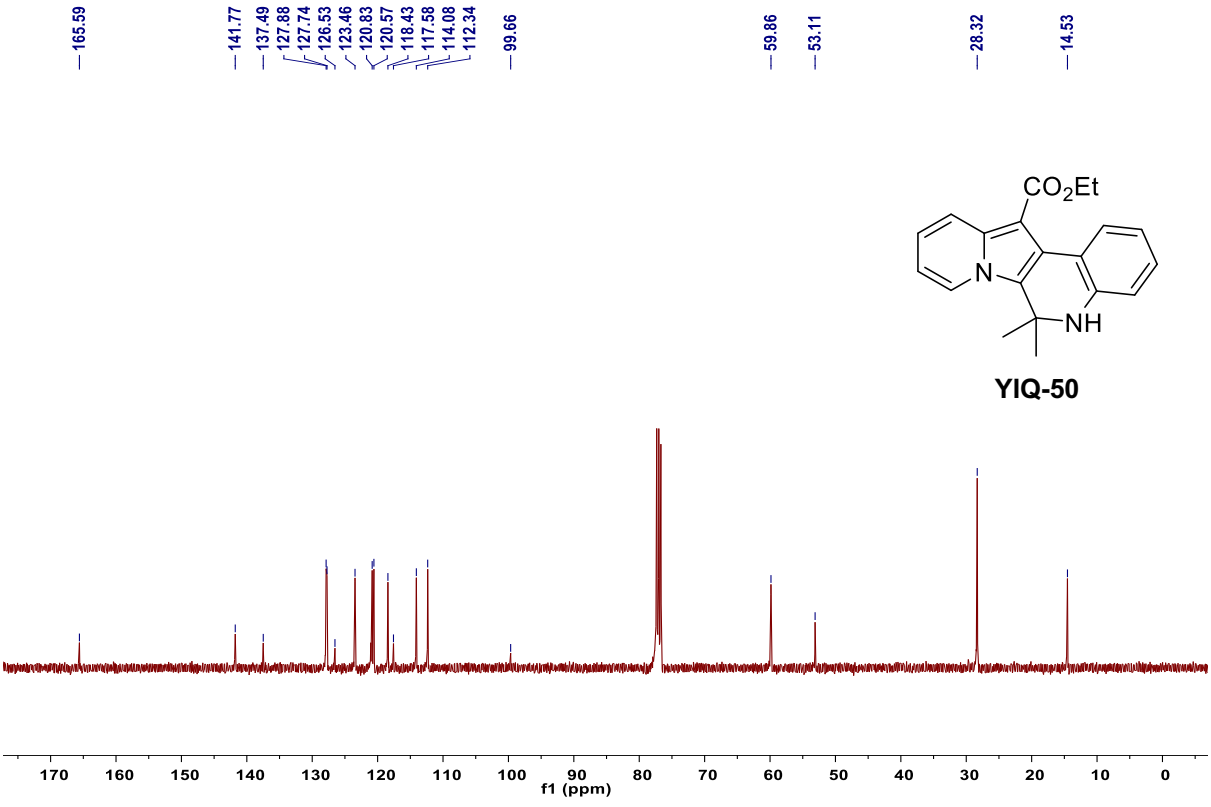
YIQ-29

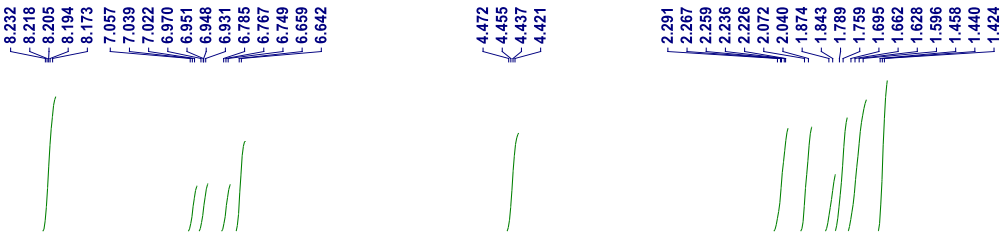

165.82
157.99
149.29
144.43
137.94
129.72
128.32
128.07
127.57
127.46
126.20
125.03
124.21
122.59
99.34
51.41
f1 (ppm)

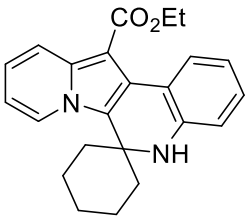
CO2Me
N
N
N

YIQ-29

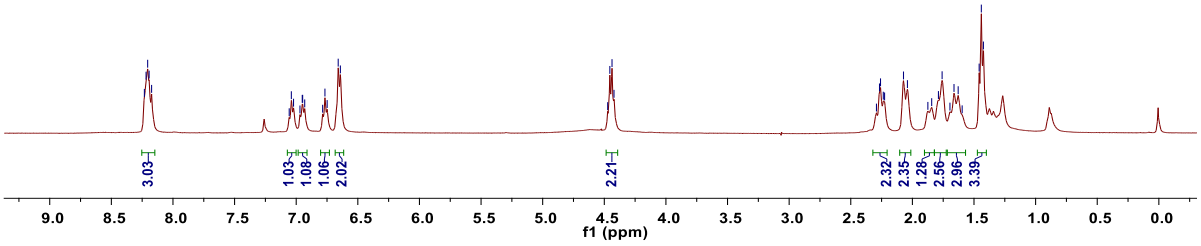

8.280
8.280
8.249
8.228
8.040
7.047
7.047
6.993
6.976
6.802
6.684
6.629
6.614
4.443
1.703
1.447
CO2Et
N
NH
YIQ-50
1.82
1.00
0.93
1.04
1.04
1.04
1.01
2.00
6.46
3.04
f1 (ppm)


165.59
141.77
137.49
127.88
127.74
126.53
123.46
120.83
120.57
118.43
117.58
114.08
112.34
99.66
59.86
53.11
28.32
14.53
CO2Et
N
NH
YIQ-50
f1 (ppm)

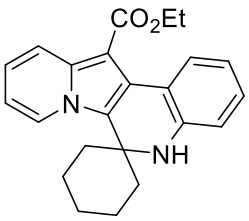

8.232
8.218
8.205
8.194
8.173
7.057
7.039
7.022
6.970
6.951
6.948
6.931
6.785
6.767
6.749
6.659
6.642
4.472
4.455
4.437
4.421
2.291
2.267
2.259
2.236
2.226
2.072
2.040
1.874
1.843
1.789
1.759
1.695
1.662
1.628
1.596
1.458
1.440
1.424


CO2Et
N
NH

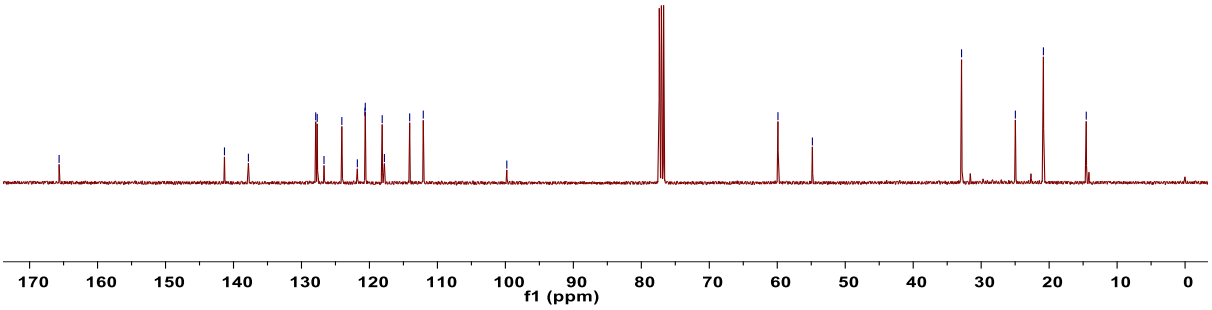
YIQ-51

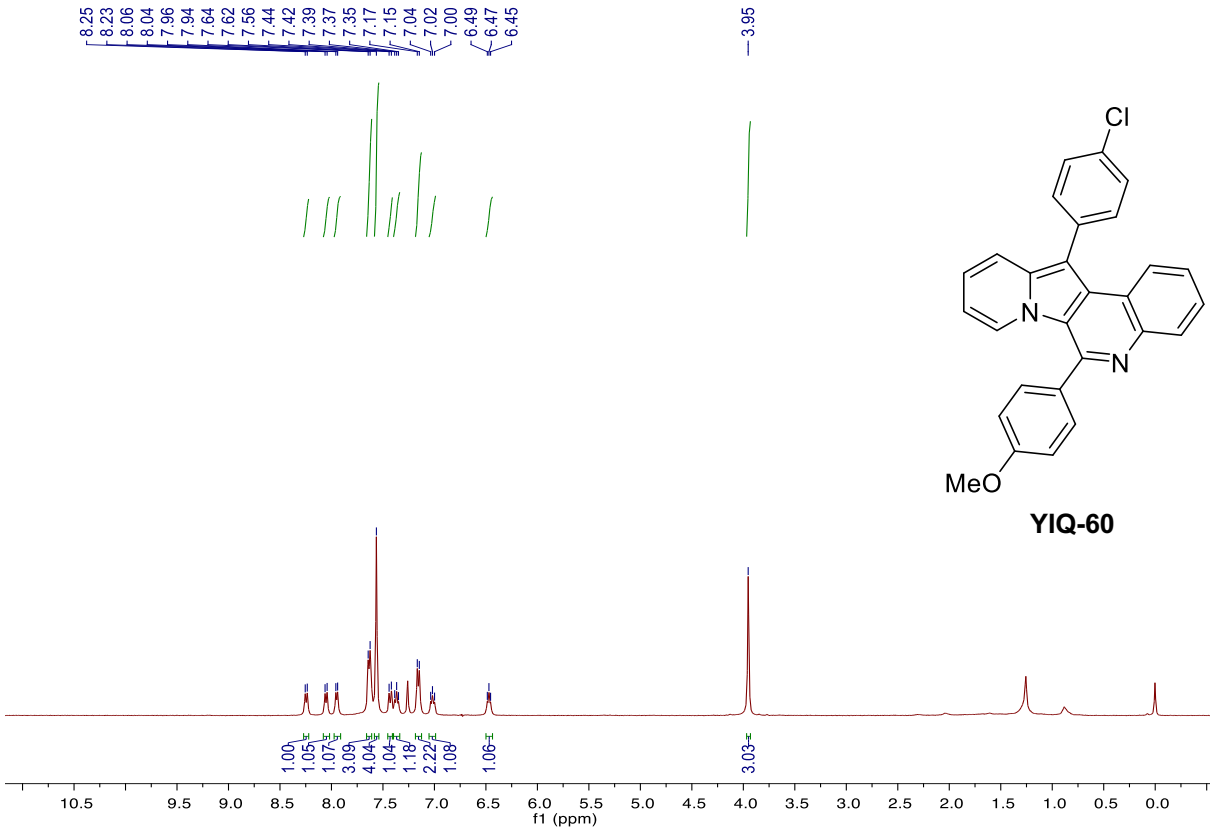

3.03
1.03
1.08
1.06
2.02
2.21
2.32
2.35
1.28
2.56
2.96
3.39
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

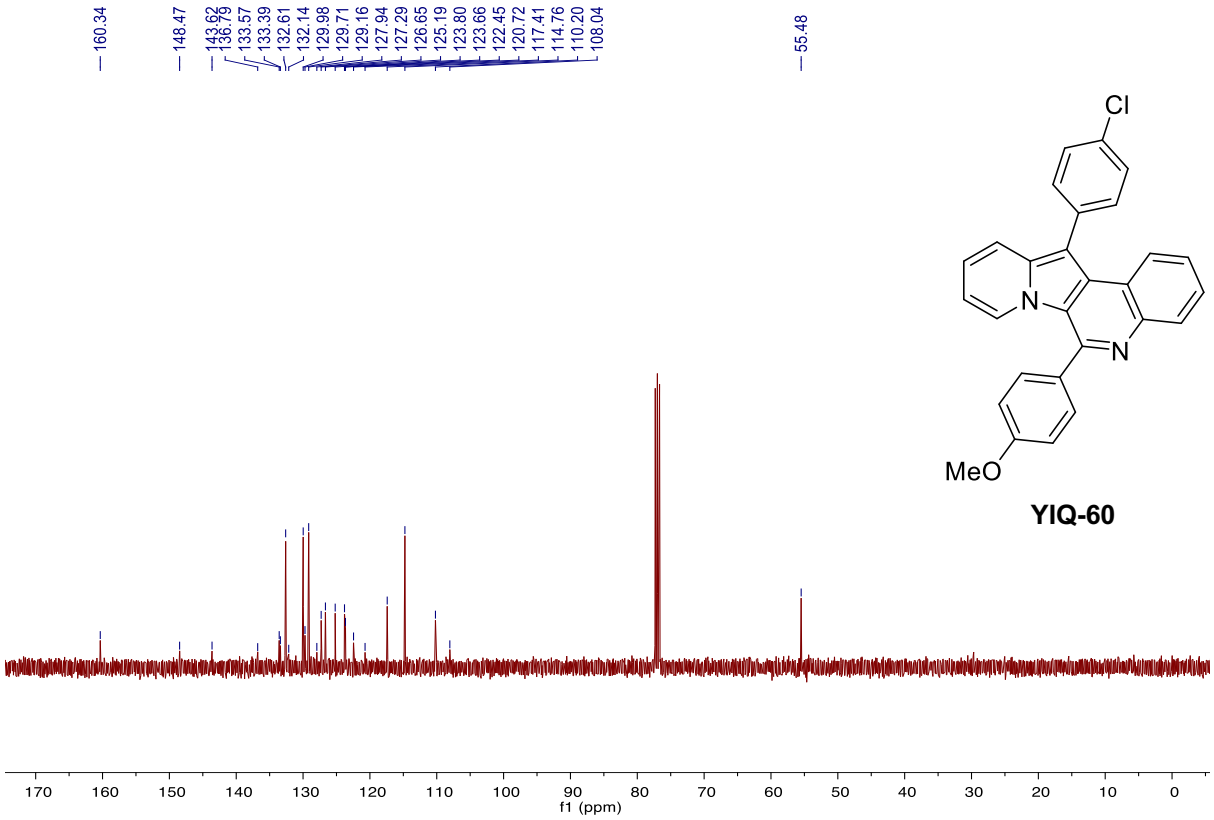

165.66
141.33
137.81
127.91
127.68
126.69
124.06
120.66
120.61
118.12
117.80
114.08
112.08
99.79
59.90
54.83
32.89
24.97
20.84
14.54

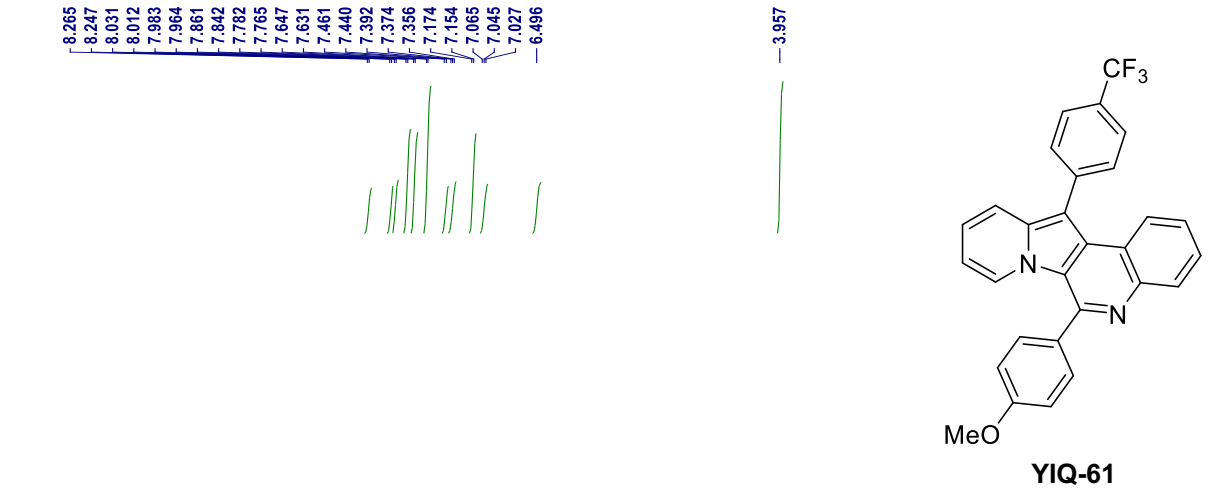

CO2Et
N
NH

YIQ-51

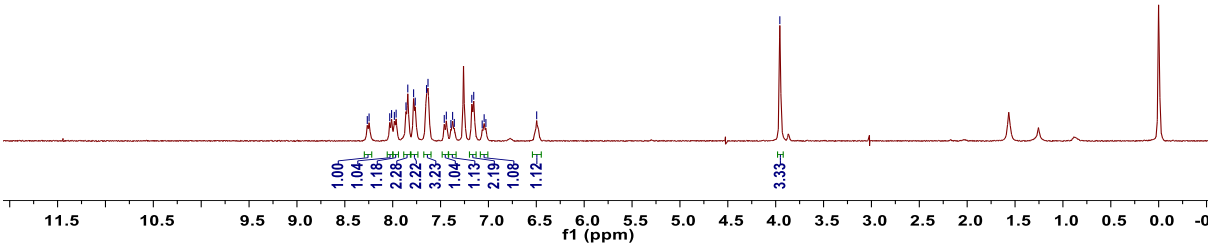

170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

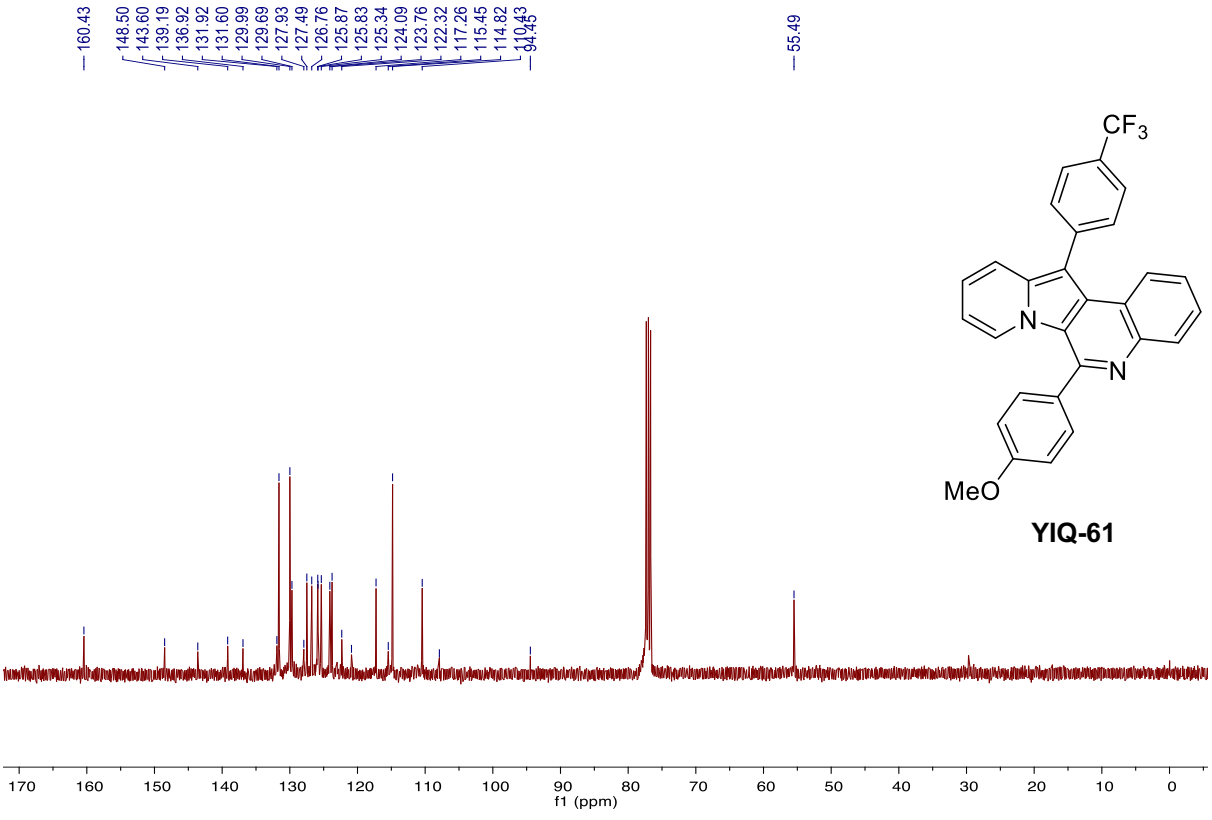

8.25
8.23
8.06
8.04
7.96
7.94
7.64
7.62
7.56
7.44
7.42
7.39
7.37
7.35
7.17
7.15
7.04
7.02
7.00
6.49
6.47
6.45
3.95
Cl
N
N
MeO
YIQ-60
1.00
1.05
1.07
3.09
4.04
1.04
1.18
2.22
1.08
1.06
3.03
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


160.34
148.47
143.62
136.79
133.57
133.39
132.61
132.14
129.98
129.71
129.16
127.94
127.29
126.65
125.19
123.80
123.66
122.45
120.72
117.41
114.76
110.20
108.04
55.48
Cl
N
N
MeO
YIQ-60
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.265
8.247
8.031
8.012
7.983
7.964
7.861
7.842
7.782
7.765
7.647
7.631
7.461
7.440
7.392
7.374
7.356
7.174
7.154
7.065
7.045
7.027
6.496
3.957
CF3
N
N
MeO

YIQ-61


1.00
1.04
1.18
2.26
2.22
3.23
1.04
1.13
2.19
1.08
1.12
3.33
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


160.43
148.50
143.60
139.19
136.92
131.92
131.60
129.99
129.69
127.93
127.49
126.76
125.87
125.83
125.34
124.09
123.76
122.32
117.26
115.45
114.82
110.43
94.45
55.49
CF3
N
N
MeO
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

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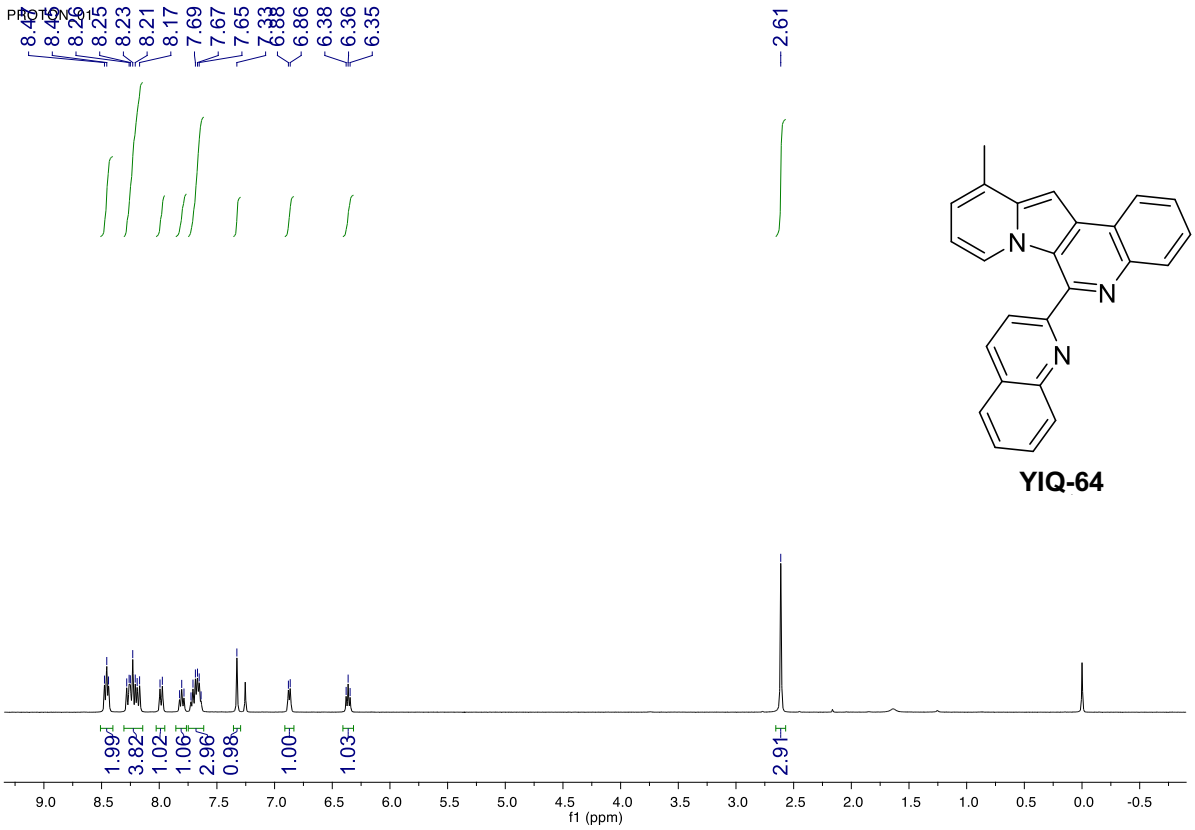
PROTON.01
8.45
8.43
8.25
8.23
8.21
8.17
7.69
7.67
7.65
7.33
6.88
6.86
6.38
6.36
6.35
2.61
N
N
N
1.99
3.82
1.02
1.06
2.96
0.98
1.00
1.03
2.91
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

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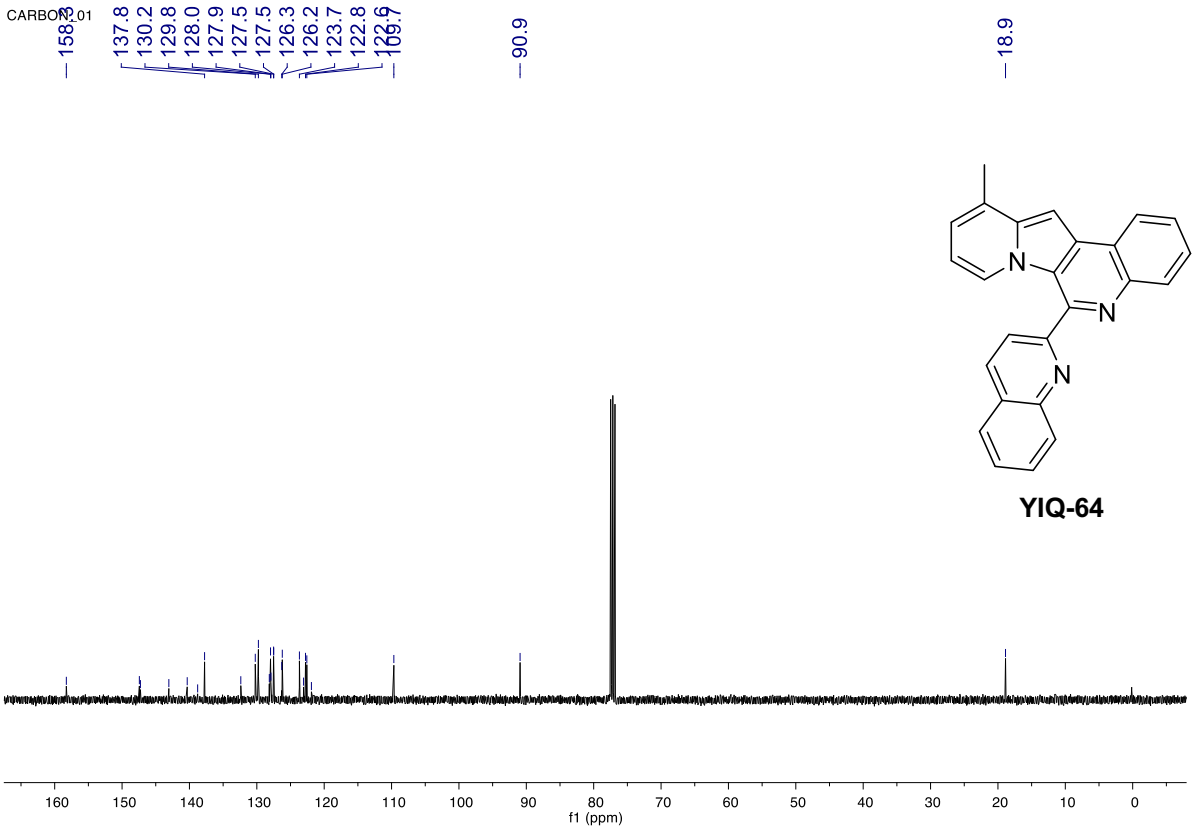
CARBON.01
158.1
137.8
130.2
129.8
128.0
127.9
127.5
127.5
126.3
126.2
123.7
122.8
122.6
109.7
90.9
18.9
N
N
N
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

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