

*Shri Datta Prasadik Shikshan Prasarak Mandal's*  
**Late Rajkamalji Bharti Arts, Commerce and Smt. Sushilabai R.  
Bharti Science College Arni, District-Yavatmal**



## **One-Day National Conference**



**on**

**“Exploring Innovative Research in Humanities,  
Commerce and Science for Sustainable Development  
(EIRHCSSD-2025)”**

**Monday, 10/03/2025**

**Conference Report**

**2024-25**

## **About Institute:**

Late Rajkamalji Bharti the founder president of Shri Datta Prasadik Shikshan Prasarak Mandal, Ami established Shri Mahant Datram Bharti Arts and Commerce College in 1984, to provide the higher education to the poor and needy students of the rural area. Today, the wards of farmers and labourers in this area are taking higher education in this college. This college has been providing the higher education to these needy students since last 40 years. The college has well infrastructural facilities. Now, the college has been renamed as Late Rajkamalji Bharti Arts, Commerce and Smt. Sushilabai R. Bharti Science College, Arni. NAAC B-Grade Accredited (Second Cycle).

Our Inspiration (EIRHCSSD-2025) Multidisciplinary National Conference organizes in the memory of our beloved former President Late Dr. Sanjay R. Bharti who had keen interest in the educational development of Arni region. This conference offers a heartily tribute to him.

## **About Conference:**

This conference is an attempt to introduce the participants to the

### **“EXPLORING INNOVATIVE RESEARCH IN HUMANITIES, COMMERCE AND SCIENCE FOR SUSTAINABLE DEVELOPMENT (EIRHCSSD-2025)”**

It aims to bring together leading academicians, researchers and students to exchange and share their experiences and research results on all aspects of recent advances and emerging trends in Arts, Commerce and Science. (any other sub theme related to the main theme of the conference not limited)

- Agriculture and Climate Change
- Bio diversity and Conservation
- Current research in life sciences
- Biotechnology for Sustainable Development
- General relativity, Astrophysics & Space Science.
- Women empowerment and political contribution
- मराठी संतांच्या विचारांची उपयुक्तता
- भारतातील वृद्धांच्या सामाजिक समस्या
- जागतिकीकरण आणि समाज विकास
- Recent Innovation in pure and applied mathematics
- Library Science
- Material Science
- Recent trends in English language and literature
- Artificial Intelligence and Library
- ICT and Library



- Digital Technology
- Library Services in new era
- Geography & Environment
- Indian Classical music
- Modern era of music
- Food & Nutrition
- Innovation in commerce
- Journey of Indian economy: Progress, prospects and challenges

All the participants are requested to register using online registration link.

Payment should be made through NEFT/RTGS online mode.

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## **Guideline for Author**

### **Call for Paper**

1. Paper should be based on original and authentic research work and case study method on theme and sub theme of the conference or any other topics.
1. The Research paper received along with the fees will be considered for publication and entire rights of publication are reserved. papers will be published in Double Blinded Peer Reviewed Online International Research Journal Having ISSN: 2347-7075 with DOI

### **-Guidelines for Author-**

1. The full-length research paper should be typed in time new roman title font size 14, paper text font size 12 for English language and Use Unicode font style, title font size 16, paper text font size 14 for Marathi and Hindi Language on A4 size Paper, MS Word file only.
2. The full paper covered up to 1500-2500 words.
3. Corresponding authors should sign the copyright license agreement & email the agreement in pdf to.... Email: eirhcssd2025@gmail.com

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1. Faculty/Delegate from Industry= 1000/-
2. PG Student/ Research Scholar= 700/-

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#### **Paper submission:**

The delegates can submit their research manuscript online to eirhcssd2025@gmail.com

Last date of paper Submission: 25 February 2025

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**Last date of paper Submission : 25 February 2025**

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Affiliated to Sant Gadge Baba Amravati University, Amravati

## ONE DAY NATIONAL CONFERENCE ON

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COMMERCE AND SCIENCE FOR SUSTAINABLE DEVELOPMENT  
(EIRHCSSD-2025)**

Monday, 10<sup>th</sup> March 2025



## ... Organised By ...

IQAC, Late Rajkamalji Bharti Arts, Commerce and  
Smt. Sushilabai R. Bharti Science College, Arni Dist. Yavatmal

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### About Institute :

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- Bio diversity and Conservation
- Current research in life sciences
- Biotechnology for Sustainable Development
- General relativity, Astrophysics & Space Science
- Women empowerment and political contribution

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- Recent Innovation in pure and applied mathematics
- Library Science
- Material Science
- Recent trends in English language and literature
- Artificial Intelligence and Library
- ICT and Library
- Digital Technology
- Library Services in new era
- Geography & Environment
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Mr. G. R. Yerawar, Arvi	Dr. Shrikant S.Nimkar Akot

## Conference Report

IQAC, Late Rajkmalji Bharti Arts, Commerce and Smt. S. R. Bharti Science College had successfully organized the national conference on “**Exploring Innovative Research in Arts, Commerce and Science for Sustainable development**” on **10<sup>th</sup> March, 2025**.

The national academic event is an attempt to create awareness among the multidisciplinary faculty members, researchers and students working together for sustainable development. The national conference also provides an opportunity to participants to contribute their findings, aware about recent approaches, study and research in arts, commerce and science in the field of conference theme.

The national conference was inaugurated at Conference Hall of the college by the hands of Chairperson of Inaugural function Hon’ble **Dr. Kirantai Bharti**, President of Shri Datta Prasadik Shikshan Prasarak Mandal’s Arni. Hon’ble Shri. Priyadarshanji Bharti, Treasurer, SDPSPM, Arni as Chief guest. Hon’ble Adv. Siddharth Bharti, Secretary, SDPSPM, Arni as the guest of Honor. The inaugurator of the function was Hon’ble Dr. Vinayak Deshpande, Vice-Chancellor, G.H. Rasoni Uni. Amravati. On the dais, many esteemed guests were present like as Hon’ble Dr. Ajay Lad, Director, IIL, SGBAU, Amravati, Hon’ble Dr. Santosh Bansod, Coordinator, BARTI, Hon’ble Dr. Mahendra Shirsat, Sr. Prof. & Head Dept. Elect., BAMU, Chatt. Sambhajinagar, Hon’ble Dr. Rahul Kamble, Prof. The English and Foreign Languages University, Hyderabad, Hon’ble Dr. Mohan R. Kherde, President, Indian Library Association, New Delhi, Hon’ble Dr. Gajanan Muley, Prof. Dept. of Physics, SGBAU, Amravati, Hon’ble Dr. Shashikant Wankhade, Director, SDPSPM, Arni, Hon’ble Dr. Nivrutti Pistulkar, Principal, LRB Arts, Comm. & SSRB Sci. Clg, Arni, Hon’ble Dr. Prashant Awate, IQAC Coordinator, LRB Arts, Comm. & SSRB Sci. Clg, Arni, Hon’ble Dr. Pratik Wankhade, Convenor, and Hon’ble Mr. Santosh Arade, Co-Convenor, National Conference (EIRHCSSD-2025).


**Anchoring: Dr. Rupali Tekade**

Dr. Pratik Wankhade, Convenor of National Conference on EIRHCSSD-2025 was briefly outline the Programme in his introductory speech. Dr. Vinayak Deshpande inaugurate the event and share his view in a very precise way. Hon’ble Dr. Ajay Lad, Director, IIL, SGBAU, Amravati congratulate the organizing committee and gave best wishes for today’s Programme Co-

Convenor of National Conference on EIRHCSSD-2025 express vote of thanks. Dr.Rupali Tekade host the function.

## **Keynote Speaker**

***Innovative Research as catalyst for sustainable development integrating  
Humanities, Commerce and Science***


	<b>Hon'ble Dr. Mahendra Shirsat,</b> Senior Prof.,Physics, Head, Dept. of Electronics & Director (RUSA, Center for Advanced Sensor Technology) and Dean, Faculty of Science and Technology BAMU, <b>Chattrapati Sambhajnagar</b>
<b>Anchoring:</b> Dr. Prashant Awate	

## **Technical Session – I**


***Creativity in Research: Exploring new narratives in literature studies***

	<b>Speaker</b> <b>Hon'ble Dr. Rahul Kamble,</b> Prof. Dept. of Indian & World Literature, The English and Foreign Languages University, Hyderabad (Telangana)
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	<p><b>Chairperson</b>  <b>Hon'ble Dr.Vinod Varghese,</b>  <i>Department of Mathematics,</i>  <i>M G.College Armori,</i>  <b>Gadchiroli MS</b></p>
<p><b>Anchoring:</b> Dr.Manoj Kakpure</p>	

**Technical Session – II**  
***Academic Integrity in Research and Publication***

	<p><b>Speaker</b>  <b>Hon'ble Dr. Mohan Kherde,</b>  President, Indian Library  Association,  <b>New Delhi</b></p>
	<p><b>Chairperson</b>  <b>Hon'ble Dr.Yuvraj Tamgadge,</b>  <i>Department of Physics,</i>  <i>Mahatma Fule Arts, Commerce and</i>  <i>Sitaramji Choudhary Science College,</i>  <b>Warud, Amarvati MS</b></p>
<p><b>Anchoring:</b>Mr.Ashay Muneshwar</p>	

## **Oral Presentations**

After this a large number of researchers participated in "Oral and Poster Presentations" which were carried in 2 different hall in parallel sessions. Total around 10 oral presentations were delivered in a days. The Jury members of Oral Presentations and Poster presentation were Hon'ble Dr. Gajanan Muley, Prof. Dept. of Physics, SGBAU, Amravati, Hon'ble Dr. Rajesh Wankhade, Prof. Dept. of Chemistry, BB Arts, NB Commerce & BP Science College, Digras Hon'ble Dr. Praveen Joshi, Prof. Dept. of Zoology, Amolakchand Mahavidhyalaya, Yavatmal and Hon'ble Dr. Kavita Tated, Prof. & Head Dept. of History, Loknayak Bapuji Aney Mahila College, Yavatmal. They had taken out their precious time and done their job efficiently with Dr. Dr. P. J. Awate, Mr. Parate, Miss. Dhakulkar and Dr. U. A. More as Incharge for those sessions.

**Anchoring: Miss. Supriya Dhakulkar**

The first three winners of oral presentations were Miss. H. S. Deshmukh, Research Scholar, Department of Physics, SGBAU Amravati as secured first position, Dr. Nikhil Bhagat Assistant Professor, Department of Physics, SPM College Manora Dist. Washim secured second position and Miss. Vanita R. Sagane Research Scholar, Department of Physics, SGBAU Amravati.

## **Valedictory Function**

In the last session, there was Valedictory function. The chairperson of the valedictory function was Hon'ble Adv. Siddharth Bharti, Secretary, SDPSPM, Arni. The chief guest Dr. S. V. Wankhade, Director SDPSPM, Arni, Guest of honor Hon'ble Dr. Gajanan Muley, Prof. Dept. of Physics, SGBAU, Amravati, our sponsor representative Hon'ble Mr. Sandesh Ramteke, Branch Manager BOM, Arni, Hon'ble Dr. Nivrutti Pistulkar, Hon'ble Dr. Prashant Awate, convenor and co-convenor were on the dais. After felicitation of guest, few participants express their opinion about today's event. Hon'ble Adv. Siddharth Bharti, congratulated the organizing committee for the success of the national conference. Dr. Pratik Wankhade-Convener had given the concluding speeching thanking everybody involved directly or indirectly in this conference.

At the last, Mr. Santosh M. Arade Co-convenor of thanks everyone in his vote of thanks.

**Anchoring: Dr. Rupali Tekade**

## Full length Paper Publication

Overall, more than 410 delegates across the country registered their names through online mode only. Eight participants registered spot registration. Special arrangement was made for spot registration and certificate distribution. All the received full length papers were published in the Special issue of **International Journal of Advance and Applied Research-A Multidisciplinary International Level Referred and Peer Reviewed Journal ISSN-2347-7075** and Impact Factor- 8.141 Published by Young Researcher Association, Kolhapur, Maharashtra, India.

## News Paper

लोकमत



मस्ट READ

# रोजगार निर्मितीसाठी संघटित प्रयत्न व्हावेत

विनायक देशपांडे यांचे  
प्रतिपादन : आर्णीत परिषद

लोकमत न्यूज नेटवर्क

**आर्णी** : भारताच्या वाढत्या लोकसंख्येला गृहीत धरून सातत्याने रोजगारनिर्मितीसाठी संघटित प्रयत्नांची आवश्यकता आहे. याकरिता कला, वाणिज्य, विज्ञान, तंत्रज्ञान या सर्व विद्याशाखांनी शाश्वत विकास हे उद्दिष्ट ठेवून एकत्रितपणे प्रयत्न करणे अत्यावश्यक आहे, असे प्रतिपादन जी. एच. रायसोनी विद्यापीठाचे कुलगुरू डॉ. विनायक देशपांडे यांनी केले.

येथील राजकमल भारती कला आणि वाणिज्य व सुशीलाबाई भारती विज्ञान महाविद्यालयाने आयोजित केलेल्या आंतरशास्त्रीय राष्ट्रीय परिषदेचे उद्घाटक म्हणून ते बोलत होते. या परिषदेचे बीजभाषक डॉ. बाबासाहेब आंबेडकर मराठवाडा विद्यापीठाचे फिजिक्स-इलेक्ट्रॉनिक्स विभागाचे प्रमुख डॉ. महेंद्र शिरसाट होते. त्यांनी

४००

प्राध्यापक,  
संशोधकांनी  
केली नोंदणी



विविध शाखांनी एकत्रितपणे केलेल्या संशोधनातून नव्या संशोधनाची निर्मिती होते, असे मत मांडले.

अध्यक्षस्थानी श्री दत्त प्रासादिक शिक्षण प्रसारक मंडळाच्या अध्यक्षा डॉ. किरणताई भारती होत्या. मानवी विकासाचा मुख्य आधार नैतिकमूल्ये असली पाहिजे, असे मत त्यांनी व्यक्त केले. परिषदेत देशभरातून ४०० प्राध्यापक व संशोधकांनी नोंद केली होती. यावेळी विविध महाविद्यालयातील प्राध्यापक, कर्मचाऱ्यांची उपस्थिती होती.

## मान्यवरांची उपस्थिती

अमरावती विद्यापीठाचे कुलसचिव डॉ. अविनाश असनारे, इंडियन लायब्ररी असोसिएशनचे अध्यक्ष डॉ. मोहन खेरडे, डॉ. अजय लाड, 'बार्टी'चे को-ऑर्डिनेटर डॉ. संतोष बनसोड, हैदराबाद युनिव्हर्सिटीचे डॉ. राहुल कांबळे, डॉ. गजानन मुळे आदींनी या परिषदेला संबोधित केले. व्यासपीठावर संस्थेचे सचिव अॅड. सिद्धार्थ भारती, कोषाध्यक्ष प्रियदर्शन भारती महाविद्यालयाचे प्राचार्य डॉ. निवृत्ती पिस्तुलकर, डॉ. शशिकांत वानखडे, डॉ. प्रशांत आवते, डॉ. व्ही. आर. माहुरे, परिषदेचे संयोजक डॉ. पी. एम. वानखडे, सहसंयोजक डॉ. एस. एम. आराडे उपस्थित होते.

## परिषदेत तीन सत्र

विषयवार विभागलेल्या परिषदेच्या तीन सत्रांचे अध्यक्षस्थान डॉ. कविता तातेड, डॉ. प्रवीण जोशी, डॉ. राजेश वानखडे यांनी भूषवले. विविध सत्रांचे डॉ. रूपाली टेकाडे, डॉ. मनोज काकपुरे, डॉ. आशय मुनेश्वर, डॉ. जितेंद्र कौसल्य, डॉ. उमेश मोरे, डॉ. अमित बागडे, प्रा. प्रफुल्ल भोकरे, डॉ. प्रतीक सोनोने यांनी संचालन केले. प्रा. मिलिंद पांडे, प्रा. उदयसिंह चव्हाण, प्रा. सदानंद बोळे यांनी आभार मानले. यशस्वितेसाठी डॉ. बबन सेलकर, डॉ. धनंजय देशमुख, प्रा. विजय टोकसे, श्रीकांत वानखडे, सूरज ढाकुलकर, विजय ठाकूर, अनिल पिल्लेवार, दिनकर वाडेकर आदींनी पुढाकार घेतला.

# देशोन्नती

## तालुका अपडेट

### भारती महाविद्यालयात आंतर विद्याशाखीय राष्ट्रीय परिषद



#### देशोन्नती वृत्तसंकलन

**आर्णी :** रोजगार निर्मिती व्हावी याकरिता संघटीत प्रयत्न होण्याची आवश्यकता असून याकरिता सर्व विद्याशाखांनी शाश्वत विकास हे उद्दिष्ट ठेवून एकत्रितपणे प्रयत्न करणे अत्यवश्यक आहे असे मत राष्ट्रीय परिषदेचे उद्घाटक डॉ. विनायक देशपांडे यांनी व्यक्त केले. ते स्व. राजकमलजी भारती कला आणि वाणिज्य व श्रीमती सुशीलाबाई भारती विज्ञान महाविद्यालयाने आयोजित केलेल्या आंतरशाखीय राष्ट्रीय परिषदेत बोलत होते.

या परिषदेत डॉ. महेंद्र शिरसाट यांनी विविध शाखांनी एकत्रितपणे केलेल्या संशोधनातून नव्या संशोधनाची निर्मिती होते. असे मत मांडले. त्यासाठी अर्थपुरवठा करणाऱ्या आर.यु.एस.ए च्या योजनांचा आढावा घेतला. याप्रसंगी त्यांनी मराठवाडा विद्यापीठातील नवीन संशोधनावर भाष्य केले.

राष्ट्रीय परिषदेच्या अध्यक्षास्थानावरून संबोधन करतांना श्री दत्तप्रासादिक शिक्षण प्रसारक मंडळाच्या अध्यक्षा डॉ. किरण भारती यांनी नैतिकमूल्ये मानवी विकासाचा मुख्य आधार

असली पाहिजेत असे मत व्यक्त केले. परिषदेला डॉ. महेंद्र शिरसाट, डॉ. अविनाश असनारे, डॉ. मोहन खेरडे, डॉ. अजय लाड, डॉ. संतोष बनसोड डॉ. राहुल कांबळे, डॉ. गजानन मुळे आदिनी संबोधित केले.

व्यासपीठावर अॅड. सिद्धार्थ भारती, प्राचार्य डॉ. निवृत्ती पिस्तुलकर, डॉ. शशिकांत वानखडे, डॉ. प्रशांत आवते, डॉ. व्ही आर. माहुरे, डॉ. पी.एम. वानखडे, डॉ. एस.एम. आराडे, डॉ. कविता तातेड, डॉ. प्रवीण जोशी, डॉ. राजेश वानखडे, डॉ. रुपाली टेकाडे, डॉ. मनोज काकपुरे, डॉ. आशय मुनेशवर, डॉ. जितेंद्र कौसल्य, डॉ. उमेश मोरे, डॉ. अमित बागडे, प्रा. प्रफुल भोकरे डॉ. प्रतिक सोनोने उपस्थित होते.

या परिषदेत देशभरातून सुमारे ४०० प्राध्यापक व संशोधकांनी नोंद केली. हा कार्यक्रम यशस्वी होण्यासाठी डॉ. सदानंद बोळे, डॉ. बबन सेलकर, डॉ. धनंजय देशमुख, प्रा. विजय टोकसे, श्रीकांत वानखडे, सुरज ढाकुलकर, विजय ठाकूर, अनिल पिल्लेवार, दिनकर वाडेकर, तसेच सर्व सीएचबी शिक्षक, शिक्षकेतर कर्मचारी यांनी परिश्रम घेतले (ता.प्र.)





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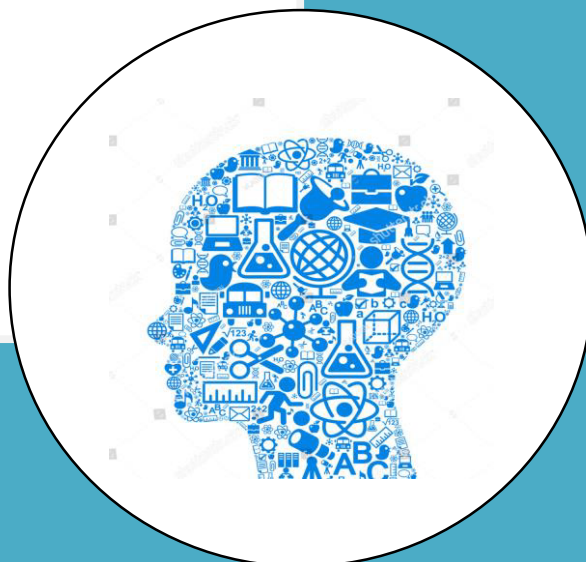






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## Spectrophotometric study of Interactions 2-[[2-(cyclohexycarbamoyl) benzoyl] amino] propanoic acid (2CMPA) with BSA: Gel exclusion chromatography and molecular modeling study.

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### Abstract:

The interaction of between 2-[[2-(cyclohexycarbamoyl) benzoyl] amino] propanoic acid (2CMPA) 2CMPA and protein BSA was studied using the gel exclusion chromatographic technique. Spectrophotometric data reveals that 2CMPA successfully binds with BSA. The effect of pH on binding affinity was also studied. The Scatchard analysis gives association constants ( $K_f$ ) values that are found to be 0.6056, 0.5809, and 0.5714 at acetate buffer pH 3, 4, and 5 respectively. It was found that 2CMPA bounds to the BSA more significantly at pH 3 than at pH 4 and 5 which shows that binding is more significant at acidic and decreases with an increase in pH. A molecular modeling study was also done which gives the efficient energy value for complex -235.41 that confirms the binding of titled 2CMPA with BSA.

**Keywords:** gel exclusion chromatography, protein-drug binding, Scatchard analysis, association constant, BSA protein, molecular modeling study.

### Introduction:

Plasma proteins are the most abundant protein in human blood. It accounts for 60% percent of total protein in the blood. Plasma proteins perform several functions such as oxygen binding, DNA binding, drug transportation, etc. Plasma proteins are mainly of three types these are alpha-1-acid glycoprotein (AGP), human serum albumin (HSA), and lipoproteins. These proteins mainly perform the function of transportation of drugs in which AGP binds mainly basic drugs and HSA binds mainly acidic drugs. HSA is a globular protein that consists of structurally (I, II, and III) sites for drug binding each site also consists of two subdomains (A and B). HSA protein shows similar bonding chemistry with bovine serum albumin (BSA) so BSA was used in place of HSA in this study because of its low cost and easy availability. The full-length precursor of BSA consists of 607 amino acids in length. An N-terminal 18-residue signal peptide is cut off from the precursor protein upon secretion; hence the initial protein contains 589 amino acid residues. An additional 4 amino acids are cleaved to yield the mature BSA protein that contains 583 amino acids.

BSA is the most studied globular protein; the Effect of binding on specific sites of BSA for ciprofloxacin and captopril drugs in the presence of a specific site probe was studied [1]. The binding interaction of gold chloroquine to BSA was analyzed in terms of binding constant, entropy, and enthalpy change [2]. Effect on the binding of

ibuprofen with normal plasma protein and plasma obtained from rheumatoid arthritis patients using ultracentrifugation technique were observed [3]. Protein binding of esmolol with BSA and AGP was studied which gives significant difference in binding with proteins [4]. The binding of propranolol with AGP was studied using the liquid-liquid interface technique [5]. capillary electrophoresis technique was also used for analyzing protein drug binding [6], Mass spectrometry-based tools were successfully used for the measurement of protein-drug binding [7] Study of binding of various 2CMPAs with serum protein using the FT-IR technique also made a valuable contribution to this study. Interactions of human serum albumin with chlorogenic acid and ferulic acid were studied using the FT-IR technique[8]. There are various forces responsible for the binding of drugs with proteins like hydrophobic interaction, hydrogen bonding, van der Waal forces, electrostatic attraction, etc. Interaction between jatrorrhizine and HSA showed that hydrophobic and electrostatic interaction play vital role in there binding [9]. The presence of foreign particles such as arsenic, lead, cadmium etc. affects the binding of drug and plasma proteins. Effect of arsenic on paracetamol binding to bovine serum albumin using site-specific probes showing a decrease in percentage of binding of paracetamol to BSA [10]. Chemical and physical properties of human plasma retinol-binding protein (RBP) and prealbumin (PA) and factors affecting their interaction with each other and with 2CMPA retinol

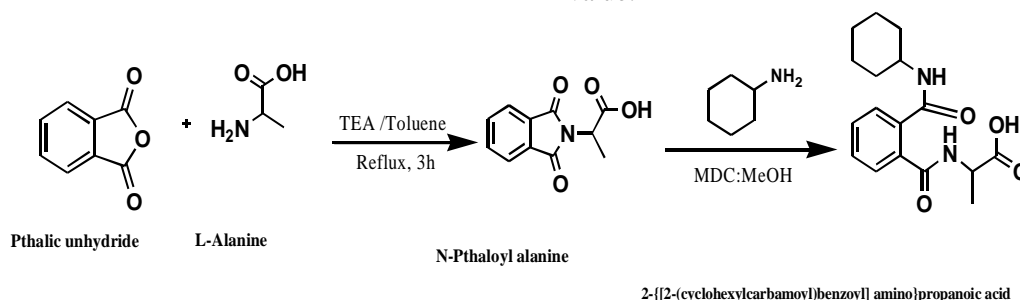
and thyroxine are observed [11]. The presence of arsenic in the complex solution of BSA and atenolol results in the free concentration of arsenic [12]. The effect of varying pH of the mobile phase on the binding of drugs shows the variation in the binding of various drugs. Thermodynamic parameters were used to rationalize the nature of binding of ciprofloxacin hydrochloride to BSA at different pH [13]. A comparative study has been done to study the accuracy and time factor for protein drug binding using various docking software [14]. Molecular docking is used for the measurement of the interaction of formononetin with HSA protein [15].

In this paper, we reported the synthesis of the 2-[[2-(cyclohexylcarbonyl) benzoyl] amino] propanoic acid by a known method and also characterized the compound by IR,  $^1\text{H}$  NMR, and Mass spectroscopy. The compound shows antibacterial activity (Pande et al. 2013) [16]. Compounds show acidic nature and affinity for the BSA protein. The binding affinity of this compound with BSA protein was then measured using gel exclusion chromatographic technique also molecular modeling software HEX 8.0 was used which confirms the binding affinity of

said 2CMPA with BSA by giving a competent energy value.

#### Materials and Methods:

For synthesis, all the chemicals used were of A.R. grade of Merck India Limited made and purchased from commercial suppliers. The purity of the synthesized compound was ascertained by thin layer chromatography on silica gel G in petroleum ether and ethyl acetate (7:3) mixture, Melting point was recorded using digital melting point apparatus Equiptronics (EQ 730). IR spectra were recorded on Bruker alpha IR Spectrometer (Germany) expressed in  $\text{cm}^{-1}$  at the Department of Chemistry J.B. College of Science Wardha.  $^1\text{H}$  NMR spectra of the compound were recorded in  $\text{CDCl}_3$  on an NMR instrument (500MHz) using TMS as an internal standard from SAIF, CDRI Lucknow. For the chromatographic experiment, Sephadex g-25 having water regain 2.5-0.2ml/g (make- sigma chemical Ltd. (Sweden), Bovine Serum Albumin ( $M_r = 66,500$ ) (make-chemsworth chemical Ltd., India) were used. 0.1M sodium acetate buffer of pH range 3, 4, and 5 were used. U.V. Visible Spectrophotometer Shimadzu Singapore (Model UV 180) was used for the measurement of absorbance value.



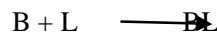
#### Scheme 1: Synthesis of 2-[[2-(cyclohexylcarbonyl) benzoyl] amino] propanoic acid

##### Measurement of binding affinity:

Sephadex g-25 was used to prepare a chromatographic column using acetate buffer solution. It was allowed to stand overnight to develop the column with continuous flow of buffer solution through the reservoir which keeps the column wet. 50  $\mu\text{M}$  BSA solution and 0.01M solution of 2-[[2-(cyclohexylcarbonyl) benzoyl] amino] propanoic acid were also prepared using sodium acetate buffer solution were prepared. A 10ml solution of BSA and drug were prepared in various ratios such as 10:0, 9:1, 8:2, 7:3, 6:4, 5:5, and 6:4. Solution was allowed to pass through the column, and eluting buffer was passed continuously which helped to run the sample solution through column. The sample solution was collected from the lower end of the column in an equal fraction and the absorbance of each collected fraction was measured on the U.V. Visible Spectrophotometer. The buffer solution of various pH was prepared and a solution of complex at different pH was made. Absorbance was recorded for the collected fraction and the effect of pH on absorbance value was observed.

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For the *Scatchards analysis* binding affinity between two molecules was expressed as an equilibrium constant and association constant which is derived from the law of mass action. BSA (B) interacts with the 2CMPA to form the complex as shown below.



So the equation for association constant

$$K_f = \frac{[BL]}{[BL] + [B]}$$

The binding strength of the 2CMPA to BSA is a measure of association constant. The fraction of binding of 2CMPA to protein BSA is represented in the term of  $[V]$  so the equation for  $[V]$  in terms of the binding is

$$V = \frac{[BL]}{[BL] + [B]}$$

Equation for  $[V]$  in terms of association constant ( $K_f$ ) given as

$$V = \frac{K_f[L]}{K_f[L] + 1}$$

Total n available sites on B out of a number of sites occupied by 2CMPA is represented in terms of  $[V']$

$$V' = \frac{nK_f[L]}{K_f[L] + 1}$$

Scatchard graph of  $[V]$  with  $[L]$  give the value for association constant ( $K_f$ ) while the graph  $[V']$  with  $V'/L$  is a measure of interacting sites that are available.

### Result and Discussion:

#### Chromatographic observation:

Initially, the absorbance value for BSA in the absence of 2CMPA was recorded at 520nm. Absorbance values for complex solution of BSA and 2CMPA at varying compositions as shown above were also recorded. Spectrophotometric values show that absorbance value continuously increases with an increase in 2CMPA concentration in a complex solution. The graph was plotted for the absorbance

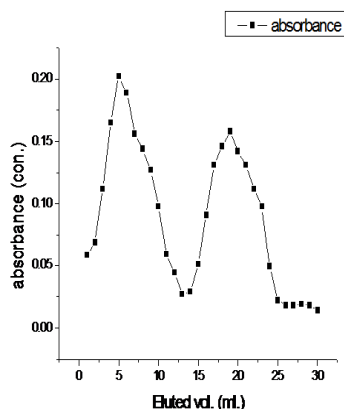


Figure 1. Graph of Absorbance Vs Eluted volume

#### Effect of pH:

The effect of binding of 2CMPA to BSA was studied at different pH 3, 4 and 5. We have prepared the complex BSA and 2CMPA solutions in a sodium acetate buffer of varying pH ranges of 3, 4, and 5. Measurement of absorbance value gives the effect of pH on binding. Association constant ( $K_f$ ) values were calculated using Scatchard analysis. It was found that binding decreases with an increase in pH value. At pH 3 binding was more significant in comparison with 4 and 5. This shows that 2CMPA binds BSA significantly at a more

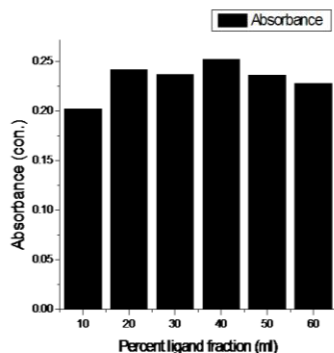


Figure 3. Graph of Absorbance Vs Percent 2CMPA fraction at pH 3

value for the collected fraction shown in Fig.1 which gives two peak. The first peak in Fig.1 shows the maximum binding of the 2CMPA with BSA while the second peak represents the unbound 2CMPA fraction. Absorbance values show a continuous increase in values of absorbance but after a particular point, a gradual increase in absorbance values shows a saturation level of 2CMPA. Chromatographic observations show that the compound 2-[[2-(cyclohexylcarbonyl) benzoyl] amino] propanoic acid binds significantly to BSA. In Figure 2 graph was plotted between the total site and to bound site, a straight line indicates that there was only one interacting site available to the 2CMPA for binding on BSA.

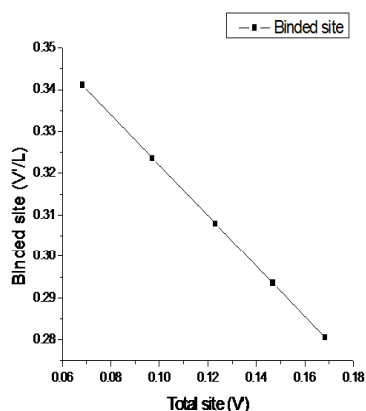


Figure 2. Graph of Total site to Binded site acidic pH. Association constant ( $K_f$ ) values at pH 3, 4, and 5 are found to be 0.6062, 0.5821, and 0.5797 respectively. Figure 3 shows the changes in absorbance value for the BSA-2CMPA complex at different compositions and Figure 4 shows the Scatchard graph at pH 3. Similarly Figure 5 and Figure 6 show changes in absorbance value for protein-2CMPA complex at different compositions and Scatchard graph at pH 4. Similarly Figure 7 and Figure 8 show changes in absorbance value for protein-2CMPA complex at different compositions and Scatchard graph at pH 5.

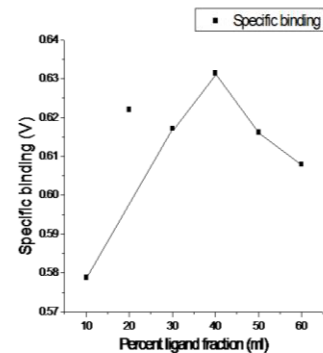


Figure 4. Specific binding Vs Percent 2CMPA fraction at pH 3

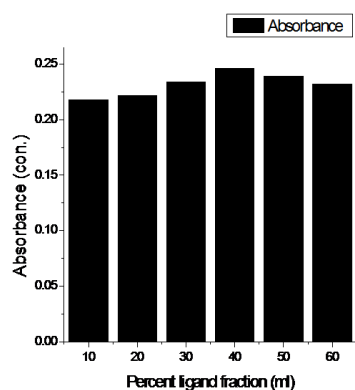


Figure 5. Graph of Absorbance Vs Percent 2CMPA fraction at pH 4

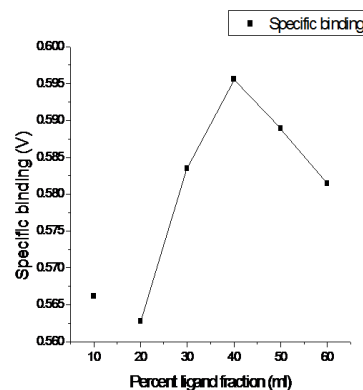


Figure 6. Specific binding Vs Percent 2CMPA fraction at pH 4

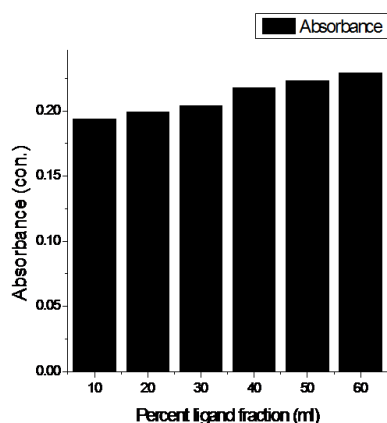


Figure 7. Graph of Absorbance Vs Percent 2CMPA fraction at pH 5

#### Molecular modeling study for interaction between BSA and said 2CMPA

Serum protein is the most studied and abundant protein in blood plasma, accounting for nearly 60% of total protein consisting of a single polypeptide chain of 589 amino acids. In serum protein, there are mainly three binding sites I, II, and III each of these contains sub-domains (A and B). Molecular modeling is also an efficient method for the measurement of interaction between protein and drug. The energy value obtained from the study is a measure of the binding of drug the drug to the

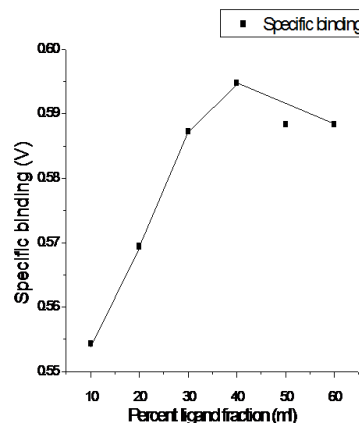


Figure 8. Specific binding Vs Percent 2CMPA fraction at pH 5

Serum protein. For the further study of the binding interaction between BSA and said 2CMPA, a molecular modeling study was done. The crystal structure of BSA was obtained from the RCSB protein data bank and 3D file for 2CMPA developed on Chem Draw Ultra 8.0. Docking was done using the software HEX 8.0. The energy value obtained was -235.41, showing that the mentioned 2CMPA efficiently binds with protein BSA. Diagrammatic representation of interaction for interaction between BSA and said 2CMPA as shown below in **Fig. 9**

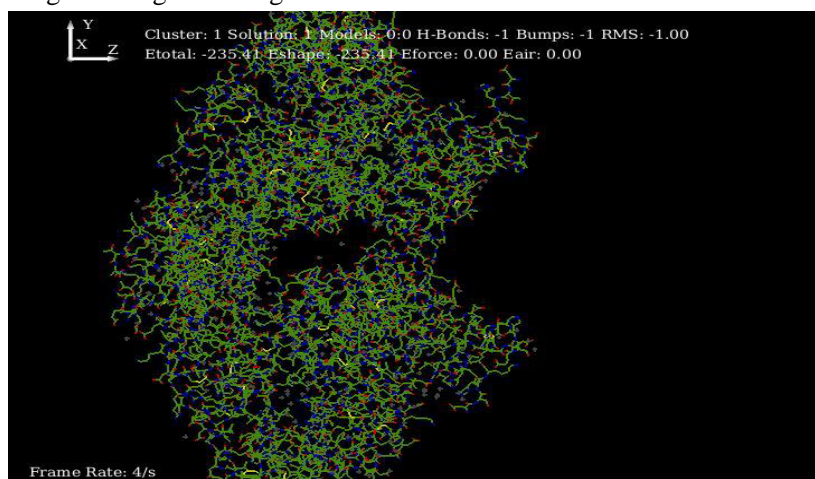


Fig. 9 Interaction between BSA and 2-[(2-(cyclohexycarbamoyl) benzoyl)amino] propanoic acid



**Conclusion:**

The chiral drug 2-[[2-(cyclohexycarbamoyl) benzoyl] amino] propanoic acid showing antibacterial activity has the efficiency to bind with protein BSA. We have studied the novel interaction of this drug with BSA protein using the gel exclusion chromatographic technique. A study of the interaction of this drug with BSA shows that the drug successfully binds with BSA. A study of binding at various buffers pH 3, 4, and 5 shows that the association constant (Kf) value was found to be more at buffer pH 3 in comparison with pH 4 and 5. The value of association constant (Kf) calculated from Scatchard analysis are found to be 0.6056, 0.5809, and 0.5714 at pH 3, 4 and 5 resp. It means that the binding of the drug with protein BSA is more efficient at acidic pH and it goes on decreasing with an increase in pH value. Furthermore, molecular docking shows the efficient energy value -235.41 which shows a confirmative binding approach of the mentioned 2CMPA with protein BSA.

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