چهاردهمین همایش
بیوشیمی فیزیک ایران

14th Conference on Biophysical Chemistry, Zabol , Iran

October 25-27, 2016

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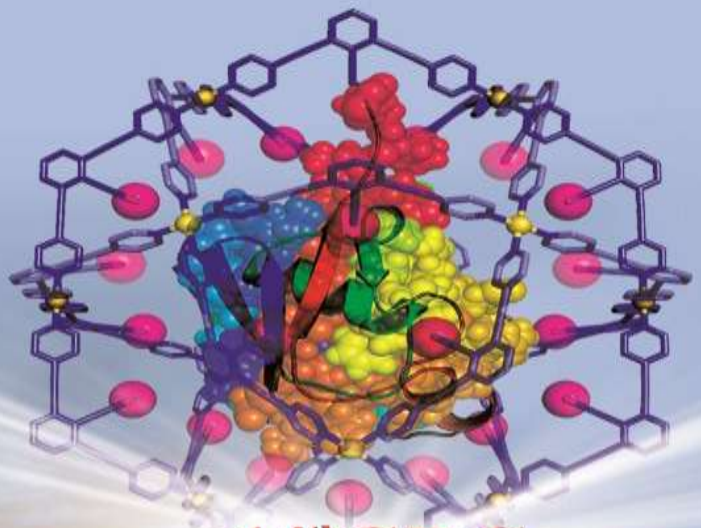

14th CBC

In the name of God

Proceeding of the

14th Iranian Biophysical Chemistry Conference

October 25-27, 2016

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The effects of electromagnetic radiation Wi-Fi devices on attention levels of girl students

Zahra Adel, Kourosh Bamdad[b] , Hamid Zare[b] , Masomeh Esmaeili [c]

[a]Department of Biology, Biophysics, Faculty of Science, Payame Noor University,Estahban Iran
[b]Department of Biology, Faculty of Science, Payame Noor University, (PNU),fars Iran
[c]Department of psychology Payame Noor Universit, fars Iran
** Corresponding author: Tel:+98 9173319213, E-mail: zbiology@hotmail.com*

Abstract

Along with the advancement of technology, the contact with different frequencies of electromagnetic field is increasing significantly. The waves despite the current very effective role in human life, creating a growing concern about potential risks on human health is [1-2]. Therefore, this study aimed to investigate the effects of electromagnetic radiation from Wi-Fi devices on attention levels were girl students in Estahban. The present study is a descriptive comparison. The study population consisted of all secondary school students and high school of 203 students Estahban are the 14- to 17-year-old were selected by cluster random sampling. After implementing the anxiety questionnaire and the selection of people without anxiety, two categories into: those with Wi-Fi modem (n = 87) and without WiFi (69 patients). Andthe software were administered divided attention. Data using SPSS software and statistical methods were analyzed MANOVA. The results showed that the two groups have Wi-Fi and non-Wi-Fi, there is a significant difference in the scattered attention test,people who use WiFi scattered from greater accuracy(sig<0/05). But in Focused attention significant difference was found between the two groups. Although the prevalence of mobile and WiFi networks less than two decades ago, the need for more longitudinal research in this field remains. But the harmful biological effects of electromagnetic field radiation are non-negligible. Exposure to the human brain near a main source of electromagnetic waves can be normal activity of brain waves hit and affect the normal operation

Keywords: Electromagnetic radiation, Wi-Fi, Attention levels

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1002CBC

Production of controlled release oral drug delivery system using β-lactoglobulin nanoparticle

Behafarid Ghalandari[a]*, *Adeleh Divsalar*[b], *Ali Akbar Saboury*[c, d]

[a]*Department of Medical Nanotechnology, Science and Research Branch, Islamic Azad University, Tehran, Iran*
[b]*Department of Cell & Molecular Biology, Faculty of Biological Sciences, Kharazmi University, Tehran, Iran*
[c]*Institute of Biochemistry and Biophysics, University of Tehran, Tehran, Iran*
[d]*Center of Excellence in Biothermodynamics, University of Tehran, Tehran, Iran*
**Corresponding Author: Email: behafarid.gh@gmail.com*

Abstract

Over the past decades many efforts have been done to producecontrolled vehicle for sustained release oral drug delivery system. The present study was performed whereas biopolymers were illustrated their ability for presence in nano-scale oral drug delivery system. Moreover, previous studies have shown β-Lactoglobulin (β-LG) as a milk whey carrier protein due to its unique physicochemical properties is known as a well promising candidate for presence in oral drug delivery system [1-3]. In this study, β-LG nanoparticles contain metal based drug were fabricated in the presence of low methoxyl pectin as extra layer at various conditions. β-LG nanoparticles were characterized by dynamic light scattering and scanning electron microscopy so that the obtained results illustrated that the particle size average is lower than 200 nm and their shape is spherically. To determine controlled release manner of drug from β-LG nanoparticles, the in vitro drug release were studied using equilibrium dialysis methods at 37 °C during in the simulation conditions of gastrointestinal (GI) tract. The results were investigated by fitting into mathematical kinetics models so that the Korsmeyer-Peppas model was the best kinetics release model. In addition, data illustrated that β-LG nanoparticles were resistance to acidic condition. Hence, anomalous non-Fickian pattern was determined for drug release in the simulation time such erosion and diffusion were occurred dependent on alkaline pH conditions of GI. Consequently, based on our findings β-LG nanoparticle is promising candidate with unique pH sensitivityfor presence in controlled release oral drug delivery system.

Keywords: β-LG nanoparticles, oral drug delivery, mathematical modeling, anomalous non-Fickian.

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1003CBC

Anti-Cancer Effect of Nilotinib, Imatinib, DasatinibandPonatinibOn theMost Effective Inhibitor ofTyrosine Kinase ABL1 andThe Introduction ofBinding Energy

Seyed Mohsen Masoumian Hosseini[*1], *Masoud Homayouni-Tabrizi*[2], *Vahid Poresmaeil*[3]

[1*] *Student Research Committee, ShahidBeheshti university of medical sciences. Tehran. Iran*
[2] *Department of Biochemistry and Biophysics, Mashhad Branch, Islamic Azad University, Mashhad, Iran*
[3] *Department of Biochemistry, Mashhad Branch, Islamic Azad University, Mashhad, Iran*
** Corresponding author Tel: 09368784499 , email: masoumian.mohsen@sbmu.ac.ir*

Abstract

The ABL1 proto-oncogene encodes a cytoplasmic and nuclear protein tyrosine kinase that has been implicated in processes of cell differentiation, cell division, cell adhesion, and stress response (1). The activity of ABL1 protein is negatively regulated by its SH3 domain (2), and deletion of the SH3 domain turns ABL1 into an oncogene (3, 4). Mutations in the ABL1 gene are associated with chronic myelogenous leukemia (CML). This, in turn, allows the cell to become cancerous. The ABL protein can be inhibited by various small molecules. One such inhibitor is imatinibmesylate, which occupies the tyrosine kinase domain and inhibits ABL's influence on the cell cycle. The second-generation ABL tyrosine-kinase inhibitors are also under development to inhibit ABL mutant's resistant to imatinib. Secondary inhibitors like nilotinib, ponatinib and dasatinib , which has the effect on tyrosine kinase , inhibits its tyrosine kinase activity. In this study, the most effective inhibitor binding affinity inhibitors are listed and described in terms of binding energy. Inhibitors were made using the software Gaussian, And docking with the software Moe was. The results of docking expression of anti-cancer compounds bind this domain tyrosine kinase ABL1 protein that is between amino acids 242-493. The results of the drug, nilotinib with a score of -8.0076 as a selective inhibitor of the best.

Keyword:*ABL1*, imatinib, ponatinib, dasatinib,nilotinib, docking

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1004CBC

Thermodynamic analysis of human serum albomin interactions with a potent anti-cancer metallodrug

Somaye Shahraki

Department of Chemistry, University of Zabol, Zabol, Iran
E-mail: s-shahraki@uoz.ac.ir

Abstract

It has been seen that the distribution, free concentration and the metabolism of various small molecules such as drugs can be significantly altered as a result of their binding to human serum albumin (HSA) [1, 2]. Therefore, the interaction of drugs with human serum albumin has major biochemical importance and can be used as a model for elucidation of the drug's protein complexation. In this research, a new zinc(II) complex [Zn(naph-dtc)(bpy)]Cl (where naph-dtc = naphthyldithiocarbamate and bpy = 2,2'-bipyridine) was synthesis and its interactions with Human serum albumin was studied by fluorescence and UV–Vis spectroscopic methods under like physiological condition in Tris–HCl buffer solution at pH 7.4 and three temperatures. Fluorescence data indicated that this Zn(II) complex strongly binds with HSA ($Kb = 2.12 \times 10^5\ M^{-1}$) and this binding is characterized by one high affinity binding site ($n \sim 1$). The Stern–Volmer analysis showed that the fluorescence quenching of protein by above complex resulted from static mechanism. Corresponding thermodynamic parameters ΔG°, ΔH° and ΔS° were calculated and revealed that hydrophobic forces played a major role when Zn(II) complex interacted with HSA. The results of UV–Vis spectra show that the secondary structure of the protein has been changed in the presence of this Zn(II) complex. Also, the distance between the acceptor, Zn(II) complex, and the donor, HSA, was estimated on the basis of the Förster resonance energy transfer (FRET).

Keywords: Dithiocarbamate, Zinc(II) complex, Human serum albumin, Spectroscopic measurements

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1005CBC

Optimization of pectinase activityfrom *Piriformospora indica*by sugar beet pulp

Parisa Fathi Rezaei, Somayyeh Kiani, Saleh Shahabivand*

Biology department, Faculty of Science, University of Maragheh, Maragheh, Iran
** Corresponding author: Tel: +98 4137278100, E-mail:* parisafathirezaei@gmail.com

Abstract

Pectinases are the growing enzymes ofbiotechnological sector, showing gradual increase in theirmarket. These enzymes areecofriendly tool of nature that are being used extensively invarious industries likefood industry; paperindustry for bleaching of pulp and waste paper recycling; inthe processing of fruit–vegetables, tea–coffee, animal feed;extraction of vegetable oil and scouring of plant fibres.Pectinases as a complex group of enzymes hydrolyze the pectin-containing substances. They have been used in several conventional industrial processes; including: juice,textile, plant fiber processing, tea, coffee and oil extraction. Fungal pectinases are among the most important industrial enzymes and are of great significance with widerange of industrial application [1-2]. Sugar-beet pulp (SBP), the main by-product of the sugar refining industry, is especially rich in pectin. In this investigation, weassayed effect of different temperature (30-90°C) and pH (4-10) on pectinase activity from *Piriformosporaindica*.First, *P. indica*was cultured onKaefer medium supplementedwith SBP powder and maintained at 30 °C under constant shakingconditions at 200 rpm on an Orbital shaker for 6 days. According to the results the optimum pH and temperature for pectinase activity was 6 and 40°C, respectively.

Keywords: Sugar beet pulp;pectinase; pectin;*Piriformospora indica*

Referees:

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1006CBC

Multi-Spectroscopic studies on the interaction of human Erythropoietin and cationic synthetic gemeni

Masuod Bagherpour[1], Kataneh Abrari[1], Adeleh Divsalar[2], Ali Akbar Saboury[3], Pouneh Pourhosseini[4]

[1]School of Biology, Damghan University, Damghan, Iran
[2]Department of Cell and Molecular Biology, Faculty of Biological Science, kharazmi University, Tehran, Iran.
[3]Institute of Biochemistry and Biophysics, Tehran University, Tehran, Iran.
[4]Faculty of Biological Sciences, Alzahra University, Tehran, Iran

Abstract

Erythropoietin (EPO) is a hematopoietic hormone, as a strong cell protector, which increases cell maintenance during different damages of central nervous system. Since the brain-blood barrier prevents the entrance of erythropoietin (with molecular weight of 34 kD) into the brain, its systemic delivery gets limited. In the present study, we have investigated the thermodynamical interaction between human EPO and gemeni using various spectroscopic techniques of fluorescence and circular dichroism (CD) at two different temperatures of 25 and 37 ˚C [1-2].Results of intrinsic fluorescence showed that the emission of EPO decreased and quenched with increasing in the gemeni concentration added to the protein solution. Analysis of quenching data indicated that there are one and two binding sites with binding constants of 3.85×10^{-5} M^{-1} and 22×10^{-5} M^{-1} on the EPO for gemeni at temperatures of 25 and 37 ˚C, respectively. Also, far-UV-CD results did not show any significant changes in the regular secondary structure of EPO upon various concentrations of this ligand. In conclusion, obtained results proposed that gemeni as a cationic surfactant can bind to EPO without inducing any adverse effects on the EPO structure.

Keywords: Erythropoietin, Gemini, intrinsic fluorescence, quenching mechanism

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1007CBC

The investigation of functional and structural effects of Phenanthroline-imidazole derivative of palladium on bovine liver catalase by spectroscopic techniques

Roohollah Ghobadi[a], Adeleh Divsalar[b], Alireza Harifi Mood[a], Ali Akbar Saboury[c], Mahboube Eslami Moghadam[d]*

[a] *Department of Chemistry, Kharazmi University, Tehran, Iran*
[b] *Department of Cell & Molecular Biology, Faculty of Biological Sciences, Kharazmi University, Tehran, Iran*
[c] *Institute of Biochemistry and Biophysics, University of Tehran, Tehran, Iran*
[d] *Chemistry & Chemical Engineering Research Center of Iran, Tehran, Iran*
** Corresponding author: Tel:+9834579600, E-mail: divsalar@khu.ac.ir*

Abstract

Successful clinical experience of using transition metal complexes in cancer therapy has encouraged scientists to synthesize new metal complexes with the aim of interacting with special targets such as proteins [1,2].In this regard, biological effects of [Pd(dach)(FIP)]$(NO_3)_2$ compound [3] which contains a novel phen-imidazole ligand, FIP, was investigated on bovine liver Catalase (BLC) structure and function. Various spectroscopic methods such as UV–visible, fluorescence, and circular dichroism (CD) were applied at different temperatures of 25 and 37 °C for kinetics and structural studies. As a consequence, the enzymatic activity slightly decreased with increasing palladium compound's concentration only to 0.03 mM and fortunately remained constant at near 70% after this concentration. Also, the fluorescence quenching measurements revealed that despite slight changes in activity, catalase experiences notable alterations in three-dimensional environment around the chromophores of the enzyme structure with increasing palladium complex concentration.Moreover, Quenching data showed that BLC has one binding sites for Pd in 25˚C and two sites in 37˚C and hydrophobic interaction play a major role in the binding process. Furthermore, CD spectroscopy data showed that Pd complex induces slight changes in the secondary structure of BLC. Regarding the vital anticancer bioactivity of catalase, i.e. breast cancer, this might be a promising outcome for chemotherapists and medicinal chemists who are investigating on metal complexes with anticancer activity and no side effects to do in vivo studies on this novel-imidazole derivative of palladium that has a notable tendency to bind to a macromolecule in the low concentrations.

Keyword:catalase, enzymatic activity; fluorescence; circular dichroism; BLC; FIP.

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1008CBC

Binding Affinity of Cationic Gemini Surfactants to Insulin: Effect of the Spacer Length

R. Ghasemi Tabesh[*,1], P.S. Pourhosseini[1], A.A. Saboury[2], and F. Najafi[3]*

[1] Faculty of Biological Sciences, Alzahra University, Tehran, Iran
[2] Institute of Biochemistry and Biophysics, University of Tehran, Tehran, Iran
[3] Department of Resin and Additives, Institute for Color Science and Technology, Tehran, Iran
** Corresponding author: r.tabesh@ student.alzahra.ac.ir*

Abstract

Gemini surfactants are composed of two surfactants that are chemically linked together by a spacer at their hydrophilic head groups.Because of their applications in academic and industrial fields, Gemini surfactants have drawn great attention of scientists of various communities, since 1991.Some of Geminis have reported as food stabilizers [1]. Others are claimed to be potential candidates for gene delivery [2]. The interaction of Gemini surfactants with nucleic acids have also studied widely. However, the interaction of Geminis with proteins has been the subject of only recent studies[3]. In this research, the interaction of two cationic Gemini surfactants with insulin is investigated by fluorescence spectroscopy. The two Gemini surfactants differ in their spacer length (C_6, C_4). Titration of insulin solution with the Gemini dispersion (C6 or C4) was performed and then, the fluorescence spectra recorded. The binding of both surfactants to the protein was evidencedby quenching the intrinsic fluorescence of protein upon addition of the surfactants.The Stern-volmer plots were applied to derive the binding parameters such as K_a and n. Results demonstrate that the longer the spacer length of the surfactant, the lower the binding affinity to insulin is. The number of binding sites for surfactant per protein molecule also decreases, as the spacer length increases.

Keyword: Cationic Gemini Surfactant; fluorescence spectroscopy; insulin; interaction.

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1009CBC

Schiff base zinc(II) complex ofthioacetamide derivatives. Synthesis, characterization and evaluation of interaction with human serum albumin

Ameneh Heidari, Somaye Shahraki

Department of Chemistry, University of Zabol, Zabol, Iran
Email: amheidari@uoz.ac.ir

Abstract

Amongst the various metal ions, zinc is an attractive prospect, being a bioessential trace element which plays a vital role in biological processes like electron transfer, endogenous oxidative DNA damage associated with aging and cancer and its complexes are preferred molecules for cancer inhibition by chemotherapy. In this study, a new water soluble zinc(II) complex 1 (Fig. 1) derived from thioacetamide and 2,3-Butanedione monoxime was synthesized and characterized by elemental analysis (CHN), molar conductance measurements and spectroscopic methods. The interaction of complex 1 with Human Serum Albumin (HSA) was investigated under like physiological condition in Tris–HCl buffer solution at pH 7.4 by means of spectroscopic methods (fluorescence, and UV-Vis).The results of fluorescence titration revealed that the complex 1 strongly quench the intrinsic fluorescence of HSA through a static quenching procedure. Binding constants (K_b) and the number of binding sites (n ~ 1) were calculated using modified Stern–Volmer equations. The thermodynamic parameters ΔG at different temperatures (298, 307, 317 K) were calculated subsequently the value of ΔH and ΔS was also calculated which revealed that the hydrophobic and hydrogen bonding interactions play a major role in HSA–complex 1 association. The distance r between donor (HSA) and acceptor (complex 1) was obtained according to fluorescence resonance energy transfer and the alterations of HSA secondary structure induced by complex 1 were confirmed by UV-Vis measurements.

Key words: Schiff base, human serum albumin, fluorescence quenching, UV-Vis spectroscopy

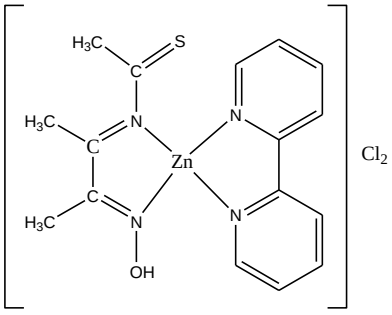

Fig. 1

1010CBC

Binding studies ofacetylacetonatopalladium(II)valine complex with CT-DNA

Ali Heydari[a], *Hassan Mansouri-Torshizi*[*a]

[a] *Department of Chemistry, University of Sistan&Baluchestan, Zahedan, Iran*
** Corresponding author: Tel:+98 54-33431146, E-mail: : hmtorshizi@hamoon.usb.ac.ir*

Abstract

The development of new metal complexes which can selectivity interact with nucleic acid is of much current interest. Among the other transition metal complexes, palladium complexes with favorable anticancer activity are good models analogues for Pt(II) complexes.[1-3] Therefore a novel palladium (II) complex has been synthesized with Valine (Val) and acetyleaceton (acac) by reaction of $Na_2[PdCl_4]$ and sodium salts of valine and acac. Thus a complex of the type [Pd(acac)(Val)] has been obtained. This water-soluble and neutral complex was characterized by spectroscopic and non-spectroscopic methods. Cytotoxicity effect of the Pd(II) complex toward cancer cell line of K_{562} was measured using MTT assay. The interaction of this complex with calf thymus DNA (CT-DNA) were investigated under physiological condition in Tris-HCl buffer using spectroscopic methods including UV-Vis absorption spectroscopy, ethidium bromide displacement and fluorescence titration spectra. The results obtained from these analyses indicated that this complex effectively interact with CT-DNA at low concentrations. Fluorescence titration revealed that binding constant (K_b), apparent biomolecular quenching constant (K_q) and number of binding sites (n) for CT-DNA. Also, thermodynamic parameters data suggested that hydrogen binding and Van der Waals force play a major role in the association of CT-DNA-Pd(II) complex. The complex exhibited groove binding mode with CT-DNA.

Keyword: Palladium(II) complex; DNA binding; cytotoxicity; Valine.

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1011CBC

Amyloid Beta (Aβ) peptide incompatibility with fibrinogen Results in Alzheimer's disease

Hossein Derakhshankhah[1], Ebrahim Barzegari[2], Rassoul Dinarvand[3],Ali Akbar Saboury[2],Mohammad Raoufi[1,3],Morteza Mahmoudi[1, 3,4]*

[1]Department of Pharmaceutical Biomaterials and Medical Biomaterials Research Center, Faculty of Pharmacy, Tehran University of Medical Sciences, Tehran, Iran ,[2]Institute of Biochemistry and Biophysics, University of Tehran, Tehran, Iran; [3]Department of Nanotechnology and Nanotechnology Research Center, Faculty of Pharmacy, Tehran University of Medical Sciences, Tehran 13169-43551, Iran;[4]Department of Anesthesiology, Brigham and Women's Hospital, Harvard Medical School, Boston, Massachusetts 02115, United States.

** Corresponding author: Tel:+98 9125290970, E-mail: derakhshankhah.hossein@gmail.com*

Abstract

Alzheimer's disease (AD) is a prevalent progressive neurodegenerative disorder, yet with undefined origin. The mostly accepted mechanism for AD pathogenesis is the Aβ hypothesis, stating that increased generation of Amyloid-β protein is responsible for the senile plaques and dementia associated with AD [1]. A milestone in study of AD etiology is the recent discovery that Aβ associates with fibrinogen and induces alterations in the structure of the fibrin clot, making it resistant to fibrinolysis [2].Designing inhibitory molecules against the interaction of Aβ with fibrinogen could be a promising approach to normalize any blood clots formed in the brain and increase their lysis. Researchers have also designed an inhibitory molecule (RU505) to suppress the proposed Aβ-fibrinogen interaction. However, the molecular mechanisms of both pathogenic Aβ-fibrinogen association and therapeutic Aβ-RU505 interaction have remained unknown [3].The present study employs molecular modeling and design methods to investigate the Aβ interactions contributing to AD progress or its treatment.These tasks are what intended by the present study, where a more potent Aβ inhibitor (T-777) is introduced. We then propose a descriptive model of the association between Aβ and fibrinogen, plus a mechanistic model for the inhibitory binding of RU505 and T-777 drug candidates.We found that most of the contacts between the Amyloid-β and fibrinogen are of the hydrogen bonding and hydrophobic nature. Though less frequent, the electrostatic contacts showed specific patterns on both molecules, which give implications for future drug design studies.

Keywords: Alzheimer's disease (AD); Amyloid-β; Fibrinogen; AD drug.

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1012CBC

NTPs in the proteins world; their prevalence & preference

Ali Golbabaie, Mehran Habibi Rezaei

Department of Biology, University of Tehran, Tehran, Iran

Abstract

Nucleoside triphosphates (NTPs) have been considered as important contributors of the metabolic systems of the cells. These molecules specifically function in the activation of proteins and supplying the energy need for many essential cell functions. Although, mostly all types of NTPs are functional but, there is an special emphasize on adenosine triphosphate (ATP) as the universal energy currency of the cell [1,2]. Nevertheless, the evolutionary reason of the selection of ATP among other NTPs has not been understood. This study aims to give some clues to shed light on the rationality of natural selection of ATP for is missions. by paying attention to the NTP binding pocket in the selected enzymes (through docking protocols). According to the results of comparing the NTP binding pockets of enzymes using different NTPs (ATP, GTP, CTP, UTP) it is noticeable that the ATP binding pockets tend to be less specific than other types. This matter is concluded regarding to the comparison of the free energy of binding of the NTP (ATP had the least free energy of binding), the variety of amino-acids in the pocket (ATP binding pockets had more diverse amino-acids), and the part of NTP from which it connects to the enzyme (ATP attaches significantly more by its phosphate groups rather than the adenosine head). It is suggestable that this non-specificity of ATP binding could work as an evolutionary advantage for ATP using a broad range of proteins with different binding pockets while other NTPs couldn't and failed to do in a similar way.

Key words: Nucleotide triphosphate, Binding pocket, Docking protocol, evolutionary aspect

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1013CBC

A Capacitance based label free aptasensor for botulinum neurotoxin detection

Jamal Rashidiani[1,2],Khadijeh Eskandary[2], Firooz Ebrahimi[1], Seyed Jafar Mousavy[1]*

[1"]Department of Biology, Faculty of Basic sciences, Imam HosseinUniversity (IHU), Tehran, Iran*
[2]Nanobiotechnology Research Centre, Baqiyatallah University of Medical Science, Tehran, Iran
*E mail of corresponding author:*jmosavi@ihu.ac.ir

Abstract

As the botulinum neurotoxins- spatially type A- have more importance for both clinically and industrially area, treeing to finding fast and fasil method to determination of this toxin is favourite for scientists and politiciansHere we reported afasil approach to achieving anano biosensor for botulinum neurotoxin type A(Bont/A). Usage a Nano electrode based on modified graphene-carbon pasteand by manse LCR meter we investigate the present of toxin in buffer media. At first graphene nanocomposites was synthesis chemically,while itshows a good conductivity witch it wassensitive for determination of Bont/A. Immobilization of aptamer has been done on the Graphene electrode in 100mM phosphate buffer solution (*p*H = 7) randomly. The Bont/A was cloned and expressed in *E.coli*, then toxin was harvested and purified and confirmed using the genetic and biotechnological methods.Graphene modified electrodes were applied as indicator for capacitance determination of Bont/A. In this study, SEM, electrochemical impedance spectroscopy and cyclic voltammetry techniques have been used to confirming the well fabrication of the nanobiosystem. The target toxin was detected in a range from $1.5\times10^{-1}$to 6.5×10^{-1} ng/mL.Through this study, BoNT/A was detected with detection limit of 0.09 $ng\cdot mL^{-1}$and correlation coefficient was about 0.964.

Keywords: Graphene, *aptamer, Botulinum, biosensor, electrochemistry*

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1014CBC

The role of free radicals resulting from acetoacetate ketone body in DNA glycation process

Mahdieh Bagherzadeh Yazdi[a]*, Mousa Bohlooli[a] and Neda Poormolaie[b]

[a]*Department of Biology, University of Zabol, Zabol, Iran*
[b]*Department of Chemistry, University of Zabol, Zabol, Iran*
** Corresponding author: Tel:+98 54 32232961, E-mail: mahdiehby777@gmail.com*

Abstract

Glucose can be covalen bond to the DNA as a non-enzymatic [1]. The persistence of DNA damage with increasing agecould exacerbate the effects of glycation nucleotides [2].Due to the structural features Ketone bodies acetoacetate and production free radical, the acetoacetatecan be effectivein the process binding glucose to DNA and proteins [3].In the study the effect of acetoacetate on the AGEs formation of DNA extractedwas studied under physiological conditions after incubation with glucose for 28 days,using various techniques such as Circular dicroism (CD), gel electrophoresis,Fluorescenceand UV-vis spectroscopy.The results of UV-vis spectroscopy show the amount of DNA-glycation in the presence of acetoacetate increased. As well as its production of reactive oxygen species, increase the complications of diabetes. A new absorbance peaks appear between 300 and 400 nm, which indicate the formation of DNA-AGEs. The modified DNA with glucose and acetoacetate had more absorbanceabout 0.5 than modified DNA with glucose alone. The DNA glycation in the presence of ketone bodies acetoacetate exacerbate structural changes in DNA, DNA single-strand break and increase of mutations and genetic instability is caused.

Keywords: Advanced glycation end products (AGEs),acetoacetate, free radicals, DNA

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1015CBC

Colloidal Hydration Layer of Heme-Imidazole SDS micelle as Efficient Nanozyme

Zainab Moosavi-Movahedi[*a], *A. A. Moosavi-Movahedi*[b]

[a]*Chemistry and Chemical Engineering Research Center of Iran, Tehran, Iran*
[b] *Institute of Biochemistry and Biophysics, University of Tehran, Tehran, Iran*
* *Corresponding author: Tel:+98 2144787797, E-mail:z.moosavi@ccerci.ac.ir*

Abstract

The thermodynamic parameters that control the non-covalent bond formation in proteins and other macromolecules can be directly studied by differential scanning calorimetry (DSC). The most factors that are responsible for the protein or colloid stability are hydrogen bonds to the solvent and intramolecular interactions. Ionic strength is an important factor in hydration layer structure, which is driving force for colloidal hydrophobic inside. Here, heme (12 μM) + imidazole (3 mM) + SDS micelle (40 mM) peroxidase-like nanozyme has shown a sharp thermal profile, observed at 66.1 ° C inside phosphate buffer 0.2 mM. However, higher PBS concentrations (5 mM, 20 mM, 30 mM) do not show any DSC thermal profile. It seems that the observed DSC profile is related to the formation of a unique, single and discrete structure of peroxidase-like biocatalyst in low ionic strength due to special order of hydration layer. It should be noted that this nanozyme (PBS 0.2 mM) has the highest catalytic activity (28.7% of native horseradish peroxidase) among the other PBS concentrations. This report discusses about Role of the hydration force in the stability of colloids at lower ionic strengths and manifests the enzymatic activity based on micelle colloidal solution in aqueous system.

Keyword: Heme-imidazole; SDS micelle, Nanozyme, DSC, hydration layer

1016CBC

A study on the interaction of two chemotherapeutic drugs of Oxali-Palladium and 5-Fluorouracil simultaneously with milk carrier protein of β-lactoglobulin

Amineh Leilabadi-Asl[a], *Adeleh divsalar*[b], *Ali Akbar Saboury*[c], *Kazem Parivar*[a]

[a]*Department of Science and Research branch, Islamic Azad University, Tehran, Iran*
[b]*Department of Cell & Molecular Biology, Faculty of Biological Sciences, Kharazmi University, Tehran, Iran*
[c]*Institute of Biochemistry and Biophysics, University of Tehran, Tehran, Iran*
** Corresponding author: Tel:9128246554, E-mail: amineh.leilabadi@srbiau.ac.ir*

Abstract

βLG is a basic element of globular protein carrier, which is the major protein in the whey of ruminant milk and is of main interest in the dairy industry. In the present study, the effects of 5-fluorouracil and oxali-palladium, as anticancer drugs, on the structure and function of βLG were investigated using different spectroscopic methods of fluorescence and circular dichroism (CD) at two temperatures of 25 and 37 °C. The resulted data from intrinsic fluorescence spectra of protein indicated that 5-Fluorouracil and oxalli-Palladium can quench the fluorescence intensity of βLG in dose-dependent manner via static mechanism of fluorescence quenching. Analysis of quenching data have represented that there are 2 and 1 binding sites on βLG for binding of oxali-palladium and 5-Fluorouracil, respectively at two temperatures of 25 and 37 °C. The analysis of circular dichroic spectra indicated reduction in stability of protein and changed the secondary structure of protein with reduction of α helical structure and increasing of β sheet structure. As a result, it can be concluded that both of the chemotherapeutic drugsof oxali-Palladium and 5-fluorouracil can bind to carrier protein of βLG and changed the secondary and tertiary structures of protein which can be considered as side effects of them.

Key words: 5-fluorouracil, Oxali-palladium, β-lactoglobulin, fluorescence, circular dichroism.

1017CBC

Effects of curcumin on beta-lactoglobulin and HSA fibrillation

Mansooreh Mazaheri[a, b]*, *Ali Akbar Moosavi -Movahedi*[b,c], *Ali Akbar Saboury*[b]

[a]*Standard Research Institute, Food Department, Karaj, Iran;*
[b]*Institute of Biochemistry and Biophysic s (IBB) , University of Tehran, Tehran, Iran*
[c]*Center of Excellence in Biothermodynamics, University of Tehran, Tehran, Iran*
** Corresponding author: Tel:+98 2632803870, E-mail: m_mazaheri@standard .ac.ir*

Abstract

Recently, amyloid fibrils formation is the subject of many scientific researchers from medicine to food science. Amyloid fibrils formation is the base of some diseases such as type II diabetes, Parkinson and Alzheimer. There are some evidences that show some biological molecules inhibited protein fibrillation and aggregation. In this study, the effect of curcumin on protein fibrillation was considered. Using a range of techniques including thioflavin T (ThT) and monitoring of the changes in reactive oxygen species (ROS) levels upon incubation of curcumin with some proteins such as beta-lactoglobulin and Human serum albumin (HSA) have been verified inhibition effects of it. The results imply two assumptions regarding the inhibition mechanism of amyloid protein fibril formation by this compound; the first is for specific structural conformation of it that is necessary for b-sheet interaction and stabilization of the inhibition–protein complex; and the second is accused to aromatic interaction between curcumin and aromatic residues in the amyloidogenic sequence that may direct the inhibitor to the amyloidogenic core and facilitate interaction, but interfere with fibril assembly. So consumption of curcumin may be effective in preventing and curing the disorders.

Keywords: polyphenol; Curcumin; Protein fibrillation; Antioxidant

1018CBC

The effects of microgravity on silver nanoparticles and DNA binding

Bahar Hajaty[a], *Azadeh Hekmat*[*a], *Farid Semsarha*[b] *and Zahra Hajebrahimi*[c]

[a.]*Department of Biology, Science and Research Branch, Islamic Azad University, Tehran, Iran.*
[b.]*Radiation Applications Research School, Nuclear Science and Technology Research Institute, Tehran, Iran.*
[c.]*Department ofPhysiology, Aerospace Research Institute, Tehran, Iran.*
** Corresponding author: Tel:+98 2144865154, E-mail: hekmat@ut.ac.ir*

Abstract

Microgravity is the condition in which objectsorpeople appear to be weightless. The effects of microgravity can be seen when astronauts and objects float in space. Microgravity can be experienced in other ways, as well. Micro- means very small, thus microgravity refers to the condition where gravity seems to be very small. Cancer harms the body when altered cells divide uncontrollably to form lumps or masses of tissue called tumors (except in the case of leukemia where cancer prohibits normal blood function by abnormal cell division in the blood stream).Chemotherapy is the treatment of cancer with one or more cytotoxic chemotherapeutic agents as part of a standardized regimen. The term encompasses a diversity of drugs, which are divided into broad categories.In this research, we have studied the effects of microgravity in the interaction between silver nanoparticles and DNA using UV-visible spectroscopy and FT-IR spectroscopyat 37 ˚C for a period of time. Our results display that silver nanoparticles have different effects on DNA structure and DNA binding in gravity and microgravity conditions. The result obtaining from this present study probably provide useful information to design better drug for cancer therapy and therefore developing more efficiency anti cancer drug in the future.

Keyword: Cancer; DNA; Silver nanoparticles; Thermodynamic parameters.

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1019CBC

The effects of microgravity on TiO_2 NPs and DNA binding

Asma Valizadeh[a], *Azadeh Hekmat*[*a] *and Zahra Hajebrahimi*[b]

[a.]*Department of Biology, Science and Research Branch, Islamic Azad University, Tehran, Iran.*
[b.]*Department ofPhysiology, Aerospace Research Institute, Tehran, Iran.*
** Corresponding author: Tel:+98 2144865154, E-mail: hekmat@ut.ac.ir*

Abstract

Microgravity which is the condition thatobjects or people appear to be weightless. The effects of microgravity can be seen when astronauts and objects float in space. The term micro-g environment is more or less a synonym of weightlessness and zero-g, but indicates that g-forces are not quite zero, just very small. Cancer cells are cells that divide persistently, forming solid tumors or flooding the blood with abnormal cells. Cell division is a normal process used by the body for growth and repair.Chemotherapy usually refers to the use of medicines or drugs to treat cancer.In this research, we have studied the effects of microgravity in the interaction between TiO_2 NPs and DNA using UV-visible spectroscopy and FT-IR spectroscopy at 37 ˚C for a period of time. Our results display that TiO_2 NPs have different effects on DNA structure and DNA binding in gravity and microgravity conditions. The result obtaining from this present study probably provide useful information to understand the effects of gravity on binding of any ligands and also to design new generation of anti cancer agents.

Keyword:DNA;Cancer; TiO_2 NPs; Thermodynamic parameters.

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1020CBC

The effects of microgravity on human serum albumin (HSA)structure

Amir Motamedzade[a], *Azadeh Hekmat*[*a] *and Zahra Hajebrahimi*[b]

[a.]*Department of Biology, Science and Research Branch, Islamic Azad University, Tehran, Iran.*
[b.]*Department ofPhysiology, Aerospace Research Institute, Tehran, Iran.*
** Corresponding author: Tel:+98 2144865154, E-mail: hekmat@ut.ac.ir*

Abstract

Microgravity is when things seem to be weightless. Gravity causes every object to pull every other object toward it.Human serum albumin (HSA) is the main protein component of blood plasma nonetheless it is also distributed in the interstitial fluid of the body tissues. HSA is often used in modeling studies due to its accessibility, low costs, stability and binding capacity. HSA is a widely studied protein as its primary structure is well known and its tertiary structure has been determined by X-ray crystallography. This globular protein consisting of a single polypeptide chain of585 amino acids, which has many significant physiological functions. In this research, we have studied the effects of microgravity on HAS structure by using UV-visible spectroscopy and FT-IR spectroscopy at 37 ˚C for a period of time. Our results indicated that the structure of human serum albumin in microgravitycondition changed. The results obtaining from this present study probably provide useful information to understand the effects of gravity on the structure of protein.

Keyword: Human Serum Albumin; gravity; UV-visible spectroscopy;FT-IR spectroscopy.

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1021CBC

Investigation the characteristics of silibinin loaded on to pegylatedniosomal nanoparticles on the human breast cancer

Leila Kanaani[1*], *Azim Akbarzadeh Khiyavi*[2], *Iraj Javadi*[1]

[1]*Department of Toxicology, Faculty of Pharmacy, Islamic Azad University, Shahreza Branch, Shahreza, Iran*
[2]*Department of Pilot Nanobiotechnology, Pasteur Institute of Iran, Tehran, Iran*
**Corresponding author: Leila Kanaani, Tel: +987144333019,E-mail: lk_rd@yahoo.com*

Abstract

Breast cancer is one of the most frequent cancer types within women population. Silibinin possesses a broad spectrum of biological applications such as anticancer activities[1]; however, poorbioavailability reducesits efficacy at the tumour sites.This study aimd to prepare nanoniosoaml silibinin and evaluate its cytotoxicity against T-47D breast cancer cell line. Niosomes were prepared by revers phase evaporation method. For this purpose, certain amount of span 80, silibinin, poly sorbet-80,PEG-3350 and cholesterol were mixed together in chloroform. The solvent phase was evaporated by rotary evaporator and the remaining gellosephasewas hydrated in phosphate buffer saline. Mean size, size distribution and zeta potential of niosomes was measured by Zetasizer instrument[2]. Releasing pattern of drug was evaluated by dialysis method and the cytotoxicity of nanoniosomes against T-47D cell line, was inspected by MTT assay[3]. Release study showed nanoparticles have proper silibinin retention capability. So our findings suggest that silibinin niosomal nanocarriers could serve as a new drug formulation for breast cancer therapy.

Keywords: Breast cancer, Silibinin, MTT assay

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1022CBC

The effect of *Rosa damascene* on lysozyme aggregation as a model system for neurodegenerative diseases

A. Naji[1,*], *A. Seyedarabi*[1], *A. A. Saboury*[1], *A. A. Meatan*[2]

[1]*Institute of Biochemistry and Biophysics, University of Tehran, Tehran, Iran*
[2]*Department of Biological Sciences, Institute of Advanced Studies in Basic Sciences (IASBS), Zanjan, Iran*
**a.naji@ut.ac.ir*

Abstract

Protein misfolding and aggregation are associated with several human diseases such as Alzheimer's, Parkinson's and etc. Alzheimer's disease affects about 5% of people over 65 years old. The effectiveness of flower scents has been mentioned in Islamic Medicine for the treatment of Alzheimer's disease.We referred to the study of *Rosa damascene* as a common flower with a desirable aroma in the forms of Rose oil, Rose water and Phenyl ethyl alcohol (as a major constituent making up 70% of rose water).In this study, anti-aggregation activity of *Rosa damascene*and its effect on the kinetics of amyloid formation on hen egg white lysozyme used as a model protein was investigated using Thioflavin T fluorescence assay, Congo red assay, dynamic light scattering and circular dichroism. Our preliminary results show phenyl ethyl alcohol to have an anti-aggregation property. Full details of our research results will be presented and discussed further in the form of a poster.

Keywords:*Rosa damascene;* Alzheimer's disease; Phenyl ethyl alcohol

1023CBC

A Reviewon Chemical stabilizationmethods of collagen

Alireza Koochakzaei [*a], *Shadpour Mallakpour*[bcd], *Hossein Ahmadi*[a]

[a]*Department of Conservation of Cultural and Historic Objects, Art University of Isfahan, Isfahan, Iran.*
[b]*Organic Polymer Chemistry Research Laboratory, Department of Chemistry, Isfahan University of Technology, Isfahan, Iran.*
[c]*Nanotechnology and Advanced Materials Institute, Isfahan University of Technology, Isfahan, Iran.*
[d]*Center of Excellence in Sensors and Green Chemistry, Department of Chemistry, Isfahan University of Technology, Isfahan, Iran.*
** Corresponding author: Tel:+98 915506 5409, E-mail: Alireza.k.1989@gmail.com*

Abstract

Collagen is an important biomaterial finding several applications as prosthesis, artificial tissue, drug carrier and cosmetics [1].Generally, the isolated collagen from skin or tendon exhibits poor thermal stability, mechanical strength and water resistance, due to the destruction of natural cross-linking and assembly structure by neutral salt, acid, alkali, or proteases during the extraction process [2].Therefore, they are often modified for practical uses by various methods. Generally, methods applied to stabilize collageninclude chemical crosslinking and/or physical treatments (dehydrothermal, radiation). Chemical reactions are favored by the largenumber of collagen functional side groups [3]. This can be achieved by a number of different cross-linking agents that react with specific amino acid residues on the collagen molecule imparting individual biochemical, thermal and mechanical characteristics to the biomaterial.Actually stabilizationof collagen reduces itsantigenicity and the rate of biodegradation and improves thethermal and mechanical stability [4].The interaction of these agents may occur with the ε-amino group of lysine residues, the carboxyl groups of glutamic and aspartic acids, or with hydroxyl groups [5].Accordingly, in this paper we review and classify chemical stabilization methods and cross-linking agents for collagen.

Keyword: Biomaterial; Collagen; Amino acid; Modification;Stabilisation; Chemical cross-linking

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1024CBC

Three dimensional pharmacophore modeling of Alpha-synuclein aggregation inhibitors

S. S. Jafarypour[1,*], *S. Gharaghani*[1], *A. A. Saboury*[1] *and A. A. Meratan*[2]

[1]*Institute of Biochemistry and Biophysics, University of Tehran, Tehran, Iran*
[2]*Department of Biological Sciences, Institute of Advanced Studies in Basic Sciences (IASBS), Zanjan, Iran*
**ssjafarypour@ut.ac.ir*

Abstract

Parkinson's disease (PD) is a progressive neurodegenerative disorder that is characterized by the deposition of misfolded α-synuclein (α-Syn) asamyloid fibrils in the various region of the brain.Therefore, preventing this process may provide an effective therapeutic approach for treatment of PD. Several experimental methods have beensuggested for inhibition of α-Syn aggregation. In the present study, pharmacophore modeling as a computational method was selected for reduction of time and cost. The pharmacophore concept has been proven to be extremely successful, not only in rationalizing structure-activity relationships, but also by its large impact on developing the appropriate 3D-tools for efficient virtual screening. Several experimental data from various types of compounds for structure–activity relationships were collected.The structure of compounds was optimized and chemical feature based on pharmacophore models of α-Syn aggregation inhibitors have been developed with the Ligandscout Program package. Our results suggest that the best pharmacophore model for α-Syn aggregation inhibitors contain three hydrogen bonds acceptor and two hydrogenbonds donor features with 0.75 score. The best pharmacophore model was validated using database of a test set consist of 48 active and inactive compounds. This well-validated model will use for 3D-query in virtual screening to identify potential hits from database.

Keywords: α-Synuclein; pharmacophore modeling; Parkinson's disease; ligandscout;virtual screening

1025CBC

DNA Binding and Biochemical Investigation of Cu (II) Complex Containing 1,10-phenanthroline and Iminolactone

Jilla Saffari[*a], *Mehri-Sadat Ekrami-Kakhki*[b]

[a]*Department of Chemistry, Islamic Azad University, Zahedan Branch, Zahedan, Iran*
[b]*Nano Technology Labratory, Esfarayen University of Technology, Esfarayen, Iran*
** Corresponding author: Tel:+98 54 31135337, E-mail: j.saffar@iauzah.ac.ir*

Abstract

Deoxyribonucleic acid (DNA) is the primary target molecule formost anticancer and antiviral therapies according to cell biologists[1]. Over the past decades, there has been a considerable interest inDNA binding properties towards different types of transition metalcomplexes under physiological conditions [2]. In this work characterization of the interaction between Cu (II) complex containing 1,10-phenanthroline and iminolactone as ligands, with DNA has been carried out by UV absorption, fluorescence spectra and viscosity measurements in order to investigate binding mode. The experimental results indicate that the Cu (II) complex binds to DNA and absorption is decreasing in charge transfer band with the increase in amount of DNA. The binding constant (K_b) at different temperatures as well as thermodynamic parameters, enthalpy change ($\Delta H°$) and entropy change ($\Delta S°$), were calculated according to relevant fluorescent data and Vant' Hoff equation. The results of interaction mechanism studies, suggested that groove binding plays a major role in the binding of the complex and DNA.

Keyword: Cu(II) complex; DNA binding; Fluorescence; Thermodynamic parameters.

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1026CBC

Study on fluorescence and DNA-binding of palladium(II) complex containing glycine and valine

Sareh Zareian-Jahromi[a] , *Hassan Mansouri-Torshizi**[a] , *Alireza Pourkarami*[b]

[a]*Department of Chemistry, University of Sistan & Baluchestan, Zahedan, Iran*
[b]*University of medical science, Zabol, Iran*
** Corresponding author: Tel:+98 54-33431146, E-mail: : hmtorshizi@hamoon.usb.ac.ir*

Abstract:

Binding of small molecules with DNA has been studied extensively since DNA is the material of inheritance and controls the structure and function of cells [1-3]. The new Palladium(II) complex, [Pd(Gly)(Val)] ,(where Gly is glycine, Val is valine)has been synthesized and characterized by elemental analyses, molar conductivity measurements and spectroscopic methods (FT-IR, ^{1}H NMR, UV–Vis). Both ligands coordinate to Pd(II) center as bidentate chelates. This complex is non-ionic in nature and possess square planer geometry around Pd(II) metal ion. The binding properties of this complex with Calf Thymus DNA (CT-DNA) have been investigated by UV–Vis absorption and competitive DNA-binding studies with ethidium bromide (EB) by fluorescence. The results obtained from these analyses indicated that this complex effectively interact with CT-DNA at low concentration. Binding constant (K_b), apparent biomolecular quenching constant (K_q) and number of binding sites (n) for CT-DNA were calculated using Stern-Volmer equation. Also, The thermodynamic parameters (ΔH^o, ΔS^o and ΔG^o) indicated that the vander Waals and hydrogen binding might play a major role in the interaction of this complex with CT-DNA. The above mentioned physical measurements indicate that the Pd(II) complex bind to calf thymus DNA, presumably via groove binding mode. In addition, the binding forces are spontaneous owing to -ΔG°.

Keywords: DNA-binding ; Pd(II) complex; Amino acids.

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1027CBC

The state of glycation due to some small molecules: Bovine Serum Albumin as a case study

Loghman Alaei[a]*, Saeid Hadi-Alijanvand[a], Fereshteh Taghavi[b], Ali Akbar Moosavi-Movahedi[a]

[a]*Institute of Biochemistry and Biophysics, University of Tehran, Tehran, Iran*
[b]*Faculty of Biological Sciences, Tarbiat Modares University, Tehran, Iran*
** Corresponding author: Tel:+98 2161113381, E-mail: l.alaei@ut.ac.ir*

Abstract

Appearance of advanced glycation end products (AGEs) is an importantfactor in the development of various disorders such asAlzheimer's disease, cataract, Diabetes, Parkinson's disease and chronickidney disease [1-2]. Hyperglycemic conditions when the bloodglucose goes above normal results in increased flux of glucoseand its metabolic intermediates toward different pathwayscontributing to the formation of highly toxic pro-oxidants calledAGEs [1-3]. One of the main targets of these events are proteins which are glycated at lysine and arginine residues [3-4]. The glycation induced changes in the secondarystructure and conformation and drug binding ability of themolecular structure can be studied.Currently, Molecular Dynamics simulations are extensively used in the study ofstructure, dynamics, and function of many biomacromolecules [2-3]. The present study employs experimental methods like UV-visible, Circular dichroism, Fluorescence and docking tools to investigate the changes occurred in secondary and tertiary structures of the bovine serum albumin (BSA) together with its interactions with glucose, potassium sorbate, and sodium benzoate molecules. The two later molecules are widely used in cosmetics, tooth pastes and food products as preservatives. Data showed that sodium benzoate is able to react with Lys residues in BSA via covalent bonds. Fluorescence spectroscopy results revealed partial unfolding of BSA when incubated with sodium benzoate in the presence or absence of glucose. The results showed that potassium sorbate shortens the glycation time for BSA. In addition, secondary and tertiary structural changes were also observed in different intervals of incubation with glucose in the presence or absence of each of potassium sorbate and sodium benzoate.

Keywords: Diabetes; Glycation; Bovine Serum Albumin; Preservatives; Sodium Benzoate; Potassium Sorbate

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1093-CBC

1028CBC

Synthesis, characterization and DNA-binding studies of a Palladium(II) complexcontaining mixed-ligands of 1,10-phenanthroline and salicylic acid

Mahin Dustkami[*a], *Hassan Mansouri-Torshizi*[a]

[a]*Department of Chemistry, University of Sistan & Baluchestan, Zahedan, Iran*
[*]*Corresponding: Tel: 09151499257, E-mail: dostkami@yahoo.com*

Abstract

The novel antitumor Pd(II) complex of formula [Pd(phen)(SA)] (where, phen=1,10-phenanthroline, SA=Salicylato) from the interaction of molecules $[Pd(phen)(H_2O)_2](NO_3)_2$ and sodium salt of salicylic acid(SA.Na) have been synthesized. The complex has been characterized by conductivity, elemental analysis,UV-Vis, FT-IR and ^{1}H-NMR techniques. The studies indicated thatthis complex is nonelectrolyte and the salicylato ligand is bidentately bound to Pd(II) ion through two oxygen atoms. The interaction of Pd(II) complex with calf thymus DNA (CT-DNA)was investigated by UV–Vis spectroscopy. This experiment imply the Pd(II) complex interact with DNA. The intrinsicbinding constant (K_{app})of interaction between CT-DNA and mentioned complex was obtained 5.628×10^3 (M^{-1}) and 6.153×10^3 (M^{-1}) at 300K and 310K, respectively. The concentration of this complex in the midpoint of transition, $[L]_{1/2}$, at 300K and 310K are 0.019 mM and 0.015 mM, respectively. This means that the complex can unfold CT-DNA at low concentrations and if this is used as antitumor agent, very low doses will be needed, which may have fewer side effects.

Keywords: palladium (II) complex, 1,10-phenanthroline, salicylic acid, DNA-binding

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1029CBC

Comparative study of thermal domains analyzing of glycated and nonglycated human serum albumin

Mousa Bohlooli

Department of Biology, University of Zabol, Zabol, Iran
Corresponding author: Tel:+98 54 32232961, E-mail: bohlooli@ut.ac.ir

Abstract

Resistance of a protein against a denaturant agent is a useful property. Protein biological functiondepends on its native structure. The loss of this folded structure leads to inactivate of a protein.[1,2]. Protein unfolding can be reversible or irreversible. The unfolding reversibility of manyproteins has been studied using different denaturant agents such as chemical reagents andtemperature [3]. Irreversibility causes misfolding and aggregation of proteins in cells and underin vitro conditions. Most importantly, it is involved in a wide range of diseases, including someof the most prevalent neurodegenerative disorders [4]. In the current research, the domainsthermal unfolding of glycated human serum albumin (GHSA) and human serum albumin (HSA)
were studied under incubation at physiological conditions for 35 days. The domains thermalunfolding of GHSA and HSA were evaluated using differential scanning calorimetry (DSC),circular dichroism (CD), and UV–Vis spectroscopy. The results showed that the first energeticdomain of GHSA remained after cooling back from 80 ºC,while the first energetic domain ofHSA disappeared at this temperature.Moreover, the secondenergetic domain of GHSA kepton after cooling back from 90 ºC, but it disappeared in HSA atthis temperate. Also, the secondarystructure recovery after cooling back in GHSA was higherthan HSA. Therefore, according to the obtained results,glucose can act as a stabilizer for HSAdomains and can be used in food and pharmaceutical industries.

Keywords: Glycation, Domain, Human serum albumin, Thermal resistans protein, DSC

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1030CBC

Kinetic and Structural Study of α-Glucosidase via XantheneHeterocycles as Antidiabetic Inhibitors

Maryam Nourisefat[a,b], *Massoud Amanlou* [c], *Farhad Panahi* [d] *Ali Khalafi-Nezhad* [d] *and Ali Akbar Moosavi-Movahedi*[a,b]

[a]*Institute of Biochemistry and Biophysics, University of Tehran, Tehran, Iran*
[b]*UNESCO Chair on Interdisciplinary Research in Diabetes, University of Tehran, Tehran, Iran*
[c]*Department of Medicinal Chemistry, Tehran University of Medical Sciences, Tehran, Iran*
[d]*Department of Chemistry, College of Sciences, Shiraz University, Shiraz 71454, Iran*
** Corresponding author: Tel:+98 21-61113381, E-mail:* m.nourisefat@ut.ac.ir

Abstract

As a serious global health crisis, diabetes mellitus (DM) commonly referred to as diabetes is a common metabolic diseases, characterizing by abnormally high blood sugar level [1]. Therefore, avoiding wide fluctuations in blood glucose levels are important goals in the therapy of the subjects with this metabolic disorder [2]. Also, decrease of the postprandial hyperglycemia by inhibition of the carbohydrate-hydrolyzing enzymes is critical for treatment for glycemic control [3]. So, the inhibition of α-Glucosidase (α-Gls) is an effective method in both preventing and treating diabetes through improvement of postprandial hyperglycemia [4]. Therefore, beside the commercial inhibitors of α-Glucosidase such as acarbose, voglibose and miglitol which are widely in use for the treatment of diabetes, it is necessary to develop more tolerable α-Glucosidase inhibitors with less unfavorable side effects. In the present study, the object of the research was to using some synthesized heterocyclic xanthene derivatives [5-6] to access their inhibitory properties against α-Gucosidase. The results in this study may lead to present a new and more specific α-Glucosidase inhibitors with potentially therapeutic values for reducing the severity of those secondary complications, which are normally associated with type-II diabetes mellitus.

Keyword: α-Glucosidase (α-Gls); Acarbose; Diabetes mellitus; Hyperglycemia; Inhibition.

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1031CBC

Cell Phone Radiation of Effects on Cancer Risk

Fatemeh Zakieh Tohidi

Department of Medical Physics, Zahedan University of Medical Sciences, Zahedan, Iran.
** Corresponding author: Tel:09358454472, E-mail: fm.tohidi@yahoo.com*

Abstract

Several studies demonstrate strong links between electromagnetic wave radiation exposure and adverse health effects. Given the functional importance of the hippocampus, this study aimed to investigate the effects of electromagnetic waves radiated by mobile phones on hippocampal expression of P21 and P53 genes as regulators of cellular apoptosis. Forty-eight male BALB/c mice were randomly divided into six groups (n=8 each). Animals in the four experimental groups were respectively exposed for 30 minutes, one, two and four hours to electromagnetic waves radiated twice a day at the frequencies of 900 and 1800 megahertz for a period of 30 consecutive days. One of experimental group was radiated for 4 hours once a day, while the control group remains constant during the experiment. The hippocampal expression of P21and P53 mRNAs were evaluated using Real-Time PCR.The ratio expression of P53 and P21 genes was increased to greater than one (P53/P21>1) in allexperimental groups compared to controls, except for the group with 2 hours twice a day exposure. However, there was not significant differences between the expression level of P53 and P21 genes among the experimental groups using paired t test ($p>0.05$).
In fact, radio frequencies of mobile phones damage brain cells depending on the duration of the conversation (the duration of radiation). While further investigation is recommended, our results revealed that the mobile phone radiation had no effect on the hippocampus expression of P53 and P21 genes in the mice.

Keywords: Electromagnetic Waves, Mice, Apoptosis, P21and P53 Genes, Hippocampus References

1032CBC

Study of the simultaneous effect of silver nanoparticles and 3-β-hydroxybutyrate on human hemoglobin glycation process

*Sakineh Janzin**[a],Mostafa Khajeh[a], Mousa Bohlooli[b]and Mansour Ghaffari-Moghaddam[a]*

[a]*Department of Chemistry, University of Zabol, Zabol, Iran*
[b]*Department of Biology, University of Zabol, Zabol, Iran*
** Corresponding author: Tel:+98 54 32233013, E-mail:* S.janzin@uoz.ac.ir

Abstract

Hemoglobin is the first protein in the glycation studies.Glycation is sugar binds to macromolecules which cause complications of diabetes [1] such as cataract and hardening of the arteries. Several factors are effective in the protein glycationsuch as pH, temperature, concentration, chemical reagents [2]. In this study,the effect of simultaneous silver nanoparticles and 3-β-hydroxybutyratewas studied on human hemoglobin glycation process on the physiological-like conditions. All samples were dialyzed after 42 days of incubation and were characterized using various biophysical techniques such as UV–vis, circular dichroism and fluorescencespectroscopy. The results offluorescence in excitation 320 nm, showed that fluorescence intensity of hemoglobin samplesincubatedwith glucose alone showed the highest intensity among all samples. The fluorescence intensity was reduced about24% in the present of 3BHB with silver nanoparticles.The simultaneous presence of silver nanoparticles and 3-β-hydroxybutyrate could help to reduce the effects of glucose. Therefore, silver nanoparticles can reduce the glycation process which is effective in reducing complications of diabetes.

Keywords: Glycation,human hemoglobin, 3-β-Hydroxy butyrate, Silver nanoparticles

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1033CBC

Optimized method for myoglobin purification and the study of physical characterization

E. Hosseini[1] *, *R. Sattari*[1] , *Sh. Ariaeenejad*[1] , *N. Poursasan, A. A. Moosavi-Movahedi*[1,2]

**hosseinielnaz@ut.ac.ir*
1. Institute of Biochemistry and Biophysics (IBB), the University of Tehran, Tehran, Iran.
2. UNESCO Chair on Interdisciplinary Research in Diabetes, University of Tehran, Tehran, Iran.

Abstract

Myoglobin is a major hemoprotein and the principal oxygen reservoir in the muscle tissues of live animals. There are different methods for isolation and purification of myoglobin but in this study a simple and rapid procedure was developed to isolate and purify myoglobin from animal muscles. This method involved fractional precipitation of a crude myoglobin extract with ammonium sulfate and purification with a single chromatographic step on a Sephadex G-100 column. Phosphate buffer and Tris-HCl buffer were used for extraction and purification. The purity of the myoglobin preparations was confirmed by SDS-polyacrylamide gel electrophoresis**.** Sephadex G-100 chromatography of crude myoglobin extracts of meat produced similar elution profiles when monitored at 412 and 525 nm that was similar to sigma myoglobin. Two kinds of different myoglobin that extracted by this method were studied by fluorescence, circular dichroism and uv-visible spectroscopic methods.

Keywords: Myoglobin; Chromatography; Sephadex G-100; Fluorescence

1034CBC

Alteration of DSC profiles for Halal and non-Halal myoglobins

R. Sattari [1], E. Hosseini [1], Sh. Ariaeenejad [1], N. Poursasan[1], F. Moosavi-Movahedi [1], H. Ghourchian[1], A. A. Moosavi-Movahedi [1,2]*

[1]Institute of Biochemistry and Biophysics, University of Tehran, Tehran, Iran.
[2]UNESCO Chair on Interdisciplinary Research in Diabetes, University of Tehran, Tehran, Iran.
**r_sattari@ut.ac.ir*

Abstract

There are several type of methods for slaughtering of animals around the world. Studies have shown that different type of slaughtering was influenced on biochemical composition and other properties of meat. The aim of this study is to analyze the effect of Halal and non-Halal slaughtering on biophysical properties of myoglobin. Myoglobin is a sarcoplasmic protein with the heme prostetic group and protein moiety in meat. For this reason myoglobin was extracted from Halal and non-Halal sheep meats and was purified by various methods of chromatography. Differential scanning calorimetry (DSC) was performed to study for thermal profiles of myoglobins from Halal and non-Halal slaughtering meats. Analysis showed that they have different thermal profiles and thermal protein stability.

Keywords: Halal slaughtering; non-Halal slaughterig; Myoglobin; Differential scanning calorimetry; Thermal profile

1035CBC

Metallo-vesicular pseudo-chloroperoxidase: A mixture of SDS/DTAB cysteine/metal

Mohammad Mahdi Kafi[a], *Zainab Moosavi-Movahedi*[*a], *Yazdan Sajadimehr*[a] *and Ali Akbar Moosavi-Movahedi*[b]

[a] *Chemistry and Chemical Engineering Research Center of Iran, Tehran, Iran*
[b] *Institute of Biochemistry and Biophysics, University of Tehran, Tehran, Iran*
** Corresponding author: Te: 021 44787797, E-mail :z.moosavi@ccerci.ac.ir*

Abstract

Biomimetics, simply, is the attempt to mimic physiological properties and functions. Using biology as aguide, we can now understand, engineer, and control bioactive molecular interactions and assemble them into novel systems or materials.Catalytic nano-architectonics is the art of assembling the desired functionalcomponents according to the scale of catalytic events [1].Herein, a cysteine-metal complex was designed and encapsulated in avesicular mixture (1:4; SDS/DTAB) in order to imitate a chloroperoxidase (CLP) nanozyme via chlorinationof thionine at pH 3. In these experiments, different metals nitrates, zinc, iron, nickel and cobalt were used. First, as biomimetally predicted, Iron chloroperoxidase reactionis done more quickly than the cobalt,nickel and zinc, respectively.Second, the presentation of mixed SDS/DTAB colloid evolutes the reaction performance because of charges available on surface of hydrophobic nano-envelop that provides a particular interface structure for positioning the charged or hydrophobic parts of active-site and substrate to locate next to each other at proper direction.

Keywords: cysteine/metal, SDS/ DTAB, vesicle, biomimetic, chloroperoxidase, nanozyme.

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1036CBC

Spectroscopic evaluation of Isoxsuprine hyreochloride interactions with human serum albumin

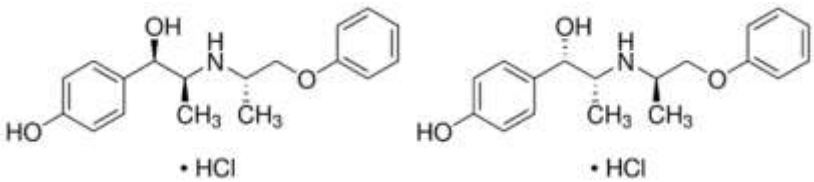
Amin Shahriar, Somaye Shahraki, Fereshteh Shiri, Mostafa Heidari Majd

Department of Chemistry, University of Zabol, Zabol, Iran
Email: amin.shahryar10@gmail.com

Abstract

Isoxsuprine (Fig. 1) is a drug that used as a vasodilator in human. It causes a direct relaxation of vascular and uterine smooth muscles [1]. Human serum albumin (HSA) acts as a reservoir and transport protein for endogenous (e.g. fatty acids or bilirubin) and exogenous compounds (e.g. drugs or nutrients) in the blood [2]. The binding of a drug to albumin is a major determinant of its pharmacokinetic and pharmacodynamic profile. In this study, the interaction between of Isoxsuprine and human serum albumins at physiological like conditions was investigated. Spectroscopic methods such as Fourier transform infrared (FT-IR), UV–Vis, fluorescence and circular dichroism (CD) spectroscopy were used to analysis of this interaction. The results indicate that there is a considerable quenching of the intrinsic fluorescence of HSA on binding with drug. The binding of drug with protein is characterized by one high affinity binding site with the association constants of the order of 105. Thermodynamic analysis showed that HSA was combined with Drug, mainly by van der Waals or hydrogen interactions. The molecular distance, r, between protein (Donor) and Isoxsuprine (acceptor) was obtained according to Forster's theory of non-radiation energy transfer. The circular dichroism results represented that Isoxsuprine induced a decrease in content of the α-helical structure of protein. We hope that results of our study make a better understanding of the extent of distribution of many drugs in the blood and the interaction with proteins.

Keyword: Isoxsuprine hydrochloride, Human serum albumin, Fluorescence, Fourier transform infrared



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1037CBC

Crystal Structure, DNA Binding andCytotoxicity of a New Hydroxyl-Quinolinato-Palladium Complex

Ziba Sorinezami, Hassan Mansouri-Torshizi

[a]*Department of Chemistry, University of Zabol, P.O. Box 98615-538, Zabol, Iran*
[b] *Department of Chemistry, University of Sistan&Baluchestan, Zahedan, Iran*

Abstract

The development of palladium anticancer drugs has been promising and their design has been based mainly on the structure-activity relationship used for platinum anticancer drugs as well as good models for the analogous Pt(II) complexes in solution[1-3].Thus our research in this area is focused on the interaction of Calf Thymus DNA (CT-DNA)with a new palladium(II) anticancer complex of[Pd(8Q)(bpy)]NO_3 (where 8Q = 8-hydroxyquinolin and bpy = 2, 2'-bipyridine).There is a set of 4 binding sits(g) for the complex on the DNA with positive cooperativity in binding. n,the Hill coefficient find out to be 5.25 at 300 and 4.36 at 310Krespectively. K_{app} the apparent equilibrium constant are 45.58 and 79.31 mM^{-1} respectively.The above compound can denature the DNA and the concentration of this ligand in the midpoint of transition ($[L]_{1/2}$), is decreased by improving temperature, from 0.066 at 300to 0.060 mmol/L at 310K. (ΔG^0_{H2O}) determined to be 31.64 and 25.19 kJ/mol at 300K and 310K respectively. values for m, are 462.19and 381.51 at 300K and 310K respectively.$\Delta H^0_{coformation}$ in the range of 300K and 310K is find out to be 220.02 kJ/mol. $\Delta S^0_{H2O}$of DNA denaturation by complex is 0.627 kJ/mol at 300K. Fluorescence titration spectra and fluorescence Scatchard plots suggest that the Pd(II) complex intercalate in DNA. The cytotoxicity assay of the complex has been performed on human breast adenocarcinoma MCF7 cell line, at micromolar concentration.

Keywords: Thermodinamic parameters, spectroscopic techniques,anti-tumor, Palladium (II) complex

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1038CBC

Interaction studies between a[(phen)Pd(8Q)]NO_3 anti-tumor complex and calf thymus DNA

Ziba Sorinezami, Hassan Mansouri-Torshizi

[a]*Department of Chemistry, University of Zabol, P.O. Box 98615-538, Zabol, Iran*
[b] *Department of Chemistry, University of Sistan&Baluchestan, Zahedan, Iran*

Abstract

Among transition metal complexes palladium(II) complexes are very interesting candidates for alternative metal-based drugs, because the coordination geometry and complex forming processes of palladium(II) are very similar to those of platinum(II)[1-3].Thus our research in this area is focused on the interaction of Calf Thymus DNA (CT-DNA)with a new palladium(II) anticancer complex of[Pd(8Q)(phen)]NO_3 (where 8Q = 8-hydroxyquinolin and phen = 1,10-phenanthroline).There is a set of 4 binding sits(g) for the complex on the DNA with positive cooperativity in binding. n,the Hill coefficient find out to be 2.59 at 300 K and 2.34 at 310K respectively. K_{app} are 76.58 and 83.03 mM^{-1} at 300K and 310K respectively. The above compound can denature the DNA and the concentration of this ligand in the midpoint of transition ($[L]_{1/2}$), is decreased by improving temperature, from 0.057 at 300to 0.054mmol/L at 310K. the ΔG^0_{H2O} determined to be 47.63 and 46.68 kJ/mol at 300and 310K respectively. values for m, are 846.8and 881.3 (kJ/mol).$(mol/L)^{-1}$ at 300K and 310K respectively. $\Delta H^0_{coformation}$ in the range of 300K and 310K is find out to be 75.44 kJ/mol. ΔS^0_{H2O} of DNA denaturation by complex is 0.092 kJ/mol at 300K. Fluorescence titration spectra and fluorescence Scatchard plots suggest that the Pd(II) complex intercalate in DNA. The cytotoxicity assay of the complex has been performed on human breast adenocarcinoma MCF7 cell line, at micromolar concentration.

Keywords: Thermodinamic parameters, spectroscopic techniques,anti-tumor, Palladium (II) complex

References

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1039CBC

Chaperone activity of antioxidant compounds to prevent the Aggregationof unfold proteins

Abbas Heidari[1]. Arezou Ghahghaei[2]

[1]PHD student, Department of Biology, Faculty of Science, ferdowsi university of mashhad
[2]Department of Biology, Faculty of Science, University of Sistanand Baluchestan

Abstract

Chaperone molecules play an important role in the proper folding of proteins and preventing proteinaggregation**.** Protein aggregation, a process which unnatural molecules connect together and create soluble small oligomers or insoluble aggregations, depends on resistance conformation and colloidal characteristics of proteins. Finding proper ways to soften or gravel of proteins aggregation would be important in the control of diseases (e.g. Alzeimer's disease, Parkinsonism) that are related to this situation.Seidlitziarosmarinus extract has antioxidant compounds which can cause increase in proteins resistance and preventing from proteins aggregation. The aim of this study is to survey the effects of antioxidant compounds in Seidlitziarosmarinus on proteins aggregation. In this research antioxidant properties of Seidlitziarosmarinus extract was evaluated on ovotransferin, insulin, and alpha lacto albumin in the presence of DTT as an aggregation and settlement inducer factor, using visible light spectroscopy, indigenous florescence spectroscopy, ANS, and Near-UV spectroscopy. Results indicated that the extract of Seidlitziarosmarinus could prevent protein aggregation which was different between three subjects of proteins and also there was a dose dependent manner about the extract; increase in concentration of extract would promote the level of conservation.

Keywords:.

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1040CBC

DNA binding properties of combination Co^{3+}, Cu^{2+}, Zn^{2+} and Pd^{2+} complexes

Fatemeh Khosravi[a], *Hassan Mansouri-Torshizi*[*a], *Alireza pourkarami*[b]

[a] *Department of Chemistry, University of Sistan&Baluchestan, Zahedan, Iran*
[b] *University of medical science, Zabol, Iran*
** Corresponding author: Tel:+98 54-33431146, E-mail: : hmtorshizi@hamoon.usb.ac.ir*

Abstract

Combination therapies are quite common.as anti-cancers, anti-microbials and etc... For instance cisplatin, ($[PtCl_2(NH_3)_2]$ or CDDP), is frequently used in combination with one, two, three, or even four other drugs, with positive results.[1] Also, kinetic studies of the interaction between DNA and combinations of the metal complexes under physiological condition are important for the development of combinations based new metallo-pharmaceuticals.[2] Therefore four Co^{3+}, Cu^{2+}, Zn^{2+} and Pd^{2+} complexes of formula $K_3[Co(ox)_3].3H_2O$ (**I**) (ox=oxalate), $[Cu(phen)_2Cl]Cl$ (**II**), $[Zn(phen)_3]Cl_2$ (**III**), $[Pd(phen)_2](NO_3)_2$ (**IV**) (phen=1,10-phenanthroline) were synthesized and characterized analytically and spectroscopically by elemental analysis (C, H, N), FT-IR, UV-Vis, resonance signals in the ^{1}H-NMR and conductivity measurements. The interaction each of four series of the metal complexes with calf thymus DNA (CT-DNA) were investigated under physiological condition in Tris-HCl buffer using spectroscopic methods including UV-Vis absorption spectroscopy, ethidium bromide displacement and fluorescence titration spectra. The results obtained from these binding studies indicated that all the series effectively interact with CT-DNA. Fluorescence titration revealed that the complexes strongly quench DNA bound ethidium bromide (EB) through static quenching procedures. The Binding constant (K_b), apparent biomolecular quenching constant (Kq) and number of binding sites (n) at different temperatures were determined according to relevant fluorescent data. Thermodynamic parameters, enthalpy change ($\Delta H°$), entropy change ($\Delta S°$) and Gibss free energy ($\Delta G°$) were calculated using K_b and Vant' Hoff equation. These parameters suggested that hydrogen binding and Van der Waals force play the major role in the association of each series of metal complexes with CT-DNA.

Keyword: Combination therapy, DNA binding, 1,10-phenanthroline

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1041CBC

Investigation of the interaction between Propyl Acridone and Butyl8chloro Acridone with ct-DNA by circular dichroism spectroscopy

Firoozeh Malekzadeh, Mehran Gholamin, Jamshid Khan Chamani*

Department of Biochemistry and Biophysics, Faculty of Sciences, Mashhad Branch, Islamic AzadUniversity, Mashhad, Iran
** E-mail:malekzadeh.firoozeh@gmail.com*

Abstract

Due to the sensitivity of CD signal to subtle variation of DNA chiral conformation, CD is useful technique to follow the complex-DNA interaction via investigation the changes in the DNA Morphology[1].In particular B-DNA shows two CD bands:a positive band at 278 nm due to base-stacking and a negative band at 246 nm due to the right handed helicity[2]. Classical interaction tend to enhance the intensities of bands due to strong base stacking interaction and stable DNA conformation ,while simple groove binding and electrostatic interaction show less perturbation or no perturbation on the base stacking and helicity bands[3]. The result indicate that in the present of two drugs both positive and negative bands are increase and decrease respectively and this type of changes in the CD bands was regarded that B-DNA changes conformation to A-DNA in intercalative binding mode .The enhancement of positive bands was due to drugs that stacked in to the base pairs of duplex DNA,which prevented the adjacent base pairs from close stacking[4].

Keyword : Intercalation;Circular dichroism; B-DNA; right handed helicity; base-stacking

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Monovalent cation effects on conformation of glucose oxidase enzyme

Fatemeh Janati-Fard[*a], *Mohammad Reza Housaindokht*[a,b], *Hassan Monhemi*[a]

[a] *Biophysical Chemistry Laboratory, Department of Chemistry, Faculty of Science, Ferdowsi University of Mashhad, Mashhad, Iran*
[b] *Research and Technology Center of Biomolecules, Faculty of Science, Ferdowsi University of Mashhad, Mashhad, Iran*
** Corresponding author: Tel:+98 38804082, E-mail: fjanatifard@gmail.com*

Abstract

Glucose oxidase (GOx) is a flavoenzyme having applications in medical industries. Here, the structure of GOxin the presence ofmonovalent Cation (NaCl) has been studied. MD simulations were carried out by GROMACS 5.0.4 with a GROMOS 43a1 forcefiled. Parameters for flavin adenine dinucleotide (FAD) were taken from the work of van den Berg et al. and protein(pdb code: 1GPE) was placed in a cubic box center consisting SPC216 water molecules. About 2000NaCl were placed inthe box.Simulations were performed for 100 ns with a timestep of dt = 0.002 ps[1-3].According tormsf analysis some secondary structures of GOx are destructed while some structures are formed on treatment with NaCl. The analysis of active site structure in chain A of GOx revealed that hydrogen bonding between His563 at $N^{\varepsilon 2}$ and Glu416 $O^{\varepsilon 2}$(5.2 Aº) is increased to the high value in GOx-NaCl which is deviated from crystal (2.5 Aº). The flavin O_4 is connected by hydrogen bonds to the backbone N atoms of Ser114 (7.5 Aº) and Gly112 (8.3 Aº) in GOx-NaCl which have high value in comparison with the crystal (3Aº and 3.3Aº forSer114 and Gly112, respectively)[4].These results are in agreement with experimental dataaboutthe structure of GOx [5]. NaCl could enter the active pocket of GOx,leading to a change in the orientation of FAD and an alteration in conformation of GOx.The structural details would be important for rational enzyme design.

Keyword: Glucose oxidase, monovalent Cation, Structural property, Molecular dynamics simulation

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1043CBC

Investigation of Intramolecular Hydrogen Bond in Malonaldehyde Derivatives: An AIM and NBO Study

Abdorahman Malekpoor, Ali Reza Nowroozi, Halime Kord – Tamandani*

Department of Chemistry, Faculty of Science, University of Sistan and Baluchestan,
P O Box 98135-674, Zahedan, Iran
**Corresponding author: Tel: +98 541 2446565; fax: +98 541 2446565;*
E-mail: eidozehi1239@gmail.com

Abstract

All the plausible conformations of tautomeric structures (Keto and Enol) of malonaldehyde (MA) have been investigated by the Bekes-Lee-Yang-Parr (B3LYP) nonlocal density functional with extended 6-311++G basis set for studying the stability order of conformers and the various possibilities of intramolecular hydrogen bonding formation. The results show that the chelated enol structur (E11) is more stable than the order conformers. This is mainly due to the formation of intramolecular hydrogen bond. Furthermore, the effect of halogen substitution (F,Cl and Br) on intramolecular hydrogen bond and π-electron delocalization were also investigated. The contribution of resonance to the stability of chelated MA conformers is greater than that of the hydrogen bond energy. Finally, the computational results with AIM and NBO analyses were compared. The topological properties of the electron density contributions for various type of intramolecular hydrogen bond have been analyzed in term of the Bader theory of atoms in molecules (AIM).

Keywords: malonaldehyde (MA);intramolecular hydrogen bond; halogen substitution; AIM; NBO

1044CBC

Alterations in the structure of blood carrier protein of Albumin upon interaction with new synthesized Pt(II) complex

Akram Najaran[1], Adeleh Divsalar[2], Ali Akbar Saboury[3], Mahbubeh Eslami-Moghadam[4]

[1]Department of Science and Research branch, Islamic Azad University, Tehran, Iran
[2]Department of Cell & Molecular Biology, Faculty of Biological Sciences, Kharazmi University, Tehran, Iran
[3] Institute of Biochemistry and Biophysics, University of Tehran, Tehran, Iran
[4] Chemistry and Engineer Chemistry Research Center, Tehran, Iran

Abstract

In recent years, using heavy metal compounds such as platinum as anticancer agent is one of the common ways in cancer chemical therapy. In this study, the biological evaluation of a new anticancer compound of glycine derivative of Pt(II) complex was investigated again Human serum albumin (HSA) as a most abundant and carrier protein in plasma. The side effects of this novel compound was checked via its ability on the alterations in the function and structure of HSA at different temperatures of 25 and 37°C by applying various spectroscopic (fluorescence, Far UV circular dichroism (CD) and UV visible) methods. Fluorescence data indicated the strong ability of Pt(II) complex to quench the intrinsic fluorescence of HSA.The binding parameters and thermodynamic parameters, including ΔH°, ΔS°, and ΔG° were also calculated by the fluorescence quenching method.The Fluorescence results have shown that there is one binding site on HSA forbinding of this complex. Also, thermal denaturation data of the protein in the absecnce and presence of this complex represented the reduction of protein thermal stability upon interaction with the Pt(II) complex via reducing of T_m value of protein. Our results suggest that the new synthesized Pt(II) complex can bind to the blood carrier protein of HSA and change the stability and tertiarystructures of protein without any alterations in secondary structure, which can be considered as the side effects of this new synthesized drugs.

Keywords: Human serum albumin, Pt(II) complex, cancer, fluorescence quenching

1045CBC

An explorative study on potent gram-negative specific LpxC inhibitors using molecular docking and molecular modeling

Rahmat A. Dijoor[a], *Fereshteh Shiri**[a], *Maryam Salahinejad*[b], *Massoud Nejati-Yazdinejad*[a]

[a]*Department of Chemistry, University of Zabol, Zabol, Iran*
[b]*Nuclear Science and Technology Research Institute, Tehran, Iran*
Fereshteh.shiri@uoz.ac.ir

Abstract

Pathogenic Gram-negative bacteria, including Pseudomonas aeruginosa and Escherichia coli are responsible for nearly half of the serious human infections and sepsis is a common complication from Gram-negative. Therefore, there is already an urgent need for identification and development of novel antibiotics particularly those effective for the treatment of Gram-negative bacterial infections. Gram-negative bacteria hasouter membrane containing lipopolysaccharides (LPS) which consists of lipid A in its outer leaflet. Lipid A is necessary to protect Gram-negative bacteria against external agents such as antibiotics and detergents. The unique and essential zinc-dependent metalloamidase UDP-3-*O*-(*R*-3-hydroxymyristoyl)-*N*-acetylglucosamine deacetylase (LpxC), which catalyzes the committed step of lipid A biosynthesis, has emerged as an attractive antibiotic target.CoMFA, CoMSIA, HQSAR, molecular docking and *in silico* ADMET prediction have been performed for LpxC inhibitors. This study has been carried out to determine the binding mode and drug likeliness nature of compounds.CoMFA, CoMSIA, HQSAR models were generated using 32 compounds. The generated models were found to be statistically significant as CoMFA model had (R^2=0.967, Q^2=0.804, R^2_{PRED}=0.827); CoMSIA model had (R^2=0.963, Q^2=0.752 R^2_{PRED}=0.857)andHQSARmodel had (R^2=0.969 Q^2=0.937 R^2_{PRED}=0.892). In order to evaluate the effectiveness of the docking protocol, co-crystallized ligand was extracted from the ligand binding domain of the protein and was re-docked into the same position. The conformer obtained on re-docking and the co-crystallized ligand were superimposed and the root mean square deviation between the two was found to be 1.21 Å. Outcomes of this study provide an insight for designing novel LpxC inhibitors.

Keyword: gram-negative specific LpxC inhibitors, CoMFA, CoMSIA, HQSAR, molecular docking

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1046CBC

Production of pectinase from sugar beet pulp by*Piriformospora indica* under submerged fermentation

Parisa Fathi Rezaei, Somayyeh Kiani, Saleh Shahabivand*

Biology department, Faculty of Science, University of Maragheh, Maragheh, Iran
** Corresponding author: Tel: +98 4137278100, E-mail:* parisafathirezaei@gmail.com

Abstract

The biotechnological potential of pectinolytic enzymes from microorganisms has drawn a great deal of attention from various researchers. Pectinases are one of the upcoming enzymes in food processing industries and they hydrolyze pectin substances. Pectinases production could be induced by agricultural wastes containing pectin such as, sugar beet pulp, apple pomace and citrus peel by various microorganisms. Sugar beet pulp (SBP) is by- product of sugar factory and especially rich in pectin. In this study, submerged fermentation was used for the production of pectinase by *Piriformospora indica* fungus with sugar beet pulp powder [1-3]. For further analysis the effect of supplementation of medium with glucose (0-10%) and ammonium sulfate (0.1-0.5 %) were evaluated. At the 6^{th} day of culture, the cell growth, growth yield, specific growth rate, spore yield, total protein content and pectinase activity were estimated. According to the results, maximum fungal biomass production, protein content and enzyme activity were determined at glucose 6% and ammonium sulfate 0.4%. Moreover, the highest pectinase activity at glucose 6% and ammonium sulfate 0.4% was calculated 4.82 U/ml and 4.29 U/ml respectively. All together, SBP could be a good inducer for pectinase production by *P. indica* and further investigation is running.

Keywords: submerged fermentation,sugar beet pulp**;** *Piriformospora indica***;** pectinase; pectin

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1047CBC

The effect of fluorineon conformation stability of organic compounds

Ashraf Moradi[*a], *Fatemeh Pirani*[b], *Ali Kakeshpour*[c], *Somayeh Ghorbani*[d], *Ameneh Ghoreishvandi*[e]

Department of Chemistry, University of Zabol, Zabol, Iran
[c]*Department of Chemistry, University of Tehtan, Tehtan, Iran*
** Corresponding author: Tel: +98 541 2449807, E-mail: ash.moradi@yahoo.com*

Abstract

Nowadays, with development of biochemistry knowledge and Access to more detailed information biological interactions all of comments are toward study on this field, Despite the scarcity of natural fluorinated compounds, they have shown many potent biological activitiesand they can make a high communicate between Many of the compounds and biological structures. Thus, fluorination of already known drugs has become an essential tool in drug discovery [1].Currently, twenty percent of commercialized drugs contain fluorine [2]. Therefore, Deeper understanding of structural consequences of fluorination in drugs is of importance. Several strategies used in the rational design and synthesis of fluorinated compounds as potential therapeutic agents are reviewed. In this research, we study the effect of fluorine in conformational stability of model compounds to understand its electronic effects in terms of dipole interaction, Hyperconjugation, and hydrogen bonding. Study on these effects can terminate to Precise control and discuss on all of interactions molecule-molecule and internal-reaction in Various sectors of biochemistry.

Keyword: Fluorine chemistry; Drugs; Quantum chemistry; Conformational analysis.

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1048CBC

Design of new Alzheimer's drugs using human's complex of Aricept by cheminformatics analysis of molecular dynamics simulation

Fereshteh Shiri[a], Somayeh Pirhadi[b], Jahan B Ghasemi[c], Fatemeh Pirani[a]*

[a]*Department of Chemistry, University ofZabol, Zabol, Iran*
[b]*Young Researchers and Elites Club, Science and Research Branch, Islamic Azad University, Tehran, Iran*
[c]*Faculty of Chemistry, University of Tehran, Tehran, Iran*
Fereshteh.shiri@uoz.ac.ir

Abstract

Alzheimer's Disease (AD) is a type of dementia that causes problems with memory, thinking and behavior. Symptoms usually develop slowly and get worse over time, becoming severe enough to interfere with daily tasks. The development of acetylcholinesterase (AChe) inhibitor drugs has followed the finding that cholinergic pathways in the cerebral cortex and basal forebrain are compromised in AD. The X-ray crystal structure of human AChe in complex with Aricept (a potent and specific inhibitor ofAChe) has been recently released in protein data bank with the PDB code of 4EY7. To regard the flexibility of the enzyme in the process of rational drug design, a 100 ns molecular dynamics simulation of this complex has been carried out using the AMBER simulation program. The trajectory then was clustered to output 10 representative structures of the complex to account the flexibility of the protein in the process of drug design. The resulted structures were used as the input to the Pharmit server to screen the NCI library by constructing structure based pharmacophre models. Shape filters for protein and ligand and also Lipinski rule of five were used to filter the output of virtual screening from pharmacophore models. The pharmacokinetic studies of the retrieved hits from the screening were carried out by regarding different critical factors like solubility, and blood brain barrier. The acceptable compounds were then docked into the protein structure using sminato investigate the important interactions and five ligands showing appropriate interactions with the target were subjected to experimental studies.

Keyword: Acetylcholinesterase; Pharmacophore; Molecular dynamics simulation; Aricept; Pharmit

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1049CBC

Inhibitory effect of boldine on TERT: In Silico study

Fatemeh Masoumi, Sakine Kazemi Noureini, Mitra Kheirabadi**

Department Basic Science,HakimSabzevari University, Sabzevar, Iran
** Corresponding author: Tel: +98 54 44013010, E-mail: kheirabadi@hsu.ac.ir, kazemibio@gmail.com*

Abstract

Telomerase has an essential RNA and a protein reverse transcriptase subunit. The telomerase maintains telomere length stability in almost all cancer cells that cause to their immortality. Human telomeres(hTERT) contain long stretches of the repetitive sequence TTAGGG which are bound by specific proteins. Cancer cells stabilize telomer length by adding TTAGGG repeats onto the telomers. Telomerase activity has been found in almost all human tumors but not in adjacent normal cells. Natural alkaloids potentially are able to inhibit telomerase. Boldine is a natural alkaloid that is found in abundance in the leaves and bark of *Peumusboldus*. It is an aporphine alkaloid showed an interesting dose and time dependent anti-proliferative effect in several cancer cell lines. In this study, binding mode of boldine-telomerase and their interactions was investigated in detail using in silico methods. There is no experimentally 3D-structure of human telomerase (hTERT). A 3D-strucutre model for human telomerase was constructed. Autodock software was used to study inhibitory binding mode telomerase-Boldine. Based on results, boldine inhibit telomerase with Ki: ????and binding energy: ???. Amino acids of active site of telomerasecontaines of 343 Asp, 344 Asp, 251 Asp, lys372, Asn369, Ala 255. Boldine sit on telomerase active site and formed three H-bonds to lys372and Asn369 andAla 255 in telomerase active site.

Keyword: Telomerase, Boldine, Autodock , Crystal structure

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1050CBC

The effects of removal of manganese ions on the structure of the enzyme chloroperoxidase

Maryam Ghorbani[*a], *Mohammad Reza Housaindokht*[b], *Mohammad Reza Bozorgmehr*[c]

[a] *Department of Chemistry, Ferdowsi University of Mashhad, International Campus, Mashhad, Iran*
[b] *Department of Chemistry, Faculty of Sciences, Ferdowsi University of Mashhad, Mashhad, Iran*
[c]*Department of Chemistry, Faculty of Sciences, Mashhad Branch, Islamic Azad University, Mashhad, Iran*
** Corresponding author: Tel:+98 9151888902, E-mail: ghorbani.chem2010@gmail.com*

Abstract

Chloroperoxidase (CPO) is the most versatile of the knownheme enzymes [1]. This enzyme has a manganese ions in its structure [2]. We have carried out molecular dynamics (MD) simulation studies on the removal of manganese(Mn^{2+}) and studied its effect on the CPO. In this study protein secondary structure, root-mean-square deviation of atomic positions(RMSD), root mean square fluctuation (RMSF) and contact map were studied before and after the removal of manganese and corresponding graphs were drawn. The study of secondary structure of protein showed that with manganese removal, three of amino acids were rearranged in 3.1 Helix, and the percent of alpha helix, extended and isolated bridge in the protein secondary structure are decreased, while the percent of coil and turn are increased. The results of the RMSD diagram showed that the presence of manganese does not have a large impact on the on the stability of the tertiary structure of the CPO. The results of the RMSF diagram showed that the removal of manganese very effective on amino acid binding site and C-terminal.

Keyword: Chloroperoxidase; molecular dynamics simulation; manganese; protein secondary structure; contact map.

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1051CBC

Discovery of new chemical scaffolds for none-nucleoside reverse transcriptase inhibitors using chemoinformatic methods

Azita Rahmani [a], *Somayeh Pirhadi*[b], *Fereshteh Shiri**[a], *Fatemeh Pirani*[a]

[a]*Department of Chemistry, University ofZabol, Zabol, Iran*
[b]*Young Researchers and Elites Club, Science and Research Branch, Islamic Azad University, Tehran, Iran*
Fereshteh.shiri@uoz.ac.ir

Abstract

Non-nucleoside reverse transcriptase inhibitors (NNRTIs) have gained a definitive place due to their uniqueantiviral potency, high specificity and low toxicity in antiretroviralcombination therapies used to treat HIV. To design more specific HIV-1 inhibitors, 218 Non-nucleoside reverse transcriptase inhibitorswith their EC_{50} values were collected from different literature sources. Then, different types of fingerprint descriptors were calculated by PaDel descriptor and afterwards enhanced replacement method (ERM) was used as the variable selection approach to choose more relevant variables. Based on selected descriptors, a classification SVM model was constructed to categorize compounds into two groups of active and inactive.The most potent inhibitor available in the set was used to carry out a similarity search in PubChem server to retrieve compounds similar to the hit compound. The screened compounds with above 85 percent of similarity to the hit compound were used as the input to the SVM model. Likewise, the most active compound in the set has been used as the input to the Pharmit web server to screen the Molport library by constructing structure based pharmacophre models. Shape filters for protein and ligand and also Lipinski rule of five were used to filter the output of virtual screening from resulted pharmacophore models. 53 compounds from the structure based pharmacophore search and the active compounds form the SVM model were docked into the protein with the PDB code of 3DLG to investigate the important molecular interactions and five ligands showing appropriate interactions with the target were subjected to experimental studies.

Keyword: Similarity search; Pharmacophore modeling; SVM; Docking

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High level expression, refolding and characterization of diphtheria fusion toxin: $DAB_{389}IL\text{-}2$

Azadeh Azizi, Shiva Bayat, Mehdi Zeinoddini, Mehrnosh Ebrahimi, Majideh Fasihi*

Department of Bioscience and Biotechnology, Malek Ashtar University of Technology
** Corresponding author: zeinoddini@modares.ac.ir*

Abstract

$DAB_{389}IL\text{-}2$ with the trade name" denileukin diftitox and ontak" is the first recombinant immunotoxin that produced using genetic engineering [1]. In this commercial fusion protein binding domain of diphtheria toxin (DT) replaced by the amino acid sequence of human interleukin-2 (IL-2) [2,3]. The aim of this work is high level expression, refolding and characterization of this diphtheria fusion toxin. For this, expressed $DAB_{389}IL\text{-}2$ was refolded and purified in thepresence of two anti-aggregators, sorbitol and L-arginine. Refolding of protein have been investigated using native-PAGE, fluorescence and circular dichroism (CD) spectroscopy. Finally the proper functioning was determined by nuclease activity assay.The results revealed that the fluorescence intensity of protein decreased in the presence of both anti-aggregators. Far-UV CD spectra indicated that the protein has some conformational alterations upon interacting with these anti-aggregators in comparison with the unfolded structure. In fact, in the presence of two refolding buffer the intensity of far-UV CD signals have been increased at the regions of 208 and 222 nm. Moreover, native-gel electrophoresis data demonstrated that the refolded configuration of protein has been formed in the both refolding buffers. Finally we have found that the refolded proteins have proper activity as indicated by nuclease activity. Therefore, addition of sorbitol and L-arginine perhaps increase the viscosity and surface tension of solvent which leads to increase the strength of hydrogen bonds and then stabilizes the refolded structure.Results of this research could give more insights about the refolding mechanism of immunotoxin in the presence of anti-aggregators [4,5].

Keyword: Immunotoxin, Refolding, Circular dichroism (CD), Anti-aggregators

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1053CBC

Porphyrins: Synthesis, Geometry, Stability, H-H Intramolecular coupling constant, Aromaticity, and Intramolecular hydrogen bonding

Ali Reza Oveisi[*a], *Saba Daliran*[b], *Poya Karimi*[a], *and Hojat Samareh Delarami*[a]

[a]*Department of Chemistry, University of Zabol, Zabol, Iran*
[b]*Faculty of Chemistry, Bu-Ali Sina university, Hamedan, Iran*
** Corresponding author: Tel:+98 915 542 8132, E-mail: alir.oveisi@gmail.com*

Abstract

Porphyrins are relevant examples of macrocycles compounds, also known as annulenes with 18-π electron systems [1], that have obtained significant attention because of their vital role in biological processes, such as photosynthesis (chlorophyll and bacteriochlorophyll), oxygen transportation, and oxygen activation (heme) [2-4].*meso*-Substituted trans-porphyrinderivativies are crucialbuilding blocks in porphyrin-based biomimetic systemsand molecular materials and can be used forthe construction of well-defined porphyrin-based architectures.As part of an ongoing project, *meso*-substituted porphyrins bearing specific patterns of substituents were synthesized and characterized by ^{1}H NMR, ^{13}C NMR, ^{1}H-^{1}H COSY, and MALDI-ToF mass spectra. Also, a modification of the Adler method for THPP (*meso*-tetrakis(4-hydroxyphenyl)porphyrin) and a purification method for TAPP (*meso*-tetrakis(4-aminophenyl) porphyrin) were reported. Furthermore, theoretical calculationssuch as H-H Intramolecular coupling constant, Intramolecular hydrogen bonding, and aromaticitywere performed to determine effects of various factors on stability of the porphyrins. Results of computed total spin-spin coupling constants and corresponding components were considered to connect stability of porphyrin derivatives to the obtained data.

Keyword: Porphyrin;Density functional calculations; Stability;H-H Intramolecular coupling constant; Aromaticity.

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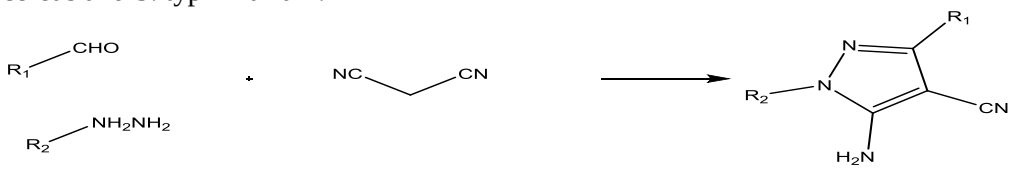
Synthesis of new pyrazole derivatives in glycerol-potassium carbonate as eutectic solventandstudy of their antibacterial effects

Zahra Motraqi[*] *, H. Beyzaei*

Department of chemistry, Faculty of scince, University of Zabol, Zabol, Iran
[*]*Corresponding auther e-mail: motraghizahra@yahoo.com*

Abstract

One of the most important and most widely ring systems, heterocyclic compounds that are the foundation of manyChemical form of the derivatives of pyrazole according to many applications in agriculture, pharmacy and color are particularly important.pharmacological properties such as antitumor, antimicrobial, anti-inflammatory [1], antiviral , antifungal, analgesic, and anti-hyperglycemic activity. The pyrazole motif makes up the core structure of numerous biologically active compounds. One area that has been intensely studied is their anticancer activity [2].In order to find better antitumor agents, a large number of pyrazole derivatives were synthesized and examined over the past several years [3]. So the use of this pharmacophore is still very powerful.An increase in regulatory restrictions on the use, manufacture and disposal of organic solvents has motivated the development of non-hazardous options for the development of green chemical processes. In this study, novel derivatives of 5-amino-1-(2,4-dinitriphenyl)-1H-pyrazole-4-carbonitrile 3-substituted a multicomponent reaction solvent one-pot eutectic glycerol-potassium carbonate was synthesized.The main feature of this method to carry out the reaction at temperatures near room temperature, high efficiency, being an ecological process.Finallyin this research project, we studied antibacterial effects of some newly synthesized pyrazole against B. cereus and S. typhimurium.



R_2: $C_6H_3N_2O_4$

Keyword: Eutectic Solvents, Green Chemist, Pyrazole Derivatives

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1055CBC

An *in-silico* expression assay of the MAGE family in malignances

Zohreh Sargazi[1], Aliakbar Haddad-Mashadrizeh[1, 2]*, Mansour Mashreghi[1]

[1]Cell and Molecular Biotechnology Research Group, Institute of Biotechnology, Ferdowsi University of Mashhad, Mashhad, Iran
[2]Department of Biology, Faculty of Science, Ferdowsi University of Mashhad, Mashhad, Iran
*Correspondence to: Aliakbar Haddad-Mashadrizeh, Cell and Molecular Biotechnology Research Group, Institute of Biotechnology, Ferdowsi University of Mashhad, Mashhad, Iran. E-mail: a.haddad@um.ac.ir, Fax: 00985118762227

Abstract

Structural analysis and expression evaluation of the cell surface specific antigens of malignances could be providing new molecular approaches for diagnosis and target therapy of cancers. In this regard, MAGE family with 25 known members and specific expression on the surface of cancerous cells provided a promising perspective for these aims. Bearing in mind, an *in-silico* expression of these antigens on the cell surface of 20 type of common cancerous and normal tissues were assessment and equilibrated via version 21 of SPSS. On the other hand, topology structures of the antigens were modeled on the surface of the cancerous cells. Moreover, the binding affinity of the selected antigen with corresponding ligands was assessment via molecular docking process. The results of this study led to revealed the different expression of these antigens on the surface of cancers. However, the MAGE-A4 showed the highest expression in the head and neck cancer. Moreover, topology features of this antigen leading to provided several oligopeptides with expression capacity on the surface of cancerous cells with connected to HLA family.In general, the results of this study in addition to detection the expression rate of MAGE family antigens on the surface of cancerous and non-cancerous cells, led to presented the *in-silico* modeling expression of MAGE-A4 antigen on the surface of cancerous cells for the first time.

Keywords: Cancer, Antigen, MAGE, Docking, Modeling

1056CBC

Detection of ascorbic acid in biological samples by a new modified glassy carbon electrode

S. Saber[1], F. Hosseini Narouei[2], M. Noroozifar [2], M. Khorasani-Motlagh[2],*

[1] Department of Agriculture, University of Zabol, Zabol, Iran
[2] Department of chemistry, University of Zabol, Zabol, Iran
[3]Department of Chemistry, University of Sistan and Baluchestan, Zahedan, Iran.
[*]Corresponding author: Tel: +98 54 31232100, Email: fnarui@gmail.com

Abstract

The present work describes the construction of a new modified electrode by casting the appropriate mixture of a metallocene, which has been introduced in the experimental part, as a mediator at the surface of glassy carbon (GC) electrode. The proposed modified GC electrode was used for the determination of ascorbic acid (AA) in phosphate buffer (PB) solution (pH = 4.0). When compared to bare GC electrode, the modified electrode not only shifted the oxidation potential of AA towards less positive potential but also enhanced its oxidation peak current. Further, the oxidation of AA was highly stable at modified electrode. The optimum analytical conditions were sought. The oxidation peak of AA increases linearly while increasing its concentration with a correlation coefficient of 0.9993 and a detection limit (3σ) was found to be quite desirable. The present modified electrode was also successfully used for the determination of AA in the presence of common interferences such as starch, glucose, citric acid Na^{+}, K^{+}, $Mg^{2+}$and Ca^{2+}. The proposed modified electrode was successfully demonstrated towards the determination of AA in pharmaceutical samples. It should be noted that procedure for preparation of this modified electrode is simple, inexpensive and rapid.

Keywords: Ascorbic acid; sensor; Chloromercuriferrocene; Nafion; electro catalytic; Glassy carbon electrode.

1057CBC

Inhibitory Influence of 3-β-hydroxybutyrate on Calf Thymus DNA Glycation by Glucose

Mahdi Miri[*a], *Mousa Bohlooli*[a], *Mostafa Khajeh*[b] *and Neda Poormolaie*[b]

[a]*Department of Biology, University of Zabol, Zabol, Iran*
[b]*Department of Chemistry, University of Zabol, Zabol, Iran*
** Corresponding author: Tel:+98 5632434012, E-mail:* mahdi.miri17@yahoo.com

Abstract

Reactions of reducing sugars with free amino groups of proteins can produce advanced glycation end products (AGEs). DNA can react with sugars in a similar way as proteins [1]. AGEs have a significant role in the pathophysiology of aging and diabetic late complications because of their genotoxic effect[2]. The 3-β-hydroxybutyrate (3BHB), a ketone body which is produced by the liver, can be detected in increased concentrations in individuals post fasting and prolonged exercises and in diabetic (type I) patients[3]. Although several studies have been done on protein glycation, but fewer studies were carried outregarding DNA glycation. In this study,to check the inhibitory effect of 3BHB on DNA-AGEs formation, Calf Thymus DNA with glucose in presence and absence 3BHB was incubated on the physiological-likeconditions for 4 weeks.After dialysis of samples,to monitor the non-enzymatic glycation of DNA nucleosides and to characterize the formation of nucleoside AGEs, the biophysical techniques such as circular dichroism (CD), agarose gel electrophoresis, UV–vis and fluorescence spectroscopy were used.The results ofCDshowed,native DNA had a negative peak of -6.1 mdeg at 245 nm, and a positive peak of +16.4 mdeg at 275 nm. DNA modified with glucose alone and DNA modified with glucose+3BHB showed -3.4 and -4.5 mdeg for negative peaks at 245 nm, and 10.9 and 13.2 for positive peaks at 275 nm, respectively.Thus, 3BHB with decrease AGEs formations can decrease the structure changes of DNA and can prevent from breaking of DNA in diabetic conditions.

Keywords: DNA,Glycation, 3-β-hydroxybutyrate, Ketone body

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1058CBC

Molecular docking study on the interaction of DNA with some natural anthraquinone derivatives

Hojat Samareh Delarami[*a], *Ali Ebrahimi*[b], *Sedigheh Mirjahanshahi*

[a]*Department of Chemistry, University of Zabol, Zabol, Iran*
[b] *Department of Chemistry, University of Sistan&Baluchestan, Zahedan, Iran*
** Corresponding author: Tel:+98 541 2449807, E-mail:hsd102012@gmail.com*

Abstract

Investigation of the drug–DNA interaction has a key role in pharmacology because DNA is often the prime target for majority of anticancer and antibiotic drugs. Anthraquinones derivatives are known to have several biological activities including antitumor properties. In this study, some natural anthraquinone derivatives were analyzed for its possible interaction with DNA targets through molecular docking and quantum mechanical calculations. The effects of noncovalent interactions on the intercalation of these compounds have also been investigated using the geometrical parameters data, AIM and NCI index analyses.Based on molecular docking and QM results, it can be concluded that the π–π interactions between the ligands aromatic ring(s) and the aromatic ring(s) of the DNA nucleobases are the major contributor to the potency of inhibition toward DNA targets. This study assists us to gain a more detailed consideration of the noncovalent interactions within the active site, which can improve our insight for the rational design of more powerful and selective anticancer agents.

Keyword: Anthraquinones, Molecular Docking, DNA, intercalation, DFT.

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1059CBC

Kinetic aspects of tetrahydrobenzo[b]pyran formation in the presence ofCaffeine as a green catalyst: a mechanistic investigation

Younes Ghalandarzehi[*a], Sayyed Mostafa Habibi-Khorassani[a],Halime Kord Tamandani[a],Mehdi Shahraki[a], Farideh Hosseani – Naruoei[b]*

[a]*Department of Chemistry, Faculty of Science, University of Sistan and Baluchestan, Zahedan, Iran*
[b]*Department of Chemistry, Faculty of Science, University of Zabol, Zabol, Iran*
**Corresponding author: Tel: +98 541 2446565; fax: +98 541 2446565; E-mail: younes.ghalandarzehi50@gmail.com*

Abstract

In this study for the first time, kinetics and mechanism of reaction between 4-methoxybenzaldehyde 1, malononitrile 2, and dimedone 3 in the presence of caffeine as a catalystusing conventional UV/vis spectrophotometry has been reported. Based on the data which has been obtained from experimental study, the overall order of the reaction is two. The second-order rate constant dependency on the temperature was in agreement with the Arrhenius and Eyring equations.The kinetic and thermodynamic parameters of the reaction have been calculated. Furthermore, useful information was obtained from studies of the effect of solvent and concentration of reactants on the reaction rate. The results showed that the second step of the reaction mechanism is a rate-determining step (*RDS*). The proposed mechanism was also confirmed according to the obtained results and the steady state approximation. In the kinetics study, activation energy and other parameters (Ea, $\Delta H^{\ddagger}$, $\Delta S^{\ddagger}$ and $\Delta G^{\ddagger}$) were determined.

Keywords: Kinetics;4-methoxybenzaldehyde; caffeine; dimedone;UV/vis spectrophotometry

1060CBC

UV-Vis Spectrophotometry as a Useful Technique to Study the Heme-containing Proteins: Structural and Functional Characteristics ofGamma Irradiated Hemoglobin

Javad Rafiei[*a, b], *Aliakbar Moosavi-Movahedi*[a], *Kamal Yavari*[b]

[a]*Institute of Biochemistry and Biophysics, University of Tehran, Tehran, Iran*
[b]*Nuclear Material and Fuel School, Nuclear Science and Technology Research Institute (NSTRI), Tehran, Iran*
** Corresponding author: Tel:+98 2161113381, E-mail: jrafiei@ut.ac.ir*

Abstract

UV-Visible spectrophotometry is a general and useful analytical instrument which is found in every chemical and biological laboratory. This simple and low cost apparatus play a key role in quantitative analysis, qualification and kinetic study of biological processes. One of the most important classes of biological molecules is the heme containing proteins. Hemeproteins have diverse biological functions including oxygen transport, catalysis, electron transfer and biological defense. All these diverse abilities are originated from approximately the same prosthetic heme group.The heme group shows some characteristic bands at UV-Vis spectra of haemproteins. In this study,the UV-Vis spectroscopy was applied to study the structural changeof hemoglobin affected by gamma irradiation. Some functional behaviors such as aggregation and oxygen affinity of hemoglobin were studied using UV-Vis spectrophotometry. The UV-Vis spectra of hemoglobin could be categorized in some structural and functional characteristic regions. The globin band at 280nm is completely structural while the Q band at 500-600 nm is exactly a functional peak, and the soret band at 370-450 nm shows both behaviors.The irradiation dose up to 190 Gy changes just functional part but upper doses affect the structural globin part too.Position of the bands, relative intensity of the structural and functional peaks to each other and the presence or absence of some peaks could predict some structural and functional changes in other hemoproteins.

Keyword: Hemoprotein; UV-Vis Spectroscopy; Gamma Radiation; Hemoglobin; Aggregation.

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1061CBC

Protective effect of albumin on the glycation of hemoglobin

Mohsen Falahat Pisheh[1],*Sajjad Shojei*[1], *Mehran Habibi-Rezaei*[1,*]

[1]*School of Biology, College of Science, University of Tehran,Tehran, Iran*
** Corresponding author: Tel: +98-21-61113214, Fax:+98-21-66971941, email: mhabibi@ut.ac.ir*

Abstract

Glycated proteins such as hemoglobin and albumin are very important for diagnosing insulin resistance related conditions(IRRC; e.g. type 2 diabetes mellitus, cardiovascular diseases, nephropathy and retinopathy). The albumin glycation assay indicates the average level of blood glucose in past 2-3 weeks[1]; albumin also protects other proteins against glycation. A special kind of glycated hemoglobin called HbA1c was discovered in the 60s[2]. HbA1c indicates average blood sugar levels in past 3-4 months.Currently the HbA1c assay is used as a gold standard for confirming IRRC[3]. To date the protective effect of albumin onhemoglobin has not been investigated. We first extracted hemoglobin from human whole blood. Then hemoglobin wasco-incubated with fructoseat different concentrations of albumin. Hemoglobin concentration was adjusted close to the physiological level (15 µL) while fructose concentration wasthat of diabetic state (30 mM). Albumin was incubated with different concentrations: Low, normal and high related to physiological state(0.5, 0.75 and 1.25 mM respectively).The first control was only hemoglobin and the second control was hemoglobin with fructose. Incubation period was 21 days. Samples were taken every 5 days with 3 repetitions and the absorption of hemoglobin from 200 to 650 nM was measured.The hemoglobin absorption spectrum has a peak from 350 to 450 nm.Glycation reduces total absorption within this range. We found that albumin prevented absorption drop within hemoglobin absorption curve.These results suggest that albumin has a protective effect against glycation of the hemoglobin.

Keywords: HbA1c, Glycation, Hemoglobin, Albumin, Diabetes, Insulin resistance

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1062CBC

Fast detection of miRNA-155 by an aptasensor based on gold nanoparticles and $MnCl_2$

Fatemeh Hakimian[1], *Hedayatollah Ghourchian*[1*], *Azam Sadat Hashemi*[2]

[1]*Institute of Biochemistry and Biophysics, University of Tehran, Tehran, Iran*
[2]*Hematology, Oncology & Genetics Research Center, Shahid Sadoughi University of Medical Sciences, Yazd, Iran*

Abstract

MicroRNAs (miRNAs) are a class of non-coding RNA molecules (containing about 22 nucleotides) found in plants, animals and some viruses, that functions in RNA silencing and post-transcriptional regulation of gene expression. miRNAs represent one of the novel strategies for cancer screening. At present, in studies that focused on the association between miRNAs and tumors, abnormal expression of miRNA-155 in patients with breast cancer has have attracted considerable attentions. As an oncogene, high expression of miR-155 was considered as a breast cancer risk factor. Experiments was carried out using ELISA Plate Reader and nanoparticles size distributions were measured with dynamic light scattering. Here, we introduce an optical aptasensor based on gold nanoparticles and $MnCl_2$ salt. In this simple method, detection of miRNA-155 was done with increasing of $MnCl_2$ salt to a solution containing gold nanoparticles that conjugated with thiolated probe. With this method even 6 pM concentration of miRNA-155 were detected. For test selectivity of the system, response of biosensor against three-base-pair mismatch, also investigated. Results exhibited high selectivity for miRNA-155 over three-base-pair mismatch.

Keywords: Gold nanoparticle- $MnCl_2$ salt-miRNA 155- aptasensor.

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1063CBC

Studies on secondary structures of Horseradish peroxidase immobilized on reduced graphene oxide nanoparticle

Monireh Besharati Vineh [a,*], *Ali* Akbar Saboury [b], Leila Ma'mani [c] and *Ali Morad Rashidi* [d]

[a] *Department of Biology, Science and Research Branch, Islamic Azad University, Tehran, Iran*
[b] *Institute of Biochemistry and Biophysics, University of Tehran, Tehran, Iran*
[c] *Department of Nanotechnology, Agricultural Biotechnology Research Institute of Iran (ABRII), Agricultural Research, Education and Extension Organization (AREEO), Karaj, Iran*
[d] *Nanotechnology Research Center, Research Institute of Petroleum Industry (RIPI), West Blvd. of Azadi Sports Complex, Tehran, P.O. Box 14665-1998, Iran*
** Corresponding author: Tel: +98 21 6695698. E-mail: m.besharati@srbiau.ac.ir*

Abstract

Horseradish peroxidase (HRP) (EC 1.11.1.7) is an oxidoreductase enzyme that oxidases a variety of organic and inorganic compounds**.** HRP is normally applied to catalyze the oxidation of substrates such as phenols and aromatic amines by H_2O_2. The free enzyme is not stable under different normal conditions, so immobilization of the enzyme may be applied to keep the stability and reduce the cost of their applications significantly. During the past decades, nanoparticles are developed to support for enzyme immobilization**.** In this study, we attempt to immobilize HRP on reduced graphene oxide (RGO) functionalized nanoparticles to be used in removing aromatic pollutants from wastewater. RGO can interact to HRP primarily through electrostatic interactions and hydrogen bonding because this nanoparticle contains greater amounts of O-containing functional groups. The secondary structure of the free and immobilized enzymes was also evaluated by using the circular dichroism (CD) spectrometer. The far-UV region was scanned between 195 and 250 nm. The relative contents of secondary structures, including α-helix, β-sheet, β-turn and random coil were calculated. Results obtained from CD spectra demonstrated that physical adsorption during the process of enzyme immobilization leads to a decrease in α-helical structure and an increase in β-sheet, β-turn and random coil structural amounts. The experimental observations also indicated that both activity and stability of immobilized enzyme is promoted. In conclusion, it can be implied that RGO has a good potential to improve the preservation of HRP activity.

Keyword: Horseradish peroxidase, Physical adsorption, Reduced graphene oxide, CD spectroscopy analysis.

1064CBC

Computational Design of some Piperine Derivatives as Novel Survivin Inhibitors

Elham Sattarinezhad, Najmeh Fani and Abdol-Khalegh Bordbar

Address: Department of Chemistry, University of Isfahan, Isfahan, 81746-73441, Iran.
Email:bordbar@chem.ui.ac.ir and akbordbar@gmail.com

Abstract

In the first part of this study, two of the most potent docking programs, AutoDock and AutoDock Vina, have been selected for virtual screening of a library of 2497 commercially available drug like derivatives of Piperine. Since AutoDock Vina is faster than AutoDock, first of all, the selected compounds were docked into the binding site of Survivin by using AutoDock Vina program. Based on the predicted binding energies, the compounds were ranked and the top 100 compounds were selected for more screening using AutoDock program. Considering the obtained binding energies, the top two highest ranked compounds, as well as Piperine, were selected and subjected to a 10 ns molecular dynamics simulation for further validate the proposed binding modes and interactions. In the last part of this study, the binding free energies were calculated using the MMPBSA and MMGBSA methods. Moreover normal-mode analyses were carried out using the *nabnmode* module of AMBER in order to estimate the conformational entropy (TΔS) to binding free energies. In addition to MMBP-GBSA methods, by using alanine scanning, ten residues in the active site of Survivin were systematically substituted with alanine and subsequently assayed to evaluate the contribution of each residue to the total binding free energy in order to determine the critical and noncritical residues in the active site.

Key words: Survivin, Piperine, Anticancer Drug, Molecular Docking, Virtual Screening, Molecular Dynamics Simulation

1065CBC

Geraphene oxide (GO) modulates the activity of Thermomyceslanuginosus lipase (TLL)

*Omid Kalji and Yahya Sefidbakht**

Protein Research Center, Shahid Beheshti University, G.C.Velenjak, Tehran, Iran
** Corresponding author:y_sefidbakht@sbu.ac.ir, Tel 021- 29905021*

Abstract

Enzymes are biocatalysts with high-performance under mild conditions.Lipases (triacylglycerol hydrolase, E.C. 3.1.1.3) are the enzymesthat catalyze hydrolysis of triacylglycerides into free fatty acids and glycerol at the lipid–water interface. lipases are frequently used in various industrial process like detergent formulations, oleochemical industry[1], biofuels, food and dairy, agro-chemical, paper manufacturing, nutrition, cosmetics and pharmaceuticals. Lipases are well known industrial biocatalyst due to their ability to carry out multitude of bioconversion reactions[2]. Recently, immobilization of enzymes has studied to improve enzymes economic efficiency such as storage capacitance,enhance activity and stability under different conditions,and so on. Geraphene oxide has shown promising application as support for heterogeneous catalysts[3][4]Graphene oxide (GO), possess large specific surface area, the abundant oxygen-containing surface functionalities, such as, epoxide, hydroxyl and carboxylic groups, and high water solubility. These features provides an ideal substrate for study enzyme immobilization. However, few studies about the interaction of biomacromolecules, such an enzymes, to GO have been reported to date.We demonstrated that the lipase from TLL adsorption immobilization on the GO sheets could take place readily without using any cross-linking reagents and additional surface modification. The catalytic properties of Go-Lipase nanocomposite shows its possible application and storage capability.

Keyword: Enzyme. Lipase. Gerapheneoxide. Immpbilization.

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1066CBC

Defining the architecture of KPC-2 carbapenemase

Hamidreza Afsharikho and Shozeb Haider

UCL School of Pharmacy, University College London, London, UK

Abstract

The rise of multi-drugresistanceinbacterial pathogensis one ofthe grandchallenges facing medical science. A main concern is the speed of development of KPC carbapenemases resistance, thus putting at risk the efficacy of the most recently approved inhibitors, including carbapenems and avibactam.New strategies to overcome resistance are urgentlyrequired, which will ultimately be facilitated by a deeper understanding of the mechanisms that regulate KPC carbapenemase function.Using enhancedsamplingcomputational methods together with site directed mutagenesis,we report the identification of “hydrophobic networks”, whose integrity has been found to be essential for KPC-2 resistance. Present throughout the structure, they are responsible for structural integrity and allosteric signalling and when disrupted lead to a complete loss of the KPC-2 mediated resistance phenotype, leading to the recovery of β-lactam sensitivity.

1067CBC

Consistency of fitting the DSC data to complete Lumry-Eyring and Two-state models

Mojtaba Amani

Department of Biochemistry, Faculty of Medicine, Ardabil university of Medical Sciences (ArUMS), Ardabil, Iran

Abstract

The consistency of the results of fitting the DSC data to complete Lumry-Eyring and Two-state models was assessed for cupper containing amine oxidase from *Euphorbia characias* (ELAO). Thermal denaturation of ELAO was reported to be irreversible two-state. Least square fitting of experimental and models were done using Solver function of Excel software. Results showed that fitting parameters for two models are in very good agreement, but two extra parameters are obtained in Lumry-Eyring model, T1/2 and □H. Lumry-Eyring model gives large difference between T1/2 and T* separating thermal effects of two steps. The low values of □H and T1/2 cause that the thermal effects of first step (Equilibrium) of lumry-Eyring model to be omitted. This means that in low temperatures, the unfolded and fold states are in fast equilibrium.

1068CBC

A hypothetical evolutionary relationship between the phylogeny position and the hydrophobic properties of fish's hemoglobin

Shohreh Ariaeenejad [1, 2], *Kaveh Kavousi* [3] *and Ali A. Moosavi-Movahedi* [1*]

[1] *Institute of Biochemistry and Biophysics, University of Tehran, Tehran, Iran*
[2] *Agricultural Biotechnology Research Institute of Iran (ABRII), Karaj, Iran*
[3] *Laboratory of Complex Biological systems and Bioinformatics (CBB), Institute of Biochemistry and Biophysics, University of Tehran, Tehran, Iran*

Abstract

Evolution involves a change over time in organisms including anatomical, biochemical or behavioral characteristics. The natural selection and genetic drift are known as two main causes of evolution. Fishes are diversified and complicated with a huge variety of adaptations. A common classification of fishes suggests that they can be divided into three different classes including Cyclostomata, Chondrichthyes, and Osteichthyes (bony fishes). In this study, globin proteins are investigated to elucidate structure-function relationships and illuminate the trend of evolution in globin proteins. The complete gene and protein sequences of all available fish α-globin sequences were analyzed to reveal their phylogenetic relationships and shed light on the speciation process. Estimating the divergence time of α-globin genes for different fish families can be done by building molecular evolutionary trees scaled to time based on the α-globin exons. The results support the hypothesis of concurrency between time of morphological speciation and α-globin divergence and this concurrency can be interpreted as a sign of struggling to acquire more fitness to changing environment. Investigation on the fish globins as well as the evolutionary studies and computational analysis of available globin proteins reveals that the hydrophobicity has a key role in the evolution process of fish hemoglobins. Our findings confirm the existence of a strong relationship between the evolutions of fish globin proteins with their hydrophobic properties. It has been shown that difference between the structural properties of Hbs is related to their adaptation with habitat environmental conditions such as depth, partial oxygen pressure, temperature and salinity.

Keywords: α-globin, hemoglobin, molecular phylogenetic, hydrophobicity.

1069CBC

Significance of Protein Aggregation via Different Oxidative Reagents

F. Taghavi*[1,2], M. Bohlooli[3], M. Habibi-Rezaei[4], A. A.Moosavi-Movahedi[1]

[1.] Institute of Biochemistry and Biophysics, University of Tehran, Tehran, Iran.
[2.] Faculty of Science, Tarbiat Modares University, Tehran, Iran.
[3.] School of Science, University of Zabol, Zabol, Iran.
[4.] Schools of Biology, University of Tehran, Tehran, Iran.

Abstract

Any changes in protein normal conformation and configuration can lead to toxic aggregation events and produce conformational diseases[1,2]. Regards to widespread usage of potassium sorbate(PS) and sodium benzoate(SB) in nowadays human life style and their possible risks, we studied the effect of them on human serum albumin structural changes and their interference with Maillard reaction in presence and absence of glucose during some incubation time. All of these studies were done via biophysical techniques including fluorescence and circular dichroism spectroscopy (CD), differential scanning calorimetry (DSC), AFM, surface tension, molecular docking and LIGPLOT studies. TNBSA assay showed that both of SB[3]and PS [4]had binding potential to HSA Lys residues through covalent bonds, triggered diabetes and formed glycotoxins especially PS. The docking and LIGPLOT studies revealed two different physical interaction sites between HSA–PS/SB.The DSC results demonstrated different HSA energetic domains and intermediate formation due to HSA incubation with PS or SB with or without glucose[3,4]. CD demonstrated the main differences in HSA secondary elements(helicity via SB or β-sheet via PS). The Th T and AFM resuls showed significant impact of PS on different amyloid fibril formation[4] with or without glucose than SB.The surface tension confirmed the destructive effect of PS on HSA structure than glucose. Also we see that some natural products (3-β- hydroxybutyrate[5] and ellagic acid[6])can inhibit the AGEs and fibril formation due to glucose and PS. This report shows a review on HSA aggregation via above oxidative reagents and outline how to inhibit the aggregation by antioxidants.

Keywords: Oxidative agents, Protein aggregation,glycation,hydrophobic area,abnormal intermediates.

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1070CBC

The effect of iron oxide nanoparticles on laccase function for biodegradation of anthracene

Elaheh Pourfakhraei[a], *Jalil Badraghi*[a]*, *Fatemeh Mamashli*[a]

[a]*Research Institute of Applied Sciences, ACECR, Shahid Beheshti University, Tehran, Iran*

Abstract

Laccase is one of the best enzymes for biodegradation of aromatic compounds. Anthracene is a poly aromatic hydrocarbon with high toxicity for environment. Degradation of anthracene has a high priority. A lot of Basidiomycetes can degrade anthracene with producing laccase and other ligninolytic enzymes. In this study laccase was isolated from a local wood decaying fungus. Effect of the enzyme was studied on biodegradation of anthracene in different temperatures and pH by gas chromatography analysis in presence and absence of iron oxide nanoparticles. The best temperature for biodegradation in presence of nanoparticles increased, but optimized pH didn't change. Biodegradation of anthracene efficiencies was obtained 73% in absence to 88% in presence of nanoparticles. Laccase has improved function by Iron oxide nanoparticles and this function remained more time. This study showed the application of laccase with iron oxide nanoparticles for improved anthracene pollutant control.

Keywords: Laccase, Biodegradation, Anthracene, Iron oxide nanoparticles.

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Single point mutation effects in the flexible area on the stability of luciferase

Mahdie Rahban [a*], *Najmeh Salehi* [a], *Mohammad Hossein Karimi- Jafari* [a], *Ali Akbar Saboury* [a], *Saman Hosseinkhani* [b]

[a] *Institute of Biochemistry and Biophysics, University of Tehran, Tehran, Iran*
[b] *Department of Biochemistry, Faculty of Biological Sciences, Tarbiat Modares University, Tehran, Iran*
** Corresponding author: Tel: +98 2161113377, E-mail: mrohban@ut.ac.ir*

Abstract

Luciferase, bioluminescence enzyme, is one of the most useful enzymes for various applications in fields of biotechnology and molecular biology. Enhancing of thermostability of luciferase is required for these applications. Studies on hyperthermophile proteins have been shown that increasing thermal stability of hyperthermophile proteins is related to their enhancing of the conformational rigidity. In the present study, molecular dynamics simulation was carried out to assess the molecular stability and flexibility profile of the luciferase structure. Firefly luciferase is a protein with a large N-terminal and a small C-terminal domain. Molecular dynamics simulation at two temperatures was used to investigate the common fluctuation sites in *p.pyralis* luciferase, which are considered to be thermally weak points. Two mutations (H489K and H489M) in the most flexible region of firefly luciferase were designed. Thermostability analysis showed that H489M mutation doesn't have any significant effect but H489K slightly stabilizes the protein slightly. The optimum temperature for activity of H489K was increased. Intrinsic and ANS fluorescence studies also demonstrated that little structural changes for these two mutate proteins were occurred. Therefore, this study shows that replacing the histidine amino acid by lysine amino acid within flexible area will increase the thermalstability while the enzyme function remains active.

Keyword: Luciferase, Thermal stability, Molecular Dynamics simulation, Fluorescence

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Evaluation of Semi-Empirical Methods for pi-conjugation Energy Profiles for proteins

Ali Kakeshpour[*a], *Fatemeh Pirani*[b]

[a]*Department of Chemistry, University of Tehtan, Tehtan, Iran*
[b] *Department of Chemistry, University of University of Zabol, Zabol, Iran*
** Corresponding author: E-mail: alikakeshpour@yahoo.com*

Abstract

This century has been an adventure for biochemists to understand protein folding and biomolecular interactions using NMR and X-ray spectroscopy methods.[1,2] Quantum chemical methods, as a compliment to experiment, offer a deeper insight into understanding structural and energetic features interaction and folding phenomenon.[3] The large size of biomolecules, however, limits the applicability of benchmark methods used in small molecule systems. Semi-empirical methods, which use Hartree-Fock formalism with approximations driven from experimental data, are one solution to this problem by decreasing the cost of calculations substantially. In this research and our studies, we assess the ability of semi-empirical[4] methods in predicting the energy profile of pi-conjugated systems and their derivatives. These interactions are important since they determine secondary, tertiary and quaternary structures of proteins by determining the amide geometry, i.e. the out-of-plane twist. Based on the research we can study these interactions by computational chemistry which leads to Careful examination interactions.

Keyword: Pi-Conjugation; Quantum Chemistry; Semi-empirical.

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