Supporting Information
for DOI: 10.1055/s-0030-1259299
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Experimental

General methods
NMR spectra were determined on a Bruker Avance II 300 MHz spectrometer (using TMS as an internal standard), 2D-NMR experiments (COSY, HMBC, HSQC) were carried out on Varian Inova 600 MHz spectrometer. IR spectra were measured using a FT-IR spectrometer Nicolet IR200 with a single-reflection ATR head. Microanalyses were carried out using CHNS Vario Micro Cube analyzer and their results were in good agreement with the calculated values. Gas chromatography was performed using PerkinElmer Clarus 500 apparatus equipped with Elite-5MS capillary column. Column chromatography was performed using commercial Merck silica gel 60 (230-400 mesh ASTM). Melting points were measured on an Electrothermal 9100 apparatus.

Synthesis of ethyl 5-oxo-2,4-diphenyl-2,5-dihydro-1H-imidazol-2-carboxylate 3a

![3a](image)

Ethyl α-bromophenylacetate 5a (1.7 mL, 2.36 g; 9.72 mmol) and 1.58 g sodium azide NaN₃ (24.3 mmol; 2.5 eq) were added to DMF (30 mL). The suspension was stirred and heated 5 hours at 80 °C. After cooling the reaction mixture was poured into 100 mL of water and extracted three times with 30 mL portions of ethyl acetate. The combined extracts were washed two times with 50 mL of water and dried over anhydrous Na₂SO₄. Then the mixture was filtered with suction and the solvent was removed under reduced pressure. The crude product was purified by column chromatography using Merck silica gel (230-400 mesh; chloroform-methanol 30:1) to give 3a as colorless, crystalline product (TLC silica gel; Fluka 60778; chloroform-methanol 30:1; Rᵣ = 0.45).

¹H-nmr (DMSO-d₆, 300 MHz); δ[ppm] 11.25 (br.s, 1H, NH), 8.38 (d, 2H, J_HH = 6.85 Hz, CH aromatic protons), 7.62 (m, 2H, CH aromatic protons), 7.50 (m, 6H, CH aromatic protons), 4.16 (ddq, 2H, J_HH = 7.13 and 10.65 Hz, OCH₂), 1.14 (t, 6H, J_HH = 7.13 Hz, CH₃).

¹³C-nmr (DMSO-d₆, 75 MHz); δ[ppm] 167.7 (COOEt), 164.8 (CO-NH), 162.9 -(C=N), 137.4 (C1-A), 132.3 (para-CH-B), 129.6 (C1-B), 128.8 (para-CH-A), 128.7 (meta-CH-B), 128.4 (meta-CH-A), 128.3 (ortho-CH-B), 126.5 (ortho-CH-A), 86.9 (C2-het), 62.5 (OCH₂), 13.8 (CH₃).

HMBC: H-C correlation list:
11.25 ppm (NH) → 162.9, 164.9, 86.5
8.38 ppm (CH aromatic proton) → 162.9, 132.3, 128.3
(162.9 ppm: signal of C=N carbon atom)
7.62 ppm (CH aromatic proton) → 86.5, 126.5, 128.3 and 128.8 ppm
7.54 ppm (CH aromatic proton) → 129.6, 162.9 and 128.7 ppm
7.44 ppm (CH aromatic proton) → 137.4, 126.5 and 128.4 ppm
7.40 ppm (CH aromatic proton) → 126.5 ppm
4.17 ppm (CH aromatic proton) → 167.7 and 13.8 ppm
(167.7 ppm: signal of COOEt carbon atom)
1.14 ppm (CH aromatic proton) → 62.5 ppm
Synthesis of ethyl 5-oxo-2,4-di(4-bromophenyl)-2,5-dihydro-1H-imidazol-2-carboxylate 3b

Ethyl 2-bromo-(4-bromophenyl)acetate 5b (1.83 g; 5.67 mmol) and 0.92 g sodium azide \( \text{NaN}_3 \) (14.2 mmol; 2.5 eq) were added to DMF (40 mL). The suspension was stirred and heated 30 hours at 80 °C. After the standard workup, the crude product was purified by column chromatography using Merck silica gel (230-400 mesh; chloroform-methanol 30:1) to give 3b as colorless, crystalline product (TLC silica gel; Fluka 60778; chloroform-methanol 30:1; \( R_f = 0.48 \)).

\[ \text{H-nmr (CDCl}_3, 300 MHz); \sigma[ppm] 8.97 \text{ (br.s, 1H, NH), 8.37 \text{ (d, 2H, J_HH = 8.82 Hz, CH aromatyczne), 7.72 \text{ (d, 1H, J_HH = 8.76 Hz, CH aromatic protons), 7.63 \text{ (d, 1H, J_HH = 8.76 Hz, CH aromatic protons), 7.62 \text{ (d, 2H, J_HH = 8.82 Hz, CH aromatic protons), 7.53 \text{ (m, 2H, CH aromatic protons), 4.26 \text{ (ddq, 2H, J/browse/10.70 Hz, OCH}_2)\), 1.26 \text{ (t, 3H, J_HH = 7.16 Hz, CH}_3)\).} ]\]

\[ \text{C-nmr (CDCl}_3, 75 MHz); \sigma[ppm] 167.3 \text{ (COOEt), 165.4 (CO-NH), 162.2 \text{ (C=N), 135.7 (C1-A), 132.1 \text{ (meta-CH-B), 131.9 (meta-CH-A), 130.4 (ortho-CH-B), 128.3 (C1-B), 128.0 (ortho-CH-A), 127.7 (para-CH-A), 123.7 (para-CH-B), 86.4 (C2-het), 63.4 (OCH}_2)\), 13.9 \text{ (CH}_3\text{, ester group).} ]\]
IR (ATR):

Synthesis of ethyl 5-oxo-2,4-di(4-methylphenyl)-2,5-dihydro-1H-imidazol-2-carboxylate 3c

Ethyl 2-bromo-(4-methylphenyl)acetate 5c (0.41 g; 1.60 mmol) and 0.26 g sodium azide NaN₃ (4.0 mmol; 2.5 eq) were added to DMF (10 mL). The suspension was stirred and heated 18 hours at 80 °C. After standard workup, the crude product was purified by column chromatography using Merck silica gel (230-400 mesh; chloroform-methanol 30:1) to give 3c as colorless product (TLC silica gel; Fluka 60778; chloroform-methanol 30:1; Rᵣ = 0.65).

¹H-nmr (CDCl₃, 300 MHz); δ[ppm] 8.75 (br.s, 1H, NH), 8.51 (d, 2H, J_HH = 8.22 Hz, CH aromatic protons), 7.45 (d, 2H, J_HH = 8.22 Hz, CH aromatic protons), 7.22 (d, 2H, J_HH = 8.58 Hz, CH aromatic protons), 7.15 (d, 2H, J_HH = 7.96 Hz, CH aromatic protons), 4.21 (ddq, 2H, J_HH = 7.16 and 10.80 Hz, OCH₂), 2.37 (s, 3H, CH₃), 2.31 (s, 3H, CH₃), 1.21 (t, 3H, J_HH = 7.16 Hz, CH₃).

¹³C-nmr (CDCl₃, 75 MHz); δ[ppm] 168.1 (COOEt), 165.7 (CO-NH), 165.2 (C=N), 142.8 (para-CH-B), 139.1 (para-CH-A), 134.1 (C1-A), 129.4 (C1-B), 129.3 (para-CH-A), 129.2 (meta-CH-B), 128.9 (meta-CH-A), 128.5 (ortho-CH-B), 126.0 (ortho-CH-A), 86.5 (C2-het), 62.9 (OCH₂), 21.7 (CH₃), 21.1 (CH₃), 13.9 (CH₃, ester group).
Synthesis of ethyl 5-oxo-2,4-di(4-nitrophenyl)-2,5-dihydro-1H-imidazol-2-carboxylate 3e

![Chemical Structure](image)

Ethyl 2-bromo-(4-nitrophenyl)acetate 5e (1.04 g; 3.61 mmol) and 0.60 g sodium azide NaN$_3$ (9.23 mmol; 2.5 eq) were added to DMF (20 mL). The suspension was stirred and heated 30 hours at 80 °C. After standard workup, the crude product was purified by column chromatography using Merck silica gel (230-400 mesh; chloroform-methanol 30:1) to give 3e as orange, amorphous product (TLC silica gel; Fluka 60778; chloroform-methanol 30:1; $R_f$ = 0.30).

$^1$H-nmr (CDCl$_3$, 300 MHz); $\delta$[ppm] 9.14 (br.s, 1H, NH), 8.70 (d, 2H, $J_{HH}$ = 9.03 Hz, CH aromatic protons), 8.33 (d, 2H, $J_{HH}$ = 9.03 Hz, CH aromatic protons), 8.28 (d, 2H, $J_{HH}$ = 8.94 Hz, CH aromatic protons), 7.89 (d, 2H, $J_{HH}$ = 8.94 Hz, CH aromatic protons), 4.29 (ddq, 2H, $J_{HH}$ = 7.14 and 10.80 Hz, OCH$_2$), 1.27 (t, 3H, $J_{HH}$ = 7.14 Hz, CH$_3$).

$^{13}$C-nmr (CDCl$_3$, 75 MHz); $\delta$[ppm] 166.4 (COOEt), 165.0 (CO-NH), 162.0 (C=N), 150.2 (para-CH-B), 148.4 (para-CH-A), 142.6 (C1-A), 134.4 (C1-B), 130.1 (ortho-CH-B), 127.7 (ortho-CH-A), 124.0 (meta-CH-B), 123.7 (meta-CH-A), 86.7 (C2-het), 64.1 (OCH$_2$), 13.9 (CH$_3$, ester group).

IR (ATR):
Synthesis of ethyl 5-oxo-2,4-di(2-pirydyl)-2,5-dihydro-1H-imidazol-2-carboxylate 3f

Ethyl 2-bromo-(2-pirydyl)acetate 5f (1.88 g; 7.70 mmol) and 1.25 g sodium azide NaN₃ (19.2 mmol; 2.5 eq) were added to DMF (25 mL). The suspension was stirred and heated 8 hours at 80 °C. After standard workup, the crude product was purified by column chromatography using Merck silica gel (230-400 mesh; chloroform-methanol 30:1) to give 3f as yellow, crystalline product (TLC silica gel; Fluka 60778; chloroform-methanol 30:1; Rₖ = 0.22).

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\text{\textsuperscript{1}H-nmr (CDCl₃, 300 MHz); } \sigma[\text{ppm}] 9.17 (br.s, 1H, NH), 8.88 (d, 1H, \text{\textsuperscript{3}J_HH} = 4.74 Hz, \text{\textsuperscript{4}J_HH} = 1.81 Hz, \text{\textsuperscript{5}J_HH} = 0.90 Hz, CH aromatic protons), 8.70 (d, 1H, \text{\textsuperscript{3}J_HH} = 7.71 Hz, \text{\textsuperscript{4}J_HH} = 1.11 Hz, CH aromatic protons), 8.67 (d, 1H, \text{\textsuperscript{3}J_HH} = 4.86 Hz, \text{\textsuperscript{4}J_HH} = 1.78 Hz, \text{\textsuperscript{5}J_HH} = 0.93 Hz, CH aromatic protons), 7.87 (d, 1H, \text{\textsuperscript{3}J_HH} = 7.82 Hz, CH aromatic protons), 7.85 (m, 1H, CH aromatic protons), 7.83 (d, 1H, \text{\textsuperscript{3}J_HH} = 7.85 Hz, \text{\textsuperscript{4}J_HH} = 1.83 Hz, CH aromatic protons), 7.74 (t, 1H, \text{\textsuperscript{3}J_HH} = 7.55 Hz, \text{\textsuperscript{4}J_HH} = 1.81 Hz, CH aromatic protons), 7.46 (dd, 1H, \text{\textsuperscript{3}J_HH} = 7.80 and 4.80 Hz, \text{\textsuperscript{4}J_HH} = 1.21 Hz, CH aromatic protons), 7.31 (dd, 1H, \text{\textsuperscript{3}J_HH} = 7.50 and 4.80 Hz, \text{\textsuperscript{4}J_HH} = 1.25 Hz, CH aromatic protons), 4.19 (ddq, 2H, \text{\textsuperscript{3}J_HH} = 7.15 and 10.80 Hz, OCH₂), 1.16 (t, 3H, \text{\textsuperscript{3}J_HH} = 7.15 Hz, CH₃).
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\[
\text{\textsuperscript{13}C-nmr (CDCl₃, 75 MHz); } \sigma[\text{ppm}] 166.7 (COOEt), 164.5 (CO-NH), 164.4 (C=N), 155.5 (C2-A), 150.8, 149.1, 148.0 (C2-B), 137.2, 136.7, 126.3, 125.9, 124.1, 122.4, 88.1 (C2-het), 63.3 (OCH₂), 13.8 (CH₃).
\]
Synthesis of ethyl 5-oxo-2,4-di(2-thienyl)-2,5-dihydro-1H-imidazol-2-carboxylate 3g

Ethyl 2-bromo-(2-thienyl)acetate 5g (0.93 g; 3.73 mmol) and 0.68 g sodium azide NaN₃ (10.45 mmol; 2.8 eq) were added to DMF (10 mL). The suspension was stirred and heated 18 hours at 80 °C. After standard workup, the crude product was purified by column chromatography using Merck silica gel (230-400 mesh; chloroform-methanol 30:1) to give 3g as red, amorphous product (TLC silica gel; Fluka 60778; chloroform-methanol 30:1; Rₑ = 0.35).

¹H-nmr (CDCl₃, 300 MHz); δ[ppm] 8.69 (br.s, 1H, NH), 8.41 (d, 1H, J₃₄ = 3.78 Hz, J₅₃ = 1.17 Hz, CH aromatic protons), 7.64 (d, 1H, J₅₄ = 5.00 Hz, J₃₅ = 1.17 Hz, CH aromatic protons), 7.33 (d, 1H, J₃₄ = 5.10 Hz, J₃₅ = 1.24 Hz, CH aromatic protons), 7.28 (d, 1H, J₅₄ = 3.68 Hz, J₃₅ = 1.24 Hz, CH aromatic protons), 7.17 (d, 1H, J₄₃ = 3.78 Hz, J₄₅ = 5.00 Hz, CH aromatic protons), 7.00 (d, 1H, J₄₅ = 3.68 Hz, J₄₃ = 5.10 Hz, CH aromatic protons), 4.31 (ddq, 2H, J₉₁₂ = 7.14 and 10.70 Hz, OCH₂), 1.30 (t, 3H, J₉₃ = 7.14 Hz, CH₃).

¹³C-nmr (CDCl₃, 75 MHz); δ[ppm] 167.1 (COOEt), 164.4 (CO-NH), 158.6 (C=N), 138.9 (C₂-A), 136.6, 132.8, 131.8, 129.6 (C₂-B), 128.2, 126.9, 126.3, 84.9 (C₂-het), 63.5 (OCH₂), 13.9 (CH₃).

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