One Pot Synthesis of 6,7-Diimino imidazo[2,3-b]pyrimido[5,6-e]pyrimido[2,3-b][1,3]benzothiazole Derivatives

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ABSTRACT
We have reported the synthesis of 6,7-Diimino imidazo[2,3-b]pyrimido[5,6-e]pyrimido[2,3-b][1,3]benzothiazole derivatives by condensing 3-Cyano-4-imino-2-methylthio-4H-pyrimido[1,2-a]benzimidazole with 2-Amino benzothiazole derivatives in presence of N,N'-dimethyl formamide and anhydrous potassium carbonate as a catalyst under reflux condition. The structures of all newly synthesized cyclic compounds were confirmed on the basis of spectral analysis, IR, 1H NMR and Mass spectral properties.

Keywords: Benzothiazole, Pyrimido, DMF, Potassium Carbonate, Spectral Properties.

I. INTRODUCTION
Benzothiazole derivatives are significant class of fused heterocycles due to their extensive range of pharmacological potential, in addition to this its value in the synthesis of drug molecules and natural products. It shows anti-inflammatory1, analgesic2, antioxidant3, antidiabetics4, antimicrobial5, antituberculosis6, vasodilator7, antitumor8, antiproliferative9, anticancer activity10. These things inspire us to synthesize some pyrimido-benzothiazole derivatives.

II. Material and Methods
All the chemicals used in present works are from analytical grade and used without further purification. Melting points of the products were determined in open capillary tubes on an electrothermal melting point apparatus and were uncorrected. All these reactions were monitored by TLC. IR spectra were recorded on Shimadzu FT-IR spectrophotometer, 1H NMR spectra were obtained on Bruker avance spectrophotometer 500 MHz in DMSO-d6 using TMS as an internal standard. Mass spectrums were analyzed on GC-MS spectrometer using the ESI 70 eV technique.

III. General Procedure
Synthesis of 6,7-Diiminoimidazo[2,3-b]pyrimido[5,6-e]pyrimido[2,3-b][1,3]benzothiazole and their substituted derivatives (3B.40a-g).

The parent compound (1) (0.001 mol) and 2-Amino benzothiazole derivatives such as 2-amino benzothiazole (2a), 2-amino-6-methylbenzothiazole (2b), 2-amino-6-methoxy benzothiazole (2c), 2-amino-4-methyl-6-nitrobenzothiazole (2d), 2-amino-6-fluoro benzothiazole (2e), 2-amino-6-chlorobenzothiazole (2f) and 2-amino-6-bromo-4-fluoro benzothiazole (2g) (0.001 mol) in 15 ml of DMF and anhydrous K2CO3 (10 mg) were refluxed for 5-6 hours. Reaction content cooled at room temperature and mixed with ice cold water then separated solid was filtered, rinse with water and recrystallized using DMF-ethanol mixture to give pure (3a-g) respectively.

IV. Result and Discussion
In the present research, we reported one pot synthesis of 6,7-diimino imidazo[2,3-b]pyrimido[5,6-e]pyrimido[2,3-b][1,3]benzothiazole and their
substituted derivatives (3a-g). The reaction started with 3-cyano-4-imino-2-methylthio-4H-pyrimido[1,2-a]benzimidazole (2) were condensed with dissimilar substituted benzothiazoles in presence of refluxing N,N'-dimethyl formamide and anhydrous potassium carbonate to accomplish corresponding target compounds (3a-g) shown in scheme-I.

The reaction started with an initial attack of amino group of benzothiazoles on carbon attached to -SCH3 group resulting in loss of the thiomethyl group in the form of methyl mercaptan. Resulting secondary amine polarizes on to nitrile carbon to give cyclized compounds

The structures of all newly synthesized cyclic compounds (3Ba-g) were confirmed on the basis of spectral analysis, IR, 1H NMR and Mass spectral data. IR spectra of compounds showed the presence of absorption bands between 3400-3436 cm⁻¹ which can be assigned to (=NH stretch). The 1H NMR showed a singlet at δ 3.81 and δ 8.6 which can be assigned to (-NH & =NH) proton. Mass spectra of compounds exhibited the molecular ion peaks which correspond to their molecular weights.

6,7-Diiminoimidazo[2,3-b]pyrimido[5,6-e]pyrimido[2,3-b][1,3]benzothiazole (3B.40a)

IR:

1577-1662 cm⁻¹ (Ar C=C stretch), 3436 cm⁻¹ (=NH stretch), 1H NMR: (500 MHz, DMSO) δ: 3.81 (s, 1H, Ar C-NH), 7.3-8.4 (m, 8H, Ar-H), 8.6 - 9.3 (s, 1H, two =NH) ppm, Mass: m/z=358 (M+1).

Plausible mechanism of compound (3a-g) (Scheme-I).

Table 1. Physico-chemical properties of synthesized compounds (3a-g).

<table>
<thead>
<tr>
<th>Sr. No</th>
<th>Compound</th>
<th>Color</th>
<th>M.F.</th>
<th>M.W.</th>
<th>M.P. (°C)</th>
<th>Yield (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>3a</td>
<td>Yello w</td>
<td>C18H11N7S3</td>
<td>357</td>
<td>316-318</td>
<td>80</td>
</tr>
<tr>
<td>2.</td>
<td>3b</td>
<td>Brow n</td>
<td>C19H12N7S3</td>
<td>371</td>
<td>325-327</td>
<td>72</td>
</tr>
<tr>
<td>3.</td>
<td>3c</td>
<td>Yello w</td>
<td>C19H13N7OS</td>
<td>387</td>
<td>314-317</td>
<td>70</td>
</tr>
<tr>
<td>4.</td>
<td>3d</td>
<td>Yello w</td>
<td>C19H12N8O2S</td>
<td>416</td>
<td>322-324</td>
<td>65</td>
</tr>
<tr>
<td>5.</td>
<td>3e</td>
<td>Yello w</td>
<td>C18H10FN7S</td>
<td>375</td>
<td>312-315</td>
<td>68</td>
</tr>
<tr>
<td>6.</td>
<td>3f</td>
<td>Brow n</td>
<td>C18H10ClN7S</td>
<td>391</td>
<td>321-323</td>
<td>73</td>
</tr>
<tr>
<td>7.</td>
<td>3g</td>
<td>Brow n</td>
<td>C18H9BrFN7S</td>
<td>454</td>
<td>318-320</td>
<td>78</td>
</tr>
</tbody>
</table>
V. Conclusion

In the present work we have synthesized 6,7-dimino imidazo[2,3-b]pyrimido[5,6-e]pyrimido[2,3-b][1,3]benzothiazole and their substituted derivatives (3a-g) in good yields. We have used inorganic base potassium carbonate as a catalyst for transformation instead of many other organic bases due to its distinctive features and DMF as refluxing solvent. We have achieved this synthesis in single step rather than multiple steps with minimum reaction time.

VI. Acknowledgement

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VII. REFERENCES