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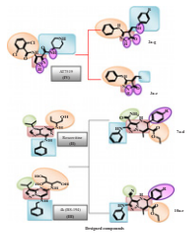
REGULAR ARTICLES

Design, synthesis and biological evaluation of certain CDK2 inhibitors based on pyrazole and pyrazolo[1,5-a] pyrimidine scaffold with apoptotic activity

Bioorganic Chemistry 86 (2019) pp. 1–14

Ghada M.E. Ali[a], Diaa A. Ibrahim[a], Amira M. Elmetwali[a], Nasser S.M. Ismail[b,*]

[a]*National Organization for Drug Control & Research, P.O. Box: 29, Cairo, Egypt*
[b]*Pharmaceutical Chemistry Department, Faculty of Pharmaceutical Sciences and Pharmaceutical Industries, Future University in Egypt, Cairo 12311, Egypt*

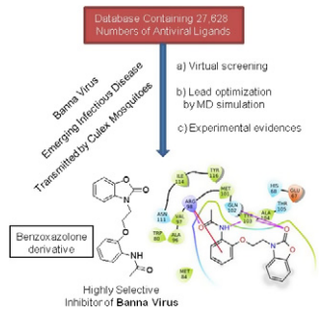


A combinatorial approach of structure-based virtual screening and molecular dynamics simulation towards the discovery of a highly selective inhibitor for VP9 coat protein of Banna virus

Bioorganic Chemistry 86 (2019) pp. 15–27

Parikshit Moitra

Technical Research Centre, Indian Association for the Cultivation of Science, 2A & 2B Raja SC Mullick Road, Jadavpur, Kolkata 700032, West Bengal, India

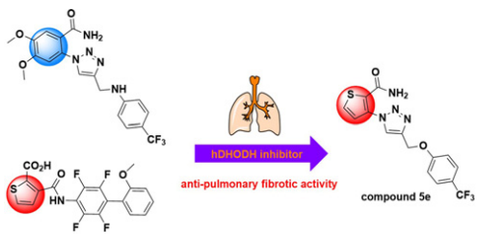


Discovery of a novel series of hDHODH inhibitors with anti-pulmonary fibrotic activities

Bioorganic Chemistry 86 (2019) pp. 44–51

Kuan Lu[a,b], Yanfang Zhao[a], Guodong Wu[a], Hao Hu[a], Mingzhong Wang[b], Guowei Gong[e,*], Yuyang Jiang[a,c,d,*]

[a]*Department of Pharmaceutical Engineering, Shenyang Pharmaceutical University, Shenyang, Liaoning 110016, PR China*
[b]*Shenzhen Kivita Innovative Drug Discovery Institute, Shenzhen 518057, PR China*
[c]*National & Local United Engineering Lab for Personalized Anti-tumor Drugs, The Graduate School at Shenzhen, Tsinghua University, Shenzhen 518055, PR China*
[d]*Department of Pharmacology and Pharmaceutical Sciences, School of Medicine, Tsinghua University, Beijing 100084, PR China*
[e]*Department of Bioengineering, Zunyi Medical University, Zhuhai Campus, Zhuhai 519041, Guangdong, PR China*

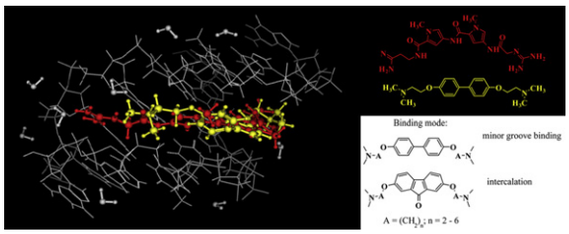


Aminoalkoxyfluorenones and aminoalkoxybiphenyls: DNA binding modes

Bioorganic Chemistry 86 (2019) pp. 52–60

Svitlana O. Zanoza[a], Kyrylo O. Klimenko[a,b], George V. Maltzev[a], Tetiana I. Bykova[c], Igor A. Levandovskiy[d], Sergiy A. Lyakhov[a], Sergiy A. Andronati[a], Mikhail L. Bondarev[e,*]

[a]A. V. Bogatsky Physico-Chemical Institute of the National Academy of Science of Ukraine, 86 Lyustdorfskaya doroga, Odessa 65080, Ukraine
[b]Laboratoire de Chemoinformatique, (UMR 7140 CNRS/UniStra) Université de Strasbourg, 1, rue B. Pascal, Strasbourg 67000, France
[c]I. I. Mechnikov National University, Department of Chemistry, 2 Dvoryanskaya, Odessa 65026, Ukraine
[d]Department of Organic Chemistry, National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", 37 Pr. Pobedy, Kyiv, Ukraine
[e]Department of Pharmaceutical Sciences, School of Pharmacy, Hampton University, Kittrell Hall, Hampton, VA 23668, USA

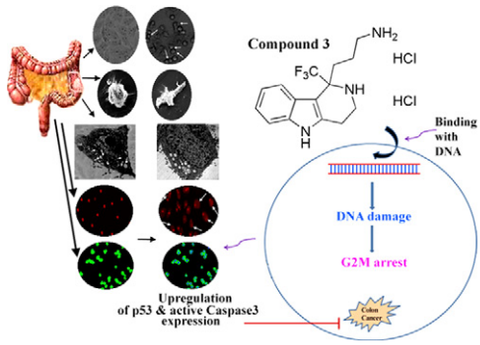


Trifluoromethylated carboline compounds targeting DNA: Synthesis, binding and anti-proliferative effects on human cancer cell lines

Bioorganic Chemistry 86 (2019) pp. 61–79

Sarita Sarkar[a], Olga I. Shmatova[b], Valentine G. Nenajdenko[b], Kakali Bhadra[a,*]

[a]Department of Zoology, University of Kalyani, Nadia, West Bengal 741235, India
[b]Department of Chemistry, Lomonosov Moscow State University, Moscow 119991, Russia

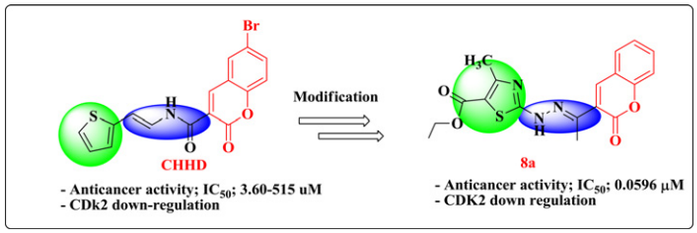


New thiazol-hydrazono-coumarin hybrids targeting human cervical cancer cells: Synthesis, CDK2 inhibition, QSAR and molecular docking studies

Bioorganic Chemistry 86 (2019) pp. 80–96

Somaia S. Abd El-Karim[a], Yasmin M. Syam[a,*], Ahmed M. El Kerdawy[b,c,d], Tamer M. Abdelghany[e]

[a]Therapeutical Chemistry Department, National Research Centre, Dokki, Cairo, P. O. Box 12622, Egypt
[b]Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Cairo University, Kasr El-Aini Street, Cairo, P.O. Box 11562, Egypt
[c]Molecular Modeling Unit, Faculty of Pharmacy, Cairo University, Kasr El-Aini Street, Cairo, P.O. Box 11562, Egypt
[d]Department of Pharmaceutical Chemistry, Faculty of Pharmacy, New Giza University, Newgiza, km 22 Cairo–Alexandria Desert Road, Cairo, Egypt
[e]Department of Pharmacology, Faculty of Pharmacy, Al-Azhar University, Nasr City, Cairo, P.O. Box 11787, Egypt

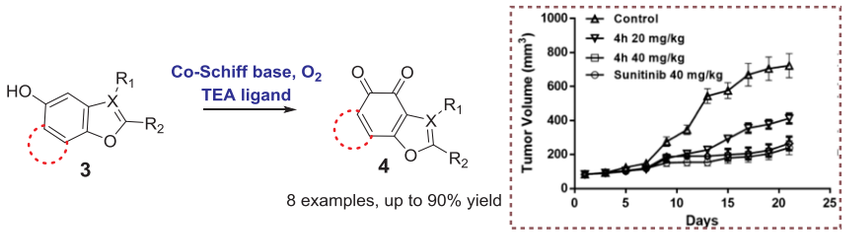


Identification of *ortho*-naphthoquinones as anti-AML agents by highly efficient oxidation of phenols

Bioorganic Chemistry 86 (2019) pp. 97–102

Huidan Huang[a], Ming Yan[a], Jianqiu Chen[a], Biao Yuan[c], Guitang Chen[c], Shujie Cheng[c], Dechun Huang[a], Zhen Gao[b,*], Chongjiang Cao[a,*]

[a]Department of Pharmaceutical Engineering, China Pharmaceutical University, Nanjing 210009, China
[b]College of Biotechnology and Pharmaceutical Engineering, Nanjing Tech University, Nanjing 211816, China
[c]Department of Food Quality and Safety, School of Engineering, China Pharmaceutical University, Nanjing 211816, China

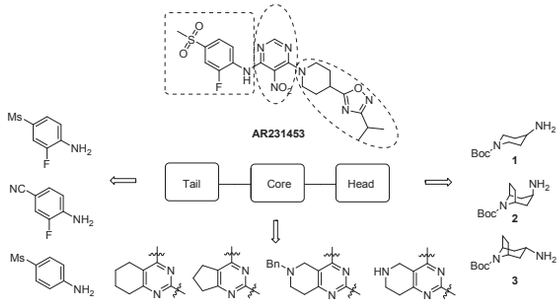


Synthesis and evaluation of novel fused pyrimidine derivatives as GPR119 agonists

Bioorganic Chemistry 86 (2019) pp. 103–111

Yuanying Fang[a,1], Lijuan Xiong[b,1], Jianguo Hu[b], Shaokun Zhang[a], Saisai Xie[a], Liangxing Tu[a], Yang Wan[a], Yi Jin[a,*], Xiang Li[a], Shaojie Hu[b], Zunhua Yang[b,*]

[a]National Engineering Research Center for Manufacturing Technology of TCM Solid Preparation, Jiangxi University of Traditional Chinese Medicine, Nanchang 330006, China
[b]College of Pharmacy, Jiangxi University of Traditional Chinese Medicine, Nanchang 330004, China

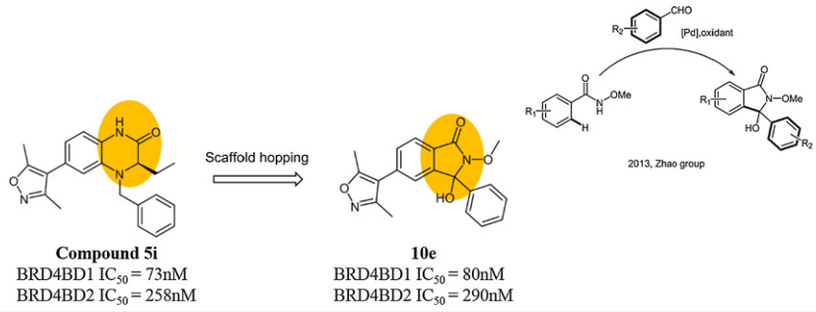


3-Hydroxyisoindolin-1-one derivates: Synthesis by palladium-catalyzed C—H activation as BRD4 inhibitors against human acute myeloid leukemia (AML) cells

Bioorganic Chemistry 86 (2019) pp. 119–125

Pan Chen[a,1], Yifei Yang[a,1], Lingyun Yang[b], Jiping Tian[b], Fangqing Zhang[b], Jinpei Zhou[a,*], Huibin Zhang[b,*]

[a]Department of Medicinal Chemistry, China Pharmaceutical University, 24 Tongjiaxiang, Nanjing 210009, PR China
[b]Center of Drug Discovery, State Key Laboratory of Natural Medicines, China Pharmaceutical University, 24 Tongjiaxiang, Nanjing 210009, PR China

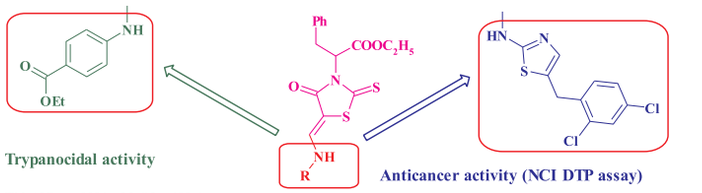


Synthesis of 5-enamine-4-thiazolidinone derivatives with trypanocidal and anticancer activity

Bioorganic Chemistry 86 (2019) pp. 126–136

Serhii Holota[a,f], Anna Kryshchyshyn[a], Halyna Derkach[b], Yaroslava Trufin[a], Inna Demchuk[a], Andrzej Gzella[c], Philippe Grellier[d], Roman Lesyk[a,e,*]

[a]Department of Pharmaceutical, Organic and Bioorganic Chemistry, Danylo Halytsky Lviv National Medical University, 69 Pekarska, Lviv 79010, Ukraine
[b]Department of Chemistry, Ivano-Frankivsk National Medical University, 2 Halytska, Ivano-Frankivsk 76018, Ukraine
[c]Department of Organic Chemistry, Poznan University of Medical Sciences, Grunwaldzka 6, 60-780 Poznan, Poland
[d]National Museum of Natural History, UMR 7245 CNRS-MNHN, Team APE, CP 52, 57 Rue Cuvier, Paris 75005, France
[e]Department of Public Health, Dietetics and Lifestyle Disorders, Faculty of Medicine, University of Information Technology and Management in Rzeszow, Sucharskiego 2, 35-225 Rzeszow, Poland
[f]Department of Organic Chemistry and Pharmacy, Lesya Ukrainka Eastern European National University, Volya Avenue 13, 43025 Lutsk, Ukraine

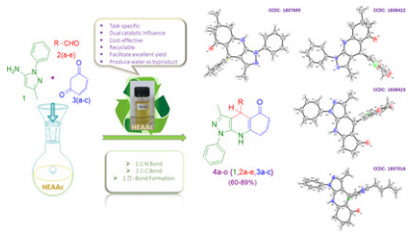


Hydroxyl alkyl ammonium ionic liquid assisted green and one-pot regioselective access to functionalized pyrazolodihydropyridine core and their pharmacological evaluation

Bioorganic Chemistry 86 (2019) pp. 137–150

Divyang M. Patel[a], Mayank G. Sharma[a], Ruturajsinh M. Vala[a], Irene Lagunes[b], Adrián Puerta[b], José M. Padrón[b], Dhanji P. Rajani[c], Hitendra M. Patel[a,*]

[a]Department of Chemistry, Sardar Patel University, Vallabh Vidyanagar 388120, Gujarat, India
[b]BioLab, Instituto Universitario de Bio-Orgánica Antonio González, CIBICAN, Universidad de La Laguna, Avda. Astrofísico Francisco Sánchez 2, 38206 La Laguna, Spain
[c]Microcare Laboratory and Tuberculosis Diagnosis & Research Center, Surat, India

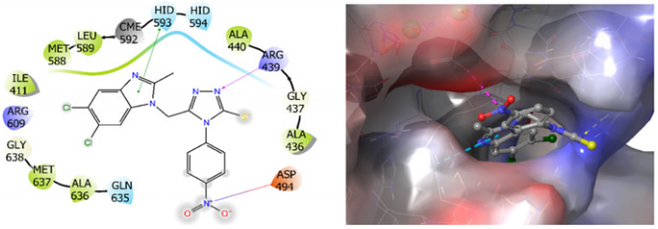


Design, molecular docking and synthesis of novel 5,6-dichloro-2-methyl-1*H*-benzimidazole derivatives as potential urease enzyme inhibitors

Bioorganic Chemistry 86 (2019) pp. 151–158

Emre Menteşe[a,*], Mustafa Emirik[a], Bahar Bilgin Sökmen[b]

[a]Department of Chemistry, Art and Science Faculty, Recep Tayyip Erdogan University, Rize, Turkey
[b]Department of Chemistry, Faculty of Arts and Sciences, Giresun University, 28049 Giresun, Turkey

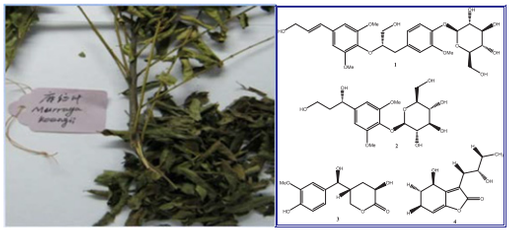


Structures and biological evaluation of phenylpropanoid derivatives from *Murraya koenigii*

Bioorganic Chemistry 86 (2019) pp. 159–165

Qinge Ma[a,1,*], Rongrui Wei[a,1,*], Ming Yang[a,*], Xiaoying Huang[a], Guoyue Zhong[a], Zhipei Sang[c], Jianghong Dong[d], Jicheng Shu[a], Jianqun Liu[a], Rui Zhang[a], Jianbo Yang[b], Aiguo Wang[b], Tengfei Ji[b], Yalun Su[b,*]

[a]State Key Laboratory of Innovative Drugs and High Efficiency Energy Saving and Consumption Reduction Pharmaceutical Equipment, Key Laboratory of Modern Preparation of TCM of Ministry of Education, Research Center of Natural Resources of Chinese Medicinal Materials and Ethnic Medicine, Jiangxi University of Traditional Chinese Medicine, Nanchang 330004, China
[b]State Key Laboratory of Bioactive Substance and Function of Natural Medicines, Institute of Materia Medica, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing 100050, China
[c]College of Chemistry and Pharmaceutical Engineering, Nanyang Normal University, Nanyang 473061, China
[d]College of Chemistry and Pharmaceutical Engineering, Huanghuai University, Zhumadian 463000, China

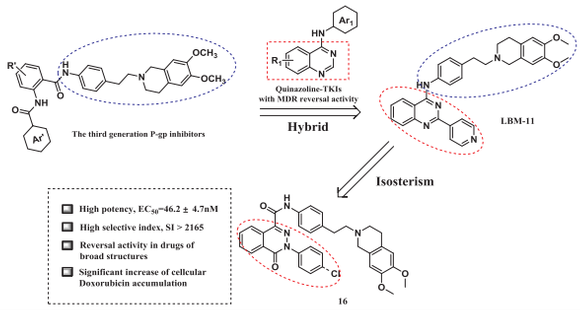


Design, synthesis and biological evaluation of N-(4-(2-(6,7-dimethoxy-3,4-dihydroisoquinolin-2(1H)-yl)ethyl)phenyl)-4-oxo-3,4-dihydrophthalazine-1-carboxamide derivatives as novel P-glycoprotein inhibitors reversing multidrug resistance

Bioorganic Chemistry 86 (2019) pp. 166–175

Qianqian Qiu[a,1], Jiaqi Zhou[b,1], Wei Shi[b], Mutta Kairuki[b], Wenglong Huang[b,c,*], Hai Qian[b,c,*]

[a]*School of Pharmacy, Jiangsu Provincial Key Laboratory of Coastal Wetland Bioresources and Environmental Protection, Yancheng Teachers' University, Yancheng 224007, PR China*
[b]*Center of Drug Discovery, State Key Laboratory of Natural Medicines, China Pharmaceutical University, 24 Tongjiaxiang, Nanjing 210009, PR China*
[c]*Jiangsu Key Laboratory of Drug Discovery for Metabolic Disease, China Pharmaceutical University, 24 Tongjiaxiang, Nanjing 210009, PR China*

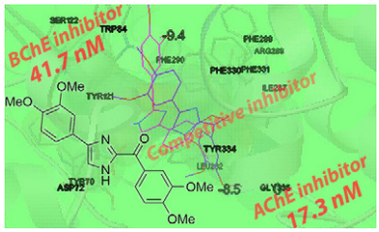


Mono- or di-substituted imidazole derivatives for inhibition of acetylcholine and butyrylcholine esterases

Bioorganic Chemistry 86 (2019) pp. 187–196

Burak Kuzu[a,b], Meltem Tan[a,b], Parham Taslimi[c], İlhami Gülçin[c], Mehmet Taşpınar[d], Nurettin Menges[a,b,*]

[a]*Pharmaceutical Chemistry Section, Van Yuzuncu Yil University, 65080 Van, Turkey*
[b]*SAFF Chemical Reagent R&D Lab. YYU-TEKNOKENT, 65080 Van, Turkey*
[c]*Department of Chemistry, Atatürk University, 25240 Erzurum, Turkey*
[d]*Department of Medicinal Biology, Van Yuzuncu Yil University, 65080 Van, Turkey*

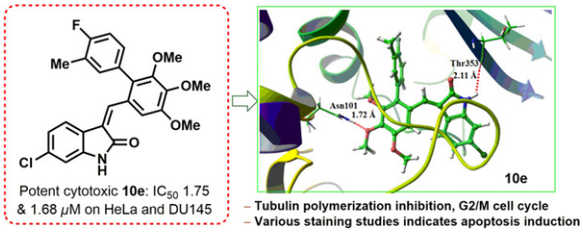


Synthesis of substituted biphenyl methylene indolinones as apoptosis inducers and tubulin polymerization inhibitors

Bioorganic Chemistry 86 (2019) pp. 210–223

Kavitha Donthiboina[a], Pratibha Anchi[b], P.V. Sri Ramya[a], Shailaja Karri[b], Gannoju Srinivasulu[a], Chandraiah Godugu[b], Nagula Shankaraiah[a,*], Ahmed Kamal[a,c,*]

[a]*Department of Medicinal Chemistry, National Institute of Pharmaceutical Education and Research (NIPER), Hyderabad 500 037, India*
[b]*Department of Regulatory Toxicology, National Institute of Pharmaceutical Education and Research (NIPER), Hyderabad 500 037, India*
[c]*School of Pharmaceutical Education and Research (SPER), Jamia Hamdard, New Delhi 110062, India*

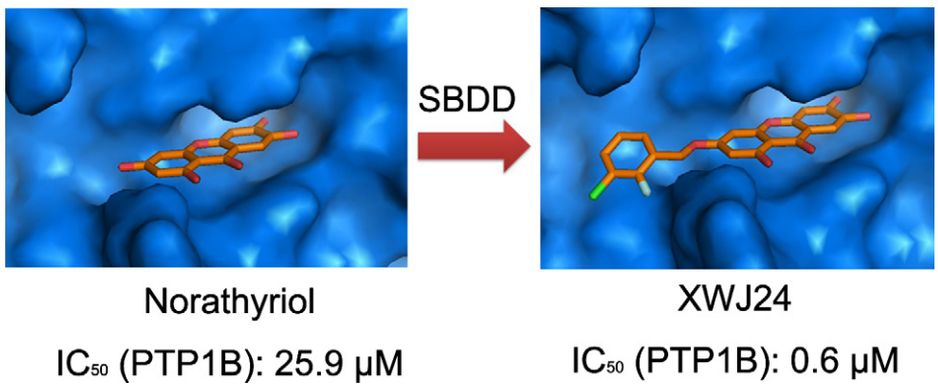


Discovery of potent PTP1B inhibitors via structure-based drug design, synthesis and *in vitro* bioassay of Norathyriol derivatives

Bioorganic Chemistry 86 (2019) pp. 224–234

Wenjie Xue[a], Jinlong Tian[a], Xiang Simon Wang[b], Jie Xia[a,*], Song Wu[a,*]

[a]*State Key Laboratory of Bioactive Substance and Function of Natural Medicines, Department of New Drug Research and Development, Institute of Materia Medica, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing 100050, China*
[b]*Department of Pharmaceutical Sciences, College of Pharmacy, Howard University, Washington DC 20059, USA*

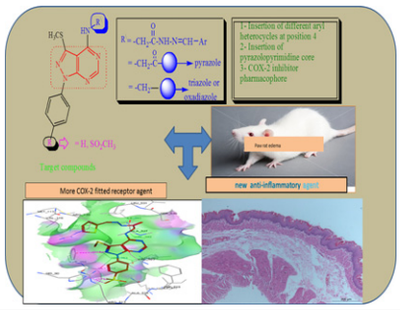


COX-1/COX-2 inhibition assays and histopathological study of the new designed anti-inflammatory agent with a pyrazolopyrimidine core

Bioorganic Chemistry 86 (2019) pp. 235–253

Eman K.A. Abdelall[a,*], Phoebe F. Lamie[a], Amira K.M. Ahmed[a], EL-Shaymaa EL-Nahass[b]

[a]Department of Pharmaceutical Organic Chemistry, Faculty of Pharmacy, Beni-Suef University, Beni-Suef 62514, Egypt
[b]Department of Pathology, Faculty of Veterinary Medicine, Beni-suef University, 62511, Egypt

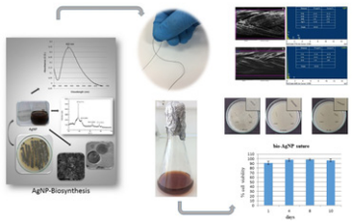


Antimicrobial characteristics and biocompatibility of the surgical sutures coated with biosynthesized silver nanoparticles

Bioorganic Chemistry 86 (2019) pp. 254–258

Tuba Baygar[a,*], Nurdan Sarac[b], Aysel Ugur[c], Inci Rana Karaca[d]

[a]Material Research Laboratory, Research Laboratories Center, Mugla Sitki Kocman University, Mugla, Turkey
[b]Department of Biology, Faculty of Science, Mugla Sitki Kocman University, Mugla, Turkey
[c]Section of Medical Microbiology, Department of Basic Sciences, Faculty of Dentistry, Gazi University, Ankara, Turkey
[d]Department of Oral and Maxillofacial Surgery, Faculty of Dentistry, Gazi University, Ankara, Turkey

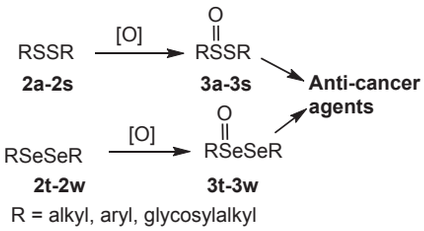


Natural product inspired allicin analogs as novel anti-cancer agents

Bioorganic Chemistry 86 (2019) pp. 259–272

Ishani Bhaumik[a,1], Kunal Pal[a,1], Utsab Debnath[a], Parimal Karmakar[b], Kuladip Jana[a], Anup Kumar Misra[a,*]

[a]Bose Institute, Division of Molecular Medicine, P-1/12, C.I.T. Scheme VII M, Kolkata 700054, India
[b]Department of Life Science and Biotechnology, Jadavpur University, Kolkata 700 032, India

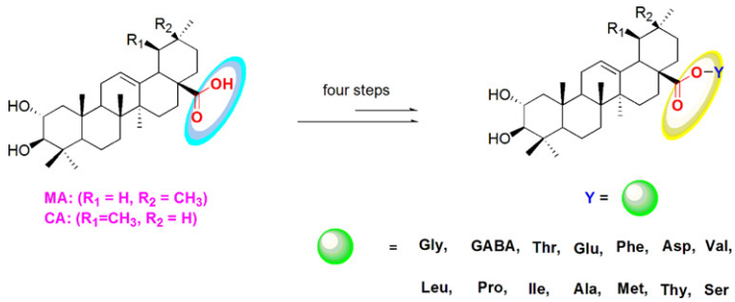


Synthesis of water soluble pentacyclic dihydroxyterpene carboxylic acid derivatives coupled amino acids and their inhibition activities on α-glucosidase

Bioorganic Chemistry 86 (2019) pp. 277–287

Zhen Zeng[a], Xiaoli Yin[b], Xueyuan Wang[a], Wuying Yang[a,*], Xiaoqin Liu[a], Yanping Hong[a,*]

[a]Jiangxi Key Laboratory of Natural Product and Functional Food, College of Food Science and Engineering Jiangxi Agricultural University, Nanchang 33045, China
[b]Library of Jiangxi Agricultural University, Nanchang 330045, China

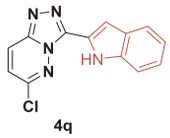


Synthesis and bioevaluation of 6-chloropyridazin-3-yl hydrazones and 6-chloro-3-substituted-[1,2,4]triazolo[4,3-*b*]pyridazines as cytotoxic agents

Bioorganic Chemistry 86 (2019) pp. 288–295

Mamta[a], Ranjana Aggarwal[a,*], Rachna Sadana[b], Jeziel Ilag[b], Garima Sumran[c]

[a]*Department of Chemistry, Kurukshetra University, Kurukshetra 136119, India*
[b]*Department of Natural Sciences, University of Houston, Downtown, Houston 77002, USA*
[c]*Department of Chemistry, D. A. V. College (Lahore), Ambala City 134 002, Haryana, India*



4q

IC_{50} = 1.64 ± 0.74 μM (SB-ALL)
= 1.14 ± 0.24 μM (NALM-6)
= 3.55 ± 0.54 μM (MCF-7)

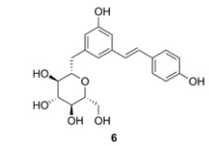
33 compounds screened using MTT assay

Tyrosinase and α-glucosidase inhibitory potential of compounds isolated from *Quercus coccifera* bark: *In vitro* and *in silico* perspectives

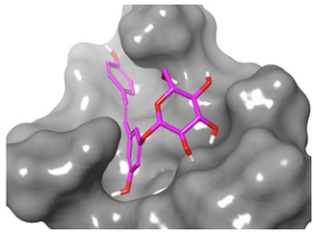
Bioorganic Chemistry 86 (2019) pp. 296–304

Suat Sari[a], Burak Barut[b], Arzu Özel[b,c], Ayşe Kuruüzüm-Uz[d], Didem Şöhretoğlu[d,*]

[a]*Hacettepe University, Faculty of Pharmacy, Department of Pharmaceutical Chemistry, Sıhhiye, Ankara, TR-06100 Ankara, Turkey*
[b]*Karadeniz Technical University, Faculty of Pharmacy, Department of Biochemistry, Trabzon, Turkey*
[c]*Karadeniz Technical University, Drug and Pharmaceutical Technology Application and Research Center, Trabzon, Turkey*
[d]*Hacettepe University, Faculty of Pharmacy, Department of Pharmacognosy, Sıhhiye, Ankara, TR-06100 Ankara, Turkey*



6
Mushroom tyrosinase IC_{50}: 4.05 ± 0.30 μg/mL

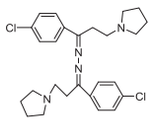


Investigation of inhibitory properties of some hydrazone compounds on hCA I, hCA II and AChE enzymes

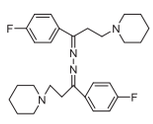
Bioorganic Chemistry 86 (2019) pp. 316–321

Kaan Kucukoglu[a,*], Halise Inci Gul[b], Parham Taslimi[c], Ilhami Gulcin[c], Claudiu T. Supuran[d]

[a]*Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Selcuk University, Konya, Turkey*
[b]*Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Atatürk University, Erzurum, Turkey*
[c]*Department of Chemistry, Faculty of Science, Atatürk University, Erzurum, Turkey*
[d]*Neurofarba Department, Section of Pharmaceutical and Nutriceutical Sciences, Universita degli Studi di Firenze, Florence, Italy*



R5 (K_i 203±55 nM against hCA I)
(K_i 200±34 nM against hCA II)



P7 (K_i 66±20 nM against AChE)

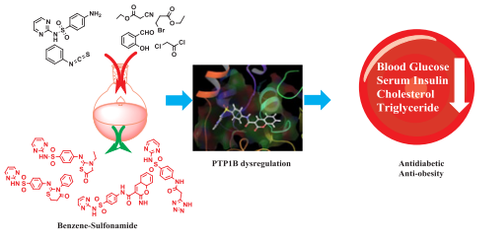
Lead compounds of the study

Toward a treatment of diabesity: Rational design, synthesis and biological evaluation of benzene-sulfonamide derivatives as a new class of PTP-1B inhibitors

Bioorganic Chemistry 86 (2019) pp. 322–338

Nagat Ghareb[a,b], Norhan M. El-Sayed[c], Reda Abdelhameed[f], Koji Yamada[d], Mohamed Saleh Elgawish[e,*]

[a]*Pharmaceutical Organic Chemistry Department, Faculty of Pharmacy, Suez Canal University, Ismailia 41522, Egypt*
[b]*Chemistry Department, College of Sciences, Prince Sattam bin Abdul-Aziz University, Saudi Arabia*
[c]*Pharmacology and Toxicology Department, Faculty of Pharmacy, Suez Canal University, Ismailia 41522, Egypt*
[d]*Graduate School of Biomedical Sciences, Nagasaki University, 1-14 Bunkyo-machi, Nagasaki 852-8521, Japan*
[e]*Medicinal Chemistry Department, Faculty of Pharmacy, Suez Canal University, Ismailia 41522, Egypt*
[f]*Graduate school of biomedical sciences, Nagasaki University to Pharmacognosy Department, Faculty of Pharmacy, Suez Canal University, Ismailia 41522, Egypt*

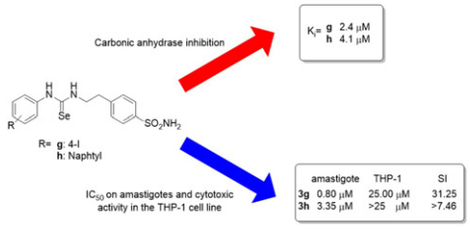


Discovery of new organoselenium compounds as antileishmanial agents

Bioorganic Chemistry 86 (2019) pp. 339–345

Abdul-Malek S. Al-Tamimi[a,1], Mikel Etxebeste-Mitxeltorena[b,1], Carmen Sanmartín[b], Antonio Jiménez-Ruiz[c], Leo Syrjänen[d], Seppo Parkkila[e], Silvia Selleri[f], Fabrizio Carta[f,*], Andrea Angeli[f,*], Claudiu T. Supuran[f,*]

[a]*Department of Pharmaceutical Chemistry, College of Pharmacy, Prince Sattam Bin Abdulaziz University, P.O. Box 173, Alkharj 11942, Saudi Arabia*
[b]*University of Navarra, School of Pharmacy and Nutrition, Department of Pharmaceutical Technology and Chemistry, Irunlarrea 1, 31008 Pamplona, Spain*
[c]*Departamento de Biología de Sistemas, Universidad de Alcala, E-28805 Alcala de Henares, Madrid, Spain*
[d]*Department of Otorhinolaryngology, Faculty of Medicine and Life Sciences, University of Tampere and Tampere University Hospital, Finland*
[e]*Faculty of Medicine and Life Sciences, University of Tampere and Fimlab Ltd, Tampere University Hospital, Finland*
[f]*Department of Neuroscience, Psychology, Drug Research and Child's Health (NEUROFARBA), Section of Pharmaceutical and Nutraceutical Sciences, Via Ugo Schiff 6, 50019, Sesto Fiorentino, Italy*

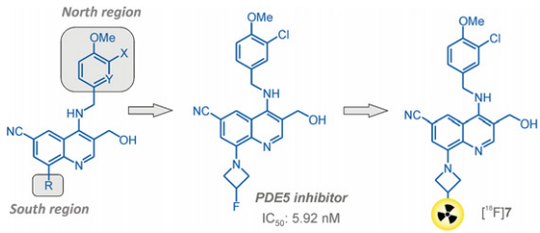


Targeting cyclic nucleotide phosphodiesterase 5 (PDE5) in brain: Toward the development of a PET radioligand labeled with fluorine-18

Bioorganic Chemistry 86 (2019) pp. 346–362

Barbara Wenzel[a,*,1], Jianrong Liu[b,1], Sladjana Dukic-Stefanovic[a], Winnie Deuther-Conrad[a], Rodrigo Teodoro[a], Friedrich-Alexander Ludwig[a], Jean-Michel Chezal[b], Emmanuel Moreau[b], Peter Brust[a], Aurelie Maisonial-Besset[b]

[a]*Helmholtz-Zentrum Dresden-Rossendorf, Institute of Radiopharmaceutical Cancer Research, Department of Neuroradiopharmaceuticals, Leipzig, Germany*
[b]*UMR 1240 INSERM IMOST, Université Clermont-Auvergne, Clermont-Ferrand, France*

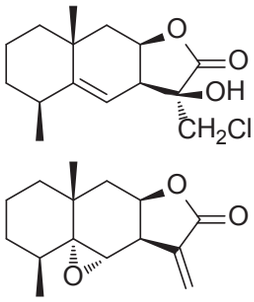


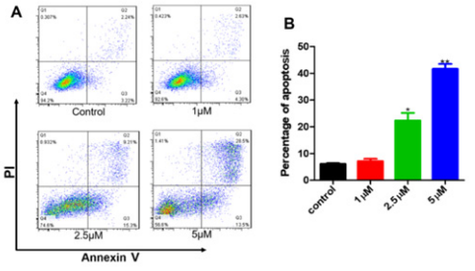
Sesquiterpenoids from the roots of *Inula helenium* inhibit acute myelogenous leukemia progenitor cells

Bioorganic Chemistry 86 (2019) pp. 363–367

Yahui Ding[a,1], Wenwei Pan[a,1], Junqing Xu[b,1], Tianpeng Wang[a], Tianyang Chen[a], Zhongquan Liu[a], Chunfeng Xie[a,*], Quan Zhang[a,*]

[a]*State Key Laboratory of Medicinal Chemical Biology, College of Pharmacy and Tianjin Key Laboratory of Molecular Drug Research, Nankai University, Tianjin 300071, People's Republic of China*
[b]*Department of Hematology, Yantai Yuhuangding Hospital, Qingdao University Medical College, Yantai 264000, People's Republic of China*



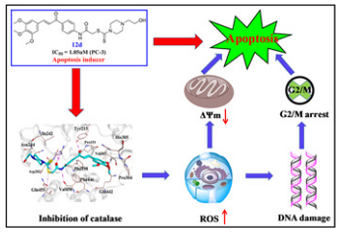


Discovery of novel chalcone-dithiocarbamates as ROS-mediated apoptosis inducers by inhibiting catalase

Bioorganic Chemistry 86 (2019) pp. 375–385

Dong-Jun Fu[a,b,d,1], Jia-Huan Li[b,1], Jia-Jia Yang[b,1], Ping Li[b], Yan-Bing Zhang[b], Simeng Liu[c], Zhong-Rui Li[b], Sai-Yang Zhang[a,b,*]

[a]School of Basic Medical Science, Zhengzhou University, Zhengzhou 450001, China
[b]School of Pharmaceutical Sciences & Collaborative Innovation Center of New Drug Research and Safety Evaluation, Zhengzhou University, Zhengzhou 450001, China
[c]Department of Gastroenterology, The Fifth Affiliated Hospital of Zhengzhou University, Zhengzhou 450052, China
[d]Department of Urology, University of California, Irvine, Orange, CA 92868, USA

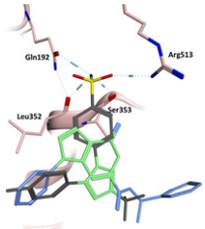


Anti-inflammatory drug approach: Synthesis and biological evaluation of novel pyrazolo [3,4-*d*] pyrimidine compounds

Bioorganic Chemistry 86 (2019) pp. 393–400

Noor Atatreh[a], Amal M. Youssef[a,b,*], Mohammad A. Ghattas[a], Mohammad Al Sorkhy[a], Sara Alrawashdeh[a], Khaled B. Al-Harbi[c], Ibrahim M. El-Ashmawy[c,d], Tariq I. Almundarij[c], Amani A. Abdelghani[e], Alaa S. Abd-El-Aziz[e]

[a]College of Pharmacy, Al Ain University of Science and Technology, Al Ain, United Arab Emirates
[b]Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Alexandria University, Alexandria, Egypt
[c]Department of Veterinary Medicine, College of Agricultural and Veterinary Medicine, Al Qassim University, Saudi Arabia
[d]Department of Pharmacology, Faculty of Veterinary Medicine, Alexandria University, Alexandria, Egypt
[e]Department of Chemistry, University of Prince Edward Island, Charlottetown, Prince Edward Island C1A 4P3, Canada

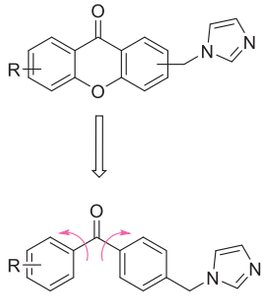


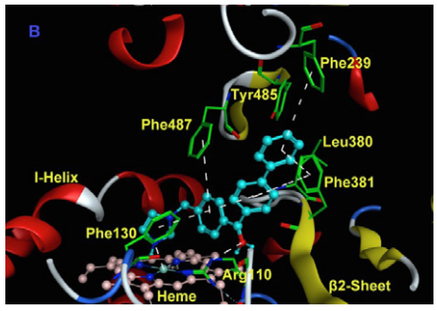
Benzophenones as xanthone-open model CYP11B1 inhibitors potentially useful for promoting wound healing

Bioorganic Chemistry 86 (2019) pp. 401–409

Silvia Gobbi[a,*,1], Qingzhong Hu[b], Giacomo Foschi[a], Elena Catanzaro[c], Federica Belluti[a], Angela Rampa[a], Carmela Fimognari[c], Rolf W. Hartmann[d], Alessandra Bisi[a,*,1]

[a]Department of Pharmacy and Biotechnology, Alma Mater Studiorum-University of Bologna, Via Belmeloro, 6, I-40126 Bologna, Italy
[b]Guangzhou University of Chinese Medicine, Guangzhou, China
[c]Department for Life Quality Studies, Alma Mater Studiorum-University of Bologna, corso d'Augusto 237, 47921 Rimini, Italy
[d]Helmholtz Institute for Pharmaceutical Research Saarland (HIPS), Universitätscampus E8 1, 66123 Saarbrücken, Germany



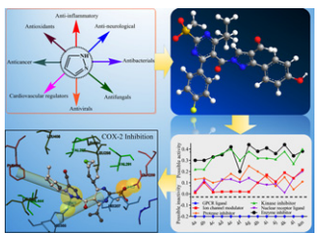


Discovery, synthesis and molecular corroborations of medicinally important novel pyrazoles; drug efficacy determinations through *in silico*, *in vitro* and cytotoxicity validations

Bioorganic Chemistry 86 (2019) pp. 410–419

P. Thangarasu[a], A. Manikandan[b], S. Thamaraiselvi[c,*]

[a]Research and Development Centre, Bharathiar University, Coimbatore 641046, India
[b]Department of Biotechnology, School of Bio-Sciences and Technology, VIT University, Vellore 632014, India
[c]PG & Research Department of Chemistry, Government Arts College, Coimbatore 641018, Tamil Nadu, India

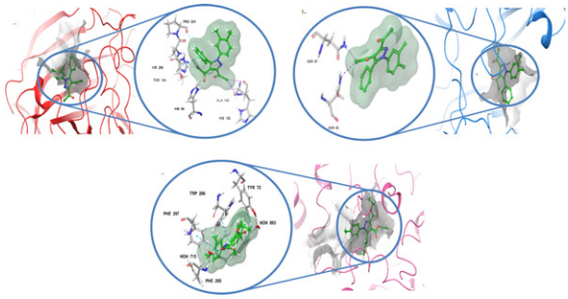


Synthesis, biological evaluation and molecular docking of novel pyrazole derivatives as potent carbonic anhydrase and acetylcholinesterase inhibitors

Bioorganic Chemistry 86 (2019) pp. 420–427

Fikret Turkan[a], Adnan Cetin[b], Parham Taslimi[c,*], Muhammet Karaman[d], İlhami Gulçin[c]

[a]Health Services Vocational School, Igdır University, 76000 Igdır, Turkey
[b]Department of Science, Faculty of Education, Muş Alparslan University, 49250 Muş, Turkey
[c]Department of Chemistry, Faculty of Science, Ataturk University, 25240 Erzurum, Turkey
[d]Department of Molecular Biology and Genetics, Faculty of Arts and Science, Kilis 7 Aralik University, 79000 Kilis, Turkey

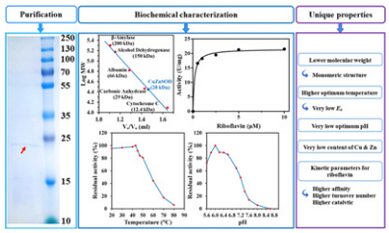


Purification and biochemical characterization of a novel copper, zinc superoxide dismutase from liver of camel *(Camelus dromedarius)*: An antioxidant enzyme with unique properties

Bioorganic Chemistry 86 (2019) pp. 428–436

Abdelbasset Chafik[a,*], Abdelkhalid Essamadi[a], Safinur Yildirim Çelik[b], Ahmet Mavi[c]

[a]Laboratory of Biochemistry and Neuroscience, Team of Applied Biochemistry and Toxicology, Faculty of Science and Technology, University Hassan First, 577 Settat, Morocco
[b]College of Education, Bayburt University, 69000 Bayburt, Turkey
[c]Chemistry Education, Kazim Karabekir Education Faculty, Atatürk University, 25240 Erzurum, Turkey

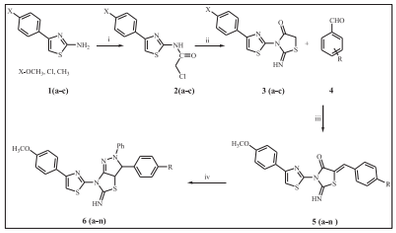


Design, synthesis and molecular docking of pyrazolo [3,4d] thiazole hybrids as potential anti-HIV-1 NNRT inhibitors

Bioorganic Chemistry 86 (2019) pp. 437–444

H.M. Kasralikar[a], S.C. Jadhavar[a], S.V. Goswami[a], N.S. Kaminwar[b], S.R. Bhusare[a,*]

[a]Department of Chemistry, Dnyanopasak College, Parbhani 431 401, MS, India
[b]Department of Chemistry, L. B. S. Mahavidyalaya, Dharmabad, Dist. Nanded, MS, India

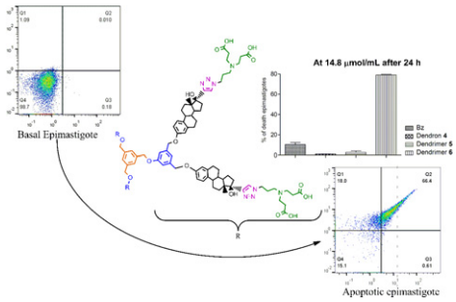


In vitro activity of steroidal dendrimers on *Trypanosoma cruzi* epimastigote form with PAMAM dendrons modified by "click" chemistry

Bioorganic Chemistry 86 (2019) pp. 452–458

Laura Juárez-Chávez[a], Socorro Pina-Canseco[b], Delia Soto-Castro[c,*], Rosa Santillan[d], Nancy E. Magaña-Vergara[e], Paz María Salazar-Schettino[f], Margarita Cabrera-Bravo[f], Eduardo Pérez-Campos[a,b,*]

[a]Unidad de Bioquímica e Inmunología, División de Estudios de Posgrado e Investigación, Instituto Tecnológico de Oaxaca, Av. Ing. Víctor Bravo Ahuja #125 esq, Clz. Tecnológico, C.P. 68030 Oaxaca, Mexico
[b]Centro de Investigación Facultad de Medicina UNAM-UABJO, Facultad de Medicina y Cirugía, Universidad Autónoma "Benito Juárez" de Oaxaca, Ex Hacienda de Aguilera S/N, Carretera a San Felipe del Agua, C.P. 68020 Oaxaca, Mexico
[c]CONACyT-Instituto Politécnico Nacional, CIIDIR Unidad Oaxaca, Hornos 1003, Santa Cruz Xoxocotlán, Oaxaca C.P. 771230, Mexico
[d]Departamento de Química, Centro de Investigación y de Estudios Avanzados del IPN, México, D.F, Apdo. Postal 14-740, 07000 Ciudad de México, Mexico
[e]Facultad de Ciencias Químicas, Universidad de Colima, km 9 Carretera Colima-Coquimatlán, Colima 28400, Mexico
[f]Facultad de Medicina, Departamento de Microbiología y Parasitología, UNAM, Ciudad de México 04510, Mexico

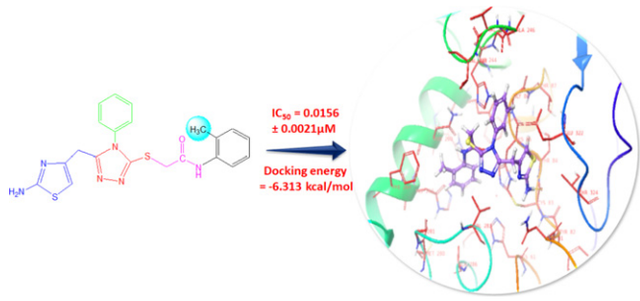


Synthesis and structure-activity relationship of tyrosinase inhibiting novel bi-heterocyclic acetamides: Mechanistic insights through enzyme inhibition, kinetics and computational studies

Bioorganic Chemistry 86 (2019) pp. 459–472

Abdul Rehman Sadiq Butt[a], Muhammad Athar Abbasi[a,b,*], Aziz-ur-Rehman[a], Sabahat Zahra Siddiqui[a], Hussain Raza[b], Mubashir Hassan[b], Syed Adnan Ali Shah[c], Muhammad Shahid[d], Sung-Yum Seo[b,*]

[a]Department of Chemistry, Government College University, Lahore 54000, Pakistan
[b]College of Natural Sciences, Department of Biological Sciences, Kongju National University, Gongju 32588, South Korea
[c]Faculty of Pharmacy and Atta-ur-Rahman Institute for Natural Products Discovery (AuRIns), Level 9, FF3, Universiti Teknologi MARA, Puncak Alam Campus, 42300 Bandar Puncak Alam, Selangor Darul Ehsan, Malaysia
[d]Department of Biochemistry, University of Agriculture, Faisalabad 38040, Pakistan

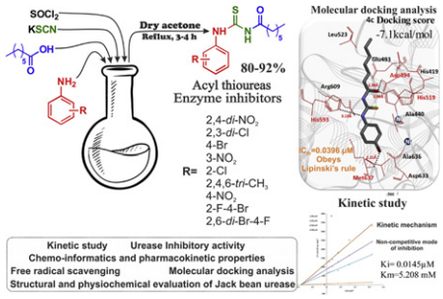


Investigation on the effect of alkyl chain linked mono-thioureas as Jack bean urease inhibitors, SAR, pharmacokinetics ADMET parameters and molecular docking studies

Bioorganic Chemistry 86 (2019) pp. 473–481

Fayaz Ali Larik[a,*], Muhammad Faisal[a,*], Aamer Saeed[a,*], Pervaiz Ali Channar[a], Jan Korabecny[b], Farukh Jabeen[e], Ihsan Ali Mahar[a], Mehar Ali Kazi[d], Qamar Abbas[g], Ghulam Murtaza[a], Gul Shahzada Khan[f], Mubashir Hassan[c], Sung-Yum Seo[c]

[a]Department of Chemistry, Quaid-I-Azam University, Islamabad 45320, Pakistan
[b]Biomedical Research Centre, University Hospital Hradec Kralove, Sokolska 581, 500 05 Hradec Kralove, Czech Republic
[c]Department of Biological Sciences, College of Natural Sciences, Kongju National University, 56 Gongjudehak-Ro, Gongju, Chungnam 314-701, Republic of Korea
[d]Institute of biochemistry, University of Sindh, Jamshoro 76080, Pakistan
[e]Cardiovascular and Metabolic Research Unit, Laurentian University, 935 Ramsey Lake Road, Sudbury, ON P3E 2C6, Canada
[f]Department of Chemistry, Abdul Wali Khan University, Mardan, Khybder Pakhtunkhwa, Pakistan
[g]Department of Physiology, University of Sindh, Jamshoro 76080, Pakistan

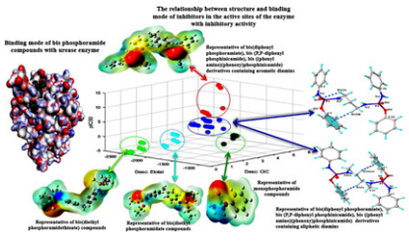


Synthesis, crystal structure and biological evaluation of new phosphoramide derivatives as urease inhibitors using docking, QSAR and kinetic studies

Bioorganic Chemistry 86 (2019) pp. 482–493

Khodayar Gholivand[a,*], Mahsa Pooyan[a], Fahimeh Mohammadpanah[a], Foroogh Pirastefar[a], Peter C. Junk[b], Jun Wang[b], Ali Asghar Ebrahimi Valmoozi[a], Ahmad Mani-Varnosfaderani[a]

[a]Department of Chemistry, Faculty of Science, Tarbiat Modares University, Tehran, Iran
[b]College of Science & Engineering, James Cook University, Townsville, Queensland 4811, Australia

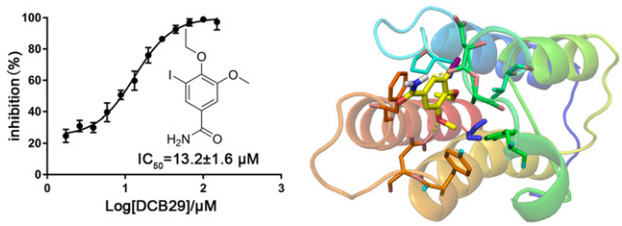


Discovery of alkoxy benzamide derivatives as novel BPTF bromodomain inhibitors via structure-based virtual screening

Bioorganic Chemistry 86 (2019) pp. 494–500

Dan Zhang[a,b,i,1], Jie Han[b,c,i,1], Wenchao Lu[b,c,i,1], Fulin Lian[b,c], Jun Wang[b,d], Tian Lu[b,d], Hongru Tao[b,e], Senhao Xiao[b,g], Fengcai Zhang[b,h], Yu-Chih Liu[f], Rongfeng Liu[f], Naixia Zhang[b,c], Hualiang Jiang[b,c,g,i], Kaixian Chen[b,c,g,i], Chunshen Zhao[a,*], Cheng Luo[b,c,g,i,*]

[a]*Guizhou Engineering Laboratory for Synthetic Drugs, Key Laboratory of Guizhou for Fermentation Engineering and Biomedicine, School of Pharmaceutical Sciences, Guizhou University, Guizhou 550025, China*
[b]*State Key Laboratory of Drug Research, CAS Key Laboratory of Receptor Research, Shanghai Institute of Materia Medica, Chinese Academy of Sciences, 555 Zuchongzhi Road, Shanghai 201203, China*
[c]*University of Chinese Academy of Sciences, 19 Yuquan Road, Beijing 100049, China*
[d]*Jiangsu Key Laboratory for High Technology Research of TCM Formulae, Nanjing University of Chinese Medicine, 138 Xianlin Road, Nanjing 210023, China*
[e]*School of Life Sciences, Shanghai University, 99 Shangda Road, Shanghai 200444, China*
[f]*Shanghai ChemPartner Co., LTD., Zhangjiang Hi-Tech Park, Shanghai 201203, China*
[g]*School of Life Science and Technology, ShanghaiTech University, 100 Haike Road, Shanghai 201210, China*
[h]*School of Pharmacy, Nanchang University, 461 Bayi Road, Nanchang 330006, China*
[i]*Open Studio for Druggability Research of Marine Natural Products, Pilot National Laboratory for Marine Science and Technology (Qingdao), 1 Wenhai Road, Aoshanwei, Jimo, Qingdao 266237, China*

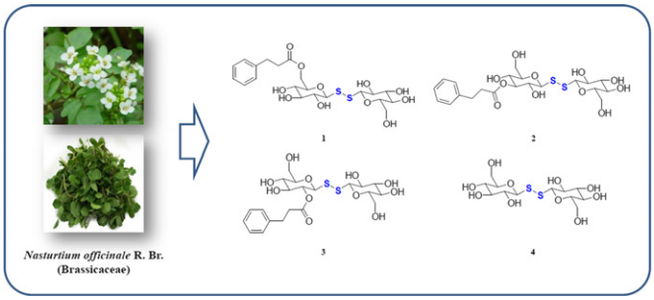


New bis-thioglycosyl-1,1′-disulfides from *Nasturtium officinale* R. Br. and their anti-neuroinflammatory effect

Bioorganic Chemistry 86 (2019) pp. 501–506

Tae Hyun Lee[a], Zahra Khan[b,c], Lalita Subedi[b,c], Sun Yeou Kim[b,c], Kang Ro Lee[a,*]

[a]*Natural Products Laboratory, School of Pharmacy, Sungkyunkwan University, Suwon 16419, Republic of Korea*
[b]*Gachon Institute of Pharmaceutical Science, Gachon University, 191 Hambakmoero, Yeonsu-gu, Incheon 21936, Republic of Korea*
[c]*College of Pharmacy, Gachon University, 191 Hambakmoero, Yeonsu-gu, Incheon 21936, Republic of Korea*

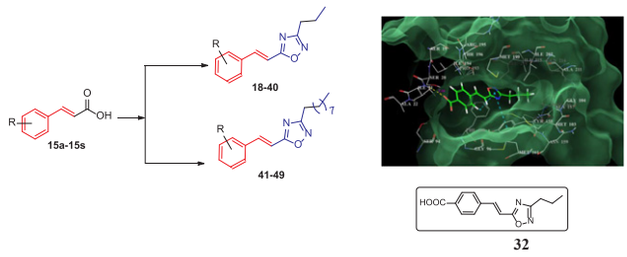


Design, synthesis and biological evaluation of (E)-5-styryl-1,2,4-oxadiazoles as anti-tubercular agents

Bioorganic Chemistry 86 (2019) pp. 507–512

Abhay Atmaram Upare[a,e], Pradip K. Gadekar[a], H. Sivaramakrishnan[a], Nishigandha Naik[b], Vijay M. Khedkar[c], Dhiman Sarkar[d], Amit Choudhari[d], S. Mohana Roopan[e,*]

[a]*Department of Process Development, Piramal Enterprises Ltd., Lighthall A wing, Hiranandani Business Park, Sakivihar road, Chandivali, Andheri (East), Mumbai 400072, India*
[b]*Haffkine Institute for Training, Research and Testing, Acharya Donde MargParel, Mumbai 400012, India*
[c]*Department of Pharmaceutical Chemistry, Shri Vile Parle Kelavani Mandal's Institute of Pharmacy, Mumbai - Agra National Hwy, Dhule, Maharashtra 424001, India*
[d]*Combi Chem-Bio Resource Centre, Division of Organic Chemistry, CSIR-National Chemical Laboratory, Dr. Homi Bhabha Road, Pune 411 008, India*
[e]*Chemistry of Heterocycles & Natural Product Research Laboratory, Department of Chemistry, School of Advanced Sciences, Vellore Institute of Technology, Vellore 632014, Tamil Nadu, India*

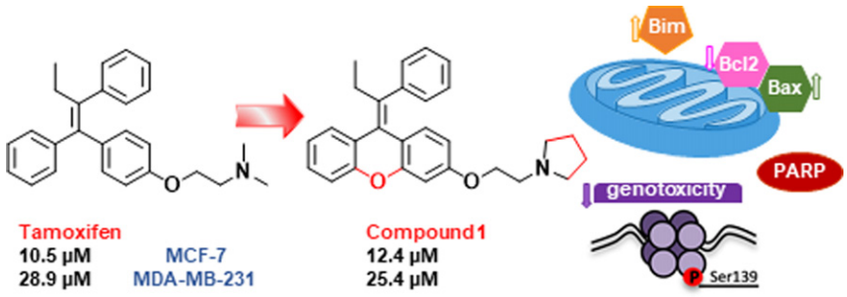


Identification of a new tamoxifen-xanthene hybrid as pro-apoptotic anticancer agent

Bioorganic Chemistry 86 (2019) pp. 538–549

Elena Catanzaro[a], Francesca Seghetti[b], Cinzia Calcabrini[a], Angela Rampa[b], Silvia Gobbi[b], Piero Sestili[c], Eleonora Turrini[a], Francesca Maffei[a], Patrizia Hrelia[d], Alessandra Bisi[b], Federica Belluti[b,*,1], Carmela Fimognari[a,*,1]

[a]Department for Life Quality Studies, Alma Mater Studiorum-University of Bologna, Corso d'Augusto 237, 47921 Rimini, Italy
[b]Department of Pharmacy and Biotechnology, Alma Mater Studiorum-University of Bologna, Via Belmeloro 6, 40126 Bologna, Italy
[c]Department of Biomolecular Sciences, University of Urbino Carlo Bo, Via I Maggetti 26, 61029 Urbino (PU), Italy
[d]Department of Pharmacy and Biotechnology, Alma Mater Studiorum-University of Bologna, Via Irnerio 48, 40126 Bologna, Italy

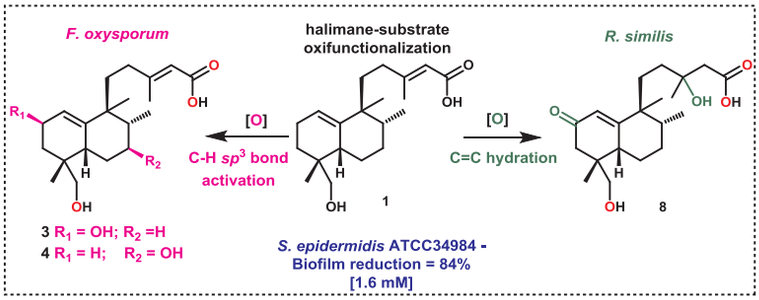


Oxidative functionalization of a halimane diterpenoid achieved by fungal transformation

Bioorganic Chemistry 86 (2019) pp. 550–556

Afif Felix Monteiro[a,1,*], Gabriela Marinho Righetto[b], Laura Vilar Simões[a], Larissa Costa de Almeida[c], Letícia Veras Costa-Lotufo[c], Ilana Lopes Baratella da Cunha Camargo[b], Ian Castro-Gamboa[a,*]

[a]Núcleo de Bioensaios, Biossíntese e Ecofisiologia de Produtos Naturais (NuBBE), Universidade Estadual Paulista (UNESP), Instituto de Química, Departamento de Química Orgância, Francisco Degni, 55, 14800-900, Araraquara, SP, Brazil
[b]São Carlos Institute of Physics, University of São Paulo, PO Box 369, 135560-970, São Carlos, SP, Brazil
[c]Universidade de São Paulo (USP), Instituto de Ciências Biomédicas, Av. Lineu Prestes, 1524, 05508-900, São Paulo, SP, Brazil

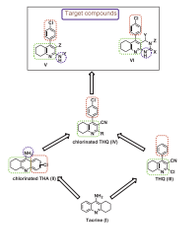


Chlorinated tacrine analogs: Design, synthesis and biological evaluation of their anti-cholinesterase activity as potential treatment for Alzheimer's disease

Bioorganic Chemistry 86 (2019) pp. 557–568

Hanan.M. Ragab[a,*], Mohamed Teleb[a], Hassan R. Haidar[b], Noha Gouda[c]

[a]Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Alexandria University, Alexandria 21521, Egypt
[b]Department of Pharmacology and Therapeutics, Faculty of Pharmacy, Beirut Arab University, Beirut, Lebanon
[c]Noha Gouda, Department of Pharmaceutics, Faculty of Pharmacy, Alexandria University, Alexandria 21521, Egypt

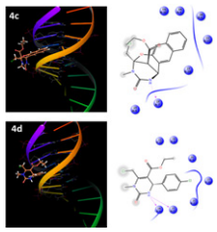


Discovery of the Biginelli hybrids as novel caspase-9 activators in apoptotic machines: Lipophilicity, molecular docking study, influence on angiogenesis gene and miR-21 expression levels

Bioorganic Chemistry 86 (2019) pp. 569–582

Nenad Janković[a,*], Jovana Trifunović Ristovski[b], Milan Vraneš[c], Aleksandar Tot[c], Jelena Petronijević[a], Nenad Joksimović[a], Tatjana Stanojković[d], Marija Đorđić Crnogorac[d], Nina Petrović[d,e], Ivana Boljević[d], Ivana Z. Matić[d], Goran A. Bogdanović[e], Momir Mikov[b], Zorica Bugarčić[a]

[a]Department of Chemistry, Faculty of Science, University of Kragujevac, Radoja Domanovića 12, 34000 Kragujevac, Serbia
[b]Department of Pharmacology, Toxicology and Clinical Pharmacology, Faculty of Medicine, University of Novi Sad, Hajduk Veljkova 3, 21000 Novi Sad, Serbia
[c]Department of Chemistry, Biochemistry and Environmental Protection, University of Novi Sad, Trg Dositeja Obradovića 3, 21000 Novi Sad, Serbia
[d]Institute for Oncology and Radiology of Serbia, Pasterova 14, 11000 Belgrade, Serbia
[e]Vinča Institute of Nuclear Science, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia

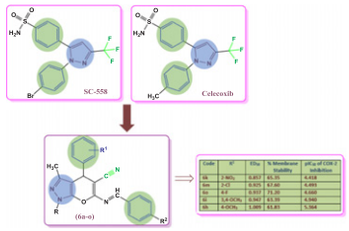


Ligand based design and synthesis of pyrazole based derivatives as selective COX-2 inhibitors

Bioorganic Chemistry 86 (2019) pp. 583–597

Manikanta Murahari[a], Vivek Mahajan[b], Sreenivasulu Neeladri[b], Maushmi S. Kumar[c], Y.C. Mayur[c,*]

[a]Pharmacological Modelling & Simulation Centre, M.S. Ramaiah University of Applied Sciences, Bangalore 560 054, India
[b]Medicinal Chemistry Research Division, VL College of Pharmacy, Raichur 584103, India
[c]Department of Pharmaceutical Chemistry, SPP School of Pharmacy & Technology Management, SVKM's NMIMS, Mumbai 400 056, India

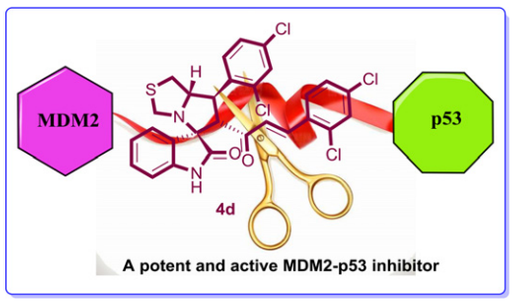


Design and synthesis of new substituted spirooxindoles as potential inhibitors of the MDM2–p53 interaction

Bioorganic Chemistry 86 (2019) pp. 598–608

Assem Barakat[a,b,*], Mohammad Shahidul Islam[a], Hussien Mansur Ghawas[a], Abdullah Mohammed Al-Majid[a], Fardous F. El-Senduny[c], Farid A. Badria[d], Yaseen A.M.M. Elshaier[e], Hazem A. Ghabbour[f]

[a]Department of Chemistry, College of Science, King Saud University, P.O. Box 2455, Riyadh 11451, Saudi Arabia
[b]Department of Chemistry, Faculty of Science, Alexandria University, P.O. Box 426, Ibrahimia, Alexandria 21321, Egypt
[c]Department of Chemistry, Faculty of Science, Mansura University, Mansura, Egypt
[d]Department of Pharmacognosy, Faculty of Pharmacy, Mansoura University, Mansoura 35516, Egypt
[e]Department of Organic and Medicinal Chemistry, Faculty of Pharmacy, University of Sadat City, Menoufiya 32958, Egypt
[f]Department of Medicinal Chemistry, Faculty of Pharmacy, University of Mansoura, Mansoura 35516, Egypt

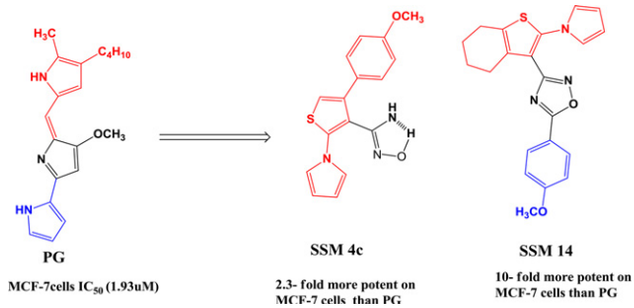


Design, synthesis, and cytotoxicity screening of 5-aryl-3-(2-(pyrrolyl) thiophenyl)-1, 2, 4-oxadiazoles as potential antitumor molecules on breast cancer MCF-7 cells

Bioorganic Chemistry 86 (2019) pp. 609–623

Mohammed K. Abd el hameid[a,*], Manal R. Mohammed[b]

[a]Organic Pharmaceutical Chemistry Department, Faculty of Pharmacy, Cairo University, Egypt
[b]Department of Radiation Biology, National Center for Radiation Research and Technology, Cairo, Egypt

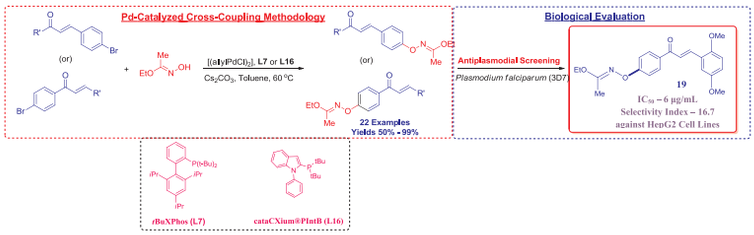


Synthesis of novel chalcones through palladium-catalyzed C—O cross-coupling reaction of bromo-chalcones with ethyl acetohydroxamate and their antiplasmodial evaluation against *Plasmodium falciparum in vitro*

Bioorganic Chemistry 86 (2019) pp. 631–640

Reeta[a,b], Rajendran Vinoth[c], T.M. Rangarajan[d,*], Ayushee[b], Rishi Pal Singh[d,*], Manjula Singh[e]

[a]*Fluoroorganic Laboratory, Centre for Fire, Explosive and Environment Safety, DRDO, Delhi, India*
[b]*Department of Chemistry, University of Delhi, Delhi, India*
[c]*Department of Biochemistry, University of Delhi South Campus, Benito Juarez Road, New Delhi, India*
[d]*Department of Chemistry, Sri Venkateswara College, University of Delhi, New Delhi, India*
[e]*Department of Chemistry, Shivaji College, University of Delhi, New Delhi, India*

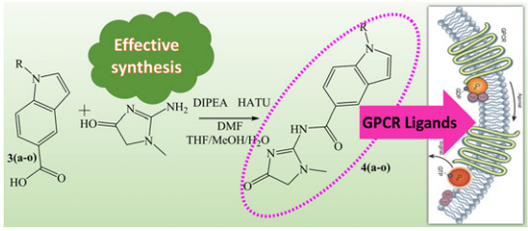


Discovery and synthesis of 2-amino-1-methyl-1H-imidazol-4(5H)-ones as GPCR ligands; an approach to develop breast cancer drugs via GPCR associated PAR1 and PI3Kinase inhibition mechanism

Bioorganic Chemistry 86 (2019) pp. 641–651

S.R. Ashok[a], M.K. Shivananda[a,*], A. Manikandan[b,**], R. Chandrasekaran[c]

[a]*Dept of Studies & Research in Chemistry, Tumkur University, Tumkur 572102, Karnataka, India*
[b]*Dept. of Biotech, Vellore Institute of Technology (VIT), Vellore 632014, Tamil Nadu, India*
[c]*Sai Supreme Chemicals, Gummidipoondi, Chennai 601201, Tamil Nadu, India*

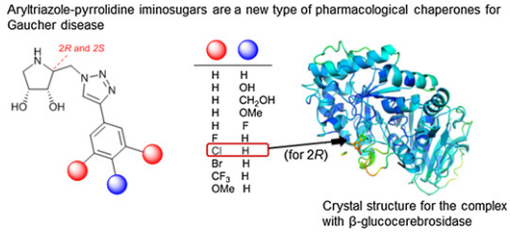


Exploring substituent diversity on pyrrolidine-aryltriazole iminosugars: Structural basis of β-glucocerebrosidase inhibition

Bioorganic Chemistry 86 (2019) pp. 652–664

Macarena Martínez-Bailén[a], Ana T. Carmona[a,*], Athéna C. Patterson-Orazem[b], Raquel L. Lieberman[b], Daisuke Ide[c], Moemi Kubo[c], Atsushi Kato[c], Inmaculada Robina[a], Antonio J. Moreno-Vargas[a,*]

[a]*Department of Organic Chemistry, Faculty of Chemistry, University of Seville, C/Prof. García González, 1, 41012-Seville, Spain*
[b]*School of Chemistry & Biochemistry, Georgia Institute of Technology, Atlanta 30332-0400, GA, United States*
[c]*Department of Hospital Pharmacy, University of Toyama, Toyama 930-0194, Japan*

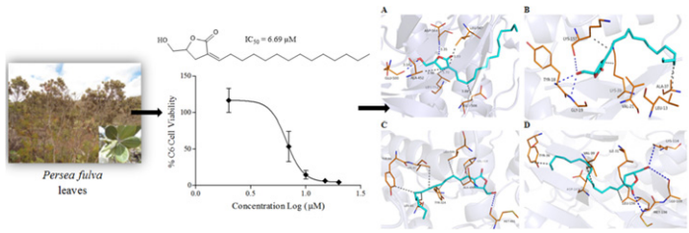


Alkene lactones from *Persea fulva* (Lauraceae): Evaluation of their effects on tumor cell growth *in vitro* and molecular docking studies

Bioorganic Chemistry 86 (2019) pp. 665–673

Isabella Mary Alves Reis[a], Rodrigo Souza Conceição[a], Rafael Short Ferreira[b], Cleonice Creusa dos Santos[b], Girliane Regina da Silva[c], Larissa de Mattos Oliveira[a], Dayse Santos Almeida Cassiano[a], Manoelito Coelho dos Santos Junior[a], Mariana Borges Botura[a], Victor Diogenes Amaral da Silva[b], Silvia Lima Costa[b], Tania Maria Sarmento da Silva[c], Ivo José Curcino Vieira[d], Raimundo Braz-Filho[e,f], Alexsandro Branco[a,*]

[a]*Departamento de Saúde, Universidade Estadual de Feira de Santana, Av. Transnordestina s/n, 44036-900 Feira de Santana, BA, Brazil*
[b]*Laboratório de Neuroquímica e Biologia Celular, Instituto de Ciências da Saúde, Universidade Federal da Bahia – UFBA, Av. Reitor Miguel Calmon s/n, Vale do Canela, 41100-100 Salvador, BA, Brazil*
[c]*Programa de Pós-Graduação em Desenvolvimento e Inovação Tecnológica em Medicamentos, Departamento de Ciências Molecular, Universidade Federal Rural de Pernambuco, Campus Dois Irmãos, 52171-900 Recife, PE, Brazil*
[d]*Laboratório de Ciências Químicas, Centro de Ciências e Tecnologia, Universidade Estadual do Norte Fluminense-Darcy Ribeiro, Av. Alberto Lamego, 2000-Parque Califórnia, 28013-602 Campos dos Goytacazes, RJ, Brazil*
[e]*PVE-FAPERJ/DEQUIM-ICE-Universidade Federal Rural do Rio de Janeiro (UFRRJ), CP 74541, 23894-374 Seropédica, RJ, Brazil*
[f]*LCQUI-CCT-Universidade Estadual do Norte Fluminense Darcy Ribeiro, 28013-600 Campos dos Goytacazes, RJ, Brazil*

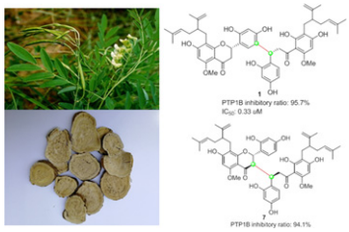


Eight new biflavonoids with lavandulyl units from the roots of *Sophora flavescens* and their inhibitory effect on PTP1B

Bioorganic Chemistry 86 (2019) pp. 679–685

Hai-Wei Yan[a], Hui Zhu[a], Xiang Yuan[a], Ya-Nan Yang[a,b], Zi-Ming Feng[a], Jian-Shuang Jiang[a], Pei-Cheng Zhang[a,*]

[a]*State Key Laboratory of Bioactive Substance and Function of Natural Medicines, Institute of Materia Medica, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing 100050, PR China*
[b]*State Key Laboratory of Functions and Applications of Medicinal Plants, Guizhou Medical University, Guizhou 550025, PR China*

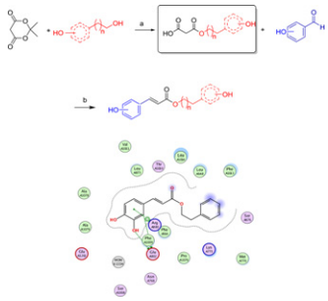


Synthesis and characterization of CAPE derivatives as xanthine oxidase inhibitors with radical scavenging properties

Bioorganic Chemistry 86 (2019) pp. 686–695

Wonbeen Choi[a], Valente Villegas[a], Hannah Istre[b], Ben Heppler[b], Niki Gonzalez[b], Nicole Brusman[b], Lindsey Snider[b], Emily Hogle[b], Janelle Tucker[b], Alma Oñate[b], Sandra Oñate[b], Lili Ma[b], Stefan Paula[a,c,*]

[a]*Department of Chemistry, Purdue University, 560 Oval Drive, West Lafayette, IN 47907-2084, USA*
[b]*Department of Chemistry and Biochemistry, Northern Kentucky University, Nunn Drive, Highland Heights, KY 41099-1905, USA*
[c]*Department of Biochemistry, Purdue University, 175 South University Street, West Lafayette, IN 47907-2063, USA*

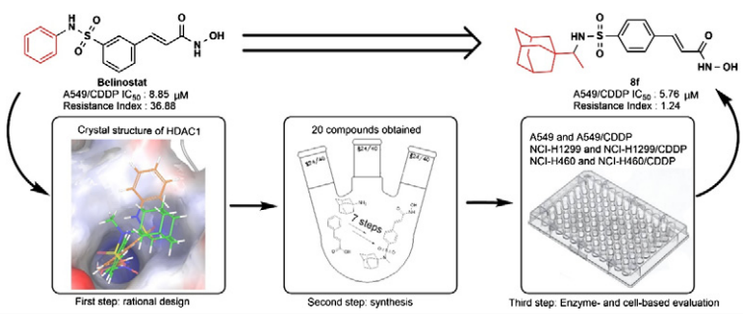


Design, synthesis and evaluation of *N*-hydroxypropenamides based on adamantane to overcome resistance in NSCLC

Bioorganic Chemistry 86 (2019) pp. 696–704

Xuefei Bao[a,1], Yuhong Sun[b,c,1], Changshun Bao[a], Jiayu Zhang[b,c], Shenglan Zou[a], Jingyu Yang[b,c], Chunfu Wu[b,c], Lihui Wang[b,c,*], Guoliang Chen[a,*]

[a]*Key Laboratory of Structure-Based Drugs Design and Discovery of Ministry of Education, Shenyang Pharmaceutical University, Shenyang, PR China*
[b]*Department of Pharmacology, Shenyang Pharmaceutical University, Shenyang, PR China*
[c]*Benxi Institute of Pharmaceutical Research, Shenyang Pharmaceutical University, Shenyang, PR China*

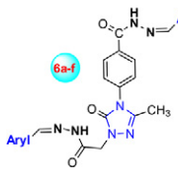


Synthesis of 5-methyl-2,4-dihydro-3*H*-1,2,4-triazole-3-one's aryl Schiff base derivatives and investigation of carbonic anhydrase and cholinesterase (AChE, BuChE) inhibitory properties

Bioorganic Chemistry 86 (2019) pp. 705–713

Musa Özil[a,*], Halis Türker Balaydın[b], Murat Şentürk[c]

[a]*Recep Tayyip Erdogan University, Faculty of Arts and Sciences, Department of Chemistry 53100 Rize, Turkey*
[b]*Recep Tayyip Erdogan University, Education Faculty, 53200 Rize, Turkey*
[c]*Agri Ibrahim Cecen University, Pharmacy Faculty, 04100 Agri, Turkey*



Inhibitor	Aryl	IC_{50} (μM) hCA I	hCA II	AChE	BChE
6a	$-C_6H_5$	-	-	0.0465	-
6e	$-C_6H_4$(p-OCH_3)	0.0538	0.0514	-	-
6f	$-C_6H_3$(2-OH, 4-Br)	-	-	-	0.0486

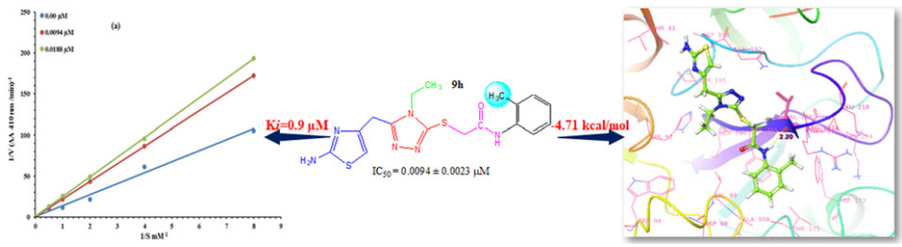
REVIEW ARTICLES

Synthesis and structure-activity relationship of elastase inhibiting novel ethylated thiazole-triazole acetamide hybrids: Mechanistic insights through kinetics and computational contemplations

Bioorganic Chemistry 86 (2019) pp. 197–209

Abdul Rehman Sadiq Butt[a], Muhammad Athar Abbasi[a,b,*], Aziz-ur-Rehman[a], Sabahat Zahra Siddiqui[a], Mubashir Hassan[b], Hussain Raza[b], Syed Adnan Ali Shah[c], Sung-Yum Seo[a,*]

[a]*Department of Chemistry, Government College University, Lahore 54000, Pakistan*
[b]*College of Natural Sciences, Department of Biological Sciences, Kongju National University, Gongju 32588, South Korea*
[c]*Faculty of Pharmacy and Atta-ur-Rahman Institute for Natural Products Discovery (AuRIns), Level 9, FF3, Universiti Teknologi MARA, Puncak Alam Campus, 42300 Bandar Puncak Alam, Selangor Darul Ehsan, Malaysia*

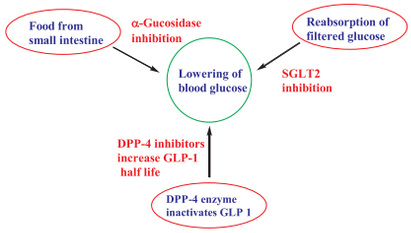


The management of diabetes mellitus-imperative role of natural products against dipeptidyl peptidase-4, α-glucosidase and sodium-dependent glucose co-transporter 2 (SGLT2)

Bioorganic Chemistry 86 (2019) pp. 305–315

Ghulam Abbas[a,b,c,*], Ahmed Al Harrasi[c], Hidayat Hussain[c,d], Ahmed Hamaed[b], Claudiu T. Supuran[a,*]

[a]Università degli Studi di Firenze, NEUROFARBA Dept., Sezione di Scienze Farmaceutiche, Via Ugo Schiff 6, 50019 Sesto Fiorentino (Florence), Italy
[b]Department of Biological Sciences and Chemistry, University of Nizwa, Birkat Al-Mauz, P.O.Box 33, Nizwa 616, Oman
[c]Natural and Medical Sciences Research Center, University of Nizwa, PC 616, Nizwa, Oman
[d]Department of Bioorganic Chemistry, Leibniz Institute of Plant Biochemistry, Weinberg 3, D-06120 Halle, (Salle), Germany

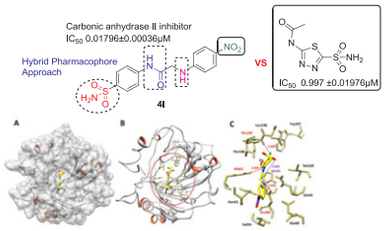


Synthesis of sulfonamide, amide and amine hybrid pharmacophore, an entry of new class of carbonic anhydrase II inhibitors and evaluation of chemo-informatics and binding analysis

Bioorganic Chemistry 86 (2019) pp. 624–630

Attique Ahmed[a], Pervaiz Ali Channar[a], Aamer Saeed[a,*], Markus Kalesse[b], Mehar Ali Kazi[c], Fayaz Ali Larik[a], Qamar Abbas[d], Mubashir Hassan[e], Hussain Raza[e], Sung-Yum Seo[e]

[a]Department of Chemistry, Quaid-I-Azam University, Islamabad 45320, Pakistan
[b]Institut für Organische Chemie, Schneiderberg 1 B, 30167 Hannover, Germany
[c]Institute of Biochemistry, University of Sindh, Jamshoro 76080, Pakistan
[d]Department of Physiology, University of Sindh, Jamshoro 76080, Pakistan
[e]Department of Biological Sciences, College of Natural Sciences, Kongju National University, 56 Gongjudehak-Ro, Gongju, Chungnam 32588, Republic of Korea



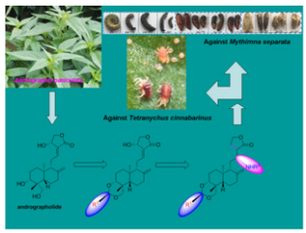
PRELIMINARY COMMUNICATIONS

Evaluation of andrographolide-based analogs derived from *Andrographis paniculata* against *Mythimna separata* Walker and *Tetranychus cinnabarinus* Boisduval

Bioorganic Chemistry 86 (2019) pp. 28–33

Ming Xu, Jianwei Xu, Meng Hao, Kong Zhang, Min Lv*, Hui Xu*

Research Institute of Pesticidal Design & Synthesis, College of Plant Protection/Chemistry and Pharmacy, Northwest A&F University, Yangling 712100, Shaanxi Province, PR China

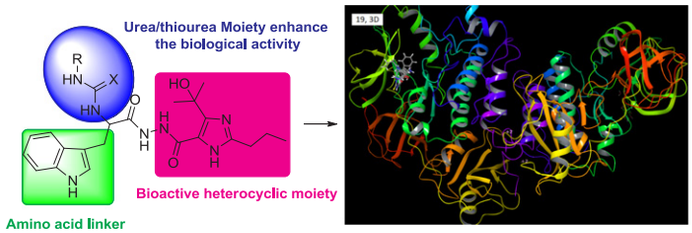


Imidazolo and tryptophan-imidazolo hybrid derived ureas/thioureas as potent bioactive agents – SAR and molecular modelling studies

Bioorganic Chemistry 86 (2019) pp. 34–38

H.K. Kumara, R. Suhas, D.M. Suyoga Vardhan, M. Shobha, D. Channe Gowda*

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

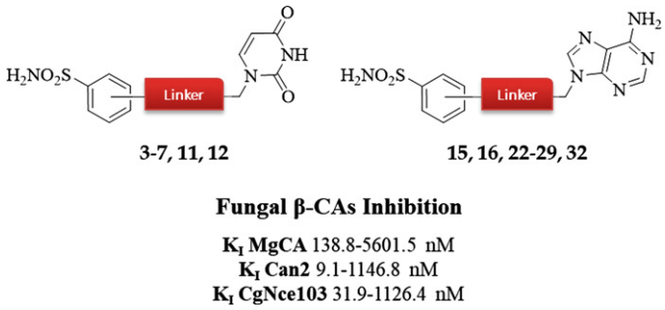


Benzenesulfonamides incorporating nitrogenous bases show effective inhibition of β-carbonic anhydrases from the pathogenic fungi *Cryptococcus neoformans*, *Candida glabrata* and *Malassezia globosa*

Silvia Bua[a], Sameh M. Osman[b], Zeid AlOthman[b], Claudiu T. Supuran[a,b,*], Alessio Nocentini[a,*]

[a]*University of Florence, NEUROFARBA Department, Via Ugo Schiff 6, 50019 Sesto Fiorentino, Italy*
[b]*Department of Chemistry, College of Science, King Saud University, Riyadh, Saudi Arabia*

Bioorganic Chemistry 86 (2019) pp. 39–43

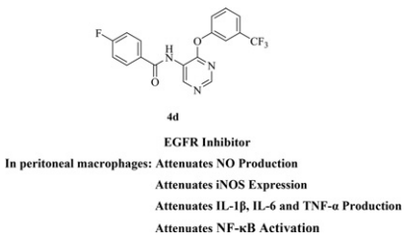


EGFR inhibitors from cancer to inflammation: Discovery of 4-fluoro-*N*-(4-(3-(trifluoromethyl)phenoxy)pyrimidin-5-yl)benzamide as a novel anti-inflammatory EGFR inhibitor

Ahmed Elkamhawy[a,b,*,1], Ahmed H.E. Hassan[c,d,*,1], Sora Paik[e,1], Yong Sup Lee[d,e,f], Hwi-Ho Lee[f,g], Ji-Sun Shin[f,g], Kyung-Tae Lee[f,g,*], Eun Joo Roh[a,h,*]

[a]*Chemical Kinomics Research Center, Korea Institute of Science and Technology (KIST), Seoul 02792, Republic of Korea*
[b]*Department of Pharmaceutical Organic Chemistry, Faculty of Pharmacy, Mansoura University, Mansoura 35516, Egypt*
[c]*Department of Medicinal Chemistry, Faculty of Pharmacy, Mansoura University, Mansoura 35516, Egypt*
[d]*Medicinal Chemistry Laboratory, Department of Pharmacy, College of Pharmacy, Kyung Hee University, Seoul 02447, Republic of Korea*
[e]*Department of Fundamental Pharmaceutical Sciences, College of Pharmacy, Kyung Hee University, Seoul 02447, Republic of Korea*
[f]*Department of Life and Nanopharmaceutical Science, College of Pharmacy, Kyung Hee University, Seoul 02447, Republic of Korea*
[g]*Department of Pharmaceutical Biochemistry, College of Pharmacy, Kyung Hee University, Seoul 02447, Republic of Korea*
[h]*Division of Bio-Medical Science & Technology, KIST School, Korea University of Science and Technology, Seoul 02792, Republic of Korea*

Bioorganic Chemistry 86 (2019) pp. 112–118

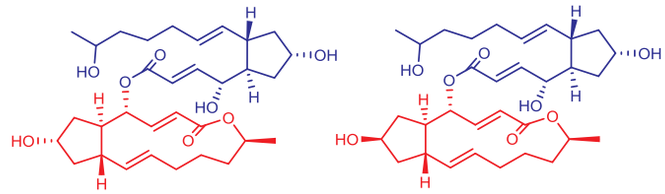


Dibrefeldins A and B, A pair of epimers representing the first brefeldin A dimers with cytotoxic activities from *Penicillium janthinellum*

Fanrong Zeng[1], Chunmei Chen[1], Ali Adhab Al Chnani, Qun Zhou, Qingyi Tong, Wenjing Wang, Yi Zang, Jiaojiao Gong, Zhaodi Wu, Junjun Liu, Jianping Wang, Hucheng Zhu[*], Yonghui Zhang[*]

Hubei Key Laboratory of Natural Medicinal Chemistry and Resource Evaluation, School of Pharmacy, Tongji Medical College, Huazhong University of Science and Technology, Wuhan 430030, People's Republic of China

Bioorganic Chemistry 86 (2019) pp. 176–182



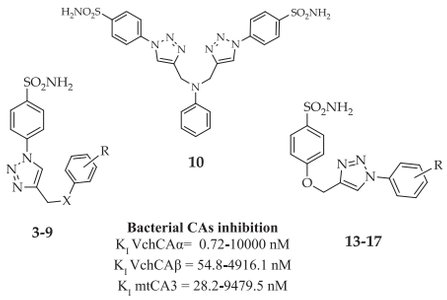
Dibrefeldins A and B (1 and 2)

Click-tailed benzenesulfonamides as potent bacterial carbonic anhydrase inhibitors for targeting *Mycobacterium tuberculosis* and *Vibrio cholerae*

Bioorganic Chemistry 86 (2019) pp. 183–186

Silvia Bua[a], Sameh M. Osman[b], Sonia Del Prete[c], Clemente Capasso[c], Zeid AlOthman[b], Alessio Nocentini[a,*], Claudiu T. Supuran[a,b,*]

[a]*University of Florence, Department of Neuroscience, Psychology, Drug Research and Child's Health, Section of Pharmaceutical and Nutraceutical Sciences, via Ugo Schiff 6, 50019 Sesto Fiorentino, Italy*
[b]*Department of Chemistry, College of Science, King Saud University, Riyadh, Saudi Arabia*
[c]*Istituto di Bioscienze e Biorisorse, CNR, Napoli, Italy*

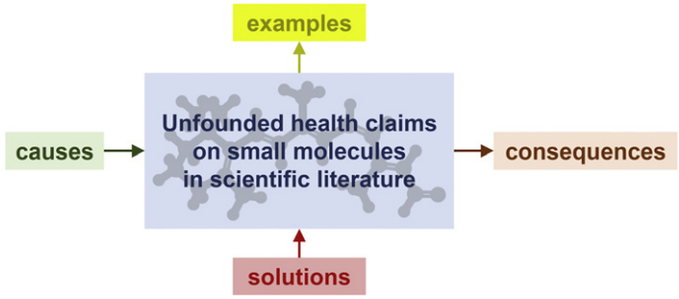


Essay: Avoiding unfounded health claims on small molecules in scientific literature

Bioorganic Chemistry 86 (2019) pp. 273–276

Bart I. Roman[*]

Department of Green Chemistry and Technology, Coupure Links 653, 9000 Gent, Belgium
Cancer Research Institute Gent (CRIG), Corneel Heymanslaan 10, 9000 Gent, Belgium

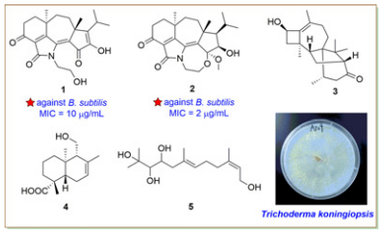


Three new diterpenes and two new sesquiterpenoids from the endophytic fungus *Trichoderma koningiopsis* A729

Bioorganic Chemistry 86 (2019) pp. 368–374

Shanchong Chen[a,b], Haohua Li[a], Yuchan Chen[a], Saini Li[a], Jianlin Xu[a,b], Heng Guo[a,b], Zhaoming Liu[a], Shuang Zhu[b], Hongxin Liu[a,*], Weimin Zhang[a,*]

[a]*State Key Laboratory of Applied Microbiology Southern China, Guangdong Provincial Key Laboratory of Microbial Culture Collection and Application, Guangdong Open Laboratory of Applied Microbiology, Guangdong Institute of Microbiology, Guangzhou 510070, China*
[b]*School of Biosciences and Biopharmaceutics, Guangdong Pharmaceutical University, Guangzhou 510006, China*

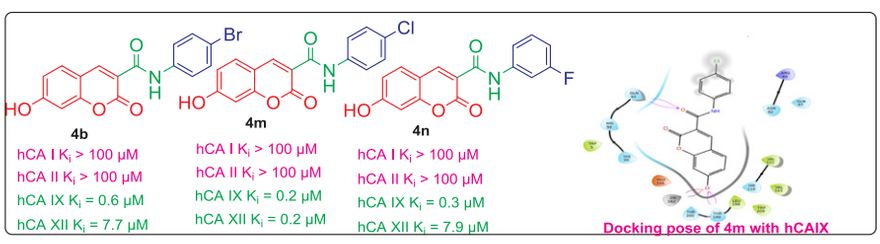


Design, synthesis and biological evaluation of coumarin-3-carboxamides as selective carbonic anhydrase IX and XII inhibitors

Bioorganic Chemistry 86 (2019) pp. 386–392

Pavitra S. Thacker[a], Mallika Alvala[a], Mohammed Arifuddin[a,*], Andrea Angeli[b], Claudiu T. Supuran[b,*]

[a]*Department of Medicinal Chemistry, National Institute of Pharmaceutical Education and Research (NIPER), Balanagar, Hyderabad 500037, India*
[b]*Università degli Studi di Firenze, Neurofarba Dept., Sezione di Scienze Farmaceutiche e Nutraceutiche, Via Ugo Schiff 6, 50019 Sesto Fiorentino, Florence, Italy*

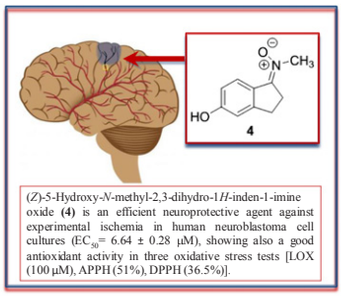


Synthesis, neuroprotective and antioxidant capacity of PBN-related indanonitrones

Bioorganic Chemistry 86 (2019) pp. 445–451

Alicia Jiménez-Almarza[a,b,c,1], Daniel Diez-Iriepa[a,d,1], Mourad Chioua[a,1], Beatriz Chamorro[c], Isabel Iriepa[d], Ricardo Martínez-Murillo[b], Dimitra Hadjipavlou-Litina[e,*], María Jesús Oset-Gasque[c,f,*], José Marco-Contelles[a,*]

[a]*Laboratory of Medicinal Chemistry, Institute of Organic Chemistry (CSIC), Juan de la Cierva 3, 28006 Madrid, Spain*
[b]*The Neurovascular Research Group, Department of Translational Neurobiology, Cajal Institute (CSIC), Madrid, Spain*
[c]*Department of Biochemistry and Molecular Biology, Faculty of Pharmacy, Complutense University of Madrid, Plaza Ramón y Cajal s/n, Ciudad Universitaria, 28040 Madrid, Spain*
[d]*Departamento de Química Orgánica and Química Inorgánica, Ctra. Madrid-Barcelona, Km. 33.6, 28871, Universidad de Alcalá, Madrid, Spain*
[e]*Department of Pharmaceutical Chemistry, Faculty of Health Sciences, Aristotle University of Thessaloniki, Thessaloniki 54124, Greece*
[f]*Instituto de Investigación en Neuroquímica, Universidad Complutense de Madrid, Ciudad Universitaria, 28040 Madrid, Spain*



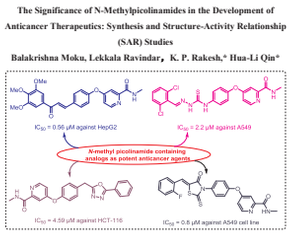
(*Z*)-5-Hydroxy-*N*-methyl-2,3-dihydro-1*H*-inden-1-imine oxide **(4)** is an efficient neuroprotective agent against experimental ischemia in human neuroblastoma cell cultures (EC_{50}= 6.64 ± 0.28 μM), showing also a good antioxidant activity in three oxidative stress tests [LOX (100 μM), APPH (51%), DPPH (36.5%)].

The significance of *N*-methylpicolinamides in the development of anticancer therapeutics: Synthesis and structure-activity relationship (SAR) studies

Bioorganic Chemistry 86 (2019) pp. 513–537

Balakrishna Moku, Lekkala Ravindar, K.P. Rakesh*, Hua-Li Qin*

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

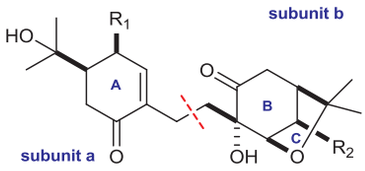


Cordatols A–D, four new anti-inflammatory bis-monoterpenoids from *Illigera cordata*

Bioorganic Chemistry 86 (2019) pp. 674–678

Min Zhou[a,b], Ruiqi Zhang[a], Xiaoli Zeng[a], Shengyong Zhang[a], Miao Dong[a,b], Xiangzhong Huang[a,b,*]

[a]*Key Laboratory of Chemistry in Ethnic Medicinal Resources, State Ethnic Affairs Commission and Ministry of Education, Yunnan Minzu University, Kunming 650031, PR China*
[b]*School of Ethnic Medicine, Yunnan Minzu University, Kunming 650031, PR China*



	R_1	R_2
1	A	A
2	B	A
3	A	B
4	B	B
5	OH	OH

A = cinnamoyloxy
B = dihydrocinnamoyloxy