Tropical Disease Initiative

www.tropicaldisease.org

Marc A. Marti-Renom

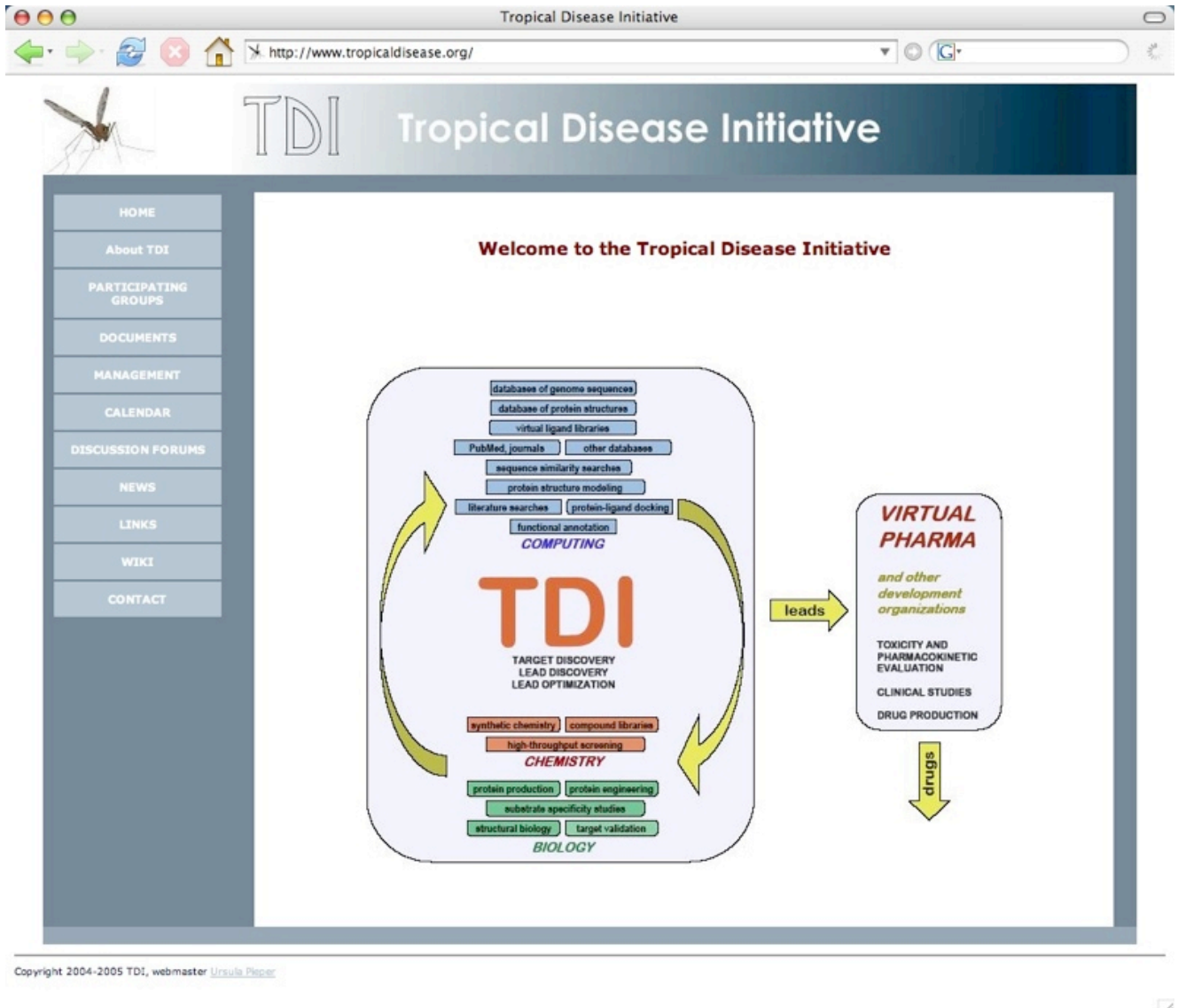
http://salilab.org/~marcius

UCSF
University of California
San Francisco

Depts. of Biopharmaceutical Sciences and Pharmaceutical Chemistry
California Institute for Quantitative Biomedical Research
University of California at San Francisco

TDI web site

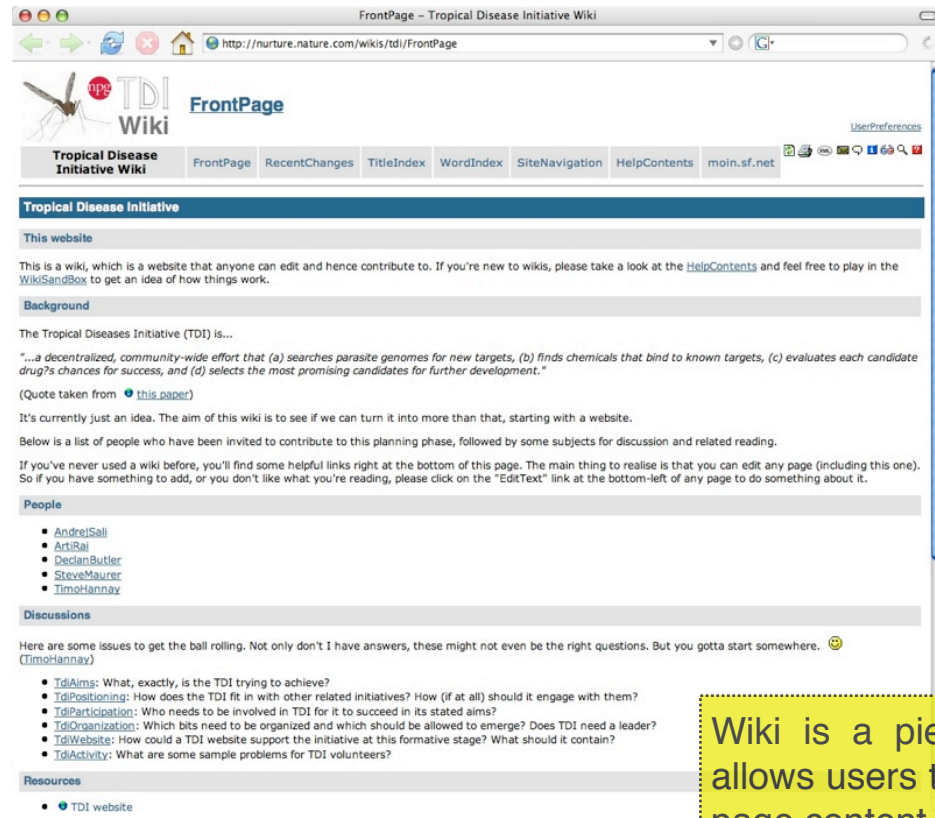
http://www.tropicaldisease.org/



HOME
About TDI
PARTICIPATING GROUPS
DOCUMENTS
MANAGEMENT
CALENDAR
DISCUSSION FORUMS
NEWS
LINKS
WIKI
CONTACT

TDI wiki site

http://nurture.nature.com/wikis/tdi/



Wiki is a piece of server software that allows users to freely create and edit Web page content using any Web browser.

- **Fill Important Gap in Existing R&D Efforts.**
- **Tip Economics.**
- **Experiment in Open Science.**

TDI mailing list

http://salilab.org/mailman/listinfo/tdi-discuss

TDI-discuss -- Tropical Disease Initiative discussion forum

About TDI-discuss

View this page in English (USA)

This list will be for discussing open source drug discovery efforts for tropical diseases.

To see the collection of prior postings to the list, visit the TDI-discuss Archives.

Using TDI-discuss

To post a message to all the list members, send email to tdi-discuss@tropicaldisease.org.

You can subscribe to the list, or change your existing subscription, in the sections below.

Subscribing to TDI-discuss

Subscribe to TDI-discuss by filling out the following form. You will be sent email requesting confirmation, to prevent others from gratuitously subscribing you. This is a hidden list, which means that the list of members is available only to the list administrator.

Your email address:	
Your name (optional):	

You may enter a privacy password below. This provides only mild security, but should prevent others from messing with your subscription. **Do not use a valuable password** as it will occasionally be emailed back to you in cleartext.

If you choose not to enter a password, one will be automatically generated for you, and it will be sent to you once you've confirmed your subscription. You can always request a mail-back of your password when you edit your personal options. Once a month, your password will be emailed to you as a reminder.

Pick a password:	
Reenter password to confirm:	
Which language do you prefer to display your messages?	English (USA)
Would you like to receive list mail batched in a daily digest?	No Yes

Subscribe

TDI mailing list

http://salilab.org/mailman/listinfo/tdi-discuss

14 Mar 2005

I think TDI is a unique and very interesting project. I would like so much to make something for it...

So, where are we going? What's happening? What can we do?

I still trust in open source drug discovery. :-))

Luca Brivio

t, if any, the bottlenecks are?
g ideas and potential avenues to explore,
n Action Plan!

disease for underserved popu
however, confused.
If someone will tell me wher
begin on, I'd be greatful.

Regards,
Jacob Lester

Thank you kindly,
Adam Huber

9 Mar 2005
I'm a programmer, not
something to keep the

GNU started with RM
Linux started with Li
You need someone g
people start sending patches...

I know this is chicken-egg, but someone needs to point this out, since I haven't seen this brought up in the papers or the website.

And you might consider merging into the bios.net effort mentioned already. Together, you just might reach the critical mass for things to take off. Consider this like when people jumped off the HURD project to come together and make linux work.

Daniel Amelang

mistic that the

Stephen Mark Maurer

TDI mailing list

http://salilab.org/mailman/listinfo/tdi-discuss

14 Mar 2005

I think TDI is a unique and very interesting proje
something for it...

So, where are we going? What's happening?

I still trust in open source drug discovery. :-))

Luca Brivio

16 Feb 2005

Hi,

It would be interesting to know what, if any, the bottlenecks are?
The Wiki site contains many interesting ideas and potential avenues to explore, but from what I can see it is **lacking an Action Plan!**

Regards,
Jacob Lester

disease for underserved popu
however, confused.
**If someone will tell me wher
begin on, I'd be greatful.**

Thank you kindly,
Adam Huber

9 Mar 2005
I'm a programmer, not
something to keep the

**GNU started with RM
Linux started with Li
You need someone g
people start sending patches...**

I know this is chicken-egg, but someone needs to point this out, since I haven't seen this brought up in the papers or the website.

And you might consider merging into the bios.net effort mentioned already. Together, you just might reach the critical mass for things to take off. Consider this like when people jumped off the HURD project to come together and make linux work.

Daniel Amelang

mistic that the

Stephen Mark Maurer

TDI mailing list

http://salilab.org/mailman/listinfo/tdi-discuss

14 Mar 2005

I think TDI is a unique and very interesting proje
something for it...

So, where are w

I still trust in open

Luca Brivio

16 Feb 2005

Hi

lenecks are?
tial avenues to explore,

10 Feb 2005

Hello,
My name is Adam Huber and I am a medical student at UNSW in Sydney Australia. I am interested in beginning research focused on tropical and infectious disease for underserved populations (A mission that seemingly matches TDI). I am, however, confused.
If someone will tell me where to sign up and give me some research topics to begin on, I'd be greatful.

Thank you kindly,
Adam Huber

9 Mar 2005
I'm a programmer, not
something to keep the

GNU started with RM
Linux started with Li
You need someone g
people start sending patches...

I know this is chicken-egg, but someone needs to point this out, since I haven't seen this brought up in the papers or the website.

And you might consider merging into the bios.net effort mentioned already. Together, you just might reach the critical mass for things to take off. Consider this like when people jumped off the HURD project to come together and make linux work.

Daniel Amelang

mistic that the

Stephen Mark Maurer

TDI mailing list

http://salilab.org/mailman/listinfo/tdi-discuss

14 Mar 2005

I think TDI is a unique and very interesting proje
something for it...

So, where are w

I still trust in open

Luca Brivio

16 Feb 2005

Hi

lenecks are?
tial avenues to explore,

10 Feb 2005

Hello,
My name is Adam Huber and I am a medical student at UNSW in Sydney Australia. I am interested in beginning research focused on tropical and infectious disease for underserved populations (A mission that seemingly matches TDI). I am,

s to

9 Mar 2005
I'm a programmer, not a bioinformatician, but I stumbled across your site and thought I'd say something to keep the list active :)

GNU started with RMS. He gave us programming/administration tools to play with.
Linux started with Linus. He released an operating system for us to play with.
You need someone great in the field to release something for everyone to 'play with'. Then people start sending patches...

I know this is chicken-egg, but someone needs to point this out, since I haven't seen this brought up in the papers or the website.

And you might consider merging into the bios.net effort mentioned already. Together, you just might reach the critical mass for things to take off. Consider this like when people jumped off the HURD project to come together and make linux work.

Daniel Amelang

mistic that the

Stephen Mark Maurer

TDI mailing list

http://salilab.org/mailman/listinfo/tdi-discuss

14 Mar 2005

I think TDI is a unique and very interesting proje
something for it...

So, where are w

I still trust in open

Luca Brivio

16 Feb 2005

Hi

lenecks are?
tial avenues to explore,

10 Feb 2005

Hello,
My name is Adam Huber and I am a medical student at UNSW in Sydney Australia.
I am interested in beginning research focused on tropical and infectious
disease for underserved populations (A mission that seemingly matches TDI). I am,

s to

9 Mar 2005
I'm a programmer, not a bioinformatician, but I stumbled across your site and thought I'd say
something to keep the list active :)

GNU started with RMS. He gave us programming/administration tools to play with.
Linux started with Linus. He released an operating system for us to play with.
You need someone great in the field to release something for everyone to 'play with'. Then people start sending patches...

I know this is chicken-egg, but someone
in the papers or the website.

And you might consider merging into the
reach the critical mass for things to take
project to come together and make linux

Daniel Amelang

19 Jan 2005

If we do the science well, I'm optimistic that the rest of TDI will fall into place.

Stephen Mark Maurer

Science @ Tropical Disease Initiative

www.tropicaldisease.org

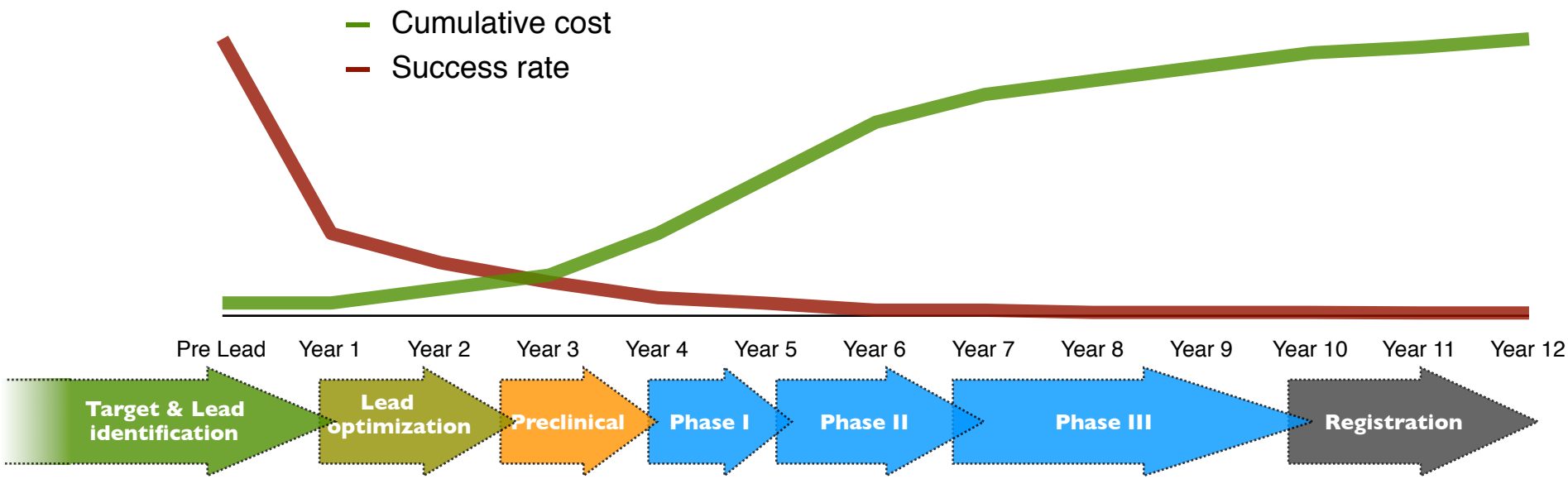
Marc A. Marti-Renom

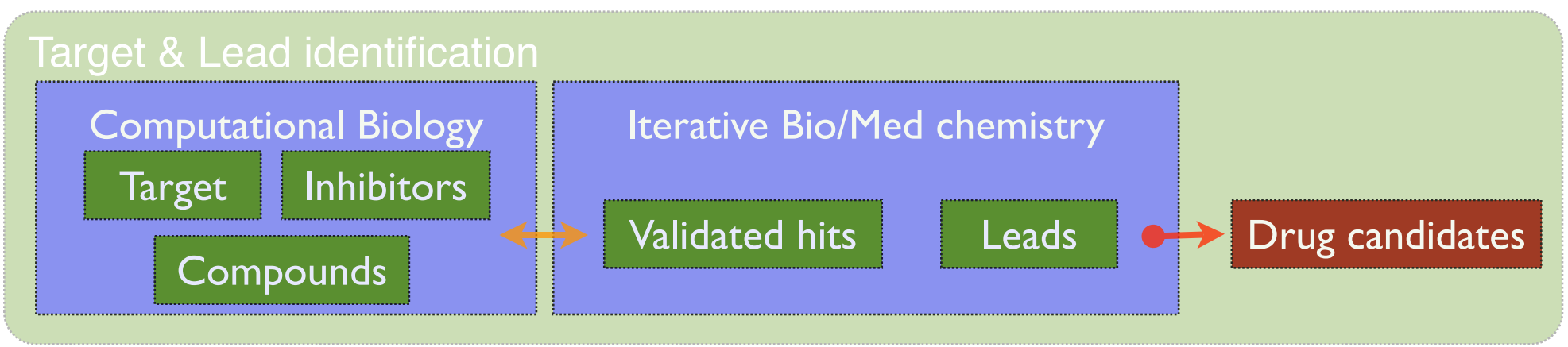
http://salilab.org/~marcius

University of California
San Francisco

Depts. of Biopharmaceutical Sciences and Pharmaceutical Chemistry
California Institute for Quantitative Biomedical Research
University of California at San Francisco

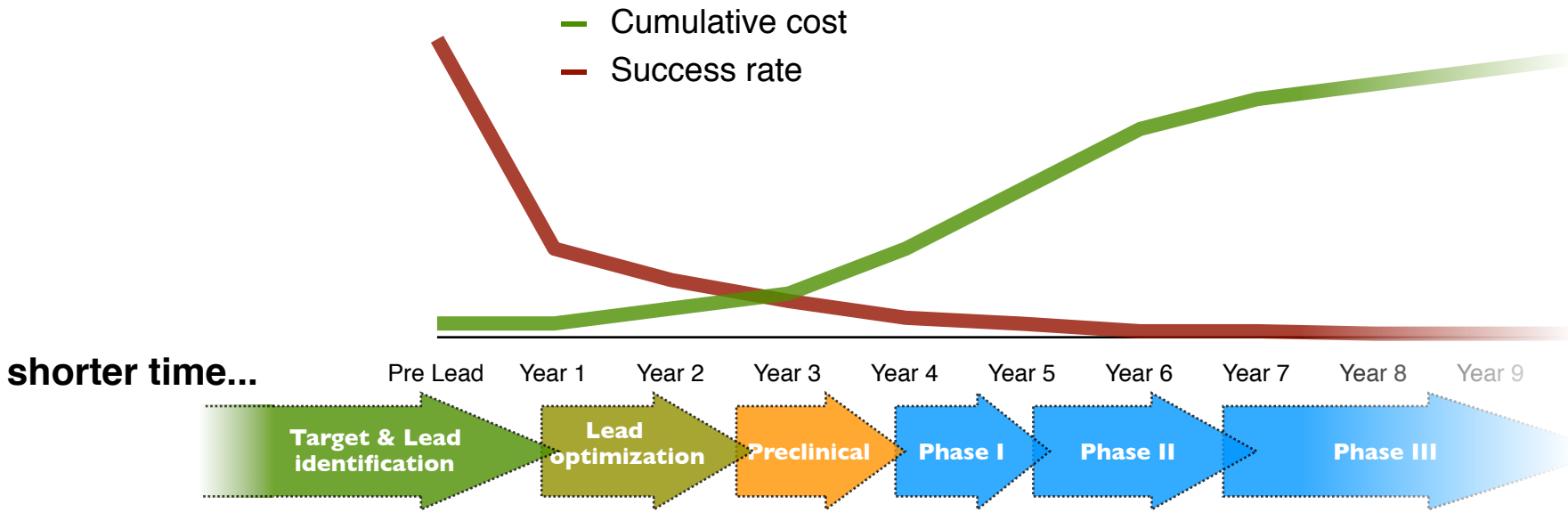
Drug Discovery pipeline





Adapted from: - Nwaka & Ridley. (2003) *Nature Reviews. Drug Discovery.* **2**:919
- Austin, Brady, Insel & collins. (2004) *Science*. **306**:1138

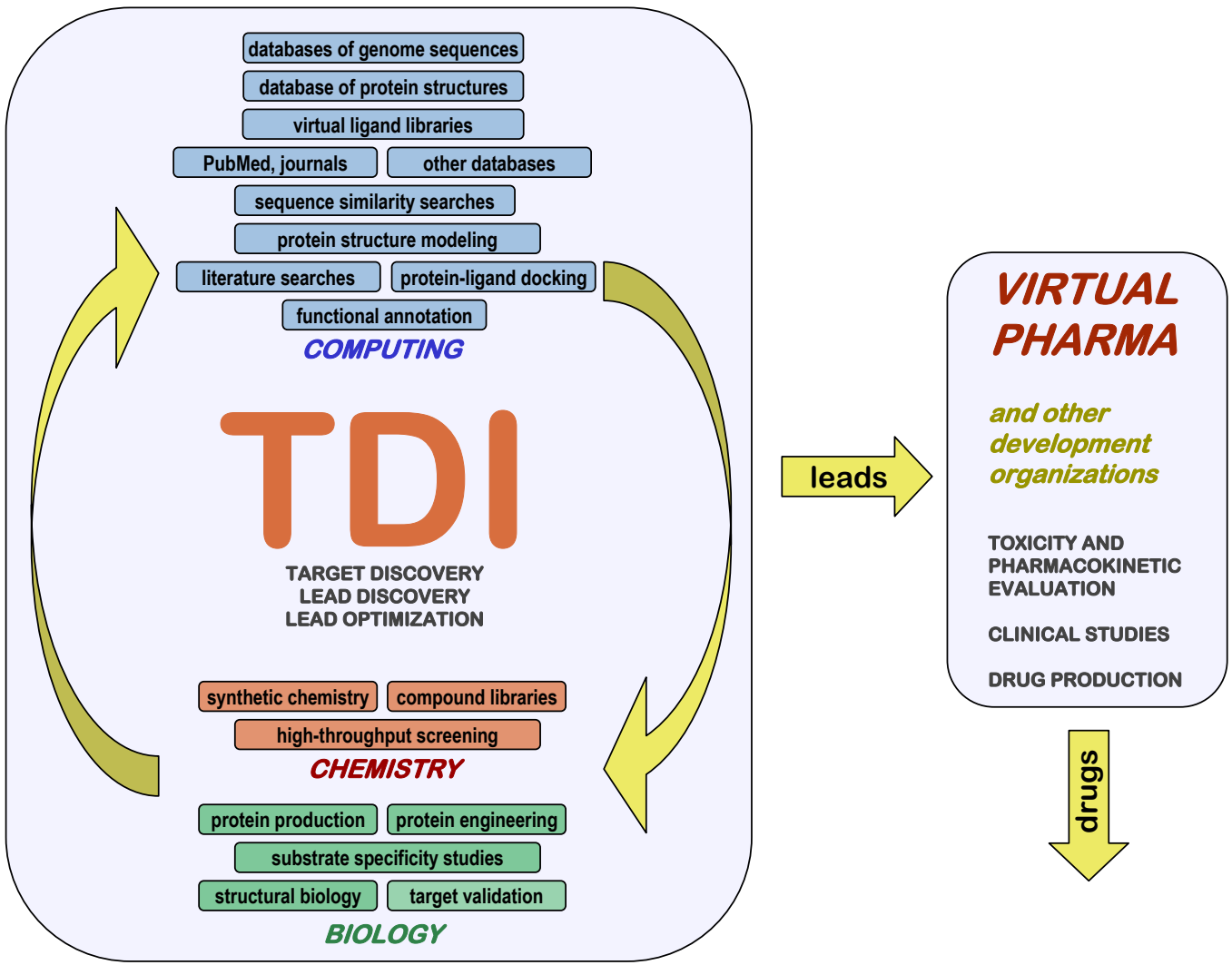
Drug Discovery pipeline



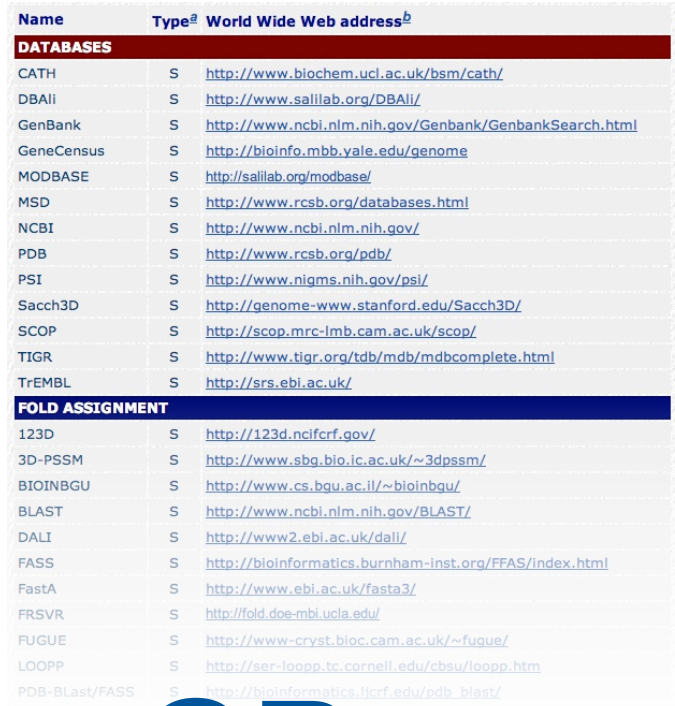
+ Completeness of genome projects (Malaria)
+ New and more complete biological databases
+ New software and computers (cheaper and faster)
+ Internet == more people

- Computational Biology **alone** is not enough
- TDI needs chemistry and biology! **(How?)**

TDI flowchart



http://salilab.org/bioinformatics_resources.shtml



Name	Type[a]	World Wide Web address[b]
DATABASES		
CATH	S	http://www.biochem.ucl.ac.uk/bsm/cath/
DBAli	S	http://www.salilab.org/DBAli/
GenBank	S	http://www.ncbi.nlm.nih.gov/Genbank/GenbankSearch.html
GeneCensus	S	http://bioinfo.mbb.yale.edu/genome
MODBASE	S	http://salilab.org/modbase/
MSD	S	http://www.rcsb.org/databases.html
NCBI	S	http://www.ncbi.nlm.nih.gov/
PDB	S	http://www.rcsb.org/pdb/
PSI	S	http://www.nigms.nih.gov/psi/
Sacch3D	S	http://genome-www.stanford.edu/Sacch3D/
SCOP	S	http://scop.mrc-lmb.cam.ac.uk/scop/
TIGR	S	http://www.tigr.org/tdb/mdb/mdbcomplete.html
TrEMBL	S	http://srs.ebi.ac.uk/
FOLD ASSIGNMENT		
123D	S	http://123d.ncifcrf.gov/
3D-PSSM	S	http://www.sbg.bio.ic.ac.uk/~3dpssm/
BIOINBGU	S	http://www.cs.bgu.ac.il/~bioinbgu/
BLAST	S	http://www.ncbi.nlm.nih.gov/BLAST/
DALI	S	http://www2.ebi.ac.uk/dali/
FASS	S	http://bioinformatics.burnham-inst.org/FFAS/index.html
FastA	S	http://www.ebi.ac.uk/fasta3/
FRSVR	S	http://fold.doe-mbi.ucla.edu/
FUGUE	S	http://www-cryst.bioc.cam.ac.uk/~fugue/
LOOPP	S	http://ser-loopp.tc.cornell.edu/cbsu/loopp.htm
PDB-BLast/FASS	S	http://bioinformatics.ljcrf.edu/pdb_blast/
PHDTHTS		

What CB can do?

Available computational biology resources for TDI

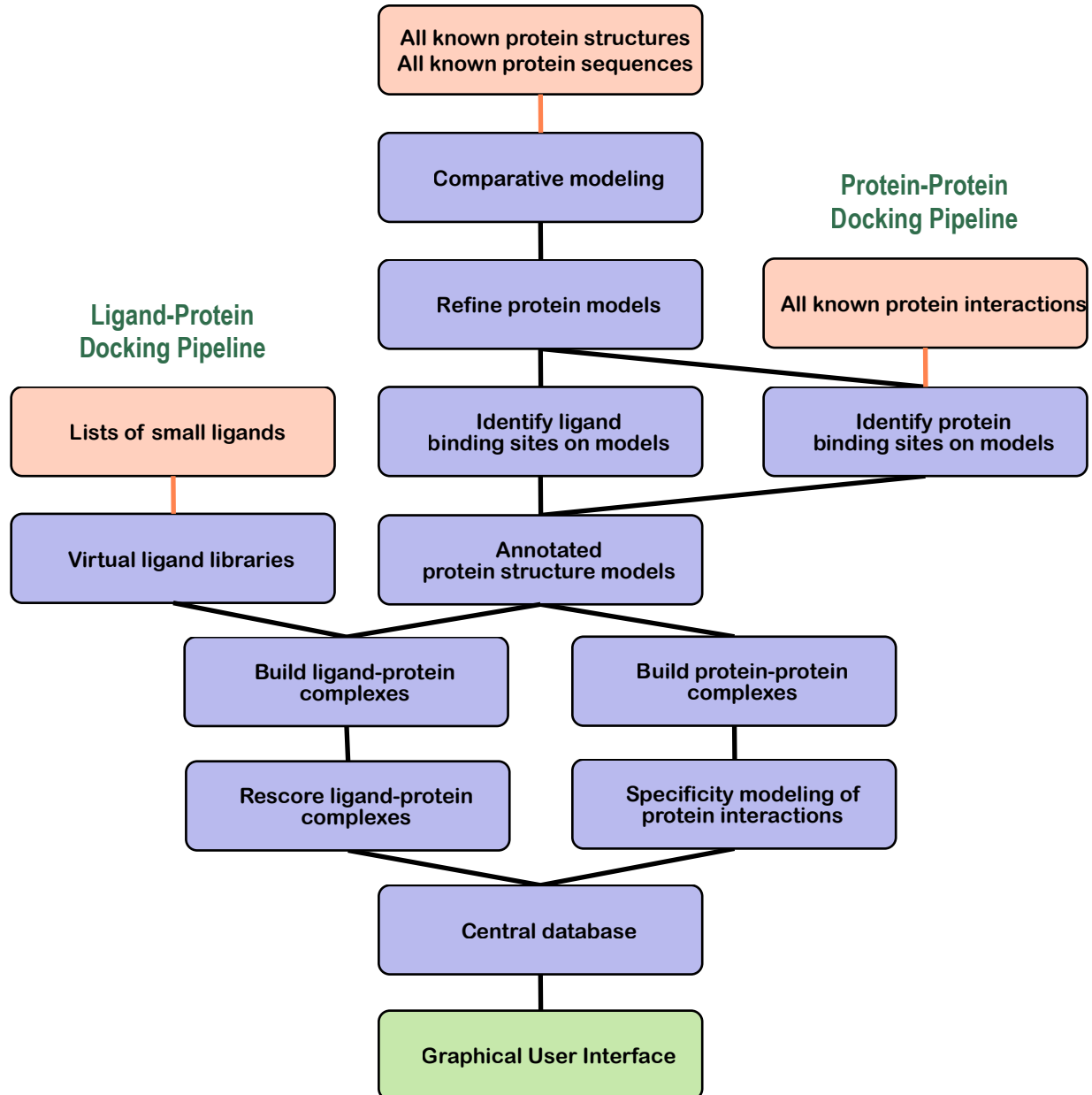
Protein-Ligand Universe

Center for Computational Proteomics Research (CCPR)

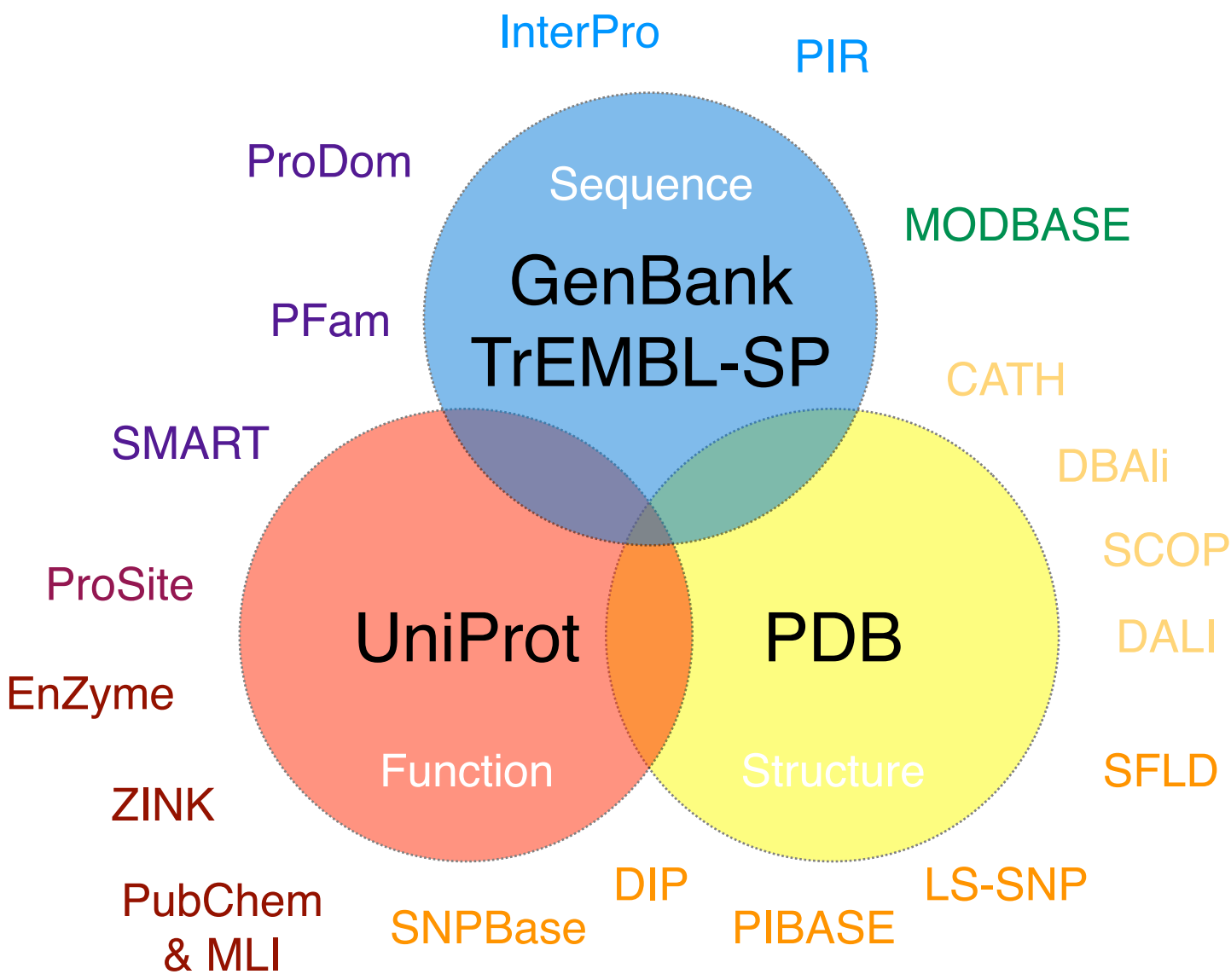
The California Institute for Quantitative Biomedical Research

Patsy Babbitt, Fred Cohen, Ken Dill, Tom Ferrin, John Irwin, Matt Jacobson, Tack Kuntz, Marc A. Marti-Renom, Andrej Sali, Brian Shoichet, Chris Voigt

http://www.ccpr.ucsf.edu/

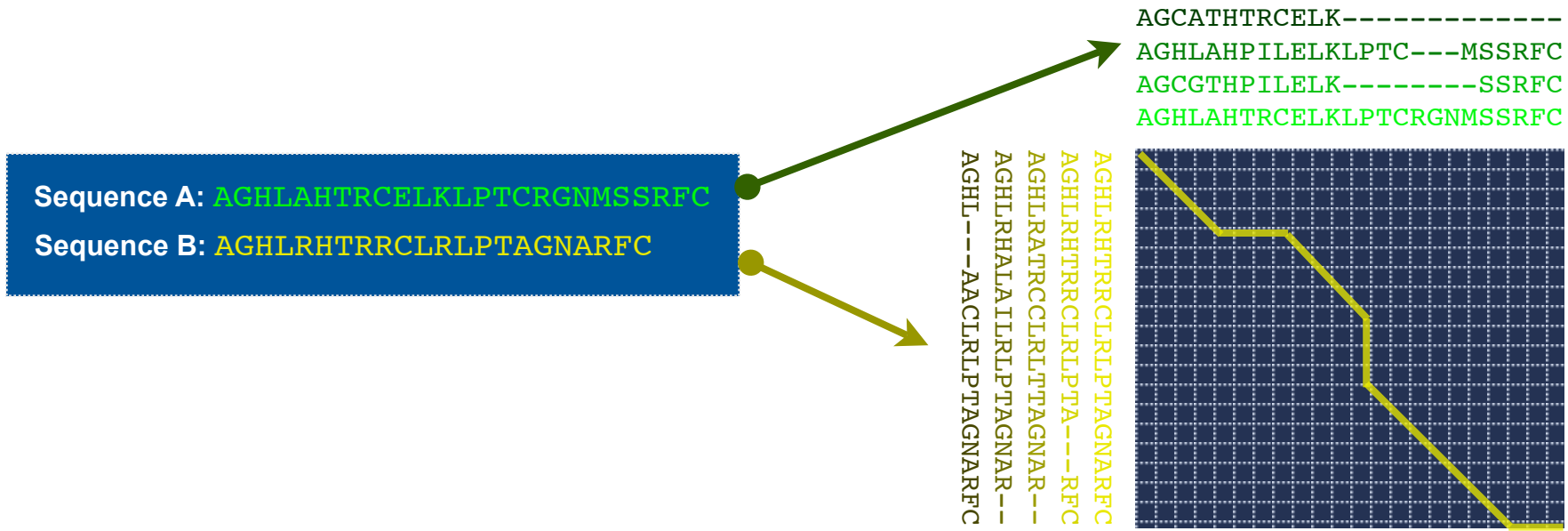


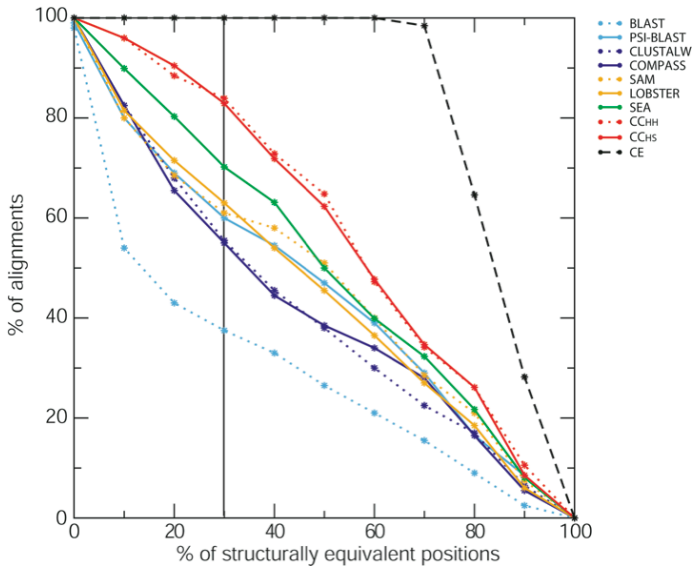
Databases

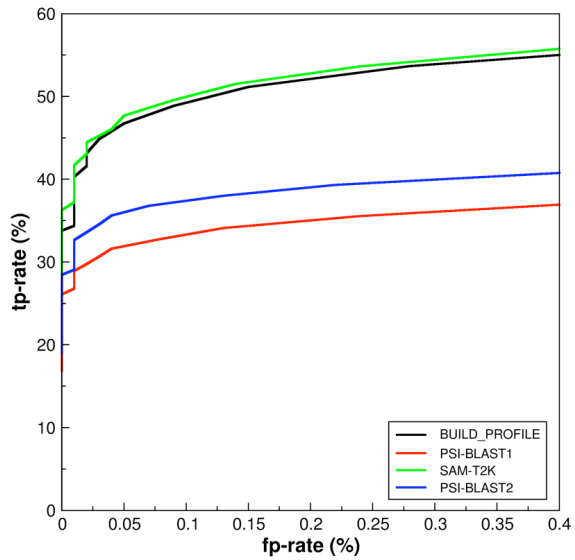

InterPro
PIR
ProDom
Sequence
MODBASE
GenBank
TrEMBL-SP
PFam
CATH
SMART
DBAli
SCOP
ProSite
UniProt
PDB
DALI
EnZyme
Function
Structure
SFLD
ZINK
DIP
LS-SNP
PubChem
& MLI
SNPBase
PIBASE

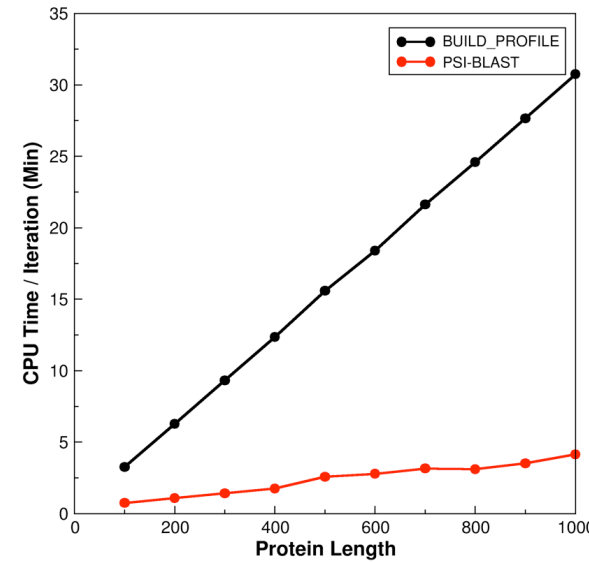
Sequence search

Profile based homology detection





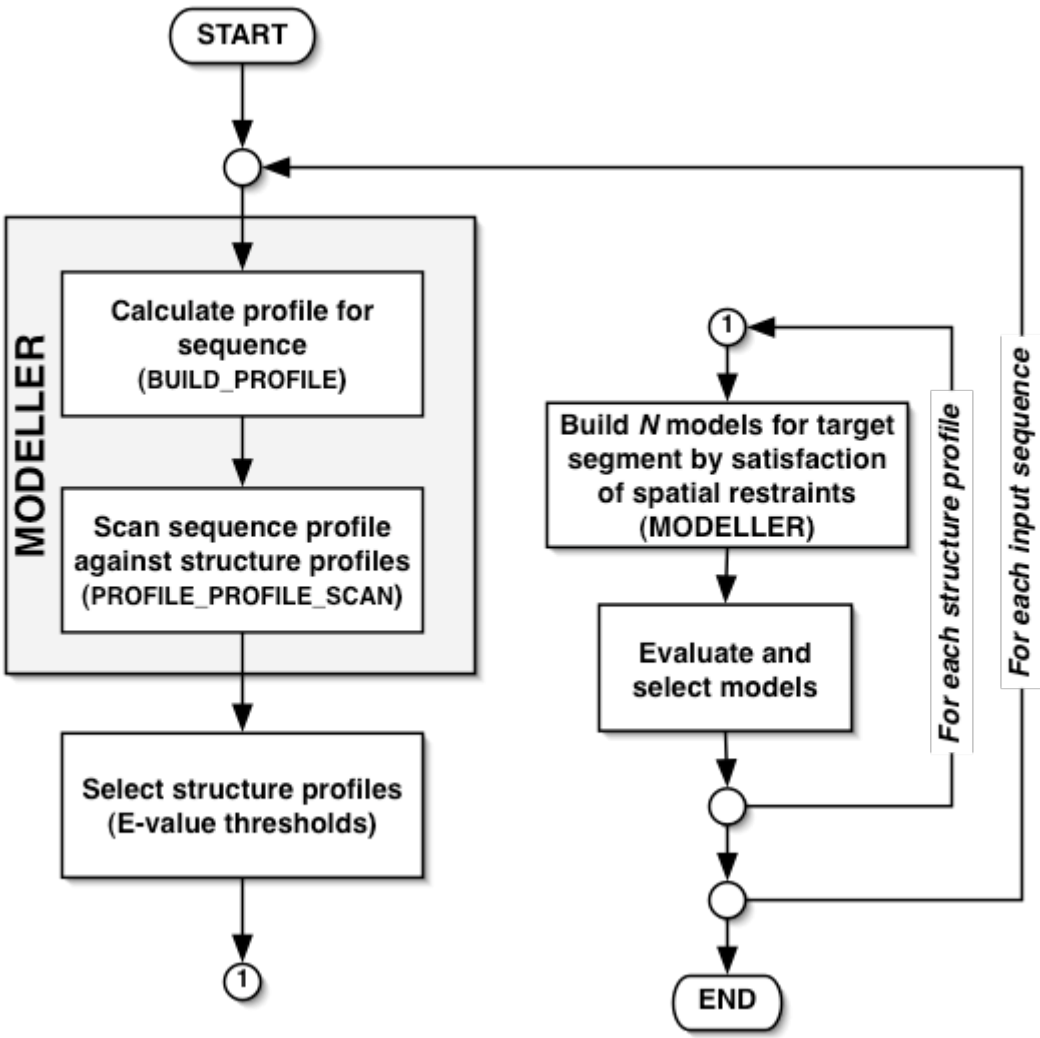


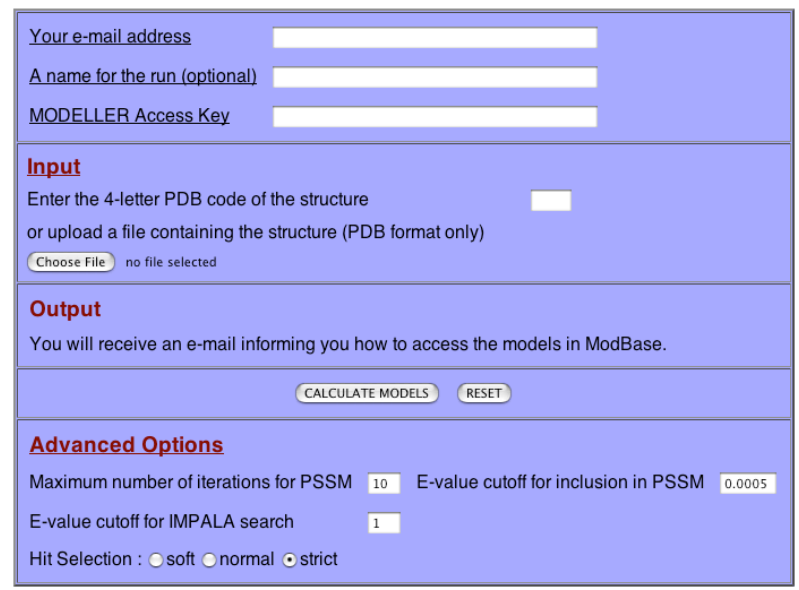


*Marti-Renom etal. (2004) Prot. Sci. **13**:1071*

Protein Structure Modeling

ModPipe & ModWeb





http://www.salilab.org/modweb/

Eswar et.al., (2003) Nucl.Acids.Res. 31(13)

Protein Structure Modeling

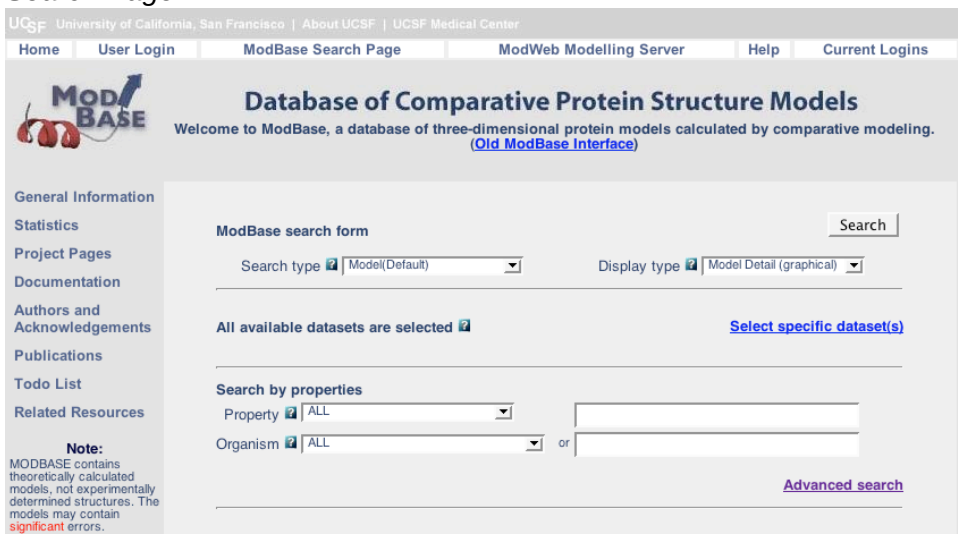
Large-Scale prediction

Sequences	1,679,742
Modeled sequences	964,442
Models	2,947,461
ModWeb datasets	1,506
ModWeb Models	387,403

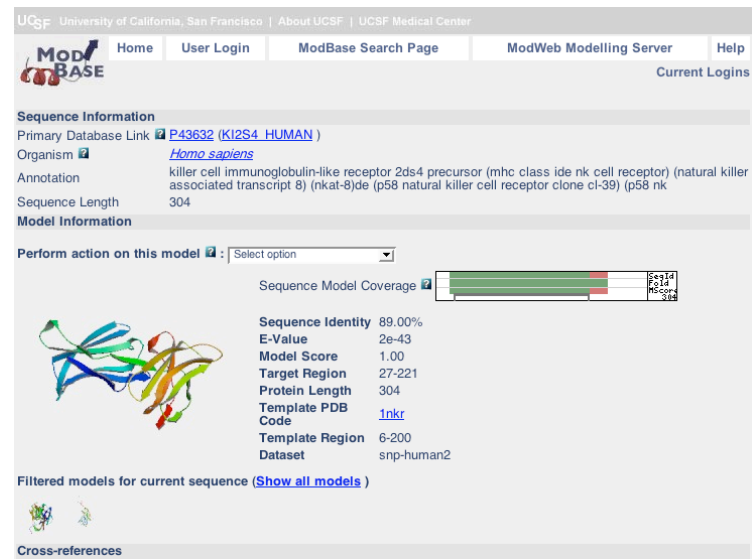
Protein Structure Modeling

MODBASE (http://www.salilab.org/modbase/)

Search Page



Model Details



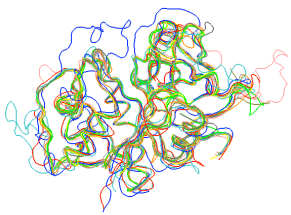
Sequence Overview

Model Overview

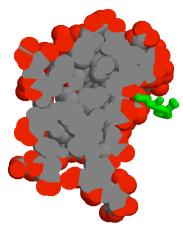
Functional Annotation

Binding site prediction

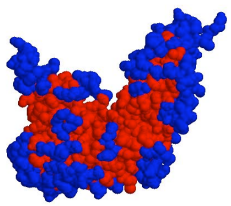
Structure conservation



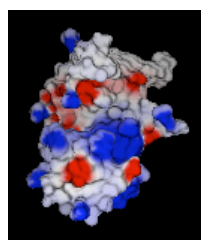
Solvent accessibility



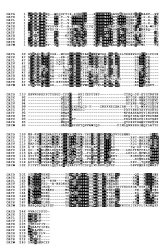
Surface geometry

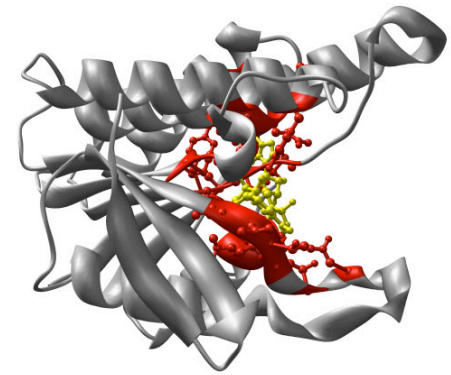


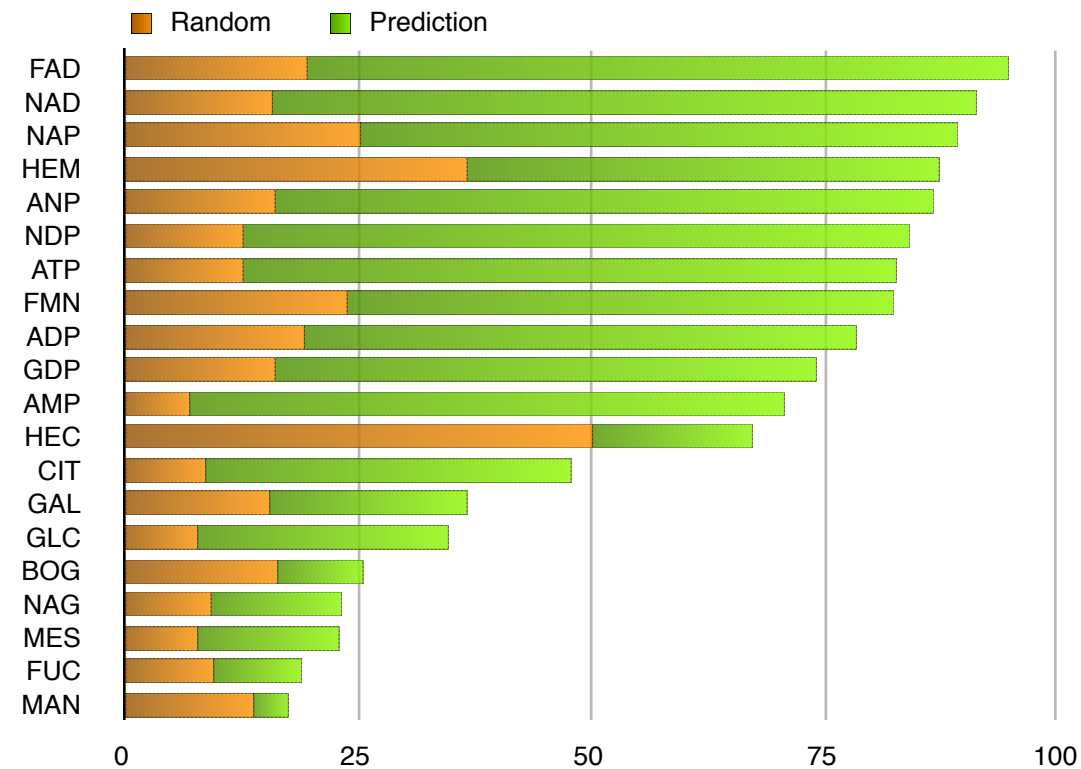
Electrostatics



Sequence conservation

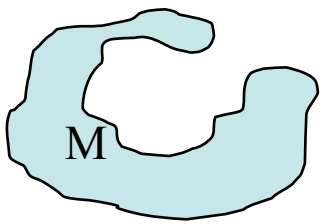






Rossi, Marti-Renom and Sali (2005) Submitted for publication

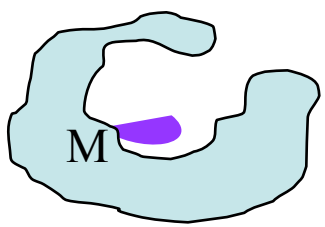
Protein-Ligand Docking

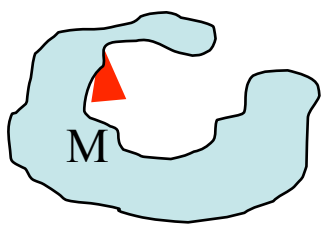


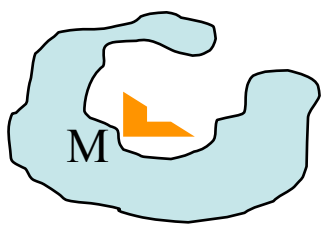
Structure of target protein

http://blaster.docking.org

Dock into site







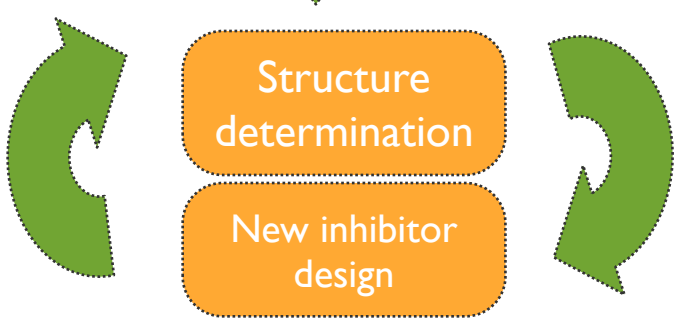
Test high-scoring molecules

Docking .vs. HTS

Target: reductase TB
Library: Merk chemical

IC_{50} < 100μM hit rates

HTS	Dock
<0.2%	~6%



Paiva et al. (2001) Biochem. Biophys. Acta. ***1545****:67-77*
Shoichet, McGovern,Wei, Irwin (2002) Curr Opin Chem Biol. ***6****:439-46*

Courtesy of John Irwin, UCSF http://www.docking.org

Protein-Ligand Docking

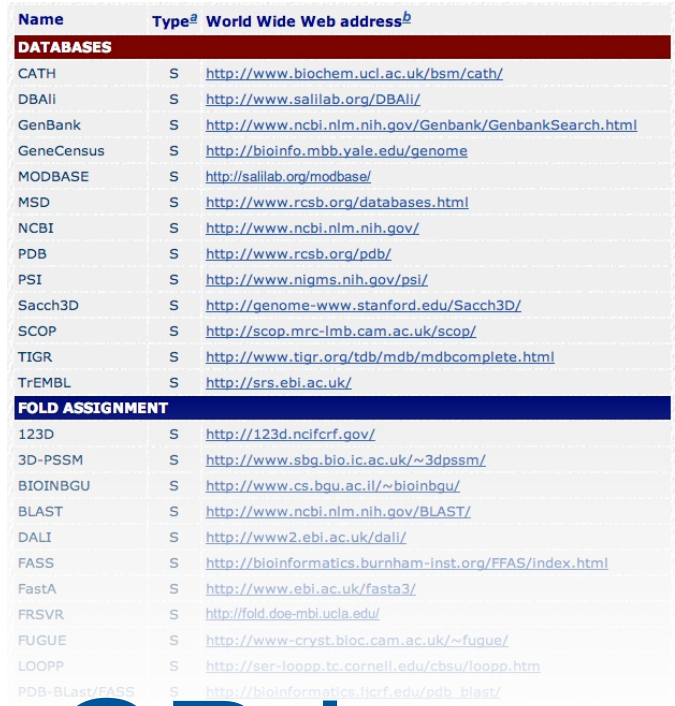
Successfully applied

Target	Best hit IC_{50} (μM)	Docking program	Structure solved?
Aldose reductase	4.3	Adam & Eve	No
CDK4	**44**	**Legend**	**Yes**
Matriptase	**0.9**	**DOCK**	**No**
Bcl-2	**10.4**	**DOCK**	**No**
Adenovirus protease	3.1	EUDOC	No
AmpC	26[a]	DOCK3.5.54	Yes
Retinoic acid receptor	**2**	**ICM**	**No**
TH receptor	1.5	ICM	No
TGT	8.3	LUDI/ FlexX	Yes
Carbonic anhydrase	0.0008	FlexX	Yes
HPRTase	2.2 [a]	DOCK3.5.54	No
Lysozyme cavity site	56 [b]	DOCK3.5.54	Yes
H_2picolinate reductase	7.2	FLOG	No
PTP-1B	0.5	DOCK3.5.54	No
Edema Factor	25 [a]	DOCK3.5.54	No
CDK2	0.08	DOCK4	No

Some recent docking successes (a. K_i. b. K_d.).

Shoichet, McGovern,Wei, Irwin (2002) Curr Opin Chem Biol. ***6****:439-46*

http://salilab.org/bioinformatics_resources.shtml



Name	Type[a]	World Wide Web address[b]
DATABASES		
CATH	S	http://www.biochem.ucl.ac.uk/bsm/cath/
DBAli	S	http://www.salilab.org/DBAli/
GenBank	S	http://www.ncbi.nlm.nih.gov/Genbank/GenbankSearch.html
GeneCensus	S	http://bioinfo.mbb.yale.edu/genome
MODBASE	S	http://salilab.org/modbase/
MSD	S	http://www.rcsb.org/databases.html
NCBI	S	http://www.ncbi.nlm.nih.gov/
PDB	S	http://www.rcsb.org/pdb/
PSI	S	http://www.nigms.nih.gov/psi/
Sacch3D	S	http://genome-www.stanford.edu/Sacch3D/
SCOP	S	http://scop.mrc-lmb.cam.ac.uk/scop/
TIGR	S	http://www.tigr.org/tdb/mdb/mdbcomplete.html
TrEMBL	S	http://srs.ebi.ac.uk/
FOLD ASSIGNMENT		
123D	S	http://123d.ncifcrf.gov/
3D-PSSM	S	http://www.sbg.bio.ic.ac.uk/~3dpssm/
BIOINBGU	S	http://www.cs.bgu.ac.il/~bioinbgu/
BLAST	S	http://www.ncbi.nlm.nih.gov/BLAST/
DALI	S	http://www2.ebi.ac.uk/dali/
FASS	S	http://bioinformatics.burnham-inst.org/FFAS/index.html
FastA	S	http://www.ebi.ac.uk/fasta3/
FRSVR	S	http://fold.doe-mbi.ucla.edu/
FUGUE	S	http://www-cryst.bioc.cam.ac.uk/~fugue/
LOOPP	S	http://ser-loopp.tc.cornell.edu/cbsu/loopp.htm
PDB-BLast/FASS	S	http://bioinformatics.ljcrf.edu/pdb_blast/

What CB has done?

Success stories in structure-based drug design...

Examples

HIV Proteinase inhibitors (1989)

Knowledge-based protein modelling and design.

Blundell T, et al Eur J Biochem. 1988 ***15****:513*

"A systematic technique for protein modelling that is applicable to the design of drugs, peptide vaccines and novel proteins is described. We have modelled an analogous protein, HIV viral proteinase on the basis of aspartic proteinases".

X-ray analysis of HIV-1 proteinase at 2.7 A resolution confirms structural homology among retroviral enzymes.

Lapatto et al Nature. 1989 Nov 16;342(6247):299-302.

"Knowledge of the tertiary structure of the proteinase from human immunodeficiency virus HIV-1 is important to the design of inhibitors that might possess antiviral activity and thus be useful in the treatment of AIDS. The conserved Asp-Thr/Ser-Gly sequence in retroviral proteinases suggests that they exist as dimers similar to the ancestor proposed for the pepsins."

HIV Proteinase structure

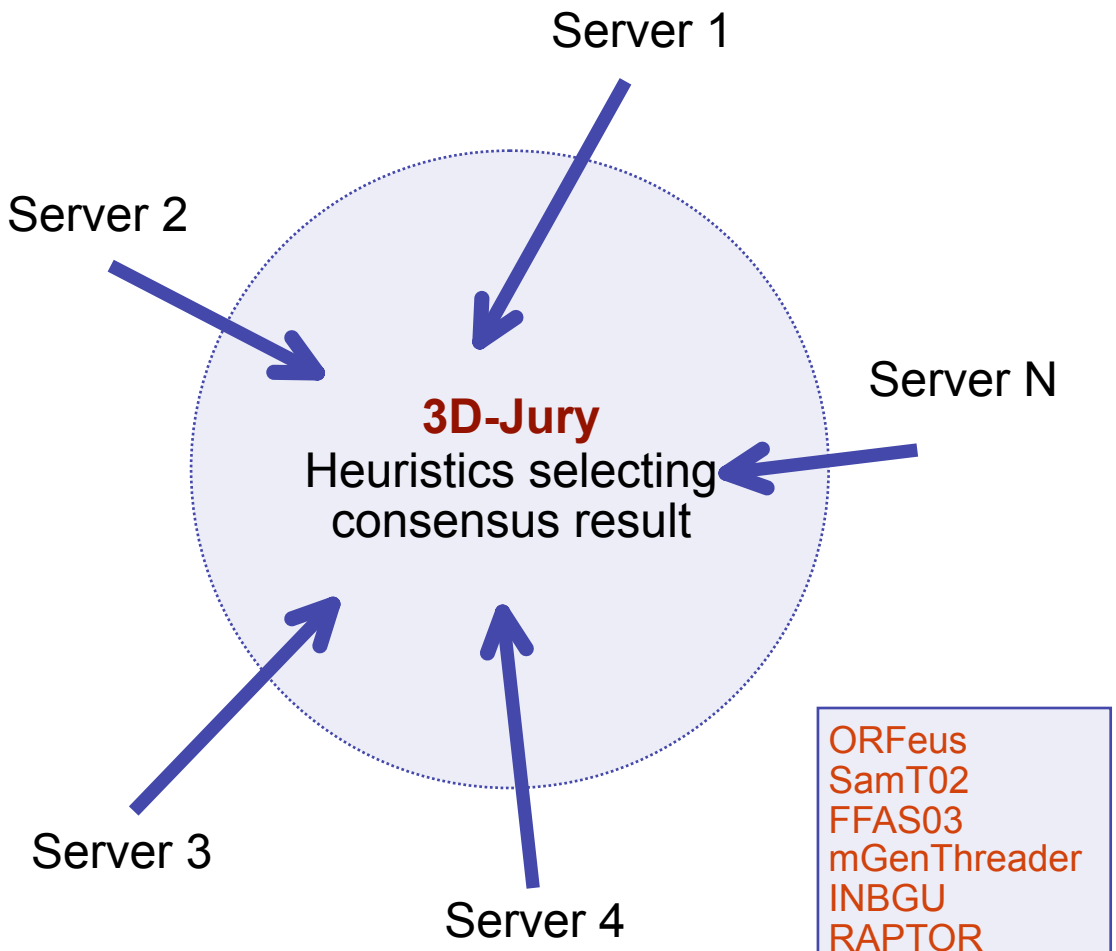
The 3-D structure of HIV-1 proteinase and the design of antiviral agents for the treatment of AIDS.

Blundell et al Trends Biochem Sci. 1990 Nov;15(11):425-30.

"Analogies between the structures of HIV-1 proteinase and the mammalian enzyme renin have given **important clues** concerning the design of specific inhibitors that have antiviral activity."

Examples

mRNA Cap-1 Methyltransferase in SARS (2003)



ORFeus
SamT02
FFAS03
mGenThreader
INBGU
RAPTOR
FUGUE-2
3D-PSSM

Cell, Vol. 113, 701–702, June 13, 2003, Copyright ©2003 by Cell Press

Letter to the Editor

mRNA Cap-1 Methyltransferase in the SARS Genome

The 3D jury system has predicted the methyltransferase fold for the nsp13 protein of the SARS coronavirus. Based on the conservation of a characteristic tetrad of residues, the mRNA cap-1 methyltransferase function has been assigned to this protein, which has potential implications for antiviral therapy.

The latest outbreak of the severe acute respiratory syndrome (SARS) epidemic has led to thousands of potentially lethally infected patients and hundreds of deaths. These numbers are likely to rise, and the spreading disease is already causing major medical and economical concerns. Meanwhile, the SARS coronavirus identified as the pathogen responsible for the disaster has been isolated, and its genome sequenced (Marra et al., 2003; Rota et al., 2003).

We have applied the 3D jury meta predictor (Ginalski et al., 2003) to annotate the structure and function of proteins encoded by the viral positive-strand ssRNA. Novel fold recognition methods utilize the global network of independent structure prediction servers. Detection of patterns of structural similarity between diverse models is used to consistently select the correct fold from a set of borderline predictions. Such methods made a dramatic impact on the last critical assessment of protein structure prediction (CASP-5 experiment) conducted in the summer of 2002. One of the most interesting findings obtained during the SARS genome annotation process is a surprisingly reliable (3D jury score >100) assignment of the methyltransferase fold to the nsp13 (GI:30133975) domain located in the C-terminal part of the almost 7000 amino acid large pp1ab viral polyprotein (Figure 1). Standard sequence comparison tools such as PSI-BLAST or RPS-BLAST applied using the conserved domain database (Marchler-Bauer et al., 2003) failed to assign any function to this domain. The domain belongs to the ancient family of AdoMet-dependent ribose 2′-O-methyltransferases, which has been adapted by numerous viruses before the three domains of life evolved form the last universal common ancestor (LUCA) (Feder et al., 2003). The enzymatic role of the protein was confirmed by the presence of the conserved tetrad of residues K-D-K-E essential for mRNA cap-1 (mGpppNm) formation.

The mRNA cap methylation is found indispensable for efficient replication of many viruses (Bach et al., 1995; Woyciniuk et al., 1995; Vlot et al., 2002) and represents an active area for drug development. Nevertheless, direct inhibitors of the nsp13 enzyme may fail to suppress viral replication, as the cap-1 formation seems to be less critical than the preceding cap-0 (mGpppN) formation (Latner et al., 2002; Wu and Guarino, 2003). The existence of the cap-1-forming enzyme in the genome would suggest that the virus also requires the AdoMet-dependent cap-0 methyltransferase. Both functions can be inhibited by carbocyclic analogs of adenosine, such as Neplanocin A or 3-deazaneplanocin A, which interfere with the AdoMet-AdoHcy metabolism of the host cell (De Clercq, 1998; Bray et al., 2002). Those compounds could complement other therapeutic strategies aimed at blocking enzymatic functions such as the RNA-dependent RNA polymerase, the protease, or the helicase encoded by the SARS virus.

Marcin von Grotthuss, Lucjan S. Wyrwicz, and Leszek Rychlewski*
BioInfoBank Institute
Limanowskiego 24A
60-744 Poznan
Poland

*Correspondence: leszek@bioinfo.pl

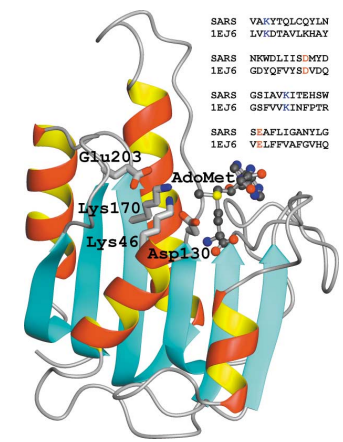


Figure 1. 3D Model of the nsp13 Domain of the SARS Coronavirus pp1ab Polyprotein

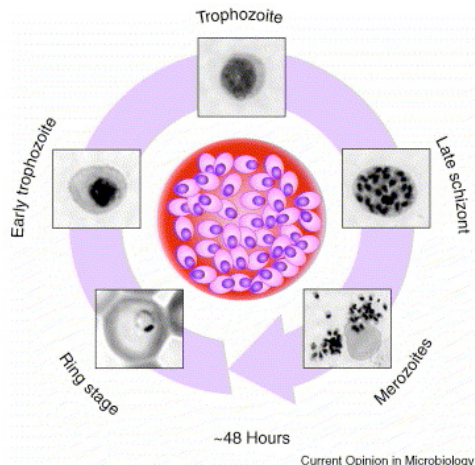
This model is based on the reassigned (Bujnicki and Rychlewski, 2001) cap-1 methyltransferase of the reovirus λ2 protein (1ej6 [Reinisch et al., 2000]). While other templates (1eiz or 1ej0) obtained marginally higher 3D jury scores, the selected template had the lowest number of insertions and deletions. Side chains of the conserved tetrad of residues (K-D-K-E) essential for cap-1 methylation and the docked AdoMet cofactor are shown. Four blocks of aligned motifs containing the conserved, function-specific residues are shown in upper right corner.

*von Grotthuss M. et al. (2003) Cell **113** pp**701***

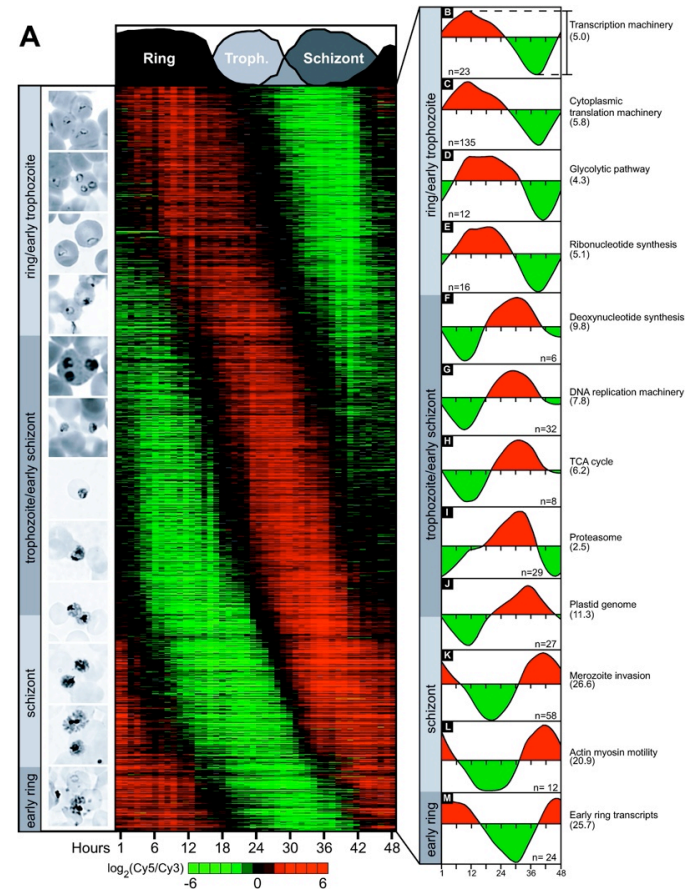
*Ginalski K, et al. (2003) Bioinformatics **19** pp**1015***

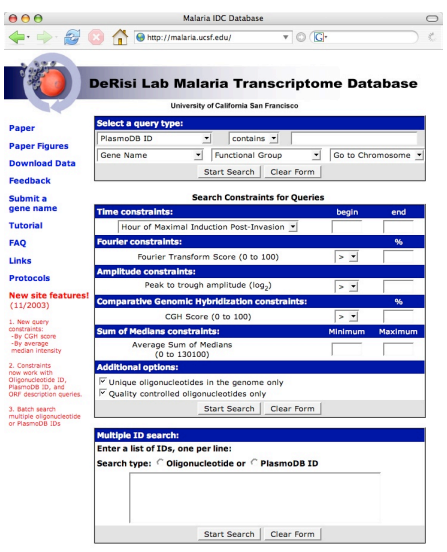
Examples

Genomic research on Malaria (2003)



Intraerythrocytic developmental cycle IDC





1. **Periodic and continuum** nature of the *P. falciparum* transcriptome (for at least 80% of the genes)
2. Potential for **characterizing** ~60% genes of unknown function

*Bozdech et al. (2003). PLoS Biology **1**(1):e5*
*Llinas & DeRisi (2004). Current Opinion in Microbiology **7**:382*

Structure-based DD

in companies...

inpharmatica

	cloning	Tissue distribution	Disease association	expression	1° assay	2° assay	screening	Hit optimisation	Lead optimisation
Nuclear Receptors									
P450s									
Ion-channels									
Progestin GPCRs									
Metalloproteinases									

VERTEX™

Viral Diseases	Preclinical	Phase I	Phase II	Phase III	Market
Agenerase® *HIV Infection*					
Lexiva®/Telzir® *HIV Infection*					
VX-385 *HIV Infection*					
merimepodib *HCV Infection*					
VX-950 *HCV Infection*					
Inflammation and Autoimmune Diseases					
VX-702 *Rheumatoid Arthritis*					
VX-765 *Psoriasis*					
pralnacasan *Inflammatory Diseases*					
Cancer					
VX-680 *Oncology*					
VX-322 *Oncology*					
VX-944 *Oncology*					
Other					
VX-409 *Pain*					
VX-692 *Bacterial Infection*					

Predix Pharmaceuticals

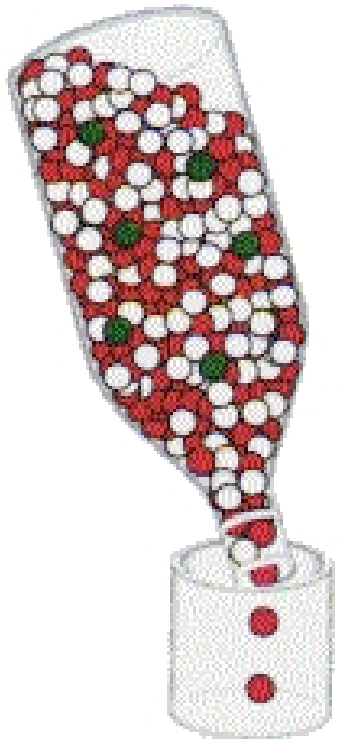
Predix' Clinical Development Programs

Indication	Target	Drug Discovery	Lead Optimization	Pre-Clinical	IND	Phase I	Phase II
PRX-00023 Anxiety/Depression	5-HT1A			Phase I Complete		1H	
PRX-03140 Alzheimer's Disease	5-HT4			Phase I		1H	
PRX-08066 Pulmonary Hypertension	5-HT2B			Pre-Clinical		Q2	

February 2005 | 2005 Anticipated Milestones

SGX

Our lead product candidate Troxatyl,™ is currently being evaluated in Phase I trials for the treatment of relapsed AML and various solid tumors.



TDI

which problems we face?

TDI scientific bottle necks

???

9 Mar 2005

GNU started with RMS. He gave us programming/administration tools to play with.
Linux started with Linus. He released an operating system for us to play with.
You need someone great in the field to release something for everyone to 'play with'.

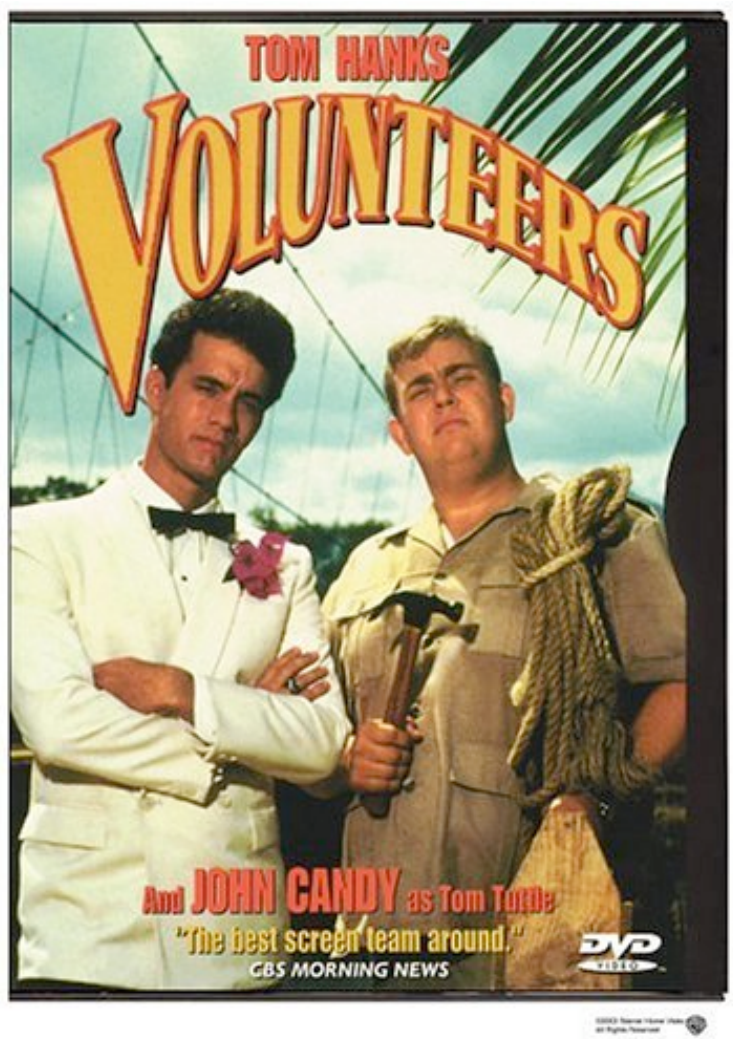
Daniel Amelang

- TOP-TEN scientific questions
- Road-Map to TOP-TEN answers
- Initial set of data and tools
- Initial set of contributors

TDI bottle necks

Gene

Lead



Acknowledgments

The Sali Lab
Andrej Sali
Frank Alber
Ranyee Chiang
Fred Davis
Damien Devos
David Eramian
Libusha Kelly
Michael F. Kim
Rachel Karchin
Dmitry Korkin
M.S. Madhusudhan
Eswar Narayanan
Mark Peterson
Ursula Pieper
Min-yi Shen
Maya Topf
Ben Webb

Tropical Disease Initiative
Stephen Maurer
Arti Rai
Andrej Sali

Ligand Docking
John Irwin
Brian Shoichet

Wiki site at NPG
Timo Hannay
Declan Butler