Molecular docking and uv-visibal spectroscopy characterisation of the complex formed between ferrocene derrivative and DNA

Adaika aicha
faculty of exactes sciences,departement of chemestry
Laboratory of Valorisation and Technologie of Sahariennes Ressources, university of Eloued
Eloued, Algeria
Mail: adaika-aicha@univ-eloued.dz

Tedjani aicha
Département of sciences of nature et de la vie Laboratoire of biologie, Université of Ouergla
Ouergla, Algeria
Mail:aichatd@gmail.com

Lanez touhami
faculty of exactes sciences,departement of chemestry
Laboratory of Valorisation and Technologie of Sahariennes Ressources, university of Eloued
Eloued, Algeria
Mail: lanez-touhami@univ-eloued.dz

***Abstract*—** In this study the ferrocene derrivative was characterized for interaction with DNA using theoretical and experimental methods. UV-visible spectroscopy was used for the experimental account of Fc-DNA complex. The experimental result showed that the Fc interacts by electrostatic mode. The binding constant (K) and Gibbs free energy (ΔG) for the Fc-DNA complex have been estimated as 5,25 x 104 mol-1 and -26,9 KJ.mol-1 respectively. The theoretical DNA binding of Fc was investigated by performing docking studies using AutoDock molecular docking software. The docking studies yield good approximation with experimental data and explain the sites of binding.

Keywords—DNA, ferrocene derivative, Gibbs free energy, The binding constant, AutoDock.

I. INTRODUCTION

Genetic material in living cells is made up of deoxyribonucleic acid (DNA), a storage site for nucleotide sequence information, the integrity and retrieval finity of which rely on its interaction with proteins and other ligands [1]. Ferrocene and its derivatives have played an important role in many areas [2]. However, much attention has been given to their biological activities, such as antitumour, antimicrobial, cytotoxic, and DNA-binding agents (3). DNA binding is a pre-requisite for a compound to be used as an antitumor agent. Some ferrocene derivatives have also been evaluated for their DNA binding affinity and display good DNA binding constants [4]. Variety of techniques is available to study the small molecule-DNA interaction. UV-visible spectroscopy was well established in this regard. The virtual screening of compounds for their interaction with bimolecular is becoming popular day by day [2]. Molecular docking is replacing the expensive experimental techniques for the screening of drug potency. In this paper we have utilized AutoDock software for the virtual binding of the studied compound with DNA. The results of the computational studies are compared with well established experimental techniques [5].

II. MATERIALS AND METHODS

A. Chemical materials

DMF, synthesis product Fc, DNA.

B. Methodology

UV-vis spectrometry: Absorption spectra were measured on a UV-vis spectrometer Shimadzu 1800. The electronic spectrum of a known concentration of the test compounds (10-3M) was obtained without DNA. The spectroscopic response of the same amount of the test sample was then monitored by addition of various concentrations of DNA in the solution. All samples were allowed to equilibrate for 5 min prior to every spectroscopic measurement.

III. RESULTS

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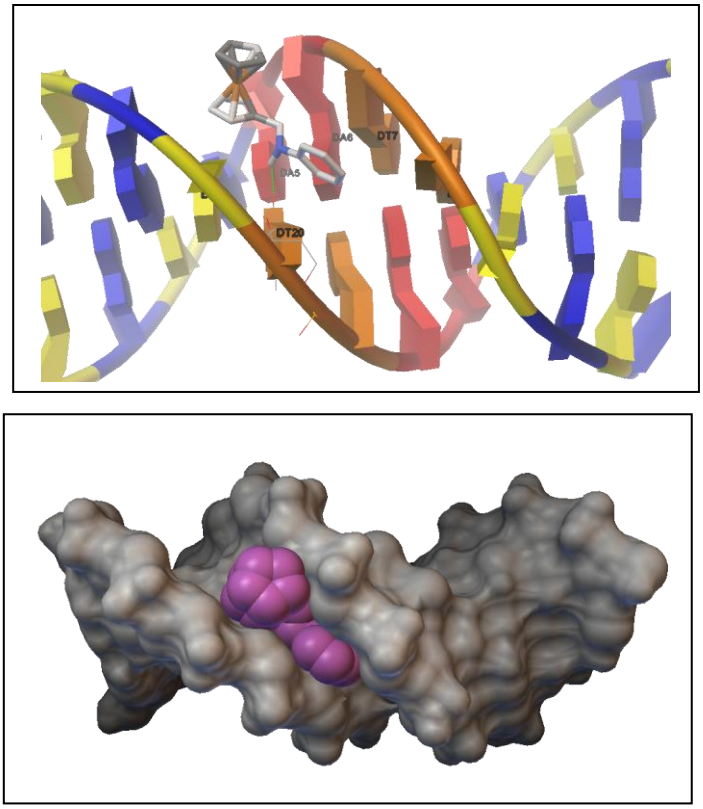

Fig.1 *Interaction of FMA with DNA, (A) : molecular docking of the between interaction FMA-ADN, désoxyadénosine (DA) : red, désoxycytosine (DC) : yellow, désoxyguanine (DG) : blue, désoxythymidine (DT) : brown, (B) : surface view of FMA docked with DNA*

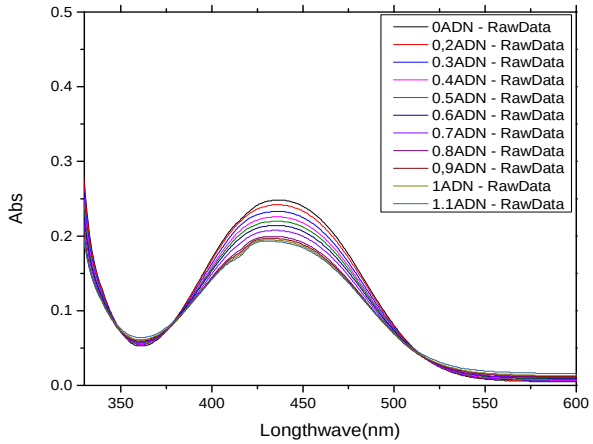

Fig.2**:** *Results of test of the interaction activity DNA-Fc using experimental methods UV-Vis spectroscopy*

TABLE I. RESULTS OF THE INTERACTION PARAMETERS K AND **ΔG** OF DNA-FC

Calcul of K and ΔG		
[ADN] mol/l ×10-5	***K (mol-1)***	***ΔG (KJ.mol-1)***
1,684	***5.25 x 104***	***-26.9***
1,846		
2		
2,146		

IV. CONCLUSION

The result of the interaction of DNA and the ferrocene derivative using theorical and experimental methods showed that these ferrocene derivative has an antitumoral activity.

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