

## SUPPLEMENTARY MATERIAL TO

## Hindered phenolic aminothiazoles – Synthesis, $\alpha$ -glucosidase, $\alpha$ -amylase inhibitory and antioxidant activities

VYJAYANTHY SATHEESH SANDHYA, VIJAYAN RADHA AKHILA, KRISHNAN  
NAIR GIRIJA KRISHNAPRIYA, KALLIKAT NARAYANAN RAJASEKHARAN,  
MAHESWARI PRIYA RANI\*

*Department of Chemistry, University of Kerala, Trivandrum, Kerala, 695581, India*

## ANALYTICAL AND SPECTRAL DATA OF THE SYNTHESISED COMPOUNDS

**4-Amino-5-(3,5-di-*t*-butyl-4-hydroxybenzoyl)-2-phenylaminothiazole (5a).** Method A: 360 mg (85 %); Method B: Yield 390 mg (93 %); yellow crystals; m.p.: 135-136 °C; Calcd. for C<sub>24</sub>H<sub>29</sub>N<sub>3</sub>O<sub>2</sub>S: C, 68.05; H, 6.90; N, 9.02 %; Found: C, 68.21; H, 6.65; N, 8.94 %; IR spectrum ( $\nu_{\text{max}}$ , cm<sup>-1</sup>): 683; 759; 1109; 1238; 1308; 1532; 1700 (C=O); 2958 (C-H); 3333 (N-H); 3617 (N-H); 3739 (O-H); <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>,  $\delta$  / ppm) : 1.33 (9H, s, Me); 5.71 (1H, s, ArOH); 7.15-7.22 (2H, *m*, ArH); 7.30-7.48 (3H, *m*, ArH); 7.51 (1H, s, NH); <sup>13</sup>C NMR spectrum (125 MHz, CDCl<sub>3</sub>,  $\delta$  / ppm): 30.1; 34.3; 120.0; 124.8; 126.1; 128.8; 128.9; 129.5; 132.5; 135.76; 135.9; 138.6; 156.4; 158.4; 163.9; 185.5; MS (*m/z*): 425.16.

*4-Amino-5-(3,5-di-*t*-butyl-4-hydroxybenzoyl)-2-(4-methoxyphenylamino)thiazole* (5b).  
d A: Yield 281 mg (62 %); Method B: Yield 326 mg (72 %); orange crystals; m.p.: 130–132 °C; Anal. Calcd. for C<sub>25</sub>H<sub>31</sub>N<sub>3</sub>O<sub>3</sub>S: C, 66.20; H, 6.89; N, 9.26 %; Found: C, 66.32; H, 7.04; N, 9.28 %; IR spectrum, ( $\nu_{\text{max}}$  cm<sup>−1</sup>): 763; 832; 1026; 1110; 1242; 1304; 1463; 1743 (C=O); 2924 (C—H); 3432 (N—H); 3615 (N—H); 3738 (O—H); <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>, δ / ppm): 1.28 (9H, s, Me); 3.83 (3H, s, OMe); 5.73 (1H, s, ArOH); 6.89 (2H, d, *J* = 7.5 Hz, ArH); 7.28 (2H, d, *J* = 7.5 Hz, ArH); 7.60 (1H, s, NH); 7.96 (2H, s, ArH); <sup>13</sup>C NMR spectrum (125 MHz, CDCl<sub>3</sub>, δ / ppm): 30.1; 34.3; 55.6; 99.9; 106.7; 114.8; 125.9; 120.5; 123.6; 124.9; 127.7; 135.8; 156.5; 157.9; 158.7; 171.2; 185.4; MS (*m/z*): 453.74.

*4-Amino-5-(3,5-di-*t*-butyl-4-hydroxybenzoyl)-2-(4-chlorophenylamino)thiazole* (5c).  
d A: Yield 288 mg (59 %); Method B: Yield 366 mg (80 %); yellowish orange crystals;  
131–133 °C. Anal. Calcd for C<sub>24</sub>H<sub>28</sub>ClN<sub>3</sub>O<sub>3</sub>S: C, 62.94; H, 6.16; N, 9.17 %; Found: C,  
H, 5.92; N, 9.03 %; IR spectrum ( $\nu_{\text{max}}$  cm<sup>−1</sup>): 825; 1019; 1099; 1211; 1488; 1542; 1741  
; 2925 (C-H); 3345 (N-H); 3611 (N-H); <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>,  $\delta$  / ppm):  
8H, s, Me); 5.53 (1H, s, ArOH); 7.30 (2H, d,  $J$  = 9 Hz, ArH); 7.36 (2H, d,  $J$  = 9 Hz, ArH);

34 7.65 (2H, *s*, ArH); 8.2 (1H, *s*, NH);  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{CDCl}_3$ ,  $\delta$  / ppm): 30.2; 34.5;  
35 94.3; 120.9; 125.0; 129.5; 129.6; 128.8; 132.4; 135.6; 137.3; 156.5; 158.4; 164.0; 167.9; 185.6;  
36 MS (*m/z*): 457.5.

37 4-Amino-5-(3,5-di-*t*-butyl-4-hydroxybenzoyl)-2-(4-methylphenylamino)thiazole (**5d**).  
38 Method A: Yield 232 mg (53 %); Method B: Yield 263 mg (60 %); yellow crystals; m.p.:  
39 123-125 °C; Anal. Calcd. For  $\text{C}_{25}\text{H}_{31}\text{N}_3\text{O}_2\text{S}$ : C, 68.62; H, 7.14; N, 9.60 %; Found: C, 68.70;  
40 H, 6.99; N, 9.46 %; IR spectrum ( $\nu_{\text{max}}$  cm $^{-1}$ ): 616; 774; 814; 888; 930; 1117; 1159; 1202;  
41 1237; 1363; 1433; 1514; 1562; 1745 (C=O); 2871; 2959 (C-H); 3288 (N-H); 3619 (N-H);  $^1\text{H}$   
42 NMR spectrum (500 MHz,  $\text{CDCl}_3 + \text{DMSO-}d_6$ ,  $\delta$  / ppm): 1.48 (18H, *s*, Me); 2.40 (3H, *s*,  
43 Me); 5.91 (1H, *s*, ArOH); 6.65 (2H, *d*, *J* = 8.5 Hz, ArH); 6.94 (2H, *d*, *J* = 8 Hz, ArH); 7.74  
44 (2H, *s*, ArH); 8.04 (1H, *broad s*, NH).

45 4-Amino-5-(3,5-di-*t*-butyl-4-hydroxybenzoyl)-2-(4-ethoxyphenylamino)thiazole (**5e**).  
46 Method A: Yield 248 mg (53 %); Method B: Yield 304 mg (65 %); yellow crystals; m.p.: 123-  
47 125 °C. Anal. Calcd. for  $\text{C}_{26}\text{H}_{33}\text{N}_3\text{O}_3\text{S}$ : C, 66.78; H, 7.11; N, 8.99 %; Found: C, 66.63; H, 6.89;  
48 N, 8.91 %; IR spectrum ( $\nu_{\text{max}}$  cm $^{-1}$ ): 768; 830; 892; 1064; 1111; 1168; 1239; 1305; 1514; 1730  
49 (C=O); 2959 (C-H); 3282 (N-H); 3619 (N-H);  $^1\text{H}$ NMR (500 MHz,  $\text{CDCl}_3$ ,  $\delta$  / ppm): 1.32-1.42  
50 (21H, *m*, Me of *t*-Bu and Et); 4.03 (2H, *q*, *J* = 7 Hz, OCH $_2$ ); 5.49 (1H, *broad s*, ArOH); 6.88-6.90  
51 (2H, *m*, ArH); 7.26-7.28 (2H, *m*, ArH); 7.63 (2H, *s*, ArH); 8.11 (1H, *s*, NH);  $^{13}\text{C}$  NMR (125  
52 MHz,  $\text{CDCl}_3$ ,  $\delta$  / ppm): 14.7; 30.2; 34.5; 63.8; 115.3; 123.5; 124.9; 131.2; 132.6; 135.5; 156.2;  
53 156.9; 164.3; 170.6; 185.3. MS (*m/z*) 469.00.

54