Electronic Supporting Information

Phenalenyl-ruthenium synergism for effectual catalytic transformations of primary amines to amides

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1. Characterization of PLY-ligands and their ruthenium complexes 1-3:

1.1. Characterization of PLY-ligands:

Figure S1. $^1$H NMR spectrum of HO,O-PLY.[1]

Figure S2. $^{13}$C{$^1$H} NMR spectrum of HO,O-PLY.[1]
Figure S3. $^1$H NMR spectrum of HO,O-PLY-Br.\cite{2}

Figure S4. $^{13}$C{$^1$H} NMR spectrum of HO,O-PLY-Br.\cite{2}
Figure S5. $^1$H NMR spectrum of HO,O-PLY-Ph.$^{[2]}$

Figure S6. $^{13}$C{$^1$H} NMR spectrum of HO,O-PLY-Ph.$^{[2]}$
1.2. Characterization data for complex 1-3:

**Figure S7.** $^1$H NMR spectrum of complex 1.

**Figure S8.** $^{13}$C{$^1$H} NMR spectrum of complex 1.
Figure S9. Mass spectrum of complex 1 in acetonitrile.

Figure S10. $^1$H NMR spectrum of complex 2.
Figure S11. $^{13}$C {$^1$H} NMR spectrum of complex 2.

Figure S12. Mass spectrum of complex 2 in acetonitrile.
Figure S13. $^1$H NMR spectrum of complex 3.

Figure S14. $^{13}$C{$^1$H} NMR spectrum of complex 3.
Figure S15. Mass spectrum of complex 3 in acetonitrile.

Figure S16. IR of spectra of complex 1-3.

Figure S17. UV-Vis spectra of complex 1-3.
2. X-ray structural details of complex 1-3:

**Table S1.** X-ray structural data of complex 1-3.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Complex 1</th>
<th>Complex 2</th>
<th>Complex 3</th>
</tr>
</thead>
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<td>C$<em>{29}$H$</em>{25}$ClO$_2$Ru</td>
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<td><strong>Formula weight</strong></td>
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<td><strong>T (K)</strong></td>
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<td><strong>Space group</strong></td>
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<td>P 2$_1$/n</td>
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<td>F(000)</td>
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<td>3.3,  33.1</td>
<td>4.0,  78.4</td>
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<td>-16: 15 ; -13: 11 ; -21: 21</td>
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<td>4746</td>
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<td>R1 = 0.0291,</td>
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<td>wR2 = 0.0777,</td>
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Table S2. Selected X-ray crystallographic bond lengths (Å) of complex 1-3.

<table>
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<th>Bond lengths</th>
<th>Complex 1</th>
<th>Complex 2</th>
<th>Complex 3</th>
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<td>Ru1-O1</td>
<td>2.051(3)</td>
<td>2.048(3)</td>
<td>2.0556(16)</td>
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<tr>
<td>Ru1-O2</td>
<td>2.057(4)</td>
<td>2.052(3)</td>
<td>2.0704(16)</td>
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<tr>
<td>Ru1-C10</td>
<td>2.187(4)</td>
<td>2.169(5)</td>
<td>2.194(2)</td>
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<td>Ru1-C11</td>
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<td>Ru1-C13</td>
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<td>Ru1-C14</td>
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<td>Ru1-C15</td>
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<td>C1-O1</td>
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<td>C9-O2</td>
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<td>C1-C2</td>
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<td>1.443(6)</td>
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<td>C8-C9</td>
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<td>1.436(3)</td>
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<td>C1-C9A</td>
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<td>1.428(5)</td>
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<td>C9-C9A</td>
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<td>C2-C3</td>
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<td>1.356(6)</td>
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<td>C7-C8</td>
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<td>1.354(3)</td>
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<tr>
<td>C9A-C9B</td>
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<td>1.440(6)</td>
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<tr>
<td>C3-C3A</td>
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<td>C7-C6A</td>
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<td>C3A-C9B</td>
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<td>C6A-C9B</td>
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<td>C5-C6</td>
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Table S3. Selected X-ray crystallographic bond angles (°) of complex 1-3.

<table>
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<th>Bond angles</th>
<th>Complex 1</th>
<th>Complex 2</th>
<th>Complex 3</th>
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</thead>
<tbody>
<tr>
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<td>Cl1-Ru1-O2</td>
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<td>O1-Ru1-O2</td>
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<td>87.77(11)</td>
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3. CD spectra of complex 1-3:

**Figure S18.** CD spectrum of complex 1.

**Figure S19.** CD spectrum of complex 2.

**Figure S20.** CD spectrum of complex 3.
4. Cyclic voltammograms of PLY-ligands (H-PLY, H-PLY-Br and H-PLY-Ph) and their metal complexes (1-3):

**Figure S21.** Cyclic voltammograms of 1-3 in DCM/0.1 M Bu$_4$NPF$_6$ at 298 K vs Ag/AgCl.

**Figure S22.** Cyclic voltammograms of PLY-ligands in DCM/0.1 M Bu$_4$NPF$_6$ at 298 K vs Ag/AgCl.
5. Reaction optimization table:

Table S4. Optimization of the aerial oxidation of benzylamine (4a) into benzamide (5a)[a]

<table>
<thead>
<tr>
<th>Entry</th>
<th>Catalyst (x mol %)</th>
<th>Base (y mol %)</th>
<th>Temp. (°C)</th>
<th>Solvent</th>
<th>Yield of 5a[b] (%)</th>
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<tr>
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<td>1 (3)</td>
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<td>2</td>
<td>1 (3)</td>
<td>KO'Bu (40)</td>
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<tr>
<td>3</td>
<td>—</td>
<td>KO'Bu (40)</td>
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<td>Toluene</td>
<td>—</td>
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<tr>
<td>4</td>
<td>[Cl(η⁶-Cym)Ru(μ-Cl)_2Ru(η⁶-Cym)Cl] (1.5)</td>
<td>KO'Bu (40)</td>
<td>90</td>
<td>Toluene</td>
<td>29</td>
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<td>5</td>
<td>KO'Bu (40)</td>
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<td>Toluene</td>
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<td>KO'Bu (40)</td>
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<td>7</td>
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<td>Ethyl-acetate</td>
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<td>KO'Bu (40)</td>
<td>90</td>
<td>i'PrOH</td>
<td>18</td>
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</table>

[a] PhCH₂NH₂ (0.5 mmol), catalyst (1.5-3 mol%), base (20-40 mol%), solvent (3mL) for 15 h at 90 °C under aerobic conditions followed by extraction from ethylacetate-H₂O mixture. [b] Isolated yield of PhCONH₂. [c],[d] Reaction time 6h and 12h respectively.
6. Kinetics of 1-catalyzed aerial oxidation of amine to amide:

Table S5. Yield of benzamide (5a) at different time intervals.

<table>
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<tr>
<th>Entry</th>
<th>Reaction time</th>
<th>Yield (%)</th>
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<td>2</td>
<td>4 h</td>
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<tr>
<td>3</td>
<td>6 h</td>
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<td>4</td>
<td>8 h</td>
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<td>5</td>
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<td>6</td>
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<td>14 h</td>
<td>93</td>
</tr>
<tr>
<td>8</td>
<td>16 h</td>
<td>93</td>
</tr>
</tbody>
</table>

Figure S23. Graphical representation of yield of benzamide (5a) vs time.
7. **Procedure for gram-scale synthesis of amide:**

In a 250 ml round bottom flask containing a magnetic stirring bar, catalyst 1 (3 mol%, 129 mg) and KOtBu (40 mol%, 415 mg) were dissolved in 80 mL of toluene. Then substrate benzylamine (1 g, 9.26 mmol) was added to it and allowed to stir for 15 h at 90 °C under aerobic conditions. After that the mixture was allowed to cool down to room temperature and the amide product was extracted with 225 mL (3 x 75 mL) of ethyl acetate. The combined organic extracts were dried over anhydrous Na2SO4 and filtered. The removal of the solvents under reduced pressure leads to the crude amide which was further purified by column chromatography using silica (hexane/ethyl acetate). Yields: 857 mg, 85%.

![Scheme S1](image)

**Scheme S1.** Aerial oxidation of benzylamine (4a) to benzamide (5a) in gram-scale.

8. **Mechanistic studies:**

8.1. **1-catalyzed aerial oxidation of amine in base free condition:**

In a 25 ml round bottom flask containing a magnetic stirring bar, catalyst 1 (3 mol%, 14 mg) and benzylamine, 4a (107 mg, 1 mmol) and toluene (5 mL) were added and then allowed to stir for 15 h at 90 °C under aerobic conditions. After that the mixture was allowed to cool down to room temperature and the amide product was extracted with 60 mL (3 x 20 mL) of ethyl acetate. The combined organic extracts were dried over anhydrous Na2SO4 and filtered. The removal of the solvents under reduced pressure leads to the mixture of mainly three products (5a, 7a and 8a). These products were separated by column chromatography using silica (hexane/ethyl acetate).

![Scheme S2](image)

**Scheme S2.** Aerial oxidation of benzylamine (4a) in absence of base.
Compound **5a**\[^{[3]}\]: Isolated as white crystalline solid with 26% yield. \[^{1}\]H NMR (400 MHz, CDCl\(_3\), Figure S24) \(\delta/\text{ppm}: 7.84 – 7.79 (m, 2H), 7.55 – 7.50 (m, 1H), 7.47 – 7.41 (m, 2H), 6.23 (s, 2H). \[^{13}\]C\{\[^{1}\]H\} NMR (101 MHz, CDCl\(_3\), Figure S25) \(\delta/\text{ppm}: 169.84, 133.40, 131.99, 128.62, 127.36.

Compound **7a**\[^{[4]}\]: Colourless liquid, Yield: 18\%. \[^{1}\]H NMR (400 MHz, CDCl\(_3\), Figure S1) \(\delta/\text{ppm}: 8.45 (s, 1H), 7.90 – 7.87 (m, 2H), 7.52 – 7.46 (m, 3H), 7.44 (d, \(J = 4.1\) Hz, 4H), 7.37 – 7.34 (m, 1H), 4.91 (s, 2H). \[^{13}\]C\{\[^{1}\]H\} NMR (101 MHz, CDCl\(_3\), Figure S27) \(\delta/\text{ppm}: 162.12, 139.24, 136.11, 129.49, 128.63, 128.51, 128.31, 127.02, 65.02.

Compound **8a**\[^{[4]}\]: Pale yellow liquid, Yield: 22\%. \[^{1}\]H NMR (400 MHz, CDCl\(_3\), Figure S1) \(\delta/\text{ppm}: 7.68 – 7.64 (m, 2H), 7.63 – 7.60 (m, 1H), 7.49 (t, \(J = 7.8\) Hz, 2H). \[^{13}\]C\{\[^{1}\]H\} NMR (101 MHz, CDCl\(_3\), Figure S2) \(\delta/\text{ppm}: 132.98, 132.29, 129.30, 119.04, 112.52.

![Figure S24. \(^{1}\)H NMR spectra of 5a.](image-url)
Figure S25. $^{13}\text{C}^{1\text{H}}$ NMR spectra of 5a.

Figure S26. $^{1\text{H}}$ NMR spectra of 7a.
Figure S27. $^{13}$C{$^{1}$H} NMR spectra of 7a.

Figure 28. $^{1}$H NMR spectra of 8a.
8.2. Procedure for 1-catalyzed aerial oxidation of nitrile to amide:

In a 10 ml round bottom flask containing a magnetic stirring bar, catalyst 1 (3 mol%, 7 mg), benzonitrile, 8a (52 mg, 0.5 mmol), KOtBu (40 mol%, 23 mg) and toluene (3 mL) were added and then allowed to stir for 15 h at 90 °C under aerobic conditions. After that, the mixture was allowed to cool down to room temperature and the amide product was extracted with 15 mL (3 x 5 mL) of ethyl acetate. The desired benzaamide, 5a was purified according to the above mentioned procedure. Yields: 58 mg, 97%.

Scheme S3. Aerial oxidation of 1-catalyzed nitrile to amide in presence of base KOtBu.

8.3. Procedure for KOtBu-catalyzed aerial oxidation of nitrile to amide:

In a 10 ml round bottom flask containing a magnetic stirring bar, benzonitrile, 8a (52 mg, 0.5 mmol), KOtBu (40 mol%, 23 mg) and toluene (3 mL) were added and then allowed to stir for 15 h at 90 °C under aerobic conditions. After that, the mixture was allowed to cool down to room temperature and the product was extracted with 15 mL (3 x 5 mL) of ethyl
acetate. The desired benzamide, 5a was purified according to the above mentioned procedure. Yields: 21 mg, 34%.

\[
\text{Scheme S4. Nitrile to amide transformation using KO\textsuperscript{t}Bu.}
\]

8.4. Procedures for deuterium-labeling experiment:

In a 15 ml schlenk tube containing a magnetic stirring bar, catalyst 1 (3 mol\%, 7 mg), benzylamine, 4a (54 mg, 0.5 mmol) and KO\textsuperscript{t}Bu (40 mol\%, 23 mg) were dissolved in the mixture of solvents dry-toluene (3 mL) and D\textsubscript{2}O (0.5 mL) under nitrogen-atmosphere. Then the reaction mixture was heated at 90 °C for 15 h under the dry atmospheric air. After that the desired amide product was extracted and purified according to the above mentioned procedure.

\[
\text{Scheme S5. 1-catalysed amine to amide transformation in presence of KO\textsuperscript{t}Bu and D\textsubscript{2}O.}
\]
8.5. Oxidation of amine to amide in presence of excess TEMPO:

In a 10 ml round bottom flask containing a magnetic stirring bar, catalyst 1 (3 mol%, 7 mg), benzylamine, 4a (54 mg, 0.5 mmol), KOtBu (40 mol%, 23 mg), required amount of TEMPO were dissolved in 3 mL toluene. Then the reaction mixture was stirred at 90 °C for 15 h under aerobic conditions. After that the mixture was allowed to cool down to room temperature and the amide product was extracted with 15 mL (3 x 5 mL) of ethyl acetate and purified by column chromatography using silica (hexane/ethyl acetate). Yields: 52 mg, 86%.

Scheme S6. Reaction of 1.5 equivalents TEMPO with benzylamine in presence of 3 mol% 1, 40 mol% KOtBu at 90 °C for 15 h.
8.6. UV-Vis spectroscopic studies:

**Figure S31.** UV-Vis-NIR spectra of complex 1 with different reagents used in amine oxidation recorded after 4 h at RT.

**Figure S32.** UV-Vis-NIR spectra of complex 1 with different reagents used in amine oxidation. All the data recorded after heating at 90 °C for 15 min.
8.7. Mass spectroscopic studies:

**Figure S33.** Mass spectra of the green solution obtained by heating the mixture of 1 and benzylamine at 90 °C for 15 min under inert conditions.
(c) \[ \text{RuO}_2 \text{O} \text{II} \text{H} + \text{MeCN} \rightarrow 1\text{d} - \text{H}_2 + \text{MeCN} \]

(d) \[ \text{RuO}_2 \text{O} \text{II} \text{L} + \text{H}_2 \text{N} + \text{MeCN} + \text{NaOH} \]
Figure S34. Mass spectra of the hot (90 °C) reaction mixture (3 mol% 1, 40 mol% KOtBu, 0.5 mmol benzylamine and 3 mL toluene) recorded at different time intervals.

Figure S35. EPR spectra of the reaction mixture (Condition) recorded at different time intervals at temperature 100 K.
8.8. Visible light mediated catalytic oxidation of amine to amide:

In a 15 ml schlenk tube containing a magnetic stirring bar, catalyst 1 (3 mol%, 7 mg), benzylamine, 4a (54 mg, 0.5 mmol) and KOtBu (40 mol%, 23 mg) were dissolved in 3 mL toluene under nitrogen-atmosphere. Then the reaction mixture was heated at 90 °C for 15 minutes and followed by stirring at RT for 15 h under aerobic conditions in front of a red-light source (5W-lamp). After that the desired amide product was extracted and purified according to the above mentioned procedure. Yields: 45 mg, 74%. We repeated the same reaction with sunlight (16 h) instead of a red light source and isolated the desired amide with an 81% yield (Scheme S9).

\[
\text{NH}_2 \quad \text{4a} \quad \text{NH}_2 \quad \text{5a}
\]

Scheme S7. Visible light mediated catalytic oxidation of amine to amide.

i) 1 (3 mol%) KOtBu (40 mol%), Toluene (90 °C, N2, 15 min.

ii) hv, air-O2, 15 h Red light

Yield: 74%

Scheme S8. Sun light mediated catalytic oxidation of amine to amide.

i) 1 (3 mol%) KOtBu (40 mol%), Toluene (90 °C, N2, 15 min.

ii) hv, air-O2, 16 h Sun light

Yield: 81%

Scheme S9. Oxidation of amine to amide under dark conditions.

8.8.1. Fluorescence study for understanding how visible light excite the molecule.

![Figure S36](image)

Figure S36. (a) Emission spectrum of HO,O-PLY. (b) The quenching of emission due to the metal to ligand (MLCT) charge transfer transition observed when irradiating the green reaction mixture obtained by heating 1 with benzylamine at 90 °C for 15 minutes was carried out.
8.9. Detection of \( \text{H}_2\text{O}_2 \) by iodide oxidation method:

After completing the amine-to-amide aerial oxidation under our ideal conditions (entry 2, Table S4), we added 3 ml of water and used ethyl acetate three times to extract the organic part. The remaining aqueous part was collected, followed by acidification with \( \text{H}_2\text{SO}_4 \) to maintain \( \text{pH}=2 \) to stop further oxidation. We added 1 ml of a 10% KI solution and three drops of a 3% ammonium molybdate solution to the acidic aqueous part. The formation of \( \text{I}^{3^-} \) could be monitored by UV-Vis spectroscopy. The characteristic band appears at 285 nm and 353 nm for \( \text{I}^{3^-} \), indirectly confirm the presence of \( \text{H}_2\text{O}_2 \) in our catalytic reaction mixture.

![Figure S37. UV-Vis spectrum of \( \text{I}^{3^-} \) obtained by the oxidation of \( \text{I}^{3^-} \) using the side product \( \text{H}_2\text{O}_2 \) produced in 1-catalysed aerial oxidation amine to amide.](image)

9. Characterization data of amides:

![Benzamide, 5a](image)

**Benzamide, 5a**\(^{[5,5]}\)

Colourless solid, Yield: 93%. \(^1\text{H} \text{NMR} \) (400 MHz, CDCl\(_3\)): \( \delta \) 7.85 (dd, \( J = 5.2, 3.3 \) Hz, 2H), 7.57 (ddd, \( J = 6.4, 3.7, 1.1 \) Hz, 1H), 7.51-7.40 (m, 2H), 6.27 (s, 2H); \(^{13}\text{C}\{^1\text{H}\} \text{NMR} \) (101 MHz, CDCl\(_3\)): \( \delta \) 169.7, 133.3, 131.9, 128.5, 127.2.
2-Bromobenzamide, 5b[3]
Colourless solid, Yield: 95%. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 7.39 (d, $J$ = 10.7, 4.1 Hz, 1H), 7.64 (dd, $J$ = 12.2, 4.8 Hz, 2H), 7.31 (td, $J$ = 7.7, 1.4 Hz, 1H), 6.25 (s, 1H), 6.18 (s, 1H) $^{13}$C{$^1$H} NMR (101 MHz, CDCl$_3$): $\delta$ 169.6, 137.0, 133.3, 131.6, 129.9, 127.9, 119.2.

3-Bromobenzamide, 5c[5]
Colourless solid, Yield: 94%. $^1$H NMR (400 MHz, DMSO-d$_6$): $\delta$ 8.09 (s, 1H), 7.91 (dd, $J$ = 19.0, 7.9 Hz, 2H), 7.57 (t, $J$ = 7.9 Hz, 1H), 9.49 (s, 2H); $^{13}$C{$^1$H} NMR (101 MHz, DMSO-d$_6$): $\delta$ 164.9, 136.8, 131.5, 131.2, 130.5, 127.7, 122.4.

4-Bromobenzamide, 5d[3,5]
Colourless solid, Yield: 96%. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 7.68 (d, $J$ = 8.4, 2H), 7.54 (d, $J$ = 8.4 Hz, 2H), 6.08 (s, 1H), 5.86 (s, 1H); $^{13}$C{$^1$H} NMR (101 MHz, CDCl$_3$): $\delta$ 168.4, 132.2, 131.9, 129.08, 126.9.

2-Chlorobenzamide, 5e[6]
Colourless solid, Yield: 94%. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 7.80 (dd, $J$ = 7.5, 1.6 Hz, 1H), 7.47-7.33 (m, 3H), 6.35 (s, 2H); $^{13}$C{$^1$H} NMR (101 MHz, CDCl$_3$): $\delta$ 168.2, 133.7, 131.8, 130.8, 130.6, 130.4, 127.1.
4-Chlorobenzamide, 5f[^3-5]
Colourless solid, Yield: 95%. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 7.78-7.73 (m, 2H), 7.45-7.39 (m, 2H), 6.04 (s, 1H), 5.83 (s, 1H); $^{13}$C{$^1$H} NMR (101 MHz, CDCl$_3$): $\delta$ 168.2, 138.3, 131.7, 128.9, 128.8.

2,6-Dichlorobenzamide, 5g[^7]
Colourless solid, Yield: 95%. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 7.36-7.33 (m, 2H), 7.30-7.27 (m, 1H), 6.08 (s, 1H), 5.78 (s, 1H); $^{13}$C{$^1$H} NMR (101 MHz, CDCl$_3$): $\delta$ 169.2, 160.9 135.5, 105.2, 104.1.

3,5-Dichlorobenzamide, 5h[^8]
Colourless solid, Yield: 96%. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 7.70 (d, $J = 1.9$ Hz, 2H), 7.54 (t, $J = 1.8$ Hz, 1H), 6.12 (s, 2H); $^{13}$C{$^1$H} NMR (101 MHz, CDCl$_3$): $\delta$ 163.7, 135.6, 134.9, 132.0, 126.1.

2-Fluorobenzamide, 5i[^3,8]
Colourless solid, Yield: 98%. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 8.11 (td, $J = 7.8, 1.6$ Hz, 1H), 7.55-7.45 (m, 1H), 7.27 (dd, $J = 8.8$, 6.4 Hz, 1H), 7.14 (dd, $J = 12.0$, 8.4 Hz, 1H), 6.70 (s, 2H); $^{13}$C{$^1$H} NMR (101 MHz, CDCl$_3$): $\delta$ 165.3, 162.2, 159.8, 134.0, 133.9, 132.3, 124.9, 116.3, 116.0.
2,6-Difluorobenzamide, 5j[9]

Colourless solid, Yield: 98%. $^1\text{H}\text{ NMR}$ (400 MHz, CDCl$_3$): $\delta$ 7.47-7.33 (m, 1H), 6.97 (t, $J$ = 8.5 Hz, 2H), 6.36 (s, 1H), 6.08 (s, 1H); $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl$_3$): $\delta$ 162.3, 161.4, 158.9, 132.2, 113.1, 112.3, 112.0.

3,5-Bis(trifluoromethyl)benzamide, 5k[10]

Colourless solid, Yield: 96%. $^1\text{H}\text{ NMR}$ (400 MHz, CDCl$_3$): $\delta$ 8.29 (s, 2H), 8.07 (s, 1H), 6.17 (s, 1H), 5.93 (s, 1H); $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl$_3$): $\delta$ 166.2, 135.4, 132.2, 127.8, 125.6, 124.1.

2-(Trifluoromethoxy)benzamide, 5l[11]

Colourless solid, Yield: 93%. $^1\text{H}\text{ NMR}$ (400 MHz, CDCl$_3$): $\delta$ 8.09 (dd, $J$ = 7.8, 1.3 Hz, 1H), 7.60-7.51 (m, 1H), 7.44 (t, $J$ = 7.4 Hz, 1H), 7.34 (d, $J$ = 8.2 Hz, 1H), 6.59 (s, 1H), 6.27 (s, 1H); $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, CDCl$_3$): $\delta$ 166.0, 146.4, 132.9, 132.1, 127.4, 127.0, 121.6, 121.0. $^{19}\text{F}\text{ NMR}$ (376 MHz, MeCN): $\delta$ 58.22.

4-Nitrobenzamide, 5m[5,12]

Colourless solid, Yield: 93%. $^1\text{H}\text{ NMR}$ (400 MHz, DMSO-$d_6$): $\delta$ 8.31 (s, 1H), 8.28 (d, $J$ = 8.6 Hz, 2H), 8.09 (d, $J$ = 8.6 Hz, 2H), 7.75 (s, 1H); $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, DMSO-$d_6$): $\delta$ 166.8, 149.5, 140.4, 129.4, 123.9.
2-Methylbenzamide, 5n\textsuperscript{[5,8]}

Colourless solid, Yield: 68%. \textbf{\textsuperscript{1}H NMR} (400 MHz, CDCl\textsubscript{3}): \(\delta 7.47\) (d, \(J = 7.6\) Hz, 1H), 7.36 (t, \(J = 7.5\) Hz, 1H), 7.25 (dd, \(J = 14.2, 7.2\) Hz, 2H), 5.91 (s, 1H), 5.83 (s, 1H) 3.11 (s, 3H); \textbf{\textsuperscript{13}C\{}\textsuperscript{\textsuperscript{1}H}\textbf{ NMR} (101 MHz, CDCl\textsubscript{3}): \(\delta 172.0, 136.3, 135.1, 131.2, 130.3, 126.9, 125.7, 19.9\).

3,4-Dimethylbenzamide, 5o\textsuperscript{[13]}

Colourless solid, Yield: 66%. \textbf{\textsuperscript{1}H NMR} (400 MHz, CDCl\textsubscript{3}): \(\delta 7.61\) (s, 1H), 7.52 (dd, \(J = 7.8, 1.7\) Hz, 1H), 7.19 (d, \(J = 7.8\) Hz, 1H), 6.15 (s, 2H), 2.30 (s, 6H); \textbf{\textsuperscript{13}C\{}\textsuperscript{\textsuperscript{1}H}\textbf{ NMR} (101 MHz, CDCl\textsubscript{3}): \(\delta 169.7, 141.2, 137.0, 130.8, 129.8, 128.7, 124.7, 19.8, 19.7\).

3-Aminobenzamide, 5p\textsuperscript{[3]}

Colourless solid, Yield: 69%. \textbf{\textsuperscript{1}H NMR} (400 MHz, DMSO-\textit{d}_6): \(\delta 7.73\) (s, 1H), 6.73-6.64 (m, 1H), 7.05 (dd, \(J = 9.0, 6.3\) Hz, 2H), 7.15 (s, 1H), 7.00-6.94 (m, 1H), 5.19 (s, 2H); \textbf{\textsuperscript{13}C\{}\textsuperscript{\textsuperscript{\textsuperscript{1}H}\textbf{ NMR} (101 MHz, DMSO-\textit{d}_6): \(\delta 169.3, 149.1, 135.7, 129.1, 117.0, 115.2, 113.6\).

4-Aminobenzamide, 5q\textsuperscript{[12,12]}

Colourless solid, Yield: 72%. \textbf{\textsuperscript{1}H NMR} (400 MHz, DMSO-\textit{d}_6): \(\delta 7.59\) (d, \(J = 8.5\) Hz, 2H), 7.54 (s, 1H), 6.88 (s, 1H), 6.53 (d, \(J = 8.5\) Hz, 2H), 5.61 (s, 2H), 3.93 (d, \(J = 5.6\) Hz, 2H); \textbf{\textsuperscript{13}C\{}\textsuperscript{\textsuperscript{\textsuperscript{1}H}\textbf{ NMR} (101 MHz, DMSO-\textit{d}_6): \(\delta 168.6, 152.2, 129.6, 121.4, 113.0\).
2-Methoxybenzamide, 5r

Colourless solid, Yield: 71%. \( ^1H\) NMR (400 MHz, CDCl\(_3\)): \( \delta \ 8.22 \) (dd, \( J = 7.8, 1.7 \) Hz, 1H), 7.75 (s, 1H), 7.53-7.44 (m, 1H), 7.09 (t, \( J = 7.6 \) Hz, 1H), 7.00 (d, \( J = 8.3 \) Hz, 1H), 6.11 (s, 1H), 3.98 (s, 3H); \( ^{13}C\{^1H\} \) NMR (101 MHz, CDCl\(_3\)): \( \delta \ 167.1, 157.9, 133.5, 132.6, 121.3, 120.7, 111.4, 56.0. \)

3-Methoxybenzamide, 5s

Colourless solid, Yield: 68%. \( ^1H\) NMR (400 MHz, CDCl\(_3\)): \( \delta \ 7.43-7.38 \) (m, 1H), 7.38-7.31 (m, 2H), 7.07 (dt, \( J = 7.1, 2.5 \) Hz, 1H), 6.14 (s, 1H), 6.00 (s, 1H), 3.85 (s, 1H); \( ^{13}C\{^1H\} \) NMR (101 MHz, CDCl\(_3\)): \( \delta \ 169.3, 159.8, 133.8, 129.6, 119.1, 118.3, 112.6, 55.4. \)

3,5-Dimethoxybenzamide, 5t

Colourless solid, Yield: 66%. \( ^1H\) NMR (400 MHz, CDCl\(_3\)): \( \delta \ 6.94 \) (d, \( J = 2.3 \) Hz, 2H), 6.61(t, \( J = 2.3 \) Hz, 1H), 6.09 (s, 1H), 5.87 (s, 1H), 3.83 (s, 6H); \( ^{13}C\{^1H\} \) NMR (101 MHz, CDCl\(_3\)): \( \delta \ 166.1, 135.3, 131.9, 130.7, 128.1, 51.5. \)

2-Ethoxybenzamide, 5u

Colourless solid, Yield: 65%. \( ^1H\) NMR (400 MHz, CDCl\(_3\)): \( \delta \ 8.24 \) (dd, \( J = 7.8, 1.8 \) Hz, 1H), 7.90 (s, 1H), 7.51-7.42 (m, 1H), 7.08 (dd, \( J = 11.2, 3.9 \) Hz, 1H), 6.98 (d, \( J = 8.3 \) Hz,
1H), 6.31 (s, 1H), 4.22 (q, \( J = 7.0 \) Hz, 2H), 1.53 (t, \( J = 7.0 \) Hz, 3H); \(^{13}\text{C}^{1}\text{H}\) NMR (101 MHz, CDCl\(_3\)): \( \delta \) 167.3, 157.3, 133.3, 132.5, 121.1, 120.8, 112.3, 64.71, 14.85.

4-Ethoxybenzamide, 5v\(^{[10]}\)

Colourless solid, Yield: 67%. \(^{1}\text{H} \) NMR (400 MHz, CDCl\(_3\)): \( \delta \) 7.79 (d, \( J = 8.8 \) Hz, 2H), 6.95 (d, \( J = 8.8 \) Hz, 2H), 5.92 (s, 1H), 5.67 (s, 1H), 4.11 (q, \( J = 7.0 \) Hz, 2H), 1.46 (t, \( J = 7.0 \) Hz, 3H); \(^{13}\text{C}^{1}\text{H}\) NMR (101 MHz, CDCl\(_3\)): \( \delta \) 168.9, 162.0, 129.2, 125.0, 114.2, 63.7, 14.6.

4-Hydroxybenzamide, 5w\(^{[11]}\)

Colourless solid, Yield: 65%. \(^{1}\text{H} \) NMR (400 MHz, DMSO-\( d_6 \)): \( \delta \) 9.98 (s, 1H), 7.75 (d, \( J = 8.5 \) Hz, 3H), 7.12 (s, 1H), 6.79 (d, \( J = 8.5 \) Hz, 2H); \(^{13}\text{C}^{1}\text{H}\) NMR (101 MHz, DMSO-\( d_6 \)): \( \delta \) 168.3, 160.7, 130.0, 125.4, 115.2.

1-Naphthamide, 6a\(^{[15]}\)

Colourless solid, Yield: 90%. \(^{1}\text{H} \) NMR (400 MHz, CDCl\(_3\)): \( \delta \) 8.45 (d, \( J = 8.4 \) Hz, 1H), 7.97 (d, \( J = 8.2 \) Hz, 1H), 7.93-7.88 (m, 1H), 7.73 (dd, \( J = 7.0, 0.8 \) Hz, 1H), 7.64-7.53 (m, 2H), 7.49 (dd, \( J = 8.0, 7.2 \) Hz, 1H), 6.01 (s, 2H); \(^{13}\text{C}^{1}\text{H}\) NMR (101 MHz, CDCl\(_3\)): \( \delta \) 171.5, 134.0, 133.8, 132.0, 131.3, 130.0, 128.4, 127.4, 126.6, 125.4, 124.7.

Benzo[b]thiophene-2-carboxamide, 6b\(^{[16]}\)

Colourless solid, Yield: 82%. \(^{1}\text{H} \) NMR (400 MHz, CDCl\(_3\)): \( \delta \) 7.93-7.76 (s, 3H), 7.52-7.37 (m, 2H), 6.01 (s, 2H); \(^{13}\text{C}^{1}\text{H}\) NMR (101 MHz, CDCl\(_3\)): \( \delta \) 164.1, 141.2, 139.1, 137.4, 126.7, 126.5, 125.3, 125.1, 122.8.
Thiophene-2-carboxamide, 6c\textsuperscript{[5,12,14]}

Colourless solid, Yield: 87%. $^1$H NMR (400 MHz, DMSO-$d_6$): $\delta$ 7.97 (s, 1H), 7.74 (t, $J$ = 4.4 Hz, 2H), 7.38 (s, 1H), 7.13 (t, $J$ = 4.2 Hz, 1H), $^{13}$C{$^1$H} NMR (101 MHz, DMSO-$d_6$): $\delta$ 163.4, 140.8, 131.5, 129.2, 128.4.

Furan-2-carboxamide, 6d\textsuperscript{[5,14]}

Colourless solid, Yield: 89%. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 7.57-7.54 (m, 2H), 7.12 (dd, $J$ = 4.9, 3.9 Hz, 1H), 5.82 (s, 1H); $^{13}$C{$^1$H} NMR (101 MHz, CDCl$_3$): $\delta$ 163.6, 137.7, 131.0, 129.4, 127.9.

Nicotinamide, 6e\textsuperscript{[13]}

Colourless solid, Yield: 93%. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 9.05 (s, 1H), 8.79 (d, $J$ = 3.9 Hz, 1H), 8.26-8.12 (m, 1H), 7.45 (dd, $J$ = 7.9, 4.8 Hz, 1H), 6.25 (s, 1H), 6.00 (s, 1H); $^{13}$C{$^1$H} NMR (101 MHz, CDCl$_3$): $\delta$ 167.4, 152.9, 148.1, 135.2, 128.9, 123.7.

Pyrazine-2-carboxamide, 6f\textsuperscript{[6,17]}

Colourless solid, Yield: 94%. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 9.44 (d, $J$ = 1.3 Hz, 1H), 8.79 (d, $J$ = 2.5 Hz, 1H), 8.61-8.55 (m, 1H), 7.68 (s, 1H), 6.10 (s, 1H); $^{13}$C{$^1$H} NMR (101 MHz, CDCl$_3$): $\delta$ 165.5, 147.6, 144.6, 144.2, 142.8.

2-phenylacetamide, 6g\textsuperscript{[3,14,17]}
Colourless solid, Yield: 84%. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 7.38 (dd, $J = 11.1$, 4.3 Hz 2H), 7.34-7.28 (m, 3H), 5.93 (s, 1H), 5.46 (s, 1H), 3.60 (s, 2H); $^{13}$C$^1$H NMR (101 MHz, CDCl$_3$): $\delta$ 173.7, 134.8, 129.4, 129.0, 127.4, 43.33.

\[ \text{2-(Thiophene-2-yl)acetamide, 6h}^{[14]} \]

Colourless solid, Yield: 86%. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 7.28 (d, $J = 2.7$ Hz, 1H), 7.00 (dd, $J = 10.6$, 5.7 Hz, 2H), 5.92 (s, 1H), 5.69 (s, 1H), 3.80 (s, 2H); $^{13}$C$^1$H NMR (101 MHz, CDCl$_3$): $\delta$ 172.6, 136.1, 128.7, 127.5, 125.7, 37.1.

\[ \text{2-(Naphthalene-1-yl)acetamide, 6i}^{[16]} \]

Colourless solid, Yield: 87%. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 8.01 (d, $J = 8.1$ Hz, 1H), 7.94-7.89 (m, 1H), 7.86 (d, $J = 7.9$ Hz, 1H), 7.57 (dq, $J = 6.7$, 5.2 Hz, 2H), 7.51-7.43 (m, 2H), 5.42 (s, 1H), 5.32 (s, 1H), 4.06 (s, 2H); $^{13}$C$^1$H NMR (101 MHz, CDCl$_3$): $\delta$ 173.3, 134.0, 131.9, 131.1, 128.8, 128.6, 128.2, 126.9, 126.2, 125.6, 123.7, 41.4.

\[ \text{Cyclohexanecarboxamide, 6j}^{[5,13,14]} \]

Colourless solid, Yield: 81%. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 5.61 (s, 1H), 5.48 (s, 1H), 2.15 (tt, $J = 11.7$, 3.5 Hz, 1H), 1.96-1.85 (m, 2H), 1.83-1.77 (m, 2H), 1.72-1.63 (m, 1H), 1.51-1.36 (m, 2H), 1.34-1.15 (m, 3H); $^{13}$C$^1$H NMR (101 MHz, CDCl$_3$): $\delta$ 178.7, 44.8, 29.7, 25.7, 25.7.

\[ \text{Cyclopropanecarboxamide, 6k}^{[17]} \]
Colourless solid, Yield: 64%. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 5.84 (s, 2H), 2.15 (dq, $J$ = 8.0, 4.6 Hz, 1H), 1.00-0.91 (m, 2H), 0.83-0.72 (m, 2H); $^{13}$C{$^1$H} NMR (101 MHz, CDCl$_3$): $\delta$ 176.4, 14.0, 7.6,

Pivalamide, 6$^{[15]}$
Colourless solid, Yield: 68%. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ 6.23 (s, 1H), 5.73 (s, 1H), 1.20 (s, 9H); $^{13}$C{$^1$H} NMR (101 MHz, CDCl$_3$): $\delta$ 181.9, 38.6, 27.6.

10. $^1$H NMR and $^{13}$C NMR spectra of amides:

![Figure S38](image_url1)  $^1$H NMR spectrum (CDCl$_3$) of benzamide, 5a.

![Figure S39](image_url2)  $^{13}$C{$^1$H} NMR spectrum (CDCl$_3$) of benzamide, 5a.
Figure S40. $^1$H NMR spectrum (CDCl$_3$) of 2-bromobenzamide, 5b.

Figure S41. $^{13}$C{$^1$H} NMR spectrum (CDCl$_3$) of 2-bromobenzamide, 5b.
**Figure S42.** $^1$H NMR spectrum (DMSO-$d_6$) of 3-bromobenzamide, 5c.

**Figure S43.** $^{13}$C ($^1$H) NMR spectrum (DMSO-$d_6$) of 3-bromobenzamide, 5c.
Figure S44. $^1$H NMR spectrum (CDCl$_3$) of 4-bromobenzamide, 5d.

Figure S45. $^{13}$C{$^1$H} NMR spectrum (CDCl$_3$) of 4-bromobenzamide, 5d.
Figure S46. $^1$H NMR spectrum (CDCl$_3$) of 2-chlorobenzamide, 5e.

Figure S47. $^{13}$C{$^1$H} NMR spectrum (CDCl$_3$) of 2-chlorobenzamide, 5e.
Figure S48. $^1$H NMR spectrum (CDCl$_3$) of 4-chlorobenzamide, 5f.

Figure S49. $^{13}$C{$^1$H} NMR spectrum (CDCl$_3$) of 4-chlorobenzamide, 5f.
**Figure S50.** $^1$H NMR spectrum ($\text{CDCl}_3$) of 2,6-dichlorobenzamide, $5g$.

**Figure S51.** $^{13}$C {$^1$H} NMR spectrum ($\text{CDCl}_3$) of 2,6-dichlorobenzamide, $5g$. 
Figure S52. $^1$H NMR spectrum (CDCl$_3$) of 3,5-dichlorobenzamide, 5h.

Figure S53. $^{13}$C($^1$H) NMR spectrum (CDCl$_3$) of 3,5-dichlorobenzamide 5h.
Figure S54. $^1$H NMR spectrum (CDCl$_3$) of 2-fluorobenzamide, 5i.

Figure S55. $^{13}$C ($^1$H) NMR spectrum (CDCl$_3$) of 2-fluorobenzamide, 5i.
Figure S56. $^1$H NMR spectrum (CDCl$_3$) of 2,6-difluorobenzamide, 5j.

Figure S57. $^{13}$C{$^1$H} NMR spectrum (CDCl$_3$) of 2,6-difluorobenzamide, 5j.
Figure S58. $^1$H NMR spectrum (CDCl$_3$) of 3,5-bis(trifluoromethyl)benzamide, 5k.

Figure S59. $^{13}$C{$^1$H} NMR spectrum (CDCl$_3$) of 3,5-bis(trifluoromethyl)benzamide, 5k.
Figure S60. $^1$H NMR spectrum (CDCl$_3$) of 2-(trifluoromethoxy)benzamide, 5l.

Figure S61. $^{13}$C{$^1$H} NMR spectrum (CDCl$_3$) of 2-(trifluoromethoxy)benzamide, 5l.

Figure S62. $^{19}$F NMR spectrum (376 MHz, CD$_3$CN) of 2-(trifluoromethoxy)benzamide, 5l.
Figure S63. $^1$H NMR spectrum (CDCl$_3$) of 4-nitrobenzamide, 5m.

Figure S64. $^{13}$C $^{1}$H NMR spectrum (CDCl$_3$) of 4-nitrobenzamide, 5m.
Figure S65. $^1$H NMR spectrum (CDCl$_3$) of 2-methylbenzamide, 5n.

Figure S66. $^{13}$C($^1$H) NMR spectrum (CDCl$_3$) of 2-methylbenzamide, 5n.
Figure S67. $^1$H NMR spectrum (CDCl$_3$) of 3,4-dimethylbenzamide, 50.

Figure S68. $^{13}$C{$^1$H} NMR spectrum (CDCl$_3$) of 3,4-dimethylbenzamide, 50.
Figure S69. $^1$H NMR spectrum (DMSO-$d_6$) of 3-aminobenzamide, 5p.

Figure S70. $^{13}$C ($^1$H) NMR spectrum (DMSO-$d_6$) of 3-aminobenzamide, 5p.
Figure S71. $^1$H NMR spectrum (DMSO-$d_6$) of 4-aminobenzamide, 5q.

Figure S72. $^{13}$C{$^1$H} NMR spectrum (DMSO-$d_6$) of 4-aminobenzamide, 5q.
Figure S73. $^1$H NMR spectrum ($\text{CDCl}_3$) of 2-methoxybenzamide, 5r.

Figure S74. $^{13}$C{$_1^1$H} NMR spectrum ($\text{CDCl}_3$) of 2-methoxybenzamide, 5r.
**Figure S75.** $^1$H NMR spectrum (CDCl$_3$) of 3-methoxybenzamide, 5s.

**Figure S76.** $^{13}$C-$^1$H NMR spectrum (CDCl$_3$) of 3-methoxybenzamide, 5s.
Figure S77. $^1$H NMR spectrum (CDCl$_3$) of 3,5-dimethoxybenzamide, 5t.

Figure S78. $^{13}$C{$^1$H} NMR spectrum (CDCl$_3$) of 3,5-dimethoxybenzamide, 5t.
Figure S79. $^1$H NMR spectrum (CDCl$_3$) of 2-ethoxybenzamide, 5u.

Figure S80. $^{13}$C{$^1$H} NMR spectrum (CDCl$_3$) of 2-ethoxybenzamide, 5u.
Figure S81. $^1$H NMR spectrum (CDCl$_3$) of 4-ethoxybenzamide, 5v.

Figure S82. $^{13}$C{$^1$H} NMR spectrum (CDCl$_3$) of 4-ethoxybenzamide, 5v.
**Figure S83.** $^1$H NMR spectrum (DMSO-$d_6$) of 4-hydroxybenzamide, 5w.

**Figure S84.** $^{13}$C{$^1$H} NMR spectrum (DMSO-$d_6$) of 4-hydroxybenzamide, 5w.
**Figure S85.** $^1$H NMR spectrum (CDCl$_3$) of 1-naphthamide, 6a.

**Figure S86.** $^{13}$C{$^1$H} NMR spectrum (CDCl$_3$) of 1-naphthamide, 6a.
Figure S87. $^1$H NMR spectrum (CDCl$_3$) of benzo[b]thiophene-2-carboxamide, 6b.

Figure S88. $^{13}$C{$^1$H} NMR spectrum (CDCl$_3$) of benzo[b]thiophene-2-carboxamide, 6b.
Figure S89. $^1$H NMR spectrum (DMSO-d$_6$) of thiophene-2-carboxamide, 6c.

Figure S90. $^{13}$C{$^1$H} NMR spectrum (DMSO-d6) of thiophene-2-carboxamide, 6c.
Figure S91. $^{1}H$ NMR spectrum (CDCl$_3$) of furan-2-carboxamide, 6d.

Figure S92. $^{13}C${$^{1}H$} NMR spectrum (CDCl$_3$) of furan-2-carboxamide, 6d.
Figure S93. $^1$H NMR spectrum (CDCl$_3$) of nicotinamide, 6e.

Figure S94. $^{13}$C($^1$H) NMR spectrum (CDCl$_3$) of nicotinamide, 6e.
**Figure S95.** $^1$H NMR spectrum (CDCl$_3$) of pyrazine-2-carboxamide, 6f.

**Figure S96.** $^{13}$C{$^1$H} NMR spectrum (CDCl$_3$) of pyrazine-2-carboxamide, 6f.
**Figure S97.** $^1$H NMR spectrum (CDCl$_3$) of 2-phenylacetamide, 6g.

**Figure S98.** $^{13}$C{$^1$H} NMR spectrum (CDCl$_3$) of 2-phenylacetamide, 6g.
**Figure S99.** $^1$H NMR spectrum (CDCl$_3$) of 2-(thiophene-2-yl)acetamide, 6h.

**Figure S100.** $^{13}$C{$^1$H} NMR spectrum (CDCl$_3$) of 2-(thiophene-2-yl)acetamide, 6h.
Figure S101. $^1$H NMR spectrum (CDCl$_3$) of 2-(naphthalen-1-yl)acetamide, 6i.

Figure S102. $^{13}$C {$^1$H} NMR spectrum (CDCl$_3$) of 2-(naphthalen-1-yl)acetamide, 6i.
Figure S103. \(^1\)H NMR spectrum (CDCl\(_3\)) of cyclohexanecarboxamide, 6j.

Figure S104. \(^{13}\)C\{\(^1\)H\} NMR spectrum (CDCl\(_3\)) of cyclohexanecarboxamide, 6j.
Figure S105. $^1$H NMR spectrum (CDCl$_3$) of cyclopropanecarboxamide, 6k.

Figure S106. $^{13}$C{$^1$H} NMR spectrum (CDCl$_3$) of cyclopropanecarboxamide, 6k.
Figure S107. $^1$H NMR spectrum (CDCl$_3$) of pivalamide, 6l.

Figure S108. $^{13}$C\{$^1$H\} NMR spectrum (CDCl$_3$) of pivalamide, 6l.
11. Theoretical calculation:

Geometry optimization of the complex I was carried out with the help of Gaussian16\(^{[1]}\) at \textit{ub3lyp} level of theory with basis set lanl2dz for transition metals Ru and 6-31g(d) for other elements.

Coordinates of optimized structure I:

\[
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\text{O} & \quad 4.741000 \quad 12.324000 \quad 5.775000 \\
\text{O} & \quad 4.604000 \quad 10.264000 \quad 7.722000 \\
\text{C} & \quad 5.569000 \quad 9.005000 \quad 4.415000 \\
\text{C} & \quad 4.947000 \quad 9.526000 \quad 6.733000 \\
\text{C} & \quad 5.452000 \quad 13.958000 \quad 8.149000 \\
\text{C} & \quad 4.723000 \quad 12.293000 \quad 9.817000 \\
\text{H} & \quad 4.942000 \quad 11.595000 \quad 10.392000 \\
\text{C} & \quad 5.708000 \quad 7.637000 \quad 4.749000 \\
\text{C} & \quad 5.469000 \quad 7.224000 \quad 6.084000 \\
\text{H} & \quad 5.547000 \quad 6.325000 \quad 6.311000 \\
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\text{H} & \quad 6.616000 \quad 12.591000 \quad 9.110000 \\
\text{C} & \quad 5.160000 \quad 9.969000 \quad 5.392000 \\
\text{C} & \quad 5.065000 \quad 11.341000 \quad 5.005000 \\
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12. References:


