Supporting Information for

Gold-Catalyzed formation of aryl-fused pyrazolooxazepines via intramolecular regioselective 7-exo-dig cyclization†

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1.1 General
Reactions were carried out in oven dried reaction flasks under nitrogen atmosphere and also solvents and reagents were transferred by oven-dried syringes to ambient temperature. TLC was performed on Merck silica gel aluminium sheets using UV as a visualizing agent and a 0.5% aqueous potassium permanganate solution and heat as developing agents. Solvents were removed under reduced pressure. Columns were packed as slurry of silica gel in hexane and ethyl acetate solvent mixture. The elution was assisted by applying pressure with an air pump. $^{13}$C NMR spectra were recorded on 75 and 125 MHz spectrometers. $^1$HNMR spectra were recorded on 300 MHz and 500 MHz spectrometers in appropriate solvents using TMS as internal standard. The following abbreviations were used to explain multiplicities: s = singlet, d = doublet, dd = double doublet, t = triplet, m = multiplet. All reactions were performed under nitrogen atmosphere with freshly distilled and dried solvents. All solvents were distilled using standard procedures. Unless otherwise noted, reagents were obtained from Aldrich, Alfa Aesar, and TCI used without further purification. Synthesis of aryl-fused pyrazolooxazepines (1a-1ab) were prepared by following reported procedures.\(^1\)

1.2 General procedure for synthesis of ortho-O-propargyl aryl pyrazoles (1a-1aa).

1.2.1 Synthesis of 5-phenyl-3-(2-(prop-2-yn-1-yloxy)phenyl)-1H-pyrazole-1a

\[
\begin{align*}
\text{CHO} & \xrightarrow{\text{Br} \text{K}_2\text{CO}_3, \text{DMF}, 28^\circ\text{C}, 4\text{hr}} \text{CHO} & \xrightarrow{n\text{-BuLi}, -78^\circ\text{C}, (2\text{hr})} \xrightarrow{\text{DMP}, \text{DCM}, 0^\circ\text{C}, \text{then} 28^\circ\text{C}, 3\text{hr}} \xrightarrow{\text{NH}_2\text{NH}_2\text{H}_2\text{O} (24-26\% \text{ in H}_2\text{O}), \text{THF}, 28^\circ\text{C}, 2\text{hr}} \text{1a}
\end{align*}
\]
Procedure for synthesis of 2-(prop-2-yn-1-yloxy)benzaldehyde - S1

To a stirred solution of 2-hydroxy benzaldehyde (1g, 8.19 mmol) in DMF (20 mL) added potassium carbonate (1.69g, 12.29 mmol) under nitrogen atmosphere. Resulting solution was stirred for 15 min. to this reaction mixture propargyl bromide (1.2mL, 10.65 mmol) was added dropwise and stirred for 4 hrs at 28 °C. After completion of reaction (monitored by TLC), it was quenched by ice water (20 mL) and extracted with ethyl acetate (2x25 mL). The organic layer was washed with brine solution (20 mL) and dried over anhydrous Na₂SO₄. The combined organic layer was evaporated under reduced pressure to afford a crude residue. The crude product was purified on SiO₂ (100-200 mesh) using hexane/EtOAc mixture (94:6) as eluents to afford the pure 2-(prop-2-yn-1-yloxy)benzaldehyde (S1) as white solid (1.15g, 88% yield).

Procedure for synthesis of 3-phenyl-1-(2-(prop-2-yn-1-yloxy)phenyl)prop-2-yn-1-ol - S2

To a 50 mL round-bottomed flask equipped with magnetic stir bar added THF (20 mL) and allowed to stirred at -78 °C. n-Butyl lithium (2.5M) (3.3 mL, 8.25 mmol) was added dropwise under nitrogen atmosphere. To this reaction mixture phenyl acetylene (0.9 mL, 8.25 mmol) was added dropwise and the reaction mixture stirred at -78 °C for 2 hrs. To this reaction mixture S1 (1.1g, 6.87 mmol) was added, the resulting reaction mixture allowed to stir at 28 °C for 2 hrs. After completion of reaction (monitored by TLC), it was quenched by ice water (10 mL) and the reaction mixture was extracted with ethyl acetate (2x25 mL). The combined organic layer was washed with brine solution (20 mL) and dried over anhydrous Na₂SO₄. The solution was concentrated under reduced pressure and the crude residue was purified by silica gel flash column chromatography (Hexane/EtOAc mixture = 90:10), affording 3-phenyl-1-(2-(prop-2-yn-1-yloxy)phenyl)prop-2-yn-1-ol (S2) as Yellow liquid (1.33g, 74 % yield).

Procedure for synthesis of 3-phenyl-1-(2-(prop-2-yn-1-yloxy) phenyl) prop-2-yn-1-one - S3

To a solution of 3-phenyl-1-(2-(prop-2-yn-1-yloxy) phenyl) prop-2-yn-1-one (S2) (1.2g, 4.58 mmol) in DCM (20 mL) added DMP (2.52g, 5.95 mmol) at 0 °C. Then the reaction mixture warmed to room temperature (28 °C) and stirred for 3 hrs. After completion of the reaction (monitored by TLC), reaction mixture was quenched by 10% sodium thiosulphate solution (10 mL) and saturated sodium bicarbonate solution (10 mL) (to neutralize the reaction mixture). Then the organic layer was extracted with DCM (2x25 mL) and washed with brine solution (20 mL). The organic layer was dried over anhydrous Na₂SO₄ and solvent was evaporated under reduced pressure to afford a crude residue. The crude residue was purified by silica gel flash column chromatography (Hexane/EtOAc mixture = 95:5), affording, 3-phenyl-1-(2-(prop-2-yn-1-yloxy) phenyl) prop-2-yn-1-one (S3) as Yellow solid (0.84g, 71% yield).

Procedure for synthesis of 5-phenyl-3-(2-(prop-2-yn-1-yloxy) phenyl)-1H-pyrazole - 1a

To a solution of 3-phenyl-1-(2-(prop-2-yn-1-yloxy) phenyl) prop-2-yn-1-one (S3) (0.8g, 3.07 mmol) in THF (8 mL) added hydrazine hydrate solution (0.67 mL, 3.38 mmol). Then the reaction mixture was stirred at 28 °C for 2 hrs. After completion of the reaction (monitored by TLC), reaction mixture was extracted with ethyl acetate (2x25 mL) and dried over anhydrous Na₂SO₄. The solvent was evaporated under reduced pressure to afford a crude residue and purified by silica gel flash column chromatography (Hexane/EtOAc mixture = 90:10), affording, 5-phenyl-3-(2-(prop-2-yn-1-yloxy) phenyl)-1H-pyrazole (1a) as light Yellow solid (0.72g,
85% yield). The above similar synthetic procedure was followed for the synthesis of the starting materials 1b - 1z.

1.2.2 General procedure for synthesis of 5-phenyl-3-(2-((3-phenylprop-2-yn-1-yl)oxy)phenyl)-1H-pyrazole - 1aa

Procedure for synthesis of 3-phenyl-1-(2-((3-phenylprop-2-yn-1-yl)oxy)phenyl)prop-2-yn-1-one - S4

To a solution of 3-phenyl-1-(2-(prop-2-yn-1-yloxy) phenyl) prop-2-yn-1-one (S3) (0.5g, 1.92 mmol) in triethyl amine (5 mL) added iodobenzene (0.26 mL, 2.3 mmol). To this reaction mixture tetrakis(triphenylphosphine)palladium(0) (0.044g, 0.038 mmol) and copper iodide (0.014g, 0.076 mmol) was added. The resulting reaction mixture was stirred at room temperature (28 °C) for 2hrs. After completion of the reaction (monitored by TLC), reaction mixture was extracted with ethyl acetate (2x5 mL). Then the organic layer was washed with ice water and brine solution (10 mL). The combined organic layer was dried over anhydrous Na₂SO₄ and solvent was evaporated under reduced pressure to afford a crude residue. The crude residue was purified by silica gel flash column chromatography (Hexane/EtOAc mixture = 94:6), affording 3-phenyl-1-(2-((3-phenylprop-2-yn-1-yl)oxy)phenyl)prop-2-yn-1-one (S4) as brown liquid (0.41g, 64% yield).

Procedure for synthesis of 5-phenyl-3-(2-((3-phenylprop-2-yn-1-yl)oxy)phenyl)-1H-pyrazole - 1aa

To a solution of 3-phenyl-1-(2-((3-phenylprop-2-yn-1-yl)oxy)phenyl)prop-2-yn-1-one (S4) (0.4g, 1.19 mmol) in THF (4 mL) added hydrazine hydrate solution (0.26 mL, 1.309 mmol). Then the reaction mixture was stirred at 28 °C for 2hrs. After completion of the reaction (monitored by TLC), reaction mixture was extracted with ethyl acetate (2x5 mL) and dried over anhydrous Na₂SO₄. The solvent was evaporated under reduced pressure to afford a crude residue and purified by silica gel flash column chromatography (Hexane/EtOAc mixture = 91:9), affording, 5-phenyl-3-(2-((3-phenylprop-2-yn-1-yl)oxy)phenyl)-1H-pyrazole (1aa) as yellow solid (0.35g, 84% yield). A similar procedure was followed for the synthesis of substrate 1ab.
1.3 Spectroscopic data of ortho-\(O\)-propargyl aryl pyrazole derivatives (1a-1ab).

<table>
<thead>
<tr>
<th>Compound</th>
<th>Molecular Formula</th>
<th>R&lt;sub&gt;f&lt;/sub&gt;</th>
<th>Solvent</th>
<th>Yield</th>
<th>Color</th>
<th>Melting Point</th>
<th>(^1)H NMR (CDCl&lt;sub&gt;3&lt;/sub&gt;, MHz)</th>
<th>(^{13})C NMR (CDCl&lt;sub&gt;3&lt;/sub&gt;, MHz)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5-Phenyl-3-(2-(prop-2-yn-1-yloxy)phenyl)-1(H)-pyrazole: 1a</td>
<td>C&lt;sub&gt;27&lt;/sub&gt;H&lt;sub&gt;21&lt;/sub&gt;FN&lt;sub&gt;3&lt;/sub&gt;O</td>
<td>0.45</td>
<td>Hexane: Ethyl acetate mixture (10 : 1)</td>
<td>85%</td>
<td>Light Yellow solid</td>
<td>84-86 °C</td>
<td>(\delta) 7.89-7.86 (m, 2H), 7.78-7.75 (m, 1H), 7.45-7.41 (m, 2H), 7.35-7.31 (m, 2H), 7.14-7.10 (m, 2H), 6.97 (s, 1H), 4.87 (d, (J = 2.4) Hz, 2H), 2.61 (t, (J = 2.4) Hz, 1H) ppm</td>
<td>(\delta) 153.8, 151.3, 141.7, 133.2, 129.1, 128.6, 128.2, 127.7, 125.6, 122.3, 118.3, 113.0, 100.2, 77.6, 76.6, 56.5 ppm</td>
</tr>
<tr>
<td>3-(2-(Prop-2-yn-1-yloxy)phenyl)-5-(p-tolyl)-1(H)-pyrazole: 1b</td>
<td>C&lt;sub&gt;30&lt;/sub&gt;H&lt;sub&gt;25&lt;/sub&gt;FN&lt;sub&gt;3&lt;/sub&gt;O</td>
<td>0.65</td>
<td>Hexane: Ethyl acetate mixture (10 : 0.7)</td>
<td>87%</td>
<td>Yellow liquid</td>
<td>84-86 °C</td>
<td>(\delta) 7.78-7.74 (m, 3H), 7.33-7.28 (m, 1H), 7.25-7.22 (d, (J = 7.8) Hz, 2H), 7.12-7.07 (d, (J = 8.4) Hz, 2H), 6.93 (s, 1H), 4.83 (d, (J = 2.4) Hz, 2H), 2.59 (t, (J = 2.4) Hz, 1H), 2.38 (s, 3H) ppm</td>
<td>(\delta) 153.8, 151.3, 141.7, 137.4, 130.4, 129.3, 129.0, 128.2, 125.5, 122.3, 118.4, 113.0, 100.0, 77.6, 76.6, 56.5, 21.2 ppm</td>
</tr>
<tr>
<td>5-(4-Fluorophenyl)-3-(2-(prop-2-yn-1-yloxy)phenyl)-1(H)-pyrazole: 1c</td>
<td>C&lt;sub&gt;29&lt;/sub&gt;H&lt;sub&gt;20&lt;/sub&gt;FN&lt;sub&gt;3&lt;/sub&gt;O</td>
<td>0.5</td>
<td>Hexane: Ethyl acetate mixture (10 : 0.6)</td>
<td>78%</td>
<td>White solid</td>
<td>133-135 °C</td>
<td>(\delta) 7.86-7.82 (m, 2H), 7.75-7.73 (m, 1H), 7.35-7.31 (m, 2H) ppm</td>
<td>(\delta) 153.8, 151.3, 141.7, 137.4, 130.4, 129.0, 128.2, 125.5, 122.3, 118.4, 113.0, 100.0, 77.6, 76.6, 56.5, 21.2 ppm</td>
</tr>
</tbody>
</table>
3-(2-(Prop-2-yn-1-yloxy)phenyl)-1H-pyrazole : **1d**

R$_f$: 0.7; Hexane: Ethyl acetate mixture (10 : 0.7); Yield: 63%, Colorless liquid; $^1$H NMR (CDCl$_3$, 400 MHz): $\delta$ 7.73-7.70 (dd, $J = 7.7$, 9.4 Hz, 1H), 7.62 (d, $J = 1.9$ Hz, 1H), 7.33-7.28 (m, 1H), 7.12-7.07 (m, 2H), 6.67 (d, $J = 1.9$ Hz, 1H), 4.83 (d, $J = 2.3$ Hz, 2H), 2.69 (t, $J = 7.7$ Hz, 2H), 2.58 (t, $J = 2.3$ Hz, 1H), 1.73-1.65 (m, 2H), 0.95 (t, $J = 7.3$ Hz, 3H) ppm; $^{13}$C NMR (CDCl$_3$, 125 MHz): $\delta$ 153.7, 140.7, 138.7, 128.9, 128.2, 122.2, 118.6, 112.9, 103.2, 77.6, 76.5, 56.4 ppm.

5-Butyl-3-(2-(prop-2-yn-1-yloxy)phenyl)-1H-pyrazole : **1e**

R$_f$: 0.45; Hexane: Ethyl acetate mixture (10 : 0.6); Yield: 81%, Yellow liquid; $^1$H NMR (CDCl$_3$, 400 MHz): $\delta$ 7.70-7.67 (m, 1H), 7.31-7.27 (m, 1H), 7.10-7.05 (m, 2H), 6.47 (s, 1H), 4.83 (d, $J = 2.3$ Hz, 2H), 2.69 (t, $J = 7.7$ Hz, 2H), 2.58 (t, $J = 2.3$ Hz, 1H), 1.73-1.65 (m, 2H), 1.47-1.37 (m, 2H), 0.95 (t, $J = 7.3$ Hz, 3H) ppm; $^{13}$C NMR (CDCl$_3$, 125 MHz): $\delta$ 153.8, 128.7, 128.2, 122.2, 119.0, 112.9, 102.0, 77.7, 76.4, 56.5, 31.7, 27.6, 22.4, 13.9 ppm.

5-Pentyl-3-(2-(prop-2-yn-1-yloxy)phenyl)-1H-pyrazole : **1f**

R$_f$: 0.4; Hexane: Ethyl acetate mixture (10 : 0.9); Yield: 65%, white solid; Melting Point: 80-82 °C; $^1$H NMR (CDCl$_3$, 500 MHz): $\delta$ 7.70-7.68 (m, 1H), 7.30-7.27 (m, 1H), 7.09-7.06 (m, 2H),
6.46 (s, 1H), 4.83 (d, J = 2.4 Hz, 2H), 2.68 (t, J = 7.7 Hz, 2H), 2.58 (t, J = 2.4 Hz, 1H), 1.74-1.68 (m, 2H), 1.40-1.35 (m, 4H), 0.91 (t, J = 7.3 Hz, 3H) ppm; $^{13}$C NMR (CDCl$_3$, 100 MHz): $\delta$ 153.8, 152.5, 141.4, 128.7, 128.1, 122.2, 119.0, 112.9, 102.0, 77.7, 76.4, 56.4, 31.5, 29.2, 27.8, 22.4, 14.0 ppm.

5-Hexyl-3-(2-(prop-2-yn-1-yloxy)phenyl)-1$H$-pyrazole: 1g

R$_f$: 0.3; Hexane: Ethyl acetate mixture (10 : 0.8); Yield: 73%, Yellow liquid; $^1$H NMR (CDCl$_3$, 300 MHz): $\delta$ 7.72-7.66 (m, 1H), 7.33-7.27 (m, 1H), 7.12-7.04 (m, 2H), 6.46 (s, 1H), 4.84 (d, J = 2.4 Hz, 2H), 2.68 (t, J = 7.7 Hz, 2H), 2.58 (t, J = 2.4 Hz, 1H), 1.75-1.64 (m, 2H), 1.43-1.30 (m, 6H), 0.89 (t, J = 6.9 Hz, 3H) ppm; $^{13}$C NMR (CDCl$_3$, 125 MHz): $\delta$ 153.8, 152.5, 141.3, 128.7, 128.2, 122.2, 119.0, 113.0, 102.0, 77.7, 76.4, 56.5, 31.6, 29.5, 29.1, 27.9, 22.5, 14.0 ppm.

5-Octyl-3-(2-(prop-2-yn-1-yloxy)phenyl)-1$H$-pyrazole: 1h

R$_f$: 0.4; Hexane: Ethyl acetate mixture (10 : 0.8); Yield: 76%, white solid; Melting Point: 67-69 °C; $^1$H NMR (CDCl$_3$, 400 MHz): $\delta$ 7.70-7.67 (m, 1H), 7.31-7.27 (m, 1H), 7.09-7.05 (m, 2H), 6.46 (s, 1H), 4.82 (d, J = 2.4 Hz, 2H), 2.68 (t, J = 7.7 Hz, 2H), 2.58 (t, J = 2.4 Hz, 1H), 1.74-1.66 (m, 2H), 1.43-1.22 (m, 10H), 0.88 (t, J = 7.3 Hz, 3H) ppm; $^{13}$C NMR (CDCl$_3$, 100 MHz): $\delta$ 153.8, 152.6, 141.3, 128.7, 128.1, 122.2, 119.0, 112.9, 101.9, 77.7, 76.4, 56.5, 31.8, 29.5, 29.4, 29.2, 27.9, 22.6, 14.0 ppm.
5-Phenyl-3-(2-(prop-2-yn-1-yloxy)naphthalen-1-yl)-1H-pyrazole : \textbf{II}

\[ \text{Rf: 0.5; Hexane: Ethyl acetate mixture (10 : 0.6); Yield: 62\%, Yellow semi solid; } \]
\[ ^1H \text{ NMR (CDCl}_3, 500 \text{ MHz): } \delta 8.04 (d, J = 8.5 \text{ Hz, 1H}), 7.92 (d, J = 9.0 \text{ Hz, 1H}), 7.90-7.88 (m, 2H), 7.85 (d, J = 7.6 \text{ Hz, 1H}), 7.49-7.40 (m, 5H), 7.36-7.32 (m, 1H), 6.87 (s, 1H), 4.78 (d, J = 2.4 \text{ Hz, 2H}), 2.50 (t, J = 2.4 \text{ Hz, 1H}) \text{ ppm; } ^{13}C \text{ NMR (CDCl}_3, 100 \text{ MHz): } \delta 152.8, 150.7, 138.9, 133.0, 132.9, 130.6, 129.6, 128.6, 128.0, 127.7, 127.2, 125.6, 124.9, 124.5, 115.2, 114.9, 105.1, 78.5, 76.1, 57.4 \text{ ppm.} \]

3-(2-(Prop-2-yn-1-yloxy)naphthalen-1-yl)-5-(p-tolyl)-1H-pyrazole : \textbf{Ij}

\[ \text{Rf: 0.3; Hexane: Ethyl acetate mixture (10 : 0.8); Yield: 70\%, light yellow solid; Melting Point: } 172-174 \text{ °C; } ^1H \text{ NMR (CDCl}_3, 500 \text{ MHz): } \delta 8.04 (d, J = 8.3 \text{ Hz, 1H}), 7.90 (d, J = 9.0 \text{ Hz, 1H}), 7.83 (d, J = 7.7 \text{ Hz, 1H}), 7.75 (d, J = 7.4 \text{ Hz, 2H}), 7.47-7.38 (m, 3H), 7.21 (d, J = 7.0 \text{ Hz, 2H}), 6.82 (s, 1H), 4.74 (s, 2H), 2.48 (s, 1H), 2.38 (s, 3H) \text{ ppm; } ^{13}C \text{ NMR (CDCl}_3, 100 \text{ MHz): } \delta 152.8, 150.6, 139.0, 137.5, 133.0, 130.5, 130.0, 129.6, 129.3, 128.0, 127.2, 125.5, 125.0, 124.5, 115.2, 104.9, 78.5, 76.1, 57.4, 21.2 \text{ ppm.} \]
5-(4-Fluorophenyl)-3-(2-(prop-2-yn-1-yloxy)naphthalen-1-yl)-1H-pyrazole: \textbf{1k}

\[ \text{\textit{R}}_f: 0.4; \text{Hexane: Ethyl acetate mixture (10 : 0.8); \textit{Yield}: 66\%, \text{white solid; Melting Point: 189-191 °C; \textit{\textit{H NMR (CDCl}_3+\text{DMSO, 300 MHz): \delta 12.48 (s, 1H), 7.96-7.83 (m, 5H), 7.53-7.49 (m, 1H), 7.47-7.37 (m, 2H), 6.73 (s, 1H), 4.79 (d, \textit{J} = 2.2 Hz, 2H), 2.66 (t, \textit{J} = 2.2 Hz, 1H) ppm; \textit{\textit{13C NMR (CDCl}_3+\text{DMSO, 75 MHz): \delta 161.5 (d, \textit{J} = 245.930 Hz, 1C), 152.5, 132.8, 129.7, 128.8, 127.3, 126.5 (d, \textit{J} = 7.703 Hz, 1C), 126.3, 124.4, 123.7, 114.7 (d, \textit{J} = 20.907 Hz, 2C), 103.8, 78.2, 75.7, 56.8 ppm.}}\]

5-Hexyl-3-(2-(prop-2-yn-1-yloxy)naphthalen-1-yl)-1H-pyrazole: \textbf{1l}

\[ \text{\textit{R}}_f: 0.4; \text{Hexane: Ethyl acetate mixture (10 : 2); \textit{Yield}: 91\%, \text{Yellow liquid; \textit{\textit{H NMR (CDCl}_3, 500 MHz): \delta 7.94 (d, \textit{J} = 8.3 Hz, 1H), 7.86 (d, \textit{J} = 9.0 Hz, 1H), 7.80 (d, \textit{J} = 8.5 Hz, 1H), 7.44-7.36 (m, 3H), 6.30 (s, 1H), 4.71 (d, \textit{J} = 2.2 Hz, 2H), 2.65 (t, \textit{J} = 7.6 Hz, 2H), 2.47 (t, \textit{J} = 2.2 Hz, 1H), 1.72-1.65 (m, 2H), 1.40-1.34 (m, 2H), 1.33-1.28 (m, 4H), 0.90 (t, \textit{J} = 7.0 Hz, 3H) ppm; \textit{\textit{13C NMR (CDCl}_3, 100 MHz): \delta 152.8, 150.4, 140.0, 133.3, 130.1, 129.7, 127.9, 126.8, 125.2, 124.3, 115.6, 106.2, 78.7, 75.8, 57.5, 31.6, 29.2, 29.1, 27.3, 22.5, 14.0 ppm.}}\]

5-Octyl-3-(2-(prop-2-yn-1-yloxy)naphthalen-1-yl)-1H-pyrazole: \textbf{1m}

\[ \text{\textit{R}}_f: 0.3; \text{Hexane: Ethyl acetate mixture (10 : 0.9); \textit{Yield}: 87\%, \text{brown liquid; \textit{\textit{H NMR (CDCl}_3, 500 MHz): \delta 7.95 (d, \textit{J} = 8.3 Hz, 1H), 7.87 (d, \textit{J} = 9.0 Hz, 1H), 7.81 (d, \textit{J} = 7.9 Hz, 1H), 7.44-7.36 (m, 3H), 6.30 (s, 1H), 4.71 (d, \textit{J} = 2.4 Hz, 2H), 2.67 (t, \textit{J} = 7.6 Hz, 2H), 2.47 (t, \textit{J} = 2.4 Hz, 1H), 1.73-1.66 (m, 2H), 1.41-1.27 (m, 10H), 0.89 (t, \textit{J} = 7.0 Hz, 3H) ppm; \textit{\textit{13C NMR (CDCl}_3,}}\]
$\delta 152.8, 150.6, 139.9, 133.3, 130.1, 129.7, 127.9, 126.9, 125.2, 124.3, 115.5, 106.3, 78.7, 75.8, 57.5, 31.8, 29.4, 29.3, 29.2, 27.4, 22.6, 14.0$ ppm.

$\text{3-(3,5-Di-tert-butyl-2-(prop-2-yn-1-yloxy)phenyl)-5-phenyl-1H-pyrazole : In}$

$\text{R_f: 0.4; Hexane: Ethyl acetate mixture (10 : 0.9); Yield: 59%, light Yellow solid; Melting Point: 151-153 °C; }^{1} \text{H NMR (CDCl}_3, 400 MHz): \delta 7.8 \text{ (d, } J = 7.3 \text{ Hz, 2H), 7.46-7.38 (m, 4H), 7.33(t, } J = 7.3 \text{ Hz, 1H), 6.90 (s, 1H), 4.24 (d, } J = 2.2 \text{ Hz, 2H), 2.50 (t, } J = 2.2 \text{ Hz, 1H), 1.48 (s, 9H), 1.34 (s, 9H) ppm; }^{13} \text{C NMR (CDCl}_3, 125 MHz): \delta 152.2, 151.0, 147.2, 143.0, 132.7, 128.6, 127.8, 125.6, 125.0, 124.8, 123.4, 101.6, 78.5, 75.4, 60.7, 35.4, 34.6, 31.3, 31.0$ ppm.

$\text{3-(3,5-Di-tert-butyl-2-(prop-2-yn-1-yloxy)phenyl)-5-(p-tolyl)-1H-pyrazole : Io}$

$\text{R_f: 0.5; Hexane: Ethyl acetate mixture (10 : 0.9); Yield: 71%, Yellow solid; Melting Point: 173-175 °C; }^{1} \text{H NMR (CDCl}_3, 500 MHz): \delta 7.76 \text{ (d, } J = 8.1 \text{ Hz, 2H), 7.43-7.38 (m,2H), 7.24 (d, } J = 7.9 \text{ Hz, 2H), 6.87 (s, 1H), 4.24 (d, } J = 2.4 \text{ Hz, 2H), 2.49 (t, } J = 2.4 \text{ Hz, 1H), 2.39 (s, 3H), 1.48 (s, 9H), 1.34(s, 9H) ppm; }^{13} \text{C NMR (CDCl}_3, 125 MHz): \delta 152.2, 147.1, 143.0, 137.7, 129.7, 129.3, 125.5, 125.0, 124.7, 101.5, 78.6, 75.3, 60.8, 35.4, 34.6, 31.4, 31.0, 21.2$ ppm.
3-(3,5-Di-tert-butyl-2-(prop-2-yn-1-yloxy)phenyl)-5-octyl-1H-pyrazole : 1p

![Chemical structure of 1p](image1.png)

Rf: 0.4; Hexane: Ethyl acetate mixture (10 : 0.8); Yield: 68%, brown liquid; $^1$H NMR (CDCl$_3$, 500 MHz): $\delta$ 7.38 (d, $J = 2.4$ Hz, 1H), 7.35 (d, $J = 2.4$ Hz, 1H), 6.43 (s, 1H), 4.19 (d, $J = 2.4$ Hz, 2H), 2.69 (t, $J = 7.6$ Hz, 2H), 2.48 (t, $J = 2.4$ Hz, 1H), 1.74-1.68 (m, 2H), 1.46 (s, 9H), 1.44-1.35 (m, 4H), 1.32 (s, 9H), 1.31-1.27 (m, 6H), 0.88 (t, $J = 7.0$ Hz, 3H) ppm; $^{13}$C NMR (CDCl$_3$, 125 MHz): $\delta$ 152.3, 146.8, 142.7, 124.8, 124.5, 123.7, 106.3, 103.2, 99.1, 78.8, 74.9, 60.4, 35.3, 35.1, 34.5, 31.8, 31.4, 31.0, 30.2, 29.2, 28.3, 27.4, 22.6, 14.0 ppm.

3-(5-Bromo-2-(prop-2-yn-1-yloxy)phenyl)-5-phenyl-1H-pyrazole : 1q

![Chemical structure of 1q](image2.png)

Rf: 0.3; Hexane: Ethyl acetate mixture (10 : 1); Yield: 78%, white semi solid; $^1$H NMR (CDCl$_3$, 400 MHz): $\delta$ 7.89-7.83 (m, 3H), 7.45-7.38 (m, 3H), 7.36-7.31 (m, 1H), 6.98 (d, $J = 8.8$ Hz, 1H), 6.95 (s, 1H), 4.82 (d, $J = 2.4$ Hz, 2H), 2.61 (t, $J = 2.4$ Hz, 1H) ppm; $^{13}$C NMR (CDCl$_3$, 125 MHz): $\delta$ 152.8, 151.0, 140.7, 132.8, 131.5, 130.7, 128.6, 127.9, 125.6, 120.6, 114.8, 114.7, 100.9, 77.1, 76.9, 56.8 ppm.

3-(5-Bromo-2-(prop-2-yn-1-yloxy)phenyl)-5-((p-tolyl)-1H-pyrazole : 1r

![Chemical structure of 1r](image3.png)

Rf: 0.45; Hexane: Ethyl acetate mixture (10 : 0.9); Yield: 77%, Yellow solid; Melting Point: 106-108°C; $^1$H NMR (CDCl$_3$, 400 MHz): $\delta$ 7.87 (d, $J = 2.4$ Hz, 1H), 7.73 (d, $J = 8.0$ Hz, 2H), 7.41-7.37 (m, 1H), 7.24 (d, $J = 7.9$ Hz, 2H), 6.97(d, $J = 8.8$ Hz, 1H), 6.92 (s, 1H), 4.81 (s, 2H), 2.6 (s,
1H), 2.39 (s, 3H) ppm; $^{13}$C NMR (CDCl$_3$, 100 MHz): $\delta$ 152.9, 137.7, 131.4, 130.7, 129.9, 129.3, 125.5, 120.7, 114.8, 114.7, 100.7, 77.1, 76.9, 56.8, 21.2 ppm.

3-(5-Bromo-2-(prop-2-yloxy)phenyl)-5-pentyl-1H-pyrazole : 1s

$^{1}$H NMR (CDCl$_3$, 500 MHz): $\delta$ 7.83 (d, $J$ = 2.4 Hz, 1H), 7.37 (dd, $J$ = 2.4, 8.8 Hz, 1H), 6.97 (d, $J$ = 8.8 Hz, 1H), 6.48 (s, 1H), 4.80 (d, $J$ = 2.4 Hz, 2H), 2.68 (t, $J$ = 7.7 Hz, 2H), 2.59 (t, $J$ = 2.4 Hz, 1H), 1.73-1.67 (m, 2H), 1.39-1.34 (m, 4H), 0.91 (t, $J$ = 7.0 Hz, 3H) ppm; $^{13}$C NMR (CDCl$_3$, 100 MHz): $\delta$ 152.9, 151.8, 140.9, 131.1, 130.8, 121.5, 114.8, 114.6, 102.7, 77.3, 76.7, 56.7, 31.5, 29.1, 27.6, 22.4, 14.0 ppm.

3-(5-Nitro-2-(prop-2-yloxy)phenyl)-5-phenyl-1H-pyrazole : 1t

$^{1}$H NMR (CDCl$_3$, 400 MHz): $\delta$ 8.69 (d, $J$ = 2.8 Hz, 1H), 8.22 (dd, $J$ = 2.8, 9.1 Hz, 1H), 7.85-7.81 (m, 2H), 7.47-7.42 (m, 2H), 7.38-7.34 (m, 1H), 7.21 (d, $J$ = 9.1 Hz, 1H), 7.09 (s, 1H), 4.97 (d, $J$ = 2.3 Hz, 2H), 2.67 (t, $J$ = 2.3 Hz, 1H) ppm; $^{13}$C NMR (CDCl$_3$, 100 MHz): $\delta$ 158.0, 150.4, 142.5, 140.9, 132.0, 128.8, 128.2, 125.6, 124.4, 123.9, 120.1, 112.8, 102.0, 77.8, 76.3, 57.2 ppm.
<table>
<thead>
<tr>
<th>Compound</th>
<th>Rf</th>
<th>Hexane: Ethyl acetate mixture</th>
<th>Yield</th>
<th>Melting Point</th>
<th>1H NMR (CDCl$_3$, 500 MHz)</th>
<th>13C NMR (CDCl$_3$, 75 MHz)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3-(5-Nitro-2-(prop-2-yn-1-yloxy)phenyl)-5-(p-tolyl)-1H-pyrazole : 1u</td>
<td>0.45</td>
<td>10 : 0.8</td>
<td>73%</td>
<td>186-188 °C</td>
<td>δ 8.68 (s, 1H), 8.22-8.17 (m, 1H), 7.70 (d, J = 7.7 Hz, 2H), 7.25-7.17 (m, 3H), 7.05 (s, 1H), 4.94 (s, 2H), 2.66 (s, 1H), 2.39 (s, 3H) ppm</td>
<td>δ 158.1, 141.7, 137.2, 129.0, 128.1, 125.0, 123.6, 123.4, 112.3, 102.4, 76.9, 76.7, 56.4, 20.8 ppm</td>
</tr>
<tr>
<td>5-Butyl-3-(5-nitro-2-(prop-2-yn-1-yloxy)phenyl)-1H-pyrazole : 1v</td>
<td>0.2</td>
<td>10 : 2</td>
<td>65%</td>
<td>125-127 °C</td>
<td>δ 8.67 (d, J = 2.7 Hz, 1H), 8.18 (dd, J = 2.8, 9.1 Hz, 1H), 7.18 (d, J = 9.1 Hz, 1H), 6.61 (s, 1H), 4.94 (d, J = 2.2 Hz, 2H), 2.71 (t, J = 7.7 Hz, 2H), 2.64 (t, J = 2.2 Hz, 1H), 1.73-1.67 (m, 2H), 1.46-1.39 (m, 2H), 0.96 (t, J = 7.3 Hz, 3H) ppm</td>
<td>δ 158.2, 142.3, 124.1, 124.0, 121.4, 112.7, 103.9, 77.4, 77.2, 57.0, 31.4, 26.8, 22.3, 13.8 ppm</td>
</tr>
<tr>
<td>3-(5-Nitro-2-(prop-2-yn-1-yloxy)phenyl)-5-octyl-1H-pyrazole : 1w</td>
<td>0.4</td>
<td>10 : 1.2</td>
<td>83%</td>
<td>92-94 °C</td>
<td>δ 8.67 (d, J = 2.8 Hz, 1H), 8.18 (dd, J = 2.8, 9.1 Hz, 1H), 7.18 (d, J = 9.1 Hz, 1H), 6.61 (s, 1H), 4.93 (d, J = 2.4 Hz, 2H), 2.70 (t, J = 7.7 Hz, 2H), 2.64 (t, J = 2.4 Hz, 1H), 1.75-1.66 (m, 2H), 1.42-1.27 (m, 10H), 0.88 (t, J = 7.0 Hz, 3H) ppm</td>
<td>δ 158.2, 142.3, 124.1, 124.0, 121.4, 112.7, 103.8, 77.4, 77.1, 57.0, 31.8, 29.4, 29.3, 29.2, 27.1, 22.6, 14.0 ppm</td>
</tr>
</tbody>
</table>
3-(3,5-Dichloro-2-(prop-2-yn-1-yloxy)phenyl)-5-phenyl-1H-pyrazole : **1x**

![Chemical Structure of 1x](image)

R<sub>f</sub>: 0.4; Hexane: Ethyl acetate mixture (10 : 0.9); Yield: 74%, white solid; Melting Point: 177-179 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>+DMSO, 300 MHz): δ 13.38 (s, 1H), 7.85-7.77 (m, 2H), 7.47-7.30 (m, 5H), 7.20 (s, 1H), 4.64 (d, J = 2.2 Hz, 2H), 2.93 (t, J = 2.2 Hz, 1H) ppm; <sup>13</sup>C NMR (CDCl<sub>3</sub>+DMSO, 75 MHz): δ 147.9, 128.6, 128.3, 127.4, 127.2, 126.6, 125.3, 124.0, 101.6, 77.1, 76.0, 58.9 ppm.

5-Butyl-3-(3,5-dichloro-2-(prop-2-yn-1-yloxy)phenyl)-1H-pyrazole : **1y**

![Chemical Structure of 1y](image)

R<sub>f</sub>: 0.45; Hexane: Ethyl acetate mixture (10 : 0.8); Yield: 80%, light yellow solid; Melting Point: 83-85 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ 7.66 (d, J = 2.4 Hz, 1H), 7.34 (d, J = 2.4 Hz, 1H), 6.57 (s, 1H), 4.62 (d, J = 2.4 Hz, 2H), 2.70 (t, J = 7.7 Hz, 2H), 2.50 (t, J = 2.4 Hz, 1H), 1.73-1.65 (m, 2H), 1.47-1.37 (m, 2H), 0.95(t, J = 7.3 Hz, 3H) ppm; <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): δ 149.2, 130.5, 129.7, 129.0, 128.5, 103.9, 77.5, 76.4, 60.6, 31.3, 26.4, 22.2, 13.8 ppm.

3-(3,5-Dichloro-2-(prop-2-yn-1-yloxy)phenyl)-5-octyl-1H-pyrazole : **1z**

![Chemical Structure of 1z](image)

R<sub>f</sub>: 0.5; Hexane: Ethyl acetate mixture (10 : 1); Yield: 67%, light yellow solid; Melting Point: 56-58 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 500 MHz): δ 7.6 (d, J = 2.5 Hz, 1H), 7.33 (d, J = 2.5 Hz, 1H), 6.57 (s, 1H), 4.61 (d, J = 2.4 Hz, 2H), 2.68 (t, J = 7.6 Hz, 2H), 2.49 (t, J = 2.4 Hz, 1H), 1.72-1.65 (m, 2H), 1.43-1.27 (m, 10H), 0.88 (t, J = 7.0 Hz, 3H) ppm; <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): δ 149.2, 142.6, 130.6, 129.7, 129.0, 128.4, 126.9, 103.9, 77.5, 76.5, 60.6, 31.8, 29.6, 29.4, 29.3, 29.2, 26.8, 22.4, 14.0 ppm.
5-Phenyl-3-(2-((3-phenylprop-2-yn-1-yl)oxy)phenyl)-1H-pyrazole : \textbf{1aa}

\[ \text{R}^f: 0.45; \text{Hexane: Ethyl acetate mixture (10 : 0.9); Yield: 84\%, yellow solid; Melting Point: 134-136 \degree C; } \]
\[ ^1\text{H NMR (CDCl}_3, 400 \text{ MHz): } \delta 7.89-7.86 (m, 2H), 7.77 (dd, } J = 1.7, 7.8 \text{ Hz, 1H), 7.46-7.40 (m, 4H), 7.37-7.28 (m, 5H), 7.22-7.19 (m, 1H), 7.14-7.10 (m, 1H), 6.97 (s, 1H), 5.08 (s, 2H) ppm; } \]
\[ ^{13}\text{C NMR (CDCl}_3, 100 \text{ MHz): } \delta 154.1, 151.3, 141.8, 133.3, 131.8, 129.1, 128.8, 128.5, 128.2, 128.1, 127.6, 125.6, 122.2, 121.8, 118.3, 113.3, 100.2, 88.1, 82.8, 57.5 \text{ ppm.} \]

5-(4-Fluorophenyl)-3-(2-((3-(4-methoxyphenyl)prop-2-yn-1-yl)oxy)phenyl)-1H-pyrazole : \textbf{1ab}

\[ \text{R}^f: 0.3; \text{Hexane: Ethyl acetate mixture (10 : 1); Yield: 67\%, light yellow solid; Melting Point: 141-143 \degree C; } \]
\[ ^1\text{H NMR (CDCl}_3, 400 \text{ MHz): } \delta 7.86-7.81 (m, 2H), 7.74 (dd, } J = 1.7, 7.8 \text{ Hz, 1H), 7.41-7.32 (m, 3H), 7.22-7.19 (m, 1H), 7.14-7.08 (m, 3H), 6.91 (s, 1H), 6.86-6.81 (m,2H), 5.08 (s, 2H), 3.81 (s, 3H) ppm; } \]
\[ ^{13}\text{C NMR (CDCl}_3, 100 \text{ MHz): } \delta 162.5 (d, } J = 246.488 \text{ Hz, 1C), 160.0, 154.2, 141.9, 133.4, 129.6, 129.2, 128.0, 127.2 (d, } J = 8.070 \text{ Hz, 1C), 122.1, 118.1, 115.4 (d, } J = 22.008 \text{ Hz, 2C), 113.9, 113.8, 113.3, 99.9, 88.2, 81.4, 57.6, 55.2 \text{ ppm.} \]

1.4 Copies of $^1$H and $^{13}$C NMR spectra (2a-2ab)

5-Methylene-2-phenyl-5,6-dihydrobenzo[f]pyrazolo[1,5-\textit{d}][1,4]oxazepine: 2a

$^1$H NMR, CDCl$_3$, 400 MHz

$^{13}$C NMR, CDCl$_3$, 125 MHz
5-Methylene-2-(p-tolyl)-5,6-dihydrobenzo[f]pyrazolo[1,5-d][1,4]oxazepine: 2b

$\text{HNMR, CDCl}_3$, 400 MHz

$^{13}\text{CNMR, CDCl}_3$, 100 MHz
2-(4-Fluorophenyl)-5-methylene-5,6-dihydrobenzo[f]pyrazolo[1,5-d][1,4]oxazepine: 2c
5-Methylene-5,6-dihydrobenzo[f]pyrazolo[1,5-d][1,4]oxazepine: 2d

$^{1}H$NMR, CDCl$_3$, 500 MHz

$^{13}$CNMR, CDCl$_3$, 125 MHz
2-Butyl-5-methylene-5,6-dihydrobenzo[f]pyrazolo[1,5-d][1,4]oxazepine: 2e

\[\text{NMR, CDCl}_3, 400 \text{ MHz}\]

\[\text{NMR, CDCl}_3, 100 \text{ MHz}\]
5-Methylene-2-penty-5,6-dihydrobenzo[f]pyrazolo[1,5-d][1,4]oxazepine: 2f
2-Hexyl-5-methylene-5,6-dihydrobenzo[f]pyrazolo[1,5-d][1,4]oxazepine: 2g

$\begin{align}
\text{HNMR, CDCl}_3, 400 \text{ MHz} \\
\text{C}_{11}H_{13}N_{2}O_2
\end{align}$

$\begin{align}
\text{CNMR, CDCl}_3, 100 \text{ MHz} \\
\text{C}_{11}H_{13}N_{2}O_2
\end{align}$
5-Methylene-2-octyl-5,6-dihydrobenzo[f]pyrazolo[1,5-d][1,4]oxazepine: 2h

$^1$HNMR, CDCl$_3$, 500 MHz

$^{13}$CNMR, CDCl$_3$, 100 MHz
5-Methylene-2-phenyl-5,6-dihyronaphtho[1,2-f]pyrazolo[1,5-\textit{d}][1,4]oxazepine: 2i

\(^1\text{H}NMR, \text{CDCl}_3, 400 \text{ MHz}\)

\(^{13}\text{C}NMR, \text{CDCl}_3, 125 \text{ MHz}\)
5-Methylene-2-(p-tolyl)-5,6-dihyronaphtho[1,2-f]pyrazolo[1,5-d'][1,4]oxazepine: 2j

$^1$H NMR, CDCl$_3$, 400 MHz

$^{13}$C NMR, CDCl$_3$, 100 MHz
2-(4-Fluorophenyl)-5-methylene-5,6-dihydropyrazolo[1,2-\(f\)]pyrazolo[1,5-\(d\)][1,4]oxazine: 2k
2-Hexyl-5-methylene-5,6-dihydronaphtho[1,2-f]pyrazolo[1,5-d][1,4]oxazepine: 2I

$^{1} \text{HNMR, CDCl}_3, 400 \text{ MHz}$

$^{13} \text{CNMR, CDCl}_3, 100 \text{ MHz}$
5-Methylene-2-octyl-5,6-dihydropynaphtho[1,2-f]pyrazolo[1,5-d][1,4]oxazepine: 2m

$\text{C}_8\text{H}_17$

$^1$HNMR, CDCl$_3$, 400 MHz

$^{13}$CNMR, CDCl$_3$, 125 MHz
8,10-Di-tert-butyl-5-methylene-2-phenyl-5,6-dihydrobenzo[f]pyrazolo[1,5-d][1,4]oxazepine: 2n
8,10-Di-tert-butyl-5-methylene-2-octyl-5,6-dihydrobenzo[f]pyrazolo[1,5-d][1,4]oxazepine: 2p
10-Bromo-5-methylene-2-phenyl-5,6-dihydrobenzo[f]pyrazolo[1,5-d][1,4]oxazepine: 2q
10-Bromo-5-methylene-2-(p-tolyl)-5,6-dihydrobenzo[f]pyrazolo[1,5-d][1,4]oxazepine: 2r

$^1$H NMR, CDCl$_3$, 500 MHz

$^{13}$C NMR, CDCl$_3$, 125 MHz
10-Bromo-5-methylene-2-pentyl-5,6-dihydrobenzo[f]pyrazolo[1,5-d][1,4]oxazepine: 2s
5-Methylene-10-nitro-2-phenyl-5,6-dihydrobenzo[/]pyrazolo[1,5-d][1,4]oxazepine: 2t

$\text{HNMR, CDCl}_3, 500 \text{ MHz}$

$\text{CNMR, CDCl}_3, 100 \text{ MHz}$
5-Methylene-10-nitro-2-(p-tolyl)-5,6-dihydrobenzo[f]pyrazolo[1,5-d][1,4]oxazepine: 2u

\[
\text{HNMR, CDCl}_3, 500 \text{ MHz}
\]

\[
\text{CNMR, CDCl}_3, 125 \text{ MHz}
\]
2-Butyl-5-methylene-10-nitro-5,6-dihydrobenzo[f]pyrazolo[1,5-d][1,4]oxazepine: 2v

$\text{HNMR, CDCl}_3, 300 \text{ MHz}$

$\text{CNMR, CDCl}_3, 100 \text{ MHz}$
5-Methylene-10-nitro-2-octyl-5,6-dihydrobenzo[f]pyrazolo[1,5-d][1,4]oxazepine: 2w

$^1$H NMR, CDCl$_3$, 500 MHz

$^{13}$C NMR, CDCl$_3$, 100 MHz
8,10-Dichloro-5-methylene-2-phenyl-5,6-dihydrobenzo[f]pyrazolo[1,5-d][1,4]oxazepine: 2x
2-Butyl-8,10-dichloro-5-methylene-5,6-dihydrobenzo[\(f\)]pyrazolo[1,5-\(d\)][1,4]oxazepine: \(2y\)

\[\text{\(1^H\)NMR, CDCl}_3, 500 MHz}\]

\[\text{\(13^{C}\)NMR, CDCl}_3, 125 MHz}\]
8,10-Dichloro-5-methylene-2-octyl-5,6-dihydrobenzo[f]pyrazolo[1,5-\(d\)][1,4]oxazepine: 2z

\[\text{\textsuperscript{1}H NMR, CDCl\textsubscript{3}, 400 MHz}\]

\[\text{\textsuperscript{13}C NMR, CDCl\textsubscript{3}, 100 MHz}\]
(E)-5-Benzylidene-2-phenyl-5,6-dihydrobenzo[f]pyrazolo[1,5-d][1,4]oxazepine: 2aa

$\text{^1H} \text{NMR, CDCl}_3, 400 \text{ MHz}$

$\text{^13C} \text{NMR, CDCl}_3, 100 \text{ MHz}$
(E)-2-(4-Fluorophenyl)-5-(4-methoxybenzylidene)-5,6-dihydrobenzo[f]pyrazolo[1,5-
\textit{d}][1,4]oxazepine: 2\textit{ab}
1.5  X-ray crystallography data of compound 2u.

X-ray data for the compound KA263 was collected at 100 K on a Bruker D8 QUEST instrument with an IμS Mo microsource ($\lambda = 0.7107$ Å) and a PHOTON-100 detector. The raw data frames were reduced and corrected for absorption effects using the Bruker Apex 3 software suite programs. The structure was solved using intrinsic phasing method and further refined with the SHELXL program and expanded using Fourier techniques. Anisotropic displacement parameters were included for all non-hydrogen atoms. All C bound H atoms were positioned geometrically and treated as riding on their parent C atoms [C-H = 0.93-0.97 Å, and $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H or $1.2U_{eq}(C)$ for other H atoms].

Crystal Data for KA263: C_{19}H_{15}N_{3}O_{3} ($M =333.35$ g/mol): monoclinic, space group P2_1/c (no. 14), $a = 7.021(9)$ Å, $b = 20.14(3)$ Å, $c = 21.54(3)$ Å, $\beta = 95.79(2)\degree$, $V = 3030(7)$ Å³, $Z = 8$, $T = 100.0$ K, $\mu$(Mo Kα) = 0.101 mm$^{-1}$, $Dcalc = 1.4612$ g/cm³, 38713 reflections measured ($4.46\degree \leq 2\Theta \leq 61.62\degree$), 9422 unique ($R_{int} = 0.0356$, $R_{sigma} = 0.0330$) which were used in all calculations. The final $R_1$ was 0.0454 (I>2σ(I)) and $wR_2$ was 0.1193 (all data). CCDC 1574971 contains supplementary Crystallographic data for the structure. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html [or from the Cambridge Crystallographic Data Centre (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(0) 1223 336 033; email: deposit@ccdc.cam.ac.uk].

![Figure 1](image.png)

**Figure 1.** A view of KA263, showing the atom-labelling scheme. Two molecules were present in the asymmetric unit. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented by circles of arbitrary radii.

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