Supporting Information for

Direct amination of nitroquinoline derivatives via nucleophilic displacement of an aromatic hydrogen

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Table S1. Selected bond lengths (**Å**) and angles (°) for **4b** and **4c**.

Bond lengths [Å]					
4b		**4c**			
N2—C8	1.473(4)	N12—C15	1.464(3)	N22—C25	1.467(3)
C3—Cl1	1.733(3)	C18—C110	1.533(4)	C28—C210	1.542(2)
N2—O1	1.213(4)	N12—O11	1.218(3)	N22—O22	1.233(3)
N2—O2	1.208(3)	N12—O12	1.228(3)	N22—O21	1.213(3)
N1—C9	1.365(4)	N11—C12	1.316(3)	N21—C22	1.316(3)
N1—C1	1.316(4)	N11—C18A	1.368(2)	N21—C28A	1.371(3)
Angles (°)					
4b		**4c**			
N2—C8—C9	119.0(2)	N12—C15—C16	117.4(2)	N22—C25—C24A	121.3(2)
N2—C8—C7	117.7(3)	C14A—C15—N12	121.8(2)	C26—C25—N22	116.6(2)
C2—C3—Cl1	120.1(3)	C210—C28—C28A	122.4(2)	C18A—C18—C110	122.4(2)
C4—C3—Cl1	119.3(2)	C27—C28—C210	120.2(2)	C17—C18—C110	120.9(2)
O2—N2—O1	123.7(3)	O12—N12—O11	123.5(2)	O21—N22—O22	123.5(2)

Table S2. Selected bond lengths (**Å**) and angles (°) for **5a**.

Bond lengths [Å]					
5a					
N120—C117	1.466(4)	N220—C217	1.472(5)	N320—C317	1.464(6)
N316—C318	1.362(5)	N316—C315	1.318(5)	N39—C310	1.419(4)
N216—C215	1.317(5)	N216—C219	1.359(4)	N29—C210	1.414(4)
N116—C115	1.323(6)	N116—C118	1.362(4)	N19—C110	1.423(5)
Angles (°)					
5a					
C118—C117—N120	118.5(3)	C110—C117—N120	119.3(3)	C110—N19—C19A	126.8(3)
C210—C217—N220	120.4(3)	C219—C217—N220	116.6(3)	C110—N19—C18A	124.6(3)
C310—C317—N320	119.7(3)	C210—N29—C28A	124.1(3)	C210—N29—C29B	124.2(3)
C318—C317—N320	117.3(3)	C310—N39—C39B	126.4(3)	C310—N39—C38A	123.4(3)

Table S3. Selected bond lengths (**Å**) and angles (°) for **5b**.

Bond lengths [Å]					
5b					
C110—N19	1.416(4)	C210—N29	1.413(4)		
N120—O11	1.355(4)	N220—O21	1.365(4)		
C117—N120	1.304(4)	C217—N220	1.297(4)		
C112—O12	1.228(4)	C212—O22	1.219(4)		
Angles (°)					
5b					
N120—C117—C110	115.2(3)	C218—C217—N220	127.2(3)	C110—N19—C19A	124.7(2)
C118—C117—N120	127.3(3)	C210—C217—N220	115.4(3)	C110—N19—C18A	126.3(2)
C119—C112—O12	121.1(3)	O22—C212—C211	122.2(3)	C210—N29—C28A	126.2(2)
C111—C112—O12	121.2(3)	O22—C212—C219	120.9(3)	C210—N29—C29A	125.6(2)

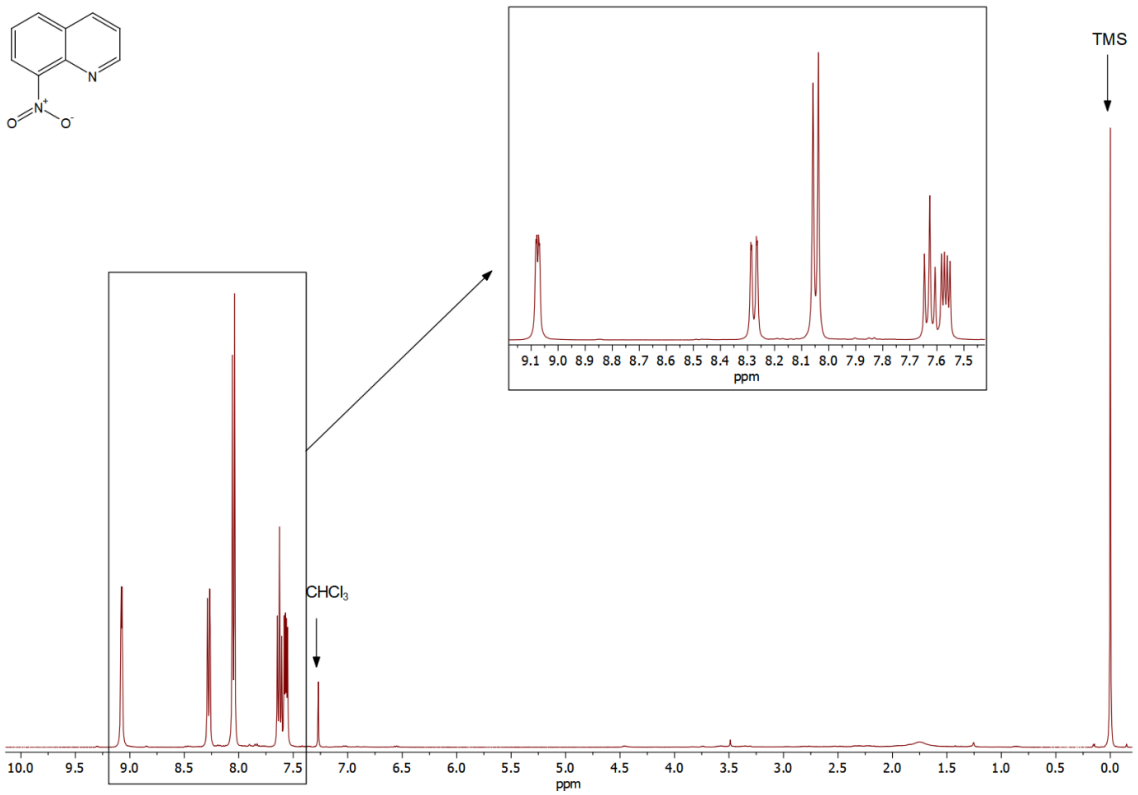

Figure S1a. ^{1}H-NMR ($CDCl_3$; 400.2 MHz) spectrum of the **4a**.

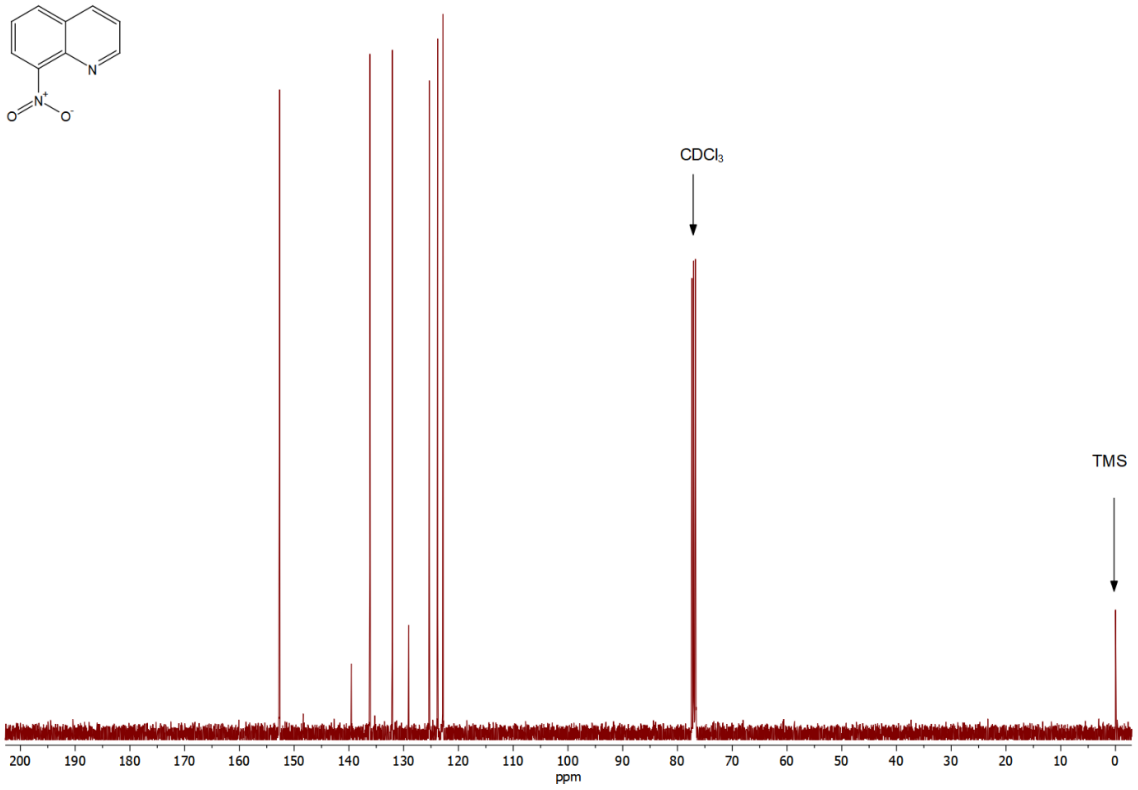

Fig. S1b. $^{13}C\{^{1}H\}$ NMR ($CDCl_3$; 100.6 MHz) spectrum of the **4a**.

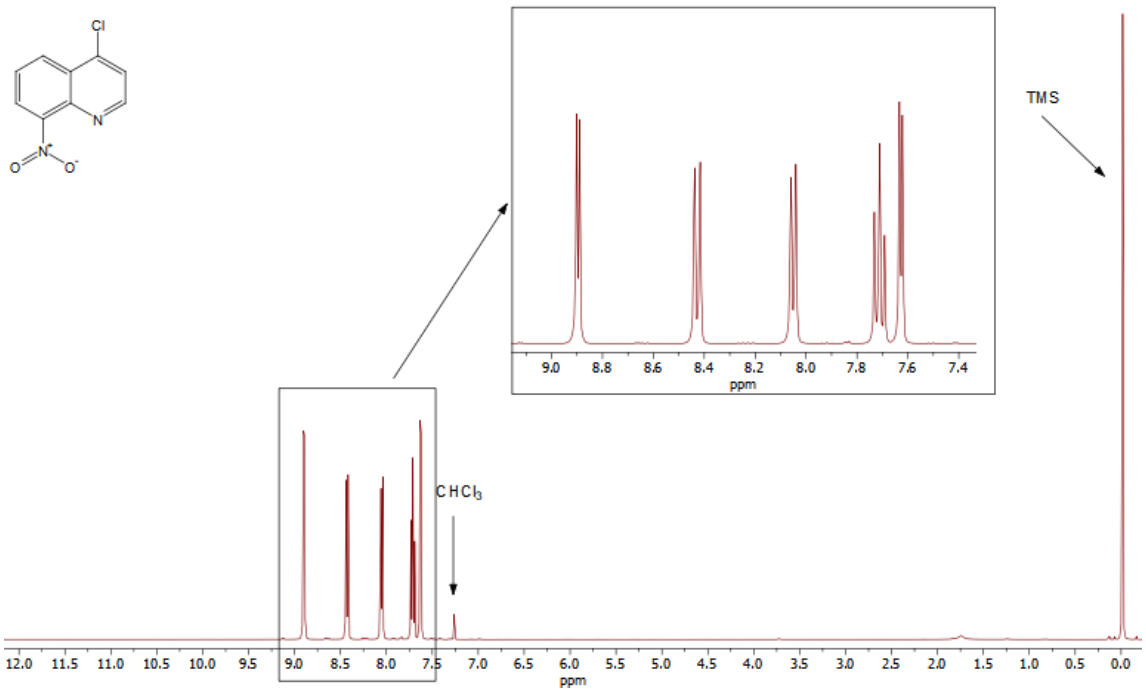

Fig. S2a. ^{1}H NMR ($CDCl_3$; 400.2 MHz) spectrum of the **4b**.

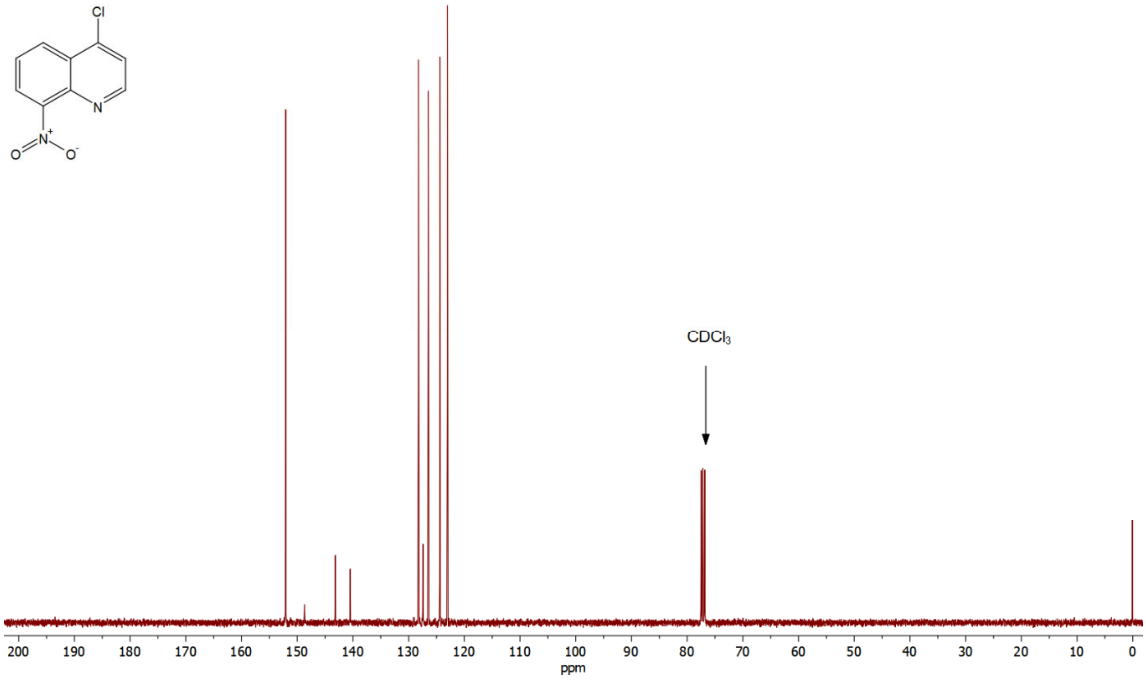

Fig. S2b. $^{13}C\{^{1}H\}$ NMR ($CDCl_3$; 100.6 MHz) spectrum of the **4b**.

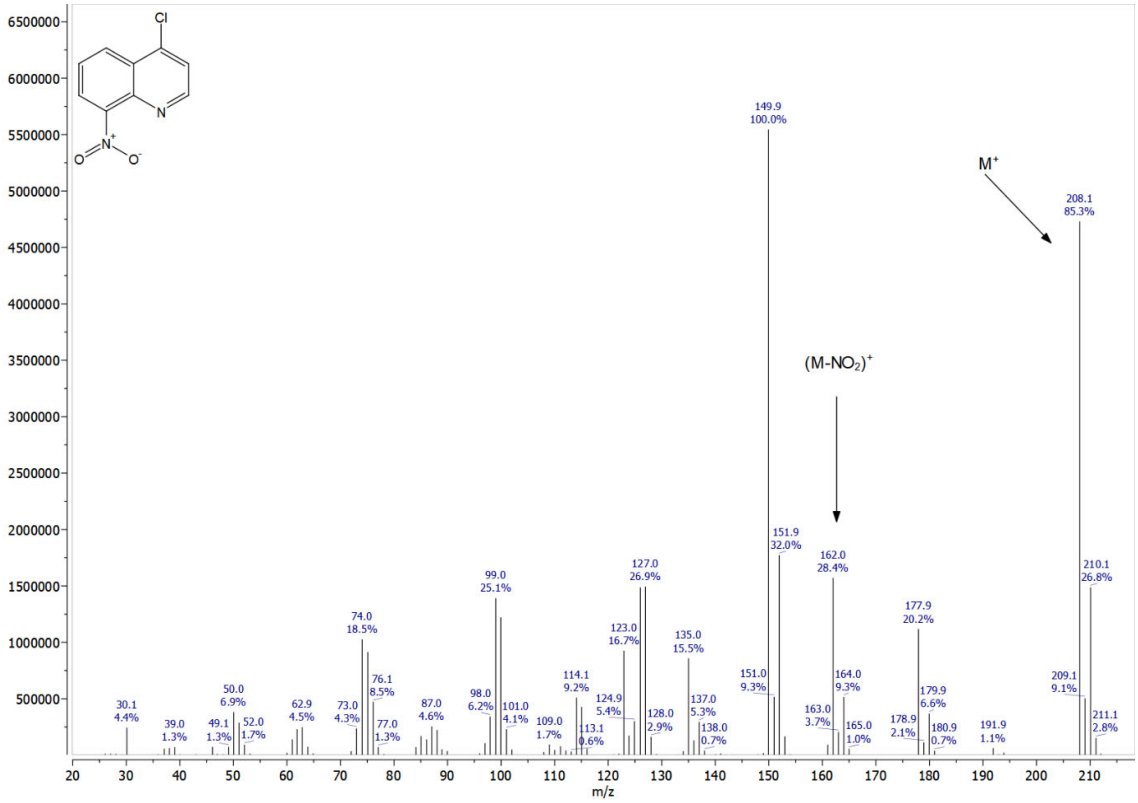

Fig. S2c. MS spectrum of the **4b**.

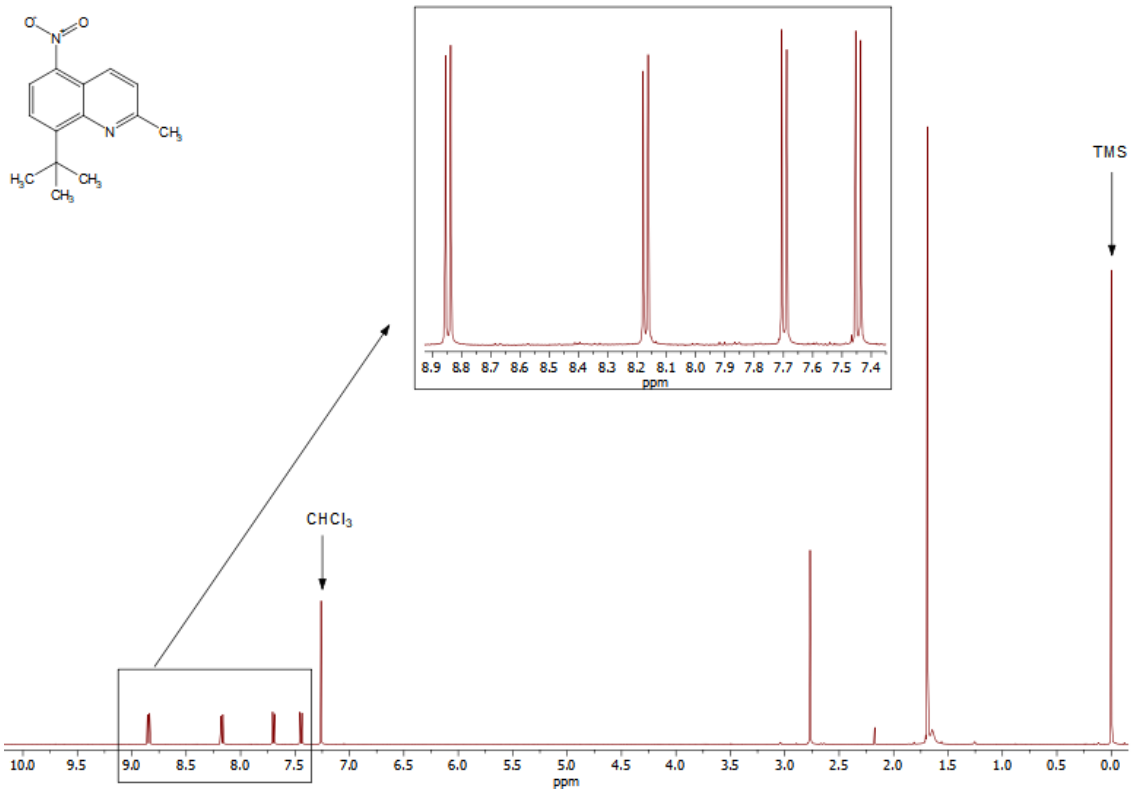

Fig. S3a. ^{1}H NMR ($CDCl_3$; 500.2 MHz) spectrum of the **4c**.

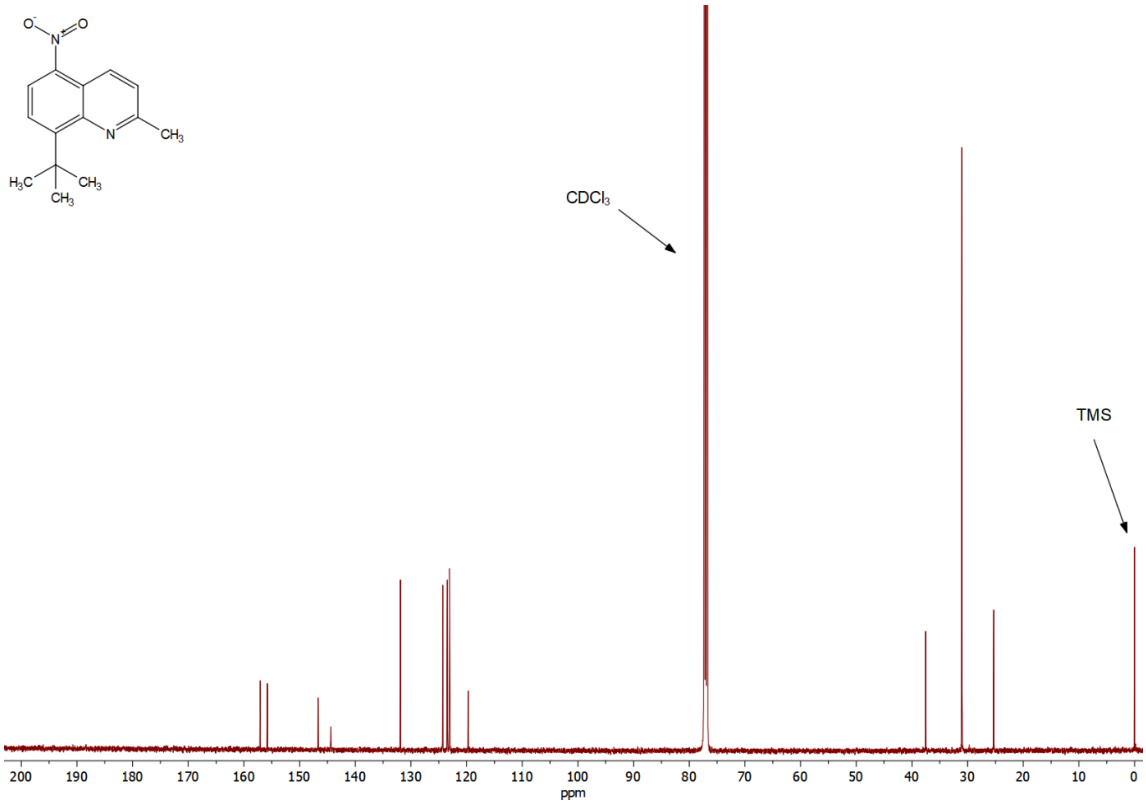

Fig. S3b. $^{13}C\{^{1}H\}$ NMR ($CDCl_3$; 125.8 MHz) spectrum of the **4c**.

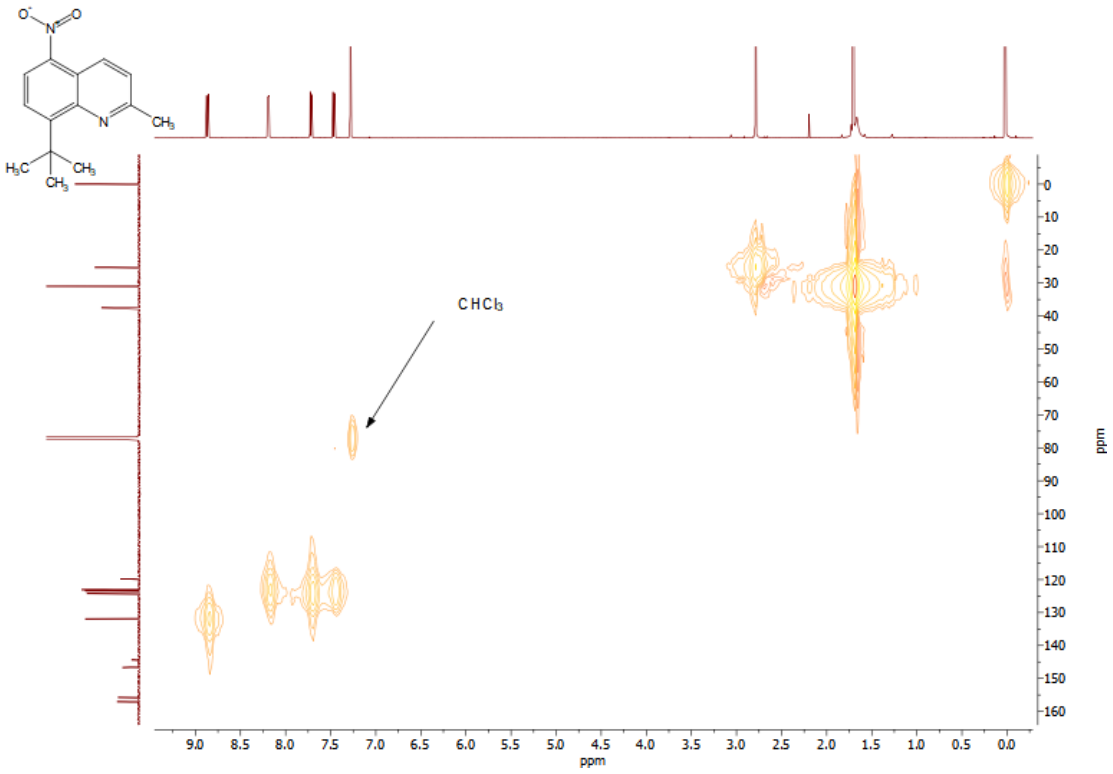

Fig. S3c. ^{1}H - ^{13}C HMQC spectrum of the **4c**.

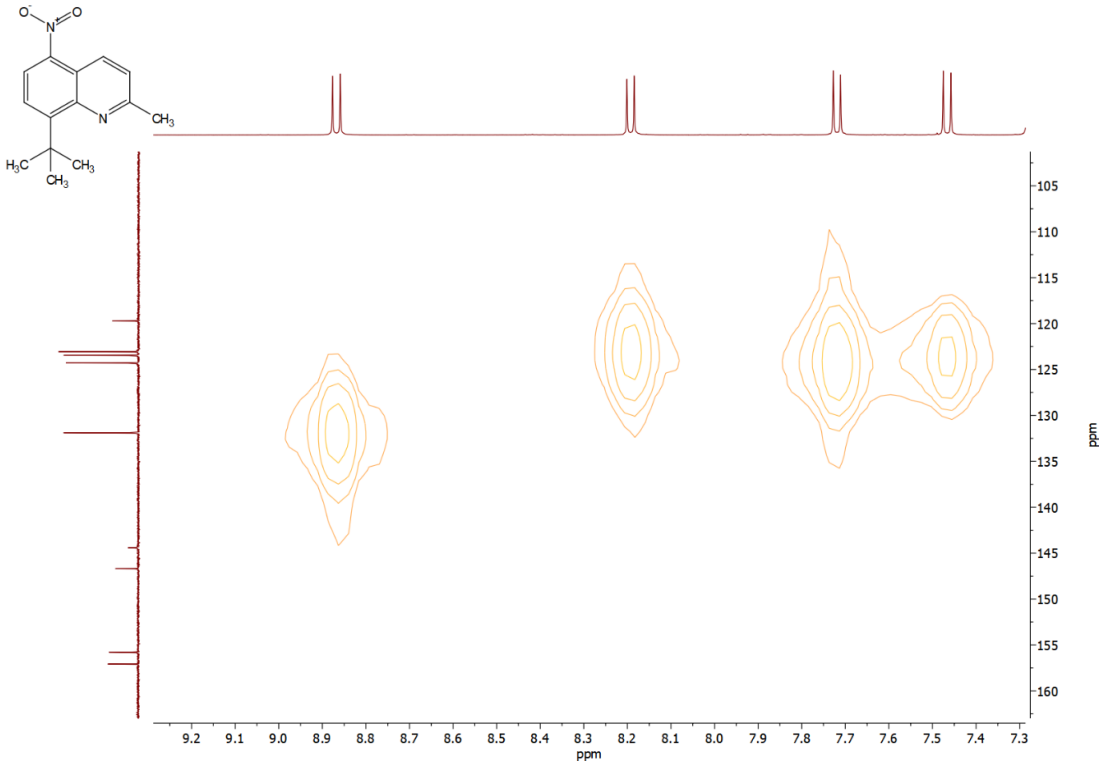

Fig. S3d. ^{1}H – ^{13}C HMQC spectrum (aromatic range) of the **4c**.

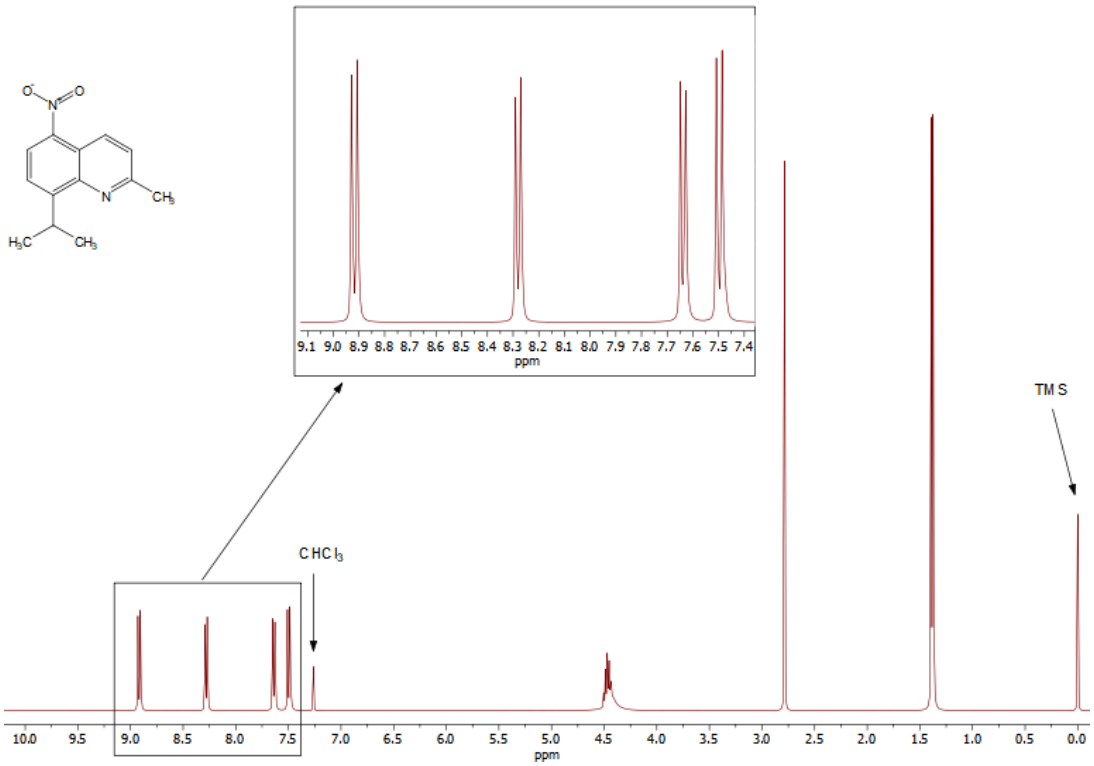

Fig. S4a. ^{1}H NMR ($CDCl_3$; 400.2 MHz) spectrum of the **4d**.

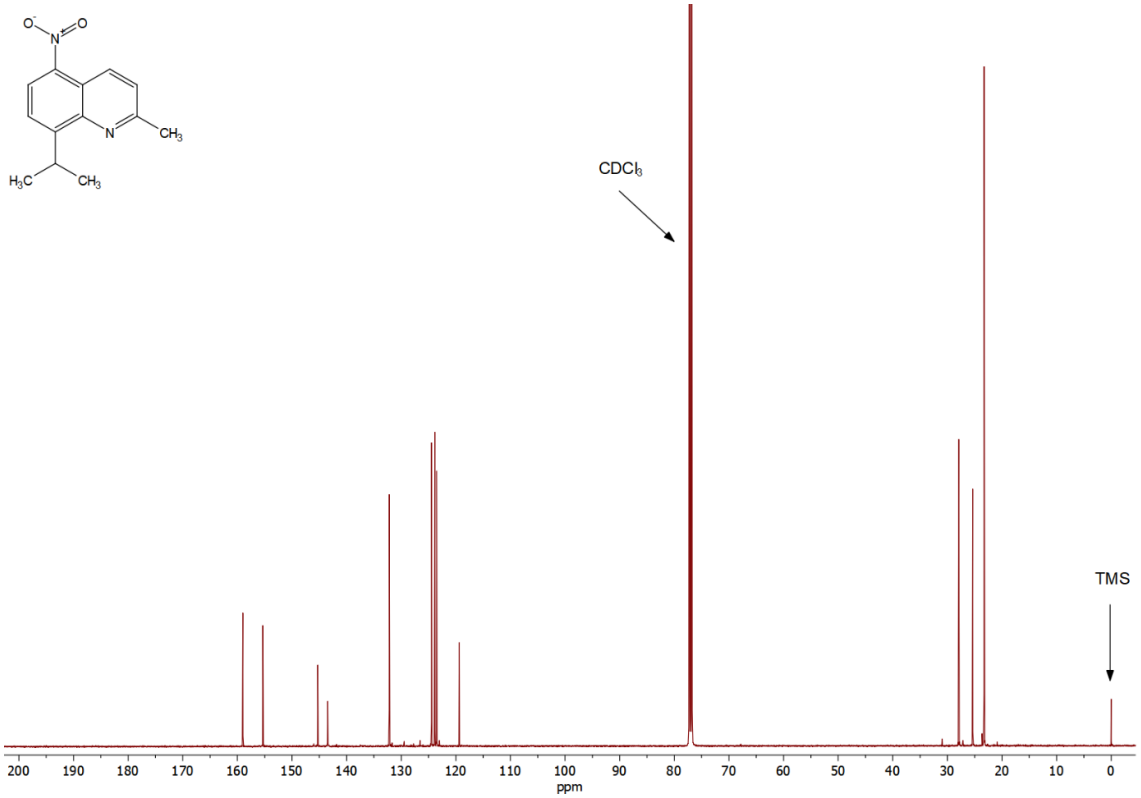

Fig. S4b. $^{13}C\{^{1}H\}$ NMR ($CDCl_3$; 125.8 MHz) spectrum of the **4d**.

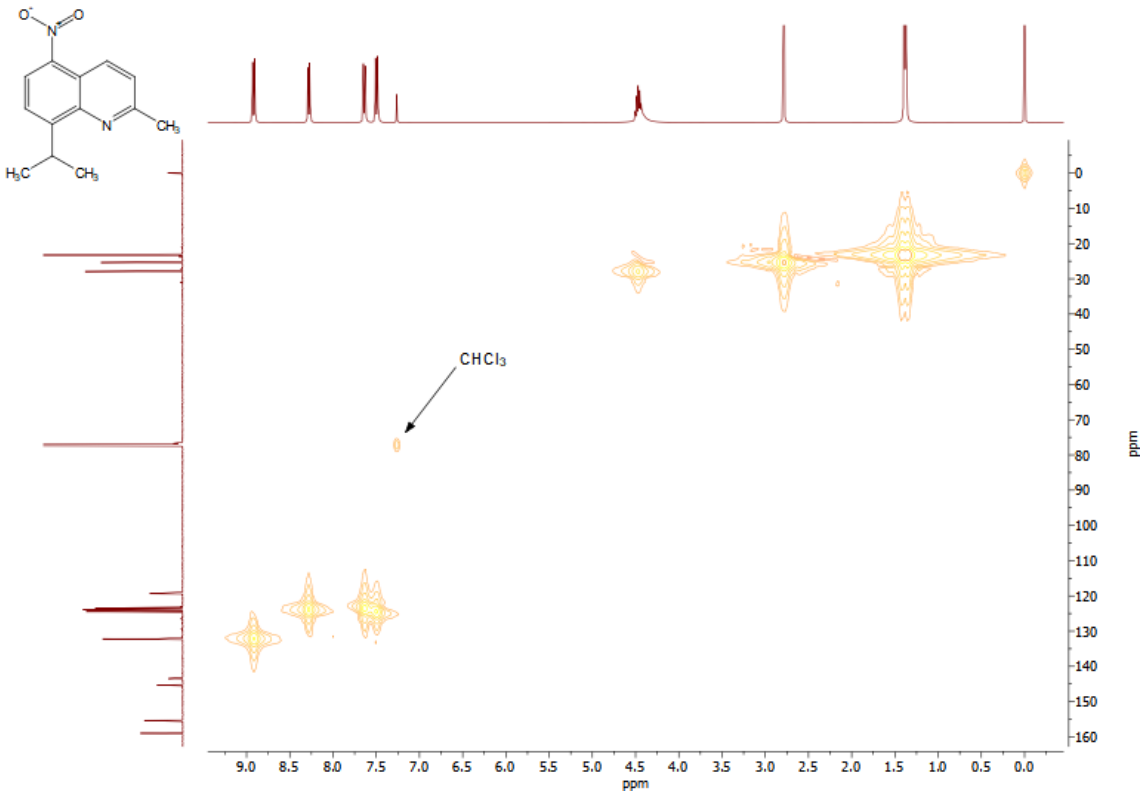

Fig. S4c. ^{1}H - ^{13}C HMQC spectrum of the **4d**.

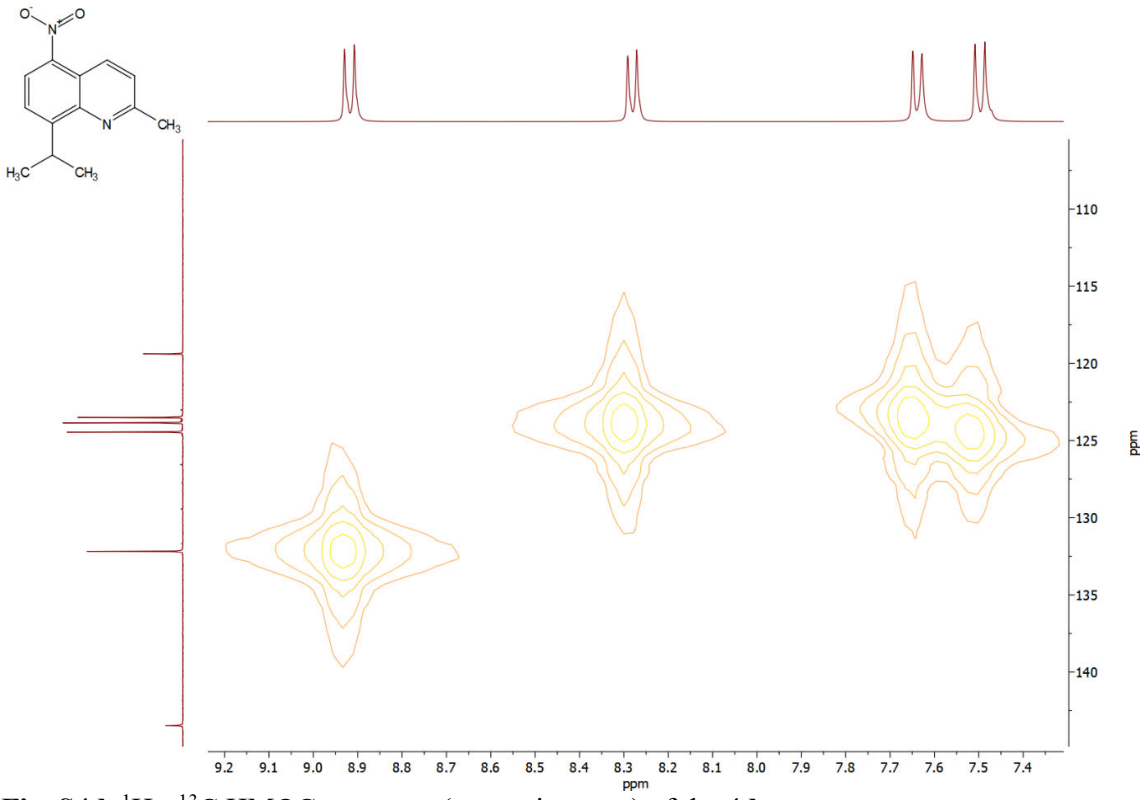

Fig. S4d. ^{1}H - ^{13}C HMQC spectrum (aromatic range) of the **4d**.

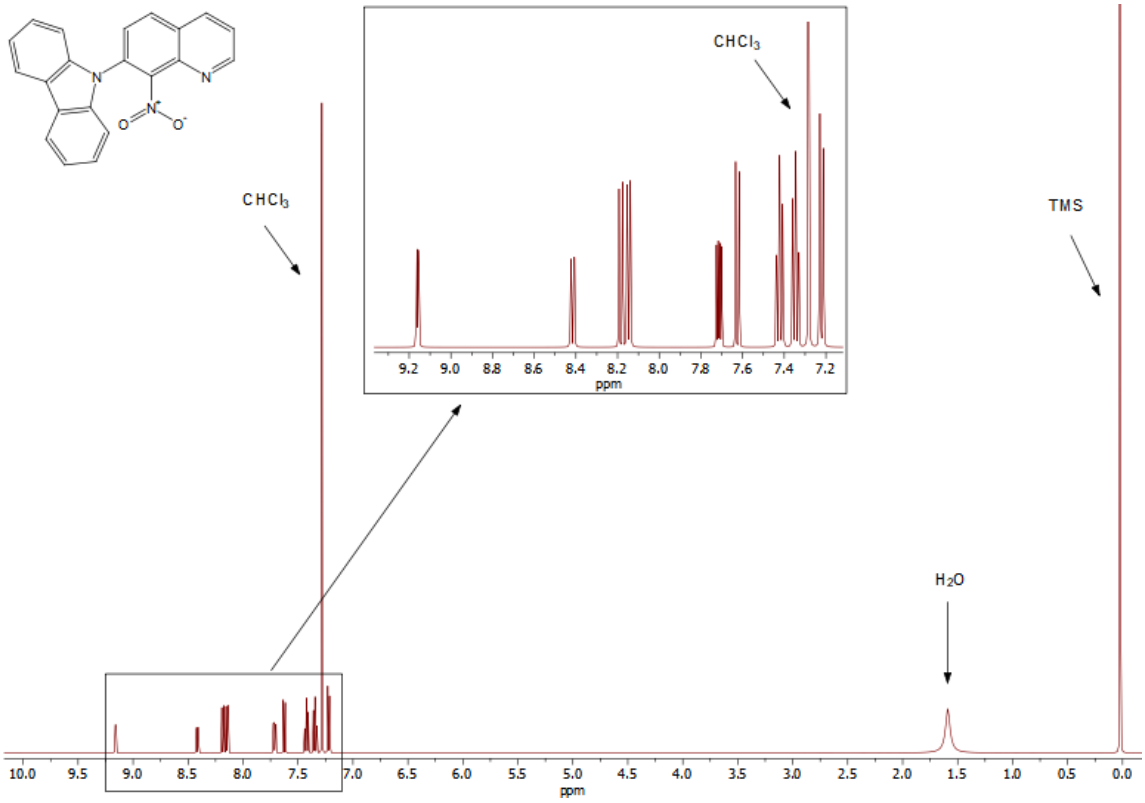

Fig. S5a. ^{1}H NMR ($CDCl_3$; 500.2 MHz) spectrum of the **5a**.

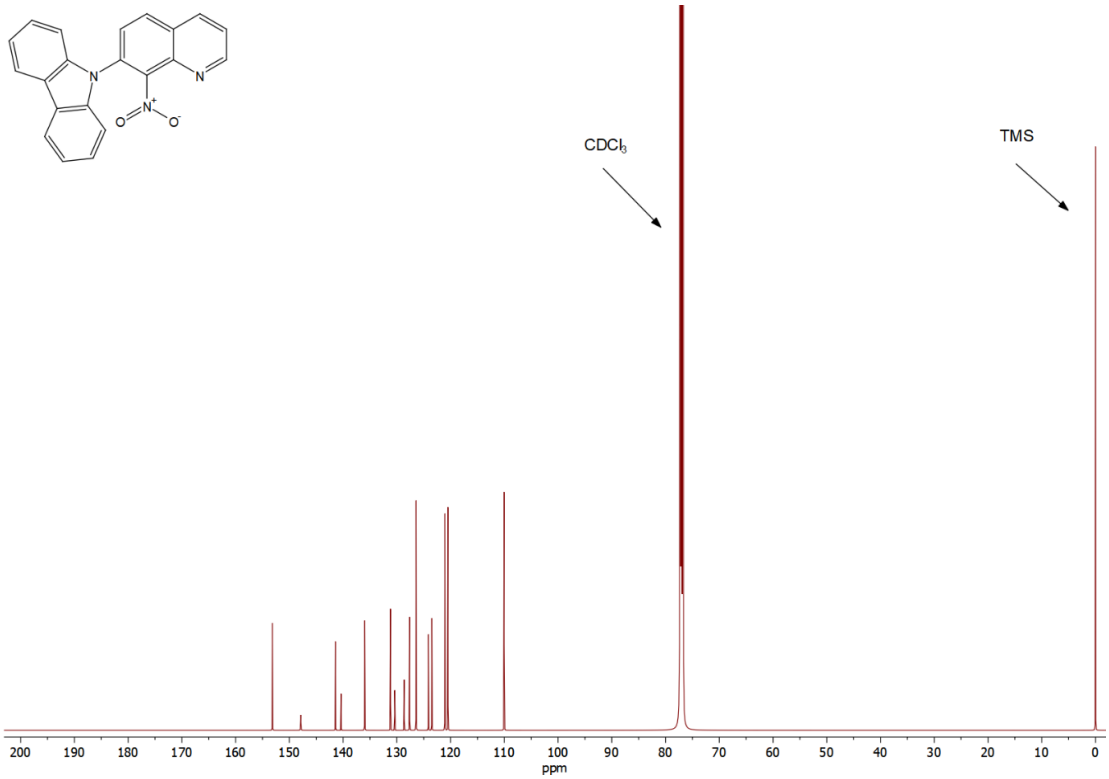

Fig. S5b. $^{13}C\{^{1}H\}$ NMR ($CDCl_3$; 125.8 MHz) spectrum of the **5a**.

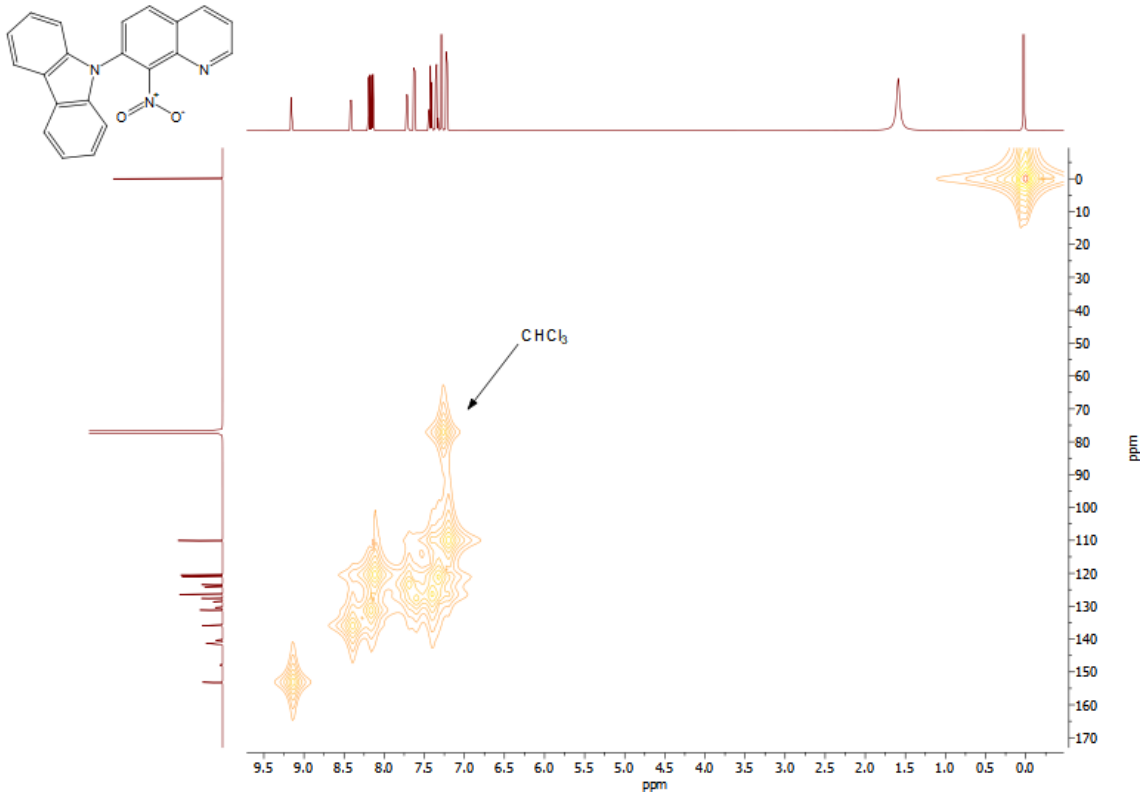

Fig. S5c. ^{1}H - ^{13}C HMQC spectrum of the **5a**.

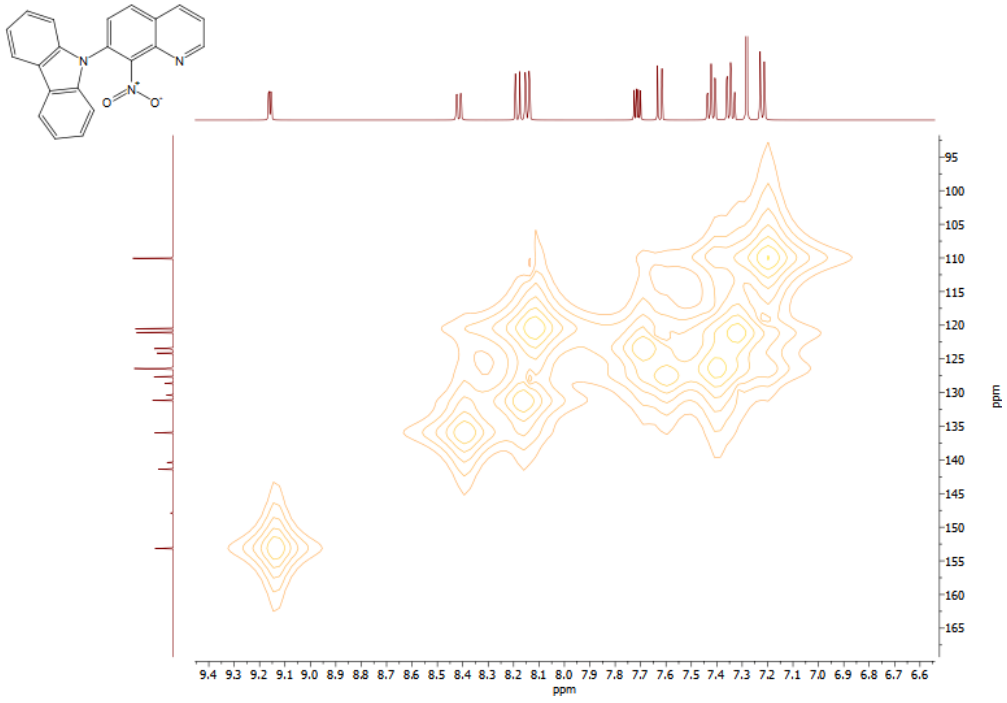

Fig. S5d. ^{1}H - ^{13}C HMQC spectrum (aromatic range) of the **5a**.

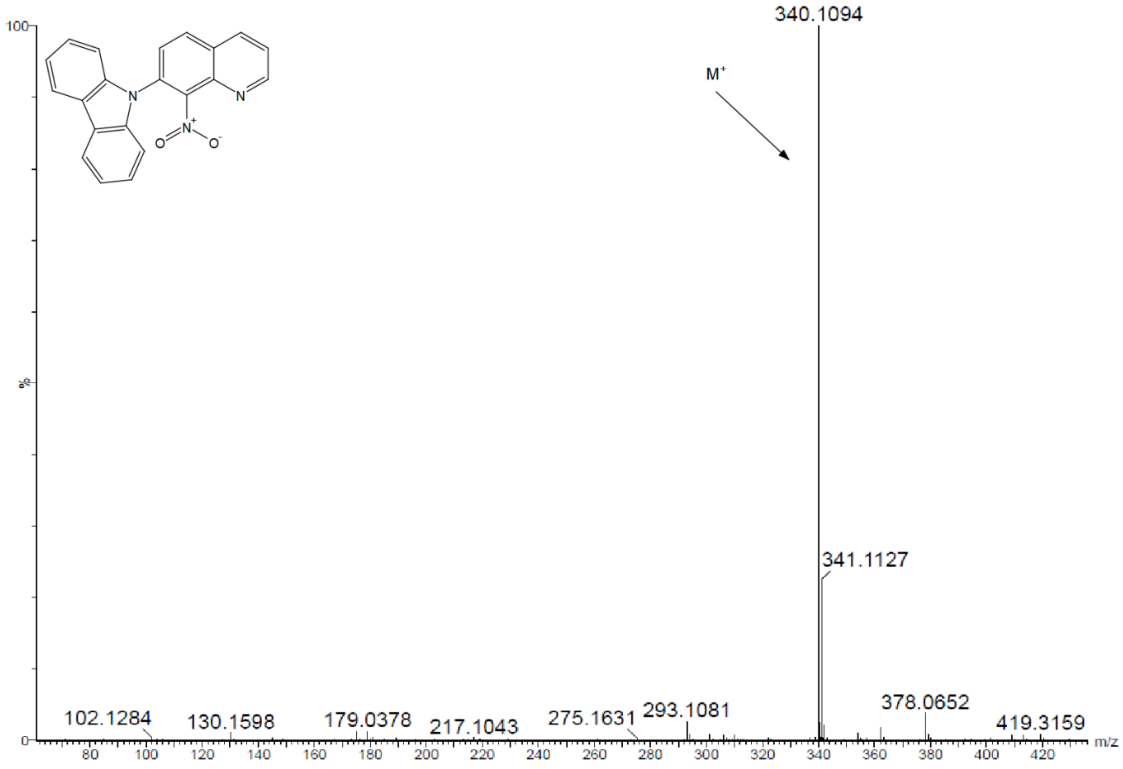

Fig. S5e. MS spectrum of the **5a**.

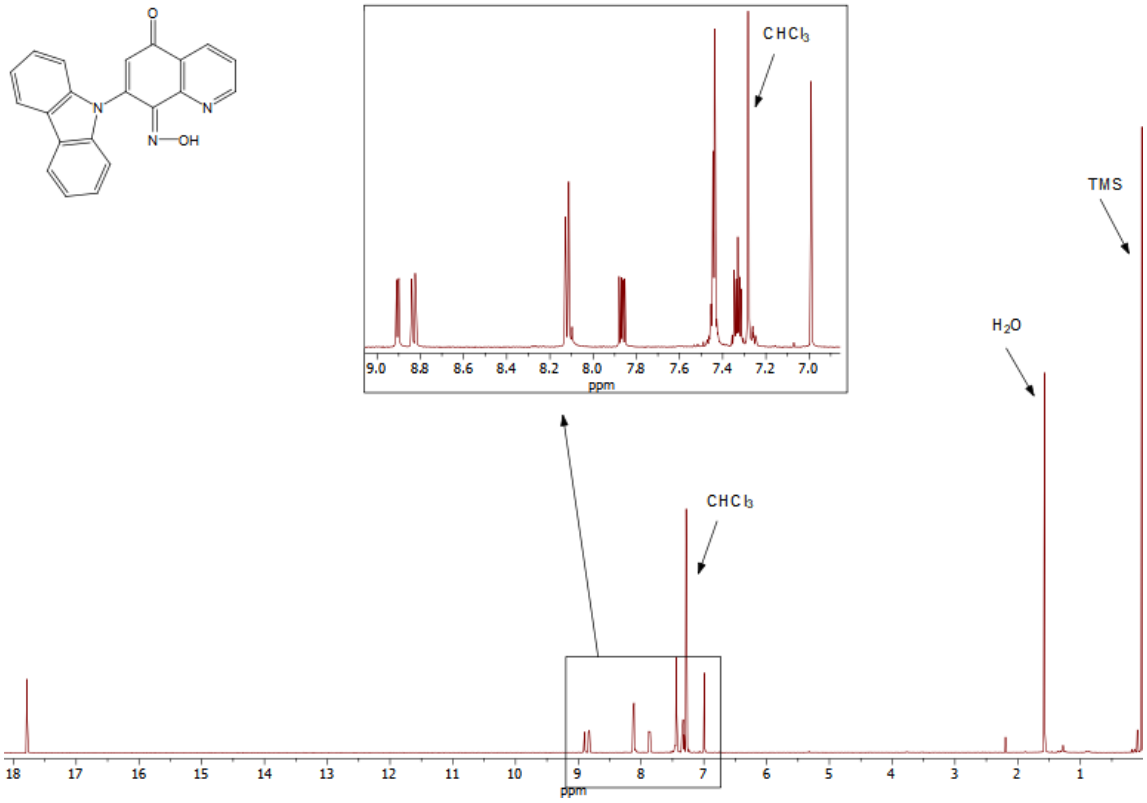

Fig. S6a. ^{1}H NMR ($CDCl_3$; 500.2 MHz) spectrum of the **5b**.

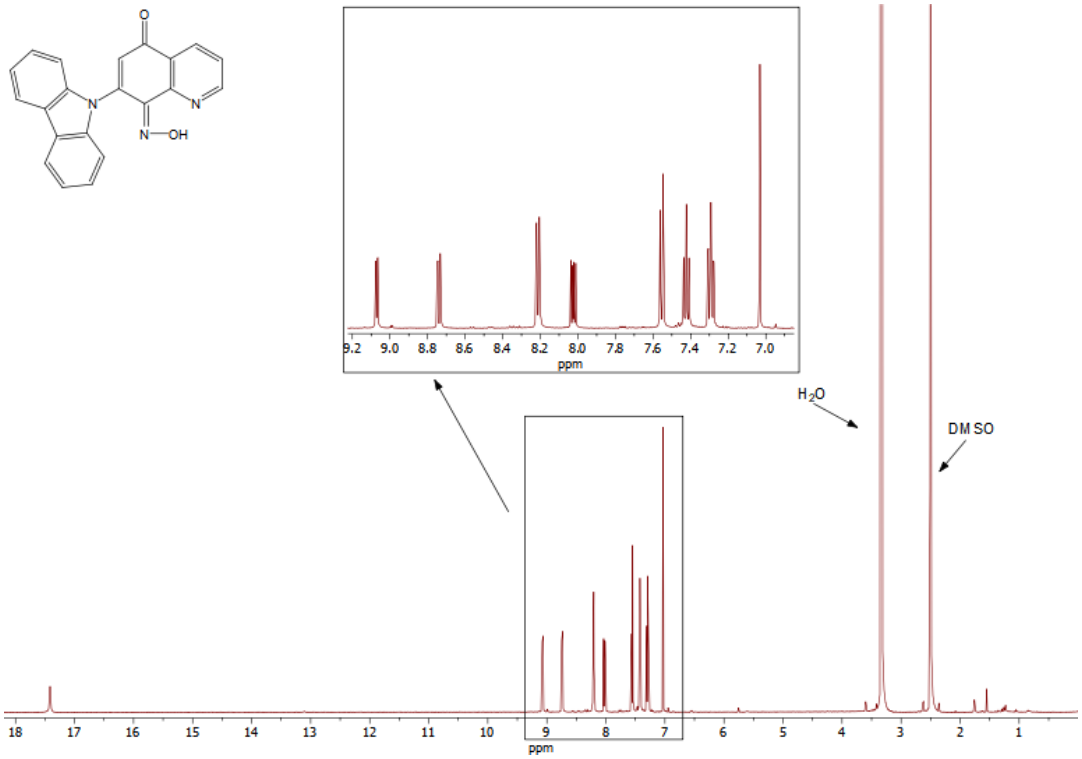

Fig. S6b. ^{1}H NMR (DMSO-d_6; 500.2 MHz) spectrum of the **5b**.

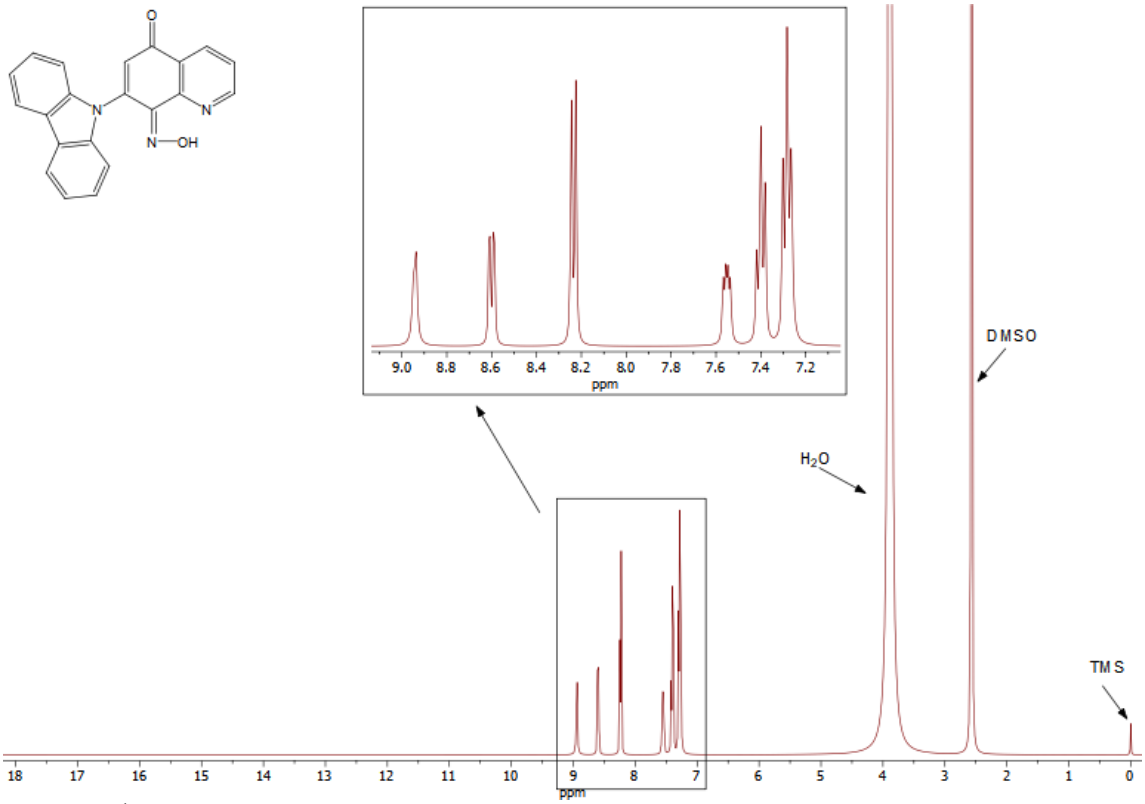

Fig. S6c. ^{1}H NMR (DMSO–d6/KOD/D_2O; 500.2 MHz) spectrum of the **5b**

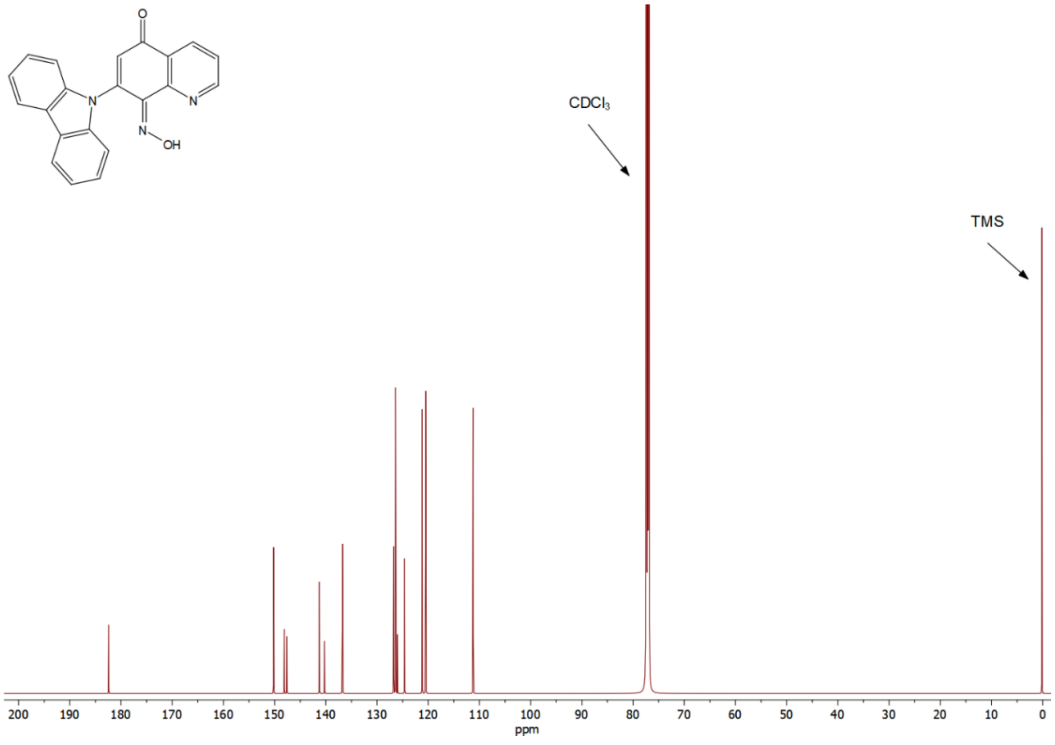

Fig. S6d. $^{13}C\{^{1}H\}$ NMR ($CDCl_3$; 125.8 MHz) spectrum of the **5b**.

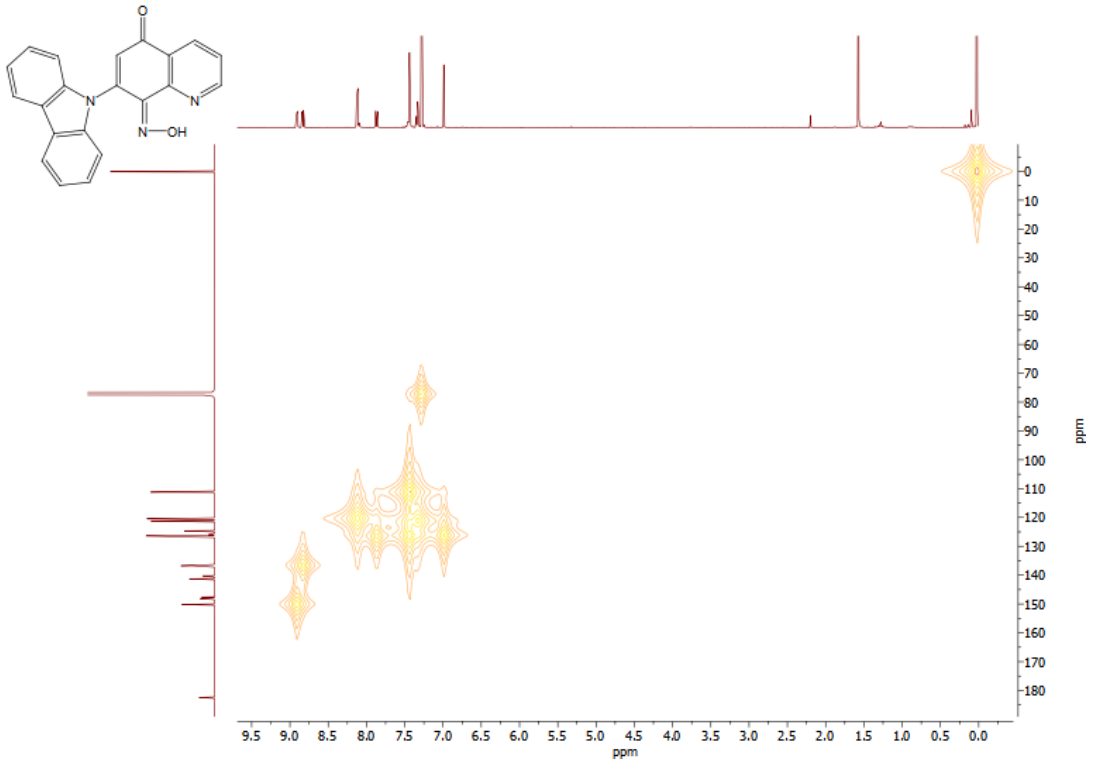

Fig. S6e. ^{1}H - ^{13}C HMQC spectrum of the **5b**.

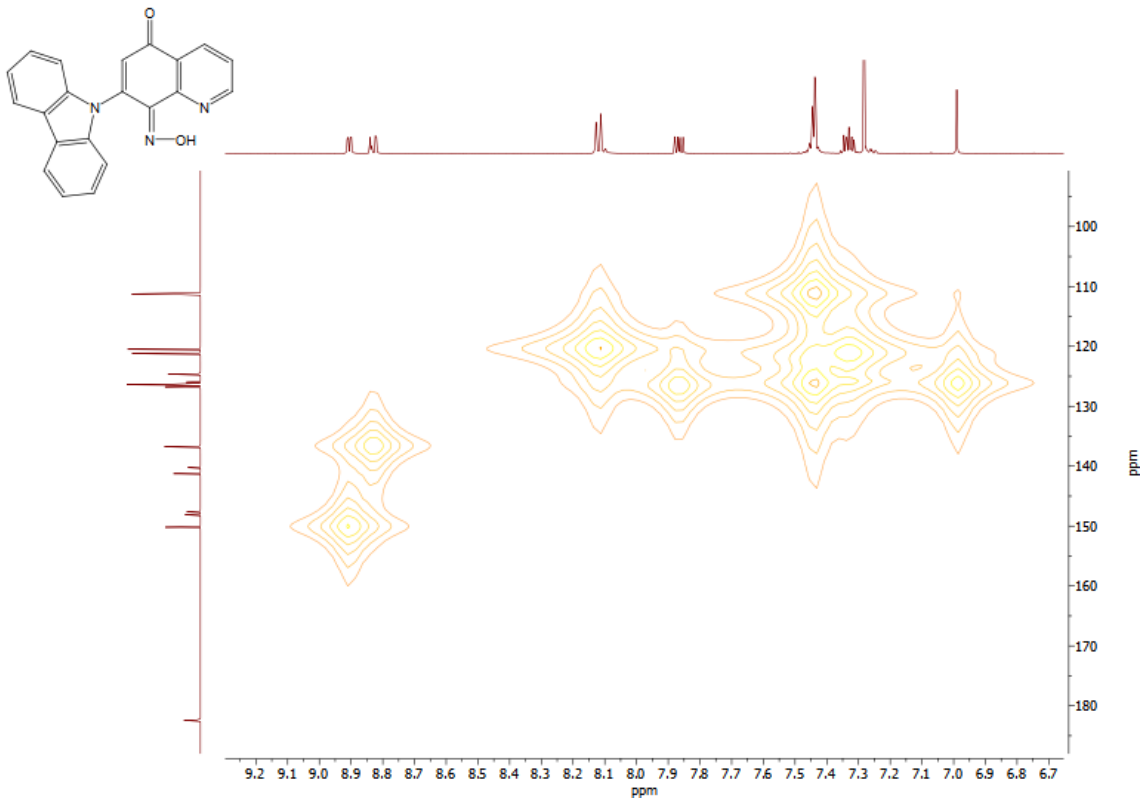

Fig. S6f. ^{1}H - ^{13}C HMQC spectrum (aromatic range) of the **5b**.

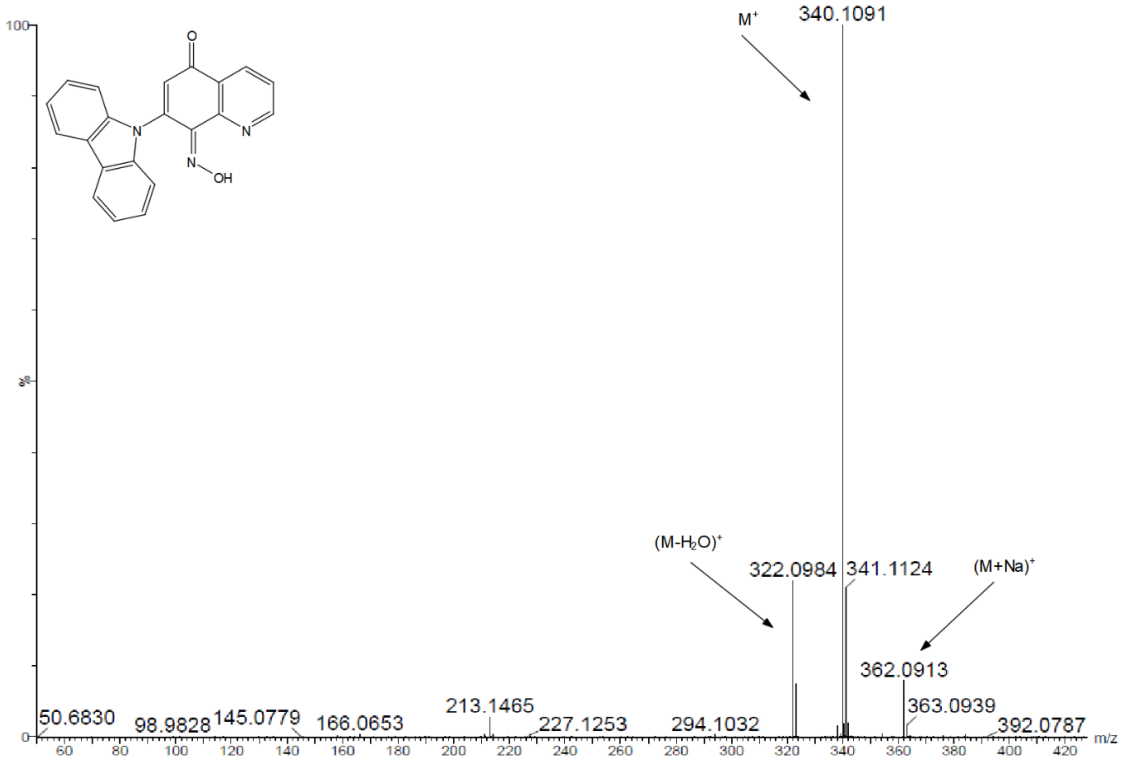

Fig. S6g. MS spectrum of the **5b**.

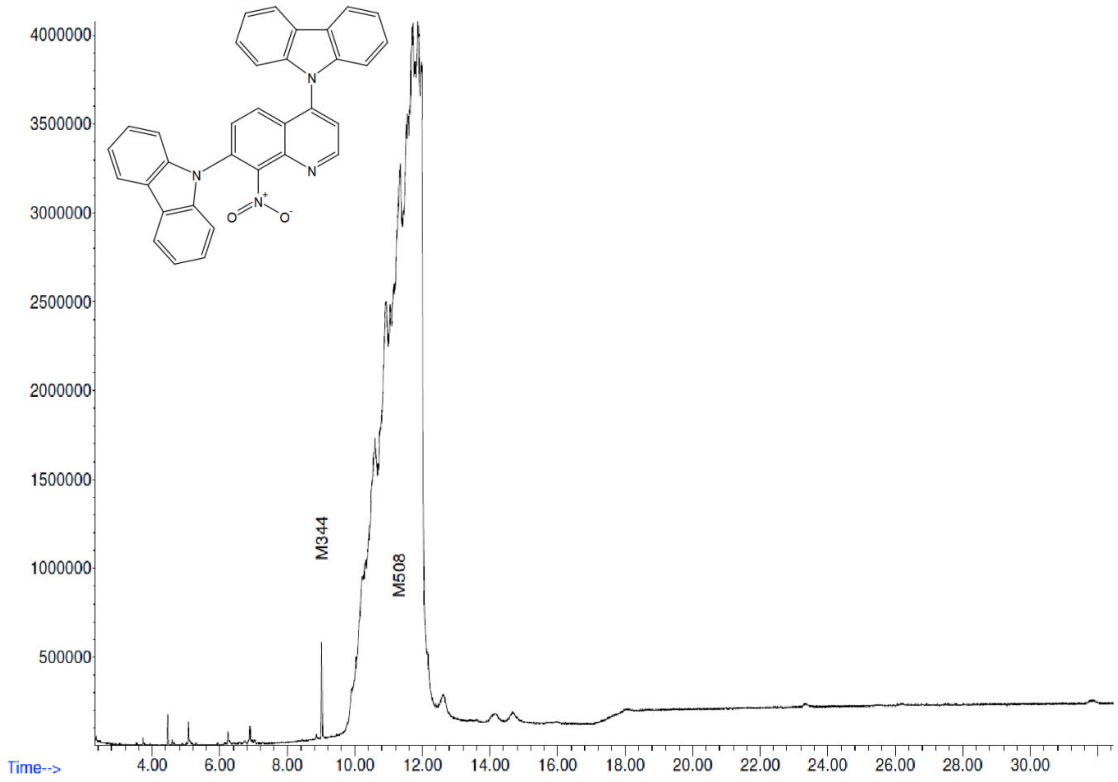

Fig. S7a. Chromatogram of the structure similar to molecule **5c**.

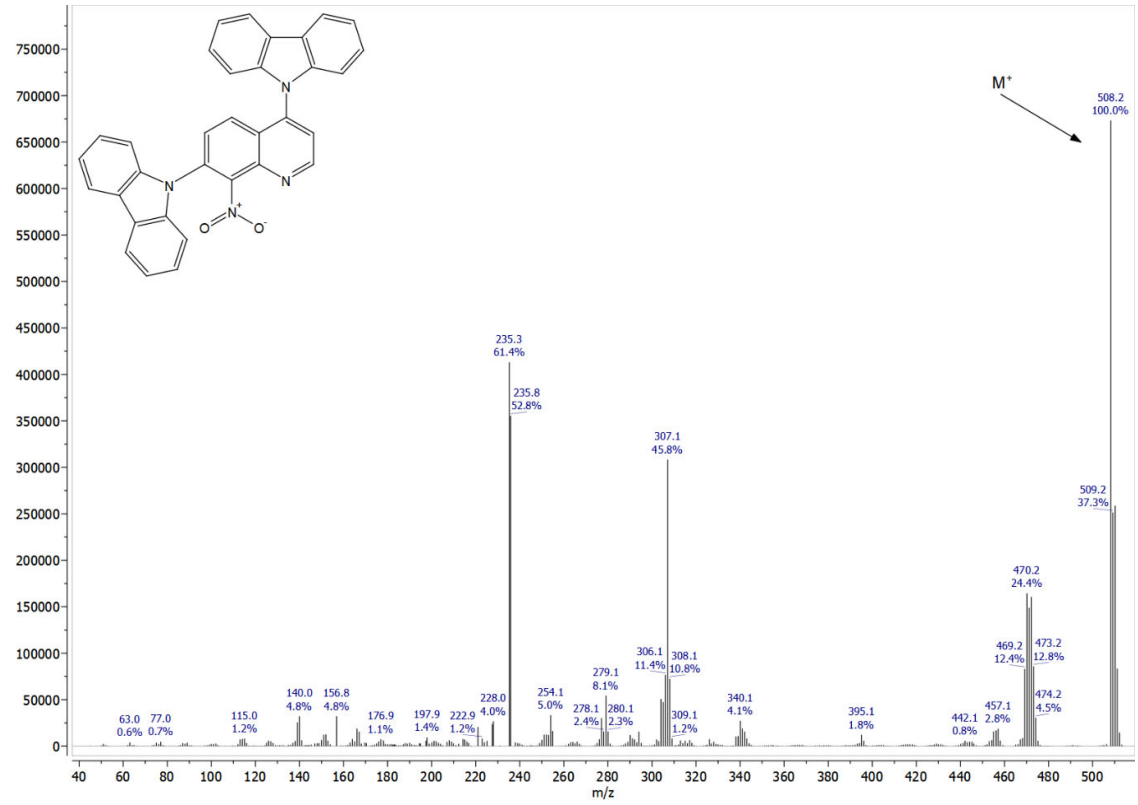

Fig. S7b. MS of the structure similar to molecule **5c**.

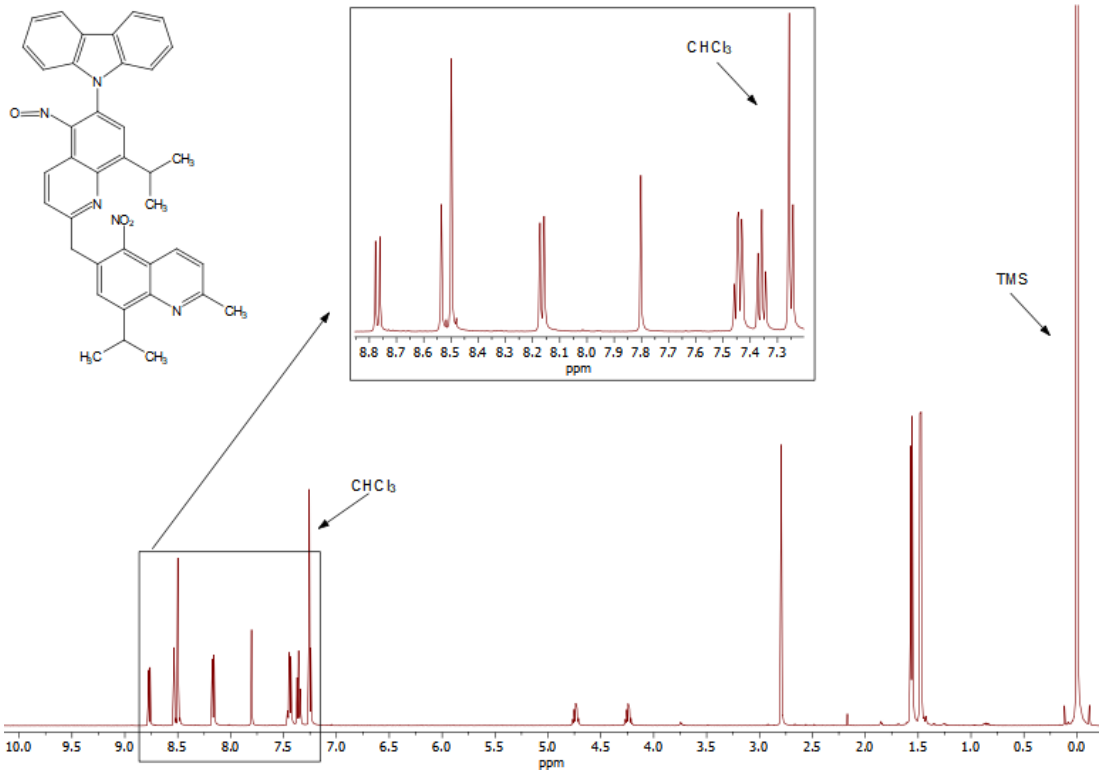

Fig. S8a. ^{1}H NMR ($CDCl_3$; 500.2 MHz) spectrum of the **5d**.

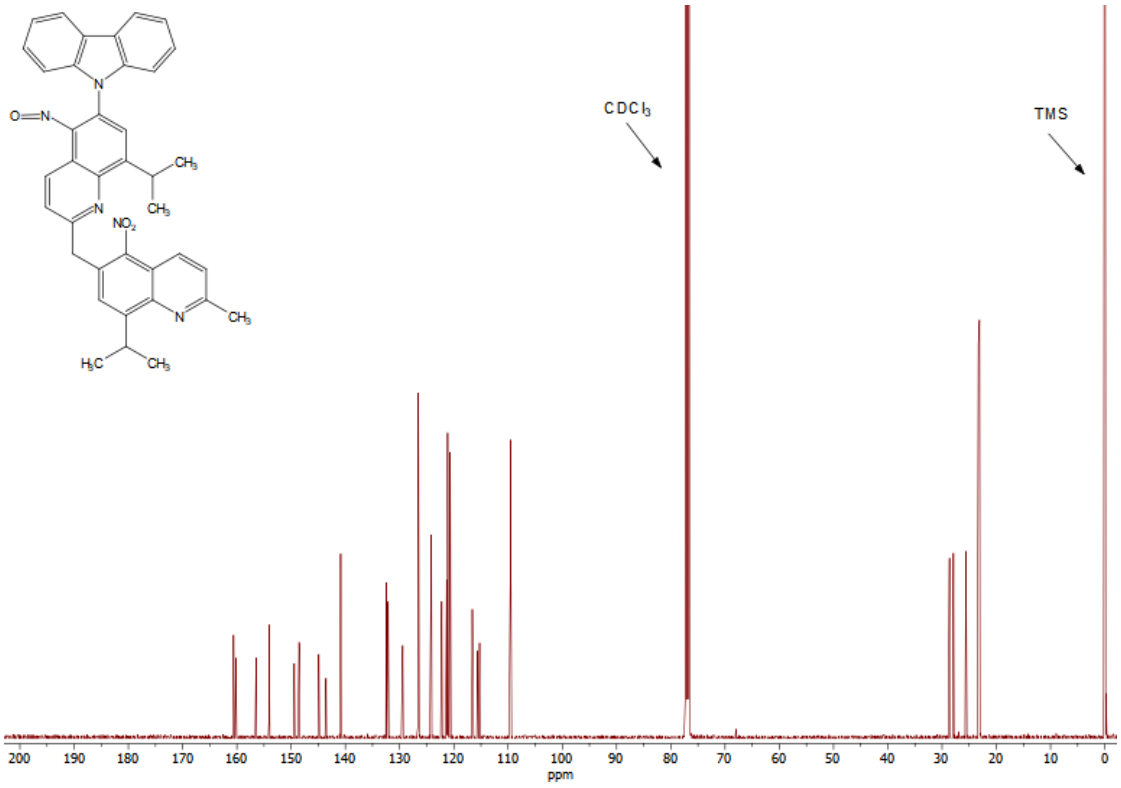

Fig. S8b. $^{13}C\{^{1}H\}$ NMR ($CDCl_3$; 125.8 MHz) spectrum of the **5d**.

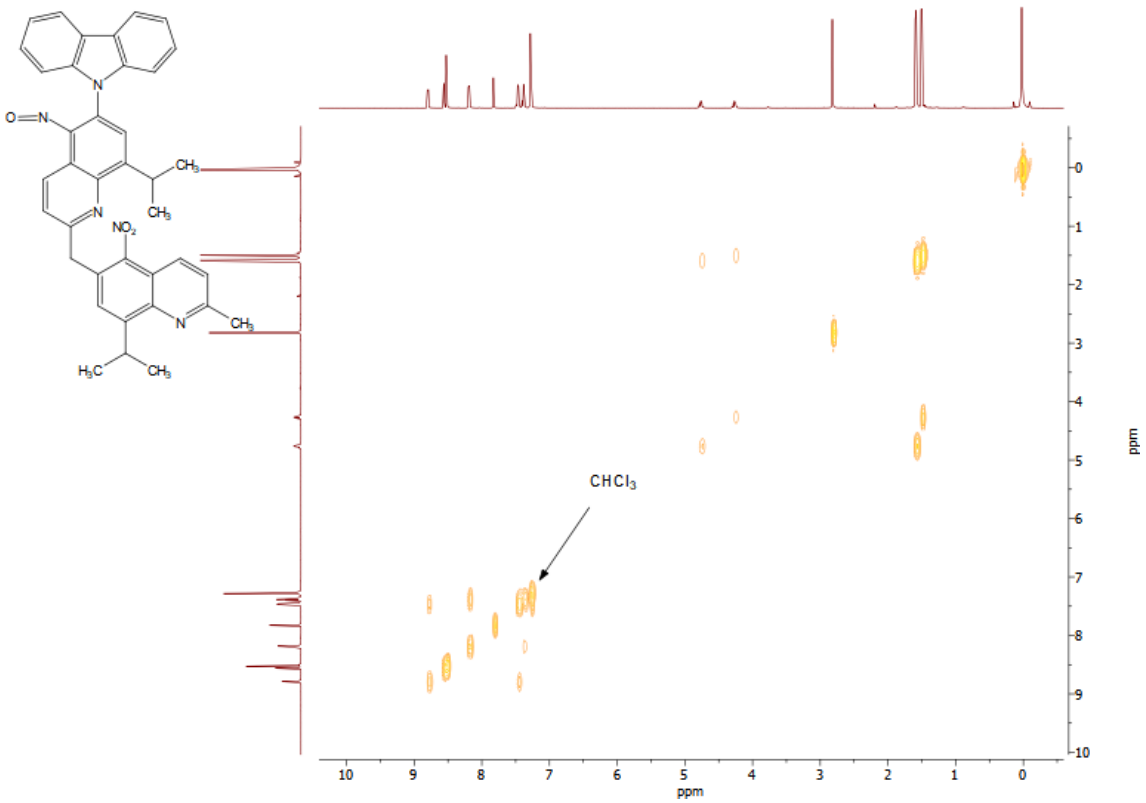

Fig. S8c. $^{1}H - {}^{1}H$ COSY spectrum of the **5d**.

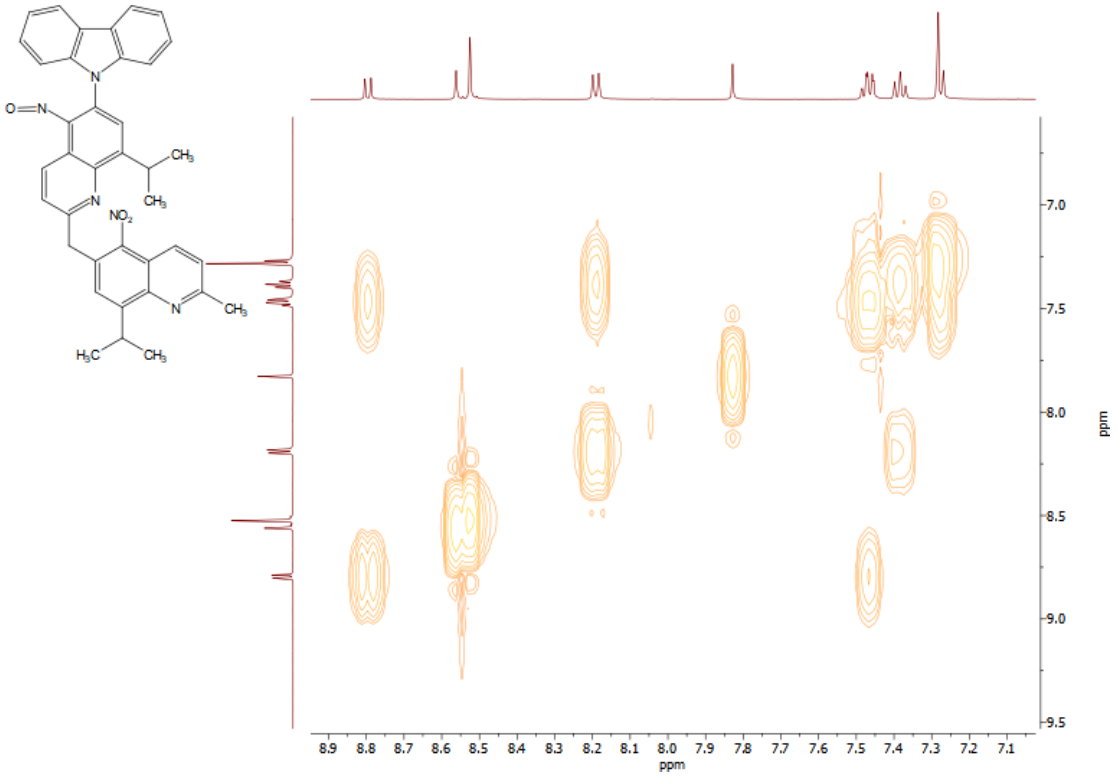

Fig. S8d. $^{1}H - {}^{1}H$ COSY spectrum (aromatic range) of the **5d**.

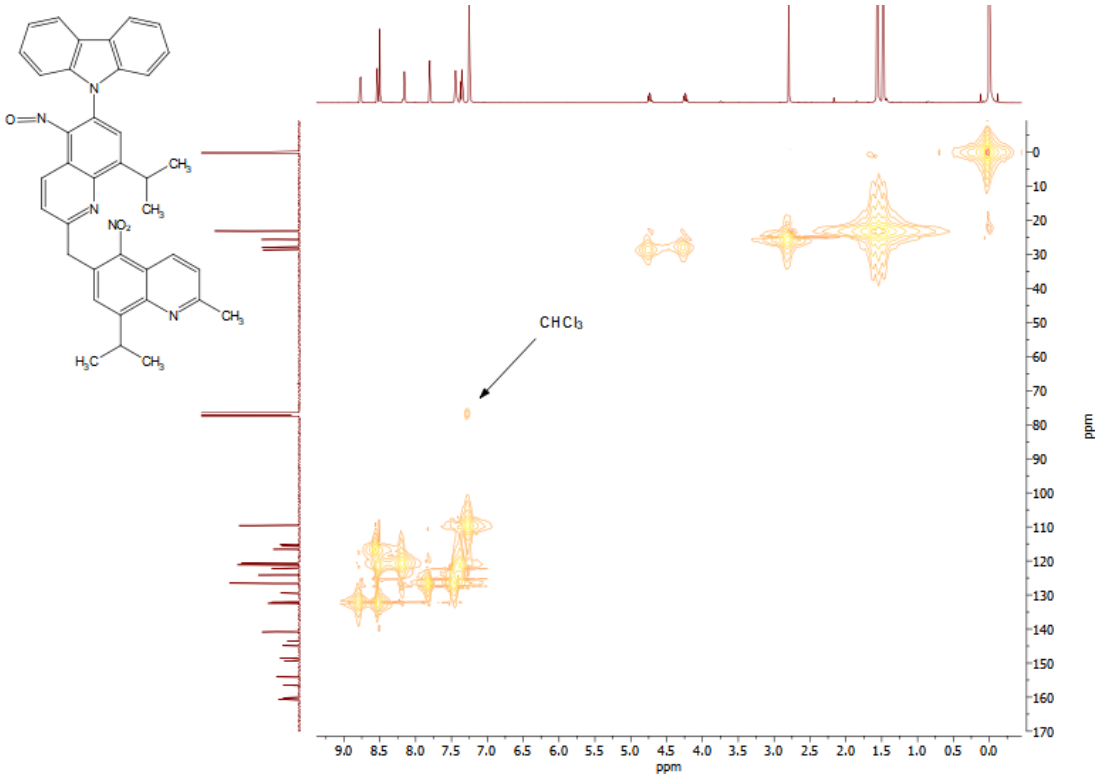

Fig. S8e. ^{1}H - ^{13}C HMQC spectrum of the **5d**.

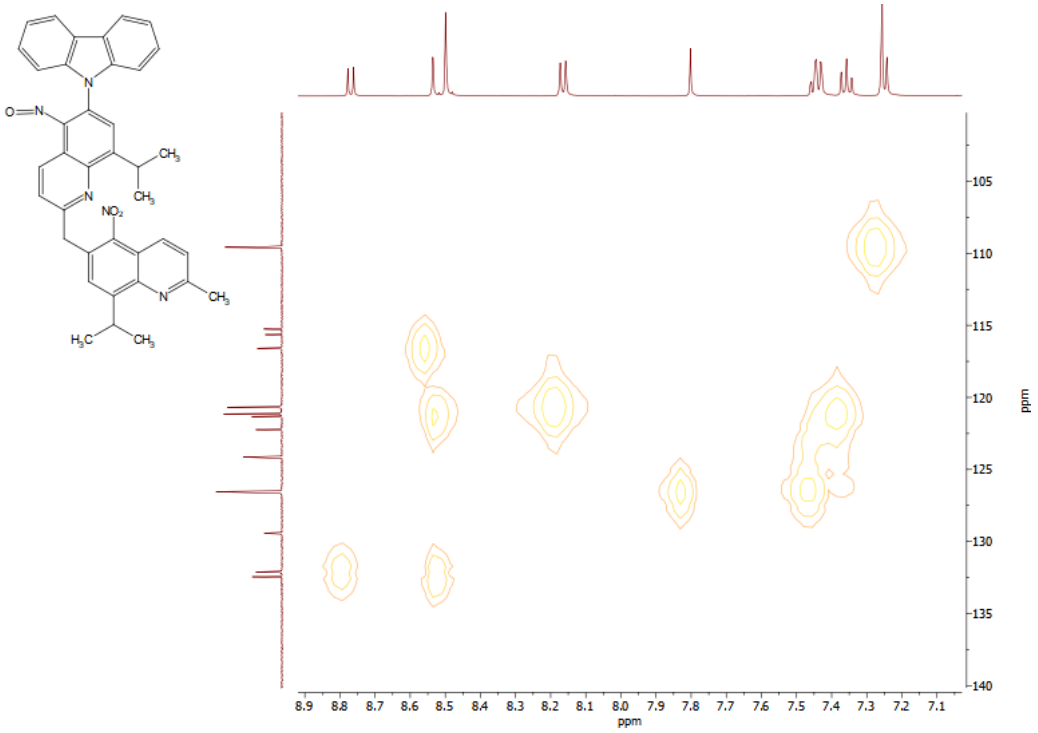

Fig. S8f. ^{1}H - ^{13}C HMQC spectrum (aromatic range) of the **5d**.

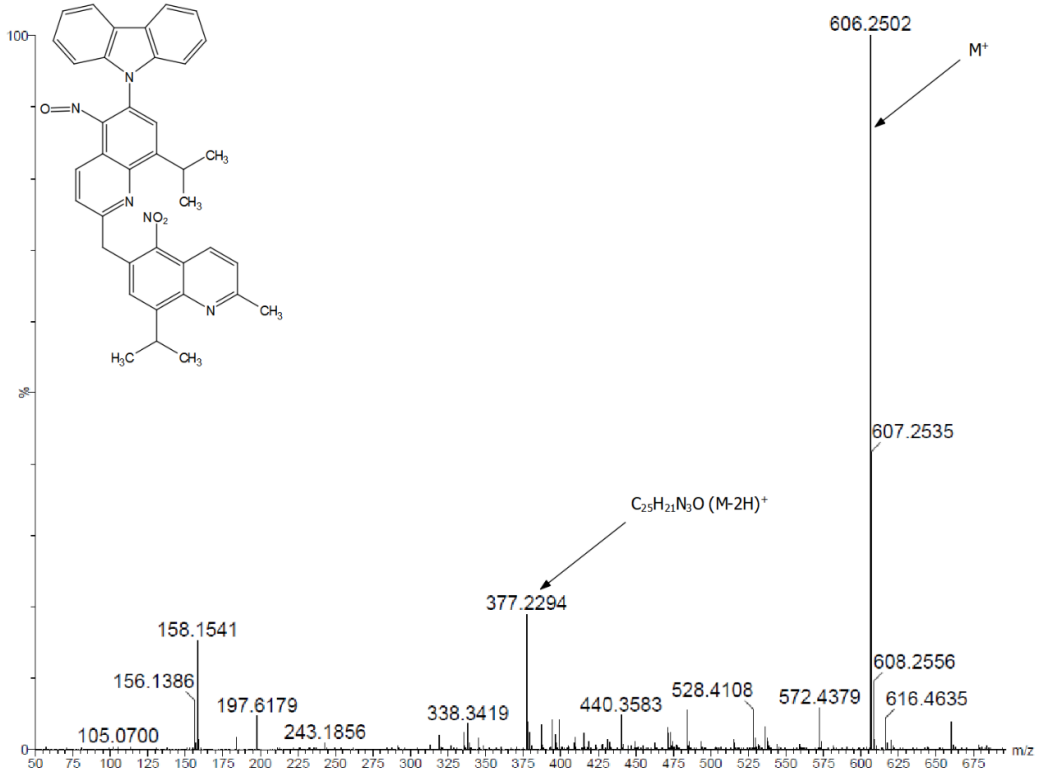

Fig. S8g. MS (ES-TOF) spectrum of the **5d**.

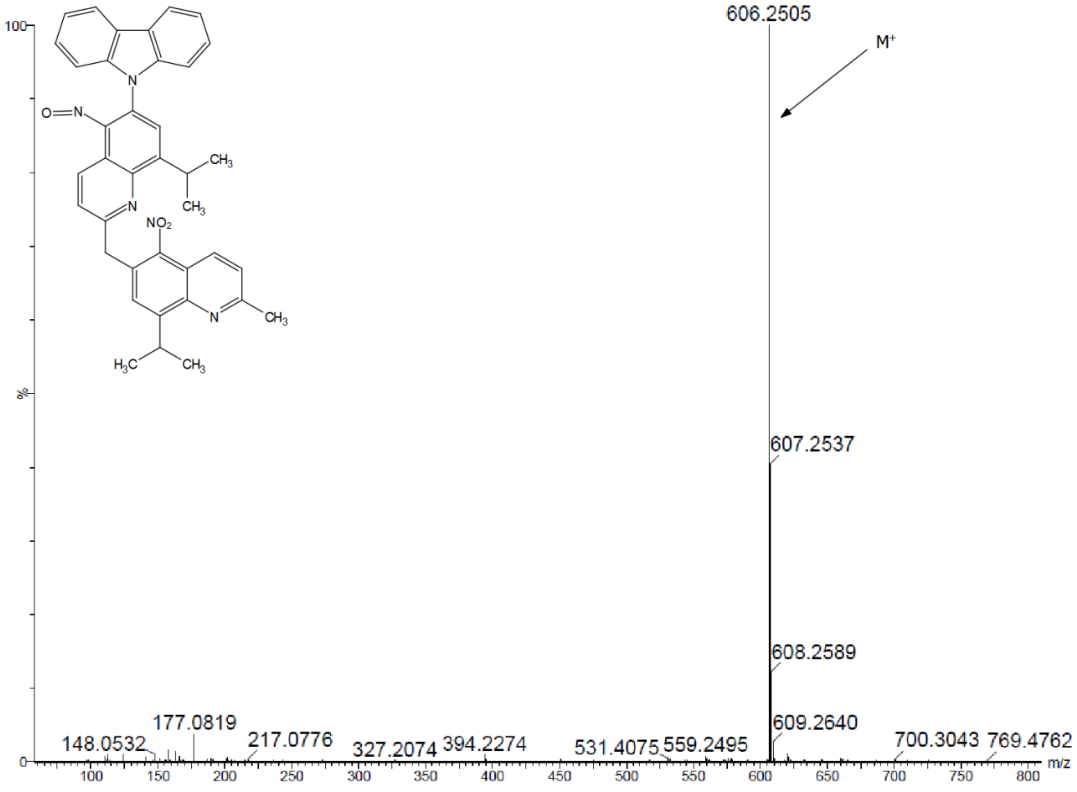

Fig. S8e. MS (AP-TOF) spectrum of the **5d**.

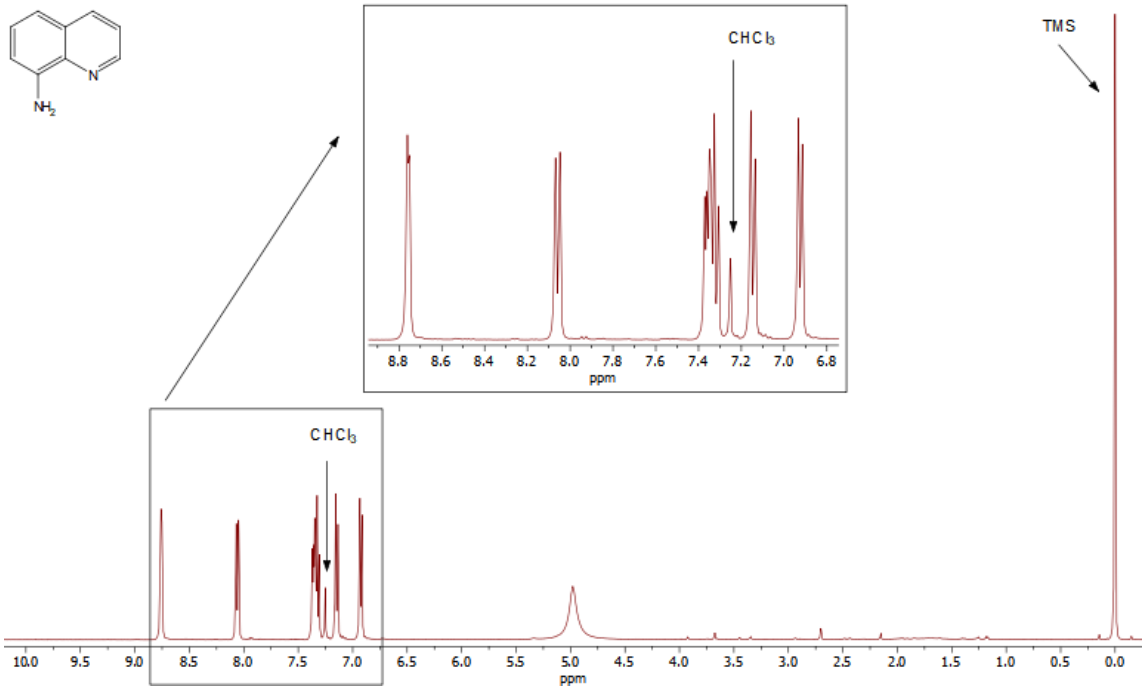

Fig. S9. ^{1}H NMR ($CDCl_3$; 400.2 MHz) spectrum of the **6a**.

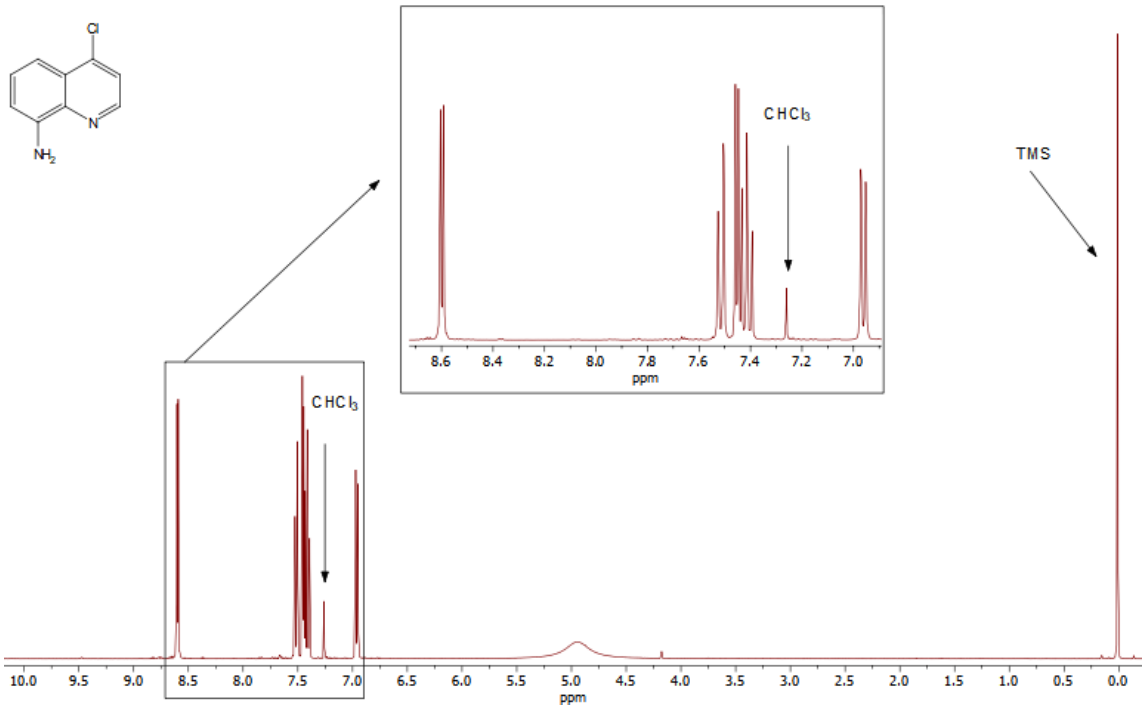

Fig. S10a. ^{1}H NMR ($CDCl_3$; 400.2 MHz) spectrum of the **6b**.

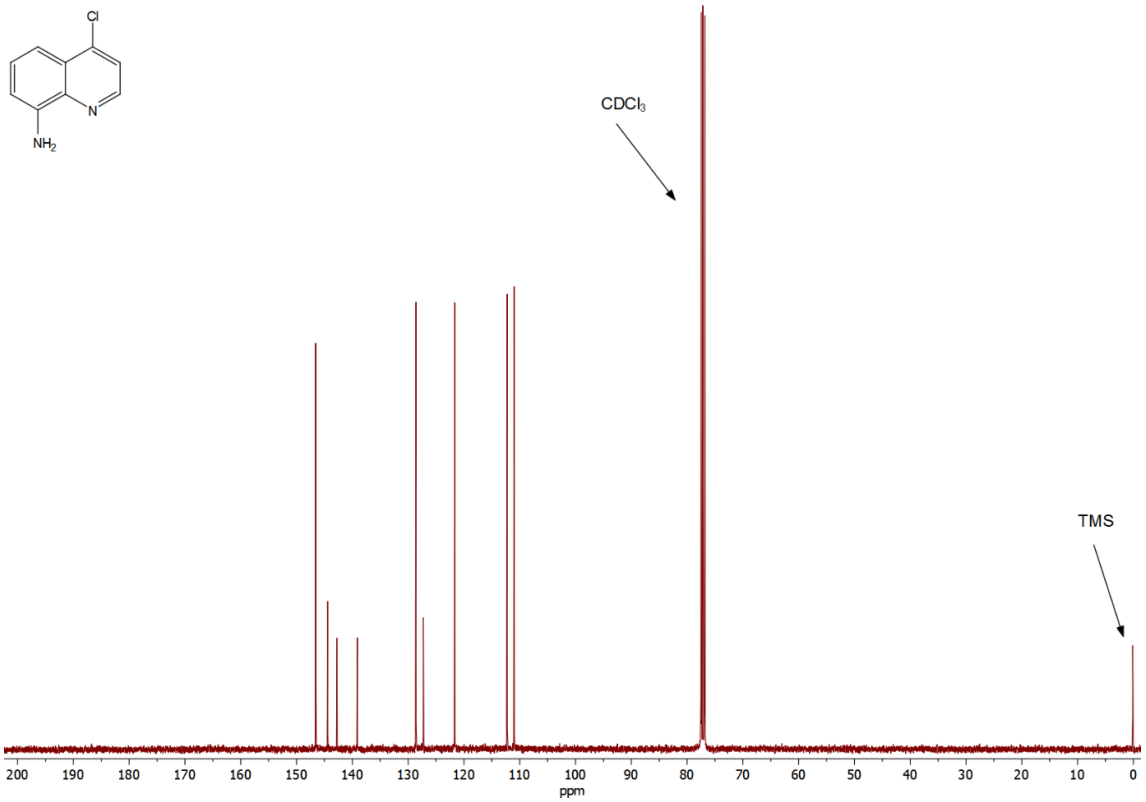

Fig. S10b. $^{13}C\{^{1}H\}$ NMR ($CDCl_3$; 100.6 MHz) spectrum of the **6b**.

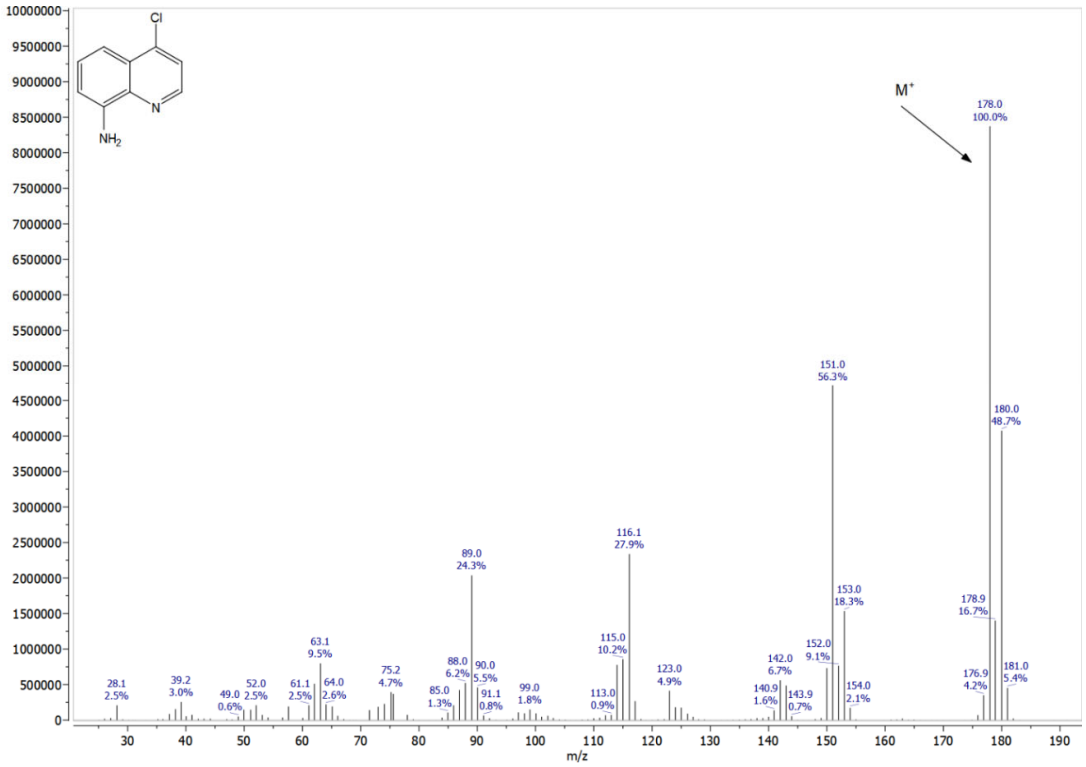

Fig. S10c. MS spectrum of the **6b**.

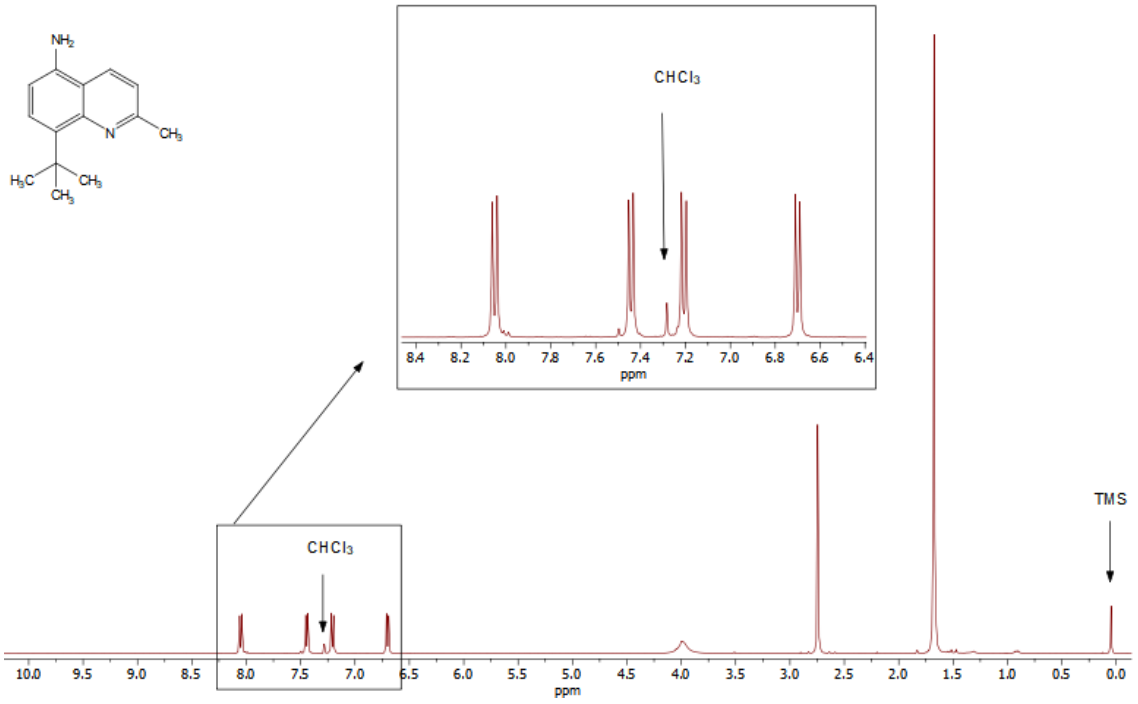

Fig. S11a. ^{1}H NMR ($CDCl_3$; 400.2 MHz) spectrum of the **6c**.

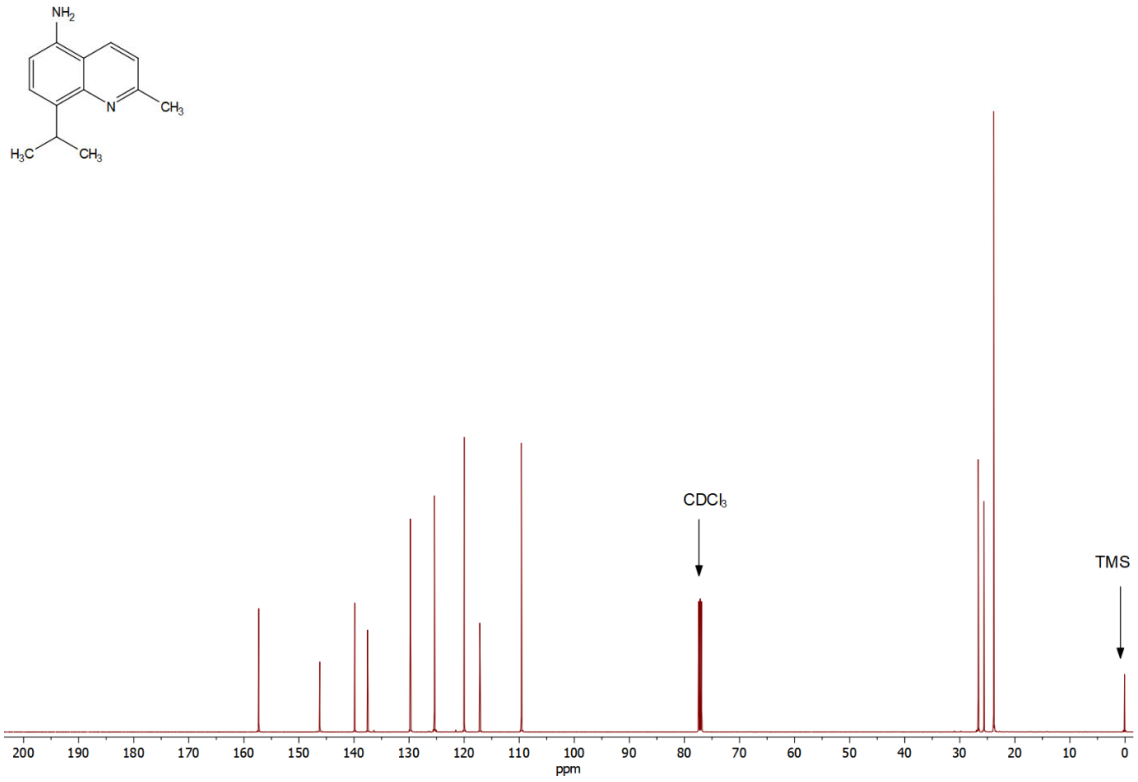

Fig. S11b. $^{13}C\{^{1}H\}$ NMR ($CDCl_3$; 100.6 MHz) spectrum of the **6c**.

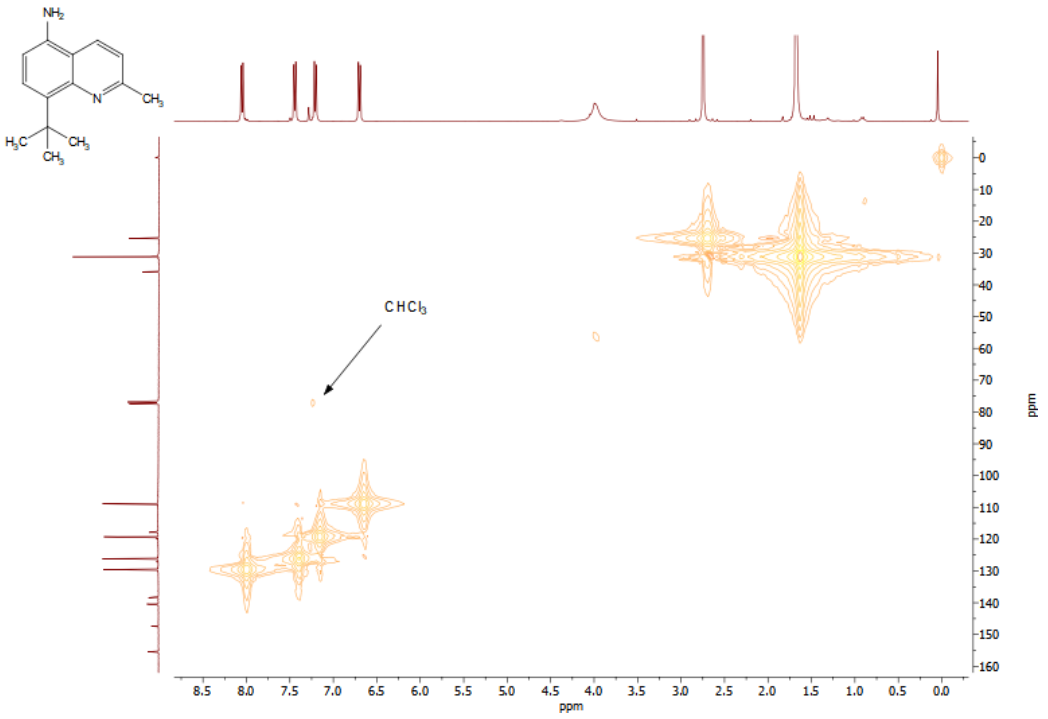

Fig. S11c. ^{1}H - ^{13}C HMQC spectrum of the **6c**.

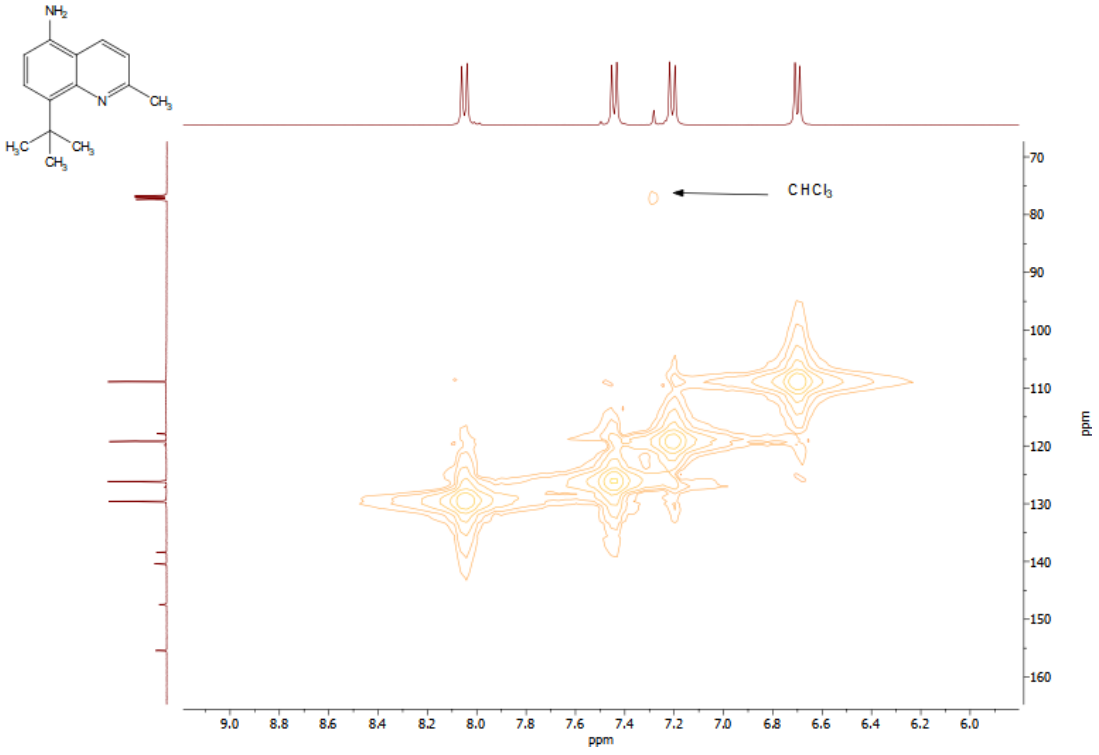

Fig. S11d. ^{1}H - ^{13}C HMQC spectrum (aromatic range) of the **6c**.

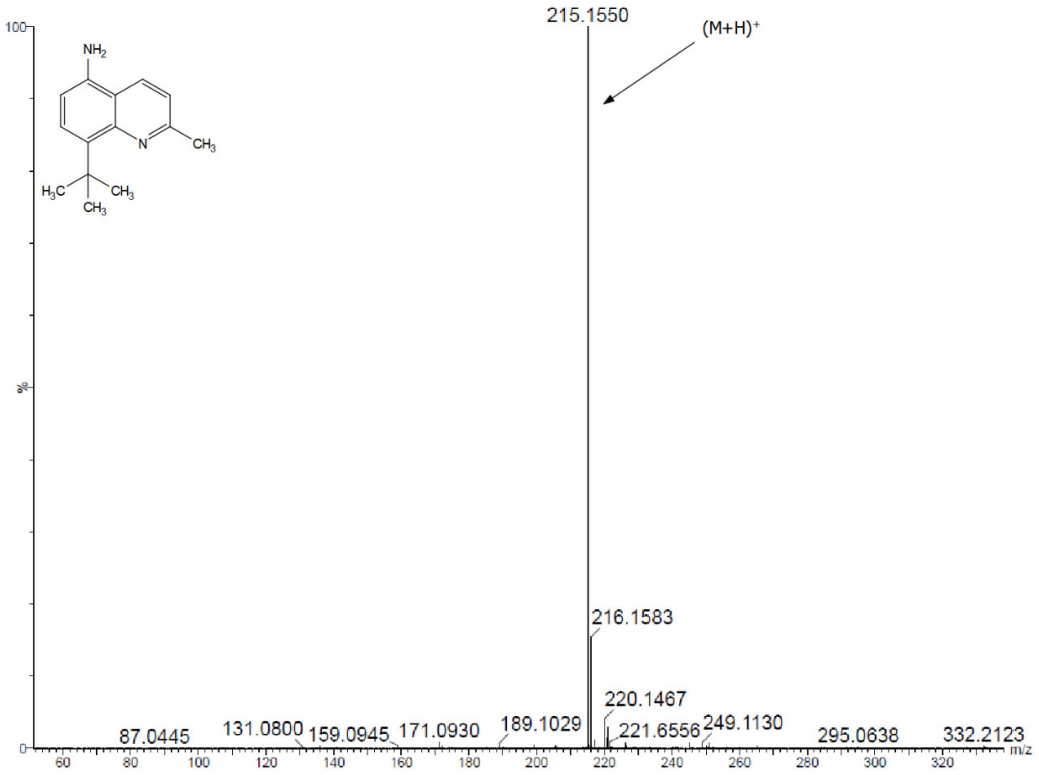

Fig. S11e. MS spectrum of the **6c**.

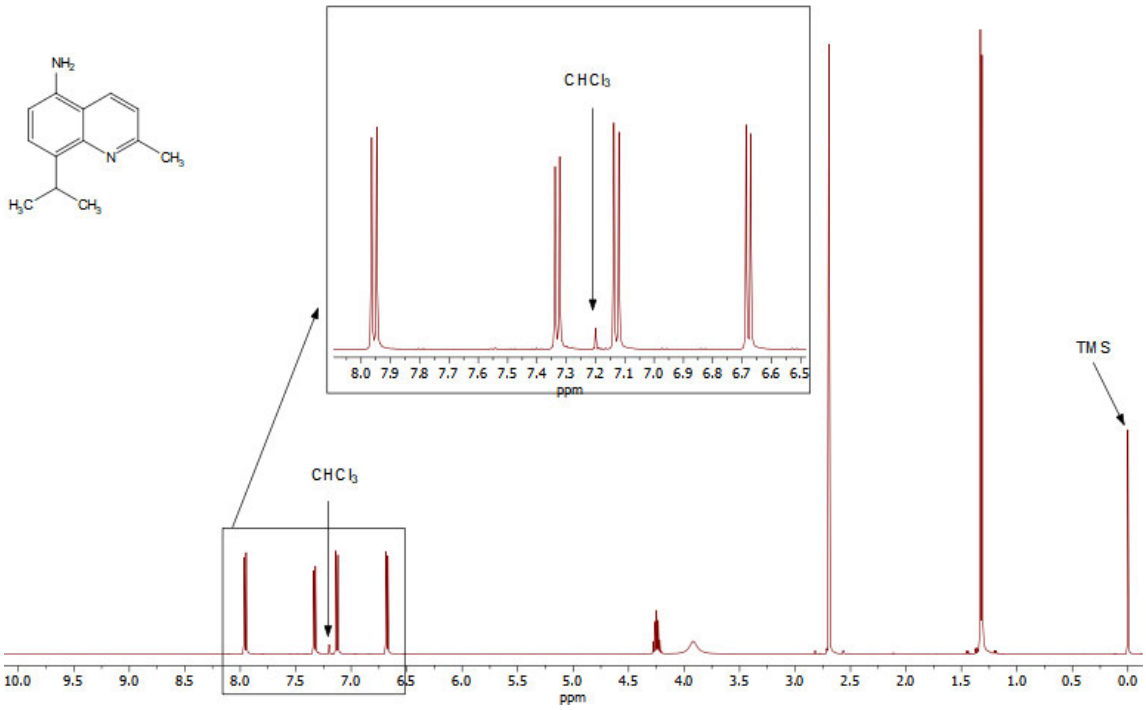

Fig. S12a. ^{1}H NMR ($CDCl_3$; 500.2 MHz) spectrum of the **6d**.

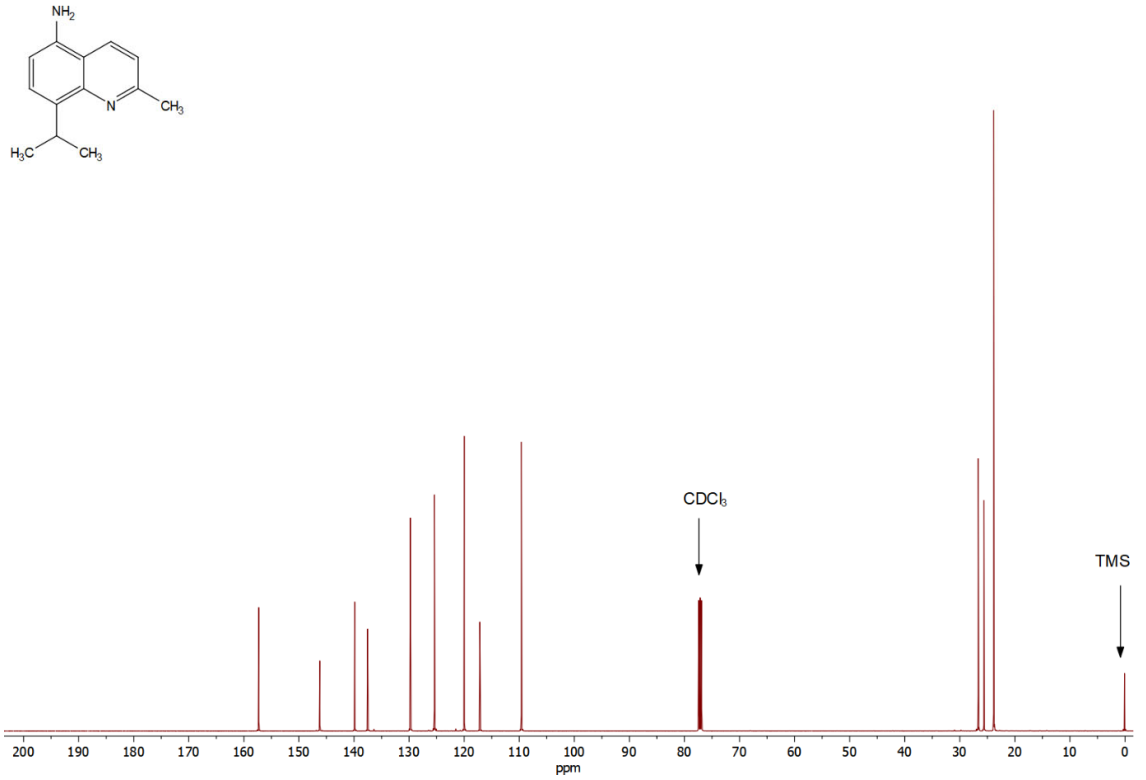

Fig. S12b. $^{13}C\{^{1}H\}$ NMR ($CDCl_3$; 125.8 MHz) spectrum of the **6d**.

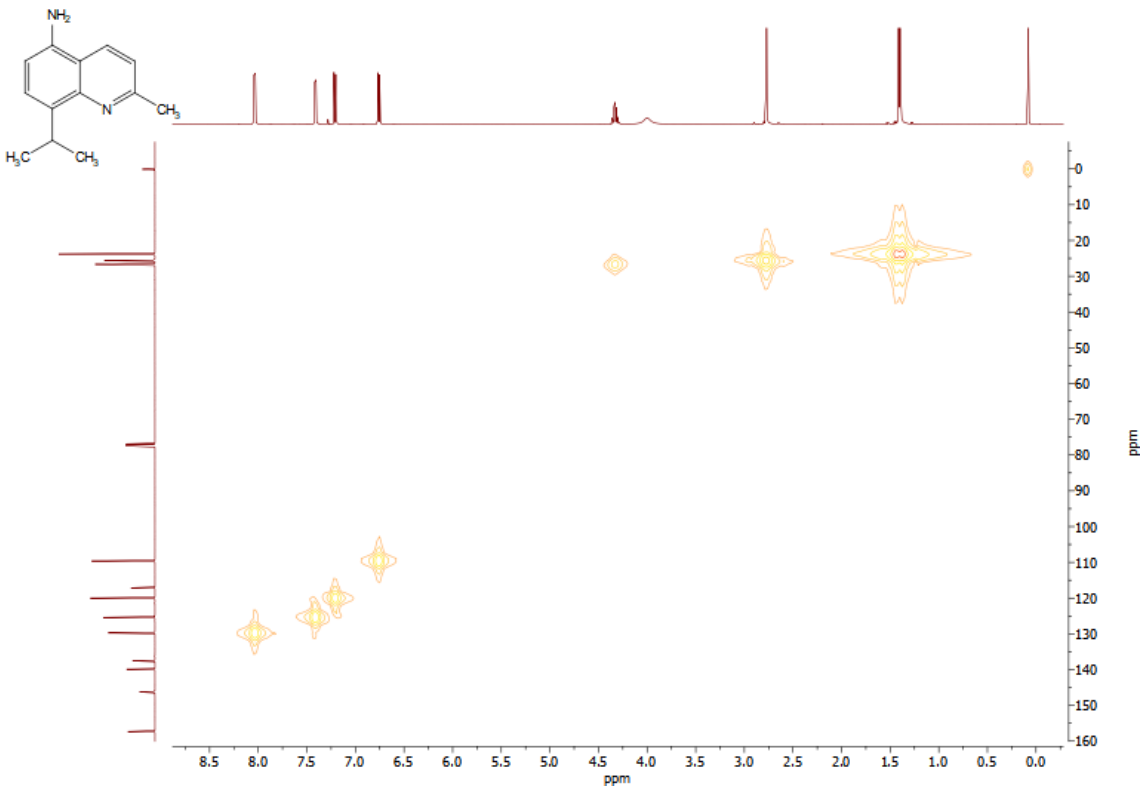

Fig. S12c. ^{1}H - ^{13}C HMQC spectrum of the **6d**.

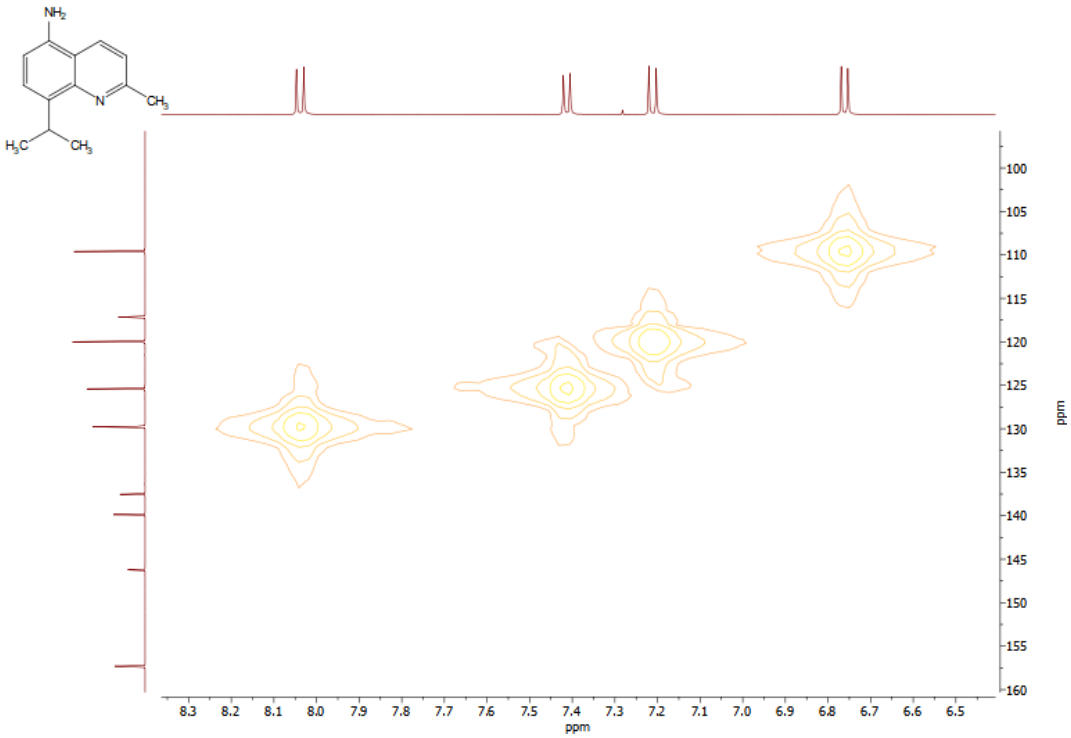

Fig. S12d. ^{1}H - ^{13}C HMQC spectrum (aromatic range) of the **6d**.

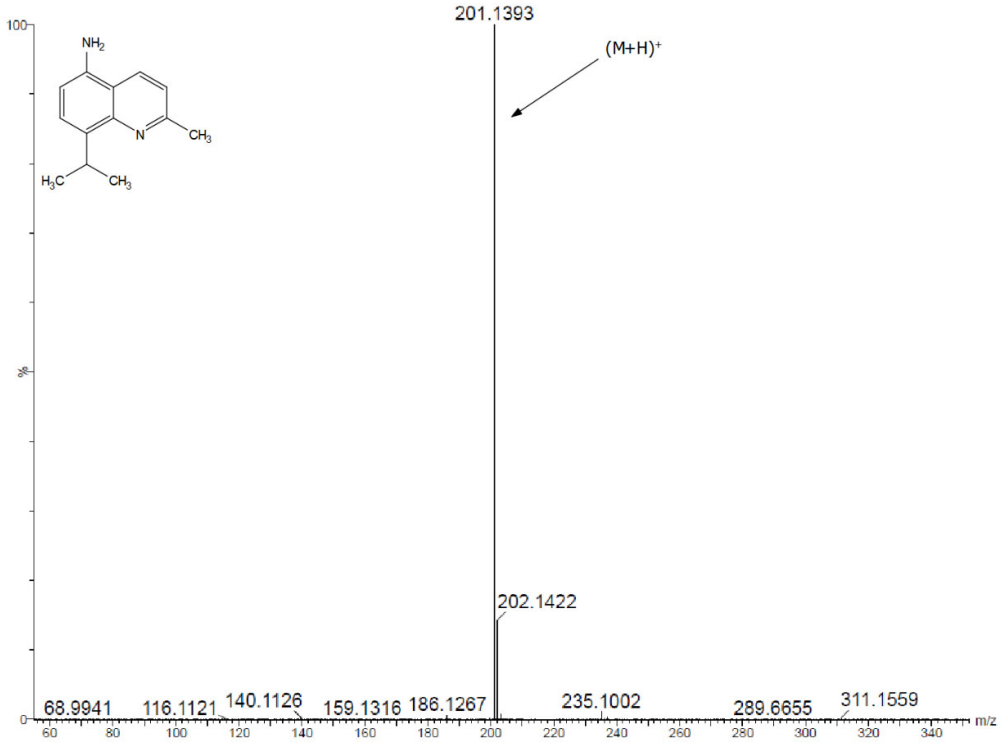

Fig. S12e. MS spectrum of the **6d**.