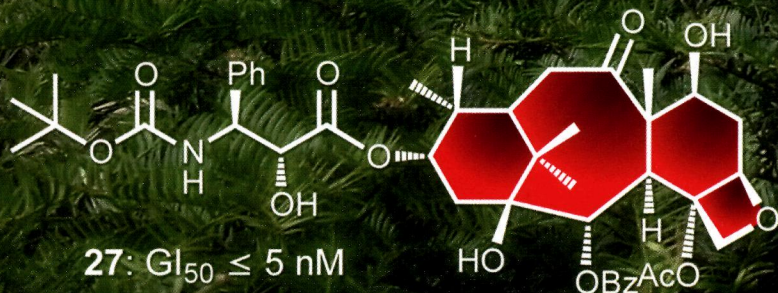
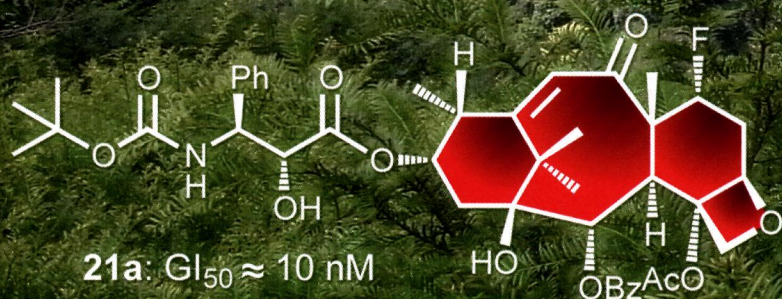


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Organic & Biomolecular Chemistry

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PAPER

Kyriacos C. Nicolaou and Roman A. Valiulin
Synthesis and biological evaluation of new paclitaxel analogs and discovery of
potent antitumor agents



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Organic & Biomolecular Chemistry

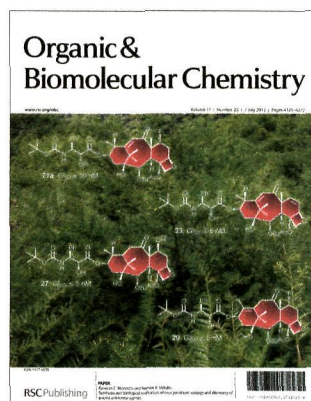
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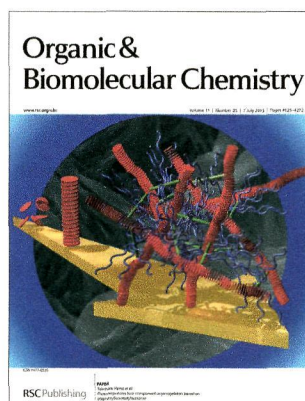


Cover

See Kyriacos C. Nicolaou and Roman A. Valiulin, pp. 4154–4163.

The cover portrays potent Taxol analogs overlying a forest of *Taxus chinensis*, the producer of 10-deacetylbaccatin III, precursor to the synthesized analogs (photo by Nicolaou during a recent visit to Fujian Province, China).

Image reproduced by permission of Kyriacos C. Nicolaou from *Org. Biomol. Chem.*, 2013, **11**, 4154.



Inside cover

See Takeharu Haino *et al.*, pp. 4164–4170.

Image reproduced by permission of Takeharu Haino from *Org. Biomol. Chem.*, 2013, **11**, 4164.

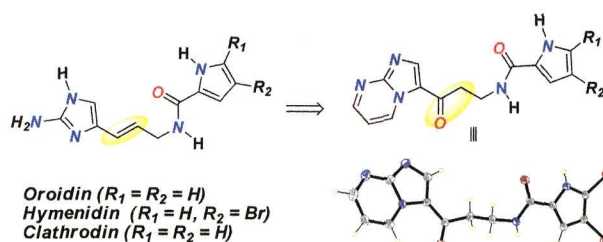
COMMUNICATIONS

4133

Total syntheses of oroidin, hymenidin and clathrocin

Sivappa Rasapalli,* Venkatreddy Kumbam, Abasaheb N. Dhawane, James A. Golen, Carl J. Lovely and Arnold L. Rheingold

The total syntheses of oroidin, hymenidin and clathrocin are reported *via* the intermediacy of a novel acyl imidazo-[1,2-*a*]pyrimidine derivative that obviates the need for expensive guanidine reagents and 2-aminoimidazole synthons and offers the opportunity for scale up.

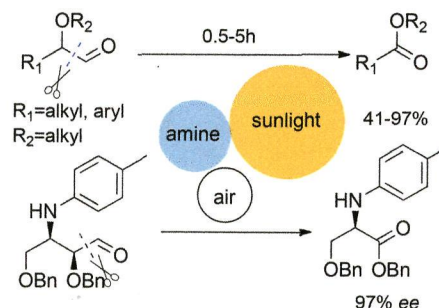


4138

Aniline mediated oxidative C–C bond cleavage of α -alkoxy aldehydes in air and a model reaction for the synthesis of α -(D)-amino acid derivatives

Bin Hu, Yunfeng Li, Zhongjun Li* and Xiangbao Meng*

A clean procedure for C–C cleavage provides a route from amino acid catalysis to amino acid ester!

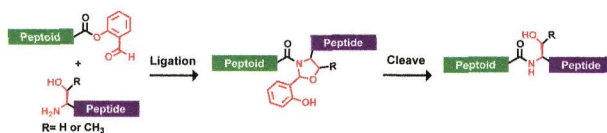


4142

Chemoselective fragment condensation between peptide and peptidomimetic oligomers

Paul M. Levine, Timothy W. Craven, Richard Bonneau and Kent Kirshenbaum*

Peptoid oligomers containing C-terminal salicylaldehyde esters can be ligated to peptides bearing N-terminal serine or threonine residues, establishing native amide linkages between unprotected oligomer fragments.

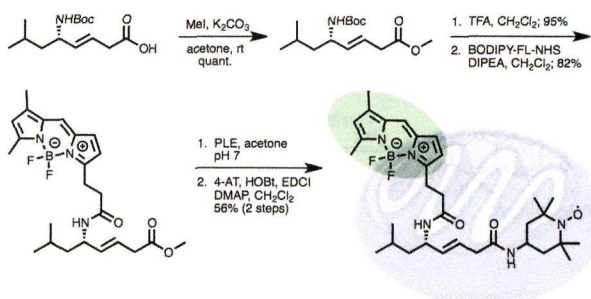


4147

Synthesis of analogs of the radiation mitigator JP4-039 and visualization of BODIPY derivatives in mitochondria

Marie-Céline Frantz, Erin M. Skoda, Joshua R. Sacher, Michael W. Epperly, Julie P. Goff, Joel S. Greenberger and Peter Wipf*

The SAR of new mitochondrially targeted nitroxide conjugates was investigated and fluorophore-tagged analogs provided the opportunity for visualization in mitochondria.



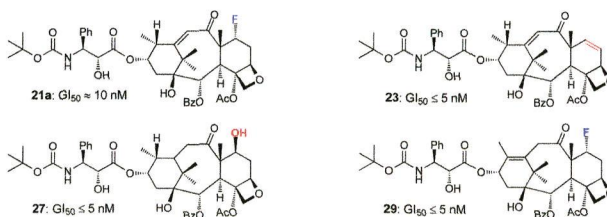
PAPERS

4154

Synthesis and biological evaluation of new paclitaxel analogs and discovery of potent antitumor agents

Kyriacos C. Nicolaou* and Roman A. Valiulin

Synthesis and biological evaluation of a series of paclitaxel analogs revealed a number of potent antitumor agents, including **21a**, **23**, **27**, and **29**.

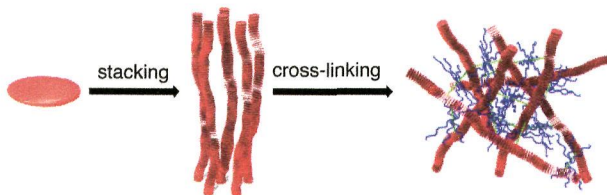


4164

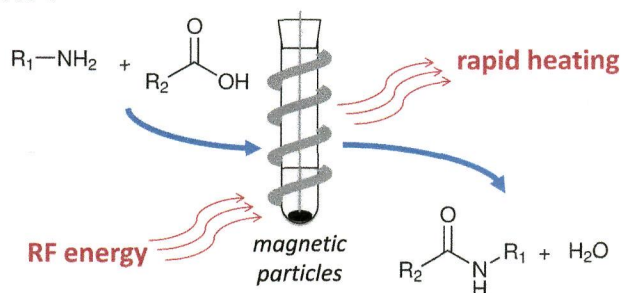
Photoresponsive two-component organogelators based on tris(phenylisoxazoly)benzene

Takeharu Haino,* Yuko Hirai, Toshiaki Ikeda and Hiroshi Saito

New photoresponsive two-component organogels were developed by photochromic tris(phenylisoxazoly)benzene and bipyridine derivatives.



4171

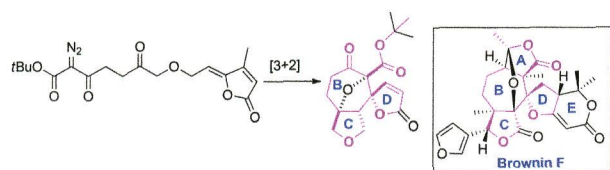


Direct amide formation using radiofrequency heating

Thomas K. Houlding, Kirill Tchabanenko, Md. Taifur Rahman and Evgeny V. Rebrov*

We present a simple method for the direct and solvent-free formation of amides from carboxylic acids and amines using radiofrequency heating.

4178

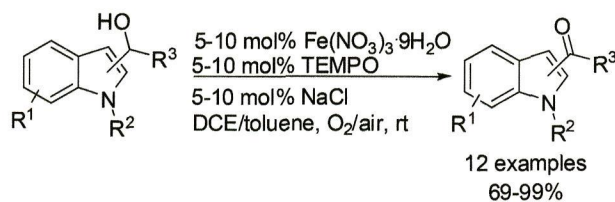


First studies directed towards the diastereoselective synthesis of the BCD tricyclic core of brownin F

Fabien Rodier, Jean-Luc Parrain, Gaëlle Chouraqui* and Laurent Commeiras*

The BCD tricyclic core of brownin F was prepared in eight synthetic operations for the first time. Our synthesis features a diastereo-, chemo- and regioselective intramolecular [3 + 2] cycloaddition between a cyclic carbonyl ylide and a γ -alkylidenebutenolide.

4186

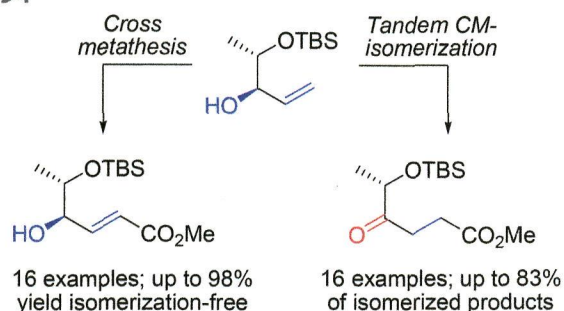


Aerobic oxidation of indole carbinols using $Fe(NO_3)_3 \cdot 9H_2O/TEMPO/NaCl$ as catalysts

Jinxian Liu and Shengming Ma*

A practical method for the aerobic oxidation of indole carbinols using $Fe(NO_3)_3 \cdot 9H_2O/TEMPO/NaCl$ as catalysts under mild conditions was developed, affording aldehydes or ketones in good to excellent yields.

4194



Cross metathesis of allyl alcohols: how to suppress and how to promote double bond isomerization

Bernd Schmidt* and Sylvia Hauke

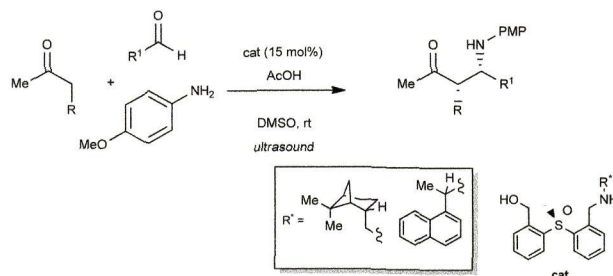
Redox isomerization as a consecutive reaction in the cross metathesis of allyl alcohols can be effectively suppressed or deliberately promoted to obtain γ -hydroxy enoates or γ -oxo-esters selectively.

4207

Efficient catalysts for asymmetric Mannich reactions

Michał Rachwałski,* Tim Leenders, Sylwia Kaczmarczyk, Piotr Kielbasiński, Stanisław Leśniak and Floris P. J. T. Rutjes

Efficient chiral catalysts for asymmetric Mannich reactions have been developed. The reaction conditions have been optimized by invoking ultrasonication.

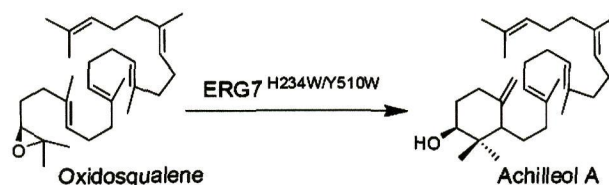


4214

Protein engineering of oxidosqualene-lanosterol cyclase into triterpene monocyclase

Cheng-Hsiang Chang, Hao-Yu Wen, Wen-Shiang Shie, Ching-Ting Lu, Meng-Erh Li, Yuan-Ting Liu, Wen-Hsuan Li and Tung-Kung Wu*

An ERG7^{H234W/Y510W} double mutant generates achilleol A as the sole product, supporting the concept of reverse evolution of triterpene cyclase.

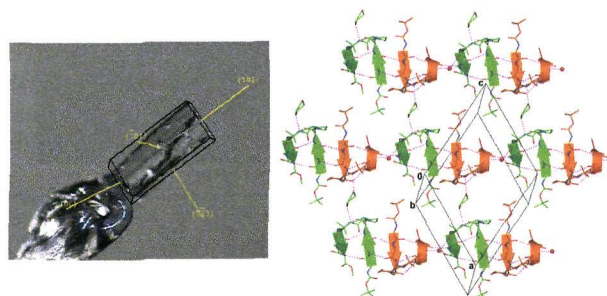


4220

Analysis of designed β -hairpin peptides: molecular conformation and packing in crystals

Subrayashastry Aravinda, Upadhyayula S. Raghavender, Rajkishor Rai, Veldore V. Harini, Narayanaswamy Shamala* and Padmanabhan Balaram*

Crystal structure determination of several designed β -hairpin peptides reveal three broad modes of association: parallel packing, antiparallel packing and orthogonal packing.

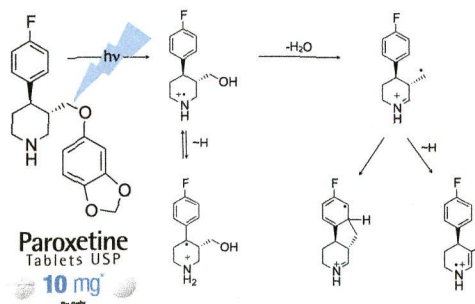


4232

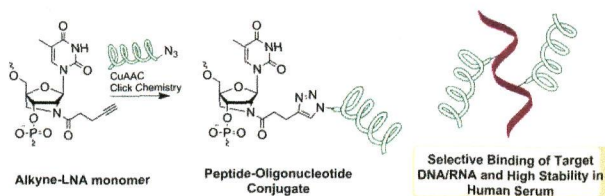
The chemical fate of paroxetine metabolites. Dehydration of radicals derived from 4-(4-fluorophenyl)-3-(hydroxymethyl)piperidine

Davor Šakić, Florian Achrainner, Valerije Vrček* and Hendrik Zipse

The light-induced dehydration of paroxetine metabolites is a radical-mediated process which can be modeled computationally. Several structures, not considered earlier, are proposed as probable photoproducts in aqueous environments.



4240



Peptide-LNA oligonucleotide conjugates

I. Kira Astakhova,* Lykke Hastrup Hansen, Birte Vester and Jesper Wengel

Herein we reveal how the CuAAC click reaction on a 2'-alkyne-2'-amino-LNA scaffold can be applied for preparation of peptide-oligonucleotide conjugates demonstrating high target binding affinity and selectivity, and remarkable stability in human serum.

4250

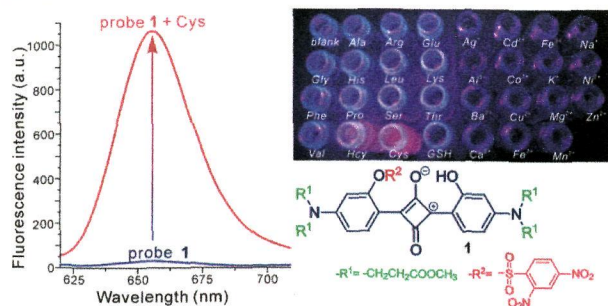


Cooperative enhancement of optical nonlinearities in a porphyrin derivative bearing a pyrimidine chromophore at the periphery

Aijian Wang, Lingliang Long, Suci Meng, Xiufen Li, Wei Zhao, Yinglin Song, Marie P. Cifuentes, Mark G. Humphrey and Chi Zhang*

Enhanced optical nonlinearities were observed for compound **6** due to a combination of different nonlinear mechanisms.

4258

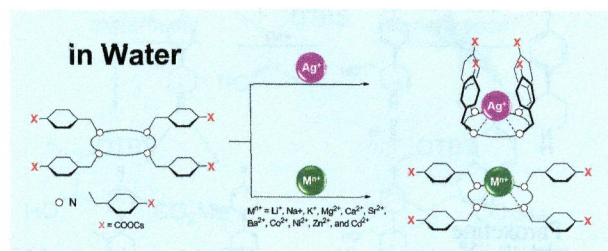


A squaraine-based red emission off-on chemosensor for biothiols and its application in living cells imaging

Xiao-Dong Liu, Ru Sun, Jian-Feng Ge,* Yu-Jie Xu,* Ying Xu and Jian-Mei Lu*

A squaraine-based fluorescent turn-on red-emitting probe for cysteine and homocysteine in biological conditions.

4265



The water-soluble argentivorous molecule: Ag^+ - π interactions in water

Yoichi Habata,* Yoko Okeda, Mari Ikeda and Shunsuke Kuwahara

Ag^+ - π interactions between Ag^+ ions and a water-soluble tetra-armed cyclen bearing aromatic side-arms (tetracesium 4,4',4'',4'''-((1,4,7,10-tetraazacyclododecane-1,4,7,10-tetrayl)tetrakis(methylene))tetrabenzoate, Cs_4L) are reported.