

Organic & Biomolecular Chemistry

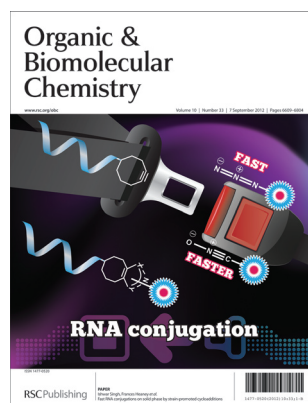
An international journal of synthetic, physical and biomolecular organic chemistry

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IN THIS ISSUE

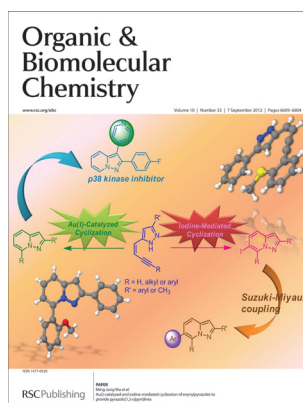
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Cover

See Ishwar Singh, Frances Heaney *et al.*, pp. 6633–6639.

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Inside cover

See Ming-Jung Wu *et al.*, pp. 6640–6648.

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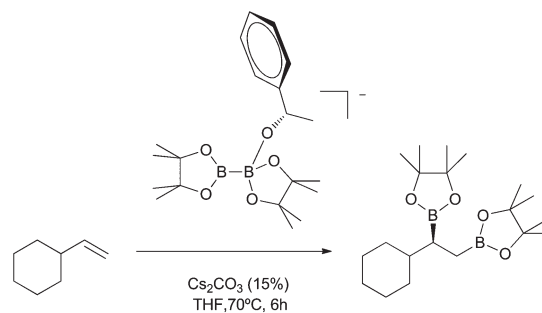
COMMUNICATIONS

6621

Asymmetric organocatalytic diboration of alkenes

Amadeu Bonet, Cristina Sole, Henrik Gulyás* and Elena Fernández*

The use of chiral alcohols to form the Lewis acid–base $^*RO^- \rightarrow$ bis(pinacolato)diboron adduct, *in situ*, provides an opportunity to induce asymmetry in the organocatalytic diboration of alkenes and complements the well established transition metal-mediated enantioselective diboration.

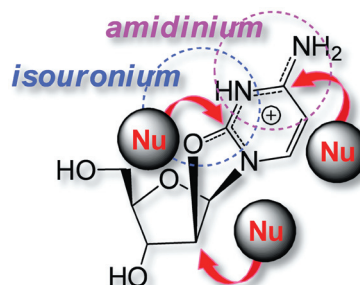


6624

Essential reactive intermediates in nucleoside chemistry: cyclonucleoside cations

Anatoly M. Belostotskii,* Elisheva Genizi and Alfred Hassner

Cyclonucleoside cations are reactive intermediates in a broad group of nucleoside reactions.



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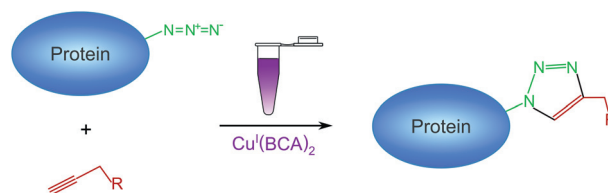
COMMUNICATIONS

6629

Evaluation of bicinchoninic acid as a ligand for copper(I)-catalyzed azide–alkyne bioconjugations

Erik H. Christen, Raphael J. Gübeli, Beate Kaufmann, Lars Merkel, Ronald Schoenmakers, Nediljko Budisa, Martin Fussenegger, Wilfried Weber* and Birgit Wiltschi

The Cu(I)–bicinchoninic acid (BCA) complex is an efficient catalyst for azide–alkyne bioconjugations.



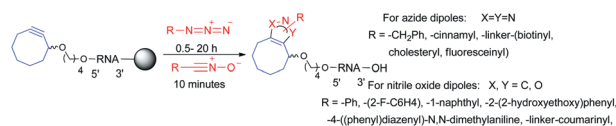
PAPERS

6633

Fast RNA conjugations on solid phase by strain-promoted cycloadditions

Ishwar Singh,* Colin Freeman, Annemieke Madder, Joseph S. Vyle and Frances Heaney*

An RNA-conjugation tool box has been developed using strain-promoted azide–alkyne cycloaddition (SPAAC) and more rapid strain-promoted nitrile oxide cycloaddition (SPNOAC) chemistries on solid-supported substrates. The conjugation is clean and easily executed under very mild conditions within minutes.

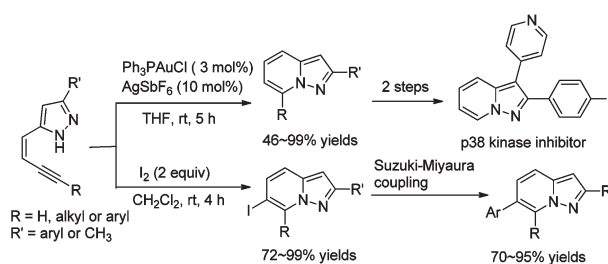


6640

Au(I)-catalyzed and iodine-mediated cyclization of enynylpyrazoles to provide pyrazolo[1,5-*a*]pyridines

Hung-Chou Wu, Chia-Wen Yang, Long-Chih Hwang and Ming-Jung Wu*

Pyrazolo[1,5-*a*]pyridines and 6-iodopyrazolo[1,5-*a*]pyridines were synthesized by gold-catalyzed and iodine-mediated cyclization of enynylpyrazoles in good to excellent yields. The adducts were converted to 6-arylpyrazolo[1,5-*a*]pyridines via Suzuki–Miyaura coupling, and 6-cyanopyrazolo[1,5-*a*]pyridines by Ullmann condensation. One of the cyclization adducts was converted to a p38 kinase inhibitor in two steps.

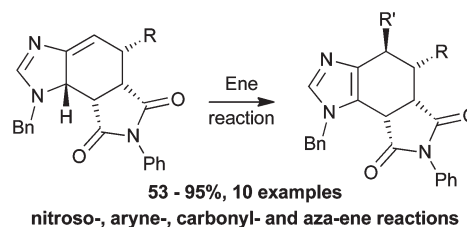


6649

Diastereoselective intermolecular ene reactions: synthesis of 4,5,6,7-tetrahydro-1*H*-benzo[*d*]imidazoles

Lynsey J. Watson, Ross W. Harrington, William Clegg and Michael J. Hall*

D–A cycloadducts of 4-vinylimidazoles and *N*-phenylmaleimide undergo high-yielding ene reactions generating, over two steps, up to 5 new stereocentres.



New process for crystal data files

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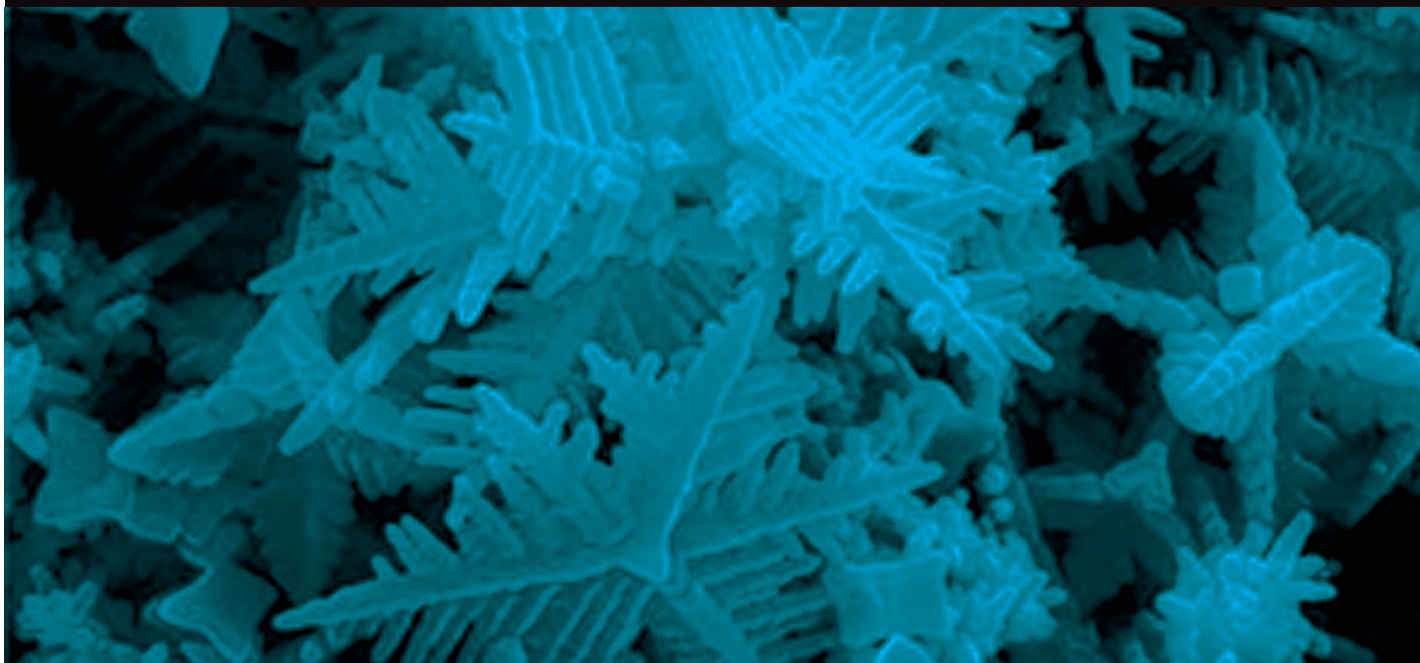


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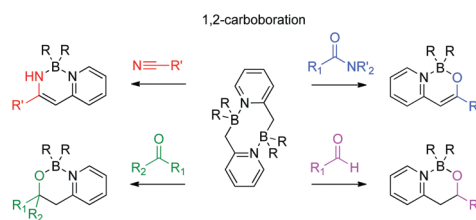
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6656

1,2-Nucleophilic addition of 2-(picolyl)organoboranes to nitrile, aldehyde, ketone, and amide

Jung-Ho Son and James D. Hoefelmeyer*

Reaction of 2-(picolyl)boranes with polar unsaturated bonds leads to 1,2-nucleophilic addition.

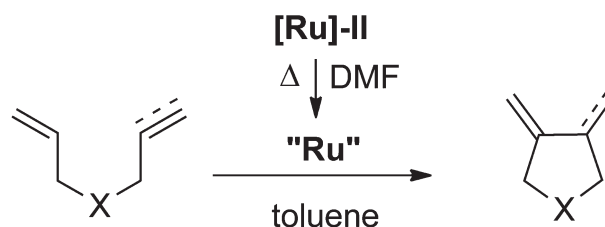


6665

Cycloisomerization of dienes and enynes catalysed by a modified ruthenium carbene species

Álvaro Mallagaray, Kazem Mohammadianejad-Abbasabadi, Sandra Medina, Gema Domínguez and Javier Pérez-Castells*

Modified [Ru]-II catalyse cycloisomerization of dienes and enynes.

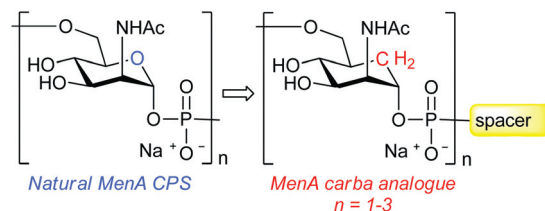


6673

Synthesis and preliminary biological evaluation of *carba* analogues from *Neisseria meningitidis* A capsular polysaccharide

Qi Gao, Cristina Zaccaria, Marta Tontini, Laura Poletti, Paolo Costantino and Luigi Lay*

The synthesis of phosphodiester-linked *carba* analogues of the corresponding *Neisseria meningitidis* A capsular polysaccharide fragments, and their preliminary biological evaluation is described.

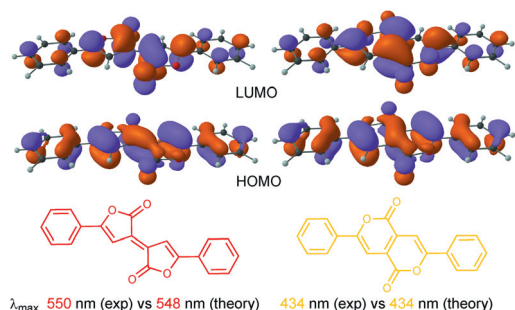


6682

Time-dependent density functional theory (TDDFT) modelling of Pechmann dyes: from accurate absorption maximum prediction to virtual dye screening

Eric Assen B. Kantchev,* Tyler B. Norsten* and Michael B. Sullivan

An accurate computational (TDDFT) method for the estimation of λ_{\max} of Pechmann dye and related compounds was evaluated and then applied to virtual screening of novel heterocycle-substituted Pechmann dyes.



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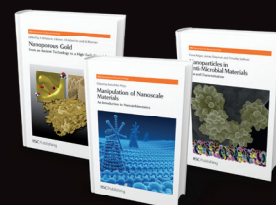
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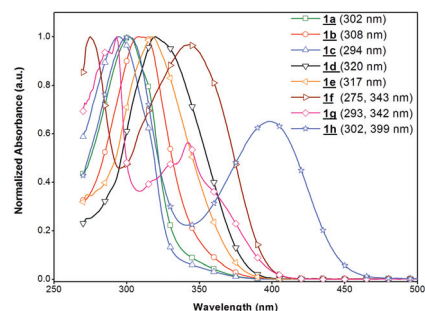
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6693

Novel multifunctional organic semiconductor materials based on 4,8-substituted 1,5-naphthyridine: synthesis, single crystal structures, opto-electrical properties and quantum chemistry calculation

Kun-Yan Wang, Chen Chen, Jin-Fang Liu, Qin Wang, Jin Chang, Hong-Jun Zhu* and Chong Li

A series of 4,8-substituted 1,5-naphthyridines have been successfully synthesised by a Suzuki cross-coupling between 4,8-dibromo-1,5-naphthyridine and the corresponding boronic acids in the presence of catalytic palladium acetate in yields of 41.4–75.8%.

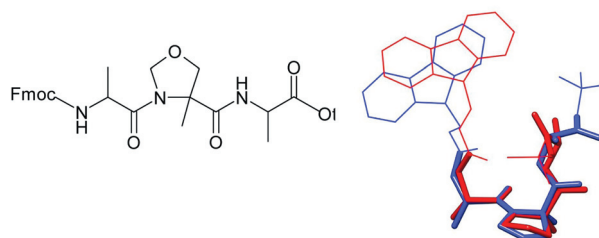


6705

4-Methylpseudoproline derived from α -methylserine – synthesis and conformational studies

Joanna Katarzyńska, Adam Mazur, Wojciech M. Wolf, Simon J. Teat, Stefan Jankowski,* Mirosław T. Leplawy and Janusz Zabrocki*

Synthesis and preferred conformation of two diastereomeric tripeptides, containing a central, novel C α -tetrasubstituted pseudoproline residue (*R*) or (*S*)-(α Me)Ser($\Psi^{H,H}$ Pro) are presented. The conformational analysis is based on NMR, X-ray diffraction experiments and on theoretical energy calculations.

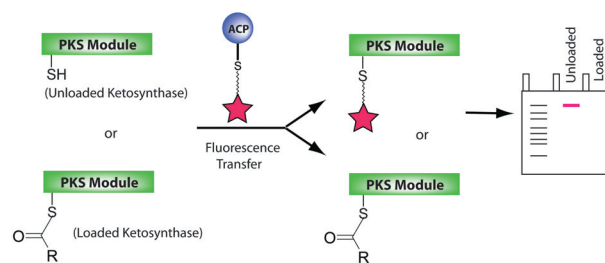


6717

A mechanism-based fluorescence transfer assay for examining ketosynthase selectivity

Gitanjali Prasad, Lawrence S. Borketey, Tsung-Yi Lin and Nathan A. Schnarr*

We have developed a mechanism-based, fluorescence transfer assay for a key enzyme component of all polyketide synthases, the ketosynthase domain. This method can be used with both ketosynthase-containing didomains and full modules.

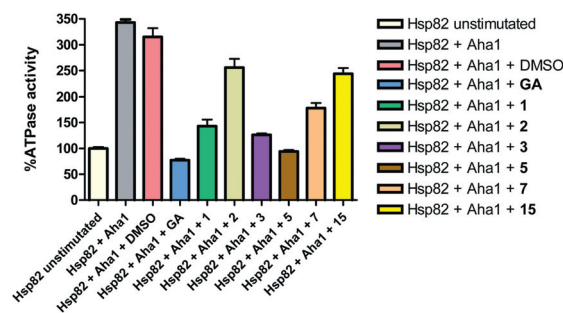


6724

Fluorine- and rhenium-containing geldanamycin derivatives as leads for the development of molecular probes for imaging Hsp90

Frank Wuest,* Vincent Bouvet, BaoChan Mai and Paul LaPointe

This work describes the development of various fluorine-containing and rhenium-containing geldanamycin derivatives as leads for the development of corresponding ^{18}F -labeled and $^{99\text{m}}\text{Tc}$ -labeled PET and SPECT probes for molecular imaging of Hsp90 expression.



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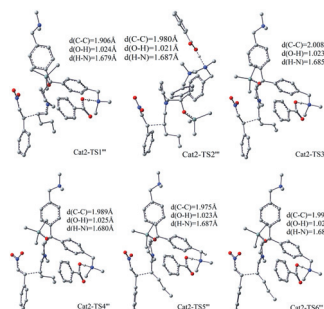
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6732

The roles of benzoic acid and water on the Michael reactions of pentanal and nitrostyrene catalyzed by diarylprolinol silyl ether

Jin Zhou, Qing Chang, Li-Hua Gan* and Yun-Gui Peng

The optimized structures and the key bond lengths of the transition states in Michael reactions between pentanal and nitrostyrene catalyzed by Cat2 with benzoic acid attached at the B3LYP/6-31G(d,p) level of theory.

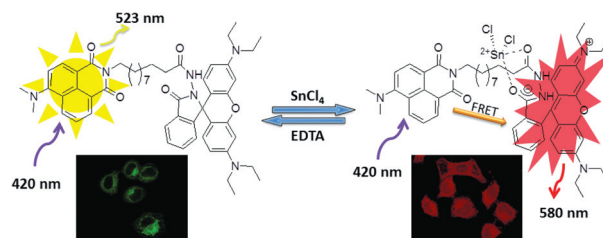


6740

A highly selective fluorescence sensor for Tin (Sn⁴⁺) and its application in imaging live cells

Qi Wang, Chunyan Li, Ying Zou, Haoxuan Wang, Tao Yi* and Chunhui Huang

A naphthalimide–rhodamine B derivative was synthesized as a fluorescence turn-ON chemodosimeter for Sn⁴⁺ in both solution and living cells.

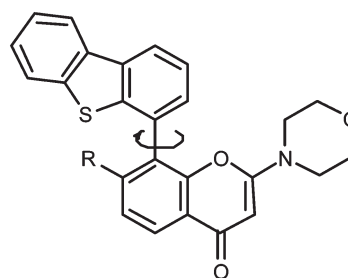


6747

Potent enantioselective inhibition of DNA-dependent protein kinase (DNA-PK) by atropisomeric chromenone derivatives

Kate M. Clapham, Tommy Rennison, Gavin Jones, Faye Craven, Julia Bardos, Bernard T. Golding, Roger J. Griffin, Karen Haggerty, Ian R. Hardcastle, Pia Thommes, Attila Ting and Céline Cano*

We describe the development and resolution of atropisomeric DNA-PK inhibitors. As predicted, only one enantiomer showed inhibitory activity against DNA-PK.



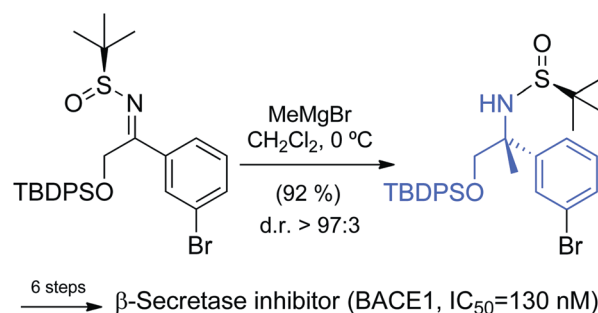
NU7441; R = H
1; R = *n*-propyl
2; R = allyl
3; R = methyl

6758

A practical entry to β -aryl- β -alkyl amino alcohols: application to the synthesis of a potent BACE1 inhibitor

Oscar Delgado,* Antonio Monteagudo, Michiel Van Gool, Andrés A. Trabanco and Santos Fustero*

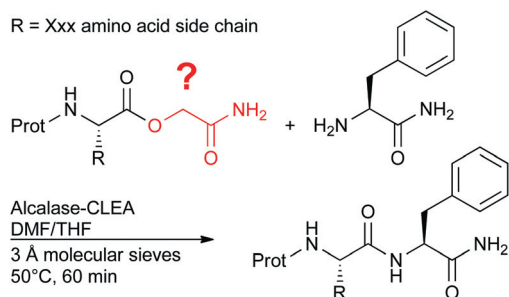
An efficient protocol for the diastereoselective preparation of β -aryl- β -alkyl amino alcohols, useful intermediates for the synthesis of potent β -secretase inhibitors, has been developed.



PAPERS

6767

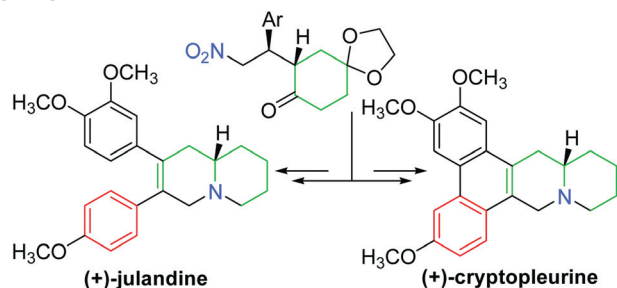
R = Xxx amino acid side chain

**Improving the carboxyamidomethyl ester for subtilisin A-catalysed peptide synthesis**

Roseri J. A. C. de Beer, Timo Nuijens, Lotte Wiermans, Peter J. L. M. Quaedflieg and Floris P. J. T. Rutjes*

Novel activating esters have been evaluated for efficiency in a chemoenzymatic subtilisin A-CLEA-catalysed approach to synthesise peptides.

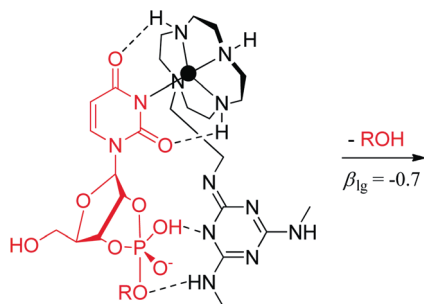
6776

**Enantioselective approach to functionalized quinolizidines: synthesis of (+)-julandine and (+)-cryptopleurine**

Sunil V. Pansare* and Rajendar Dyapa

An enantioselective synthesis of the diaryl quinolizidine alkaloid (+)-julandine and the phenanthroquinolizidine (+)-cryptopleurine was achieved from a key γ -nitroketone which is readily prepared by an organocatalytic Michael addition.

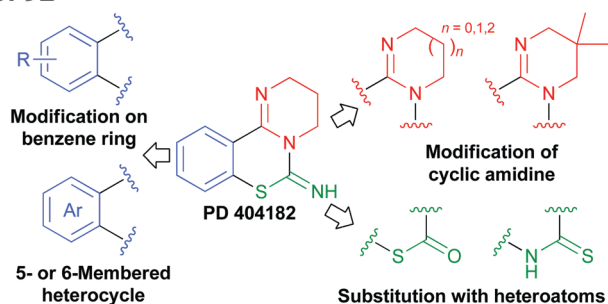
6785

**Intracomplex general acid/base catalyzed cleavage of RNA phosphodiester bonds: the leaving group effect**

Tuomas Lönnberg* and Mikko Luomala

A β_{lg} value of -0.7 has been determined for intracomplex general acid/base catalyzed hydrolysis of uridine-3'-phosphodiester, consistent with proton transfer to the leaving group taking place concerted with rate-limiting P–O bond cleavage.

6792

**Concise synthesis and anti-HIV activity of pyrimido[1,2-c]-[1,3]benzothiazin-6-imines and related tricyclic heterocycles**

Tsukasa Mizuhara, Shinya Oishi,* Hiroaki Ohno, Kazuya Shimura, Masao Matsuoka and Nobutaka Fujii*

Structure-activity relationship study of PD 404182 derivatives for anti-HIV agents was carried out using facile synthetic approaches.