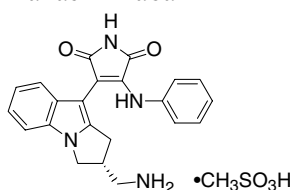


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ARTICLES

- Synthesis, SAR studies, and pharmacological evaluation of 3-anilino-4-(3-indolyl) maleimides with conformationally restricted structure as orally bioavailable PKC β -selective inhibitors** pp 5781–5794

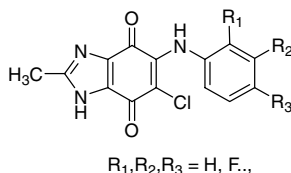
Masahiro Tanaka, Shoichi Sagawa, Jun-ichi Hoshi, Fumito Shimoma, Katsutaka Yasue, Minoru Ubukata, Tomoyuki Ikemoto, Yasunori Hase, Mitsuru Takahashi, Tomohiko Sasase, Nobuhisa Ueda, Mutsuyoshi Matsushita and Takashi Inaba*



IC₅₀ values (nM (at isozymes)): 4.0 (β 1), 2.3 (β 2), 86 (α), 110 (γ), 54 (δ), 490 (ϵ), 1700 (ζ), 1000 (μ)

- Synthesis and biological evaluation of 5-arylamino-1*H*-benzo[d]imidazole-4,7-diones as inhibitor of endothelial cell proliferation** pp 5795–5801

Kwang-Hoe Chung, Sung-Yu Hong, Hea-Jung You, Rae-Eun Park and Chung-Kyu Ryu*

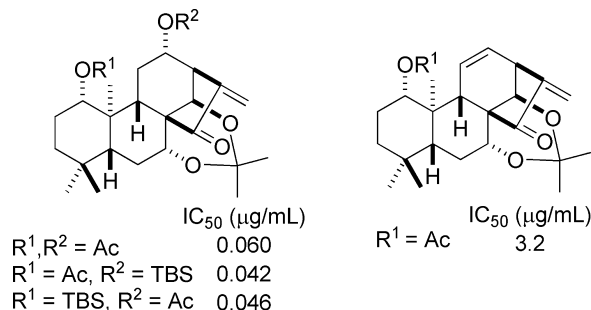


5-Arylamino-1*H*-benzo[d]imidazole-4,7-diones were synthesized and tested for their inhibitory activities on the proliferation of human umbilical vein endothelial cells. Among them, several 1*H*-benzo[d]imidazole-4,7-diones exhibited potent antiproliferative activity.

- Synthesis of 1-*O*-monoacyl or 12-*O*-monoacyl, 1-,12-*O*-diacyl-, and 11,12-dehydrated excisanin A 7,14-acetonides and their cytotoxic activity** pp 5802–5811

Yutaka Aoyagi, Yumi Nishioka, Fukuya Tobe, Tomoyo Hasuda, Koichi Takeya,*
Ming-Yu Gui, Yong-Ri Jin and Xu-Wen Li

1-*O*-Monoacyl, 12-*O*-monoacyl, 1-,12-*O*-diacyl, and 11,12-dehydrated excisanin A 7,14-acetonides were synthesized from excisanin A isolated from *Rabdosia excisa*. The structure and cytotoxic activity relationships (SAR) of the natural parent *ent*-kaurene diterpenes and these semisynthetic analogues were studied by using P388 murine leukemia cells.

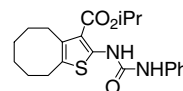


A new class of small molecule RNA polymerase inhibitors with activity against Rifampicin-resistant *Staphylococcus aureus*

pp 5812–5832

Francis Arhin, Odette Bélanger, Stéphane Ciblat, Mohammed Dehbi, Daniel Delorme, Evelyne Dietrich, Dilip Dixit, Yanick Lafontaine, Dario Lehoux, Jing Liu, Geoffrey A. McKay, Greg Moeck, Ranga Reddy, Yannick Rose, Ramakrishnan Srikumar, Kelly S.E. Tanaka, Daniel M. Williams, Philippe Gros, Jerry Pelletier, Thomas R. Parr and Adel Rafai Far*

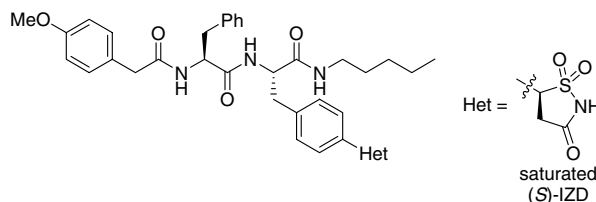
The structure–activity relationships around a *Staphylococcus aureus* RNA polymerase inhibitor in terms of inhibitory and antibacterial activities are presented. The antibacterial activity of selected members of this class of compounds, including some nanomolar inhibitors of the polymerase, is characterized. Several features of this class of compounds as antibacterials are highlighted.



Isothiazolidinone heterocycles as inhibitors of protein tyrosine phosphatases: Synthesis and structure–activity relationships of a peptide scaffold

pp 5833–5849

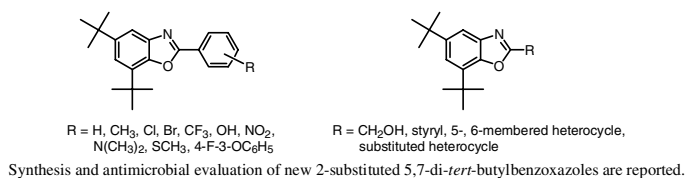
Eddy W. Yue,* Brian Wayland, Brent Douty, Matthew L. Crawley, Erin McLaughlin, Amy Takvorian, Zelda Wasserman, Michael J. Bower, Min Wei, Yanlong Li, Paul J. Ala, Lucie Gonneville, Richard Wynn, Timothy C. Burn, Phillip C.C. Liu and Andrew P. Combs



Synthesis and antimicrobial evaluation of new 2-substituted 5,7-di-*tert*-butylbenzoxazoles

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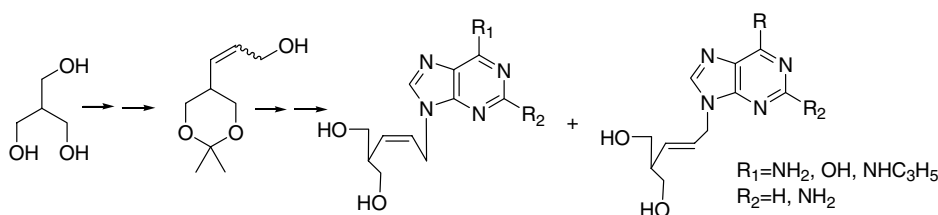
Jarmila Vinsova,* Katerina Cermakova, Alexandra Tomeckova, Martina Ceckova, Josef Jampilek, Pavel Cermak, Jiri Kunes, Martin Dolezal and Frantisek Staud



Synthesis and biological evaluation of carboacyclic nucleosides with (*Z*) and (*E*)-9-[4,4-bis(hydroxymethyl)]-2-butenyl side chain

pp 5866–5875

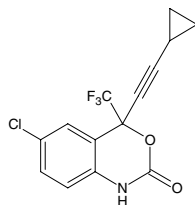
Ye Tang, Ramaiah Muthyala* and Robert Vince*



A series of carboacyclic nucleosides with (*Z*) and (*E*)-9-[4,4-bis(hydroxy-methyl)]-2-butenyl side chains were synthesized as potential antiviral compounds.

QSAR for non-nucleoside inhibitors of HIV-1 reverse transcriptase

pp 5876–5889

Pablo R. Duchowicz,* Michael Fernández, Julio Caballero,
Eduardo A. Castro and Francisco M. Fernández

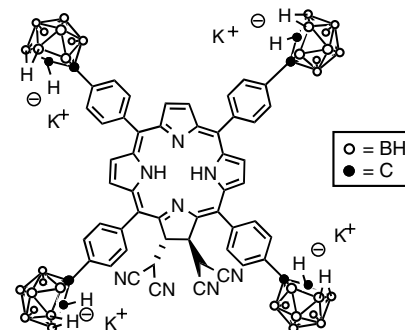
QSAR modeling the inhibitory potency pIC_{90} [mM] of 154 NNRTI of wild-type HIV-1 RT and 56 NNRTI of K-103N mutant form, using forward stepwise regression, the replacement method, and genetic algorithms. Different parallelisms are argued between the activities and the optimal molecular descriptors. Inhibition = function (molecular structural descriptors).

Synthesis and cellular studies of a carboranylchlorin for the PDT and BNCT of tumors

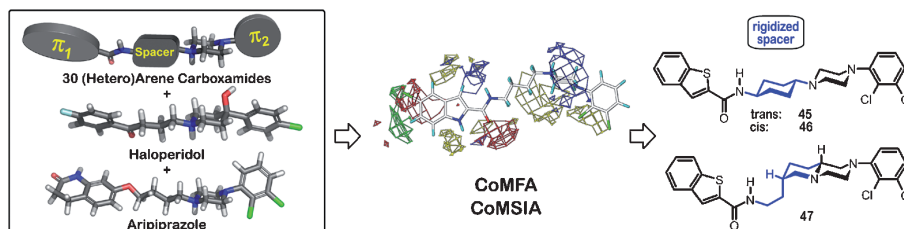
pp 5890–5897

Raymond Luguya, Timothy J. Jensen, Kevin M. Smith and M. Graça H. Vicente*

The syntheses of a water-soluble carboranylchlorin are described. This compound has low dark cytotoxicity but is toxic in the presence of light. The new carboranylchlorin is efficiently taken up by T98G cells and it localizes intracellularly preferentially within the lysosomes.

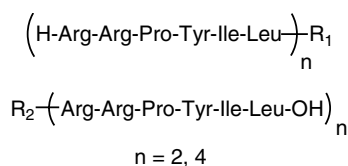
**CoMFA and CoMSIA investigations of dopamine D3 receptor ligands leading to the prediction, synthesis, and evaluation of rigidized FAUC 365 analogues**

pp 5898–5912

Ismail Salama, Karin Schlotter, Wolfgang Utz, Harald Hübner,
Peter Gmeiner and Frank Boeckler***Synthesis and evaluation of novel multimeric neurotensin(8–13) analogs**

pp 5913–5920

Christina Hultsch, Beate Pawelke, Ralf Bergmann and Frank Wuest*



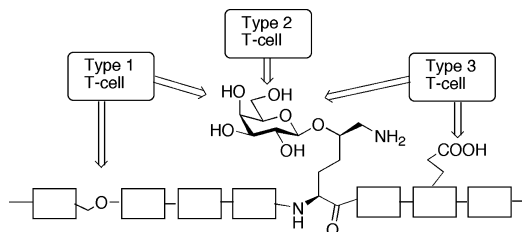
Different dimeric and tetrameric neurotensin(8–13) derivatives containing a lysine (R_1) or a glutamic acid (R_2) core unit were synthesized and evaluated concerning their binding affinity toward the neurotensin receptor.



Side-chain and backbone amide bond requirements for glycopeptide stimulation of T-cells obtained in a mouse model for rheumatoid arthritis

pp 5921–5932

Lotta Holm, Robert Bockermann, Erik Wellner, Johan Bäcklund, Rikard Holmdahl and Jan Kihlberg*

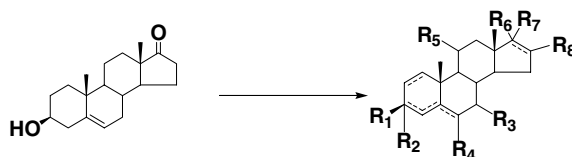


Alanine substituted glycopeptide based on the immunodominant type II collagen epitope, and a methylene ether amide bond isomer was used to probe the T-cell contact points needed for T-cell stimulation.

C₁₉-Steroids as androgen receptor modulators: Design, discovery, and structure-activity relationship of new steroidal androgen receptor antagonists

pp 5933–5947

Padma Marwah, Ashok Marwah, Henry A. Lardy,* Hiroshi Miyamoto and Chawnsang Chang

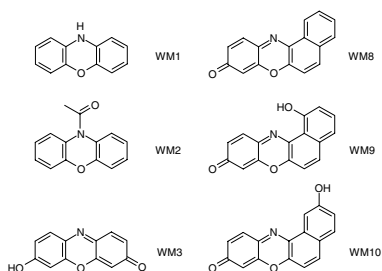


Synthesis and evaluation of a variety of C₁₉-steroids in prostate cancer cell lines. Three steroids were identified that antagonized the effects of DHT and Adiol on the androgen receptor transactivation.

A study on the perturbation of model lipid membranes by phenoxazines

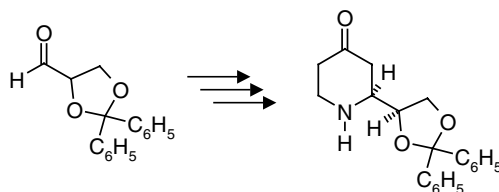
pp 5948–5954

Andrzej B. Hendrich,* Kamila Stańczak, Małgorzata Komorowska, Noboru Motohashi, Masami Kawase and Krystyna Michalak


Synthesis and NMDA-receptor affinity of 4-oxo-dexoxadrol derivatives

pp 5955–5962

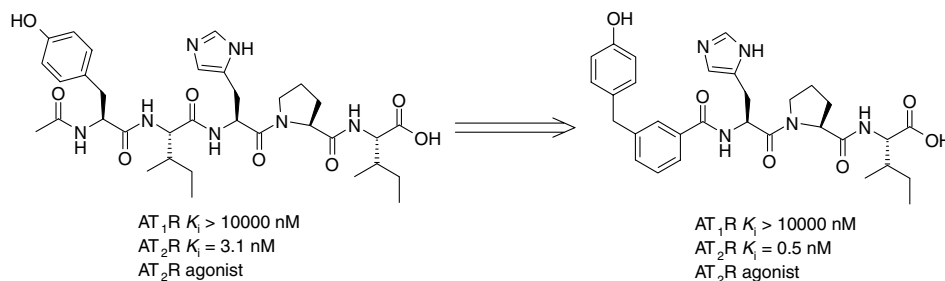
Michael Sax, Kirstin Ebert, Dirk Schepmann, Birgit Wibbeling and Bernhard Wünsch*



Short pseudopeptides containing turn scaffolds with high AT₂ receptor affinity

pp 5963–5972

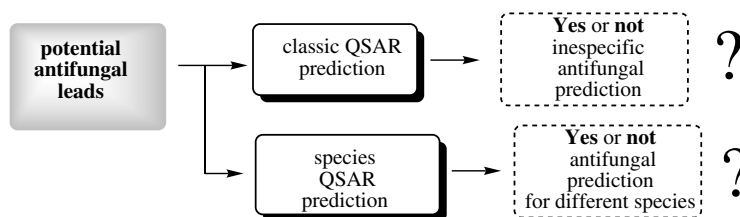
Jennie Georgsson, Ulrika Rosenström, Charlotta Wallinder, Hélène Beaudry, Bianca Plouffe, Gunnar Lindeberg, Milad Botros, Fred Nyberg, Anders Karlén, Nicole Gallo-Payet* and Anders Hallberg*



Unify QSAR approach to antimicrobials. Part 1: Predicting antifungal activity against different species

pp 5973–5980

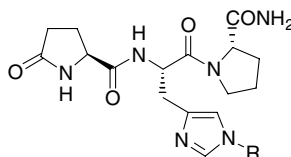
Humberto González-Díaz,* Francisco J. Prado-Prado, Lourdes Santana and Eugenio Uriarte



Synthesis, receptor binding, and activation studies of N(1)-alkyl-L-histidine containing thyrotropin-releasing hormone (TRH) analogues

pp 5981–5988

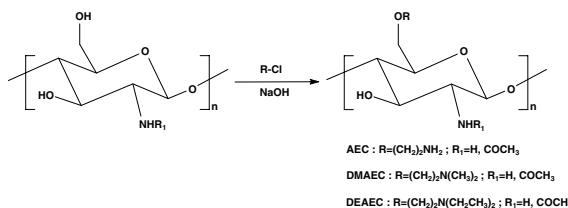
Navneet Kaur, Vikramdeep Monga, Jatinder S. Josan, Xiping Lu, Marvin C. Gershengorn and Rahul Jain*



Reactive oxygen species scavenging activity of aminoderivatized chitosan with different degree of deacetylation

pp 5989–5994

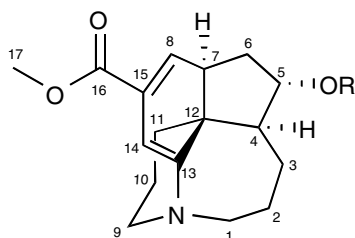
Jae-Young Je and Se-Kwon Kim*



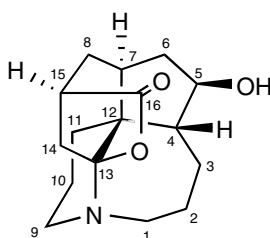
Lycopladienes B–D and lyconadin B, new alkaloids from *Lycopodium complanatum*

pp 5995–6000

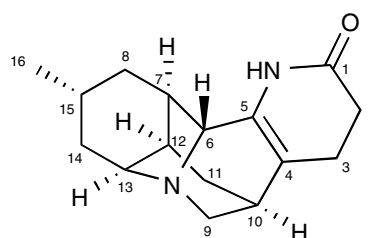
Kan'ichiro Ishiuchi, Takaaki Kubota, Tomohiro Hoshino, Yutaro Obara,
Norimichi Nakahata and Jun'ichi Kobayashi*



lycopladiene B : R = H
lycopladiene C : R = Ac



lycopladiene D



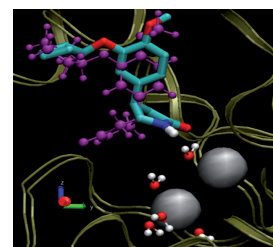
lyconadin B

Molecular docking study and development of an empirical binding free energy model for phosphodiesterase 4 inhibitors

pp 6001–6011

Fernanda G. Oliveira, Carlos M. R. Sant'Anna, Ernesto R. Caffarena,
Laurent E. Dardenne and Eliezer J. Barreiro*

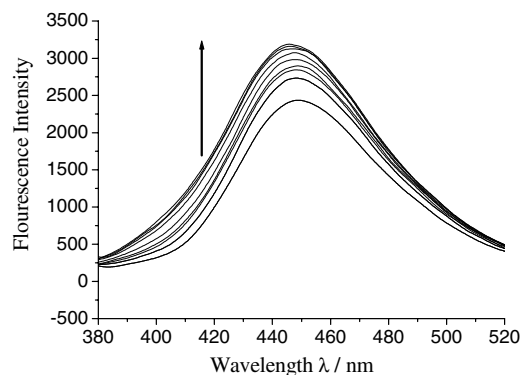
Molecular docking, molecular dynamics, and semiempirical quantum calculations were combined to develop an empirical free energy model for the prediction of PDE4B inhibitors' activity.

**Synthesis, characterization, and DNA-binding properties of the Ln(III) complexes with 6-hydroxy chromone-3-carbaldehyde-(2'-hydroxy) benzoyl hydrazone**

pp 6012–6021

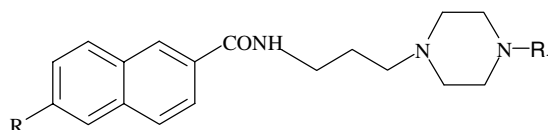
Bao-dui Wang, Zheng-Yin Yang* and Tian-rong Li

6-Hydroxy chromone-3-carbaldehyde-(2'-hydroxy) benzoyl hydrazone and its Ln(III) complexes have been prepared and characterized. The intrinsic binding constants of Eu(III) complex and ligand with DNA were 3.55×10^6 and $1.33 \times 10^6 \text{ M}^{-1}$, respectively. All the compounds have shown considerable antioxidant activity, and the suppression rate of the complexes tested are higher than that of the ligand itself.

**Design, synthesis and evaluation of naphthalene-2-carboxamides as reversal agents in MDR cancer**

pp 6022–6026

Tushar N. Lokhande,* C. L. Viswanathan, Advait Joshi and Aarti Juvekar

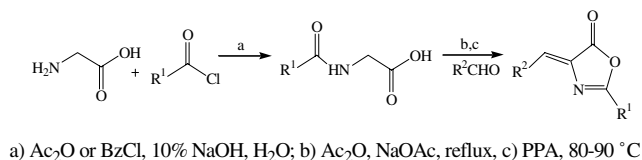


Novel six compounds with structure *N*-[3-(4-substituted-1-piperazinyl) propyl]-6-methoxy naphthalene-2-carboxamides were designed, synthesized, and evaluated for MDR reversal activity by MTT assay. Test compounds reversed adriamycin resistance and compounds **2**, **3**, and **5** exhibited better activity as compared to Verapamil.

Oxazolones: New tyrosinase inhibitors; synthesis and their structure–activity relationships

pp 6027–6033

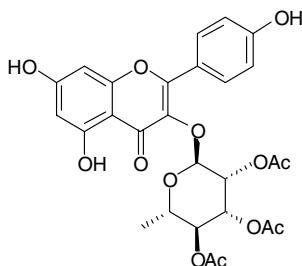
Khalid Mohammed Khan,* Uzma Rasool Mughal, Mahmud Tareq Hassan Khan, Zia-Ullah, Shahnaz Perveen and Muhammad Iqbal Choudhary



Seventeen oxazolone derivatives were synthesized, characterized, and screened for tyrosinase inhibition.

Influence of rhamnose substituents on the potency of SL0101, an inhibitor of the Ser/Thr kinase, RSK pp 6034–6042

Jeffrey A. Smith, David J. Maloney, David E. Clark, Yaming Xu, Sidney M. Hecht and Deborah A. Lannigan*

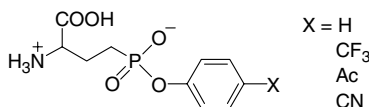


3Ac-SL0101, a specific inhibitor of RSK activity, selectively reduces the growth of human breast cancer cells.

γ-(Monophenyl)phosphono glutamate analogues as mechanism-based inhibitors of γ-glutamyl transpeptidase

pp 6043–6054

Liyoun Han, Jun Hiratake,* Norihito Tachi, Hideyuki Suzuki, Hidehiko Kumagai and Kanzo Sakata

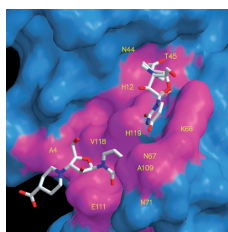


A series of hydrolytically stable monophenyl phosphonoates has been synthesized and found to serve as irreversible and mechanism-based inhibitors of *Escherichia coli* and human γ-glutamyl transpeptidase.

The binding of 3'-N-piperidine-4-carboxyl-3'-deoxy-*ara*-uridine to ribonuclease A in the crystal

pp 6055–6064

Demetres D. Leonidas,* Tushar Kanti Maiti, Anirban Samanta, Swagata Dasgupta, Tanmaya Pathak, Spyros E. Zographos and Nikos G. Oikonomakos

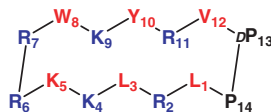


The binding of 3'-N-piperidine-4-carboxyl-3'-deoxy-*ara*-uridine to ribonuclease A, a member of a novel class of ribonucleolytic inhibitors, has been studied by X-ray crystallography at 1.7 Å resolution.

QSAR analysis of antimicrobial and haemolytic effects of cyclic cationic antimicrobial peptides derived from protegrin-1

pp 6065–6074

Vladimir Frečer*

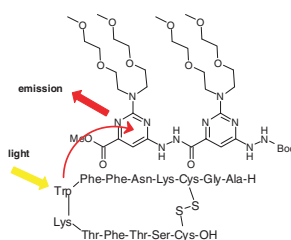


In this paper, we quantitatively analyse antimicrobial and haemolytic activities of porcine protegrin-1 mimetics—cyclic cationic peptides with β -hairpin fold synthesised by Robinson et al. [*Bioorg. Med. Chem.* **2005**, *13*, 2055] The presented QSAR models, which use molecular properties related to possible mechanisms of cell membrane disruption that can be easily calculated from readily available data on amino acids, rationalize the relationships between sequences and antimicrobial and haemolytic potencies of the peptides.

Luminescent pyrimidine hydrazide oligomers with peptide affinity

pp 6075–6084

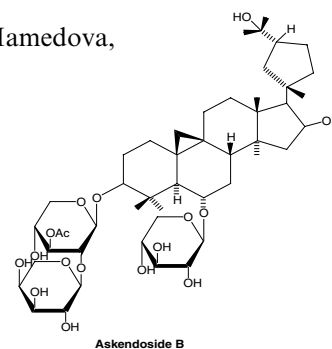
Xiaoqiang Li, Stefan Miltschitzky and Burkhard König*



Tyrosinase inhibition studies of cycloartane and cucurbitane glycosides and their structure–activity relationships

pp 6085–6088

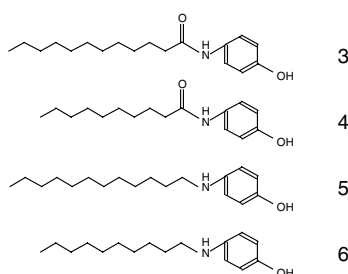
Mahmud Tareq Hassan Khan,* M. Iqbal Choudhary, Atta-ur-Rahman, Reyhan P. Mamedova, Manzura A. Agzamova, Mukhlis N. Sultankhodzhaev and Mahamed I. Isaev



Antioxidant and anticancer activities of novel *p*-alkylaminophenols and *p*-acylaminophenols (aminophenol analogues)

pp 6089–6096

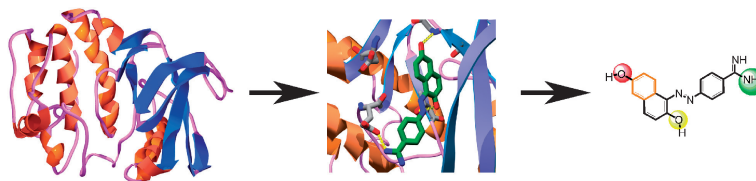
Noriko Takahashi,* Toshihiro Ohba, Takayasu Yamauchi and Kimio Higashiyama



Homology model of RSK2 N-terminal kinase domain, structure-based identification of novel RSK2 inhibitors, and preliminary common pharmacophore

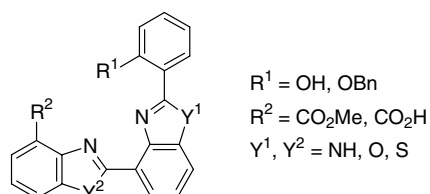
pp 6097–6105

Tam Luong Nguyen,* Rick Gussio, Jeffrey A. Smith, Deborah A. Lannigan, Sidney M. Hecht, Dominic A. Scudiero, Robert H. Shoemaker and Daniel W. Zaharevitz

**Synthesis and anticancer evaluation of bis(benzimidazoles), bis(benzoxazoles), and benzothiazoles**

pp 6106–6119

Shu-Ting Huang, I-Jen Hsei and Chinpiao Chen*

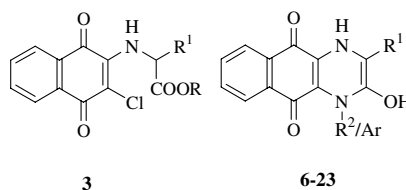


The syntheses of nineteen bis(benzimidazoles), bis(benzoxazoles), benzothiazoles, and their derivatives are described, and their *in vitro* antitumor activities (Against A-549, BFTC-905, RD, MES-SA, and HeLa cell lines) are evaluated.

Design, synthesis, and biological evaluation of 1,2,3-trisubstituted-1,4-dihydrobenzo[g]quinoxaline-5,10-diones and related compounds as antifungal and antibacterial agents

pp 6120–6126

Vishnu K. Tandon,* Dharmendra B. Yadav, Hardesh K. Maurya, Ashok K. Chaturvedi and Praveen K. Shukla



The synthesis, antifungal, and antibacterial activities of **3–23** are described.

OTHER CONTENTS**Summary of instructions to authors**

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*Corresponding author

+ Supplementary data available via ScienceDirect

COVER

Collagen induced arthritis is a common mouse model for rheumatoid arthritis. Presentation of a glycopeptide fragment from type II collagen by MHC molecules on antigen presenting cells (APCs) for recognition by T cell receptors (TCRs) is a key step in induction of disease. The roles of individual glycopeptide side-chains, in particular galactosylated hydroxylysine 264 and glutamic acid 266, as well as one of the amide bonds for T cell recognition has now been established. [Holm, L.; Bockermann, R.; Wellner, E.; Bäcklund, J.; Holmdahl, R. and Kihlberg, J. *Bioorg. Med. Chem.* **2006**, *15*, 5921.]



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