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Aerobic oxidative C–H/C–H coupling of azaaromatics with indoles and pyrroles in the presence of TiO_2 as a photocatalyst

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Supporting Information

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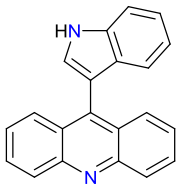
1. Synthesis of compounds 6a-e and 8a-e

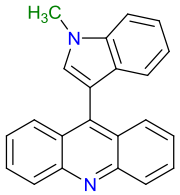
A quartz tube containing a solution of acridine **4a** (1 mmol) or 6-phenyl-1,2,5-oxadiazolo[3,4-*b*]pyrazine **4c** (1 mmol), nucleophile **5a-e** (1 mmol) and TiO_2 (10 mass.%, anatase) in acetic acid (10 mL) was treated in ultrasonic bath for 5 min to obtain a suspension. The resulting mixture was exposed to Xe lamp (5000 K, 35 W) under air oxygen, bubbling through the reaction mixture at room temperature for 5 h. The reaction mixture was concentrated under a reduce pressure.

9-(1*H*-Indol-3-yl)acridine (6a)



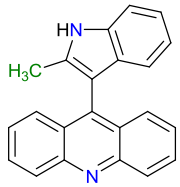
The residue was purified by column chromatography on silica gel eluting with mixture hexane/ethyl acetate 8/2 to give compound **6a** as a yellow solid (157 mg, 60%), mp 257-258 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) ppm: δ 6.96-7.01 (m, 2H, 5′-H, 6′-H), 7.21-7,23 (m, 1H, 7′-H), 7.47-7.49 (m, 2H, 2-H, 7-H), 7.63 (d, 1H, ^3J(H,H) = 12.00 Hz, 4′-H), 7.80-7,81 (m, 3H, 2′-H, 3-H, 6-H), 7.92-7,94 (d, 2H, ^3J(H,H) = 8.00 Hz, 1-H, 8-H), 8.21-8.24 (d, 2H, ^3J(H,H) = 12.00 Hz, 4-H, 5-H), 11.86 (s, 1H, N′-H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) ppm: δ 108.94 (C3′); 112.61 (C4′); 119.41 (C6′); 120.26 (C5′), 122.29 (C7′), 125.92 (C2, C7); 126.03 (C1a, C8a); 127.64 (C1, C8); 127.68 (C2′); 128.33 (C7a′); 129.86 (C4, C5); 130.54 (C3, C6); 136.68 (C4a′); 141.73 (C9); 148.95 (C4a, C5a). ESI-MS: *m/z* (%): 294 (100) [M^+]. Anal. Found: C, 85.70; H, 4.76; N, 9.54. Calc for $C_{21}H_{14}N_2$: C, 85.69; H, 4.79; N, 9.52.

9-(1-Methyl-1*H*-indol-3-yl)acridine (6b)



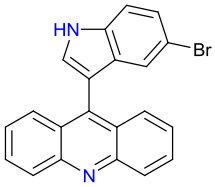
The residue was purified by column chromatography on silica gel eluting with mixture hexane/ethyl acetate 8/2 to give compound **6b** as a yellow solid (295 mg, 86%), mp 259-260 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) ppm: δ 4.02 (s, 3H, N'-Me), 6.97-7.04 (m, 2H, 5′-H, 6′-H), 7.27-7.30 (m, 1H, 7′-H), 7.46-7.7.49 (m, 2H, 2-H, 7-H), 7.65-7.67 (d, 1H, ^3J(H,H) = 8.00 Hz, 4′-H), 7.77 (s, 1H, 2′-H), 7.81-7.84 (m, 2H, 3-H, 6-H), 7.93-7.95 (d, 2H, ^3J(H,H) = 8.00 Hz, 4-H, 5-H), 8.20-8.22 (d, ^3J(H,H) = 8.00 Hz, 2H, 1-H, 8-H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) ppm: δ 33.31 (N′-Me); 108.15 (C3′); 110.89 (C4′); 119.65 (C6′); 120.42 (C5′); 122.38 (C7′), 125.93 (C1a, C8a); 125.99 (C2, C7); 127.58 (C4, C5); 128.65 (C4a′); 129.89 (C1, C8); 130.50 (C3, C6); 131.62 (C2′); 137.23 (C7a′); 141.20 (C9); 148.97 (C4a, C5a). ESI-MS: *m/z* (%): 308 (100) [M^+]. Anal. Found: C, 85.74; H, 5.21; N, 9.05. Calc for $C_{22}H_{16}N_2$: C, 85.69; H, 5.23; N, 9.08.

9-(2-Methyl-1*H*-indol-3-yl)acridine (6c)



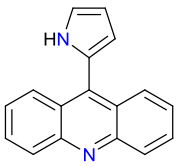
The residue was purified by column chromatography on silica gel eluting with mixture hexane/ethyl acetate 8/2 to give compound **6c** as a light-brown solid (292 mg, 85%), mp 277-278 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) ppm: δ 2.12 (s, 3H, C′-Me), 6.73-6.75 (m, 1H, 5′-H), 6.86-6.90 (m, 1H, 6′-H), 7.09-7.13 (m, 1H, 7′-H), 7.46-7.48 (m, 3H, 4′-H, 2-H,7-H), 7.70-7.72 (m, 2H, 4-H, 5-H), 7.82 (m, 2H, 3-H, 6-H), 8.20-8.22 (m, 2H, 1-H, 8-H), 11.44 (s, 1H, N′-H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) ppm: δ 12.70 (C′-Me); 106.34 (C3′); 111.57 (C4′); 118.35 (C5′); 120.03 (C6′); 121.54 (C7′); 126.17 (C2, C7); 127.47 (C4, C5); 129.32 (C2′); 129.72 (C1, C8); 130.78 (C3, C6); 135.52 (C7a′); 135.88 (C4a′); 141.97 (C9); 148.79 (C1a, C8a). ESI-MS: *m/z* (%): 308 (100) [M^+]. Anal. Found: C, 85.68; H, 5.20; N, 9.12. Calc for $C_{22}H_{16}N_2$: C, 85.69; H, 5.23; N, 9.08.

9-(5-Bromo-1*H*-indol-3-yl)acridine (6d)



The residue was purified by column chromatography on silica gel eluting with mixture hexane/ethyl acetate 8/2 to give compound **6d** as a yellow solid (158 mg, 38%), mp 242-244 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) ppm: δ 7.08-7.09 (m, 1H, 4′-H), 7.36 (m, 1H, 7′-H), 7.50-7.54 (t, 2H, ^{3}J(H,H) = 8.00 Hz, 2-H, 7-H), 7.62-7.64 (d, 1H, ^{3}J(H,H) = 8.00 Hz, 6′-H), 7.86-7,89 (m, 5H, 2′-H, 1-H, 3-H, 6-H, 8-H), 8.23-8,25 (d, 2H, ^{3}J(H,H) = 8.00 Hz, 4-H, 5-H), 12.06 (s, 1H, N′-H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) ppm: δ 108.10 (C3′); 112.32 (C5′); 114.23 (C6′); 120.88 (C4′), 124.39 (C7′), 125.53 (C1a, C8a); 125.69 (C2, C7); 126.84 (C1, C8); 128.67 (C2′); 129.41 (C4, C5); 129.55 (C7a′); 130.11 (C3, C6); 134.93 (C4a′); 140.21 (C9); 148.39 (C4a, C5a). ESI-MS: *m/z* (%): 372 (100) [M^+]. Anal. Found: C, 67.56; H, 3.55; N, 7.48. Calc for $C_{21}H_{13}BrN_2$: C, 67.58; H, 3.51; N, 7.51.

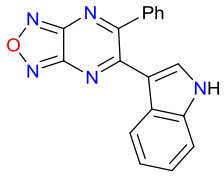
9-(1*H*-Pyrrol-2-yl)acridine (6e)



The residue was purified by column chromatography on silica gel eluting with mixture hexane/ethyl acetate 8/2 to give compound **6e** as a yellow solid (134 mg, 49%), mp 217-218 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) ppm: δ 6.44-6.46 (m, 1H, 4′-H), 6.52-6.53 (m, 1H, 5′-H), 7.19-7,20 (m, 1H,

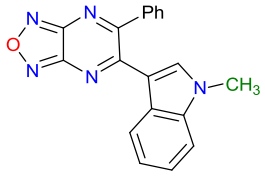
3′-H), 7.57-7.61 (m, 2H, 2-H, 7-H), 7.85-7,87 (m, 2H, 3-H, 6-H), 8.06-8,08 (d, 2H, ^{3}J(H,H) = 8.00 Hz, 4-H, 5-H), 8.19-8.21 (d, 2H, ^{3}J(H,H) = 8.00 Hz, 1-H, 8-H), 11.62 (s, 1H, N′-H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) ppm: δ 108.83 (C4′); 112.31 (C5′); 120.38 (C3′), 123.79 (C2′), 125.05 (C1a, C8a); 125.87 (C2, C7); 126.96 (C4, C5); 129.24 (C1, C8); 130.08 (C3, C6); 139.14 (C9); 148.40 (C4a, C5a). ESI-MS: *m/z* (%): 244 (100) [M$^+$]. Anal. Found: C, 83.56; H, 4.99; N, 11.45. Calc for $C_{17}H_{12}N_2$: C, 83.58; H, 4.95; N, 11.47.

5-(1*H*-Indol-3-yl)-6-phenyl-[1,2,5]oxadiazolo[3,4-*b*]pyrazine (8a)



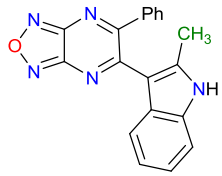
The residue was purified by column chromatography on silica gel eluting with mixture hexane/ethyl acetate 8/2 to give compound **8a** as a red solid (180 mg, >99% yield), mp 245-246 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) ppm: δ 6.61 (s, 1H, 2′-H), 7.26-7.32 (m, 2H, 5′-H, 6′-H), 7.44-7.48 (m, 1H, 7′-H), 7.54-7.58 (m, 2H, Ph), 7.62-7.69 (m, 3H, Ph), 8.59-8.61 (m, 1H, 4′-H), 11.89 (s, 1H, N′-H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) ppm: δ 112.90 (C7′); 114.05 (C3′); 122.66 (C6′); 123.18 (4′-H), 124.21 (C5′), 126.68 (C4a′); 128.91, 129.52, 131.00 (Ph); 134.67 (C2′); 136.77 (C7a′); 139.45 (Ph); 150.79 (C5); 152.37 (C3a); 158.39 (C6a); 165.23 (C4). ESI-MS: *m/z* (%): 313 (100) [M$^+$]. Anal. Found: C, 69.01; H, 3.51; N, 22.39. Calc for $C_{18}H_{11}N_5O$: C, 69.00; H, 3.54; N, 22.35.

5-(1-Methyl-1*H*-indol-3-yl)-6-phenyl-[1,2,5]oxadiazolo[3,4-*b*]pyrazine (8b)



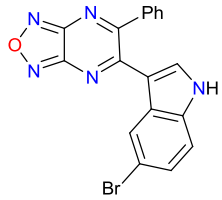
The residue was purified by column chromatography on silica gel eluting with mixture hexane/ethyl acetate 8/2 to give compound **8b** as a red solid (180 mg, >99% yield), mp 227-228 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) ppm: δ 3.61 (s, 3H, N'-Me), 6.59 (s, 1H, 2′-H), 7.31-7.35 (m, 2H, Ph), 7.51-7.57 (m, 3H, Ph), 7.66-7.69 (m, 3H, 4′-H, 5′-H, 6′-H), 8.54-8.56 (m, 1H, 7′-H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) ppm: δ 29.41 (N′-Me); 111.31 (C-Ph); 113.23 (C3′); 122.92 (C-Ph); 123.24 (C7′), 124.20 (C-Ph), 127.16 (C7a′); 128.87 (2C-Ph); 129.54 (C4′, C5′); 131.08 (C6′); 137.55 (C4a′); 137.86 (C2′); 139.18 (C2); 150.80 (C7a); 152.30 (C3a); 157.95 (C-Ph); 165.02 (C1). ESI-MS: *m/z* (%): 327 (100) [M$^+$]. Anal. Found: C, 69.75; H, 4.02; N, 21.36. Calc for $C_{13}H_{13}N_5O$: C, 69.71; H, 4.00; N, 21.39.

5-(2-Methyl-1*H*-indol-3-yl)-6-phenyl-[1,2,5]oxadiazolo[3,4-*b*]pyrazine (8c)



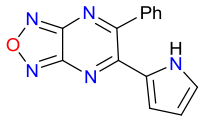
The residue was purified by column chromatography on silica gel eluting with mixture hexane/ethyl acetate 8/2 to give compound **8c** as a dark-red solid (180 mg, >99%), mp 181-182 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) ppm: δ 2.10 (s, 3H, C'-Me), 6.89-6.93 (m, 1H, 6′-H), 7.04-7.08 (m, 1H, 5′-H), 7.30-7.34 (m, 3H, Ph), 7.40-7.45 (m, 2H, Ph), 7.58-7.60 (m, 2H, 4′-H, 7′-H); 11.68 (s, 1H, N′-H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) ppm: δ 13.37 (C′-Me); 111.49 (C-Ph); 119.97 (C-Ph); 120.69 (C6′); 122.15 (C5′); 127.37 (C7a′); 128.38, 128.77 (C-Ph); 129.96 (C4′, C7′); 131.01 (C4a′); 135.74 (C3′); 138.63 (C2); 140.71 (C2′); 151.74 (C7a); 152.24 (C3a); 164.64 (C1). ESI-MS: *m/z* (%): 327 (100) [M^{+}]. Anal. Found: C, 69.66; H, 4.05; N, 21.37. Calc for $C_{13}H_{13}N_5O$: C, 69.71; H, 4.00; N, 21.39.

5-(5-Bromo-1*H*-indol-3-yl)-6-phenyl-[1,2,5]oxadiazolo[3,4-*b*]pyrazine (8d)



The residue was purified by column chromatography on silica gel eluting with mixture hexane/ethyl acetate 8/2 to give compound **8d** as a red solid (176 mg, 89%), mp 276-278 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) ppm: δ 6.66 (s, 1H, 4′-H), 7.43-7.50 (m, 2H, 6′-H, 7′-H), 7.58-7.62 (m, 2H, Ph), 7.66-7.72 (m, 3H, Ph), 8.73 (s, 1H, 2′-H); 12.07 (s, 1H, N′-H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) ppm: δ 112.91 (C3′); 114.49 (C6′); 114.85 (C5′); 124.65 (C2′); 126.18 (C7′); 127.87 (C4a′); 128.45 (2C-Ph); 129.04 (2C-Ph); 130.58 (C-Ph); 134.97 (C4′); 135.01 (C7a′); 138.63 (C-Ph); 150.35 (C3a); 151.71 (C6a); 157.64 (C5); 164.56 (C4). ESI-MS: *m/z* (%): 392 (100) [M^{+}]. Anal. Found: C, 55.05; H, 2.59; N, 17.92. Calc for $C_{18}H_{10}BrN_5O$: C, 55.12; H, 2.57; N, 17.86.

5-Phenyl-6-(1*H*-pyrrol-2-yl)-[1,2,5]oxadiazolo[3,4-*b*]pyrazine (8e)



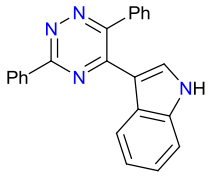
The residue was purified by column chromatography on silica gel eluting with mixture hexane/ethyl acetate 8/2 to give compound **8e** as a yellow solid (126 mg, 98%), mp 188-189 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) ppm: δ 5.48-5.49 (m, 1H, 4′-H), 6.08-6.10 (m, 1H, 5′-H), 7.24 (m, 1H, 3′-H), 7.59-7.63 (m, 2H, Ph), 7.67-7.71 (m, 3H, Ph), 12.41 (s, 1H, N′-H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) ppm: δ 111.24 (C5′); 120.00 (C4′); 128.09 (C3′); 128.19(2C-Ph); 128.61 (2C-Ph); 128.99 (C2′); 130.33 (C-Ph); 138.42 (C5); 150.72 (C-Ph); 151.68 (C3a); 151.81 (C6a); 163.97 (C4). ESI-MS:

m/z (%): 363 (100) [M^+]. Anal. Found: C, 63.85; H, 3.42; N, 26.65. Calc for $C_{13}H_{13}N_5O$: C, 63.87; H, 3.45; N, 26.60.

2. Synthesis of compounds 7a-e

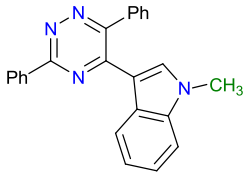
A quartz tube containing a solution of 3,6-diphenyl-1,2,4-triazine **4b** (1 mmol), nucleophile **5a-e** (2 mmol) and TiO_2 (10 mass.%, anatase) in acetic acid (10 mL) was treated in ultrasonic bath for 5 min to obtain a suspension. The resulting mixture was exposed to Xe lamp (5000 K, 35 W) under air oxygen, bubbling through the reaction mixture and was held at boiling for 5 h. The reaction mixture was concentrated under a reduce pressure.

3,6-Diphenyl-5-(1*H*-Indol-3-yl)-1,2,4-triazine (7a)



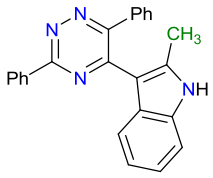
The residue was purified by column chromatography on silica gel eluting with mixture hexane/ethyl acetate 8/2 to give compound **7a** as a light-brown solid (200 mg, 82%). The product was identified as a compound **7a** by comparing its ^{1}H NMR spectra with its given in the literature. Satisfactory elemental analysis for C, H and N were obtained for compound **7a**; none of the experimentally found percentages deviated from the theoretical values by more than 0.3%.[1]

3,6-Diphenyl-5-(1-Methyl-1*H*-indol-3-yl)-1,2,4-triazine (7b)



The residue was purified by column chromatography on silica gel eluting with mixture hexane/ethyl acetate 8/2 to give compound **7b** as a yellow solid (202 mg, 65%). The product was identified as a compound **7b** by comparing its ^{1}H NMR spectra with its given in the literature. Satisfactory elemental analysis for C, H and N were obtained for compound **7b**; none of the experimentally found percentages deviated from the theoretical values by more than 0.3%.[1]

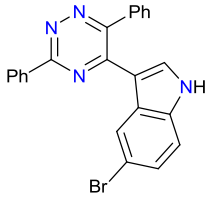
3,6-Diphenyl-5-(2-Methyl-1*H*-indol-3-yl)-1,2,4-triazine (7c)



The residue was purified by column chromatography on silica gel eluting with mixture hexane/ethyl acetate 8/2 to give compound **7c** as a yellow solid (217 mg, 70%). The product was identified as a compound **7c** by comparing its ^{1}H NMR spectra with its given in the literature.

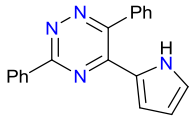
Satisfactory elemental analysis for C, H and N were obtained for compound **7c**; none of the experimentally found percentages deviated from the theoretical values by more than 0.3%.[1]

3,6-Diphenyl-5-(5-bromo-1*H*-indol-3-yl)-1,2,4-triazine (7d)



The residue was purified by column chromatography on silica gel eluting with mixture hexane/ethyl acetate 8/2 to give compound **7d** as a yellow solid (128 mg, 35%), mp 192-194 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) ppm: δ 6.94-6.95 (m, 1H, 4′-H), 7.38-7.40 (m, 1H, 7′-H), 7.45-7.48 (m, 1H, 6′-H), 7.59-7,60 (m, 3H, Ph), 7.67-7,70 (m, 5H, Ph), 8.53-8.56 (m, 2H, Ph), 8.70-8.71 (m, 1H, 2′-H), 11.98 (s, 1H, N′-H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) ppm: δ 109.85 (C3′); 114.17 (C5′); 114.42 (C6′); 124.49 (C2′), 125.46 (C7′), 127.58 (2C-Ph); 127.83 (C3); 128.77 (2C-Ph); 129.03 (2C-Ph); 129.05 (2C-Ph); 129.57 (C-Ph); 131.43 (C-Ph); 132.80 (C4′); 135.19 (C7a′); 135.39 (C4a′); 136.97 (C5); 152.05 (C-Ph); 154.80 (C-Ph); 160.41 (C6). ESI-MS: *m/z* (%): 427 (100) [M^+]. Anal. Found: C, 64.70; H, 3.58; N, 13.06. Calc for $C_{23}H_{15}BrN_4$: C, 64.65; H, 3.54; N, 13.11.

3,6-Diphenyl-5-(1*H*-pyrrol-2-yl)-1,2,4-triazine (7e)

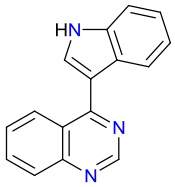


The residue was purified by column chromatography on silica gel eluting with mixture hexane/ethyl acetate 8/2 to give compound **7e** as a light-brown solid (131 mg, 51%). The product was identified as a compound **7e** by comparing its ^{1}H NMR spectra with its given in the literature. Satisfactory elemental analysis for C, H and N were obtained for compound **7e**; none of the experimentally found percentages deviated from the theoretical values by more than 0.3%.[1]

3. Synthesis of compounds 9a, 10a, 19

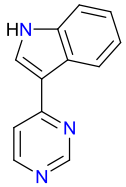
To a round bottom flask were added a solution of quinazoline **4d** (1 mmol) or pyrimidine **4e** (1 mmol), indole **5a** (1 mmol) or *N*,*N*-diethylaniline **18b** (1,5 mmol) in mixture trifluoroacetic acid/benzene 1/2 (10 mL). The reaction mixture was stirred at room temperature for 5 h. The solvent was further removed under vacuum. A quartz tube containing a solution of residue in ethanol, aqueous NaOH (2 equiv.) and TiO_2 (10 mass.%, anatase) was treated in ultrasonic bath for 5 min to obtain a suspension. The resulting mixture was exposed to Xe lamp (5000 K, 35 W) under air oxygen, bubbling through the reaction mixture at room temperature for 5 h. The reaction mixture was then transferred to separatory funnel. The aqueous layer was extracted with $CHCl_3$ (3 x 10 mL). The organic extracts were combined and dried over Na_2SO_4, filtered and concentrated under a reduce pressure.

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



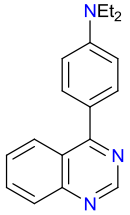
The residue was purified by column chromatography on silica gel eluting with mixture ethyl acetate/methanol 10/1 to give compound **9a** as a yellow solid (264 mg, 70%). The product was identified as a compound **9a** by comparing its ^{1}H NMR spectra with its given in the literature. Satisfactory elemental 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%.[2]

4-(1*H*-Indol-3-yl)pyrimidine (10a)



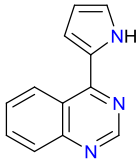
The residue was purified by column chromatography on silica gel eluting with mixture ethyl acetate/methanol 10/1 to give compound **10a** as a red-brown solid (341 mg, 70%).The product was identified as a compound **10a** by comparing its ^{1}H NMR spectra with its given in the literature. Satisfactory elemental analysis for C, H and N were obtained for compound **10a**; none of the experimentally found percentages deviated from the theoretical values by more than 0.3%.[3]

4-(4'-*N*,*N*-Diethylaminophenyl)quinazoline (19)



The residue was purified by column chromatography on silica gel eluting with mixture hexane/ethyl acetate 1/1 to give compound **19** as a yellow solid (238 mg, 56%).The product was identified as a compound **19** by comparing its ^{1}H NMR spectra with its given in the literature. Satisfactory elemental analysis for C, H and N were obtained for compound **19**; none of the experimentally found percentages deviated from the theoretical values by more than 0.3%.[4]

4. Synthesis of compound 9e (4-(1*H*-pyrrol-2-yl)quinazoline)

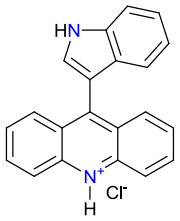


To a round bottom flask were added a solution of quinazoline **4d** (1 mmol), pyrrole **5e** (1 mmol) in mixture HCl/MeOH 1/2 (2 mL). The reaction mixture was stirred at room temperature for 10 h. The solvent was further removed under vacuum. A quartz tube containing a solution of residue in ethanol, aqueous NaOH (2 equiv.) and TiO_2 (10 mass.%, anatase) was treated in ultrasonic bath for 5 min to obtain a suspension. The resulting mixture was exposed to Xe lamp (5000 K, 35 W) under air oxygen, bubbling through the reaction mixture at room temperature for 5 h. The reaction mixture was then transferred to separatory funnel. The aqueous layer was extracted with $CHCl_3$ (3 x 10 mL). The organic extracts were combined and dried over Na_2SO_4, filtered and concentrated under a reduce pressure. The residue was purified by column chromatography on silica gel eluting with mixture ethyl acetate/methanol 10/1 to give compound **9e** as a brown solid (112 mg, 74%), mp 192-194 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) ppm: δ 5.68 (m, 1H, 4′-H), 5.89 (m, 1H, 7-H), 6.63 (m, 1H, 5′-H), 6.84-6.92 (m, 3H, 3′-H, 6-H, 8-H), 7.06-7.10 (m, 1H, 5-H), 7.18 (s, 1H, 2-H), 10.79 (s, 1H, N′-H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) ppm: δ 99.49 (C2′); 104.99 (C4′); 106.88 (C7); 117.31 (C5′); 123.32 (C3′); 126.73 (C6, C8); 127.40 (C2); 135.54 (C4a, C8a); 147.24 (C4). ESI-MS: *m/z* (%): 195 (100) [M^+]. Anal. Found: C, 73.89; H, 4.58; N, 21.54. Calc for $C_{12}H_9N_3$: C, 73.83; H, 4.65; N, 21.52.

5. Synthesis of compounds 11a-e, 12a-e, 13a-e, 20, 21

A quartz tube containing a solution of 10-hydroacridinium chloride **4g,** 10-methylacridinium iodide **4h** or 1-methylquinoxalinum iodide **4i** (1 mmol), nucleophile **5a-e** (2 mmol) or **19a,b** (2 mmol) in *n*-BuOH (10 mL) and TiO_2 (10 mass.%, anatase) was treated in ultrasonic bath for 5 min to obtain a suspension. The resulting mixture was exposed to Xe lamp (5000 K, 35 W) under air oxygen, bubbling through the reaction mixture at room temperature for 5 h. The reaction mixture was concentrated under a reduce pressure. Then dry diethyl ether was added to a solution and the form suspension was filtered. The residue was recrystallized from suitable solvent.

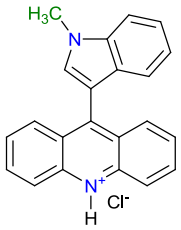
9-(1*H*-Indol-3-yl)acridinium chloride (11a)



The residue was recrystallized from acetonitrile to give compound **11a** as a dark red solid (199 mg, 65%), mp 201-203 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) ppm: δ 7.07-7.11 (m, 1H, 6′-H), 7.17-7.19 (m, 1H, 5′-H), 7.27-7.31 (m, 1H, 7′-H), 7.67-7.69 (d, 1H, ^3J(H,H) = 8.00 Hz, 4′-H), 7.75-7.79 (t, 2H, ^3J(H,H) = 4.00 Hz, 2-H, 7-H), 8.10-8.11 (d, 1H, ^3J(H,H) = 4.00 Hz, 2′-H), 8.22-8.27 (m, 4H, 3-H, 4-H, 5-H, 6-H), 8.57-8.60 (d, ^3J(H,H) = 12.00 Hz, 2H, 1-H, 8-H), 12.48 (s, 1H, N′-H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) ppm: δ 108.32 (C3′); 113.12 (C4′); 119.59 (C6′); 121.06 (C1, C8); 121.41 (C5′); 123.20

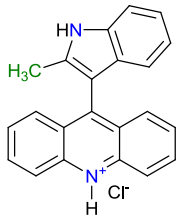
(C7′); 125.34 (C8a, C10a); 127.67 (C2, C7); 127.99(C3a′, C7a′); 129.41 (C4, C5); 130.99 (C2′); 136.51 (C3, C6); 137.02 (C4a, C9a); 140.57 (C9). ESI-MS: *m/z* (%): 295 (100) [M^+]. Anal. Found: C, 76.26; H, 4.58; N, 8.42. Calc for $C_{21}H_{15}ClN_2$: C, 76.24; H, 4.57; N, 8.47.

9-(1-Methyl-1*H*-indol-3-yl)acridinium chloride (11b)



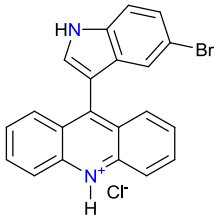
The residue was recrystallized from benzene to give compound **11b** as a red solid (217 mg, 70%), mp 209-211 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) ppm: δ 4.08 (s, 3H, N'-Me), 7.11-7.20 (m, 2H, 5′-H, 6′-H), 7.34-7.38 (m, 1H, 7′-H), 7.72-7.77 (m, 3H, 4′-H, 2-H, 7-H), 8.08 (s, 1H, 2′-H), 8.19-8.23 (t, 2H, ^3J(H,H) = 8.00 Hz, 3-H, 6-H), 8.26-8.28 (d, 2H, ^3J(H,H) = 8.00 Hz, 4-H, 5-H), 8.58-8.60 (d, ^3J(H,H) = 8.00 Hz, 2H, 1-H, 8-H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) ppm: δ 33.69 (N′-Me); 107.59 (C3′); 111.40 (C4′); 119.82 (C6′); 121.52 (C5′); 122.13 (C1, C8), 123.20 (C7′); 125.45 (C8a, C10a); 127.44 (C2, C7); 128.39 (C3a′); 128.74 (C4a, C9a); 129.19 (C4, C5); 134.27 (C2′); 135.77 (C3, C6); 137.60 (C7a′); 141.61 (C9). ESI-MS: *m/z* (%): 309 (100) [M^+]. Anal. Found: C, 76.68; H, 4.95; N, 10.30. Calc for $C_{22}H_{17}ClN_2$: C, 76.63; H, 4.97; N, 10.28.

9-(2-Methyl-1*H*-indol-3-yl)acridinium chloride (11c)



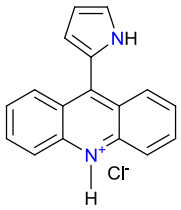
The residue was recrystallized from mixture benzene-acetonitrile to give compound **11c** as a dark red solid (203 mg, 64%), mp 178-180 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) ppm: δ 2.24 (s, 3H, C′-Me), 6.96-6.97 (m, 2H, 5′-H, 6′-H), 7.15-7.19 (m, 1H, 7′-H), 7.54-7.56 (d, 1H, ^3J(H,H) = 8.00 Hz, 4′-H), 7.73-7.77 (t, 2H, ^3J(H,H) = 8.00 Hz, 2-H, 7-H), 8.02-8.04 (d, 2H, ^3J(H,H) = 8.00 Hz, 4-H, 5-H), 8.22-8.26 (t, 2H, ^3J(H,H) = 8.00 Hz, 3-H, 6-H), 8.66-8.68 (d, ^3J(H,H) = 8.00 Hz, 2H, 1-H, 8-H), 12.30 (s, 1H, N′-H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) ppm: δ 13.20 (C′-Me); 106.07 (C3′); 111.98 (C4′); 118.53 (C6′); 120.87 (C1, C8); 121.05 (C5′); 122.31 (C7′); 125.85 (C8a, C10a); 127.83 (C2, C7); 129.19 (C3a′); 129.30 (C4, C5); 136.26 (C4a, C9a); 136.60 (C3, C6); 138.56 (C2′); 137.60 (C7a′); 140.40 (C9). ESI-MS: *m/z* (%): 309 (100) [M^+]. Anal. Found: C, 76.65; H, 4.98; N, 10.26. Calc for $C_{22}H_{17}ClN_2$: C, 76.63; H, 4.97; N, 10.28.

9-(5-Bromo-1*H*-indol-3-yl)acridinium chloride (11d)



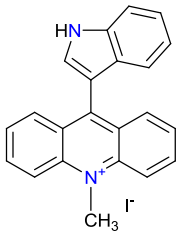
The residue was recrystallized from mixture benzene-acetonitrile to give compound **11d** as a red solid (175 mg, 46%), mp 213-215 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) ppm: δ 7.32 (s, 1H, 4′-H), 7.38-7.41 (m, 1H, 7′-H), 7.66-7.68 (d, 1H, ^{3}J(H,H) = 8.00 Hz, 6′-H), 7.76-7.79 (m, 2H, 2-H, 7-H), 8.07 (m, 1H, 2′-H), 8.16-8.24 (m, 4H, 3-H, 4-H, 5-H, 6-H), 8.64-8.66 (d, 2H, ^{3}J(H,H) = 8.00 Hz, 1-H, 8-H), 12.52 (s, 1H, N′-H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) ppm: δ 107.39 (C3′); 113.25 (C5′); 114.55 (C6′); 121.27 (C1, C8, C4′); 125.18 (C7′); 125.35 (C3a′, C7a′); 127.20 (C2, C7); 128.41 (C4, C5); 129.39 (C8a, C10a); 130.82 (C2′); 135.29 (C4a, C9a); 135.54 (C3, C6); 140.81 (C9). ESI-MS: *m/z* (%): 374 (100) [M^{+}]. Anal. Found: C, 61.60; H, 3.47; N, 6.78. Calc for $C_{21}H_{14}BrClN_2$: C, 61.56; H, 3.44; N, 6.84.

9-(1*H*-Pyrrol-2-yl)acridinium chloride (11e)



The residue was recrystallized from acetonitrile to give compound **11e** as a brown solid (183 mg, 70%), mp 231-232 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) ppm: δ 6.57 (m, 1H, 5′-H), 6.83 (s, 1H, 4′-H), 7.44 (s, 1H, 3′-H), 7.78-7.81 (t, ^{3}J(H,H) = 8.00 Hz, 2H, 2-H, 7-H), 8.11-8.15 (t, ^{3}J(H,H) = 8.00 Hz, 2H, 3-H, 6-H), 8.32-8.34 (d, ^{3}J(H,H) = 8.00 Hz, 2H, 4-H, 5-H), 8.42-8.44 (d, ^{3}J(H,H) = 8.00 Hz, 2H, 1-H, 8-H), 12.10 (s, 1H, N′-H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) ppm: δ 60.88 (C2′); 95.95 (C8a, C10a); 99.99 (C4a, C9a); 110.85 (C5′); 116.92 (C4′); 123.86(C1, C8); 124.73 (C3); 127.50 (C2, C7); 128.88 (C4, C5); 134.61 (C3, C6); 143.17 (C9). ESI-MS: *m/z* (%): 245 (100) [M^{+}]. Anal. Found: C, 72.69; H, 4.69; N, 9.94. Calc for $C_{17}H_{13}ClN_2$: C, 72.73; H, 4.67; N, 9.98.

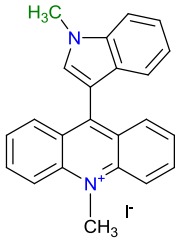
9-(1*H*-Indol-3-yl)-10-methylacridinium iodide (12a)



The residue was recrystallized from ethanol to give compound **12a** as a red solid (341 mg, >99%). The product was identified as a compound **12a** by comparing its ^{1}H NMR spectra with its given in the

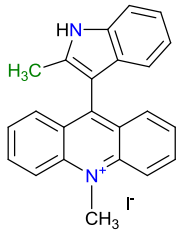
literature. Satisfactory elemental analysis for C, H and N were obtained for compound **12a**; none of the experimentally found percentages deviated from the theoretical values by more than 0.3%.[4]

10-Methyl-9-(1-methyl-1*H*-indol-3-yl)acridinium iodide (12b)



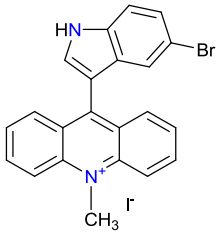
The residue was recrystallized from ethanol to give compound **12b** as a red solid (238 mg, 85%), mp 218-220 ºC. ^{1}H NMR (400 MHz, DMSO-d_6/CCl_4, 1:1) ppm: δ 4.10 (s, 3H, N′-Me), 4.86 (s, 3H, N-Me), 7.15-7.16 (d, 2H, ^{3}J(H,H) = 4.00 Hz, 5′-H, 6′-H), 7.37-7.41 (m, 1H, 7′-H), 7.76-7.78 (d, 2H, ^{3}J(H,H) = 8.40 Hz, 4′-H), 7.85-7.89 (t, 2H, ^{3}J(H,H) = 8.00 Hz, 2-H, 7-H), 8.16 (s, 1H, 2′-H), 8.38-8.44 (m, 4H, 4-H, 5-H, 3-H, 6-H), 8.77-8.80 (d, ^{3}J(H,H) = 9.20 Hz, 2H, 1-H, 8-H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6/CCl_4, 1:1) ppm: δ 33.86 (N'-Me); 39.10 (N-Me); 107.47 (C3′); 111.65 (C4′); 119.54 (C1, C8), 119.59 (C6′); 121.95 (C5′); 123.48 (C7′); 126.03 (C8a, C10a); 127.57 (C2, C7); 128.72 (C3a′); 131.05 (C4, C5); 135.28 (C2′); 137.54 (C7a′); 138.38 (C3, C6); 141.69 (C4a, C9a); 156.09 (C9). ESI-MS: *m/z* (%): 323 (100) [M^+]. Anal. Found: C, 61.27; H, 4.24; N, 6.35. Calc for $C_{23}H_{19}N_2I$: C, 61.33; H, 4.22; N, 6.22.

10-Methyl-9-(2-methyl-1*H*-indol-3-yl)acridinium iodide (12c)



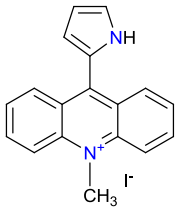
The residue was recrystallized from ethanol to give compound **12c** as a red solid (252 mg, 90%), mp 205-207 ºC. ^{1}H NMR (400 MHz, DMSO-d_6/CCl_4, 1:1) ppm: δ 2.24 (s, 3H, C′-Me), 4.89 (s, 3H, N-Me), 6.97-7.01 (m, 2H, 5′-H, 6′-H), 7.22 (m, 1H, 7′-H), 7.56-7.58 (d, 1H, ^{3}J(H,H) = 8.00 Hz, 4′-H), 7.86 (m, 2H, 2-H, 7-H), 8.18-8.20 (d, 2H, ^{3}J(H,H) = 8.00 Hz, 4-H, 5-H), 8.40 (m, 2H, 3-H, 6-H), 8.81-8.83 (d, ^{3}J(H,H) = 8.00 Hz, 2H, 1-H, 8-H), 12.18 (s, 1H, N′-H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6/CCl_4, 1:1) ppm: δ 12.69 (C'-Me); 39.19 (N-Me); 105.77 (C2′); 111.57 (C4′); 117.85 (C6′); 119.26 (C1, C8); 120.65 (C5′); 122.07 (C7′); 126.10 (C8a, C10a); 127.32 (C2, C7); 129.11 (C7a′); 130.36 (C4, C5); 135.72 (C3a′); 138.00 (C3′); 138.55 (C3, C6); 141.17 (C4a, C9a); 156.47 (C9). ESI-MS: *m/z* (%): 323 (100) [M^+]. Anal. Found: C, 61.03; H, 4.32; N, 6.29. Calc for $C_{23}H_{19}N_2I$: C, 61.33; H, 4.22; N, 6.22.

9-(5-Bromo-1*H*-indol-3-yl)-10-methylacridinium iodide (12d)



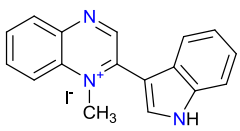
The residue was recrystallized from *i*-propanol to give compound **12d** as a red solid (232 mg, 73%), mp 180-182 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) ppm: δ 4.92 (s, 3H, N-Me), 7.26-7.30 (m, 1H, 4′-H), 7.36-7.39 (m, 1H, 7′-H), 7.64-7.66 (d, 2H, ^{3}J(H,H) = 8.00 Hz, 6′-H), 7.86-7.90(m, 2H, 2-H, 7-H), 8.05-8.06 (m, 1H, 2′-H), 8.39-8.43 (m, 4H, 4-H, 5-H, 3-H, 6-H), 8.80-8.82 (d, 2H, ^{3}J(H,H) = 8.00 Hz, 1-H, 8-H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) ppm: δ 38.91 (N-Me); 99.48 (C3′); 113.47 (C5′); 114.67 (C6′), 119.13 (C1, C8); 121.06 (C4′); 125.32 (C3a′); 125.42 (C7′); 125.99 (C8a, C10a); 127.30 (C2, C7); 129.75 (C7a′); 130.17 (C2′); 135.12 (C9); 138.04 (C4, C5, C3, C6); 141.22 (C4a, C9a). ESI-MS: *m/z* (%): 386 (100) [M^{+}]. Anal. Found: C, 51.35; H, 3.06; N, 5.48. Calc for $C_{22}H_{16}BrN_2I$: C, 51.29; H, 3.13; N, 5.44.

10-Methyl-9-(1*H*-pyrrol-2-yl)acridinium iodide (12e)



The residue was recrystallized from mixture benzene/acetonitrile to give compound **12e** as a dark-red solid (206 mg, 86% yield). The product was identified as a compound **12e** by comparing its ^{1}H NMR spectra with its given in the literature. Satisfactory elemental analysis for C, H and N were obtained for compound **12e**; none of the experimentally found percentages deviated from the theoretical values by more than 0.3%.[4]

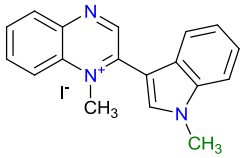
2-(1*H*-Indol-3-yl)-1-methylquinoxalin-1-ium iodide (13a)



The residue was recrystallized from ethanol to give compound **13a** as a brown solid (285 mg, 75%), mp 272-274 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) ppm: δ 4.66 (s, 3H, N-Me), 7.30-7.36 (m, 2H, 5′-H, 6′-H), 7.56-7.60 (m, 1H, 7′-H), 8.01-8.05 (m, 1H, 4′-H), 8.12-8.16 (m, 1H, 6-H), 8.38-8.44 (m, 2H, 7-H, 8-H), 8.68 (d, 1H, ^{3}J(H,H) = 4.00 Hz, 2′-H), 8.72-8.74 (m, 1H, 5-H),10.09 (s, 1H, 3-H), 12.24 (s, 1H, N′-H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) ppm: δ 45.32 (N-Me); 112.27 (C7a′); 112.46 (C4′); 119.02 (C7); 121.91 (C8), 121.96 (C6′), 123.63 (C5′); 124.75 (C4a′); 127.91 (C1a); 129.51 (C5); 131.43 (C7′);

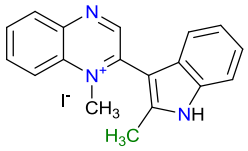
131.66 (C2′); 133.21 (C6); 137.27 (C2); 141.75 (C3); 144.56 (C4a); 152.00 (C3′). ESI-MS: *m/z* (%): 260 (100) [M^+]. Anal. Found: C, 52.71; H, 3.62; N, 10.91. Calc for $C_{17}H_{14}IN_3$: C, 52.73; H, 3.64; N, 10.85.

1-Methyl-2-(1-methyl-1*H*-indol-3-yl)quinoxalin-1-ium iodide (13b)



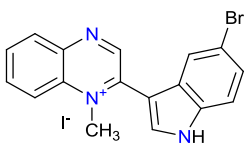
The residue was recrystallized from acetonitrile to give compound **13b** as a red solid (161 mg, 78%), mp 176-178 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) ppm: δ 3.93 (s, 3H, N′-Me), 4.61 (s, 3H, N-Me), 7.32-7.40 (m, 2H, 5′-H, 6′-H), 7.59-7.61 (d, 1H, ^3J(H,H) = 8.00 Hz, 4′-H), 7.99-8.03 (m, 1H, 7′-H), 8.10-8.14 (t, 1H, ^3J(H,H) = 8.00 Hz, 6-H), 8.33-8.40 (m, 2H, 5-H, 7-H), 8.60 (s, 1H, 2′-H), 8.67-8.68 (d, 1H, ^3J(H,H) = 4.00 Hz, 8-H), 9.99 (s, 1H, 3-H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) ppm: δ 32.44 (N′-Me); 44.27 (N-Me), 109.87 (C7a′); 110.11 (C4′); 117.94 (C7); 120.94 (C8), 121.15 (C6′); 122.59 (C5′); 123.92 (C4a′); 126.71 (C1a); 128.36 (C5); 130.35 (C7′); 132.16 (C6); 133.87 (C2′); 136.69 (C2); 140.43 (C3); 143.36 (C4a); 150.38 (C3′). ESI-MS: *m/z* (%): 274 (100) [M^+]. Anal. Found: C, 53.92; H, 4.03; N, 10.43. Calc for $C_{18}H_{16}IN_3$: C, 53.88; H, 4.02; N, 10.47.

1-Methyl-2-(2-methyl-1*H*-indol-3-yl)quinoxalin-1-ium iodide (13c)



The residue was recrystallized from ethanol to give compound **13c** as a brown solid (174 mg, 74%), mp 270-272 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) ppm: δ 2.89 (s, 3H, C′-Me), 4.77 (s, 3H, N-Me), 7.22-7.27 (m, 2H, 5′-H, 6′-H), 7.45-7.49 (m, 1H, 7′-H), 8.09-8.13 (m, 1H, 4′-H), 8.16-8.20 (m, 1-H, 5-H), 8.35-8.41 (m, 2H, 6-H, 7-H), 8,48-8.50 (d, 1H, ^3J(H,H) = 8.00 Hz, 8-H), 9,60 (s, 1H, 3-H), 12.05 (s, 1H, N′-H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) ppm: δ 14.71 (C′-Me); 46.23 (N-Me); 108.95 (C2′); 112.03 (C7′); 119.66 (C8), 120.50 (C6), 121.88 (C5′); 123.10 (C6′); 126.61 (C3′); 128.40 (C1a); 130.18 (C7); 132.78 (C4′); 133.98 (C5); 136.02 (C4a′, C7a′); 142.25 (C3); 145.32 (C4a); 153.04 (C2). ESI-MS: *m/z* (%): 274 (100) [M^+]. Anal. Found: C, 53.89; H, 3.99; N, 10.51. Calc for $C_{18}H_{16}IN_3$: C, 53.88; H, 4.02; N, 10.47.

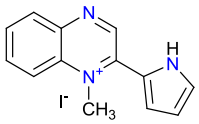
1-Methyl-2-(5-bromo-1*H*-indol-3-yl)quinoxalin-1-ium iodide (13d)



The residue was recrystallized from acetonitrile to give compound **13d** as a brown solid (178 mg, 52%), mp 304-306 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) ppm: δ 4.68 (s, 3H, N-Me), 7.49-7.51 (m, 1H, 4′-

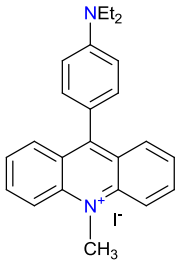
H), 7.60-7.62 (m, 1H, 7′-H), 8.07-8.11 (m, 1H, 7-H), 8.16-8.19 (m, 1-H, 6-H), 8.47-8.49 (d, 2H, ^{3}J(H,H) = 8.00 Hz, 5-H, 8-H), 8,72-8.73 (m, 1H, 6′-H), 8.88 (s, 1H, 2′-H), 10.12 (s, 1H, 3-H), 12.48 (s, 1H, N′-H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) ppm: δ 45.87 (N-Me); 112.83 (C3′); 113.02 (C7′); 115.04 (C5′); 119.58 (C8); 122.52 (C2′); 124.18 (C4′); 125.31 (C7a′); 128.47 (C1a); 130.07 (C5); 131.99 (C7); 133.22 (C6′); 133.77 (C6); 137.83 (C4a′); 142.30 (C3); 145.12 (C2); 152.56 (C4a). ESI-MS: *m/z* (%): 339 (100) [M^+]. Anal. Found: C, 43.87; H, 2.73; N, 9.04. Calc for $C_{17}H_{13}BrIN_3$: C, 43.81; H, 2.81; N, 9.01.

1-Methyl-2-(1*H*-pyrrol-2-yl)quinoxalin-1-ium iodide (13e)



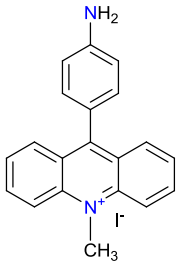
The residue was recrystallized from mixture benzene/acetonitrile to give compound **13e** as a dark-brown solid (110 mg, 46% yield). The product was identified as a compound **13e** by comparing its ^{1}H NMR spectra with its given in the literature. Satisfactory elemental analysis for C, H and N were obtained for compound **13e**; none of the experimentally found percentages deviated from the theoretical values by more than 0.3%.[4]

9-(4'-(Diethylaminophenyl)-10-methylacridinium iodide (20)



The residue was recrystallized from ethanol to give compound **20** as a dark blue solid. Yield 167 mg (80%). The product was identified as a compound **20** by comparing its ^{1}H NMR spectra with its given in the literature. Satisfactory elemental analyses for C, H and N were obtained for compound **20**; none of the experimentally found percentages deviated from the theoretical values by more than 0.3%.[4]

9-(4'-Aminophenyl)-10-methylacridinium iodide (21)



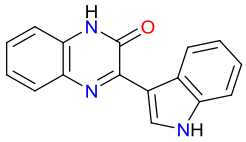
The residue was recrystallized from ethanol to give compound **21** as a dark blue solid. Yield 245 mg (96%). The product was identified as a compound **21** by comparing its ^{1}H NMR spectra with its

given in the literature. Satisfactory elemental analyses for C, H and N were obtained for compound **21**; none of the experimentally found percentages deviated from the theoretical values by more than 0.3%.[5]

6. Synthesis of compounds 14a-e, 15a-e, 22

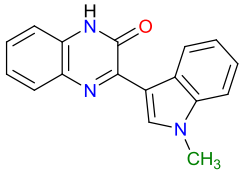
A quartz tube containing a solution of quinoxalin-2-one **4j** (1 mmol) or 3-(pyridine-2-yl)-1,2,4-triazin-5(2*H*)-one **4k** (1 mmol), nucleophile **5a-e** (1 mmol) or **18b** (2 mmol) and TiO_2 (10 mass.%, anatase) in acetic acid (10 mL) was treated in ultrasonic bath for 5 min to obtain a suspension. The resulting mixture was exposed to Xe lamp (5000 K, 35 W) under air oxygen, bubbling through the reaction mixture and was held at boiling for 5 h. The reaction mixture was concentrated under a reduce pressure.

3-(1*H*-Indol-3-yl)quinoxalin-2(1*H*)-one (14a)



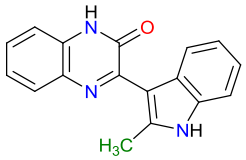
The residue was purified by column chromatography on silica gel eluting with mixture hexane/ethyl acetate 8/2 to give compound **14a** as a brown solid (201 mg, >99%). The product was identified as a compound **14a** by comparing its ^{1}H NMR spectra with its given in the literature. Satisfactory elemental analysis for C, H and N were obtained for compound **14a**; none of the experimentally found percentages deviated from the theoretical values by more than 0.3%.[5]

3-(1-Methyl-1*H*-indol-3-yl)quinoxalin-2(1*H*)-one (14b)



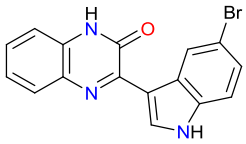
The residue was purified by column chromatography on silica gel eluting with mixture hexane/ethyl acetate 8/2 to give compound **14b** as a light brown solid (200 mg, >99%), mp 287-288 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) ppm: δ 3.91 (s, 3H, N′-Me), 7.26-7.33 (m, 4H, 5-H, 6-H, 7-H, 8-H), 7.40-7.44 (m, 1H, 5′-H), 7.54-7.56 (m, 1H, 6′-H), 7.85-7.87 (m, 1-H, 4′-H), 8.90-8.92 (m, 1H, 7′-H), 8.94 (s, 1H, 8.94), 12.41 (s, 1H, N-H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) ppm: δ 33.46 (N-Me); 110.64 (C3); 110.80 (C6′); 115.39 (C6), 121.74 (C7), 123.08 (C5); 123.59 (C5a); 123.68 (C8); 127.17 (C7a′); 128.03 (C4′); 128.41 (C5′); 130.64 (C4a′); 133.14 (C8a); 137.27 (C7′); 137.33 (C2′); 152.13 (C3′); 154.81 (C2). ESI-MS: *m/z* (%): 275 (100) [M^+]. Anal. Found: C, 74.12; H, 4.78; N, 15.24. Calc for $C_{17}H_{13}N_3O$: C, 74.17; H, 4.76; N, 15.26.

3-(2-Methyl-1*H*-indol-3-yl)quinoxalin-2(1*H*)-one (14c)



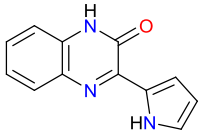
The residue was purified by column chromatography on silica gel eluting with mixture hexane/ethyl acetate 8/2 to give compound **14c** as a brown solid (169 mg, 90%). The product was identified as a compound **14c** by comparing its ^{1}H NMR spectra with its given in the literature. Satisfactory elemental analysis for C, H and N were obtained for compound **14c**; none of the experimentally found percentages deviated from the theoretical values by more than 0.3%.[5]

3-(5-Bromo-1*H*-indol-3-yl)quinoxalin-2(1*H*)-one (14d)



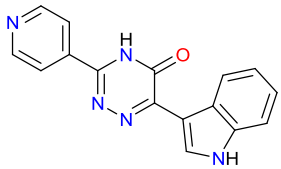
The residue was purified by column chromatography on silica gel eluting with mixture hexane/ethyl acetate 8/2 to give compound **14d** as a brown solid (203 mg, 87%). The product was identified as a compound **14d** by comparing its ^{1}H NMR spectra with its given in the literature. Satisfactory elemental analysis for C, H and N were obtained for compound **14d**; none of the experimentally found percentages deviated from the theoretical values by more than 0.3%.[5]

3-(1*H*-Pyrrol-2-yl)quinoxalin-2(1*H*)-one (14e)



The residue was purified by column chromatography on silica gel eluting with mixture hexane/ethyl acetate 8/2 to give compound **14e** as a brown solid (144 mg, 99%). The product was identified as a compound **14e** by comparing its ^{1}H NMR spectra with its given in the literature. Satisfactory elemental analysis for C, H and N were obtained for compound **14e**; none of the experimentally found percentages deviated from the theoretical values by more than 0.3%.[6]

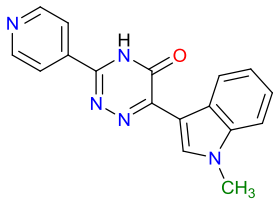
6-(1*H*-Indol-3-yl)-3-(pyridin-4-yl)-1,2,4-triazin-5(4*H*)-one (15a)



The residue was purified by column chromatography on silica gel eluting with mixture ethyl acetate/methanol 10/1 to give compound **15a** as a light brown solid (207 mg, 62%), mp 305-306 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) ppm: δ 7.14-7.18 (m, 2H, 5′-H, 6′-H), 7.45-7.48 (m, 1H, 7′-H), 8.11-8.15

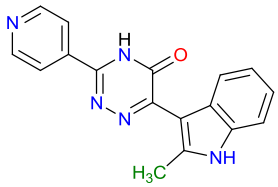
(m, 2H, Pyr), 8.47-8.49 (m, 1H, 4′-H), 8.75-8.77 (m, 2H, Pyr), 8.83-8.88 (d, 1H, ^{3}J(H,H) = 4.00 Hz, 2′-H), 11.64 (s, 1H, N′-H), 14.07 (s, 1H, N-H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) ppm: δ 108.65 (C3′); 112.46 (C7′); 121.12 (C6′); 121.75 (2C-Pyr), 122.81 (C5′), 122.87 (C4′); 125.94 (C4a′); 132.72 (C2′); 136.83 (C7a′); 140.13 (C-Pyr); 149.50 (C6); 150.82 (2C-Pyr); 153.99 (C3); 161.03 (C5). ESI-MS: *m/z* (%): 289 (100) [M^+]. Anal. Found: C, 66.39; H, 3.81; N, 24.25. Calc for $C_{16}H_{11}N_5O$: C, 66.43; H, 3.83; N, 24.21.

6-(1-Methyl-1*H*-indol-3-yl)-3-(pyridin-4-yl)-1,2,4-triazin-5(4*H*)-one (15b)



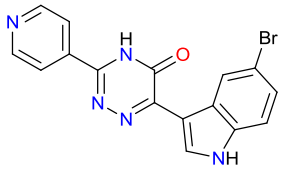
The residue was purified by column chromatography on silica gel eluting with mixture ethyl acetate/methanol 10/1 to give compound **15b** as a light brown solid (208 mg, 60%), mp 229-230 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) ppm: δ 3.94 (s, 3H, N′-Me), 7.20-7.29 (m, 2H, 5′-H, 6′-H), 7.48-7.50 (m, 1H, 7′-H), 8.08-8.10 (m, 2H, Pyr), 8.43-8.45 (m, 1H, 4′-H), 8.84-8.79 (m, 3H, 2′-H, Pyr), 14.33 (s, 1H, N-H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) ppm: δ 32.94 (N′-Me); 99.49 (C3′); 107.06 (C-Pyr); 110.30 (C7′); 120.98 (C6′); 121,25 (2C-Pyr), 121.42 (C5′); 122,48 (C4′); 125.86 (C4a′); 136.05 (C7a′); 136.87 (C2′); 148.67 (C6); 149.96 (C3); 150.34 (2C-Pyr); 153.39 (C5). ESI-MS: *m/z* (%): 303 (100) [M^+]. Anal. Found: C, 67.38; H, 4.37; N, 23.05. Calc for $C_{17}H_{13}N_5O$: C, 67.32; H, 4.32; N, 23.09.

6-(2-Methyl-1*H*-indol-3-yl)-3-(pyridin-4-yl)-1,2,4-triazin-5(4*H*)-one (15c)



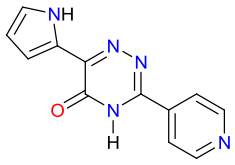
The residue was purified by column chromatography on silica gel eluting with mixture ethyl acetate/methanol 10/1 to give compound **15c** as a light brown solid (199 mg, 62%), mp 277-278 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) ppm: δ 2.55 (s, 3H, C′-Me), 6.98-7.07 (m, 2H, 5′-H, 6′-H), 7.32-7.33 (d, 1H, ^{3}J(H,H) = 4.00 Hz, 7′-H), 7.67-7.69 (d, 1H, ^{3}J(H,H) = 8.00 Hz, 4′-H), 8.10-8.11 (m, 2H, Pyr), 8.79-8.81 (d, 2H, ^{3}J(H,H) = 8.00 Hz, Pyr), 11.39 (s, 1H, N′-H), 14.28 (s, 1H, N-H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) ppm: δ 14.49 (C′-Me); 105.75 (C3′); 111.20 (C7′); 119.97 (C6′); 120.78 (C4′); 121,39 (C5′), 121,75 (2C-Pyr), 127.95 (C4a′), 135.73 (C7a′); 139.04 (C-Pyr); 139.24 (C2′); 150.74 (C6); 150.99 (2C-Pyr); 154.83 (C3); 160.99 (C5). ESI-MS: *m/z* (%): 303 (100) [M^+]. Anal. Found: C, 67.30; H, 4.30; N, 23.08; O, 5.32. Calc for $C_{17}H_{13}N_5O$: C, 67.32; H, 4.32; N, 23.09; O, 5.27.

6-(5-Bromo-1*H*-indol-3-yl)-3-(pyridin-4-yl)-1,2,4-triazin-5(4*H*)-one (15d)



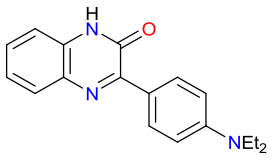
The residue was purified by column chromatography on silica gel eluting with mixture ethyl acetate/methanol 10/1 to give compound **15d** as a yellow solid (202 mg, 48%), mp 268-270 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) ppm: δ 7.36-7.38 (m, 1H, 4′-H), 7.50-7.52 (m, 1H, 7′-H), 8.07-8.08 (m, 2H, Pyr), 8.66 (m, 1H, 6′-H), 8.84-8.89 (m, 3H, 2′-H, Pyr), 11.99 (s, 1H, N′-H), 14.33 (s, 1H, N-H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) ppm: δ 99.49 (C3′); 107.21 (C4a′); 113.61 (C7a′); 114.14 (C7′), 121.12 (2C-Pyr), 124.31 (C6′); 124.99 (C4′); 126.98 (C5); 133.76 (C2′); 135.09 (C6); 138.20 (C3); 150.53 (3C-Pyr); 153.08 (C5). ESI-MS: *m/z* (%): 367 (100) [M$^+$]. Anal. Found: C, 52.16; H, 2.70; N, 19.09. Calc for $C_{16}H_{10}BrN_5O$: C, 52.19; H, 2.74; N, 19.02.

6-(1*H*-Pyrrol-2-yl)-3-(pyridin-4-yl)-1,2,4-triazin-5(4*H*)-one (15e)



The residue was purified by column chromatography on silica gel eluting mixture ethyl acetate/methanol 10/1 to give compound **15e** as a light brown solid (179 mg, 65%), mp 245-246 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) ppm: δ 6.24-6.26 (m, 1H, 4′-H), 7.07-7.09 (m, 1H, 5′-H), 7.31 (s, 1H, 3′-H), 8.03-8.05 (m, 2H, Pyr), 8.82-8.83 (m, 2H, Pyr), 11.68 (s, 1H, N′-H), 14.24 (s, 1H, N-H) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) ppm: δ 99.49 (C2′); 109.75 (C4′); 114.96 (C3′); 121.22 (2C-Pyr); 121,34 (C3), 123,63 (C5′), 124.31 (C6), 138.18 (C-Pyr); 150.16 (C5); 150.44 (2C-Pyr). ESI-MS: *m/z* (%): 239 (100) [M$^+$]. Anal. Found: C, 60.29; H, 3.76; N, 29.30; O, 6.65. Calc for $C_{17}H_{13}N_5O$: C, 60.25; H, 3.79; N, 29.27; O, 6.69.

3-(4'-Diethylaminophenyl)quinoxalin-2(1*H*)-one (22)

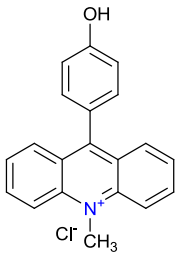


The residue was purified by column chromatography on silica gel eluting with mixture hexane/ethyl acetate 8/2 to give compound **22** as a brown solid (190 mg, 95%). The product was identified as a compound **22** by comparing its ^{1}H NMR spectra with its given in the literature. Satisfactory elemental analysis for C, H and N were obtained for compound **22**; none of the experimentally found percentages deviated from the theoretical values by more than 0.3%.[7]

7. Synthesis of compound 25a,b

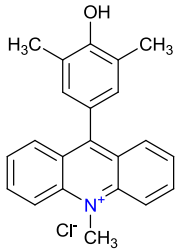
To a round bottom flask were added a solution of phenol **23a** (1 mmol) or 2,6-dimethylphenol **23b** (1 mmol) in dry ethanol and NaOH. The reaction mixture was refluxed for 2 h. The hot solution of N-methylacridinium iodide **4h** was added in solution of phenol and refluxing was continued for 4 h. The reaction mixture was further concentrated under a reduce pressure. A quartz tube containing solution of residue and TiO_2 (10 mass.%, anatase) in *n*-BuOH and HCl (2 equiv.) was treated in ultrasonic bath for 5 min to obtain a suspension. The resulting mixture was exposed to Xe lamp (5000 K, 35 W) under air oxygen, bubbling through the reaction mixture at room temperature for 4 h. The reaction mixture was filtered. The solvent from filtrate was removed under vacuum. Then dry diethyl ether was added to resulting mixture and the form suspension was filtered.

9-(4'-Hydroxyphenyl)-10-methylacridinium chloride (25a)



The residue was recrystallized from ethyl mixture acetate/methanol to give compound **25a** as a orange solid. Yield 206 mg (80%). The product was identified as a compound **25a** by comparing its ^{1}H NMR spectra with its given in the literature. Satisfactory elemental analyses for C, H and N were obtained for compound **25a**; none of the experimentally found percentages deviated from the theoretical values by more than 0.3%.[4]

9-(4'-Hydroxy-3',5'-dimethylphenyl)-10-methylacridinium chloride (25b)



The residue was recrystallized from mixture ethyl acetate/methanol to give compound **25b** as a orange solid. Yield 191 mg (90%), mp 192-193 ºC. ^{1}H NMR (400 MHz, DMSO-d_6) ppm: δ 2.33 (s, 6H, 2C′-CH_3), 4.91 (s, 3H, N-CH_3), 7.15 (s, 2H, 2′-H, 6′-H), 7.90-7,94 (t, ^3J(H,H) = 8.00 Hz, 2H, 2-H, 7-H), 8.10-8.12 (d, 2H, ^3J(H,H) = 8.00 Hz, 4-H, 5-H), 8.41-8.45 (m, 2H, 3-H, 6-H), 8.82-8.85 (d, ^3J(H,H) = 12.00 Hz, 2H, 1-H, 8-H), 9.16 (s, 1H, OH) ppm. ^{13}C NMR (100 MHz, DMSO-d_6) ppm: δ 16.72 ($2CH_3$); 38.88 (N-Me); 119.08 (C1, C8); 123.47 (C1′); 124.90 (C3′, C5′); 125.67 (C8a, C10a); 127.60 (C2, C7); 130.12 (C2′, C6′); 130.29 (C4, C5); 138.19 (C3, C6); 141.15 (C4a, C9a); 155.27 (C4′); 161.53 (C9). ESI-

MS: *m/z* (%): 314 (100) [M^+]. Anal. Found: C, 75.56; H, 5.74; N, 4.02. Calc for $C_{22}H_{20}ClNO$: C, 75.53; H, 5.76; N, 4.00.

NMR ^{1}H Spectra

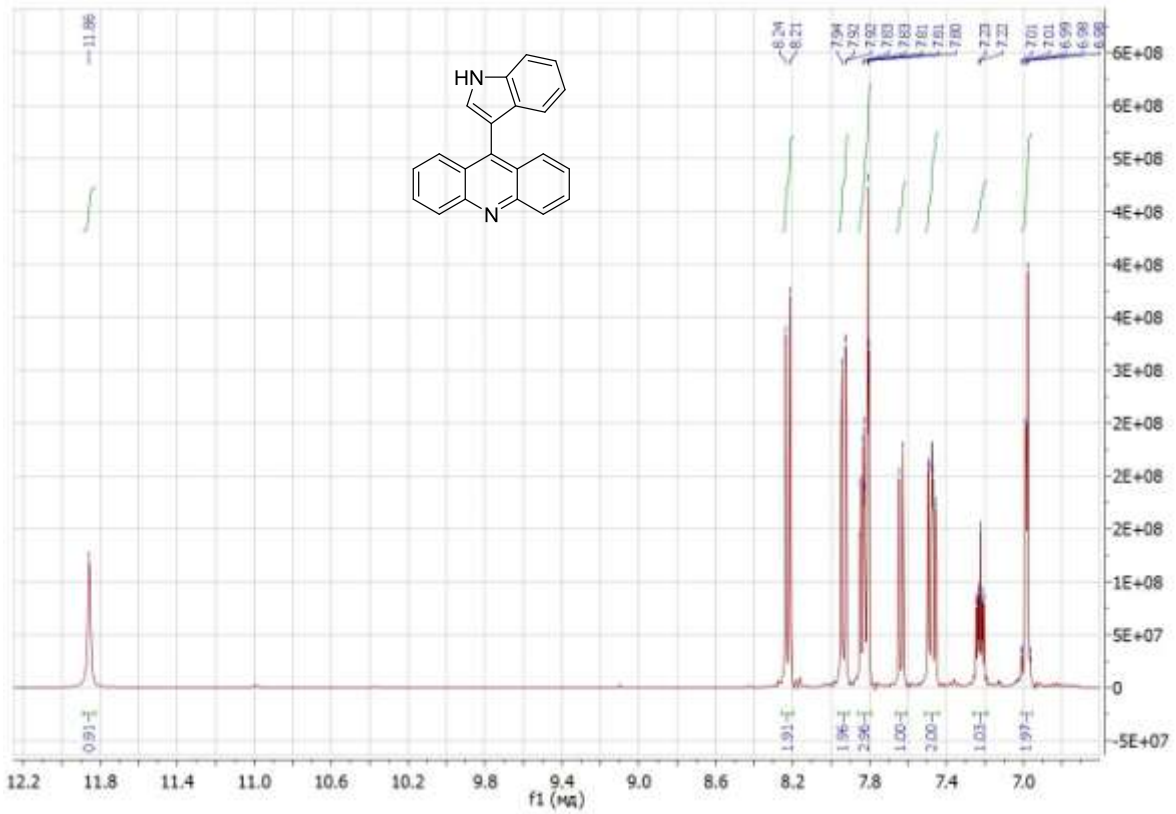


Figure S1. ^{1}H NMR Spectrum of 9-(1*H*-indol-3-yl)acridine (6a)

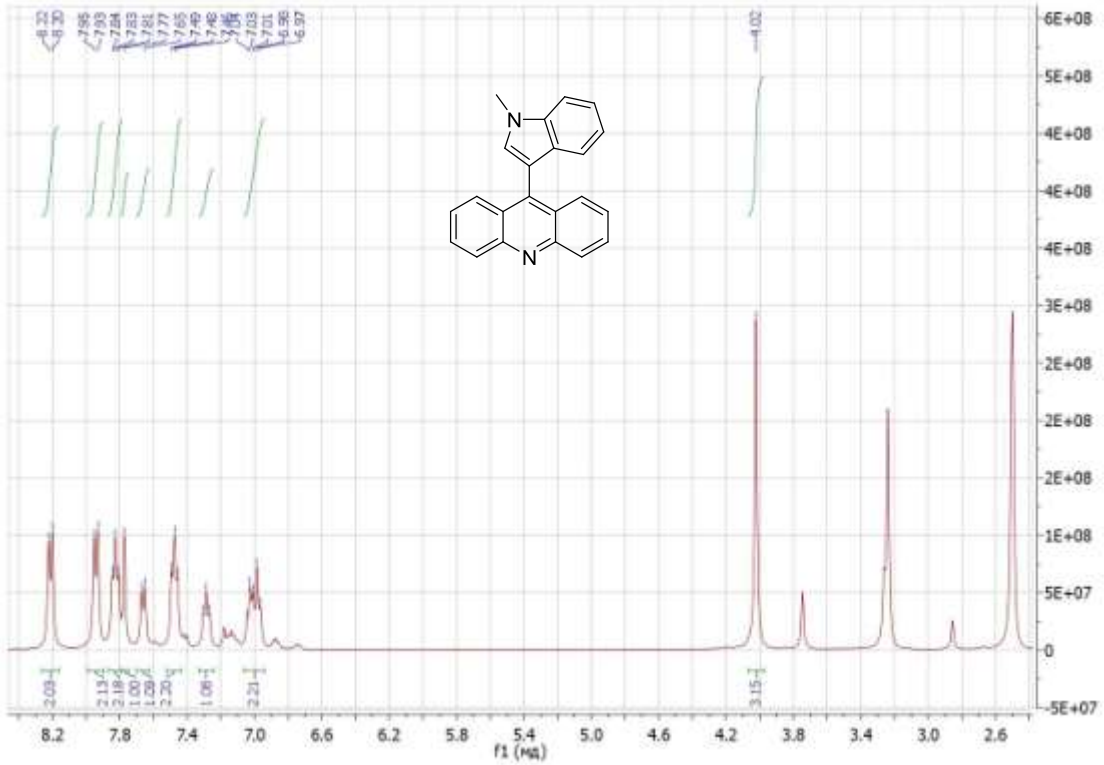


Figure S2. ^{1}H NMR Spectrum of 9-(N-methylindol-3-yl)acridine (6b)

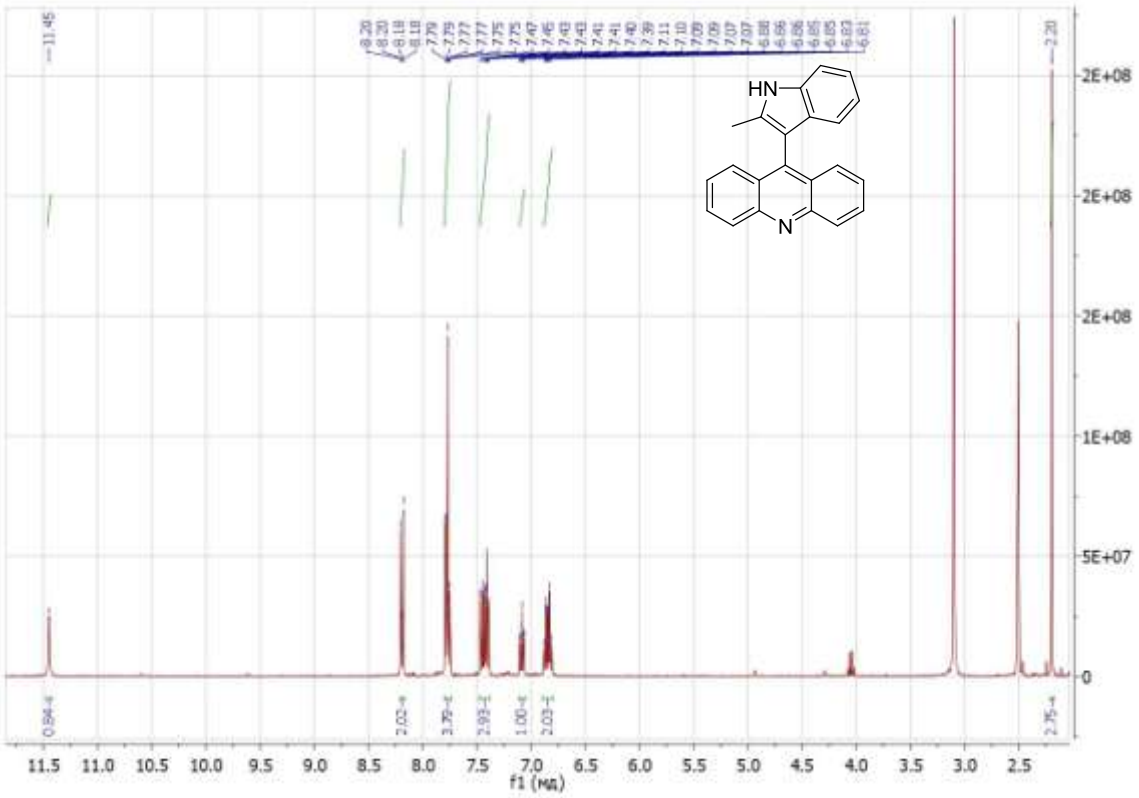


Figure S3. ^{1}H NMR Spectrum of 9-(2-methylindol-3-yl)acridine (6c)

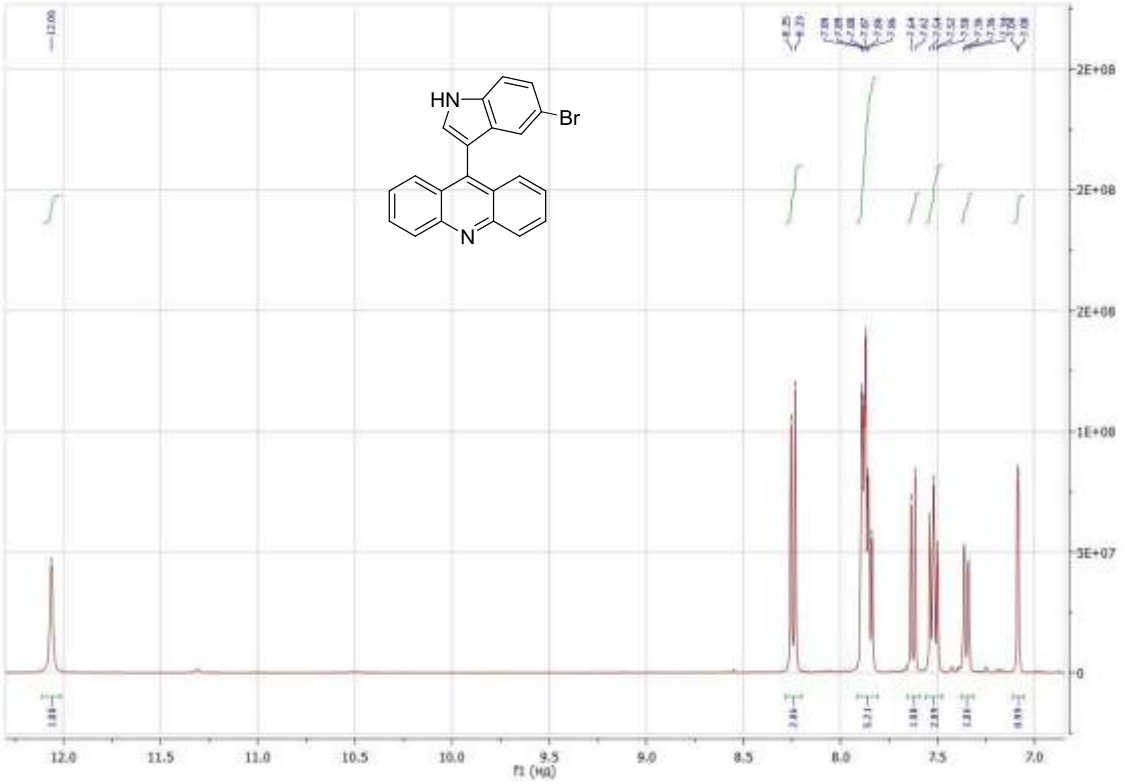


Figure S4. ^{1}H NMR Spectrum of 9-(5-bromo-1*H*-indol-3-yl)acridine (6d)

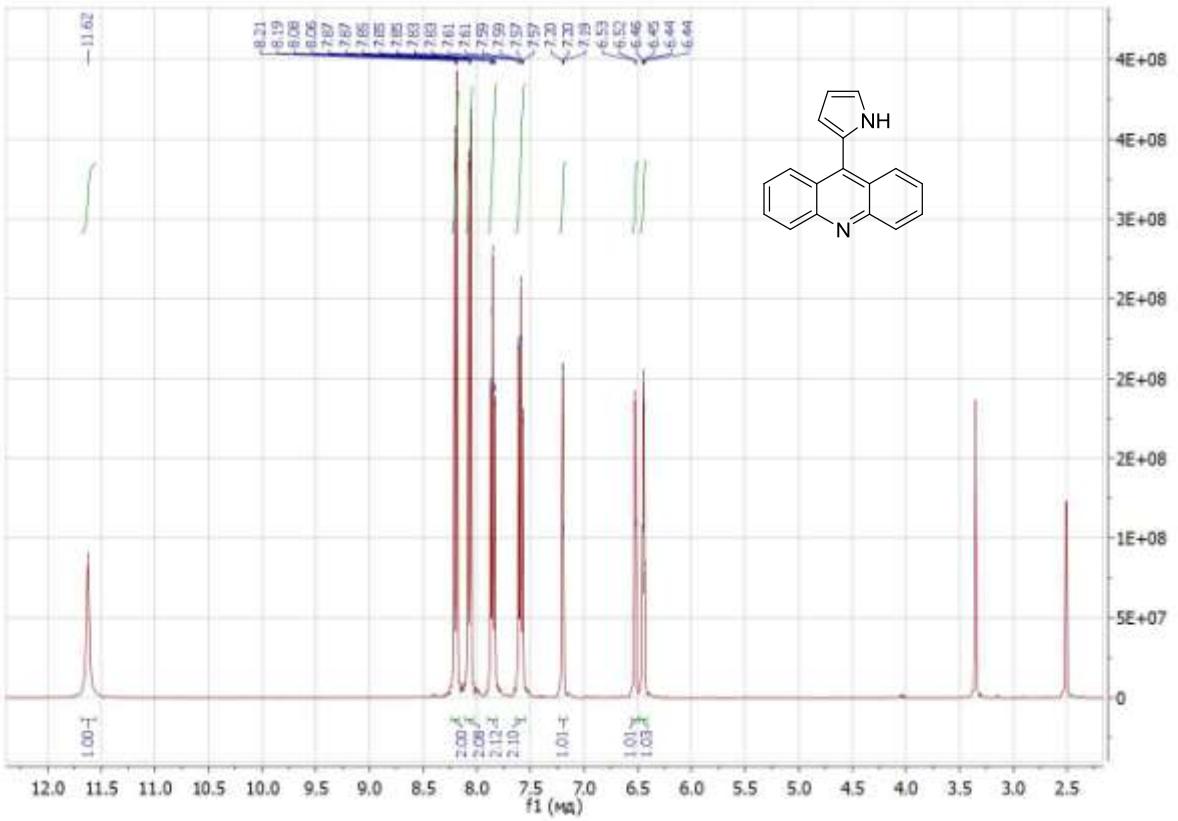


Figure S5. ^{1}H NMR Spectrum of 9-(1*H*-pyrrol-2-yl)acridine (6e)

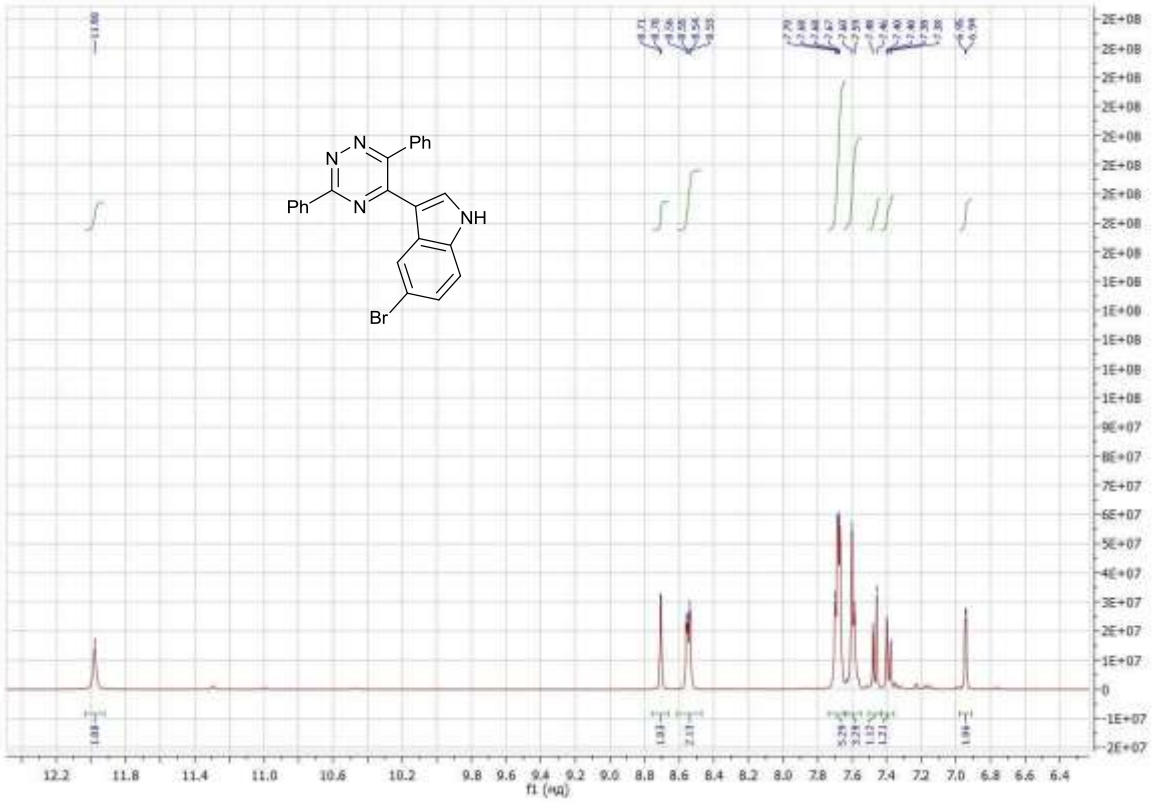


Figure S6. ^{1}H NMR Spectrum of 3,6-diphenyl-5-(5-bromo-1*H*-indol-3-yl)-1,2,4-triazine (7d)

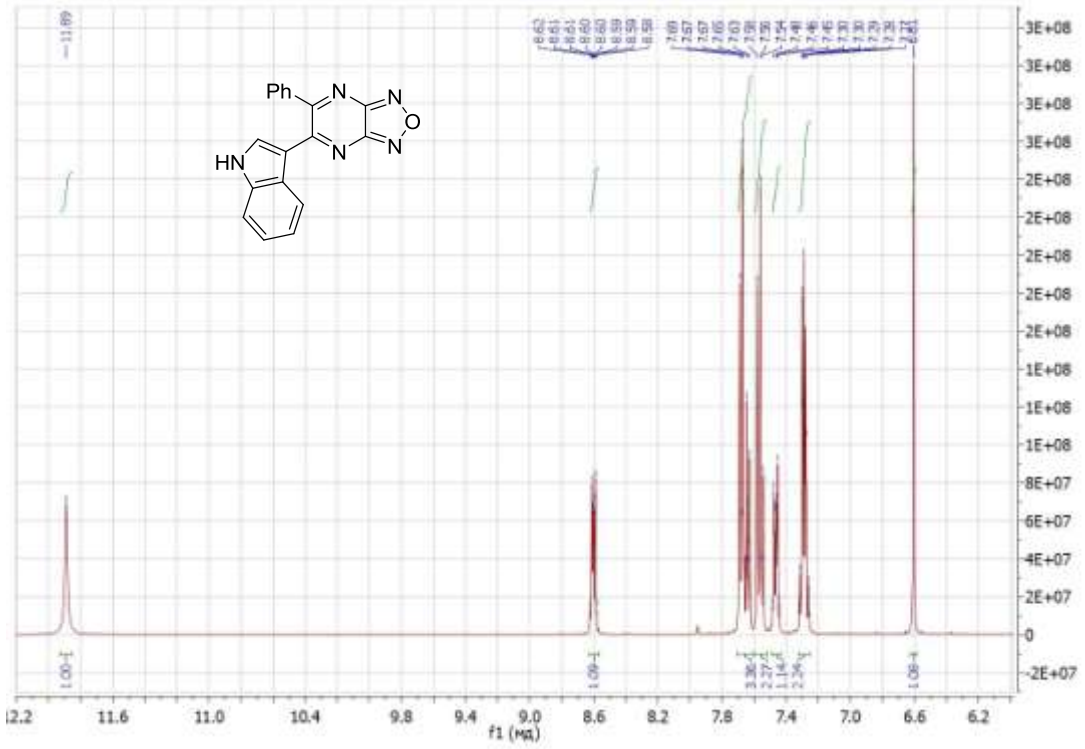


Figure S7. ^{1}H NMR Spectrum of 5-(1*H*-indol-3-yl)-6-phenyl-1,2,5-oxadiazolo[3,4-*b*]pyrazine (8a)

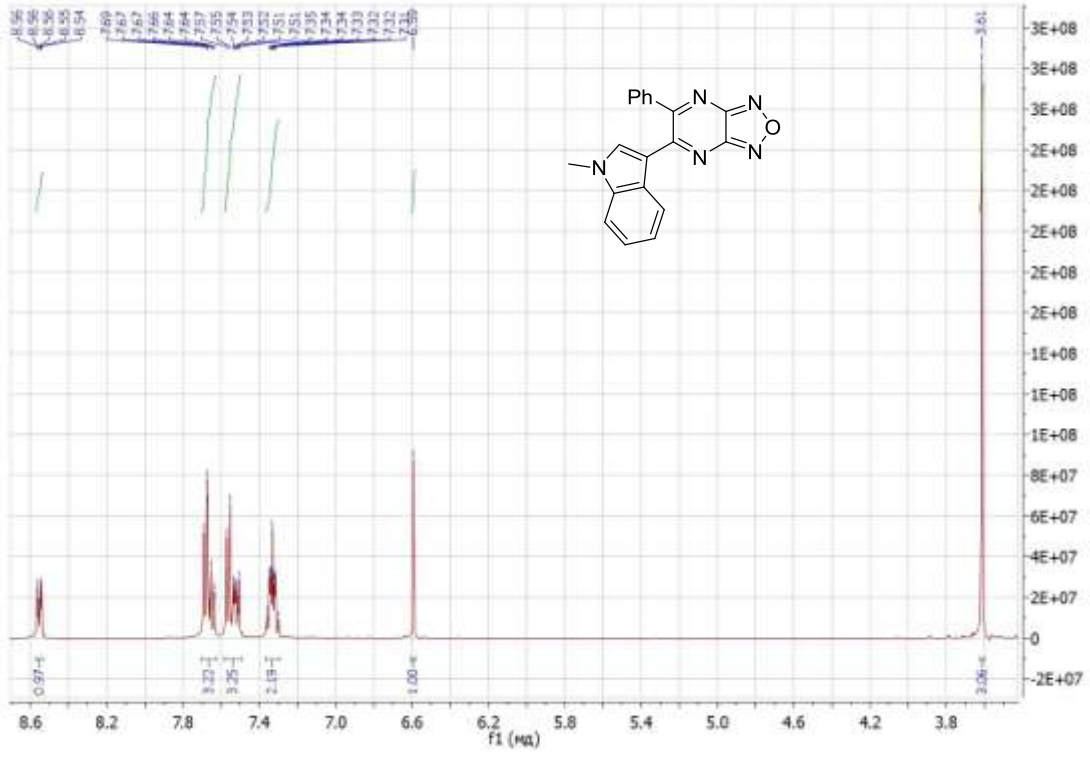


Figure S8. ^{1}H NMR Spectrum of 5-(N-methylindol-3-yl)-6-phenyl-1,2,5-oxadiazolo[3,4-*b*]pyrazine (8b)

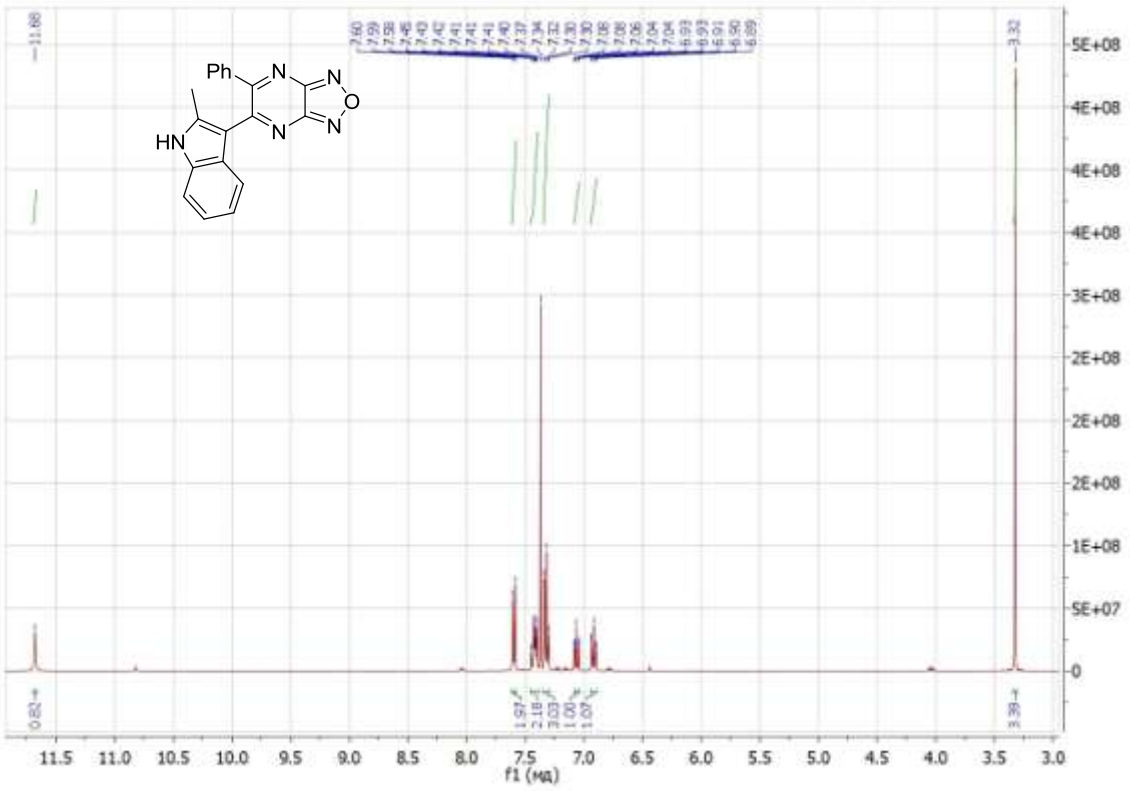


Figure S9. ^{1}H NMR Spectrum of 5-(2-methyl-1*H*-indol-3-yl)-6-phenyl-1,2,5-oxadiazolo[3,4-*b*]pyrazine (8c)

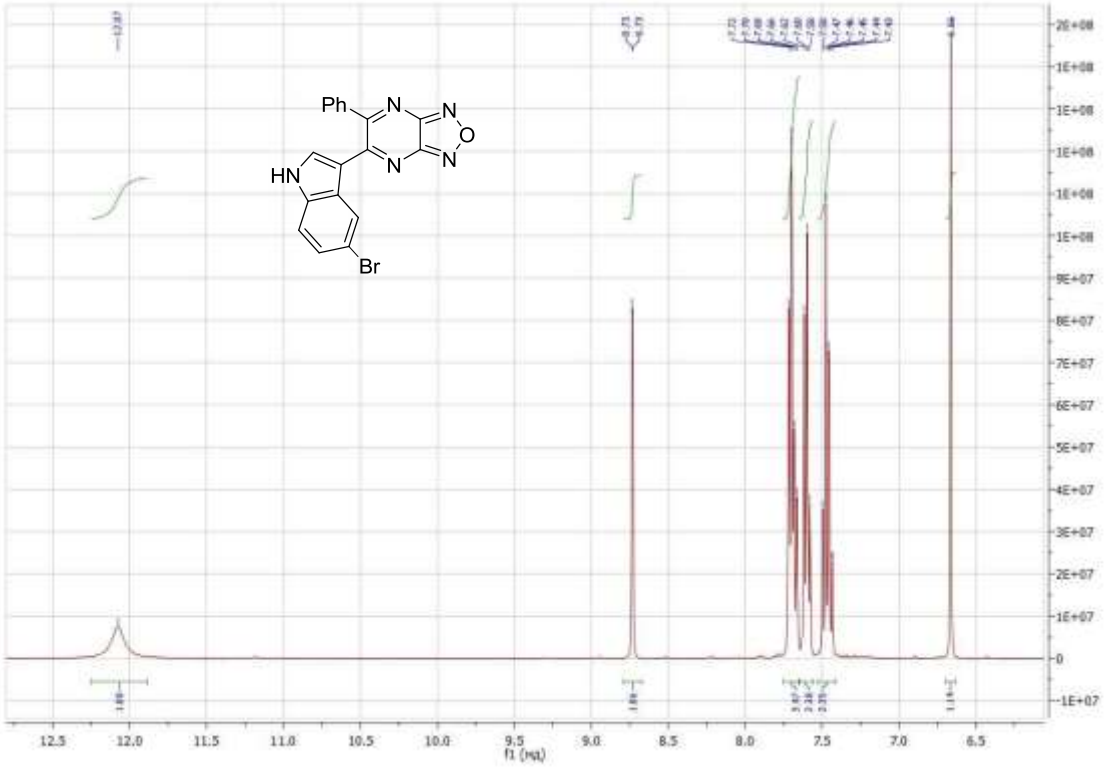


Figure S10. ^{1}H NMR Spectrum of 5-(5-bromo-1*H*-indol-3-yl)-6-phenyl-1,2,5-oxadiazolo[3,4-*b*]pyrazine (8d)

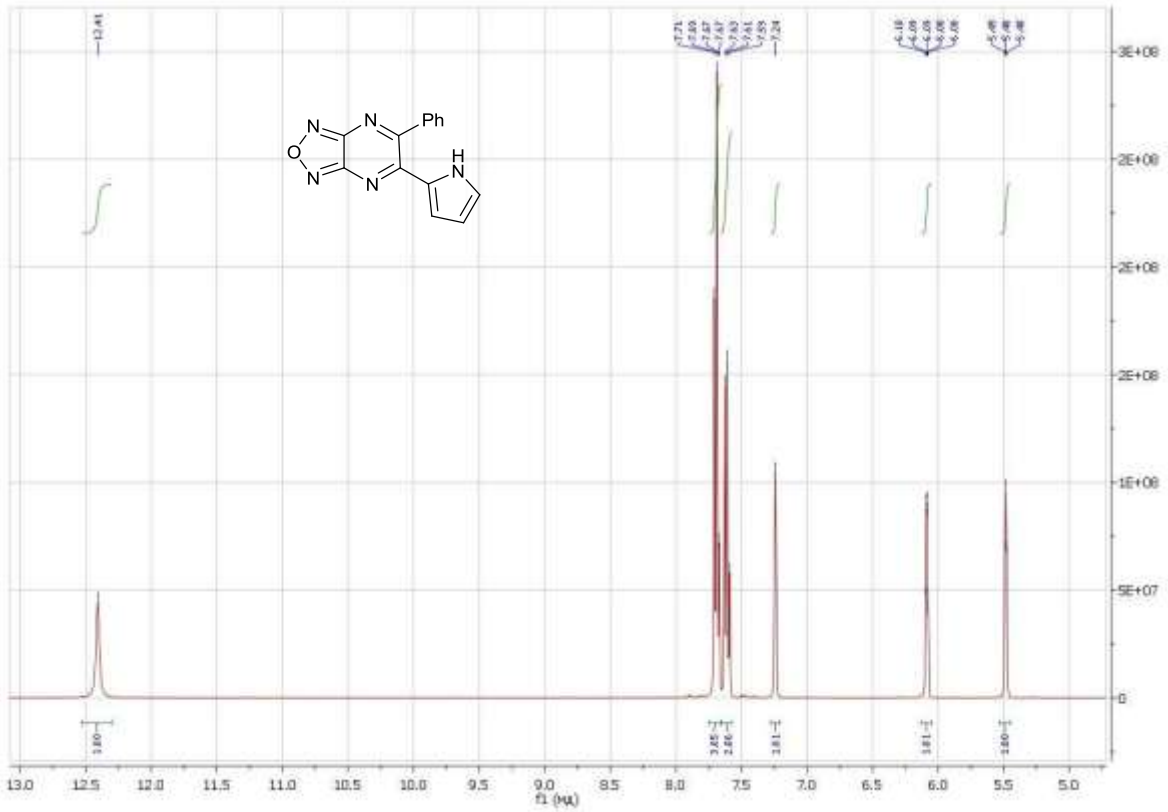


Figure S11. ^{1}H NMR Spectrum of 5-phenyl-6-(1*H*-pyrrol-2-yl)-[1,2,5]oxadiazolo[3,4-*b*]pyrazine (8e)

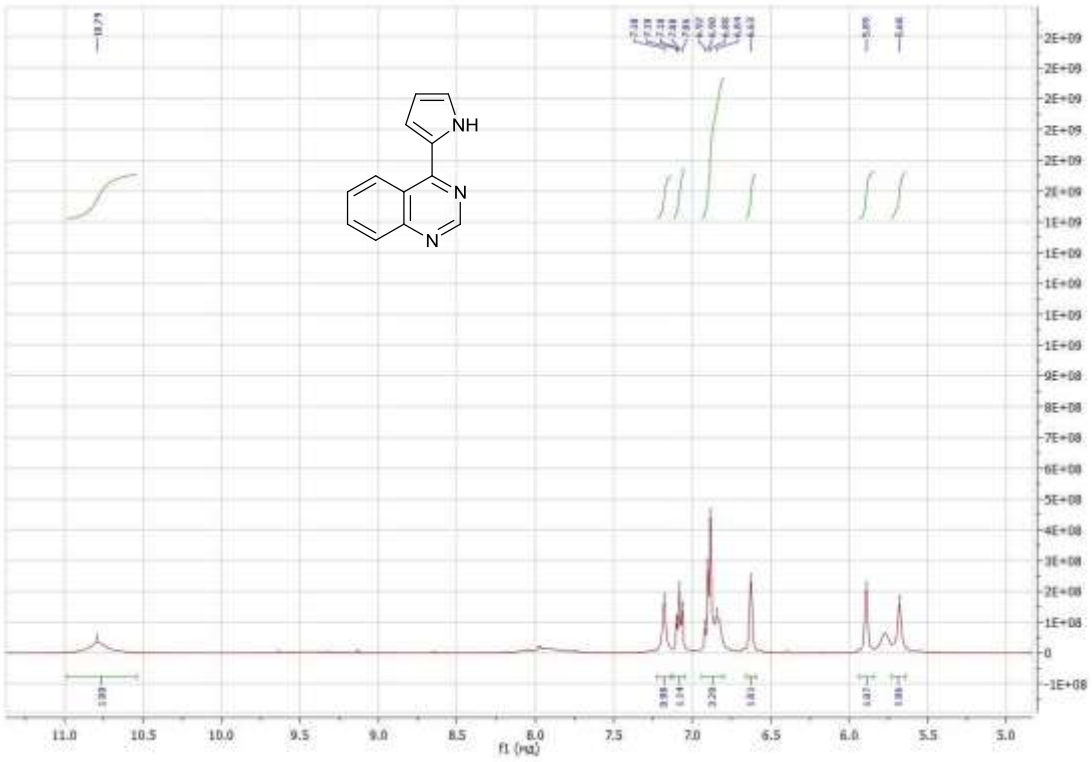
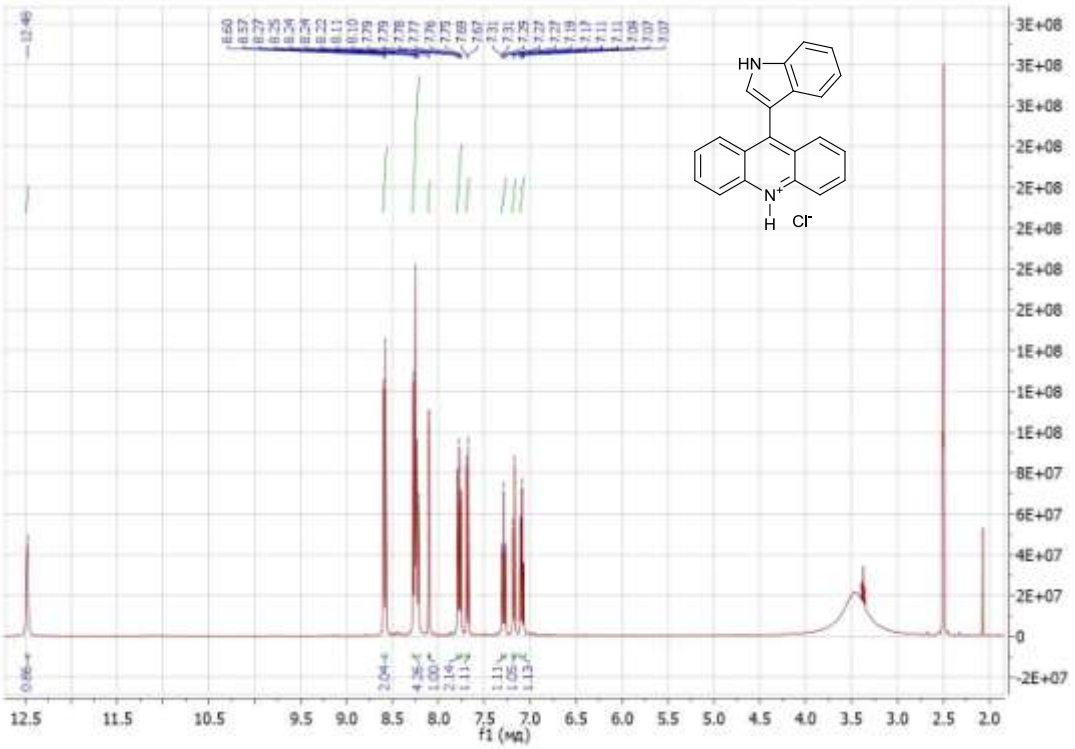


Figure S12. ^{1}H NMR Spectrum of 4-(1*H*-pyrrol-2-yl)quinazoline (9e)



S13. Figure ^{1}H NMR Spectrum of 9-(1*H*-indol-3-yl)-10-hydroacridinum chloride (11a)

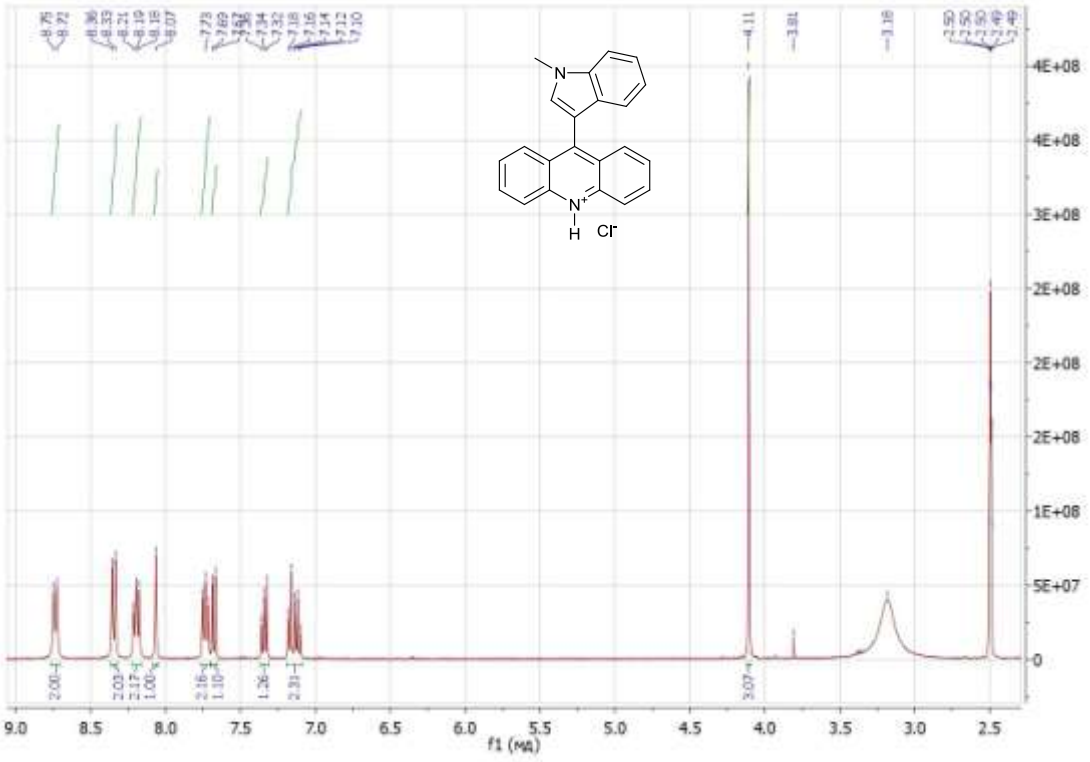


Figure S14. ^{1}H NMR Spectrum of 9-(N-methylindol-3-yl)-10-hydroacridinum chloride (11b)

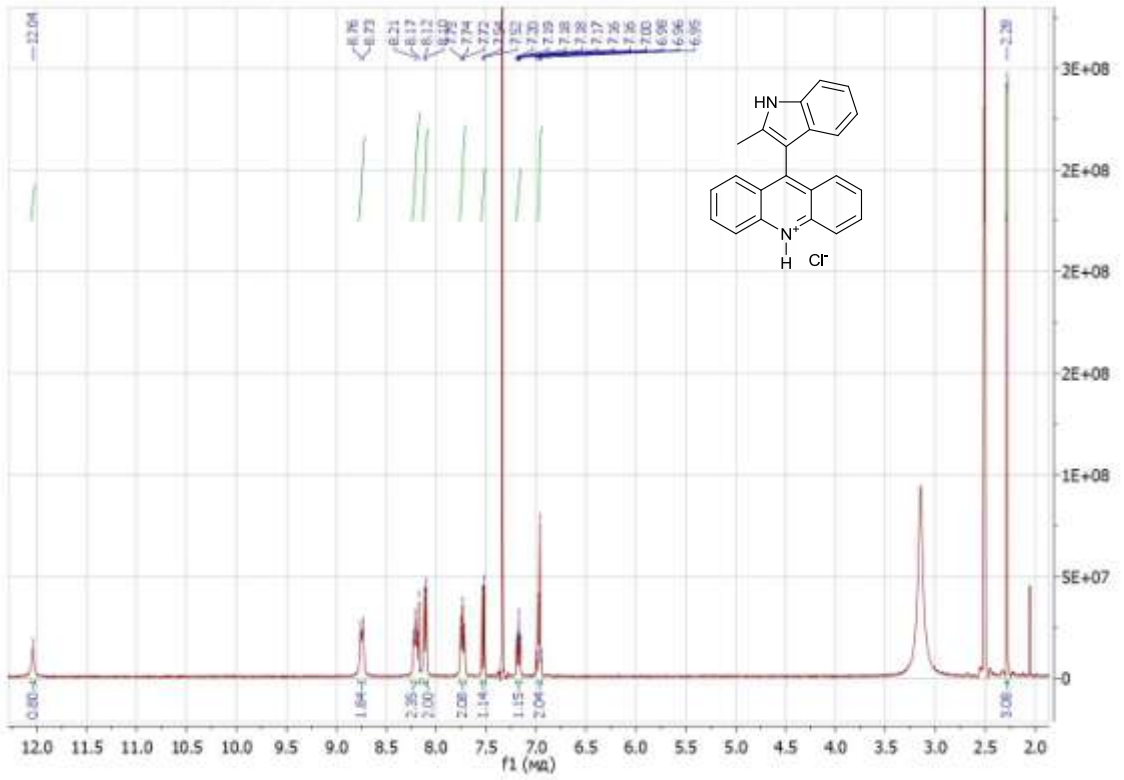


Figure S15. ^{1}H NMR Spectrum of 9-(2-methyl-1*H*-indol-3-yl)-10-hydroacridinum chloride (11c)

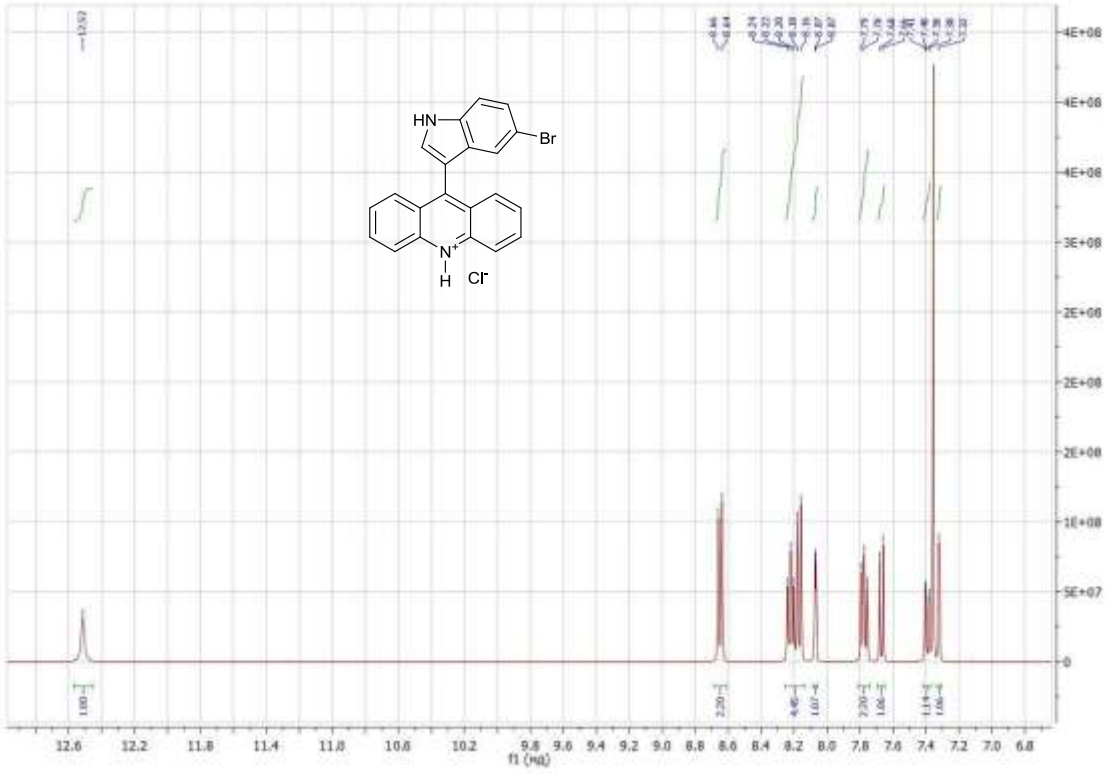


Figure S16. ^{1}H NMR Spectrum of 9-(5-bromo-1*H*-indol-3-yl)-10-hydroacridinum chloride (11d)

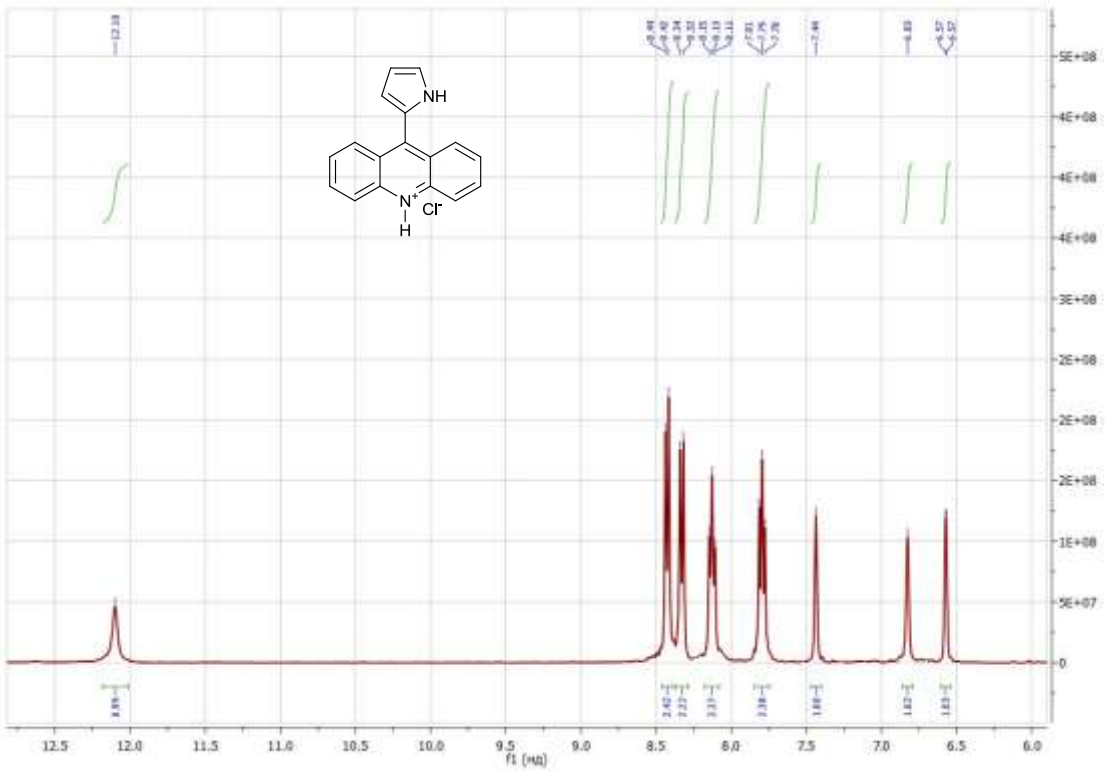


Figure S17. ^{1}H NMR Spectrum of 9-(1*H*-pyrrol-2-yl)-10-hydroacridinum chloride (11d)

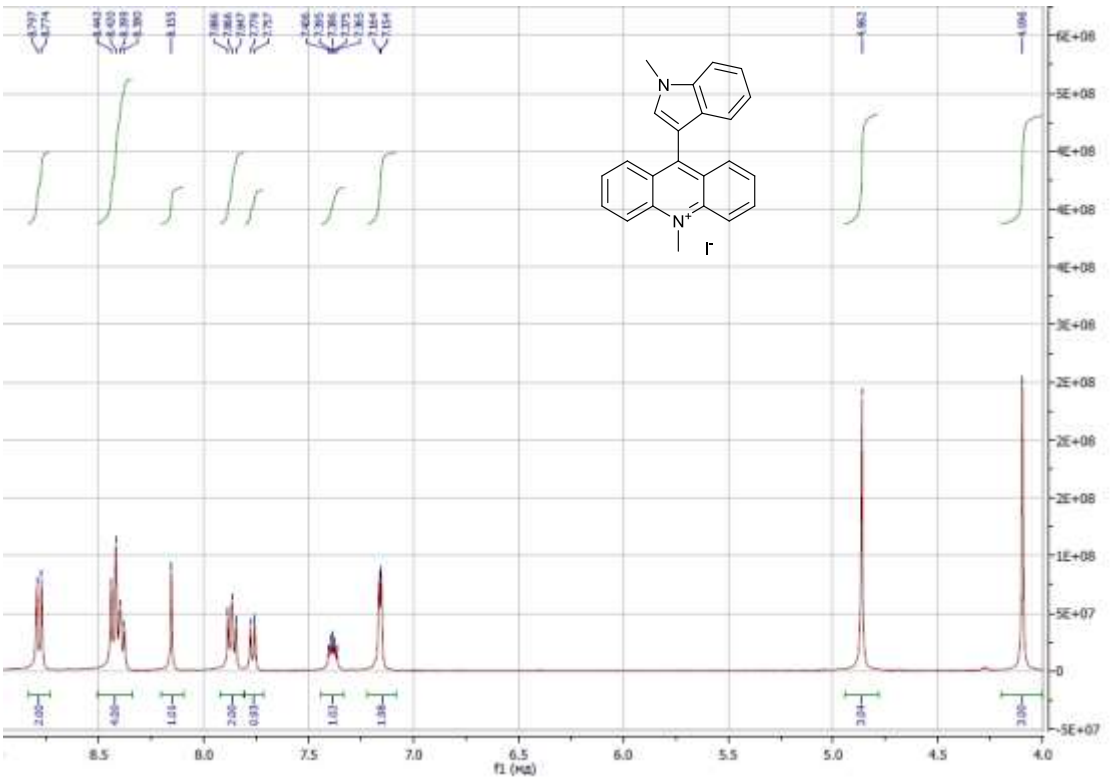


Figure S18. ^{1}H NMR Spectrum of 9-(N-methylindol-3-yl)-10-methylacridinum iodide (12b)

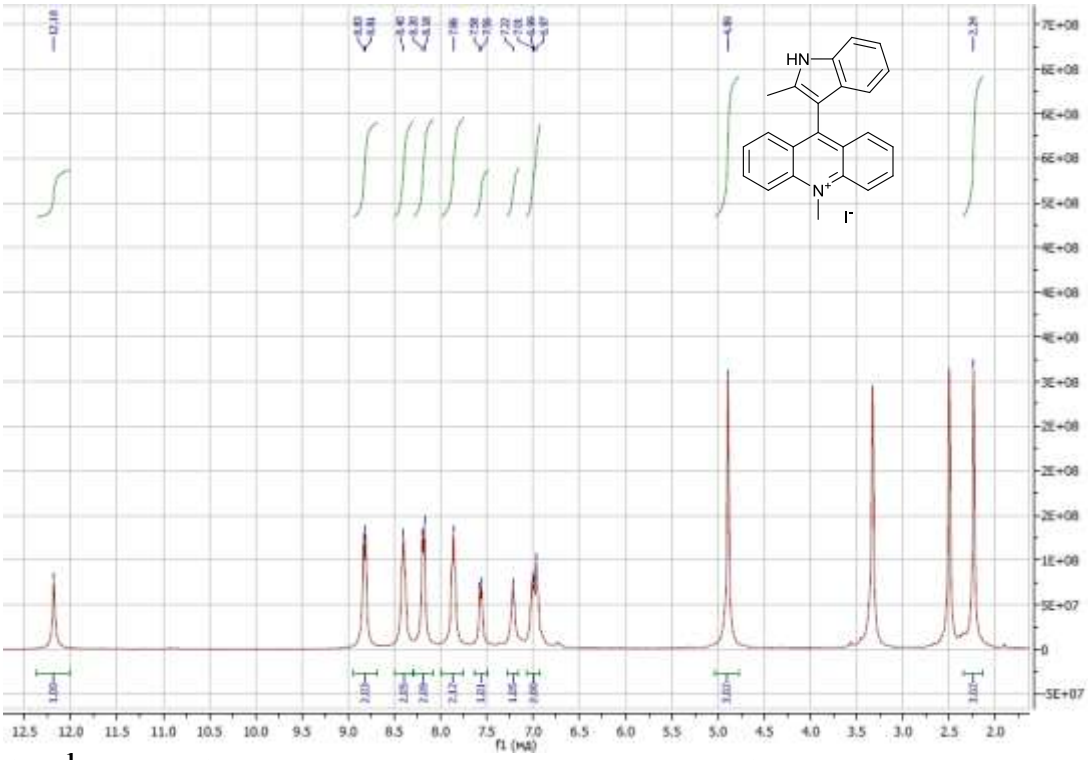


Figure S19. ^{1}H NMR Spectrum of 9-(2-methyl-1*H*-indol-3-yl)-10-methylacridinum iodide (12c)

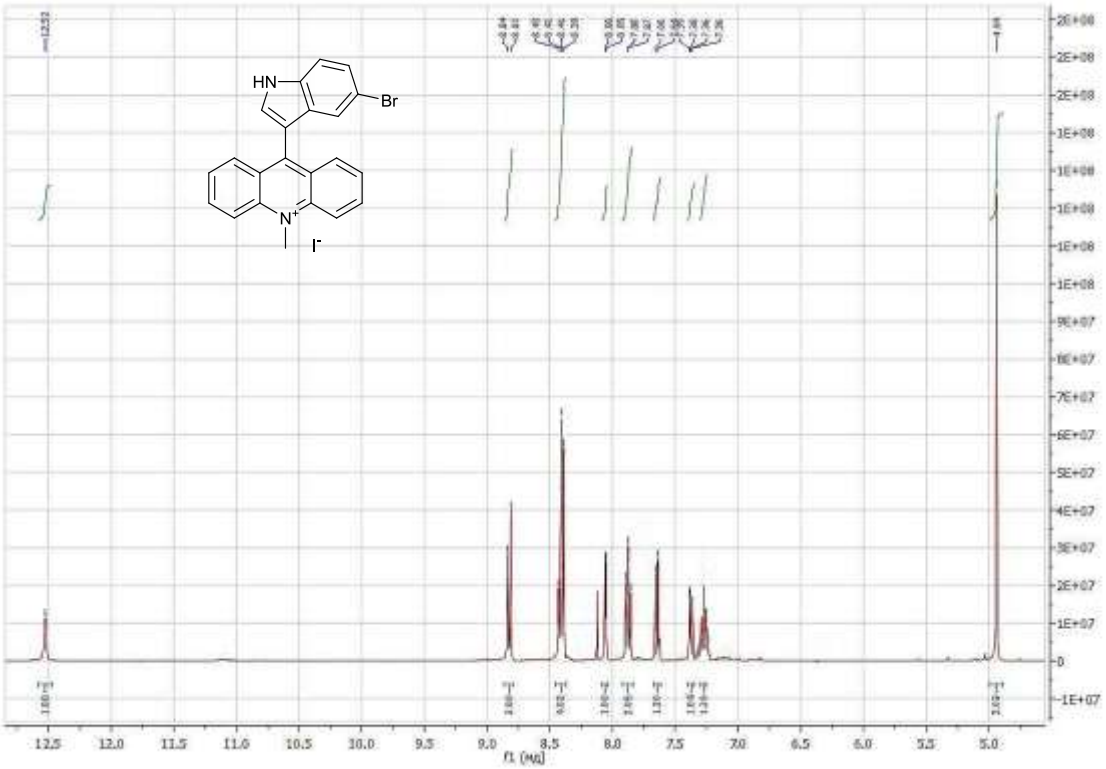


Figure S20. ^{1}H NMR Spectrum of 9-(5-bromo-1*H*-indol-3-yl)-10-methylacridinum iodide (12d)

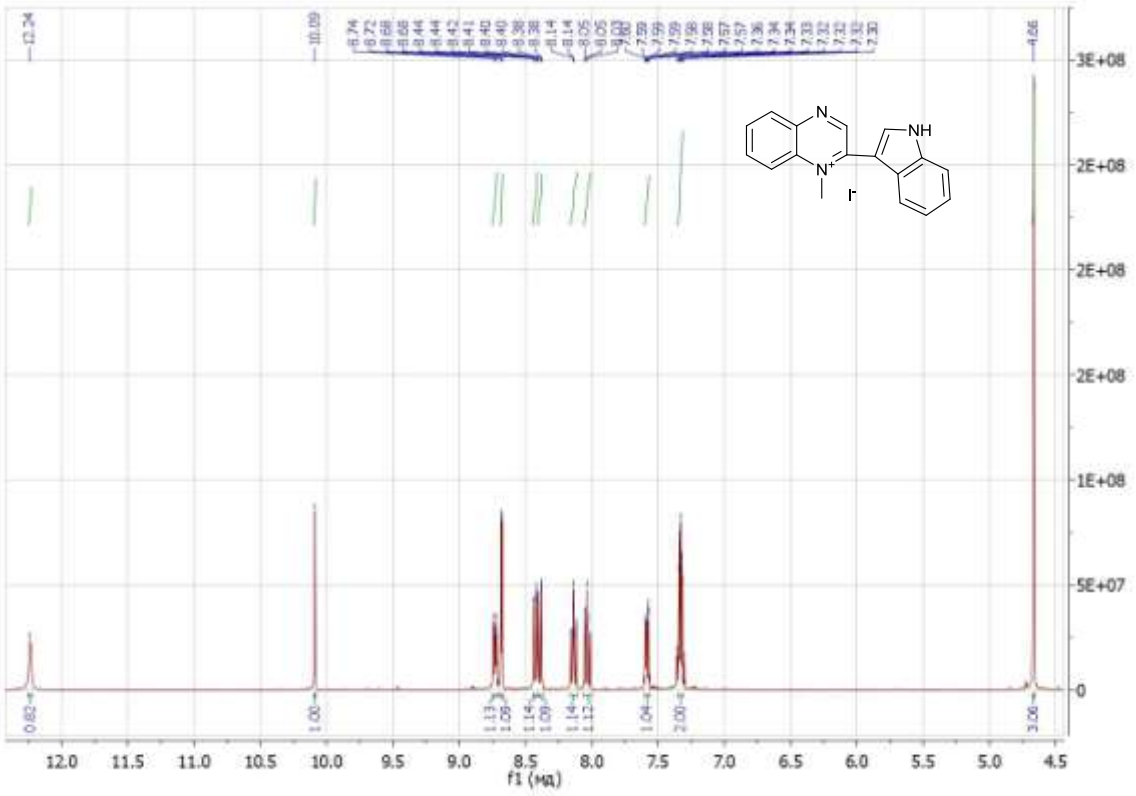


Figure S21. ^{1}H NMR Spectrum of 2-(1*H*-indol-3-yl)-1-methylquinoxalin-1-ium iodide (13a)

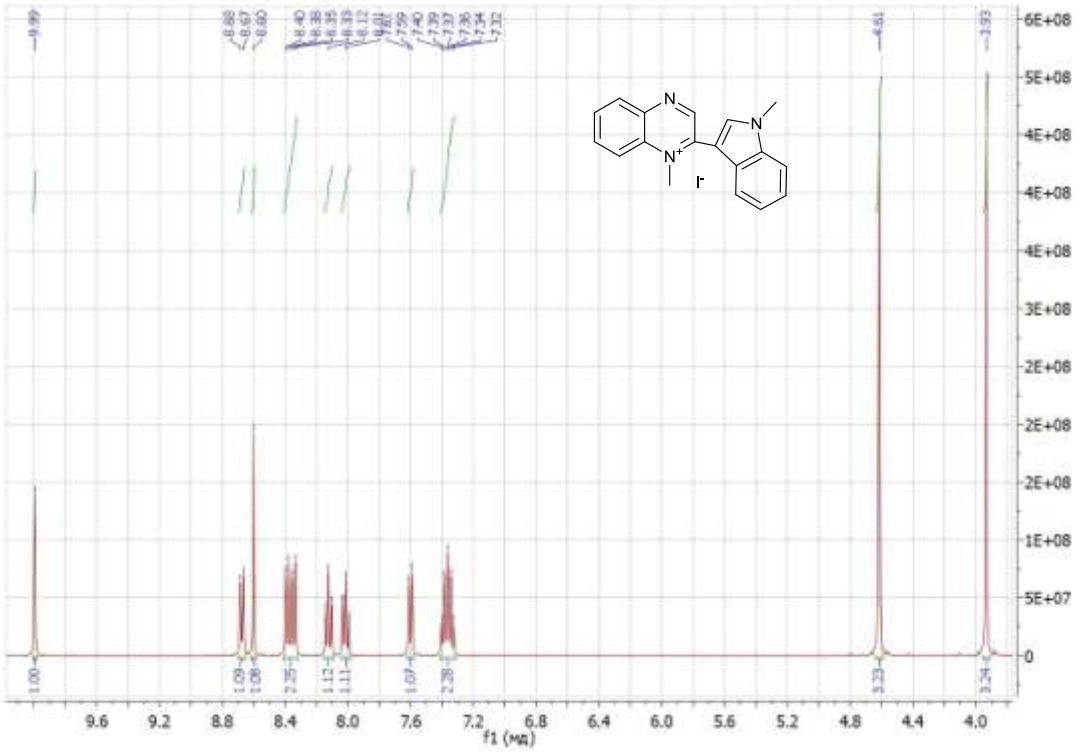


Figure S22. ^{1}H NMR Spectrum of 2-(N-methylindol-3-yl)-1-methylquinoxalin-1-ium iodide (13b)

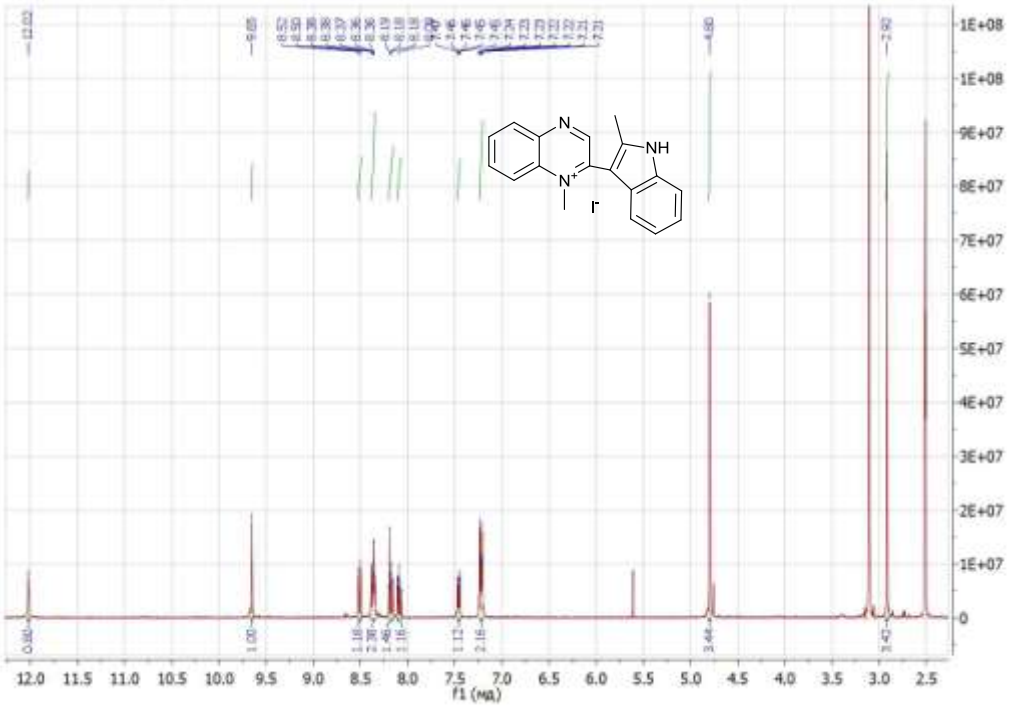


Figure S23. ^{1}H NMR Spectrum of 2-(2-methyl-1*H*-indol-3-yl)-1-methylquinoxalinum iodide (13c)

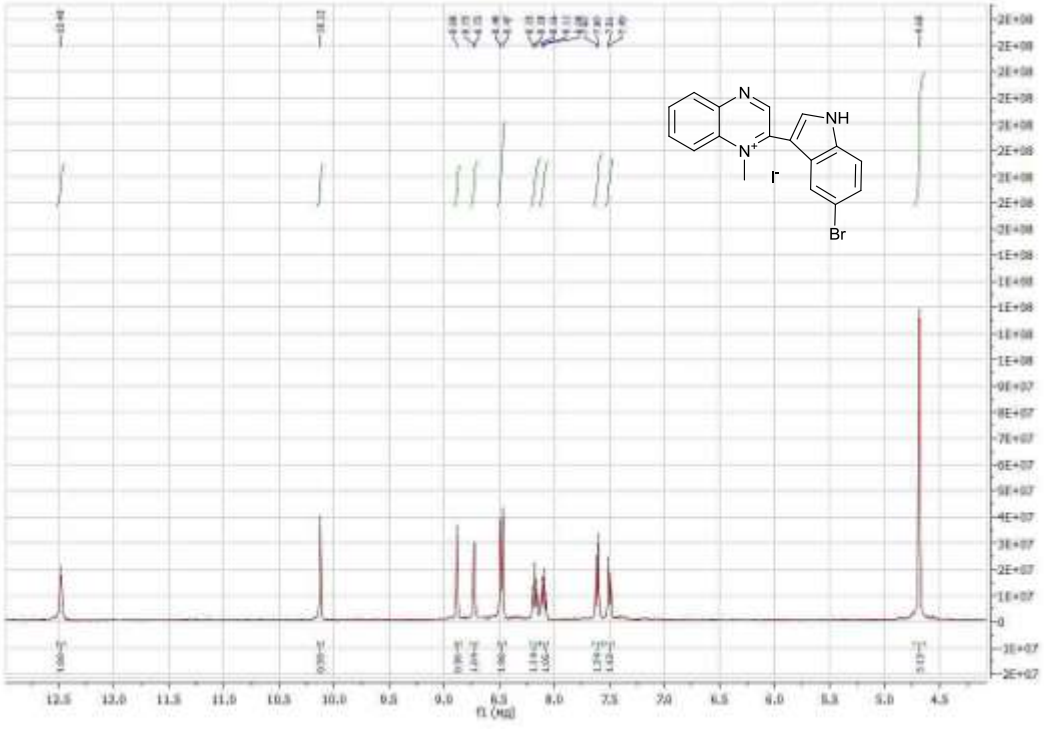


Figure S24. ^{1}H NMR Spectrum of 2-(5-bromo-1*H*-indol-3-yl)-1-methylquinoxalinum iodide (13d)

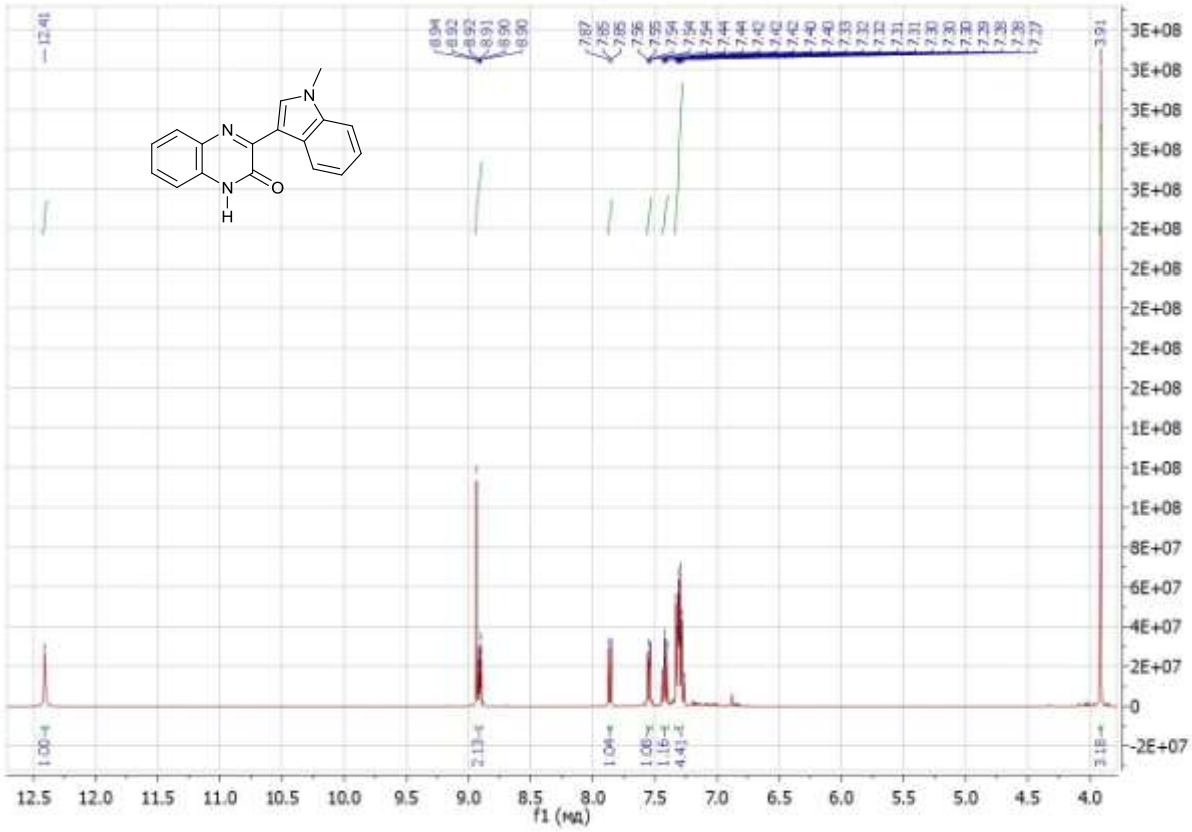


Figure S25. ^{1}H NMR Spectrum of 3-(N-methylindol-3-yl)quinoxalin-2(1*H*)-one (14b)

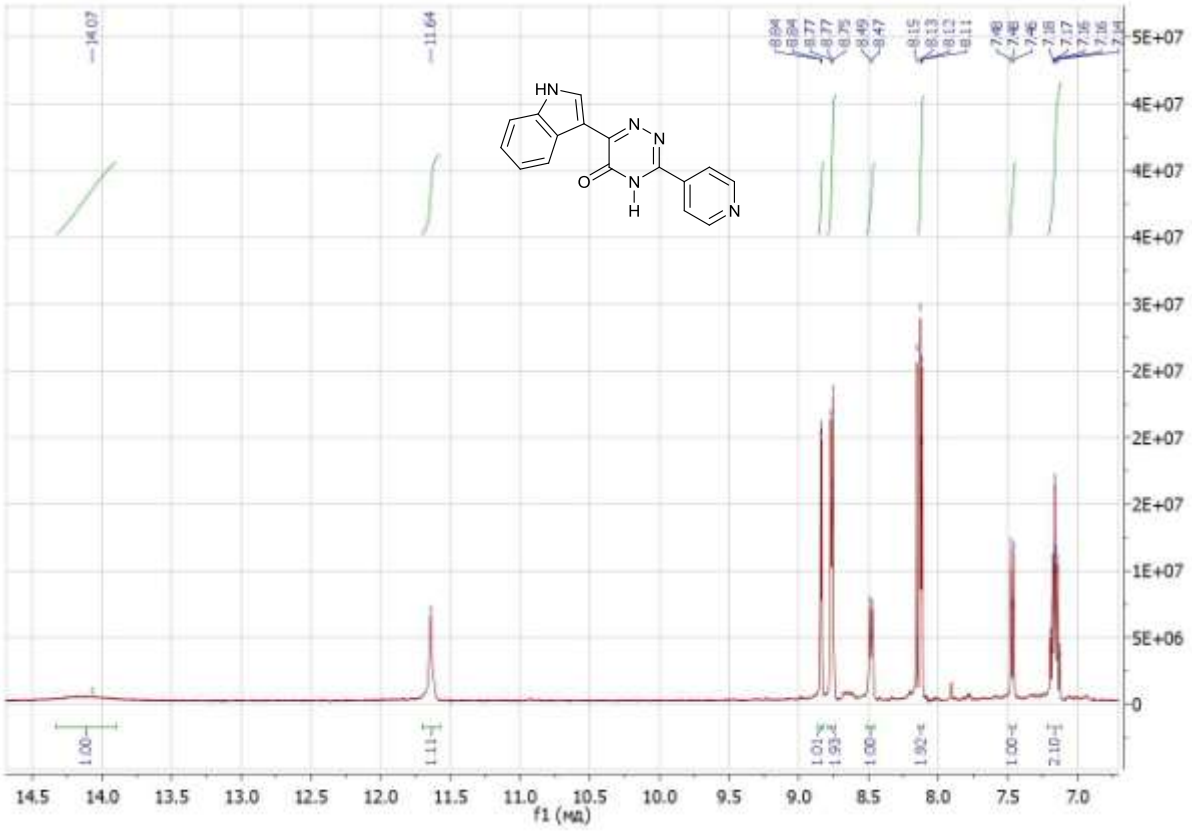


Figure S26. ^{1}H NMR Spectrum of 6-(1*H*-indol-3-yl)-3-(pyridin-4-yl)-1,2,4-triazin-5(4*H*)-one (15a)

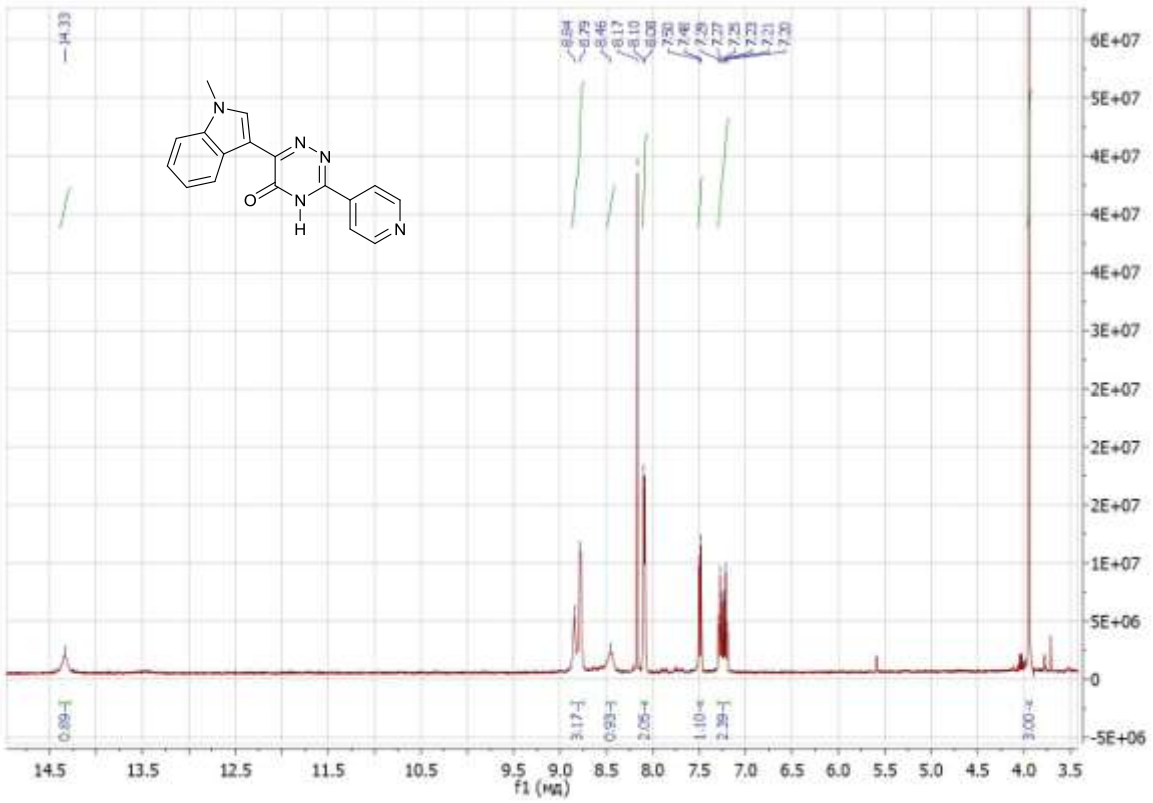


Figure S27. ^{1}H NMR Spectrum of 6-(N-methylindol-3-yl)-3-(pyridin-4-yl)-1,2,4-triazin-5(4*H*)-one (15b)

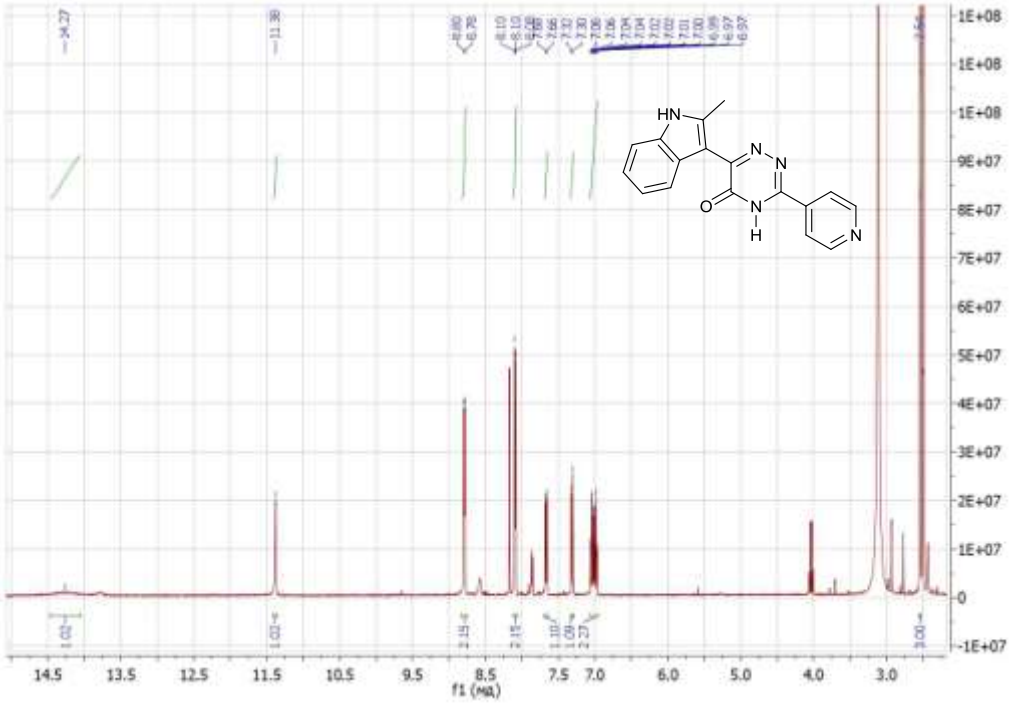


Figure S28. ^{1}H NMR Spectrum of 6-(2-methyl-1*H*-indol-3-yl)-3-(pyridin-4-yl)-1,2,4-triazin-5(4*H*)-one (15c)

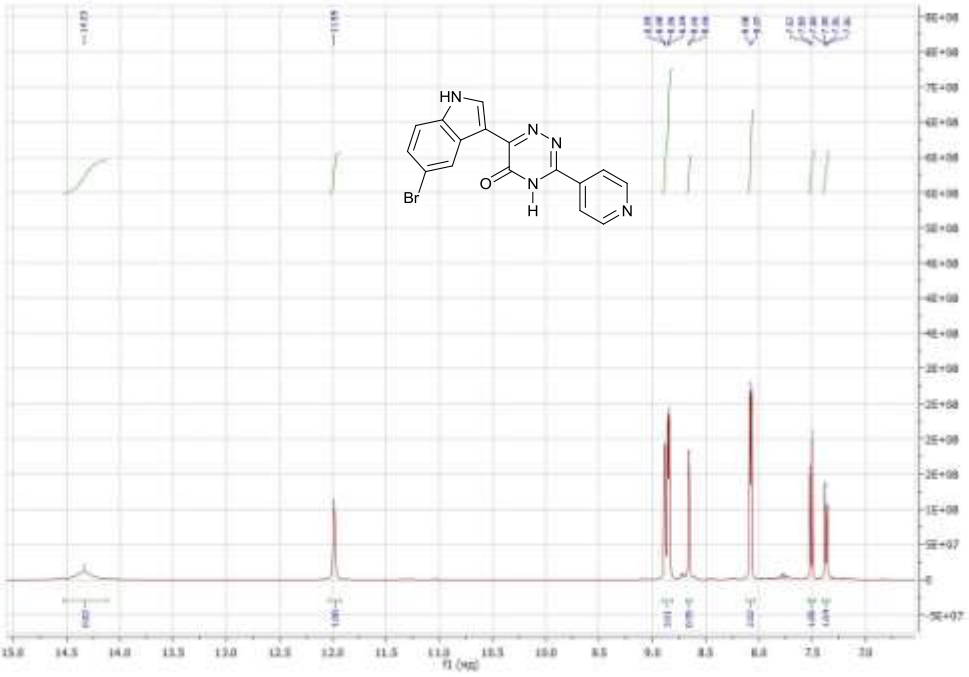


Figure S29. ^{1}H NMR Spectrum of 6-(5-bromo-1*H*-indol-3-yl)-3-(pyridin-4-yl)-1,2,4-triazin-5(4*H*)-one (15d)

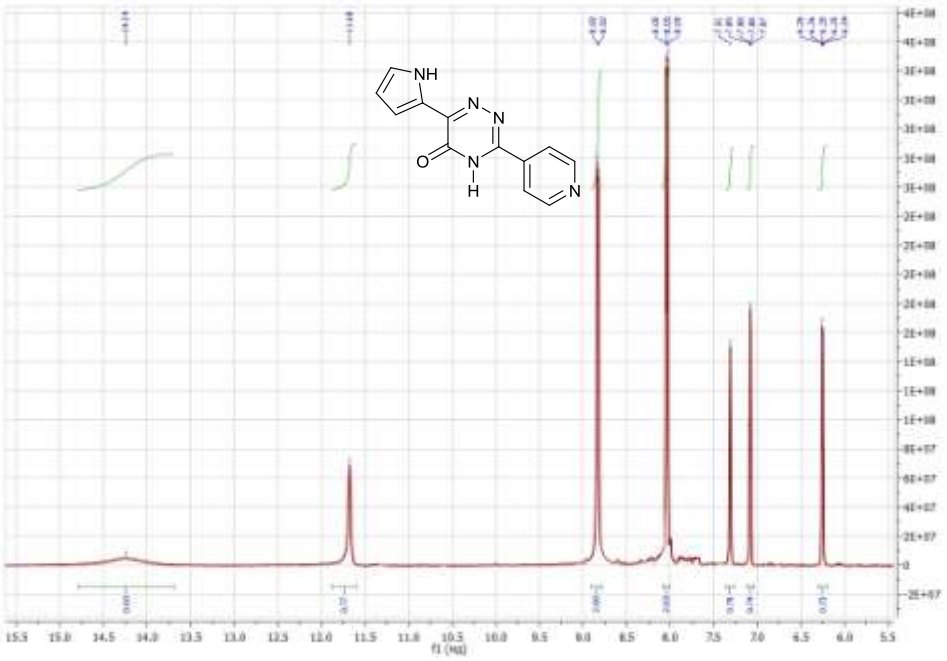


Figure S30. ^{1}H NMR Spectrum of 6-(1*H*-pyrrol-2-yl)-3-(pyridin-4-yl)-1,2,4-triazin-5(4*H*)-one (15e)

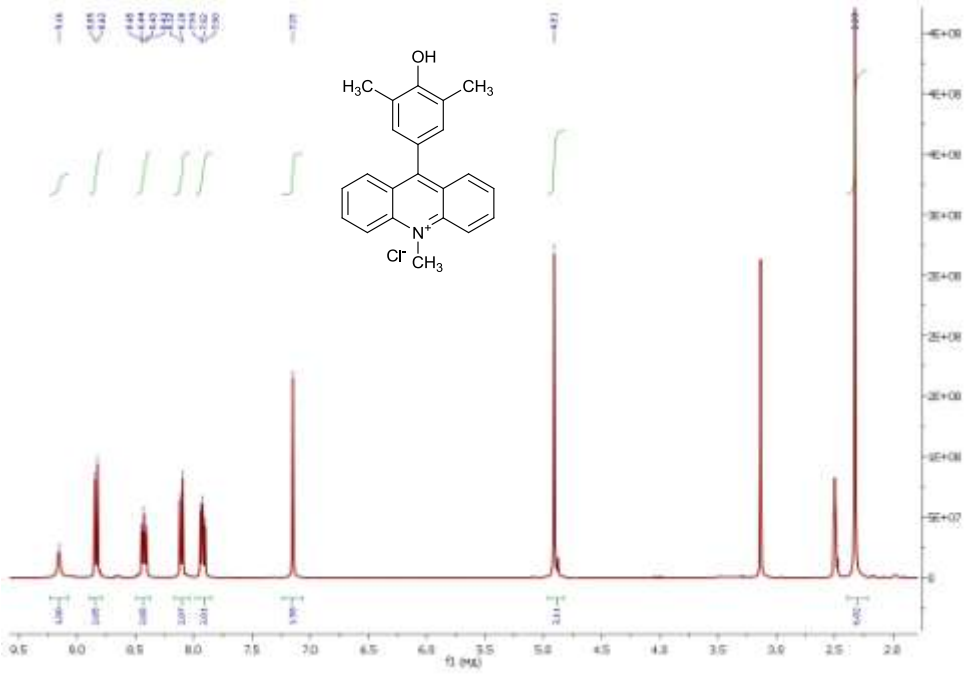


Figure S31. ^{1}H NMR Spectrum of 9-(4'-hydroxy-3',5'-dimethylphenyl)-10-methylacridinium chloride (25b)

NMR ^{13}C Spectra

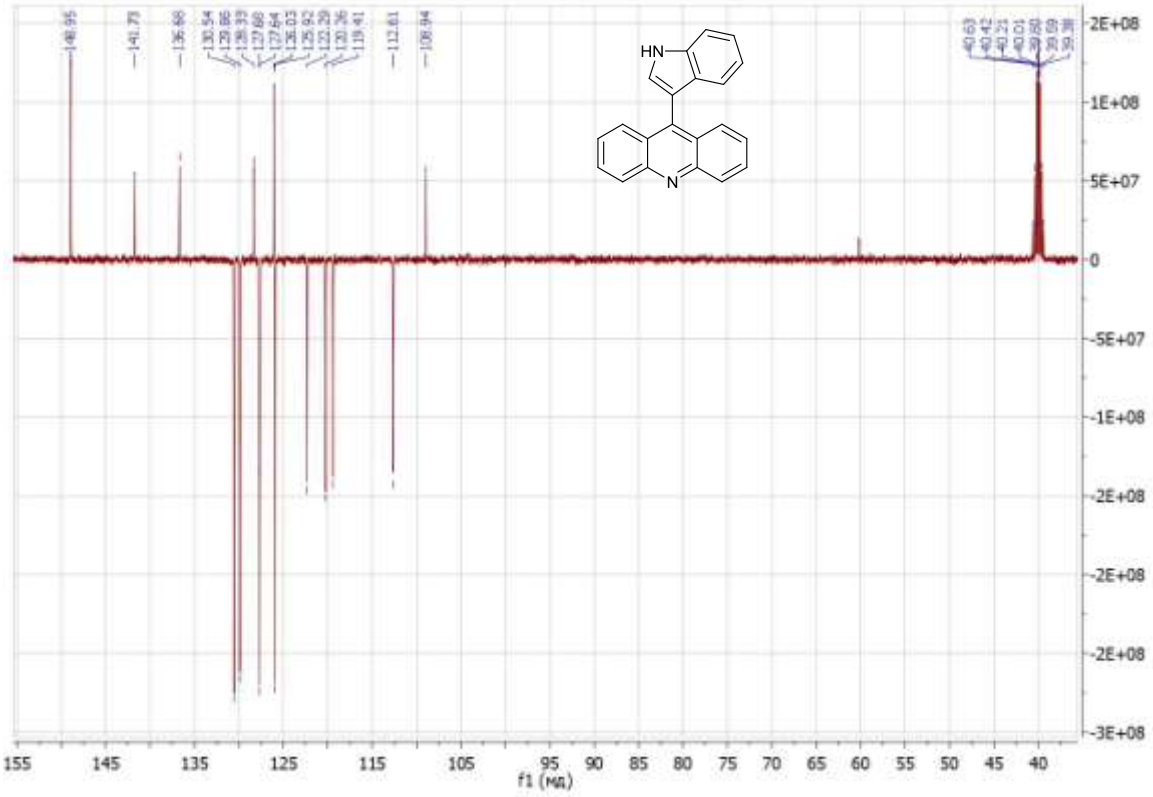


Figure S32. ^{13}C NMR Spectrum of 9-(1*H*-indol-3-yl)acridine (6a)

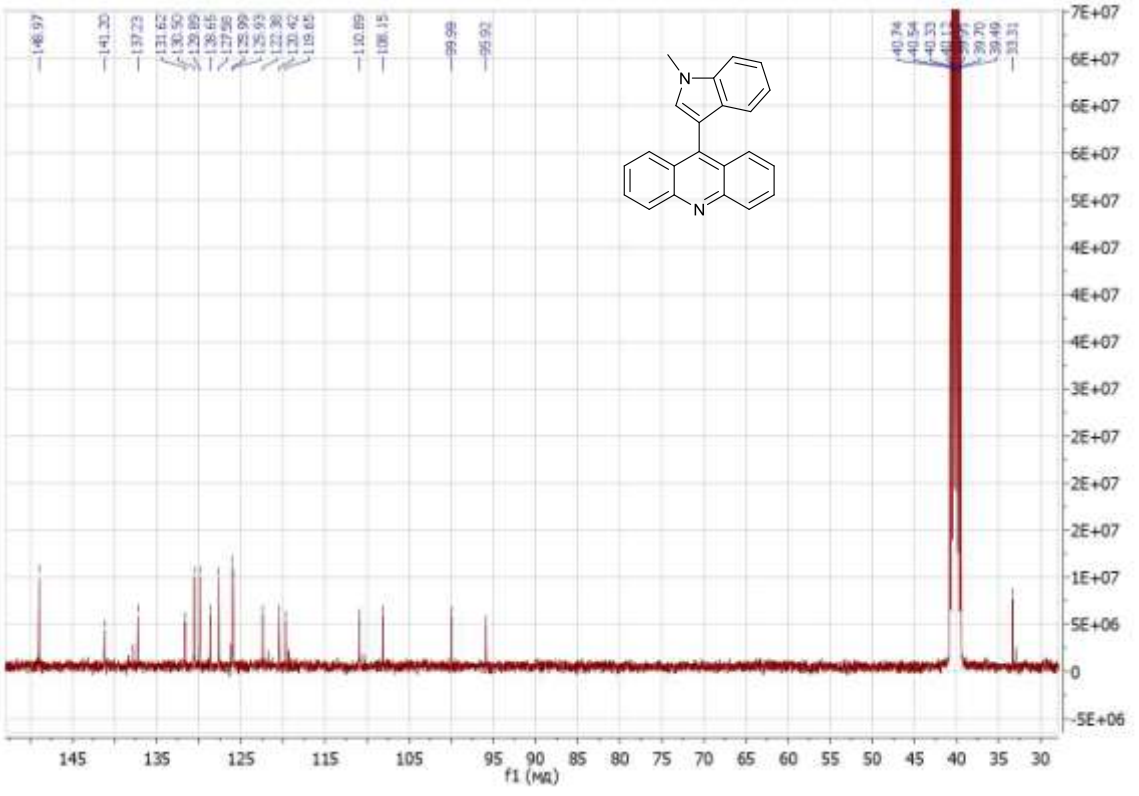


Figure S33. ^{13}C NMR Spectrum of 9-(N-methylindol-3-yl)acridine (6b)

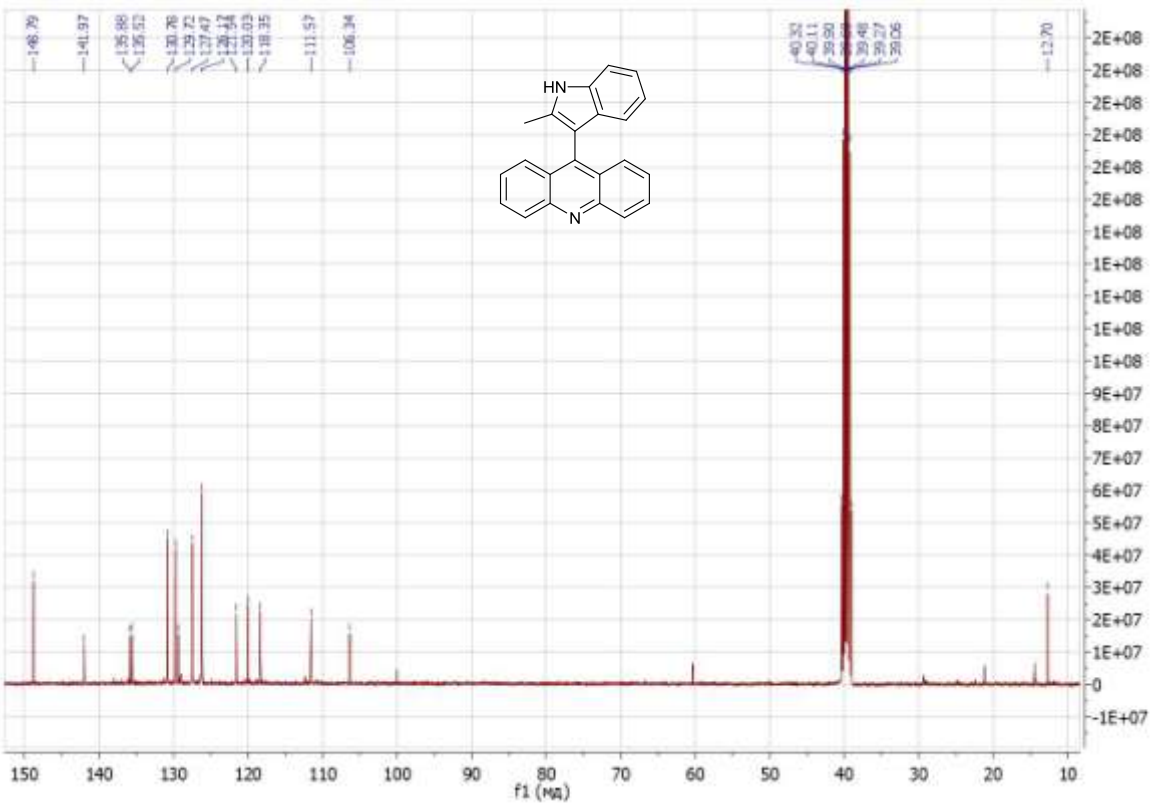


Figure S34. ^{13}C NMR Spectrum of 9-(2-methylindol-3-yl)acridine (6c)

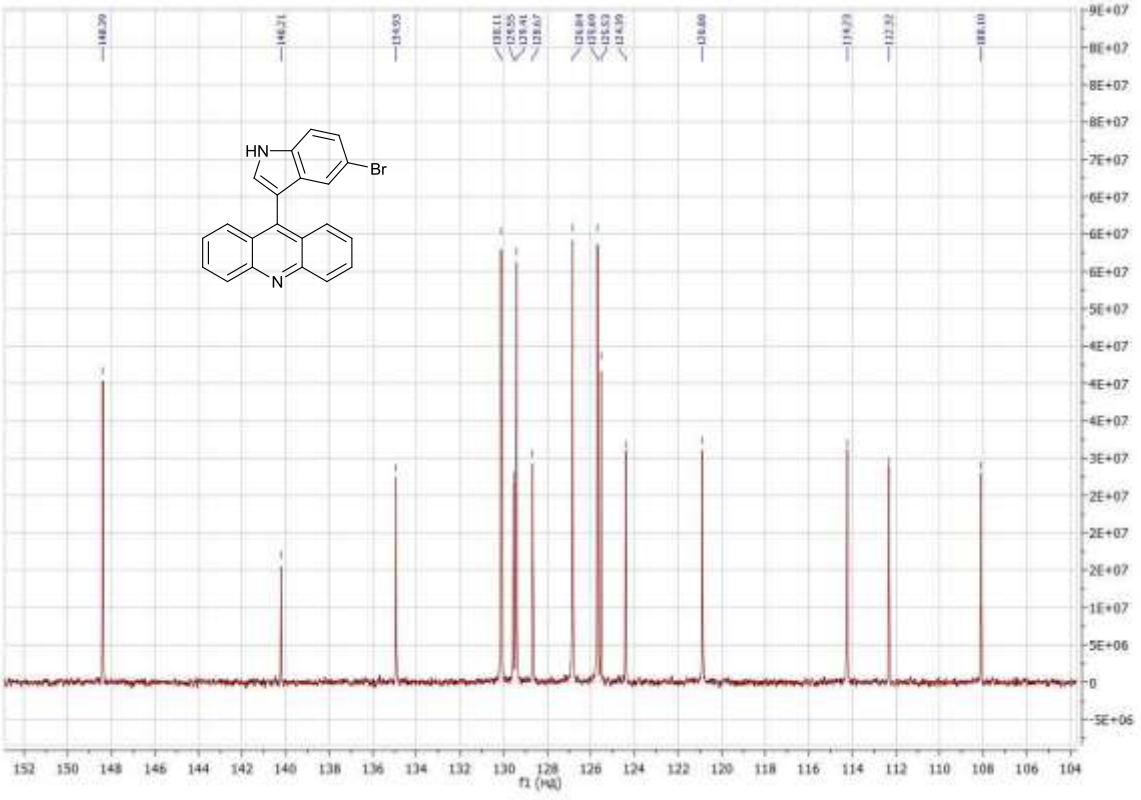


Figure S35. ^{13}C NMR Spectrum of 9-(5-bromo-1*H*-indol-3-yl)acridine (6d)

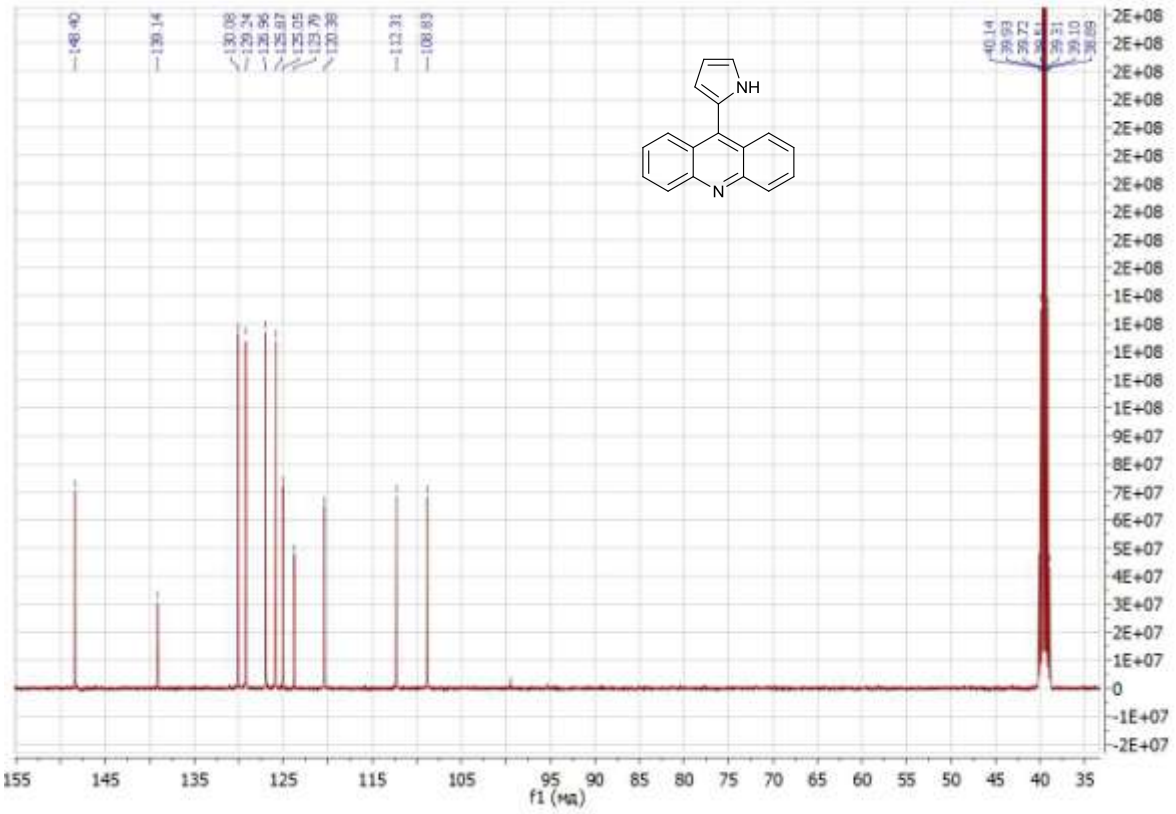


Figure S36. ^{13}C NMR Spectrum of 9-(1*H*-pyrrol-2-yl)acridine (6e)

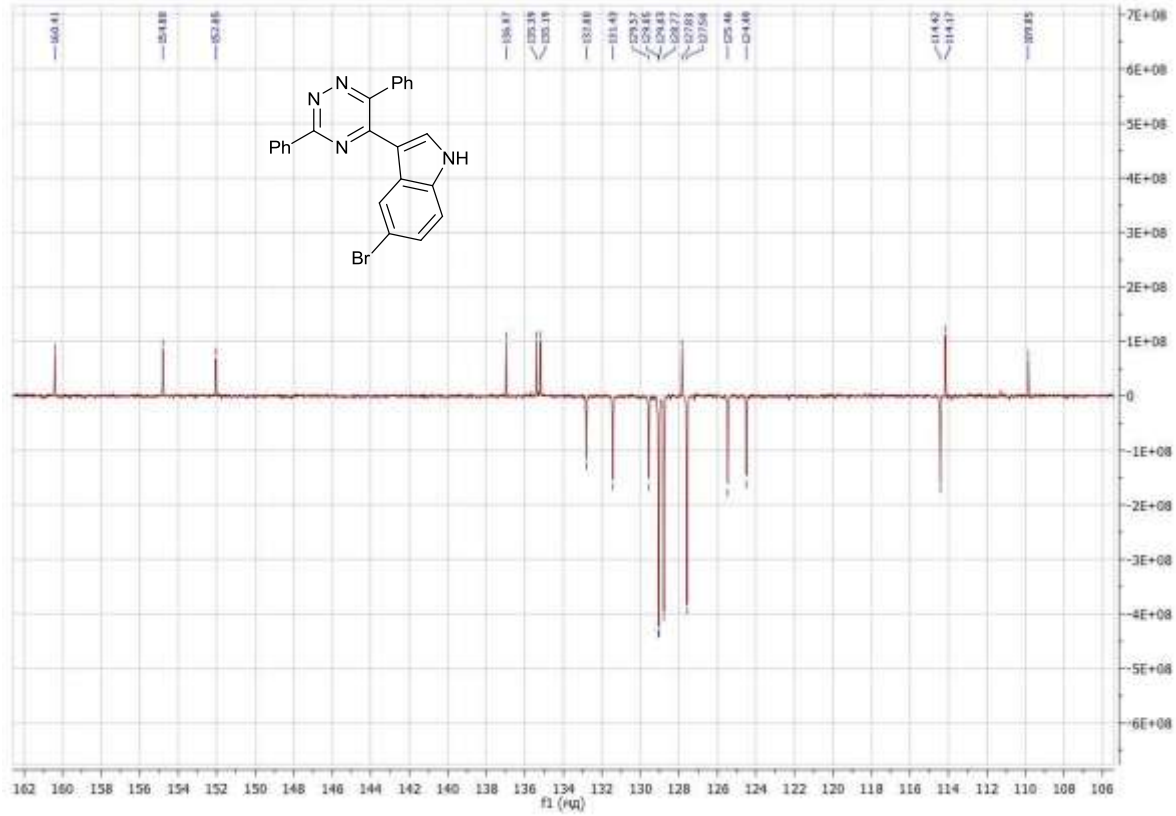


Figure S37. ^{13}C NMR Spectrum of 3,6-diphenyl-5-(5-bromo-1*H*-indol-3-yl)-1,2,4-triazine (7d)

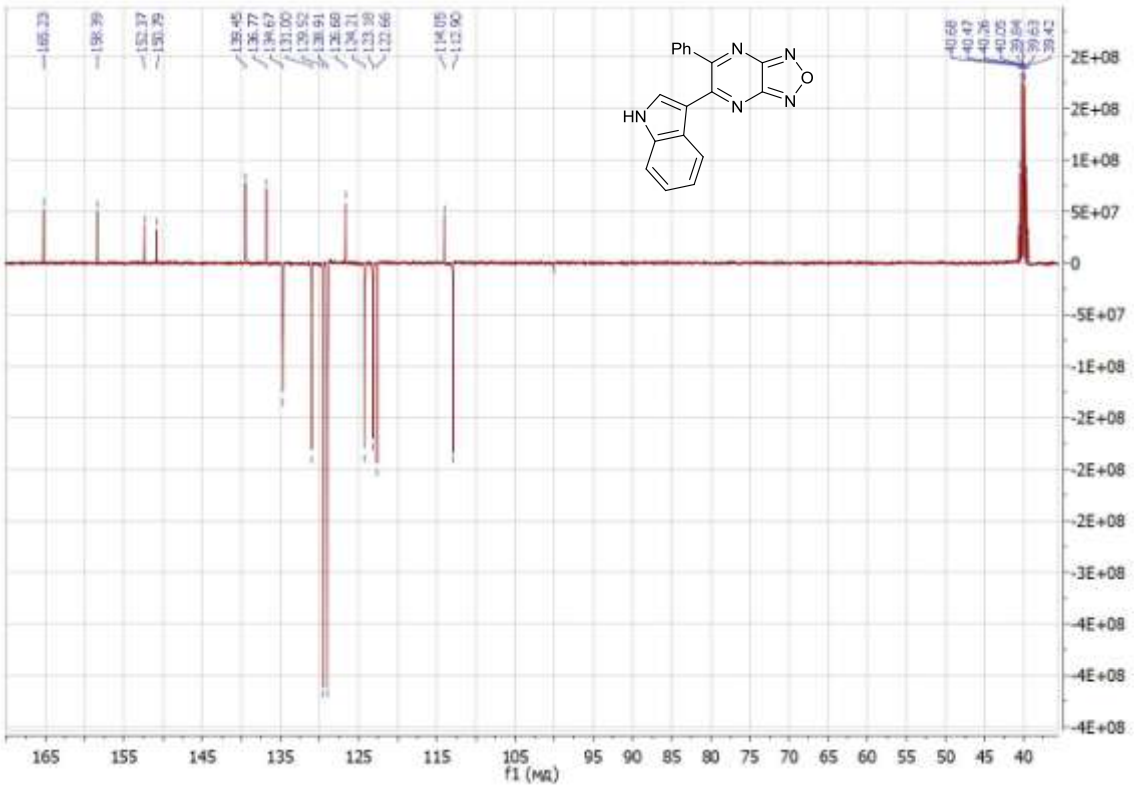


Figure S38. ^{13}C NMR Spectrum of 5-(1*H*-indol-3-yl)-6-phenyl-1,2,5-oxadiazolo[3,4-*b*]pyrazine (8a)

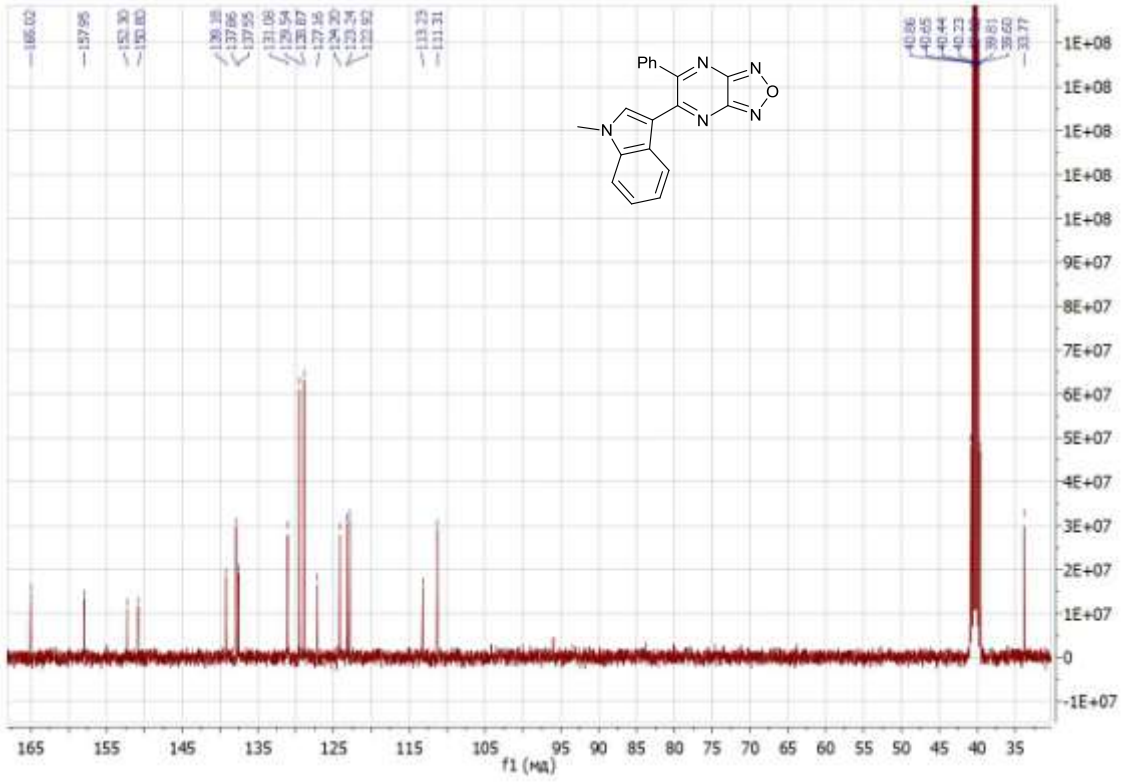


Figure S39. ^{13}C NMR Spectrum of 5-(N-methylindol-3-yl)-6-phenyl-1,2,5-oxadiazolo[3,4-*b*]pyrazine (8b)

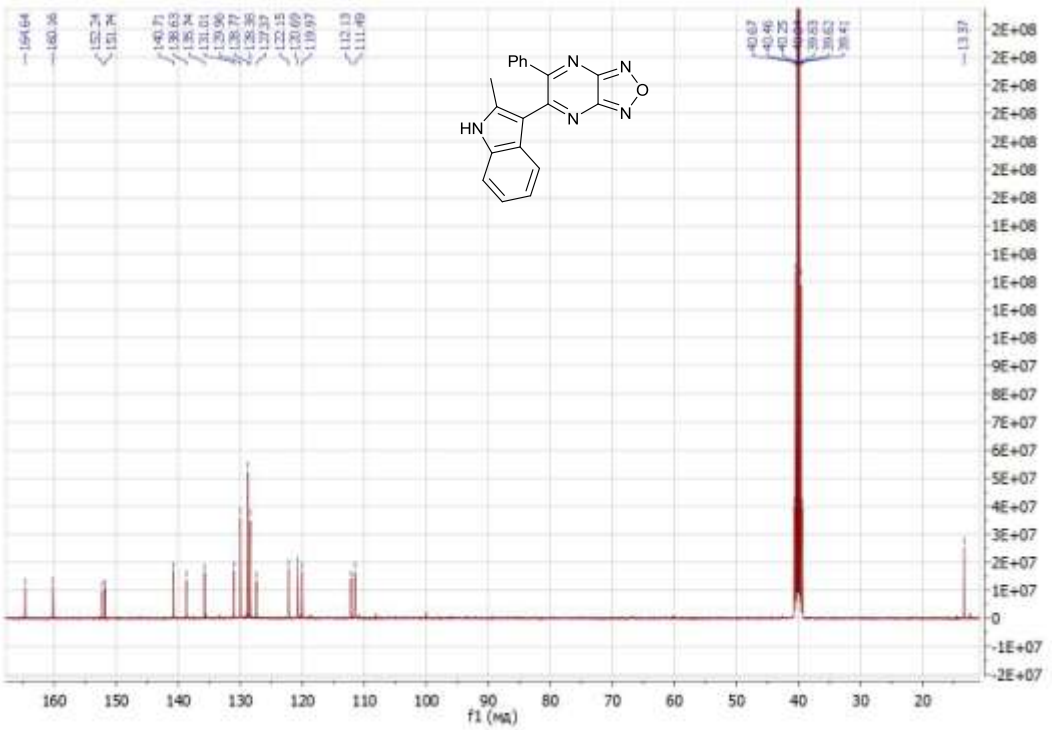


Figure S40. ^{13}C NMR Spectrum of 5-(2-methy-1*H*-lindol-3-yl)-6-phenyl-1,2,5-oxadiazolo[3,4-*b*]pyrazine (8c)

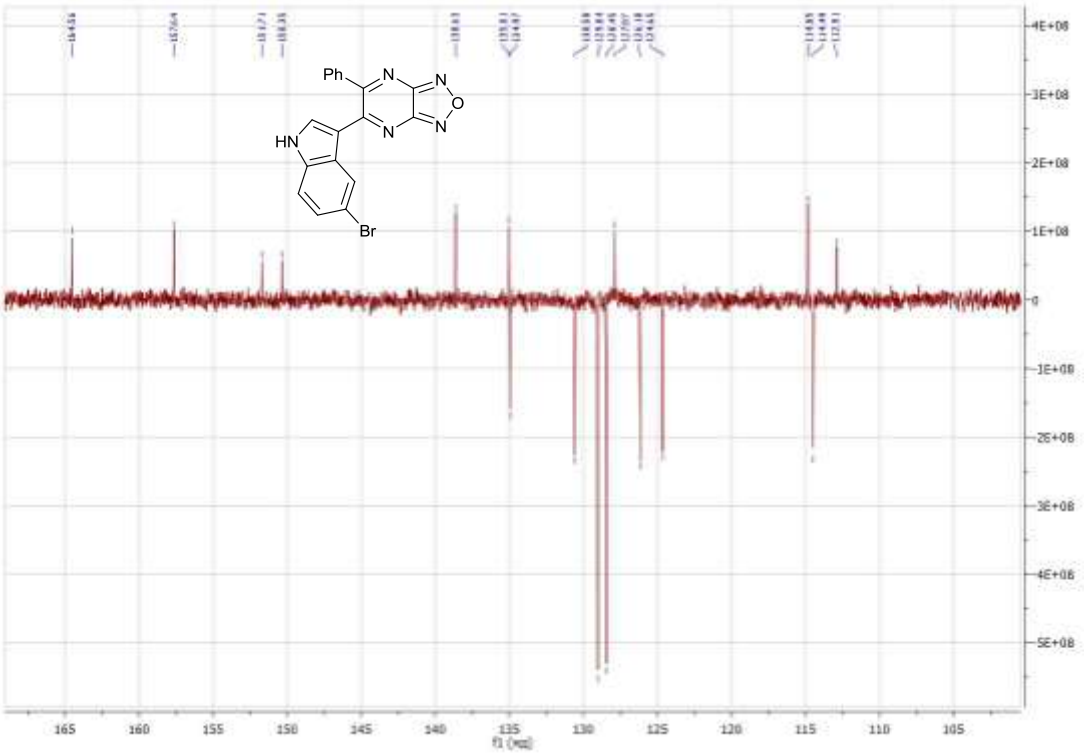


Figure S41. ^{13}C NMR Spectrum of 5-(5-bromo-1*H*-indol-3-yl)-6-phenyl-1,2,5-oxadiazolo[3,4-*b*]pyrazine (8d)

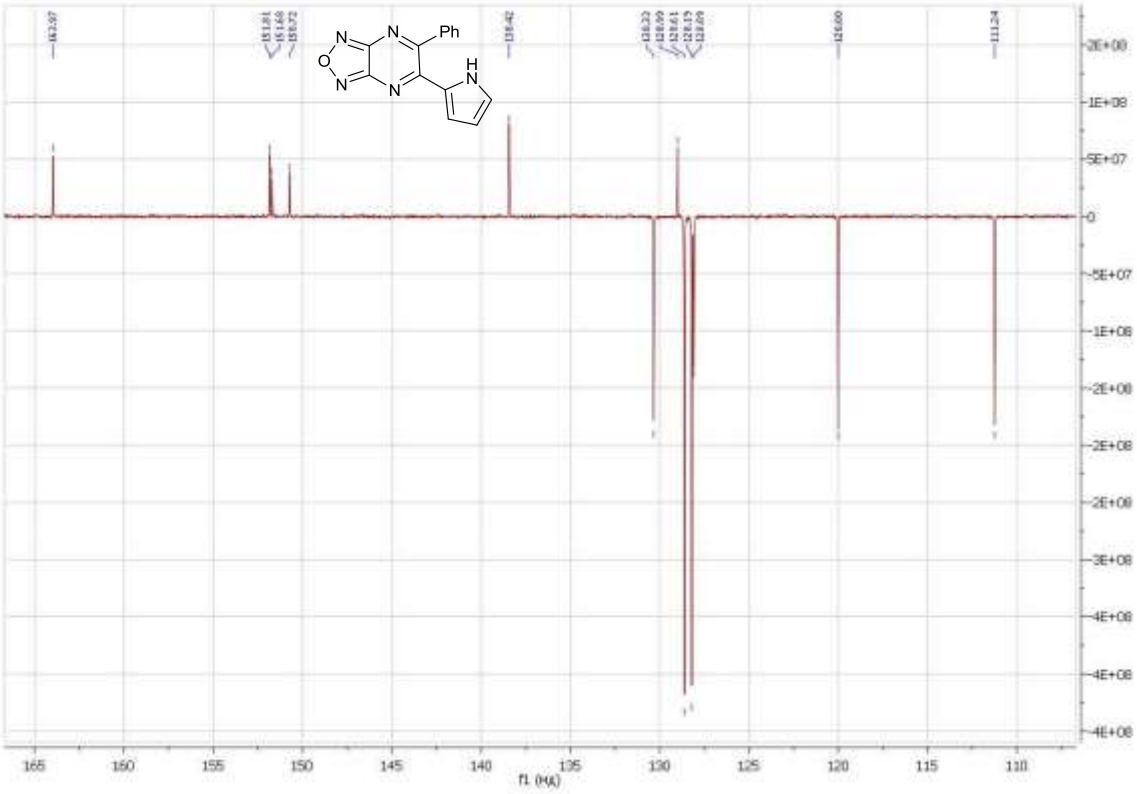


Figure S42. ^{13}C NMR Spectrum of 5-phenyl-6-(1*H*-pyrrol-2-yl)-[1,2,5]oxadiazolo[3,4-*b*]pyrazine (8e)

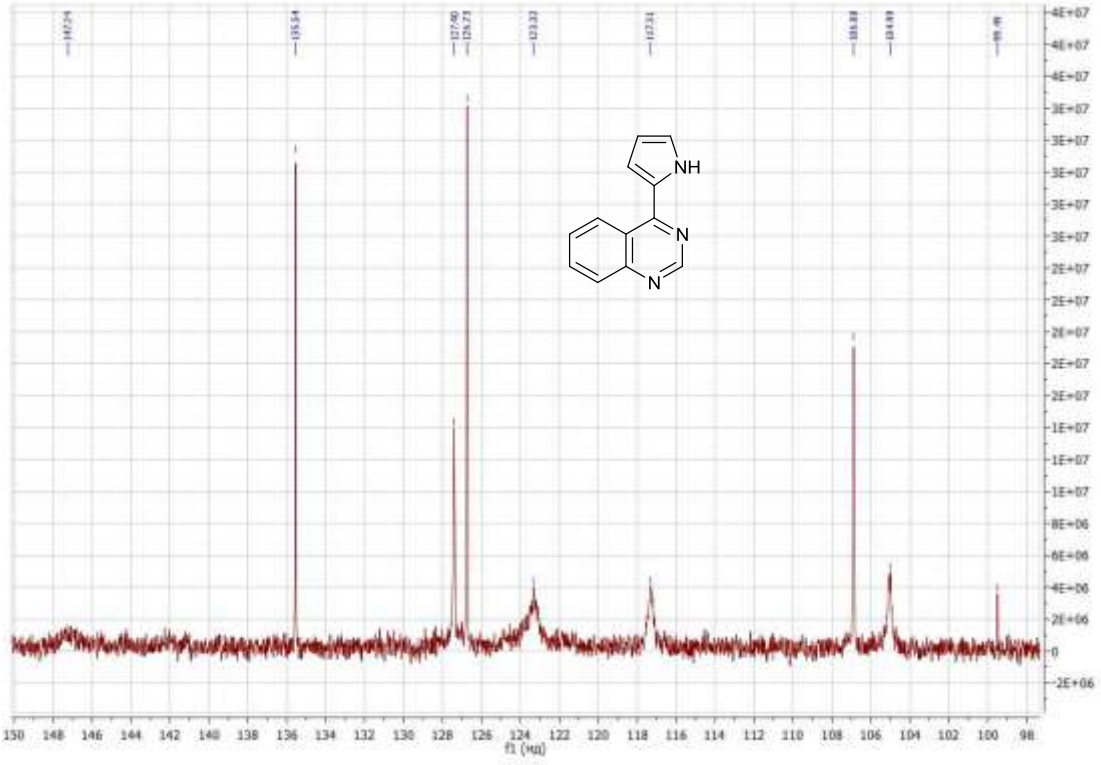


Figure S43. ^{13}C NMR Spectrum of 4-(1*H*-pyrrol-2-yl)quinazoline (9e)

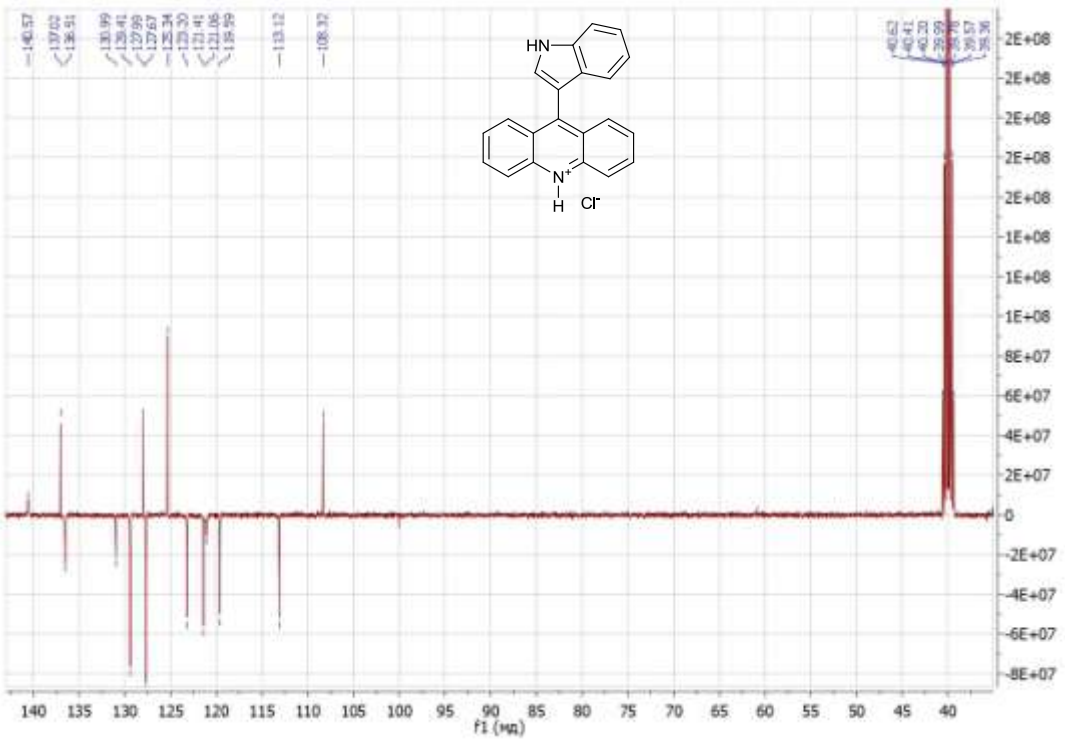


Figure S44. ^{13}C NMR Spectrum of 9-(1*H*-indol-3-yl)-10-hydroacridinum chloride (11a)

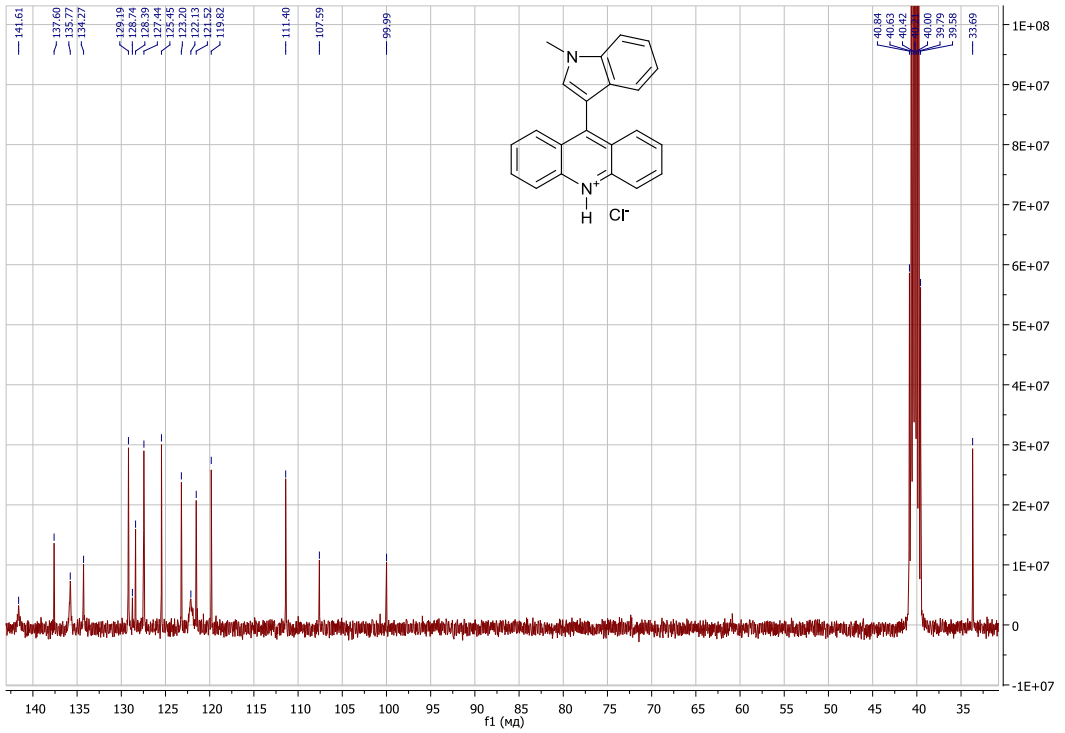


Figure S45. ^{13}C NMR Spectrum of 9-(N-methylindol-3-yl)-10-hydroacridinum chloride (11b)

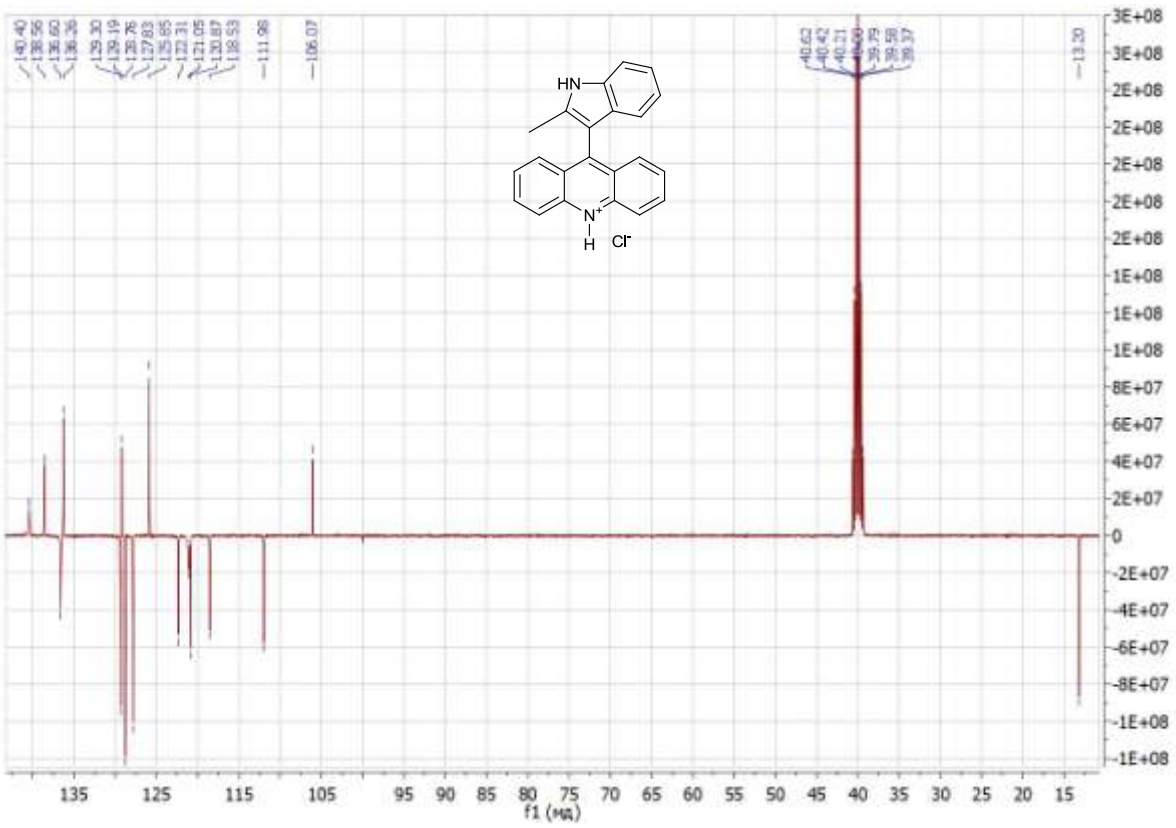


Figure S46. ^{13}C NMR Spectrum of 9-(2-methyl-1*H*-indol-3-yl)-10-hydroacridinum chloride (11c)

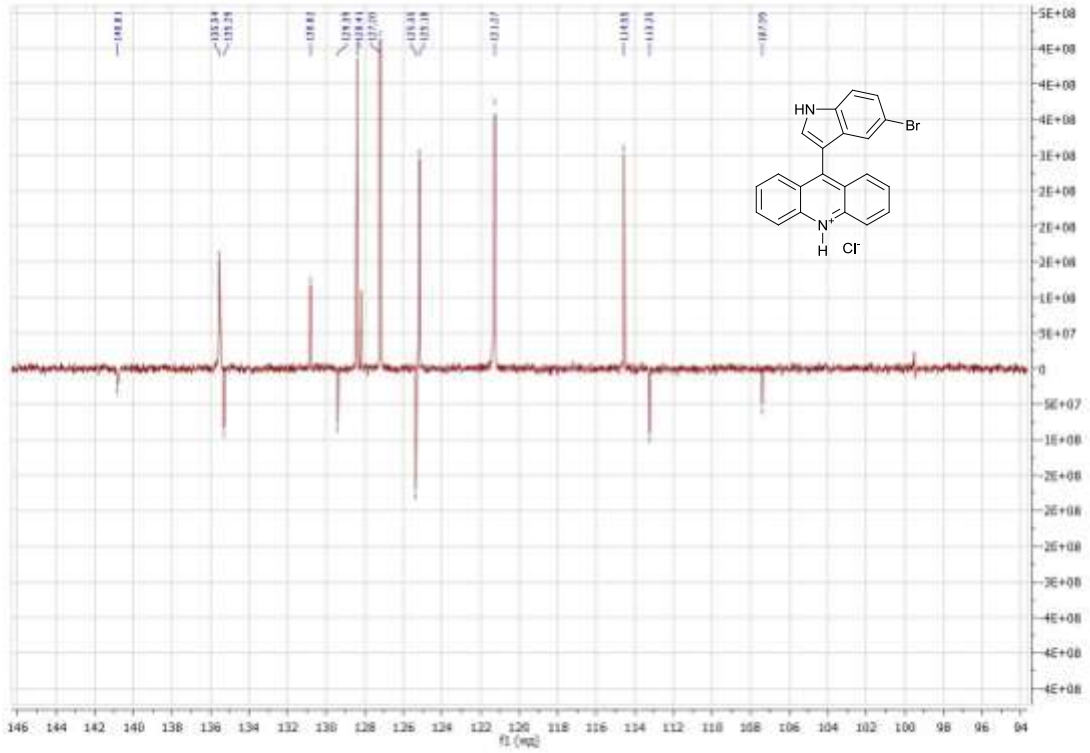


Figure S47. ^{13}C NMR Spectrum of 9-(5-bromo-1*H*-indol-3-yl)-10-hydroacridinum chloride (11d)

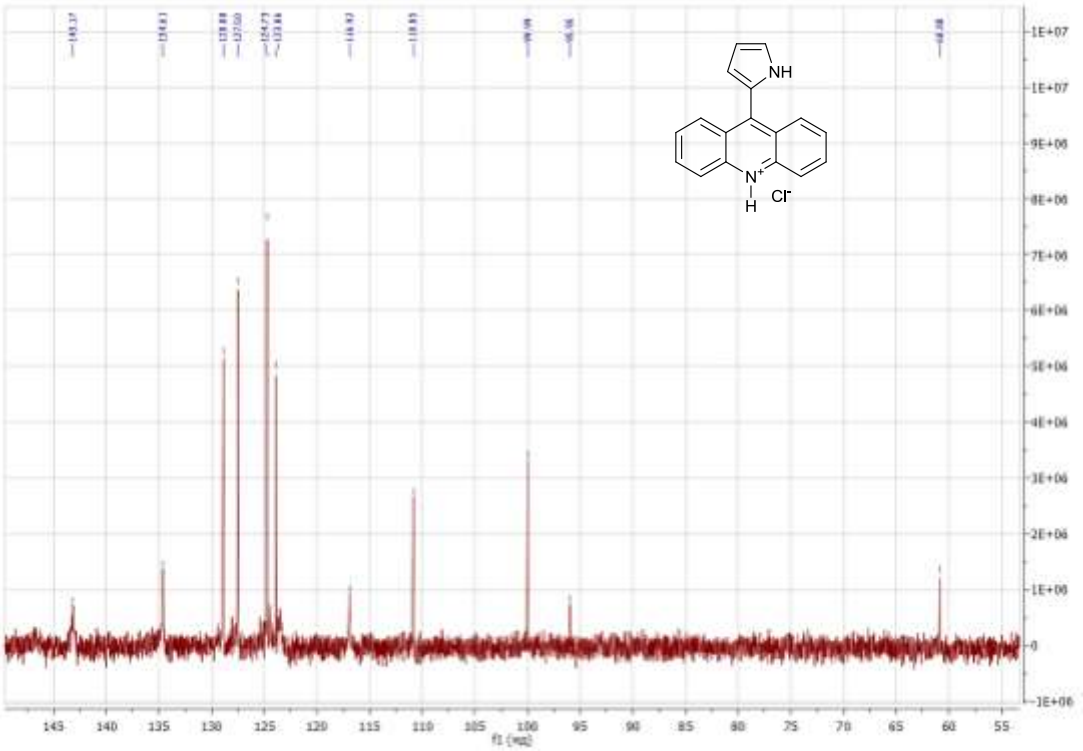


Figure S48. ^{13}C NMR Spectrum of 9-(1*H*-pyrrol-2-yl)-10-hydroacridinum chloride (11e)

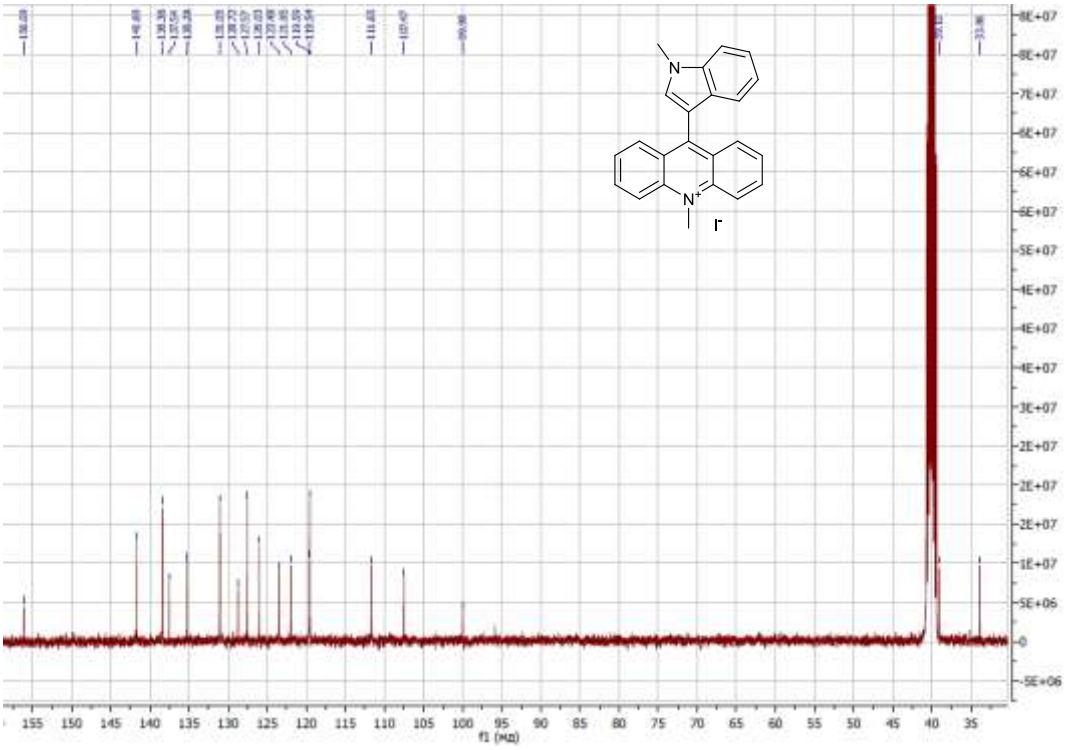


Figure S49. ^{13}C NMR Spectrum of 9-(N-methylindol-3-yl)-10-methylacridinum iodide (12b)

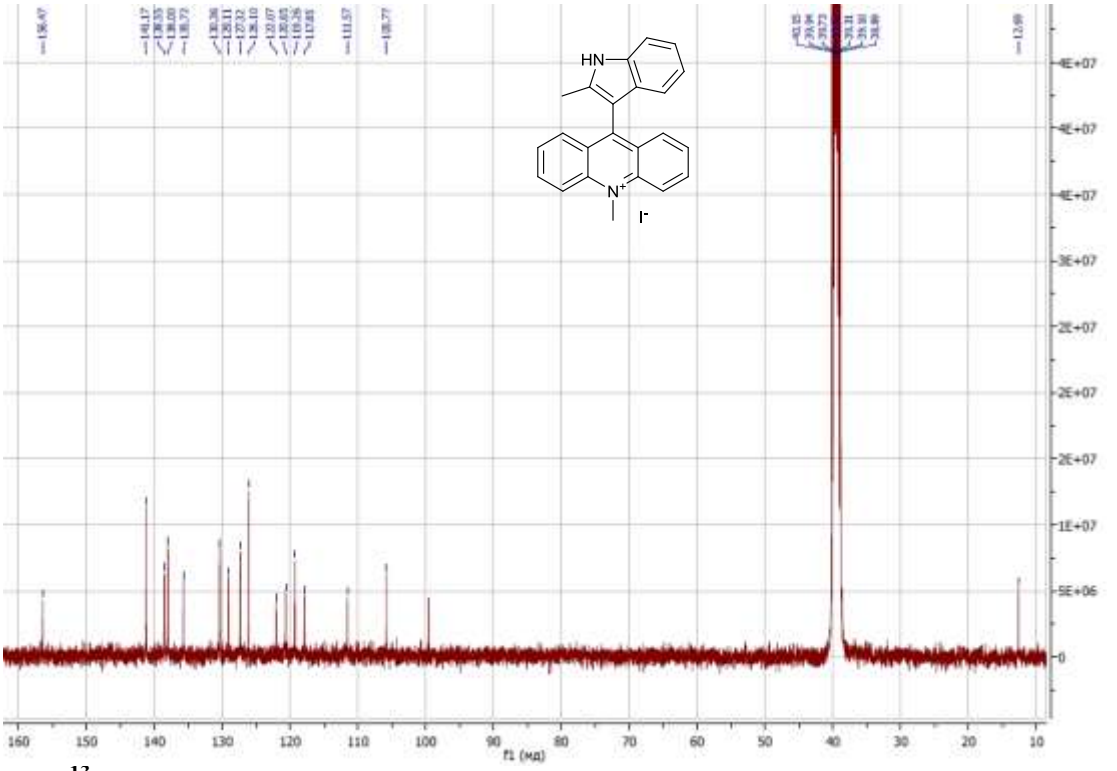


Figure S50. ^{13}C NMR Spectrum of 9-(2-methyl-1*H*-indol-3-yl)-10-methylacridinum iodide (12c)

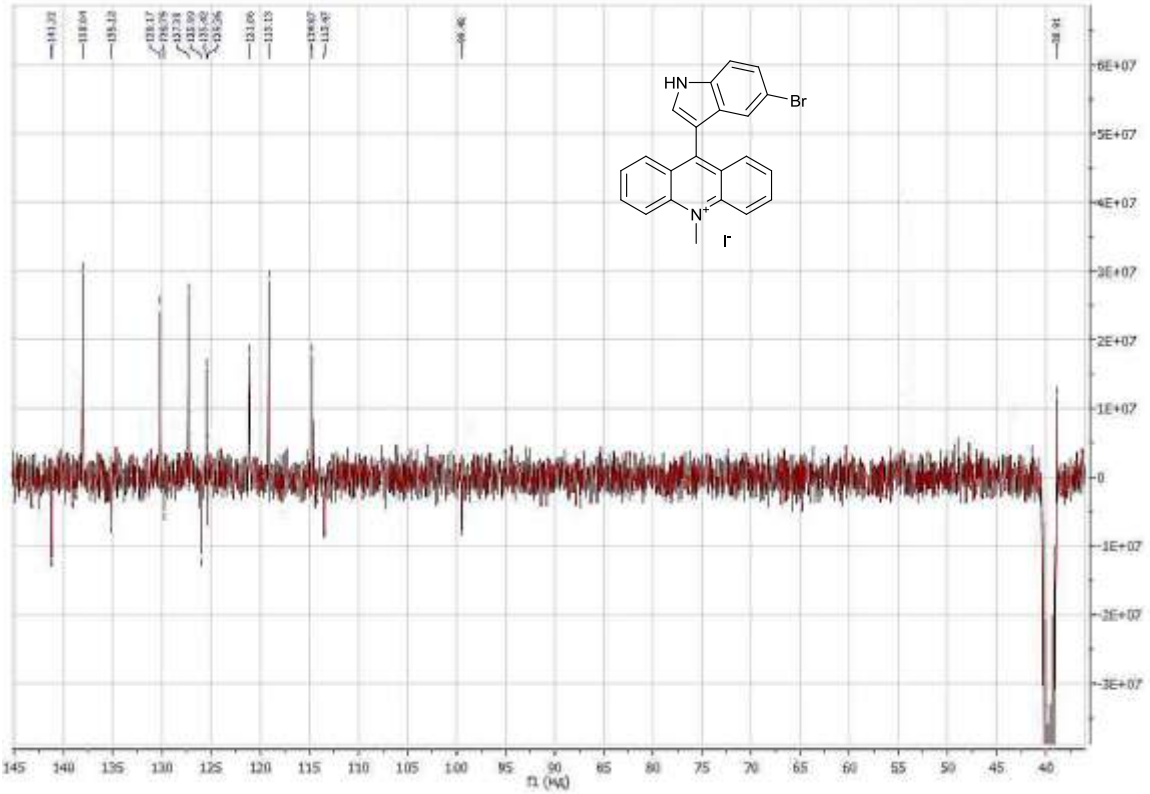


Figure S51. ^{13}C NMR Spectrum of 9-(5-bromo-1*H*-indol-3-yl)-10-methylacridinum iodide (12d)

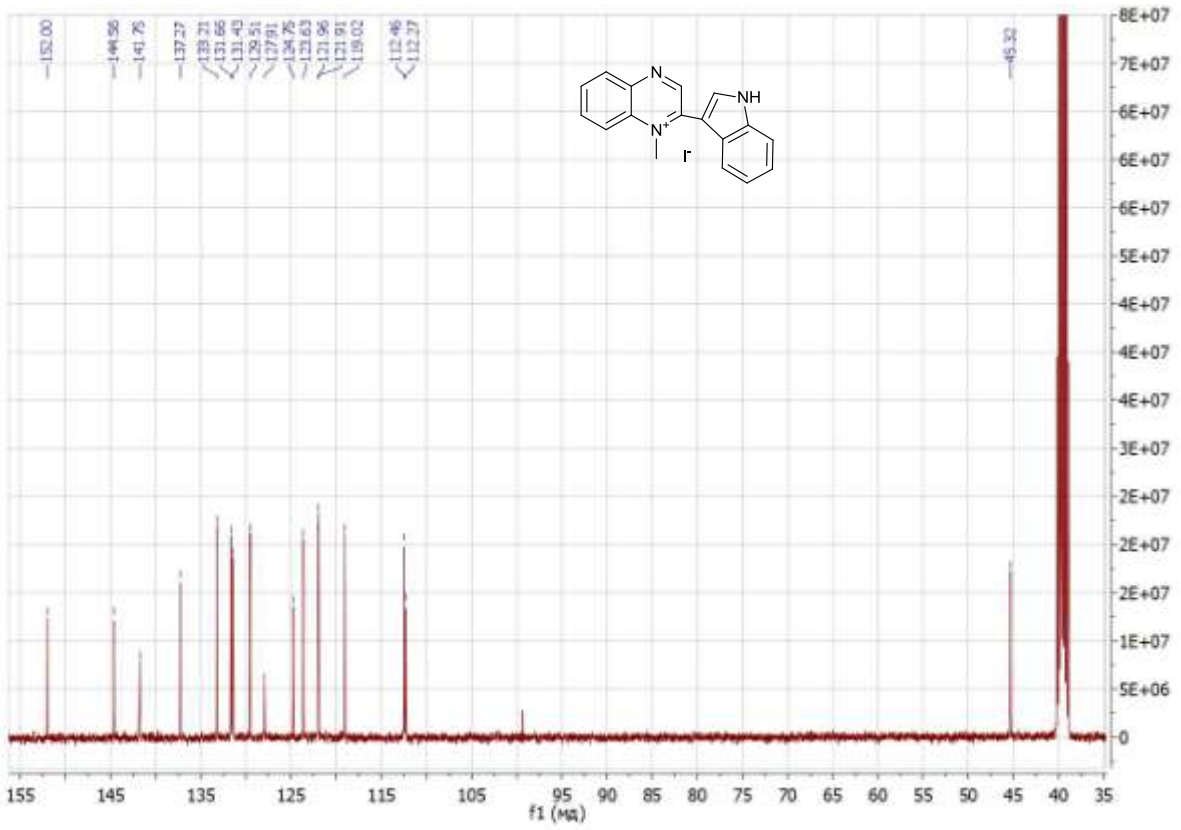


Figure S52. ^{13}C NMR Spectrum of 2-(1*H*-indol-3-yl)-1-methylquinoxalin-1-ium iodide (13a)

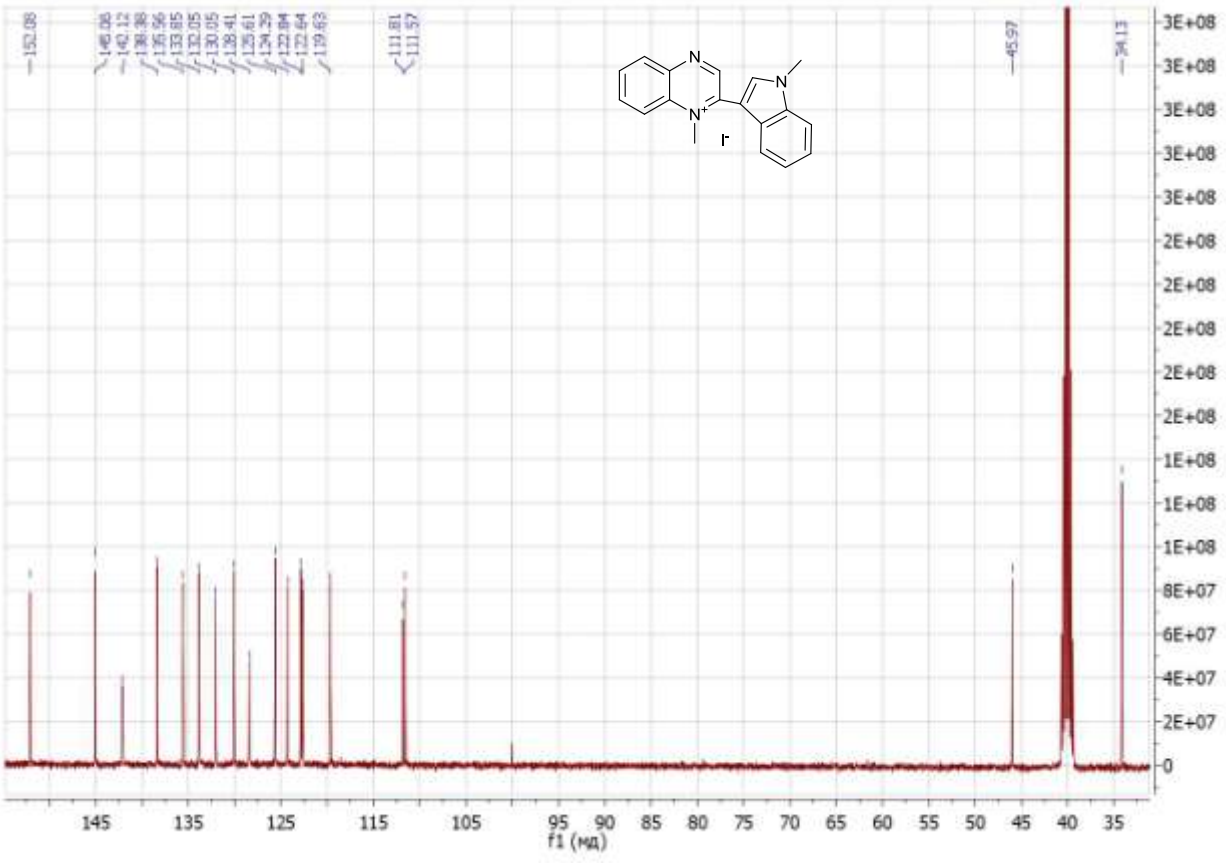


Figure S53. ^{13}C NMR Spectrum of 2-(N-methylindol-3-yl)-1-methylquinoxalin-1-ium iodide (13b)

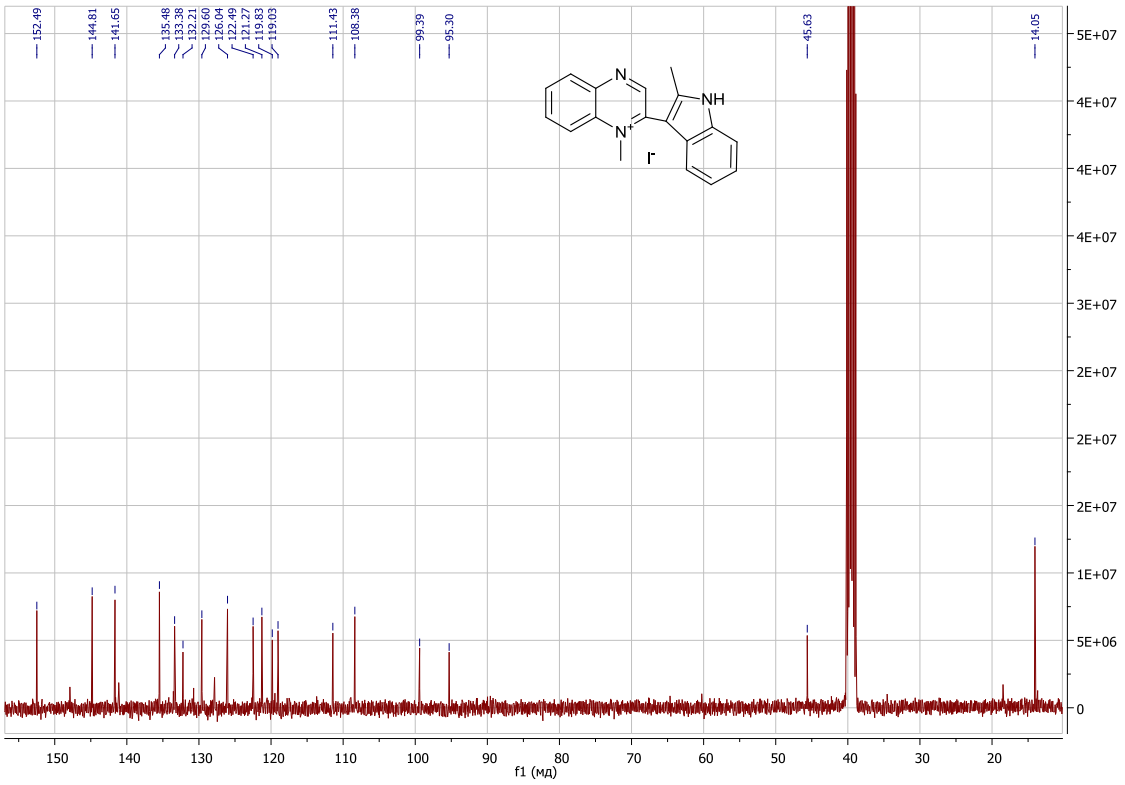


Figure S54. ^{13}C NMR Spectrum of 2-(2-methyl-1*H*-indol-3-yl)-1-methylquinoxalin-1-ium iodide (13c)

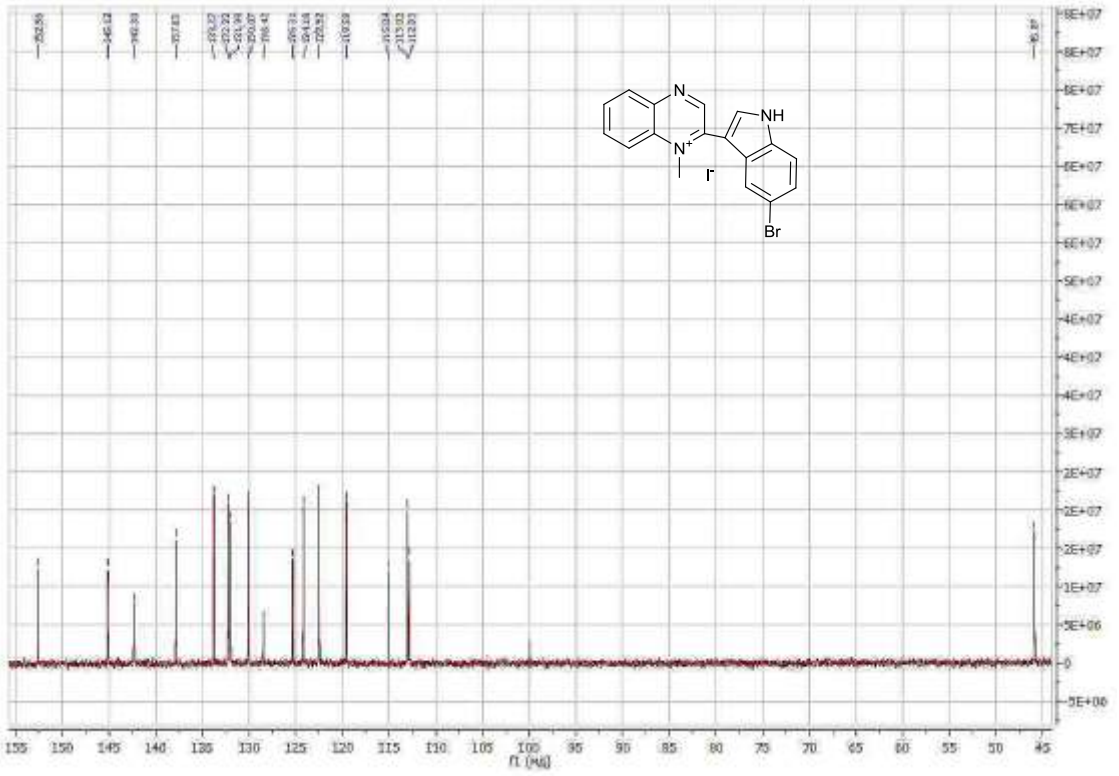


Figure S55. ^{13}C NMR Spectrum of 2-(5-bromo-1*H*-indol-3-yl)-1-methylquinoxalin-1-ium iodide (13d)

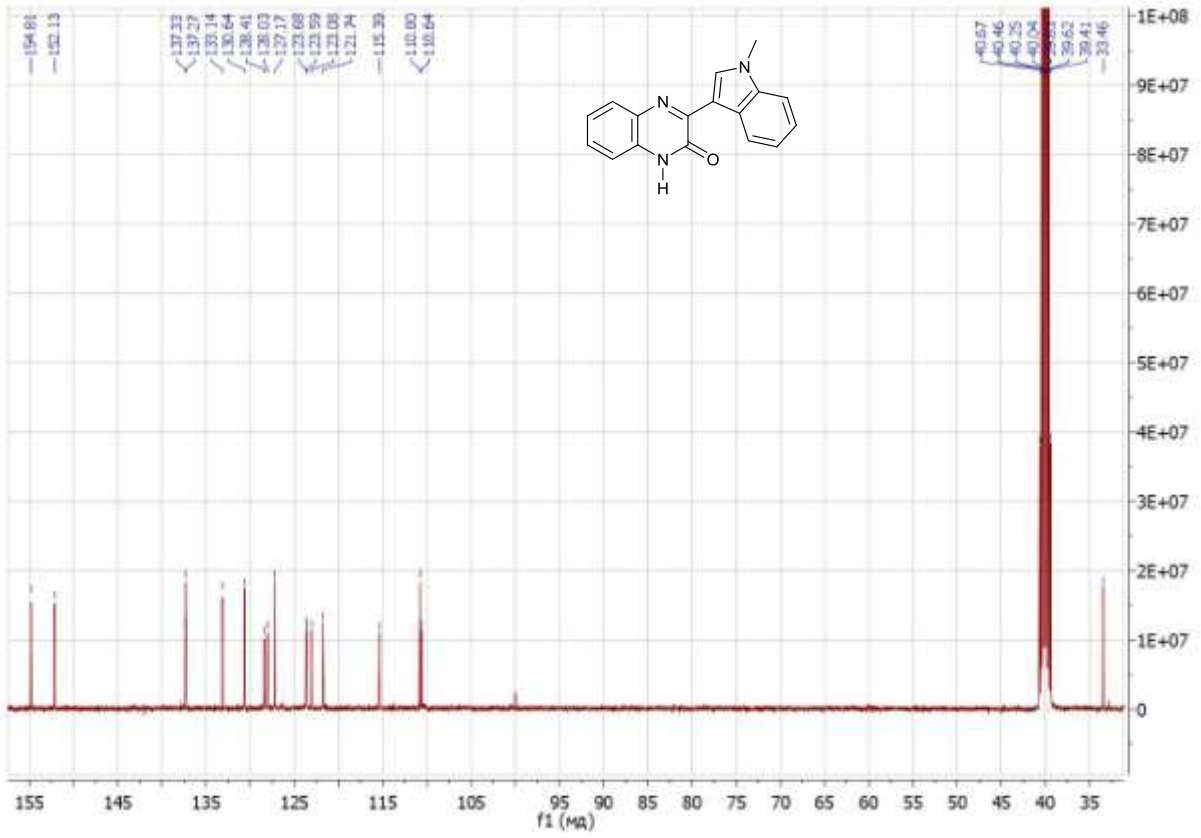


Figure S56. ^{13}C NMR Spectrum of 3-(N-methylindol-3-yl)quinoxalin-2(1*H*)-one (14b)

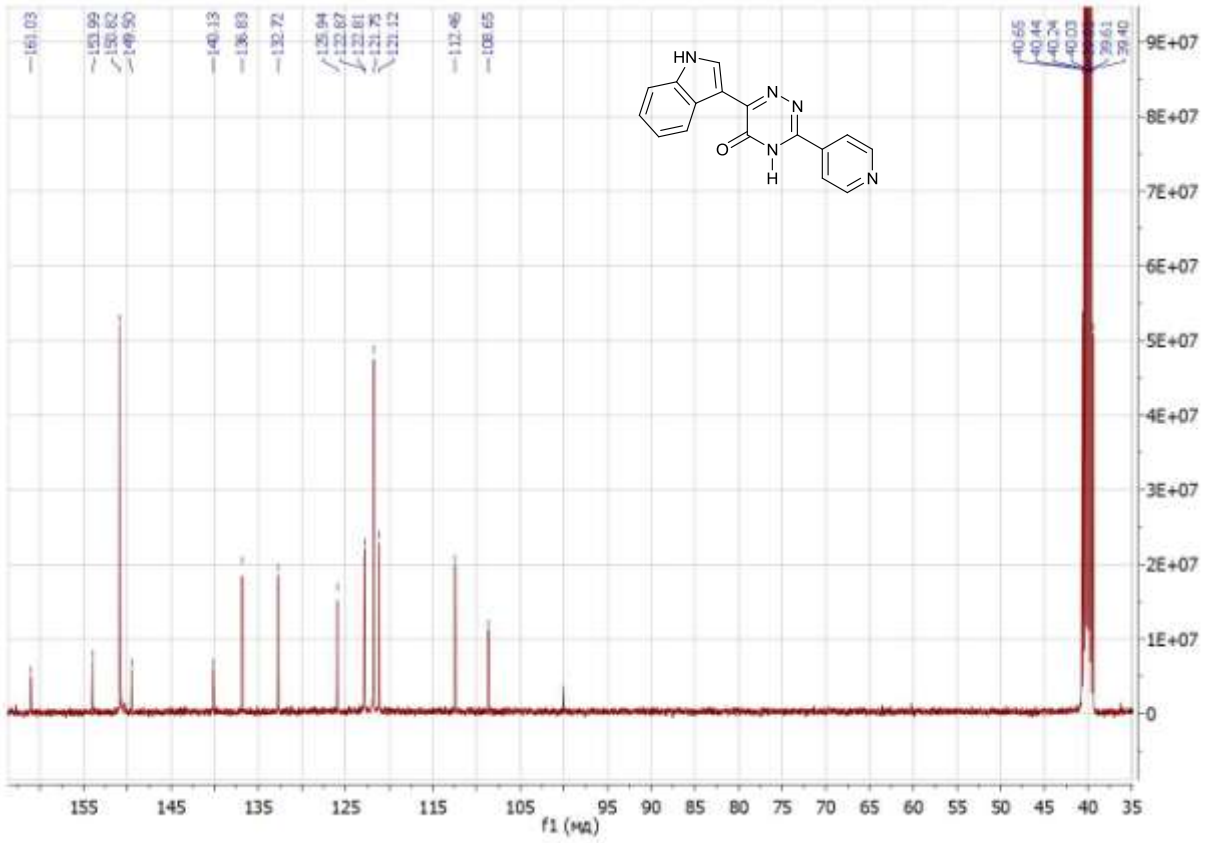


Figure S57. ^{13}C NMR Spectrum of 6-(1*H*-indol-3-yl)-3-(pyridin-4-yl)-1,2,4-triazin-5(4*H*)-one (15a)

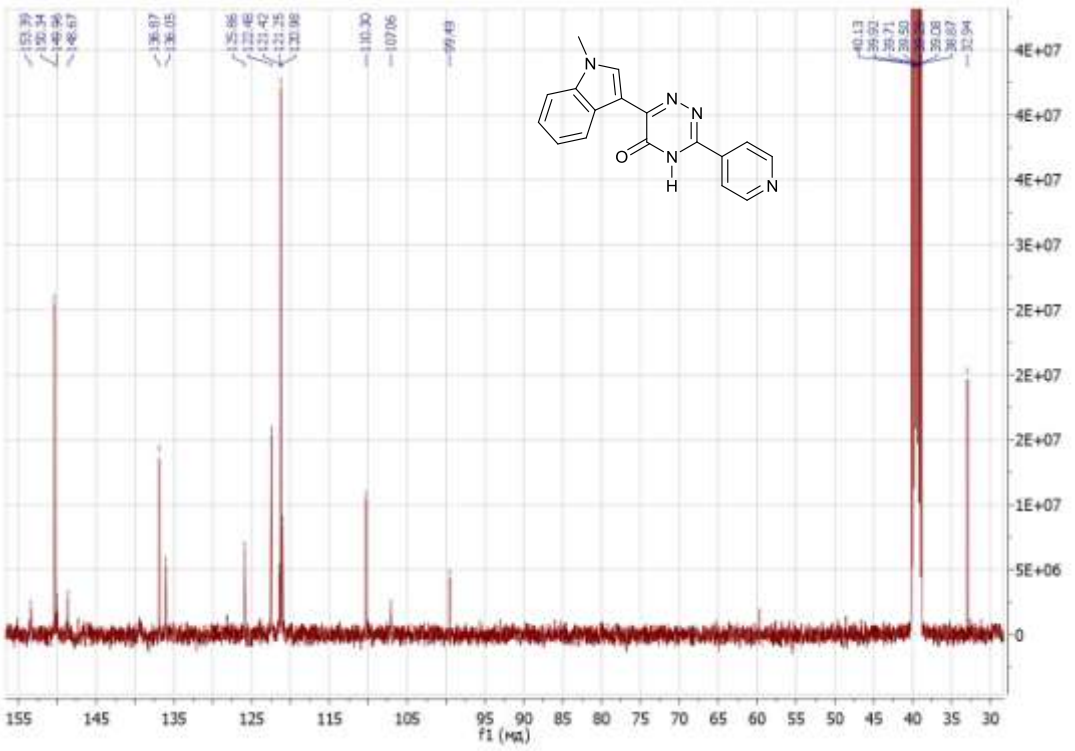


Figure S58. ^{13}C NMR Spectrum of 6-(N-methylindol-3-yl)-3-(pyridin-4-yl)-1,2,4-triazin-5(4*H*)-one (15b)

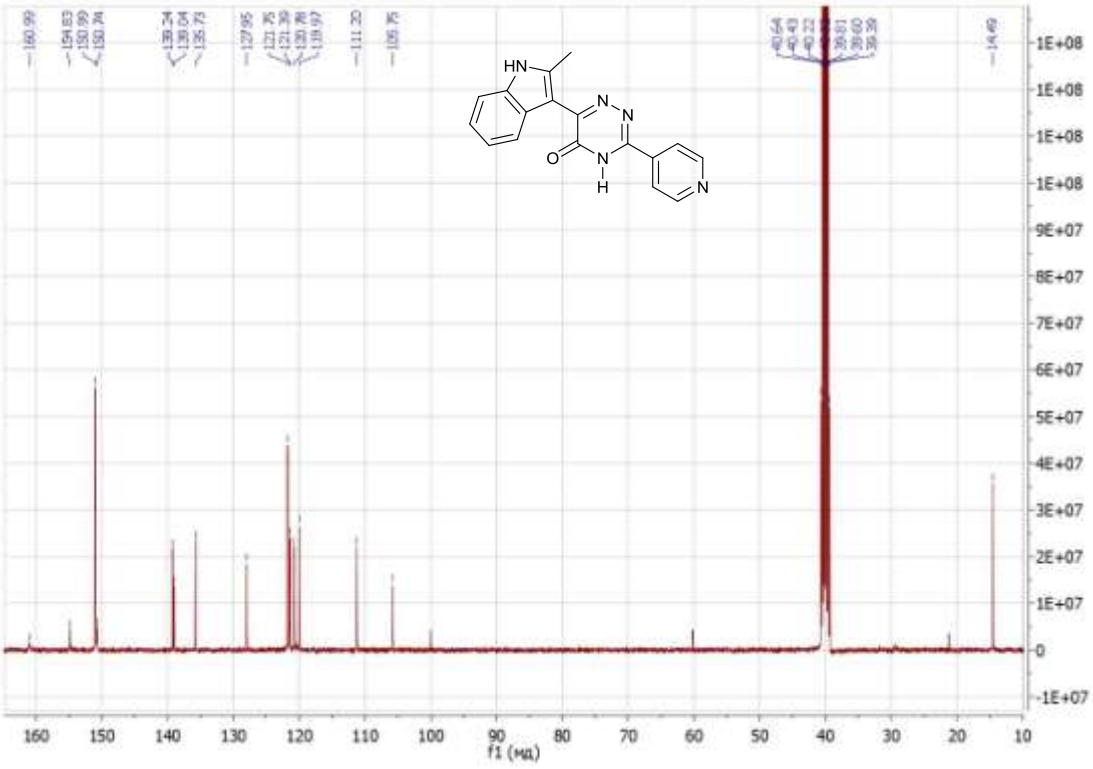


Figure S59. ^{13}C NMR Spectrum of 6-(2-methyl-1*H*-indol-3-yl)-3-(pyridin-4-yl)-1,2,4-triazin-5(4*H*)-one (15c)

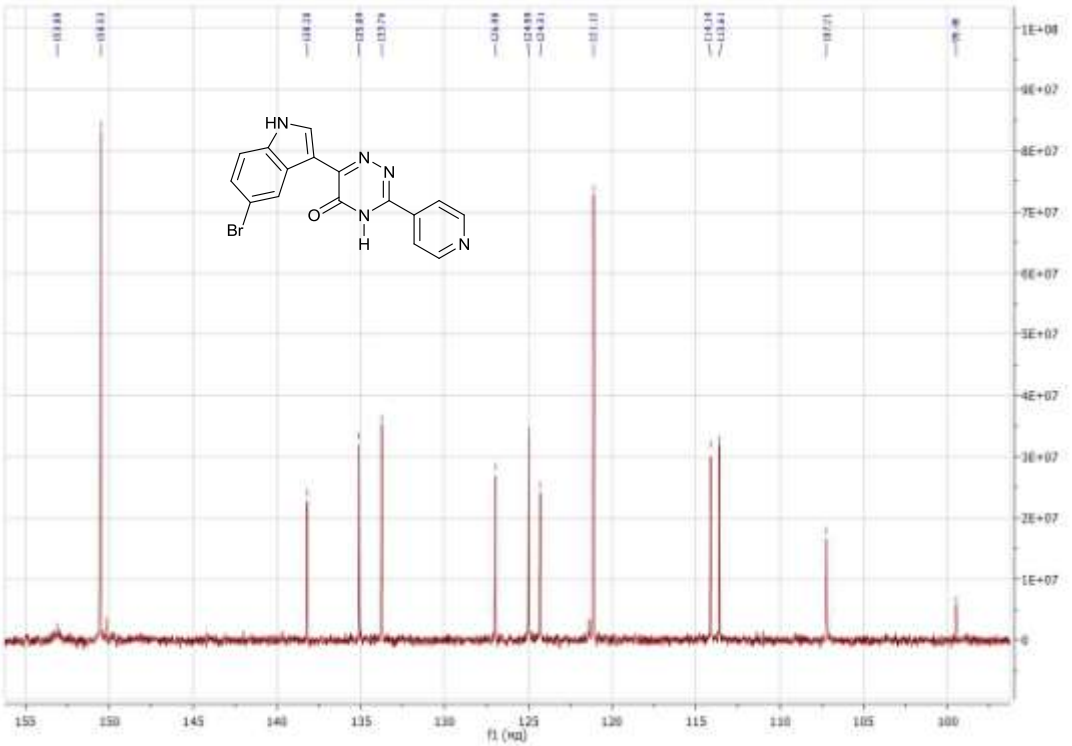


Figure S60. ^{13}C NMR Spectrum of 6-(5-bromo-1*H*-indol-3-yl)-3-(pyridin-4-yl)-1,2,4-triazin-5(4*H*)-one (15d)

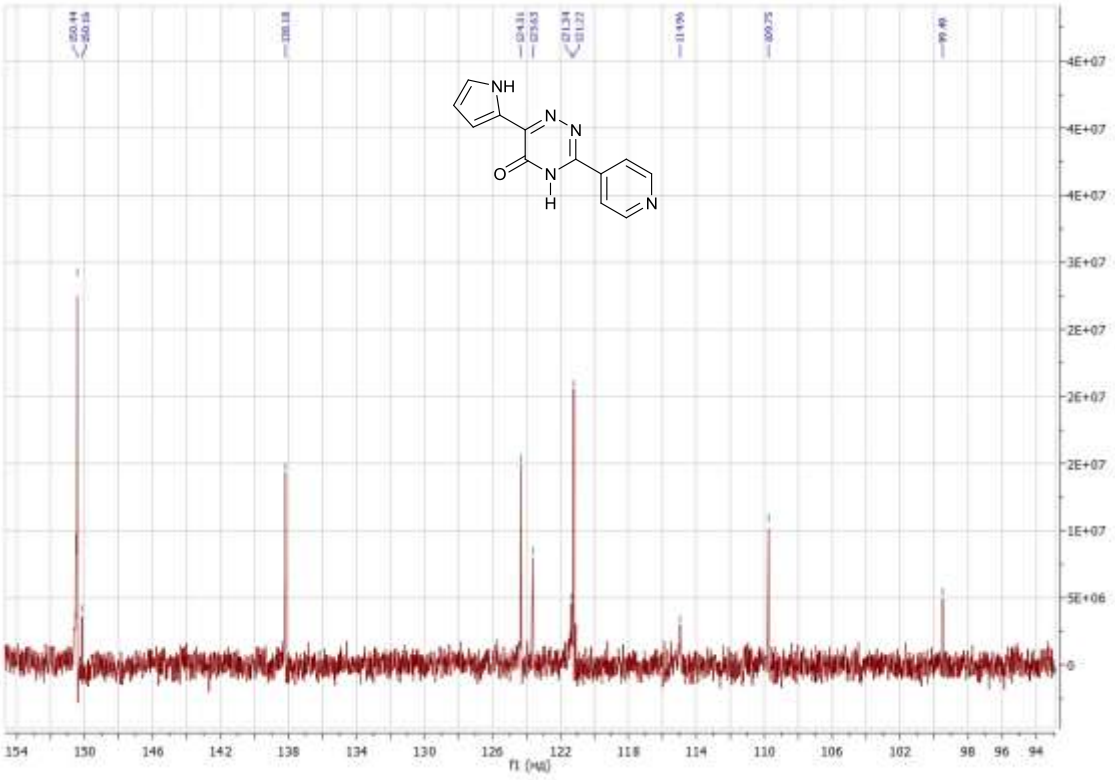


Figure S61. ^{13}C NMR Spectrum of 6-(1*H*-pyrrol-2-yl)-3-(pyridin-4-yl)-1,2,4-triazin-5(4*H*)-one (15e)

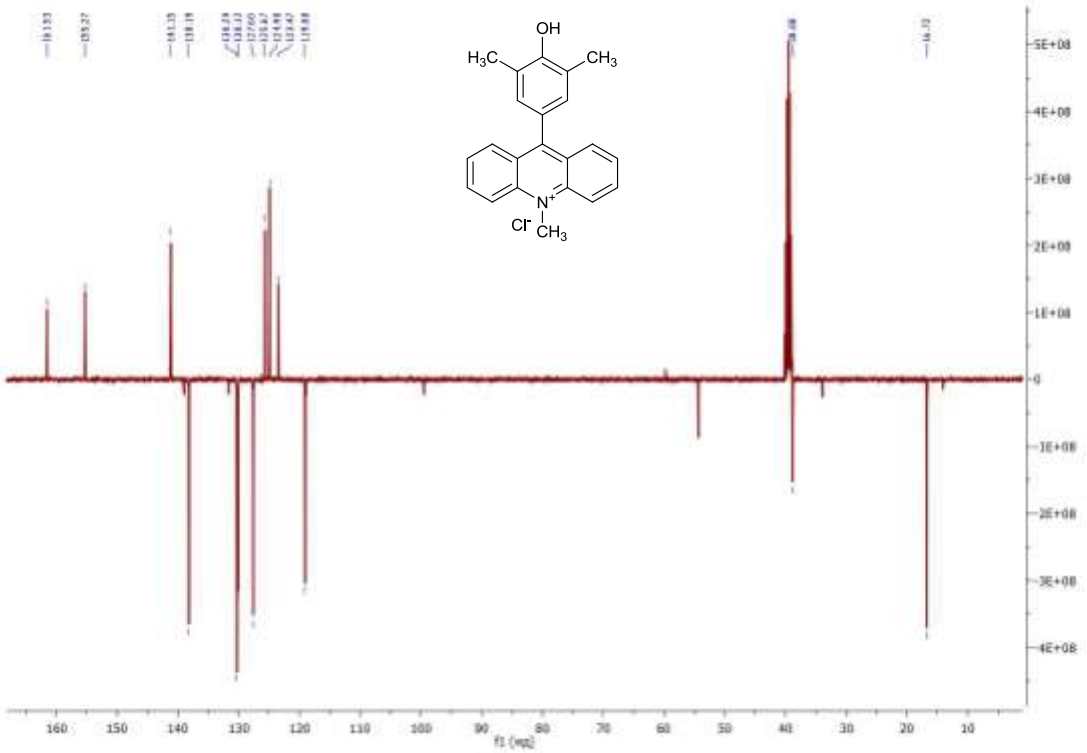


Figure S62. ^{13}C NMR Spectrum of 9-(4-hydroxy-3,5-dimethylphenyl)-10-methylacridinium chloride (25b)

NOESY Spectra

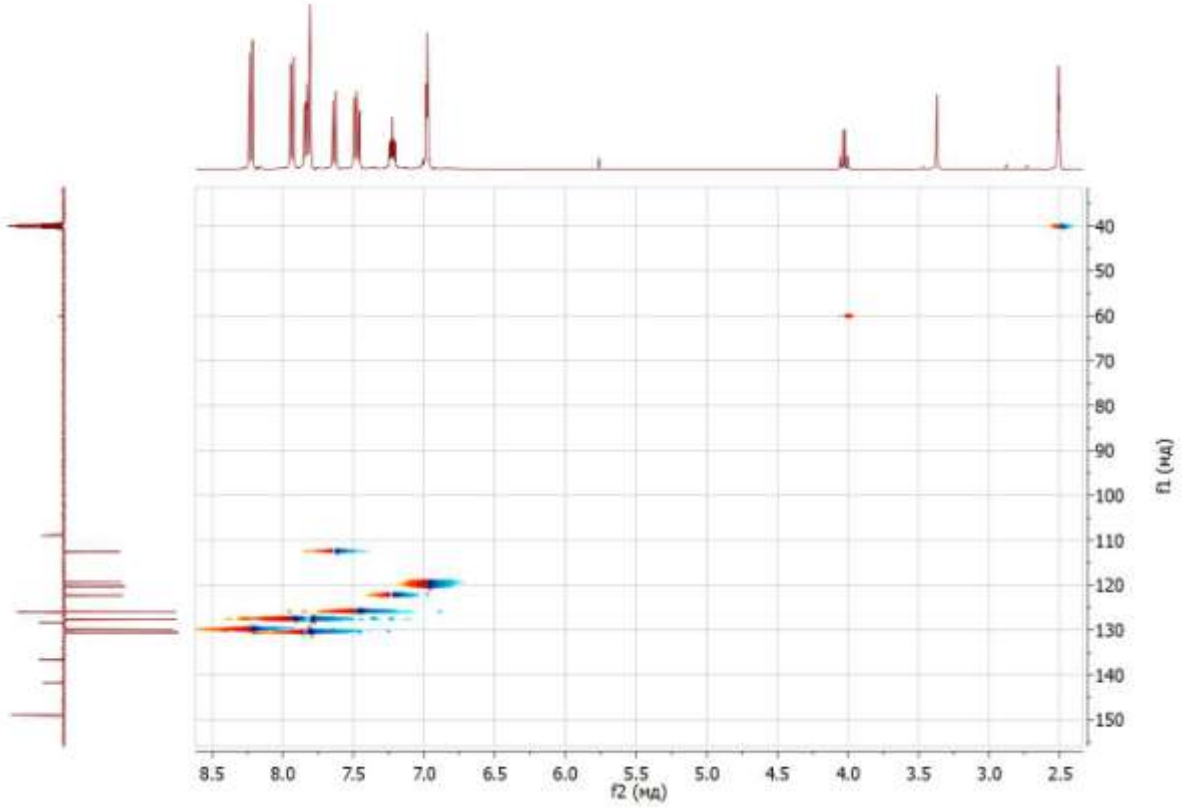


Figure S64. 2D ^{1}H-^{13}C HSQC Spectrum of 9-(1*H*-indol-3-yl)-acridine (6a)

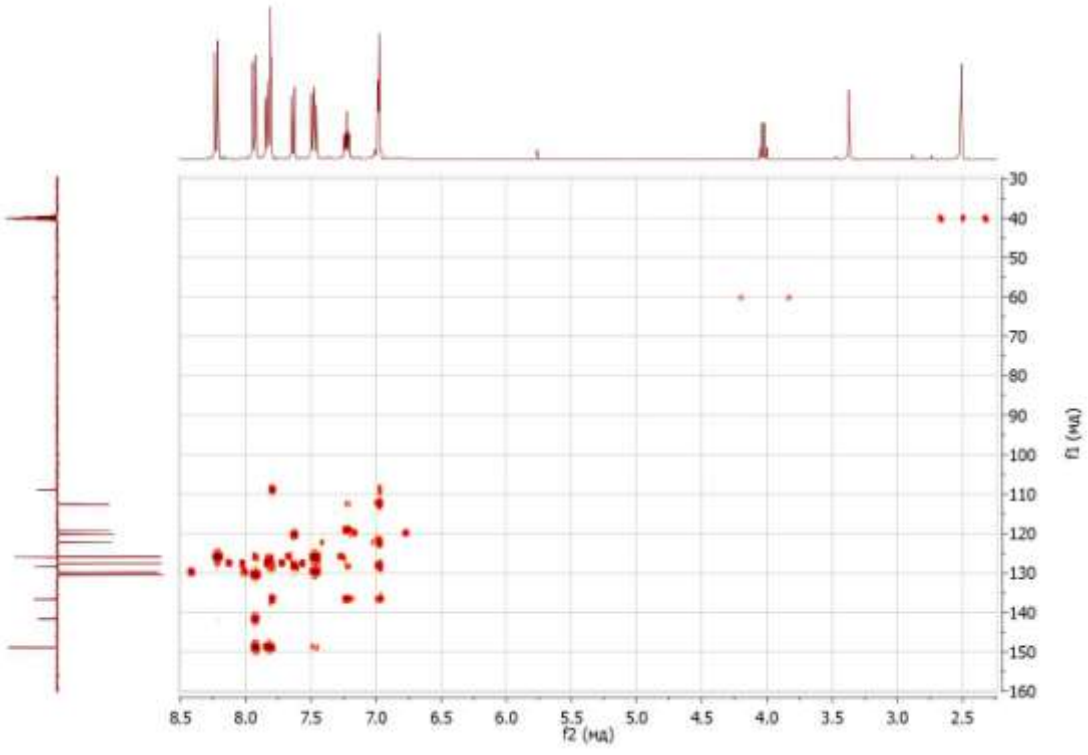


Figure S65. 2D ^{1}H-^{13}C HMBC Spectrum of 9-(1*H*-indol-3-yl)-acridine (6a)

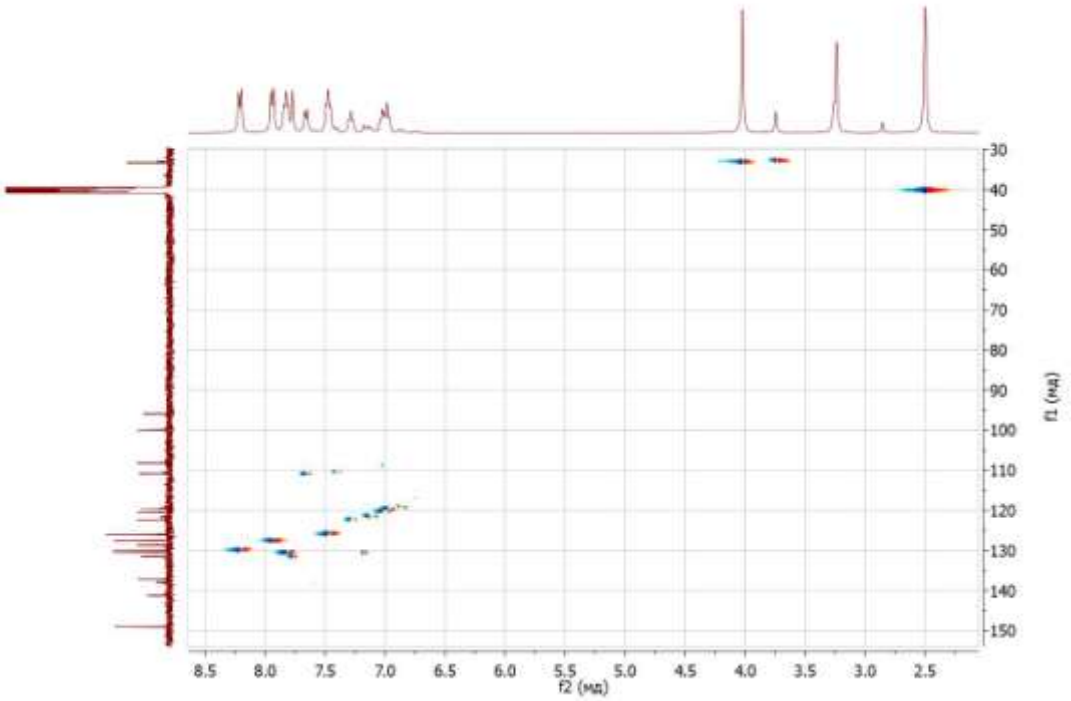


Figure S66. 2D ^{1}H-^{13}C HSQC Spectrum of 9-(N-methylindol-3-yl)-acridine (6b)

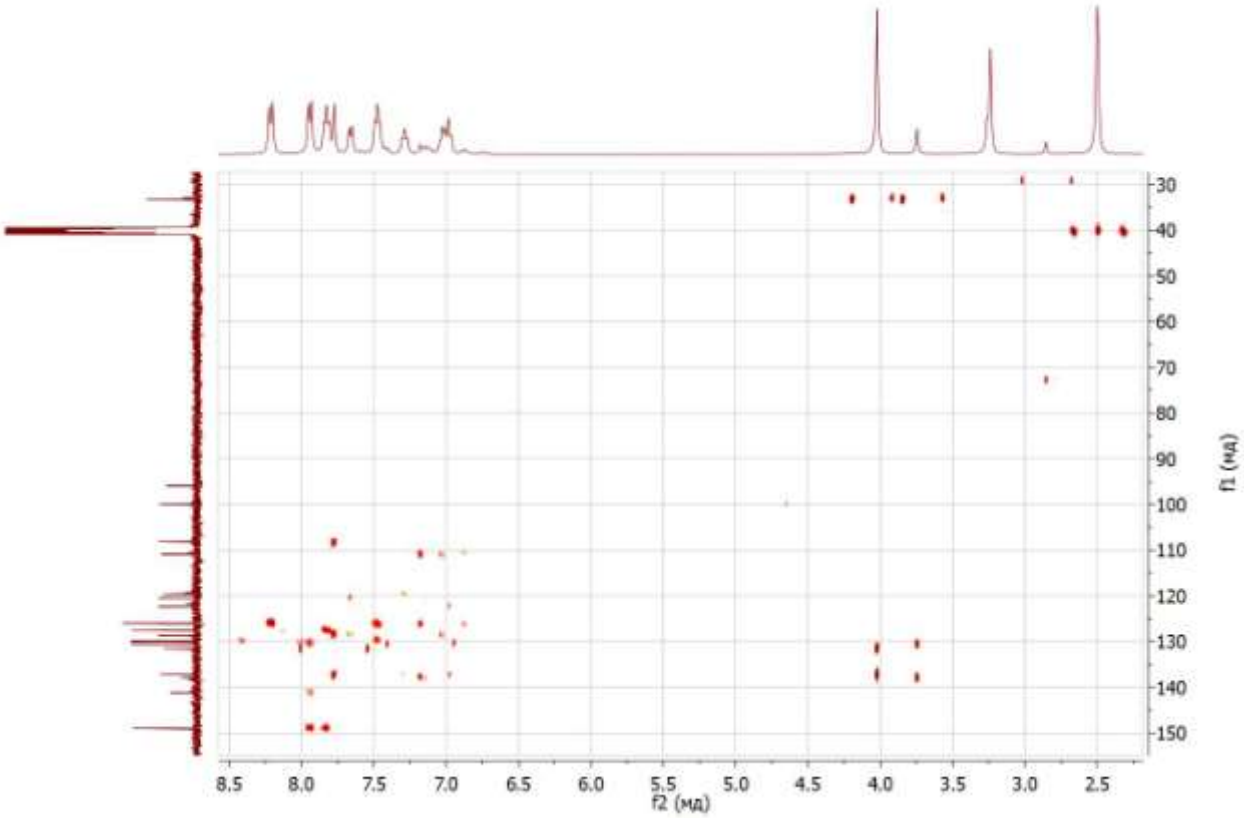


Figure S67. 2D ^{1}H-^{13}C HMBC Spectrum of 9-(N-methylindol-3-yl)-acridine (6b)

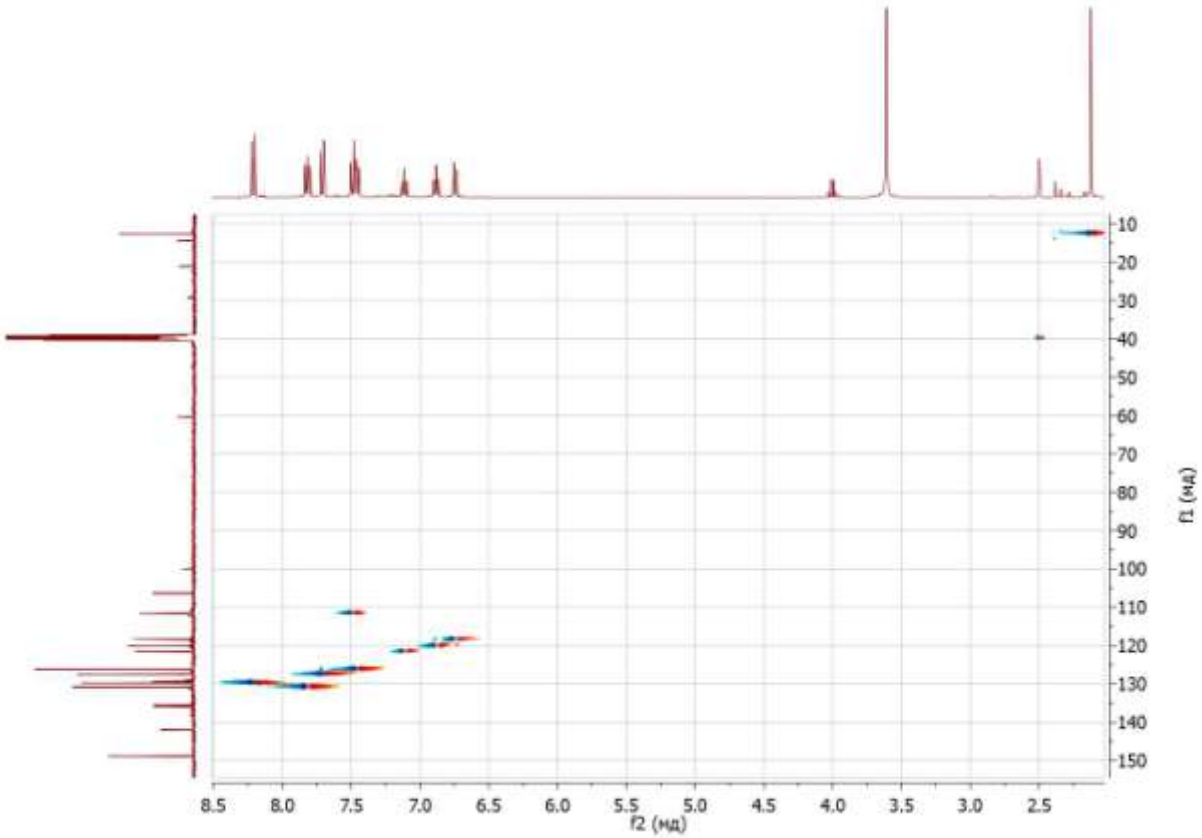


Figure S68. 2D ^{1}H-^{13}C HSQC Spectrum of 9-(2-methyl-1*H*-indol-3-yl)-acridine (6c)

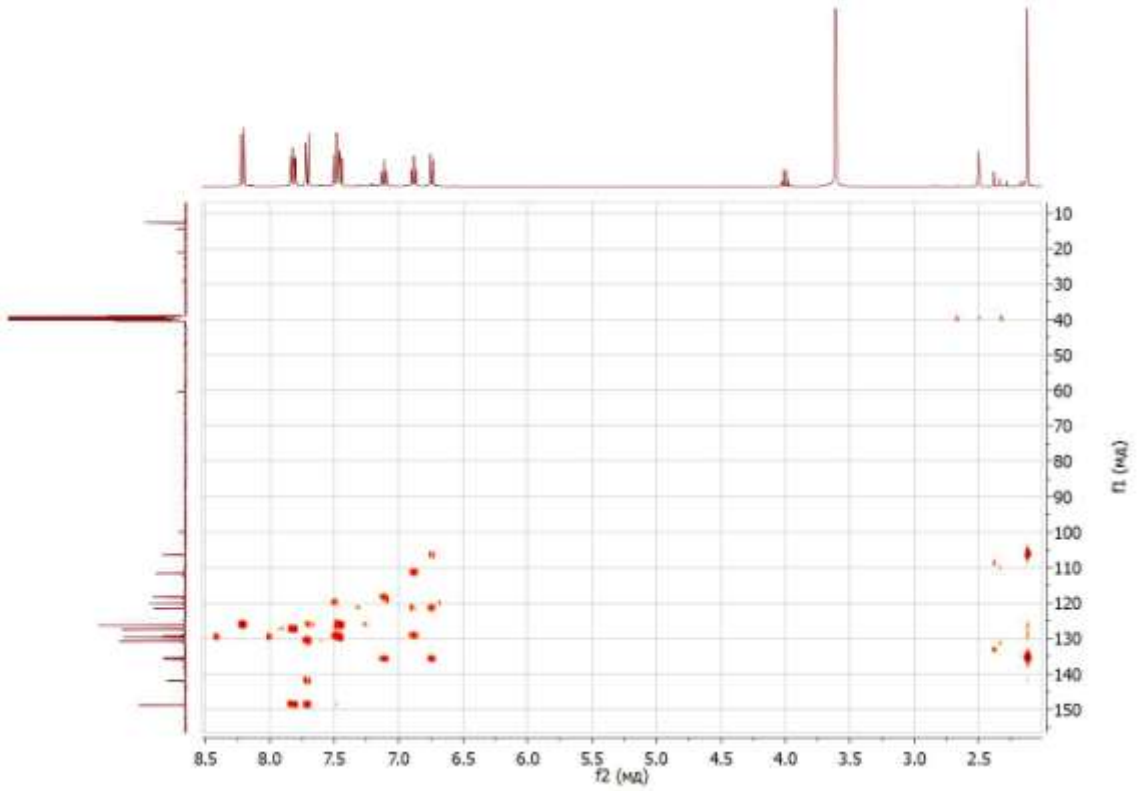


Figure S69. 2D ^{1}H-^{13}C HMBC Spectrum of 9-(2-methyl-1*H*-indol-3-yl)-acridine (6c)

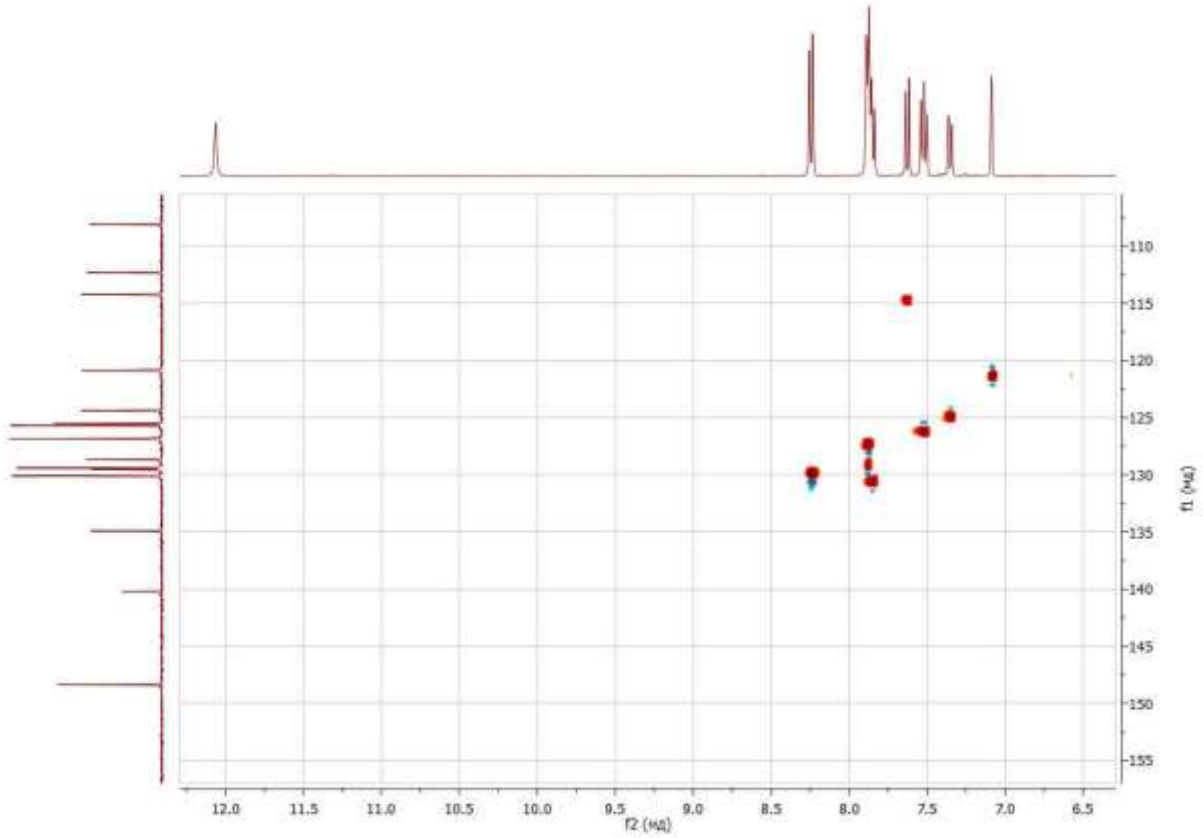


Figure S70. 2D ^{1}H-^{13}C HSQC Spectrum of 9-(5-bromo-1*H*-indol-3-yl)-acridine (6d)

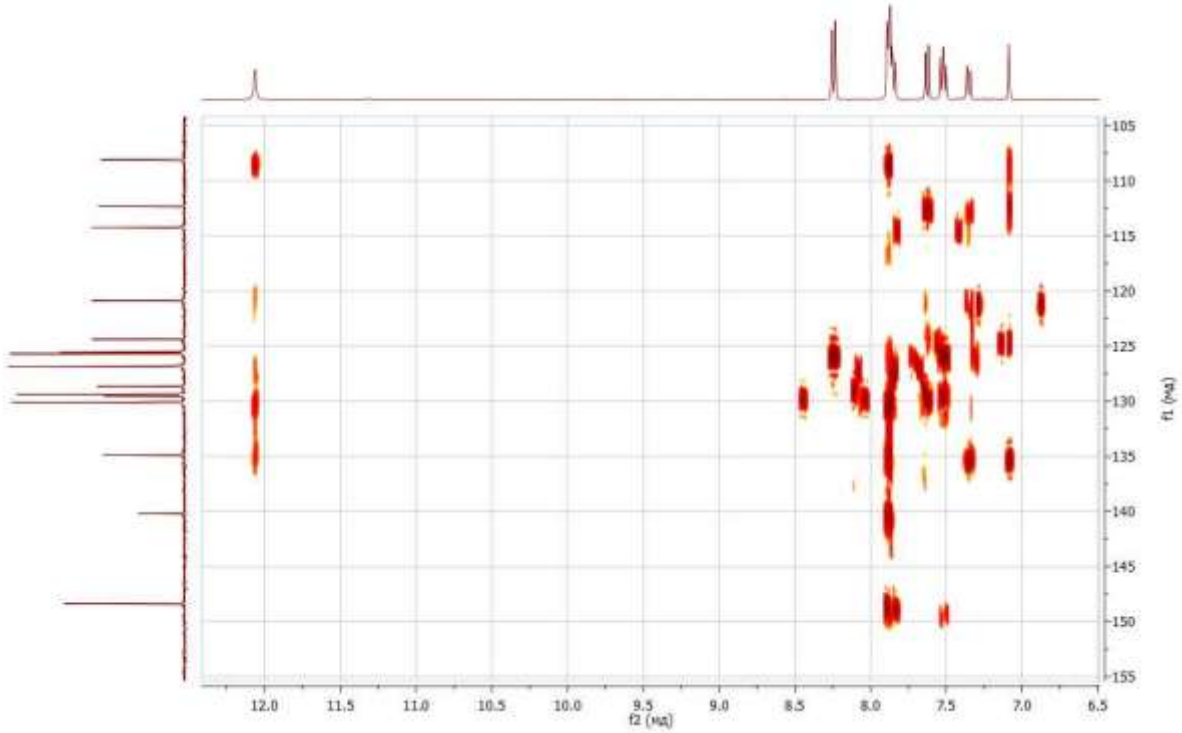


Figure S71. 2D ^{1}H-^{13}C HMBC Spectrum of 9-(2-bromo-1*H*-indol-3-yl)-acridine (6d)

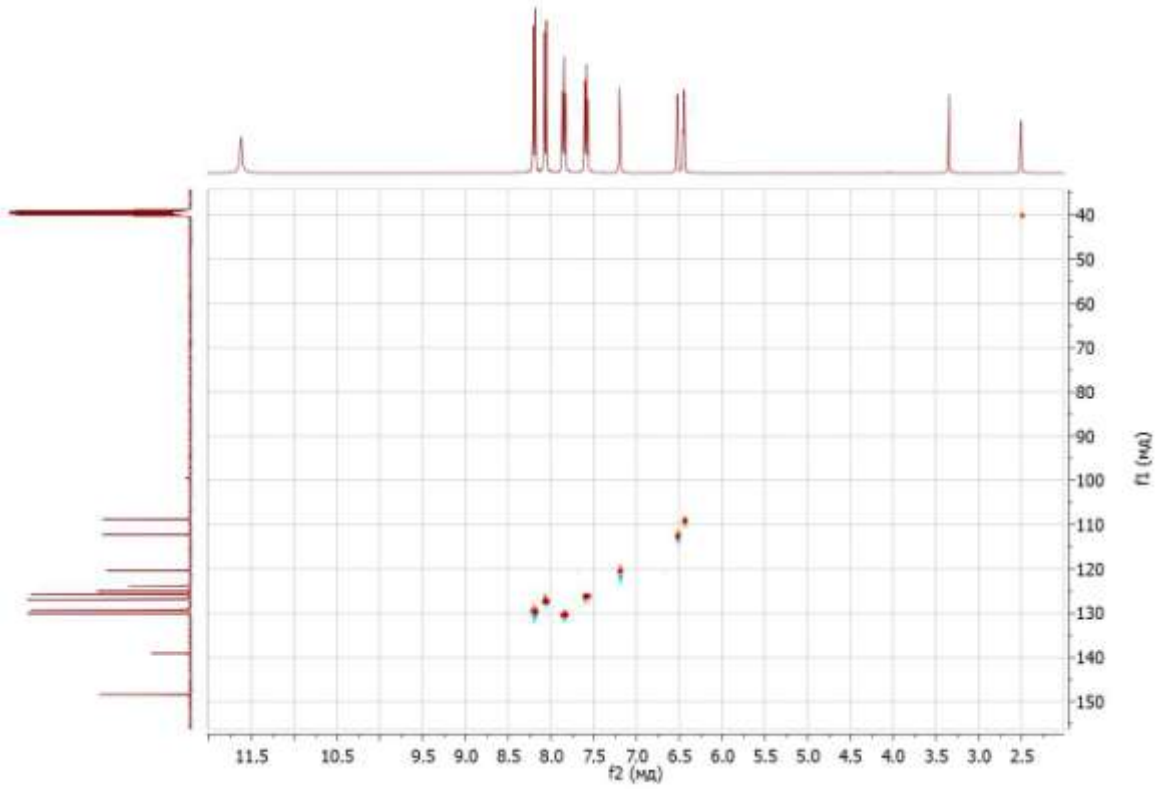


Figure S72. 2D ^{1}H-^{13}C HSQC Spectrum of 9-(1*H*-pyrrol-2-yl)-acridine (6e)

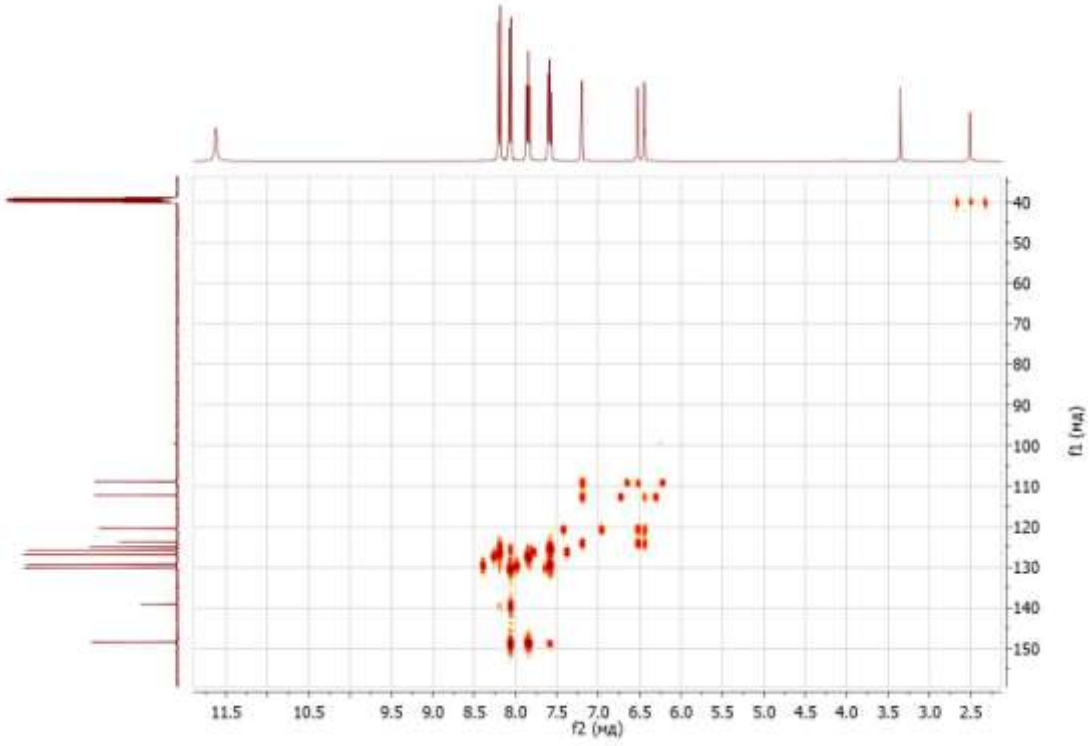


Figure S73. 2D ^{1}H-^{13}C HMBC Spectrum of 9-(1*H*-pyrrol-2-yl)-acridine (6e)

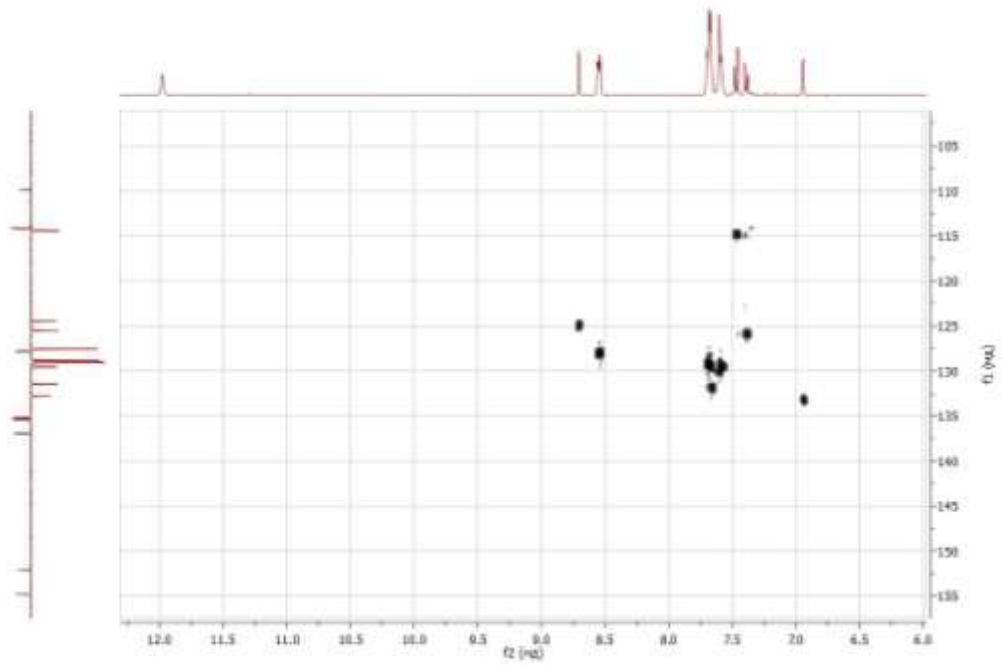


Figure S74. 2D ^{1}H-^{13}C HSQC Spectrum of 3,6-diphenyl-5-(5-bromo-1*H*-indol-3-yl)-1,2,4-triazine (7d)

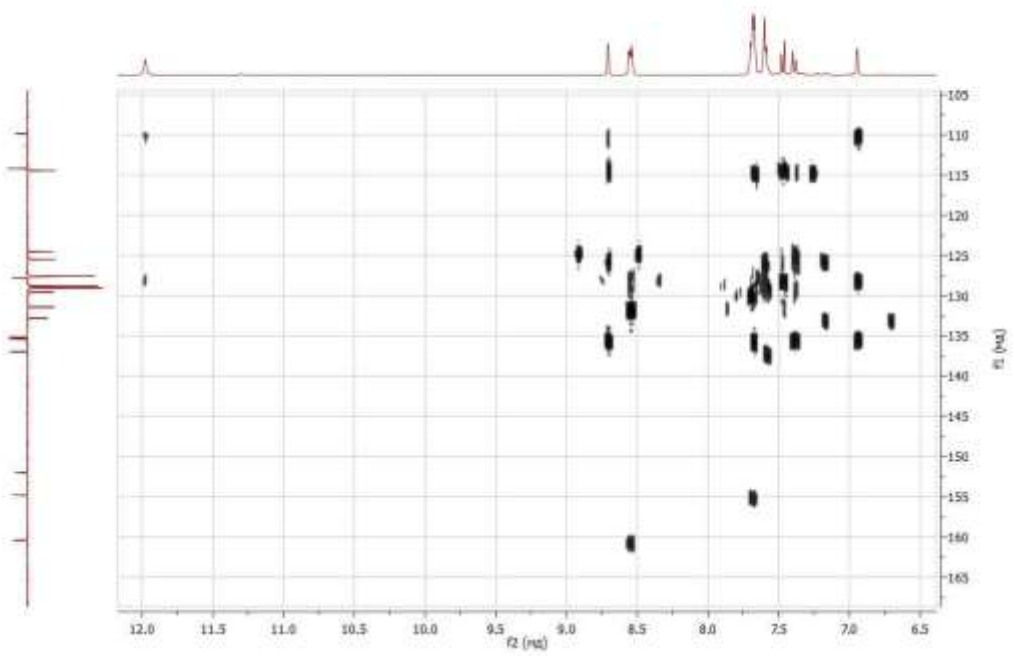


Figure S75. 2D ^{1}H-^{13}C HMBC Spectrum of 3,6-diphenyl-5-(5-bromo-1*H*-indol-3-yl)-1,2,4-triazine (7d)

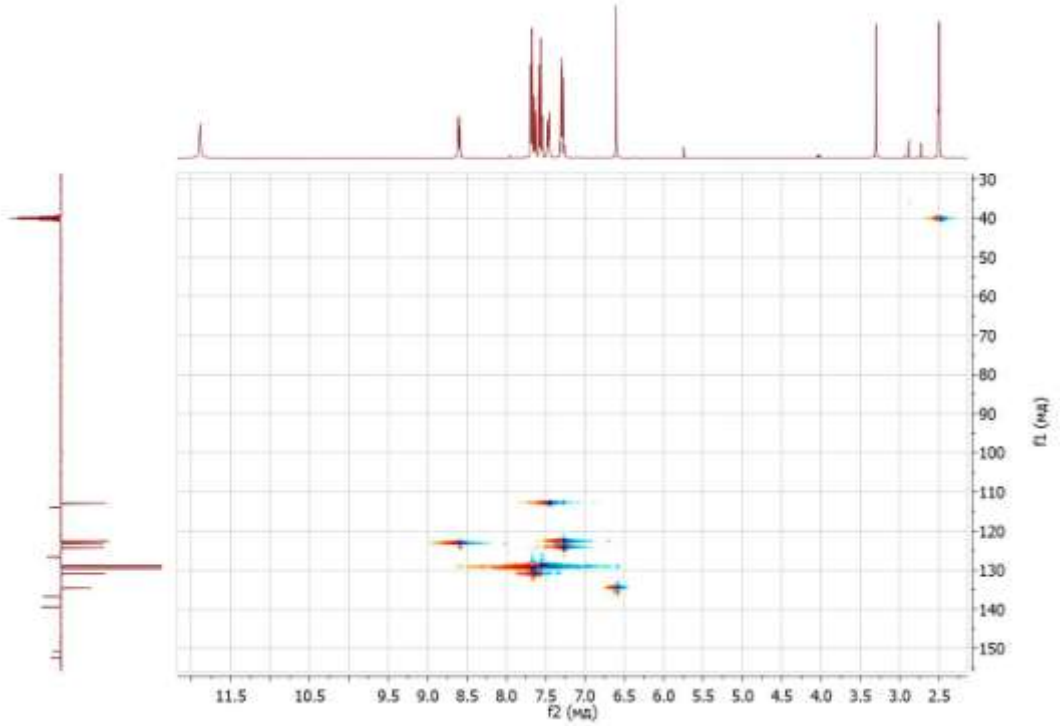


Figure S76. 2D ^{1}H-^{13}C HSQC Spectrum of 5-(1*H*-indol-3-yl)-6-phenyl-1,2,5-oxadiazolo[3,4-*b*]pyrazine (8a)

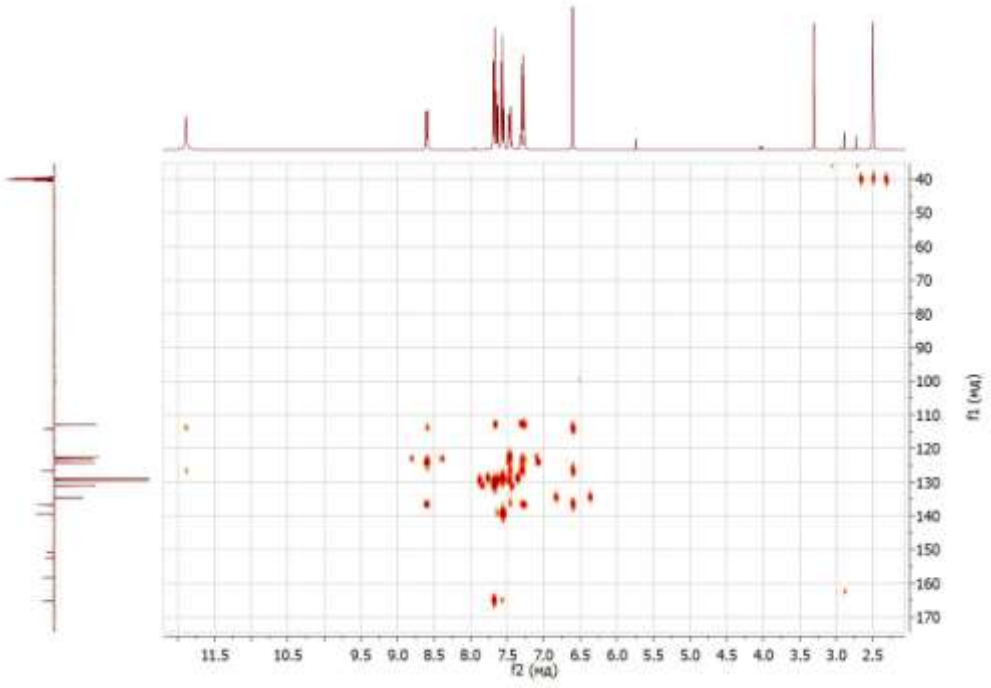


Figure S77. 2D ^{1}H-^{13}C HMBC Spectrum of 5-(1*H*-indol-3-yl)-6-phenyl-1,2,5-oxadiazolo[3,4-*b*]pyrazine (8a)

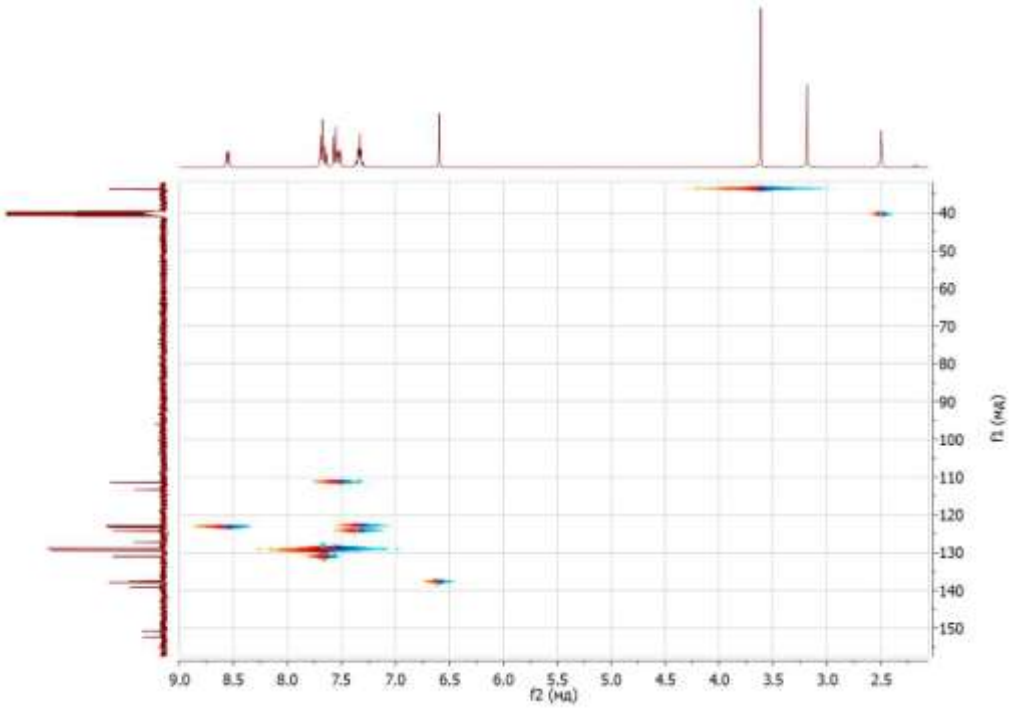


Figure S78. 2D ^{1}H-^{13}C HSQC Spectrum of 5-(N-methylindol-3-yl)-6-phenyl-1,2,5-oxadiazolo[3,4-*b*]pyrazine (8b)

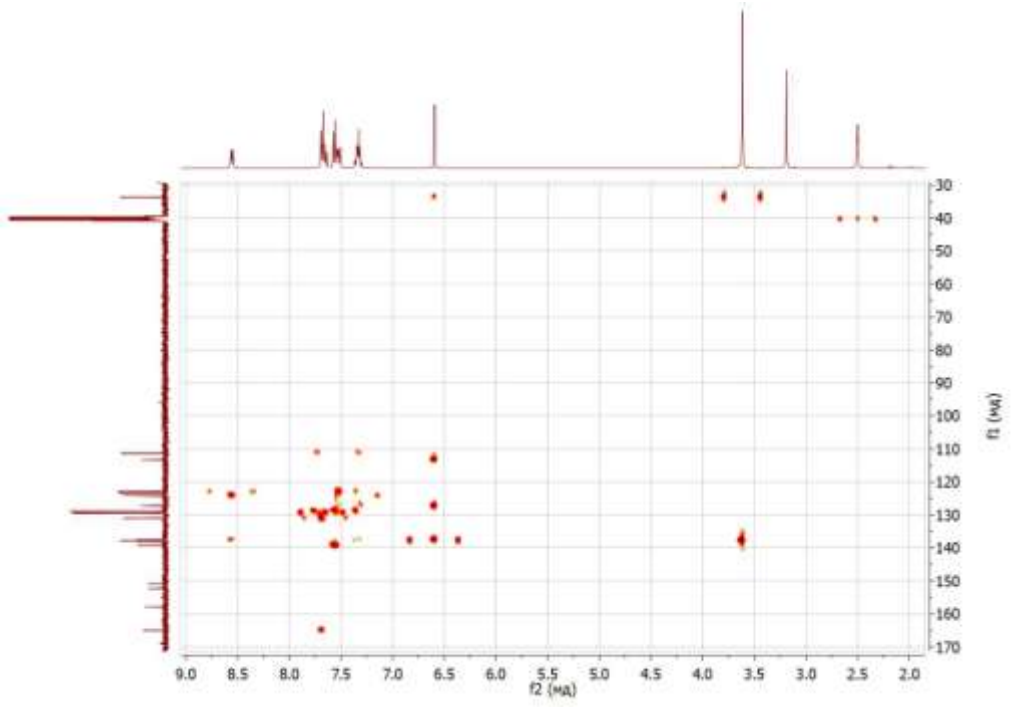


Figure S79. 2D ^{1}H-^{13}C HMBC Spectrum of 5-(N-methylindol-3-yl)-6-phenyl-1,2,5-oxadiazolo[3,4-*b*]pyrazine (8b)

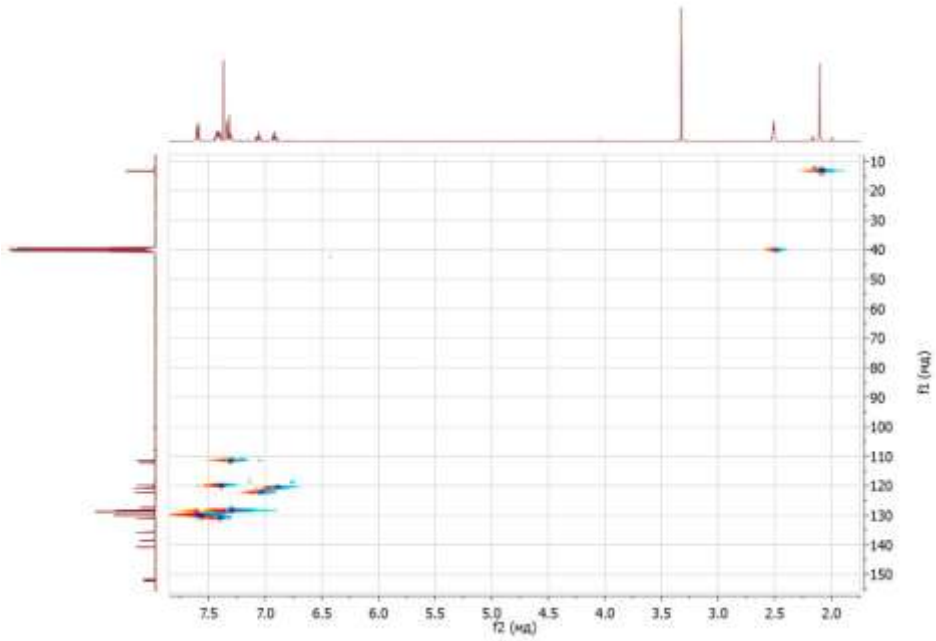


Figure S80. 2D ^{1}H-^{13}C HSQC Spectrum of 5-(2-methyl-1*H*-indol-3-yl)-6-phenyl-1,2,5-oxadiazolo[3,4-*b*]pyrazine (8c)

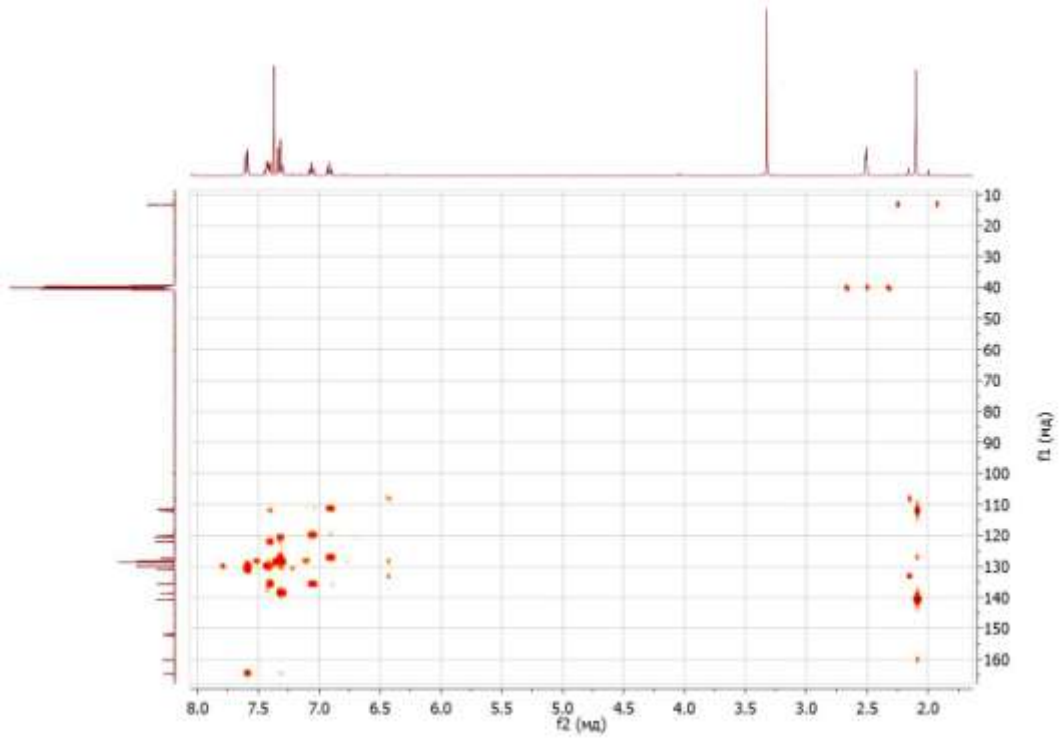


Figure S81. 2D ^{1}H-^{13}C HMBC Spectrum of 5-(2-methyl-1*H*-indol-3-yl)-6-phenyl-1,2,5-oxadiazolo[3,4-*b*]pyrazine (8c)

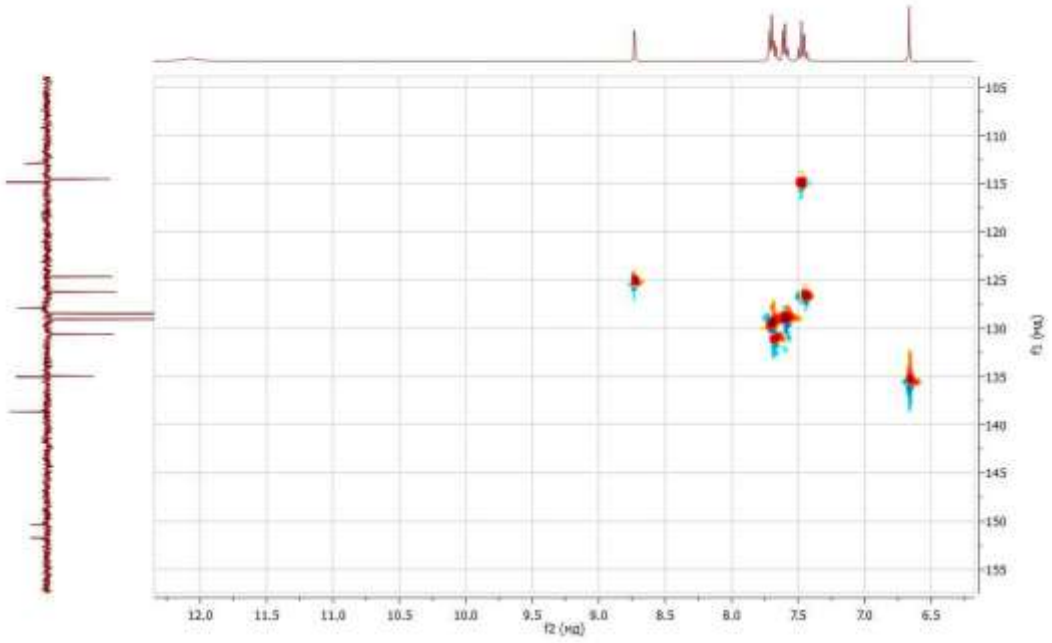


Figure S82. 2D ^{1}H-^{13}C HSQC Spectrum of 5-(5-bromo-1*H*-indol-3-yl)-6-phenyl-1,2,5-oxadiazolo[3,4-*b*]pyrazine (8d)

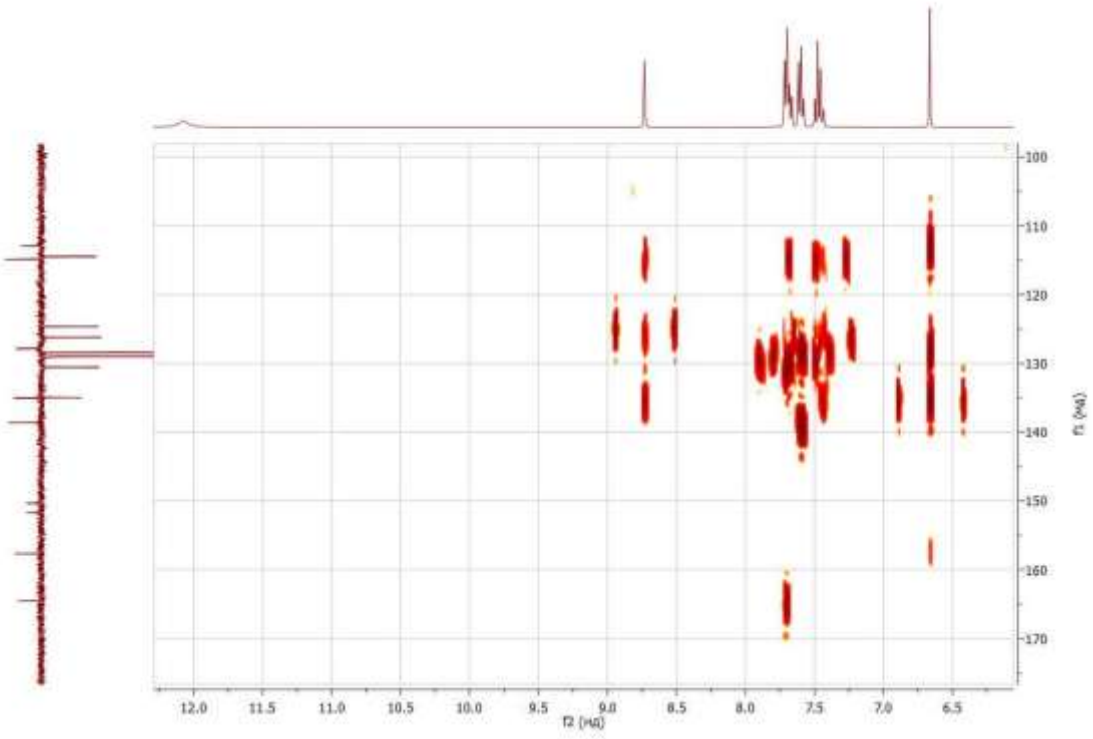


Figure S83. 2D ^{1}H-^{13}C HMBC Spectrum of 5-(5-bromo-1*H*-indol-3-yl)-6-phenyl-1,2,5-oxadiazolo[3,4-*b*]pyrazine (8d)

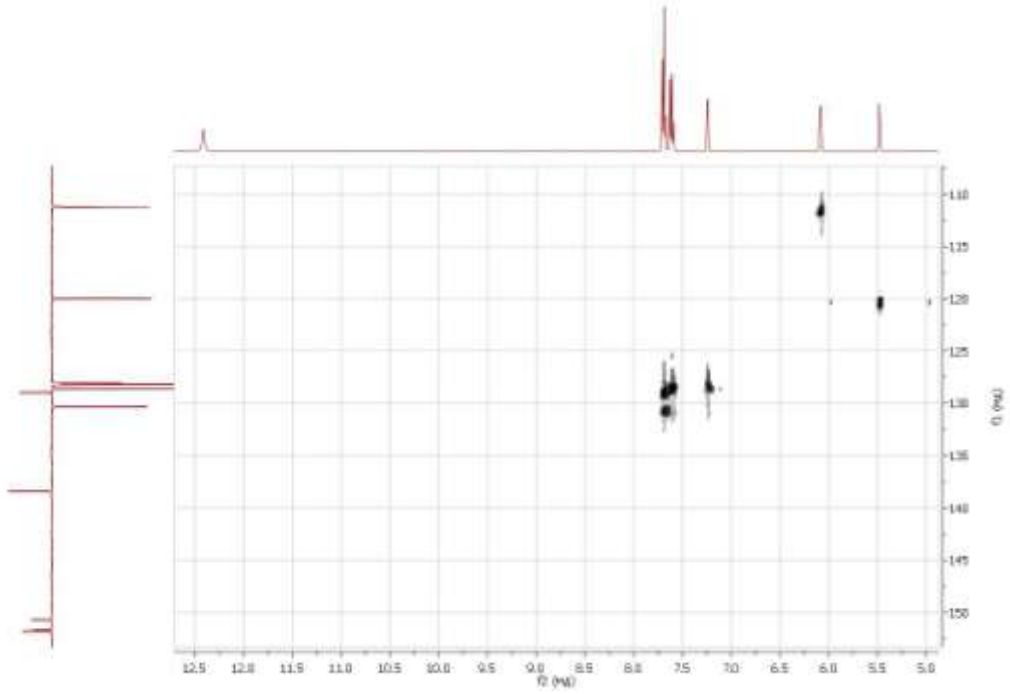


Figure S84. 2D ^{1}H-^{13}C HSQC Spectrum of 5-phenyl-6-(1*H*-pyrrol-2-yl)-[1,2,5]oxadiazolo[3,4-*b*]pyrazine (8e)

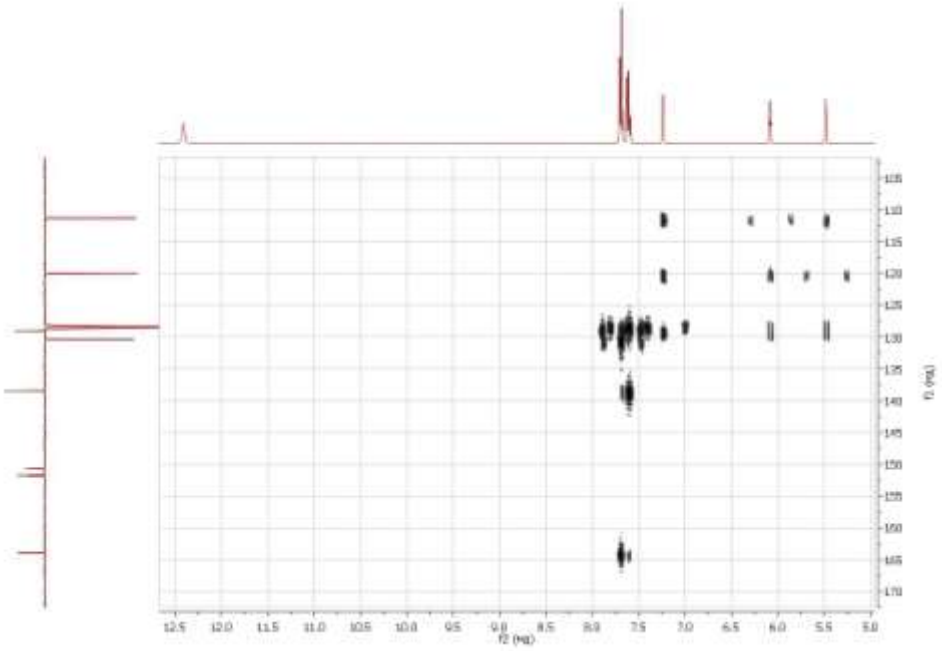


Figure S85. 2D ^{1}H-^{13}C HMBC Spectrum of 5-phenyl-6-(1*H*-pyrrol-2-yl)-[1,2,5]oxadiazolo[3,4-*b*]pyrazine (8e)

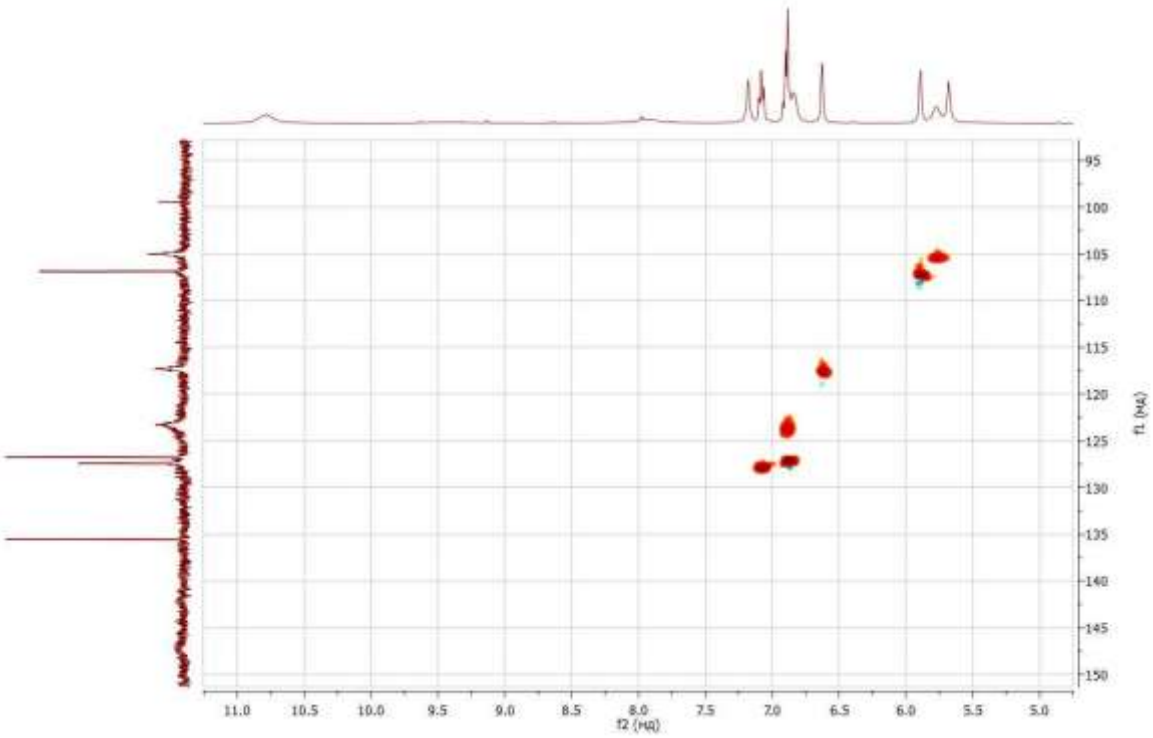


Figure S86. 2D ^{1}H-^{13}C HSQC Spectrum of 4-(1*H*-pyrrol-2-yl)quinazoline (9e)

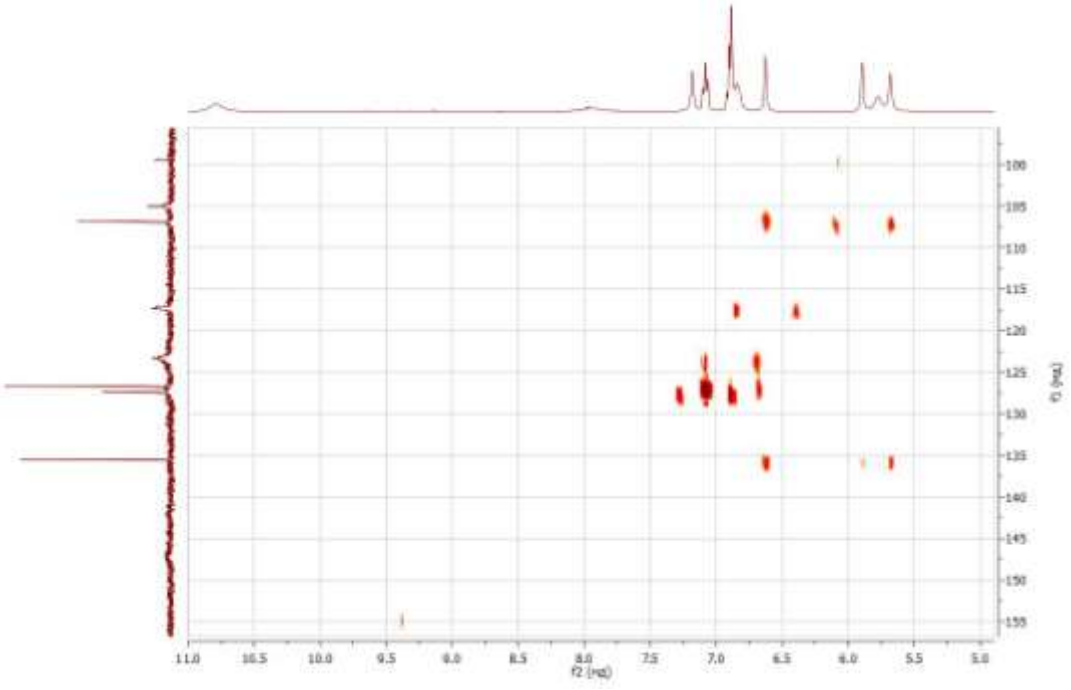


Figure S87. 2D ^{1}H-^{13}C HMBC Spectrum of 4-(1*H*-pyrrol-2-yl)quinazoline (9e)

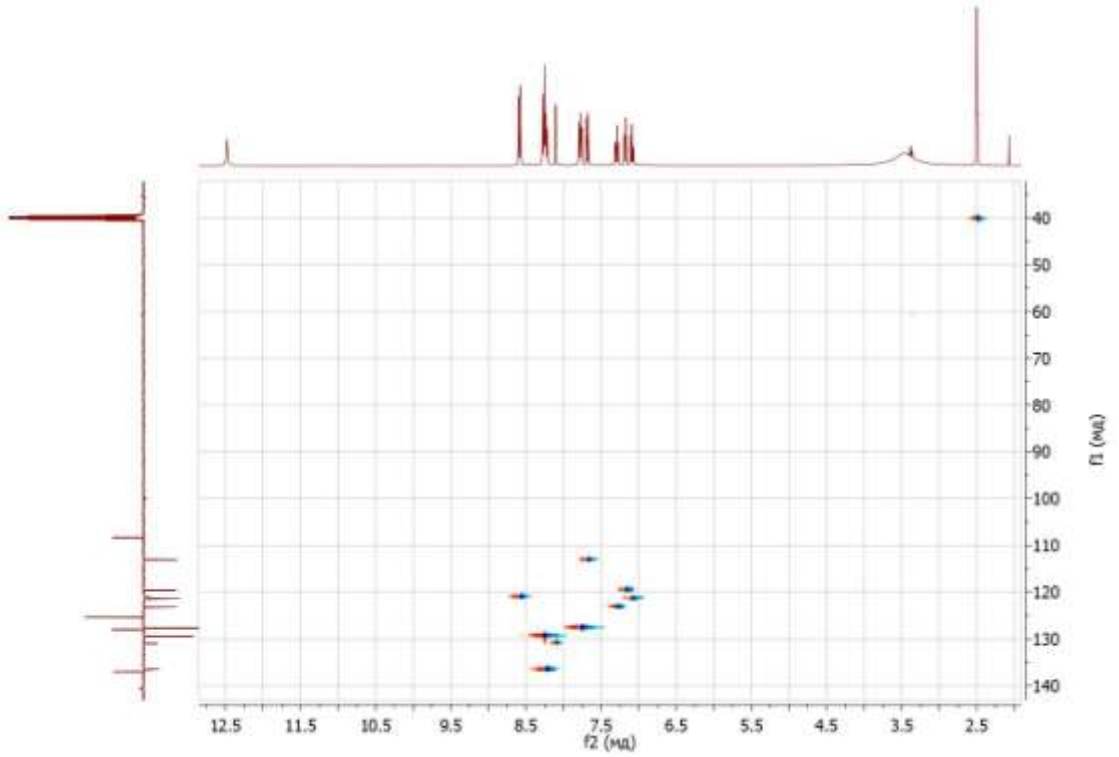


Figure S88. 2D ^{1}H-^{13}C HSQC Spectrum of 9-(1*H*-indol-3-yl)-10-hydroacridinum chloride (11a)

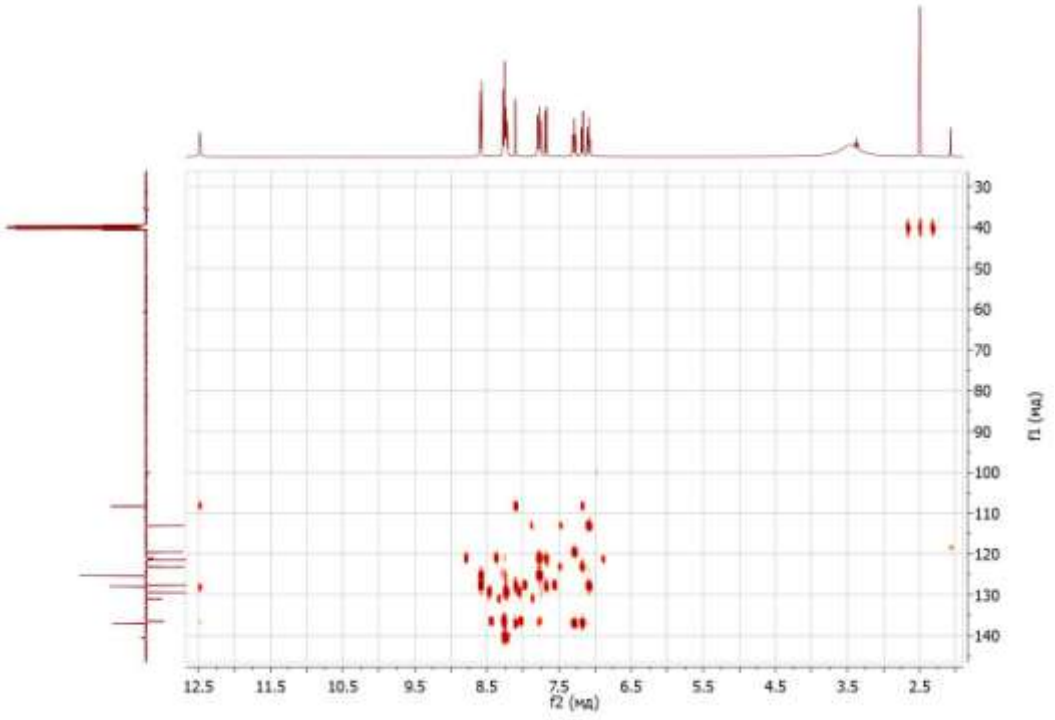


Figure S89. 2D ^{1}H-^{13}C HMBC Spectrum of 9-(1*H*-indol-3-yl)-10-hydroacridinum chloride (11a)

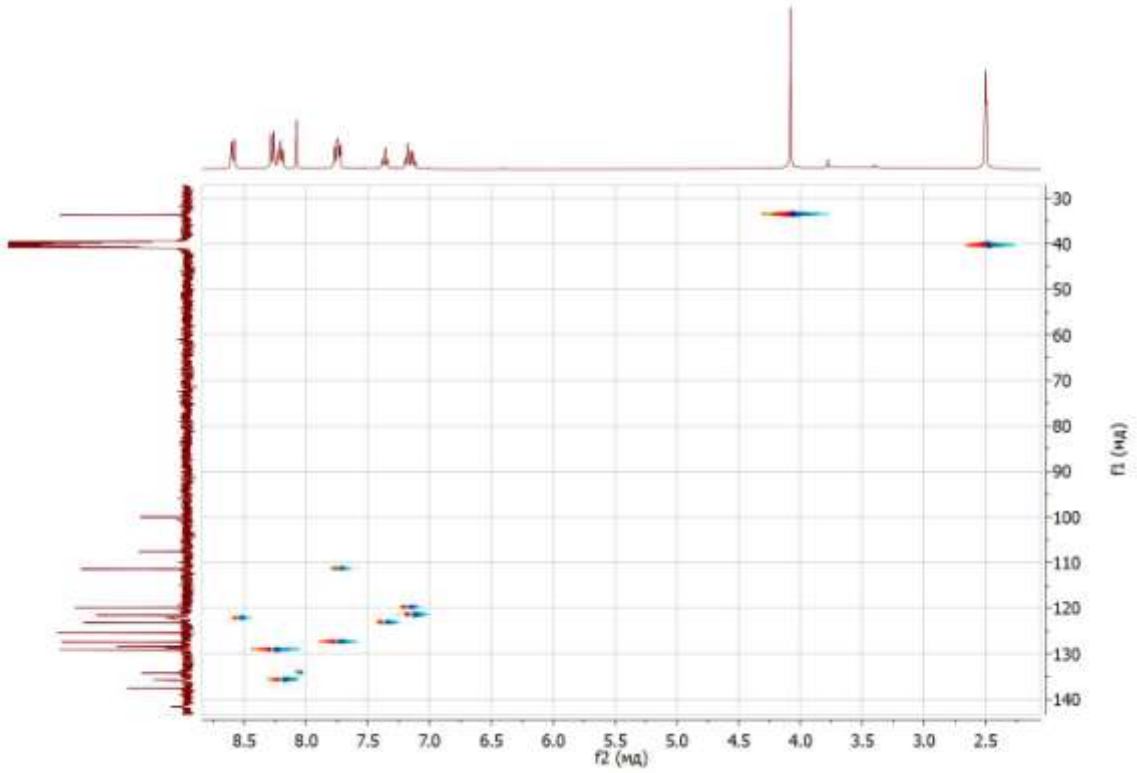


Figure S90. 2D ^{1}H-^{13}C HSQC Spectrum of 9-(N-methylindol-3-yl)-10-hydroacridinum chloride (11b)

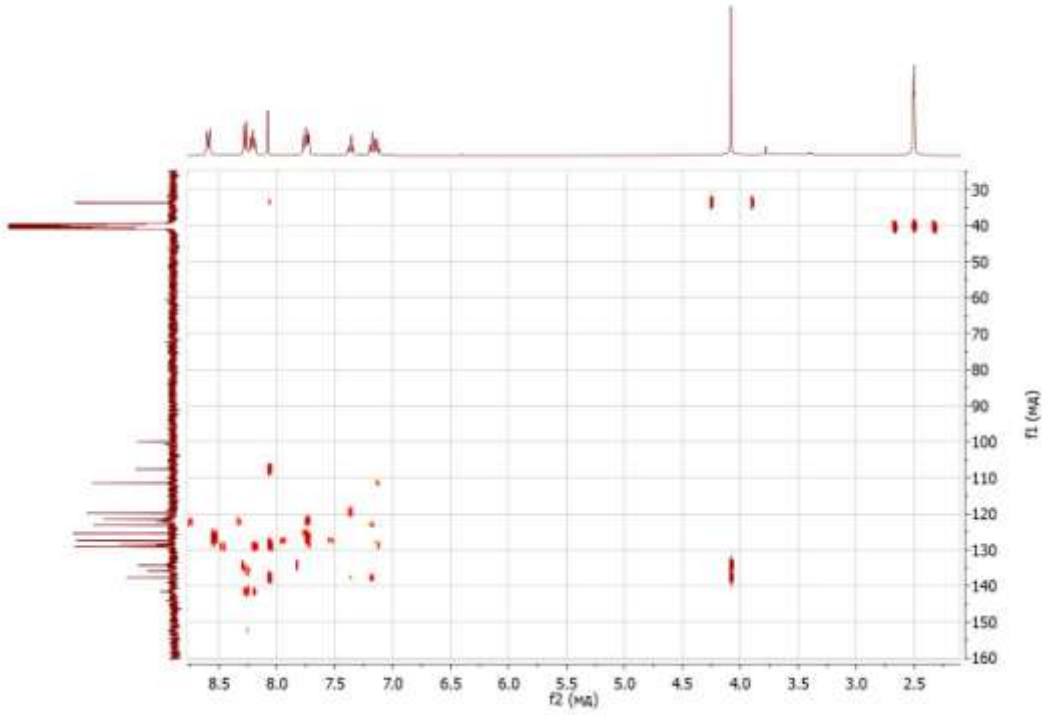


Figure S91. 2D ^{1}H-^{13}C HMBC Spectrum of 9-(N-methylindol-3-yl)-10-hydroacridinum chloride (11b)

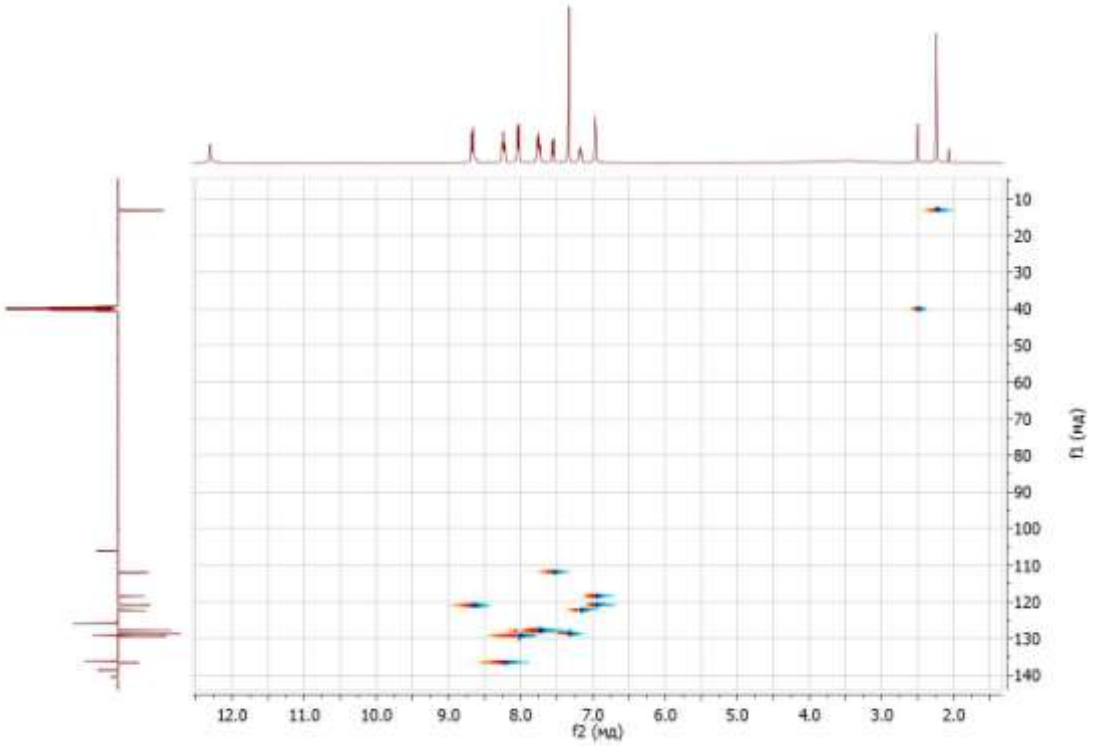


Figure S92. 2D ^{1}H-^{13}C HSQC Spectrum of 9-(2-methyl-1*H*-indol-3-yl)-10-hydroacridinum chloride (11c)

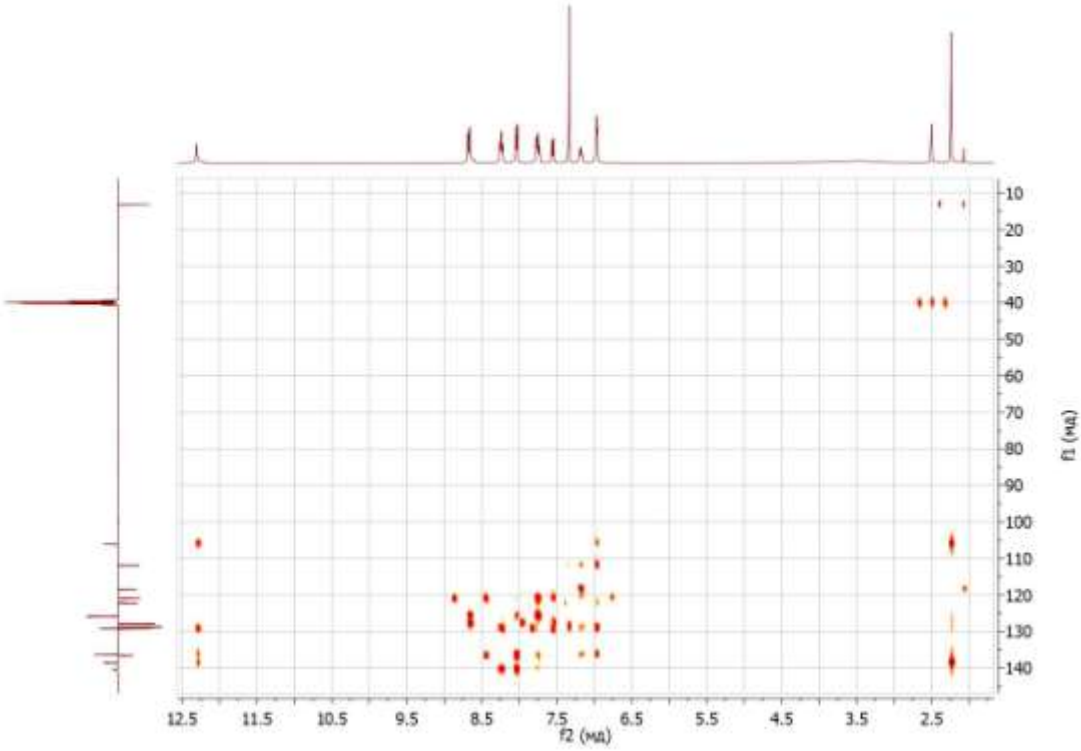


Figure S93. 2D ^{1}H-^{13}C HMBC Spectrum of 9-(2-methyl-1*H*-indol-3-yl)-10-hydroacridinum chloride (11c)

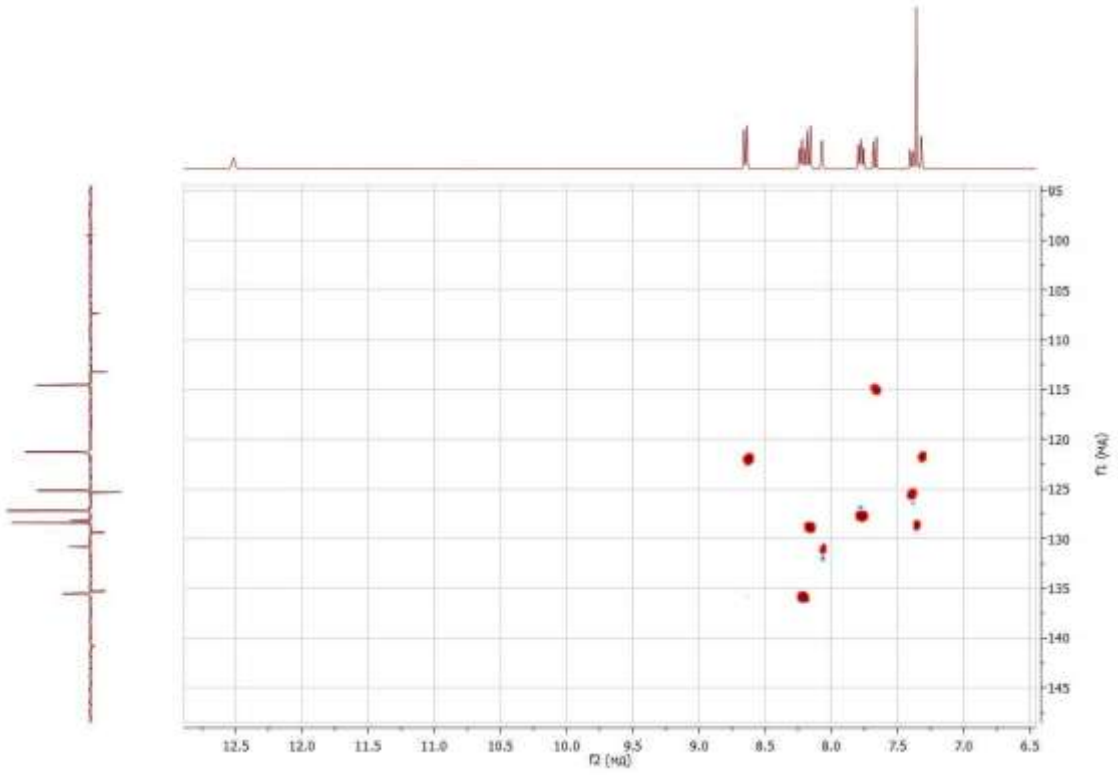


Figure S94. 2D ^{1}H-^{13}C HSQC Spectrum of 9-(5-bromo-1*H*-indol-3-yl)-10-hydroacridinum chloride (11d)

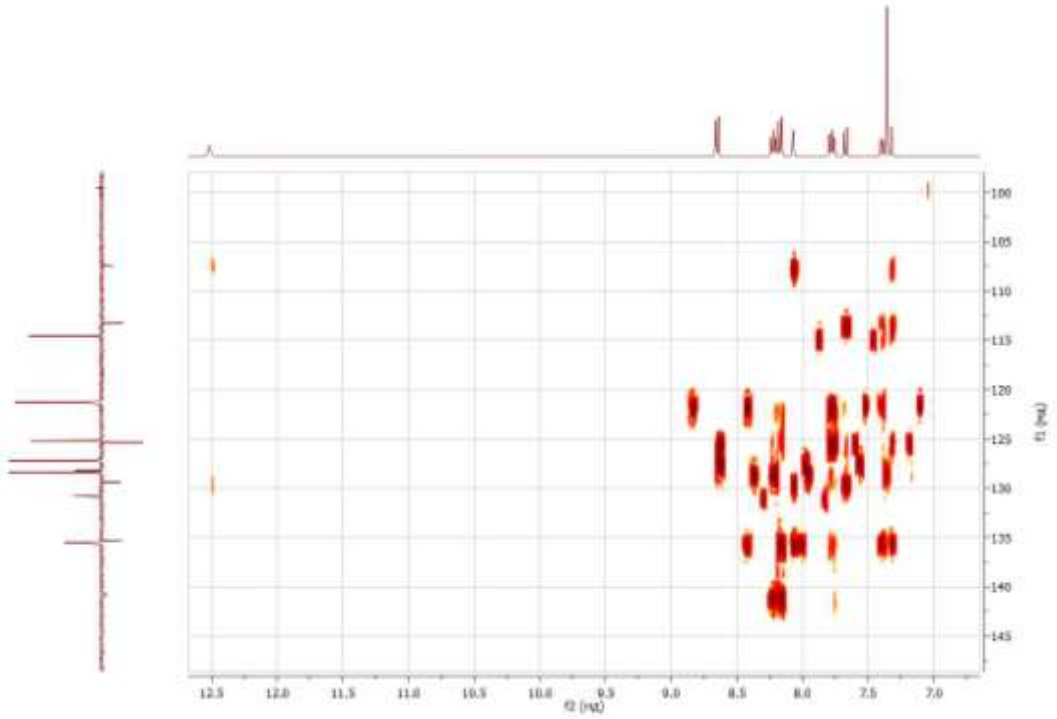


Figure S95. 2D ^{1}H-^{13}C HMBC Spectrum of 9-(5-bromo-1*H*-indol-3-yl)-10-hydroacridinum chloride (11d)

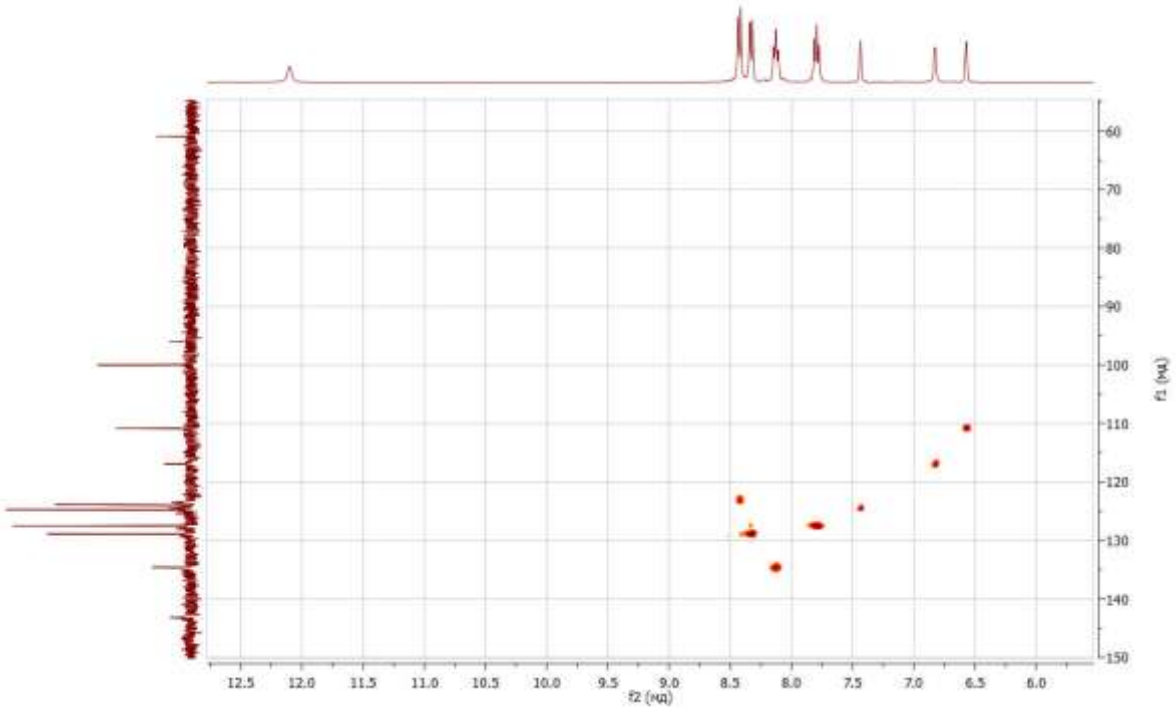


Figure S96. 2D ^{1}H-^{13}C HSQC Spectrum of 9-(1*H*-pyrrol-2-yl)-10-hydroacridinum chloride (11e)

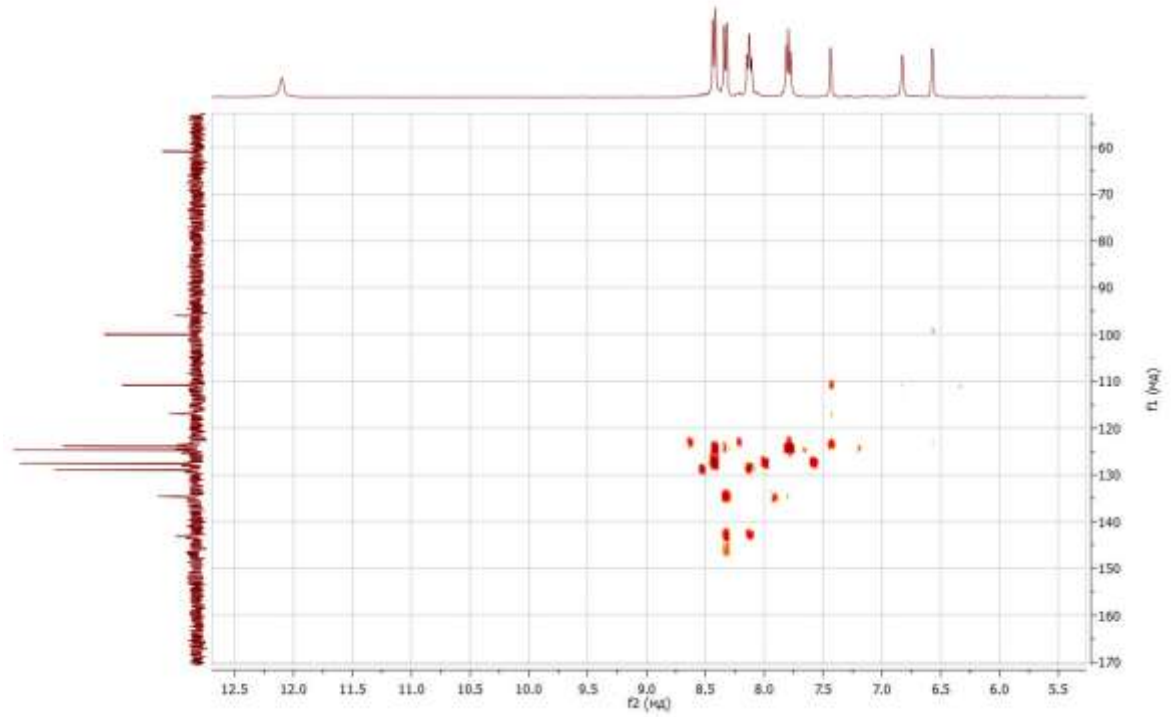


Figure S97. 2D ^{1}H-^{13}C HMBC Spectrum of 9-(1*H*-pyrrol-2-yl)-10-hydroacridinum chloride (11e)

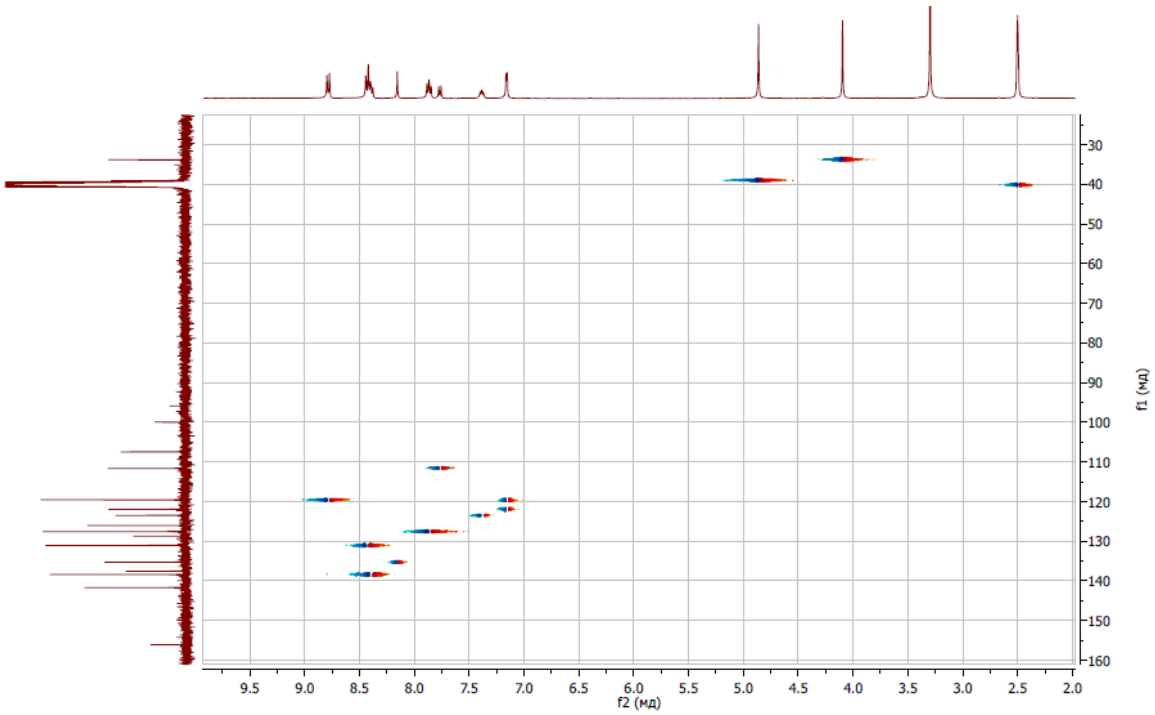


Figure S98. 2D ^{1}H-^{13}C HSQC Spectrum of 9-(N-methylindol-3-yl)-10-methylacridinum iodide (12b)

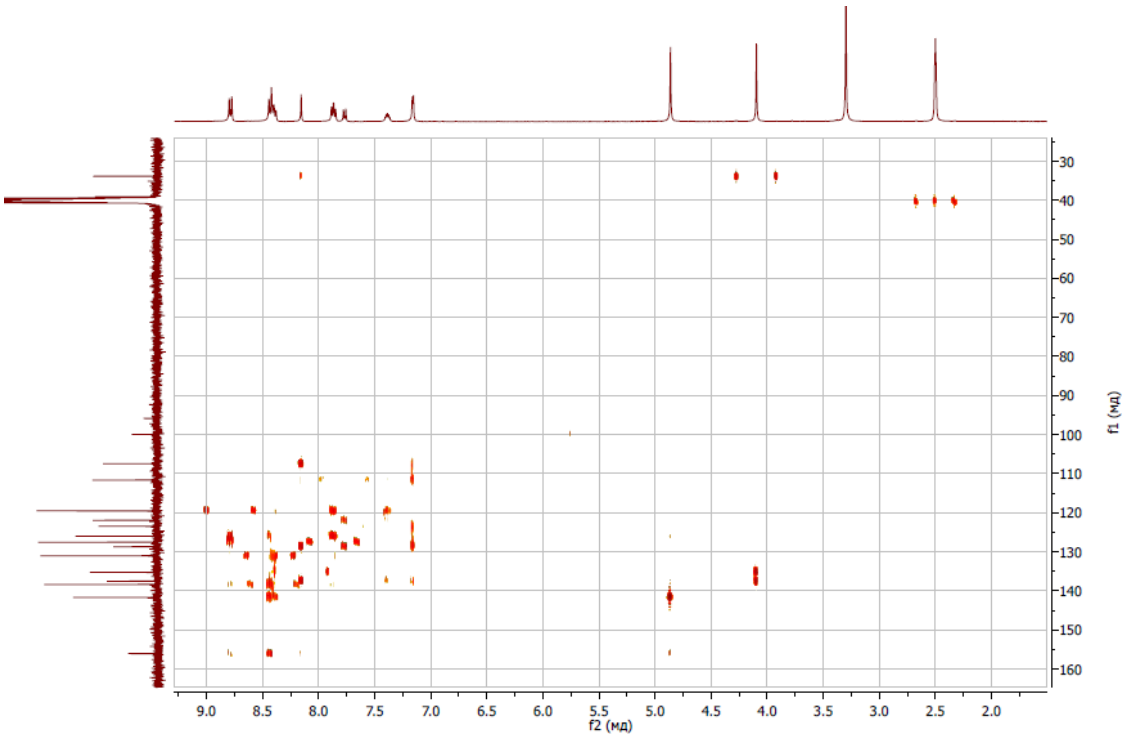


Figure S99. 2D ^{1}H-^{13}C HMBC Spectrum of 9-(N-methylindol-3-yl)-10-methylacridinum iodide (12b)

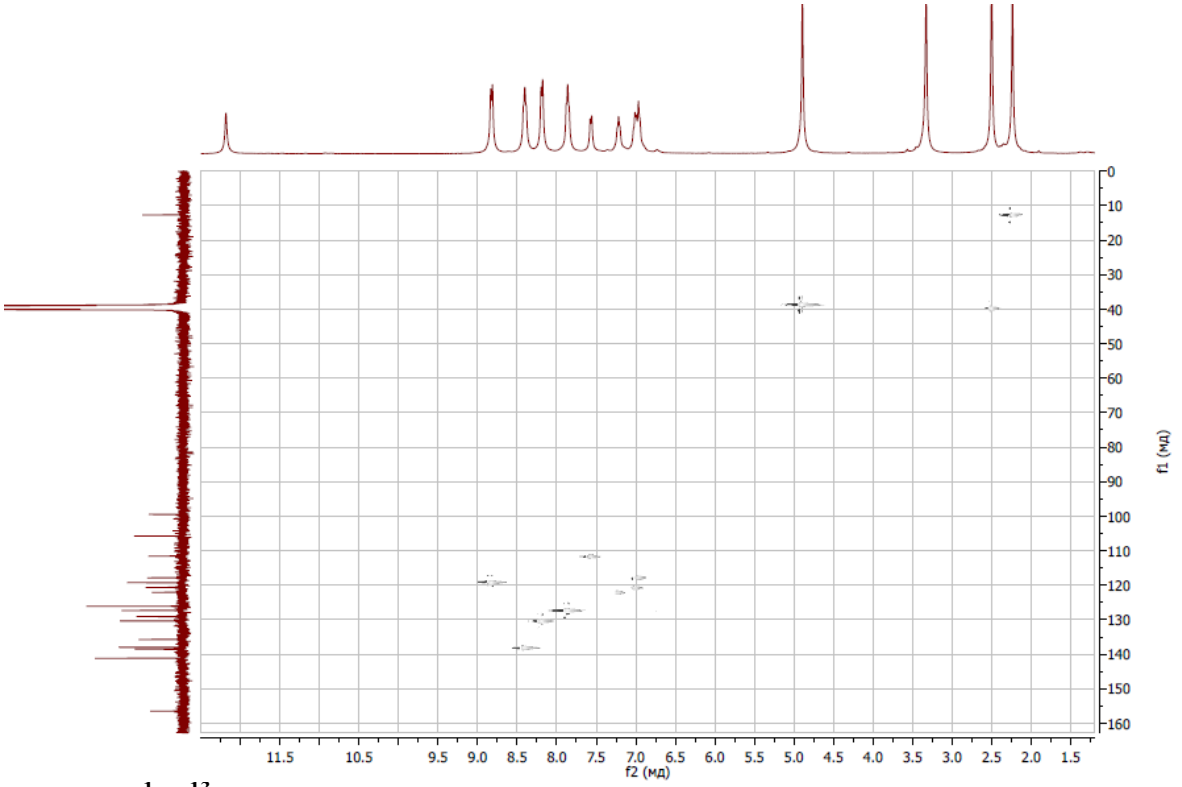


Figure S100. 2D ^{1}H-^{13}C HSQC Spectrum of 9-(2-methyl-1*H*-indol-3-yl)-10-methylacridinum iodide (12c)

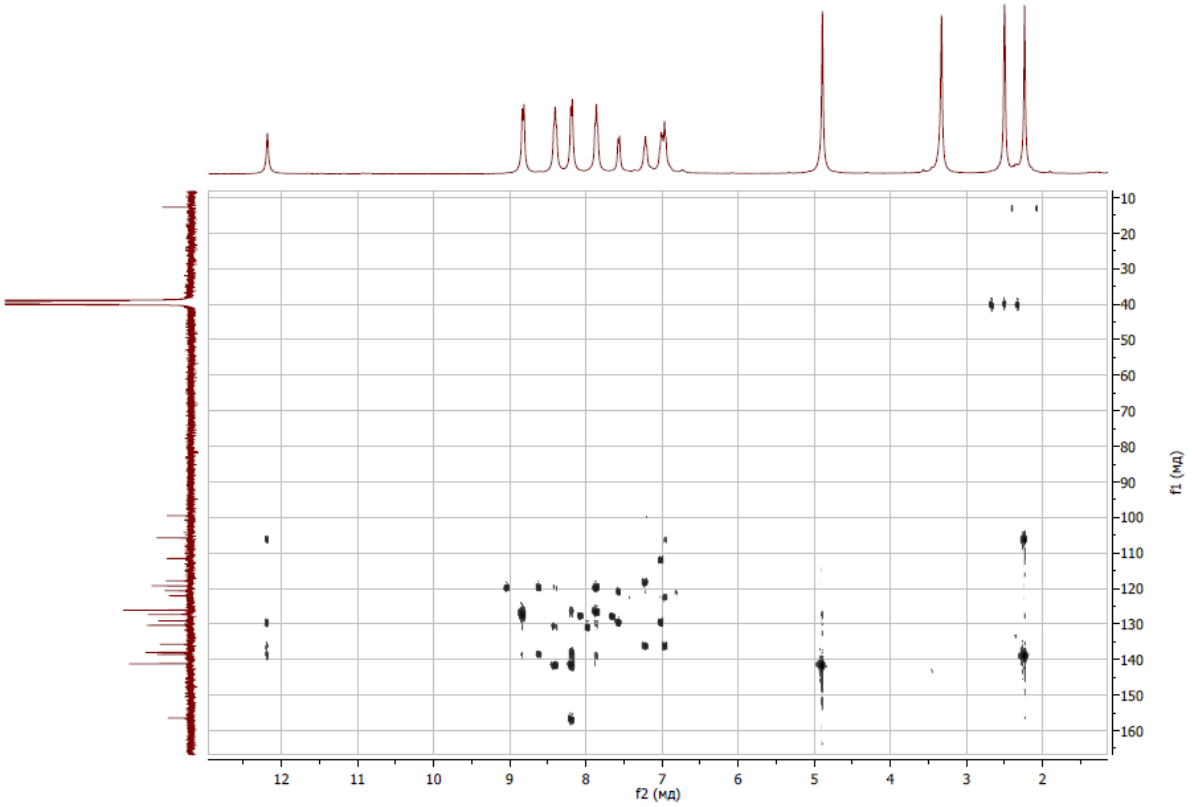


Figure S101. 2D ^{1}H-^{13}C HMBC Spectrum of 9-(2-methyl-1*H*-indol-3-yl)-10-methylacridinum iodide (12c)

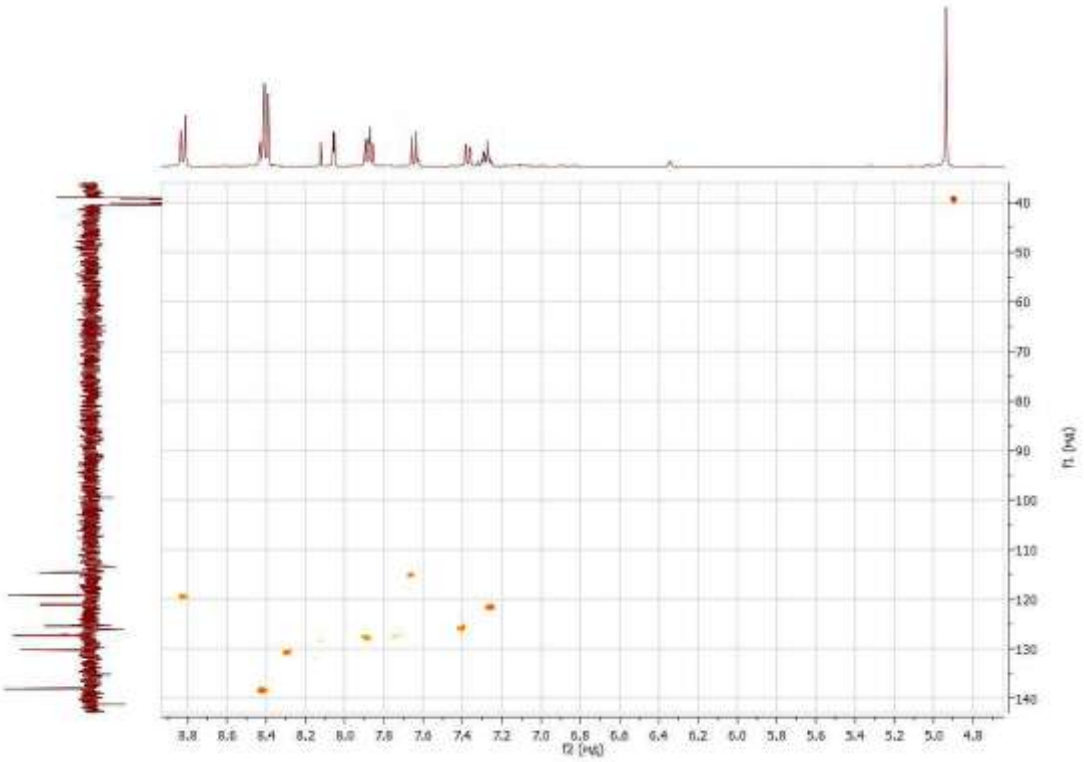


Figure S102. 2D ^{1}H-^{13}C HSQC Spectrum of 9-(5-bromo-1*H*-indol-3-yl)-10-methylacridinum iodide (12d)

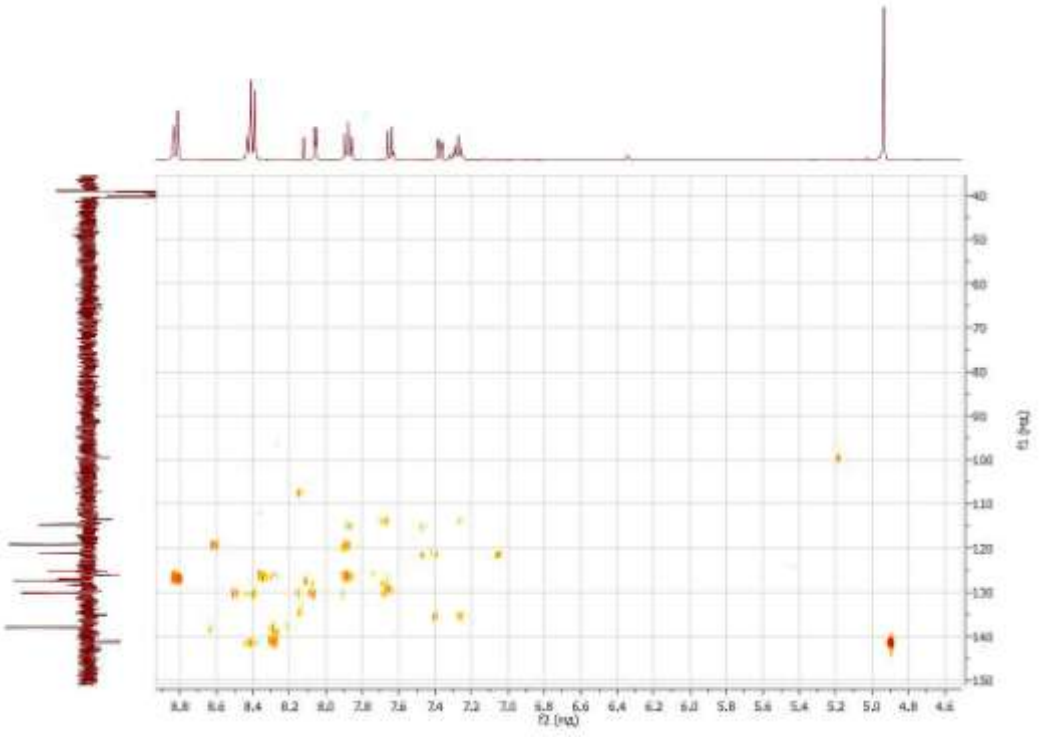


Figure S103. 2D ^{1}H-^{13}C HMBC Spectrum of 9-(5-bromo-1*H*-indol-3-yl)-10-methylacridinum iodide (12d)

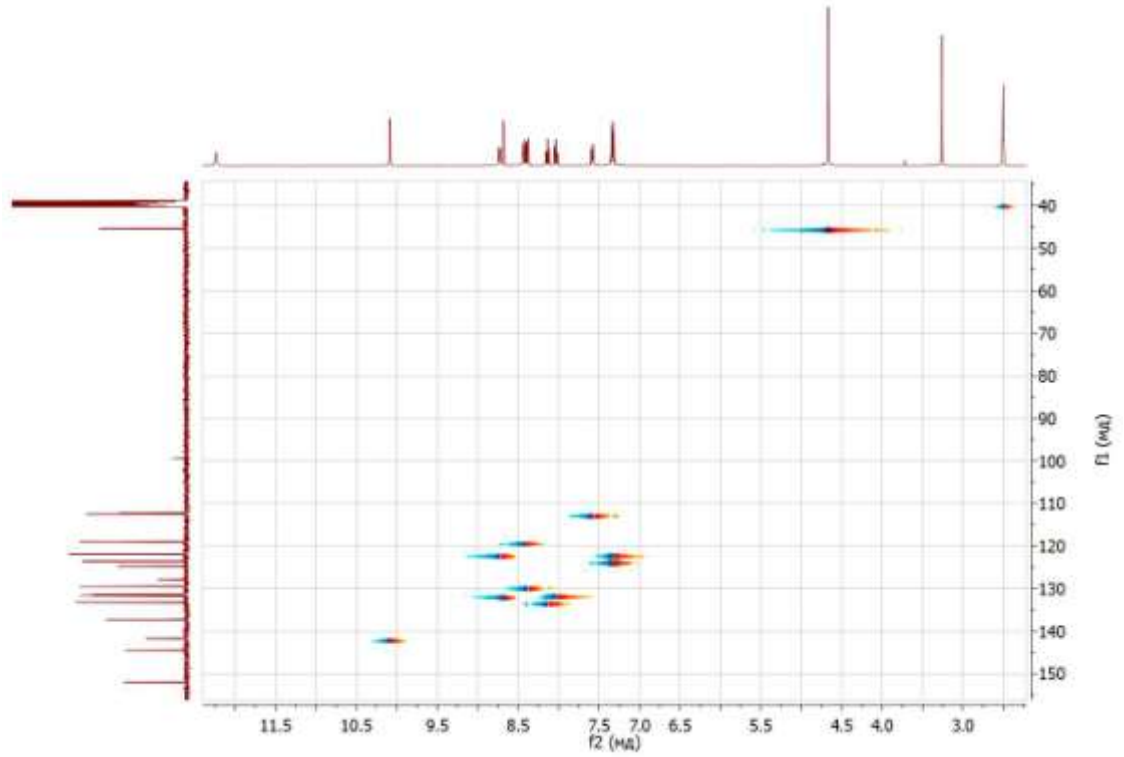


Figure S104. 2D ^{1}H-^{13}C HSQC Spectrum of 2-(1*H*-indol-3-yl)-1-methylquinoxalin-1-ium iodide (13a)

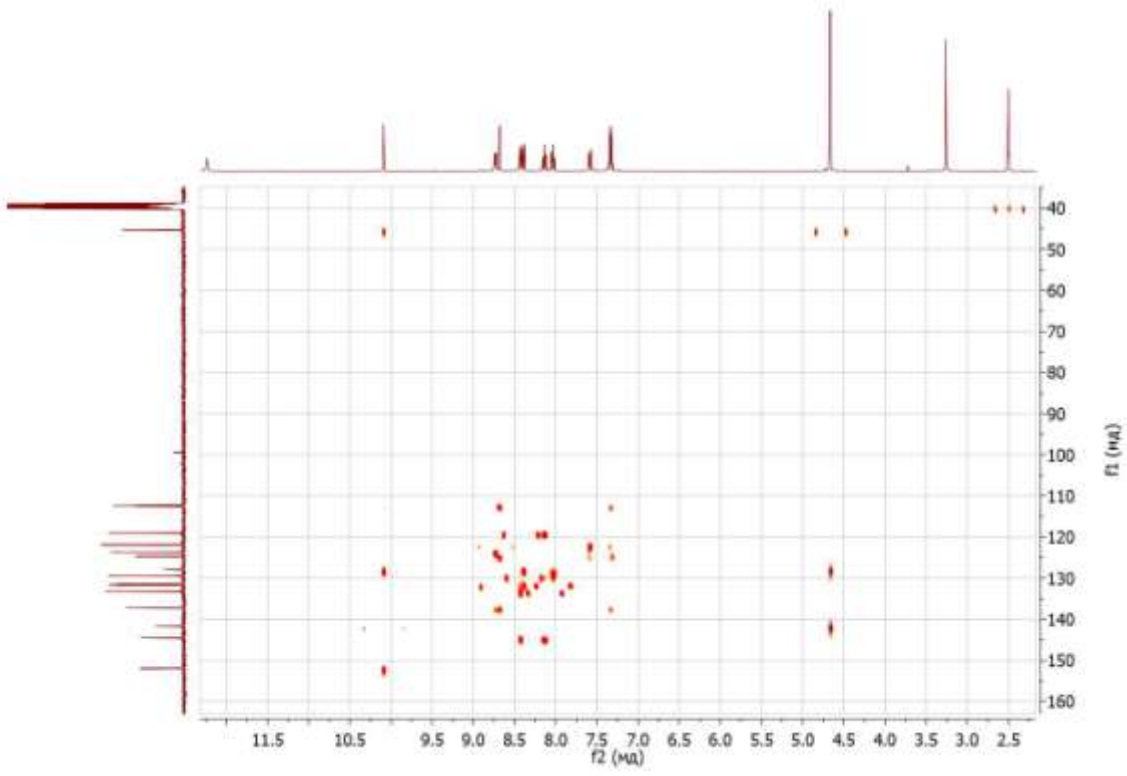


Figure S105. 2D ^{1}H-^{13}C HMBC Spectrum of 2-(1*H*-indol-3-yl)-1-methylquinoxalin-1-ium iodide (13a)

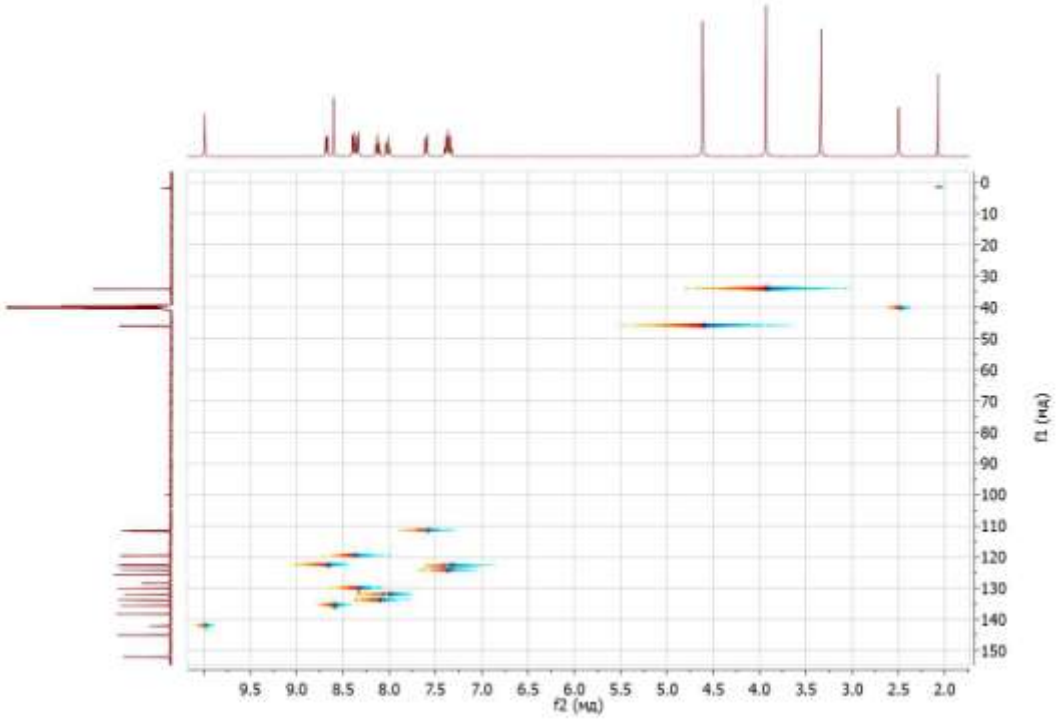


Figure S106. 2D ^{1}H-^{13}C HSQC Spectrum of 2-(N-methylindol-3-yl)-1-methylquinoxalin-1-ium iodide (13b)

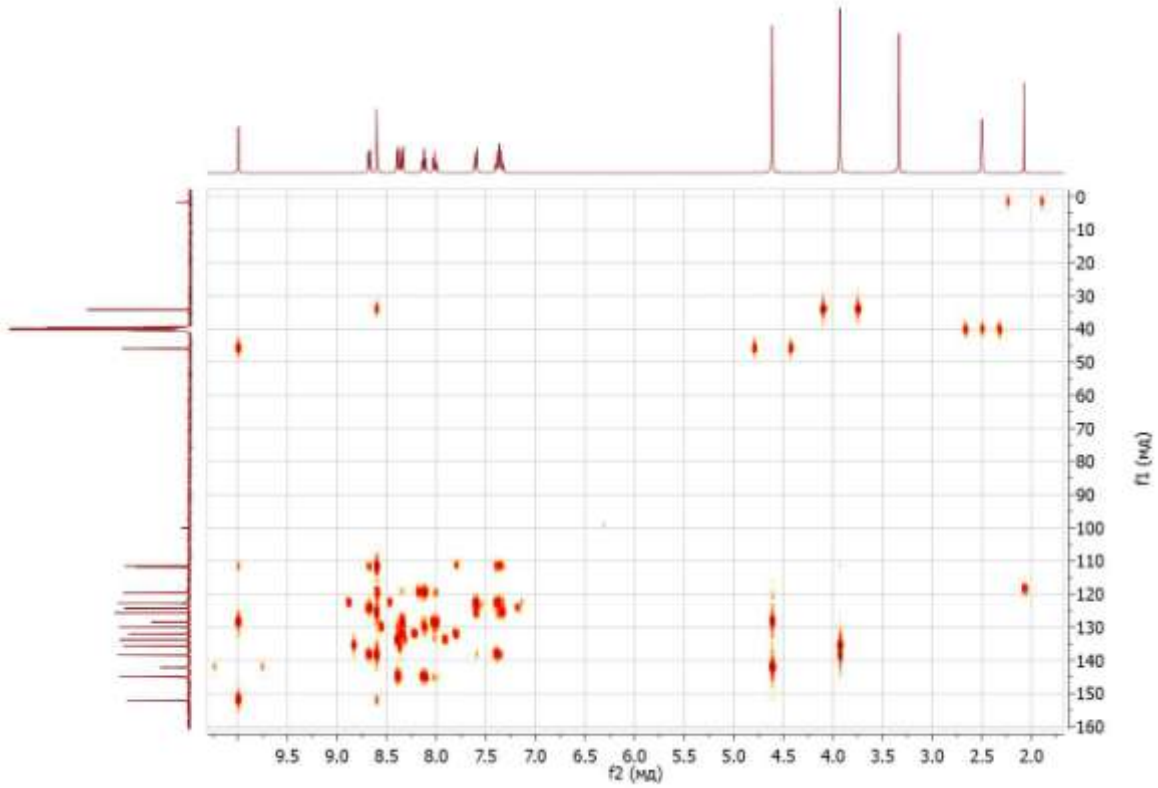


Figure S107. 2D ^{1}H-^{13}C HMBC Spectrum of 2-(N-methylindol-3-yl)-1-methylquinoxalin-1-ium iodide (13b)

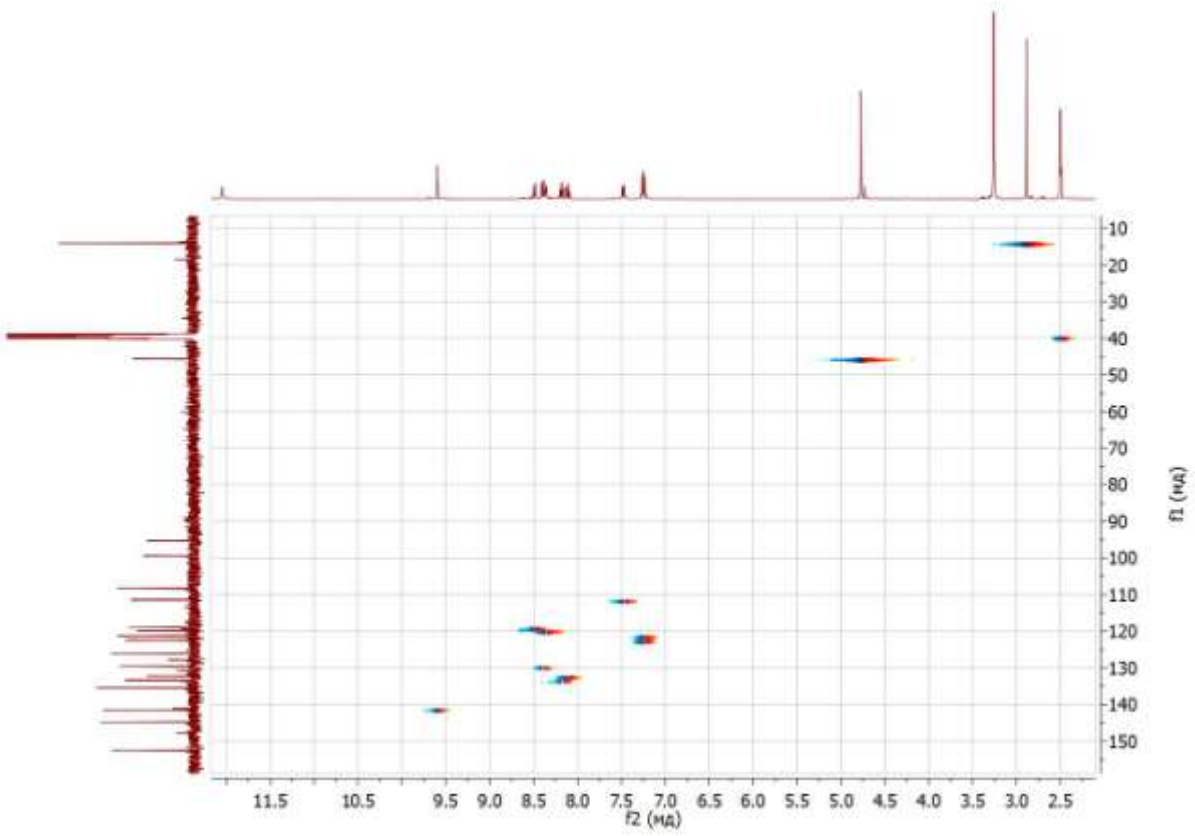


Figure S108. 2D ^{1}H-^{13}C HSQC Spectrum of 2-(2-methyl-1*H*-indol-3-yl)-1-methylquinoxalin-1-ium iodide (13c)

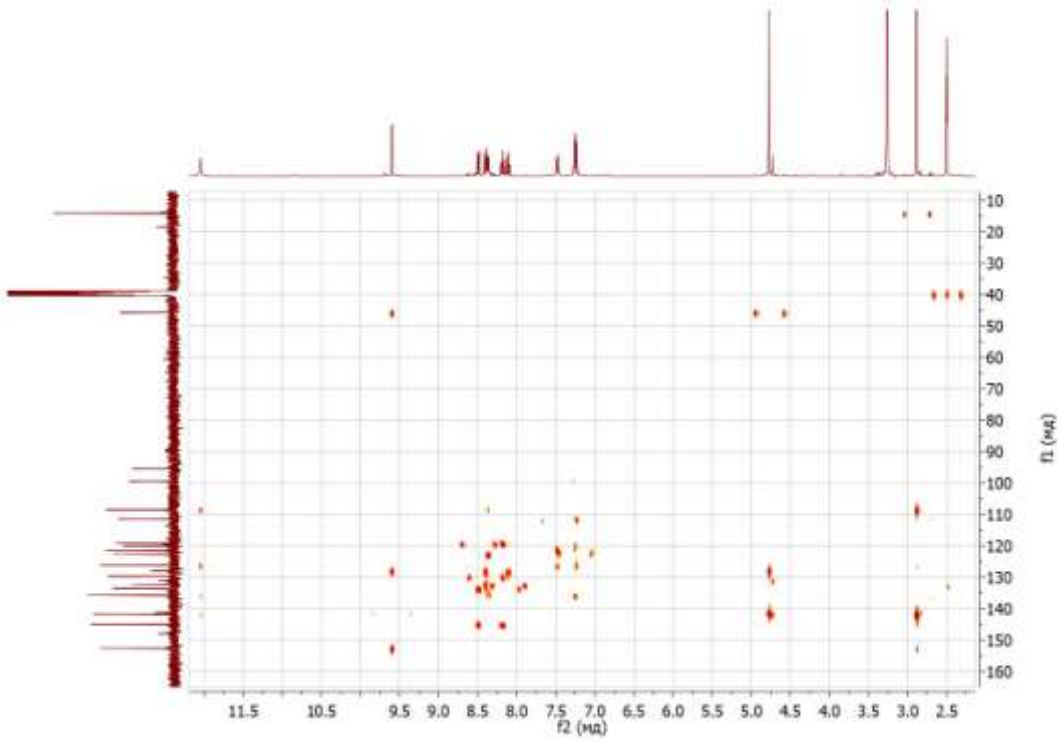


Figure S109. 2D ^{1}H-^{13}C HMBC Spectrum of 2-(2-methyl-1*H*-indol-3-yl)-1-methylquinoxalin-1-ium iodide (13c)

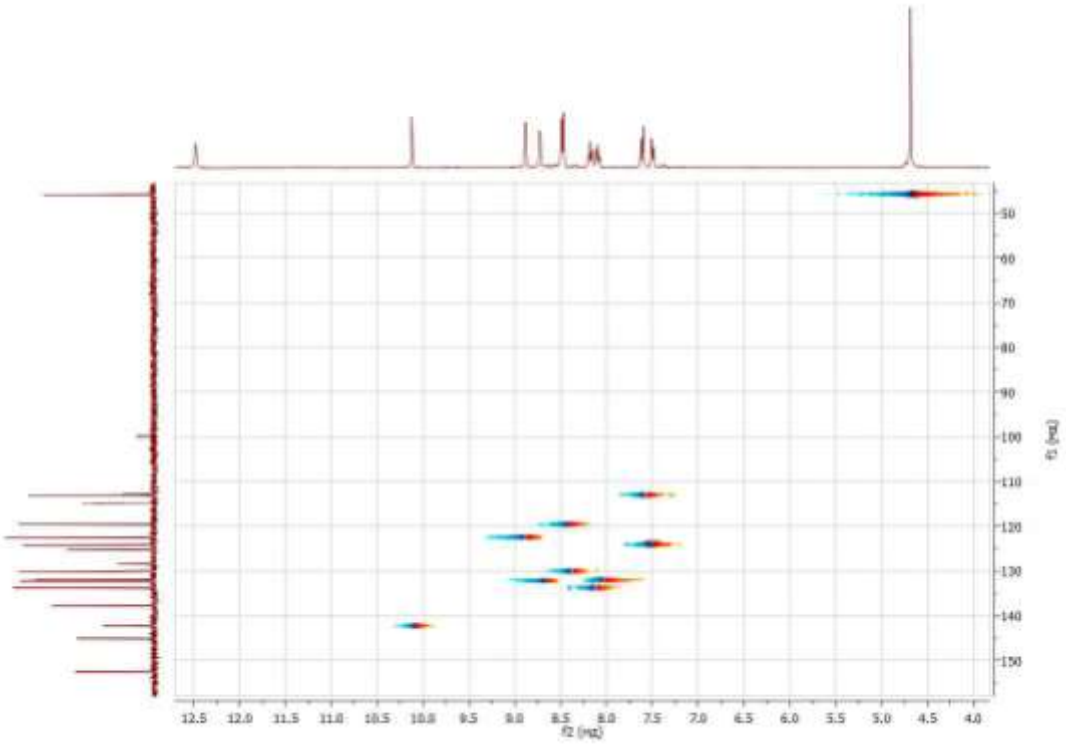


Figure S110. 2D ^{1}H-^{13}C HSQC Spectrum of 2-(5-bromo-1*H*-indol-3-yl)-1-methylquinoxalin-1-ium iodide (13d)

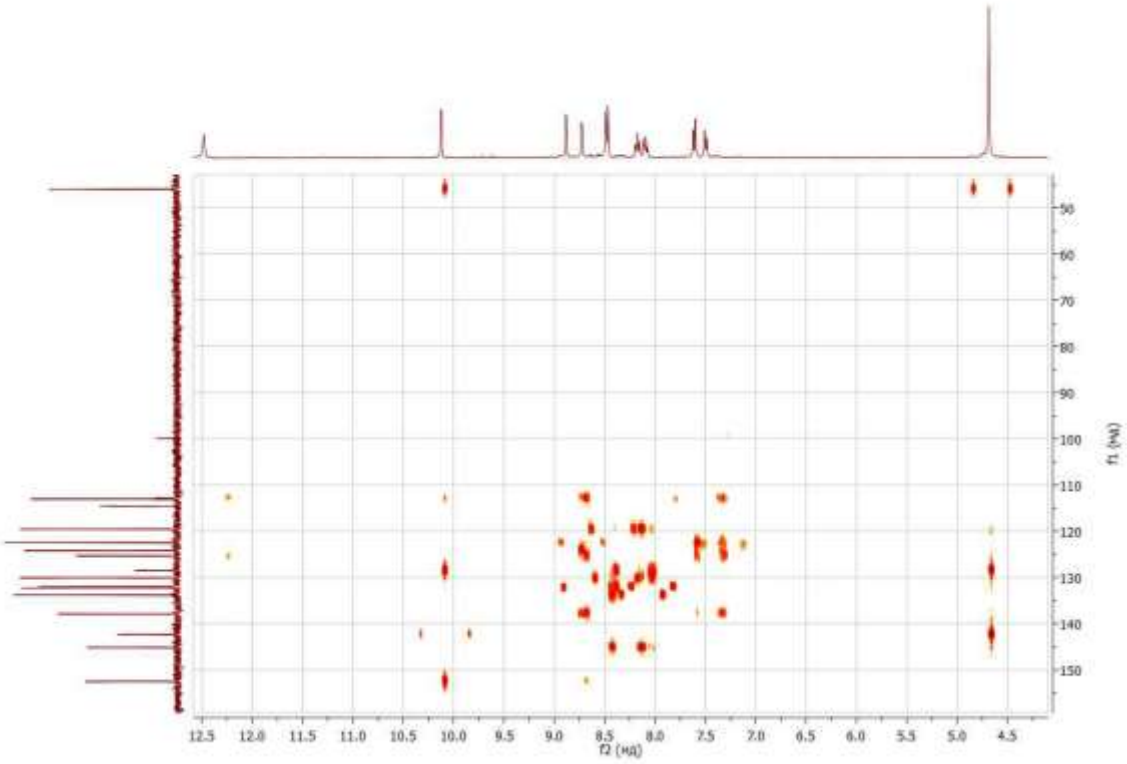


Figure S111. 2D ^{1}H-^{13}C HMBC Spectrum of 2-(5-bromo-1*H*-indol-3-yl)-1-methylquinoxalin-1-ium iodide (13d)

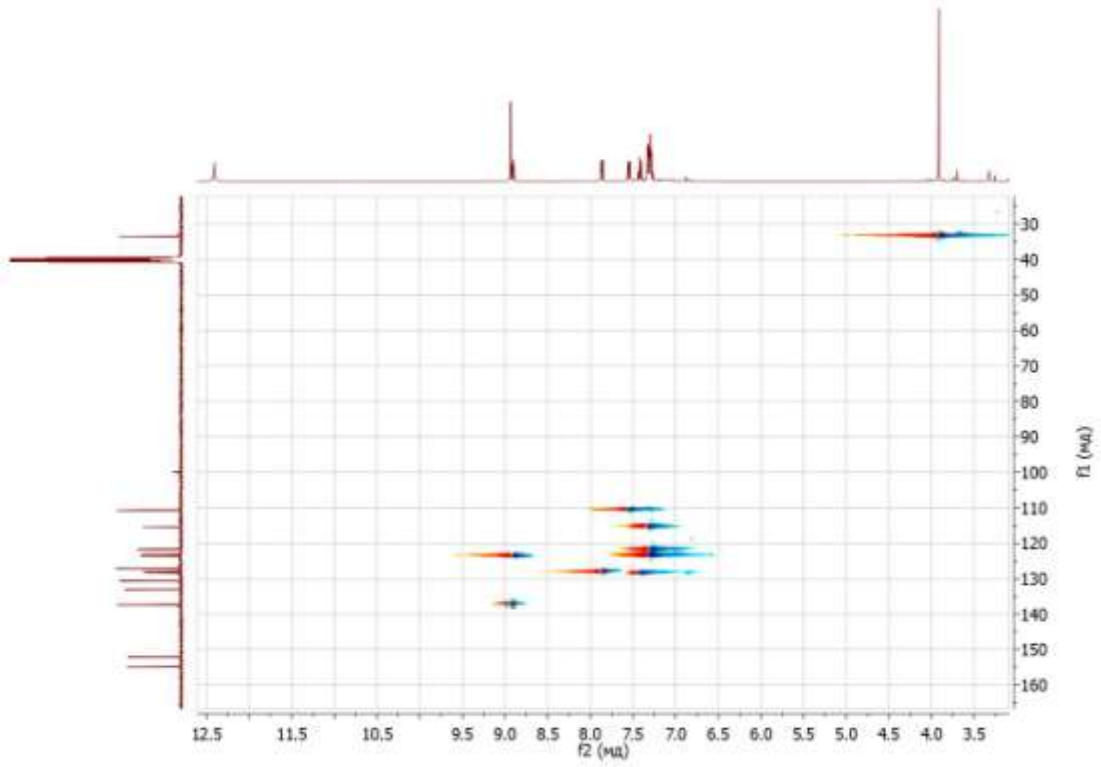


Figure S112. 2D ^{1}H-^{13}C HSQC Spectrum of 3-(N-methylindol-3-yl)-quinoxalin-2(1*H*)-one (14b)

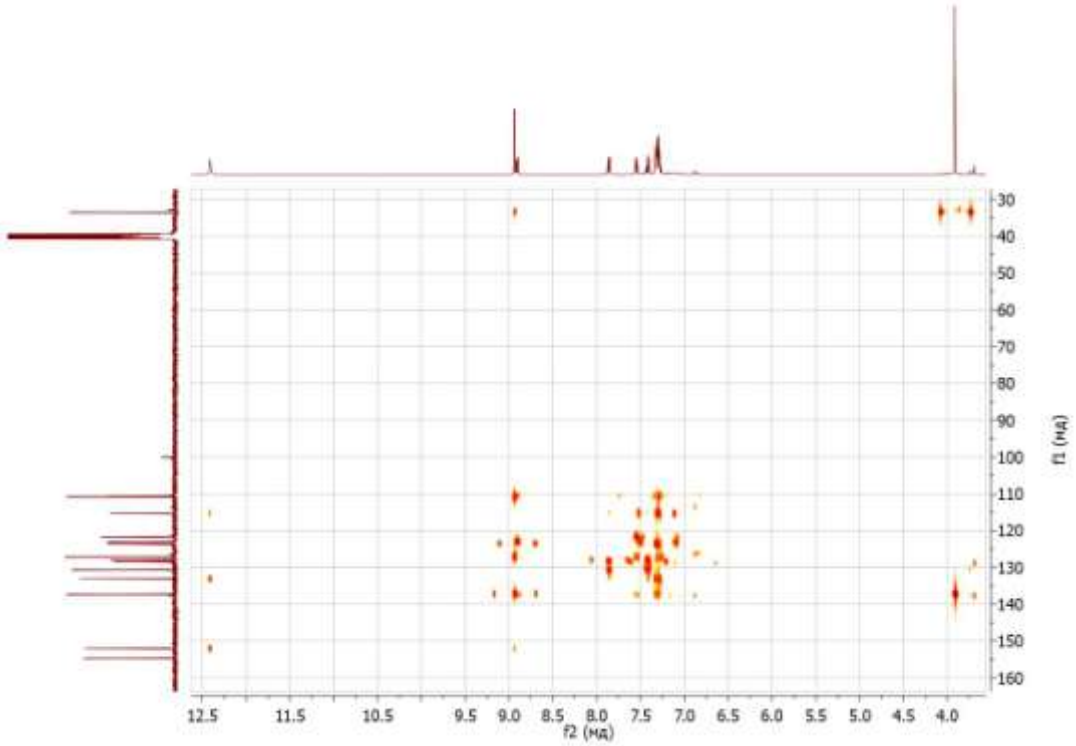


Figure S113. 2D ^{1}H-^{13}C HMBC Spectrum of 3-(N-methylindol-3-yl)-quinoxalin-2(1*H*)-one (14b)

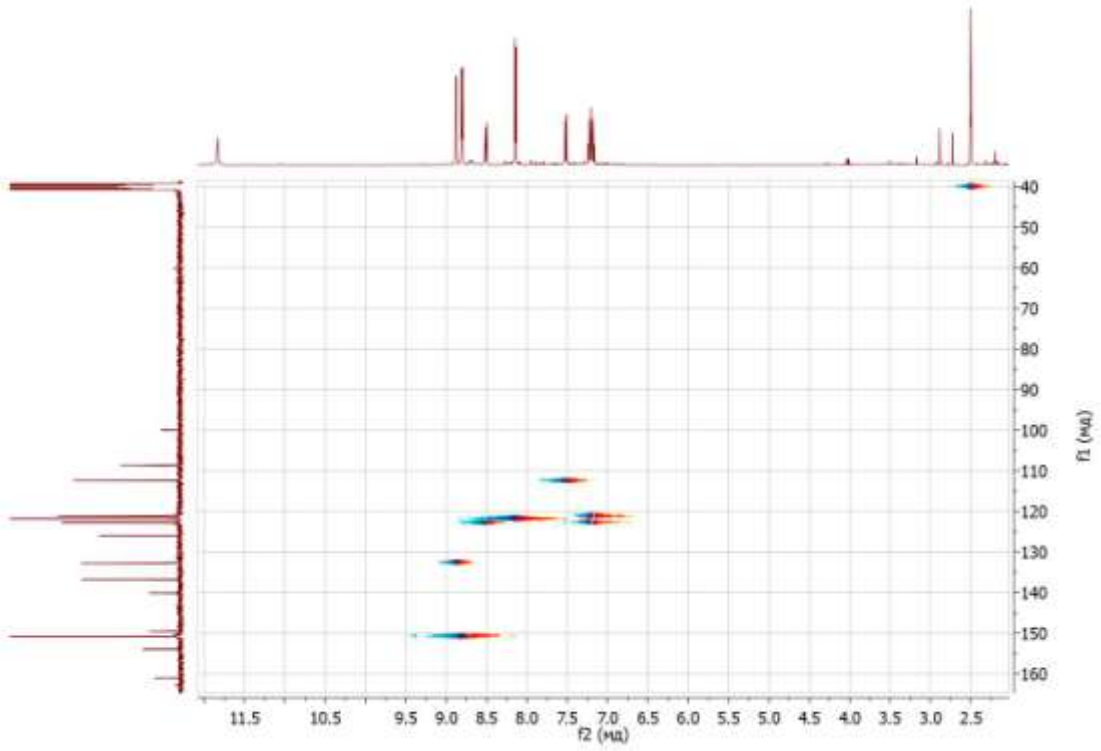


Figure S114. 2D ^{1}H-^{13}C HSQC Spectrum of 6-(1*H*-indol-3-yl)-3-(pyridin-4-yl)-1,2,4-triazin-5(4*H*)-one (15a)

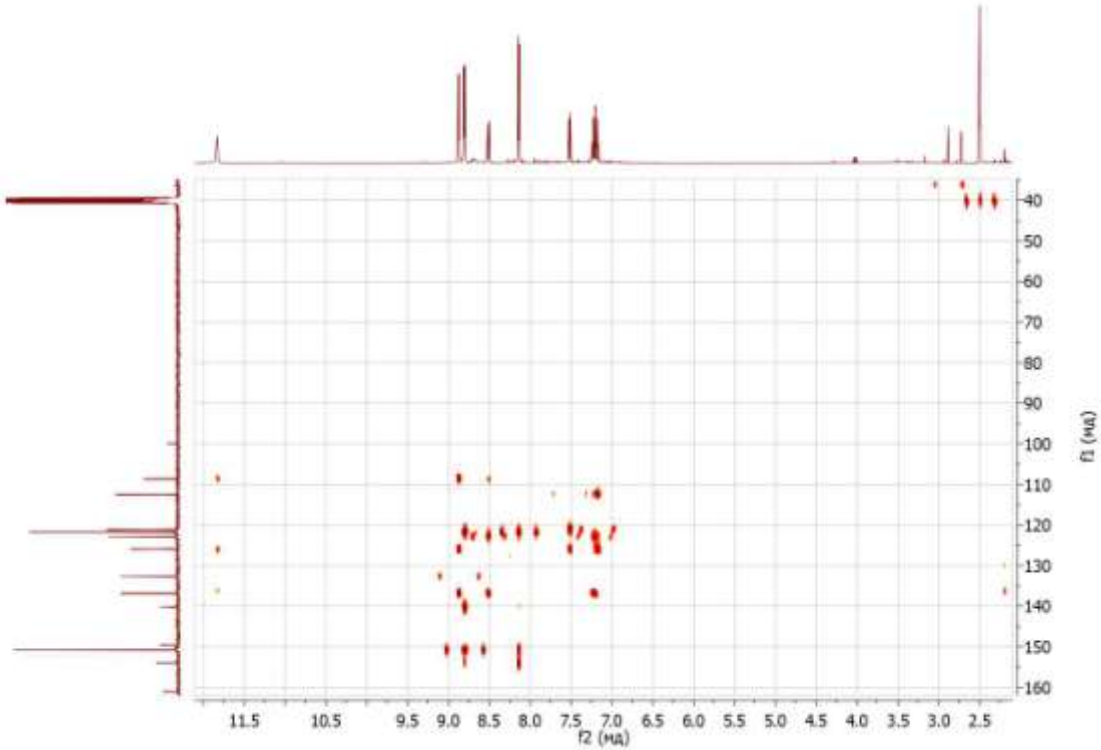


Figure S115. 2D ^{1}H-^{13}C HMBC Spectrum of 6-(1*H*-indol-3-yl)-3-(pyridin-4-yl)-1,2,4-triazin-5(4*H*)-one (15a)

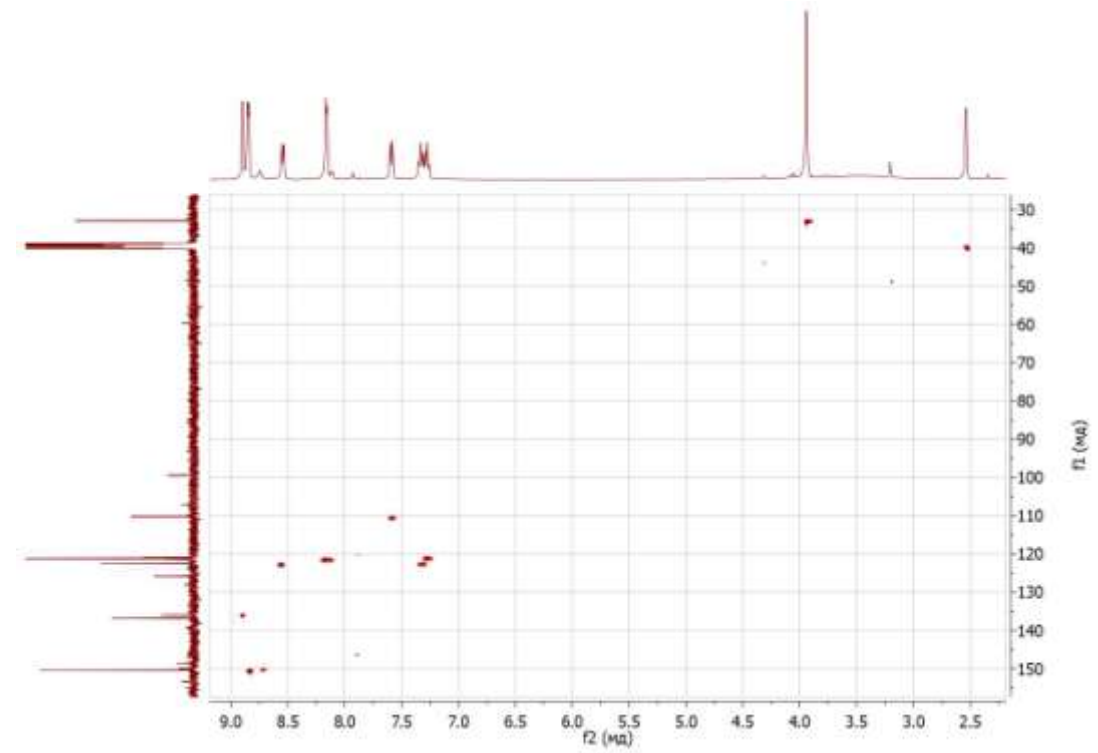


Figure S116. 2D ^{1}H-^{13}C HSQC Spectrum of 6-(N-methylindol-3-yl)-3-(pyridin-4-yl)-1,2,4-triazin-5(4*H*)-one (15b)

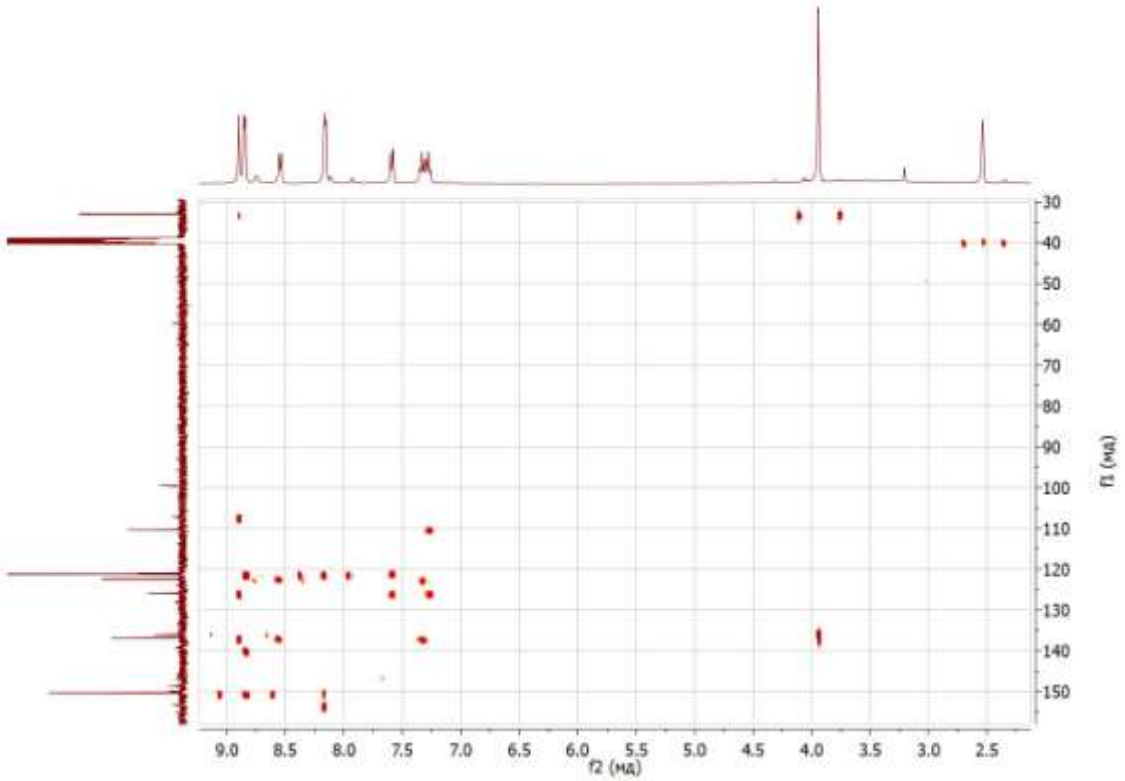


Figure S117. 2D ^{1}H-^{13}C HMBC Spectrum of 6-(N-methylindol-3-yl)-3-(pyridin-4-yl)-1,2,4-triazin-5(4*H*)-one (15b)

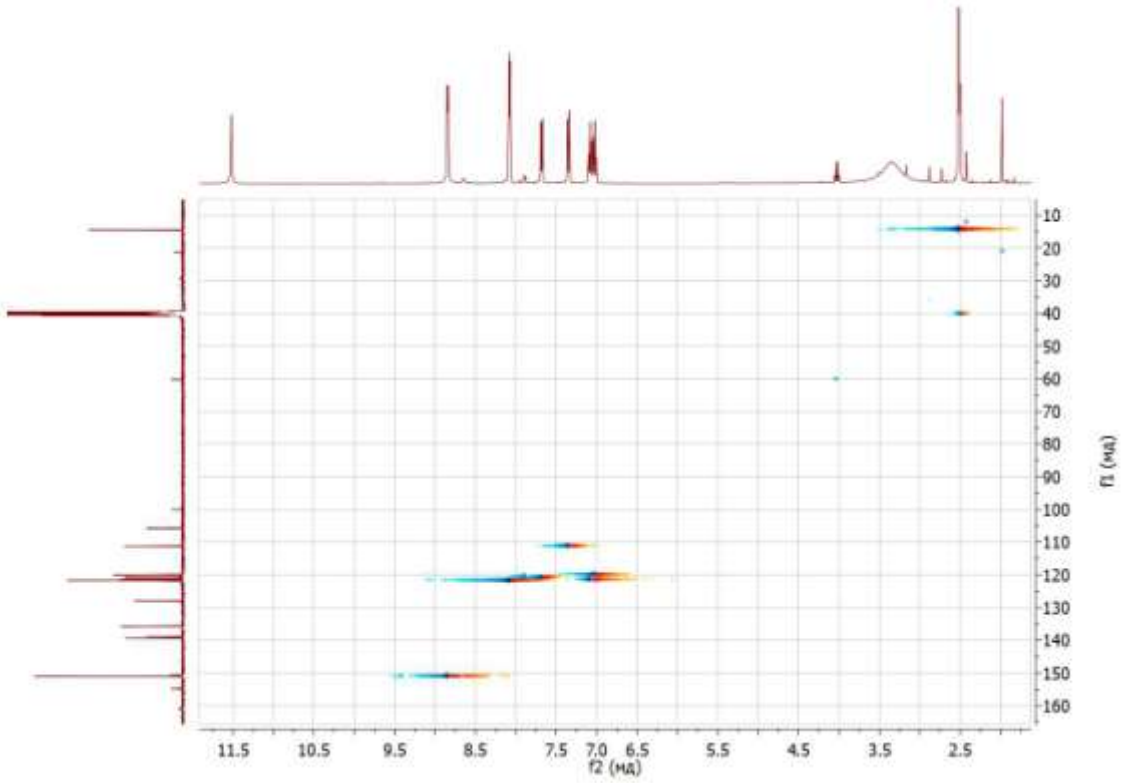


Figure S118. 2D ^{1}H-^{13}C HSQC Spectrum of 6-(2-methyl-1*H*-indol-3-yl)-3-(pyridin-4-yl)-1,2,4-triazin-5(4*H*)-one (15c)

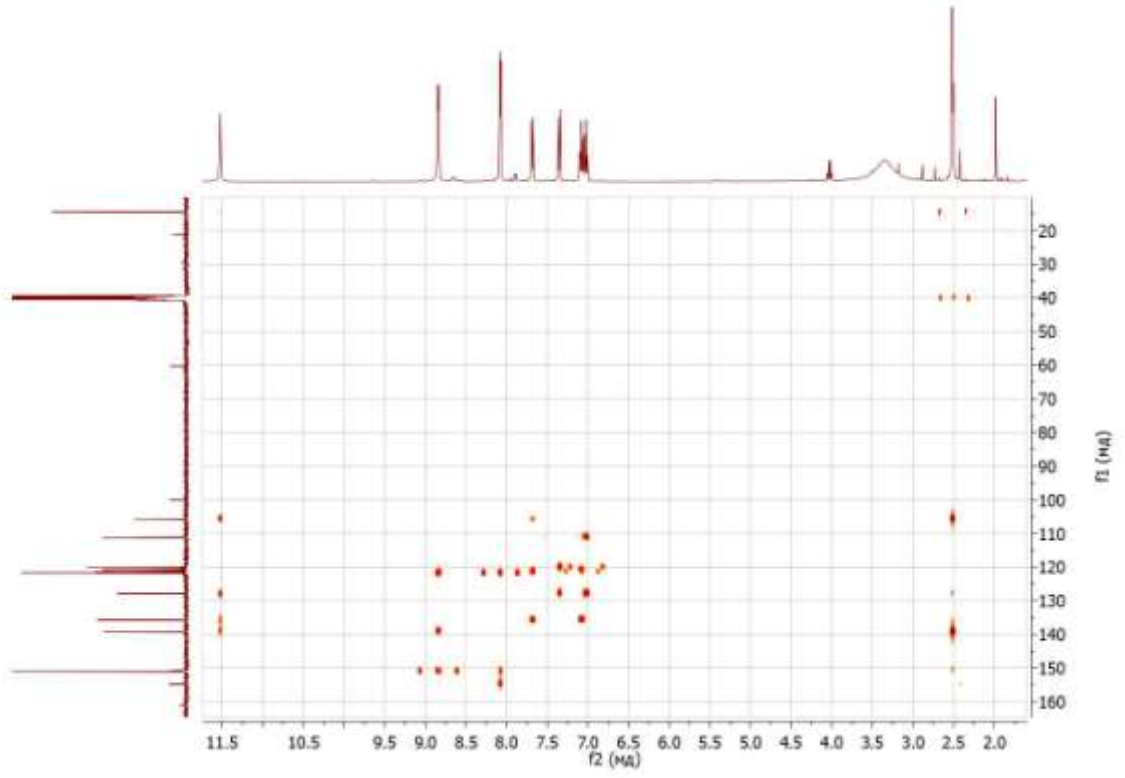


Figure S119. 2D ^{1}H-^{13}C HMBC Spectrum of 6-(2-methyl-1*H*-indol-3-yl)-3-(pyridin-4-yl)-1,2,4-triazin-5(4*H*)-one (15c)

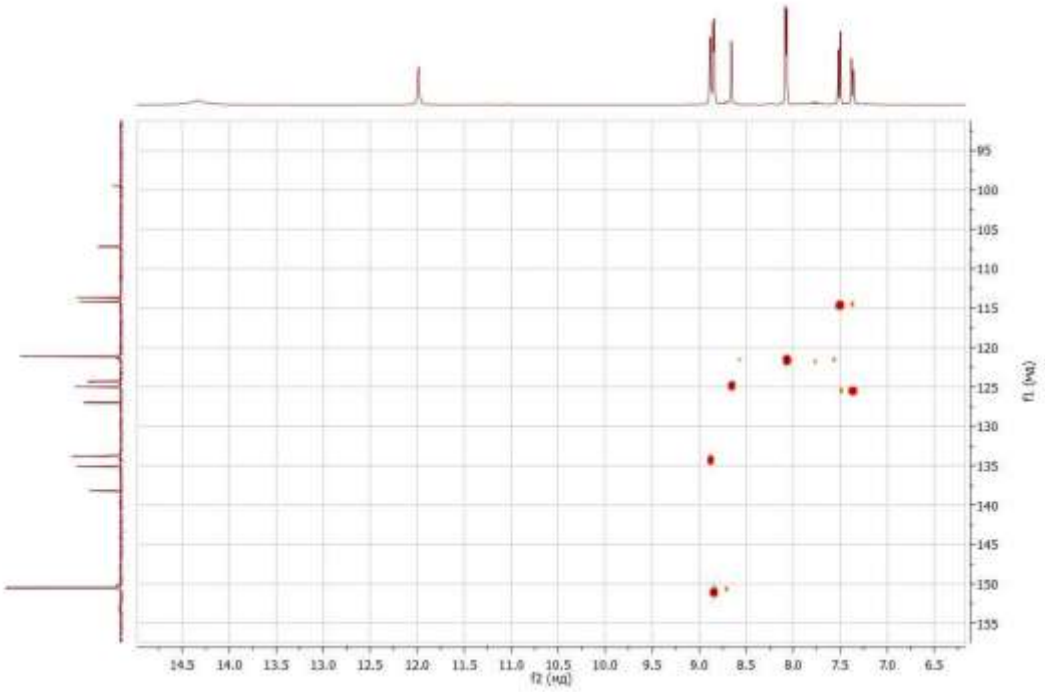


Figure S120. 2D ^{1}H-^{13}C HSQC Spectrum of 6-(5-bromo-1*H*-indol-3-yl)-3-(pyridin-4-yl)-1,2,4-triazin-5(4*H*)-one (15d)

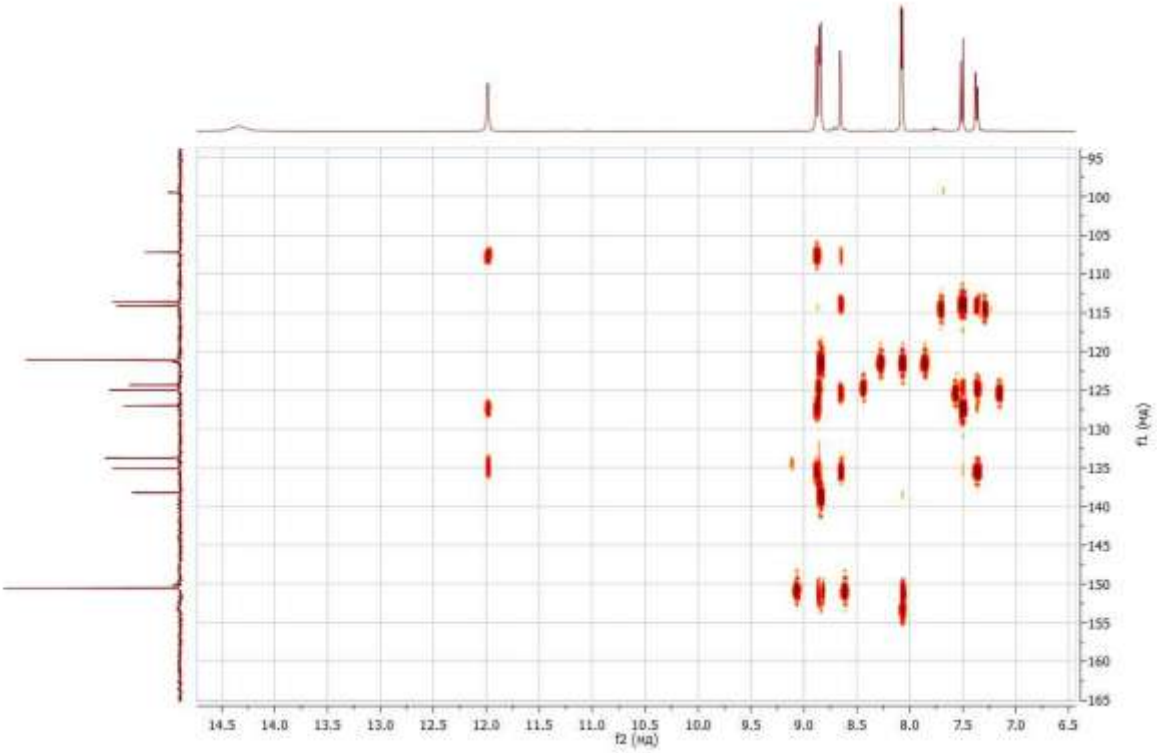


Figure S121. 2D ^{1}H-^{13}C HMBC Spectrum of 6-(5-bromo-1*H*-indol-3-yl)-3-(pyridin-4-yl)-1,2,4-triazin-5(4*H*)-one (15d)

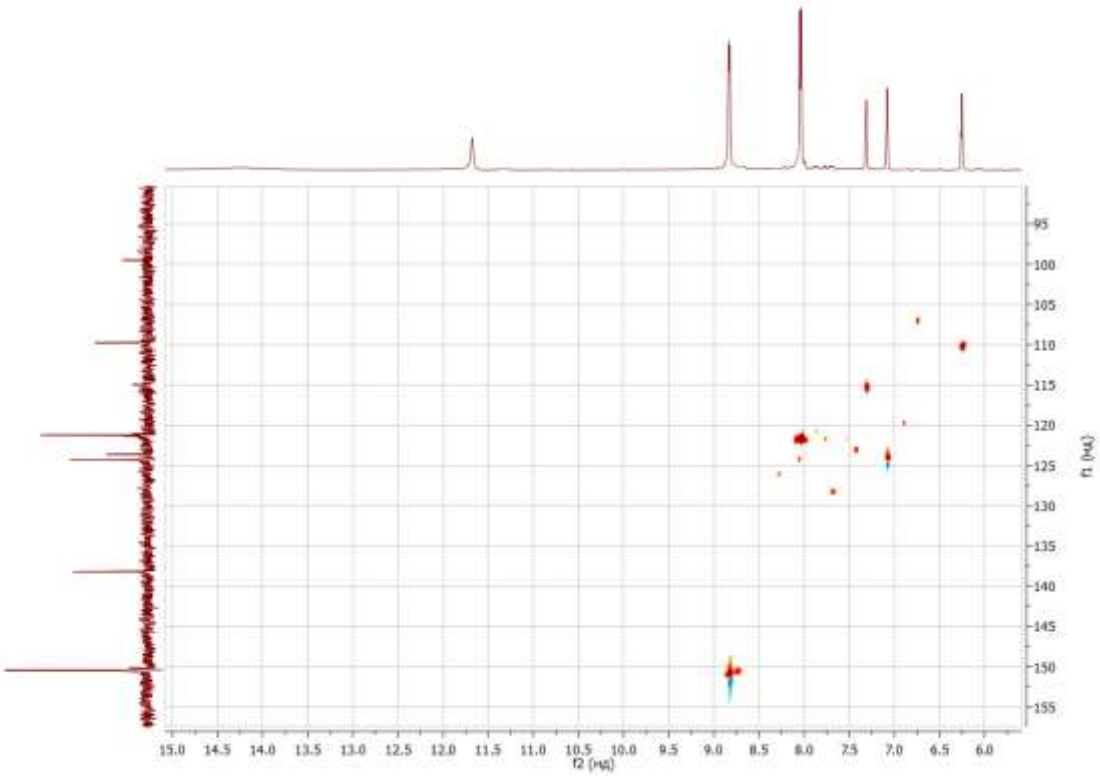


Figure S122. 2D ^{1}H-^{13}C HSQC Spectrum of 6-(1*H*-pyrrol-2-yl)-3-(pyridin-4-yl)-1,2,4-triazin-5(4*H*)-one (15e)

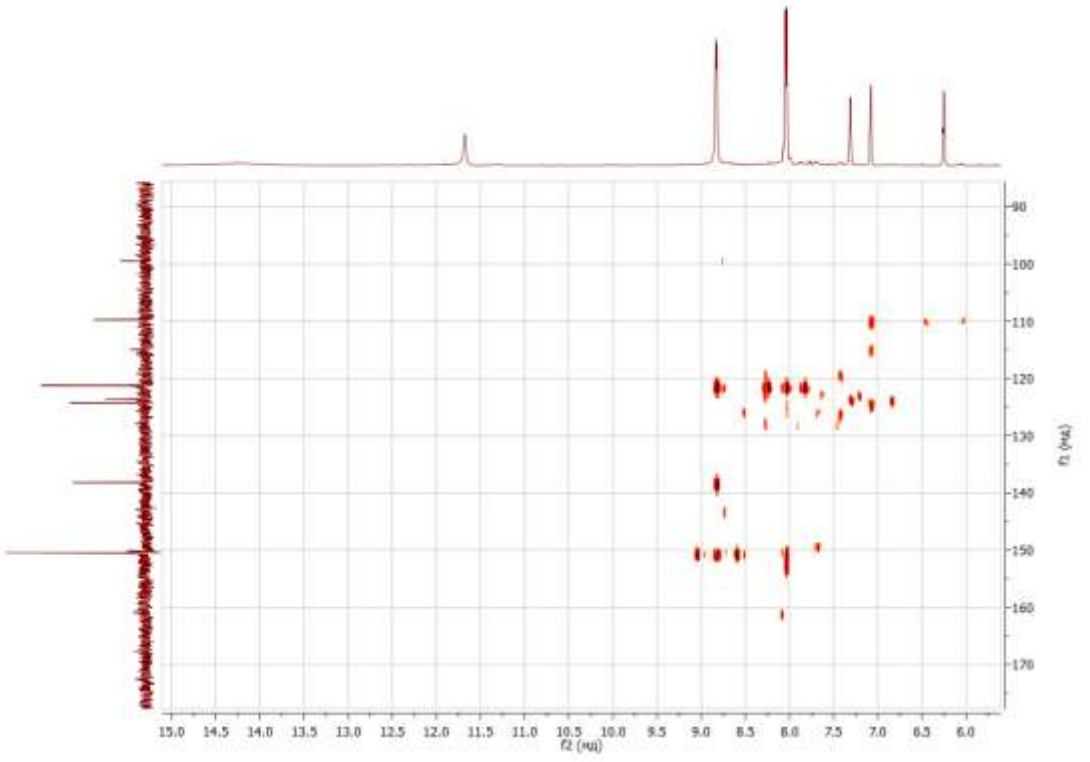


Figure S123. 2D ^{1}H-^{13}C HMBC Spectrum of 6-(1*H*-pyrrol-2-yl)-3-(pyridin-4-yl)-1,2,4-triazin-5(4*H*)-one (15e)

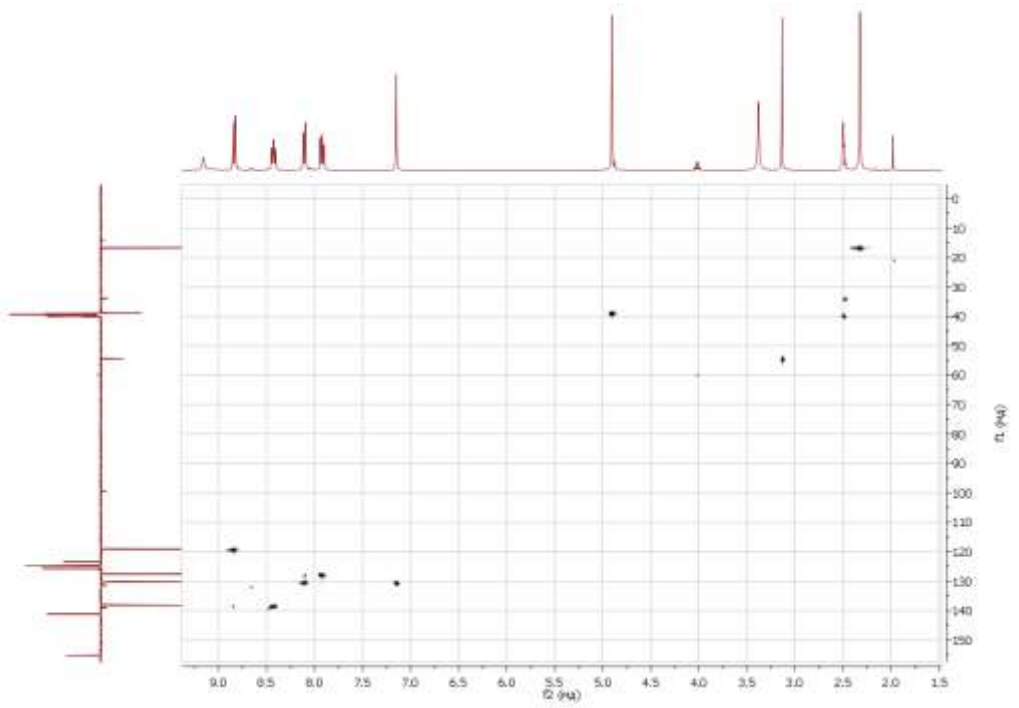


Figure S124. 2D ^{1}H-^{13}C HSQC Spectrum of 9-(4'-hydroxy-3',5'-dimethylphenyl)-10-methylacridinium chloride (25b)

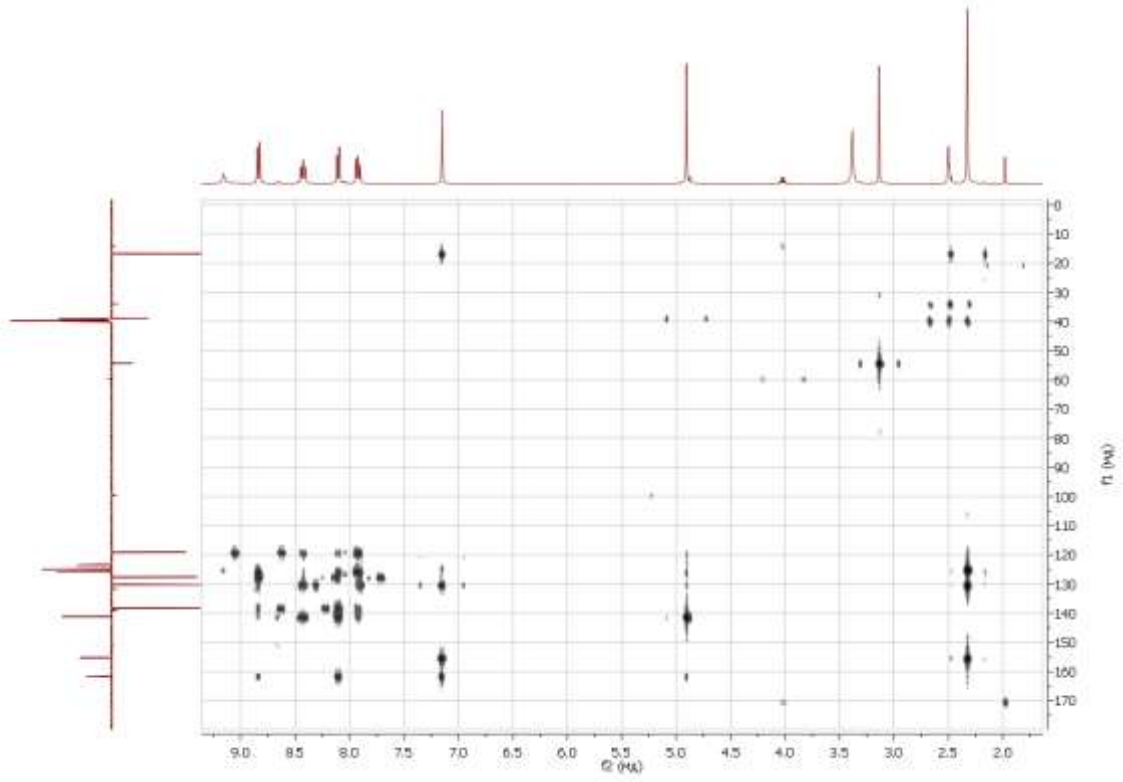


Figure S125. 2D ^{1}H-^{13}C HMBC Spectrum of 9-(4'-hydroxy-3',5'-dimethylphenyl)-10-methylacridinium chloride (25b)

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