Bioorganic & Medicinal Chemistry 16 (2008) 6651–6662

Contents lists available at ScienceDirect

Bioorganic & Medicinal Chemistry

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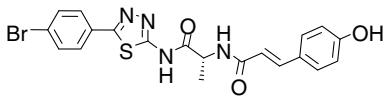
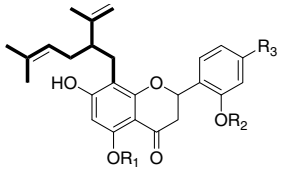
Novel aminopeptidase N inhibitors derived from 1,3,4-thiadiazole scaffold **pp 6663–6668**
GuoGang Tu, ShaoHua Li, HuiMing Huang, Gang Li, Fang Xiong, Xi Mai, HuaWei Zhu, BinHai Kuang, Wen Fang Xu*



2d

The synthesis and biological activity of a new series of 1,3,4-thiadiazole scaffold is described.

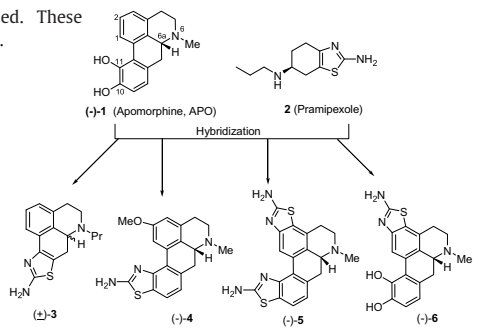
BACE1 inhibitory effects of lavandulyl flavanones from *Sophora flavescens* **pp 6669–6674**
Eun Mi Hwang, Young Bae Ryu, Hoi Young Kim, Dong-Gyu Kim, Seong-Geun Hong, Jin Hwan Lee, Marcus J. Curtis-Long, Seong Hun Jeong, Jae-Yong Park*, Ki Hun Park*



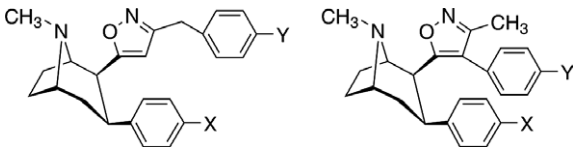
The β-secretase inhibitory capacity of flavanone from *Sophora flavescens* was studied, flavanone involving lavandulyl appendage showed significant BACE1 inhibition.

Synthesis and pharmacological investigation of novel 2-aminothiazole-privileged aporphines **pp 6675–6681**
Zhili Liu, Xuetao Chen, Leiping Yu, Xuechu Zhen*, Ao Zhang*

A series of 2-aminothiazole-privileged aporphine analogues were designed and synthesized. These compounds displayed variant binding affinity at dopamine D_1, D_2 and serotonin 5-HT_{1A} receptors.

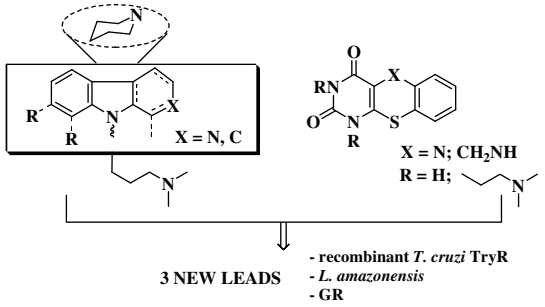


Synthesis and monoamine transporter binding properties of 2β-[3′-(substituted benzyl)isoxazol-5-yl]- and 2β-[3′-methyl-4′-(substituted phenyl)isoxazol-5-yl]-3β-(substituted phenyl)tropanes **pp 6682–6688**
Chunyang Jin, Hernán A. Navarro, Kevin Page, F. Ivy Carroll*

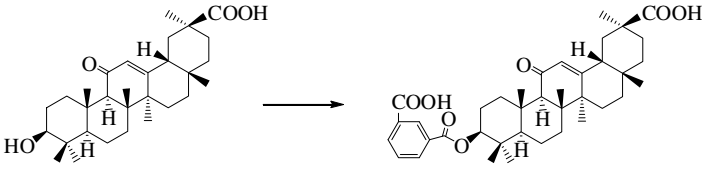


A series of novel 2β-[3′-(substituted benzyl)isoxazol-5-yl]- and 2β-[3′-methyl-4′-(substituted phenyl)isoxazol-5-yl]-3β-(substituted phenyl)tropane derivatives have been synthesized and evaluated for their monoamine transporter binding properties.

The use of natural product scaffolds as leads in the search for trypanothione reductase inhibitors **pp 6689–6695**
Betty C. Galarreta, Roxana Sifuentes, Angela K. Carrillo, Luis Sanchez, Maria del Rosario I. Amado, Helena Maruenda*

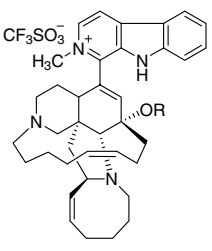


Synthesis and proteasome inhibition of glycyrrhetinic acid derivatives **pp 6696–6701**
Li Huang, Donglei Yu, Phong Ho, Keduo Qian, Kuo-Hsiung Lee, Chin-Ho Chen*



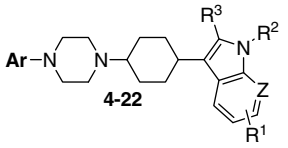
2-*N*-Methyl modifications and SAR studies of manzamine A **pp 6702–6706**
Mohamed A. Ibrahim, Abbas G. Shilabin, Sivaprakasam Prasanna, Melissa Jacob, Shabana I. Khan, Robert J. Doerksen, Mark T. Hamann*

Mono- and di-methylated quaternary carbolinium salts of manzamine A were synthesized and evaluated for their antimalarial activity and cytotoxicity and their potential to bind with GSK-3β using docking. These modifications were made based on previous studies suggesting N-alkylation of β-carbolines improves malaria activity and reduces toxicity.



Studies toward the discovery of the next generation of antidepressants. Part 6: Dual 5-HT$_{1A}$ receptor and serotonin transporter affinity within a class of arylpiperazinyl-cyclohexyl indole derivatives **pp 6707–6723**

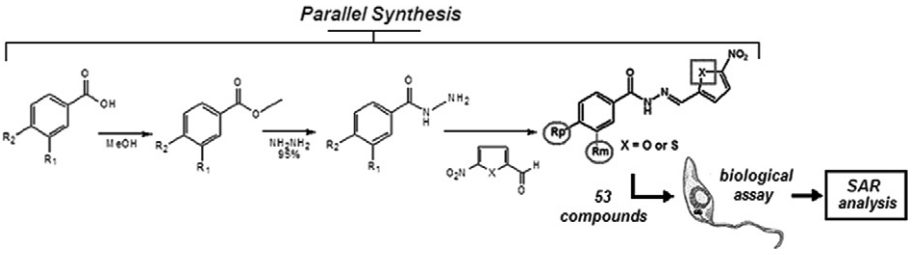
Dahui Zhou*, Ping Zhou, Deborah A. Evrard, Kristin Meagher, Michael Webb, Boyd L. Harrison, Donna M. Huryn, Jeannette Golembieski, Geoffrey A. Hornby, Lee E. Schechter, Deborah L. Smith, Terrance H. Andree, Richard E. Mewshaw*



Based on the previously reported discovery lead, 3-(*cis*-4-(4-(1*H*-indol-4-yl)piperazin-1-yl)cyclohexyl)-5-fluoro-1*H*-indole (**2**), a series of related arylpiperazin-4-yl-cyclohexyl indole analogs were synthesized then evaluated as 5-HT transporter inhibitors and 5-HT$_{1A}$ receptor antagonists. The investigation of the structure–activity relationships revealed the optimal pharmacophoric elements required for activities in this series. The best example from this study, 5-(piperazin-1-yl)quinoline analog (*trans*-**20**), exhibited equal binding affinities at 5-HT transporter (K_i = 4.9 nM), and 5-HT$_{1A}$ receptor (K_i = 6.2 nM), and functioned as a 5-HT$_{1A}$ receptor antagonist.

Antileishmanial activity screening of 5-nitro-2-heterocyclic benzylidene hydrazides **pp 6724–6731**

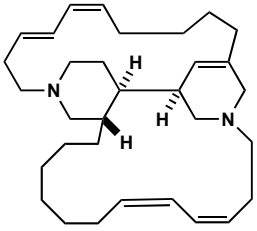
Daniela G. Rando*, Mitchell A. Avery, Babu L. Tekwani, Shabana I. Khan, Elizabeth I. Ferreira



Halicyclamine A, a marine spongean alkaloid as a lead for anti-tuberculosis agent **pp 6732–6736**

Masayoshi Arai, Mari Sobou, Catherine Vilchéze, Anthony Baughn, Hiroyuki Hashizume, Patamaporn Pruksakorn, Shunsuke Ishida, Makoto Matsumoto, William R. Jacobs Jr., Motomasa Kobayashi*

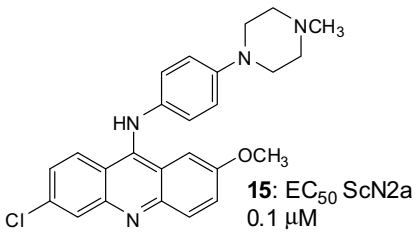
Halicyclamine A was re-discovered from the marine sponge *Haliclona* sp. as a new lead of anti-mycobacterial agent, which is effective to *Mycobacterium tuberculosis* in both active and dormant states. The detailed anti-mycobacterial activity are presented.



halicyclamine A

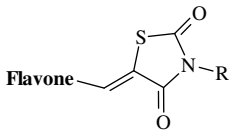
Antiprion activity of functionalized 9-aminoacridines related to quinacrine **pp 6737–6746**

Hanh Thuy Nguyen Thi, Chong-Yew Lee, Kenta Teruya, Wei-Yi Ong, Katsumi Doh-ura*, Mei-Lin Go*



Structural modification of the 9-substituted amino side chain of quinacrine resulted in compounds with better potencies and selectivities than quinacrine.

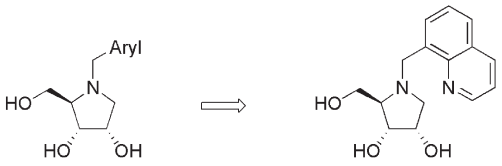
Synthesis and biological activity of some new flavonyl-2,4-thiazolidinediones **pp 6747–6751**
Oya Bozdağ-Dündar*, Eugen J. Verspohl, Net Daş-Evcimen, Rebecca M. Kaup, Katrin Bauer, Mutlu Sarıkaya, Begüm Evranos, Rahmiye Ertan



R=H, CH_2COOH, $CH_2COOC_2H_5$

A new series of flavonyl-2,4-thiazolidinediones were prepared by Knoevenagel reaction. The prepared compounds were tested for their aldose reductase inhibitory and insulinotropic activities.

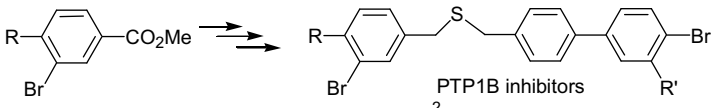
***N*-Arylmethyl substituted iminoribitol derivatives as inhibitors of a purine specific nucleoside hydrolase** **pp 6752–6763**
Annelies Goeminne, Maya Berg, Michael McNaughton, Gunther Bal, Georgiana Surpateanu, Pieter Van der Veken, Stijn De Prol, Wim Versées, Jan Steyaert, Achiel Haemers, Koen Augustyns*



K_i (*Tv*NH): 0.0108 μM

N-Arylmethyl-iminoribitols were developed and tested as inhibitors against a purine specific nucleoside hydrolase from *Trypanosoma vivax*.

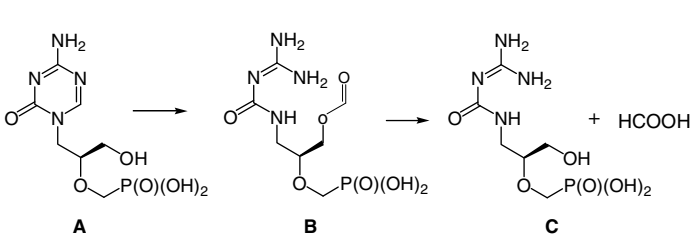
A re-examination of the difluoromethylenesulfonic acid group as a phosphotyrosine mimic for PTP1B inhibition **pp 6764–6777**
Munawar Hussain, Vanessa Ahmed, Bryan Hill, Zaheer Ahmed, Scott D. Taylor*



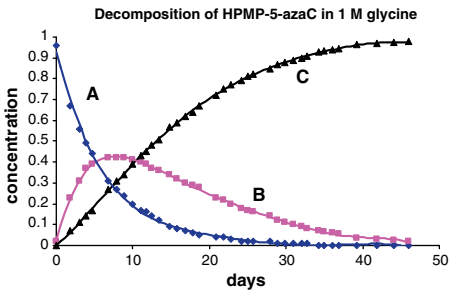
R = $CH_2PO(OEt)_2$, CH_2SO_3nPt

R = $CF_2PO_3^{-2}$, SO_2NH_2 (IC_{50} = 6 nM)
$CF_2SO_3^-$, SO_2NH_2, (IC_{50} = 13 μM)
$CH_2SO_3^-$, SO_2NH_2, (IC_{50} = 19 μM)
$CF_2PO_3^{-2}$, $CF_2SO_2NH_2$, (IC_{50} = 30 nM)
$CF_2SO_3^-$, $CF_2SO_2NH_2$, (IC_{50} = 6 μM)

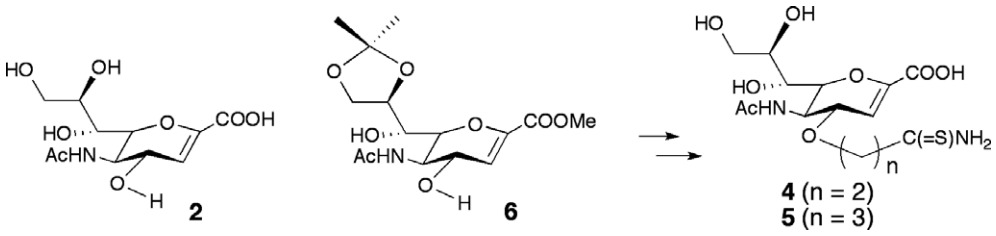
Study of chemical stability of antivirally active 5-azacytosine acyclic nucleoside phosphonates using NMR spectroscopy **pp 6778–6782**
Martin Dračínský*, Marcela Krečmerová, Antonín Holý



$t_{1/2}$ = 4.6 days $t_{1/2}$ = 6.4 days

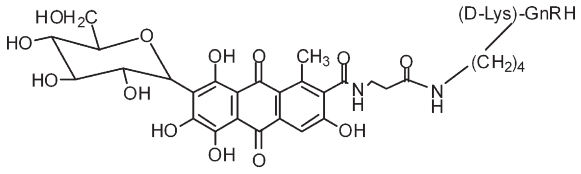


2-Deoxy-2,3-didehydro-*N*-acetylneuraminic acid analogs structurally modified by thiocarbamoylalkyl groups at the C-4 position: Synthesis and biological evaluation as inhibitors of human parainfluenza virus type 1 **pp 6783–6788**
Kiyoshi Ikeda*, Kazuki Sato, Reiko Nishino, Shinya Aoyama, Takashi Suzuki, Masayuki Sato



We synthesized analogs having thiocarbamoylethyl- **4** and thiocarbamoylpropyl group **5** at the C-4 position of **2** via the key compound **6**. Compounds **4** and **5** showed the inhibitory activities against human parainfluenza virus type 1 (hPIV-1) sialidase.

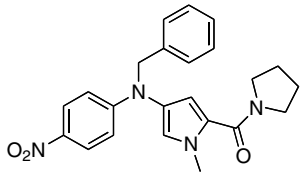
Conjugates of gonadotropin releasing hormone (GnRH) with carminic acid: Synthesis, generation of reactive oxygen species (ROS) and biological evaluation **pp 6789–6798**
Vered Lev-Goldman, Brenda Mester, Nurit Ben-Aroya, Tamar Hanoch, Barbara Rupp, Tsvetanka Stanoeva, Georg Gescheidt, Rony Seger, Yitzhak Koch, Lev Weiner*, Mati Fridkin*



Carminic acid-GnRH

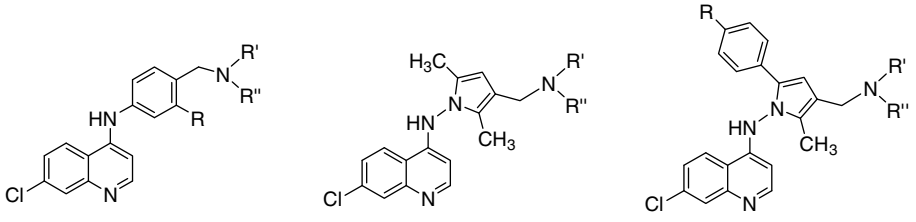
A natural anthraquinone, carminic acid, was conjugated to GnRH peptide hormone to be used as a model for potential photoactive targeted compounds.

4-(Anilino)pyrrole-2-carboxamides: Novel non-steroidal/non-anilide type androgen antagonists effective upon human prostate tumor LNCaP cells with mutated nuclear androgen receptor **pp 6799–6812**
Ken-ichi Wakabayashi, Keisuke Imai, Hiroyuki Miyachi, Yuichi Hashimoto, Aya Tanatani*

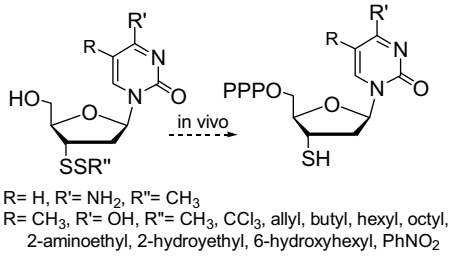


Novel 4-(anilino)pyrrole-2-carboxamides were designed and synthesized as non-steroidal/non-anilide type AR antagonists.

Novel amodiaquine congeners as potent antimalarial agents **pp 6813–6823**
Manolo Casagrande, Nicoletta Basilico, Silvia Parapini, Sergio Romeo, Donatella Taramelli, Anna Sparatore*

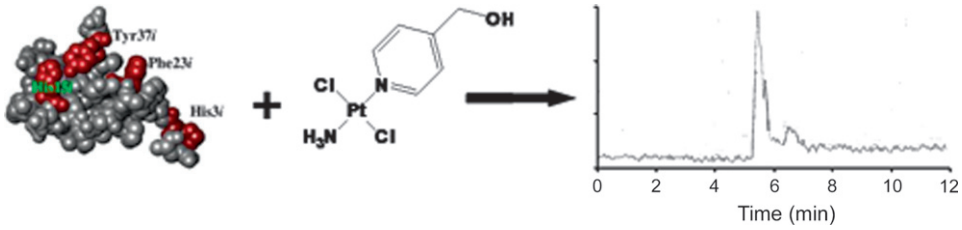


Anti-retroviral and cytostatic activity of 2′,3′-dideoxyribonucleoside 3′-disulfides **pp 6824–6831**
Béatrice Gerland, Jérôme Désiré, Jan Balzarini, Jean-Luc Décout*



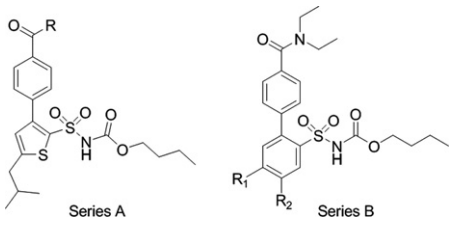
R= H, R'= NH_2, R"= CH_3
R= CH_3, R'= OH, R"= CH_3, CCl_3, allyl, butyl, hexyl, octyl, 2-aminoethyl, 2-hydroyethyl, 6-hydroxyhexyl, $PhNO_2$

Study by HPLC-MS of the interaction of platinum antitumor complexes with potato carboxypeptidase inhibitor (PCI) **pp 6832–6840**
Alberto Martínez, Virtudes Moreno*, Laura Sanglas, Rafael de Llorens, Francesc X. Avilés, Julia Lorenzo*

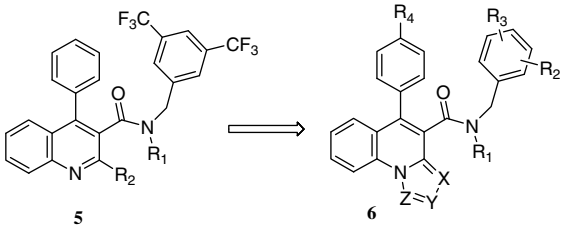


The binding of two platinum antitumor complexes to PCI protein (wild type and mutated) was proved by HPLC-MS and the cytotoxic activity of the adducts was measured by the typical MTT assay.

Selective angiotensin II AT_2 receptor agonists: Benzamide structure–activity relationships **pp 6841–6849**
Charlotta Wallinder, Milad Botros, Ulrika Rosenström, Marie-Odile Guimond, Hélène Beaudry, Fred Nyberg, Nicole Gallo-Payet, Anders Hallberg, Mathias Alterman*

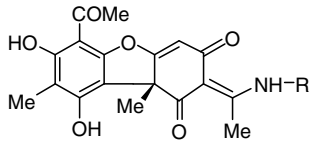


Design, synthesis, and structure–affinity relationship studies in NK_1 receptor ligands based on azole-fused quinolinecarboxamide moieties **pp 6850–6859**
Andrea Cappelli*, Germano Giuliani, Maurizio Anzini, Daniela Riitano, Gianluca Giorgi, Salvatore Vomero



5 6

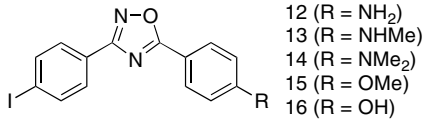
Synthesis and cytotoxic activities of usnic acid derivatives **pp 6860–6866**
Marc-Antoine Bazin, Anne-Cécile Le Lamer, Jean-Guy Delcros, Isabelle Rouaud, Philippe Uriac, Joël Boustie, Jean-Charles Corbel, Sophie Tomasi*



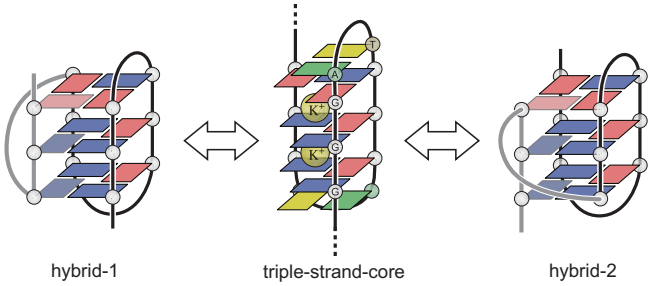
R=amine, polyamine, alcohol, amino acid moiety

Cytotoxic evaluation of enamines derived from (+)-usnic acid led us to the selection of the diaminooctane derivative as active towards cancer cell lines ($2.7 < IC_{50} < 14.1$ μM). Apoptotic effect was also observed.

Development of novel β-amyloid probes based on 3,5-diphenyl-1,2,4-oxadiazole **pp 6867–6872**
Masahiro Ono*, Mamoru Haratake, Hideo Saji, Morio Nakayama

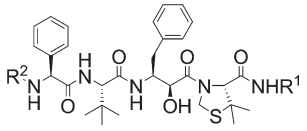


G-quadruplex structures of human telomere DNA examined by single molecule FRET and BrG-substitution **pp 6873–6879**
Kenji Okamoto, Yuta Sannohe, Tomoko Mashimo, Hiroshi Sugiyama, Masahide Terazima*



The G-quadruplex structure of human telomere DNA was investigated by single molecule FRET measurement with the aid of structural modification by bromoguanine-substitutions and explained by newly introduced triple-strand-core model.

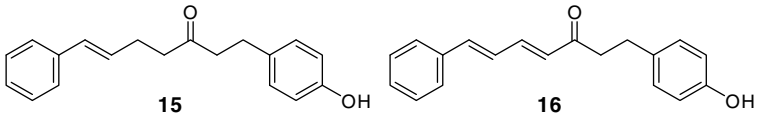
Locking the two ends of tetrapeptidic HTLV-I protease inhibitors inside the enzyme **pp 6880–6890**
Meihui Zhang, Jeffrey-Tri Nguyen, Henri-Obadja Kumada, Tooru Kimura, Maosheng Cheng, Yoshio Hayashi, Yoshiaki Kiso*



Structure–activity relationship studies were performed on 44 novel tetrapeptidic HTLV-I protease inhibitors possessing different hydrophobic P_3-cap and P_1'-cap moieties.

Diarylheptanoids, new phytoestrogens from the rhizomes of *Curcuma comosa*: Isolation, chemical modification and estrogenic activity evaluation **pp 6891–6902**

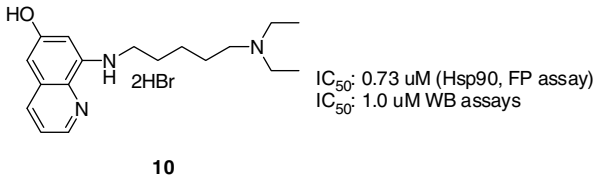
Apichart Suksamrarn*, Mathurose Ponglikitmongkol, Kanjana Wongkrajang, Anon Chindaduang, Suthadta Kittidanairak, Aroon Jankam, Boon-ek Yingyongnarongkul, Narin Kittipanumat, Ratchanaporn Chokchaisiri, Pichit Khetkam, Pawinee Piyachaturawat



Five new naturally occurring and nine known diarylheptanoids were isolated. Some of them exhibited higher estrogenic activity than the phytoestrogen genistein.

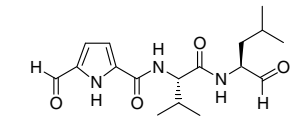
Discovery of aminoquinolines as a new class of potent inhibitors of heat shock protein 90 (Hsp90): Synthesis, biology, and molecular modeling **pp 6903–6910**

Thota Ganesh, Jaeki Min, Pahk Thepchatri, Yuhong Du, Lian Li, Iestyn Lewis, Larry Wilson, Haian Fu, Gabriela Chiosis, Raymond Dingledine, Dennis Liotta, James P. Snyder, Aiming Sun*



Synthesis, biological evaluation and molecular modelling of *N*-heterocyclic dipeptide aldehydes as selective calpain inhibitors **pp 6911–6923**

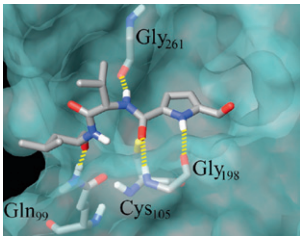
Matthew A. Jones, James D. Morton*, James M. Coxon, Stephen B. McNabb, Hannah Y.-Y. Lee, Steven G. Aitken, Janna M. Mehrtens, Lucinda J. G. Robertson, Axel T. Neffe, Shigeru Miyamoto, Roy Bickerstaffe, Karl Gately, Jacqueline M. Wood, Andrew D. Abell*



IC_{50} (o-CAPN1) = 290 nM

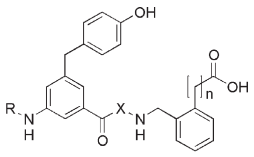
IC_{50} (o-CAPN2) = 25 nM

Selectivity o-CAPN2 over o-CAPN1 > 11 fold



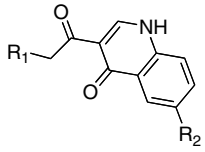
Ligands to the (IRAP)/AT4 receptor encompassing a 4-hydroxydiphenylmethane scaffold replacing Tyr^2 **pp 6924–6935**

Hanna Andersson, Heidi Demaegdt, Georges Vauquelin, Gunnar Lindeberg, Anders Karlén, Mathias Hallberg*



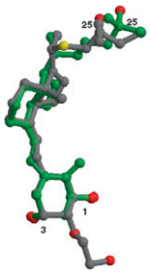
R = Val, Nle, H
X = Ile, Leu, Pro, nothing
n = 0, 1

Affinity of 3-acyl substituted 4-quinolones at the benzodiazepine site of $GABA_A$ receptors **pp 6936–6948**
Erik Lager, Jakob Nilsson, Elsebet Østergaard Nielsen, Mogens Nielsen, Tommy Liljefors, Olov Sterner*



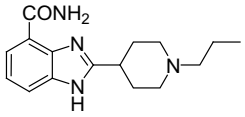
24 3-acyl-4-quinolones with various substituents in position 6 were synthesized and assayed for affinity at the benzodiazepine site of $GABA_A$ receptors.

2-Substituted-16-ene-22-thia-1α,25-dihydroxy-26,27-dimethyl-19-norvitamin D_3 analogs: Synthesis, biological evaluation, and crystal structure **pp 6949–6964**
Masato Shimizu, Yukiko Miyamoto, Hajime Takaku, Mayumi Matsuo, Makoto Nakabayashi, Hiroyuki Masuno, Nobuyuki Udagawa, Hector F. DeLuca, Teikichi Ikura*, Nobutoshi Ito*



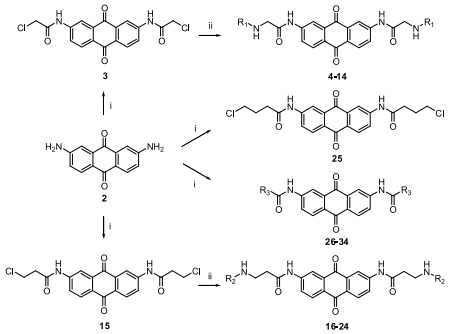
2-Substituted-16-ene-22-thia-1α,25-dihydroxy-26,27-dimethyl-19-norvitamin D_3 analogs (grey) exhibited an extremely higher level of potency than the natural hormone (green). X-ray crystallography revealed the key interactions between the ligands and the receptor.

Discovery and SAR of 2-(1-propylpiperidin-4-yl)-1*H*-benzimidazole-4-carboxamide: A potent inhibitor of poly(ADP-ribose) polymerase (PARP) for the treatment of cancer **pp 6965–6975**
Thomas D. Penning*, Gui-Dong Zhu, Viraj B. Gandhi, Jianchun Gong, Sheela Thomas, Wilfried Lubisch, Roland Grandel, Wolfgang Wernet, Chang H. Park, Elizabeth H. Fry, Xuesong Liu, Yan Shi, Vered Klinghofer, Eric F. Johnson, Cherrie K. Donawho, David J. Frost, Velitchka Bontcheva-Diaz, Jennifer J. Bouska, Amanda M. Olson, Kennan C. Marsh, Yan Luo, Saul H. Rosenberg, Vincent L. Giranda

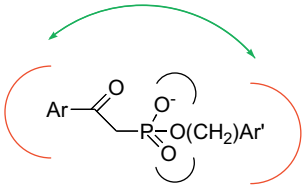


The SAR of a series of cyclic amine-containing benzimidazole carboxamide PARP inhibitors is described.

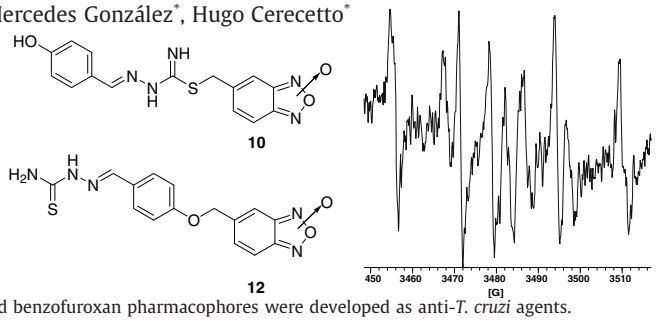
Synthesis, human telomerase inhibition and anti-proliferative studies of a series of 2,7-bis-substituted amido-anthraquinone derivatives **pp 6976–6986**
Hsu-Shan Huang*, Kuo-Feng Huang, Cho-Lu Li, Yi-Yuan Huang, Yi-Hsuan Chiang, Fong-Chun Huang, Jing-Jer Lin*



β-Ketophosphonates as β-lactamase inhibitors: Intramolecular cooperativity between the hydrophobic subsites of a class D β-lactamase **pp 6987–6994**
Senthil K. Perumal, S. A. Adediran, R. F. Pratt*

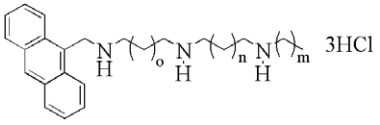


New trypanocidal hybrid compounds from the association of hydrazone moieties and benzofuroxan heterocycle **pp 6995–7004**
Williams Porcal, Paola Hernández, Lucía Boiani, Mariana Boiani, Ana Ferreira, Agustina Chidichimo, Juan J. Cazzulo, Claudio Olea-Azar, Mercedes González*, Hugo Cerecetto*



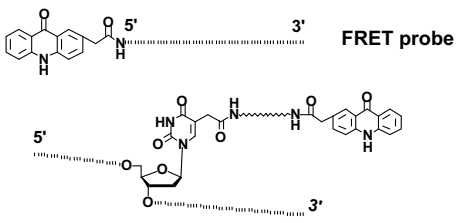
Hybrid compounds containing hydrazones and benzofuroxan pharmacophores were developed as anti-*T. cruzi* agents.

Synthesis and evaluation of unsymmetrical polyamine derivatives as antitumor agents **pp 7005–7012**
Jianhong Wang, Songqiang Xie, Yanjie Li, Yongjun Guo, Yuanfang Ma, Jin Zhao, Otto Phanstiel IV, Chaojie Wang*



2a: m=1, n=2, o=1 **2e**: m=2, n=1, o=2
2b: m=1, n=1, o=2 **2f**: m=1, n=2, o=2
2c: m=2, n=1, o=1 **2g**: m=2, n=2, o=2
2d: m=2, n=2, o=1

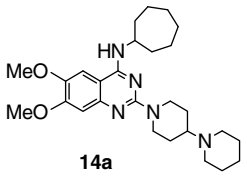
Acridone-tagged DNA as a new probe for DNA detection by fluorescence resonance energy transfer and for mismatch DNA recognition **pp 7013–7020**
Yasuhisa Hagiwara, Tomoya Hasegawa, Atushi Shoji, Masayasu Kuwahara, Hiroaki Ozaki, Hiroaki Sawai*



Acridone was incorporated in to modified DNA at 5′-terminal or at C5 position of thymidine by post-modification method. Acridone-tagged DNA at 5′-terminal can be used as a probe for DNA detection by FRET with dabcyl-tagged DNA. Moreover, acridone-tagged DNA at C5 position of inside thymidine showed T-T mismatch discrimination.

Discovery of potent CCR4 antagonists: Synthesis and structure–activity relationship study of 2,4-diaminoquinazolines **pp 7021–7032**

Kazuhiro Yokoyama*, Noriko Ishikawa, Susumu Igarashi, Noriyuki Kawano, Kazuyuki Hattori, Takahiro Miyazaki, Shin-ichi Ogino, Yuzo Matsumoto, Makoto Takeuchi, Mitsuaki Ohta



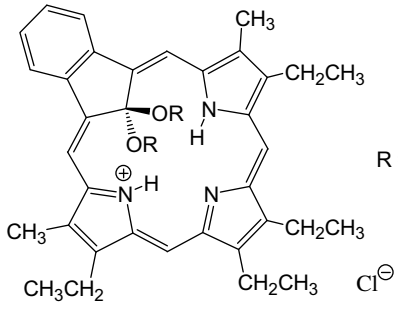
14a

A new series of potent competitive CCR4 antagonists were discovered. Compound **14a** showed potent inhibition in the [^{35}S]GTPγS-binding assay, and blocked the chemotaxis of human and mouse CCR4-expressing cells.

Carbaporphyrin ketals as potential agents for a new photodynamic therapy treatment of leishmaniasis **pp 7033–7038**

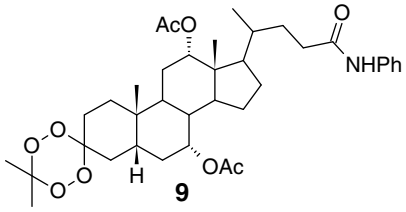
Justin B. Morgenthaler, Steven J. Peters, David L. Cedeño, Manuel H. Constantino, Kevin A. Edwards, Erin M. Kamowski, Jennifer C. Passini, Brian E. Butkus, Alexandra M. Young, Timothy D. Lash, Marjorie A. Jones*

Dimethyl and diethyl carbaporphyrin ketals inhibit the growth of *Leishmania tarentolae* promastigotes in vitro. These unique porphyrinoids show promise as potent inhibitors of *Leishmania*.



Mixed tetraoxanes containing the acetone subunit as antimalarials **pp 7039–7045**

Dejan M. Opsenica, Nataša Terzić, Philip L. Smith, Youngsun Yang, Lalaine Anova, Kirsten S. Smith, Bogdan A. Šolaja*



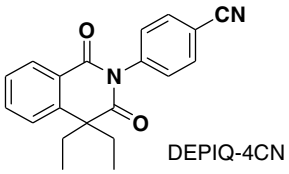
9

P. falciparum	D6	W2	TM91C235	RCS
IC_{50} (nM)	9.97	5.02	15.75	1.89
IC_{90} (nM)	20.84	14.35	20.89	4.45

P. berghei $_{KBG173}$ MCD ≤ 20 mg/kg/day (p.o.)

Progesterone receptor antagonists with a 3-phenylquinazoline-2,4-dione/2-phenylisoquinoline-1,3-dione skeleton **pp 7046–7054**

Aya Nakagawa*, Shigeyuki Uno, Makoto Makishima, Hiroyuki Miyachi, Yuichi Hashimoto*

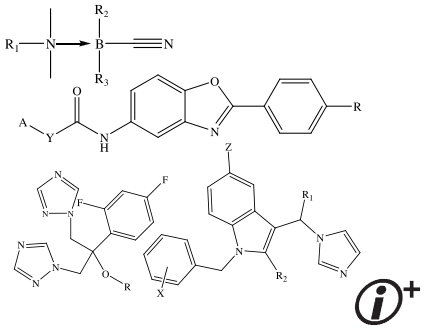


DEPIQ-4CN

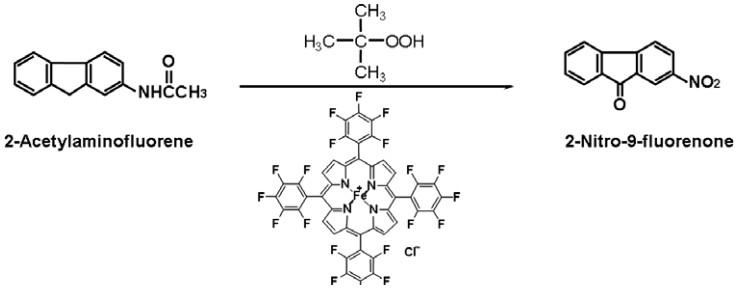
Novel non-steroidal progesterone receptor antagonists, including 4-(4,4-diethyl-3,4-dihydro-1,3-dioxoquinolin-2(1*H*)-yl)benzonitrile (DEPIQ-4CN), which has IC_{50} values of 74–78 nM in alkaline phosphatase activity and reporter gene assays, were developed.

QSAR modeling of the antifungal activity against *Candida albicans* for a diverse set of organic compounds **pp 7055–7069**
Alan R. Katritzky*, Svetoslav H. Slavov, Dimitar A. Dobchev, Mati Karelson

Experimentally measured minimum inhibitory concentrations for a series of 83 cyanoborane, fluconazole, carbonylaminobenzoxazole and imidazolylmethylindole derivatives were studied by the methods of QSAR. A good explanatory model with R^2 = 0.788 was obtained and reported.



Oxidative transformation of 2-acetylaminofluorene by a chemical model for cytochrome P450: A water-insoluble porphyrin and *tert*-butyl hydroperoxide **pp 7070–7077**
Keiko Inami*, Masataka Mochizuki



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*Corresponding author
ⓘ+ Supplementary data available via ScienceDirect

COVER

An insight into biologically relevant chemical space showing the scaffolds of potential natural-product based inhibitors orbiting their target, the protein structure of protein 11-beta steroid dehydrogenase (PDB code 1xu7). Graphic produced using Pymol (http://www.pymol.org). [M. A. Koch, A. Schuffenhauer, M. Scheck, S. Wetzel, M. Casaulta, A. Odermatt, P. Ertl, H. Waldmann, Charting biologically relevant chemical space: A structural classification of natural products (SCONP), *PNAS* **2005**, *102*, 17272–17277 and S. Wetzel, H. Waldmann, Cheminformatic analysis of natural products and their chemical space, *Chimia* **2007**, *61*(6), 355–360].

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ISSN 0968-0896