

ACCELRYS Inc &
Institute of Bioinformatics and Applied Biotechnology (IBAB)
Bangalore
Present

GENES to DRUGS: In-Silico Drug Discovery

DATES: 26 June – 15 July 2006

VENUE: IBAB, ITPL, Bangalore

Last Date for registration:

15 June 2006

(Limited Participation,

On a First Come First Served Basis)

For further information contact:

Dr. Nishi Mahapatra/ Ms. Shamala Prasad
Institute of Bioinformatics and Applied
Biotechnology
G 05, Tech Park Mall, International Tech
Park, Whitefield Road
Bangalore 560 066
India

**For map & other information visit our
website: www.ibab.ac.in**

**Telephone: +91-80-2841 0029/ 2841
6034/ 2841 2769**

Fax: +91-80-2841 2761

**Mail: nishi@ibab.ac.in/
shamala@ibab.ac.in**

In today's drug discovery process software tools play a major role as they accelerate the drug discovery cycle. Worldwide Pharmaceutical and Biotechnology Companies are recruiting people with knowledge on using software tools in drug discovery as well as scientific knowledge

Accelrys is the world leader in providing software tools for modeling, computation, simulation, and the management and mining of scientific data used by scientists for product design as well as drug discovery and development.

IBAB is a young institute set up as a Government of Karnataka and ICICI public-private partnership. It started operations in 2002, in Bangalore, India. It has had the involvement of leading academic institutes and industry, which has enabled it to attain high standards in a short period of time. IBAB's mandate is to help grow the biotech industry. The immediate objectives of the institute is to run post graduate programs in bioinformatics and biotechnology, carry out contract research, undertake executive education and promote entrepreneurship.

This course intends to cover sequence analysis, protein modeling and simulation, structure based drug design, QSAR, pharmacophore design, ADME properties and toxicity prediction using Accelrys' world renowned software tools.

The course features:

GCG: a comprehensive sequence analysis tool used by scientists for over 20 years at over 1000 institutions worldwide

Insight II: enables homology modeling, protein modeling and simulation.

Cerius2: offers tools that provide a process for lead design and generation from virtual/real libraries. Quantitative Structure Activity Relationship, Structure based drug design and De novo drug design.

Catalyst: the most used and most successful pharmacophore and 3D database management tool with its patented algorithms.

Fee: Rs. 25,000/- per attendee (Academics)

Rs. 35,000/- per attendee (Corporates/ Other professionals)



GENES to DRUGS In-Silico Drug Discovery

26 June – 15 July 2006

Day – 1: 26 June 2006 (Monday)

S. No.	Module	Start	Speaker	Organization
	Registration	09:00		
Lecture 1	Basic concepts in biology Central dogma of molecular biology	09:30		
	Coffee break	11:00		
Lecture 2	Human Genome project	11:15		
	Lunch break	13:00		
Lecture 3	Introduction to Bioinformatics	14:00		
	Coffee break	15:30		
Lecture 4	Introduction to sequence analysis-1: Sequence based Biological databases, Basic concepts of sequence similarity, identity and homology. Definition of homologues, orthologues and paralogs	15:45		

Day – 2: 27 June 2006 (Tuesday)

S. No.	Module	Start	Speaker	Organization
Lecture 5	Introduction to Sequence Analysis-2: Scoring matrices Dynamic programming; Pairwise sequence alignment (Global)	09:30		
	Coffee break	11:00		
Lecture 6	Pairwise sequence alignment (Local)	11:15		
	Lunch break	13:00		
Lecture 7	Introduction to GCG Software	14:00		
	Coffee break	15:30		
HS-1	Hands on Session-GCG	15:45		

Day – 3: 28 June 2006 (Wednesday)

S. No.	Module	Start	Speaker	Organization
Lecture 8	Introduction to Sequence Analysis-3: Scoring Matrices	09:30		

	Coffee break	11:00		
Lecture 9	Multiple sequence alignment; Need for MSA, Progressive & hierarchical MSA,	11:15		
	Lunch break	13:00		
<i>HS-2</i>	Hands on Session-GCG	14:00		
	Coffee break	15:30		
<i>HS-3</i>	Hands on Session-GCG	15:45		
Day – 4 : 29 June 2006 (Thursday)				
S. No.	Module	Start	Speaker	Organization
Lecture 10	Phylogenetic analysis	09:30		
	Coffee break	11:00		
Lecture 11	Hidden Markov Models	11:15		
	Lunch break	13:00		
<i>HS-4</i>	Hands on Session-GCG	14:00		
	Coffee break	15:30		
<i>HS-5</i>	Hands on Session-GCG	15:45		
Day – 5: 30 June 2006 (Friday)				
S. No.	Module	Start	Speaker	Organization
Lecture 12	Genetic algorithms	09:30		
	Coffee break	11:00		
Lecture 13	DNA Microarray: Basic principles	11:15		
	Lunch break	13:00		
Lecture 14	Gene Annotations	14:00		
	Coffee break	15:30		
<i>HS-6</i>	Hands on Session-GCG	15:45		
Day – 6: 1 July 2006 (Saturday)				
S. No.	Module	Start	Speaker	Organization
<i>HS-7</i>	Hands on Session-GCG (Exercise)	09:00	Participants	

Day – 7: 2 July 2006 (Sunday)				
Day – 8: 3 July 2006 (Monday)				
S. No.	Module	Start	Speaker	Organization
Lecture 15	Principles of Macromolecule structure and function : Proteins	09:30		
	Coffee break	11:00		
Lecture 16	Principles of Macromolecule structure and function : Nucleic Acids	11:15		
	Lunch	13:00		
Demo	Introduction to IinsightII interface	14:00		
	Coffee break	15:30		
HS-8	Hands On – InsightII (Biopolymer Modeling)	15:45		
Day – 9: 4 July 2006 (Tuesday)				
S. No.	Module	Start	Speaker	Organization
Lecture 17	Protein structure prediction (Identification of remote homologue's, Threading)	09:30		
	Coffee break	11:00		
Lecture 18	Homology modeling	11:15		
	Lunch	13:00		
HS-9	InsightII hands: Homology modeling	14:00		
Day – 10: 5 July 2006 (Wednesday)				
S. No.	Module	Start	Speaker	Organization
Lecture 19	Protein Fold recognition and Classification	09:30		
	Coffee break	11:00		
Lecture 20	Structural alignment DALI databases	11:15		
	Lunch	13:00		
HS-10	InsightII: Delphi (Electrostatic surface diagrams)	14:00		
	Coffee break	15:30		
HS-11	InsightII: Delphi	15:45		
Day –11: 6 July 2006 (Thursday)				

S. No.	Module	Start	Speaker	Organization
Lecture 21	Molecular modeling and Simulations: Concepts of Force field	09:30		
	Coffee break	11:00		
Lecture 22	Molecular modeling and Simulations: Energy minimization algorithms	11:15		
	Lunch	13:00		
HS-12	InsightII: Energy minimization and molecular dynamics	14:00		
	Coffee break	15:30		
HS-13	InsightII: Energy minimization and molecular dynamics	15:45		
Day -12: 7 July 2006 (Friday)				
S. No.	Module	Start	Speaker	Organization
Lecture 23	Introduction to Drug Design: An Overview	09:30		
	Coffee break	11:00		
Lecture 24	Docking algorithms	11:15		
	Lunch break	13:00		
HS-14	Hands on session-Cerius2	14:00		
	Coffee break	15:30		
HS-15	Hands on session-Cerius2	15:45		
Day -13: 8 July 2006 (Saturday)				
S. No.	Module	Start	Speaker	Organization
Lecture 25	Structure Based Drug Design-1	09:30		
	Overview of Drug Design			
	Structural information and role of computation			
	Structures in target identification and target validation			
	Molecular recognition-protein small molecule recognition			
	Principles of drug action, Active site detection and characterization			
	Coffee break	11:00		
Lecture 26	Structure Based Drug Design-2	11:15		
	Concepts of ab-initio ligand design, docking			

	Algorithms, ligand conformation, issues for high throughput docking			
	Virtual screening, Lead optimisation			
	Pharmacokinetic and pharmacodynamic issues, structure-based vaccine design, future projections			
	Lunch break	13:00		
Lecture 27	Ligand fit – presentation	14:00		
	Coffee break	15:30		
<i>HS-16</i>	Hands on Session-Cerius2	15:45		
<i>HS-17</i>	Ligand fit contd.			
Day –14: 9 July 2006 (Sunday)				
Day –15: 10 July 2006 (Monday)				
S. No.	Module	Start	Speaker	Organization
<i>HS-18</i>	Ligand fit contd.	09:30		
	Coffee break	11:00		
Lecture 28	De Novo Drug Design- Ludi	11:15		
	Lunch break	13:00		
<i>HS-19</i>	Hands on Session-Cerius2	14:00		
<i>HS-20</i>	Ludi			
	Coffee break	15:30		
<i>HS-21</i>	Ludi	15:45		
Day –16: 11 July 2006 (Tuesday)				
S. No.	Module	Start	Speaker	Organization
Lecture 29	QSAR-I: Property based and topological QSAR	09:30		
	Coffee break	11:00		
Lecture 30	QSAR-2: 3-D QSAR (MSA, MFA, RSA)	11:15		
	Lunch break	13:00		
<i>HS-22</i>	Hands on Session-Cerius2 (QSAR -MFA)	14:00		
	Coffee break	15:30		
<i>HS-23</i>	QSAR -Regression technique	15:45		

Day –17: 12 July 2006 (Wednesday)				
S. No.	Module	Start	Speaker	Organization
<i>HS-24</i>	Hands on Session-Cerius2: QSAR contd- Regression technique	09:30		
	Coffee break	11:00		
<i>HS-25</i>	QSAR contd -Genetic Function Approximation	11:15		
	Lunch break	13:00		
Lecture 31	ADME: Introduction	14:00		
	Coffee break	15:30		
<i>HS-26</i>	ADME – Hands on	15:45		
Day –18: 13 July 2006 (Thursday)				
S. No.	Module	Start	Speaker	Organization
Lecture 32	Introduction to catalyst	09:30		
	Coffee break	11:00		
Lecture 33	Autodock	11:00		
	Lunch break	13:00		
<i>HS-27</i>	hands on	14:00		
	Coffee break	15:30		
<i>HS-28</i>	hands on			
Day –19: 14 July 2006 (Friday)				
S. No.	Module	Start	Speaker	Organization
Lecture 33	Introduction to Discovery Studio	09:30		
	Coffee break	11:00		
Demo	Introduction to Discovery Studio	11:15		
	Lunch break	13:00		
<i>HS-29</i>	Hands on	14:00		
	Coffee break	15:30		
<i>HS-30</i>	Hands on	15:45		

Day -20: 15 July 2006 (Saturday)

S. No.	Module	Start	Speaker	Organization
Lecture 34	In-Silico Drug Designing for Tuberculosis	09:30		
	Coffee break	11:00		
Lecture 35	Significance of identifying SNPs	11:15		
	Lunch break	13:00		
Lecture 36	Structural genomics, Protein arrays	14:00		
	Coffee break	15:30		
Lecture 37	Functional genomics	15:45		



Registration form

GENES to DRUG In-Silico Drug Discovery

26 June - 15 July, 2006

Name: _____ Designation: _____

Education: Current: _____

Last degree: _____

Current Company/ Institute/ College: _____

Residential address: _____

City/ Pin: _____ Phone: _____

Email: _____

Please repeat the same e-mail: _____

Payment details: DDs favouring “Institute of Bioinformatics and Applied Biotechnology” payable at Bangalore.

DD no: _____ Bank: _____ Amount: _____

I wish to participate in the above-specified lab course. Please register me for the same. I have understood the objectives, contents and other details of the course, which was available via the poster and the website or the course co-ordinator at IBAB. I understand that the fees won't be refunded under any circumstances. I certify that all the above information is correct to the best of my knowledge.

Signature: _____ Date: _____

Registration: Send the filled form along with the DD to

Dr. Nishi Mahapatra

Co-ordinator, Lab Procedures in Biotechnology and Bioinformatics

Institute of Bioinformatics and Applied Biotechnology

G-05, Tech Park Mall, ITPL

Whitefield Road, Bangalore – 560 066

Additional Information:

Current Research/work Area:
