



Bioorganic & Medicinal Chemistry Volume 20, Issue 19, 2012

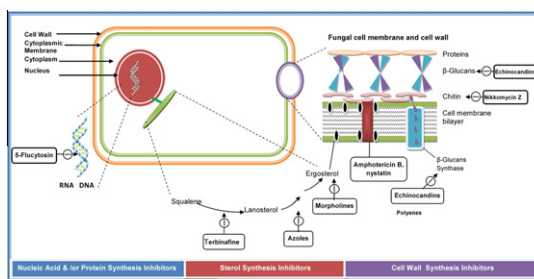
Contents

REVIEW

The biology and chemistry of antifungal agents: A review

pp 5678–5698

Muthu K Kathiravan*, Amol B Salake, Aparna S Chothe, Prashik B Dudhe, Rahul P Watode, Maheshwar S Mukta, Sandeep Gadhwe

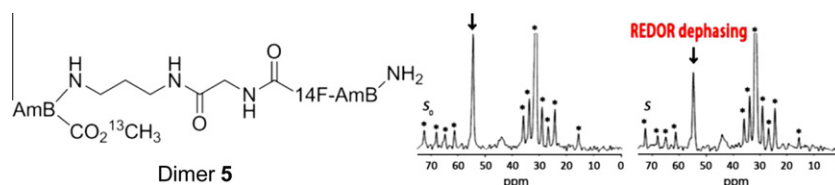


ARTICLES

Possible conformation of amphotericin B dimer in membrane-bound assembly as deduced from solid-state NMR

pp 5699–5704

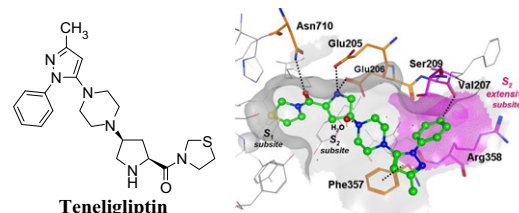
Yuichi Umegawa, Takeshi Adachi, Nobuaki Matsumori*, Michio Murata*



Discovery and preclinical profile of teneligliptin (3-[(2S,4S)-4-[4-(3-methyl-1-phenyl-1H-pyrazol-5-yl)piperazin-1-yl]pyrrolidin-2-ylcarbonyl]thiazolidine): A highly potent, selective, long-lasting and orally active dipeptidyl peptidase IV inhibitor for the treatment of type 2 diabetes

pp 5705–5719

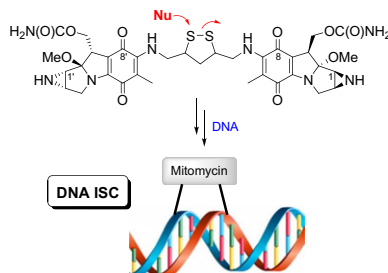
Tomohiro Yoshida, Fumihiko Akahoshi*, Hiroshi Sakashita, Hiroshi Kitajima, Mitsuharu Nakamura, Shuji Sonda, Masahiro Takeuchi, Yoshihito Tanaka, Naoko Ueda, Sumie Sekiguchi, Takayuki Ishige, Kyoko Shima, Mika Nabeno, Yuji Abe, Jun Anabuki, Aki Soejima, Kumiko Yoshida, Yoko Takashina, Shinichi Ishii, Satoko Kiuchi, Sayaka Fukuda, Reiko Tsutsumiuchi, Keigo Kosaka, Takahiro Murozono, Yoshinobu Nakamaru, Hiroyuki Utsumi, Naoya Masutomi, Hiroyuki Kishida, Ikuko Miyaguchi, Yoshiharu Hayashi



Studies on synthesis and activation mechanism of mitomycin dimers connected by 1,2-dithiolane and diol linkers

pp 5720–5729

Hyoung Rae Kim, Jae Jin Kim, Jung Jae Park, Sang Hyup Lee*

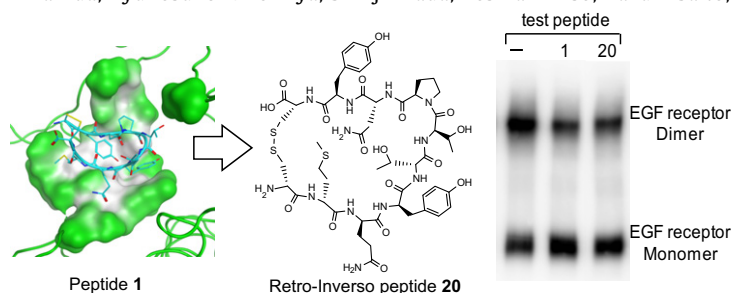


A mitomycin dimer connected by a 1,2-dithiolane (a five-membered cyclic disulfide) linker was highly efficient for nucleophilic activation and corresponding production of DNA interstrand cross-link (DNA ISC) adducts.

Evaluation of dimerization–inhibitory activities of cyclic peptides containing a β -hairpin loop sequence of the EGF receptor

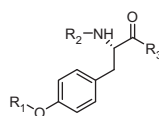
pp 5730–5737

Takaaki Mizuguchi, Naho Ohara, Mika Iida, Ryunosuke Ninomiya, Shinji Wada, Yoshiaki Kiso, Kazuki Saito, Kenichi Akaji*

**Design, synthesis and evaluation of novel metalloproteinase inhibitors based on L-tyrosine scaffold**

pp 5738–5744

Xian-Chao Cheng, Run-Ling Wang*, Zhen-Ke Dong, Jing Li, Yao-Yuan Li, Rong-Rong Li

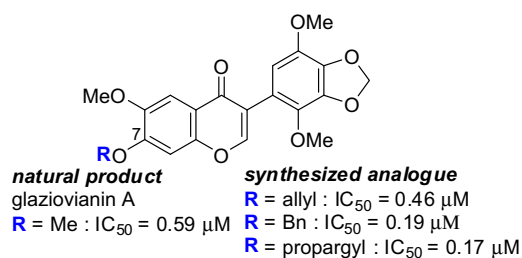


A series of novel L-tyrosine derivatives were designed, synthesized and assayed for their inhibitory activities on matrix metalloproteinase 2 (MMP-2) and histone deacetylase 8 (HDAC-8).

Design, synthesis, and biological evaluation of the analogues of glaziovianin A, a potent antitumor isoflavone

pp 5745–5756

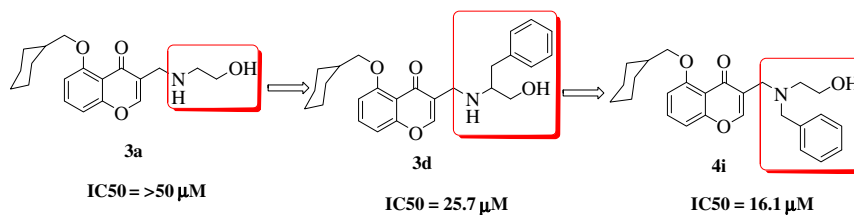
Ichiro Hayakawa*, Akiyuki Ikedo, Takumi Chinen, Takeo Usui, Hideo Kigoshi*



Novel interleukin-5 inhibitors based on hydroxyethylaminomethyl-4H-chromen-4-one scaffold

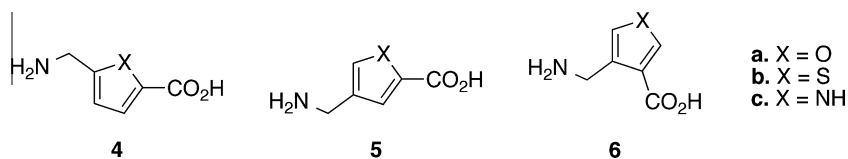
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Cheonik Joo, Eeda Venkateswararao, Ki-Cheul Lee, Vinay K. Sharma, Min-Sik Kyung, Youngsoo Kim, Sang-Hun Jung*

**Synthesis and evaluation of novel heteroaromatic substrates of GABA aminotransferase**

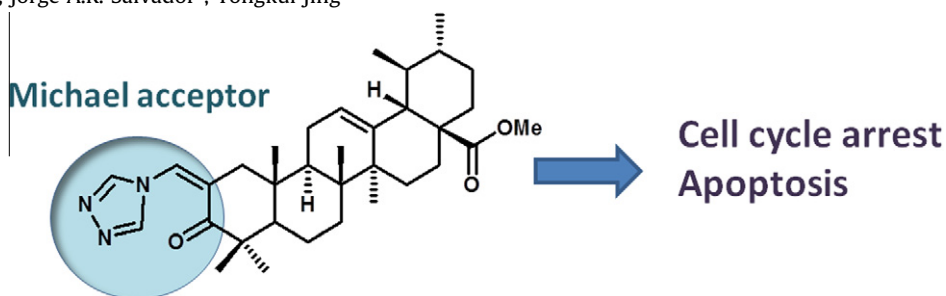
pp 5763–5773

Dustin D. Hawker, Richard B. Silverman*

**Synthesis of novel ursolic acid heterocyclic derivatives with improved abilities of antiproliferation and induction of p53, p21^{waf1} and NOXA in pancreatic cancer cells**

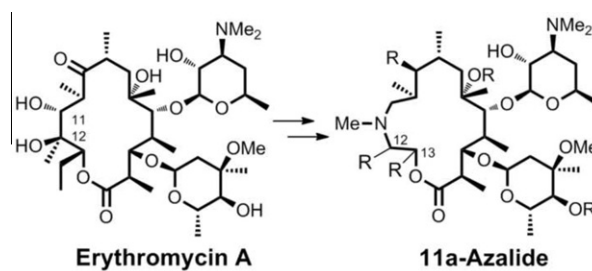
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Ana S. Leal, Rui Wang, Jorge A.R. Salvador*, Yongkui Jing*

**Synthesis and structure–activity relationship of a novel class of 15-membered macrolide antibiotics known as ‘11a-azalides’**

pp 5787–5801

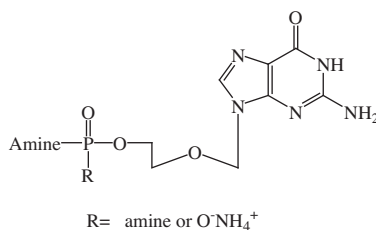
Tomohiro Sugimoto*, Tetsuya Tanikawa, Keiko Suzuki, Yukiko Yamasaki



Phosphoramidate derivatives of acyclovir: Synthesis and antiviral activity in HIV-1 and HSV-1 models in vitro

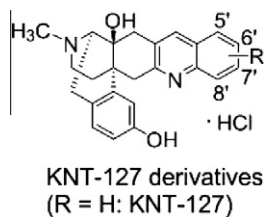
pp 5802–5809

Natalia F. Zakirova*, Alexander V. Shipitsyn, Maxim V. Jasko, Maria M. Prokofjeva, Valeria L. Andronova, Georgiy A. Galegov, Vladimir S. Prassolov, Sergey N. Kochetkov

**Synthesis of quinolinomorphinan derivatives as highly selective δ opioid receptor ligands**

pp 5810–5831

Yoshihiro Ida, Ayaka Matsubara, Toru Nemoto, Manabu Saito, Shigeto Hirayama, Hideaki Fujii, Hiroshi Nagase*

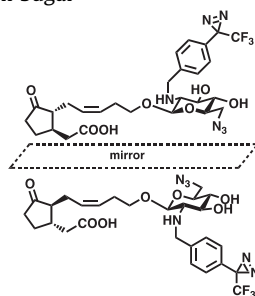


The study of the structure–activity relationship of KNT-127 derivatives showed that the 5'- and 8'-positions on the quinoline ring would be the most appropriate sites for modification to enhance the affinity and selectivity for the δ receptor.

Hybrid stereoisomers of a compact molecular probe based on a jasmonic acid glucoside: Syntheses and biological evaluations

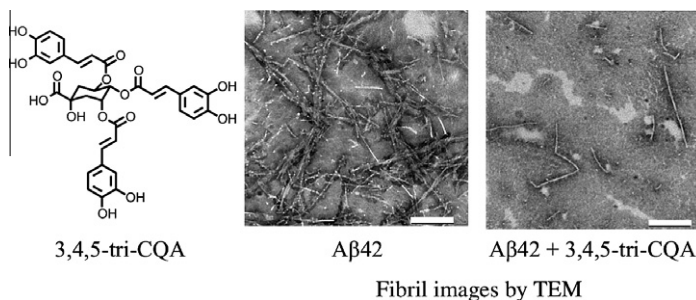
pp 5832–5843

Minoru Ueda*, Gangqiang Yang, Yasuhiro Ishimaru, Tetsuya Itabashi, Satoru Tamura, Hiromasa Kiyota, Shigefumi Kuwahara, Sho Inomata, Mitsuru Shoji, Takeshi Sugai

**Protective effects of caffeoylquinic acids on the aggregation and neurotoxicity of the 42-residue amyloid β -protein**

pp 5844–5849

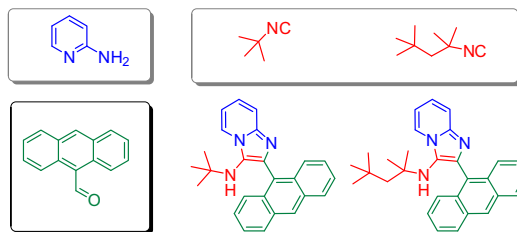
Yusaku Miyamae, Manami Kurisu, Kazuma Murakami, Junkyu Han, Hiroko Isoda, Kazuhiro Irie, Hideyuki Shigemori*



Antibacterial activities of Groebke–Blackburn–Bienaymé-derived imidazo[1,2-*a*]pyridin-3-amines

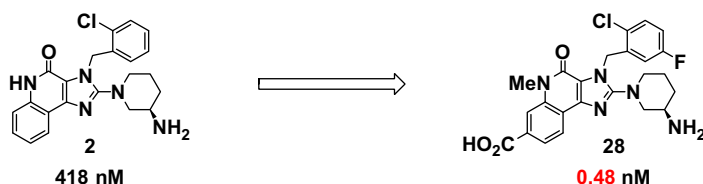
pp 5850–5863

Nikunj M. Shukla, Deepak B. Salunke, Euna Yoo, Cole A. Mutz, Rajalakshmi Balakrishna, Sunil A. David*

MIC: 3.91 $\mu\text{g/mL}$ (MRSA)**Discovery of 3*H*-imidazo[4,5-*c*]quinolin-4(5*H*)-ones as potent and selective dipeptidyl peptidase IV (DPP-4) inhibitors**

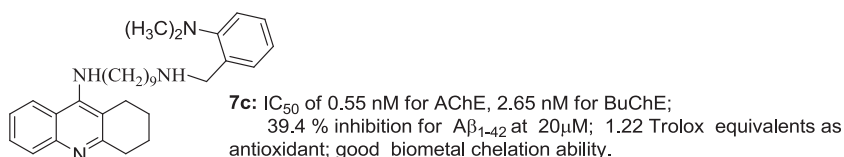
pp 5864–5883

Yohei Ikuma*, Hitoshi Hochigai, Hidenori Kimura, Noriko Nunami, Tomonori Kobayashi, Katsuya Uchiyama, Yudai Furuta, Mutsuko Sakai, Masakuni Horiguchi, Yumi Masui, Kazuhiko Okazaki, Yasuhiro Sato, Hiroyuki Nakahira

***O*-Hydroxyl- or *o*-amino benzylamine-tacrine hybrids: Multifunctional biometals chelators, antioxidants, and inhibitors of cholinesterase activity and amyloid- β aggregation**

pp 5884–5892

Fei Mao, Ling Huang, Zonghua Luo, Anqiu Liu, Chuanjun Lu, Zhiyong Xie*, Xingshu Li*

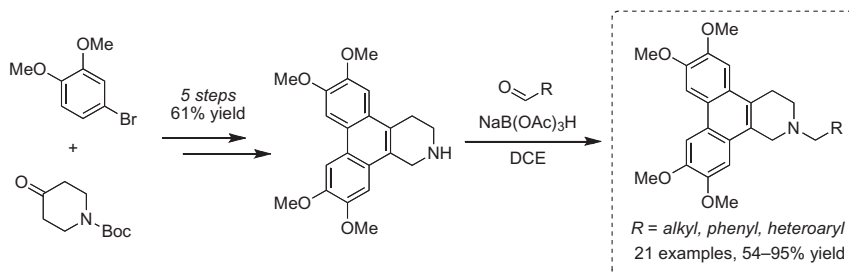


A series of hybrid molecules were synthesised by reacting *N*-(aminoalkyl)tacrine with salicylic aldehyde or derivatives of 2-aminobenzaldehyde. All of the hybrids are potential biometal chelators, and in addition, most of them were better antioxidants and inhibitors of cholinesterases and amyloid- β ($\text{A}\beta$) aggregation than the lead compound tacrine. Compound 7c has the potential to be a candidate for AD therapy: it is a much better inhibitor of acetylcholinesterase (AChE) than tacrine (IC_{50} : 0.55 nM vs 109 nM), has good biometal chelation ability, is able to inhibit $\text{A}\beta$ aggregation and has moderate antioxidant activity (1.22 Trolox equivalents).

Synthesis and evaluation of the anti-proliferative and NF- κB activities of a library of simplified tylophorine analogs

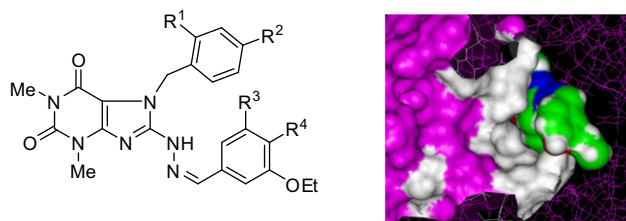
pp 5893–5900

Micah J. Niphakis, Bryant C. Gay, Kwon Ho Hong, Nicholas P. Bleeker, Gunda I. Georg*

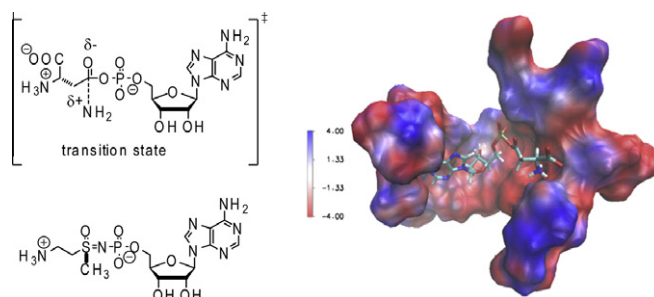


Design and synthesis of EGFR dimerization inhibitors and evaluation of their potential in the treatment of psoriasis pp 5901–5914

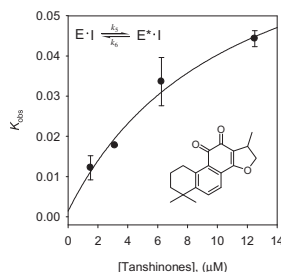
Donna Petch, Rosaleen J. Anderson, Anne Cunningham, Suja E. George, David E. Hibbs, Ran Liu, Simon P. Mackay, Andrew Paul, David A.P. Small, Paul W. Groundwater*

**A sulfoximine-based inhibitor of human asparagine synthetase kills L-asparaginase-resistant leukemia cells** pp 5915–5927

Hideyuki Ikeuchi, Yong-Mo Ahn, Takuya Otokawa, Bunta Watanabe, Lamees Hegazy, Jun Hiratake*, Nigel G.J. Richards*

**Tanshinones as selective and slow-binding inhibitors for SARS-CoV cysteine proteases** pp 5928–5935

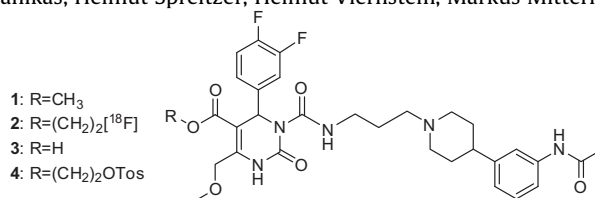
Ji-Young Park, Jang Hoon Kim, Young Min Kim, Hyung Jae Jeong, Dae Wook Kim, Ki Hun Park, Hyung-Jun Kwon, Su-Jin Park, Woo Song Lee*, Young Bae Ryu*



This is first report to describe the specific and selective inhibition effects of tanshinones against SARS-CoV 3CL^{pro} and PL^{pro} with deubiquitination. In detail kinetic mechanism, tanshinones manifest a slow-binding inhibition profile.

**[¹⁸F]FE@SNAP—A new PET tracer for the melanin concentrating hormone receptor 1 (MCHR1): Microfluidic and vessel-based approaches** pp 5936–5940

Cécile Philippe, Johanna Ungersboeck, Eva Schirmer, Milica Zdravkovic, Lukas Nics, Markus Zeilinger, Karem Shanab, Rupert Lanzenberger, Georgios Karanikas, Helmut Spreitzer, Helmut Viernstein, Markus Mitterhauser, Wolfgang Wadsak*



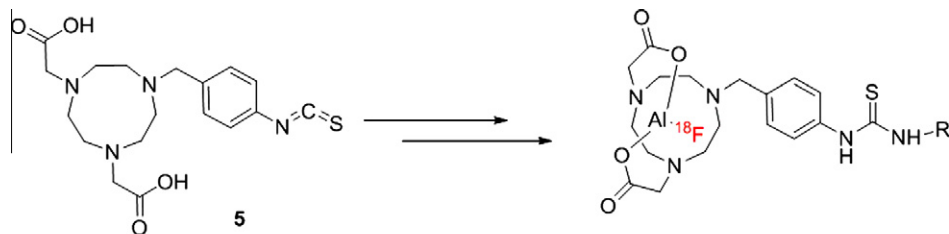
SNAP-7941 derivatives 1–4 (1: SNAP-7941; 2: [¹⁸F]FE@SNAP; 3: SNAP-acid; 4: Tos@SNAP).

SNAP-7941 derivatives 1–4 (1: SNAP-7941; 2: [¹⁸F]FE@SNAP; 3: SNAP-acid; 4: Tos@SNAP).



Development of a bifunctional chelating agent containing isothiocyanate residue for one step F-18 labeling of peptides and application for RGD labeling pp 5941–5947

Dinesh Shetty, Jae Min Jeong*, Young Ju Kim, Ji Youn Lee, Lathika Hoigebazar, Yun-Sang Lee, Dong Soo Lee, June-Key Chung

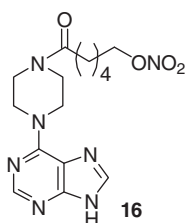


R = Peptide, protein and other molecules

**Discovery of 6-[4-(6-nitroxyhexanoyl)piperazin-1-yl]-9H-purine, as pharmacological post-conditioning agent**

pp 5948–5956

Maria Koufaki*, Theano Fotopoulou, Efstathios K. Iliodromitis, Sophia-Iris Bibli, Anastasia Zoga, Dimitrios Th. Kremastinos, Ioanna Andreadou

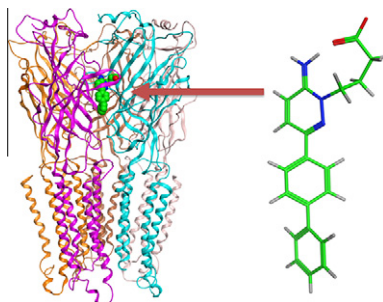


Administration of the analogue **16** in anesthetized rabbits, at a dose of 3.8 $\mu\text{mol/kg}$, resulted on a significant reduction of infarct size, compared to PostC group ($13.4 \pm 1.9\%$ vs $26.4 \pm 2.3\%$).

**Competitive antagonism of insect GABA receptors by iminopyridazine derivatives of GABA**

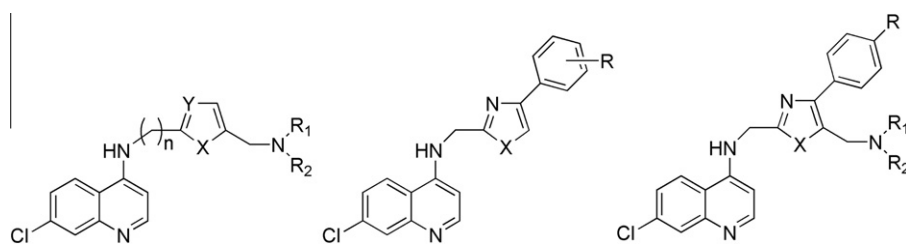
pp 5957–5964

Mohammad Mostafizur Rahman, Yuki Akiyoshi, Shogo Furutani, Kazuhiko Matsuda, Kenjiro Furuta, Izumi Ikeda, Yoshihisa Ozoe*

**Synthesis and antiparasmodial activity of new heteroaryl derivatives of 7-chloro-4-aminoquinoline**

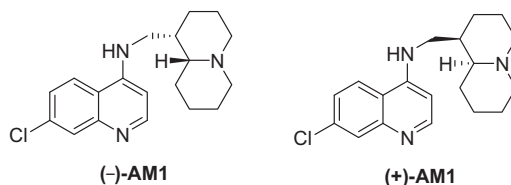
pp 5965–5979

Manolo Casagrande, Anna Barteselli, Nicoletta Basilico, Silvia Parapini, Donatella Taramelli, Anna Sparatore*

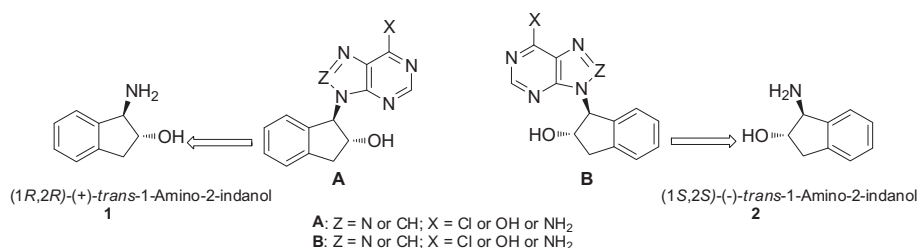


Synthesis and comparison of antiparasmodial activity of (+), (–) and racemic 7-chloro-4-(N-lupinyl)aminoquinoline**pp 5980–5985**

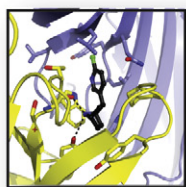
Chiara Rusconi, Nadia Vaiana, Manolo Casagrande, Nicoletta Basilico, Silvia Parapini, Donatella Taramelli, Sergio Romeo, Anna Sparatore*

**Synthesis and biological evaluation of novel homochiral carbocyclic nucleosides from 1-amino-2-indanols****pp 5986–5991**

Esteban A. Ugliarolo, Dolores Gagey, Beatriz Lantaño, Graciela Y. Moltrasio, Rodolfo H. Campos, Lucía V. Cavallaro*, Albertina G. Moglioni*

**Identification of novel $\alpha 7$ nicotinic receptor ligands by in silico screening against the crystal structure of a chimeric $\alpha 7$ receptor ligand binding domain****pp 5992–6002**

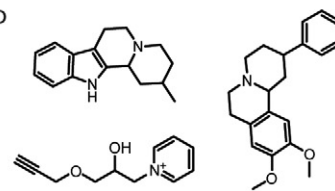
Atilla Akdemir, Ewald Edink, Andrew J. Thompson, Sarah C.R. Lummis, Albert J. Kooistra, Chris de Graaf, Iwan J.P. de Esch*

 $\alpha 7$ /Ls-AChBP chimeric crystal structure:

Compound Collection:



Docking-based in silico screening protocol:

Novel Chemotypes for human $\alpha 7$ nAChR:**OTHER CONTENTS****Corrigendum****p 6003****Bioorganic & Medicinal Chemistry Reviews and Perspectives****pp I–III**

*Corresponding author

 Supplementary data available via SciVerse ScienceDirect

COVER

The cover image shows the structures of (-)-7-chloro-4-(*N*-lupinyl)aminoquinoline, a semisynthetic derivative of the natural alkaloid (-)-lupinine isolated from *Lupinus luteus*, and of its enantiomer, which are new potential antimalarial compounds, exhibiting potent activity against different strains of *Plasmodium falciparum*. [Rusconi, C.; Vaiana, N.; Casagrande, M.; Basilio, N.; Parapini, S.; Taramelli, D.; Romeo, S.; Sparatore, A. *Bioorg. Med. Chem.*, **2012**, 20, 5979–5984.]

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