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# Green Synthesis Of New (E)-3-methyl-6-((naphthalene-1-ylimino)methyl)benzo[d]thiazol-2(3h)-one Schiff Base, ADME Study

Aya Alem[1*], Yasser Bouchebcheb [1] , Dalila Fedaoui[1], Messaoud Liachaa[1]

•[1]Laboratory of Synthesis and Organic Biocatalysis (LSBO), Department of chemistry, Faculty of Science, University of Badji Mokhtar Annaba - Algeria.BP 12 – 23200 Sidi-Ammar

## INTRODUCTION & AIM

The chemistry of heterocycles has received a great deal of attention in recent times due to their importance, and among these heterocycles is benzothiazolinone, which has received a great deal of attention due to its biological, pharmacological [1], [2], and agricultural [3] benefits.
Schiff bases, which are molecules whose structure contains imine functions (C=N), have also been the subject of constant attention and development due to their different biological properties [4], [5].

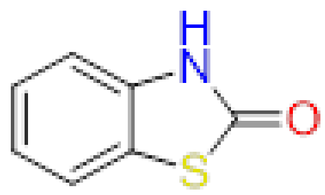


**Fig.**2-oxo-3H-benzothiazole

Our goal was to use green chemistry to synthesize a Schiff base benzothiazolinone derivative with a high yield and short turnaround time. The derivative's were theoretically investigated using SwissADME webservice, and its structure was determined using IR, $^{1}$HNMR, and $^{13}$C NMR spectroscopy.

## METHOD

**Chemistry**

To synthesize (E)-3-methyl-6-((naphthalene-1-ylimino)methyl)benzo[d]thiazol-2(3h)-one Schiff Base, amine (1 equiv) and 6-carbaldehyde (1 equiv) are reacted using EtOH as solvent. The reaction takes place at 80°C under ultrasonic irradiation for 23 min. After monitoring the progress of the reaction by TLC, the mixture is allowed to cool, resulting in the formation of a precipitate. The solid is then filtered on filter paper and washed with a little water. This method has a number of advantages: it's easy to set up, enables direct recovery of the pure product, requires a short reaction time and, above all, offers high yields 65% .

**Theorical examination**

The pharmacokinetical properties performed using SwissADME web [6] to investigate the of compound (a).

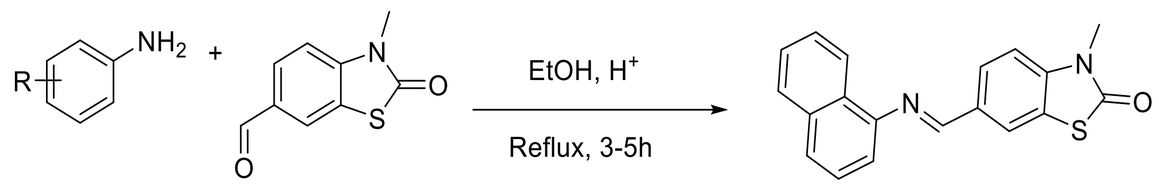
## RESULTS & DISCUSSION

**Spectroscopic caracterisation**

**$^{1}$H NMR spectroscopy**

The disappearance of the CHO proton signal characteristic of the aldehyde function of the aldehyde (1) around 9.93 ppm compared with the synthesized compound (a), and the appearance of the HC=N proton signals in the 8.58-8.77 ppm region confirm the formation of the imine function for the derivative.
The methyl group bound to the nitrogen atom appears as a singlet in the strong fields, at 3.44-3.51 ppm.

**RMN $^{1}$H(400 MHz, Chloroform-d):** δ, ppm (J, Hz): 8.52 (1H, s, **H**C=N), 8.39 – 8.29 (1H, m, **H-**Ar), 8.18 (1H, d, J = 1.6 Hz, **H-**7), 7.92 (1H, dd, J = 8.3, 1.7 Hz, **H**-5), 7.92 – 7.82 (1H, m, **H-**Ar), 7.77 – 7.69 (1H, m, **H-**Ar), 7.58 – 7.40 (3H, m, **H-**Ar), 7.15 (1H, d, J = 8.3 Hz, **H**-4), 7.06 (1H, dd, J = 7.3, 1.1 Hz, **H-**Ar), 3.52 (3H, s, N–C**H$_3$**).




(1) (a)

**Schema.1.** the reaction pathway.

**$^{13}$C NMR spectroscopy**

The disappearance of the signal characteristic of the CHO carbon of the aldehyde around 191.70 ppm compared with the synthesized compound (a) and the appearance of the signals characteristic of the HC=N carbon in the 156.69-159.89 ppm region confirm the formation of the imine function. In addition, the characteristic signals from the carbon atoms of the benzothiazolinone aromatic ring vary in the range δ = 111.77-140.58 ppm, and the carbonyl function (C=O) of the compound appears at 169.41-169.50 ppm. Signals from methyl carbons bonded to the N atom appear in a strong field at 29.66-29.86 ppm.

**FT-IR(KBr, *v*cm$^{-1}$ ):** 1681.58 (C=O), 1622.14 (C=N).

**Theorical examination**

| Parameter | Criteria | Observed Value | Status |
|---|---|---|---|
| Molecular Weight | ≤ 500 g/mol | 318.39 g/mol | Meets Criteria |
| LogP (Consensus) | ≤ 5.0 | 4.22 | Meets Criteria |
| Hydrogen Bond Donors (HBD) | ≤ 5 | 2 | Meets Criteria |
| Hydrogen Bond Acceptors (HBA) | ≤ 10 | 2 | Meets Criteria |
| Topological Polar Surface Area (TPSA) | ≤ 140 Å2 (bonus criterion) | 62.60 Å2 | Meets Criteria |

**Table.** Lipinski Rule of Five Analysis results.

This compound adheres to Lipinski's Rule of Five, with no violations, making it a promising candidate for oral bioavailability. Its favorable molecular weight, lipophilicity, and hydrogen bonding properties suggest good membrane permeability and absorption potential.

## CONCLUSION

In conclusion, this work successfully demonstrates a green chemistry approach for the synthesis of the imine benzothiazolinone derivative, using EtOH and ultrasound-assisted method. This strategy not only achieves high yield and faster reaction time but also facilitates an easy and pure recovery of the product. The structure of the synthesized derivative was confirmed through IR, $^{1}$H NMR, and $^{13}$C NMR spectroscopic techniques. Additionally, theoretical analysis for pharmacokinetical propreties was done.

## FUTURE WORK / REFERENCES

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