

*Supporting Material*

# Design, Synthesis, and Antiviral Activities of New Benzotriazole-Based Derivatives

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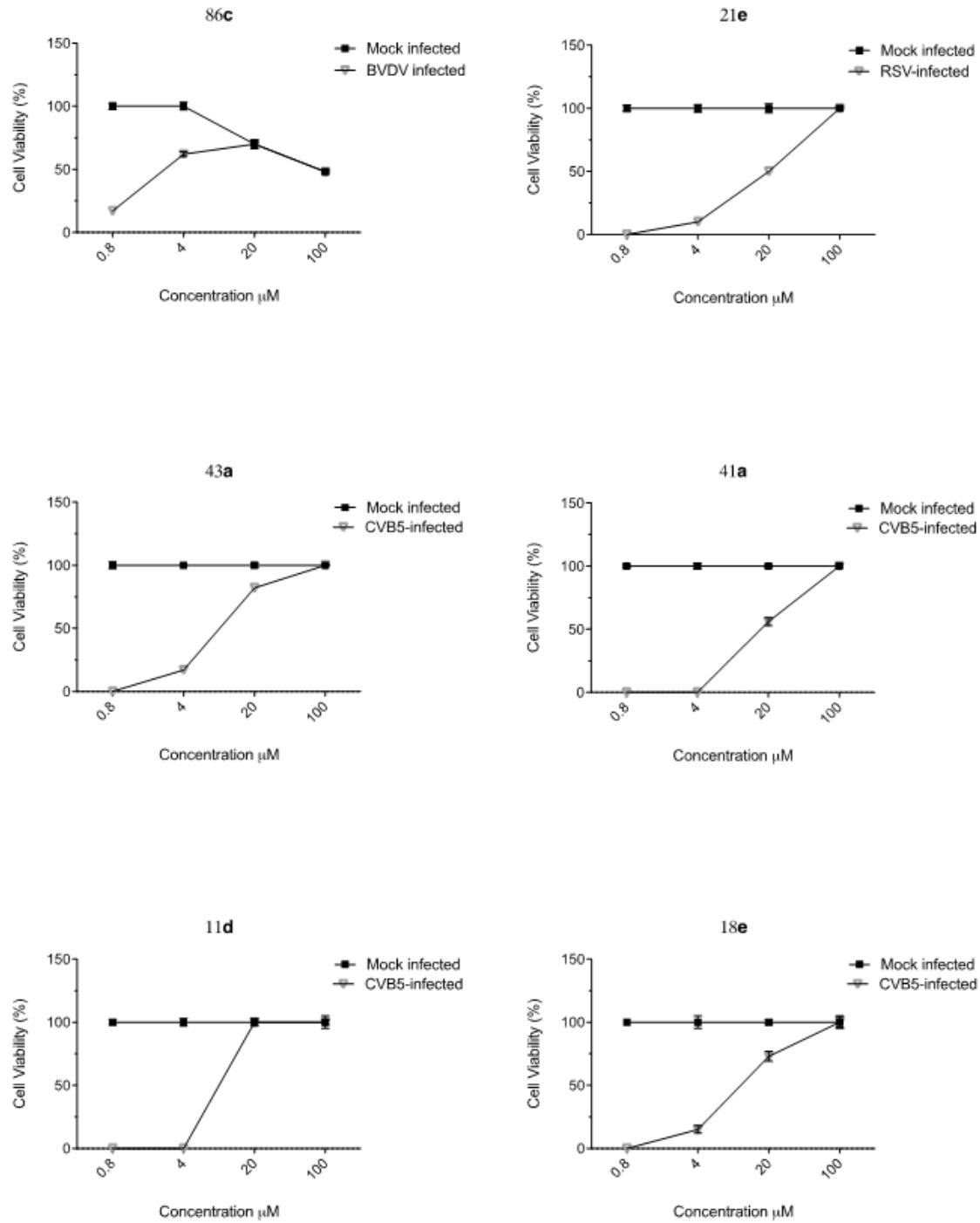
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## Supporting Material

*Dose-response curves for 6 most active compounds*



**Figure S1.** Cytotoxicity and broad-spectrum antiviral activity of selected benzotriazole derivatives (86c, 21e, 43a, 41a, 11d, 18e). The viability of mock-infected cells was estimated by MTT assay, three days after-infection. The number of live cells was expressed as a percentage of mock-infected, untreated control cells. Data are expressed as means  $\pm$  SD of at least two independent measurements.

*Experimental – chemical characterization*

**5,6-dichloro-2-(3-nitrobenzyl)-2H-benzo [d][1,2,3]triazole (3a).**

Compound **3a** was obtained in 5% total yield; m.p. : 237-239 °C; TLC (petroleum ether/ethyl acetate = 7/3)  $R_f$ : 0.58;  $^1\text{H-NMR}$  (400 MHz, DMSO- $d_6$ )  $\delta$ : 8.43 (2H, s, H-4,7), 8.34 (1H, s, H-2'), 8.24 (1H, d,  $J$  = 8.0 Hz, H-4'), 7.85 (1H, d,  $J$  = 7.6 Hz, H-6'), 7.70 (1H, t,  $J$  = 8.0 Hz, H-5'), 6.22 (2H, s, CH<sub>2</sub>).  $^{13}\text{C-NMR}$  (DMSO- $d_6$ )  $\delta$ : 142.9 (2C), 136.6 (2C), 136.5 (CH), 130.1 (CH), 129.9 (2C), 123.5 (CH), 123.4 (CH), 119.5 (2CH), 58.7 (CH<sub>2</sub>). LC/MS  $m/z$  323, 325 [M+H]<sup>+</sup>.

#### **5,6-dimethyl-2-(3-nitrobenzyl)-2H-benzo [d][1,2,3]triazole (3b)**

Compound **3b** was obtained in 12% total yield; m.p.: 145-148 °C TLC (petroleum ether/ethyl acetate = 8,5/1,5)  $R_f$  : 0.40;  $^1\text{H-NMR}$  (400 MHz, DMSO- $d_6$ )  $\delta$ : 10.59 (1H, s, NH), 8.35 (2H, d,  $J$  = 8.4 Hz, H-3'',5''), 8.15 (2H, d,  $J$  = 8.4 Hz, H-2'',6''), 7.77 (1H, d,  $J$  = 7.6 Hz, H-4'), 7.32 (1H, s, H-2'), 7.66 (2H, s, H-4,7), 7.15 (1H, d,  $J$  = 7.6 Hz, H-6'), 5.91 (2H, s, CH<sub>2</sub>), 2.36 (6H, s, CH<sub>3</sub>).  $^{13}\text{C-NMR}$  (DMSO- $d_6$ )  $\delta$ : 163.9 (C=O), 149.1 (C), 143.3 (C), 140.4 (C), 139.0 (C), 136.6 (3C), 136.2 (C), 129.2 (C), 129.2 (2CH), 129.0 (CH), 123.9 (CH), 123.5 (CH), 120.2 (CH), 119.8 (CH), 116.2 (CH), 59.1 (CH<sub>2</sub>), 20.3 (CH<sub>3</sub>); LC/MS  $m/z$  283 [M+H]<sup>+</sup>.

#### **5,6-dichloro-1-(3-nitrobenzyl)-1H-benzo [d][1,2,3]triazole (4a)**

Compound **4a** was obtained in 44% total yield; m.p.: 156-157 °C TLC (petroleum ether/ethyl acetate = 7/3)  $R_f$ : 0.46;  $^1\text{H-NMR}$  (400 MHz, DMSO- $d_6$ )  $\delta$ : 8.50 (1H, s, H-4), 8.48 (1H, s, H-7), 8.30 (1H, s, H-2'), 8.17 (1H, d,  $J$  = 8.0 Hz, H-4'), 7.78 (1H, d,  $J$  = 7.8 Hz, H-6'), 7.65 (1H, t,  $J$  = 8.0 Hz, H-5'), 6.14 (2H, s, CH<sub>2</sub>).  $^{13}\text{C-NMR}$  (DMSO- $d_6$ )  $\delta$ : 143.1 (2C), 136.6 (2C), 135.7 (CH), 130.9 (CH), 130.1 (2C), 123.5 (CH), 123.4 (CH), 119.5 (2CH), 58.1 (CH<sub>2</sub>). LC/MS  $m/z$  323, 325 [M+H]<sup>+</sup>.

#### **5,6-dimethyl-1-(3-nitrobenzyl)- 1H-benzo [d][1,2,3]triazole (4b)**

Compound **4b** was obtained in 40% total yield; m.p.: 130-132 °C; TLC (petroleum ether/ethyl acetate = 8,5/1,5)  $R_f$ : 0.16;  $^1\text{H-NMR}$  (400 MHz, DMSO- $d_6$ )  $\delta$ : 8.15-8.24 (2H, m, H-4',6'), 7.80 (1H, 1, H-2'), 7.76-7.67 (3H, m, H-4,7,5') 6.10 (2H, s, CH<sub>2</sub>), 2.34 (6H, s, 2CH<sub>3</sub>).  $^{13}\text{C-NMR}$  (DMSO- $d_6$ )  $\delta$ : 149.0 (C), 144.5 (C), 138.3 (C), 137.8 (C), 134.6 (CH), 134.1 (C), 131.7 (C), 130.4 (CH), 122.6 (CH), 122.3 (CH), 116.2 (CH), 109.5 (CH), 49.6 (CH<sub>2</sub>), 20.4 (CH<sub>3</sub>), 19.8 (CH<sub>3</sub>). LC/MS  $m/z$  283 [M+H]<sup>+</sup>.

#### **3-((5,6-dimethyl-2H-benzo[d][1,2,3]triazol-2-yl)methyl)aniline (5b)**

Compound **5b** was obtained in 93% total yield; m.p.: 140-144 °C; TLC (petroleum ether/ethyl acetate 6/4)  $R_f$  : 0.56;  $^1\text{H-NMR}$  (400 MHz, DMSO- $d_6$ )  $\delta$ : 7.63 (2H, s, H-4,7), 6.95 (3H, t, H-5'), 6.45 (3H, m, H-2',4',6'), 5.68 (2H, s, CH<sub>2</sub>), 5.13 (2H, s, NH<sub>2</sub>), 2.34 (6H, s, 2CH<sub>3</sub>);  $^{13}\text{C-NMR}$  (DMSO- $d_6$ )  $\delta$ : 148.9 (C), 143.2 (2C), 136.4 (2C), 136.1 (C), 129.0 (CH), 115.8 (CH), 115.2 (CH), 113.6 (CH), 113.0 (CH), 112.6 (CH), 59.5 (CH<sub>2</sub>), 23.2 (CH<sub>3</sub>), 20.3 (CH<sub>3</sub>). LC/MS  $m/z$  253 [M+H]<sup>+</sup>.

#### **3-((5,6-dichloro-1H-benzo[d][1,2,3]triazol-1-yl)methyl)aniline (6a)**

Compound **6a** was obtained in 55% total yield; m.p. 161-162 °C; TLC: (petroleum ether/ethyl acetate 7/3)  $R_f$  : 0.29;  $^1\text{H-NMR}$  (400 MHz, DMSO- $d_6$ )  $\delta$ : 8.49 (1H, s, H-4), 8.30 (1H, s, H-7), 6.97 (1H, t,  $J$  = 7.5 Hz, H-5'), 6.45-6.43 (2H, m, H-4',6'), 6.40 (1H, s, H-2'), 5.80 (2H, s, CH<sub>2</sub>), 5.15 (2H, s, NH<sub>2</sub>);  $^{13}\text{C-NMR}$  (DMSO- $d_6$ ) 149.1 (C), 144.2 (C), 135.9 (C), 132.1 (C), 130.6 (C), 129.3 (CH), 127.1 (C), 120.6 (CH), 114.9 (CH), 113.7 (CH), 112.5 (CH), 112.5 (CH), 51.1 (CH<sub>2</sub>). LC/MS:  $m/z$  293, 295 [M+H]<sup>+</sup>.

#### **3-((5,6-dimethyl-1H-benzo[d][1,2,3]triazol-1-yl)methyl)aniline (6b)**

Compound **6b** was obtained in 90% total yield; m.p. 146-149 °C; TLC (petroleum ether/ethyl acetate 6/4)  $R_f$  : 0.32;  $^1\text{H-NMR}$  (400 MHz, DMSO- $d_6$ )  $\delta$ : 7.78 (1H, s, H-4), 7.52 (1H, s, H-7), 6.96 (3H, t,  $J$  = 8,0 Hz, H-5'), 6.43 (2H, m, H-4',6'), 6.37 (1H, s, H-2'), 5.71 (2H, s, CH<sub>2</sub>), 5.10 (2H, s, NH<sub>2</sub>), 2.34 (6H, s, 2CH<sub>3</sub>);  $^{13}\text{C-NMR}$  (DMSO- $d_6$ )  $\delta$ : 149.0 (C), 144.5 (C), 137.2 (C), 136.6 (C), 133.4 (C), 131.8 (C), 129.1 (C), 118.1 (C), 114.7 (C), 113.4 (C), 112.3 (C), 109.8 (C), 51.0 (C), 20.4 (C), 19.8 (C). LC/MS  $m/z$  253 [M+H]<sup>+</sup>.

#### **5,6-dichloro-2-(4-nitrobenzyl)-2H-benzo [d][1,2,3]triazole (8a)**

Compound **8a** was obtained in 14% total yield; m.p.: 146-148 °C; TLC (petroleum ether/ethyl acetate = 7,5/2,5)  $R_f$  : 0.58;  $^1\text{H-NMR}$  (400 MHz, CDCl<sub>3</sub>)  $\delta$ : 8.35-8.23 (4H, m, H-3',5', H-7, H-4), 7.63 (2H, d,  $J$  = 8.4, H-2',6'), 5.51 (2H, s, CH<sub>2</sub>);  $^{13}\text{C-NMR}$  (DMSO- $d_6$ )  $\delta$ : 146.8 (2C), 145.9 (C), 141.2 (C), 133.4 (2C), 129.9 (2CH), 127.2 (2CH), 123.8 (2CH), 61.3 (CH<sub>2</sub>). LC/MS  $m/z$  323, 325 [M+H]<sup>+</sup>.

#### **5,6-dimethyl-2-(4-nitrobenzyl)- 2H-benzo [d][1,2,3]triazole (8b)**

Compound **8b** was obtained in 37% total yield; m.p.: 140-142 °C; TLC (petroleum ether/ethyl acetate 8 / 2)  $R_f$  : 0.46;  $^1\text{H-NMR}$  (400 MHz, DMSO- $d_6$ )  $\delta$ : 8.28 (2H, d,  $J$  = 8.6 Hz, H-3',5'), 7.76 (2H, d,  $J$  = 8.6 Hz, H-2',6'), 7.67 (1H, s, H-4,7), 5.55 (2H, s, CH<sub>2</sub>), 2.35 (6H, s, 2CH<sub>3</sub>).  $^{13}\text{C-NMR}$  (DMSO- $d_6$ )  $\delta$ : 147.2 (C), 146.9 (2C), 141.5 (C), 138.2 (2C), 127.9 (2CH), 125.5 (2CH), 116.5 (2CH), 55.4 (CH<sub>2</sub>), 18.8 (2CH<sub>3</sub>); LC/MS  $m/z$  283 [M+H]<sup>+</sup>.

#### **2-(4-nitrobenzyl)-2H-benzo [d][1,2,3]triazole (8c)**

Compound **8c** was obtained in 20% total yield; m.p.: 118-122 °C;(petroleum ether/ethyl acetate 8/2)  $R_f$  : 0.39;  $^1\text{H-NMR}$  (200 MHz, DMSO- $d_6$ )  $\delta$ : 8.37 (2H, d,  $J$  = 8.6 Hz, H-3',5'), 8.29-8.26 (4H, m, arom), 7.79 (2H, d,  $J$  = 8.8 Hz, H-2',6'),

5.56 (2H, s, CH<sub>2</sub>); <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>) δ: 145.6 (C), 144.9 (2C), 142.3 (C), 128.9 (2CH), 126.3 (2CH), 123.8 (2CH), 118.5 (2CH), 58.2 (CH<sub>2</sub>). LC/MS *m/z* 255 [M+H]<sup>+</sup>.

#### 5,6-difluoro-2-(4-nitrobenzyl)-1H-benzo[d][1,2,3]triazole (8d)

Compound **8d** was obtained in 27% total yield; m.p.: 179–180 °C; TLC (petroleum ether/ethyl acetate 7/3) *R<sub>f</sub>*: 0.63; <sup>1</sup>H-NMR (200 MHz, DMSO-*d*<sub>6</sub>) δ: 8.23 (2H, d, *J* = 7.8 Hz, H-3', 5'), 8.10–7.81 (2H, m, H-4, 7), 7.56 (2H, d, *J* = 7.8 Hz, H-2', 6'), 6.16 (2H, s, CH<sub>2</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>) δ: 149.5 (2C), 145.5 (C), 145.4 (C), 132.8 (C), 126.2 (C), 129.8 (2CH), 117.1 (2CH), 115.1 (2CH), 54.7 (CH<sub>2</sub>). LC/MS *m/z* : 291 [M+H]<sup>+</sup>.

#### 4-fluoro-2-(4-nitrobenzyl)-2H-benzo[d][1,2,3]triazole (8e)

Compound **8e** was obtained in 3% total yield; mp: 136–139 °C; TLC (petroleum ether/ethyl acetate 8:2) *R<sub>f</sub>*: 0.33; <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ: 8.25 (2H, d, *J* = 8.4 Hz, H-3', 5'), 7.80 (1H, d, *J* = 8.4 Hz, H-7), 7.64 (2H, d, *J* = 8.4 Hz, H-2', 6'), 7.48–7.43 (1H, m, H-6), 7.29 (1H, t, H-5), 6.23 (2H, s, CH<sub>2</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>) δ: 151.4 (C), 147.4 (C), 146.6 (C), 142.1 (C), 134.9 (C), 129.6 (2CH), 127.1 (CH), 123.9 (2CH), 114.5 (CH), 110.2 (CH), 58.8 (CH<sub>2</sub>). LC/MS: *m/z* 273 [M+H]<sup>+</sup>.

#### 5,6-dichloro-1-(4-nitrobenzyl)-1H-benzo[d][1,2,3]triazole (9a)

Compound **9a** was obtained in 32% total yield; m.p.: 158–160 °C; TLC (petroleum ether/ethyl acetate 7.5/2.5) *R<sub>f</sub>*: 0.42; <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) δ: 8.21 (3H, d, *J* = 7.8 Hz, H-3', 5', H-4), 7.88 (1H, s, H-7), 7.51 (2H, d, *J* = 8.6 Hz, H-2', 6'), 6.03 (2H, s, CH<sub>2</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>) δ: 145.9 (C), 145.3 (C), 142.5 (C), 133.8 (2C), 132.6 (C), 128.6 (2CH), 126.5 (2CH), 124.3 (2CH), 52.0 (CH<sub>2</sub>). LC/MS *m/z* 323, 325 [M+H]<sup>+</sup>.

#### 5,6-dimethyl-1-(4-nitrobenzyl)-1H-benzo[d][1,2,3]triazole (9b)

Compound **9b** was obtained in 45% total yield; m.p.: 143–145 °C; TLC (petroleum ether/ethyl acetate 8/2) *R<sub>f</sub>*: 0.17; <sup>1</sup>H-NMR (200 MHz, DMSO-*d*<sub>6</sub>) δ: 8.28 (2H, d, *J* = 8.8 Hz, H-3', 5'), 7.82 (1H, s, H-4) 7.62 (1H, s, H-7), 7.48 (2H, d, *J* = 8.8 Hz, H-2', 6'), 6.10 (2H, s, CH<sub>2</sub>), 2.35 (6H, s, 2CH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>) δ: 145.6 (C), 144.9 (C), 142.2 (C), 132.9 (C), 131.9 (2C), 127.9 (2CH), 118.5 (2CH), 116.5 (2CH), 52.1 (CH<sub>2</sub>), 18.8 (2CH<sub>3</sub>). LC/MS *m/z* 283 [M+H]<sup>+</sup>.

#### 1-(4-nitrobenzyl)-1H-benzo[d][1,2,3]triazole (9c) [34]

Compound **9c** was obtained in 44% total yield; m.p.: 126–128 °C; TLC (petroleum ether/ethyl acetate 8/2) *R<sub>f</sub>*: 0.13; <sup>1</sup>H-NMR (200 MHz, DMSO-*d*<sub>6</sub>) δ: 8.22 (2H, d, *J* = 8.4 Hz, H-3', 5'), 8.09 (1H, d, *J* = 8.2 Hz, H-4), 7.87 (1H, d, *J* = 8.2 Hz, H-7), 7.70–7.60 (1H, m, H arom), 7.54 (2H, d, *J* = 8.4 Hz, H-2', 6'), 7.47–7.43 (1H, m, H arom), 6.19 (2H, s, CH<sub>2</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>) δ: 145.6 (C), 144.9 (C), 142.3 (C), 132.9 (C), 128.9 (2CH), 126.3 (2CH), 123.8 (2CH), 118.5 (CH), 110.5 (CH), 52.2 (CH<sub>2</sub>). LC/MS *m/z* 283 [M+H]<sup>+</sup>.

#### 5,6-difluoro-1-(4-nitrobenzyl)-1H-benzo[d][1,2,3]triazole (9d)

Compound **9d** was obtained in 73 % total yield; m.p.: 139–140 °C; TLC (petroleum ether/ethyl acetate 7/3) *R<sub>f</sub>*: 0.37; <sup>1</sup>H-NMR (200 MHz, DMSO-*d*<sub>6</sub>) δ: 8.30–8.14 (4H, m, H-4, 7, 3', 5'), 7.56 (2H, d, *J* = 8.8 Hz, H-2', 6'), 6.14 (2H, s, CH<sub>2</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>) δ: 149.5 (2C), 145.5 (C), 144.9 (C), 142.3 (C), 132.8 (C), 128.9 (2CH), 123.8 (2CH), 117.1 (2CH), 54.7 (CH<sub>2</sub>). LC/MS *m/z*: 291 [M+H]<sup>+</sup>.

#### 4-fluoro-1-(4-nitrobenzyl)-1H-benzo[d][1,2,3]triazole (9e)

Compound **9e** was obtained in 15% total yield; mp: 161–164 °C; TLC (petroleum ether/ethyl acetate 8:2): *R<sub>f</sub>*: 0.10. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ: 8.22 (2H, d, *J* = 8.8 Hz, H-3,5), 7.73 (1H, d, *J* = 8.4 Hz, H-7), 7.56 (2H, d, *J* = 8.8 Hz, H-2', 6' + 1H, H-6), 7.26 (1H, t, H-5), 6.21 (2H, s, CH<sub>2</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>): 152.3 (C), 147.3 (C), 142.9 (C), 135.8 (C), 135.2 (C), 128.9 (CH), 128.9 (2CH), 123.8 (2CH), 108.8 (CH), 107.2 (CH), 50.3 (CH<sub>2</sub>). LC/MS: *m/z* 273 [M+H]<sup>+</sup>.

#### 7-fluoro-1-(4-nitrobenzyl)-1H-benzo[d][1,2,3]triazole(10e)

Compound **10e** was obtained in 13% total yield; mp: 155–158 °C; TLC (petroleum ether/ethyl acetate 8:2) *R<sub>f</sub>*: 0.22. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ: 8.22 (2H, d, *J* = 8 Hz, H-3,5), 7.95 (1H, d, *J* = 7.2 Hz, H-4), 7.48 (2H, d, *J* = 8 Hz, H-2', 6'), 7.43–7.39 (2H, m, H-5,6), 6.20 (2H, s, CH<sub>2</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>) δ: 148.8 (C), 148.3 (C), 146.5 (C), 143.3 (C), 128.4 (2CH), 125.2 (CH), 124.0 (2CH), 122.5 (C), 115.8 (CH), 112.6 (CH), 52.0 (CH<sub>2</sub>). LC/MS: *m/z* 273 [M+H]<sup>+</sup>.

#### 4-((5,6-dichloro-2H-benzo[d][1,2,3]triazol-2-yl)methyl)aniline (11a)

Compound **11a** was obtained in 10% total yield; m.p. 247–250 °C; TLC: (petroleum ether/ethyl acetate 7/3) *R<sub>f</sub>*: 0.49; <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ: 8.03 (2H, s, H-4,7), 7.10 (2H, d, *J* = 8.2 Hz, H-2', 6'), 6.48 (2H, d, *J* = 8.4 Hz, H-3', 5'), 5.74 (2H, s, CH<sub>2</sub>), 5.26 (2H, s, NH<sub>2</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>) δ: 145.9 (2C), 145.2 (C), 133.8 (2C), 129.0 (2CH), 126.3 (2CH), 125.0 (C), 114.9 (2CH), 58.7 (CH<sub>2</sub>). LC/MS: *m/z* 293, 295 [M+H]<sup>+</sup>.

#### 4-((5,6-dimethyl-2H-benzo[d][1,2,3]triazol-2-yl)methyl)aniline (11b)

Compound **11b** was obtained in 27% total yield; m.p. 169–171°C; TLC (petroleum ether/ethyl acetate 6/4); *R<sub>f</sub>*: 0.45; <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ: 7.62 (1H, s, H-4,7), 7.07 (2H, d, *J* = 8.2 Hz, H-2', 6'), 6.50 (2H, d, *J* = 8.4 Hz, H-3', 5'), 5.63 (2H, s, CH<sub>2</sub>), 5.16 (2H, s, NH<sub>2</sub>), 2.34 (6H, s, 2CH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>) δ: 145.5 (2C), 145.4 (C), 136.8 (2C), 129.8 (2CH), 124.4 (C), 124.1 (2CH), 115.1 (2CH), 61.6 (CH<sub>2</sub>), 18.8 (2CH<sub>3</sub>). LC/MS *m/z* 253 [M+H]<sup>+</sup>.

#### **4-((5,6-difluoro-2H-benzo[d][1,2,3]triazol-2-yl)methyl)aniline (11d)**

Compound **11d** was obtained in 20% total yield; m.p.: 149–150 °C; TLC (petroleum ether/ethyl acetate 7/3);  $R_f$ : 0.34;  $^1\text{H-NMR}$  (400 MHz, DMSO- $d_6$ )  $\delta$ : 8.04 (2H, t, H-4,7), 7.11 (2H, d,  $J$  = 8.00 Hz, H-2',6'), 6.52 (2H, d,  $J$  = 8.4 Hz, H-3',5'), 5.71 (2H, s, CH<sub>2</sub>), 5.19 (2H, s, NH<sub>2</sub>).  $^{13}\text{C-NMR}$  (DMSO- $d_6$ )  $\delta$ : 149.5 (2C), 145.5 (2C), 145.4 (C), 129.8 (2CH), 124.4 (C), 117.1 (2CH), 115.1 (2CH), 61.6 (CH<sub>2</sub>). LC/MS:  $m/z$  261 [M+H]<sup>+</sup>.

#### **4-((5,6-dichloro-1H-benzo[d][1,2,3]triazol-1-yl)methyl)aniline (12a)**

Compound **12a** was obtained in 30% total yield; m.p.: 203–206 °C; TLC (petroleum ether/ethyl acetate 7/3);  $R_f$ : 0.29;  $^1\text{H-NMR}$  (400 MHz, CDCl<sub>3</sub>)  $\delta$ : 8.45 (1H, s, H-4), 8.32 (1H, s, H-7), 7.11 (2H, d,  $J$  = 8.4 Hz, H-2',6'), 6.51 (2H, d,  $J$  = 8.4 Hz, H-3',5'), 5.75 (2H, s, CH<sub>2</sub>), 5.13 (2H, s, NH<sub>2</sub>),  $^{13}\text{C-NMR}$  (DMSO- $d_6$ )  $\delta$ : 145.7 (C), 144.9 (C), 133.8 (2C), 133.0 (C), 129.5 (2CH), 126.6 (2CH), 125.9 (C), 115.4 (2CH), 52.3 (CH<sub>2</sub>). LC/MS:  $m/z$  293, 295 [M+H]<sup>+</sup>.

#### **4-((5,6-dimethyl-1H-benzo[d][1,2,3]triazol-1-yl)methyl)aniline (12b)**

Compound **12b** was obtained in 88% total yield; m.p.: 184–186 °C; TLC (petroleum ether/ethyl acetate 6/4);  $R_f$ : 0.17;  $^1\text{H-NMR}$  (200 MHz, DMSO- $d_6$ )  $\delta$ : 7.76 (1H, s, H-4), 7.57 (1H, s, H-7), 7.06 (2H, d,  $J$  = 8.6 Hz, H-2',6'), 6.48 (2H, d,  $J$  = 8.6 Hz, H-3',5'), 5.65 (2H, s, CH<sub>2</sub>), 5.13 (2H, s, NH<sub>2</sub>), 2.36 (6H, s, 2CH<sub>3</sub>).  $^{13}\text{C-NMR}$  (DMSO- $d_6$ )  $\delta$ : 149.2 (C), 145.5 (C), 132.5 (2C), 132.2 (C), 128.8 (C), 128.2 (2CH), 124.2 (2CH), 114.3 (2CH), 52.3 (CH<sub>2</sub>), 18.8 (2CH<sub>3</sub>). LC/MS  $m/z$  253 [M+H]<sup>+</sup>.

#### **4-((1H-benzo[d][1,2,3]triazol-1-yl)methyl) aniline (12c)**

Compound **12c** was obtained in 78% total yield; m.p.: 151–153 °C; TLC (petroleum ether/ethyl acetate 4/6);  $R_f$ : 0.47;  $^1\text{H-NMR}$  (400 MHz, DMSO- $d_6$ )  $\delta$ : 8.03 (1H, d,  $J$  = 8.4 Hz, H-4), 7.81 (1H, d,  $J$  = 8.4 Hz, H-7), 7.50 (1H, t, H-5), 7.41 (1H, t, H-6) 7.07 (2H, d,  $J$  = 8.2 Hz, H-3',5'), 6.49 (2H, d,  $J$  = 8.2 Hz, H-2',6'), 5.74 (2H, s, CH<sub>2</sub>), 5.15 (2H, s, NH<sub>2</sub>).  $^{13}\text{C-NMR}$  (DMSO- $d_6$ )  $\delta$ : 149.2 (C), 145.5 (C), 132.4 (C), 132.8 (C), 128.7 (2CH), 126.6 (2CH), 119.7 (CH), 114.6 (2CH), 110.3 (CH), 52.3 (CH<sub>2</sub>). LC/MS  $m/z$  225 [M+H]<sup>+</sup>.

#### **4-((5,6-difluoro-1H-benzo[d][1,2,3]Triazol-1-yl)methyl)aniline (12d)**

Compound **12d** was obtained in 70% total yield; m.p.: 116–117 °C; TLC (petroleum ether/ethyl acetate 8/2);  $R_f$ : 0.14;  $^1\text{H-NMR}$  (400 MHz, CDCl<sub>3</sub>)  $\delta$ : 8.20 (H, t, H-4), 8.07 (H, t, H-7), 7.11 (2H, d,  $J$  = 8.6 Hz, H-2', 6'), 6.51 (2H, d,  $J$  = 8.6 Hz, H-2', 5'), 5.71 (2H, s, CH<sub>2</sub>), 5.18 (2H, s, NH<sub>2</sub>).  $^{13}\text{C-NMR}$  (DMSO- $d_6$ )  $\delta$ : 149.5 (2C), 145.5 (C), 145.4 (C), 132.8 (C), 129.8 (2CH), 126.2 (C), 117.1 (2CH), 115.1 (2CH), 54.7 (CH<sub>2</sub>). LC/MS:  $m/z$  [M+H]<sup>+</sup>.

#### **4-((4-fluoro-1H-benzo[d][1,2,3]triazol-1-yl)methyl)aniline (12e)**

Compound **12e** was obtained in 43% total yield; mp 164–167 °C; TLC (dichloromethane/ethyl acetate 9.5/0.5)  $R_f$ : 0.17;  $^1\text{H NMR}$  (400 MHz, CDCl<sub>3</sub>):  $\delta$  7.65 (1H, d,  $J$  = 7.0 Hz, H-7), 7.53–7.48 (1H, m, H-6), 7.20 (1H, t, H-5), 7.09 (2H, d,  $J$  = 8.0 Hz, H-3',5'), 6.51 (2H, d,  $J$  = 8.0 Hz, H-2',6'), 5.77 (2H, s, CH<sub>2</sub>), 5.16 (2H, s, NH<sub>2</sub>).  $^{13}\text{C-NMR}$  (400 MHz, CDCl<sub>3</sub>)  $\delta$ : 152.1 (C), 148.6 (C), 135.3 (C), 135.2 (C), 129.1 (2CH), 128.3 (CH), 122.0 (C), 113.8 (2CH), 108.4 (CH), 107.4 (CH), 51.5 (CH<sub>2</sub>). LC/MS:  $m/z$  243 [M+H]<sup>+</sup>.

#### **N-(4-((4-fluoro-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)acetamide (15e)**

Compound **15e** was obtained in 11% total yield; m.p.: 233–234 °C; TLC (dichloromethane/ethyl acetate 7:3);  $R_f$ : 0.37.  $^1\text{H NMR}$  (400 MHz, DMSO- $d_6$ )  $\delta$ : 9.97 (1H, br s, NH), 7.68 (1H, d,  $J$  = 8.4 Hz, H-7), 7.54 (2H, d,  $J$  = 7.6 Hz, H-3',5' and H-6), 7.30 (2H, d,  $J$  = 7.6 Hz, H-2',6'), 7.23 (1H, t, H-5), 5.94 (2H, s, CH<sub>2</sub>), 2.01 (3H, s, CH<sub>3</sub>).  $^{13}\text{C-NMR}$  (DMSO- $d_6$ )  $\delta$ : 168.5 (C), 152.2 (C), 139.0 (C), 135.5 (C), 129.7 (C), 128.6 (2CH), 124.0 (CH), 119.2 (2CH), 110.6 (CH), 108.5 (CH), 107.3 (CH), 50.9 (CH<sub>2</sub>), 23.8 (CH<sub>3</sub>). LC/MS:  $m/z$  285 [M+H]<sup>+</sup>.

#### **N-(4-((4-fluoro-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)propionamide(16e)**

Compound **16e** was obtained, in 78% total yield; mp: 244–246 °C. TLC (petroleum ether /ethyl acetate 7:3);  $R_f$ : 0.19.  $^1\text{H NMR}$  (400 MHz, DMSO- $d_6$ )  $\delta$ : 9.89 (1H, br s), 7.91 (1H, d,  $J$  = 8.8 Hz, H-7), 7.68 (2H, d,  $J$  = 8.4 Hz, H-3',4'), 7.57–7.50 (1H, m, H-6), 7.37 (2H, d,  $J$  = 8.4Hz, H-2',6'), 7.25–7.20 (1H, m, H-5), 5.93 (2H, s, CH<sub>2</sub>), 2.29 (2H, d, CH<sub>2</sub>), 1.033 (3H, t, CH<sub>3</sub>).  $^{13}\text{C-NMR}$  (DMSO- $d_6$ )  $\delta$ : 172.0 (C), 152.2 (C), 139.3 (C), 135.5 (C), 135.3 (C), 129.6 (C), 129.1 (3CH), 119.2 (2CH), 108.5 (CH), 107.4 (CH), 51.3 (CH<sub>2</sub>), 29.4 (CH<sub>2</sub>), 9.6 (CH<sub>3</sub>). LC/MS:  $m/z$  299 [M+H]<sup>+</sup>.

#### **N-(4-((4-fluoro-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)butyramide (17e)**

Compound **17e** was obtained, in 40% total yield; mp: 215–216 °C; TLC (petroleum ether /ethyl acetate 7:3);  $R_f$ : 0.16.  $^1\text{H NMR}$  (400 MHz, DMSO- $d_6$ )  $\delta$ : 9.91 (1H, br s, NH), 7.66 (1H, d,  $J$  = 8.4 Hz, H-5), 7.56–7.49 (3H, m, H-3',5' and 7'), 7.30 (2H, d,  $J$  = 8.4 Hz, H- 2',6'), 7.22 (1H, dd,  $J$  = 3.2 e  $J$  = 7.6 Hz, H-6), 5.92 (2H, s, CH<sub>2</sub>), 2.24 (2H, t, CH<sub>2</sub>), 1.57 (2H, d, CH<sub>2</sub>), 0.87 (3H, t, CH<sub>3</sub>).  $^{13}\text{C-NMR}$  (DMSO- $d_6$ )  $\delta$ : 171.5 (C), 152.1 (C), 139.1 (C), 139.0 (C), 135.4 (C), 129.7 (C), 128.6 (CH), 128.5 (2CH), 119.3 (2CH), 108.6 (CH), 107.3 (CH), 51.0 (CH<sub>2</sub>), 18.5 (CH<sub>2</sub>), 13.5 (CH<sub>3</sub>). LC/MS:  $m/z$  313 [M+H]<sup>+</sup>.

#### **N-(4-((4-fluoro-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)benzamide (19e)**

Compound **19e** was obtained, in 89% total yield; mp: 214–217 °C; TLC (dichloromethane/ethyl acetate 9:1);  $R_f$ : 0.59.  $^1\text{H NMR}$  (400 MHz, DMSO- $d_6$ )  $\delta$ : 10.29 (1H, br s, NH), 7.96 (2H, d,  $J$  = 7.2 Hz, H-2",6"), 7.77 (2H, d,  $J$  = 8 Hz, H-3',5'), 7.71 (1H, d,  $J$  = 8.4 Hz, H-7), 7.58–7.50 (4H, m, H-3",4",5",6), 7.37 (2H, d,  $J$  = 8 Hz, H-2',6'), 7.23 (1H, t, H-5), 5.98

(2H, s, CH<sub>2</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>) δ: 166.0 (C), 152.7 (C), 139.6 (C), 136.0 (C), 135.8 (C), 135.2 (C), 132.1 (CH), 130.9 (C), 129.0 (CH), 128.9 (3CH), 128.1 (2CH), 121.0 (2CH), 109.1 (CH), 108.9 (CH), 17.8 (CH), 51.5 (CH<sub>2</sub>). LC/MS *m/z* 347 [M+H]<sup>+</sup>.

***N*-(4-((4-fluoro-1*H*-benzo[*d*][1,2,3]triazol-1-yl)methyl)phenyl)-4-methoxybenzamide (20e)**

Compound 20e was obtained, in 94% total yield; mp: 266–268 °C; TLC (petroleum ether/ethyl acetate 6:4): R<sub>f</sub>: 0.29. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ: 10.13 (1H, br s, NH), 7.93 (2H, d, *J* = 8.8 Hz, H-2'',6''), 7.75 (2H, d, *J* = 8 Hz, H-3',5'), 7.71 (1H, d, *J* = 8.4 Hz, H-7), 7.57–7.53 (1H, m, H-6), 7.36 (2H, d, *J* = 8.4 Hz, H-2'',6''), 7.23 (1H, t, H-5), 7.05 (2H, d, *J* = 8.8 Hz, H-3'',5''), 5.97 (2H, s, CH<sub>2</sub>), 3.83 (3H, s, OCH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>) δ: 164.9 (C), 161.9 (C), 152.2 (C), 139.3 (C), 135.6 (C), 135.2 (C), 130.1 (C), 129.6 (2CH), 128.5 (CH), 128.3 (2CH), 126.7 (C), 120.5 (2CH), 113.6 (2CH), 108.5 (CH), 107.4 (CH), 55.4 (CH<sub>3</sub>), 51.1 (CH<sub>2</sub>). LC/MS *m/z* 377 [M+H]<sup>+</sup>.

***N*-(4-((4-fluoro-1*H*-benzo[*d*][1,2,3]triazol-1-yl)methyl)phenyl)-3,4,5-trimethoxybenzamide (21e)**

Compound 21e was obtained, in 94% total yield; mp: 177–179 °C; TLC (dichloromethane/ethyl acetate 9:1): R<sub>f</sub>: 0.22. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ: 10.16 (1H, br s, NH), 7.73–7.70 (3H, d, *J* = 8.8 Hz, H-7-2'',6''), 7.57–7.52 (1H, m, H-6), 7.36 (2H, d, *J* = 8.4 Hz, H-3',5'), 7.25–7.21 (3H, m, H-5, 2',6'), 5.99 (2H, s, CH<sub>2</sub>), 3.86 (6H, s, 3,5-OCH<sub>3</sub>), 3.73 (3H, s, OCH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>) δ: 164.9 (C), 152.6 (C), 152.2 (C), 140.3 (C), 139.0 (C), 135.4 (C), 135.4 (C), 135.2 (C), 130.5 (C), 129.8 (C), 128.6 (CH), 128.5 (2CH), 120.8 (2CH), 108.6 (CH), 107.3 (CH), 105.3 (2CH), 60.1 (CH<sub>3</sub>), 56.1 (2CH<sub>3</sub>), 51.0 (CH<sub>2</sub>). LC/MS *m/z* 437 [M+H]<sup>+</sup>.

***N*-(4-((4-fluoro-1*H*-benzo[*d*][1,2,3]triazol-1-yl)methyl)phenyl)-4-nitrobenzamide (22e)**

Compound 22e was obtained, in 91% total yield; mp: 272–274 °C; TLC (dichloromethane/ethyl acetate 9:1): R<sub>f</sub>: 0.33. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ: 10.61 (1H, br s, NH), 8.36 (2H, d, *J* = 8.8 Hz, H-2'',6''), 8.16 (2H, d, *J* = 8.8 Hz, H-3'',5''), 7.76 (2H, d, *J* = 8.4 Hz, H-3',5'), 7.71 (1H, d, *J* = 8.4 Hz, H-7), 7.57–7.52 (1H, m, H-6), 7.39 (2H, d, *J* = 8.4 Hz, H-2',6'), 7.24 (1H, t, H-5), 6.00 (2H, s, CH<sub>2</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>) δ: 163.9 (C), 152.2 (C), 149.2 (C), 140.4 (C), 138.6 (C), 135.5 (C), 135.2 (C), 131.0 (C), 129.2 (3CH), 128.5 (2CH), 123.5 (2CH), 120.7 (2CH), 108.6 (CH), 107.4 (CH), 51.0 (CH<sub>2</sub>). LC/MS *m/z* 392 [M+H]<sup>+</sup>.

***N*-(3-((5,6-dimethyl-2*H*-benzo[*d*][1,2,3]triazol-2-yl)methyl)phenyl)acetamide (23b)**

Compound 23b was obtained, in 43% total yield; mp: 184–187 °C; TLC (petroleum ether /ethyl acetate 6:4): R<sub>f</sub>: 0.13. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ: 9.94 (1H, s, NH), 7.65 (2H, s, H-4,7), 7.55 (1H, d, *J* = 8Hz, H-4'), 7.49 (1H, s, H-2'), 7.27 (1H, t, *J* = 7.8 Hz, H-5'), 7.02 (1H, d, *J* = 7.6 Hz, H-6'), 5.85 (2H, s, CH<sub>2</sub>), 2.35 (6H, s, 2CH<sub>3</sub>), 1.99 (3H, s, CO-CH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>) δ: 168.3 (CO), 145.5 (2C), 138.4 (C), 136.8 (2C), 136.4 (C), 128.8 (CH), 122.6 (CH), 118.6 (CH), 118.2 (CH), 116.2 (2CH), 59.2 (CH<sub>2</sub>), 23.9 (CO-CH<sub>3</sub>), 20.3 (2CH<sub>3</sub>). LC/MS *m/z* 295 [M+H]<sup>+</sup>, 317 [M+Na]<sup>+</sup>.

***N*-(3-((5,6-dimethyl-2*H*-benzo[*d*][1,2,3]triazol-2-yl)methyl)phenyl)propionamide (24b)**

Compound 24b was obtained, in 80% total yield; mp: 178–182 °C; TLC (petroleum ether /ethyl acetate 6:4): R<sub>f</sub>: 0.40. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ: 9.94 (1H, s, NH), 7.84 (2H, s, H-4,7), 7.65 (1H, d, *J* = 7.5 Hz, H-2'',6''), 7.55 (1H, s, H-2'), 7.30 (1H, t, *J* = 7.30 Hz, H-5'), 7.02 (1H, d, *J* = 7.0 Hz, H-4'), 6.85 (2H, d, *J* = 6.80 Hz, H-3'',5''), 6.57 (1H, d *J* = 6.6 Hz, H-6'), 5.86 (2H, s, CH<sub>2</sub>), 2.34 (6H, s, 2CH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>) δ: 165.2 (CO), 154.9 (C), 140.2 (C), 137.3 (C), 136.3 (C), 133.4 (C), 131.7 (C), 128.8 (CH), 128.8 (2CH), 124.4 (C), 123.5 (CH), 119.8 (CH), 119.3 (CH), 118.1 (CH), 112.5 (CH), 111.2 (CH), 109.7 (CH), 50.9 (CH<sub>2</sub>), 20.4 (CH<sub>3</sub>), 19.8 (CH<sub>3</sub>). LC/MS *m/z* 309 [M+H]<sup>+</sup>, 332 [M+Na]<sup>+</sup>.

***N*-(3-((5,6-dimethyl-2*H*-benzo[*d*][1,2,3]triazol-2-yl)methyl)phenyl)-4-fluorobenzamide (25b)**

Compound 25b was obtained, in 27% total yield; mp: 211–212 °C; TLC (petroleum ether/ethyl acetate = 7/3) R<sub>f</sub>: 0.10. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ: 10.16 (1H, s, NH), 8.23 (1H, s, H-2'), 7.99 (1H, t, *J* = 8 Hz, H-5'), 7.65(2H, s, H-4,7), 7.55 (2H, d, *J* = 7.5 Hz, H-2'',6''), 7.32 (3H, m, H-4', 3'', 5''), 7.05 (1H, d, *J* = 7.6 Hz, H-6'), 5.86 (2H, s, CH<sub>2</sub>), 2.35 (6H, s, 2CH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>) δ: 166.2 (CO), 143.3 (2C), 138.5 (C), 136.5 (3C), 136.3 (C), 132.1 (CH), 132.0 (CH), 129.4 (CH), 123.3 (CH), 119.5 (CH), 118.8 (CH), 116.2 (2CH), 115.7 (CH), 115.5 (CH), 59.0 (CH<sub>2</sub>), 20.30 (CH<sub>3</sub>). LC/MS 300 *m/z* 375 [M+H]<sup>+</sup>, 397 [M+Na]<sup>+</sup>.

***N*-(3-((5,6-dimethyl-2*H*-benzo[*d*][1,2,3]triazol-2-yl)methyl)phenyl)-4-chlorobenzamide (26b)**

Compound 26b was obtained, in 56% total yield; mp: 246–247 °C; TLC (petroleum ether/ethyl acetate = 7/3) R<sub>f</sub>: 0.50. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ: 10.33 (1H, s, NH), 7.95 (2H, d, *J* = 7.95 Hz, H-2'',6''), 7.75 (2H, m, H-2',4'), 7.66 (2H, s, H-4,7), 7.59 (2H, d, *J* = 7.6 Hz, H-3'',5''), 7.35 (1H, t, *J* = 7.35 Hz, H-5'), 7.12 (1H, d, *J* = 7.1, H-6'), 5.89 (2H, s, CH<sub>2</sub>), 2.36 (6H, s, 2CH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>) δ: 164.4 (CO), 143.3 (C), 139.3 (C), 137.7 (2C), 136.5 (C), 136.1 (C), 131.0 (2CH), 129.6 (2C), 129.6 (CH), 129.2 (2CH), 123.4 (CH), 119.9 (CH), 118.6 (CH), 116.2 (2CH), 59.1 (CH<sub>2</sub>), 20.3 (2CH<sub>3</sub>). LC/MS 300 *m/z* 391 [M+H]<sup>+</sup>, 413 [M+Na]<sup>+</sup>.

***N*-(3-((5,6-dimethyl-2*H*-benzo[*d*][1,2,3]triazol-2-yl)methyl)phenyl)-4-bromobenzamide (27b)**

Compound 27b was obtained, in 17% total yield; mp: 267–268 °C; TLC (petroleum ether/ethyl acetate = 7/3) R<sub>f</sub>: 0.85. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ: 10.34 (1H, s, NH), 7.87 (2H, s, H-4,7), 7.74 (4H, s, H-2'',3'',5'',6''), 7.66 (2H, s,

H-2',4'), 7.35 (1H, s, H-5'), 7.13 (1H, s, H-6'), 5.89 (2H, s, CH<sub>2</sub>), 2.35 (6H, s, CH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-d<sub>6</sub>) δ: 164.5 (CO), 143.3 (C), 139.3 (C), 136.8 (2C), 136.4 (C), 136.1 (C), 133.8 (C), 131.3 (2CH), 129.8 (2CH), 128.9 (CH), 125.4 (C), 123.6 (CH), 120.1 (CH), 119.7 (CH), 116.2 (CH), 59.2 (CH<sub>2</sub>), 20.3 (2CH<sub>3</sub>). LC/MS 300 m/z 436 [M+H]<sup>+</sup>, 458 [M+Na]<sup>+</sup>.

#### *N*-(3-((5,6-dimethyl-2H-benzo[d][1,2,3]triazol-2-yl)methyl)phenyl)-4-trifluoromethyl benzamide (28b)

Compound **28b** was obtained, in 18% total yield; mp: 237–239 °C; TLC (petroleum ether/ethyl acetate = 6/4) R<sub>f</sub>: 0.64. <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) δ: 10.49 (1H, s, NH), 8.11 (2H, d, J = 8.1 Hz, H-2'',6''), 7.89 (2H, d, J = 7.95 Hz, H-3'',5''), 7.79–7.74 (3H, m, H-2',4'), 7.66 (2H, s, H-4,7), 7.37 (1H, t, J = 7.3 Hz, H-5'), 7.14 (1H, d, J = 7.1 Hz, H-6'), 5.90 (2H, s, CH<sub>2</sub>), 2.35 (6H, s, 2CH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-d<sub>6</sub>) δ: 164.4 (CO), 143.3 (2C), 139.1 (2C), 138.6 (C), 136.6 (2C), 136.1 (C), 131.5 (CF<sub>3</sub>), 129.0 (CH), 128.6 (2CH), 125.3 (2CH), 123.7 (CH), 122.5 (CH), 120.2 (CH), 116.2 (2CH), 59.2 (CH<sub>2</sub>), 20.3 (CH<sub>3</sub>). LC/MS m/z 425 [M+H]<sup>+</sup>.

#### *N*-(3-((5,6-dimethyl-2H-benzo[d][1,2,3]triazol-2-yl)methyl)phenyl)-4-nitrobenzamide (29b)

Compound **29b** was obtained, in 43% total yield; mp: 184–187 °C; TLC (petroleum ether/ethyl acetate = 6/4) R<sub>f</sub>: 0.13. <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) δ: 10.59 (1H, s, NH), 8.35 (2H, d, J = 8.4 Hz, H-2'',6''), 8.15 (2H, d, J = 8.4 Hz, H-3'',5''), 7.77 (1H, d, J = 7.6 Hz, H-4'), 7.73 (1H, s, H-2'), 7.66 (2H, s, H-4,7), 7.38 (1H, t, J = 7.8 Hz, H-5'), 5.91 (2H, s, CH<sub>2</sub>), 2.36 (6H, s, 2CH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-d<sub>6</sub>) δ: 163.9 (CO), 149.1 (C), 143.3 (C), 140.4 (C), 139.0 (C), 136.6 (3C), 136.2 (C), 129.2 (2CH), 129.0 (CH), 123.9 (CH), 123.5 (2CH), 120.2 (CH), 119.8 (CH), 116.2 (2CH), 59.1 (CH<sub>3</sub>), 20.3 (CH<sub>3</sub>). LC/MS m/z 402 [M+H]<sup>+</sup>, 424 [M+Na]<sup>+</sup>.

#### *1*-(3-((5,6-dimethyl-2H-benzo[d][1,2,3]triazol-2-yl)methyl)phenyl)-3-ethylurea (30b)

Compound **30b** was obtained, in 32% total yield; mp: 218–219 °C; TLC (petroleum ether/ethyl acetate = 6/4) R<sub>f</sub>: 0.15. <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) δ: 8.45 (1H, s, NH), 7.65 (2H, s, H-4,7), 7.34 (1H, d, J = 8.4 Hz, H-4'), 7.32 (1H, s, H-2'), 7.18 (1H, t, H-5'), 6.86 (1H, d, J = 7.2 Hz, H-6'), 6.02 (1H, t, NH), 5.81 (2H, s, CH<sub>2</sub>), 3.07 (2H, q, CH<sub>2</sub>), 2.35 (6H, s, 2CH<sub>3</sub>), 1.02 (3H, t, CH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-d<sub>6</sub>) δ: 154.9 (CO), 143.3 (C), 140.9 (C), 136.5 (2C), 136.0 (2C), 128.9 (CH), 120.5 (CH), 117.2 (CH), 116.8 (CH), 116.2 (2CH), 59.3 (CH<sub>2</sub>), 33.9 (CH<sub>2</sub>), 20.3 (2CH<sub>3</sub>), 15.4 (CH<sub>3</sub>). LC/MS m/z: 324 [M+H]<sup>+</sup>.

#### *1*-(3-((5,6-dimethyl-2H-benzo[d][1,2,3]triazol-2-yl)methyl)phenyl)-3-propylurea (31b)

Compound **31b** was obtained, in 48% total yield; mp: 204–206 °C; TLC (petroleum ether/ethyl acetate = 6/4) R<sub>f</sub>: 0.21. <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) δ: 8.44 (1H, s, NH), 7.65 (2H, s, H-4,7), 7.34 (1H, d, J = 8.0 Hz, H-4'), 7.31 (1H, s, H-2'), 7.18 (1H, t, H-5'), 6.86 (1H, d, J = 7.6 Hz, H-6'), 6.06 (1H, t, NH), 5.81 (2H, s, CH<sub>2</sub>), 3.07 (2H, q, CH<sub>2</sub>-NH), 2.35 (6H, s, 2CH<sub>3</sub>), 1.41–1.35 (2H, m, CH<sub>2</sub>), 0.87–0.82 (3H, m, CH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-d<sub>6</sub>) δ: 155.0 (CO), 143.3 (C), 140.9 (C), 136.5 (2C), 136.0 (2C), 128.9 (CH), 120.5 (CH), 117.5 (CH), 117.2 (CH), 116.2 (2CH), 59.3 (CH<sub>2</sub>), 40.8 (CH<sub>2</sub>), 22.9 (CH<sub>2</sub>), 20.3 (2CH<sub>3</sub>), 11.3 (CH<sub>3</sub>). LC/MS m/z: 338 [M+H]<sup>+</sup>.

#### *1-butyl-3-(3-((5,6-dimethyl-2H-benzo[d][1,2,3]triazol-2-yl)methyl)phenyl)urea (32b)*

Compound **32b** was obtained, in 10% total yield; mp: 288–289 °C; TLC (petroleum ether/ethyl acetate = 6/4) R<sub>f</sub>: 0.35. <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) δ: 8.65 (1H, s, NH), 7.66 (2H, s, H-4,7), 7.37 (1H, s, H-2'), 7.38 (1H, d, J = 8 Hz H-4'), 7.20 (1H, t, H-5'), 6.94 (1H, d, J = 7.6 Hz H-6'), 6.04 (1H, t, NH), 5.81 (2H, s, CH<sub>2</sub>), 3.04 (2H, q, CH<sub>2</sub>), 1.38–1.27 (6H, m, 2CH<sub>2</sub>), 0.87 (3H, t, CH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-d<sub>6</sub>) δ: 155.0 (CO), 143.3 (C), 140.9 (C), 139.9 (C), 136.5 (C), 136.2 (2C), 129.1 (CH), 121.5 (CH), 117.8 (CH), 117.5 (CH), 116.2 (2CH), 59.2 (2CH<sub>2</sub>), 31.8 (CH<sub>2</sub>), 20.3 (3CH<sub>3</sub>), 19.5 (CH<sub>2</sub>). LC/MS m/z: 352 [M+H]<sup>+</sup>.

#### *1-cyclopentyl-3-(3-((5,6-dimethyl-2H-benzo[d][1,2,3]triazol-2-yl)methyl)phenyl)urea (33b)*

Compound **33b** was obtained, in 33% total yield; mp: 298–299 °C; TLC (petroleum ether/ethyl acetate = 6/4) R<sub>f</sub>: 0.46. <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) δ: 8.28 (1H, s, NH), 7.65 (2H, s, H-4,7), 7.38 (1H, d, J = 7.6 Hz, H-4'), 7.19 (1H, t, H-5'), 7.03 (1H, s, H-2'), 6.86 (1H, d, J = 6.8 Hz, H-6'), 6.08 (1H, d, J = 6.0 Hz, NH), 5.81 (2H, s, CH<sub>2</sub>), 3.89 (1H, s, CH), 2.36 (6H, s, 2CH<sub>3</sub>), 1.88–1.75 (2H, m, CH<sub>2</sub>), 1.65–1.45 (4H, m, 2CH<sub>2</sub>), 1.35–1.25 (2H, m, CH<sub>2</sub>). <sup>13</sup>C-NMR (DMSO-d<sub>6</sub>) δ: 155.1 (CO), 143.7 (C), 141.3 (C), 140.3 (C), 137.0 (2C), 136.5 (C), 129.6 (CH), 129.4 (CH), 121.0 (CH), 117.6 (CH), 117.2 (CH), 116.7 (2CH), 59.7 (CH<sub>2</sub>), 33.2 (2CH<sub>2</sub>), 23.6 (2CH<sub>2</sub>), 20.8 (2CH<sub>3</sub>). LC/MS m/z: 364 [M+H]<sup>+</sup>.

#### *1-cyclohexyl-3-(3-((5,6-dimethyl-2H-benzo[d][1,2,3]triazol-2-yl)methyl)phenyl)urea (34b)*

Compound **34b** was obtained, in 73% total yield; mp: 299–300 °C; TLC (petroleum ether/ethyl acetate = 6/4) R<sub>f</sub>: 0.26. <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) δ: 8.33 (1H, s, NH), 7.65 (2H, s, H-4,7), 7.32 (2H, d, J = 8.4 Hz, H-2,4'), 7.29 (1H, s, H-2'), 7.19 (1H, t, H-5'), 6.86 (1H, d, J = 7.2 Hz, H-6'), 5.99 (1H, d, J = 7.6 Hz, NH-CH), 5.81 (1H, s, CH<sub>2</sub>), 2.36 (6H, s, 2CH<sub>3</sub>), 1.80–1.46 (4H, m, 2CH<sub>2</sub>), 1.35–1.05 (6H, m, 3CH<sub>2</sub>). <sup>13</sup>C-NMR (DMSO-d<sub>6</sub>) δ: 154.2 (CO), 143.2 (C), 140.8 (C), 136.5 (2C), 136.0 (2C), 128.9 (CH), 120.5 (CH), 117.9 (CH), 117.2 (CH), 116.7 (CH), 116.2 (2CH), 59.3 (CH<sub>2</sub>), 47.5 (CH), 33.3 (CH<sub>2</sub>), 25.2 (2CH<sub>2</sub>), 24.3 (2CH<sub>2</sub>), 20.3 (2CH<sub>3</sub>). LC/MS m/z: 378 [M+H]<sup>+</sup>.

#### *N*-(3-((5,6-dichloro-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)acetamide (35a)

Compound **35** was obtained, in 42% total yield; mp: 196–196 °C; TLC (petroleum ether /ethyl acetate 7:3):  $R_f$ : 0.09.  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 9.93 (1H, s, NH), 8.49 (1H, s, H-4), 8.35 (1H, s, H-7), 7.55 (1H, d,  $J$  = 8.0 Hz, H-4'), 7.46 (1H, s, H-2'), 7.28 (1H, t,  $J$  = 7.8 Hz, H-5'), 7.05 (1H, d,  $J$  = 7.6 Hz, H-6'), 5.97 (2H, s, CH<sub>2</sub>), 1.99 (3H, s, CH<sub>3</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ ): 168.3 (CO), 144.2 (C), 139.7 (C), 135.9 (CH), 132.1 (C), 130.8 (C), 129.2 (CH), 127.2 (C), 122.3 (CH), 120.6 (CH), 118.7 (C), 117.8 (CH), 112.5 (CH), 51.1 (CH<sub>2</sub>), 23.9 (2CH<sub>3</sub>). LC/MS  $m/z$  335, 337 [M+H]<sup>+</sup>.

**N-(3-((5,6-dichloro-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)propionamide (36a)**

Compound **36** was obtained, in 51% total yield; mp: 145–146 °C; TLC (petroleum ether /ethyl acetate 7:3):  $R_f$ : 0.21.  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 9.86 (1H, s, NH), 8.49 (1H, s, H-2'), 8.35 (1H, s, H-4), 7.57 (1H, t,  $J$  = 8 Hz, H-4'), 7.49 (1H, s, H-7), 7.28 (1H, t,  $J$  = 7.8 Hz, H-5'), 7.05 (1H, d,  $J$  = 7.2 Hz, H-6'), 5.96 (2H, s, CH<sub>2</sub>), 2.29–2.24 (2H, m, CH<sub>2</sub>–CH<sub>3</sub>), 1.04 (3H, t,  $J$  = 7.4 Hz, CH<sub>3</sub>–CH<sub>2</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ ): 172.0 (CO), 144.2 (C), 139.8 (C), 135.9 (CH), 132.1 (C), 130.8 (C), 129.1 (CH), 127.2 (C), 122.2 (CH), 120.6 (CH), 118.7 (C), 117.9 (CH), 112.5 (CH), 51.1 (CH<sub>2</sub>), 29.4 (CH<sub>2</sub>), 9.5 (CH<sub>3</sub>). LC/MS  $m/z$  349, 351 [M+H]<sup>+</sup>.

**N-(3-((5,6-dimethyl-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)acetamide (37b)**

Compound **37b** was obtained, in 66% total yield; mp: 198–200 °C; TLC (petroleum ether /ethyl acetate 6:4):  $R_f$ : 0.10.  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 9.91 (1H, s, NH), 7.80 (1H, s, H-4), 7.53 (3H, m, H-2,2',4'), 7.40 (1H, s, H-7), 7.26 (1H, t,  $J$  = 8 Hz, H-5'), 6.98 (1H, d,  $J$  = 7.6 Hz, H-6'), 5.84 (2H, s, CH<sub>2</sub>), 2.35 (6H, s, 2CH<sub>3</sub>), 1.98 (3H, s, CH<sub>3</sub>CO).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ ): 168.3 (CO), 144.5 (C), 139.7 (C), 137.3 (C), 136.6 (C), 133.5 (C), 131.7 (C), 129.0 (CH), 122.1 (CH), 118.5 (CH), 118.1 (CH), 117.7 (CH), 109.7 (CH), 50.7 (CH<sub>2</sub>), 23.9 (CH<sub>3</sub>), 20.1 (2CH<sub>3</sub>). LC/MS  $m/z$  295 [M+H]<sup>+</sup>, 317 [M+Na]<sup>+</sup>.

**N-(3-((5,6-dimethyl-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)propionamide (38b)**

Compound **38b** was obtained, in 25% total yield; mp: 155–157 °C; TLC (petroleum ether /ethyl acetate 6:4):  $R_f$ : 0.25.  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 9.8 (1H, s, NH), 7.79 (1H, s, H-4), 7.55 (2H, m, H-4',2'), 7.44 (1H, s, H-7), 7.27 (1H, t,  $J$  = 7.8 Hz, H-5'), 6.98 (1H, d,  $J$  = 7.6 Hz, H-6'), 5.86 (2H, s, CH<sub>2</sub>), 2.35 (6H, s, 2CH<sub>3</sub>), 2.26 (2H, q,  $J$  = 7.4 Hz, CH<sub>2</sub>–CH<sub>3</sub>), 1.02 (3H, J = 7.8 Hz, CH<sub>3</sub>–CH<sub>2</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ ): 172.0 (CO), 144.6 (C), 139.7 (C), 137.3 (C), 136.5 (C), 133.4 (C), 131.7 (C), 129.0 (CH), 122.5 (CH), 118.5 (CH), 118.1 (CH), 118.0 (CH), 117.7 (CH), 50.8 (CH<sub>2</sub>), 29.4 (CH<sub>2</sub>), 20.4 (CH<sub>3</sub>), 20.6 (CH<sub>3</sub>), 10.8 (CH<sub>3</sub>–CH<sub>2</sub>). LC/MS  $m/z$  309 [M+H]<sup>+</sup>, 331 [M+Na]<sup>+</sup>.

**N-(3-((5,6-dichloro-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-4-methylbenzamide (39a)**

Compound **39a** was obtained, in 41% total yield; mp: 199–200 °C; TLC (petroleum ether/ethyl acetate = 7/3)  $R_f$ : 0.50.  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 10.17 (1H, s, NH), 8.51 (1H, s, H-4), 8.39 (1H, s, H-7), 7.83 (2H, d,  $J$  = 7.6 Hz, H-2'',6''), 7.75 (1H, d,  $J$  = 8 Hz, H-4'), 7.71 (1H, s, H-2'), 7.36 (1H, t,  $J$  = 8 Hz, H-5'), 7.32 (2H, d,  $J$  = 8 Hz, H-3'',5''), 7.13 (1H, d,  $J$  = 7.6 Hz, H-6'), 6.00 (2H, s, CH<sub>2</sub>), 2.38 (3H, s, CH<sub>3</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ ): 165.4 (CO), 144.3 (C), 141.6 (C), 139.7 (C), 135.8 (CH), 132.1 (C), 131.8 (C), 130.8 (C), 129.1 (CH), 128.8 (2CH), 127.7 (2CH), 127.2 (C), 122.9 (C), 120.6 (CH), 120.1 (CH), 119.3 (CH), 112.5 (CH), 51.2 (CH<sub>2</sub>), 21.0 (CH<sub>3</sub>). LC/MS  $m/z$  410 [M+H]<sup>+</sup>, 423 [M+Na]<sup>+</sup>.

**N-(3-((5,6-dichloro-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-4-methoxybenzamide (40a)**

Compound **40a** was obtained, in 21% total yield; mp: 221–223 °C; TLC (petroleum ether/ethyl acetate = 7/3)  $R_f$ : 0.25.  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 10.10 (1H, s, NH), 8.52 (1H, s, H-4), 8.39 (1H, s, H-7), 7.92 (2H, d,  $J$  = 8.4 Hz, H-2'',6''), 7.74 (1H, d,  $J$  = 8.4 Hz, H-4'), 7.71 (1H, s, H-2'), 7.35 (1H, t,  $J$  = 8.0 Hz, H-5'), 7.12 (1H, d,  $J$  = 7.2 Hz, H-6'), 7.06 (2H, d,  $J$  = 8.4 Hz, H-3'',-5''), 6.00 (2H, s, CH<sub>2</sub>), 3.83 (3H, s, OCH<sub>3</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ ): 164.9 (CO), 161.9 (C), 144.3 (C), 139.8 (C), 135.8 (CH), 132.1 (C), 130.8 (C), 129.6 (2CH), 129.0 (CH), 127.2 (C), 126.7 (C), 122.8 (C), 120.6 (CH), 120.1 (CH), 119.3 (CH), 113.5 (2CH), 112.5 (CH), 55.4 (CH<sub>3</sub>), 51.2 (CH<sub>2</sub>). LC/MS  $m/z$  426, [M+H]<sup>+</sup>.

**N-(3-((5,6-dichloro-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-3,4,5-trimethoxybenzamide (41a)**

Compound **41a** was obtained, in 22% total yield; mp: 142–144 °C; TLC (petroleum ether/ethyl acetate = 7/3)  $R_f$ : 0.15.  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 10.15 (1H, s, NH), 8.52 (1H, s, H-4), 8.39 (1H, s, H-7), 7.70 (2H, s, H-2',4'), 7.37 (1H, t,  $J$  = 8 Hz, H-5'), 7.23 (2H, s, H-2'',6''), 7.15 (1H, d,  $J$  = 7.2 Hz, H-6'), 6.00 (2H, s, CH<sub>2</sub>), 3.86 (6H, s, 2OCH<sub>3</sub>), 3.73 (3H, s, OCH<sub>3</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ ): 165.0 (CO), 152.6 (2CH), 144.3 (C), 140.3 (C), 139.5 (C), 135.8 (C), 132.0 (C), 130.8 (C), 129.8 (C), 129.1 (CH), 127.3 (C), 123.2 (C), 120.6 (CH), 120.4 (C), 119.7 (CH), 112.5 (CH), 105.3 (2CH), 60.1 (OCH<sub>3</sub>), 56.1 (2OCH<sub>3</sub>), 51.2 (CH<sub>2</sub>). LC/MS  $m/z$  487, 489 [M+H]<sup>+</sup>.

**N-(3-((5,6-dichloro-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-4-fluorobenzamide (42a)**

Compound **42a** was obtained, in 94% total yield; mp: 184–186 °C; TLC (petroleum ether/ethyl acetate = 7/3)  $R_f$ : 0.35.  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 10.28 (1H, s, NH), 8.52 (1H, s, H-4), 8.39 (1H, s, H-7), 7.99 (2H, d,  $J$  = 8 Hz, H-2'',6''), 7.74 (1H, d,  $J$  = 8.4 Hz, H-4'), 7.69 (1H, s, H-2'), 7.38–7.33 (3H, m, H-3'',5'',5'), 7.15 (1H, d,  $J$  = 7.6 Hz, H-6'), 6.00 (2H, s, CH<sub>2</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ ): 164.5 (CO), 164.1 (C), 144.3 (C), 139.5 (C), 135.9 (C), 132.1 (C), 131.2 (C), 130.8 (C), 130.4 (CH), 130.3 (CH), 129.1 (CH), 127.2 (C), 123.1 (CH), 120.6 (CH), 120.1 (CH), 119.3 (CH), 115.4 (CH), 115.2 (CH), 112.5 (CH), 51.2 (CH<sub>2</sub>). LC/MS  $m/z$  415, 417 [M+H]<sup>+</sup>.

**N-(3-((5,6-dichloro-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-4-bromobenzamide (44a)**

Compound **44a** was obtained, in 23% total yield; mp: 221–223 °C; TLC (petroleum ether/ethyl acetate = 7/3)  $R_f$ : 0.46.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 10.32 (1H, s, NH), 8.51 (1H, s, H-4), 8.39 (1H, s, H-7), 7.87 (2H, d,  $J$  = 8.4 Hz, H-2'',6''), 7.8–7.0 (3H, m, H-4',3'',5''), 7.72 (1H, s, H-2'), 7.37 (1H, t,  $J$  = 8 Hz, H-5'), 7.16 (1H, d,  $J$  = 7.6 Hz, H-6'), 6.00 (2H, s, CH<sub>2</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ ): 164.6 (CO), 144.3 (C), 139.4 (C), 135.9 (CH), 133.8 (C), 132.1 (C), 131.4 (2CH), 130.8 (C), 129.8 (2CH), 129.1 (CH), 127.2 (C), 125.4 (C), 123.2 (C), 120.6 (CH), 120.1 (CH), 119.3 (CH), 112.5 (CH), 51.1 (CH<sub>2</sub>). LC/MS  $m/z$  477, 475 [M+H]<sup>+</sup>.

#### *4-cyano-N-(3-((5,6-dichloro-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)benzamide (45a)*

Compound **45a** was obtained, in 24% total yield; mp: 167–169 °C; TLC (petroleum ether/ethyl acetate = 7/3)  $R_f$ : 0.37.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 10.48 (1H, s, NH), 8.51 (1H, s, H-4), 8.39 (1H, s, H-7), 8.06 (2H, d,  $J$  = 8 Hz, H-2'',6''), 8.0 (2H, d,  $J$  = 8.4 Hz, H-3'',5''), 7.75 (1H, d,  $J$  = 8.0 Hz, H-4'), 7.69 (1H, s, H-2'), 7.38 (1H, t,  $J$  = 7.8 Hz, H-5'), 7.18 (1H, d,  $J$  = 7.6 Hz, H-6'), 6.02 (2H, s, CH<sub>2</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ )  $\delta$ : 164.2 (CO), 144.3 (C), 139.2 (C), 138.7 (C), 136.0 (C), 132.4 (2CH), 132.1 (C), 130.8 (C), 129.2 (CH), 128.5 (2CH), 127.2 (C), 123.5 (CH), 120.6 (CH), 120.2 (CH), 119.3 (CH), 118.3 (C≡N), 113.9 (C), 112.5 (CH), 51.1 (CH<sub>2</sub>). LC/MS  $m/z$  422, 424 [M+H]<sup>+</sup>.

#### *N-(3-((5,6-dichloro-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-4-(trifluoromethyl)benzamide (46a)*

Compound **46a** was obtained, in 44% total yield; mp: 211–213 °C; TLC (petroleum ether/ethyl acetate = 7/3)  $R_f$ : 0.67.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 10.47 (1H, s, NH), 8.52 (1H, s, H-4), 8.39 (1H, s, H-7), 8.11 (2H, d,  $J$  = 7.6 Hz, H-2'',6''), 7.90 (2H, d,  $J$  = 8 Hz, H-3'',5''), 7.76 (1H, d,  $J$  = 8 Hz, H-4'), 7.69 (1H, d, H-2'), 7.39 (1H, t,  $J$  = 7.8 Hz, H-5'), 7.17 (1H, d,  $J$  = 6.8 Hz, H-6'), 6.02 (2H, s, CH<sub>2</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ )  $\delta$ : 164.7 (CO), 145.7 (C), 139.1 (C), 137.8 (C), 137.5 (C), 135.9 (C), 133.2 (C), 131.4 (2C), 130.4 (CH), 130.5 (CH), 127.9 (CH), 127.2 (C), 123.8 (CH), 120.6 (CH), 120.3 (CH), 119.3 (CH), 115.4 (CH), 115.2 (CH), 113.0 (CH), 51.2 (CH<sub>2</sub>). LC/MS  $m/z$  465, 467 [M+H]<sup>+</sup>.

#### *N-(3-((5,6-dichloro-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-4-nitrobenzamide (47a)*

Compound **47a** was obtained, in 14% total yield; mp: 217–218 °C; TLC (petroleum ether/ethyl acetate = 7/3)  $R_f$ : 0.29.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 10.57 (1H, s, NH), 8.52 (1H, s, H-4), 8.40 (1H, s, H-7), 8.35 (2H, d,  $J$  = 8.8 Hz, H-3'',5''), 8.14 (1H, d,  $J$  = 8.4 Hz, H-2'',6''), 7.77 (1H, s, H-4'), 7.69 (1H, s, H-2'), 7.40 (1H, t,  $J$  = 7.8 Hz, H-5'), 7.19 (1H, d,  $J$  = 7.6 Hz, H-6'), 6.02 (2H, s, CH<sub>2</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ )  $\delta$ : 164.0 (CO), 149.2 (C), 144.3 (C), 140.4 (C), 139.2 (C), 136.0 (C), 132.1 (C), 130.8 (C), 129.2 (CH), 129.2 (2CH), 127.3 (C), 123.9 (CH), 123.5 (2CH), 120.7 (CH), 120.2 (CH), 119.4 (CH), 112.5 (CH), 51.1 (CH<sub>2</sub>). LC/MS  $m/z$  442, 444 [M+H]<sup>+</sup>.

#### *4-amino-N-(3-((5,6-dichloro-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)benzamide (48a)*

This compound was obtained starting from compound **47a** (7.43 mmol) in 50 ml of ethanol and 0.88 mL of methylhydrazine. It was heated in autoclave for 24 h at 100 °C. In the end, the mother was evaporated in vacuo and the crude residue is triturated with petrol ether to obtain compound **48**. The crude product was not further purified.

Compound **48a** was obtained, in 66% total yield; mp: 101–102 °C; TLC (petroleum ether/ethyl acetate = 6/4)  $R_f$ : 0.18.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 9.77 (1H, s, NH), 8.50 (1H, s, H-4), 8.37 (1H, s, H-7), 7.73–7.66 (4H, m, H-6',2',2'',6''), 7.31 (1H, t,  $J$  = 7.8 Hz, H-5'), 7.06 (1H, d,  $J$  = 7.2 Hz, H-4'), 6.58 (2H, d,  $J$  = 8 Hz, H-3'',5''), 5.98 (2H, s, CH<sub>2</sub>), 5.76 (2H, s, NH<sub>2</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ )  $\delta$ : 165.3 (CO), 152.2 (C), 144.3 (C), 140.2 (C), 135.7 (C), 132.1 (C), 130.7 (C), 129.3 (2CH), 128.9 (CH), 127.2 (C), 122.3 (CH), 120.8 (C), 120.6 (CH), 119.8 (CH), 119.1 (CH), 112.5 (CH), 112.5 (2CH), 51.3 (CH<sub>2</sub>). LC/MS  $m/z$  412, 414 [M+H]<sup>+</sup>.

#### *N-(3-((5,6-dimethyl-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-4-methylbenzamide (49b)*

Compound **49b** was obtained, in 57% total yield; mp: 211–212 °C; TLC (petroleum ether/ethyl acetate = 7/3)  $R_f$ : 0.27.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 10.16 (1H, s, NH), 7.82 (3H, m, H-2'',6'',4), 7.3 (2H, d,  $J$  = 8.4 Hz, H-4'), 7.7 (1H, s, H-7), 7.58 (1H, s, H-2'), 7.32 (3H, m, H-3'',5'',5'), 7.05 (1H,  $J$  = 7.2 Hz, 6'), 5.89 (2H, s, CH<sub>2</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ )  $\delta$ : 165.3 (CO), 144.6 (C), 141.6 (C), 139.6 (C), 137.3 (C), 136.5 (C), 133.5 (C), 131.7 (C), 131.7 (C), 128.9 (CH), 127.7 (CH), 122.7 (CH), 119.9 (CH), 119.2 (CH), 118.1 (CH), 109.7 (CH), 50.8 (CH<sub>2</sub>), 21.0 (CH<sub>3</sub>), 20.4 (CH<sub>3</sub>), 19.8 (CH<sub>3</sub>). LC/MS  $m/z$  371 [M+H]<sup>+</sup>.

#### *N-(3-((5,6-dimethyl-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-4-methoxylbenzamide (50b)*

Compound **50b** was obtained, in 17% total yield; mp: 203–206 °C; TLC (petroleum ether/ethyl acetate = 6/4)  $R_f$ : 0.36.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 10.09 (1H, s, NH), 7.91 (2H, d,  $J$  = 7.9 Hz, H-2'',6''), 7.80 (1H, s, H-4'), 7.72 (1H, d,  $J$  = 7.7 Hz, H-4'), 7.68 (1H, s, H-2'), 7.59 (1H, s, H-7), 7.32 (1H, t,  $J$  = 7.3 Hz, H-5'), 7.04 (3H, m, H-6',3'',5''), 5.89 (2H, s, CH<sub>2</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ )  $\delta$ : 164.9 (CO), 161.9 (C), 144.6 (C), 139.7 (C), 137.3 (C), 136.4 (C), 133.5 (C), 131.7 (C), 129.6 (CH), 129.3 (CH), 128.9 (CH), 126.7 (C), 122.6 (CH), 119.9 (CH), 119.2 (CH), 118.1 (CH), 113.7 (CH), 113.5 (CH), 109.7 (CH), 55.4 (OCH<sub>3</sub>), 50.8 (CH<sub>2</sub>), 20.1 (2CH<sub>3</sub>). LC/MS  $m/z$  387 [M+H]<sup>+</sup>, 409 [M+Na]<sup>+</sup>.

#### *N-(3-((5,6-dimethyl-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-3,4,5-trimethoxylbenzamide (51b)*

Compound **51b** was obtained, in 20% total yield; mp: 160–162 °C; TLC (petroleum ether/ethyl acetate = 6/4)  $R_f$ : 0.21.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 10.13 (NH), 7.80 (1H, s, H-4), 7.67 (2H, m, H-4',2'), 7.59 (1H, s, H-7), 7.35 (3H,

$t, J = 8.0$  Hz, H-5'), 7.24 (2H, s, H-2'',6''), 7.08 (1H, d,  $J = 7.2$ , H-6') 5.9 (2H, s, CH<sub>2</sub>) 3.85 (6H, s, 2OCH<sub>3</sub>), 3.72 (3H, s, OCH<sub>3</sub>), 2.35 (6H, s, 2CH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>)  $\delta$ : 165.3 (CO), 152.7 (C), 152.6 (C), 144.6 (C), 140.4 (C), 139.4 (C), 137.4 (C), 136.5 (C), 133.5 (C), 131.7 (C), 129.8 (C), 129.0 (CH), 127.6 (CH), 123.0 (CH), 120.2 (CH), 119.5 (CH), 118.1 (CH), 109.7 (CH), 105.3 (CH), 105.0 (CH), 60.1 (OCH<sub>3</sub>), 56.1 (OCH<sub>3</sub>), 56.0 (OCH<sub>3</sub>), 50.8 (CH<sub>2</sub>), 20.1 (CH<sub>3</sub>). LC/MS *m/z* 447 [M+H]<sup>+</sup>, 469 [M+Na]<sup>+</sup>.

#### *N*-(3-((5,6-dimethyl-1*H*-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-4-fluorobenzamide (52b)

Compound **52b** was obtained, in 98% total yield; mp: 143–147 °C; TLC (petroleum ether/ethyl acetate = 7/3) *R*<sub>f</sub> 0.22. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 10.26 (1H, s, NH), 7.99 (2H, t, H-3'',5''), 7.72 (1H, d,  $J = 7.72$  Hz, H-4'), 7.66 (1H, s, H-7), 7.58 (1H, s, H-2'), 7.34 (3H, m, H-2'',6''), 7.08 (1H, d,  $J = 7.08$ , H-6'), 5.90 (2H, s, 2CH<sub>2</sub>), 2.35 (6H, s, 2CH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>)  $\delta$ : 164.1 (CO), 144.6 (C), 139.5 (C), 137.4 (C), 136.5 (C), 133.5 (C), 131.7 (C), 131.2 (C), 130.4 (2CH), 129.0 (CH), 122.9 (CH), 119.9 (CH), 119.2 (CH), 118.1 (CH), 115.2 (CH), 109.7 (CH), 50.8 (CH<sub>2</sub>), 20.4 (CH<sub>3</sub>), 19.8 (CH<sub>3</sub>). LC/MS *m/z* 375 [M+H]<sup>+</sup>.

#### *N*-(3-((5,6-dimethyl-1*H*-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-4-chlorobenzamide (53b)

Compound **53b** was obtained, in 56% total yield; mp: 227–229 °C; TLC (petroleum ether/ethyl acetate = 7/3) *R*<sub>f</sub> 0.30. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 10.65 (1H, s, NH), 7.94 (2H, d,  $J = 8$  Hz, H-3'',5''), 7.80 (1H, s, H-2'), 7.730 (1H, d,  $J = 8$  Hz, H-4'), 7.59 (2H, d,  $J = 7.2$  Hz, H-3'',5''), 7.08 (1H, d,  $J = 7.6$  Hz, H-6'), 5.90 (2H, s, CH<sub>2</sub>), 2.36 (6H, s, 2CH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>)  $\delta$ : 169.9 (CO), 149.8 (C), 144.6 (C), 142.6 (C), 141.8 (C), 141.7 (C), 138.7 (C), 138.7 (C), 137.0 (C), 134.8 (2CH), 134.3 (CH), 133.6 (2CH), 128.3 (CH), 125.2 (CH), 124.5 (CH), 123.4 (CH), 115.0 (CH), 56.0 (CH<sub>2</sub>), 25.6 (CH<sub>3</sub>), 25.1 (CH<sub>3</sub>). LC/MS *m/z* 391 [M+H]<sup>+</sup>, 413 [M+Na]<sup>+</sup>.

#### *N*-(3-((5,6-dimethyl-1*H*-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-4-bromobenzamide (54b)

Compound **54b** was obtained, in 15% total yield; mp: 237–238 °C; TLC (petroleum ether/ethyl acetate = 7/3) *R*<sub>f</sub> 0.25. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 7.78 (2H, d,  $J = 8.4$  Hz, H-3'',5''), 7.80 (1H, s, H-4), 7.72 (3H, m, H-4',2'',6''), 7.65 (1H, s, H-2'), 7.59 (1H, s, H-7), 7.34 (1H, t,  $J = 7.6$  Hz, H-5'), 7.08 (2H, d,  $J = 7.6$  Hz, H-6'), 5.9 (2H, s, 2CH<sub>2</sub>), 2.35 (6H, s, 2CH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>)  $\delta$ : 164.5 (CO), 144.6 (C), 139.4 (C), 137.4 (C), 136.6 (CH), 133.8 (C), 133.5 (C), 131.7 (C), 131.3 (2CH), 129.8 (2CH), 129.0 (CH), 125.4 (C), 123.0 (C), 119.9 (CH), 118.1 (CH), 109.7 (CH), 50.8 (CH<sub>2</sub>), 20.1 (CH<sub>3</sub>). LC/MS *m/z* 436 [M+H]<sup>+</sup>.

#### *4-cyano-N*-(3-((5,6-dimethyl-1*H*-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)benzamide (55b)

Compound **55b** was obtained, in 26% total yield; mp: 242–247 °C; TLC (petroleum ether/ethyl acetate = 6/4) *R*<sub>f</sub> 0.3. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 7.85 (2H, d,  $J = 7.9$  Hz, H-2'',6''), 7.86 (2H, d,  $J = 7.76$ , H-3'',5''), 7.28 (1H, s, H-2'), 7.62 (1H, d,  $J = 7.6$  Hz, H-4'), 7.52 (1H, s, H-4), 7.38 (1H, s, H-7), 7.27 (1H, t,  $J = 7.3$  Hz, H-5'), 7.00 (1H, d,  $J = 7.03$  Hz, H-6'), 5.71 (2H, s, CH<sub>2</sub>), 2.35 (6H, s, 2CH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>)  $\delta$ : 164.2 (CO), 144.6 (C), 139.1 (C), 138.8 (C), 136.8 (C), 136.6 (C), 133.5 (C), 132.4 (2CH), 131.7 (C), 129.3 (CH), 128.5 (CH), 132.3 (CH), 120.0 (CH), 119.3 (CH), 118.2 (CN), 118.1 (CH), 113.8 (C), 109.7 (CH), 50.6 (CH<sub>2</sub>), 20.4 (CH<sub>3</sub>), 19.8 (CH<sub>3</sub>). LC/MS *m/z* 382 [M+H]<sup>+</sup>.

#### *N*-(3-((5,6-dimethyl-1*H*-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-4-(trifluoromethyl)benzamide (56b)

Compound **56b** was obtained, in 20% total yield; mp: 201–203 °C; TLC (petroleum ether/ethyl acetate = 6/4) *R*<sub>f</sub> 0.84. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 10.47 (1H, s, NH), 8.10 (2H, d,  $J = 8$  Hz, H-2'',6''), 7.89 (2H, d,  $J = 8.4$  Hz, H-3'',5''), 7.80 (1H, s, H-4), 7.74 (1H, d,  $J = 8$  Hz, H-6'), 7.66 (1H, s, H-2'), 7.59 (1H, s, H-7), 7.36 (1H, t,  $J = 8.0$  Hz, H-5'), 7.12 (1H, d,  $J = 7.1$  Hz, H-4'), 5.91 (2H, s, CH<sub>2</sub>), 2.36 (6H, s, 2CH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>)  $\delta$ : 164.4 (CO), 145.5 (C), 137.5 (C), 136.8 (2C), 136.4 (C), 135.8 (C), 134.4 (C), 132.8 (C), 128.8 (CH), 127.8 (2CH), 125.2 (2CH), 124.1 (2CH), 123.2 (CH), 121.3 (CH), 118.6 (CH), 50.7 (CH<sub>2</sub>), 20.4 (CH<sub>3</sub>), 19.8 (CH<sub>3</sub>). LC/MS *m/z* 425 [M+H]<sup>+</sup>.

#### *N*-(3-((5,6-dimethyl-1*H*-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-4-nitrobenzamide (57b)

Compound **57b** was obtained, in 31% total yield; mp: 227–230 °C; TLC (petroleum ether/ethyl acetate = 4/6) *R*<sub>f</sub> 0.76. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 10.57 (1H, s, NH), 8.34 (2H, d,  $J = 8.2$  Hz, 3'',5''), 8.12 (2H, d,  $J = 8.2$  Hz, H-2'',6''), 7.80 (1H, s, H-2'), 7.75 (1H, d,  $J = 9.2$  Hz, H-4'), 7.64 (1H, s, H-4), 7.59 (1H, s, H-7), 7.36 (1H, t,  $J = 8$  Hz, H-5'), 7.12 (1H, d,  $J = 7.6$  Hz, H-6'), 5.92 (2H, s, CH<sub>2</sub>), 2.35 (2CH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>)  $\delta$ : 163.9 (CO), 149.1 (C), 144.6 (C), 140.4 (C), 139.1 (C), 137.4 (C), 136.7 (C), 133.5 (C), 131.7 (C), 129.2 (2CH), 129.1 (CH), 123.5 (CH), 123.3 (CH), 122.7 (CH), 120.0 (CH), 119.3 (CH), 118.1 (CH), 109.7 (CH), 50.7 (CH<sub>2</sub>), 20.1 (2CH<sub>3</sub>). LC/MS *m/z* 402 [M+H]<sup>+</sup>.

#### *1*-(3-((5,6-dichloro-1*H*-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-3-ethylurea (58a)

Compound **58a** was obtained, in 44% total yield; mp: 244–245 °C; TLC (petroleum ether/ethyl acetate = 6/4) *R*<sub>f</sub> 0.15. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>)  $\delta$ : 8.49 (1H, s, H-4), 8.44 (1H, s, NH), 8.37 (1H, s, H-7), 7.33 (1H, d,  $J = 8.4$  Hz, H-4'), 7.31 (1H, s, H-2'), 7.19 (1H, t, H-5'), 6.88 (1H, d,  $J = 7.6$  Hz, H-6'), 6.03 (1H, t, NH), 5.92 (2H, s, CH<sub>2</sub>), 3.07 (2H, q, CH<sub>2</sub>), 1.02 (3H, t, CH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>)  $\delta$ : 154.9 (CO), 144.2 (C), 141.1 (C), 135.8 (C), 132.0 (C), 130.7 (C), 129.1 (CH), 127.2 (C), 120.6 (CH), 120.2 (CH), 117.3 (CH), 116.5 (CH), 112.5 (CH), 51.3 (CH<sub>2</sub>), 34.0 (CH<sub>2</sub>), 15.4 (CH<sub>3</sub>). LC/MS *m/z* 364 [M+H]<sup>+</sup>.

**1-(3-((5,6-dichloro-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-3-propylurea (59a)**

Compound **59a** was obtained, in 45% total yield; mp: >300 °C; TLC (petroleum ether/ethyl acetate = 6/4)  $R_f$ : 0.38.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 8.50 (1H, s, H-4), 8.43 (1H, s, NH), 8.37 (1H, s, H-7), 7.33 (1H, d,  $J$  = 8.0 Hz, H-4'), 7.32 (1H, s, H-2'), 7.20 (1H, t, H-5'), 6.88 (1H, d,  $J$  = 7.6 Hz, H-6'), 6.07 (1H, t, NH), 5.92 (2H, s, CH<sub>2</sub>), 3.00 (2H, q, CH<sub>2</sub>), 1.43-1.38 (2H, m, CH<sub>2</sub>), 0.85 (3H, t, CH<sub>3</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ )  $\delta$ : 155.0 (CO), 144.2 (C), 141.1 (C), 135.8 (C), 132.1 (C), 130.7 (C), 129.1 (CH), 127.2 (C), 121.2 (CH), 120.6 (CH), 117.3 (CH), 116.5 (CH), 112.5 (CH), 51.3 (CH<sub>2</sub>), 40.8 (CH<sub>2</sub>), 22.9 (CH<sub>2</sub>), 11.3 (CH<sub>3</sub>). LC/MS  $m/z$ : 378 [M+H]<sup>+</sup>.

**1-butyl-3-(3-((5,6-dichloro-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)urea (60a)**

Compound **60a** was obtained, in 19% total yield; mp: 232-233 °C; TLC (petroleum ether/ethyl acetate = 6/4)  $R_f$ : 0.41.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 8.49 (1H, s, H-4), 8.42 (1H, s, NH), 8.35 (1H, s, H-7), 7.33 (1H, d,  $J$  = 8.0 Hz, H-4'), 7.30 (1H, s, H-2'), 7.19 (1H, t, H-5'), 6.88 (1H, d,  $J$  = 7.6 Hz, H-6'), 6.05 (1H, t, NH), 5.92 (2H, s, CH<sub>2</sub>), 3.04 (2H, q, CH<sub>2</sub>-CH<sub>3</sub>), 1.41-1.31 (2H, m, CH<sub>2</sub>), 1.31-1.27 (2H, m, CH<sub>2</sub>), 0.87 (3H, t, CH<sub>3</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ )  $\delta$ : 155.5 (CO), 144.7 (C), 141.5 (C), 136.3 (C), 132.5 (C), 131.2 (C), 129.6 (CH), 127.7 (C), 121.1 (CH), 120.7 (CH), 117.7 (CH), 116.9 (CH), 113.0 (CH), 51.7 (CH<sub>2</sub>), 32.3 (CH<sub>2</sub>), 19.9 (CH<sub>2</sub>), 14.1 (CH<sub>3</sub>). LC/MS  $m/z$ : 392, 394 [M+H]<sup>+</sup>.

**1-cyclopentyl-3-(3-((5,6-dichloro-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)urea (61a)**

Compound **61a** was obtained, in 10% total yield; mp: 231-232 °C; TLC (petroleum ether/ethyl acetate = 6/4)  $R_f$ : 0.36.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 8.49 (1H, s, H-4), 8.34 (1H, s, NH), 8.28 (1H, s, H-7), 7.28 (1H, s, H-2'), 7.31 (1H, d,  $J$  = 8.0 Hz, H-4'), 7.19 (1H, t, H-5'), 6.87 (1H, d,  $J$  = 7.6 Hz, H-6'), 6.08 (1H, d,  $J$  = 6.8 Hz, NH), 5.92 (2H, s, CH<sub>2</sub>), 1.83-1.78 (1H, m, CH), 1.61-1.59 (2H, m, CH<sub>2</sub>), 1.53-1.50 (2H, m, CH<sub>2</sub>), 1.34-1.30 (4H, m, 2CH<sub>2</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ )  $\delta$ : 154.6 (CO), 144.2 (C), 141.0 (C), 135.8 (C), 132.0 (C), 130.7 (C), 129.2 (CH), 127.2 (C), 120.6 (CH), 120.2 (CH), 117.2 (CH), 116.4 (CH), 112.5 (CH), 51.3 (CH<sub>2</sub>), 50.8 (CH), 32.7 (2CH<sub>2</sub>), 23.1 (2CH<sub>2</sub>). LC/MS  $m/z$ : 404 [M+H]<sup>+</sup>.

**1-cyclohexyl-3-(3-((5,6-dichloro-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)urea (62a)**

Compound **62a** was obtained, in 10% total yield; mp: 200-201 °C; TLC (petroleum ether/ethyl acetate = 6/4)  $R_f$ : 0.18.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 10.17 (1H, s, NH), 8.49 (1H, s, H-4), 8.37 (1H, s, H-7), 7.52 (1H, s, H-2'), 7.37-7.27 (2H, m, H-4',5'), 7.06 (1H, d,  $J$  = 6.8 Hz, H-6'), 6.08-5.87 (1H, m, NH-CH), 5.56 (2H, d,  $J$  = 5.2 Hz, CH<sub>2</sub>), 1.73-1.42 (4H, m, 2CH<sub>2</sub>), 1.23-1.03 (6H, m, 3CH<sub>2</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ )  $\delta$ : 156.6 (CO), 144.2 (C), 138.6 (C), 136.2 (C), 132.1 (C), 130.8 (C), 129.4 (CH), 129.2 (C), 122.9 (CH), 120.6 (CH), 118.9 (CH), 118.1 (CH), 112.5 (CH), 51.0 (CH<sub>2</sub>), 47.5 (CH-N), 33.3 (3CH<sub>2</sub>), 24.4 (2CH<sub>2</sub>). LC/MS  $m/z$ : 404 [M+H]<sup>+</sup>.

**1-(3-((5,6-dimethyl-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-3-ethylurea (63b)**

Compound **63b** was obtained, in 79% total yield; mp: 271-273 °C; TLC (petroleum ether/ethyl acetate = 6/4)  $R_f$ : 0.07.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 8.45 (1H, s, NH), 7.79 (1H, s, H-4), 7.55 (1H, s, H-7), 7.33 (1H, d,  $J$  = 9.2 Hz, H-6'), 7.23 (1H, s, H-2'), 7.17 (1H, t, H-5'), 6.81 (1H, d,  $J$  = 7.6 Hz, H-4'), 6.03 (1H, t, NH), 5.82 (2H, s, CH<sub>2</sub>), 3.12-3.00 (2H, m, CH<sub>2</sub>), 2.35 (6H, s, 2CH<sub>3</sub>), 1.01 (3H, t, CH<sub>3</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ )  $\delta$ : 155.0 (CO), 144.5 (C), 140.9 (C), 137.4 (C), 136.4 (C), 133.5 (C), 131.7 (C), 129.0 (CH), 120.0 (CH), 118.1 (CH), 117.1 (CH), 116.4 (CH), 109.7 (CH), 50.9 (CH<sub>2</sub>), 33.9 (CH<sub>2</sub>), 20.4 (CH<sub>3</sub>), 19.8 (CH<sub>3</sub>), 15.4 (CH<sub>3</sub>). LC/MS  $m/z$ : 324 [M+H]<sup>+</sup>.

**1-(3-((5,6-dimethyl-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-3-propylurea (64b)**

Compound **64b** was obtained, in 31% total yield; mp: 189-191 °C; TLC (petroleum ether/ethyl acetate = 6/4)  $R_f$ : 0.14.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 8.42 (1H, s, NH), 7.79 (1H, s, H-4), 7.55 (1H, s, H-7), 7.33 (1H, d,  $J$  = 8.8 Hz, H-6'), 7.22 (1H, s, H-2'), 7.17 (1H, t, H-5'), 6.81 (1H, d,  $J$  = 7.6 Hz, H-4'), 6.06 (1H, t, NH), 5.82 (2H, s, CH<sub>2</sub>), 3.05-2.95 (2H, m, CH<sub>2</sub>), 2.35 (6H, s, 2CH<sub>3</sub>), 1.40 (2H, q, CH<sub>2</sub>-NH), 0.84 (3H, t, CH<sub>3</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ )  $\delta$ : 155.0 (CO), 144.5 (C), 141.0 (C), 137.4 (C), 136.5 (C), 133.5 (C), 131.7 (C), 129.2 (CH), 120.0 (CH), 118.1 (CH), 117.1 (CH), 116.3 (CH), 109.7 (CH), 50.8 (CH<sub>2</sub>), 40.8 (CH<sub>2</sub>), 22.9 (CH<sub>2</sub>), 20.4 (CH<sub>3</sub>), 19.8 (CH<sub>3</sub>), 11.3 (CH<sub>3</sub>). LC/MS  $m/z$ : 338 [M+H]<sup>+</sup>.

**1-(sec-butyl)-3-(3-((5,6-dimethyl-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)urea (65b)**

Compound **65b** was obtained, in 31% total yield; mp: 202-204 °C; TLC (petroleum ether/ethyl acetate = 6/4)  $R_f$ : 0.22.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 8.31 (1H, s, NH), 7.79 (1H, s, H-4), 7.55 (1H, s, H-7), 7.31 (1H, d,  $J$  = 7.6 Hz, H-6'), 7.22 (1H, s, H-2'), 7.17 (1H, t, H-5'), 6.81 (1H, d,  $J$  = 7.6 Hz, H-4'), 5.86 (1H, q, NH), 5.82 (2H, s, CH<sub>2</sub>), 2.35 (6H, s, 2CH<sub>3</sub>), 1.45-1.38 (1H, m, CH), 1.02 (3H, t, CH<sub>3</sub>), 0.83 (2H, t, CH<sub>2</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ )  $\delta$ : 154.5 (CO), 144.5 (C), 140.9 (C), 137.4 (C), 136.5 (C), 133.5 (C), 131.7 (C), 129.0 (CH), 120.0 (CH), 118.1 (CH), 117.0 (CH), 116.2 (CH), 109.7 (CH), 50.8 (CH<sub>2</sub>), 46.0 (CH), 29.2 (CH<sub>2</sub>), 20.6 (CH<sub>3</sub>), 20.4 (CH<sub>3</sub>), 19.8 (CH<sub>3</sub>), 10.2 (CH<sub>3</sub>). LC/MS  $m/z$ : 352 [M+H]<sup>+</sup>.

**1-butyl-3-(3-((5,6-dimethyl-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)urea (66b)**

Compound **66b** was obtained, in 37% total yield; mp: 195-197 °C; TLC (petroleum ether/ethyl acetate = 6/4)  $R_f$ : 0.18.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 8.40 (1H, s, NH), 7.79 (1H, s, H-4), 7.55 (1H, s, H-7), 7.33 (1H, d,  $J$  = 8.0 Hz, H-6'), 7.22 (1H, s, H-2'), 7.17 (1H, t, H-5'), 6.81 (1H, d,  $J$  = 7.6 Hz, H-4'), 6.03 (1H, t, NH), 5.82 (2H, s, CH<sub>2</sub>), 3.04 (2H, q, CH<sub>2</sub>), 2.35 (6H, s, 2CH<sub>3</sub>), 1.45-1.39 (2H, m, CH<sub>2</sub>), 1.39-1.20 (2H, m, CH<sub>2</sub>), 0.87 (3H, t, CH<sub>3</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ )  $\delta$ :

160.2 (CO), 149.8 (C), 146.2 (C), 142.6 (C), 141.7 (C), 138.7 (C), 137.0 (C), 134.3 (CH), 125.2 (CH), 123.3 (CH), 122.3 (CH), 121.5 (CH), 115.0 (CH), 56.1 (CH<sub>2</sub>), 43.9 (CH<sub>2</sub>), 37.0 (CH<sub>3</sub>), 25.6 (CH<sub>3</sub>), 25.1 (CH<sub>3</sub>), 24.7 (CH<sub>2</sub>), 18.9 (CH<sub>3</sub>). LC/MS *m/z*: 352 [M+H]<sup>+</sup>.

#### **1-(*tert*-butyl)-3-(3-((5,6-dimethyl-1*H*-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)urea (67b)**

Compound **67b** was obtained, in 22% total yield; mp: 189–191 °C; TLC (petroleum ether/ethyl acetate = 6/4) *R<sub>f</sub>*: 0.33. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ: 8.24 (1H, s, NH), 7.79 (1H, s, H-4), 7.56 (1H, s, H-7), 7.26 (1H, d, *J* = 8.4 Hz, H-6'), 7.23 (1H, s, H-2'), 7.16 (1H, t, H-5'), 6.78 (1H, d, *J* = 7.6 Hz, H-4'), 5.91 (1H, s, NH), 5.82 (2H, s, CH<sub>2</sub>), 2.35 (6H, s, CH<sub>3</sub>), 1.26 (9H, s, CH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>) δ: 159.4 (CO), 149.8 (C), 146.2 (C), 142.6 (C), 141.7 (C), 138.7 (C), 137.0 (C), 134.3 (C), 125.1 (CH), 123.3 (CH), 122.1 (CH), 121.4 (CH), 115.0 (CH), 56.1 (C), 54.6 (CH<sub>2</sub>), 34.2 (3CH<sub>3</sub>), 25.6 (CH<sub>3</sub>), 25.1 (CH<sub>3</sub>). LC/MS *m/z*: 352 [M+H]<sup>+</sup>.

#### **1-cyclopentyl-3-(3-((5,6-dimethyl-1*H*-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)urea (68b)**

Compound **68b** was obtained, in 33% total yield; mp: 290–292 °C; TLC (petroleum ether/ethyl acetate = 6/4) *R<sub>f</sub>*: 0.21. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ: 8.25 (1H, s, NH), 7.79 (1H, s, H-4), 7.55 (1H, s, H-7), 7.31 (1H, d, *J* = 8.4 Hz, H-6'), 7.20 (1H, s, H-2'), 7.17 (1H, t, H-5'), 6.81 (1H, d, *J* = 7.6 Hz, H-4'), 6.06 (1H, d, NH), 3.95–3.8 (1H, m, CH), 2.35 (6H, s, CH<sub>3</sub>), 1.89–1.72 (2H, m, CH<sub>2</sub>), 1.68–1.48 (4H, m, 2CH<sub>2</sub>), 1.33 (2H, t, CH<sub>2</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>) δ: 154.6 (CO), 144.5 (C), 140.9 (C), 137.3 (C), 136.5 (C), 133.4 (C), 131.7 (C), 129.0 (CH), 120.0 (CH), 118.1 (CH), 117.0 (CH), 116.2 (CH), 109.7 (CH), 50.8 (CH), 50.8 (CH<sub>2</sub>), 32.8 (2CH<sub>2</sub>), 23.1 (2CH<sub>2</sub>), 20.4 (CH<sub>3</sub>), 19.8 (CH<sub>3</sub>). LC/MS *m/z*: 364 [M+H]<sup>+</sup>.

#### **1-cyclohexyl-3-(3-((5,6-dimethyl-1*H*-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)urea (69b)**

Compound **69b** was obtained, in 25% total yield; mp: 233–235 °C; TLC (petroleum ether/ethyl acetate = 6/4) *R<sub>f</sub>*: 0.26. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ: 8.30 (1H, s, NH), 7.79 (1H, s, H-4), 7.55 (1H, s, H-7), 7.31 (1H, d, *J* = 8.8 Hz, H-6'), 7.22–7.11 (2H, m, H-5'/H-2'), 6.81 (1H, d, *J* = 7.6 Hz, H-4'), 5.98 (1H, d, *J* = 7.6 Hz, NH), 5.82 (2H, s, CH<sub>2</sub>), 3.54 (1H, m, CH), 2.35 (6H, s, 2CH<sub>3</sub>), 1.8–1.48 (4H, m, 2CH<sub>2</sub>), 1.35–1.05 (6H, m, 3CH<sub>2</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>) δ: 154.2 (CO), 144.5 (C), 140.9 (C), 137.3 (C), 136.5 (C), 133.5 (C), 131.7 (C), 129.0 (CH), 120.0 (CH), 118.1 (CH), 117.0 (CH), 116.2 (CH), 109.7 (CH), 50.8 (CH<sub>2</sub>), 47.5 (CH), 32.8 (CH<sub>2</sub>), 25.2 (2CH<sub>2</sub>), 24.2 (2CH<sub>2</sub>), 20.4 (CH<sub>3</sub>), 19.8 (CH<sub>3</sub>). LC/MS *m/z*: 378 [M+H]<sup>+</sup>.

#### **1-(3-((5,6-dimethyl-1*H*-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-3-(4-methoxyphenyl)urea (70b)**

Compound **70b** was obtained, in 29% total yield; mp: 233–235 °C; TLC (petroleum ether/ethyl acetate = 6/4) *R<sub>f</sub>*: 0.15. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ: 8.65 (1H, s, NH), 8.43 (1H, d, NH), 7.85 (1H, s, H-4), 7.64 (1H, s, H-7), 7.44 (1H, d, *J* = 8.00 Hz, H-6'), 7.40–7.32 (3H, m, H-2', H-2'', H-6''), 7.29 (1H, t, H-5'), 6.98–6.85 (3H, m, H-4', H-3'', H-5''), 5.92 (1H, s, CH<sub>2</sub>), 3.76 (3H, s, OCH<sub>3</sub>), 2.41 (6H, s, 2CH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>) δ: 154.5 (CO), 152.5 (C), 144.5 (C), 140.3 (C), 137.3 (C), 136.7 (C), 133.5 (C), 132.5 (C), 131.8 (C), 129.2 (CH), 120.7 (CH), 120.0 (2CH), 118.1 (CH), 117.5 (CH), 116.8 (CH), 113.9 (2CH), 109.7 (CH), 55.1 (OCH<sub>3</sub>), 50.8 (CH<sub>2</sub>), 20.4 (CH<sub>3</sub>), 19.8 (CH<sub>3</sub>). LC/MS *m/z*: 402 [M+H]<sup>+</sup>.

#### **1-(3-((5,6-dimethyl-1*H*-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-3-(3,4,5-trimethoxyphenyl)urea (71b)**

Compound **71b** was obtained, in 43% total yield; mp: 206–208 °C; TLC (petroleum ether/ethyl acetate = 6/4) *R<sub>f</sub>*: 0.05. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ: 8.64 (1H, s, NH), 8.53 (1H, s, NH), 7.80 (1H, s, H-4), 7.60 (1H, s, H-7), 7.30–7.40 (2H, m, H-2', H-6'), 7.24 (1H, t, H-5'), 6.88 (1H, d, *J* = 7.2 Hz, H-4'), 6.77 (2H, s, H-2'', H-6''), 5.87 (2H, s, CH<sub>2</sub>), 3.74 (6H, s, CH<sub>3</sub>), 3.60 (3H, s, CH<sub>3</sub>), 2.35 (6H, s, 2CH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>) δ: 152.8 (CO), 152.4 (C), 144.5 (C), 150.0 (C), 139.9 (C), 137.4 (C), 136.7 (C), 133.6 (C), 135.7 (C), 135.6 (C), 133.5 (C), 132.5 (C), 131.7 (C), 129.2 (CH), 120.9 (CH), 118.1 (CH), 117.8 (CH), 117.1 (CH), 109.8 (CH), 96.0 (CH), 60.1 (OCH<sub>3</sub>), 55.7 (2OCH<sub>3</sub>), 50.8 (CH<sub>2</sub>), 20.4 (CH<sub>3</sub>), 19.8 (CH<sub>3</sub>). LC/MS *m/z*: 462 [M+H]<sup>+</sup>.

#### **1-(3-((5,6-dimethyl-1*H*-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-3-(4-fluorophenyl)urea (72b)**

Compound **72b** was obtained, in 38% total yield; mp: 245–247 °C; TLC (petroleum ether/ethyl acetate = 6/4) *R<sub>f</sub>*: 0.18. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ: 8.68 (1H, s, NH), 8.60 (1H, s, NH), 7.80 (1H, s, H-4), 7.58 (1H, s, H-7), 7.48–7.34 (3H, d, H-6', H-2'', H-6''), 7.30 (1H, s, H-2'), 7.25 (1H, t, H-5'), 7.10 (2H, t, H-3'', H-5''), 6.90 (1H, d, *J* = 7.6 Hz, H-4'), 5.87 (1H, s, CH<sub>2</sub>), 2.35 (6H, s, 2CH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>) δ: 157.3 (C-F), 152.5 (CO), 140.1 (C), 137.4 (C), 136.7 (C), 133.5 (C), 131.8 (C), 129.2 (CH), 120.9 (CH), 120.0 (CH), 119.9 (CH), 118.1 (CH), 117.7 (CH), 116.9 (CH), 115.3 (CH), 115.1 (CH), 109.7 (CH), 50.8 (CH<sub>2</sub>), 20.4 (CH<sub>3</sub>), 19.8 (CH<sub>3</sub>). LC/MS *m/z*: 390 [M+H]<sup>+</sup>.

#### **1-(3-((5,6-dimethyl-1*H*-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-3-(4-chlorophenyl)urea (73b)**

Compound **73b** was obtained, in 17% total yield; mp: 249–251 °C; TLC (petroleum ether/ethyl acetate = 6/4) *R<sub>f</sub>*: 0.20. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ: 8.72 (2H, s, 2NH), 7.80 (1H, s, H-4), 7.58 (1H, s, H-7), 7.45 (2H, d, *J* = 8.8 Hz, H-3'', H-5''), 7.40 (1H, d, *J* = 8.00 Hz, H-6'), 7.35–7.28 (3H, m, H-2', H-2'', H-6''), 7.26 (1H, t, H-5'), 6.91 (1H, d, *J* = 7.6 Hz, H-4'), 5.87 (1H, s, CH<sub>2</sub>), 2.35 (6H, s, 2CH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>) δ: 152.3 (CO), 144.5 (C), 139.9 (C), 138.5 (C), 137.4 (C), 136.7 (C), 133.5 (C), 131.7 (C), 129.2 (CH), 128.6 (2CH), 125.4 (CH), 121.0 (CH), 119.7 (2CH), 118.1 (CH), 117.8 (CH), 117.0 (CH), 109.7 (CH), 50.7 (CH<sub>2</sub>), 20.4 (CH<sub>3</sub>), 19.8 (CH<sub>3</sub>). LC/MS *m/z*: 406 [M+H]<sup>+</sup>.

#### **1-(3-((5,6-dimethyl-1*H*-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-3-(4-(trifluoromethyl)phenyl)urea (74b)**

Compound **74b** was obtained, in 33% total yield; mp: 290–292 °C; TLC (petroleum ether/ethyl acetate = 6/4)  $R_f$ : 0.18.  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 9.03 (1H, s, NH), 8.85 (1H, s, NH), 7.80 (1H, s, H-4), 7.62 (4H, s, H-2'', H-3'', H-5'', H-6''), 7.59 (1H, s, H-7), 7.41 (1H, d,  $J$  = 8.4 Hz, H-6'), 7.33 (1H, s, H-2'), 7.27 (1H, t, H-5'), 6.93 (1H, d,  $J$  = 7.2 Hz, H-4'), 5.88 (1H, s, CH<sub>2</sub>), 2.35 (6H, s, 2CH<sub>3</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ )  $\delta$ : 152.1 (CO), 144.5 (C), 143.3 (C), 139.7 (2C), 137.4 (C), 136.8 (2C), 133.5 (C), 131.8 (C), 129.2 (CH), 126.0 (CH), 121.3 (CH), 118.1 (CH), 117.8 (4CH), 117.2 (CH), 109.7 (CH), 50.7 (CH<sub>2</sub>), 20.4 (CH<sub>3</sub>), 19.8 (CH<sub>3</sub>). LC/MS  $m/z$ : 440 [M+H]<sup>+</sup>.

#### *N-(4-(5,6-dimethyl-2H-benzo[d][1,2,3]triazol-2-yl)phenyl)acetamide (75b)*

Compound **75b** was obtained, in 89% total yield; mp: 166–168 °C; TLC (petroleum ether /ethyl acetate 1:1):  $R_f$ : 0.22.  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 9.98 (1H, s, NH), 7.64 (1H, s, H-4,7), 7.53 (2H, d,  $J$  = 8.8, H-2',6'), 7.27 (2H, d,  $J$  = 8.4, H-3',5'), 5.80 (2H, s, CH<sub>2</sub>), 2.34 (6H, s, 2CH<sub>3</sub>), 2.01 (3H, s, CH<sub>3</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ ): 168.9 (C), 145.5 (2C), 136.6 (2C), 135.2 (C), 130.9 (C), 128.8 (2CH), 124.1 (CH), 121.5 (2CH), 61.6 (CH<sub>2</sub>), 24.0 (CH<sub>3</sub>), 18.8 (2CH<sub>3</sub>). LC/MS  $m/z$  295 [M+H]<sup>+</sup>.

#### *N-(4-(5,6-dimethyl-2H-benzo[d][1,2,3]triazol-2-yl)phenyl)propionamide (76b)*

Compound **76b** was obtained, in 82% total yield; mp: 177–179 °C; TLC (petroleum ether /ethyl acetate 6:4):  $R_f$ : 0.29.  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 9.91 (1H, s, NH), 7.64 (1H, s, H-4,7), 7.56 (2H, d,  $J$  = 7.8, H-2',6'), 7.29 (2H, d,  $J$  = 7.8, H-3',5'), 5.81 (2H, s, CH<sub>2</sub>), 2.46 (2H, q, CH<sub>2</sub>CH<sub>3</sub>), 2.35 (6H, s, 2CH<sub>3</sub>), 1.06 (3H, t, CH<sub>2</sub>CH<sub>3</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ ): 168.9 (C), 145.5 (2C), 136.6 (2C), 135.2 (C), 130.9 (C), 128.8 (2CH), 124.1 (CH), 121.5 (2CH), 61.6 (CH<sub>2</sub>), 30.0 (CH<sub>2</sub>), 18.8 (2CH<sub>3</sub>), 10.4 (CH<sub>3</sub>). LC/MS  $m/z$  309 [M+H]<sup>+</sup>.

#### *N-(4-(5,6-dimethyl-1H-benzo[d][1,2,3]triazol-1-yl)phenyl)acetamide (77b)*

Compound **77b** was obtained, in 90% total yield; mp: 205–207 °C; TLC (petroleum ether /ethyl acetate 4:6):  $R_f$ : 0.24.  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 9.96 (1H, s, NH), 7.77 (1H, s, H-4), 7.58 (1H, s, H-7), 7.51 (2H, d,  $J$  = 8.0, H-2',6'), 7.24 (2H, d,  $J$  = 8.4, H-3',5'), 5.81 (2H, s, CH<sub>2</sub>), 2.34 (6H, s, 2CH<sub>3</sub>), 2.00 (3H, s, CH<sub>3</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ ): 168.9 (C), 145.6 (C), 136.6 (2C), 135.2 (C), 132.8 (C), 130.9 (C), 128.8 (2CH), 124.1 (CH), 121.5 (2CH), 61.6 (CH<sub>2</sub>), 24.0 (CH<sub>3</sub>), 18.8 (2CH<sub>3</sub>). LC/MS  $m/z$  295 [M+H]<sup>+</sup>.

#### *N-(4-(5,6-dimethyl-1H-benzo[d][1,2,3]triazol-1-yl)phenyl)propionamide (78b)*

Compound **78b** was obtained, in 30% total yield; mp: 218–220 °C; TLC (petroleum ether /ethyl acetate 1:1):  $R_f$ : 0.32.  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 9.89 (1H, s, NH), 7.78 (1H, s, H-4), 7.58 (1H, s, H-7), 7.54 (2H, d,  $J$  = 8.6, H-2',6'), 7.24 (2H, d,  $J$  = 8.6, H-3',5'), 5.81 (2H, s, CH<sub>2</sub>), 2.34 (6H, s, 2CH<sub>3</sub>), 2.32 (2H, q, CH<sub>2</sub>CH<sub>3</sub>), 1.04 (3H, t, CH<sub>2</sub>CH<sub>3</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ ): 168.9 (C), 145.6 (C), 136.6 (2C), 135.2 (C), 132.8 (C), 130.9 (C), 128.8 (2CH), 124.1 (CH), 121.5 (2CH), 61.6 (CH<sub>2</sub>), 32.0 (CH<sub>2</sub>), 18.8 (2CH<sub>3</sub>), 10.4 (CH<sub>3</sub>). LC/MS  $m/z$  309 [M+H]<sup>+</sup>.

#### *N-(4-((1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)acetamide (79c)*

Compound **79c** was obtained, in 75% total yield; mp: 187–189 °C; TLC (petroleum ether /ethyl acetate 6:4):  $R_f$ : 0.10.  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 9.97 (1H, s, NH), 8.04 (1H, d,  $J$  = 8.2, H-4), 7.82 (1H, d,  $J$  = 8.2, H-7), 7.53–7.48 (3H, m, H-3',5',H-5), 7.40 (1H, t, H-6), 7.28 (2H, d,  $J$  = 8.6, H-2',6'), 5.90 (2H, s, CH<sub>2</sub>), 2.00 (3H, s, CH<sub>3</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ ): 168.9 (CO), 145.5 (C), 132.8 (C), 131.8 (C), 135.5 (C), 129.2 (2CH), 126.2 (2CH), 121.5 (2CH), 119.6 (CH), 110.0 (CH), 54.7 (CH<sub>2</sub>), 24.0 (CH<sub>3</sub>). LC/MS  $m/z$  267 [M+H]<sup>+</sup>.

#### *N-(4-((1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)propionamide (80c)*

Compound **80c** was obtained, in 73% total yield; mp: 192–195 °C; TLC (petroleum ether /ethyl acetate 6:4):  $R_f$ : 0.32.  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 9.90 (1H, s, NH), 8.04 (1H, d,  $J$  = 8.0, H-4), 7.82 (1H, d,  $J$  = 8.0, H-7), 7.59–7.48 (3H, m, H-3',5',H-5), 7.36 (1H, t, H-6), 7.28 (2H, d,  $J$  = 8.0, H-2',6'), 5.90 (2H, s, CH<sub>2</sub>), 2.31 (2H, q, CH<sub>2</sub>CH<sub>3</sub>), 1.04 (3H, t, CH<sub>2</sub>CH<sub>3</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ ): 168.8 (CO), 145.5 (C), 132.8 (C), 131.8 (C), 135.5 (C), 129.2 (2CH), 126.2 (2CH), 121.5 (2CH), 119.6 (CH), 110.0 (CH), 54.7 (CH<sub>2</sub>), 30.6 (CH<sub>2</sub>), 10.0 (CH<sub>3</sub>). LC/MS  $m/z$  281 [M+H]<sup>+</sup>.

#### *N-(4-((5,6-difluoro-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)acetamide (81d)*

Compound **81d** was obtained, in 50% total yield; mp: 242–243 °C; TLC (petroleum ether /ethyl acetate 6:4):  $R_f$ : 0.10.  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 9.97 (H, s, NH), 8.21 (H, t, H-4), 8.13 (H, t, H-7), 7.53 (2H, d,  $J$  = 8.0 Hz, H-3',5'), 7.31 (2H, d,  $J$  = 8.0 Hz, H-2',6'), 5.87 (2H, s, CH<sub>2</sub>), 2.00 (3H, s, CH<sub>3</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ ):  $\delta$  168.9 (C), 149.5 (2C), 145.5 (C), 135.5 (C), 132.8 (C), 131.8 (C), 129.2 (2CH), 121.5 (2CH), 117.1 (2CH), 54.7 (CH<sub>2</sub>), 24.0 (CH<sub>3</sub>). LC/MS:  $m/z$  303 [M+H]<sup>+</sup>.

#### *N-(4-((5,6-difluoro-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)propionamide (82d)*

Compound **82d** was obtained, in 22% total yield; mp: 240–242 °C; TLC (petroleum ether /ethyl acetate 6:4):  $R_f$ : 0.24.  $^1\text{H}$  NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 9.90 (H, s, NH), 8.19 (H, t, H-4), 8.10 (H, t, H-7), 7.55 (2H, d,  $J$  = 8.0 Hz, H-3',5'), 7.31 (2H, d,  $J$  = 8.0 Hz, H-2',6'), 5.87 (2H, s, CH<sub>2</sub>), 2.28 (2H, q, CH<sub>2</sub>), 1.05 (3H, s, CH<sub>3</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ ):  $\delta$  172.0 (C), 149.5 (2C), 145.5 (C), 135.5 (C), 132.8 (C), 131.8 (C), 129.2 (2CH), 121.5 (2CH), 117.1 (2CH), 54.7 (CH<sub>2</sub>), 30.6 (CH<sub>2</sub>), 10.0 (CH<sub>3</sub>). LC/MS:  $m/z$  317 [M+H]<sup>+</sup>.

***N-(4-((5,6-dimethyl-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-4-methoxybenzamide (83b)***

Compound **83b** was obtained, in 53% total yield; mp: 196–198 °C; TLC (petroleum ether/ethyl acetate = 1/1)  $R_f$ : 0.30.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 10.13 (1H, s, NH), 7.93 (2H, d,  $J$  = 8.6 Hz, H-2'', 6''), 7.80 (1H, s, H-4), 7.73 (2H, d,  $J$  = 8.2 Hz, H-3', 5'), 7.61 (1H, s, H-7), 7.30 (2H, d,  $J$  = 8.2 Hz, H-2', 6'), 7.05 (2H, d,  $J$  = 8.4 Hz, H-3'', 5''), 5.86 (2H, s, CH<sub>2</sub>), 3.83 (3H, s, OCH<sub>3</sub>), 2.36 (6H, s, 2CH<sub>3</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ )  $\delta$ : 164.9 (CO), 161.9 (C), 144.6 (C), 139.7 (C), 137.3 (C), 136.4 (C), 133.5 (C), 131.7 (C), 129.6 (CH), 129.3 (CH), 128.9 (CH), 126.7 (C), 122.6 (CH), 119.9 (CH), 119.2 (CH), 118.1 (CH), 113.7 (CH), 113.5 (CH), 109.7 (CH), 55.4 (OCH<sub>3</sub>), 50.8 (CH<sub>2</sub>), 20.1 (2CH<sub>3</sub>). LC/MS *m/z* 387 [M+H]<sup>+</sup>.

***N-(4-((5,6-dimethyl-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-4-nitrobenzamide (84b)***

Compound **84b** was obtained, in 34% total yield; mp: 192–194 °C; TLC (petroleum ether/ethyl acetate = 1/1)  $R_f$ : 0.28.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 10.19 (1H, s, NH), 8.21 (1H, s, H-4), 7.76 (1H, s, H-7), 7.58–7.60 (6H, m, H-3', 5', 2'', 3'', 5'', 6''), 7.25 (2H, d,  $J$  = 8.2 Hz, H-2', 6'), 5.81 (2H, s, CH<sub>2</sub>), 2.33 (6H, s, 2CH<sub>3</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ )  $\delta$ : 163.9 (CO), 149.1 (C), 144.6 (C), 140.4 (C), 139.1 (C), 137.4 (C), 136.7 (C), 133.5 (C), 131.7 (C), 129.2 (2CH), 129.1 (CH), 123.5 (CH), 123.4 (CH), 122.7 (CH), 120.0 (CH), 119.3 (CH), 118.1 (CH), 109.7 (CH), 50.7 (CH<sub>2</sub>), 20.1 (2CH<sub>3</sub>). LC/MS *m/z* 402 [M+H]<sup>+</sup>.

***N-(4-((1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-4-nitrobenzamide (85c)***

Compound **85c** was obtained, in 34% total yield; mp: 245–246 °C; TLC (petroleum ether/ethyl acetate = 4/6)  $R_f$ : 0.68.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 10.62 (1H, s, NH), 8.36 (2H, d,  $J$  = 7.8, H-3'', 5''), 8.15 (2H, d,  $J$  = 7.8, H-2'', 6''), 8.06 (1H, d,  $J$  = 7.6, H-4), 7.85 (1H, d,  $J$  = 7.6, H-7), 7.75 (2H, d,  $J$  = 7.8, H-3', 5'), 7.55 (1H, t, H-5), 7.44–7.36 (3H, m, H-6, 2', 6'), 5.97 (2H, s, CH<sub>2</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ )  $\delta$ : 163.9 (CO), 149.1 (C), 144.6 (C), 140.4 (C), 139.1 (C), 133.5 (C), 131.7 (C), 129.2 (2CH), 129.1 (CH), 123.5 (C), 129.2 (CH), 129.1 (CH), 126.2 (2CH), 123.5 (CH), 123.3 (CH), 122.7 (CH), 120.0 (CH), 119.3 (CH), 118.1 (CH), 109.7 (CH), 50.7 (CH<sub>2</sub>). LC/MS *m/z* 374, 375 [M+H]<sup>+</sup>.

***N-(4-((1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-4-methoxybenzamide (86c)***

Compound **86c** was obtained, in 41% total yield; mp: 172–174 °C; TLC (petroleum ether/ethyl acetate = 6/4)  $R_f$ : 0.21.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 10.14 (1H, s, NH), 8.06 (1H, d,  $J$  = 8.2, H-4), 7.94 (2H, d,  $J$  = 8.4, H-2'', 6''), 7.85 (1H, d,  $J$  = 9.0, H-7), 7.75 (2H, d,  $J$  = 7.6, H-3', 5'), 7.56 (1H, t, H-5), 7.44–7.33 (3H, m, H-6 e 2', 6'), 7.04 (2H, d,  $J$  = 8.0, H-3'', 5''), 5.95 (2H, s, CH<sub>2</sub>), 3.84 (3H, s, OCH<sub>3</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ )  $\delta$ : 163.9 (CO), 154.1 (C), 144.6 (C), 140.4 (C), 139.1 (C), 137.4 (C), 136.7 (C), 133.5 (C), 131.7 (C), 129.2 (2CH), 129.1 (CH), 126.2 (2CH), 123.5 (CH), 123.3 (CH), 122.7 (CH), 120.0 (CH), 119.3 (CH), 118.1 (CH), 109.7 (CH), 60.1 (OCH<sub>3</sub>), 50.7 (CH<sub>2</sub>). LC/MS *m/z* 359 [M+H]<sup>+</sup>.

***N-(4-((1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-3, 4, 5-trimethoxybenzamide (87c)***

Compound **87c** was obtained, in 54% total yield; mp: 147–149 °C; TLC (petroleum ether/ethyl acetate = 4/6)  $R_f$ : 0.35.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 10.17 (1H, s, NH), 8.05 (1H, d,  $J$  = 8.0, H-4), 7.95 (1H, s, H-2''), 7.86 (1H, d,  $J$  = 8.0, H-7), 7.70 (2H, d,  $J$  = 8.0, H-3', 5'), 7.53 (1H, t, H-5), 7.40–7.26 (3H, m, H-6, 2', 6'), 7.24 (1H, s, H-6''), 5.95 (2H, s, CH<sub>2</sub>), 3.84 (6H, s, 2OCH<sub>3</sub>), 3.71 (3H, s, OCH<sub>3</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ )  $\delta$ : 165.0 (CO), 152.6 (2CH), 144.3 (C), 140.3 (C), 139.5 (C), 135.8 (C), 129.8 (C), 129.1 (CH), 127.3 (C), 126.1 (CH), 126.3 (CH), 123.2 (C), 120.6 (CH), 120.4 (C), 119.7 (CH), 112.5 (CH), 105.3 (2CH), 60.1 (OCH<sub>3</sub>), 56.1 (2OCH<sub>3</sub>), 51.2 (CH<sub>2</sub>). LC/MS *m/z* 419 [M+H]<sup>+</sup>.

***N-(4-((1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-4-(trifluoromethoxy)benzamide (88c)***

Compound **88c** was obtained, in 63% total yield; mp: 229–231 °C; TLC (petroleum ether/ethyl acetate = 6/4)  $R_f$ : 0.55.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 10.52 (1H, s, NH), 8.14–8.00 (4H, m, H arom), 7.94–7.83 (4H, m, H arom) 7.80–7.72 (2H, m, H arom), 7.42–7.35 (2H, m, H arom), 5.96 (2H, s, CH<sub>2</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ )  $\delta$ : 163.9 (CO), 154.1 (C), 144.6 (C), 140.4 (C), 139.1 (C), 137.4 (C), 136.7 (C), 133.5 (C), 131.7 (C), 129.7 (C), 129.2 (2CH), 129.1 (CH), 126.2 (2CH), 123.5 (CH), 123.3 (CH), 122.7 (CH), 120.0 (CH), 119.3 (CH), 118.1 (CH), 109.7 (CH), 50.7 (CH<sub>2</sub>). LC/MS *m/z* 413 [M+H]<sup>+</sup>.

***N-(4-((5,6-difluoro-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-4-methylbenzamide (89d)***

Compound **89d** was obtained, in 12% total yield; mp: 297–299 °C; TLC (petrol ether/ethyl acetate = 7/3)  $R_f$ : 0.47.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 10.70 (H, s, NH), 8.28–8.10 (2H, m, H-4, 7), 7.94 (2H, t, H-3'', 5''), 7.70 (2H, d,  $J$  = 7.8 Hz, H-3', 5'), 7.35 (2H, d,  $J$  = 6.6 Hz, H-2', 6'), 7.35 (2H, d,  $J$  = 6.6 Hz, H-2'', 6''), 6.00 (2H, s, CH<sub>2</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ )  $\delta$ : 164.7 (C), 149.5 (2C), 145.5 (C), 139.3 (C), 134.9 (C), 132.8 (C), 132.3 (C), 131.8 (C), 129.3 (2CH), 129.2 (2CH), 127.5 (2CH), 121.5 (2CH), 54.7 (CH<sub>2</sub>). LC/MS: *m/z* 379 [M+H]<sup>+</sup>.

***N-(4-((5,6-difluoro-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-4-nitrobenzamide (90d)***

Compound **90d** was obtained, in 53% total yield; mp: 240–242 °C; TLC (chloroform/methanol = 99.5/0.5)  $R_f$ : 0.67.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 10.67 (H, s, NH), 8.35 (2H, d,  $J$  = 6.6 Hz, H-3'', 5''), 8.34–8.19 (4H, m, H-4, 7, 2'', 6''), 7.81 (2H, d,  $J$  = 6.6 Hz, H-3', 5'), 7.42 (2H, d,  $J$  = 6.6 Hz, H-2', 6'), 5.99 (2H, s, CH<sub>2</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ )  $\delta$ : 164.7 (C), 151.3 (C), 149.5 (2C), 145.5 (C), 136.8 (C), 134.9 (C), 132.8 (C), 131.8 (C), 129.6 (2CH), 129.2 (2CH), 124.0 (2CH), 121.5 (2CH), 117.1 (2CH) 57.7 (CH<sub>2</sub>). LC/MS: *m/z* 410 [M+H]<sup>+</sup>.

***N-(4-((5,6-difluoro-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-3, 4, 5-trimethoxybenzamide (91d)***

Compound **91d** was obtained, in 53% total yield; mp: 134–136 °C; TLC (chloroform/methanol = 99.5/0.5)  $R_f$ : 0.46.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 10.16 (H, s, NH), 8.27 (H, td, H-4), 8.19 (H, td, H-7), 7.70 (2H, d,  $J$  = 8.4 Hz, H-3', 5'), 7.38 (2H, d,  $J$  = 8.6 Hz, H-2', 6'), 7.24 (2H, s, H-2'', 6''), 5.91 (2H, s, CH<sub>2</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ ):  $\delta$  164.7 (C), 153.2 (2C), 149.5 (2C), 145.5 (C), 142.6 (C), 134.9 (C), 132.8 (C), 131.8 (C), 124.1 (C), 129.2 (2CH), 121.5 (2CH), 117.1 (2CH), 106.6 (2CH), 60.8 (CH<sub>3</sub>), 56.1 (2CH<sub>3</sub>), 54.7 (CH<sub>2</sub>). LC/MS: *m/z* 455 [M+H]<sup>+</sup>.

#### *N*-(4-((5,6-difluoro-1*H*-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-4-fluorobenzamide (92d)

Compound **92d** was obtained, in 50% total yield; mp: 241–242 °C; TLC (petroleum ether/ethyl acetate = 7/3)  $R_f$ : 0.21.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 10.33 (H, s, NH), 8.30–8.05 (2H, m, H-4, 7), 7.98 (2H, t, H-3'', 5''), 7.74 (2H, d,  $J$  = 7.8 Hz, H-3', 5'), 7.46–7.30 (4H, m, H-2', 6', 2'', 6''), 5.91 (2H, s, CH<sub>2</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ ):  $\delta$  166.3 (C), 149.5 (2C), 145.5 (C), 134.9 (C), 132.8 (C), 131.8 (C), 129.8 (C), 129.2 (2CH), 129.1 (2CH), 121.5 (2CH), 117.1 (2CH) 115.6 (2CH), 54.7 (CH<sub>2</sub>). LC/MS: *m/z* 383 [M+H]<sup>+</sup>.

#### *N*-(4-((5,6-difluoro-1*H*-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-4-chlorobenzamide (93d)

Compound **93d** was obtained, in 20% total yield; mp: 263–264 °C; TLC (chloroform/methanol = 99/1))  $R_f$ : 0.35.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 10.70 (H, s, NH), 8.28–8.10 (2H, m, H-4, 7), 8.08 (2H, t, H-3'', 5''), 7.70 (2H, d,  $J$  = 7.8 Hz, H-3', 5'), 7.42 (2H, d,  $J$  = 6.6 Hz, H-2', 6'), 7.35 (2H, d,  $J$  = 6.6 Hz, H-2'', 6''), 6.00 (2H, s, CH<sub>2</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ ):  $\delta$  164.7 (C), 149.5 (2C), 145.5 (C), 137.7 (C), 134.9 (C), 132.8 (C), 132.3 (C), 131.8 (C), 130.1 (2CH), 129.2 (2CH), 128.2 (2CH), 121.5 (2CH), 54.7 (CH<sub>2</sub>). LC/MS: *m/z* 400 [M+H]<sup>+</sup>.

#### *N*-(4-((5,6-difluoro-1*H*-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-4-bromobenzamide (94d)

Compound **94d** was obtained, in 20% total yield; mp: 235–236 °C; TLC (petroleum ether/ethyl acetate = 7/3)  $R_f$ : 0.42.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 10.70 (H, s, NH), 8.30–8.10 (2H, m, H-4, 7), 8.10 (2H, t, H-3'', 5''), 7.72 (2H, d,  $J$  = 7.8 Hz, H-3', 5'), 7.40 (2H, d,  $J$  = 6.6 Hz, H-2', 6'), 7.38 (2H, d,  $J$  = 6.6 Hz, H-2'', 6''), 5.98 (2H, s, CH<sub>2</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ ):  $\delta$  164.7 (C), 149.5 (2C), 145.5 (C), 134.9 (C), 133.2 (C), 132.8 (C), 131.8 (C), 126.5 (C), 131.7 (2CH), 129.7 (2CH), 129.2 (2CH), 121.5 (2CH), 117.1 (2CH) 54.7 (CH<sub>2</sub>). LC/MS: *m/z* 444 [M+H]<sup>+</sup>.

#### 1-(4-((5,6-dichloro-1*H*-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-3-ethylurea (95a)

Compound **95a** was obtained, in 80% total yield; mp: 211–212 °C; TLC (petroleum ether/ethyl acetate = 6/4)  $R_f$ : 0.15.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 8.47 (2H, s, H-4 and NH-Ph), 8.36 (1H, s, H-7), 7.36 (2H, d,  $J$  = 7.2 Hz, H-3', 5'), 7.26 (2H, d,  $J$  = 7.2 Hz, H-2', 6'), 6.09 (H, t, NH-CH<sub>2</sub>), 5.86 (2H, s, CH<sub>2</sub>), 3.08 (2H, q, CH<sub>2</sub>), 1.02 (3H, t, CH<sub>3</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ ):  $\delta$  155.0 (CO), 144.3 (C), 140.7 (C), 131.8 (C), 130.6 (C), 128.6 (2CH), 127.5 (C), 127.1 (C), 120.6 (CH), 117.7 (2CH), 112.5 (CH), 51.0 (CH<sub>2</sub>-Ph), 33.9 (CH<sub>2</sub>), 15.4 (CH<sub>3</sub>). LC/MS *m/z*: 364, 366 [M+H]<sup>+</sup>.

#### 1-(4-((5,6-dichloro-1*H*-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-3-propylurea (96a)

Compound **96a** was obtained, in 12% total yield; mp: 213–214 °C; TLC (petroleum ether/ethyl acetate = 6/4)  $R_f$ : 0.21.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 8.46 (2H, s, H-4 and NH-Ph), 8.36 (1H, s, H-7), 7.36 (2H, d,  $J$  = 8.0 Hz, H-3', 5'), 7.25 (2H, d,  $J$  = 8.0 Hz, H-2', 6'), 6.12 (H, t, NH-CH<sub>2</sub>), 5.86 (2H, s, CH<sub>2</sub>), 3.01 (2H, q, CH<sub>2</sub>-NH), 1.41 (2H, q, CH<sub>2</sub>-CH<sub>3</sub>), 0.85 (3H, t, CH<sub>3</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ ):  $\delta$  155.0 (CO), 144.3 (C), 140.7 (C), 131.8 (C), 130.6 (C), 128.5 (2CH), 127.5 (C), 127.1 (C), 120.5 (CH), 117.7 (2CH), 112.5 (CH), 51.0 (CH<sub>2</sub>-Ph), 40.8 (CH<sub>2</sub>), 22.9 (CH<sub>2</sub>), 11.3 (CH<sub>3</sub>). LC/MS *m/z*: 378, 380 [M+H]<sup>+</sup>.

#### 1-butyl-3-(4-((5,6-dichloro-1*H*-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)urea (97a)

Compound **97a** was obtained, in 20% total yield; mp: 216–217 °C; TLC (petroleum ether/ethyl acetate = 6/4)  $R_f$ : 0.37.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 8.52 (H, s, H-4), 8.49 (7H, s, NH-Ph), 8.42 (H, s, H-7), 7.41 (2H, d,  $J$  = 8.4 Hz, H-3', 5'), 7.31 (2H, d,  $J$  = 8.4 Hz, H-2', 6'), 6.15 (H, t, NH-CH<sub>2</sub>), 5.92 (2H, s, CH<sub>2</sub>), 3.10 (2H, q, CH<sub>2</sub>-NH), 1.46–1.38 (2H, m, CH<sub>2</sub>-CH<sub>2</sub>), 1.37–1.31 (2H, m, CH<sub>2</sub>-CH<sub>3</sub>), 0.92 (3H, t, CH<sub>3</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ ):  $\delta$  155.0 (CO), 144.3 (C), 140.7 (C), 131.8 (C), 130.6 (C), 128.6 (2CH), 127.5 (C), 127.1 (C), 120.6 (CH), 117.6 (2CH), 112.5 (CH), 51.0 (CH<sub>2</sub>-Ph), 38.6 (CH<sub>2</sub>), 31.8 (CH<sub>2</sub>), 19.5 (CH<sub>2</sub>), 13.6 (CH<sub>3</sub>). LC/MS *m/z*: 392, 394 [M+H]<sup>+</sup>.

#### 1-cyclohexyl-3-(4-((5,6-dichloro-1*H*-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)urea (98a)

Compound **98a** was obtained, in 80% total yield; mp: 130–132 °C; TLC (petroleum ether/ethyl acetate = 6/4)  $R_f$ : 0.46.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 8.47 (H, s, H-4), 8.35 (H, s, H-7), 8.36 (H, s, NH-Ph), 7.34 (2H, d,  $J$  = 8 Hz, H-3', 5'), 7.25 (2H, d,  $J$  = 8 Hz, H-2', 6'), 6.08 (H, d, NH-CH), 5.86 (2H, s, CH<sub>2</sub>), 3.35–3.20 (H, m, CH-NH), 1.78–1.49 (6H, m, 3CH<sub>2</sub>), 1.30–1.16 (4H, m, 2CH<sub>2</sub>).  $^{13}\text{C}$ -NMR (DMSO- $d_6$ ):  $\delta$  156.6 (CO), 154.2 (C), 144.3 (C), 140.6 (C), 131.8 (C), 130.6 (C), 128.6 (2CH), 127.3 (C), 120.7 (CH), 117.6 (2CH), 112.5 (CH), 51.0 (CH<sub>2</sub>-Ph), 47.5 (CH-NH), 33.3 (2CH<sub>2</sub>), 32.9 (CH<sub>2</sub>), 25.3 (CH<sub>2</sub>), 24.4 (CH<sub>2</sub>). LC/MS *m/z*: 418, 421 [M+H]<sup>+</sup>.

#### 1-(4-((5,6-dimethyl-1*H*-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-3-propylurea (99b)

Compound **99b** was obtained, in 63% total yield; mp: 190–192 °C; TLC (petroleum ether/ethyl acetate = 6/4)  $R_f$ : 0.29.  $^1\text{H}$ -NMR (400 MHz, DMSO- $d_6$ )  $\delta$ : 8.42 (1H, s, NH-Ph), 7.78 (1H, s, H-4), 7.57 (1H, s, H-7), 7.33 (2H, d,  $J$  = 8.0, H-2', 6'), 7.17 (2H, d,  $J$  = 8.0, H-3', 5'), 6.14–6.05 (1H, m, NH-CH<sub>2</sub>), 5.77 (2H, s, CH<sub>2</sub>), 3.10–2.90 (2H, m, CH<sub>2</sub>-NH), 2.31 (6H,

s, 2CH<sub>3</sub>), 1.80-1.40 (4H, m, 2CH<sub>2</sub>), 1.42-1.30 (2H, q, CH<sub>2</sub>CH<sub>3</sub>), 0.85 (3H, t, CH<sub>2</sub>CH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-d<sub>6</sub>) δ: 155.0 (CO), 144.3 (C), 140.7 (C), 134.6 (C), 133.8 (C), 128.5 (2CH), 127.5 (C), 127.1 (C), 120.5 (CH), 116.7 (2CH), 112.5 (CH), 51.0 (CH<sub>2</sub>-Ph), 40.8 (CH<sub>2</sub>), 22.9 (CH<sub>3</sub>), 11.3 (CH<sub>3</sub>). LC/MS *m/z* 338 [M+H]<sup>+</sup>.

#### **1-cyclohexyl-3-(4-((5,6-dimethyl-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)urea (100b)**

Compound **100b** was obtained, in 48% total yield; mp: 216-218 °C; TLC (petroleum ether/ethyl acetate = 6/4) R<sub>f</sub> : 0.23. <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) δ: 8.29 (1H, s, NH-Ph), 7.74 (1H, s, H-4), 7.55 (1H, s, H-7), 7.28 (2H, d, *J* = 8.2, H-2', 6'), 7.15 (2H, d, *J* = 8.0, H-3', 5'), 6.01 (1H, d, *J* = 7.6, NH-CH), 5.74 (2H, s, CH<sub>2</sub>), 3.51-3.25 (1H, m, CH), 2.31 (6H, s, 2CH<sub>3</sub>), 1.80-1.40 (4H, m, 2CH<sub>2</sub>), 1.35-1.00 (6H, m, 3CH<sub>2</sub>). <sup>13</sup>C-NMR (DMSO-d<sub>6</sub>) δ: 156.6 (CO), 154.2 (C), 144.3 (C), 140.6 (C), 131.8 (C), 130.6 (C), 128.6 (2CH), 127.3 (C), 121.7 (CH), 118.6 (2CH), 112.5 (CH), 51.0 (CH<sub>2</sub>-Ph), 47.5 (CH-NH), 33.3 (2CH<sub>2</sub>), 32.9 (CH<sub>2</sub>), 25.3 (CH<sub>2</sub>), 24.4 (CH<sub>2</sub>). LC/MS *m/z* 378 [M+H]<sup>+</sup>.

#### **1-(4-((1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-3-propylurea (101c)**

Compound **101c** was obtained, in 39% total yield; mp: 165-167 °C; TLC (diethyl ether) R<sub>f</sub> : 0.35. <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) δ: 8.45 (1H, s, NH-Ph), 8.03 (1H, d, *J* = 7.8, H-4), 7.83 (1H, d, *J* = 7.4, H-7), 7.52 (1H, t, H-5), 7.42 (1H, t, H-6), 7.34 (2H, d, *J* = 8.4, H-3', 5'), 7.23 (2H, d, *J* = 8.4, H-2', 6'), 6.13 (1H, t, NH-CH<sub>2</sub>), 5.86 (2H, s, CH<sub>2</sub>), 3.10-2.88 (2H, m, CH<sub>2</sub>-NH), 1.48-1.35 (2H, q, CH<sub>2</sub>CH<sub>3</sub>), 0.84 (3H, t, CH<sub>2</sub>CH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-d<sub>6</sub>) δ: 168.9 (CO), 145.5 (C), 132.8 (C), 131.8 (C), 135.5 (C), 129.2 (2CH), 126.2 (2CH), 121.5 (2CH), 119.6 (CH), 110.0 (CH), 54.7 (CH<sub>2</sub>), 40.8 (CH<sub>2</sub>), 22.9 (CH<sub>2</sub>), 11.3 (CH<sub>3</sub>). LC/MS *m/z* 310 [M+H]<sup>+</sup>.

#### **1-(4-((1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-3-cyclohexylurea (102c)**

Compound **102c** was obtained, in 66% total yield; mp: 141-143 °C; TLC (diethyl ether/ petroleum ether = 8/2) R<sub>f</sub> : 0.28. <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) δ: 8.32 (1H, s, NH-Ph), 8.03 (1H, d, *J* = 8.4, H-4), 7.55 (1H, d, *J* = 8. H-7), 7.55-7.38 (2H, m, H-5,6), 7.32 (2H, d, *J* = 8.2, H-2', 6'), 7.22 (2H, d, *J* = 8.4, H-3', 5'), 6.06 (1H, d, *J* = 7.6, NH-CH), 5.86 (2H, s, CH<sub>2</sub>), 3.51-3.25 (1H, m, CH), 1.80-1.40 (4H, m, 2CH<sub>2</sub>), 1.35-1.00 (6H, m, 3CH<sub>2</sub>). <sup>13</sup>C-NMR (DMSO-d<sub>6</sub>) δ: 168.9 (CO), 145.5 (C), 132.8 (C), 131.8 (C), 135.5 (C), 129.2 (2CH), 126.2 (2CH), 121.5 (2CH), 119.6 (CH), 110.0 (CH), 54.7 (CH<sub>2</sub>), 47.5 (CH-NH), 33.3 (2CH<sub>2</sub>), 32.9 (CH<sub>2</sub>), 25.3 (CH<sub>2</sub>), 24.4 (CH<sub>2</sub>). LC/MS *m/z* 350 [M+H]<sup>+</sup>.

#### **1-(4-((1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-3-phenylurea (103c)**

Compound **103c** was obtained, in 16% total yield; mp: 159-161 °C; TLC (diethyl ether/ petroleum ether = 8/2) R<sub>f</sub> : 0.31. <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) δ: 10.24 (1H, s, NH), 8.25 (1H, s, NH-Ph), 8.04 (1H, d, *J* = 8.2, H-4), 7.82 (1H, d, *J* = 8.2, H-7), 7.55 (2H, d, *J* = 8.6, H-3', 5'), 7.48-7.38 (4H, m, arom), 7.32 (2H, d, *J* = 8.4, H-2', 6'), 7.18-7.14 (1H, m, arom), 5.92 (2H, s, CH<sub>2</sub>). <sup>13</sup>C-NMR (DMSO-d<sub>6</sub>) δ: 168.9 (CO), 145.5 (C), 139.4 (C), 132.8 (C), 131.8 (C), 135.5 (C), 129.2 (2CH), 128.9 (2CH), 126.2 (2CH), 126.10 (CH), 121.8 (2CH), 121.5 (2CH), 119.6 (CH), 110.0 (CH), 54.7 (CH<sub>2</sub>). LC/MS *m/z* 344 [M+H]<sup>+</sup>.

#### **1-(4-((5,6-difluoro-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-3-ethylurea (104d)**

Compound **104d** was obtained, in 47% total yield; mp: 286-287 °C; TLC (petroleum ether/ethyl acetate = 6/4) R<sub>f</sub> : 0.11. <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) δ: 8.46 (H, s, NH-Ph), 8.21 (H, t, H-4), 8.10 (H, t, H-7), 7.36 (2H, d, *J* = 8.4 Hz, H-3',5'), 7.27 (2H, d, *J* = 8.4 Hz, H-2',6'), 6.08 (H, t, NH-CH<sub>2</sub>), 5.83 (2H, s, CH<sub>2</sub>-Ph), 3.11-3.04 (2H, m, CH<sub>2</sub>), 1.03 (3H, t, CH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-d<sub>6</sub>) δ: 151.6 (CO), 149.1 (2CF), 140.6 (C), 140.5 (C), 128.7 (C), 128.6 (2CH), 128.5 (C), 118.4 (2CH), 106.0 (CH), 98.5 (CH), 51.0 (CH<sub>2</sub>-Ph), 33.9 (CH<sub>2</sub>), 15.4 (CH<sub>3</sub>). LC/MS *m/z* 332 [M+H]<sup>+</sup>.

#### **1-(4-((5,6-difluoro-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)-3-propylurea (105d)**

Compound **105d** was obtained, in 41% total yield; mp: 286-287 °C; TLC (petroleum ether/ethyl acetate = 6/4) R<sub>f</sub> : 0.17. <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) δ: 8.45 (H, s, NH-Ph), 8.21 (H, t, H-4), 8.10 (H, t, H-7), 7.35 (2H, d, *J* = 8.8 Hz, H-3',5'), 7.30 (2H, d, *J* = 8.8 Hz, H-2',6'), 6.12 (H, t, NH-CH<sub>2</sub>), 5.83 (2H, s, CH<sub>2</sub>), 3.00 (2H, q, CH<sub>2</sub>-NH), 1.41 (2H, q, CH<sub>2</sub>-CH<sub>3</sub>), 0.84 (3H, t, CH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-d<sub>6</sub>) δ: 152.3 (CO), 149.2 (2CF), 140.6 (2C), 128.7 (2CH), 127.5 (2C), 117.7 (2CH), 106.1 (CH), 98.4 (CH), 51.0 (CH<sub>2</sub>), 40.8 (CH<sub>2</sub>), 22.9 (CH<sub>2</sub>), 11.3 (CH<sub>3</sub>). LC/MS *m/z* 345 [M+H]<sup>+</sup>.

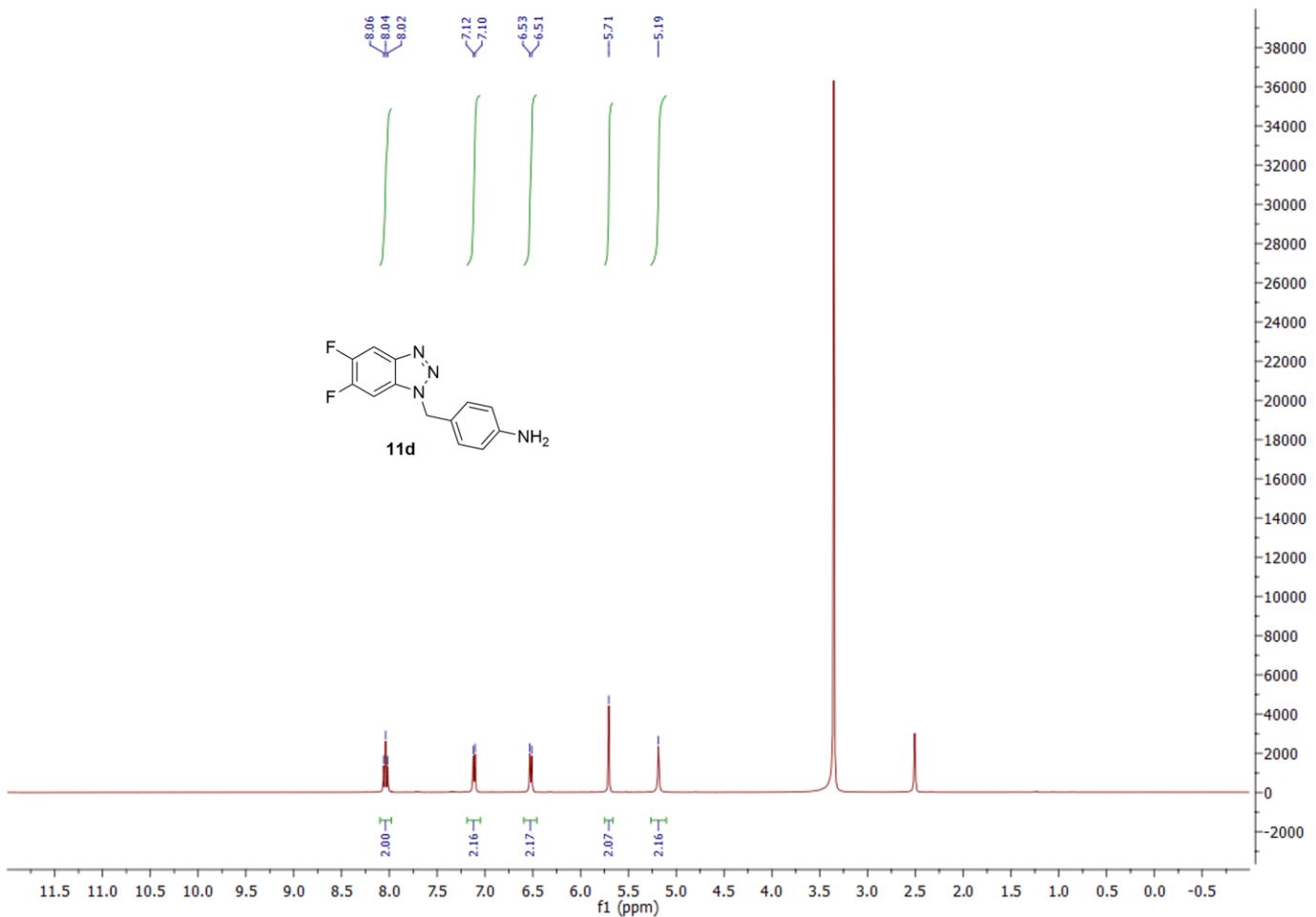
#### **1-butyl-3-(4-((5,6-difluoro-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)urea (106d)**

Compound **106d** was obtained, in 18% total yield; mp: 193-194 °C; TLC (petroleum ether/ethyl acetate = 6/4) R<sub>f</sub> : 0.26. <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) δ: 8.44 (H, s, NH-Ph), 8.21 (H, t, H-4), 8.10 (H, t, H-7), 7.35 (2H, d, *J* = 8.4 Hz, H-3',5'), 7.26 (2H, d, *J* = 8.4 Hz, H-2',6'), 6.10 (H, t, NH-CH<sub>2</sub>), 5.83 (2H, s, CH<sub>2</sub>), 3.05 (2H, t, CH<sub>2</sub>-NH), 1.38 (2H, q, CH<sub>2</sub>-CH<sub>2</sub>), 1.33-1.23 (2H, m, CH<sub>2</sub>-CH<sub>2</sub>-CH<sub>3</sub>), 0.88 (3H, t, CH<sub>3</sub>). <sup>13</sup>C-NMR (DMSO-d<sub>6</sub>) δ: 155.0 (CO), 149.2 (2CF), 140.6 (2C), 128.7 (2CH), 127.5 (2C), 177.6 (2CH), 106.1 (CH), 98.5 (CH), 51.0 (CH<sub>2</sub>-Ph), 32.1 (CH<sub>2</sub>), 31.8 (CH<sub>2</sub>), 19.5 (CH<sub>2</sub>), 13.7 (CH<sub>3</sub>). LC/MS *m/z* 360 [M+H]<sup>+</sup>.

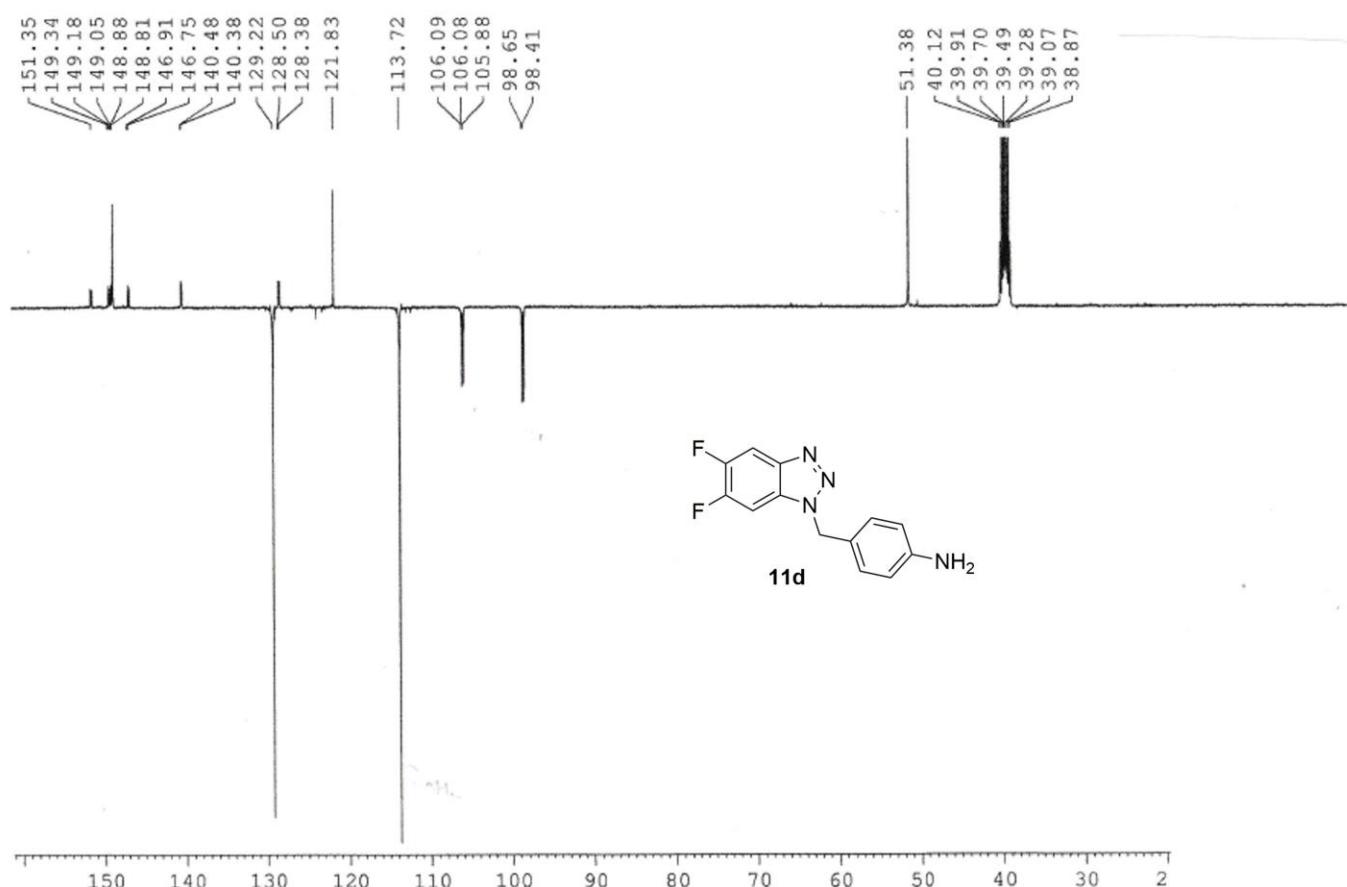
#### **1-cyclohexyl-3-(4-((5,6-difluoro-1H-benzo[d][1,2,3]triazol-1-yl)methyl)phenyl)urea (107d)**

Compound **107d** was obtained, in 16% total yield; mp: 203-204 °C; TLC (petroleum ether/ethyl acetate = 6/4) R<sub>f</sub> : 0.32. <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) δ: 8.36 (H, s, NH-Ph), 8.21 (H, t, H-4), 8.10 (H, t, H-7), 7.34 (2H, d, *J* = 8.8 Hz, H-

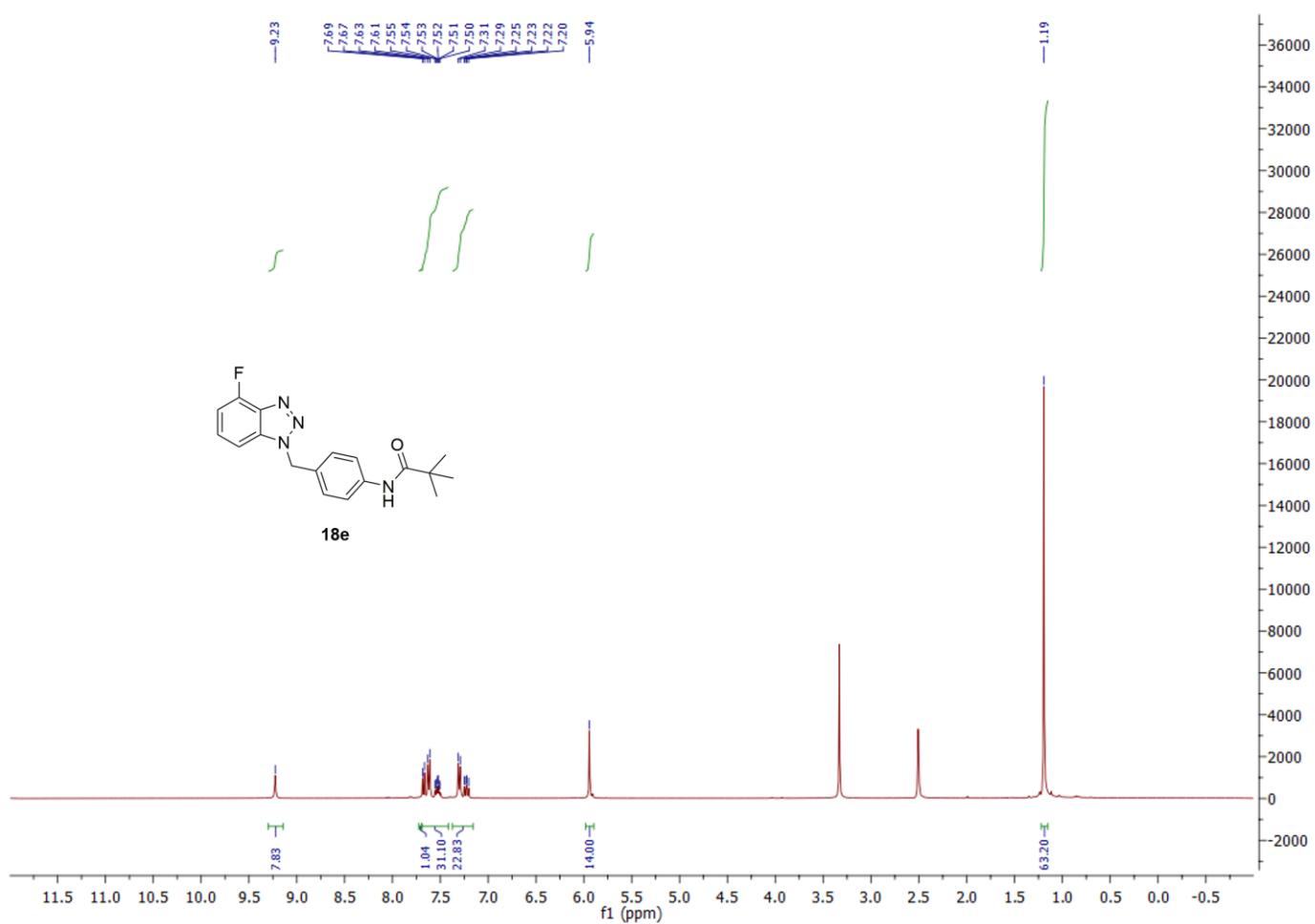
3',5'), 7.26 (2H, d,  $J = 8.8$  Hz, H-2',6'), 6.08 (H, d, NH-CH), 5.80 (2H, s, CH<sub>2</sub>), 3.44-3.40 (H, m, CH-NH), 1.82-1.45 (6H, m, 3CH<sub>2</sub>), 1.30-0.98 (4H, m, 2CH<sub>2</sub>). <sup>13</sup>C-NMR (DMSO-*d*<sub>6</sub>)  $\delta$ : 156.6 (CO), 154.2 (C), 149.2 (2CF), 140.6 (C), 140.4 (C), 128.7 (2CH), 128.6 (C), 117.6 (2CH), 106.1 (CH), 98.5 (CH), 51.0 (CH<sub>2</sub>), 47.5 (CH), 33.3 (2CH<sub>2</sub>), 32.9 (CH<sub>2</sub>), 25.2 (CH<sub>2</sub>), 24.3 (CH<sub>2</sub>). LC/MS *m/z* 386 [M+H]<sup>+</sup>.



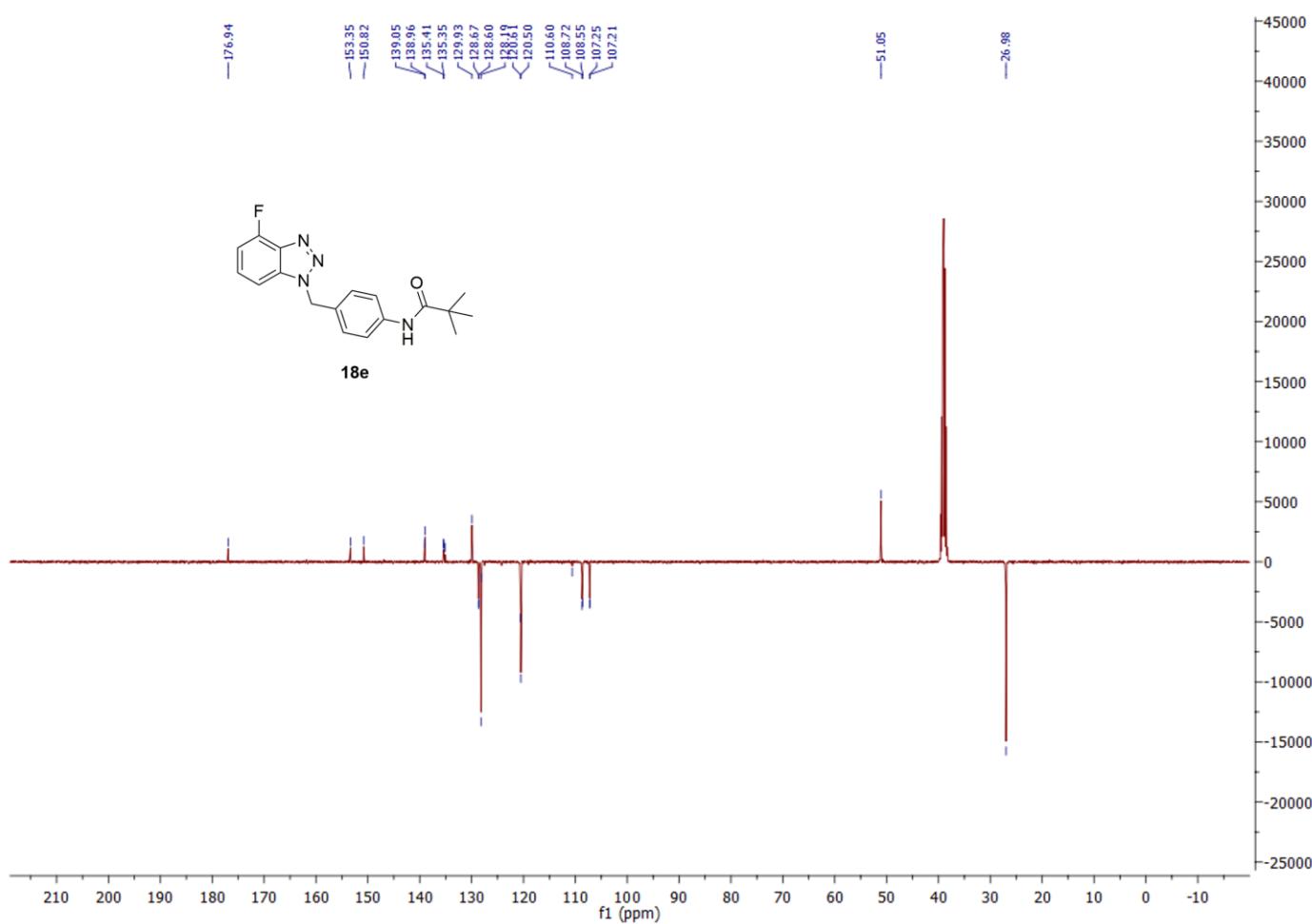
**Figure S2.** <sup>1</sup>H-NMR for compound 11d.



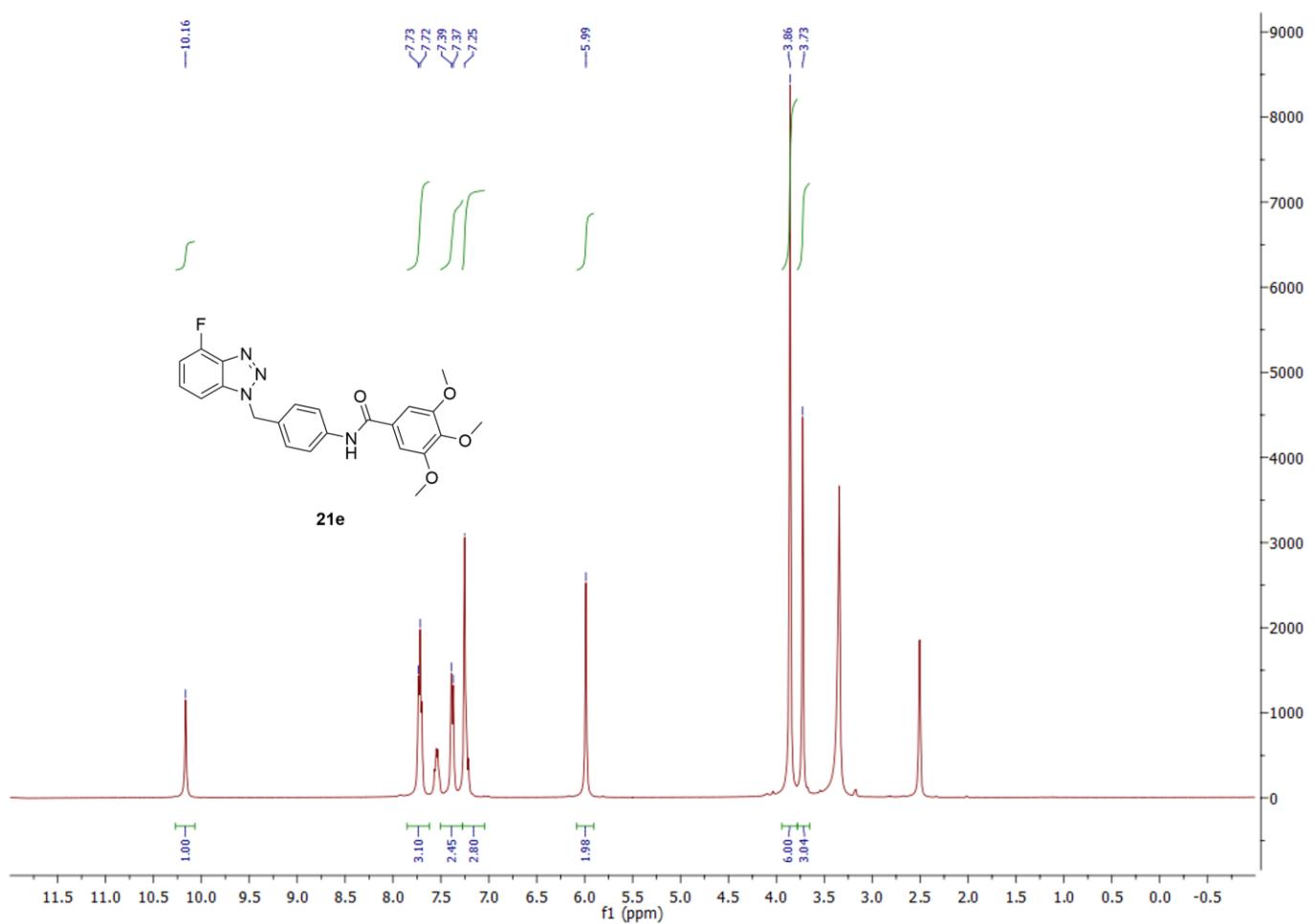
**Figure S3.**  $^{13}\text{C}$ -NMR for compound **11d**.



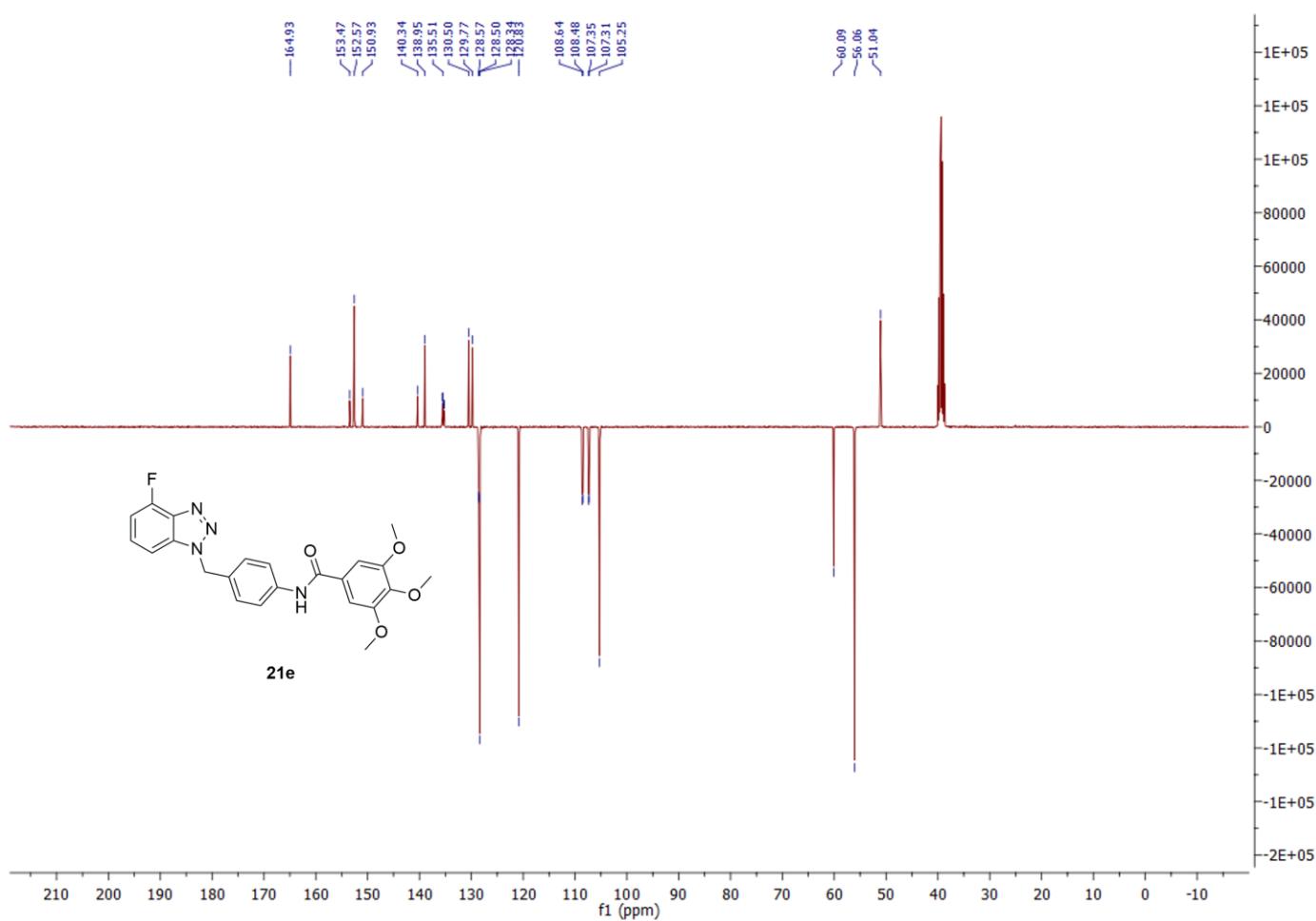
**Figure S4.**  $^1\text{H}$ -NMR for compound **18e**.



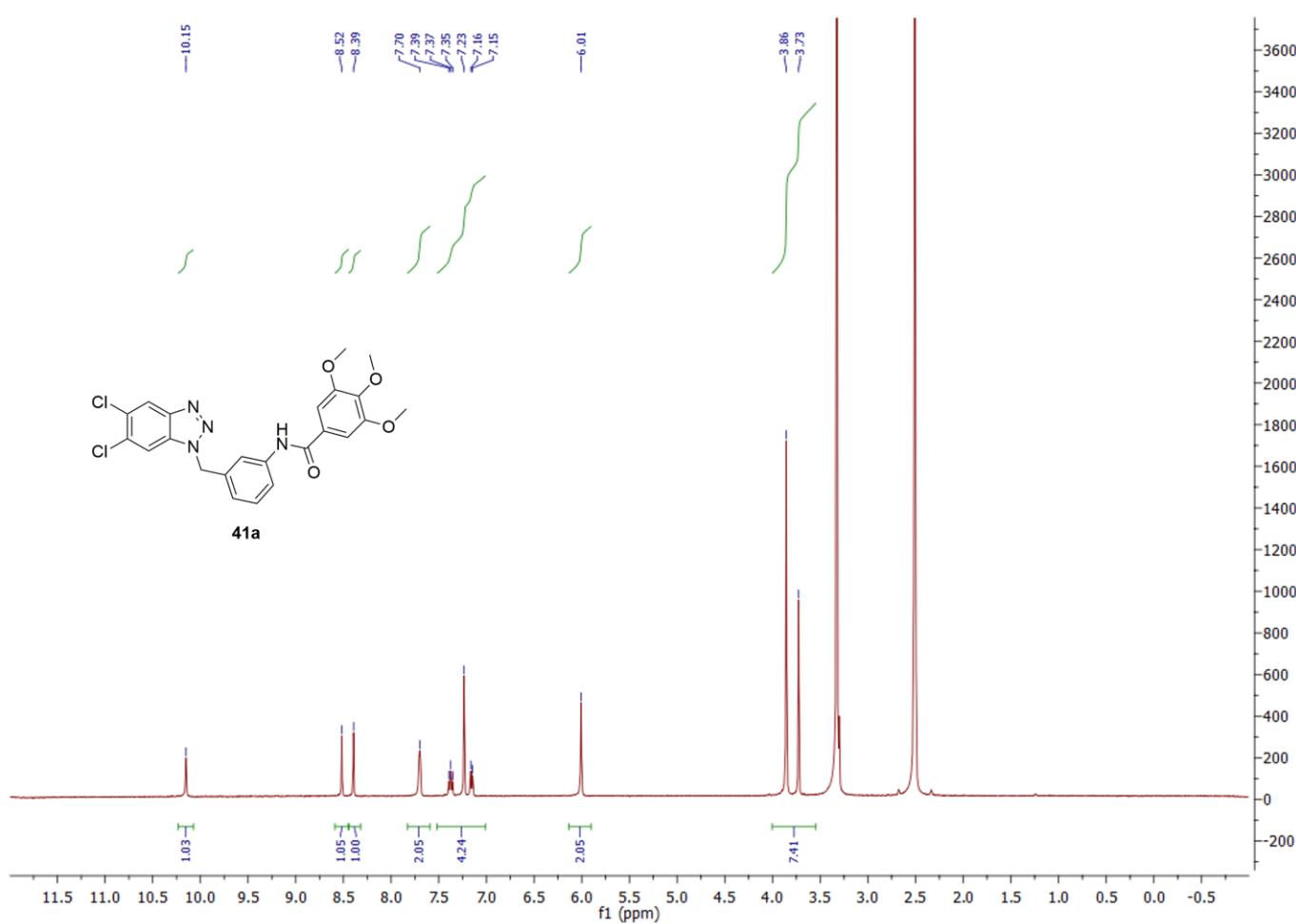
**Figure S5.**  $^{13}\text{C}$ -NMR for compound **18e**.



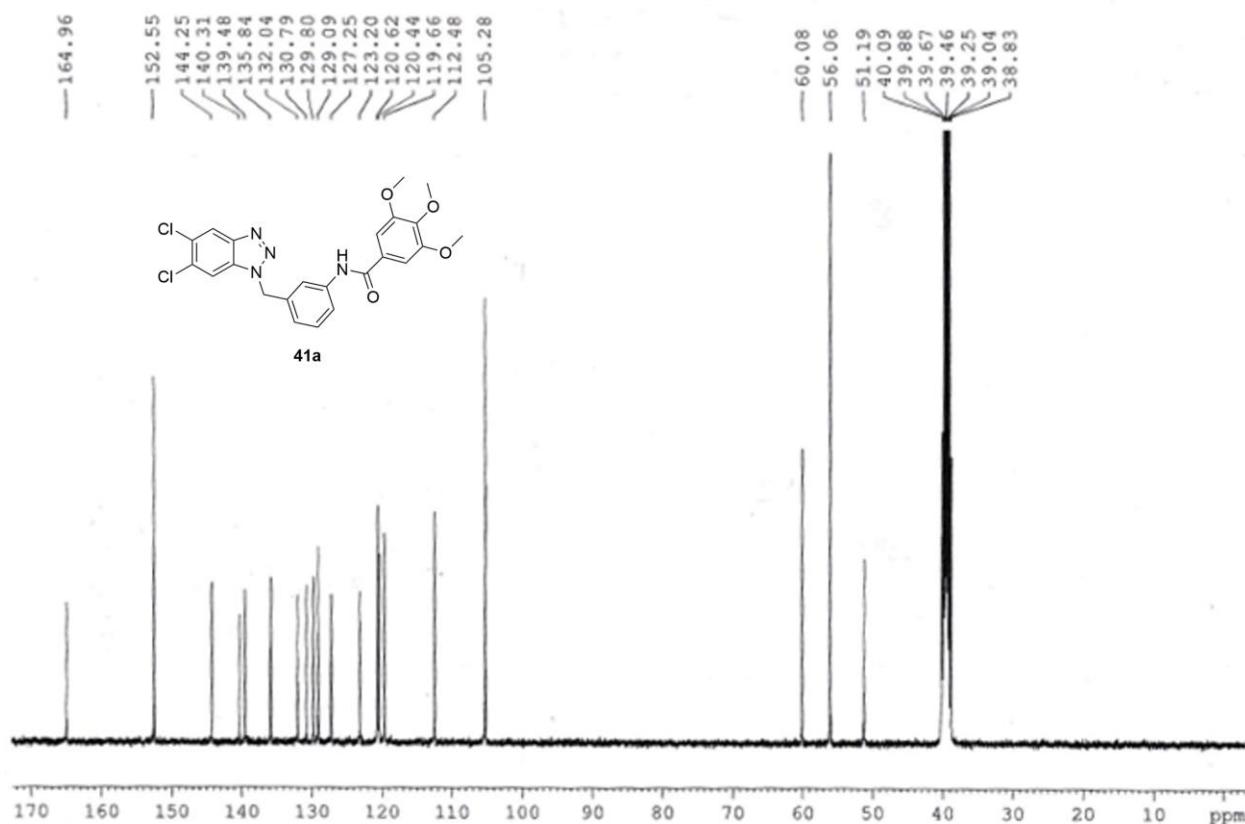
**Figure S6.**  $^1\text{H}$ -NMR for compound **21e**.



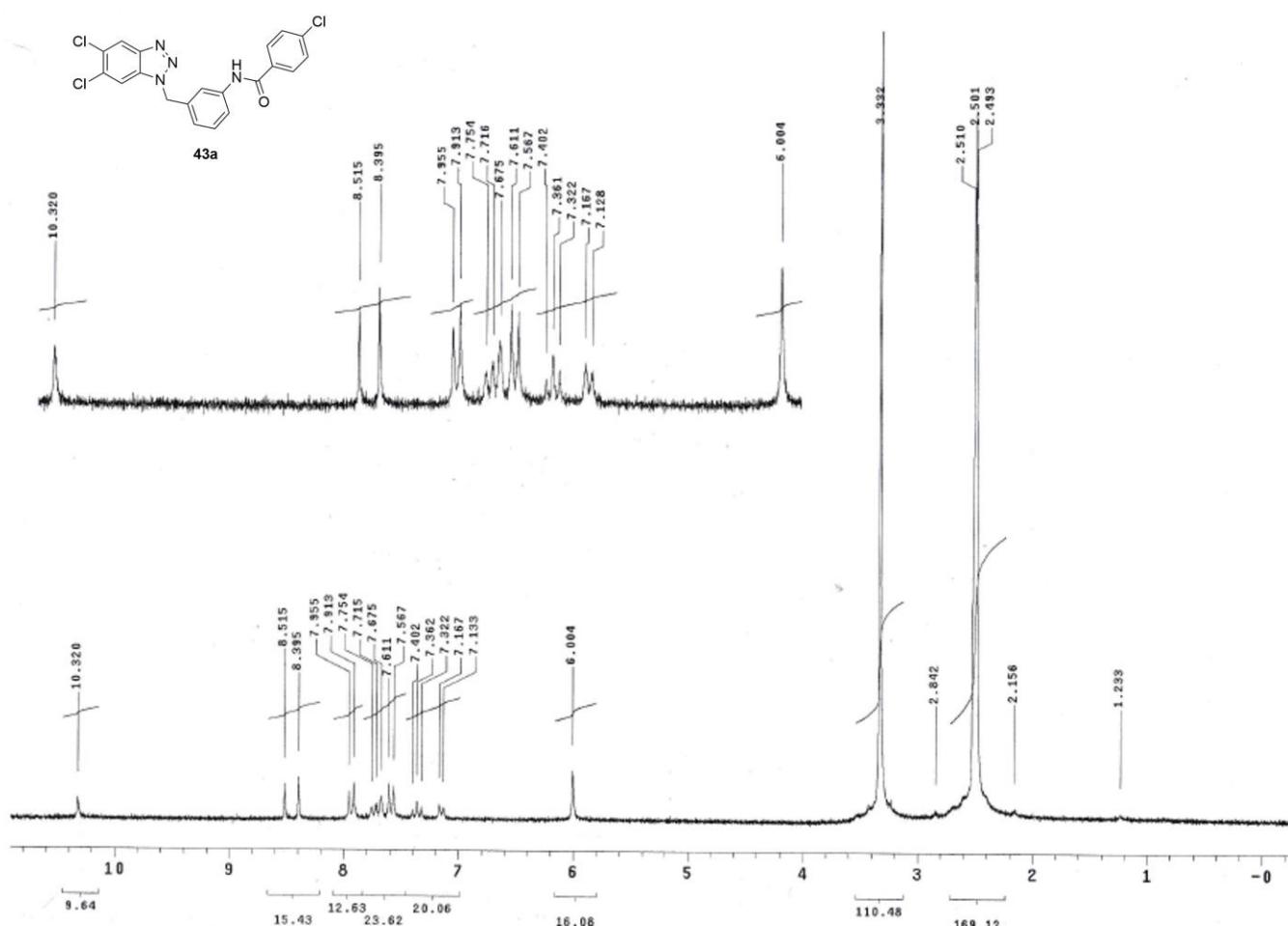
**Figure S7.**  $^{13}\text{C}$ -NMR for compound **21e**.



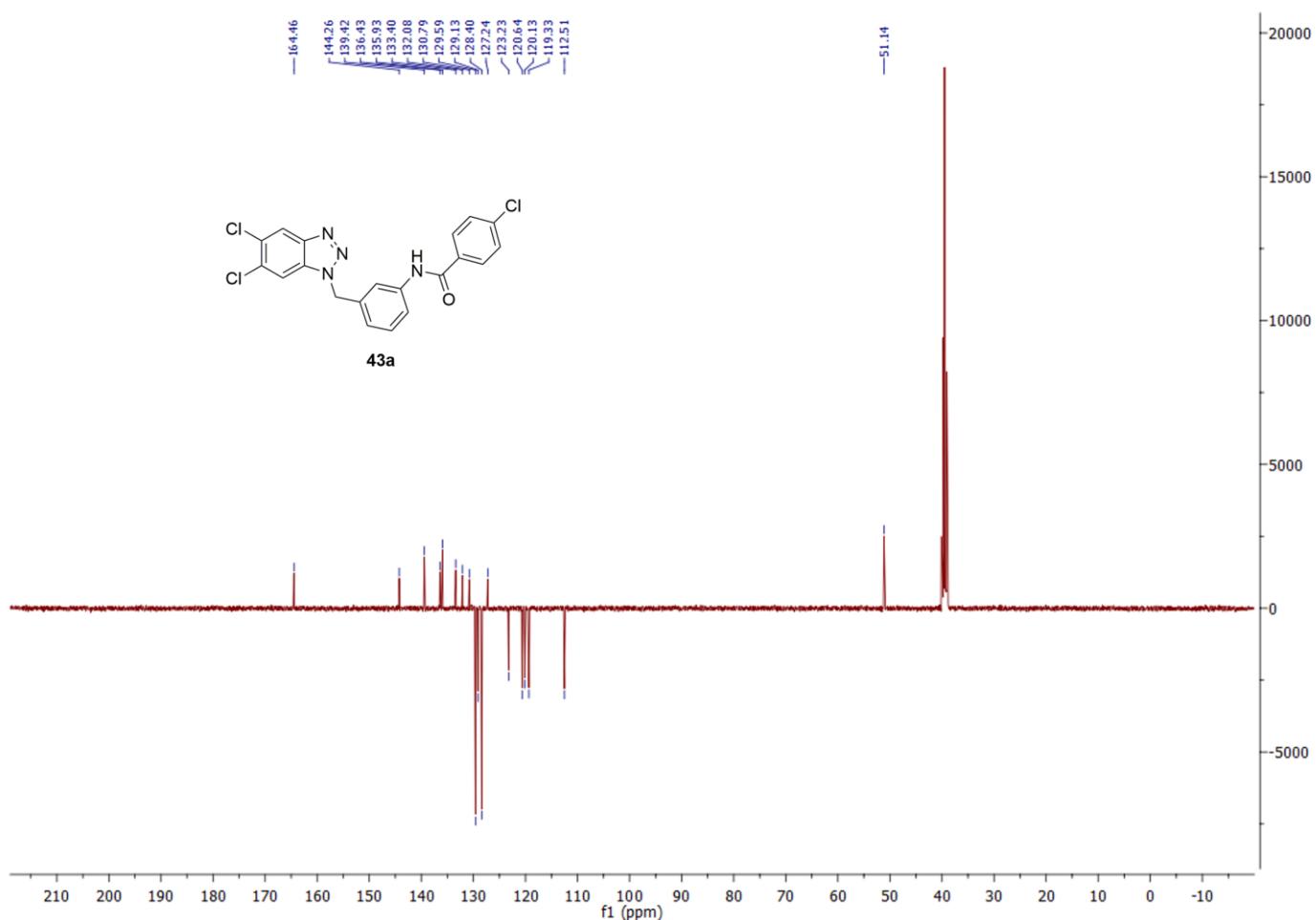
**Figure S8.**  $^1\text{H}$ -NMR for compound 41a.



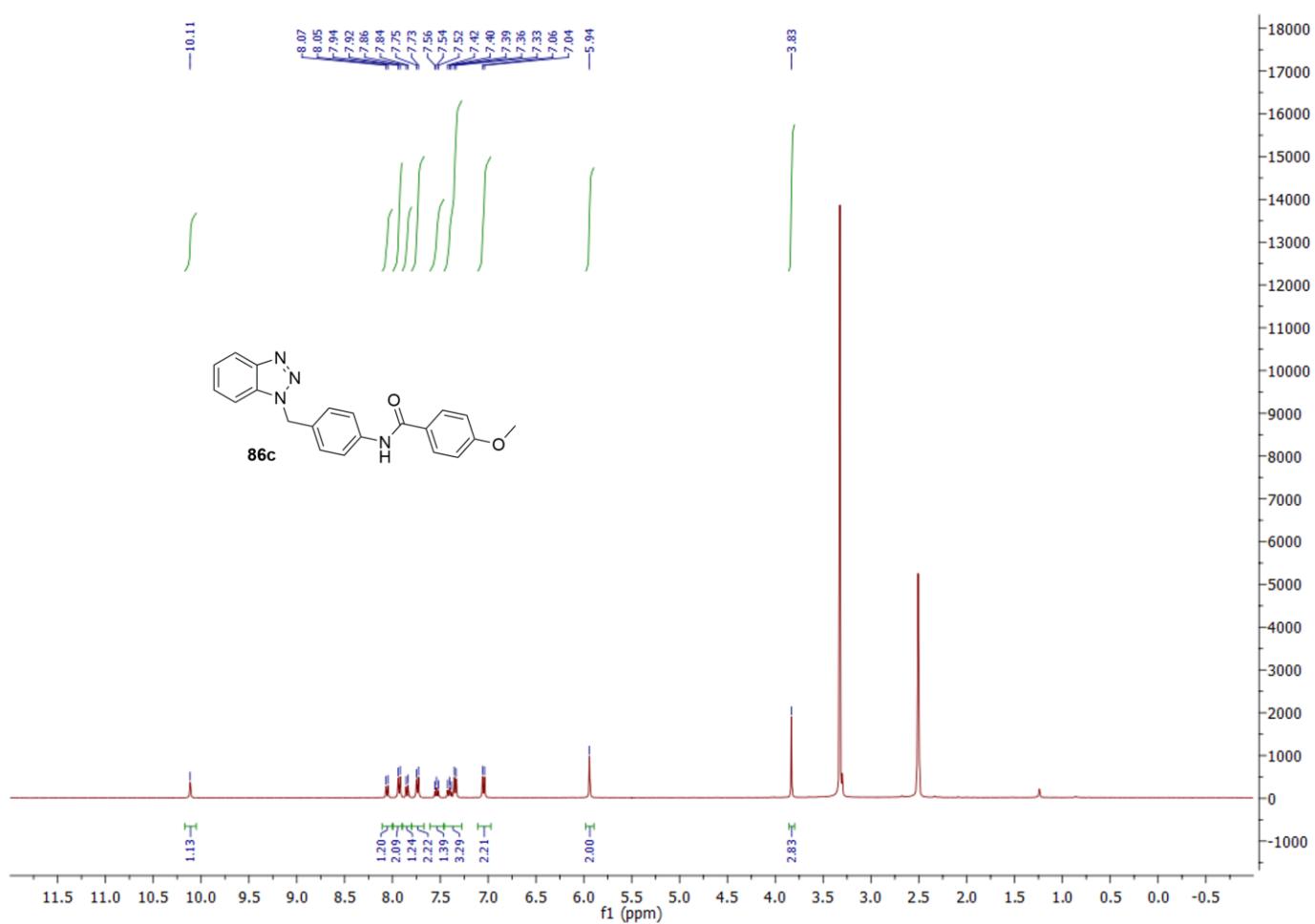
**Figure S9.**  $^{13}\text{C}$ -NMR for compound 41a.



**Figure S10.**  $^1\text{H}$ -NMR for compound 43a.



**Figure S11.**  $^{13}\text{C}$ -NMR for compound 43a.



**Figure S12.**  $^1\text{H}$ -NMR for compound 86c.