**Mohan Rao, Ph.D (Computational Biology)**
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## Professional Experience

**Principal Research Scientist**, TransTech Pharma, High Point, North Carolina, USA (2002-)

**Senior Research Scientist,** Inflazyme Pharmaceutical Ltd, Vancouver, Canada (2001-2002)

**Research Scientist,** GlycoDesign Inc, Toronto, Canada (1999-2001)

**Research Associate, The Scripps Research Institute,** La Jolla, California, USA (1994-1999)

**Citizenship: CANADA**

## Education

**Ph.D** in Computational biology, Thesis " **Computer Modeling of Protein-Ligand interactions" Indian Institute of Science**, Molecular Biophysics, Bangalore, India.

The project was to model the interactions of lectin, Wheat Germ Agglutinin with various saccharide inhibitors; carried out high temperature molecular dynamics studies on saccharides to exhaustively search the conformational space. Later I docked these saccharide conformers to the lectin by using stereochemical contact criteria as preliminary screening and positioning method and subsequently refining the complex by using potential energy minimization in Torsional angle-rigid body rotation space.

**M.S**. in Physics, "A" grade

**B.S**. in Physics, Chemistry and Mathematics, "A" grade.

## Highlights of Qualifications

Extensive experience in Computer Aided Drug Design approach, Pharmacophore, ADMET modeling, Insilico high-throughput screening,

Structure based protein design

Expert in Protein-Protein and Protein-Ligand docking methods/applications

Outstanding skills in researching all aspects of bimolecular interactions.

Extremely well organized; follow through the last detail.

## Grants

i. SBIR, **"Accelerated Drug Discovery Through Computational Biology"** (2004-2006)

ii. Small Business biodefense Program (administered by NIH)], **"Novel Orthopox Small Molecule Antivirus"** (2004-2006)

**US Patents**

i. Modulators of galactosyltransferases. Inventors: Mohan Rao and Igor Tvaroska. (2001)
ii. Computational design of glycosylatransferase active sites and their modulators. Inventors: Mohan Rao,Isabelle Andrea, Tobor Kozar and Igor Tavroska. (2002)
iii. Aryl and heteroaryl compounds, compositions, and methods of use (2005)
iv. Ligands for I7L as modulators of orthopox viruses and methods for drug discovery thereof (WO2005/069012 A12)(2005)

## Selected Research Publications


1. Bolken, T., Byrd, C., Mjalli, A., Arimilli, A., Andrews, R., Rothelein, R., **Andrea, T., Rao, M.S**, Hruby., D. Optimization of orthopoxvirus antiviral drugs that block viral maturation. , (Nov 2004). J. of Virology,Vol78,p12147-12156.

2. Jian Cui' David Crich, Donald Wink, Matthew Lam, Arnold L. Rheingold, David A. Case, WenTao Fu, Yasheen Zhou, **Mohan Rao, Arthur J. Olson** and Michael E. Johnson. Design and synthesis of highly constrained factor Xa inhibitors: amidine-Substituted bis(benzoyl)-[1 and 3]-diazepan-2-ones and bis(benzylidene)-bis(*gem*-dimethyl)cycloketones, Biorg Med.chemistry,2003, 11:3376.

3. **Rao, M.S**.,and Tvaroska,I. Structure of alpha 1-3 Galactosyltransferase and its complexes. -Proteins 2001 44:428.

4. Yong-Mei Zhang, **Mohan S. Rao,** Richard J. Heath, Allen C. Price, **Arthur J. Olson**, Charles O. Rock, and Stephen W. White. Identification and Analysis of the Acyl Carrier Protein (ACP) Docking Site on-Ketoacyl ACP Synthase III -J.Biol.Chem. 2001 276: 8231

5. **Rao, M.S**., Olson, A.J. Modeling of factor Xa-inhibitor complexes: A computational flexible docking approach. -Proteins 1999 34:173.

6. Coombs, G.S., **Rao, M.S., Olson, A.J**., Dawson, P.E., Madison, E.L. Revisiting catalysis by chymotrypsin family serine proteases using peptide substrates and inhibitors with unnatural main chains. -J.Biol.Chem. 1999 274:24074.

7. Ruf, W., Shobe, J., **Rao, S.M.,** Dickinson, C.D., **Olson, A., Edgington, T.S**. Importance of factor VII Gla-domain residue Arg-36 for recognition of the macromolecular substrate factor X Gla-domain. -Biochemistry 2000 38:1957.

8. Molecular docking programs successfully predict the binding of b-lactamase inhibitory protein to TEM-1 b- lactamase. Nature str. Biology 1996 Vol 3 ,p 233-239.

**Conference papers**

15 conference posters and presentations based on my industrial computational modeling projects.

**Membership of Professional Associations**

The Protein Society

American Chemical Society

Society of Glycobiology

## Relevant Experience

Expert in use of several commercially available molecular modeling packages including InsightII, Discover, LUDI (de novo design), Pharmacophore modeling, Cerius 2, Catalyst , Modeler, QSAR, AutoDock, Dock, Schrodinger, Moe Suite of programs and cheminformatics tools

Programming ability in Fortran, Pascal and C. Knowledge in Tcl, JAVA ,SQL/PL SQL, and HTML.

Experience in UNIX, Linux, MSDOS, WINDOWS' NT and 2000. Worked on a variety of computer platforms such as SGI, SUN Spark, HP, CONVEX, VAX and IBM compatible machines

Successful completion of **Laboratory to Leadership course**

References:

**Prof. Arthur J. Olson**,
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**Prof. Thomas S. Edgington**,
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**Prof. Melvin Okamura**
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