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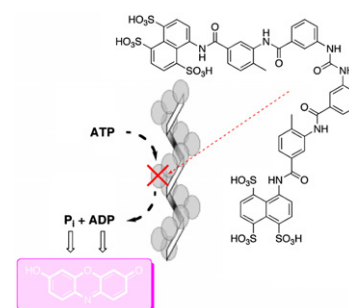
ARTICLES

Directed molecular screening for RecA ATPase inhibitors

Tim J. Wigle and Scott F. Singleton*

To improve the efficacy of existing antibacterial drugs by countering bacterial mechanisms of drug resistance, three suramin-like inhibitory agents were discovered using two new fluorescence-based assays for RecA's ATPase activity.

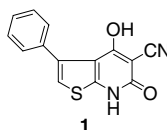
pp 3249–3253



Discovery and SAR development of thienopyridones: A class of small molecule AMPK activators

Gang Zhao,* Rajesh R. Iyengar, Andrew S. Judd, Barbara Cool, William Chiou, Lemma Kifle, Ernst Frevert, Hing Sham and Philip R. Kym

pp 3254–3257

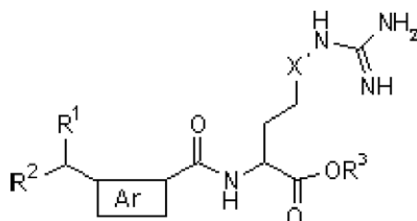


AMPK Rat Liver EC 50 38 uM

Discovery of new C3aR ligands. Part 1: Arginine derivatives

Frédéric Denonne,* Sophie Binet, Maggi Burton, Philippe Collart, Alan Dipesa, Tanmoy Ganguly, Alexander Giannaras, Seema Kumar, Timothy Lewis, Florence Maounis, Jean-Marie Nicolas, Tamsin Mansley, Patrick Pasau, Dorin Preda, Karin Stebbins, Alexander Volosov and Dong Zou

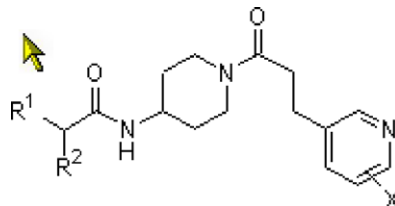
pp 3258–3261



Discovery of new C3aR ligands. Part 2: Amino-piperidine derivatives

pp 3262–3265

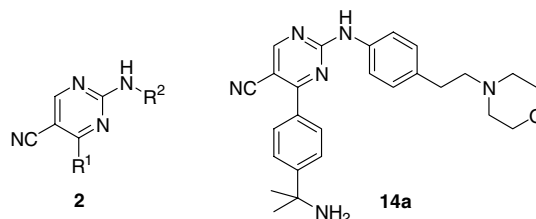
Frédéric Denonne,* Sophie Binet, Maggi Burton, Philippe Collart, Sabine Defays, Alan Dipesa, Maria Eckert, Alexander Giannaras, Seema Kumar, Beth Levine, Jean-Marie Nicolas, Patrick Pasau, Cécile Pégurier, Dorin Preda, Nathalie Van houtvin, Andrew Volosov and Dong Zou

**4-Aryl-5-cyano-2-aminopyrimidines as VEGF-R2 inhibitors: Synthesis and biological evaluation**

pp 3266–3270

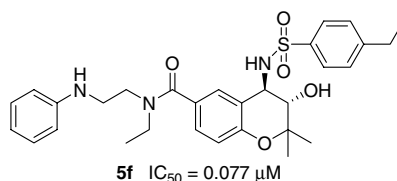
Terry V. Hughes,* Stuart L. Emanuel, Amanda K. Beck, Steven K. Wetter, Peter J. Connolly, Prabha Karnachi, Michael Reuman, Javed Seraj, Angel R. Fuentes-Pesquera, Robert H. Gruninger, Steven A. Middleton, Ronghui Lin, Jeremy M. Davis and David F. C. Moffat

A novel series of 4-aryl-5-cyano-2-aminopyrimidines **2** were synthesized and found to have potent VEGF-R2 kinase inhibitory activity. Structure–activity relationships were investigated and compound **14a** was shown to be efficacious in a mouse model of corneal neovascularization.

**Benzopyran sulfonamides as K_v1.5 potassium channel blockers**

pp 3271–3275

John Lloyd,* Karnail S. Atwal, Heather J. Finlay, Michael Nyman, Tram Huynh, Rao Bhandaru, Alexander Kover, Joan Schmidt, Wayne Vaccaro, Mary Lee Conder, Tonya Jenkins-West and Paul Levesque

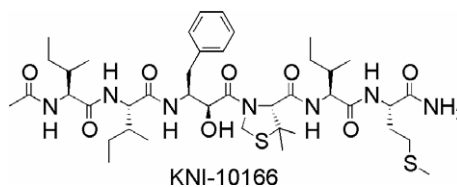


K_v1.5 blockers have the potential to be selective agents for the treatment of atrial fibrillation. Benzopyrans provide a template for the synthesis of potent and selective K_v1.5 blockers.

Chipping at large, potent human T-cell leukemia virus type 1 protease inhibitors to uncover smaller, equipotent inhibitors

pp 3276–3280

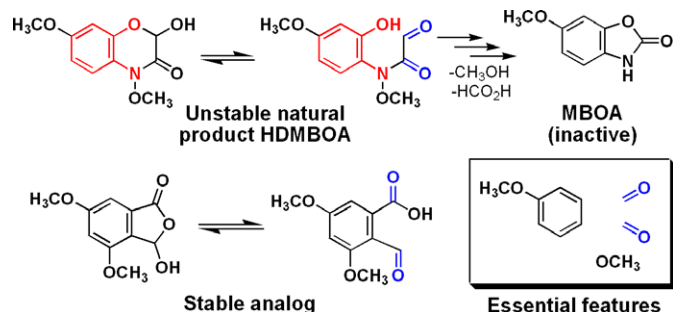
Tooru Kimura, Jeffrey-Tri Nguyen, Hikoichiro Maegawa, Keiji Nishiyama, Yasuhiro Arai, Yasuko Matsui, Yoshio Hayashi and Yoshiaki Kiso*



Rational design of inhibitors of VirA–VirG two-component signal transduction

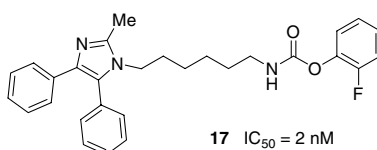
pp 3281–3286

Justin Maresh, Jin Zhang, Yih-Ling Tzeng, Nora A. Goodman and David G. Lynn*

**Novel inhibitors of fatty acid amide hydrolase**

pp 3287–3291

S. Y. Sit,* Charlie Conway, Robert Bertekap, Kai Xie, Clotilde Bourin, Kevin Burris and Hongfeng Deng

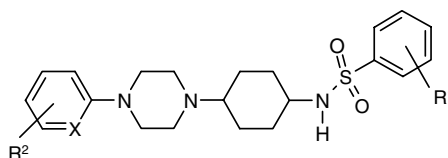


A class of bisarylimidazole derivatives are identified as potent inhibitors of the enzyme fatty acid amide hydrolase (FAAH).

(Arylpiperazinyl)cyclohexylsulfonamides: Discovery of $\alpha_{1a/1d}$ -selective adrenergic receptor antagonists for the treatment of Benign Prostatic Hyperplasia/Lower Urinary Tract Symptoms (BPH/LUTS)

pp 3292–3297

George Chiu,* Shengjian Li, Peter J. Connolly, Virginia Pulito, Jingchun Liu and Steven A. Middleton



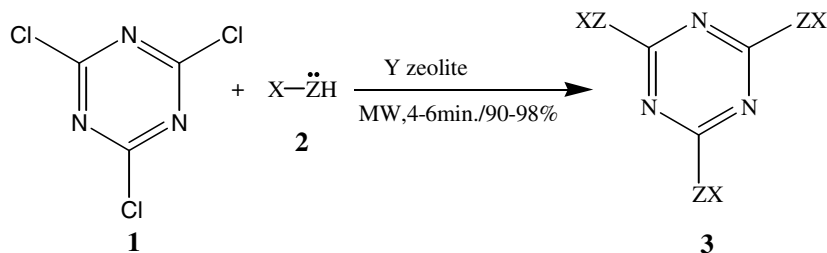
A series of (arylpiperazinyl)cyclohexylsulfonamides that show selectivity to human $\alpha_{1a/1d}$ -adrenergic receptors was developed. These compounds have potential for the treatment of BPH/LUTS.

**Synthesis and cytotoxic activity of trisubstituted-1,3,5-triazines**

pp 3298–3304

Kapil Arya* and Anshu Dandia

A simple and environmentally friendly procedure has been developed for the synthesis of 2,4,6-trisubstituted-1,3,5-triazines using HY zeolite under microwaves and synthesized compounds screened for cytotoxic, antimicrobial, and photo-synthesis-inhibiting activities.

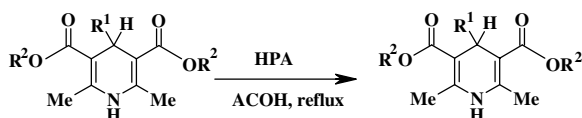


$\text{X} = \text{Ar}/\text{CH}_3\text{Ar}/(\text{C}_2\text{H}_5)_2/(\text{CH}_3)_2/\text{CH}_3\text{CO}/\text{CH}_3/\text{OCH}_3\text{Ar}/\text{NO}_2\text{Ar}/\text{ClAr}/\text{H}$, $\text{Z} = \text{O}, \text{NH}$

Oxidative aromatization of Hantzsch 1,4-dihydropyridines in the presence of mixed-addenda vanadomolybdophosphate heteropolyacid, $H_6PMo_9V_3O_{40}$

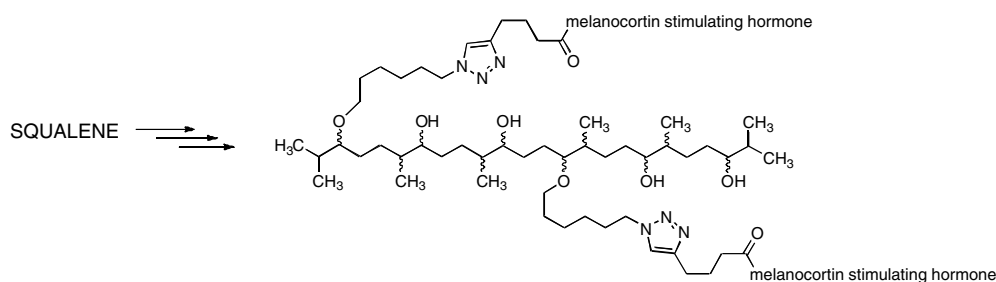
pp 3305–3309

Majid M. Heravi,* Fatemeh Derikvand, Shahla Hassan-Pour, Khadijeh Bakhtiari, Fatemeh F. Bamoharram and Hossein A. Oskooie


Squalene-derived flexible linkers for bioactive peptides

pp 3310–3313

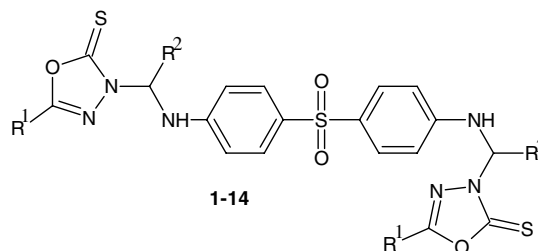
Bhumasamudram Jagadish, Rajesh Sankaranarayanan, Liping Xu, Reyniak Richards, Josef Vagner, Victor J. Hruby, Robert J. Gillies and Eugene A. Mash*


Oxadiazole mannich bases: Synthesis and antimycobacterial activity

pp 3314–3316

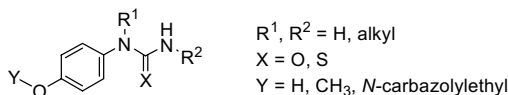
Mohamed Ashraf Ali and Mohammad Shaharyar*

A series of oxadiazole mannich bases were synthesized by reacting oxadiazole derivatives, dapsone and appropriate aldehyde in the presence of methanol. The synthesized compounds were evaluated for antimycobacterial activity against *Mycobacterium tuberculosis* H₃₇Rv and INH resistant *M. tuberculosis*. Among the synthesized compounds, compound (4) 3-{2-furyl[4-(4-{2-furyl[5-(2-naphthyloxymethyl)-2-thioxo-2,3-dihydro-1,3,4-oxadiazol-3-yl]methylamino}-phenylsulfonyl)anilino]methyl}-5-(2-naphthyloxymethyl)-2,3-dihydro-1,3,4-oxadiazole-2-thione was found to be the most promising compound active against *M. tuberculosis* H₃₇Rv and isoniazid (INH) resistant *M. tuberculosis* with minimum inhibitory concentration (MIC) 0.1 μ M & 1.10 μ M respectively.


Design and synthesis of urea and thiourea derivatives and their inhibitory activities on lipopolysaccharide-induced NO production

pp 3317–3321

Yoon Jung Kim, Jae-Ha Ryu, Ye Jin Cheon, Hyo Jin Lim and Raok Jeon*



Synthesis of series of ureas and thioureas and their inhibitory activities of NO production in lipopolysaccharide-activated macrophages are reported.

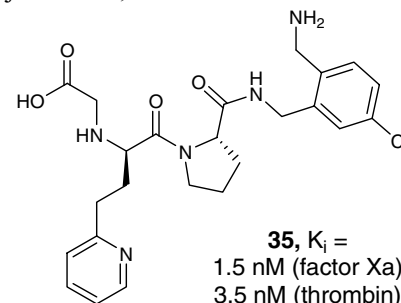


From selective substrate analogue factor Xa inhibitors to dual inhibitors of thrombin and factor Xa. Part 3

pp 3322–3329

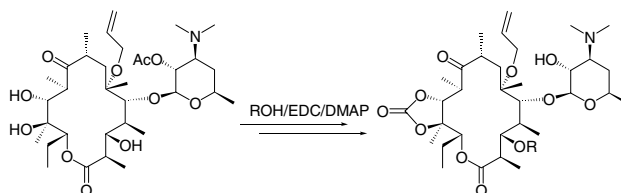
Daniel Dönnecke, Andrea Schweinitz, Anne Stürzebecher, Peter Steinmetzer, Maj Schuster, Uta Stürzebecher, Silke Nicklisch, Jörg Stürzebecher and Torsten Steinmetzer*

Highly potent and selective substrate analogue inhibitors of factor Xa containing weakly basic P1 residues were converted to dual inhibitors of thrombin and factor Xa by simple replacement of the P2 and P3 amino acids. The most potent inhibitors have K_i values in the low nanomolar range for both proteases and possess excellent anticoagulant activity in human plasma.

**Synthesis and antibacterial activity of derivatives of 6-*O*-allylic acylides**

pp 3330–3334

Peng Xu, Lu Liu, Zhiping Jin and Pingsheng Lei*

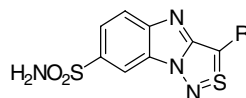


A facile way to assemble a series of potent acylide derivatives against both macrolide-susceptible and macrolide-resistant strains was reported.

**Benzimidazo[1,2-*c*][1,2,3]thiadiazole-7-sulfonamides as inhibitors of carbonic anhydrase**

pp 3335–3338

Virginija Dudutienė, Lina Baranauskienė and Daumantas Matulis*

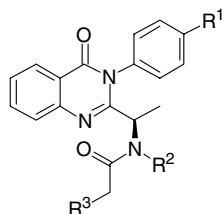


Synthesis and binding of the novel carbonic anhydrase inhibitors are described.

Discovery and optimization of a series of quinazolinone-derived antagonists of CXCR3

pp 3339–3343

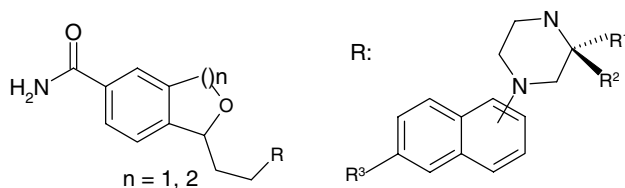
Michael Johnson, An-Rong Li, Jiwen Liu, Zice Fu, Liusheng Zhu, Shichang Miao, Xuemei Wang, Qingge Xu, Alan Huang, Andrew Marcus, Feng Xu, Karen Ebsworth, Emmanuel Sablan, Jay Danao, Jeff Kumer, Dan Dairaghi, Chris Lawrence, Tim Sullivan, George Tonn, Thomas Schall, Tassie Collins and Julio Medina*



Naphthyl piperazines with dual activity as 5-HT_{1D} antagonists and 5-HT reuptake inhibitors

pp 3344–3348

Ana B. Bueno,* Jeremy Gilmore, John Boot, Richard Broadmore, Jane Cooper, Jeremy Findlay, Lorna Hayhurst, Alicia Marcos, Carlos Montero, Stephen Mitchell, Graham Timms, Rosemarie Tomlinson, Louise Wallace and Leslie Walton



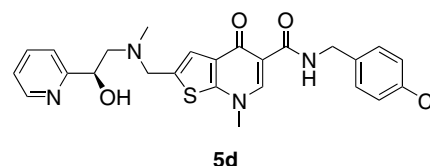
A series of compounds with dual activity as 5-HT_{1D} antagonists and 5-HT reuptake inhibitors were prepared by incorporating naphthylpiperazines to substituted isochromans and dihydroisobenzofurans.

2-Aryl-2-hydroxyethylamine substituted 4-oxo-4,7-dihydrothieno[2,3-*b*]pyridines as broad-spectrum inhibitors of human herpesvirus polymerases

pp 3349–3353

Mark E. Schnute,* David J. Anderson, Roger J. Brideau, Fred L. Ciske, Sarah A. Collier, Michele M. Cudahy, MariJean Eggen, Michael J. Genin, Todd A. Hopkins, Thomas M. Judge, Euibong J. Kim, Mary L. Knechtel, Sajiv K. Nair, James A. Nieman, Nancee L. Oien, Allen Scott, Steven P. Tanis, Valerie A. Vaillancourt, Michael W. Wathen and Janet L. Wieber

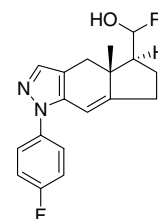
A potent series of broad-spectrum antivirals against human herpesviruses has been identified which inhibit HCMV, HSV-1, EBV, and VZV polymerases.

**Novel glucocorticoids containing a 6,5-bicyclic core fused to a pyrazole ring: Synthesis, in vitro profile, molecular modeling studies, and in vivo experiments**

pp 3354–3361

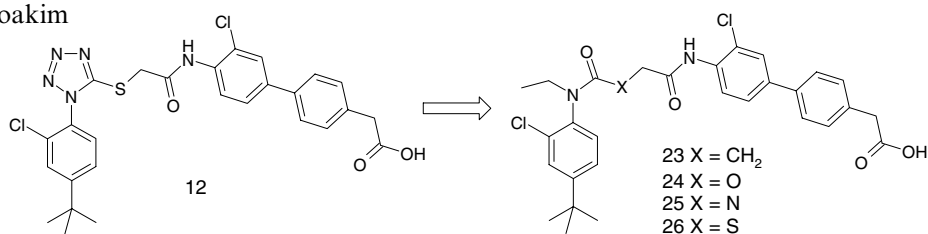
Christopher F. Thompson,* Nazia Quraishi, Amjad Ali, Ralph T. Mosley, James R. Tata, Milton L. Hammond, James M. Balkovec, Monica Einstein, Lan Ge, Georgianna Harris, Terri M. Kelly, Paul Mazur, Shilpa Pandit, Joseph Santoro, Ayesha Sitlani, Chuanlin Wang, Joanne Williamson, Douglas K. Miller, Ting-ting D. Yamin, Chris M. Thompson, Edward A. O'Neill, Dennis Zaller, Michael J. Forrest, Ester Carballo-Jane and Silvi Luell

Compounds containing the depicted core were synthesized. These compounds were evaluated for binding to the glucocorticoid receptor in cell based transactivation and transrepression assays. Molecular modeling and in vivo data are also provided.

**Scaffold hopping in the rational design of novel HIV-1 non-nucleoside reverse transcriptase inhibitors**

pp 3362–3366

Jeff A. O'Meara,* Araz Jakalian, Steven LaPlante, Pierre R. Bonneau, René Coulombe, Anne-Marie Faucher, Ingrid Guse, Serge Landry, Jennifer Racine, Bruno Simoneau, Bounkham Thavonekham and Christiane Yoakim

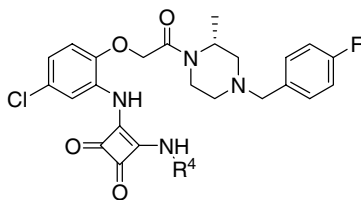


Tetrazole thioacetanilides such as **12** were identified as potent NNRTIs via high-throughput screening. Analysis of the binding mode of these inhibitors permitted the successful scaffold hop to tertiary amides (**23**), carbamates (**24**), and thiocarbamates (**26**).

Structure–activity relationships of novel, highly potent, selective, and orally active CCR1 antagonists pp 3367–3372

Yun Feng Xie, Kirk Lake, Kathleen Ligsay, Mallareddy Komandla, Ila Sircar, Gobi Nagarajan, Jian Li, Kui Xu, Jason Parise, Lisa Schneider, Ding Huang, Juping Liu, Kevin Dines, Naoki Sakurai, Miguel Barbosa and Rick Jack*

Design, synthesis, and structure–activity relationships of a series of 3-amino-4-(2-(2-(4-benzylpiperazin-1-yl)-2-oxoethoxy)phenylamino)cyclobut-3-ene-1,2-diones are described. Compound **22** demonstrated high potency and excellent selectivity for the CCR1 and desirable pharmacokinetic profiles. Compound **22** was efficacious in the mouse collagen-induced arthritis model.



Compound **22** ($R^4 = H$)

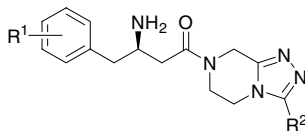
IC_{50} (CCR1 binding): 10 nM (human)
260 nM (mouse)
20 nM (rat)

IC_{50} (Ca^{2+} flux): 4 nM (human)

IC_{50} (Chemotaxis): 7 nM (human)

Triazolopiperazine-amides as dipeptidyl peptidase IV inhibitors: Close analogs of JANUVIA™ (sitagliptin phosphate) pp 3373–3377

Dooseop Kim,* Jennifer E. Kowalchick, Scott D. Edmondson, Anthony Mastracchio, Jinyou Xu, George J. Eiermann, Barbara Leiting, Joseph K. Wu, KellyAnn D. Pryor, Reshma A. Patel, Huaibing He, Kathryn A. Lyons, Nancy A. Thornberry and Ann E. Weber

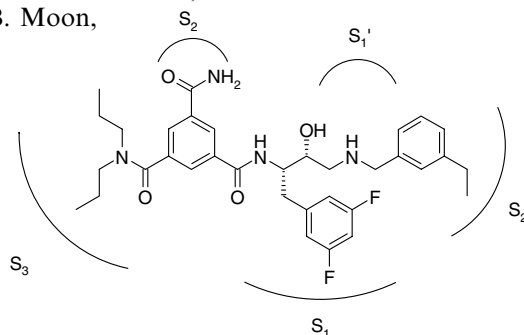


A series of β -aminoamides bearing triazolopiperazines has been prepared and evaluated as potent, selective, orally active dipeptidyl peptidase IV (DPP-4) inhibitors.

Potent and selective isophthalamide S_2 hydroxyethylamine inhibitors of BACE1 pp 3378–3383

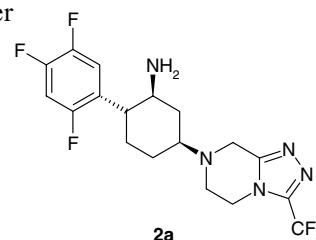
Steven W. Kortum,* Timothy E. Benson, Michael J. Bienkowski, Thomas L. Emmons, D. Bryan Prince, Donna J. Paddock, Alfredo G. Tomasselli, Joseph B. Moon, Alice LaBorde and Ruth E. TenBrink

The design and synthesis of a novel series of potent BACE1 hydroxyethylamine inhibitors. These inhibitors feature hydrogen bonding substituents at the C-5 position of the isophthalamide ring with improved selectivity over cathepsin D.

**Rational design of a novel, potent, and orally bioavailable cyclohexylamine DPP-4 inhibitor by application of molecular modeling and X-ray crystallography of sitagliptin** pp 3384–3387

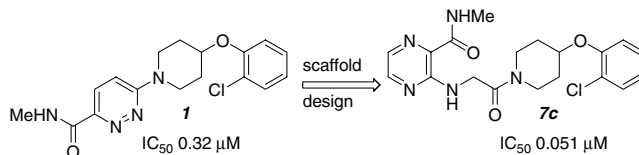
Tesfaye Biftu,* Giovanna Scapin, Suresh Singh, Dennis Feng, Joe W. Becker, George Eiermann, Huaibing He, Kathy Lyons, Sangita Patel, Aleksandr Petrov, Ranabir Sinha-Roy, Bei Zhang, Joseph Wu, Xiaoping Zhang, George A. Doss, Nancy A. Thornberry and Ann E. Weber

Molecular modeling was used to design a rigid analog of sitagliptin **1**. The X-ray crystal structure of sitagliptin bound to DPP-4 suggested that the central β -amino butyl amide moiety could be replaced with a cyclohexylamine group. This was confirmed by structural analysis and the resulting analog **2a** was synthesized and found to be a potent DPP-4 inhibitor ($IC_{50} = 21$ nM) with excellent in vivo activity and pharmacokinetic profile.



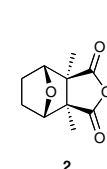
Discovery of 1-(4-phenoxy-piperidin-1-yl)-2-arylaminoethanone stearyl-CoA desaturase 1 inhibitors pp 3388–3391

Hongyu Zhao,* Michael D. Serby, Harriet T. Smith, Ning Cao, Tom S. Suhar, Teresa K. Surowy, Heidi S. Camp, Christine A. Collins, Hing L. Sham and Gang Liu

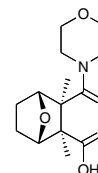
**Heterocyclic substituted cantharidin and norcantharidin analogues—synthesis, protein phosphatase (1 and 2A) inhibition, and anti-cancer activity** pp 3392–3397

Timothy A. Hill, Scott G. Stewart, Benjamin Sauer, Jayne Gilbert, Stephen P. Ackland, Jennette A. Sakoff and Adam McCluskey*

In this work, we report the first improvement in protein phosphatase inhibition by a cantharidin analogue. Compound **19** is approximately twice as potent as cantharidin against both PP1 and PP2A. Additionally **19** displays excellent broad spectrum cytotoxicity.



PP2A $IC_{50} = 1.2 \pm 0.1 \mu M$
PP1 $IC_{50} = 11.3 \pm 1.97 \mu M$

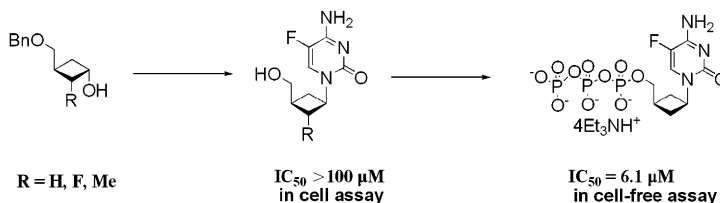


19
PP2A $IC_{50} = 0.79 \pm 0.1 \mu M$
PP1 $IC_{50} = 5.9 \pm 2.2 \mu M$

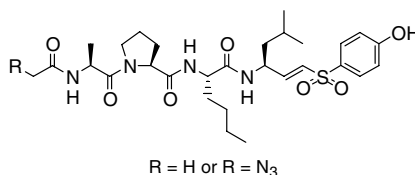
Synthesis and evaluation of 2'-substituted cyclobutyl nucleosides and nucleotides as potential anti-HIV agents pp 3398–3401

Yongfeng Li, Shuli Mao, Michael W. Hager, Kimberlynne D. Becnel, Raymond F. Schinazi and Dennis C. Liotta*

Several 2'-substituted cyclobutyl nucleosides were synthesized and evaluated as anti-HIV agents. Whereas the cyclobutyl nucleosides were not active against HIV in culture, the triphosphate forms were quite active against wild-type and mutant forms of HIV reverse transcriptase (RT).

**A cell-permeable inhibitor and activity-based probe for the caspase-like activity of the proteasome** pp 3402–3405

Paul F. van Swieten, Emllyn Samuel, Rosa Orient Hernández, Adrianus M. C. H. van den Nieuwendijk, Michiel A. Leeuwenburgh, Gijsbert A. van der Marel, Benedikt M. Kessler, Herman S. Overkleeft* and Alexei F. Kisselev*



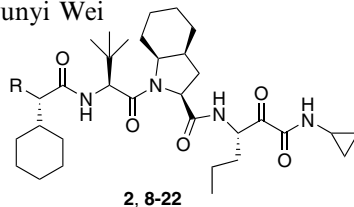
A subunit-specific proteasome inhibitor was developed and its specificity was assayed both by fluorescent substrate hydrolysis and by visualization of the targeted subunits via an activity-based probe approach.



Inhibitors of hepatitis C virus NS3-4A protease. Effect of P4 capping groups on inhibitory potency and pharmacokinetics

pp 3406–3411

Robert B. Perni,* Gurudatt Chandorkar, Kevin M. Cottrell, Cynthia A. Gates, Chao Lin, Kai Lin, Yu-Ping Luong, John P. Maxwell, Mark A. Murcko, Janos Pitlik, Govinda Rao, Wayne C. Schairer, John Van Drie and Yunyi Wei

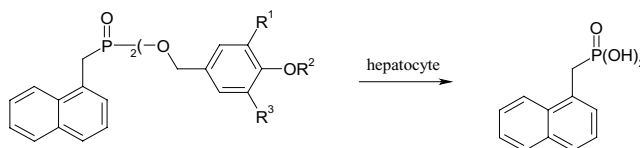


A series of tetrapeptide HCV NS3-4A protease inhibitors with varying P4 capping groups were prepared. The SAR and pharmacokinetic properties of these inhibitors are discussed.

Bis[(para-methoxy)benzyl] phosphonate prodrugs with improved stability and enhanced cell penetration

pp 3412–3416

Qun Dang,* Yan Liu, Robert M. Rydzewski, Brian S. Brown, Edward Robinson, Paul D. van Poelje, Timothy J. Colby and Mark D. Erion*



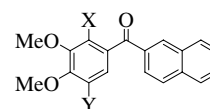
A series of bis[(para-methoxy)benzyl] phosphonate esters were synthesized and evaluated as phosphonate prodrugs. Two esters (**4b** and **4c**) were identified with significantly improved aqueous stability and enhanced penetration to primary rat hepatocytes.

Synthesis and biological activity of naphthalene analogues of phenstatins: Naphthylphenstatins

pp 3417–3420

Concepción Álvarez, Raquel Álvarez, Purificación Corchete, Concepción Pérez-Melero, Rafael Peláez* and Manuel Medarde*

The synthesis and biological activity of a new family of phenstatin analogues, carrying a 2-naphthyl moiety, is reported. Compound **7** ($IC_{50}[TPI] = 1.1 \mu M$) is more potent than combretastatin A4 ($IC_{50}[TPI] = 3 \mu M$) in tubulin polymerization inhibition assays (TPI). The replacement of the 3-hydroxy-4-methoxyphenyl ring by a 2-naphthyl system is more favourable in the phenstatin than in the combretastatin series.

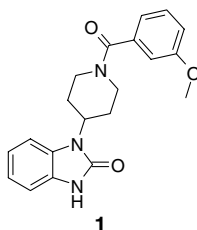


Naphthylphenstatins
 X or Y = MeO
7 X = H, Y = OMe
 IC_{50} (TPI) = 1.1 μM

**Piperidine amides as 11 β -hydroxysteroid dehydrogenase type 1 inhibitors**

pp 3421–3425

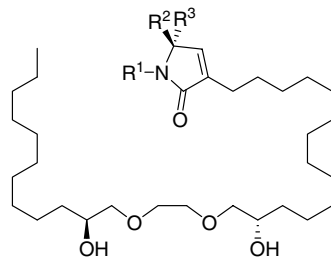
Katarina Flyrén,* Lars O. Bergquist, Victor M. Castro, Christopher Fotsch, Lars Johansson, David J. St. Jean, Jr., Lori Sutin and Meredith Williams



Compound **1** was identified as a potent 11 β -HSD1 inhibitor in a HTS screen. Synthesis and inhibitory potency of analogs to **1** are reported.

Annonaceous acetogenin mimics bearing a terminal lactam and their cytotoxicity against cancer cells pp 3426–3430

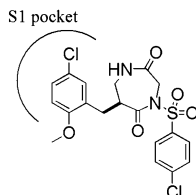
Hai-Xia Liu, Guo-Rui Huang, Huan-Ming Zhang, Jia-Rui Wu* and Zhu-Jun Yao*



A new series of annonaceous acetogenin mimics containing a terminal lactam were designed, synthesized, and evaluated.

Identification of 6-substituted 4-arylsulfonyl-1,4-diazepane-2,5-diones as a novel scaffold for human chymase inhibitors pp 3431–3434

Taisaku Tanaka,* Tsuyoshi Muto,* Hiroshi Maruoka, Seiichi Imajo, Harukazu Fukami, Yoshiaki Tomimori, Yoshiaki Fukuda and Takashi Nakatsuka

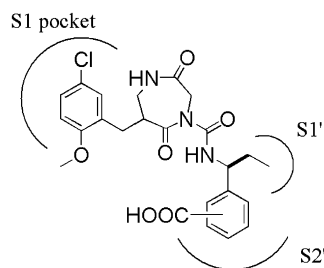


A novel series of 6-substituted 4-sulfonyl-1,4-diazepane-2,5-diones were designed, synthesized, and evaluated as human chymase inhibitors. Structure–activity relationship studies led to the identification of a potent inhibitor, (6*S*)-6-(5-chloro-2-methoxybenzyl)-4-[(4-chlorophenyl)sulfonyl]-1,4-diazepane-2,5-dione, with an IC_{50} of 0.027 μ M.

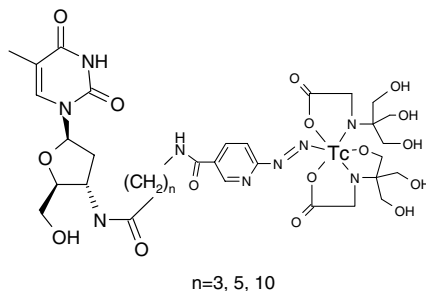
Development of 6-benzyl substituted 4-aminocarbonyl-1,4-diazepane-2,5-diones as orally active human chymase inhibitors pp 3435–3439

Hiroshi Maruoka,* Tsuyoshi Muto,* Taisaku Tanaka, Seiichi Imajo, Yoshiaki Tomimori, Yoshiaki Fukuda and Takashi Nakatsuka

A novel series of 6-benzyl substituted 4-aminocarbonyl-1,4-diazepane-2,5-diones was designed, synthesized, and evaluated as human chymase inhibitors. From this series, we identified several compounds which were effective, via oral administration, in a mouse model of chronic dermatitis.

**Technetium-99m-labeling and synthesis of thymidine analogs: Potential candidates for tumor imaging** pp 3440–3444

Bao Teng, Yunpeng Bai, Yu Chang, Shizhen Chen and Zhaolong Li*



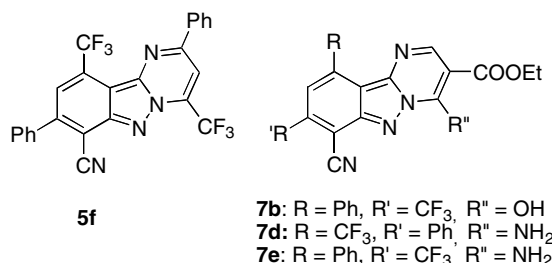
The synthesis and labeling of a series of thymidine analogs were reported.



Synthesis and structure–activity relationships of novel pyrimido[1,2-*b*]indazoles as potential anticancer agents against A-549 cell lines

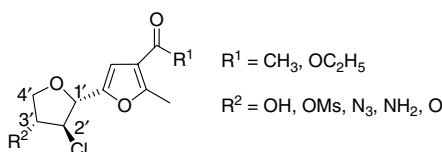
pp 3445–3453

T. Yakaiah, B. P. V. Lingaiah, B. Narsaiah,* B. Shireesha, B. Ashok Kumar, S. Gururaj, T. Parthasarathy and B. Sridhar

**Synthesis of furanosyl α -C-glycosides derived from 4-chloro-4-deoxy- α -D-galactose and their cytotoxic activities**

pp 3454–3457

Lin Yan, Gui-Fu Dai, Jian-Li Yang, Feng-Wu Liu and Hong-Min Liu*



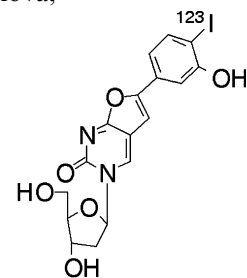
Some new furanosyl α -C-glycoside derivatives were synthesized and tested for in vitro cytotoxicity against human lung adenocarcinoma cell lines.

Synthesis and biological evaluation of an ¹²³I-labeled bicyclic nucleoside analogue (BCNA) as potential SPECT tracer for VZV-tk reporter gene imaging

pp 3458–3462

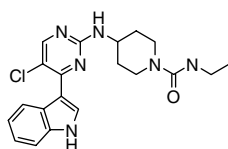
Satish K. Chitneni, Christophe M. Deroose, Humphrey Fonge, Rik Gijssbers, Natalia Dyubankova, Jan Balzarini, Zeger Debyser, Luc Mortelmans, Alfons M. Verbruggen and Guy M. Bormans*

An ¹²³I-labeled BCNA that has good affinity for VZV-TK (IC₅₀: 4.2 μ M) is synthesized and evaluated.

**Synthesis and SAR of aminopyrimidines as novel c-Jun N-terminal kinase (JNK) inhibitors**

pp 3463–3467

Mahbub Alam, Rebekah E. Beevers, Tom Ceska, Richard J. Davenport, Karen M. Dickson, Mara Fortunato, Lewis Gowers, Alan F. Haughan, Lynwen A. James, Mark W. Jones, Natasha Kinsella,* Christopher Lowe, Johannes W. G. Meissner, Anne-Lise Nicolas, Benjamin G. Perry, David J. Phillips, William R. Pitt, Adam Platt, Andrew J. Ratcliffe, Andrew Sharpe and Laura J. Tait

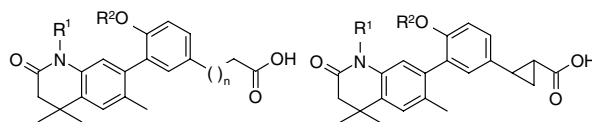


A series of novel aminopyrimidines is reported which exhibits JNK1 and JNK2 inhibitory activity.

Dihydro-[1H]-quinolin-2-ones as retinoid X receptor (RXR) agonists for potential treatment of dyslipidemia

pp 3491–3496

Bharat Lagu,* Rimma Lebedev, Barbara Pio, Maria Yang and Patricia D. Pelton

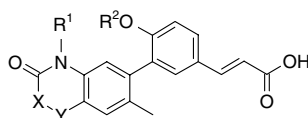


A number of RXR modulators with novel structural features were synthesized and screened in the functional assays. The synthesis and the structure–activity relationship within the series of compounds will be presented. Some in vivo data generated in the models for dyslipidemia and diabetes will also be presented.

RXR–LXR heterodimer modulators for the potential treatment of dyslipidemia

pp 3497–3503

Bharat Lagu,* Barbara Pio, Rimma Lebedev, Maria Yang and Patricia D. Pelton

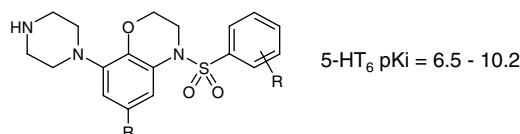


A number of RXR agonists were synthesized and screened in functional assays. The synthesis and the structure–activity relationship (SAR) within the series of compounds will be presented. Some in vivo data in rodent models for dyslipidemia and diabetes will also be presented.

3,4-Dihydro-2H-benzo[1,4]oxazine derivatives as 5-HT₆ receptor antagonists

pp 3504–3507

Shu-Hai Zhao,* Jacob Berger, Robin D. Clark, Steven G. Sethofer, Nancy E. Krauss, Julie M. Brothers, Renee S. Martin, Dinah L. Misner, Dietmar Schwab and Ludmila Alexandrova

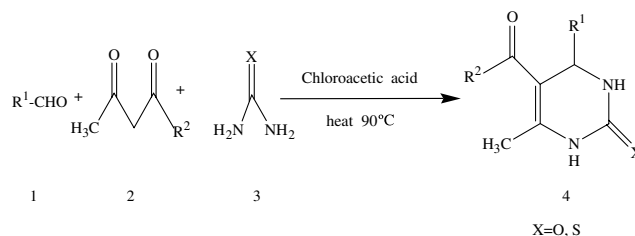


The synthesis and structure–activity relationships of a series of 3,4-dihydro-2H-benzo[1,4]oxazine based 5-HT₆ antagonists are described.

One-pot synthesis of 3,4-dihydropyrimidin-2(1H)-ones using chloroacetic acid as catalyst

pp 3508–3510

Yang Yu, Di Liu, Chunsheng Liu and Genxiang Luo*

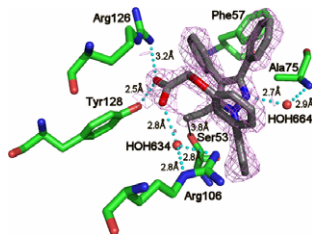


A simple and effective synthesis of 3,4-dihydropyrimidin-2(1H)-one derivatives from aldehydes, 1,3-dicarbonyl compounds and urea or thiourea using chloroacetic acid as catalyst under solvent-free conditions is reported.

Potent and selective biphenyl azole inhibitors of adipocyte fatty acid binding protein (aFABP)

pp 3511–3515

Richard Sulsky,* David R. Magnin, Yanting Huang, Ligaya Simpkins, Prakash Taunk, Manorama Patel, Yeheng Zhu, Terry R. Stouch, Donna Bassolino-Klimas, Rex Parker, Thomas Harrity, Robert Stoffel, David S. Taylor, Thomas B. Lavoie, Kevin Kish, Bruce L. Jacobson, Steven Sheriff, Leonard P. Adam,* William R. Ewing and Jeffrey A. Robl



X-ray crystal structure of an FABP inhibitor bound to the active site of aFABP.

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Summary of instructions to authors

p I

*Corresponding author

①⁺ 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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