Supporting Information

Triazine diphosphonium tetrachloroferrate ionic liquid immobillized on functionalized halloysite nanotubes as an efficient and reusable catalyst for the synthesis of mono-, bis- and tris-benzothiazoles

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1. Spectroscopic data of the products:

2-Phenylbenzo[d]thiazole (3a)



White solid. 95% yield; m.p: 108-110 °C (Lit. [1] 110-112 °C). IR (KBr): $v_{max} = 3063$, 2926, 1553, 1506, 1473, 1310, 1222, 1159, 1069, 960, 758, 687, 619 cm⁻¹. ¹H NMR (400 MHz, DMSO-*d*₆): $\delta = 8.23$ (dd, ^{*l*}J = 8.1 Hz, ²J = 1.3 Hz, 1H), 8.21-8.13 (m, 3H), 7.69-7.61 (m, 4H), 7.55 (td, ^{*l*}J = 7.5 Hz, ²J = 1 Hz, 1H).

2-(2-Chlorophenyl)benzo[d]thiazole (3b)



Yellow solid. 90% yield; m.p: 84-85 °C (Lit. [1] 83-84 °C). IR (KBr): $v_{max} = 3062, 2923, 1557, 1425, 1312, 1218, 964, 755, 726 cm^{-1}.$ ¹H NMR (400 MHz, DMSO-*d*₆): $\delta = 8.33-8.27$ (m, 2H), 8.22 (d, *J* = 7.6 Hz, 1H), 7.83 (dd, ^{*i*}*J* = 7.6 Hz, ²*J* = 1.8 Hz, 1H), 7.72-7.58 (m, 4H).

2-(3-Chlorophenyl)benzo[d]thiazole (3c)



Yellow solid. 92% yield; m.p: 95-97 °C (Lit. [1] 97-99 °C). IR (KBr): $v_{max} = 3053$, 2919, 1914, 1567, 1501, 1424, 1312, 1229, 1074, 885, 729 cm⁻¹. ¹H NMR (400 MHz, DMSO- d_6): $\delta = 8.20$ (d, J = 8.1 Hz, 1H), 8.13-8.13 (m, 1H), 8.11 (d, J = 8.1, 1H), 8.06 (dt, ${}^{1}J = 7.5$ Hz, ${}^{2}J = 1.5$ Hz, 1H), 7.68-7.56 (m, 3H), 7.51 (td, ${}^{1}J = 7.6$ Hz, ${}^{2}J = 1.3$ Hz, 1H).

2-(4-Chlorophenyl)benzo[d]thiazole (3d)



Yellow solid. 96% yield; m.p: 112-114 °C (Lit. [1] 115-117 °C). IR (KBr): $v_{max} = 3054$, 2923, 1643, 1587, 1506, 1471, 1312, 1249, 1086, 968, 826, 756, 689 cm⁻¹. ¹H NMR (400 MHz, DMSO-*d*₆): $\delta = 8.18$ (d, J = 7.8 Hz, 1H), 8.15-8.11 (m, 2H), 8.10 (d, J = 7.4 Hz, 1H), 7.68-7.63 (m, 2H), 7.58 (td, ${}^{1}J = 7.2$ Hz, ${}^{2}J = 1.3$ Hz, 1H), 7.50 (td, ${}^{1}J = 7.4$ Hz, ${}^{2}J = 1.2$ Hz, 1H).

2-(3-Bromophenyl)benzo[d]thiazole (3e)



white solid. 92% yield; m.p: 90-92 °C (Lit. [2] 88 °C). IR (KBr): $v_{max} = 3056$, 2921, 1587, 1498, 1460, 1218, 1066, 971, 751, 673 cm⁻¹. ¹H NMR (400 MHz, DMSO- d_6): $\delta = 8.25$ (t, J = 1.9 Hz, 1H), 8.18 (d, J = 7.4 Hz, 1H), 8.08 (m, 2H), 7.88 (dd, $^{J}J = 7.8$ Hz, $^{2}J = 1.7$ Hz, 1H), 7.61-7.47 (m, 3H).

2-(4-Bromophenyl)benzo[d]thiazole (3f)



Yellow solid. 95% yield; m.p: 109-110 °C (Lit. [3] 105-107 °C). IR (KBr): $v_{max} = 3055$, 2919, 1661, 1581, 1476, 1224, 1066, 967, 827, 753, 732, 687 cm⁻¹. ¹H NMR (400 MHz, DMSO-*d*₆): $\delta = 8.18$ (d, J = 8.0 Hz, 1H), 8.12-8.04 (m, 3H), 7.84-7.77 (m, 2H), 7.58 (td, $^{1}J = 7.2$ Hz, $^{2}J = 1.3$ Hz, 1H), 7.50 (td, $^{1}J = 7.2$ Hz, $^{2}J = 1.3$ Hz, 1H).

2-(4-Fluorophenyl)benzo[d]thiazole (3g)



White solid. 92% yield; m.p: 97-99 °C (Lit. [1] 98-100 °C). IR (KBr): $v_{max} = 3055$, 2923, 1598, 1480, 1226, 967, 757, 689 cm⁻¹. ¹H NMR (400 MHz, DMSO- d_6): $\delta = 8.20$ -8.14 (m, 3H), 8.08 (d, J = 7.9 Hz, 1H), 7.57 (td, ${}^{I}J = 7.3$ Hz, ${}^{2}J = 1.3$ Hz, 1H), 7.51-7.46 (m, 3H).

4-(benzo[d]thiazol-2-yl)benzonitrile (3h)



White solid. 92% yield; m.p: 165-167 °C (Lit. [1] 165-167 °C). IR (KBr): $v_{max} = 3059$, 2921, 2864, 2223, 1928, 1602, 1556, 1477, 1430, 1222, 905, 761 cm⁻¹. ¹H NMR (400 MHz, DMSO- d_6): $\delta = 8.28$ (d, J = 7.9 Hz, 2H), 8.22 (d, J = 7.6 Hz, 1H), 8.14 (d, J = 7.5 Hz, 1H), 8.05 (d, J = 7.8 Hz, 2H), 7.61 (t, J = 7.5 Hz, 1H), 7.53 (t, J = 7.5 Hz, 1H).

2-(o-Tolyl)benzo[d]thiazole (3i)



Yellow solid. 90% yield; m.p: 55-57 °C (Lit. [1] 52-54 °C). IR (KBr): $v_{max} = 3063$, 2926, 1600, 1479, 1429, 1212, 953, 866, 760, 723, 686 cm⁻¹. ¹H NMR (400 MHz, DMSO-*d*₆): $\delta = 8.17$ (dd, ^{*1*}*J* = 8.0 Hz, ²*J* = 1.3 Hz, 1H), 8.10 (dd, ^{*1*}*J* = 7.5 Hz, ²*J* = 1.3 Hz, 1H), 7.81 (d, *J* = 8.0 Hz, 1H), 7.57 (td, ^{*1*}*J* = 7.2 Hz, ²*J* = 1.3 Hz, 1H), 7.53-7.37 (m, 4H), 2.64 (s, 3H).

2-(p-Tolyl)benzo[d]thiazole (3j)

Me

Yellow solid. 90% yield; m.p: 83-85°C (Lit. [2] 86 °C). IR (KBr): $v_{max} = 3023$, 2912, 1606, 1482, 1431, 1312, 1225, 959, 816, 759 cm⁻¹. ¹H NMR (400 MHz, DMSO-*d*₆): $\delta = 7.86$ (d, J = 7.9 Hz, 1H), 7.80 (d, J = 8.0 Hz, 1H), 7.72 (d, J = 8.1 Hz, 2H), 7.29 (td, ${}^{1}J = 7.5$ Hz, ${}^{2}J = 1.3$ Hz, 1H), 7.19 (td, ${}^{1}J = 7.7$ Hz, ${}^{2}J = 1.3$ Hz, 1H), 7.10 (d, J = 8.0 Hz, 2H), 2.11 (s, 3H).

3-(Benzo[d]thiazol-2-yl)aniline (3k)



Pale yellow solid. 90% yield; m.p: 135-137 °C (Lit. [3] 138-139 °C). IR (KBr): $v_{max} = 3314$, 3213, 2923, 1628, 1604, 1482, 1201, 993, 761, 635 cm⁻¹.¹H NMR 400 MHz, DMSO-*d*₆): $\delta = 8.20$ (dd, ${}^{1}J = 7.2$ Hz, ${}^{2}J = 0.5$ Hz, 1H), 8.10 (dd, ${}^{1}J = 7.2$ Hz, ${}^{2}J = 0.5$ Hz, 1H), 7.61 (td, d, ${}^{1}J = 7.5$ Hz, ${}^{2}J = 1.3$ Hz, 1H), 7.53 (td, ${}^{1}J = 7.7$ Hz, ${}^{2}J = 1.3$ Hz, 1H), 7.45-7.41 (m, 1H), 7.30-7.24 (m, 2H), 6.82 (m, 1H), 5.55 (s, 2H).

2-(4-methoxyphenyl)benzo[d]thiazole (3l)



White solid. 95% yield; m.p: 123-125 °C (Lit. [1] 123-125 °C). IR (KBr): $v_{max} = 3056, 2993, 2935, 1908, 1650, 1601, 1519, 1481, 1256, 757 cm⁻¹.¹H NMR (400 MHz, DMSO-$ *d* $₆): <math>\delta = 8.17$ (d, J = 8.0 Hz, 1H), 8.13-8.02 (m, 3H), 7.58 (t, J = 7.8 Hz, 1H), 7.49 (t, J = 7.6 Hz, 1H), 7.23-7.15 (m, 2H), 3.92 (s, 3H).

2-(Pyridin-2-yl)benzo[d]thiazole (3m)

White solid. 95% yield; m.p: 127-129 °C (Lit. [4] 129-131 °C). IR (KBr): $v_{max} = 3053, 3004, 1582, 1458, 1429, 1314, 1233, 976, 781, 617 cm⁻¹. ¹H NMR (400 MHz, DMSO-$ *d* $₆): <math>\delta = 8.75$ (d, J = 4.8 Hz, 1H), 8.35

(d, *J* = 7.7 Hz, 1H), 8.19 (d, *J* = 7.9 Hz, 1H), 8.12 (d, *J* = 8.1 Hz, 1H), 8.06 (td, ^{*I*}*J* = 7.7 Hz, ^{*2*}*J* = 1.5 Hz, 1H), 7.65-7.55 (m, 2H), 7.51 (t, *J* = 7.5 Hz, 1H).

2-(Pyridin-3-yl)benzo[d]thiazole (3n)



White solid. 95% yield; m.p: 124-126°C (Lit. [5] 129-131 °C). IR (KBr): $v_{max} = 3053$, 2919, 1613, 1574, 1426, 1237, 961, 763, 691 cm⁻¹. ¹H NMR (400 MHz, DMSO-*d*₆): $\delta = 9.39-9.32$ (m, 1H), 8.84 (dd, ^{*1*}*J* = 4.8 Hz, ²*J* = 1.7 Hz, 1H), 8.54 (dt, ^{*1*}*J* = 7.7 Hz, ²*J* = 1.5 Hz, 1H), 8.29 (d, *J* = 7.7 Hz, 1H), 8.20 (d, *J* = 7.6 Hz, 1H), 7.70 (td, ^{*1*}*J* = 7.7 Hz, ²*J* = 1.3 Hz, 1H), 7.66 (td, ^{*1*}*J* = 7.7 Hz, ²*J* = 1.3 Hz, 1H), 7.59 (td, ^{*1*}*J* = 7.5 Hz, ²*J* = 1.3 Hz, 1H).

2-benzylbenzo[d]thiazole (5a)



Yellow liquid (Lit. [6] liquid). 90% yield; IR (KBr): $v_{max} = 3061$, 3033, 2955, 2892, 1945, 1726, 1598, 1514, 1433, 1107, 758, 702 cm⁻¹. ¹H NMR (400 MHz, DMSO- d_6): $\delta = 8.07$ (d, J = 7.9, 1H), 8.01 (d, J = 8.1 Hz, 1H), 7.54 (t, J = 7.6, 1.3 Hz, 1H), 7.50-7.39 (m, 5H), 7.37 -7.30 (m, 1H), 4.53 (s, 2H).

2-(4-Chlorobenzyl)benzo[d]thiazole (5b)



Bright yellow solid, 90% yield; m.p: 61-63 °C (Lit. [7] 64 °C). IR (KBr): $v_{max} = 3062, 2916, 1781, 1646, 1591, 1489, 1311, 1092, 937, 839, 759 cm^{-1}.$ ¹H NMR (400 MHz, DMSO-*d*₆): $\delta = 8.00-8.02$ (m, 1H), 7.96 (d, J = 8.1 Hz, 1H), 7.48 (td, ${}^{1}J = 7.5$ Hz, ${}^{2}J = 1.2$ Hz, 1H), 7.44-7.36 (m, 5H), 4.48 (s, 2H).

2-(4-Methoxybenzyl)benzo[d]thiazole (5c)



Yellow solid. 90% yield; m.p: 50-52 °C (Lit. [8] 60-62 °C). IR (KBr): $v_{max} = 3461$, 3065, 2960, 2926, 1611, 1510, 1294, 1026, 939, 810, 758, 623 cm⁻¹. ¹H NMR (400 MHz, DMSO-*d*₆): $\delta = 8.00$ (d, J = 7.9 Hz, 1H), 7.95 (d, J = 7.9 Hz, 1H), 7.48 (td, ${}^{1}J = 7.7$ Hz, ${}^{2}J = 1.3$ Hz, 1H), 7.38 (td, ${}^{1}J = 7.8$ Hz, ${}^{2}J = 1.3$ Hz, 1H), 7.34-7.29 (m, 2H), 6.96-6.89 (m, 2H), 4.40 (s, 2H), 3.75 (s, 3H).

2-(4-methylbenzyl)benzo[d]thiazole (5d)



Yellow liquid. 90% yield; m.p: 43-45 °C (Lit. [9] 46-47 °C). IR (KBr): $v_{max} = 3055$, 2918, 2857, 1898, 1613, 1511, 1433, 1131, 814, 757, 628 cm⁻¹. ¹H NMR (400 MHz, DMSO-*d*₆): $\delta = 8.05$ (d, J = 8.0 Hz, 1H), 8.01 (d, J = 8.1 Hz, 1H), 7.53 (t, J = 7.0 Hz, 1H), 7.44 (t, J = 6.9 Hz, 1H), 7.33 (d, J = 7.8 Hz, 2H), 7.21 (d, J = 7.7 Hz, 2H), 4.47 (s, 2H), 2.33 (s, 3H).

2-benzhydrylbenzo[d]thiazole (5e)



Yellow liquid. 90% yield; m.p: 75-77 °C (Lit. [10] 78-79 °C). IR (KBr): $v_{max} = 3060, 3028, 2923, 1949, 1714, 1598, 1495, 1451, 1312, 1136, 758, 700 cm⁻¹. ¹H NMR (400 MHz, DMSO-$ *d* $₆): <math>\delta = 8.04$ (d, J = 7.8 Hz, 1H), 7.97 (d, J = 7.6 Hz, 1H), 7.49 (t, J = 8.1 Hz, 1H), 7.43-7.36 (m, 9H), 7.30-7.26 (m, 2H), 6.12 (s, 1H).

3-(Benzo[d]thiazol-2-yl)benzonitrile (30)

White solid. 90% yield; m.p: 154-156 °C (Lit. [11] 156-158 °C). IR (KBr): $v_{max} = 3057$, 2924, 2227, 1578, 1504, 1424, 1313, 1255, 1155, 918, 795, 754, 681 cm⁻¹. ¹H NMR (400 MHz, DMSO- d_6): $\delta = 8.51-8.52$ (m, 1H), 8.43 (dt, ¹J = 7.8 Hz, ²J = 1.4 Hz, 1H), 8.22 (d, J = 7.8 Hz, 1H), 8.12 (d, J = 7.8 Hz, 1H), 8.06 (dt, ¹J = 7.6 Hz, ²J = 1.2 Hz, 1H), 7.8 (t, J = 7.8 Hz, 1H), 7.61 (td, ¹J = 7.6 Hz, ²J = 1.2 Hz, 1H), 7.53 (td, ¹J = 7.6 Hz, ²J = 1.2 Hz, 1H).

1,3-Bis(benzo[d]thiazol-2-yl)benzene (3p)



Off-white solid. 80% yield; m.p: 173-175 °C (Lit. [12] 170-172 °C). IR (KBr): $v_{max} = 3054$, 3019, 1555, 1508, 1428, 1313, 1262, 957, 750 cm⁻¹. ¹H NMR (400 MHz, CDCl₃): $\delta = 8.82-8.83$ (m, 1H), 8.26 (dd, ^{*1*}J = 7.8 Hz, ²J = 1.6 Hz, 2H), 8.16 (d, J = 7.6 Hz, 2H), 7.98 (d, J = 7.6 Hz, 2H), 7.67 (t, J = 7.8 Hz, 1H), 7.56 (td, ^{*1*}J = 7.6 Hz, ²J = 1.3 Hz, 2H), 7.46 (td, ^{*1*}J = 7.6 Hz, ²J = 1.2 Hz, 2H).

2-(4-(Benzo[d]thiazol-2-ylmethyl)phenyl)acetonitrile (5f)



Light brown oil. 85% yield; IR (KBr): $v_{max} = 3061$, 2923, 2251, 1615, 1515,1436, 1104, 760, 463 cm⁻¹.¹H NMR (400 MHz, DMSO-*d*₆): $\delta = 8.03$ (d, J = 7.8 Hz, 1H), 7.97 (d, J = 7.8 Hz, 1H), 7.49 (td, ${}^{1}J = 7.6$ Hz, ${}^{2}J = 1.3$ Hz, 1H), 7.45-7.34 (m, 4H), 7.28 (d, J = 7.1 Hz, 1H), 4.51 (s, 2H), 4.06 (s, 2H). 13 C NMR (100 MHz, DMSO-*d*₆): $\delta = 170.55$, 152.81, 138.33, 135.00, 131.72, 129.35, 128.70, 128.47, 126.83, 126.12, 124.92, 122.31, 122.12, 119.19, 39.10, 22.23. Anal. Calcd for C₁₆H₁₂N₂S: C, 72.70; H, 4.58; N, 10.60; S, 12.13. Found: C, 72.81; H, 4.56; N, 10.54; S, 12.04.

1,3-Bis(benzo[d]thiazol-2-ylmethyl)benzene (5g)



Yellow oil. 78% yield; IR (KBr): $v_{max} = 3057$, 2924, 1720, 1512, 1430, 1241, 1131, 1055, 861, 760, 722, 618 cm⁻¹.¹H NMR (400 MHz, DMSO-*d*₆): $\delta = 8.02$ (d, J = 7.7 Hz, 2H), 7.95 (d, J = 7.8 Hz, 2H), 7.49 (td, ${}^{1}J = 7.6$ Hz, ${}^{2}J = 1.3$ Hz, 2H), 7.44 (s, 1H), 7.43-7.31 (m, 5H), 4.48 (s, 4H). 13 C NMR (100 MHz, DMSO-*d*₆): $\delta = 170.83$, 152.81, 137.99, 135.00, 129.87, 129.11, 127.94, 126.09, 124.87, 122.28, 122.11, 39.50. Anal. Calcd for C₂₂H₁₆N₂S₂: C, 70.94; H, 4.33; N, 7.52; S, 17.21. Found: C, 71.03; H, 4.30; N, 7.57; S, 17.14.

2,2',2''-(benzene-1,3,5-triyl)triacetonitrile (4h)



White solid. 80% yield; m.p: 125-127 °C (Lit. [13] 123-125 °C). IR (KBr): $v_{max} = 3040, 2947, 2918, 2249, 1611, 1464, 1410, 943, 829, 685 cm⁻¹.¹H NMR (400 MHz, DMSO-$ *d* $₆): <math>\delta = 7.31$ (s, 3H), 4.13 (s, 6H).

1,3,5-tris(benzo[d]thiazol-2-ylmethyl)benzene (5h)



White solid. 75% yield; m.p: 121-122 °C. IR (KBr): $v_{max} = 3061$, 2908, 1600, 1506, 1428, 1127, 757, 727 cm⁻¹. ¹H NMR (400 MHz, CDCl₃): $\delta = 8.00$ (d, J = 8.0 Hz, 3H), 7.80 (d, J = 8.1 Hz, 3H), 7.47 (t, J = 7.8 Hz, 3H), 7.38-7.33 (m, 6H), 4.50 (s, 6H). ¹³C NMR (100 MHz, CDCl₃): $\delta = 170.46$, 153.25, 138.48, 135.68, 129.02, 126.02, 124.88, 122.85, 121.56, 40.36. Anal. Calcd for C₃₀H₂₁N₃S₃: C, 69.33; H, 4.07; N, 8.09; S, 18.51. Found: C, 69.22; H, 4.10; N, 8.02; S, 18.43.

2. ¹H NMR and ¹³C NMR Spectra of the Products:



2-Phenylbenzo[d]thiazole (Scheme 3, 3a);¹H NMR (400 MHz, DMSO-*d*₆)



2-(2-Chlorophenyl)benzo[d]thiazole (Scheme 3, 3b);¹H NMR (400 MHz, DMSO-*d*₆)



2-(3-Chlorophenyl)benzo[d]thiazole (Scheme 3, 3c);¹H NMR (400 MHz, DMSO-d₆)



2-(4-Chlorophenyl)benzo[d]thiazole (Scheme 3, 3d);¹H NMR (400 MHz, DMSO-d₆)



2-(3-Bromophenyl)benzo[d]thiazole (Scheme 3, 3e);¹H NMR (400 MHz, DMSO-d₆)



2-(4-Bromophenyl)benzo[d]thiazole (Scheme 3, 3f); ¹H NMR (400 MHz, DMSO-d₆)



2-(4-Fluorophenyl)benzo[d]thiazole (Scheme 3, 3g); ¹H NMR (400 MHz, DMSO-d₆)



4-(benzo[d]thiazol-2-yl)benzonitrile (Scheme 3, 3h);¹H NMR (400 MHz, DMSO-d₆)



2-(o-Tolyl)benzo[d]thiazole (Scheme 3, 3i);¹H NMR (400 MHz, DMSO-d₆)



2-(p-Tolyl)benzo[d]thiazole (Scheme 3, 3j);¹H NMR (400 MHz, DMSO-d₆)



3-(Benzo[d]thiazol-2-yl)aniline (Scheme 3, 3k);¹H NMR (400 MHz, DMSO-d₆)



2-(4-methoxyphenyl)benzo[d]thiazole (Scheme 3, 3l);¹H NMR (400 MHz, DMSO-d₆)



2-(Pyridin-2-yl)benzo[d]thiazole (Scheme 3, 3m);¹H NMR (400 MHz, DMSO-d₆)







2-benzylbenzo[d]thiazole (Scheme 3, 5a);¹H NMR (400 MHz, DMSO-d₆)



2-(4-Chlorobenzyl)benzo[d]thiazole (Scheme 3, 5b);¹H NMR (400 MHz, DMSO-d₆)



2-(4-Methoxybenzyl)benzo[d]thiazole (Scheme 3, 5c);¹H NMR (400 MHz, DMSO-d₆)



2-(4-methylbenzyl)benzo[d]thiazole (Scheme 3, 5d);¹H NMR (400 MHz, DMSO-d₆)



2-benzhydrylbenzo[d]thiazole (Scheme 3, 5e);¹H NMR (400 MHz, DMSO-d₆)



3-(Benzo[d]thiazol-2-yl)benzonitrile (Scheme 3, 30);¹H NMR (400 MHz, DMSO-d₆)



1,3-Bis(benzo[d]thiazol-2-yl)benzene (Scheme 3, 3p);¹H NMR (400 MHz, CDCl₃)



2-(4-(Benzo[d]thiazol-2-ylmethyl)phenyl)acetonitrile (Scheme 3, 5f);¹H NMR (400 MHz, DMSO-*d*₆)



2-(4-(Benzo[d]thiazol-2-ylmethyl)phenyl)acetonitrile (Scheme 3, 5f); ¹³C NMR (100 MHz, DMSO-d₆)



1,3-Bis(benzo[d]thiazol-2-ylmethyl)benzene (Scheme 3, 5g);¹H NMR (400 MHz, DMSO-d₆)



1,3-Bis(benzo[d]thiazol-2-ylmethyl)benzene (Scheme 3, 5g); ¹³C NMR (100 MHz, DMSO-d₆)



2,2',2''-(benzene-1,3,5-triyl)triacetonitrile (Scheme 3, 4h);¹H NMR (400 MHz, DMSO-d₆)



1,3,5-tris(benzo[d]thiazol-2-ylmethyl)benzene (Scheme 3, 5h);¹H NMR (400 MHz, CDCl₃)



1,3,5-tris(benzo[d]thiazol-2-ylmethyl)benzene (Scheme 3, 5h); ¹³C NMR (100 MHz, CDCl₃)

3. References:

1. Y. Gao, Q. Song, G. Cheng, and X. Cui, Org. Biomol. Chem., 2014, 12 (7), 1044-1047.

2. I. Choi, V. Müller, G. Lole, R. Köhler, V. Karius, W. Viöl, C. Jooss, and L. Ackermann, *Chem. Eur. J.*, 2020, **26 (16)**, 3509-3514.

3. R. Openshaw, K. Maepa, S. J. Benjamin, L. Wainwright, J. M. Combrinck, R. Hunter, and T. J. Egan, *ACS infect. Dis.*, 2021, **7** (2), 362-376.

4. M. Teramoto, M. Imoto, M. Takeda, T. Mizuno, A. Nomoto, and A. Ogawa, *J. Org. Chem.*, 2020, **85** (23), 15213-15220.

5. R. R. Putta, S. Chun, S. H. Choi, S. B. Lee, D. C. Oh, and S. Hong, *J. Org. Chem.*, 2020, **85 (23)**, 15396-15405.

6. Y. Sun, H. Jiang, W. Wu, W. Zeng, and X. Wu, Org. lett., 2013, 15 (7), 1598-1601.

7. R. Guglielmetti, et al. Bulletin de la Societe Chimique de France, 1967, 2812-2823.

8. P. Boggu, E. Venkateswararao, M. Manickam, D. Kwak, Y. Kim, and S. H. Jung, *Bioorg. Med. Chem.*, 2016, **24 (8)**, 1872-1878.

9. A. Samat, R. Guglielmetti, and J. Metzger, Helv. Chim. Acta., 1972, 55 (5), 1782-1801.

10. X. Zhao, G. Wu, Y. Zhang, and J. Wang, J. Am. Chem. Soc., 2011, 133 (10), 3296-3299.

11. N. Mishra, A. S. Singh, A. K. Agrahari, S. K. Singh, M. Singh, and V. K. Tiwari, ACS Comb. Sci., 2019, **21** (5), 389-399.

12. T. C. Harrop, K. Rodriguez, and P. K. Mascharak, Synth. Commun., 2003, 33 (11), 1943-1949.

13. M. Kanishi, J. I. Kunizaki, J. Inanaga, and M.Yamaguchi, *Bull. Chem. Soc. Japan*, 1981, **54 (12)**, 3828-3831.