



## Graphical Abstracts/Bioorganic Chemistry 85 (2019) ii–xvii

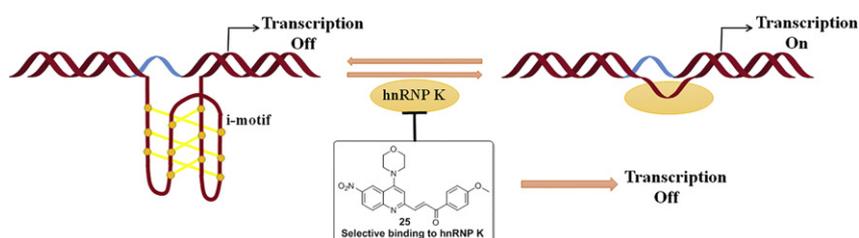
## REGULAR ARTICLES

### Syntheses and evaluation of new Quinoline derivatives for inhibition of hnRNP K in regulating oncogene *c-myc* transcription

Bing Shu<sup>a,b</sup>, Ping Zeng<sup>a</sup>, Shuangshuang Kang<sup>a</sup>, Peng-Hui Li<sup>a</sup>, Dexuan Hu<sup>a</sup>, Guotao Kuang<sup>a</sup>, Jiaojiao Cao<sup>a</sup>, Xiaoya Li<sup>a</sup>, Meiling Zhang<sup>a</sup>, Lin-Kun An<sup>a</sup>, Zhi-Shu Huang<sup>a</sup>, Ding Li<sup>a,\*</sup>

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Bioorganic Chemistry 85 (2019) pp. 1–17

### Ursolic and oleanolic acid derivatives with cholinesterase inhibiting potential

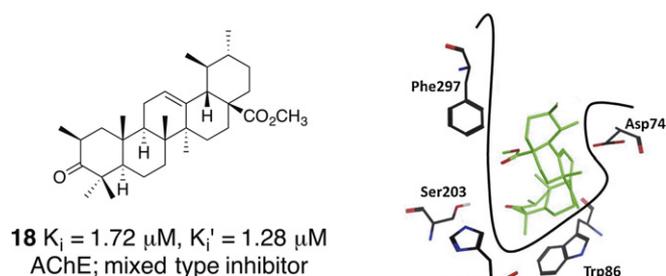
Anne Loesche<sup>a</sup>, Alexander Köwitsch<sup>a</sup>, Susana D. Lucas<sup>b</sup>, Zayan Al-Halabi<sup>c</sup>, Wolfgang Sippl<sup>c</sup>, Ahmed Al-Harrasi<sup>d</sup>, René Csuk<sup>a,\*</sup>

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<sup>b</sup>Universidade de Lisboa, Faculdade de Farmácia, Instituto de Investigação do Medicamento (iMed.U.Lisboa), Av. Prof. Gama Pinto, 1649-003 Lisboa, Portugal

<sup>c</sup>Martin-Luther-University Halle-Wittenberg, Institute of Pharmacy, Wolfgang-Langenbeck-Str. 4, D-06120 Halle (Saale), Germany

<sup>d</sup>University of Nizwa, Chair of Oman's Medicinal Plants and Marine Natural Products, PO Box 33, Birkat Al-Mauz, Nizwa, Oman



Bioorganic Chemistry 85 (2019) pp. 23–32

### Synthesis of benzothiazole derivatives as a potent $\alpha$ -glucosidase inhibitor

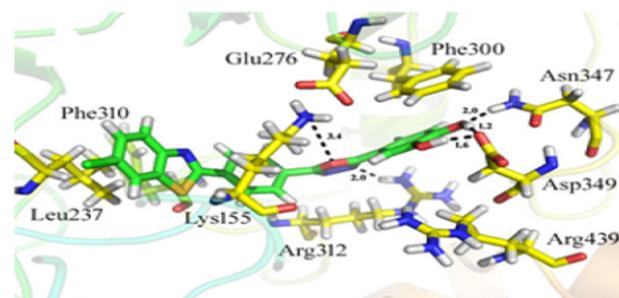
Mohammed Gollapalli<sup>a</sup>, Muhammad Taha<sup>b,\*</sup>, Muhammad Tariq Javid<sup>c</sup>, Noor Barak Almandil<sup>b</sup>, Fazal Rahim<sup>c</sup>, Abdul Wadood<sup>d</sup>, Ashik Mosaddik<sup>b</sup>, Mohamed Ibrahim<sup>b</sup>, Mohammed A. Alqahtani<sup>a</sup>, Yasser A. Bamarouf<sup>f</sup>

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<sup>b</sup>Department of Clinical Pharmacy, Institute for Research and Medical Consultations (IRMC), Imam Abdulrahman Bin Faisal University, P.O. Box 1982, Dammam 31441, Saudi Arabia

<sup>c</sup>Department of Chemistry, Hazara University, Mansehra-21300, Khyber Pakhtunkhwa, Pakistan

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



Bioorganic Chemistry 85 (2019) pp. 33–48

### Synthesis, molecular properties prediction and biological evaluation of indole-vinyl sulfone derivatives as novel tubulin polymerization inhibitors targeting the colchicine binding site

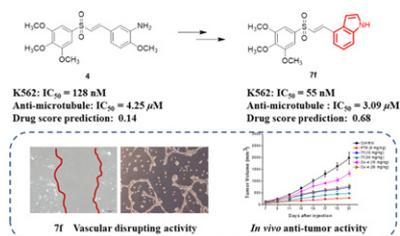
Wenlong Li<sup>a</sup>, Honghao Sun<sup>a</sup>, Feijie Xu<sup>a</sup>, Wen Shuai<sup>a</sup>, Jie Liu<sup>a</sup>, Shengtao Xu<sup>a,\*</sup>, Hequan Yao<sup>a</sup>, Cong Ma<sup>b</sup>, Zheyang Zhu<sup>c,\*</sup>, Jinyi Xu<sup>a,\*</sup>

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<sup>b</sup>State Key Laboratory of Chemical Biology and Drug Discovery, and Department of Applied Biology and Chemical Technology, The Hong Kong Polytechnic University, Kowloon, Hong Kong

<sup>c</sup>Division of Molecular Therapeutics & Formulation, School of Pharmacy, The University of Nottingham, University Park Campus, Nottingham NG7 2RD, UK

Bioorganic Chemistry 85 (2019) pp. 49–59

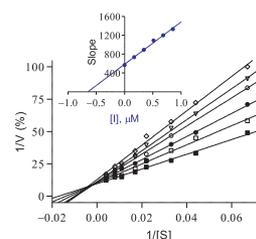
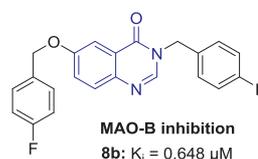


### The monoamine oxidase inhibition properties of C6-mono- and N3/C6-disubstituted derivatives of 4(3H)-quinazolinone

Malikotsi A. Qhobosheane<sup>a</sup>, Lesetja J. Legoabe<sup>a,\*</sup>, Anél Petzer<sup>a,b</sup>, Jacobus P. Petzer<sup>a,b</sup>

<sup>a</sup>Centre of Excellence for Pharmaceutical Sciences, North-West University, Private Bag X6001, Potchefstroom 2520, South Africa

<sup>b</sup>Pharmaceutical Chemistry, School of Pharmacy, North-West University, Private Bag X6001, Potchefstroom 2520, South Africa



Bioorganic Chemistry 85 (2019) pp. 60–65

### Synthesis and biological activity of a potent optically pure autoinducer-2 quorum sensing agonist

Osvaldo S. Ascenso<sup>a,1</sup>, Inês M. Torcato<sup>a,b,1</sup>, Ana Sofia Miguel<sup>a</sup>, João C. Marques<sup>c</sup>, Karina B. Xavier<sup>b</sup>, M. Rita Ventura<sup>a,\*</sup>, Christopher D. Maycock<sup>a,d,\*</sup>

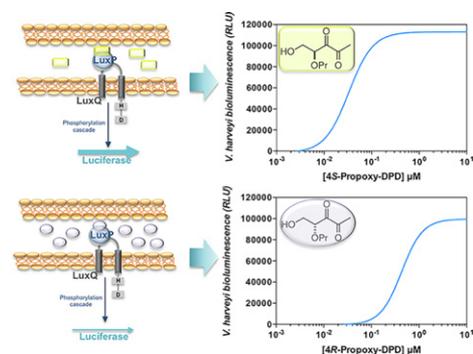
<sup>a</sup>Instituto de Tecnologia Química e Biológica, Universidade Nova de Lisboa, Apartado 127, 2780-901 Oeiras, Portugal

<sup>b</sup>Instituto Gulbenkian de Ciência, 2781-901 Oeiras, Portugal

<sup>c</sup>Rowland Institute at Harvard, 100 Edwin H. Land Boulevard, Cambridge, MA 02142, USA<sup>2</sup>

<sup>d</sup>Faculdade de Ciências da Universidade de Lisboa, Departamento de Química e Bioquímica, 1749-016 Lisboa, Portugal

Bioorganic Chemistry 85 (2019) pp. 75–81



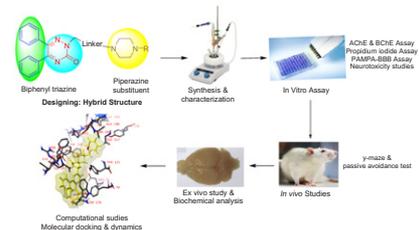
### Biphenyl-3-oxo-1,2,4-triazine linked piperazine derivatives as potential cholinesterase inhibitors with anti-oxidant property to improve the learning and memory

Prabhash Nath Tripathi<sup>a</sup>, Pavan Srivastava<sup>a</sup>, Piyoosh Sharma<sup>a</sup>, Manish Kumar Tripathi<sup>a</sup>, Ankit Seth<sup>a</sup>, Avanish Tripathi<sup>a</sup>, Sachchida Nand Rai<sup>b</sup>, Surya Pratap Singh<sup>b</sup>, Sushant K. Shrivastava<sup>a,\*</sup>

<sup>a</sup>Pharmaceutical Chemistry Research Laboratory, Department of Pharmaceutical Engineering & Technology, Indian Institute of Technology (Banaras Hindu University), Varanasi 221 005 India

<sup>b</sup>Department of Biochemistry, Institute of Science, Banaras Hindu University, Varanasi 221005, India

Bioorganic Chemistry 85 (2019) pp. 82–96



### ***In vitro* and *in silico* evaluation of new thiazole compounds as monoamine oxidase inhibitors**

*Bioorganic Chemistry 85 (2019) pp. 97–108*

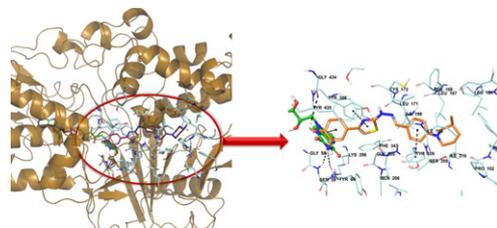
Begüm Nurpelin Sağlık<sup>a,b,\*</sup>, Betül Kaya Çavuşoğlu<sup>a</sup>, Derya Osmaniye<sup>a,b</sup>, Serkan Levent<sup>a,b</sup>, Ulviye Acar Çevik<sup>a,b</sup>, Sinem Ilgin<sup>c</sup>, Yusuf Özkay<sup>a,b</sup>, Zafer Asım Kaplancıklı<sup>a</sup>, Yusuf Öztürk<sup>d</sup>

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

<sup>b</sup>Doping and Narcotic Compounds Analysis Laboratory, Faculty of Pharmacy, Anadolu University, Eskişehir, Turkey

<sup>c</sup>Department of Pharmaceutical Toxicology, Faculty of Pharmacy, Anadolu University, Eskişehir, Turkey

<sup>d</sup>Department of Pharmacology, Faculty of Pharmacy, Anadolu University, Eskişehir, Turkey



### **Synthesis of novel quinoline-based thiadiazole, evaluation of their antileishmanial potential and molecular docking studies**

*Bioorganic Chemistry 85 (2019) pp. 109–116*

Noor Barak Almandil<sup>a</sup>, Muhammad Taha<sup>a,\*</sup>, Fazal Rahim<sup>b</sup>, Abdul Wadood<sup>c</sup>, Syahrul Imran<sup>d</sup>, Mohammed A. Alqahtani<sup>e</sup>, Yasser A. Bamarouf<sup>e</sup>, Mohamed Ibrahim<sup>a</sup>, Ashik Mosaddik<sup>a</sup>, Mohammed Gollapalli<sup>e</sup>

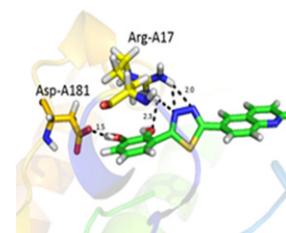
<sup>a</sup>Department of Clinical Pharmacy, Institute for Research and Medical Consultations (IRMC), Imam Abdulrahman Bin Faisal University, P.O. Box 1982, Dammam 31441, Saudi Arabia

<sup>b</sup>Department of Chemistry, Hazara University, Mansehra 21300, Pakistan

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

<sup>d</sup>Atta-ur-Rahman Institute for Natural Product Discovery, Universiti Teknologi MARA (UiTM), Puncak Alam Campus, 42300 Bandar Puncak Alam, Selangor D.E., Malaysia

<sup>e</sup>College of Computer Science & Information Technology (CCSIT), Imam Abdulrahman Bin Faisal University, P.O. Box 1982, Dammam 31441, Saudi Arabia



### **Expansion of the scaffold diversity for the development of highly selective butyrylcholinesterase (BChE) inhibitors: Discovery of new hits through the pharmacophore model generation, virtual screening and molecular dynamics simulation**

*Bioorganic Chemistry 85 (2019) pp. 117–127*

Xin Lu<sup>a</sup>, Hongyu Yang<sup>a</sup>, Qihang Li<sup>a</sup>, Yao Chen<sup>b</sup>, Qi Li<sup>a</sup>, You Zhou<sup>c</sup>, Feng Feng<sup>d</sup>, Wenyuan Liu<sup>e</sup>, Qinglong Guo<sup>f</sup>, Haopeng Sun<sup>a,\*</sup>

<sup>a</sup>Department of Medicinal Chemistry, China Pharmaceutical University, Nanjing 211198, People's Republic of China

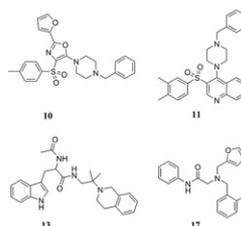
<sup>b</sup>School of Pharmacy, Nanjing University of Chinese Medicine, Nanjing 210023, People's Republic of China

<sup>c</sup>College of Biotechnology, Southwest University, Chongqing 400715, People's Republic of China

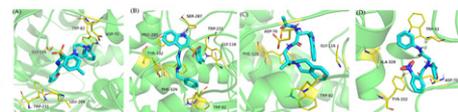
<sup>d</sup>Department of Natural Medicinal Chemistry, China Pharmaceutical University, Nanjing 211198, People's Republic of China

<sup>e</sup>Department of Analytical Chemistry, China Pharmaceutical University, Nanjing 210009, People's Republic of China

<sup>f</sup>State Key Laboratory of Natural Medicines, Jiangsu Key Laboratory of Carcinogenesis and Intervention, School of Basic Medicine and Clinical Pharmacy, China Pharmaceutical University, Nanjing 210009, People's Republic of China



Compound	ACHE IR (%) at 10µM	BChE IC <sub>50</sub> (µM)	
		cy BChE	hu BChE
<b>10</b>	18.7 ± 0.7	2.2 ± 0.2	7.5 ± 5.0
<b>11</b>	22.5 ± 1.7	0.7 ± 0.2	1.3 ± 0.6
<b>13</b>	11.8 ± 0.2	0.7 ± 0.2	1.4 ± 1.9
<b>17</b>	9.3 ± 0.4	1.3 ± 0.3	1.7 ± 2.7



### The first synthesis, carbonic anhydrase inhibition and anticholinergic activities of some bromophenol derivatives with S including natural products

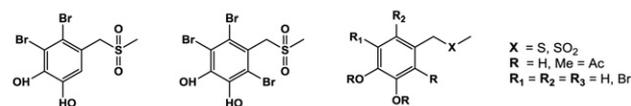
Bioorganic Chemistry 85 (2019) pp. 128–139

Cetin Bayrak<sup>a,b</sup>, Parham Taslimi<sup>a</sup>, Halide Sedef Karaman<sup>a</sup>, İlhami Gulcin<sup>a</sup>, Abdullah Menzek<sup>a,\*</sup>

<sup>a</sup>Department of Chemistry, Faculty of Science, Ataturk University, 25240-Erzurum, Turkey  
<sup>b</sup>Dogubayazit Ahmed-i Hani Vocational School, Agri Ibrahim Cecen University, 04400-Agri, Turkey

### The first synthesis, carbonic anhydrase inhibition and anticholinergic activities of some bromophenol derivatives with S including natural products

Cetin Bayrak, Parham Taslimi, Halide Sedef Karamana, İlhami Gulcin, Abdullah Menzek



### 3, 9-di-O-substituted coumestrols incorporating basic amine side chains act as novel apoptosis inducers with improved pharmacological selectivity

Bioorganic Chemistry 85 (2019) pp. 140–151

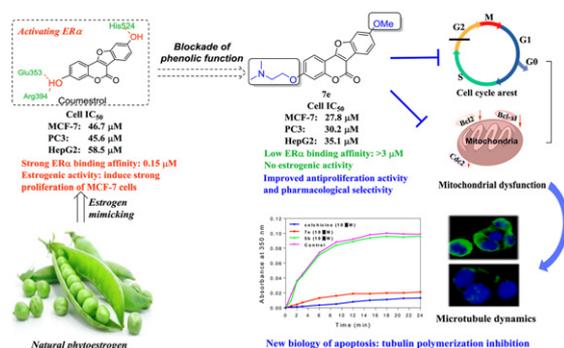
Guoshun Luo<sup>a,b,1</sup>, Zhengpu Tang<sup>a,b,1</sup>, Xinyu Li<sup>a,b</sup>, Qiangqiang Hou<sup>a,b</sup>, Yu Chen<sup>b,c</sup>, Kejing Lao<sup>d</sup>, Hua Xiang<sup>a,b,\*</sup>

<sup>a</sup>State Key Laboratory of Natural Medicines, Jiangsu Key Laboratory of Drug Design and Optimization, China Pharmaceutical University, Nanjing 210009, China

<sup>b</sup>Department of Medicinal Chemistry, School of Pharmacy, China Pharmaceutical University, Nanjing 210009, China

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<sup>d</sup>Shaanxi Key Laboratory of Brain Disorders and Institute of Basic and Translational Medicine, Xi'an Medical University, Xi'an, Shaanxi 710021, China



### Cloning, overexpression and characterization of a thermostable β-xylosidase from *Thermotoga petrophila* and cooperated transformation of ginsenoside extract to ginsenoside 20(S)-Rg3 with a β-glucosidase

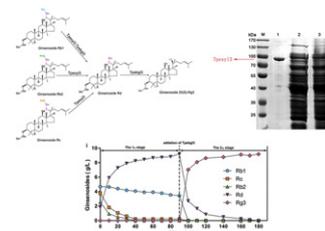
Bioorganic Chemistry 85 (2019) pp. 159–167

Shanshan Zhang<sup>a,b</sup>, Jingcong Xie<sup>a,b</sup>, Linguo Zhao<sup>a,b,\*</sup>, Jianjun Pei<sup>a,b</sup>, Erzhen Su<sup>a,b</sup>, Wei Xiao<sup>c,\*</sup>, Zhenzhong Wang<sup>c</sup>

<sup>a</sup>Co-Innovation Center for Sustainable Forestry in Southern China, Nanjing Forestry University, 159 Long Pan Road, Nanjing 210037, China

<sup>b</sup>College of Chemical Engineering, Nanjing Forestry University, 159 Long Pan Road, Nanjing 210037, China

<sup>c</sup>Jiangsu Kanion Pharmaceutical Co., Ltd., 58 Haichang South Road, Lianyungang 222001, China



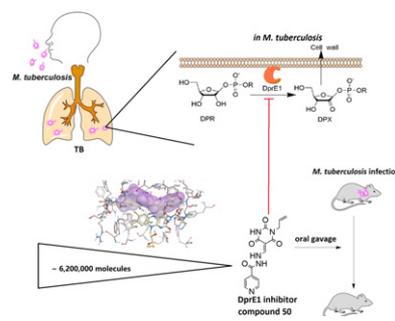
### Identification of a pyrimidinetrione derivative as the potent DprE1 inhibitor by structure-based virtual ligand screening

Bioorganic Chemistry 85 (2019) pp. 168–178

Ya Gao<sup>a</sup>, Jinshan Xie<sup>a</sup>, Ruotian Tang<sup>a</sup>, Kaiyin Yang<sup>a</sup>, Yahan Zhang<sup>a</sup>, Lixia Chen<sup>b,\*</sup>, Hua Li<sup>a,b,\*</sup>

<sup>a</sup>Hubei Key Laboratory of Natural Medicinal Chemistry and Resource Evaluation, School of Pharmacy, Tongji Medical College, Huazhong University of Science and Technology, Wuhan 430030, China

<sup>b</sup>Wuya College of Innovation, School of Traditional Chinese Materia Medica, Key Laboratory of Structure-Based Drug Design & Discovery, Ministry of Education, Shenyang Pharmaceutical University, Shenyang 110016, China



### Mitochondria-targeted triphenylphosphonium conjugated glycyrrhetic acid derivatives as potent anticancer drugs

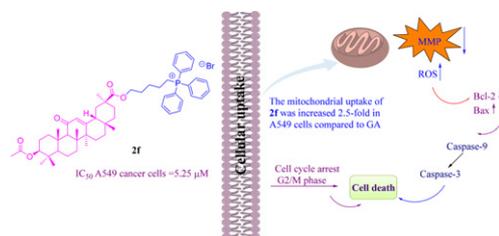
Bioorganic Chemistry 85 (2019) pp. 179–190

Le Jin<sup>a,1</sup>, Lumei Dai<sup>b,1</sup>, Min Ji<sup>a,\*</sup>, Hengshan Wang<sup>c,\*</sup>

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<sup>b</sup>Key Laboratory of Tropical Marine Bio-resources and Ecology, South China Sea Institute of Oceanology, Chinese Academy of Sciences, Guangzhou 510301, China

<sup>c</sup>State Key Laboratory for the Chemistry and Molecular Engineering of Medicinal Resources, School of Chemistry and Pharmaceutical Sciences of Guangxi Normal University, Guilin 541004, China



### Synthesis and biological evaluation of novel tris-chalcones as potent carbonic anhydrase, acetylcholinesterase, butyrylcholinesterase and $\alpha$ -glycosidase inhibitors

Bioorganic Chemistry 85 (2019) pp. 191–197

Serdar Burmaoglu<sup>a,b,\*</sup>, Ali Osman Yilmaz<sup>b</sup>, M. Fatih Polat<sup>c</sup>, Rüya Kaya<sup>d</sup>, İlhami Gulcin<sup>b</sup>, Oztekin Algul<sup>e,\*</sup>

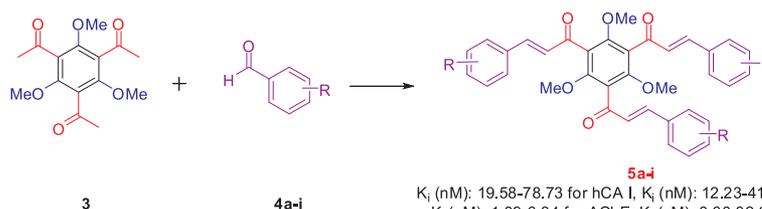
<sup>a</sup>Tercan Vocational High School, Erzincan Binali Yildirim University, Erzincan 24800, Turkey

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

<sup>c</sup>Department of Pharmaceutical Basic Sciences, Faculty of Pharmacy, Erzincan Binali Yildirim University, Erzincan 24100, Turkey

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

<sup>e</sup>Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Mersin University, Mersin 33169, Turkey



**5a-i**  
 $K_i$  (nM): 19.58-78.73 for hCA I,  $K_i$  (nM): 12.23-41.70 for hCA II,  
 $K_i$  (nM): 1.09-6.84 for AChE,  $K_i$  (nM): 8.30-32.30 for BChE,  
 $K_i$  (nM): 0.93±0.20-18.53±5.06 for  $\alpha$ -GLY

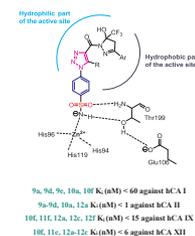
### Synthesis of novel benzenesulfonamide bearing 1,2,3-triazole linked hydroxy-trifluoromethylpyrazolines and hydrazones as selective carbonic anhydrase isoforms IX and XII inhibitors

Bioorganic Chemistry 85 (2019) pp. 198–208

Vikas Sharma<sup>a</sup>, Rajiv Kumar<sup>a</sup>, Silvia Bua<sup>b</sup>, Claudiu T. Supuran<sup>b,\*</sup>, Pawan K. Sharma<sup>a,\*</sup>

<sup>a</sup>Department of Chemistry, Kurukshetra University, Kurukshetra 136119, India

<sup>b</sup>Università degli Studi di Firenze, Laboratorio di Chimica Bioinorganica, Rm 188, and Neurofarba Department, Sezione di Scienze Farmaceutiche, Via U. Schiff 6, I-50019 Sesto Fiorentino, Firenze, Italy



### Identification of 1,2,4-triazoles as new thymidine phosphorylase inhibitors: Future anti-tumor drugs

Bioorganic Chemistry 85 (2019) pp. 209–220

Sohail Anjum Shahzad<sup>a,\*</sup>, Muhammad Yar<sup>b,\*</sup>, Zulfiqar Ali Khan<sup>c</sup>, Lubna Shahzadi<sup>b</sup>, Syed Ali Raza Naqvi<sup>c</sup>, Adeem Mahmood<sup>d</sup>, Sami Ullah<sup>a</sup>, Ahson Jabbar Shaikh<sup>a</sup>, Tauqir Ali Sherazi<sup>a</sup>, Adebayo Tajudeen Bale<sup>a</sup>, Jędrzej Kukulowicz<sup>e</sup>, Marek Bajda<sup>e</sup>

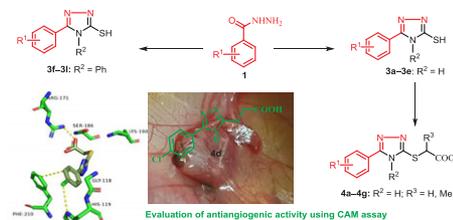
<sup>a</sup>Department of Chemistry, COMSATS University Islamabad, Abbottabad Campus, Abbottabad 22060, Pakistan

<sup>b</sup>Interdisciplinary Research Center in Biomedical Materials, COMSATS University Islamabad, Lahore Campus, Lahore 54000, Pakistan

<sup>c</sup>Department of Chemistry, Government College University, Faisalabad 38000, Pakistan

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

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



### Docking- and pharmacophore-based virtual screening for the identification of novel *Mycobacterium tuberculosis* protein tyrosine phosphatase B (MtpB) inhibitor with a thiobarbiturate scaffold

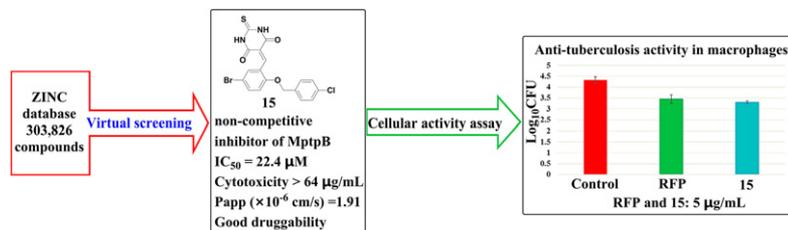
Dongfeng Zhang<sup>a</sup>, Yun Lin<sup>b</sup>, Xi Chen<sup>c</sup>, Wenting Zhao<sup>a</sup>, Dongni Chen<sup>b</sup>, Meng Gao<sup>a</sup>, Qinglin Wang<sup>b</sup>, Bin Wang<sup>c</sup>, Haihong Huang<sup>a,\*</sup>, Yongjun Lu<sup>b,\*</sup>, Yu Lu<sup>c,\*</sup>

<sup>a</sup>State Key Laboratory of Bioactive Substances and Function of Natural Medicine, Beijing Key Laboratory of Active Substance Discovery and Druggability Evaluation, Institute of Materia Medica, Peking Union Medical College and Chinese Academy of Medical Sciences, 1 Xian Nong Tan Street, Beijing 100050, China

<sup>b</sup>School of Life Sciences, Sun Yat-sen University, 135 West Xingang Road, Guangzhou, Guangdong 510275, China

<sup>c</sup>Beijing Key Laboratory of Drug Resistance Tuberculosis Research, Department of Pharmacology, Beijing Tuberculosis and Thoracic Tumor Research Institute, Beijing Chest Hospital, Capital Medical University, 97 Ma Chang Street, Beijing 101149, China

Bioorganic Chemistry 85 (2019) pp. 229–239



### Exploring the antimalarial potential of the methoxy-thiazinoquinone scaffold: Identification of a new lead candidate

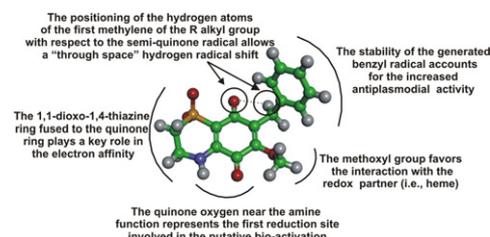
Concetta Imperatore<sup>a,1</sup>, Marco Persico<sup>a,1</sup>, Maria Senese<sup>a</sup>, Anna Aiello<sup>a</sup>, Marcello Casertano<sup>a</sup>, Paolo Luciano<sup>a</sup>, Nicoletta Basilio<sup>b,\*</sup>, Silvia Parapini<sup>b</sup>, Antonella Paladino<sup>c</sup>, Caterina Fattorusso<sup>a,\*</sup>, Marialuisa Menna<sup>a,\*</sup>

<sup>a</sup>The NeaNat Group, Department of Pharmacy, University of Naples "Federico II", Via D. Montesano 49, 80131 Napoli, Italy

<sup>b</sup>Dipartimento di Scienze Biomediche, Chirurgiche e Odontoiatriche, Università di Milano, Via Pascal 36, 20133 Milan, Italy

<sup>c</sup>Istituto di Chimica del Riconoscimento Molecolare, CNR, Via M. Bianco 9, 20131 Milano, Italy

Bioorganic Chemistry 85 (2019) pp. 240–252



### Synthesis, anticancer effect and molecular modeling of new thiazolylpyrazolyl coumarin derivatives targeting VEGFR-2 kinase and inducing cell cycle arrest and apoptosis

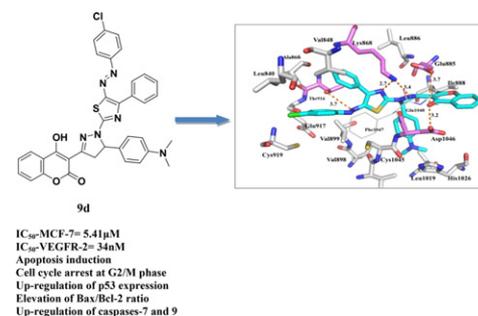
Tahia K. Mohamed<sup>a</sup>, Rasha Z. Batran<sup>a,\*</sup>, Samia A. Elseginy<sup>b</sup>, Mamdouh M. Ali<sup>c</sup>, Abeer E. Mahmoud<sup>c</sup>

<sup>a</sup>Chemistry of Natural Compounds Department, Pharmaceutical and Drug Industries Research Division, National Research Centre, 33 El Bohouth St., Dokki, P.O. Box 12622, Giza, Egypt

<sup>b</sup>Green Chemistry Department, Chemical Industries Research Division, National Research Centre, 33 El Bohouth St., Dokki, P.O. Box 12622, Giza, Egypt

<sup>c</sup>Biochemistry Department, Division of Genetic Engineering and Biotechnology, National Research Centre, 33 El Bohouth St., Dokki, P.O. Box 12622, Giza, Egypt

Bioorganic Chemistry 85 (2019) pp. 253–273



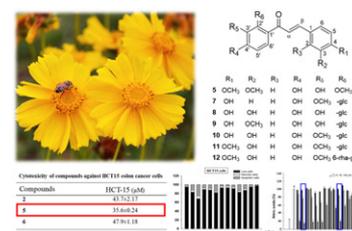
### Lanceoleins A–G, hydroxychalcones, from the flowers of *Coreopsis lanceolata* and their chemopreventive effects against human colon cancer cells

Hyoung-Geun Kim<sup>a</sup>, Hyun-Ji Oh<sup>a</sup>, Jung-Hwan Ko<sup>a</sup>, Hae Seong Song<sup>a</sup>, Yeong-Geun Lee<sup>a</sup>, Se Chan Kang<sup>a</sup>, Dae Young Lee<sup>b,\*</sup>, Nam-In Baek<sup>a,\*</sup>

<sup>a</sup>Graduate School of Biotechnology and Department of Oriental Medicine Biotechnology, Kyung-Hee University, Yongin 17104, Republic of Korea

<sup>b</sup>Department of Herbal Crop Research, National Institute of Horticultural and Herbal Science, RDA, Eumseong 27709, Republic of Korea

Bioorganic Chemistry 85 (2019) pp. 274–281



### Targeting microbial resistance: Synthesis, antibacterial evaluation, DNA binding and modeling study of new chalcone-based dithiocarbamate derivatives

Bioorganic Chemistry 85 (2019) pp. 282–292

Marwa Ayman<sup>a</sup>, Shahenda M. El-Messery<sup>b,\*</sup>, Elsayed E. Habib<sup>c,d</sup>, Sara T. Al-Rashood<sup>e</sup>,  
Abdulrahman A. Almehizia<sup>e</sup>, Hamad M. Alkahtani<sup>e</sup>, Ghada S. Hassan<sup>f,\*</sup>

<sup>a</sup>Faculty of Pharmacy, Mansoura University, P.O.Box 35516, Mansoura, Egypt

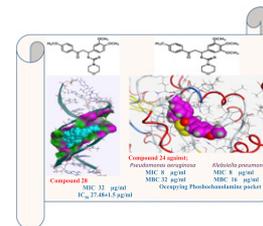
<sup>b</sup>Department of Pharmaceutical Organic Chemistry, Faculty of Pharmacy, Mansoura University, P.O.Box 35516, Mansoura, Egypt

<sup>c</sup>Department of Pharmaceutics and Pharmaceutical Technology, College of Pharmacy, Taibah University, Almadinah Almunawwarah 344, Saudi Arabia

<sup>d</sup>Department of Microbiology, Faculty of Pharmacy, Mansoura University, Mansoura 35516, Egypt

<sup>e</sup>Department of Pharmaceutical Chemistry, College of Pharmacy, King Saud University, Riyadh 11451, Saudi Arabia

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



### Design and synthesis of new phthalazine-based derivatives as potential EGFR inhibitors for the treatment of hepatocellular carcinoma

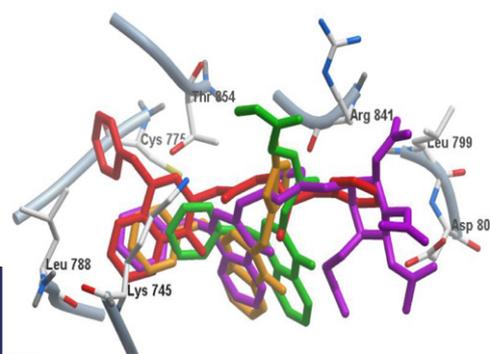
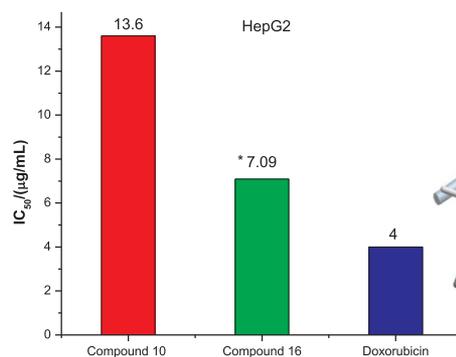
Bioorganic Chemistry 85 (2019) pp. 293–307

Ahmed T.A. Boraie<sup>a,\*</sup>, Hanaa K. Ashour<sup>a</sup>,  
El Sayed H. El Tamany<sup>a</sup>, Nahla Abdelmoaty<sup>a</sup>,  
Abdullah I. El-Falouji<sup>b</sup>, Mohamed S. Gomaa<sup>c</sup>

<sup>a</sup>Chemistry Department, Faculty of Science, Suez Canal University, Ismailia, Egypt

<sup>b</sup>Institute of Biotechnology for Postgraduate Studies and Research, Suez Canal University, Ismailia, Egypt

<sup>c</sup>Chemistry Department, College of Clinical Pharmacy, Imam Abdulrahman Bin Faisal University, Dammam, Saudi Arabia



Novel potential EGFR inhibitors for the treatment of hepatocellular carcinoma

### Synthesis and biological evaluation of some novel thio benzimidazole derivatives as anti-renal cancer agents through inhibition of c-MET kinase

Bioorganic Chemistry 85 (2019) pp. 337–348

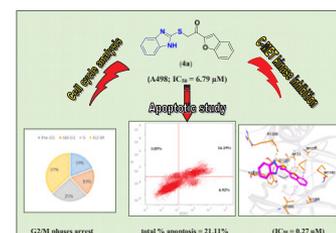
Hany S. Ibrahim<sup>a,\*</sup>, Mohamed E. Albakri<sup>a</sup>, Walaa R. Mahmoud<sup>b</sup>, Heba Abdelrasheed Allam<sup>b</sup>,  
Ahmed M. Reda<sup>c</sup>, Hatem A. Abdel-Aziz<sup>d</sup>

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

<sup>b</sup>Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Cairo University, Cairo 11562, Egypt

<sup>c</sup>Department of Biochemistry, Faculty of Pharmacy, Egyptian Russian University, Badr City, Cairo 11829, Egypt

<sup>d</sup>Department of Applied Organic Chemistry, National Research Center, Dokki, Giza, P.O. Box 12622, Egypt



### O-linked melatonin dimers as bivalent ligands targeting dimeric melatonin receptors

Bioorganic Chemistry 85 (2019) pp. 349–356

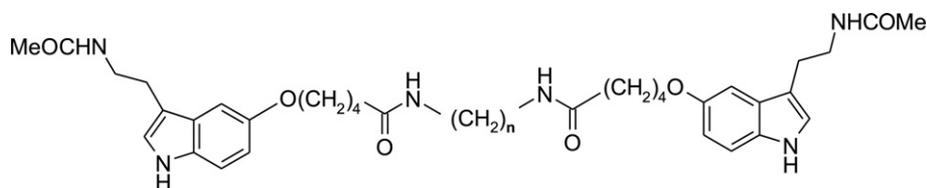
Angeliki Karamitri<sup>a,b,c</sup>, Mirna S. Sadek<sup>d</sup>,  
Anne-Sophie Journé<sup>a,b,c</sup>, Florence Gbahou<sup>a,b,c</sup>,  
Romain Gerbier<sup>a,b,c</sup>, Mai B. Osman<sup>d</sup>,  
Samy A.M. Habib<sup>d</sup>, Ralf Jockers<sup>a,b,c,1</sup>,  
Darius P. Zlotos<sup>d,s,1</sup>

<sup>a</sup>Inserm, U1016, Institut Cochin, Paris, France

<sup>b</sup>CNRS UMR 8104, Paris, France

<sup>c</sup>Univ. Paris Descartes, Sorbonne Paris Cite, Paris, France

<sup>d</sup>The German University in Cairo, Department of Pharmaceutical Chemistry, New Cairo City, 11835 Cairo, Egypt



**3a-e** (n = 4,6,8,10,12)

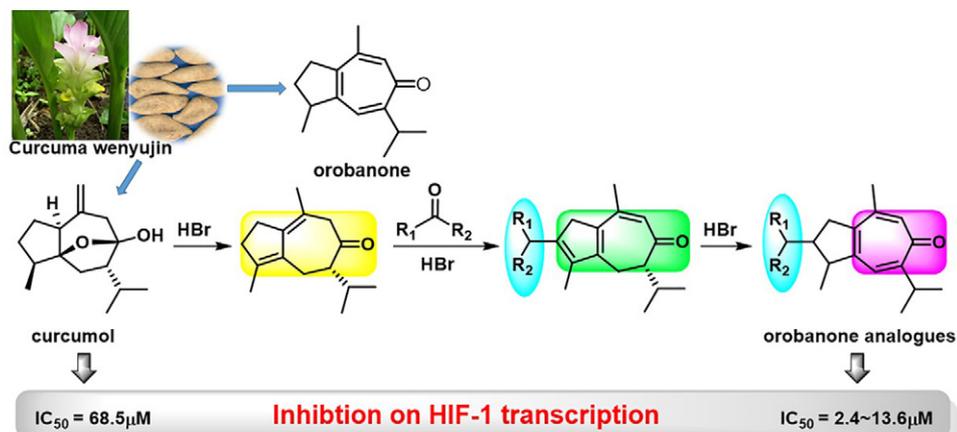
### Orobanone analogues from acid-promoted aromatization rearrangement of curcumol inhibit hypoxia-inducible factor-1 (HIF-1) in cell-based reporter assays

Bioorganic Chemistry 85 (2019) pp. 357–363

Yue-qing Li<sup>a</sup>, Guang-zhe Li<sup>a,\*</sup>, Yi Dong<sup>a</sup>,  
Xu Ma<sup>a</sup>, Hui-juan Dong<sup>a</sup>, Qian-qian Wu<sup>a</sup>,  
Wei-jie Zhao<sup>a,b,\*</sup>

<sup>a</sup>School of Pharmaceutical Science and Technology, Dalian University of Technology, No. 2 Linggong Road, Dalian 116024, China

<sup>b</sup>State Key Laboratory of Fine Chemicals, Dalian University of Technology, No. 2 Linggong Road, Dalian 116024, China

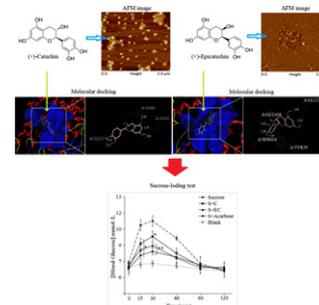


### The mechanism of interactions between flavan-3-ols against α-glucosidase and their *in vivo* antihyperglycemic effects

Bioorganic Chemistry 85 (2019) pp. 364–372

Ling-Ling Zhang<sup>1</sup>, Lin Han<sup>1</sup>, Shi-Yi Yang, Xue-Mei Meng, Wen-Fang Ma, Min Wang<sup>\*</sup>

College of Food Science and Engineering, Northwest A&F University, 712100 Yangling, PR China

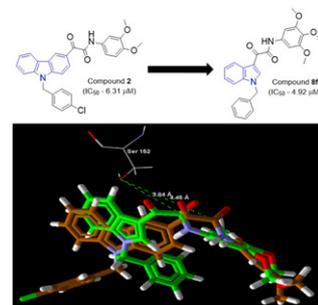


### Design, synthesis, biological evaluation and molecular modelling studies of indole glyoxylamides as a new class of potential pancreatic lipase inhibitors

S.N.C. Sridhar, Saksham Palawat, Atish T. Paul\*

Laboratory of Natural Product Chemistry, Department of Pharmacy, Birla Institute of Technology and Science, Pilani (BITS Pilani), Pilani campus, Pilani 333 031, Rajasthan, India

Bioorganic Chemistry 85 (2019) pp. 373–381

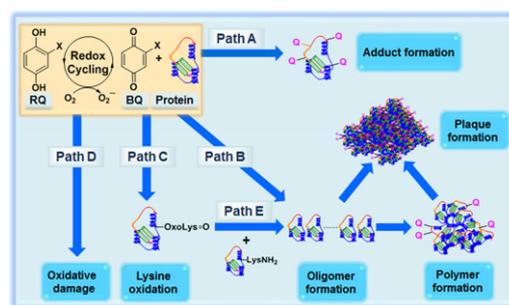


### Studies on lysozyme modifications induced by substituted *p*-benzoquinones

Jisook Kim\*, Charles A. Thomas, Jacob M. Ewald, Neethu M. Kurien, Mary E. Booker, Hendrik J. Greve, Titus V. Albu\*

Department of Chemistry and Physics, University of Tennessee at Chattanooga, Chattanooga, TN 37403, USA

Bioorganic Chemistry 85 (2019) pp. 386–398



### Design, synthesis, molecular docking and biological activity evaluation of some novel indole derivatives as potent anticancer active agents and apoptosis inducers

Ahmed M. Sh. El-Sharief<sup>a,\*</sup>, Yousry A. Ammar<sup>a,\*</sup>, Amany Belal<sup>b,c,\*</sup>, Marwa A.M. Sh. El-Sharief<sup>d,e</sup>, Yehia A. Mohamed<sup>d</sup>, Ahmed B.M. Mehany<sup>f,\*</sup>, Gameel A.M. Elhag Ali<sup>a</sup>, Ahmed Ragab<sup>a,\*</sup>

<sup>a</sup>Chemistry Department, Faculty of Science, Al-Azhar University, Nasr City, Cairo 11284, Egypt

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

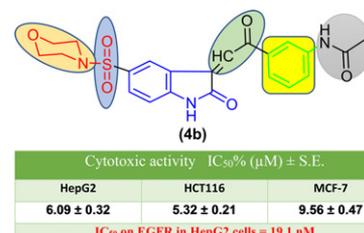
<sup>c</sup>Pharmaceutical Chemistry Department, College of Pharmacy, Taif University, Taif 21974, Saudi Arabia

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

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

<sup>f</sup>Zology Department, Faculty of Science, Al-Azhar University, Nasr City, Cairo 11284, Egypt

Bioorganic Chemistry 85 (2019) pp. 399–412



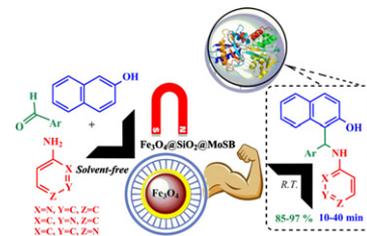
### Synthesis of 1-( $\alpha$ -aminoalkyl)-2-naphthol and $\alpha$ -aminonitrile derivatives with molybdenum Schiff base complex covalently bonded on silica-coated magnetic nanoparticles and DNA interaction study of one type of derivatives using computational and spectroscopic methods

Jamshid Rakhtshah<sup>a</sup>, Behrouz Shaabani<sup>a,b,\*</sup>, Sadegh Salehzadeh<sup>b</sup>, Neda Hosseinpour Moghadam<sup>b</sup>

<sup>a</sup>Department of Inorganic Chemistry, Faculty of Chemistry, University of Tabriz, Tabriz, Iran

<sup>b</sup>Faculty of Chemistry, Bu-Ali Sina University, Hamedan 6517838683, Iran

Bioorganic Chemistry 85 (2019) pp. 420–430

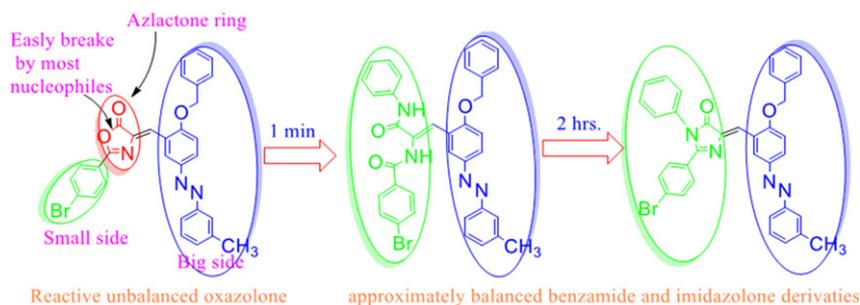


**Synthesis, characterization, antioxidant power and acute toxicity of some new azo-benzamide and azo-imidazolone derivatives with in vivo and in vitro antimicrobial evaluation**

Mohammed Kareem Samad<sup>a</sup>, Farouq Emam Hawaiz

Department of Chemistry, College of Education, Salahaddin University – Hawler, Erbil-Kurdistan, Iraq

Bioorganic Chemistry 85 (2019) pp. 431–444

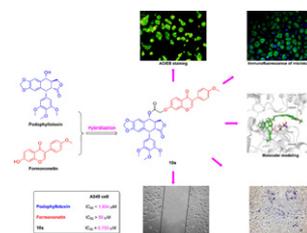


**Novel hybrids of podophyllotoxin and formononetin inhibit the growth, migration and invasion of lung cancer cells**

Chengli Yang, Qiongli Xie, Xian Zeng, Nengyin Tao, Yingshu Xu, Yongzheng Chen, Jing Wang<sup>a</sup>, Lei Zhang<sup>a</sup>

Generic Drug Research Center of Guizhou Province, Green Pharmaceuticals Engineering Research Center of Guizhou Province, School of Pharmacy, Zunyi Medical University, Zunyi 563003, PR China

Bioorganic Chemistry 85 (2019) pp. 445–454



**Novel lawsone-containing ruthenium(II) complexes: Synthesis, characterization and anticancer activity on 2D and 3D spheroid models of prostate cancer cells**

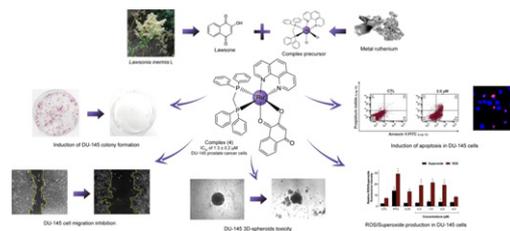
Rone Aparecido De Grandis<sup>a,\*</sup>, Patrick Wellington da Silva dos Santos<sup>b</sup>, Katia Mara de Oliveira<sup>c</sup>, Ana Rita Tomazela Machado<sup>b</sup>, Alexandre Ferro Aissa<sup>b</sup>, Alzir Azevedo Batista<sup>c</sup>, Lusânia Maria Gregg Antunes<sup>b</sup>, Fernando Rogério Pavan<sup>a,\*</sup>

<sup>a</sup>School of Pharmaceutical Sciences, São Paulo State University, Araraquara, São Paulo 14800-903, Brazil

<sup>b</sup>School of Pharmaceutical Sciences of Ribeirão Preto, University of São Paulo, Ribeirão Preto, São Paulo 14040-903, Brazil

<sup>c</sup>Department of Chemistry, Federal University of São Carlos, São Carlos, São Paulo 13561-901, Brazil

Bioorganic Chemistry 85 (2019) pp. 455–468



**Click chemistry based multicomponent approach in the synthesis of spirochromenocarbazole tethered 1,2,3-triazoles as potential anticancer agents**

Pramod V. Chavan<sup>a</sup>, Uday V. Desai<sup>a,\*</sup>, Prakash P. Wadgaonkar<sup>b</sup>, Savita R Tapase<sup>c</sup>, Kisan M. Kodam<sup>c</sup>, Amit Choudhari<sup>d</sup>, Dhiman Sarkar<sup>d,\*</sup>

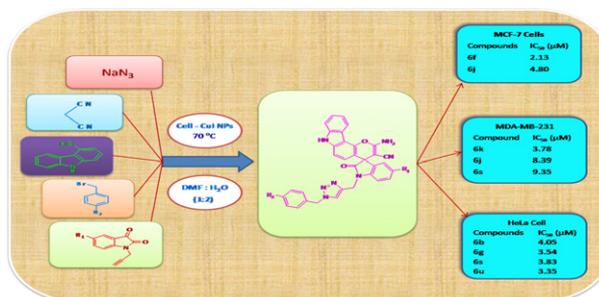
<sup>a</sup>Department of Chemistry, Shivaji University, Kolhapur 416 004, India

<sup>b</sup>Polymer Science and Engineering Division, CSIR, National Chemical Laboratory, Pune 411 008, India

<sup>c</sup>Biochemistry Division, Department of Chemistry, Savitribai Phule Pune University, Pune 411007, India

<sup>d</sup>Combi – Chem. Bio-Resource Centre, CSIR National Chemical Laboratory, Pune 411 008, India

Bioorganic Chemistry 85 (2019) pp. 475–486

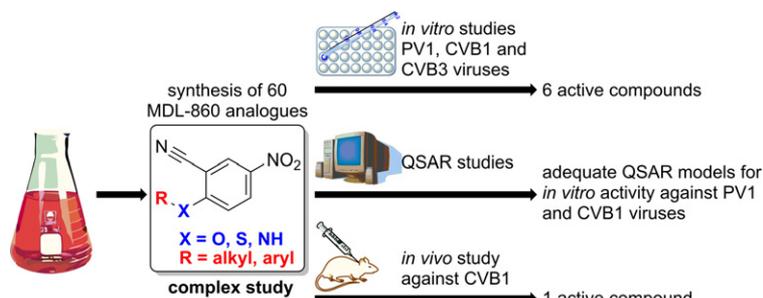


### Anti-enteroviral activity of new MDL-860 analogues: Synthesis, *in vitro/in vivo* studies and QSAR analysis

Bioorganic Chemistry 85 (2019) pp. 487–497

Ivanka Nikolova<sup>b</sup>, Ivaylo Slavchev<sup>a</sup>, Martin Ravutsov<sup>a</sup>, Miroslav Dangelov<sup>a</sup>, Yana Nikolova<sup>a</sup>, Irena Zagranjarska<sup>a</sup>, Adelina Stoyanova<sup>b</sup>, Nadya Nikolova<sup>b</sup>, Lucia Mukova<sup>b</sup>, Petar Grozdanov<sup>b</sup>, Rosica Nikolova<sup>c</sup>, Boris Shivachev<sup>c</sup>, Victor E. Kuz'min<sup>d,e</sup>, Liudmila N. Ognichenko<sup>d,e</sup>, Angel S. Galabov<sup>b,\*</sup>, Georgi M. Dobrikov<sup>a,\*</sup>

<sup>a</sup>Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences, bl. 9, Acad. G. Bonchev Str., Sofia 1113, Bulgaria  
<sup>b</sup>Stephan Angeloff Institute of Microbiology, Bulgarian Academy of Sciences, bl. 26, Acad. G. Bonchev Str., Sofia 1113, Bulgaria  
<sup>c</sup>Institute of Mineralogy and Crystallography, Bulgarian Academy of Sciences, bl. 107, Acad. G. Bonchev Str., Sofia 1113, Bulgaria  
<sup>d</sup>A.V. Bogatsky Physical-Chemical Institute NAS of Ukraine, Department of Molecular Structure and Chemoinformatics, Odessa, Ukraine  
<sup>e</sup>Odessa National Polytechnic University, Department of Theoretical Foundation of Chemistry, Odessa, Ukraine

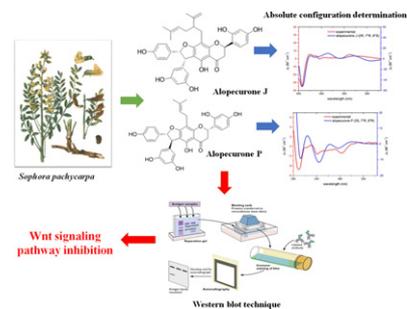


### Absolute configuration and anti-cancer effect of prenylated flavonoids and flavonostilbenes from *Sophora pachycarpa*: Possible involvement of Wnt signaling pathway

Bioorganic Chemistry 85 (2019) pp. 498–504

Motahare Boozari<sup>a</sup>, Samad Nejad Ebrahimi<sup>b</sup>, Saba Soltani<sup>c</sup>, Zahra Tayarani-Najaran<sup>d</sup>, Seyed Ahmad Emami<sup>a</sup>, Javad Asili<sup>a</sup>, Mehrdad Iranshahi<sup>e,\*</sup>

<sup>a</sup>Department of Pharmacognosy, School of Pharmacy, Mashhad University of Medical Sciences, Mashhad, Iran  
<sup>b</sup>Department of Phytochemistry, Medicinal Plants and Drugs Research Institute, Shahid Beheshti University, G.C., Evjn, Tehran, Iran  
<sup>c</sup>Department of Pharmacognosy, Faculty of Pharmacy, Tehran University of Medical Sciences, Tehran, Iran  
<sup>d</sup>Medical Toxicology Research Center, Mashhad University of Medical Sciences, Mashhad, Iran  
<sup>e</sup>Biotechnology Research Center, Pharmaceutical Technology Institute, Mashhad University of Medical Sciences, Mashhad, Iran

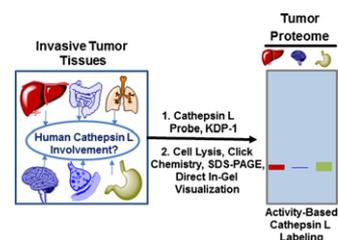


### Cell penetrable, clickable and tagless activity-based probe of human cathepsin L

Bioorganic Chemistry 85 (2019) pp. 505–514

Dibyendu Dana<sup>a,b</sup>, Jeremy Garcia<sup>c</sup>, Ashif I. Bhuiyan<sup>a,f</sup>, Pratikumar Rathod<sup>d,g</sup>, Laura Joo<sup>a</sup>, Daniel A. Novoa<sup>a</sup>, Suneeta Paroly<sup>e</sup>, Karl R. Fath<sup>c,f</sup>, Emmanuel J. Chang<sup>d,b,f</sup>, Sanjai K. Pathak<sup>a,b,f,\*</sup>

<sup>a</sup>Queens College of the City University of New York, Chemistry and Biochemistry Department, 65-30 Kissena Blvd, Flushing, NY 11367-1597, USA  
<sup>b</sup>Chemistry Doctoral Program, The Graduate Center of the City University of New York, 365 5th Ave, New York, NY 10016, USA  
<sup>c</sup>Queens College of the City University of New York, Department of Biology, 65-30 Kissena Blvd, Flushing, NY 11367-1597, USA  
<sup>d</sup>York College of the City University of New York, Department of Chemistry, 94-20 Guy R. Brewer Blvd, Jamaica, NY 11451-0001, USA  
<sup>e</sup>Bard High School Early College Queens, 30-20 Thomson Avenue, Long Island City, NY 11101, USA  
<sup>f</sup>Biochemistry Doctoral Program, The Graduate Center of the City University of New York, 365 5th Ave, New York, NY 10016, USA  
<sup>g</sup>Laguardia Community College, 31-10 Thomson Ave, Long Island City, NY 11101, USA



### Design, synthesis and biological study of hybrid drug candidates of nitric oxide releasing cucurbitacin-inspired estrone analogs for treatment of hepatocellular carcinoma

Bioorganic Chemistry 85 (2019) pp. 515–533

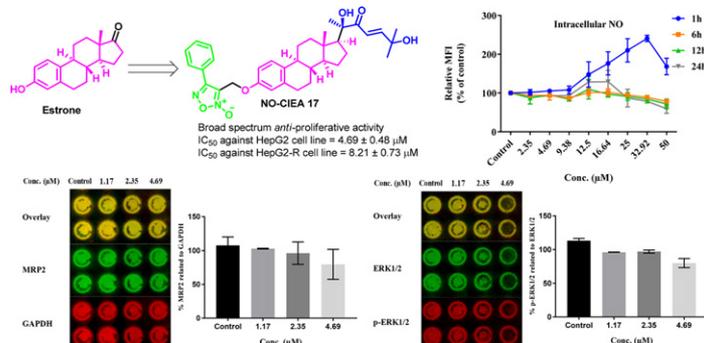
Mahrous A. Abou-Salim<sup>a,d</sup>, Mohamed A. Shaaban<sup>b</sup>,  
Mohammed K. Abd El Hameid<sup>b</sup>, Yaseen A.M.M. Elshaier<sup>c</sup>,  
Fathi Halaweish<sup>d,\*</sup>

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

<sup>b</sup>Cairo University, Faculty of Pharmacy, Pharmaceutical Organic Chemistry, Cairo 11562, Egypt

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

<sup>d</sup>South Dakota State University, Chemistry & Biochemistry, Box 2202, Brookings, SD 57007, USA



### Design, synthesis and evaluation of D-amino acid-containing peptidomimetics targeting the polo-box domain of polo-like kinase 1

Bioorganic Chemistry 85 (2019) pp. 534–540

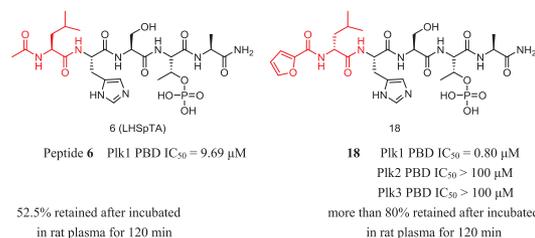
Zhiyan Li<sup>a,b,c</sup>, Zhenguo Zhang<sup>a,b,c</sup>, Yanhong Chen<sup>a,b,c</sup>, Shijun Tang<sup>a,b,c</sup>, Tongyuan Lin<sup>a,b,d</sup>,  
Jingfang Huang<sup>b,d</sup>, Bo Li<sup>b,d,\*</sup>, Cheng Jiang<sup>a,b,c,\*</sup>

<sup>a</sup>Jiangsu Key Laboratory of Drug Design and Optimization, China Pharmaceutical University, Nanjing 210009, China

<sup>b</sup>Key Laboratory on Protein Chemistry and Structural Biology, China Pharmaceutical University, Nanjing 210009, China

<sup>c</sup>Department of Medicinal Chemistry, China Pharmaceutical University, Nanjing 210009, China

<sup>d</sup>Key Laboratory of Drug Quality Control and Pharmacovigilance, China Pharmaceutical University, Nanjing 210009, China



### Pyrazoles containing thiophene, thienopyrimidine and thienotriazolopyrimidine as COX-2 selective inhibitors: Design, synthesis, *in vivo* anti-inflammatory activity, docking and *in silico* chemo-informatic studies

Bioorganic Chemistry 85 (2019) pp. 541–557

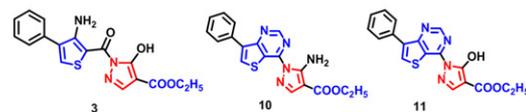
Mai S. El-Shoukrofy<sup>a,\*</sup>, Heba A. Abd El Razik<sup>a</sup>, Omaira M. AboulWafa<sup>a</sup>, Aida E. Bayad<sup>b</sup>,  
Ibrahim M. El-Ashmawy<sup>b,c</sup>

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

<sup>b</sup>Pharmacology Department, Faculty of Veterinary Medicine, Alexandria University, Alexandria, Egypt

<sup>c</sup>Department of Veterinary Medicine, Faculty of Agricultural and Veterinary Medicine, Qassim University, P.O. Box 1482, Buraydah, Al-Qassim, Saudi Arabia

The thiophene analog **3** and the thienopyrimidine derivatives **10** and **11** are promising non-toxic anti-inflammatory candidates that have moderate selectivity towards COX-2 enzyme with safe gastrointestinal profile in addition to expected good oral bioavailability and acceptable drug likeness properties.



### Cytotoxic clerodane diterpenoids from the leaves of *Casearia kurzii*

Bioorganic Chemistry 85 (2019) pp. 558–567

Jun Ma<sup>a</sup>, Xueyuan Yang<sup>a</sup>, Qi Zhang<sup>a</sup>,  
Xuke Zhang<sup>a</sup>, Chunfeng Xie<sup>a</sup>,  
Muhetaer Tuerhong<sup>b</sup>, Jie Zhang<sup>c</sup>,  
Da-Qing Jin<sup>d</sup>, Dongho Lee<sup>e</sup>, Jing Xu<sup>a,\*</sup>,  
Yasushi Ohizumi<sup>f</sup>, Yuanqiang Guo<sup>a,\*</sup>

<sup>a</sup>State Key Laboratory of Medicinal Chemical Biology, College of Pharmacy, and Tianjin Key Laboratory of Molecular Drug Research, Nankai University, Tianjin 300350, People's Republic of China

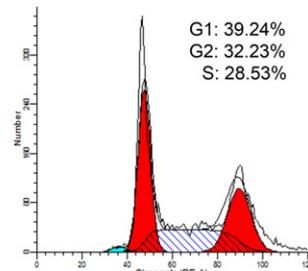
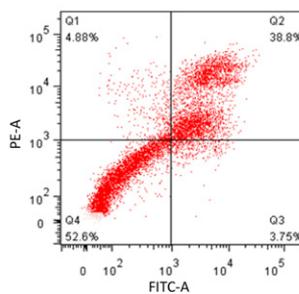
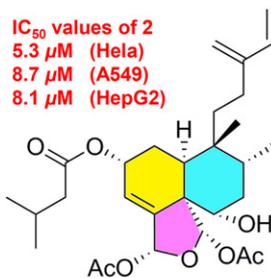
<sup>b</sup>College of Chemistry and Environmental Sciences, Laboratory of Xinjiang Native Medicinal and Edible Plant Resources Chemistry, Kashgar University, Kashgar 844000, People's Republic of China

<sup>c</sup>Key Laboratory for Green Processing of Chemical Engineering of Xinjiang Bingtuan, School of Chemistry and Chemical Engineering, Shihezi University, Shihezi 832003, People's Republic of China

<sup>d</sup>School of Medicine, Nankai University, Tianjin 300071, People's Republic of China

<sup>e</sup>Department of Biosystems and Biotechnology, College of Life Sciences and Biotechnology, Korea University, Seoul 02841, Republic of Korea

<sup>f</sup>Kansei Fukushi Research Institute, Tohoku Fukushi University, Sendai 989-3201, Japan



### Indole derivatives as multifunctional drugs: Synthesis and evaluation of antioxidant, photoprotective and antiproliferative activity of indole hydrazones

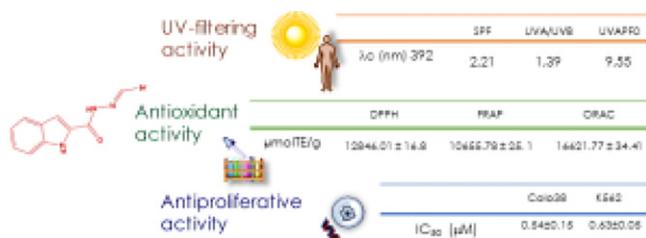
Bioorganic Chemistry 85 (2019) pp. 568–576

Monica Demurtas<sup>a,1</sup>, Anna Baldisserotto<sup>b,1</sup>, Ilaria Lampronti<sup>b</sup>, Davide Moi<sup>a</sup>,  
Gianfranco Balboni<sup>a</sup>, Salvatore Pacifico<sup>c</sup>, Silvia Vertuani<sup>b</sup>, Stefano Manfredini<sup>b</sup>,  
Valentina Onnis<sup>a,\*</sup>

<sup>a</sup>Department of Life and Environmental Sciences, Unit of Pharmaceutical, Pharmacological and Nutraceutical Sciences, University of Cagliari, via Ospedale 72, Cagliari I-09124, Italy

<sup>b</sup>Department of Life Sciences and Biotechnology, University of Ferrara, Via Fossato di Mortara 17-19, Ferrara I-44121, Italy

<sup>c</sup>Department of Chemical and Pharmaceutical Sciences, University of Ferrara, Via Fossato di Mortara 17-19, Ferrara I-44121, Italy



### Novel aryl carboximidamide and 3-aryl-1,2,4-oxadiazole analogues of naproxen as dual selective COX-2/15-LOX inhibitors: Design, synthesis and docking studies

Bioorganic Chemistry 85 (2019) pp. 577–584

Bahaa G.M. Youssif<sup>a,b,\*</sup>, Mamdouh F.A. Mohamed<sup>d,e,\*</sup>, Mohammad M. Al-Sanea<sup>b</sup>, Amr H. Moustafa<sup>d</sup>,  
Antar A. Abdelhamid<sup>d</sup>, Hesham A.M. Goma<sup>e,f</sup>

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

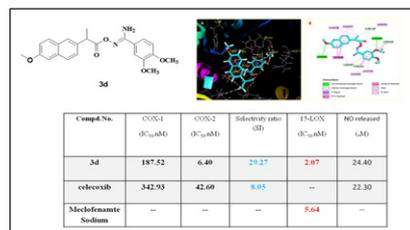
<sup>b</sup>Pharmaceutical Chemistry Department, College of Pharmacy, Jouf University, Sakaka, Aljouf 2014, Saudi Arabia

<sup>c</sup>Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Sohag University, 82524 Sohag, Egypt

<sup>d</sup>Department of Chemistry, Faculty of Science, Sohag University, Sohag 82524, Egypt

<sup>e</sup>Pharmacology Department, College of Pharmacy, Jouf University, Sakaka, Aljouf 2014, Saudi Arabia

<sup>f</sup>Biochemistry Department, Faculty of Pharmacy, Nahda University, Beni-Suef, Egypt



### Design, synthesis, and DNA interaction studies of furo-imidazo [3.3.3] propellane derivatives: Potential anticancer agents

Bioorganic Chemistry 85 (2019) pp. 585–599

Alaa A. Hassan<sup>a,\*</sup>, Ashraf A. Aly<sup>a</sup>, Nasr K. Mohamed<sup>a</sup>, Kamal M. El Shaieb<sup>a</sup>, Maysa M. Makhoulouf<sup>a</sup>, El-Shimaa M.N. Abdelhafez<sup>b</sup>, Stefan Bräse<sup>c,d</sup>, Martin Nieger<sup>e</sup>, Kevin N. Dalby<sup>f</sup>, Tamer S. Kaoud<sup>b,f,\*</sup>

<sup>a</sup>Chemistry Department, Faculty of Science, Minia University, El-Minia 61519, Egypt

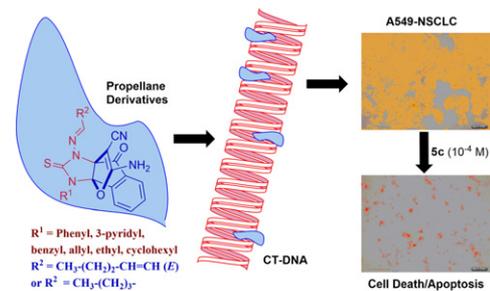
<sup>b</sup>Department of Medicinal Chemistry, Faculty of Pharmacy, Minia University, El-Minia 61519, Egypt

<sup>c</sup>Institute of Organic Chemistry, Karlsruhe Institute of Technology, Fritz-Haber-Weg 6, Karlsruhe 76131, Germany

<sup>d</sup>Institute of Toxicology and Genetics, Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen, Germany

<sup>e</sup>Department of Chemistry, University of Helsinki, P.O. Box 55, A.I. Virtasen aukio I, Helsinki 00014, Finland

<sup>f</sup>Division of Chemical Biology and Medicinal Chemistry, The University of Texas at Austin, Austin, TX 78712, USA



### REVIEW ARTICLES

### Bio-guided search of active indole alkaloids from *Tabernaemontana catharinensis*: Antitumour activity, toxicity *in silico* and molecular modelling studies

Bioorganic Chemistry 85 (2019) pp. 66–74

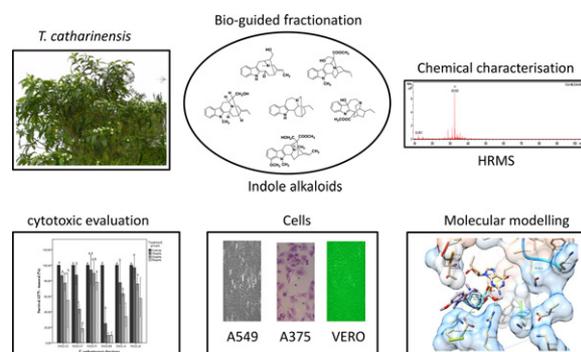
Pauline Fagundes Rosales<sup>a,b</sup>, Flavio Ferreira Marinho<sup>a</sup>, Adriana Gower<sup>a</sup>, Marilda Chiarello<sup>a</sup>, Bianca Canci<sup>c</sup>, Mariana Roesch-Ely<sup>c</sup>, Favero Reisendorfer Paula<sup>d</sup>, Sidnei Moura<sup>a,\*</sup>

<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>Laboratory of Genomics, Proteomics and DNA Repair, University of Caxias do Sul, Brazil

<sup>d</sup>Laboratory of Research and Drugs Development, Federal University of Pampa, Brazil



### Piperazine-azole-fluoroquinolone hybrids: Conventional and microwave irradiated synthesis, biological activity screening and molecular docking studies

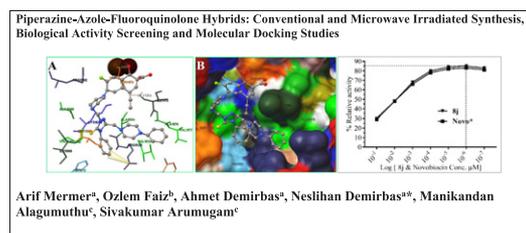
Bioorganic Chemistry 85 (2019) pp. 308–318

Arif Mermer<sup>a</sup>, Ozlem Faiz<sup>b</sup>, Ahmet Demirbas<sup>a</sup>, Neslihan Demirbas<sup>a,\*</sup>, Manikandan Alagumuthu<sup>c</sup>, Sivakumar Arumugam<sup>c</sup>

<sup>a</sup>Karadeniz Technical University, Department of Chemistry 61080 Trabzon, Turkey

<sup>b</sup>Recep Tayyip Erdogan University, Department of Chemistry, 53100 Rize, Turkey

<sup>c</sup>Dept. of Biotechnology, School of Bio-Sciences and Technology, VIT, Vellore 632014, India



### Wedtrilosides A and B, two new diterpenoid glycosides from the leaves of *Wedelia trilobata* (L.) Hitchc. with $\alpha$ -amylase and $\alpha$ -glucosidase inhibitory activities

Bioorganic Chemistry 85 (2019) pp. 319–324

Nguyen Thi Luyen<sup>a,b,c</sup>, Pham Thanh Binh<sup>a</sup>, Pham Thi Tham<sup>d</sup>, Ta Manh Hung<sup>e</sup>, Nguyen Hai Dang<sup>a,c</sup>, Nguyen Tien Dat<sup>b,c</sup>, Nguyen Phuong Thao<sup>a,\*</sup>

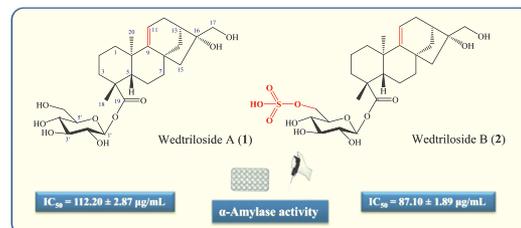
<sup>a</sup>Institute of Marine Biochemistry (IMBC), Vietnam Academy of Science and Technology (VAST), 18 Hoang Quoc Viet, Cau Giay, Hanoi, Viet Nam

<sup>b</sup>Center for Research and Technology Transfer, VAST, 18 Hoang Quoc Viet, Cau Giay, Hanoi, Viet Nam

<sup>c</sup>Graduate University of Science and Technology, VAST, 18 Hoang Quoc Viet, Cau Giay, Hanoi, Viet Nam

<sup>d</sup>Faculty of Chemical Technology, Hanoi University of Industry, 298 Cau Dien, Bactuliem, Hanoi, Viet Nam

<sup>e</sup>National Institute of Drug Quality Control (NIDQC), 48 Hai Ba Trung, Hoankiem, Hanoi, Viet Nam



## PRELIMINARY COMMUNICATIONS

## A molecular hybrid producing simultaneously singlet oxygen and nitric oxide by single photon excitation with green light

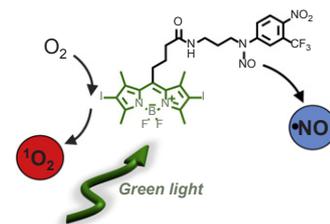
Bioorganic Chemistry 85 (2019) pp. 18–22

Cristina Parisi<sup>a,1</sup>, Mariacristina Failla<sup>b,1</sup>, Aurore Fraix<sup>a</sup>, Antonio Rescifina<sup>a</sup>, Barbara Rolando<sup>b</sup>, Loretta Lazzarato<sup>b,\*</sup>, Venera Cardile<sup>c</sup>, Adriana C.E. Graziano<sup>c</sup>, Roberta Fruttero<sup>b</sup>, Alberto Gasco<sup>b</sup>, Salvatore Sortino<sup>a,\*</sup>

<sup>a</sup>Department of Drug Sciences, University of Catania, I-95125 Catania, Italy

<sup>b</sup>Department of Drug Science and Technology, University of Torino, I-10125 Torino, Italy

<sup>c</sup>Department of Biomedical and Biotechnological Sciences, Physiology Division, University of Catania, I-95125 Catania, Italy

Radical rescues yeast cell death triggered by expression of human  $\alpha$ -synuclein and its A53T mutant, but not by human  $\beta$ A4 peptide and proapoptotic protein bax

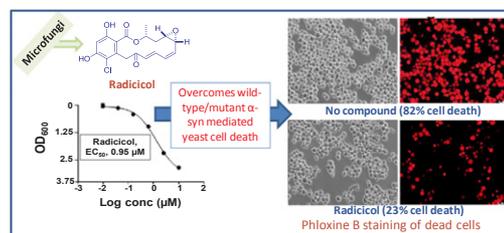
Bioorganic Chemistry 85 (2019) pp. 152–158

Asma Derf<sup>a</sup>, Shilpa A. Verekar<sup>b</sup>, Shreyans K. Jain<sup>c</sup>, Sunil K. Deshmukh<sup>b</sup>, Sandip B. Bharate<sup>c,\*</sup>, Bhabatosh Chaudhuri<sup>a,\*</sup>

<sup>a</sup>Leicester School of Pharmacy, De Montfort University, Leicester LE1 9BH, UK

<sup>b</sup>Piramal Life Sciences Limited, Goregaon (East), Mumbai 400 063, India

<sup>c</sup>CSIR-Indian Institute of Integrative Medicine, Canal Road, Jammu 180001, India

Synthesis, antioxidant and A $\beta$  anti-aggregation properties of new ferulic, caffeic and lipoic acid derivatives obtained by the Ugi four-component reaction

Bioorganic Chemistry 85 (2019) pp. 221–228

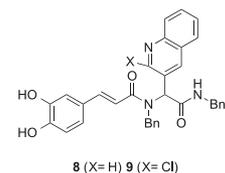
Mohamed Benchekroun<sup>a,1</sup>, Irene Pachón-Angona<sup>a</sup>, Vincent Luzet<sup>a</sup>, Helene Martin<sup>b</sup>, María-Jesús Oset-Gasque<sup>c</sup>, José Marco-Contelles<sup>d</sup>, Lhassane Ismaili<sup>a</sup>

<sup>a</sup>Laboratoire Neurosciences intégratives et cliniques EA 481, Pôle de Chimie Organique et Thérapeutique, Univ. Bourgogne Franche-Comté, UFR Santé, 19, rue Ambroise Paré, F-25000 Besançon, France

<sup>b</sup>PEPITE EA4267, Laboratoire de Toxicologie Cellulaire, Univ. Bourgogne Franche-Comté, F-25000 Besançon, France

<sup>c</sup>Faculty of Pharmacy, Department of Biochemistry and Molecular Biology, Complutense University, 28040-Madrid, Spain

<sup>d</sup>Laboratory of Medicinal Chemistry (IQOG, CSIC), Juan de la Cierva 3, 28006 Madrid, Spain



8 (X=H) 9 (X=Cl)

We have identified molecules 8 and 9 as potent antioxidant agents showing strong A $\beta$ <sub>1-40</sub> self-aggregation inhibition

## Innovative nano-carriers in anticancer drug delivery-a comprehensive review

Bioorganic Chemistry 85 (2019) pp. 325–336

Peng Dong<sup>a,b</sup>, K.P. Rakesh<sup>a,\*</sup>, H.M. Manukumar<sup>c,d,\*</sup>, Yasser Hussein Eissa Mohammed<sup>e</sup>, C.S. Karthik<sup>d</sup>, S. Sumathi<sup>f</sup>, P. Mallu<sup>d</sup>, Hua-Li Qin<sup>a,\*</sup>

<sup>a</sup>Department of Pharmaceutical Engineering, School of Chemistry, Chemical Engineering and Life Science, Wuhan University of Technology, 205 Luoshi Road, Wuhan 430070, PR China

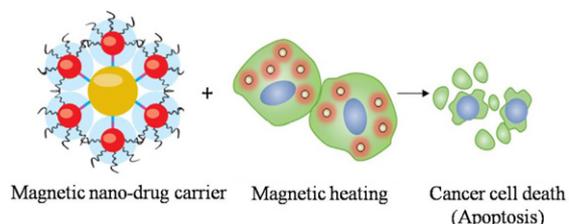
<sup>b</sup>Zhejiang Huahai Pharmaceutical Co. LTD., Chuan Nan Site No. 1 Branch Factory, Duqiao, Linhai, Zhejiang Province 317016, PR China

<sup>c</sup>Department of Studies in Biotechnology, University of Mysore, Manasagangotri, Mysuru 570006, Karnataka, India

<sup>d</sup>Department of Chemistry, Sri Jayachamarajendra College of Engineering, JSS Science and Technology University, Mysuru 570 006, Karnataka, India

<sup>e</sup>Department of Biochemistry, Faculty of Applied Science College, University of Hajjah, Yemen

<sup>f</sup>Department of Biochemistry, Biotechnology and Bioinformatics, Avinashilingam Institute for Home Science and Higher Education for Women, Coimbatore 641 043, India



### Bioactive cytosporone derivatives isolated from the mangrove-derived fungus *Dothiorella* sp. ML002

Bioorganic Chemistry 85 (2019) pp. 382–385

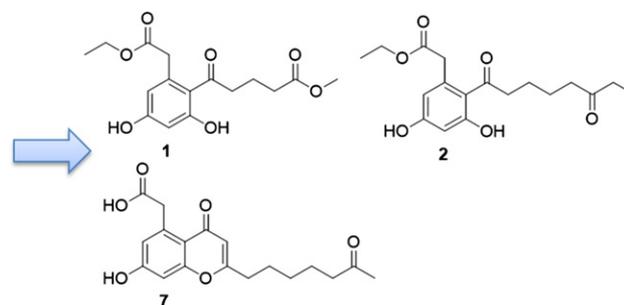
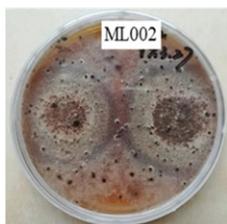
Cai-Juan Zheng<sup>a,b,c,1</sup>, Guo-Lei Huang<sup>b,c,1</sup>,  
Hai-Xia Liao<sup>c,d</sup>, Rong-Qing Mei<sup>a,b,c</sup>, You-Ping Luo<sup>b,c</sup>,  
Guang-Ying Chen<sup>a,b,c</sup>, Qing-Ying Zhang<sup>a,\*</sup>

<sup>a</sup>State Key Laboratory of Natural and Biomimetic Drugs,  
School of Pharmaceutical Sciences, Peking University  
Health Science Center, Beijing 100191, People's Republic  
of China

<sup>b</sup>Key Laboratory of Tropical Medicinal Plant Chemistry of  
Ministry of Education, Hainan Normal University, Haikou  
571158, People's Republic of China

<sup>c</sup>Key Laboratory of Tropical Medicinal Plant Chemistry of  
Hainan Province, College of Chemistry and Chemical  
Engineering, Hainan Normal University, Haikou 571158,  
People's Republic of China

<sup>d</sup>College of Chemistry and Food Sciences, Yulin Normal  
University, Yulin 537000, People's Republic of China



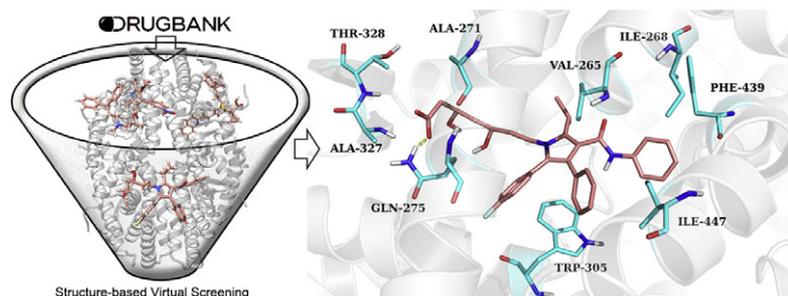
### Discovery of atorvastatin as a tetramer stabilizer of nuclear receptor RXR $\alpha$ through structure-based virtual screening

Bioorganic Chemistry 85 (2019) pp. 413–419

Xin Wang<sup>a,1</sup>, Shuyi Chong<sup>a,1</sup>, Huiyun Lin<sup>a</sup>, Zhiqiang Yan<sup>a</sup>,  
Fengyu Huang<sup>a</sup>, Zhiping Zeng<sup>a</sup>, Xiaokun Zhang<sup>a,b,\*</sup>, Ying Su<sup>b,\*</sup>

<sup>a</sup>School of Pharmaceutical Science, Fujian Provincial Key Laboratory of  
Innovative Drug Target Research, Xiamen University, Fujian  
361002, China

<sup>b</sup>Sanford Burnham Prebys Medical Discovery Institute, 10901 N.  
Torrey Pines Road, La Jolla, CA 92037, USA



### Chiral resolution and neuroprotective activities of enantiomeric dihydrobenzofuran neolignans from the fruit of *Crataegus pinnatifida*

Bioorganic Chemistry 85 (2019) pp. 469–474

Rui Guo<sup>a</sup>, Tian-Ming Lv<sup>a</sup>, Feng-Ying Han<sup>a</sup>, Bin Lin<sup>b</sup>, Guo-Dong Yao<sup>a</sup>, Xiao-Bo Wang<sup>c</sup>,  
Xiao-Xiao Huang<sup>a,c,\*</sup>, Shao-Jiang Song<sup>a,\*</sup>

<sup>a</sup>School of Traditional Chinese Materia Medica, Key Laboratory of Computational Chemistry-Based  
Natural Antitumor Drug Research & Development, Liaoning Province, Shenyang Pharmaceutical  
University, Shenyang 110016, People's Republic of China

<sup>b</sup>School of Pharmaceutical Engineering, Shenyang Pharmaceutical University, Shenyang 110016,  
People's Republic of China

<sup>c</sup>Chinese People's Liberation Army 210 Hospital, Dalian 116021, People's Republic of China

