

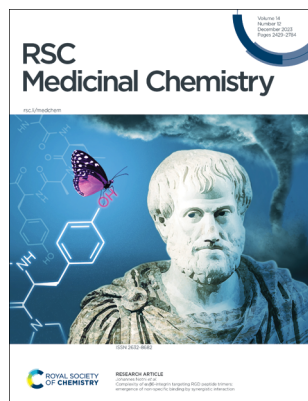
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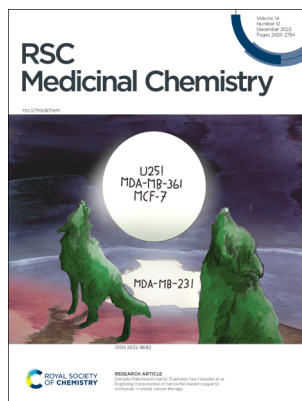
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Cover

See Johannes Notni *et al.*, pp. 2564–2573.
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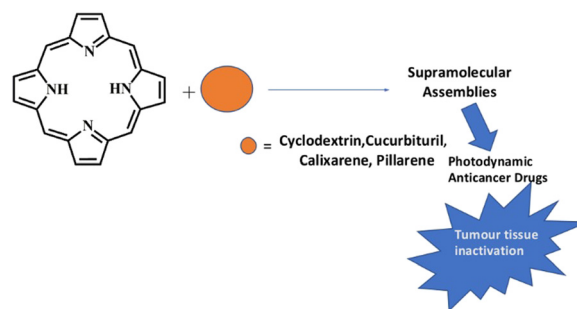
See Danijela Maksimović-Ivanić, Evamarie Hey-Hawkins *et al.*, pp. 2574–2582.
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REVIEWS

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Applications of supramolecular assemblies in drug delivery and photodynamic therapy

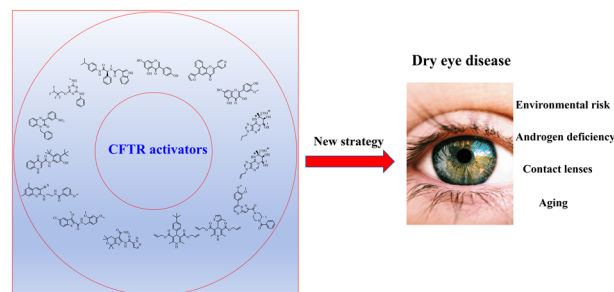
Kharu Nisa,* Ishfaq Ahmad Lone, Waseem Arif, Preeti Singh,* Sajad Ur Rehman and Ravi Kumar*



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Overview of CFTR activators and their recent studies for dry eye disease: a review

Jie Wu, Xiaoqian Wang, Yanfang Zhao, Yunlei Hou* and Ping Gong*



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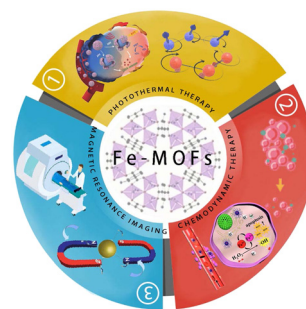


REVIEWS

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Current status of Fe-based MOFs in biomedical applications

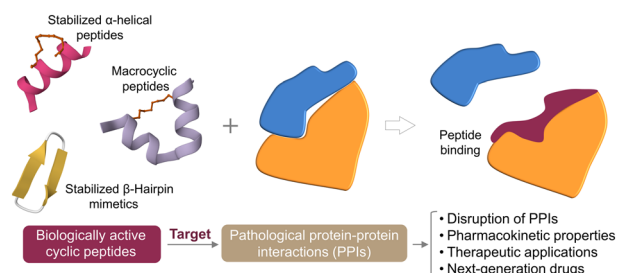
Hanping Yang, Donghui Liao, Zhidong Cai, Yuelin Zhang, Alireza Nezamzadeh-Ejhieh, Mingbin Zheng, Jianqiang Liu,* Zhi Bai* and Hailiang Song*



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Stabilized cyclic peptides as modulators of protein–protein interactions: promising strategies and biological evaluation

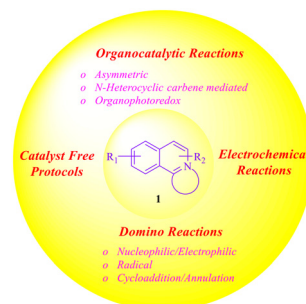
Jiongjia Cheng, Junlong Zhou, Lingyan Kong, Haiying Wang, Yuchi Zhang, Xiaofeng Wang, Guangxiang Liu* and Qian Chu*



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Diversely functionalized isoquinolines and their core-embedded heterocyclic frameworks: a privileged scaffold for medicinal chemistry

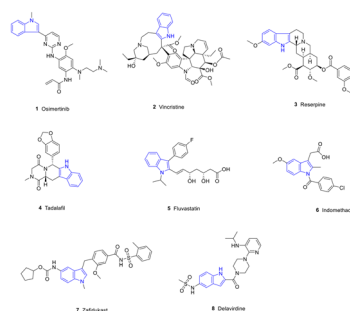
Archana Vijayakumar, M. Manod, R. Bharath Krishna, Abra Mathew and Chithra Mohan*



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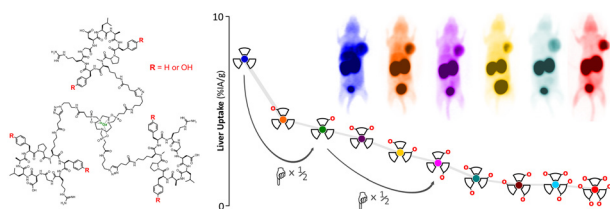
Research status of indole-modified natural products

Song-Fang Duan, Lei Song, Hong-Yan Guo, Hao Deng, Xing Huang, Qing-Kun Shen, Zhe-Shan Quan* and Xiu-Mei Yin*



RESEARCH ARTICLES

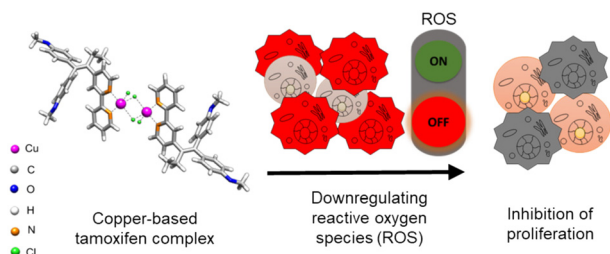
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Complexity of $\alpha_v\beta_6$ -integrin targeting RGD peptide trimers: emergence of non-specific binding by synergistic interaction

Neil Gerard Quigley, Frauke Richter, Susanne Kossatz and Johannes Notni*

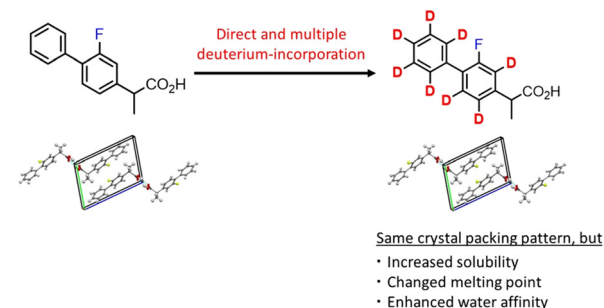
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Exploring the potential of tamoxifen-based copper(II) dichloride in breast cancer therapy

Aleksandr Kazimir, Benedikt Schwarze, Peter Lönnecke, Sanja Jelača, Sanja Mijatović, Danijela Maksimović-Ivanić* and Evamarie Hey-Hawkins*

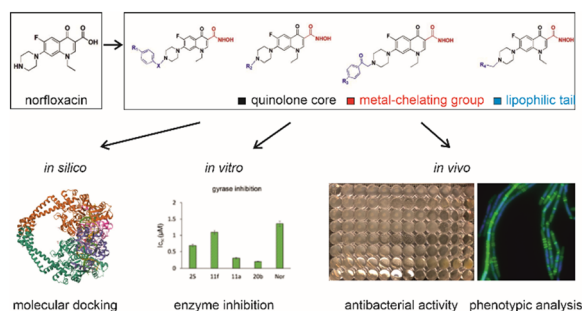
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Impact of multiple H/D replacements on the physicochemical properties of flurbiprofen

Hiromasa Uchiyama,* Kazuho Ban, Shiho Nozaki, Yui Ikeda, Takayoshi Ishimoto, Hiroyoshi Fujioka, Mako Kamiya, Ryugo Amari, Hirofumi Tsujino, Masayoshi Arai, Sachi Yamazoe, Keiko Maekawa, Takuma Kato, Mitsunobu Doi, Kazunori Kadota, Yuichi Tozuka, Naohito Tomita, Hironao Sajiki, Shuji Akai and Yoshinari Sawama*

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Rational design, synthesis, molecular modeling, biological activity, and mechanism of action of polypharmacological norfloxacin hydroxamic acid derivatives

Ahmed M. Kamal El-sagheir, Ireny Abdelmesseheh Nekhala, Mohammed K. Abd El-Gaber, Ahmed S. Aboraia, Jonatan Persson, Ann-Britt Schäfer, Michaela Wenzel* and Farghaly A. Omar*



Discovery of pyrazolopyrimidines that selectively inhibit CSF-1R kinase by iterative design, synthesis and screening against glioblastoma cells

1) Library Design & Synthesis
2) Phenotypic Assays in GBM lines
3) Phenomics in patient-derived GBM cells
4) Kinome screening

B58 (eDB333)
 EC_{50} (E21 GBM cells) = 0.9 μ M
 IC_{50} (CSF-1R) = 0.159 μ M

A silicon-containing aryl/penta-1,4-dien-3-one/amine hybrid exhibits antiproliferative effects on breast cancer cells by targeting the HSP90 C-terminus without inducing heat-shock response

penta-1,4-dien-3-one linker

Aryl part **Amine part**

- enhance the lipophilic interaction
- maintain the geometry
- enhance the hydrogen bond

↓ 1/32 compounds

1z

IC₅₀ (MCF-7) = 7.85 μM
 IC₅₀ (BT474) = 9.06 μM
 Without HSR induction
 Good thermostability
 Good *in vitro* metabolic stability

Hsp90

Chain A
 Chain B

1z (red)

110 114 115

	MCF-7				MDA-MB-231			
	CTL	NA	1z	10	CTL	NA	1z	10
Hsp90	+	+	+	+	+	+	+	+
AKT	+	+	+	+	+	+	+	+
ERK1	+	+	+	+	+	+	+	+
ERK2	+	+	+	+	+	+	+	+
MDM2	+	+	+	+	+	+	+	+
GAPDH	+	+	+	+	+	+	+	+

Merge

MDA-MB-231
 Hsp90
 DAPI

MDA-MB-231
 Hsp90
 DAPI

MDA-MB-231
 Hsp90
 DAPI

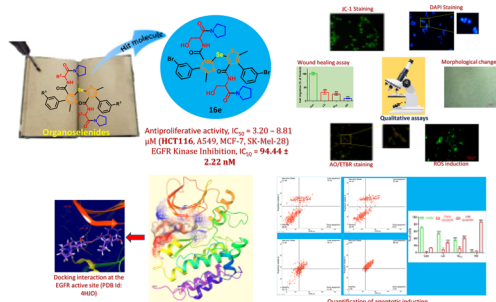
MDA-MB-231
 Hsp90
 DAPI

Novel pyrazolo[3,4-d]pyrimidine derivatives: design, synthesis, anticancer evaluation, VEGFR-2 inhibition, and antiangiogenic activity

Figure 1 illustrates the synthesis of compound 12b. The starting materials are VEGFR2 (IC₅₀ = 0.001), Sunitinib, and a sound heading. The product, 12b, is a VEGFR2 inhibitor with an IC₅₀ of 0.063. The diagram also shows the chemical structure of 12b and its cytotoxicity data (IC₅₀ = 0.063, 75.555 ± 4.11, 21.83, 3.343 ± 0.13, 15.44).

Newly synthesized 6-substituted piperazine/phenyl-9-cyclopentyl containing purine nucleobase analogs act as potent anticancer agents and induce apoptosis *via* inhibiting Src in hepatocellular carcinoma cells

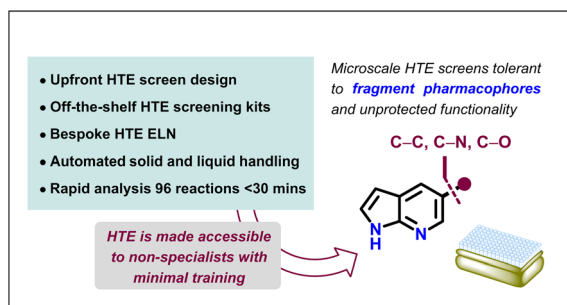
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Development of trisubstituted thiophene-3-arboxamide selenide derivatives as novel EGFR kinase inhibitors with cytotoxic activity

Priyanka N. Makhal, Anika Sood, Arbaz Sujat Shaikh, Lahu N. Dayare, Dharmendra Kumar Khatri* and Venkata Rao Kaki*

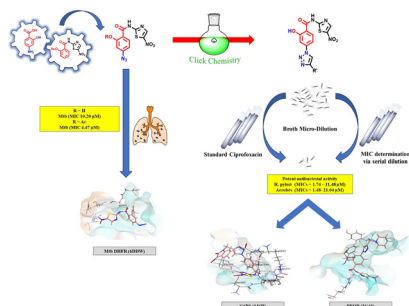
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Enabling synthesis in fragment-based drug discovery (FBDD): microscale high-throughput optimisation of the medicinal chemist's toolbox reactions

Chloe Townley, Davide Branduardi, Gianni Chessari, Benjamin D. Cons, Charlotte Griffiths-Jones, Richard J. Hall, Christopher N. Johnson, Yuji Ochi, Stuart Whibley and Rachel Grainger*

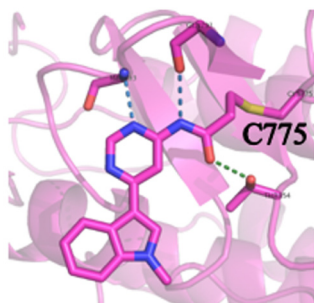
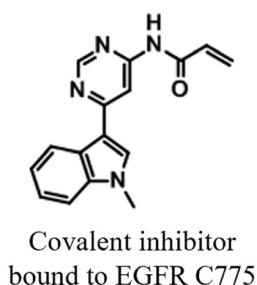
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New nitazoxanide derivatives: design, synthesis, biological evaluation, and molecular docking studies as antibacterial and antimycobacterial agents

Mahmoud Saleh, Yaser A. Mostafa, Jyothi Kumari, Momen M. Thabet, Dharmarajan Sriram, Mahmoud Kandeel and Hajjaj H. M. Abdu-Allah*

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A covalent fragment-based strategy targeting a novel cysteine to inhibit activity of mutant EGFR kinase

Naoki Kuki, David L. Walmsley, Kazuo Kanai, Sho Takechi, Masao Yoshida, Ryo Murakami, Kohei Takano, Yuichi Tominaga, Mizuki Takahashi, Shuichiro Ito, Naoki Nakao, Hayley Angove, Lisa M. Baker, Edward Carter, Pawel Dokurno, Loic Le Strat, Alba T. Macias, Carrie-Anne Molyneaux, James B. Murray, Allan E. Surgenor, Tomoaki Hamada and Roderick E. Hubbard

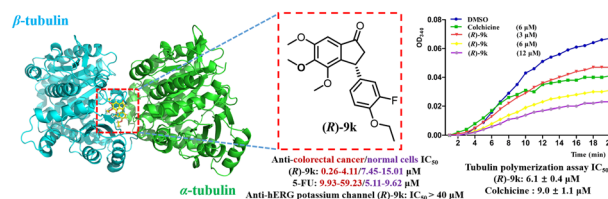


RESEARCH ARTICLES

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Discovery of novel tubulin CBSI (*R*)-9k from the indanone scaffold for the treatment of colorectal cancer

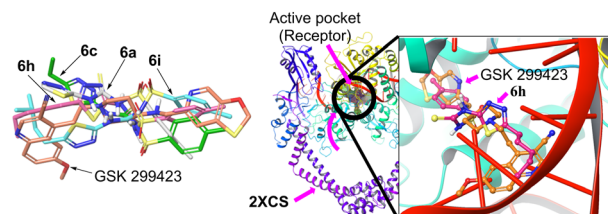
Zhipeng Huo, Delin Min, Shijie Zhang, Mei-Lin Tang* and Xun Sun*



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Synthesis, biological and molecular modelling for 1,3,4-thiadiazole sulfonyl thioureas: bacterial and fungal activity

Nguyen Dinh Thanh,* Vu Ngoc Toan, Nguyen Thi Kim Giang, Hoang Thi Kim Van, Do Son Hai, Nguyen Minh Tri and Duong Ngoc Toan



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Naphthyl bearing 1,3,4-thiadiazoleacetamides targeting the parasitic folate pathway as anti-infectious agents: *in silico*, synthesis, and biological approach

Kavita Pal, Sahil Lala, Priyanka Agarwal, Tarosh S. Patel, Jenny Legac, Md. Ataur Rahman, Saiema Ahmed, Nida Shahid, Sneha Singh, Kajal Kumari, Hari Madhav, Abhik Sen, Nikhat Manzoor, Bharat C. Dixit, Robyn Van Zyl, Philip J. Rosenthal and Nasimul Hoda*

