

A Combinatorial Approach towards a Library of Chiral γ -Lactams and 2,3-Disubstituted Pyrroles

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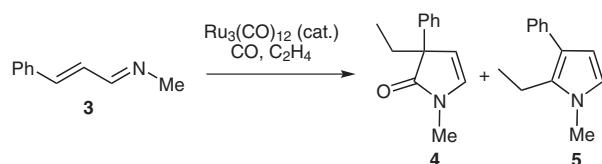
Received 20 July 2011; revised 4 October 2011

Abstract: A library of heterocyclic products with a wide variety of organic residues is produced via a four-component reaction of α,β -unsaturated aldehydes, primary amines, carbon monoxide, and ethylene using a multi-reactor station with an array of 96 autoclaves employing the same high-pressure reaction conditions for all catalytic reactions. In the presence of $\text{Ru}_3(\text{CO})_{12}$ as a precatalyst, mixtures of chiral γ -lactams and 2,3-disubstituted pyrroles are obtained. This combinatorial approach also enables us for the first time to set up rules relating to the effects of specific substituents in the substrates on the outcome of the respective catalytic reaction.

Key words: ruthenium, C–H activation, catalysis, γ -lactams, pyrroles

The direct catalytic activation of C–H bonds with the purpose of establishing new C–C bonds is a highly attractive synthetic objective in terms of avoiding synthesis and isolation of more reactive intermediates, for example, chlorinated compounds. Progress in this field has been thoroughly reviewed in recent years.^{1–8}

Some of us have developed a reaction of α,β -unsaturated imines, carbon monoxide, and ethylene (or terminal alkenes in general) to produce chiral 1,3-dihydropyrrolones as the main product in nonpolar solvents. As a side-product 2,3-disubstituted pyrroles are formed (Scheme 1).^{9–15}



Scheme 1 Ruthenium-catalyzed formation of γ -lactams and pyrroles

The formation of both products obviously proceeds via the activation of a C–H bond in the β -position relative to the imine C=N bond. The product ratio is highly dependent on the relative permittivity of the solvent used; with nonpolar solvents like, for example, hydrocarbons leading to the quantitative and selective formation of racemic lactams **4**, whereas use of more polar solvents or the presence of traces of water leads to an enhancement of the yield of the pyrrole **5** (75% in anhyd MeOH).¹⁵ γ -Lactams or γ -bu-

tyric acid derivatives have been investigated with respect to their potential as psychotropic drugs, as agents against Alzheimer's disease, Down's syndrome, osteoporosis, and cancer or as constituents of peptide mimetics exhibiting γ -turns.^{16–22} It has also been demonstrated that incorporation of γ -amino acids into protein sequences considerably enhances their stability against proteases, which is an essential prerequisite to use those proteins as drugs under physiological conditions.²³

Herein we report the combinatorial reaction of seven α,β -unsaturated aldehydes with eight different primary amines in the presence of CO and ethylene to yield the corresponding pyrrolone and pyrrole derivatives. In order to afford the same reaction conditions for all catalytic reactions we used a multi-reactor station manufactured by Advanced ChemTech Inc. This multi-reactor station is set up by 96 autoclaves with a maximum working capacity of 3.5 mL each. The reaction vessel block is covered by a top clamp plate with a septum and valve membrane sheet and is connected to a gas mixing facility allowing for the preparation of mixtures of gaseous substrates with different partial pressures (Figure 1).

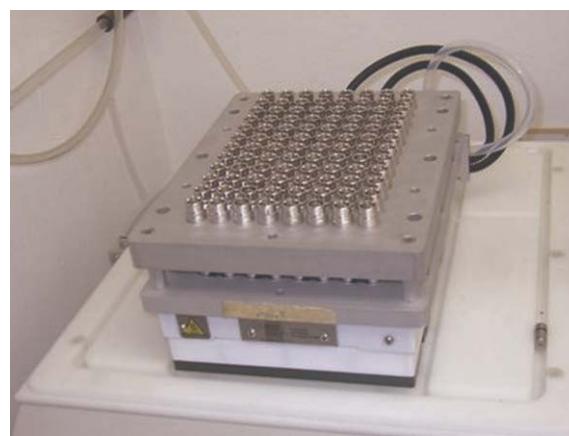
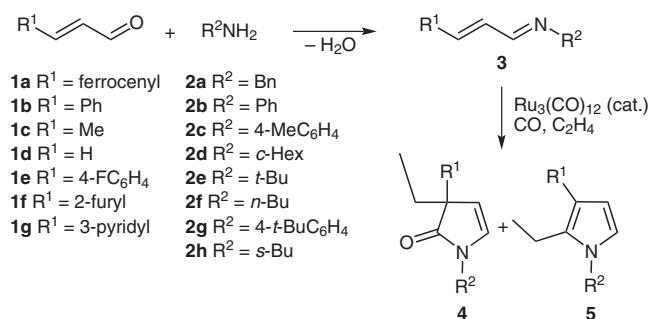


Figure 1 Multi-reactor station (without cover plate)

Initially, we planned to use ionic liquids as reaction media because we have been able to demonstrate that optimization of the reaction conditions of the reaction depicted in Scheme 1 in $[\text{C}_4\text{mim}][\text{BTA}]$ led to milder conditions with regard to reaction time and partial pressures of the gaseous substrates than when performed in classical organic solvents.²⁴ Beforehand only a limited number of transition-metal-catalyzed reactions in ionic liquids proceeding

via C–H activation steps have been reported, including activation of methane, dehydrogenation of cyclooctadiene, isomerization of alkenes, or C–H activation of terminal alkynes.^{25–29} Unfortunately, this reaction does not work in ionic liquids if the multi-reactor station shown in Figure 1 is employed. This is most probably due to the low solubility of CO in ionic liquids³⁰ in combination with the small surface, which is caused by the slim layout of the autoclaves. Nevertheless, combinatoric synthesis of heterocyclic compounds was efficiently achieved in toluene as the solvent.

Table 1 shows the primary amines and α,β -unsaturated aldehydes that have been introduced to the catalytic reaction to form the 1,3-dihydropyrrolones and 2,3-disubstituted pyrroles, respectively, after reacting with CO and ethylene in the presence of $\text{Ru}_3(\text{CO})_{12}$ as a precatalyst (Scheme 2). Exploratory analysis at the multi-reactor station showed that the temperature in the middle of the block differs about 10 °C from the reaction vessels at the outside of the block. In order to afford the same reaction conditions for all catalytic reactions the outer autoclaves were not used. Thus, eight primary amines were combined with seven α,β -unsaturated aldehydes. Workup was easily achieved by removing the solvent under reduced pressure and the oily residue was used to get an impression of the outcome of the products **4** and **5** via ^1H NMR spectroscopy. The products were finally separated by column chromatography and characterized by IR, ^1H , and ^{13}C NMR spectroscopy as well as by mass spectrometry and high-resolution mass spectrometry (cf. experimental part).



Scheme 2 Four-component reaction leading to heterocyclic products of type **4** and **5**, all combinations of R¹ and R² were used in the experiments

Table 2 shows the combination of eight amines with seven aldehydes and the yields of the corresponding products **4** and **5**. From the entries in Table 2 it can be concluded that most combinations for the catalytic transformation of primary amines and unsaturated aldehydes to the heterocyclic products work very well. Acrolein and *tert*-butylamine are the only substrates examined that did not react at all. One reason in the case of acrolein might be that it is too reactive and does not even lead to the intermediate imine after combination with an amine. The resulting ^1H NMR spectra of crude reaction mixtures showed no signals indicating the heterocyclic products of type **4** and **5**,

Table 1 Primary Amines and α,β -Unsaturated Aldehydes Used in the Experiments

Amines	Aldehydes
2a: benzylamine	1a: 3-ferrocenylpropenal
2b: aniline	1b: <i>trans</i> -cinnamaldehyde
2c: <i>p</i> -toluidine	1c: <i>trans</i> -crotonic aldehyde
2d: cyclohexylamine	1d: acrolein
2e: <i>tert</i> -butylamine	1e: <i>trans</i> -4-fluorocinnamaldehyde
2f: <i>n</i> -butylamine	1f: 3-(2-furyl)acrolein
2g: 4- <i>tert</i> -butylaniline	1g: <i>trans</i> -3-(3-pyridyl)acrolein
2h: <i>sec</i> -butylamine	

which are easily identified by two doublets in the range of 5–7 ppm. Moreover, there was also no signal corresponding to the CH function of imines or even the starting aldehyde. Signals in the aliphatic and olefinic region of the spectrum might be indicative for the formation of oligomeric or polymeric products. In contrast, in the case of the *tert*-butylamine it is most probably rather a matter of steric pressure preventing the catalytic reaction. Additional reactions combining *trans*-cinnamaldehyde with *tert*-butylamine and 2,6-diisopropylphenylamine showed that it is indeed possible to get the unsaturated imine but not at all the catalytic reaction products. Other aliphatic amines give both heterocyclic products **4** and **5** when reacted with the aldehydes used. In the case of *sec*-butylamine two diastereomeric pairs of enantiomers are produced, as can be seen from the NMR data in which signals representing atoms in close proximity to one of the stereogenic centers are doubled. Moreover, aromatic amines, for example, aniline just react with 3-ferrocenylpropenal and 3-(2-furyl)acrolein to a mixture of the corresponding lactam and pyrrole. Otherwise it can be observed that just the pyrrole derivative is formed with a yield of about 50%. There is just one exception for the combination of 3-(2-furyl)acrolein with aniline where also just the pyrrole is formed. In general, it has to be pointed out that water that is produced by the condensation reaction of the aldehyde with the respective amine leads to an enhanced yield of the corresponding pyrrole compared to the reaction conditions in which the pure imine would have been introduced to the catalytic heterocycle formation in anhydrous toluene.

All amines and aldehydes except 3-ferrocenylpropenal were purchased from Sigma-Aldrich and were used without further purification. *sec*-Butylamine was used as a racemic mixture. 3-Ferrocenylpropenal was prepared by alkylation of ferrocene with 1,1,3,3-tetramethoxypropane.³¹ All catalytic reaction procedures were carried out under an argon atmosphere in freshly distilled, anhydrous solvents.³² The multi-reactor station was purchased from Advanced ChemTech Inc. Support now is provided by Activotec Inc. (<http://www.activotec.com/>). NMR spectra were recorded at 298 K on a Bruker AC 200 spectrometer (^1H : 200 MHz; ^{13}C : 50.32 MHz; CDCl_3 as internal standard), a Bruker DRX 400 spectrometer (^1H : 400.13 MHz; ^{13}C : 100.62 MHz; CDCl_3 as internal standard) or

Table 2 Used Aldehydes and Amines, Isolated Yields of **4** and **5**, and Numbering Scheme of All Products

R ²	R ¹ = Fc		R ¹ = Ph		R ¹ = Me		R ¹ = H		R ¹ = 4-FC ₆ H ₄		R ¹ = 2-furyl		R ¹ = 3-pyridyl	
	Yield (%)		Yield (%)		Yield (%)		Yield (%)		Yield (%)		Yield (%)		Yield (%)	
	4	5	4	5	4	5	4	5	4	5	5	4	5	4
PhCH ₂ (aa–ga)	66	30	42	50	22	50	—	—	65	28	57	43	59	35
Ph (ab–gb)	45	53	—	57	—	57	—	—	—	57	—	47	55	45
4-MeC ₆ H ₄ (ac–gc)	45	52	—	47	—	47	—	—	—	57	40	55	35	54
c-Hex (ad–gd)	57	42	46	48	46	27	—	—	52	34	60	37	46	49
t-Bu (ae–ge)	—	—	—	—	—	—	—	—	—	—	—	—	—	—
n-Bu (af–gf)	67	25	58	40	50	49	—	—	55	33	60	36	54	32
4-t-BuC ₆ H ₄ (ag–gg)	54	44	—	52	—	46	—	—	—	54	42	41	64	31
s-Bu (ah–gh)	68	28	51	42	51	27	—	—	41	52	57	38	40	43

a Bruker Ultrashield 600+ (¹H: 600.15 MHz; ¹³C: 150.91 MHz; CDCl₃ as internal standard). Mass spectra were recorded on a Finnigan MAT SSQ 710 instrument using direct electron impact (DEI) techniques. High-resolution mass spectra were recorded on a Finnigan MAT 95 XL using EI techniques. IR spectra were recorded at 298 K on a Shimadzu IRAffinity-1 (FTIR) at the laboratory of the Institute of Organic Chemistry and Macromolecular Chemistry of Friedrich-Schiller-University of Jena.

One-Pot Synthesis of γ -Lactams and Pyrroles; General Procedure

Each reaction vessel was charged with a primary amine **2** (1 mmol), an α,β -unsaturated aldehyde **1** (1 mmol) as well as Ru₃(CO)₁₂ (19 mg, 0.03 mmol) and anhyd, freshly distilled toluene (1.5 mL). Afterwards, the multi-reactor station was pressurized with CO (12 bar) and ethylene (8 bar), and heated up to 140 °C for a reaction time of 16 h. After the autoclaves had cooled to r.t., the reaction mixtures were transferred to Schlenk tubes. The solvent was removed in vacuo and the remaining oily residue was used to determine yields of the products **4** and **5** by ¹H NMR spectroscopy. If resonances corresponding to the respective products were observed, the solvent used for the ¹H NMR spectroscopic investigation was removed under reduced pressure. Preparative separation of **4** and **5** was achieved by column chromatography (10 × 2 cm, silica gel). Using a mixture of light petroleum (bp 40–60 °C) and CH₂Cl₂, depending on the reaction mixture, led to elution of **5**, whereas **4** was obtained by using EtOH as eluent. The exact ratio of solvents for the elution of all derivatives of **4** and **5** are specified in connection with the physical data of each compound (vide infra). Analytical data of **4ba** and **5ba** are in accordance with values published earlier by us.¹³ All compounds were either light yellow (R¹ = aliphatic moiety) or yellow-orange (R¹ = aromatic) oils.

N-Benzyl-3-ethyl-3-ferrocenyl-1,3-dihydropyrrol-2-one (**4aa**)

Yield: 253 mg (66%); eluent: EtOH.

IR (neat): 3090 (w), 2967 (w), 2932 (w), 2874 (w), 2021 (m), 1952 (m), 1694 (s), 1605 (m), 1354 (s), 1103 (s), 999 (s), 818 (vs), 698 cm⁻¹ (vs).

¹H NMR (200 MHz, CDCl₃): δ = 0.74 (t, J = 7.4 Hz, 2 H), 1.16 (t, J = 7.5 Hz, 1 H), 1.83 (q, J = 7.4 Hz, 1.3 H), 2.23 (q, J = 7.6 Hz, 0.6 H), 4.09–4.47 (m, 4 H), 4.65 (AB spin system, J = 14.8, 51.3 Hz, 2 H), 5.45 (d, J = 4.8 Hz, 1 H), 6.44 (d, J = 4.8 Hz, 1 H), 7.28–7.31 (m, 5 H).

¹³C NMR (50 MHz, CDCl₃): δ = 9.2, 9.8, 29.6, 32.9, 43.5, 45.6, 54.2, 65.8, 66.5, 67.2, 67.8, 68.5, 87.9, 113.7, 127.7, 128.1, 128.8, 130.2, 136.7, 179.2.

MS (DEI): m/z (%) = 385 (100, [M⁺]), 356 (50, [M⁺ – Et]), 265 (21, [M⁺ – C₉H₁₂]), 91 (30, [C₇H₇⁺]).

HRMS: m/z calcd for C₂₃H₂₃⁵⁴FeNO: 383.11759; found: 383.11679, Δ = 0.80 mmu.

N-Benzyl-2-ethyl-3-ferrocenylpyrrole (**5aa**)

Yield: 110 mg (30%); eluent: light petroleum–CH₂Cl₂ (70:30).

¹H NMR (200 MHz, CDCl₃): δ = 1.12 (t, J = 7.6 Hz, 3 H), 2.68 (q, J = 7.6 Hz, 2 H), 4.07 (s, 5 H), 4.18 (t, J = 1.8 Hz, 2 H), 4.43 (t, J = 1.8 Hz, 2 H), 5.04 (s, 2 H), 6.30 (d, J = 2.8 Hz, 1 H), 6.54 (d, J = 2.8 Hz, 1 H), 6.99–7.31 (m, 5 H).

¹³C NMR (50 MHz, CDCl₃): δ = 14.9, 18.1, 50.2, 66.7, 67.2, 69.1, 83.2, 108.0, 117.1, 120.2, 126.2, 127.3, 128.7, 131.0, 138.8.

MS (DEI): m/z (%) = 369 (100, [M⁺]), 354 (6, [M⁺ – Me]), 278 (9, [M⁺ – C₇H₇]), 263 (22, [M⁺ – C₈H₁₀]), 91 (22, [C₇H₇⁺]).

HRMS: m/z calcd for C₂₃H₂₃⁵⁴FeN: 367.12267; found: 367.12247, Δ = 0.2 mmu.

3-Ethyl-3-ferrocenyl-N-phenyl-1,3-dihydropyrrol-2-one (**4ab**)

Yield: 166 mg (45%); eluent: EtOH.

IR (neat): 2955 (m), 2924 (vs), 2855 (m), 1717 (s), 1701 (s), 1597 (m), 1501 (s), 1458 (m), 1385 (m), 1273 (s), 1211 (m), 1072 (m), 741 (vs), 691 cm⁻¹ (vs).

¹H NMR (200 MHz, CDCl₃): δ = 0.80 (t, J = 7.4 Hz, 3 H), 1.86 (q, J = 7.4 Hz, 2 H), 4.05 (s, 5 H), 4.11–4.55 (m, 4 H), 5.66 (d, J = 5.2 Hz, 1 H), 6.99 (d, J = 5.2 Hz, 1 H), 7.10–7.58 (m, 5 H).

¹³C NMR (50 MHz, CDCl₃): δ = 8.3, 32.7, 54.1, 65.4, 67.3, 67.5, 86.5, 113.4, 120.3, 124.5, 128.2, 129.6, 136.0, 176.8.

MS (DEI): m/z (%) = 371 (100, [M⁺]), 342 (58, [M⁺ – Et]), 314 (6, [M⁺ – Et – CO]), 121 (6, [FeC₅H₅⁺]), 77 (7, [Ph⁺]).

HRMS: m/z calcd for C₂₂H₂₁⁵⁴FeNO: 369.10194; found: 369.10251, Δ = 0.57 mmu.

2-Ethyl-3-ferrocenyl-N-phenylpyrrole (**5ab**)

Yield: 188 mg (53%); eluent: light petroleum–CH₂Cl₂ (70:30).

¹H NMR (200 MHz, CDCl₃): δ = 0.98 (t, J = 7.4 Hz, 3 H), 2.74 (q, J = 7.4 Hz, 2 H), 4.13 (s, 5 H), 4.22 (t, J = 1.8 Hz, 2 H), 4.46 (t,

$J = 1.8$ Hz, 2 H), 6.38 (d, $J = 3.0$ Hz, 1 H), 6.68 (d, $J = 3.0$ Hz, 1 H), 7.32–7.50 (m, 5 H).

^{13}C NMR (50 MHz, CDCl_3): $\delta = 14.7, 18.2, 67.1, 67.3, 69.1, 83.0, 109.1, 117.8, 121.1, 126.4, 127.1, 129.0, 131.6, 140.5$.

MS (DEI): m/z (%) = 355 (100, $[\text{M}^+]$), 340 (14, $[\text{M}^+ - \text{Me}]$), 170 (10, $[\text{M}^+ - \text{C}_{10}\text{H}_9\text{Fe}]$).

HRMS: m/z calcd for $\text{C}_{22}\text{H}_{21}^{54}\text{FeN}$: 353.10702; found: 353.10452, $\Delta = 2.50$ mmu.

3-Ethyl-3-ferrocenyl-N-p-tolyl-1,3-dihydropyrrol-2-one (4ac)

Yield: 174 mg (45%); eluent: EtOH.

IR (neat): 2963 (w), 2924 (m), 2855 (w), 1956 (w), 1709 (s), 1612 (m), 1512 (vs), 1454 (m), 1385 (s), 1204 (s), 999 (m), 814 (vs), 702 cm^{-1} (m).

^1H NMR (200 MHz, CDCl_3): $\delta = 0.80$ (t, $J = 7.4$ Hz, 3 H), 1.85 (q, $J = 7.4$ Hz, 2 H), 2.34 (s, 3 H), 4.05 (s, 5 H), 4.11–4.56 (m, 4 H), 5.66 (d, $J = 5.0$ Hz, 1 H), 6.95 (d, $J = 5.0$ Hz, 1 H), 7.22 (dd, $J = 2.0$ Hz, $J = 6.7$ Hz, 2 H), 7.43 (dd, $J = 2.0, 6.7$ Hz, 2 H).

^{13}C NMR (50 MHz, CDCl_3): $\delta = 9.3, 20.9, 33.7, 55.0, 66.0, 68.0, 68.5, 87.5, 114.1, 120.3, 129.7, 130.9, 134.4, 135.3, 177.8$.

MS (DEI): m/z (%) = 385 (100, $[\text{M}^+]$), 356 (25, $[\text{M}^+ - \text{Et}]$), 328 (4, $[\text{M}^+ - \text{Et} - \text{CO}]$), 121 (4, $[\text{FeC}_5\text{H}_5^+]$).

HRMS: m/z calcd for $\text{C}_{23}\text{H}_{23}^{54}\text{FeNO}$: 383.11759; found: 383.11799, $\Delta = 0.40$ mmu.

2-Ethyl-3-ferrocenyl-N-p-tolylpyrrole (5ac)

Yield: 192 mg (52%); eluent: light petroleum– CH_2Cl_2 (70:30).

^1H NMR (200 MHz, CDCl_3): $\delta = 0.99$ (t, $J = 7.4$ Hz, 3 H), 2.43 (s, 3 H), 2.72 (q, $J = 7.4$ Hz, 2 H), 4.13 (s, 5 H), 4.21 (t, $J = 1.8$ Hz, 2 H), 4.46 (t, $J = 1.8$ Hz, 2 H), 6.37 (d, $J = 2.8$ Hz, 1 H), 6.65 (d, $J = 2.8$ Hz, 1 H), 7.24 (s, 4 H).

^{13}C NMR (50 MHz, CDCl_3): $\delta = 14.7, 18.2, 21.1, 67.1, 67.3, 69.1, 83.1, 108.8, 117.4, 121.1, 126.3, 129.6, 131.7, 137.0, 138.0$.

MS (DEI): m/z (%) = 369 (100, $[\text{M}^+]$), 354 (9, $[\text{M}^+ - \text{Me}]$), 339 (4, $[\text{M}^+ - \text{C}_2\text{H}_6]$), 185 (4, $[\text{FeC}_{10}\text{H}_9^+]$), 121 (7, $[\text{FeC}_5\text{H}_5^+]$).

HRMS: m/z calcd for $\text{C}_{23}\text{H}_{23}^{54}\text{FeN}$: 367.12267; found: 367.12031, $\Delta = 2.36$ mmu.

N-Cyclohexyl-3-ethyl-3-ferrocenyl-1,3-dihydropyrrol-2-one (4ad)

Yield: 216 mg (57%); eluent: EtOH.

IR (neat): 3094 (w), 2932 (m), 2855 (w), 1967 (w), 1686 (s), 1605 (m), 1450 (m), 1377 (s), 1254 (m), 999 (s), 818 (vs), 752 (vs), 691 cm^{-1} (s).

^1H NMR (400 MHz, CDCl_3): $\delta = 0.69$ (t, $J = 7.2$ Hz, 3 H), 1.12–1.70 (m, 10 H), 1.80 (q, $J = 7.2$ Hz, 2 H), 3.94–3.98 (m, 1 H), 4.03 (s, 5 H), 4.05–4.47 (m, 4 H), 5.43 (d, $J = 4.8$ Hz, 1 H), 6.60 (d, $J = 5.0$ Hz, 1 H).

^{13}C NMR (100 MHz, CDCl_3): $\delta = 9.1, 25.4, 32.0, 32.3, 33.5, 50.3, 54.6, 65.8, 66.5, 67.1, 67.8, 68.5, 87.9, 113.3, 127.8, 178.6$.

MS (DEI): m/z (%) = 377 (100, $[\text{M}^+]$), 348 (54, $[\text{M}^+ - \text{Et}]$), 266 (16, $[\text{M}^+ - \text{C}_8\text{H}_{15}]$), 83 (30, $[\text{C}_6\text{H}_{11}^+]$).

HRMS: m/z calcd for $\text{C}_{22}\text{H}_{27}^{54}\text{FeNO}$: 375.14889; found: 375.14465, $\Delta = 4.24$ mmu.

N-Cyclohexyl-2-ethyl-3-ferrocenylpyrrole (5ad)

Yield: 153 mg (42%); eluent: light petroleum– CH_2Cl_2 (70:30).

^1H NMR (400 MHz, CDCl_3): $\delta = 1.20$ (t, $J = 7.6$ Hz, 3 H), 1.38–2.03 (m, 10 H), 2.76 (q, $J = 7.6$ Hz, 2 H), 3.74–3.82 (m, 1 H), 4.09

(s, 5 H), 4.16 (t, $J = 1.6$ Hz, 2 H), 4.38 (t, $J = 1.6$ Hz, 2 H), 6.25 (d, $J = 3.2$ Hz, 1 H), 6.61 (d, $J = 3.2$ Hz, 1 H).

^{13}C NMR (100 MHz, CDCl_3): $\delta = 15.4, 17.9, 25.5, 26.1, 34.9, 54.7, 67.0, 69.0, 83.8, 107.9, 115.1, 115.5, 130.1$.

MS (DEI): m/z (%) = 361 (100, $[\text{M}^+]$), 331 (2, $[\text{M}^+ - \text{C}_2\text{H}_6]$), 279 (3, $[\text{M}^+ - \text{C}_6\text{H}_{10}]$), 264 (6, $[\text{M}^+ - \text{C}_7\text{H}_{13}]$), 83 (11, $[\text{C}_6\text{H}_{11}^+]$).

HRMS: m/z calcd for $\text{C}_{22}\text{H}_{27}^{54}\text{FeN}$: 359.15397; found: 359.15152, $\Delta = 2.45$ mmu.

N-Butyl-3-ethyl-3-ferrocenyl-1,3-dihydropyrrol-2-one (4af)

Yield: 236 mg (67%); eluent: EtOH.

IR (neat): 2959 (w), 2932 (w), 2874 (vw), 1967 (vw), 1694 (vs), 1454 (m), 1377 (m), 1261 (m), 1107 (s), 999 (s), 818 (vs), 691 cm^{-1} (m).

^1H NMR (200 MHz, CDCl_3): $\delta = 0.72$ (t, $J = 7.4$ Hz, 3 H), 0.93 (t, $J = 7.2$ Hz, 3 H), 1.33–1.37 (m, 2 H), 1.56–1.60 (m, 2 H), 1.77 (q, $J = 7.4$ Hz, 2 H), 3.28–3.64 (m, 2 H), 4.03 (s, 5 H), 4.05–4.43 (m, 4 H), 5.44 (d, $J = 5.0$ Hz, 1 H), 6.50 (d, $J = 5.0$ Hz, 1 H).

^{13}C NMR (50 MHz, CDCl_3): $\delta = 9.2, 13.7, 20.0, 31.1, 33.0, 41.5, 54.3, 65.9, 66.6, 67.1, 67.8, 68.5, 88.0, 113.3, 130.8, 179.3$.

MS (DEI): m/z (%) = 351 (100, $[\text{M}^+]$), 322 (63, $[\text{M}^+ - \text{Et}]$), 280 (9, $[\text{M}^+ - \text{C}_5\text{H}_{11}]$), 121 (5, $[\text{FeC}_5\text{H}_5^+]$).

HRMS: m/z calcd for $\text{C}_{20}\text{H}_{25}^{54}\text{FeNO}$ (349.13324): 349.13138, $\Delta = 1.86$ mmu.

N-Butyl-2-ethyl-3-ferrocenylpyrrole (5af)

Yield: 84 mg (25%); eluent: light petroleum– CH_2Cl_2 (70:30).

^1H NMR (200 MHz, CDCl_3): $\delta = 0.97$ (t, $J = 7.2$ Hz, 3 H), 1.22 (t, $J = 7.4$ Hz, 3 H), 1.39–1.43 (m, 2 H), 1.72–1.76 (m, 2 H), 2.74 (q, $J = 7.4$ Hz, 2 H), 3.79 (t, $J = 7.4$ Hz, 2 H), 4.08 (s, 5 H), 4.17 (t, $J = 1.8$ Hz, 2 H), 4.40 (t, $J = 1.8$ Hz, 2 H), 6.24 (d, $J = 3.0$ Hz, 1 H), 6.53 (d, $J = 3.0$ Hz, 1 H).

^{13}C NMR (50 MHz, CDCl_3): $\delta = 13.8, 15.0, 17.9, 20.1, 33.7, 46.2, 66.9, 67.1, 69.1, 83.6, 107.7, 116.1, 118.7, 130.2$.

MS (DEI): m/z (%) = 335 (100, $[\text{M}^+]$), 320 (9, $[\text{M}^+ - \text{Me}]$), 306 (4, $[\text{M}^+ - \text{Et}]$), 291 (2, $[\text{M}^+ - \text{C}_3\text{H}_8]$), 186 (3, $[\text{FeC}_{10}\text{H}_{10}]$).

HRMS: m/z calcd for $\text{C}_{20}\text{H}_{25}^{54}\text{FeN}$: 333.13832; found: 333.13537, $\Delta = 2.95$ mmu.

N-(4-tert-Butylphenyl)-3-ethyl-3-ferrocenyl-1,3-dihydropyrrol-2-one (4ag)

Yield: 230 mg (54%); eluent: EtOH.

IR (neat): 2962 (m), 2365 (s), 2330 (m), 1697 (vs), 1616 (m), 1516 (vs), 1454 (s), 1389 (s), 1204 (s), 999 (s), 818 (vs), 706 cm^{-1} (s).

^1H NMR (200 MHz, CDCl_3): $\delta = 0.79$ (t, $J = 7.4$ Hz, 3 H), 1.31 (s, 9 H), 1.85 (q, $J = 7.4$ Hz, 2 H), 4.05 (s, 5 H), 4.02–4.56 (m, 4 H), 5.63 (d, $J = 5.2$ Hz, 1 H), 6.96 (d, $J = 5.2$ Hz, 1 H), 7.45 (d, $J = 3.8$ Hz, 4 H).

^{13}C NMR (50 MHz, CDCl_3): $\delta = 8.3, 30.3, 32.7, 33.5, 54.0, 64.9, 65.8, 66.1, 67.0, 68.5, 86.6, 113.2, 120.0, 125.1, 129.8, 133.4, 147.6, 176.8$.

MS (DEI): m/z (%) = 427 (100, $[\text{M}^+]$), 398 (55, $[\text{M}^+ - \text{Et}]$), 370 (2, $[\text{M}^+ - \text{Et} - \text{CO}]$), 313 (2, $[\text{M}^+ - \text{Et} - \text{CO} - \text{C}_4\text{H}_9]$), 121 (11, $[\text{FeC}_5\text{H}_5^+]$).

HRMS: m/z calcd for $\text{C}_{26}\text{H}_{29}^{54}\text{FeNO}$: 425.16454; found: 425.16345, $\Delta = 1.09$ mmu.

N-(4-tert-Butylphenyl)-2-ethyl-3-ferrocenylpyrrole (5ag)

Yield: 180 mg (44%); eluent: light petroleum– CH_2Cl_2 (70:30).

¹H NMR (400 MHz, CDCl₃): δ = 1.00 (t, J = 7.6 Hz, 3 H), 1.38 (s, 9 H), 2.72 (q, J = 7.6 Hz, 2 H), 4.13 (s, 5 H), 4.21 (t, J = 1.6 Hz, 2 H), 4.46 (t, J = 1.6 Hz, 2 H), 6.37 (d, J = 2.8 Hz, 1 H), 6.66 (d, J = 2.8 Hz, 1 H), 7.26 (d, J = 2.8 Hz, 2 H), 7.45 (d, J = 2.8 Hz, 2 H).

¹³C NMR (100 MHz, CDCl₃): δ = 14.8, 18.2, 31.4, 34.6, 67.1, 67.3, 69.1, 83.2, 108.8, 117.4, 121.1, 125.8, 126.0, 131.7, 137.9, 150.2.

MS (DEI): m/z (%) = 411 (100, [M⁺]), 396 (6, [M⁺ – Me]), 339 (4, [M⁺ – C₅H₁₂]), 266 (10, [C₁₁H₁₃⁺]), 121 (6, [FeC₅H₅⁺]).

HRMS: m/z calcd for C₂₆H₂₉⁵⁴FeN: 409.16962; found: 409.16677, Δ = 2.85 mmu.

N-sec-Butyl-3-ethyl-3-ferrocenyl-1,3-dihydropyrrol-2-one (4ah)

Yield: 239 mg (68%); eluent: EtOH.

IR (neat): 3094 (vw), 2967 (w), 2932 (vw), 2874 (vw), 1967 (w), 1686 (vs), 1605 (m), 1454 (m), 1381 (s), 1258 (s), 999 (s), 818 (vs), 752 cm⁻¹ (s).

¹H NMR (600 MHz, CDCl₃): δ = 0.69 (t, J = 7.2 Hz, 3 H), 0.84 (t, J = 7.6 Hz, 3 H), 1.13 (d, J = 6.7 Hz, 1.8 H), 1.20 (d, J = 6.9 Hz, 1.2 H), 1.52–1.57 (m, 2 H), 1.69–1.88 (m, 2 H), 3.98–4.02 (m, 1 H), 4.00–4.04 (m, 2 H), 4.03 (s, 5 H), 4.23–4.27 (m, 2 H), 5.40 (d, J = 4.8 Hz, 0.6 H), 5.43 (d, J = 4.8 Hz, 0.4 H), 6.49 (d, J = 4.8 Hz, 0.6 H), 6.50 (d, J = 4.8 Hz, 0.4 H).

¹³C NMR (150 MHz, CDCl₃): δ = 8.0, 8.4, 9.8, 10.0, 18.4, 18.6, 27.5, 27.8, 31.3, 32.2, 47.1, 47.6, 53.7, 53.8, 64.8, 64.9, 65.3, 65.6, 66.1, 66.4, 66.7, 66.8, 67.5, 87.2, 87.8, 112.7, 113.0, 126.2, 126.6, 178.1, 178.2.

MS (DEI): m/z (%) = 351 (100, [M⁺]), 323 (18, [M⁺ – CO]), 322 (73, [M⁺ – Et]), 266 (18, [M⁺ – C₆H₁₃]), 121 (12, [FeC₅H₅⁺]).

HRMS: m/z calcd for C₂₀H₂₅⁵⁴FeNO: 349.13324; found: 349.13179, Δ = 1.45 mmu.

N-sec-Butyl-2-ethyl-3-ferrocenylpyrrole (5ah)

Yield: 94 mg (28%); eluent: light petroleum–CH₂Cl₂ (70:30).

¹H NMR (600 MHz, CDCl₃): δ = 0.76 (t, J = 7.2 Hz, 3 H), 1.12 (t, J = 7.2 Hz, 3 H), 1.32 (d, J = 7.2 Hz, 3 H), 1.67 (q, J = 7.2 Hz, 2 H), 2.67–2.75 (m, 2 H), 3.88 (q, J = 7.2 Hz, 1 H), 3.99 (s, 5 H), 4.10 (d, J = 7.2 Hz, 2 H), 4.33 (d, J = 7.2 Hz, 2 H), 6.17 (d, J = 3.0 Hz, 1 H), 6.47 (d, J = 3.0 Hz, 1 H).

¹³C NMR (150 MHz, CDCl₃): δ = 10.0, 14.3, 16.9, 21.2, 30.2, 51.2, 65.9, 66.1, 68.1, 82.9, 107.0, 113.4, 114.3, 129.7.

MS (DEI): m/z (%) = 335 (100, [M⁺]), 320 (6, [M⁺ – Me]), 306 (2, [M⁺ – Et]), 278 (2, [M⁺ – C₄H₉]).

HRMS: m/z calcd for C₂₀H₂₅⁵⁴FeN: 333.13832; found: 333.13618, Δ = 2.14 mmu.

2-Ethyl-N,3-diphenylpyrrole (5bb)

Yield: 140 mg (57%); eluent: light petroleum–CH₂Cl₂ (70:30).

¹H NMR (200 MHz, CDCl₃): δ = 0.92 (t, J = 7.4 Hz, 3 H), 2.78 (q, J = 7.4 Hz, 2 H), 6.39 (d, J = 2.8 Hz, 1 H), 6.76 (d, J = 2.8 Hz, 1 H), 7.35–7.50 (m, 10 H).

¹³C NMR (50 MHz, CDCl₃): δ = 14.3, 17.7, 108.5, 121.3, 122.3, 125.1, 126.3, 127.1, 127.8, 128.0, 128.8, 131.4, 137.1, 140.2.

MS (DEI): m/z (%) = 247 (100, [M⁺]), 232 (83, [M⁺ – Me]), 141 (5, [M⁺ – C₈H₁₀]), 91 (15, [C₇H₇⁺]), 77 (22, [Ph⁺]).

HRMS: m/z calcd for C₁₈H₁₇N: 247.13610; found: 247.13522 (M⁺), Δ = 0.88 mmu.

2-Ethyl-3-phenyl-N-p-tolylpyrrole (5bc)

Yield: 122 mg (47%); eluent: light petroleum–CH₂Cl₂ (70:30).

¹H NMR (200 MHz, CDCl₃): δ = 0.93 (t, J = 7.4 Hz, 3 H), 2.43 (s, 3 H), 2.76 (q, J = 7.4 Hz, 2 H), 6.37 (d, J = 2.8 Hz, 1 H), 6.73 (d, J = 2.8 Hz, 1 H), 7.22–7.49 (m, 9 H).

¹³C NMR (50 MHz, CDCl₃): δ = 14.7, 18.1, 21.1, 108.5, 121.6, 122.4, 125.3, 126.4, 128.1, 128.3, 129.6, 131.8, 137.3, 137.4, 138.0.

MS (DEI): m/z (%) = 261 (100, [M⁺]), 246 (82, [M⁺ – Me]), 168 (4, [M⁺ – C₂H₆]), 154 (4, [M⁺ – C₈H₁₁]), 91 (7, [C₇H₇⁺]).

HRMS: m/z calcd for C₁₉H₁₉N: 261.15175; found: 261.15148 (M⁺), Δ = 0.27 mmu.

N-Cyclohexyl-3-ethyl-3-phenyl-1,3-dihydropyrrol-2-one (4bd)

Yield: 125 mg (46%); eluent: EtOH.

IR (neat): 2924 (s), 2855 (m), 1967 (w), 1700 (m), 1601 (w), 1447 (m), 1377 (m), 1253 (m), 752 (s), 698 cm⁻¹ (vs).

¹H NMR (200 MHz, CDCl₃): δ = 0.78 (t, J = 7.4 Hz, 3 H), 1.11–1.78 (m, 10 H), 1.99 (q, J = 7.4 Hz, 2 H), 3.86–3.93 (m, 1 H), 5.57 (d, J = 5.0 Hz, 1 H), 6.61 (d, J = 5.0 Hz, 1 H), 7.18–7.45 (m, 5 H).

¹³C NMR (500 MHz, CDCl₃): δ = 9.0, 25.4, 31.0, 31.7, 32.1, 50.4, 58.8, 113.3, 126.6, 126.8, 128.3, 128.4, 140.2, 179.1.

MS (DEI): m/z (%) = 269 (100, [M⁺]), 240 (59, [M⁺ – Et]), 187 (13, [M⁺ – C₆H₁₀]), 172 (12, [M⁺ – C₇H₁₃]), 158 (48, [M⁺ – C₈H₁₅]), 77 (5, [Ph⁺]).

HRMS: m/z calcd for C₁₈H₂₃NO: 269.17796; found: 269.17795, Δ = 0.01 mmu.

N-Cyclohexyl-2-ethyl-3-phenylpyrrole (5bd)

Yield: 122 mg (48%); eluent: light petroleum–CH₂Cl₂ (70:30).

¹H NMR (200 MHz, CDCl₃): δ = 1.24 (t, J = 7.4 Hz, 3 H), 1.34–2.07 (m, 10 H), 2.74 (q, J = 7.4 Hz, 2 H), 3.77–3.92 (m, 1 H), 6.27 (d, J = 3.0 Hz, 1 H), 6.71 (d, J = 3.0 Hz, 1 H), 7.18–7.41 (m, 5 H).

¹³C NMR (50 MHz, CDCl₃): δ = 15.6, 17.8, 25.5, 26.1, 35.0, 55.0, 107.7, 115.8, 120.8, 125.0, 128.0, 128.2, 130.1, 137.8.

MS (DEI): m/z (%) = 253 (100, [M⁺]), 238 (18, [M⁺ – Me]), 224 (4, [M⁺ – Et]), 170 (3, [M⁺ – C₆H₁₁]), 156 (8, [M⁺ – C₇H₁₃]).

HRMS: m/z calcd for C₁₈H₂₃N: 253.18305; found: 253.18344, Δ = 0.39 mmu.

N-Butyl-3-ethyl-3-phenyl-1,3-dihydropyrrol-2-one (4bf)

Yield: 142 mg (58%); eluent: EtOH.

IR (neat): 2959 (w), 2932 (w), 2874 (vw), 1686 (s), 1447 (w), 1373 (w), 1261 (m), 1076 (m), 1015 (m), 791 (m), 698 cm⁻¹ (vs).

¹H NMR (600 MHz, CDCl₃): δ = 0.80 (t, J = 7.2 Hz, 3 H), 0.90 (t, J = 7.2 Hz, 3 H), 1.30 (q, J = 7.2 Hz, 2 H), 1.50–1.56 (m, 2 H), 2.00 (q, J = 7.2 Hz, 2 H), 3.32–3.48 (m, 2 H), 5.61 (d, J = 5.4 Hz, 1 H), 6.52 (d, J = 5.4 Hz, 1 H), 7.20–7.44 (m, 5 H).

¹³C NMR (150 MHz, CDCl₃): δ = 9.2, 13.6, 20.0, 31.0, 31.3, 41.7, 58.5, 113.2, 126.7, 126.9, 128.4, 131.5, 140.2, 179.6.

MS (DEI): m/z (%) = 243 (100, [M⁺]), 214 (76, [M⁺ – Et]), 200 (17, [M⁺ – C₃H₇]), 186 (4, [M⁺ – C₄H₉]), 172 (50, [M⁺ – C₃H₇ – CO]).

HRMS: m/z calcd for C₁₆H₂₁NO: 243.16231; found: 243.16213, Δ = 0.18 mmu.

N-Butyl-2-ethyl-3-phenylpyrrole (5bf)

Yield: 91 mg (40%); eluent: light petroleum–CH₂Cl₂ (70:30).

¹H NMR (600 MHz, CDCl₃): δ = 0.90 (t, J = 7.2 Hz, 3 H), 1.24 (t, J = 7.2 Hz, 3 H), 1.42 (dt, J = 7.2 Hz, 2 H), 1.76–1.81 (m, 2 H), 2.75 (q, J = 7.2 Hz, 2 H), 3.85 (t, J = 7.2 Hz, 2 H), 6.26 (d, J = 3.0 Hz, 1 H), 6.63 (d, J = 3.0 Hz, 1 H), 7.19–7.41 (m, 5 H).

¹³C NMR (150 MHz, CDCl₃): δ = 12.8, 14.2, 16.8, 19.2, 32.8, 45.3, 106.6, 118.3, 120.4, 124.0, 126.9, 127.2, 129.7, 136.8.

MS (DEI): m/z (%) = 227 (100, [M⁺]), 212 (72, [M⁺ – Me]), 198 (27, [M⁺ – Et]), 184 (26, [M⁺ – C₃H₇]), 170 (19, [M⁺ – C₄H₉]).

HRMS: m/z calcd for C₁₆H₂₁N: 227.16740; found: 227.16754, Δ = 0.14 mmu.

N-4-tert-Butylphenyl-2-ethyl-3-phenylpyrrole (5bg)

Yield: 158 mg (52%); eluent: light petroleum–CH₂Cl₂ (70:30).

¹H NMR (200 MHz, CDCl₃): δ = 1.35 (t, J = 7.4 Hz, 3 H), 1.41 (s, 9 H), 2.80 (q, J = 7.4 Hz, 2 H), 6.40 (d, J = 3.0 Hz, 1 H), 6.77 (d, J = 3.0 Hz, 1 H), 7.29–7.53 (m, 9 H).

¹³C NMR (50 MHz, CDCl₃): δ = 14.4, 17.8, 31.1, 34.6, 108.3, 120.3, 120.8, 121.3, 122.0, 125.0, 125.7, 127.7, 128.0, 131.5, 137.4, 150.1.

MS (DEI): m/z (%) = 303 (100, [M⁺]), 288 (40, [M⁺ – Me]), 244 (7, [M⁺ – C₄H₁₁]), 232 (22, [M⁺ – C₅H₁₁]).

HRMS: m/z calcd for C₂₂H₂₅N: 303.19870; found: 303.19795, Δ = 0.75 mmu.

N-sec-Butyl-3-ethyl-3-phenyl-1,3-dihydropyrrol-2-one (4bh)

Yield: 124 mg (51%); eluent: EtOH.

IR (neat): 2967 (m), 2916 (m), 2851 (w), 2361 (w), 1971 (w), 1686 (s), 1601 (m), 1454 (m), 1377 (s), 1253 (m), 907 (m), 752 (vs), 698 cm⁻¹ (vs).

¹H NMR (600 MHz, CDCl₃): δ = 0.70–0.83 (m, 6 H), 1.09 (d, J = 6.8 Hz, 1.5 H), 1.13 (d, J = 6.8 Hz, 1.5 H), 1.45–1.52 (m, 2 H), 1.94–1.98 (m, 2 H), 4.00 (q, J = 6.6 Hz, 1 H), 5.54 (d, J = 5.4 Hz, 0.5 H), 5.56 (d, J = 5.4 Hz, 0.5 H), 6.51 (d, J = 5.4 Hz, 1 H), 7.15 (m, 1 H), 7.22 (m, 2 H), 7.39 (m, 2 H).

¹³C NMR (50 MHz, CDCl₃): δ = 9.1, 9.3, 10.7, 10.8, 19.5, 19.6, 28.5, 29.7, 31.0, 31.2, 48.4, 59.0, 113.5, 113.7, 126.6, 126.7, 126.8, 127.9, 128.0, 128.4, 128.8, 140.2, 179.4.

MS (DEI): m/z (%) = 243 (100, [M⁺]), 214 (93, [M⁺ – Et]), 186 (17, [M⁺ – C₄H₉]), 158 (43, [M⁺ – C₄H₉ – CO]), 77 (8, [Ph⁺]).

HRMS: m/z calcd for C₁₆H₂₁NO: 243.16231; found: 243.16212, Δ = 0.19 mmu.

N-sec-Butyl-2-ethyl-3-phenylpyrrole (5bh)

Yield: 95 mg (42%); eluent: light petroleum–CH₂Cl₂ (70:30).

¹H NMR (200 MHz, CDCl₃): δ = 0.89 (t, J = 3.7 Hz, 3 H), 1.26 (t, J = 7.0 Hz, 3 H), 1.43 (d, J = 6.6 Hz, 3 H), 1.78 (q, J = 7.4 Hz, 2 H), 2.73 (q, J = 7.6 Hz, 2 H), 4.03 (q, J = 7.0 Hz, 1 H), 6.29 (d, J = 3.0 Hz, 1 H), 6.66 (d, J = 3.0 Hz, 1 H), 7.18–7.38 (m, 5 H).

¹³C NMR (50 MHz, CDCl₃): δ = 11.1, 15.6, 17.7, 22.3, 31.2, 52.5, 109.0, 115.0, 120.6, 124.9, 128.0, 128.2, 130.7, 137.9.

MS (DEI): m/z (%) = 227 (100, [M⁺]), 212 (97, [M⁺ – Me]), 198 (28, [M⁺ – Et]), 156 (48, [M⁺ – C₅H₁₁]).

HRMS: m/z calcd for C₁₆H₂₁N: 227.16740; found: 227.16730, Δ = 0.10 mmu.

N-Benzyl-3-ethyl-3-methyl-1,3-dihydropyrrol-2-one (4ca)

Yield: 47 mg (22%); eluent: light petroleum–CH₂Cl₂ (50:50).

IR (neat): 2959 (w), 2928 (m), 2859 (w), 1705 (vs), 1454 (s), 1396 (m), 1273 (s), 1072 (m), 698 cm⁻¹ (vs).

¹H NMR (200 MHz, CDCl₃): δ = 0.75 (t, J = 7.4 Hz, 3 H), 1.19 (s, 3 H), 1.63 (q, J = 7.4 Hz, 2 H), 4.60 (AB spin system, J = 15.2, 20.1 Hz, 2 H), 5.24 (d, J = 5.0 Hz, 1 H), 6.29 (d, J = 5.0 Hz, 1 H), 7.18–7.32 (m, 5 H).

¹³C NMR (50 MHz, CDCl₃): δ = 9.1, 23.8, 38.8, 45.5, 68.2, 115.5, 126.3, 127.7, 128.7, 130.8, 137.0, 177.5.

MS (DEI): m/z (%) = 215 (100, [M⁺]), 186 (11, [M⁺ – Et]), 149 (38, [M⁺ – C₅H₆]), 91 (72, [C₇H₇⁺]), 65 (8, [C₅H₅⁺]).

HRMS: m/z calcd for C₁₄H₁₇NO: 215.13101; found: 215.13078, Δ = 0.23 mmu.

N-Benzyl-2-ethyl-3-methylpyrrole (5ca)

Yield: 100 mg (50%); eluent: light petroleum–CH₂Cl₂ (70:30).

¹H NMR (200 MHz, CDCl₃): δ = 1.01 (t, J = 7.6 Hz, 3 H), 2.10 (s, 3 H), 2.52 (q, J = 7.6 Hz, 2 H), 5.03 (s, 2 H), 6.01 (d, J = 2.8 Hz, 1 H), 6.53 (d, J = 2.8 Hz, 1 H), 7.01–7.38 (m, 5 H).

¹³C NMR (50 MHz, CDCl₃): δ = 11.3, 14.6, 17.4, 50.4, 108.7, 114.6, 119.3, 126.3, 126.7, 127.2, 128.6, 130.9.

MS (DEI): m/z (%) = 199 (52, [M⁺]), 184 (62, [M⁺ – Me]), 91 (100, [C₇H₇⁺]), 65 (13, [C₅H₅⁺]).

HRMS: m/z calcd for C₁₄H₁₇N: 199.13610; found: 199.13673, Δ = 0.63 mmu.

2-Ethyl-3-methyl-N-phenylpyrrole (5cb)

Yield: 106 mg (57%); eluent: light petroleum–CH₂Cl₂ (70:30).

¹H NMR (200 MHz, CDCl₃): δ = 0.96 (t, J = 7.4 Hz, 3 H), 2.12 (s, 3 H), 2.56 (q, J = 7.4 Hz, 2 H), 6.08 (d, J = 2.8 Hz, 1 H), 6.64 (d, J = 2.8 Hz, 1 H), 7.26–7.47 (m, 5 H).

¹³C NMR (50 MHz, CDCl₃): δ = 11.3, 14.5, 17.6, 109.8, 115.5, 120.2, 126.1, 126.8, 128.9, 131.5, 140.8.

MS (DEI): m/z (%) = 185 (78, [M⁺]), 170 (100, [M⁺ – Me]), 77 (15, [Ph⁺]).

HRMS: m/z calcd for C₁₃H₁₅N: 185.12045; found: 185.11962, Δ = 0.83 mmu.

2-Ethyl-3-methyl-N-p-tolylpyrrole (5cc)

Yield: 94 mg (47%); eluent: light petroleum–CH₂Cl₂ (70:30).

¹H NMR (200 MHz, CDCl₃): δ = 0.96 (t, J = 7.4 Hz, 3 H), 2.12 (s, 3 H), 2.40 (s, 3 H), 2.55 (q, J = 7.4 Hz, 2 H), 6.06 (d, J = 2.8 Hz, 1 H), 6.61 (d, J = 2.8 Hz, 1 H), 7.14–7.24 (m, 4 H).

¹³C NMR (50 MHz, CDCl₃): δ = 11.3, 14.5, 17.6, 21.0, 109.5, 115.2, 120.2, 126.0, 129.5, 131.6, 136.7, 138.3.

MS (DEI): m/z (%) = 199 (100, [M⁺]), 184 (80, [M⁺ – Me]), 154 (18, [M⁺ – C₂H₆ – Me⁺]), 91 (17, [C₇H₇⁺]), 77 (5, [Ph⁺]).

HRMS: m/z calcd for C₁₄H₁₇N: 199.13610; found: 199.13607 (M⁺), Δ = 0.03 mmu.

N-Cyclohexyl-3-ethyl-3-methyl-1,3-dihydropyrrol-2-one (4cd)

Yield: 96 mg (46%); eluent: CH₂Cl₂.

IR (neat): 2928 (vs), 2855 (m), 1971 (m), 1937 (m), 1674 (vs), 1450 (s), 1377 (s), 1258 (s), 1188 (s), 1138 (s), 895 (m), 691 cm⁻¹ (m).

¹H NMR (200 MHz, CDCl₃): δ = 0.66 (t, J = 7.4 Hz, 3 H), 1.09 (s, 3 H), 1.53 (q, J = 7.4 Hz, 2 H), 1.20–1.75 (m, 10 H), 3.80–3.86 (m, 1 H), 5.17 (d, J = 5.0 Hz, 1 H), 6.43 (d, J = 5.0 Hz, 1 H).

¹³C NMR (50 MHz, CDCl₃): δ = 8.8, 21.9, 25.3, 25.4, 31.7, 32.1, 50.0, 51.2, 115.0, 127.3, 181.5.

MS (DEI): m/z (%) = 207 (68, [M⁺]), 192 (7, [M⁺ – Et]), 178 (100, [M⁺ – Et]).

HRMS: m/z calcd for C₁₃H₂₁NO: 207.16231; found: 207.16278, Δ = 0.47 mmu.

N-Cyclohexyl-2-ethyl-3-methylpyrrole (5cd)

Yield: 51 mg (27%); eluent: light petroleum–CH₂Cl₂ (70:30).

¹H NMR (200 MHz, CDCl₃): δ = 1.11 (t, J = 7.4 Hz, 3 H), 1.25–1.94 (m, 10 H), 2.05 (s, 3 H), 2.58 (q, J = 7.4 Hz, 2 H), 3.68–3.83 (m, 1 H), 5.96 (d, J = 2.8 Hz, 1 H), 6.58 (d, J = 2.8 Hz, 1 H).

^{13}C NMR (50 MHz, CDCl_3): δ = 11.2, 15.0, 17.4, 25.5, 26.1, 35.0, 54.9, 108.4, 113.2, 114.5, 130.0.

MS (DEI): m/z (%) = 191 (88, $[\text{M}^+]$), 176 (100, $[\text{M}^+ - \text{Me}]$), 162 (29, $[\text{M}^+ - \text{Et}]$).

HRMS: m/z calcd for $\text{C}_{13}\text{H}_{21}\text{N}$: 191.16740; found: 191.16732, Δ = 0.08 mmu.

N-Butyl-2-ethyl-3-methyl-1,3-dihydropyrrol-2-one (4cf)

Yield: 90 mg (50%); eluent: light petroleum– CH_2Cl_2 (50:50).

IR (neat): 2963 (m), 2928 (m), 2874 (w), 1694 (vs), 1458 (m), 1362 (m), 1265 (m), 1192 (m), 1111 (m), 741 (m), 691 cm^{-1} (s).

^1H NMR (200 MHz, CDCl_3): δ = 0.68 (t, J = 7.4 Hz, 3 H), 0.87 (t, J = 7.2 Hz, 3 H), 1.10 (s, 3 H), 1.20–1.31 (m, 2 H), 1.41–1.66 (m, 4 H), 3.31–3.38 (m, 2 H), 5.19 (d, J = 5.0 Hz, 1 H), 6.33 (d, J = 5.0 Hz, 1 H).

^{13}C NMR (50 MHz, CDCl_3): δ = 8.9, 13.6, 19.8, 22.0, 29.9, 30.9, 41.4, 50.9, 114.9, 130.3, 182.0.

MS (DEI): m/z (%) = 181 (58, $[\text{M}^+]$), 166 (11, $[\text{M}^+ - \text{Me}]$), 152 (100, $[\text{M}^+ - \text{Et}]$), 138 (22, $[\text{M}^+ - \text{C}_3\text{H}_7]$), 110 (62, $[\text{M}^+ - \text{C}_5\text{H}_{11}]$), 96 (17, $[\text{M}^+ - \text{C}_6\text{H}_{13}]$).

HRMS: m/z calcd for $\text{C}_{11}\text{H}_{19}\text{NO}$: 181.14666; found: 181.14621, Δ = 0.45 mmu.

N-Butyl-2-ethyl-3-methylpyrrole (5cf)

Yield: 81 mg (49%); eluent: light petroleum– CH_2Cl_2 (70:30).

^1H NMR (200 MHz, CDCl_3): δ = 0.94 (t, J = 7.4 Hz, 3 H), 1.11 (t, J = 7.4 Hz, 3 H), 1.30–1.41 (m, 2 H), 1.62–1.77 (m, 2 H), 2.04 (s, 3 H), 2.55 (q, J = 7.4 Hz, 2 H), 3.85 (t, J = 7.4 Hz, 2 H), 5.91 (d, J = 2.8 Hz, 1 H), 6.47 (d, J = 2.8 Hz, 1 H).

^{13}C NMR (50 MHz, CDCl_3): δ = 11.2, 13.7, 14.7, 17.3, 20.1, 33.9, 46.3, 108.1, 113.8, 118.0, 130.4.

MS (DEI): m/z (%) = 165 (66, $[\text{M}^+]$), 150 (100, $[\text{M}^+ - \text{Me}]$), 136 (30, $[\text{M}^+ - \text{Et}]$), 122 (20, $[\text{M}^+ - \text{C}_3\text{H}_7]$), 108 (31, $[\text{M}^+ - \text{C}_4\text{H}_9]$), 94 (22, $[\text{M}^+ - \text{C}_5\text{H}_{11}]$), 28 (24, $[\text{C}_2\text{H}_4^+]$).

HRMS: m/z calcd for $\text{C}_{11}\text{H}_{19}\text{N}$: 165.15175; found: 165.15189, Δ = 0.14 mmu.

N-(4-tert-Butylphenyl)-2-ethyl-3-methylpyrrole (5cg)

Yield: 111 mg (46%); eluent: light petroleum– CH_2Cl_2 (70:30).

^1H NMR (200 MHz, CDCl_3): δ = 0.98 (t, J = 7.4 Hz, 3 H), 1.36 (s, 9 H), 2.12 (s, 3 H), 2.56 (q, J = 7.4 Hz, 2 H), 6.06 (d, J = 2.8 Hz, 1 H), 6.63 (d, J = 2.8 Hz, 1 H), 7.21 (d, J = 8.0 Hz, 2 H), 7.43 (d, J = 8.0 Hz, 2 H).

^{13}C NMR (50 MHz, CDCl_3): δ = 11.3, 14.6, 17.6, 31.4, 34.6, 109.5, 115.2, 120.2, 125.7, 125.8, 131.6, 138.2, 149.8.

MS (DEI): m/z (%) = 241 (100, $[\text{M}^+]$), 226 (72, $[\text{M}^+ - \text{Me}]$), 196 (10, $[\text{M}^+ - \text{C}_3\text{H}_9]$), 170 (31, $[\text{M}^+ - \text{C}_5\text{H}_{11}]$), 57 (7, $[\text{C}_4\text{H}_9^+]$).

HRMS: m/z calcd for $\text{C}_{17}\text{H}_{23}\text{N}$: 241.18305; found: 241.18335, Δ = 0.30 mmu.

N-sec-Butyl-3-ethyl-3-methyl-1,3-dihydropyrrol-2-one (4ch)

Yield: 93 mg (51%); eluent: CH_2Cl_2 .

IR (neat): 2967 (m), 2928 (w), 1694 (vs), 1454 (m), 1381 (m), 1258 (s), 1069 (m), 745 (m), 691 cm^{-1} (s).

^1H NMR (200 MHz, CDCl_3): δ = 0.63–0.83 (m, 6 H), 1.10 (s, 1.8 H), 1.08–1.13 (m, 1.8 H), 1.13 (s, 1.2 H), 1.10–1.16 (m, 1.2 H), 1.41–1.71 (m, 4 H), 4.02 (q, J = 7.0 Hz, 1 H), 5.21 (d, J = 5.0 Hz, 1 H), 6.38 (d, J = 5.0 Hz, 1 H).

^{13}C NMR (50 MHz, CDCl_3): δ = 8.9, 9.1, 10.6, 10.7, 19.5, 19.7, 22.2, 22.2, 28.4, 28.5, 29.9, 47.9, 48.1, 51.3, 51.4, 115.3, 126.7, 126.8, 181.9.

MS (DEI): m/z (%) = 181 (50, $[\text{M}^+]$), 152 (100, $[\text{M}^+ - \text{Et}]$), 124 (30, $[\text{M}^+ - \text{C}_4\text{H}_9]$), 110 (7, $[\text{M}^+ - \text{C}_5\text{H}_{11}]$), 96 (42, $[\text{M}^+ - \text{C}_6\text{H}_{13}]$), 57 (11, $[\text{C}_4\text{H}_9^+]$).

HRMS: m/z calcd for $\text{C}_{11}\text{H}_{19}\text{NO}$: 181.14666; found: 181.14699, Δ = 0.33 mmu.

N-sec-Butyl-2-ethyl-3-methylpyrrole (5ch)

Yield: 45 mg (27%); eluent: light petroleum– CH_2Cl_2 (70:30).

^1H NMR (200 MHz, CDCl_3): δ = 0.84 (t, J = 7.4 Hz, 3 H), 1.10 (t, J = 7.6 Hz, 3 H), 1.37 (d, J = 6.8 Hz, 3 H), 1.66–1.81 (m, 2 H), 2.05 (s, 3 H), 2.57 (q, J = 7.6 Hz, 2 H), 3.93 (q, J = 6.8 Hz, 1 H), 5.98 (d, J = 3.0 Hz, 1 H), 6.53 (d, J = 3.0 Hz, 1 H).

^{13}C NMR (50 MHz, CDCl_3): δ = 11.0, 11.2, 15.0, 17.3, 22.2, 31.1, 52.4, 108.6, 112.9, 113.8, 130.5.

MS (DEI): m/z (%) = 165 (85, $[\text{M}^+]$), 150 (100, $[\text{M}^+ - \text{Me}]$), 136 (40, $[\text{M}^+ - \text{Et}]$), 122 (19, $[\text{M}^+ - \text{C}_3\text{H}_7]$), 108 (18, $[\text{M}^+ - \text{C}_4\text{H}_9]$), 94 (64, $[\text{M}^+ - \text{C}_5\text{H}_{11}]$), 57 (25, $[\text{C}_4\text{H}_9^+]$).

HRMS: m/z calcd for $\text{C}_{11}\text{H}_{19}\text{N}$: 165.15175; found: 165.15098, Δ = 0.77 mmu.

N-Benzyl-3-ethyl-3-(4-fluorophenyl)-1,3-dihydropyrrol-2-one (4ea)

Yield: 193 mg (65%); eluent: EtOH.

IR (neat): 2967 (w), 2932 (w), 1967 (w), 1682 (s), 1601 (s), 1508 (vs), 1393 (m), 1358 (s), 1227 (vs), 1157 (s), 1076 (m), 833 (vs), 729 (vs), 698 cm^{-1} (vs).

^1H NMR (600 MHz, CDCl_3): δ = 0.74 (t, J = 7.2 Hz, 2.25 H), 1.10 (t, J = 7.6 Hz, 0.75 H), 1.94 (q, J = 7.2 Hz, 1.5 H), 2.16 (q, J = 7.6 Hz, 0.5 H), 4.52 (AB spin system, J = 15.0, 85.1 Hz, 2 H), 5.54 (d, J = 4.8 Hz, 1 H), 6.39 (d, J = 4.8 Hz, 1 H), 6.91–7.39 (m, 9 H).

^{13}C NMR (150 MHz, CDCl_3): δ = 9.3, 9.9, 29.7, 31.6, 43.6, 45.8, 57.8, 113.3, 115.3, 127.8, 128.8, 128.3, 131.3, 135.6, 136.7, 138.4, 162.0, 179.5.

MS (DEI): m/z (%) = 295 (100, $[\text{M}^+]$), 280 (4, $[\text{M}^+ - \text{Me}]$), 266 (49, $[\text{M}^+ - \text{Et}]$), 204 (3, $[\text{M}^+ - \text{C}_7\text{H}_7]$), 91 (62, $[\text{C}_7\text{H}_7^+]$).

HRMS: m/z calcd for $\text{C}_{19}\text{H}_{18}\text{FNO}$: 295.13724; found: 295.13726, Δ = 0.02 mmu.

N-Benzyl-2-ethyl-3-(4-fluorophenyl)pyrrole (5ea)

Yield: 78 mg (28%); eluent: light petroleum– CH_2Cl_2 (70:30).

^1H NMR (200 MHz, CDCl_3): δ = 1.12 (t, J = 7.6 Hz, 3 H), 2.65 (q, J = 7.6 Hz, 2 H), 5.10 (s, 2 H), 6.26 (d, J = 2.8 Hz, 1 H), 6.61 (d, J = 2.8 Hz, 1 H), 7.00–7.36 (m, 9 H).

^{13}C NMR (150 MHz, CDCl_3): δ = 14.1, 16.8, 49.4, 107.0, 114.8, 119.6, 125.4, 126.4, 127.7, 128.3, 129.4, 130.1, 132.6, 137.4, 159.3.

MS (DEI): m/z (%) = 279 (100, $[\text{M}^+]$), 264 (22, $[\text{M}^+ - \text{Me}]$), 188 (6, $[\text{M}^+ - \text{C}_7\text{H}_7]$), 91 (95, $[\text{C}_7\text{H}_7^+]$).

HRMS: m/z calcd for $\text{C}_{19}\text{H}_{18}\text{FN}$: 279.14233; found: 279.14283, Δ = 0.50 mmu.

2-Ethyl-3-(4-fluorophenyl)-N-phenylpyrrole (5eb)

Yield: 150 mg (57%); eluent: light petroleum– CH_2Cl_2 (70:30).

^1H NMR (200 MHz, CDCl_3): δ = 0.88 (t, J = 7.4 Hz, 3 H), 2.72 (q, J = 7.4 Hz, 2 H), 6.32 (d, J = 2.8 Hz, 1 H), 6.74 (d, J = 2.8 Hz, 1 H), 7.01–7.43 (m, 9 H).

^{13}C NMR (50 MHz, CDCl_3): δ = 14.6, 18.0, 108.8, 115.1, 121.6, 126.6, 127.5, 129.1, 129.4, 129.6, 131.6, 133.4, 140.5, 163.6.

MS (DEI): m/z (%) = 265 (89, $[\text{M}^+]$), 250 (100, $[\text{M}^+ - \text{Me}]$), 235 (4, $[\text{M}^+ - \text{C}_2\text{H}_6]$), 77 (8, $[\text{Ph}^+]$), 28 (3, $[\text{C}_2\text{H}_4]$).

HRMS: m/z calcd for $\text{C}_{18}\text{H}_{16}\text{FN}$: 265.12668; found: 265.12490 (M^+), Δ = 1.78 mmu.

2-Ethyl-3-(4-fluorophenyl)-*N*-*p*-tolylpyrrole (5ec)

Yield: 140 mg (50%); eluent: light petroleum–CH₂Cl₂ (70:30).

¹H NMR (200 MHz, CDCl₃): δ = 0.90 (t, *J* = 7.4 Hz, 3 H), 2.41 (s, 3 H), 2.70 (q, *J* = 7.4 Hz, 2 H), 6.31 (d, *J* = 2.8 Hz, 1 H), 6.71 (d, *J* = 2.8 Hz, 1 H), 7.00–7.40 (m, 8 H).

¹³C NMR (50 MHz, CDCl₃): δ = 14.3, 17.7, 20.7, 108.2, 114.7, 121.3, 125.6, 126.1, 129.2, 129.3, 131.4, 133.1, 137.0, 137.6, 160.8.

MS (DEI): *m/z* (%) = 279 (100, [M⁺]), 264 (82, [M⁺ – Me]), 91 (6, [C₇H₇⁺]).

HRMS: *m/z* calcd for C₁₉H₁₈FN: 279.14233; found: 279.14268, Δ = 0.35 mmu.

***N*-Cyclohexyl-3-ethyl-3-(4-fluorophenyl)-1,3-dihydropyrrol-2-one (4ed)**

Yield: 148 mg (52%); eluent: EtOH.

IR (neat): 2963 (m), 2932 (m), 1967 (w), 1686 (m), 1601 (m), 1508 (s), 1381 (m), 1261 (vs), 1223 (s), 1161 (m), 1096 (vs), 1015 (vs), 802 (vs), 690 cm⁻¹ (s).

¹H NMR (600 MHz, CDCl₃): δ = 0.77 (t, *J* = 7.2 Hz, 3 H), 1.11–1.81 (m, 10 H), 1.95 (q, *J* = 7.2 Hz, 2 H), 3.85–3.91 (m, 1 H), 5.56 (d, *J* = 5.4 Hz, 1 H), 6.62 (d, *J* = 5.2 Hz, 1 H), 6.96 (t, *J* = 8.4 Hz, 2 H), 7.40 (t, *J* = 4.2 Hz, 2 H).

¹³C NMR (150 MHz, CDCl₃): δ = 9.1, 25.4, 25.5, 31.6, 32.1, 50.5, 58.2, 113.0, 115.1, 128.3, 128.6, 136.0, 161.9, 179.0.

MS (DEI): *m/z* (%) = 287 (100, [M⁺]), 258 (50, [M⁺ – Et]), 204 (3, [M⁺ – C₆H₁₁]), 176 (9, [M⁺ – C₆H₁₁ – C₂H₄]), 109 (4, [M⁺ – C₆H₁₁ – C₆H₄F]).

HRMS: *m/z* calcd for C₁₈H₂₂FNO: 287.16854; found: 287.16825, Δ = 0.29 mmu.

***N*-Cyclohexyl-2-ethyl-3-(4-fluorophenyl)pyrrole (5ed)**

Yield: 92 mg (34%); eluent: light petroleum–CH₂Cl₂ (70:30).

¹H NMR (600 MHz, CDCl₃): δ = 1.21 (t, *J* = 7.2 Hz, 3 H), 1.40–2.04 (m, 10 H), 2.70 (q, *J* = 7.2 Hz, 2 H), 3.80–3.84 (m, 1 H), 6.22 (d, *J* = 3.0 Hz, 1 H), 6.69 (d, *J* = 3.0 Hz, 1 H), 7.03 (t, *J* = 8.4 Hz, 2 H), 7.31 (dd, *J* = 3.0, 5.4 Hz, 2 H).

¹³C NMR (150 MHz, CDCl₃): δ = 14.6, 16.7, 24.5, 25.1, 34.0, 54.0, 106.7, 113.9, 114.8, 118.9, 128.4, 129.0, 132.8, 160.0.

MS (DEI): *m/z* (%) = 271 (100, [M⁺]), 256 (25, [M⁺ – Me]), 242 (4, [M⁺ – Et]), 188 (7, [M⁺ – C₆H₁₁]), 83 (3, [C₆H₁₁⁺]).

HRMS: *m/z* calcd for C₁₈H₂₂FN: 271.17363; found: 271.17367, Δ = 0.04 mmu.

***N*-Butyl-3-ethyl-3-(4-fluorophenyl)-1,3-dihydropyrrol-2-one (4ef)**

Yield: 144 mg (55%); eluent: EtOH.

IR (neat): 2963 (w), 2932 (w), 2874 (vw), 1967 (vw), 1686 (s), 1601 (m), 1508 (vs), 1369 (m), 1261 (w), 1223 (vs), 1161 (m), 833 (vs), 691 cm⁻¹ (w).

¹H NMR (600 MHz, CDCl₃): δ = 0.77 (t, *J* = 7.2 Hz, 3 H), 0.78 (t, *J* = 7.2 Hz, 3 H), 0.89 (t, *J* = 7.2 Hz, 3 H), 1.28 (q, *J* = 7.2 Hz, 2 H), 1.48–1.55 (m, 2 H), 1.95 (q, *J* = 7.2 Hz, 2 H), 3.69 (q, *J* = 7.2 Hz, 2 H), 5.58 (d, *J* = 4.8 Hz, 1 H), 6.53 (d, *J* = 4.8 Hz, 1 H), 6.96 (t, *J* = 9.0 Hz, 1 H), 7.42 (dd, *J* = 5.4 Hz, *J* = 8.4 Hz, 2 H).

¹³C NMR (150 MHz, CDCl₃): δ = 9.2, 13.6, 19.9, 30.9, 31.6, 41.8, 57.8, 112.8, 115.2, 128.4, 131.7, 135.9, 162.7, 179.5.

MS (DEI): *m/z* (%) = 261 (100, [M⁺]), 232 (49, [M⁺ – Et]), 218 (6, [M⁺ – C₃H₇]), 204 (4, [M⁺ – C₄H₉]), 190 (16, [M⁺ – C₅H₁₁]).

HRMS: *m/z* calcd for C₁₆H₂₀FNO: 261.15289; found: 261.15165, Δ = 1.24 mmu.

***N*-Butyl-2-ethyl-3-(4-fluorophenyl)pyrrole (5ef)**

Yield: 82 mg (33%); eluent: light petroleum–CH₂Cl₂ (70:30).

¹H NMR (600 MHz, CDCl₃): δ = 0.97 (t, *J* = 7.2 Hz, 3 H), 1.20 (t, *J* = 7.2 Hz, 3 H), 1.40 (q, *J* = 7.2 Hz, 2 H), 1.70–1.79 (m, 2 H), 2.70 (q, *J* = 7.2 Hz, 2 H), 3.83 (t, *J* = 7.2 Hz, 2 H), 6.19 (d, *J* = 3.0 Hz, 1 H), 6.61 (d, *J* = 3.0 Hz, 1 H), 7.03 (t, *J* = 9.0 Hz, 2 H), 7.31 (t, *J* = 4.2 Hz, 2 H).

¹³C NMR (150 MHz, CDCl₃): δ = 12.8, 14.2, 16.7, 19.1, 32.8, 45.3, 106.5, 114.0, 118.3, 119.4, 128.3, 129.6, 132.8, 160.00.

MS (DEI): *m/z* (%) = 245 (100, [M⁺]), 230 (74, [M⁺ – Me]), 216 (28, [M⁺ – Et]), 202 (28, [M⁺ – C₃H₇]), 188 (26, [M⁺ – C₄H₉]).

HRMS: *m/z* calcd for C₁₆H₂₀FN: 245.15798; found: 245.15760, Δ = 0.38 mmu.

***N*-(4-tert-Butylphenyl)-2-ethyl-3-(4-fluorophenyl)pyrrole (5eg)**

Yield: 174 mg (54%); eluent: light petroleum–CH₂Cl₂ (70:30).

¹H NMR (200 MHz, CDCl₃): δ = 1.26 (t, *J* = 7.2 Hz, 3 H), 1.37 (s, 9 H), 2.71 (q, *J* = 7.2 Hz, 2 H), 6.31 (d, *J* = 2.8 Hz, 1 H), 6.72 (d, *J* = 2.8 Hz, 1 H), 7.01–7.48 (m, 8 H).

¹³C NMR (50 MHz, CDCl₃): δ = 14.7, 18.0, 31.4, 34.7, 108.5, 115.1, 121.6, 126.0, 126.1, 129.4, 131.8, 133.5, 137.8, 150.6, 163.6.

MS (DEI): *m/z* (%) = 321 (100, [M⁺]), 306 (36, [M⁺ – Me]), 250 (12, [M⁺ – C₅H₁₁]), 132 (4, [C₁₀H₁₂⁺]), 57 (6, [C₄H₉⁺]).

HRMS: *m/z* calcd for C₂₂H₂₄FN: 321.18928; found: 321.18829, Δ = 0.99 mmu.

***N*-sec-Butyl-3-ethyl-3-(4-fluorophenyl)-1,3-dihydropyrrol-2-one (4eh)**

Yield: 108 mg (41%); eluent: EtOH.

IR (neat): 2967 (m), 2932 (w), 1694 (s), 1508 (s), 1381 (m), 1258 (vs), 1161 (m), 1015 (vs), 791 (vs), 694 cm⁻¹ (m).

¹H NMR (200 MHz, CDCl₃): δ = 0.70–0.89 (m, 6 H), 1.12 (d, *J* = 6.8 Hz, 1.5 H), 1.17 (d, *J* = 6.8 Hz, 1.5 H), 1.41–1.61 (m, 2 H), 1.96 (q, *J* = 7.4 Hz, 1 H), 1.96 (q, *J* = 7.4 Hz, 1 H), 4.03 (m, 1 H), 5.57 (d, *J* = 3.1 Hz, 0.5 H), 5.60 (d, *J* = 3.1 Hz, 0.5 H), 6.57 (d, *J* = 5.0 Hz, 1 H), 6.95 (t, *J* = 8.8 Hz, 2 H), 7.37–7.45 (m, 2 H).

¹³C NMR (50 MHz, CDCl₃): δ = 9.0, 9.2, 10.6, 10.7, 19.4, 19.6, 28.4, 31.3, 31.4, 48.4, 58.2, 113.1, 113.3, 114.8, 115.3, 128.1, 128.2, 128.3, 135.9, 159.3, 164.2, 179.2.

MS (DEI): *m/z* (%) = 261 (100, [M⁺]), 246 (3, [M⁺ – Me]), 232 (96, [M⁺ – Et]), 204 (20, [M⁺ – C₄H₉]), 190 (4, [M⁺ – C₅H₁₁]), 176 (52, [M⁺ – C₆H₁₃]), 57 (9, [C₄H₉⁺]), 29 (18, [Et⁺]).

HRMS: *m/z* calcd for C₁₆H₂₀FNO: 261.15289; found: 261.15237, Δ = 0.52 mmu.

***N*-sec-Butyl-2-ethyl-3-(4-fluorophenyl)pyrrole (5eh)**

Yield: 128 mg (52%); eluent: light petroleum–CH₂Cl₂ (70:30).

¹H NMR (200 MHz, CDCl₃): δ = 0.84 (t, *J* = 7.4 Hz, 3 H), 1.19 (t, *J* = 7.4 Hz, 3 H), 1.41 (d, *J* = 6.6 Hz, 3 H), 1.77 (q, *J* = 7.6 Hz, 2 H), 2.67 (q, *J* = 7.6 Hz, 2 H), 3.99 (q, *J* = 6.8 Hz, 1 H), 6.21 (d, *J* = 3.0 Hz, 1 H), 6.63 (d, *J* = 3.0 Hz, 1 H), 6.96–7.05 (m, 2 H), 7.23–7.32 (m, 2 H).

¹³C NMR (50 MHz, CDCl₃): δ = 11.0, 15.5, 17.6, 22.3, 31.1, 52.6, 107.9, 114.9, 119.7, 129.3, 129.4, 130.6, 133.9, 160.9.

MS (DEI): *m/z* (%) = 245 (100, [M⁺]), 230 (32, [M⁺ – Me]), 216 (13, [M⁺ – Et]), 188 (6, [M⁺ – C₄H₉]), 174 (20, [M⁺ – C₅H₁₁]), 95 (3, [C₆H₄F]).

HRMS: *m/z* calcd for C₁₆H₂₀FN: 245.15798; found: 245.15786, Δ = 0.12 mmu.

N-Benzyl-3-ethyl-3-furyl-1,3-dihydropyrrol-2-one (4fa)

Yield: 151 mg (57%); eluent: EtOH.

IR (neat): 2970 (w), 2932 (w), 2878 (w), 2361 (w), 2021 (m), 1952 (m), 1667 (s), 1605 (m), 1497 (s), 1454 (s), 1354 (s), 1258 (m), 1076 (m), 1011 (s), 729 (vs), 689 cm⁻¹ (vs).¹H NMR (200 MHz, CDCl₃): δ = 0.84 (t, *J* = 7.4 Hz, 1.5 H), 1.16 (t, *J* = 7.6 Hz, 1.5 H), 2.06 (q, *J* = 7.4 Hz, 1 H), 2.23 (q, *J* = 7.6 Hz, 1 H), 4.52 (AB spin system, *J* = 7.8, 36.6 Hz, 2 H), 5.46 (d, *J* = 2.8 Hz, 1 H), 6.19 (dd, *J* = 0.8, 3.2 Hz, 1 H), 6.30 (dd, *J* = 1.8, 3.3 Hz, 1 H), 6.41 (d, *J* = 2.8 Hz, 1 H), 7.21–7.32 (m, 5 H), 7.35 (dd, *J* = 0.8, 1.8 Hz, 1 H).¹³C NMR (50 MHz, CDCl₃): δ = 8.5, 9.5, 28.2, 29.3, 43.2, 43.4, 55.2, 58.0, 105.6, 109.8, 111.3, 126.0, 127.1, 127.4, 128.4, 131.5, 141.8, 152.2, 177.2.MS (DEI): *m/z* (%) = 267 (100, [M⁺]), 238 (39, [M⁺ – Et]), 200 (11, [M⁺ – C₄H₃O]), 176 (6, [M⁺ – C₇H₇]), 91 (52, [C₇H₇⁺]).HRMS: *m/z* calcd for C₁₇H₁₇NO₂: 267.12593; found: 267.12572, Δ = 0.21 mmu.**N-Benzyl-2-ethyl-3-furylpyrrole (5fa)**Yield: 109 mg (43%); eluent: light petroleum–CH₂Cl₂ (70:30).¹H NMR (200 MHz, CDCl₃): δ = 1.11 (t, *J* = 7.6 Hz, 3 H), 2.78 (q, *J* = 7.6 Hz, 2 H), 5.08 (s, 2 H), 6.24 (dd, *J* = 0.8, 3.2 Hz, 1 H), 6.43 (d, *J* = 2.8 Hz, 1 H), 6.43 (dd, *J* = 0.8, 3.2 Hz, 1 H), 6.60 (d, *J* = 2.8 Hz, 1 H), 7.03–7.33 (m, 5 H), 7.38 (dd, *J* = 0.8, 1.8 Hz, 1 H).¹³C NMR (50 MHz, CDCl₃): δ = 14.0, 18.1, 49.9, 102.0, 105.8, 110.6, 120.6, 126.0, 127.1, 128.4, 131.4, 138.0, 139.4, 151.8.MS (DEI): *m/z* (%) = 251 (100, [M⁺]), 236 (38, [M⁺ – Me]), 160 (7, [M⁺ – C₇H₇]), 91 (73, [C₇H₇⁺]).HRMS: *m/z* calcd for C₁₇H₁₇NO: 251.13101; found: 251.13106, Δ = 0.05 mmu.**2-Ethyl-3-furyl-N-phenylpyrrole (5fb)**Yield: 111 mg (47%); eluent: light petroleum–CH₂Cl₂ (70:30).¹H NMR (200 MHz, CDCl₃): δ = 1.06 (t, *J* = 7.4 Hz, 3 H), 2.80 (q, *J* = 7.4 Hz, 2 H), 6.29 (dd, *J* = 0.8, 3.4 Hz, 1 H), 6.39 (dd, *J* = 1.8, 3.2 Hz, 1 H), 6.49 (d, *J* = 3.0 Hz, 1 H), 6.70 (d, *J* = 3.0 Hz, 1 H), 7.35 (dd, *J* = 0.8, 1.8 Hz, 1 H), 7.31–7.47 (m, 5 H).¹³C NMR (50 MHz, CDCl₃): δ = 14.4, 18.6, 102.9, 106.8, 110.9, 113.2, 121.7, 126.6, 127.5, 129.1, 132.3, 140.0, 151.8.MS (DEI): *m/z* (%) = 237 (100, [M⁺]), 222 (70, [M⁺ – Me]), 208 (2, [M⁺ – Et]), 91 (3, [C₇H₇⁺]), 77 (5, [Ph⁺]).HRMS: *m/z* calcd for C₁₆H₁₅NO: 237.11536; found: 237.11537 (M⁺), Δ = 0.01 mmu.**3-Ethyl-3-furyl-N-p-tolyl-1,3-dihydropyrrol-2-one (4fc)**

Yield: 108 mg (40%); eluent: EtOH.

IR (neat): 2963 (w), 2928 (m), 2859 (w), 1717 (vs), 1612 (m), 1512 (vs), 1458 (m), 1385 (vs), 1277 (s), 1207 (s), 1072 (s), 1015 (s), 864 (s), 813 (vs), 736 (vs), 706 cm⁻¹ (s).¹H NMR (200 MHz, CDCl₃): δ = 0.89 (t, *J* = 7.4 Hz, 3 H), 2.11 (q, *J* = 7.4 Hz, 2 H), 2.32 (s, 3 H), 5.63 (d, *J* = 5.0 Hz, 1 H), 6.24 (dd, *J* = 0.8, 3.4 Hz, 1 H), 6.30 (dd, *J* = 1.8, 3.2 Hz, 1 H), 6.93 (d, *J* = 5.0 Hz, 1 H), 7.15–7.36 (m, 4 H), 7.50 (dd, *J* = 3.6, 5.6 Hz, 1 H).¹³C NMR (50 MHz, CDCl₃): δ = 8.8, 20.9, 30.4, 56.2, 106.1, 110.2, 112.1, 121.5, 128.8, 129.6, 132.5, 135.6, 142.2, 152.4, 176.0.MS (DEI): *m/z* (%) = 267 (80, [M⁺]), 252 (2, [M⁺ – Me]), 238 (100, [M⁺ – Et]), 223 (7, [M⁺ – C₃H₈]), 210 (17, [M⁺ – CO – Et]), 91 (23, [C₇H₇⁺]).HRMS: *m/z* calcd for C₁₇H₁₇NO₂: 267.12593; found: 267.12564, Δ = 0.29 mmu.**2-Ethyl-3-furyl-N-p-tolylpyrrole (5fc)**Yield: 139 mg (55%); eluent: light petroleum–CH₂Cl₂ (60:40).¹H NMR (200 MHz, CDCl₃): δ = 1.05 (t, *J* = 7.4 Hz, 3 H), 2.42 (s, 3 H), 2.77 (q, *J* = 7.4 Hz, 2 H), 6.27 (dd, *J* = 0.8, 3.2 Hz, 1 H), 6.43 (dd, *J* = 1.8, 3.4 Hz, 1 H), 6.46 (d, *J* = 2.8 Hz, 1 H), 6.67 (d, *J* = 3.0 Hz, 1 H), 7.18–7.28 (m, 4 H), 7.39 (dd, *J* = 0.8, 1.8 Hz, 1 H).¹³C NMR (50 MHz, CDCl₃): δ = 14.1, 18.3, 20.7, 102.4, 106.3, 110.6, 112.4, 121.4, 121.4, 126.1, 129.3, 132.0, 137.2, 139.6, 151.6.MS (DEI): *m/z* (%) = 251 (100, [M⁺]), 236 (98, [M⁺ – Me]), 222 (17, [M⁺ – Et]), 208 (17, [M⁺ – C₃H₇]), 91 (8, [C₇H₇⁺]).HRMS: *m/z* calcd for C₁₇H₁₇NO: 251.13101; found: 251.13079, Δ = 0.22 mmu.**N-Cyclohexyl-3-ethyl-3-furyl-1,3-dihydropyrrol-2-one (4fd)**

Yield: 155 mg (60%); eluent: EtOH.

IR (neat): 2932 (m), 2855 (w), 1967 (w), 1694 (s), 1605 (m), 1450 (m), 1381 (m), 1254 (m), 1011 (s), 730 (vs), 694 cm⁻¹ (s).¹H NMR (200 MHz, CDCl₃): δ = 0.79 (t, *J* = 7.4 Hz, 3 H), 1.12–1.80 (m, 10 H), 2.00 (q, *J* = 7.4 Hz, 2 H), 3.87–3.94 (m, 1 H), 5.43 (d, *J* = 5.0 Hz, 1 H), 6.15 (dd, *J* = 0.8, 3.2 Hz, 1 H), 6.26 (dd, *J* = 2.0, 3.2 Hz, 1 H), 6.59 (d, *J* = 5.0 Hz, 1 H), 7.31 (dd, *J* = 1.0, 1.8 Hz, 1 H).¹³C NMR (50 MHz, CDCl₃): δ = 8.6, 25.4, 28.5, 31.8, 32.1, 50.5, 55.9, 105.7, 110.1, 111.2, 129.4, 142.0, 152.9, 177.0.MS (DEI): *m/z* (%) = 259 (100, [M⁺]), 230 (44, [M⁺ – Et]), 177 (21, [M⁺ – C₆H₁₀]), 148 (62, [M⁺ – C₆H₁₁ – C₂H₄]), 120 (7, [M⁺ – C₆H₁₁ – C₂H₄ – CO]).HRMS: *m/z* calcd for C₁₆H₂₁NO₂: 259.15723; found: 259.15696, Δ = 0.27 mmu.**N-Cyclohexyl-2-ethyl-3-furylpyrrole (5fd)**Yield: 90 mg (37%); eluent: light petroleum–CH₂Cl₂ (70:30).¹H NMR (200 MHz, CDCl₃): δ = 1.20 (t, *J* = 7.4 Hz, 3 H), 1.39–2.02 (m, 10 H), 2.84 (q, *J* = 7.4 Hz, 2 H), 3.80–3.85 (m, 1 H), 6.18 (dd, *J* = 0.8, 3.4 Hz, 1 H), 6.35 (d, *J* = 3.0 Hz, 1 H), 6.39 (dd, *J* = 1.8, 3.4 Hz, 1 H), 6.65 (d, *J* = 3.0 Hz, 1 H), 7.35 (dd, *J* = 0.8, 1.8 Hz, 1 H).¹³C NMR (50 MHz, CDCl₃): δ = 14.9, 18.3, 25.5, 26.1, 34.8, 54.8, 102.2, 105.9, 110.8, 111.2, 116.1, 130.8, 139.6, 152.3.MS (DEI): *m/z* (%) = 243 (100, [M⁺]), 228 (35, [M⁺ – Me]), 214 (5, [M⁺ – Et]), 161 (9, [M⁺ – C₆H₁₀]), 146 (30, [M⁺ – C₆H₁₁ – Me]).HRMS: *m/z* calcd for C₁₆H₂₁NO: 243.16231; found: 243.16212, Δ = 0.19 mmu.**N-Butyl-3-ethyl-3-furyl-1,3-dihydropyrrol-2-one (4ff)**

Yield: 140 mg (60%); eluent: EtOH.

IR (neat): 2959 (m), 2920 (m), 2851 (m), 1701 (w), 1462 (m), 1377 (w), 1258 (vs), 1080 (s), 1015 (vs), 864 (m), 794 (vs), 729 cm⁻¹ (m).¹H NMR (200 MHz, CDCl₃): δ = 0.85 (t, *J* = 7.2 Hz, 3 H), 0.89 (t, *J* = 7.2 Hz, 3 H), 1.24–1.29 (m, 2 H), 1.49–1.55 (m, 2 H), 2.02 (q, *J* = 7.2 Hz, 2 H), 3.35–3.42 (m, 2 H), 5.45 (d, *J* = 5.0 Hz, 1 H), 6.15 (dd, *J* = 0.8, 3.2 Hz, 1 H), 6.26 (dd, *J* = 1.8, 3.2 Hz, 1 H), 6.49 (d, *J* = 5.0 Hz, 1 H), 7.31 (dd, *J* = 0.8, 1.8 Hz, 1 H).¹³C NMR (50 MHz, CDCl₃): δ = 8.7, 13.6, 19.8, 28.5, 30.9, 41.7, 55.6, 105.7, 110.1, 111.2, 132.3, 142.0, 152.8, 177.5.MS (DEI): *m/z* (%) = 233 (93, [M⁺]), 204 (86, [M⁺ – Et]), 190 (11, [M⁺ – C₃H₇]), 162 (39, [M⁺ – C₃H₇ – CO]), 151 (100, [M⁺ – C₄H₃O – Me]), 148 (26, [M⁺ – C₆H₁₃]).

HRMS: *m/z* calcd for C₁₄H₁₉NO₂: 233.14158; found: 233.14188, Δ = 0.30 mmu.

N-Butyl-2-ethyl-3-furylpyrrole (5ff)

Yield: 79 mg (36%); eluent: light petroleum–CH₂Cl₂ (80:20).

¹H NMR (200 MHz, CDCl₃): δ = 0.96 (t, *J* = 7.4 Hz, 3 H), 1.21 (t, *J* = 7.4 Hz, 3 H), 1.34–1.43 (m, 2 H), 1.70–1.78 (m, 2 H), 2.82 (q, *J* = 7.4 Hz, 2 H), 3.82 (t, *J* = 7.4 Hz, 2 H), 6.19 (dd, *J* = 0.8, 3.4 Hz, 1 H), 6.33 (d, *J* = 3.0 Hz, 1 H), 6.40 (dd, *J* = 1.8, 3.4 Hz, 1 H), 6.55 (d, *J* = 3.0 Hz, 1 H), 7.36 (dd, *J* = 0.8, 1.8 Hz, 1 H).

¹³C NMR (50 MHz, CDCl₃): δ = 13.7, 14.5, 18.3, 20.0, 33.7, 46.2, 102.1, 105.6, 110.8, 111.8, 119.6, 131.2, 139.6, 152.3.

MS (DEI): *m/z* (%) = 217 (100, [M⁺]), 202 (72, [M⁺ – Me]), 188 (16, [M⁺ – Et]), 174 (7, [M⁺ – C₃H₇]), 160 (18, [M⁺ – C₄H₉]), 146 (14, [M⁺ – C₅H₁₂]).

HRMS: *m/z* calcd for C₁₄H₁₉NO: 217.14666; found: 217.14699, Δ = 0.33 mmu.

N-(4-*tert*-Butylphenyl)-3-ethyl-3-furyl-1,3-dihydropyrrol-2-one (4fg)

Yield: 131 mg (42%); eluent: light petroleum–CH₂Cl₂ (70:30).

IR (neat): 2959 (m), 2928 (m), 2870 (w), 1717 (vs), 1609 (m), 1516 (s), 1462 (m), 1385 (s), 1269 (m), 1211 (s), 1072 (m), 1015 (m), 864 (m), 833 (s), 729 (vs), 702 cm⁻¹ (s).

¹H NMR (200 MHz, CDCl₃): δ = 0.90 (t, *J* = 7.4 Hz, 3 H), 1.30 (s, 9 H), 2.12 (q, *J* = 7.4 Hz, 2 H), 5.64 (d, *J* = 5.0 Hz, 1 H), 6.25 (dd, *J* = 0.8, 3.2 Hz, 1 H), 6.31 (dd, *J* = 1.8, 3.2 Hz, 1 H), 6.95 (d, *J* = 5.0 Hz, 1 H), 7.38 (s, 4 H), 7.36 (dd, *J* = 0.8, 2.0 Hz, 1 H).

¹³C NMR (50 MHz, CDCl₃): δ = 8.7, 29.7, 31.3, 34.5, 56.3, 106.1, 110.2, 112.1, 121.1, 126.0, 132.4, 142.2, 148.8, 152.4, 176.0.

MS (DEI): *m/z* (%) = 309 (100, [M⁺]), 294 (12, [M⁺ – Me]), 280 (46, [M⁺ – Et]), 266 (7, [M⁺ – C₃H₇]), 252 (17, [M⁺ – CO – Et]), 133 (4, [C₁₀H₁₃⁺]), 57 (14, [C₄H₉⁺]).

HRMS: *m/z* calcd for C₂₀H₂₃NO: 309.17288; found: 309.17227, Δ = 0.61 mmu.

N-(4-*tert*-Butylphenyl)-2-ethyl-3-furylpyrrole (5fg)

Yield: 121 mg (41%); eluent: light petroleum–CH₂Cl₂ (70:30).

¹H NMR (200 MHz, CDCl₃): δ = 1.08 (t, *J* = 7.4 Hz, 3 H), 1.38 (s, 9 H), 2.79 (q, *J* = 7.4 Hz, 2 H), 6.28 (dd, *J* = 0.8, 3.2 Hz, 1 H), 6.44 (dd, *J* = 1.8, 3.2 Hz, 1 H), 6.48 (d, *J* = 3.0 Hz, 1 H), 6.69 (d, *J* = 3.0 Hz, 1 H), 7.25 (d, *J* = 8.8 Hz, 2 H), 7.40 (dd, *J* = 0.8, 1.8 Hz, 1 H), 7.47 (d, *J* = 8.8 Hz, 2 H).

¹³C NMR (50 MHz, CDCl₃): δ = 14.5, 18.6, 31.4, 34.7, 102.7, 106.6, 110.9, 112.8, 121.7, 126.0, 126.1, 132.4, 137.4, 139.9, 150.6, 151.9.

MS (DEI): *m/z* (%) = 293 (100, [M⁺]), 278 (71, [M⁺ – Me]), 222 (15, [M⁺ – C₅H₁₁]).

HRMS: *m/z* calcd for C₂₀H₂₃NO: 293.17796; 293.17873, Δ = 0.77 mmu.

N-*sec*-Butyl-3-ethyl-3-furyl-1,3-dihydropyrrol-2-one (4fh)

Yield: 134 mg (57%); eluent: EtOH.

IR (neat): 2967 (w), 2936 (w), 2878 (vw), 2045 (w), 1971 (w), 1695 (vs), 1609 (m), 1462 (m), 1377 (s), 1254 (s), 1219 (s), 1011 (s), 802 (m), 735 cm⁻¹ (vs).

¹H NMR (200 MHz, CDCl₃): δ = 0.77–0.86 (m, 6 H), 1.15 (d, *J* = 2.1 Hz, 1.5 H), 1.19 (d, *J* = 2.1 Hz, 1.5 H), 1.53 (m, 2 H), 2.02 (q, *J* = 7.4 Hz, 2 H), 4.07 (m, 1 H), 5.46 (d, *J* = 2.4 Hz, 0.5 H), 5.47 (d, *J* = 2.4 Hz, 0.5 H), 6.14 (m, 1 H), 6.26 (m, 1 H), 6.54 (d, *J* = 5.0 Hz, 1 H), 7.13 (t, *J* = 0.8 Hz, 1 H).

¹³C NMR (50 MHz, CDCl₃): δ = 8.6, 8.9, 10.6, 10.8, 19.4, 19.7, 28.3, 28.4, 28.6, 48.4, 48.6, 56.0, 56.1, 105.7, 110.1, 111.5, 111.7, 128.7, 128.9, 142.0, 153.0, 177.4.

MS (DEI): *m/z* (%) = 233 (100, [M⁺]), 204 (75, [M⁺ – Et]), 190 (3, [M⁺ – C₃H₇]), 176 (15, [M⁺ – C₄H₉]), 148 (24, [M⁺ – C₄H₉ – CO]), 57 (3, [C₄H₉⁺]).

HRMS: *m/z* calcd for C₁₄H₁₉NO₂: 233.14158; found: 233.14174, Δ = 0.16 mmu.

N-*sec*-Butyl-2-ethyl-3-furylpyrrole (5fh)

Yield: 82 mg (38%); eluent: light petroleum–CH₂Cl₂ (70:30).

¹H NMR (200 MHz, CDCl₃): δ = 0.84 (t, *J* = 7.4 Hz, 3 H), 1.19 (t, *J* = 7.4 Hz, 3 H), 1.40 (d, *J* = 6.8 Hz, 2 H), 1.76 (t, *J* = 7.4 Hz, 3 H), 2.83 (q, *J* = 7.4 Hz, 2 H), 4.01 (q, *J* = 7.0 Hz, 1 H), 6.18 (dd, *J* = 0.8, 3.4 Hz, 1 H), 6.37 (d, *J* = 3.0 Hz, 1 H), 6.39 (dd, *J* = 1.8, 3.4 Hz, 1 H), 6.60 (d, *J* = 3.0 Hz, 1 H), 7.35 (dd, *J* = 0.8, 1.8 Hz, 1 H).

¹³C NMR (50 MHz, CDCl₃): δ = 10.9, 14.8, 18.2, 22.3, 30.9, 52.4, 102.1, 106.2, 110.8, 111.1, 115.3, 131.3, 139.6, 152.4.

MS (DEI): *m/z* (%) = 217 (100, [M⁺]), 202 (50, [M⁺ – Me]), 188 (10, [M⁺ – Et]), 146 (31, [M⁺ – C₅H₁₁]), 57 (6, [C₄H₉⁺]).

HRMS: *m/z* calcd for C₁₄H₁₉NO: 217.14666; found: 217.14709, Δ = 0.43 mmu.

N-Benzyl-3-ethyl-3-(3-pyridyl)-1,3-dihydropyrrol-2-one (4ga)

Yield: 163 mg (59%); eluent: EtOH.

IR (neat): 2967 (w), 2932 (w), 2874 (w), 1670 (m), 1420 (m), 1261 (m), 1026 (m), 806 (m), 748 (s), 698 cm⁻¹ (vs).

¹H NMR (400 MHz, CDCl₃): δ = 0.81 (t, *J* = 7.6 Hz, 3 H), 2.05 (q, *J* = 7.6 Hz, 2 H), 4.59 (AB spin system, *J* = 15.2, 53.9 Hz, 2 H), 5.64 (d, *J* = 5.2 Hz, 1 H), 6.49 (d, *J* = 5.2 Hz, 1 H), 7.17–7.30 (m, 5 H), 7.91–8.60 (m, 4 H).

¹³C NMR (100 MHz, CDCl₃): δ = 9.2, 31.5, 45.8, 56.7, 112.0, 123.5, 127.8, 128.3, 128.7, 131.9, 134.5, 135.7, 136.4, 148.3, 148.4, 178.9.

MS (DEI): *m/z* (%) = 278 (25, [M⁺]), 249 (25, [M⁺ – Et]), 221 (2, [M⁺ – Et – CO]), 91 (100, [C₇H₇⁺]), 77 (7, [Ph⁺]).

HRMS: *m/z* calcd for C₁₈H₁₈N₂O: 278.14191; found: 278.14185, Δ = 0.06 mmu.

N-Benzyl-2-ethyl-3-(3-pyridyl)pyrrole (5ga)

Yield: 91 mg (35%); eluent: light petroleum–CH₂Cl₂ (40:60).

¹H NMR (400 MHz, CDCl₃): δ = 1.15 (t, *J* = 7.6 Hz, 3 H), 2.65 (q, *J* = 7.6 Hz, 2 H), 5.10 (s, 2 H), 6.31 (d, *J* = 2.8 Hz, 1 H), 6.64 (d, *J* = 2.8 Hz, 1 H), 7.03–7.33 (m, 5 H), 7.25–8.67 (m, 4 H).

¹³C NMR (100 MHz, CDCl₃): δ = 15.1, 17.9, 50.5, 107.9, 121.3, 126.4, 127.6, 127.9, 128.3, 128.8, 132.0, 133.6, 134.7, 138.1, 146.4, 148.9.

MS (DEI): *m/z* (%) = 262 (100, [M⁺]), 247 (50, [M⁺ – Me]), 234 (3, [M⁺ – C₂H₄]), 91 (47, [C₇H₇⁺]).

HRMS: *m/z* calcd for C₁₈H₁₈N₂: 262.14700; found: 262.14649, Δ = 0.51 mmu.

3-Ethyl-3-(3-pyridyl)-N-phenyl-1,3-dihydropyrrol-2-one (4gb)

Yield: 146 mg (55%); eluent: EtOH.

IR (neat): 2963 (vw), 2928 (vw), 1705 (w), 1597 (m), 1497 (s), 1385 (m), 1026 (m), 806 (m), 752 (s), 691 cm⁻¹ (vs).

¹H NMR (200 MHz, CDCl₃): δ = 0.89 (t, *J* = 7.4 Hz, 3 H), 2.11 (q, *J* = 7.4 Hz, 2 H), 5.84 (d, *J* = 5.2 Hz, 1 H), 7.04 (d, *J* = 5.2 Hz, 1 H), 7.28–7.47 (m, 5 H), 7.28–7.47 (m, 1 H), 7.96 (dt, *J* = 2.0, 8.0 Hz, 1 H), 8.44–8.51 (m, 1 H), 8.63–8.70 (m, 1 H).

¹³C NMR (50 MHz, CDCl₃): δ = 9.1, 31.9, 57.5, 112.7, 121.5, 123.5, 126.0, 129.2, 132.3, 134.6, 136.7, 140.2, 148.2, 148.5, 177.5. MS (DEI): *m/z* (%) = 264 (91, [M⁺]), 235 (100 [M⁺ – Et]), 77 (19, [Ph⁺]). HRMS: *m/z* calcd for C₁₇H₁₆N₂O: 264.12626; found: 264.12627, Δ = 0.01 mmu.

2-Ethyl-N-phenyl-3-(3-pyridyl)pyrrole (5gb)

Yield: 111 mg (45%); eluent: light petroleum–CH₂Cl₂ (50:50).

¹H NMR (200 MHz, CDCl₃): δ = 0.86 (t, *J* = 7.4 Hz, 3 H), 2.72 (q, *J* = 7.4 Hz, 2 H), 6.37 (d, *J* = 3.0 Hz, 1 H), 6.77 (d, *J* = 3.0 Hz, 1 H), 7.32–7.53 (m, 5 H), 7.70 (m, 2 H), 8.38–8.45 (m, 1 H), 8.62–8.67 (m, 1 H).

¹³C NMR (50 MHz, CDCl₃): δ = 14.1, 18.1, 108.6, 122.2, 126.6, 127.7, 128.8, 129.2, 129.8, 130.9, 132.5, 135.0, 140.1, 146.6, 149.1.

MS (DEI): *m/z* (%) = 248 (100, [M⁺]), 233 (47, [M⁺ – Me]), 77 (7, [C₆H₇⁺]).

HRMS: *m/z* calcd for C₁₇H₁₆N₂: 248.13135; found: 248.13104, Δ = 0.31 mmu.

3-Ethyl-3-(3-pyridyl)-N-*p*-tolyl-1,3-dihydropyrrol-2-one (4gc)

Yield: 98 mg (35%); eluent: EtOH.

IR (neat): 2955 (w), 2920 (m), 2851 (w), 1709 (s), 1512 (vs), 1385 (s), 1026 (s), 810 (vs), 714 cm⁻¹ (vs).

¹H NMR (200 MHz, CDCl₃): δ = 0.88 (t, *J* = 7.4 Hz, 3 H), 2.05–2.14 (m, 2 H), 2.32 (s, 3 H), 5.82 (d, *J* = 5.0 Hz, 1 H), 6.99 (d, *J* = 5.0 Hz, 1 H), 7.17 (d, *J* = 8.4 Hz, 2 H), 7.31 (d, *J* = 8.4 Hz, 2 H), 7.51–7.60 (m, 1 H), 7.96 (dt, *J* = 2.0, 8.4 Hz, 1 H), 8.45–8.51 (m, 1 H), 8.62–8.69 (m, 1 H).

¹³C NMR (150 MHz, CDCl₃): δ = 9.2, 20.9, 31.9, 57.4, 112.5, 121.6, 123.5, 129.7, 132.1, 132.6, 134.2, 134.6, 135.9, 148.3, 148.5, 177.5.

MS (DEI): *m/z* (%) = 278 (100, [M⁺]), 249 (87, [M⁺ – Et]), 221 (15, [M⁺ – Et – CO]), 91 (10, [C₇H₇⁺]).

HRMS: *m/z* calcd for C₁₈H₁₈N₂O: 278.14191; found: 278.14141, Δ = 0.50 mmu.

2-Ethyl-3-(3-pyridyl)-N-*p*-tolylpyrrole (5gc)

Yield: 142 mg (54%); eluent: CH₂Cl₂.

¹H NMR (200 MHz, CDCl₃): δ = 0.90 (t, *J* = 7.4 Hz, 3 H), 2.41 (s, 3 H), 2.70 (q, *J* = 7.4 Hz, 2 H), 6.35 (d, *J* = 3.0 Hz, 1 H), 6.73 (d, *J* = 3.0 Hz, 1 H), 7.03–7.38 (m, 4 H), 7.72 (dt, *J* = 2.0, 8.0 Hz, 1 H), 8.34–8.71 (m, 3 H).

¹³C NMR (50 MHz, CDCl₃): δ = 14.7, 18.1, 21.1, 108.3, 118.6, 120.8, 122.3, 123.3, 126.5, 129.7, 130.3, 132.6, 134.9, 137.7, 146.5, 149.1.

MS (DEI): *m/z* (%) = 262 (100, [M⁺]), 247 (53, [M⁺ – Me]), 91 (4, [C₇H₇⁺]).

HRMS: *m/z* calcd for C₁₈H₁₈N₂: 262.14700; found: 262.14701, Δ = 0.01 mmu.

N-Cyclohexyl-3-ethyl-3-(3-pyridyl)-1,3-dihydropyrrol-2-one (4gd)

Yield: 146 mg (54%); eluent: EtOH.

IR (neat): 2932 (m), 2855 (w), 1686 (vs), 1605 (m), 1381 (s), 1254 (s), 1196 (m), 1138 (m), 810 (m), 694 cm⁻¹ (vs).

¹H NMR (200 MHz, CDCl₃): δ = 0.72 (t, *J* = 7.4 Hz, 3 H), 1.24–1.75 (m, 10 H), 1.92 (q, *J* = 7.4 Hz, 2 H), 3.78–3.82 (m, 1 H), 5.54 (d, *J* = 5.0 Hz, 1 H), 6.61 (d, *J* = 5.0 Hz, 1 H), 7.19 (dd, *J* = 4.8, 8.0 Hz, 1 H), 7.81 (dt, *J* = 1.8, 8.0 Hz, 1 H), 8.37 (d, *J* = 3.6 Hz, 1 H), 8.68 (d, *J* = 1.8 Hz, 1 H).

¹³C NMR (50 MHz, CDCl₃): δ = 8.57, 24.86, 25.03, 31.3, 31.7, 50.3, 56.7, 111.3, 123.0, 129.1, 134.1, 135.7, 147.8, 178.0.

MS (DEI): *m/z* (%) = 270 (100, [M⁺]), 255 (2, [M⁺ – Me]), 241 (48, [M⁺ – Et]), 188 (17, [M⁺ – C₆H₁₀]), 84 (10, [C₆H₁₂⁺]).

HRMS: *m/z* calcd for C₁₇H₂₂N₂O: 270.17321; found: 270.17314, Δ = 0.07 mmu.

N-Cyclohexyl-2-ethyl-3-(3-pyridyl)pyrrole (5gd)

Yield: 52 mg (20%); eluent: CH₂Cl₂.

¹H NMR (200 MHz, CDCl₃): δ = 1.12 (t, *J* = 7.6 Hz, 3 H), 1.30–2.03 (m, 10 H), 2.70 (q, *J* = 7.6 Hz, 2 H), 3.78–3.85 (m, 1 H), 6.25 (d, *J* = 3.0 Hz, 1 H), 6.72 (d, *J* = 3.0 Hz, 1 H), 7.20–7.26 (m, 1 H), 7.63 (dt, *J* = 2.0, 8.0 Hz, 1 H), 8.35–8.42 (m, 1 H), 8.60–8.65 (m, 1 H).

¹³C NMR (50 MHz, CDCl₃): δ = 15.6, 17.8, 25.4, 26.1, 34.9, 55.1, 107.6, 116.5, 117.1, 123.2, 128.7, 133.5, 134.9, 146.2, 149.0.

MS (DEI): *m/z* (%) = 254 (100, [M⁺]), 239 (13, [M⁺ – Me]), 156 (10, [M⁺ – C₇H₁₄]), 29 (18, [Et⁺]).

HRMS: *m/z* calcd for C₁₇H₂₂N₂: 254.17830; found: 254.17875, Δ = 0.45 mmu.

N-Butyl-3-ethyl-3-(3-pyridyl)-1,3-dihydropyrrol-2-one (4gf)

Yield: 133 mg (54%); eluent: EtOH.

IR (neat): 2959 (m), 2932 (m), 2874 (w), 1694 (vs), 1670 (vs), 1655 (vs), 1547 (m), 1416 (m), 1373 (m), 1261 (m), 1026 (m), 806 (s), 714 cm⁻¹ (vs).

¹H NMR (200 MHz, CDCl₃): δ = 0.79 (t, *J* = 7.4 Hz, 1.5 H), 0.88 (t, *J* = 7.2 Hz, 1.5 H), 0.89 (t, *J* = 7.2 Hz, 1.5 H), 1.12 (t, *J* = 7.6 Hz, 1.5 H), 1.24–1.31 (m, 2 H), 1.44–1.50 (m, 2 H), 1.98 (q, *J* = 7.4 Hz, 1 H), 2.16 (q, *J* = 7.6 Hz, 1 H), 3.18–3.24 (m, 1 H), 3.34–3.42 (m, 1 H), 5.63 (d, *J* = 5.0 Hz, 1 H), 6.57 (d, *J* = 5.0 Hz, 1 H), 7.22 (q, *J* = 4.8 Hz, 1 H), 7.89 (dt, *J* = 2.0, 8.0 Hz, 1 H), 8.39–8.43 (m, 1 H), 8.52–8.59 (m, 1 H).

¹³C NMR (50 MHz, CDCl₃): δ = 9.1, 9.9, 13.6, 13.7, 19.8, 20.0, 29.8, 30.9, 31.4, 31.7, 39.2, 41.8, 56.8, 111.6, 123.5, 132.4, 134.6, 136.5, 148.2, 178.9.

MS (DEI): *m/z* (%) = 245 (100, [M⁺ + 1]), 244 (68, [M⁺]), 215 (41, [M⁺ – Et]), 201 (4, [M⁺ – C₃H₇]), 173 (23, [M⁺ – C₅H₁₁]), 27 (60, [Et⁺]).

HRMS: *m/z* calcd for C₁₅H₂₀N₂O: 244.15756; found: 244.15759, Δ = 0.03 mmu.

N-Butyl-2-ethyl-3-(3-pyridyl)pyrrole (5gf)

Yield: 72 mg (32%); eluent: light petroleum–CH₂Cl₂ (70:30).

¹H NMR (200 MHz, CDCl₃): δ = 0.95 (t, *J* = 7.2 Hz, 3 H), 1.20 (t, *J* = 7.4 Hz, 3 H), 1.40 (q, *J* = 7.2 Hz, 2 H), 1.68–1.75 (m, 2 H), 2.69 (q, *J* = 7.4 Hz, 2 H), 3.83 (t, *J* = 7.2 Hz, 2 H), 6.22 (d, *J* = 2.8 Hz, 1 H), 6.63 (d, *J* = 2.8 Hz, 1 H), 7.50 (dd, *J* = 3.2, 5.8 Hz, 1 H), 7.64 (dt, *J* = 2.0, 8.0 Hz, 1 H), 8.34–8.41 (m, 1 H), 8.56–8.63 (m, 1 H).

¹³C NMR (50 MHz, CDCl₃): δ = 13.8, 15.2, 17.8, 20.1, 33.7, 46.4, 107.4, 119.9, 123.1, 123.6, 128.8, 130.9, 134.8, 146.0, 148.8.

MS (DEI): *m/z* (%) = 228 (100, [M⁺]), 213 (19, [M⁺ – Me]), 185 (7, [M⁺ – C₃H₇]), 157 (8, [M⁺ – C₅H₁₁]), 149 (14, [M⁺ – C₅H₅N]), 57 (6, [C₄H₉⁺]), 29 (20, [Et⁺]).

HRMS: *m/z* calcd for C₁₅H₂₀N₂: 228.16265; found: 228.16302, Δ = 0.37 mmu.

N-(4-*tert*-Butylphenyl)-3-ethyl-3-(3-pyridyl)-1,3-dihydropyrrol-2-one (4gg)

Yield: 204 mg (64%); eluent: EtOH.

IR (neat): 2920 (vs), 2851 (s), 1709 (w), 1462 (m), 1261 (w), 1022 (w), 802 (m), 718 cm⁻¹ (w).

¹H NMR (200 MHz, CDCl₃): δ = 0.88 (t, *J* = 7.4 Hz, 3 H), 1.29 (s, 9 H), 2.10 (q, *J* = 7.4 Hz, 2 H), 5.81 (d, *J* = 5.0 Hz, 1 H), 7.01 (d, *J* = 5.0 Hz, 1 H), 7.33–7.43 (m, 4 H), 7.50 (dd, *J* = 3.4, 5.8 Hz, 1 H), 7.96 (dt, *J* = 1.8, 8.0 Hz, 1 H), 8.47–8.52 (m, 1 H), 8.59–8.64 (m, 1 H).

¹³C NMR (50 MHz, CDCl₃): δ = 9.1, 31.3, 31.8, 34.5, 57.4, 112.6, 121.2, 123.3, 126.1, 130.9, 132.5, 134.1, 134.6, 148.3, 148.5, 149.1, 177.7.

MS (DEI): *m/z* (%) = 320 (100, [M⁺]), 305 (42, [M⁺ – Me]), 291 (61, [M⁺ – Et]), 277 (22, [M⁺ – C₃H₇]), 134 (95, [C₁₀H₁₄⁺]), 57 (14, [C₄H₉⁺]).

HRMS: *m/z* calcd for C₂₁H₂₄N₂O: 320.18886; found: 320.18865, Δ = 0.21 mmu.

N-(4-tert-Butylphenyl)-2-ethyl-3-(3-pyridyl)pyrrole (5gg)

Yield: 93 mg (31%); eluent: CH₂Cl₂.

¹H NMR (200 MHz, CDCl₃): δ = 0.94 (t, *J* = 7.4 Hz, 3 H), 1.36 (s, 9 H), 2.72 (q, *J* = 7.4 Hz, 2 H), 5.35 (d, *J* = 3.0 Hz, 1 H), 6.75 (d, *J* = 3.0 Hz, 1 H), 6.95–7.03 (m, 2 H), 7.32–7.39 (m, 2 H), 7.37–7.43 (m, 1 H), 8.32–8.38 (m, 1 H), 8.54–8.67 (m, 2 H).

¹³C NMR (150 MHz, CDCl₃): δ = 14.1, 19.2, 31.3, 34.4, 108.3, 114.9, 119.4, 122.3, 126.3, 128.9, 132.4, 130.9, 134.1, 134.9, 146.5, 148.0, 148.7.

MS (DEI): *m/z* (%) = 304 (100, [M⁺]), 289 (68, [M⁺ – Me]), 233 (21, [M⁺ – C₅H₁₁]), 57 (14, [C₄H₉⁺]).

HRMS: *m/z* calcd for C₂₁H₂₄N₂: 304.19395; found: 304.19406, Δ = 0.11 mmu.

N-sec-Butyl-3-ethyl-3-(3-pyridyl)-1,3-dihydropyrrol-2-one (4gh)

Yield: 98 mg (40%); eluent: EtOH.

IR (neat): 2967 (w), 2932 (vw), 2878 (vw), 1694 (vs), 1609 (m), 1458 (m), 1381 (s), 1258 (s), 1219 (s), 1026 (m), 910 (m), 806 (m), 714 cm⁻¹ (vs).

¹H NMR (200 MHz, CDCl₃): δ = 0.66–0.86 (m, 6 H), 1.10 (d, *J* = 6.8 Hz, 1.5 H), 1.15 (d, *J* = 6.8 Hz, 1.5 H), 1.44–1.51 (m, 2 H), 1.96 (q, *J* = 7.4 Hz, 2 H), 3.96–4.08 (m, 1 H), 5.59 (d, *J* = 3.0 Hz, 0.5 H), 5.62 (d, *J* = 3.0 Hz, 0.5 H), 6.59 (d, *J* = 5.2 Hz, 1 H), 7.19 (q, *J* = 4.8 Hz, 1 H), 7.79–7.83 (m, 1 H), 8.41 (dd, *J* = 1.4, 4.8 Hz, 1 H), 8.54 (d, *J* = 2.2 Hz, 1 H).

¹³C NMR (100 MHz, CDCl₃): δ = 8.9, 9.2, 10.6, 10.7, 19.4, 19.5, 28.3, 28.4, 31.1, 31.2, 48.6, 48.6, 57.1, 57.2, 111.9, 112.0, 123.4, 128.8, 128.9, 134.3, 134.4, 135.9, 136.0, 148.2, 178.6.

MS (DEI): *m/z* (%) = 244 (100, [M⁺]), 229 (3, [M⁺ – Me]), 215 (89, [M⁺ – Et]), 201 (2, [M⁺ – C₃H₇]), 187 (24, [M⁺ – C₄H₉]), 173 (6, [M⁺ – C₅H₁₁]), 159 (76, [M⁺ – C₆H₁₃]), 57 (8, [C₄H₉⁺]).

HRMS: *m/z* calcd for C₁₅H₂₀N₂O: 244.15756; found: 244.15763, Δ = 0.07 mmu.

N-sec-Butyl-2-ethyl-3-(3-pyridyl)pyrrole (5gh)

Yield: 97 mg (43%); eluent: CH₂Cl₂.

¹H NMR (200 MHz, CDCl₃): δ = 0.84 (t, *J* = 7.4 Hz, 3 H), 1.22 (t, *J* = 7.4 Hz, 3 H), 1.42 (d, *J* = 6.8 Hz, 3 H), 1.77 (q, *J* = 7.4 Hz, 2 H), 2.69 (q, *J* = 7.6 Hz, 2 H), 4.02 (q, *J* = 6.8 Hz, 1 H), 6.27 (d, *J* = 3.0 Hz, 1 H), 6.67 (d, *J* = 3.0 Hz, 1 H), 7.24 (dq, *J* = 0.8, 4.8 Hz, 1 H), 7.64 (dt, *J* = 2.0, 7.8 Hz, 1 H), 8.39 (dd, *J* = 1.6, 4.8 Hz, 1 H), 8.63 (dd, *J* = 0.8, 2.2 Hz, 1 H).

¹³C NMR (100 MHz, CDCl₃): δ = 11.0, 15.5, 17.7, 22.3, 31.1, 52.7, 107.8, 115.7, 116.9, 123.2, 131.4, 133.5, 134.9, 146.1, 149.0.

MS (DEI): *m/z* (%) = 228 (100, [M⁺]), 213 (78, [M⁺ – Me]), 199 (24, [M⁺ – Et]), 157 (41, [M⁺ – C₅H₁₁]).

HRMS: *m/z* calcd for C₁₅H₂₀N₂: 228.16265; found: 228.16293, Δ = 0.28 mmu.

Acknowledgment

The authors gratefully thank the Deutsche Bundesstiftung Umwelt (DBU) for financial support.

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