

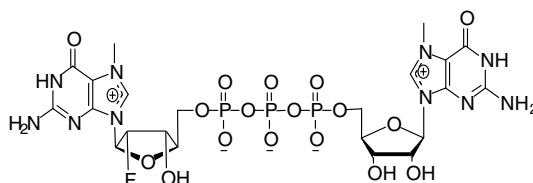
Contents

ARTICLES

Synthesis and application of 2'-fluoro-substituted cap analogs

pp 5295–5299

Anilkumar R. Kore,* Muthian Shanmugasundaram, Irudaya Charles,
Angie M. Cheng and Timothy J. Barta

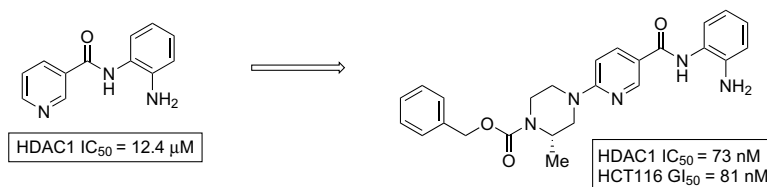


Design, synthesis, and biological evaluation of 2'-fluoro-substituted cap analogs i.e., $m^{7,2'}F$ G[5']ppp[5']G and $m^{7,2'}F$ G[5']ppp[5']m⁷G are reported.

The discovery of 6-amino nicotinamides as potent and selective histone deacetylase inhibitors

pp 5300–5309

Christopher L. Hamblett,* Joey L. Methot, Dawn M. Mampreian, David L. Sloman,
Matthew G. Stanton, Astrid M. Kral, Judith C. Fleming, Jonathan C. Cruz, Melissa Chenard,
Nicole Ozerova, Anna M. Hitz, Hongmei Wang, Sujal V. Deshmukh, Naim Nazef,
Andreas Harsch, Bethany Hughes, William K. Dahlberg, Alex A. Szewczak,
Richard E. Middleton, Ralph T. Mosley, J. Paul Secrist and Thomas A. Miller

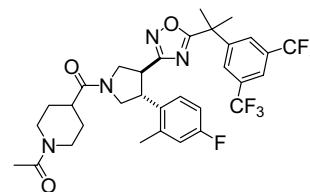


Pyrrolidine-carboxamides and oxadiazoles as potent hNK₁ antagonists

pp 5310–5315

Jonathan R. Young,* Ronsar Eid, Cherilyn Turner, Robert J. DeVita, Marc M. Kurtz,
Kwei-Lan C. Tsao, Gary G. Chicchi, Alan Wheeldon, Emma Carlson and Sander G. Mills

The preparation and structure–activity-relationships of novel pyrrolidine-carboxamides and oxadiazoles are described. Compounds in this series were found to be potent hNK₁ antagonists in vitro and efficacious in vivo with minimal interactions with P₄₅₀ liver enzymes. Oxadiazole **22** was determined to have excellent hNK₁ binding affinity, functional activity, and a good PD response in vivo.



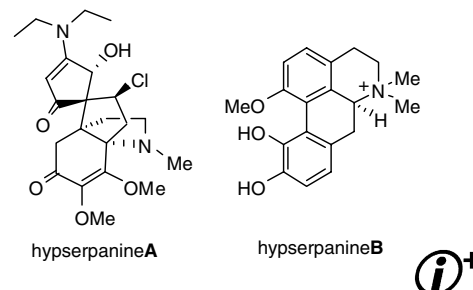
22: hNK₁ IC₅₀ = 0.03 nM
ED₅₀ (24 hr) = 6 mpk

Two new alkaloids and active anti-hepatitis B virus constituents from *Hypserpa nitida*

pp 5316–5320

Pi Cheng, Yun-bao Ma, Shu-ying Yao, Quan Zhang, En-jun Wang, Meng-hong Yan, Xue-mei Zhang, Feng-xue Zhang and Ji-jun Chen*

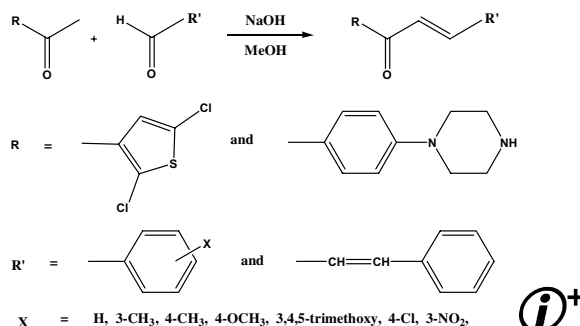
Hypserpanines **A** and **B** together with 11 known alkaloids were isolated from *Hypserpa nitida* and evaluated for their anti-HBV activities in vitro.

**Synthesis and antimicrobial evaluation of new chalcones containing piperazine or 2,5-dichlorothiophene moiety**

pp 5321–5324

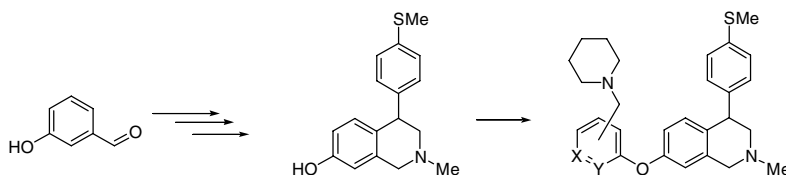
V. Tomar and G. Bhattacharjee,* Kamaluddin, Ashok Kumar

Two series of new chalcones have been synthesized and evaluated for their antimicrobial activity. Some of these derivatives are potentially active against Gram-positive bacteria; *Staphylococcus aureus* and *Escherichia coli*.

**Dual serotonin transporter inhibitor/histamine H₃ antagonists: Development of rigidified H₃ pharmacophores**

pp 5325–5329

John M. Keith,* Ann J. Barbier, Sandy J. Wilson, Kirstin Miller, Jamin D. Boggs, Ian C. Fraser, Curt Mazur, Timothy W. Lovenberg and Nicholas I. Carruthers



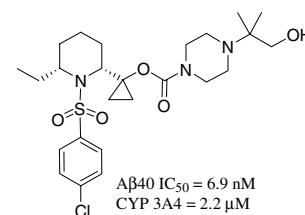
A series of tetrahydroisoquinolines acting as dual serotonin transporter inhibitor/histamine H₃ antagonists is described. The introduction of polar aromatic spacers as part of the histamine H₃ pharmacophore was explored. A convergent synthesis of the final products allowing late stage introduction of the aromatic side chain was developed. In vitro and in vivo data are discussed.

Small conformationally restricted piperidine *N*-arylsulfonamides as orally active γ -secretase inhibitors

pp 5330–5335

Hubert Josien,* Thomas Bara, Murali Rajagopalan, Theodros Asberom, John W. Clader, Leonard Favreau, William J. Greenlee, Lynn A. Hyde, Amin A. Nomeir, Eric M. Parker, Dmitri A. Pissarnitski, Lixin Song, Gwendolyn T. Wong, Lili Zhang, Qi Zhang and Zhiqiang Zhao

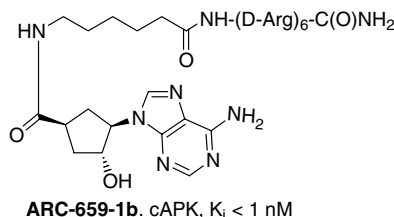
The design and development of small 2,6-disubstituted piperidine *N*-arylsulfonamide γ -secretase inhibitors is reported. Compounds active orally and with less CYP liability than earlier leads were obtained.



Carbocyclic 3'-deoxyadenosine-based highly potent bisubstrate-analog inhibitor of basophilic protein kinases

pp 5336–5339

Erki Enkvist, Gerda Raidaru, Angela Vaasa, Tõnis Pehk, Darja Lavogina and Asko Uri*

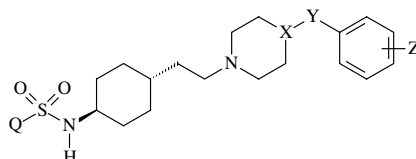


Conjugation of a nucleoside analog and a transport peptide led to a highly potent inhibitor of basophilic protein kinases.

**Novel sulfonamides having dual dopamine D2 and D3 receptor affinity show in vivo antipsychotic efficacy with beneficial cognitive and EPS profile**

pp 5340–5344

Éva Ágai-Csongor,* Katalin Nógrádi, János Galambos, István Vágó, Attila Bielik, Ildikó Magdó, Györgyi Ignác-Szendrei, György Miklós Keserű, István Greiner, István Laszlovszky, Éva Schmidt, Béla Kiss, Katalin Sághy, Judit Laszy, István Gyertyán, Mária Zájer-Balázs, Larisa Gémesi and György Domány



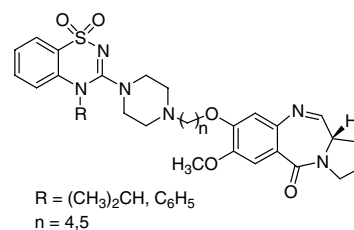
Novel arylsulfonamides were identified as high-affinity dopamine D3 and D2 receptor ligands. Some derivatives were found to be active in antipsychotic tests in vivo.

**1,2,4-Benzothiadiazine linked pyrrolo[2,1-c][1,4]benzodiazepine conjugates: Synthesis, DNA-binding affinity and cytotoxicity**

pp 5345–5348

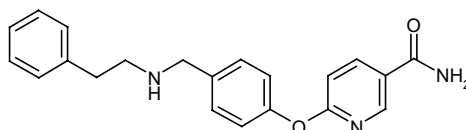
Ahmed Kamal,* M. Naseer A. Khan, K. Srinivasa Reddy, S. Kaleem Ahmed, M. Shiva Kumar, Aarti Juvekar, Subrata Sen and Surekha Zingde

Novel 1,2,4-benzothiadiazine–PBD conjugates were synthesized and displayed significant anticancer activity against selected human cancer cell lines.

**Structure–activity relationship studies of carboxamido-biaryl ethers as opioid receptor antagonists (OpRAs). Part 1**

pp 5349–5352

Kumiko Takeuchi,* William G. Holloway, Jamie H. McKinzie, Todd M. Suter, Michael A. Statnick, Peggy L. Surface, Paul J. Emmerson, Elizabeth M. Thomas, Miles G. Siegel, James E. Matt, Chad N. Wolfe and Charles H. Mitch

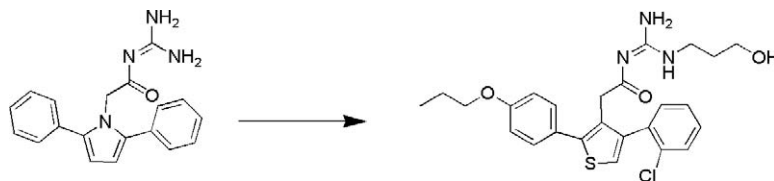


A structurally unique and new class of opioid receptor antagonists (OpRAs) that bear no structural resemblance with morphine or endogenous opioid peptides has been discovered. A series of carboxamido-biaryl ethers were identified as potent receptor antagonists against mu, kappa, and delta opioid receptors.

Thiophene substituted acylguanidines as BACE1 inhibitors

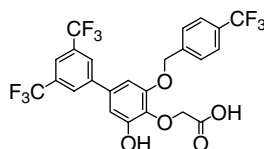
pp 5353–5356

William F. Fobare,* William R. Solvibile, Albert J. Robichaud, Michael S. Malamas, Eric Manas, Jim Turner, Yun Hu, Erik Wagner, Rajiv Chopra, Rebecca Cowling, Guixan Jin and Jonathan Bard

**2-*O*-Carboxymethylpyrogallol derivatives as PTP1B inhibitors with antihyperglycemic activity**

pp 5357–5360

Bharat Raj Bhattarai, Suja Shrestha, Seung Wook Ham, Kwang Rok Kim, Hya Gyeong Chen, Keun-Hyeung Lee and Hyeongjin Cho*



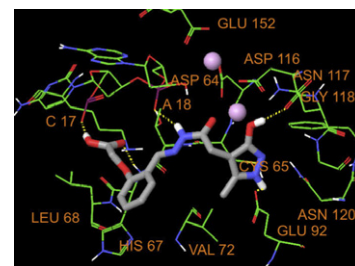
2-*O*-Carboxymethylpyrogallol derivatives were synthesized, with their in vitro inhibitory activities against PTP1B and in vivo antihyperglycemic effects examined. When compound **14** was fed to a high-fat diet-induced diabetic mouse model, significant improvements were observed in both the fasting glucose level and glucose tolerance.

Virtual screening application of a model of full-length HIV-1 integrase complexed with viral DNA

pp 5361–5365

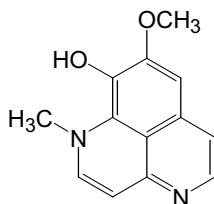
Chenzhong Liao, Rajeshri G. Karki, Christophe Marchand, Yves Pommier and Marc C. Nicklaus*

Virtual screening was performed on a model of full-length HIV-1 integrase complexed with viral DNA. Docking into the active site of this model yielded several μM level, structurally novel inhibitors of the strand transfer reaction catalyzed by wild-type HIV-1 integrase.

**Aaptamines as sortase A inhibitors from the tropical sponge *Aaptos aaptos***

pp 5366–5369

Kyoung Hwa Jang, Soon-Chun Chung, Jongheon Shin,* So-Hyoung Lee, Tae-Im Kim, Hyi-Seung Lee and Ki-Bong Oh*



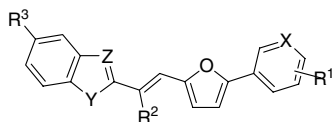
2: $\text{IC}_{50} = 3.7 \mu\text{g/mL}$

The isolation and sortase A inhibitory activity of four aaptamines are reported.

Toward novel HIV-1 integrase binding inhibitors: Molecular modeling, synthesis, and biological studies

pp 5370–5373

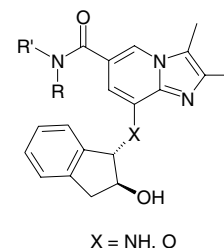
Claudia Mugnaini, Suvi Rajamaki, Cristina Tintori, Federico Corelli, Silvio Massa, Myriam Witvrouw, Zeger Debyser, Veljko Veljkovic and Maurizio Botta*

**Novel indanyl-substituted imidazo[1,2-*a*]pyridines as potent reversible inhibitors of the gastric H⁺/K⁺-ATPase**

pp 5374–5378

Peter Jan Zimmermann,* Wilm Buhr, Christof Brehm, Andreas Marc Palmer, Martin Philipp Feth, Jörg Senn-Bilfinger and Wolfgang-Alexander Simon

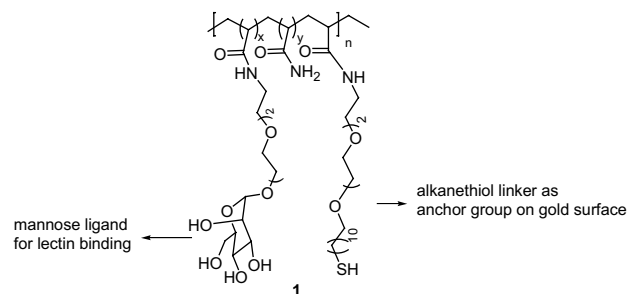
8-Indanyl-substituted imidazo[1,2-*a*]pyridines were synthesized and evaluated for their anti-secretory activity in a binding assay against H⁺/K⁺-ATPase from hog gastric mucosa.

**Alkanethiol containing glycopolymers: A tool for the detection of lectin binding**

pp 5379–5383

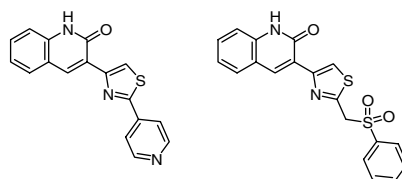
Mingchuan Huang, Zhihong Shen, Yalong Zhang, Xiangqun Zeng* and Peng George Wang*

Glycopolymers containing mannose and alkanethiol linker were synthesized through substituting preactivated poly [*N*-(acryloyloxy) succinimide] (pNAS) with amine-containing monomer. With the obtained glycopolymers, a glycosurface was generated on the gold surface of quartz crystal microbalance (QCM) through self-assembled strategy by use of alkanethiol functional group. Furthermore, the resulting glycosurface was used to detect the binding of mannose specific lectin concanavalin A (Con A).

**Design and synthesis of quinolin-2(1*H*)-one derivatives as potent CDK5 inhibitors**

pp 5384–5389

Wenge Zhong,* Hu Liu, Matthew R. Kaller, Charles Henley, Ella Magal, Thomas Nguyen, Timothy D. Osslund, David Powers, Robert M. Rzasa, Hui-Ling Wang, Weiya Wang, Xiaoling Xiong, Jiandong Zhang and Mark H. Norman



3 IC₅₀: 54 ± 33 nM

17j IC₅₀: 29 ± 19 nM

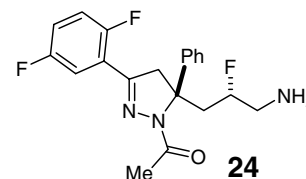
A novel series of quinolin-2(1*H*)-one derivatives were synthesized and found to have potent CDK5 inhibitory activities.

Kinesin spindle protein (KSP) inhibitors. Part 6: Design and synthesis of 3,5-diaryl-4,5-dihydropyrazole amides as potent inhibitors of the mitotic kinesin KSP

pp 5390–5395

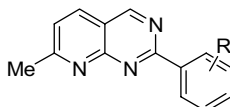
Paul J. Coleman,* John D. Schreier, Christopher D. Cox, Mark E. Fraley, Robert M. Garbaccio, Carolyn A. Buser, Eileen S. Walsh, Kelly Hamilton, Robert B. Lobell, Keith Rickert, Weikang Tao, Ronald E. Diehl, Vicki J. South, Joseph P. Davide, Nancy E. Kohl, Youwei Yan, Lawrence Kuo, Thomayant Prueksaritanont, Chunze Li, Elizabeth A. Mahan, Carmen Fernandez-Metzler, Joseph J. Salata and George D. Hartman

Dihydropyrazole amides such as **24** are potent inhibitors of KSP with favorable physical properties, pharmacokinetics, and in vivo potency. A diastereoselective synthesis of **24** is described.

**Synthesis and SAR of 2-aryl pyrido[2,3-*d*]pyrimidines as potent mGlu5 receptor antagonists**

pp 5396–5399

John A. Wendt,* Susan D. Deeter, Susan E. Bove, Christopher S. Knauer, Rachel M. Brooker, Corinne E. Augelli-Szafran, Roy D. Schwarz, Jack J. Kinsora and Kenneth S. Kilgore

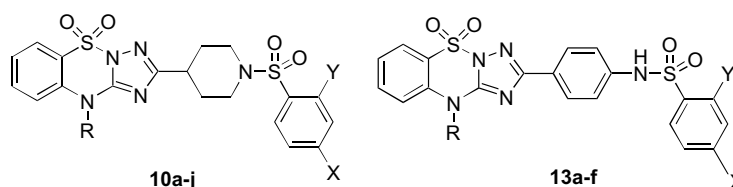


A novel series of potent 2-aryl pyrido[2,3-*d*]pyrimidine mGlu5 receptor antagonists are described. The synthesis and pharmacological activities of these analogs are discussed.

Synthesis, structure analysis, and antibacterial activity of some novel 10-substituted 2-(4-piperidyl/phenyl)-5,5-dioxo[1,2,4]triazolo[1,5-*b*][1,2,4]benzothiadiazine derivatives

pp 5400–5405

Ahmed Kamal,* M. Naseer A. Khan, K. Srinivasa Reddy, K. Rohini, G. Narahari Sastry, B. Sateesh and B. Sridhar



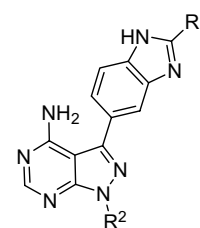
R = CH₃, C₆H₅
X = H, CH₃, F, Cl, NHAc
Y = H, Cl

**Pyrazolo[3,4-*d*]pyrimidines as potent inhibitors of the insulin-like growth factor receptor (IGF-IR)**

pp 5406–5409

Robert D. Hubbard,* Nwe Y. Bamaung, Fabio Palazzo, Qian Zhang, Peter Kovar, Donald J. Osterling, Xiaoming Hu, Julie L. Wilsbacher, Eric F. Johnson, Jennifer Bouska, Jieyi Wang, Randy L. Bell, Steven K. Davidsen and George S. Sheppard

The synthesis, in vitro and in vivo characterization of a novel class of insulin-like growth factor receptor tyrosine kinase inhibitors, the pyrazolo[3,4-*d*]pyrimidines, is disclosed.

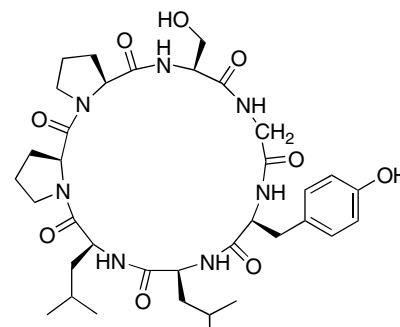


Cyclonatsudamine A, a new vasodilator cyclic peptide from *Citrus natsudaoidai*

pp 5410–5413

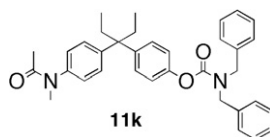
Hiroshi Morita,* Maiko Enomoto, Yusuke Hirasawa, Toru Iizuka, Kazunori Ogawa, Nobuo Kawahara, Yukihiko Goda, Teruki Matsumoto and Koichi Takeya

A new cyclic heptapeptide, cyclonatsudamine A (**1**), has been isolated from the peels of *Citrus natsudaoidai* and the structure was elucidated by 2D NMR analysis and chemical degradation. Cyclonatsudamine A relaxed norepinephrine-induced contractions of rat aorta.

**3,3-Diphenylpentane skeleton as a steroid skeleton substitute: Novel inhibitors of human 5α -reductase 1**

pp 5414–5418

Shinnosuke Hosoda and Yuichi Hashimoto*

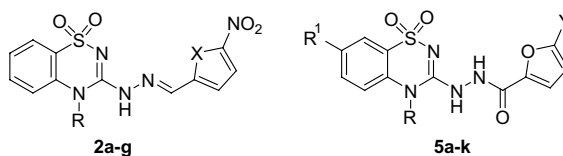


4-(3-(4-(*N*-Methylacetamido)phenyl)pentan-3-yl)phenyl dibenzylcarbamate (**11k**) is a competitive 5α -reductase inhibitor with the IC_{50} value of 0.84 μ M.

Anti-tubercular agents. Part IV: Synthesis and antimycobacterial evaluation of nitroheterocyclic-based 1,2,4-benzothiadiazines

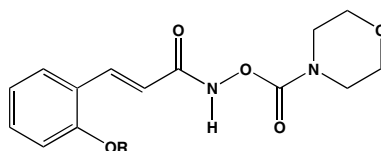
pp 5419–5422

Ahmed Kamal,* S. Kaleem Ahmed, K. Srinivasa Reddy, M. Naseer A. Khan, Rajesh V. C. R. N. C. Shetty, B. Siddhardha, U. S. N. Murthy, Inshad Ali Khan, Manoj Kumar, Sandeep Sharma and Anshu Beulah Ram

**Synthesis and biological evaluation of cinnamyl compounds as potent antitumor agents**

pp 5423–5427

Dae-Seop Shin, Jiin Kim, Dong Cho Han, Kwang-Hee Son, Chang Woo Lee, Hwan-Mook Kim, Su Hyung Hong and Byoung-Mog Kwon*

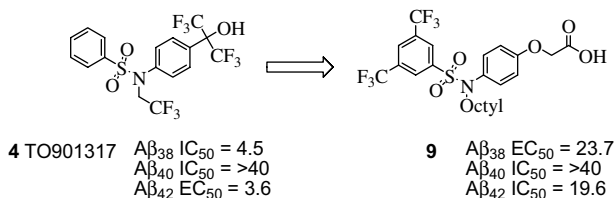


Cinnamyl compounds related to 2'-hydroxycinnamaldehyde were synthesized. The compounds inhibited the growth of human tumor cells through induction of apoptosis and arresting cell cycle at G_2/M phase.

Conversion of the LXR-agonist TO-901317—From inverse to normal modulation of γ -secretase by addition of a carboxylic acid and a lipophilic anchor

pp 5428–5431

Rajeshwar Narlawar, Karlheinz Baumann, Christian Czech and Boris Schmidt*



TO-901317 analogue derivatives, where the hexafluorocarbonyl moiety was replaced by an oxyacetic acid functionality, switch the mode of action from an inverse modulation to normal modulation of γ -secretase. As anticipated, compound **9** was found to be an effective modulator of γ -secretase and displayed activity at low micromolar concentration.

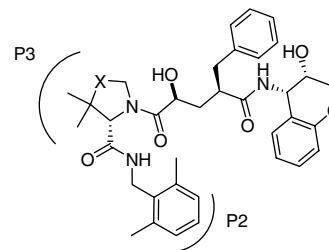


Synthesis of novel HIV protease inhibitors (PI) with activity against PI-resistant virus

pp 5432–5436

Subharekha Raghavan,* Zhijian Lu, Teresa Beeson, Kevin T. Chapman, William A. Schleif, David B. Olsen, Mark Stahlhut, Carrie A. Rutkowski, Lori Gabryelski, Emilio Emini and James R. Tata

HIV protease inhibitors with modifications on the P3 position have been designed and synthesized. These compounds exhibit excellent antiviral activity against both the wild type enzyme and PI-resistant clinical viral isolates.

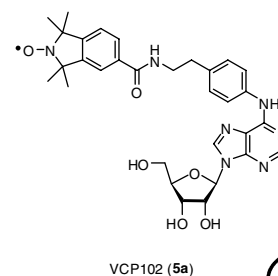


Dual acting antioxidant A_1 adenosine receptor agonists

pp 5437–5441

Alison Gregg, Steven E. Bottle, Shane M. Devine, Heidi Figler, Joel Linden, Paul White, Colin W. Pouton, Vijay Urmaliya and Peter J. Scammells*

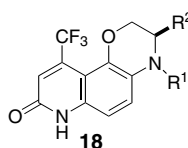
Herein we report the synthesis and biological evaluation of some potent and selective A_1 adenosine receptor agonists, which incorporate a functionalised linker attached to an antioxidant moiety. N^6 -(2,2,5,5-Tetramethylpyrrolidin-1-yloxy-3-ylmethyl)adenosine (**VCP28**, **2e**) proved to be an agonist with high affinity ($K_i = 50$ nM) and good selectivity (A_3/A_1 400) for the A_1 AR. N^6 -[4-[2-[1,1,3,3-Tetramethylisoindolin-2-yloxy]-5-amido]ethyl]phenyl]adenosine (**VCP102**, **5a**) has higher binding affinity ($K_i = 7$ nM), but lower selectivity ($A_3/A_1 = \sim 3$). All compounds bind weakly ($K_i > 1$ μ M) to A_{2A} and A_{2B} receptors. The combination of A_1 agonist activity and antioxidant activity has the potential to produce cardioprotective effects.



Potent, nonsteroidal selective androgen receptor modulators (SARMs) based on 8*H*-[1,4]oxazino[2,3-*f*]quinolin-8-ones

pp 5442–5446

Robert I. Higuchi,* Anthony W. Thompson, Jyun-Hung Chen, Thomas R. Caferro, Marquis L. Cummings, Charlotte P. Deckhut, Mark E. Adams, Christopher M. Tegley, James P. Edwards, Francisco J. López, E. Adam Kallel, Donald S. Karanewsky, William T. Schrader, Keith B. Marschke and Lin Zhi

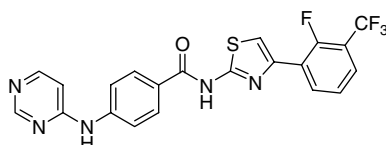


The synthesis and biological evaluation of a selective androgen receptor modulator (SARM) series is reported.

Pyrimidine benzamide-based thrombopoietin receptor agonists

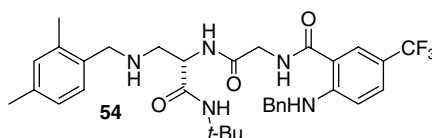
pp 5447–5454

Lawrence A. Reiter, Chakrapani Subramanyam, Emilio J. Mangual, Christopher S. Jones,*
 Marc I. Smeets, William H. Brissette, Sandra P. McCurdy, Paul D. Lira, Robert G. Linde,
 Qifang Li, Fangning Zhang, Amy S. Antipas, Laura C. Blumberg, Jonathan L. Doty,
 James P. Driscoll, Michael J. Munchhof, Sharon L. Ripp, Andrei Shavnya,
 Richard M. Shepard, Diana Sperger, Lisa M. Thomasco, Kristen A. Trevena,
 Lilli A. Wolf-Gouveia and Liling Zhang

**Capped diaminopropionamide-glycine dipeptides are inhibitors of CC chemokine receptor 2 (CCR2)**

pp 5455–5461

Percy H. Carter,* Gregory D. Brown, Sarah R. Friedrich, Robert J. Cherney, Andrew J. Tebben,
 Yvonne C. Lo, Gengjie Yang, Heather Jezak, Kimberly A. Solomon, Peggy A. Scherle and Carl P. Decicco

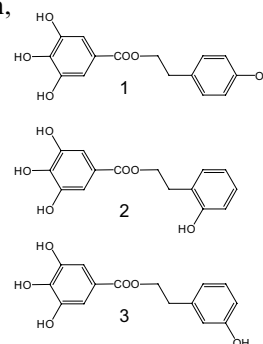


A new series of CCR2 antagonists has been discovered that incorporates intramolecular hydrogen bonding as a strategy for rigidifying the scaffold. The structure–activity relationship was established through initial systematic modification of substitution pattern and chain length, followed by independent optimization of three substituents. Compound **54** exhibited potent activity (CCR2 binding IC_{50} = 19 nM; Chemotaxis IC_{50} = 39 nM) and good selectivity over CCR1 and CCR3.

**Synthetic tyrosyl gallate derivatives as potent melanin formation inhibitors**

pp 5462–5464

Chan Woo Lee, Eun-Mi Son, Han Sung Kim, Pan Xu, Tuyagerel Batmunkh,
 Burm-Jong Lee* and Kyung Ah Koo*



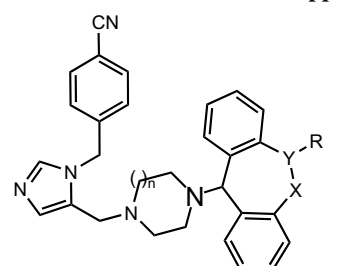
The synthesis of the potent melanin formation inhibitors (**1–3**) is reported.

Design, synthesis and biological evaluation of substituted dioxodibenzothiazepines and dibenzocycloheptanes as farnesyltransferase inhibitors

pp 5465–5471

Pauline Gilleron, Nicolas Wlodarczyk, Raymond Houssin, Amaury Farce,
 Guillaume Laconde, Jean-François Goossens, Amélie Lemoine,
 Nicole Pommery, Jean-Pierre Hénichart and Régis Millet*

The design, synthesis, inhibitory FTase activity and antiproliferative properties of the title tricyclic compounds are reported.



$n = 1$ or 2

$X = SO_2, Y = N, R = \text{alkyl or } C_3H_6-N \text{ (morpholine)}$

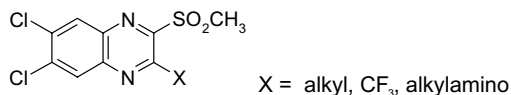
or $X = Y = CH_2$



Small molecule *ago*-allosteric modulators of the human glucagon-like peptide-1 (hGLP-1) receptor

pp 5472–5478

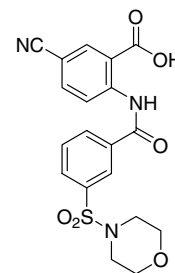
Min Teng,* Michael D. Johnson, Christine Thomas, Dan Kiel, James N. Lakis, Tim Kercher, Shelley Aytes, Jarek Kostrowicki, Dilip Bhumralkar, Larry Truesdale, John May, Ulla Sidelman, Janos T. Kodra, Anker Steen Jørgensen, Preben Houlberg Olesen, Johannes Cornelis de Jong, Peter Madsen, Carsten Behrens, Ingrid Pettersson, Lotte Bjerre Knudsen, Jens J. Holst and Jesper Lau

**Correlation of carboxylic acid pK_a to protein binding and antibacterial activity of a novel class of bacterial translation inhibitors**

pp 5479–5482

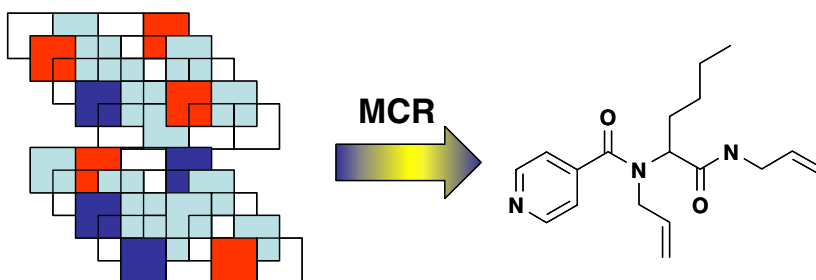
Cory M. Stiff, Min Zhong, Ronald W. Sarver, Hua Gao, Andrea M. Ho, Michael T. Sweeney, Gary E. Zurenko and Donna L. Romero*

A study of the relationship between pK_a of a compound containing a carboxylic acid, and its antibacterial activity and protein binding is reported.

**Novel anti-tuberculosis agents from MCR libraries**

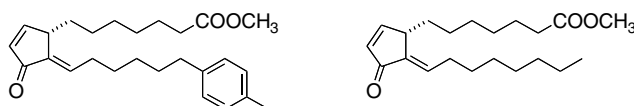
pp 5483–5491

Alexander Dömling,* Sepp Achatz and Barbara Beck

**Synthesis of neuroprotective cyclopentenone prostaglandin analogs: Suppression of manganese-induced apoptosis of PC12 cells**

pp 5487–5491


Kyoji Furuta, Masahide Maeda, Yoko Hirata, Shoko Shibata, Kazutoshi Kiuchi and Masaaki Suzuki*



The synthesis and evaluation for anti- and proapoptotic properties of cyclopentenone prostaglandin analogs are described.

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*Corresponding author

 Supplementary data available via ScienceDirect**COVER**

Typical snapshot of **7b** bound to HIV-RT from an MC simulation. Carbon atoms of **7b** are gold; from the left, Tyr181, Tyr188, Phe227, Leu100, Lys101; Trp229 at the top, Val106 at the bottom. H-bond with Lys101 O on right. Some residues in front including Glu138 have been removed for clarity. The water on N5 is also H-bonded to a carboxylate O of Glu138. [Thakur, V. T.; Kim, J. T.; Hamilton, A. D.; Bailey, C. M.; Domaoal, R. A.; Wang, L.; Anderson, K. S.; Jorgensen, W. L. *Bioorg. Med. Chem. Lett.* **2006**, 16, 5664.]

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