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Organic & Biomolecular Chemistry

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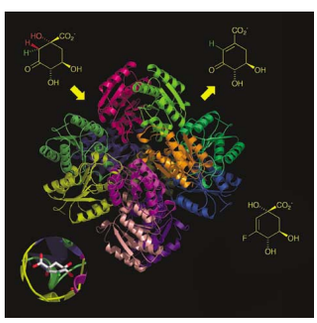
Incorporating Acta Chemica Scandinavica



Cover

See Martyn Frederickson, Aleksander W. Roszak, John R. Coggins, Adrian J. Lapthorn and Chris Abell, pp. 1592–1596.

The cover art shows the stereospecific reaction catalysed by homo-dodecameric type II dehydroquinases together with the fluoro analogue of the enolate intermediate of the reaction which is the most potent inhibitor known to date of the type II dehydroquinase from *Mycobacterium tuberculosis*. This low molecular weight inhibitor is pictured bound at the active site of a type II enzyme.

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contents

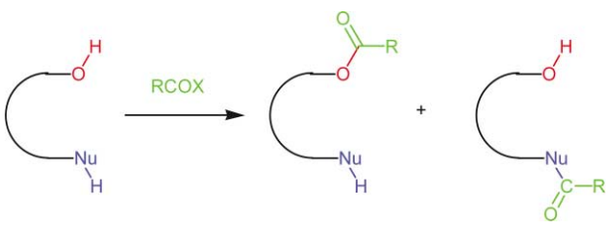
Chemical Science

June 2004/Volume 1/Issue 6

www.rsc.org/chemicalscience

Drawing together the research highlights and news from all RSC publications, *Chemical Science* provides a 'snapshot' the latest developments across the chemical sciences showcasing newsworthy articles, as well as the most significant scientific advances.

PERSPECTIVE



Chemoselectivity in reactions of esterification

Moshe Nahmany and Artem Melman

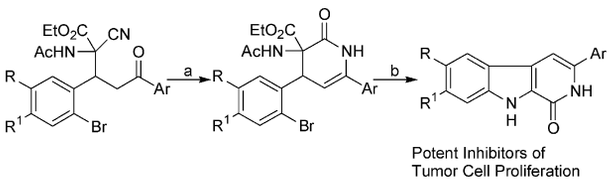
This review is devoted to the problem of chemoselective formation of ester functions in polyfunctional molecules. The review covers most typical approaches to chemoselective acylation of hydroxy groups in molecules containing an amino, mercapto, or another hydroxy functionality as well as chemoselective esterification of di- and polycarboxylic acids.

COMMUNICATIONS

CuI catalyzed *N*-arylation of amide as a key step for the preparation of 3-aryl β-carbolin-1-ones

Shaozhong Wang, Jianwei Sun, Gang Yu, Xiaoyi Hu, Jun O Liu and Yuefei Hu

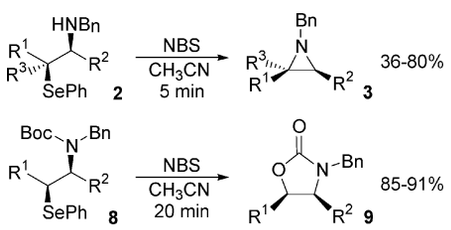
The five- and six-membered nitrogen-containing rings in the β-carbolin-1-ones were elaborated efficiently by an intramolecular ketone–nitrile annulation and an intramolecular *N*-arylation of amide respectively.



New phenylselanyl group activation: synthesis of aziridines and oxazolidin-2-ones

Catherine Miniejew, Francis Outurquin and Xavier Pannecoucke

Halogenation by *N*-bromosuccinimide has been shown to be the most suitable manner to cyclize β-phenylselanyl amines into aziridines and can also afford oxazolidin-2-ones from *N*-Boc β-phenylselanyl amines in excellent yield.

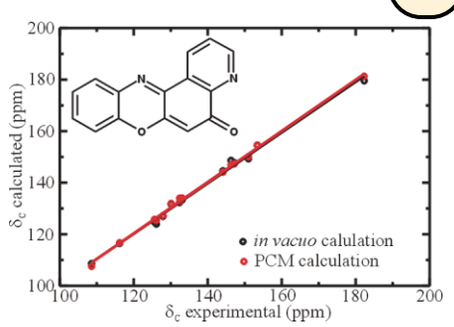


ARTICLES

Observed and calculated ^{1}H- and ^{13}C-NMR chemical shifts of substituted 5*H*-pyrido[3,2-*a*]- and 5*H*-pyrido[2,3-*a*]-phenoxazin-5-ones and of some 3*H*-phenoxazin-3-one derivatives

Orlando Crescenzi, Gaetano Correale, Adele Bolognese, Vincenzo Piscopo, Michelangelo Parrilli and Vincenzo Barone

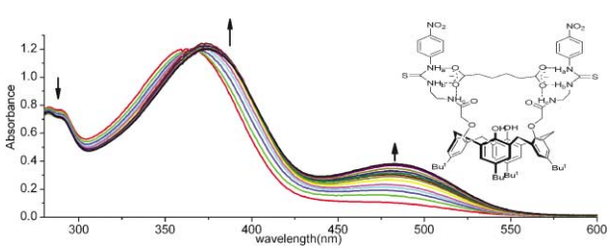
^{1}H- and ^{13}C-NMR chemical shifts of the title compounds have been assigned, and the experimental chemical shifts have been compared with the results of density functional calculations employing large basis set.



Calix[4]arenes containing thiourea and amide moieties: neutral receptors towards α,ω-dicarboxylate anions

Shun-Ying Liu, Yong-Bing He, Jin-Long Wu, Lan-Hua Wei, Hai-Juan Qin, Ling-Zhi Meng and Ling Hu

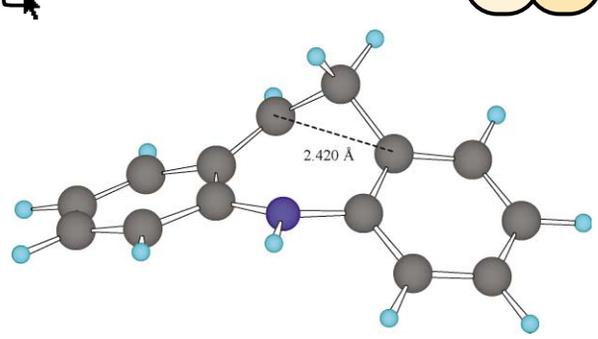
Two-armed neutral anion receptors, calix[4]arenes bearing thiourea and amide binding sites, could be used as chemical sensors for some special dicarboxylate anions.



Homoheteroaromaticity: the case study of azepine and dibenzazepine

Christophe Dardonville, María Luisa Jimeno, Ibon Alkorta and José Elguero

Azepine and dibenzazepines are antiaromatic compounds that by protonation afford homoheteroaromatic compounds. GIAO and NICS/DFT calculations have been used to calculate NMR properties and energies.



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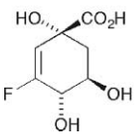
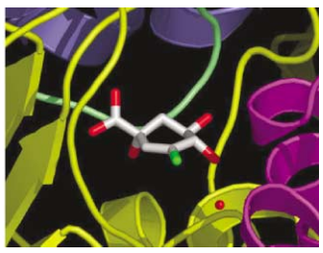
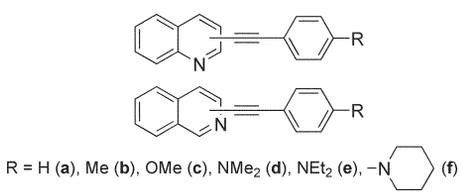




(1*R*,4*S*,5*R*)-3-Fluoro-1,4,5-trihydroxy-2-cyclohexene-1-carboxylic acid: the fluoro analogue of the enolate intermediate in the reaction catalyzed by type II dehydroquinases

Martyn Frederickson, Aleksander W. Roszak, John R. Coggins, Adrian J. Lapthorn and Chris Abell

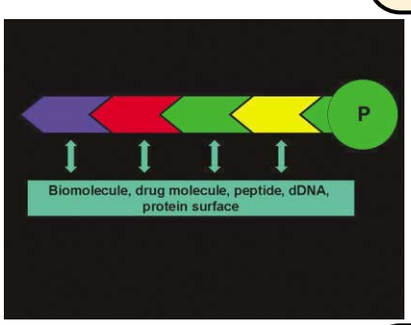
The fluoro analogue of the enolate intermediate in the reaction catalyzed by type II dehydroquinases has been prepared and has been shown to be the most potent inhibitor reported to date of the type II enzyme from *Mycobacterium tuberculosis*.



Synthesis and electrogenerated chemiluminescence of donor-substituted phenylquinolinylethynes and phenylisoquinolinylethynes: effect of positional isomerism

Arumugasamy Elangovan, Shu-Wen Yang, Jui-Hsien Lin, Kuo-Ming Kao and Tong-Ing Ho

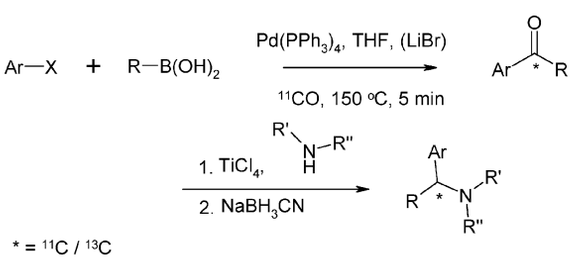
New donor-substituted phenylethynylquinolines and isoquinolines have been synthesized and their electrogenerated chemiluminescence and photophysical properties are studied.



PEG-supported synthesis of pyrazole oligoamides with peptide β-sheet affinity

Kateřina Černovská, Miriam Kemter, Hans-Christoph Gallmeier, Petra Rzepecki, Thomas Schrader and Burkhard König

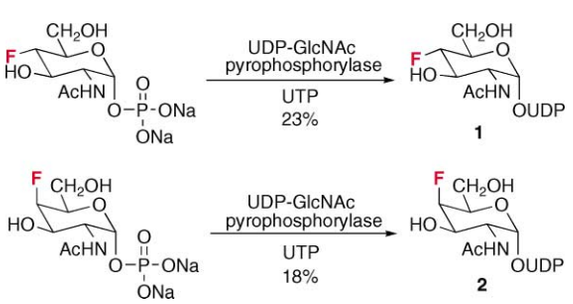
Molecules with peptide affinity are sequentially coupled on PEG as polymer support. This leads to extended water soluble synthetic receptors. We illustrate the concept using peptide binding pyrazole amino acids which are combined to oligoamides with increased affinity.



Synthesis of [^{11}C]/(^{13}C)amines *via* carbonylation followed by reductive amination

Obaidur Rahman, Tor Kihlberg and Bengt Långström

A novel approach for the preparation of ^{11}C-/^{13}C-amines has been described.



Chemo-enzymatic synthesis of fluorinated 2-*N*-acetamidosugar nucleotides using UDP-GlcNAc pyrophosphorylase

Fei Feng, Kiyoshi Okuyama, Kenichi Niikura, Takashi Ohta, Reiko Sadamoto, Kenji Monde, Toshitada Noguchi and Shin-Ichiro Nishimura

Two non-natural fluorinated 2-*N*-acetamidosugar nucleotides UDP-4-FGlcNAc **1** and its galacto isomer UDP-4-FGalNAc **2** were synthesized with UDP-GlcNAc pyrophosphorylase.

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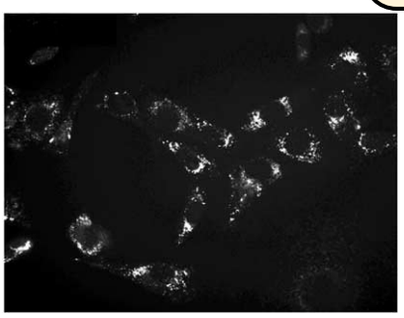
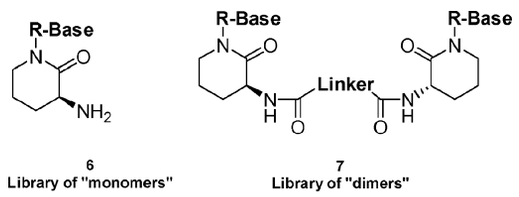


Design, synthesis and evaluation of ratiometric probes for hydrogencarbonate based on europium emission

Yann Bretonniere, Martin J. Cann, David Parker and Rachel Slater

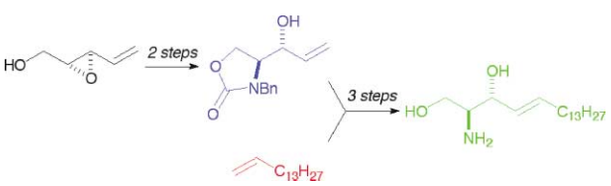
A series of emissive Eu complexes has been evaluated as probes for hydrogencarbonate and exhibit promise for intracellular ratiometric analysis.



Design, synthesis and biological activity of a targeted library of potential tryptase inhibitors

Mónica García, Xavier del Río, Sandra Silvestre, Mario Rubiralta, Estrella Lozoya, Victor Segarra, Dolors Fernández, Montserrat Miralpeix, Mònica Aparici and Anna Diez

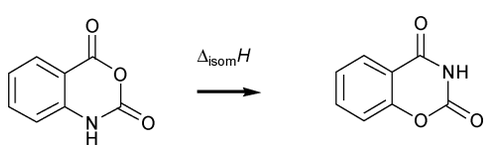
The design, synthesis and biological evaluation of two targeted libraries of potential tryptase inhibitors are presented.



A practical synthesis of D-*erythro*-sphingosine using a cross-metathesis approach

Staffan Torssell and Peter Somfai

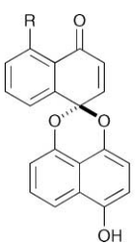
The synthesis of D-*erythro*-sphingosine was accomplished through a regioselective opening of the vinylepoxide and an *E*-selective cross-metathesis as the key steps.



The energetics of isomeric benzoxazine diones: isatoic anhydride revisited

M. Agostinha R. Matos, Margarida S. Miranda, Victor M. F. Morais and Joel F. Liebman

Thermochemistry of the isomeric compounds: 2*H*-1,3-benzoxazine-2,4(3*H*)dione and isatoic anhydride. An experimental and theoretical investigation.



S11; R = H
IC$_{50}$ *(Trx-1/TrxR)* ***340 nM***; *IC*$_{50}$ *(MCF-7)* ***2.8 μM***

S12; R = OH
IC$_{50}$ *(Trx-1/TrxR)* ***200 nM***; *IC*$_{50}$ *(MCF-7)* ***2.6 μM***

Natural product based inhibitors of the thioredoxin–thioredoxin reductase system

Peter Wipf, Stephen M. Lynch, Anne Birmingham, Giselle Tamayo, Allan Jiménez, Nefertiti Campos and Garth Powis

SAR studies of spiroketal naphthodecalins provided new nanomolar inhibitors of the Trx/TrxR redox control system.

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