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Symposium-in-Print

Chemical Proteomics

Edited by:

Herman S. Overkleeft

Leiden Inst. of Chemistry Universiteit Leiden, Postbus 9502, Leiden, 2300 RA, Netherlands

Contents

Publisher's Note

pp 550–551

SPECIAL ISSUE ARTICLES

Chemical proteomics

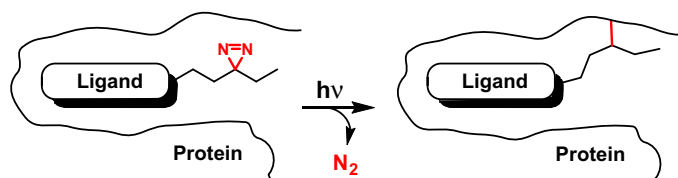
pp 552–553

Herman S. Overkleeft*

Diazirine based photoaffinity labeling

pp 554–570

Luba Dubinsky, Bastiaan P. Krom, Michael M. Meijler*



Diazirines are among the smallest photoreactive groups that form a reactive carbene upon light irradiation. This feature has been widely utilized in photoaffinity labeling to study ligand–receptor, ligand–enzyme and protein–protein interactions, and in the isolation and identification of unknown proteins. This review summarizes recent advances in the use of diazirines in photoaffinity labeling.

Cleavable linkers in chemical biology

pp 571–582

Geoffray Leriche, Louise Chisholm, Alain Wagner*



Development and characterization of improved β -lactone-based anti-virulence drugs targeting ClpP

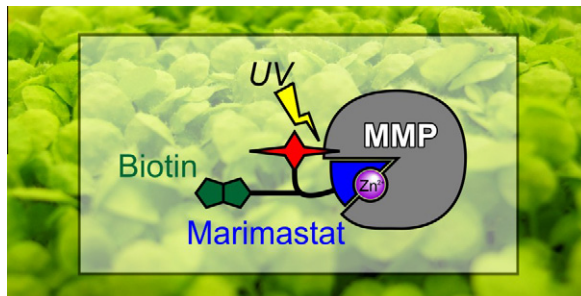
pp 583–591

Evelyn Zeiler, Vadim S. Korotkov, Katrin Lorenz-Baath, Thomas Böttcher*, Stephan A. Sieber*

**Labeling and enrichment of *Arabidopsis thaliana* matrix metalloproteases using an active-site directed, marimastat-based photoreactive probe**

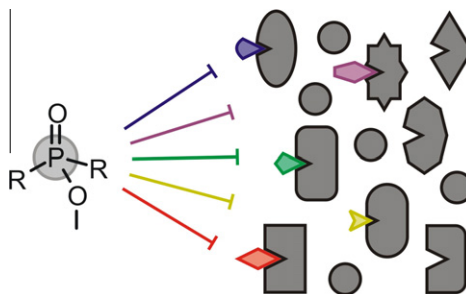
pp 592–596

Janina Lenger, Farnusch Kaschani, Thomas Lenz, Christian Dalhoff, Joji Grace Villamor, Hubert Köster, Norbert Sewald*, Renier A. L. van der Hoorn*

**Selective inhibition of plant serine hydrolases by agrochemicals revealed by competitive ABPP**

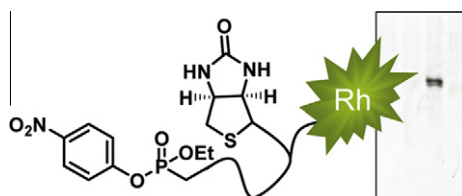
pp 597–600

Farnusch Kaschani, Sabrina Nickel, Bikram Pandey, Benjamin F. Cravatt, Markus Kaiser, Renier A. L. van der Hoorn*

**A *para*-nitrophenol phosphonate probe labels distinct serine hydrolases of *Arabidopsis***

pp 601–606

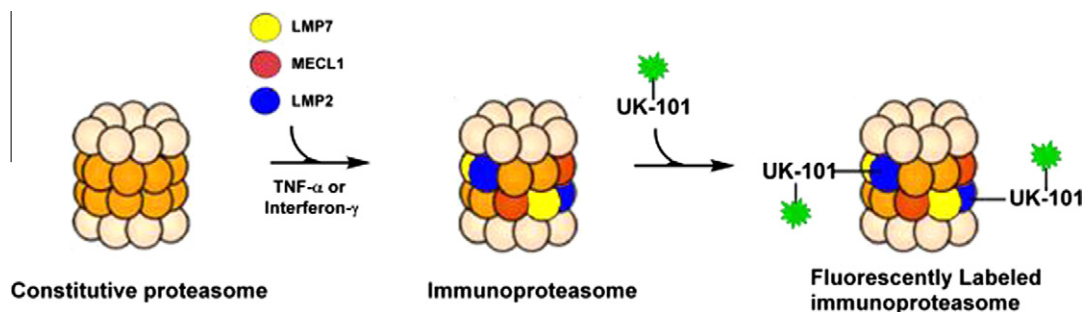
Sabrina Nickel, Farnusch Kaschani, Tom Colby, Renier A. L. van der Hoorn, Markus Kaiser*



A bright approach to the immunoproteasome: Development of LMP2/ β 1i-specific imaging probes

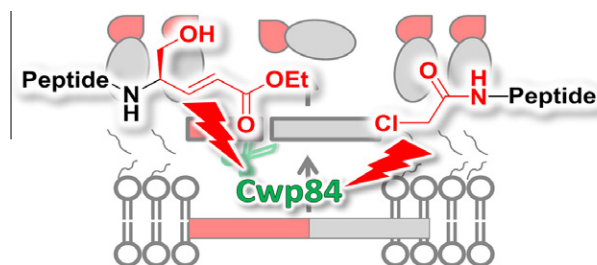
pp 607–613

Kimberly Cornish Carmony, Do-Min Lee, Ying Wu, Na-Ra Lee, Marie Wehenkel, Jason Lee, Beilei Lei, Chang-Guo Zhan, Kyung-Bo Kim*

**Novel inhibitors of surface layer processing in *Clostridium difficile***

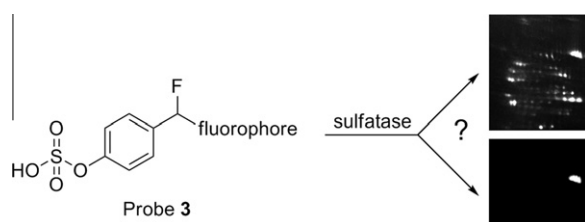
pp 614–621

T. H. Tam Dang, Robert P. Fagan, Neil F. Fairweather, Edward W. Tate*

**Evaluation of sulfatase-directed quinone methide traps for proteomics**

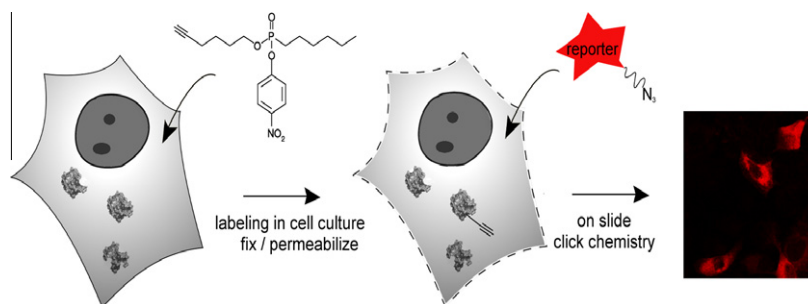
pp 622–627

Janina Lenger, Marius Schröder, Eva C. Ennemann, Benjamin Müller, Chi-Huey Wong, Thomas Noll, Thomas Dierks, Sarah R. Hanson*, Norbert Sewald*

**Activity based subcellular resolution imaging of lipases**

pp 628–632

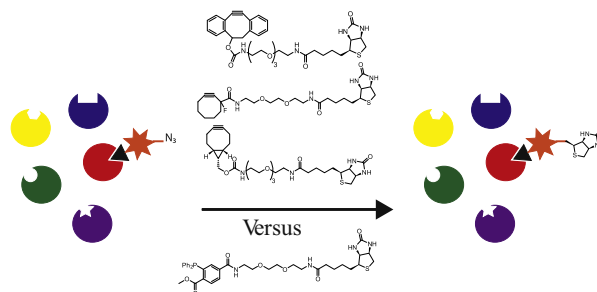
Martin Viertler, Matthias Schittmayer, Ruth Birner-Gruenberger*



Two-step bioorthogonal activity-based proteasome profiling using copper-free click reagents: A comparative study

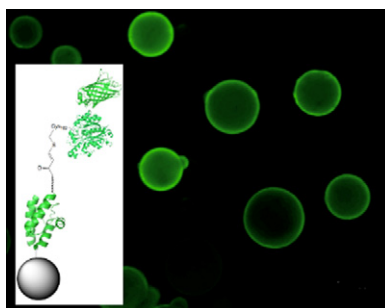
pp 662–666

Wouter A. van der Linden, Nan Li, Sascha Hoogendoorn, Mark Ruben, Martijn Verdoes, Jun Guo, Geert-Jan Boons, Gijsbert A. van der Marel, Bogdan I. Florea*, Herman S. Overkleeft*

**Resin-based investigation of acyl carrier protein interaction networks in *Escherichia coli***

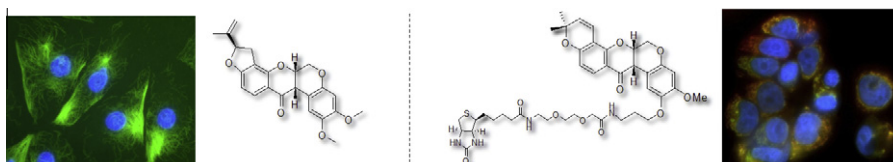
pp 667–671

Michael Rothmann, Sherry Niessen, Robert W. Haushalter, Benjamin F. Cravatt, Michael D. Burkart*

**Synthesis of deguelin–biotin conjugates and investigation into deguelin's interactions**

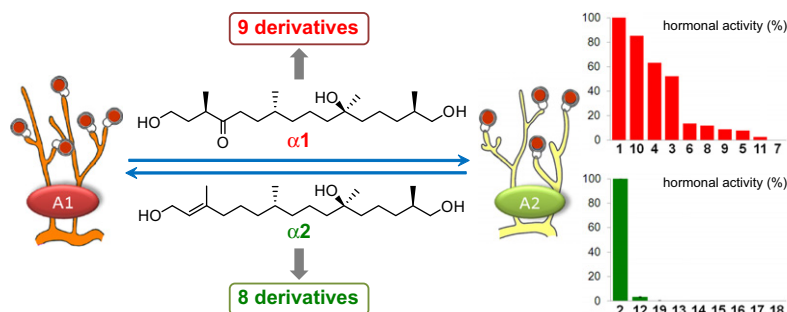
pp 672–680

José Garcia, Sofia Barluenga, Katarzyna Gorska, Florenz Sasse, Nicolas Winssinger*

**REGULAR ARTICLES****Structure–activity relationship of α hormones, the mating factors of phytopathogen *Phytophthora***

pp 681–686

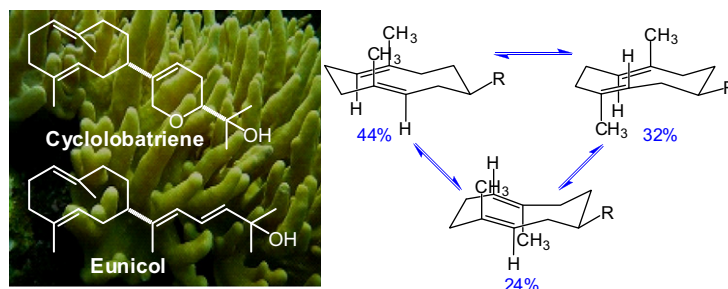
Shylaja D. Molli, Jianhua Qi, Arata Yajima, Keisuke Shikai, Tadashi Imaoka, Tomoo Nukada, Goro Yabuta, Makoto Ojika*



Cyclolobatriene, a novel prenylated germacrene diterpene, from the soft coral *Lobophytum pauciflorum*

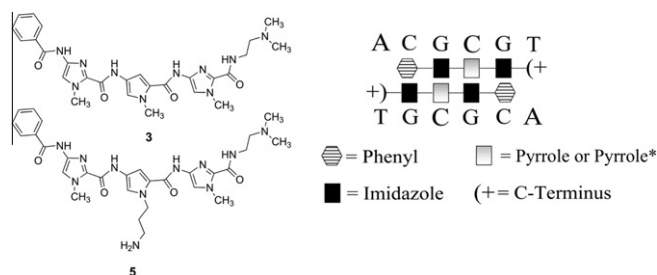
pp 687–692

Sudhakar V. S. Govindam, Yukio Yoshioka, Akihiko Kanamoto, Takeshi Fujiwara, Tetsuji Okamoto, Makoto Ojika*

**Novel diamino imidazole and pyrrole-containing polyamides: Synthesis and DNA binding studies of mono- and diamino-phenyl-lmPy*lm polyamides designed to target 5'-ACGCGT-3'**

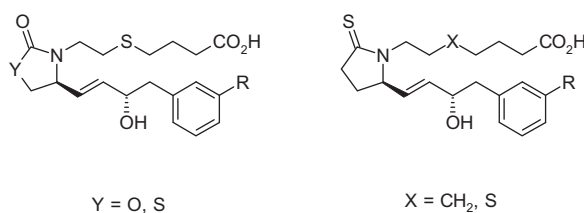
pp 693–701

Vijay Satam, Balaji Babu, Sameer Chavda, Mia Savagian, Robert Sjöholm, Samuel Tzou, Yang Liu, Konstantinos Kiakos, Shicai Lin, W. David Wilson, John A. Hartley, Moses Lee*

**Synthesis and evaluation of novel modified γ -lactam prostanoids as EP4 subtype-selective agonists**

pp 702–713

Tohru Kambe*, Toru Maruyama, Toshihiko Nagase, Seiji Ogawa, Chiaki Minamoto, Kiyoto Sakata, Takayuki Maruyama, Hisao Nakai, Masaaki Toda

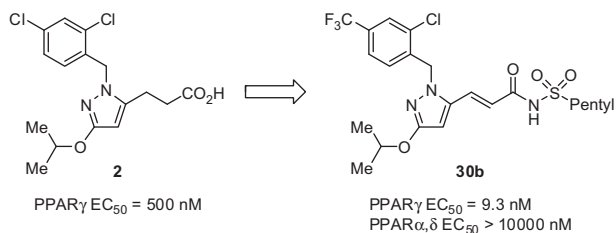


The 2-oxo-1,3-oxazoline, 2-oxo-1,3-thiazolidine and 5-thioxopyrrolidine were identified as new templates for EP4 receptor selective agonists.

A new class of non-thiazolidinedione, non-carboxylic-acid-based highly selective peroxisome proliferator-activated receptor (PPAR) γ agonists: Design and synthesis of benzylpyrazole acylsulfonamides

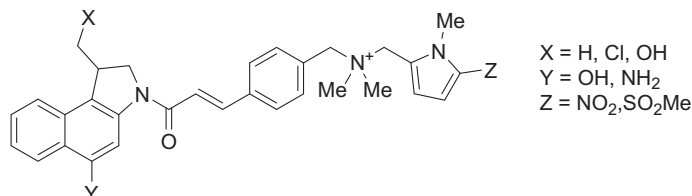
pp 714–733

Kentaro Rikimaru*, Takeshi Wakabayashi, Hidenori Abe, Hiroshi Imoto, Tsuyoshi Maekawa, Osamu Ujikawa, Katsuhito Murase, Takanori Matsuo, Mitsuharu Matsumoto, Chisako Nomura, Hiroko Tsuge, Naoto Arimura, Kazutoshi Kawakami, Junichi Sakamoto, Miyuki Funami, Clifford D. Mol, Gyorgy P. Snell, Kenneth A. Bragstad, Bi-Ching Sang, Douglas R. Dougan, Toshimasa Tanaka, Nozomi Katayama, Yoshiaki Horiguchi, Yu Momose



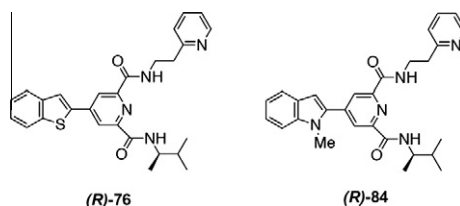
Weight loss effects of quaternary salts of 5-amino-1-(chloromethyl)-1,2-dihydro-3H-benz[e]indoles; structure–activity relationships pp 734–749

Moana Tercel, Ralph J. Stevenson, Guo-Liang Lu, Stephen M. Stribbling, William R. Wilson, Michele A. Tatnell, Rebecca N. Marnane, Kathleen G. Mountjoy, William A. Denny*

**STAT6 phosphorylation inhibitors block eotaxin-3 secretion in bronchial epithelial cells**

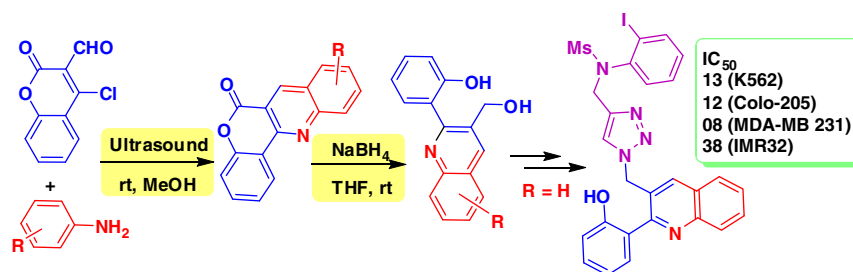
pp 750–758

Li Zhou, Tomohiko Kawate, Xiaorong Liu, Young Bae Kim, Yajuan Zhao, Guohong Feng, Julian Banerji, Huw Nash, Charles Whitehurst, Satish Jindal, Arshad Siddiqui, Brian Seed*, Jia L. Wolfe

**Ultrasound mediated catalyst free synthesis of 6H-1-benzopyrano[4,3-b]quinolin-6-ones leading to novel quinoline derivatives: Their evaluation as potential anti-cancer agents**

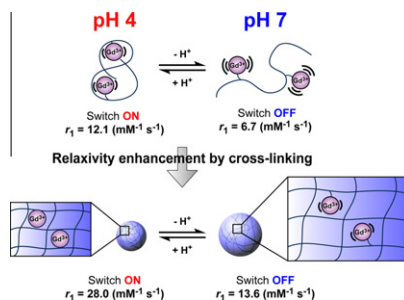
pp 759–768

Naveen Mulakayala, D. Rambabu, Mohan Rao Raja, Chaitanya M., Chitta Suresh Kumar, Arunasree M. Kalle, G. Rama Krishna, C. Malla Reddy, M. V. Basaveswara Rao, Manojit Pal*

**Switchable MRI contrast agents based on morphological changes of pH-responsive polymers**

pp 769–774

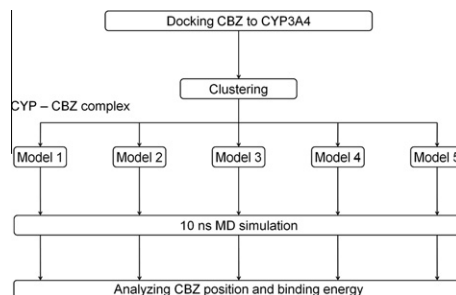
Satoshi Okada, Shin Mizukami, Kazuya Kikuchi*



Prediction of sites of metabolism in a substrate molecule, instanced by carbamazepine oxidation by CYP3A4

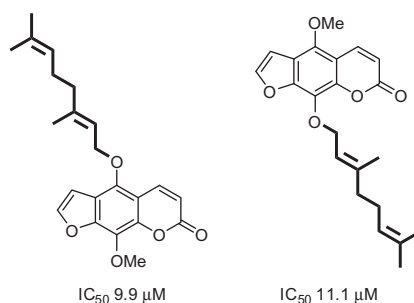
pp 775–783

Hitomi Yuki, Teruki Honma, Masayuki Hata*, Tyuji Hoshino*

**Structure–activity relationships for naturally occurring coumarins as β -secretase inhibitor**

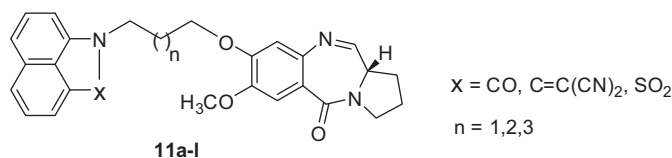
pp 784–788

Shinsuke Marumoto, Mitsuo Miyazawa*

**Design and synthesis of benzo[c,d]indolone-pyrrolobenzodiazepine conjugates as potential anticancer agents**

pp 789–800

Ahmed Kamal*, G. Ramakrishna, V. Lakshma Nayak, P. Raju, A. V. Subba Rao, A. Viswanath, M. V. P. S. Vishnuvardhan, Sistla Ramakrishna*, G. Srinivas

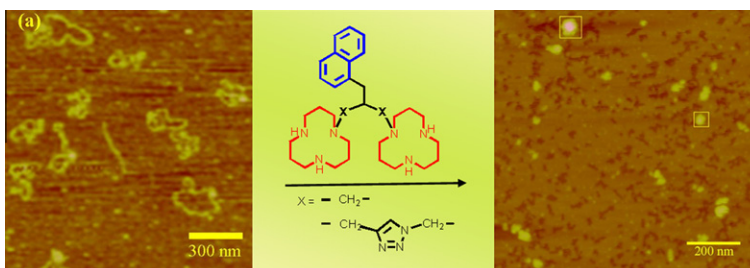


A series of benzo[c,d]indolone-pyrrolobenzodiazepine conjugates **11a–l** have been prepared and evaluated for their anticancer activity.

Effective and reversible DNA condensation induced by bifunctional molecules containing macrocyclic polyamines and naphthyl moieties

pp 801–808

Hao Yan, Zhi-Fen Li, Zhi-Fo Guo, Zhong-Lin Lu*, Feng Wang, Li-Zhu Wu*



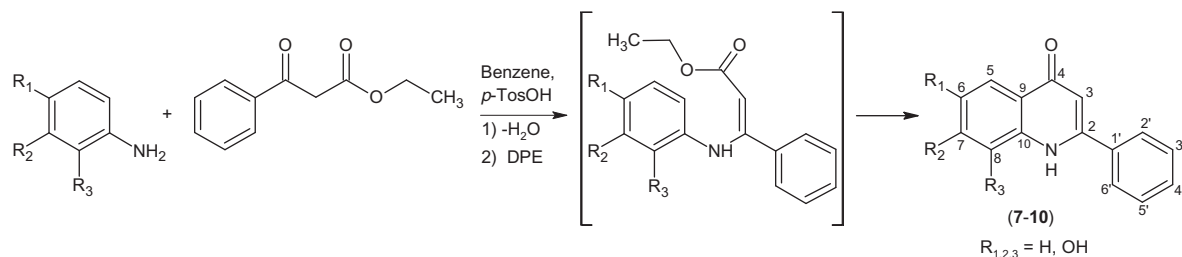
Bifunctional molecules containing naphthyl and macrocyclic polyamine [12]aneN₃ moieties have been synthesized and successfully applied in DNA condensation.



Antioxidant properties of 4-quinolones and structurally related flavones

pp 809–818

Jane Greeff, Jacques Joubert, Sarel F. Malan, Sandra van Dyk*

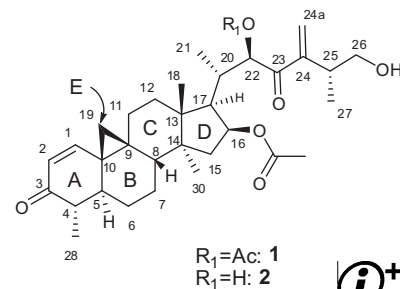


A series of synthesised 4-quinolones (7–10) were evaluated for antioxidant activity and compared to structurally related quinolines and flavones as potential neuroprotective agents.

Semisynthetic neoboutomellerone derivatives as ubiquitin-proteasome pathway inhibitors

pp 819–831

Joséphine Beck, Yves Guminski, Christophe Long, Laurence Marcourt, Fadila Derguini, Fabien Plisson, Antonio Grondin, Isabelle Vandenberghe, Stéphane Vispé, Viviane Brel, Yannick Aussagues, Frédéric Ausseil, Paola B. Arimondo, Georges Massiot, François Sautel*, Frédéric Cantagrel*

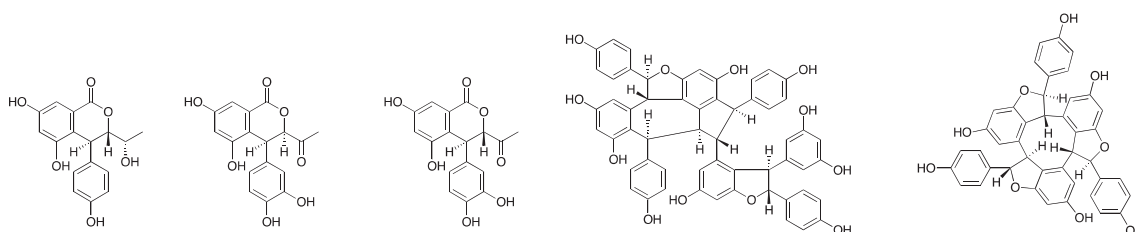


Structures of neoboutomellerones isolated from *Neoboutonia melleri*.

Antidiabetogenic oligostilbenoids and 3-ethyl-4-phenyl-3,4-dihydroisocoumarins from the bark of *Shorea roxburghii*

pp 832–840

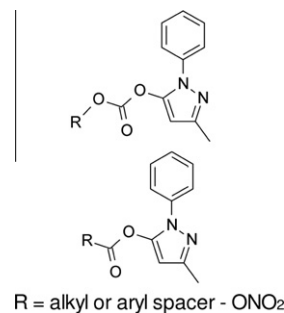
Toshio Morikawa, Saowanee Chaipetch, Hisashi Matsuda, Makoto Hamao, Yohei Umeda, Hiroki Sato, Haruka Tamura, Haruka Kon'i, Kiyofumi Ninomiya, Masayuki Yoshikawa, Yutana Pongpiriyadacha, Takao Hayakawa, Osamu Muraoka*

**Synthesis physicochemical profile and PAMPA study of new NO-donor edaravone co-drugs**

pp 841–850

Barbara Rolando, Andrea Filieri, Konstantin Chegaev, Loretta Lazzarato, Marta Giorgis, Claudio De Nardi, Roberta Fruttero*, Sophie Martel, Pierre-Alain Carrupt, Alberto Gasco

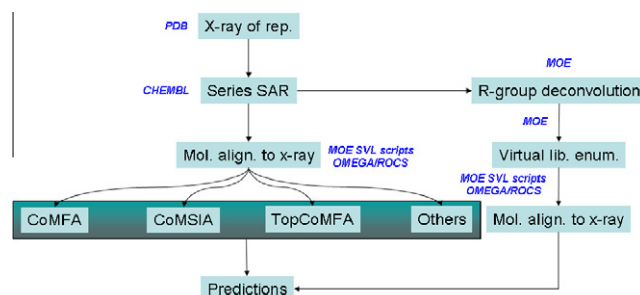
A new class of co-drugs obtained by joining antioxidant edaravone with a vasodilating substructure containing NO-donor functions, is presented. These compounds, characterized by a good gastrointestinal absorption, afford edaravone and the related NO-donor moieties when incubated in human serum and in rat liver homogenate. The title products are potentially useful for treating ROS-related conditions accompanied by decreased NO availability.



An integrated computational workflow for efficient and quantitative modeling of renin inhibitors

pp 851–858

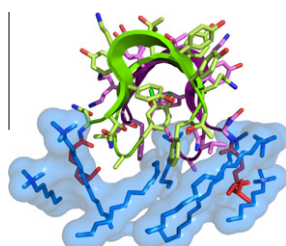
Govindan Subramanian*, Shashidhar N. Rao



Studies on the biosynthesis of the lipodepsipeptide antibiotic Ramoplanin A2

pp 859–865

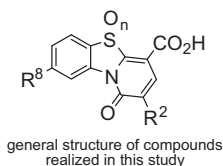
Amanda J. Hoertz, James B. Hamburger, David M. Gooden, Maria M. Bednar, Dewey G. McCafferty*



Pyridobenzothiazole derivatives as new chemotype targeting the HCV NS5B polymerase

pp 866–876

Giuseppe Manfroni*, Francesco Meschini, Maria Letizia Barreca*, Pieter Leyssen, Alberta Samuele, Nunzio Iraci, Stefano Sabatini, Serena Massari, Giovanni Maga, Johan Neyts, Violetta Cecchetti

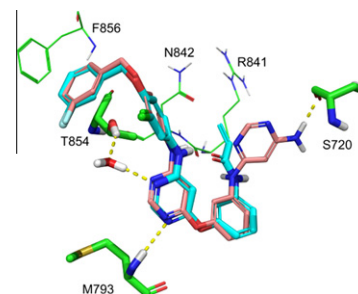


Synthesis and biological evaluation of 4-[3-chloro-4-(3-fluorobenzyloxy)anilino]-6-(3-substituted-phenoxy)pyrimidines as dual EGFR/ErbB-2 kinase inhibitors

pp 877–885

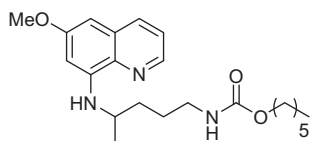
Siyuan Li, Chunying Guo, Hongli Zhao, Yun Tang, Minbo Lan*

A series of 4,6-disubstituted pyrimidines derivatives were designed and synthesized as dual EGFR/ErbB-2 inhibitors. 4-[3-Chloro-4-(3-fluorobenzyloxy)anilino]-6-(3-acrylamidophenoxy)pyrimidine and 4-[3-chloro-4-(3-fluorobenzyloxy)anilino]-6-[3-[6-(4-amino)pyrimidinyl]amino]phenoxy]pyrimidine had the best biological activities in vitro. Docking simulation was performed to explore the binding model of these compounds with EGFR.



A carbamate-based approach to primaquine prodrugs: Antimalarial activity, chemical stability and enzymatic activation pp 886–892

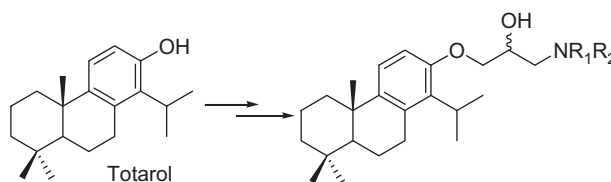
Graça Mata, Virgílio E. do Rosário, Jim Iley, Luís Constantino, Rui Moreira*



O-Alkyl carbamate derivatives of primaquine were shown to display potent transmission-blocking antimalarial activity.

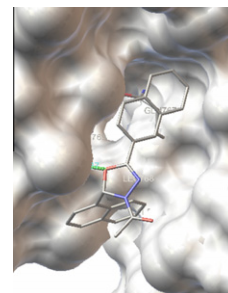
Synthesis, biological evaluation and mechanistic studies of totarol amino alcohol derivatives as potential antimalarial agents pp 893–902

Claire Tacon, Eric M. Guantai, Peter J. Smith, Kelly Chibale*

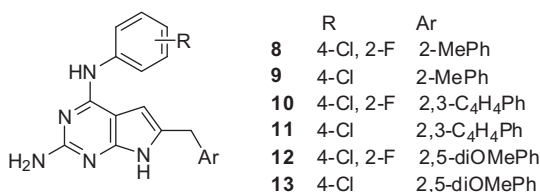
**Design, synthesis, biological evaluation and molecular modeling of 1,3,4-oxadiazoline analogs of combretastatin-A4 as novel antitubulin agents** pp 903–909

Yang Hu, Xiang Lu, Ke Chen, Ru Yan, Qing-Shan Li, Hai-Liang Zhu*

A new series of novel 1,3,4-oxadiazoline analogs (**6a–6t**) of combretastatin A-4 with naphthalene ring were designed, synthesized, and evaluated for biological activities as potential tubulin polymerization inhibitors. Among these compounds, **6n** showed the most potent antiproliferative activities against multiple cancer cell lines and retained the microtubule disrupting effects. Docking simulation was performed to insert compound **6n** into the crystal structure of tubulin to determine the probable binding model.

**N⁴-Aryl-6-substitutedphenylmethyl-7H-pyrrolo[2,3-d]pyrimidine-2,4-diamines as receptor tyrosine kinase inhibitors** pp 910–914

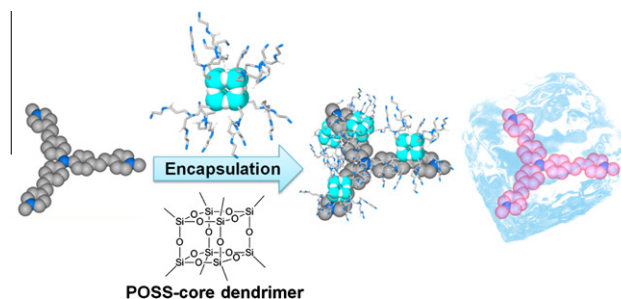
Aleem Gangjee*, Sonali Kurup, Michael A. Ihnat, Jessica E. Thorpe, Bryan Disch



Enhancement of optical properties of dyes for bioprobes by freezing effect of molecular motion using POSS-core dendrimers

pp 915–919

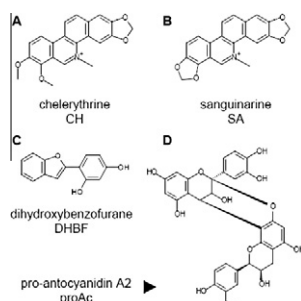
Kazuo Tanaka, Jong-Hwan Jeon, Kenichi Inafuku, Yoshiki Chujo*



Bacterial biofilm formation inhibitory activity revealed for plant derived natural compounds

pp 920–926

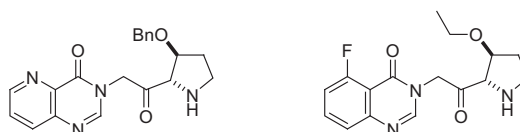
M. Artini, R. Papa, G. Barbato, G. L. Scoarughi, A. Cellini, P. Morazzoni, E. Bombardelli, L. Selan*



Febrifugine analogue compounds: Synthesis and antimalarial evaluation

pp 927–932

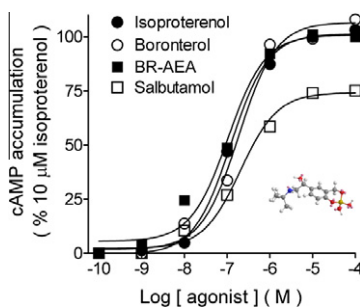
Shuren Zhu*, Gudise Chandrashekar, Li Meng, Katie Robinson, Dipsanker Chatterji



Cell-based and in-silico studies on the high intrinsic activity of two boron-containing salbutamol derivatives at the human β_2 -adrenoceptor

pp 933–941

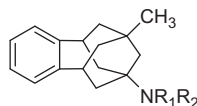
Marvin A. Soriano-Ursúa*, Daniel A. McNaught-Flores, Gustavo Nieto-Alamilla, Aldo Segura-Cabrera, José Correa-Basurto, José A. Arias-Montaño, José G. Trujillo-Ferrara



Synthesis of benzopolycyclic cage amines: NMDA receptor antagonist, trypanocidal and antiviral activities

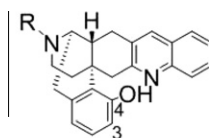
pp 942–948

Eva Torres, María D. Duque, Marta López-Querol, Martin C. Taylor, Lieve Naesens, Chunlong Ma, Lawrence H. Pinto, Francesc X. Sureda, John M. Kelly, Santiago Vázquez*

**Synthesis of quinolinomorphinan-4-ol derivatives as δ opioid receptor agonists**

pp 949–961

Yoshihiro Ida, Toru Nemoto, Shigeto Hirayama, Hideaki Fujii, Yumiko Osa, Masayuki Imai, Takashi Nakamura, Toshiyuki Kanemasa, Akira Kato, Hiroshi Nagase*



R = isobutyl: SN-24

R = methyl: SN-26

R = cyclopropylmethyl: SN-27

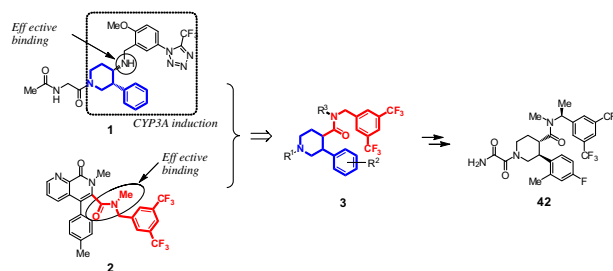
The morphinan derivatives with the 4-hydroxy group (SN-24, 26, 27) showed higher selectivities for the δ receptor over the μ receptor than the corresponding derivatives with the 3-hydroxy group. And they showed high agonist activities for the δ receptor in the [35 S]GTP γ S binding assay.

Novel 3-phenylpiperidine-4-carboxamides as highly potent and orally long-acting neurokinin-1 receptor antagonists with reduced CYP3A induction

pp 962–977

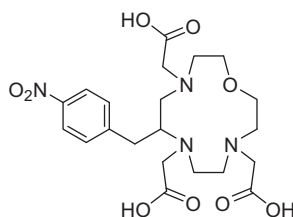
Junya Shirai*, Hideyuki Sugiyama, Shinji Morimoto, Hironobu Maezaki, Yasuharu Yamamoto, Satoshi Okanishi, Izumi Kamo, Shiho Matsumoto, Keiko Ishigami, Nobuhiro Inatomi, Akio Imanishi, Makiko Kawamoto, Naoki Tarui, Tadatoshi Hashimoto, Yoshinori Ikeura

Hybridization of the substructures from two types of tachykinin NK₁ receptor antagonists **1** and **2** generated a novel series of 3-phenylpiperidine-4-carboxamide derivatives **3**. Compound **42** showed high metabolic stability and excellent efficacy in the guinea-pig GR-73637-induced locomotive activity assay at 1 and 24 h after oral administration, exhibited good pharmacokinetic profiles in four animal species, and a low potential in a pregnane X receptor induction assay.

**Facile synthesis and evaluation of C-functionalized benzyl-1-oxa-4,7,10-triazacyclododecane-*N,N,N'*-triacetic acid as chelating agent for ^{111}In -labeled polypeptides**

pp 978–984

Hirofumi Suzuki, Ayaka Kanai, Tomoya Uehara, Francisco L. Guerra Gomez, Hirofumi Hanaoka, Yasushi Arano*

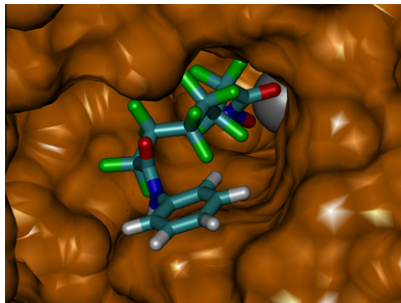


Facile synthetic procedure of the C-functionalized ODTA, and its basic study of the complex with ^{111}In are reported.

Synthesis and biochemical analysis of 2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoro-*N*-hydroxy-octanediamides as inhibitors of human histone deacetylases

pp 985–995

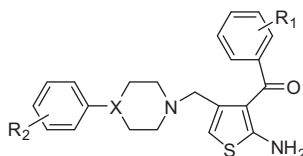
Leonhard M. Henkes, Patricia Haus, Felix Jäger, Joachim Ludwig, Franz-Josef Meyer-Almes*



Structure–activity relationships of 2-amino-3-aryl-4-[(4-arylpiperazin-1-yl)methyl]thiophenes. Part 2: Probing the influence of diverse substituents at the phenyl of the arylpiperazine moiety on allosteric enhancer activity at the A₁ adenosine receptor

pp 996–1007

Romeo Romagnoli*, Pier Giovanni Baraldi*, Maria Dora Carrion, Carlota Lopez Cara, Olga Cruz-Lopez, Maria Kimatrai Salvador, Delia Preti, Mojgan Aghazadeh Tabrizi, John C. Shryock, Allan R. Moorman, Fabrizio Vincenzi, Katia Varani, Pier Andrea Borea

R₁=4-Cl or 3-CF₃

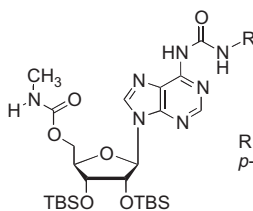
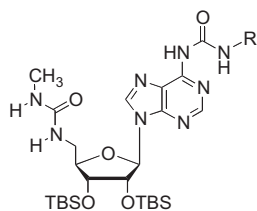
X=N or CH

R₂= one or two EWGs (Cl, F, CF₃ or NO₂)

Synthesis, SAR, and preliminary mechanistic evaluation of novel antiproliferative *N*⁶,5'-bis-ureido- and 5'-carbamoyl-*N*⁶-ureidoadenosine derivatives

pp 1008–1019

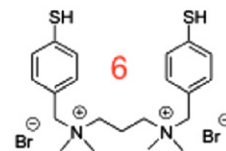
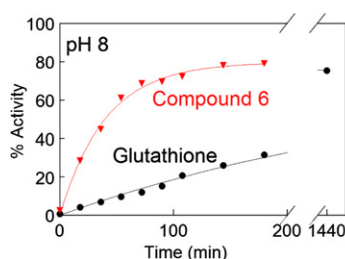
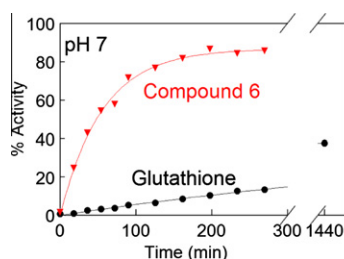
Jadd R. Shelton, Christopher E. Cutler, Marcelio Oliveira, Jan Balzarini, Matt A. Peterson*

R = Phenyl, *p*-chlorophenyl, *p*-iodophenyl, *m*-iodophenyl, *p*-nitrophenyl, *p*-methoxyphenyl, benzyl, propyl, hexyl, cyclohexyl

Oxidative folding of lysozyme with aromatic dithiols, and aliphatic and aromatic monothiols

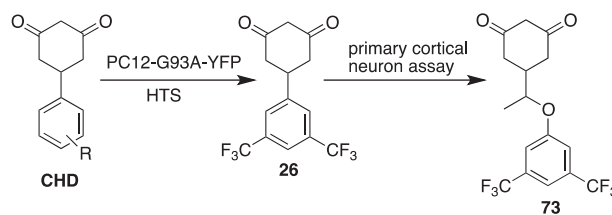
pp 1020–1028

Amar S. Patel, Watson J. Lees*



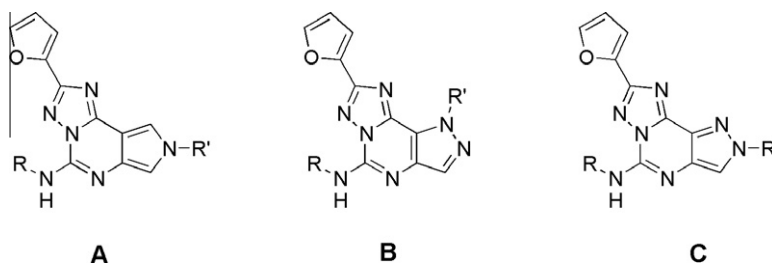
Cyclohexane 1,3-diones and their inhibition of mutant SOD1-dependent protein aggregation and toxicity in PC12 cells pp 1029–1045

Wei Zhang, Radhia Benmohamed, Anthony C. Arvanites, Richard I. Morimoto, Robert J. Ferrante, Donald R. Kirsch, Richard B. Silverman*

**Pyrrolo- and pyrazolo-[3,4-e][1,2,4]triazolo[1,5-c]pyrimidines as adenosine receptor antagonists**

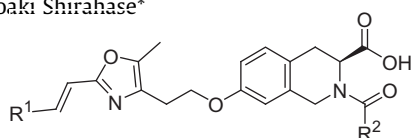
pp 1046–1059

Pier Giovanni Baraldi*, Giulia Saponaro, Mojgan Aghazadeh Tabrizi, Stefania Baraldi, Romeo Romagnoli, Allan R. Moorman, Katia Varani, Pier Andrea Borea, Delia Preti

**Novel (S)-1,2,3,4-tetrahydroisoquinoline-3-carboxylic acids: Peroxisome proliferator-activated receptor γ selective agonists with protein-tyrosine phosphatase 1B inhibition**

pp 1060–1075

Kazuya Otake, Satoru Azukizawa, Masaki Fukui, Kazuyoshi Kunishiro, Hikaru Kamemoto, Mamoru Kanda, Tomohiro Miike, Masayasu Kasai, Hiroaki Shirahase*

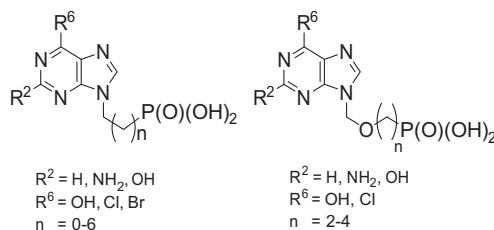
Compound **14i**:R¹ = (CH₃)₂CHCH₂CH₂-R² = CH₃CH=CH-CH=CH-

Compound	PPAR γ	PTP-1B	Cmax (μ M) (10 mg/kg, rats)
	EC ₅₀ (μ M)	IC ₅₀ (μ M)	
14i	0.03	1.18	4.5
Rosiglitazone	0.12	>30	34.7
Ertiprotafib	NT	0.41	NT

A novel series of 1,2,3,4-tetrahydroisoquinoline-3-carboxylic acid derivatives were synthesized and **14i** was identified as a potent human PPAR γ selective agonist and human PTP-1B inhibitor. Compound **14i** is a promising candidate for an efficacious and safe anti-diabetic drug targeting PPAR γ and PTP-1B.

Synthesis of 9-phosphonoalkyl and 9-phosphonoalkoxyalkyl purines: Evaluation of their ability to act as inhibitors of *Plasmodium falciparum*, *Plasmodium vivax* and human hypoxanthine-guanine-(xanthine) phosphoribosyltransferases pp 1076–1089

Michal Česnek*, Dana Hocková, Antonín Holý, Martin Dračinský, Ondřej Baszczyński, John de Jersey, Dianne T. Keough, Luke W. Guddat



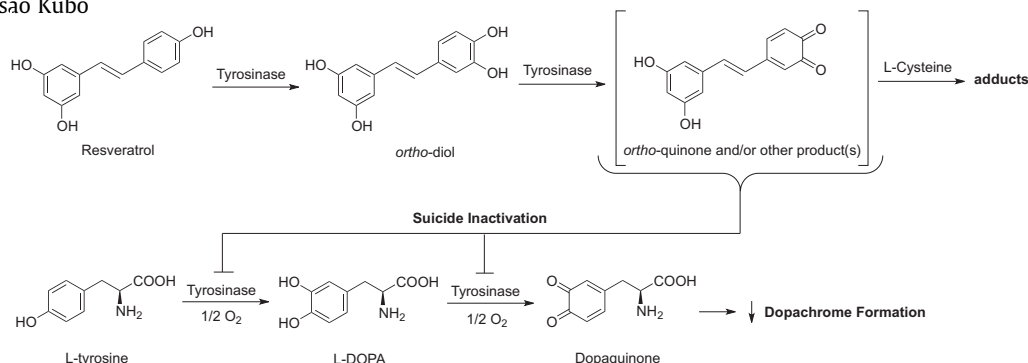
R² = H, NH₂, OH
R⁶ = OH, Cl, Br
n = 0-6

R² = H, NH₂, OH
R⁶ = OH, Cl
n = 2-4

Resveratrol as a k_{cat} type inhibitor for tyrosinase: Potentiated melanogenesis inhibitor

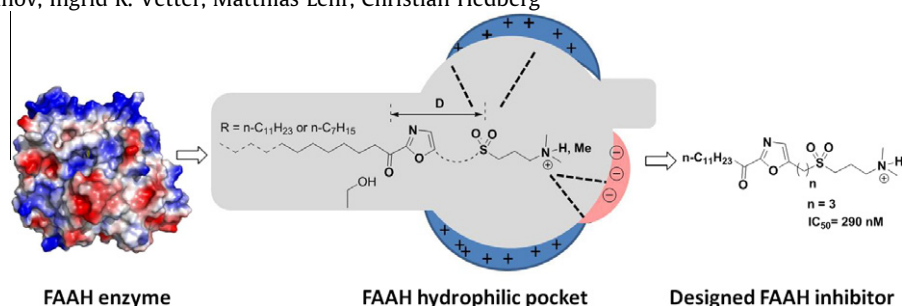
pp 1090–1099

Hiroki Satooka*, Isao Kubo

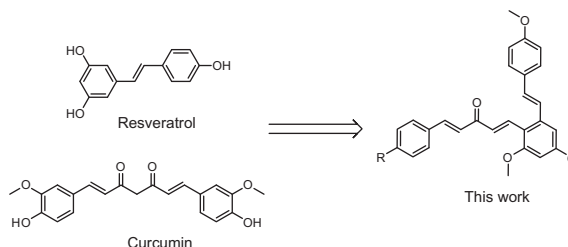
**Design, synthesis and evaluation of polar head group containing 2-keto-oxazole inhibitors of FAAH**

pp 1100–1112

Marion Rusch, Stefan Zahov, Ingrid R. Vetter, Matthias Lehr, Christian Hedberg*

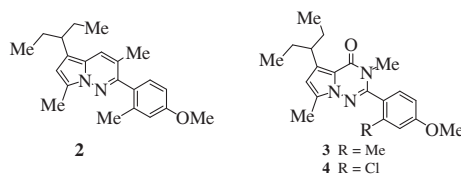
Design of α -keto oxazoles as fatty acid amide hydrolase (FAAH) inhibitors based on the electrostatic potential surface of the enzyme in its hydrophilic pocket.**Synthesis, biological evaluation and molecular docking studies of resveratrol derivatives possessing curcumin moiety as potent antitubulin agents**

Ban-Feng Ruan, Xiang Lu, Ting-Ting Li, Jian-Feng Tang, Yao Wei, Xiao-Liang Wang, Shi-Li Zheng, Ri-Sheng Yao*, Hai-Liang Zhu*

A series of resveratrol derivatives possessing curcumin moiety were synthesized and evaluated for their antiproliferative and antitubulin activity. Docking simulation was performed to position compound **C5** into the colchicine binding site to determine the probable binding mode.**Pyrrolo[1,2-*b*]pyridazines, pyrrolo[2,1-*f*]triazin-4(3*H*)-ones, and related compounds as novel corticotropin-releasing factor 1 (CRF₁) receptor antagonists**

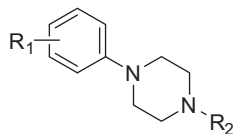
pp 1122–1138

Tetsuji Saito*, Tetsuo Obitsu, Hiroshi Kohno, Isamu Sugimoto, Takeshi Matsushita, Taihei Nishiyama, Tomoko Hirota, Hiroyuki Takeda, Naoya Matsumura, Sonoko Ueno, Akihiro Kishi, Yoshifumi Kagamiishi, Hisao Nakai, Yoshikazu Takaoka

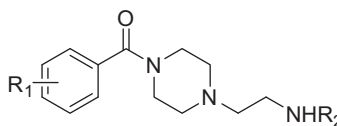


4-Aminoethylpiperazinyl aryl ketones with 5-HT_{1A}/5-HT₇ selectivity**pp 1139–1148**

Mi Kyoung Kim, Hyo Seon Lee, Sora Kim, Suh Young Cho, Bryan L. Roth, Youhoon Chong*, Hyunah Choo*




Arylpiperazine



4-Aminoethylpiperazinyl aryl ketone(1)

4-Aminoethylpiperazinyl aryl ketones were designed through homology modeling of 5-HT_{1A}R and 5-HT₇R, and synthesized compounds showed 5-HT_{1A}/5-HT₇ selectivity.

*Corresponding author

 Supplementary data available via SciVerse ScienceDirect**COVER**

Chemical Proteomics (Herman S. Overkleeft, *Bioorg. Med. Chem.* **2012**, 20, 552).

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