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INVESTIGATION OF NUCLEIC ACID TARGET TO 1,3,4-THIADIAZOLE DERIVATIVE BY USING DOCKING STUDIES

Ammar M. K. AL-Azzawi*, Tareq K. Ibraheem, Waseela A. Abdul Razaq and Ghada S. Fadil

Department of Chemistry, College of Education for Pure Science, University of Diyala, Iraq.
*e-mail : ammarmoh72@yahoo.com

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ABSTRACT : This work has been carried out in order to achieve the fullest possibilities of DNA targeting for numerous medical purposes. In this work, synthesized five membered heterocyclic derivatives via reaction terphathalic acid with two moles of thiosemicabazide in the presence POCl3 and synthesized Schiff bases from reaction compound preparation with p-ch, hlorobenzaldehyde. Interacting's between the molecule and the DNA-receptor were examined by using molecular operating program docking studies to demonstrate binding with auto dock vina by molecular docking.

Key words : 1,3,4 thiadizal, derivative, DNA, docking, vina.

INTRODUCTION

In recent years, extensive research has been carried out into various classes of thiadiazole compounds, many of which have important biological properties such as antimicrobial (Desai and Baxi, 1992; Gawande and Shingare, 1987; Mamolo *et al*, 1996), anti-tuberculosis (Shukla *et al*, 1984), anti-inflammatory (Varvaresou *et al*, 1998; Song *et al*, 1999; Mullican *et al*, 1993; Labanauskas *et al*, 2001), anticonvulsant (Chapleo *et al*, 1986; Chapleo *et al*, 1988), antihypertensive (Turner *et al*, 1988b; Turner *et al*, 1988a), local anesthetic (Mazzone *et al*, 1993), anticancer (MIYAMOTO *et al*, 1985; Chou *et al*, 2003). For medicinal uses as well, binders may be used since they are capable of binding to DNA. DNA molecules are now common in the treatments of cancer. In addition to various commercially available thiadiazole, there are a large number of biological activities such as antiarrhythmic and anti-diabetic properties, including medicines such as antiviral, analgesic, anticonvulsant and antidepressant (Hanna *et al*, 1995). Specific chemical and physical properties of the molecules are taken from these alternatives (Clerici *et al*, 2001; Gawande and Shingare, 1987).

MATERIALS AND METHODS

Merck and Sigima-Aldrich were collected and used as obtained all materials (chemicals). Melting points in an open capillary were calculated with the Thomas Hoover 6427-Fio system. IR spectra were recorded witha perkin-elmer 137A spectrometer (Pavia *et al*, 2014). HNMR spectra were recorded in DMSO-d_6 using Varian 300 MHz spectrometer the elemental analyses (CHN) were obtained from carloerba model EA 1108 analyzer carried out on Perkin – Elmer 24^0C analyzer. Intrinsic viscosity were determined in a Cannon-Fenske using DMF or DMSO as solvent (Silverstein *et al*, 2005). Thermal analysis was performed in Saljuk University (Turkey). Electrical conductivity was determined in Cond. 740 (ino Lab) Terminal WTW in 20^0C using DMF and DMSO solvents. General procedure for the first step synthesis of Schiff Bases of 1, 3, 4-thiadiazole derivatives preparation 1, 3, 4-thiadiazole derivatives from reaction (1.6gm, 10mmol) terphathalic acid with (0.9gm, 10mmol) thiosemicarbazide after added phosphorous oxychloride (5ML, 10mmol) was added drop-wise to an ice cold mixture reaction, the mixture was refluxed for 3hrs then cooling and added 20ML with stirring, reflux and continued for 5hrs then added 10% Potassium Hydroxide solution (Silverstein *et al*, 2005), filtered, washed and recrystallized from ethanol.

The FT-IR spectroscopy[17] the absence for the carboxylic group (3456 cm^{-1}) for (OH) and (1689 cm^{-1}) for carbonyl group and presence of a band at (3276-3111 cm^{-1}) to amine group asymmetric and symmetric (3049-3028 cm^{-1}) CH aromatic rings, (1622-1619 cm^{-1}) C=N, (1587-1429 cm^{-1}) C = C aromatic.

The Schiff base synthesized by reaction 1,3,4-thiadiazole derivative with p-chlorobenzaldehyde (2.8gm, 20mmol) solvolysis 10ML ethanol and added (2.6gm, 10mmol) compound [1] and some drops glacial acetic acid (GAA) and the mixture reaction refluxed for 6hrs and