

## Supporting Information

## Sodium dodecyl sulfate (SDS) Assisted Synthesis of 2'-Aminobenzothiazolo-methyl naphthols in Water

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Spectroscopic data for **4a-p**

**1-((benzo[d]thiazol-2-ylamino)(phenyl)-methyl)naphthalen-2-ol (4a):** mp 199-201 (200-201).<sup>[1a]</sup>  $\delta_{\text{H}}$  (400 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  8.44 (brs, 1H), 7.96 (s, 1H), 7.75 (d, *J* = 8.1 Hz, 1H), 7.70 (d, *J* = 8.9 Hz, 1H), 7.53 (d, *J* = 7.8 Hz, 1H), 7.47 (d, *J* = 8.0 Hz, 1H), 7.42 – 7.32 (m, 3H), 7.31 – 7.21 (m, 5H), 7.20 – 7.12 (m, 2H), 7.04 (t, *J* = 7.6 Hz, 1H).  $\delta_{\text{C}}$  (100 MHz, DMSO-*d*<sub>6</sub>) 166.77, 153.65, 152.58, 142.97, 132.60, 131.26, 130.03, 129.11, 129.01, 128.56, 126.67, 126.63, 126.51, 125.90, 124.29, 122.87, 121.45, 121.35, 119.16, 118.85, 118.57, 53.53. *m/z* (ESI) calcd. for C<sub>24</sub>H<sub>19</sub>N<sub>2</sub>OS<sup>+</sup> [M + H]<sup>+</sup> 383.1213, found 383.0871.

**1-((benzo[d]thiazol-2-ylamino)(4-methoxy-phenyl)methyl)naphthalen-2-ol (4b):** mp 165-167 (172-173).<sup>[1a]</sup>  $\delta_{\text{H}}$  8.45 (brs, 1H), 7.95 (s, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.69 (d, *J* = 8.8 Hz, 1H), 7.52 (d, *J* = 7.8 Hz, 1H), 7.48 (d, *J* = 8.0 Hz, 1H), 7.39 – 7.37 (m, 1H), 7.33 – 7.20 (m, 5H), 7.04 (d, *J* = 7.5 Hz, 2H), 6.76 (d, *J* = 8.7 Hz, 2H), 3.72 (s, 3H).  $\delta_{\text{C}}$  (100 MHz, DMSO-*d*<sub>6</sub>) 166.73, 158.17, 153.58, 152.59, 134.63, 132.59, 131.17, 129.90, 129.13, 128.99, 127.71, 126.59, 125.89, 124.41, 122.83, 121.40, 121.33, 119.21, 118.88, 118.50, 113.98, 55.42, 53.24. *m/z* (ESI) calcd. for C<sub>25</sub>H<sub>21</sub>N<sub>2</sub>O<sub>2</sub>S<sup>+</sup> [M + H]<sup>+</sup> 413.1318, found 413.1018.

**1-((benzo[d]thiazol-2-ylamino)(3-methoxy-phenyl)methyl)naphthalen-2-ol (4c):** mp 184-186.  $\delta_{\text{H}}$  (400 MHz, DMSO-*d*<sub>6</sub>) 8.49 (brs, 1H), 7.95 (s, 1H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.69 (d, *J* = 8.9 Hz, 1H), 7.53 (d, *J* = 7.8 Hz, 1H), 7.47 (d, *J* = 8.0 Hz, 1H), 7.40 – 7.34 (m, 1H), 7.26 – 7.22 (m, 3H), 7.15 (t, *J* = 7.9 Hz, 1H), 7.09 (d, *J* = 7.9 Hz, 1H), 7.04 (t, *J* = 7.7 Hz, 1H), 6.95 (s, 1H), 6.92 (d, *J* = 7.9 Hz, 1H), 6.74 – 6.68 (m, 1H), 3.69 (s, 3H).  $\delta_{\text{C}}$  (100 MHz, DMSO-*d*<sub>6</sub>) 166.72, 159.60, 153.60, 152.54, 144.67, 132.58, 131.22, 130.01, 129.68, 129.07, 128.99, 126.68, 125.90, 122.88, 121.45, 121.35, 119.09, 118.94, 118.83, 118.56, 113.08, 111.11, 55.33, 53.43. *m/z* (ESI) calcd. for C<sub>25</sub>H<sub>21</sub>N<sub>2</sub>O<sub>2</sub>S<sup>+</sup> [M + H]<sup>+</sup> 413.1318, found 413.1081.

**1-((benzo[d]thiazol-2-ylamino)(2-methoxy-phenyl)methyl)naphthalen-2-ol (4d):** mp 165-167.  $\delta_{\text{H}}$  (400 MHz, DMSO-*d*<sub>6</sub>) 10.47 (s, 2H), 8.16 (d, *J* = 8.7 Hz, 1H), 7.73 (d, *J* = 7.9 Hz, 1H), 7.67 (d, *J* = 8.8 Hz, 1H), 7.61 – 7.51 (m, 3H), 7.50 – 7.45 (m, 2H), 7.43 – 7.41 (m, 2H), 7.36 – 7.19 (m, 5H), 7.15 (t, *J* = 7.3 Hz, 1H), 7.06 (t, *J* = 7.4 Hz, 1H), 7.02 – 7.00 (m, 1H), 6.88 – 6.83 (m, 2H), 3.79 (s, 3H).  $\delta_{\text{C}}$  (100 MHz, DMSO-*d*<sub>6</sub>) 166.16, 157.20, 153.84, 152.79, 133.09, 131.06, 130.09, 129.45, 128.81, 128.71, 128.40, 126.33, 125.96, 125.79, 123.97, 122.60, 121.23, 121.14, 120.15, 119.03, 118.68, 118.40, 111.38, 55.82, 50.63. *m/z* (ESI) calcd. for C<sub>25</sub>H<sub>21</sub>N<sub>2</sub>O<sub>2</sub>S<sup>+</sup> [M + H]<sup>+</sup> 413.1318, found 413.0927.

**1-((benzo[d]thiazol-2-ylamino)(2,4-dimethoxyphenyl)methyl)naphthalen-2-ol (4e):** mp 161-163.  $\delta_{\text{H}}$  (400 MHz, DMSO-*d*<sub>6</sub>) 8.09 (d, *J* = 8.6 Hz, 1H), 7.78 – 7.71 (m, 2H), 7.68 (d, *J* = 8.9 Hz, 2H), 7.60 – 7.50 (m, 3H), 7.45 (t, *J* = 7.1 Hz, 2H), 7.36 (d, *J* = 8.5 Hz, 2H), 7.32 – 7.20 (m, 4H), 7.14 – 6.94 (m, 2H), 6.90 (s, 1H), 6.74 – 6.50 (m, 1H), 6.48 – 6.46 (m, 2H), 6.37 (dd, *J* = 8.6, 2.3 Hz, 1H), 3.90 (d, *J* = 13.3 Hz, 3H), 3.82 (s, 3H).  $\delta_{\text{C}}$  (100 MHz, DMSO-*d*<sub>6</sub>) 166.16, 160.05, 158.19, 153.72, 152.84, 133.08, 131.00, 129.51, 129.33, 128.81, 128.74, 126.33, 125.77, 123.98, 122.61, 122.12, 121.21, 121.05, 119.04, 118.83, 118.33, 104.59, 98.77, 55.96, 55.59, 50.41. *m/z* (ESI) calcd. for C<sub>26</sub>H<sub>23</sub>N<sub>2</sub>O<sub>3</sub>S<sup>+</sup> [M + H]<sup>+</sup> 443.1424, found 443.0948.

**1-((benzo[d]thiazol-2-ylamino)(p-tolyl)methyl)naphthalen-2-ol (4f):** mp 176-178 (182–183).<sup>[1b]</sup>  $\delta_{\text{H}}$  (400 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  8.52 (brs, 1H), 7.93 (brs, 1H), 7.75 (d, *J* = 8.1 Hz, 1H), 7.69 (d, *J* = 8.8 Hz, 1H), 7.52 (d, *J* = 7.9 Hz, 1H), 7.47-7.49 (m, 1H), 7.37 (t, *J* = 7.2 Hz, 1H), 7.23-7.31 (m, 5H), 7.03-7.06 (m, 4H), 2.27 (s, 3H).  $\delta_{\text{C}}$  (100 MHz, DMSO-*d*<sub>6</sub>) 166.75, 153.58, 152.57, 139.88, 135.58, 132.58, 131.20, 129.93, 129.13, 128.97, 126.59, 126.45, 125.88, 124.45, 122.83, 121.40, 121.33, 119.24, 118.85, 118.51, 53.38, 21.03. *m/z* (ESI) calcd. for C<sub>25</sub>H<sub>21</sub>N<sub>2</sub>OS<sup>+</sup> [M + H]<sup>+</sup> 397.1369, found 397.0871.

**1-((benzo[d]thiazol-2-ylamino)(4-chloro-phenyl)methyl)naphthalen-2-ol (4g):** mp 206-208 (208-209).<sup>[1a]</sup>  $\delta_{\text{H}}$  (400 MHz, DMSO-*d*<sub>6</sub>) 7.92 (s, 1H), 7.81 – 7.68 (m, 2H), 7.53 (d, *J* = 7.6 Hz, 2H), 7.47 – 7.36 (m, 2H), 7.36 – 7.24 (m, 5H), 7.22 – 7.20 (m, 2H), 7.12 – 7.04 (m, 2H).  $\delta_{\text{C}}$  (100 MHz, DMSO-*d*<sub>6</sub>) 166.66, 153.68, 152.51, 142.18, 132.48, 131.32, 131.15, 130.26, 129.08, 128.52, 128.39, 126.86, 125.91, 122.95, 121.55, 121.38, 118.82, 118.68, 53.05. *m/z* (ESI) calcd. for C<sub>24</sub>H<sub>18</sub>ClN<sub>2</sub>OS<sup>+</sup> [M + H]<sup>+</sup> 417.0823, found 417.0537.

**1-((benzo[d]thiazol-2-ylamino)(3-chloro-phenyl)methyl)naphthalen-2-ol (4h):** mp 192-194.  $\delta_{\text{H}}$  (400 MHz, DMSO-*d*<sub>6</sub>) 8.49 (brs, 1H), 8.06 – 7.84 (m, 1H), 7.83 – 7.69 (m, 2H), 7.65 – 7.55 (m, 2H), 7.49 (dd, *J* = 8.0, 2.6 Hz, 1H), 7.45 – 7.36 (m, 3H), 7.36 – 7.13 (m, 7H), 7.08 – 7.04 (m, 1H).  $\delta_{\text{C}}$  (100 MHz, DMSO-*d*<sub>6</sub>) 166.62, 153.68, 152.40, 145.86, 133.32, 132.46, 131.29, 130.52, 130.35, 129.11, 129.01, 126.99, 126.66, 126.16, 125.94, 125.30, 123.87, 123.01, 121.61, 121.42, 118.82, 118.70, 118.53, 53.13. *m/z* (ESI) calcd. for C<sub>24</sub>H<sub>18</sub>ClN<sub>2</sub>OS<sup>+</sup> [M + H]<sup>+</sup> 417.0823, found 417.0507 [M + H]<sup>+</sup>.

**1-((benzo[d]thiazol-2-ylamino)(pyridin-4-yl)methyl)naphthalen-2-ol (4i):** mp 209-211.  $\delta_{\text{H}}$  (400 MHz, DMSO-*d*<sub>6</sub>)  $\delta$  8.48 (d, *J* = 5.3 Hz, 2H), 7.94 (brs, 1H), 7.78 (d, *J* = 7.9 Hz, 1H), 7.75 (d, *J* = 8.9 Hz, 1H), 7.68 (s, 1H), 7.56 (d, *J* = 7.7 Hz, 1H), 7.47 (d, *J* = 8.1 Hz, 1H), 7.42 (d, *J* = 5.1 Hz, 2H), 7.32 – 7.22 (m, 4H), 7.06 (t, *J* = 7.4 Hz, 1H).  $\delta_{\text{C}}$  (100 MHz, DMSO-*d*<sub>6</sub>) 166.62, 153.82, 152.45, 152.41, 149.82, 132.47, 131.39, 130.55, 129.12, 129.01, 127.02, 125.93, 123.04, 121.82, 121.67, 121.42, 118.77, 117.97, 52.77. *m/z* (ESI) calcd. for C<sub>23</sub>H<sub>18</sub>N<sub>3</sub>OS<sup>+</sup> [M + H]<sup>+</sup> 384.1165, found 384.0902.

**1-((benzo[d]thiazol-2-ylamino)(4-fluoro-phenyl)methyl)naphthalen-2-ol (4j):** mp 176-178.  $\delta_{\text{H}}$  (400 MHz, DMSO-*d*<sub>6</sub>) 8.41 (s, 1H), 7.92 (s, 1H), 7.76 (d, *J* = 8.1 Hz, 1H), 7.70 (d, *J* = 8.9 Hz, 1H), 7.51 (t, *J* = 8.9 Hz, 2H), 7.44 – 7.37 (m, 1H), 7.37 – 7.31 (m, 2H), 7.30 (s, 1H), 7.29 – 7.20 (m, 3H), 7.07 – 7.03 (m, 2H), 6.94 – 6.89 (m, 2H).  $\delta_{\text{C}}$  (100 MHz, DMSO-*d*<sub>6</sub>) 166.71, 162.17, 160.25, 153.65, 152.28, 138.98, 132.50, 131.14, 130.18, 129.07, 128.43, 128.37, 126.80, 125.94, 124.11, 122.93, 121.57, 121.40, 118.84, 118.80, 118.55, 115.38, 115.21, 53.13. *m/z* (ESI) calcd. for C<sub>24</sub>H<sub>18</sub>FN<sub>2</sub>OS<sup>+</sup> [M + H]<sup>+</sup> 401.1118, found 401.0742.

**1-((benzo[d]thiazol-2-ylamino)(3-bromo-phenyl)methyl)naphthalen-2-ol (4k):** mp 202-204.  $\delta_{\text{H}}$  (400 MHz, DMSO-*d*<sub>6</sub>) 8.41 (s, 1H), 7.98 (s, 1H), 7.76 (d, *J* = 7.9 Hz, 1H), 7.71 (d, *J* = 8.8 Hz, 1H), 7.58 – 7.52 (m, 2H), 7.48 (d, *J* = 7.9 Hz, 1H), 7.42 (s, 1H), 7.34 – 7.21 (m, 5H), 7.19 (s, 1H), 7.11 (t, *J* = 7.7 Hz, 1H), 7.05 (t, *J* = 7.4 Hz, 1H).  $\delta_{\text{C}}$  (100 MHz, DMSO-*d*<sub>6</sub>) 166.59, 153.67, 152.44, 146.10, 132.46, 131.30, 130.82, 130.36, 129.55, 129.12, 129.03, 127.00, 125.93, 125.68, 123.90, 123.02, 122.02, 121.60, 121.41, 118.83, 118.71, 118.54, 53.08. *m/z* (ESI) calcd. for C<sub>24</sub>H<sub>18</sub>BrN<sub>2</sub>OS<sup>+</sup> 461.0318 [M + H]<sup>+</sup>, found 461.0076 and 462.9982.

**1-((benzo[d]thiazol-2-ylamino)(2-fluoro-phenyl)methyl)naphthalen-2-ol (4l):** mp 181-183.  $\delta_{\text{H}}$  (400 MHz, DMSO-*d*<sub>6</sub>) 8.65 (d, *J* = 8.6 Hz, 1H), 8.22 – 8.16 (m, 1H), 7.93 – 7.91 (m, 1H), 7.74 – 7.64 (m, 4H), 7.53 (d, *J* = 7.7 Hz, 1H), 7.52 – 7.43 (m, 2H), 7.33 – 7.15 (m, 4H), 7.05 (td, *J* = 7.9, 4.0 Hz, 2H), 7.00 – 6.90 (m, 1H).  $\delta_{\text{C}}$  (100 MHz, DMSO-*d*<sub>6</sub>) 166.00, 161.36, 159.41, 153.78, 152.59, 132.68, 131.23, 130.10, 129.50, 129.05, 128.82, 126.75, 125.88, 124.12, 123.48, 122.80, 121.49, 121.35, 118.90, 118.69, 117.65, 115.74, 115.56, 49.50. *m/z* (ESI) calcd. for C<sub>24</sub>H<sub>18</sub>FN<sub>2</sub>OS<sup>+</sup> [M + H]<sup>+</sup> 401.1118, found 401.0752.

**1-((benzo[d]thiazol-2-ylamino)(3-nitro-phenyl)methyl)naphthalen-2-ol (4m):** mp 191-194 (198–199).<sup>[1a]</sup>  $\delta_{\text{H}}$  (400 MHz, DMSO-*d*<sub>6</sub>) 8.31 (s, 1H), 8.05 – 7.99 (d, *J* = 9.2 Hz, 1H), 7.99 (s, 1H), 7.77 (d, *J* = 8.0 Hz, 1H), 7.72 (d, *J* = 8.9 Hz, 1H), 7.67 (d, *J* = 7.7 Hz, 1H), 7.54 (d, *J* = 7.8 Hz, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.46 – 7.41 (m, 1H), 7.38 (t, *J* = 8.0 Hz, 1H), 7.30 – 7.22 (m, 4H), 7.05 (t, *J* = 7.6 Hz, 1H).  $\delta_{\text{C}}$  (100 MHz, DMSO-*d*<sub>6</sub>) 166.58, 153.80, 152.37, 148.21, 145.84, 133.33, 132.41, 131.38, 130.66, 130.18, 129.19, 128.99, 127.22, 125.95, 123.62, 123.11, 121.83, 121.72, 121.46, 120.93, 118.83, 118.17, 53.16. *m/z* (ESI) calcd. for C<sub>24</sub>H<sub>18</sub>N<sub>3</sub>O<sub>3</sub>S<sup>+</sup> [M + H]<sup>+</sup> 428.1063, found 428.0772

**1-((benzo[d]thiazol-2-ylamino)(4-nitro-phenyl)methyl)naphthalen-2-ol (4n):** mp 189-191.  $\delta_{\text{H}}$  (400 MHz, DMSO-*d*<sub>6</sub>) 8.02 (d, *J* = 8.8 Hz, 2H), 7.81 (d, *J* = 8.0 Hz, 1H), 7.72 (d, *J* = 8.9 Hz, 1H), 7.59 – 7.54 (m, 3H), 7.48 (d, *J* = 8.0 Hz, 1H), 7.40 – 7.32 (m, 2H), 7.32 – 7.28 (m, 1H), 7.25 (s, 1H), 7.18 – 7.08 (m,

1H). 6.80 (brs, 1H).  $\delta_C$  (100 MHz, DMSO- $d_6$ ) 166.54, 153.72, 152.39, 151.64, 146.40, 132.40, 131.41, 130.63, 129.15, 129.03, 127.66, 127.11, 125.92, 123.87, 123.07, 121.70, 121.43, 118.81, 118.16, 53.37.  $m/z$  (ESI) calcd. for  $C_{24}H_{18}N_3O_3S^+$  [M + H]<sup>+</sup> 428.1063, found 428.0821.

**1-((benzo[d]thiazol-2-ylamino)(4-chloro-phenyl)methyl)-7-methoxynaphthalen-2-ol (4o):** mp 190-192.  $\delta_H$  (400 MHz, DMSO- $d_6$ ) 7.64 (d,  $J = 5.7$  Hz, 1H), 7.62 (d,  $J = 5.3$  Hz, 1H), 7.53 (t,  $J = 8.6$  Hz, 2H), 7.41 (s, 1H), 7.35 (d,  $J = 8.4$  Hz, 2H), 7.29 (t,  $J = 7.7$  Hz, 1H), 7.23 (d,  $J = 8.5$  Hz, 2H), 7.15 – 7.05 (m, 3H), 6.92 (dd,  $J = 8.9, 2.1$  Hz, 1H), 3.77 (s, 3H).  $\delta_C$  (100 MHz, DMSO- $d_6$ ) 166.62, 157.77, 154.21, 152.48, 142.40, 133.78, 131.30, 130.99, 130.52, 129.97, 128.49, 128.27, 125.91, 124.36, 121.54, 121.38, 118.59, 118.08, 116.10, 114.77, 55.31, 52.95.  $m/z$  (ESI)  $C_{25}H_{20}ClN_2O_2S^+$  [M + H]<sup>+</sup> 447.0929, found 447.0616.

**5-((benzo[d]thiazol-2-ylamino)(4-chloro-phenyl)methyl)quinolin-6-ol (4p):** mp 207-209 (209-211).<sup>[1a]</sup>  $\delta_H$  8.63 (s, 1H), 8.58 (brs, 1H), 8.34 (d,  $J = 6.9$  Hz, 1H), 7.93 – 7.81 (m, 1H), 7.50 (d,  $J = 7.7$  Hz, 1H), 7.46 (d,  $J = 9.1$  Hz, 1H), 7.37 (d,  $J = 8.0$  Hz, 1H), 7.34 – 7.27 (m, 1H), 7.25 – 7.22 (m, 2H), 7.19 – 7.11 (m, 4H), 6.97 (t,  $J = 7.5$  Hz, 1H).  $\delta_C$  (100 MHz, DMSO- $d_6$ ) 166.46, 153.74, 152.43, 147.23, 144.12, 141.68, 131.33, 131.25, 128.65, 128.40, 127.55, 125.94, 122.08, 121.64, 121.42, 118.73, 118.64, 52.81.  $m/z$  (ESI) calcd. for  $C_{23}H_{17}ClN_3OS^+$  [M + H]<sup>+</sup> 418.0775, found 418.0424.

#### Reference:

- (a) A. Ohanian, S. Javanshir, M. M. Heravi, F. F. Bamoharram, 13<sup>th</sup> *International Electronic Conference on Synthetic Organic Chemistry (ECSOC-13)*, November 1-30, **2009**.  
(b) A. Shaabani, A. Rahmati, E. Farhangi, *Tetrahedron Lett.* **2007**, 48, 7291.





















































