

**Atom- and step-economical nucleophilic arylation of azaaromatics via electrochemical  
oxidative cross C-C coupling reactions**

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**Supporting Information**

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## 1. General Information

All starting reagents and solvents were obtained from commercial sources and dried by using standard procedures before use. 10-Methylacridinium iodide was synthesized according to the known procedure,<sup>1</sup> converted to the tetrafluoroborate salt by the addition of  $\text{NH}_4\text{BF}_4$  to iodide, and purified by recrystallization from water.

$^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were recorded on a AVANCE-500 instruments using  $\text{Me}_4\text{Si}$  as an internal standard. Elemental analysis was carried out on a Eurovector EA 3000 automated analyzer. Melting points were determined on Boetius combined heating stages and were not corrected.

The GC-MS analysis of all samples was carried out using an Agilent GC 7890A MS 5975C Inert XL EI/CI GC-MS spectrometer with a quadrupole mass-spectrometric detector with electron ionization (70 eV) and scan over the total ionic current in the range  $m/z$  20–1000 and a quartz capillary column HP-5MS (30 m  $\times$  0.25 mm, film thickness 0.25 mm). Helium served as a carrier gas, the split ratio of the flow 1:50, and consumption through the column 1.0  $\text{mL min}^{-1}$ ; the initial temperature of the column 40  $^\circ\text{C}$  (storage 3 min), programming rate 10  $^\circ\text{C min}^{-1}$  to 290  $^\circ\text{C}$  (storage 20 min), the temperature of the evaporator 250  $^\circ\text{C}$ , the temperature of the source 230  $^\circ\text{C}$ , the temperature of the quadrupole 150  $^\circ\text{C}$ , and the temperature of the transition chamber 280  $^\circ\text{C}$ . Solutions of samples with concentration of 3–4  $\text{mg mL}^{-1}$  were prepared in toluene. Samples of 1 mL of the obtained solutions were analyzed.

Cyclic voltammograms were recorded by an Autolab PGSTAT128N instrument. The experiments were carried out under argon in anhydrous acetonitrile with the additives of supporting electrolyte 0.1 M  $\text{NEt}_4\text{BF}_4$  at 20  $^\circ\text{C}$  in a three-electrode system. A platinum disk electrode ( $d=2$  mm) used as a working electrode, a glass graphite rod as an auxiliary electrode,  $\text{Ag}/\text{AgNO}_3$  was a reference electrode. The scanning rate was set 100  $\text{mV/s}$ . The concentration of the samples was arbitrary.

Preparative electrolyses were carried out using Autolab PGSTAT128N in 50-mL electrode cell. The working surface of the platinum wire anode used as a working electrode was 15.0  $\text{cm}^2$ ,  $\text{Ag}/\text{AgNO}_3$  was a reference electrode. A tracing-paper was used as a membrane. A platinum wire served as a cathode, and the catholyte was a saturated solution of the background used in the catholyte in the corresponding solvent. Electrolysis was carried out in a stream of argon using a 0.1 M  $\text{NEt}_4\text{BF}_4$  solution in a  $\text{CH}_3\text{CN}-\text{CH}_3\text{OH}$  (5:1) mixture as the supporting electrolyte, in a temperature-controlled (20  $^\circ\text{C}$ ).

## 2. NMR analysis of reaction mixtures

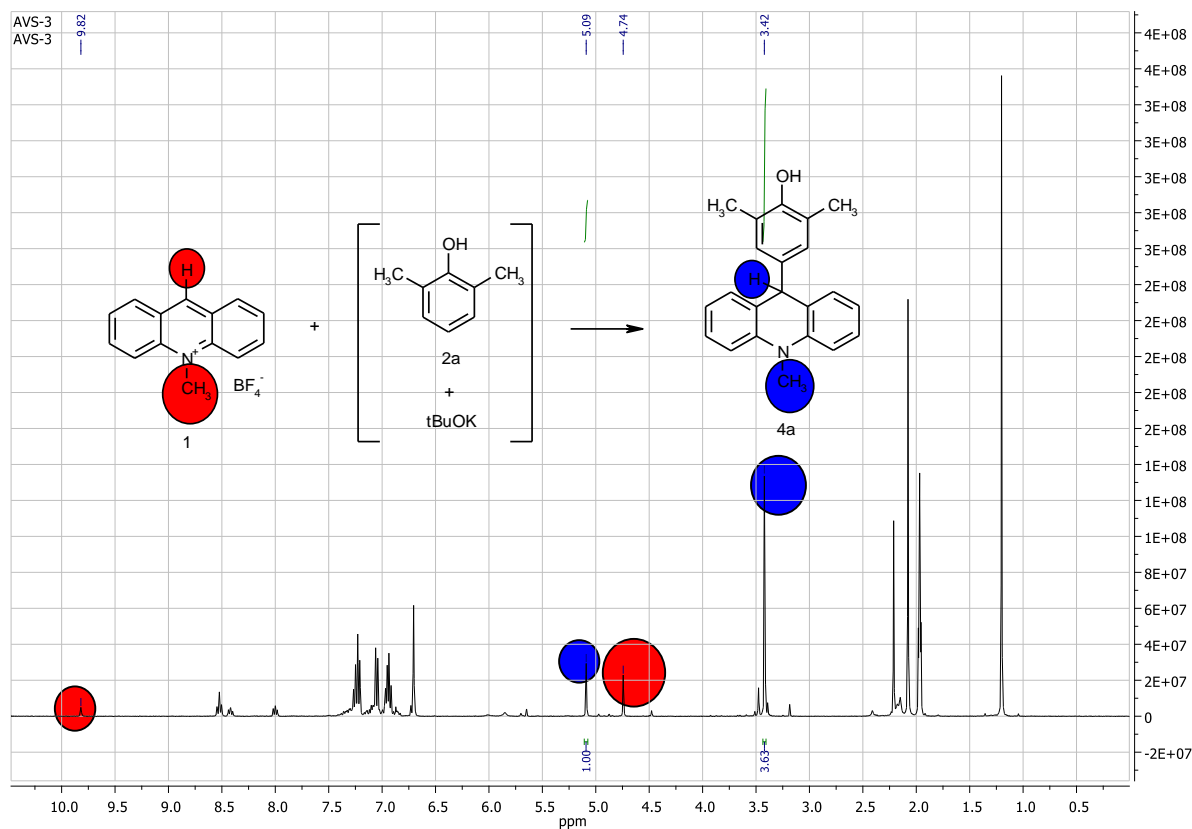


Fig 1. <sup>1</sup>H NMR spectra of a mixture of compound **1** (5mg) and phenolate **2a** (1 eq.) in 0.5 ml of CD<sub>3</sub>CN. Two minutes after mixing.

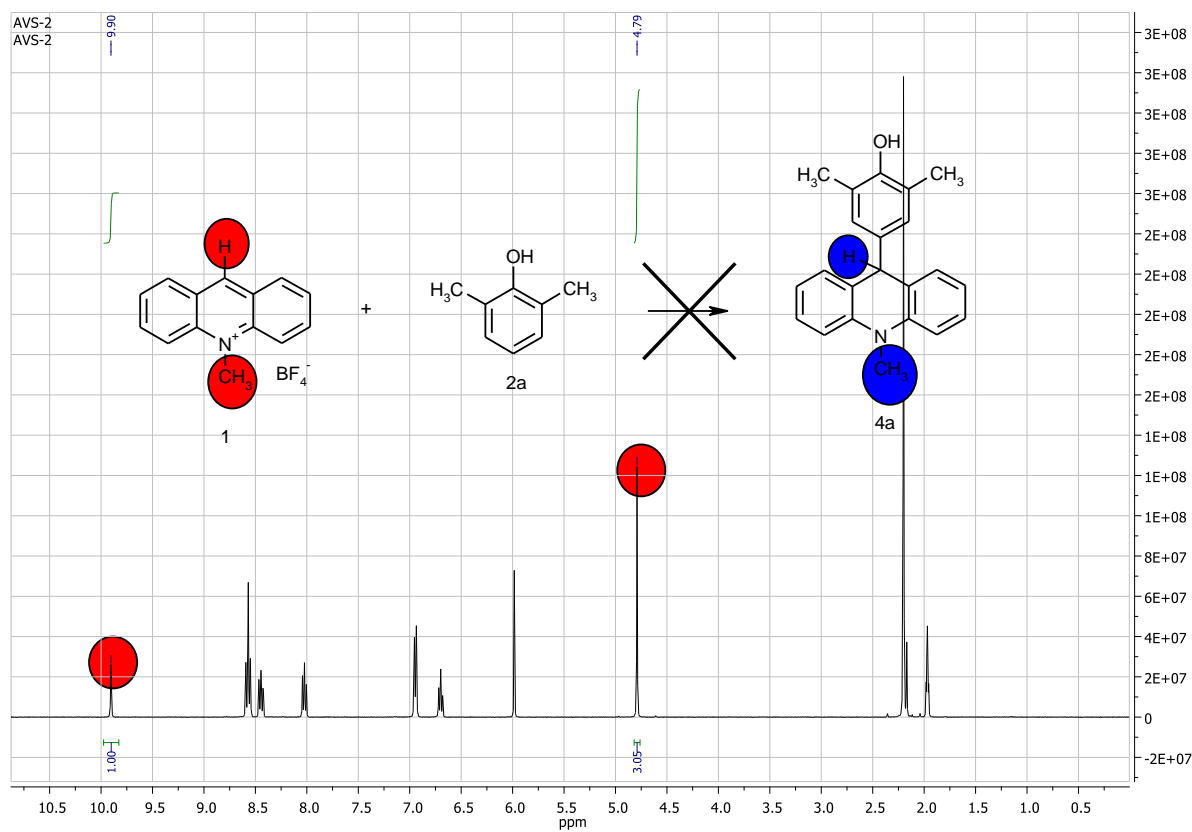


Fig 2. <sup>1</sup>H NMR spectra of a mixture of compound **1** (5mg) and phenol **2a** (1 eq.) in 0.5 ml of CD<sub>3</sub>CN. Two minutes after mixing.

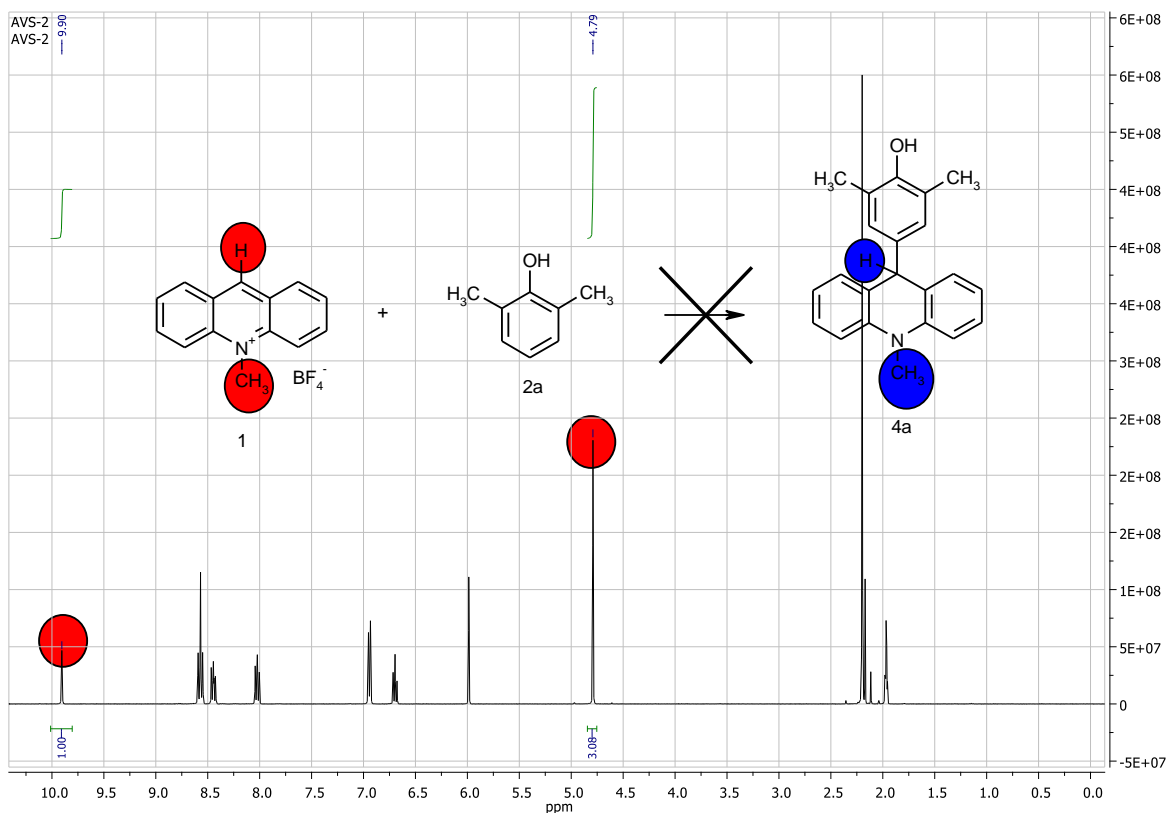


Fig 3.  $^1\text{H}$  NMR spectra of a mixture of compound **1** (5mg) and phenol **2a** (1 eq.) in 0.5 ml of  $\text{CD}_3\text{CN}$ . Sixteen hours after mixing.

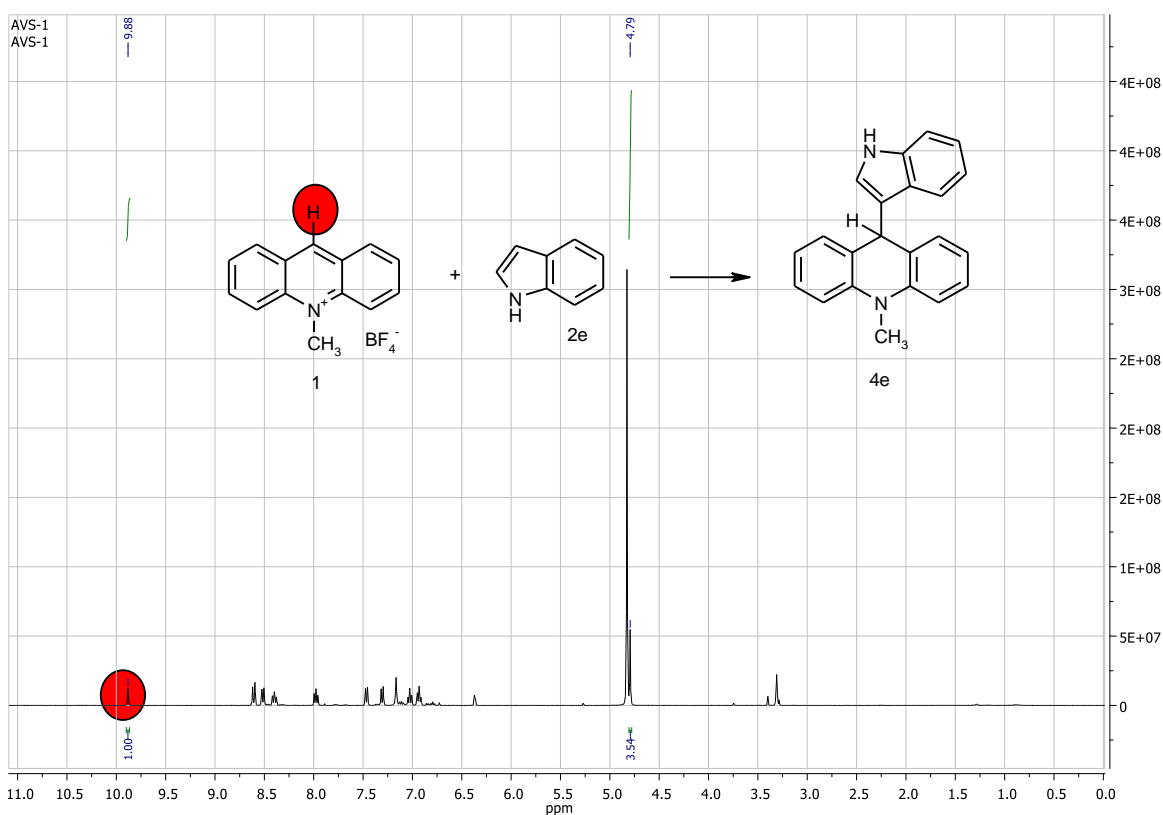


Fig 4.  $^1\text{H}$  NMR spectra of a mixture of compound **1** (5mg) and indole **2e** (1 eq.) in 0.5 ml of  $\text{CD}_3\text{OD}$ . Two minutes after mixing.

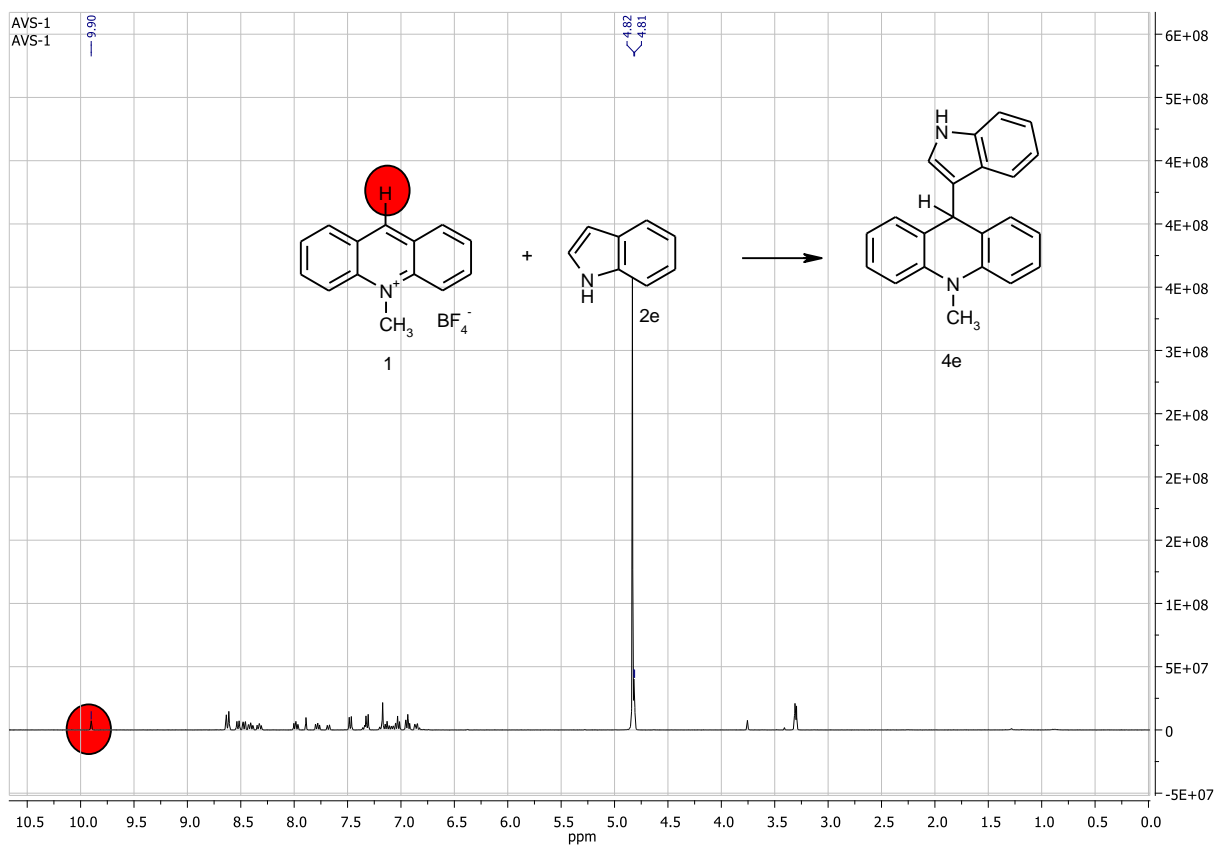


Fig 5.  $^1\text{H}$  NMR spectra of a mixture of compound **1** (5mg) and indole **2e** (1 eq.) in 0.5 ml of  $\text{CD}_3\text{OD}$ .  
One hour after mixing.

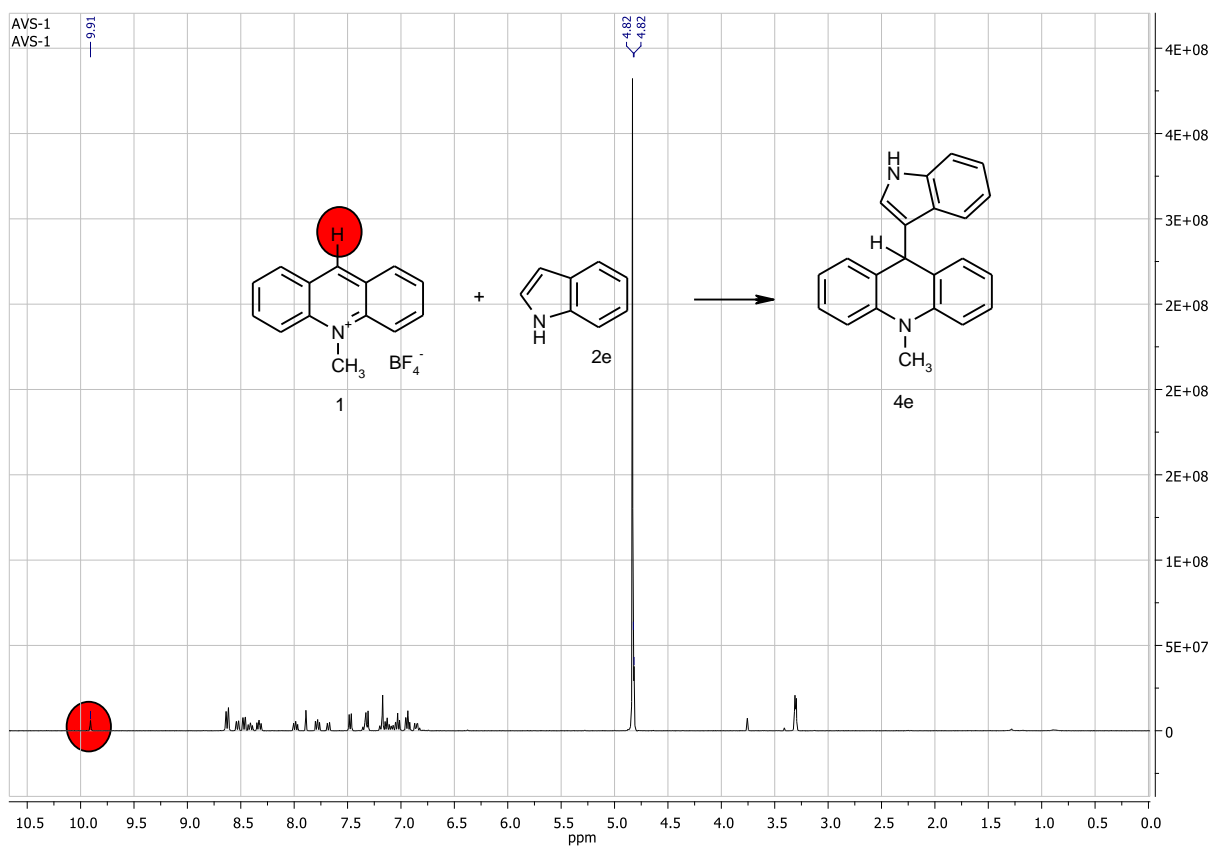


Fig 6.  $^1\text{H}$  NMR spectra of a mixture of compound **1** (5mg) and indole **2e** (1 eq.) in 0.5 ml of  $\text{CD}_3\text{OD}$ .  
Two hours after mixing.

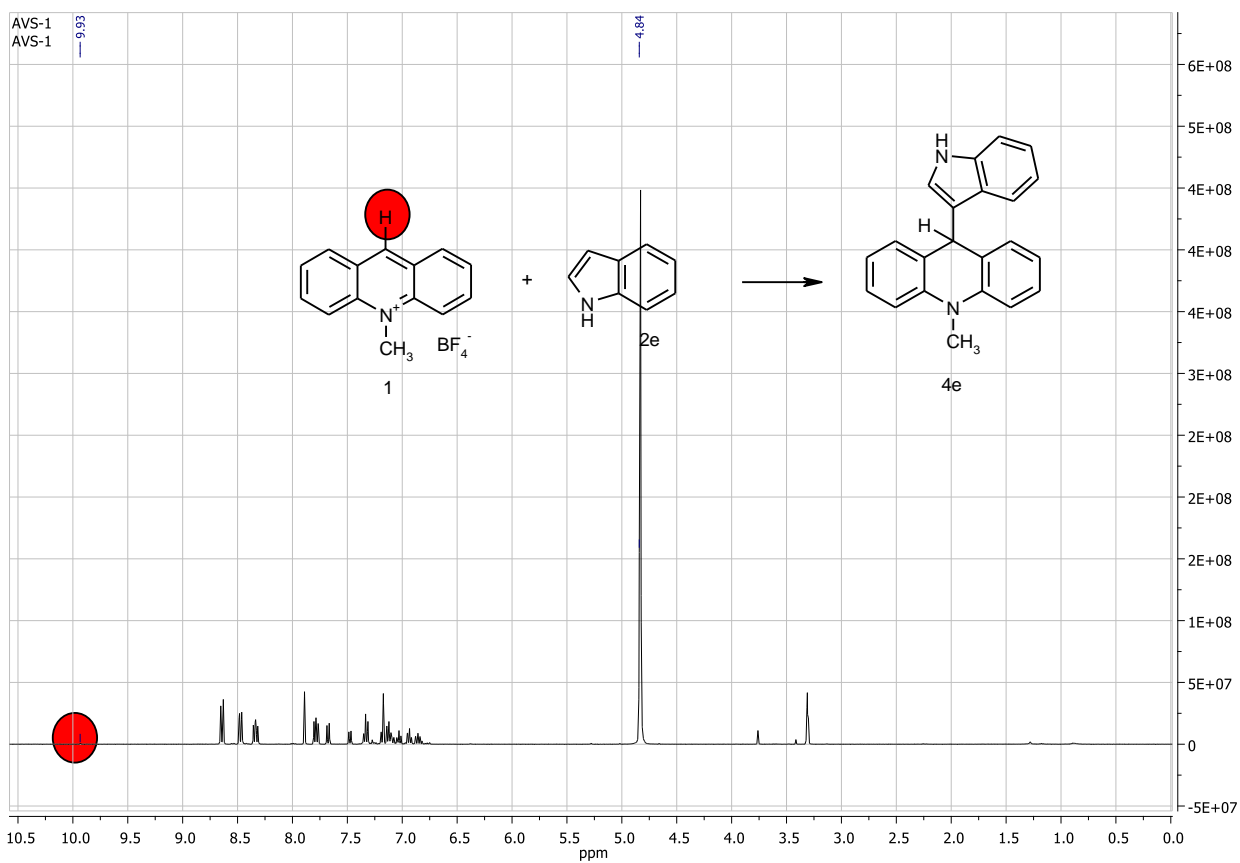
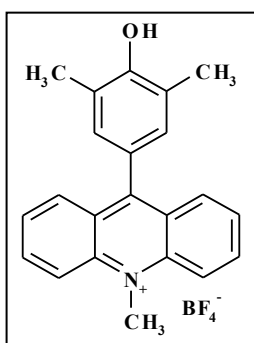


Fig 7.  $^1\text{H}$  NMR spectra of a mixture of compound **1** (5mg) and indole **2e** (1 eq.) in  $0.5\text{ ml}$  of  $\text{CD}_3\text{OD}$ . Sixteen hours after mixing.

### 3. Synthesis of compounds 3a-d

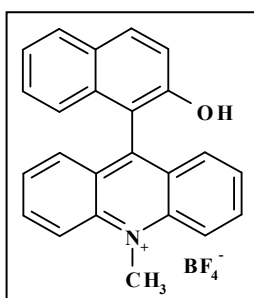
The potassium *tert*-butoxide (0.55 mmol), corresponding phenols **2a-d** (0.55 mmol) and acetonitrile (10mL) were added to electrochemical cell under argon atmosphere. The reaction mixture was stirred at room temperature for 15 min. Then 10-methylacridinium tetrafluoroborate **1** (0.5 mmol, 140 mg) was added to the reaction mixture, and stirred at room temperature for 1 h. The supporting electrolyte (40 mL) was placed in the anode and in the cathode cell compartment (10 mL). Finally, the acetic acid (1 mmol, 57  $\mu$ L) was placed in the anode cell compartment. Electrolysis was carried out at a controlled potential (reference electrode Ag/AgNO<sub>3</sub>). Upon passing 2.1F of electricity (for a two-electron process), the electrolysis was stopped, the solvent was distilled off in vacuum from the anolyte, the residue was washed with 30 ml of ether and 10 ml of water. The residue was recrystallized from water and dried on air.

#### 9-(4-Hydroxy-3,5-dimethyl-phenyl)-10-methyl-acridinium tetrafluoroborate (**3a**)



Orange needles. 195 mg (98%). The product was identified as a compound **3a** by comparing its <sup>1</sup>H NMR spectra with its given in the literature. Satisfactory elemental analysis for C, H and N were obtained for compound **3a**; none of the experimentally found percentages deviated from the theoretical values by more than 0.3%.<sup>2</sup> <sup>1</sup>H NMR (500 MHz, [D<sub>6</sub>]DMSO):  $\delta$  9.09 (s, 1H), 8.82 (d, 2H, J=9.2 Hz), 8.45-8.42 (m, 2H), 8.12-8.10 (m, 2H), 7.94-7.91 (m, 2H), 7.16 (s, 2H), 4.90 (s, 3H), 2.33 (s, 6H) ppm. <sup>13</sup>C NMR (126 MHz, [D<sub>6</sub>]DMSO):  $\delta$  161.5, 155.2, 141.1, 138.2, 130.3, 130.1, 127.6, 125.7, 124.8, 123.5, 119.0, 38.8, 16.6 ppm.

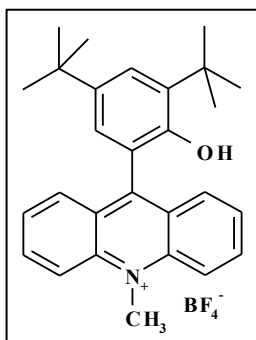
#### 9-(2-Hydroxy-1-naphthyl)-10-methyl-acridinium tetrafluoroborate (**3b**)



Red needles. 208 mg (99%). The product was identified as a compound **3b** by comparing its <sup>1</sup>H NMR spectra with its given in the literature. Satisfactory elemental analysis for C, H and N were

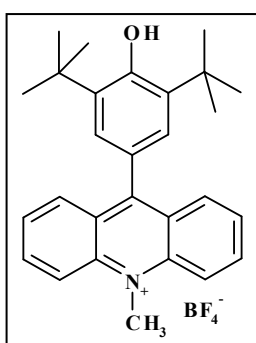
obtained for compound **3b**; none of the experimentally found percentages deviated from the theoretical values by more than 0.3%.<sup>2</sup> <sup>1</sup>H NMR (500 MHz, [D<sub>6</sub>]DMSO): δ 10.32 (s, 1H), 8.91 (d, 2H, J=9.3 Hz), 8.45-8.42 (m, 2H), 8.22 (d, 1H, J=9.0 Hz), 8.05 (d, 1H, J=8.1 Hz), 7.85-7.77 (m, 4H), 7.52 (d, 1H, J=9.0 Hz), 7.38-7.35 (m, 1H), 7.23-7.20 (m, 1H), 6.69 (d, 1H, J=8.5 Hz), 4.99 (s, 3H) ppm. <sup>13</sup>C NMR (126 MHz, [D<sub>6</sub>]DMSO): δ 158.7, 153.0, 141.3, 138.5, 133.2, 132.1, 129.1, 128.3, 128.0, 127.6, 127.5, 126.6, 123.7, 123.5, 119.5, 118.2, 111.8, 38.9 ppm.

**9-(2-Hydroxy-3,5-di-tertbutyl-phenyl)-10-methyl-acridinium tetrafluoroborate (3c)**



Yellow crystals. 230 mg (95%). The product was identified as a compound **3c** by comparing its <sup>1</sup>H NMR spectra with its given in the literature. Satisfactory elemental analysis for C, H and N were obtained for compound **3c**; none of the experimentally found percentages deviated from the theoretical values by more than 0.3%.<sup>2</sup> <sup>1</sup>H NMR (500 MHz, [D<sub>6</sub>]DMSO): δ 8.85 (d, 2H, J=9.3 Hz), 8.48-8.42 (m, 2H), 8.32 (s, 1H), 7.96-7.95 (m, 4H), 7.58 (d, 1H, J=2.4 Hz), 7.10 (d, 1H, J=2.4 Hz), 4.97 (s, 3H), 1.47 (s, 9H), 1.30 (s, 9H) ppm. <sup>13</sup>C NMR (126 MHz, [D<sub>6</sub>]DMSO): δ 159.5, 150.3, 141.3, 141.3, 138.3, 137.3, 129.6, 127.9, 126.7, 125.5, 125.4, 120.7, 119.0, 38.7, 35.0, 34.1, 31.3, 29.5 ppm.

**9-(4-Hydroxy-3,5-di-tertbutyl-phenyl)-10-methyl-acridinium tetrafluoroborate (3d)**



Yellow crystals. 232 mg (96%). The product was identified as a compound **3d** by comparing its <sup>1</sup>H NMR spectra with its given in the literature. Satisfactory elemental analysis for C, H and N were obtained for compound **3d**; none of the experimentally found percentages deviated from the theoretical values by more than 0.3%.<sup>2</sup> <sup>1</sup>H NMR (500 MHz, [D<sub>6</sub>]DMSO): δ 8.82 (d, 2H, J=9.2 Hz), 8.45-8.41 (m, 2H), 8.08 (d, 2H, J=8.6 Hz), 7.97-7.94 (m, 2H), 7.79 (s,

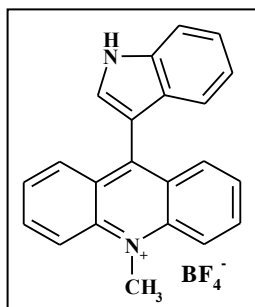


1H), 7.31 (s, 2H), 4.89 (s, 3H), 1.46 (s, 18H) ppm. <sup>13</sup>C NMR (126 MHz, [D<sub>6</sub>]DMSO): δ 141.3, 139.3, 138.1, 130.0, 127.7, 127.2, 125.7, 124.2, 119.0, 38.8, 34.8, 30.2 ppm.

#### 4. Synthesis of compounds 3e-i

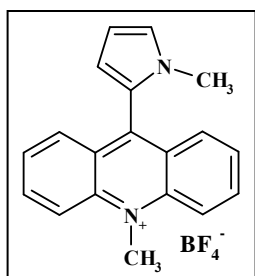
In a round bottom flask were added a solution of corresponding nucleophile **2e-i** (1 mmol) and 10-methylacridinium tetrafluoroborate **1** (0.5 mmol, 140 mg) in 10 mL methanol. The reaction mixture was refluxed for 1 h, then was transferred to an electrochemical cell. The supporting electrolyte (40 mL) was placed in the anode and in the cathode cell compartment (10 mL). Electrolysis was carried out at a controlled potential (reference electrode Ag/AgNO<sub>3</sub>). Upon passing 2.1F of electricity (for a two-electron process), the electrolysis was stopped, the solvent was distilled off in vacuum from the anolyte and the residue was washed with 30 ml of ether and 10 ml of water. The residue was recrystallized from ethanol and dried on air.

#### 9-(1*H*-Indol-3-yl)-10-methylacridinium tetrafluoroborate (**3e**)



Red crystals, 189 mg (96%). M.p.: 192-193 °C. <sup>1</sup>H NMR (500 MHz, [D<sub>6</sub>]DMSO): δ 12.44 (s, 1H), 8.80 (d, 2H, J=9.5 Hz), 8.43-8.39 (m, 4H), 8.14 (d, 1H, J=2.6 Hz), 7.90-7.86 (m, 2H), 7.70 (d, 1H, J=8.2 Hz), 7.32 (t, 1H, J=7.4 Hz), 7.17-7.10 (m, 2H), 4.88 (s, 3H) ppm. <sup>13</sup>C NMR (126 MHz, [D<sub>6</sub>]DMSO): δ 156.2, 141.2, 137.9, 136.5, 131.1, 130.5, 127.9, 127.1, 125.6, 122.9, 121.2, 119.0, 118.9, 112.7, 107.9, 38.6 ppm. Elem. Anal. Calcd. For C<sub>22</sub>H<sub>17</sub>N<sub>2</sub>BF<sub>4</sub>: C 66.69, H 4.33, N 7.07 Found: C 66.78, H 4.39, N 7.10.

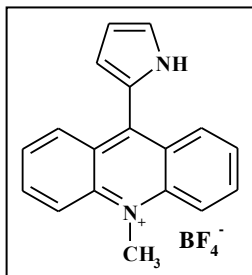
#### 10-Methyl-9-(1-methyl-1*H*-pyrrol-2-yl)acridinium tetrafluoroborate (**3f**)



Red powder, 179 mg (93%). M.p.: 174-175 °C. <sup>1</sup>H NMR (500 MHz, [D<sub>6</sub>]DMSO): δ 8.73-8.70 (m, 2H), 8.67-8.63 (m, 2H), 8.40-8.36 (m, 2H), 7.96-7.91 (m, 2H), 7.55 (t, 1H, J=1.8 Hz), 7.28 (t, 1H, J=2.4 Hz), 6.65-6.64 (m, 1H), 4.78 (s, 3H), 3.91(s, 3H) ppm. <sup>13</sup>C NMR (126 MHz, [D<sub>6</sub>]DMSO): δ 156.9, 141.2, 137.6, 130.8, 127.6, 127.0, 124.8, 124.6, 118.8, 114.9, 112.9, 38.4,

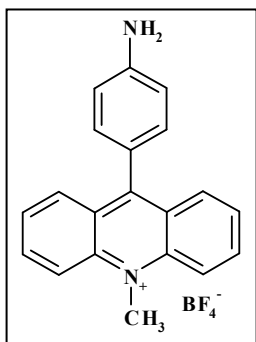
36.3 ppm. Elem. Anal. Calcd. For  $C_{19}H_{17}N_2BF_4$ : C 63.36, H 4.77, N 7.77 Found: C 63.30, H 4.83, N 7.67.

**10-Methyl-9-(1*H*-pyrrol-2-yl)acridinium tetrafluoroborate (3g)**



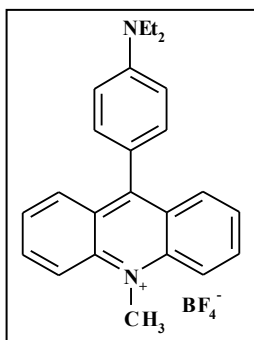
Red crystals, 162 mg (94%). M.p.: 179-181 °C.  $^1H$  NMR (500 MHz,  $[D_6]DMSO$ ):  $\delta$  12.05 (s, 1H), 8.74-8.71 (m, 2H), 8.66-8.62 (m, 2H), 8.41-8.31 (m, 2H), 7.99-7.92 (m, 2H), 7.54 (s, 1H), 7.32-7.31 (m, 1H), 6.69-6.68 (m, 1H), 4.80 (s, 3H) ppm.  $^{13}C$  NMR (126 MHz,  $[D_6]DMSO$ ):  $\delta$  157.6, 141.1, 137.7, 130.8, 127.4, 127.0, 124.5, 124.2, 118.8, 114.9, 112.5, 38.4 ppm. Elem. Anal. Calcd. For  $C_{18}H_{15}N_2BF_4$ : C 62.45, H 4.38, N 8.09 Found: C 62.37, H 4.46, N 8.11.

**9-(4-Aminophenyl)-10-methyl-acridinium tetrafluoroborate (3h)**



Dark needles. 180 mg (97%). The product was identified as a compound **3h** by comparing its  $^1H$  NMR spectra with its given in the literature. Satisfactory elemental analysis for C, H and N were obtained for compound **3h**; none of the experimentally found percentages deviated from the theoretical values by more than 0.3%.<sup>2</sup>  $^1H$  NMR (500 MHz,  $[D_6]DMSO$ ):  $\delta$  8.76 (d, 2H,  $J=9.2$  Hz), 8.42-8.38 (m, 2H), 8.24-8.22 (m, 2H), 7.93-7.90 (m, 2H), 7.31-7.29 (m, 2H), 6.92-6.89 (m, 2H), 6.02 (s, 2H), 4.83 (s, 3H) ppm.  $^{13}C$  NMR (126 MHz,  $[D_6]DMSO$ ):  $\delta$  162.0, 151.3, 141.2, 137.8, 132.6, 130.3, 127.2, 125.4, 119.1, 118.9, 113.5, 38.5 ppm.

### 9-(4-Diethylaminophenyl)-10-methyl-acridinium tetrafluoroborate (**3i**)

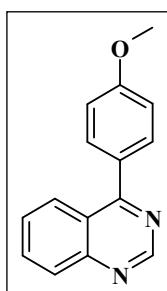


Dark violet crystals. 206 mg (97%). The product was identified as a compound **3i** by comparing its  $^1\text{H}$  NMR spectra with its given in the literature. Satisfactory elemental analysis for C, H and N were obtained for compound **3i**; none of the experimentally found percentages deviated from the theoretical values by more than 0.3%.<sup>2</sup>  $^1\text{H}$  NMR (500 MHz,  $[\text{D}_6]\text{DMSO}$ ):  $\delta$  8.77 (d, 2H,  $J=9.2$  Hz), 8.42-8.38 (m, 2H), 8.25-8.23 (m, 2H), 7.93-7.90 (m, 2H), 7.44 (d, 2H,  $J=8.8$  Hz), 7.03 (d, 2H,  $J=8.9$  Hz), 4.83 (s, 3H), 3.55-3.51 (m, 4H), 1.24-1.21 (m, 6H) ppm.  $^{13}\text{C}$  NMR (126 MHz,  $[\text{D}_6]\text{DMSO}$ ):  $\delta$  161.6, 149.0, 141.2, 137.8, 133.0, 130.3, 127.2, 125.4, 118.9, 118.5, 111.0, 43.8, 38.5, 12.4 ppm.

#### 5. Synthesis of compounds **9a**, **9b**, **10**

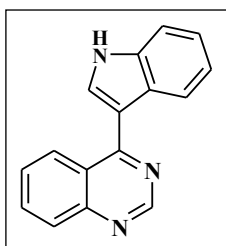
In a round bottom flask were added a solution of quinazoline **5** (1 mmol, 130 mg) or pyrimidine **6** (1 mmol, 80 mg), trifluoroacetic acid (1mmol, 74  $\mu\text{L}$ ) in 10 mL acetonitrile. Then indole **2e** (1.1 mmol, 129 mg) or anisole (1.1 mmol, 120  $\mu\text{L}$ ) was added to a solution. The reaction mixture was stirred at room temperature for 10 h, then potassium *tert*-butoxide (1 mmol, 112 mg) was added to a solution. The reaction mixture was transferred to an electrochemical cell. The supporting electrolyte (40 mL) was placed in the anode and in the cathode cell compartment (10 mL). Electrolysis was carried out at a controlled potential (reference electrode  $\text{Ag}/\text{AgNO}_3$ ). Upon passing 2.1F of electricity (for a two-electron process), the electrolysis was stopped, the solvent was distilled off in vacuum from the anolyte, the residue was extracted with ethyl acetate. The products was purified by silica gel column chromatography with ethyl acetate:methanol (10:1).

#### 4-(4-Methoxyphenyl)quinazoline (**9a**)



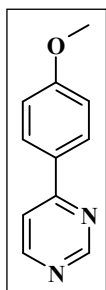
Colourless solid. 198 mg (84%). The product was identified as a compound **9a** by comparing its  $^1\text{H}$  NMR spectra with its given in the literature. Satisfactory elemental analysis for C, H and N were obtained for compound **9a**; none of the experimentally found percentages deviated from the theoretical values by more than 0.3%.<sup>3</sup> GC  $t_R$  25.04 min; MS  $m/z$  (rel intensity) 236 ( $M^+$ , 100).  $^1\text{H}$  NMR (500 MHz,  $[\text{D}_6]\text{DMSO}$ ):  $\delta$  9.31 (s, 1H), 8.16 (d,  $J=8.4$  Hz, 1H), 8.09-8.02 (m, 2H), 7.81 (d,  $J=8.6$  Hz, 2H), 7.75 (t,  $J=7.5$  Hz, 1H), 7.19 (d,  $J=8.7$  Hz, 2H), 3.89 (s, 3H) ppm.  $^{13}\text{C}$  NMR (126 MHz,  $[\text{D}_6]\text{DMSO}$ ):  $\delta$  166.9, 160.9, 154.3, 150.5, 133.9, 131.7, 128.9, 128.4, 128.1, 126.8, 122.2, 114.1, 55.4 ppm. FT-IR (DRA,  $\text{cm}^{-1}$ ): 459, 514, 551, 589, 634, 679, 731, 773, 788, 801, 816, 840, 870, 948, 959, 979, 1025, 1089, 1113, 1131, 1167, 1197, 1255, 1273, 1291, 1308, 1346, 1385, 1417, 1447, 1458, 1491, 1513, 1535, 1564, 1607, 1737, 1907, 2041, 2559, 2842, 2944, 2969, 2995, 3050.

#### 4-(1*H*-Indol-3-yl)quinazoline (**9b**)



Yellow solid. 200 mg (82%). The product was identified as a compound **9b** by comparing its  $^1\text{H}$  NMR spectra with its given in the literature. Satisfactory elemental analysis for C, H and N were obtained for compound **9b**; none of the experimentally found percentages deviated from the theoretical values by more than 0.3%.<sup>4</sup> GC  $t_R$  30.75 min; MS  $m/z$  (rel intensity) 245 ( $M^+$ , 100).  $^1\text{H}$  NMR (500 MHz,  $[\text{D}_6]\text{DMSO}$ ):  $\delta$  12.06 (s, 1H), 9.27 (s, 1H), 8.54 (d,  $J=8.4$  Hz, 1H), 8.30-8.28 (m, 2H), 8.04-7.98 (m, 2H), 7.75 (t,  $J=7.0$  Hz, 1H), 7.58 (d,  $J=8.0$  Hz, 1H), 7.27 (t,  $J=7.4$  Hz, 1H), 7.21 (t,  $J=7.4$  Hz, 1H).  $^{13}\text{C}$  NMR (126 MHz,  $[\text{D}_6]\text{DMSO}$ ):  $\delta$  162.8, 154.5, 150.4, 136.7, 133.4, 131.0, 128.3, 127.7, 126.9, 126.3, 122.5, 122.3, 121.5, 120.7, 112.1, 112.0 ppm.

#### 4-(4-Methoxyphenyl)pyrimidine (**10**)



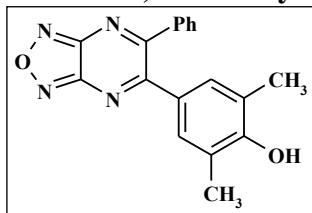
Yellow solid. 160 mg (86%). The product was identified as a compound **10** by comparing its  $^1\text{H}$  NMR spectra with its given in the literature. Satisfactory elemental analysis for C, H and N were obtained for compound **10**; none of the experimentally found percentages deviated from the theoretical values by more than 0.3%.<sup>5</sup> GC  $t_R$  20.25 min; MS  $m/z$  (rel intensity) 186 ( $M^+$ ,

100).  $^1\text{H}$  NMR (500 MHz,  $[\text{D}_6]\text{DMSO}$ ):  $\delta$  9.17 (s, 1H), 8.78 (d,  $J=5.3$  Hz, 1H), 8.20 (d,  $J=8.6$  Hz, 2H), 8.03 (d,  $J=5.2$  Hz, 1H), 7.11 (d,  $J=8.6$  Hz, 2H), 3.85 (s, 3H) ppm.  $^{13}\text{C}$  NMR (126 MHz,  $[\text{D}_6]\text{DMSO}$ ):  $\delta$  162.1, 161.8, 158.6, 157.6, 128.6, 128.2, 116.2, 114.4, 55.4 ppm. FT-IR (DRA,  $\text{cm}^{-1}$ ): 492, 580, 633, 669, 718, 732, 775, 808, 821, 830, 852, 987, 1025, 1052, 1114, 1150, 1176, 1252, 1282, 1310, 1329, 1392, 1456, 1512, 1538, 1579, 1606, 1661, 1905, 1967, 2044, 2256, 2580, 2840, 2907, 2934, 2972, 3029.

### 6. Synthesis of compounds **11a**, **11b**, **12**

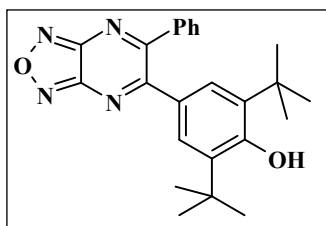
In an electrochemical cell were added a solution of 6-phenyl-1,2,5-oxadiazolo[3,4-*b*]pyrazine **7** (1 mmol, 198 mg) or 3-phenyl-1,2,4-triazin-5(2*H*)-one **8** (1 mmol, 173 mg) in 2 mL trifluoroacetic acid under argon atmosphere. Then corresponding phenols **2a** or **2d** was added to a solution. The reaction mixture was stirred at room temperature for 1 h. The supporting electrolyte (40 mL) was placed in the anode and in the cathode cell compartment (10 mL). Electrolysis was carried out at a controlled potential (reference electrode  $\text{Ag}/\text{AgNO}_3$ ). Upon passing 2.1F of electricity (for a two-electron process), the electrolysis was stopped, the solvent was distilled off in vacuum from the anolyte and the residue was washed with 30 ml of water. The products **11a**, **b** was recrystallized from ethanol and dried on air. The product **12** was recrystallized from acetonitrile.

#### 2,6-Dimethyl-4-(6-phenyl-1,2,5-oxadiazolo[3,4-*b*]pyrazin-5-yl)phenol (**11a**)



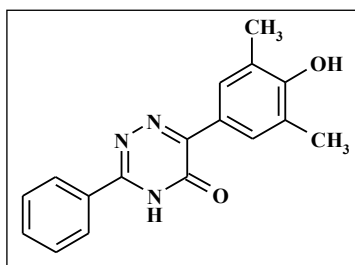
Yellow-orange crystalline powder. 276 mg (87%). The product was identified as a compound **11a** by comparing its  $^1\text{H}$  NMR spectra with its given in the literature. Satisfactory elemental analysis for C, H and N were obtained for compound **11a**; none of the experimentally found percentages deviated from the theoretical values by more than 0.3%.<sup>6</sup> GC  $t_R$  31.48 min; MS  $m/z$  (rel intensity) 318 ( $\text{M}^+$ , 100).  $^1\text{H}$  NMR (500 MHz,  $[\text{D}_6]\text{DMSO}$ ):  $\delta$  9.04 (s, 1H), 7.54-7.48 (m, 3H), 7.44-8.41 (m, 2H), 7.06 (s, 2H), 2.05 (s, 6H).  $^{13}\text{C}$  NMR (126 MHz,  $[\text{D}_6]\text{DMSO}$ ):  $\delta$  164.1, 162.9, 156.3, 151.6, 151.3, 138.1, 131.0, 130.4, 129.6, 127.9, 127.7, 123.7, 16.5 ppm.

#### 2,6-Di-*tert*-butyl-4-(6-phenyl-1,2,5-oxadiazolo[3,4-*b*]pyrazin-5-yl)phenol (**11b**)



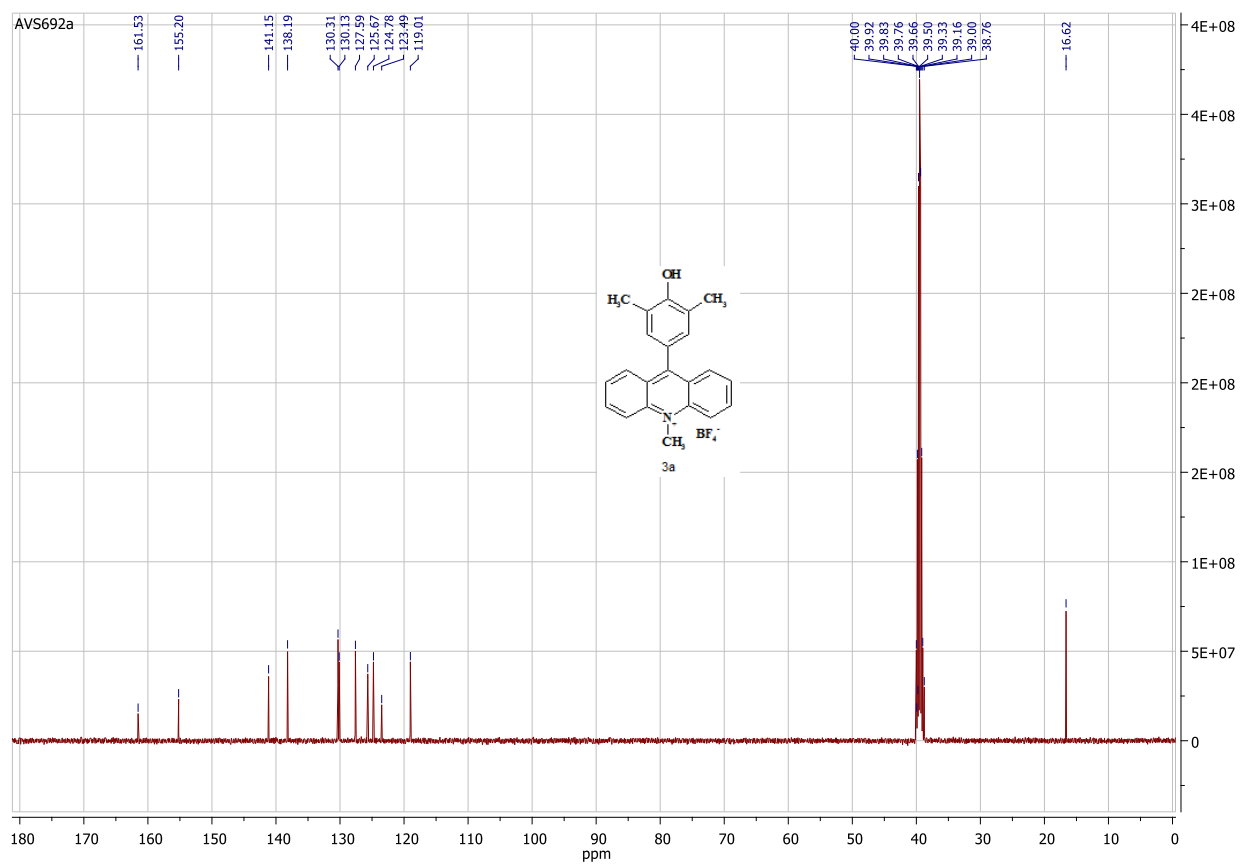
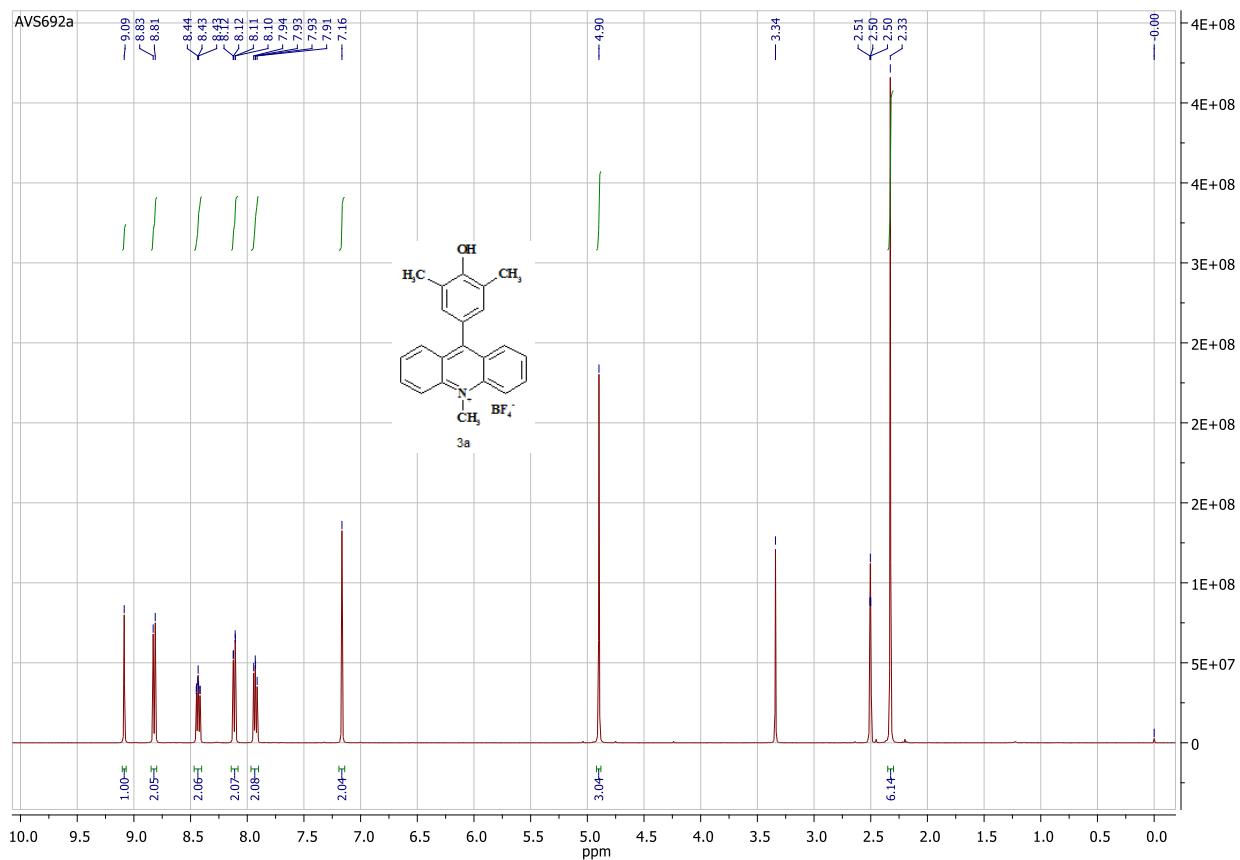
Orange crystalline powder. 361 mg (90%). The product was identified as a compound **11b** by comparing its  $^1\text{H}$  NMR spectra with its given in the literature. Satisfactory elemental analysis for C, H and N were obtained for compound **11b**; none of the experimentally found percentages deviated from the theoretical values by more than 0.3%.<sup>6</sup> GC  $t_R$  34.69 min; MS  $m/z$  (rel intensity) 402 ( $M^+$ , 100).  $^1\text{H}$  NMR (500 MHz,  $[\text{D}_6]\text{DMSO}$ ):  $\delta$  7.67 (s, 1H), 7.53-7.42 (m, 5H), 7.32 (s, 2H), 1.24 (s, 18H).  $^{13}\text{C}$  NMR (126 MHz,  $[\text{D}_6]\text{DMSO}$ ):  $\delta$  164.3, 163.3, 156.9, 151.6, 151.2, 138.5, 137.8, 130.2, 129.6, 128.0, 127.5, 34.4, 29.8 ppm. FT-IR (DRA,  $\text{cm}^{-1}$ ): 463, 511, 597, 618, 686, 694, 736, 757, 777, 814, 855, 863, 884, 904, 918, 931, 1006, 1023, 1104, 1181, 1203, 1232, 1266, 1306, 1324, 1386, 1421, 1433, 1445, 1495, 1535, 1552, 1596, 1693, 2864, 2970, 3061, 3083, 3581.

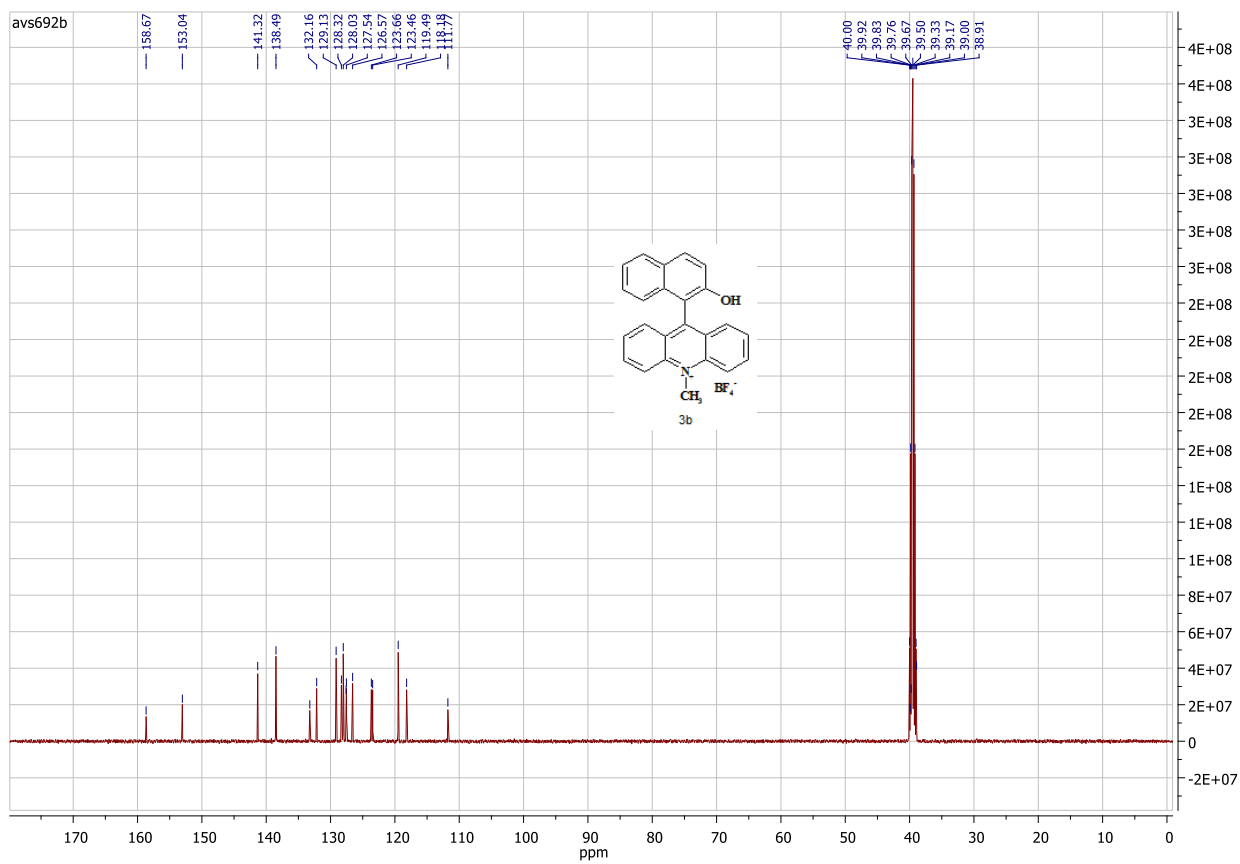
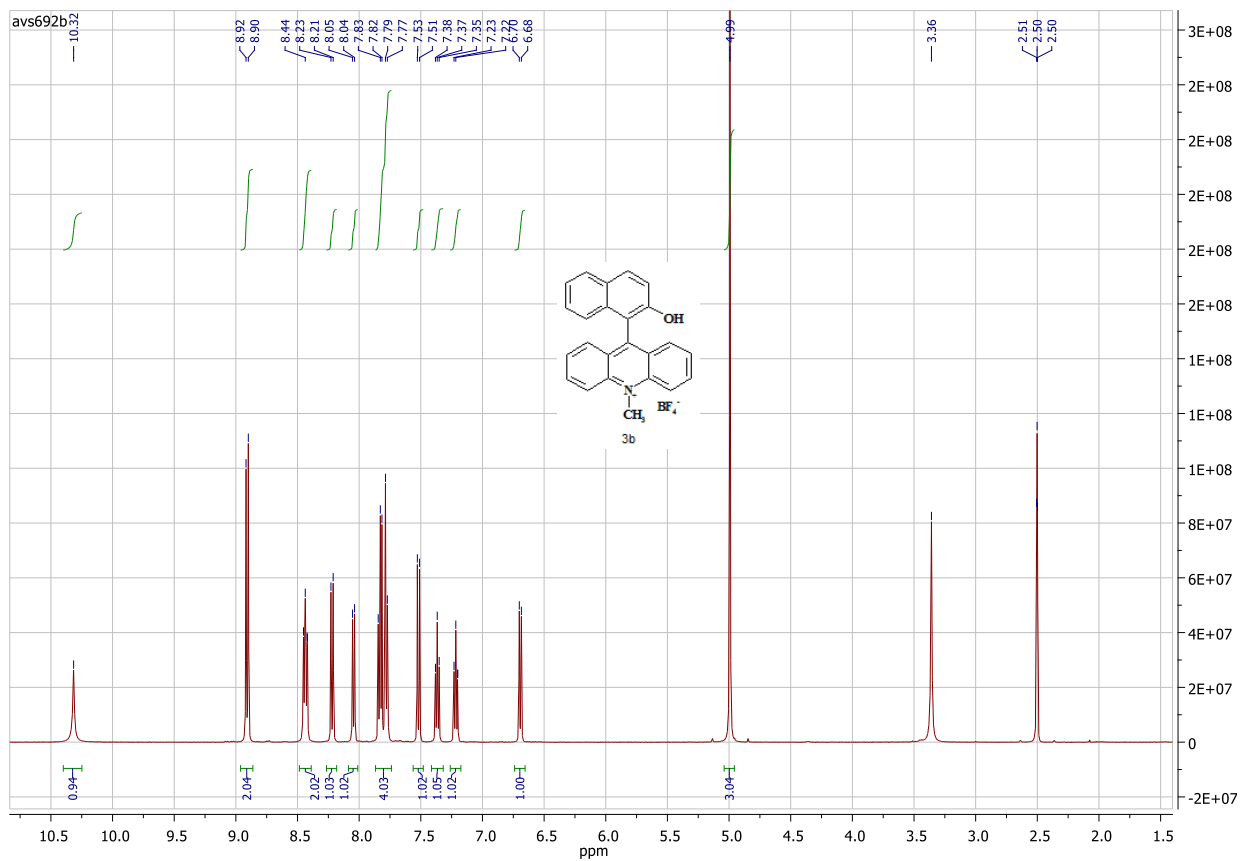
**3-Phenyl-6-(3,5-dimethyl-4-hydroxyphenyl)-1,2,4-triazin-5(2H)-one (12)**



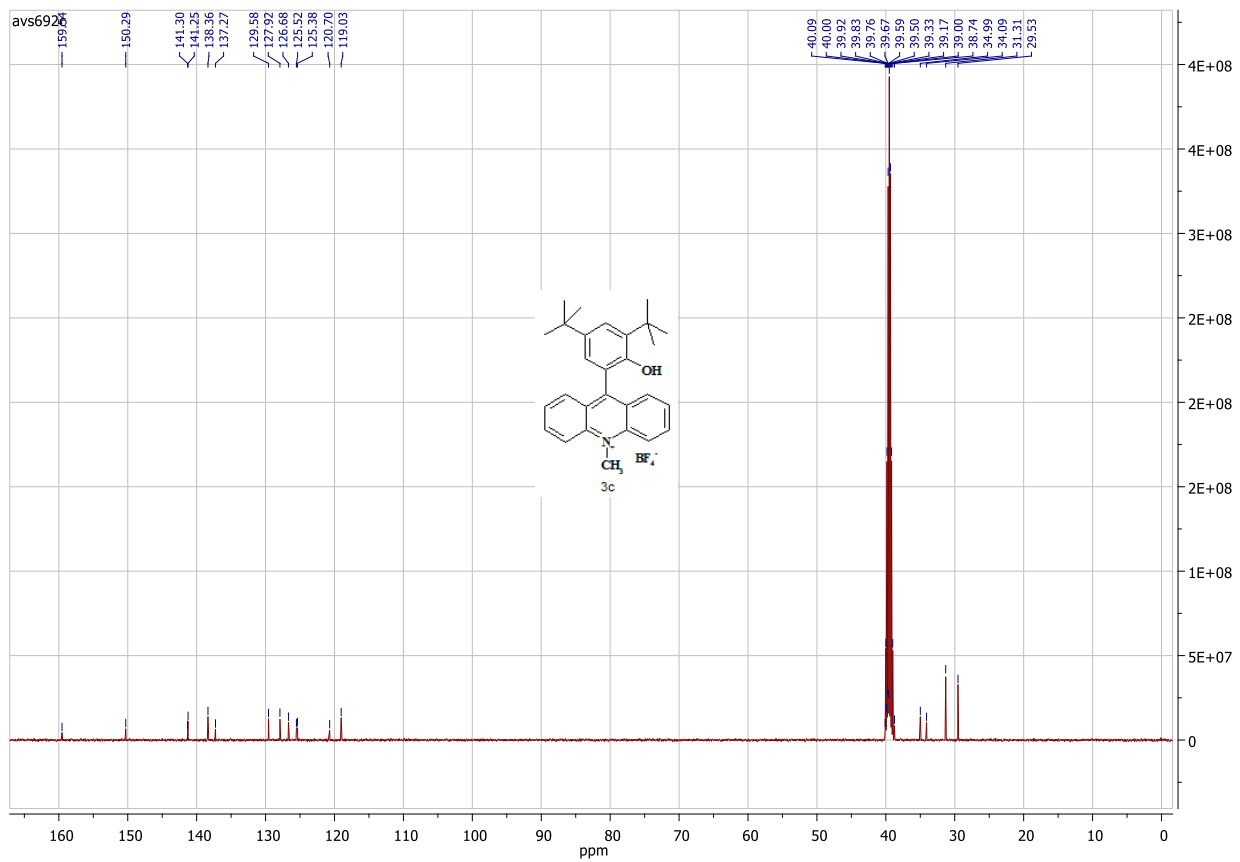
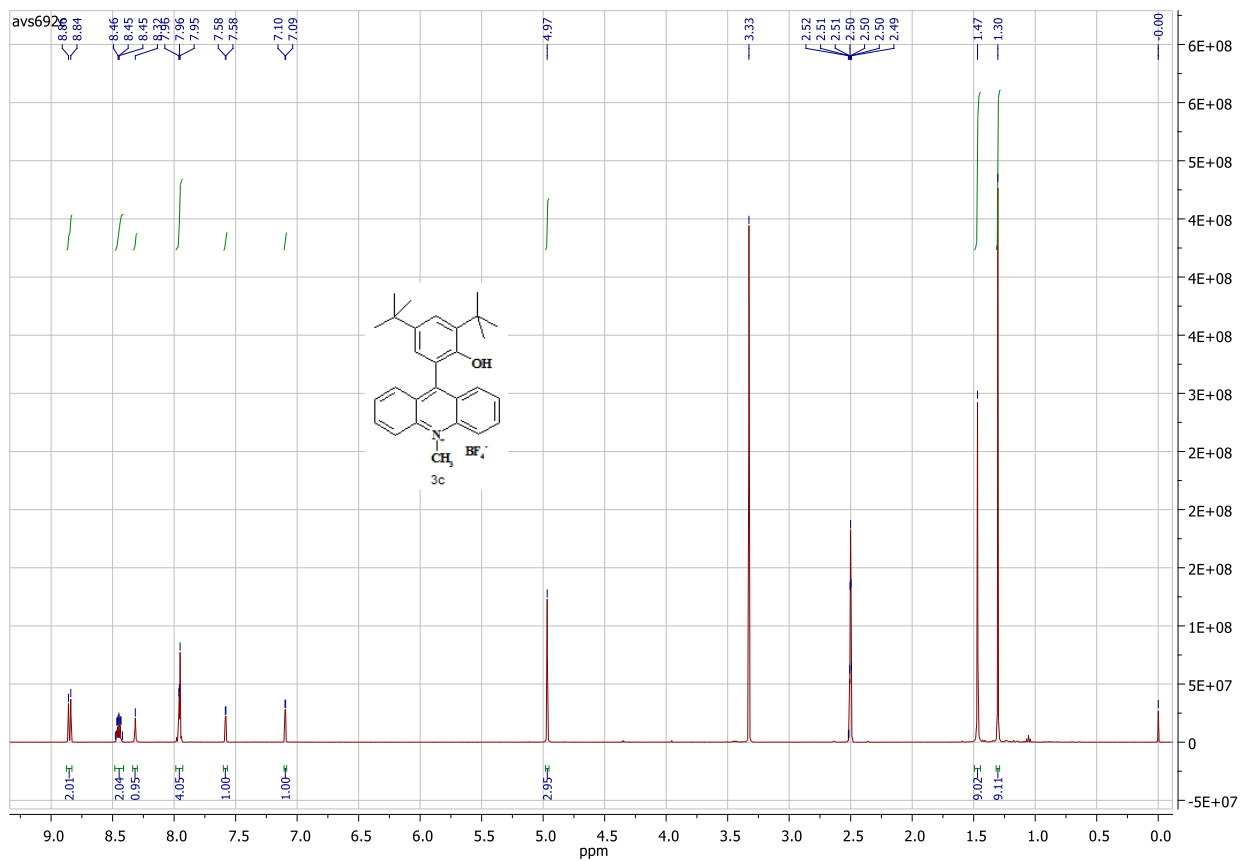
Yellow crystalline powder. 184 mg (63%). The product was identified as a compound **12** by comparing its  $^1\text{H}$  NMR spectra with its given in the literature. Satisfactory elemental analysis for C, H and N were obtained for compound **12**; none of the experimentally found percentages deviated from the theoretical values by more than 0.3%.<sup>7</sup>  $^1\text{H}$  NMR (500 MHz,  $[\text{D}_6]\text{DMSO}$ ):  $\delta$  14.18 (s, 1H), 8.79 (s, 1H), 8.11-8.10 (m, 2H), 7.87 (s, 2H), 7.67-7.61 (m, 3H), 2.24 (s, 6H).  $^{13}\text{C}$  NMR (126 MHz,  $[\text{D}_6]\text{DMSO}$ ):  $\delta$  155.5, 132.4, 130.4, 128.9, 127.6, 123.6, 16.8 ppm. FT-IR (DRA,  $\text{cm}^{-1}$ ): 410, 428, 456, 491, 508, 586, 634, 687, 701, 738, 773, 896, 949, 970, 997, 1030, 1050, 1089, 1184, 1208, 1257, 1331, 1384, 1411, 1429, 1450, 1492, 1516, 1552, 1679, 1784, 2913, 2945, 3077, 3169.

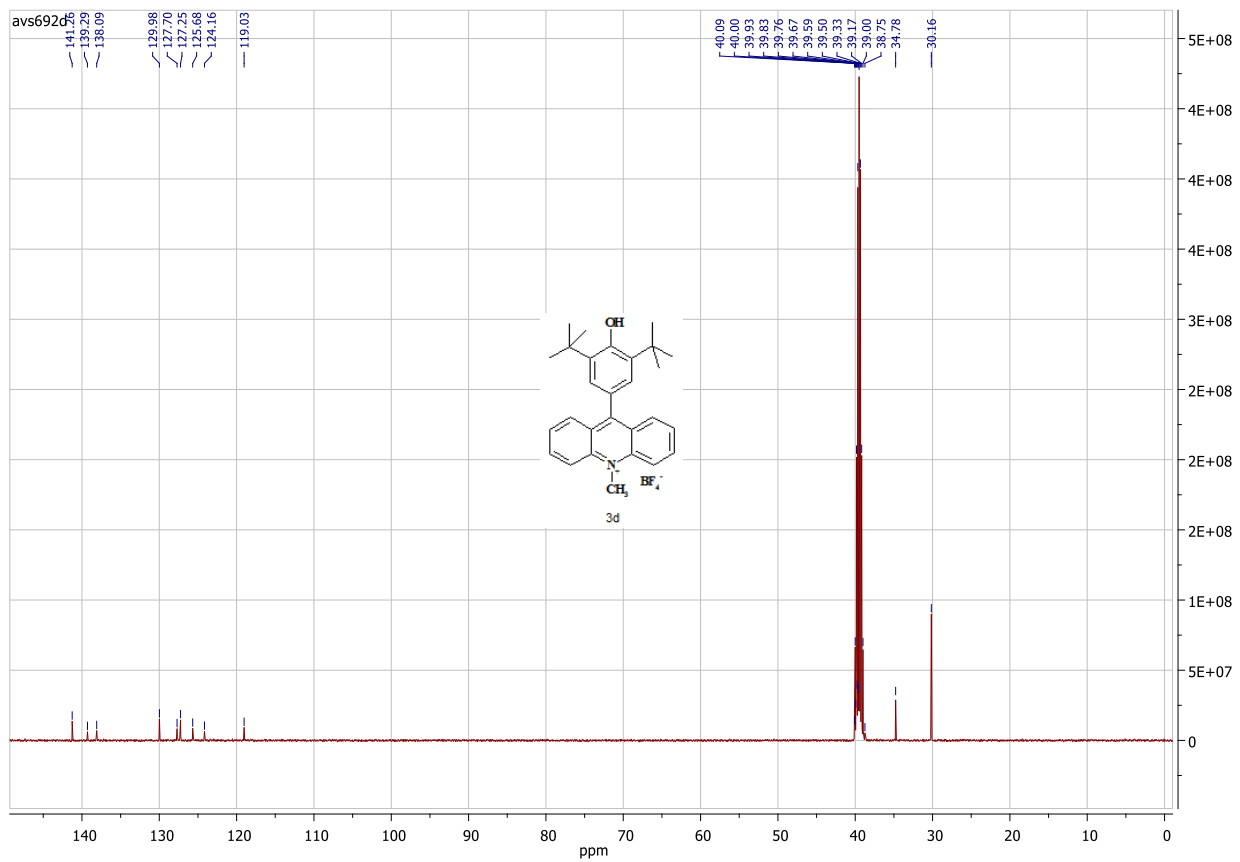
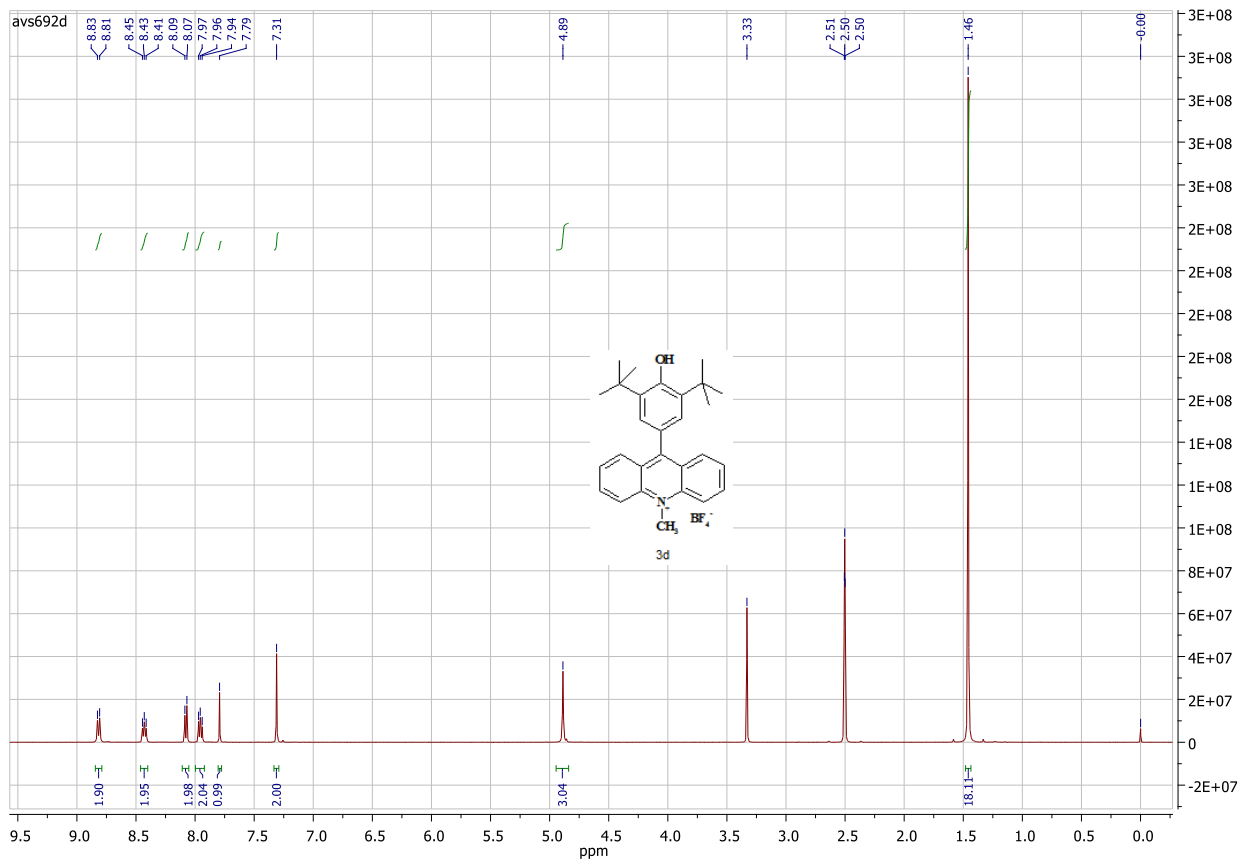
## 7. Spectra

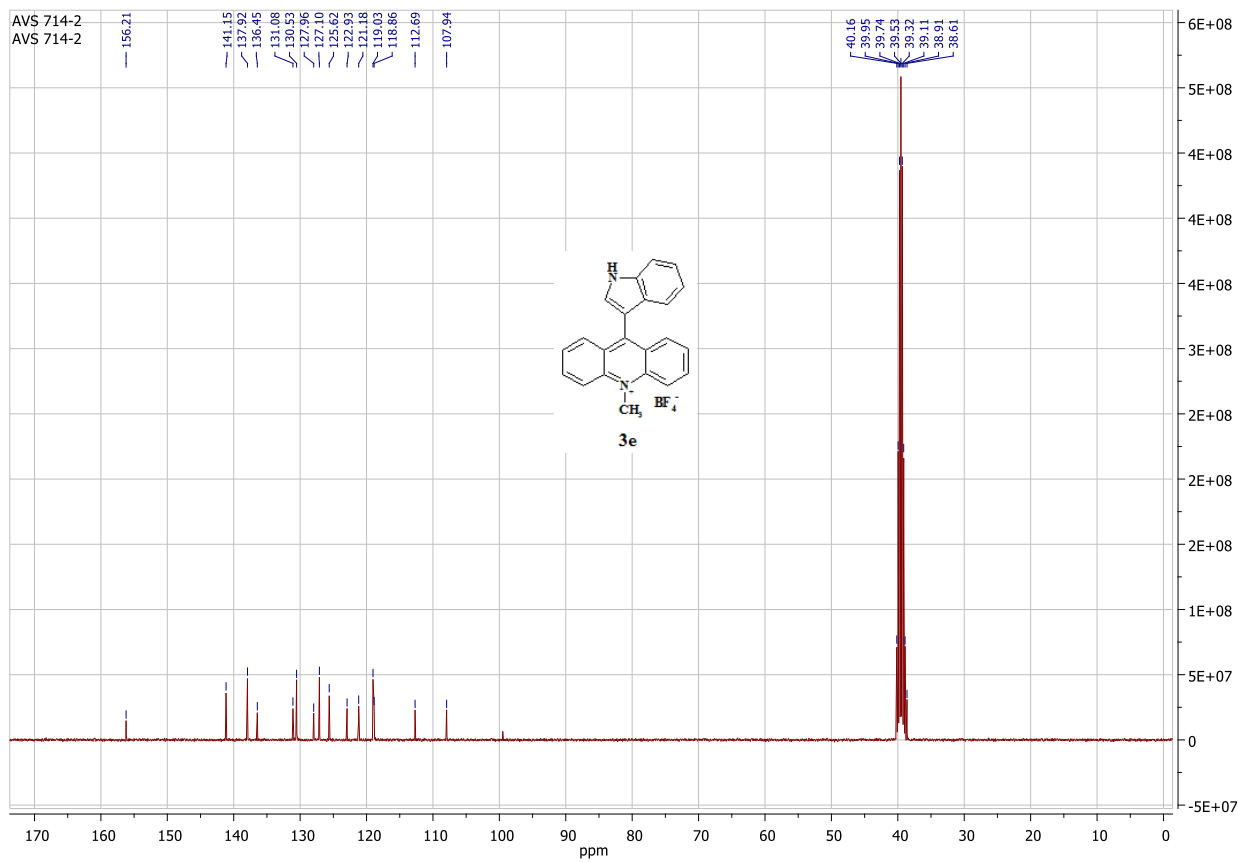
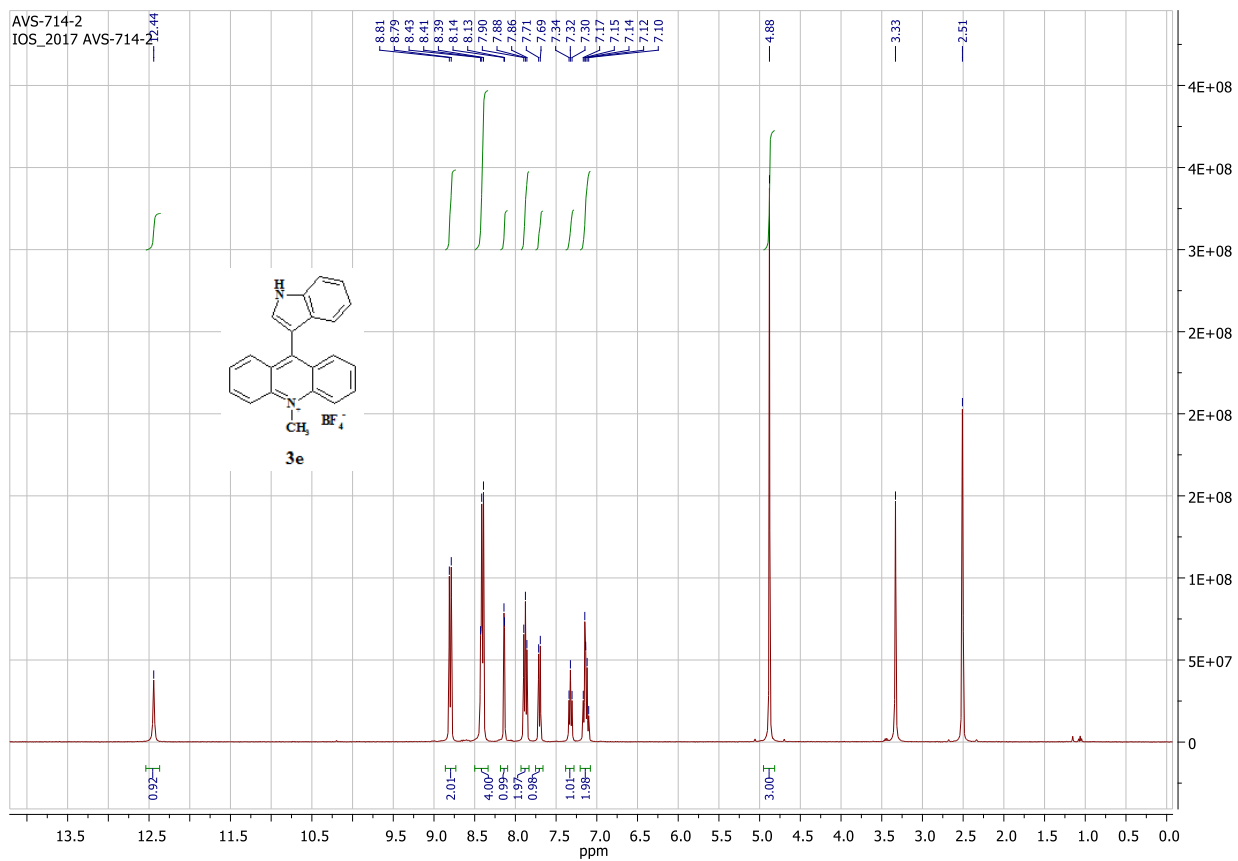


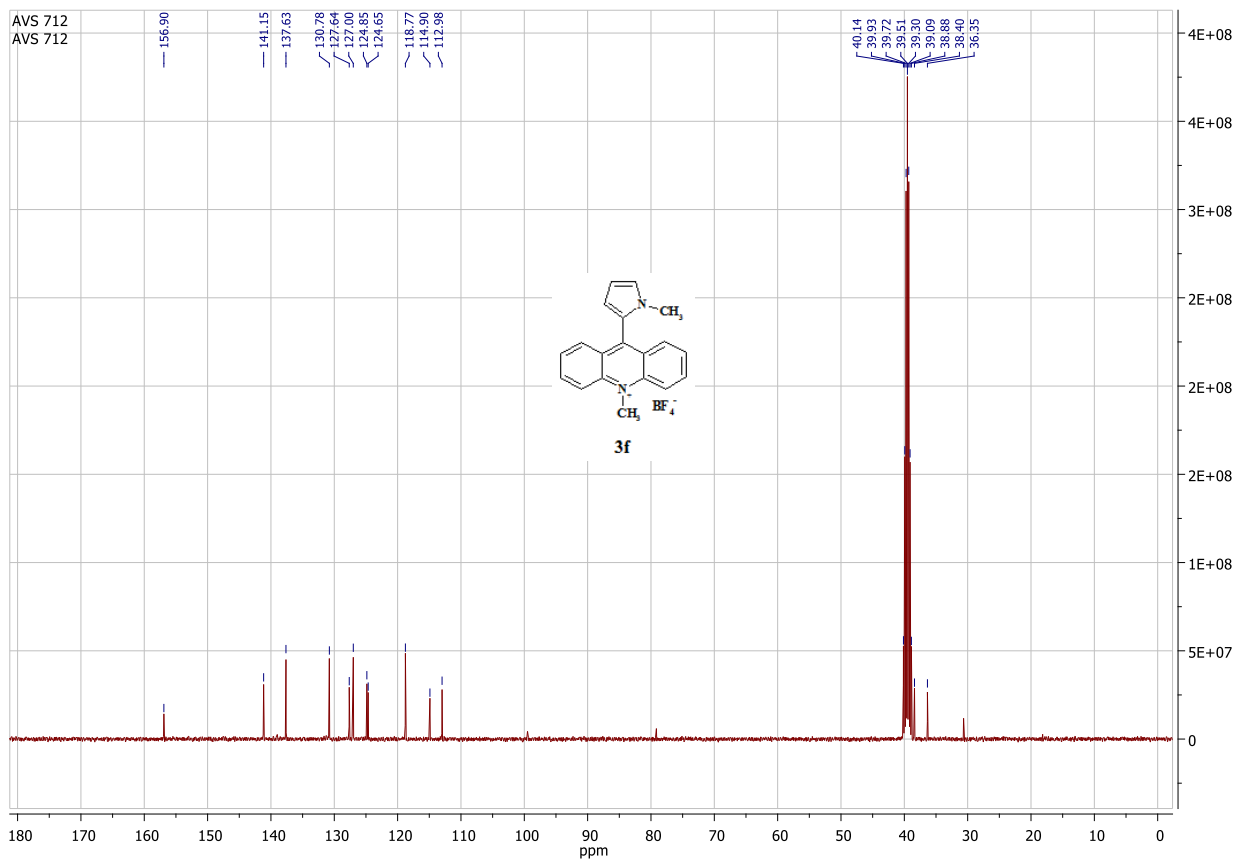
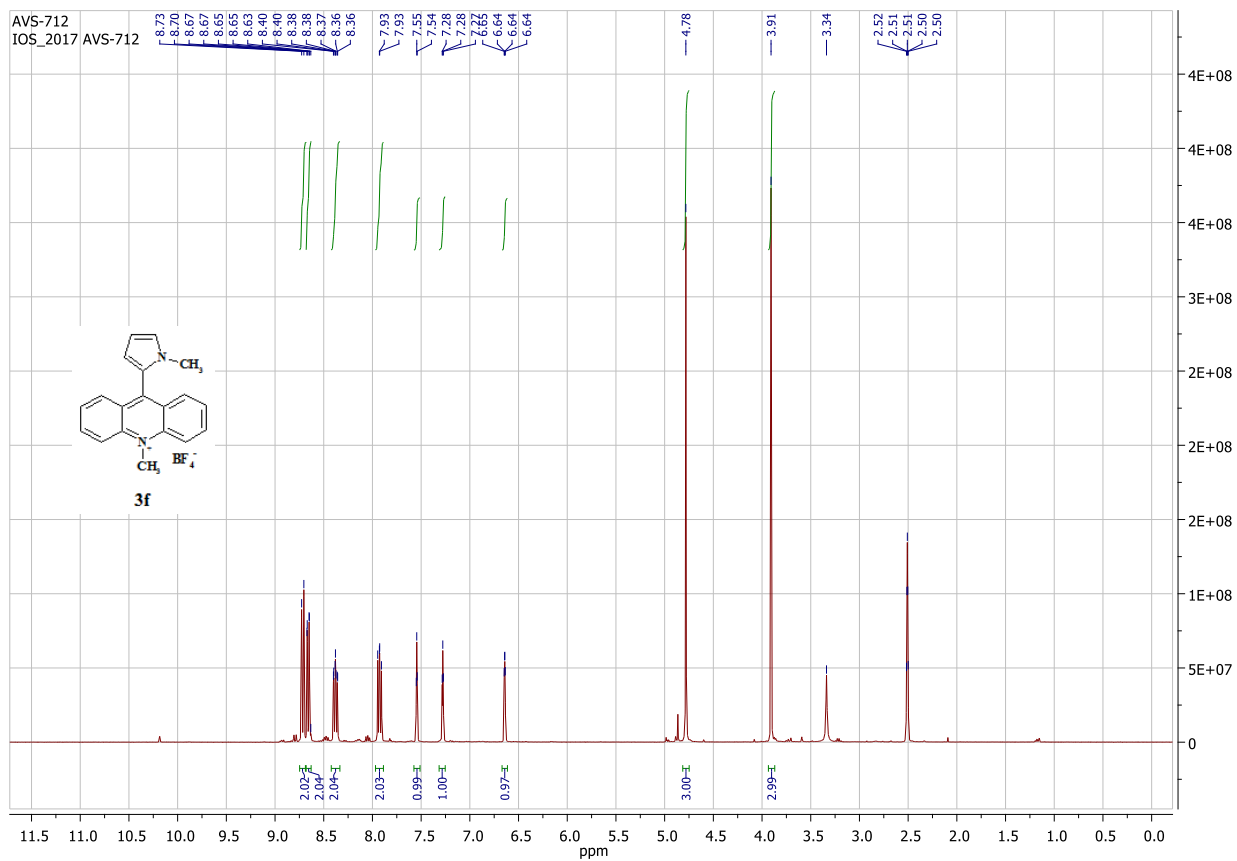


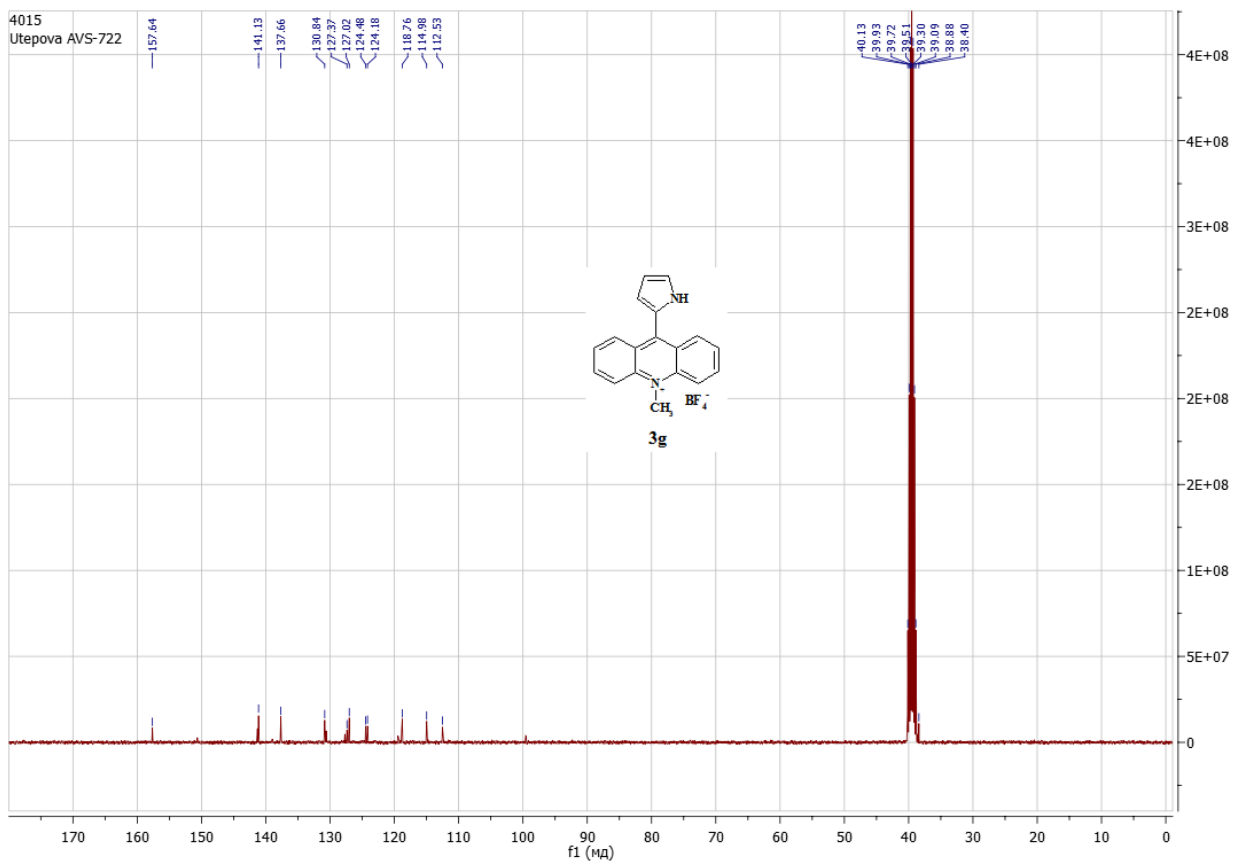
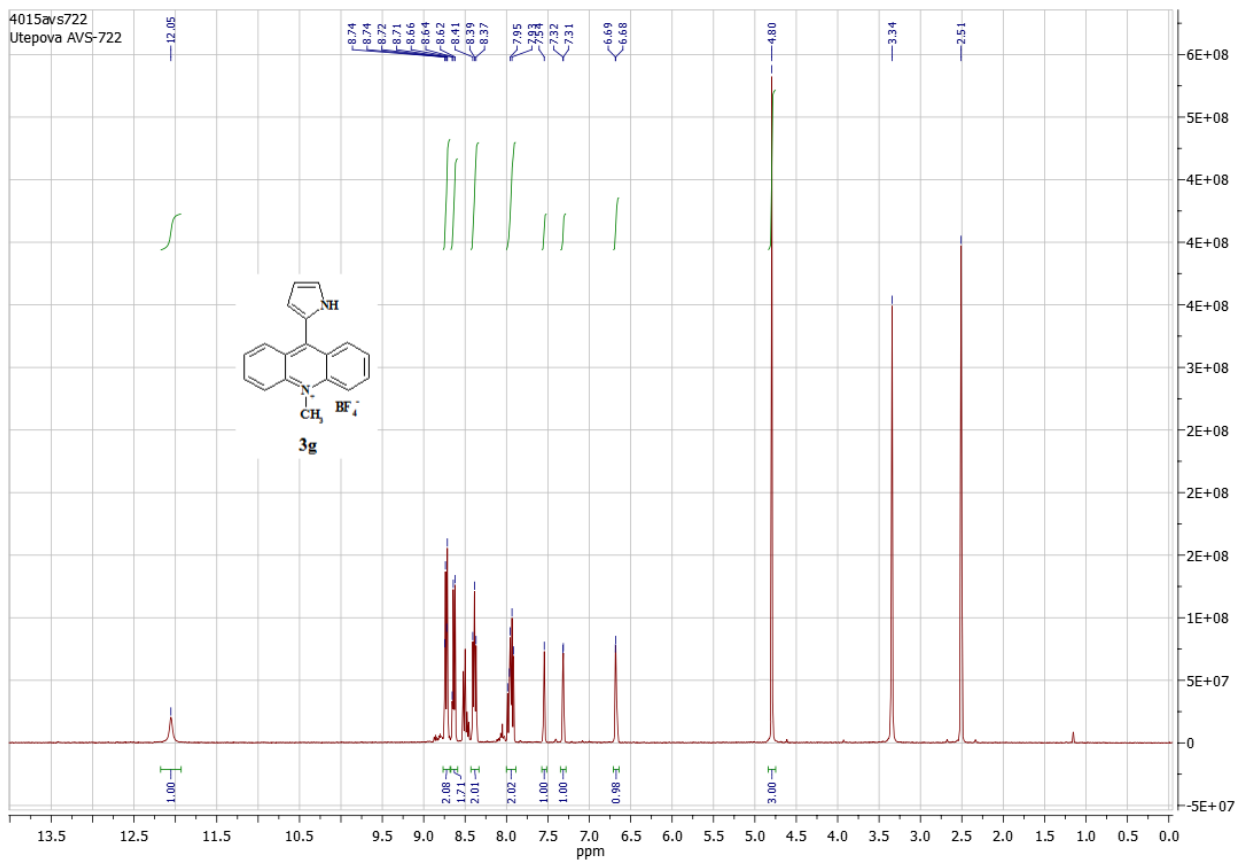


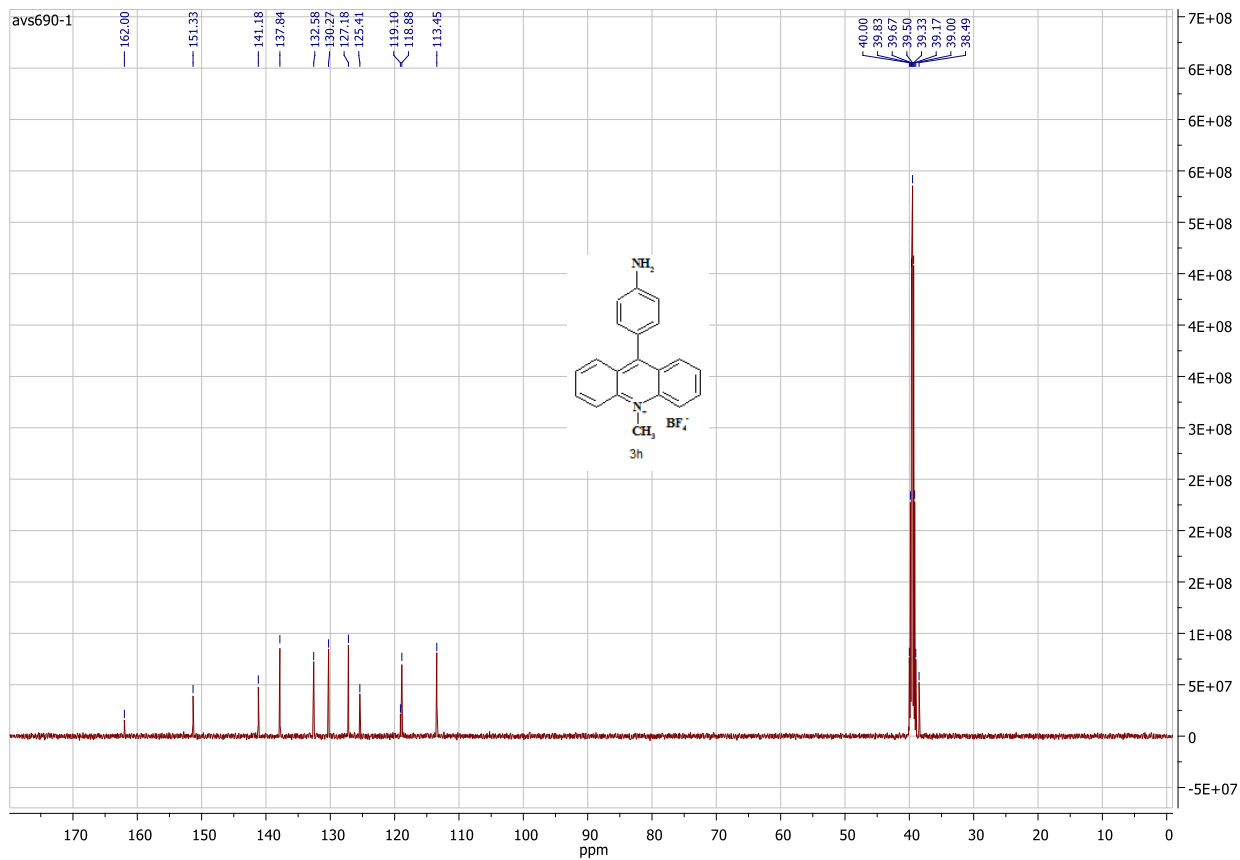
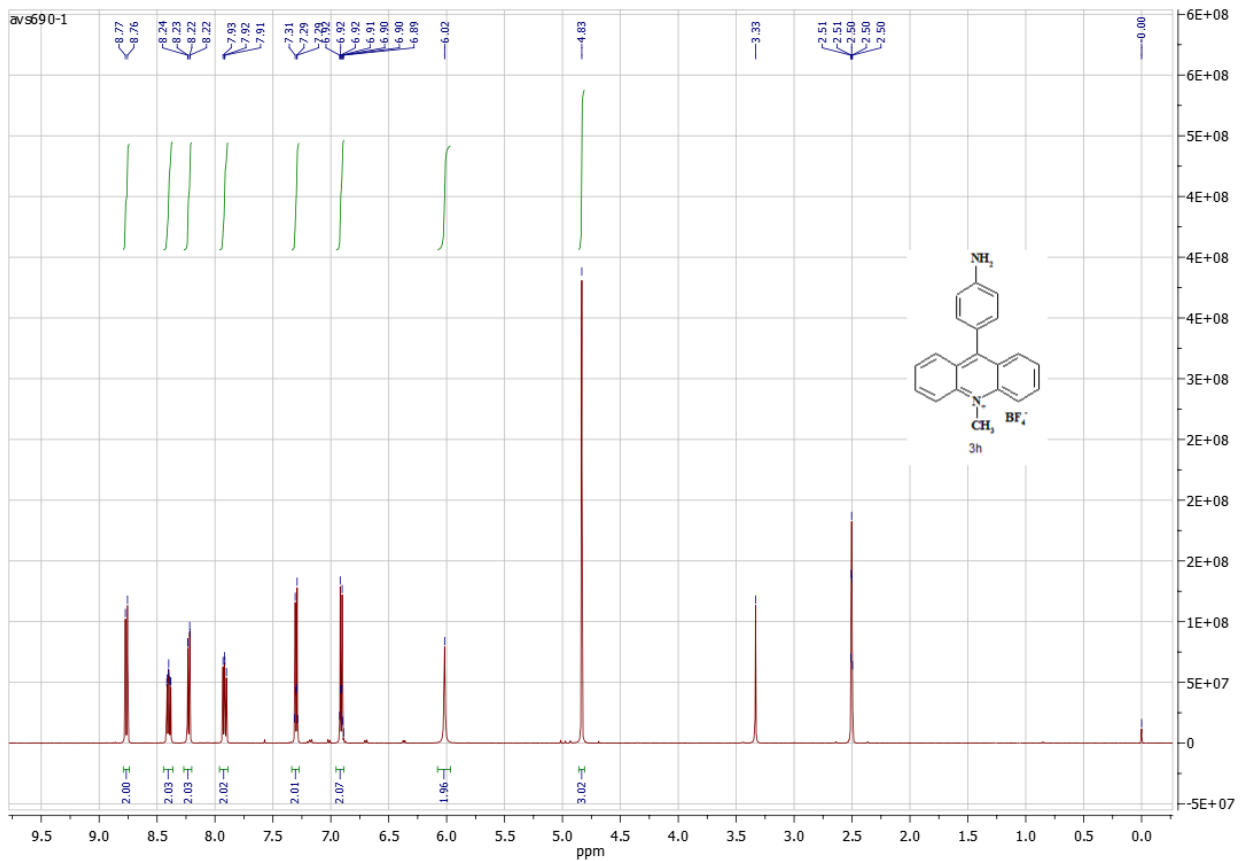


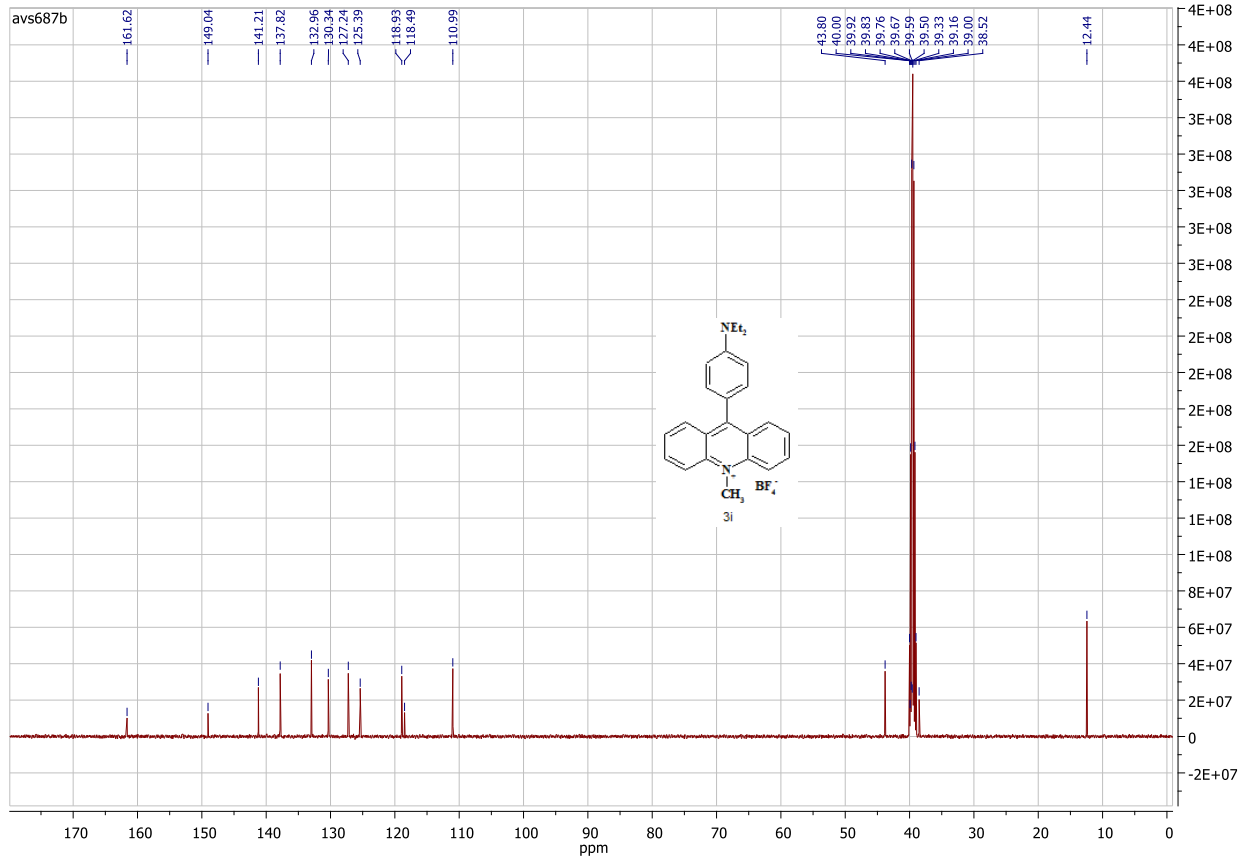
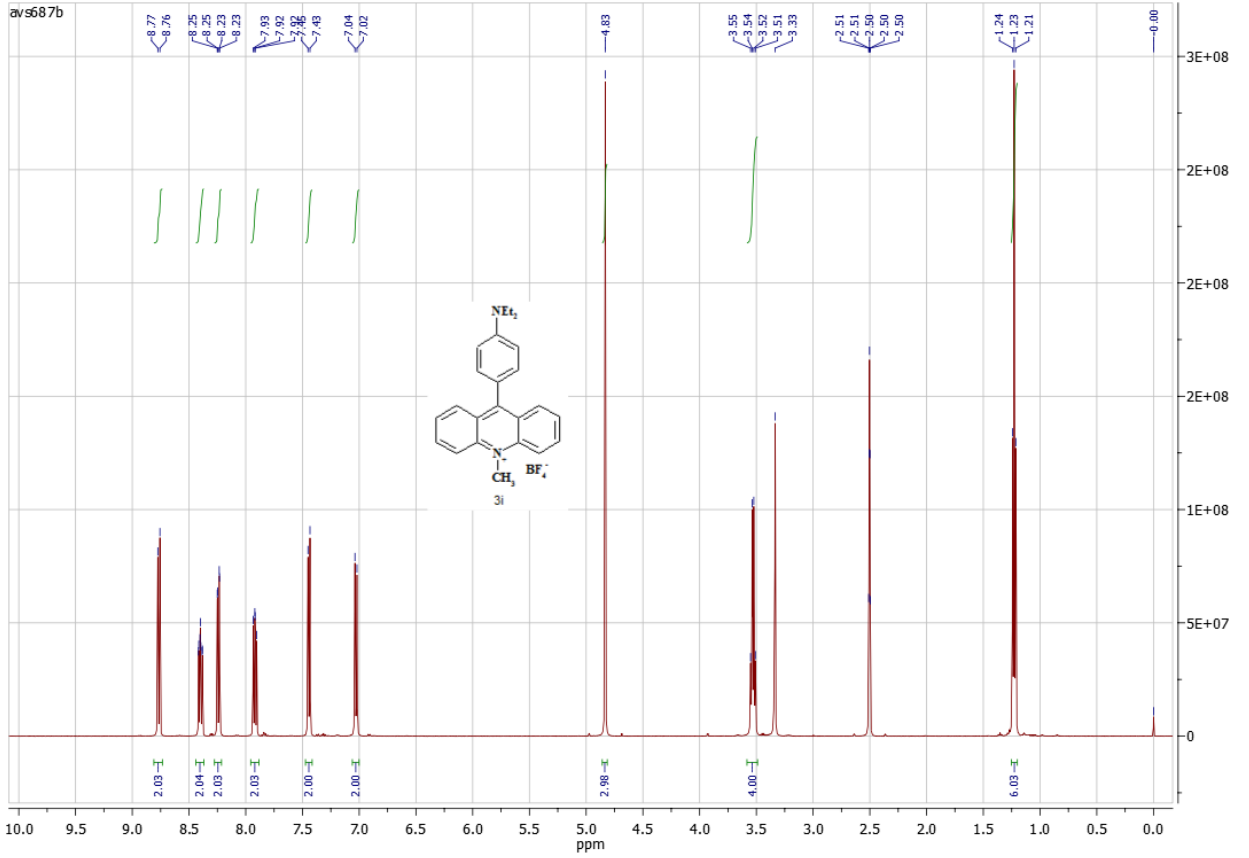


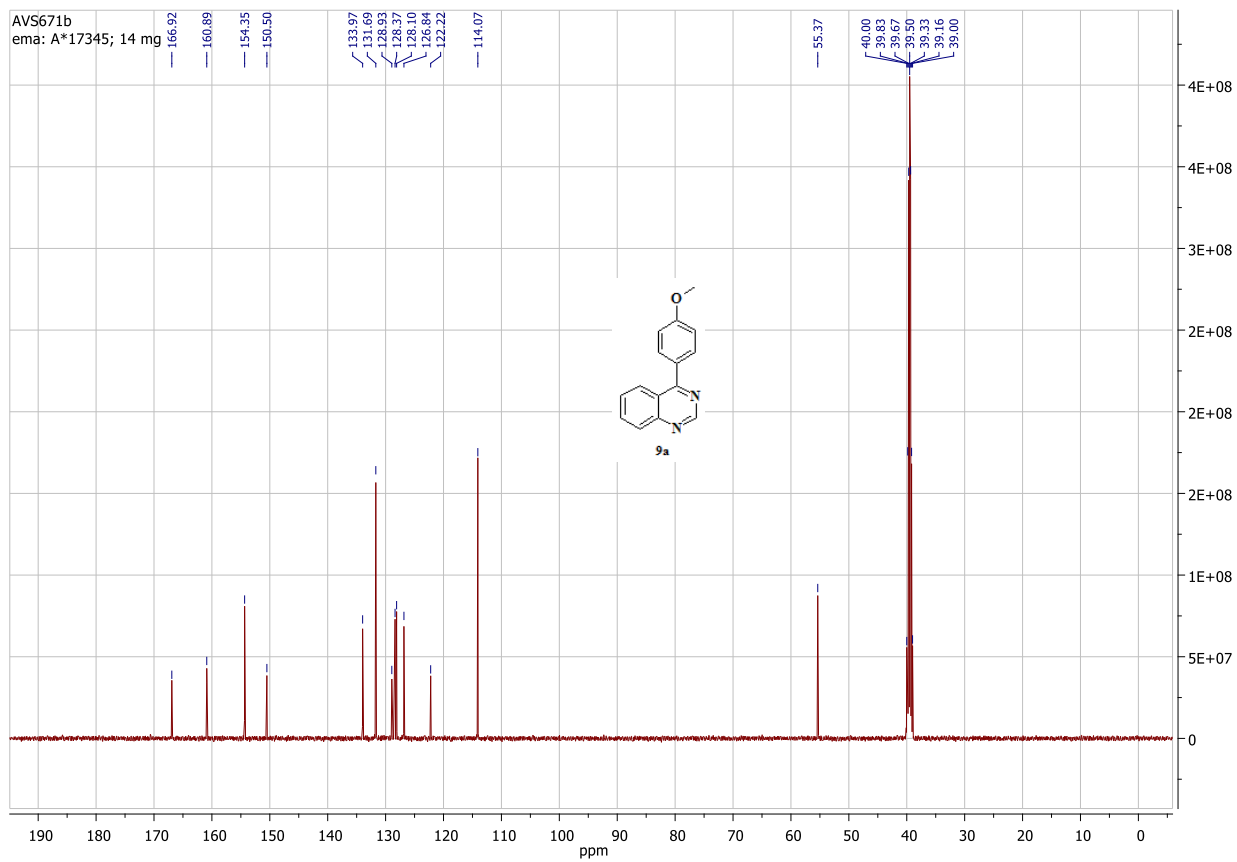
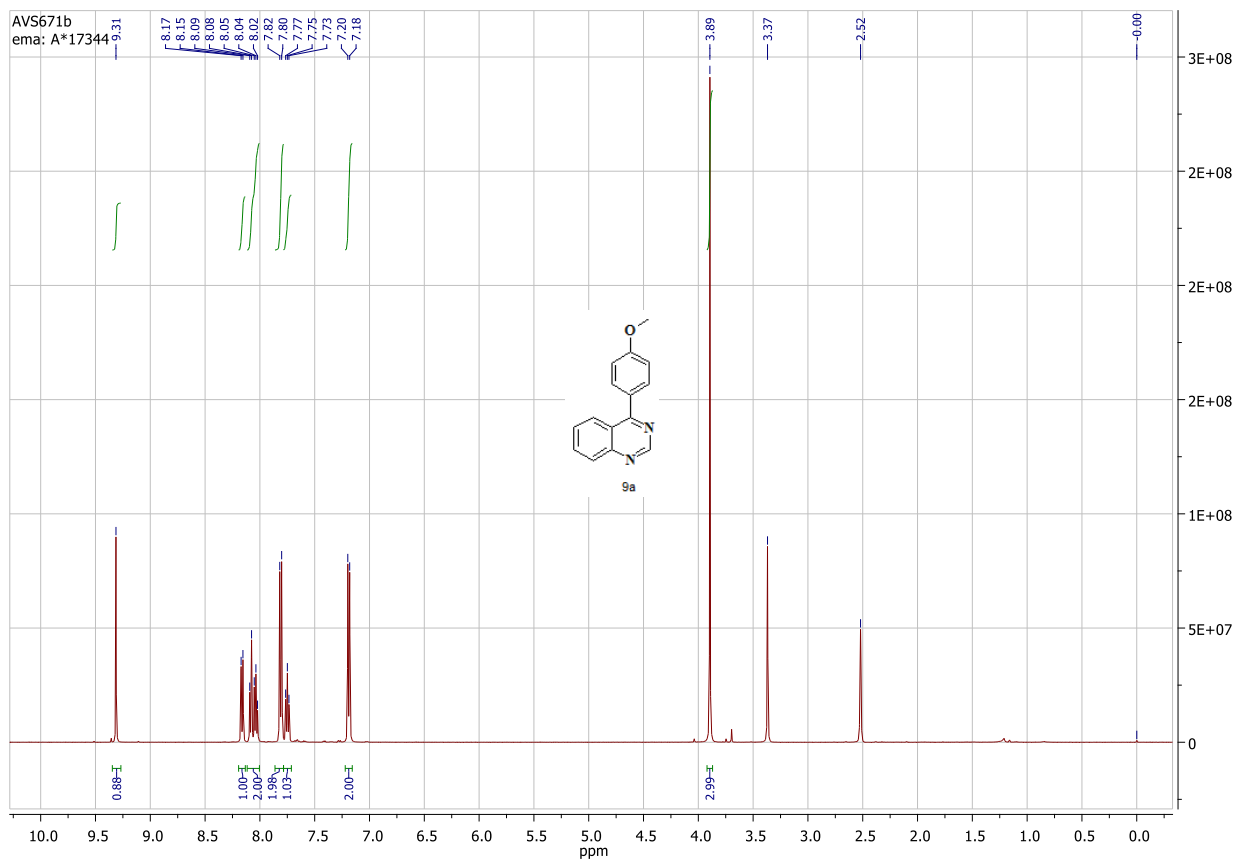




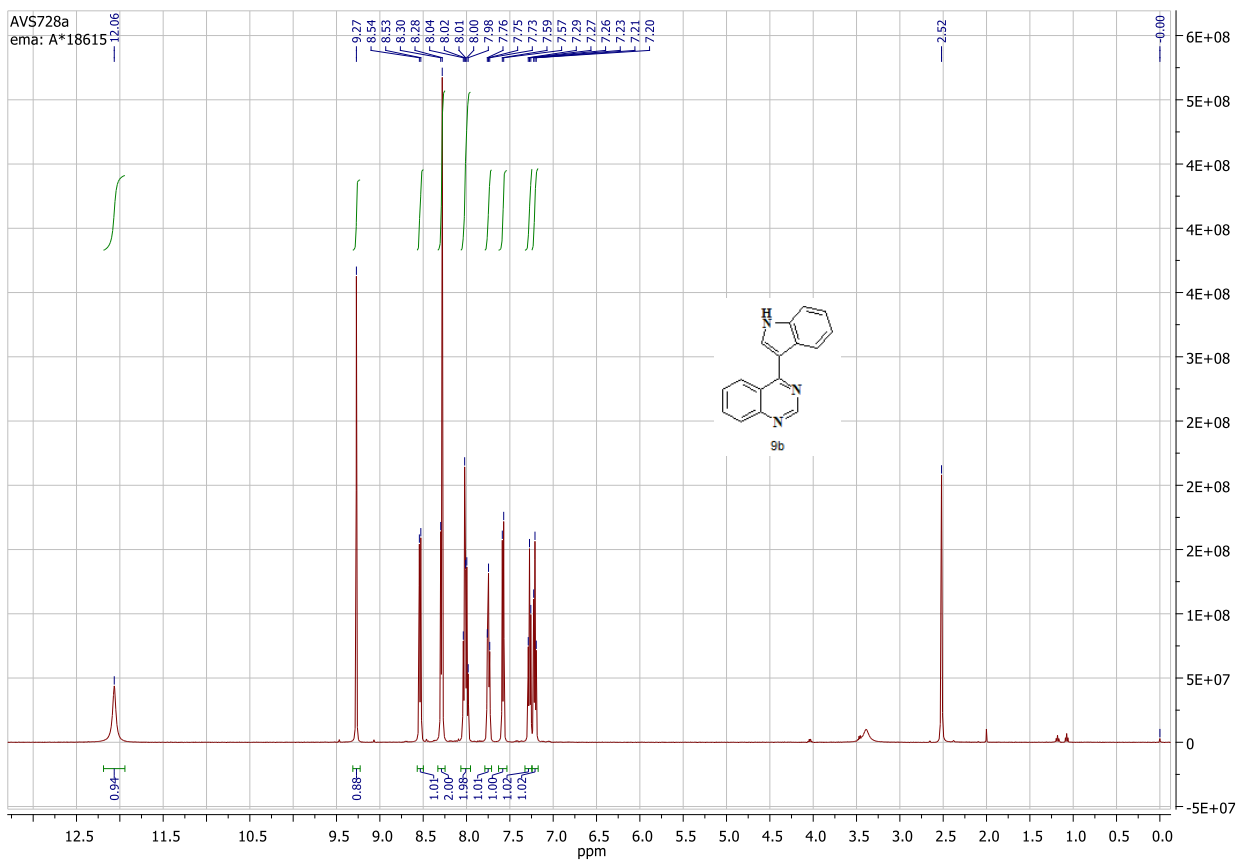
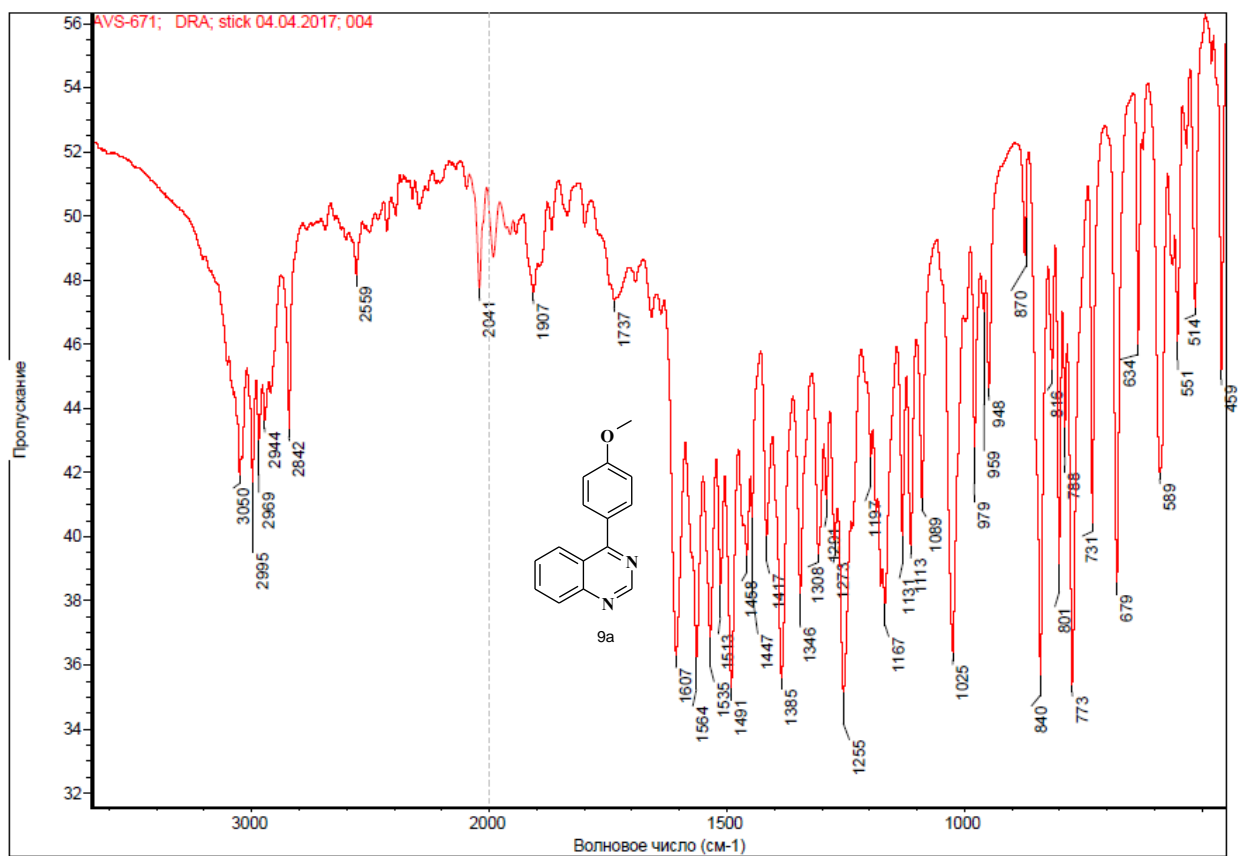


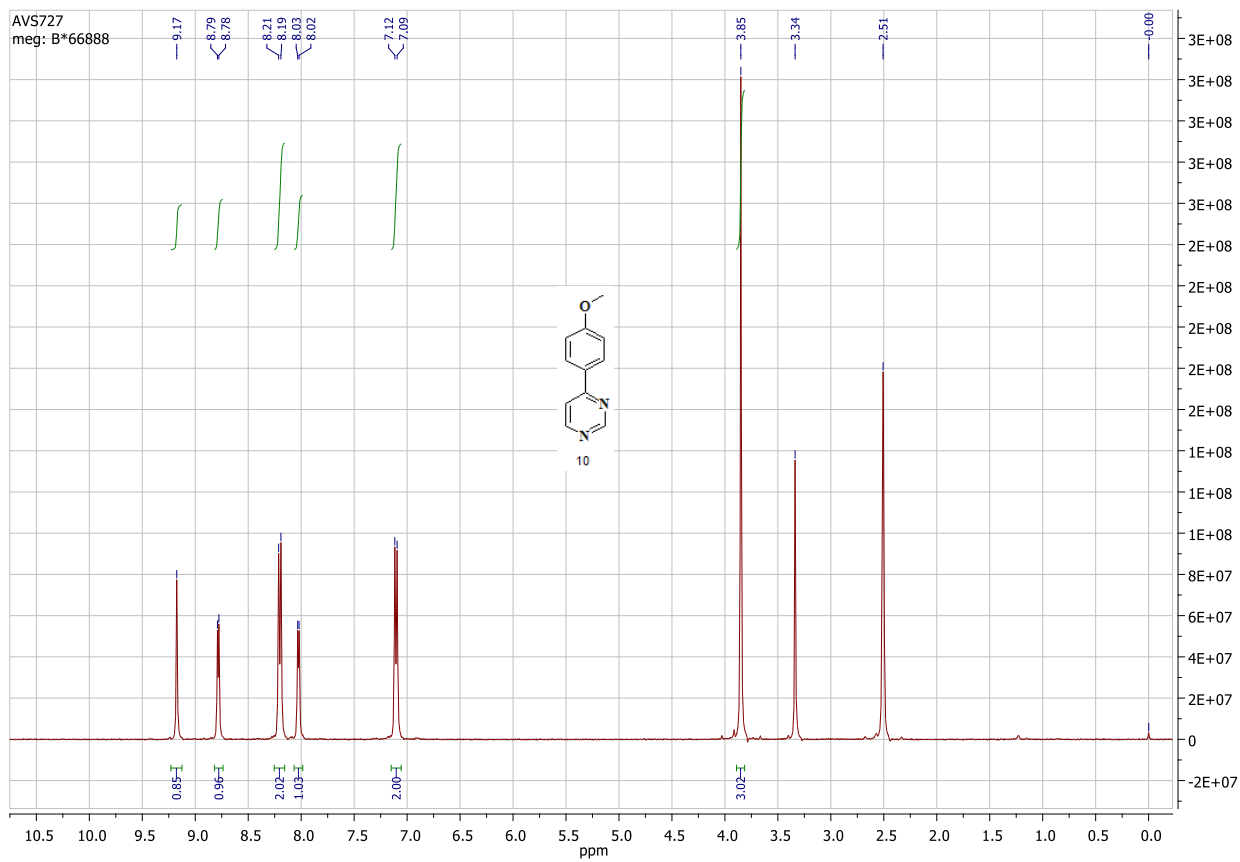
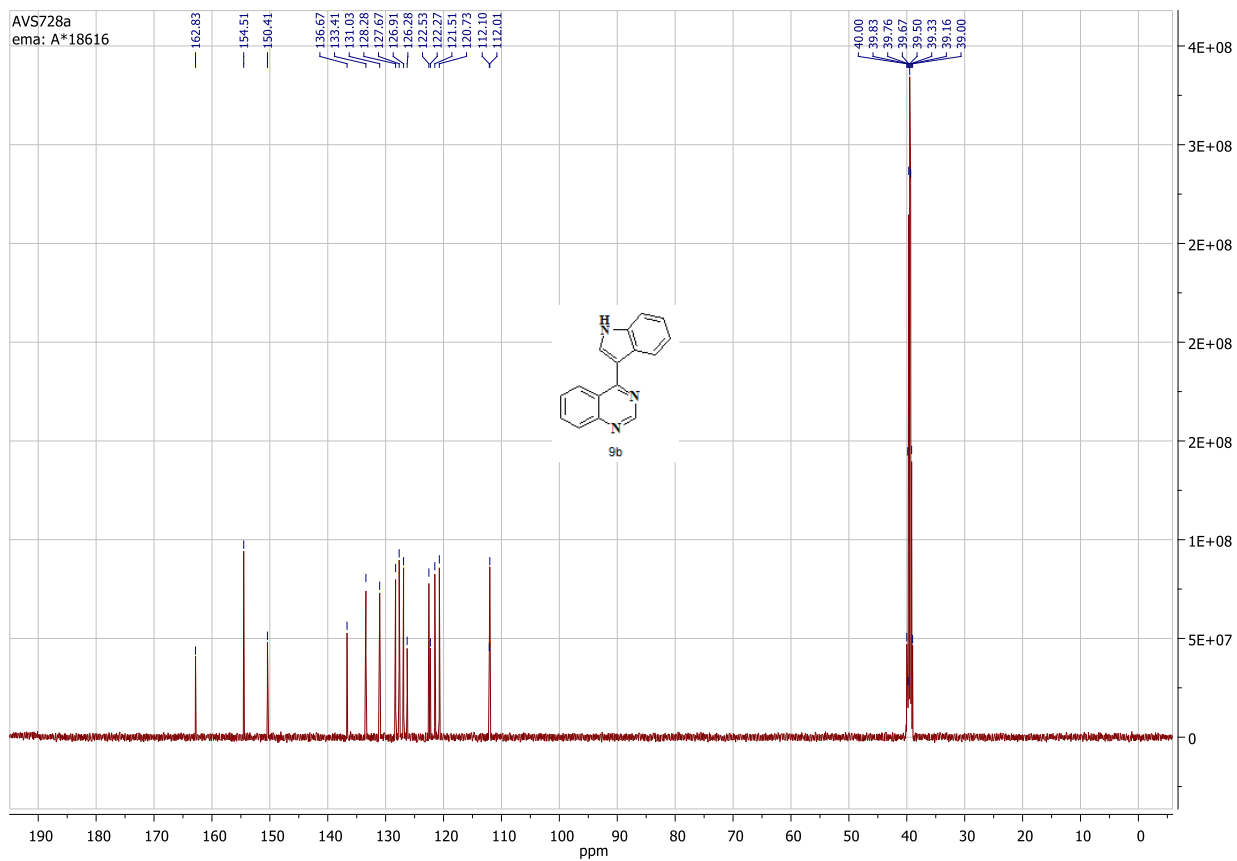


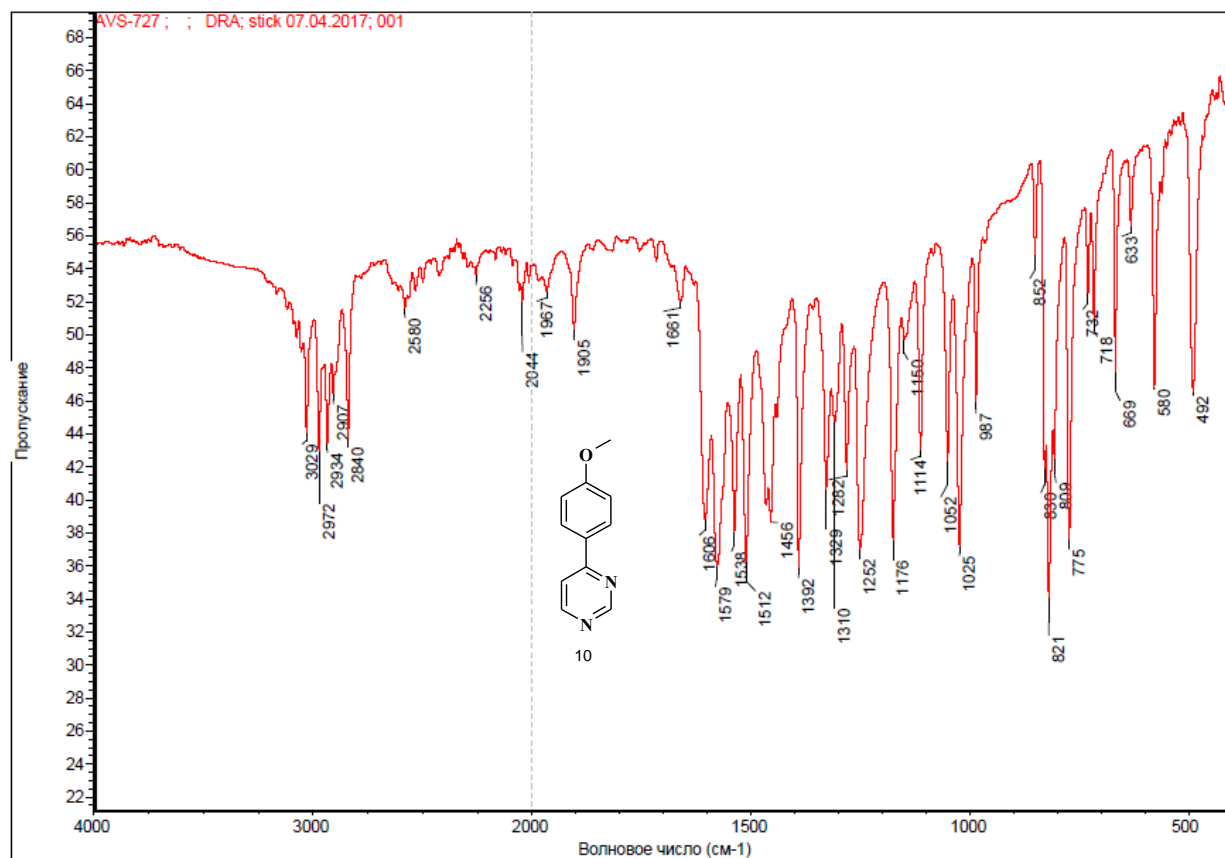
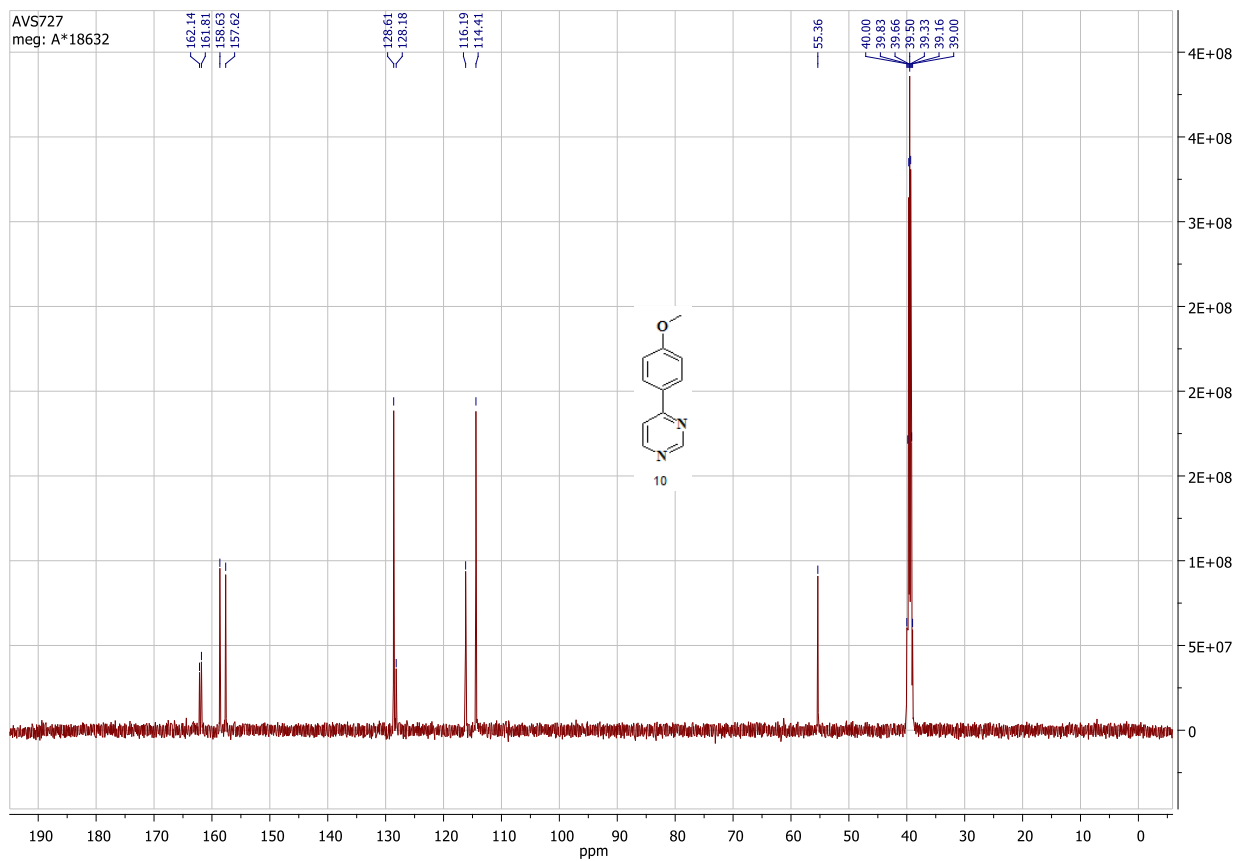


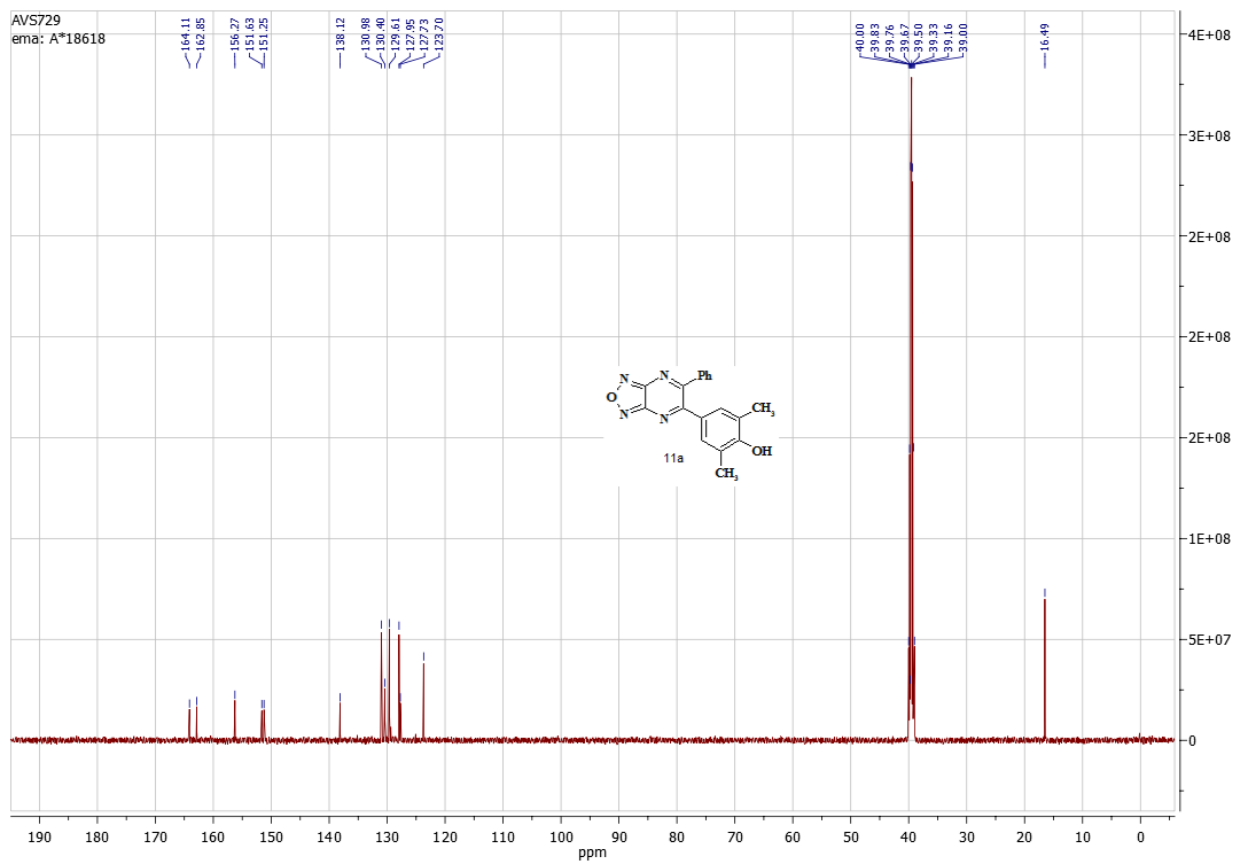
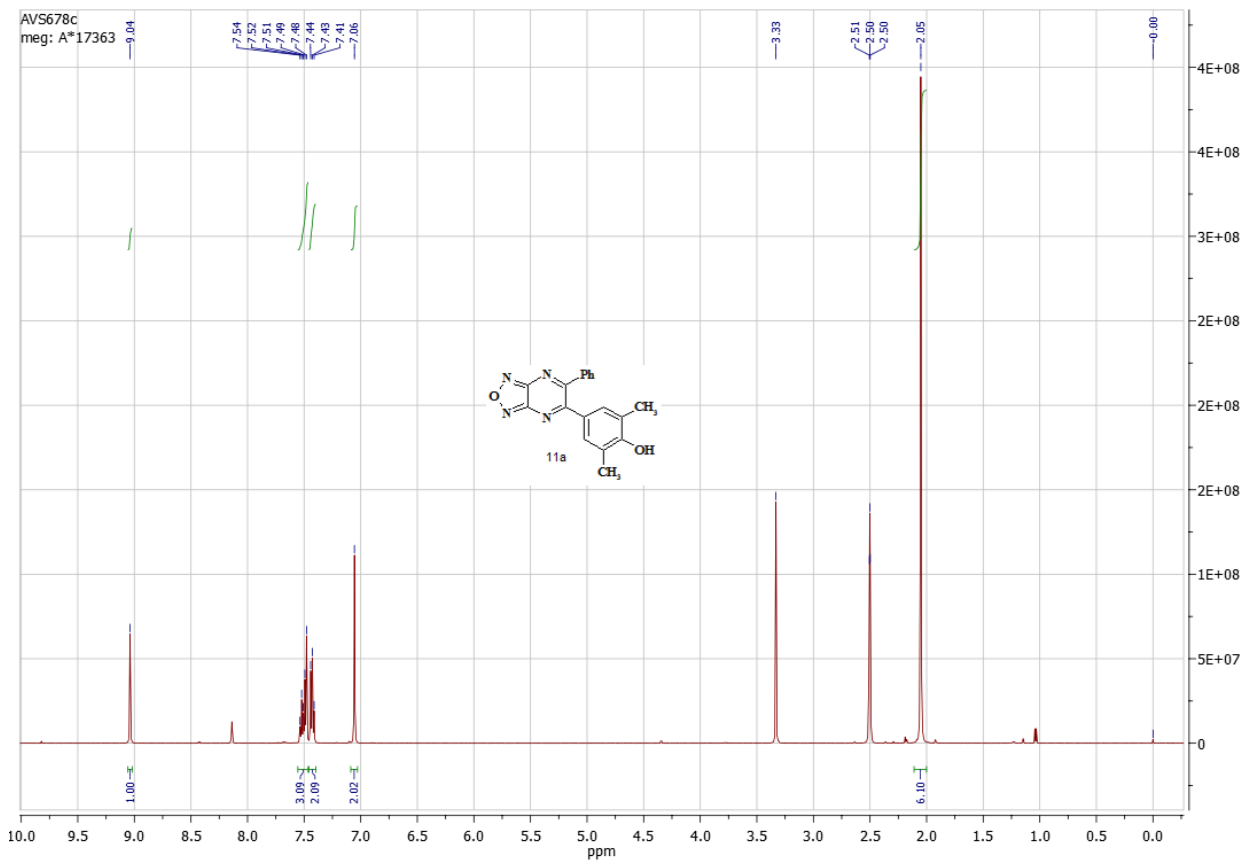


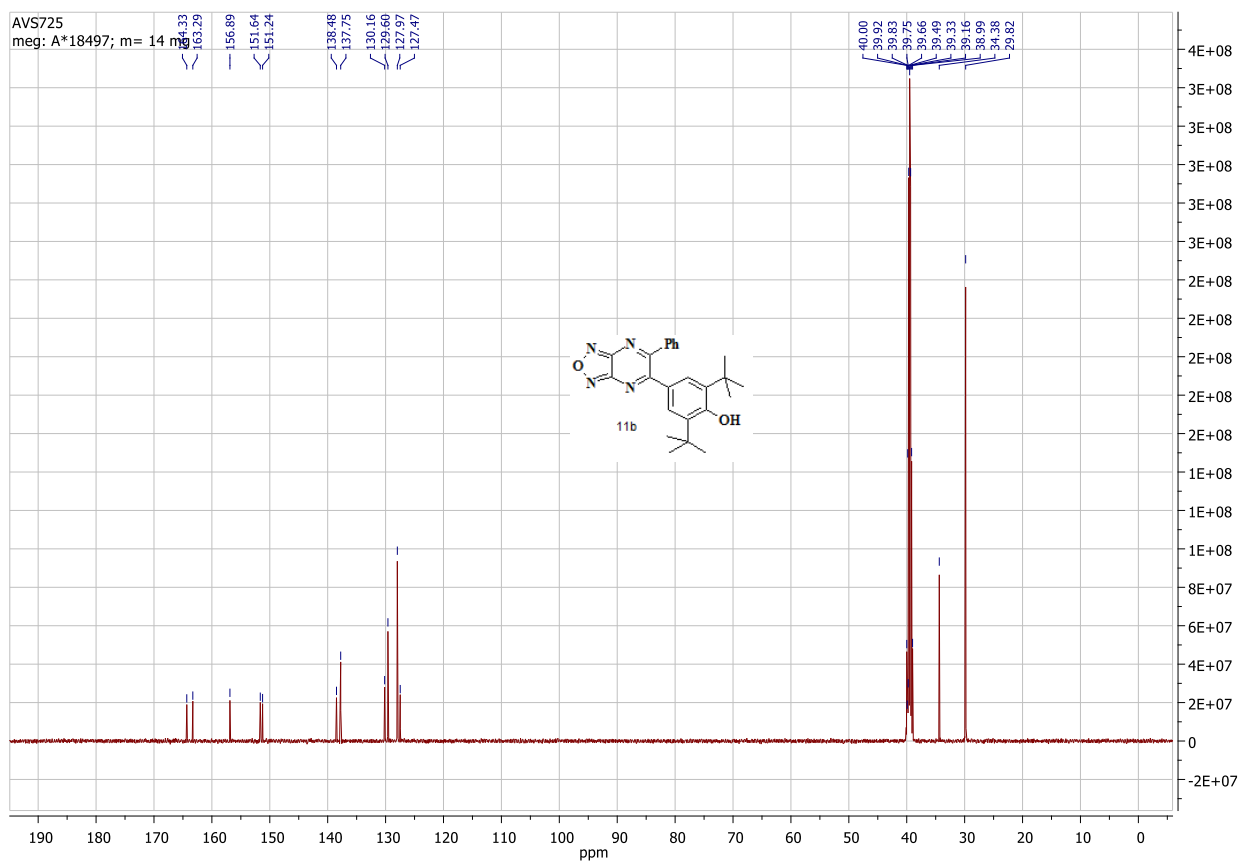
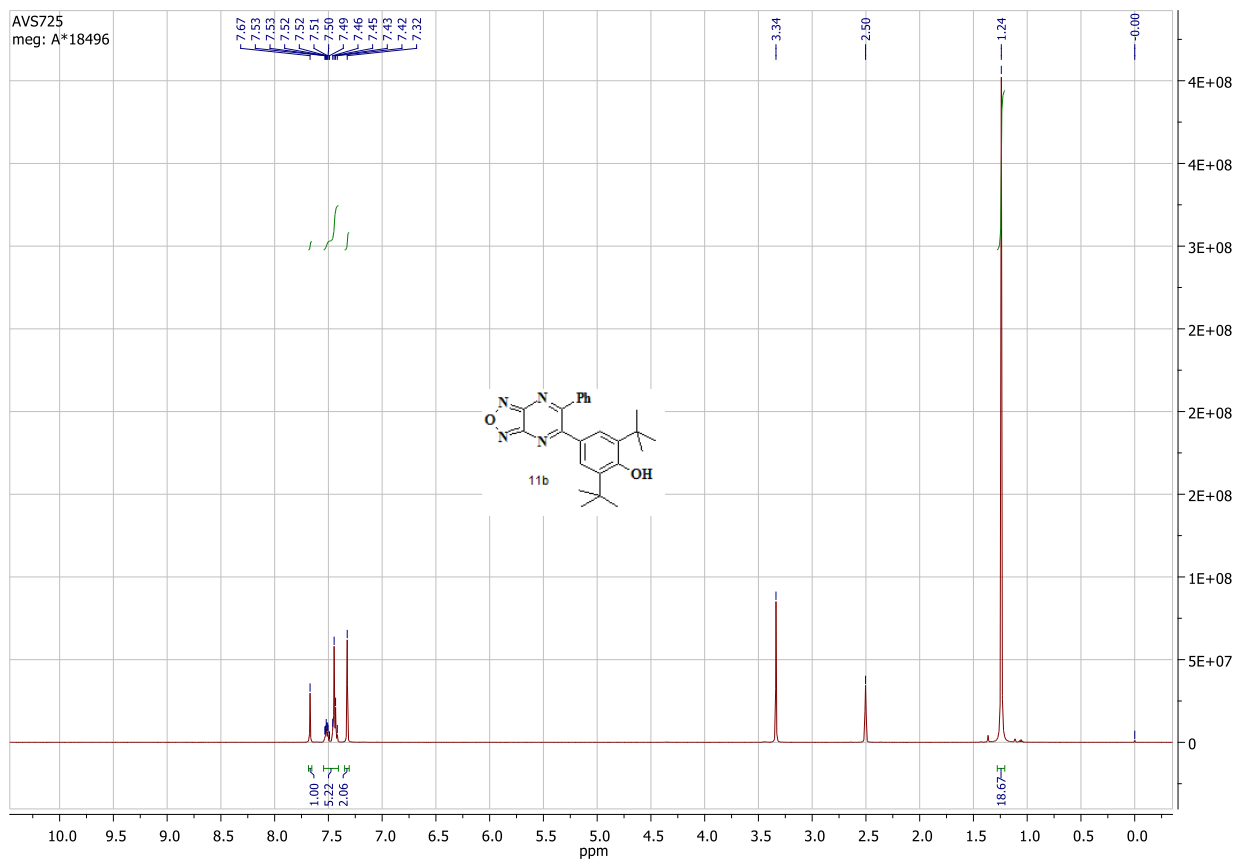


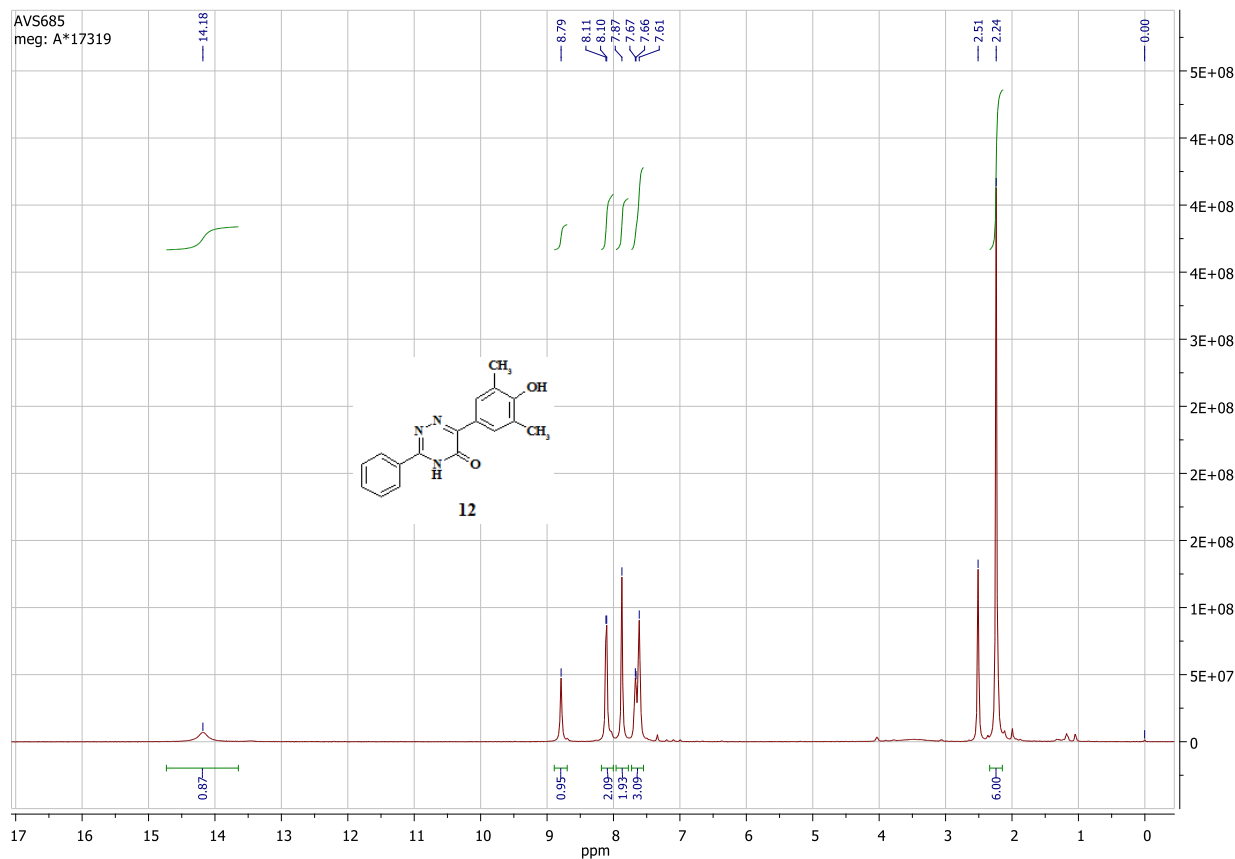
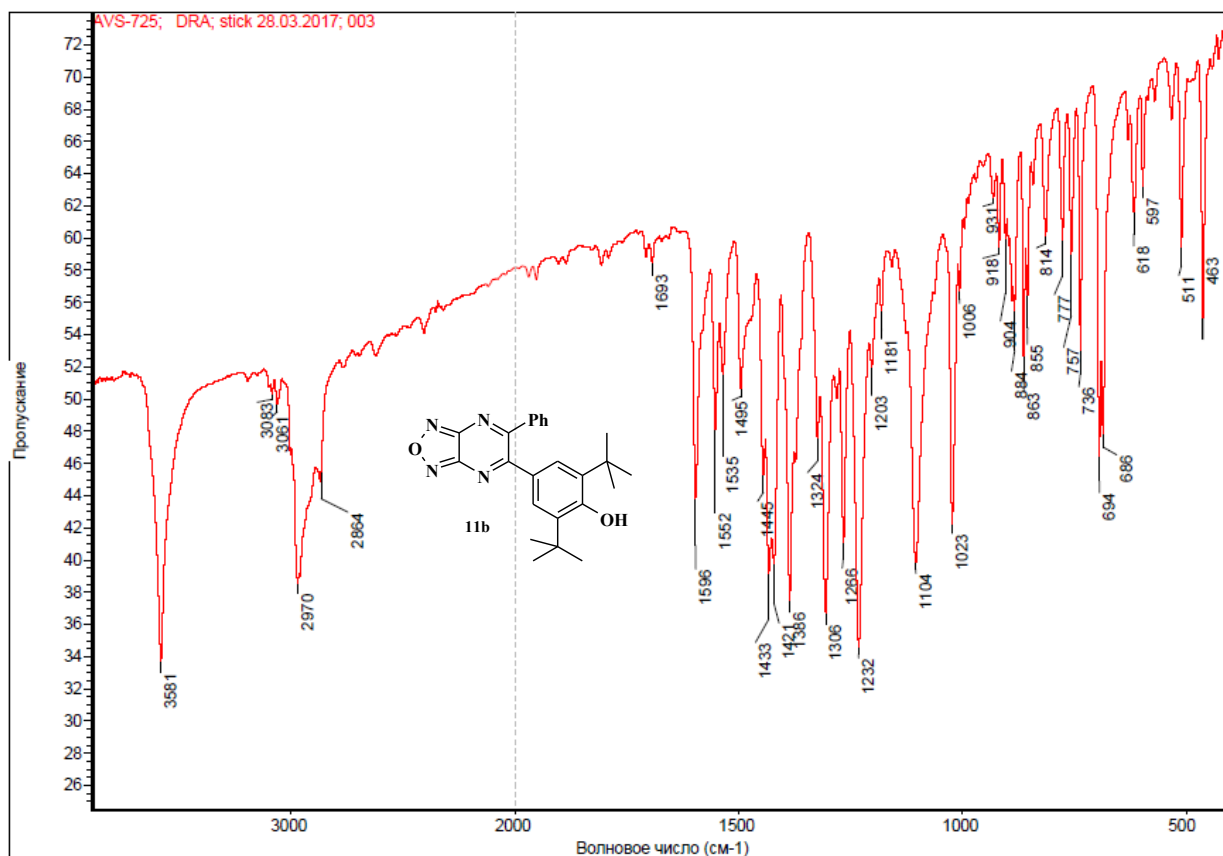


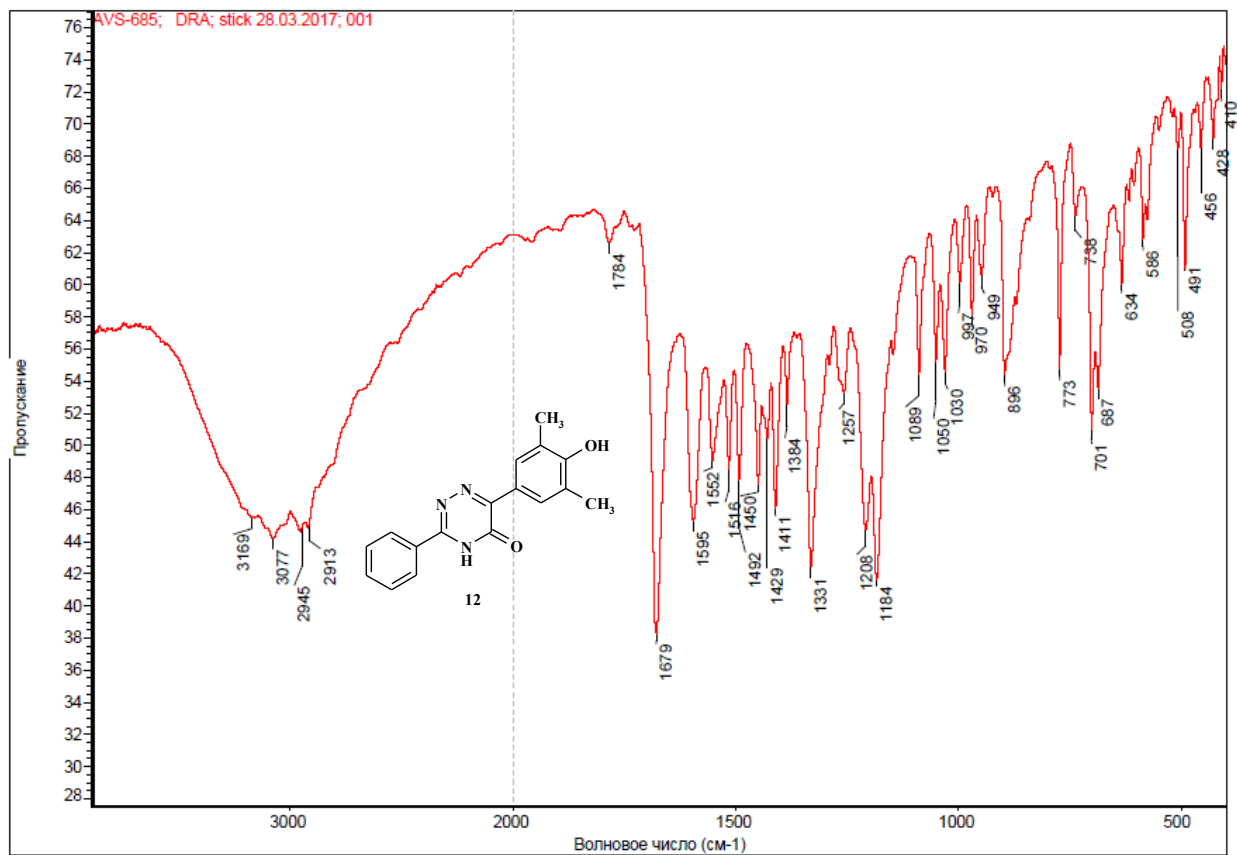
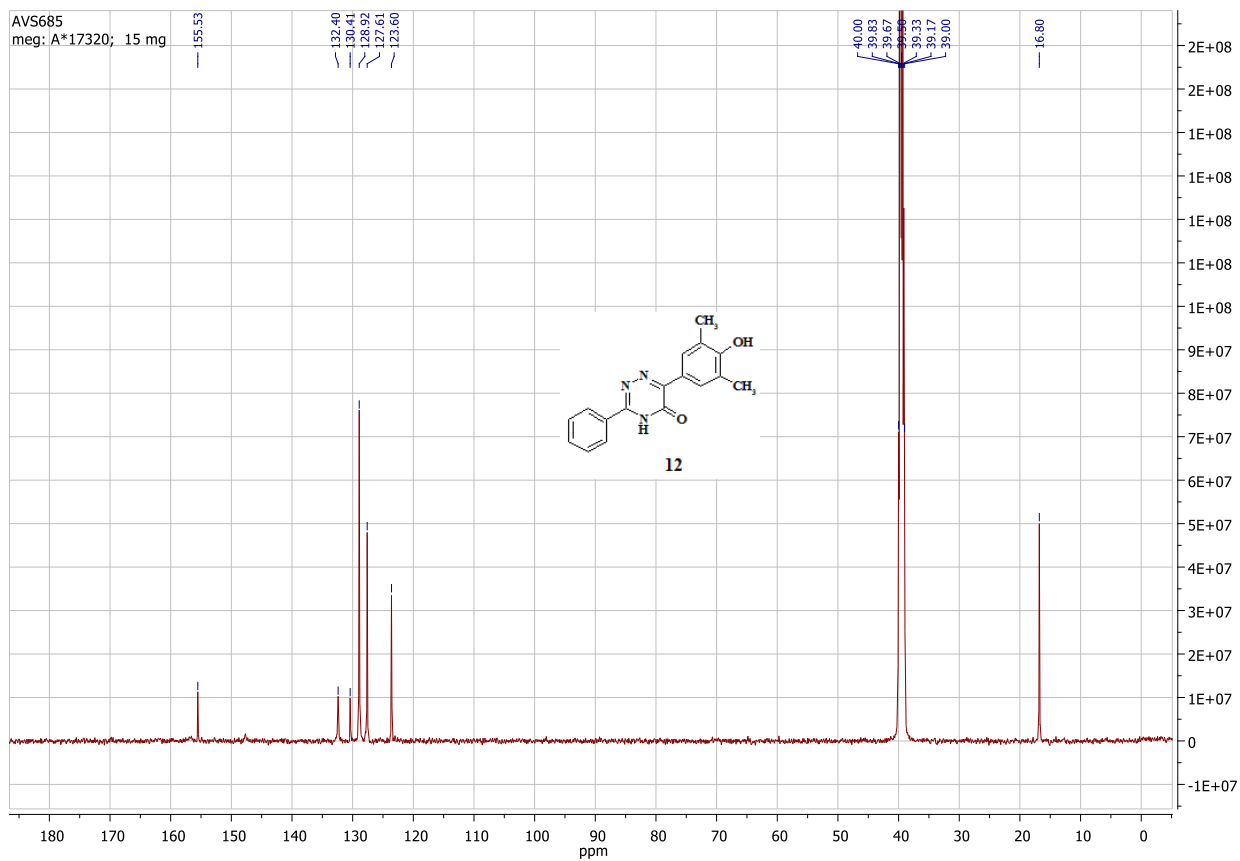












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