



# Your Preferred Knowledgeable CADD Partner



# INDRAS<sup>®</sup>

*In Silico Discovery Research Academic Research Services Pvt. Ltd.*  
44-347/6, Tirumalanagar, Moula Ali, Hyderabad-500040, TS, INDIA

**SREEDHARA RAO, VOLETI, Ph.D**  
Managing Director

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# Philosophy of INDRAS

**INDRAS**<sup>(R)</sup> - A Company Caters  
***Rational In Silico Solutions*** To  
Organizations Conduct ***Drug Design***  
***& Discovery Research***



# Vision and Mission Statement

**VISION : To Promote CADD Utility in Research & Teaching Oriented Organizations, and Generate Clinical Candidates**

**Mission : To Generate Jobs in CADD for At least 10-Scientists by 2020**



# Working Relationship

## INDRAS

- Consult : Expert CADD Consultancy
- Contract : In-source CADD Solutions
- Collaborate: Knowledgeable CADD Research

**With Academia, Institutes, and Industry  
in Research in Drug Design and Discovery**



# INDRAS Consulting Arrangements

## Consulting Modes:

1. Individual KOL to Clients in Business Meetings
2. Project-based Expert Research Advise
3. Install and Manage CADD Center at Client-Site



# INDRAS Contracting Arrangements

## Contracting Modes:

- 1. Install and Manage on-site Contract Work**
  - Enhanced CADD-Scientist Interactions
- 2. In-source Client's CADD Project Work**
  - Accomplish and Share Timely Research Outcomes



# INDRAS Collaborating Arrangements

## Collaborating Modes:

### 1. Work in Tandem with Organizations

- To Facilitate CADD Component in Research Projects of Drug Discovery.

### 2. Work with Organizations

- Analyze, Write, and Manage Research Grants Collaborating with Organizations.



# Company Information - INDARAS

- **Incorporated** - October, 2013
- **Location** - Hyderabad, TS, India.
- **Infrastructure** - CADD Computing Hardware
- **Expertise** – ~20 Years of In Silico Drug Discovery
- **Manpower** – Turn-key and PhD qualified.





# Founders & Advisor



**Dr. Sreedhara R. VOLETI**  
Founder – MD/CEO

Dr. Sreedhara Voleti has a PhD in chemistry from Indian Institute of Science (IISc), and postdoctoral research in engineering and biology with work experience in Pharma R&D of over 20+ years in USA and India. He is a passionate entrepreneur and founded INDRAS & Theraxel Discoveries.



**Mr. Ravikanth S. Bh.**  
Co-Founder – CFO

Mr. Ravi Kanth has served various business sectors like HR consulting, IT & ITES Outsourcing Services, Oil & Gas Industry products Trading, Agricultural Commodities Trading. At present Mr. Ravi Kanth stays in Malawi working as GM Operations with a reputed Agricultural chemical, Pesticides, Farm Implements.



**Dr. Uday Saxena**  
Advisor

Dr. Uday Saxena is the Co-Founder of Reagene Innovations. He has held several executive and leadership positions in pharmaceutical industry across the globe. He was associated with the Team at Parke-Davis/Pfizer that discovered Lipitor/atorvastatin, a block buster drug for cardiovascular complications.



# Founder & Promoter



**Dr. Sreedhara R. Voleti, PhD**

**Founder & Managing Director**

Sree is a specialist researcher in the fields of Molecular Modeling and computer aided drug design/discovery for ~20 years with academic, Pharmaceutical industry, and non-profit organizational settings both in USA and India. He brings valuable research and managerial expertise in this arena. Sree, published, managed, supervised CADD teams, conducted in silico rational drug discovery of various therapeutic areas. He promotes CADD in academic and industry scenario - and he is passionate about teaching, training, and parting research knowledge of CADD.

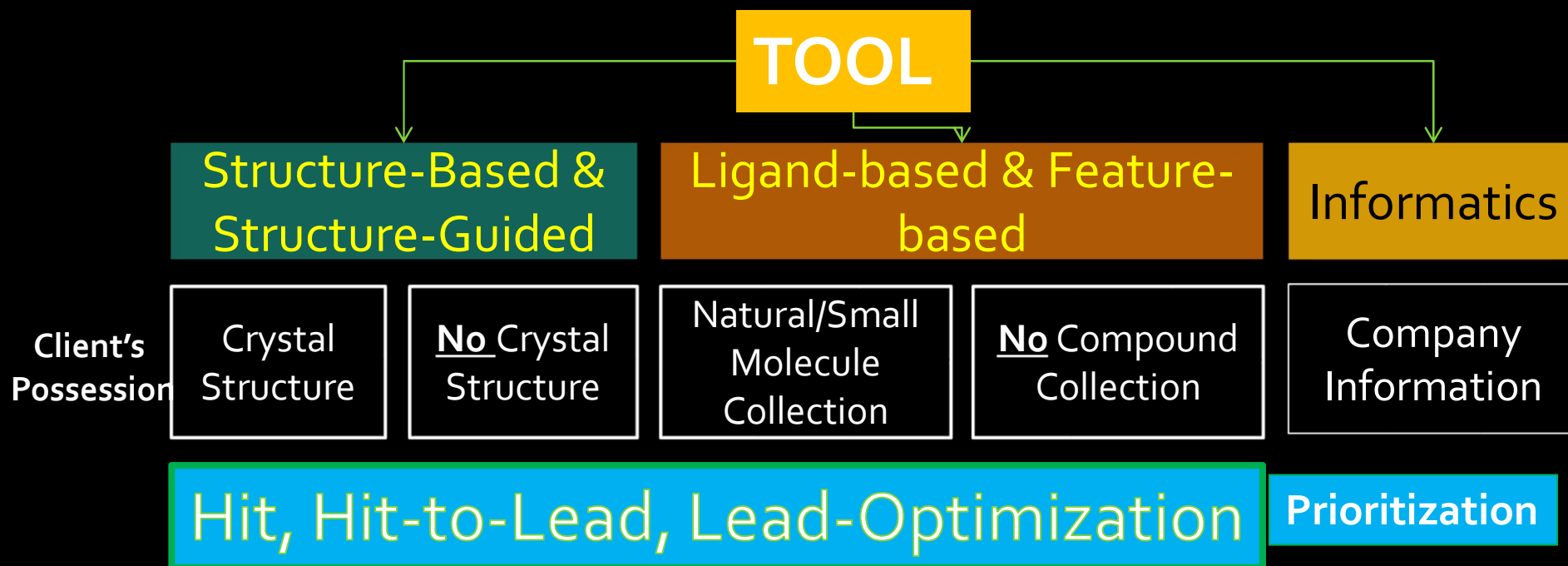


# Key Career Achievements

- **Played Key Role With Med. Chem. Teams in Discovery of MMP9-12, 5LO-H1 dual-inhibitor Clinical Candidates**
- **Successfully Optimized and Prioritized dual DPP4-ACE Inhibitor That Saved Time/Money/Resources for Research Organization**
- **Attracted Funding in Designing Selective Subtype PI3K/Mtor Inhibitors For Treatment Of Cancers**
- **Identified Potential TAK1 Receptor Antagonists as ALTERNATE THERAPY in T2DM**
- **Successfully Supported Over 30 Research Projects Across Diverse Therapeutic Areas**
- **Consulted with Camitro Corporation, Inc., now Transformed as OPTIBRIUM, UK.**
- **Recognized with APPRECIATE Award (Runner Up) by Global Ranbaxy R&D for Successful Data Management to Desktop, Corporate Data Access-to-Desktop Facilitating Over 500 Scientists of R&D**



# Key CADD Tools



- Structural Analysis
- Hit-Finding & optimization
- in silico ADMET profile
- Lead Optimization
- Lead Hopping

- Build qualified Homology Model
- Hit-finding & optimization
- in silico ADMET profile
- Lead Optimization
- Lead Hopping

- Shape/Electrostatics screening,
- Pharmacophore-based screening,
- Property-based screening for Hit-finding, Possible Therapeutic Application

- Screen Commercial Libraries (ZINC, CoCoCo) for Hit-finding



# Case Studies

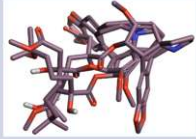
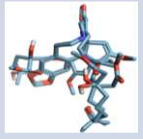
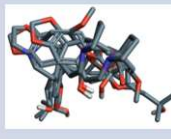

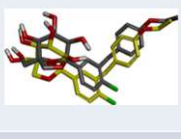
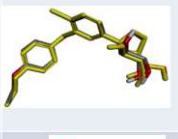
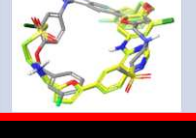
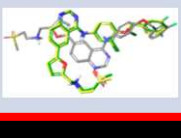
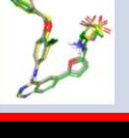
1. CHEMVEDA Life Sciences & NIPER, Hyd.
2. Connexios Life Sciecnas
3. Glenmark Pvt. Ltd.
4. Incozen Therapeutics Pvt. Ltd.
5. Laxai Avanti Life Sciences Pvt. Ltd.
6. ReaGene Innovations Pvt. Ltd. & Tech Mahindra



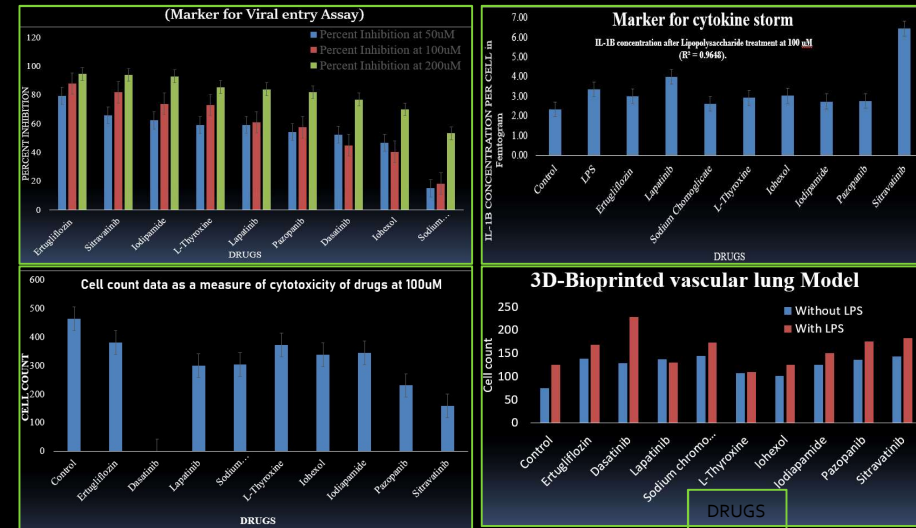
# Drug Repurposing as Therapeutics for COVID-19

With ReaGene Innovations Pvt. Ltd. & Tech Mahindra Pvt. Ltd. (2020-2021)

## Conformational Consistency of Top Repurposed Drugs

#		Mpro Site	S1-1 Site	S1-2 Site
1	Homo-harringtonine			
2	Ertugliflozin			
3	Lapatinib			

## In Vitro Results of the Prioritized Repurposed Drugs



1. Identification of SGLT2 inhibitor Ertugliflozin as a treatment for COVID-19 using computational and experimental paradigm. BioRxiv [2021.06.18.448921](https://doi.org/10.1101/2021.06.18.448921);
2. Tyrosine Kinase Inhibitor Family of Drugs as Prospective Targeted Therapy for COVID-19 Based on In Silico And 3D-Human Vascular Lung Model Studies, BioRxiv [2021.05.13.443955](https://doi.org/10.1101/2021.05.13.443955)
3. In silico and in vitro Demonstration of Homoharringtonine's Antagonism of RBD-ACE2 Binding and its Anti-inflammatory and anti-thrombogenic Properties in a 3D human vascular lung model, BioRxiv [2021.05.02.442384](https://doi.org/10.1101/2021.05.02.442384);
4. **Mini Review:** Emergence of New Drug Discovery Paradigm using Computational and Experimental Biology, Journal of Infectious Diseases and Diagnosis, Vol.6. iss.2, #152. (2022)

Patent filed:

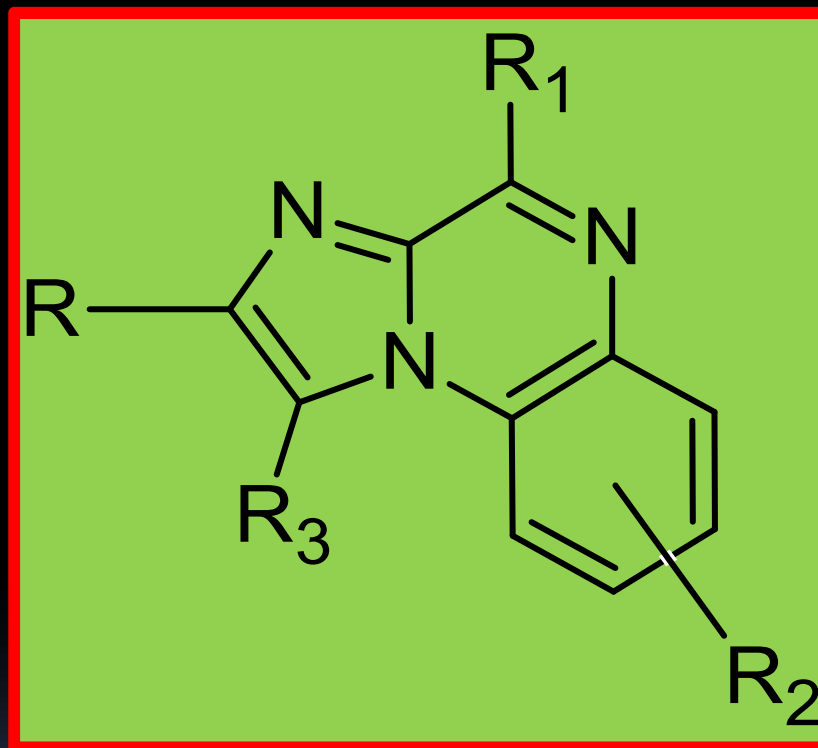
Rational Identification of FDA Approved Drugs by Computational Modelling and Inhibition of RBD/ACE2 Binding for Treatment of COVID-19., PCT/IB2021/057470, 13 August 2021



# Designed Selective Inhibitors

With CHEMVEDA Life Sciences & NIPER, Hyderabad

BIRAC – SBIRI Project (2016-18)



Designed Selective PI<sub>3</sub>K $\alpha$ -, PI<sub>3</sub>K- $\beta$ , and dual mTOR-PI<sub>3</sub>K $\alpha$ , mTOR-PI<sub>3</sub>K $\beta$  Inhibitors in Oncology



# Active Sites of PI3K isoforms & mTOR



4JPS

PI3K- $\alpha$



4BFR

PI3K- $\beta$

PI3K- $\gamma$



3L54



2WXJ

MOLCAD  
Surfaces



mTOR (4JT5)

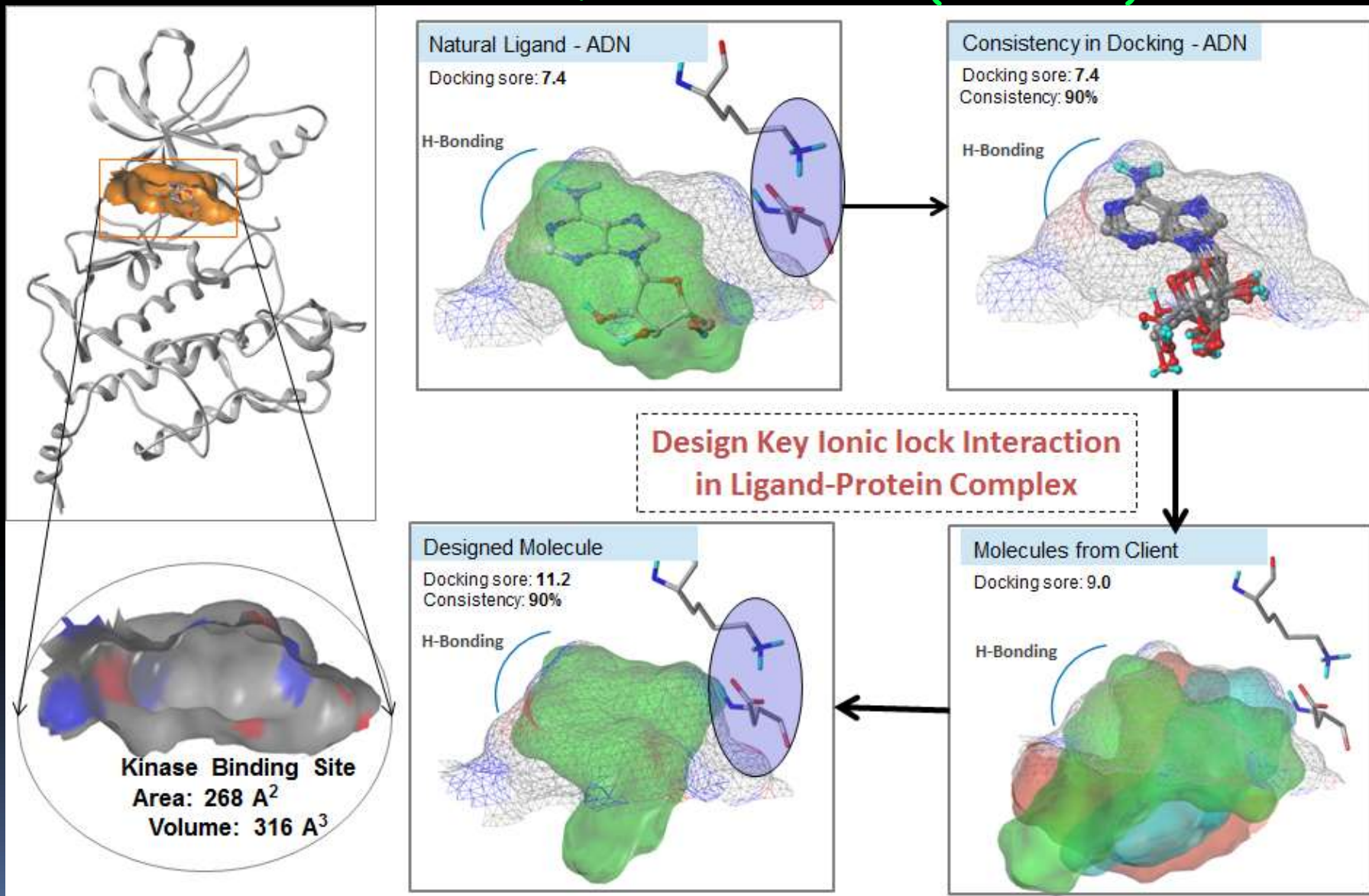
Kinase (PDB-ID)	Surface Area (Å <sup>2</sup> )	Cavity Volume (Å <sup>3</sup> )
PI3K- $\alpha$ 4JPS	406	445
PI3K- $\beta$ 4BFR	475	592
PI3K- $\gamma$ 3L54	420	531
PI3K- $\delta$ 2WXJ	336	430
mTOR 4JT5	416	521





# Design of Inhibitors to TAK1 Kinase Binding site

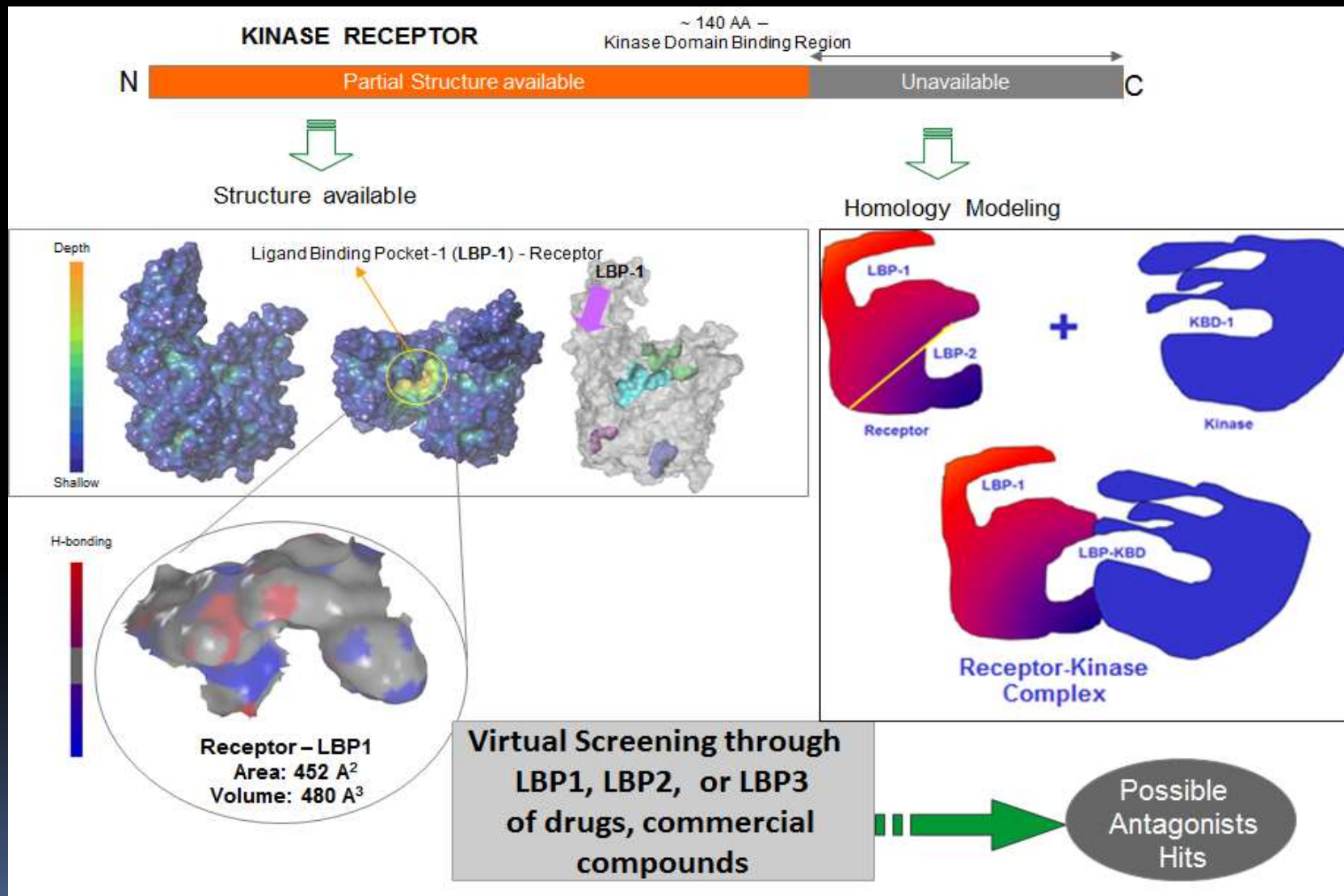
With Connexios Life Sciences Pvt. Ltd. (2014-2016)





# TAK1 Receptor Complex Antagonists & Virtual HTS

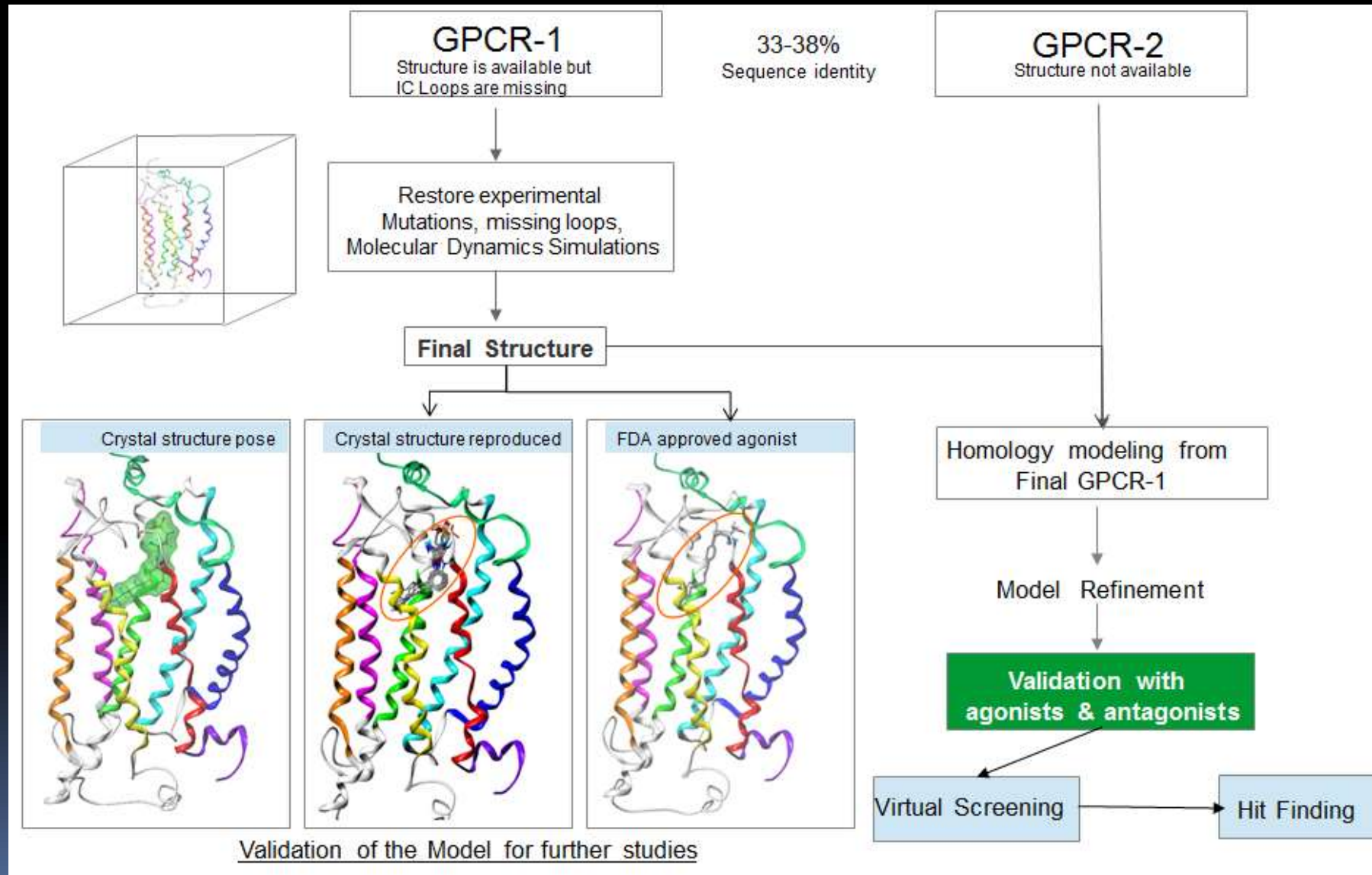
With Connexios Life Sciences Pvt. Ltd. (2014-2016)





# Modeling GPCRs in Metabolic Disorders

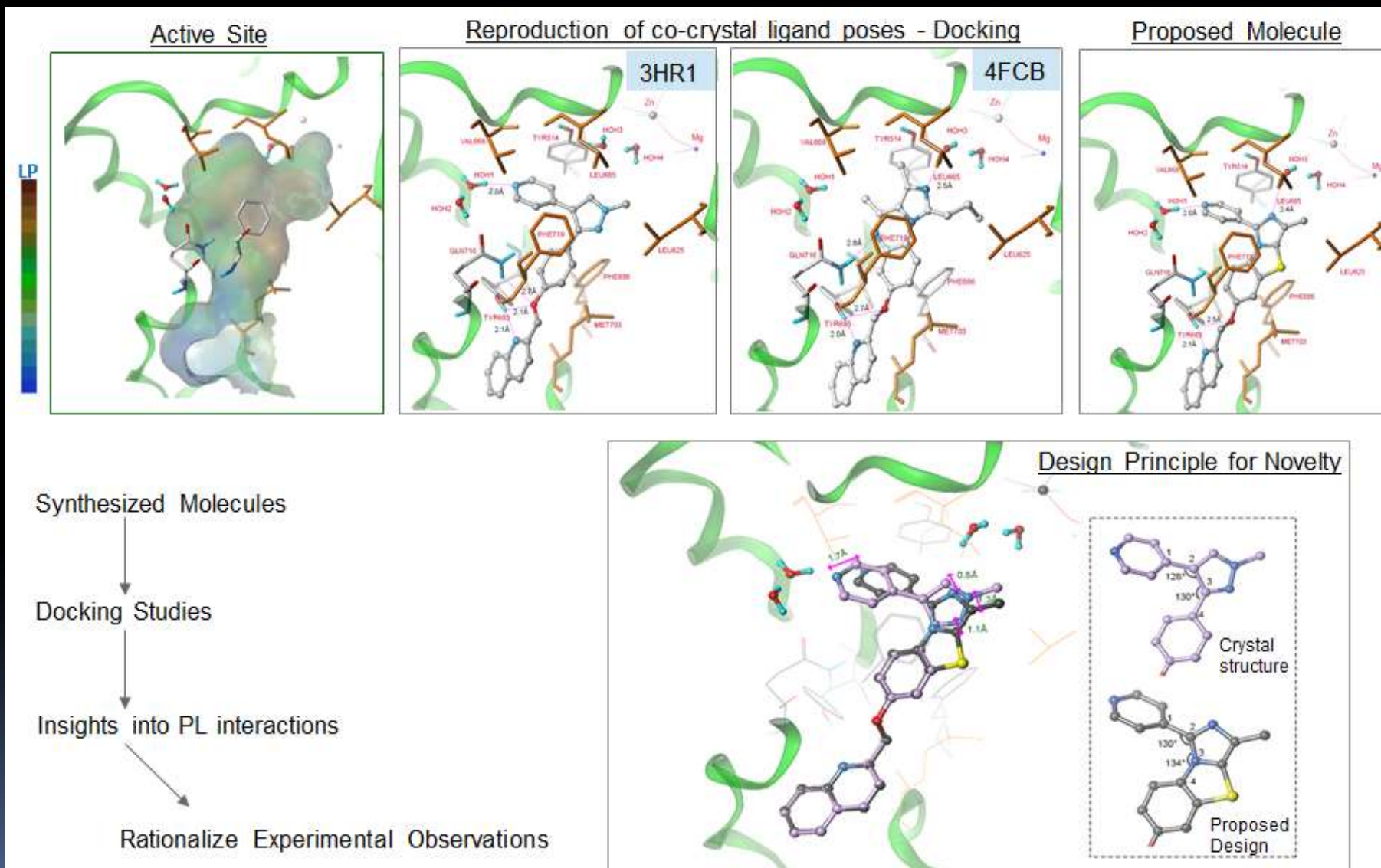
With Connexios Life Sciences Pvt. Ltd. (2014-2016)





# Rationalize Phosphodiesterase PDE10A Inhibitors

With GLENMARK Pvt. Ltd. (2014)



Biorg. Med.Chem. Let. 23, (2013) 6747-6754



## Example Slides

1. Modeling P-L-I in a Single Target (GPCR) - C<sub>3a</sub>R
2. Fragment-based P-L Interactions in an Enzyme - PTP-1B
3. Modeling P-L-I in Dual-action Targets (GPCR-Enzyme) - H1-5LO
4. vHTS in an anti-bacterial Target – Gyr-B
5. Modeling & vHTS for an anti-tuberculosis (*MTb*) Target - CM

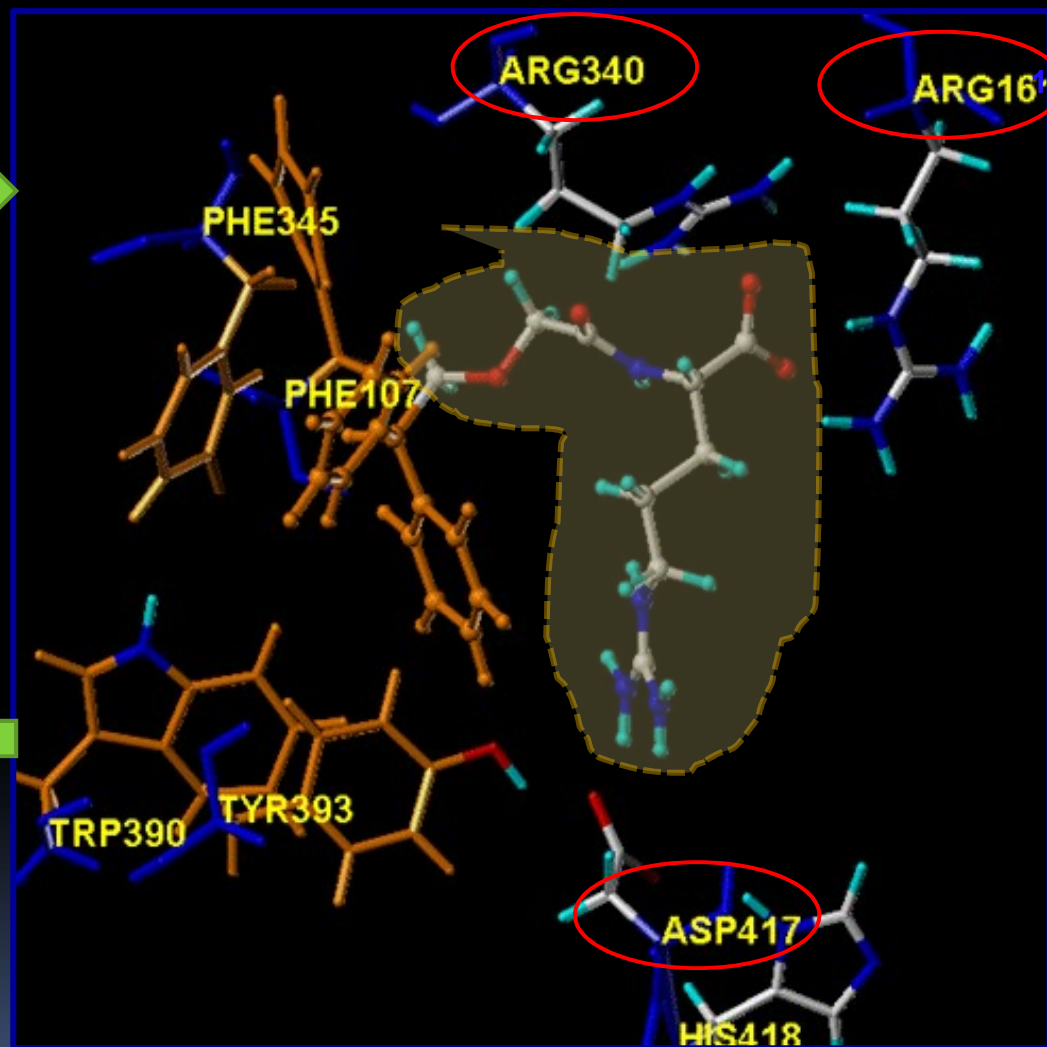
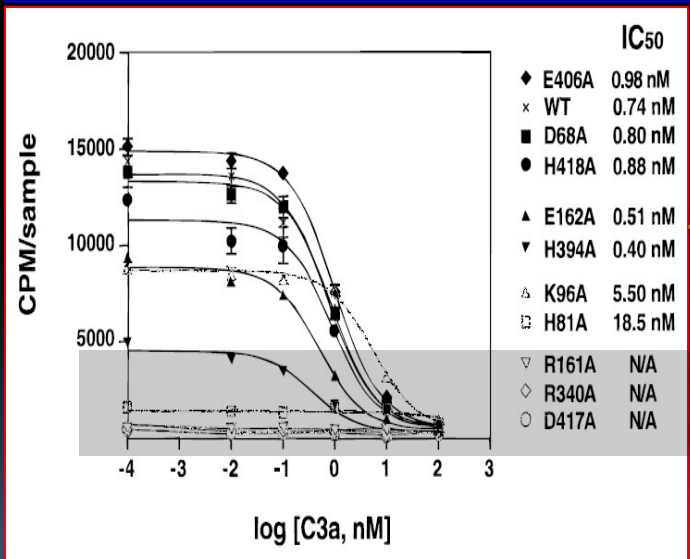
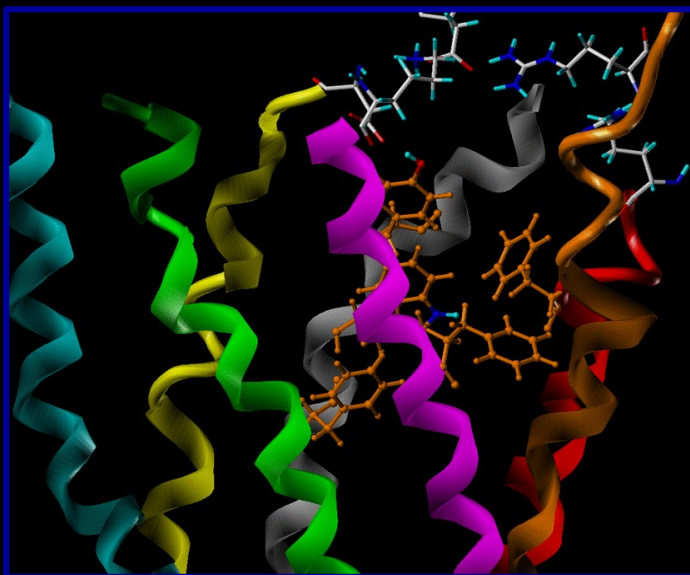
P-L-I : Protein Ligand Interactions  
vHTS:- virtual Highthroughput Screening  
GPCR: g-Protein Coupled Receptor

mTb: mycobacterium Tuberculosis  
PTP-1B: Protein-tyrosine phosphatase 1B  
Gyr-B: Gyrase-B    CM :- Chorismate Mutase

5LO : 5-Lipoxygenase  
H1 – Histamine-1



# Case Study I - GPCR - C3aR & Rationalized Interactions

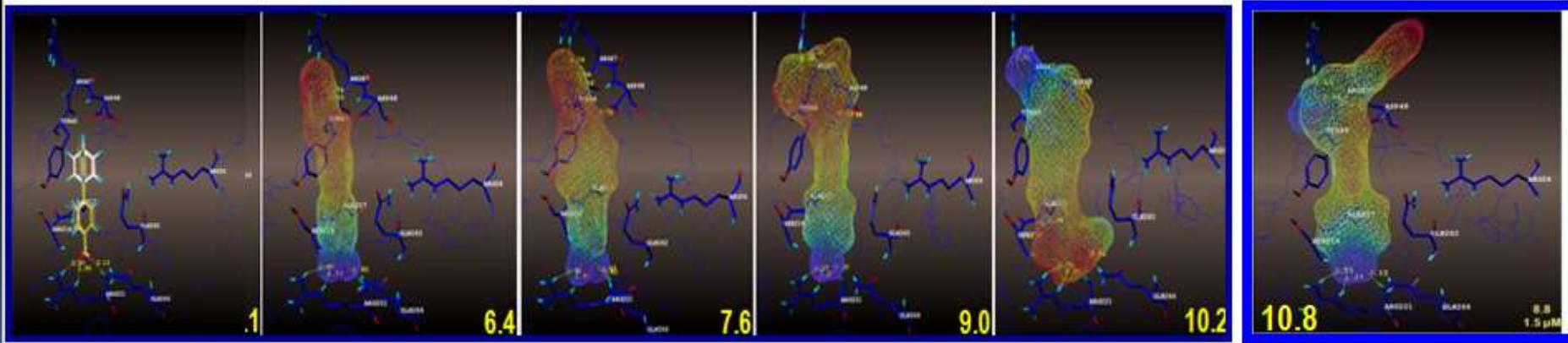
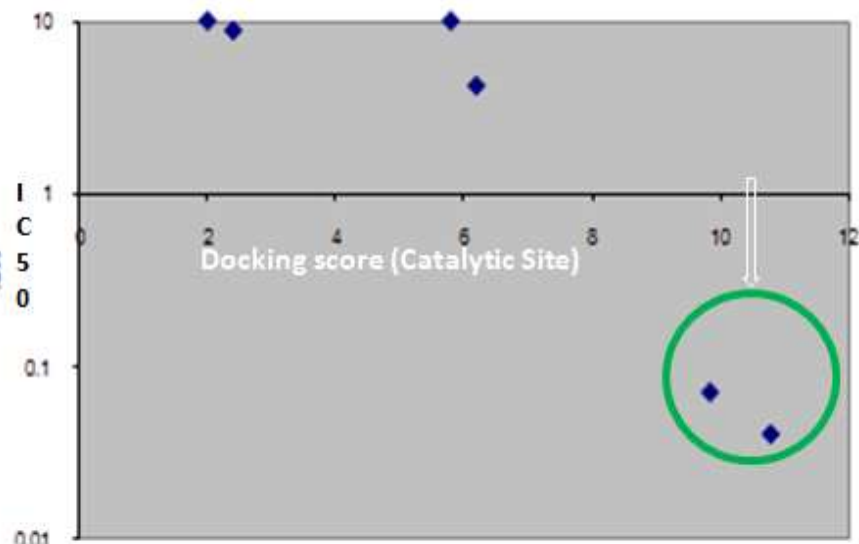
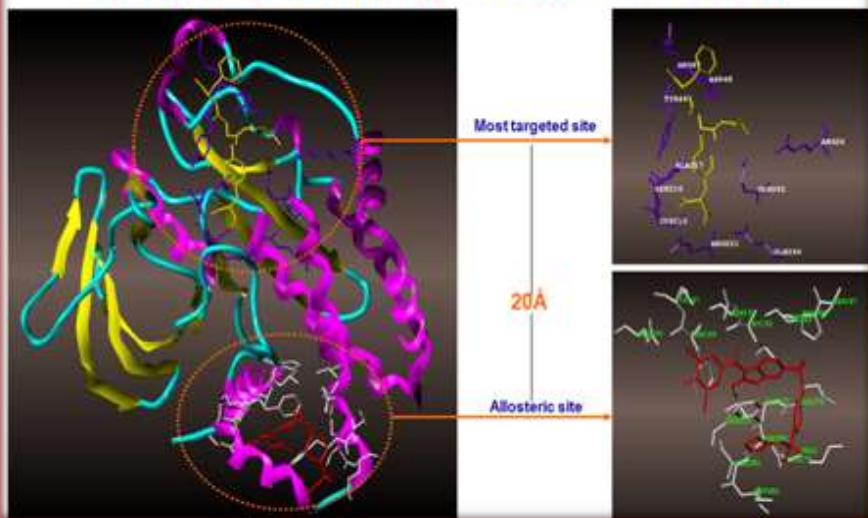


Voleti S.R., *Int. J. Drug Disc.*, 1, 128-136 (2012)



# Case Study II - Enzyme (PTP-1B)

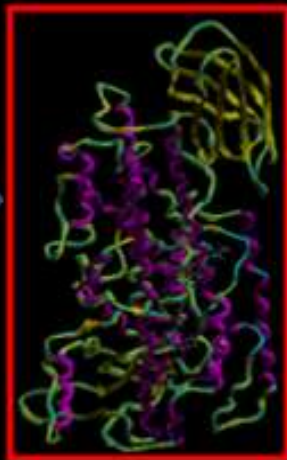
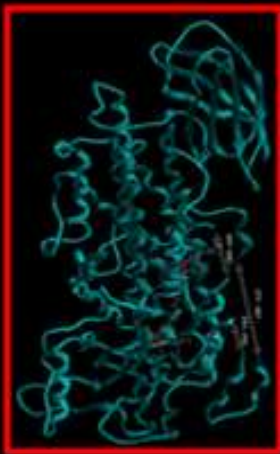
## Inhibitor Binding Site/s of PTP1B



DST Funded Project: SR-S1-OC-03/2010) – INR 5.4Mn

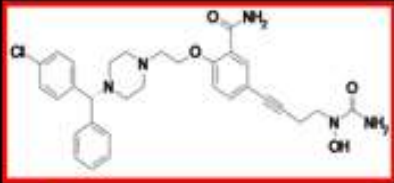
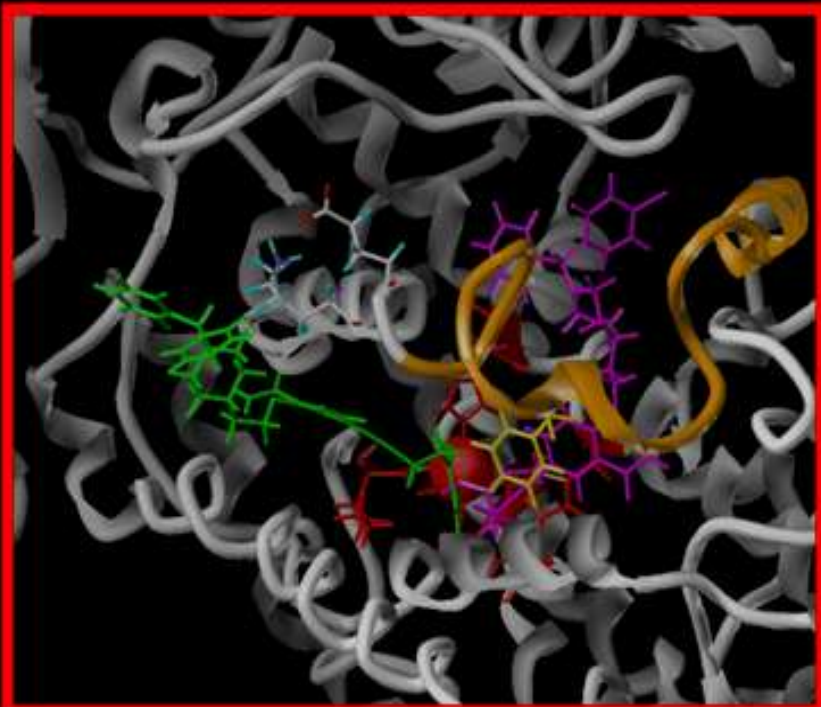
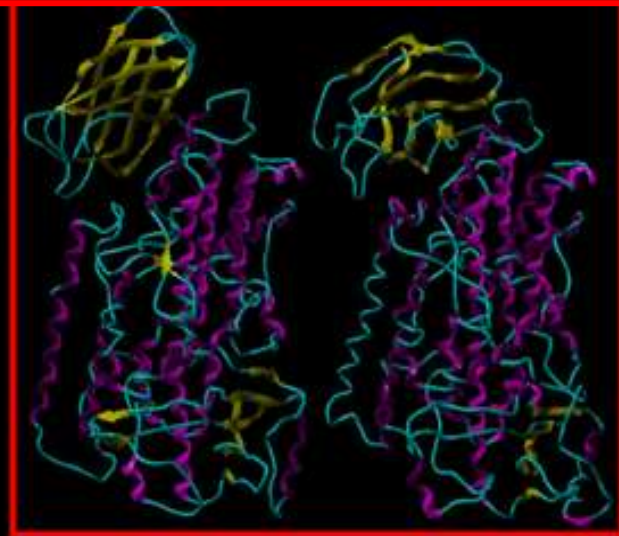


# Case Study III - GPCR and Enzyme (H1-5LO)



**Rbt 15-LO and Hum 5-LO**

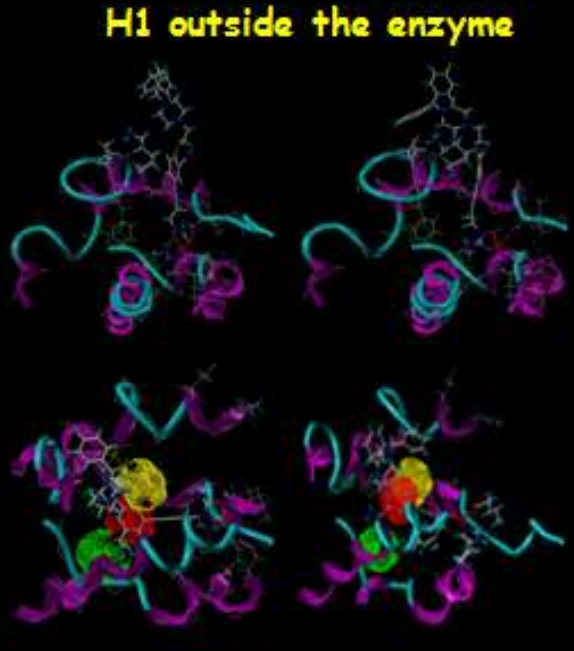
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5	U01425	344	Rattus norvegicus
6	U01426	344	Rattus norvegicus
7	U01427	344	Rattus norvegicus
8	U01428	344	Rattus norvegicus
9	U01429	344	Rattus norvegicus
10	U01430	344	Rattus norvegicus
11	U01431	344	Rattus norvegicus
12	U01432	344	Rattus norvegicus
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98	U01518	344	Rattus norvegicus
99	U01519	344	Rattus norvegicus
100	U01520	344	Rattus norvegicus



H1	RBL	HWB	Hrb5LO
Ki	IC50	IC50	IC50
(nM)	(nM)	(nM)	(nM)
110	100	109	180

**8 orientations**

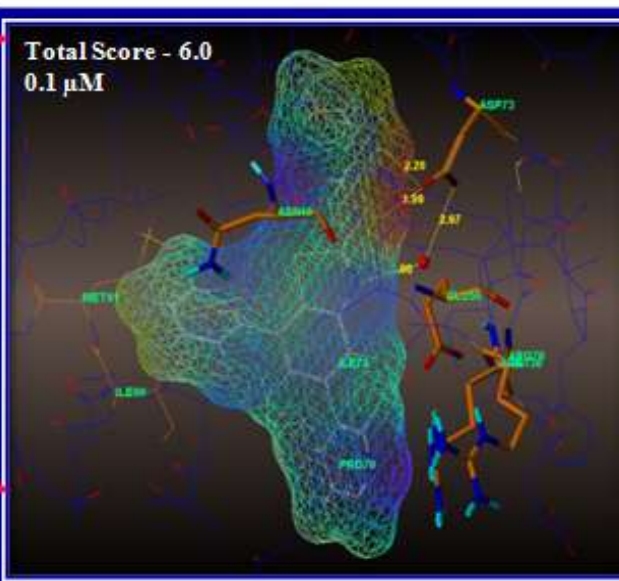
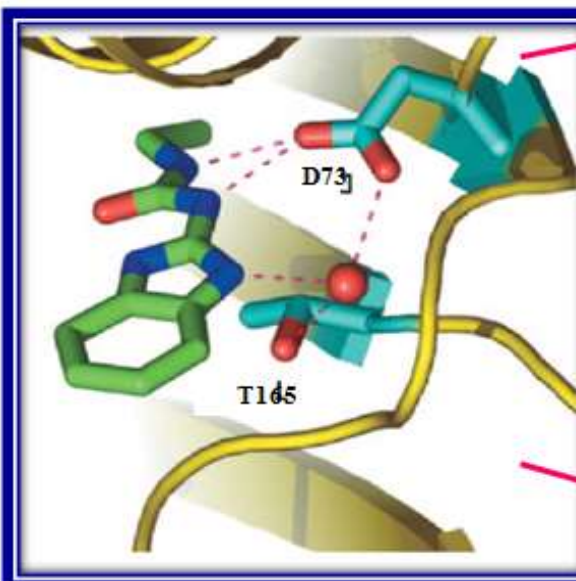
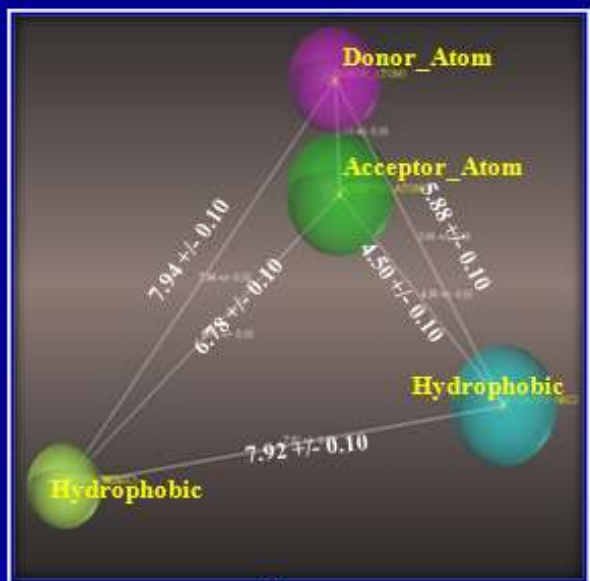
•11th Infl. Res. As. Conf., Bolton Landing, NY, USA, (2002)







# Case Study IV - Multi-CADD tool Screening (GyrB)

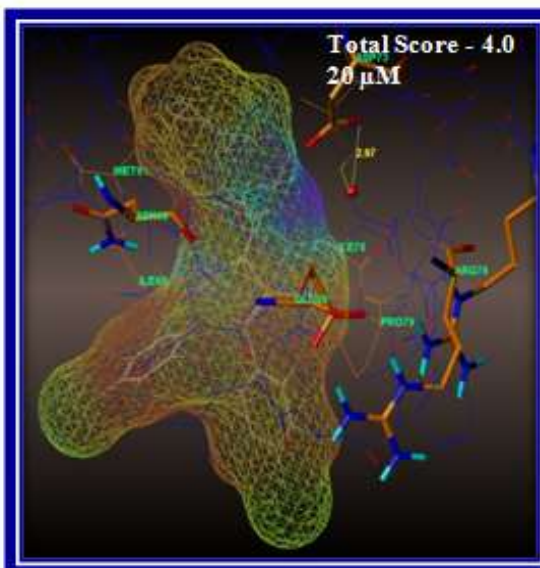


Various filters

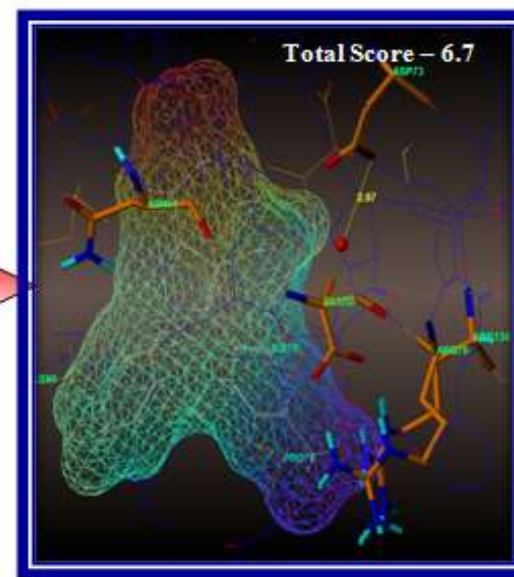
Databases Searching

Molecular Docking /  
Torsional Minimization / QFIT

Hits

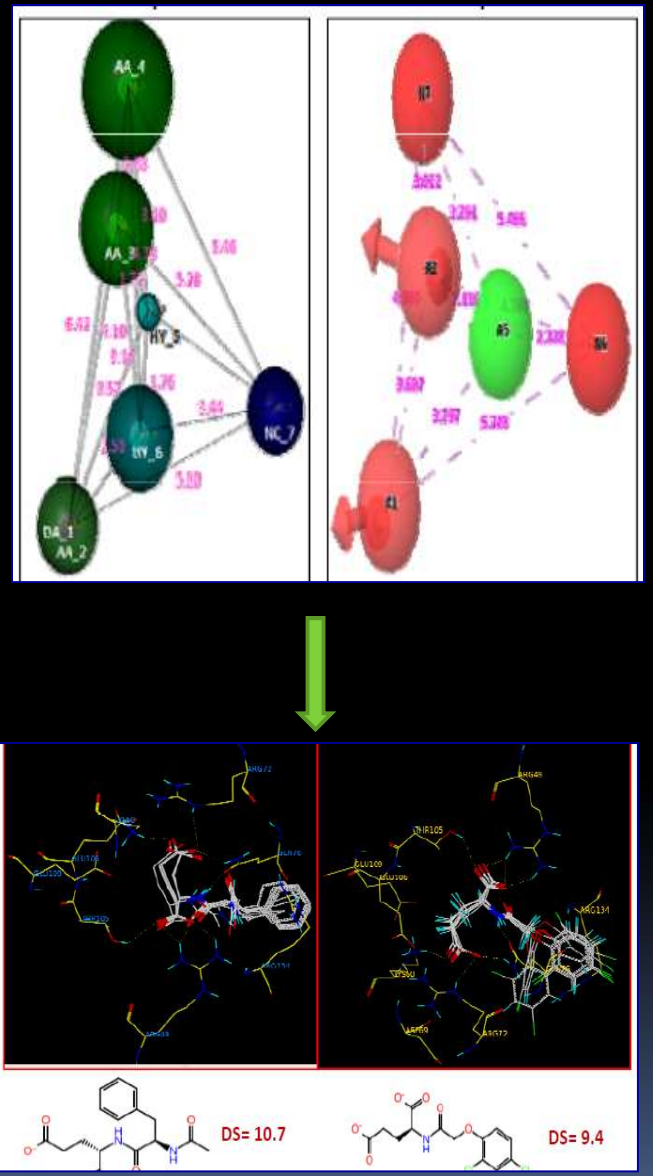
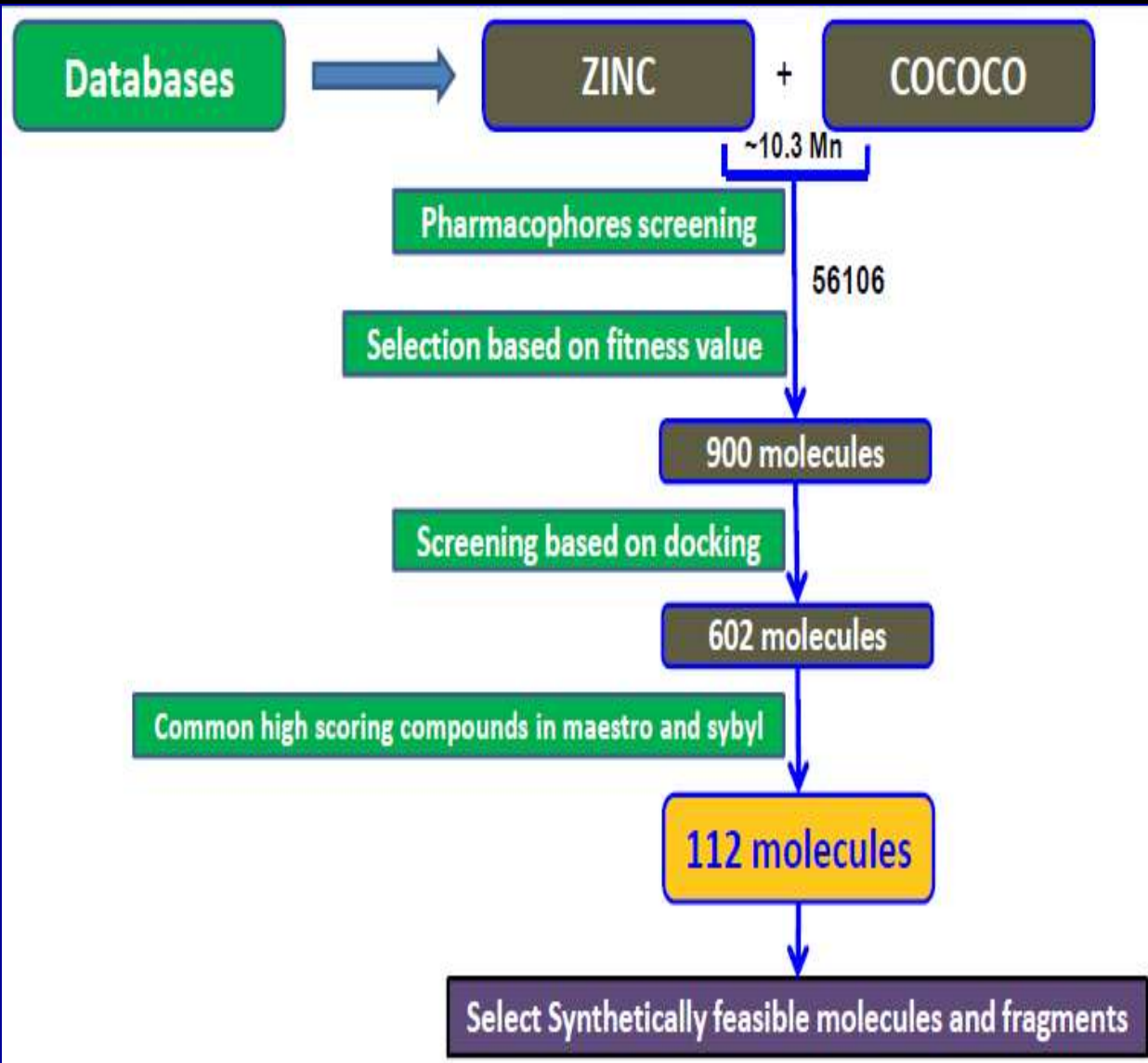


Structure Based  
Lead Opt.





# Case Study V - Multi-CADD tool Screening (CM in mTb)



Co-PI: DBT's Centre for Excellence in TB (ILS, Hyderabad)



# Informatics Capabilities

## Cheminformatics - Data Management & Visualization

The screenshot displays a comprehensive cheminformatics software interface with several key components:

- Structure Viewer:** A list of 23 marked compounds with their IDs (194, 223, 229, 231, 278, 454, 686, 723, 724, 1339, 1340, 1343, 1359, 1361, 1373, 1376, 1377, 1380, 1397, 1407, 1408, 1411, 1542) and corresponding chemical structures.
- Coincidence:** A scatter plot showing the relationship between SOM clustering (x-axis, 1-8) and K-means clustering (y-axis, 1-8). Points are colored and sized based on their cluster membership.
- Scatter Plot:** A plot of FING\_3 (y-axis, 0-180) versus SOM clustering (x-axis, 0-12). Points are colored by cluster.
- Table:** A data table with columns ID, EXTREG, and MDLNUMBER, listing 12 records.
- Query Devices:** A panel for searching and filtering data, showing SOM clustering (rank) and similarity values.
- Details-on-Demand:** A table providing detailed information for each compound, including ID, EXTREG, MDLNUMBER, FING\_3, and ATO.
- K-means clustering:** A bar chart showing the count of compounds in each of the 8 clusters.
- Self-Organizing Maps:** A grid of plots showing the distribution of compounds across different SOM clusters.

At the bottom, the status bar indicates "Ready" and "1575 out of 1575 records visible (100.00 %), 23 marked".



# Your Partner for Rational Drug Design/Discovery



Insilico Discovery Research Academic Services Pvt. Ltd.

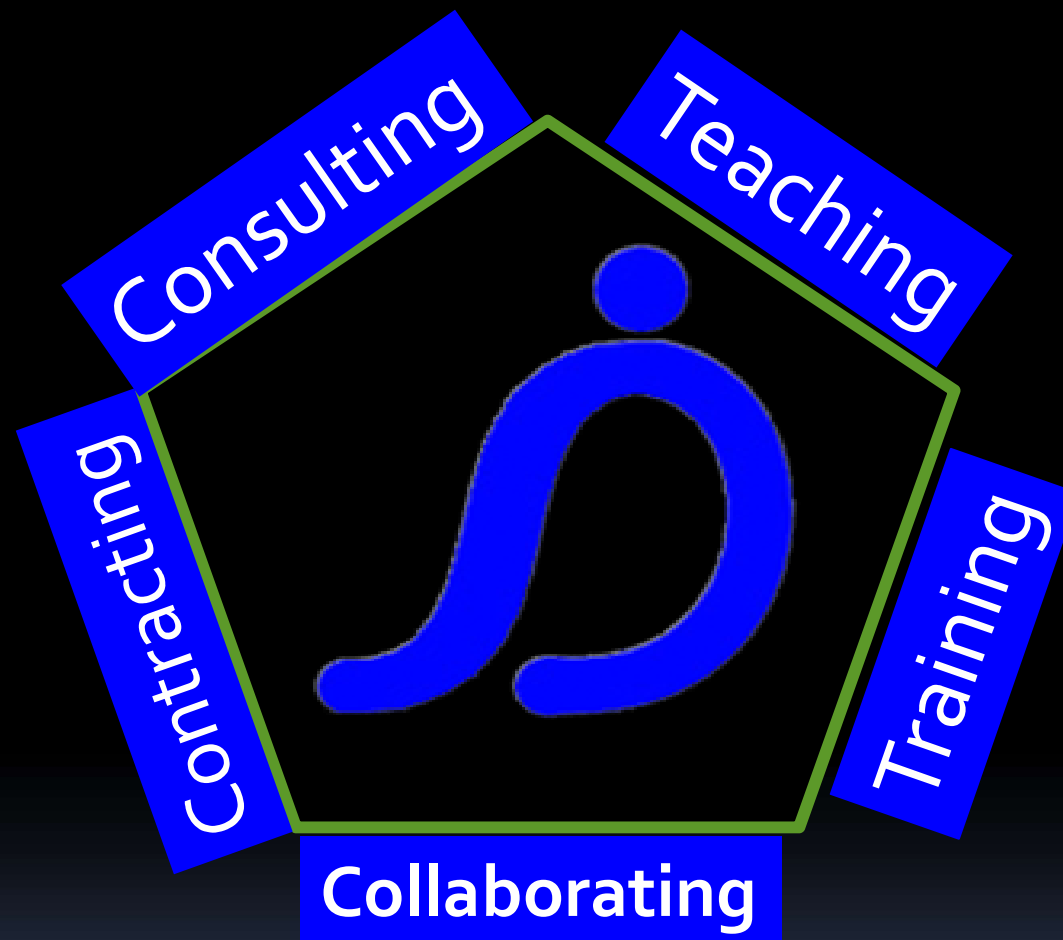
44-347/6, Sapthagiri Colony, Tirumalanagar,  
Moula Ali, Hyderabad – 500040, INDIA

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Thank You!