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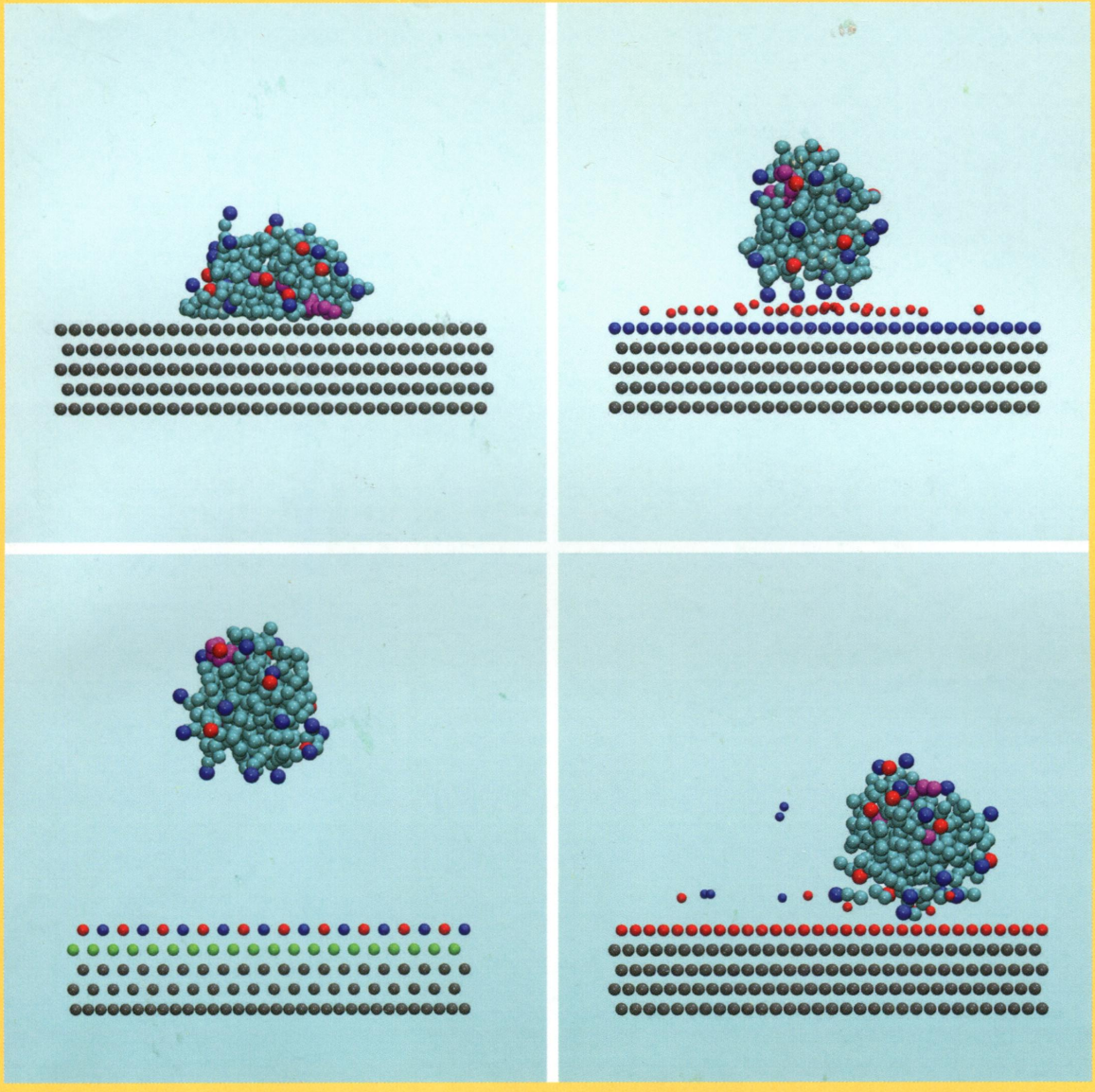

Lysozyme Adsorption on Different Surfaces by Mesoscopic Coarse-Grained Simulations (see page 5A)

BIOPHYSICAL CHEMISTRY, BIOMATERIALS, LIQUIDS, AND SOFT MATTER

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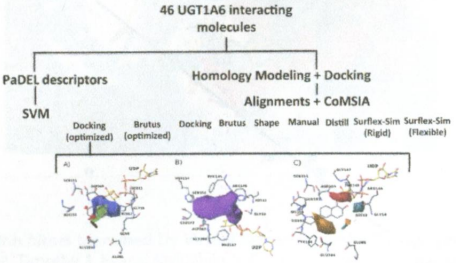
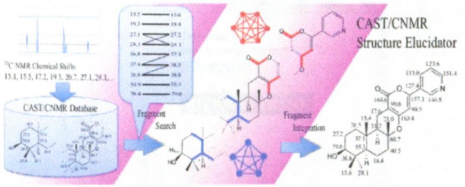
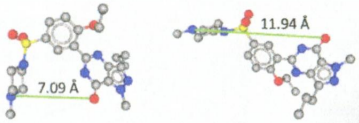
ON THE COVER: AlzPlatform (http://www.cbligand.org/AD/) is an Alzheimer's disease (AD) domain-specific chemogenomics knowledge base, featuring a large repertoire of AD drugs and small chemical molecules as well as related genes and protein targets. The comprehensive database and powerful computational 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.

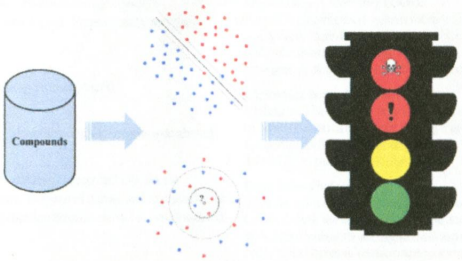
Articles

Chemical Information





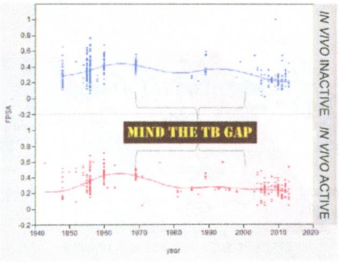




1070 S dx.doi.org/10.1021/ci500077v

Looking Back to the Future: Predicting *in Vivo* Efficacy of Small Molecules versus *Mycobacterium tuberculosis*

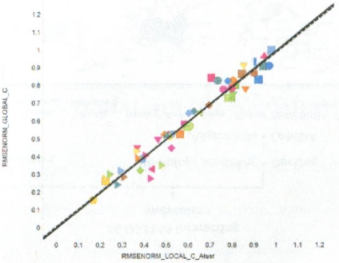
Sean Ekins,* Richard Pottorf, Robert C. Reynolds, Antony J. Williams, Alex M. Clark, and Joel S. Freundlich*



1083 S dx.doi.org/10.1021/ci500084w

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

Robert P. Sheridan*

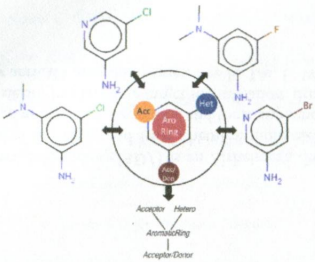


Computational Chemistry

1093 dx.doi.org/10.1021/ci400694q

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

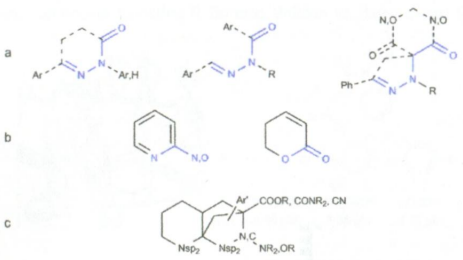
Tim Geppert* and Bernd Beck



1103 S dx.doi.org/10.1021/ci400723m

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

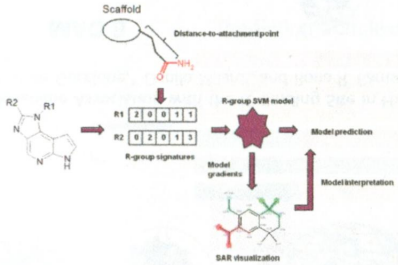
Polina V. Oliferenko, Alexander A. Oliferenko, Adel S. Girgis, Dalia O. Saleh, Aladdin M. Srour, Riham F. George, Girinath G. Pillai, Chandramukhi S. Panda, C. Dennis Hall,* and Alan R. Katritzky



1117 S dx.doi.org/10.1021/ci500075q

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*

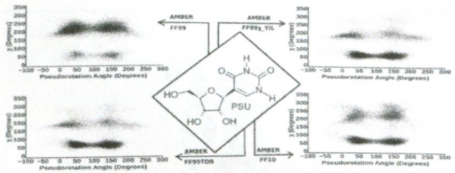


Computational Biochemistry

1129 S dx.doi.org/10.1021/ci400582a

Conformational Preferences of Modified Uridines: Comparison of AMBER Derived Force Fields

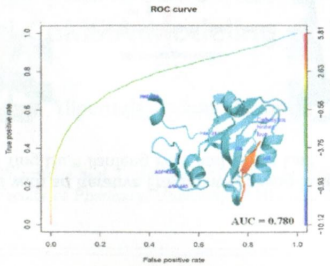
Indrajit Deb, Joanna Sarzynska, Lennart Nilsson, and Ansuman Lahiri*



1143 S dx.doi.org/10.1021/ci400627y

Structure-Based Multiscale Approach for Identification of Interaction Partners of PDZ Domains

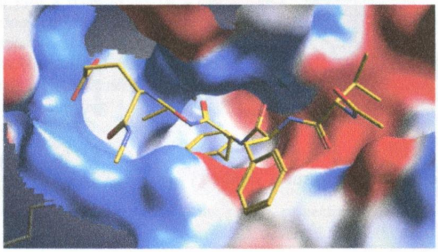
Garima Tiwari and Debasisa Mohanty*



1157 S dx.doi.org/10.1021/ci500015m

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

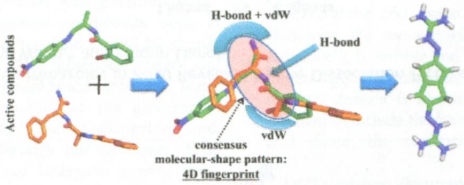
Darrick Pope, Jeffry D. Madura, and Michael Cascio*

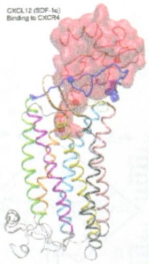


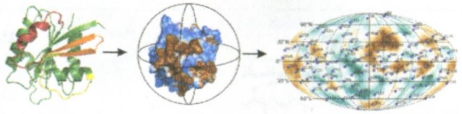
1166 S dx.doi.org/10.1021/ci500025r

Novel Mycosin Protease MycP$_1$ Inhibitors Identified by Virtual Screening and 4D Fingerprints

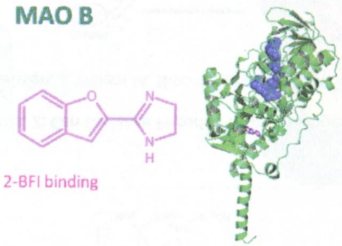
Adel Hamza, Jonathan M. Wagner, Timothy J. Evans, Mykhaylo S. Frasinyuk, Stefan Kwiatkowski, Chang-Guo Zhan, David S. Watt, and Konstantin V. Korotkov*

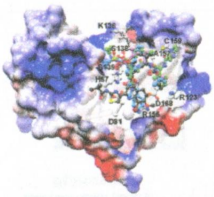


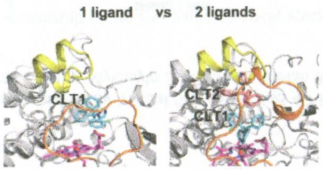


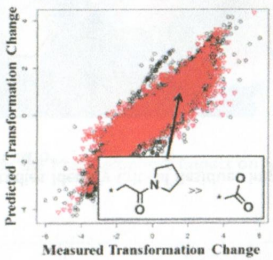


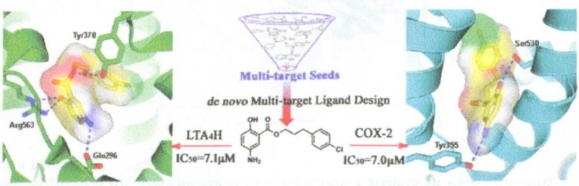
Pharmaceutical Modeling









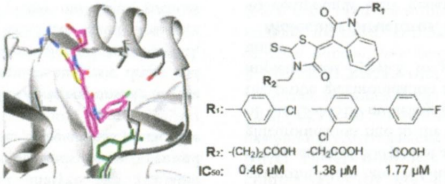


Bioinformatics

1242 Ⓢ 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*

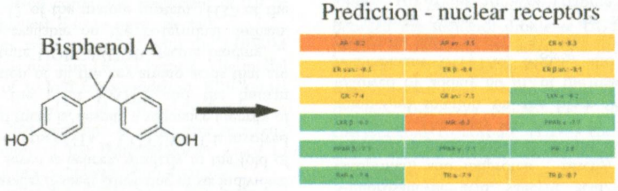


Software Description

1254 Ⓢ 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 Sollner Dolenc, Stanislav Gobec, and Samo Turk*



Ⓢ Supporting Information available via online article