

**Conference: New Trends in Bioinformatics**  
**New Methods, Softwares, Databases, web-tools of Bioinformatics from India**  
**July 30<sup>th</sup> and 31<sup>st</sup>, 2012**  
**Venue: Seminar Hall, IIT Delhi**

**Day 1 (Monday, July 30<sup>th</sup>, 2012)**

**SESSION - 1 (9:00 – 10:35): Inauguration**

**Chairperson: T. Madhan Mohan**

<b>09:00-09:15</b>	<b>Welcome by B. Jayaram, IITD</b>
<b>09:15-09:30</b>	<b>T. Madhan Mohan, DBT</b>
<b>09:30-10:30</b>	<b>Plenary Lecture : M. Vijayan, IISc</b> Development of Computational Biology and Bioinformatics in India. A Personal Perspective
<b>10:30-10:35</b>	<b>Vote of Thanks</b>

**High Tea (10:35-11:10) & Mounting of Posters in the Exhibition Hall**  
**Chairpersons for Posters: James Gomes, Archana Chugh & Khushhali Menaria**

**SESSION - 2 (11:10 – 13:00)**

**Chairperson: N. Gautham**

<b>11:10-11:40</b>	<b>Lecture 1: N. Gautham, UoM</b> Charting the conformational space of molecules using MOLS Sampling
<b>11:40-12:10</b>	<b>Lecture 2: K. GuruPrasad, CCMB</b> Certain sequence-structure relatedness in proteins
<b>12:10-12:40</b>	<b>Lecture 3: R.S. Rathore, UoH</b> Advances in Docking Methodologies: Case Studies of Fructose-1,6-Bisphosphatase, Adenosine A2A and Dopamine D3 Receptors
<b>12:40-13:00</b>	<b>Lecture 4: HPC related talk by Wipro Ltd. (Sponsor)</b>

**Lunch & Poster Presentation (13:00-14:20) in the Exhibition Hall**

**SESSION - 3 (14:20-17:00)**

**Chairperson: Manju Bansal**

<b>14:20-14:50</b>	<b>Lecture 5: Manju Bansal, IISc.</b> Sequence dependent variations in RNA double helical structures: role of non-bonded interactions
<b>14:50-15:20</b>	<b>Lecture 6: G.P.S. Raghava, IMTECH</b> Peptide Bioinformatics and its application in cancer therapeutics
<b>15:20-15:50</b>	<b>Lecture 7: Alpan Raval, DE Shaw Research</b> Refinement of protein structure homology models via long, all-atom molecular dynamics simulations
<b>15:50-16:10</b>	<b>Lecture 8: Presentation by NVIDIA on GPUs, etc (Sponsor)</b>
<b>16:10-16:30</b>	<b>Lecture 9: Presentation by NetApp (a Storage based Company) (Sponsor)</b>
<b>16:30-17:00</b>	<b>Lecture 10: HPC related talk by IBM India Ltd. (Sponsor)</b>

**Coffee Break & Poster Presentation (17:00 -17:30) in the Exhibition Hall**

**SESSION - 4 (17:30- 19:00) 10<sup>th</sup> Anniversary Celebrations of SCFBio**

**Chairperson: R. K. Shevgaonkar**

<b>17:30-17:35</b>	<b>Welcome: B. Jayaram, IITD</b>
<b>17:35-17:45</b>	<b>About <i>Dhanvantari</i> (Genome to drug software); Release of Software by Chief Guest</b>
<b>17:45-18:00</b>	<b>S. Prasad, IITD</b>
<b>18:00-18:15</b>	<b>Manju Sharma, Former Secy, DBT</b>
<b>18:15-18:30</b>	<b>Chief Guest: T. Ramasami, Secretary, DST</b>
<b>18:30-18:45</b>	<b>Chairman: R.K. Shevgaonkar, Director, IITD</b>
<b>18:45</b>	<b>Vote of Thanks &amp; High Tea</b>

**Conference Dinner (19:00-22:00)**

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**Day 2 (Tuesday, July 31<sup>st</sup>, 2012)**

**SESSION - 5 (9:00 – 11:00)**

**Chairperson: Indira Ghosh**

<b>9:00-9:30</b>	<b>Lecture 11: Indira Ghosh, JNU</b> Proton Transfer Mechanism in F <sub>1</sub> F <sub>0</sub> ATP Synthase: A Quantum Chemical and Molecular Dynamics Study
<b>9:30-10:00</b>	<b>Lecture 12: Rajendra Joshi, CDAC</b> Multiscale Modelling in Understanding the Self-Assembly Mechanism of Human $\beta$ 2-Adrenergic Receptor in Lipid Bilayer
<b>10:00-10:30</b>	<b>Lecture 13: Sreedhara Rao Voleti, ILS</b> In Silico Applications to Concept Validation in Drug Discovery - C3aR Antagonists and Dual-Action Inhibitors of DPP4-ACE
<b>10:30-11:00</b>	<b>Lecture 14: A. Mittal, IITD</b> Newest view on protein folding: Analytical and experimental evidence towards a paradigm shift

**Tea Break (11:00-11:15)**

**SESSION - 6 (11:15 – 13:15)**

**Chairperson: R. Sankararamakrishnan**

<b>11:15-11:45</b>	<b>Lecture 15: R. Sankararamakrishnan, IITK</b> The superfamily of aquaporin channels from bacteria to humans: Same fold with different transport properties
<b>11:45-12:15</b>	<b>Lecture 16: Debasish Dash, IGIB</b> GenoSuite: A Multi-algorithmic proteogenomic analysis tool
<b>12:15-12:45</b>	<b>Lecture 17: D. Sundar, IITD</b> Molecular tools for targeted genome engineering
<b>12:45-13:15</b>	<b>Lecture 18: Simon See, Shanghai Jiaotong University</b>

**Lunch & Poster (13:15-14:15) in Exhibition Hall**

**SESSION - 7 (14:15-16:15)**

**Chairperson: P. Gautam**

<b>14:15-14:45</b>	<b>Lecture 19: P. Gautam, AU</b>
<b>14:45-15:15</b>	<b>Lecture 20: Parbati Biswas, DU</b> Conformation, Entropy and Hydration Pattern of Ambivalent Helices
<b>15:15-15:45</b>	<b>Lecture 21: Surjit B. Dixit, Zymeworks</b>
<b>15:45-16:15</b>	<b>Lecture 22: James Gomes, IITD</b> Disease Implications of Inter and Intra Protein Networks

**Coffee Break (16:15-16:30)**

**SESSION - 8 (16:30-18:45)**

**Chairperson: D. Mohanty**

<b>16:30-17:00</b>	<b>Lecture 23: Dinesh Gupta, ICGB</b> Use of Plasmodium falciparum gene co-expression networks to identify hubs as potential drug targets
<b>17:00-17:30</b>	<b>Lecture 24: S. K. Saxena, CCMB</b> In silico design of novel, high-affinity neuraminidase inhibitors for Influenza A (H1N1) pdm09 (pH1N1) virus
<b>17:30-18:00</b>	<b>Lecture 25: Garima Khandelwal, Priyanka Dhingra &amp; Tanya Singh</b> SCFBio ( <i>Chemgenome, Bhageerath &amp; Sanjeevini</i> ) Genome to Hits
<b>18:00-18:30</b>	<b>Lecture 26: D. Mohanty, NII</b> Structure based approach for understanding substrate specificity of peptide recognition modules
<b>18:30-18:45</b>	<b>Best Poster Awards &amp; Valediction</b>

## **National Conference on “New Trends in Bioinformatics”**

**Theme: New Methods, Softwares, Databases, Web-tools of Bioinformatics from India**

**Dates: July 30<sup>th</sup> & 31<sup>st</sup>, 2012; Venue: Seminar Hall, IIT Delhi.**

Genomic information for more than ~ 2100 genomes, is now available. NGS technologies while expediting sequencing are posing new challenges for assembly of large genomes. The annotation methods are less than perfect. Newer regulatory and coding regions are being discovered. Eukaryotic genome annotation is still a big challenge. New ways to look at genomic information are required.

Protein secondary structure prediction methods have not evolved beyond 80% accuracy. Tertiary structure prediction methods being assessed via CASP also have reached a stage of 70% accuracy for 3 to 5 Ang structures. Structure based drug design initiatives require higher resolution targets which underscores the need for greater accuracies and precision in structure prediction. Above all, principles governing folding are still elusive.

Drug design continues to be thwarted by affinity versus selectivity and toxicity issues which are still beyond the purview of docking and scoring strategies. Even the latter need better algorithms. While it is clear that systems biology needs to be harnessed in drug discovery, its current utilization is sub-optimal.

Considering the challenges and opportunities involved in creating a pipeline for individualized medicine from the emerging genomic, proteomic and metabolomic information, it is proposed to organize a two day national conference (July 30<sup>th</sup> & 31<sup>st</sup>, 2012) on “New trends in Bioinformatics”.

The conference brings together several leading experts from the country in Bioinformatics to address what has been solved and what remains to be conquered in some key areas on the pathway to developing *in silico* suggestions of personalized medicine.

The conference will feature, 25 leading scientists from the country sharing the latest from their Laboratories, at least 75 students making poster presentations on their discoveries. Overall, about 350 participants are expected.

The conference coincides with the *tenth anniversary* of SCFBio, which has just put together ‘*Dhanvantari*’ software which integrates the latest versions of *Chemgenome*, *Bhageerath* & *Sanjeevini* for genome annotation, protein tertiary structure prediction and target directed lead molecule design respectively, into a pipeline in a high performance computing environment. The participants will have an opportunity to familiarize themselves with methods/softwares/tools/databases from SCFBio as well as from the laboratories of the invited experts.

Through this circular, we at SCFBio extend a warm welcome to all the experts and beginners in Bioinformatics to the conference.