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SUPPLEMENTARY MATERIAL TO

Trichloroisocyanuric acid as an efficient homogeneous catalyst for the chemoselective synthesis of 2-substituted oxazolines, imidazolines and thiazolines under solvent-free condition

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PHYSICAL AND SPECTRAL DATA OF SOME PRODUCTS

*2-Phenyl-4,5-dihydro-1,3-oxazole (**1c**)*. Oil; IR (neat, cm^{-1}): 1648 (C=N stretching); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 4.05 (2H, *t*, *J* = 9.5 Hz, CH_2–O), 4.41 (2H, *t*, *J* = 9.5 Hz, CH_2-N), 7.40 (2H, *t*, *J* = 7.5 Hz, aromatic), 7.46 (1H, *t*, *J* = 7.5 Hz, aromatic), 7.95 (2H, *d*, *J* = 7.5 Hz, aromatic).

*2-(3-Chlorophenyl)-4,5-dihydro-1,3-oxazole (**2c**)*. m.p. 40–42 °C; IR (KBr, cm^{-1}): 1644 (C=N stretching); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 4.04 (2H, *t*, *J* = 9.5 Hz, CH_2–O,), 4.41 (2H, *t*, *J* = 9.5 Hz, CH_2-N), 7.32 (2H, t, aromatic, *J* =7.9 Hz), 7.42 (1H, dd, aromatic, *J* = 0.8 and 7.9 Hz), 7.81 (1H, *dd*, *J* = 0.8 and 7.9 Hz, aromatic), 7.92 (1H, *s*, aromatic).

*2-(4-Chlorophenyl)-4,5-dihydro-1,3-oxazole (**3c**)*. m.p. 77–79 °C; IR (KBr, cm^{-1}): 1646 (C=N stretching); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 4.05 (2H, *t*, *J* = 9.5 Hz, CH_2–O), 4.43 (2H, *t*, *J* = 9.5 Hz, CH_2-N), 7.8 (2H, *d*, *J* =8.3 Hz, aromatic), 7.88 (2H, *d*, *J* = 8.3 Hz, aromatic).

*2-(3-Pyridyl)-4,5-dihydro-1,3-oxazole (**4c**)*. m.p. 66–68 °C; IR (KBr, cm^{-1}): 1648 (C=N stretching); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 4.06 (2H, *t*, *J* = = 9.6 Hz, CH_2–O), 4.44 (2H, *t*, *J* = 9.6 Hz, CH_2-N), 7.33 (1H, *dd*, *J* =7.9 and 4.7 Hz, aromatic), 8.20 (1H, *dd*, *J* = 1.8 and 7.9 Hz, aromatic), 8.68 (1H, *dd*, *J* = 1.8 and 4.7 Hz, aromatic), 9.13 (1H, *s*, aromatic).

*2-(4-Pyridyl)-4,5-dihydro-1,3-oxazole (**5c**)*. m.p. 109–111 °C; IR (KBr, cm^{-1}): 1648 (C=N stretching); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 4.05 (2H, *t*, *J* = = 9.6 Hz, CH_2–O), 4.42 (2H, *t*, *J* = 9.4 Hz, CH_2–N), 7.74 (2H, *d*, *J* = 5.7 Hz, aromatic), 8.67 (2H, *d*, *J* = 5.7 Hz, aromatic).

*2-(2-Thienyl)-4,5-dihydro-1,3-oxazole (**6c**)*. m.p. 58–60 °C; IR (KBr, cm^{-1}): 1642 (C=N stretching); ^{1}H NMR (500 MHz, $CDCl_3$, δ / ppm): 4.03 (2H, *t*, CH_2–O,

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J = 9.4 Hz), 4.42 (2H, *t*, CH_2–N, *J* = 9.4 Hz), 7.06 (1H, dd, aromatic, *J* =3.6 and 4.7 Hz), 7.44 (1H, *d*, aromatic, *J* = 4.7 Hz), 7.60 (1H, *d*, aromatic, *J* = 3.6 Hz).

*2-Phenyl-4,5-dihydro-1H-imidazole (**7c**)*. m.p. 100–102 °C; IR (KBr, cm^{-1}): 3190 (NH stretching), 1598 (C=N stretching); ^{1}H-NMR (80 MHz, $CDCl_3$, δ / ppm): 3.75 (4H, *s*, $2CH_2$), 4.8 (1H, *s*, NH), 7.3–7.4 (3H, *m*, aromatic), 7.7–7.8 (2H, *m*, aromatic).

*2-(3-Chlorophenyl)-4,5-dihydro-1H-imidazole (**8c**)*. m.p. 134–136 °C; IR (KBr, cm^{-1}): 3140 (NH stretching), 1595 (C=N stretching); ^{1}H-NMR (80 MHz, $CDCl_3$, δ / ppm): 3.76 (4H, *s*, $2CH_2$), 4.25 (1H, *s*, NH), 7.22–7.75(4H, *m*, aromatic).

*2-(4-Chlorophenyl)-4,5-dihydro-1H-imidazole (**9c**)*. m.p. 186–188 °C; IR (KBr, cm^{-1}): 3140 (NH stretching), 1590 (C=N stretching); ^{1}H-NMR (80 MHz, $CDCl_3$, δ / ppm): 3.75 (4H, *s*, $2CH_2$), 4.22 (1H, *s*, NH), 7.30 (2H, *d*, aromatic), 7.93 (2H, *d*, aromatic).

*2-(4-Bromophenyl)-4,5-dihydro-1H-imidazole (**10c**)*. m.p. 242–246 °C; Anal. Calcd. For $C_9H_9N_2Br$: C, 48.17; H, 4.06; N, 12.45. Found: C, 48.21; H, 4.02; N, 12.50; IR (KBr, cm^{-1}): 3130 (NH stretching), 1590 (C=N stretching); ^{1}H-NMR (80 MHz, $CDCl_3$, δ / ppm): 3.90 (4H, *s*, $2CH_2$), 7.70–7.80 (4H, *m*).

*2-(2-Pyridyl)-4,5-dihydro-1H-imidazole (**11c**)*. m.p. 100–102 °C; IR (KBr, cm^{-1}): 3240 (NH stretching), 1594 (C=N stretching); ^{1}H-NMR (80 MHz, $CDCl_3$, δ / ppm): 3.81 (4H, *s*, $2CH_2$), 5.38 (1H, *s*, NH), 7.22-7.38 (1H, *m*, aromatic), 7.62-7.85 (1H, *m*, aromatic), 8.12 (1H, *d*, aromatic). 8.55 (1H, *d*, aromatic).

*2-(3-Pyridyl)-4,5-dihydro-1H-imidazole (**12c**)*. m.p. 106–108 °C; IR (KBr, cm^{-1}): 3150 (NH stretching), 1586 (C=N stretching); ^{1}H-NMR (80 MHz, $CDCl_3$, δ / ppm): 3.78 (4H, *s*, $2CH_2$), 4.54 (1H, *s*, NH), 7.2–7.38 (1H, *m*, aromatic), 8.02––8.15 (1H, *m*, aromatic), 8.6–8.67 (1H, *m*, aromatic), 8.92 (1H, *s*, aromatic).

*2-(4-Pyridyl)-4,5-dihydro-1H-imidazole (**13c**)*. m.p. 133–135 °C; IR (KBr, cm^{-1}): 3180 (NH stretching), 1594 (C=N stretching); ^{1}H-NMR (80 MHz, $CDCl_3$, δ / ppm): 3.79 (4H, *s*, $2CH_2$), 4.3 (1H, *s*, NH), 7.61 (2H, *d*, aromatic), 8.65 (2H, *d*, aromatic).

*2-(2-Thienyl)-4,5-dihydro-1H-imidazole (**14c**)*. m.p. 174–176 °C; IR (KBr, cm^{-1}): 3140 (NH stretching), 1597 (C=N stretching); ^{1}H NMR (80 MHz, $CDCl_3$, δ / ppm): 3.75 (4H, *s*, $2CH_2$), 4.25 (1H, *s*, NH), 6.9–7.05 (1H, *m*, aromatic), 7.35––7.4 (2H, *m*, aromatic).

*2-Phenyl-4,5-dihydro-1,3-thiazole (**15c**)*. m.p. 126–128 °C; ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 3.40 (2H, *t*, CH_2–S, *J* = 8.3 Hz), 4.46 (2H, *t*, CH_2–N, *J* = = 8.3 Hz), 7.38–7.49 (3H, *m*, aromatic), 7.85 (2H, *dd*, aromatic, *J* = 1.6 and 7.6 Hz).

*2-(4-Fluorophenyl)-4,5-dihydro-1,3-thiazole (**16c**)*. Oil; Anal. Calcd. For C_9H_8NSF: C, 59.64; H, 4.45; N, 7.72. Found: C, 59.67; H, 4.42; N, 7.73; ^{1}H--NMR (500 MHz, $CDCl_3$, δ / ppm): 3.44 (2H, *t*, CH_2–S, *J* = 8.3 Hz), 4.46 (2H, *t*, CH_2–N, *J* = 8.3 Hz), 7.07–7.13 (2H, *m*, aromatic), 7.82–7.87 (2H, *m*, aromatic).

*2-(4-Chlorophenyl)-4,5-dihydro-1,3-thiazole (**17c**)*. m.p. 53–55 128 °C; ^{1}H--NMR (500 MHz, $CDCl_3$, δ / ppm): 3.45 (2H, *t*, CH_2–S, J = 8.4 Hz), 4.47 (2H, *t*, CH_2–N, J = 8.4 Hz), 7.40 (2H, *d*, aromatic, J = 8.6 Hz), 7.79 (2H, *d*, aromatic, J = 8.6 Hz).

*2-(4-Bromophenyl)-4,5-dihydro-1,3-thiazole (**18c**)*. m.p. 60–62 °C; ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 3.33 (2H, *t*, CH_2–S, J = 8.35 Hz), 4.44 (2H, *t*, CH_2–N, J = 8.4 Hz), 7.54 (2H, *d*, aromatic, J = 8.55 Hz), 7.69 (2H, *d*, aromatic, J = 8.5 Hz).

*2-(3-Nitrophenyl)-4,5-dihydro-1,3-thiazole (**19c**)*. m.p. 135–137 °C; Anal. Calcd. For $C_9H_8N_2SO_2$: C, 51.94; H, 3.81; N, 13.44. Found: C, 51.92; H, 3.85; N, 13.46; ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 3.53 (2H, *t*, CH_2–S, J = 8.4 Hz), 4.53 (2H, *t*, CH_2–N, J = 8.4 Hz), 7.63 (1H, *t*, aromatic, J = 8.0 Hz), 8.19 (1H, *d*, aromatic, J = 7.8 Hz), 8.34 (1H, *dd*, aromatic, J = 1.3 and 8.2 Hz), 8.70 (1H, *s*, aromatic, J = 1.8 Hz).

*2-(4-Hydroxyphenyl)-4,5-dihydro-1,3-thiazole (**20c**)*. m.p. 176–178 °C; ^{1}H--NMR (500 MHz, $CDCl_3$, δ / ppm): 3.43 (2H, *t*, CH_2–S, J = 8.3 Hz), 3.85 (1H, *s*, OH), 4.44 (2H, *t*, CH_2–N, J = 8.3 Hz), 6.84 (2H, *d*, aromatic, J = 8.5 Hz) 7.73 (2H, *d*, aromatic, J = 8.5 Hz); MS (*m*/*z*): 179 (M^+), 177 (M^+–2H), 151 (M^+––C_2H_4).

*2-(4-Methoxyphenyl)-4,5-dihydro-1,3-thiazole (**21c**)*. m.p. 53–55 °C; ^{1}H--NMR (500 MHz, $CDCl_3$, δ / ppm): 3.42 (2H, *t*, CH_2–S, J = 8.2 Hz), 3.86 (3H, *s*, O–CH_3), 4.44 (2H, *t*, CH_2–N, J = 8.2 Hz), 6.93 (2H, *d*, aromatic, J = 8.3 Hz), 7.81 (2H, *d*, aromatic, J = 8.3 Hz).

*2-(2-Pyridyl)-4,5-dihydro-1,3-thiazole (**22c**)*. m.p. 92–94 °C; ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 3.32 (2H, *t*, CH_2–S, J = 8.6 Hz), 4.48 (2H, *t*, CH_2–N, J = 8.6 Hz), 7.28–732 (1H, *m*, aromatic), 7.71 (1H, *dt*, aromatic, J = 1.7 and 7.7 Hz), 8.01 (1H, *d*, aromatic, J = 7.9 Hz), 8.60 (1H, *d*, aromatic, J = 4.8 Hz).

*2-(3-Pyridyl)-4,5-dihydro-1,3-thiazole (2**3c**)*. m.p. 111–113 °C; ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 3.37 (2H, *t*, CH_2–S, J = 8.4 Hz), 4.39 (2H, *t*, CH_2–N, J = 8.4 Hz), 7.27 (1H, *dd*, aromatic, J = 4.8 and 8.0 Hz), 8.02 (1H, *dt*, aromatic, J = 1.9 and 8.0 Hz), 8.60 (1H, *dd*, aromatic, J = 1.4 and 4.8 Hz), 8.96 (1H, *d*, aromatic, J = 1.9 Hz).

*2-(2-Thienyl)-4,5-dihydro-1,3-thiazole (**24c**)*. m.p. 40–42 °C; ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 3.37 (2H, *t*, CH_2–S, J = 8.4 Hz), 4.39 (2H, *t*, CH_2–N, J = 8.4 Hz), 7.27 (1H, *dd*, aromatic, J = 4.8 and 8.0 Hz), 8.02 (1H, *dt*, aromatic, J = 1.9 and 8.0 Hz), 8.60 (1H, *dd*, aromatic, J = 1.4 and 4.8 Hz), 8.96 (1H, *d*, aromatic, J = 1.9 Hz).

*3-(4,5-Dihydro-1,3-oxazole-2-yl)benzonitrile (**1f**)*. m.p. 98–100 °C; IR (KBr, cm^{-1}): 1647 (C=N stretching); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 4.08 (2H, *t*, CH_2–O, J = 9.6 Hz), 4.47 (2H, *t*, CH_2–N, J = 9.4 Hz), 7.53 (1H, *t*, aromatic, J =7.8), 7.74 (1H, *d*, aromatic, J = 7.7 Hz), 8.18 (1H, *d*, aromatic, J = 7.8 Hz), 8.22 (1H, *s*, aromatic).

4-(4,5-Dihydro-1,3-oxazol-2-yl)benzonitrile (***2f***). m.p. 112–114 °C; IR (KBr, cm^{-1}): 1641 (C=N stretching); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 4.09 (2H, *t*, CH_2–O, *J* = 9.6 Hz), 4.426 (2H, *t*, CH_2–N, *J* = 9.6 Hz), 7.68 (2H, *d*, aromatic, *J* =8.3 Hz), 8.03 (2H, *d*, aromatic, *J* = 8.3 Hz).

2,2'-(1,3-Phenylene)bis[4,5-dihydrooxazole] (***3f***). m.p. 137–139 °C; IR (KBr, cm^{-1}): 1657 (C=N stretching); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 4.09 (4H, *t*, $2CH_2$–O, *J* = 9.5 Hz), 4.46 (4H, *t*, $2CH_2$–N, *J* = 9.5 Hz), 7.48 (1H, *t*, aromatic, *J* = 7.8 Hz), 8.10 (2H, *dd*, aromatic, *J* = 1.4 and 7.8 Hz), 8.50 (1H, *s*, aromatic).

2,2'-(1,4-Phenylene)bis[4,5-dihydrooxazole] (***4f***). m.p. 238–240 °C; IR (KBr, cm^{-1}): 1640 (C=N stretching); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 4.10 (4H, *t*, $2CH_2$–O, *J* = 9.6 Hz), 4.48 (4H, *t*, $2CH_2$–N, *J* = 9.6 Hz), 8.01 (4H, *s*, aromatic).

*3-(4,5-Dihydro-1*H*-imidazol-2-yl)benzonitrile* (***5f***). m.p. 133–134 °C; ^{1}H--NMR (500 MHz, $CDCl_3$, δ / ppm): 3.81 (4H, *s*, $2CH_2$), 4.2 (1H, *s*, NH), 7.51 (1H, *t*, aromatic, *J* = 7.8 Hz), 7.71 (1H, *d*, aromatic, *J* = 7.7 Hz), 8.01 (1H, *d*, aromatic, *J* = 7.9 Hz), 8.05 (1H, *s*, aromatic); MS (*m*/*z*): 171 (M^+), 169 (M^+–2H), 142 (M^+–C_2H_5).

*4-(4,5-Dihydro-1*H*-imidazole-2-yl)benzonitrile* (***6f***). m.p. 207–209 °C; ^{1}H--NMR (500 MHz, $CDCl_3$, δ / ppm): 3.83 (4H, *s*, $2CH_2$), 4.2 (1H, *s*, NH), 7.71 (2H, *d*, aromatic, *J* = 8.4 Hz), 7.90 (2H, *d*, aromatic, *J* = 8.4 Hz); MS (*m*/*z*): 171 (M^+), 169 (M^+–2H), 142 (M^+–C_2H_5).

2,2'-(1,3-Phenylene)bis[4,5-dihydrothiazole] (***7f***). m.p. 111–113 °C; ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 3.46 (4H, *t*, $2CH_2$–S, *J* = 8.4 Hz), 4.49 (4H, *t*, $2CH_2$–N, *J* = 8.4 Hz), 7.48 (1H, *dd*, aromatic, *J* = 7.8 and 8.0 Hz), 7.95 (2H, *dd*, aromatic, *J* = 1.5 and 7.8 Hz), 8.27 (1H, *s*, aromatic); MS (*m*/*z*): 248 (M^+), 246 (M^+–2H), 244 (M^+–4H), 220 (M^+–C_2H_4), 192 (M^+–$2C_2H_4$).

2,2'-(1,4-Phenylene)bis[4,5-dihydrothiazole] (***8f***). m.p. 105–107 °C; ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 3.45 (4H, *t*, $2CH_2$–S, *J* = 8.3 Hz), 4.49 (4H, *t*, $2CH_2$–N, *J* = 8.3 Hz), 7.88 (4H, *s*, aromatic).