Supporting Information

Effect of Fe(III)-based MOFs on catalytic efficiency of Tandem cyclooxidative reaction between 2-aminobenzamide and alcohols

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Section 1: Materials and General Methods

Chemicals used in this work. 1,3,5-triphenylbenzene (97% purity), iron (III) chloride hexahydrate, terephthalic acid (98% purity) were obtained from Aldrich Chemical Co. Hydrofluoric acid, hydrochloric acid, ethanol (99.5% purity), methanol (99.8% purity), sodium hydroxide (97% purity) and sodium sulfate (97% purity) were purchased from Fisher Scientific. 2,6-naphthalenedicarboxylic acid (98% purity), biphenyl-4,4′-dicarboxylic acid (99% purity) were purchased from TCI America. 3-nitrobenzoic acid (99% purity), d-glucose (97% purity), ethyl acetate (anhydrous, purity ≥ 99%), n-hexane (anhydrous, purity ≥ 99.5%), Silica gel 230–400 mesh for flash chromatography, TLC plates (silica gel 60 F254) were purchased from Merck Millipore Co. 1,4-dioxane (99.9% extra dry grade), 1-butanol (purity ≥ 99%), 1-phenylethanol (purity ≥ 98%), 2-aminobenzamide (purity ≥ 98%), 2-propanol (purity ≥ 99%), 4-nitrobenzoic acid (99% purity), 4-methylbenzyl alcohol (purity ≥ 98%), 4-methoxybenzyl alcohol (purity ≥ 98%), aluminum chloride (anhydrous), acetic acid (99.5% purity), acetone (99.8% extra dry grade), Acetyl chloride (99.5% purity), benzyl alcohol (purity ≥ 98%), cyclohexanol (purity ≥ 99%), cycloheptanol (purity ≥ 97%), cyclooctanol (purity ≥ 97%), dichloromethane (99.8% extra dry grade), furfuryl alcohol (purity ≥ 98%), iron (III) nitrate nonahydrate (98% purity), N,N-dimethylformamide (DMF; 99.8% extra dry grade) were purchased from Acros Organics. NMR solvents: Deuterated solvents D₂O, NaOD/D₂O 40 wt%, and dimethyl sulfoxide-d₆ (DMSO-d₆; 99.9% purity) were purchased from Cambridge Isotope Laboratories. Water used in this work was double distilled and filtered through an Amillipore membrane.

Analytical techniques. Powder X-ray diffraction data for refinement was collected on a Bruker D8 Advance employing Ni filtered Cu Kα (λ = 1.54059 Å) radiation (Section 3). A liquid N₂ bath was used for measurements at 77 K. Helium was used as estimation of dead space. Ultrahigh-purity-grade N₂ and He (99.999% purity) were used throughout adsorption experiments. Thermogravimetric analysis (TGA) curves were recorded on a TA Q500 thermal analysis system under airflow (Section 4). The air used has a purity of 99.99%. The chemicals were measured by using Sartorius balance. Low-pressure N₂ adsorption measurements were carried out on a Micromeritics 3Flex surface characterization analyzer (Section 5). The reactions were conducted on a CEM Discover SP microwave system. The products were centrifuged by Mikro 200 machine and analyzed by Agilent GC-MS system or thin-layer chromatography.
(TCL) performed on F-254 silica gel coated aluminum plates from Merck (Section 6). Column chromatography was performed on silica gel 60, 0.04–0.06 mm (230–400 mesh). Melting points were recorded with a Buchi B-545 melting point Apparatus. Fourier transform infrared (FT-IR) spectra were measured on a Bruker E400 FT-IR spectrometer (Section 7 and 8). Nuclear magnetic resonance (\(^1\)H and \(^{13}\)C NMR) spectra were acquired on a Bruker advance II 500 MHz NMR spectrometer (Section 7 and 8). Chemical shifts were quoted in parts per million (ppm) and referenced to the appropriate solvent peak. Gas chromatography-mass spectrometry (GC-MS) measurements were carried out on an Agilent GC System 7890 equipped with a mass selective detector (Agilent 5973N) and a capillary DB-5MS column (30 m × 250 µm × 0.25 µm)(Section 7).


**Linkers**

- **H$_3$BTC**
- **H$_3$BTB**
- **H$_2$BDC**
- **H$_2$NDC**
- **H$_3$BPDC**
- **3,3’-Azo BDC**
- **4,4’-Azo BDC**
Figure S1. Linkers have been used for the synthesis of Fe-MOFs. Triangular linkers (Benzene-1,3,5-tricarboxylic acid (H$_3$BTC), 4,4’,4”-benzene-1,3,5-triyl-tris(benzoic acid) (H3BTB) ) and linear linkers (Benzene-1,4-dicarboxylic acid linker (H$_2$BDC), and 2,6-naphthalenedicarboxylic acid (H$_2$NDC), 4,4’-biphenyldicarboxylic acid(H$_2$BPDC), 3,3’-azobenzene dicarboxylic acid (3,3’-AzoBDC), 4,4’-azobenzene dicarboxylic acid (4,4’-AzoBDC)).

1,3,5-tris(4-carboxyphenyl)benzene (H$_3$BTB),azobenzene-3,3’-dicarboxylic acid (3,3’-azoBDC) and azobenzene-4,4’-dicarboxylic acid (4,4’-azoBDC) were synthesized following the reported procedure.[1-3]

Synthesis of MOF-907:

MOF-907 was synthesized according to a literature procedure.[4]
A mixture of Fe(NO$_3$)$_3$·9H$_2$O (0.600 g, 1.5 mmol), 1,3,5-tris(4-carboxyphenyl) benzene (H$_3$BTB) (0.360 g, 0.81 mmol), and 2,6-Naphthalenedicarboxylic acid (H$_2$NDC) (0.300 g,1.38 mmol) in N,N-dimethylformamide (DMF) (120 mL) was added to a 200-mL glass bottle. The procedure was followed by the addition of 6 mL of acetic acid. The mixture was then sonicated for 1 min and isothermally heated at 120 °C for 24 h. The orange powder was cooled down to room temperature and the solid product is washed with DMF (3× 10 mL, each day) for 3 days. After that, the sample was exchanged solvent by acetone (3 × 10 mL, each day) for 3 days. Finally, the sample was activated by heating at 100 °C under low pressure for 24 h leading to obtain109 mg of activated MOF(22.95% yield based on Fe(NO$_3$)$_3$·9H$_2$O).

Synthesis of MOF-908:

MOF-908 was synthesized according to a literature procedure.[5]
A mixture of Fe(NO$_3$)$_3$·9H$_2$O (0.03686g, 0.0912mmol), 1,3,5-tris(4-carboxyphenyl) benzene (H$_3$BTB) (0.020 g, 0.046 mmol), 4,4’-biphenyldicarboxylic acid (H$_2$BPDC) (0.0055 g, 0.023 mmol), and 3,3’-azobenzene dicarboxylic acid (3,3’-AzoBDC) (0.00681 g, 0.025 mmol) was dissolved in a mixture of N,N-dimethylformamide (DMF, 3.5 mL), 0.5 mL of methanol and 0.2 mL of acetic acid in a 8-mL glass vial. The reaction solution was then heated at 120 °C in an isothermal oven for 24 h to obtain orange shaped crystals. The crystals were thoroughly washed with DMF (3× 10 mL) per day for three days total. After that, the solid was then immersed in acetone (3×
10 mL) per day over a total of three days. The solvent exchanged sample was activated under vacuum at ambient temperature for 24 h, followed by heating at 100 °C under vacuum for 24 h, obtained 14mg of activated MOF (40.64 % yield based on Fe(NO$_3$)$_3$·9H$_2$O).

**Synthesis of MOF-909:**

MOF-909 was synthesized according to a literature procedure.[5]

Fe(NO$_3$)$_3$·9H$_2$O (0.03686 g, 0.0912 mmol), 1,3,5-tris(4-carboxyphenyl) benzene (H$_3$BTB) (0.020 g, 0.046 mmol), and 3,3’-azobenzene dicarboxylic acid (3,3’-AzoBDC) (0.01362 g, 0.050 mmol) were added in the mixed of 3.5 mLDMF, 0.5mL methanol and 0.2 mLacetic acid. This mixture was then sonicated for 1 min and introduced to an 8-mL glass vial. The solution was heated at 120 °C in an isothermal oven for 24 h. The reaction was then cooled down to room temperature and the solid product is washed with DMF (5 × 3 mL, each day) for 3 days and afterward, the MOF material was exchanged by acetone for 3 days (5 × 3 mL, each day). Finally, The solvent exchanged sample was activated under vacuum at ambient temperature for 24 h, followed by heating at 100 °C under vacuum for an additional 24 h, obtained 9.0mg of activated MOF (27 % yield based on Fe(NO$_3$)$_3$·9H$_2$O).

**Synthesis of PCN-280:**

The synthetic procedure of PCN-280 was slightly modified comparing to the original report.[6]

Fe(NO$_3$)$_3$·9H$_2$O (0.03686 g, 0.0912 mmol), 1,3,5-tris(4-carboxyphenyl) benzene (H$_3$BTB) (0.020 g, 0.046 mmol), and biphenyl-4,4′-dicarboxylic acid (H$_2$BPDC) (0.011 g, 0.046 mmol) were added in the mixture of N,N-dimethylformamide (DMF, 3.5 mL), methanol (0.5 mL) and acetic acid (0.2 mL) and then introduced to an 8-mL glass vial. The mixture was sonicated for 1 min to obtain a clear solution. Subsequently, this solution was placed in an isothermal oven at 120 °C for 24 h to obtain the orange shaped crystals of PCN-280. The solid was washed with DMF (5 × 3 mL, each day) for 3 days. After that, the sample was exchanged solvent by acetone for 3 days (5 × 3 mL, each day). The solvent-exchanged sample was activated by heating at 80 °C under low pressure for 24 h producing 14mg of activated MOF (53% yield based on Fe(NO$_3$)$_3$·9H$_2$O).

**Synthesis of PCN-285:**

The synthetic procedure of PCN-285 was slightly modified comparing to the original report.[6]
A solid mixture of Fe(NO$_3$)$_3$·9H$_2$O, 1,3,5-tris(4-carboxyphenyl) benzene (H$_3$BTB) (0.020 g, 0.046 mmol), and 4,4’-azobenzene dicarboxylic acid (4,4’-AzoBDC) (0.01362 g, 0.050 mmol) was dissolved in N,N-dimethylformamide (DMF, 3.5 mL) in a 8-mL glass vial. The procedure was followed by the addition of 6 mL of acetic acid. The mixture was then sonicated for 1 min and isothermally heated at 120 °C for 24 h. The orange crystalline product was collected after cooling down to room temperature and washed with DMF (5 × 3 mL, each day) for 3 days, exchanged with acetone (5 × 3 mL, each day) for 3 days. The solvent-exchanged sample was activated by heating at 80 °C under low pressure for 24 h producing 6mg of activated MOF (36% yield based on Fe(NO$_3$)$_3$·9H$_2$O).

**Synthesis of MIL-126, MIL-88B, MIL-100 (Fe), MIL-101 (Fe)**

Mil-126,Mil-88B,Mil-100 (Fe), MIL-101 (Fe) were synthesized according to the reported procedure.[7-10]

**Section 3: Powder X-ray Diffraction Patterns of Fe-MOF Materials**

PXRD data was collected using a Bruker D8 Advance diffractometer in reflectance Bragg-Brentano geometry employing Ni filtered Cu Kα focused radiation (1.54059 Å, 1.54439 Å) at 1600 W (40 kV, 40 mA) power. The PXRD instrument is equipped with a LynxEye detector. The best counting statistics were achieved by collecting samples using a 0.02° 2θ step scan from 3 – 30° with exposure time of 0.25 s per step. The measurement was performed at room temperature and atmospheric pressure.
**Figure S2.** PXRD of simulated MOF-907 compared to as-synthesized and activated PXRD patterns.

**Figure S3.** PXRD of simulated MOF-908 compared to as-synthesized and activated PXRD patterns.
Figure S4. PXRD of simulated MOF-909 compared to as-synthesized and activated PXRD patterns.

Figure S5. PXRD of simulated PCN-280 compared to as-synthesized and activated PXRD patterns.
Figure S6. PXRD of simulated PCN-285 compared to as-synthesized and activated PXRD patterns

Figure S7. PXRD of simulated MIL-126 compared to as-synthesized and activated PXRD patterns
**Figure S8.** PXRD of simulated MIL-88 compared to as-synthesized and activated PXRD patterns

**Figure S9.** PXRD of simulated MIL-100 compared to as-synthesized and activated PXRD patterns
Figure S10. PXRD of simulated MIL-101 compared to as-synthesized and activated PXRD patterns

Section 4: Thermogravimetric Analysis (TGA)

The thermal stability MOF materials were examined by thermogravimetric analysis. In this measurement, an activated sample of MOF was heated under air flow (60 mL min$^{-1}$) from 30 to 600 °C with a gradient of 5 °C min$^{-1}$.

Figure S11. Thermogravimetric analysis of activated MOF-907 under air flow.
**Figure S12.** Thermogravimetric analysis of activated MOF-908 under air flow.

**Figure S13.** Thermogravimetric analysis of activated MOF-909 under air flow.
Figure S14. Thermogravimetric analysis of activated PCN-280 under air flow.

Figure S15. Thermogravimetric analysis of activated PCN-285 under air flow.
Figure S16. Thermogravimetric analysis of activated MIL-126 under air flow.

Figure S17. Thermogravimetric analysis of activated MIL-88B under air flow.
Section 5: N\textsubscript{2} adsorption isotherm

The permanent porosity of activated MOF was proven by N\textsubscript{2} adsorption at 77 K, measured by a Micromeritics 3Flex surface characterization analyzer.
Figure S20. \( N_2 \) sorption isotherms of activated MOF-907 at 77 K. The filled and open circles represent the adsorption and desorption branches, respectively. The connecting line is provided as a guide for the eyes.

Figure S21. \( N_2 \) sorption isotherms of activated MOF-908 at 77 K. The filled and open circles represent the adsorption and desorption branches, respectively. The connecting line is provided as a guide for the eyes.
**Figure S22.** $\text{N}_2$ sorption isotherms of activated MOF-909 at 77 K. The filled and open circles represent the adsorption and desorption branches, respectively. The connecting line is provided as a guide for the eyes.

**Figure S23.** $\text{N}_2$ sorption isotherms of activated PCN-280 at 77 K. The filled and open circles represent the adsorption and desorption branches, respectively. The connecting line is provided as a guide for the eyes.
Figure S24. N$_2$ sorption isotherms of activated PCN-285 at 77 K. The filled and open circles represent the adsorption and desorption branches, respectively. The connecting line is provided as a guide for the eyes.

Figure S25. N$_2$ sorption isotherms of activated MIL-126 at 77 K. The filled and open circles represent the adsorption and desorption branches, respectively. The connecting line is provided as a guide for the eyes.
Figure S26. $N_2$ sorption isotherms of activated MIL-88B at 77 K. The filled and open circles represent the adsorption and desorption branches, respectively. The connecting line is provided as a guide for the eyes.

Figure S27. $N_2$ sorption isotherms of activated MIL-100 at 77 K. The filled and open circles represent the adsorption and desorption branches, respectively. The connecting line is provided as a guide for the eyes.
Figure S28. N$_2$ sorption isotherms of activated MIL-101 at 77 K. The filled and open circles represent the adsorption and desorption branches, respectively. The connecting line is provided as a guide for the eyes.

Table S1. Summary of surface areas and Pore size of Fe-MOFs (cluster Fe$^{3+}$)

<table>
<thead>
<tr>
<th>Name</th>
<th>Theoretical value (m$^2$ g$^{-1}$)</th>
<th>Langmuir (m$^2$ g$^{-1}$)</th>
<th>BET (m$^2$ g$^{-1}$)</th>
<th>Pore size Distribution (Å)</th>
<th>Ref</th>
</tr>
</thead>
<tbody>
<tr>
<td>MOF-909</td>
<td>2350</td>
<td>2450</td>
<td>1900</td>
<td>24</td>
<td>[5]</td>
</tr>
<tr>
<td>MOF-908</td>
<td>2300</td>
<td>2150</td>
<td>1800</td>
<td>23</td>
<td>[5]</td>
</tr>
<tr>
<td>PCN-280</td>
<td>1800</td>
<td>1750</td>
<td>1600</td>
<td>12</td>
<td>[5]</td>
</tr>
<tr>
<td>PCN-285</td>
<td>1900</td>
<td>1750</td>
<td>1680</td>
<td>22</td>
<td>[4]</td>
</tr>
<tr>
<td>MIL-88B</td>
<td>450</td>
<td>300</td>
<td>164</td>
<td>19</td>
<td>[8,11]</td>
</tr>
<tr>
<td>MIL-100</td>
<td>-</td>
<td>2450</td>
<td>2235</td>
<td>25;29</td>
<td>[10]</td>
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</tbody>
</table>
Section S6: Oxidative cyclization reaction data

Table S2. Summary of active site density of mixed linker-based Fe-MOFs

<table>
<thead>
<tr>
<th>Cat.</th>
<th>Cell volume</th>
<th>Volume (cm³)</th>
<th>Density (g cm⁻³)</th>
<th>Molar catalyst (10⁻⁵ mol)</th>
<th>Pore size Distribution (Å)</th>
<th>Active site density (10¹⁸ cluster Å⁻³)</th>
<th>Space group (N°)</th>
<th>Ref</th>
</tr>
</thead>
<tbody>
<tr>
<td>PCN-285</td>
<td>46525.1</td>
<td>0.047</td>
<td>0.347</td>
<td>1.51009</td>
<td>22</td>
<td>0.909</td>
<td>R3 (146)</td>
<td>[6]</td>
</tr>
<tr>
<td>MOF-909</td>
<td>43939.4</td>
<td>0.047</td>
<td>0.3569</td>
<td>1.55318</td>
<td>23.5</td>
<td>0.963</td>
<td>R3 (146)</td>
<td>[5]</td>
</tr>
<tr>
<td>MOF-908</td>
<td>43191.9</td>
<td>0.047</td>
<td>0.3534</td>
<td>1.57888</td>
<td>23</td>
<td>0.979</td>
<td>R3 (146)</td>
<td>[5]</td>
</tr>
<tr>
<td>MOF-907</td>
<td>87991.1</td>
<td>0.047</td>
<td>0.43</td>
<td>2.10526</td>
<td>19</td>
<td>1.269</td>
<td>Im-3m (229)</td>
<td>[4]</td>
</tr>
<tr>
<td>MIL-101</td>
<td>701861</td>
<td>0.047</td>
<td>0.4659</td>
<td>3.02514</td>
<td>34</td>
<td>1.821</td>
<td>Fd -3m (#227-2)</td>
<td>[13]</td>
</tr>
<tr>
<td>PCN-280</td>
<td>21525</td>
<td>0.047</td>
<td>0.731</td>
<td>3.28821</td>
<td>12</td>
<td>1.965</td>
<td>R3m (160)</td>
<td>[6]</td>
</tr>
<tr>
<td>MIL-126</td>
<td>16826.8</td>
<td>0.047</td>
<td>0.752</td>
<td>3.71261</td>
<td>-</td>
<td>2.235</td>
<td>P43212 (#96-1)</td>
<td>[14, 15]</td>
</tr>
<tr>
<td>MIL-88</td>
<td>3251.9</td>
<td>0.047</td>
<td>0.7787</td>
<td>2.42279</td>
<td>19</td>
<td>3.018</td>
<td>P63/mmc (#1941)</td>
<td>[16]</td>
</tr>
<tr>
<td>MIL-100</td>
<td>394481</td>
<td>0.047</td>
<td>0.7447</td>
<td>3.98804</td>
<td>29</td>
<td>3.241</td>
<td>Fd -3m (#227-2)</td>
<td>[10]</td>
</tr>
</tbody>
</table>
The calculation of active site density (ASD) was followed by the equation:

\[ ASD = \frac{V \times N_{Fe}}{3 \times V_{Cell}} \]

Where:

\( V \): Volume of materials

\( N_{Fe} \): Number of Fe atoms in one unit cell

\( V_{Cell} \): Cell volume of materials

**Procedure for the synthesis of 2-phenylquinazolin-4(3H)-one**

The reaction included benzyl alcohol (1.5 mmol), 2-aminobenzamide (0.5 mmol), Fe-MOF (4.2 mol\%) and tert-butyl hydroperoxide (TBHP) (70\% in water) (2 mmol) was heated by microwave irradiation system at 120 \(^\circ\)C for 1.5 minutes. After reaction completion, the mixture was dissolved with ethyl acetate and centrifuged to remove catalyst. The pure product was refined by column chromatography (9:1 ratio of n-hexane/ethyl acetate). 2-Phenylquinazolin-4(3H)-one compound was confirmed via melting point, FT-IR, \(^1\)H and \(^{13}\)C NMR, GC-MS. For the reusable survey, the catalyst was washed with ethyl acetate (3 x 2 mL) and dried at 80 \(^\circ\)C for next cycle.

**Table S3. Effects of the other catalyst on the synthesis of 2-phenylquinazolin-4(3H)-one**

<table>
<thead>
<tr>
<th>Entry</th>
<th>Cat.</th>
<th>Volume (mL)</th>
<th>Density (g/mL)</th>
<th>Mass (mg)</th>
<th>GC Yield (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>PCN-285</td>
<td>0.047</td>
<td>0.347</td>
<td>16.31</td>
<td>95</td>
</tr>
<tr>
<td>2</td>
<td>MOF-909</td>
<td>0.047</td>
<td>0.357</td>
<td>16.78</td>
<td>13</td>
</tr>
<tr>
<td>3</td>
<td>MOF-908</td>
<td>0.047</td>
<td>0.353</td>
<td>16.59</td>
<td>40</td>
</tr>
<tr>
<td>4</td>
<td>MOF-907</td>
<td>0.047</td>
<td>0.430</td>
<td>20.21</td>
<td>95</td>
</tr>
<tr>
<td>5</td>
<td>MIL-101</td>
<td>0.047</td>
<td>0.466</td>
<td>21.90</td>
<td>95</td>
</tr>
<tr>
<td>6</td>
<td>PCN-280</td>
<td>0.047</td>
<td>0.731</td>
<td>34.36</td>
<td>45</td>
</tr>
<tr>
<td>7</td>
<td>MIL-126</td>
<td>0.047</td>
<td>0.752</td>
<td>35.34</td>
<td>18</td>
</tr>
<tr>
<td>8</td>
<td>MIL-88B</td>
<td>0.047</td>
<td>0.779</td>
<td>36.61</td>
<td>40</td>
</tr>
<tr>
<td>Entry</td>
<td>Cat.</td>
<td>Volume (mL)</td>
<td>Density (g/mL)</td>
<td>Mass (mg)</td>
<td>GC Yield (%)</td>
</tr>
<tr>
<td>-------</td>
<td>-----------</td>
<td>-------------</td>
<td>----------------</td>
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<td>--------------</td>
</tr>
<tr>
<td>1</td>
<td>PCN-285</td>
<td>0.047</td>
<td>0.347</td>
<td>16.3</td>
<td>8</td>
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<tr>
<td>2</td>
<td>MOF-907</td>
<td>0.047</td>
<td>0.430</td>
<td>20</td>
<td>15</td>
</tr>
<tr>
<td>3</td>
<td>MIL-101</td>
<td>0.047</td>
<td>0.466</td>
<td>21.9</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>MIL-100</td>
<td>0.047</td>
<td>0.745</td>
<td>35</td>
<td>0</td>
</tr>
</tbody>
</table>

*Reaction condition: 1-phenylethanol (1.5 mmol, 183 mg), anthranilamide (0.5 mmol, 68 mg), TBHP (2 mmol, 277 µL), were heated by microwave irradiation system at 120°C in 1.5 minutes.*
Figure S29. Structures of MOF materials a) PCN-285 have structure meso MOFs b) MOF-907 MOF-907 possesses 1-D interconnected channels. C) MIL-101 have structure Cage-type meso MOFs. Atom colors: Fe: blue polyhedral. C: black, and O: red. All H atoms are omitted for clarity.

Table S5. Optimization of reaction condition on the synthesis of 2-phenylquinazolin-4(3H)-one.

<table>
<thead>
<tr>
<th>Entry</th>
<th>MOF-907 catalyst (mol%)</th>
<th>Oxidant</th>
<th>Molar of oxidant</th>
<th>Reaction Condition °C (min)</th>
<th>GC Yield (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>TBHP</td>
<td>2.0</td>
<td>120 (15)</td>
<td>0</td>
</tr>
<tr>
<td>2</td>
<td>2.1</td>
<td>TBHP</td>
<td>2.0</td>
<td>120 (15)</td>
<td>18</td>
</tr>
<tr>
<td>3</td>
<td>2.7</td>
<td>TBHP</td>
<td>2.0</td>
<td>120 (15)</td>
<td>24</td>
</tr>
<tr>
<td>4</td>
<td>3.2</td>
<td>TBHP</td>
<td>2.0</td>
<td>120 (15)</td>
<td>47</td>
</tr>
<tr>
<td>5</td>
<td>3.6</td>
<td>TBHP</td>
<td>2.0</td>
<td>120 (15)</td>
<td>60</td>
</tr>
<tr>
<td>6</td>
<td>4.2</td>
<td>TBHP</td>
<td>2.0</td>
<td>120(15)</td>
<td>95</td>
</tr>
<tr>
<td>7</td>
<td>4.2</td>
<td>TBHP</td>
<td>2.0</td>
<td>60 (15)</td>
<td>0</td>
</tr>
<tr>
<td>8</td>
<td>4.2</td>
<td>TBHP</td>
<td>2.0</td>
<td>70 (15)</td>
<td>0</td>
</tr>
<tr>
<td>9</td>
<td>4.2</td>
<td>TBHP</td>
<td>2.0</td>
<td>80 (15)</td>
<td>Trace</td>
</tr>
<tr>
<td>10</td>
<td>4.2</td>
<td>TBHP</td>
<td>2.0</td>
<td>100 (15)</td>
<td>60</td>
</tr>
<tr>
<td>11</td>
<td>4.2</td>
<td>TBHP</td>
<td>2.0</td>
<td>110 (15)</td>
<td>65</td>
</tr>
<tr>
<td>12</td>
<td>4.2</td>
<td>TBHP</td>
<td>2.0</td>
<td>120(10)</td>
<td>95</td>
</tr>
<tr>
<td>13</td>
<td>4.2</td>
<td>TBHP</td>
<td>2.0</td>
<td>120(5.0)</td>
<td>93</td>
</tr>
<tr>
<td>14</td>
<td>4.2</td>
<td>TBHP</td>
<td>2.0</td>
<td>120(2.0)</td>
<td>95</td>
</tr>
<tr>
<td>15</td>
<td>4.2</td>
<td>TBHP</td>
<td>2.0</td>
<td>120(1.5)</td>
<td>95</td>
</tr>
<tr>
<td>16</td>
<td>4.2</td>
<td>TBHP</td>
<td>2.0</td>
<td>120 (1.0)</td>
<td>83</td>
</tr>
<tr>
<td>17</td>
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<td>TBHP</td>
<td>2.0</td>
<td>120(0.5)</td>
<td>55</td>
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<tr>
<td>18</td>
<td>4.2</td>
<td>TBHP</td>
<td>1.5</td>
<td>120(1.5)</td>
<td>83</td>
</tr>
<tr>
<td>Entry</td>
<td>Alcohols</td>
<td>Products</td>
<td>Yield&lt;sup&gt;b&lt;/sup&gt; (%)</td>
<td>TOF</td>
<td></td>
</tr>
<tr>
<td>-------</td>
<td>----------------</td>
<td>----------</td>
<td>------------------------</td>
<td>-------</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>Ph-CH₂OH</td>
<td><img src="image1.png" alt="Product 1" /></td>
<td>95&lt;sup&gt;a&lt;/sup&gt;</td>
<td>902.5</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>2-Meth-OH</td>
<td><img src="image2.png" alt="Product 2" /></td>
<td>95&lt;sup&gt;a&lt;/sup&gt;</td>
<td>902.5</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>4-Meth-OH</td>
<td><img src="image3.png" alt="Product 3" /></td>
<td>88&lt;sup&gt;a&lt;/sup&gt;</td>
<td>835.9</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>Fur-OH</td>
<td><img src="image4.png" alt="Product 4" /></td>
<td>85&lt;sup&gt;a&lt;/sup&gt;</td>
<td>807.4</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>1-OH</td>
<td><img src="image5.png" alt="Product 5" /></td>
<td>70&lt;sup&gt;a&lt;/sup&gt;</td>
<td>664.9</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>1-Methyl-OH</td>
<td><img src="image6.png" alt="Product 6" /></td>
<td>95&lt;sup&gt;b&lt;/sup&gt;</td>
<td>67.7</td>
<td></td>
</tr>
</tbody>
</table>

**Table S6.** Synthesis of 2-phenylquinazolin-4(3H)-one and 2,3-dihydroquinazolin-4-one derivatives

\[ R-OH + \text{MOF-907 TBHP} \rightarrow \text{products} \]

\[ 120 \degree C, 1.5 \text{ min} \]
Table 1: Products from the reaction between 1-butanol and 2-aminobenzamide

<table>
<thead>
<tr>
<th></th>
<th>Structure 1</th>
<th>Structure 2</th>
<th>Yield (%)</th>
<th>TOF ($h^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>![Structure 1 Image]</td>
<td>![Structure 2 Image]</td>
<td>70&lt;sup&gt;b&lt;/sup&gt;</td>
<td>49.9</td>
</tr>
<tr>
<td>8</td>
<td>![Structure 1 Image]</td>
<td>![Structure 2 Image]</td>
<td>40&lt;sup&gt;b&lt;/sup&gt;</td>
<td>22.8</td>
</tr>
<tr>
<td>9</td>
<td>![Structure 1 Image]</td>
<td>![Structure 2 Image]</td>
<td>50&lt;sup&gt;b&lt;/sup&gt;</td>
<td>35.6</td>
</tr>
<tr>
<td>10</td>
<td>![Structure 1 Image]</td>
<td>![Structure 2 Image]</td>
<td>25&lt;sup&gt;b&lt;/sup&gt;</td>
<td>10.7</td>
</tr>
</tbody>
</table>

Reaction condition: 2-aminobenzamide (0.5 mmol, 68 mg), TBHP (2 mmol, 277 µL) were heated by microwave irradiation system at 120 °C. Holding time microwave irradiation was 1.5 min<sup>a</sup> and 20 min<sup>b</sup>

**Equation 1:** The calculation formula of TOF

\[
\text{TOF (} h^{-1} \text{)} = \frac{\text{moles of product}}{\text{moles of cat.} \times h}
\]

**Scheme S1.** The by-product formation of the reaction between 1-butanol and 2-aminobenzamide
Figure S30. (A) P-XRD analysis of MOF-907 before (blue) and after (black) reaction in comparison to the simulated pattern. (B) Reusable ability of MOF-907. (C), (D) SEM images of MOF-907 before and after the catalysis.

Section 7. IR, NMR data of quinazolin-4(3H)-ones and 2,3-dihydroquinazolin-4-ones

2-phenylquinazolin-4(3H)-one

![Chemical Structure](image)

Yield: 95%

Color: White solid

Melting point: 230-232°C

FT-IR (ATR, 4000 – 600 cm⁻¹): 3167, 2921, 2851, 1660, 1597, 1288.
\( ^1H \text{ NMR (500 MHz, DMSO-} \, d_6) \): \( \delta \) 12.48 (s, 1H), 8.15 – 8.11 (m, 3H), 7.85 – 7.82 (m, 1H), 7.74 (d, \( J = 8.0 \) Hz, 1H), 7.60 – 7.51 (m, 4H).

\( ^{13}C \text{ NMR (125 MHz, DMSO-} \, d_6) \): \( \delta \) 162.8, 152.9, 149.1, 135.1, 133.0, 131.8, 129.1, 128.1, 127.7, 127.1, 126.2, 121.1.

GC-MS (EI, 70 eV) \( m/z \): 222 ([M]⁺)

2-(\( p \)-tolyl)quinazolin-4(3H)-one

![Chemical structure of 2-(\( p \)-tolyl)quinazolin-4(3H)-one]

Yield: 95%
Color: White solid
Melting point: 231-233°C

FT-IR (ATR, 4000 – 600 cm\(^{-1}\)): 3173, 3065, 2920, 2852, 1657, 1599, 1285.

\( ^1H \text{ NMR (500 MHz, DMSO-} \, d_6) \): \( \delta \) 12.4 (s, 1H), 8.13 (dd, \( J = 8.0, 1.5 \) Hz, 1H), 8.03 (d, \( J = 8.0 \) Hz, 2H), 7.82 (td, \( J = 8.0, 1.5 \) Hz, 1H), 7.72 (d, \( J = 8.0 \) Hz, 1H), 7.52 – 7.48 (m, 1H), 7.34 (d, \( J = 8.0 \) Hz, 2H), 2.37 (s, 3H).

\( ^{13}C \text{ NMR (125 MHz, DMSO-} \, d_6) \): \( \delta \) 162.8, 152.7, 149.1, 142.0, 135.1, 130.1, 129.6, 128.0, 127.7, 126.9, 126.2, 125.0, 23.1.

GC-MS (EI, 70 eV) \( m/z \): 236 ([M]⁺)

2-(4-methoxyphenyl)quinazolin-4(3H)-one

![Chemical structure of 2-(4-methoxyphenyl)quinazolin-4(3H)-one]

Yield: 88%
Color: White solid
Melting point: 240-243°C

FT-IR (ATR, 4000 – 600 cm\(^{-1}\)): 3153, 3064, 2918, 2850, 1672, 1598, 1244, 1029.
$^1$H NMR (500 MHz, DMSO-$d_6$): $\delta$ 12.4 (s, 1H), 8.19 (d, $J = 8.5$ Hz, 2H), 8.13 (dd, $J = 8.0$, 1.0 Hz, 1H), 7.83 – 7.79 (m, 1H), 7.70 (d, $J = 8.0$ Hz, 1H), 7.50 – 7.46 (m, 1H), 7.10 – 7.08 (m, 2H), 3.85 (s, 3H).

$^{13}$C NMR (125 MHz, DMSO-$d_6$): $\delta$ 162.8, 162.3, 152.4, 149.3, 135.0, 129.3, 127.7, 126.6, 126.3, 125.3, 121.2, 114.5, 55.9.

GC-MS (EI, 70 eV) m/z: 252 ([M]$^+$)

2-(furan-2-yl)quinazolin-4(3H)-one

Yield: 85%
Color: White solid
Melting point: 215-217°C

FT-IR (ATR, 4000 – 600 cm$^{-1}$): 3123, 2954, 2920, 2852, 1676, 1600, 1459, 1266, 1021.

$^1$H NMR (500 MHz, DMSO-$d_6$): $\delta$ 12.5 (s, 1H), 8.13 (dd, $J = 8.0$, 1.0 Hz, 1H), 8.00 (d, $J = 1.0$ Hz, 1H), 7.83 – 7.80 (m, 1H), 7.69 (d, $J = 8.0$ Hz, 1H), 7.63 (d, $J = 3.0$ Hz, 1H), 7.51 – 7.48 (m, 1H), 6.75 (dd, $J = 3.0$, 1.0 Hz, 1H).

$^{13}$C NMR (125 MHz, DMSO-$d_6$): $\delta$ 162.0, 149.1, 147.0, 146.6, 144.5, 135.1, 127.7, 127.0, 126.4, 121.6, 115.0, 113.0.

GC-MS (EI, 70 eV) m/z: 212 ([M]$^+$)

2-propylquinazolin-4(3H)-one

Yield: 70%
Color: White solid
Melting point: 192-194°C

FT-IR (ATR, 4000 – 600 cm$^{-1}$): 3166, 3033, 2961, 2920, 1672, 1617, 1501, 1251.
\textbf{\textit{H} NMR (500 MHz, DMSO- \textit{d}_6):} \delta 12.1 (s, 1H), 8.07 (dd, \textit{J} = 8.0, 1.0 Hz, 1H), 7.78 – 7.74 (m, 1H), 7.58 (d, \textit{J} = 8.0 Hz, 1H), 7.46 – 7.43 (m, 1H), 2.57 (t, \textit{J} = 7.5 Hz, 2H), 1.74 (sex, \textit{J} = 7.5 Hz, 2H), 0.93 (t, \textit{J}= 7.5 Hz, 3H).

\textbf{\textit{C} NMR (125 MHz, DMSO- \textit{d}_6):} \delta 162.3, 157.8, 149.4, 134.7, 127.3, 126.4, 126.1, 121.3, 36.8, 20.7, 13.9.

\textbf{GC-MS (EI, 70 eV) \textit{m/z}:} 188 ([M]+)

2-methyl-2-phenyl-2,3-dihydroquinazolin-4(1\textit{H})-one

Yield: 25%

Color: Brown solid

Melting point: 223-225°C

IR (ATR, 4000-600 cm\textsuperscript{-1}): 3398, 3177, 2927, 1657, 1610, 1489, 1150, 1025.

\textbf{\textit{H} NMR (500 MHz, DMSO- \textit{d}_6):} \delta 8.73 (s, 1H), 7.60 (s, 1H), 7.48 – 7.45 (m, 3H), 7.26 (t, \textit{J} = 8.0 Hz, 2H), 7.20 – 7.14 (m, 2H), 6.75 (d, \textit{J} = 8.0 Hz, 1H), 6.58 – 6.54 (m, 1H), 1.62 (s, 3H).

\textbf{\textit{C} NMR (125 MHz, DMSO- \textit{d}_6):} \delta 164.2, 148.1, 147.6, 133.7, 128.4, 127.7, 127.5, 125.6, 117.3, 115.5, 114.7, 70.6, 31.2.

\textbf{GC-MS (EI, 70 eV) \textit{m/z}:} 238 ([M]+)

1’\textit{H}-spiro[cyclohexane-1,2’quinazolin]-4’(3’\textit{H})-one

Yield: 95%

Color: White solid

Melting point: 217-220°C

IR (ATR 4000-600 cm\textsuperscript{-1}): 3360, 3164, 2924, 1642, 1604, 1473, 1034.
\(^1^H\) NMR (500 MHz, DMSO-\(d_6\)):\(\delta\) 7.87 (s, 1H), 7.54 (dd, \(J = 8.0, 1.5\) Hz, 1H), 7.19 (td, \(J = 8.0, 1.5, 1\)H), 6.78 (d, \(J = 8.0\) Hz, 1H), 6.61 – 6.58 (m, 2H), 1.75 – 1.70 (m, 2H), 1.61 – 1.48 (m, 6H), 1.44 – 1.38 (m, 1H), 1.27 – 1.19 (m, 1H).

\(^1^3^C\) NMR (125 MHz, DMSO-\(d_6\)):\(\delta\) 163.6, 147.2, 133.6, 127.6, 116.9, 115.0, 114.9, 68.3, 37.6, 25.1, 21.4.

GC-MS (EI, 70 eV) \(m/z\):216 ([M]+)

\(1'\)-H-spiro[cycloheptane-1,2'-quinazolin]-4'(3'H)-one

Yield: 70%
Color: White solid
Melting point: 219-222°C
IR (ATR 4000-600 cm\(^{-1}\)): 3332, 3173, 2922, 1609, 1487, 1038.

\(^1^H\) NMR (500 MHz, DMSO-\(d_6\)):\(\delta\) 7.98 (s, 1H), 7.52 (dd, \(J = 8.0, 1.5\) Hz, 1H), 7.20 – 7.16 (m, 1H), 6.70 –6.98 (m, 2H); 6.60 – 6.56 (m, 1H), 1.91 – 1.80 (m, 4H), 1.49 (s, 8H).

\(^1^3^C\) NMR (125 MHz, DMSO-\(d_6\)):\(\delta\) 163.4, 147.2, 133.6, 127.53, 116.8, 114.8, 72.4, 41.5, 29.6, 21.3.

GC-MS (EI, 70 eV) \(m/z\):230 ([M]+)

\(1'\)-H-spiro[cyclooctane-1,2'-quinazolin]-4'(3'H)-one

Yield: 40%
Color: White solid
Melting point: 219-223°C
IR (ATR 4000-600 cm\(^{-1}\)): 3354, 3222, 2916, 1643, 1633, 1482, 1421, 1011.
$^1$H NMR (500 MHz, DMSO- $d_6$): $\delta$ 7.92 (s, 1H), 7.52 (dd, $J = 8.0$, 1.5 Hz, 1H), 7.20 – 7.16 (m, 1H), 6.71 (d, $J = 8.0$ Hz, 1H), 6.60 – 6.56 (m, 2H), 1.91 – 1.80 (m, 4H), 1.52 – 1.49 (m, 10H).

$^{13}$C NMR (125 MHz, DMSO- $d_6$): $\delta$ 163.4, 147.3, 133.6, 127.5, 116.7, 114.8, 71.8, 36.1; 28.2, 24.6, 21.2.

GC-MS (EI, 70 eV) $m/z$:244 ([M]$^+$)

2,2-dimethyl-2,3-dihydroquinazolin-4(1H)-one

Yield: 50%

Color: White solid

Melting point: 195-198°C

IR (ATR 4000-600 cm$^{-1}$): 3326, 3174, 2924, 1606, 1478, 1424, 1025.

$^1$H NMR (500 MHz, DMSO- $d_6$): $\delta$ 7.89 (s, 1H), 7.55 (dd, $J = 8$, 1.5 Hz, 1H), 7.21 – 7.18 (m, 1H), 6.62 – 6.58 (m, 3H), 1.36 (s, 6H).

$^{13}$C NMR (125 MHz, DMSO- $d_6$): $\delta$ 163.5, 147.5, 133.6, 127.64, 116.9, 114.7, 114.3, 67.3, 29.47.

GC-MS (EI, 70 eV) $m/z$:176 ([M]$^+$)
Section 8. Copies of $^1$H, $^{13}$C NMR and HRMS spectra of all products

Figure S31. $^1$H (top) and $^{13}$C (bottom) NMR spectra of 2-phenylquinazolin-4(3$H$)-one
Figure S32. $^1$H (top) and $^{13}$C (bottom) NMR spectra of 2-(p-tolyl)quinazolin-4(3$H$)-one
Figure S33. $^1$H (top) and $^{13}$C (bottom) NMR spectra of 2-(4-methoxyphenyl)quinazolin-4(3$H$)-one
Figure S34. $^1$H (top) and $^{13}$C (bottom) NMR spectra of 2-(furan-2-yl)quinazolin-4(3H)-one
Figure S35. $^1$H (top) and $^{13}$C (bottom) NMR spectra of 2-propylquinazolin-4(3$H$)-one
Figure S36. $^1$H (top) and $^{13}$C (bottom) NMR spectra of 2-methyl-2-phenyl-2,3-dihydroquinoxalin-4(1$H$)-one
**Figure S37.** $^1$H (top) and $^{13}$C (bottom) NMR spectra of 1'-$H$-spiro[cyclohexane-1,2'-quinazolin]-4'(3'-$H$)-one
Figure S38. $^1$H (top) and $^{13}$C (bottom) NMR spectra of 1'H-spiro[cycloheptane-1,2'-quinazolin]-4'(3'H)-one
Figure S39. $^1$H (top) and $^{13}$C (bottom) NMR spectra of 1'H-spiro[cyclooctane-1,2'-quinazolin]-4(3'H)-one
Figure S40. $^1$H (top) and $^{13}$C (bottom) NMR spectra of 2,2-dimethyl-2,3-dihydroquinazolin-4($^1$H)-one
Section 9: References