



SUPPLEMENTARY MATERIAL TO  
**Hindered phenolic aminothiazoles – Synthesis,  $\alpha$ -glucosidase and  
 $\alpha$ -amylase inhibitory and antioxidant activities**

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J. Serb. Chem. Soc. 82 (10) (2017) 1087–1095

ANALYTICAL AND SPECTRAL DATA FOR THE SYNTHESISED COMPOUNDS

*[4-Amino-2-(phenylamino)-5-thiazolyl](3,5-di-*t*-butyl-4-hydroxyphenyl)-methanone (5a)*. Method A, yield: 360 mg (85 %); method B, yield 390 mg (93 %). yellow crystals; m.p.: 135–136 °C; Anal. 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, 9.19 %; IR (KBr, cm<sup>-1</sup>): 3739m, 3617m, 3433m, 2958m, 1700s, 1532s, 1428s, 1308m, 1238s, 1109m, 759w, 683w; <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>,  $\delta$  / ppm): 8.78 (1H, s, NH), 7.66 (2H, s, Ar-H), 7.36 (4H, d, *J* = 5.6 Hz, Ar-H), 7.13–7.16 (1H, m, Ar-H), 5.51 (1H, s, Ar-OH), 1.43 (18H, s, CH<sub>3</sub>); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>,  $\delta$  / ppm): 185.5, 168.9, 164.1, 156.4, 138.7, 135.9, 135.6, 132.5, 129.6, 125.0, 124.9, 120.1, 94.2, 34.5, 30.2; (+)ESI-HRMS (*m/z*): Calcd. for [C<sub>24</sub>H<sub>29</sub>N<sub>3</sub>O<sub>2</sub>S + H]<sup>+</sup>: 424.20587. Found: 424.20619.

*{4-Amino-2-[(4-methoxyphenyl)amino]-5-thiazolyl}(3,5-di-*t*-butyl-4-hydroxyphenyl)methanone (5b)*. Method 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, 9.18 %; IR (KBr, cm<sup>-1</sup>): 3738m, 3615m, 3432w, 2924m, 1743m, 1520s, 1463s, 1304m, 1242s, 1110m, 1026m, 832w, 763w; <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>,  $\delta$  / ppm): 7.62 (2H, s, Ar-H), 7.30 (2H, d, *J* = 8.8 Hz, Ar-H), 6.89 (2H, d, *J* = 8.8 Hz, Ar-H), 5.49 (1H, s, Ar-OH), 3.81 (3H, s, OCH<sub>3</sub>), 1.45 (18H, s, CH<sub>3</sub>); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>,  $\delta$  / ppm): 185.3, 170.6, 164.4, 157.5, 156.3, 135.5, 132.6, 131.5, 124.9, 123.4, 114.8, 94.1, 55.6, 34.5, 30.2; FABMS (thioglycerol matrix) (*m/z*): Calcd. for [C<sub>25</sub>H<sub>31</sub>N<sub>3</sub>O<sub>3</sub>S]<sup>+</sup>: 453.20. Found: 453.74.

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*{4-Amino-2-[(4-chlorophenyl)amino]-5-thiazolyl}(3,5-di-*t*-butyl-4-hydroxyphenyl)methanone (5c)*. Method A, yield: 288 mg (59 %); method B, yield: 366 mg (80 %); yellowish orange crystals; m.p.: 131–133 °C; Anal. calcd. for C<sub>24</sub>H<sub>28</sub>ClN<sub>3</sub>O<sub>2</sub>S: C, 62.94; H, 6.16; N, 9.17 %. Found: C, 62.71; H, 5.92; N, 9.03 %; IR (KBr, cm<sup>-1</sup>): 3611w, 3345w, 2925m, 1741m, 1542s, 1488s, 1211s, 1099m, 1019m, 825w; <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>, δ / ppm): 8.72 (1H, *s*, NH), 7.65 (2H, *s*, Ar-H), 7.35 (2H, *d*, *J* = 8.8 Hz, Ar-H), 7.27 (2H, *d*, *J* = 4.8 Hz, Ar-H), 5.52 (1H, *s*, Ar-OH), 1.42 (18H, *s*, CH<sub>3</sub>); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>, δ / ppm): 185.6, 168.2, 164.2, 156.5, 137.4, 135.7, 132.4, 129.5, 129.4, 125.0, 121.0, 94.3, 34.5, 30.2; FABMS (thioglycerol matrix) (*m/z*): Calcd. for [C<sub>24</sub>H<sub>28</sub>ClN<sub>3</sub>O<sub>2</sub>S]<sup>+</sup>: 457.16. Found: 457.16.

*{4-Amino-2-[(4-methylphenyl)amino]-5-thiazolyl}(3,5-di-*t*-butyl-4-hydroxyphenyl)methanone (5d)*. Method A, yield: 232 mg (53 %); method B, yield: 263 mg (60 %); yellow crystals: m.p.: 123–125 °C; Anal. calcd. for C<sub>25</sub>H<sub>31</sub>N<sub>3</sub>O<sub>2</sub>S: C, 68.62; H, 7.14; N, 9.60 %. Found: C, 68.70; H, 6.99; N, 9.46 %; IR (KBr, cm<sup>-1</sup>): 3619m, 3288m, 2959s, 2871s, 1745m, 1562s, 1514s, 1433s, 1363s, 1237s, 1202s, 1159s, 1117s, 930w, 888m, 814m, 774m, 616w; <sup>1</sup>H-NMR (400 MHz, CDCl<sub>3</sub>, δ / ppm): 7.66 (2H, *s*, Ar-H), 7.25 (2H, *d*, *J* = 8.8 Hz, Ar-H), 7.17 (2H, *d*, *J* = 8.4 Hz, Ar-H), 5.50 (1H, *s*, Ar-OH), 2.34 (3H, *s*, CH<sub>3</sub>), 1.45 (18H, *s*, CH<sub>3</sub>); <sup>13</sup>C-NMR (100 MHz, CDCl<sub>3</sub>, δ / ppm): 185.4, 169.3, 164.1, 156.4, 135.9, 135.6, 135.0, 132.6, 130.1, 124.9, 120.5, 94.2, 34.5, 30.2, 20.9; (+)ESI-HRMS (*m/z*): Calcd. for [C<sub>25</sub>H<sub>31</sub>N<sub>3</sub>O<sub>2</sub>S + H]<sup>+</sup>: 438.22152. Found: 438.22227.

*{4-Amino-2-[(4-ethoxyphenyl)amino]-5-thiazolyl}(3,5-di-*t*-butyl-4-hydroxyphenyl)methanone (5e)*. Method A, yield: 248 mg (53 %); method B, yield: 304 mg (65 %); yellow crystals; m.p.: 123–125 °C; Anal. calcd. for C<sub>26</sub>H<sub>33</sub>N<sub>3</sub>O<sub>3</sub>S: C, 66.78; H, 7.11; N, 8.99 %. Found: C, 66.63; H, 6.89; N, 8.91 %; IR (KBr, cm<sup>-1</sup>): 3619m, 3282w, 2959m, 1730m, 1514s, 1305m, 1239s, 1168m, 1111m, 1064m, 892w, 830w, 768w; <sup>1</sup>H-NMR (500 MHz, CDCl<sub>3</sub>, δ / ppm): 8.11 (1H, *s*, NH), 7.63 (2H, *s*, Ar-H), 7.28–7.26 (2H, *m*, Ar-H), 6.90–6.88 (2H, *m*, Ar-H), 5.49 (1H, *s*, Ar-OH), 4.03 (2H, *q*, *J* = 7.0 Hz, OCH<sub>2</sub>), 1.66 (18H, *s*, CH<sub>3</sub>), 1.42 (3H, *t*, *J*<sub>1</sub> = 8.0 Hz, *J*<sub>2</sub> = 7.0 Hz, CH<sub>3</sub>); <sup>13</sup>C-NMR (125 MHz, CDCl<sub>3</sub>, δ / ppm): 185.3, 170.7, 164.4, 156.9, 156.3, 135.5, 132.6, 131.2, 124.9, 123.5, 115.3, 63.8, 34.5, 30.2, 14.8; FABMS (thioglycerol matrix) (*m/z*): Calcd. for [C<sub>26</sub>H<sub>33</sub>N<sub>3</sub>O<sub>3</sub>S + H]<sup>+</sup>: 468.23. Found: 469.00.

<sup>13</sup>C- AND <sup>1</sup>H-NMR SPECTRA OF COMPOUNDS 5a-e

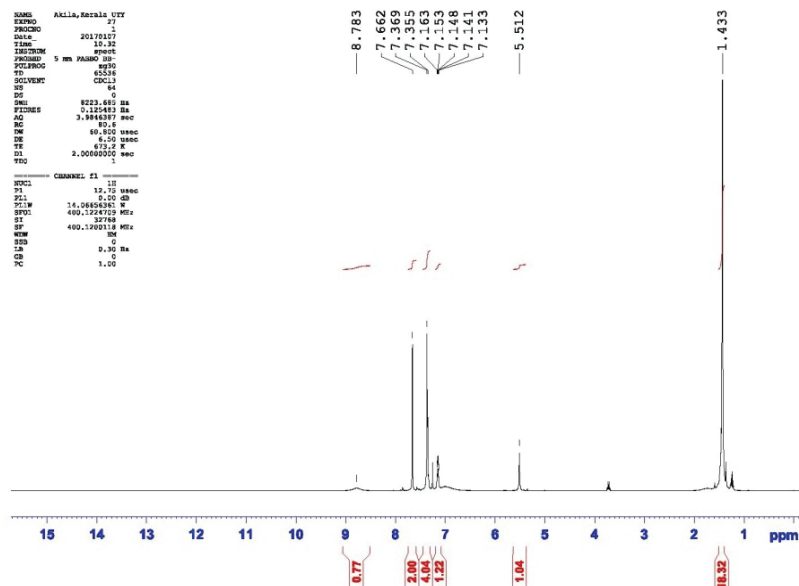


Fig. S-1. <sup>1</sup>H-NMR spectrum (400 MHz, CDCl<sub>3</sub>) of 5a.

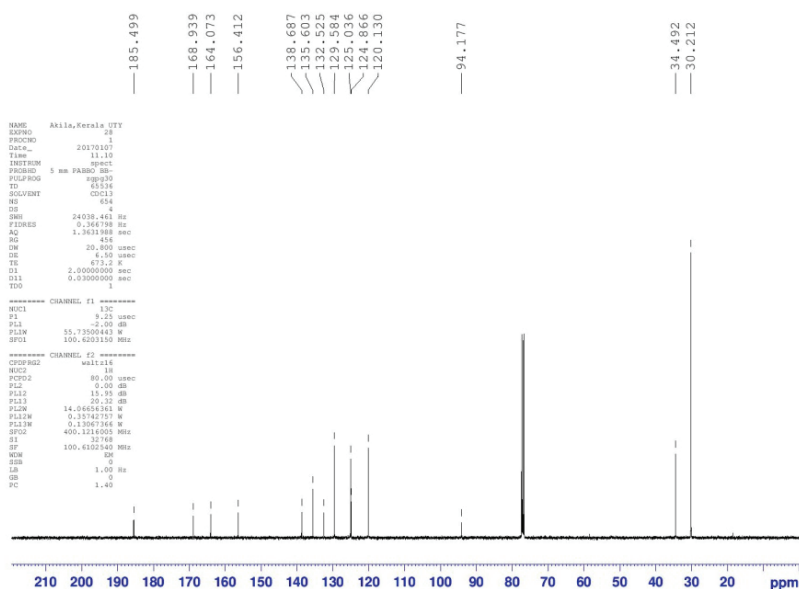
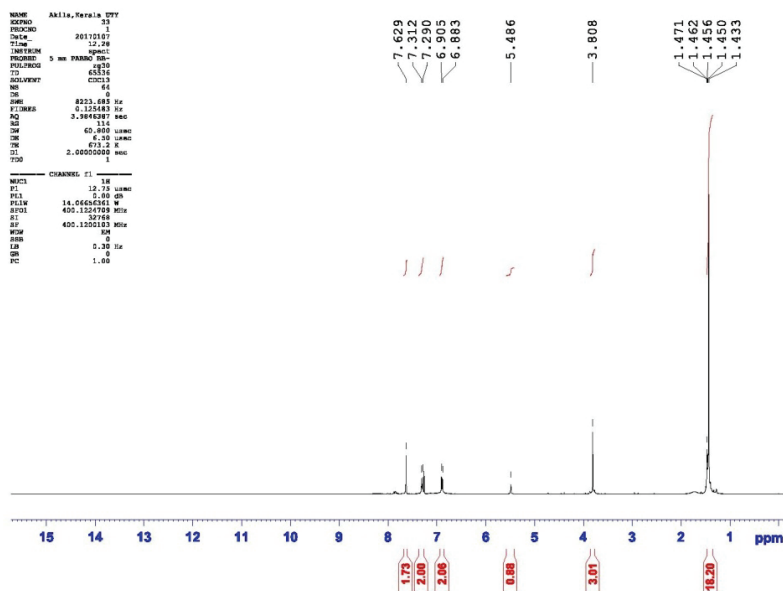
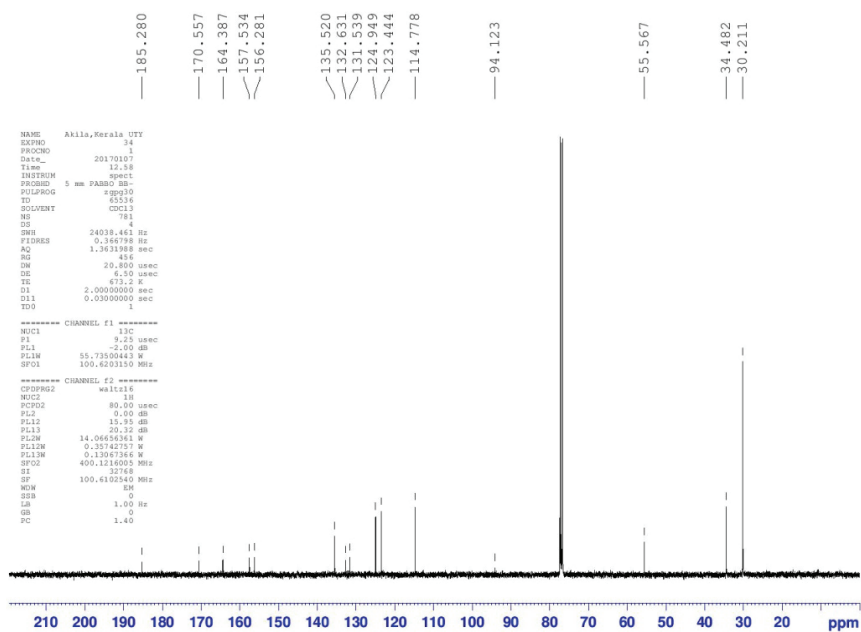


Fig. S-2. <sup>13</sup>C-NMR spectrum (100 MHz, CDCl<sub>3</sub>) of 5a.

Fig. S-3.  $^1\text{H-NMR}$  spectrum (400 MHz,  $\text{CDCl}_3$ ) of **5b**.Fig. S-4.  $^{13}\text{C-NMR}$  spectrum (100 MHz,  $\text{CDCl}_3$ ) of **5b**.

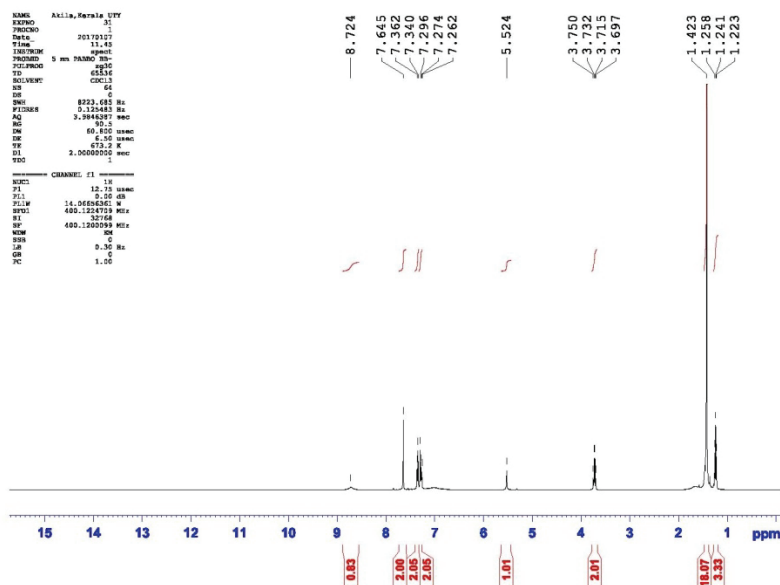


Fig. S-5. <sup>1</sup>H-NMR spectrum (400 MHz, CDCl<sub>3</sub>) of 5c.

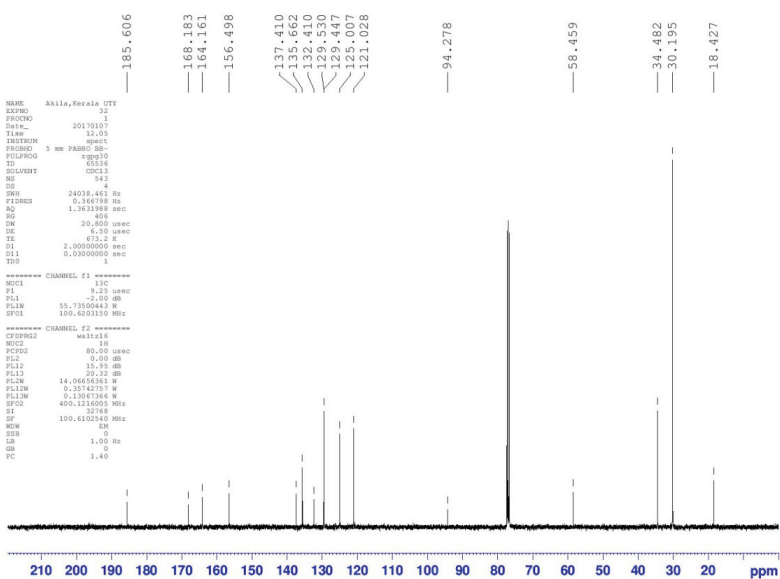
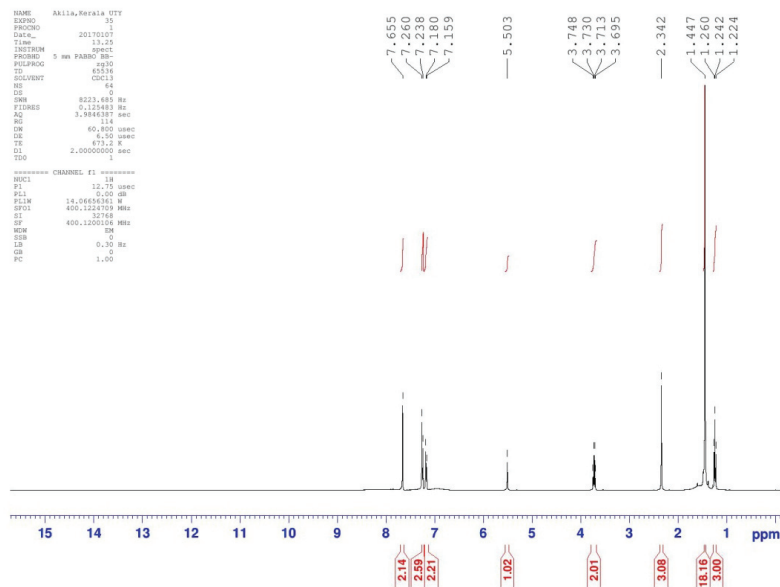
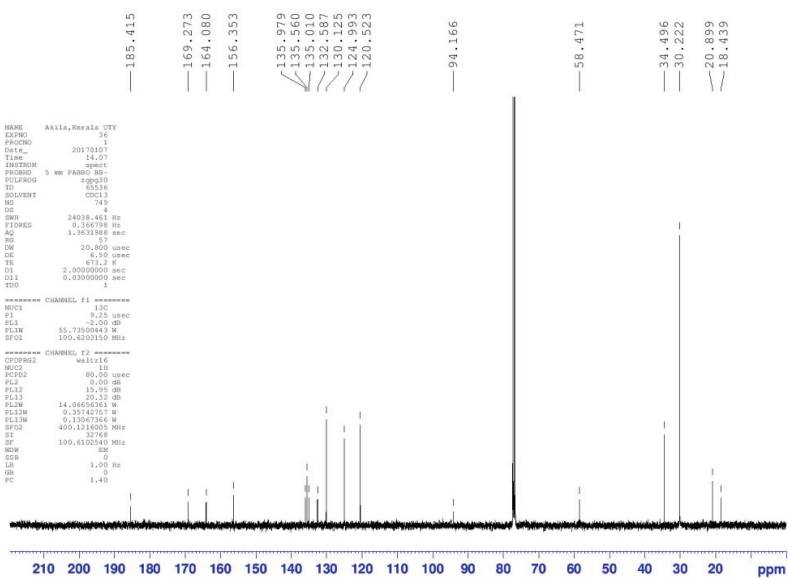


Fig. S-6. <sup>13</sup>C-NMR spectrum (100 MHz, CDCl<sub>3</sub>) of 5c.

Fig. S-7.  $^1\text{H-NMR}$  spectrum (400 MHz,  $\text{CDCl}_3$ ) of **5d**.Fig. S-8.  $^{13}\text{C-NMR}$  spectrum (100 MHz,  $\text{CDCl}_3$ ) of **5d**.

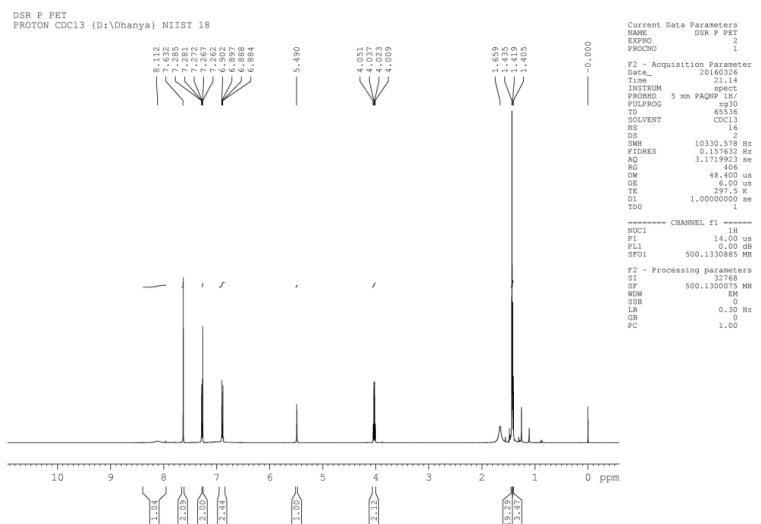


Fig. S-9. <sup>1</sup>H-NMR spectrum (500 MHz, CDCl<sub>3</sub>) of **5e**.

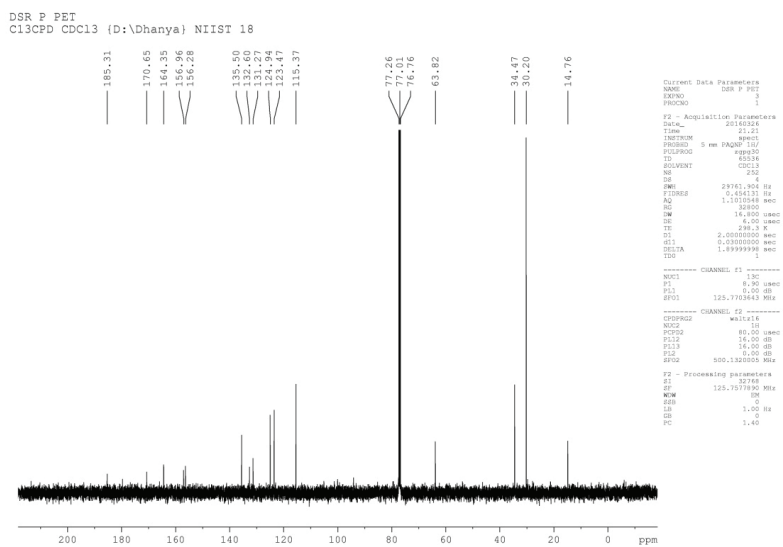


Fig. S-10. <sup>13</sup>C-NMR spectrum (125 MHz, CDCl<sub>3</sub>) of **5e**.