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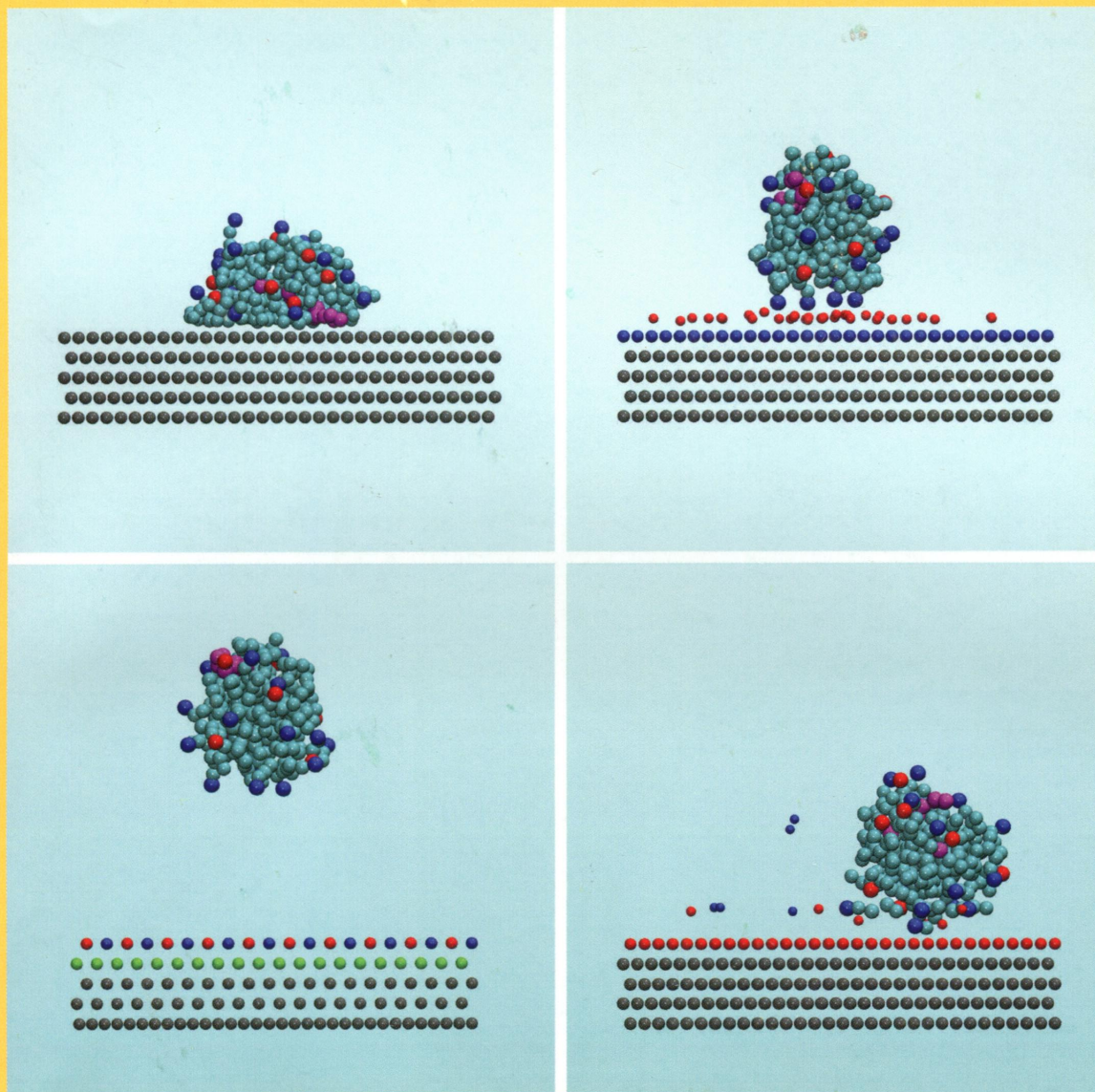
VOLUME 118

NUMBER 17

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THE JOURNAL OF PHYSICAL CHEMISTRY

B



Lysozyme Adsorption
on Different Surfaces
by Mesoscopic
Coarse-Grained
Simulations
(see page 5A)

BIOPHYSICAL CHEMISTRY, BIOMATERIALS, LIQUIDS, AND SOFT MATTER



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ON THE COVER: AlzPlatform (<http://www.cbligand.org/AD/>) is an Alzheimer's disease (AD) domain-specific chemogenomics knowledge base, featuring a large repertoire of AD drugs and small chemical molecules as well as related genes and protein targets. The comprehensive database and powerful computational algorithms and tools implemented have been developed and maintained by Xie's laboratory (<http://www.cbligand.org/xielab/>) to facilitate target identification, drug repurposing, and system polypharmacology analyses on a chemogenomics scale for new anti-AD drug discoveries. See H. Liu, L. Wang, M. Lv, R. Pei, P. Li, Z. Pei, Y. Wang, W. Su, and X.-Q. Xie, pp 1050–1060.

Articles

Chemical Information

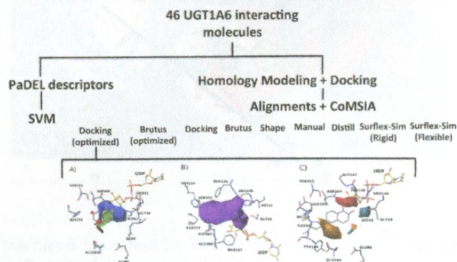
1011



[dx.doi.org/10.1021/ci400577a](https://doi.org/10.1021/ci400577a)

SVM Classification and CoMSIA Modeling of UGT1A6 Interacting Molecules

Leo Ghemto, Anne Soikkeli, Marjo Yliperttula, Jouni Hirvonen, Moshe Finel, and Henri Xhaard*



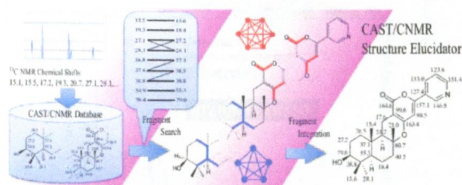
1027



[dx.doi.org/10.1021/ci400601c](https://doi.org/10.1021/ci400601c)

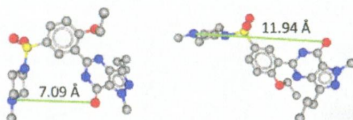
Chemical Structure Elucidation from ^{13}C NMR Chemical Shifts: Efficient Data Processing Using Bipartite Matching and Maximal Clique Algorithms

Shungo Koichi,* Masaki Arisaka, Hiroyuki Koshino, Atsushi Aoki, Satoru Iwata, Takeaki Uno, and Hiroko Satoh

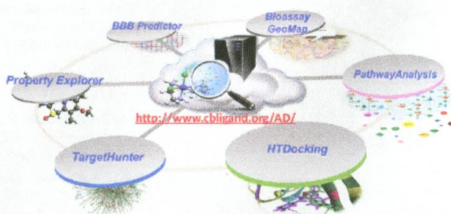


Screen3D: A Novel Fully Flexible High-Throughput Shape-Similarity Search Method

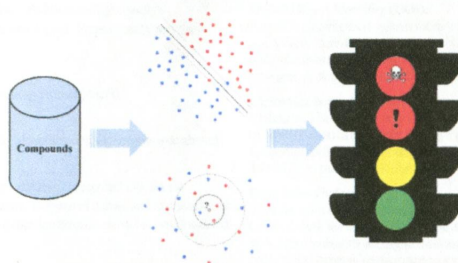
Adrián Kalászi,* Dániel Szisz, Gábor Imre, and Tímea Polgár*

**AlzPlatform: An Alzheimer's Disease Domain-Specific Chemogenomics Knowledgebase for Polypharmacology and Target Identification Research**

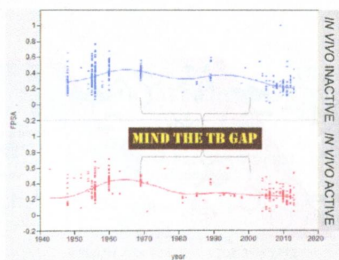
Haibin Liu, Lirong Wang, Mingliang Lv, Rongrong Pei, Peibo Li, Zhong Pei, Yonggang Wang, Weiwei Su,* and Xiang-Qun Xie*

**In Silico Prediction of Chemical Acute Oral Toxicity Using Multi-Classification Methods**

Xiao Li, Lei Chen, Feixiong Cheng, Zengrui Wu, Hanping Bian, Congying Xu, Weihua Li, Guixia Liu, Xu Shen, and Yun Tang*

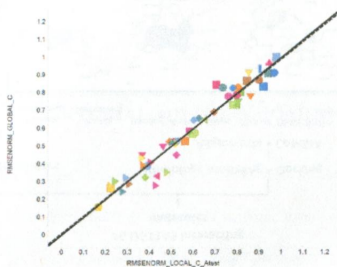


Looking Back to the Future: Predicting *in Vivo* Efficacy of Small Molecules versus *Mycobacterium tuberculosis*
 Sean Ekins,* Richard Pottorf, Robert C. Reynolds, Antony J. Williams, Alex M. Clark, and Joel S. Freundlich*



Global Quantitative Structure–Activity Relationship Models vs Selected Local Models as Predictors of Off-Target Activities
 for Project Compounds

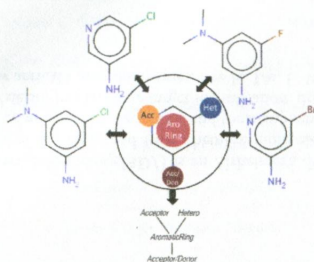
Robert P. Sheridan*



Computational Chemistry

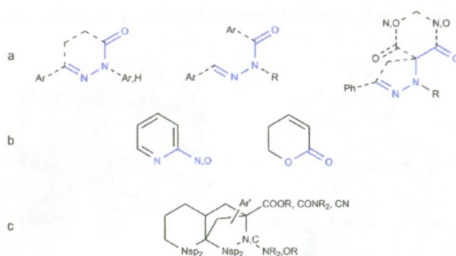
Fuzzy Matched Pairs: A Means To Determine the Pharmacophore Impact on Molecular Interaction

Tim Geppert* and Bernd Beck

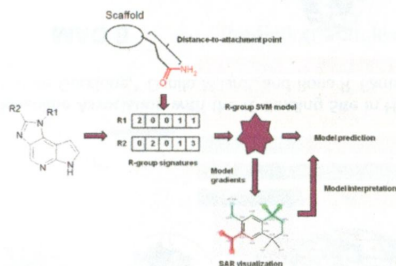


Synthesis, Bioassay, and Molecular Field Topology Analysis of Diverse Vasodilatory Heterocycles

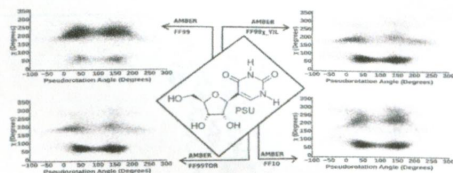
Polina V. Oliferenko, Alexander A. Oliferenko, Adel S. Gergis, Dalia O. Saleh, Aladdin M. Srour, Riham F. George, Girinath G. Pillai, Chandramukhi S. Panda, C. Dennis Hall,* and Alan R. Katritzky

**Beyond the Scope of Free-Wilson Analysis. 2: Can Distance Encoded R-Group Fingerprints Provide Interpretable Nonlinear Models?**

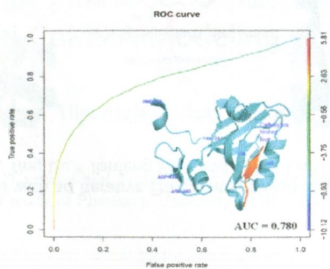
Mats Eriksson, Hongming Chen,* Lars Carlsson, J. Willem M. Nissink, John G. Cumming, and Ingemar Nilsson*

**Computational Biochemistry****Conformational Preferences of Modified Uridines: Comparison of AMBER Derived Force Fields**

Indrajit Deb, Joanna Sarzynska, Lennart Nilsson, and Ansuman Lahiri*

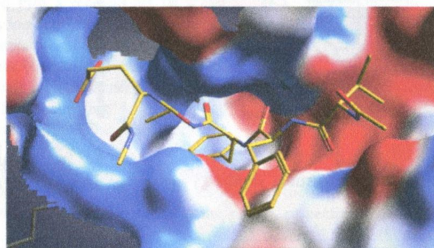


Structure-Based Multiscale Approach for Identification of Interaction Partners of PDZ Domains
Garima Tiwari and Debasisa Mohanty*



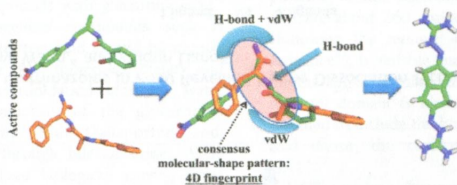
β -Amyloid and Nephrilysin Computational Studies Identify Critical Residues Implicated in Binding Specificity

Darrick Pope, Jeffrey D. Madura, and Michael Cascio*

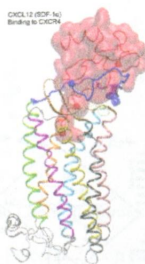


Novel Mycosin Protease MycP₁ Inhibitors Identified by Virtual Screening and 4D Fingerprints

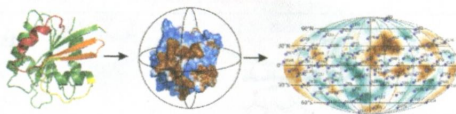
Adel Hamza, Jonathan M. Wagner, Timothy J. Evans, Mykhaylo S. Frasinuk, Stefan Kwiatkowski, Chang-Guo Zhan, David S. Watt, and Konstantin V. Korotkov*



Elucidating a Key Component of Cancer Metastasis: CXCL12 (SDF-1 α) Binding to CXCR4
Phanourios Tamamis and Christodoulos A. Floudas*



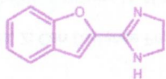
Deciphering Fine Molecular Details of Proteins' Structure and Function with a *Protein Surface Topography (PST)* Method
Anna D. Koromysova, Anton O. Chugunov,* and Roman G. Efremov



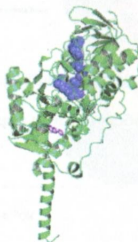
Pharmaceutical Modeling

Computational Comparison of Imidazoline Association with the I2 Binding Site in Human Monoamine Oxidases
Livia Basile, Matteo Pappalardo, Salvatore Guccione,* Danilo Milardi, and Rona R. Ramsay*

MAO B

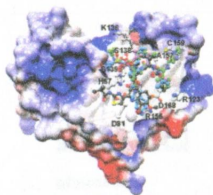


2-BFI binding



Key Binding and Susceptibility of NS3/4A Serine Protease Inhibitors against Hepatitis C Virus

Arthitaya Meeprasert, Supot Hannongbua, and Thanyada Rungrotmongkol*



A Cooperative Mechanism of Clotrimazoles in P450 Revealed by the Dissociation Picture of Clotrimazole from P450

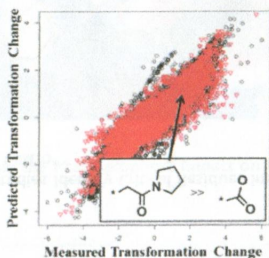
Mian Wang, Marc Baaden, Jianyi Wang,* and Zhiqun Liang*

1 ligand vs 2 ligands



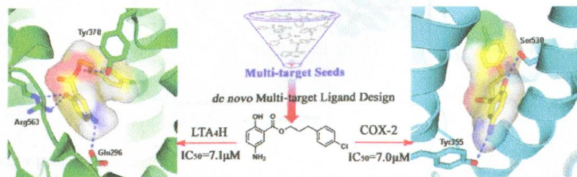
Quantitative Structure–Activity Relationship Models of Chemical Transformations from Matched Pairs Analyses

Jeremy M. Beck and Clayton Springer*



De Novo Design of Multitarget Ligands with an Iterative Fragment-Growing Strategy

Erchang Shang, Yaxia Yuan, Xinyi Chen, Ying Liu,* Jianfeng Pei,* and Luhua Lai*

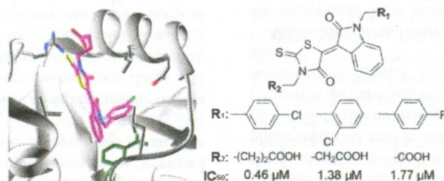


1242 **S**

dx.doi.org/10.1021/ci400686d

Identification of Novel Potential Antibiotics against *Staphylococcus* Using Structure-Based Drug Screening Targeting Dihydrofolate Reductase

Maiko Kobayashi, Tomohiro Kinjo, Yuji Koseki, Christina R. Bourne, William W. Barrow, and Shunsuke Aoki*



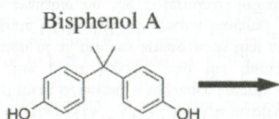
Software Description

1254 **S**

dx.doi.org/10.1021/ci400649p

Endocrine Disruptome—An Open Source Prediction Tool for Assessing Endocrine Disruption Potential through Nuclear Receptor Binding

Katra Kolšek, Janez Mavri, Marija Šollner Dolenc, Stanislav Gobec, and Samo Turk*



Prediction - nuclear receptors

ER α -0.2	ER α -0.1	ER α -0.3
ER α -0.2	ER β -0.4	ER β -0.1
ER γ -0.4	ER γ -0.3	ER γ -0.1
AR -0.1	AR -0.2	AR -0.1
PRAR -0.2	PRAR -0.1	PR -0.1
TR α -0.4	TR α -0.4	TR β -0.7