Supporting Information

I$_2$-Catalyzed One-pot Synthesis of Pyrrolo[1,2-a]quinoxaline and Imidazo[1,5-a]quinoxaline Derivatives via sp$^3$ and sp$^2$ C-H Cross-Dehydrogenative Coupling

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Table of Contents

1. General information………………………………………………………………………………S2
2. Preparation of starting material……………………………………………………………S2
3. General experimental procedures for the synthesis of Pyrrolo[1,2-a]quinoxaline and Imidazo[1,5-a]quinoxaline 4…………………………………………………………… S3
4. Spectra data……………………………………………………………………………………S4
5. References……………………………………………………………………………………S12
6. $^1$H NMR and $^{13}$C NMR spectra……………………………………………………………S13
1. General information

2-(1H-pyrrol-1-yl)aniline, 2-(1H-indol-1-yl)aniline and 2-(1H-imidazol-1-yl)aniline were prepared according to literature procedures. Other reagents were commercially available and were used without further purification. All reactions were monitored by thin-layer chromatography (TLC). \(^1\)H NMR spectra were recorded on a Bruker Avance 300 spectrometer at 300 MHz, using CDCl\(_3\), CD\(_2\)Cl\(_2\) and DMSO-\(d_6\) as solvent and tetramethylsilane (TMS) as internal standard. \(^13\)C NMR spectra were run in the same instrument at 75 MHz. HRMS spectra were determined on a Q-TOF6510 spectrograph (Agilent).

2. Preparation of starting material

2.1 General procedure for preparation of 1-(2-nitrophenyl)-1H-pyrrole IV

\[
\begin{align*}
\text{I} \quad &+ \quad \text{AcOH} \\
\rightarrow \quad &\text{IV}
\end{align*}
\]

A mixture of \(\alpha\)-nitroaniline I (10.00 mmol) and 2,5-dimethoxytetrahydrofuran (10.00 mmol) in acetic acid was refluxed for 1 h with vigorous stirring. The reaction mixture was cooled to ambient temperature and then poured into water. The precipitate was filtered and washed with water. The precipitate thus obtained was dissolved in ethyl acetate, dried over MgSO\(_4\) and evaporated to dryness under reduced pressure. The residue thus obtained was filtered through a short pad of silica gel, using hexane/ethyl acetate as eluent, to afford compound IV which were directly used for next step without further purification.

2.2 General procedure for preparation of 1-(2-nitrophenyl)-1H-indole V and 1-(2-nitrophenyl)-1H-imidazole VI

\[
\begin{align*}
\text{F} \quad &+ \quad \text{NaOH} \\
\rightarrow \quad &\text{V or VI}
\end{align*}
\]

To a well-stirred solution of N-heterocycle (1.0 mmol) in DMSO (1.0 mL), NaOH (1.0 equiv.) and 1-fluoro-2-nitrobenzene (1.0 mmol) were added slowly. The reaction mixture was
stirred vigorously for 1–1.5 h at room temperature until no more starting material was detectable by TLC analysis. The reaction mixture was extracted with ethyl acetate and water and dried with MgSO₄. The solvent was evaporated in vacuo and the solid obtained was purified by column chromatography (petroleum ether/ethyl acetate) on silica gel to afford V or VI which were directly used for next step without further purification.

2.3 General procedure for preparation of 2-(1H-N-heterocyc-1-yl)aniline 2

A mixture of iron powder (38.2 mmol), NH₄Cl (5.1 mmol) in H₂O (10 mL) was heated to 100 °C for 15 min. Then the mixture was added in substituted nitrobenzene IV, V or VI (10.0 mmol), and stirred for corresponding time (TLC monitored). Then the mixture was cooled to room temperature and neutralized with 5% NaHCO₃ solution(V/V) and extracted with ethyl acetate (4 × 30 mL) and dried with MgSO₄. The solvent was evaporated in vacuo and the solid obtained was purified by column chromatography (petroleum ether/ethyl acetate) on silica gel to afford 2 with good yields.

3. General experimental procedures for the synthesis of Pyrrolo[1,2-a]quinoxaline and Imidazo[1,5-a]quinoxaline 3

A mixture of arylethanone 1 (0.5 mmol), I₂ (0.1 mmol) in DMSO (2 mL) was heated to 120 °C (TLC monitored). Then the mixture was added in substituted aniline 2 (0.5 mmol), and stirred for corresponding time (TLC monitored). Then the mixture was cooled to room temperature and diluted with water (30 mL) and extracted with dichloromethane twice (2 × 30 mL). The extract was washed with 10% Na₂S₂O₃ solution(V/V), dried over anhydrous MgSO₄ and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel to afford 3.
4. Spectra data

Phenyl(pyrrrolo[1,2-a]quinoxalin-4-yl)methanone 3aa

The title compound 3aa was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether : ethyl acetate : dichloromethane = 8 : 1 : 1 gave 3aa as a Yellow solid (0.118 g, 87%). $^1$H NMR (300 M, DMSO-d$_6$): $\delta$ 8.64 (1H, $J = 1.2, 2.7$ Hz, dd), 8.41 (1H, $J = 0.9, 8.4$ Hz, dd), 8.07-8.04 (2H, m), 7.96 (1H, $J = 1.5, 8.1$ Hz, dd), 7.77-7.71 (2H, m), 7.61-7.53 (3H, m), 7.11 (1H, $J = 1.2, 4.2$ Hz, dd); $^{13}$C NMR (75 MHz, DMSO-d$_6$): $\delta$ 192.12, 149.53, 135.48, 134.03, 133.85, 130.45, 130.27, 129.81, 128.56, 127.52, 125.78, 123.36, 116.83, 115.03, 114.87, 108.25; HRMS calcd for C$_{18}$H$_{12}$N$_2$O (M+H)$^+$ 273.1022; found: 273.1009.

(4-Methoxyphenyl)(pyrrrolo[1,2-a]quinoxalin-4-yl)methanone 3ab

The title compound 3ab was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether : ethyl acetate : dichloromethane = 8 : 1 : 1 gave 3ab as a Yellow solid (0.128 g, 85%). $^1$H NMR (300 M, CDCl$_3$): $\delta$ 8.23-8.18 (2H, m), 8.08-8.04 (2H, m), 7.95 (1H, $J = 0.9, 8.1$ Hz, dd), 7.67-7.61 (1H, m), 7.54-7.48 (1H, m), 7.18 (1H, $J = 1.2, 4.2$ Hz, dd), 7.03-6.96 (3H, m), 3.92 (3H, s); $^{13}$C NMR (75 MHz, CDCl$_3$): $\delta$ 190.81, 164.21, 150.76, 134.89, 133.45, 131.01, 129.17, 128.70, 127.97, 125.44, 124.51, 114.79, 114.69, 113.87, 113.76, 108.87, 55.55; HRMS calcd for C$_{19}$H$_{14}$N$_2$O$_2$ (M+H)$^+$ 303.1128; found: 303.1157.

Pyrrolo[1,2-a]quinoxalin-4-yl(p-tolyl)methanone 3ac

The title compound 3ac was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether : ethyl acetate : dichloromethane = 8 : 1 : 1 gave 3ac as a Yellow solid (0.123 g, 86%). $^1$H NMR (300 M, CDCl$_3$): $\delta$ 8.10-8.05 (4H, m), 7.93 (1H, $J = 0.6, 2.1$ Hz, dd), 7.65-7.60 (1H, m), 7.52-7.46 (1H, m), 7.30 (2H, $J = 8.1$ Hz, d), 7.19 (1H, $J = 1.2, 4.2$ Hz, dd), 6.97 (1H, $J = 2.7, 4.2$ Hz, dd); $^{13}$C NMR (75 MHz, CDCl$_3$): $\delta$ 191.74, 150.25, 144.80, 131.68, 131.64, 131.59, 131.48, 131.29, 129.59, 127.99, 127.91, 125.57, 124.35, 115.03, 113.90, 109.34, 21.84; HRMS calcd for C$_{19}$H$_{14}$N$_2$O (M+H)$^+$ 287.1179; found: 287.1174.

Pyrrolo[1,2-a]quinoxalin-4-yl(o-tolyl)methanone 3ad

The title compound 3ad was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether : ethyl acetate : dichloromethane = 8 : 1 : 1 gave 3ad as a Yellow solid (0.123 g, 88%). $^1$H NMR (300 M, CDCl$_3$): $\delta$ 8.03-8.02 (1H, m), 7.97 (1H, $J = 1.2, 8.1$ Hz, d), 7.92 (1H, $J = 8.1$ Hz, d), 7.65-7.58 (2H, m), 7.45 (2H, $J = 7.8$ Hz, t), 7.34-7.31 (2H, m), 7.28-7.23 (1H, m), 6.98 (1H, $J = 3.0, 4.2$ Hz, dd), 2.54 (3H, s); $^{13}$C NMR (75 MHz, CDCl$_3$): $\delta$ 195.79, 150.18, 139.37, 139.33, 136.66, 136.61, 134.86, 131.68, 131.64, 131.59, 131.55, 131.48, 131.29, 129.59, 127.99, 125.40, 125.18, 124.26, 115.05,
(4-Fluorophenyl)(pyrrolo[1,2-a]quinoxalin-4-yl)methanone 3ae

The title compound 3ae was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether : ethyl acetate : dichloromethane = 8 : 1 : 1 gave 3ae as a Yellow solid (0.116 g, 80%). $^1$H NMR (300 MHz, CDCl$_3$): $\delta$ 8.26-8.21 (2H, m), 8.10 (1H, $J$ = 1.5 Hz, d), 8.03-7.93 (2H, m), 7.70-7.65 (1H, m), 7.55-7.50 (1H, m), 7.26-7.19 (3H, m), 7.01-6.99 (1H, m); $^{13}$C NMR (75 MHz, CDCl$_3$): $\delta$ 190.91, 166.41 ($J_{CF}$ = 253.5, d), 149.77, 134.94, 134.06 ($J_{CF}$ = 9, d), 132.87 ($J_{CF}$ = 4, d), 131.20, 130.04, 128.36, 125.92, 124.67, 115.76 ($J_{CF}$ = 21.75, d), 115.50, 115.23, 114.43, 109.30; HRMS calcd for C$_{19}$H$_{14}$N$_2$O (M+H)$^+$ 287.1179; found: 287.1195.

(4-Nitrophenyl)(pyrrolo[1,2-a]quinoxalin-4-yl)methanone 3af

The title compound 3af was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether : ethyl acetate : dichloromethane = 5 : 1 : 1 gave 3af as a Yellow solid (0.130 g, 82%). $^1$H NMR (300 MHz, CDCl$_3$): $\delta$ 8.38-8.32 (4H, m), 8.15 (1H, $J$ = 1.2, 2.7 Hz, dd), 8.05-8.00 (2H, m), 7.75-7.69 (1H, m), 7.58-7.52 (1H, m), 7.45 (1H, $J$ = 0.9, 4.2 Hz, dd), 7.07 (1H, $J$ = 2.7, 3.9 Hz, dd); $^{13}$C NMR (75 MHz, CDCl$_3$): $\delta$ 191.10, 148.11, 141.88, 134.69, 132.34, 131.39, 130.76, 128.48, 126.10, 124.40, 123.52, 115.77, 115.68, 114.54, 109.78; HRMS calcd for C$_{18}$H$_{11}$N$_3$O$_3$ (M+H)$^+$ 318.0873; found: 318.0857.

(2-Fluorophenyl)(pyrrolo[1,2-a]quinoxalin-4-yl)methanone 3ag

The title compound 3ag was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether : ethyl acetate : dichloromethane = 8 : 1 : 1 gave 3ag as a Yellow solid (0.117 g, 81%). $^1$H NMR (300 MHz, CDCl$_3$): $\delta$ 8.04 (1H, $J$ = 0.9, 2.7 Hz, dd), 7.97 (1H, $J$ = 1.5, 2.1 Hz, dd), 7.91 (1H, $J$ = 0.9, 8.1 Hz, dd), 7.88-7.83 (1H, m), 7.64-7.54 (2H, m), 7.48-7.41 (2H, m), 7.33-7.27 (1H, m), 7.17-7.11 (1H, m), 7.00 (1H, $J$ = 2.7, 4.2 Hz, dd); $^{13}$C NMR (75 MHz, CDCl$_3$): $\delta$ 191.71, 161.54 ($J_{CF}$ = 258.8, d), 148.96, 134.78, 134.19 ($J_{CF}$ = 8.3, d), 131.67 ($J_{CF}$ = 2.3, d), 131.26, 129.84, 128.18, 126.29 ($J_{CF}$ = 12.8, d), 125.45, 124.10 ($J_{CF}$ = 3.8, d), 123.67, 116.30 ($J_{CF}$ = 21.8, d), 115.21, 114.79, 113.89, 109.06; HRMS calcd for C$_{18}$H$_{11}$FN$_2$O (M+H)$^+$ 291.0928; found: 291.0935.

(4-Chlorophenyl)(pyrrolo[1,2-a]quinoxalin-4-yl)methanone 3ah

The title compound 3ah was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether : ethyl acetate : dichloromethane = 8 : 1 : 1 gave 3ah as a Yellow solid (0.127 g, 83%). $^1$H NMR (300 MHz, CDCl$_3$): $\delta$ 8.16-8.12 (2H, m), 8.08-8.05 (2H, m), 7.94 (1H, $J$ = 10.8 Hz, t), 7.68-7.62 (1H, m), 7.54-7.47 (3H, m), 7.29-7.26 (1H, m), 7.00 (1H, $J$ = 2.7, 3.9 Hz, dd); $^{13}$C NMR (75 MHz,
CDCl₃): δ 190.79, 157.87, 149.01, 140.18, 134.27, 132.47, 130.93, 129.79, 128.70, 125.69, 115.26, 115.18, 113.96, 109.50; HRMS calcd for C₁₈H₁₁ClN₂O (M+H)⁺ 307.0633; found: 307.0607.

Benzo[d][1,3]dioxol-5-yl(pyrrolo[1,2-a]quinoxalin-4-yl)methanone 3ai

The title compound 3ai was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether : ethyl acetate : dichloromethane = 8 : 1 : 1 gave 3ai as a Yellow solid (0.135 g, 86%). ¹H NMR (300 M, CDCl₃): δ 8.04 (2H, J = 1.2, 8.4 Hz, dd), 7.92 (1H, J = 0.9, 8.1 Hz, dd), 7.79 (1H, J = 1.5, 8.1 Hz, dd), 7.69 (1H, J = 1.5 Hz, d), 7.65-7.59 (1H, m), 7.52-7.46 (1H, m), 7.13 (1H, J = 1.2, 4.2 Hz, dd), 6.95 (1H, J = 3.0, 4.2 Hz, dd), 6.88 (1H, J = 8.4 Hz, d), 6.07 (2H, s); ¹³C NMR (75 MHz, CDCl₃): δ 190.35, 152.54, 150.54, 148.04, 134.74, 130.97, 130.28, 129.25, 128.33, 127.91, 125.48, 124.41, 114.83, 114.79, 113.87, 110.23, 108.85, 107.98, 101.93; HRMS calcd for C₁₉H₁₂N₂O₃ (M+H)⁺ 317.0921; found: 317.0897.

Naphthalen-1-yl(pyrrolo[1,2-a]quinoxalin-4-yl)methanone 3aj

The title compound 3aj was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether : ethyl acetate : dichloromethane = 8 : 1 : 1 gave 3aj as a Yellow solid (0.135 g, 81%). ¹H NMR (300 M, CDCl₃): δ 8.62-8.58 (1H, m), 8.16 (1H, J = 1.2, 2.7 Hz, dd), 8.12 (1H, J = 8.1 Hz, d), 8.07-7.98 (2H, m), 7.95 (J = 1.2, 8.1 Hz, dd), 7.87 (J = 1.2, 7.2 Hz, dd), 7.71-7.60 (3H, m), 7.58-7.47 (2H, m), 7.40 (J = 1.2, 4.2 Hz, dd), 7.06 (J = 2.7, 3.9 Hz, dd); ¹³C NMR (75 MHz, CDCl₃): δ 194.75, 154.89, 150.42, 133.87, 133.07, 131.60, 131.27, 130.64, 129.79, 128.56, 127.91, 126.49, 125.61, 124.25, 115.38, 115.17, 114.07, 109.46; HRMS calcd for C₂₂H₁₄N₂O (M+H)⁺ 323.1179; found: 323.1172.

Naphthalen-2-yl(pyrrolo[1,2-a]quinoxalin-4-yl)methanone 3ak

The title compound 3ak was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether : ethyl acetate : dichloromethane = 8 : 1 : 1 gave 3ak as a Yellow solid (0.136 g, 85%). ¹H NMR (300 M, CDCl₃): δ 8.69 (1H, s), 8.24 (1H, J = 1.8, 8.7 Hz, dd), 8.07-8.04 (2H, m), 7.97-7.89 (4H, m), 7.68-7.59 (2H, m), 7.56-7.48 (2H, m), 7.23 (1H, J = 1.2, 3.9 Hz, dd), 6.98 (1H, J = 2.7, 3.9 Hz, dd); ¹³C NMR (75 MHz, CDCl₃): δ 192.13, 150.14, 135.80, 134.76, 133.55, 133.36, 132.34, 130.85, 129.78, 129.46, 128.80, 128.11, 128.00, 127.74, 126.73, 125.49, 124.44, 115.07, 114.76, 114.03, 108.77; HRMS calcd for C₂₂H₁₄N₂O (M+H)⁺ 323.1179; found: 323.1176.

Pyrrolo[1,2-a]quinoxalin-4-yl(thiophen-2-yl)methanone 3al

The title compound 3al was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether : ethyl acetate : dichloromethane = 8 : 1 : 1 gave 3al as a Yellow solid.
(7-Methoxypyrrolo[1,2-a]quinoxalin-4-yl)(phenyl)methanone 3ba

The title compound 3ba was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether : ethyl acetate : dichloromethane = 10 : 1 : 1 gave 3ba as a Yellow solid (0.129 g, 86%). 1H NMR (300 MHz, CDCl3): δ 8.12-8.10 (2H, m), 8.02 (1H, J = 1.5 Hz, d), 7.89 (1H, J = 9.0 Hz, d), 7.33 (2H, J = 8.1 Hz, d), 7.25 (1H, J = 2.7, 9.0 Hz, dd), 7.13 (1H, J = 1.2, 4.2 Hz, dd), 6.93 (1H, J = 2.7, 4.2 Hz, dd); 13C NMR (75 MHz, CDCl3): δ 192.31, 157.82, 149.98, 134.04 (3J C,F = 9.8, d), 124.50, 122.62, 118.87, 115.31, 115.06, 114.80, 112.13, 108.72, 56.19; HRMS calcd for C19H14NO2 (M+H)+ 317.1285; found: 317.1286.

(7-Methoxypyrrolo[1,2-a]quinoxalin-4-yl)(p-tolyl)methanone 3bc

The title compound 3bc was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether : ethyl acetate : dichloromethane = 10 : 1 : 1 gave 3bc as a Yellow solid (0.129 g; 82%). 1H NMR (300 MHz, CDCl3): δ 8.03-8.00 (3H, m), 7.88 (1H, J = 9.0 Hz, d), 7.47 (1H, J = 2.7 Hz, d), 7.33 (2H, J = 8.1 Hz, d), 7.25 (1H, J = 2.7, 9.0 Hz, dd), 7.13 (1H, J = 1.2, 4.2 Hz, dd), 6.93 (1H, J = 2.7, 4.2 Hz, dd); 13C NMR (75 MHz, CDCl3): δ 192.31, 157.82, 149.98, 133.79, 131.16, 128.67, 124.55, 122.66, 119.08, 115.33, 115.07, 114.88, 112.18, 108.77, 56.20; HRMS calcd for C20H16N2O2 (M+H)+ 331.1285; found: 317.1286.

(4-Fluorophenyl)(7-methoxypyrrolo[1,2-a]quinoxalin-4-yl)methanone 3be

The title compound 3be was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether : ethyl acetate : dichloromethane = 10 : 1 : 1 gave 3be as a Yellow solid (0.137 g; 86%). 1H NMR (300 MHz, CDCl3): δ 8.21 (2H, J = 2.7, 8.7 Hz, dd), 8.02 (1H, J = 1.2 Hz, d), 7.89 (1H, J = 9.0 Hz, d), 7.47 (1H, J = 2.7 Hz, d), 7.33 (2H, J = 8.1 Hz, d), 7.25 (1H, J = 2.7, 9.0 Hz, dd), 7.13 (1H, J = 2.7, 4.2 Hz, dd); 13C NMR (75 MHz, CDCl3): δ 192.21, 157.85, 149.98, 133.79, 129.42, 124.57, 122.62, 118.87, 115.31, 115.06, 114.80, 112.13, 108.72, 56.19, 21.91; HRMS calcd for C19H13FN2O2 (M+H)+ 331.1285; found: 317.1286.

(7-Methylpyrrolo[1,2-a]quinoxalin-4-yl)(phenyl)methanone 3ca

The title compound 3ca was prepared according to general procedure 3. A purification by flash
chromatography in petroleum ether : ethyl acetate : dichloromethane = 8 : 1 : 1 gave 3ca as a Yellow solid (0.121 g, 85%). \(^1\)H NMR (300 M, CDCl\(_2\)): \(\delta\) 8.14-8.10 (2H, m), 8.05 (1H, \(J = 1.5, 2.7\) Hz, dd), 7.87 (1H, \(J = 8.7\) Hz, d), 7.81 (1H, \(J = 0.6\) Hz, d), 7.68-7.63 (1H, m), 7.54-7.47 (3H, m), 7.20 (1H, \(J = 1.2, 4.2\) Hz, dd), 6.96 (1H, \(J = 2.4, 3.9\) Hz, dd), 2.51 (3H, s); \(^{13}\)C NMR (75 MHz, CDCl\(_2\)): \(\delta\) 192.74, 149.99, 136.62, 136.00, 134.96, 133.74, 131.18, 131.12, 130.89, 128.61, 126.22, 124.67, 115.16, 114.91, 114.11, 108.89, 21.10; HRMS calcd for C\(_{19}\)H\(_{14}\)N\(_2\)O (M+H)\(^+\) 287.1179; found: 287.1184.

(7-Chloropyrrolo[1,2-a]quinoxalin-4-yl)(phenyl)methanone 3da

The title compound 3da was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether : ethyl acetate : dichloromethane = 8 : 1 : 1 gave 3da as a Yellow solid (0.119 g, 78%). \(^1\)H NMR (300 M, CDCl\(_2\)): \(\delta\) 8.13-8.10 (4H, m), 8.06 (2H, \(J = 0.9, 2.4\) Hz, dd), 7.99-7.99 (2H, \(J = 0.9, 2.4\) Hz, d), 7.91 (2H, \(J = 9.0\) Hz, d), 7.69-7.64 (2H, m), 7.60 (2H, \(J = 2.4, 8.7\) Hz, dd), 7.55-7.50 (4H, m), 7.22 (2H, \(J = 2.7, 3.9\) Hz, dd), 7.00 (2H, \(J = 2.7, 3.9\) Hz, dd); \(^{13}\)C NMR (75 MHz, CDCl\(_2\)): \(\delta\) 192.34, 151.14, 136.22, 136.02, 134.00, 131.18, 130.90, 130.39, 129.74, 128.71, 127.04, 124.68, 115.88, 115.73, 115.57, 109.80; HRMS calcd for C\(_{18}\)H\(_{11}\)ClN\(_2\)O (M+H)\(^+\) 307.0633; found: 307.0610.

(7-Chloropyrrolo[1,2-a]quinoxalin-4-yl)(4-methoxyphenyl)methanone 3db

The title compound 3db was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether : ethyl acetate : dichloromethane = 8 : 1 : 1 gave 3db as a Yellow solid (0.129 g, 77%). \(^1\)H NMR (300 M, CDCl\(_2\)): \(\delta\) 8.05-8.01 (2H, m), 7.96 (1H, \(J = 0.9, 2.4\) Hz, dd), 7.92 (1H, \(J = 9.0\) Hz, d), 7.51 (H, \(J = 2.4, 9.0\) Hz, dd), 7.05 (1H, \(J = 1.2, 4.2\) Hz, dd), 6.93-6.88 (3H, m), 3.81(3H, s); \(^{13}\)C NMR (75 MHz, CDCl\(_2\)): \(\delta\) 190.63, 164.73, 151.95, 136.05, 133.58, 130.86, 130.22, 129.47, 128.83, 126.99, 124.74, 115.87, 115.71, 115.44, 114.09, 109.74, 56.00; HRMS calcd for C\(_{19}\)H\(_{13}\)ClN\(_2\)O\(_2\) (M+H)\(^+\) 337.0738; found: 337.0730.

(7-Chloropyrrolo[1,2-a]quinoxalin-4-yl)(p-tolyl)methanone 3dc

The title compound 3dc was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether : ethyl acetate : dichloromethane = 8 : 1 : 1 gave 3dc as a Yellow solid (0.123 g, 77%). \(^1\)H NMR (300 M, CDCl\(_2\)): \(\delta\) 8.08 (1H, \(J = 1.2, 2.7\) Hz, dd), 8.06-8.02 (3H, m), 7.94 (1H, \(J = 9.0\) Hz, d), 7.63 (1H, \(J = 2.4, 8.7\) Hz, dd), 7.36 (2H, \(J = 7.8\) Hz, d), 7.20 (1H, \(J = 1.2, 3.9\) Hz, dd), 7.02 (1H, \(J = 2.7, 3.9\) Hz, dd); \(^{13}\)C NMR (75 MHz, CDCl\(_2\)): \(\delta\) 191.90, 151.60, 145.37, 136.06, 133.55, 131.25, 130.87, 130.31, 129.58, 129.47, 127.02, 124.70, 115.84, 115.71, 115.48, 109.73, 21.92; HRMS calcd for C\(_{19}\)H\(_{13}\)ClN\(_2\)O (M+H)\(^+\) 321.0789; found: 321.0762.

(7-Chloropyrrolo[1,2-a]quinoxalin-4-yl)(4-fluorophenyl)methanone 3de

The title compound 3de was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether : ethyl acetate : dichloromethane = 8 : 1 : 1 gave 3de as a Yellow solid (0.123 g, 77%). \(^1\)H NMR (300 M, CDCl\(_2\)): \(\delta\) 8.08 (1H, \(J = 1.2, 2.7\) Hz, dd), 8.06-8.02 (3H, m), 7.94 (1H, \(J = 9.0\) Hz, d), 7.63 (1H, \(J = 2.4, 8.7\) Hz, dd), 7.36 (2H, \(J = 7.8\) Hz, d), 7.20 (1H, \(J = 1.2, 3.9\) Hz, dd), 7.02 (1H, \(J = 2.7, 3.9\) Hz, dd); \(^{13}\)C NMR (75 MHz, CDCl\(_2\)): \(\delta\) 191.90, 151.60, 145.37, 136.06, 133.55, 131.25, 130.87, 130.31, 129.58, 129.47, 127.02, 124.70, 115.84, 115.71, 115.48, 109.73, 21.92; HRMS calcd for C\(_{19}\)H\(_{13}\)ClN\(_2\)O (M+H)\(^+\) 321.0789; found: 321.0762.
The title compound 3de was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether : ethyl acetate : dichloromethane = 8 : 1 : 1 gave 3de as a Yellow solid (0.126 g, 78%). ¹H NMR (300 M, CD₂Cl₂): δ 8.24-8.18 (4H, m), 8.07 (2H, J = 1.2, 2.7 Hz, dd), 8.01 (2H, J = 2.4 Hz, d), 7.93 (2H, J = 8.7 Hz, d), 7.62 (2H, J = 2.1, 8.7 Hz, dd), 7.26-7.17 (6H, m), 7.01 (2H, J = 3.0, 4.2 Hz, dd); ¹³C NMR (75 MHz, CD₂Cl₂): δ 190.61, 166.51 (¹J_C,F = 253.5, d), 150.78, 135.91, 134.12, 133.99, 132.59⁴(¹J_C,F = 3.0, d), 130.96, 130.13 (¹J_C,F = 37.5, d), 127.06, 124.62, 115.98, 115.71⁵(¹J_C,F = 8.3, d), 115.69, 109.93; HRMS calcd for C₁₈H₁₀ClFN₂O (M+H)⁺ 325.0539; found: 325.0549.

(7-Chloropyrrolo[1,2-a]quinoxalin-4-yl)(furan-2-yl)methanone 3dm

The title compound 3dm was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether : ethyl acetate : dichloromethane = 8 : 1 : 1 gave 3dm as a Yellow solid (0.126 g, 85%). ¹H NMR (300 M, CD₂Cl₂): δ 8.06-8.04 (2H, m), 7.91 (1H, J = 3.3 Hz, t), 7.87 (1H, s), 7.81 (1H, s), 7.60 (1H, J = 2.1, 9.0 Hz, dd), 7.48 (1H, J = 3.6 Hz, d), 7.02-7.00 (1H, m), 6.67 (1H, J = 1.8 Hz, d); ¹³C NMR (75 MHz, CD₂Cl₂): δ 191.17, 185.01, 178.50, 151.49, 149.45, 148.67, 146.87, 135.95, 130.90, 130.47, 130.05, 127.24, 124.62, 124.19, 115.82, 112.90, 110.38; HRMS calcd for C₁₆H₉ClN₂O₂ (M+H)⁺ 297.0425; found: 297.0405.

Imidazo[1,5-a]quinoxalin-4-yl(phenyl)methanone 3ea

The title compound 3ea was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether : ethyl acetate : dichloromethane = 5 : 1 : 1 gave 3ea as a Yellow solid (0.114 g, 84%). ¹H NMR (300 M, CD₂Cl₂): δ 8.79 (1H, s), 8.23-8.19 (3H, m), 8.07-8.02 (2H, m), 7.75-7.58 (3H, m), 7.57-7.52 (2H, m); ¹³C NMR (75 MHz, CD₂Cl₂): δ 191.17, 185.01, 178.50, 151.49, 149.45, 148.67, 135.95, 130.90, 130.47, 130.05, 127.24, 124.62, 124.19, 115.82, 112.90, 110.38; HRMS calcd for C₁₇H₁₁N₃O (M+H)⁺ 274.0975; found: 274.0959.

Imidazo[1,5-a]quinoxalin-4-yl(naphthalen-2-yl)methanone 3ej

The title compound 3ej was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether : ethyl acetate : dichloromethane = 5 : 1 : 1 gave 3ej as a Yellow solid (0.135 g, 84%). ¹H NMR (300 M, CD₂Cl₂): δ 8.72 (2H, J =4.2 Hz, d), 8.17-8.10 (2H, m), 8.02-7.96 (2H, m), 7.92-7.85 (3H, m), 7.68-7.63 (1H, m), 7.60-7.46 (3H, m); ¹³C NMR (75 MHz, CD₂Cl₂): δ 191.31, 150.14, 136.17, 135.42, 134.13, 133.29, 132.69, 131.76, 131.09, 130.25, 129.85, 129.31, 129.25, 128.52, 128.15, 127.66, 127.19, 126.07, 125.86, 114.99; HRMS calcd for C₂₁H₁₁N₃O (M+H)⁺ 324.1131; found: 324.1136.

(1-Methylimidazo[1,5-a]quinoxalin-4-yl)(phenyl)methanone 3fa

59
The title compound 3fa was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether : ethyl acetate : dichloromethane = 5 : 1 : 1 gave 3fa as a Yellow solid (0.126 g, 88%). 1H NMR (300 M, CDCl2): δ 8.30 (1H, J = 0.6, 8.4 Hz, dd), 8.21-8.19 (2H, m), 8.07-8.04 (2H, m), 7.73-7.68 (2H, m), 7.63-7.54 (3H, m), 3.16 (3H, s); 13C NMR (75 MHz, CDCl2): δ 191.69, 150.21, 142.64, 136.45, 136.14, 133.89, 131.55, 131.27, 130.20, 128.66, 128.04, 127.56, 126.94, 124.33, 19.01; HRMS calcd for C18H13N3O (M+H)+ 288.1131; found: 288.1149.

(1-Methylimidazo[1,5-a]quinoxalin-4-yl)(p-tolyl)methanone 3fc

The title compound 3fc was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether : ethyl acetate : dichloromethane = 5 : 1 : 1 gave 3fc as a Yellow solid (0.129 g, 86%). 1H NMR (300 M, CDCl2): δ 8.31 (1H, J = 1.2, 8.4 Hz, dd), 8.12-8.09 (2H, m), 8.06 (1H, J = 1.8, 8.1 Hz, dd), 7.99 (1H, s), 7.74-7.68 (1H, m), 7.64-7.58 (1H, m), 7.37 (2H, J = 8.1 Hz, d), 3.16 (3H, s), 2.50 (3H, s); 13C NMR (75 MHz, CDCl2): δ 191.26, 150.63, 145.25, 142.59, 136.51, 133.45, 131.49, 131.36, 130.05, 129.42, 128.01, 127.37, 126.94, 124.38, 116.23, 21.91, 18.96; HRMS calcd for C19H15N3O (M+H)+ 302.1288; found: 302.1289.

(4-Fluorophenyl)(1-methylimidazo[1,5-a]quinoxalin-4-yl)methanone 3fe

The title compound 3fe was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether : ethyl acetate : dichloromethane = 5 : 1 : 1 gave 3fe as a Yellow solid (0.126 g, 83%). 1H NMR (300 M, CDCl2): δ 8.35-8.28 (3H, m), 8.09-8.05 (2H, m), 7.76-7.70 (1H, m), 7.65-7.59 (1H, m), 7.29-7.22 (2H, m), 3.17 (3H, s); 13C NMR (75 MHz, CDCl2): δ 189.91, 166.46 (J_{C,F} = 253.5, d), 149.96, 142.67, 136.38, 134.25 (J_{C,F} = 9.8, d), 132.54 (J_{C,F} = 3.0, d), 131.58, 130.34, 128.03, 127.54, 127.02, 124.24, 116.26, 115.92, 115.63 (J_{C,F} = 21.8, d), 18.94; HRMS calcd for C18H12FN3O (M+H)+ 306.1037; found: 306.1036.

(3-Methylimidazo[1,5-a]quinoxalin-4-yl)(phenyl)methanone 3ga

The title compound 3ga was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether : ethyl acetate : dichloromethane = 5 : 1 : 1 gave 3ga as a Yellow solid (0.129 g, 90%). 1H NMR (300 M, CDCl2): δ 8.68 (1H, s), 8.07-8.04 (2H, m), 7.99-7.93 (2H, m), 7.72-7.61 (2H, m), 7.58-7.51 (3H, m), 2.35 (3H, s); 13C NMR (75 MHz, CDCl2): δ 192.23, 152.78, 153.95, 137.95, 135.48, 135.34, 134.80, 130.89, 130.76, 129.84, 129.17, 128.68, 127.36, 125.89, 119.14, 114.63, 15.18; HRMS calcd for C18H13N3O (M+H)+ 288.1131; found: 288.1125.

(4-Methoxyphenyl)(3-methylimidazo[1,5-a]quinoxalin-4-yl)methanone 3gb
The title compound 3gb was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether:ethyl acetate:dichloromethane = 5:1:1 gave 3gb as a Yellow solid (0.138 g, 87%). 1H NMR (300 M, CDCl₃): δ 8.70 (1H, s), 8.08-8.04 (2H, m), 8.01-7.96 (2H, m), 7.69-7.63 (1H, m), 7.60-7.55 (1H, m), 7.05-7.02 (2H, m), 3.93 (3H, s), 2.37 (3H, s); 13C NMR (75 MHz, CDCl₃): δ 190.78, 165.20, 153.22, 137.83, 135.46, 133.29, 130.69, 129.62, 128.59, 128.40, 127.31, 125.85, 119.14, 114.61, 114.50, 15.05; HRMS calcd for C₁₉H₁₅N₃O₂ (M+H)⁺ 318.1237; found: 318.1238.

Indolo[1,2-a]quinoxalin-6-yl(phenyl)methanone 3ha

The title compound 3ha was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether:ethyl acetate:dichloromethane = 8:1:1 gave 3ha as a Red solid (0.116 g, 72%). 1H NMR (300 M, CDCl₃): δ 8.63 (1H, J = 0.9, 8.4 Hz, dd), 8.57 (1H, J = 0.6, 8.7 Hz, dd), 8.22-8.18 (2H, m), 8.10-8.04 (2H, m), 7.83-7.77 (1H, m), 7.75-7.64 (2H, m), 7.60-7.51 (5H, m); 13C NMR (75 MHz, CDCl₃): δ 192.35, 152.10, 136.30, 135.19, 134.04, 133.13, 131.68, 131.47, 131.17, 130.85, 129.88, 128.78, 127.91, 125.17, 124.73, 123.50, 123.39, 115.38, 114.91, 102.64; HRMS calcd for C₂₂H₁₄N₂O (M+H)⁺ 323.1179; found: 323.1180.

(7-Methylindolo[1,2-a]quinoxalin-6-yl)(phenyl)methanone 3ia

The title compound 3ia was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether:ethyl acetate:dichloromethane = 8:1:1 gave 3ia as a Red solid (0.146 g, 81%). 1H NMR (300 M, CDCl₃): δ 8.55-8.49 (2H, m), 8.08-8.05 (2H, m), 7.97-7.93 (2H, m), 7.72-7.60 (3H, m), 7.56-7.41 (4H, m), 2.35 (3H, s); 13C NMR (75 MHz, CDCl₃): δ 193.40, 154.89, 135.80, 135.21, 134.78, 132.58, 131.44, 130.79, 130.75, 130.19, 129.84, 129.27, 125.47, 124.41, 124.35, 122.73, 121.23, 115.16, 114.75, 110.47, 10.15; HRMS calcd for C₂₃H₁₆N₂O (M+H)⁺ 337.1335; found: 337.1320.

(4-Fluorophenyl)(7-methylindolo[1,2-a]quinoxalin-6-yl)methanone 3ie

The title compound 3ie was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether:ethyl acetate:dichloromethane = 8:1:1 gave 3ie as a Red solid (0.141 g, 80%). 1H NMR (300 M, CDCl₃): δ 8.54-8.48 (2H, m), 8.16-8.09 (2H, m), 7.95 (2H, J = 1.8, 8.1 Hz, dd), 7.72-7.60 (2H, m), 7.52-7.41 (2H, m), 7.25-7.17 (2H, m), 2.35 (3H, s); 13C NMR (75 MHz, CDCl₃): δ 191.73, 166.96 (3J_CF = 255.0, d), 154.44, 135.04, 133.76 (3J_CF = 9.8, d), 132.60, 132.31 (3J_CF = 3.0, d), 131.43, 130.75, 130.18, 129.96, 125.58, 124.39, 124.29, 122.79, 121.25, 116.50 (3J_CF = 21.8, d), 115.18, 114.75, 110.59, 10.17; HRMS calcd for C₂₃H₁₅FN₂O (M+H)⁺ 355.1241; found: 355.1243.

(7-fluoropyrrolo[1,2-a]quinoxalin-4-yl)(phenyl)methanone 3ia

The title compound 3ia was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether:ethyl acetate:dichloromethane = 8:1:1 gave 3ia as a Red solid (0.146 g, 81%). 1H NMR (300 M, CDCl₃): δ 8.55-8.49 (2H, m), 8.08-8.05 (2H, m), 7.97-7.93 (2H, m), 7.72-7.60 (3H, m), 7.56-7.41 (4H, m), 2.35 (3H, s); 13C NMR (75 MHz, CDCl₃): δ 193.40, 154.89, 135.80, 135.21, 134.78, 132.58, 131.44, 130.79, 130.75, 130.19, 129.84, 129.27, 125.47, 124.41, 124.35, 122.73, 121.23, 115.16, 114.75, 110.47, 10.15; HRMS calcd for C₂₃H₁₆N₂O (M+H)⁺ 337.1335; found: 337.1320.
The title compound 3la was prepared according to general procedure 3. A purification by flash chromatography in petroleum ether : ethyl acetate : dichloromethane = 8 : 1 : 1 gave 3la as a yellow solid (0.109 g, 75%). 1H NMR (300 M, CD₂Cl₂): δ 8.12-8.10 (3H, m), 8.07 (2H, J = 1.8, 2.7 Hz, dd), 7.95 (1H, J = 5.1, 9.3 Hz, dd), 7.71-7.64 (2H, m), 7.55-7.50 (2H, m), 7.44-7.37 (1H, m), 7.20 (1H, J = 1.2, 3.9 Hz, dd), 6.99 (1H, J = 2.7, 4.2 Hz, dd); 13C NMR (75 MHz, CD₂Cl₂): δ 192.37, 160.30 (J_C,F = 242.3, d), 151.23, 136.23, 136.20 (J_C,F = 11.3, d), 134.02, 131.14, 128.73, 125.08, 124.59, 117.54 (J_C,F = 24.0, d), 116.14 (J_C,F = 22.5, d), 115.84, 115.71, 115.35, 109.64; HRMS calcd for C₁₈H₁₁FN₂O (M+H)+ 291.0928; found: 291.0911.

5. References

6. HRMS, ¹H NMR and ¹³C NMR spectra
Phenyl[pyrrolo[1,2-a]quinazalin-4-yl]methanone (3aa).
(4-Methoxyphenyl)(pyrrolo[1,2-a]quinoxalin-4-yl)methanone (3ab).
Pyrrolo[1,2-a]quinazolin-4-yl(p-tolyl)methanone (3ac).
Pyrrolo[1,2-a]quinoxalin-4-yl(o-tolyl)methanone (3ad).
(4-Fluorophenyl)(pyrrolo[1,2-a]quinazolin-4-yl)methanone (3ae).
(4-Nitrophenyl)(pyrrolo[1,2-a]quinoxalin-4-yl)methanone (3af).
(2-Fluorophenyl)pyrrol[1,2-α]quinoxalin-4-yl)methanone (3ag).
(4-Chlorophenyl)[pyrrolo[1,2-a]quinoxalin-4-yl]methanone (3ah).
Benzo[d][1,3]dioxol-5-yl(pyrrolo[1,2-a]quinoxalin-4-yl)methanone (3ai).
Naphthalen-1-yl(pyrrrolo[1,2-a]quinoxalin-4-yl)methanone (3a).
Naphthalen-2-yl(pyrrolo[1,2-a]quinaxalin-4-yl)methanone (3ak).
Pyrrolo[1,2-a]quinoxalin-4-yl(thiophen-2-yl) methanone (3a1).
(7-Methoxypyrrrolo[1,2-a]quinazolin-4-yl)(phenyl)methanone (3ba)
(7-Methoxypyrrolo[1,2-a]quinoxalin-4-yl)(p-tolyl)methanone (3bc)
(4-Fluorophenyl)(7-methoxypyrrolo[1,2-a]quinoxalin-4-yl)methanone (3be)
(7-Methylpyrrolo[1,2-a]quinoxalin-4-yl)(phenyl)methanone (3ca)
(7-Chloropyrrolo[1,2-a]quinazolin-4-yl)(phenyl)methanone (3da)
(7-Chloropyrrolo[1,2-a]quinoxalin-4-yl)(4-methoxyphenyl)methanone (3db)
(7-Chloropyrrolo[1,2-a]quinoxalin-4-yl)(p-tolyl)methanone (3dc)
(7-Chloropyrrolo[1,2-a]quinoxalin-4-yl)(4-fluorophenyl)methanone (3de)
(7-Chloropyrrolo[1,2-a]quinazolin-4-yl)(furan-2-yl)methanone (3dm)
Imidazo[1,5-a]quinoxalin-4-yl(phenyl)methanone (3ea)
Imidazo[1,5-a]quinoxalin-4-yl(naphthalen-2-yl)methanone (3ej)
(1-Methylimidazo[1,5-a]quinoxalin-4-yl)(phenyl)methanone (3fa)
(1-Methylimidazo[1,5-a]quinoxalin-4-yl)(p-tolyl)methanone (3c)
(4-Fluorophenyl)(1-methylimidazo[1,5-a]quinoxalin-4-yl)methanone (3fe)
(3-Methylimidazo[1,5-a]quinolin-4-yl)(phenyl)methanone (3ga)
(4-Methoxyphenyl)(3-methylimidazo[1,5-a]quinoxalin-4-yl)methanone (3gb)
Indolo[1,2-a]quinazalin-6-yl(phenyl)methanone (3ha)
(7-Methylindolo[1,2-a]quinoxalin-6-yl)(phenyl)methanone (3ia)
(4-Fluorophenyl)(7-methylindolo[1,2-a]quinazolin-6-yl)methanone (3le)
(7-fluoropyrrolo[1,2-a]quinolin-4-yl)(phenyl)methanone (3la)