Molecular BioSystems

Interfacing chemical biology with the -omic sciences and systems biology

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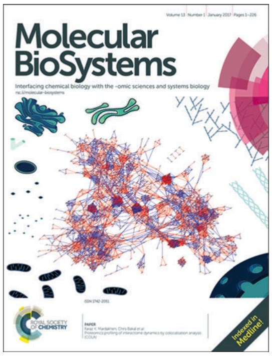
IN THIS ISSUE

ISSN 1742–2051 CODEN MBOIBW 13(1) 1–226 (2017)



Cover
See Faraz K. Mardakhe, Chris Bakal *et al.*, pp. 92–105.
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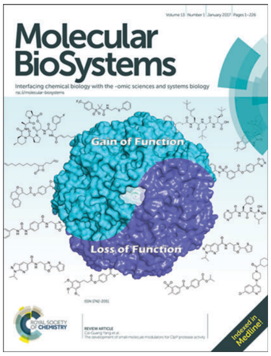

Inside cover
See Cai-Guang Yang *et al.*, pp. 23–31.
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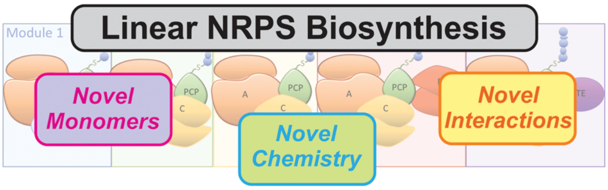
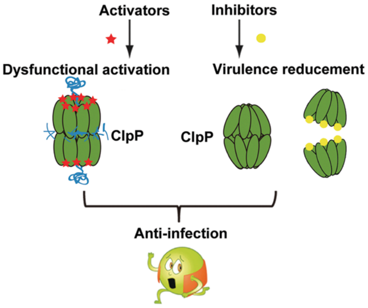
OPINION



REVIEWS



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Molecular BioSystems (electronic: ISSN 1742-2051) is published 12 times a year by the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, UK CB4 0WF.

All orders, with cheques made payable to the Royal Society of Chemistry, should be sent to the Royal Society of Chemistry Order Department, Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK Tel +44 (0)1223 432398; E-mail **orders@rsc.org**

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REVIEWS

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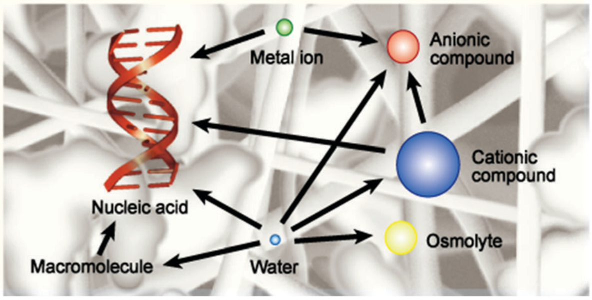
Model studies of the effects of intracellular crowding on nucleic acid interactions

Shu-ichi Nakano* and Naoki Sugimoto*

Studies using experimental model systems have revealed significant effects of the intracellular environment on the interactions of DNA and RNA.



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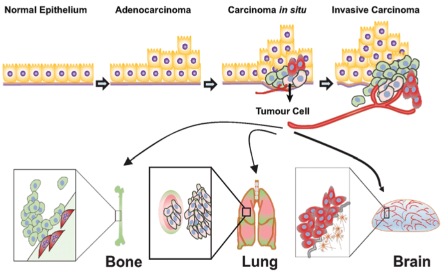
Advancement of mass spectrometry-based proteomics technologies to explore triple negative breast cancer

Sayem Miah, Charles A. S. Banks, Mark K. Adams, Laurence Florens, Kiven E. Lukong and Michael P. Washburn*

Understanding the complexity of cancer biology requires extensive information about the cancer proteome over the course of the disease.



Progression of human breast cancer.

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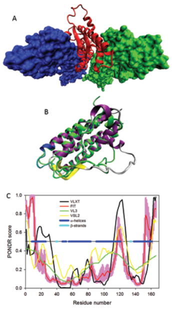
Erythropoietin and co.: intrinsic structure and functional disorder

Vladimir N. Uversky* and Elrashdy M. Redwan*

Erythropoietin (Epo) is a glycoprotein with important roles in erythropoiesis and other biological processes by serving as a hormone, a cytokine, or a growth factor. At least in part, the Epo multifunctionality is driven by its partners. The goal of this article is to evaluate the roles of intrinsic disorder in the functions of Epo and its primary interactors, EpoR, βCR, and HIF-1α.



COMMUNICATIONS

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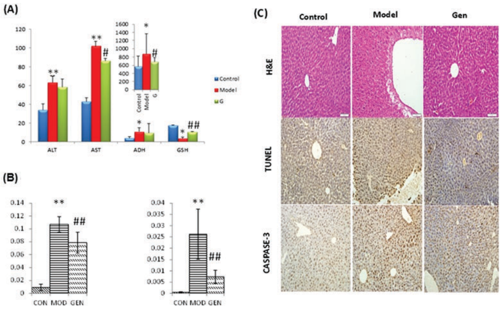
High-throughput metabolomics approach reveals new mechanistic insights for drug response of phenotypes of geniposide towards alcohol-induced liver injury by using liquid chromatography coupled to high resolution mass spectrometry

Tianlei Zhang, Aihua Zhang, Shi Qiu, Hui Sun, Ying Han, Yu Guan and Xijun Wang*

Alcohol-induced liver injury (ALD) shows obvious metabolic disorders, categorized by a wide range of metabolite abnormalities.



COMMUNICATIONS

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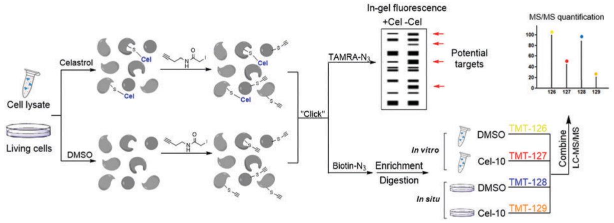

Competitive profiling of celastrol targets in human cervical cancer HeLa cells *via* quantitative chemical proteomics

Yiqing Zhou, Weichao Li, Mingli Wang, Xixi Zhang,
Haibing Zhang, Xiaofeng Tong and Youli Xiao*

We reported the proteome-wide profiling of cellular targets of celastrol in HeLa cells *via* competitive chemoproteomics approach utilizing a cysteine-targeting activity-based probe.

PAPERS

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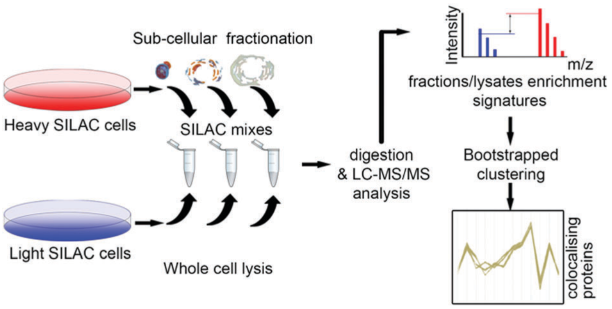

Proteomics profiling of interactome dynamics by colocalisation analysis (COLA)

Faraz K. Mardakheh,* Heba Z. Sailem, Sandra Kümper,
Christopher J. Tape, Ryan R. McCully, Angela Paul,
Sara Anjomani-Virmouni, Claus Jørgensen,
George Poulogiannis, Christopher J. Marshall and
Chris Bakal*

A combined proteomics and bioinformatics strategy for mapping interactome dynamics *via* assessment of subcellular protein–protein colocalisations.

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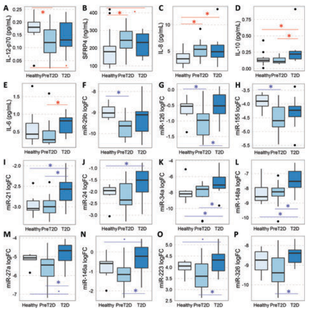

Altered levels of circulating cytokines and microRNAs in lean and obese individuals with prediabetes and type 2 diabetes

Yury O. Nunez Lopez, Gabriella Garufi and
Attila A. Seyhan*

Today obesity and type 2 diabetes (T2D) have both reached epidemic proportions.

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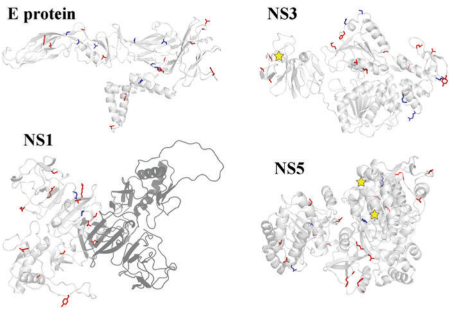

Analysis of worldwide sequence mutations in Zika virus proteins E, NS1, NS3 and NS5 from a structural point of view

C. F. Baez, V. A. Barel, A. M. T. de Souza, C. R. Rodrigues,
R. B. Varella and N. Cirauqui*

A structural and mutational analysis of ZIKV identifies some protein regions as potential anti-ZIKV targets.

PAPERS

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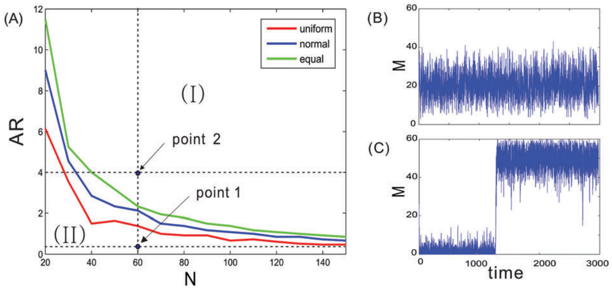
Random positioning of nucleosomes enhances heritable bistability

Heli Tan, Tuoqi Liu, Jiajun Zhang and Tianshou Zhou*

Chromosomal regions are often dynamically modified by histones, leading to the uncertainty of nucleosome positions.



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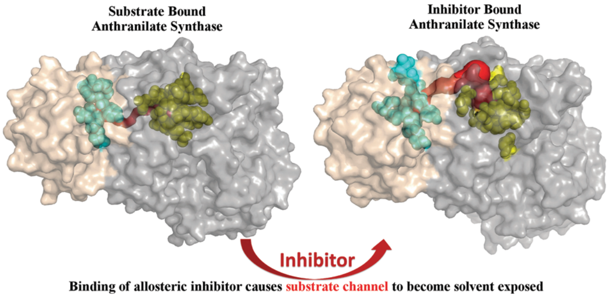
Uncoupling of an ammonia channel as a mechanism of allosteric inhibition in anthranilate synthase of *Serratia marcescens*: dynamic and graph theoretical analysis

Ashutosh Srivastava and Somdatta Sinha*

Network modeling and molecular dynamic studies reveal the perturbation in communication pathways as a mechanism of allosteric inhibition in anthranilate synthase.



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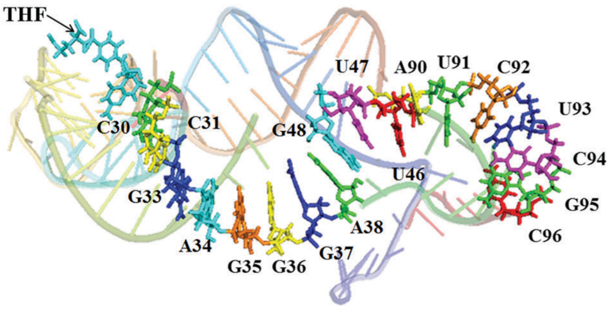
Allosteric pathways in tetrahydrofolate sensing riboswitch with dynamics correlation network

Jin-Mai Zhang, Cheng Jiang, Wei Ye, Ray Luo* and Hai-Feng Chen*

The allosteric pathway of a THF riboswitch is from the allosteric site of THF to the expression platform.



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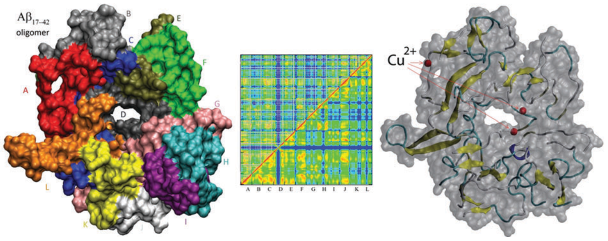
Probing oligomerization of amyloid beta peptide *in silico*

L. Dorosh and M. Stepanova*

Simulations reveal molecular-level details of aggregation of amyloid β peptide that is implicated in fatal Alzheimer's disease.



PAPERS

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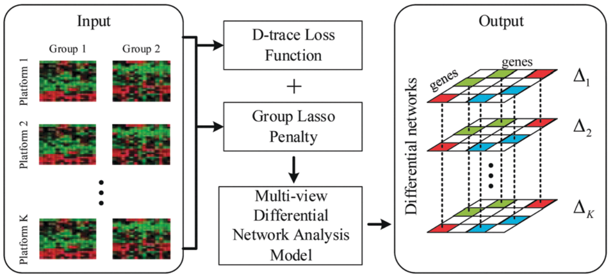

Identifying differential networks based on multi-platform gene expression data

Le Ou-Yang, Hong Yan and Xiao-Fei Zhang*

Exploring how the structure of a gene regulatory network differs between two different disease states is fundamental for understanding the biological mechanisms behind disease development and progression.

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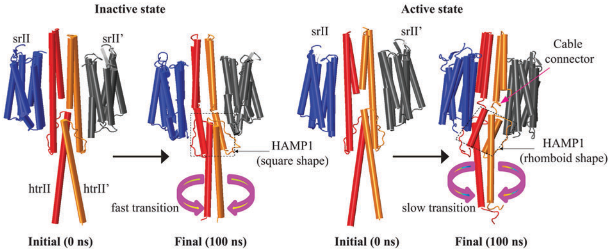

Conformational states of HAMP domains interacting with sensory rhodopsin membrane systems: an integrated all-atom and coarse-grained molecular dynamics simulation approach

Bikash Ranjan Sahoo and Toshimichi Fujiwara*

The mechanistic and structural basis of srII–htrII signaling mediated by a HAMP four-helix bundle in *Natronomonas pharaonis*.

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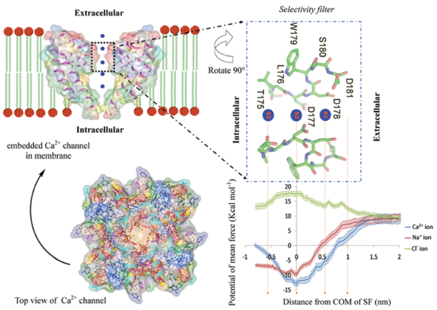

Modeling ion permeation through a bacterial voltage-gated calcium channel Ca_VAb using molecular dynamics simulations

Jamal Adiban, Yousef Jamali and Hashem Rafii-Tabar*

Ca^{2+} ion binds tightly to the center of the selectivity filter of voltage-gated calcium channels.

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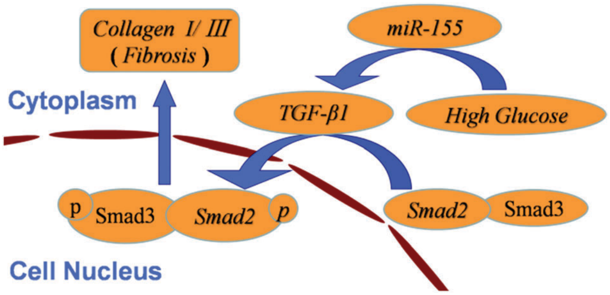

miR-155 regulates high glucose-induced cardiac fibrosis *via* the TGF-β signaling pathway

Dong Zhang, Yongchun Cui, Bin Li, Xiaokang Luo, Bo Li and Yue Tang*

miR-155 regulates high glucose-induced cardiac fibrosis *via* the TGF-β/Smad 2 pathway.