Supporting Information

p-TsOH-promoted synthesis of (*E*)-6-phenyl-7-styryl-5,6-dihydrodibenzo[*b,h*][1,6]naphthyridines via cascade intramolecular aza-Michael addition/Friedlander condensation of 2'-aminochalcones in a SDS/H_2O system

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Experimental Section

General Information.

Melting points were determined in capillary tubes on an electrically heated block and are uncorrected. IR spectra were recorded using a FTIR spectrophotometer. NMR spectra were recorded at 300 MHz and 400 MHz for ^{1}H NMR, 75 and 100 MHz for ^{13}C NMR using $CDCl_3$/DMSO-d_6 as the solvent and tetramethylsilane as the internal reference. Chemical shifts are reported in parts per million. Splitting patterns are described as singlet (s), doublet (d), triplet (t), multiplet (m) and broad (br). HRMS was recorded using a Q-TOF mass spectrometer. Column chromatography was performed over flash silica gel (230-400 Mesh). All chemicals and reagents were purchased from commercial sources and used without purification.

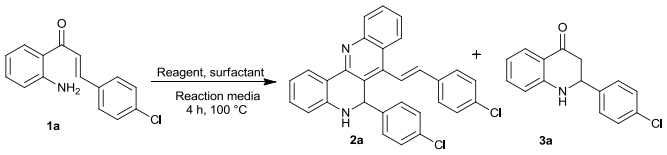
General procedure for the synthesis of (*E*)-6-phenyl-7-styryl-5,6-dihydro dibenzo[*b,h*]naphthyridine (2a-2s).

To a solution of 2'-aminochalcone **1** (1.0 mmol) in water (10 mL) was added *p*-TsOH (1.0 mmol) and SDS (0.20 mmol). The solution was stirred at 100 °C for 3-5 h and brought to room temperature. The solidified product was filtered and washed with ethyl acetate (2×10 mL), which was further purified by column chromatography over silica gel (DCM/MeOH = 10:0.1 v/v) to give compound **2** and **3** as yellow solids.

General procedure for the synthesis of (*E*)-6-phenyl-7-styryl-dibenzo[*b,h*][1,6]naphthyridines (4a, 4i and 4m).

To a solution of (*E*)-6-phenyl-7-styryl-5,6-dihydrodibenzo[*b,h*][1,6]naphthyridine **2** (0.2 mmol) in dry DCM (15 mL) was added DDQ (0.5 mmol). The solution was stirred at room temperature for 5-10 min. The reaction mixture was diluted with saturated K_2CO_3 solution (40 mL) and extracted with DCM (2×20 mL). The organic layer was further washed with brine solution (3×30 mL), dried over anhydrous $MgSO_4$ and the solvent removed under reduced pressure to give the final product. The product was further washed with MeOH to give compound **4** as yellow solid.

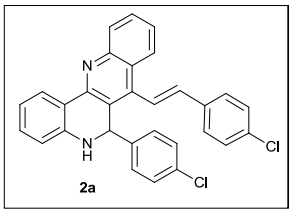
Table 1 Optimization of reaction conditions.



Entry	Reagent (equiv)	Surfactant SDS (20 mol%)	Reaction media	Temperature (˚C)	Yield[b]	
					2a	**3a**
17	*p*-TsOH (1)	SLS	Water	100	75	22
18	*p*-TsOH (1)	PF-127	Water	100	10	12
19	*p*-TsOH (1)	Tween 80	Water	100	12	10
20	*p*-TsOH (1)	Triton X-100	Water	100	75	22
21	*p*-TsOH (1)	TBAI	Water	100	41	28
22	*p*-TsOH (1)	-	MeOH	60	60	25
23	*p*-TsOH (1)	-	IPA	80	30	55
24	*p*-TsOH (1)	-	CH_3CN	80	-	90
25	*p*-TsOH (1)	-	Toluene	100	-	85

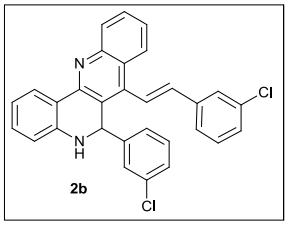
[a]Reaction condition: [g]Abbreviations: SDS = sodium dodecyl sulfate; SLS = sodium lauryl sulphate; PF-127 = pluronic F-127; Tween 80 = polyoxyethylene(20)sorbitanmonooleate (Polysorbate 80); Triton X-100 = $[C_{14}H_{22}O(C_2H_4O)n]$ where n = 9–10; TBAI = tetra-n-butyl ammonium iodide,

(*E*)-6-(4-chlorophenyl)-7-(4-chlorostyryl)-5,6-dihydrodibenzo[*b,h*][1,6]naphthyridine (2a).



Yellow solid (187 mg, 78%), mp 180-183 ºC; FT-IR (KBr, cm^{-1}) 3398, 3019, 1637, 758; ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.40 (s, 1H), 5.87 (s, 1H), 6.50-6.54 (brd, 2H), 6.93 (t, *J* = 5.80 Hz, 1H), 7.08-7.19 (m, 6H), 7.36-7.46 (m, 5H), 7.69 (t, *J* = 7.40 Hz, 1H), 7.95 (d, *J* = 8.08 Hz, 1H), 8.17 (d, *J* = 8.08 Hz, 1H), 8.56 (d, *J* = 6.96 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 56.6 (CH), 115.3 (CH), 119.5 (CH), 121.4 (C), 122.6 (CH), 125.27 (CH), 125.32 (C), 125.9 (CH), 126.1 (CH), 126.3 (C), 127.8 (2×CH), 128.1 (2×CH), 129.0 (2×CH), 129.1 (2×CH), 129.5 (CH), 129.9 (CH), 131.6 (CH), 133.7 (C), 134.4 (C), 134.6 (C), 136.5 (CH), 141.3 (C), 142.2 (C), 144.6 (C), 148.1 (C), 149.6 (C), ESI-MS (m/z): 479 $(M+H)^+$; HRMS (ESI) calculated for $C_{30}H_{21}Cl_2N_2$ $(M+H)^+$: 479.1082, found 479.1079.

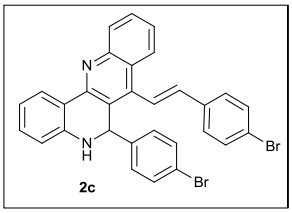
(*E*)-6-(3-chlorophenyl)-7-(3-chlorostyryl)-5,6-dihydrodibenzo[*b,h*][1,6]naphthyridine (2b).



Yellow solid (172 mg, 72%), mp 215-218 ºC; FT-IR (KBr, cm^{-1}) 3391, 3021, 1615, 769; ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.44 (s, 1H), 5.86 (s, 1H), 6.48 (d, *J* = 16.7 Hz, 1H), 6.54-6.56 (dd, *J* = 8.0, 0.68 Hz, 1H), 6.92-6.96 (m, 1H), 7.01-7.04 (m, 1H), 7.09-7.15 (m, 3H), 7.17-7.22 (m, 2H), 7.27-7.29 (m, 1H), 7.32-7.37 (m, 2H), 7.43-7.47 (m, 2H), 7.68-7.72 (m, 1H), 7.94-7.96 (dd, *J* = 8.4, 0.8 Hz, 1H), 8.16-8.18 (dd, *J* = 8.48 Hz, 0.56 Hz, 1H), 8.56-8.58 (dd, *J* = 7.84 Hz, 1.4 Hz, 1H); ^{13}C NMR δ 56.9 (CH), 115.2 (CH), 119.5 (CH), 121.3 (C), 123.5 (CH), 124.9 (CH), 124.9 (CH), 125.1 (C), 125.2 (CH), 126.0 (CH), 126.1 (CH), 126.3 (C), 126.5 (CH), 126.9 (CH), 128.0 (CH), 128.6 (CH),129.6 (CH), 129.9 (CH), 130.2 (CH), 130.3 (CH), 131.6 (CH), 134.7 (C), 134.9 (C), 136.5 (CH), 137.9 (C),

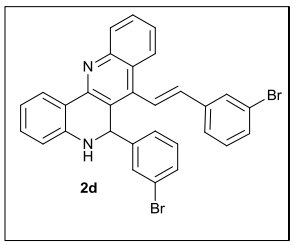
141.3 (C), 144.5 (C), 145.6 (C), 148.1 (C), 149.6 (C), ESI-MS (m/z): 479 $(M+H)^+$; HRMS (ESI) calculated for $C_{30}H_{21}Cl_2N_2$ $(M+H)^+$: 479.1082, found 479.1085.

(*E*)-6-(4-bromophenyl)-7-(4-bromostyryl)-5,6-dihydrodibenzo[*b,h*][1,6]naphthyridine (2c).



Yellow solid (216 mg, 76%), mp 156-159 ^oC; FT-IR (KBr, cm^{-1}) 3394, 3019, 1630, 752; ^1H NMR (400 MHz, $CDCl_3$): δ 4.40 (s, 1H), 5.85 (s, 1H), 6.49-6.55 (m, 2H), 6.93 (t, *J* = 7.28 Hz, 1H), 7.01 (d, *J* = 7.96 Hz, 2H), 7.10 (d, *J* = 16.72 Hz, 1H), 7.19 (t, *J* = 7.6 Hz, 1H), 7.28-7.32 (m, 4H merge with solvent), 7.44 (t, *J* = 7.72 Hz, 1H), 7.54 (d, *J* = 7.8 Hz, 2H), 7.69 (t, *J* = 7.76 Hz, 1H), 7.95 (d, *J* = 8.36 Hz, 1H), 8.16 (d, *J* = 8.28 Hz, 1H), 8.55 (d, *J* = 7.68 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 56.7 (CH), 115.3 (CH), 119.6 (CH), 121.4 (C), 121.8 (C), 122.7 (C&CH), 125.2 (C&CH), 126.0 (CH), 126.1 (CH), 126.3 (C), 128.1 (2×CH), 128.4 (2×CH), 129.5 (CH), 129.9 (CH), 131.6 (CH), 132.0 (2×CH), 132.1 (2×CH), 134.9 (C), 136.6 (CH), 141.3 (C), 142.6 (C), 144.5 (C), 148.1 (C), 149.6 (C), ESI-MS (m/z): 569 (M+H)+; HRMS (ESI) calculated for $C_{30}H_{21}Br_2N_2$ $(M+H)^+$: 569.0051, found 569.0053.

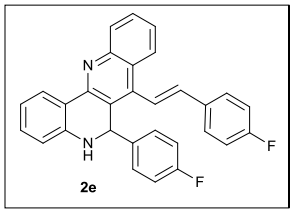
(*E*)-6-(3-bromophenyl)-7-(3-bromostyryl)-5,6-dihydrodibenzo[*b,h*][1,6]naphthyridine (2d).



Yellow solid (199 mg, 70%), mp 168-170 ^oC; FT-IR (KBr, cm^{-1}) 3367, 3019, 1567, 771; ^1H NMR (400 MHz, $CDCl_3$): δ 4.43 (s, 1H), 5.85 (s, 1H), 6.47 (d, *J* = 16.68 Hz, 1H), 6.56 (d, *J* = 7.88 Hz, 1H), 6.92-6.96 (m, 1H), 7.03-7.09 (m, 2H), 7.12 (d, *J* = 16.68 Hz, 1H), 7.18-7.22 (m, 1H), 7.28-7.35 (m, 4H), 7.43-7.49 (m, 2H), 7.59 (s, 1H), 7.68-7.72 (m, 1H), 7.94 (d, *J* = 8.4 Hz, 1H), 8.17 (d, *J* = 8.44 Hz, 1H), 8.55-8.58 (dd, *J* = 7.84, 1.16 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 56.9 (CH), 115.2 (CH),

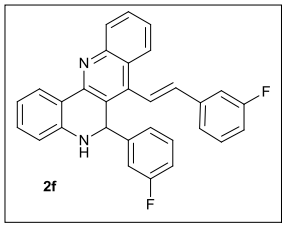
119.5 (CH), 121.2 (C), 122.8 (C), 123.2 (C), 123.5 (CH), 125.1 (C), 125.2 (CH), 125.4 (CH), 125.5 (CH), 126.0 (CH), 126.1 (CH), 126.3 (C), 129.5 (CH), 129.6 (CH), 129.8 (CH), 129.9 (CH), 130.5 (CH), 130.7 (CH), 130.9 (CH), 131. 5 (CH), 131.7 (CH), 136.4 (CH), 138.1 (C), 141.3 (C), 144.5 (C), 145.9 (C), 148.1 (C), 149.6 (C), ESI-MS (m/z): 569 $(M+H)^+$; HRMS (ESI) calculated for $C_{30}H_{21}Br_2N_2$ $(M+H)^+$: 569.0051, found 569.0052.

(*E*)-6-(4-fluorophenyl)-7-(4-fluorostyryl)-5,6-dihydrodibenzo[*b,h*][1,6]naphthyridine (2e).



Yellow solid (147 mg, 66%), mp 184-186 ^oC; FT-IR (KBr, cm^{-1}) 3392, 3019, 1637, 757; ^1H NMR (400 MHz, $CDCl_3$): δ 4.41 (s, 1H), 5.89 (s, 1H), 6.49-6.55 (m, 2H), 6.85-6.95 (m, 3H), 7.01-7.21 (m, 6H), 7.38-7.46 (m, 3H), 7.69 (t, *J* = 7.4 Hz, 1H), 7.97 (d, *J* = 8.32 Hz, 1H), 8.17 (d, *J* = 8.4 Hz, 1H), 8.57 (d, *J* = 7.68 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 56.5 (CH), 115.6 (d, *J* = 22.09 Hz, 2×CH), 115.8 (CH), 116.1 (d, *J* = 21.66 Hz, 2×CH), 119.4 (CH), 121.5 (C), 121.7 (d, *J* = 2.09 Hz, CH), 125.3 (CH), 125.6 (C), 125.9 (CH), 126.1 (CH), 126.5 (C), 128.3 (d, *J* = 8.09 Hz, 2×CH), 128.5 (d, *J* = 8.03 Hz, 2×CH), 129.4 (CH), 129.9 (CH), 131.6 (CH), 132.4 (d, *J* = 3.34 Hz, C), 136.5 (CH), 139.8 (d, *J* = 3.26 Hz, C), 141.4 (C), 144.7 (C), 148.1 (C), 149.7 (C), 163.8 (d, *J* = 245.27 Hz, C-F), 164.6 (d, *J* = 247.24 Hz, C-F), ESI-MS (m/z): 447 $(M+H)^+$; HRMS (ESI) calculated for $C_{30}H_{21}F_2N_2$ $(M+H)^+$: 447.1673, found 447.1672.

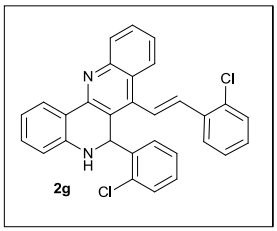
(*E*)-6-(3-fluorophenyl)-7-(3-fluorostyryl)-5,6-dihydrodibenzo[*b,h*][1,6]naphthyridine (2f).



Yellow solid (160 mg, 72%), mp 228-230 ^oC; FT-IR (KBr, cm^{-1}) 3390, 3019, 1651, 770; ^1H NMR (400 MHz, $CDCl_3$): δ 4.46 (s, 1H), 5.89 (s, 1H), 6.51-6.57 (m, 2H), 6.82-6.85 (m, 1H), 6.87-6.95 (m, 3H), 7.03-7.08 (m, 1H), 7.12-7.22 (m, 5H), 7.34-7.39 (m, 1H), 7.43-7.47 (m, 1H), 7.68-7.72 (m, 1H), 7.95-7.98 (dd, *J* = 8.4, 0.8 Hz, 1H), 8.16-8.19 (dd, *J* = 8.44, 0.6 Hz, 1H), 8.55-8.58 (d, *J* = 7.84, 1.4

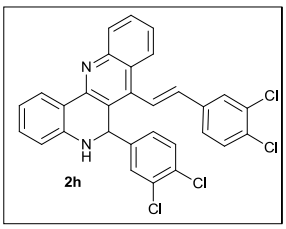
Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 56.76 (CH), 113.15 (d, *J* = 21.79 Hz, CH), 113.91 (d, *J* = 21.54 Hz, CH), 114.93 (d, *J* = 20.99 Hz, CH), 115.24 (CH), 115.62 (d, *J* = 21.27 Hz, CH), 119.57 (CH), 121.41 (C), 122.39 (CH), 122.62 (CH), 123.36 (CH), 125.13 (C), 125.26 (CH), 126.11 (d, *J* = 10.52 Hz, 2×CH), 126.32 (C), 129.53 (CH), 129.95 (CH), 130.49 (d, *J* = 8.09 Hz, 2×CH), 130.61 (CH), 136.70 (CH), 138.41 (d, *J* = 7.6 Hz, C), 141.22 (C), 144.56 (C), 146.11 (d, *J* = 5.75 Hz, C), 148.13 (C), 149.67 (C), 164.21 (d, *J* = 245.06 Hz, C-F), 164.45 (d, *J* = 245.06 Hz, C-F), ESI-MS (m/z): 447 $(M+H)^+$; HRMS (ESI) calculated for $C_{30}H_{21}F_2N_2$ $(M+H)^+$: 447.1673, found 447.1667.

(*E*)-6-(2-chlorophenyl)-7-(2-chlorostyryl)-5,6-dihydrodibenzo[*b,h*][1,6]naphthyridine (2g).



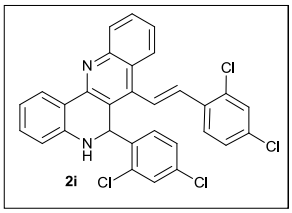
Yellow solid (124 mg, 52%), mp 211-213 ^oC; FT-IR (KBr, cm^{-1}) 3391, 3019, 1634, 762; ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.88 (s, 1H), 6.43 (s, 1H), 6.54 (d, *J* = 7.96 Hz, 1H), 6.73-6.75 (dd, *J* = 7.76, 1.4 Hz, 1H), 6.88-6.97 (m, 3H), 7.09-7.18 (m, 3H), 7.23-7.32 (m, 3H merge with solvent), 7.36-7.39 (m, 2H), 7.49 (t, *J* = 7.8 Hz, 1H), 7.65-7.67 (dd, *J* = 7.56, 1.4 Hz, 1H), 7.73 (t, *J* = 7.28 Hz, 1H), 8.07 (d, *J* = 8.4 Hz, 1H), 8.21 (d, *J* = 8.4 Hz, 1H), 8.56 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 53.3 (CH), 115.4 (CH), 119.4 (CH), 121.6 (C), 124.3 (CH), 124.6 (C), 125.3 (CH), 126.0 (CH), 126.0 (CH), 126.3 (C), 126.8 (CH), 127.0 (CH), 127.3 (CH), 129.0 (CH), 129.5 (CH), 129.5 (CH), 129.7 (CH), 129.9 (CH), 129.9 (CH), 130.0 (CH), 131.5 (CH), 131.7 (C), 133.7 (C), 134.3 (CH), 134.6 (C), 139.8 (C), 141.3 (C), 144.6 (C), 148.3 (C), 150.6 (C), ESI-MS (m/z): 479 (M+H)+; HRMS (ESI) calculated for $C_{30}H_{21}Cl_2N_2$ $(M+H)^+$:479.1082, found 479.1083.

(*E*)-6-(3,4-dichlorophenyl)-7-(3,4-dichlorostyryl)-5,6-dihydrodibenzo[*b,h*][1,6]naphthyridine (2h).



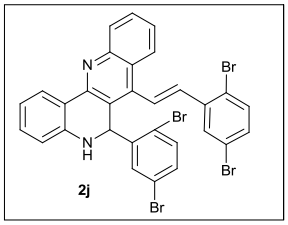
Yellow solid (208 mg, 76%), mp 212-215 °C; FT-IR (KBr, cm^{-1}) 3399, 3020, 1608, 758; ^{1}H NMR (400 MHz, DMSO-d_6): δ 6.13 (d, *J* = 2.2 Hz, 1H), 6.70 (d, *J* = 16.72 Hz, 1H), 6.74-6.78 (m, 2H), 6.95-6.98 (dd, *J* = 8.44, 2.08 Hz, 1H), 7.08 (d, *J* = 2.2 Hz, 1H), 7.16-7.20 (m, 1H), 7.40 (d, *J* = 8.36 Hz, 1H), 7.44 (d, *J* = 2.0 Hz, 1H), 7.52-7.56 (m, 1H), 7.61-7.64 (m, 1H), 7.66-7.72 (m, 2H), 7.74-7.79 (m, 1H), 7.99 (d, *J* = 1.8 Hz, 1H), 8.05-8.09 (m, 2H), 8.33-8.35 (dd, *J* = 7.96, 1.28 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 54.2 (CH), 115.6 (CH), 118.1 (CH), 120.0 (C), 125.0 (CH), 125.2 (C), 125.8 (C, CH), 126.1 (CH), 126.6 (CH), 127.3 (CH), 127.6 (CH), 129.1 (CH), 129.2 (CH), 129.7 (CH), 130.2 (C&CH), 131.2 (C&CH), 131.3 (CH), 131.3 (C), 132.1 (C), 132.2 (CH), 135.9 (CH), 137.3 (C), 141.5 (C), 145.2 (C), 146.4 (C), 147.9 (C), 149.7 (C); ESI-MS(m/z): 549 $(M+H)^+$; HRMS (ESI) calculated for $C_{30}H_{19}Cl_4N_2$ $(M+H)^+$: 549.0273, found 549.0264.

(*E*)-6-(2,4-dichlorophenyl)-7-(2,4-dichlorostyryl)-5,6dihydrodibenzo[*b,h*][1,6]naphthyridine (2i).



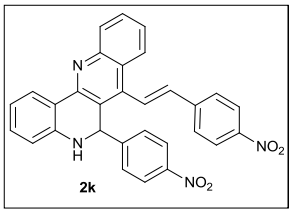
Yellow solid (178 mg, 65%), mp 220-222 °C; FT-IR (KBr, cm^{-1}) 3400, 3020, 1608, 760; ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.78 (s, 1H), 6.35 (s, 1H), 6.54 (d, *J* = 7.84 Hz, 1H), 6.68 (d, *J* = 8.4 Hz, 1H), 6.80 (d, *J* = 16.64 Hz, 1H), 6.94 (d, *J* = 7.60 Hz, 2H), 7.10 (d, *J* = 16.64 Hz, 1H), 7.18 (t, *J* = 7.32 Hz, 1H), 7.30 (d, *J* = 8.28 Hz, 1H), 7.40 (d, *J* = 2.44 Hz, 2H), 7.49 (t, *J* = 7.52 Hz, 1H), 7.60 (d, *J* = 8.4 Hz, 1H), 7.74 (t, *J* = 7.6 Hz, 1H), 8.01 (d, *J* = 8.28 Hz, 1H), 8.21 (d, *J* = 8.4 Hz, 1H), 8.55 (d, *J* = 7.76 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 52.8 (CH), 115.4 (CH), 119.7 (CH), 121.5 (C), 124.2 (C), 124.7 (CH), 125.2 (CH), 126.1 (CH), 126.1 (C), 126.2 (CH), 127.5 (CH), 127.5 (CH), 127.7 (CH), 129.7 (3×CH), 130.0 (CH), 130.4 (CH), 131.6 (CH), 132.2 (C), 132.9 (C), 133.2 (CH), 134.2 (2×C), 134.7 (C), 138.4 (C), 141.0 (C), 144.3 (C), 148.3 (C), 150.3 (C); ESI-MS(m/z): 549 $(M+H)^+$; HRMS (ESI) calculated for $C_{30}H_{19}Cl_4N_2$ $(M+H)^+$: 549.0273, found 549.0263.

(*E*)-6-(2,5-dibromophenyl)-7-(2,5-dibromostyryl)-5,6-dihydrodibenzo[*b,h*][1,6]naphthyridine (2j).



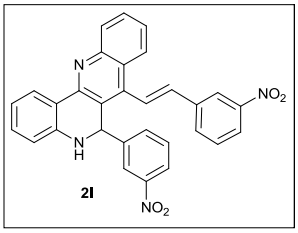
Yellow solid (254 mg, 70%), mp 200-203 ^{o}C; FT-IR (KBr, cm^{-1}) 3396, 3020, 1610, 762; ^{1}H NMR (400 MHz, DMSO-d_6): δ 6.39 (d, J = 2.2 Hz, 1H), 6.52 (d, J = 16.56 Hz, 1H), 6.75-6.81 (m, 3H), 6.90 (d, J = 2.44 Hz, 1H), 7.15-7.19 (m, 1H), 7.31-7.34 (dd, J = 8.52, 2.44 Hz, 1H), 7.46-7.49 (dd, J = 8.56, 2.36 Hz, 1H), 7.53-7.59 (m, 4H), 7.78-7.81 (m, 1H), 8.04 (d, J = 7.8 Hz, 1H), 8.09-8.15 (m, 2H), 8.40 (d, J = 7.12 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 55.7 (CH), 115.3 (CH), 119.7 (CH), 120.8 (C), 121.2 (C), 121.6 (C), 122.4 (C), 122.5 (C), 123.9 (C), 125.3 (CH), 125.8 (CH), 125.9 (C), 126.2 (CH), 126.3 (CH), 129.8 (CH), 129.9 (CH), 130.1 (CH), 131.7 (CH), 132.5 (CH), 132.6 (CH), 132.7 (CH), 134.4 (CH), 134.6 (CH), 135.8 (CH), 138.1 (C), 140.9 (C), 143.3 (C), 143.9 (C), 148.4 (C), 150.1 (C), ESI-MS (m/z): 726 $(M+H)^+$; HRMS (ESI) calculated for $C_{30}H_{19}Br_4N_2$ $(M+H)^+$: 726.8241, found 726.8239.

(*E*)-6-(4-nitrophenyl)-7-(4-nitrostyryl)-5,6-dihydrodibenzo[*b,h*][1,6]naphthyridine (2k).



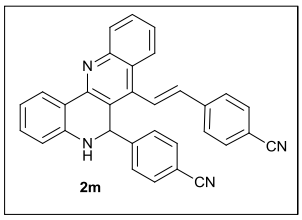
Yellow solid (155 mg, 62%), mp: 150-152 ^{o}C; FT-IR (KBr, cm^{-1}) 3365, 2918, 1594, 1402, 1219, 771; ^{1}H NMR (400 MHz, DMSO-d_6): δ 6.23 (d, J = 2.2 Hz, 1H), 6.75-6.78 (m, 2H), 6.84 (d, J = 16.72 Hz, 1H), 7.15-7.19 (m, 2H), 7.38 (d, J = 8.76 Hz, 2H), 7.53-7.57 (m, 1H), 7.76-7.80 (m, 1H), 7.84 (d, J = 16.72 Hz, 1H), 7.89 (d, J = 8.8 Hz, 2H), 8.03-8.09 (m, 4H), 8.25 (d, J = 8.76 Hz, 2H), 8.34-8.36 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 54.8 (CH), 115.7 (CH), 118.2 (CH), 120.1 (C), 124.2 (2×CH), 124.4 (2×CH), 125.1 (C), 125.8 (C&CH), 126.0 (CH), 126.7 (CH), 127.4 (CH), 128.3 (2×CH), 128.4 (2×CH), 129.8 (CH), 130.3 (CH), 132.2 (CH), 136.4 (CH), 141.4 (C), 142.9 (C), 146.3 (C), 147.1 (C), 147.4 (C), 147.9 (C), 149.8 (C), 151.2 (C), ESI-MS(m/z): 501 $(M+H)^+$; HRMS (ESI) calculated for $C_{30}H_{21}N_4O_4$ $(M+H)^+$: 501.1563, found 501.1565.

(*E*)-6-(3-nitrophenyl)-7-(3-nitrostyryl)-5,6-dihydrodibenzo[*b,h*][1,6]naphthyridine (2l).



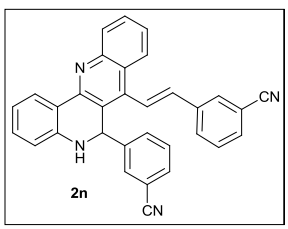
Brown solid (170 mg, 68%), mp 230-233 ^{o}C; FT-IR (KBr, cm^{-1}) 3398, 3021, 1641, 1405, 1215, 760; ^{1}H NMR (400 MHz, DMSO-d_6): δ 6.32 (d, J = 2.2 Hz, 1H), 6.75-6.84 (m, 3H), 7.19-7.22 (m, 2H), 7.45-7.55 (m, 3H), 7.68 (t, J = 8.0 Hz, 1H), 7.78-7.79 (m, 1H), 7.86 (d, J = 16.76 Hz, 1H), 7.97-7.99 (m, 1H), 8.07-8.13 (m, 4H), 8.17-8.19 (dd, J = 8.16, 1.56 Hz, 1H), 8.35-8.37 (dd, J = 7.96, 1.24 Hz, 1H), 8.47-8.48 (m, 1H); ^{13}C NMR (75 MHz, DMSO-d_6): δ 54.6 (CH), 115.6 (CH), 118.1 (C), 119.9 (CH), 121.8 (C&CH), 121.9 (CH), 122.7 (CH), 123.4 (CH), 125.4 (CH), 125.8 (2×CH), 126.1 (C&CH), 126.6 (CH), 129.7 (CH), 130.3 (CH), 130.6 (2×CH), 132.2 (CH), 133.6 (CH), 136.3 (CH), 138.3 (C), 141.7 (C), 146.4 (C), 146.4 (C), 147.9 (2×C), 148.8 (C), 149.7 (C), ESI-MS(m/z): 501 $(M+H)^+$; HRMS (ESI) calculated for $C_{30}H_{21}N_4O_4$ $(M+H)^+$: 501.1563, found 501.1560.

(*E*)-4-(2-(6-(4-cyanophenyl)-5,6-dihydrodibenzo[*b,h*][1,6]naphthyridin-7-yl)vinyl)benzonitrile (2m).



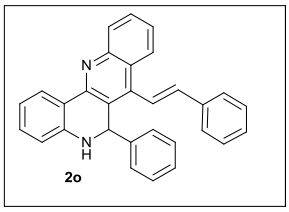
Yellow solid (172 mg, 75%), mp 250-252 ^{o}C; FT-IR (KBr, cm^{-1}) 3399, 3019, 2399, 1606, 757; ^{1}H NMR (300 MHz, $CDCl_3$): δ 4.47 (s, 1H), 5.92 (s, 1H), 6.52-6.58 (m, 2H), 6.96 (t, J = 7.53 Hz, 1H), 7.19-7.29 (m, 4H merge with solvent), 7.47-7.51 (m, 5H), 7.69-7.72 (m, 3H), 7.91 (d, J = 8.28 Hz, 1H), 8.18 (d, J = 8.37 Hz, 1H), 8.56 (d, J = 7.38 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 56.8 (CH), 111.9 (C), 112.2 (C), 115.3 (CH), 118.3 (C), 118.5 (C), 119.9 (CH), 121.3 (C), 124.5 (C), 125.0 (CH), 125.6 (CH), 125.9 (C), 126.1 (CH), 126.4 (CH), 127.0 (2×CH), 127.4 (2×CH), 129.9 (CH), 130.1 (CH), 131.9 (CH), 132.8 (4×CH), 136.3 (CH), 140.0 (C), 140.7 (C), 144.0 (C), 148.1 (C), 148.2 (C), 149.5 (C), ESI-MS (m/z): 461 $(M+H)^+$; HRMS (ESI) calculated for $C_{32}H_{21}N_4$ $(M+H)^+$: 461.1766, found 461.1758.

(*E*)-3-(2-(6-(3-cyanophenyl)-5,6-dihydrodibenzo[*b,h*][1,6]naphthyridin-7-yl)vinyl)benzonitrile (2n).



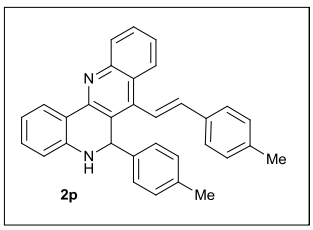
Yellow solid (175 mg, 76%), mp 258-261 ^{o}C; FT-IR (KBr, cm^{-1}) 3395, 3022, 2291, 1618, 789; ^{1}H NMR (400 MHz, DMSO-d_6): 6.19 (d, J = 2.32 Hz, 1H), 6.70 (d, J = 16.76, 1H), 6.75-6.78 (m, 2H), 7.11 (d, J = 2.32 Hz, 1H), 7.16-7.20 (m, 1H), 7.34-7.36 (m, 2H), 7.52-7.63 (m, 4H), 7.74-7.81 (m, 3H), 7.92 (d, J = 7.96 Hz , 1H), 8.06-8.11 (m, 2H), 8.19 (s, 1H), 8.33-8.36 (dd, J = 8.0, 1.28 Hz, 1H); ^{13}C (100 MHz, DMSO-d_6): 54.6 (CH), 111.6 (C), 112.4 (C), 115.6 (CH), 118.1 (CH), 118.9 (C), 119.2 (C), 120.1 (C), 125.2 (C&CH), 125.8 (CH), 125.9 (C), 126.1 (CH), 126.6 (CH), 129.7 (CH), 130.3 (2×CH), 130.4 (CH), 130.7 (2×CH), 131.5 (CH), 131.8 (CH), 132.1 (CH), 132.2 (CH), 132.2 (CH), 136.3 (CH), 137.7 (C), 141.6 (C), 145.7 (C), 146.4 (C), 147.9 (C), 149.7 (C), ESI-MS (m/z): 461 (M+H)$^{+}$; HRMS (ESI) calculated for $C_{32}H_{21}N_4$ (M+H)$^{+}$: 461.1766, found 461.1759.

(*E*)-6-phenyl-7-styryl-5,6-dihydrodibenzo[*b,h*][1,6]naphthyridine (2o).



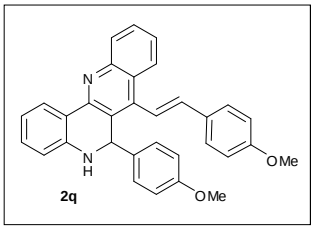
Yellow solid (107 mg, 52%), mp 156-159 ^{o}C; FT-IR (KBr, cm^{-1}) 3392, 3019, 1644, 769; ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.45 (s, 1H), 5.93 (s, 1H), 6.53-6.61 (m, 2H), 6.90-6.94 (m, 1H), 7.12-7.21 (m, 7H), 7.35-7.44 (m, 6H), 7.66-7.70 (m, 1H), 8.00 (d, J = 7.84 Hz, 1H), 8.17 (d, J = 8.4 Hz, 1H), 8.56-8.58 (dd, J = 7.8, 1.32 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 57.3 (CH), 115.2 (CH), 119.2 (CH), 121.5 (C), 122.1 (CH), 125.4 (CH), 125.7 (CH), 126.0 (CH), 126.6 (C), 126.7 (C&2×CH), 126.8 (2×CH), 127.8 (CH), 128.6 (CH), 128.9 (4×CH), 129.3 (CH), 129.8 (CH), 131.4 (CH), 136.3 (C), 137.7 (CH), 141.7 (C), 143.8 (C), 144.9 (C), 148.1 (C), 149.8 (C), ESI-MS (m/z): 411 (M+H)+; HRMS (ESI) calculated for $C_{30}H_{23}N_2$ (M+H)$^{+}$:411.1861, found 411.1853.

(*E*)-7-(4-methylstyryl)-6-(p-tolyl)-5,6-dihydrodibenzo[*b,h*][1,6]naphthyridine (2p).



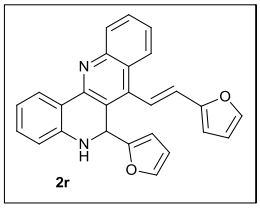
Yellow solid (77 mg, 35%), mp 172-174 ^{o}C; FT-IR (KBr, cm^{-1}) 3392, 3019, 1650, 771; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.25 (s, 3H), 2.40 (s, 3H), 4.42 (s, 1H), 5.88 (s, 1H), 6.53 (d, *J* = 7.84 Hz, 1H), 6.60 (d, *J* = 16.72 Hz, 1H), 6.91 (t, *J* = 7.4 Hz, 1H), 6.98-7.10 (m, 5H), 7.15-7.22 (m, 3H), 7.34 (d, *J* = 7.96 Hz, 2H), 7.41 (t, *J* = 7.16 Hz, 1H), 7.67 (t, *J* = 7.12 Hz, 1H), 8.00 (d, *J* = 8.28 Hz, 1H), 8.16 (d, *J* = 8.44 Hz, 1H), 8.56 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.0 (CH_3), 21.3 (CH_3), 56.9 (CH), 115.2 (CH), 119.2 (CH), 121.1 (CH), 121.6 (C), 125.5 (CH), 125.6 (CH), 125.9 (C), 125.9 (CH), 126.6 (C&2×CH), 126.7 (2×CH), 129.2 (CH), 129.5 (2×CH), 129.6 (2×CH), 129.8 (CH), 131.4 (CH), 133.6 (C), 137.4 (C), 137.5 (CH), 138.6 (C), 140.9 (C), 141.7 (C), 145.1 (C), 148.1 (C), 149.8 (C), ESI-MS (m/z): 439 (M+H)+; HRMS (ESI) calculated for $C_{30}H_{27}N_2$ $(M+H)^+$:439.2174, found 439.2171.

(*E*)-6-(4-methoxyphenyl)-7-(4-methoxystyryl)-5,6-dihydrodibenzo[*b,h*][1,6]naphthyridine (2q).



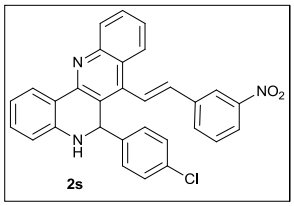
Yellow solid (56 mg, 24%), mp 164-166 ^{o}C; FT-IR (KBr, cm^{-1}) 3395, 3021, 1648, 778; ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.71 (s, 3H), 3.86 (s, 3H), 4.41 (s, 1H), 5.87 (s, 1H), 6.53 (t, *J* = 8.12 Hz, 2H), 6.71 (d, *J* = 8.36 Hz, 2H), 6.89-7.00 (m, 4H), 7.07-7.18 (m, 3H), 7.37-7.43 (m, 3H), 7.67 (t, *J* = 7.72 Hz, 1H), 8.00 (d, *J* = 8.28 Hz, 1H), 8.16 (d, *J* = 8.4 Hz, 1H), 8.56 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 55.2 (CH_3), 55.4 (CH_3), 56.6 (CH), 114.1 (2×CH), 114.3 (2×CH), 115.2 (CH), 119.2 (CH), 119.8 (CH), 121.6 (C), 125.5 (CH), 125.6 (CH), 126.0 (CH), 126.7 (C), 127.9 (2×CH), 128.0 (2×CH), 129.1 (CH), 129.8 (CH), 131.3 (CH), 136.4 (C), 137.1 (CH), 141.8 (C), 145.0 (C), 148.1 (C), 149.8 (C), 159.0 (2×C), 160.0 (2×C); ESI-MS (m/z): 471 (M+H)+; HRMS (ESI) calculated for $C_{32}H_{27}N_2O_2$ $(M+H)^+$:471.2073, found 471.2067.

(*E*)-6-(furan-2-yl)-7-(2-(furan-2-yl)vinyl)-5,6-dihydrodibenzo[*b,h*][1,6]naphthyridine (2r).



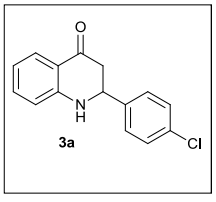
Yellow solid (70 mg, 36%), mp 162-164 ºC; FT-IR (KBr, cm^{-1}) 3395, 3019, 1649, 779; ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.69 (s, 1H), 5.71 (t, *J* = 0.64 Hz, 1H), 5.99 (s, 1H), 6.12 (d, *J* = 1.8 Hz, 1H), 6.37 (d, *J* = 3.2 Hz, 1H), 6.47 (t, *J* = 1.84 Hz, 1H), 6.55 (d, *J* = 16.48 Hz, 1H), 6.68 (d, *J* = 7.92 Hz, 1H), 6.94 (t, *J* = 7.28 Hz, 1H), 7.21 (t, *J* = 7.72 Hz, 1H), 7.26-7.32 (m, 2H), 7.45-7.48 (m, 2H), 7.70 (t, *J* = 8.12 Hz, 1H), 8.07-8.17 (dd, *J* = 28.64, 8.36 Hz, 2H), 8.51 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 50.7 (CH), 108.0 (CH), 110.3 (CH), 110.4 (CH), 111.8 (CH), 115.4 (CH), 119.8 (2×CH), 122.1 (C), 123.3 (C), 125.5 (CH), 125.7 (CH), 125.8 (CH), 126.0 (CH), 126.2 (C), 129.4 (CH), 129.9 (CH), 131.2 (CH), 141.0 (C), 142.1 (CH), 143.0 (CH), 145.2 (C), 148.2 (C), 149.9 (C), 152.0 (C), 155.3 (C), ESI-MS (m/z): 391 (M+H)+; HRMS (ESI) calculated for $C_{26}H_{19}N_2O_2$ $(M+H)^+$:391.1447, found 391.1446.

(*E*)-6-(4-chlorophenyl)-7-(3-nitrostyryl)-5,6-dihydrodibenzo[*b,h*][1,6]naphthyridine (2s).



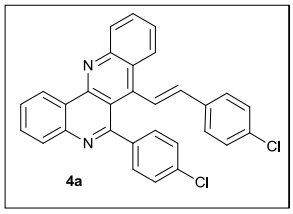
Yellow solid (245 mg, 50%), mp 170-172 ºC; FT-IR (KBr, cm^{-1}) 3394, 3020, 1638, 1407, 1211, 759; ^{1}H NMR (400 MHz, $CDCl_3$): δ 4.42 (s, 1H), 5.87 (s, 1H), 6.55 (d, *J* = 7.96 Hz, 1H), 6.62 (d, *J* = 16.68 Hz, 1H), 6.94 (t, *J* = 7.48 Hz, 1H), 7.08 (d, *J* = 8.32 Hz, 2H), 7.17-7.22 (m, 3H), 7.24-7.28 (m, 1H), 7.46 (t, *J* = 7.68 Hz, 1H), 7.59 (t, *J* = 7.84 Hz, 1H), 7.67-7.73 (m, 2H), 7.93 (d, *J* = 8.4 Hz, 1H), 8.19 (t, *J* = 8.48 Hz, 2H), 8.32 (s, 1H), 8.56 (d, *J* = 7.68 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 56.7 (CH), 115.3 (CH), 119.6 (CH), 121.0 (CH), 121.3 (C), 123.1 (CH), 125.0 (CH), 125.4 (C&CH), 126.1 (C&CH), 126.2 (CH), 128.1 (2×CH), 129.2 (2×CH), 129.6 (CH), 129.9 (CH), 130.0 (CH), 131.7 (CH), 132.5 (CH), 133.9 (C), 135.4 (CH), 137.8 (C), 140.5 (C), 142.0 (C), 144.5 (C), 148.1 (C), 148.8 (C), 149.6 (C), ESI-MS (m/z): 490 $(M+H)^+$; HRMS (ESI) calculated for $C_{30}H_{21}ClN_3O_2$ $(M+H)^+$: 490.1322, found 490.1302.

2-(4-chlorophenyl)-2,3-dihydroquinolin-4(*1H*)-one (3a).[1]



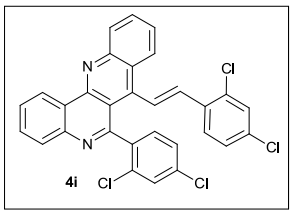
Yellow solid (51 mg, 20%), mp 164-166ºC; FT-IR (KBr, cm^{-1}) 3398, 3019, 1668, 1215; ^1H NMR (400 MHz, $CDCl_3$): δ 2.72-2.87 (m, 2H), 4.50 (s, 1H), 4.71-4.75 (dd, *J* = 13.08, 4.2 Hz, 1H), 6.73 (d, *J* = 8.2 Hz, 1H), 6.78-6.82 (m, 1H), 7.33-7.41 (m, 5H), 7.85-7.88 (dd, *J* = 7.9, 1.52 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 46.4 (CH_2), 57.9 (CH), 115.9 (CH), 118.7 (CH), 119.1 (C), 127.6 (CH), 128.0 (2×CH), 129.2 (2×CH), 134.2 (C), 135.5 (CH), 139.6 (C), 151.4 (C), 192.9 (C), ESI-MS(m/z): 258 $(M+H)^+$; HRMS (ESI) calculated for $C_{15}H_{13}ClNO$ $(M+H)^+$: 258.0686, found 258.0693.

(*E*)-6-(4-chlorophenyl)-7-(4-chlorostyryl)dibenzo[*b,h*][1,6]naphthyridine (4a).



Yellow solid (91 mg, 95%), mp 184-185 ºC; FT-IR (KBr, cm^{-1}) 3020, 1632, 1536, 757; ^1H NMR (400 MHz, $CDCl_3$): δ 6.22 (d, *J* = 16.52 Hz, 1H), 7.00 (d, *J* = 8.44 Hz, 2H), 7.15 (d, *J* = 16.48 Hz, 1H), 7.28-7.31 (m, 4H), 7.39-7.42 (m, 2H), 7.57-7.61 (m, 1H), 7.77-7.81 (m, 1H), 7.84-7.88 (m, 1H), 7.91-7.95 (m, 1H), 8.15-8.17 (dd, *J* = 7.96, 0.76 Hz, 1H), 8.21-8.23 (dd, *J* = 8.64, 0.56 Hz, 1H), 8.40 (d, *J* = 8.24 Hz, 1H), 9.37-9.39 (dd, *J* = 8.08, 1.32 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 116.7 (C), 124.6 (CH), 124.7 (C), 125.9 (CH), 126.3 (C), 126.5 (2×CH), 127.6 (2×CH), 127.8 (CH), 128.8 (2×CH), 128.9 (2×CH), 129.2 (CH), 130.0 (CH), 130.2 (2×CH), 130.9 (CH), 131.7 (CH), 134.5 (2×C), 134.5 (C), 136.6 (CH), 142.2 (C), 144.4 (C), 145.9 (C), 148.8 (C), 149.4 (C), 160.5 (C), ESI-MS(m/z): 477 $(M+H)^+$; HRMS (ESI) calculated for $C_{30}H_{19}Cl_2N_2$ $(M+H)^+$: 477.0925, found 477.0915.

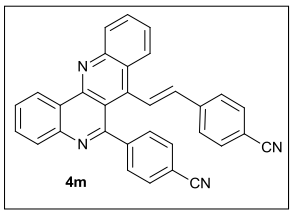
(*E*)-6-(2,4-dichlorophenyl)-7-(2,4-dichlorostyryl)dibenzo[*b,h*][1,6]naphthyridine (4i).



Yellow solid (105 mg, 96%) , mp 240-243 °C; FT-IR (KBr, cm^{-1}) 3019, 1581, 1537, 758; ^1H NMR (400 MHz, $CDCl_3$): δ 6.87 (d, *J* = 16.64 Hz, 1H), 7.05 (d, *J* = 16.6 Hz, 1H), 7.11 (d, *J* = 8.48 Hz, 1H), 7.24-7.25 (m, 2H), 7.27-7.29 (m, 1H), 7.42-7.48 (m, 2H), 7.59-7.63 (m, 1H), 7.81-7.89 (m, 2H), 7.92-

7.96 (m, 1H), 8.16-8.18 (dd, *J* = 7.72, 0.8 Hz, 1H), 8.27 (d, *J* = 8.44 Hz, 1H), 8.42 (d, *J* = 8.48 Hz, 1H), 9.44-9.46 (dd, *J* = 8.0, 1.52 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 116.8 (C), 124.8 (CH), 125.1 (C), 125.9 (C), 126.4 (CH), 126.7 (CH), 126.8 (CH), 126.9 (CH), 127.3 (CH), 127.6 (CH), 128.2 (CH), 129.3 (CH), 129.5 (CH), 129.8 (CH), 130.1 (CH), 130.9 (CH), 131.3 (CH), 131.9 (CH), 131.9 (CH), 132.4 (C), 133.9 (C), 134.1 (C), 134.8 (C), 135.1 (C), 140.9 (C), 144.4 (C), 145.2 (C), 148.1 (C), 149.8 (C), 157.9 (C), ESI-MS(m/z): 547 $(M+H)^+$; HRMS (ESI) calculated for $C_{30}H_{17}Cl_4N_2$ $(M+H)^+$: 547.0116, found 547.0129.

(*E*)-4-(2-(6-(4-cyanophenyl)dibenzo[*b,h*][1,6]naphthyridin-7-yl)vinyl)benzonitrile (4m).



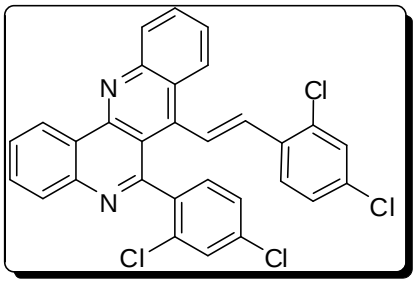
Yellow solid (89 mg, 97%), mp 280-282 ^oC; FT-IR (KBr, cm^{-1}) 3019, 2224, 1604, 1560, 758; ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.27 (d, *J* = 16.52 Hz, 1H), 7.16 (d, *J* = 8.24 Hz, 2H), 7.35 (d, *J* = 16.48 Hz, 1H), 7.61-7.66 (m, 7H), 7.81-7.85 (m, 1H), 7.88-7.92 (m, 1H), 7.95-7.99 (m, 1H), 8.15-8.18 (m, 2H), 8.44 (d, *J* = 8.44 Hz, 1H), 9.39-9.41 (dd, *J* = 8.0, 1.32 Hz, 1H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 111.9 (C), 112.5 (C), 116.2 (C), 118.1 (C), 118.4 (C), 124.7 (C&CH), 125.9 (CH), 126.0 (C), 126.7 (2×CH), 127.0 (CH), 128.3 (CH), 128.8 (CH), 129.4 (CH), 129.6 (2×CH), 130.2 (CH), 131.2 (CH), 132.1 (CH), 132.4 (2×CH), 132.5 (2×CH), 136.5 (CH), 139.8 (C), 144.3 (C), 144.4 (C), 148.3 (C), 148.8 (C), 149.4 (C), 159.2 (C), ESI-MS (m/z): 459 $(M+H)^+$; HRMS (ESI) calculated for $C_{32}H_{19}N_4$ $(M+H)^+$: 459.1610, found 459.1611.

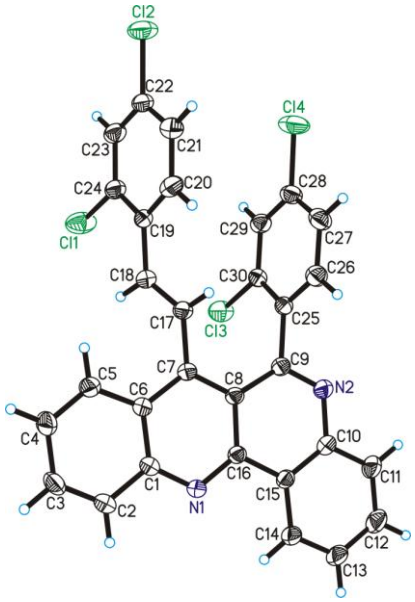
X-Ray Data Collection and Structure Refinement Details:

A good quality single crystal of size 0.54 x 0.46 x 0.44 mm, was selected under a polarizing microscope and was mounted on a glass fiber for data collection. Single crystal X-ray data for compound **4i** were collected on the Rigaku Kappa 3 circle diffractometer equipped with the AFC12 goniometer and enhanced sensitivity (HG) Saturn724+CCD detector in the 4x4 bin mode using the monochromated Mo-Kα radiation generated from the microfocus sealed tube MicroMax-003 X-ray generator equipped with specially designed confocal multilayer optics. Data collection was performed using ω-scans of 0.5^o steps at 293(2) K. Cell determination, data collection and data reduction was

performed using the Rigaku CrystalClear-SM Expert 2.1 b24[2] software. Structure solution and refinement were performed by using SHELX-97[3]. Refinement of coordinates and anisotropic thermal parameters of non-hydrogen atoms were carried out by the full-matrix least-squares method. The hydrogen atoms attached to carbon atoms were generated with idealized geometries and isotropically refined using a riding model.

ORTEP diagram of compound 4i (CCDC 1025096)**:**





ORTEP diagram drawn with 30% ellipsoid probability for non-H atoms of the crystal structure of compound **4i** determined at 293 K.

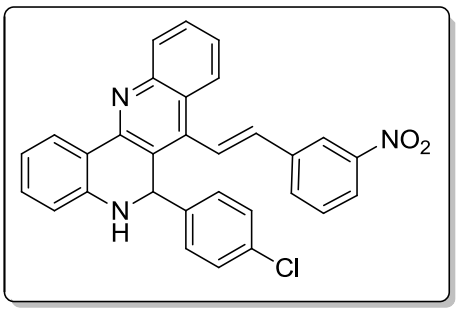
Table 1 Crystal data and structure refinement details for compound **4i**

Compound	**4i**
Empirical formula	C_{30} H_{16} Cl_4 N_2
Formula weight	546.25
Crystal System	Triclinic
Space group	*P*-1
a (Å)	8.336(2)
b (Å)	9.118(3)
c (Å)	17.445(5)
α (°)	103.692(17)
β (°)	93.563(17)
γ (°)	107.081(14)

V (Å^3)	1219.0(6)
Z	2
D_c (g/cm^3)	1.488
F_{000}	556
μ (mm^{-1})	0.510
θ_{max} (°)	25.42
Total reflections	9490
Unique reflections	4345
Reflections [$I > 2\sigma(I)$]	2787
Parameters	325
R_{int}	0.0273
Goodness-of-fit	0.973
R [$F^2 > 2\sigma(F^2)$]	0.0383
wR (F^2, all data)	0.1070
CCDC No.	1025096

X-Ray Data Collection and Structure Refinement Details:

A good quality yellow color single crystal of size 0.43 x 0.40 x 0.16 mm, was selected under a polarizing microscope and was mounted on a glass fiber for data collection. Single crystal X-ray data for compound **2s** were collected on the Rigaku Kappa 3 circle diffractometer equipped with the AFC12 goniometer and enhanced sensitivity (HG) Saturn724+ CCD detector in the 4x4 bin mode using the monochromated Mo-Kα radiation generated from the microfocus sealed tube MicroMax-003 X-ray generator equipped with specially designed confocal multilayer optics. Data collection was performed using ω-scans of 0.5° steps at 293(2) K. Cell determination, data collection and data reduction was performed using the Rigaku CrystalClear-SM Expert 2.1 b24[2] software. Structure solution and refinement were performed by using SHELX-97[3]. Refinement of coordinates and anisotropic thermal parameters of non-hydrogen atoms were carried out by the full-matrix least-squares method. The hydrogen atoms attached to carbon atoms were generated with idealized geometries and isotropically refined using a riding model.



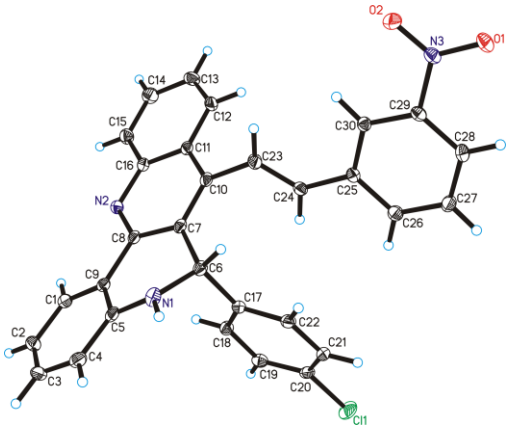
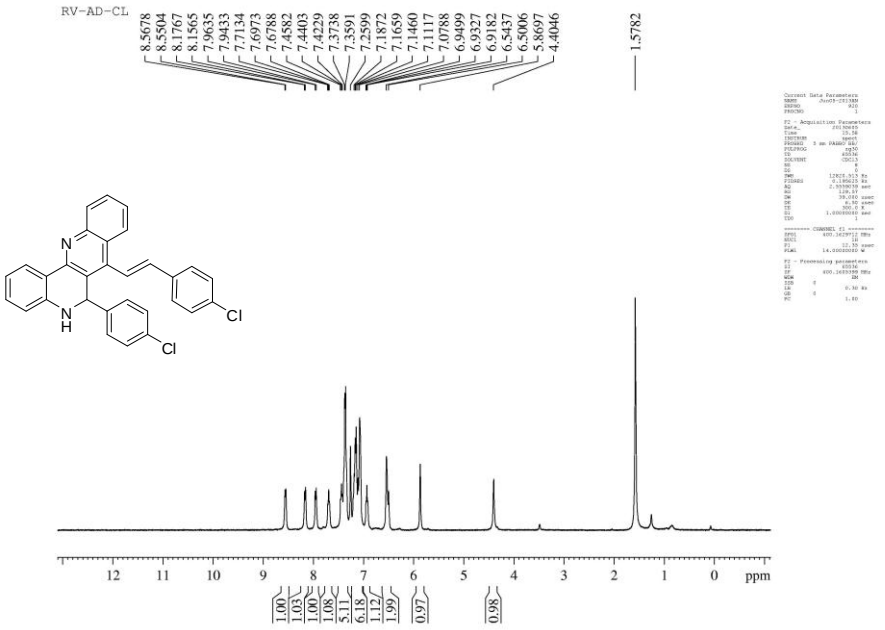


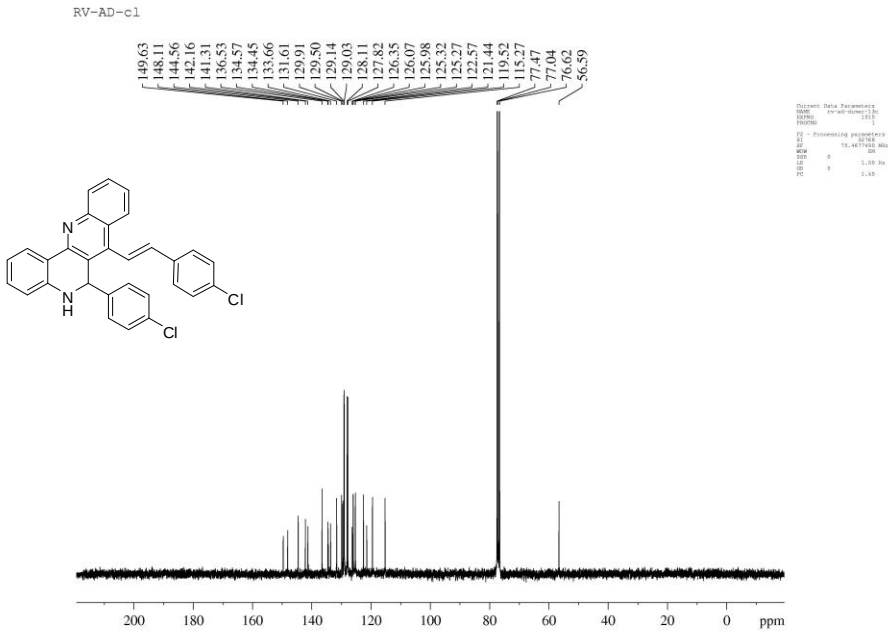
Table 1 Crystal data and structure refinement details for **2s**.

Compound	**2s**
Empirical formula	C_{30} H_{20} Cl N_3 O_2
Formula weight	489.94
Crystal System	Triclinic
Space group	*P*-1
a (Å)	9.823(3)
b (Å)	10.668(2)
c (Å)	11.585(3)
α (°)	95.708(3)
β (°)	105.487(5)
γ (°)	94.881(3)
V (Å^3)	1156.2(5)
Z	2
D_c (g/cm^3)	1.407
F_{000}	508
μ (mm^{-1})	0.201
θ_{max} (°)	25.38
Total reflections	7875
Unique reflections	3911
Reflections [$I > 2\sigma(I)$]	3176
Parameters	329
R_{int}	0.0363
Goodness-of-fit	0.975
R [$F^2 > 2\sigma(F^2)$]	0.0397
wR (F^2, all data)	0.1128
CCDC No.	1058218

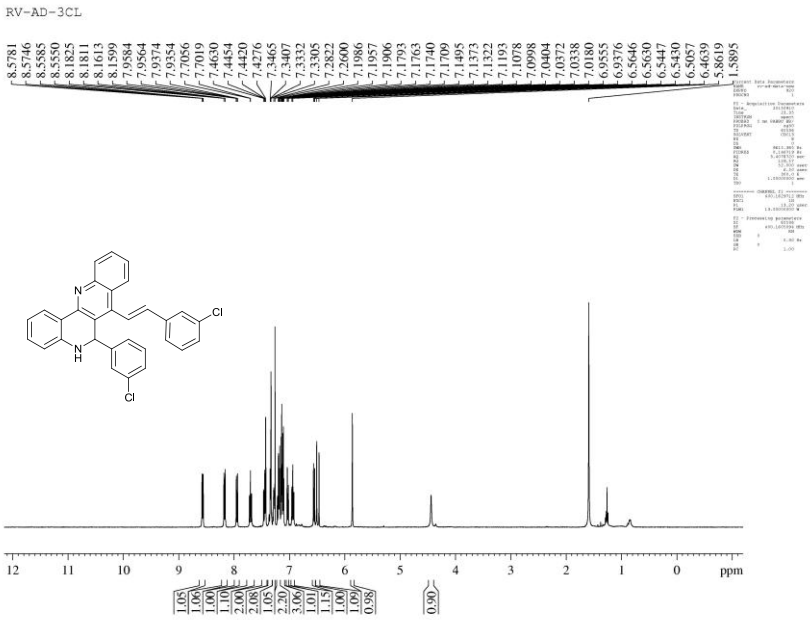
1. N. Ahmed and J. E. van Lier, *Tetrahedron Lett*., 2006, **47**, 2725.
2. CrystalClear 2.1, Rigaku Corporation, Tokyo, Japan.
3. Sheldrick, G. M. Acta Crystallogr., Sect. A 2008, **64**, 112–122.



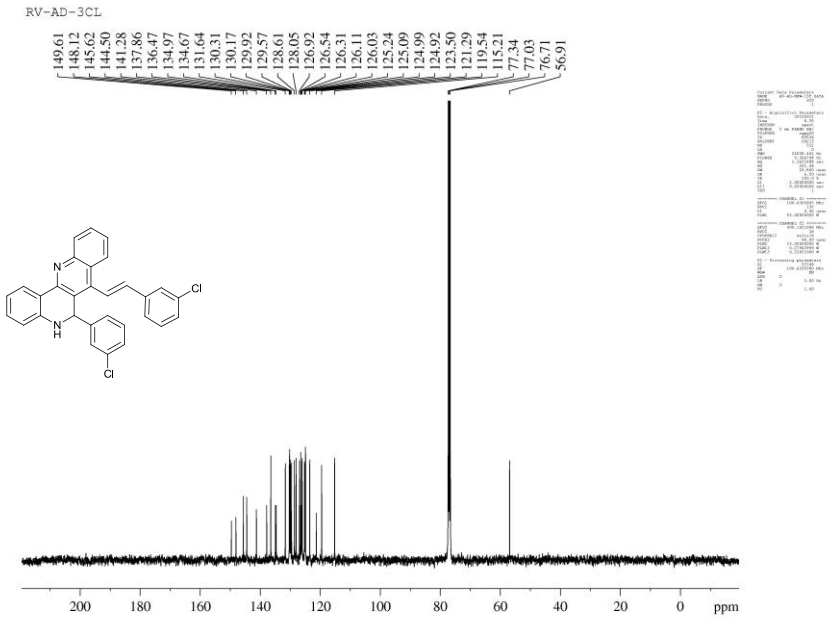
^{1}H NMR Spectra of **2a** (400 MHz, $CDCl_3$)



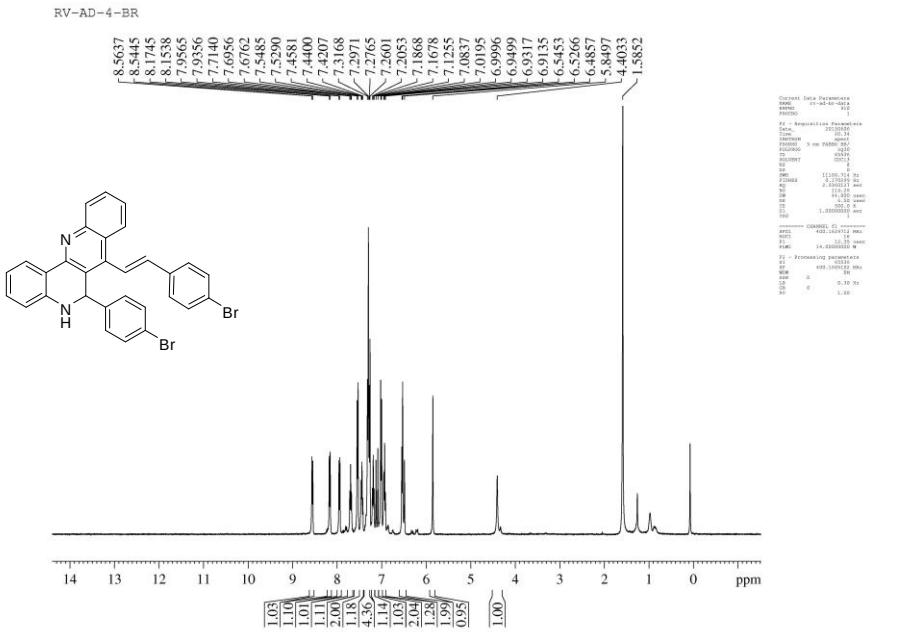
^{13}C NMR Spectra of **2a** (75 MHz, $CDCl_3$)



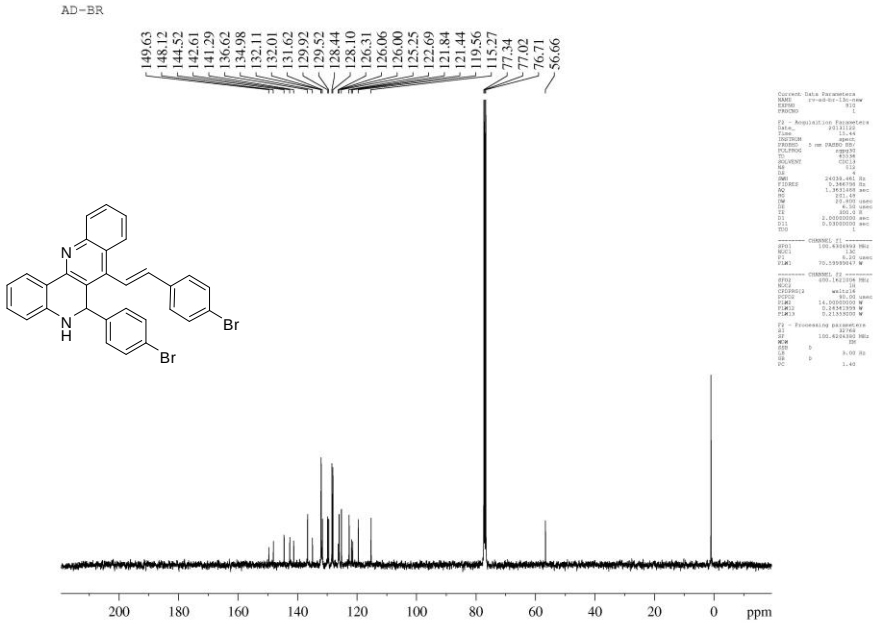
^{1}H NMR Spectra of **2b** (400 MHz, $CDCl_3$)



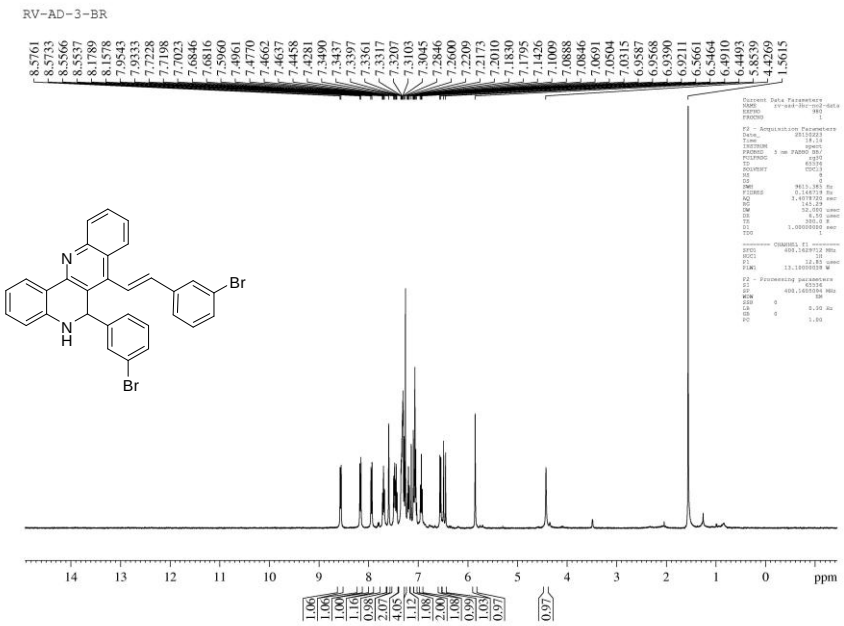
^{13}C NMR Spectra of **2b** (100 MHz, $CDCl_3$)



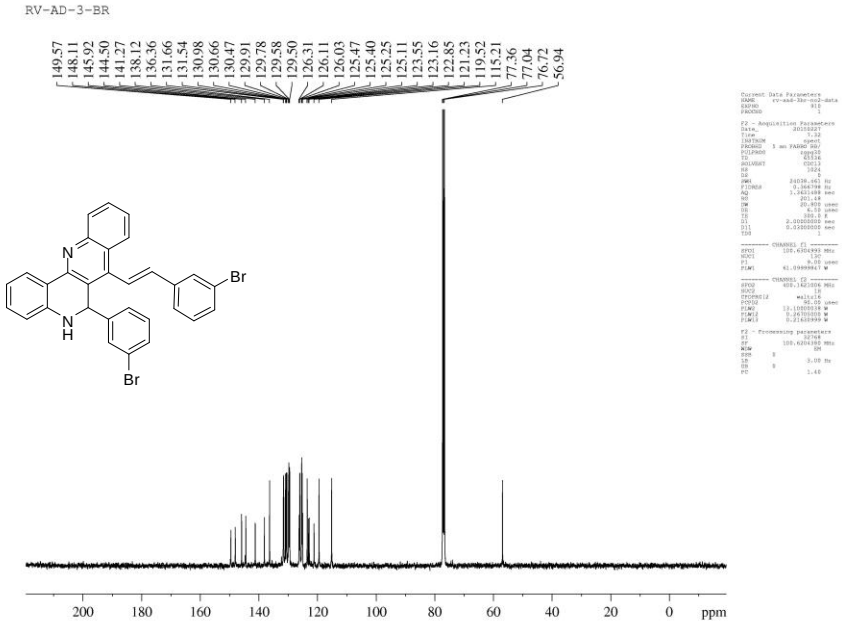
^{1}H NMR Spectra of **2c** (400 MHz, $CDCl_3$)



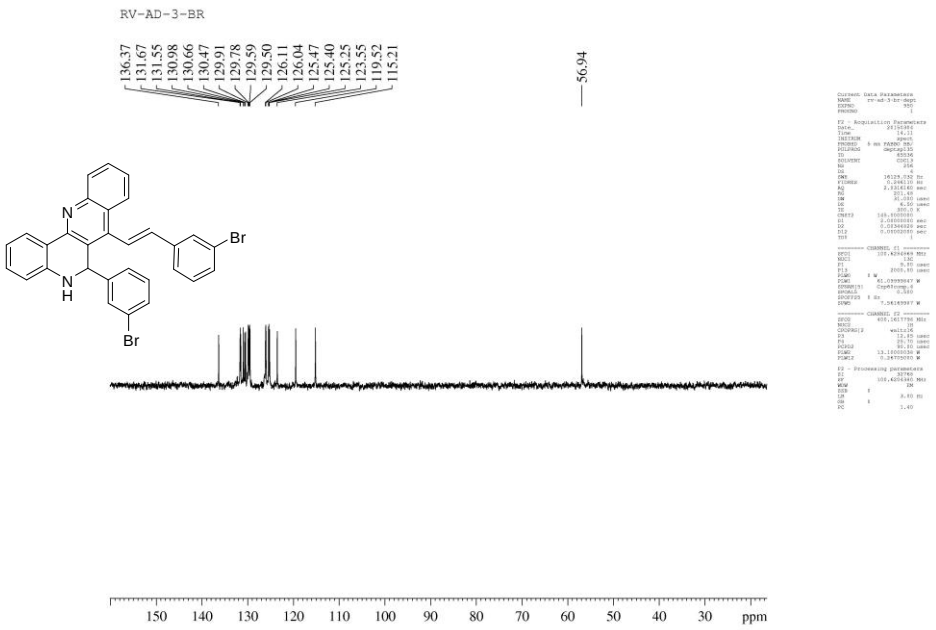
^{13}C NMR Spectra of **2c** (100 MHz, $CDCl_3$)



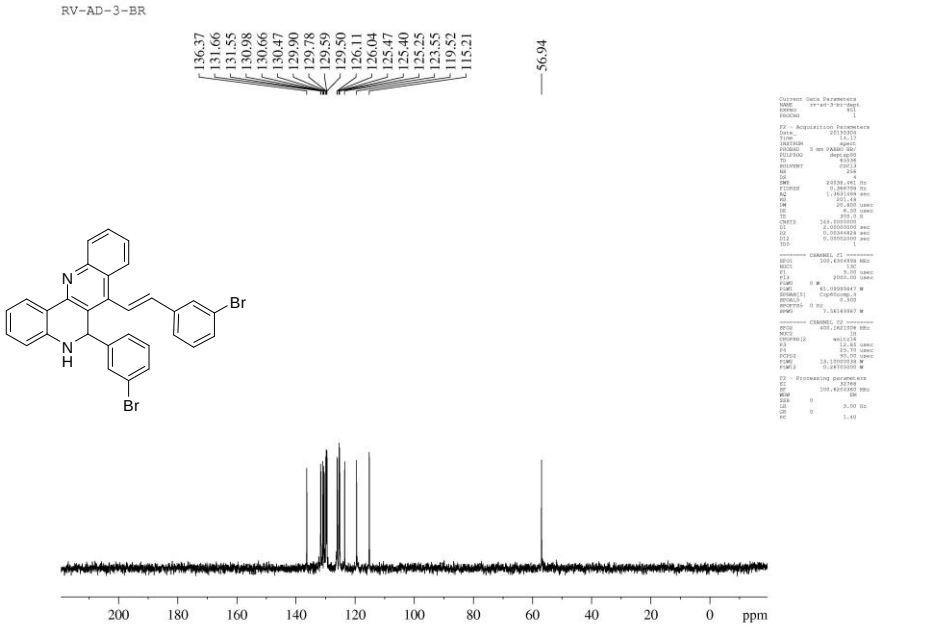
^{1}H NMR Spectra of **2d** (400 MHz, $CDCl_3$)



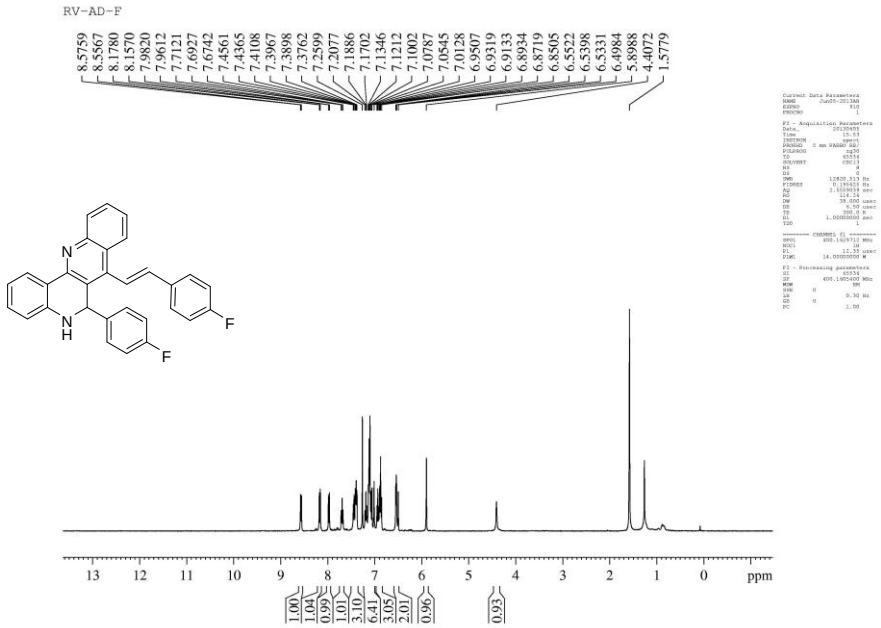
^{13}C NMR Spectra of **2d** (100 MHz, $CDCl_3$)



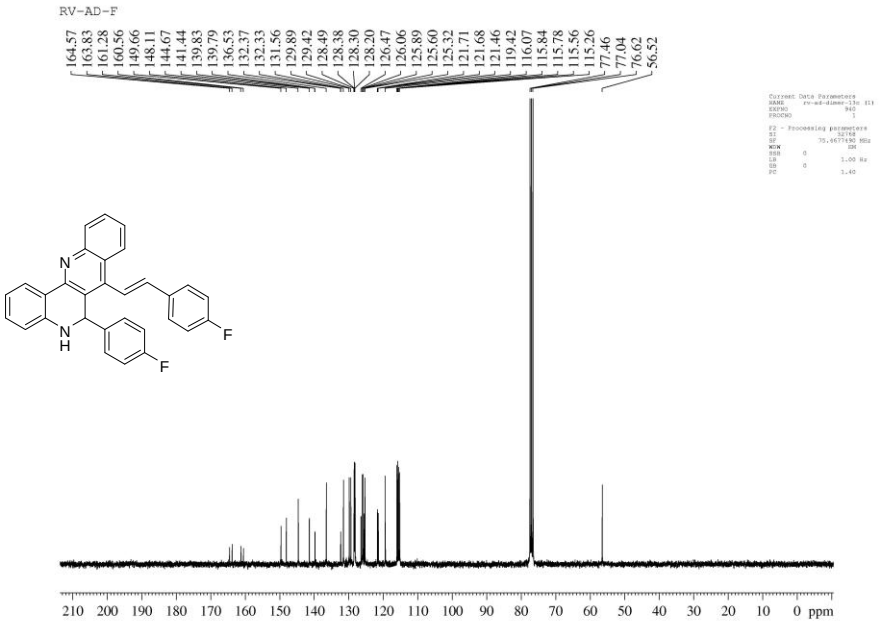
DEPT 135 ^{O} of **2d** (100 MHz, $CDCl_3$)



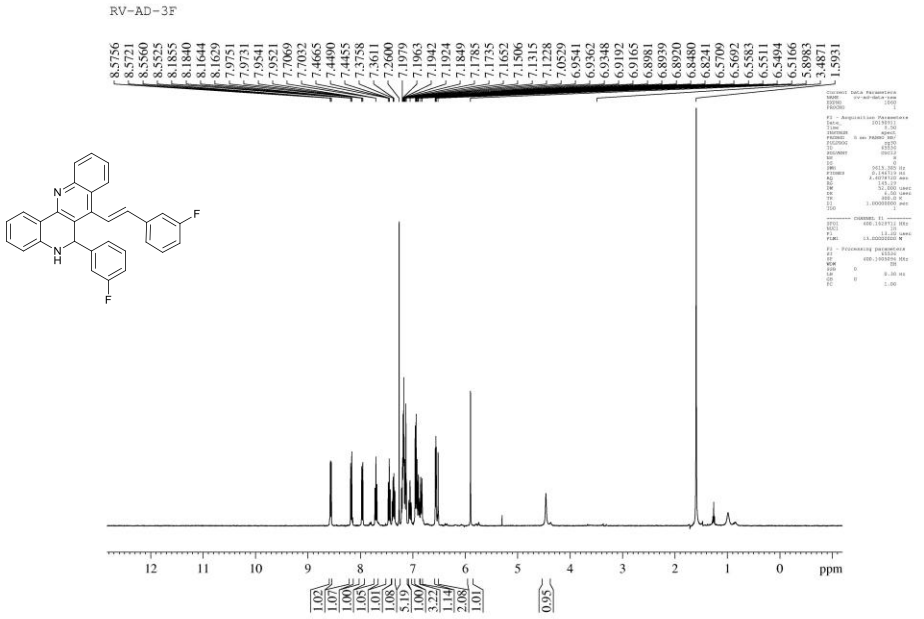
DEPT 90 ^{O} of **2d** (100 MHz, $CDCl_3$)



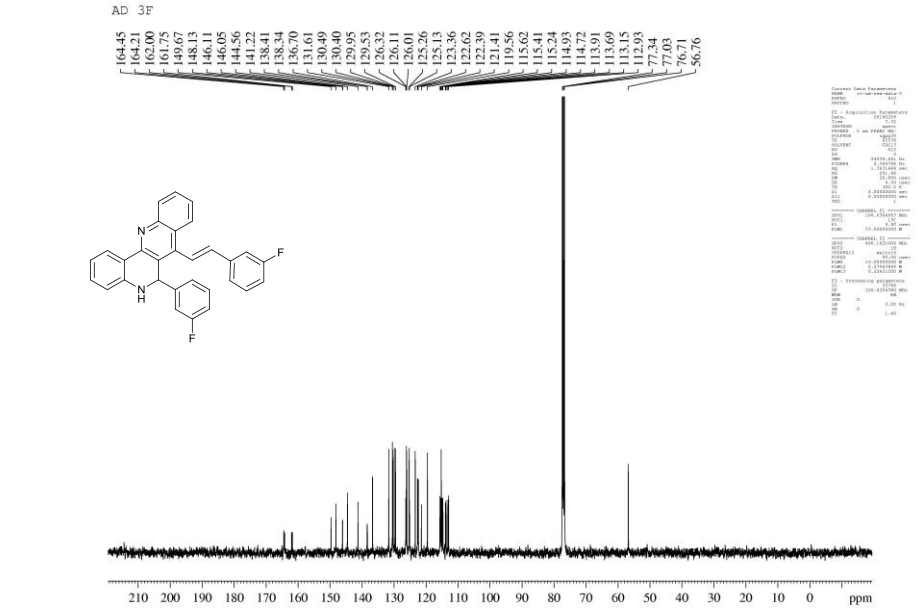
^{1}H NMR Spectra of **2e** (400 MHz, $CDCl_3$)



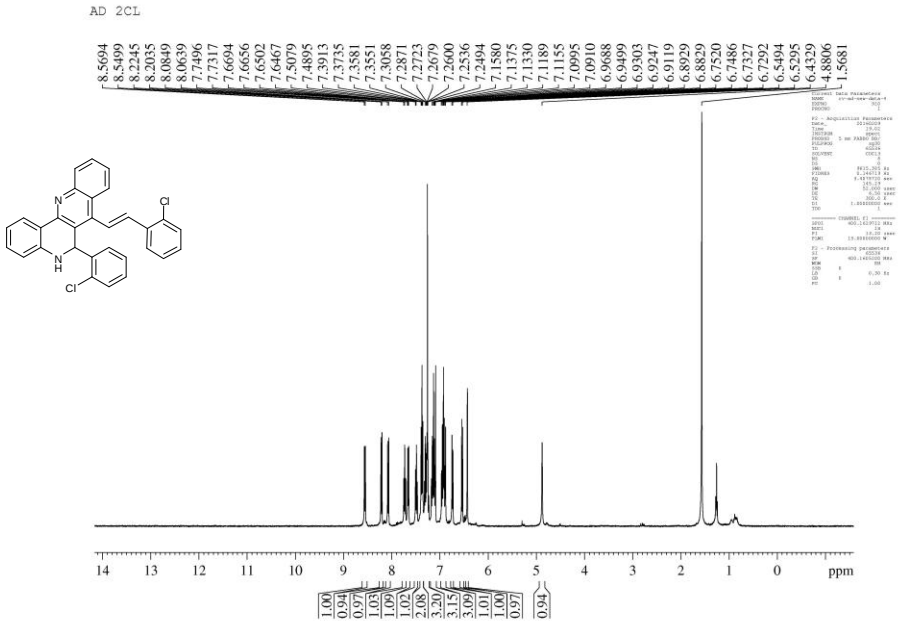
^{13}C NMR Spectra of **2e** (75 MHz, $CDCl_3$)



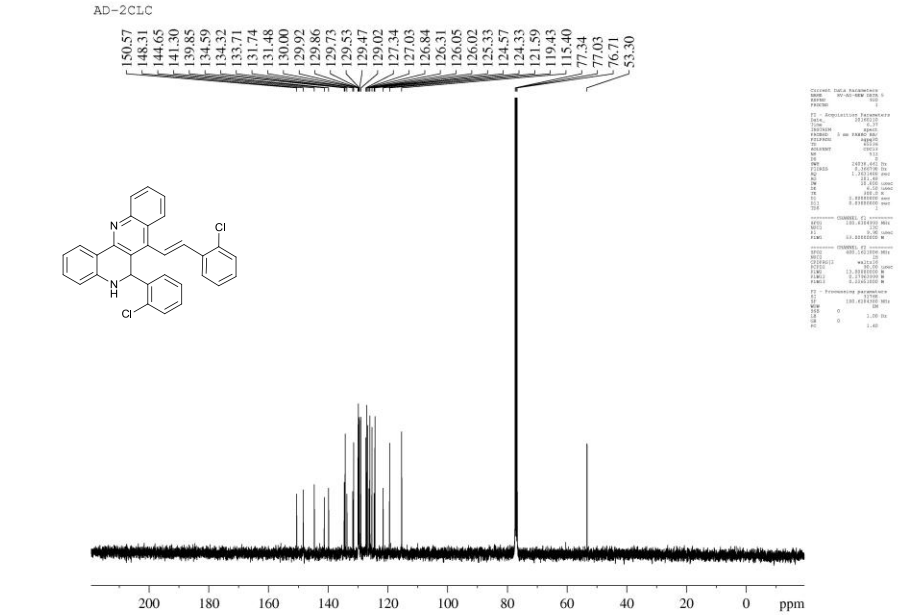
^{1}H NMR Spectra of **2f** (400 MHz, $CDCl_3$)



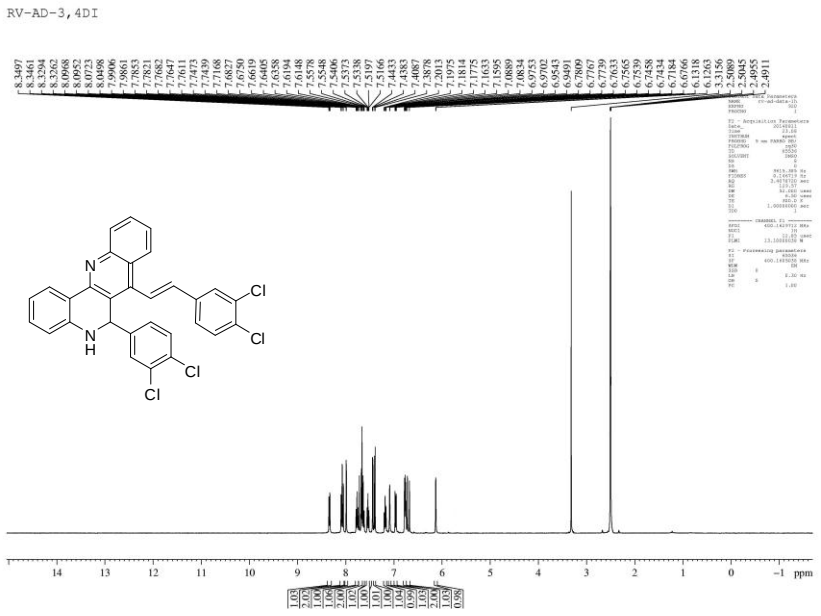
^{13}C NMR Spectra of **2f** (100 MHz, $CDCl_3$)



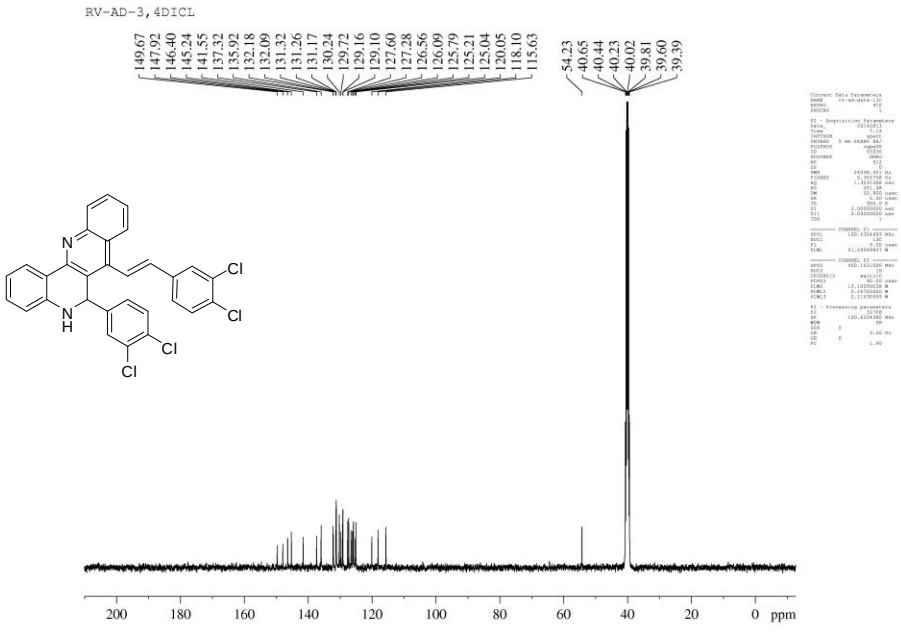
^{1}H NMR Spectra of **2g** (400 MHz, $CDCl_3$)



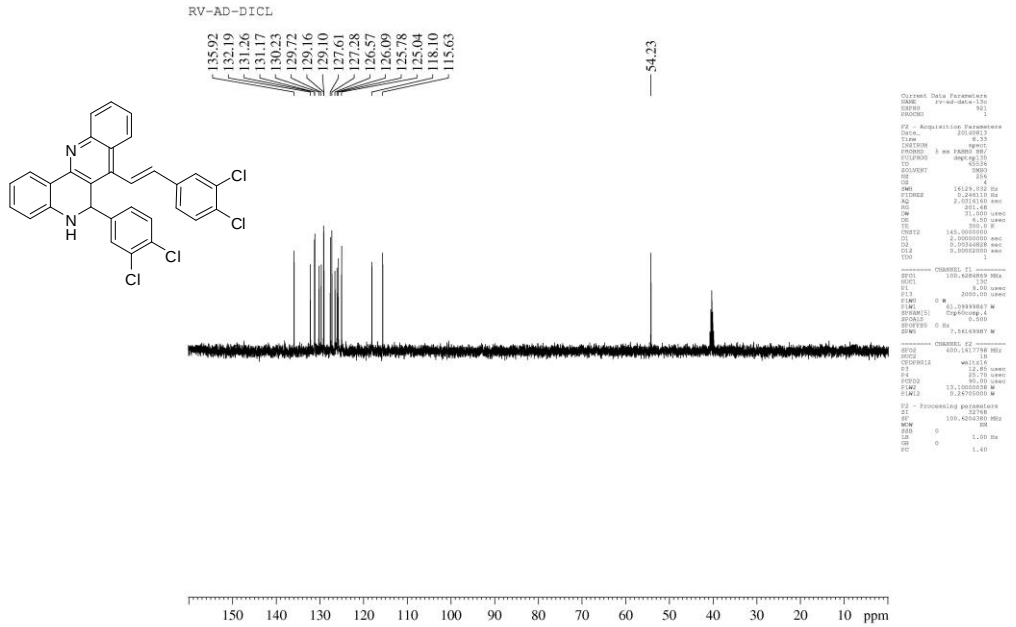
^{13}C NMR Spectra of **2g** (100 MHz, $CDCl_3$)



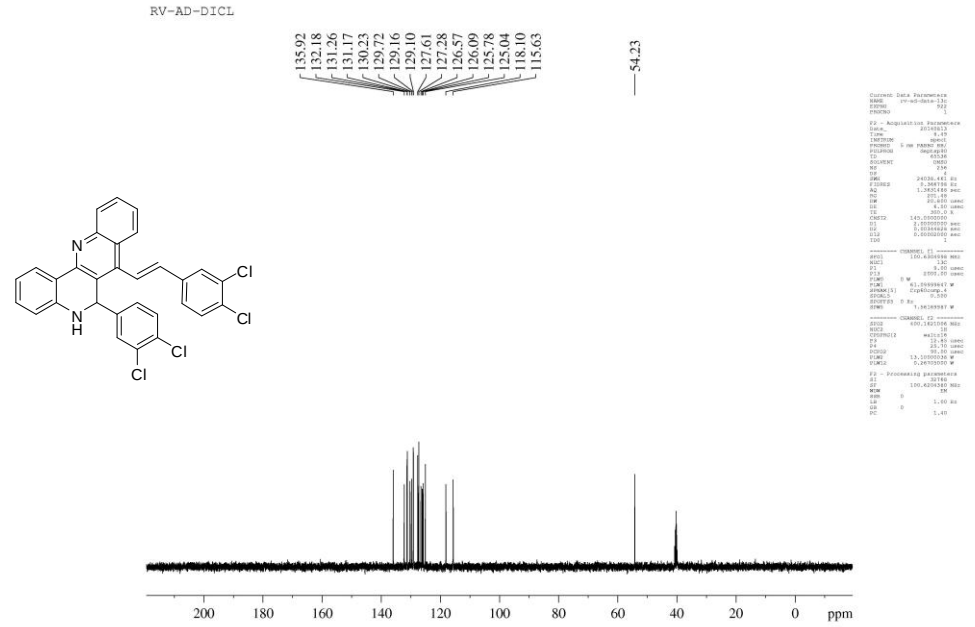
^{1}H NMR Spectra of **2h** (400 MHz, DMSO-d_6)



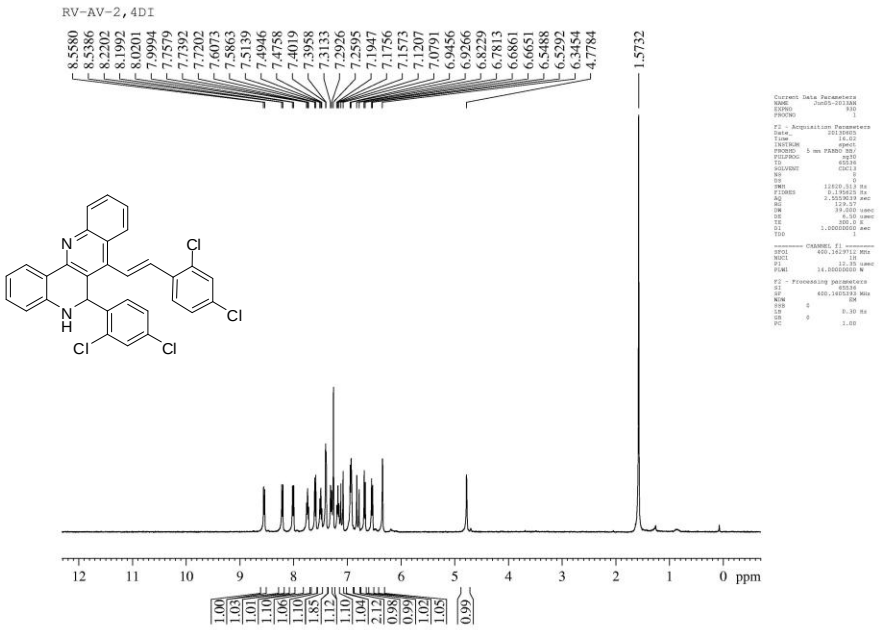
^{13}C NMR Spectra of **2h** (100 MHz, DMSO-d_6)



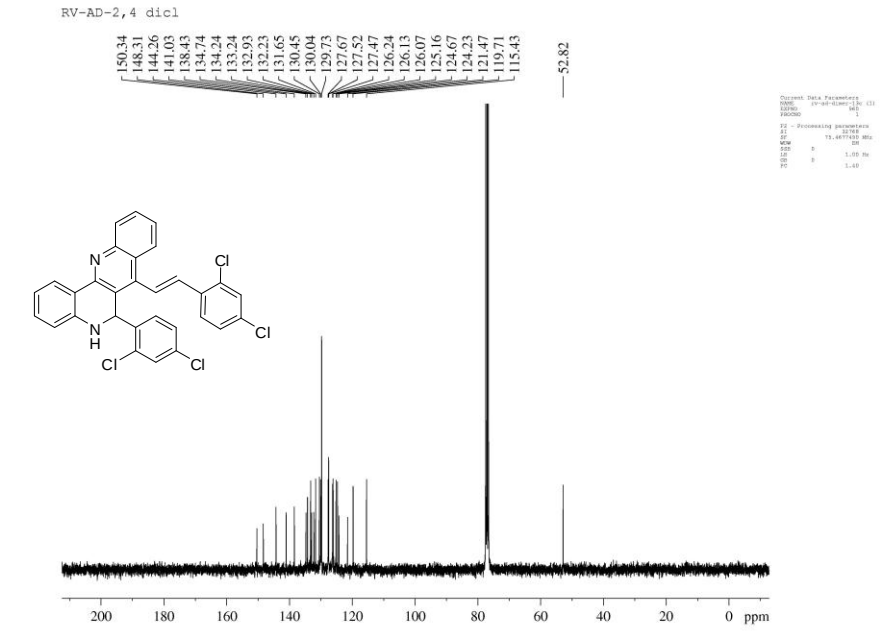
DEPT 135 ^{O} of **2h** (100 MHz, DMSO-d_6)



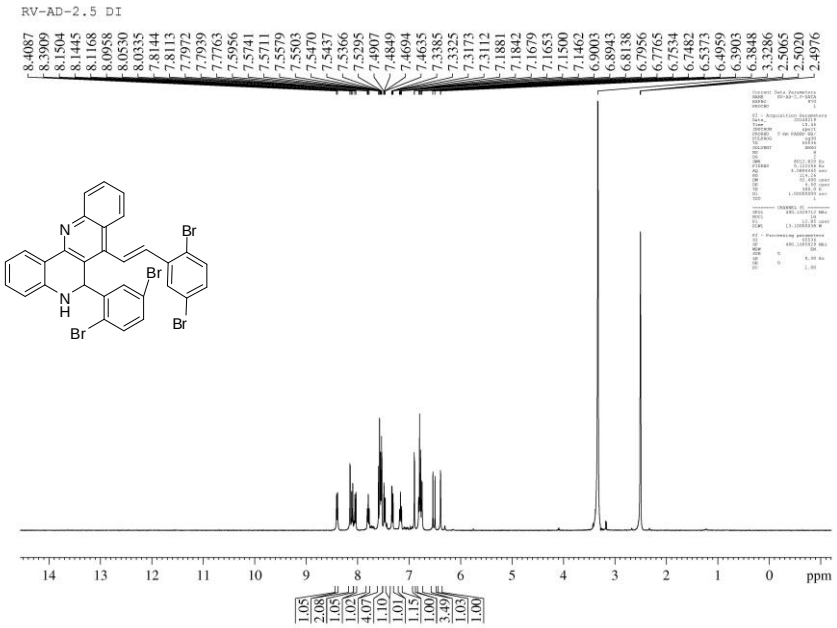
Dept 90 ^{O} of **2h** (100 MHz, DMSO-d_6)



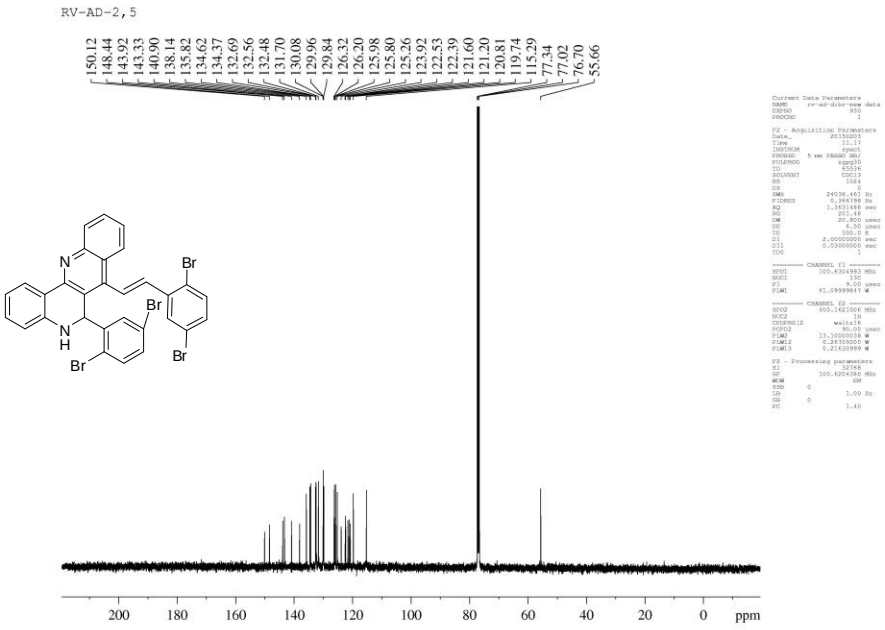
^{1}H NMR Spectra of **2i** (400 MHz, $CDCl_3$)



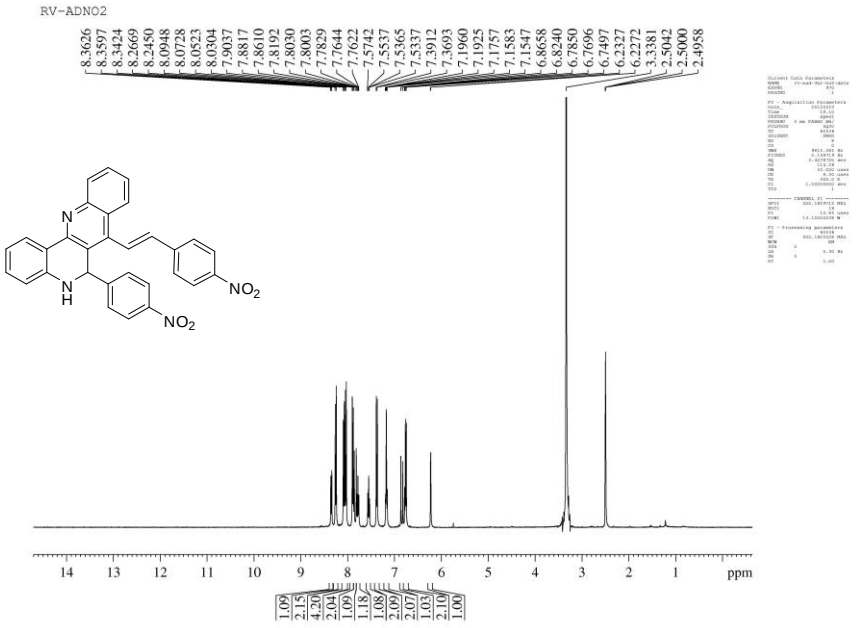
^{13}CNMR Spectra of **2i** (75 MHz, $CDCl_3$)



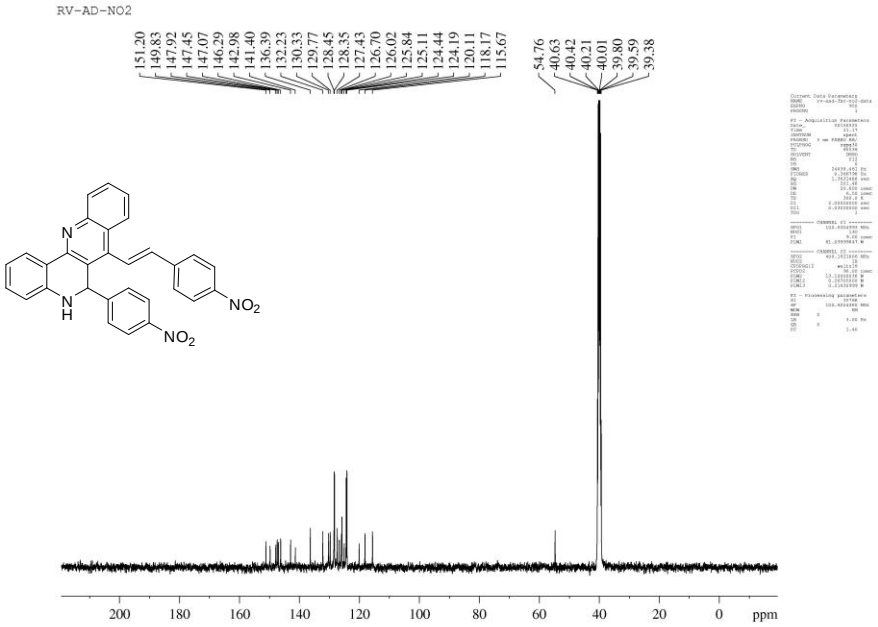
^{1}H NMR Spectra of **2j** (400 MHz, DMSO-d_6)



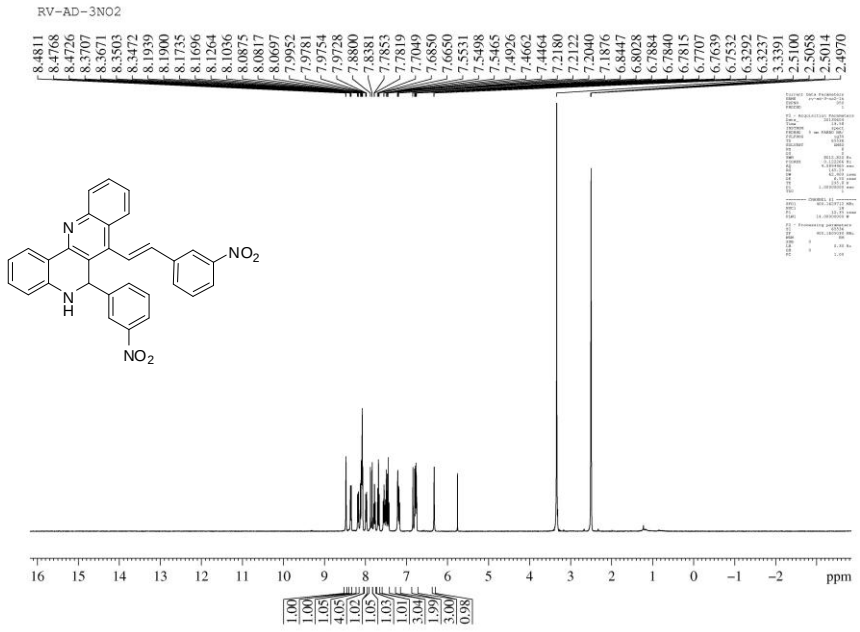
^{13}C NMR Spectra of **2j** (100 MHz, $CDCl_3$)



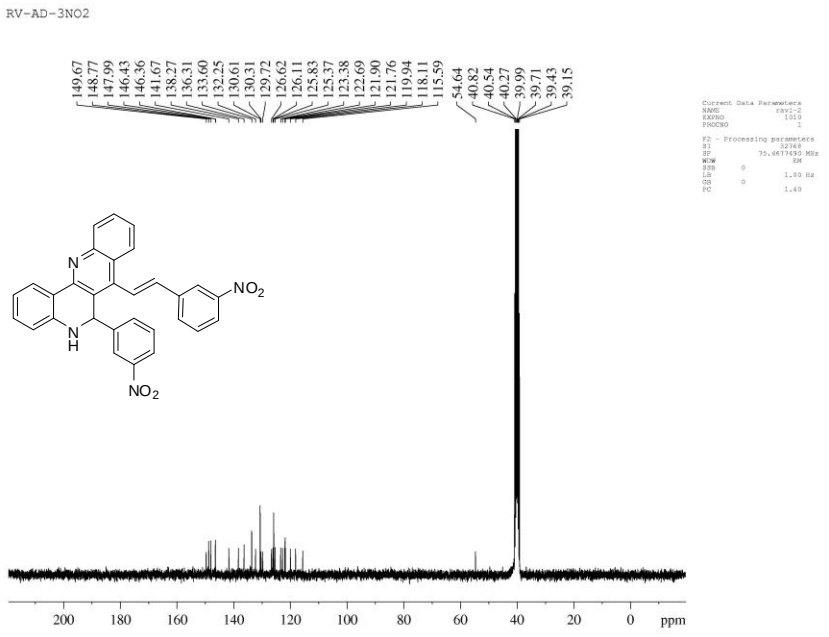
^{1}H NMR Spectra of **2k** (400 MHz, DMSO-d_6)



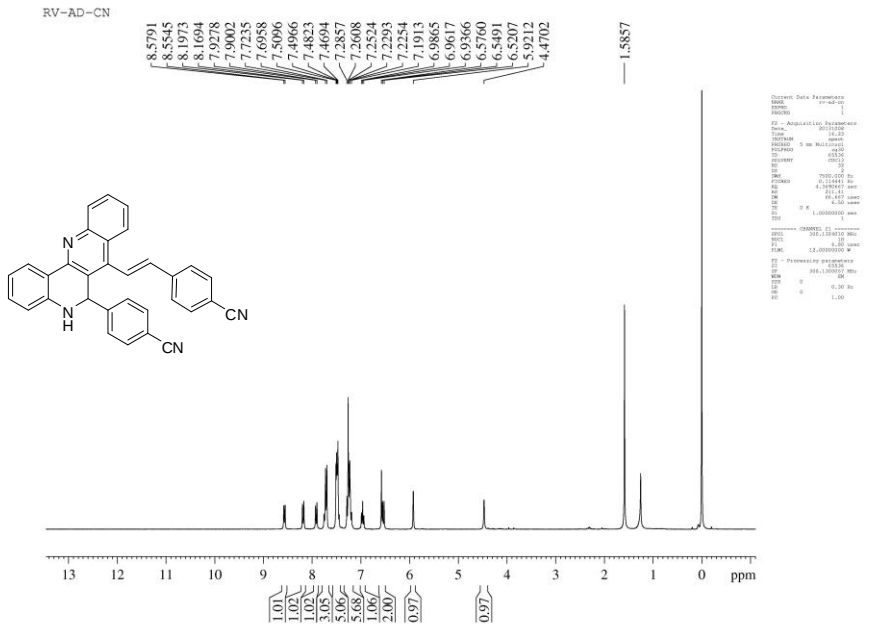
^{13}C NMR Spectra of **2k** (100 MHz, DMSO-d_6)



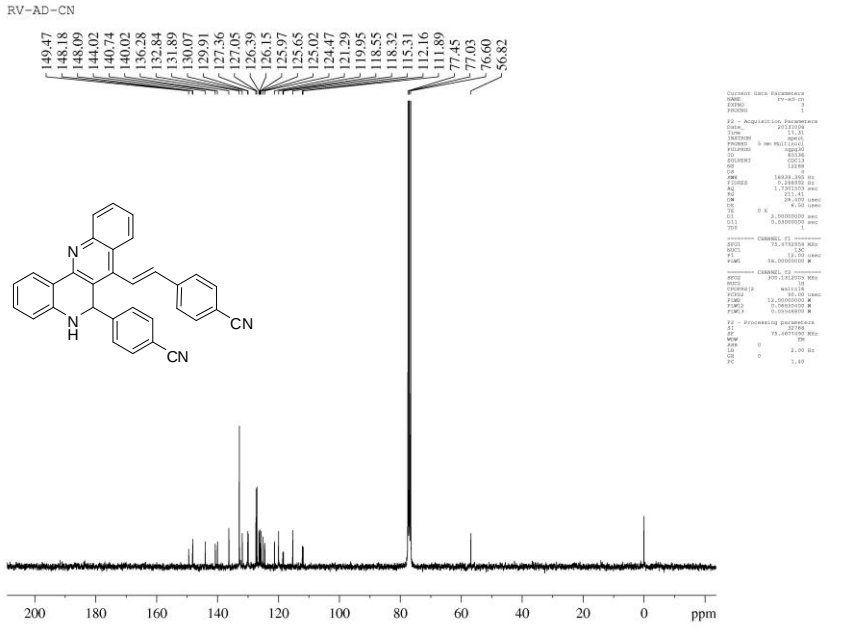
^{1}H NMR Spectra of **2l** (400 MHz, DMSO-d_6)



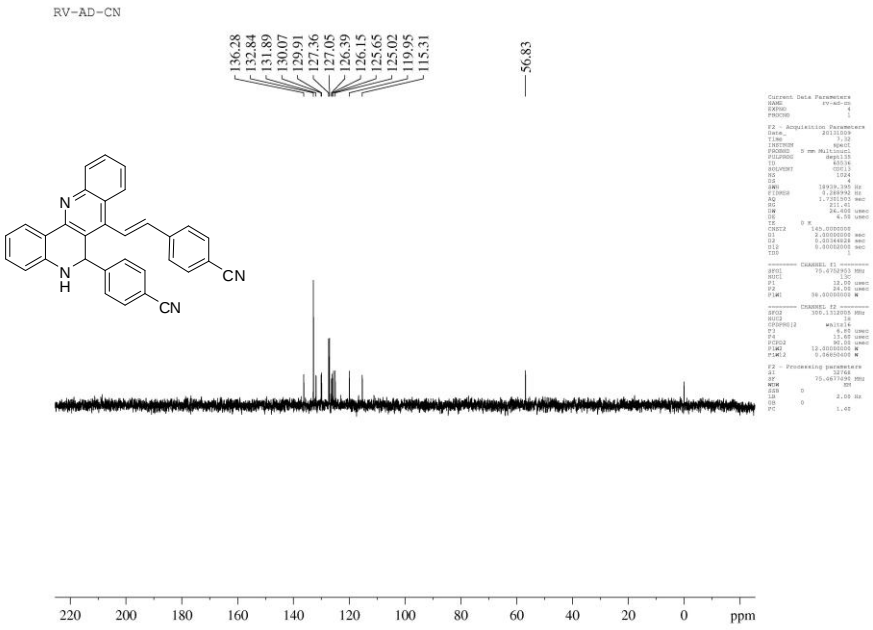
^{13}C NMR Spectra of **2l** (75 MHz, DMSO-d_6)



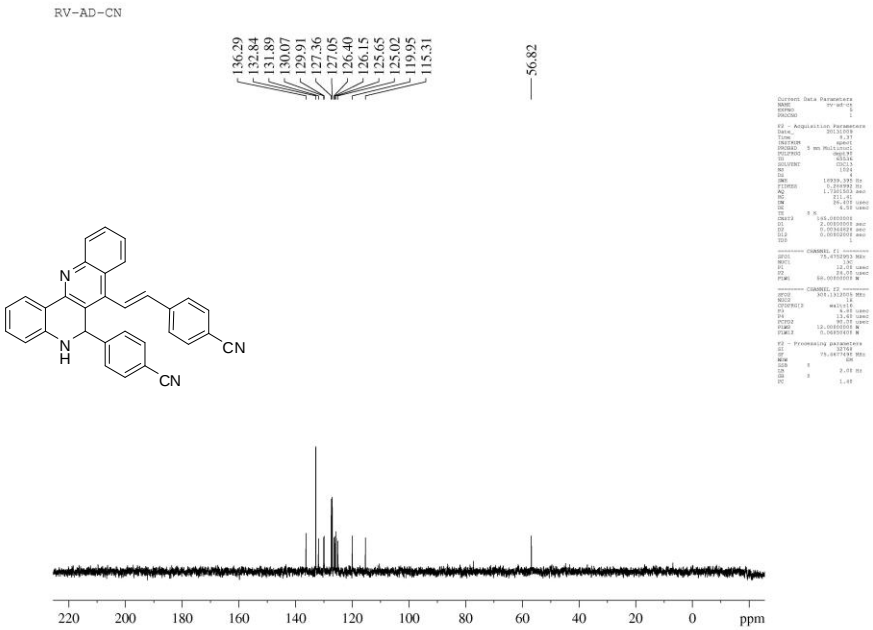
^{1}H NMR Spectra of **2m** (300 MHz, $CDCl_3$)



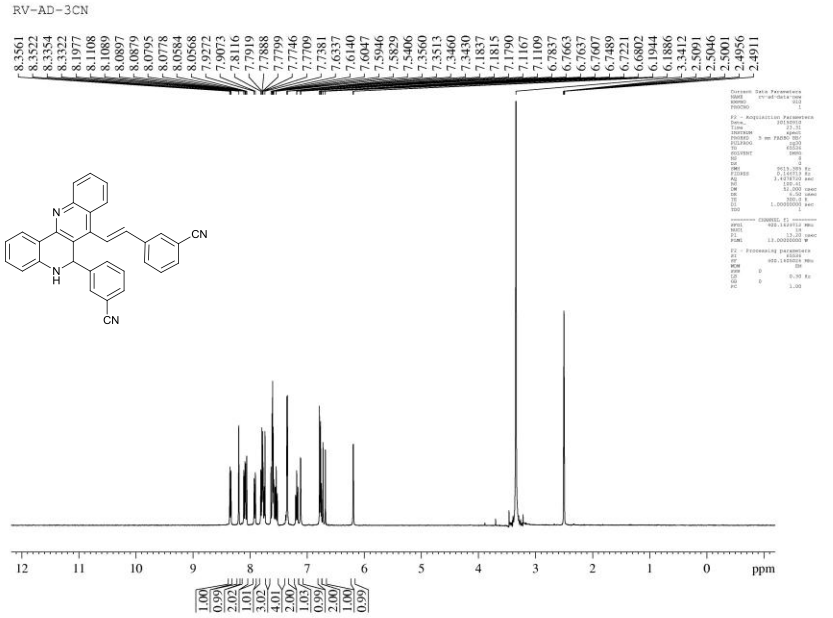
^{13}C NMR Spectra of **2m** (75 MHz, $CDCl_3$)



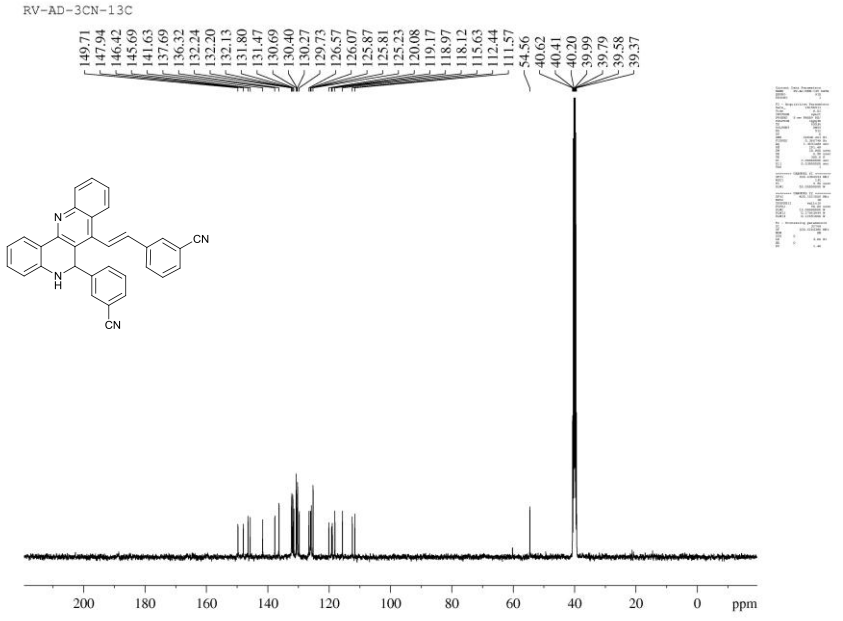
DEPT 135 ^{O} of **2m** (75 MHz, $CDCl_3$)



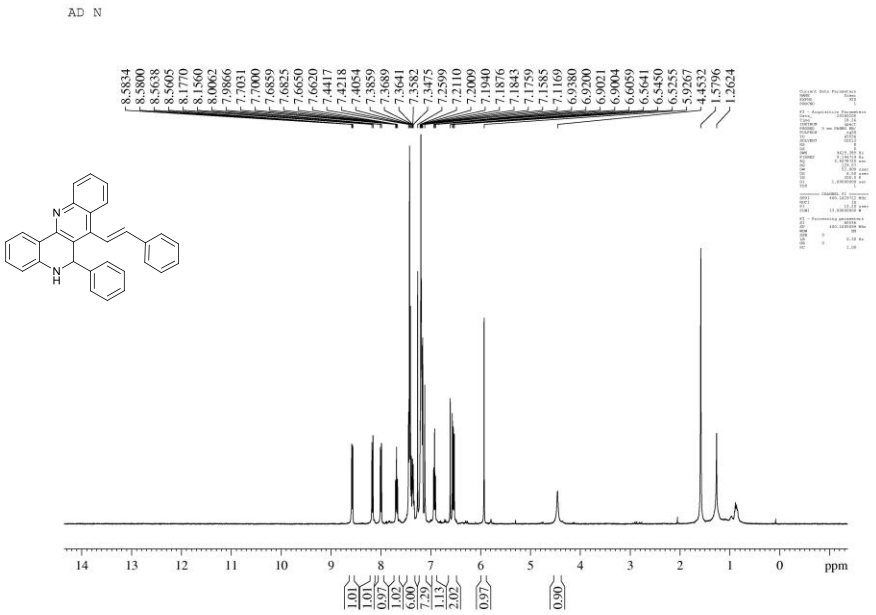
DEPT 90 ^{O} of **2m** (75 MHz, $CDCl_3$)



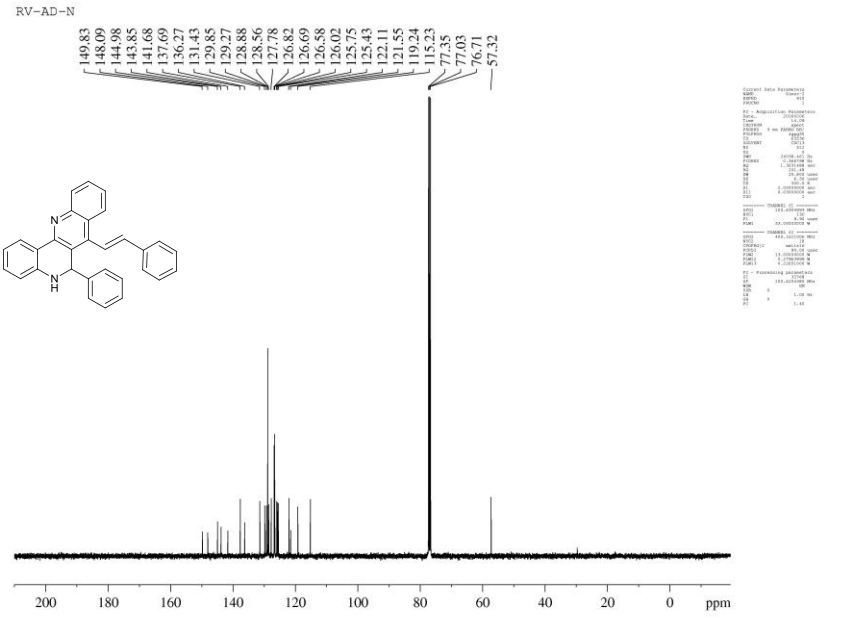
^{1}H NMR Spectra of **2n** (400 MHz, DMSO-d_6)



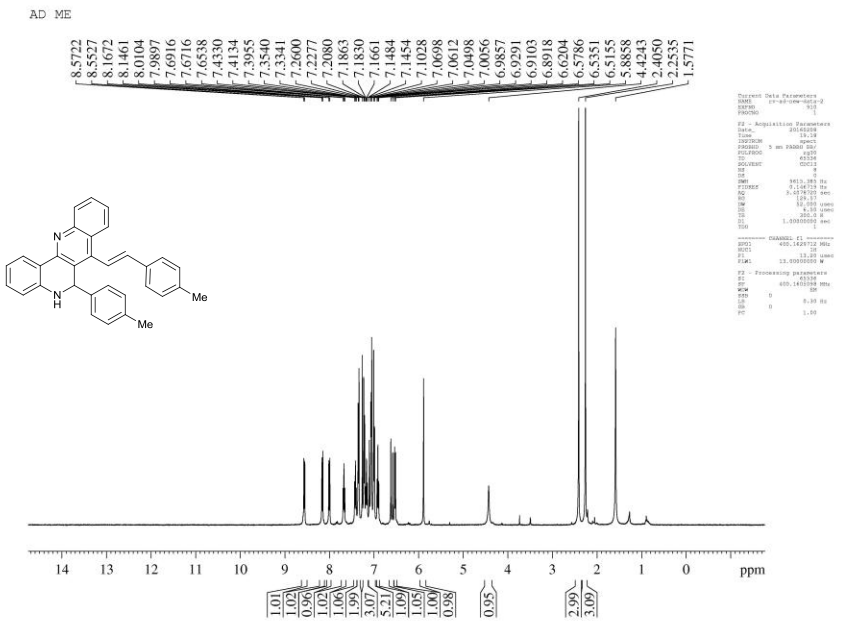
^{13}C NMR Spectra of **2n** (100 MHz, DMSO-d_6)



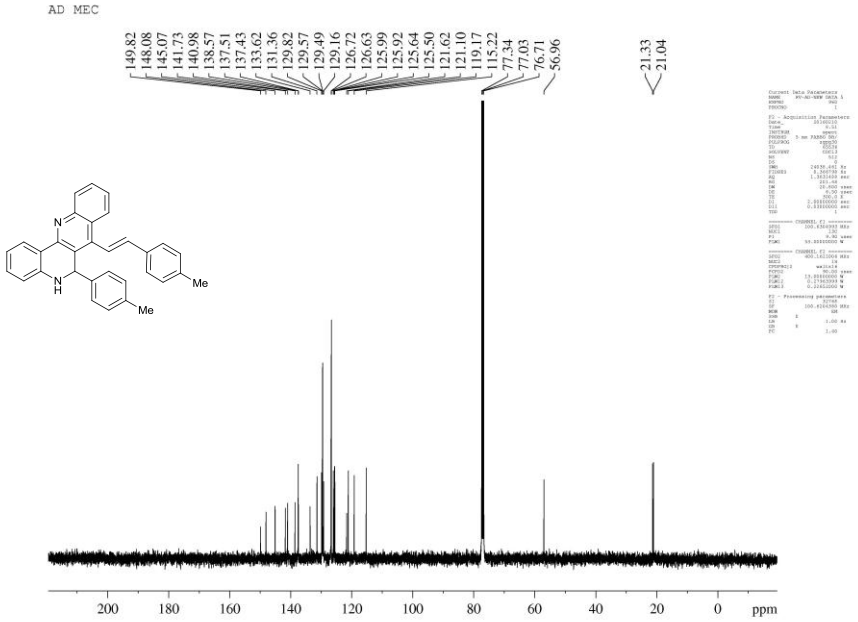
^{1}H NMR Spectra of **2o** (400 MHz, $CDCl_3$)



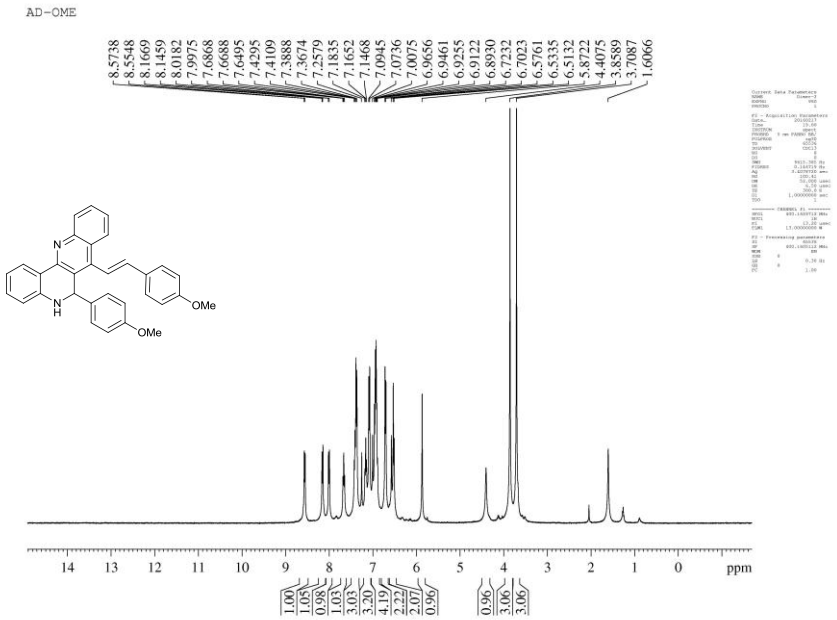
^{13}C NMR Spectra of **2o** (100 MHz, $CDCl_3$)



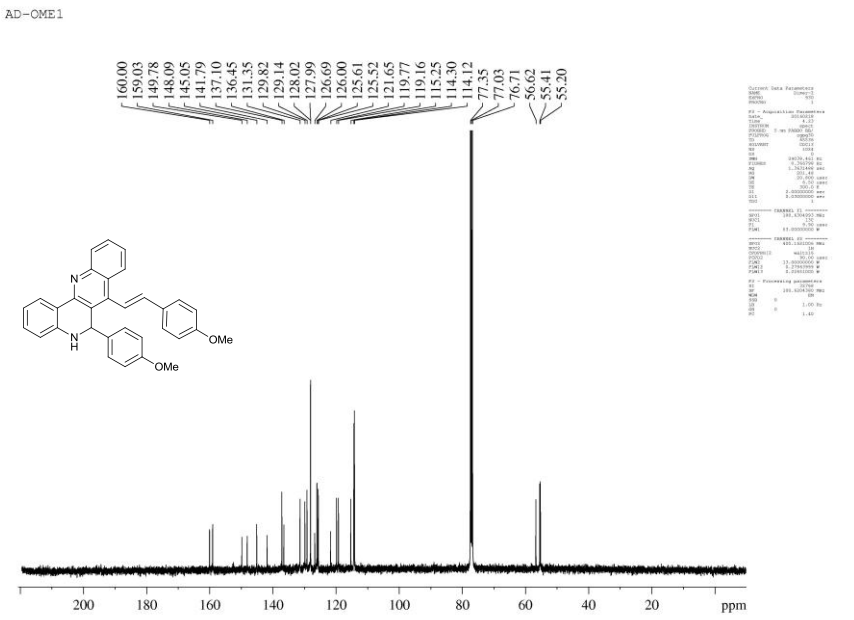
^{1}H NMR Spectra of **2p** (400 MHz, $CDCl_3$)



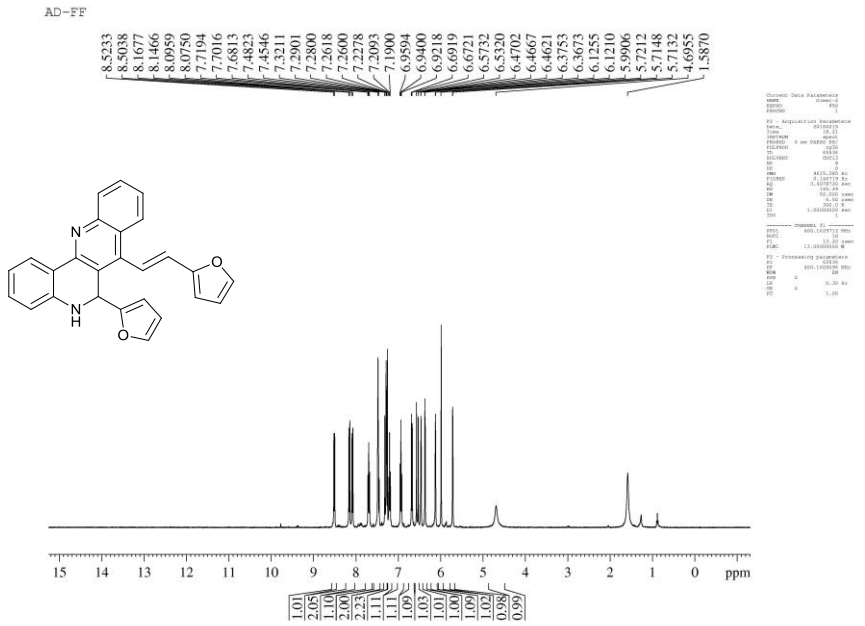
^{13}C NMR Spectra of **2p** (100 MHz, $CDCl_3$)



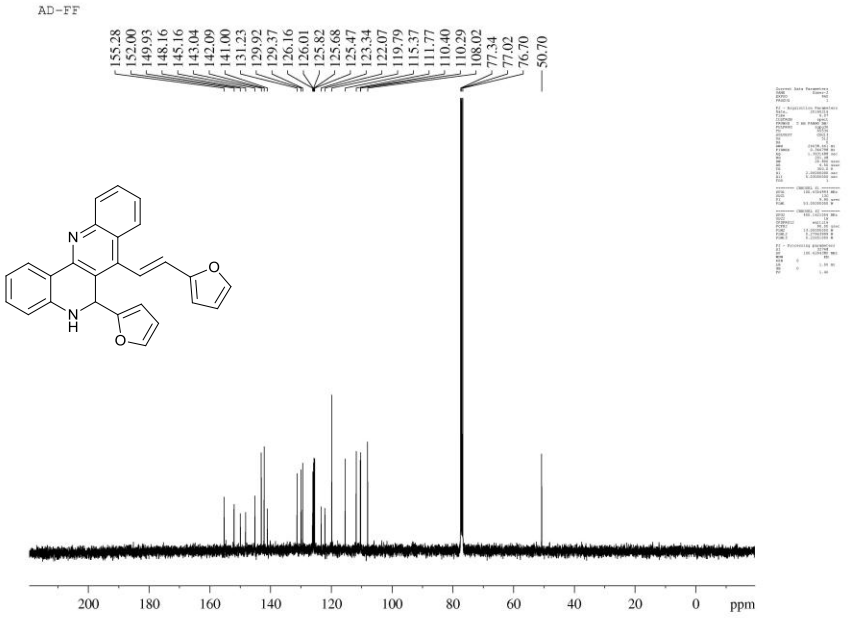
^{1}H NMR Spectra of **2q** (400 MHz, $CDCl_3$)



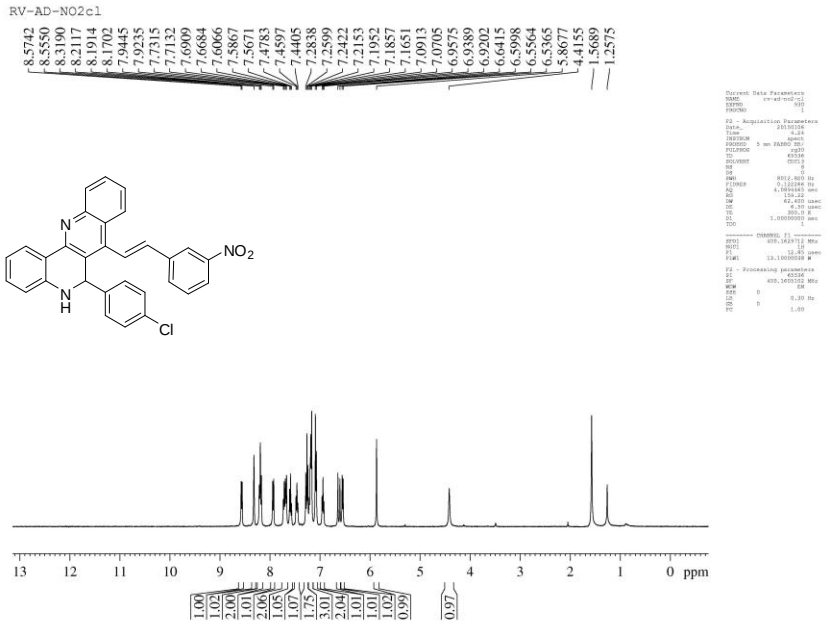
^{13}C NMR Spectra of **2q** (100 MHz, $CDCl_3$)



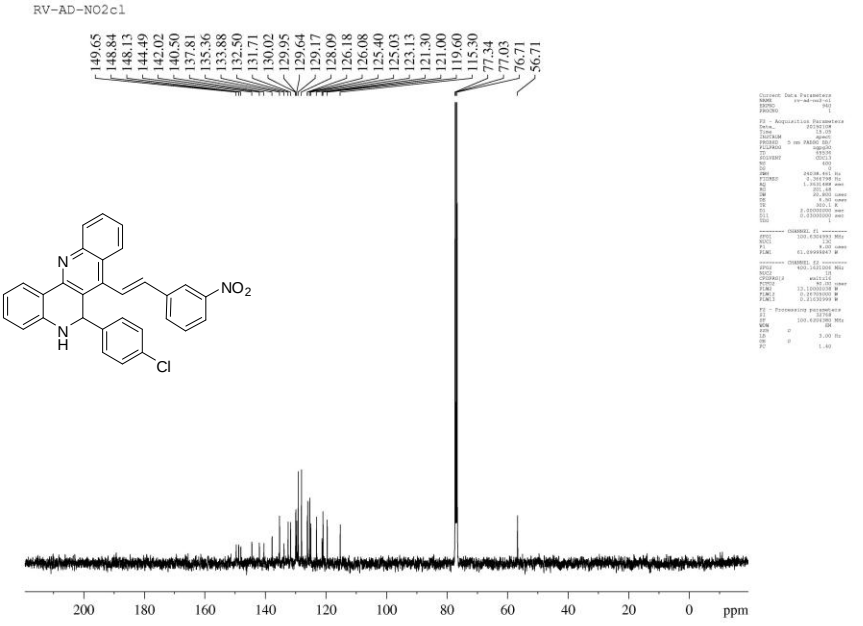
^{1}H NMR Spectra of **2r** (400 MHz, $CDCl_3$)



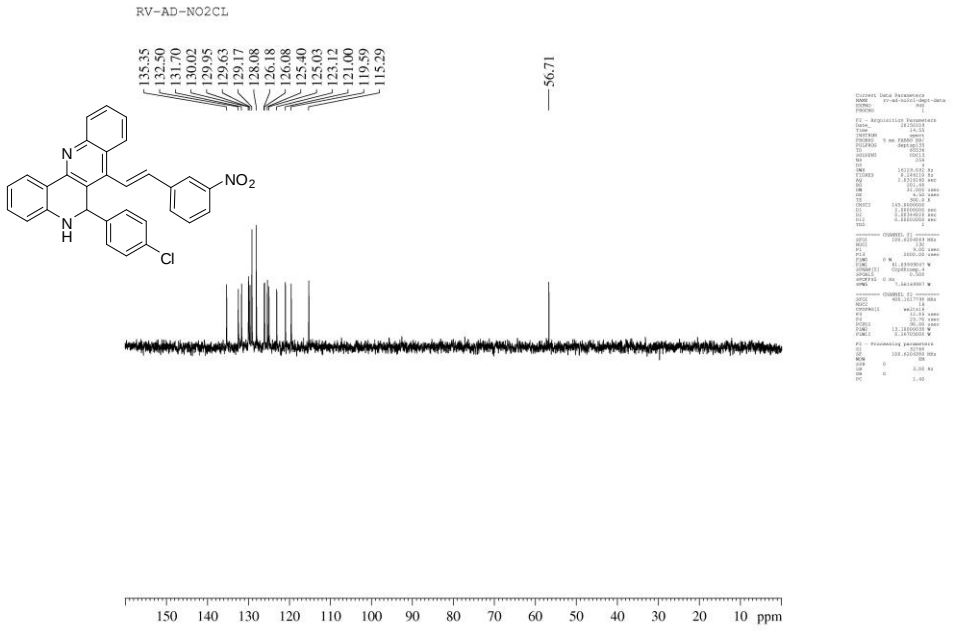
^{13}C NMR Spectra of **2r** (100 MHz, $CDCl_3$)



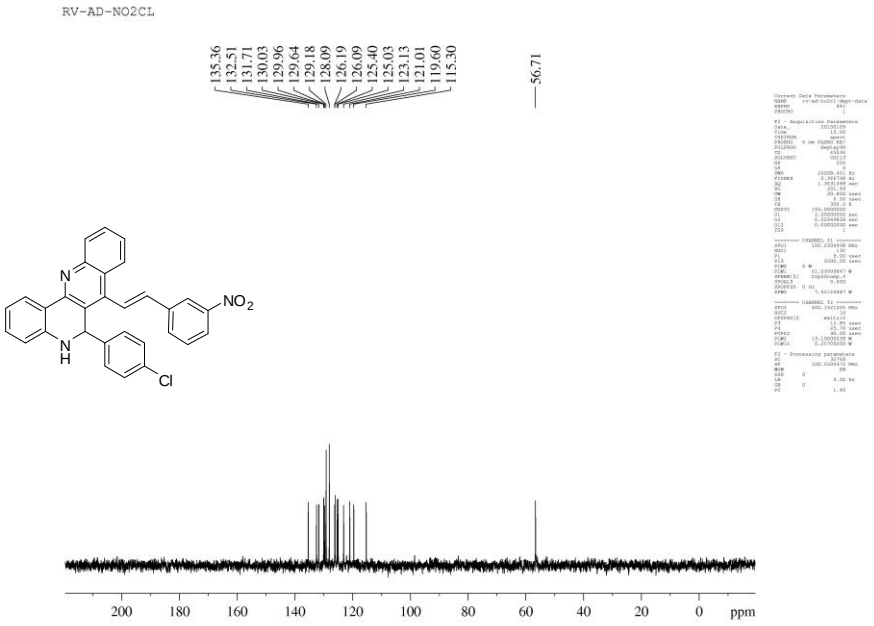
^{1}H NMR Spectra of **2s** (400 MHz, $CDCl_3$)



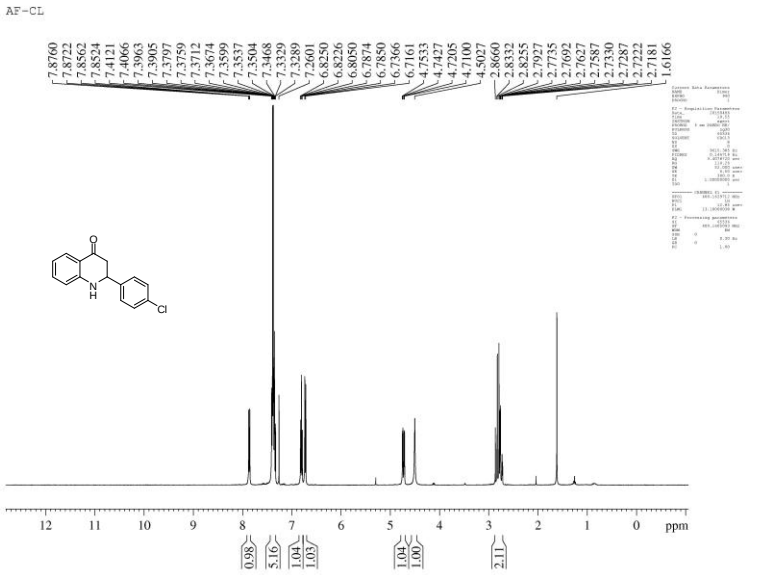
^{13}C NMR Spectra of **2s** (100 MHz, $CDCl_3$)



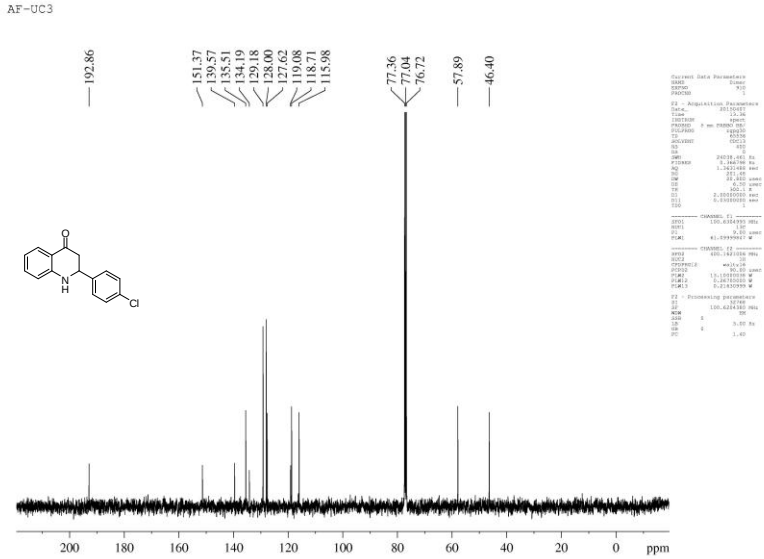
DEPT 135 ^{O} of **2s** (100 MHz, $CDCl_3$)



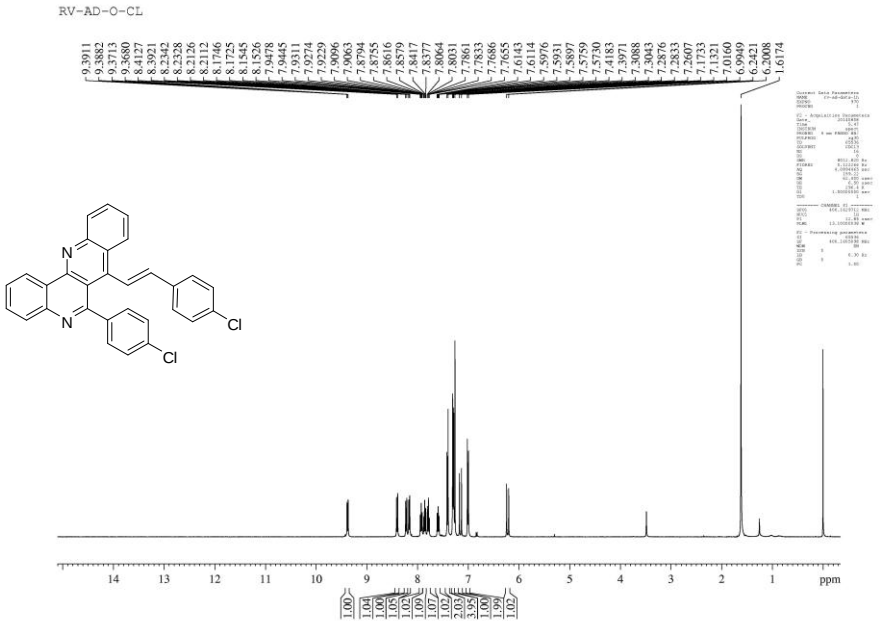
DEPT 90 ^{O} of **2s** (100 MHz, $CDCl_3$)



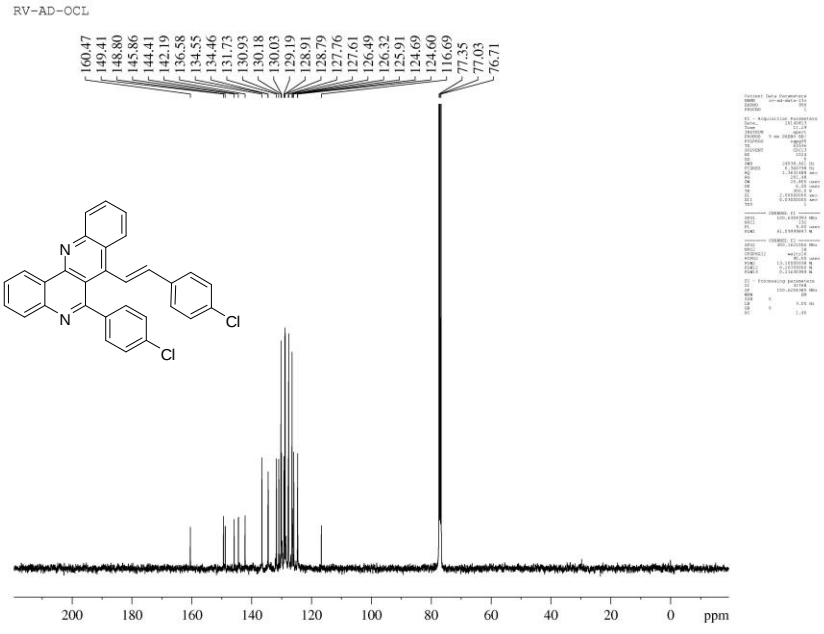
^{1}H NMR Spectra of **3a** (400 MHz, $CDCl_3$)



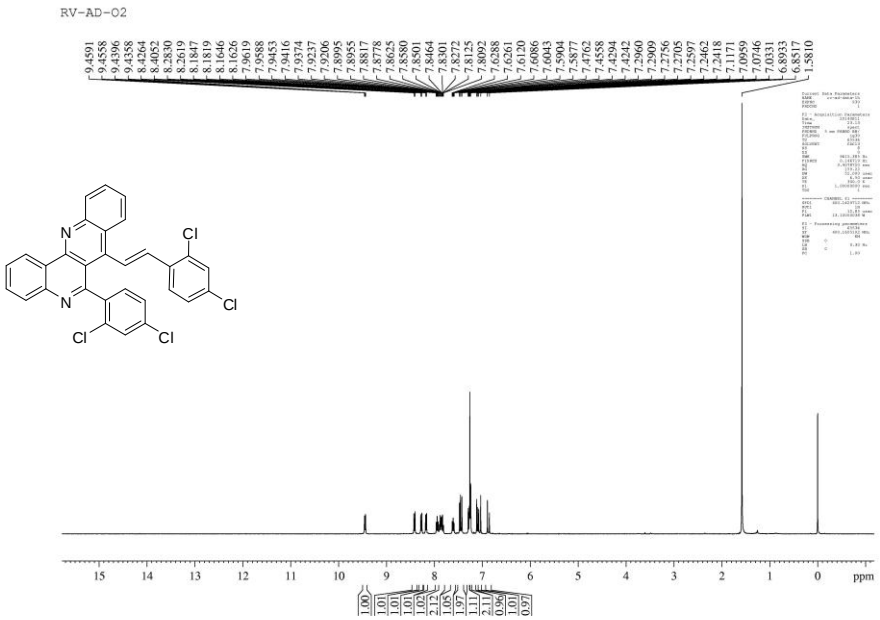
^{13}C NMR Spectra of **3a** (100 MHz, $CDCl_3$)



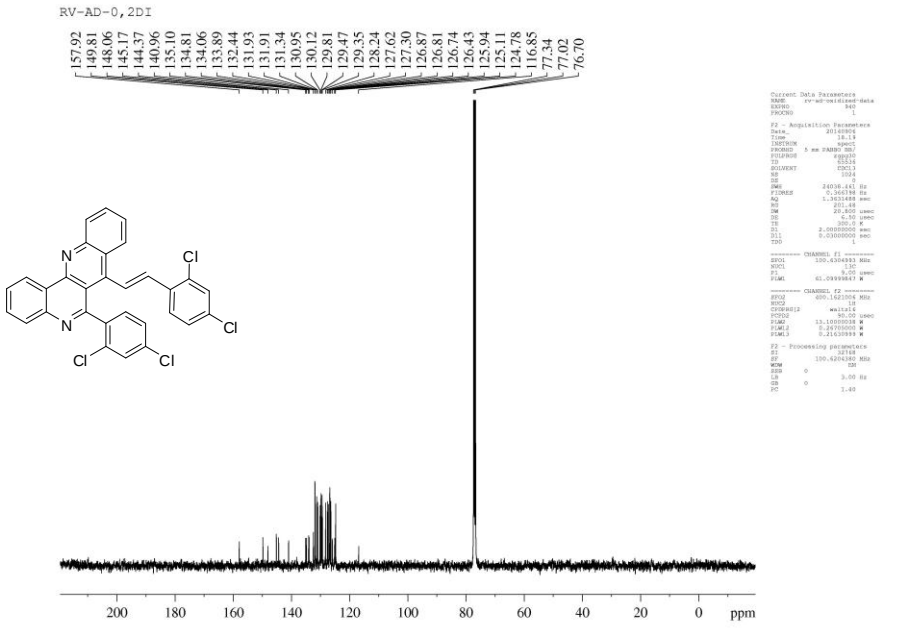
^{1}H NMR Spectra of **4a** (400 MHz, $CDCl_3$)



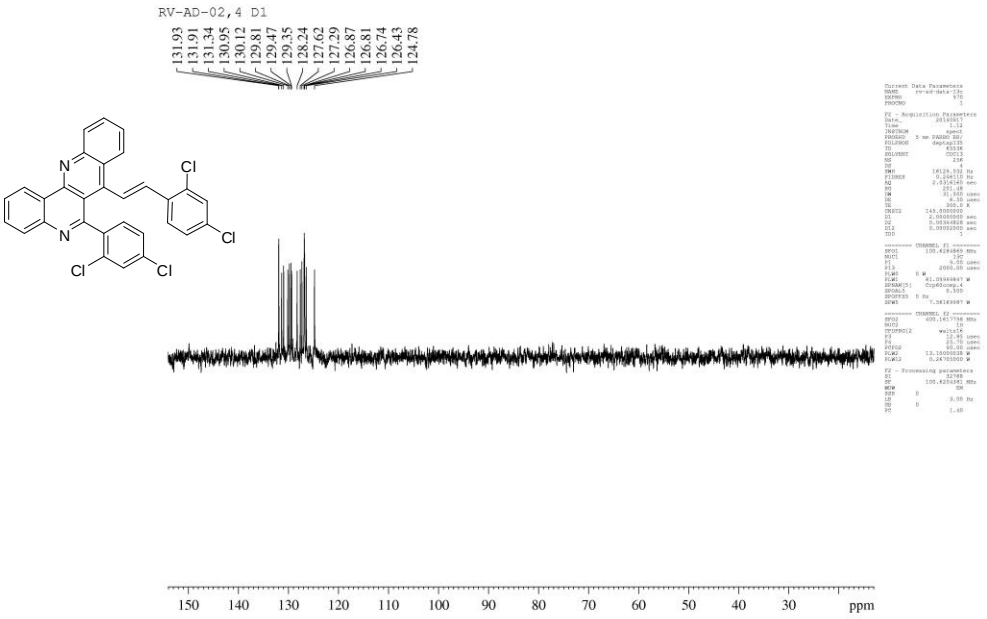
^{13}C NMR Spectra of **4a** (100 MHz, $CDCl_3$)



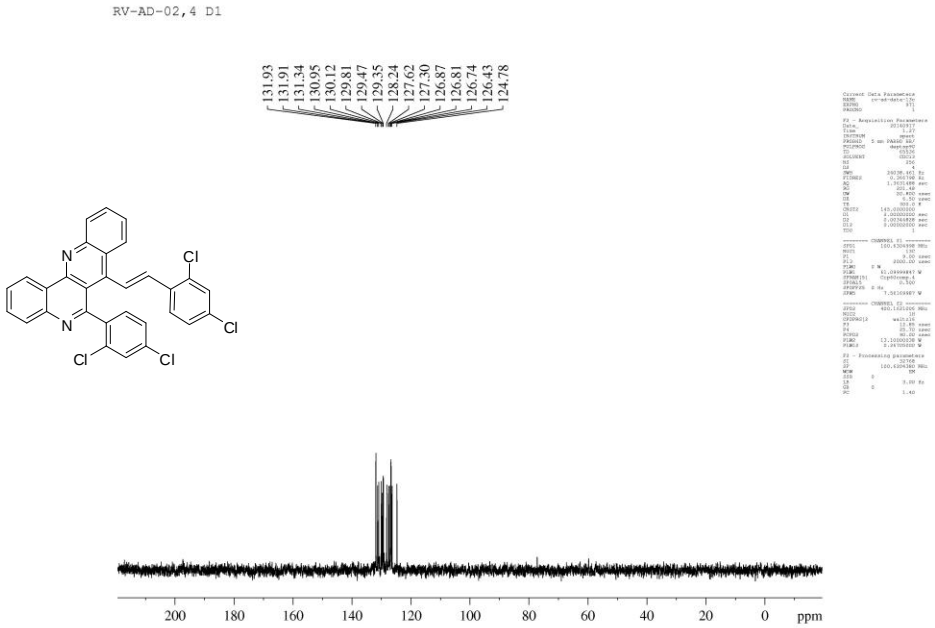
^{1}H NMR Spectra of **4i** (400 MHz, $CDCl_3$)



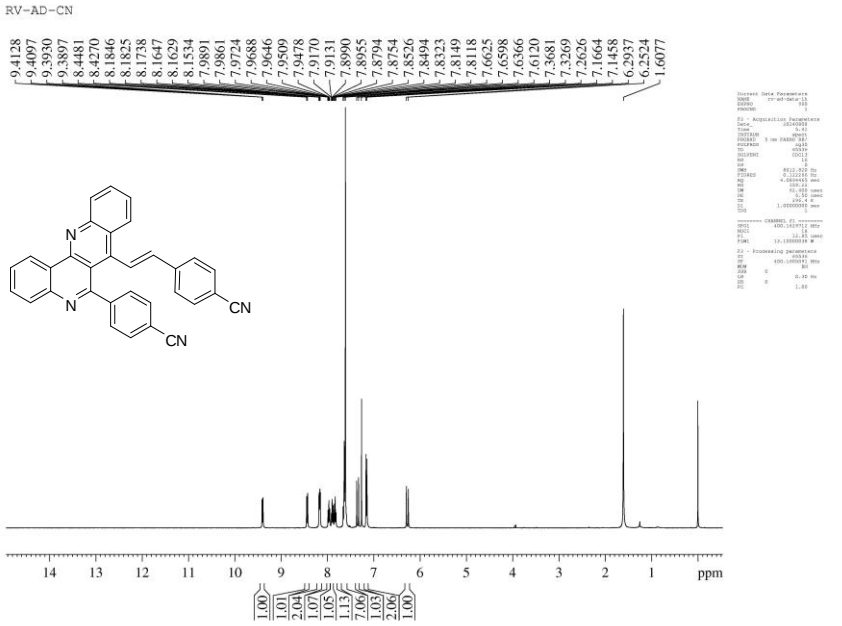
^{13}C NMR Spectra of **4i** (100 MHz, $CDCl_3$)



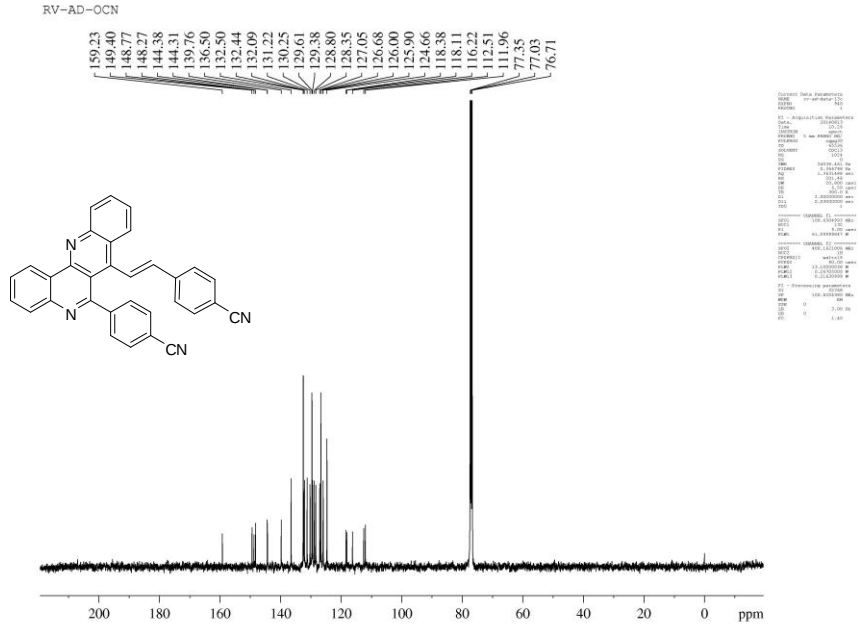
DEPT 135 ^{O} of **4i** (100 MHz, $CDCl_3$)



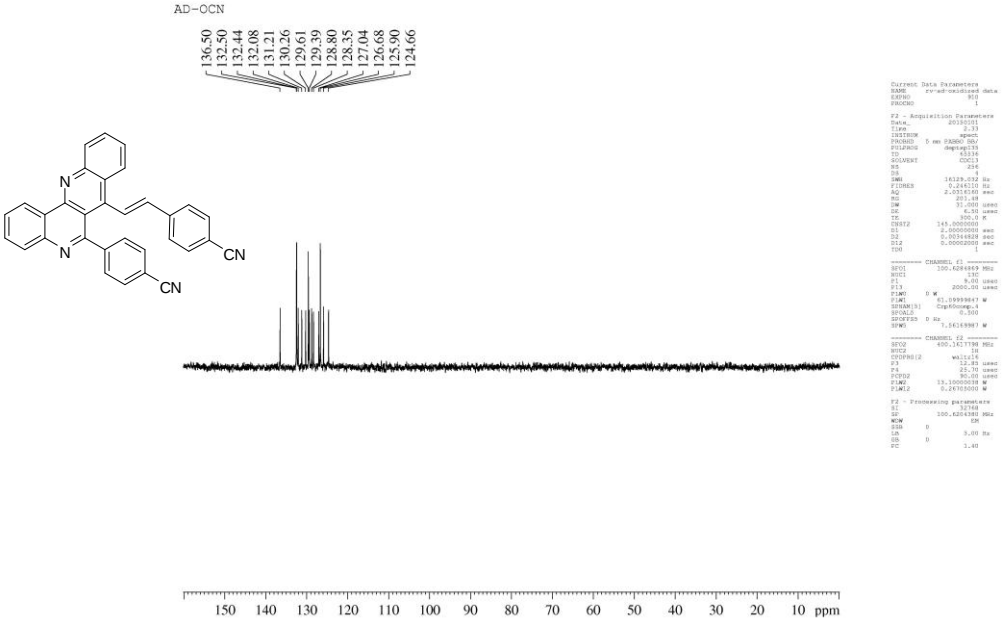
DEPT 90 ^{O} of **4i** (100 MHz, $CDCl_3$)



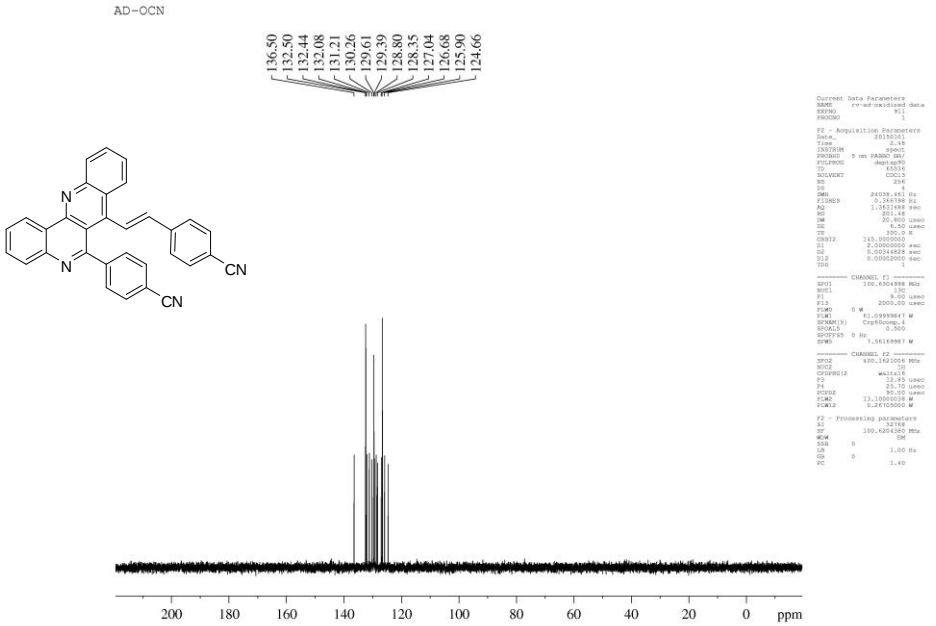
^{1}H NMR Spectra of **4m** (400 MHz, $CDCl_3$)



^{13}C NMR Spectra of **4m** (100 MHz, $CDCl_3$)



DEPT 135 ^{O} of **4m** (100 MHz, $CDCl_3$)



DEPT 90 ^{O} of **4m** (100 MHz, $CDCl_{3}$`)