



## Graphical Abstracts/Bioorganic Chemistry 88 (2019) i-xxii

## PUBLISHER'S NOTE

Introducing article numbering to Journal of Bioorganic Chemistry

Bioorganic Chemistry 88 (2019) 103041

## REGULAR ARTICLES

**Targeting hepatocellular carcinoma:  
Synthesis of new pyrazole-based  
derivatives, biological evaluation,  
DNA binding, and molecular  
modeling studies**

Dina M. Omran<sup>a</sup>, Mariam A. Ghaly<sup>a,\*</sup>,  
Shahenda M. El-Messery<sup>b</sup>, Farid A. Badria<sup>c</sup>,  
Ehab Abdel-Latif<sup>d</sup>, Ihsan A. Shehata<sup>a</sup>

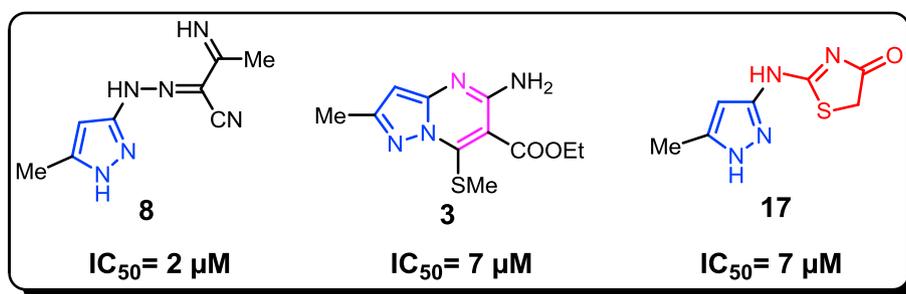
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Bioorganic Chemistry 88 (2019) 102917



### Probing the high potency of pyrazolyl pyrimidinetriones and thioxopyrimidinediones as selective and efficient non-nucleotide inhibitors of recombinant human ectonucleotidases

Bioorganic Chemistry 88 (2019) 102893

Hina Andleeb<sup>a,b</sup>, Shahid Hameed<sup>a,\*</sup>, Syeda Abida Ejaz<sup>c</sup>, Imtiaz Khan<sup>a,d,e</sup>, Sumera Zaib<sup>c</sup>, Joanna Lecka<sup>f,g</sup>, Jean Sévigny<sup>f,g</sup>, Jamsheed Iqbal<sup>e,\*</sup>

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<sup>b</sup>Sulaiman Bin Abdullah Aba Al-Khail – Centre for Interdisciplinary Research in Basic Science (SA-CIRBS), Faculty of Basic and Applied Sciences, International Islamic University, Islamabad, Pakistan

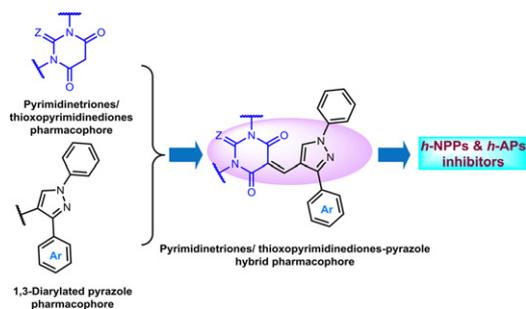
<sup>c</sup>Centre for Advanced Drug Research, COMSATS Institute of Information Technology, Abbottabad 22060, Pakistan

<sup>d</sup>School of Chemistry, The University of Manchester, Oxford Road, Manchester M13 9PL, United Kingdom

<sup>e</sup>Manchester Institute of Biotechnology, The University of Manchester, 131 Princess Street, Manchester M1 7DN, United Kingdom

<sup>f</sup>Département de microbiologie-infectiologie et d'immunologie, Faculté de Médecine, Université Laval, Québec, QC G1V 0A6, Canada

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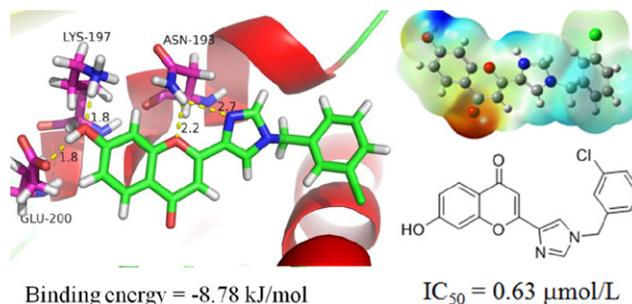
### Identification of novel imidazole flavonoids as potent and selective inhibitors of protein tyrosine phosphatase

Bioorganic Chemistry 88 (2019) 102900

Ling Zhang<sup>a,\*</sup>, Yu Ge<sup>a</sup>, Qing Ming Wang<sup>a,\*</sup>, Cheng-He Zhou<sup>b</sup>

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<sup>b</sup>Laboratory of Bioorganic & Medicinal Chemistry, School of Chemistry and Chemical Engineering, Southwest University, Chongqing 400715, People's Republic of China



### Vieloplains A-G, seven new guaiane-type sesquiterpenoid dimers from *Xylopiia vihana*

Bioorganic Chemistry 88 (2019) 102891

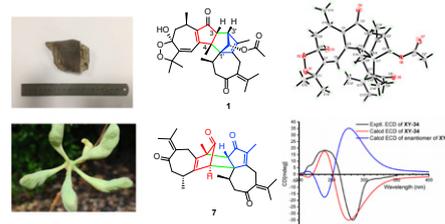
Yangguo Xie<sup>a</sup>, Xianglong Zhong<sup>d</sup>, Yongzhen Xiao<sup>a</sup>, Shenglan Zhu<sup>a</sup>, Ishaq Muhammad<sup>a</sup>, Shikai Yan<sup>a</sup>, Huizi Jin<sup>a,\*</sup>, Weidong Zhang<sup>a,b,c,\*</sup>

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<sup>c</sup>School of Pharmacy, Second Military Medical University, Shanghai 200433, PR China

<sup>d</sup>Department of Pharmacy, Anhui University of Chinese Medicine, HeFei 320000, PR China



### Synthesis and anti-tumor activity of [1,4] dioxino [2,3-f] quinazoline derivatives as dual inhibitors of c-Met and VEGFR-2

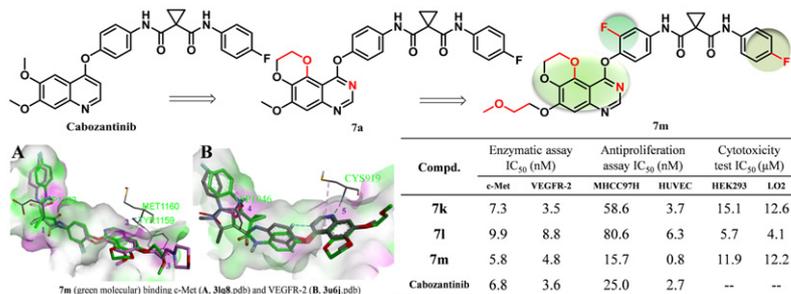
Bioorganic Chemistry 88 (2019) 102916

Dengshuai Wei<sup>a</sup>, Haoru Fan<sup>a</sup>, Kun Zheng<sup>b</sup>, Xuemei Qin<sup>c</sup>, Leifu Yang<sup>b</sup>, Yajuan Yang<sup>b</sup>, Ye Duan<sup>b</sup>, Qiang Zhang<sup>b</sup>, Chengchu Zeng<sup>a</sup>, Liming Hu<sup>a,\*</sup>

<sup>a</sup>College of Life Science and Bioengineering & Beijing Key Laboratory of Environmental and Oncology, Beijing University of Technology, Beijing 100124, China

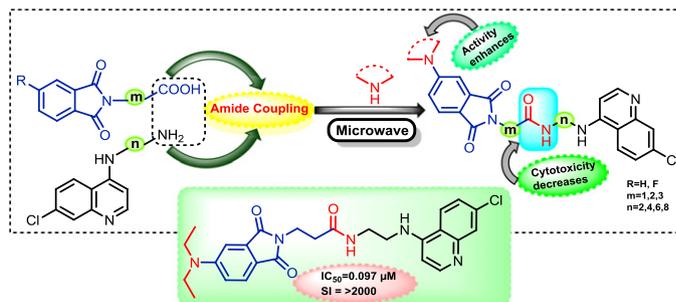
<sup>b</sup>Beijing Scitech-MQ Pharmaceuticals Limited, Beijing 101320, China

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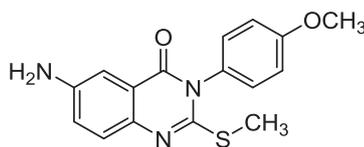
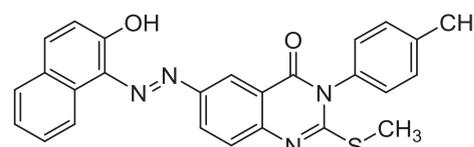
### Substituted 1,3-dioxoisindoline-4-aminoquinolines coupled via amide linkers: Synthesis, antiparasmodial and cytotoxic evaluation

Bioorganic Chemistry 88 (2019) 102912

Anu Rani<sup>a</sup>, Jenny Legac<sup>b</sup>, Philip J. Rosenthal<sup>b</sup>, Vipin Kumar<sup>a,\*</sup><sup>a</sup>Department of Chemistry, Guru Nanak Dev University, Amritsar 143005, Punjab, India<sup>b</sup>Department of Medicine, University of California, San Francisco, CA, USA

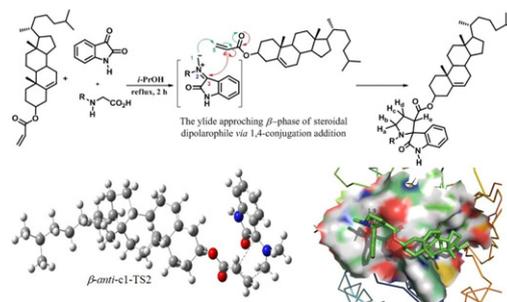
### Synthesis, antitumor testing and molecular modeling study of some new 6-substituted amido, azo or thioureido-quinazolin-4(3H)-ones

Bioorganic Chemistry 88 (2019) 102923

Mohamed A. Sabry<sup>a,\*</sup>, Heba A. Ewida<sup>b</sup>, Ghada S. Hassan<sup>a</sup>, Mariam A. Ghaly<sup>a</sup>, Hussein I. El-Subbagh<sup>a,\*</sup><sup>a</sup>Department of Medicinal Chemistry, Faculty of Pharmacy, Mansoura University, P.O. Box 35516, Mansoura, Egypt<sup>b</sup>Department of Pharmacology and Biochemistry, Faculty of Pharmaceutical Sciences & Pharmaceutical Industries, Future University in Egypt, 12311 Cairo, Egypt21: Average IC<sub>50</sub> 6.7 μM53: Average IC<sub>50</sub> 7.6 μM

### Glucosamine-6-phosphate synthase inhibiting C3-β-cholesterol tethered spiro heterocyclic conjugates: Synthesis and their insight of DFT and docking study

Bioorganic Chemistry 88 (2019) 102920

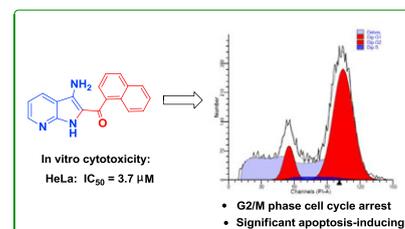
Govindasami Periyasami<sup>a,b,\*</sup>, Subban Kamalraj<sup>c,f</sup>, Ramanathan Padmanaban<sup>d</sup>, Santhakumar Yeswanth Kumar<sup>d</sup>, Antony Stalin<sup>e,f</sup>, Natarajan Arumugam<sup>a</sup>, Raju Suresh Kumar<sup>a</sup>, Mostafizur Rahaman<sup>a</sup>, Periyar Durairaju<sup>g</sup>, Abdulaziz Alrehaili<sup>a</sup>, Ali Aldalbahi<sup>a,\*</sup><sup>a</sup>Department of Chemistry, College of Science, King Saud University, Riyadh, Saudi Arabia<sup>b</sup>Department of Organic Chemistry, University of Madras, Guindy Campus, Chennai, India<sup>c</sup>Department of Biochemistry, Indian Institute of Science, Bangalore, Karnataka, India<sup>d</sup>Department of Chemistry, School of Physical, Chemical & Applied Sciences, Pondicherry University, Puducherry, India<sup>e</sup>Division of Bioinformatics, Entomology Research Institute, Loyola College, Chennai 600 034, Tamil Nadu, India<sup>f</sup>Centre for Advanced Studies in Botany & Centre for Herbal Sciences, University of Madras, Guindy Campus, Chennai 600 025, Tamil Nadu, India<sup>g</sup>Department of Chemistry, Thiruvallur Government Arts College, Periyar University, Raisenpura, India

### Facile one-pot synthesis, antiproliferative evaluation and structure-activity relationships of 3-amino-1H-indoles and 3-amino-1H-7-azaindoles

Bioorganic Chemistry 88 (2019) 102914

Peng-Cheng Diao, Meng-Jin Hu, Hai-Kui Yang, Wen-Wei You, Pei-Liang Zhao<sup>\*</sup>

Guangdong Provincial Key Laboratory of New Drug Screening, School of Pharmaceutical Science, Southern Medical University, Guangzhou 510515, PR China



### Potent and selective EGFR inhibitors based on 5-aryl-7H-pyrrolopyrimidin-4-amines

Bioorganic Chemistry 88 (2019) 102918

Ann Christin Reiersølmoen<sup>a</sup>,  
Thomas Ihle Aarhus<sup>a,b</sup>, Sarah Eckelt<sup>a,c</sup>,  
Kristin Gabestad Nørsett<sup>d,e</sup>, Eirik Sundby<sup>b</sup>,  
Bård Helge Hoff<sup>a,\*</sup>

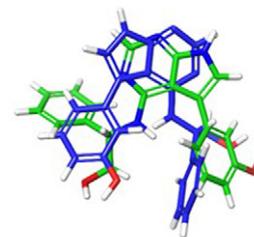
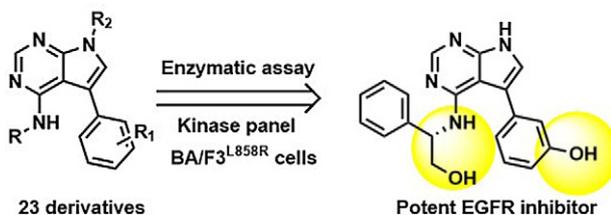
<sup>a</sup>Department of Chemistry, Norwegian University of Science and Technology (NTNU), NO-7491 Trondheim, Norway

<sup>b</sup>Department of Material Science, Norwegian University of Science and Technology (NTNU), NO-7491 Trondheim, Norway

<sup>c</sup>Institute of Organic Chemistry, Universität Hamburg, Welckerstrasse 8, 201354 Hamburg, Germany

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<sup>e</sup>Department of Computer Science, Norwegian University of Science and Technology (NTNU), NO-7491 Trondheim, Norway



### 6-Methoxyflavonols from the aerial parts of *Tetragonia tetragonoides* (Pall.) Kuntze and their anti-inflammatory activity

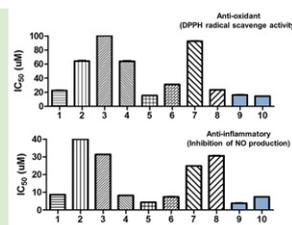
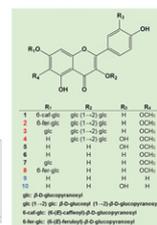
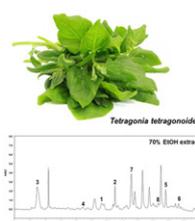
Bioorganic Chemistry 88 (2019) 102922

Yeong-Geun Lee<sup>a</sup>, Hwan Lee<sup>b</sup>, Jin Ah Ryuk<sup>c</sup>, Joo Tae Hwang<sup>c</sup>,  
Hyoung-Geun Kim<sup>a</sup>, Dong-Sung Lee<sup>b</sup>, Yeon-Ju Kim<sup>a</sup>, Deok-Chun Yang<sup>a</sup>,  
Byoung Seob Ko<sup>c,\*</sup>, Nam-In Baek<sup>a,\*</sup>

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<sup>b</sup>College of Pharmacy, Chosun University, Gwangju 61452, Republic of Korea

<sup>c</sup>Korea Institute of Oriental Medicine, Daejeon 34054, Republic of Korea



### Hydrazones as novel epigenetic modulators: Correlation between TET 1 protein inhibition activity and their iron(II) binding ability

Bioorganic Chemistry 88 (2019) 102809

Milan Jakubek<sup>a,b,c</sup>, Zdeněk Kejřík<sup>c</sup>, Robert Kapláneš<sup>a,b</sup>, Veronika Antonyovš<sup>a,b,c</sup>, Róbert Hromádka<sup>c,d</sup>,  
Viera Šandrikovš<sup>d</sup>, David Šykora<sup>b</sup>, Pavel Martásek<sup>c,e</sup>, Vladimír Král<sup>a,b,c,\*</sup>

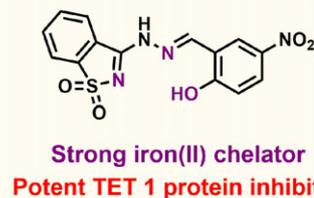
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<sup>d</sup>Research and Development Center C2P s.r.o., Jungmannovš 101, 503 51 Chlumec nad Cidlinovš, Czech Republic

<sup>e</sup>General University Hospital in Prague, U nemocnice 2, 121 08 Prague 2, Czech Republic



### Synthesis of some new C2 substituted dihydropyrimidines and their electrophysiological evaluation as L-/T-type calcium channel blockers

Mohamed Teleb<sup>a,b</sup>, Ola H. Rizk<sup>b,c</sup>,  
Fang-Xiong Zhang<sup>d</sup>, Frank R. Fronczek<sup>e</sup>,  
Gerald W. Zamponi<sup>d</sup>, Hesham Fahmy<sup>a,\*</sup>

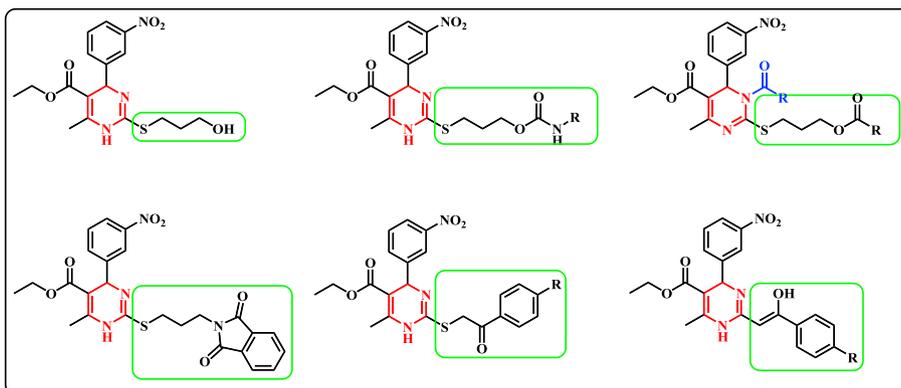
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<sup>c</sup>Department of Pharmaceutical Chemistry, Faculty of Pharmacy and Drug Manufacturing, Pharos University in Alexandria, Alexandria 21311, Egypt

<sup>d</sup>Department of Physiology & Pharmacology, Hotchkiss Brain Institute, University of Calgary, 3330 Hospital Drive NW, Calgary T2N 4N1, Canada

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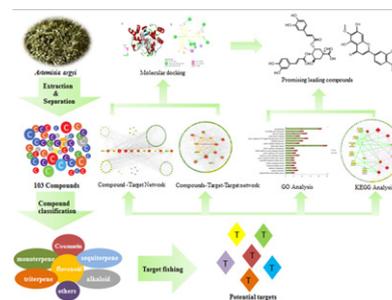
Bioorganic Chemistry 88 (2019) 102915

### Virtual screening of active compounds from *Artemisia argyi* and potential targets against gastric ulcer based on Network pharmacology

Yue Wang<sup>a,b</sup>, Yi-wei Sun<sup>a</sup>, Yu-meng Wang<sup>a</sup>, Yan Ju<sup>a</sup>, Da-li Meng<sup>a,b,\*</sup>

<sup>a</sup>School of Traditional Chinese Materia Medica, Shenyang Pharmaceutical University, Shenyang 110016, PR China

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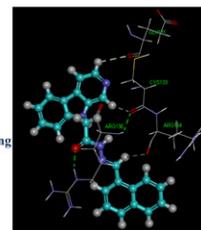
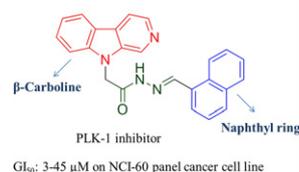
### *In-silico* design and synthesis of N9-substituted $\beta$ -Carbolines as PLK-1 inhibitors and their *in-vitro/in-vivo* tumor suppressing evaluation

Gomathi Priya Jeyapal<sup>a</sup>, Rajendiran Krishnasamy<sup>b</sup>, Carolyn K. Suzuki<sup>c</sup>, Sundararajan Venkatesh<sup>c</sup>, M.J.N. Chandrasekar<sup>a,\*</sup>

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<sup>c</sup>Department of Microbiology, Biochemistry & Molecular Genetics, New Jersey Medical School-Rutgers, The State University of New Jersey, Newark, NJ, USA



Bioorganic Chemistry 88 (2019) 102913

### Novel eugenol bearing oxypropanolamines: Synthesis, characterization, antibacterial, antidiabetic, and anticholinergic potentials

Hayriye Genç Bilgiçli<sup>a,\*</sup>, Ali Kestane<sup>a</sup>, Parham Taslimi<sup>b</sup>, Oguz Karabay<sup>c</sup>, Arlinda Bytyqi-Damoni<sup>d</sup>, Mustafa Zengin<sup>a</sup>, İlhami Gulçin<sup>e</sup>

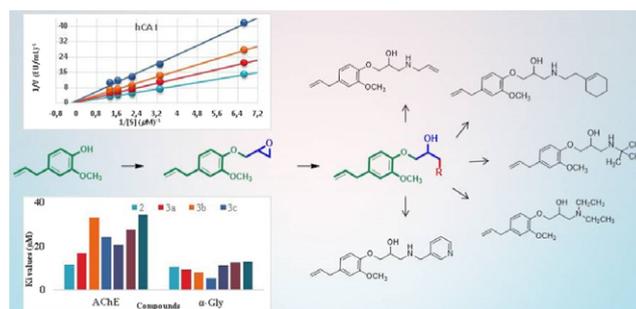
<sup>a</sup>Sakarya University, Science and Arts Faculty Chemistry Department, 54187-Serdivan Sakarya, Turkey

<sup>b</sup>Department of Biotechnology, Faculty of Science, Bartın University, 74100 Bartın, Turkey

<sup>c</sup>Sakarya University, Faculty of Medicine Infectious Diseases and Clinical Microbiology Department, 54290-Adapazarı Sakarya, Turkey

<sup>d</sup>University of Pristina, Faculty of Education, Department of Chemistry, Pristina, Kosovo

<sup>e</sup>Department of Chemistry, Faculty of Science, Atatürk University, 25240-Erzurum, Turkey



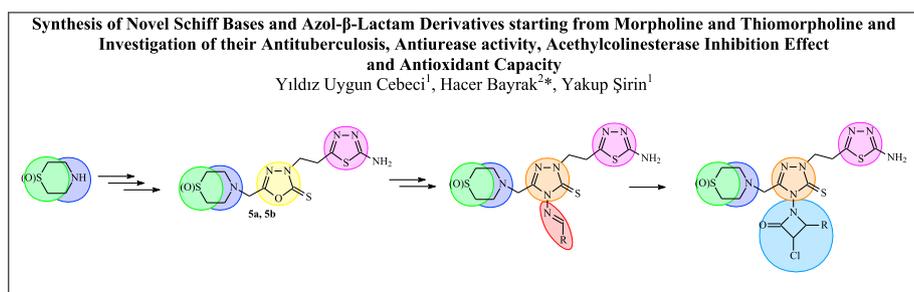
Bioorganic Chemistry 88 (2019) 102931

### Synthesis of novel Schiff bases and azol-β-lactam derivatives starting from morpholine and thiomorpholine and investigation of their antitubercular, antiurease activity, acetylcholinesterase inhibition effect and antioxidant capacity

Yıldız Uygun Cebeci<sup>a</sup>, Hacer Bayrak<sup>b,\*</sup>, Yakup Şirin<sup>a</sup>

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<sup>b</sup>Department of Chemistry and Chemical Processing Technology, Karadeniz Technical University, 61080 Trabzon, Turkey



Bioorganic Chemistry 88 (2019) 102928

### Synthesis and *in vitro* antitumor activity of novel acylspermidine derivative N-(4-aminobutyl)-N-(3-aminopropyl)-8-hydroxy-dodecanamide (AAHD) against HepG2 cells

Abdulrahman L. Al-Malki<sup>a,b,c</sup>, Syed Shoeb Razvi<sup>a</sup>, Furkhan Ahmed Mohammed<sup>d</sup>, Mazin A. Zamzami<sup>a,e,f</sup>, Hani Choudhry<sup>a,b,e,f</sup>, Taha A. Kumosani<sup>a,b,g</sup>, Khadijah S. Balamash<sup>a</sup>, Fawzia A. Alshubaily<sup>a</sup>, Shareefa A. ALGhamdi<sup>a</sup>, Khalid O. Abualnaja<sup>a,b,c</sup>, Wesam H. Abdulaal<sup>a,b,e,f</sup>, Mustafa A. Zeyadi<sup>a</sup>, Maryam H. Al-Zahrani<sup>a</sup>, Mahmoud Alhosin<sup>a,e,f</sup>, Tadao Asami<sup>a,b,h,\*</sup>, Said S. Moselhy<sup>a,b,c,i,\*</sup>

<sup>a</sup>Department of Biochemistry, Faculty of Science, King Abdulaziz University, Jeddah, Saudi Arabia

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<sup>d</sup>Department of Biology, Faculty of Science, King Abdulaziz University, Jeddah, Saudi Arabia

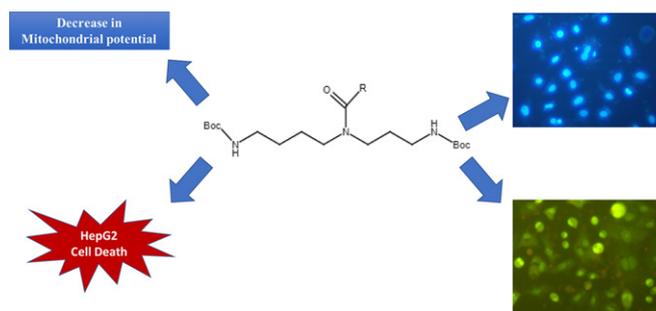
<sup>e</sup>Cancer Metabolism and Epigenetic Unit, Faculty of Science, King Abdulaziz University, Jeddah, Saudi Arabia

<sup>f</sup>Cancer and Mutagenesis Unit, King Fahd Medical Research Center, King Abdulaziz University, Jeddah, Saudi Arabia

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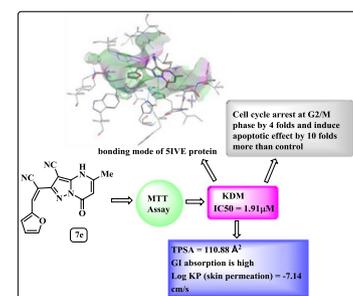
Bioorganic Chemistry 88 (2019) 102937

### Design, synthesis, anticancer evaluation, molecular docking and cell cycle analysis of 3-methyl-4,7-dihydropyrazolo [1,5-*a*] pyrimidine derivatives as potent histone lysine demethylases (KDM) inhibitors and apoptosis inducers

Nadia Hanafy Metwally<sup>a</sup>, Mona Said Mohamed, Eman Ali Ragb

Department of Chemistry, Faculty of Science, Cairo University, Giza, Egypt

Bioorganic Chemistry 88 (2019) 102929



### Synthesis and molecular docking study of some 3,4-dihydrothieno [2,3-*d*] pyrimidine derivatives as potential antimicrobials

Omaima G. Shaaban<sup>a,b,\*</sup>, Doaa A.E. Issa<sup>c</sup>, Alaa A. El-Tombary<sup>a</sup>, Shrouk M. Abd El Wahab<sup>d</sup>, Abeer E. Abdel Wahab<sup>e</sup>, Ibrahim A. Abdelwahab<sup>f</sup>

<sup>a</sup>Department of Pharmaceutical Chemistry, Faculty of Pharmacy, University of Alexandria, Alexandria 21521, Egypt

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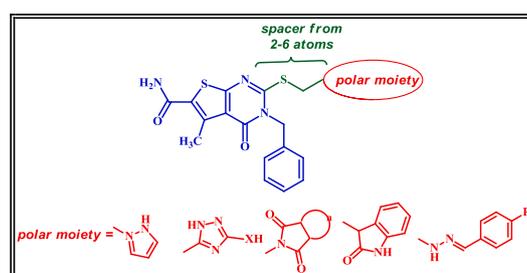
<sup>c</sup>Department of Pharmaceutical Sciences, Faculty of Pharmacy, Beirut Arab University, Beirut, Lebanon

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Bioorganic Chemistry 88 (2019) 102934



New target 2- substituted thieno[2,3-*d*]pyrimidine-6-carboxamides as antimicrobials

### Isolation, identification, and quantification of Pentylcurcumene from *Geophila repens*: A new class of cholinesterase inhibitor for Alzheimer's disease

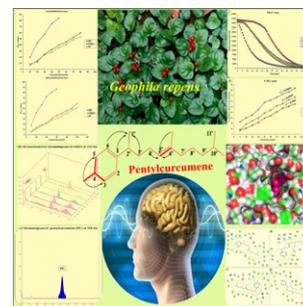
Umesh Chandra Dash<sup>a</sup>, Satish Kanhar<sup>a</sup>, Anshuman Dixit<sup>b</sup>, Jagnehswar Dandapat<sup>c</sup>, Atish Kumar Sahoo<sup>a,\*</sup>

<sup>a</sup>Medicinal & Aromatic Plant Division, Regional Plant Resource Centre, Forest & Environment Department, Govt. of Odisha, Nayapalli, Bhubaneswar 751015, India

<sup>b</sup>Institute of Life Sciences (ILS), NALCO Square, Bhubaneswar-751023, Odisha, India

<sup>c</sup>Department of Biotechnology, Utkal University, Vani Vihar, Bhubaneswar 751004, India

Bioorganic Chemistry 88 (2019) 102947



### Phenanthroimidazole derivatives act as potent inducer of autophagy by activating DNA damage pathway

Hao Zhang<sup>a,1</sup>, Yue Song<sup>a,1</sup>, Li Li<sup>b,c</sup>, Shuang-Yan Zhang<sup>b,c</sup>, Qiong Wu<sup>b,c,\*</sup>, Wen-Jie Mei<sup>b,c,d,\*</sup>, Hui-Min Liu<sup>a</sup>, Xi-Cheng Wang<sup>a,\*</sup>

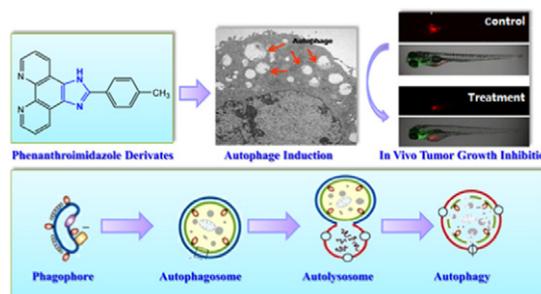
<sup>a</sup>The First Affiliated Hospital of Guangdong Pharmaceutical University, Guangzhou 510006, PR China

<sup>b</sup>School of Pharmacy, Guangdong Pharmaceutical University, Guangzhou 510006, PR China

<sup>c</sup>Guangdong Province Engineering Technology Centre for Molecular Probe and Biomedicine Imaging, Guangzhou 510006, PR China

<sup>d</sup>Guangzhou Key Laboratory of Construction and Application of New Drug Screening Model Systems, Guangdong Pharmaceutical University, Guangzhou 510006, China

Bioorganic Chemistry 88 (2019) 102940



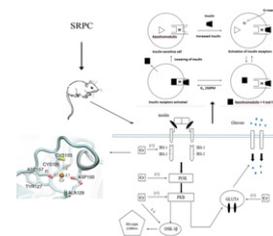
### Hypoglycemic activity and mechanism of the sulfated rhamnose polysaccharides chromium (III) complex in type 2 diabetic mice

Bioorganic Chemistry 88 (2019) 102942

Han Ye<sup>a</sup>, Zhaopeng Shen<sup>b</sup>, Jiefen Cui<sup>a</sup>, Yujie Zhu<sup>a</sup>, Yuanyuan Li<sup>a</sup>, Yongzhou Chi<sup>a</sup>, Jingfeng Wang<sup>a</sup>, Peng Wang<sup>a,\*</sup>

<sup>a</sup>College of Food Science and Engineering, Ocean University of China, Qingdao 266003, PR China

<sup>b</sup>College of Medicine and Pharmacy, Ocean University of China, Qingdao 266003, PR China

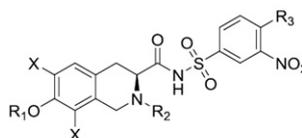


### Discovery and development of 1,2,3,4-tetrahydroisoquinoline-3-carboxylic acid derivatives as Bcl-2/Mcl-1 inhibitors

Bioorganic Chemistry 88 (2019) 102938

Renshuai Liu, Lulu Liu, Xinying Yang, Hao Fang<sup>\*</sup>

Department of Medicinal Chemistry, Key Laboratory of Chemical Biology (Ministry of Education), School of Pharmacy, Shandong University, Ji'nan, Shandong 250012, PR China



11t R<sub>1</sub>=4-Ph-Bn- X=Br  
R<sub>2</sub>=4-CN-Bn- R<sub>3</sub>=Cl

K <sub>i</sub> /μM			IC <sub>50</sub> /μM				
Bcl-2	Bcl-X <sub>L</sub>	Mcl-1	Jurkat	RS4;11	KG1	Molt-4	HL-60
0.45±0.02	N.A.	0.35±0.06	15.50±1.50	12.81±0.72	17.68±1.52	13.96±4.00	21.97±1.96

### Synthesis and systemic toxicity assessment of quinine-triazole scaffold with antiprotozoal potency

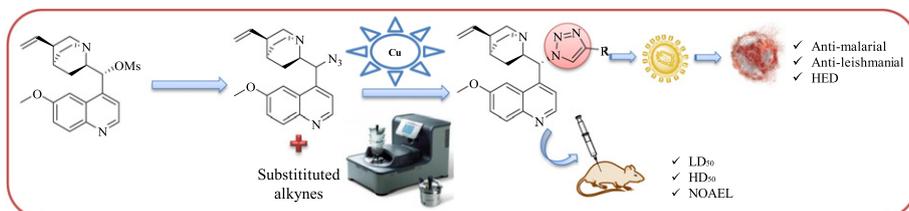
Bioorganic Chemistry 88 (2019) 102939

Adarsh Sahu<sup>a,\*</sup>, Ram Kishore Agrawal<sup>a</sup>, RajKishor Pandey<sup>b</sup>

<sup>a</sup>Department of Pharmaceutical Sciences, Dr.

Harisingh Gour Vishwavidyalaya, Sagar, MP, India

<sup>b</sup>National Institute of Pharmaceutical Education and Research, Hajipur, India



### Design, synthesis and photoinduced DNA cleavage studies of [1,2,4]-triazolo[4,3-a]quinoxalin-4(5H)-ones

Bioorganic Chemistry 88 (2019) 102932

Garima Sumran<sup>a,\*</sup>, Ranjana Aggarwal<sup>b</sup>, Ashwani Mittal<sup>c</sup>, Aviral Aggarwal<sup>d</sup>, Amit Gupta<sup>e</sup>

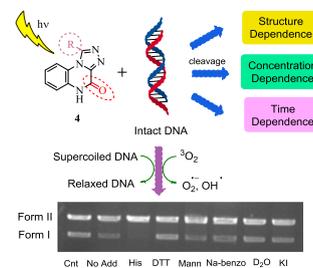
<sup>a</sup>Department of Chemistry, D. A. V. College (Lahore), Ambala City 134 002, Haryana, India

<sup>b</sup>Department of Chemistry, Kurukshetra University, Kurukshetra 136 119, India

<sup>c</sup>Biochemistry Department, University College, Kurukshetra University, Kurukshetra 136 119, India

<sup>d</sup>Birla Institute of Technology and Science, Pilani-K. K. Birla Goa Campus, Goa 403 726, India

<sup>e</sup>Department of Chemistry, Dronacharya Government College, Gurgaon 122 001, India



### $\alpha$ -bisabolol $\beta$ -D-fucopyranoside as a potential modulator of $\beta$ -amyloid peptide induced neurotoxicity: An *in vitro* & *in silico* study

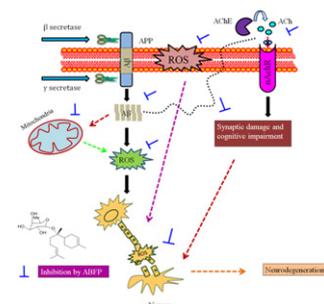
Bioorganic Chemistry 88 (2019) 102935

Mahalingam Jeyakumar<sup>a</sup>, Sethuraman Sathya<sup>a</sup>, Soniya Gandhi<sup>b</sup>, Prabhakararao Tharra<sup>b</sup>, Venkatesan Suryanarayanan<sup>c</sup>, Sanjeev Kumar Singh<sup>c</sup>, Beeraiah Baire<sup>b</sup>, Kasi Pandima Devi<sup>a,\*</sup>

<sup>a</sup>Department of Biotechnology, Alagappa University, Karaikudi 630003, Tamil Nadu, India

<sup>b</sup>Department of Chemistry, Indian Institute of Technology Madras, Chennai 600036, Tamil Nadu, India

<sup>c</sup>Computer Aided Drug Design and Molecular Modeling Lab, Department of Bioinformatics, Alagappa University, Karaikudi 630003, Tamil Nadu, India



### Design, synthesis and molecular docking of new *N*-4-piperazinyl ciprofloxacin-triazole hybrids with potential antimicrobial activity

Bioorganic Chemistry 88 (2019) 102952

Hamada H.H. Mohammed<sup>a,b</sup>, El-Shimaa M.N. Abdelhafez<sup>a</sup>, Samar H. Abbas<sup>a</sup>, Gamal A.I. Moustafa<sup>a</sup>, Glenn Hauk<sup>c</sup>, James M. Berger<sup>c</sup>, Satoshi Mitarai<sup>d</sup>, Masayoshi Arai<sup>e</sup>, Rehab M. Abd El-Baky<sup>f</sup>, Gamal El-Din A. Abu-Rahma<sup>a,\*</sup>

<sup>a</sup>Department of Medicinal Chemistry, Faculty of Pharmacy, Minia University, Minia 61519, Egypt

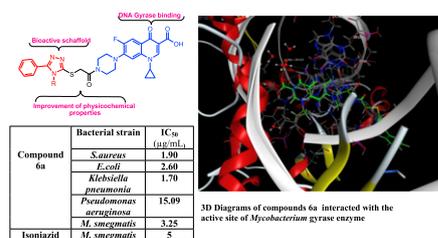
<sup>b</sup>Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Deraya University, New-Minia 61519, Egypt

<sup>c</sup>Department of Biophysics and Biophysical Chemistry, Johns Hopkins University School of Medicine, Baltimore, MD, USA

<sup>d</sup>Bacteriology Division, Department of Mycobacterium Reference and Research, Research Institute of Tuberculosis, Japan Anti-Tuberculosis Association, Kiyose 204-8533, Japan

<sup>e</sup>Graduate School of Pharmaceutical Sciences, Osaka University, 1-6 Yamadaoka, Suita, Osaka 565-0871, Japan

<sup>f</sup>Department of Microbiology & Immunology, Faculty of Pharmacy, Minia University, Minia 61519, Egypt



### Fluoro-benzimidazole derivatives to cure Alzheimer's disease: *In-silico* studies, synthesis, structure-activity relationship and *in vivo* evaluation for $\beta$ secretase enzyme inhibition

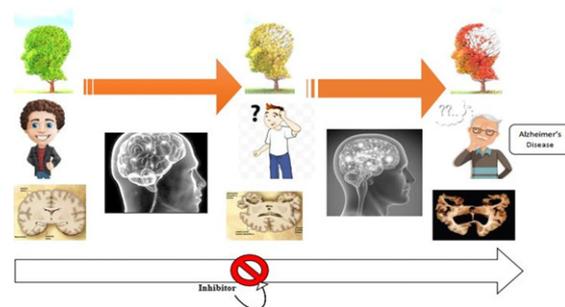
Bioorganic Chemistry 88 (2019) 102936

Sayyad Ali<sup>a,b</sup>, Muhammad Hassham Hassan Bin Asad<sup>a,c,\*</sup>, Soham Maity<sup>b</sup>, Wahid Zada<sup>a</sup>, Albert A. Rizvanov<sup>c</sup>, Jamshed Iqbal<sup>a</sup>, Borhan Babak<sup>b</sup>, Izhar Hussain<sup>a,\*</sup>

<sup>a</sup>Department of Pharmacy, COMSATS University Islamabad, Abbottabad Campus, 22060, Pakistan

<sup>b</sup>Department of Chemistry, Michigan State University, East Lansing, MI 48824, USA

<sup>c</sup>Department of Genetics, Institute of Fundamental Medicine and Biology, Kazan Federal University, 420021, Russia



### Synthesis and biological evaluation of 3-functionalized 2-phenyl- and 2-alkylbenzo [b] furans as antiproliferative agents against human melanoma cell line

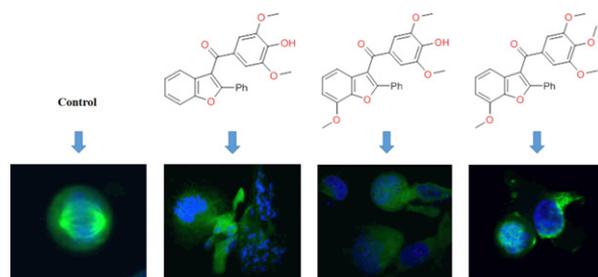
Bioorganic Chemistry 88 (2019) 102930

Halina Kwiecień<sup>a,\*</sup>, Magdalena Perużyńska<sup>b</sup>, Karolina Stachowicz<sup>a</sup>, Katarzyna Piotrowska<sup>c</sup>, Joanna Bujak<sup>c</sup>, Patrycja Kopytko<sup>c</sup>, Marek Drożdżik<sup>b</sup>

<sup>a</sup>West Pomeranian University of Technology in Szczecin, Department of Organic Synthesis and Drug Technology, Al. Piastów 42, 71-065 Szczecin, Poland

<sup>b</sup>Pomeranian Medical University, Department of Experimental & Clinical Pharmacology, Powstańców Wlkp. 72, 70-111 Szczecin, Poland

<sup>c</sup>Pomeranian Medical University, Department of Physiology, Powstańców Wlkp. 72, 70-111 Szczecin, Poland



Microtubule and chromosome organization in A375 cells

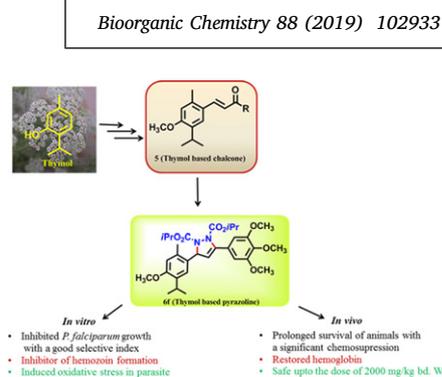
### Synthesis of thymol-based pyrazolines: An effort to perceive novel potent-antimalarials

Dushyant Singh Raghuvanshi<sup>a,\*</sup>, Narsingh Verma<sup>a,c</sup>, Shiv Vardan Singh<sup>b</sup>, Sonam Khare<sup>b</sup>, Anirban Pal<sup>b,c,\*</sup>, Arvind Singh Negi<sup>a,c</sup>

<sup>a</sup>Department of Medicinal Chemistry, CSIR-Central Institute of Medicinal and Aromatic Plants, P.O. CIMAP, Kukrail Road, Lucknow 226015, India

<sup>b</sup>Molecular Bioprospection Department, CSIR-Central Institute of Medicinal and Aromatic Plants, P.O. CIMAP, Kukrail Road, Lucknow 226015, India

<sup>c</sup>Academy of Scientific and Innovative Research (AcSIR), Ghaziabad 221002, India

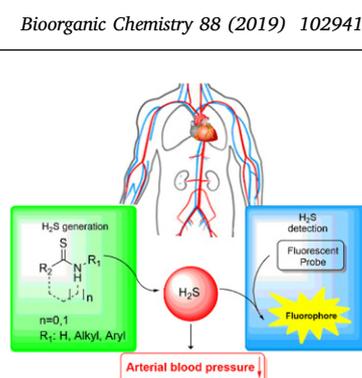


### Evaluation of thioamides, thiolactams and thioureas as hydrogen sulfide (H<sub>2</sub>S) donors for lowering blood pressure

Ewelina Zaorska<sup>a</sup>, Tomasz Hutsch<sup>a</sup>, Marta Gawryś-Kopczyńska<sup>a</sup>, Ryszard Ostaszewski<sup>b</sup>, Marcin Ufnal<sup>a,\*</sup>, Dominik Koszelewski<sup>b,\*</sup>

<sup>a</sup>Department of Experimental Physiology and Pathophysiology, Laboratory of Centre for Preclinical Research, Medical University of Warsaw, Pawińskiego 3c, 02-106 Warsaw, Poland

<sup>b</sup>Institute of Organic Chemistry, Polish Academy of Sciences Kasprzaka 44/52, 01-224 Warsaw, Poland



### Design, synthesis and anticancer evaluation of thieno[2,3-d]pyrimidine derivatives as dual EGFR/HER2 inhibitors and apoptosis inducers

Souad A. Elmetwally<sup>a</sup>, Khaled F. Saied<sup>b,\*</sup>, Ibrahim H. Eissa<sup>c</sup>, Eslam B. Elkaeed<sup>d,\*</sup>

<sup>a</sup>Department of Basic Science, Higher Technological Institute, 10<sup>th</sup> of Ramadan City 228, Egypt

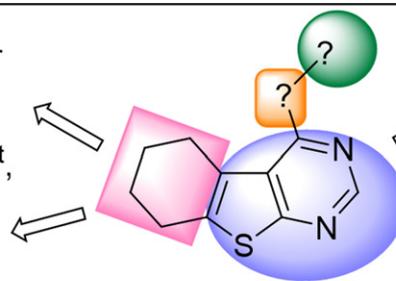
<sup>b</sup>Department of Basic Science, Oral and Dental Medicine, Nahda University, East Beni-Suef, 62511 Beni-Suef, Egypt

<sup>c</sup>Department of Pharmaceutical Chemistry, Faculty of Pharmacy (Boys), Al-Azhar University, Nasr City, 11884 Cairo, Egypt

<sup>d</sup>Department of Pharmaceutical Organic Chemistry, Faculty of Pharmacy (Boys), Al-Azhar University, Nasr City, 11884 Cairo, Egypt

Tested against four cancer cell lines.

*In vitro* anti EGFR<sup>wt</sup>, EGFR<sup>T790M</sup> and HER2 activity



Cell cycle analysis & apoptosis

Molecular docking against EGFR<sup>wt</sup> and EGFR<sup>T790M</sup>

Bioorganic Chemistry 88 (2019) 102944

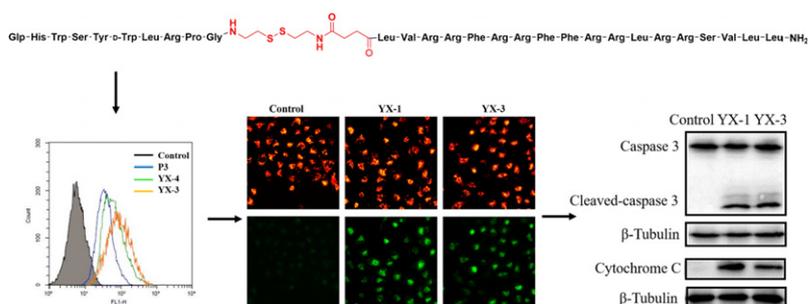
### Synthesis and evaluation of redox-sensitive gonadotropin-releasing hormone receptor-targeting peptide conjugates

*Bioorganic Chemistry 88 (2019) 102945*

Yuxuan Dai<sup>a</sup>, Na Yue<sup>a</sup>, Chunxia Liu<sup>a</sup>, Xingguang Cai<sup>a</sup>,  
Xin Su<sup>a</sup>, Xinzhou Bi<sup>a</sup>, Qifei Li<sup>a</sup>, Chengye Li<sup>a</sup>,  
Wenlong Huang<sup>a,b</sup>, Hai Qian<sup>a,b,\*</sup>

<sup>a</sup>Center of Drug Discovery, State Key Laboratory of Natural Medicines, China Pharmaceutical University, 24 Tongjiaxiang, Nanjing 210009, PR China

<sup>b</sup>Jiangsu Key Laboratory of Drug Discovery for Metabolic Disease, China Pharmaceutical University, 24 Tongjiaxiang, Nanjing 210009, PR China



### Synthesis, antimicrobial, antioxidant, cytotoxic, antiurease and molecular docking studies of *N*-(3-trifluoromethyl)benzoyl-*N'*-aryl thiourea derivatives

*Bioorganic Chemistry 88 (2019) 102946*

Aneela Maalik<sup>a,\*</sup>, Hina Rahim<sup>b</sup>,  
Muhammad Saleem<sup>c</sup>, Nighat Fatima<sup>d</sup>,  
Abdur Rauf<sup>e</sup>, Abdul Wadood<sup>e</sup>,  
Muhammad Imran Malik<sup>f</sup>, Ayaz Ahmed<sup>g</sup>,  
Hummera Rafique<sup>b</sup>,  
Muhammad Naveed Zafar<sup>j</sup>, Muhammad Riaz<sup>e</sup>,  
Lubna Rasheed<sup>i</sup>, Amara Mumtaz<sup>b,\*</sup>

<sup>a</sup>Department of Chemistry, COMSATS University Islamabad, Islamabad Campus, Park Road, Chak Shahzad, 45550 Islamabad, Pakistan

<sup>b</sup>Department of Chemistry, COMSATS University, Abbottabad Campus, 22060 Abbottabad, Pakistan

<sup>c</sup>Department of Chemistry, University of Education, Lahore, Dera Ghazi Khan Campus, 32200 Punjab, Pakistan

<sup>d</sup>Department of Pharmacy, COMSATS University, Abbottabad Campus, 22060 Abbottabad, Pakistan

<sup>e</sup>Department of Chemistry, University of Swabi, 23561 Ambar, Khyber Pakhtunkhwa, Pakistan

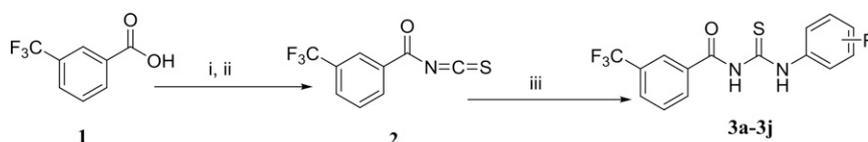
<sup>f</sup>HEJ Research Institute of Chemistry, International Centre for Chemical and Biological Sciences, University of Karachi, 75270 Karachi, Pakistan

<sup>g</sup>Panjwani Center for Molecular Medicine and Drug Research, International Center for Chemical and Biological Sciences, University of Karachi, Pakistan

<sup>h</sup>Department of Chemistry, University of Gujrat, 50700 Gujrat, Pakistan

<sup>i</sup>Department of Chemistry, Quaid-i-Azam University, Islamabad, Pakistan

<sup>j</sup>Department of Chemistry, University of Education, Township Campus, Lahore, Pakistan



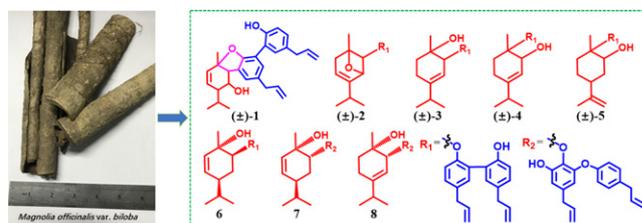
- |                           |                            |
|---------------------------|----------------------------|
| <b>3a.</b> R=2,6-Dichloro | <b>3f.</b> R=4-Cyano       |
| <b>3b.</b> R=3-Chloro     | <b>3g.</b> R=H             |
| <b>3c.</b> R=2,5-Dichloro | <b>3h.</b> R=2,4-Dinitro   |
| <b>3d.</b> R=4-Nitro      | <b>3i.</b> R=3,4-Dimethoxy |
| <b>3e.</b> R=2-Fluoro     | <b>3j.</b> R=3-Bromo       |

### Magmenthanes A-H: Eight new meroterpenoids from the bark of *Magnolia officinalis* var. *Biloba*

*Bioorganic Chemistry 88 (2019) 102948*

Chuan Li, Chuang-Jun Li, Jie Ma, Ji-Wu Huang, Xu-Yan Wang,  
Xiao-Liang Wang, Fei Ye, Dong-Ming Zhang<sup>\*</sup>

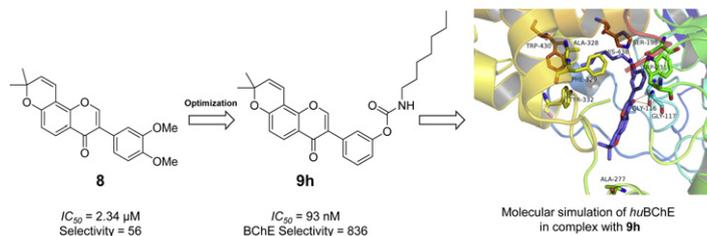
State Key Laboratory of Bioactive Substance and Function of Natural Medicines, Institute of Materia Medica, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing 100050, People's Republic of China



### Highly selective carbamate-based butyrylcholinesterase inhibitors derived from a naturally occurring pyranoisoflavone

Chuanhai Wu, Yan-bei Tu, Ziyuan Li\*, Yan-fang Li\*

School of Chemical Engineering, Sichuan University, Chengdu 610065, China



### Design and synthesis of the novel oleanolic acid-cinnamic acid ester derivatives and glycyrrhetic acid-cinnamic acid ester derivatives with cytotoxic properties

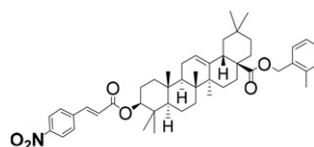
Rui Wang<sup>a,b,1</sup>, Wei Yang<sup>a,1</sup>, Yiqing Fan<sup>a</sup>, Wim Dehaen<sup>b</sup>, Yang Li<sup>c</sup>, Huijing Li<sup>d</sup>, Wei Wang<sup>a</sup>, Qingxuan Zheng<sup>a</sup>, Qiyong Huai<sup>a,\*</sup>

<sup>a</sup>Marine College, Shandong University, Weihai 264209, China

<sup>b</sup>Molecular Design and Synthesis, Department of Chemistry, KU Leuven, Celestijnenlaan 200F, B-3001 Heverlee, Belgium

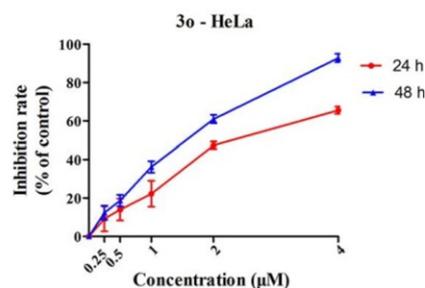
<sup>c</sup>Zhong Yuan Academy of Biological Medicine, Liaocheng People's Hospital/Affiliated Liaocheng Hospital, Taishan Medical University, Liaocheng, China

<sup>d</sup>School of Marine Science and Technology, Harbin Institute of Technology at Weihai, Weihai 264209, China



HeLa cells ( $IC_{50} = 1.35 \mu\text{M}$ )

L-O2 cells ( $IC_{50} > 100 \mu\text{M}$ )



### Discovery of Baicalin as NDM-1 inhibitor: Virtual screening, biological evaluation and molecular simulation

Cheng Shi, Jingxiao Bao, Ying Sun, Xinyue Kang, Xingzhen Lao\*, Heng Zheng\*

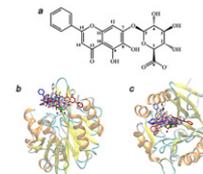
School of Life Science and Technology, China Pharmaceutical University, Nanjing 210009, P.R. China

*Bioorganic Chemistry 88 (2019) 102953*

Discovery of Baicalin as NDM-1 inhibitor: Virtual screening, biological evaluation and molecular simulation

Cheng Shi (Shi C), Ying Sun (Sun Y), Jingxiao Bao (Bao JX), Xinyue Kang (Kang XY), Xingzhen Lao (Lao XZ)\*, Heng Zheng (Zheng H)\*

School of Life Science and Technology, China Pharmaceutical University, Nanjing 210009, P.R. China



In this study, structure-based virtual screening method led to the identification of Baicalin as a novel NDM-1 inhibitor. Inhibitory assays showed that Baicalin possessed a good inhibition of NDM-1 with  $IC_{50}$  values of  $3.89 \pm 1.1 \mu\text{M}$  and restored the susceptibility of *E. coli* BL21(DE3) pET28a-NDM-1 to clinically used  $\beta$ -lactam antibiotics. Molecular docking and molecular dynamics simulations obtained a complex structure between the relatively stable inhibitor molecule Baicalin and NDM-1 enzyme.

### Synthesis, characterization, anticancer evaluation and mechanisms of cytotoxic activity of novel 3-hydroxy-3-pyrrolin-2-ones bearing thenoyl fragment: DNA, BSA interactions and molecular docking study

Bioorganic Chemistry 88 (2019) 102954

Nenad Joksimović<sup>a</sup>, Jelena Petronijević<sup>a</sup>, Nenad Janković<sup>a</sup>, Dejan Baskić<sup>b</sup>, Suzana Popović<sup>b</sup>, Danijela Todorović<sup>c</sup>, Sanja Matic<sup>d</sup>, Goran A. Bogdanović<sup>e</sup>, Milan Vraneš<sup>f</sup>, Aleksandar Tot<sup>f</sup>, Zorica Bugarčić<sup>a,\*</sup>

<sup>a</sup>University of Kragujevac, Faculty of Science, Department of Chemistry, Radoja Domanovića 12, 34000 Kragujevac, Serbia

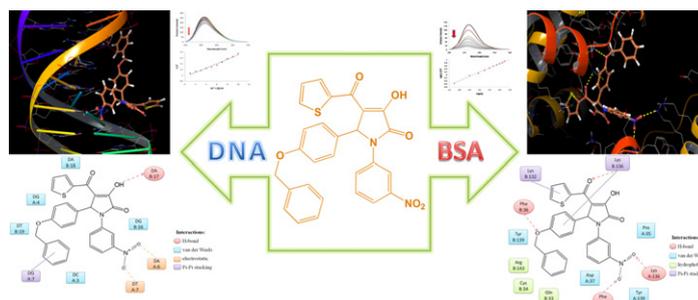
<sup>b</sup>University of Kragujevac, Faculty of Medical Sciences, Centre for Molecular Medicine and Stem Cell Research, Svetozara Markovića 69, 34000 Kragujevac, Serbia

<sup>c</sup>University of Kragujevac, Faculty of Medical Sciences, Department of Genetics, Svetozara Markovića 69, 34000 Kragujevac, Serbia

<sup>d</sup>Doctoral Academic Study, Faculty of Medical Sciences, University of Kragujevac, Svetozara Markovića 69, 34000 Kragujevac, Serbia

<sup>e</sup>Vinča Institute of Nuclear Science University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia

<sup>f</sup>University of Novi Sad, Department of Chemistry, Biochemistry and Environmental Protection, Trg Dositeja Obradovića 3, 21000 Novi Sad, Serbia



### Natural urease inhibitors from *Aloe vera* resin and *Lycium shawii* and their structural-activity relationship and molecular docking study

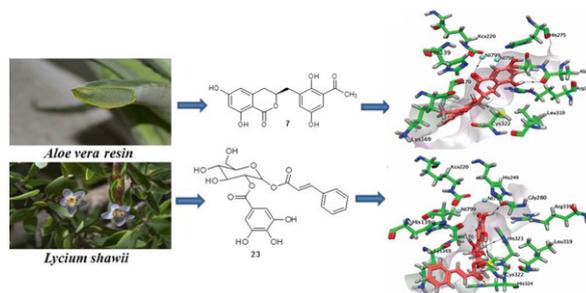
Bioorganic Chemistry 88 (2019) 102955

Najeeb Ur Rehman<sup>a</sup>, Ajmal Khan<sup>a</sup>, Ahmed Al-Harrasi<sup>a,\*</sup>, Mohammed Khiat<sup>a</sup>, Hidayat Hussain<sup>a,c</sup>, Abdul Wadood<sup>b</sup>, Muhammad Riaz<sup>b</sup>

<sup>a</sup>Natural and Medical Sciences Research Center, University of Nizwa, P.O. Box 33, Postal Code 616, Birkat Al Mauz, Nizwa, Oman

<sup>b</sup>Department of Biochemistry, Abdul Wali Khan University Mardan, Mardan 23200, Pakistan

<sup>c</sup>Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry, Halle, Germany

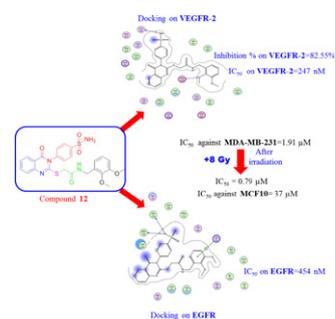


### Exploration of *N*-alkyl-2-[(4-oxo-3-(4-sulfamoylphenyl)-3,4-dihydroquinazolin-2-yl)thio]acetamide derivatives as anticancer and radiosensitizing agents

Bioorganic Chemistry 88 (2019) 102956

Aiten M. Soliman, Mostafa M. Ghorab<sup>\*</sup>

Department of Drug Radiation Research, National Center for Radiation Research and Technology (NCRRT), Egyptian Atomic Energy Authority (EAEA), Nasr City, P.O. Box 29, Cairo, Egypt

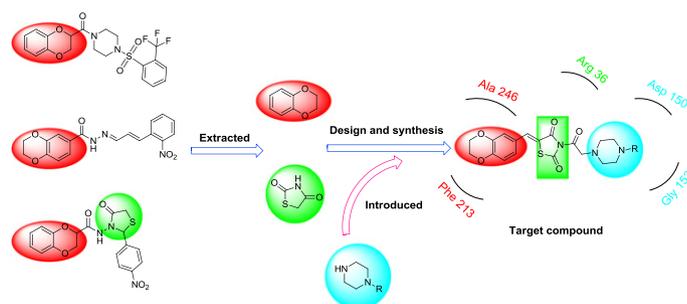


### Design, synthesis and molecular docking of 1,4-benzodioxane thiazolidinedione piperazine derivatives as FabH inhibitors

Juan Sun<sup>a</sup>, Wen He<sup>a</sup>, Han-Yu Liu<sup>b</sup>, Jie Qin<sup>b</sup>, Chun-Lin Ye<sup>a,\*</sup>

<sup>a</sup>School of Biological & Chemical Engineering, Zhejiang University of Science & Technology, Hangzhou 310023, People's Republic of China

<sup>b</sup>School of Life Science, Shandong University of Technology, Zibo 255049, People's Republic of China



### Excavating precursors from the traditional Chinese herb *Polygala tenuifolia* and *Gastrodia elata*: Synthesis, anticonvulsant activity evaluation of 3,4,5-trimethoxycinnamic acid (TMCA) ester derivatives

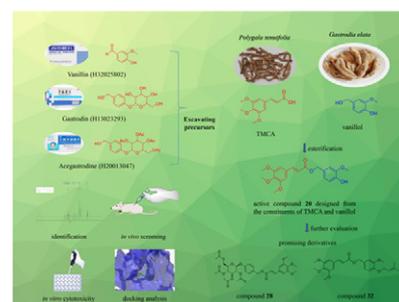
Zefeng Zhao<sup>a,1</sup>, Yajun Bai<sup>a,b,1</sup>, Jing Xie<sup>a</sup>, Xufei Chen<sup>a</sup>, Xirui He<sup>c,\*</sup>, Ying Sun<sup>a</sup>, Yujun Bai<sup>a</sup>, Yangyang Zhang<sup>a</sup>, Shaoping Wu<sup>a,\*</sup>, Xiaohui Zheng<sup>a,\*</sup>

<sup>a</sup>School of Pharmacy, Biomedicine Key Laboratory of Shaanxi Province, Northwest University, Xi'an 710069, China

<sup>b</sup>College of Chemistry and Materials Science, Northwest University, Xi'an 710069, China

<sup>c</sup>Honghui Hospital, Xi'an Jiaotong University, Xi'an 710054, China

*Bioorganic Chemistry 88 (2019) 102832*



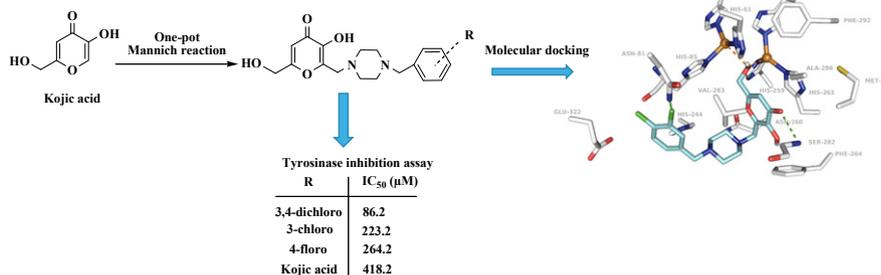
### Synthesis, computational molecular docking analysis and effectiveness on tyrosinase inhibition of kojic acid derivatives

Gülşah Karakaya<sup>a</sup>, Aslı Türe<sup>b</sup>, Ayşe Ercan<sup>c</sup>, Selin Öncül<sup>c</sup>, Mutlu Dilsiz Aytemir<sup>a,\*</sup>

<sup>a</sup>Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Hacettepe University, Ankara, Turkey

<sup>b</sup>Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Marmara University, İstanbul, Turkey

<sup>c</sup>Department of Biochemistry, Faculty of Pharmacy, Hacettepe University, Ankara, Turkey



### Multifunctional nanoparticles from albumin for stimuli-responsive efficient dual drug delivery

Hamed Nosrati<sup>a,b</sup>, Fatemeh Abhari<sup>c</sup>,  
Jalil Charmi<sup>d</sup>, Soodabeh Davaran<sup>e</sup>,  
Hossein Danafar<sup>a,b,\*</sup>

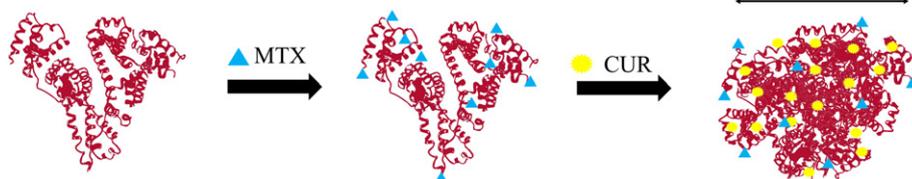
<sup>a</sup>Zanjan Pharmaceutical Nanotechnology Research Center, Zanjan University of Medical Sciences, Zanjan, Iran

<sup>b</sup>Department of Pharmaceutical Biomaterials, School of Pharmacy, Zanjan University of Medical Sciences, Zanjan, Iran

<sup>c</sup>Department of Medical Physics, School of Medicine, Tabriz University of Medical Sciences, Tabriz, Iran

<sup>d</sup>Department of Physics, Faculty of Science, University of Zanjan, Zanjan 45371-38791, Iran

<sup>e</sup>Drug Applied Research Center, Tabriz University of Medical Sciences, P.O. Box: 51656-65811, Tabriz, Iran



Bioorganic Chemistry 88 (2019) 102959

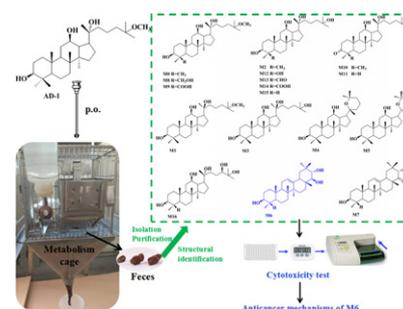
### New perspective on the metabolism of AD-1 *in vivo*: Characterization of a series of dammarane-type derivatives with novel metabolic sites and anticancer mechanisms of active oleanane-type metabolites

Meng Ding<sup>a</sup>, Xude Wang<sup>a</sup>, Yumeng Zhang<sup>a</sup>, Weihui Yuan<sup>a</sup>, Huixing Zhang<sup>a</sup>, Lei Xu<sup>a</sup>, Ziyi Wang<sup>b</sup>, Jincal Lu<sup>a,\*</sup>,  
Wei Li<sup>a,c,\*</sup>, Yuqing Zhao<sup>a,c,\*</sup>

<sup>a</sup>Shenyang Pharmaceutical University, Shenyang 110016, China

<sup>b</sup>Guangxi University of Chinese Medicine, Nanning 530200, China

<sup>c</sup>Key Laboratory of Structure-based Drug Design and Discovery of Ministry of Education, Shenyang Pharmaceutical University, Shenyang 110016, China



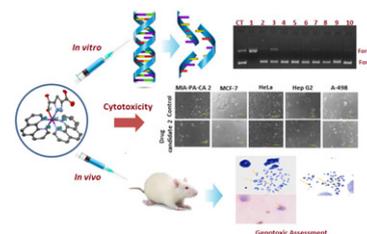
Bioorganic Chemistry 88 (2019) 102961

### Evaluation of cytotoxic activity and genotoxicity of structurally well characterized potent cobalt(II) phen-based antitumor drug entities: An *in vitro* and *in vivo* approach

Huzaiifa Yasir Khan<sup>a</sup>, Mohd Owais Ansari<sup>b</sup>, G.G.H.A. Shadab<sup>b</sup>, Sartaj Tabassum<sup>a</sup>, Farukh Arjmand<sup>a,\*</sup>

<sup>a</sup>Department of Chemistry, Aligarh Muslim University, Aligarh 202002, Uttar Pradesh, India

<sup>b</sup>Cytogenetics and Molecular Toxicology Laboratory, Section of Genetics, Department of Zoology, Aligarh Muslim University, Aligarh 202002, Uttar Pradesh, India



Bioorganic Chemistry 88 (2019) 102963

### Selective cyclooxygenase inhibition and ulcerogenic liability of some newly prepared anti-inflammatory agents having thiazolo [4,5-d] pyrimidine scaffold

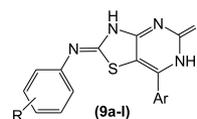
*Bioorganic Chemistry 88 (2019) 102964*

 Rania B. Bakr<sup>a,b,\*</sup>, Amira A. Ghoneim<sup>c,d</sup>, Amany A. Azouz<sup>e</sup>
<sup>a</sup>Department of Pharmaceutical Chemistry, College of Pharmacy, Jouf University, Sakaka, Al Jouf-2014, Saudi Arabia

<sup>b</sup>Department of Pharmaceutical Organic Chemistry, Faculty of Pharmacy, Beni-Suef University, Beni-Suef 62514, Egypt

<sup>c</sup>Chemistry Department, Faculty of Science, Jouf University, P.O. Box, 2014, Aljouf, Saudi Arabia

<sup>d</sup>Chemistry Department, Faculty of Science, Zagazig University, Zagazig, Egypt

<sup>e</sup>Department of Pharmacology and Toxicology, Beni-Suef University, Beni-Suef 62514, Egypt


	R	Ar	R	Ar
9a	3-COCH <sub>3</sub>	4-F-C <sub>6</sub> H <sub>4</sub>	9h	4-COCH <sub>3</sub>
9b	3-COCH <sub>3</sub>	4-Cl-C <sub>6</sub> H <sub>4</sub>	9i	4-COOC <sub>2</sub> H <sub>5</sub>
9c	3-COCH <sub>3</sub>	4-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub>	9j	4-COOC <sub>2</sub> H <sub>5</sub>
9d	3-COCH <sub>3</sub>	3,4,5-(OCH <sub>3</sub> ) <sub>3</sub> -C <sub>6</sub> H <sub>2</sub>	9k	4-COOC <sub>2</sub> H <sub>5</sub>
9e	4-COCH <sub>3</sub>	4-F-C <sub>6</sub> H <sub>4</sub>	9l	4-COOC <sub>2</sub> H <sub>5</sub>
9f	4-COCH <sub>3</sub>	4-Cl-C <sub>6</sub> H <sub>4</sub>		
9g	4-COCH <sub>3</sub>	4-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub>		
				3,4,5-(OCH <sub>3</sub> ) <sub>3</sub> -C <sub>6</sub> H <sub>2</sub>
				4-F-C <sub>6</sub> H <sub>4</sub>
				4-Cl-C <sub>6</sub> H <sub>4</sub>
				4-(NO <sub>2</sub> )-C <sub>6</sub> H <sub>4</sub>
				3,4,5-(OCH <sub>3</sub> ) <sub>3</sub> -C <sub>6</sub> H <sub>2</sub>

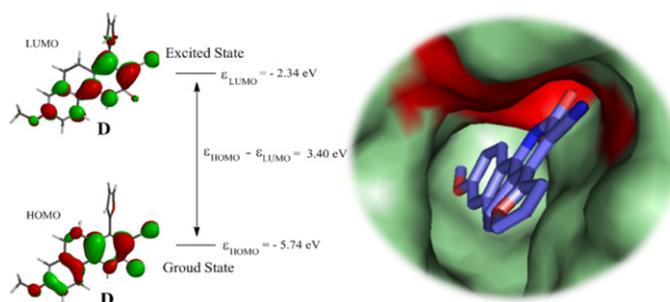
### Synthesis and evaluation of Quinoline-3-carbonitrile derivatives as potential antibacterial agents

*Bioorganic Chemistry 88 (2019) 102968*

 Salman A. Khan<sup>a,\*</sup>, Abdullah M. Asiri<sup>a,b</sup>, Hadi Mussa Basisi<sup>a</sup>,  
 Mohammad Asad<sup>a</sup>, Mohie E.M. Zayed<sup>a</sup>, Kamlesh Sharma<sup>c</sup>,  
 Mohmmad Younus Wani<sup>d,\*</sup>
<sup>a</sup>Chemistry Department, Faculty of Science, King Abdulaziz University, P.O. Box 80203, Jeddah 21589, Saudi Arabia

<sup>b</sup>Center of Excellence for Advanced Materials Research (CEAMR), King Abdulaziz University, P.O. Box 80203, Jeddah 21589, Saudi Arabia

<sup>c</sup>Department of Chemistry, Faculty of Sciences, Shree Guru Gobind Singh Tricentenary University, Gurugram 122505, Haryana, India

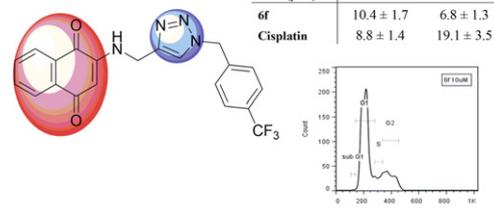
<sup>d</sup>Chemistry Department, Faculty of Science, University of Jeddah, P.O. Box 80327, Jeddah 21589, Saudi Arabia


### Click chemistry-assisted synthesis of novel aminonaphthoquinone-1,2,3-triazole hybrids and investigation of their cytotoxicity and cancer cell cycle alterations

*Bioorganic Chemistry 88 (2019) 102967*

 Maryam Gholampour<sup>a</sup>, Sara Ranjbar<sup>b</sup>, Najmeh Edraki<sup>c</sup>, Maryam Mohabbati<sup>c</sup>, Omidreza Firuzi<sup>c</sup>,  
 Mehdi Khoshneviszadeh<sup>a,c,\*</sup>
<sup>a</sup>Department of Medicinal Chemistry, Faculty of Pharmacy, Shiraz University of Medical Sciences, Shiraz, Iran

<sup>b</sup>Pharmaceutical Sciences Research Center, Shiraz University of Medical Sciences, Shiraz, Iran

<sup>c</sup>Medicinal and Natural Products Chemistry Research Center, Shiraz University of Medical Sciences, Shiraz, Iran


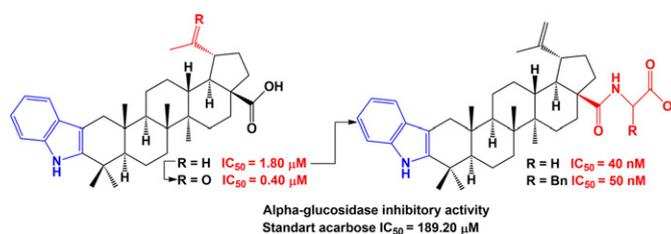
### Structural modifications of 2,3-indolobetulinic acid: Design and synthesis of highly potent α-glucosidase inhibitors

*Bioorganic Chemistry 88 (2019) 102957*

 Elmira F. Khusnutdinova<sup>a,\*</sup>, Anastasiya V. Petrova<sup>a,b</sup>, Ha Nguyen Thi Thu<sup>c</sup>,  
 Anh Le Thi Tu<sup>c</sup>, Tra Nguyen Thanh<sup>c</sup>, Cham Ba Thi<sup>c</sup>, Denis A. Babkov<sup>d</sup>,  
 Oxana B. Kazakova<sup>a</sup>
<sup>a</sup>Ufa Institute of Chemistry UFRS RAS, 71 pr. Oktyabrya, Ufa 450054, Russian Federation

<sup>b</sup>Bashkir State University, 32 Validy Str., Ufa 450076, Russian Federation

<sup>c</sup>Institute of Chemistry, Vietnamese Academy of Science and Technology, 18 Hoang Quoc Viet Str., Cau Giay Dist., Hanoi, Viet Nam

<sup>d</sup>Scientific Center for Innovative Drugs, Volgograd State Medical University, Novorossiyskaya st. 39, Volgograd 400087, Russian Federation


### Synthesis and biological evaluation of flavone-8-acrylamide derivatives as potential multi-target-directed anti Alzheimer agents and investigation of binding mechanism with acetylcholinesterase

Bioorganic Chemistry 88 (2019) 102960

Jeelan Basha Shaik<sup>a</sup>, Daniel Pushparaju Yeggoni<sup>b</sup>, Yelamanda Rao Kandrakonda<sup>a</sup>, Mohan Penumala<sup>a</sup>, Raveendra Babu Zinka<sup>a</sup>, Kasi Viswanath Kotapati<sup>c</sup>, Mark Manidhar Darla<sup>d</sup>, Dinakara Rao Ampasala<sup>c</sup>, Rajagopal Subramanyam<sup>b</sup>, Damu Gangaiah Amooru<sup>a,\*</sup>

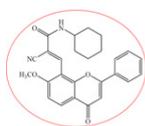
<sup>a</sup>Department of Chemistry, Yogi Vemana University, Kadapa, Andhra Pradesh, India

<sup>b</sup>Department of Plant Sciences, School of Life Sciences, University of Hyderabad, Hyderabad, India

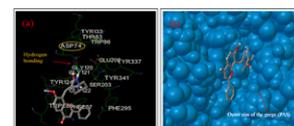
<sup>c</sup>Centre for Bioinformatics, School of Life Sciences, Pondicherry Central University, Puducherry, India

<sup>d</sup>Department of Chemistry, Sri Venkateswara University, Tirupati, Andhra Pradesh, India

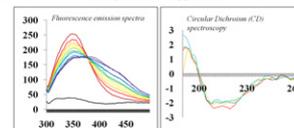
#### Binding mechanism with AChE



**Compound 8e**  
 hAChE IC<sub>50</sub> = 1.25 μM  
 Ee AChE IC<sub>50</sub> = 0.064 μM  
 ABTS radical scavenging activity IC<sub>50</sub> = 0.626 μM  
 Non toxic to SK N SH cells



#### Computational approach



Biophysical approach

### Identification of anti-inflammatory polyketides from the coral-derived fungus *Penicillium sclerotiorin*: *In vitro* approaches and molecular-modeling

Bioorganic Chemistry 88 (2019) 102973

Zhaoming Liu<sup>a,b,1</sup>, Pei Qiu<sup>a,1</sup>, Hongju Liu<sup>c</sup>, Jing Li<sup>c</sup>, Changlun Shao<sup>d,\*</sup>, Tao Yan<sup>e</sup>, Wenhao Cao<sup>e</sup>, Zhigang She<sup>a,\*</sup>

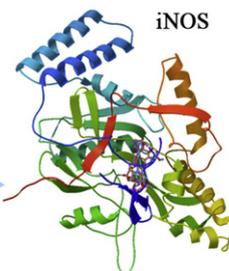
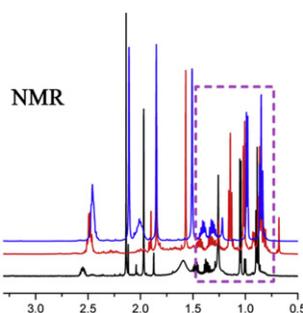
<sup>a</sup>School of Chemistry, Sun Yat-Sen University, Guangzhou 510275, PR China

<sup>b</sup>State Key Laboratory of Applied Microbiology Southern China, Guangdong Provincial Key Laboratory of Microbial Culture Collection and Application, Guangdong Open Laboratory of Applied Microbiology, Guangdong Institute of Microbiology, 100 Central Xianlie Road, Yuexiu District, Guangzhou 510070, PR China

<sup>c</sup>School of Pharmacy, Guangdong Medical University, Dongguan 523808, PR China

<sup>d</sup>Key Laboratory of Marine Drugs, The Ministry of Education of China, School of Medicine and Pharmacy, Ocean University of China, Qingdao 266003, PR China

<sup>e</sup>CAS Key Laboratory of Tropical Marine Bio-resources and Ecology, Guangdong Key Laboratory of Marine Materia Medica, RNAM Center for Marine Microbiology, South China Sea Institute of Oceanology, Chinese Academy of Sciences, 164 West Xingang Road, Guangzhou 510301, PR China



### Novel 9-(2-(1-arylethylidene)hydrazinyl)acridine derivatives: Target Topoisomerase 1 and growth inhibition of HeLa cancer cells

Bioorganic Chemistry 88 (2019) 102962

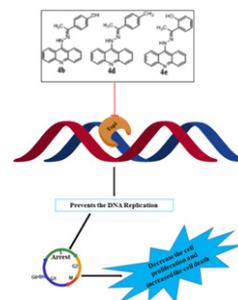
Md Rafi Haider<sup>a</sup>, Kamal Ahmad<sup>a</sup>, Nadeem Siddiqui<sup>a</sup>, Zulphikar Ali<sup>a</sup>, Md Jawaid Akhtar<sup>a,d</sup>, Neeraj Fuloria<sup>b</sup>, Shivkanya Fuloria<sup>b</sup>, Manickam Ravichandran<sup>c</sup>, M. Shahar Yar<sup>a,\*</sup>

<sup>a</sup>Department of Pharmaceutical Chemistry, School of Pharmaceutical Education and Research (SPER), Jamia Hamdard, Hamdard Nagar, New Delhi 110062, India

<sup>b</sup>Department of Pharmaceutical Chemistry, Faculty of Pharmacy, AIMST University, Semeling Campus, Jalan Bedong-Semeling, Bedong, Kedah Darul Aman 08100, Malaysia

<sup>c</sup>Faculty of Applied Science, AIMST University, Semeling Campus, Jalan Bedong-Semeling, Bedong, Kedah Darul Aman 08100, Malaysia

<sup>d</sup>School of Pharmacy, Bharat Institute of Technology, NH 58, Partapur Bypass, Meerut 250103, India



### Dipyridamole inhibits $\alpha$ -amylase/ $\alpha$ -glucosidase at sub-micromolar concentrations; *in-vitro*, *in-vivo* and theoretical studies

Bioorganic Chemistry 88 (2019) 102972

Sajjad Esmaeili<sup>a,\*</sup>, Sarwar Azizian<sup>b</sup>, Bahareh Shahmoradi<sup>c</sup>,  
Sajad Moradi<sup>d</sup>, Mohsen Shahlaei<sup>e</sup>, Reza Khodarahmi<sup>a,b,\*</sup>

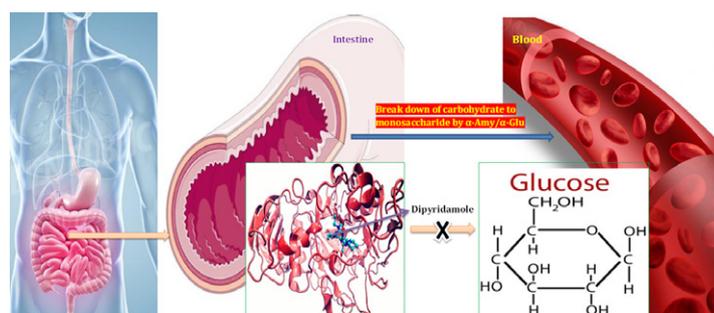
<sup>a</sup>Medical Biology Research Center, Health Technology Institute, Kermanshah University of Medical Sciences, Kermanshah, Iran

<sup>b</sup>Department of Pharmacognosy and Biotechnology, Faculty of Pharmacy, Kermanshah University of Medical Sciences, Kermanshah, Iran

<sup>c</sup>Department of Biology, Faculty of Sciences, University of Isfahan, Isfahan, Iran

<sup>d</sup>Nano Drug Deliver Research Center, Health Technology Institute, Kermanshah University of Medical Sciences, Kermanshah, Iran

<sup>e</sup>Pharmaceutical Sciences Research Center, Health Institute, Kermanshah University of Medical Sciences, Kermanshah, Iran



### Design, synthesis and molecular modeling studies on novel moxifloxacin derivatives as potential antibacterial and antituberculosis agents

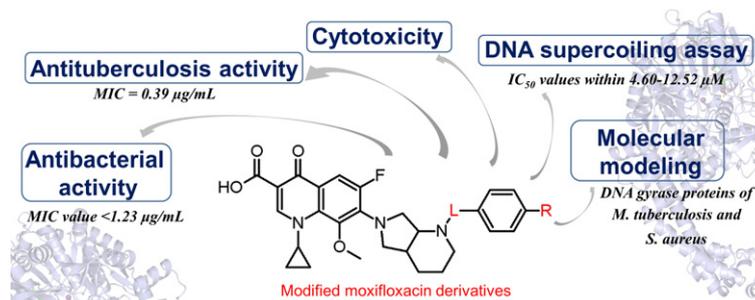
Bioorganic Chemistry 88 (2019) 102965

Ashlı Türe<sup>a</sup>, Necla Kulabaş<sup>a</sup>, Serap İpek Dingiş<sup>a</sup>, Kaan Birgül<sup>a,1</sup>,  
Arif Bozdeveci<sup>b</sup>, Şengül Alpay Karaoğlu<sup>b</sup>, Vagolu Siva Krishna<sup>c</sup>,  
Dharmarajan Sriram<sup>c</sup>, İlkyay Küçükgüzel<sup>a,\*</sup>

<sup>a</sup>Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Marmara University, Haydarpaşa 34668, İstanbul, Turkey

<sup>b</sup>Department of Biology, Recep Tayyip Erdoğan University, 53100 Rize, Turkey

<sup>c</sup>Medicinal Chemistry Research Laboratory, Pharmacy group, Birla Institute of Technology and Science, 333031 Pilani, India



### Synthesis and identification of quinoline derivatives as topoisomerase I inhibitors with potent antipsoriasis activity in an animal model

Bioorganic Chemistry 88 (2019) 102899

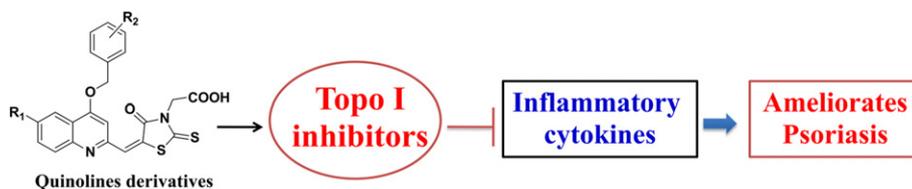
Wen-Jin Zhang<sup>a,1</sup>, Peng-Hui Li<sup>a,b,1</sup>,  
Min-Cong Zhao<sup>a</sup>, Yao-Hao Gu<sup>a</sup>,  
Chang-Zhi Dong<sup>a,c</sup>, Hui-Xiong Chen<sup>a,d</sup>,  
Zhi-Yun Du<sup>a,\*</sup>

<sup>a</sup>Institute of Natural Medicine & Green Chemistry, School of Chemical Engineering and Light Industry, Guangdong University of Technology, Guangzhou 510006, China

<sup>b</sup>School of Life Science, Huizhou University, Huizhou 516001, China

<sup>c</sup>Universite Paris Diderot, Sorbonne Paris Cite, ITODYS, UMR 7086 CNRS, 15 rue J-A de Baif, 75270 Paris Cedex 13, France

<sup>d</sup>CNRS, UMR8601, Laboratoire de Chimie et Biochimie Pharmacologiques et Toxicologiques, CBNIT, Université Paris Descartes PRES Sorbonne Paris Cite, UFR Biomedicale, 45 rue des Saints-Peres, 75270 Paris Cedex 06, France



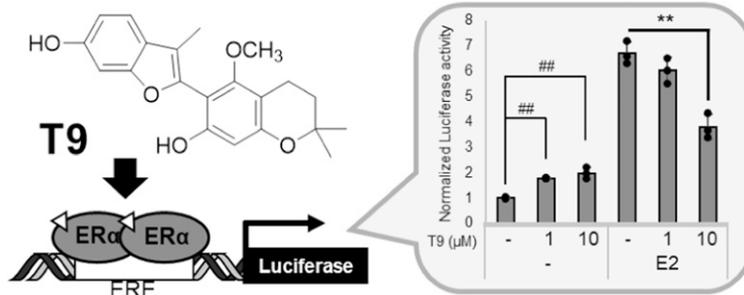
### Identification of 10-dehydroxyglycyuralin E as a selective human estrogen receptor alpha partial agonist

Nao Saito<sup>a</sup>, Keiko Kawase<sup>a</sup>, Naoya Yamashita<sup>a</sup>, Yingzhan Tang<sup>b</sup>, Ying Wang<sup>b</sup>, Jian Wang<sup>b</sup>, Yongxiang Liu<sup>b</sup>, Ning Li<sup>b</sup>, Wei Li<sup>b,c,\*</sup>, Mao-Sheng Cheng<sup>b,\*</sup>, Kazuo Koike<sup>c</sup>, Yuichiro Kanno<sup>a,\*</sup>, Kiyomitsu Nemoto<sup>a</sup>

<sup>a</sup>Department of Molecular Toxicology, Faculty of Pharmaceutical Sciences, Toho University, Miyama 2-2-1, Funabashi, Chiba 274-8510, Japan

<sup>b</sup>Key Laboratory of Structure-Based Drug Design & Discovery, Ministry of Education, Shenyang Pharmaceutical University, Shenyang 110016, Liaoning, PR China

<sup>c</sup>Faculty of Pharmaceutical Sciences, Toho University, Miyama 2-2-1, Funabashi, Chiba 274-8510, Japan

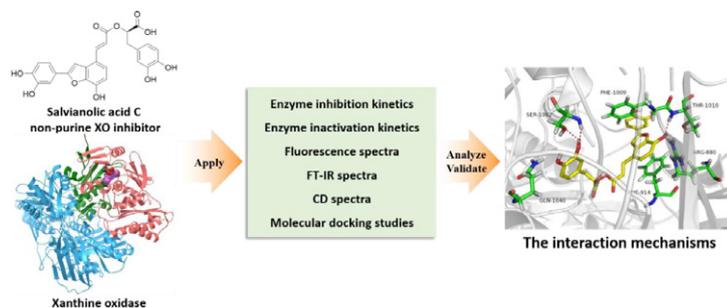


### Investigation of the interaction between salvianolic acid C and xanthine oxidase: Insights from experimental studies merging with molecular docking methods

Hongjin Tang<sup>a,\*</sup>, Dongsheng Zhao<sup>b</sup>

<sup>a</sup>College of Biological and Chemical Engineering, Anhui Polytechnic University, Wuhu 241000, PR China

<sup>b</sup>College of Pharmacy, Shandong University of Traditional Chinese Medicine, Jinan 250355, PR China

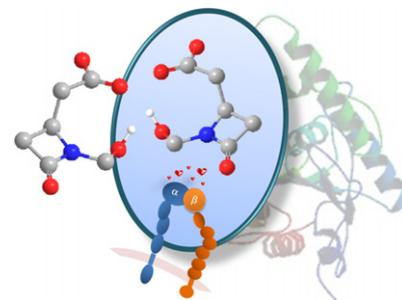


### Chiral β-lactam-based integrin ligands through Lipase-catalysed kinetic resolution and their enantioselective receptor response

Giulia Martelli<sup>a</sup>, Paola Galletti<sup>a</sup>, Monica Baiula<sup>b</sup>, Luca Calcinari<sup>a</sup>, Giacomo Boschi<sup>a</sup>, Daria Giacomini<sup>a,\*</sup>

<sup>a</sup>Department of Chemistry "G. Ciamician", University of Bologna, Via Selmi 2, 40126 Bologna, Italy

<sup>b</sup>Department of Pharmacy and Biotechnology, University of Bologna, Via Imerio, 48, 40126 Bologna, Italy



### Synthesis of oxazolidinone from enantiomerically enriched allylic alcohols and determination of their molecular docking and biologic activities

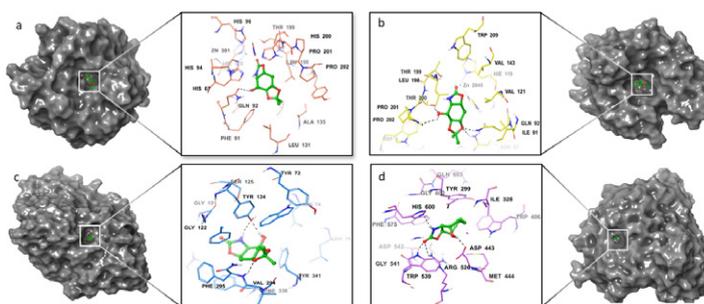
Bioorganic Chemistry 88 (2019) 102980

Ufuk Atmaca<sup>a,b</sup>, Rüya Kaya<sup>a,c</sup>, Halide Sedef Karaman<sup>a</sup>, Murat Çelik<sup>a,\*</sup>, İlhami Gülçin<sup>a,\*</sup>

<sup>a</sup>Department of Chemistry, Faculty of Sciences, Ataturk University, 25240 Erzurum, Turkey

<sup>b</sup>Oltu Vocational School, Ataturk University, 25400 Oltu-Erzurum, Turkey

<sup>c</sup>Central Research and Application Laboratory, Agri Ibrahim Cecen University, 04100 Agri, Turkey



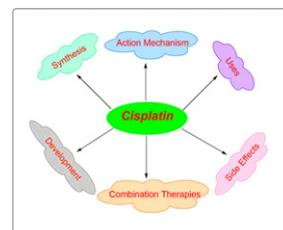
### REVIEW ARTICLES

### Cisplatin: The first metal based anticancer drug

Bioorganic Chemistry 88 (2019) 102925

Sumit Ghosh

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### Nimesulide analogues: From anti-inflammatory to antitumor agents

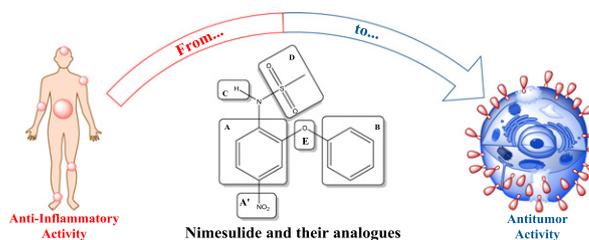
Bioorganic Chemistry 88 (2019) 102966

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### Current development of 5-nitrofuran-2-yl derivatives as antitubercular agents

Bioorganic Chemistry 88 (2019) 102969

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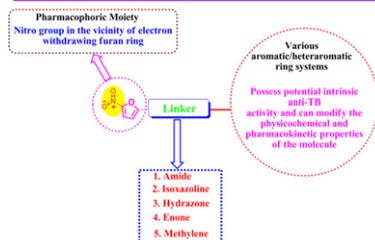
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We report herein the main efforts made to design and develop 5-nitrofurano-2-yl derivatives with promising antitubercular activity against drug-sensitive and resistant MTB.



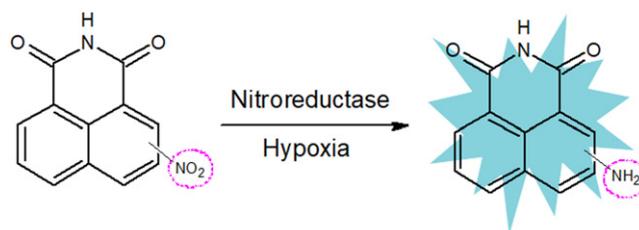
## Naphthalimides in fluorescent imaging of tumor hypoxia – An up-to-date review

Bioorganic Chemistry 88 (2019) 102979

Rashmi Kumari<sup>a</sup>, Dhanya Sunil<sup>a,\*</sup>, Raghunani S. Ningthoujam<sup>b</sup>

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## PRELIMINARY COMMUNICATIONS

### Chemical constituents from Vietnamese mangrove *Calophyllum inophyllum* and their anti-inflammatory effects

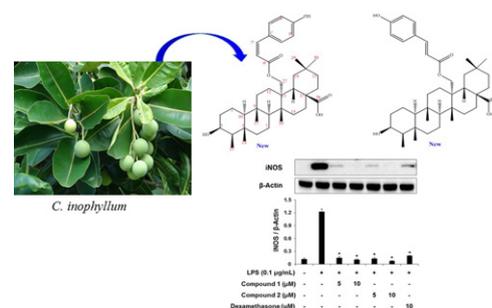
Bioorganic Chemistry 88 (2019) 102921

Nguyen Van Thanh<sup>b,1</sup>, Hyun-Jae Jang<sup>c,1</sup>, Le Ba Vinh<sup>a,b,1</sup>, Kieu Thi Phuong Linh<sup>b</sup>, Phan Thi Thanh Huong<sup>b</sup>, Nguyen Xuan Cuong<sup>b</sup>, Nguyen Hoai Nam<sup>b</sup>, Chau Van Minh<sup>b</sup>, Young Ho Kim<sup>a,\*</sup>, Seo Young Yang<sup>a,\*</sup>

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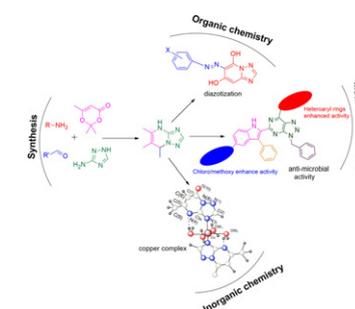


### An exhaustive compilation on chemistry of triazolopyrimidine: A journey through decades

Bioorganic Chemistry 88 (2019) 102919

Pankaj Kumar Singh, Shalki Choudhary, Aanchal Kashyap, Himanshu Verma, Swati Kapil, Manoj Kumar, Mohit Arora, Om Silakari<sup>\*</sup>

Molecular Modeling Lab (MML), Department of Pharmaceutical Sciences and Drug Research, Punjabi University, Patiala, Punjab 147002, India



### Discovery of cycloneolignan enantiomers from *Isatis indigotica* Fortune with neuroprotective effects against MPP<sup>+</sup>-induced SH-SY5Y cell injury

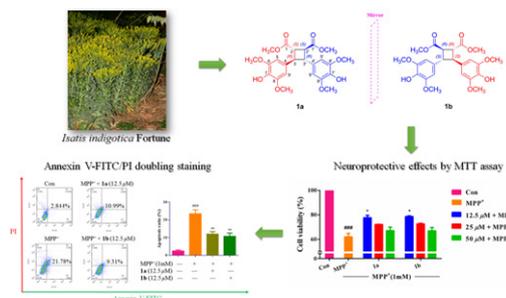
Bioorganic Chemistry 88 (2019) 102926

Yu-Fei Xi<sup>a,1</sup>, Si-Fan Liu<sup>a,1</sup>, Wei Hong<sup>a</sup>, Xiao-Yu Song<sup>a</sup>, Li-Li Lou<sup>a</sup>, Le Zhou<sup>a</sup>, Guo-Dong Yao<sup>a</sup>, Bin Lin<sup>b</sup>, Xiao-Bo Wang<sup>c</sup>, Xiao-Xiao Huang<sup>a,c,\*</sup>, Shao-Jiang Song<sup>a,\*</sup>

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**Phytosynthesis of silver nanoparticles using *Mangifera indica* flower extract as bioreductant and their broad-spectrum antibacterial activity**

*Bioorganic Chemistry* 88 (2019) 102970

Fuad Ameen<sup>a</sup>, P. Srinivasan<sup>b</sup>, T. Selvankumar<sup>b</sup>, S. Kamala-Kannan<sup>c</sup>, S. Al Nadhari<sup>d</sup>, A. Almansob<sup>a</sup>, T. Dawoud<sup>a</sup>, M. Govarthan<sup>e,\*</sup>

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