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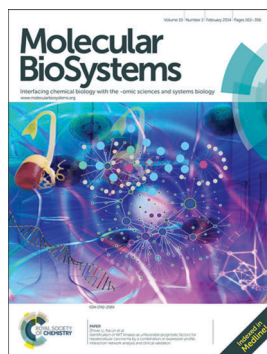
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ISSN 1742–206X CODEN MBOIBW 10(2) 163–356 (2014)



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See Stephen Kwok-Wing Tsui, Simon Ming-Yuen Lee *et al.*, pp. 206–214. Image reproduced by permission of Simon Ming-Yuen Lee from *Mol. BioSyst.*, 2014, 10, 206.



Inside cover

See Zhiwei Li, Na Lin *et al.*, pp. 215–222. Image reproduced by permission of Yanqiong Zhang from *Mol. BioSyst.*, 2014, 10, 215.

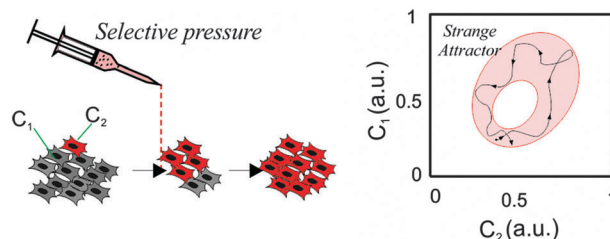
OPINION

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Tumors as chaotic attractors

Svetoslav Nikolov, Olaf Wolkenhauer and Julio Vera*

Tumors are envisioned as nonlinear dynamical systems that behave like strange attractors, a dynamical behavior displayed by some chaotic systems.



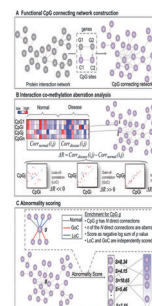
METHOD

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A network-based, integrative approach to identify genes with aberrant co-methylation in colorectal cancer

Yongsheng Li, Juan Xu, Huanyu Ju, Yun Xiao, Hong Chen, Junying Lv, Tingting Shao, Jing Bai, Yunpeng Zhang, Li Wang, Xishan Wang,* Huan Ren* and Xia Li*

A novel method which integrates DNA methylation and a protein interaction network to identify genes in colorectal cancers is reported.



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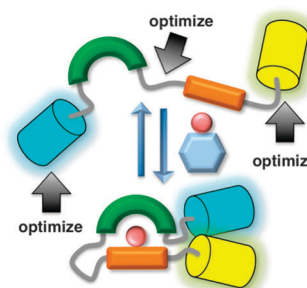
COMMUNICATIONS

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Optimization of a genetically encoded biosensor for cyclin B1-cyclin dependent kinase 1

Ahmed Saied F. Belal, Brittney R. Sell, Hiofan Hoi, Michael W. Davidson and Robert E. Campbell*

Optimization of a fluorescent protein-based biosensor of kinase activity can be achieved by screening libraries in *E. coli* with an inducible kinase.

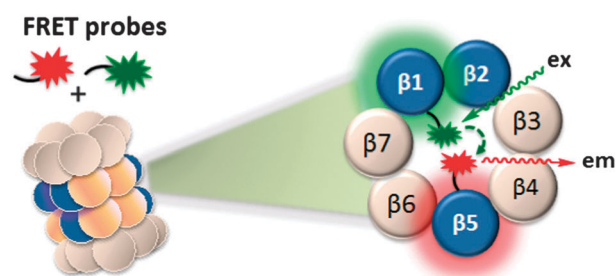


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A FRET-based approach for identification of proteasome catalytic subunit composition

Ji Eun Park, Ying Wu, Kimberly Cornish Carmony, Zachary Miller, Lalit Kumar Sharma, Do-Min Lee, Doo-Young Kim, Woojin Lee and Kyung-Bo Kim*

Proteasome anatomy revealed: FRET pairs that target proteasome catalytic subunits have been developed. Upon excitation, FRET between a donor-acceptor pair bound to two different catalytic subunits within a single 20S proteasome occurs, revealing the catalytic subunit composition.

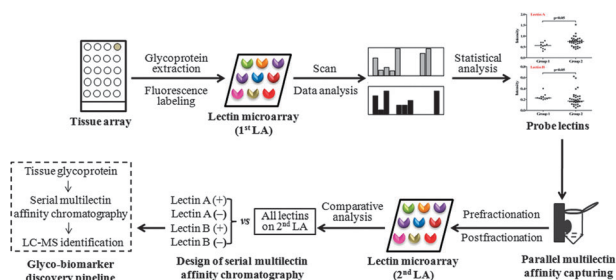


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Multilectin-assisted fractionation for improved single-dot tissue glycome profiling in clinical glycoproteomics

Binbin Tan, Atsushi Matsuda, Yan Zhang, Atsushi Kuno and Hisashi Narimatsu*

An ultrasensitive and universal platform for glyco-biomarker discovery based on lectin microarrays and lectin-assisted fractionation.



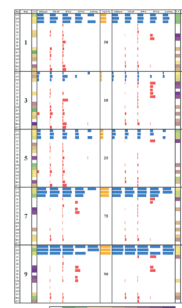
PAPERS

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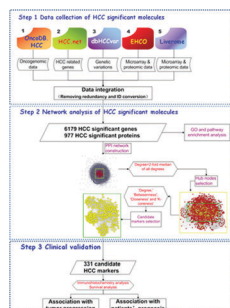
Quick, sensitive and specific detection and evaluation of quantification of minor variants by high-throughput sequencing

Ross Ka-Kit Leung, Zhi Qiang Dong, Fei Sa, Cheong Meng Chong, Si Wan Lei, Stephen Kwok-Wing Tsui* and Simon Ming-Yuen Lee*

Minor variants have significant implications in quasispecies evolution, early cancer detection and non-invasive fetal genotyping but their accurate detection by next-generation sequencing (NGS) is hampered by sequencing errors.



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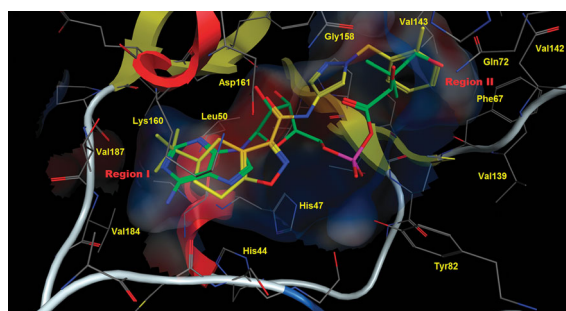


Identification of AKT kinases as unfavorable prognostic factors for hepatocellular carcinoma by a combination of expression profile, interaction network analysis and clinical validation

Yanqiong Zhang, Xiaodong Guo, Mei Yang, Lingxiang Yu, Zhiwei Li* and Na Lin*

This study provided an integrated analysis to identify a list of biologically significant HCC related markers and pathways. Further experimental validation identified AKT proteins as novel unfavorable prognostic factors for HCC.

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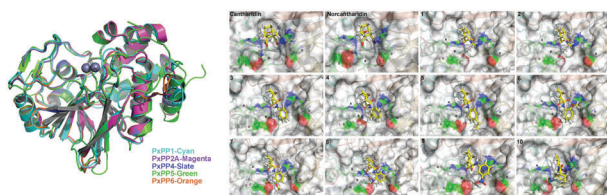


Binding of pyrazole-based inhibitors to Mycobacterium tuberculosis pantothenate synthetase: docking and MM-GB(PB)SA analysis

Fidele Ntie-Kang,* Srinivasaraghavan Kannan, Kanin Wichapong, Luc C. Owono Owono, Wolfgang Sippl and Eugene Megnassan

A virtual screening method for searching for potential inhibitors of Mycobacterium tuberculosis pantothenate synthetase has been developed based on docking, pharmacophore modelling and MM-GBSA/MM-PBSA.

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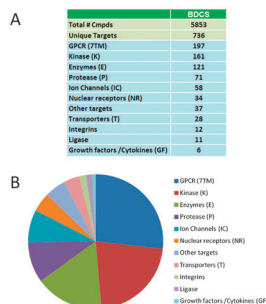


Cantharidin impedes the activity of protein serine/threonine phosphatase in Plutella xylostella

Xi'en Chen, Jiyuan Liu and Yalin Zhang*

Cantharidin and its 11 analogs could anchor to the active sites of PxPSPs exerting their insecticidal activity.

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A novel approach applying a chemical biology strategy in phenotypic screening reveals pathway-selective regulators of histone 3 K27 tri-methylation

Yan Liu,* Michael Platchek, Burcu Kement, Weilin T. Bee, Maggie Truong, Xin Zeng, Sunny Hung, Hong Lin, Dwight Morrow, Lorena A. Kallal, Qing Xie, Pankaj Agarwal, Andrew J. Pope and Zining Wu

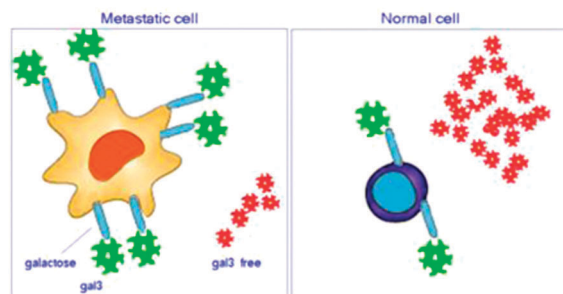
Epigenetic regulation by histone methylation is crucial for proper programming of the genome during development.

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Galectin-3 coats the membrane of breast cells and makes a signature of tumours

Giuseppina Simone,* Natalia Malara, Valentina Trunzo, Maria Renne, Gerardo Perozziello, Enzo Di Fabrizio and Andreas Manz

The galactose-based assay exploiting a microfluidic approach displays high sensitivity in highlighting the galectin-3 phenotype. The galectin-3 that coats the cellular membrane displays metastatic potential and can provide new insight into metastatisation of the breast cells.



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Predicting genetic and ecological characteristics of bacterial species by comparing the trajectories of dN/dS and dI/dS in bacterial genomes

Ye Feng and Cheng-Hsun Chiu*

Indel (insertion/deletion) causes gene disruption and is considered to be deleterious like non-synonymous mutation during the evolution of bacterial genomes.

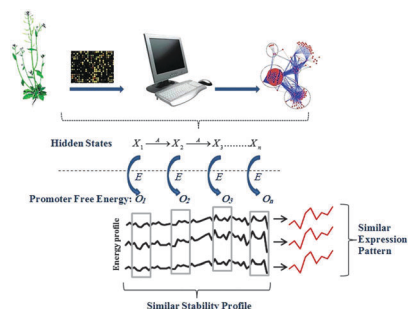


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The structural properties of DNA regulate gene expression

Sattar Soltani,* Hossein Askari,* Nasim Ejlali and Rosa Aghdam

The graphical abstract illustrates how structural properties of DNA regulatory sequences control gene expression based on our suggested hidden Markov model.

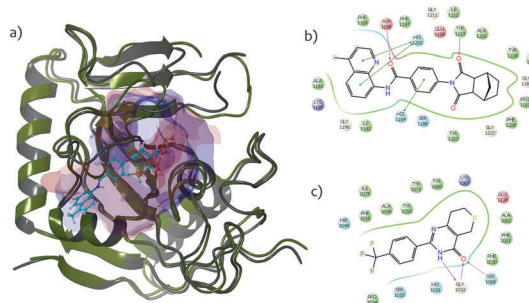


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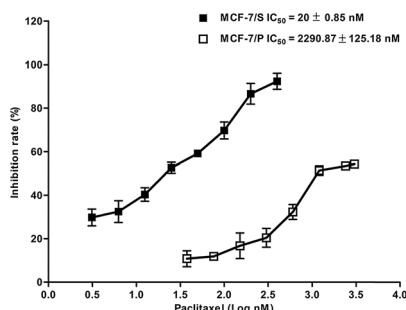
Molecular insights on TNKS1/TNKS2 and inhibitor-IWR1 interactions

Palani Kirubakaran, Gugan Kothandan, Seung J. Cho and Karthikeyan Muthusamy*

Tankyrases (TNKS) belong to the poly(ADP-ribose)-polymerase (PARP) protein super family and play a vital role in the Wnt/ β -catenin signaling pathway.



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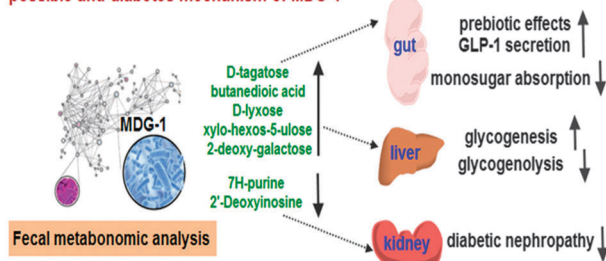
Proteomic analysis of the proteins that are associated with the resistance to paclitaxel in human breast cancer cells

Siying Chen, Qian Dong, Sasa Hu, Jiangxia Cai, Weipeng Zhang, Jinyao Sun, Taotao Wang, Jiao Xie, Hairong He, Jianfeng Xing, Jun Lu* and Yalin Dong*

Cancers frequently develop resistance to paclitaxel but the underlying molecular mechanisms remain to be determined.

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possible anti-diabetes mechanism of MDG-1

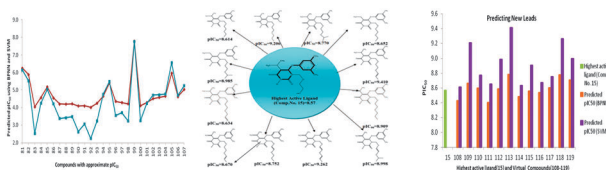


Fecal metabonomic study of a polysaccharide, MDG-1 from *Ophiopogon japonicus* on diabetic mice based on gas chromatography/time-of-flight mass spectrometry (GC TOF/MS)

Yunyun Zhu, Wenjuan Cong,* Lan Shen, Hai Wei, Yuan Wang, Lingyi Wang, Kefeng Ruan, Fei Wu and Yi Feng*

Fecal metabonomics elucidated a possible anti-diabetic mechanism of a non-digestible polysaccharide MDG-1 from the MDG-1-gut-microbe-interaction perspective.

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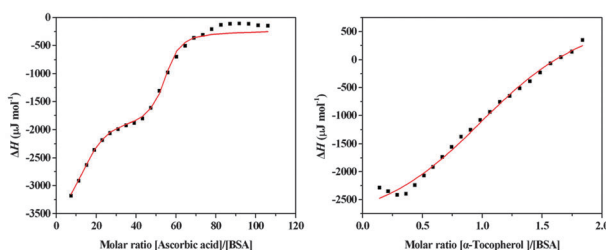


Design of novel leads: ligand based computational modeling studies on non-nucleoside reverse transcriptase inhibitors (NNRTIs) of HIV-1

Nilanjana Jain (Pancholi), Swagata Gupta, Neelima Sapre and Nitin S. Sapre*

Ligand based molecular modeling studies performed on NNRTIs of HIV-1 have resulted in extraction of novel lead molecules with high anti HIV-1 inhibitory activity.

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Binding of ascorbic acid and α -tocopherol to bovine serum albumin: a comparative study

Xiangrong Li, Gongke Wang, Dejun Chen and Yan Lu*

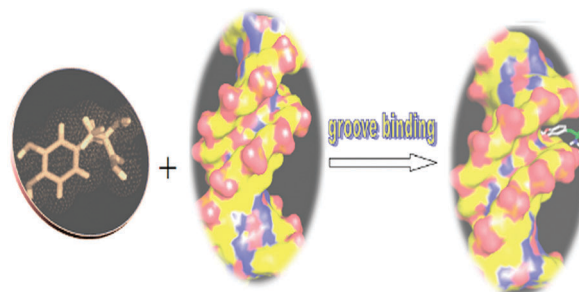
The study provides the full basic data for clarifying the different binding mechanisms of ascorbic acid and α -tocopherol to BSA.

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Multi-spectroscopic and molecular modeling studies on the interaction of antihypertensive drug; methyldopa with calf thymus DNA

Nahid Shahabadi* and Maryam Maghsudi

A combination of experimental and computational methods were employed, in order to determine where and how MDP binds to DNA.



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A model of glycosylated human butyrylcholinesterase

Lei Fang, Fang Zheng and Chang-Guo Zhan*

A three-dimensional model of glycosylated human BChE has been developed to investigate the influence of glycans on the PEGylation modification.

