

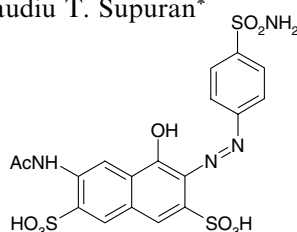
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ARTICLES

Carbonic anhydrase inhibitors: Cloning, characterization, and inhibition studies of the cytosolic isozyme III with sulfonamides

pp 7229–7236

Isao Nishimori, Tomoko Minakuchi, Saburo Onishi, Daniela Vullo, Alessandro Cecchi, Andrea Scozzafava and Claudiu T. Supuran*



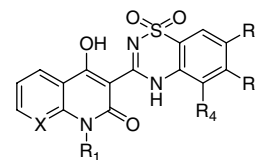
Ki (CA III) = 2.3 μ M

Identification of a series of novel derivatives as potent HCV inhibitors by a ligand-based virtual screening optimized procedure

pp 7237–7247

Georgia Melagraki, Antreas Afantitis, Haralambos Sarimveis,* Panayiotis A. Koutentis, John Markopoulos and Olga Igglessi-Markopoulou

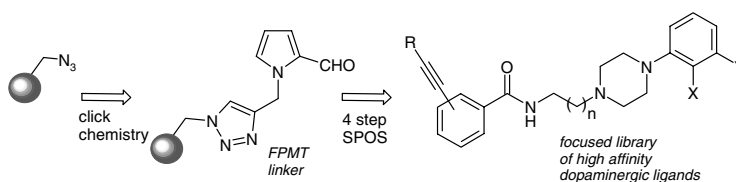
An accurate and reliable QSAR model involving five descriptors that is able to predict successfully the HCV inhibitory potency against genotype 1 HCV polymerase is presented. The effects of various structural modifications on biological activity are investigated and biological activities of novel structures are estimated using the developed QSAR model. More specifically a search for optimized pharmacophore patterns by insertions, substitutions, and ring fusions of pharmacophoric substituents of the main building block scaffolds is described.



Click chemistry based solid phase supported synthesis of dopaminergic phenylacetynes

pp 7248–7257

Pilar Rodriguez Loaiza, Stefan Löber, Harald Hübner and Peter Gmeiner*

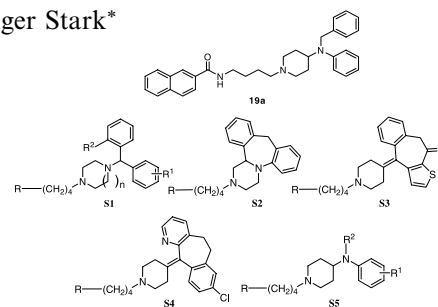


Hybrid approach for the design of highly affine and selective dopamine D₃ receptor ligands using privileged scaffolds of biogenic amine GPCR ligands

pp 7258–7273

Britta C. Sasse, Ulrich R. Mach, Jukka Leppanen, Thierry Calmels and Holger Stark*

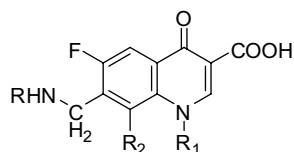
The design and optimization of dopamine D₃ receptor ligands has been performed applying a hybrid structure development. Novel ligands were synthesized containing privileged scaffolds of known histamine H₁ receptor antagonists and fragments of dopamine D₃ receptor-preferring ligands. Compounds were screened in vitro for binding affinities at dopamine D₂ and D₃ receptors, recognizing the most promising compound with a K_i (hD₃) = 0.3 nM and a selectivity ratio of 2343.



Synthesis and structure–activity relationship of 7-(substituted)-aminomethyl-4-quinolone-3-carboxylic acid derivatives

pp 7274–7280

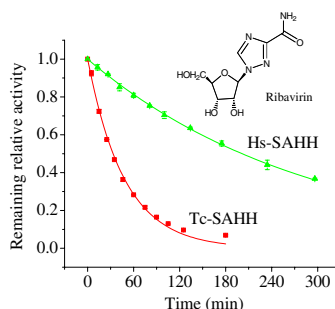
Zhenfa Zhang,* Aizhen Yu and Weicheng Zhou



The antiviral drug ribavirin is a selective inhibitor of S-adenosyl-L-homocysteine hydrolase from *Trypanosoma cruzi*

pp 7281–7287

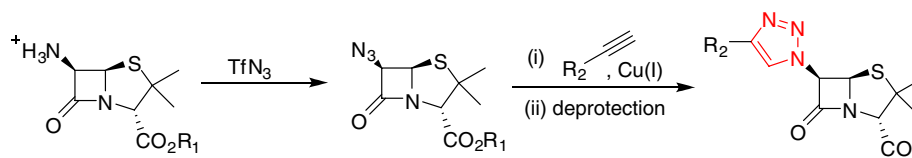
Sumin Cai, Qing-Shan Li, Ronald T. Borchardt, Krzysztof Kuczera and Richard L. Schowen*



Direct diazo-transfer reaction on β -lactam: Synthesis and preliminary biological activities of 6-triazolypenicillanic acids

pp 7288–7300

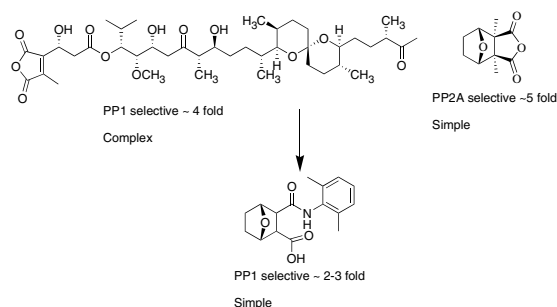
Po C. Chen, Rebekah E. Wharton, Pratiq A. Patel and Adegboyega K. Oyelere*



Synthesis and biological evaluation of norcantharidin analogues: Towards PP1 selectivity

pp 7301–7310

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

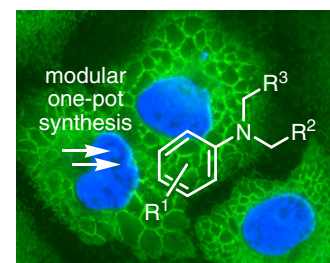


Efficient one-pot synthesis of biologically active polysubstituted aromatic amines

pp 7311–7317

Dirk Menche,* Fatih Arikan, Jun Li, Sven Rudolph and Florenz Sasse

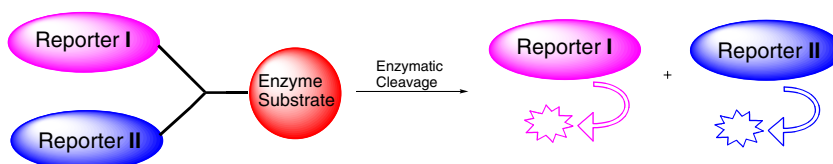
An efficient and modular one-pot synthesis of polysubstituted aromatic amines by a mild reductive amination procedure is described and the biological potential of these nitrogen-centered compounds is demonstrated by growth inhibition of murine connective tissue cells and microscopy-based morphological studies.



Molecular probe for enzymatic activity with dual output

pp 7318–7324

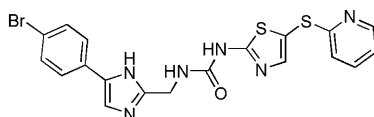
Eyal Danieli and Doron Shabat*



Phenylimidazole derivatives as specific inhibitors of bacterial enoyl-acyl carrier protein reductase FabK

pp 7325–7336

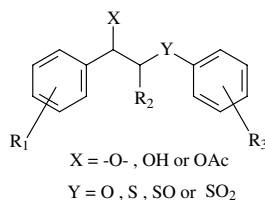
Tomohiro Ozawa, Hideo Kitagawa,* Yasuo Yamamoto, Sho Takahata, Maiko Iida, Yumi Osaki and Keiko Yamada



Streptococcus pneumoniae FabK IC_{50} = 2.4 nM
 MIC_{50} = 1 μ g/mL, MIC_{90} = 4 μ g/mL (against 29 clinical isolates of *S. pneumoniae*)

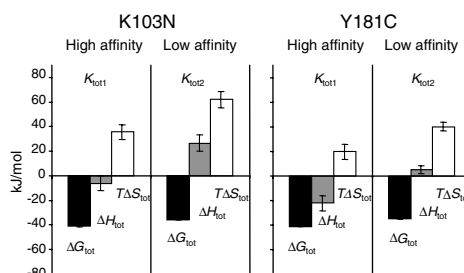
Structure–activity relationship of antileishmanials neolignan analogues

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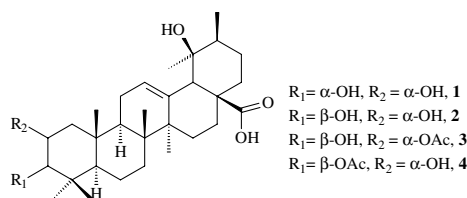
 Mário Aveniente, Eduardo F. Pinto, Lourivaldo S. Santos,
 Bartira Rossi-Bergmann and Lauro E. S. Barata*

Additional level of information about complex interaction between non-nucleoside inhibitor and HIV-1 reverse transcriptase using biosensor-based thermodynamic analysis

pp 7344–7354

Matthis Geitmann* and U. Helena Danielson


Natural triterpenoids from *Cecropia lyratiloba* are cytotoxic to both sensitive and multidrug resistant leukemia cell lines

pp 7355–7360

 Gleice da Graça Rocha, Marisol Simões, Kelly Araujo Lúcio, Rodrigo Rodrigues Oliveira,
 Maria Auxiliadora Coelho Kaplan and Cerli Rocha Gattass*


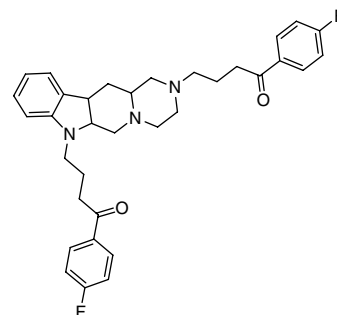
In vitro cytotoxicity of *Cecropia lyratiloba* triterpenoids, euscaphic acid (**1**), tormentic acid (**2**), 2 α -acetyl tormentic acid (**3**), and 3 β -acetyl tormentic acid (**4**) against K562 and K562/VCR leukemia cell lines.

Rational design, synthesis and evaluation of (6a*R,11b*S**)-1-(4-fluorophenyl)-4-{7-[4-(4-fluorophenyl)-4-oxobutyl]1,2,3,4,6,6a,7,11b,12,12a(*RS*)-decahydropyrazino[2',1':6,1]pyrido[3,4-*b*]indol-2-yl}-butan-1-one as a potential neuroleptic agent**

pp 7361–7367

 Ruchika Chakrabarty, Jyoti Rao, Aparna Anand, Abhijeet Deb Roy,
 Raja Roy, G. Shankar, P. R. Dua and Anil K. Saxena*

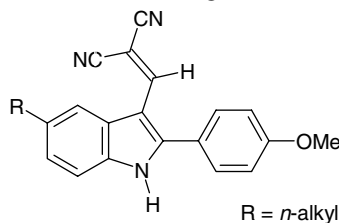
Synthesis and potent neuroleptic activity of a novel 1,2,3,4,6,6a,7,11b,12,12a-decahydropyrazino[2',1':6,1]pyrido[3,4-*b*]indole derivative having *D*₁, *D*₂, and 5-HT_{2A} receptor blocking activity (p*K*_i (5-HT_{2A})/p*K*_i (*D*₂) = 1.42) is reported.



[(2-Phenylindol-3-yl)methylene]propanedinitriles inhibit the growth of breast cancer cells by cell cycle arrest in G₂/M phase and apoptosis

pp 7368–7379

Michaela Pojarová, Doris Kaufmann, Robert Gastpar, Tsuyuki Nishino, Przemyslaw Reszka, Patrick J. Bednarski and Erwin von Angerer*

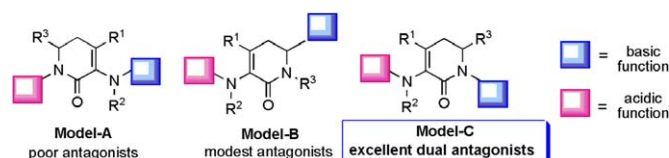


[(5-*n*-Alkyl-2-phenylindol-3-yl)methylene]propane-dinitriles strongly inhibit the growth of human breast cancer cells (IC₅₀: 13–200 nM) by blockade of the cell cycle in G₂/M phase.

**Synthesis and biological evaluation of non-peptide $\alpha_v\beta_3/\alpha_5\beta_1$ integrin dual antagonists containing 5,6-dihydropyridin-2-one scaffolds**

pp 7380–7390

Fides Benfatti, Giuliana Cardillo,* Serena Fabbri, Patrizia Galzerano, Luca Gentilucci, Riccardo Juris, Alessandra Tolomelli, Monica Baiula, Antonino Spartà and Santi Spampinato*

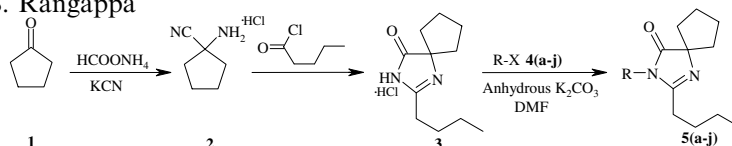


The 5,6-dihydropyridin-2-one was identified as a scaffold to turn into potential integrin ligands, introducing a carboxylic acid and a basic appendage. The synthesis and the antiadhesion activity of a small library of peptidomimetics capable to recognize $\alpha_v\beta_3$ and $\alpha_5\beta_1$ integrins has been herein reported.

Synthesis and screening for acetylcholinesterase inhibitor activity of some novel 2-butyl-1,3-diaza-spiro[4,4]non-1-en-4-ones: Derivatives of irbesartan key intermediate

pp 7391–7398

C. V. Kavitha, S. L. Gaonkar, J. N. Narendra Sharath Chandra, C. T. Sadashiva and K. S. Rangappa*

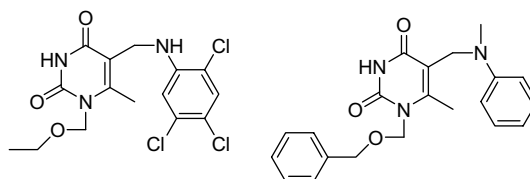


A series of novel 2-butyl-1,3-diaza-spiro[4,4]non-1-en-4-one derivatives have been synthesized by interaction of 2-butyl-1,3-diaza-spiro[4,4]non-1-en-4-one with different bioactive aralkyl halides by two different methods viz., conventional and microwave irradiation. All the synthesized compounds have been screened for their efficacy as acetylcholinesterase (AChE) inhibitor. AChE inhibitory activity was carried out by using Ellman colorimetric assay with neostigmine as a reference standard. Among the compounds synthesized, compounds **5a**, **5b**, **5j** showed good inhibition against AChE.

The design and synthesis of N-1-alkylated-5-aminoaryalkylsubstituted-6-methyluracils as potential non-nucleoside HIV-1 RT inhibitors

pp 7399–7407

Xiao Lu, Yanli Chen, Ying Guo, Zhenming Liu, Yawei Shi, Yang Xu, Xiaowei Wang, Zhili Zhang and Junyi Liu*

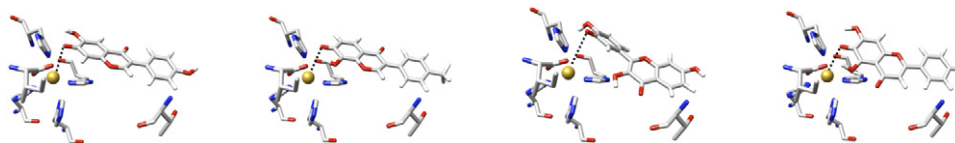


A synthesis route to get a novel series of hydrid analogues of MKC-442 and pyridinon as inhibitors of HIV-1 reverse transcripts and evaluate results about their potent inhibiting activity against HIV-RT.

Structure–activity relationship studies of flavonoids as potent inhibitors of human platelet 12-hLO, reticulocyte 15-hLO-1, and prostate epithelial 15-hLO-2

pp 7408–7425

Yesseny Vasquez-Martinez, Rachana V. Ohri, Victor Kenyon, Theodore R. Holman* and Silvia Sepúlveda-Boza*



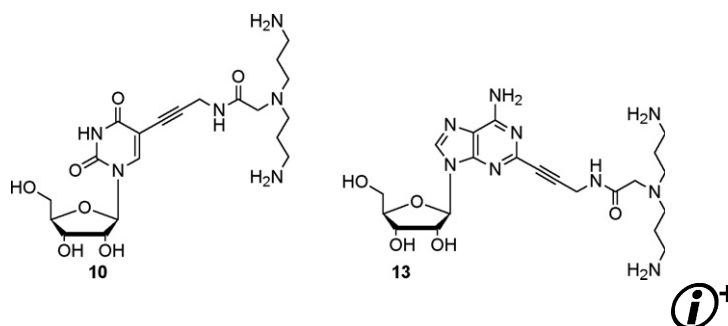
Possible docking modes to 15-hLO-1 for 4 potent, reductive flavonoid inhibitors.

Construction of polyamine-modified uridine and adenosine derivatives—evaluation of DNA binding capacity and cytotoxicity in vitro

pp 7426–7433

Johannes Ghatnekar, Margareta Hägerlöf, Stina Oredsson, Kersti Alm, Sofi K. C. Elmroth* and Tina Persson

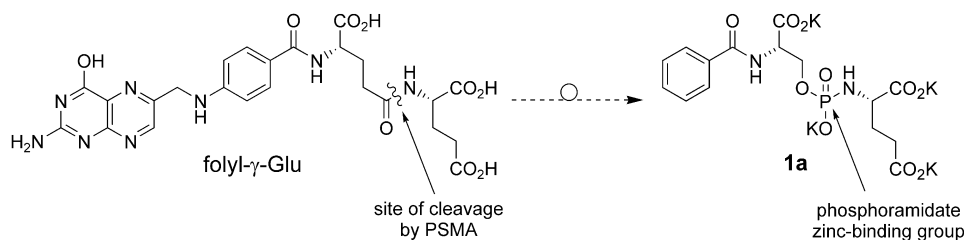
Two novel nucleoside-based polyamine derivatives were synthesized. Their cell growth inhibitory effects and their structural and thermodynamic influence on DNA were investigated.



The molecular pruning of a phosphoramidate peptidomimetic inhibitor of prostate-specific membrane antigen

pp 7434–7443

Lisa Y. Wu, Marc O. Anderson, Yoko Toriyabe, Jack Maung, Tammy Y. Campbell, Cheryl Tajon, Marat Kazak, Jamie Moser and Clifford E. Berkman*

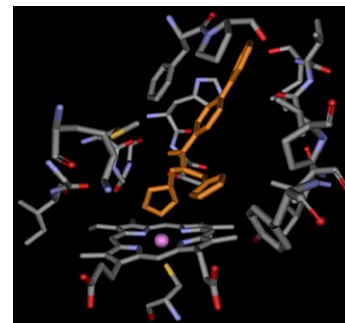


Synthesis, antifungal and antimycobacterial activities of new bis-imidazole derivatives, and prediction of their binding to P450_{14DM} by molecular docking and MM/PBSA method

pp 7444–7458

Daniele Zampieri, Maria Grazia Mamolo,* Luciano Vio, Elena Banfi, Giuditta Scialino, Maurizio Fermeiglia, Marco Ferrone and Sabrina Pricl

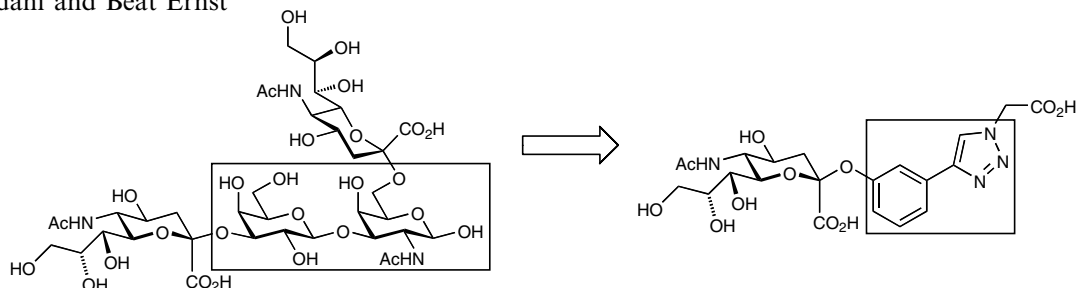
1-Aryl-3-(1H-imidazol-1-yl)-2-[(1H-imidazol-1-yl)methyl]-propan-1-one and 3-(1H-imidazol-1-yl)-2-[(1H-imidazol-1-yl)methyl]-1-(thiophen-2-yl)-propan-1-one derivatives were synthesized and tested for their in vitro antifungal and antimycobacterial activity. Molecular modeling investigations showed that the active compounds may interact at the active site of the fungal cytochrome P450-dependent sterol 14 α -demethylase in the sterol biosynthesis pathway and that their binding free energy values are in agreement with their MIC values.



Mimetics of the tri- and tetrasaccharide epitope of GQ1b α as myelin-associated glycoprotein (MAG) ligands

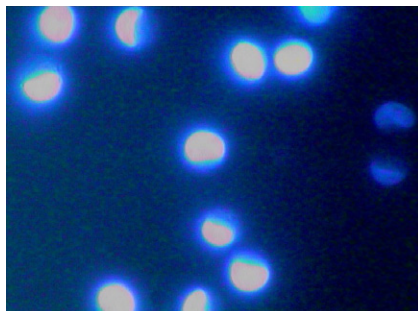
pp 7459–7469

Ganpan Gao, Martin Smiesko, Oliver Schwardt, Heiko Gäthje, Soerge Kelm, Angelo Vedani and Beat Ernst*

**New functional assay of P-glycoprotein activity using Hoechst 33342**

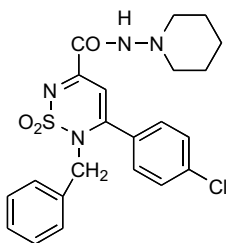
pp 7470–7479

Henrik Müller, Werner Klinkhammer, Christoph Globisch, Matthias U. Kassack, Ilza K. Pajeva and Michael Wiese*

**Discovery of 1,1-dioxo-1,2,6-thiadiazine-5-carboxamide derivatives as cannabinoid-like molecules with agonist and antagonist activity**

pp 7480–7493

Carolina Cano, Pilar Goya, Juan Antonio Paez,* Rocío Girón, Eva Sánchez and María Isabel Martín

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*Corresponding author

i+ Supplementary data available via ScienceDirect

COVER

An efficient and modular one-pot synthesis of polysubstituted aromatic amines by a mild reductive amination procedure is described and the biological potential of these nitrogen-centered compounds is demonstrated by growth inhibition of murine connective tissue cells and microscopy-based morphological studies. [Menche, D.; Arian, F.; Li, J.; Rudolph, S.; Sasse, F. *Bioorg. Med.* **2007**, *15*, 7311–7317].

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