**Supporting Information**

**1,2,3-Triazole Derivatives as Antitubercular Agents: Synthesis, Biological Evaluation and Molecular Docking Study**

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1. Synthesis of Benzyl azides (8-12):

1.1. Synthesis of benzyl alcohols:

Various substituted benzaldehydes (1 equiv.) were taken in round bottom flask, methanol used as a solvent and allowed reaction mixture for stirring below 0 °C. Then, NaBH\(_4\) (3 equiv.) were added slowly with constant stirring and maintaining the temperature below 0 °C. The progress of the reaction was monitored by thin layer chromatography (TLC) using ethyl acetate: hexane as a solvent system. After completion of the reaction as indicated by TLC, the reaction mixture was then poured on crushed ice and extracted in ethylacetate (3 x 10 mL). The combined organic layer was dried over MgSO\(_4\). Solvent was removed under reduced pressure, and the substituted benzyl alcohols were sufficiently pure to use without further work up.

1.1.2. Synthesis of benzyl bromides:

These benzyl alcohols (1 equiv.) were taken in RBF and dichloromethane as a solvent. This reaction allowed to stir below 5 °C, then drop by drop added phosphorus tribromide (PBr\(_3\)) (1 equiv). The progress of the reaction was monitored by thin layer chromatography (TLC) using ethyl acetate: hexane as a solvent system. After completion of reaction as indicated by TLC, the reaction mass was then poured on crushed ice. Ethylacetate was added to the mixture and the organic layer was separated. The aqueous layer was extracted with 3 x 10 mL of ethylacetate and the combined organic layers were dried over MgSO\(_4\). Solvent was removed under reduced pressure, and the substituted benzyl bromides were sufficiently pure to use without further purification.
1.1.3. **Synthesis of benzyl azides:**  
To a stirred solution of the corresponding bromide (1.0 equiv) in a 50 mL water/acetone mixture (1:4) was added NaN₃ (1.5 equiv). The resulting suspension was stirred at room temperature for 24 hours. The progress of the reaction was monitored by thin layer chromatography (TLC) using ethyl acetate:hexane as a solvent system. After the completion of reaction as indicated by TLC, the reaction mixture was then poured on crushed ice. Ethyl acetate was added to the mixture and the organic layer was separated. The aqueous layer was extracted with 3 x 10 mL of ethylacetate and the combined organic layers were dried over MgSO₄. Solvent was removed under reduced pressure, and the azides were 8-12 sufficiently pure to use without further purification.

![Figure S1. Synthesized alkynes and azide derivatives 1-12.](image-url)
Figure S2. Synthesized 1-(substituted benzyl)-4-(substituted phenoxymethyl)-1H-1,2,3-triazole analogs 13-19.
### Table S1 Anti-tubercular activity of compounds against avirulent strain of dormant MTB H37Ra

<table>
<thead>
<tr>
<th>Compound</th>
<th>% Inhibition of MTB H37Ra growth in presence of compounds</th>
<th>Activity</th>
<th>% Inhibition of MTB H37Ra growth in presence of compounds</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>30 μg/ml 10 μg/ml 3 μg/ml</td>
<td>+/-</td>
<td>30 μg/ml 10 μg/ml 3 μg/ml</td>
</tr>
<tr>
<td>13a</td>
<td>92.16 70.29 67.58 +</td>
<td>16a</td>
<td>13.79 -0.21 -0.11 -</td>
</tr>
<tr>
<td>13b</td>
<td>67.15 66.44 65.61 -</td>
<td>16b</td>
<td>1.66 0.47 18.37 -</td>
</tr>
<tr>
<td>13c</td>
<td>90.07 62.24 55.75 +</td>
<td>16c</td>
<td>27.79 16.25 31.92 -</td>
</tr>
<tr>
<td>13d</td>
<td>91.48 71.82 70.67 +</td>
<td>16d</td>
<td>56.04 43.04 29.17 -</td>
</tr>
<tr>
<td>13e</td>
<td>91.36 77.74 66.32 +</td>
<td>16e</td>
<td>34.97 24.07 11.79 -</td>
</tr>
<tr>
<td>14a</td>
<td>90.07 73.54 70.45 +</td>
<td>17a</td>
<td>91.59 74.87 72.14 +</td>
</tr>
<tr>
<td>14b</td>
<td>74.34 71.82 60.72 -</td>
<td>17b</td>
<td>80.06 77.81 69.83 -</td>
</tr>
<tr>
<td>14c</td>
<td>95.30 76.29 67.93 +</td>
<td>17c</td>
<td>91.33 80.98 75.45 +</td>
</tr>
<tr>
<td>14d</td>
<td>91.52 70.64 71.67 +</td>
<td>17d</td>
<td>79.99 75.64 60.90 -</td>
</tr>
<tr>
<td>14e</td>
<td>66.20 63.92 48.11 -</td>
<td>18a</td>
<td>80.40 73.56 71.63 -</td>
</tr>
<tr>
<td>15a</td>
<td>91.63 73.32 25.85 +</td>
<td>18b</td>
<td>70.81 68.37 63.49 -</td>
</tr>
<tr>
<td>15b</td>
<td>91.36 56.75 50.57 +</td>
<td>18c</td>
<td>91.14 84.73 81.09 +</td>
</tr>
<tr>
<td>15c</td>
<td>95.87 94.61 73.62 +</td>
<td>18d</td>
<td>76.78 71.44 68.76 -</td>
</tr>
<tr>
<td>15d</td>
<td>92.01 80.72 71.86 +</td>
<td>18e</td>
<td>90.90 87.64 71.40 +</td>
</tr>
<tr>
<td>15e</td>
<td>94.15 95.18 77.99 +</td>
<td>19a</td>
<td>71.63 68.46 60.56 -</td>
</tr>
<tr>
<td></td>
<td>19b 52.46 47.65 39.02 -</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The % Inhibition in the presence of test material is calculated by following formula:

\[
\% \text{ inhibition} = \left( \frac{\text{Average of Control} - \text{Average of Compound}}{\text{Average of Control} - \text{Average of Blank}} \right) \times 100
\]

where control is culture medium with cells and DMSO and blank is culture medium without cells. Compounds were considered inactive if %I <90 at 30 μg/mL. For all samples, each compound concentration was tested in triplicates in a single experiment.
Table S2 Experimentally determined Anti-tubercular activity of the key compounds

<table>
<thead>
<tr>
<th>Compound</th>
<th>IC&lt;sub&gt;50&lt;/sub&gt; and IC&lt;sub&gt;90&lt;/sub&gt; values (µg/mL) of compounds with SD values</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>M. tuberculosis H37Ra (ATCC 25177)</td>
</tr>
<tr>
<td></td>
<td>In Vitro (Dormant)</td>
</tr>
<tr>
<td></td>
<td>IC&lt;sub&gt;50&lt;/sub&gt;</td>
</tr>
<tr>
<td>13a</td>
<td>1.70 ± 0. 31</td>
</tr>
<tr>
<td>13c</td>
<td>3.54 ± 0. 93</td>
</tr>
<tr>
<td>13d</td>
<td>2.28 ± 0. 81</td>
</tr>
<tr>
<td>13e</td>
<td>3.16 ± 0. 12</td>
</tr>
<tr>
<td>14a</td>
<td>1.12 ± 0. 33</td>
</tr>
<tr>
<td>14c</td>
<td>2.48 ± 0. 77</td>
</tr>
<tr>
<td>14d</td>
<td>3.06 ± 0. 59</td>
</tr>
<tr>
<td>15a</td>
<td>3.64 ± 0. 29</td>
</tr>
<tr>
<td>15b</td>
<td>2.57 ± 0. 28</td>
</tr>
<tr>
<td>15c</td>
<td>0.74 ± 0. 30</td>
</tr>
<tr>
<td>15d</td>
<td>2.87 ± 0. 85</td>
</tr>
<tr>
<td>15e</td>
<td>0.52 ± 0. 63</td>
</tr>
<tr>
<td>17a</td>
<td>0.74 ± 0. 34</td>
</tr>
<tr>
<td>17c</td>
<td>0.16 ± 0. 04</td>
</tr>
<tr>
<td>18c</td>
<td>0.83 ± 0. 10</td>
</tr>
<tr>
<td>18e</td>
<td>0.92 ± 0. 50</td>
</tr>
</tbody>
</table>

<sup>b</sup>Rifampicin 0.0014± 0.62 0.043± 0.15 0.0018± 0.13 0.048±0.44

<sup>a</sup>IC<sub>50</sub>/IC<sub>90</sub> in µg/mL. Antitubercular activity of each agent was determined by serial dose dependent dilutions. <sup>b</sup>Standard antitubercular drugs and positive controls. Data were expressed as the means of triplication. SD (±): Standard Deviation.
13a. HRMS

13a. $^1$H NMR, 200 MHz, CDCl$_3$
13a. $^{13}$C NMR, 50 MHz, CDCl$_3$

![13C NMR spectrum of compound 13a.](image)

13a. DEPT, 50 MHz, CDCl$_3$

![DEPT spectrum of compound 13a.](image)
13b.HRMS

[Graphical representation of a molecular structure with peaks at 333.0980, 311.1155, 189.0893, and 443.0159 m/z values]
13b. $^1$H NMR, 200 MHz, CDCl$_3$
13b. $^{13}$C NMR, 50 MHz, CDCl$_3$

![C NMR Spectrum for 13b]

13b. DEPT, 50 MHz, CDCl$_3$

![DEPT Spectrum for 13b]
13c. HRMS

13c. $^1$H NMR, 200 MHz, CDCl$_3$
13c. $^{13}$C NMR, 50 MHz, CDCl$_3$
$^{13}$c DEPT, 50 MHz, CDCl$_3$
13c. HRMS

13c. $^1$H NMR, 200 MHz, CDCl$_3$
13e. $^{13}$C NMR, 50 MHz, CDCl$_3$

[Chemical Structure Image]

13e.DEPT, 50 MHz, CDCl$_3$

[Chemical Structure Image]
14a. $^1$H NMR, 200 MHz, CDCl$_3$

14a. $^{13}$C NMR, 50 MHz, CDCl$_3$
14a. DEPT, 50 MHz, CDCl$_3$
$^{1}H$ NMR, 200 MHz, CDCl$_3$
14c. $^{13}$C NMR, 50 MHz, CDCl$_3$

14c. DEPT, 50 MHz, CDCl$_3$
14d. $^1$H NMR, 200 MHz, CDCl$_3$

14d. $^{13}$C NMR, 50 MHz, CDCl$_3$
14d.DEPT, 50 MHz, CDCl$_3$
14e. $^1$H NMR, 200 MHz, CDCl$_3$

14e. $^{13}$C NMR, 200 MHz, CDCl$_3$
14c.DEPT, 50 MHz, CDCl$_3$
15a. HRMS

15a. $^1$H NMR, 200 MHz, CDCl$_3$
15a. $^{13}$C NMR, 100 MHz, CDCl$_3$

![NMR spectrum of 15a]

15a. DEPT, 100 MHz, CDCl$_3$

![DEPT spectrum of 15a]
15b. HRMS

15b. $^1$H NMR, 400 MHz, CDCl$_3$
15b. $^{13}$C NMR, 100 MHz, CDCl$_3$

[Diagram of $^{13}$C NMR spectrum with chemical structures and peak assignments]

15b. DEPT, 100 MHz, CDCl$_3$

[Diagram of DEPT spectrum with chemical structures and peak assignments]
$^{15}\text{c} \cdot \text{HRMS}$

![HRMS spectrum](image)

$^{15}\text{c} \cdot {^1}\text{H NMR, 200 MHz, CDCl}_3$

![NMR spectrum](image)
$^{15c}$H NMR, 200 MHz, CDCl$_3$

$^{13c}$C NMR, 50 MHz, CDCl$_3$
15d. $^{13}$C NMR, 50 MHz, CDCl$_3$

15d. DEPT, 50 MHz, CDCl$_3$
15e. HRMS

15e. $^1$H NMR, 400 MHz, CDCl$_3$
$^{13}$C NMR, 100 MHz, CDCl$_3$

$^{13}$C NMR, 100 MHz, CDCl$_3$

DEPT, 100 MHz, CDCl$_3$
**16c. HRMS**

![HRMS spectrum](image)

**16c. $^1$H NMR, 200 MHz, CDCl$_3$**

![NMR spectrum](image)
16c. $^{13}$C NMR, 50 MHz, CDCl$_3$

![Carbon NMR spectrum](image)

16c.DEPT, 50 MHz, CDCl$_3$

![DEPT spectrum](image)
16d. HRMS

16d. $^1$H NMR, 200 MHz, CDCl$_3$
16d. $^{13}$C NMR, 50 MHz, CDCl$_3$

[Diagram of $^{13}$C NMR spectrum]

16d. DEPT, 50 MHz, CDCl$_3$

[Diagram of DEPT spectrum]
16e. $^{13}$C NMR, 50 MHz, CDCl$_3$

![Carbon NMR spectrum](image1)

16e. DEPT, 50 MHz, CDCl$_3$

![DEPT spectrum](image2)
17b. HRMS

\[ \text{Intens.} \]

136.0404
180.0665
334.0506
381.0720

359.0 (HRMS, 0.1-0.4min #5-23, 100%=56457)
C17H16ClN4O3, 359.0000

17b. \textsuperscript{1}H NMR, 200 MHz, CDCl$_3$

\[ \text{Chemical Shift (ppm)} \]
17b. $^{13}$C NMR, 100 MHz, CDCl$_3$

![Carbon NMR spectrum](image1)

17b. DEPT, 100 MHz, CDCl$_3$

![DEPT spectrum](image2)
17c. HRMS

17c. $^1$H NMR, 200 MHz, CDCl$_3$
$^{13}$C NMR, 100 MHz, CDCl$_3$

17c.

DEPT, 100 MHz, CDCl$_3$

17c.
18b. HRMS

18b. $^1$H NMR, 200 MHz, CDCl$_3$
18b. $^{13}$C NMR, 50 MHz, CDCl$_3$

![Chemical Spectrum 1](image1)

18b. DEPT, 50 MHz, CDCl$_3$

![Chemical Spectrum 2](image2)
18c. HRMS

18c. $^1$H NMR, 400 MHz, CDCl$_3$
18c. $^{13}$C NMR, 100 MHz, CDCl$_3$

18c. DEPT, 100 MHz, CDCl$_3$
$^{1}H$ NMR, 400 MHz, CDCl$_3$
19a. $^{13}$C NMR, 50 MHz, CDCl$_3$

19a. DEPT, 50 MHz, CDCl$_3$
19b. HRMS

19b. $^1$H NMR, 400 MHz, CDCl$_3$
19b. $^{13}$C NMR, 100 MHz, CDCl$_3$

19b. DEPT, 100 MHz, CDCl$_3$