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### *A Journal of the Proteomics Society, India (PSI)*

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**Cover page figure:** Electrostatic map depicting the positively charged active site cavity containing Lys 12 (blue coloured lines of force) in the structure of triose-phosphate isomerase wherein S-glycosylation of cysteine 217 allosterically inhibits the enzyme (details, M.SS. Hameed pp 133-146)



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## GENERAL INFORMATION

**The Journal:** Journal of Proteins and Proteomics (JPP), with its genesis in India, is a peer reviewed journal envisaged to serve the world wide community of researchers and teachers dealing with the challenges of proteins and proteomics resulting in an improved understanding of protein science in general. Published bi-annually, the aim is also to supplement the regular issues with special issues in selected, relevant topics of protein science. The journal has an online presence at <http://www.jpp.org.in>.

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## WELCOME TO THE FIRST ISSUE FROM PROTEOMICS SOCIETY, INDIA (PSI) (TWENTIETH ISSUE OVERALL)

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Journal of Proteins and Proteomics is now an official journal of the Proteomics Society, India (PSI). We are happy to publish the second issue of the journal, duly chaperoned by the society. The new section on *Messages and Motivation* this time carries a thought provoking message by Prof. Utpal Tatu, IISc., Bangalore. His message will motivate one to think about the role of science societies, and thus PSI, in the changed scenario of e-age. Hope the message sets in discussions and new ideas to adapt to the demands of the modern times.

The issue presents *six articles*, which are diverse and covers both protein science in general and proteomics research in particular. The *first article* is a review that highlights the current status of research in alpha-synuclein structure, a protein responsible for various neurodegenerative disorders mainly through formation of specialized aggregates called amyloid fibrils. The article attempts to scan the investigations that have proposed and validated means to block the aggregation process in an effort to put forth meaningful new ways to deal with the proteinopathies caused by alpha-synuclein.

The next four articles represent the largest density of proteomics based research articles in a single issue of JPP. The first of this series - *second article* in the issue - presents a comparative evaluation of seven isoforms of serum sirtuins with the purpose of developing protein marker for frailty. Frailty is an adverse health condition, especially in the elderly, and no diagnostic biomarker has been identified for the same. The levels of sirtuin proteins have been estimated in the blood plasma of patients using surface plasmon resonance and compared to those of normal individuals. The data was validated by western blots and it was evident that SIRT 1 and SIRT 3 may be used as biomarkers.

The *third article* also had a clinical base and investigated the role of certain proteins and their complexes in human sperm motility and capacitation. The target protein included prolactin inducible protein (PIP), which is expressed in human body fluids. PIP was recently isolated from human semen in complex with human serum albumin (HSA). In this article the comparative expression of this complex was analyzed using co-immunoprecipitation and western blot methods in human seminal plasma samples of infertile individuals against fertile controls. Results indicated that HSA-PIP complex was downregulated in azoospermia conditions and the complex maybe a positive regulator of sperm motility and capacitation.

The *fourth article* describes a mass spectrometry intensive investigation, where the authors evaluated the accuracy and consistency of SWATH-MS based quantification. The article addresses the challenges that proteomics researchers face with regard to the accurate and sensitive quantitation of low abundant proteins using mass spectrometry with high degree of reproducibility. The study aptly proves that SWATH-MS based quantification can be achieved to as low as 2.5 fmoles of peptides. Given the fact that of late proteomics has emerged as the dependable source of information for biological interactions and mass spectrometry lies at the heart of proteomics research, the method described in this paper is a significant advance in quantifying low abundant proteins.

The *fifth article* is unique since this is the first time that the journal carries a mass spectrometry based plant proteomics investigation. Leaf proteins of spinach have been profiled using mass spectrometry based identification of the proteins. As many as 639 proteins were identified using LC-

ESI-MS/MS technology. The study unraveled the diversity and complexity of leaf proteins and will provide insight into the protein networks that control biological processes in leaf.

The *last article* of the issue is a structure based study that elegantly demonstrates *in silico* how a post-translational modification of an amino acid side chain allosterically inhibits the catalytic activity of an enzyme, a novel method of enzyme regulation. Triose- phosphate isomerase was used as a model enzyme and it was shown using molecular dynamics investigation that glutathionylation of cysteine 217 in the enzyme allosterically inhibits its activity. This study will throw light on some aspects of redox signaling and its regulation. This *article won the cover page* due to its elegance and significance and the in-depth analysis of the intended biological process.

The issue also contains *two technical notes* from a commercial organization. Both the notes describe mass spectrometry based technology and we hope that they are useful to our readers.

We also take the opportunity to thank the sponsors, who supported the printing cost of the issue, such that authors could publish their manuscripts without any charge and the readers can access them without any charge either. We hope you will like our effort and provide us with your suggestions, opinions, inputs and whatsoever. We welcome everyone associated with the journal to send in their ideas and thoughts.

**Suman Kundu**  
*Editor- in-Chief*  
30<sup>th</sup> June, 2016

## **CHANGING ROLE OF SCIENCE SOCIETIES AND PSI**

Scientific societies have played an important role in the history of science. During renaissance, science societies and academies is where actual scientific discoveries took place. University, on the other hand, was the place where one learnt what was already known. The trend has now turned around. Societies are now playing more of a supporting role such as publishing journals, organizing meetings and have become the place for scientific networking. In US and in Europe, societies also lobby with the corridors of power to help formulate science policies.

In the face of communication through e-mails, face book, skype, video conferencing and easy access to scientific journals on your computers, what role can societies continue to play? Judging from the dwindling memberships to the scientific societies and the competition among their large numbers, science societies will have to transform and adapt in order to continue remaining relevant in the 21<sup>st</sup> century. What should be the role of a scientific society in the rapidly changing world of science?

In light of these provocative challenges faced by scientific societies all around the world I am going to present my views on what PSI can do in our country to carve a new mould for engagement of scientific community and policy makers with itself. Since its inception in the year 2009, PSI has played a key role in popularization of the science of proteomics at the national level. In addition to organizing annual meetings in different parts of the country, the society has also organized large numbers of hands-on workshops and seminar series in different colleges and universities. Thousands of students from different institutions, including those from remote regions in the country have received exposure to modern tools in proteomic research through the above activities. Most recently PSI has adopted the Journal of Proteins and Proteomics (JPP) under its banner. JPP will provide a wonderful opportunity to students in India to publish their research and ideas in this upcoming journal. Clearly PSI will continue to play a pivotal role in proteomic education and training in the country. While highlighting the achievements of PSI in educational activities, I take this opportunity to share my views on the roles that PSI can and should play in spreading proteomic technologies and encouraging proteomic researchers in various institutions in the country.

I am going to highlight two important opportunities of immediate relevance that PSI has in providing thrust to proteomic research in the country. These are: 1) efficient utilization of proteomic technologies in academia and 2) making proteomic technologies available to support industry.

India has over 800 universities hosting several thousand research laboratories in different disciplines broadly categorized under bio medical sciences, agricultural sciences and fisheries. Of the thousands of research laboratories about 500 laboratories are equipped with the state of the art facilities, such as mass spectrometry, for carrying out proteomic research. Despite this large number of mass spectrometers, the actual number of research groups having proteomic capabilities is relatively low. Only about 25 laboratories carry the necessary expertise required to employ proteomic methods and make use of the modern mass spectrometry facilities that are available. This means that large numbers of expensive instruments purchased with government funded programs remain under-utilized. PSI carries a tremendous responsibility of filling this gap. Can we ensure efficient utilization of currently available facilities by facilitating training of scientists in Institutions that have the required facility but not the required training to efficiently use them?

There is a big divide between research carried out in academia and activities in the industry in our country. The knowledge exchange between academia and industry is abysmal in our country. This gap is not unique to the field of proteomics but spreads across disciplines. However, there is an opportunity for PSI to address this problem through the area of proteomics. PSI is ideally placed to play an important role in galvanizing knowledge exchange and collaborations between industry and academia. By organizing interactive sessions and inviting industry to collaborate with academia in the area of proteomics PSI can facilitate this exchange that may lead to successful examples of public-private partnerships in our country.

PSI has a wonderful opportunity to learn from experiences of older science societies in our country. PSI has an opportunity to break the traditional pattern, be agile and adapt to the needs of students, researchers and science policy makers. Only time will tell if PSI is able to rise to the occasion and pull proteomic researchers in the country together to support a common national science agenda.

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