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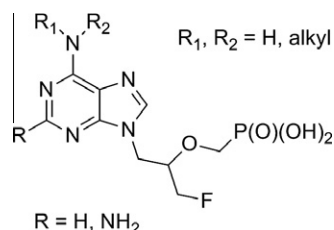
Bioorganic & Medicinal Chemistry Volume 19, Issue 7, 2011

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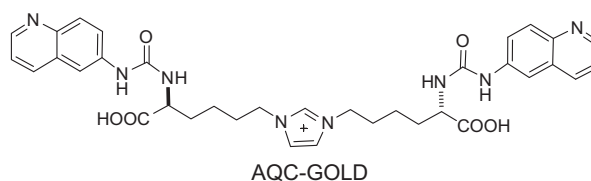
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Ondřej Baszczyński, Petr Jansa, Martin Dračinský, Blanka Klepetářová, Antonín Holý, Ivan Votruba, Erik de Clercq, Jan Balzarini, Zlatko Janeba*



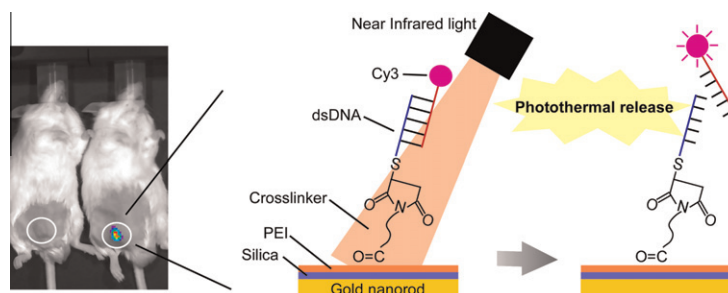
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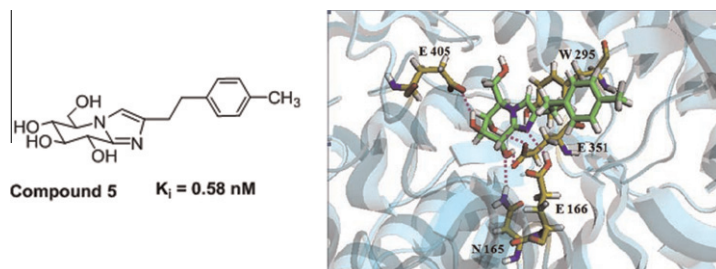
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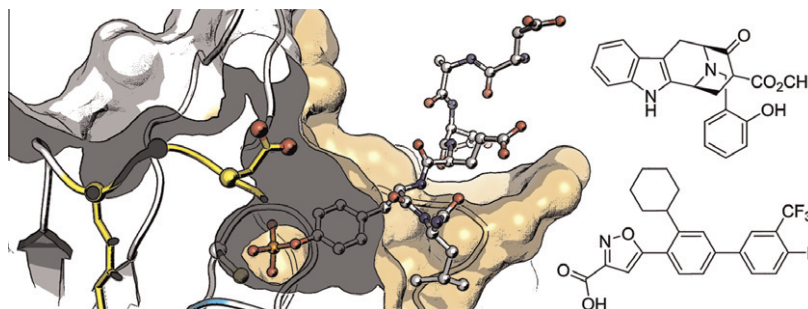
Tiehai Li, Lina Guo, Yan Zhang, Jiajia Wang, Zhenxing Zhang, Jing Li, Wenpeng Zhang, Jianping Lin, Wei Zhao*, Peng George Wang*



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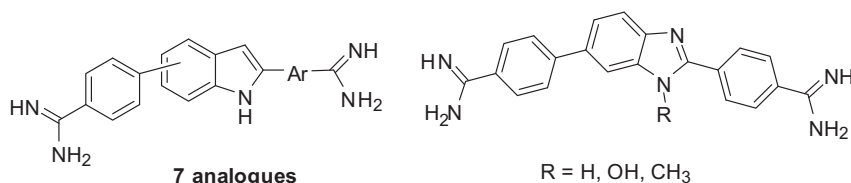
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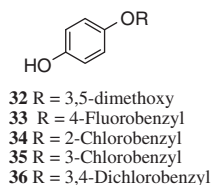
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Synthesis and anti-melanogenic activity of hydroxyphenyl benzyl ether analogues

pp 2168–2175

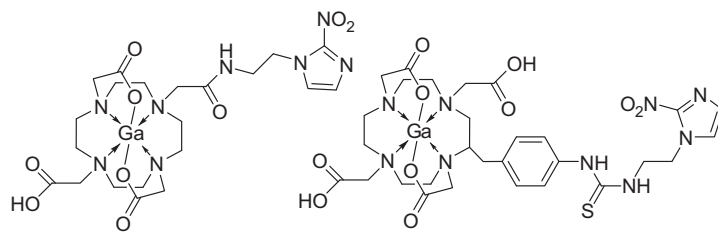
Kiran Sapkota, Eunmiri Roh, Eunyoung Lee, Eun-Mi Ha, Jae-Ho Yang, Eung-Seok Lee, Youngjoo Kwon, Youngsoo Kim*, Younghwa Na*



Synthesis of ^{68}Ga -labeled DOTA-nitroimidazole derivatives and their feasibilities as hypoxia imaging PET tracers

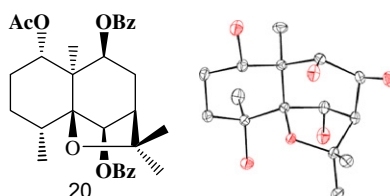
pp 2176–2181

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

**Dihydro- β -agarofuran sesquiterpenes isolated from *Celastrus vulcanicola* as potential anti-*Mycobacterium tuberculosis* multidrug-resistant agents**

pp 2182–2189

David Torres-Romero, Ignacio A. Jiménez, Rosario Rojas, Robert H. Gilman, Matías López, Isabel L. Bazzocchi*

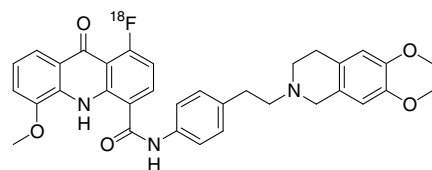
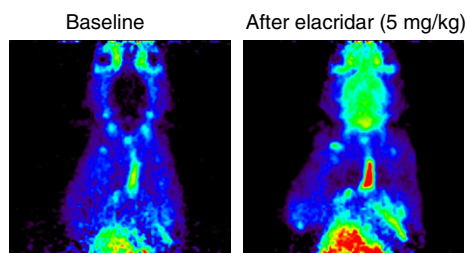


A series of natural and derivative dihydro- β -agarofuran sesquiterpenes have been tested against sensitive and resistant *Mycobacterium tuberculosis* strains. Among those tested, **20** exhibited promising anti-MDR TB activity. Their stereostructures were elucidated by NMR and X-ray analysis.

**Radiosynthesis and in vivo evaluation of 1- ^{18}F fluoroelacridar as a positron emission tomography tracer for P-glycoprotein and breast cancer resistance protein**

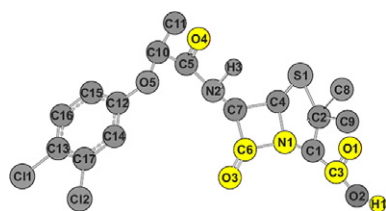
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Bernd Dörner, Claudia Kuntner, Jens P. Bankstahl, Thomas Wanek, Marion Bankstahl, Johann Stanek, Julia Müllauer, Florian Bauer, Severin Mairinger, Wolfgang Löscher, Donald W. Miller, Peter Chiba, Markus Müller, Thomas Erker*, Oliver Langer

1- ^{18}F Fluoroelacridar ([^{18}F]4b)**4D-QSAR analysis and pharmacophore modeling: Electron conformational-genetic algorithm approach for penicillins**

pp 2199–2210

Ersin Yanmaz, Emin Sarıpinar*, Kader Şahin, Nazmiye Geçen, Fatih Çopur



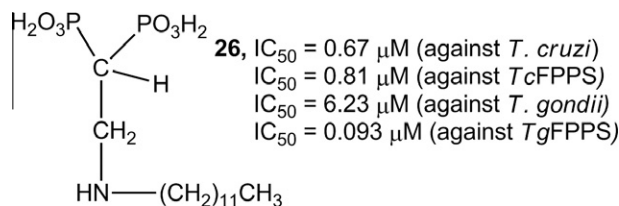
Pharmacophore Atoms and Electron Conformational Submatrices of Activity

N1	C6	C3	O1	H1	O3	O4	
-0.110	0.935	2.430	2.934	4.215	2.425	4.968	N1
	0.274	3.767	4.372	5.404	1.953	4.152	C6
		0.384	1.833	1.906	4.322	7.319	C3
			-0.362	2.226	5.075	7.523	O1
				0.230	5.693	9.166	H1
					-0.247	4.784	O3
						-0.351	O4



Synthesis and biological evaluation of new 2-alkylaminoethyl-1,1-bisphosphonic acids against *Trypanosoma cruzi* and *Toxoplasma gondii* targeting farnesyl diphosphate synthase

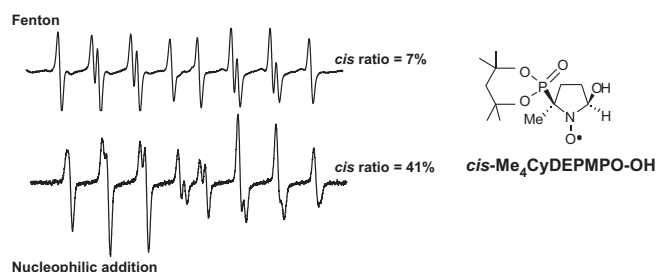
Valeria S. Rosso, Sergio H. Szajnman, Leena Malayil, Melina Galizzi, Silvia N. J. Moreno, Roberto Docampo, Juan B. Rodriguez*



CyDEPMPOs: A class of stable cyclic DEPMPO derivatives with improved properties as mechanistic markers of stereoselective hydroxyl radical adduct formation in biological systems

pp 2218–2230

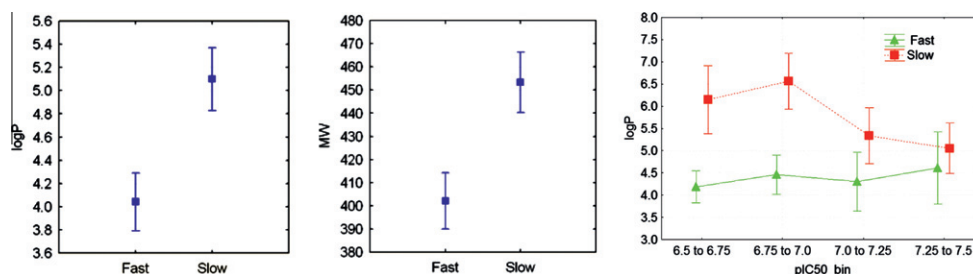
Gaëlle Gosset, Jean-Louis Clément, Marcel Culcasi*, Antal Rockenbauer, Sylvia Pietri



Molecular properties affecting fast dissociation from the D₂ receptor

pp 2231–2241

Gary Tresadern*, Jose Manuel Bartolome, Gregor J. Macdonald, Xavier Langlois*



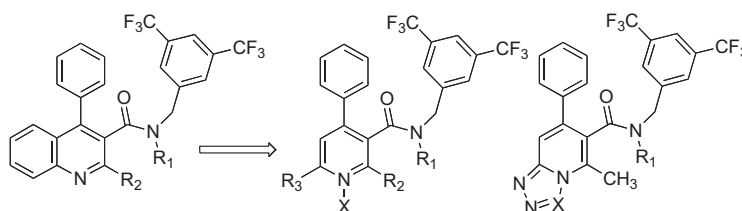
Statistical analysis reveals the important molecular properties affecting fast and slow dissociating D₂ receptor antagonists.



Non-peptide NK₁ receptor ligands based on the 4-phenylpyridine moiety

pp 2242–2251

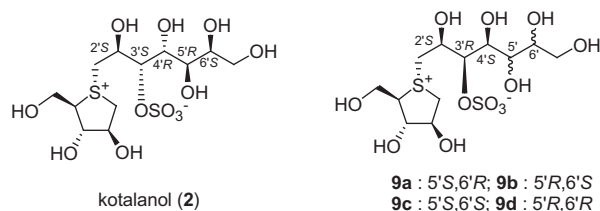
Germano Giuliani, Andrea Cappelli*, Mario Matarrese, Valeria Masiello, Elia Anna Turolla, Cristina Monterisi, Ferruccio Fazio, Maurizio Anzini, Galia Pericot Mohr, Daniela Riitano, Federica Finetti, Lucia Morbidelli, Marina Ziche, Gianluca Giorgi, Salvatore Vomero



Role of the side chain stereochemistry in the α -glucosidase inhibitory activity of kotalanol, a potent natural α -glucosidase inhibitor

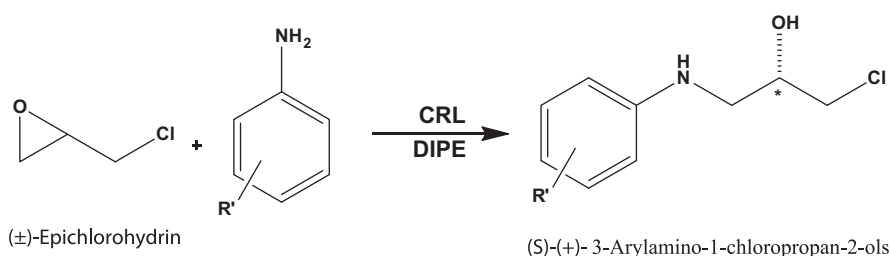
pp 2252–2262

Weijia Xie, Genzoh Tanabe, Kanjyun Matsuoka, Mumen F. A. Amer, Toshie Minematsu, Xiaoming Wu, Masayuki Yoshikawa, Osamu Muraoka*

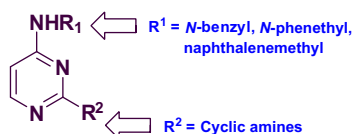
**Selective biocatalytic aminolysis of ($\pm$)-epichlorohydrin: Synthesis and ICAM-1 inhibitory activity of (*S*)-(+)-3-arylamino-1-chloropropan-2-ols**

Pankaj Gupta, Sumati Bhatia, Ashish Dhawan, Sakshi Balwani, Shatrughan Sharma, Raju Brahma, Rajpal Singh, Balaram Ghosh, Virinder S. Parmar, Ashok K. Prasad*

Regio- and enantioselective synthesis of (*S*)-(+)-3-arylamino-1-chloropropan-2-ols has been achieved by epoxide ring opening of ($\pm$)-epichlorohydrin with different aromatic amines in the presence of *Candida rugosa* lipase. Activity of seven model (*S*)-(+)-3-arylamino-1-chloropropan-2-ols, out of 10 compounds synthesized, has been evaluated for the inhibition of tumor necrosis factor- α (TNF- α) induced expression of cell adhesion molecule, that is, intercellular adhesion molecule-1 (ICAM-1) and structure-activity relationship has been established.

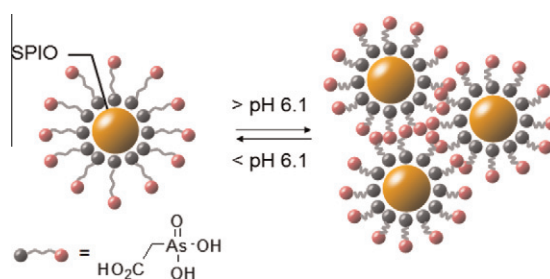
**Design, synthesis and structure-activity relationship (SAR) studies of 2,4-disubstituted pyrimidine derivatives: Dual activity as cholinesterase and A β -aggregation inhibitors**

Tarek Mohamed, Xiaobei Zhao, Lila K. Habib, Jerry Yang, Praveen P. N. Rao*

Novel ring scaffold as dual cholinesterase and A β -aggregation inhibitors.**Arsonic acid-presenting superparamagnetic iron oxide for pH-responsive aggregation under slightly acidic conditions**

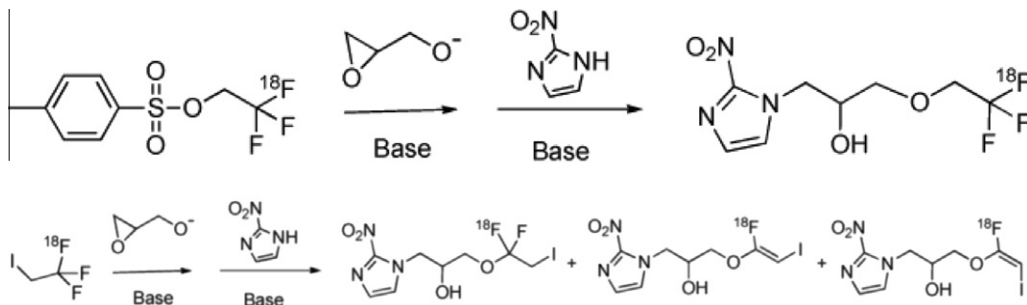
pp 2282–2286

Hiroki Minehara, Kensuke Naka, Kazuo Tanaka, Asako Narita, Yoshiki Chujo*



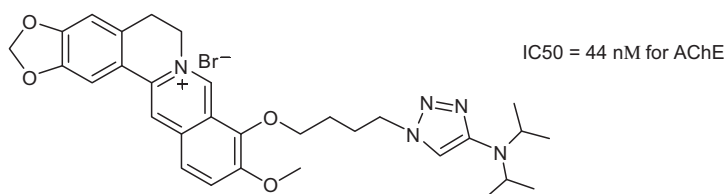
Radiosynthesis of the tumor hypoxia marker [^{18}F]TFMISO via O-[^{18}F]trifluoroethylation reveals a striking difference between trifluoroethyl tosylate and iodide in regiochemical reactivity toward oxygen nucleophiles pp 2287–2297

Makiko Suehiro*, Guangbin Yang, Geralda Torchon, Ellen Ackerstaff, John Humm, Jason Koutcher, Ouathék Ouerfelli



Synthesis, biological evaluation and molecular modeling of novel triazole-containing berberine derivatives as acetylcholinesterase and β -amyloid aggregation inhibitors pp 2298–2305

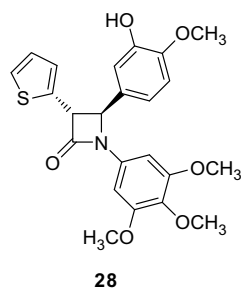
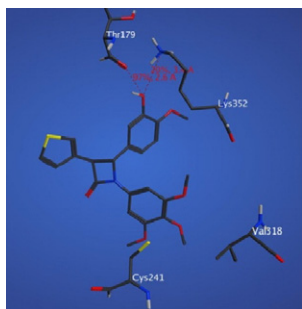
Anding Shi, Ling Huang, Chuanjun Lu, Feng He*, Xingshu Li*



A series of novel triazole-containing berberine derivatives were designed, synthesized, and biologically evaluated as inhibitors of acetylcholinesterase (AChE), butyrylcholinesterase (BuChE) and β -amyloid aggregation.

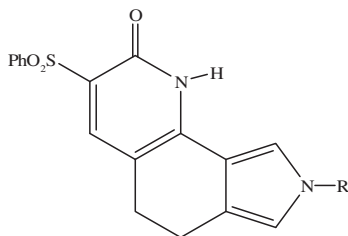
Synthesis, evaluation and structural studies of antiproliferative tubulin-targeting azetidin-2-ones pp 2306–2325

Niamh M. O'Boyle*, Lisa M. Greene, Orla Bergin, Jean-Baptiste Fichet, Thomas McCabe, David G. Lloyd, Daniela M. Zisterer, Mary J. Meegan*



Pyrrolo[3,4-*h*]quinolinones a new class of photochemotherapeutic agents pp 2326–2341

Paola Barraja, Patrizia Diana, Alessandra Montalbano, Anna Carbone, Giampietro Viola, Giuseppe Basso, Alessia Salvador, Daniela Vedaldi, Francesco Dall'Acqua, Girolamo Cirrincione*

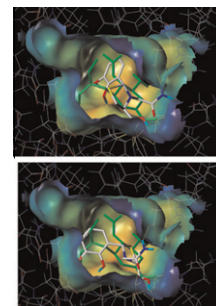


A new series of pyrroloquinolinones were synthesised and evaluated for their phototoxic activity. Some of the title compounds showed, upon UVA irradiation, IC_{50} values comparable or lower than angelicin used as reference drug.

Design, synthesis and biological activity of thiazolidine-4-carboxylic acid derivatives as novel influenza neuraminidase inhibitors pp 2342–2348

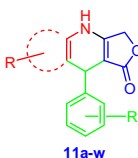
Yu Liu, Fanbo Jing, Yingying Xu, Yuanchao Xie, Fangyuan Shi, Hao Fang, Minyong Li, Wenfang Xu*

Docking result of compound **4f** and oseltamivir (**4f** is displayed by atom type while oseltamivir is shown in lime line). The active pocket is displayed using Channel pattern (Type: Cavity Depth) with the program MOLCAD Surfaces of Sybyl8.1.

**Synthesis of a new 4-aza-2,3-didehydropodophyllotoxin analogues as potent cytotoxic and antimitotic agents**

pp 2349–2358

Ahmed Kamal*, Paidakula Suresh, Adla Mallareddy, Banala Ashwini Kumar, Papagari Venkat Reddy, Paidakula Raju, Jaki R. Tamboli, Thokhir B. Shaik, Nishant Jain, Shasi V. Kalivendi*



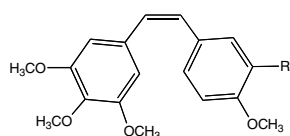
R = 2,4-dimethoxy-5-pyrimidyl, 5-indyl, 2-methyl-5-indyl, 5-indazolyl, 6-benzthiazolyl, 2-methyl-6-benzthiazolyl, 2-mercapto-5-imidazolyl, 5-triazolyl, 3-(4-methoxyaryl)5-isoxazolyl, 3-(4-chloroaryl)5-isoxazolyl, 2,3,4-trimethoxyaryl;

R¹ = 3,4,5-trimethoxy, 4-hydroxy-3-methoxy, 3-hydroxy-4-methoxy, 4-fluoro-3-methoxy, 3-nitro-4-methoxy, 2-fluoro-4-methoxy;

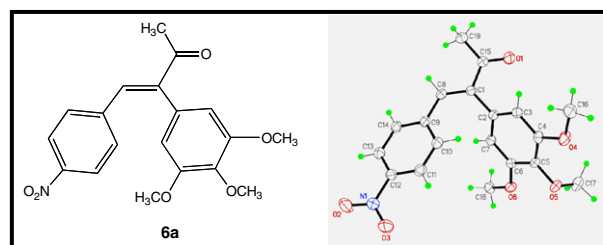
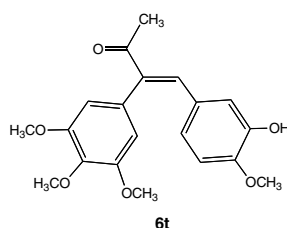
Acetyl analogs of combretastatin A-4: Synthesis and biological studies

pp 2359–2367

Balaji Babu, Megan Lee, Lauren Lee, Raymond Strobel, Olivia Brockway, Alexis Nickols, Robert Sjöholm, Samuel Tzou, Sameer Chavda, Dereje Desta, Gregory Fraley, Adam Siegfried, William Pennington, Rachel M. Hartley, Cara Westbrook, Susan L. Mooberry, Konstantinos Kiakos, John A. Hartley, Moses Lee*

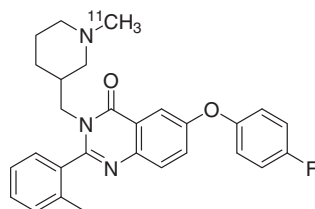


- 1, R = OH, combretastatin A-4
- 2, R = phosphate
- 3, R = NH₂, AC-7739
- 4, R = NHCOCHNH₂CH₂OH, AVE-8062

**Synthesis and in vivo evaluation of (S)-6-(4-fluorophenoxy)-3-((1-[¹¹C]methylpiperidin-3-yl)methyl)-2-o-tolylquinazolin-4(3H)-one, a potential PET tracer for growth hormone secretagogue receptor (GHSR)**

pp 2368–2372

Rachel Potter, Andrew G. Horti*, Hayden T. Ravert, Daniel P. Holt, Paige Finley, Ursula Scheffel, Robert F. Dannals, Richard L. Wahl



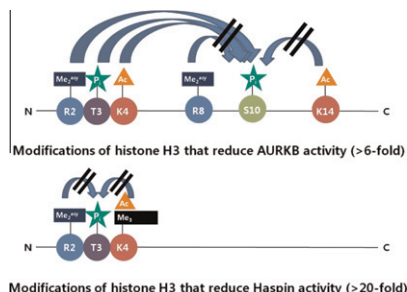
We report the synthesis, in vitro, and in vivo evaluation of 6-(4-fluorophenoxy)-3-((1-[¹¹C]methylpiperidin-3-yl)methyl)-2-o-tolylquinazolin-4(3H)-one ([¹¹C]) as a potential PET radiotracer for imaging of the Ghrelin Secretagogue Receptor (GHSR).



Methylation-mediated control of aurora kinase B and Haspin with epigenetically modified histone H3 N-terminal peptides

pp 2373–2377

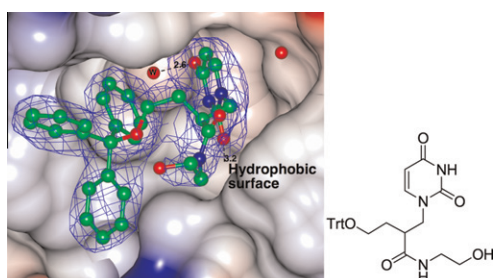
Areum Han, Kyung Hyun Lee, Soonsil Hyun, Nam Joo Lee, Su Jin Lee, Heeyong Hwang, Jaehoon Yu*



β -Branched acyclic nucleoside analogues as inhibitors of *Plasmodium falciparum* dUTPase

pp 2378–2391

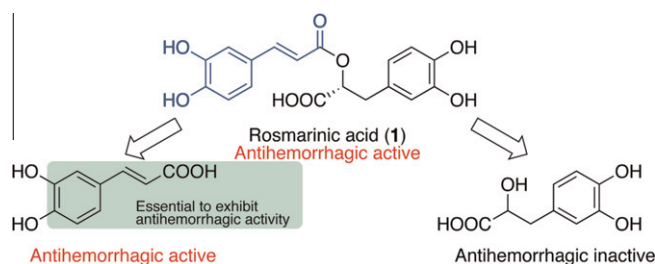
Beatriz Baragaña, Orla McCarthy, Paula Sánchez, Cristina Bosch-Navarrete, Marcel Kaiser, Reto Brun, Jean L. Whittingham, Shirley M. Roberts, Xiao-Xiong Zhou, Keith S. Wilson, Nils Gunnar Johansson, Dolores González-Pacanowska, Ian H. Gilbert*



Contribution of cinnamic acid analogues in rosmarinic acid to inhibition of snake venom induced hemorrhage

pp 2392–2396

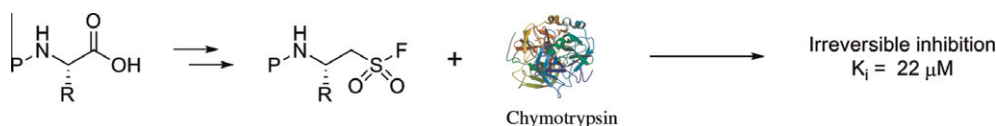
Hnin Thanda Aung, Tadashi Furukawa, Toshiaki Nikai, Masatake Niwa, Yoshiaki Takaya*



Synthesis and biological evaluation of novel irreversible serine protease inhibitors using amino acid based sulfonyl fluorides as an electrophilic trap

pp 2397–2406

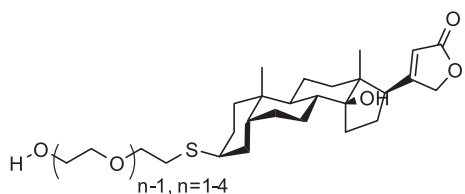
Arwin J. Brouwer, Tarik Ceylan, Anika M. Jonker, Tima van der Linden, Rob M. J. Liskamp*



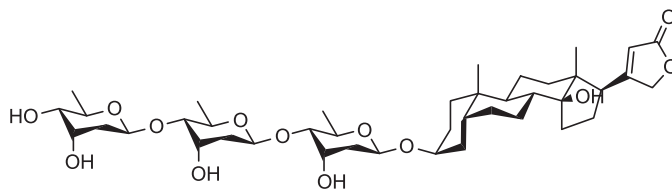
Synthesis and evaluation of cardiac glycoside mimics as potential anticancer drugs

pp 2407–2417

Marie Jensen, Steffen Schmidt, Natalya U. Fedosova, Jan Mollenhauer, Henrik H. Jensen*



Digitoxin Mimics: K_{app} (Na^+ , K^+ ATPase) 0.48–2.1 μM
 IC_{50} (MCF-7 breast cancer) 0.2–1.4 μM

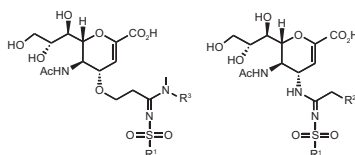


Digitoxin: K_{app} (Na^+ , K^+ ATPase) 0.99 μM
 IC_{50} (MCF-7 breast cancer) 0.02 μM

Syntheses of 2-deoxy-2,3-didehydro-N-acetylneuraminic acid analogues modified by N-sulfonylamidino groups at the C-4 position and biological evaluation as inhibitors of human parainfluenza virus type 1

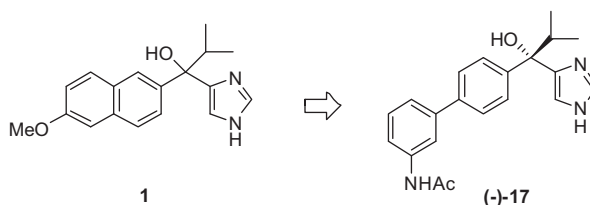
pp 2418–2427

Reiko Nishino, Kiyoshi Ikeda*, Takuya Hayakawa, Tadanobu Takahashi, Takashi Suzuki, Masayuki Sato

**17,20-Lyase inhibitors. Part 3: Design, synthesis, and structure–activity relationships of biphenylmethylimidazole derivatives as novel 17,20-lyase inhibitors**

pp 2428–2442

Tomohiro Kaku*, Saori Tsujimoto, Nobuyuki Matsunaga, Toshimasa Tanaka, Takahito Hara, Masuo Yamaoka, Masami Kusaka, Akihiro Tasaka

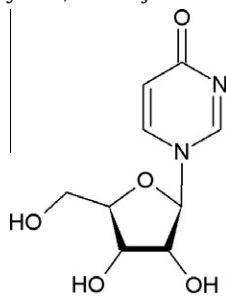


A novel series of biphenylmethylimidazole derivatives were synthesized as inhibitors of 17,20-lyase, and their biological activities were evaluated.

Desulfurization of 2-thiouracil nucleosides: Conformational studies of 4-pyrimidinone nucleosides

pp 2443–2449

Karina Kraszewska, Iwona Kaczyńska, Stefan Jankowski, Janina Karolak-Wojciechowska, Elzbieta Sochacka*



Synthesis, crystal structures and conformations in aqueous solution of 4-pyrimidinone nucleosides were presented

4-pyrimidinone ribofuranoside ($\text{H}^2\text{O}^4\text{U}$)

4-pyrimidinone 2'-deoxyribofuranoside ($\text{dH}^2\text{O}^4\text{U}$)

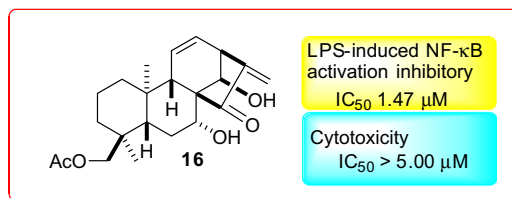
Synthesis, crystal structures and conformations in aqueous solution of 4-pyrimidinone nucleosides were presented.



Synthesis of rabdokunmin C analogues and their inhibitory effect on NF- κ B activation

pp 2450–2457

Yutaka Aoyagi, Yoshiyuki Adachi, Kei Ozawa, Chihiro Yokomizo, Ming-Yu Gui, Yong-Ri Jin, Xu-Wen Li, Naohito Ohno, Koichi Takeya*

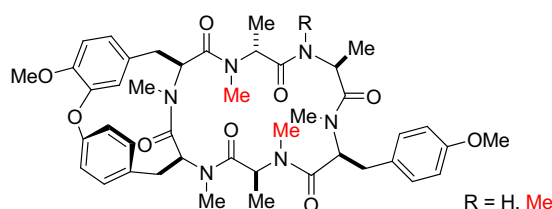


Synthesis of rabdokunmin C analogues was carried out. SAR study of their analogues on inhibitory activity of NF- κ B activation was also reported.

Per-N-methylated analogues of an antitumor bicyclic hexapeptide RA-VII

pp 2458–2463

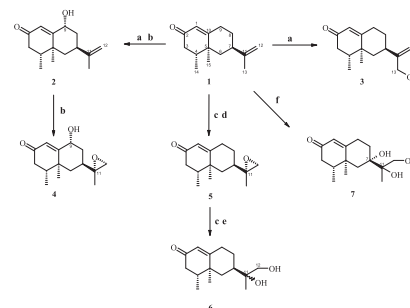
Yukio Hitotsuyanagi, Ji-Ean Lee, Saori Kato, Ik-Hwi Kim, Hideyuki Kohashi, Haruhiko Fukaya, Koichi Takeya*

**Microbial transformation of (+)-nootkatone and the antiproliferative activity of its metabolites**

pp 2464–2469

Anna Gliszczynska, Agnieszka Łysek, Tomasz Janeczko, Marta Świtalska, Joanna Wietrzyk, Czesław Wawrzęńczyk*

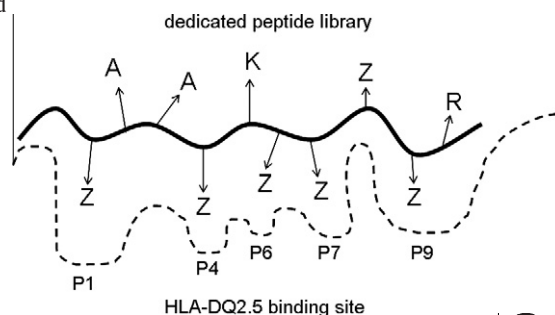
We report the microbial transformation of natural bicyclic ketone (+)-nootkatone (**1**). We proposed the metabolic pathway of (+)-nootkatone in fungal culture studied and showed the antiproliferative activity of obtained metabolites towards cancer cell lines A549 (human lung adenocarcinoma) and HL-60 (human promyelocytic leukemia).

**Assessing high affinity binding to HLA-DQ2.5 by a novel peptide library based approach**

pp 2470–2477

Ulrike Jüse*, Magnus Arntzen, Peter Højrup, Burkhard Fleckenstein, Ludvig M. Sollid

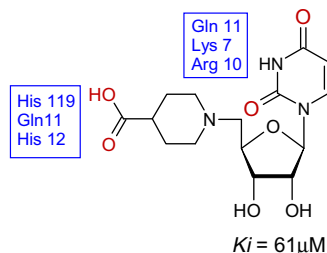
A novel method using soluble peptide libraries with dedicated positions (Z) and soluble recombinant HLA-DQ2.5 for HLA class II peptide binding motif refinement and peptide blocker development.



5'-Modified pyrimidine nucleosides as inhibitors of ribonuclease A

pp 2478–2484

Anirban Samanta, Swagata Dasgupta*, Tanmaya Pathak*



Inhibition of the ribonucleolytic activity of ribonuclease A by 5'-modified pyrimidine nucleosides having free carboxyl groups is reported for the first time.



*Corresponding author

Supplementary data available via ScienceDirect

COVER

The known veterinary anthelmintic and proton ionophore, closantel, was recently discovered to also exhibit potent chitinase inhibition activity and inhibit molting in the parasitic nematode, *Onchocerca volvulus*, the causative agent of the neglected tropical disease onchocerciasis. [C. Gloeckner, A. L. Garner, F. Mersha, Y. Oksov, N. Tricoche, L. M. Eubanks, S. Lustigman, G. F. Kaufmann, K. D. Janda, Repositioning of an existing drug for the neglected tropical disease Onchocerciasis, *Proc. Natl. Acad. Sci., U.S.A.* **2010**, 107, 3424.]

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