Supporting Information

Ruthenium-catalysed one-pot regio- and diastereoselective synthesis of pyrrolo[1,2-a]indoles via cascade C-H functionalization/annulation

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General Information

Materials

All the starting materials, reagents and catalysts were purchased from Aldrich or Acros and used as such. For thin layer chromatography, analytical TLC plates (Alugram SIL G/UV254 and 70-230 mesh silica gel (E. M. Merck) were used). Column chromatography was performed using silica gel (Merck, 60-120 mesh size). Anhydrous solvents were purchased from Acros Organics and stored over molecular sieves. The chromatographic solvents used for isolation/purification of compounds were distilled prior to use. The chromatographic solvents are mentioned as volume: volume ratios. Reactions were typically run in oven-dried screw-cap vial under inert atmosphere. All reactions were carried out in 5 mL glass microwave vials equipped with air tight teflon caps or a 100 mL round bottomed flask and sealed with a glass stopper and heated in oil baths with a thermocouple temperature control. Toluene, THF and dichloromethane were freshly distilled over sodium or calcium hydride and stored under N₂. 1,2-dichloroethane used for the catalytic reactions was analytical grade (99.5%) and was purged with N₂ for 30 min and stored over dried MS 4 Å. Other solvents, unless otherwise stated, were purchased in reagent grade or anhydrous quality and used as received. Reagents were either purchased directly from commercial suppliers or prepared according to literature procedures. Yields refer to isolated compounds.

Apparatus

¹H and ¹³C NMR spectra were recorded on a 400 MHz & 300 MHz instrument using CDCl₃ and DMSO-d₆ as a solvent. The ¹H and ¹³C NMR chemical shifts are reported in parts per million relative to tetramethylsilane using the residual solvent signal as the internal reference. The following abbreviations were used to designate chemical shift multiplicities: s = singlet, bs = broad singlet, d = doublet, dd = double doublet, dt = doublet of a triplet, t = triplet, q = quartet, m = multiplet. The ¹³C NMR spectra are proton decoupled. The melting points were determined on a digital Barnsted Electrothermal 9200 apparatus and are uncorrected. Mass spectra were recorded by using a Kratos MS50TC and a Kratos Mach III system. The ion source temperature was 150-250 °C, as required. High resolution EI-mass spectra were performed with a resolution of 10,000. The low-resolution spectra were obtained with a HP5989A MS instrument. The low resolution ESI-MS were obtained with a Thermo Scientific instrument.
Experimental Section

Synthesis of Starting materials

Table 1. Chemicals used for synthesis of starting materials 1a-1r

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**General procedure for synthesis of compounds 1a-1r**

**Step-1**: Thionyl chloride (0.15 ml, 2.0 mmol) was added to substituted phenylacetic acid S2a-S2j (1.2 mmol) dropwise at room temperature and reaction mixture was stirred for 30 min. Then, the reaction mixture was heated at 80 °C for 30 min and then cooled to room temperature. The excess thionyl chloride was removed under vacuum and the resulting crude acid chloride was used in next step without further purification.

**Step-2**: Under nitrogen atmosphere, the above acid chloride in CH$_2$Cl$_2$ (5 mL) was added to a solution of indoline S1a-S1c (1.0 mmol), DMAP (0.05 mmol), Et$_3$N (2.0 mmol) in CH$_2$Cl$_2$ (10 mL) at -20 °C dropwise. After stirring at -20 °C for 30 min and then at room temperature overnight, the reaction mixture was quenched with saturated NaHCO$_3$, extracted with CH$_2$Cl$_2$ (2 x 15 mL). The combined organic layer was washed with brine, dried over Na$_2$SO$_4$ and evaporated under vacuum to give crude amide product S4a-S4p which was used in next step without further purification.

**Step-3**: Crude amide product S4a-S4p obtained in Step-2 above, was dissolved in dry toluene (10 mL) and added DDQ (2,3-Dichloro-5,6-dicyano-1,4-benzoquinone) (1.2 mmol). The reaction mixture was then refluxed at 110 °C for overnight and then cooled to room temperature. The toluene was removed under vacuum and the resulting residue was subjected to silica gel column chromatography (20-40% Ethyl acetate in heptane) to afford the desired product 1a-1r.
Compound 1a: (1-(1H-indol-1-yl)-2-phenylethanone)

![Chemical structure of Compound 1a](image)

Compound 1a was obtained as colorless solid. Yield: 68%, Melting point: 62-64 ºC. \( ^1\text{H} \) NMR (300 MHz, CDCl\textsubscript{3})  δ 8.50 (d, 1H, \( J = 8.2 \) Hz), 7.57-7.53 (m, 1H), 7.49 (d, 1H, \( J = 4.0 \) Hz), 7.40-7.23 (m, 7H), 6.62 (dd, 1H, \( J = 4.0 \) Hz, 0.6 Hz), 4.24 (s, 2H). \( ^{13}\text{C} \) NMR (75 MHz, CDCl\textsubscript{3})  δ 169.53, 136.00, 133.62, 130.52, 129.30, 129.12, 127.62, 125.46, 125.06, 124.05, 121.01, 116.98, 109.69, 43.24. HRMS (EI): Calculated for C\textsubscript{16}H\textsubscript{13}NO [M]+ 235.0997, found 235.0960.

Compound 1b: (1-(1H-indol-1-yl)-2-(4-methoxyphenyl)ethanone)

![Chemical structure of Compound 1b](image)

Compound 1b was obtained as colorless solid. Yield: 30%, Melting point: 77-79 ºC. \( ^1\text{H} \) NMR (300 MHz, CDCl\textsubscript{3})  δ 8.49 (d, 1H, \( J = 8.2 \) Hz), 7.59-7.53 (m, 1H), 7.51 (d, 1H, \( J = 3.8 \) Hz), 7.39-7.21 (m, 4H), 6.89 (d, 2H, \( J = 8.9 \) Hz), 6.62 (d, 1H, \( J = 3.8 \) Hz), 4.19 (s, 2H), 3.79 (s, 3H). \( ^{13}\text{C} \) NMR (75 MHz, CDCl\textsubscript{3})  δ 169.89, 159.08, 136.01, 130.50, 130.38, 125.57, 125.43, 125.05, 124.00, 121.00, 116.98, 114.56, 109.61, 55.50, 42.37. HRMS (EI): Calculated for C\textsubscript{17}H\textsubscript{15}NO\textsubscript{2} [M]+ 265.1103, found 265.1130.

Compound 1c: (1-(1H-indol-1-yl)-2-(4-nitrophenyl)ethanone)
Compound 1c was obtained as colorless solid. Yield: 76%, Melting point: 110-112 °C. $^1$H NMR (300 MHz, CDCl$_3$) δ 8.44 (d, 1H, $J = 8.1$ Hz), 8.24 (d, 1H, $J = 8.8$ Hz), 7.58 (d, 1H, $J = 7.7$ Hz), 7.54-7.47 (m, 3H), 7.41-7.33 (m, 1H), 7.33-7.26 (m, 1H), 6.70 (dd, 1H, $J = 3.8$ Hz, 0.6 Hz), 4.37 (s, 2H). $^{13}$C NMR (75 MHz, CDCl$_3$) δ 168.00, 147.58, 140.79, 135.93, 130.69, 130.55, 129.35, 129.03, 125.81, 124.43, 124.25, 124.20, 121.25, 116.88, 110.53, 42.58. HRMS (EI): Calculated for C$_{16}$H$_{12}$N$_2$O$_3$ [M]$^+$ 280.0848, found 280.0874.

Compound 1d: (2-(3,4-dichlorophenyl)-1-(1H-indol-1-yl)ethanone)

Compound 1d was obtained as colorless solid. Yield: 60%, Melting point: 93-95 °C. $^1$H NMR (300 MHz, CDCl$_3$) δ 8.45 (d, 1H, $J = 8.2$ Hz), 7.57 (d, 1H, $J = 7.4$ Hz), 7.47-7.40 (m, 3H), 7.39-7.26 (m, 2H), 7.16 (dd, 1H, $J = 8.2$ Hz, 2.1 Hz), 6.67 (dd, 1H, $J = 3.8$ Hz, 0.4 Hz), 4.19 (s, 2H). $^{13}$C NMR (75 MHz, CDCl$_3$) δ 168.37, 135.95, 133.53, 133.06, 131.99, 131.54, 130.93, 130.53, 128.97, 125.69, 124.48, 124.30, 121.17, 116.90, 110.26, 41.93. HRMS (EI): Calculated for C$_{16}$H$_{11}$Cl$_2$NO [M]$^+$ 303.0218, found 302.9811.

Compound 1e: (2-(3-chlorophenyl)-1-(1H-indol-1-yl)ethanone)
Compound 1e was obtained as pale yellow liquid. Yield: 63%. \(^1\)H NMR (300 MHz, CDCl\(_3\)) \(
\delta 8.47 (d, 1H, J = 8.2 Hz), 7.56 (d, 1H, J = 7.3 Hz), 7.46 (d, 1H, J = 3.7 Hz), 7.39-7.16 (m, 6H), 6.65 (d, 1H, J = 4.0 Hz), 4.20 (s, 2H).\)

\(^{13}\)C NMR (75 MHz, CDCl\(_3\)) \(
\delta 168.76, 135.95, 135.39, 134.85, 130.52, 130.28, 129.60, 127.91, 127.64, 125.59, 124.73, 124.20, 121.10, 116.94, 110.03, 42.60.\)

HRMS (EI): Calculated for C\(_{16}\)H\(_{12}\)ClNO [M]+ 269.0607, found 269.0649.

**Compound 1f**: (2-(2-bromophenyl)-1-(1H-indol-1-yl)ethanone)

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\begin{array}{c}
\text{\includegraphics[width=0.2\textwidth]{compound1f.png}}
\end{array}
\end{center}
}
\]

Compound 1f was obtained as colorless solid. Yield: 52%, Melting point: 102-104 °C. \(^1\)H NMR (300 MHz, CDCl\(_3\)) \(
\delta 8.48 (d, 1H, J = 8.2 Hz), 7.64 (d, 1H, J = 3.8 Hz), 7.45 (d, 1H, J = 3.8 Hz), 7.39-7.14 (m, 5H), 6.68 (d, 1H, J = 3.8 Hz), 4.40 (s, 2H).\)

\(^{13}\)C NMR (75 MHz, CDCl\(_3\)) \(
\delta 168.47, 136.00, 133.83, 133.18, 131.55, 130.58, 129.47, 128.04, 125.54, 125.14, 124.83, 124.12, 121.09, 116.96, 109.92, 43.33.\)

HRMS (EI): Calculated for C\(_{16}\)H\(_{12}\)BrNO [M]+ 313.0102, found 313.0128.

**Compound 1g**: (1-(5-methyl-1H-indol-1-yl)-2-phenylethanone)

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\begin{array}{c}
\text{\includegraphics[width=0.2\textwidth]{compound1g.png}}
\end{array}
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}
\]

Compound 1g was obtained as colorless solid. Yield: 40%, Melting point: 72-74 °C. \(^1\)H NMR (300 MHz, CDCl\(_3\)) \(
\delta 8.35 (d, 1H, J = 8.4 Hz), 7.45 (d, 1H, J = 3.8 Hz), 7.39-7.27 (m, 6H), 7.16 (d, 1H, J = 8.5 Hz), 6.54 (d, 1H, J = 3.8 Hz), 4.22 (s, 2H), 2.43 (s, 3H).\)

\(^{13}\)C NMR (75 MHz, CDCl\(_3\)) \(
\delta 169.16, 134.01, 133.55, 133.45, 130.60, 129.13, 128.92, 127.40, 126.57, 124.93, 120.78, 116.41, 109.30, 42.95, 21.39.\)

HRMS (EI): Calculated for C\(_{17}\)H\(_{15}\)NO [M]+ 249.1154, found 249.1172.
Compound 1h: (1-(5-bromo-1H-indol-1-yl)-2-phenylethanone)

![1h structure]

Compound 1h was obtained as colorless solid. Yield: 51%, Melting point: 72-74 °C. $^1$H NMR (300 MHz, CDCl$_3$) δ 8.37 (d, 1H, $J = 8.9$ Hz), 7.68 (d, 1H, $J = 2.0$ Hz), 7.51 (d, 1H, 3.8 Hz), 7.44 (dd, 1H, $J = 8.9$ Hz, 1.9 Hz), 7.39-7.28 (m, 5H), 6.56 (d, 1H, $J = 3.8$ Hz), 4.24 (s, 2H). $^{13}$C NMR (75 MHz, CDCl$_3$) δ 169.45, 134.71, 133.29, 132.23, 129.28, 129.21, 128.31, 127.77, 126.13, 123.71, 118.38, 117.37, 108.84, 43.14. HRMS (EI): Calculated for C$_{18}$H$_{12}$BrNO [M]$^+$ 313.0102, found 313.0130.

Compound 1i: (2-(3-chlorophenyl)-1-(5-methyl-1H-indol-1-yl)ethanone)

![1i structure]

Compound 1i was obtained as colorless solid. Yield: 40%, Melting point: 67-69 °C. $^1$H NMR (300 MHz, CDCl$_3$) δ 8.33 (d, 1H, $J = 8.5$ Hz), 7.43 (d, 1H, $J = 3.8$ Hz), 7.34 (d, 2H, $J = 5.1$ Hz), 7.30-7.27 (m, 2H), 7.23-7.14 (m, 2H), 6.58 (d, 1H, $J = 3.9$ Hz), 4.20 (s, 2H), 2.44 (s, 3H). $^{13}$C NMR (75 MHz, CDCl$_3$) δ 168.57, 135.52, 134.86, 134.17, 133.82, 130.79, 130.27, 129.62, 127.89, 127.65, 126.89, 124.78, 121.06, 116.56, 109.86, 42.54, 21.58. HRMS (EI): Calculated for C$_{17}$H$_{14}$ClNO [M]$^+$ 283.0764, found 283.0761.

Compound 1j: (2-(4-methoxyphenyl)-1-(5-methyl-1H-indol-1-yl)ethanone)

![1j structure]
Compound 1j was obtained as colorless solid. Yield: 41%, Melting point: 95-197 °C. $^1$H NMR (300 MHz, CDCl$_3$) δ 8.34 (d, 1H, J = 8.5 Hz), 7.46 (d, 1H, J = 3.9 Hz), 7.33 (t, 1H), 7.23 (d, 2H, J = 9.2 Hz), 7.16 (d, 1H, J = 8.5 Hz), 6.88 (d, 1H, J = 8.6 Hz), 6.54 (d, 1H, J = 3.8 Hz), 4.16 (s, 2H), 3.79 (s, 3H), 2.43 (s, 3H). $^{13}$C NMR (75 MHz, CDCl$_3$) δ 169.69, 159.04, 134.18, 133.55, 130.74, 130.37, 126.70, 125.68, 125.08, 120.92, 116.56, 114.51, 109.38, 55.48, 42.23, 21.56. HRMS (EI): Calculated for C$_{18}$H$_{17}$NO$_2$ [M]$^+$ 279.1259, found 279.1296.

**Compound 1k:** (2-(3,4-dichlorophenyl)-1-(5-methyl-1H-indol-1-yl)ethanone)

Compound 1k was obtained as colorless solid. Yield: 31%, Melting point: 112-114 °C. $^1$H NMR (300 MHz, CDCl$_3$) δ 8.30 (d, 1H, J = 8.7 Hz), 7.46-7.38 (m, 3H), 7.36-7.32 (m, 1H), 7.21-7.12 (m, 2H), 6.60 (d, 1H, J = 3.8 Hz), 4.18 (s, 2H), 2.44 (s, 3H). $^{13}$C NMR (75 MHz, CDCl$_3$) δ 168.19, 134.14, 133.93, 133.65, 133.05, 131.95, 131.55, 130.91, 130.79, 128.98, 126.97, 124.53, 121.12, 116.51, 110.08, 41.84, 21.58. HRMS (EI): Calculated for C$_{17}$H$_{13}$Cl$_2$NO [M]$^+$ 317.0374, found 317.0372.

**Compound 1l:** (1-(1H-indol-1-yl)-2-(4-(trifluoromethyl)phenyl)ethanone)
Compound 1l was obtained as pale yellow solid. Yield: 29%, Melting point: 92-94 °C. $^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 8.46 (d, 1H, $J = 8.1$ Hz), 7.64 (d, 2H, $J = 8.2$ Hz), 7.57 (d, 1H, $J = 7.7$ Hz), 7.52-7.26 (m, 5H), 6.67 (d, 1H, $J = 3.6$ Hz), 4.31 (s, 2H). $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 168.59, 137.49, 135.97, 130.54, 129.95, 129.82, 126.03, 125.98, 125.69, 124.59, 124.28, 121.16, 116.93, 110.20, 42.75. HRMS (EI): Calculated for C$_{17}$H$_{12}$F$_{3}$NO [M]$^+$ 303.0871, found 303.0844.

**Compound 1m:** (2-(4-fluorophenyl)-1-(1H-indol-1-yl)ethanone)

Compound 1m was obtained as pale yellow solid. Yield: 84%, Melting point: 79-81 °C. $^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 8.47 (d, 1H, $J = 8.2$ Hz), 7.56 (d, 1H, $J = 7.2$ Hz), 7.48 (d, 1H, $J = 3.8$ Hz), 7.40-7.21 (m, 4H), 7.04 (t, 2H), 6.64 (d, 1H, $J = 3.8$ Hz), 4.20 (s, 2H). $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 169.32, 162.33 (d, $J = 247.0$ Hz, CF), 135.98, 131.03 (d, $J = 8.0$ Hz), 130.51, 129.24 (d, $J = 3.0$ Hz), 125.55, 124.78, 124.13, 121.08, 116.93, 116.13, 115.85, 109.88, 42.20. HRMS (EI): Calculated for C$_{16}$H$_{12}$FNO [M]$^+$ 253.0903, found 253.0919.

**Compound 1n:** (1-(1H-indol-1-yl)-2-(p-tolyl)ethanone)
Compound 1n was obtained as pale yellow solid. Yield: 35%, Melting point: 70-72 °C. $^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 8.49 (d, 1H, $J = 8.2$ Hz), 7.54 (d, 1H, $J = 7.6$ Hz), 7.49 (d, 1H, $J = 3.8$ Hz), 7.39-7.10 (m, 6H), 6.61 (d, 1H, $J = 3.8$ Hz), 4.20 (s, 2H), 2.33 (s, 3H). $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 169.75, 137.29, 136.00, 130.51, 129.82, 129.14, 125.42, 125.10, 124.00, 120.98, 116.98, 109.58, 42.88, 21.30. HRMS (EI): Calculated for C$_{17}$H$_{15}$NO [M]$^+$ 249.1154, found 249.1144.

**Compound 1o**: (1-(1H-indol-1-yl)-2,2-diphenylethanone)

![Compound 1o](image)

Compound 1o was obtained as colorless solid. Yield: 45%, Melting point: 91-93 °C. $^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 8.56 (d, 1H, $J = 8.4$ Hz), 7.52 (d, 1H, $J = 7.4$ Hz), 7.45 (d, 1H, $J = 3.8$ Hz), 7.40-7.21 (m, 12H), 6.54 (d, 1H, $J = 3.9$ Hz), 5.76 (s, 2H). $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 170.60, 138.50, 136.22, 130.43, 129.10, 128.45, 127.80, 125.52, 125.22, 124.15, 120.98, 117.20, 109.77, 58.02. HRMS (EI): Calculated for C$_{22}$H$_{17}$NO [M]$^+$ 311.1310, found 311.1312.

**Compound 1p**: (2,2-bis(4-chlorophenyl)-1-(1H-indol-1-yl)ethanone)

![Compound 1p](image)

Compound 1p was obtained as colorless solid. Yield: 78%, Melting point: 46-48 °C. $^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 8.52 (d, 1H, $J = 8.5$ Hz), 7.53 (d, 1H, $J = 7.7$ Hz), 7.42-7.11 (m, 11H), 6.56 (d, 1H, $J = 3.5$ Hz), 5.68 (s, 1H). $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 169.75, 136.58, 136.13, 134.06, 130.45, 130.34, 129.40, 125.74, 124.78, 124.43, 121.15, 117.11, 110.32, 56.54. HRMS (EI): Calculated for C$_{22}$H$_{15}$Cl$_2$NO [M]$^+$ 379.0531, found 379.0564.
Compound 1r: (1-(5-methyl-1H-indol-1-yl)-2,2-diphenylethanone)

Compound 1r was obtained as pale yellow solid. Yield: 28%, Melting point: 73-75 °C. $^1$H NMR (300 MHz, CDCl$_3$) $\delta$ 8.42 (d, 1H, $J = 8.5$ Hz), 7.81 (dd, 1H, $J = 8.1$ Hz, 1.2 Hz), 7.49 (d, 1H, $J = 7.9$ Hz), 7.41 (d, 1H, $J = 3.8$ Hz), 7.38-7.25 (m, 9H), 7.17 (d, 1H, $J = 8.4$ Hz), 6.47 (d, 1H, $J = 3.8$ Hz), 5.75 (s, 1H), 2.42 (s, 3H). $^{13}$C NMR (75 MHz, CDCl$_3$) $\delta$ 170.22, 138.43, 137.63, 134.22, 133.58, 132.45, 130.52, 130.10, 128.92, 128.31, 127.59, 126.62, 125.10, 120.76, 116.64, 109.41, 57.74, 21.38. HRMS (EI): Calculated for C$_{23}$H$_{19}$NO [M]$^+$ 325.1467, found 325.1484.
Optimization of reaction conditions for compound 3a

1. Screening of solvents:

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<th>Solvent</th>
<th>% yield</th>
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<td>Dioxane</td>
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<td>THF</td>
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<td>t-AmOH</td>
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<tr>
<td>HFIP</td>
<td>34</td>
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Reactions carried out with 0.2 mmol of 1a, 3 equiv of acrylate 2a, Ru cat (10 mol %), AgSbF₆ (40 mol%) and Cu(OAc)₂·H₂O (2 equiv) in 1 mL of solvent in a sealed vial for 24 h at 120 ºC. nd = not detected.

Comments: DCM, THF, HFIP showed similar conversion on LCMS, but due to pressure generation in DCM and expensiveness of HFIP, THF was elected for further optimization.

2. Screening of catalyst:

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<th>Catalyst</th>
<th>% yield⁴</th>
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</tr>
<tr>
<td>Ru(PPh₃)₃Cl₂</td>
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<tr>
<td>[Rut(Cp*)Cl₂]₂</td>
<td>nd</td>
</tr>
<tr>
<td>RuCl₃ + PPh₃</td>
<td>Nd</td>
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</tbody>
</table>

⁴ Reaction conditions: 0.2 mmol of 1a, 3 equiv of acrylate 2a, Ru cat (10 mol %), AgSbF₆ (40 mol%) and Cu(OAc)₂·H₂O (2 equiv) in 1 mL of solvent in a sealed vial for 24 h at 120 ºC.
Reactions carried out with 0.2 mmol of 1a, 3 equiv of acrylate 2a, cat (10 mol %), AgSbF$_6$ (40 mol%) and Cu(OAc)$_2$.H$_2$O (2 equiv) in 1 mL dry THF in a sealed vial for 24 h at 120 °C. nd = not detected. bOnly alkenylated product was found as palladium was reported earlier for C-2 alkenylation of indole.

Comments: Use of an analagous Rh-catalyst afforded the same isolated yield of desired compound in comparison with the Ru-catalyst. Loading of the expensive Rh-catalyst did not make sense as other cheaper source was working effectively.

3. Screening of time and temperature:

<table>
<thead>
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<th>Temperature (°C)</th>
<th>Time (h)</th>
<th>% yield</th>
</tr>
</thead>
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<tr>
<td>120</td>
<td>24</td>
<td>37</td>
</tr>
<tr>
<td>120</td>
<td>48</td>
<td>40</td>
</tr>
<tr>
<td>100</td>
<td>48</td>
<td>47</td>
</tr>
</tbody>
</table>

Reactions carried out with 0.2 mmol of 1a, 3 equiv of acrylate 2a, Ru cat (5 mol %), AgSbF$_6$ (20 mol%) and Cu(OAc)$_2$.H$_2$O (2 equiv) in 1 mL dry THF in a sealed vial.

Comments: Lowering the temperature and twice the reaction run time favoured the product formation.

4. Screening of acid additive:

<table>
<thead>
<tr>
<th>Additive acid (equiv)</th>
<th>% yield</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pivalic acid (3 equiv)</td>
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</tr>
<tr>
<td>Pivalic acid (5 equiv)</td>
<td>63</td>
</tr>
<tr>
<td>Acetic acid (5 equiv)</td>
<td>61</td>
</tr>
<tr>
<td>Acetic acid:THF (1:1)</td>
<td>52</td>
</tr>
</tbody>
</table>

Reactions carried out with 0.2 mmol of 1a, 3 equiv of acrylate 2a, Ru cat (5 mol %), AgSbF$_6$ (20 mol%) and Cu(OAc)$_2$.H$_2$O (2 equiv) in 1 mL dry THF in a sealed vial at 100 °C for 48 h.

Comments: Addition of pivalic or acetic acid helps the formation of product in better yields through Concerted-Metallation Deprotonation (CMD) path.
General procedure for the synthesis of compounds 3a-3u

To an oven dried 5 mL microwave vial containing a stir bar was added 1-(1H-indol-1-yl)-2-arylethanone 1a-1r (0.5 mmol), Ru[(p-cymene)Cl]2 (15 mg, 5 mol%), Cu(OAc)2•H2O (200 mg), silver source (20 mol%) in dry solvent (2 mL) was added to this vial and the mixture was stirred for 10 min at room temperature. Then acrylate 2a-2f (1.00 mmol) and Acetic acid (150 μL) was added via syringe and the vial was sealed with taflon cap. The vial was tightly sealed and the mixture was heated with stirring in a preheated oil bath at 100 °C for stipulated time. After allotted time the mixture was cooled to room temperature, diluted with EtOAc (5 mL) and filtered through celite pad. The pad was further washed with EtOAc (25 mL) and the combined organic solvent was evaporated in vacuo to afford a crude mixture which was purified by silica gel flash column chromatography using pet.ether/EtOAc (9:1) as eluent to afford compound 3a-3u (cis-diastereomer) along with inseparable diastereomer 4a-4u. The structure of compound 3a was confirmed on the basis of its XRD analysis and by analogy, structures of rest of compounds 3b-3u were established.

Compound 3a: (methyl 2-(3-oxo-2-phenyl-2,3-dihydro-1H-pyrrolo[1,2-a]indol-1-yl)acetate)

Compound 3a obtained as pale yellow solid along with its diastereomer 4a in ratio 3a:4a = 4.3:1. Combined yield: 65%. 1H NMR (300 MHz, CDCl3) (major diastereomer) δ 8.17-8.04 (m, 1H), 7.58-7.51 (m, 1H), 7.41-7.22 (m, 7H), 6.38 (s, 1H), 4.07 (d, 1H, J = 5.2 Hz), 3.94-3.86 (m, 1H), 3.67 (s, 3H), 2.97-2.77 (m, 2H). 13C NMR (75 MHz, CDCl3) (major
Compound 3b: (ethyl 2-(3-oxo-2-phenyl-2,3-dihydro-1H-pyrrolo[1,2-a]indol-1-yl)acetate)

Compound 3b obtained as pale yellow viscous liquid along with its diastereomer 4b in ratio 3b:4b = 4:1. Combined yield: 63%. \(^1\)H NMR (300 MHz, CDCl\(_3\)) (major diastereomer) \(\delta\) 8.15-8.05 (m, 1H), 7.57-7.51 (m, 1H), 7.44-7.21 (m, 6.6H), 7.13-7.02 (m, 0.4H), 6.39 (s, 0.8H), 6.35 (s, 0.2H), 4.64 (d, \(J = 8.7\) Hz, 0.2H), 4.35-4.23 (m, 0.2H), 4.17-4.05 (m, 2.8H), 3.95-3.85 (m, 0.8H), 2.91-2.82 (m, 1.6H), 2.45 (dd, \(J = 16.9\) Hz, 7.7 Hz, 0.2H), 2.20 (dd, \(J = 16.8\) Hz, 7.8 Hz, 0.2H), 1.23-1.13 (m, 3H). \(^{13}\)C NMR (75 MHz, CDCl\(_3\)) (major diastereomer) \(\delta\) 171.54, 171.45, 170.96, 170.87, 145.24, 144.39, 137.44, 135.30, 135.23, 134.87, 130.74, 129.75, 129.32, 129.05, 128.29, 128.17, 124.57, 124.06, 121.13, 114.25, 114.18, 101.41, 61.16, 60.96, 59.64, 56.80, 39.51, 38.72, 36.19, 34.59, 14.28. HRMS (EI): Calculated for C\(_{16}\)H\(_{13}\)NO \([M]^+\) 319.1208, found 319.1172.

Compound 3c: (butyl 2-(3-oxo-2-phenyl-2,3-dihydro-1H-pyrrolo[1,2-a]indol-1-yl)acetate)

Compound 3c obtained as pale yellow viscous liquid along with its diastereomer 4c in ratio 3c:4c = 4:1. Combined yield: 61%. \(^1\)H NMR (300 MHz, CDCl\(_3\)) (major diastereomer) \(\delta\) 8.15-8.05 (m, 1H), 7.57-7.51 (m, 1H), 7.42-7.21 (m, 6.6H), 7.13-7.04 (m, 0.4H), 6.39 (s, 0.8H), 6.34 (s, 0.2H), 4.64 (d, \(J = 8.78\) Hz, 0.2H), 4.34-4.24 (m, 0.2H), 4.10-4.02 (m, 2.8H), 3.94-3.86 (m, 0.8H), 2.90-2.82 (m, 1.6H), 2.46 (dd, \(J = 16.9\) Hz, 7.5 Hz, 0.2H), 2.21 (dd, \(J = 17.0\) Hz, 7.8 Hz, 0.2H), 1.58-1.45 (m, 2H), 1.40-1.23 (m, 2H), 0.93-0.85 (m, 3H). \(^{13}\)C NMR
(75 MHz, CDCl₃) (major diastereomer) δ 171.55, 171.06, 170.87, 145.27, 144.39, 135.32, 135.23, 134.89, 130.75, 129.74, 129.34, 129.06, 128.30, 128.18, 128.30, 128.00, 127.96, 127.88, 124.57, 124.06, 121.13, 114.26, 114.19, 101.40, 65.10, 64.99, 64.89, 59.64, 56.84, 39.53, 38.69, 36.11, 34.62, 30.70, 19.28, 13.85.

HRMS (EI): Calculated for C₂₃H₂₃NO₃ [M]⁺ 361.1678, found 361.1671.

**Compound 3d**: (isobutyl 2-(3-oxo-2-phenyl-2,3-dihydro-1H-pyrrolo[1,2-a]indol-1-yl)acetate)

![Compound 3d](image)

Compound 3d obtained as pale yellow viscous liquid along with its diastereomer 4d in ratio 3d:4d = 3:1. Combined yield: 66%. **¹H NMR (300 MHz, CDCl₃) (major diastereomer)** δ 8.15-8.05 (m, 1H), 7.57-7.52 (m, 1H), 7.41-7.26 (m, 6.5H), 7.11-7.03 (m, 0.5H), 6.39 (s, 0.8H), 6.35 (s, 0.2H), 4.65 (d, J = 8.8 Hz, 0.2H), 4.3 -4.26 (m, 0.25H), 4.08 (d, J = 5.2 Hz, 0.8H), 3.96-3.74 (m, 1.5H), 2.54-2.42 (m, 0.25H), 2.28-2.17 (m, 0.25H), 1.93-1.77 (m, 1H), 0.90-0.85 (m, 6H). **¹³C NMR (75 MHz, CDCl₃) (major diastereomer)** δ 171.54, 171.07, 170.84, 145.28, 144.40, 137.44, 135.33, 135.25, 134.92, 130.78, 129.73, 129.34, 129.07, 128.30, 128.18, 124.57, 124.06, 121.13, 114.26, 114.20, 101.42, 71.32, 71.17, 59.62, 56.86, 39.54, 38.65, 36.01, 34.63, 27.80, 22.53, 19.22, 14.25. **HRMS (EI)**: Calculated for C₂₃H₂₃NO₃ [M]⁺ 361.1678, found 361.1659.

**Compound 3e**: (cyclohexyl 2-(3-oxo-2-phenyl-2,3-dihydro-1H-pyrrolo[1,2-a]indol-1-yl)acetate)

![Compound 3e](image)

Compound 3e obtained as pale yellow viscous liquid along with its diastereomer 4e in ratio 3e:4e = 6.7:1. Combined yield: 67%. **¹H NMR (300 MHz, CDCl₃) (major diastereomer)** δ
8.21-7.98 (m, 1H), 7.57-7.51 (m, 1H), 7.40-7.21 (m, 6.5H), 7.09-7.03 (m, 0.5H), 6.38 (s, 0.75H), 6.34 (s, 0.25H), 4.81-4.66 (m, 1H), 4.63 (d, J = 8.7 Hz, 0.25H), 4.33-4.22 (m, 0.25H), 4.07 (d, J = 5.1 Hz, 0.75H), 3.93-3.85 (m, 0.75H), 2.92-2.76 (m, 1.5H), 2.44 (dd, J = 16.9 Hz, 7.5 Hz, 0.25H), 2.19 (dd, J = 16.9 Hz, 7.5 Hz, 0.25H), 1.85-1.77 (m, 1H), 1.76-1.59 (m, 3H), 1.56-1.45 (m, 1H), 1.42-1.14 (m, 6H). 

$^{13}$C NMR (75 MHz, CDCl$_3$) (major diastereomer) $\delta$ 171.59, 170.91, 170.38, 145.38, 144.49, 137.50, 135.31, 135.23, 134.98, 130.72, 129.68, 129.30, 129.05, 128.29, 128.12, 124.52, 123.99, 121.09, 114.21, 114.15, 101.35, 73.75, 73.48, 59.61, 56.85, 39.53, 39.03, 36.31, 34.61, 31.73, 31.65, 25.41, 23.89.

HRMS (EI): Calculated for C$_{25}$H$_{25}$NO$_3$ [M]$^+$ 387.1834, found 387.1836.

Compound 3h: (methyl 2-((3-chlorophenyl)-3-oxo-2,3-dihydro-1H-pyrrolo[1,2-a]indol-1-yl)acetate)

![Chemical structure of compound 3h](image.png)

Compound 3h obtained as pale yellow viscous liquid along with its diastereomer 4h in ratio 3h:4h = 5.7:1. Combined yield: 67%. 

$^1$H NMR (300 MHz, CDCl$_3$) (major diastereomer) $\delta$ 8.13-8.02 (m, 1H), 7.56-7.50 (m, 1H), 7.34-7.23 (m, 5H), 7.16-7.10 (m, 1H), 6.38 (s, 0.85H), 6.34 (s, 0.15H), 4.60 (d, J = 8.9 Hz, 0.1H), 4.04 (d, J = 5.3 Hz, 0.9H), 3.67 (s, 2.6H), 3.58 (s, 0.4H), 2.85 (d, J = 7.1 Hz, 1.7H), 2.48 (dd, J = 16.9 Hz, 7.5 Hz, 0.15H), 2.19 (dd, J = 16.9 Hz, 8.0 Hz, 0.15H). 

$^{13}$C NMR (75 MHz, CDCl$_3$) (major diastereomer) $\delta$ 171.64, 171.27, 170.66, 170.05, 144.59, 143.83, 139.24, 136.71, 135.25, 135.16, 135.04, 134.88, 130.67, 130.55, 130.25, 130.05, 128.50, 128.39, 127.77, 126.49, 124.69, 124.18, 121.19, 114.20, 114.14, 101.69, 101.63, 60.55, 59.06, 56.22, 52.15, 39.29, 38.24, 35.90, 34.44. HRMS (EI): Calculated for C$_{20}$H$_{16}$ClNO$_3$ [M]$^+$ 353.0819, found 353.0869.

Compound 3i: (methyl 2-((4-fluorophenyl)-3-oxo-2,3-dihydro-1H-pyrrolo[1,2-a]indol-1-yl)acetate)
Compound 3i obtained as pale yellow viscous liquid along with its diastereomer 4i in ratio 3i:4i = 4:1. Combined yield: 59%. \(^1\)H NMR (300 MHz, CDCl\(_3\)) (major diastereomer) \(\delta\) 8.13-8.03 (m, 1H), 7.56-7.51 (m, 1H), 7.42-7.15 (m, 3.5H), 7.11-6.98 (m, 2.5H), 6.38 (s, 0.8H), 6.34 (s, 0.2H), 4.63 (d, \(J = 8.8\) Hz, 0.2H), 4.31-4.20 (m, 0.2H), 4.05 (d, \(J = 5.3\) Hz, 0.8H), 3.89-3.80 (m, 0.8H), 3.67 (s, 2.4H), 3.58 (s, 0.6H), 2.86 (d, \(J = 7.1\) Hz, 1.6H), 2.47 (dd, \(J = 17.2\) Hz, 7.3 Hz, 0.20H), 2.19 (dd, \(J = 17.0\)Hz, 8.1 Hz, 0.20H). \(^{13}\)C NMR (75 MHz, CDCl\(_3\)) (major diastereomer) \(\delta\) 171.35, 170.55, 163.38, 161.75, 143.95, 135.24, 133.15, 133.13, 131.51, 131.45, 130.70, 129.99, 129.94, 124.69, 124.64, 124.14, 121.16, 116.29, 116.15, 116.06, 115.91, 114.19, 114.13, 111.58, 101.52, 58.78, 55.95, 52.12, 51.97, 39.48, 38.26, 35.90, 34.52. HRMS (EI): Calculated for C\(_{20}\)H\(_{16}\)FNO\(_3\) [M]+ 337.1114, found 337.1135.

Compound 3j: (methyl 2-(2-(2-bromophenyl)-3-oxo-2,3-dihydro-1H-pyrrolo[1,2-a]indol-1-yl)acetate)

Compound 3j obtained as pale yellow viscous liquid along with its diastereomer 4j in ratio 3j:4j = 15.7:1. Combined yield: 58%. \(^1\)H NMR (300 MHz, CDCl\(_3\)) (major diastereomer) \(\delta\) 8.14-8.04 (m, 1H), 7.61 (d, \(J = 7.6\) Hz, 0.7H), 7.54-7.50 (m, 1H), 7.40-7.14 (m, 5.3H), 6.37 (s, 1H), 4.53 (d, \(J = 5.8\) Hz, 0.7H), 4.06 (d, \(J = 5.1\) Hz, 0.3H), 3.98-3.85 (m, 1H), 3.66 (s, 3H), 3.06-2.82 (m, 2H). \(^{13}\)C NMR (75 MHz, CDCl\(_3\)) (major diastereomer) \(\delta\) 171.42, 170.78, 169.98, 144.26, 144.10, 137.35, 136.92, 135.26, 135.12, 133.69, 130.95, 130.71, 130.63, 129.86, 129.30, 128.32, 128.26, 128.16, 124.56, 124.06, 121.12, 114.14, 101.44, 59.56, 59.36, 52.11, 39.48, 39.08, 38.31, 38.07. HRMS (EI): Calculated for C\(_{20}\)H\(_{16}\)BrNO\(_3\) [M]+ 397.0314, found 397.0317.
**Compound 3k**: (methyl 2-(3-oxo-2-(4-(trifluoromethyl)phenyl)-2,3-dihydro-1H-pyrrolo[1,2-a]indol-1-yl)acetate)

Compound 3k obtained as pale yellow viscous liquid along with its diastereomer 4k in ratio 3k:4k = 11.5:1. Combined yield: 58%.  

\[ ^1H \text{ NMR (300 MHz, CDCl}_3 \] major diastereomer \[ \delta \]

- 8.13-8.03 (m, 1H)
- 7.64 (d, J = 8.2 Hz, 2H)
- 7.57-7.52 (m, 1H)
- 7.40 (d, J = 8.0 Hz, 2H)
- 7.35-7.29 (m, 2H)
- 6.41 (s, 0.92H)
- 6.37 (s, 0.08H)
- 4.72 (d, J = 7.9 Hz, 0.08H)
- 4.38-4.27 (m, 0.08H)
- 4.16 (d, J = 5.2 Hz, 0.92H)
- 3.94-3.86 (m, 0.92H)
- 3.67 (s, 2.83H)
- 3.54 (s, 0.17H)
- 2.89 (d, J = 7.2 Hz, 1.84H)
- 2.49 (dd, J = 16.8 Hz, 7.6 Hz, 0.08H)
- 2.19 (dd, J = 17.0 Hz, 8.2 Hz, 0.08H)

\[ ^13C \text{ NMR (75 MHz, CDCl}_3 \] major diastereomer \[ \delta \]

- 171.26
- 169.94
- 143.75
- 141.36
- 135.29
- 130.71
- 128.77
- 126.31
- 126.27
- 124.82
- 124.31
- 121.27
- 101.79
- 59.27
- 52.21
- 39.23
- 38.35

HRMS (EI): Calculated for C\textsubscript{21}H\textsubscript{16}F\textsubscript{3}NO\textsubscript{3} [M\textsuperscript{+}] 387.1082, found 387.1077.

**Compound 3l**: (ethyl 2-(2-(3,4-dichlorophenyl)-3-oxo-2,3-dihydro-1H-pyrrolo[1,2-a]indol-1-yl)acetate)

Compound 3l obtained as pale yellow viscous liquid along with its diastereomer 4l in ratio 3l:4l = 6.1:1. Combined yield: 60%.  

\[ ^1H \text{ NMR (300 MHz, CDCl}_3 \] major diastereomer \[ \delta \]

- 8.11-8.01 (m, 1H)
- 7.56-7.51 (m, 1H)
- 7.43 (d, J = 8.1 Hz, 1H)
- 7.38 (d, J = 2.1 Hz, 1H)
- 7.34-7.28 (m, 2H)
- 7.11 (dd, J = 8.3 Hz, 2.1 Hz, 0.88H)
- 6.91 (dd, J = 8.3 Hz, 2.1 Hz, 0.12H)
- 6.39 (s, 0.88H)
- 6.36 (s, 0.12H)
- 4.60 (d, J = 8.8 Hz, 0.1H)
- 4.19-4.07 (q, 2H)
- 4.05 (d, J = 5.1 Hz, 1H)
- 3.88-3.81 (m, 0.9H)
- 2.85 (dd, J = 6.9 Hz, 1.9 Hz, 1.7H)
- 2.49 (dd, J = 17.1 Hz, 7.4 Hz, 0.15H)
- 2.20 (dd, J = 17.0 Hz, 8.2 Hz, 0.15H)

\[ ^13C \text{ NMR (75 MHz, CDCl}_3 \] major diastereomer \[ \delta \]

- 171.26
- 169.94
- 143.75
- 141.36
- 135.29
- 130.71
- 128.77
- 126.31
- 126.27
- 124.82
- 124.31
- 121.27
- 101.79
- 59.27
- 52.21
- 39.23
- 38.35

HRMS (EI): Calculated for C\textsubscript{21}H\textsubscript{16}Cl\textsubscript{2}NO\textsubscript{3} [M\textsuperscript{+}] 386.0915, found 386.0916.
**Compound 3m**: (methyl 2-(3-oxo-2-(p-tolyl)-2,3-dihydro-1H-pyrrolo[1,2-a]indol-1-yl)acetate)

Compound 3m obtained as pale yellow viscous liquid along with its diastereomer 4m in ratio 3m:4m = 2.3:1. Combined yield: 51%. **1H NMR (300 MHz, CDCl₃) (major diastereomer)** δ 8.14-8.04 (m, 1H), 7.56-7.50 (m, 1H), 7.32-7.25 (m, 2H), 7.19-7.09 (m, 3.5H), 6.93 (d, J = 8.2 Hz, 0.5H), 6.36 (s, 0.75H), 6.33 (s, 0.25H), 4.59 (d, J = 8.7 Hz, 0.25H), 4.30-4.19 (m, 0.25H), 4.01 (d, J = 5.3 Hz, 0.75H), 3.90-3.80 (m, 0.75H), 3.66 (s, 2.3H), 3.57 (s, 0.7H), 2.93-2.77 (m, 1.4H), 2.44 (dd, J = 16.8 Hz, 7.9 Hz, 0.30H), 2.33 (s, 2.2H), 231 (s, 0.8H), 2.21 (dd, J = 16.8 Hz, 7.5 Hz, 0.30H). **13C NMR (75 MHz, CDCl₃) (major diastereomer)** δ 171.93, 171.66, 171.47, 170.98, 145.23, 144.34, 137.92, 135.24, 135.18, 134.28, 131.71, 130.72, 129.97, 129.70, 129.55, 128.13, 124.50, 124.00, 121.09, 114.21, 114.15, 101.32, 59.23, 56.41, 52.09, 54.65, 39.50, 38.37, 35.96, 34.58, 21.29, 14.25. **HRMS (EI)**: Calculated for C₂₁H₁₇Cl₂NO₃ [M⁺] 401.0585, found 401.0531.

**Compound 3n**: (methyl 2-(2-(4-methoxyphenyl)-3-oxo-2,3-dihydro-1H-pyrrolo[1,2-a]indol-1-yl)acetate)
Compound 3n obtained as colorless solid along with its diastereomer 4n in ratio 3n:4n = 9:1. Combined yield: 40%. Melting point: 110-112 °C. $^1$H NMR (300 MHz, CDCl$_3$) (major diastereomer) δ 8.14-8.04 (m, 1H), 7.57-7.51 (m, 1H), 7.34-7.27 (m, 2H), 7.18 (d, $J$ = 8.8 Hz, 1.9H), 6.98 (d, $J$ = 8.7 Hz, 0.1H), 6.90 (d, $J$ = 8.7 Hz, 1.9H), 6.84 (d, $J$ = 8.7 Hz, 0.1H), 6.38 (s, 0.9H), 6.34 (s, 0.1H), 4.60 (d, $J$ = 8.8 Hz, 0.1H), 4.30-4.20 (m, 0.1H), 4.01 (d, $J$ = 5.4 Hz, 0.9H), 3.90-3.82 (m, 0.9H), 3.79 (s, 2.7H), 3.78 (s, 0.3H), 3.67 (s, 2.7H), 3.58 (s, 0.3H), 2.94-2.78 (m, 1.9H), 2.46 (dd, $J$ = 16.8 Hz, 7.7 Hz, 0.1H), 2.23 (dd, $J$ = 17.0 Hz, 7.8 Hz, 0.1H).

$^{13}$C NMR (75 MHz, CDCl$_3$) (major diastereomer) δ 171.52, 171.11, 159.51, 144.27, 135.24, 130.85, 130.75, 129.41, 129.32, 124.54, 124.06, 121.12, 114.74, 114.47, 114.19, 101.37, 58.89, 55.52, 52.15, 39.59, 38.31. HRMS (EI): Calculated for C$_{21}$H$_{19}$NO$_4$ [M]$^+$ 349.1314, found 349.1310.

**Compound 3o:** (methyl 2-(2-(4-nitrophenyl)-3-oxo-2,3-dihydro-1H-pyrrolo[1,2-a]indol-1-yl)acetate)

![Compound 3o](image)

Compound 3o obtained as pale yellow viscous liquid along with its diastereomer 4o in ratio 3o:4o = 6.7:1. Combined yield: 38%. $^1$H NMR (300 MHz, CDCl$_3$) (major diastereomer) δ 8.22 (d, $J$ = 8.7 Hz, 2H), 8.11-8.00 (m, 1H), 7.57-7.53 (m, 1H), 7.46 (d, $J$ = 8.6Hz, 2H), 7.35-7.29 (m, 2H), 6.42 (s, 0.9H), 6.39 (s, 0.1H), 4.23 (d, $J$ = 5.1 Hz, 1H), 3.98-3.84 (m, 1H), 3.68 (s, 2.75H), 3.56 (s, 0.25H), 2.99-2.82 (m, 1.74H), 2.52 (dd, $J$ = 17.1 Hz, 7.3 Hz, 0.13H), 2.17 (dd, $J$ = 17.2 Hz, 8.2 Hz, 0.13H). $^{13}$C NMR (75 MHz, CDCl$_3$) (major diastereomer) δ 171.17, 169.34, 147.73, 144.65, 143.42, 135.28, 130.67, 129.35, 124.93, 129.43, 121.33, 114.16, 101.97, 59.16, 52.26, 39.04, 38.38. HRMS (EI): Calculated for C$_{20}$H$_{16}$N$_2$O$_5$ [M]$^+$ 364.1059, found 364.1049.

**Compound 3p:** (methyl 2-(7-methyl-3-oxo-2-phenyl-2,3-dihydro-1H-pyrrolo[1,2-a]indol-1-yl)acetate)
Compound 3p obtained as pale yellow viscous liquid along with its diastereomer 4p in ratio 3p:4p = 3.3:1. Combined yield: 65%. 1H NMR (300 MHz, CDCl3) (major diastereomer) δ 7.99 (d, J = 8.3 Hz, 0.25H), 7.94 (d, J = 8.3 Hz, 0.75H), 7.40-7.22 (m, 5.5H), 7.17-7.10 (m, 1H), 7.09-7.01 (m, 0.5H), 6.30 (s, 0.75H), 6.26 (s, 0.25H), 4.61 (d, J = 8.8 Hz, 0.20H), 4.30-4.19 (m, 0.20H), 4.03 (d, J = 5.1 Hz, 0.8H), 3.91-3.82 (m, 0.8H), 3.65 (s, 2.3H), 3.55 (s, 0.7H), 2.88-2.82 (m, 1.5H), 2.50-2.39 (m, 3.25H), 2.19 (dd, J = 16.9 Hz, 7.8 Hz, 0.25H). 13C NMR (75 MHz, CDCl3) (major diastereomer) δ 171.90, 171.46, 171.28, 170.60, 145.26, 144.40, 137.48, 135.56, 135.48, 134.91, 134.32, 134.26, 129.72, 129.29, 129.00, 128.90, 128.26, 128.13, 125.33, 121.10, 113.81, 113.74, 101.20, 59.58, 56.75, 52.08, 51.92, 39.54, 38.39, 35.93, 34.59, 21.85. HRMS (EI): Calculated for C21H19NO3 [M]+ 333.1365, found 333.1365.

Compound 3q: (ethyl 2-(7-methyl-3-oxo-2-phenyl-2,3-dihydro-1H-pyrrolo[1,2-a]indol-1-yl)acetate)

Compound 3q obtained as pale yellow viscous liquid along with its diastereomer 4q in ratio 3q:4q = 3:1. Combined yield: 58%. 1H NMR (300 MHz, CDCl3) (major diastereomer) δ 8.00 (d, J = 8.4 Hz, 0.25H), 7.94 (d, J = 8.2 Hz, 0.75H), 7.40-7.22 (m, 5.5H), 7.17-7.02 (m, 1.5H), 6.31 (s, 0.75H), 6.27 (s, 0.25H), 4.62 (d, J = 8.6 Hz, 0.25H), 4.32-4.22 (m, 0.25H), 4.17-3.97 (m, 2.7H), 3.92-3.83 (m, 0.75H), 2.85 (d, J = 7.0 Hz, 1.5H), 2.50-2.39 (m, 3.25H), 2.19 (dd, J = 17.0 Hz, 7.8 Hz, 0.25H), 1.22-1.13 (m, 2.5H), 0.88 (t, 0.50H). 13C NMR (75 MHz, CDCl3) (major diastereomer) δ 171.47, 171.34, 170.98, 170.67, 145.39, 144.52, 137.57, 135.59, 135.51, 134.99, 134.30, 134.24, 129.74, 129.29, 129.02, 128.90, 128.28, 128.12, 125.31, 121.09, 113.82, 113.74, 101.18, 61.13, 60.92, 59.64, 56.80, 39.54, 38.76,
36.16, 34.61, 34.31, 22.53, 21.85, 14.28. **HRMS (EI):** Calculated for C_{22}H_{21}NO_3 [M]^+ 347.1521, found 347.1517.

**Compound 3r:** (methyl 2-(2-(3,4-dichlorophenyl)-7-methyl-3-oxo-2,3-dihydro-1H-pyrrolo[1,2-a]indol-1-yl)acetate)

![Chemical structure of compound 3r]

Compound 3r obtained as pale yellow viscous liquid along with its diastereomer 4r in ratio 3r:4r = 9:1. Combined yield: 59%. **1H NMR (300 MHz, CDCl_3)** (major diastereomer) \( \delta \) 7.97 (d, \( J = 8.1 \) Hz, 0.1H), 7.92 (d, \( J = 8.1 \) Hz, 0.9H), 7.44 (d, \( J = 8.3 \) Hz, 1H), 7.39-7.34 (m, 1H), 7.32 (s, 1H), 7.22 (d, \( J = 2.1 \) Hz, 0.1H), 7.17-7.07 (m, 1.8H), 6.90 (dd, \( J = 8.3 \) Hz, 2.1 Hz, 0.1H), 6.31 (s, 0.9H), 6.28 (s, 0.1H), 4.59 (d, \( J = 8.8 \) Hz, 0.1H), 4.31-4.21 (m, 0.1H), 4.03 (d, \( J = 5.2 \) Hz, 0.9H), 3.86-3.77 (m, 0.9H), 3.68 (s, 2.7H), 3.59 (s, 0.3H), 2.93-2.77 (m, 1.9H), 2.45 (s, 3H), 2.19 (dd, \( J = 17.1 \) Hz, 8.2 Hz, 0.1H). **13C NMR (75 MHz, CDCl_3)** (major diastereomer) \( \delta \) 171.26, 169.50, 143.67, 137.58, 135.55, 134.59, 133.32, 132.44, 131.22, 130.36, 128.85, 127.67, 125.59, 121.24, 113.77, 101.63, 58.57, 52.24, 39.22, 38.36, 21.86. **HRMS (EI):** Calculated for C_{21}H_{17}Cl_2NO_3 [M]^+ 401.0585, found 401.0559.

**Compound 3s:** (methyl 2-(2-(4-methoxyphenyl)-7-methyl-3-oxo-2,3-dihydro-1H-pyrrolo[1,2-a]indol-1-yl)acetate)

![Chemical structure of compound 3s]

Compound 3s obtained as colorless solid along with its diastereomer 4s in ratio 3s:4s = 9:1. Combined yield: 44%. Melting point: 106-108 °C. **1H NMR (300 MHz, CDCl_3)** (major diastereomer) \( \delta \) 7.99 (d, 1H, \( J = 8.4 \) Hz, 0.1H), 7.94 (d, \( J = 8.3 \) Hz, 0.9H), 7.32 (s, 1H), 7.17 (d, \( J = 8.9 \) Hz, 1.8H), 7.12 (dd, \( J = 8.1 \) Hz, 0.9 Hz, 0.9H), 6.97 (d, \( J = 8.8 \) Hz, 0.2H), 6.89 (d, \( J = 8.8 \) Hz, 1.8H), 6.84 (d, \( J = 8.6 \) Hz, 0.2H), 6.29 (s, 0.9H), 6.26 (s, 0.1H), 4.59 (d, \( J = 8.7 \) Hz, 0.1H), 4.49 (s, 1H), 4.19 (s, 1H), 3.83 (s, 6H), 3.65 (s, 3H), 2.91 (s, 3H), 2.19 (dd, \( J = 17.1 \) Hz, 8.2 Hz, 0.1H).
Hz, 0.1H), 4.27-4.18 (m, 0.1H), 3.99 (d, J = 5.4 Hz, 0.9H), 3.87-3.81 (m, 0.9H), 3.79 (s, 2.7H), 3.78 (s, 0.3H), 3.67 (s, 2.7H), 3.58 (s, 0.3H), 2.92-2.78 (m, 1.9H), 2.45 (s, 3H), 2.21 (dd, J = 17.0 Hz, 7.9 Hz, 0.1H). $^{13}$C NMR (75 MHz, CDCl$_3$) (major diastereomer) $\delta$ 171.56, 170.94, 159.48, 159.41, 144.41, 135.54, 134.24, 130.85, 129.64, 129.40, 128.92, 125.33, 121.09, 114.73, 114.55, 114.45, 113.77, 101.17, 58.90, 55.52, 52.14, 39.64, 38.37, 21.87. HRMS (EI): Calculated for C$_{22}$H$_{21}$NO$_4$ [M]$^+$ 363.1471, found 363.1489.

**Compound 3t:** (methyl 2-(2-(3-chlorophenyl)-7-methyl-3-oxo-2,3-dihydro-1H-pyrrolo[1,2-a]indol-1-yl)acetate)

![Compound 3t](image)

Compound 3t obtained as pale yellow viscous liquid along with its diastereomer 4t in ratio 3t:4t = 6.1:1. Combined yield: 60%. $^1$H NMR (300 MHz, CDCl$_3$) (major diastereomer) $\delta$ 7.98 (d, J = 8.2 Hz, 0.15H), 7.93 (d, J = 8.3 Hz, 0.85H), 7.35-7.23 (m, 4H), 7.16-7.08 (m, 2H), 6.31 (s, 0.85H), 6.28 (s, 0.15H), 4.60 (d, J = 8.8 Hz, 0.15H), 4.32-4.21 (m, 0.15H), 4.03 (d, J = 5.2 Hz, 0.85H), 3.89-3.79 (m, 0.85H), 3.67 (s, 2.60H), 3.58 (s, 0.40H), 2.85 (d, J = 7.1 Hz, 1.85H), 2.45 (s, 3H), 2.19 (dd, J = 17.0 Hz, 8.2 Hz, 0.15H). $^{13}$C NMR (75 MHz, CDCl$_3$) (major diastereomer) $\delta$ 171.33, 169.89, 143.96, 139.39, 135.56, 135.07, 134.47, 130.56, 128.87, 128.51, 128.40, 126.51, 125.49, 121.19, 113.77, 101.47, 59.12, 52.18, 39.37, 38.38, 21.86. HRMS (EI): Calculated for C$_{21}$H$_{18}$ClNO$_3$ [M]$^+$ 367.0975, found 367.0943.

**Compound 3u:** (methyl 2-(7-bromo-3-oxo-2-phenyl-2,3-dihydro-1H-pyrrolo[1,2-a]indol-1-yl)acetate)

![Compound 3u](image)

Compound 3u obtained as pale yellow viscous liquid along with its diastereomer 4u in ratio 3u:4u = 6.1:1. Combined yield: 63%. $^1$H NMR (300 MHz, CDCl$_3$) (major diastereomer) $\delta$
7.97 (d, J = 8.6 Hz, 0.2H), 7.92 (d, J = 8.5 Hz, 0.8H), 7.66 (s, 1H), 7.45-7.19 (m, 5.5H), 7.09-6.99 (m, 0.5H), 6.32 (s, 0.8H), 6.28 (s, 0.2H), 4.63 (d, J = 8.8 Hz, 0.2H), 4.31-4.20 (m, 0.2H), 4.05 (d, J = 5.3 Hz, 0.8H), 3.92-3.83 (m, 0.8H), 3.66 (s, 2.4H), 3.56 (s, 0.6H), 2.86 (dd, J = 7.2 Hz, 3.1 Hz, 1.7H), 2.44 (dd, J = 17.0 Hz, 7.9 Hz, 0.15H), 2.20 (dd, J = 16.9 Hz, 7.7 Hz, 0.15H). 13C NMR (75 MHz, CDCl3) (major diastereomer) δ 171.58, 171.19, 170.67, 170.56, 146.29, 145.42, 136.84, 136.74, 129.55, 129.37, 129.23, 129.18, 128.95, 128.63, 128.15, 128.13, 126.80, 123.75, 120.99, 117.70, 115.23, 115.18, 100.66, 100.60, 59.18, 56.41, 52.02, 51.86, 39.32, 37.85, 35.70, 34.45. HRMS (EI): Calculated for C20H16BrNO3 [M]+ 397.0314, found 397.0347.

General procedure for the synthesis of compounds 5a-5d

To an oven dried 5 mL microwave vial containing a stir bar was added 1-(1H-indol-1-yl)-2-arylethanone 1s-1u (0.5 mmol), Ru[(p-cymene)Cl]2 (15 mg, 5 mol%), Cu(OAc)2•H2O (200 mg), silver source (20 mol%) in dry solvent (2 mL) was added to this vial and the mixture was stirred for 10 min at room temperature. Then acrylate 2a-2b (1.00 mmol) and Acetic acid (150 μL) was added via syringe and the vial was sealed with taflon cap. The vial was tightly sealed and the mixture was heated with stirring in a preheated oil bath at 100 °C for stipulated time. After allotted time the mixture was cooled to room temperature, diluted with EtOAc (5 mL) and filtered through celite pad. The pad was further washed with EtOAc (25 mL) and the combined organic solvent was evaporated in vacuo to afford a crude mixture which was purified by silica gel flash column chromatography using pet.ether/EtOAc (9:1) as eluent to afford compound 5a-5d. The structure of compound 5a was confirmed on the basis of its XRD analysis and by analogy, structures of rest of compounds 5b-5d were established.

Compound 5a: (methyl 6-oxo-6a-phenyl-6,6a,11,11a-tetrahydroindenol[2′,1′:3,4]pyrrolo[1,2-a]indole-11-carboxylate)
Compound 5a obtained as colorless solid. Yield: 72%, Melting point: 100-104 °C. \(^1\)H NMR (300 MHz, CDCl\(_3\)) \(\delta\) 8.13-8.07 (m, 1H), 7.64-7.60 (m, 1H), 7.54-7.45 (m, 2H), 7.39-7.36 (m, 2H), 7.34-7.27 (m, 5H), 7.24-7.19 (m, 2H), 6.44 (s, 1H), 4.58 (t, 1H), 4.39 (d, \(J = 2.3\) Hz, 1H), 3.73 (s, 3H). \(^{13}\)C NMR (75 MHz, CDCl\(_3\)) \(\delta\) 171.85, 171.47, 143.64, 140.91, 140.32, 135.00, 130.92, 129.27, 128.56, 128.51, 128.29, 127.81, 127.59, 124.47, 123.96, 121.00, 114.14, 101.68, 66.91, 51.88, 40.39, 38.45. HRMS (EI): Calculated for C\(_{26}\)H\(_{19}\)NO\(_3\) [M]+ 393.1365, found 393.1486.

**Compound 5b:** (ethyl 6-oxo-6a-phenyl-6,6a,11,11a-tetrahydroinden[2’,1’:3,4]pyrrolo[1,2-a]indole-11-carboxylate)

Compound 4b obtained as colorless solid. Yield: 65%, Melting point: 130-132 °C. \(^1\)H NMR (300 MHz, CDCl\(_3\)) \(\delta\) 8.12-8.07 (m, 1H), 7.66-7.58 (m, 1H), 7.55-7.46 (m, 2H), 7.40-7.35 (m, 2H), 7.34-7.27 (m, 5H), 7.24-7.19 (m, 2H), 6.44 (s, 1H), 4.58 (t, 1H), 4.36 (d, \(J = 2.3\) Hz, 1H), 4.21-4.11 (dq, 2H), 1.19 (t, 3H). \(^{13}\)C NMR (75 MHz, CDCl\(_3\)) \(\delta\) 172.24, 171.86, 143.64, 141.72, 141.34, 140.09, 135.43, 130.76, 129.60, 129.31, 128.84, 127.79, 127.62, 126.71, 126.09, 124.67, 124.12, 121.11, 114.22, 101.25, 72.96, 61.86, 56.98, 51.20, 14.26. HRMS (EI): Calculated for C\(_{27}\)H\(_{21}\)NO\(_3\) [M]+ 407.1521, found 407.1490.

**Compound 5c:** methyl 2-methyl-6-oxo-6a-phenyl-6,6a,11,11a-tetrahydroinden[2’,1’:3,4]pyrrolo[1,2-a]indole-11-carboxylate)
Compound 5c obtained as colorless solid. Yield: 69%. Melting point: 80-82 °C. **H NMR (300 MHz, CDCl$_3$) $\delta$ 7.98-7.93 (m, 1H), 7.65-7.65 (m, 1H), 7.49-7.44 (m, 1H), 7.39-7.34 (m, 2H), 7.33-7.27 (m, 4H), 7.24-7.16 (m, 2H), 7.13-7.09 (m, 1H), 6.83 (s, 0.1H), 6.36 (s, 0.9H), 4.68 (d, $J = 8.9$ Hz, 0.1H), 4.59-4.51 (m, 0.9H), 4.37 (d, $J = 9.0$ Hz, 1.4 Hz, 0.1H), 4.3 (d, $J = 2.3$ Hz, 0.9H), 3.78 (s, 0.3H), 3.73 (s, 2.7H), 2.43 (s, 3H). **C NMR (75 MHz, CDCl$_3$) $\delta$ 172.44, 171.98, 144.61, 141.79, 141.48, 139.88, 135.71, 134.42, 129.56, 129.35, 128.93, 128.84, 127.76, 127.58, 126.72, 126.12, 125.40, 121.09, 113.79, 101.06, 72.92, 56.79, 52.86, 51.19, 21.86. HRMS (EI): Calculated for C$_{27}$H$_{21}$NO$_3$ [M]$^+$ 407.1521, found 407.1510.

Compound 5d: (methyl 9-chloro-6a-(4-chlorophenyl)-2-methyl-6-oxo-6a,11,11a-tetrahydroindeno[2',1':3,4]pyrrolo[1,2-a]indole-11-carboxylate)

Compound 5d obtained as colorless solid. Yield: 64%. Melting point: 88-90 °C. **H NMR (300 MHz, CDCl$_3$) $\delta$ 7.94 (d, $J = 8.2$ Hz, 0.8H), 7.90 (d, $J = 8.3$ Hz, 0.2H), 7.54-7.41 (m, 2H), 7.37-7.27 (m, 4H), 7.23-7.01 (m, 3H), 6.37 (s, 0.8H), 6.34 (s, 0.2 H), 4.53 (t, 1H), 4.33 (d, $J = 2.3$ Hz, 1H), 3.77 (s, 2.6H), 3.63 (s, 0.4H), 2.44 (s, 3H). **C NMR (75 MHz, CDCl$_3$) $\delta$ 171.73, 171.07, 143.69, 141.52, 139.78, 139.74, 135.89, 135.66, 134.75, 134.01, 129.98, 129.13, 128.99, 128.89, 127.58, 126.40, 125.69, 121.24, 113.80, 101.58, 71.77, 56.49, 53.20, 51.21, 21.87. HRMS (EI): Calculated for C$_{27}$H$_{19}$Cl$_2$NO$_3$ [M]$^+$ 475.0742, found 475.0758.
**Crystal Data of Compound 3a and 5a**

CCDC 1567079 and 1567080 contain the supplementary crystallographic data for compound 3a and 5a, respectively. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via [www.ccdc.cam.ac.uk/data_request/cif](http://www.ccdc.cam.ac.uk/data_request/cif).

**Figure 1:** Crystal structure of compound 3a

![Crystal structure of compound 3a](image1)

**Figure 2:** Crystal structure of compound 5a

![Crystal structure of compound 5a](image2)
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**References:**


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$^1$H and $^{13}$C NMR of compound 3b
$^1$H and $^{13}$C NMR of compound 3c
$^1$H and $^{13}$C NMR of compound 3d
$^1$H and $^{13}$C NMR spectra of compound 3e
$^1$H and $^{13}$C NMR of compound 3h

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$^1$H and $^{13}$C NMR of compound 3i
$^1$H and $^{13}$C NMR spectra of compound 3j
$^1$H and $^{13}$C NMR spectra of compound 3k
\( ^1H \) and \( ^13C \) NMR of compound 3l

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$^1$H and $^{13}$C NMR of compound 3m

S59
\(^1\)H and \(^{13}\)C NMR of compound 3n

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$^1$H and $^{13}$C NMR of compound 3o
$^1$H and $^{13}$C NMR of compound 3p
$^1$H and $^{13}$C NMR of compound 3q
$^{1}$H and $^{13}$C NMR of compound 3r
$^1$H and $^{13}$C NMR of compound 3s
$^1$H and $^{13}$C NMR spectra of compound 3t
$^1$H and $^{13}$C NMR of compound 3u
$^1$H and $^{13}$C NMR spectra of compound 5a
$^1$H and $^{13}$C NMR spectra of compound 5b
$^1$H and $^{13}$C NMR spectra of compound 5c

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$^1$H and $^{13}$C NMR spectra of compound 5d