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2-[SUBSTITUTEDTHIOCARBAMIDO-11-(PIPERAZIN-1-YL)DIBENZO[b,f][1,4] OXAZEPINES

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ABSTRACT

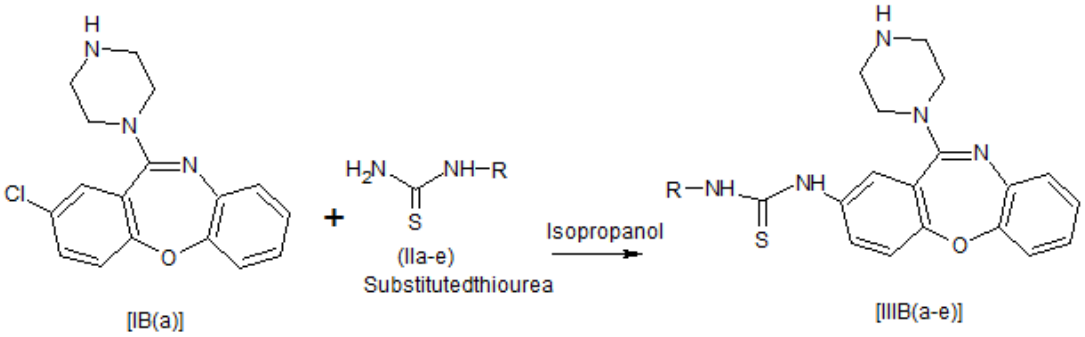
Recently in this laboratory a novel series of 2-[substitutedthiocarbamido-11-(piperazin-1-yl) dibenzo[b,f][1,4]oxazepines **[IIIB(a-e)]** was successfully synthesized by the interactions of 2-chloro-11-(piperazin-1-yl)dibenzo[b,f][1,4]oxazepine **(IB)** with various thioureas **(IIa-e)** in isopropanol medium. The structure determination and justification of the synthesized compounds were done on the basis of chemical characteristics, elemental analysis and spectral studies.

INTRODUCTION

Oxazepine and their derivatives have some important biological pharmacological activities[1] such as enzyme inhibitors[2], analgesic[3], anti-depressant[4] and psychoactive drugs[5]. Oxazepine nucleus is used for treatment of depression, anxiety and agitation[6-7]. Recently new series of 1,2,4-thiadiazoles, 1,3,5-thiadiazines and 1,3,5-dithiazines were synthesized by exploring the synthetic applications of -thiocarbamido, -amino, -halo, -cyano, etc. and their antimicrobial, antifungal, antibacterial, analgesic physiochemical parameters[8-11] were studied. 2-Chloro-11-(piperazin-1-yl)dibenzo [b,f] [1,4] oxazepine **(IB)** and their derivatives showed agricultural, medicinal, biological, pharmaceutical, industrial significances and applications.

2-chloro-11-(piperazin-1-yl)dibenzo[b,f][1,4]oxazepine and their derivatives showed agricultural, medicinal, biological, pharmaceutical, industrial significances and applications. By considering all these facts this research scheme was designed.

The main objective of the work is to synthesize a novel series of 2-[substitutedthio- carbamido-11-(piperazin-1-yl)dibenzo[b,f][1,4] oxazepines **[IIIB(a-e)].** This was synthesized by the interactions of 2-choloro-11-(piperazin-1-yl)dibenzo [b,f] [1,4] oxazepine **(IB)** with various thioureas **(IIa-e)** in isopropanol medium **Scheme-I.**



2-Chloro-11-(piperazin-1-yl)dibenzo [b,f][1,4] oxazepine

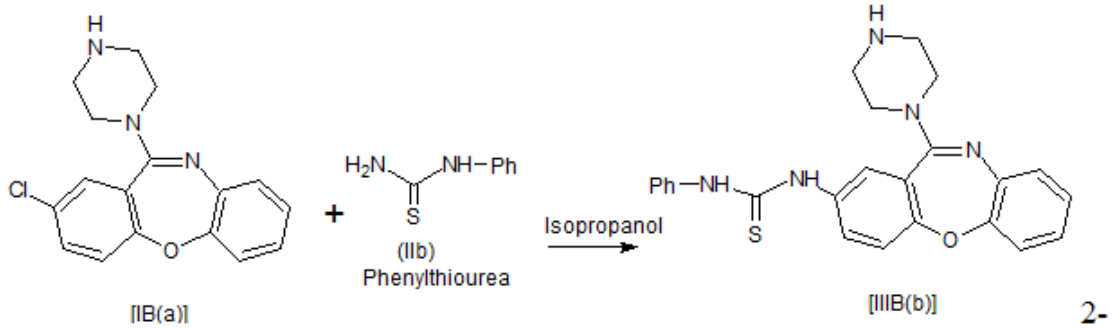
2-[Substitutedthiocarbamido-11 -(piperazin-1-yl)dibenzo[b,f][1,4]oxazepine

Scheme-I

Synthesis of 2-[phenylthiocarbamido-11-(piperazin-1-yl)dibenzo[b,f] [1,4] oxazepine

2-[Phenylthiocarbamido-11-(piperazin-1-yl)dibenzo[b,f][1,4]oxazepine was synthesized by refluxing 2-chloro-11-(piperazin-1-yl)dibenzo[b,f][1,4]oxazepine **(IB)** and phenylthiourea **[IIA]** in isopropanol medium for 4 hours on water bath, dark brown crystals were separated out at room conditions, filtered, dried and were recrystallized from aqueous ethanol. Yield 87%, M.P. 248^0C.

The formation of **[IIIB(b)]**is depicted as below,



Chloro-11-(piperazin-1-yl)dibenzo [b,f][1,4] oxazepine

2-[Phenylthiocarbamido-11 (piperazin-1-yl)dibenzo[b,f][1,4]oxazepine

[IIIB(b)]

Properties of [IIIB(b)]

It is dark brown colour crystalline solid having melting point 248^0C. It gave positive test for nitrogen and sulphur. It was desulphurized by sodium plumbite solution which clearly indicate the presence of C=S group. It was soluble in water, ethanol, DMSO-d_6 while insoluble in carbon tetrachloride, chloroform, benzene, petroleum ether. It formed picrate having melting point 180^0C. **Elemental analysis: [**C: 66.40% (found), 67.13% (calculated)], [H: 04.40% (found), 05.36% (calculated)], [N: 16.31% (found), 16.31% (calculated)], [S: 06.53% (found), 07.45% (calculated)]. **IR Spectrum**: The IR spectrum was carried out in KBr-pellets. The important absorptions are correlated as (cm^{-1}) 3423.65 N–H stretching, 2889.33 C-H stretching, 1681.93 N=C-N stretching, 1562.34 N-C=S stretching, 1145.72 C-N stretching. **NMR Spectrum:** The NMR spectrum was carried out in DMSO-d_6 and $CDCl_3$. This spectrum distinctly displayed the

signals due to Ar-H protons at δ 9.6791-6.9518 ppm, -NH proton at δ 4.2485-3.2303 ppm, -CH_2 protons at δ 2.8934-1.0556 ppm.

Similarly, 2-[thiocarbamido-11-(piperazin-1-yl)dibenzo[b,f][1,4] oxazepine **[IIIB(a)],** 2-[ethylthiocarbamido-11-(piperazin-1-yl)dibenzo [b,f] [1,4] oxazepine **[IIIB(b)],** 2-[methylthiocarbamido-11-(piperazin-1-yl)dibenzo [b,f] [1,4] oxazepine **[IIIB(d)],** 2-[allylthiocarbamido-11-(piperazin-1-yl) dibenzo[b,f] [1,4] oxazepine **[IIIB(e)]** were prepared by the interactions of 2-chloro-11-(piperazin-1-yl)dibenzo[b,f][1,4] oxazepine **(IB)** and ethylthiourea **(IIb)** thiourea, **(IIc)**, methylthiourea **(IId)** allylthiourea **(IIe)** respectively by the above mentioned method and enlisted in **Table No. I**

Table No. I

Sr. No.	2-[**Substituted**thiocarbamido-11-(piperazin -1-yl)dibenzo[b,f][1,4] oxazepine	**Yield (%)**	**M.P. ˚C**
1.	2-[Thiocarbamido-11-(piperazin-1-yl) dibenzo[b,f][1,4]oxazepine **[IIIB(a)]**	95	204
2.	2-[**Ethyl**----------oxazepine **[IIIB(b)]**	85	154
3.	2-[**Methyl**----------oxazepine **[IIIB(d)]**	82	178
4.	2-[**Allyl**----------oxazepine **[IIIB(e)]**	78	157

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