Heterogeneous recyclable nano-CeO2 catalyst: Efficient and eco-friendly synthesis of novel fused triazolo and tetrazolo pyrimidine derivatives in aqueous medium

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Supplementary Information

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1. Reusability study of nano-CeO₂ Catalyst:

The catalyst recycling experiment was done using the model reaction of the reaction of benzoylacetonitrile 1 (1 mmol), benzaldehyde 2a (1 mmol) and 5-aminotriazole 3 (1 mmol) and 20 mol% of the catalyst in H₂O at 80 °C. After completion of the reaction, the catalyst was easily separated by filtration and washed with hot ethanol, dried under oven and reused in the subsequent reaction. Almost quantifiable catalyst could be recovered from each run. The reusability of the catalyst was tested up to 5 successive runs (Table 1).

**Table 1: Reusability of nano-CeO₂ in the synthesis of title compounds 4a**

<table>
<thead>
<tr>
<th>Entry</th>
<th>Run</th>
<th>Yields (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Fresh</td>
<td>92</td>
</tr>
<tr>
<td>2</td>
<td>1ˢᵗ</td>
<td>91</td>
</tr>
<tr>
<td>3</td>
<td>2ⁿᵈ</td>
<td>89</td>
</tr>
<tr>
<td>4</td>
<td>3ʳᵈ</td>
<td>88</td>
</tr>
<tr>
<td>5</td>
<td>4ᵗʰ</td>
<td>86</td>
</tr>
</tbody>
</table>

2. Copies of Mass, ¹H and ¹³C NMR spectra of all the compounds

![Mass Spectrum of compound 5a](image-url)
$^1$H NMR Spectrum of compound 5a
$^{13}$C NMR Spectrum of compound 5a

Mass Spectrum of compound 5b

$^1$H NMR Spectrum of compound 5b
$^{13}$C NMR Spectrum of compound 4b

Mass Spectrum of compound 5c
$\text{H NMR Spectrum of compound 5c}$

$\text{C NMR Spectrum of compound 4c}$

$\text{H NMR Spectrum of compound 5c}$

$\text{C NMR Spectrum of compound 4c}$
Mass Spectrum of compound 5d

\[ \text{H NMR Spectrum of compound 5d} \]
$^{13}$C NMR Spectrum of compound 4d

Mass Spectrum of compound 5e
$^{1}$H NMR Spectrum of compound 5e

Mass Spectrum of compound 5f
$^1$H NMR Spectrum of compound 5f

$^{13}$C NMR Spectrum of compound 4f
Mass Spectrum of compound 5g

$^1$H NMR Spectrum of compound 5g
Mass Spectrum of compound 5h

$^1$H NMR Spectrum of compound 5h
Mass Spectrum of compound 5k

$^1$H NMR Spectrum of compound 5k
$^{13}$C NMR Spectrum of compound 4k

Mass Spectrum of compound 5m
$^1$H NMR Spectrum of compound 5m

$^{13}$C NMR Spectrum of compound 4m
Mass Spectrum of compound 5n

$^1$H NMR Spectrum of compound 5n
\(^{13}\)C NMR Spectrum of compound 4n

Mass Spectrum of compound 6a
$^{1}H$ NMR Spectrum of compound 6a

$^{13}C$ NMR Spectrum of compound 6a
Mass Spectrum of compound 6b

$^1$H NMR Spectrum of compound 6b
$^{13}$C NMR Spectrum of compound 6b

Mass Spectrum of compound 6c
$^1$H NMR Spectrum of compound 6c

$^{13}$C NMR Spectrum of compound 6c
Mass Spectrum of compound 6e

$^1$H NMR Spectrum of compound 6e
Mass Spectrum of compound 6f

$^1$H NMR Spectrum of compound 6f
$^{13}$C NMR Spectrum of compound 6f

Mass Spectrum of compound 6k
$^{13}$C NMR Spectrum of compound 6k