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Bioorganic & Medicinal Chemistry Vol. 16, No. 23, 2008

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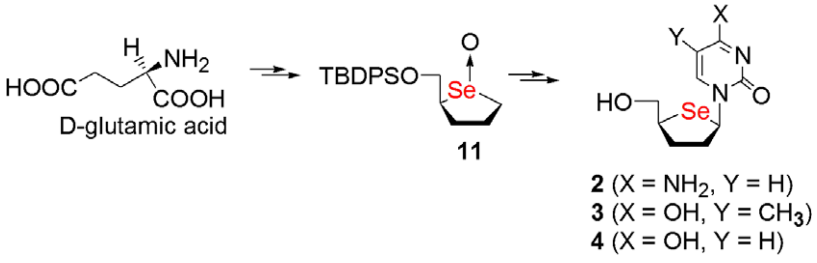
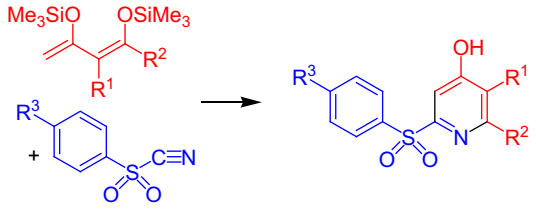
ARTICLES

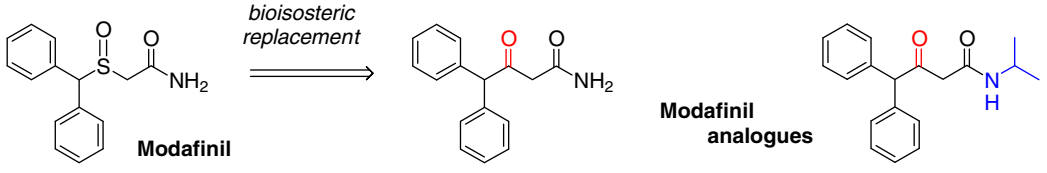
Design and synthesis of novel 2′,3′-dideoxy-4′-selenonucleosides as potential antiviral agents **pp 9891–9897**
Lak Shin Jeong *, Yoo Na Choi, Dilip K. Tosh, Won Jun Choi, Hea Ok Kim, Jungwon Choi



Hetero-Diels–Alder reaction of 1,3-bis(trimethylsilyloxy)-1,3-butadienes with arylsulfonylcyanides. Synthesis and antimicrobial activity of 4-hydroxy-2-(arylsulfonyl)pyridines **pp 9898–9903**
Ibrar Hussain, Mirza Arfan Yawer, Michael Lalk, Ulrike Lindequist, Alexander Villinger, Christine Fischer, Peter Langer *



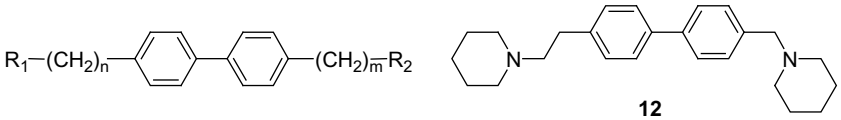
Efficient synthesis and biological evaluation of two modafinil analogues **pp 9904–9910**
Carmela De Risi *, Luca Ferraro, Gian P. Pollini, Sergio Tanganelli, Filippo Valente, Augusto C. Veronese



Non classical bioisosters of modafinil were synthesized through replacement of the sulfoxide function with a carbonyl group and modification of the carboxylic acid amide functionality, and evaluated for their effects on the spontaneous and the electrically-evoked tritiated serotonin ([3H]5-HT) efflux from rat cortical slices.

Synthesis and structure–activity relationships for biphenyl H_3 receptor antagonists with moderate anti-cholinesterase activity pp 9911–9924

Giovanni Morini, Mara Comini, Mirko Rivara, Silvia Rivara*, Fabrizio Bordi, Pier Vincenzo Plazzi, Lisa Flammini, Francesca Saccani, Simona Bertoni, Vigilio Ballabeni, Elisabetta Barocelli, Marco Mor



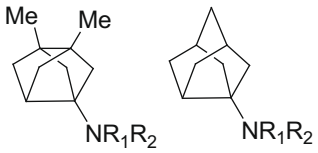
12

rH_3 pK_i=8.08 hH_3 pK_i=8.70
Cholinesterase inhibition pIC_{50}=5.96

A series of H_3-antagonists with a 4,4′-biphenyl scaffold was developed, in which the terminal groups were modulated, providing compounds with high H_3 receptor binding affinity and antagonist potency, together with moderate anti-cholinesterase activity.

Synthesis and pharmacological evaluation of several ring-contracted amantadine analogs pp 9925–9936

Pelayo Camps, María D. Duque, Santiago Vázquez*, Lieve Naesens, Erik De Clercq, Francesc X. Sureda, Marta López-Querol, Antoni Camins, Mercè Pallàs, S. Radhika Prathalingam, John M. Kelly, Vanessa Romero, Dolores Ivorra, Diego Cortés

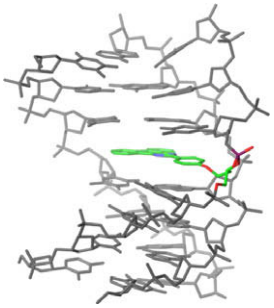


Several bisnoradamantylamines and noradamantylamines have been synthesized and their antiviral, trypanocidal, NMDA receptor antagonist, and dopamine reuptake inhibitory activities have been studied.

Using an aryl phenanthroimidazole moiety as a conjugated flexible intercalator to improve the hybridization efficiency of a triplex-forming oligonucleotide pp 9937–9947

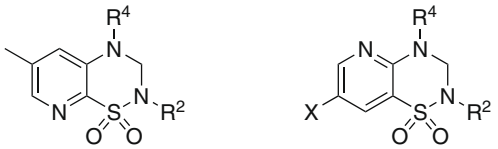
Amany M. A. Osman, Per T. Jørgensen, Niels Bomholt, Erik B. Pedersen*

New intercalating monomer with a phenanthroimidazole moiety show extraordinary high thermal stability of the corresponding Hoogsteen-type triplexes and Hoogsteen-type parallel duplexes with high discrimination to Hoogsteen mismatches.



Synthesis and pharmacological evaluation of a second generation of pyridothiadiazine 1,1-dioxides acting as AMPA potentiators pp 9948–9956

Pierre Francotte*, Pascal de Tullio, Tchao Podona, Ousmane Diouf, Pierre Fraikin, Pierre Lestage, Laurence Danober, Jean-Yves Thomas, Daniel-Henri Caignard, Bernard Pirotte

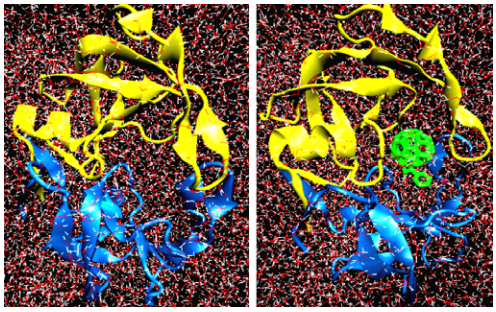


X = F, Cl, Br, CH_3
R^2 = H, CH_3
R^4 = CH_3, CH_2CH_3

Computational design of novel fullerene analogues as potential HIV-1 PR inhibitors: Analysis of the binding interactions between fullerene inhibitors and HIV-1 PR residues using 3D QSAR, molecular docking and molecular dynamics simulations **pp 9957–9974**

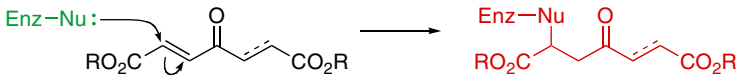
Serdar Durdagi *, Thomas Mavromoustakos, Nikos Chronakis, Manthos G. Papadopoulos *

A series of experimentally reported as well as computationally designed [60]fullerene analogues have been used in order to analyze the binding interactions between fullerene based inhibitors and HIV-1 PR with employing combined docking, MD simulations and 3D QSAR studies.



Irreversible inhibition of dihydrodipicolinate synthase by 4-oxo-heptenedioic acid analogues **pp 9975–9983**

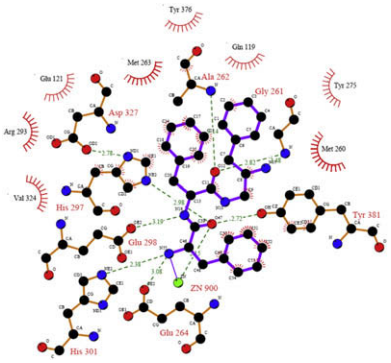
Berin A. Boughton, Michael D. W. Griffin, Paul A. O'Donnell, Renwick C. J. Dobson, Matthew A. Perugini, Juliet A. Gerrard, Craig A. Hutton *



Novel 3-phenylpropane-1,2-diamine derivates as inhibitors of aminopeptidase N (APN) **pp 9984–9990**

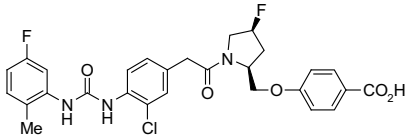
Luqing Shang, Qiang Wang, Hao Fang, Jiajia Mu, Xuejian Wang, Yumei Yuan, Binghe Wang, Wenfang Xu *

The most active compound **12i** was built and docked into the active site of APN (PDB code: 2DQM) using Sybyl7.0. The docking result was showed by LIGPLOT.



Identification of 4-[1-[3-chloro-4-[*N*′-(5-fluoro-2-methylphenyl)ureido]phenylacetyl]-(4*S*)-fluoro-(2*S*)-pyrrolidinylmethoxy]benzoic acid as a potent, orally active VLA-4 antagonist **pp 9991–10000**

Fumihito Muro *, Shin Iimura, Yoshiyuki Yoneda, Jun Chiba, Toshiyuki Watanabe, Masaki Setoguchi, Yutaka Iigou, Gensuke Takayama, Mika Yokoyama, Tohru Takashi, Atsushi Nakayama, Nobuo Machinaga



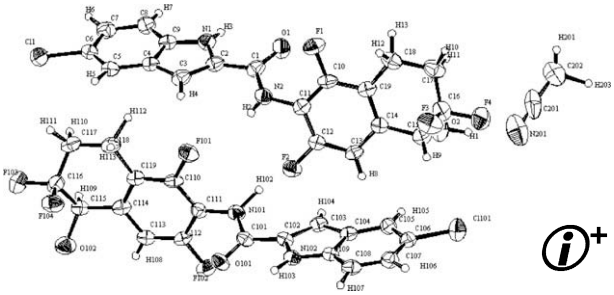
20l: VLA-4/VCAM-1 binding assay, IC_{50}= 1.6 nM

A series of benzoic acid derivatives were synthesized and evaluated for VLA-4 inhibitory activity in a receptor binding assay. A representative compound **20l** demonstrated efficacy in murine asthma model by oral dosing.

Design, synthesis, and pharmacological evaluation of *N*-bicyclo-5-chloro-1*H*-indole-2-carboxamide derivatives as potent glycogen phosphorylase inhibitors pp 10001–10012

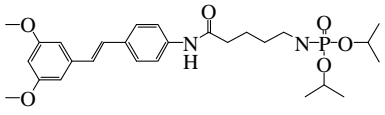
Kenichi Onda *, Ryota Shiraki, Takashi Ogiyama, Kazuhiro Yokoyama, Kazuhiro Momose, Naoko Katayama, Masaya Orita, Tomohiko Yamaguchi, Masako Furutani, Noritaka Hamada, Makoto Takeuchi, Minoru Okada, Mitsuaki Ohta, Shin-ichi Tsukamoto

5-Chloro-*N*-[(5*R*)-1,3,6,6-tetrafluoro-5-hydroxy-5,6,7,8-tetrahydronaphthalen-2-yl]-1*H*-indole-2-carboxamide are potent inhibitors of human liver glycogen phosphorylase *a* (hLGPa) that inhibited glucagon-induced glucose output in cultured primary hepatocytes and showed oral hypoglycemic activity in diabetic db/db mice.



The design, synthesis, and anti-tumor mechanism study of *N*-phosphoryl amino acid modified resveratrol analogues pp 10013–10021

Huachen Liu, Aijun Dong, Chunmei Gao, Chunyan Tan, Hongxia Liu, Xuyu Zu, Yuyang Jiang *

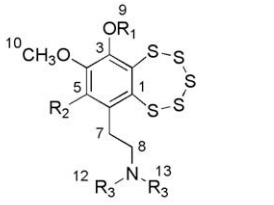


IC_{50} 3.45 ± 0.82 μM

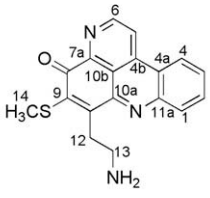
Twenty novel *N*-phosphoryl amino acid modified resveratrol analogues have been synthesized and characterized. Among them, compound **8d** has the most potent anti-proliferative activity against CNE-2 cells with IC_{50} value at 3.45 ± 0.82 μM. Further mechanism study has suggested that **8d** can induce cells apoptosis through the mitochondrial pathway.

Discovery of new pyridoacridine alkaloids from *Lissoclinum* cf. *badium* that inhibit the ubiquitin ligase activity of Hdm2 and stabilize p53 pp 10022–10028

Jason A. Clement, Jirouta Kitagaki, Yili Yang, Carrie J. Saucedo, Barry R. O'Keefe, Allan M. Weissman *, Tawnya C. McKee *, James B. McMahon



1 $R_1 = R_2 = H$; $R_3 = CH_3$
2 $R_1 = CH_3$; $R_2 = R_3 = H$
3 $R_1 = CH_3$; $R_2 = SCH_3$; $R_3 = CH_3$



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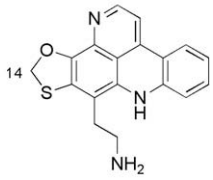
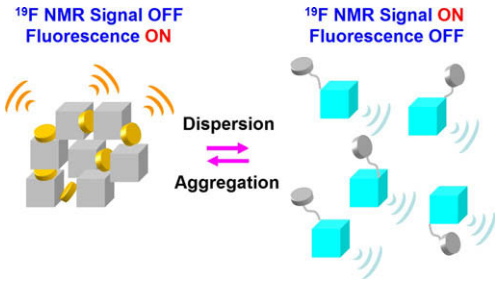


5

Ratiometric multimodal chemosensors based on cubic silsesquioxanes for monitoring solvent polarity pp 10029–10033

Kazuo Tanaka, Kenichi Inafuku, Yoshiki Chujo *

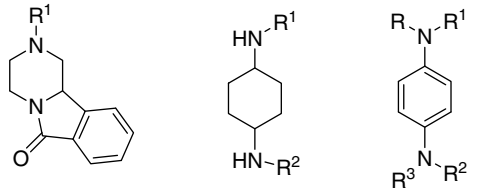


We report the multi-functionalized cubic silsesquioxane (POSS) as the ratiometric multimodal chemosensors for monitoring solvent polarity with fluorescence and ^{19}F NMR.

Design, synthesis and preliminary pharmacological evaluation of new analogues of DM232 (unifiram) and DM235 (sunifiram) as cognition modulators **pp 10034–10042**

Elisabetta Martini, Monica Norcini, Carla Ghelardini, Dina Manetti, Silvia Dei, Luca Guandalini, Michele Melchiorre, Simona Pagella, Serena Scapecchi, Elisabetta Teodori, Maria Novella Romanelli *

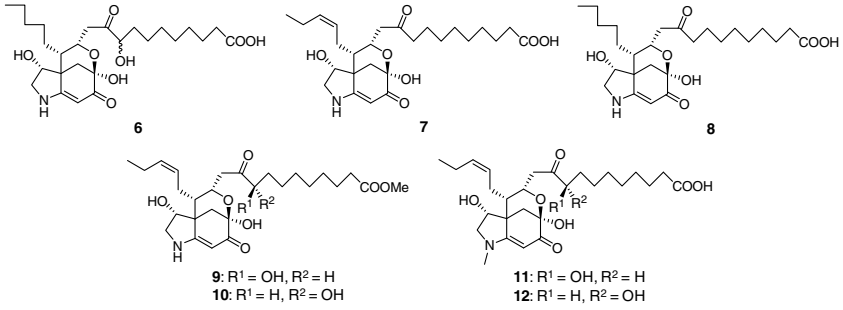
A series of 1,2,3,4-tetrahydropyrazino[2,1-*a*]isoindol-6(2*H*)-one, 1,4-diamino-cyclohexane or 1,4-diaminobenzene derivatives have been synthesized and tested in the mouse passive-avoidance test. Some compounds display good cognition-enhancing activity, while other are endowed with amnesia inducing properties.



R^1, R^2 = MeCO, EtCO, PhCO, $iPrSO_2$, 4-F-$C_6H_4SO_2$
R, R^3 = H, CH_3

Structure and biological activity of novel FN analogs as flowering inducers **pp 10043–10048**

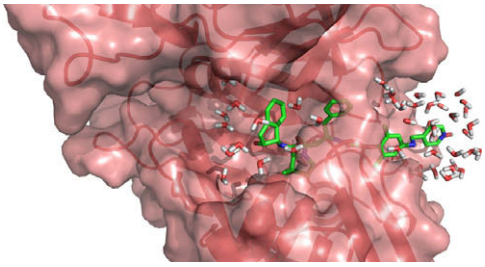
Kenji Kai, Jun Takeuchi, Taichi Kataoka, Mineyuki Yokoyama, Naoharu Watanabe *



Antimalarial activity enhancement in hydroxymethylcarbonyl (HMC) isostere-based dipeptidomimetics targeting malarial aspartic protease plasmepsin **pp 10049–10060**

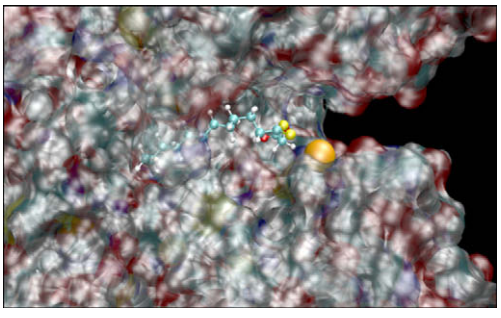
Koushi Hidaka, Tooru Kimura, Adam J. Ruben, Tsuyoshi Uemura, Mami Kamiya, Aiko Kiso, Tetsuya Okamoto, Yumi Tsuchiya, Yoshio Hayashi, Ernesto Freire, Yoshiaki Kiso *

We identified mono-substituted amino derivatives of an allophenylnorstatine-containing plasmepsin inhibitor with promising anti-malarial activity and low cytotoxicity.

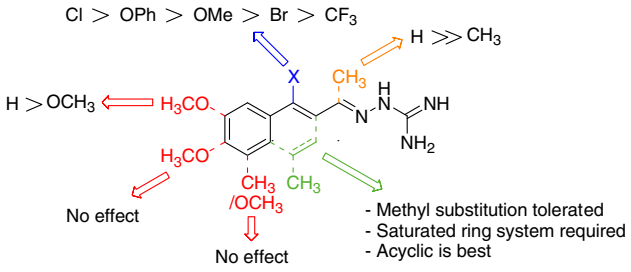


Substituted hippurates and hippurate analogs as substrates and inhibitors of peptidylglycine α-hydroxylating monooxygenase (PHM) **pp 10061–10074**

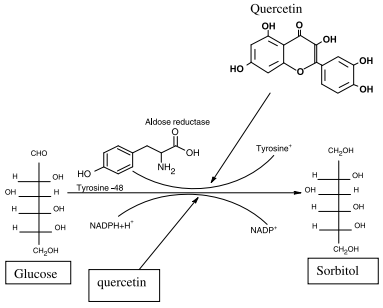
David J. Merkler *, Alexander S. Asser, Laura E. Baumgart, Natalie Carballo, Sarah E. Carpenter, Geoffrey H. Chew, Casey C. Cosner, Jodi Dusi, Lamar C. Galloway, Andrew B. Lowe, Edward W. Lowe Jr., Lawrence King III, Robert D. Kendig, Paul C. Kline, Robert Malka, Kathleen A. Merkler, Neil R. McIntyre, Mindy Romero, Benjamin J. Wilcox, Terence C. Owen



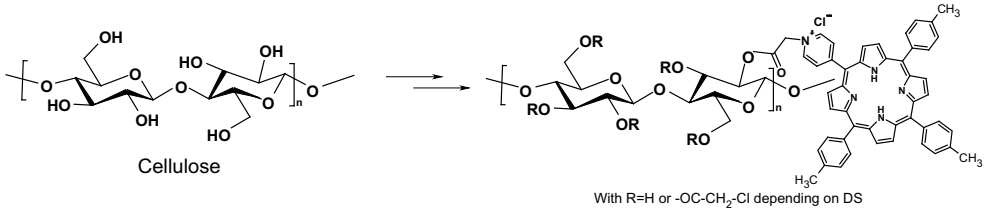
Synthesis and biological evaluation of guanylhydrazone coactivator binding inhibitors for the estrogen receptor **pp 10075–10084**
Andrew L. LaFrate, Jillian R. Gunther, Kathryn E. Carlson, John A. Katzenellenbogen *



Inhibition of aldose reductase from cataracted eye lenses by finger millet (*Eleusine coracana*) polyphenols **pp 10085–10090**
S. Chethan, Shylaja M. Dharmesh *, Nagappa G. Malleshi

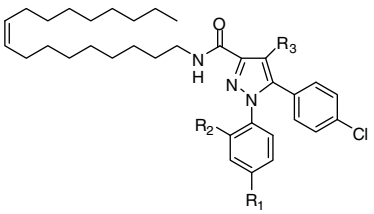


Photobactericidal plastic films based on cellulose esterified by chloroacetate and a cationic porphyrin **pp 10091–10097**
Mohammed Krouit, Robert Granet, Pierre Krausz *



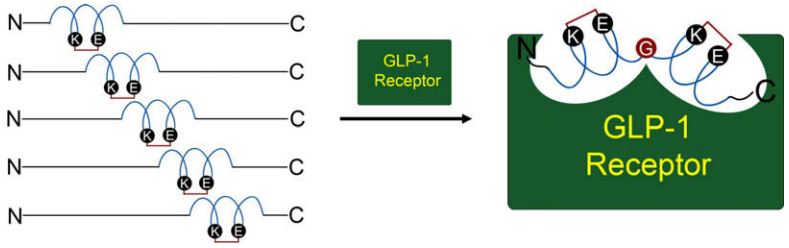
Plastic films obtained by cellulose acylation with chloroacetyl chloride were further modified by reaction with *para*-5-pyridyl-10,15,20-tritolylporphyrin. The resulting material displayed photobactericidal activity against *Staphylococcus aureus* and *Escherichia coli*.

Antiobesity designed multiple ligands: Synthesis of pyrazole fatty acid amides and evaluation as hypophagic agents **pp 10098–10105**
Mario Alvarado, Pilar Goya *, Manuel Macías-González, Francisco Javier Pavón, Antonia Serrano, Nadine Jagerovic, Jose Elguero, Angel Gutiérrez-Rodríguez, Santiago García-Granda, Margarita Suardíaz, Fernando Rodríguez de Fonseca *

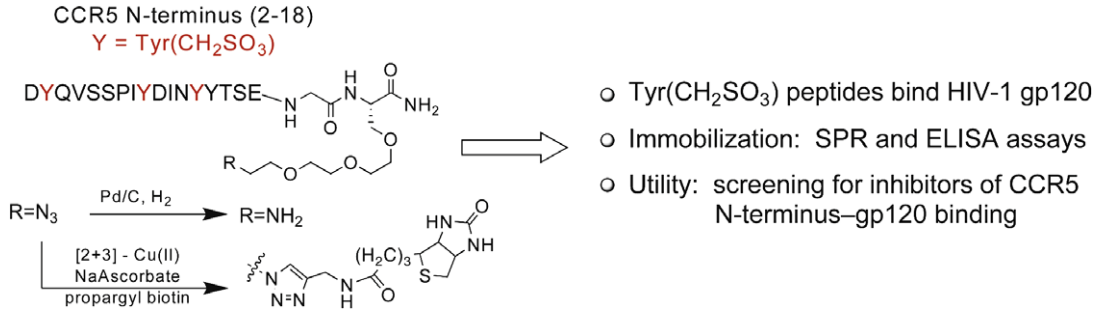


Pyrazole fatty acid amides have been synthesized from suitable pyrazole esters, and oleyl and hexadecyl amines. The compounds reduce food intake in rats. The oleyl derivatives are PPARα activators.

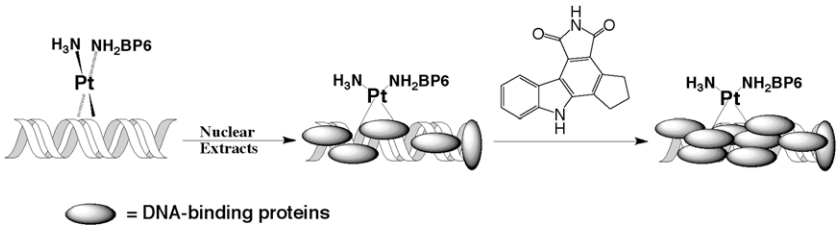
Search for α-helical propensity in the receptor-bound conformation of glucagon-like peptide-1 **pp 10106–10112**
Eunice N. Murage, Jonathan C. Schroeder, Martin Beinborn, Jung-Mo Ahn *



Tyrosine-sulfate isosteres of CCR5 N-terminus as tools for studying HIV-1 entry **pp 10113–10120**
Son N. Lam, Priyamvada Acharya, Richard Wyatt, Peter D. Kwong, Carole A. Bewley *

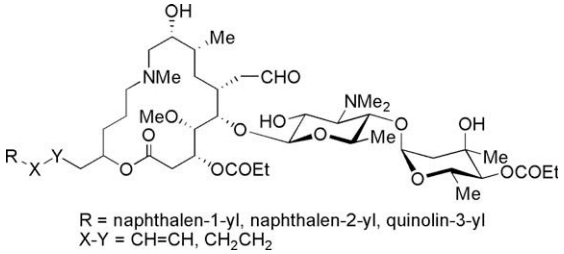


Poly(ADP-ribose) polymerase-1 activity facilitates the dissociation of nuclear proteins from platinum-modified DNA **pp 10121–10128**
Evan R. Guggenheim, Alison E. Ondrus, Mohammad Movassaghi, Stephen J. Lippard *



Inhibitors of the enzyme poly(ADP-ribose) polymerase-1 were synthesized; these inhibitors increase the ability of nuclear proteins to bind Pt-modified DNA.

Novel azalides derived from 16-membered macrolides. Part II: Isolation of the linear 9-formylcarboxylic acid and its sequential macrocyclization with an amino alcohol or an azidoamine **pp 10129–10156**
Tomoaki Miura *, Kenichi Kanemoto, Satomi Natsume, Kunio Atsumi, Hideki Fushimi, Takuji Yoshida, Keiichi Ajito *



The design and synthesis of novel 14- to 16-membered 11-azalides and 11-azalactams starting from 16-membered macrolides are described. Fifteen-substituted 16-membered azalides exhibited more potent antibacterial activities against resistant bacteria of *Streptococcus pneumoniae*.

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Instructions to contributors **p I**

*Corresponding author
ⓘ+ Supplementary data available via ScienceDirect

COVER

An insight into biologically relevant chemical space showing the scaffolds of potential natural-product based inhibitors orbiting their target, the protein structure of protein 11-beta steroid dehydrogenase (PDB code 1xu7). Graphic produced using Pymol (http://www.pymol.org). [M. A. Koch, A. Schuffenhauer, M. Scheck, S. Wetzel, M. Casaulta, A. Odermatt, P. Ertl, H. Waldmann, Charting biologically relevant chemical space: A structural classification of natural products (SCONP), *PNAS* **2005**, *102*, 17272–17277 and S. Wetzel, H. Waldmann, Cheminformatic analysis of natural products and their chemical space, *Chimia* **2007**, *61*(6), 355–360].

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