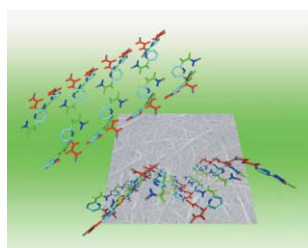


# Organic & Biomolecular Chemistry

FORMERLY PERKIN TRANSACTIONS 1 AND 2

Incorporating Acta Chemica Scandinavica

**Cover**

See Kazuhiro Yabuuchi, Emmanuel Marfo-Owusu and Takashi Kato, page 3464.

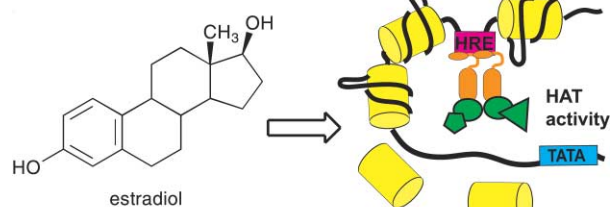
Hydrogen-bonded 1D molecular array of a pyridine-based bisurea compound: the zigzag layered sheet formed through intra- and intermolecular hydrogen bonds.

Chemical biology articles published in this journal also appear in the *Chemical Biology Virtual Journal*: [www.rsc.org/chembiol](http://www.rsc.org/chembiol)

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## EMERGING AREA

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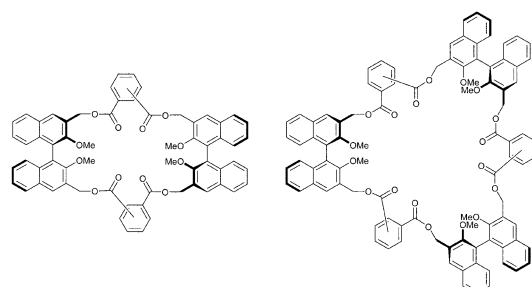
**Chemical approaches to studying transcription**

Ross V. Weatherman

Small molecule modulators and new analytical techniques have greatly aided in the study of the complex process of gene transcription.

## COMMUNICATIONS

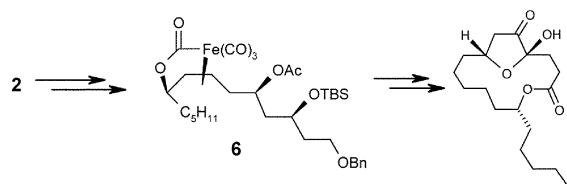
3261 3262

**Rigid optically-active  $D_2$  and  $D_3$  macrocycles**

Marina Ricci and Dario Pasini

Direct condensation of an optically-active binaphthyl-containing diol with either phthalic or terephthalic acids yield macrocycles of differing sizes, shapes and symmetry ( $D_2$  or  $D_3$ ). NMR and circular dichroism spectroscopies show how these macrocycles, although possessing the same elemental composition, have greatly differing shape persistency characteristics.

3263 3264

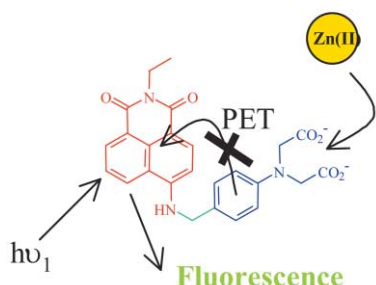


### Synthesis of (-)-Gloeosporone, a fungal autoinhibitor of spore germination using a $\pi$ -allyltricarboxyliron lactone complex as a templating architecture for 1,7-diol construction

Steven V. Ley, Ed Cleator, Jürgen Harter and Christopher J. Hollowood

The synthesis of the fungal autoinhibitor (-)-Gloeosporone is described. The key step involves reductive removal of the ligating iron, used to instil the embedded 1,7-diol functionality species, by treatment of **6** with lithium naphthalenide.

3265 3267

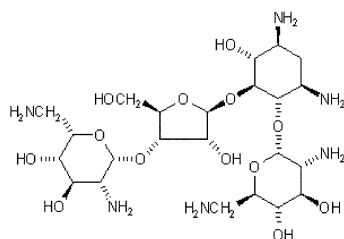


### A highly selective and sensitive fluorescent PET (photoinduced electron transfer) chemosensor for Zn(II)

Thorfinnur Gunnlaugsson, T. Clive Lee and Raman Parkesh

We report the design and synthesis of a new, highly Zn(II) selective and sensitive fluorescent PET chemosensor, synthesised in high yields in a few steps; it does not respond to  $\text{Ca}^{2+}$  and  $\text{Mg}^{2+}$ , and many other transition metal ions.

3268 3270



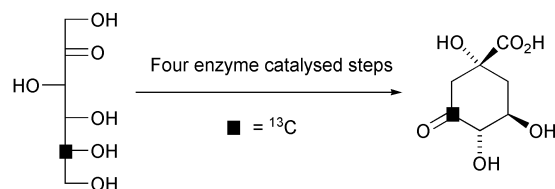
Streptomycin

### Binding affinity and inhibitory potency of neomycin and streptomycin on the Tat peptide interaction with HIV-1 TAR RNA detected by on-line acoustic wave sensor

Nardos Tassew and Michael Thompson

The binding of neomycin and streptomycin to a segment of the transactivation responsive region (TAR) RNA of the human immunodeficiency virus, and their inhibitory potency to disrupt the interaction of the RNA with a regulatory Tat protein-derived peptide, have been studied.

3271 3273

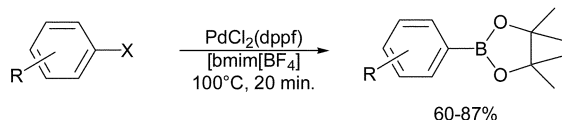


### Enzymic synthesis of 3-[3- $^{13}\text{C}$ ]dehydroquinic acid

Martyn Frederickson, Emily J. Parker, John R. Coggins and Chris Abell

3-[ $^{13}\text{C}$ ]Dehydroquinic acid has been prepared from commercially available D-5-[ $^{13}\text{C}$ ]fructose over four enzyme catalysed steps.

3274 3276



R = H, 4-Me, 4-OMe, 2-Me, 2-OMe, 2-NH<sub>2</sub>; X = I  
R = H, 4-Me; X = Br

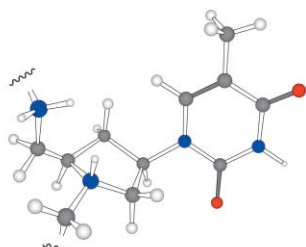
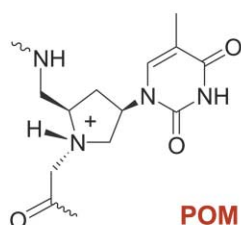
### Synthesis of arylboronates by the palladium catalysed cross-coupling reaction in ionic liquids

Andrzej Wolan and Marek Zaidlewicz

Synthesis of arylboronates from aryl iodides and bromides, and pinacolborane in ionic liquids is described.



3277 3292

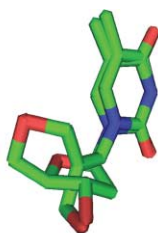
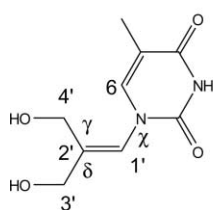


### Design, synthesis, conformational analysis and nucleic acid hybridisation properties of thymidyl pyrrolidine-amide oligonucleotide mimics (POM)

David T. Hickman, T. H. Samuel Tan, Jordi Morral, Paul M. King, Matthew A. Cooper and Jason Micklefield

Cationic POM are stereochemically and conformationally similar to natural nucleic acids, but exhibit superior affinity for complementary ssDNA and RNA.

3293 3296



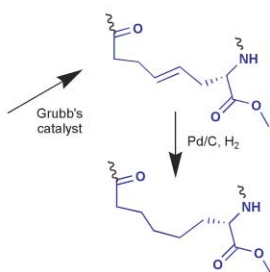
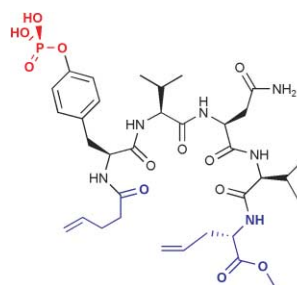
**1** + DNA A-helix thymidine  
(from a RNA/DNA A-helix)

### Acyclic, achiral enamide nucleoside analogues. The importance of the C=C bond in the analogue for its ability to mimic natural nucleosides

Asger B. Petersen, Michael Å. Petersen, Ulla Henriksen, Steen Hammerum and Otto Dahl

The nucleoside analogue **1** is shown to be able to mimic dT conformations in A- or B-type helices quite well.

3297 3303



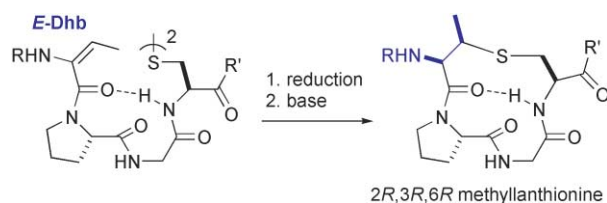
### Cyclic phosphopeptides for interference with Grb2 SH2 domain signal transduction prepared by ring-closing metathesis and phosphorylation

Frank J. Dekker, Nico J. de Mol, Marcel J. E. Fischer, Johan Kemmink and Rob M. J. Liskamp

The design, synthesis (featuring ring-closing metathesis) and interaction analysis of cyclic phosphopeptides that bind to the Grb2 SH2 domain is described.



3304 3315



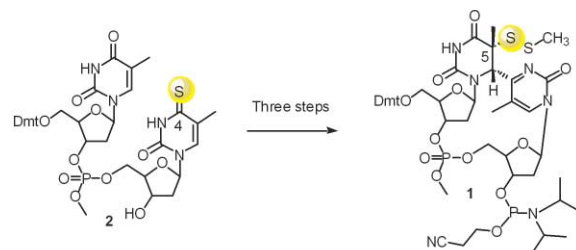
### Biomimetic studies on the mechanism of stereoselective lanthionine formation

Yantao Zhu, Matt D. Gieselman, Hao Zhou, Olga Averin and Wilfred A. van der Donk

Oxidative elimination of *syn*-3-methyl-*Se*-phenylselenocysteine provided *E*-dehydrobutyrine containing peptides that were cyclized to stereodefined methylanthionines.



3316 3320



### Synthesis of the TT pyrimidine (6-4) pyrimidone photoproduct-thio analogue phosphoramidite building block

Sandra Karina Angulo Matus, Jean-Louis Fourrey and Pascale Clivio

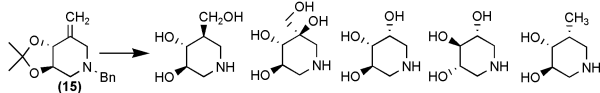
The phosphoramidite of the TpT (6-4) photoproduct-C5 thio analogue is readily obtained in three steps from *P*-methyl-5'-*O*-dimethoxytritylthymidyl(3'→5')-4-thiothymidine.

3321 3326

### A new access to polyhydroxy piperidines of the azasugar class: synthesis and glycosidase inhibition studies

Ganesh Pandey, Manmohan Kapur, M. Islam Khan and Sushama M. Gaikwad

A new synthetic strategy has been devised to access a variety of polyhydroxylated piperidines belonging to the azasugar class of glycosidase inhibitors.

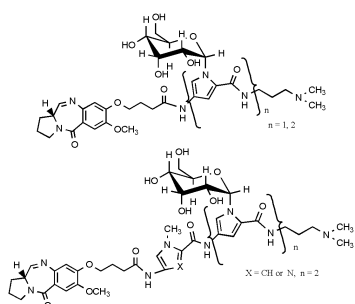


3327 3342

### Design, synthesis and *in vitro* cytotoxicity studies of novel pyrrolo [2,1][1,4] benzodiazepine-glycosylated pyrrole and imidazole polyamide conjugates

Rohtash Kumar and J. William Lown

The design, synthesis and biological evaluation of novel pyrrolo [2,1][1,4] benzodiazepine-water insoluble and water soluble glycosylated pyrrole and imidazole polyamide conjugates are described.

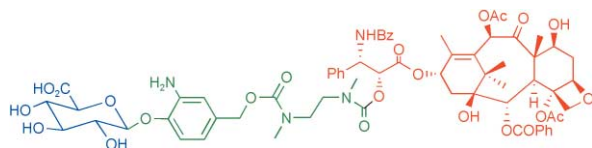


3343 3352

### A new paclitaxel prodrug for use in ADEPT strategy

Emmanuel Bouvier, Sylvie Thiroit, Frédéric Schmidt and Claude Monneret

A tripartite paclitaxel prodrug has been synthesized. *In vivo* tests showed good kinetics of drug liberation by  $\beta$ -glucuronidase.

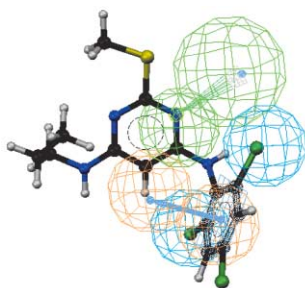


3353 3361

### Synthesis, molecular modeling and biological activity of methyl and thiomethyl substituted pyrimidines as corticotropin releasing hormone type 1 antagonists

Adam McCluskey, Paul A. Keller, Jody Morgan and James Garner

The thiomethyl moiety contributes to activity, and statistical validity of our CRH<sub>1</sub> pharmacophore but is not selected as important for activity.

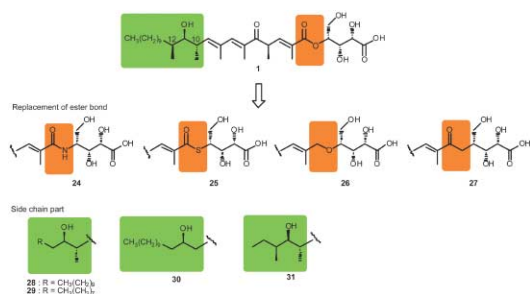


3362 3376

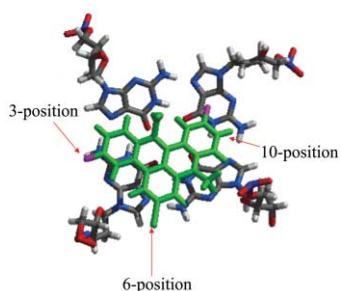
### Chemistry and biology of khafrefungin. Large-scale synthesis, design, and structure-activity relationship of khafrefungin, an antifungal agent

Masayuki Nakamura, Yuichiro Mori, Kennichi Okuyama, Kunihiko Tanikawa, Satoshi Yasuda, Kentaro Hanada and Shū Kobayashi

Multigram-scale synthesis, design and structure-activity relationship of khafrefungin, an antifungal agent that inhibits inositol phosphorylceramide (IPC) synthase, are described.



3377 3389

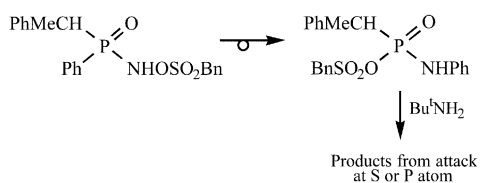


### Antitumour polycyclic acridines. Palladium(0) mediated syntheses of quino[4,3,2-*kl*]acridines bearing peripheral substituents as potential telomere maintenance inhibitors

Robert A. Heald and Malcolm F. G. Stevens

Pentacyclic quino[4,3,2-*kl*]acridines substituted in the 3-, 6- and 10-positions have been prepared by Pd(0) mediated coupling reactions and may be converted to 8,13-dimethylquinoacridinium salts with telomerase-inhibitory activity.

3390 3395

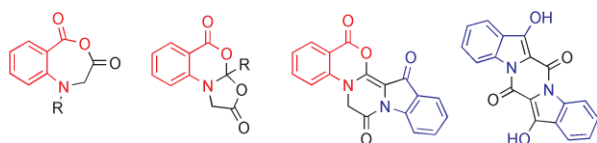


### Competing sulfonylation and phosphorylation following rearrangement of an *O*-sulfonyl-*N*-phosphinoylhydroxylamine with *tert*-butylamine: demonstration of a phosphonamidic-sulfonic anhydride intermediate and <sup>18</sup>O-labelling evidence on how it may be formed

Martin J. P. Harger

The observed products correspond to attack at sulfur or phosphorus in a phosphonamidic-sulfonic anhydride.

3396 3403

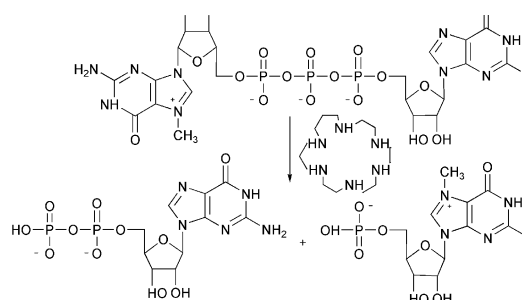


### Products from dehydration of dicarboxylic acids derived from anthranilic acid

Per Wiklund, Ivan Romero and Jan Bergman

Treatment of dicarboxylic acids derived from anthranilic acids with several dehydrating agents, gave cyclic ortho amides, 7-membered anhydrides and diketopiperazine indole dimers. Literature structures of products from such reactions have been revised.

3404 3409

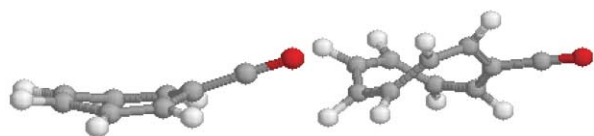


### Macrocyclic amines as catalysts of the hydrolysis of the triphosphate bridge of the mRNA 5'-cap structure

Zhibo Zhang, Harri Lönnberg and Satu Mikkola

Three macrocyclic amines are found to enhance the hydrolysis of the triphosphate bridge of a 5'-cap model compound, *P*<sup>1</sup>-(7-methylguanosine) *P*<sup>3</sup>-guanosine 5',5'-triphosphate.

3410 3417

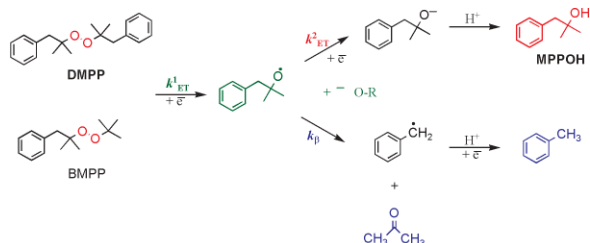


### Aromaticity and antiaromaticity in fulvenes, ketocyclopolynes, fulvenones, and diazocyclopolynes

Katayoun Najafian, Paul von Ragué Schleyer and Thomas T. Tidwell

Computational studies reveal the degree of aromaticity/antiaromaticity in the 3, 5, 7 and 9-membered ring members of the fulvene family.

3418 3429

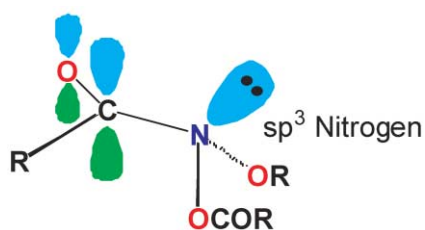


### Model dialkyl peroxides of the Fenton mechanistic probe 2-methyl-1-phenyl-2-propyl hydroperoxide (MPPH): kinetic probes for dissociative electron transfer

David C. Magri and Mark S. Workentin

Two dialkyl peroxides, DMPP and BMPP, were devised as kinetic probes to investigate the partitioning between electron transfer and  $\beta$ -scission fragmentation of the generated alkoxy radical after dissociative electron transfer to the O–O bond using heterogeneous and homogeneous electrochemical techniques.

3430 3437

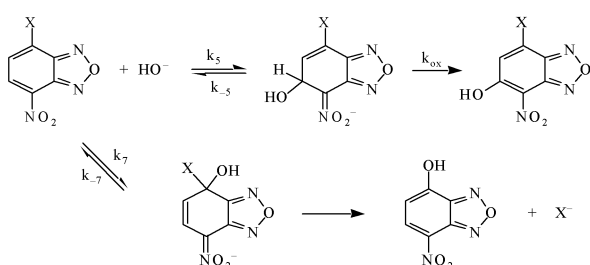


### Crystal structures and properties of mutagenic *N*-acyloxy-*N*-alkoxyamides — “most pyramidal” acyclic amides

Ashley-Mae E. Gillson, Stephen A. Glover, David J. Tucker and Peter Turner

*N*-Acyloxy-*N*-alkoxyamides are the “most pyramidal” acyclic amides. X-ray structures confirm the dramatic influence of bisoxo-substitution at the amide nitrogen.

3438 3443

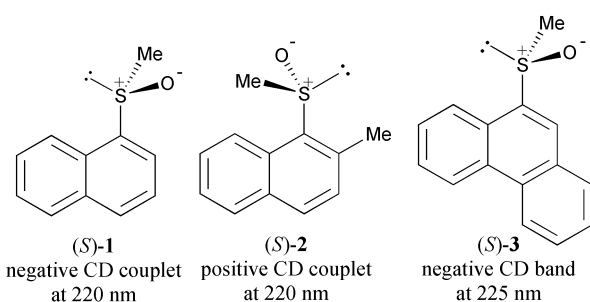


### $\sigma$ -Adduct formation and oxidative substitution in the reactions of 4-nitrobenzofurazan and some derivatives with hydroxide ions in water

Michael R. Crampton, Rachel E. A. Lunn and David Lucas

Reaction of 4-nitrobenzofurazan and its derivatives with hydroxide ions yields  $\sigma$ -adducts which may be oxidised to hydroxynitrobenzofurazans.

3444 3449

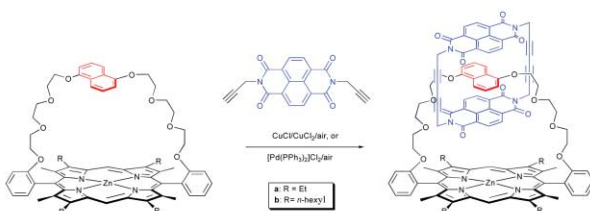


### Circular dichroism spectra and absolute configuration of some aryl methyl sulfoxides

Maria Irene Donnoli, Egidio Giorgio, Stefano Superchi and Carlo Rosini

The absolute configurations of **1**, **2** and **3** were assigned by coupled oscillator calculations of their circular dichroism spectra.

3450 3457



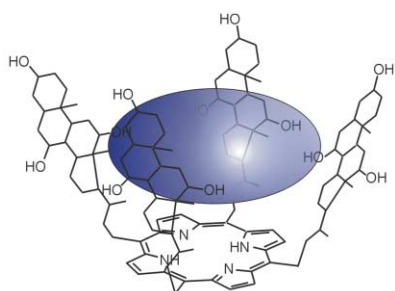
### Neutral $\pi$ -associated porphyrin [2]catenanes

Maxwell J. Gunter and Sandra M. Farquhar

The synthesis is described of a series of neutral porphyrin-containing catenanes, consisting of a zinc porphyrin strapped by a polyethylene glycol chain incorporating a central naphthoquinol unit, interlinked with a naphthalene diimide macrocycle.



3458 3463



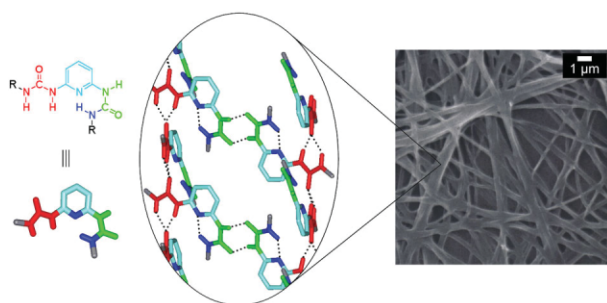
### Steroid–porphyrin conjugate for saccharide sensing in protic media

Mykhaylo Dukh, David Šaman, Kamil Lang, Vladimír Pouzar, Ivan Černý, Pavel Drašar and Vladimír Král

Oligosaccharides are preferentially bound by the steroid–porphyrin receptor in aqueous solutions. Binding to the solid receptor films is also reported.



3464 3469



### A new urea gelator: incorporation of intra- and intermolecular hydrogen bonding for stable 1D self-assembly

Kazuhiro Yabuuchi, Emmanuel Marfo-Owusu and Takashi Kato

The incorporation of intra- and intermolecular hydrogen bonding plays a key role for the fibrous self-assembly along with the gelation.

3470

Nam-Cheol Kim, Tyler N. Graf,  
Charles M. Sparacino, Mansukh C. Wani  
and Monroe E. Wall

### Complete isolation and characterization of silybins and isosilybins from milk thistle (*Silybum marianum*)

Naoko Tanaka, Zulfiqar Hasan, Aloysius F. Hartog,  
Teunie van Herk and Ron Wever

### Phosphorylation and dephosphorylation of polyhydroxy compounds by class A bacterial acid phosphatases

David H. Grayson, Úna McCarthy and  
Edwin D. Roycroft

### Intramolecular acylative ring-switching reactions of 3-(tetrahydro-2'-furyl)propanoic acid derivatives to give butanolides: mechanism and scope

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