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Bioorganic Chemistry

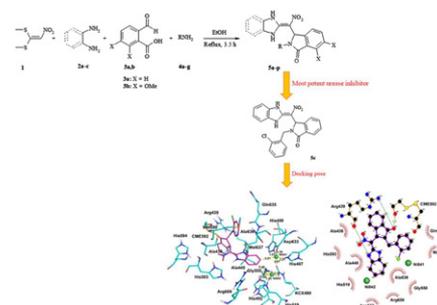
journal homepage: www.elsevier.com/locate/bioorg

Graphical Abstracts/Bioorganic Chemistry 87 (2019) ii-xxvii

REGULAR ARTICLES

Isoindolin-1-one derivatives as urease inhibitors: Design, synthesis, biological evaluation, molecular docking and *in-silico* ADME evaluation

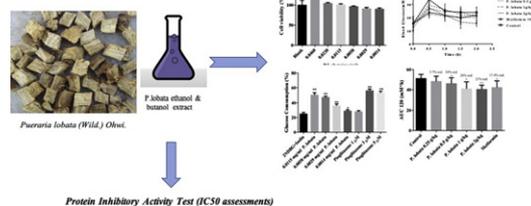
Bioorganic Chemistry 87 (2019) pp. 1–11

Fariba Peytam^a, Mehdi Adib^{a,*}, Shabnam Mahernia^b, Mahmoud Rahmanian-Jazi^a, Mehdi Jahani^a, Behrad Masoudi^a, Mohammad Mahdavi^c, Massoud Amanlou^{b,d,*}^aSchool of Chemistry, College of Science, University of Tehran, PO Box 14155-6455, Tehran, Iran^bComputational Chemistry Group, The Institute of Pharmaceutical Sciences (TIPS), Tehran University of Medical Sciences, Tehran, Iran^cEndocrinology and Metabolism Research Center, Endocrinology and Metabolism Clinical Sciences Institute, Tehran University of Medical Sciences, Tehran, Iran^dDepartment of Medicinal Chemistry, Faculty of Pharmacy, Tehran University of Medical Sciences, Tehran, IranAnti-diabetic potential of *Pueraria lobata* root extract through promoting insulin signaling by PTP1B inhibition

Bioorganic Chemistry 87 (2019) pp. 12–15

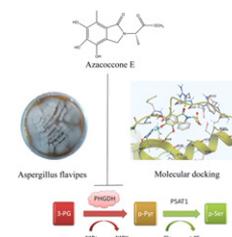
Ran Sun, Xinxian Deng, Dongdong Zhang, Fangzhou Xie, Di Wang, Juntao Wang, Mojdeh S. Tavallaie, Faqin Jiang^{*}, Lei Fu^{*}

Shanghai Key Laboratory for Molecular Engineering of Chiral Drugs, School of Pharmacy, Shanghai Jiao Tong University (SJTU), 800 Dongchuan Road, Shanghai 200240, China



Azacoccone E inhibits cancer cell growth by targeting 3-phosphoglycerate dehydrogenase

Bioorganic Chemistry 87 (2019) pp. 16–22

Jing Guo^{a,1}, Xiaoxia Gu^{a,1}, Mengzhu Zheng^{a,1}, Yonghui Zhang^{a,*}, Lixia Chen^{b,*}, Hua Li^{a,b,*}^aHubei Key Laboratory of Natural Medicinal Chemistry and Resource Evaluation, School of Pharmacy, Tongji Medical College, Huazhong University of Science and Technology, Wuhan 430030, China^bWuya College of Innovation, Key Laboratory of Structure-Based Drug Design & Discovery, Ministry of Education, Shenyang Pharmaceutical University, Shenyang 110016, China

Cucurbitane-type compounds from *Momordica charantia*: Isolation, *in vitro* antidiabetic, anti-inflammatory activities and *in silico* modeling approaches

Siddanagouda R. Shivanagoudra^a,
Wilmer H. Perera^a, Jose L. Perez^a,
Giridhar Athrey^b, Yuxiang Sun^c,
G.K. Jayaprakasha^{a,*},
Bhimanagouda S. Patil^{a,*}

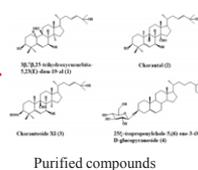
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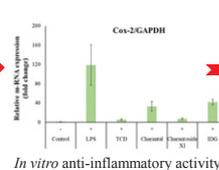
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Texas A&M University, College Station, TX
77843, United States



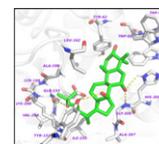
Bitter melons



Purified compounds



In vitro anti-inflammatory activity



Molecular docking

Bioorganic Chemistry 87 (2019) pp. 31–42

Tyrosinase inhibition and anti-melanin generation effect of cinnamamide analogues

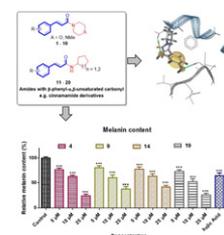
Sultan Ullah^a, Chaeun Park^a, Muhammad Ikram^{b,c}, Dongwan Kang^a, Sanggwon Lee^a, Jungho Yang^a,
Yujin Park^a, Sik Yoon^b, Pusoon Chun^d, Hyung Ryong Moon^{a,*}

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South Korea



Synthesis of benzenesulfonamides linked to quinazoline scaffolds as novel carbonic anhydrase inhibitors

Bioorganic Chemistry 87 (2019) pp. 78–90

Adel S. El-Azab^{a,*}, Alaa A.-M. Abdel-Aziz^a, Sivia Bua^b, Alessio Nocentini^b, Manal A. El-Gendy^a, Menshawy A. Mohamed^{c,d}, Taghreed Z. Shawer^e, Nawaf A. AlSaif^a, Claudiu T. Supuran^{b,*}

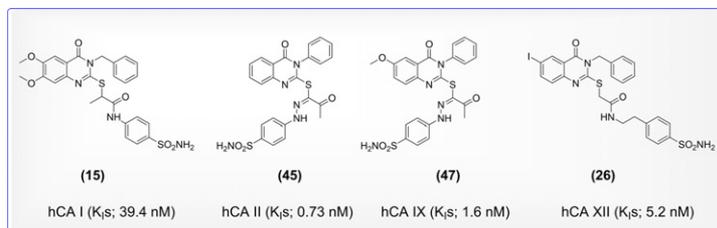
^aDepartment of Pharmaceutical Chemistry, College of Pharmacy, King Saud University, Riyadh, Saudi Arabia

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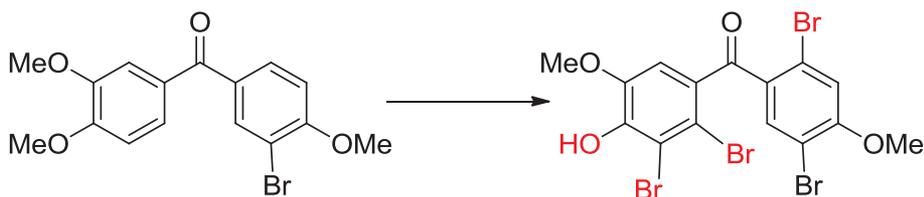


Synthesis and characterization of novel bromophenols: Determination of their anticholinergic, antidiabetic and antioxidant activities

Bioorganic Chemistry 87 (2019) pp. 91–102

Necla Öztaşkın^{*}, Rüya Kaya, Ahmet Maraş^{*}, Ertan Şahin, İlhami Gülcin, Süleyman Gökso

Atatürk University, Faculty of Science, Department of Chemistry, 25240 Erzurum, Turkey



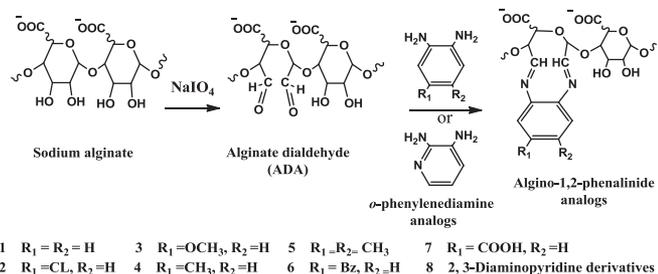
Synthesis of compounds having antimicrobial activity from alginate

Bioorganic Chemistry 87 (2019) pp. 103–111

Dalia M.S.A. Salem^{a,*}, Mohammed A.E. Sallam^{b,*}, Trevena N.M.A. Youssef^b

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Synthesis and antiproliferative activity of new 2-glyco-3-nitro-2H-chromenes

Bioorganic Chemistry 87 (2019) pp. 112–116

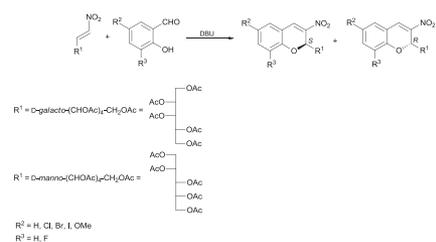
Verónica Luque-Agudo^{a,d}, Jesús Albarrán-Velo^a, Mark E. Light^b, José M. Padrón^c, Emilio Román^a, José A. Serrano^a, M. Victoria Gil^{b,*}

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^dCentro de Investigación Biomédica en Red. Bioingeniería, Biomateriales y Nanomedicina CIBER-BBN, Badajoz, Spain



Sesquiterpenes from *Curcuma zedoaria* rhizomes and their cytotoxicity against human gastric cancer AGS cells

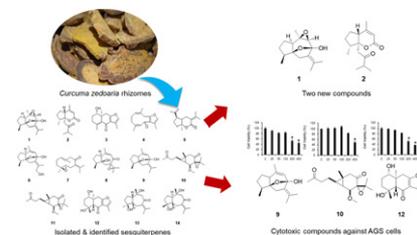
Tae Kyoung Lee^a, Dahae Lee^a, Seoung Rak Lee^a, Yoon-Joo Ko^b, Ki Sung Kang^c, Sang Jeon Chung^a, Ki Hyun Kim^{a,*}

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^cCollege of Korean Medicine, Gachon University, Seongnam 13120, Republic of Korea

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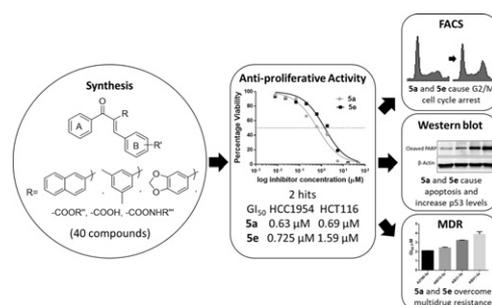
Synthesis and evaluation of novel α -substituted chalcones with potent anti-cancer activities and ability to overcome multidrug resistance

Sharon Riaz^a, Maheen Iqbal^b, Rahim Ullah^b, Rida Zahra^b, Ghayoor Abbas Chotana^a, Amir Faisal^{b,*}, Rahman Shah Zaib Saleem^{a,*}

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Bioorganic Chemistry 87 (2019) pp. 123–135



Iridoids from *Valeriana jatamansi* induce autophagy-associated cell death via the PDK1/Akt/mTOR pathway in HCT116 human colorectal carcinoma cells

Yu-Zhu Tan^{a,b}, Cheng Peng^{a,b,*}, Chang-Jiang Hu^b, Hong-Xiang Li^c, Wen-Bing Li^d, Jun-Lin He^{a,b}, Yu-Zhi Li^{a,b}, Hai Zhang^{a,b}, Ruo-Qi Zhang^{a,b}, Li-Xia Wang^{a,b}, Zhi-Xing Cao^{a,b,*}

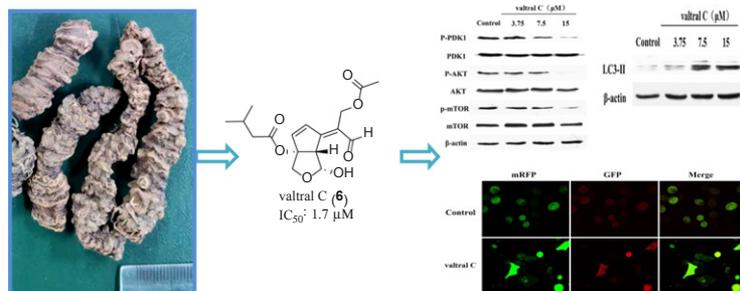
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Bioorganic Chemistry 87 (2019) pp. 136–141



Synthesis of C–C, C–N coupled novel substituted dibutyl benzothiazepinone derivatives and evaluation of their thrombin inhibitory activity

Bioorganic Chemistry 87 (2019) pp. 142–154

C.P. Baburajeev^{a,1}, Chakrabhavi Dhananjaya Mohan^{b,1}, Vijay Pandey^c, Shobith Rangappa^d, Naveen Shivalingegowda^e, Leen Kalash^f, Sannaningaiah Devaraja^g, Andreas Bender^f, Peter E. Lobie^c, Kanchugarakoppal S. Rangappa^{h,*}, Basappa^{a,1,*}

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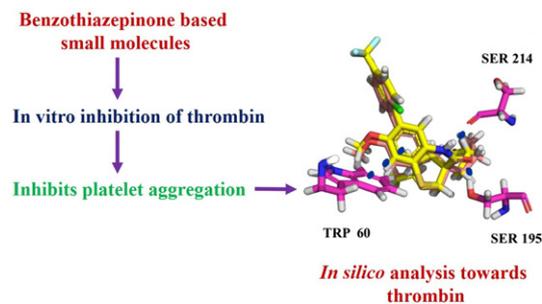
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Synthesis and characterization of new thiosemicarbazones, as potent urease inhibitors: *In vitro* and *in silico* studies

Bioorganic Chemistry 87 (2019) pp. 155–162

Muhammad Islam^{a,b}, Ajmal Khan^b, Muhammad Tariq Shehzad^a, Abdul Hameed^c, Nadeem Ahmed^a, Sobia Ahsan Halim^b, Mohammed Khat^b, Muhammad Usman Anwar^d, Javid Hussain^d, René Csuk^e, Zahid Shafiq^{a,*}, Ahmed Al-Harrasi^{b,*}

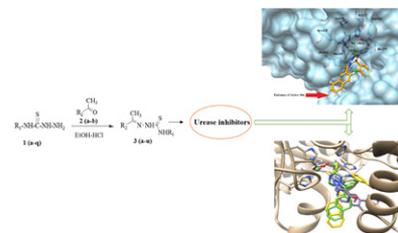
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Synthesis and evaluation of novel benzotropolones as Atg4B inhibiting autophagy blockers

Bioorganic Chemistry 87 (2019) pp. 163–168

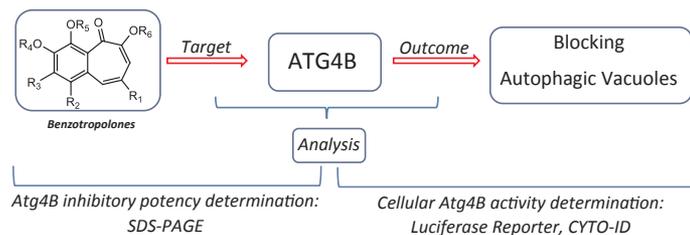
Muhammet Tanc^{a,1}, Matthias Cleenewerck^{a,1}, Ammar Kurdi^b, Ria Roelandt^{c,d}, Wim Declercq^{c,d}, Guido De Meyer^b, Koen Augustyns^a, Wim Martinet^{b,*}, Pieter Van der Veken^{a,*}

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Evaluation of guanyldihydrazone derivatives as inhibitors of *Candida rugosa* digestive lipase: Biological, biophysical, theoretical studies and biotechnological application

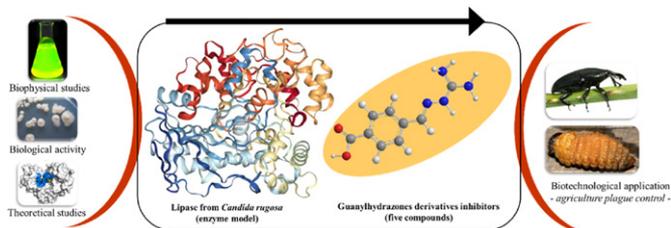
Bioorganic Chemistry 87 (2019) pp. 169–180

Camilla C. Santana^a, Edeildo F. Silva-Júnior^{a,b}, João César N. Santos^b, Érica E. da S. Rodrigues^a, Isabella M. da Silva^b, João X. Araújo-Júnior^{a,b}, Ticiano G. do Nascimento^a, Leandro A. Oliveira Barbosa^c, Camila B. Dornelas^a, Isis M. Figueiredo^b, Josué Carinhanha C. Santos^{b,c}, Luciano Aparecido M. Grillo^{a,*}

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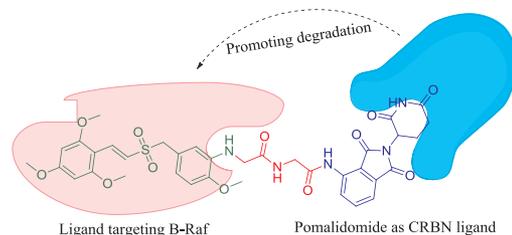


Pomalidomide hybrids act as proteolysis targeting chimeras: Synthesis, anticancer activity and B-Raf degradation

Bioorganic Chemistry 87 (2019) pp. 191–199

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Development of a versatile DNMT and HDAC inhibitor C02S modulating multiple cancer hallmarks for breast cancer therapy

Bioorganic Chemistry 87 (2019) pp. 200–208

Zigao Yuan^{a,b,1}, Shaopeng Chen^{b,c,1}, Chunmei Gao^{b,d}, Qiuzi Dai^b, Cunlong Zhang^b, Qinsheng Sun^b, Jin-Shun Lin^b, Chun Guo^a, Yuzong Chen^{b,e}, Yuyang Jiang^{a,b,f,*}

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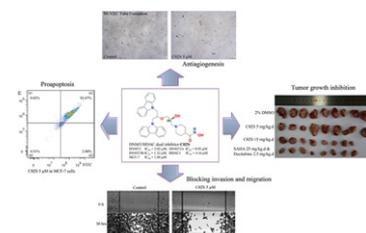
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Rhamnolipid inspired lipopeptides effective in preventing adhesion and biofilm formation of *Candida albicans*

Bioorganic Chemistry 87 (2019) pp. 209–217

Milos Jovanovic^a, Jelena Radivojevic^b, Kevin O'Connor^c, Stevan Blagojevic^d, Biljana Begovic^d, Vera Lukic^e, Jasmina Nikodinovic-Runic^{b,*}, Vladimir Savic^{a,*}

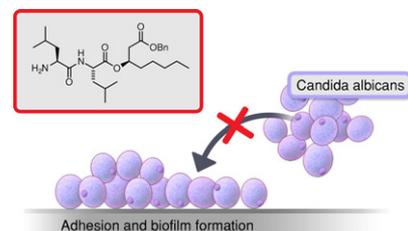
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Nitrogen-containing derivatives of *O*-tetramethylquercetin: Synthesis and biological profiles in prostate cancer cell models

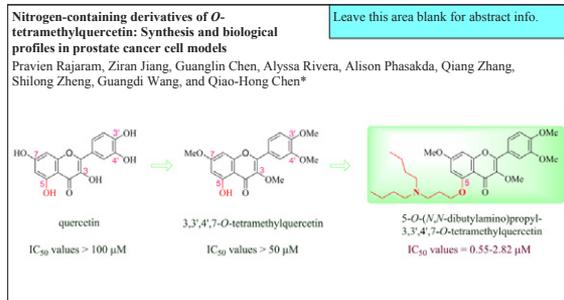
Bioorganic Chemistry 87 (2019) pp. 227–239

Pravien Rajaram^a, Ziran Jiang^a, Guanglin Chen^a, Alyssa Rivera^a, Alison Phasakda^a, Qiang Zhang^{b,c}, Shilong Zheng^{b,c}, Guangdi Wang^{b,c}, Qiao-Hong Chen^{a,*}

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Structure-based design, synthesis and biological evaluation of a newer series of pyrazolo [1,5-*a*] pyrimidine analogues as potential anti-tubercular agents

Bioorganic Chemistry 87 (2019) pp. 240–251

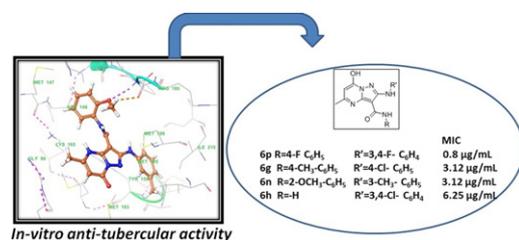
Palmi Modi^{a,b,d}, Shivani Patel^{a,c}, Mahesh Chhabria^{a,*}

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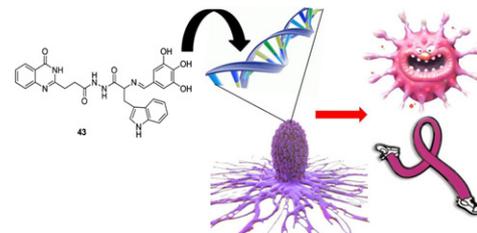


Anticancer and DNA binding studies of potential amino acids based quinazolinone analogs: Synthesis, SAR and molecular docking

Bioorganic Chemistry 87 (2019) pp. 252–264

K.P. Rakesh, H.K. Kumara, H.M. Manukumar, D. Channe Gowda*

Department of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, Karnataka, India



Characterization, quantitation, similarity evaluation and combination with Na⁺, K⁺-ATPase of cardiac glycosides from *Streblus asper*

Bioorganic Chemistry 87 (2019) pp. 265–275

Yidan Bai^{a,b}, Wanfang Zhu^a, Yunhui Xu^c, Zijian Xie^c, Toshihiro Akihisa^d, Jiradej Manosroi^{e,f}, Haopeng Sun^b, Feng Feng^a, Wenyuan Liu^{b,*}, Jie Zhang^{a,*}

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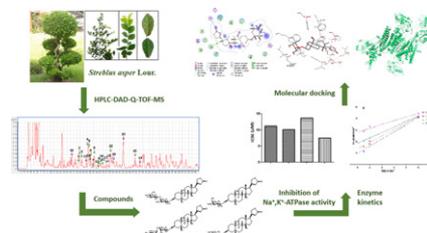
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Interaction of C20-substituted derivative of pregnenolone acetate with copper (II) leads to ROS generation, DNA cleavage and apoptosis in cervical cancer cells: Therapeutic potential of copper chelation for cancer treatment

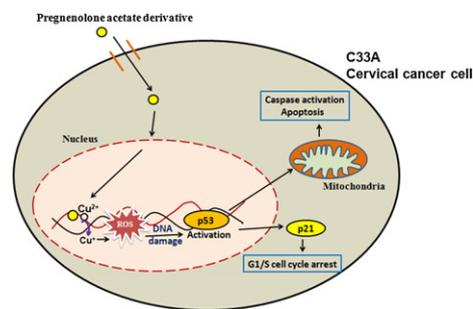
Atif Zafar^a, Swarnendra Singh^b, Sabahuddin Ahmad^c, Saman Khan^a, Mohammad Imran Siddiqi^c, Imrana Naseem^{a,*}

^aDepartment of Biochemistry, Faculty of Life Sciences, Aligarh Muslim University, Aligarh 202002, Uttar Pradesh, India

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Bioorganic Chemistry 87 (2019) pp. 276–290

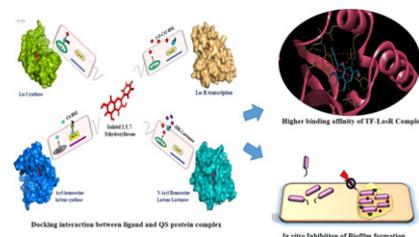


Inhibition of biofilm formation, quorum sensing activity and molecular docking study of isolated 3, 5, 7-Trihydroxyflavone from *Alstonia scholaris* leaf against *P. aeruginosa*

M. Abinaya, M. Gayathri*

Department of Biotechnology, School of Biosciences & Technology, Vellore Institute of Technology (VIT), Vellore 632014, Tamil Nadu, India

Bioorganic Chemistry 87 (2019) pp. 291–301



Synthesis, molecular docking studies, and antimicrobial evaluation of new structurally diverse ureas

Mahadev Patil^a, Anurag Noonikara Poyil^b, Shrinivas D. Joshi^c, Shivaputra A. Patil^d, Siddappa A. Patil^{a,*}, Alejandro Bugarin^{b,*}

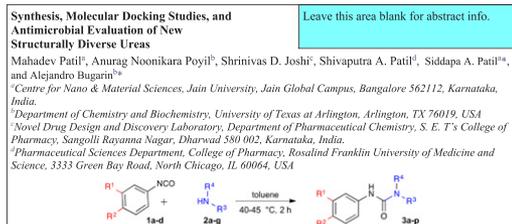
^aCentre for Nano & Material Sciences, Jain University, Jain Global Campus, Bangalore 562112, Karnataka, India

^bDepartment of Chemistry & Biochemistry, University of Texas at Arlington, Arlington, TX 76019, USA

^cNovel Drug Design and Discovery Laboratory, Department of Pharmaceutical Chemistry, S. E. T's College of Pharmacy, Sangolli Rayanna Nagar, Dharwad 580 002, Karnataka, India

^dPharmaceutical Sciences Department, College of Pharmacy, Rosalind Franklin University of Medicine and Science, 3333 Green Bay Road, North Chicago, IL 60064, USA

Bioorganic Chemistry 87 (2019) pp. 302–311



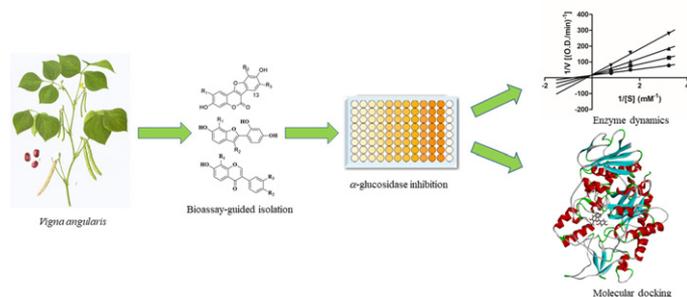
Bioassay-guided isolation of antioxidant and α -glucosidase inhibitory constituents from stem of *Vigna angularis*

Feng Guo^a, Shuoyang Zhang^a, Xiuying Yan^a, Yuhan Dan^a, Jian Wang^b, Yunli Zhao^{a,*}, Zhiguo Yu^{a,*}

^aDepartment of Pharmaceutical Analysis, School of Pharmacy, Shenyang Pharmaceutical University, Shenyang 110016, China

^bSchool of Pharmaceutical Engineering, Shenyang Pharmaceutical University, Shenyang 110016, China

Bioorganic Chemistry 87 (2019) pp. 312–320



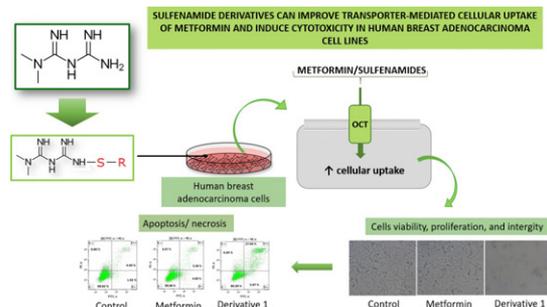
Sulfenamide derivatives can improve transporter-mediated cellular uptake of metformin and induce cytotoxicity in human breast adenocarcinoma cell lines

Magdalena Markowicz-Piasecka^{a,*}, Johanna Huttunen^b, Joanna Sikora^a,
Kristiina M. Huttunen^b

^aLaboratory of Bioanalysis, Department of Pharmaceutical Chemistry, Drug Analysis and Radiopharmacy, Medical University of Lodz, ul. Muszyńskiego1, 90-151 Lodz, Poland

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Bioorganic Chemistry 87 (2019) pp. 321–334



Synthesis of TPEN variants to improve cancer cells selective killing capacity

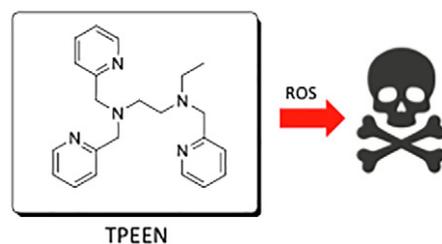
Stephanie Schaefer-Ramadan^a, Maciej Barlog^b, Jim Roach^c, Mohammed Al-Hashimi^b, Hassan S. Bazzi^b,
Khaled Machaca^{a,*}

^aDepartment of Physiology and Biophysics, Weill Cornell Medicine – Qatar, Doha, Qatar

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^cPre-Medical Education, Weill Cornell Medicine – Qatar, Doha, Qatar

Bioorganic Chemistry 87 (2019) pp. 366–372



Cytotoxic polyhydroxy serratene triterpenoids from *Lycopodium complanatum*

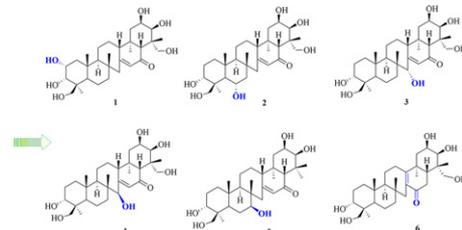
Qiuzhu Dong^a, Zhenxing Zou^a, Xiaohui Jia^c, Xia Yu^a, Jing Li^a, Wenhao Zhou^a,
Huihui Sun^a, Wei Wu^a, Guishan Tan^{a,b}, Kangping Xu^{a,*}

^aXiangya School of Pharmaceutical Sciences, Central South University, Changsha 410013, PR China

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^cSchool of Chemistry and Chemical Engineering, University of South China, Hengyang 421001, PR China

Bioorganic Chemistry 87 (2019) pp. 373–379



Novel 8-amino-1,2,4-triazolo[4,3- α]pyrazin-3-one derivatives as potent human adenosine A₁ and A_{2A} receptor antagonists. Evaluation of their protective effect against β -amyloid-induced neurotoxicity in SH-SY5Y cells

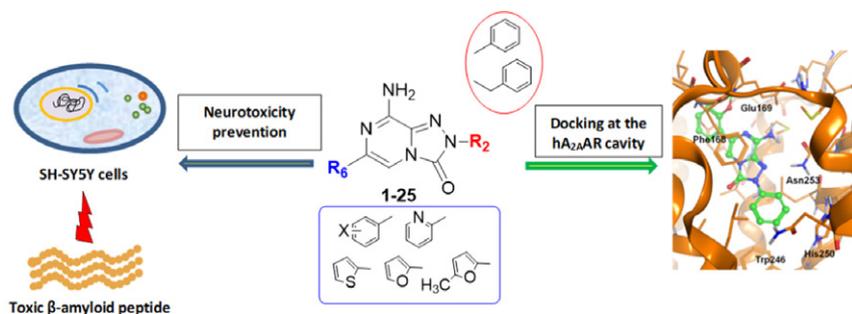
Bioorganic Chemistry 87 (2019) pp. 380–394

Matteo Falsini^a, Daniela Catarzi^a, Flavia Varano^a, Diego Dal Ben^b, Gabriella Marucci^b, Michela Buccioni^b, Rosaria Volpini^b, Lorenzo Di Cesare Mannelli^c, Carla Ghelardini^c, Vittoria Colotta^{a,*}

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^bScuola di Scienze del Farmaco e dei Prodotti della Salute, Università degli Studi di Camerino, via S. Agostino 1, 62032 Camerino, MC, Italy

^cDipartimento di Neuroscienze, Psicologia, Area del Farmaco e Salute del Bambino, Sezione di Farmacologia, Università degli Studi di Firenze, Viale Pieraccini 5, 50139 Firenze, Italy

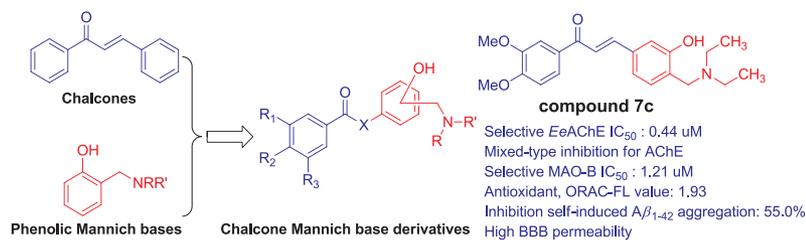


Design, synthesis and evaluation of chalcone Mannich base derivatives as multifunctional agents for the potential treatment of Alzheimer's disease

Bioorganic Chemistry 87 (2019) pp. 395–408

Xiaoyu Zhang, Qing Song, Zhongcheng Gao, Yan Li, Chaoquan Tian, Ziyi Yang, Heng Zhang, Yong Deng^{*}

Department of Medicinal Chemistry, Key Laboratory of Drug-Targeting and Drug Delivery System of the Education Ministry, Sichuan Engineering Laboratory for Plant-Sourced Drug and Sichuan Research Center for Drug Precision Industrial Technology, West China School of Pharmacy, Sichuan University, Chengdu 610041, PR China

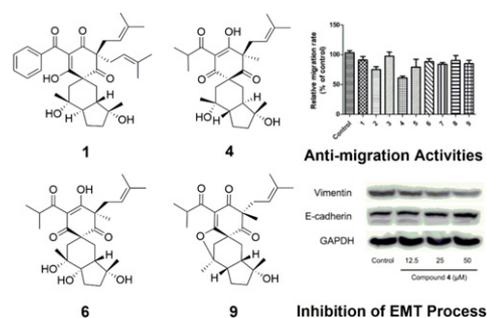


Hyperpatulols A–I, spirocyclic acylphloroglucinol derivatives with anti-migration activities from the flowers of *Hypericum patulum*

Bioorganic Chemistry 87 (2019) pp. 409–416

Yang-Yang Liu, Zhen Ao, Qi-Qi Xu, Dong-Rong Zhu, Chen Chen, Xiao-Bing Wang, Jian-Guang Luo^{*}, Ling-Yi Kong^{*}

Jiangsu Key Laboratory of Bioactive Natural Product Research and State Key Laboratory of Natural Medicines, School of Traditional Chinese Pharmacy, China Pharmaceutical University, 24 Tong Jia Xiang, Nanjing 210009, People's Republic of China



NO inhibitory phytochemicals as potential anti-inflammatory agents from the twigs of *Trigonostemon heterophyllus*

Yaru Xi^{a,1}, Lijun An^{a,1}, Xueyuan Yang^a, Ziteng Song^a, Jie Zhang^b, Muhetaer Tuerhong^c, Da-Qing Jin^d, Yasushi Ohizumi^e, Dongho Lee^f, Jing Xu^{a,*}, Yuanqiang Guo^{a,*}

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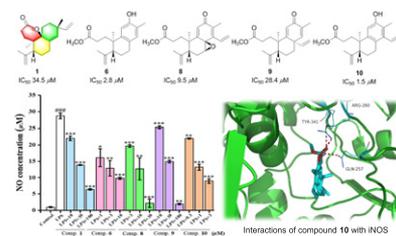
^cCollege of Chemistry and Environmental Sciences, Laboratory of Xinjiang Native Medicinal and Edible Plant Resources Chemistry, Kashgar University, Kashgar 844000, China

^dSchool of Medicine, Nankai University, Tianjin 300071, China

^eKansei Fukushi Research Institute, Tohoku Fukushi University, Sendai 989-3201, Japan

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Bioorganic Chemistry 87 (2019) pp. 417–424



Design, synthesis, and carbonic anhydrase inhibition activity of benzenesulfonamide-linked novel pyrazoline derivatives

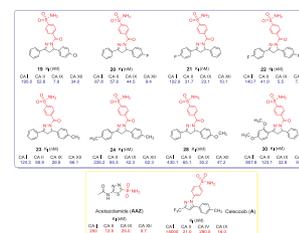
Alaa A.-M. Abdel-Aziz^{a,*}, Adel S. El-Azab^a, Silvia Bua^b, Alessio Nocentini^b, Mohamed A. Abu El-Enin^c, Mohammed M. Alanazi^a, Nawaf A. AlSai^a, Mohamed M. Hefnawy^a, Claudiu T. Supuran^{b,*}

^aDepartment of Pharmaceutical Chemistry, College of Pharmacy, King Saud University, Riyadh, Saudi Arabia

^bUniversità degli Studi di Firenze, NEUROFARBA Dept., Sezione di Scienze Farmaceutiche, Via Ugo Schiff 6, 50019 Sesto Fiorentino, Florence, Italy

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Bioorganic Chemistry 87 (2019) pp. 425–431



Organometallic ruthenium(II)-arene complexes with triphenylphosphine amino acid bioconjugates: Synthesis, characterization and biological properties

Margareta Pernar^{a,1}, Zoran Kokan^{b,1}, Juran Kralj^a, Zoran Glasovac^c, Lidija-Marija Tumir^c, Ivo Piantanida^c, Domagoj Eljuga^d, Iztok Turel^e, Anamaria Brozovic^{a,*}, Srečko I. Kirin^{b,*}

^aDivision of Molecular Biology, Ruđer Bošković Institute, Bijenička cesta 54, HR-10000 Zagreb, Croatia

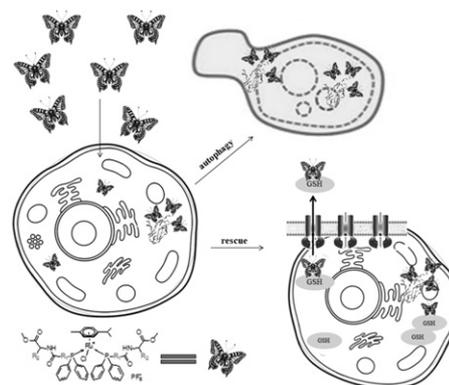
^bDivision of Materials Chemistry, Ruđer Bošković Institute, Bijenička cesta 54, HR-10000 Zagreb, Croatia

^cDivision of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, Bijenička cesta 54, HR-10000 Zagreb, Croatia

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^eFaculty of Chemistry and Chemical Technology, University of Ljubljana, Večna pot 113, SLO-1000 Ljubljana, Slovenia

Bioorganic Chemistry 87 (2019) pp. 432–446



Bioactive terpenoids from *Euonymus verrucosus* var. *pauciflorus* showing NO inhibitory activities

Yuling Yang^{a,1}, Xueyuan Yang^{a,1}, Xuke Zhang^a, Ziteng Song^a,
Feng Liu^a, Yue Liang^a, Jie Zhang^b, Da-Qing Jin^c, Jing Xu^{a,*},
Dongho Lee^d, Muhetaer Tuerhong^e, Yasushi Ohizumi^f,
Yuanqiang Guo^{a,*}

^aState 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

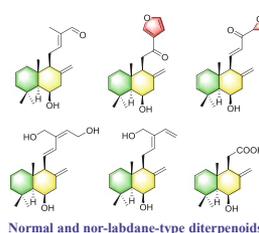
^bKey Laboratory for Green Processing of Chemical Engineering of Xinjiang Bingtuan, School of Chemistry and Chemical Engineering, Shihezi University, Shihezi 832003, People's Republic of China

^cSchool of Medicine, Nankai University, Tianjin 300071, People's Republic of China

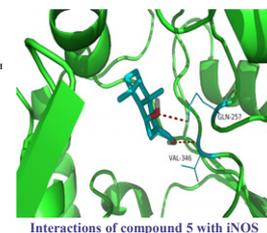
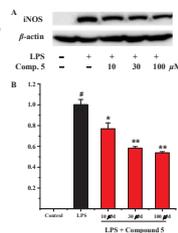
^dDepartment of Biosystems and Biotechnology, College of Life Sciences and Biotechnology, Korea University, Seoul 02841, Republic of Korea

^eCollege of Chemistry and Environmental Sciences, Laboratory of Xinjiang Native Medicinal and Edible Plant Resources Chemistry, Kashgar University, Kashgar 844000, People's Republic of China

^fKansei Fukushi Research Institute, Tohoku Fukushi University, Sendai 989-3201, Japan



Normal and non-labdane-type diterpenoids



Interactions of compound 5 with iNOS

Bioorganic Chemistry 87 (2019) pp. 447–456

Design and synthesis of mono- and di-pyrazolyl-s-triazine derivatives, their anticancer profile in human cancer cell lines, and *in vivo* toxicity in zebrafish embryos

Muhammad Farooq^a, Anamika Sharma^b, Zainab Almarhoon^c, Abudalla Al-Dhfyhan^{d,e},
Ayman El-Faham^{e,f,*}, Nael Abu Taha^a, Mohammad A.M. Wadaan^a, Beatriz G. de la Torre^{b,g},
Fernando Albericio^{b,c,h,i,j}

^aBioproducts Research Chair, College of Science, Department of Zoology, King Saud University, P.O. Box 2455, Riyadh 11451, Saudi Arabia

^bCatalysis and Peptide Research Unit, School of Health Sciences, University of KwaZulu-Natal, University Road, Westville, Durban 4001, South Africa

^cDepartment of Chemistry, College of Science, King Saud University, P.O. Box 2455, Riyadh 11451, Saudi Arabia

^dDepartment of Pharmacology and Toxicology, College of Pharmacy, King Saud University, P. O. Box 2457, Riyadh, Saudi Arabia

^eStem Cell & Tissue Re-Engineering, King Faisal Specialist Hospital and Research Center, Riyadh 11211, Saudi Arabia

^fDepartment of Chemistry, Faculty of Science, Alexandria University, P.O. Box 426, Alexandria 21321, Egypt

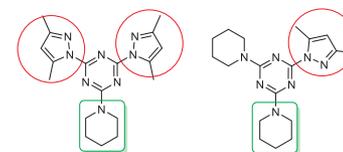
^gKRISP, College of Health Sciences, University of KwaZulu-Natal, Westville, Durban 4001, South Africa

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Bioorganic Chemistry 87 (2019) pp. 457–464



	MCF7	MDA-MB-231	HepG2	LoVo	K-562
4a	7.5 ± 0.43	14 ± 0.21	17.5 ± 0.25	6.1 ± 0.24	9.8 ± 0.04
6g	5 ± 0.04	15 ± 0.24	21.2 ± 0.13	8.4 ± 0.16	5.9 ± 0.21

Meglumine as a green, efficient and reusable catalyst for synthesis and molecular docking studies of bis(indolyl)methanes as antioxidant agents

Bakthavatchala Reddy Nemallapudi^a,
Grigory V. Zyryanov^{a,b}, Balakrishna Avula^c,
Mallikarjuna Reddy Guda^a,
Suresh Reddy Cirandur^d,
Chintha Venkataramaiah^e,
Wudayagiri Rajendra^e, Sravya Gundala^{a,*}

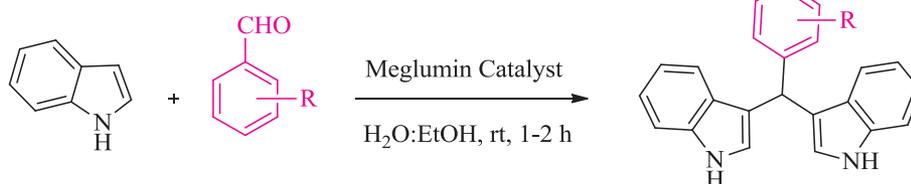
^aChemical Engineering Institute, Ural Federal University, Yekaterinburg 620002, Russian Federation

^bUral Division of the Russian Academy of Sciences, I. Ya. Postovskiy Institute of Organic Synthesis, 22 S. Kovalevskoy Street, Yekaterinburg 620219, Russian Federation

^cRajeev Gandhi Memorial College of Engineering and Technology (Autonomous), Nandyal 518501, Andhra Pradesh, India

^dDepartment of Chemistry, Sri Venkateswara University, Tirupati 517 502, Andhra Pradesh, India

^eDivision of molecular biology, Department of Zoology, Sri Venkateswara University, Tirupati 517502, Andhra Pradesh, India



Bioorganic Chemistry 87 (2019) pp. 465–473

Semi-synthetic isoflavones as BACE-1 inhibitors against Alzheimer's disease

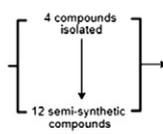
Giovanni Ribauda^{a,1}, Paolo Coghi^{b,1},
Enrico Zanforlin^{a,1}, Betty Yuen Kwan Law^b,
Yuki Yu Jun Wu^b, Yu Han^b,
Alena Congling Qiu^b, Yuan Qing Qu^b,
Giuseppe Zagotto^{a,*}, Vincent Kam Wai Wong^{b,*}

^aDepartment of Pharmaceutical and Pharmacological Sciences, University of Padova, Via Marzolo 5, 35131 Padova, Italy

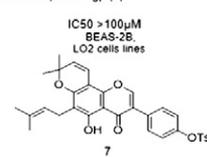
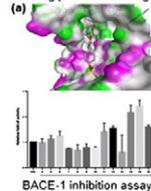
^bState Key Laboratory of Quality Research in Chinese Medicine, Macau University of Science and Technology, Avenida Wai Long, Taipa, Macau



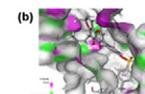
Maclura Pomifera (Osage Orange)



Docking pose of 7 on target BACE-1 (a) and P-gp (b)



IC50 >100µM
BEAS-2B,
LO2 cell lines



P-gp GLO activity assay (ATP assay)

Bioorganic Chemistry 87 (2019) pp. 474–483

Synthesis and biological evaluation of new bisindole-imidazopyridine hybrids as apoptosis inducers

Satish Sunkari^{a,b}, Srinivasa Reddy Bonam^{b,c,1}, A.V. Subba Rao^{a,2}, Sd Riyaz^d, V. Lakshma Nayak^a,
Halmuthur Mahabalarao Sampath Kumar^{b,c}, Ahmed Kamal^{a,b,e,*}, Bathini Nagendra Babu^{a,b,*}

^aCentre for Semio Chemicals, CSIR-Indian Institute of Chemical Technology (IICT), Hyderabad 500007, India

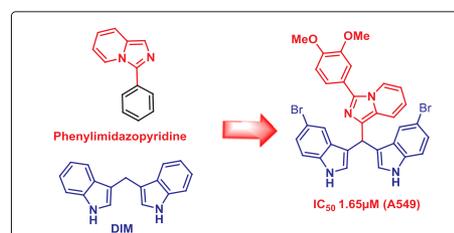
^bAcademy of Scientific and Innovative Research, New Delhi 110 025, India

^cVaccine Immunology Laboratory, Natural Product Chemistry Division, CSIR-Indian Institute of Chemical Technology (IICT), Hyderabad 500007, India

^dDepartment of Chemistry, Jawaharlal Nehru Technological University, Hyderabad 500085, India

^eSchool of Pharmaceutical Education and Research (SPER), Jamia Hamdard, New Delhi 110062, India

Bioorganic Chemistry 87 (2019) pp. 484–494

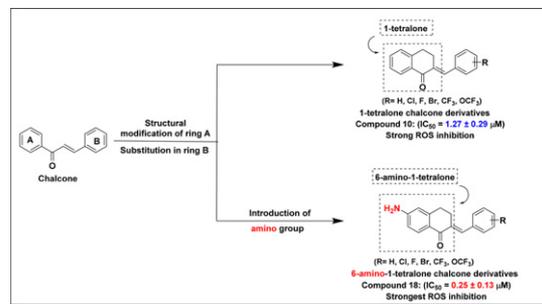


Introduction of amino moiety enhances the inhibitory potency of 1-tetralone chalcone derivatives against LPS-stimulated reactive oxygen species production in RAW 264.7 macrophages

Pramila Katila¹, Aastha Shrestha¹, Aarajana Shrestha, Ritina Shrestha, Pil-Hoon Park^{*}, Eung-Seok Lee^{*}

College of Pharmacy, Yeungnam University, Gyeongsan 38541, Republic of Korea

Bioorganic Chemistry 87 (2019) pp. 495–505



New benzyl pyridinium derivatives bearing 2,4-dioxochroman moiety as potent agents for treatment of Alzheimer's disease: Design, synthesis, biological evaluation, and docking study

Marjan Mollazadeh^a, Maryam Mohammadi-Khanaposhtani^b, Afsaneh Zonouzi^{b,*}, Hamid Nadri^c, Zahra Najafi^{d,e}, Bagher Larijani^f, Mohammad Mahdavi^{f,*}

^aSchool of Chemistry, College of Science, University of Tehran, Tehran, Iran

^bCellular and Molecular Biology Research Center, Health Research Institute, Babol University of Medical Sciences, Babol, Iran

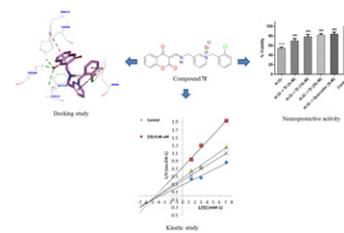
^cDepartment of Medicinal Chemistry, Faculty of Pharmacy and Pharmaceutical Sciences Research Center, Shahid Sadoughi University of Medical Sciences, Yazd, Iran

^dDepartment of Medicinal Chemistry, School of Pharmacy, Hamadan University of Medical Sciences, Hamadan, Iran

^eMedicinal Plants and Natural Products Research Center, Hamadan University of Medical Sciences, Hamadan, Iran

^fEndocrinology and Metabolism Research Center, Endocrinology and Metabolism Clinical Sciences Institute, Tehran University of Medical Sciences, Tehran, Iran

Bioorganic Chemistry 87 (2019) pp. 506–515



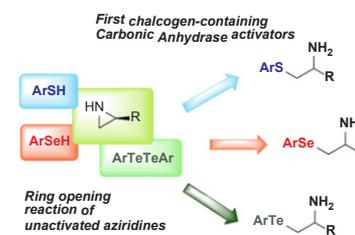
Sulfur, selenium and tellurium containing amines act as effective carbonic anhydrase activators

Damiano Tanini^a, Antonella Capperucci^a, Claudiu T. Supuran^{b,*}, Andrea Angeli^{b,*}

^aUniversity of Florence, Department of Chemistry "Ugo Schiff", Via della Lastruccia 3-13, I-50019 Sesto Fiorentino, Italy

^bUniversity of Florence, NEUROFARBA Dept., Sezione di Scienze Farmaceutiche, Via Ugo Schiff 6, 50019 Sesto Fiorentino, Florence, Italy

Bioorganic Chemistry 87 (2019) pp. 516–522



Natural product-based design, synthesis and biological evaluation of 2',3,4'-tetrahydrochalcone analogues as antiviral agents

Hui Zhong^a, Jia Zhou^{a,*}, Xiao-Hong An^a, Ying-Rong Hua^a, Yi-Fan Lai^a, Rui Zhang^a, Owais Ahmad^a, Ye Zhang^{b,c,*}, Jing Shang^{a,*}

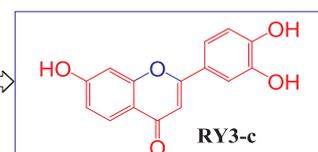
^aState Key Laboratory of Natural Medicines, Jiangsu Key Laboratory of TCM Evaluation and Translational Research, School of Traditional Chinese Pharmacy, China Pharmaceutical University, Nanjing 211198, China

^bSchool of Pharmacy, Guilin Medical University, Guilin 541004, China

^cState Key Laboratory for Chemistry and Molecular Engineering of Medicinal Resources, School of Chemistry and Pharmacy, Guangxi Normal University, Guilin 541004, China



Design & Synthesis



Bioorganic Chemistry 87 (2019) pp. 523–533

Dual targeting of PTP1B and glucosidases with new bifunctional iminosugar inhibitors to address type 2 diabetes

Bioorganic Chemistry 87 (2019) pp. 534–549

Xhenti Ferhati^{a,1}, Camilla Matassini^{a,1}, Maria Giulia Fabbrini^a, Andrea Goti^{a,b},
Amelia Morrone^c, Francesca Cardona^{a,b,e}, Antonio J. Moreno-Vargas^d, Paolo Paoli^{c,e*}

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^cPaediatric Neurology Unit and Laboratories, Neuroscience Department, Meyer Children's Hospital, and Department of Neurosciences, Pharmacology and Child Health, University of Florence, Viale Pieraccini n. 24, 50139 Firenze, Italy

^dDepartamento de Química Orgánica, Facultad de Química, Universidad de Sevilla, n/Prof. García González 1, E-41012 Sevilla, Spain

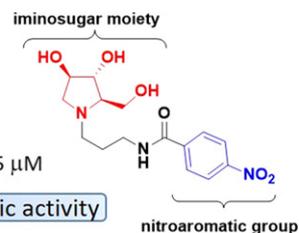
^eDepartment of Experimental and Clinical Biomedical Sciences, University of Florence, Viale Morgagni 50, 50134 Florence, Italy

A new bifunctional inhibitor to address type 2 diabetes

PTP1B $IC_{50} = 31 \mu M$

α -glucosidase $IC_{50} = 25 \mu M$

ex vivo insulino-mimetic activity

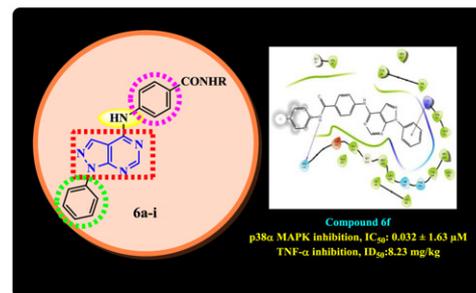


Synthesis, evaluation and docking of novel pyrazolo pyrimidines as potent p38 α MAP kinase inhibitors with improved anti-inflammatory, ulcerogenic and TNF- α inhibitory properties

Bioorganic Chemistry 87 (2019) pp. 550–559

Kanagasabai Somakala, Sana Tariq, Mohd. Amir*

Department of Pharmaceutical Chemistry, School of Pharmaceutical Education and Research, Jamia Handard, New Delhi 110062, India



Antiproliferative effect, cell cycle arrest and apoptosis generation of novel synthesized anticancer heterocyclic derivatives based 4H-benzo [h] chromene

Bioorganic Chemistry 87 (2019) pp. 560–571

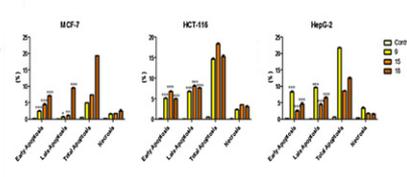
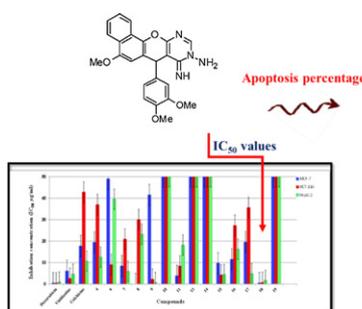
Fawzia F. Alblewi^{a,*}, Rawda M. Okasha^a, Zainab M. Hritani^a,
Hany M. Mohamed^{b,c}, Mohammed A.A. El-Nassag^{b,c},
Ahmed H. Halawa^c, Ahmed Mora^c, Ahmed M. Fouda^d,
Mohammed A. Assiri^d, Al-Anood M. Al-Dies^d, Tarek H. Afifi^a,
Ahmed M. El-Agrody^c

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^cChemistry Department, Faculty of Science, Al-Azhar University, Nasr City 11884, Cairo, Egypt

^dChemistry Department, Faculty of Science, King Khalid University, Abha, 61413, P.O. Box 9004, Saudi Arabia



Multi-target-directed triazole derivatives as promising agents for the treatment of Alzheimer's disease

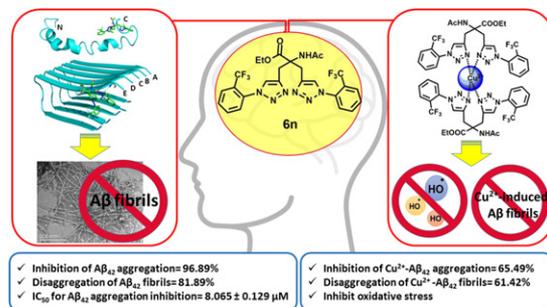
Bioorganic Chemistry 87 (2019) pp. 572–584

Anupamjeet Kaur^a, Sukhmani Mann^a, Amandeep Kaur^a, Nitesh Priyadarshi^c, Bhupesh Goyal^{b,*}, Nitin Kumar Singhal^{c,*}, Deepti Goyal^{a,*}

^aDepartment of Chemistry, Faculty of Basic and Applied Sciences, Sri Guru Granth Sahib World University, Fatehgarh Sahib 140406, Punjab, India

^bSchool of Chemistry and Biochemistry, Thapar Institute of Engineering & Technology, Patiala 147004, Punjab, India

^cNational Agri-Food Biotechnology Institute, S.A.S. Nagar, Punjab, India



Withanolides from *Physalis peruviana* showing nitric oxide inhibitory effects and affinities with iNOS

Bioorganic Chemistry 87 (2019) pp. 585–593

Bangjian Dong^a, Lijun An^a, Xueyuan Yang^a, Xuke Zhang^a, Jie Zhang^b, Muhetaer Tuerhong^c, Da-Qing Jin^d, Yasushi Ohizumi^e, Dongho Lee^f, Jing Xu^{a,*}, Yuanqiang Guo^{a,*}

^aState Key Laboratory of Medicinal Chemical Biology, College of Pharmacy, and Tianjin Key Laboratory of Molecular Drug Research, Nankai University, Tianjin 300050, People's Republic of China

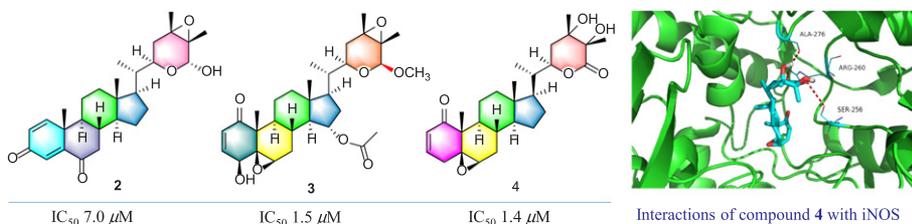
^bKey Laboratory for Green Processing of Chemical Engineering of Xinjiang Bingtuan, School of Chemistry and Chemical Engineering, Shihezi University, Shihezi 832003, People's Republic of China

^cCollege of Chemistry and Environmental Sciences, Laboratory of Xinjiang Native Medicinal and Edible Plant Resources Chemistry, Kashgar University, Kashgar 844000, People's Republic of China

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^eDepartment of Medical Biochemistry, School of Pharmaceutical Sciences, University of Shizuoka, Shizuoka 422-8526, Japan

^fDepartment of Biosystems and Biotechnology, College of Life Sciences and Biotechnology, Korea University, Seoul 136-713, Republic of Korea

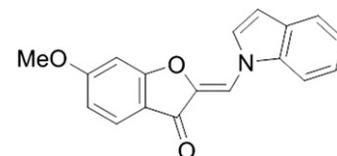


Design, synthesis and evaluation of 2-(indolylmethylidene)-2,3-dihydro-1-benzofuran-3-one and 2-(indolyl)-4H-chromen-4-one derivatives as novel monoamine oxidases inhibitors

Bioorganic Chemistry 87 (2019) pp. 594–600

Koichi Takao^{*}, Shiori U, Hitoshi Kamauchi, Yoshiaki Sugita

Laboratory of Bioorganic Chemistry, Department of Pharmaceutical Sciences, Faculty of Pharmacy and Pharmaceutical Sciences, Josai University, 1-1 Keyaki-dai, Sakado, Saitama 350-0295, Japan



9a: IC₅₀ = 0.0026 μM

Aureone-indole hybrids

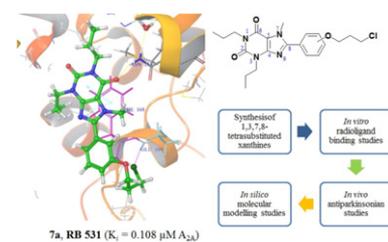
Synthesis, biological evaluation and molecular modelling studies of 1,3,7,8-tetrastituted xanthenes as potent and selective A_{2A} AR ligands with *in vivo* efficacy against animal model of Parkinson's disease

Suman Rohilla^a, Ranju Bansal^{a,*}, Sonja Kachler^b, Karl-Norbert Klotz^b

^aUniversity Institute of Pharmaceutical Sciences, Panjab University, Chandigarh

^bInstitut für Pharmakologie und Toxikologie, Universität Würzburg, Germany

Bioorganic Chemistry 87 (2019) pp. 601–612



New phosphate derivatives of betulin as anticancer agents: Synthesis, crystal structure, and molecular docking study

Elwira Chrobak^{a,*}, Monika Kadela-Tomanek^a, Ewa Bębenek^a, Krzysztof Marciniak^a, Joanna Wietrzyk^b, Justyna Trynda^b, Bartosz Pawełczak^c, Joachim Kusz^d, Janusz Kasperczyk^{e,f}, Ewa Chodurek^e, Piotr Padaszyński^e, Stanisław Boryczka^a

^aMedical University of Silesia in Katowice, School of Pharmacy with the Division of Laboratory Medicine in Sosnowiec, Department of Organic Chemistry, 4 Jagiellońska Str., 41-200 Sosnowiec, Poland

^bPolish Academy of Sciences, Ludwik Hirszfeld Institute of Immunology and Experimental Therapy, Department of Experimental Oncology, 12 R. Weigla Str., 53-114 Wrocław, Poland

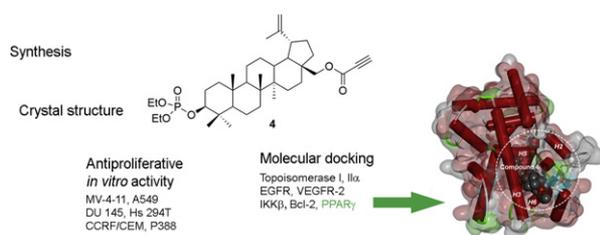
^cRainbow Pharmacy, 25 Jana Matejki Str., 43-600 Jaworzno, Poland

^dUniversity of Silesia, Institute of Physics, 1 75 Pułku Piechoty Str., 41 500 Chorzów, Poland

^eMedical University of Silesia in Katowice, School of Pharmacy with the Division of Laboratory Medicine in Sosnowiec, Department of Biopharmacy, 8 Jedności Str., 41-200 Sosnowiec, Poland

^fCentre of Polymer and Carbon Materials, Polish Academy of Sciences, 34 Curie-Skłodowska Str., 41-819 Zabrze, Poland

Bioorganic Chemistry 87 (2019) pp. 613–628



Tick-borne flavivirus reproduction inhibitors based on isoxazole core linked with adamantane

Dmitry A. Vasilenko^a, Evgenia V. Dueva^{a,b,1}, Liubov I. Kozlovskaya^{b,c}, Nikolay A. Zefirov^{a,d}, Yuri K. Grishin^a, Gennady M. Butov^e, Vladimir A. Palyulin^{a,d}, Tamara S. Kuznetsova^a, Galina G. Karganova^{b,c}, Olga N. Zefirova^{a,d}, Dmitry I. Osolodkin^{a,b,c,*}, Elena B. Averina^{a,d,*}

^aDepartment of Chemistry, Lomonosov Moscow State University, Leninskie Gory 1 bd. 3, Moscow 119991, Russia

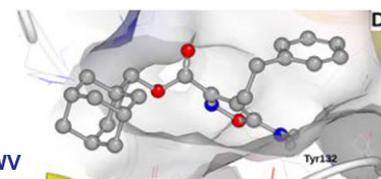
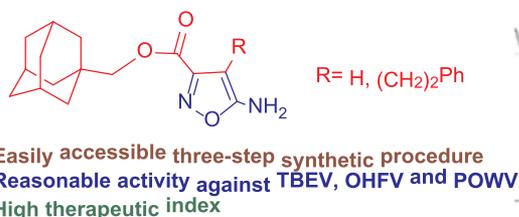
^bFSBSI "Chumakov FSC R&D IBP RAS", Moscow 108819, Russia

^cSechenov First Moscow State Medical University, Moscow 119991, Russia

^dInstitute of Physiologically Active Compounds, Severny Proezd 1, Chernogolovka, Moscow Region 142432, Russia

^eVolgograd State Technical University, Lenina Avenue 28, Volgograd 400005, Russia

Bioorganic Chemistry 87 (2019) pp. 629–637



Discovery of new inhibitors against both NF- κ B and osteoclastogenesis from in-house library with α , β -unsaturated-enone fragment

Chao Zhao^a, Dane Huang^{a,b}, Ruyue Li^{b,d}, Jiake Xu^e, Qiong Gu^{a,*}, Jun Xu^{a,c,*}

^aResearch Center for Drug Discovery, School of Pharmaceutical Sciences, Sun Yat-sen University, Guangzhou 510006, People's Republic of China

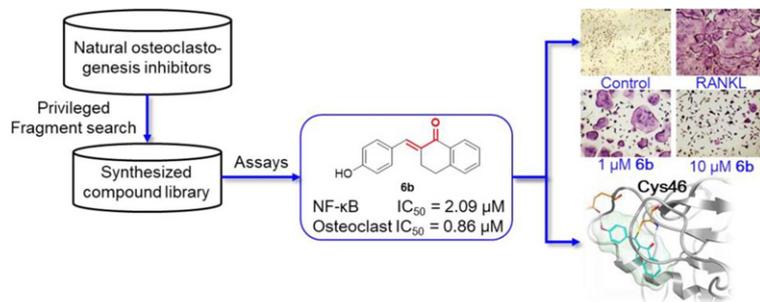
^bGuangdong Province Engineering Technology Research Institute of T. C. M., Guangdong Provincial Key Laboratory of Research and Development in Traditional Chinese Medicine, Guangzhou 510095, People's Republic of China

^cSchool of Biotechnology and Health Sciences, Wuyi University, 99 Yingbin Road, Jiangmen 529020, People's Republic of China

^dGuangzhou University of Chinese Medicine, Guangdong Second Traditional Chinese Medicine Hospital, Guangzhou 510095, People's Republic of China

^eMolecular Laboratory, School of Biomedical Science, University of Western Australia, Perth, Western Australia, Australia

Bioorganic Chemistry 87 (2019) pp. 638–646



In vitro and in silico studies of novel synthetic ACE-inhibitory peptides derived from *Saccharomyces cerevisiae* protein hydrolysate

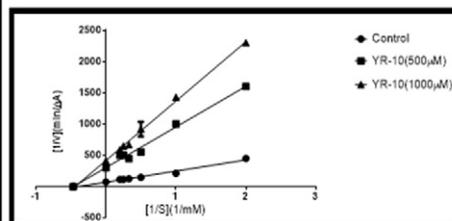
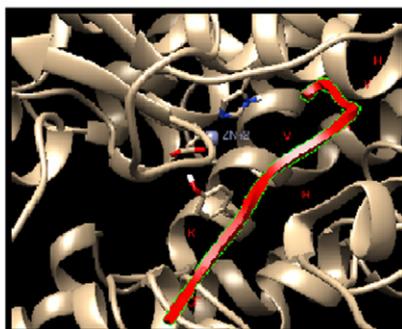
Mahta Mirzaei^{a,*}, Saeed Mirdamadi^{b,*}, Maliheh Safavi^b, Mahnaz Hadizadeh^b

^aDepartment of Food Science and Technology, Shahr-e-Qods Branch, Islamic Azad University, Tehran, Iran

^bDepartment of Biotechnology, Iranian Research Organization for Science & Technology (IROST), Tehran, Iran

Bioorganic Chemistry 87 (2019) pp. 647–654

YR-10	Y	G	K	P	V	A	V	P	A	R
GA-8		G	K	P	V	A	V	P	A	
GHA-8		G	K	H	V	A	V	H	A	
YHR-10	Y	G	K	H	V	A	V	H	A	R
PAR-3								P	A	R

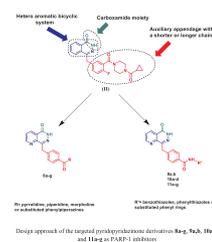


Design and synthesis of novel PARP-1 inhibitors based on pyridopyridazinone scaffold

Ghada F. Elmasry^{*}, Enayat E. Aly, Fadi M. Awadallah, Samir M. El-Moghazy

Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Cairo University, El-Kasr El-Eini Street, P.O. Box 11562, Cairo, Egypt

Bioorganic Chemistry 87 (2019) pp. 655–666



Unveiling novel diphenyl-1H-pyrazole based acrylates tethered to 1,2,3-triazole as promising apoptosis inducing cytotoxic and anti-inflammatory agents

Bioorganic Chemistry 87 (2019) pp. 667–678

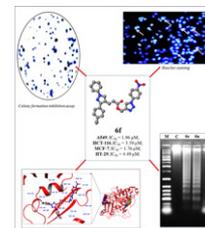
Mohammed Faraz Khan^a, Tarique Anwer^b, Afroz Bakht^c, Garima Verma^a, Wasim Akhtar^a, M. Mumtaz Alam^a, Moshahid Alam Rizvi^d, Mymoon Akhter^a, Mohammad Shaquiquzzaman^{a,*}

^aDrug Design and Medicinal Chemistry Lab, Department of Pharmaceutical Chemistry, School of Pharmaceutical Education and Research, Jamia Hamdard, New Delhi 110062, India

^bDepartment of Pharmacology, College of Pharmacy, Jazan University, PO Box 114, Gizan, Saudi Arabia

^cDepartment of Chemistry, College of Science and Humanities, Prince Sattam bin Abdulaziz University, P.O. Box- 173, Al-Kharj, Saudi Arabia

^dThe Genome Biology Lab, Department of Biosciences, Jamia Millia Islamia, New Delhi 110025, India



5-Thioxoimidazolidine-2-one derivatives: Synthesis, anti-inflammatory activity, analgesic activity, COX inhibition assay and molecular modelling study

Bioorganic Chemistry 87 (2019) pp. 679–687

Marwa A.M.Sh. El-Sharief^{a,b,*}, Samir Y. Abbas^{c,*}, Ahmed M.Sh. El-Sharief^d, Nermien M. Sabry^a, Ziad Moussa^e, Shahenda M. El-Messery^f, Ahmed R. Elsheikh^g, Ghada S. Hassan^{h,*}, Mardia T. El Sayed^a

^aApplied Organic Chemistry Department, National Research Centre, Cairo, Egypt

^bFaculty of Science and Arts, Mohail Asser, King Khalid University, Saudi Arabia

^cOrganometallic and Organometalloid Chemistry Department, National Research Centre, Cairo, Egypt

^dChemistry Department, Faculty of Science, Al-Azhar University (Boys), Cairo, Egypt

^eDepartment of Chemistry, College of Science, United Arab Emirates University, P.O. Box 15551, Al-Ain, United Arab Emirates

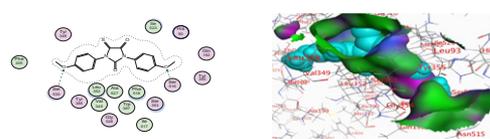
^fDepartment of Pharmaceutical Organic Chemistry, Faculty of Pharmacy, Mansoura University, Mansoura, Egypt

^gDepartment of Pharmacology and Toxicology, Faculty of Pharmacy, Mansoura University, Mansoura, Egypt

^hDepartment of Medicinal Chemistry, Faculty of Pharmacy, Mansoura University, Mansoura, Egypt

5-Thioxoimidazolidine-2-one derivatives: Synthesis, anti-inflammatory activity, analgesic activity, COX inhibition assay and molecular modelling study

Marwa A. M. Sh. El-Sharief^{a,b,*}, Samir Y. Abbas^{c,*}, Ahmed M. Sh. El-Sharief^d, Nermien M. Sabry^a, Ziad Moussa^e, Shahenda M. El-Messery^f, Ahmed R. Elsheikh^g, Ghada S. Hassan^{h,*}, Mardia T. El Sayed^a



Sangganen O induced apoptosis of A549 cells is counterbalanced by protective autophagy

Bioorganic Chemistry 87 (2019) pp. 688–698

Zhong-Rui Li¹, Ting Ma¹, Yan-Jia Guo, Bo Hu, Sheng-Hui Niu, Feng-Zhi Suo, Lin-Na Du, Ying-Hua You, Wen-Ting Kang, Shuan Liu, MAA Mamun, Qi-Meng Song, Jing-Ru Pang, Yi-Chao Zheng², Hong-Min Liu²

Collaborative Innovation Center of New Drug Research and Safety Evaluation, Henan Province, PR China

Key Laboratory of Advanced Drug Preparation Technologies (Zhengzhou University), Ministry of Education of China, PR China

Key Laboratory of Henan Province for Drug Quality and Evaluation, PR China

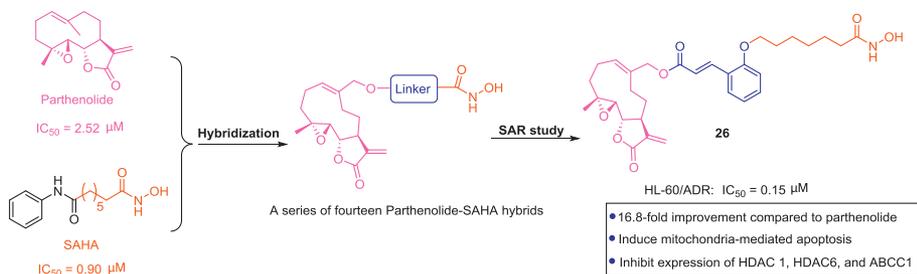
School of Pharmaceutical Sciences, Zhengzhou University, Zhengzhou 450001, PR China



Design and synthesis of parthenolide-SAHA hybrids for intervention of drug-resistant acute myeloid leukemia

Weizhi Ge^a, Zhongquan Liu^a, Yu Sun^b, Tianpeng Wang^a, Hongyu Guo^a, Xinyi Chen^a, Shengzu Li^a, Mengmeng Wang^c, Yue Chen^{a,*}, Yahui Ding^{a,*}, Quan Zhang^{a,*}

^aState Key Laboratory of Medicinal Chemical Biology, College of Pharmacy and Tianjin Key Laboratory of Molecular Drug Research, Nankai University, Haihe Education Park, 38 Tongyan Road, Tianjin 300353, People's Republic of China
^bCollege of Life Sciences, Nankai University, Tianjin 300353, People's Republic of China
^cAccurate Company, Ltd., Tianjin 300384, People's Republic of China

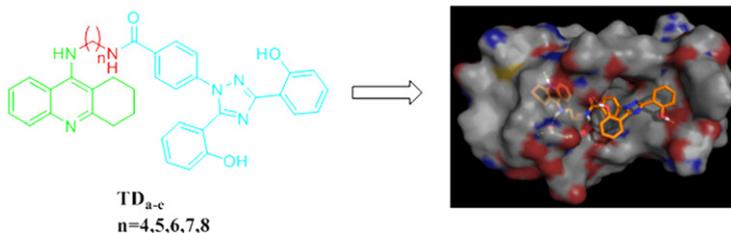


Bioorganic Chemistry 87 (2019) pp. 699–713

Design, synthesis and evaluation of a novel metal chelator as multifunctional agents for the treatment of Alzheimer's disease

Yingying Wang^a, Yue Yang^a, Kwon Ho Hong^b, Yao Ning^a, Ping Yu^a, Jinghui Ren^a, Min Ji^{c,d}, Jin Cai^{a,d,*}

^aSchool of Chemistry and Chemical Engineering, Southeast University, Nanjing, Jiangsu 211189, PR China
^bDepartment of Medicinal Chemistry and the Institute for Therapeutics Discovery and Development, University of Minnesota, Minneapolis, MN 55414, USA
^cSchool of Biological Science & Medical Engineering, Southeast University, Nanjing 210096, PR China
^dSuzhou Key Laboratory of Biomaterials and Technologies & Collaborative Innovation Center of Suzhou Nano Science and Technology, Suzhou 215123, PR China

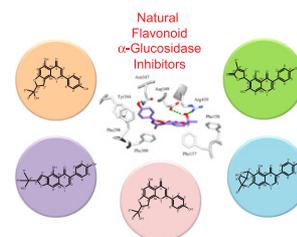


Bioorganic Chemistry 87 (2019) pp. 720–727

Natural flavonoid α -glucosidase inhibitors from *Retama raetam*: Enzyme inhibition and molecular docking reveal important interactions with the enzyme active site

Usman Ghani^{a,*}, Mohammad Nur-e-Alam^b, Muhammad Yousaf^b, Zaheer Ul-Haq^c, Omar M. Noman^b, Adnan J. Al-Rehaily^b

^aClinical Biochemistry Unit, Department of Pathology, College of Medicine, King Saud University, Riyadh 11461, Saudi Arabia
^bDepartment of Pharmacognosy, College of Pharmacy, King Saud University, P.O. Box. 2457, Riyadh 11451, Saudi Arabia
^cDr. Panjwani Center for Molecular Medicine and Drug Research, International Center for Chemical and Biological Sciences, University of Karachi, Karachi 75210, Pakistan



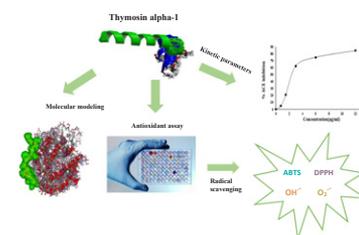
Bioorganic Chemistry 87 (2019) pp. 736–742

Antioxidant and angiotensin-converting enzyme (ACE) inhibitory activity of thymosin alpha-1 (Th α 1) peptide

Jasmin Kharazmi-Khorassani^a, Ahmad Asoodeh^{a,*}, Hamid Tanzadehpanah^b

^aDepartment of Chemistry, Faculty of Science, Ferdowsi University of Mashhad, Mashhad, Iran
^bResearch Center for Molecular Medicine, Hamadan University of Medical Sciences, Hamadan, Iran

Bioorganic Chemistry 87 (2019) pp. 743–752



Design, synthesis and biological evaluation of *Helicobacter pylori* inosine 5'-monophosphate dehydrogenase (HpIMPDH) inhibitors. Further optimization of selectivity towards HpIMPDH over human IMPDH2

Bioorganic Chemistry 87 (2019) pp. 753–764

Chetan P. Shah^a, Gayathri Purushothaman^b, Vijay Thiruvankatam^{b,c}, Sivapriya Kirubakaran^{b,d}, Kapil Juvale^a, Prashant S. Kharkar^{a,*}

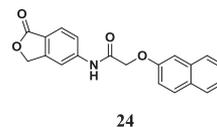
^aShobhaben Pratapbhai Patel School of Pharmacy and Technology Management, SVKM's NMIMS

(Deemed to be University), V. L. Mehta Road, Vile Parle (West), Mumbai 400 056, India

^bBiological Engineering, Indian Institute of Technology Gandhinagar, Palaj, Gandhinagar 382355, India

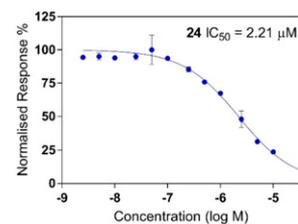
^cPhysics, Indian Institute of Technology Gandhinagar, Palaj, Gandhinagar 382355, India

^dChemistry, Indian Institute of Technology Gandhinagar, Palaj, Gandhinagar 382355, India



24

Inhibition: HpIMPDH: ~87%
hIMPDH2: <0.1%
(@ 10 M)



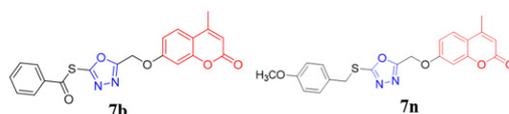
Synthesis and biological evaluation of coumarin-1,3,4-oxadiazole hybrids as selective carbonic anhydrase IX and XII inhibitors

Bioorganic Chemistry 87 (2019) pp. 765–772

Sridhar Goud Narella^a, Mohammed Ghouse Shaik^a, Arifuddin Mohammed^a, Mallika Alvala^{a,*}, Andrea Angel^b, Claudiu T. Supuran^{b,*}

^aDepartment of Medicinal Chemistry, National Institute of Pharmaceutical Education and Research (NIPER), Balanagar, Hyderabad 500037, India

^bUniversità degli Studi di Firenze, Neurofarba Dept., Sezione di Scienze Farmaceutiche e Nutraceutiche, Via Ugo Schiff 6, 50019 Sesto Fiorentino, Florence, Italy



7b
hCA I K_i > 100 μM hCA II K_i > 100 μM
hCA IX K_i = 7.83 μM hCA XII K_i = 0.16 μM

7n
hCA I K_i > 100 μM hCA II K_i > 100 μM
hCA IX K_i = 2.34 μM hCA XII K_i = 9.67 μM

Probing the antibacterial and anticancer potential of tryptamine based mixed ligand Schiff base Ruthenium(III) complexes

Bioorganic Chemistry 87 (2019) pp. 773–782

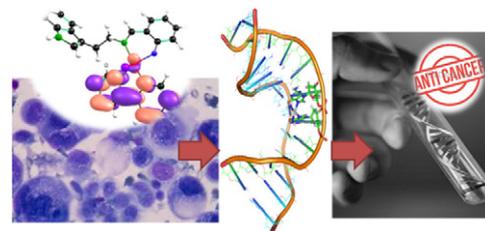
Manzoor Ahmad Malik^a, Md Kausar Raza^b, Ovas Ahmad Dar^a, Amadudin^c, Mohammad Abid^c, Mohammad Younus Wani^{d,*}, Abdullah Saad Al-Bogami^d, Athar Adil Hashmi^{a,*}

^aBioinorganic Lab., Department of Chemistry, Jamia Millia Islamia, New Delhi 110025, India

^bDepartment of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore 560012, India

^cMedicinal Chemistry Lab., Department of Biosciences, Jamia Millia Islamia, New Delhi 110025, India

^dChemistry Department, Faculty of Science, University of Jeddah, P.O. Box 80327, Jeddah 21589, Saudi Arabia



Furofuran lignans as a new series of antidiabetic agents exerting α-glucosidase inhibition and radical scavenging: Semisynthesis, kinetic study and molecular modeling

Bioorganic Chemistry 87 (2019) pp. 783–793

Wisuttaya Worawalai^a, Titiruetai Doungwichitrkul^a, Warin Rangubpit^b, Panyakorn Taweachat^b, Pornthep Sompornpisut^b, Preecha Phuwapraisiran^{a,*}

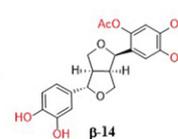
^aCenter of Excellence in Natural Product, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

^bCenter of Excellence in Computational Chemistry, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

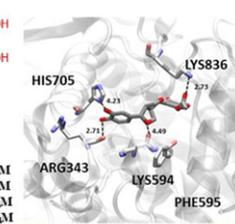


IC₅₀ (yeast) = 205.8 ± 1.1 μM
(maltase) = >1000 μM
(sucrase) = >1000 μM
SC₅₀ (DPPH) = 420.3 ± 4.3 μM

methylenedioxy
cleavage



IC₅₀ (yeast) = 5.3 ± 0.6 μM
(maltase) = 25.7 ± 1.0 μM
(sucrase) = 12.9 ± 0.4 μM
SC₅₀ (DPPH) = 11.2 ± 0.8 μM



Novel synthesized SLC-0111 thiazole and thiaziazole analogues: Determination of their carbonic anhydrase inhibitory activity and molecular modeling studies

Mahmoud F. Abo-Ashour^a, Wagdy M. Eldehna^{b,*}, Alessio Nocentini^c, Hany S. Ibrahim^a, Silvia Bua^c, Hatem A. Abdel-Aziz^d, Sahar M. Abou-Seri^{e,*}, Claudiu T. Supuran^{c,*}

^aDepartment of Pharmaceutical Chemistry, Faculty of Pharmacy, Egyptian Russian University, Badr City, Cairo 11829, Egypt

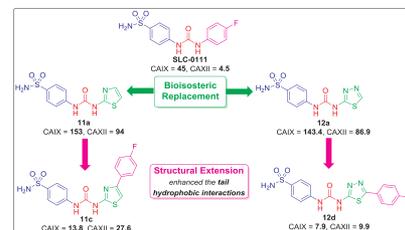
^bDepartment of Pharmaceutical Chemistry, Faculty of Pharmacy, Kafrelsheikh University, Kafrelsheikh, P.O. Box 33516, Egypt

^cDepartment of NEUROFARBA, Section of Pharmaceutical and Nutraceutical Sciences, University of Florence, Polo Scientifico, Via U. Schiff 6, 50019, Sesto Fiorentino, Firenze, Italy

^dDepartment of Applied Organic Chemistry, National Research Center, Dokki, Cairo 12622, Egypt

^eDepartment of Pharmaceutical Chemistry, Faculty of Pharmacy, Cairo University, Kasr El-Aini Street, Cairo, P.O. Box 11562, Egypt

Bioorganic Chemistry 87 (2019) pp. 794–802



Mechanistic investigation of anthocyanidin derivatives as α -glucosidase inhibitors

Jang Hoon Kim, Hyo Young Kim, Chang Hyun Jin^{*}

Advanced Radiation Technology Institute, Korea Atomic Energy Research Institute, Jeongseup 56212, Republic of Korea

Bioorganic Chemistry 87 (2019) pp. 803–809



Evaluation of angularly condensed diquinothiazines as potential anticancer agents

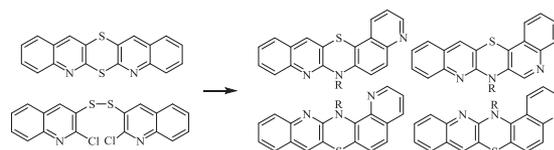
Małgorzata Jeleń^a, Krystian Pluta^{a,*}, Małgorzata Latocha^b, Beata Morak-Młodawska^a, Kinga Suwińska^{c,d}, Dariusz Kuśmierz^b

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2D NMR: ROESY, COSY, HSQC, HMBC X-ray analysis

Anticancer activity $IC_{50} < 1 \mu\text{g/mL}$

SNB-19, Caco-2, MDA-MB-231, A549

H3, TP53, CDKN1A, BAX, BACL-2

Synthesis and biological evaluation of purine-pyrazole hybrids incorporating thiazole, thiazolidinone or rhodanine moiety as 15-LOX inhibitors endowed with anticancer and antioxidant potential

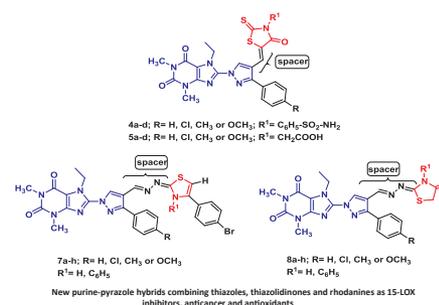
Ola S. Afifi^a, Omaima G. Shaaban^{a,b,*}, Heba A. Abd El Razik^a, Shams El-Dine A. Shams El-Dine^a, Fawzia A. Ashour^a, Alaa A. El-Tombary^a, Marwa M. Abu-Serie^c

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Synthesis, biological activity and multiscale molecular modeling studies of bis-coumarins as selective carbonic anhydrase IX and XII inhibitors with effective cytotoxicity against hepatocellular carcinoma

Belma Zengin Kurt^{a,*}, Aydan Dag^a,
Berna Doğan^b, Serdar Durdagi^{b,*},
Andrea Angeli^c, Alessio Nocentini^c,
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Department of Pharmaceutical Chemistry, 34093
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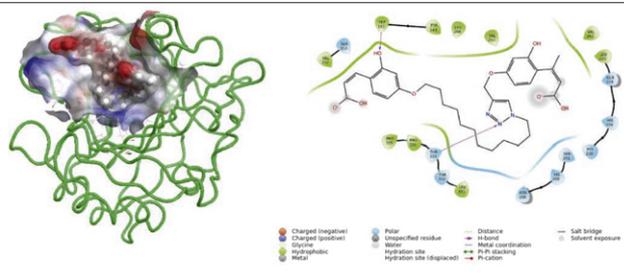
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Synthesis, Biological Activity and
Multiscale Molecular Modeling Studies of
Bis-coumarins as Selective Carbonic
Anhydrase IX and XII Inhibitors with
Effective Cytotoxicity against
Hepatocellular Carcinoma

Belma Zengin Kurt^a, Aydan Dag^a, Berna Doğan,
Serdar Durdagi^a, Andrea Angeli, Alessio
Nocentini, Claudiu T. Supuran, Fatih Sonmez



Xanthine oxidase inhibitors from an endophytic fungus *Lasiodiplodia pseudotheobromae*

Sanjay Kumar^a, Amol Dilip Pagar^a, Furkan Ahmad^d,
Vagish Dwibedi^b, Aabid Wani^c, Prasad V. Bharatam^c,
Manmohan Chhibber^d, Sanjai Saxena^{b,*},
Inder Pal Singh^{a,*}

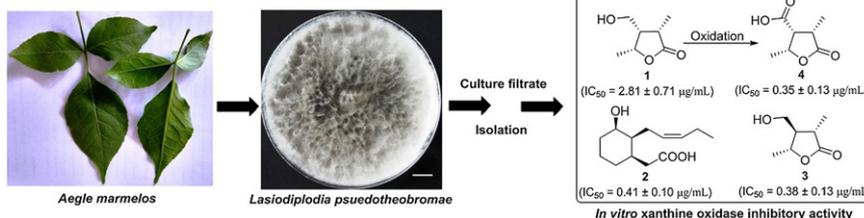
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Benzoxazinone-thiosemicarbazones as antidiabetic leads via aldose reductase inhibition: Synthesis, biological screening and molecular docking study

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Abdul Hameed^c, Muhammad Islam^a, Mariya al-Rashida^d, Maliha Uroos^e,
Asnuzilawati Asari^f, Zahid Shafiq^{a,*}, Jamshed Iqbal^{b,*}

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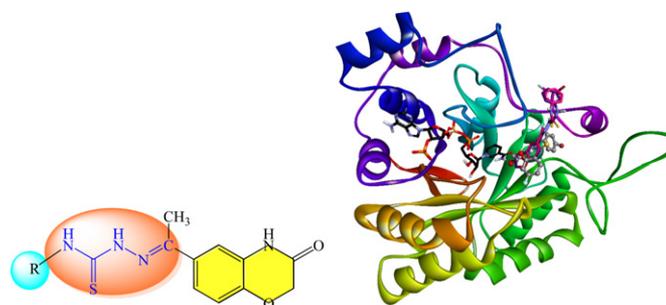
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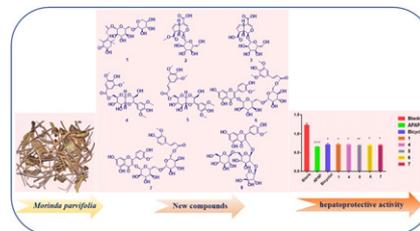


Eight new glycosides with hepatoprotective activity isolated from the aerial parts of *Morinda parvifolia*

Xianming Su, Li Li, Hua Sun, Fan Zhang, Changkang Li, Fenghua Li, Hongqing Wang, Baoming Li, Ruoyun Chen, Jie Kang*

State Key Laboratory of Bioactive Substances and Functions of Natural Medicines, Institute of Materia Medica, Chinese Academy of Medical Sciences & Peking Union Medical College, No. 1 Xiannongtan Street, Beijing 100050, China

Bioorganic Chemistry 87 (2019) pp. 867–875



Fluorescent labeling of ursolic acid with FITC for investigation of its cytotoxic activity using confocal microscopy

Tatiana S. Frolova^{a,b,c,d,*}, Alla V. Lipeeva^b, Dmitry S. Baev^{b,c}, Sergey I. Baiborodin^a, Konstantin E. Orishchenko^a, Alexey V. Kochetov^{a,c}, Olga I. Sinitsyna^{a,c}

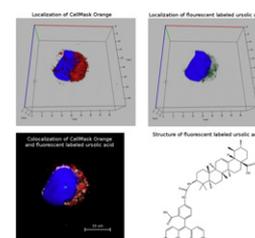
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Synthesis, bioactivity and molecular modeling studies on potential anti-Alzheimer piperidinehydrazide-hydrazones

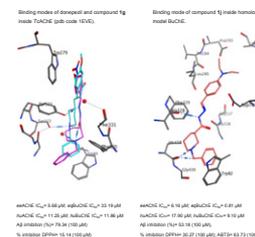
Sulunay Parlara^a, Gozde Sayar^a, Ayse Hande Tarikogullari^a, Sumru Sozer Karadagli^b, Vildan Alptuzun^{a,*}, Ercin Erciyas^a, Ulrike Holzgrabe^c

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REVIEW ARTICLES

Promising anti-inflammatory effects of chalcones via inhibition of cyclooxygenase, prostaglandin E₂, inducible NO synthase and nuclear factor κB activities

Haroon ur Rashid^{a,d}, Yiming Xu^a, Nasir Ahmad^c, Yaseen Muhammad^a, Lisheng Wang^{a,b,*}

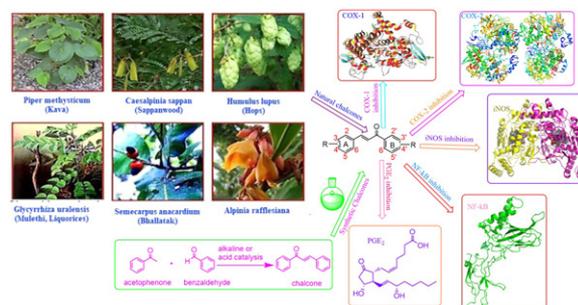
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PRELIMINARY COMMUNICATIONS

Phenylsulfonyl piperazine bridged [1,3] dioxolo [4,5-g] chromenones as promising antiproliferative and antioxidant agents

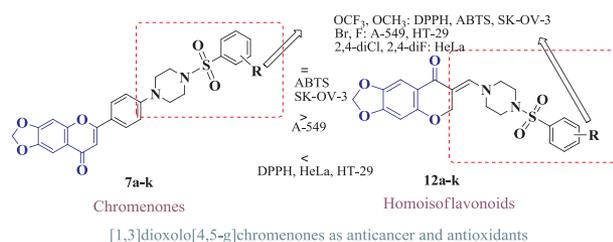
Rahul V. Patel^a, Bhupendra M. Mistry^a, Riyaz Syed^b, Nikhil M. Parekh^c, Han-Seung Shin^{a,*}

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Natural and semisynthetic oxyprenylated aromatic compounds as stimulators or inhibitors of melanogenesis

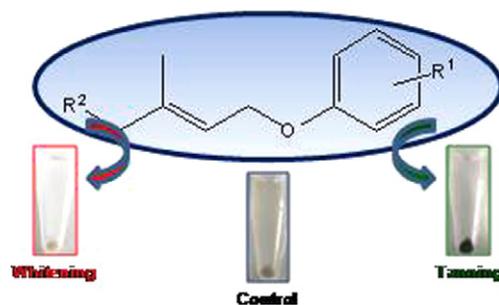
Salvatore Genovese^a, Francesco Epifano^{b,*}, Philippe de Medina^c, Nicolas Caron^b, Arnaud Rives^b, Marc Poirot^c, Sandrine Silvente-Poirot^c, Serena Fiorito^a

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Investigation of new quinoline derivatives as promising inhibitors of NTPDases: Synthesis, SAR analysis and molecular docking studies

Komal Hayat^a, Saira Afzal^b, Altaf Saeed^a, Amna Murtaza^a, Shafiq Ur Rahman^b, Khalid Mohammed Khan^{c,d}, Aamer Saeed^a, Sumera Zaib^b, Joanna Lecka^{e,f}, Jean Sévigny^{e,f}, Jamshed Iqbal^{b,*}, Abbas Hassan^{a,*}

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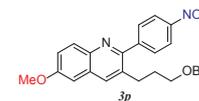
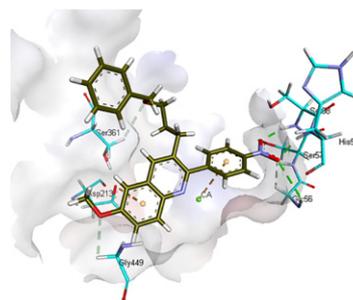
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<i>h</i> -NTPDase1	
IC ₅₀ (μM) ^a ± SEM / %inhibition	
3p	0.23 ± 0.09
Suramin	16.1 ± 1.08

Glycopentanolones A-D, four new geranylated quinolone alkaloids from *Glycosmis pentaphylla*

Yun-Hyeok Choi^{a,b,1}, Changon Seo^{a,1}, Wonsik Jeong^a, Ji Eun Lee^a, Jae Yeon Lee^a, Eun-Kyung Ahn^a, Jae-Shin Kang^c, Jae-Ho Lee^c, Chun Whan Choi^a, Joa Sub Oh^d, Dongho Lee^{b,*}, Seong Su Hong^{a,*}

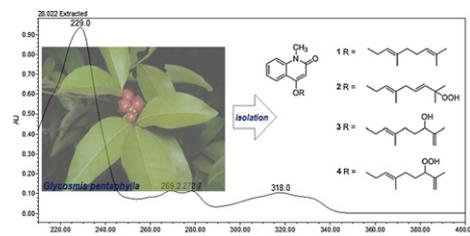
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Lithocarols A-F, six tenellone derivatives from the deep-sea derived fungus *Phomopsis lithocarpus* FS508

Jianlin Xu^{a,b}, Zhaoming Liu^a, Yuchan Chen^a, Haibo Tan^c, Haohua Li^a, Saini Li^a, Heng Guo^{a,b}, Zilei Huang^a, Xiaoxia Gao^b, Hongxin Liu^{a,*}, Weimin Zhang^{a,*}

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