



SUPPLEMENTARY MATERIAL TO  
**Synthesis of new functionalized derivatives of  
1,2,4-triazolo[4',3':2,3][1,2,4]triazino[5,6-*b*]indole**

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ANALYTIC AND SPECTRAL DATA OF THE PREPARED COMPOUNDS

(2*H*-1,2,4-Triazino[5,6-*b*]indol-3-yl)2-oxo-*N*-phenyl propanehydrazonothioate (**6b**). Yield: 75 %; m.p.: 236 °C (EtOH); Anal. Calcd. for C<sub>18</sub>H<sub>14</sub>N<sub>6</sub>OS (FW: 362): C, 59.32; H, 3.76; N, 22.87 %. Found: C, 59.11; H, 3.56; N, 22.56 %; IR (KBr, cm<sup>-1</sup>): 3423, 3288 (2NH), 1697 (CO); <sup>1</sup>H-NMR (300 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 2.70 (3H, *s*), 6.76–8.12 (9H, *m*, ArH), 10.34 (1H, *s*), 11.51 (1H, *s*); <sup>13</sup>C-NMR (75 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 178.6 (COPh), 158.2, 155.3, 152.1, 149.2, 143.2, 136.8, 136.2, 134.0, 133.9, 131.2, 130.8, 129.6, 125.7, 123.4, 24.3; MS (*m/z* (relative abundance, %)): 362 (M<sup>+</sup>, 19), 279 (34), 129 (46), 77 (100).

Ethyl 2-(phenylhydrazono)-2-(2*H*-1,2,4-triazino[5,6-*b*]indol-3-ylthio)-acetate (**6e**). Yield: 80 %; m.p.: 218 °C (DMF); Anal. Calcd. for C<sub>19</sub>H<sub>16</sub>N<sub>6</sub>O<sub>2</sub>S (FW: 392): C, 58.01; H, 3.91; N, 21.127 %. Found: C, 57.86; H, 3.87; N, 21.00 %; IR (KBr, cm<sup>-1</sup>): 3433, 3318 (2NH), 1723 (CO); <sup>1</sup>H-NMR (300 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 1.33 (3H, *t*, *J* = 7.1 Hz), 4.43 (2H, *q*, *J* = 7.1 Hz), 6.87–8.31 (9H, *m*, ArH), 10.31 (1H, *s*), 11.21 (1H, *s*); <sup>13</sup>C-NMR (75 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 164.5 (CONHPh), 155.4, 156.4, 150.3, 146.3, 143.8, 137.6, 136.0, 135.3, 132.5, 131.9, 131.4, 130.4, 128.4, 126.3, 126.1, 123.6, 120.5, 118.9; MS (*m/z* (relative abundance, %)): 392 (M<sup>+</sup>, 9), 235 (17), 131 (79), 103 (92), 77 (100).

(2*H*-1,2,4-Triazino[5,6-*b*]indol-3-yl)2-oxo-*N*-phenyl 2-(phenylamino)ethanehydrazonothioate (**6h**). Yield: 70 %; m.p.: 254 °C (EtOH); Anal. Calcd. for C<sub>32</sub>H<sub>17</sub>N<sub>7</sub>OS (FW: 439): C, 62.59; H, 3.78; N, 15.98 %. Found: C, 62.46; H, 3.85; N, 15.77 %; IR (KBr, cm<sup>-1</sup>): 3440, 3376, 3263 (3NH), 1689 (CO); <sup>1</sup>H-NMR (300 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 6.88–8.18 (14H, *m*, ArH), 10.43 (1H, *s*), 11.04 (1H, *s*), 11.32 (1H, *s*); <sup>13</sup>C-NMR (75 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 178.6

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(COPh), 158.2, 155.3, 152.1, 149.2, 143.2, 136.8, 136.2, 134.0, 133.9, 131.2, 130.8, 129.6, 125.7, 123.4, 24.3; MS ( $m/z$  (relative abundance, %)): 439 ( $M^+$ , 100), 237 (33), 118 (26), 77 (45).

*1,3-Diphenyl-1H-1,2,4-triazolo[4',3':2,3][1,2,4]triazino[5,6-b]indole (8a)*. Yield: 70 %; m.p.: 284 °C (DMF); Anal. Calcd. for  $C_{22}H_{14}N_6$  (FW: 362): C, 72.46; H, 3.66; N, 22.89 %. Found: C, 72.26; H, 3.68; N, 22.42 %;  $^1H$ -NMR (300 MHz, DMSO- $d_6$ ,  $\delta$  / ppm): 6.64–8.20 (14H, *m*, ArH);  $^{13}C$ -NMR (75 MHz, DMSO- $d_6$ ,  $\delta$  / ppm): 158.5, 156.7, 153.3, 151.2, 149.3, 139.7, 138.7, 138.3, 134.4, 133.2, 133.1, 132.4, 132.1, 130.8, 127.8, 127.1, 125.7, 124.9; MS ( $m/z$  (relative abundance, %)): 362 ( $M^+$ , 38), 315 (17), 251 (11.8), 121 (30), 92 (70), 77 (100), 51 (64).

*1-(1-Phenyl-1H-1,2,4-triazolo[4',3':2,3][1,2,4]triazino[5,6-b]indol-3-yl)ethanone (8b)*. Yield: 72 %; m.p.: 269 °C (DMF); Anal. Calcd. for  $C_{18}H_{12}N_6O$  (FW: 328): C, 65.63; H, 3.59; N, 25.44 %. Found: C, 65.85; H, 3.46; N, 25.03 %; IR (KBr,  $cm^{-1}$ ): 1693 (CO);  $^1H$ -NMR (300 MHz, DMSO- $d_6$ ,  $\delta$  / ppm): 2.74 (3H, *s*), 6.60–8.14 (9H, *m*, ArH);  $^{13}C$ -NMR (75 MHz, DMSO- $d_6$ ,  $\delta$  / ppm): 172.2 (COCH<sub>3</sub>), 158.8, 155.4, 152.1, 151.2, 148.3, 139.8, 138.3, 134.4, 133.3, 132.4, 130.0, 128.8, 127.1, 124.7, 29.4; MS ( $m/z$  (relative abundance, %)): 328 ( $M^+$ , 100), 267 (25), 125 (62), 76 (66), 99 (41), 77 (28).

*1-[1-(4-Methylphenyl)-1H-1,2,4-triazolo[4',3':2,3][1,2,4]triazino[5,6-b]indol-3-yl]ethanone (8c)*. Yield: 78 %; m.p.: 254 °C (DMF); Anal. Calcd. for  $C_{19}H_{14}N_6O$  (FW: 342): C, 66.45; H, 4.09; N, 24.23 %. Found: C, 66.33; H, 4.02; N, 24.12 %; IR (KBr,  $cm^{-1}$ ): 1703, (CO);  $^1H$ -NMR (300 MHz, DMSO- $d_6$ ,  $\delta$  / ppm): 2.23 (3H, *s*), 2.57 (3H, *s*), 6.80–8.16 (4H, *m*, ArH), 7.62 (2H, *d*,  $J = 8$  Hz), 7.81 (2H, *d*,  $J = 8$  Hz);  $^{13}C$ -NMR (75 MHz, DMSO- $d_6$ ,  $\delta$  / ppm): 174.6 (COCH<sub>3</sub>), 163.4, 158.2, 153.7, 150.8, 149.7, 142.3, 139.6, 137.6, 135.4, 134.2, 133.4, 129.2, 126.7, 122.5, 29.1, 18.4; MS ( $m/z$  (relative abundance, %)): 342 ( $M^+$ , 100), 259 (18), 118 (60), 90 (41), 77 (22).

*1-[1-(4-Chlorophenyl)-1H-1,2,4-triazolo[4',3':2,3][1,2,4]triazino[5,6-b]indol-3-yl]ethanone (8d)*. Yield: 70 %; m.p.: 276 °C (DMF); Anal. Calcd. for  $C_{18}H_{11}ClN_6O$  (FW: 362): C, 59.43; H, 3.17; N, 21.80 %. Found: C, 59.13; H, 3.06; N, 21.83 %; IR (KBr,  $cm^{-1}$ ): 1693 (CO);  $^1H$ -NMR (300 MHz, DMSO- $d_6$ ,  $\delta$  / ppm): 2.64 (3H, *s*), 6.80–8.29 (4H, *m*, ArH), 7.74 (2H, *d*,  $J = 8$  Hz), 7.84 (2H, *d*,  $J = 8$  Hz);  $^{13}C$ -NMR (75 MHz, DMSO- $d_6$ ,  $\delta$  / ppm): 174.5 (COCH<sub>3</sub>), 161.9, 159.8, 154.5, 151.2, 151.0, 139.9, 139.2, 135.7, 133.9, 133.6, 131.0, 129.9, 124.3, 120.4, 30.4; MS ( $m/z$  (relative abundance, %)): 364 ( $M^+ + 2$ , 8.5), 363 ( $M^+ + 1$ , 17), 362 ( $M^+$ , 26), 169 (57), 125 (62), 118 (85), 90 (55), 76 (66), 63 (98), 50 (100).

*Ethyl 1-phenyl-1H-1,2,4-triazolo[4',3':2,3][1,2,4]triazino[5,6-b]indole-3-carboxylate (8e)*. Yield: 80 %; m.p.: 234 °C (DMF); Anal. Calcd. for  $C_{19}H_{14}N_6O_2$  (FW: 358): C, 63.11; H, 3.68; N, 23.36 %. Found: C, 63.10; H, 3.42; N, 23.23 %;

IR (KBr,  $\text{cm}^{-1}$ ): 1741 (CO);  $^1\text{H-NMR}$  (300 MHz,  $\text{DMSO-}d_6$ ,  $\delta$  / ppm): 1.43 (3H, *t*,  $J = 7$  Hz), 4.40 (2H, *q*,  $J = 7$  Hz), 6.45–8.30 (9H, *m*, ArH);  $^{13}\text{C-NMR}$  (75 MHz,  $\text{DMSO-}d_6$ ,  $\delta$  / ppm): 171.2 (COEt), 155.1, 148.1, 142.4, 139.2, 138.1, 137.3, 136.0, 135.2, 134.1, 131.5, 130.3, 129.2, 128.1, 119.1, 53.3, 13.4; MS ( $m/z$  (relative abundance, %)): 358 ( $\text{M}^+$ , 9), 235 (50), 131 (79), 103 (92), 91 (40), 77 (100).

*Ethyl 1-(4-Methylphenyl)-1H-1,2,4-triazolo[4',3':2,3][1,2,4]triazino[5,6-b]indole-3-carboxylate (8f)*. Yield: 78 %; m.p.: 242 °C (DMF /  $\text{H}_2\text{O}$ ); Anal. Calcd. for  $\text{C}_{20}\text{H}_{16}\text{N}_6\text{O}_2$  (FW: 372): C, 64.31; H, 3.68; N, 23.36 %. Found: C, 63.10; H, 4.21; N, 22.30 %; IR (KBr,  $\text{cm}^{-1}$ ): 1751 (CO);  $^1\text{H-NMR}$  (300 MHz,  $\text{DMSO-}d_6$ ,  $\delta$  / ppm): 1.44 (3H, *t*,  $J = 7$  Hz), 2.4 (3H, *s*), 4.43 (2H, *q*,  $J = 7$  Hz), 6.69–8.26 (4H, *m*, ArH), 7.49 (2H, *d*,  $J = 8$  Hz), 7.52 (2H, *d*,  $J = 8$  Hz);  $^{13}\text{C-NMR}$  (75 MHz,  $\text{DMSO-}d_6$ ,  $\delta$  / ppm): 170.6 (COEt), 156.5, 148.8, 144.2, 139.9, 139.2, 137.7, 136.4, 136.9, 134.6, 133.1, 132.4, 127.6, 124.8, 119.6, 56.2, 18.8, 13.9; MS ( $m/z$  (relative abundance, %)): 372 ( $\text{M}^+$ , 100), 260 (50), 220 (17), 158 (12), 104 (14), 91 (40), 77 (32).

*Ethyl 1-(4-Chlorophenyl)-1H-1,2,4-triazolo[4',3':2,3][1,2,4]triazino[5,6-b]indole-3-carboxylate (8g)*. Yield: 75 %; m.p.: 248 °C (DMF /  $\text{H}_2\text{O}$ ); Anal. Calcd. for  $\text{C}_{19}\text{H}_{13}\text{ClN}_6\text{O}_2$  (FW: 392): C, 57.92; H, 3.21; N, 21.14 %. Found: C, 57.76; H, 3.32; N, 20.84 %; IR (KBr,  $\text{cm}^{-1}$ ): 1742 (CO);  $^1\text{H-NMR}$  (300 MHz,  $\text{DMSO-}d_6$ ,  $\delta$  / ppm): 1.43 (3H, *t*,  $J = 7$  Hz), 4.41 (2H, *q*,  $J = 7$  Hz), 6.74–8.21 (4H, *m*, ArH), 7.74 (2H, *d*,  $J = 8$  Hz), 8.11 (2H, *d*,  $J = 8$  Hz);  $^{13}\text{C-NMR}$  (75 MHz,  $\text{DMSO-}d_6$ ,  $\delta$  / ppm): 171.2 (COEt), 158.8, 149.9, 146.4, 141.0, 139.4, 138.2, 137.6, 136.3, 135.6, 133.5, 133.1, 126.8, 124.8, 118.9, 55.6, 13.9; MS ( $m/z$  (relative abundance, %)): 394 ( $\text{M}^{+2}$ , 25), 393 ( $\text{M}^{+1}$ , 28), 392 ( $\text{M}^+$ , 70), 192 (21), 103 (92), 77 (100)

*N,1-Diphenyl-1H-1,2,4-triazolo[4',3':2,3][1,2,4]triazino[5,6-b]indole-3-carboxylate (8h)*. Yield: 75 %; m.p.: 236 °C (AcOH); Anal. Calcd. for  $\text{C}_{24}\text{H}_{17}\text{N}_7\text{O}$  (FW: 419): C, 68.31; H, 3.87; N, 23.10 %. Found: C, 68.22; H, 3.80; N, 22.89 %; IR (KBr,  $\text{cm}^{-1}$ ): 3256 (NH), 1673 (CO);  $^1\text{H-NMR}$  (300 MHz,  $\text{DMSO-}d_6$ ,  $\delta$  / ppm): 6.80–8.20 (14H, *m*, ArH), 11.03 (1H, *s*, NH);  $^{13}\text{C-NMR}$  (75 MHz,  $\text{DMSO-}d_6$ ,  $\delta$  / ppm): 163.2, 155.8, 155.7, 154.2, 149.1, 146.2, 143.3, 139.8, 139.2, 138.3, 129.8, 129.7, 129.1, 128.8, 128.3, 128.1, 125.5, 124.6, 120.5; MS ( $m/z$  (relative abundance, %)): 419 ( $\text{M}^+$ , 17), 551 (14), 287 (16), 201 (18), 119 (8), 91 (31), 77 (100).

*1-(4-Methylphenyl)-N-phenyl-1H-1,2,4-triazolo[4',3':2,3][1,2,4]triazino[5,6-b]indole-3-carboxylate (8i)*. Yield: 77 %; m.p. 260 °C (DMF); Anal. Calcd. for  $\text{C}_{24}\text{H}_{17}\text{N}_7\text{O}$  (FW: 419): C, 68.51; H, 4.10; N, 23.10 %. Found: C, 68.31; H, 4.00; N, 22.90 %; IR (KBr,  $\text{cm}^{-1}$ ): 3260 (NH), 1678 (CO);  $^1\text{H-NMR}$  (300 MHz,  $\text{DMSO-}d_6$ ,  $\delta$  / ppm): 2.40 (3H, *s*), 6.72–8.28 (9H, *m*, ArH), 7.81 (2H, *d*,  $J = 8$  Hz), 8.11 (2H, *d*,  $J = 8$  Hz), 11.05 (1H, *s*);  $^{13}\text{C-NMR}$  (75 MHz,  $\text{DMSO-}d_6$ ,  $\delta$  /

/ ppm): 162.4, 156.5, 156.2, 154.8, 150.3, 148.6, 144.5, 140.3, 139.7, 136.4, 131.8, 129.8, 129.0, 128.8, 128.3, 126.8, 124.6, 122.4, 120.5, 17.9; MS ( $m/z$  (relative abundance, %)): 419 ( $M^+$ , 10), 237 (11.4), 152 (13), 118 (100), 91 (43), 77 (93).

*1-(4-Chlorophenyl)-N-phenyl-1H-1,2,4-triazolo[4',3':2,3][1,2,4]triazino[5,6-b]indole-3-carboxylate (8j)*. Yield: 65 %; m.p.: 268 °C (DMF); Anal. Calcd. for  $C_{23}H_{14}ClN_7O$  (FW: 439): C, 62.58; H, 3.01; N, 22.01 %. Found: C, 62.39; H, 3.23; N, 21.71 %; IR (KBr,  $cm^{-1}$ ): 3249 (NH), 1662 (CO);  $^1H$ -NMR (300 MHz, DMSO- $d_6$ ,  $\delta$  / ppm): 6.72–8.20 (9H, *m*, ArH), 7.59 (2H, *d*,  $J = 8$  Hz), 7.61 (2H, *d*,  $J = 8$  Hz), 11.05 (1H, *s*);  $^{13}C$ -NMR (75 MHz, DMSO- $d_6$ ,  $\delta$  / ppm): 163.7, 156.8, 155.2, 154.7, 149.9, 147.0, 143.8, 140.1, 139.5, 138.7, 127.6, 126.2, 124.7, 124.3, 124.0, 123.8, 123.5, 120.6, 118.4; MS ( $m/z$  (relative abundance, %)): 441 ( $M^{+2}$ , 6), 440 ( $M^{+1}$ , 8), 439 ( $M^+$ , 19), 313 (10), 239 (11), 119 (19), 91 (29), 77 (100).

*Phenyl(1-phenyl-1H-1,2,4-triazolo[4',3':2,3][1,2,4]triazino[5,6-b]indol-3-yl)methanone (8k)*. Yield: 75 %; m.p.: 282 °C (DMF); Anal. Calcd. for  $C_{23}H_{14}N_6O$  (FW: 390): C, 70.44; H, 3.36; N, 21.35 %. Found: C, 63.10; H, 3.42; N, 23.23 %; IR (KBr,  $cm^{-1}$ ): 1694 (CO);  $^1H$ -NMR (300 MHz, DMSO- $d_6$ ,  $\delta$  / ppm): 6.89–8.30 (14H, *m*, ArH);  $^{13}C$ -NMR (75 MHz, DMSO- $d_6$ ,  $\delta$  / ppm): 176.6 (COPh), 156.3, 154.3, 152.1, 149.3, 146.2, 143.1, 139.8, 139.2, 138.3, 137.1, 134.2, 133.8, 132.8, 132.2, 131.3, 128.8, 127.1, 125.5; MS ( $m/z$  (relative abundance, %)): 390 ( $M^+$ , 20), 279 (12), 129 (17), 105 (8.4), 91 (7.1), 77 (100).

*[1-(4-Methylphenyl)-1H-1,2,4-triazolo[4',3':2,3][1,2,4]triazino[5,6-b]indol-3-yl]phenylmethanone (8l)*. Yield: 77 %; m.p.: 276 °C (DMF); Anal. Calcd. for  $C_{24}H_{16}N_6O$  (FW: 404): C, 70.89; H, 3.78; N, 20.28 %. Found: C, 63.10; H, 3.42; N, 23.23 %; IR (KBr,  $cm^{-1}$ ): 1696 (CO);  $^1H$ -NMR (300 MHz, DMSO- $d_6$ ,  $\delta$  / ppm): 2.44 (3H, *s*), 6.89–8.28 (9H, *m*, ArH), 7.88 (2H, *d*,  $J = 8$  Hz), 8.18 (2H, *d*,  $J = 8$  Hz);  $^{13}C$ -NMR (75 MHz, DMSO- $d_6$ ,  $\delta$  / ppm): 175.4 (COPh), 157.6, 154.8, 152.5, 150.6, 147.2, 144.4, 140.4, 139.8, 138.9, 138.5, 134.7, 133.0, 132.6, 132.1, 130.3, 128.2, 122.3, 120.5, 17.9; MS ( $m/z$  (relative abundance, %)): 404 ( $M^+$ , 16), 341 (31), 192 (23), 118 (43), 91 (33), 77 (53), 63 (100).

*[1-(4-Chlorophenyl)-1H-1,2,4-triazolo[4',3':2,3][1,2,4]triazino[5,6-b]indol-3-yl]phenylmethanone (8m)*. Yield: 65 %; m.p.: 294 °C (DMF); Anal. Calcd. for  $C_{23}H_{13}ClN_6O$  (FW: 424): C, 65.50; H, 3.11; N, 19.01 %. Found: C, 65.23; H, 3.03; N, 18.81 %; IR (KBr,  $cm^{-1}$ ): 1698 (CO);  $^1H$ -NMR (300 MHz, DMSO- $d_6$ ,  $\delta$  / ppm): 6.82–8.29 (9H, *m*, ArH), 7.69 (2H, *d*,  $J = 8$  Hz), 7.84 (2H, *d*,  $J = 8$  Hz);  $^{13}C$ -NMR (75 MHz, DMSO- $d_6$ ,  $\delta$  / ppm): 176.8 (COPh), 157.7, 154.8, 153.5, 149.8, 147.6, 144.1, 139.6, 139.0, 138.1, 137.6, 134.0, 133.6, 133.5, 132.1, 130.7, 128.2, 123.3, 120.5; MS ( $m/z$  (relative abundance, %)): 426 ( $M^{+2}$ , 6), 425 ( $M^{+1}$ , 8), 424 ( $M^+$ , 19), 320 (32), 302 (48), 167 (19), 111 (100), 77 (54).

*3-[(2H-1,2,4-triazino[5,6-b]indol-3-yl)thio]-2,4-pentanedione (Iib)*. Yield: 60 %; m.p.: 198 °C (DMF / EtOH); Anal. Calcd. for C<sub>14</sub>H<sub>12</sub>N<sub>4</sub>O<sub>2</sub>S (FW: 300): C, 55.99; H, 4.03; N, 18.65 %. Found: C, 55.76; H, 4.00; N, 18.43 %; IR (KBr, cm<sup>-1</sup>): 3410 (NH), 1712, 1702, (2CO); <sup>1</sup>H-NMR (300 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 2.51 (6H, *s*), 5.4 (1H, *s*), 6.91–7.66 (4H, *m*, ArH), 11.17 (1H, *s*); <sup>13</sup>C-NMR (75 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 187.6, 167.4 (2CO), 156.7, 150.1, 145.6, 132.9, 132.2, 130.4, 124.1, 121.4, 118.6, 66.3, 49.8, 24.8, 14.6; MS (*m/z* (relative abundance, %)): 330 (M<sup>+</sup>, 21), 202 (100), 65 (63), 50 (18).

*Ethyl 3-oxo-2-[(2H-1,2,4-triazino[5,6-b]indol-3-yl)thio]butanoate (Iie)*. Yield: 75 %; m.p.: 180 °C (DMF / EtOH); Anal. Calcd. for C<sub>15</sub>H<sub>14</sub>N<sub>4</sub>O<sub>3</sub>S (FW: 330): C, 54.53; H, 4.27; N, 16.96 %. Found: C, 54.33; H, 4.43; N, 16.76 %; IR (KBr, cm<sup>-1</sup>): 3417 (NH), 1743, 1712 (CO); <sup>1</sup>H-NMR (300 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 1.33 (3H, *t*, *J* = 7.2 Hz), 2.51 (3H, *s*), 4.47 (2H, *q*, *J* = 7.2 Hz), 5.21 (1H, *s*), 6.88–8.15 (4H, *m*, ArH), 11.31 (1H, *s*); <sup>13</sup>C-NMR (75 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 188.2 (CO), 156.4, 150.9, 145.7, 133.9, 132.8, 130.4, 125.4, 120.8, 118.9, 68.9, 24.8; MS (*m/z* (relative abundance, %)): 330 (M<sup>+</sup>, 19), 317 (16), 202 (31), 150 (16), 77 (56), 60 (100).

*3-Oxo-N-phenyl-2-[(2H-1,2,4-triazino[5,6-b]indol-3-yl)thio]butanoate (Iih)*. Yield: 80 %; m.p.: 215 °C (DMF / EtOH); Anal. Calcd. for C<sub>19</sub>H<sub>15</sub>N<sub>5</sub>O<sub>3</sub>S (FW: 377): C, 60.46; H, 4.01; N, 18.56 %. Found: C, 60.76; H, 3.96; N, 18.28 %; IR (KBr, cm<sup>-1</sup>): 3417, 3321 (2NH), 1712, 1640 (CO); <sup>1</sup>H-NMR (300 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 2.53 (3H, *s*), 4.52 (*s*, 1H), 6.86–8.11 (*m*, 9H, ArH), 11.04 (*s*, 1H), 11.32 (*s*, 1H); <sup>13</sup>C-NMR (75 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 189.8, 166.4 (2CO), 159.4, 154.4, 150.9, 144.2, 136.4, 135.8, 132.9, 131.8, 131.0, 130.4, 127.4, 126.7, 120.8, 117.6, 67.8, 24.6; MS (*m/z* (relative abundance, %)): 377 (M<sup>+</sup>, 32), 202 (100), 167 (65), 134 (10), 118 (52), 63 (67).