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Symposium-in-Print

Tetrahedron Young Investigator Award 2010 Peter Seeberger

Edited by: Prof. Herbert Waldmann

Max-Planck-Institute for Molecular Physiology, Dept of Chemical Biology, Otto-Hahn-Strasse 11, 44227 Dortmund, Germany

Contents

Preface

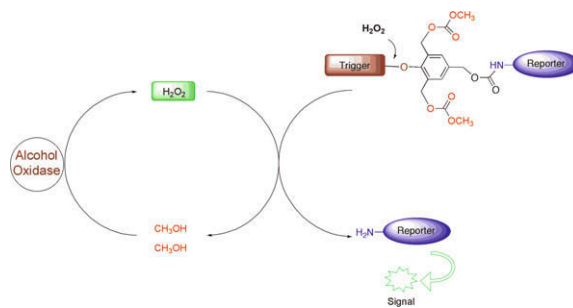
p 3642

SPECIAL ISSUE ARTICLES

Dendritic chain reaction: Responsive release of hydrogen peroxide upon generation and enzymatic oxidation of methanol

pp 3643–3647

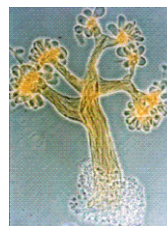
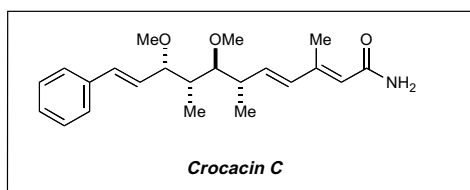
Michal Avital-Shmilovici, Doron Shabat*



Total synthesis of (+)-crocacin C

pp 3648–3655

Gopal Sirasani, Tapas Paul, Rodrigo B. Andrade*

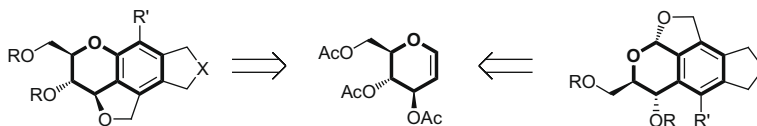


Chondromyces crocatus

Hybrids of sugars and aromatics: A Pd-catalyzed modular approach to chromans and isochromans

pp 3656–3667

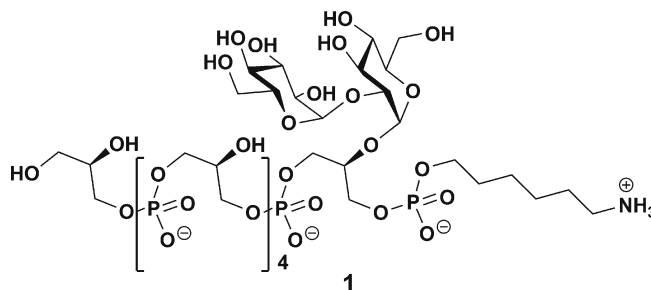
Markus Leibeling, Dennis C. Koester, Martin Pawliczek, Daniel Kratzert, Birger Dittrich, Daniel B. Werz*



Synthesis of an α -kojibiosyl substituted glycerol teichoic acid hexamer

pp 3668–3678

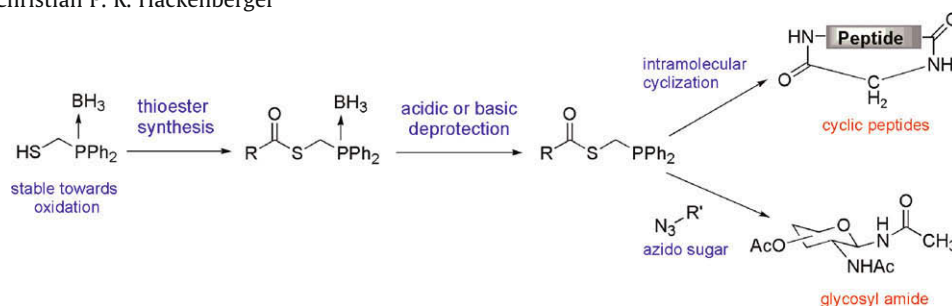
Wouter F. J. Hogendorf, Leendert J. Van den Bos, Herman S. Overkleeft, Jeroen D. C. Codée*, Gijsbert A. Van der Marel*



Acidic and basic deprotection strategies of borane-protected phosphinothioesters for the traceless Staudinger ligation

pp 3679–3686

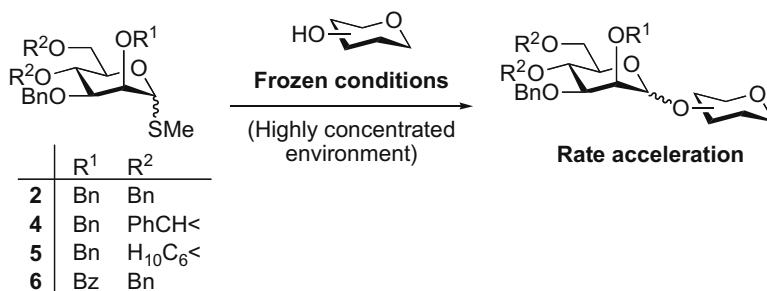
Michaela Mühlberg, Da'san M. M. Jaradat, Rolf Kleineweischede, Ilona Papp, Decha Dechtrirat, Silvia Muth, Malgorzata Broncel, Christian P. R. Hackenberger*



Effects of frozen conditions on stereoselectivity and velocity of O-glycosylation reactions

pp 3687–3695

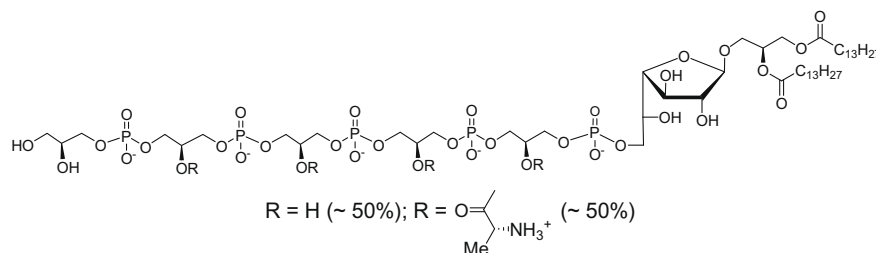
Akihiro Ishiwata*, Ayaka Sakurai, Katharina Dürr, Yukishige Ito*



Synthesis of the lipoteichoic acid of the *Streptococcus* species DSM 8747

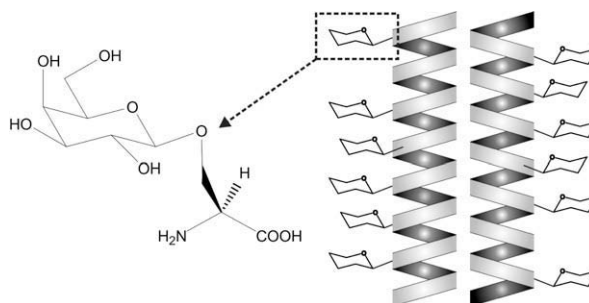
pp 3696–3702

Yan Qiao, Buko Lindner, Ulrich Zähringer, Peter Truog, Richard R. Schmidt*

**Multiple glycosylation of de novo designed α -helical coiled coil peptides**

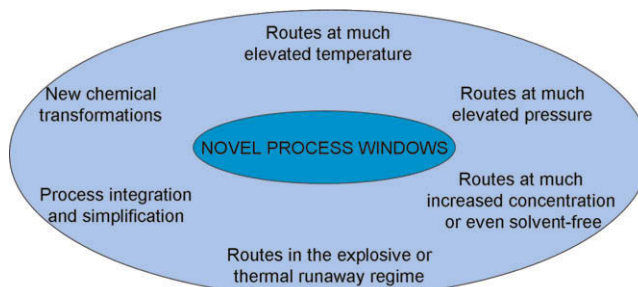
pp 3703–3706

Jessica A. Falenski, Ulla I. M. Gerling, Beate Kokschi*

**Flow chemistry using milli- and microstructured reactors—From conventional to novel process windows**

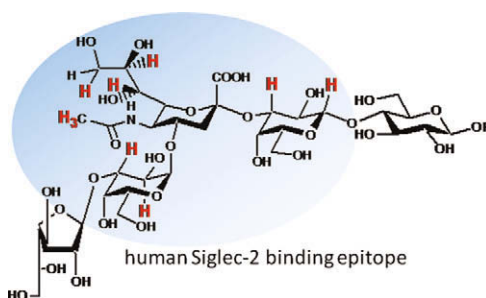
pp 3707–3719

Tobias Illg, Patrick Löb, Volker Hessel*

**Synthesis and binding analysis of unique AG2 pentasaccharide to human Siglec-2 using NMR techniques**

pp 3720–3725

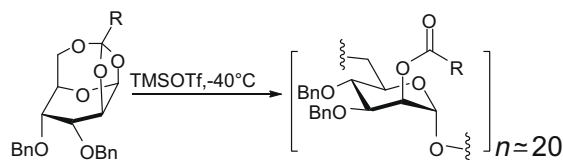
Shinya Hanashima, Ken-ichi Sato, Yuko Naito, Hiromu Takematsu, Yasunori Kozutsumi, Yukishige Ito, Yoshiki Yamaguchi*



Polymerization of mannosyl tricyclic orthoesters for the synthesis of $\alpha(1-6)$ mannopyranan—the backbone of lipomannan

pp 3726–3734

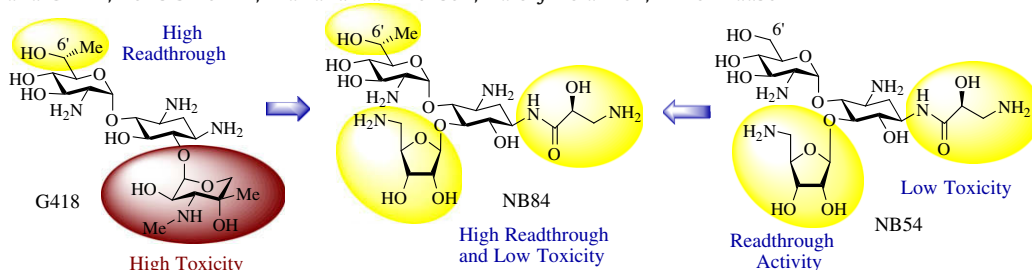
Chanokpon Yongyat, Somsak Ruchirawat, Siwarutt Boonyarattanakalin*



Repairing faulty genes by aminoglycosides: Development of new derivatives of geneticin (G418) with enhanced suppression of diseases-causing nonsense mutations

pp 3735–3746

Igor Nudelman, Dana Glikin, Boris Smolkin, Mariana Hainrichson, Valery Belakhov, Timor Baasov*



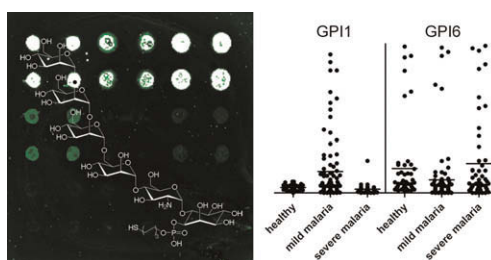
Introduction of (*R*)-6'-methyl group of the aminoglycoside G418 onto the recent lead NB54, lead to the development of the new compound NB84 exhibiting significantly improved readthrough activity and reduced toxicity.



Synthetic glycosylphosphatidylinositol microarray reveals differential antibody levels and fine specificities in children with mild and severe malaria

pp 3747–3752

Marco Tamborrini, Xinyu Liu, Joseph Paschal Mugasa, Yong-Uk Kwon, Faustin Kamena, Peter H. Seeberger, Gerd Pluschke*

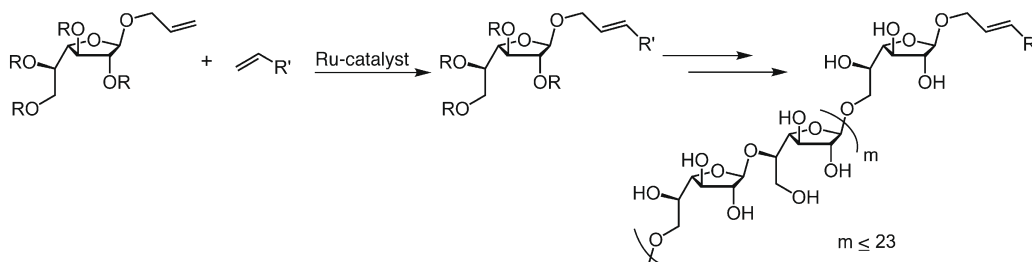


A carbohydrate microarray spotted with synthetic GPI-glycans provides insights into the anti-malarial antibody response in healthy and malaria diseased individuals.

Synthesis of galactofuranose-based acceptor substrates for the study of the carbohydrate polymerase GltT2

pp 3753–3759

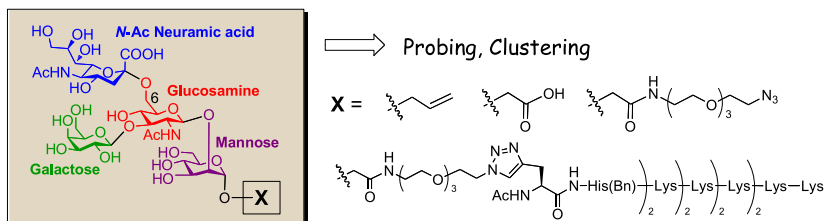
Rebecca A. Splain, Laura L. Kiessling*



Probe design and synthesis of Gal β (1 \rightarrow 3)[NeuAc α (2 \rightarrow 6)]GlcNAc β (1 \rightarrow 2)Man motif of N-glycan

pp 3760–3766

Guang-ming Bao, Katsunori Tanaka, Kazuhiro Ikenaka, Koichi Fukase*

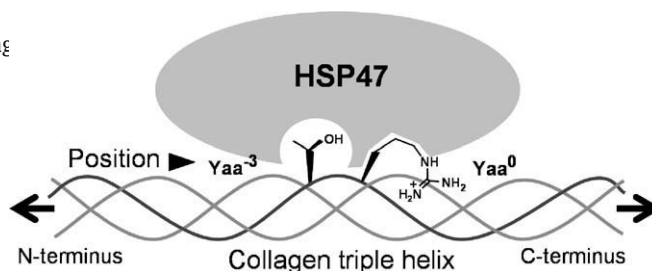


Synthesis and clusterization of Gal β (1 \rightarrow 3)[NeuAc α (2 \rightarrow 6)]GlcNAc β (1 \rightarrow 2)Man motif of the N-glycan, as the molecular probes for their biological evaluation, are reported.

REGULAR ARTICLES**A structure–activity relationship study elucidating the mechanism of sequence-specific collagen recognition by the chaperone HSP47**

pp 3767–3775

Yoshimi Nishikawa, Yoshifumi Takahara, Shinichi Asada, Akira Shigenag, Akira Otaka, Kouki Kitagawa, Takaki Koide*

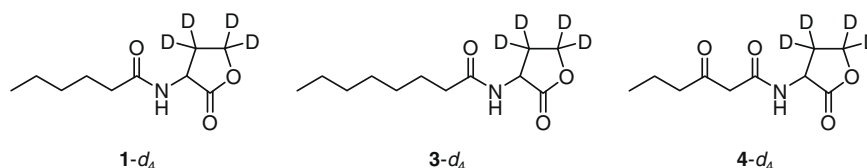


HSP47 binds to triple-helical collagen, recognizing Yaa⁰ and Yaa⁻³ side-chains in the Xaa-Yaa⁻³-Gly-Xaa-Yaa⁰-Gly sequence. Structural preferences for Yaa⁰ and Yaa⁻³ were determined using synthetic collagen-mimetic peptides.

**Facile preparation of deuterium-labeled N-acylhomoserine lactones as internal standards for isotope dilution mass spectrometry**

pp 3776–3782

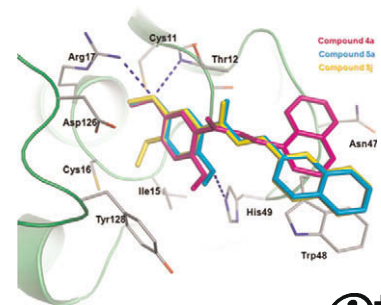
Kenji Kai*, Ayaka Tani, Hideo Hayashi

**Inhibition of *Mycobacterium tuberculosis* tyrosine phosphatase PtpA by synthetic chalcones: Kinetics, molecular modeling, toxicity and effect on growth**

pp 3783–3789

Alessandra Mascarello, Louise Domeneghini Chiaradia, Javier Vernal, Andrea Villarino, Rafael V. C. Guido, Paulo Perizzolo, Valerie Poirier, Dennis Wong, Priscila Graziela Alves Martins, Ricardo José Nunes, Rosendo Augusto Yunes, Adriano Defini Andricopulo, Yossef Av-Gay*, Hernán Terenzi*

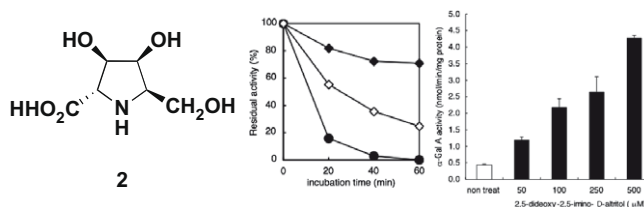
We have recently identified five synthetic chalcones which inhibit the activity of *Mycobacterium tuberculosis* protein tyrosine phosphatase A (PtpA), an enzyme associated with *M. tuberculosis* infectivity, and we carried out the analysis of the molecular recognition of these inhibitors on their macromolecular target through Structure–Activity Relationship (SAR) studies and molecular modeling.



2,5-Dideoxy-2,5-imino-D-altritol as a new class of pharmacological chaperone for Fabry disease

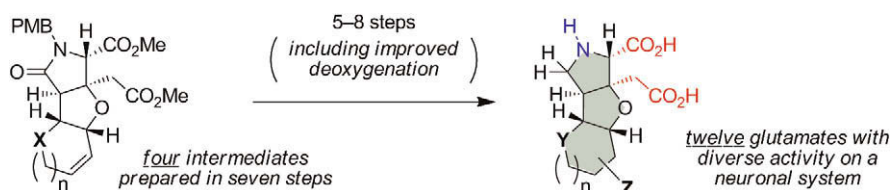
pp 3790–3794

Atsushi Kato*, Yukiko Yamashita, Shinpei Nakagawa, Yuriko Koike, Isao Adachi, Jackie Hollinshead, Robert J. Nash, Kyoko Ikeda, Naoki Asano

**Improved synthesis and in vitro/in vivo activities of natural product-inspired, artificial glutamate analogs**

pp 3795–3804

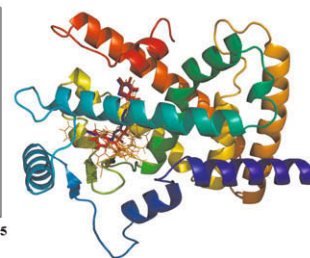
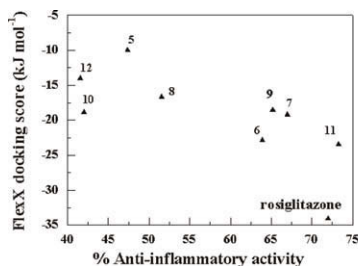
Masato Oikawa*, Minoru Ikoma, Makoto Sasaki, Martin B. Gill, Geoffrey T. Swanson, Keiko Shimamoto, Ryuichi Sakai

**Synthesis and anti-inflammatory activity of new arylidene-thiazolidine-2,4-diones as PPAR_γ ligands**

pp 3805–3811

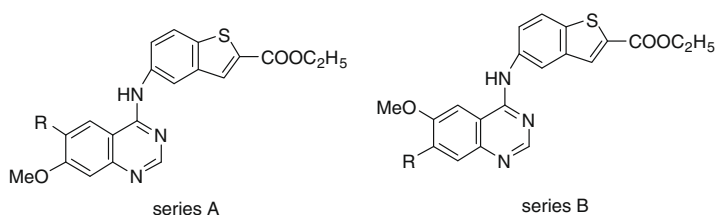
Cleiton Diniz Barros, Angélica Amorim Amato, Tiago Bento de Oliveira, Karime Bicas Rocha Iannini, Anekécia Lauro da Silva, Teresinha Gonçalves da Silva, Elisa Soares Leite, Marcelo Zaldini Hernandez, Maria do Carmo Alves de Lima, Suely Lins Galdino, Francisco de Assis Rocha Neves, Ivan da Rocha Pitta*

Trend between the docking scores (PPAR_γ receptor) and the anti-inflammatory activity of eight new synthesized 5-arylidene-3-benzyl-thiazolidine-2,4-diones compounds. The compound **11** exhibited an anti-inflammatory activity slightly higher than the reference drug, rosiglitazone, a well-known potent agonist of the PPAR_γ.

**Design and synthesis of novel Gefitinib analogues with improved anti-tumor activity**

pp 3812–3822

Xiaoqing Wu, Mingdong Li, Yang Qu, Wenhua Tang, Youguang Zheng, Jiqin Lian, Min Ji*, Liang Xu*

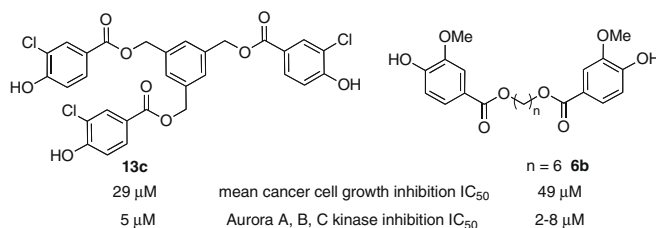


Two series of 4-benzothienyl amino quinazolines were designed and synthesized as new analogues of the EGFR inhibitor Gefitinib, with improved anti-tumor and pro-apoptotic activity.

Simple di- and trivanillates exhibit cytostatic properties toward cancer cells resistant to pro-apoptotic stimuli

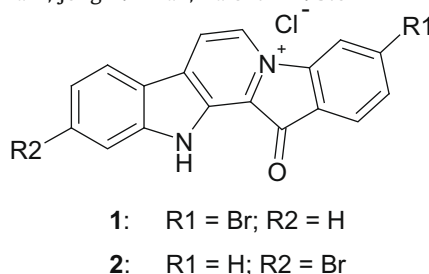
pp 3823–3833

Delphine Lamoral-Theys, Laurent Pottier, Frédéric Kerff, François Dufrasne, Fabien Proutière, Nathalie Wauthoz, Philippe Neven, Laurent Ingrassia, Pierre Van Antwerpen, Florence Lefranc, Michel Gelbcke, Bernard Pirotte, Jean-Louis Kraus, Jean Nève, Alexander Kornienko, Robert Kiss*, Jacques Dubois

**The anticancer activity of 3- and 10-bromofascaplysins is mediated by caspase-8, -9, -3-dependent apoptosis**

pp 3834–3840

Alexandra S. Kuzmich, Sergey N. Fedorov*, Valeria V. Shastina, Larisa K. Shubina, Oleg S. Radchenko, Nadezda N. Balaneva, Maxim E. Zhidkov, Joo-In Park, Jong Y. Kwak, Valentin A. Stonik

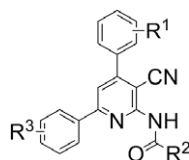


Cancer-preventive and cytotoxic activities of 3- and 10-bromofascaplysins (**1** and **2**) are mediated, at least in part, through the induction of caspase-dependent apoptosis.

Synthesis and structure–activity relationships of 2-acylamino-4,6-diphenylpyridine derivatives as novel antagonists of GPR54

pp 3841–3859

Toshitake Kobayashi*, Satoshi Sasaki, Naoki Tomita, Seiji Fukui, Noritaka Kuroda, Masaharu Nakayama, Atsushi Kiba, Yoshihiro Takatsu, Tetsuya Ohtaki, Fumio Itoh, Atsuo Baba

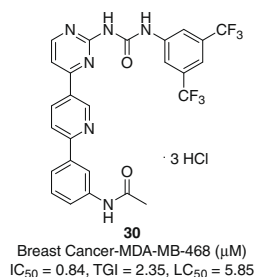


Synthesis and structure–activity relationships of 2-acylamino-4,6-diphenylpyridines as novel small molecule GPR54 antagonists are reported.

Design and synthesis of new anticancer pyrimidines with multiple-kinase inhibitory effect

pp 3860–3874

Ibrahim Mustafa El-Deeb, So Ha Lee*



A new series of N-substituted-2-aminopyrimidines has been designed, synthesized, and tested over a panel of 60 cancer cell lines. Compound **30** has showed multiple inhibitions over a number of oncogenic kinases. A molecular modeling study was made by docking of the most active compound **30** into the kinase domain of ABL1 to investigate its possible binding interactions.

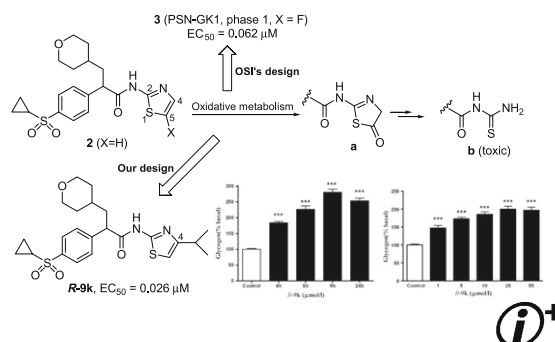


Design, synthesis, and pharmacological evaluation of *N*-(4-mono and 4,5-disubstituted thiazol-2-yl)-2-aryl-3-(tetrahydro-2*H*-pyran-4-yl)propanamides as glucokinase activators

pp 3875–3884

Fuying Li, Qingzhang Zhu, Yi Zhang, Ying Feng, Ying Leng*, Ao Zhang*

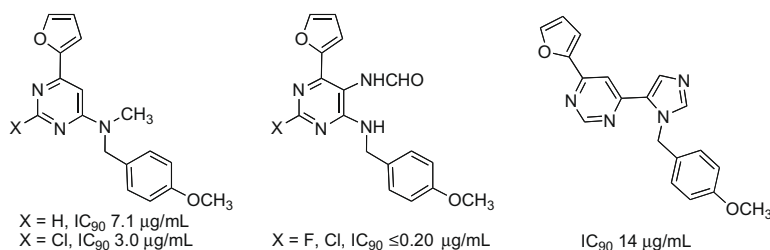
A series of *N*-thiazole substituted arylacetamides were designed as metabolic stable glucokinase (GK) activators for the treatment of type 2 diabetes. Compound **9-9k**, with an EC₅₀ of 0.026 μM significantly increased both glucose uptake and glycogen synthesis in rat primary cultured hepatocytes. Single oral administration of compound **9-9k** exerted significant reduction of blood glucose levels in both ICR and *ob/ob* mice.



Synthesis and biological evaluation of pyrimidine analogs of antimycobacterial purines

pp 3885–3897

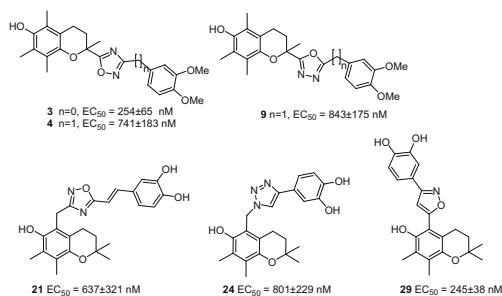
Matthew L. Read, Morten Brændvang, Pedro O. Miranda, Lise-Lotte Gundersen*



Synthesis of a second generation chroman/catechol hybrids and evaluation of their activity in protecting neuronal cells from oxidative stress-induced cell death

pp 3898–3909

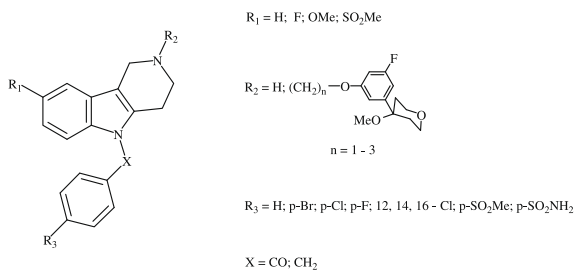
Maria Koufaki*, Elissavet Theodorou, Xanthippi Alexi, Michael N. Alexis



Synthesis and biological activity of *N*-aroyl-tetrahydro- γ -carbolines

pp 3910-3924

Alexandre Bridoux*, Régis Millet, Jean Pommery, Nicole Pommery, Jean-Pierre Henichart



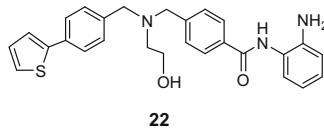
Tetrahydro- γ -carboline derivatives exhibited potent inhibitory activity with IC_{50} values in the range of 3.0–6.0 μ M.



New orally bioavailable 2-aminobenzamide-type histone deacetylase inhibitor possessing a (2-hydroxyethyl)-(4-(thiophen-2-yl)benzyl)amino group

pp 3925–3933

Shingo Kiyokawa, Yoshiyuki Hirata, Yasuo Nagaoka, Makio Shibano, Masahiko Taniguchi, Masahide Yasuda, Kimiye Baba, Shinichi Uesato*

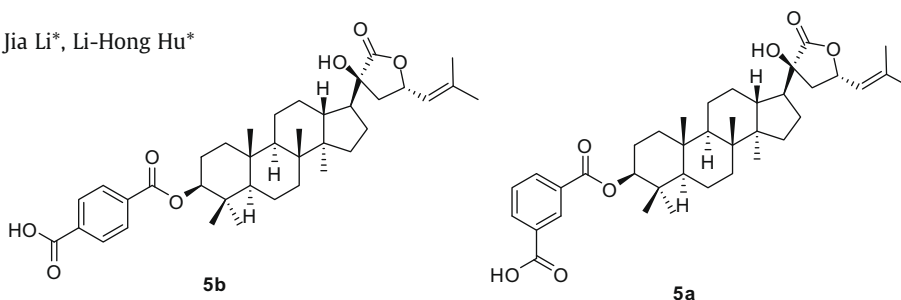


A sulfur-containing HDAC inhibitors were designed. Compound **22** reduced the growth of HCT116 xenografts in nude mice to T/C 67% by oral administration (at 45 mg/kg), which was similar to the value for MS-275.

Dammaranes from *Gynostemma pentaphyllum* and synthesis of their derivatives as inhibitors of protein tyrosine phosphatase 1B

pp 3934–3939

Ji-Qing Xu, Qiang Shen, Jia Li*, Li-Hong Hu*



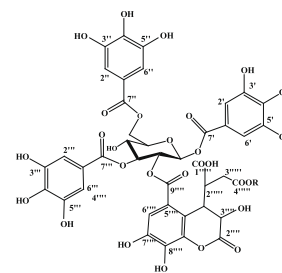
We reported the dammaranes inhibitors of PTP1B and concluded the SAR. Compound **5b** was found with the best activity ($IC_{50} = 0.27 \mu M$) and **5a** exhibited the best selectivity (nearly fivefolds) between PTP1B and TCPTP.

**Insulinomimetic activity of two new gallotannins from the fruits of *Capparis moonii***

pp 3940–3945

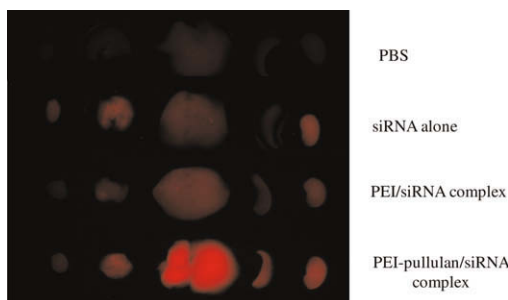
Anil Kanaujia*, Rajeev Duggar, Steve Thomas Pannakal, Satyapal Singh Yadav, Chandra Kant Katiyar, Vinay Bansal, S. Anand, S. Sujatha, B. S. Lakshmi

Bioassay guided fractionation of the hydro-alcoholic extract of *Capparis moonii* fruit, led to the isolation of two new Chebulinic acid derivatives. The compounds, **1** and **2** showed significant glucose uptake effect of 223% and 219% over the control at the 10 ng/ml and 100 ng/ml concentration, respectively. The increased glucose uptake effects of the compounds, were associated with significant IR and IRS-1 phosphorylation, GLUT4 and PI3-kinase mRNA expression in the L6 cells.

**Liver-targeted siRNA delivery by polyethylenimine (PEI)-pullulan carrier**

pp 3946–3950

Jeong-Hun Kang, Yoichi Tachibana, Wakako Kamata, Atsushi Mahara, Mariko Harada-Shiba, Tetsuji Yamaoka*



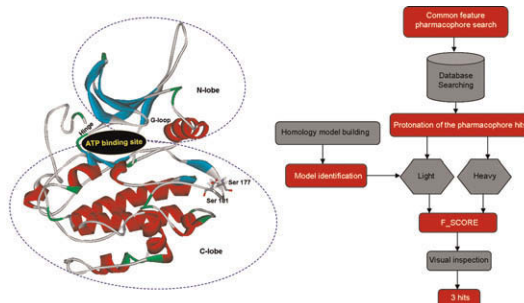
After systemic injection, the PEI-pullulan/siRNA complex led to an increased fluorescence level in the liver.



IKK β inhibitors identification part II: Ligand and structure-based virtual screening

pp 3951–3960

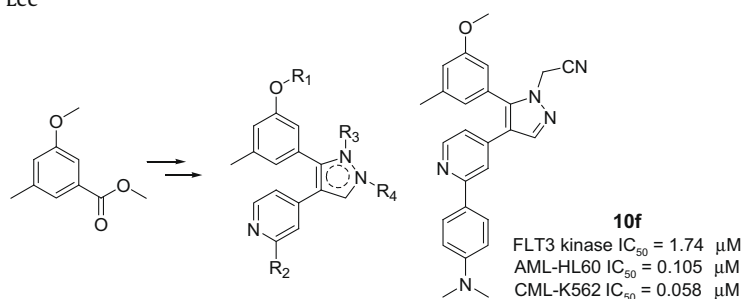
Shanthi Nagarajan, Hyunah Choo, Yong Seo Cho, Kwang-Seok Oh, Byung Ho Lee, Kye Jung Shin, Ae Nim Pae*



Design and synthesis of new potent anticancer pyrazoles with high FLT3 kinase inhibitory selectivity

pp 3961–3973

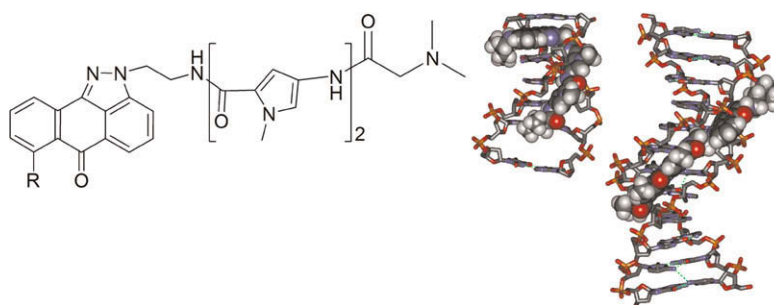
Ibrahim Mustafa El-Deeb, So Ha Lee*



Design, synthesis and biological evaluation of a novel series of anthrapyrazoles linked with netropsin-like oligopyrrole carboxamides as anticancer agents

pp 3974–3984

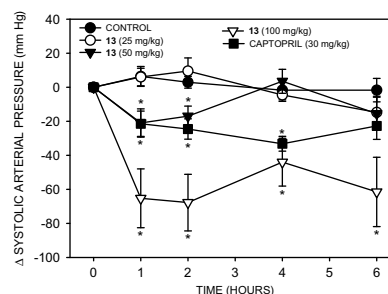
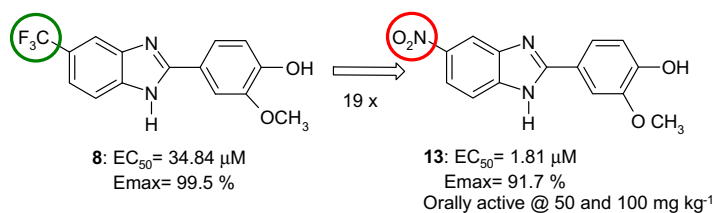
Rui Zhang, Xing Wu, Lynn J. Guziec, Frank S. Guziec, Gaik-Lean Chee, Jack C. Yalowich, Brian B. Hasinoff*



Synthesis, vasorelaxant activity and antihypertensive effect of benzo[d]imidazole derivatives

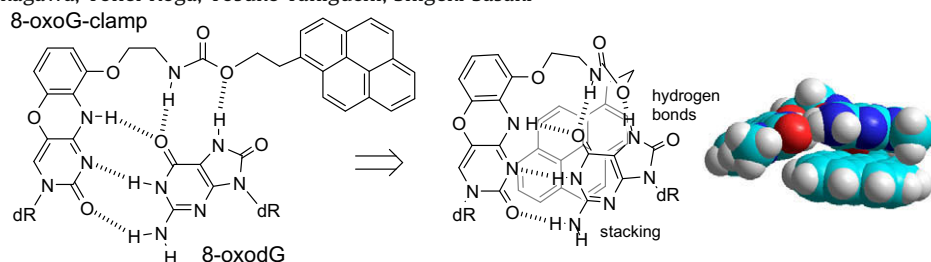
pp 3985–3991

Gabriel Navarrete-Vázquez*, Sergio Hidalgo-Figueroa, Mariana Torres-Piedra, Jorge Vergara-Galicia, Julio Cesar Rivera-Leyva, Samuel Estrada-Soto*, Ismael León-Rivera, Berenice Aguilar-Guardarrama, Yolanda Ríos-Gómez, Rafael Villalobos-Molina, Maximiliano Ibarra-Barajas



Synthesis of new derivatives of 8-oxoG-Clamp for better understanding the recognition mode and improvement of selective affinity pp 3992–3998

Zhichun Li, Osamu Nakagawa, Yohei Koga, Yosuke Taniguchi, Shigeki Sasaki*

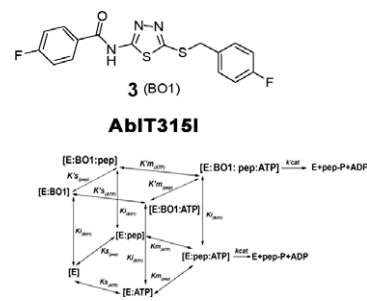


8-OxoG-clamp derivatives having a variety of *N*-functional groups were synthesized to clarify the suitable structure for more selective recognition, and 2-pyrene-1-yl-ethoxycarbonyl unit was found to produce higher stability with 8-oxoG.

Dual Src and Abl inhibitors target wild type Abl and the AbIT315I Imatinib-resistant mutant with different mechanisms pp 3999–4008

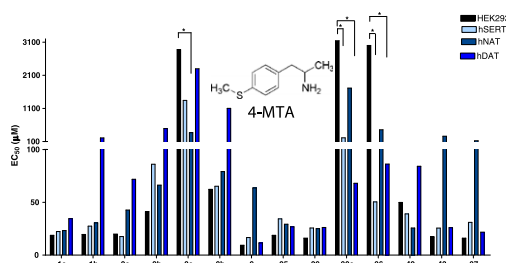
Emmanuele Crespan, Marco Radi, Samantha Zanolli, Silvia Schenone, Maurizio Botta*, Giovanni Maga*

The dual Src-Abl inhibitor BO1 targets AbIT315I through a non-competitive mechanism with limited loss of potency.



Synthesis and in vitro toxicity of 4-MTA, its characteristic clandestine synthesis byproducts and related sulfur substituted α -alkylthioamphetamines pp 4009–4031

Suzanne M. Cloonan, John J. Keating, Desmond Corrigan, John E. O'Brien, Pierce V. Kavanagh, D. Clive Williams, Mary J. Meegan*

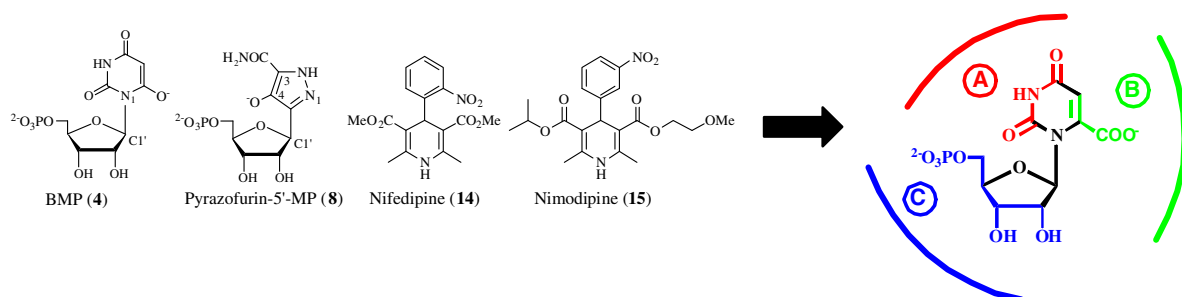


Impurities isolated from clandestine 4-MTA synthesis show cytotoxicity to cells expressing the human serotonin, noradrenaline and dopamine transporters.



Structural determinants for the inhibitory ligands of orotidine-5'-monophosphate decarboxylase pp 4032–4041

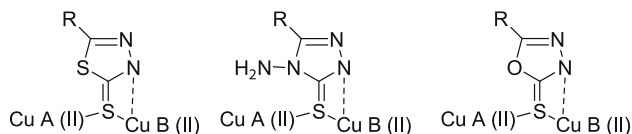
Maria Elena Meza-Avina, Lianhu Wei, Yan Liu, Ewa Poduch, Angelica M. Bello, Ram K. Mishra, Emil F. Pai*, Lakshmi P. Kotra*



New potent inhibitors of tyrosinase: Novel clues to binding of 1,3,4-thiadiazole-2(3*H*)-thiones, 1,3,4-oxadiazole-2(3*H*)-thiones, 4-amino-1,2,4-triazole-5(4*H*)-thiones, and substituted hydrazides to the dicopper active site

pp 4042–4048

Usman Ghani*, Nisar Ullah

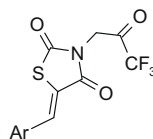


Kinetic and enzyme binding studies provide novel clues to mono-dentate binding of a series of substituted thiadiazole, oxadiazole, and triazole moieties to the active site dicopper center of tyrosinase including hydrophobicity mainly contributing to the potent inhibition of the enzyme.

Identification of new non-carboxylic acid containing inhibitors of aldose reductase

pp 4049–4055

Rosanna Maccari*, Rosella Ciurleo, Marco Giglio, Mario Cappiello, Roberta Moschini, Antonella Del Corso, Umberto Mura, Rosaria Ottanà



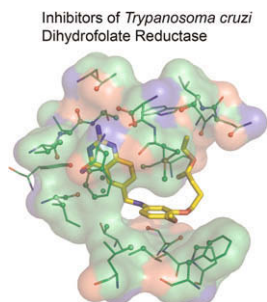
New non-carboxylic acid containing 5-arylidene-2,4-thiazolidinedione derivatives have been identified as aldose reductase inhibitors active at low micromolar doses.



Synthesis and characterization of potent inhibitors of *Trypanosoma cruzi* dihydrofolate reductase

pp 4056–4066

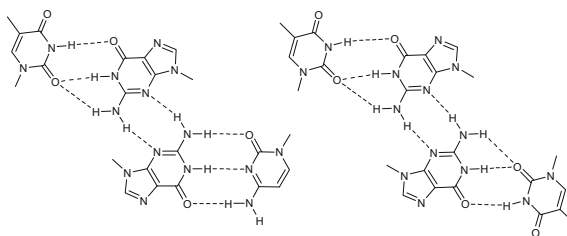
Norbert Schormann, Sadanandan E. Velu, Srinivasan Murugesan, Olga Senkovich, Kiera Walker, Bala C. Chenna, Bidhan Shinkre, Amar Desai, Debasish Chattopadhyay*



Self-association of cyclic oligonucleotides through G:T:G:T minor groove tetrads

pp 4067–4073

Júlia Viladoms, Núria Escaja, Enrique Pedrosa*, Carlos González*



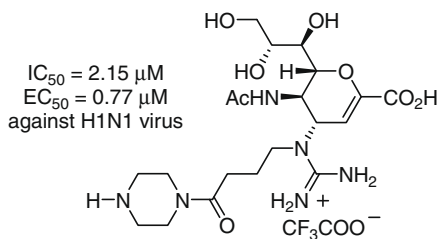
G–T mismatches can form minor groove aligned tetrads (G:C:G:T or G:T:G:T) of similar structure and stability to those formed by G–C Watson–Crick base pairs.



Analogs of zanamivir with modified C4-substituents as the inhibitors against the group-1 neuraminidases of influenza viruses

pp 4074–4084

Wen-Hsien Wen, Shi-Yun Wang, Keng-Chang Tsai, Yih-Shyun E. Cheng, An-Suei Yang, Jim-Min Fang*, Chi-Huey Wong

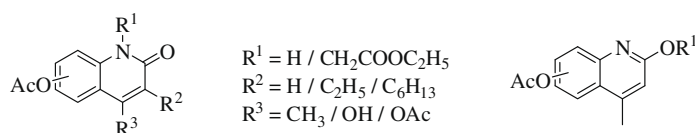


Zanamivir derivative having an extended (piperazinocarbonyl)propyl substituent at the internal N-position of the guanidinium group is designed as an inhibitor specifically against the group-1 neuraminidases of influenza viruses.

**Characterization of 4-methyl-2-oxo-1,2-dihydroquinolin-6-yl acetate as an effective antiplatelet agent**

pp 4085–4094

Nivedita Priya, Anjali Gupta, Karam Chand, Prabhjot Singh, Abha Kathuria, Hanumantharao G. Raj*, Virinder S. Parmar, Sunil K. Sharma*

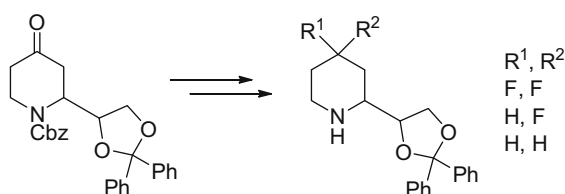


A series of novel quinolin-2-one derivatives were synthesized and examined for their antiplatelet action by virtue of causing Calreticulin Transacetylase catalyzed activation of platelet Nitric Oxide Synthase.

**Synthesis and NMDA receptor affinity of fluorinated dioxadrol analogues**

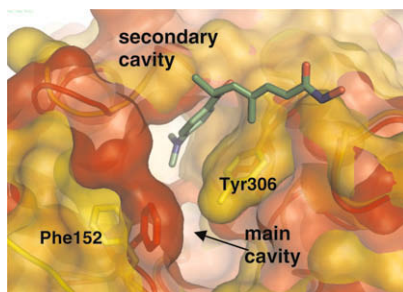
pp 4095–4102

Ashutosh Banerjee, Dirk Schepmann, Bernhard Wünsch*

**On the inhibition of histone deacetylase 8**

pp 4103–4110

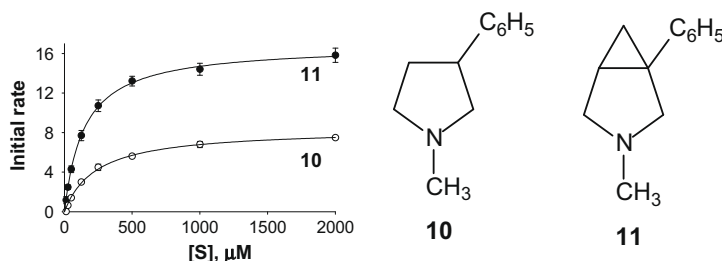
Guillermina Estiu, Nathan West, Ralph Mazitschek, Edward Greenberg, James E. Bradner, Olaf Wiest*



Interactions of 1-methyl-3-phenylpyrrolidine and 3-methyl-1-phenyl-3-azabicyclo[3.1.0]hexane with monoamine oxidase B

pp 4111–4118

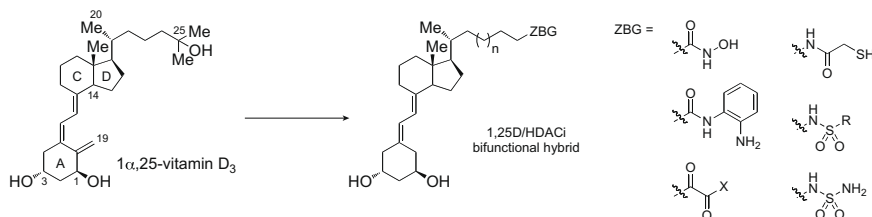
Anél Pretorius, Modupe O. Ogunrombi, Hendrik Fourie, Gisella Terre'Blanche, Neal Castagnoli Jr., Jacobus J. Bergh, Jacobus P. Petzer*



Vitamin D receptor agonist/histone deacetylase inhibitor molecular hybrids

pp 4119–4137

Marc Lamblin, Basel Dabbas, Russell Spingarn, Rodrigo Mendoza-Sanchez, Tian-Tian Wang, Beum-Soo An, Dao Chao Huang, Richard Kremer, John H. White*, James L. Gleason*



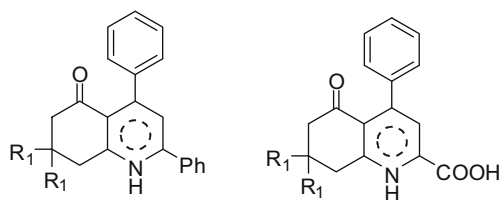
Incorporation of zinc-binding groups into the side-chain of 1 α ,25-dihydroxyvitamin D₃ (1,25D) fully bifunctional hybrid molecules which act both as vitamin D receptor agonists and histone deacetylase inhibitors. These bifunctional hybrids display in vitro antiproliferative activity against the AT84 squamous carcinoma cell line while lacking the in vivo hypercalcemic effects of 1,25D.



Design and synthesis of 2,4-disubstituted polyhydroquinolines as prospective antihyperglycemic and lipid modulating agents

pp 4138–4148

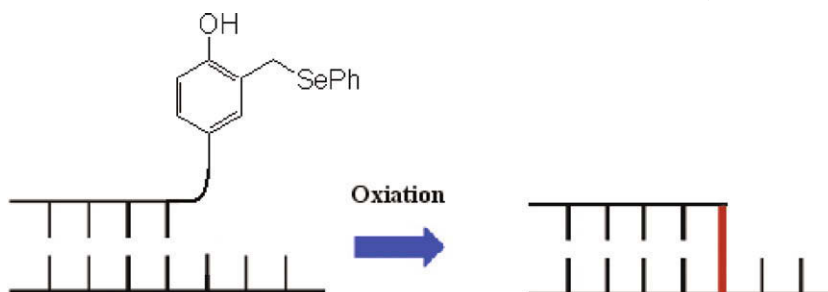
Atul Kumar*, Siddharth Sharma, Vishwa Deepak Tripathi, Ram Awatar Maurya, Swayam Prakash Srivastava, Gitika Bhatia, A. K. Tamrakar, Arvind Kumar Srivastava



Oligonucleotide-selenide conjugate: Synthesis and its inducible sequence-specific alkylation of DNA

pp 4149–4153


Yuhao Du, Xiaocheng Weng, Jing Huang, Dan Zhang, Heng Ma, Dong Chen, Xiang Zhou*, Jean-François Constant*



Oligonucleotide-selenium conjugate was designed and synthesized and its sequence-specific cross-linking ability was investigated.



*Corresponding author

+ Supplementary data available via ScienceDirect

COVER

The cover shows the binding surface of the monoclonal antibody raised against the anthrax tetrasaccharide that recognizes *Bacillus anthracis* spores shown as background. The STD NMR structure and the image were generated by Dr. Heiko Möller (Uni Konstanz). The cover was designed by Marie-Lyn Hecht and Peter H. Seeberger.

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