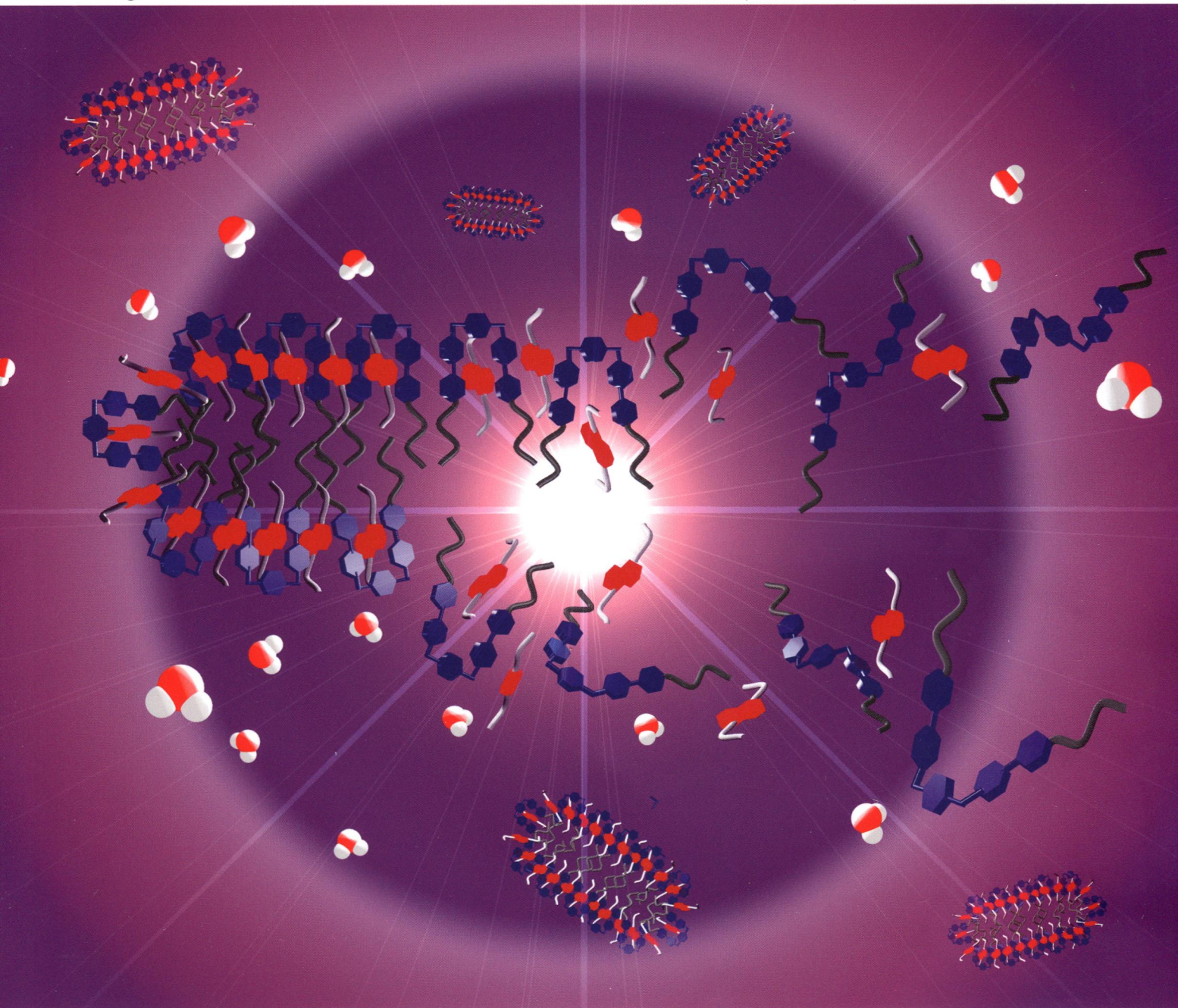


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# Organic & Biomolecular Chemistry

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ISSN 1477-0520

**PAPER**

Mark A. Olson *et al.*

Template-directed self-assembly by way of molecular recognition at the micellar-solvent interface: modulation of the critical micelle concentration



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# Organic & Biomolecular Chemistry

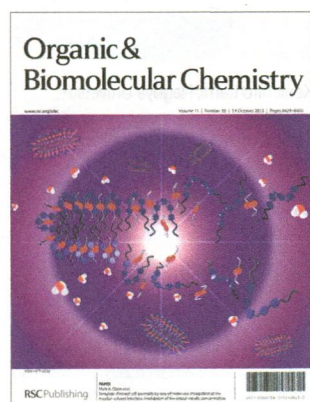
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## IN THIS ISSUE

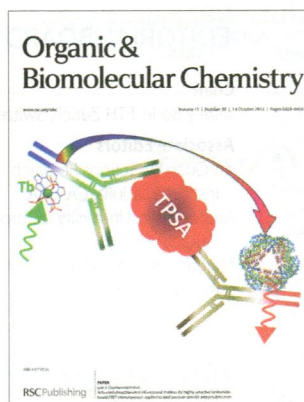
ISSN 1477-0520 CODEN OBCRAK 11(38) 6429–6660 (2013)



### Cover

See Mark A. Olson *et al.*, pp. 6483–6492.

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### Inside cover

See Loïc J. Charbonnière *et al.*, pp. 6493–6501.

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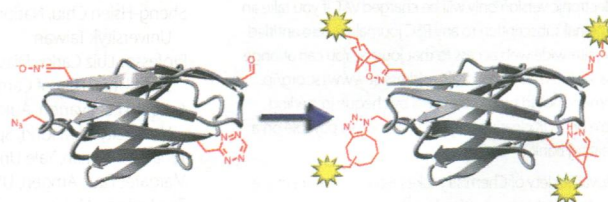
## PERSPECTIVE

6439

### Bioorthogonal labelling of biomolecules: new functional handles and ligation methods

Marjoke F. Debets, Jan C. M. van Hest and Floris P. J. T. Rutjes\*

In this review recent developments in bioorthogonal chemistry are described with a focus on newly developed reactions and their mutual orthogonality.



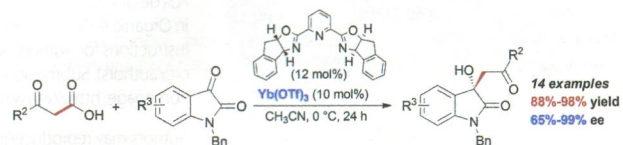
## COMMUNICATIONS

6456

### Enantioselective synthesis of 3-hydroxy oxindoles by ytterbium-catalysed decarboxylative addition of $\beta$ -ketoacids to isatins

Zhiqiang Duan, Jianlin Han, Ping Qian, Zirui Zhang, Yi Wang\* and Yi Pan

A ytterbium(III)-indapybox catalysed enantioselective decarboxylative addition reaction of  $\beta$ -ketoacids to isatins is described. The biologically important 3-hydroxy oxindoles were obtained in high yields and excellent enantioselectivities.



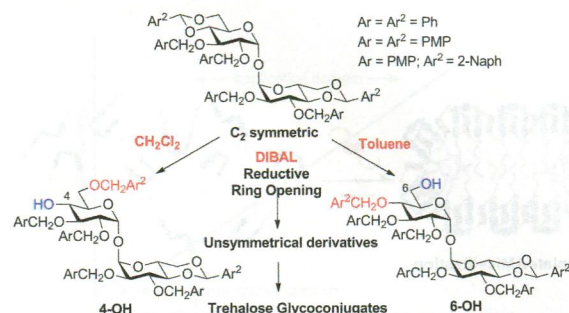
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Центральная научная библиотека  
Уральского отделения  
Российской академии наук (ЦНБ УрО РАН)

6460

### Desymmetrization of trehalose via regioselective DIBAL reductive ring opening of benzylidene and substituted benzylidene acetals

Vikram A. Sarpe and Suvarn S. Kulkarni\*

Regioselective DIBAL-reductive ring opening of trehalose dibenzylidene and substituted dibenzylidene acetals at O6 or O4 gives access to unsymmetrical trehalose glycoconjugates.

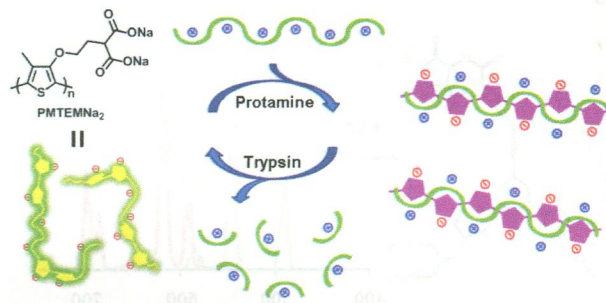


6466

### Colorimetric and fluorescent detection of protamines with an anionic polythiophene derivative

Zhiyi Yao, Wenjuan Ma, Yan Yang, Xueliang Chen, Li Zhang, Chen Lin and Hai-Chen Wu\*

The colorimetric and fluorescent dual detection of protamines based on an anionic polythiophene derivative with high sensitivity and selectivity.

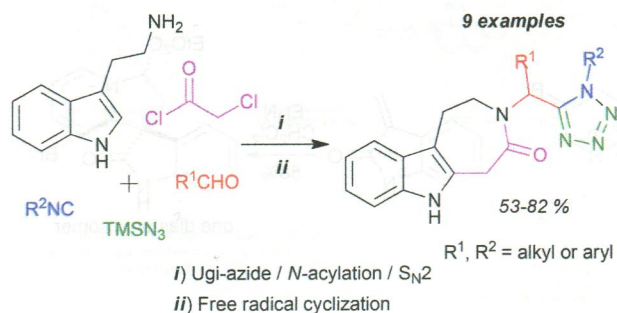


6470

### Synthesis of 3-tetrazolymethyl-azepino[4,5-*b*]-indol-4-ones in two reaction steps: (Ugi-azide/*N*-acylation/*S<sub>N</sub>2*)/free radical cyclization and docking studies to a 5-Ht<sub>6</sub> model

Raul E. Gordillo-Cruz, Angel Rentería-Gómez, Alejandro Islas-Jácome, Carlos J. Cortes-García, Erik Díaz-Cervantes, Juvencio Robles and Rocío Gámez-Montaño\*

Synthesis of nine novel 3-tetrazolymethyl-azepino[4,5-*b*]-indol-4-ones in two reaction steps.

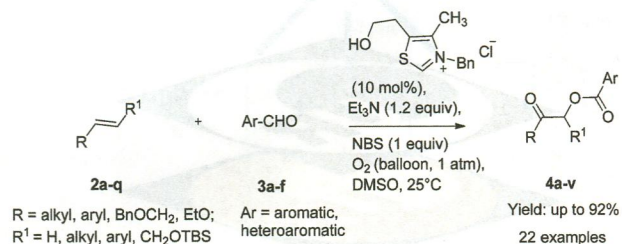


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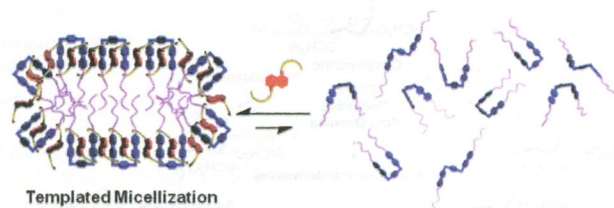
### *N*-Heterocyclic carbene catalyzed regioselective oxo-acyloxylation of alkenes with aromatic aldehydes: a high yield synthesis of $\alpha$ -acyloxy ketones and esters

Rambabu N. Reddi, Pushpa V. Malekar and Arumugam Sudalai\*

An *N*-heterocyclic carbene (NHC)-catalyzed reaction of alkenes with aromatic aldehydes providing for a high yield synthesis of  $\alpha$ -acyloxy ketones and esters has been described.



6483

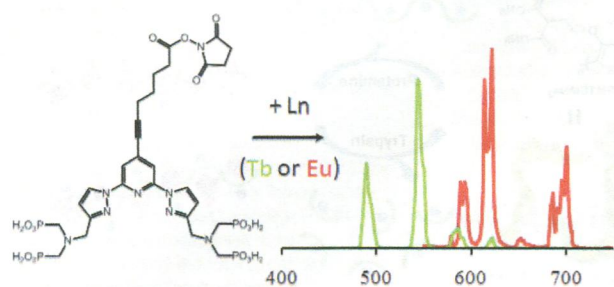


### Template-directed self-assembly by way of molecular recognition at the micellar–solvent interface: modulation of the critical micelle concentration

Mark A. Olson,\* Jonathan R. Thompson, Trenton J. Dawson, Christopher M. Hernandez, Marco S. Messina and Travis O'Neal

Templated micellisation of bipyridinium-based amphiphiles triggered by donor–acceptor interactions results in augmented properties and more.

6493

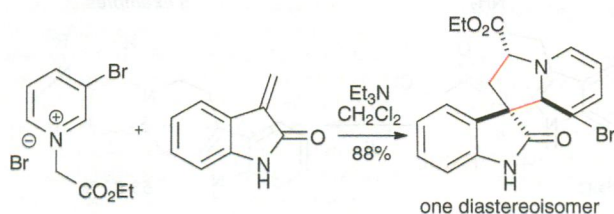


### Activated phosphonated trifunctional chelates for highly sensitive lanthanide-based FRET immunoassays applied to total prostate specific antigen detection

Katia Nchimi-Nono, K. David Wegner, Stina Lindén, Alexandre Lecoindre, Laurence Ehret-Sabatier, Shakir Shakir, Niko Hildebrandt and Loïc J. Charbonnière\*

The first example of an activated phosphonated chelate for lanthanide labeling was applied to TPSA detection.

6502



### Alkaloid inspired spirocyclic oxindoles from 1,3-dipolar cycloaddition of pyridinium ylides

Jonathan Day, Maliha Uroos, Richard A. Castledine, William Lewis, Ben McKeever-Abbas and James Dowden\*

Alkaloid-like spirooxindoles are obtained in good yield as single diastereoisomers by 1,3-dipolar cycloaddition between pyridinium ylides and 3-alkenyloxindoles.

6510



### Photocatalytic surface patterning of cellulose using diazonium salts and visible light

Peter Schroll, Charlie Fehl, Stephan Dankesreiter and Burkhard König\*

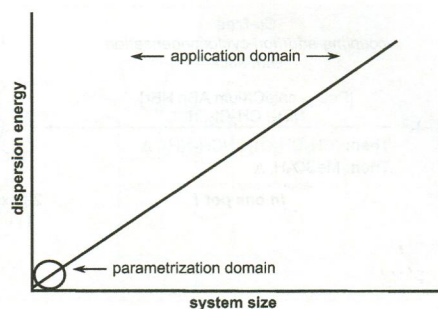
The Photo-Meerwein reaction allows a selective arylation of the functionalized surface.

6515

### Error estimates for (semi-)empirical dispersion terms and large biomacromolecules

Martin Korth

Error estimates for the dispersion terms of DFT, SQM and MM methods applied to really large biomolecules are derived using error statistics for smaller systems and dispersion contribution estimates for the PDBbind database of protein–ligand interactions. It is found that dispersion terms will usually not be a limiting factor for reaching chemical accuracy, though some force fields and large ligand sizes are problematic.

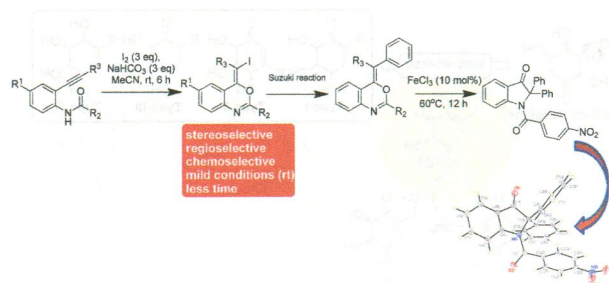


6520

### A convenient method to construct (Z)-oxazines via 6-exo-dig iodocyclization and synthesis of indolin-3-one

Jaya Kishore Vandavasi, Kung-Kai Kuo, Wan-Ping Hu, Ho-Chanu Shen, Wei-Sheng Lo and Jeh-Jeng Wang\*

A mild and efficient method to synthesize iodine substituted 1,3-benzoxazines with high regio-, stereo- and chemoselectivity is described.

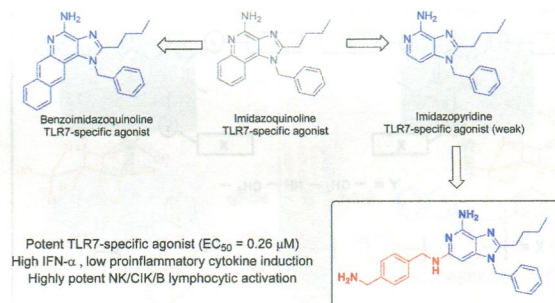


6526

### Structure–activity relationships in Toll-like receptor 7 agonistic 1*H*-imidazo[4,5-*c*]pyridines

Euna Yoo, Breanna M. Crall, Rajalakshmi Balakrishna, Subbalakshmi S. Malladi, Lauren M. Fox, Alec R. Hermanson and Sunil A. David\*

SAR exploration in 1*H*-imidazo[4,5-*c*]pyridines yielded pure TLR7 agonists, which induced prominent IFN- $\alpha$ , but negligible proinflammatory cytokines in human peripheral blood mononuclear cells.

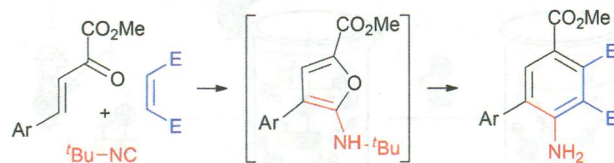


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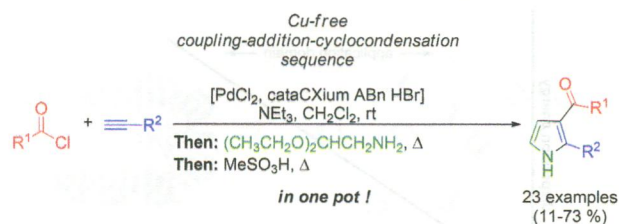
### Elusive 2-aminofuran Diels–Alder substrates for a straightforward synthesis of polysubstituted anilines

Ana G. Neo, Ana Bornadiego, Jesús Díaz, Stefano Marcaccini and Carlos F. Marcos\*

Three-component tandem [4 + 1]/[4 + 2] cycloaddition/aromatisation/dealkylation affords polyfunctionalised *N*-unsubstituted anilines in one-pot.



6556

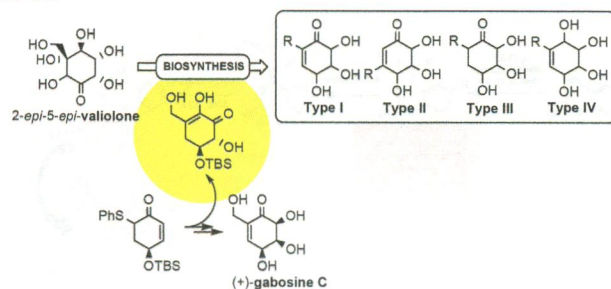


### A one-pot coupling–addition–cyclocondensation sequence (CACS) to 2-substituted 3-acylpyrroles initiated by a copper-free alkylation

Jan Nordmann and Thomas J. J. Müller\*

A novel Cu-free coupling–addition–cyclocondensation sequence (CACS) furnishes 2-substituted 3-acylpyrroles in a consecutive three-component synthesis in moderate to good yields and with a broad scope of diversity.

6562

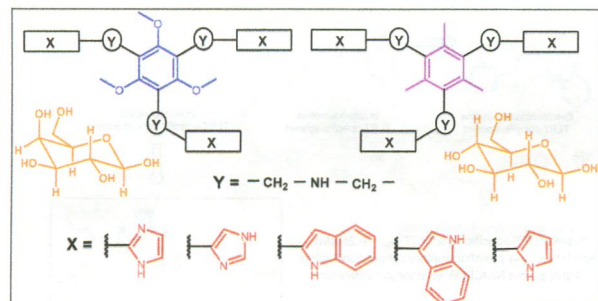


### How a diversity-oriented approach has inspired a new hypothesis for the gabosine biosynthetic pathway. A new synthesis of (+)-gabosine C

Miguel Ángel Fresneda, Ramon Alibés, Josep Font, Pau Bayón\* and Marta Figueredo\*

A diversity-oriented approach to gabosines inspired a new hypothesis for their biosynthesis, based on a keto–enol equilibrium cascade pathway.

6569

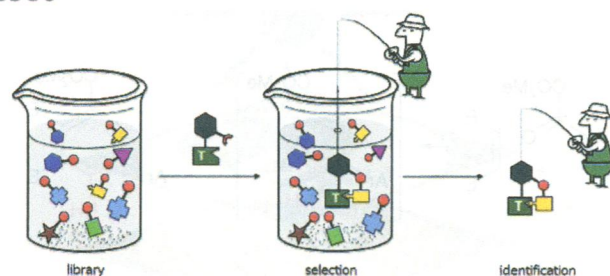


### Trimethoxybenzene- and trimethylbenzene-based compounds bearing imidazole, indole and pyrrole groups as recognition units: synthesis and evaluation of the binding properties towards carbohydrates

Jan-Ruven Rosien, Wilhelm Seichter and Monika Mazik\*

Ten new trimethoxybenzene- and trimethylbenzene-based receptors bearing imidazole or indole groups as recognition sites are described.

6580



### Dynamic covalent capture of hydrazides by a phosphonate-target immobilized on resin

Giulio Gasparini, Federico Rastrelli and Leonard J. Prins\*

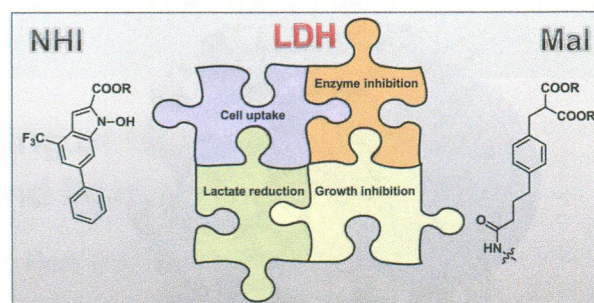
A protocol is described that permits the self-selection of hydrazides from a combinatorial library by a target immobilized on resin.

6588

### Assessing the differential action on cancer cells of LDH-A inhibitors based on the *N*-hydroxyindole-2-carboxylate (NHI) and malonic (Mal) scaffolds

Carlotta Granchi, Emilia C. Calvaresi, Tiziano Tuccinardi, Ilaria Paterni, Marco Macchia, Adriano Martinelli, Paul J. Hergenrother\* and Filippo Minutolo\*

Anti-glycolytic effects and mechanisms of action of *N*-hydroxyindoles (NHI) and malonates (Mal) displaying efficient LDH-A inhibitory properties were comparatively assessed in cancer cells.

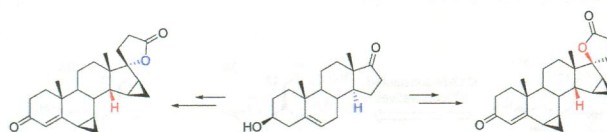


6597

### A facile total synthesis of drospirenone isomers containing 14 $\beta$ -hydrogen configuration

Wen Wan,\* Guobin Ma, Wei Gao, Jing Wang, Lei Li, Shangqin Rao, Chunfang Zheng, Haizhen Jiang, Hongmei Deng and Jian Hao\*

Two isomeric drospirenone derivatives **13** and **16** possessing a 14 $\beta$ -hydrogen were prepared in 8 steps.

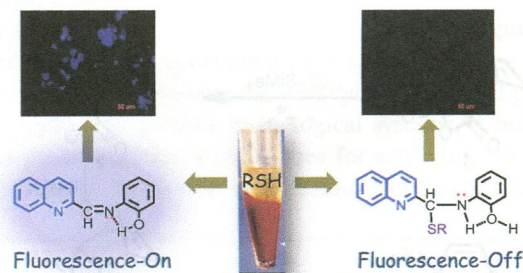


6604

### Designing a thiol specific fluorescent probe for possible use as a reagent for intracellular detection and estimation in blood serum: kinetic analysis to probe the role of intramolecular hydrogen bonding

Priyadip Das, Amal Kumar Mandal, Upendar Reddy G., Mithu Baidya, Sudip K. Ghosh\* and Amitava Das\*

**L**<sub>1</sub> could be utilized for chemodosimetric detection of certain GSH, Cys and Hcy in blood plasma as well as in live HeLa cells.

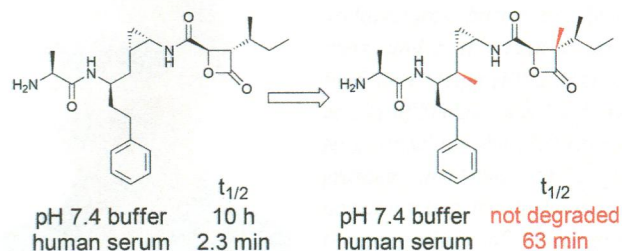


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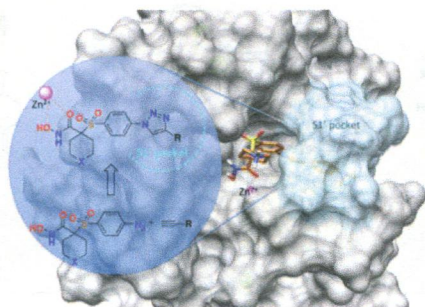
### Design and synthesis of the stabilized analogs of belactosin A with the unnatural *cis*-cyclopropane structure

Shuhei Kawamura, Yuka Unno, Akira Asai, Mitsuhiro Arisawa and Satoshi Shuto\*

Strategic improvement of chemical and biological stabilities by introducing two methyl groups.



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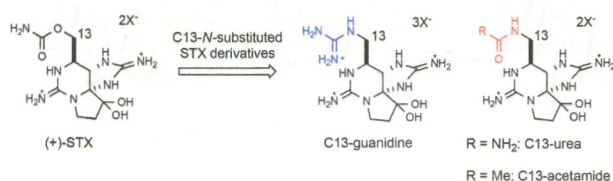


### Progress towards water-soluble triazole-based selective MMP-2 inhibitors

Benjamin Fabre, Kamila Filipiak, José María Zapico, Natalia Díaz, Rodrigo J. Carbajo, Anne K. Schott, María Paz Martínez-Alcázar, Dimas Suárez, Antonio Pineda-Lucena, Ana Ramos\* and Beatriz de Pascual-Teresa\*

Design and synthesis of water soluble  $\alpha$ -piperidine- $\alpha$ -sulfone hydroxamic acids with potent inhibition of MMP-2, a good selectivity profile and improved LE index and drug-like properties.

6642

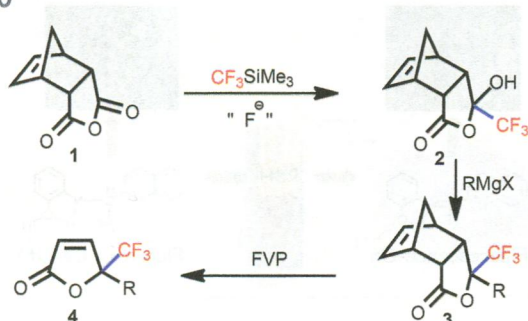


### Synthesis of saxitoxin derivatives bearing guanidine and urea groups at C13 and evaluation of their inhibitory activity on voltage-gated sodium channels

Takafumi Akimoto, Asako Masuda, Mari Yotsu-Yamashita, Takatsugu Hirokawa and Kazuo Nagasawa\*

Here, we describe the synthesis of the first C13-*N*-substituted STX derivatives **4**, **5**, and **6** bearing a guanidine, a urea group, and an acetamide **8**.

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### A synthesis of $\gamma$ -trifluoromethyl $\alpha,\beta$ -unsaturated $\gamma$ -butyrolactones using $\text{CF}_3\text{SiMe}_3$ as a trifluoromethylating agent

Chonticha Masusai, Darunee Soorukram, Chutima Kuhakarn, Patoomratana Tuchinda, Chaveng Pakawatchai, Saowanit Saithong, Vichai Reutrakul and Manat Pohmakotr\*

A general synthesis of  $\gamma$ -trifluoromethyl  $\alpha,\beta$ -unsaturated  $\gamma$ -butyrolactones is described.