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Photoconversion of an anthraquinone derivative in the presence of human serum albumin

Fatemeh Isfahani [a], Davood Ajloo [a,b,*], Ayoub Kanaani [a], Ali A. Saboury [c]

[a] School of Chemistry, Damghan University, Damghan, Iran
[b] Institute of Biological Science, Damghan University, Damghan, Iran
[c] Institute of Biochemistry and Biophysics, University of Tehran, Tehran, Iran

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ABSTRACT

Photconversion of an anthraquinone photochrome (AQP) from Trans to Ana forms were studied by different methods and techniques. Solution of AQP was irradiated under UV light in buffer condition, pH = 7.5, 10 mM phosphate buffer in the absence and presence of human serum albumin at 27 and 37 °C. The results showed that a new peak at higher wavelength was observed that indicative of producing the Ana form. Rate of Trans to Ana conversion increases in the presence of human serum albumin (HSA). Electron transport calculations were carried out from the first principles with a method based on non-equilibrium Green's functions (NEGF) combined with DFT. The results showed that electron transport is easier in Ana form due to increasing the resonance length and electron delocalization. Binding study by docking and spectroscopy showed that Trans form has more tendency to interact with HSA due to higher number of HSA-Trans hydrogen bond. Structural studies by circular dichroism and molecular dynamics results show that at lower concentration of AQP, percentage of helix was increased and then decreases at higher concentration. In addition structural parameters such as RMSD, accessible surface area, hydrogen bond, in associated with experimental results showed that protein folded at low concentration.

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1. Introduction

Photochromism does not have a rigorous definition, but is usually used to describe compounds that undergo a reversible photochemical reaction where an absorption band in the visible part of the electromagnetic spectrum changes dramatically in strength or wavelength. Some of the most common processes involved in photochromism are pericyclic reaction, intramolecular hydrogen transfer, intramolecular group transfers, dissociation electron transfer processes and (oxidation-reduction). Another requirement of photochromism is two states of the molecule should be thermally stable under ambient conditions for a reasonable time. All photochromic molecules back-isomerize to their more stable form at some rate, and this back-isomerization is accelerated by heating. There is therefore a close relationship between photochromic and thermochromic compounds [1].

Photochromic compounds can be used in drug delivery, molecular logic gates [2], molecular switches [3], photo-controllable biological processes [4,5], optoelectronic devices [6], molecular machines [7] photo-controllable drug or ion delivery [8], optical data storage [9] and photoresponsive supramolecular self-assembly, [10]. Among them, organic photochromic molecules, including anthraquinones undergo color changes upon photo irradiation, and have shown good performance in their chemical, biological, physical, and nanotechnology applications [11]. Anthraquinone are photochromic material with its trans and ana isomers interchanged by light irradiation and heat, making it a very useful platform for photo-triggered biological systems.

The transport properties of fulgide-based photochromic switches are investigated in the framework of DFT calculations. Light activated furyl fulgide molecules are coupled to nanoscopic metallic electrodes. The electrocyclization process under UV light converts the open-ring into a closed-ring conformation. Conversely, the reverse process takes place by visible light illumination [12].

The molecular structure, vibrational frequencies of benzaldehyde derivatives of dihydroanthracene as a photochrome in “trans” and “ana” forms have been investigated by UV–Vis, FT-IR and NMR spectroscopy as well as DFT B3LYP method with 6-311++G(d,p) basis set [13,14]. Transition structures were calculated by QST3 and IRC methods which yielded the potential energy surface and activation energy. Upon irradiation with 300 nm light, the camel solid turned orange, in which a visible absorption band was observed at 475 nm. Our results show, current through the ana form is higher than that trans form.

* Corresponding author.
E-mail address: ajloo@du.ac.ir (D. Ajloo).

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Table 1
Thermodynamic functions at B3LYP/6-311++G(d,p) level of theory for "Trans" and "Ana" forms.

Parameters	"Trans" form	"Ana" form
Dipole moment, μ (D)	3.98	3.7372
SCF energy (a.u.)	−1108.6459	−1108.5990
Zero-point vibrational energy (kcal/mol)	170.8993	170.8621
Thermal energy (kcal/mol)	182.890	182.850
Enthalpy, H (cal/mol K)	75.363	75.528
Entropy, S (cal/mol K)	147.458	145.644

Transport properties of diazabicyclo molecular optical switch was analyzed using first-principles calculations [15,16]. Multiple attributes such as I–V characteristics, electronic transmission coefficients T(E), the effect of electrode materials (Au, Ag, and Pt) on electronic transport properties, on-off ratio and spatial distribution of molecular projected self-consistent Hamiltonian (MPSH) orbitals corresponding to the closed and open forms were studied [16–18].

An approach to generate materials with programmable thermochromic transition temperatures (TTTs), based on the reversible microcrystallization of anthraquinone dyes with the assistance of blended Pluronic block copolymers was reported [19].

The application of photochromic compounds to biological systems has recently attracted considerable attention [20]. The enantioselective photochromism of diarylethenes incorporated in human serum albumin (HSA) in buffered aqueous media to elucidate the effect, on the photochromism of diarylethenes, of the chiral peptides in HSA was reported [21]. It is widely used as a predominant stimulus to control chemical reactions, special physical properties, and biological evolutions [22]. Hence, light is very crucial to the biological system in any creature.

The interaction of a naturally occurring chromene, flindersine (FL), and bovine serum albumin (BSA) has been investigated by UV-vis

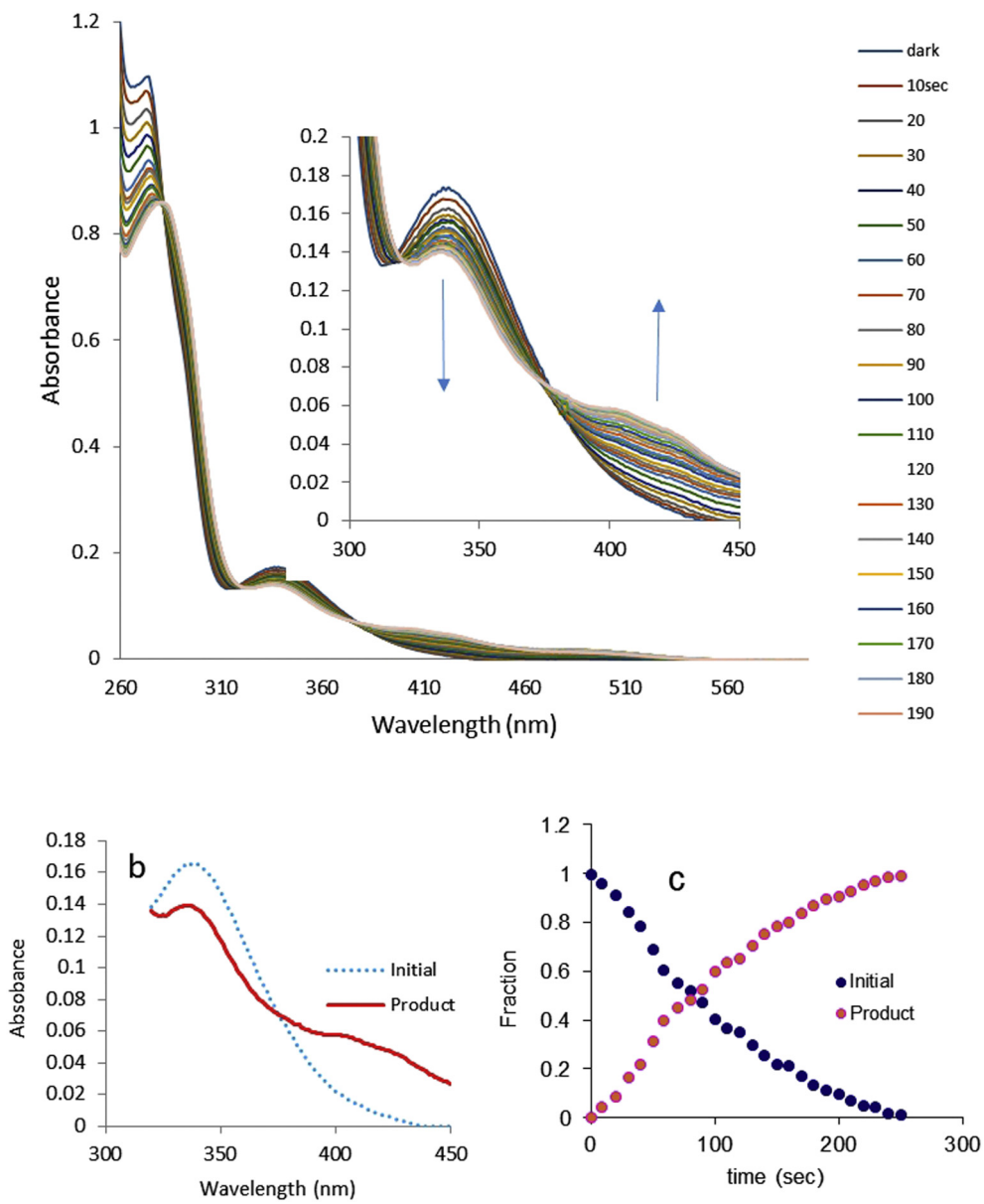

Fig. 1. a) Uv-Vis spectrum of photochrome after irradiation under UV-light in different period of time, Inset, expanded part of spectra for conversion of Trans to Ana forms, b) initial (trans) and final (Ana) spectrum, c) variation of Trans and Ana fraction obtained by MCR-ALS optimization.

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