Pd-Catalyzed Triple-Fold C(sp²) -H Activation with Enaminones and Alkenes for Pyrrole Synthesis via Hydrogen Evolution

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General experimental information
All experiments were carried out under air atmosphere. All enaminones 1 were synthesized following literature process,¹ and other chemicals and solvents used in the experiments were obtained from commercial sources and used directly without further treatment. ¹H and ¹³C NMR spectra were recorded in 400 MHz apparatus and the
frequencies for $^1$H NMR and $^{13}$C NMR test are 400 MHz and 100 MHz, respectively. The chemical shifts were reported in ppm with TMS as internal standard. Melting points were tested in X-4A instrument without correcting temperature and the HRMS were obtained under ESI model with TOF analyzer.

Table S1 Optimization of the reaction conditions$^a$

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\begin{array}{cccc}
\text{Entry} & \text{Pd-Catalyst} & T (^\circ \text{C}) & \text{Solvent} & \text{Yield (\%)}^b \\
1 & \text{Pd(OAc)}_2 & 80 & \text{DMF} & 24 \\
2^c & \text{Pd(OAc)}_2 & 80 & \text{DMF} & 0 \\
3 & \text{no} & 80 & \text{DMF} & 0 \\
4 & \text{PdCl}_2 & 80 & \text{DMF} & 33 \\
5 & \text{Pd(PPh}_3)_4 & 80 & \text{DMF} & \text{trace} \\
6 & \text{PdCl}_2(\text{PPh}_3)_2 & 80 & \text{DMF} & 21 \\
7 & \text{Pd(acac)}_2 & 80 & \text{DMF} & 17 \\
8^d & \text{PdCl}_2 & 80 & \text{DMF} & 39 \\
9^e & \text{PdCl}_2 & 80 & \text{DMF} & 28 \\
10^d,f & \text{PdCl}_2 & 80 & \text{DMF} & 43 \\
11^d,f & \text{PdCl}_2 & 40 & \text{DMF} & 44 \\
12^d,f & \text{PdCl}_2 & 60 & \text{DMF} & 48 \\
13^d,f,g & \text{PdCl}_2 & 60 & \text{DMF} & 49 \\
14^d,f,h & \text{PdCl}_2 & 60 & \text{DMF} & 51 \\
15^d,f,i & \text{PdCl}_2 & 60 & \text{DMF} & 55 \\
16^d,f,i & \text{PdCl}_2 & 60 & \text{DMF} & 52 \\
17^d,f,i & \text{PdCl}_2 & 60 & \text{DMSO} & \text{trace} \\
18^d,f,i & \text{PdCl}_2 & 60 & \text{toluene} & \text{trace} \\
19^d,f,i,k,l & \text{PdCl}_2 & 60 & \text{DMF} & 63 \\
20^d,f,i,k,l,m & \text{PdCl}_2 & 60 & \text{DMF} & 71 \\
21^f,i,k,l,m & \text{PdCl}_2 & 60 & \text{DMF} & \text{trace} \\
\end{array}
\]
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$^a$General conditions: $1\text{a}$ (0.2 mmol), $2\text{a}$ (0.4 mmol), Pd-cat. (0.01 mmol) and CuBr$_2$ (0.1 mmol) in solvent (2 mL), stirred under air atmosphere for 12 h. $^b$Yield of isolated product based on $1\text{a}$. $^c$Without CuBr$_2$. $^d$With CuBr$_2$ (0.2 mmol). $^e$With CuBr$_2$ (0.3 mmol). $^f$With PdCl$_2$ (0.02 mmol). $^g$With $2\text{a}$ (0.5 mmol). $^h$With $2\text{a}$ (0.6 mmol). $^i$With $2\text{a}$ (0.7 mmol). $^j$With $2\text{a}$ (0.8 mmol). $^k$AgOAc (0.03 mmol) was additionally employed. $^l$With 0.5 mL DMF. $^m$CuI (0.2 mmol) instead of CuBr$_2$. 

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Scheme S1 Hydrogen gas detection

The detected result of hydrogen before the reaction of 1a and 2a for 3a synthesis

The detected result of hydrogen after the reaction completion of 1a and 2a

The detected result of hydrogen before synthesis of 3a by using 5a

The detected result of hydrogen after the completion of 3a synthesis with 5a
HRMS (ESI) for the detection of dienamine 5b

Reaction of 1a and 2b at room temperature (evident signal of dienamine 5b)

Scheme S2 Collection of unsuccessful reactions

standard conditions: the conditions used in Scheme 1 of the manuscript
General procedure for the pyrrole synthesis with enaminones and alkenes

To a 25 mL round-bottom flask were added enaminone 1 (0.2 mmol), acrylate 2 (0.7 mmol), PdCl₂ (0.02 mmol), CuBr₂ (0.2 mmol), AgOAc (0.03 mmol) and DMF (0.5 mL). Then, the mixture was stirred at 60 °C with oil bath heating for 12 h. Upon completion, the vessel was allowed to cool down to room temperature. After 5 mL of saturated brine was added, the resulting mixture was extracted with ethyl acetate (3 × 8 mL). The organic phases were combined and washed with small amount of water for three times. After drying with anhydrous Na₂SO₄, the solid was filtered and the solvent in the acquired solution was removed under reduced pressure. The resulting residue was subjected to flash silica gel column chromatography to provide pure products with the elution of mixed petroleum ether/ethyl acetate (v/v = 5:1-3:1).

Procedure for the 1 mmol scale synthesis of 3a

To a 50 mL round-bottom flask were added enaminone 1a (1 mmol), methyl acrylate 2a (3.5 mmol), PdCl₂ (0.1 mmol), CuBr₂ (1 mmol), AgOAc (0.15 mmol) and DMF (2.5 mL). The mixture was stirred at 60 °C with oil bath heating for 12 h. After cooling down to room temperature. Saturated brine (15 mL) was added, and the resulting mixture was extracted with ethyl acetate (3 × 15 mL). The organic phases were combined and washed with small amount of water for three times. After drying with anhydrous Na₂SO₄, the solid was filtered and the solvent in the acquired solution was removed under reduced pressure. The resulting residue was subjected to flash silica gel column chromatography to provide pure products 3a (128.8 mg, 53%) with the elution of mixed petroleum ether/ethyl acetate (v/v = 5:1).

General procedure for the synthesis of dienamines 5

To a 25 mL round-bottom flask were added enaminone 1 (0.2 mmol), propiolate 4 (0.4 mmol), CuI (0.1 mmol) and MeCN (2.0 mL). The mixture was then stirred at 80 °C with oil bath heating for 24 h. After adding 5 mL brine, the resulting mixture was extracted with ethyl acetate (3 × 8 mL). The organic phases were combined and washed with small amount of water for three times. After drying with anhydrous Na₂SO₄, the solid was filtered and the solvent in the acquired solution was removed under reduced pressure. The resulting residue was subjected to flash silica gel column chromatography.
chromatography to provide pure products with the elution of mixed petroleum ether/ethyl acetate (v/v = 5:1-3:1).

**General procedure for pyrrole synthesis with dienamines**

To a 25 mL round-bottom flask were added dienamines 5 (0.2 mmol), PdCl₂ (0.02 mmol), CuBr₂ (0.2 mmol), AgOAc (0.03 mmol) and DMF (0.5 mL). The mixture was stirred at 60 °C with oil bath heating for 12 h. After adding 5 mL brine, and the resulting mixture was extracted with ethyl acetate (3 × 8 mL). The organic phases were combined and washed with small amount of water for three times. After drying with anhydrous Na₂SO₄, the solid was filtered and the solvent in the acquired solution was removed under reduced pressure. The resulting residue was subjected to flash silica gel column chromatography to provide pure products with the elution of mixed petroleum ether/ethyl acetate (v/v = 5:1-3:1).

**Characterization data for all products**

**Methyl 4-benzoyl-5-methyl-1H-pyrrole-2-carboxylate (3a).** Eluent: V_{PET}/V_{EA} = 5:1; white solid (34.5 mg, 71% yield); mp 201-203 °C; ¹H NMR (400 MHz, CDCl₃) δ 9.53 (s, 1 H), 7.80 (d, J = 7.0 Hz, 2 H), 7.55 (t, J = 7.2 Hz, 1 H), 7.47 (t, J = 7.4 Hz, 2 H), 7.09 (d, J = 2.4 Hz, 1 H), 3.86 (s, 3 H), 2.65 (s, 3 H); ¹³C NMR (100 MHz, CDCl₃) δ 191.9, 161.4, 140.7, 139.6, 131.7, 129.0, 128.2, 121.5, 120.0, 119.0, 51.7, 14.0.

**Ethyl 4-benzoyl-5-methyl-1H-pyrrole-2-carboxylate (3b).** Eluent: V_{PET}/V_{EA} = 5:1; white solid (32.3 mg, 63% yield); mp 123-125°C; ¹H NMR (400 MHz, CDCl₃) δ 9.76 (s, 1 H), 7.80 (d, J = 7.0 Hz, 2 H), 7.55 (t, J = 7.2 Hz, 1 H), 7.47 (t, J = 7.4 Hz, 2 H), 7.09 (d, J = 2.4 Hz, 1 H), 4.33 (q, J = 7.0 Hz, 2 H), 2.65 (s, 3 H), 1.36 (t, J = 7.0 Hz, 3 H); ¹³C NMR (100 MHz, CDCl₃) δ 191.9, 161.2, 140.6, 139.8, 131.6, 129.0, 128.2,
121.4, 120.4, 118.7, 60.8, 14.4, 13.9; HRMS (ESI) m/z: [M + H]⁺ Calcd for C₁₅H₁₆NO₃ 258.1125; Found 258.1126.

**Butyl 4-benzoyl-5-methyl-1H-pyrrole-2-carboxylate (3c).** Eluent: Vₚₑᵗ/Vₑₐ = 5:1; white solid (37.0 mg, 65% yield); mp 103-105°C; ¹H NMR (400 MHz, CDCl₃) δ 9.97 (s, 1 H), 7.80 (d, J = 7.0Hz, 2 H), 7.49-7.46 (m, 3 H), 7.09 (d, J = 2.4 Hz, 1 H), 4.28 (t, J = 6.8 Hz, 2 H), 2.65 (s, 3 H), 1.74-1.67 (m, 2 H), 1.47-1.38 (m, 2 H), 0.95 (t, J = 7.4 Hz, 3 H); ¹³C NMR (100 MHz, CDCl₃) δ 191.9, 161.4, 140.8, 139.8, 131.6, 129.0, 128.2, 121.4, 120.3, 118.8, 64.7, 30.8, 19.2, 13.9, 13.7; HRMS (ESI) m/z: [M + H]⁺ Calcd for C₁₇H₂₀NO₃ 286.1438; Found 286.1439.

**Tert-butyl 4-benzoyl-5-methyl-1H-pyrrole-2-carboxylate (3d).** Eluent: Vₚₑᵗ/Vₑₐ = 5:1; white solid (39.9 mg, 70% yield); mp 143-145°C; ¹H NMR (400 MHz, CDCl₃) δ 9.79 (s, 1 H), 7.80 (d, J = 7.0 Hz, 2 H), 7.55 (t, J = 7.2 Hz, 1 H), 7.47 (t, J = 7.2 Hz, 2 H), 7.00 (d, J = 2.4 Hz, 1 H), 2.63 (s, 3 H), 1.56 (s, 9 H); ¹³C NMR (100 MHz, CDCl₃) δ 192.0, 160.6, 140.1, 139.9, 131.5, 129.0, 128.2, 121.8, 121.2, 118.2, 81.6, 28.3, 13.9; HRMS (ESI) m/z: [M + H]⁺ Calcd for C₁₇H₂₀NO₃ 286.1438; Found 286.1439.

**Benzyl 4-benzoyl-5-methyl-1H-pyrrole-2-carboxylate (3e).** Eluent: Vₚₑᵗ/Vₑₐ = 5:1; white solid (47.2 mg, 74% yield); mp 138-140°C; ¹H NMR (400 MHz, CDCl₃) δ 10.14 (s, 1 H), 7.82-7.75 (m, 2 H), 7.57-7.50 (m, 1 H), 7.49-7.43 (m, 2 H), 7.42-7.31 (m, 5 H), 7.14 (d, J = 2.4 Hz, 1 H), 5.32 (s, 2 H), 2.61 (s, 3 H); ¹³C NMR (100 MHz, CDCl₃) δ 192.0, 161.1, 141.3, 139.7, 135.7, 131.7, 129.1, 128.7, 128.4, 128.3, 128.2, 121.5, 120.0, 119.4, 66.4, 13.9; HRMS (ESI) m/z: [M + H]⁺ Calcd for C₂₀H₁₈NO₃ 320.1281; Found 320.1283.
Methyl 4-(4-fluorobenzoyl)-5-methyl-1H-pyrrole-2-carboxylate (3f). Eluent: V_{PET/V_EA} = 5:1; white solid (27.7 mg, 53% yield); mp 187-189 °C; ¹H NMR (400 MHz, CDCl₃) δ 9.86 (s, 1 H), 7.85-7.82 (m, 2 H), 7.15 (t, J = 8.6 Hz, 2 H), 7.07 (d, J = 2.4 Hz, 1 H), 3.88 (s, 3 H), 2.65 (s, 3 H); ¹³C NMR (100 MHz, CDCl₃) δ 190.3, 166.2, 162.6 (d, J_C-F = 214 Hz), 140.9, 135.8 (d, J_C-F = 3 Hz), 131.5 (d, J_C-F = 9 Hz), 121.2, 120.1, 118.7, 115.3 (d, J_C-F = 21 Hz), 51.8, 13.9; HRMS (ESI) m/z: [M + H]^+ Calcd for C₁₄H₁₃FNO₃ 262.0874; Found 262.0875.

Butyl 4-(4-fluorobenzoyl)-5-methyl-1H-pyrrole-2-carboxylate (3g). Eluent: V_{PET/V_EA} = 5:1; white solid (34.0 mg, 56% yield); mp 101-103°C; ¹H NMR (400 MHz, CDCl₃) δ 10.12 (s, 1 H), 7.89-7.79 (m, 2 H), 7.19-7.13 (m, 2 H), 7.05 (d, J = 2.4 Hz, 1 H), 4.29 (t, J = 6.8 Hz, 2 H), 2.64 (s, 3 H), 1.77-1.67 (m, 2 H), 1.48-1.37 (m, 2 H), 0.96 (t, J = 7.4 Hz, 3 H); ¹³C NMR (100 MHz, CDCl₃) δ 190.4, 164.9 (d, J_C-F = 251 Hz), 161.5, 141.0, 135.8 (d, J_C-F = 3 Hz), 131.5 (d, J_C-F = 9 Hz), 121.2, 120.4, 118.5, 115.3 (d, J_C-F = 21 Hz), 64.8, 30.8, 19.2, 13.9, 13.7; HRMS (ESI) m/z: [M - H]^− Calcd for C₁₇H₁₇FNO₃ 302.1198; Found 302.1199.

Methyl 4-(4-chlorobenzoyl)-5-methyl-1H-pyrrole-2-carboxylate (3h). Eluent: V_{PET/V_EA} = 5:1; white solid (32.1 mg, 58% yield); mp 231-233 °C; ¹H NMR (400 MHz, DMSO-d₆) δ 12.53 (s, 1 H), 7.65 (d, J = 8.2 Hz, 2 H), 7.53 (d, J = 8.4 Hz, 2 H), 6.82 (d, J = 2.0 Hz, 1 H), 3.70 (s, 3 H), 2.42 (s, 3 H); ¹³C NMR (100 MHz, DMSO-d₆) δ 189.8, 160.9, 141.9, 138.7, 136.8, 130.8, 129.0, 120.6, 120.4, 118.5, 51.8, 13.8; HRMS (ESI) m/z: [M + H]^+ Calcd for C₁₄H₁₃ClNO₃ 278.0578; Found 278.0580.
**Butyl 4-(4-chlorobenzoyl)-5-methyl-1H-pyrrole-2-carboxylate (3i).** Eluent: V_{PET}/V_{EA} = 5:1; white solid (40.2 mg, 63% yield); mp 135-137°C; $^1$H NMR (400 MHz, DMSO-$_d$$_6$) δ 12.53 (s, 1 H), 7.73-7.69 (m, 2 H), 7.61-7.57 (m, 2 H), 6.87 (d, $J$ = 2.4 Hz, 1 H), 4.20 (t, $J$ = 6.6 Hz, 2 H), 2.49 (s, 3 H), 1.67-1.58 (m, 2 H), 1.42-1.31 (m, 2 H), 0.90 (t, $J$ = 7.4 Hz, 3 H); $^{13}$C NMR (100 MHz, DMSO-$_d$$_6$) δ 189.9, 160.6, 141.8, 138.7, 136.8, 130.8, 129.0, 120.8, 120.4, 118.2, 64.1, 30.8, 19.1, 14.0, 13.8; HRMS (ESI) m/z: [M + H]$^+$ Calcd for C$_{17}$H$_{19}$ClNO$_3$ 320.1048; Found 320.1050.

**Methyl 4-(4-bromobenzoyl)-5-methyl-1H-pyrrole-2-carboxylate (3j).** Eluent: V_{PET}/V_{EA} = 5:1; white solid (36.6 mg, 57% yield); mp 247-249 °C; $^1$H NMR (400 MHz, DMSO-$_d$$_6$) δ 12.53 (s, 1 H), 7.67 (d, $J$ = 8.4 Hz, 2 H), 7.57 (d, $J$ = 8.4 Hz, 2 H), 6.82 (s, 1 H), 3.70 (s, 3 H), 2.42 (s, 3 H); $^{13}$C NMR (100 MHz, DMSO-$_d$$_6$) δ 189.9, 160.9, 141.9, 139.0, 131.9, 131.0, 125.8, 120.6, 120.4, 118.5, 51.8, 13.8; ESI-HRMS HRMS (ESI) m/z: [M + H]$^+$ Calcd for C$_{14}$H$_{13}$BrNO$_3$ 322.0073; Found 322.0075.

**Tert-butyl 4-(4-bromobenzoyl)-5-methyl-1H-pyrrole-2-carboxylate (3k).** Eluent: V_{PET}/V_{EA} = 5:1; white solid (47.9 mg, 66% yield); mp 173-175°C; $^1$H NMR (400 MHz, DMSO-$_d$$_6$) δ 12.33 (s, 1 H), 7.74 (d, $J$ = 8.4 Hz, 2 H), 7.62 (d, $J$ = 8.4 Hz, 2 H), 6.76 (d, $J$ = 1.2 Hz, 1 H), 2.48 (s, 3 H), 1.50 (s, 9 H); $^{13}$C NMR (100 MHz, DMSO-$_d$$_6$) δ 190.1, 160.0, 141.3, 139.2, 131.9, 130.9, 125.7, 122.2, 120.2, 117.7, 80.9, 28.4, 13.8; HRMS (ESI) m/z: [M + H]$^+$ Calcd for C$_{17}$H$_{19}$BrNO$_3$ 364.0543; Found 364.0542.
Methyl 4-(4-iodobenzoyl)-5-methyl-1H-pyrrole-2-carboxylate (3l). Eluent: V_{PET}/V_{EA} = 5:1; white solid (38.4 mg, 52% yield); mp 264-266 °C; \(^1^H\) NMR (400 MHz, DMSO-\(d_6\)) \(\delta\) 12.57 (s, 1 H), 7.91 (d, \(J = 8.2\) Hz, 2 H), 7.47 (d, \(J = 8.2\) Hz, 2 H), 6.88 (d, \(J = 2.2\) Hz, 1 H), 3.77 (s, 3 H), 2.48 (s, 3 H); \(^1^C\) NMR (100 MHz, DMSO-\(d_6\)) \(\delta\) 190.2, 160.9, 141.8, 139.3, 137.8, 130.8, 120.6, 120.4, 118.5, 99.8, 51.8, 13.8; HRMS (ESI) m/z: [M + H]\(^+\) Calcd for C\(_{14}\)H\(_{13}\)INO\(_3\) 369.9935; Found 369.9936.

Methyl 4-(4-cyanobenzoyl)-5-methyl-1H-pyrrole-2-carboxylate (3m). Eluent: V_{PET}/V_{EA} = 5:1; white solid (27.3 mg, 51% yield); mp 215-217 °C; \(^1^H\) NMR (400 MHz, CDCl\(_3\)) \(\delta\) 9.68 (s, 1 H), 7.79 (d, \(J = 8.0\) Hz, 2 H), 7.71 (d, \(J = 8.0\) Hz, 2 H), 6.92 (s, 1 H), 3.80 (s, 3 H), 2.60 (s, 3 H); \(^1^C\) NMR (100 MHz, CDCl\(_3\)) \(\delta\) 188.9, 160.2, 142.3, 140.5, 131.1, 128.2, 119.6, 119.5, 117.4, 117.1, 113.9, 50.8, 13.0; HRMS (ESI) m/z: [M + H]\(^+\) Calcd for C\(_{15}\)H\(_{13}\)N\(_2\)O\(_3\) 269.0921; Found 269.0922.

Ethyl 4-(4-cyanobenzoyl)-5-methyl-1H-pyrrole-2-carboxylate (3n). Eluent: V_{PET}/V_{EA} = 5:1; white solid (31.0 mg, 55% yield); mp 199-201°C; \(^1^H\) NMR (400 MHz, CDCl\(_3\)) \(\delta\) 10.38 (s, 1 H), 7.87 (d, \(J = 8.2\) Hz, 2 H), 7.79 (d, \(J = 8.2\) Hz, 2 H), 7.00 (d, \(J = 2.4\) Hz, 1 H), 4.36 (q, \(J = 7.0\) Hz, 2 H), 2.68 (s, 3 H), 1.38 (t, \(J = 7.0\) Hz, 3 H); \(^1^C\) NMR (100 MHz, CDCl\(_3\)) \(\delta\) 190.1, 161.3, 143.4, 141.9, 132.2, 129.3, 120.8, 120.5, 118.4, 118.2, 114.9, 61.1, 14.4, 14.0; HRMS (ESI) m/z: [M + H]\(^+\) Calcd for C\(_{16}\)H\(_{15}\)N\(_2\)O\(_3\) 283.1077; Found 283.1079.

Methyl 4-(4-methoxybenzoyl)-5-methyl-1H-pyrrole-2-carboxylate (3o). Eluent: V_{PET}/V_{EA} = 3:1; white solid (37.1 mg, 68% yield); mp 213-215 °C; \(^1^H\) NMR (400 MHz, DMSO-\(d_6\)) \(\delta\) 12.47 (s, 1 H), 7.72 (d, \(J = 8.6\) Hz, 2 H), 7.06 (d, \(J = 8.6\) Hz, 2 H),
6.91 (d, \( J = 1.2 \text{ Hz}, 1 \text{ H} \)), 3.85 (s, 3 H), 3.78 (s, 3 H), 2.47 (s, 3 H); \(^{13}\text{C NMR (100 MHz, DMSO-}d_6\text{)} \delta 189.7, 162.5, 161.0, 141.1, 132.4, 131.3, 120.9, 120.2, 118.3, 114.1, 55.9, 51.8, 13.6; \text{HRMS (ESI) m/z: [M + H]}^+ \text{ Calcd for C}_{15}\text{H}_{16}\text{NO}_{4} 274.1074; \text{Found 274.1075.}

\text{Tert-butyl 4-(4-methoxybenzoyl)-5-methyl-1H-pyrrole-2-carboxylate (3p). Eluent: V}_{\text{PET}}/\text{VEA} = 3:1; \text{white solid (39.7 mg, 63% yield); mp 210-212}^\circ\text{C; }\text{^1H NMR (400 MHz, CDCl}_3\text{)} \delta 9.64 (s, 1 H), 7.83 (d, \( J = 8.8 \text{ Hz}, 2 \text{ H} \)), 7.00 (d, \( J = 2.4 \text{ Hz}, 1 \text{ H} \)), 6.97 (d, \( J = 8.8 \text{ Hz}, 2 \text{ H} \)), 3.89 (s, 3 H), 2.60 (s, 3 H), 1.57 (s, 9 H); \text{^13C NMR (100 MHz, CDCl}_3\text{)} \delta 190.8, 162.6, 160.6, 139.6, 132.4, 131.4, 121.7, 121.4, 118.0, 113.5, 81.5, 55.4, 28.4, 13.8; \text{HRMS (ESI) m/z: [M + H]}^+ \text{ Calcd for C}_{18}\text{H}_{22}\text{NO}_{4} 316.1543; \text{Found 316.1545.}

\text{Methyl 5-methyl-4-(4-methylbenzoyl)-1H-pyrrole-2-carboxylate (3q). Eluent: V}_{\text{PET}}/\text{VEA} = 5:1; \text{white solid (36.0 mg, 70% yield); mp 199-201}^\circ\text{C; }\text{^1H NMR (400 MHz, DMSO-}d_6\text{)} \delta 12.43 (s, 1 H), 7.54 (d, \( J = 7.8 \text{ Hz}, 2 \text{ H} \)), 7.26 (d, \( J = 7.8 \text{ Hz}, 2 \text{ H} \)), 6.82 (d, \( J = 1.6 \text{ Hz}, 1 \text{ H} \)), 3.70 (s, 3 H), 2.41 (s, 3 H), 2.32 (s, 3 H); \text{^13C NMR (100 MHz, DMSO-}d_6\text{)} \delta 190.8, 160.9, 142.1, 141.4, 137.4, 129.4, 129.1, 120.9, 120.3, 118.5, 51.8, 21.5, 13.7; \text{HRMS (ESI) m/z: [M + H]}^+ \text{ Calcd for C}_{15}\text{H}_{16}\text{NO}_{3} 258.1125; \text{Found 258.1126.}

\text{Ethyl 5-methyl-4-(4-methylbenzoyl)-1H-pyrrole-2-carboxylate (3r). Eluent: V}_{\text{PET}}/\text{VEA} = 5:1; \text{white solid (39.6 mg, 73% yield); mp 149-151}^\circ\text{C; }\text{^1H NMR (400 MHz, CDCl}_3\text{)} \delta 10.07 (s, 1 H), 7.72 (d, \( J = 8.0 \text{ Hz}, 2 \text{ H} \)), 7.28 (d, \( J = 8.4 \text{ Hz}, 2 \text{ H} \)), 7.10 (d, \( J = 2.4 \text{ Hz}, 1 \text{ H} \)), 4.33 (q, \( J = 7.0 \text{ Hz}, 2 \text{ H} \)), 2.64 (s, 3 H), 2.43 (s, 3 H), 1.36 (t,
$J = 7.0 \text{ Hz}, 3 \text{ H});^{13}\text{C NMR (100 MHz, CDCl}_3\delta 191.7, 161.4, 142.2, 140.7, 137.0, 129.3, 128.9, 121.5, 120.2, 118.9, 60.8, 21.6, 14.4, 13.8; \text{HRMS (ESI) m/z: } [M + H]^+ \text{ Calcd for } C_{16}H_{18}NO_3 272.1281; \text{Found 272.1283.}

Butyl 5-methyl-4-(4-methylbenzoyl)-1H-pyrrole-2-carboxylate (3s). Eluent: $\text{VPET/VEA} = 5:1$; white solid (42.5 mg, 71% yield); mp 99-101°C; $^1\text{H NMR (400 MHz, CDCl}_3\delta 9.81 (s, 1 H), 7.72 (d, J = 8.0 Hz, 2 H), 7.28 (d, J = 8.0 Hz, 2 H), 7.09 (d, J = 2.6 Hz, 1 H), 4.28 (t, J = 6.8 Hz, 2 H), 2.63 (s, 3 H), 2.44 (s, 3 H), 1.72-1.66 (m, 2 H), 1.48-1.39 (m, 2 H), 0.95 (t, J = 7.4 Hz, 3 H); ^{13}\text{C NMR (100 MHz, CDCl}_3\delta 161.4, 142.3, 140.5, 137.0, 129.3, 128.9, 121.6, 120.3, 118.7, 64.6, 30.8, 21.6, 19.2, 13.9, 13.7; \text{HRMS (ESI) m/z: } [M + H]^+ \text{ Calcd for } C_{18}H_{22}NO_3 300.1594; \text{Found 300.1596.}

Tert-butyl 5-methyl-4-(4-methylbenzoyl)-1H-pyrrole-2-carboxylate (3t). Eluent: $\text{VPET/VEA} = 5:1$; white solid (44.8 mg, 75% yield); mp 210-212°C; $^1\text{H NMR (400 MHz, CDCl}_3\delta 9.61 (s, 1 H), 7.72 (d, J = 8.0 Hz, 2 H), 7.27 (d, J = 8.0 Hz, 2 H), 7.00 (d, J = 2.4 Hz, 1 H), 2.62 (s, 3 H), 2.43 (s, 3 H), 1.56 (s, 9 H); ^{13}\text{C NMR (100 MHz, CDCl}_3\delta 191.8, 160.6, 142.2, 139.9, 137.1, 129.3, 128.9, 121.7, 121.4, 118.2, 81.5, 28.4, 21.6, 13.9; \text{HRMS (ESI) m/z: } [M + H]^+ \text{ Calcd for } C_{18}H_{22}NO_3 300.1594; \text{Found 300.1596.}

Benzyl 5-methyl-4-(4-methylbenzoyl)-1H-pyrrole-2-carboxylate (3u). Eluent: $\text{VPET/VEA} = 5:1$; white solid (50.6 mg, 76% yield); mp 93-95°C; $^1\text{H NMR (400 MHz, CDCl}_3\delta 9.68 (s, 1 H), 7.70 (d, J = 8.0 Hz, 2 H), 7.45-7.32 (m, 5 H), 7.25 (d, J = 8.0 Hz, 2 H), 7.13 (d, J = 2.4 Hz, 1 H), 5.31 (s, 2 H), 2.60 (s, 3 H), 2.42 (s, 3 H); ^{13}\text{C NMR (100 MHz, CDCl}_3\delta 191.6, 160.9, 142.3, 140.7, 136.9, 135.8, 129.3, 129.0,
128.6, 128.4, 128.3, 121.7, 119.9, 119.2, 66.4, 21.6, 13.9; HRMS (ESI) m/z: [M + H]⁺
Calcd for C₂₁H₂₀NO₃ 334.1438; Found 334.1441.

**Methyl 4-(3-chlorobenzoyl)-5-methyl-1H-pyrrole-2-carboxylate (3v).**
Eluent: Vₚₑᵗ/VEₐ = 5:1; white solid (31.0 mg, 56% yield); mp 186-188 °C; ¹H NMR (400 MHz, CDCl₃) δ 10.03 (s, 1 H), 7.76 (s, 1 H), 7.66 (d, J = 7.6 Hz, 1 H), 7.52 (d, J = 8.0 Hz, 1 H), 7.41 (t, J = 7.8 Hz, 1 H), 7.06 (d, J = 1.8 Hz, 1 H), 3.88 (s, 3 H), 2.65 (s, 3 H); ¹³C NMR (100 MHz, CDCl₃) δ 190.2, 161.6, 141.4, 141.3, 134.4, 131.6, 129.6, 128.9, 127.1, 121.0, 120.3, 118.7, 51.8, 13.9; HRMS (ESI) m/z: [M + H]⁺ Calcd for C₁₄H₁₃ClNO₃ 278.0578; Found 278.0580.

**Benzyl 4-(3-chlorobenzoyl)-5-methyl-1H-pyrrole-2-carboxylate (3w).**
Eluent: Vₚₑᵗ/VEₐ = 5:1; white solid (45.3mg, 64% yield); mp 127-129 °C; ¹H NMR (400 MHz, CDCl₃) δ 9.83 (s, 1 H), 7.77-7.73 (m, 1 H), 7.68-7.62 (m, 1 H), 7.53-7.48 (m, 1 H), 7.43-7.33 (m, 6 H), 7.09 (d, J = 2.4 Hz, 1 H), 5.32 (s, 2 H), 2.61 (s, 3 H); ¹³C NMR (100 MHz, CDCl₃) δ 190.3, 160.8, 141.3, 141.3, 135.6, 134.5, 131.6, 129.6, 128.9, 128.7, 128.5, 128.3, 127.1, 121.1, 120.2, 119.0, 66.5, 14.0; HRMS (ESI) m/z: [M + H]⁺ Calcd for C₂₀H₁₇ClNO₃ 354.0891; Found 354.0891.

**Methyl 4-(3-bromobenzoyl)-5-methyl-1H-pyrrole-2-carboxylate (3x).**
Eluent: Vₚₑᵗ/VEₐ = 5:1; white solid (37.8 mg, 59% yield); mp 182-184 °C; ¹H NMR (400 MHz, CDCl₃) δ 10.01 (s, 1 H), 7.91 (s, 1 H), 7.73-7.62 (m, 2 H), 7.35 (t, J = 7.8 Hz, 1 H), 7.06 (d, J = 2.4 Hz, 1 H), 3.88 (s, 3 H), 2.65 (s, 3 H); ¹³C NMR (100 MHz, CDCl₃)
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δ 190.1, 161.6, 141.6, 141.3, 134.5, 131.8, 129.8, 127.5, 122.5, 121.0, 120.3, 118.7, 51.8, 13.9; HRMS (ESI) m/z: [M + H]⁺ Calcd for C₁₄H₁₃BrNO₃ 322.0073; Found 322.0075.

Benzyl 4-(3-bromobenzoyl)-5-methyl-1H-pyrrole-2-carboxylate (3y). Eluent: Vₚₑᵗ/Vₑₐ = 5:1; white solid (53.2 mg, 67% yield); mp 146-148°C; ¹H NMR (400 MHz, CDCl₃) δ 9.80 (s, 1 H), 7.90 (t, J = 1.6 Hz, 1 H), 7.72-7.63 (m, 2 H), 7.43-7.30 (m, 6 H), 7.09 (d, J = 2.4 Hz, 1 H), 5.32 (s, 2 H), 2.61 (s, 3 H); ¹³C NMR (100 MHz, CDCl₃) δ 190.2, 160.8, 141.5, 141.3, 135.7, 134.5, 131.8, 129.9, 128.7, 128.5, 128.3, 127.5, 122.6, 121.0, 120.3, 118.9, 66.5, 14.0; HRMS (ESI) m/z: [M - H]⁻ Calcd for C₂₀H₁₅BrNO₃ 396.0241; Found 396.0240.

Methyl 4-(3-methoxybenzoyl)-5-methyl-1H-pyrrole-2-carboxylate (3z). Eluent: Vₚₑᵗ/Vₑₐ = 5:1; white solid (35.5 mg, 65% yield); mp 147-149 °C; ¹H NMR (400 MHz, CDCl₃) δ 9.94 (s, 1 H), 7.38-7.36 (m, 2 H), 7.33 (s, 1 H), 7.12-7.07 (m, 2 H), 3.87 (s, 3 H), 3.86 (s, 3 H), 2.65 (s, 3 H); ¹³C NMR (100 MHz, CDCl₃) δ 191.6, 161.7, 159.6, 141.0, 141.0, 129.2, 121.7, 121.5, 120.0, 119.0, 118.0, 113.6, 55.4, 51.7, 13.9; HRMS (ESI) m/z: [M + H]⁺ Calcd for C₁₅H₁₆NO₄ 274.1074; Found 274.1075.

Butyl 4-(3-methoxybenzoyl)-5-methyl-1H-pyrrole-2-carboxylate (3aa). Eluent: Vₚₑᵗ/Vₑₐ = 3:1; white solid (39.7 mg, 63% yield); mp 105-107°C; ¹H NMR (400 MHz, CDCl₃) δ 10.33 (s, 1 H), 7.45-7.36 (m, 2 H), 7.36-7.32 (m, 1 H), 7.16-7.03 (m, 2 H), 4.29 (t, J = 6.8 Hz, 2 H), 3.86 (s, 3 H), 2.65 (s, 3 H), 1.76-1.66 (m, 2 H),
1.48-1.37 (m, 2 H), 0.95 (t, J = 7.4 Hz, 3 H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) δ 191.7, 161.6, 159.5, 141.2, 141.1, 129.2, 121.7, 121.4, 120.3, 118.9, 118.0, 113.5, 64.7, 55.4, 30.8, 19.2, 13.9, 13.7; HRMS (ESI) m/z: [M - H] - Calcd for C\(_{18}\)H\(_{20}\)NO\(_4\) 314.1398; Found 314.1408.

Methyl 5-methyl-4-(3-methylbenzoyl)-1H-pyrrole-2-carboxylate (3ab). Eluent: V\(_{PET}/\)V\(_{EA}\) = 5:1; white solid (32.9 mg, 64% yield); mp 155-157°C; \(^1\)H NMR (400 MHz, DMSO-\(d_6\)) δ 12.52 (s, 1 H), 7.48-7.46 (m, 2 H), 7.41-7.40 (m, 2 H), 6.87 (d, J = 2.2 Hz, 1 H), 3.77 (s, 3 H), 2.48 (s, 3 H), 2.38 (s, 3 H); \(^{13}\)C NMR (100 MHz, DMSO-\(d_6\)) δ 191.3, 160.9, 141.5, 140.2, 138.2, 132.6, 129.2, 128.7, 126.1, 120.9, 120.4, 118.6, 51.8, 21.4, 13.7; HRMS (ESI) m/z: [M + H]\(^+\) Calcd for C\(_{15}\)H\(_{16}\)NO\(_3\) 258.1125; Found 258.1126.

Ethyl 5-methyl-4-(3-methylbenzoyl)-1H-pyrrole-2-carboxylate (3ac). Eluent: V\(_{PET}/\)V\(_{EA}\) = 5:1; white solid (33.1 mg, 61% yield); mp 134-136°C; \(^1\)H NMR (400 MHz, CDCl\(_3\)) δ 9.94 (s, 1 H), 7.64-7.55 (m, 2 H), 7.40-7.32 (m, 3 H), 7.09 (d, J = 2.4 Hz, 1 H), 4.34 (q, J = 7.0 Hz, 2 H), 2.64 (s, 3 H), 2.43 (s, 3 H), 1.36 (t, J = 7.0 Hz, 3 H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) δ 192.2, 161.3, 140.7, 139.8, 138.1, 132.4, 129.4, 128.0, 126.3, 121.5, 120.3, 118.9, 60.8, 21.4, 14.4, 13.9; HRMS (ESI) m/z: [M + H]\(^+\) Calcd for C\(_{16}\)H\(_{18}\)NO\(_3\) 272.1281; Found 272.1283.

Methyl 5-methyl-4-(2-methylbenzoyl)-1H-pyrrole-2-carboxylate (3ad). Eluent: V\(_{PET}/\)V\(_{EA}\) = 5:1; white solid (28.8 mg, 56% yield); mp 167-169°C; \(^1\)H NMR (400
MHz, CDCl$_3$) $\delta$ 10.16 (s, 1 H), 7.35-7.32 (m, 2 H), 7.24-7.21 (m, 2 H), 6.87 (d, $J = 2.4$ Hz, 1 H), 3.83 (s, 3 H), 2.62 (s, 3 H), 2.35 (s, 3 H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 194.3, 161.6, 140.7, 140.4, 135.7, 130.9, 129.6, 127.6, 125.2, 122.8, 120.2, 119.3, 51.7, 19.6, 13.9; HRMS (ESI) m/z: [M + H]$^+$ Calcd for C$_{15}$H$_{16}$NO$_3$ 258.1125; Found 258.1126.

Methyl 4-(1-naphthoyl)-5-methyl-1H-pyrrole-2-carboxylate (3ae). Eluent: V$_{PET}$/V$_{EA}$ = 5:1; white solid (36.3 mg, 62% yield); mp 184-186°C; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 9.81 (s, 1 H), 8.11 (d, $J = 8.6$ Hz, 1 H), 7.95 (d, $J = 8.0$ Hz, 1 H), 7.89 (d, $J = 7.2$ Hz, 1 H), 7.59 (d, $J = 6.8$ Hz, 1 H), 7.54-7.44 (m, 3 H), 6.88 (d, $J = 2.6$ Hz, 1 H), 3.80 (s, 3 H), 2.66 (s, 3 H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 193.4, 161.4, 140.8, 138.2, 133.8, 130.4, 128.3, 126.9, 126.3, 126.2, 125.6, 124.5, 123.3, 120.2, 119.3, 51.7, 14.1; HRMS (ESI) m/z: [M + H]$^+$ Calcd for C$_{18}$H$_{16}$NO$_3$ 294.1125; Found 294.1126.

Tert-butyl 4-(1-naphthoyl)-5-methyl-1H-pyrrole-2-carboxylate (3af). Eluent: V$_{PET}$/V$_{EA}$ = 5:1; white solid (38.2 mg, 57% yield); mp 213-215°C; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 9.85 (s, 1 H), 8.15-8.09 (m, 1 H), 7.96 (d, $J = 8.2$ Hz, 1 H), 7.92-7.87 (m, 1 H), 7.62-7.58 (m, 1 H), 7.55-7.48 (m, 3 H), 6.82 (d, $J = 2.6$ Hz, 1 H), 2.62 (s, 3 H), 1.51 (s, 9 H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 193.6, 160.7, 140.4, 138.3, 133.8, 130.4, 130.4, 128.3, 126.9, 126.3, 126.2, 125.6, 124.5, 123.1, 122.0, 118.5, 81.7, 28.3, 14.2; HRMS (ESI) m/z: [M + H]$^+$ Calcd for C$_{21}$H$_{22}$NO$_3$ 336.1594; Found 336.1596.
Methyl 4-(2-naphthoyl)-5-methyl-1H-pyrrole-2-carboxylate (3ag). Eluent: $V_{PET}/V_{EA} = 5:1$; white solid (40.4 mg, 69% yield); mp 216-218 °C; $^1H$ NMR (400 MHz, CDCl$_3$) $\delta$ 9.65 (s, 1 H), 8.30 (s, 1 H), 8.00-7.85 (m, 4 H), 7.66-7.47 (m, 2 H), 7.16 (s, 1 H), 3.86 (s, 3 H), 2.68 (s, 3 H); $^{13}C$ NMR (100 MHz, CDCl$_3$) $\delta$ 191.8, 161.5, 140.7, 136.9, 135.0, 132.4, 130.1, 129.3, 128.2, 127.8, 127.8, 126.6, 125.4, 120.1, 119.0, 51.7, 13.9; HRMS (ESI) m/z: [M + H]$^+$ Calcd for C$_{18}$H$_{16}$NO$_3$ 294.1125; Found 294.1126.

Butyl 4-(2-naphthoyl)-5-methyl-1H-pyrrole-2-carboxylate (3ah). Eluent: $V_{PET}/V_{EA} = 5:1$; white solid (42.9 mg, 64% yield); mp 158-160 °C; $^1H$ NMR (400 MHz, CDCl$_3$) $\delta$ 10.09 (s, 1 H), 8.31 (s, 1 H), 7.99-7.88 (m, 4 H), 7.63-7.52 (m, 2 H), 7.16 (d, $J = 2.4$ Hz, 1 H), 4.29 (t, $J = 6.8$ Hz, 2 H), 2.68 (s, 3 H), 1.74-1.66 (m, 2 H), 1.47-1.36 (m, 2 H), 0.94 (t, $J = 7.4$ Hz, 3 H); $^{13}C$ NMR (100 MHz, CDCl$_3$) $\delta$ 191.9, 161.5, 140.9, 137.0, 135.0, 132.4, 130.2, 129.3, 128.2, 127.8, 127.8, 126.6, 125.4, 121.6, 120.4, 118.9, 64.8, 30.8, 19.2, 13.9, 13.7; HRMS (ESI) m/z: [M + H]$^+$ Calcd for C$_{21}$H$_{22}$NO$_3$ 336.1594; Found 336.1596.

Methyl 5-methyl-4-(thiophene-2-carbonyl)-1H-pyrrole-2-carboxylate (3ai). Eluent: $V_{PET}/V_{EA} = 5:1$; white solid (36.4 mg, 73% yield); mp 230-232 °C; $^1H$ NMR (400 MHz, DMSO-$d_6$) $\delta$ 12.54 (s, 1 H), 7.96 (d, $J = 5.0$ Hz, 1 H), 7.79 (d, $J = 3.6$ Hz, 1 H), 7.27-7.21 (m, 2 H), 3.80 (s, 3 H), 2.48 (s, 3 H); $^{13}C$ NMR (100 MHz, DMSO-$d_6$) $\delta$ 181.9, 161.0, 145.1, 141.5, 133.8, 133.1, 128.9, 120.7, 120.4, 117.3, 51.8, 13.6; HRMS (ESI) m/z: [M + H]$^+$ Calcd for C$_{12}$H$_{12}$NO$_3$S 250.0532; Found 250.0534.
Ethyl 5-methyl-4-(thiophene-2-carbonyl)-1H-pyrrole-2-carboxylate (3aj). Eluent: \( V_{\text{PET}}/V_{\text{EA}} = 5:1 \); white solid (36.3 mg, 69% yield); mp 148-150°C; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 9.62 (s, 1 H), 7.77 (dd, \( J = 3.8, 1.0 \) Hz, 1 H), 7.64 (dd, \( J = 5.0, 1.0 \) Hz, 1 H), 7.35 (d, \( J = 2.4 \) Hz, 1 H), 7.18-7.14 (m, 1 H), 4.36 (q, \( J = 7.0 \) Hz, 2 H), 2.63 (s, 3 H), 1.38 (t, \( J = 7.0 \) Hz, 3 H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \( \delta \) 182.6, 161.0, 145.2, 140.4, 132.6, 127.8, 121.2, 120.6, 117.4, 60.8, 14.4, 13.8; HRMS (ESI) m/z: [M + H]\(^+\) Calcd for C\(_{13}\)H\(_{14}\)NO\(_3\)S 264.0689; Found 264.0690.

Benzyl 5-methyl-4-(thiophene-2-carbonyl)-1H-pyrrole-2-carboxylate (3ak). Eluent: \( V_{\text{PET}}/V_{\text{EA}} = 5:1 \); white solid (46.8 mg, 72% yield); mp 107-109°C; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 10.06 (s, 1 H), 7.74 (dd, \( J = 3.6, 1.0 \) Hz, 1 H), 7.62 (dd, \( J = 5.0, 1.0 \) Hz, 1 H), 7.46-7.30 (m, 6 H), 7.14 (dd, \( J = 4.8, 3.8 \) Hz, 1 H), 5.34 (s, 2 H), 2.60 (s, 3 H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \( \delta \) 182.6, 161.1, 145.1, 141.1, 135.7, 132.6, 128.7, 128.5, 128.2, 127.8, 121.3, 120.2, 118.0, 66.5, 13.8; HRMS (ESI) m/z: [M + H]\(^+\) Calcd for C\(_{18}\)H\(_{16}\)NO\(_3\)S 326.0845; Found 326.0848.

Methyl 4-(benzo[d][1,3]dioxole-5-carbonyl)-5-methyl-1H-pyrrole-2-carboxylate (3al). Eluent: \( V_{\text{PET}}/V_{\text{EA}} = 5:1 \); white solid (36.2 mg, 63% yield); mp 216-218°C; \(^1\)H NMR (400 MHz, DMSO-\(d_6\)) \( \delta \) 12.47 (s, 1 H), 7.36-7.26 (m, 1 H), 7.24-7.16 (m, 1 H), 7.03 (d, \( J = 8.0 \) Hz, 1 H), 6.90 (s, 1 H), 6.13 (s, 2 H), 3.78 (s, 3 H), 2.46 (s, 3 H); \(^{13}\)C NMR (100 MHz, DMSO-\(d_6\)) \( \delta \) 189.3, 161.0, 150.8, 147.9, 141.2, 134.2, 125.0, 120.8, 120.2, 118.3, 108.8, 108.3, 102.3, 51.8, 13.6; HRMS (ESI) m/z: [M + H]\(^+\) Calcd for C\(_{15}\)H\(_{14}\)NO\(_5\) 288.0866; Found 288.0868.

Methyl 4-(3,4-dimethoxybenzoyl)-5-methyl-1H-pyrrole-2-carboxylate (3am).
Eluent: \( V_{PET}/V_{EA} = 3:1 \); white solid (36.9 mg, 61% yield); mp 185-187°C; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 9.89 (s, 1 H), 7.51-7.39 (m, 2 H), 7.14 (d, \( J = 2.4 \) Hz, 1 H), 6.92 (d, \( J = 8.2 \) Hz, 1 H), 3.96 (s, 3 H), 3.94 (s, 3 H), 3.87 (s, 3 H), 2.63 (s, 3 H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \( \delta \) 190.5, 161.6, 152.4, 148.9, 140.4, 132.3, 123.9, 121.6, 119.9, 118.7, 111.7, 109.9, 56.0, 56.0, 51.7, 13.7; HRMS (ESI) \( m/z: [M + H]^+ \) Calcd for C\(_{16}\)H\(_{18}\)NO\(_5\) 304.1179; Found 304.1181.

Methyl 4-(3,4-dichlorobenzoyl)-5-methyl-1H-pyrrole-2-carboxylate (3an). Eluent: \( V_{PET}/V_{EA} = 5:1 \); white solid (44.8 mg, 72% yield); mp 217-219°C; \(^1\)H NMR (400 MHz, DMSO-\( d_6 \)) \( \delta \) 12.64 (s, 1 H), 7.84 (d, \( J = 2.0 \) Hz, 1 H), 7.78 (d, \( J = 8.2 \) Hz, 1 H), 7.65 (dd, \( J = 8.2, 2.0 \) Hz, 1 H), 6.90 (s, 1 H), 3.78 (s, 3 H), 2.49 (s, 3 H); \(^{13}\)C NMR (100 MHz, DMSO-\( d_6 \)) \( \delta \) 188.5, 160.9, 142.21, 140.28, 140.28, 134.73, 131.87, 131.23, 130.57, 129.05, 120.75, 118.41, 51.87, 13.79; HRMS (ESI) \( m/z: [M + H]^+ \) Calcd for C\(_{14}\)H\(_{12}\)Cl\(_2\)NO\(_3\) 312.0189; Found 312.0191.

Tert-butyl 4-(3,4-dichlorobenzoyl)-5-methyl-1H-pyrrole-2-carboxylate (3ao). Eluent: \( V_{PET}/V_{EA} = 5:1 \); white solid (52.9 mg, 75% yield); mp 164-166°C; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \( \delta \) 10.00 (s, 1 H), 7.89 (d, \( J = 2.0 \) Hz, 1 H), 7.63 (dd, \( J = 8.2, 2.0 \) Hz, 1 H), 7.56 (d, \( J = 8.2 \) Hz, 1 H), 6.93 (d, \( J = 2.4 \) Hz, 1 H), 2.64 (s, 3 H), 1.58 (s, 9 H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \( \delta \) 189.3, 160.6, 140.8, 139.5, 135.9, 132.8, 130.9, 130.3, 128.2, 122.2, 120.5, 117.7, 81.9, 28.3, 14.0; HRMS (ESI) \( m/z: [M + H]^+ \) Calcd for C\(_{17}\)H\(_{18}\)Cl\(_2\)NO\(_3\) 354.0658; Found 354.0642.
Methyl 4-(furan-2-carbonyl)-5-methyl-1H-pyrrole-2-carboxylate (3ap). Eluent: 
$V_{PET}/V_{EA} = 5:1$; white solid (31.2 mg, 67% yield); mp 237-239°C; $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 12.52 (s, 1 H), 8.04-7.99 (m, 1 H), 7.47 (d, $J = 2.4$ Hz, 1 H), 7.30 (d, $J = 3.4$ Hz, 1 H), 6.75-6.69 (m, 1 H), 3.80 (s, 3 H), 2.50 (s, 3 H); $^{13}$C NMR (100 MHz, DMSO-$d_6$) $\delta$ 181.1, 165.8, 158.4, 152.0, 147.0, 125.5, 124.4, 122.8, 122.3, 117.5, 56.6, 18.7; HRMS (ESI) m/z: [M - H]$^-\text{Calcd}$ for C$_{12}$H$_{10}$NO$_4$ 232.0615; Found 232.0615.

![Methyl 4-(furan-2-carbonyl)-5-methyl-1H-pyrrole-2-carboxylate (3ap) structure](image)

4-Ethyl 2-methyl 5-phenyl-1H-pyrrole-2,4-dicarboxylate (3aq). Eluent: $V_{PET}/V_{EA} = 5:1$; white solid (37.7 mg, 69% yield); mp 123-125°C; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 9.71 (s, 1 H), 7.67-7.58 (m, 2 H), 7.48-7.35 (m, 4 H), 4.22 (q, $J = 7.0$ Hz, 2 H), 3.81 (s, 3 H), 1.26 (t, $J = 7.0$ Hz, 3 H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 164.0, 161.4, 140.8, 130.8, 129.2, 129.1, 128.2, 121.9, 118.6, 114.3 60.0, 51.8, 14.2; HRMS (ESI) m/z: [M + H]$^+$ Calcd for C$_{15}$H$_{16}$NO$_4$ 274.1074; Found 274.1075.

![4-Ethyl 2-methyl 5-phenyl-1H-pyrrole-2,4-dicarboxylate (3aq) structure](image)

Methyl 4-benzoyl-5-propyl-1H-pyrrole-2-carboxylate (3ar). Eluent: $V_{PET}/V_{EA} = 5:1$; white solid (38.5 mg, 71% yield); mp 118-120°C; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 9.66 (s, 1 H), 7.79 (d, $J = 7.2$ Hz, 2 H), 7.54 (t, $J = 7.2$ Hz, 1 H), 7.47 (t, $J = 7.4$ Hz, 2 H), 7.09 (d, $J = 2.4$ Hz, 1 H), 3.86 (s, 3 H), 3.03 (t, $J = 7.6$ Hz, 2 H), 1.82-1.72 (m, 2 H), 1.00 (t, $J = 7.2$ Hz, 3 H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 191.8, 161.5, 145.2, 139.8, 131.6, 129.1, 128.2, 121.1, 120.0, 119.1, 51.7, 29.6, 22.3, 13.9; HRMS (ESI) m/z: [M + H]$^+$ Calcd for C$_{16}$H$_{18}$NO$_3$ 272.1281; Found 272.1283.

![Methyl 4-benzoyl-5-propyl-1H-pyrrole-2-carboxylate (3ar) structure](image)

Methyl 4-benzoyl-5-phenyl-1H-pyrrole-2-carboxylate (3as). Eluent: $V_{PET}/V_{EA} = 5:1$; white solid (44.5 mg, 73% yield); mp 119-121°C; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$
9.66 (s, 1 H), 7.79 (d, J = 7.2 Hz, 2 H), 7.54-7.46 (m, 3 H), 7.40-7.32 (m, 5 H), 7.22 (d, J = 2.6 Hz, 1 H), 3.85 (s, 3 H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 191.6, 161.3, 140.5, 138.8, 132.1, 130.7, 129.6, 129.0, 128.6, 128.5, 128.1, 121.9, 119.4, 51.9; HRMS (ESI) m/z: [M + H]$^+$ Calcd for C$_{19}$H$_{16}$NO$_3$ 306.1125; Found 306.1126.

**Methyl (2E, 4E)-5-amino-4-benzoylhexa-2,4-dienoate (5a).** Eluent: V$_{PET}$/V$_{EA}$ = 5:1; white solid (42.6 mg, 87% yield); mp 170-172$^\circ$C; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.68 (d, J = 15.8 Hz, 1 H), 7.51-7.45 (m, 2 H), 7.42-7.33 (m, 3 H), 5.14 (d, J = 15.8 Hz, 1 H), 3.62 (s, 3 H), 2.31 (s, 3 H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 196.1, 168.4, 165.4, 143.4, 141.4, 130.4, 128.2, 128.1, 113.5, 103.9, 51.2, 22.9; HRMS (ESI) m/z: [M + H]$^+$ Calcd for C$_{14}$H$_{16}$NO$_3$ 246.1125; Found 246.1126.

**Ethyl (2E, 4E)-5-amino-4-benzoylhexa-2,4-dienoate (5b).** Eluent: V$_{PET}$/V$_{EA}$ = 5:1; white solid (46.1 mg, 89% yield); mp 137-139$^\circ$C; $^1$H NMR (400 MHz, DMSO-$d_6$) $\delta$ 7.60 (d, J = 15.8 Hz, 1 H), 7.51-7.29 (m, 5 H), 5.03 (d, J = 15.8 Hz, 1 H), 3.97 (q, J = 7.0 Hz, 2 H), 2.29 (s, 3 H), 1.10 (t, J = 7.0 Hz, 3 H); $^{13}$C NMR (100 MHz, DMSO-$d_6$) $\delta$ 195.0, 168.2, 167.6, 144.3, 142.4, 130.3, 128.6, 128.1, 110.3, 102.8, 59.4, 22.2 14.7; HRMS (ESI) m/z: [M + H]$^+$ Calcd for C$_{15}$H$_{18}$NO$_3$ 260.1281; Found 260.1283.

**Tert-butyl (2E, 4E)-5-amino-4-benzoylhexa-2,4-dienoate (5c).** Eluent: V$_{PET}$/V$_{EA}$ = 5:1; white solid (48.2 mg, 84% yield); mp 119-121$^\circ$C; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.56 (d, J = 15.8 Hz, 1 H), 7.46 (d, J = 7.6 Hz, 2 H), 7.41-7.33 (m, 3 H), 5.13 (d, J = 15.8 Hz, 1 H), 2.25 (s, 3 H), 1.39 (s, 9 H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 196.0,
167.5, 165.7, 142.6, 141.5, 130.1, 128.0, 115.5, 103.7, 79.4, 28.2, 22.9; HRMS (ESI) m/z: [M + H]^+ Calcd for C_{17}H_{22}NO_{3} 288.1594; Found 288.1597.

Methyl (2E, 4E)-5-amino-4-(4-chlorobenzoyl)hexa-2,4-dienoate (5d). Eluent: V_{PET}/V_{EA} = 5:1; white solid (48.0 mg, 86% yield); mp 182-184°C; ^1H NMR (400 MHz, CDCl₃) δ 7.66 (d, J = 15.8 Hz, 1 H), 7.44 (d, J = 8.4 Hz, 2 H), 7.34 (d, J = 8.4 Hz, 2 H), 5.18 (d, J = 15.8 Hz, 1 H), 3.65 (s, 3 H), 2.31 (s, 3 H); ^13C NMR (100 MHz, CDCl₃) δ 194.4, 168.3, 165.7, 143.1, 139.7, 136.5, 129.7, 128.4, 114.0, 103.6, 51.2, 22.8; HRMS (ESI) m/z: [M + H]^+ Calcd for C_{14}H_{15}ClNO_{3} 280.0735; Found 280.0737.

Methyl (2E, 4E)-5-amino-4-(4-methylbenzoyl)hexa-2,4-dienoate (5e). Eluent: V_{PET}/V_{EA} = 5:1; white solid (43.0 mg, 83% yield); mp 163-165°C; ^1H NMR (400 MHz, CDCl₃) δ 7.70 (d, J = 15.8 Hz, 1 H), 7.40 (d, J = 7.8 Hz, 2 H), 7.16 (d, J = 7.8 Hz, 2 H), 5.17 (d, J = 15.8 Hz, 1 H), 3.63 (s, 3 H), 2.37 (s, 3 H), 2.28 (s, 3 H); ^13C NMR (100 MHz, CDCl₃) δ 196.1, 168.5, 165.0, 143.7, 140.8, 138.5, 128.8, 128.4, 113.0, 104.0, 51.1, 22.7, 21.5; HRMS (ESI) m/z: [M + H]^+ Calcd for C_{15}H_{18}NO_{3} 260.1281; Found 260.1283.

Methyl (2E, 4E)-5-amino-4-(3-bromobenzoyl)hexa-2,4-dienoate (5f). Eluent: V_{PET}/V_{EA} = 5:1; white solid (56.9 mg, 88% yield); mp 129-131°C; ^1H NMR (400 MHz, CDCl₃) δ 7.68-7.58 (m, 2 H), 7.54 (d, J = 7.8 Hz, 1 H), 7.37 (d, J = 7.8 Hz, 1 H), 7.23 (t, J = 7.8 Hz, 1 H), 5.16 (d, J = 15.8 Hz, 1 H), 3.64 (s, 3 H), 2.29 (s, 3 H); ^13C NMR (100 MHz, CDCl₃) δ 193.8, 168.3, 166.3, 143.3, 143.0, 133.2, 131.0, 129.7, 126.7, 122.3, 114.0, 103.4, 51.3, 22.8; HRMS (ESI) m/z: [M + H]^+ Calcd for C_{14}H_{15}BrNO_{3} 324.0230; Found 324.0231.
Methyl (2E, 4E)-5-amino-4-(3-methoxybenzoyl)hexa-2,4-dienoate (5g). Eluent: 
$V_{PET}/V_{EA} = 3:1$; white solid (44.0 mg, 80% yield); mp 140-142°C; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.67 (d, $J = 15.8$ Hz, 1 H), 7.29-7.25 (m, 1 H), 7.10-6.99 (m, 2 H), 6.99-6.92 (m, 1 H), 5.19 (d, $J = 15.8$ Hz, 1 H), 3.81 (s, 3 H), 3.63 (s, 3 H), 2.33 (s, 3 H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 195.8, 168.3, 165.1, 159.4, 143.3, 142.7, 129.1, 120.6, 116.7, 113.6, 112.9, 104.0, 55.4, 51.1, 23.0; HRMS (ESI) m/z: [M + H]$^+$ Calcd for C$_{15}$H$_{18}$NO$_4$ 276.1230; Found 276.1232.

Methyl (2E, 4E)-5-amino-4-(furan-2-carbonyl)hexa-2,4-dienoate (5h). Eluent: 
$V_{PET}/V_{EA} = 5:1$; white solid (36.7 mg, 78% yield); mp 123-125°C; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.90 (d, $J = 15.8$ Hz, 1 H), 7.54 (d, $J = 1.6$ Hz, 1 H), 6.93 (d, $J = 3.6$ Hz, 1 H), 6.48 (dd, $J = 3.6$, 1.8 Hz, 1 H), 5.56 (d, $J = 15.8$ Hz, 1 H), 3.74 (s, 3 H), 2.29 (s, 3 H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 180.7, 168.2, 164.8, 152.8, 152.8, 145.0, 143.1, 117.2, 115.1, 111.7, 103.3, 51.4, 23.2; HRMS (ESI) m/z: [M + H]$^+$ Calcd for C$_{12}$H$_{14}$NO$_4$ 236.0917; Found 236.0919.

5-Ethyl 1-methyl (2E, 4E)-4-(amino(phenyl)methylene)pent-2-enedioate (5i). 
Eluent: $V_{PET}/V_{EA} = 5:1$; white solid (41.3 mg, 75% yield); mp 107-109°C; $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 9.43 (s, 1 H), 7.51-7.40 (m, 3 H), 7.37-7.31 (m, 2 H), 7.27 (d, $J = 15.6$ Hz, 1 H), 6.12 (d, $J = 15.6$ Hz, 1 H), 5.69 (s, 1H), 4.30 (q, $J = 7.0$ Hz, 2 H), 3.54 (s, 3 H), 1.39 (t, $J = 7.0$ Hz, 3 H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 169.9, 169.5, 167.3, 142.3, 136.8, 130.2, 128.8, 128.2, 110.8, 95.3, 60.1, 50.9, 14.4; HRMS (ESI) m/z: [M + H]$^+$ Calcd for C$_{15}$H$_{18}$NO$_4$ 276.1230; Found 276.1240.
Methyl (2E, 4E)-5-amino-4-benzoylocta-2,4-dienoate (5j). Eluent: $V_{PET}/V_{EA} = 5:1$; white solid (44.2 mg, 81% yield); mp 79-81°C; $^1$H NMR (400 MHz, CDCl$_3$) δ 7.72 (d, $J = 15.8$ Hz, 1 H), 7.48 (d, $J = 7.0$ Hz, 2 H), 7.42 -7.31 (m, 3 H), 5.03 (d, $J = 15.8$ Hz, 1 H), 3.61 (s, 3 H), 2.56 (t, $J = 7.6$ Hz, 2 H), 1.78-1.63 (m, 2 H), 1.06 (t, $J = 7.3$ Hz, 3 H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 196.5, 168.6, 168.5, 142.8, 141.5, 130.5, 128.2, 128.1, 114.0, 103.3, 51.2, 36.8, 21.6, 13.8; HRMS (ESI) m/z: [M + H]$^+$ Calcd for C$_{16}$H$_{20}$NO$_3$ [M + H]$^+$ 274.1438; Found 274.1441.

Methyl (2E, 4E)-5-amino-4-benzoyl-5-phenylpenta-2,4-dienoate (5k). Eluent: $V_{PET}/V_{EA} = 5:1$; white solid (47.3 mg, 77% yield); mp 100-102°C; $^1$H NMR (400 MHz, CDCl$_3$) δ 7.63 (d, $J = 7.4$ Hz, 2 H), 7.56-7.36 (m, 9 H), 4.81 (d, $J = 15.8$ Hz, 1 H), 3.49 (s, 3 H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 197.1, 168.2, 165.7, 144.0, 136.4, 131.1, 130.7, 129.1, 128.5, 128.4, 128.3, 113.6, 104.5, 51.0; HRMS (ESI) m/z: [M + H]$^+$ Calcd for C$_{19}$H$_{18}$NO$_3$ 308.1281; Found 308.1283.

References


The $^1$H and $^{13}$C NMR spectra of all products

$^1$H NMR spectrum of 3a (400 MHz, CDCl$_3$)

$^{13}$C NMR spectrum of 3a (100 MHz, CDCl$_3$)
$\text{S26}$

$\text{H NMR spectrum of 3b (400 MHz, CDCl}_3$  

$\text{C NMR spectrum of 3b (100 MHz, CDCl}_3$
$^{1}$H NMR spectrum of 3c (400 MHz, CDCl$_3$)

$^{13}$C NMR spectrum of 3c (100 MHz, CDCl$_3$)
$^1$H NMR spectrum of 3d (400 MHz, CDCl$_3$)

$^{13}$C NMR spectrum of 3d (100 MHz, CDCl$_3$)
$^1$H NMR spectrum of 3e (400 MHz, CDCl$_3$)

$^{13}$C NMR spectrum of 3e (100 MHz, CDCl$_3$)
$^1$H NMR spectrum of 3f (400 MHz, CDCl$_3$)

$^{13}$C NMR spectrum of 3f (100 MHz, CDCl$_3$)
$^{1}$H NMR spectrum of 3g (400 MHz, CDCl$_3$)

$^{13}$C NMR spectrum of 3g (100 MHz, CDCl$_3$)
$^1$H NMR spectrum of 3h (400 MHz, DMSO-$d_6$)

$^{13}$C NMR spectrum of 3h (100 MHz, DMSO-$d_6$)
$^1$H NMR spectrum of 3i (400 MHz, DMSO-$d_6$)

$^{13}$C NMR spectrum of 3i (100 MHz, DMSO-$d_6$)
$^1$H NMR spectrum of 3j (400 MHz, DMSO-$d_6$)

$^{13}$C NMR spectrum of 3j (100 MHz, DMSO-$d_6$)
$^1$H NMR spectrum of 3k (400 MHz, DMSO-$d_6$)

$^{13}$C NMR spectrum of 3k (100 MHz, DMSO-$d_6$)
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$^{13}$C NMR spectrum of 3I (100 MHz, DMSO-$d_6$)
1H NMR spectrum of 3m (400 MHz, CDCl₃)

13C NMR spectrum of 3m (100 MHz, CDCl₃)
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$^{13}$C NMR spectrum of 3n (100 MHz, CDCl$_3$)
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$^1$H NMR spectrum of 3p (400 MHz, CDCl$_3$)

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$^1$H NMR spectrum of 3q (400 MHz, DMSO-$d_6$)

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$^1$H NMR spectrum of $3r$ (400 MHz, CDCl$_3$)

$^{13}$C NMR spectrum of $3r$ (100 MHz, CDCl$_3$)

542
$\textbf{1H NMR spectrum of 3s (400 MHz, CDCl}_3}$

$\textbf{13C NMR spectrum of 3s (100 MHz, CDCl}_3$
$^1$H NMR spectrum of 3t (400 MHz, CDCl$_3$)

$^{13}$C NMR spectrum of 3t (100 MHz, CDCl$_3$)
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$^1$H NMR spectrum of 3x (400 MHz, CDCl$_3$)

$^{13}$C NMR spectrum of 3x (100 MHz, CDCl$_3$)
$^1$H NMR spectrum of 3y (400 MHz, CDCl$_3$)

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$^{13}$C NMR spectrum of 3aq (100 MHz, CDCl₃)
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$^1$H NMR spectrum of 5a (400 MHz, CDCl$_3$)

$^{13}$C NMR spectrum of 5a (100 MHz, CDCl$_3$)
$^1$H NMR spectrum of 5b (400 MHz, DMSO-$d_6$)

$^{13}$C NMR spectrum of 5b (100 MHz, DMSO-$d_6$)
$^1$H NMR spectrum of 5c (400 MHz, CDCl₃)

$^{13}$C NMR spectrum of 5c (100 MHz, CDCl₃)
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$^{13}$C NMR spectrum of 5e (100 MHz, CDCl$_3$)
\(^1\)H NMR spectrum of 5f (400 MHz, CDCl\(_3\))

\(^{13}\)C NMR spectrum of 5f (100 MHz, CDCl\(_3\))
1H NMR spectrum of 5g (400 MHz, CDCl₃)

13C NMR spectrum of 5g (100 MHz, CDCl₃)
$\text{H NMR spectrum of } 5h \text{ (400 MHz, CDCl$_3$)}$

$\text{C NMR spectrum of } 5h \text{ (100 MHz, CDCl$_3$)}$
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$^{13}$C NMR spectrum of 5j (100 MHz, CDCl$_3$)
$^{1}$H NMR spectrum of 5k (400 MHz, CDCl$_3$)

$^{13}$C NMR spectrum of 5k (100 MHz, CDCl$_3$)
Single crystal information

The preparation of single crystal of 3ag. The pure product 3ag (~40 mg) was dissolved in dichloromethane (2 mL) in the test tube. To the tube was additionally added petroleum ether (2 mL) and shook the tube to make the liquids completely mix with each other. The tube was then sealed with plastic membrane. After poking a few small holes on the membrane with needle, the tube was located under room temperature for slow epuration until the occurrence of proper single crystal sample.

X-ray Crystallography measurement. The structure of single crystals was determined by X-ray single crystal diffraction with graphite-monochromated Mo Kα radiation (\(\lambda = 0.71073 \text{ Å}\)). The reflection intensity in the \(\theta\) range 3.00-27.48° for 3ag was collected at 295(2) K. The employed single crystal exhibits no detectable decay during the data collection. The data were corrected for \(Lp\) and absorption effects. The direct method employing the SHELXS-97 program gave the initial positions for part of non-hydrogen atoms, and the subsequent difference Fourier syntheses using SHELXL-2016 program resulted in initial positions for the rest non-hydrogen atoms. The full-matrix least-squares technique was applied for refinement of positions and anisotropic displacement parameters of all the non-hydrogen atoms, as well as the positions of the hydrogen atoms using riding mode with isotropic displacement parameters set to 1.2 times and 1.5 times of the values for aromatic and methyl C atoms, respectively. Detailed information about the crystal data and structure determination is summarized in Table S2.

Figure S1  ORTEP view of the structure for compound 3ag with thermal ellipsoids at 45 % probability level
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<td>$R_1$, $wR_2$ (all data)</td>
<td>0.0821, 0.1443</td>
</tr>
<tr>
<td>A, B values in $w$</td>
<td>0.0676, 0</td>
</tr>
<tr>
<td>$\delta \rho_{max}$, $\delta \rho_{min}$ (e Å⁻³)</td>
<td>0.258, -0.199</td>
</tr>
</tbody>
</table>

$a) R_1 = \sum(|F_o| - |F_c|)/\sum|F_o|$, $wR_2 = [\sum w(F_o^2 - F_c^2)^2/\sum w(F_o^2)^2]^{1/2}$

$b) w = [\sum w(F_o^2 + (AP)^2 + BP)^{-1}$ with $P = (F_o^2 + 2F_c^2)/3$