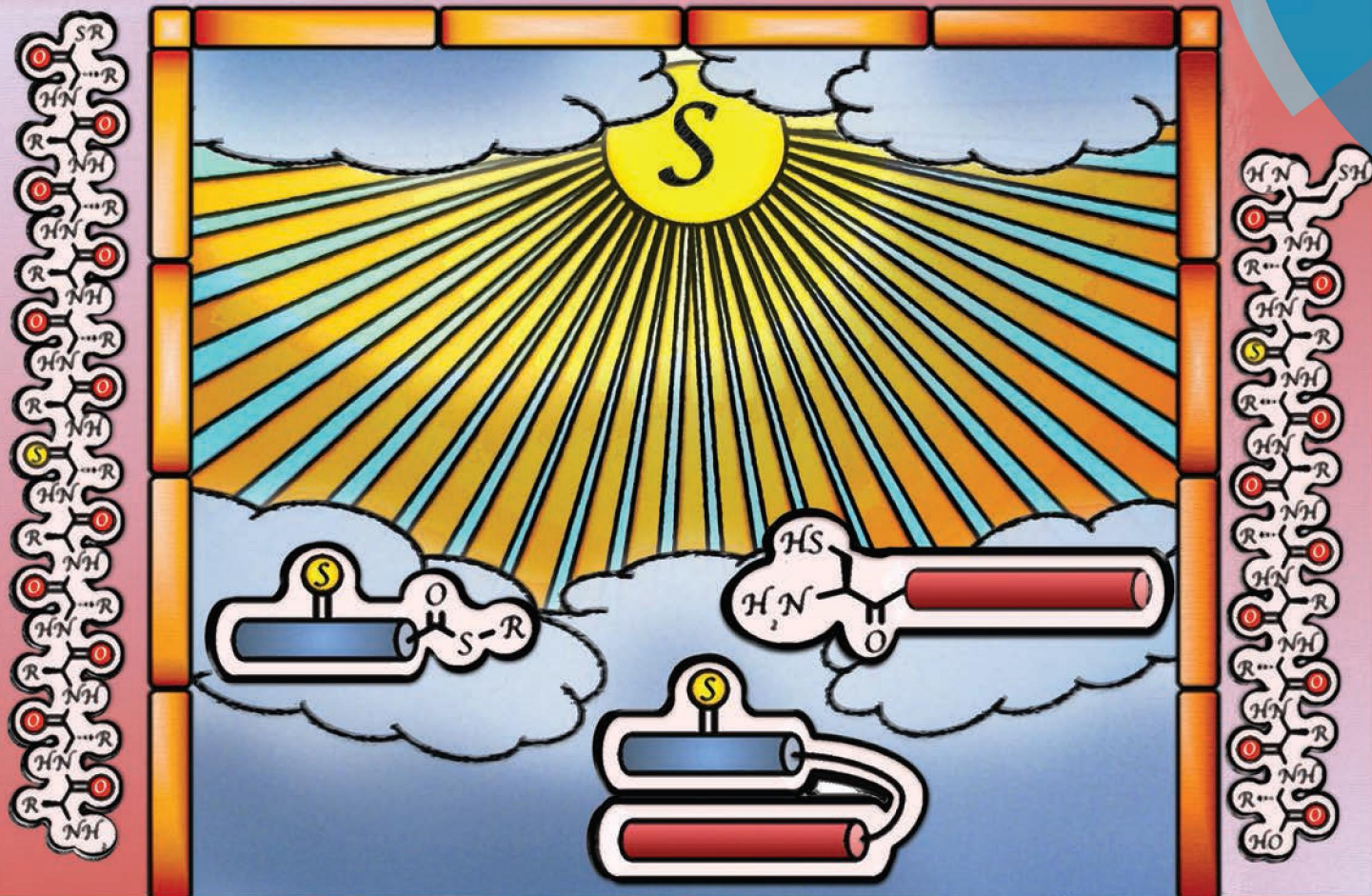


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Thioprotein Semisynthesis



ISSN 1477-0520



PERSPECTIVE

E. James Petersson *et al.*

Semi-synthesis of thioamide containing proteins

Organic & Biomolecular Chemistry

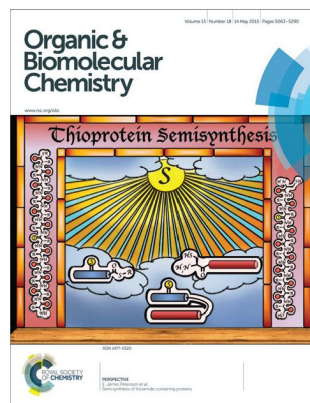
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Cover

See E. James Petersson *et al.*, pp. 5074–5081.

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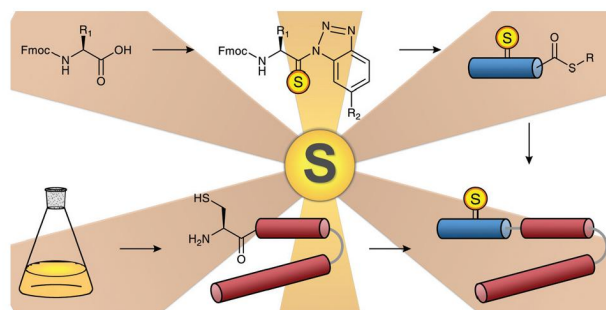
PERSPECTIVE

5074

Semi-synthesis of thioamide containing proteins

Yanxin J. Wang, D. Miklos Szantai-Kis and E. James Petersson*

To make thioamide protein folding experiments applicable to full-sized proteins, our laboratory has used a combination of native chemical ligation of thiopeptide fragments, unnatural amino acid mutagenesis to install fluorophore partners in expressed protein fragments, and chemoenzymatic protein modification to render these expressed protein ligations traceless.



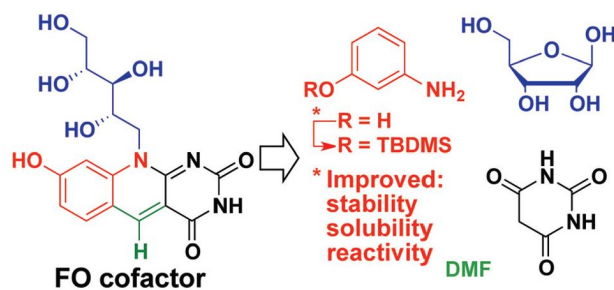
COMMUNICATIONS

5082

Convenient synthesis of deazaflavin cofactor FO and its activity in F₄₂₀-dependent NADP reductase

Mohammad S. Hossain, Cuong Q. Le, Ebenezer Joseph, Toan Q. Nguyen, Kayunta Johnson-Winters* and Frank W. Foss Jr.*

Revised synthesis of FO, a 5-deazaflavin cofactor, and its activity as a surrogate for the F₄₂₀ cofactor in Fno.



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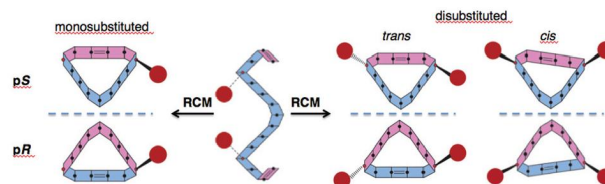
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5086

Stereogenic α -carbons determine the shape and topology of [13]-macrolactones

Anniefer N. Magpusao, Kelli Rutledge,
Brandon Q. Mercado and Mark W. Peczu*^{*}

The configuration of α -stereogenic centers affects the shape and topology of [13]-macrolactones. When one α -stereogenic center is substituted, it directs the planar chirality of the macrocycle; when two centers are substituted, both the shape and the topology are influenced.

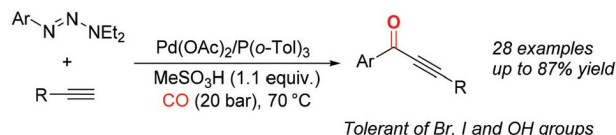


5090

Palladium-catalyzed carbonylative Sonogashira coupling between aryl triazenes and alkynes

Wanfang Li and Xiao-Feng Wu*^{*}

We developed an interesting palladium-catalyzed carbonylative Sonogashira reaction with aryl triazenes and alkynes as substrates and methanesulfonic acid as the additive. A series of α,β -ynones were synthesized by this alternative procedure. Notably, bromides, iodides and hydroxyl groups could be well-tolerated under these reaction conditions.

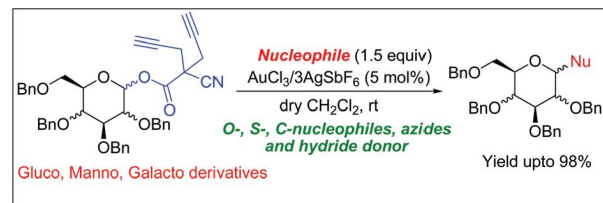


5094

Gold-catalysed glycosylation reaction using an easily accessible leaving group

Srinivasa Rao Koppolu, Ramana Niddana and
Rengarajan Balamurugan*^{*}

Development of a simple leaving group for the gold-catalysed glycosylation has been achieved.

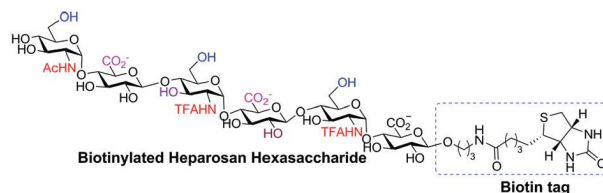


5098

Facile chemoenzymatic synthesis of biotinylated heparosan hexasaccharide

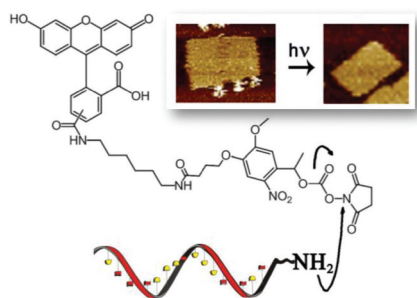
Baolin Wu, Na Wei, Vireak Thon, Mohui Wei, Zaikuan Yu,
Yongmei Xu, Xi Chen, Jian Liu, Peng George Wang* and
Tiehai Li*^{*}

A biotinylated heparosan hexasaccharide was synthesized by a facile chemoenzymatic approach in a one-pot multi-enzyme fashion.



COMMUNICATIONS

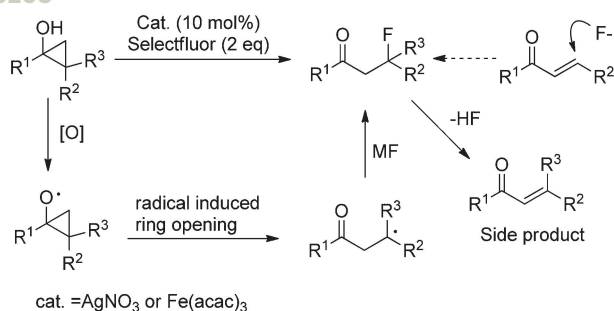
5102

**Photocleavable ligands for protein decoration of DNA nanostructures**

Josipa Brglez, Ishtiaq Ahmed and Christof M. Niemeyer*

Amino-reactive, photocleavable modifiers bearing small-molecule hapten groups were incorporated into DNA origami to control binding of cognate proteins.

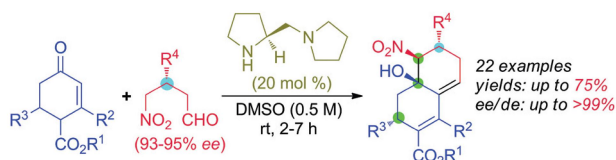
5105

**Iron- or silver-catalyzed oxidative fluorination of cyclopropanols for the synthesis of β -fluoroketones**

Shichao Ren, Chao Feng* and Teck-Peng Loh*

The Fe^{III}- or Ag^I-catalyzed oxidative fluorination of cyclopropanols *via* radical rearrangement is disclosed.

5110

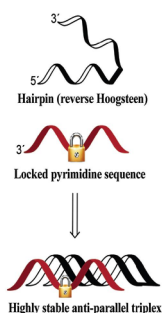
**Organocatalytic diastereoselective synthesis of chiral decalines through the domino Claisen–Schmidt/Henry reaction**

Adhuri B. Shashank and Dhevalapally B. Ramachary*

General and operative domino Claisen–Schmidt/Henry (CS/H) reaction has been revealed to obtain highly substituted chiral decalines in good yields with excellent ees and des by using push–pull enamine catalysis.

PAPERS

5115

**Thermal stability of G-rich anti-parallel DNA triplexes upon insertion of LNA and α -L-LNA**

Tamer R. Kosbar, Mamdouh A. Sofan, Laila Abou-Zeid and Erik B. Pedersen*

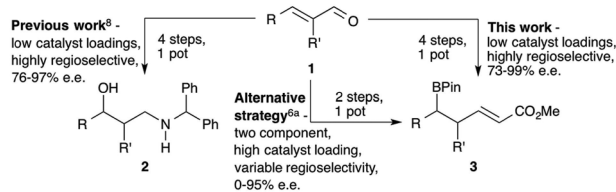
G-rich anti-parallel DNA triplexes were modified with LNA or α -L-LNA in their Watson–Crick and TFO strands.

5122

One-pot catalytic asymmetric borylation of unsaturated aldehyde-derived imines; functionalisation to homoallylic boronate carboxylate ester derivatives

Alba Pujol, Adam D. J. Calow, Andrei S. Batsanov and Andrew Whiting*

The β -borylation reaction of α,β -unsaturated aldehyde-derived imines, formed *in situ*, has been studied using a one-pot methodology, as a route to homoallylic boronates through the β -boryl aldehydes.

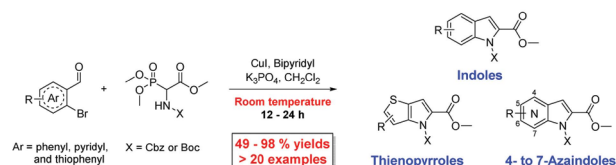


5131

Mild one-pot Horner–Wadsworth–Emmons olefination and intramolecular N-arylation for the syntheses of indoles, all regio-isomeric azaindoles, and thienopyrroles

Ji Hye Choi and Hwan Jung Lim*

Indoles, azaindoles, and thienopyrroles have been successfully synthesized using mild one-pot Horner–Wadsworth–Emmons olefination and intramolecular N-arylations.

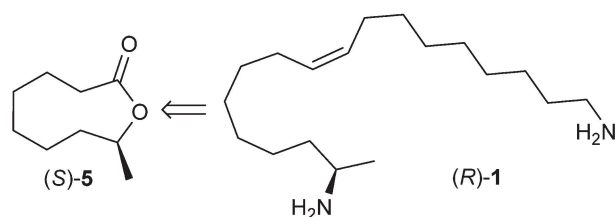


5139

Efficient synthesis of (*R*)-harmonine – the toxic principle of the multicolored Asian lady beetle (*Harmonia axyridis*)

Nadja C. Nagel, Anita Masic, Uta Schurig and Wilhelm Boland*

An efficient and flexible synthesis of (*R*)-harmonine and putative biosynthetic precursors has been developed. Furthermore, its antimicrobial activity against *Leishmania major* is demonstrated.

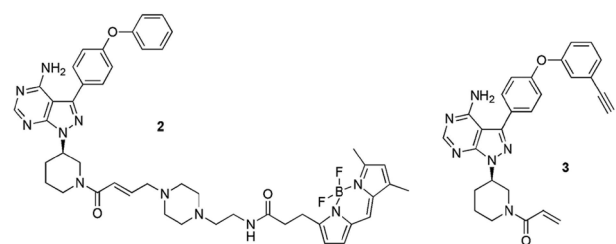


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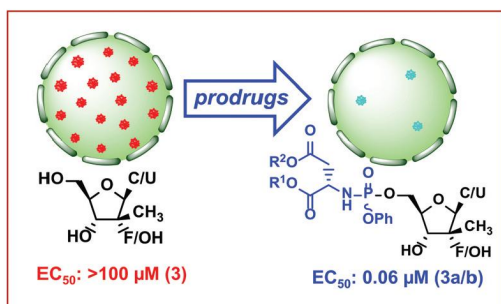
Direct and two-step bioorthogonal probes for Bruton's tyrosine kinase based on ibrutinib: a comparative study

Nora Liu, Sascha Hoogendoorn, Bas van de Kar, Allard Kaptein, Tjeerd Barf, Christoph Driessen, Dmitri V. Filippov, Gijsbert A. van der Marel, Mario van der Stelt* and Herman S. Overkleeft*

Direct and two-step activity-based probes allow for profiling of Bruton's tyrosine kinase *in vitro* and *in situ*.



5158

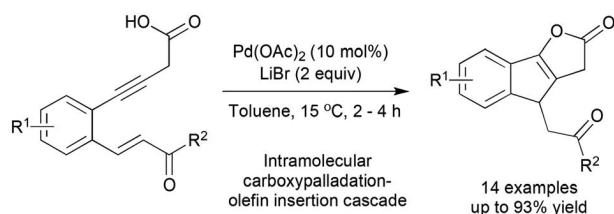


Aspartic acid based nucleoside phosphoramidate prodrugs as potent inhibitors of hepatitis C virus replication

Munmun Maiti, Mohitosh Maiti, Jef Rozenski, Steven De Jonghe and Piet Herdewijn*

A series of novel nucleoside phosphoramidate prodrugs has been synthesized and shown as potent inhibitors of hepatitis C virus replication. The conjugates are having a diverse structural variation in the promoiety part and can be catalytically processed to deliver active nucleotides.

5175

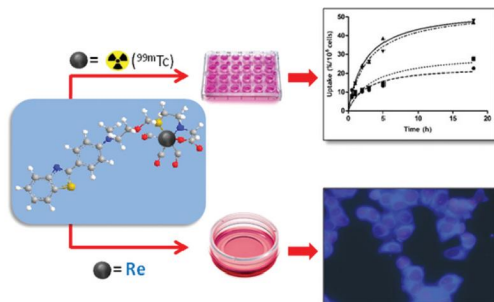


Palladium(II)-catalyzed intramolecular carboxypalladation-olefin insertion cascade: direct access to indeno[1,2-*b*]furan-2-ones

Perumal Vinoth, Thavaraj Vivekanand, Padmakar A. Suryavanshi, J. Carlos Menéndez, Hiroaki Sasai and Vellaisamy Sridharan*

An efficient intramolecular carboxypalladation-olefin insertion cascade was developed for the synthesis of indeno[1,2-*b*]furan-2-ones.

5182

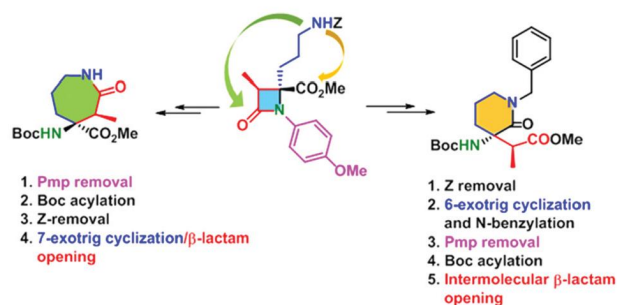


Isostructural Re(I)/^{99m}Tc(I) tricarbonyl complexes for cancer theranostics

Patrique Nunes, Goreti Ribeiro Morais, Elisa Palma, Francisco Silva, Maria Cristina Oliveira, Vera F. C. Ferreira, Filipa Mendes, Lurdes Gano, Hugo Vicente Miranda, Tiago F. Outeiro, Isabel Santos and António Paulo*

Novel cysteamine-based (N,S,O)-chelators were successfully applied in the synthesis of isostructural M(I) (M = Re, ^{99m}Tc) tricarbonyl complexes for cancer theranostics.

5195



Divergent, stereoselective access to heterocyclic α,α -quaternary- and $\beta^{2,3,3}$ -amino acid derivatives from a *N*-Pmp-protected Orn-derived β -lactam

Diego Núñez-Villanueva, M. Teresa García-López, Mercedes Martín-Martínez and Rosario González-Muñiz*

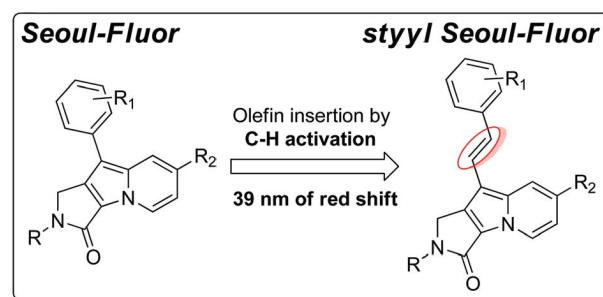
A unique *N*-*p*-methoxybenzyl Orn-derived (3*S*,4*S*)- β -lactam was divergently transformed into (3*S*,4*S*)-2-oxoazepane- α,α - and (2*S*,3*S*)-2-oxopiperidine- $\beta^{2,3,3}$ -amino acid derivatives.

5202

Unique photophysical properties of 9-styryl-1,2-dihydropyrrolo[3,4- β]indolizin-3-one and its efficient synthesis *via* direct C–H activation

Eun Joung Choi and Seung Bum Park*

A styryl Seoul-Fluor (SF) skeleton was rationally designed by introducing an olefin unit at the C-9 of 1,2-dihydropyrrolo[3,4- β]indolizin-3-one *via* regioselective direct C–H activation, affording average 39 nm of bathochromic shift.

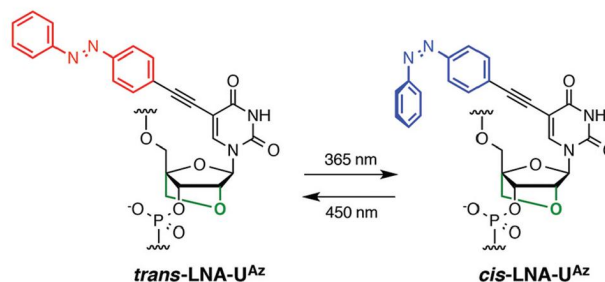


5209

C5-azobenzene-functionalized locked nucleic acid uridine: isomerization properties, hybridization ability, and enzymatic stability

K. Morihiro,* O. Hasegawa, S. Mori, S. Tsunoda and S. Obika*

C5-azobenzene-functionalized locked nucleic acid uridine (LNA-U^{Az}) shows effective photo-isomerization properties, RNA-selective hybridization ability, and high enzymatic stability.

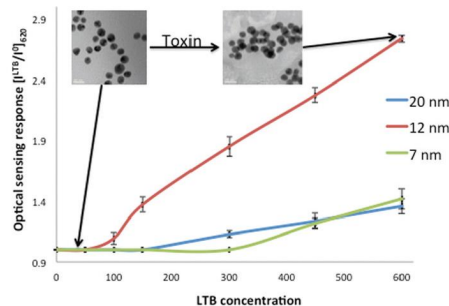


5215

Size-optimized galactose-capped gold nanoparticles for the colorimetric detection of heat-labile enterotoxin at nanomolar concentrations

Vivek Poonthiyil, Vladimir B. Golovko* and Antony J. Fairbanks*

Galactose-capped gold nanoparticles size-dependently sense the bacterial lectin, heat-labile enterotoxin, allowing selective colorimetric toxin detection at 100 nM.

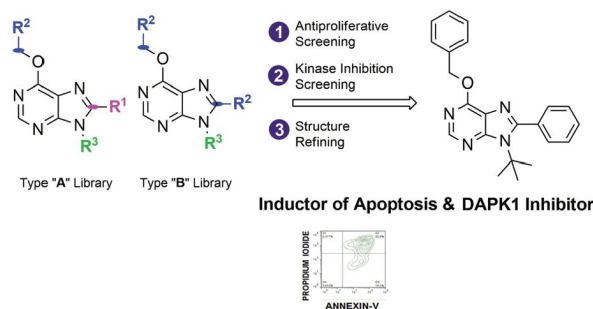


5224

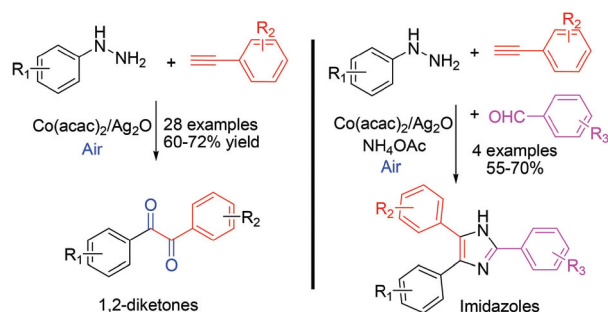
Synthesis of 6,8,9 poly-substituted purine analogue libraries as pro-apoptotic inducers of human leukemic lymphocytes and DAPK-1 inhibitors

Maria J. Pineda de las Infantas,* Sara Torres-Rusillo, Juan Diego Unciti-Broceta, Pablo Fernandez-Rubio, Maria Angelica Luque-Gonzalez, Miguel A. Gallo, Asier Unciti-Broceta, Ignacio J. Molina* and Juan J. Diaz-Mochon*

Purines to study DAPK1 role in apoptosis.



5235

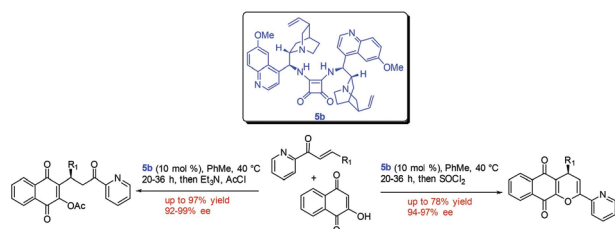


Cobalt(II) catalyzed C(sp)-H bond functionalization of alkynes with phenyl hydrazines: facile access to diaryl 1,2-diketones

Jaideep B. Bharate, Sheenu Abbat, Rohit Sharma, Prasad V. Bharatam,* Ram A. Vishwakarma* and Sandip B. Bharate*

A cobalt acetylacetonate catalyzed oxidative diketonation of alkynes via C(sp)-H bond functionalization has been described. Its application to the synthesis of imidazoles has also been demonstrated.

5243

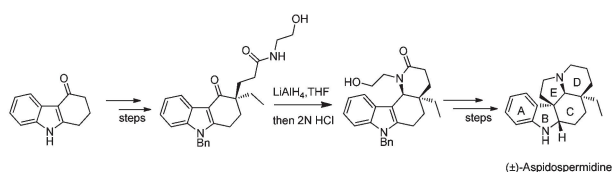


Highly enantioselective synthesis of naphthoquinones and pyranonaphthoquinones catalyzed by bifunctional chiral bis-squaramides

Nagaraju Molleti and Vinod K. Singh*

A variety of enantioenriched naphthoquinones has been synthesized in high yields and excellent enantioselectivities (up to >99% ee) using a bifunctional chiral bis-squaramide catalyzed conjugate addition of 2-hydroxy-1,4-naphthoquinone to 2-enoylpyridines.

5255

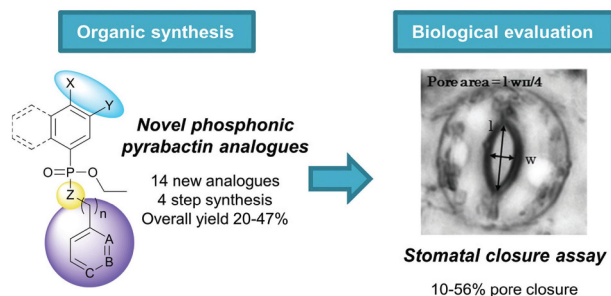


Concise total synthesis of (+)-aspidospermidine

Haichen Ma, Xingang Xie, Peng Jing, Weiwei Zhang and Xuegong She*

(+)-Aspidospermidine (**1**) has been synthesized from the commercially available 2,3-dihydro-1H-carbazol-4(9H)-one **6** in 10 steps with 20% overall yield. The key step of the strategy is a one-pot carbonyl reduction/iminium formation/intramolecular conjugate addition reaction that may be applied for the synthesis of other kinds of *Aspidosperma* alkaloids.

5260



Phosphonamide pyrabactin analogues as abscisic acid agonists

M. Van Overtveldt, T. S. A. Heugebaert, I. Verstraeten, D. Geelen and C. V. Stevens*

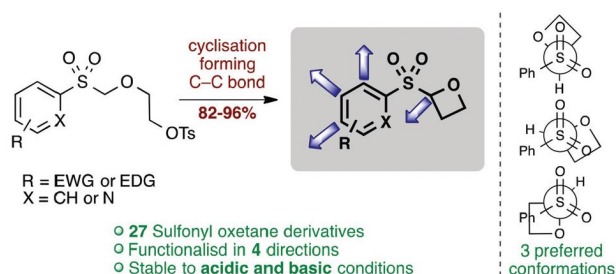
A 4-step synthesis towards phosphonic pyrabactin analogues is presented. Via a stomatal closure and germination assay, their ability to selectively induce the ABA-signaling pathway was demonstrated.

5265

Studies on the synthesis, stability and conformation of 2-sulfonyl-oxetane fragments

K. F. Morgan, I. A. Hollingsworth and J. A. Bull*

A library of 2-sulfonyl oxetane fragments has been synthesised and elaborated into lead-like compounds. The oxetane derivatives were stable to acidic and basic conditions and have 3-preferred conformations.

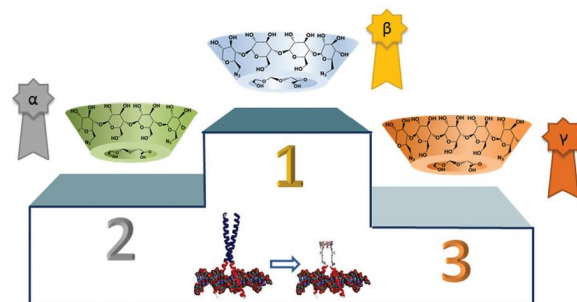


5273

Cyclodextrin-peptide conjugates for sequence specific DNA binding

Yara Ruiz García, Jan Zelenka, Y. Vladimir Pabon, Abhishek Iyer, Miloš Buděšínský, Tomáš Kraus, C. I. Edvard Smith and Annemieke Madder*

CD-peptide conjugates were synthesized *via* CuAAC. Though the CD cavity size was shown to influence the binding affinity of the compounds, all constructs recognize and bind the cognate CRE dsDNA.

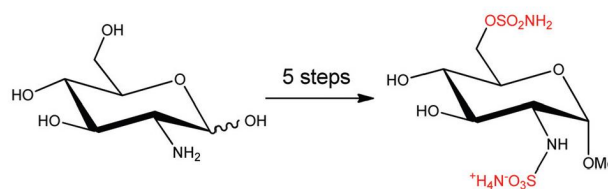


5279

Regioselective sulfamoylation at low temperature enables concise syntheses of putative small molecule inhibitors of sulfatases

Duncan C. Miller,* Benoit Carbain, Gary S. Beale, Sari F. Alhasan, Helen L. Reeves, Ulrich Baisch, David R. Newell, Bernard T. Golding* and Roger J. Griffin

An improved synthesis from D-glucosamine of a purported Sulf-2 inhibitor is described, with assay data for this compound and analogues showing only weak inhibition of Sulf-2, and sulfatases ARSA or ARSB.



5285

Metal-free cascade cyclization of alkenes toward perfluorinated oxindoles

Shi Tang,* Zhi-Hao Li, Ming-Wei Wang, Zhi-Ping Li and Rui-Long Sheng

A simple AIBN-mediated cyclization reaction of activated alkenes toward perfluorinated oxindoles is developed.

