



## Graphical Abstracts/ Bioorganic Chemistry 90 (2019) ii-xviii

## REGULAR ARTICLES

**Discovery of novel indole-based aroylhydrazones as anticonvulsants: Pharmacophore-based design**

Bioorganic Chemistry 90 (2019) 103028

Violina T. Angelova<sup>a</sup>, Miroslav Rangelov<sup>b</sup>, Nadezhda Todorova<sup>c</sup>, Miroslav Dangelov<sup>b</sup>, Pavlina Andreeva-Gateva<sup>d</sup>, Magdalena Kondeva-Burdina<sup>a</sup>, Valentin Karabeliov<sup>a</sup>, Boris Shivachev<sup>e</sup>, Jana Tchekekarova<sup>f</sup>

<sup>a</sup>Faculty of Pharmacy, Medical University-Sofia (MU-Sofia), Bulgaria

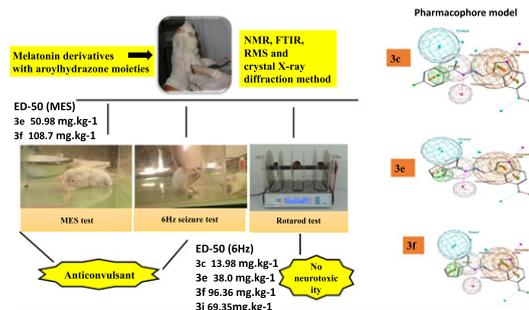
<sup>b</sup>Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences (BAS), Sofia, Bulgaria

<sup>c</sup>Institute of Biodiversity and Ecosystem Research, BAS, Sofia, Bulgaria

<sup>d</sup>Department of Pharmacology and Toxicology, Medical University of Sofia, Bulgaria

<sup>e</sup>Institute of Mineralogy and Crystallography, BAS, Sofia, Bulgaria

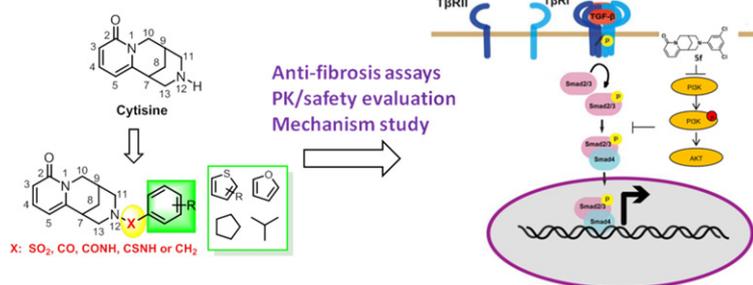
<sup>f</sup>Institute of Neurobiology, BAS, 1113 Sofia, Bulgaria


**Novel cytosine derivatives exert anti-liver fibrosis effect via PI3K/Akt/Smad pathway**

Bioorganic Chemistry 90 (2019) 103032

Sheng Tang, Yinghong Li, Yunyang Bao, Zhiting Dai, Tianyu Niu, Kun Wang, Hongwei He, Danqing Song

Institute of Medicinal Biotechnology, Peking Union Medical College and Chinese Academy of Medical Sciences, Beijing 100050, China


**Green synthesis of selenium-N-heterocyclic carbene compounds: Evaluation of antimicrobial and anticancer potential**

Bioorganic Chemistry 90 (2019) 103042

Amna Kamal<sup>a</sup>, Mansoureh Nazari V.<sup>b</sup>, Muhammad Yaseen<sup>d</sup>, Muhammad Adnan Iqbal<sup>a,c</sup>, Mohamed B. Khadeer Ahamed<sup>e</sup>, Aman Shah Abdul Majid<sup>f</sup>, Haq Nawaz Bhatti<sup>a</sup>

<sup>a</sup>Department of Chemistry, University of Agriculture, Faisalabad 38040, Pakistan

<sup>b</sup>Department of Pharmacology, School of Pharmaceutical Sciences, Universiti Sains Malaysia, Minden, 11800 Pulau Penang, Malaysia

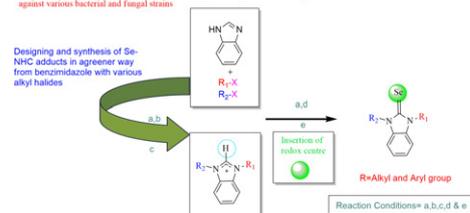
<sup>c</sup>Organometallic and Coordination Chemistry Laboratory, Department of Chemistry, University of Agriculture, Faisalabad 38040, Pakistan

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<sup>e</sup>EMAN Biodiscoveries Sdn. Bhd., A1-4, Lot 5, Persiaran 2/1, Kedah Halal Park, Kawasan Perindustrian Sungai Petani, 08000 Sungai Petani, Kedah, Malaysia

<sup>f</sup>Faculty of Medicine, Qest International University Perak, Ipoh, Perak, Malaysia

Se-NHC adducts were designed and synthesized in greener way and evaluated against various cancer cell lines and in addition against various bacterial and fungal strains



### Repurposing the scorpion venom peptide VmCT1 into an active peptide against Gram-negative ESKAPE pathogens

Cibele Nicolaski Pedron<sup>a</sup>, Iris Araújo<sup>a</sup>,  
Pedro Ismael da Silva Junior<sup>c</sup>,  
Fernanda Dias da Silva<sup>a</sup>,  
Marcelo Der Torossian Torres<sup>d,e</sup>,  
Vani Xavier Oliveira Junior<sup>a,b</sup>

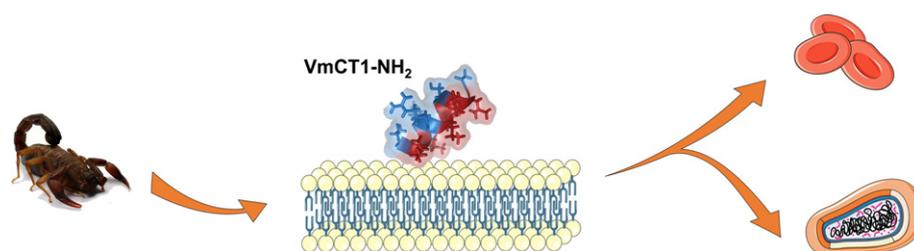
<sup>a</sup>Universidade Federal do ABC, Centro de Ciências Naturais e Humanas, 5001 Avenida dos Estados, Santo André, 09210580 SP, Brazil

<sup>b</sup>Universidade Federal de São Paulo, 100 Rua 3 de Maio, 04044020 São Paulo, SP, Brazil

<sup>c</sup>Instituto Butantan, Laboratório Especial de Toxinologia Aplicada, 1500 Avenida Vital Brasil, 05503900 São Paulo, SP, Brazil

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<sup>e</sup>Department of Bioengineering, University of Pennsylvania, Philadelphia 19104, PA, United States

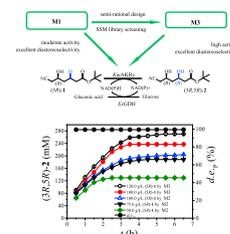


Bioorganic Chemistry 90 (2019) 103038

### Improving the catalytic efficiency of aldo-keto reductase KmAKR towards *t*-butyl 6-cyano-(3*R*,5*R*)-dihydroxyhexanoate via semi-rational design

Han Yu, Shuai Qiu, Feng Cheng, Ying-Nan Cheng, Ya-Jun Wang, Yu-Guo Zheng

Key Laboratory of Bioorganic Synthesis of Zhejiang Province, College of Biotechnology and Bioengineering, Zhejiang University of Technology, Hangzhou 310014, PR China  
Engineering Research Center of Bioconversion and Biopurification of the Ministry of Education, Zhejiang University of Technology, Hangzhou, Zhejiang 310014, PR China  
The National and Local Joint Engineering Research Center for Biomufacturing of Chiral Chemicals, Zhejiang University of Technology, Hangzhou 310014, PR China



Bioorganic Chemistry 90 (2019) 103018

### Cytotoxic and neuroprotective activities of constituents from *Alternaria alternate*, a fungal endophyte of *Psidium littorale*

Jian Xu<sup>a</sup>, Yun-Wei Hu<sup>b</sup>, Wei Qu<sup>a,c</sup>, Ming-Hua Chen<sup>e</sup>, Liang-Sheng Zhou<sup>f</sup>, Qi-Rui Bi<sup>a</sup>,  
Jian-Guang Luo<sup>a</sup>, Wen-Yuan Liu<sup>b</sup>, Feng Feng<sup>a,c,d</sup>, Jie Zhang<sup>a</sup>

<sup>a</sup>Department of Natural Medicinal Chemistry, School of Traditional Chinese Pharmacy, China Pharmaceutical University, Nanjing 210009, People's Republic of China

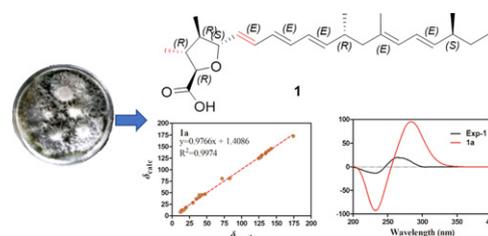
<sup>b</sup>Key Laboratory of Drug Quality Control and Pharmacovigilance (China Pharmaceutical University), Ministry of Education, China Pharmaceutical University, Nanjing 210009, People's Republic of China

<sup>c</sup>Key Laboratory of Biomedical Functional Materials, China Pharmaceutical University, Nanjing 211198, People's Republic of China

<sup>d</sup>Jiangsu Food & Pharmaceutical Science College, Huaian 223003, People's Republic of China

<sup>e</sup>NHC Key Laboratory for Microbial Drug Biotechnology, Institute of Medicinal Biotechnology, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing 100050, People's Republic of China

<sup>f</sup>College of Health Sciences, Jiangsu Normal University, Xuzhou 221116, People's Republic of China

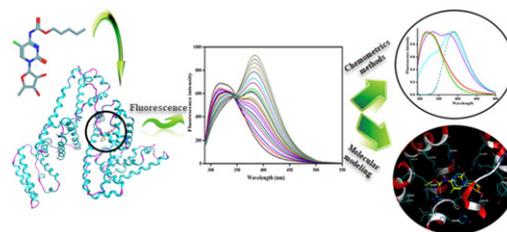


Bioorganic Chemistry 90 (2019) 103046

### Probing the binding mechanism of capecitabine to human serum albumin using spectrometric methods, molecular modeling, and chemometrics approach

S. Fatemeh Mousavi, Mohammad Hossein Fatemi

Chemometrics Laboratory, Faculty of Chemistry, University of Mazandaran, Babolsar, Iran



Bioorganic Chemistry 90 (2019) 103037

### New phenolic Mannich bases with piperazines and their bioactivities

Halise Inci Gul<sup>a</sup>, Mehtap Tugrak<sup>a</sup>, Mustafa Gul<sup>b</sup>, Sertac Mazlumoglu<sup>a</sup>, Hiroshi Sakagami<sup>c</sup>, Ilhami Gulcin<sup>d</sup>, Claudiu T. Supuran<sup>e</sup>

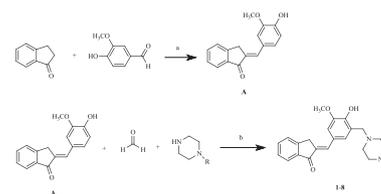
<sup>a</sup>Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Ataturk University, Erzurum, Turkey

<sup>b</sup>Department of Physiology, Faculty of Medicine, Ataturk University, Erzurum, Turkey

<sup>c</sup>Meikai University Research Institute of Odontology (M-RIO), Sakado, Saitama, Japan

<sup>d</sup>Faculty of Science, Department of Chemistry, Ataturk University, Erzurum, Turkey

<sup>e</sup>Neurofarba Department and Laboratorio di Chimica Bioorganica Universita' degli Studi di Firenze, Sesto Fiorentino, Italy



Reagents and conditions: a) EtOH, 10% NaOH, RT, b) CH<sub>3</sub>CN, 200 Watt, 120°C, 13.8 bar.  
R = Methyl (1), Phenyl (2), Benzyl (3), 2-Methoxyphenyl (4), 3-Methoxyphenyl (5), 2-Fluorophenyl (6), 4-Fluorophenyl (7), 3-Trifluoromethylphenyl (8)

Bioorganic Chemistry 90 (2019) 103057

### Investigation of potent inhibitors of cholinesterase based on thiourea and pyrazoline derivatives: Synthesis, inhibition assay and molecular modeling studies

Amara Mumtaz<sup>a</sup>, Abdul Majeed<sup>a</sup>, Sumera Zaib<sup>b</sup>, Shafiq Ur Rahman<sup>b</sup>, Saba Hameed<sup>a</sup>, Aamer Saeed<sup>c</sup>, Hummera Rafique<sup>d</sup>, Ehsanullah Mughal<sup>d</sup>, Aneela Maalik<sup>e</sup>, Izhar Hussain<sup>f</sup>, Jamshed Iqbal<sup>b,f</sup>

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

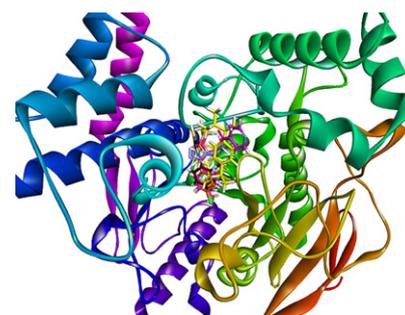
<sup>b</sup>Centre for Advanced Drug Research, COMSATS University Islamabad, Abbottabad Campus, Abbottabad 22060, Pakistan

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

<sup>d</sup>Department of Chemistry, University of Gujrat, Gujrat, Pakistan

<sup>e</sup>Department of Chemistry, COMSATS University Islamabad, Islamabad Campus, 45550-Islamabad, Pakistan

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

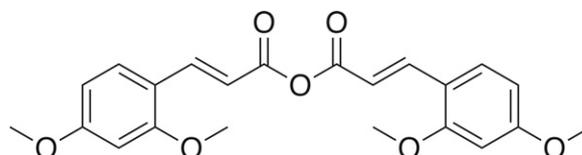


Bioorganic Chemistry 90 (2019) 103036

### Substituted cinnamic anhydrides act as selective inhibitors of acetylcholinesterase

Josephine M. Gießel, Immo Serbian, Anne Loesche, René Csuk

Martin-Luther-University Halle-Wittenberg, Organic Chemistry, Kurt-Mothes Str. 2, D-06120 Halle (Saale), Germany



$K_i = 8.30 \mu\text{M}$ ,  $K_i' = 9.54 \mu\text{M}$   
ee-acetylcholinesterase

Bioorganic Chemistry 90 (2019) 103058

### Cytotoxicity of oleanolic and ursolic acid derivatives toward hepatocellular carcinoma and evaluation of NF- $\kappa$ B involvement

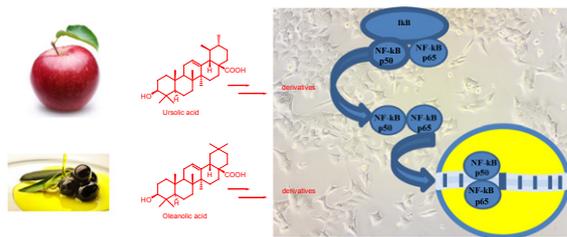
Bioorganic Chemistry 90 (2019) 103054

Gianfranco Fontana<sup>a</sup>, Maurizio Bruno<sup>a</sup>, Monica Notarbartolo<sup>a</sup>, Manuela Labbozzetta<sup>a</sup>, Paola Poma<sup>a</sup>, Alberto Spinella<sup>b</sup>, Sergio Rosselli<sup>c</sup>

<sup>a</sup>Dipartimento di Scienze e Tecnologie Biologiche, Chimiche e Farmaceutiche (STEBICEF), Università degli Studi di Palermo, Viale delle Scienze, ed. 17, I-90128 Palermo, Italy

<sup>b</sup>Centro Grandi Apparecchiature (CGA) – ATen Center, University of Palermo, via F. Marini 14, 90128 Palermo, Italy

<sup>c</sup>Dipartimento di Scienze Agrarie, Alimentari e Forestali (SAAF), Università degli Studi di Palermo, Viale delle Scienze, ed. 4, I-90128 Palermo, Italy



### Exploiting the 7-methylimidazo [1,5-a] pyrazin-8(7H)-one scaffold for the development of novel chemical inhibitors for Bromodomain and Extraterminal Domain (BET) family

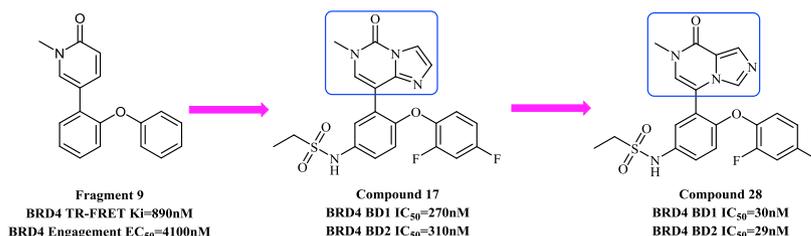
Bioorganic Chemistry 90 (2019) 103044

Yifei Yang<sup>a</sup>, Pan Chen<sup>a</sup>, Leilei Zhao<sup>b</sup>, Fangqing Zhang<sup>b</sup>, Bing Zhang<sup>b</sup>, Changliang Xu<sup>c</sup>, Huibin Zhang<sup>b</sup>, Jinpei Zhou<sup>a</sup>

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

<sup>c</sup>Jiangsu Collaborative Innovation Center of Traditional Chinese Medicine Prevention and Treatment of Tumor, Nanjing University of Chinese Medicine, Nanjing, Jiangsu 210023, PR China

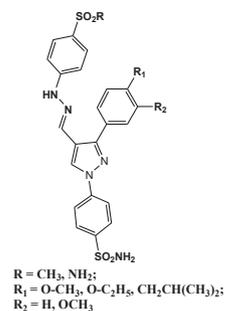


### Design, synthesis of celecoxib-tolmetin drug hybrids as selective and potent COX-2 inhibitors

Bioorganic Chemistry 90 (2019) 103029

Khaled R.A. Abdellatif, Eman K.A. Abdelall, Madlen B. Labib, Wael A.A. Fadaly, Taha H. Zidan

Pharmaceutical Organic Chemistry Department, Faculty of Pharmacy, Beni-Suef University, Beni-Suef, Egypt



### Novel Pyrazoloquinolin-2-ones: Design, synthesis, docking studies, and biological evaluation as antiproliferative EGFR-TK inhibitors

Bioorganic Chemistry 90 (2019) 103045

Mohammed A.I. Elbastawesy<sup>a</sup>, Ashraf A. Aly<sup>b</sup>, Mohamed Ramadan<sup>a</sup>, Yaseen A.M.M. Elshaiher<sup>c</sup>, Bahaa G.M. Youssif<sup>d</sup>, Alan B. Brown<sup>e</sup>, Gamal El-Din A Abu-Rahma<sup>f</sup>

<sup>a</sup>Department of Pharmaceutical Organic Chemistry, Faculty of Pharmacy, Al-Azhar University, 71524 Assiut, Egypt

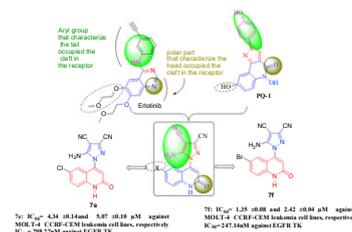
<sup>b</sup>Department of Chemistry, Faculty of Science, Minia University, 61519 Minia, Egypt

<sup>c</sup>Department of Organic and Medicinal Chemistry, Faculty of Pharmacy, University of Sadat City, 32958 Menoufia, Egypt

<sup>d</sup>Department of Pharmaceutical Organic Chemistry, Faculty of Pharmacy, Assiut University, 71526 Assiut, Egypt

<sup>e</sup>Program in Chemistry, Florida Institute of Technology, Melbourne, FL 32901, USA

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



### Protective effect of hypoxylonol C and 4,5,4',5'-tetrahydroxy-1,1'-binaphthyl isolated from *Annulohyphylon annulatum* against streptozotocin-induced damage in INS-1 cells

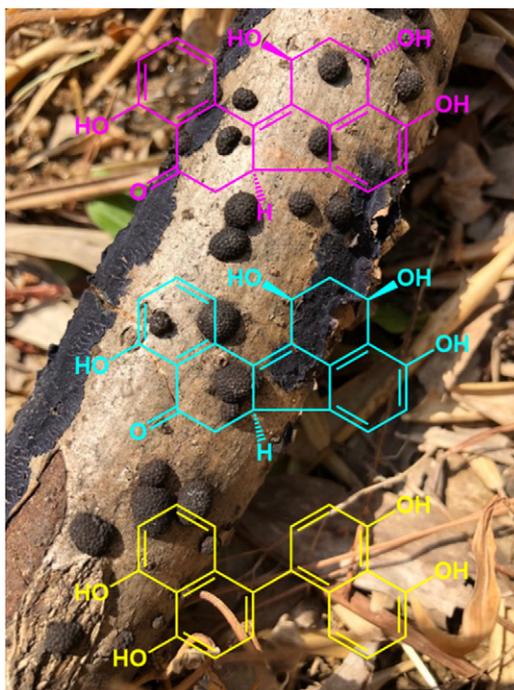
Dahae Lee<sup>a</sup>, Pilju Choi<sup>b,c</sup>,  
Buyng Su Hwang<sup>c</sup>, Taejung Kim<sup>c</sup>,  
Youngseok Kim<sup>c</sup>, Jin-Chul Kim<sup>c</sup>,  
Ji Hoon Song<sup>b</sup>, Jung Sik Park<sup>b</sup>,  
Gwi Seo Hwang<sup>b</sup>, Noriko Yamabe<sup>b</sup>,  
Ki Sung Kang<sup>b</sup>, Jungyeob Ham<sup>c,d</sup>

<sup>a</sup>School of Pharmacy, Sungkyunkwan University, Suwon 16419, Republic of Korea

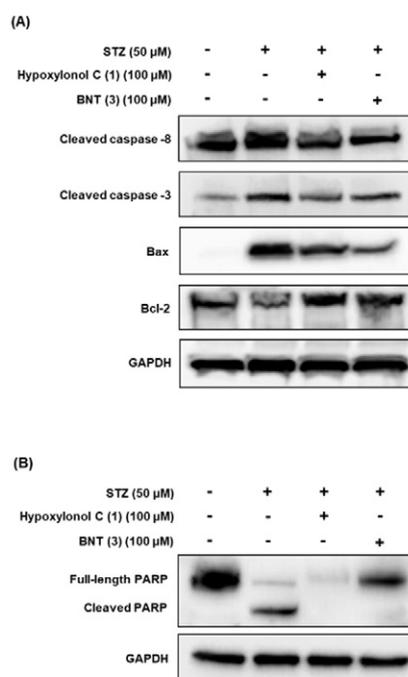
<sup>b</sup>College of Korean Medicine, Gachon University, Seongnam 13120, Republic of Korea

<sup>c</sup>Natural Products Research Institute, Korea Institute of Science and Technology, 679 Saimdang-ro, Gangneung 25451, Republic of Korea

<sup>d</sup>Division of Bio-Medical Science and Technology, University of Science and Technology, Daejeon 34113, Republic of Korea



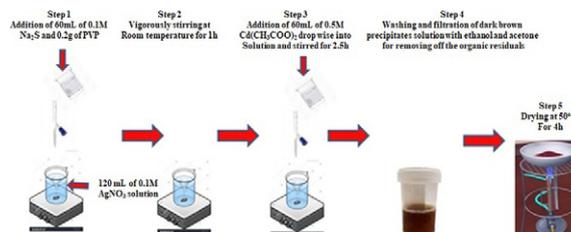
Bioorganic Chemistry 90 (2019) 103053



### Facile synthesis and antimicrobial activity of CdS-Ag<sub>2</sub>S nanocomposites

Tahir Iqbal, Faisal Ali, N.R. Khalid, M. Bilal Tahir, Mohsin Ijaz

Department of Physics, Faculty of Sciences, University of Gujrat, Hafiz Hayat Campus, Gujrat 50700, Pakistan



Bioorganic Chemistry 90 (2019) 103064

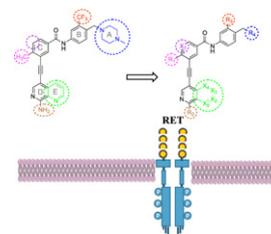
### Identification of nicotinamide aminonaphthyridine compounds as potent RET kinase inhibitors and antitumor activities against RET rearranged lung adenocarcinoma

Modi Wang<sup>a,b</sup>, N. Naganna<sup>a,b</sup>, Herman O. Sintim<sup>a,b,c</sup>

<sup>a</sup>Purdue Institute for Drug Discovery, West Lafayette, IN 47907, USA

<sup>b</sup>Department of Chemistry, Purdue University, West Lafayette, IN 47907, USA

<sup>c</sup>Purdue University Center for Cancer Research, Purdue University, West Lafayette, IN 47907, USA



Bioorganic Chemistry 90 (2019) 103052

### Isolation and characterization of three pairs of indoleketopiperazine enantiomers containing infrequent N-methoxy substitution from the marine algal-derived endophytic fungus *Acrostalagmus luteoalbus* TK-43

*Bioorganic Chemistry 90 (2019) 103030*

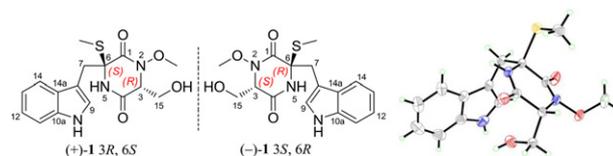
Jin Cao<sup>a,b</sup>, Xiao-Ming Li<sup>a</sup>, Ling-Hong Meng<sup>a</sup>, Belma Konuklugil<sup>c</sup>, Xin Li<sup>a,d</sup>, Hong-Lei Li<sup>a,d</sup>, Bin-Gui Wang<sup>a,d</sup>

<sup>a</sup>Key Laboratory of Experimental Marine Biology, Institute of Oceanology, Chinese Academy of Sciences, and Laboratory of Marine Biology and Biotechnology, Qingdao National Laboratory for Marine Science and Technology, Nanhai Road 7, Qingdao 266071, People's Republic of China

<sup>b</sup>University of Chinese Academy of Sciences, Yuquan Road 19A, Beijing 100049, People's Republic of China

<sup>c</sup>Department of Pharmacognosy, Faculty of Pharmacy, Ankara University, 06110 Ankara, Turkey

<sup>d</sup>Center for Ocean Mega-Science, Chinese Academy of Sciences, Nanhai Road 7, Qingdao 266071, People's Republic of China



### Anticancer properties of N-alkyl-2, 4-diphenylimidazo [1, 2-a] quinoxalin-1-amine derivatives; kinase inhibitors

*Bioorganic Chemistry 90 (2019) 103055*

Zahra Rezaei<sup>a</sup>, Mir Mahdi Didehvar<sup>b</sup>, Mohammad Mahdavi<sup>c</sup>, Homa Azizian<sup>d</sup>, Haleh Hamedifar<sup>e</sup>, Eman H.M. Mohammed<sup>f</sup>, Sayednaser Ostad<sup>g</sup>, Mohsen Amini<sup>h</sup>

<sup>a</sup>Department of Medicinal Chemistry, Faculty of Pharmacy, Tehran University of Medical Sciences, 14176 Tehran, Iran

<sup>b</sup>School of Chemistry, University College of Science, University of Tehran, PO Box 14155-6455, Tehran, Iran

<sup>c</sup>Endocrinology and Metabolism Research Center, Endocrinology and Metabolism Research Institute, Tehran University of Medical Sciences, Tehran, Iran

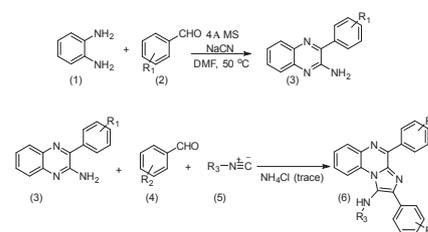
<sup>d</sup>Department of Medicinal Chemistry, School of Pharmacy-International Campus, Iran University of Medical Sciences, Tehran, Iran

<sup>e</sup>CinnaGen Medical Biotechnology Research Center, Alborz University of Medical Sciences, Karaj, Iran

<sup>f</sup>Department of Chemistry, Faculty of Sciences, Menoufia University, Shebin El-Koam, Egypt

<sup>g</sup>Department of Toxicology & Pharmacology, Faculty of Pharmacy, Tehran University of Medical Sciences, Tehran, Iran

<sup>h</sup>Department of Medicinal Chemistry, Faculty of Pharmacy and Drug Design and Development Research Center, The Institute of Pharmaceutical Sciences (TIPS), Tehran, Iran



### Ultrasound-assisted synthesis of novel chalcone, heterochalcone and bis-chalcone derivatives and the evaluation of their antioxidant properties and as acetylcholinesterase inhibitors

*Bioorganic Chemistry 90 (2019) 103034*

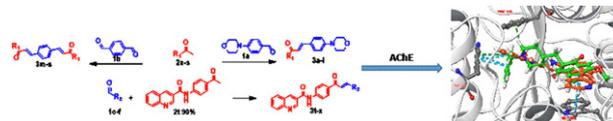
Efraín Polo<sup>a</sup>, Nicol Ibarra-Arellano<sup>a</sup>, Luis Prent-Peñaloza<sup>a</sup>, Alejandro Morales-Bayuelo<sup>b</sup>, José Henao<sup>c</sup>, Antonio Galdámez<sup>d</sup>, Margarita Gutiérrez<sup>a</sup>

<sup>a</sup>Laboratorio de Síntesis Orgánica, Instituto de Química de Recursos Naturales, Universidad de Talca, Casilla 747, Talca 3460000, Chile

<sup>b</sup>Ciencias de la Salud, Grupo de Investigaciones Básicas y Clínicas de la Universidad del Sinú (GIBACUS), escuela de medicina, Universidad del Sinú, seccional Cartagena, Colombia

<sup>c</sup>Grupo de Investigación en Química Estructural (GIQUE), Escuela de Química, Facultad de Ciencias, Universidad Industrial de Santander, A.A. 678, Carrera 27, Calle 9 Ciudadela Universitaria, Bucaramanga, Colombia

<sup>d</sup>Departamento de Química, Facultad de Ciencias, Universidad de Chile, Santiago 7800003, Chile



### Synthesis, molecular docking and kinetic studies of novel quinolinyl based acyl thioureas as mushroom tyrosinase inhibitors and free radical scavengers

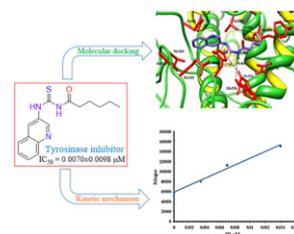
Bioorganic Chemistry 90 (2019) 103063

Muhammad Naeem Mustafa<sup>a</sup>, Aamer Saeed<sup>a</sup>, Pervaiz Ali Channar<sup>a</sup>, Fayaz Ali Larik<sup>a</sup>,  
Muhammad Zain-ul abideen<sup>a</sup>, Ghulam Shabir<sup>a</sup>, Qamar Abbas<sup>c</sup>, Mubashir Hassan<sup>b</sup>, Hussain Raza<sup>b</sup>, Sung-Yum Seo<sup>b</sup>

<sup>a</sup>Department of Chemistry, Quaid-I-Azam University, Islamabad 45320, Pakistan

<sup>b</sup>Department of Biological Sciences, College of Natural Sciences, Kongju National University, 56 Gongjudehak-Ro, Gongju, Chungnam 314-701, Republic of Korea

<sup>c</sup>Department of Physiology, University of Sindh, Jamshoro 76080, Pakistan



### Synthesis, modeling and biological evaluation of some pyrazolo [3,4-d] pyrimidinones and pyrazolo [4,3-e] [1,2,4] triazolo [4,3-a] pyrimidinones as anti-inflammatory agents

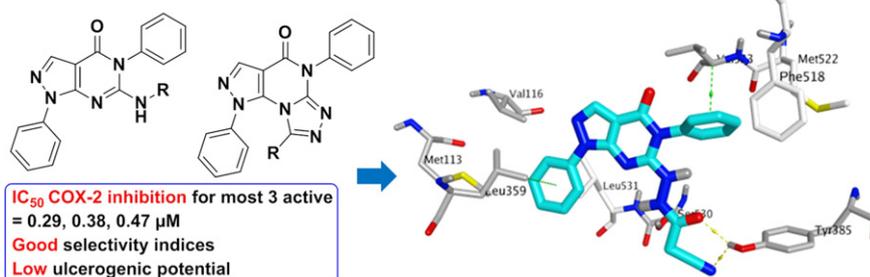
Bioorganic Chemistry 90 (2019) 102844

Gina N. Tageldin<sup>a</sup>, Tamer M. Ibrahim<sup>b</sup>,  
Salwa M. Fahmy<sup>a</sup>, Hayam M. Ashour<sup>a</sup>,  
Mounir A. Khalil<sup>a</sup>, Rasha A. Nassra<sup>c</sup>,  
Ibrahim M. Labouta<sup>a</sup>

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

<sup>b</sup>Pharmaceutical Chemistry Department, Faculty of Pharmacy, Kafrelsheikh University, Kafr El-Sheikh 33516, Egypt

<sup>c</sup>Department of Medical Biochemistry, Faculty of Medicine, Alexandria University, Alexandria, Egypt



### New potent antifungal triazole alcohols containing N-benzylpiperazine carbodithioate moiety: Synthesis, *in vitro* evaluation and *in silico* study

Bioorganic Chemistry 90 (2019) 103060

Yaser Mahmoudi<sup>a</sup>, Hamid Badali<sup>b</sup>, Seyedeh Mahdieh Hashemi<sup>c</sup>, Mahsa Ansari<sup>d</sup>, Hamed Fakhim<sup>e</sup>, Marjan Fallah<sup>f</sup>,  
Mohammad Shokrzadeh<sup>f</sup>, Saeed Emami<sup>c</sup>

<sup>a</sup>Student Research Committee, Faculty of Pharmacy, Mazandaran University of Medical Sciences, Sari, Iran

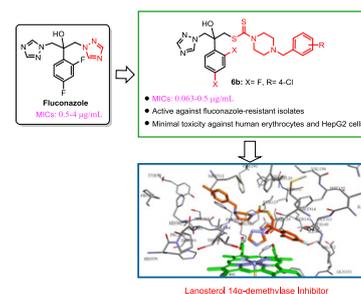
<sup>b</sup>Department of Medical Mycology/Invasive Fungi Research Center, School of Medicine, Mazandaran University of Medical Sciences, Sari, Iran

<sup>c</sup>Department of Medicinal Chemistry and Pharmaceutical Sciences Research Center, Faculty of Pharmacy, Mazandaran University of Medical Sciences, Sari, Iran

<sup>d</sup>Pharmaceutical Sciences Research Center, Student Research Committee, Faculty of Pharmacy, Mazandaran University of Medical Sciences, Sari, Iran

<sup>e</sup>Department of Medical Parasitology & Mycology/Cellular and Molecular Research Center, Urmia University of Medical Sciences, Urmia, Iran

<sup>f</sup>Department of Toxicology and Pharmacology, Faculty of Pharmacy, Mazandaran University of Medical Sciences, Sari, Iran



### Antibacterial activity of 3,3'-dihydroxycurcumin (DHC) is associated with membrane perturbation

Bioorganic Chemistry 90 (2019) 103031

Carlos R. Polaquini<sup>a</sup>, Luana G. Morão<sup>b</sup>, Ana C. Nazaré<sup>a</sup>, Guilherme S. Torrezan<sup>a</sup>, Guilherme Dilari<sup>b</sup>, Lúcia B. Cavalca<sup>b,c</sup>, Débora L. Campos<sup>d</sup>, Isabel C. Silva<sup>b,d</sup>, Jessé A. Pereira<sup>e</sup>, Dirk-Jan Scheffers<sup>c</sup>, Cristiane Duque<sup>e</sup>, Fernando R. Pavan<sup>d</sup>, Henrique Ferreira<sup>b</sup>, Luis O. Regasini<sup>a</sup>

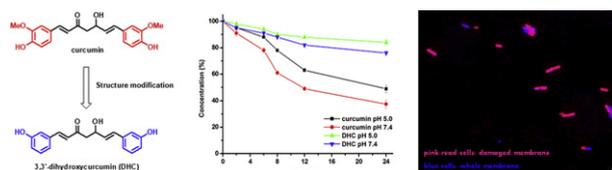
<sup>a</sup>Department of Chemistry and Environmental Sciences, Institute of Biosciences, Humanities and Exact Sciences, São Paulo State University (Unesp), São José do Rio Preto 15054-000, Brazil

<sup>b</sup>Department of Biochemistry and Microbiology, Institute of Biosciences, São Paulo State University (Unesp), Rio Claro 13506-900, Brazil

<sup>c</sup>Department of Molecular Microbiology, Groningen Biomolecular Sciences and Biotechnology Institute, University of Groningen, Groningen 9747, the Netherlands

<sup>d</sup>Department of Biological Sciences, School of Pharmaceutical Sciences, São Paulo State University (Unesp), Araraquara 14800-903, Brazil

<sup>e</sup>Department of Pediatric Dentistry and Public Health, School of Dentistry, São Paulo State University (Unesp), Araçatuba 16015-050, Brazil



### A competent synthesis and efficient anti-inflammatory responses of isatinimino acridinedione moiety via suppression of *in vivo* NF-κB, COX-2 and iNOS signaling

Bioorganic Chemistry 90 (2019) 103047

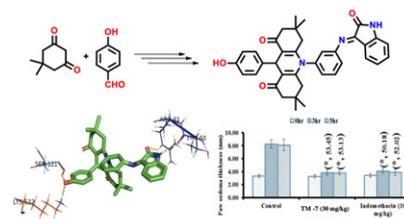
Govindasami Periyasami<sup>a</sup>, Paulrayer Antonisamy<sup>b</sup>, Karthikeyan Perumal<sup>c</sup>, Antony Stalin<sup>d</sup>, Mostafizur Rahaman<sup>a</sup>, Asma A. Alothman<sup>a</sup>

<sup>a</sup>Department of Chemistry, College of Science, King Saud University, Riyadh 11451, Saudi Arabia

<sup>b</sup>Department of Korean Physiology, Wonkwang University School of Korean Medicine, 460 Iksan-daero, Iksan City, Jeonbuk 570-749, Republic of Korea

<sup>c</sup>Department of Chemistry, The Ohio State University, 170A CBEC, 151 West Woodruff Avenue, Columbus, OH 43210, United States

<sup>d</sup>Department of Traditional Chinese Medicine, Zhejiang A&F University, Hangzhou 311300, China



### One-step synthesis of methylene-bridged bis-carbazole and evaluation of its antitumor activity and G-quadruplex DNA binding property

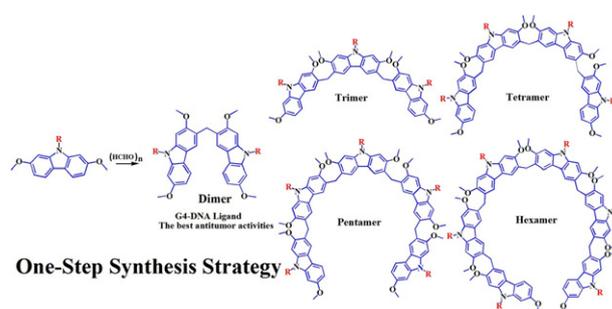
Bioorganic Chemistry 90 (2019) 103074

Gang Li<sup>c</sup>, Haodong Tang<sup>a</sup>, Chuanfeng Liu<sup>a</sup>, Xiaoyu Liao<sup>c</sup>, Sicong Li<sup>a</sup>, Zhengning Shu<sup>a</sup>, Hui Yu<sup>b</sup>, Peng Yang<sup>a,c</sup>

<sup>a</sup>Wuyi College of Innovation, Shenyang Pharmaceutical University, Shenyang 110016, China

<sup>b</sup>School of Textile Materials and Engineering, Wuyi University, Jiangmen 529020, China

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



### Synthesis, anti-diabetic evaluation and molecular docking studies of 4-(1-aryl-1H-1, 2, 3-triazol-4-yl)-1,4-dihydropyridine derivatives as novel 11-β hydroxysteroid dehydrogenase-1 (11β-HSD1) inhibitors

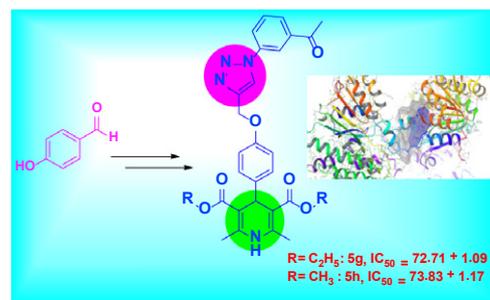
Bioorganic Chemistry 90 (2019) 103056

E. Praveenkumar<sup>a</sup>, Nirmala Gurrappu<sup>a</sup>, Prashanth Kumar Kolluri<sup>a</sup>, Vishwanadham Yerragunta<sup>b</sup>, Bharathi Reddy Kunduru<sup>c</sup>, N.J.P. Subhashini<sup>a</sup>

<sup>a</sup>Department of Chemistry, University College of Science, Osmania University, Hyderabad, Telangana 500 007, India

<sup>b</sup>Bio-organic & Medicinal Chemistry Research Division, Vishnu Institute of Pharmaceutical Education and Research (VIPER), Narsapur, Medak, Telangana 502 313, India

<sup>c</sup>Department of Genetics and Biotechnology, University College of Science, Osmania University, Hyderabad, Telangana 500 007, India



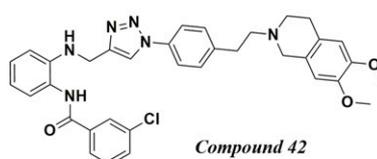
### Discovery of aromatic amides with triazole-core as potent reversal agents against P-glycoprotein-mediated multidrug resistance

Qianqian Qiu<sup>a</sup>, Jilan Zhu<sup>a</sup>, Qitong Chen<sup>a</sup>, Ziqian Jiang<sup>a</sup>, Jiting Xu<sup>a</sup>, Xueting Jiang<sup>a</sup>, Wenlong Huang<sup>b,c</sup>, Zhongquan Liu<sup>a</sup>, Jing Ye<sup>a</sup>, Xiaojuan Xu<sup>a</sup>

<sup>a</sup>School of Pharmacy, Jiangsu Provincial Key Laboratory of Coastal Wetland Bioresources and Environmental Protection, Yancheng Teachers' University, Yancheng, PR China

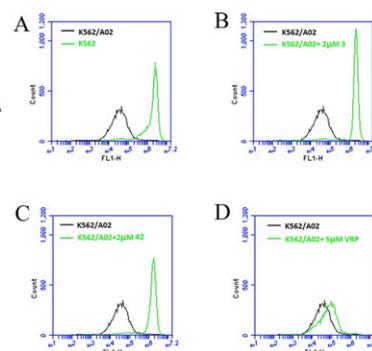
<sup>b</sup>Center of Drug Discovery, State Key Laboratory of Natural Medicines, China Pharmaceutical University, Nanjing, PR China

<sup>c</sup>Jiangsu Key Laboratory of Drug Discovery for Metabolic Disease, China Pharmaceutical University, Nanjing, PR China



- ◆ High potency,  $EC_{50} = 78.1 \pm 5.4$  nM
- ◆ Long activity duration, > 24h
- ◆ Great suppression of P-gp function
- ◆ No effect on CYP3A4 activity

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### Extraction, isolation and *in vitro* evaluation of affinisine from *Tabernaemontana catharinensis* in human melanoma cells

Pauline Fagundes Rosales<sup>a,b</sup>, Adriana Gower<sup>a</sup>, Martha Lucia Ruiz Benitez<sup>c</sup>, Bruna Silveira Pacheco<sup>c</sup>, Natália Vieira Segatto<sup>c</sup>, Mariana Roesch-Ely<sup>d</sup>, Tiago Collares<sup>c</sup>, Fabiana Kömmling Seixas<sup>c</sup>, Sidnei Moura<sup>a</sup>

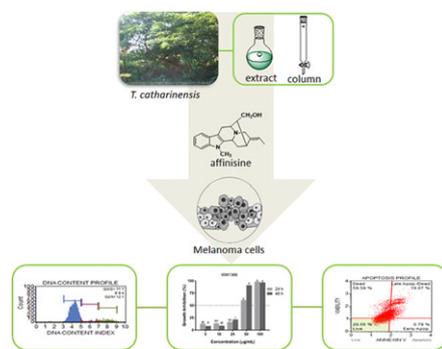
<sup>a</sup>Laboratory of Biotechnology of Natural and Synthetics Products - University of Caxias do Sul – Brazil

<sup>b</sup>Federal Institute of Education, Science and Technology of Rio Grande do Sul- Campus Bento Gonçalves – Brazil

<sup>c</sup>Research Group on Cellular and Molecular Oncology, Postgraduate Program in Biotechnology- Federal University of Pelotas – Brazil

<sup>d</sup>Laboratory of Genomics, Proteomics and DNA Repair - University of Caxias do Sul – Brazil

Bioorganic Chemistry 90 (2019) 103079

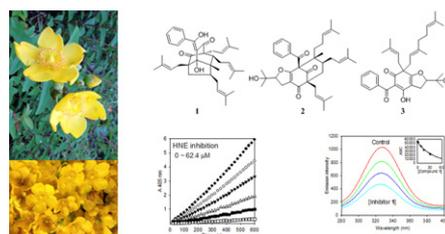


### Human neutrophil elastase (HNE) inhibitory polyprenylated acylphloroglucinols from the flowers of *Hypericum ascyron*

Zuo Peng Li, Jeong Yoon Kim, Yeong Jun Ban, Ki Hun Park

Division of Applied Life Science (BK21 plus), IALS, Gyeongsang National University, Jinju 52828, Republic of Korea

Bioorganic Chemistry 90 (2019) 103075



### 6-Substituted purines as ROCK inhibitors with anti-metastatic activity

Jiří Voller<sup>a,b</sup>, Lenka Zahajská<sup>c</sup>, Lucie Plíhalová<sup>a,d</sup>, Jana Jeřábková<sup>a</sup>, David Burget<sup>a</sup>, Andreea Csilla Pataki<sup>e</sup>, Vladimír Kryštof<sup>a</sup>, Marek Zatloukal<sup>d</sup>, Jan Brábek<sup>e</sup>, Daniel Rösel<sup>e</sup>, Václav Mik<sup>d</sup>, Martin Tkáč<sup>a</sup>, Tomáš Pospíšil<sup>d</sup>, Tomáš Gucký<sup>d</sup>, Karel Doležal<sup>a,d</sup>, Miroslav Strnad<sup>a</sup>

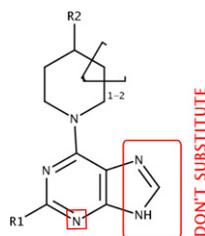
<sup>a</sup>Laboratory of Growth Regulators, The Czech Academy of Sciences, Institute of Experimental Botany & Palacký University, Šlechtitelů 27, CZ-78371 Olomouc, Czech Republic

<sup>b</sup>Department of Clinical and Molecular Pathology, Institute of Molecular and Translational Medicine, Faculty of Medicine and Dentistry, Palacký University, Hněvotínská 3, 775 15 Olomouc, Czech Republic

<sup>c</sup>Isotope Laboratory, The Czech Academy of Sciences, Institute of Experimental Botany, Vídeňská 1083, 142 00 Prague 4, Czech Republic

<sup>d</sup>Department of Chemical Biology and Genetics, Centre of the Region Haná for Biotechnological and Agricultural Research, Palacký University, Šlechtitelů 27, CZ-78371 Olomouc, Czech Republic

<sup>e</sup>Department of Cell Biology, Faculty of Science, Charles University in Prague, Viničná 7, 12843, Prague 2, Czech Republic



Bioorganic Chemistry 90 (2019) 103005

✖ ROCK2 activity

melanoma cell lines:

- ✖ MLC2 phosphorylation
- ✖ ameoboid morphology
- ✖ 3D collagen gel invasion

### Muscle extract of *Arothron immaculatus* regulates the blood glucose level and the antioxidant system in high-fat diet and streptozotocin induced diabetic rats

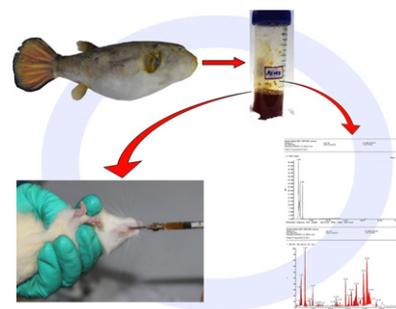
Karunanidhi Kaleshkumar<sup>a</sup>, Rajendran Rajaram<sup>a</sup>, Nambirajan Gayathri<sup>b</sup>, Thilagar Sivasudha<sup>b</sup>, Ganesan Arun<sup>a</sup>, Govindaraju Archunan<sup>c</sup>, Balázs Gulyás<sup>d</sup>, Parasuraman Padmanabhan<sup>d</sup>

<sup>a</sup>DNA Barcoding and Marine Genomics Laboratory, Department of Marine Science, School of Marine Sciences, Bharathidasan University, Tiruchirappalli 620 024, Tamil Nadu, India

<sup>b</sup>Department of Environmental Biotechnology, Bharathidasan University, Tiruchirappalli 620 024, Tamil Nadu, India

<sup>c</sup>Department of Animal Science, Bharathidasan University, Tiruchirappalli 620 024, Tamil Nadu, India

<sup>d</sup>Lee Kong Chian School of Medicine, Nanyang Technological University (NTU), 59, Nanyang Drive, Experimental Medicine Building, Singapore 636921, Singapore

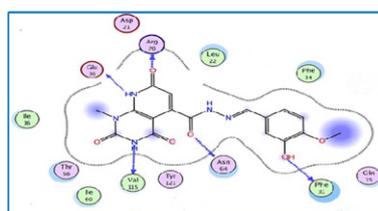


Bioorganic Chemistry 90 (2019) 103072

### Dihydrofolate reductase inhibition effect of 5-substituted pyrido [2,3-*d*] pyrimidines: Synthesis, antitumor activity and molecular modeling study

Ola A. Abdelaziz, Walaa M. El Hussein, Khalid B. Selim, Hassan M. Eisa

Department of Pharmaceutical Organic Chemistry, Faculty of Pharmacy, Mansoura University, Mansoura 35516, Egypt



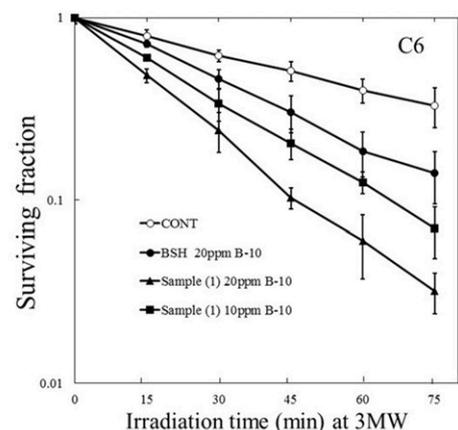
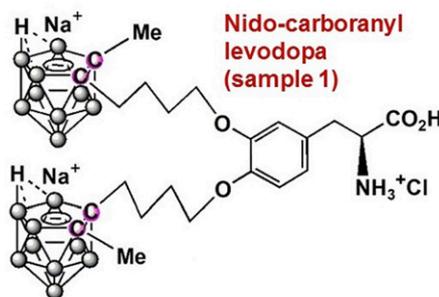
### Synthesis and *in vitro* anti-tumor activity of carboranyl levodopa

Yinghui Zhu<sup>a</sup>, Yongxiang Lin<sup>b</sup>,  
Narayan S. Hosmane<sup>c</sup>

<sup>a</sup>School of Pharmacy, Macau University of Science and Technology, Avenida Wai Long, Taipa 999078, Macau

<sup>b</sup>Institute of Chemical and Engineering Sciences, No. 1 Pesek Road, Jurong Island 627833, Singapore

<sup>c</sup>Department of Chemistry and Biochemistry, Northern Illinois University, DeKalb, IL 60115, USA

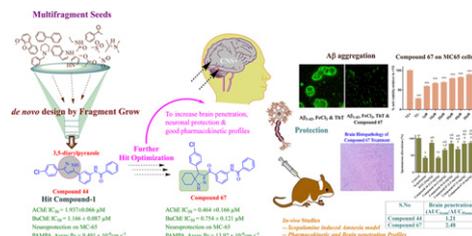


Bioorganic Chemistry 90 (2019) 103090

### Development of pyrazole and spiro-pyrazoline analogs as multifunctional agents for treatment of Alzheimer's disease

Gopichand Gutti, Devendra Kumar, Pankaj Paliwal, Ankit Ganeshpurkar, Khemraj Lahre, Ashok Kumar, Sairam Krishnamurthy, Sushil Kumar Singh

Department of Pharmaceutical Engineering & Technology, Indian Institute of Technology (Banaras Hindu University), Varanasi 221005, India



Bioorganic Chemistry 90 (2019) 103080

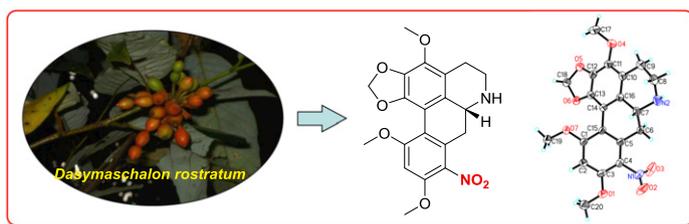
### Bioactive aporphine alkaloids from the stems of *Dasymaschalon rostratum*

Zhangxin Yu<sup>a,b</sup>, Changri Han<sup>a,c</sup>, Xiaoping Song<sup>a,c</sup>, Guangying Chen<sup>a</sup>, Jinxiong Chen<sup>a</sup>

<sup>a</sup>Key Laboratory of Tropical Medicinal Resource Chemistry of Ministry of Education, College of Chemistry and Chemical Engineering, Hainan Normal University, Haikou 571158, China

<sup>b</sup>Hainan Provincial Key Laboratory of Resources Conservation and Development of Southern Medicine, Hainan Branch of the Institute of Medicinal Plant Development, Chinese Academy of Medical Sciences and Peking Union Medical College, Haikou 570311, China

<sup>c</sup>Key Laboratory of Medicinal and Edible Plant Resources of Hainan Province, School of Chemical and Material Engineering, Hainan Institute of Science and Technology, Haikou 571126, China



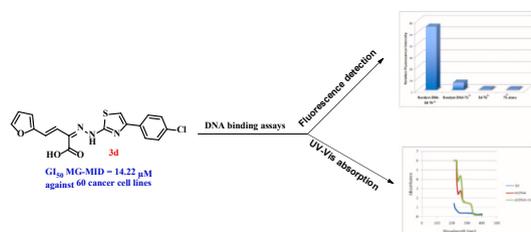
Bioorganic Chemistry 90 (2019) 103066

### Discovery of a novel DNA binding agent via design and synthesis of new thiazole hybrids and fused 1,2,4-triazines as potential antitumor agents: Computational, spectrometric and *in silico* studies

Marwa H. El-Wakil<sup>a</sup>, Amira F. El-Yazbi<sup>b</sup>, Hayam M.A. Ashour<sup>a</sup>, Mounir A. Khalil<sup>a</sup>, Khadiga A. Ismail<sup>a</sup>, Ibrahim M. Labouta<sup>a</sup>

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

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



Bioorganic Chemistry 90 (2019) 103089

### Search for multifunctional agents against Alzheimer's disease among non-imidazole histamine H3 receptor ligands. *In vitro* and *in vivo* pharmacological evaluation and computational studies of piperazine derivatives

Bioorganic Chemistry 90 (2019) 103084

Jakub Jończyk<sup>a</sup>, Krzysztof Lodarski<sup>a</sup>, Marek Staszewski<sup>b</sup>, Justyna Godyń<sup>a</sup>, Paula Zaręba<sup>a</sup>, Ondrej Soukup<sup>c,d</sup>, Jana Janockova<sup>c</sup>, Jan Korabecny<sup>c,d</sup>, Kinga Sałat<sup>e</sup>, Natalia Malikowska-Racia<sup>e</sup>, Michalina Hebda<sup>a</sup>, Natalia Szałaj<sup>a</sup>, Barbara Filipek<sup>e</sup>, Krzysztof Walczyński<sup>b</sup>, Barbara Malawska<sup>a</sup>, Marek Bajda<sup>a</sup>

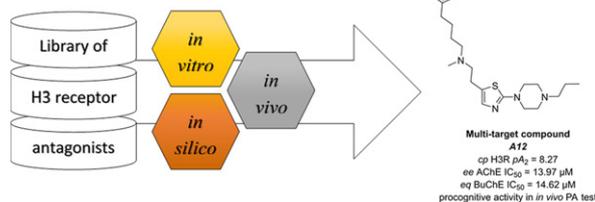
<sup>a</sup>Department of Physicochemical Drug Analysis, Faculty of Pharmacy, Jagiellonian University Medical College, Medyczna 9, 30-688 Kraków, Poland

<sup>b</sup>Department of Synthesis and Technology of Drugs, Medical University of Łódź, Muszyńskiego 1, 90-145 Łódź, Poland

<sup>c</sup>Biomedical Research Center, University Hospital Hradec Kralove, Sokolska 581, 500 05 Hradec Kralove, Czech Republic

<sup>d</sup>National Institute of Mental Health, Topolova 748, 250 67 Klecany, Czech Republic

<sup>e</sup>Department of Pharmacodynamics, Jagiellonian University Medical College, Medyczna 9, 30-688 Kraków, Poland



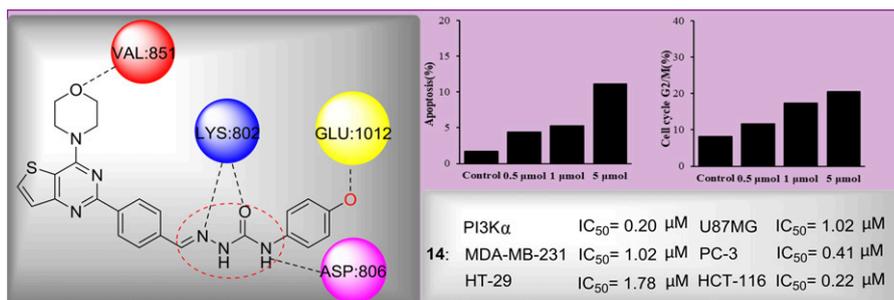
### Design, synthesis and biological evaluation of novel thieno [3,2-d] pyrimidine and quinazoline derivatives as potent antitumor agents

Bioorganic Chemistry 90 (2019) 103086

Hao Hu, Yuhong Dong, Ming Li, Ruxin Wang, Xian Zhang, Ping Gong, Yanfang Zhao

Key Laboratory of Structure-Based Drug Design and Discovery (Shenyang Pharmaceutical University), Ministry of Education, 103 Wenhua Road, Shenhe District, Shenyang 110016, PR China

Department of Pharmacology, Shenyang Pharmaceutical University, 103 Wenhua Road, Shenhe District, Shenyang 110016, PR China



### 5,6,7,8-Tetrahydrobenzo [4,5] thieno [2,3-d] pyrimidine derivatives as inhibitors of full-length ROR $\gamma$ t

Bioorganic Chemistry 90 (2019) 103077

Chuyu Lao, Xiaoqing Zhou, Huanpeng Chen, Fengjiao Wei, Zhaofeng Huang, Chuan Bai

Institute of Human Virology, Guangdong Engineering Research Center for Antimicrobial Agent and Immunotechnology, Zhongshan School of Medicine, Sun Yat-sen University, Guangzhou, Guangdong 510080, China

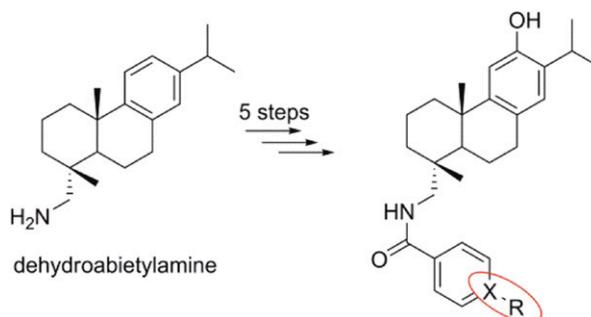


### Novel 12-hydroxydehydroabietylamine derivatives act as potent and selective butyrylcholinesterase inhibitors

Anne Loesche<sup>a</sup>, Jana Wiemann<sup>a</sup>,  
Matthias Rohmer<sup>a</sup>, Wolfgang Brandt<sup>b</sup>,  
René Csuk<sup>a</sup>

<sup>a</sup>Martin-Luther-University Halle-Wittenberg,  
Organic Chemistry, Kurt-Mothes-Str. 2, D-06120  
Halle (Saale), Germany

<sup>b</sup>Leibniz Institute of Plant Biochemistry, Bioorganic  
Chemistry, Weinberg 3, D-06120 Halle (Saale),  
Germany



13 X = C R = NO<sub>2</sub>  
K<sub>i</sub> = 0.72 ± 0.06

17 X = N  
K<sub>i</sub> = 0.86 ± 0.19

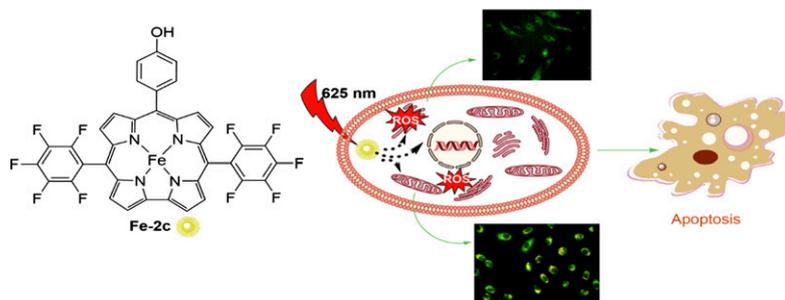
Bioorganic Chemistry 90 (2019) 103092

### DNA interaction and photodynamic antitumor activity of transition metal mono-hydroxyl corrole

Yan-Mei Sun<sup>a</sup>, Waseem Akram<sup>a</sup>, Fan Cheng<sup>a</sup>, Ze-Yu Liu<sup>a</sup>,  
Yu-Hui Liao<sup>b</sup>, Yong Ye<sup>a</sup>, Hai-Yang Liu<sup>a</sup>

<sup>a</sup>School of Chemistry and Chemical Engineering, Key Laboratory of  
Functional Molecular Engineering of Guangdong Province, South  
China University of Technology, Guangzhou 510641, China

<sup>b</sup>Molecular Diagnosis and Treatment Center for Infectious Diseases,  
Dermatology Hospital, Southern Medical University, Guangzhou  
510091, China



Bioorganic Chemistry 90 (2019) 103085

### The green synthesis and molecular docking of novel N-substituted rhodanines as effective inhibitors for carbonic anhydrase and acetylcholinesterase enzymes

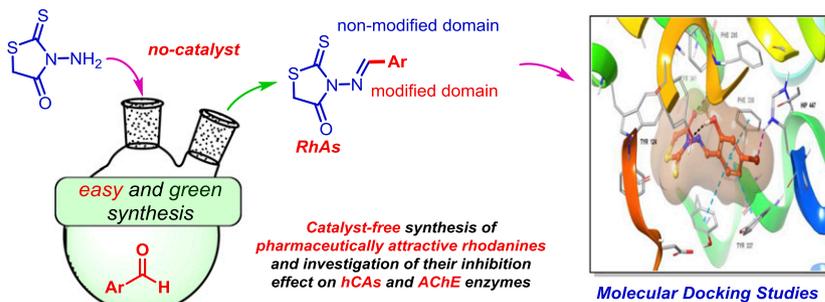
Sinan Bayindir<sup>a</sup>, Cuneyt Caglayan<sup>b</sup>,  
Muhammet Karaman<sup>c</sup>, İlhami Gülcin<sup>d</sup>

<sup>a</sup>Department of Chemistry, Faculty of Sciences and Arts, Bingöl  
University, 12000-Bingöl, Turkey

<sup>b</sup>Department of Biochemistry, Faculty of Veterinary Medicine,  
Bingöl University, 12000-Bingöl, Turkey

<sup>c</sup>Department of Molecular Biology and Genetics, Faculty of Arts  
and Science, Kilis 7 Aralık University, 79000-Kilis, Turkey

<sup>d</sup>Department of Chemistry, Faculty of Sciences, Atatürk  
University, 25240-Erzurum, Turkey



Bioorganic Chemistry 90 (2019) 103096

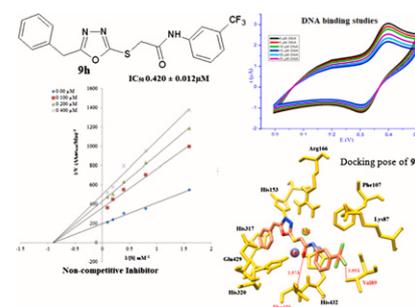
### Substituted phenyl [(5-benzyl-1,3,4-oxadiazol-2-yl)sulfanyl] acetates/acetamides as alkaline phosphatase inhibitors: Synthesis, computational studies, enzyme inhibitory kinetics and DNA binding studies

Zafar Iqbal<sup>a</sup>, Zaman Ashraf<sup>a</sup>, Mubashir Hassan<sup>b</sup>, Qamar Abbas<sup>c</sup>, Erum Jabeen<sup>a</sup>

<sup>a</sup>Department of Chemistry, Allama Iqbal Open University, Islamabad 44000, Pakistan

<sup>b</sup>Institute of Molecular Biology and Biotechnology, The University of Lahore, Pakistan

<sup>c</sup>Department of Physiology, University of Sindh, Jamshoro, Pakistan

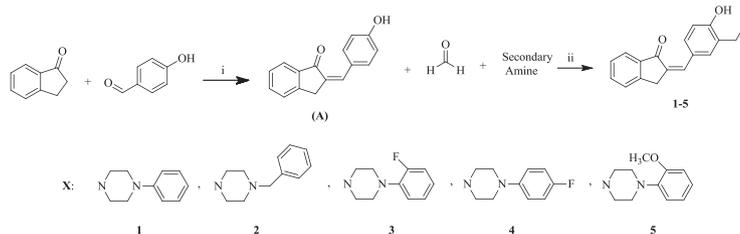


Bioorganic Chemistry 90 (2019) 103108

### Synthesis and biological evaluation of some new mono Mannich bases with piperazines as possible anticancer agents and carbonic anhydrase inhibitors

Bioorganic Chemistry 90 (2019) 103095

Mehtap Tugrak<sup>a</sup>, Halise Inci Gul<sup>a</sup>, Kenjiro Bandow<sup>b</sup>, Hiroshi Sakagami<sup>c</sup>, Ilhami Gulcin<sup>d</sup>, Yusuf Ozkay<sup>e</sup>, Claudiu T. Supuran<sup>f</sup>



<sup>a</sup>Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Ataturk University, Erzurum, Turkey

<sup>b</sup>Division of Biochemistry, Meikai University School of Dentistry, Sakado, Saitama, Japan

<sup>c</sup>Meikai University Research Institute of Odontology (M-RIO), Meikai University School of Dentistry, Sakado, Saitama, Japan

<sup>d</sup>Faculty of Science, Department of Chemistry, Ataturk University, Erzurum, Turkey

<sup>e</sup>Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Anadolu University, Eskişehir, Turkey

<sup>f</sup>Neurofarba Department, Sezione di Scienza Farmaceutica e Nutraceutica, Università degli Studi di Firenze, Via U. Schiff 6, 50019 Sesto Fiorentino (Florence), Italy

### Triazole substituted metal-free, metallo-phthalocyanines and their water soluble derivatives as potential cholinesterases inhibitors: Design, synthesis and *in vitro* inhibition study

Bioorganic Chemistry 90 (2019) 103100

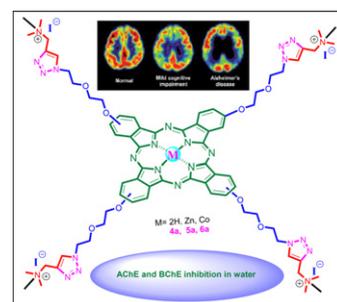
Tayfun Arslan<sup>a,b</sup>, Nezaket Çakır<sup>a</sup>, Turgut Keleş<sup>c</sup>, Zekeriya Biyiklioglu<sup>c</sup>, Murat Senturk<sup>d</sup>

<sup>a</sup>Giresun University, Faculty of Science, Department of Chemistry, 28200 Giresun, Turkey

<sup>b</sup>Giresun University, Technical Sciences Vocational School, Department of Textile, Giresun University, 28049 Giresun, Turkey

<sup>c</sup>Karadeniz Technical University, Faculty of Science, Department of Chemistry, 61080 Trabzon, Turkey

<sup>d</sup>Agri Ibrahim Cecen University, Faculty of Pharmacy, Department of Basic Sciences of Pharmacy, 04100 Agri, Turkey



### Synthesis, biological evaluation and *in silico* studies with 4-benzylidene-2-phenyl-5(4H)-imidazolone-based benzenesulfonamides as novel selective carbonic anhydrase IX inhibitors endowed with anticancer activity

Bioorganic Chemistry 90 (2019) 103102

Wagdy M. Eldehna<sup>a</sup>, Mohamed A. Abdelrahman<sup>b</sup>, Alessio Nocentini<sup>c,d</sup>, Silvia Bua<sup>c</sup>, Sara T. Al-Rashood<sup>e</sup>, Ghada S. Hassan<sup>f</sup>, Alessandro Bonardi<sup>c,d</sup>, Abdulrahman A. Almehizia<sup>e</sup>, Hamad M. Alkahtani<sup>e</sup>, Amal Alharbi<sup>e</sup>, Paola Gratteri<sup>d</sup>, Claudiu T. Supuran<sup>c</sup>

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

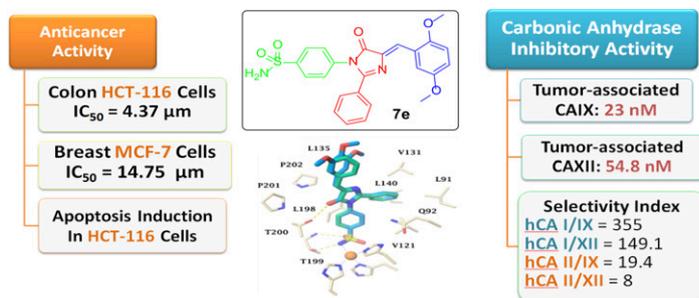
<sup>b</sup>Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Egyptian Russian University, Badr City, Cairo 11829, Egypt

<sup>c</sup>Department of NEUROFARBA, Section of Pharmaceutical and Nutraceutical Sciences, University of Florence, Polo Scientifico, Via U. Schiff 6, 50019, Sesto Fiorentino, Firenze, Italy

<sup>d</sup>Department of NEUROFARBA, Section of Pharmaceutical and Nutraceutical Sciences, Laboratory of Molecular Modeling Cheminformatics & QSAR, University of Florence, Polo Scientifico, Via U. Schiff 6, 50019, Sesto Fiorentino, Firenze, Italy

<sup>e</sup>Department of Pharmaceutical Chemistry, College of Pharmacy, King Saud University, P.O. Box 2457, Riyadh 11451, Saudi Arabia

<sup>f</sup>Department of Medicinal Chemistry, Faculty of Pharmacy, Mansoura University, Mansoura 35516, Egypt

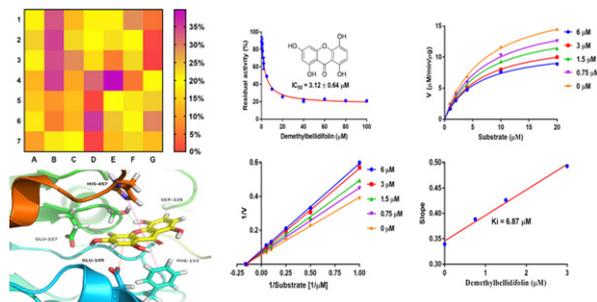


### Demethylbellidifolin isolated from *Swertia bimaculata* against human carboxylesterase 2: Kinetics and interaction mechanism merged with docking simulations

Tian-Tian Liu<sup>a</sup>, Xiao-Kui Huo<sup>a</sup>, Xiang-Ge Tian<sup>a</sup>, Jia-Hao Liang<sup>a</sup>, Jing Yi<sup>a</sup>, Xin-Yue Zhang<sup>a</sup>, Song Zhang<sup>a</sup>, Lei Feng<sup>a</sup>, Jing Ning<sup>a</sup>, Bao-Jing Zhang<sup>a</sup>, Cheng-Peng Sun<sup>a</sup>, Xiao-Chi Ma<sup>a,b</sup>

<sup>a</sup>College of Pharmacy, College (Institute) of Integrative Medicine, The National & Local Joint Engineering Research Center for Drug Development of Neurodegenerative Disease, Dalian Medical University, Dalian, China

<sup>b</sup>Jiangsu Key Laboratory of New Drug Research and Clinical Pharmacy, Xuzhou Medical University, Xuzhou, China



Bioorganic Chemistry 90 (2019) 103101

### Synthesis and anticancer activity of bis-benzo [d] [1,3] dioxol-5-yl thiourea derivatives with molecular docking study

Reem A.K. Al-Harbi<sup>a</sup>, Marwa A.M.Sh. El-Sharief<sup>b,c</sup>, Samir Y. Abbas<sup>d</sup>

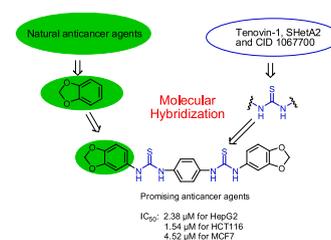
<sup>a</sup>Department of Chemistry, Faculty of Science, Taibah University, Almadinah Almunawarrah, Saudi Arabia

<sup>b</sup>Applied Organic Chemistry Department, National Research Centre, Cairo, Egypt

<sup>c</sup>Faculty of Science and Arts, Mohail Asser, King Khalid University, Saudi Arabia

<sup>d</sup>Organometallic and Organometalloid Chemistry Department, National Research Centre, Cairo, Egypt

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## REVIEW ARTICLES

### Potential chemical transformation of phosphinic acid derivatives and their applications in the synthesis of drugs

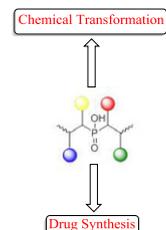
Moaz M. Abdou<sup>a,b</sup>, Rasha A. El-Saeed<sup>c</sup>

<sup>a</sup>Egyptian Petroleum Research Institute, Nasr City, P.O. 11727, Cairo, Egypt

<sup>b</sup>Department of Chemistry, University of Liverpool, Liverpool L69 7ZD, UK

<sup>c</sup>Department of Chemistry, Faculty of Science, Mansoura University, ET-35516 Mansoura, Egypt

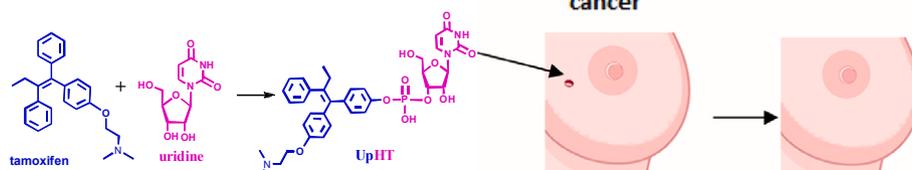
Bioorganic Chemistry 90 (2019) 103039



### The stilbene derivatives, nucleosides, and nucleosides modified by stilbene derivatives

Hanna Krawczyk

Department of Organic Chemistry, Faculty of Chemistry, Warsaw University of Technology, Noakowskiego 3, 00-664 Warsaw, Poland



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## PRELIMINARY COMMUNICATIONS

### Synthesis and antitumor activity of three novel ginsenoside M1 derivatives with 3'-ester modifications

Ke-Ke Li<sup>a</sup>, Xiao-Mei Yan<sup>b</sup>, Zheng-Ning Li<sup>c</sup>, Qiu Yan<sup>d</sup>, Xiao-Jie Gong<sup>a</sup>

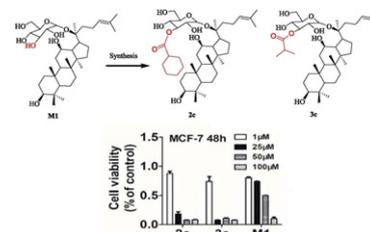
<sup>a</sup>College of Life Science, Dalian Minzu University, Dalian 116600, China

<sup>b</sup>College of Laboratory Medicine, Dalian Medical University, Dalian 116044, China

<sup>c</sup>College of Environmental and Chemical Engineering, Dalian University, Dalian 116622, China

<sup>d</sup>College of Basic Medical Sciences, Dalian Medical University, Dalian 116044, China

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### Synthesis and biological evaluation of indoloquinoline alkaloid cryptolepine and its bromo-derivative as dual cholinesterase inhibitors

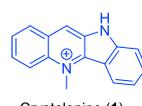
Vijay K. Nuthakki<sup>a</sup>, Ramesh Mudududdla<sup>a,b</sup>, Ankita Sharma<sup>b,c</sup>, Ajay Kumar<sup>b,c</sup>, Sandip B. Bharate<sup>a,b</sup>

<sup>a</sup>Medicinal Chemistry Division, CSIR-Indian Institute of Integrative Medicine, Canal Road, Jammu 180001, India

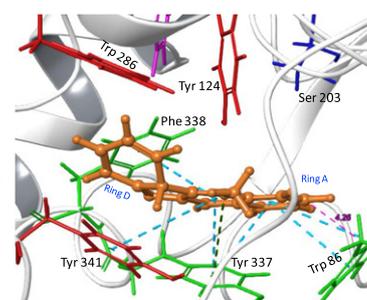
<sup>b</sup>Academy of Scientific & Innovative Research, CSIR-Indian Institute of Integrative Medicine, Canal Road, Jammu 180001, India

<sup>c</sup>PKPD Toxicology & Formulation Division, CSIR-Indian Institute of Integrative Medicine, Canal Road, Jammu 180001, India

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$IC_{50}$  ( $\mu M$ )  
 EeAChE: 0.27 ( $k_i = 0.34 \mu M$ )  
 rHuAChE: 0.48 ( $k_i = 0.88 \mu M$ )  
 eqBChE: 0.70 ( $k_i = 0.51 \mu M$ )  
 P-gp induction at 0.1  $\mu M$   
 BACE-1 inhibition at 100  $\mu M$   
 LS-180:  $GI_{50} > 12.5 \mu M$   
 SH-SY5Y:  $GI_{50} > 5 \mu M$



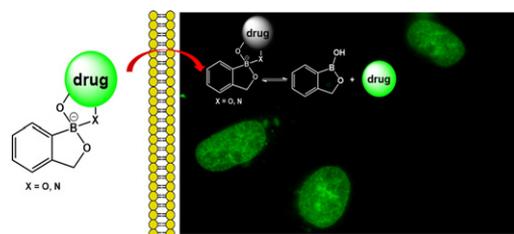
### Benzoxaboroles as dynamic covalent receptors for bioconjugation and transport of nucleosides and related drugs: Proof of action in HeLa cells

Cecilia Samaniego Lopez<sup>a</sup>, Jimena H. Martínez<sup>b</sup>, Sofía L. Acebedo<sup>a</sup>, Carla C. Spagnuolo<sup>a</sup>

<sup>a</sup>Departamento de Química Orgánica, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, CIHIDECAR-CONICET-UBA, Int. Güiraldes 2160, 3er piso, Ciudad Autónoma de Buenos Aires CC1428EHA, Argentina

<sup>b</sup>Departamento de Química Biológica, IQUIBICEN, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Int. Güiraldes 2160, 4to piso, Ciudad Autónoma de Buenos Aires CC1428EHA, Argentina

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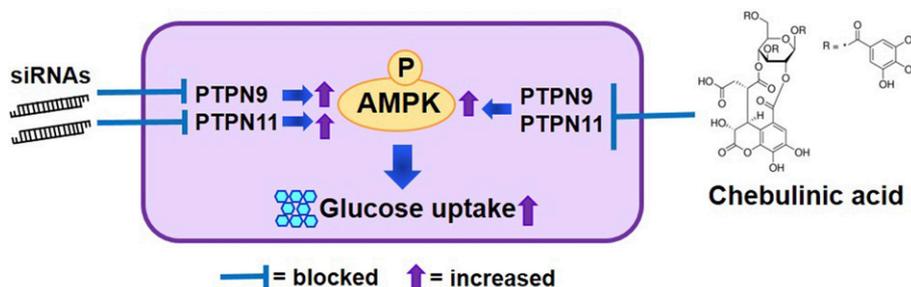
### Identification of chebulinic acid as a dual targeting inhibitor of protein tyrosine phosphatases relevant to insulin resistance

Sun-Young Yoon<sup>a</sup>, Hyo Jin Kang<sup>b</sup>, Dohee Ahn<sup>a</sup>, Ji Young Hwang<sup>a</sup>, Se Jeong Kwon<sup>a</sup>, Sang J. Chung<sup>a</sup>

<sup>a</sup>School of Pharmacy, Sungkyunkwan University, Suwon 16419, Republic of Korea

<sup>b</sup>Department of Chemistry, Dongguk University, Seoul 100-715, Republic of Korea

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**(±)-Meliviticines A and B:  
Rearranged prenylated  
acetophenone derivatives from  
*Melicope viticina* and their  
antimicrobial activity**

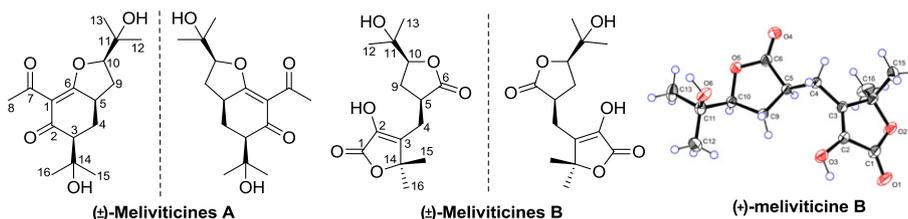
Wei Li<sup>a,b</sup>, Li Rao<sup>a</sup>, Yu Liu<sup>a</sup>, Qian He<sup>a</sup>, Yue Fan<sup>a</sup>,  
Yun-Xia You<sup>a</sup>, Yu Su<sup>a</sup>, Feng Hu<sup>a</sup>, You-Kai Xu<sup>c</sup>,  
Bin Lin<sup>d</sup>, Sheng Yin<sup>b</sup>, Chuan-Rui Zhang<sup>a</sup>

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<sup>c</sup>Key Laboratory of Tropical Plant Resource and  
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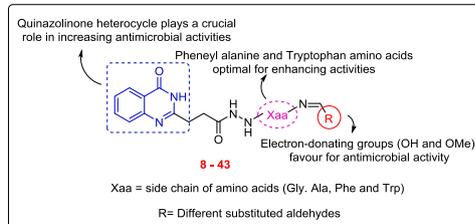
*Bioorganic Chemistry* 90 (2019) 103099

**Amino acids conjugated quinazolinone-Schiff's bases as potential antimicrobial agents: Synthesis, SAR and molecular docking studies**

K.P. Rakesh<sup>a</sup>, H.K. Kumara<sup>b</sup>, B.J. Ullas<sup>a</sup>, J. Shivakumara<sup>a</sup>, D. Channe Gowda<sup>a</sup>

<sup>a</sup>Department of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, Karnataka, India

<sup>b</sup>Department of Chemistry, KLE Society's Jagadguru Tontadarya College, Gadag-582101, Karnataka, India



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**SPECIAL ISSUE ON BIOCATALYSIS**

**Preface**

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