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 Supplementary material

J. Serb. Chem. Soc. 82 (3) 889–8153 (2017)

# SUPPLEMENTARY MATERIAL TO Synthesis of novel pyrazoline-based bis(1,2,3-triazole) scaffolds *via* click chemistry

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J. Serb. Chem. Soc. 82 (3) (2017) 241–251

# ANALYTICAL AND SPECTRAL DATA FOR THE SYNTHESIZED COMPOUNDS

(*E*)-1,3-Bis(2-hydroxyphenyl)prop-2-en-1-one (3). Yellow solid; yield: 85 %; m.p. 158–161 °C; IR (KBr, cm<sup>-1</sup>): 3277 (OH), 1629 (C=O), 1573 (C=C), 1263 (Ar-O); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>,  $\delta$  / ppm): 5.62 (1H, *s*, OH), 6.85 (1H, *d*, *J* = 8.0 Hz, Ar-H), 6.92–6.97 (1H, *m*, Ar-H), 6.99–7.04 (2H, *m*, Ar-H), 7.27– -7.32 (1H, *m*, Ar-H), 7.47–7.52 (1H, *m*, Ar-H), 7.61 (1H, *d*, *J* = 7.6 Hz, Ar-H), 7.84 (1H, *d*, *J* = 15.6 Hz, H<sub>a</sub>), 7.94 (1H, *d*, *J* = 8.0 Hz, Ar-H), 8.19 (1H, *d*, *J* = 15.6 Hz, H<sub>β</sub>), 12.88 (1H, *s*, OH); MS: *m/z*, 241.0 [M+H]<sup>+</sup> (100 %).

2,2'-(1-Methyl-4,5-dihydro-1H-pyrazole-3,5-diyl)diphenol (4). Off white solid; yield: 82%; m.p. 120–124 °C; Anal. Calcd. for C<sub>16</sub>H<sub>16</sub>N<sub>2</sub>O<sub>2</sub>: C, 71.62; H, 6.01; N, 10.44 %. Found: C, 71.64; H, 6.04; N, 10.47 %. IR (KBr, cm<sup>-1</sup>): 3054 (OH, H-bonded), 1590 (C=N), 1253 (Ar-O); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>,  $\delta$  / ppm): 2.91 (3H, *s*, NCH<sub>3</sub>), 3.23 (1H, *dd*, *J* = 16.6, 14.9 Hz, H<sub>A</sub>), 3.54 (1H, *dd*, *J* = 16.6, 9.6 Hz, H<sub>B</sub>), 4.11 (1H, *dd*, *J* = 14.9, 9.6 Hz, H<sub>X</sub>), 6.85–6.94 (3H, *m*, Ar-H), 7.02 (1H, *d*, *J* = 8.7 Hz, Ar-H), 7.08 (1H, *dd*, *J* = 7.8, 1.7 Hz, Ar-H), 7.15 (1H, *dd*, *J* = 7.8, 1.7 Hz, Ar-H), 7.22–7.25 (1H, *m*, Ar-H), 7.26–7.31 (1H, *m*, Ar-H), 9.17 (1H, *s*, OH), 10.73 (1H, *s*, OH); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>,  $\delta$  / ppm): 41.9, 42.4, 72.5, 115.6, 117, 117.7, 119.4, 119.9, 121.3, 128.2, 129.5, 129.7, 131.6, 156.1, 158, 159.8. MS: *m*/z, 269.0 [M+H]<sup>+</sup> (100 %).

*1-Methyl-3,5-bis{2-[(prop-2-ynyl)oxy]phenyl}-4,5-dihydro-1H-pyrazole (5).* Pale brown solid; yield: 62 %; m.p. 71–73 °C; Anal. Calcd. for C<sub>22</sub>H<sub>20</sub>N<sub>2</sub>O<sub>2</sub>: C, 76.72; H, 5.85; N, 8.13 %. Found: C, 76.74; H, 5.87; N, 8.14 %. IR (KBr, cm<sup>-1</sup>): 3290 (C=C–H), 1592 (C=N), 1225 (C–O–C); <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>,

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δ / ppm): 2.47 (1H, *t*, *J* = 2.6 Hz, C≡CH), 2.50 (1H, *t*, *J* = 2.6 Hz, C≡CH), 2.85 (3H, *s*, NCH<sub>3</sub>), 2.92 (1H, *dd*, *J* = 16.6 Hz, *J* = 14.9, H<sub>A</sub>), 3.79 (1H, *dd*, *J* = 16.6, 9.6 Hz, H<sub>B</sub>), 4.51 (1H, *dd*, *J* = 14.9, 9.6 Hz, H<sub>X</sub>), 4.70 (2H, *d*, *J* = 2.4 Hz, OCH<sub>2</sub>), 4.73 (2H, *d*, *J* = 2.4 Hz, OCH<sub>2</sub>), 6.98–7.07 (4H, *m*, Ar-H), 7.24–7.30 (2H, *m*, Ar-H), 7.67 (1H, *dd*, *J* = 7.8, 1.7 Hz, Ar-H), 7.81 (1H, *dd*, *J* = 7.8, 1.7 Hz, Ar-H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>, δ / ppm ): 41.9, 44.7, 56.2, 56.3, 67.1, 75.4, 75.6, 78.5, 78.7, 112.1, 113.4, 121.8, 121.9, 123.5, 127.5, 127.9, 129.1, 129.5, 130.2, 149.5, 155.4, 155.6 MS: *m/z*, 345.2 [M+H]<sup>+</sup> (100 %).

(2E)-1,3-Bis{2-[(prop-2-yn-1-yl)oxy]phenyl}prop-2-en-1-one (8). Viscous liquid; yield: 82 %; <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>,  $\delta$  / ppm): 2.51 (1H, d, J = 2.4 Hz, C=CH), 2.52 (1H, d, J = 2.4 Hz, C=CH), 4.77 (2H, d, J = 2.4 Hz, OCH<sub>2</sub>), 4.79 (2H, d, J = 2.4 Hz, OCH<sub>2</sub>), 7.01–7.13 (4H, m, Ar-H), 7.34–7.38 (1H, m, Ar-H), 7.43–7.49 (2H, m, Ar-H and H<sub>a</sub>), 7.50–7.65 (2H, m, Ar-H), 7.96 (1H, d, J = 16.4 Hz, H<sub>β</sub>); MS: m/z, 317.1 [M+H]<sup>+</sup> (100 %).

(2*E*)-1,3-Bis{2-[(1-benzyl-1H-1,2,3-triazol-4-yl)methoxy]phenyl}prop-2-en--1-one (**9**). Viscous liquid; yield: 85 %; Anal. Calcd. for C<sub>35</sub>H<sub>30</sub>N<sub>6</sub>O<sub>3</sub>: C, 72.15; H, 5.19; N, 14.42 %. Found: C, 72.17; H, 5.20; N, 14.45 %. <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 5.23 (2H, *s*, OCH<sub>2</sub>), 5.25 (2H, *s*, OCH<sub>2</sub>), 5.49 (2H, *s*, NCH<sub>2</sub>), 5.61 (2H, *s*, NCH<sub>2</sub>), 6.97 (1H, *t*, *J* = 7.6 Hz, Ar-H), 7.05 (1H, *t*, *J* = 7.2 Hz, Ar-H), 7.15-7.17 (2H, *m*, Ar-H), 7.27–7.30 (6H, *m*, Ar-H), 7.33–7.35 (3H, *m*, Ar-H), 7.37–7.44 (2H, *m*, Ar-H), 7.48–7.55 (3H, *m*, Ar-H and H<sub>α</sub>), 7.60 (1H, *d*, *J* = 7.6 Hz, Ar-H), 7.75 (1H, *d*, *J* = 16 Hz, H<sub>β</sub>), 8.15 (1H, *s*, triazole-H), 8.26 (1H, *s*, triazole-H); MS: *m/z*, 583.2 [M+H]<sup>+</sup> (100%).

*1-Benzyl-4-{[2-(5-{2-[(1-benzyl-1H-1,2,3-triazol-4-yl)methoxy]phenyl}-1-methyl-4,5-dihydro-1H-pyrazol-3-yl)phenoxy]methyl}-1H-1,2,3-triazole* (7*a*). Yellow solid; yield: 90 %; m.p. 104–108 °C; Anal. Calcd. for C<sub>36</sub>H<sub>34</sub>N<sub>8</sub>O<sub>2</sub>: C, 70.80; H, 5.61; N, 18.35 %. Found: C, 70.82; H, 5.62; N, 18.37 %. IR (KBr, cm<sup>-1</sup>): 1598 (C=N), 1229 (C-O-C); <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>,  $\delta$  / ppm): 2.61 (3H, *s*, NCH<sub>3</sub>), 2.67 (1H, *dd*, *J* = 16.8, 14.8 Hz, H<sub>A</sub>), 3.52 (1H, *dd*, *J* = 16.8, 9.6 Hz, H<sub>B</sub>), 4.24 (1H, *dd*, *J* = 14.8, 9.6 Hz, H<sub>X</sub>), 5.16 (2H, *s*, OCH<sub>2</sub>), 5.17 (2H, *s*, OCH<sub>2</sub>), 5.54 (2H, *s*, NCH<sub>2</sub>), 5.57 (2H, *s*, NCH<sub>2</sub>), 6.94–7.01 (2H, *m*, Ar-H), 7.16–7.33 (14H, *m*, Ar-H), 7.44 (1H, *d*, *J* = 7.2 Hz, Ar-H), 7.63 (1H, *dd*, *J* = 8.0, 1.2 Hz, Ar-H), 8.18 (1H, *s*, triazole-H), 8.25 (1H, *s*, triazole-H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>,  $\delta$  / ppm): 41.5, 43.9, 52.7, 52.8, 61.6, 61.7, 66.6, 112.7, 113.7, 120.9, 121.2, 122.4, 124.4, 124.5, 126.7, 127.6, 127.8, 128, 128.2, 128.3, 128.6, 129.0, 129.8, 135.8, 135.9, 142.9, 143.2, 148.3, 155.6, 155.9. MS: *m/z*, 611.4 [M+H]<sup>+</sup> (100%).

 $I-[(4-Bromophenyl)methyl]-4-[(2-{5-[2-({1-[(4-bromophenyl)methyl]-1H -1,2,3-triazol-4-yl}methoxy)phenyl]-1-methyl-4,5-dihydro-1H-pyrazol-3-yl}phen$ oxy)methyl]-1H-1,2,3-triazole (7b). Pale brown solid; yield: 90 %; m.p. 145–-147 °C; Anal. Calcd. for C<sub>36</sub>H<sub>32</sub>Br<sub>2</sub>N<sub>8</sub>O<sub>2</sub>: C, 56.26; H, 4.20; N, 14.58 %. Found:

C, 56.28; H, 4.19; N, 14.60 %. IR (KBr, cm<sup>-1</sup>): 1588 (C=N), 1232 (C–O–C); <sup>1</sup>H-NMR (400 MHz, DMSO- $d_6$ ,  $\delta$  / ppm): 2.61 (3H, s, NCH<sub>3</sub>), 2.68 (1H, dd, J = 16.6, 14.9 Hz, H<sub>A</sub>), 3.52 (1H, dd, J = 16.6, 9.6 Hz, H<sub>B</sub>), 4.24 (1H, dd, J = 14.9, 9.6 Hz, H<sub>X</sub>), 5.16 (2H, s, OCH<sub>2</sub>), 5.17 (2H, s, OCH<sub>2</sub>), 5.53 (2H, s, NCH<sub>2</sub>), 5.56 (2H, s, NCH<sub>2</sub>), 6.94–7.01 (2H, m, Ar-H), 7.12 (2H, d, J = 8.8 Hz, Ar-H), 7.18–7.22 (4H, m, Ar-H), 7.23–7.34 (3H, m, Ar-H), 7.44–7.48 (4H, m, Ar-H), 7.63 (1H, dd, J = 7.8 and 1.6 Hz, Ar-H), 8.18 (1H, s, triazole-H), 8.25 (1H, s, triazole-H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>,  $\delta$  / ppm): 41.9, 44.3, 53.3, 53.4, 62.4, 62.5, 67.9, 112, 113.3, 121.5, 121.6, 122.8, 122.9, 123, 123.1, 127.7, 128.3, 128.9, 129.4, 129.6, 129.8, 132.1, 132.2, 133.6, 133.7, 144.4, 144.6, 149.3, 155.8, 156.2. MS: m/z, 767.2 [M+1]<sup>+</sup> (40 %), 768.1 [M+2]<sup>+</sup> (15 %), 769.2 [M+3]<sup>+</sup> (100 %), 771.2 [M+4]<sup>+</sup> (50 %).

*I*-[(4-tert-*Butylphenyl*)*methyl*]-4-[(2-{5-[2-({*I*-[(4-tert-*butylphenyl*)*methyl*]--*I*H-*I*, 2, 3-triazol-4-yl}*methoxy*)phenyl]-*I*-*methyl*-4, 5-dihydro-*I*H-pyrazol-3-yl}phenoxy)*methyl*]-*I*H-*I*, 2, 3-triazole (7c). Off white solid; yield: 89 %; m.p. 73–76 °C; Anal. Calcd. for C<sub>44</sub>H<sub>50</sub>N<sub>8</sub>O<sub>2</sub>: C, 73.10; H, 6.97; N, 15.50 %. Found: C, 73.14; H, 6.99; N, 15.52 %. IR (KBr, cm<sup>-1</sup>): 1592 (C=N), 1234 (C–O–C); <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 1.20 (9H, *s*, (CH<sub>3</sub>)<sub>3</sub>), 1.22 (9H, *s*, (CH<sub>3</sub>)<sub>3</sub>), 2.61 (3H, *s*, NCH<sub>3</sub>), 2.67 (1H, *dd*, *J* = 16.6, 14.9 Hz, H<sub>A</sub>), 3.57 (1H, *dd*, *J* = 16.6, 9.6 Hz, H<sub>B</sub>), 4.24 (1H, *dd*, *J* = 14.9, 9.6 Hz, H<sub>X</sub>), 5.16 (2H, *s*, OCH<sub>2</sub>), 5.17 (2H, *s*, OCH<sub>2</sub>), 5.48 (2H, *s*, NCH<sub>2</sub>), 5.51 (2H, *s*, NCH<sub>2</sub>), 6.93–7.01 (2H, *m*, Ar-H), 7.11 (2H, *d*, *J* = 7.9 Hz, Ar-H), 7.16–7.31 (10H, *m*, Ar-H), 7.44 (1H, *d*, *J* = 7.9 Hz, Ar-H), 7.64 (1H, *d*, *J* = 7.9 Hz, Ar-H), 8.14 (1H, *s*, triazole-H), 8.22 (1H, *s*, triazole-H); <sup>13</sup>C-NMR (100 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 30.9, 34.2, 41.5, 43.9, 52.5, 61.6, 61.8, 66.7, 112.7, 113.7, 120.9, 121.1, 122.3, 124.3, 124.4, 125.4, 126.6, 127.5, 127.6, 128.2, 129.0, 129.8, 132.9, 133.0, 142.9, 143.2, 148.2, 150.5, 155.6, 155.9. MS: *m*/z, 723.5 [M+H]<sup>+</sup> (100 %).

*I*-[(3-Fluorophenyl)methyl]-4-[(2-{5-[2-({*I*-[(3-fluorophenyl)methyl]-1H--1,2,3-triazol-4-yl}methoxy)phenyl]-1-methyl-4,5-dihydro-1H-pyrazol-3-yl}phenoxy)methyl]-1H-1,2,3-triazole (7d). Pale yellow solid; yield: 75 %; m.p. 56–59 °C; Anal. Calcd. for C<sub>36</sub>H<sub>32</sub>F<sub>2</sub>N<sub>8</sub>O<sub>2</sub>: C, 66.86; H, 4.99; N, 17.33 %. Found: C, 66.89; H, 5.02; N, 17.36 %. IR (KBr, cm<sup>-1</sup>): 1592 (C=N), 1252 (C=O–C); <sup>1</sup>H-NMR (400 MHz, DMSO-d<sub>6</sub>,  $\delta$  / ppm): 2.61 (3H, *s*, NCH<sub>3</sub>), 2.68 (1H, *dd*, *J* = 16.6, 14.03 Hz, H<sub>A</sub>), 3.55 (1H, *dd*, *J* = 16.6, 9.6 Hz, H<sub>B</sub>), 4.26 (1H, *dd*, *J* = 14.03, 9.6 Hz, H<sub>X</sub>), 5.17 (2H, *s*, OCH<sub>2</sub>), 5.18 (2H, *s*, OCH<sub>2</sub>), 5.58 (2H, *s*, NCH<sub>2</sub>), 5.60 (2H, *s*, NCH<sub>2</sub>), 6.95–7.13 (8H, *m*, Ar-H), 7.18–7.33 (6H, *m*, Ar-H), 7.44 (1H, *d*, *J* = 7.9 Hz, Ar-H), 7.63 (1H, *dd*, *J* = 7.9 and 1.7 Hz, Ar-H), 8.21 (1H, *s*, triazole-H), 8.27 (1H, *s*, triazole-H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>,  $\delta$  / ppm): 41.8, 44.2, 53.3, 62.2, 62.4, 67.6, 111.9, 113.2, 114.7, 114.8, 114.9, 115.0, 115.5, 115.6, 121.4, 121.5, 123.0, 123.1, 123.2, 123.3, 123.33, 123.37, 123.4, 127.5, 128.2,

128.9, 129.5, 129.7, 130.5, 130.6, 130.63, 130.7, 136.8, 136.9, 137.0, 144.3, 144.5, 149.2, 155.7, 156.0, 161.5, 164.0; MS: *m*/*z*, 647.3 [M+H]<sup>+</sup> (100 %).

2-({4-[(2-{5-[2-({1-[(2-Hvdroxy-5-nitrophenyl)methyl]-1H-1,2,3-triazol-4--yl}methoxy)phenyl]-1-methyl-4,5-dihydro-1H-pyrazol-3-yl}phenoxy)methyl]--IH-1,2,3-triazol-1-yl{methyl)-4-nitrophenol (7e). A yellow solid; yield: 80 %; m.p. 105-110 °C; Anal. Calcd. for C<sub>36</sub>H<sub>32</sub>N<sub>10</sub>O<sub>8</sub>: C, 59.01; H, 4.40; N, 19.12 %. Found: C, 59.04; H, 4.42; N, 19.16 %. IR (KBr, cm<sup>-1</sup>): 3435 (OH), 1594 (C=N), 1340 (N=O), 1289 (C–O–C); <sup>1</sup>H-NMR (400 MHz, DMSO- $d_6$ ,  $\delta$  / ppm): 2.61 (3H, s, NCH<sub>3</sub>), 2.69 (1H, dd, J = 16.6, 14.03 Hz, H<sub>A</sub>), 3.56 (1H, dd, J = 16.6, 9.6 Hz,  $H_B$ ), 4.26 (1H, dd, J = 14.03, 9.6 Hz,  $H_X$ ), 5.16 (2H, s, OCH<sub>2</sub>), 5.17 (2H, s, OCH2), 5.54 (2H, s, NCH2), 5.57 (2H, s, NCH2), 6.92-7.00 (4H, m, Ar-H), 7.16--7.29 (4H, *m*, Ar-H), 7.42 (1H, *d*, *J* = 7.9 Hz, Ar-H), 7.61 (1H, *dd*, *J* = 7.9, 1.7 Hz, Ar-H), 7.97 (2H, dd, J = 8.7, 2.6 Hz, Ar-H), 8.05–8.09 (2H, m, Ar-H), 8.17 (1H, s, triazole-H), 8.21 (1H, s, triazole-H), 11.53 (2H, bs, OH); <sup>13</sup>C-NMR (100 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 41.4, 43.9, 47.8, 48.5, 61.5, 61.6, 66.4, 112.6, 113.7, 115.7, 120.9, 121, 122.4, 122.9, 123, 124.7, 124.8, 125.9, 126.2, 126, 126.7, 128.2, 128.3, 128.9, 129.7, 139, 142.7, 142.9, 148.2, 155.6, 155.9, 162.1. MS: m/z, 733.3,  $[M+H]^+$  (100 %).

1-[(3-Chlorophenyl)methyl]-4-[(2-{5-[2-({1-[(3-chlorophenyl)methyl]-1H--1,2,3-triazol-4-yl}methoxy)phenyl]-1-methyl-4,5-dihydro-1H-pyrazol-3-yl}phenoxy)methyl]-1H-1,2,3-triazole (7f). Pale yellow solid; yield: 86 %; m.p. 85-89 °C; Anal. Calcd. for C<sub>36</sub>H<sub>32</sub>Cl<sub>2</sub>N<sub>8</sub>O<sub>2</sub>: C, 63.62; H, 4.75; N, 16.49 %. Found: C, 63.64; H, 4.76; N, 16.51 %. IR (KBr, cm<sup>-1</sup>): 1598 (C=N), 1228 (C-O-C); <sup>1</sup>H--NMR (400 MHz, DMSO-d<sub>6</sub>, δ / ppm): 2.61 (3H, s, NCH<sub>3</sub>), 2.69 (1H, dd,  $J = 16.6, 14.9 \text{ Hz}, \text{H}_{A}$ ), 3.53 (1H, dd,  $J = 16.6, 9.6 \text{ Hz}, \text{H}_{B}$ ), 4.26 (1H, dd, J = 14.9, 9.6 Hz, H<sub>x</sub>), 5.17 (2H, s, OCH<sub>2</sub>), 5.18 (2H, s, OCH<sub>2</sub>), 5.57 (2H, s, NCH<sub>2</sub>), 5.60 (2H, s, NCH<sub>2</sub>), 6.93–7.00 (2H, m, Ar-H), 7.10 (1H, d, J = 7.01 Hz, Ar-H), 7.18– -7.36 (11H, m, Ar-H), 7.45 (1H, dd, J = 7.01, 1.7 Hz, Ar-H), 7.63 (1H, dd, J = 7.01, 1.7 Hz, Ar-H), 8.22 (1H, s, triazole-H), 8.28 (1H, s, triazole-H); <sup>13</sup>C--NMR (100 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 41.5, 43.9, 51.9, 52, 61.5, 61.7, 66.5, 112.7, 113.7, 120.9, 121.2, 122.4, 124.6, 124.7, 126.3, 126.4, 126.5, 126.6, 127.7, 128.0, 128.2, 128.3, 129, 129.7, 130.5, 130.6, 133.2, 138.2, 138.3, 143, 143.3, 148.2, 155.6, 155.9. MS: m/z, 679.3  $[M+1]^+$  (100 %), 680.3  $[M+2]^+$  (45 %),  $681.3 [M+3]^+ (75\%), 682.2 [M+4]^+ (30\%).$ 

4-[(2-{1-Methyl-5-[2-({1-[(3-methylphenyl)methyl]-1H-1,2,3-triazol-4-yl}methoxy)phenyl]-4,5-dihydro-1H-pyrazol-3-yl}phenoxy)methyl]-1-[(3-methylphenyl)methyl]-1H-1,2,3-triazole (7g). Pale yellow solid; yield: 72 %; m.p. 79– -82 °C; Anal. Calcd. for  $C_{38}H_{38}N_8O_2$ : C, 71.45; H, 6.00; N, 17.54 %. Found: C, 71.46; H, 6.02; N, 17.56 %. IR (KBr, cm<sup>-1</sup>): 2930 (C–C), 1591 (C=N), 1237 (C–O–C); <sup>1</sup>H-NMR (400 MHz, DMSO- $d_6$ ,  $\delta$  / ppm): 2.20 (6H, s, Ar CH<sub>3</sub>), 2.61 (3H, s, NCH<sub>3</sub>), 2.68 (1H, dd, J = 16.6, 14.9 Hz, H<sub>A</sub>), 3.53 (1H, dd, J = 16.6, 9.6

Hz, H<sub>B</sub>), 4.25 (1H, *dd*, J = 14.9, 9.6 Hz, H<sub>X</sub>), 5.15 (2H, *s*, OCH<sub>2</sub>), 5.16 (2H, *s*, OCH<sub>2</sub>), 5.48 (2H, *s*, NCH<sub>2</sub>), 5.52 (2H, *s*, NCH<sub>2</sub>), 6.93–7.10 (8H, *m*, Ar-H), 7.12–7.30 (6H, *m*, Ar-H), 7.44 (1H, *d*, J = 7.9 Hz, Ar-H), 7.63 (1H, *d*, J = 7.9 Hz, Ar-H), 8.15 (1H, *s*, triazole-H), 8.22 (1H, *s*, triazole-H); <sup>13</sup>C-NMR (125 MHz, CDCl<sub>3</sub>,  $\delta$  / ppm): 21.2, 21.3, 41.9, 44.3, 54.0, 62.4, 62.6, 67.5, 112, 113.2, 121.4, 121.5, 122.8, 122.9, 123.1, 124.9, 125.0, 127.5, 128.2, 128.6, 128.7, 128.9, 128.9, 129.0, 129.4, 129.6, 129.7, 134.4, 134.5, 138.8, 144.3, 144.4, 149.4, 155.9, 156.2; MS: *m/z*, 639.4 [M+H]<sup>+</sup> (100 %).

1-{[2-Fluoro-5-(trifluoromethyl)phenyl]methyl}-4-{[2-(5-{2-[(1-{[2-fluoro--5-(trifluoromethyl)phenyl]methyl}-1H-1,2,3-triazol-4-yl)methoxy]phenyl}-1--methyl-4,5-dihydro-1H-pyrazol-3-yl)phenoxy]methyl}-1H-1,2,3-triazole (7**h**). Pale yellow solid; yield: 70 %; m.p. 68-70 °C; Anal. Calcd. for C38H30F8N8O2: C, 58.31; H, 3.86; N, 14.32 %. Found: C, 58.34; H, 3.89; N, 14.33 %. IR (KBr, cm<sup>-1</sup>): 1600 (C=N), 1119 (C–O–C); <sup>1</sup>H-NMR (400 MHz, DMSO- $d_6$ ,  $\delta$  / ppm): 2.60 (3H, s, NCH<sub>3</sub>), 2.67 (1H, dd, J = 16.6, 14.03 Hz, H<sub>A</sub>), 3.52 (1H, dd, J = 16.6, 9.6 Hz,  $H_B$ ), 4.25 (1H, dd, J = 14.03, 9.6 Hz,  $H_X$ ), 5.17 (2H, s, OCH<sub>2</sub>), 5.18 (2H, s, OCH<sub>2</sub>), 5.70 (2H, s, NCH<sub>2</sub>), 5.73 (2H, s, NCH<sub>2</sub>), 6.92–7.00 (2H, m, Ar-H), 7.18– -7.31 (4H, *m*, Ar-H), 7.38–7.45 (3H, *m*, Ar-H), 7.62 (1H, *d*, *J* = 7.9 Hz, Ar-H), 7.74–7.79 (4H, m, Ar-H), 8.25 (1H, s, triazole-H), 8.30 (1H, s, triazole-H); <sup>13</sup>C--NMR (100 MHz, DMSO-*d*<sub>6</sub>, δ / ppm): 41.4, 43.9, 46.5, 46.6, 61.4, 61.6, 66.5, 112.6, 113.6, 116.8, 117, 120.9, 121.1, 122.2, 122.4, 124, 124.1, 124.2, 124.3, 124.7, 124.8, 124.9, 126.6, 128.2, 128.9, 129.7, 142.8, 143.2, 148.2, 155.5, 155.8. MS: m/z, 783.3  $[M+H]^+$  (100 %).

 $1-[(3,5-Difluorophenyl)methyl]-4-[(2-{5-[2-({1-[(3,5-difluorophenyl)$ methyl]-1H-1,2,3-triazol-4-yl}methoxy)phenyl]-1-methyl-4,5-dihydro-1H-pyrazol-3-yl}phenoxy)methyl]-1H-1,2,3-triazole (7i). Pale green solid; yield: 74 %; m.p. 72-75 °C; Anal. Calcd. for C<sub>36</sub>H<sub>30</sub>F<sub>4</sub>N<sub>8</sub>O<sub>2</sub>: C, 63.34; H, 4.43; N, 16.41 %. Found: C, 63.36; H, 4.45; N, 16.42 %. IR (KBr, cm<sup>-1</sup>): 1628 (C=N), 1119 (C-O-C); <sup>1</sup>H-NMR (400 MHz, DMSO- $d_6$ ,  $\delta$  / ppm): 2.60 (3H, s, NCH<sub>3</sub>), 2.67 (1H, dd,  $J = 17.1, 14.4 \text{ Hz}, H_A$ , 3.53 (1H, dd,  $J = 17.1, 10.09 \text{ Hz}, H_B$ ), 4.24 (1H, dd,  $J = 14.4, 10.09 \text{ Hz}, \text{H}_{X}$ ), 5.17 (2H, s, OCH<sub>2</sub>), 5.19 (2H, s, OCH<sub>2</sub>), 5.59 (2H, s, NCH<sub>2</sub>), 5.61 (2H, s, NCH<sub>2</sub>), 6.88–6.95 (4H, m, Ar-H), 6.98 (2H, q, J = 7.4 Hz, Ar-H), 7.08–7.34 (6H, m, Ar-H), 7.42 (1H, dd, J = 7.4, 1.7 Hz, Ar-H), 7.61 (1H, dd, J = 7.4, 1.7 Hz, Ar-H), 8.23 (1H, s, triazole-H), 8.28 (1H, s, triazole-H); <sup>13</sup>C--NMR (100 MHz, DMSO- $d_6$ ,  $\delta$  / ppm): 41.4, 43.9, 51.6, 61.5, 61.7, 66.5, 103.4, 103.6, 103.9, 110.8, 110.9, 111, 111.07, 111.1, 111.2, 112.7, 113.7, 120.9, 121.1, 122.4, 124.7, 124.8, 126.6, 128.2, 128.3, 129, 129.7, 139.9, 140, 140.1, 140.2, 143, 143.3, 148.2, 155.5, 155.8, 161, 161.2, 163.5, 163.6. MS: m/z, 683.3  $[M+H]^+$  (100 %).

 $I-\{[2,5-Bis(trifluoromethyl)phenyl]methyl\}-4-\{[2-(5-\{2-[(1-\{[2,5-bis(trifluoromethyl)phenyl]methyl\}-IH-1,2,3-triazol-4-yl)methoxy]phenyl\}-1-methyl-4,5-$ 

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-*dihydro-1*H-*pyrazol-3-yl)phenoxy]methyl}-1*H-*1*,*2*,*3-triazole* (7*j*). Off white solid; yield: 85 %; m.p. 77–80 °C; Anal. Calcd. for C<sub>40</sub>H<sub>30</sub>F<sub>12</sub>N<sub>8</sub>O<sub>2</sub>: C, 54.43; H, 3.43; N, 12.69 %. Found: C, 54.45; H, 3.44; N, 12.71 %. IR (KBr, cm<sup>-1</sup>): 1595 (C=N), 1127 (C–O–C); <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>,  $\delta$  / ppm): 2.61 (3H, *s*, NCH<sub>3</sub>), 2.67 (1H, *dd*, *J* = 16.6, 14.9 Hz, H<sub>A</sub>), 3.43 (1H, *dd*, *J* = 16.6, 9.6 Hz, H<sub>B</sub>), 4.24 (1H, *dd*, *J* = 14.9, 9.6 Hz, H<sub>X</sub>), 5.17 (2H, *s*, OCH<sub>2</sub>), 5.19 (2H, *s*, OCH<sub>2</sub>), 5.83 (2H, *s*, NCH<sub>2</sub>), 5.87 (2H, *s*, NCH<sub>2</sub>), 6.92–6.98 (2H, *m*, Ar-H), 7.15–7.31 (4H, *m*, Ar-H), 7.43 (1H, *dd*, *J* = 7.9, 1.7 Hz, Ar-H), 7.50 (2H, *d*, *J* = 14.0 Hz, Ar-H), 7.62 (1H, *dd*, *J* = 7.9, 1.7 Hz, Ar-H), 7.91–7.95 (2H, *m*, Ar-H), 7.99–8.01 (2H, *m*, Ar-H), 8.26 (1H, *s*, triazole-H), 8.32 (1H, *s*, triazole-H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>,  $\delta$  / ppm): 41.8, 44.3, 49.7, 62.2, 62.5, 67.6, 111.8, 113.2, 121.4, 121.5, 121.6, 121.9, 123.2, 123.6, 124.1, 124.6, 125.7, 126.8, 127, 127.1, 127.6, 128.3, 129, 129.6, 129.7, 130.9, 131.2, 134.6, 134.7, 135, 144.8, 144.9, 149.2, 155.8, 156.1. MS: *m/z*, 883.2 [M+H]<sup>+</sup> (100 %).

1-[(4-Fluorophenyl)methyl]-4-[(2-{5-[2-({1-[(4-fluorophenyl)methyl]-1H--1,2,3-triazol-4-yl{methoxy)phenyl]-1-methyl-4,5-dihydro-1H-pyrazol-3-yl{phenoxy)methyl]-1H-1,2,3-triazole (7k). A brown solid; yield: 70 %; m.p. 70-74 °C; Anal. Calcd. for C<sub>36</sub>H<sub>32</sub>F<sub>2</sub>N<sub>8</sub>O<sub>2</sub>: C, 66.86; H, 4.99; F, 5.88; N, 17.33 %. Found: C, 66.89; H, 4.97; F, 5.90; N, 17.35 %. IR (KBr, cm<sup>-1</sup>): 1595 (C=N), 1227 (C-O-C); <sup>1</sup>H-NMR (400 MHz, DMSO- $d_6$ ,  $\delta$  / ppm): 2.61 (3H, s, NCH<sub>3</sub>), 2.67 (1H, dd,  $J = 16.6, 14.9 \text{ Hz}, \text{H}_{A}$ , 3.51 (1H, dd,  $J = 16.6, 9.6 \text{ Hz}, \text{H}_{B}$ ), 4.24 (1H, dd, J == 14.9, 9.6 Hz, H<sub>x</sub>), 5.16 (2H, s, OCH<sub>2</sub>), 5.17 (2H, s, OCH<sub>2</sub>), 5.53 (2H, s, NCH<sub>2</sub>), 5.56 (2H, s, NCH<sub>2</sub>), 6.94–7.06 (2H, m, Ar-H), 7.07–7.12 (4H, m, Ar-H), 7.19– -7.33 (8H, *m*, Ar-H), 7.44 (1H, *dd*, *J* = 7.9, 1.7 Hz, Ar-H), 7.63 (1H, *dd*, *J* = 7.9, 1.7 Hz, Ar-H), 8.17 (1H, s, triazole-H), 8.24 (1H, s, triazole-H); <sup>13</sup>C-NMR (125 MHz, CDCl<sub>3</sub>, δ / ppm): 41.8, 44.1, 53.1, 53.2, 62.2, 62.4, 67.6, 111.9, 113.1, 115.8, 115.8, 115.9, 116.0, 121.4, 121.5, 121.6, 121.7, 122.9, 123.0, 127.5, 128.2, 128.8, 129.4, 129.5, 129.6, 129.71, 129.73, 129.77, 129.8, 129.9, 130.37, 130.39, 130.4, 130.5, 144.2, 144.4, 149.2, 155.7, 156.1, 161.63, 161.64, 163.6; MS: m/z, 647.3 [M+H]<sup>+</sup> (100 %).

*1-[(3-Fluoro-4-methoxyphenyl)methyl]-4-[(2-{5-[2-({1-[(3-fluoro-4-methoxyphenyl)methyl]-1*H-1,2,3-triazol-4-yl}methoxy)phenyl]-1-methyl-4,5-dihydro--*1*H-pyrazol-3-yl}phenoxy)methyl]-1H-1,2,3-triazole (7I). Grey solid; yield: 86 %; m.p. 88–92 °C; Anal. Calcd. for  $C_{38}H_{36}F_2N_8O_4$ : C, 64.58; H, 5.13; N, 15.85 %. Found: C, 64.60; H, 5.15; N, 15.88 %. IR (KBr, cm<sup>-1</sup>): 1589 (C=N), 1277 (C–O–C); <sup>1</sup>H-NMR (500 MHz, DMSO-*d*<sub>6</sub>,  $\delta$  / ppm): 2.61 (3H, *s*, NCH<sub>3</sub>), 2.68 (1H, *dd*, *J* = 16.6, 14.1 Hz, H<sub>A</sub>), 3.54 (1H, *dd*, *J* = 16.6, 10.2 Hz, H<sub>B</sub>), 3.77 (3H, *s*, OCH<sub>3</sub>), 3.78 (3H, *s*, OCH<sub>3</sub>), 4.23 (1H, *dd*, *J* = 14.1, 10.2 Hz, H<sub>x</sub>), 5.16 (2H, *s*, OCH<sub>2</sub>), 5.17 (2H, *s*, OCH<sub>2</sub>), 5.47 (2H, *s*, NCH<sub>2</sub>), 5.50 (2H, *s*, NCH<sub>2</sub>), 6.93–7.06 (6H, *m*, Ar-H), 7.13–7.30 (6H, *m*, Ar-H), 7.43 (1H, *d*, *J* = 7.8 Hz, Ar-H), 7.62 (1H, *d*, *J* = 7.8 Hz, Ar-H), 8.18 (1H, *s*, triazole-H), 8.24 (1H, *s*, triazole-H); <sup>13</sup>C-

-NMR (125 MHz, CDCl<sub>3</sub>,  $\delta$  / ppm): 41.9, 44.2, 53.2, 56.2, 62.4, 62.6, 67.7, 111.9, 113.2, 113.5, 113.6, 115.8, 115.9, 116, 116.1, 121.4, 121.5, 122.8, 122.9, 123.1, 124.11, 124.14, 124.169, 127.2, 127.3, 127.4, 127.6, 128.2, 128.9, 129.6, 129.8, 144.3, 144.5, 147.9, 148.1, 149.4, 151.3, 153.2, 155.9, 156.2; MS: *m*/*z*, 707.3 [M+H]<sup>+</sup> (100 %).

*1-{[4-(1-Methylethyl]phenyl]methyl}-4-{[2-(1-methyl-5-{2-[(1-{[4-(1--methylethyl]phenyl]methyl}-1H-1,2,3-triazol-4-yl]methoxy]phenyl}-4,5-dihydro-*-*1*H-*pyrazol-3-yl)phenoxy]methyl}-1*H-*1,2,3-triazole* (7*m*). Grey solid; yield: 75 %; m.p. 84–88 °C; Anal. Calcd. for C<sub>42</sub>H<sub>46</sub>N<sub>8</sub>O<sub>2</sub>: C, 72.60; H, 6.67; N, 16.13 %. Found: C, 72.62; H, 6.66; N, 16.14 %. IR (KBr, cm<sup>-1</sup>): 1591 (C=N), 1235 (C–O–C); <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>,  $\delta$  / ppm): 1.13 (12H, *t*, *J* = 6.4 Hz, (CH<sub>3</sub>)<sub>2</sub>), 2.61 (3H, *s*, NCH<sub>3</sub>), 2.67 (1H, *dd*, *J* = 16.6, 14.0 Hz, H<sub>A</sub>), 2.78–2.84 (2H, *m*, CH(CH<sub>3</sub>)<sub>2</sub>), 3.53 (1H, *dd*, *J* = 16.6, 9.6 Hz, H<sub>B</sub>), 4.23 (1H, *dd*, *J* = 14.0, 9.6 Hz, H<sub>X</sub>), 5.16 (2H, *s*, OCH<sub>2</sub>), 5.17 (2H, *s*, OCH<sub>2</sub>), 5.48 (2H, *s*, NCH<sub>2</sub>), 5.51 (2H, *s*, NCH<sub>2</sub>), 6.94–7.01 (2H, *m*, Ar-H), 7.10–7.33 (12H, *m*, Ar-H), 7.43 (1H, *dd*, *J* = 7.9, 1.7 Hz, Ar-H), 7.64 (1H, *dd*, *J* = 7.9, 1.7 Hz, Ar-H), 8.15 (1H, *s*, triazole-H); 8.23 (1H, *s*, triazole-H); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>,  $\delta$  / ppm): 23.8, 33.8, 42.0, 44.3, 53.9, 62.3, 62.6, 67.4, 112.0, 113.3, 121.5, 122.9, 127.1, 127.2, 127.5, 128.1, 128.2, 128.3, 129.0, 129.6, 129.9, 131.7, 131.9, 149.5, 155.9, 156.2; MS: *m/z*, 695.4 [M+H]<sup>+</sup> (100 %).



IR, NMR AND MASS SPECTRA FOR THE SYNTHESIZED COMPOUNDS

Fig. S-1. IR spectrum of compound 3.

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Fig. S-2. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) spectrum of compound  $\mathbf{3}$ .



Fig. S-3. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) spectrum of compound **3**.



Fig. S-4. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) spectrum of compound **3**.



Fig. S-5. Mass spectrum of compound **3**.

SUPPLEMENTARY MATERIAL





SUPPLEMENTARY MATERIAL



Fig. S-10. Mass spectrum of compound 4.



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Fig. S-16. Mass spectrum of compound 5.



Fig. S-17. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) spectrum of compound 8.



Fig. S-18. <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>) spectrum of compound 8.



Fig. S-19. Mass spectrum of compound 8.



Fig. S-20. <sup>1</sup>H-NMR (400 MHz, DMSO- $d_6$ ) spectrum of compound 9.





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Fig. S-22. <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound **9**.

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Fig. S-23. Mass spectrum of compound 9.

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Fig. S-25. <sup>1</sup>H-NMR (400 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound 7a.









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Fig. S-31. Mass spectrum of compound 7a.



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Fig. S-34. <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) spectrum of compound 7b.





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Fig. S-36. <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) spectrum of compound **7b**.



Fig. S-37. Mass spectrum of compound 7b.

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Fig. S-41. <sup>13</sup>C-NMR (100 MHz, DMSO- $d_6$ ) spectrum of compound 7c.

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Fig. S-42. <sup>13</sup>C-NMR (100 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound 7c.



Fig. S-43. Mass spectrum of compound 7c.



Fig. S-45. <sup>1</sup>H-NMR (400 MHz, DMSO- $d_6$ ) spectrum of compound 7d.





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Fig. S-48. <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) spectrum of compound 7d.

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Fig. S-49. Mass spectrum of compound 7d.

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Fig. S-52. <sup>13</sup>C-NMR (100 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound 7e.



Fig. S-53. <sup>13</sup>C-NMR (100 MHz, DMSO- $d_6$ ) spectrum of compound 7e.





Fig. S-55. IR spectrum of compound 7f.



Fig. S-57. <sup>13</sup>C-NMR (100 MHz, DMSO- $d_6$ ) spectrum of compound 7f.



Fig. S-59. <sup>13</sup>C-NMR (100 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound 7f.

SUPPLEMENTARY MATERIAL











Fig. S-64. <sup>13</sup>C-NMR (125 MHz, CDCl<sub>3</sub>) spectrum of compound 7g.



Fig. S-65.  $^{13}\text{C-NMR}$  (125 MHz, CDCl\_3) spectrum of compound 7g.



Fig. S-66. Mass spectrum of compound 7g.



Fig. S-68. <sup>1</sup>H-NMR (400 MHz, DMSO- $d_6$ ) spectrum of compound **7h**.

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Fig. S-70. <sup>13</sup>C-NMR (100 MHz, DMSO- $d_6$ ) spectrum of compound 7h.



Fig. S-71. <sup>13</sup>C-NMR (100 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound 7h.



Fig. S-72. Mass spectrum of compound 7h.

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Fig. S-77. <sup>13</sup>C-NMR (100 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound 7i.

SUPPLEMENTARY MATERIAL



Fig. S-78. Mass spectrum of compound 7i.

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Fig. S-81. <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>) spectrum of compound 7j.







Fig. S-83. Mass spectrum of compound 7j.



Fig. S-84. IR spectrum of compound 7k.



Fig. S-86. <sup>13</sup>C-NMR (125 MHz, CDCl<sub>3</sub>) spectrum of compound 7k.

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-163.608 < 161.647 161.636156.117 155.769 -115.976 -115.845 -115.803 -113.115 -111.944 -144.410-144.207130.442 130.416 130.397 130.370 129.927 129.840 129.840 129.644 129.587 129.471 128.859 128.859 -149.283 29.734 2 Compound 7k 155 150 145 140 135 130 125 120 115 ppm 165 160 Fig. S-87. <sup>13</sup>C-NMR (125 MHz, CDCl<sub>3</sub>) spectrum of compound 7k. 44.164 -77.247 -76.993 -76.738  $< 62.424 \\ 62.251$ 53.204 41.851 





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SUPPLEMENTARY MATERIAL



Fig. S-89. Mass spectrum of compound 7k.





Fig. S-91. <sup>1</sup>H-NMR (500 MHz, DMSO- $d_6$ ) spectrum of compound 7l



Fig. S-93. <sup>13</sup>C-NMR (125 MHz, CDCl<sub>3</sub>) spectrum of compound 71.

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 62. -56.225 -67.693 N Compound 7I 70 75 60 80 65 55 50 45 ppm

Fig. S-94.  $^{13}$ C-NMR (125 MHz, CDCl<sub>3</sub>) spectrum of compound 71.



Fig. S-95. Mass spectrum of compound 7l.

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Fig. S-99.  $^{13}$ C-NMR (100 MHz, CDCl<sub>3</sub>) spectrum of compound 7m.





Fig. S-101. Mass spectrum of compound 7m.