



SUPPLEMENTARY MATERIAL TO

**An efficient synthesis of novel triazoles incorporating barbituric motifs via [3+2] cycloaddition reactions: an experimental and theoretical study**

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CHARACTERIZATION DATA FOR THE PREPARED COMPOUNDS

2-(Prop-2-yn-1-yloxy)benzaldehyde (**2a**).<sup>1</sup> Yield: 93 %; white solid; m.p.: 69–70 °C.

4-(Prop-2-yn-1-yloxy)benzaldehyde (**2b**). Yield: 90 %; white solid; m.p.: 68–69.5 °C; <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 2.59 (1H, s), 4.86 (2H, s), 7.11 (2H, *d*, *J* = 7.7 Hz), 7.9 (2H, *d*, *J* = 7.7 Hz), 10.5 (1H, s).

5-(2-(Prop-2-yn-1-yloxy)benzylidene)pyrimidine-2,4,6(1H,3H,5H)-trione (**4a**).<sup>1</sup> Yield: 85 %; yellow solid; m.p.: 207–208.3 °C; IR (KBr, cm<sup>-1</sup>): 3310, 3155, 3010, 1771, 1642.

5-(4-(Prop-3-yn-1-yloxy)benzylidene)pyrimidine-2,4,6(1H,3H,5H)-trione (**4b**). Yield: 90 %; yellow solid; m.p.: 217.5–219.4 °C; IR (KBr, cm<sup>-1</sup>): 3262, 2091, 1751, 1666; <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 11.17 (1H, s, NH), 10.97 (1H, s, NH), 8.32 (2H, *m*, Ar-H), 8.30 (1H, s, CH), 7.10 (2H, *d*, *J* = 8.4 Hz), 4.96 (2H, s, CH<sub>2</sub>), 3.66 (1H, s, CH); <sup>13</sup>C-NMR (100 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 161.02, 160.58, 159.21, 149.33, 136.58, 133.32, 128.28, 117.45, 115.06, 79.07, 56.21.

5-(2-(Prop-2-yn-1-yloxy)benzylidene)-2-thioxodihydropyrimidine-4,6(1H,5H)-dione (**4c**). Yield: 80 %; yellow solid; m.p.: 228–230 °C; IR (KBr, cm<sup>-1</sup>): 3249, 2095, 1670; <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 11.41 (1H, s, NH), 11.36 (1H, s, NH), 8.30 (1H, s, CH), 7.71 (2H, *d*, *J* = 8.4 Hz, Ar-H), 7.21 (2H, *d*, *J* = 8.4 Hz, Ar-H), 4.91 (2H, s, CH<sub>2</sub>), 3.66 (1H, s, CH); <sup>13</sup>C-NMR (100 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 173.02, 164.58, 162.21, 151.93, 150.58, 137.32, 126.28, 117.45, 115.06, 79.07, 56.21.

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5-(4-(prop-3-yn-1-yloxy)benzylidene)-2-thioxodihydropyrimidine-4,6(1H,5H)-dione (**4d**). Yield: 87 %; yellow solid; m.p.: 196–198 °C; IR (KBr,  $\text{cm}^{-1}$ ): 3230, 2119, 1678;  $^1\text{H-NMR}$  (400 MHz,  $\text{DMSO-}d_6$ ,  $\delta$  / ppm): 11.37(1H, s, NH), 11.17 (1H, s, NH), 8.25 (1H, s, CH), 7.83–7.80 (2H, m, Ar-H), 7.22 (2H, d,  $J = 8.4$  Hz), 4.90 (2H, s,  $\text{CH}_2$ ), 3.66 (1H, s, CH);  $^{13}\text{C-NMR}$  (100 MHz,  $\text{DMSO-}d_6$ ,  $\delta$  / ppm): 173.02, 164.58, 162.21, 151.93, 150.58, 137.32, 126.28, 117.45, 115.06, 79.07, 56.21.

1,3-Dimethyl-5-(2-(prop-2-yn-1-yloxy)benzylidene)pyrimidine-2,4,6(1H,3H,5H)-trione (**4e**).<sup>78</sup> Yield: 84 %; yellow solid; m.p.: 141.5–143.0 °C; IR (KBr,  $\text{cm}^{-1}$ ): 3345, 1770, 1684.

1,3-Dimethyl-5-(4-(prop-3-yn-1-yloxy)benzylidene)pyrimidine-2,4,6(1H,3H,5H)-trione (**4f**). Yield: 79 %; yellow solid; m.p.: 172.5–173.8 °C; IR (KBr,  $\text{cm}^{-1}$ ): 3245, 2115, 1684;  $^1\text{H-NMR}$  (400 MHz,  $\text{DMSO-}d_6$ ,  $\delta$  / ppm): 8.33 (2H, d, Ar-H), 8.30 (1H, s, CH), 7.11 (2H, d,  $J = 8.4$  Hz), 4.95 (2H, s,  $\text{CH}_2$ ), 3.66 (1H, s, CH), 3.25 (3H, s,  $\text{CH}_3$ ), 3.21 (3H, s,  $\text{CH}_3$ );  $^{13}\text{C-NMR}$  (100 MHz,  $\text{DMSO-}d_6$ ,  $\delta$  / ppm): 163.02, 161.58, 161.21, 155.93, 151.58, 137.36, 126.26, 116.45, 115.06, 79.34, 56.29, 29.10, 28.49.

5-(2-((1-Benzyl-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)pyrimidine-2,4,6(1H,3H,5H)-trione (**7a**). Yellow solid; m.p.: 281.3–283.2 °C; Anal. Calcd. for  $\text{C}_{21}\text{H}_{17}\text{N}_5\text{O}_4$  ( $FW$ : 403.4): C, 62.53; H, 4.25; N, 17.36 %. Found: C, 62.48; H, 4.22; N, 17.38 %; IR (KBr,  $\text{cm}^{-1}$ ): 3438, 2925, 1677, 1597, 1159;  $^1\text{H-NMR}$  (400 MHz,  $\text{DMSO}$ ,  $\delta$  / ppm): 10.99 (1H, s, NH), 10.75 (1H, s, NH), 8.32 (1H, s, CH), 8.07 (1H, s, CH), 7.86 (1H, bs, Ar-H), 7.51–7.06 (7H, m, Ar-H), 5.62 (2H, s,  $\text{OCH}_2$ ), 5.27 (2H, s,  $\text{CH}_2$ );  $^{13}\text{C-NMR}$  (100 MHz,  $\text{DMSO}$ ): 163.39, 162.79, 159.23, 148.05, 143.09, 136.41, 132.23, 131.71, 130.33, 129.24, 128.65, 128.27, 126.47, 125.43, 115.68, 115.44, 115.14, 61.92, 53.34; MS ( $m/z$ ): 402.1 ( $\text{M}^+$ ).

5-(2-((1-(4-Bromobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)pyrimidine-2,4,6(1H,3H,5H)-trione (**7b**). Yellow solid; m.p.: 279.2–280.3 °C; Anal. Calcd. for  $\text{C}_{21}\text{H}_{16}\text{BrN}_5\text{O}_4$  ( $FW$ : 482.3): C, 52.30; H, 3.34; N, 14.52 %. Found: C, 52.37; H, 3.37; N, 14.48 %; IR (KBr,  $\text{cm}^{-1}$ ): 3438, 2926, 1715, 1685, 1598, 1161;  $^1\text{H-NMR}$  (400 MHz,  $\text{DMSO}$ ,  $\delta$  / ppm): 11.20 (1H, s, NH), 10.99 (1H, s, NH), 8.35 (1H, s, CH), 8.07 (1H, s, CH), 7.87 (1H, d,  $J = 8$  Hz, Ar-H), 7.53–7.21 (5H, m, Ar-H), 7.15–7.01 (2H, m, Ar-H), 5.67 (2H, s,  $\text{OCH}_2$ ), 5.28 (2H, s,  $\text{CH}_2$ );  $^{13}\text{C-NMR}$  (100 MHz,  $\text{DMSO}$ ,  $\delta$  / ppm): 164.59, 163.37, 161.08, 148.08, 135.19, 132.23, 130.34, 129.87, 129.33, 129.25, 128.90, 128.79, 128.46, 128.06, 125.54, 115.73, 115.67, 61.89, 53.41; MS ( $m/z$ ): 483.3 ( $\text{M}^+$ ).

5-(2-((1-Benzyl-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (**7c**). Cream solid; m.p.: 289.0–290.5 °C; Anal. Calcd. for  $\text{C}_{23}\text{H}_{21}\text{N}_5\text{O}_4$  ( $FW$ : 431.5): C, 64.03; H, 4.91; N, 16.23 %. Found: C, 64.08; H, 4.93; N, 16.25 %; IR (KBr,  $\text{cm}^{-1}$ ): 3439, 2956, 1629, 1524, 1144;  $^1\text{H-NMR}$  (400 MHz,  $\text{DMSO}$ ,  $\delta$  / ppm): 8.37 (1H, s, CH), 8.07 (1H, s, CH), 7.87

(2H, *d*, *J* = 8.8 Hz, Ar-H), 7.52 (1H, *t*, *J* = 8.8 Hz, Ar-H), 7.42 (1H, *m*, Ar-H), 7.23 (1H, *d*, *J* = 8.4 Hz, Ar-H), 7.18–7.11 (2H, *m*, Ar-H), 7.10–7.06 (1H, *m*, Ar-H), 7.01 (1H, *m*, Ar-H), 5.65 (2H, *s*, OCH<sub>2</sub>), 5.28 (2H, *s*, CH<sub>2</sub>), 3.23 (3H, *s*, CH<sub>3</sub>), 3.21 (3H, *s*, CH<sub>3</sub>); <sup>13</sup>C-NMR (100 MHz, DMSO,  $\delta$  / ppm): 163.37, 161.58, 161.21, 155.95, 137.64, 132.22, 131.30, 130.35, 128.27, 126.27, 125.60, 124.52, 116.45, 115.69, 115.19, 115.06, 61.91, 52.63, 29.09, 28.49; MS (*m/z*): 430.0 (M<sup>+</sup>).

5-(2-((1-(3-Fluorobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (**7d**). Yellow solid; m.p.: 273.2–274.9 °C; Anal. Calcd. for C<sub>23</sub>H<sub>20</sub>FN<sub>5</sub>O<sub>4</sub> (*FW*: 449.4): C, 61.47; H, 4.49; N, 15.58 %. Found: C, 61.50; H, 4.53; N, 15.54 %; IR (KBr, cm<sup>-1</sup>): 3427, 2926, 1602, 1485, 1127; <sup>1</sup>H-NMR (400 MHz, DMSO,  $\delta$  / ppm): 8.37 (1H, *s*, CH), 8.06 (1H, *s*, CH), 7.96 (1H, *s*, Ar-H), 7.87 (2H, *bs*, Ar-H), 7.36–7.33 (3H, *m*, Ar-H), 7.23–7.16 (2H, *m*, Ar-H), 5.67 (2H, *s*, OCH<sub>2</sub>), 5.29 (2H, *s*, CH<sub>2</sub>), 2.88 (3H, *s*, CH<sub>3</sub>), 2.72 (3H, *s*, CH<sub>3</sub>); <sup>13</sup>C-NMR (100 MHz, DMSO,): 163.01, 161.58, 161.21, 148.46, 136.32, 135.60, 132.23, 130.48, 130.34, 129.25, 128.68, 128.61, 128.47, 127.99, 115.75, 115.68, 115.44, 62.39, 56.57, 36.25, 31.23; MS (*m/z*): 451.0 (M<sup>+</sup>).

5-(2-((1-Benzyl-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)-2-thioxodihydropyrimidine-4,6(1H,5H)-dione (**7e**). Yellow solid; m.p.: 251.6–252.9 °C; Anal. Calcd. for C<sub>21</sub>H<sub>17</sub>N<sub>5</sub>O<sub>3</sub>S (*FW*: 419.4): C, 60.13; H, 4.09; N, 16.70 %. Found: C, 60.08; H, 4.07; N, 16.72 %; IR (KBr, cm<sup>-1</sup>): 3439, 2924, 1710, 1660, 1597, 1220, 1166; <sup>1</sup>H-NMR (400 MHz, DMSO,  $\delta$  / ppm): 11.22 (1H, *s*, NH), 11.08 (1H, *s*, NH), 8.39 (1H, *s*, CH), 8.24 (1H, *s*, CH), 7.66 (1H, *d*, *J* = 7.6 Hz, Ar-H), 7.37–7.34 (3H, *m*, Ar-H), 7.32–7.29 (2H, *m*, Ar-H), 7.29–7.24 (2H, *m*, Ar-H), 6.98 (1H, *t*, *J* = 7.2 Hz, Ar-H), 5.62 (2H, *s*, OCH<sub>2</sub>), 5.21 (2H, *s*, CH<sub>2</sub>); <sup>13</sup>C-NMR (100 MHz, DMSO,  $\delta$  / ppm): 168.04, 163.37, 156.06, 143.85, 137.39, 136.46, 131.13, 129.22, 128.60, 128.34, 126.83, 125.93, 125.22, 121.90, 121.61, 115.73, 113.88, 62.31, 53.32, MS (*m/z*): 420.1 (M<sup>+</sup>).

5-(2-((1-(3-Fluorobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)-2-thioxodihydropyrimidine-4,6(1H,5H)-dione (**7f**). Yellow solid; m.p.: 271.7–273.2 °C; Anal. Calcd. for C<sub>21</sub>H<sub>16</sub>FN<sub>5</sub>O<sub>3</sub>S (*FW*: 437.5): C, 57.66; H, 3.69; N, 16.01 %. Found: C, 57.70; H, 3.71; N, 15.97 %; IR (KBr, cm<sup>-1</sup>): 3441, 2920, 1726, 1627, 1597, 1250, 1166; <sup>1</sup>H-NMR (400 MHz, DMSO,  $\delta$  / ppm): 11.82 (1H, *s*, NH), 11.22 (1H, *s*, NH), 8.35 (1H, *s*, CH), 8.24 (1H, *s*, CH), 7.66 (1H, *d*, *J* = 7.6 Hz, Ar-H), 7.43–7.31 (2H, *m*, Ar-H), 7.25 (1H, *d*, *J* = 8.0 Hz, Ar-H), 7.19–7.08 (3H, *m*, Ar-H), 6.98 (1H, *t*, *J* = 7.6 Hz, Ar-H), 5.65 (2H, *s*, OCH<sub>2</sub>), 5.22 (2H, *s*, CH<sub>2</sub>); <sup>13</sup>C-NMR (100 MHz, DMSO,  $\delta$  / ppm): 163.10, 159.28, 156.69, 154.10, 146.84, 137.83, 136.45, 131.13, 125.92, 125.41, 124.44, 121.62, 120.78, 119.89, 115.61, 115.34, 115.12, 114.96, 113.88, 113.23, 63.49, 52.63; MS (*m/z*): 438.1 (M<sup>+</sup>).

5-(2-((1-(4-Bromobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)-2-thioxodihydropyrimidine-4,6(1H,5H)-dione (**7g**). Yellow solid; m.p.: 275.0–276.9 °C; Anal. Calcd. for C<sub>21</sub>H<sub>16</sub>BrN<sub>5</sub>O<sub>3</sub>S (*FW*: 498.3): C, 50.61; H, 3.24; N, 14.05 %. Found: C, 50.67; H, 3.27; N, 14.02 %; IR (KBr, cm<sup>-1</sup>): 3439, 2925, 1729, 1627, 1485, 1238, 1166; <sup>1</sup>H-NMR (400 MHz, DMSO, δ / ppm): 11.47 (1H, *s*, NH), 11.10 (1H, *s*, NH), 8.40 (1H, *s*, CH), 8.23 (1H, *s*, CH), 7.84 (2H, *d*, *J* = 8.8 Hz, Ar-H), 7.44–7.41 (1H, *m*, Ar-H), 7.39–7.27 (2H, *m*, Ar-H), 7.18 (2H, *d*, *J* = 8.8 Hz, Ar-H), 7.07 (1H, *m*, Ar-H), 5.60 (2H, *s*, OCH<sub>2</sub>), 5.20 (2H, *s*, CH<sub>2</sub>); <sup>13</sup>C-NMR (100 MHz, DMSO, δ / ppm): 167.53, 161.35, 159.73, 138.82, 131.37, 131.29, 130.29, 126.51, 125.71, 125.51, 125.48, 124.45, 124.42, 117.69, 115.60, 115.40, 115.34, 115.12, 113.50, 63.13, 52.67; MS (*m/z*): 497.4 (M<sup>+</sup>).

5-(4-((1-Benzyl-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)pyrimidine-2,4,6-(1H,3H,5H)-trione (**8a**). Yellow solid; m.p.: 254–255.1 °C; Anal. Calcd. for C<sub>21</sub>H<sub>17</sub>N<sub>5</sub>O<sub>4</sub> (*FW*: 403.4): C, 62.53; H, 4.25; N, 17.36 %. Found: C, 62.41; H, 4.15; N, 17.46 %; IR (KBr, cm<sup>-1</sup>): 3439, 2924, 1718, 1680, 1597, 1166; <sup>1</sup>H-NMR (400 MHz, DMSO, δ / ppm): 10.99 (1H, *s*, NH), 10.97 (1H, *s*, NH), 8.37 (1H, *s*, CH), 8.06 (1H, *s*, CH), 7.87 (2H, *d*, *J* = 8.8 Hz, Ar-H), 7.72 (2H, *d*, *J* = 8.8 Hz, Ar-H), 7.39–7.25 (3H, *m*, Ar-H), 7.22 (2H, *d*, *J* = 8.8 Hz, Ar-H), 5.71 (2H, *s*, OCH<sub>2</sub>), 5.22 (2H, *s*, CH<sub>2</sub>); <sup>13</sup>C-NMR (100 MHz, DMSO, δ / ppm): 163.32, 162.79, 159.23, 148.03, 137.39, 137.23, 132.22, 131.36, 130.20, 129.12, 128.29, 126.47, 115.76, 115.68, 61.89, 52.04; MS (*m/z*): 402.2 (M<sup>+</sup>).

5-(4-((1-(2-Chlorobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)pyrimidine-2,4,6-(1H,3H,5H)-trione (**8b**). Yellow solid; m.p.: 241.5–243.2 °C; Anal. Calcd. for C<sub>21</sub>H<sub>16</sub>ClN<sub>5</sub>O<sub>4</sub> (*FW*: 437.9): C, 57.61; H, 3.68; N, 16.00 %. Found: C, 57.65; H, 3.71; N, 16.05 %; IR (KBr, cm<sup>-1</sup>): 3503, 2923, 1715, 1628, 1593, 1170; <sup>1</sup>H-NMR (400 MHz, DMSO, δ / ppm): 11.02 (1H, *s*, NH), 10.97 (1H, *s*, NH), 8.35 (1H, *s*, CH), 8.06 (1H, *s*, CH), 7.87 (2H, *d*, *J* = 8.0 Hz, Ar-H), 7.52 (1H, *d*, *J* = 7.2 Hz, Ar-H), 7.35–7.42 (1H, *m*, Ar-H), 7.24 (2H, *dd*, *J* = 12.8, 8.0 Hz, Ar-H), 6.99–7.05 (2H, *m*, Ar-H), 5.74 (2H, *s*, OCH<sub>2</sub>), 5.32 (2H, *s*, CH<sub>2</sub>); <sup>13</sup>C-NMR (100 MHz, DMSO, δ / ppm): 163.49, 162.21, 159.37, 159.28, 133.49, 133.14, 132.06, 131.87, 131.05, 130.84, 130.55, 130.13, 128.27, 128.22, 128.15, 115.71, 115.49, 62.49, 51.32; MS (*m/z*): 437.0 (M<sup>+</sup>).

5-(4-((1-(3-Fluorobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)pyrimidine-2,4,6-(1H,3H,5H)-trione (**8c**). Yellow solid; m.p.: 259.2–260.1 °C; Anal. Calcd. for C<sub>21</sub>H<sub>16</sub>FN<sub>5</sub>O<sub>4</sub> (*FW*: 421.4): C, 59.86; H, 3.83; N, 16.62 %. Found: C, 59.91; H, 3.88; N, 16.56 %; IR (KBr, cm<sup>-1</sup>): 3461, 2932, 1684, 1502, 1159; <sup>1</sup>H-NMR (400 MHz, DMSO, δ / ppm): 11.07 (1H, *s*, NH), 10.97 (1H, *s*, NH), 8.37 (1H, *s*, CH), 8.08 (1H, *s*, CH), 7.87 (2H, *d*, *J* = 8.4 Hz, Ar-H), 7.43–7.35 (1H, *m*, Ar-H), 7.23 (2H, *d*, *J* = 8.8 Hz, Ar-H), 7.20–7.14 (3H, *m*, Ar-H), 5.65 (2H, *s*, OCH<sub>2</sub>), 5.29 (2H, *s*, CH<sub>2</sub>); <sup>13</sup>C-NMR (100 MHz, DMSO, δ / ppm): 163.80, 163.36, 161.37, 142.93, 139.07, 138.99, 132.24, 131.39, 131.31, 125.60,

124.55, 124.52, 116.30, 115.68, 115.64, 115.42, 61.88, 52.65; MS ( $m/z$ ): 421.2 ( $M^+$ ).

5-(4-((1-(4-Bromobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)pyrimidine-2,4,6(1H,3H,5H)-trione (**8d**). Yellow solid; m.p.: 235.5–237 °C; Anal. Calcd. for  $C_{21}H_{16}BrN_5O_4$  ( $FW$ : 482.3): C, 52.30; H, 3.34; N, 14.52 %. Found: C, 52.24; H, 3.41; N, 14.58 %; IR (KBr,  $cm^{-1}$ ): 3440, 2918, 1761, 1650, 1156;  $^1H$ -NMR (400 MHz, DMSO,  $\delta$  / ppm): 11.23 (1H, *s*, NH), 11.19 (1H, *s*, NH), 8.33 (1H, *s*, CH), 8.23 (1H, *s*, CH), 7.67 (2H, *d*,  $J = 8.4$  Hz, Ar-H), 7.58 (2H, *d*,  $J = 8.0$  Hz, Ar-H), 7.34 (2H, *d*,  $J = 8.0$  Hz, Ar-H), 7.26 (2H, *d*,  $J = 8.4$  Hz, Ar-H), 5.61 (2H, *s*,  $OCH_2$ ), 5.33 (2H, *s*,  $CH_2$ );  $^{13}C$ -NMR (100 MHz, DMSO,  $\delta$  / ppm): 168.53, 164.90, 163.37, 149.86, 138.90, 135.19, 132.23, 130.34, 129.06, 128.46, 128.05, 125.54, 125.06, 115.73, 115.57, 63.03, 52.64; MS ( $m/z$ ): 481.3 ( $M^+$ ).

5-(4-((1-(2-Chlorobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)-1,3-dimethylpyrimidine-2,4,6(1H,3H,5H)-trione (**8e**). Yellow solid; m.p.: 246.5–248.2 °C; Anal. Calcd. for  $C_{23}H_{20}ClN_5O_4$  ( $FW$ : 465.9): C, 59.30; H, 4.33; N, 15.03 %. Found: C, 59.21; H, 4.30; N, 15.11 %; IR (KBr,  $cm^{-1}$ ): 3447, 2923, 1670, 1597, 1178;  $^1H$ -NMR (400 MHz, DMSO,  $\delta$  / ppm): 8.38 (1H, *s*, CH), 7.97 (1H, *s*, CH), 7.87 (2H, *m*, Ar-H), 7.28–7.15 (4H, *m*, Ar-H), 7.06–6.88 (2H, *m*, Ar-H), 5.66 (2H, *s*,  $OCH_2$ ), 5.10 (2H, *s*,  $CH_2$ ), 2.87 (3H, *s*,  $CH_3$ ), 2.71 (3H, *s*,  $CH_3$ );  $^{13}C$ -NMR (100 MHz, DMSO,  $\delta$  / ppm): 162.79, 161.24, 159.45, 147.39, 137.39, 132.23, 131.96, 131.36, 130.68, 129.19, 128.97, 128.28, 126.47, 115.91, 115.76, 61.59, 52.51, 35.25, 33.21; MS ( $m/z$ ): 465.3 ( $M^+$ ).

5-(4-((1-Benzyl-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)-2-thioxodihydropyrimidine-4,6(1H,5H)-dione (**8f**). Yellow solid. m.p.: 229.9–231.5 °C; Anal. Calcd. for  $C_{21}H_{17}N_5O_4$  ( $FW$ : 419.4): C, 60.13; H, 4.09; N, 16.70 %. Found: C, 60.19 ; H, 4.13; N, 16.81 %; IR (KBr,  $cm^{-1}$ ): 3438, 2925, 1677, 1597, 1159;  $^1H$ -NMR (400 MHz, DMSO,  $\delta$  / ppm): 11.06 (1H, *s*, NH), 10.98 (1H, *s*, NH), 8.34 (1H, *s*, CH), 8.06 (1H, *s*, CH), 7.87 (2H, *d*,  $J = 8.4$  Hz, Ar-H), 7.57 (2H, *d*,  $J = 8.0$  Hz, Ar-H), 7.51 (1H, *t*,  $J = 8.4$  Hz, Ar-H), 7.22 (2H, *d*,  $J = 8.0$  Hz, Ar-H), 7.04 (2H, *d*,  $J = 8.4$  Hz, Ar-H), 5.60 (2H, *s*,  $OCH_2$ ), 5.27 (2H, *s*,  $CH_2$ );  $^{13}C$ -NMR (100 MHz, DMSO,  $\delta$  / ppm): 176.80, 163.37, 159.28, 148.04, 135.83, 135.79, 132.23, 132.17, 130.71, 130.69, 130.33, 128.27, 126.42, 121.94, 115.67, 61.91, 52.60; MS ( $m/z$ ): = 421.1 ( $M^+$ ).

5-(4-((1-(4-Bromobenzyl)-1H-1,2,3-triazol-4-yl)methoxy)benzylidene)-2-thioxodihydropyrimidine-4,6(1H,5H)-dione (**8g**). Yellow solid; m.p.: 267.3–269.5 °C; Anal. Calcd. for  $C_{21}H_{16}BrN_5O_3S$  ( $FW$ : 498.3): C, 50.61; H, 3.24; N, 14.05 %. Found: C, 50.55; H, 3.18; N, 14.13 %; IR (KBr,  $cm^{-1}$ ): 3439, 2925, 1728, 1627, 1238, 1130;  $^1H$ -NMR (400 MHz, DMSO,): 11.47 (1H, *s*, NH), 11.44 (1H, *s*, NH), 8.37 (1H, *s*, CH), 8.16 (1H, *s*, CH), 7.74 (2H, *d*,  $J = 8.0$  Hz, Ar-H), 7.57 (2H, *d*,  $J = 8.0$  Hz, Ar-H), 7.45–7.42 (2H, *m*, Ar-H), 7.26 (2H, *d*,  $J = 8.8$  Hz, Ar-H), 5.61 (2H, *s*,  $OCH_2$ ), 5.23 (2H, *s*,  $CH_2$ );  $^{13}C$ -NMR (100 MHz, DMSO,

$\delta$  / ppm): 177.41, 162.19, 155.72, 142.69, 138.88, 136.85, 133.36, 132.15, 131.77, 130.59, 127.94, 125.35, 124.25, 121.89, 116.52, 113.50, 62.68, 52; MS ( $m/z$ ): 497.0 ( $M^+$ ).

## REFERENCES

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