Organic & Biomolecular Chemistry

An international journal of synthetic, physical and biomolecular organic chemistry

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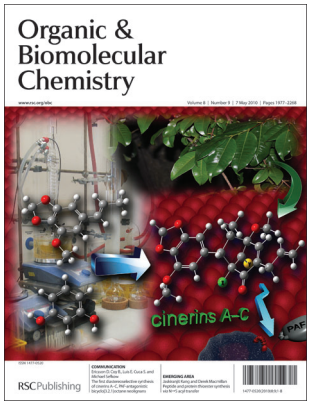
IN THIS ISSUE

ISSN 1477-0520 CODEN OBCRAK 8(9) 1977–2268 (2010)



Cover
See Michael Sefkow *et al.*, pp. 2003–2005.
The first total synthesis of PAF-antagonistic cinerins A–C, isolated from the leaves of *Pleurothyrium cinereum*, is reported by Coy *et al.* on page 2003.

Image reproduced by permission of Michael Sefkow from *Org. Biomol. Chem.*, 2010, **8**, 2003.

Inside cover
See Werner M. Nau *et al.*, pp. 2037–2042.
Cucurbiturils are promising macrocycles for drug delivery, which have now been shown to display very low, if not negligible, toxicity in cell and animal studies.

Image reproduced by permission of Werner M. Nau from *Org. Biomol. Chem.*, 2010, **8**, 2037.

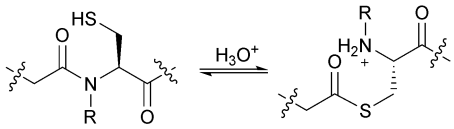
EMERGING AREA

1993

Peptide and protein thioester synthesis *via* N→S acyl transfer

Jaskiranjit Kang and Derek Macmillan*

Peptide thioesters are playing an increasingly prominent role in the chemical toolbox for protein assembly and modification through Native Chemical Ligation (NCL). In this article we highlight recent developments in thioester production through selective disruption of amide bonds.



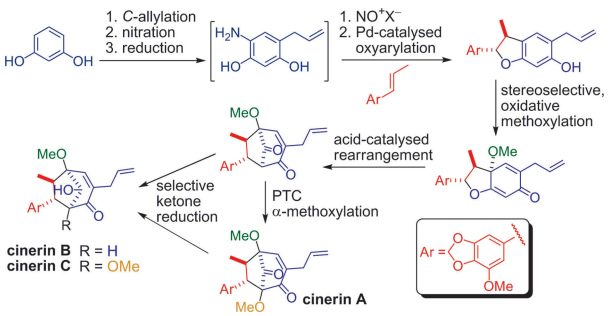
COMMUNICATIONS

2003

The first diastereoselective synthesis of cinerins A–C, PAF-antagonistic macrophyllin-type bicyclo[3.2.1]octane neolignans, using a novel Pd-catalysed oxyarylation

Ericsson D. Coy B.,* Luis E. Cuca S. and Michael Sefkow*

The first diastereoselective synthesis of PAF-antagonistic cinerins A–C, macrophyllin-type bicyclo[3.2.1]octane neolignans from *Pleurothyrium cinereum*, has been accomplished using a novel Pd-catalysed oxyarylation to afford a 2,3-dihydrobenzofuran as the key intermediate.



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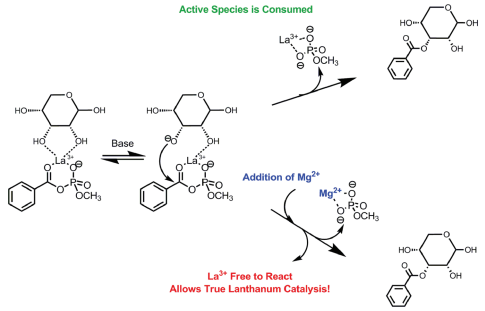
2006

Magnesium ion enhances lanthanum-promoted monobenzoylation of a monosaccharide in water

Raj S. Dhiman and Ronald Kluger*

Monobenzoylation of sugars is promoted by lanthanum triflate. Addition of magnesium ion produces a precipitate from the phosphate monoester by-product that allows lanthanum to function at low catalyst loading.

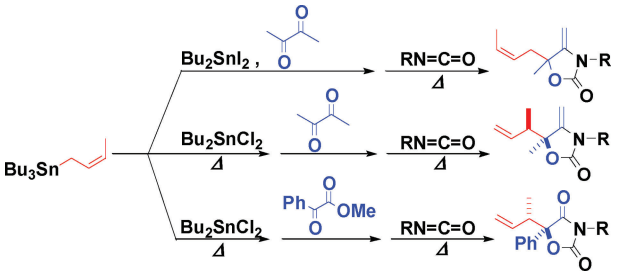


2009

Synthesis of oxazolidinones initiated by regio- and diastereo-controlled crotylation of α-dicarbonyl compounds

Ikuya Shibata,* Ryota Kojima, Shinji Tsunoi, Takashi Nozaki, Tomonari Watanabe, Atsushi Ninomiya, Makoto Yasuda and Akio Baba

One-pot synthesis of oxazolidinones was established initiated by allylation of α-dicarbonyl compounds, accompanying regio- and diastereo-controlled carbon–carbon bond formation on the side chains of the oxazolidinones.

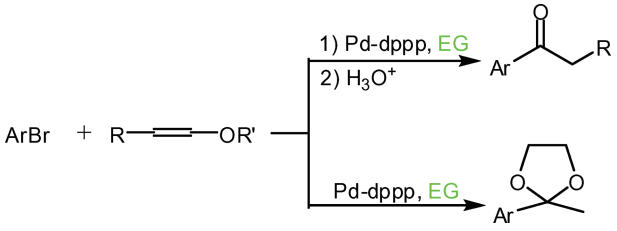


2012

Efficient synthesis of alkyl aryl ketones & ketals *via* palladium-catalyzed regioselective arylation of vinyl ethers

Mingcui Liu, Zeynab Hyder, Yawei Sun, Weijun Tang, Lijin Xu* and Jianliang Xiao

The combination of $Pd(OAc)_2$ with 1,3-bis(diphenylphosphino)propane in ethylene glycol constitutes a high-performance catalytic system for highly regioselective arylation of a range of electron-rich vinyl ethers by aryl bromides to provide, upon hydrolysis, alkyl aryl ketones and cyclic ketals in good yields with up to 3.75×10^5 TON and 15625 h^{-1} TOF.

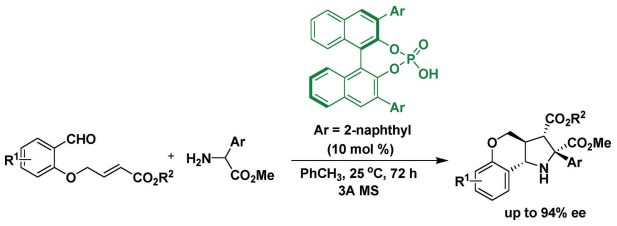


2016

Organocatalytic asymmetric intramolecular [3+2] cycloaddition: A straightforward approach to access multiply substituted hexahydrochromeno[4,3-b]pyrrolidine derivatives in high optical purity

Nan Li, Jin Song, Xi-Feng Tu, Bin Liu, Xiao-Hua Chen and Liu-Zhu Gong*

Asymmetric organocatalytic intramolecular 1,3-dipolar cycloaddition of 4-(2-formylphenoxy)butenoates with amino esters provides hexahydromeno[4,3-b]pyrrolidine derivatives in high ee (up to 94% ee).

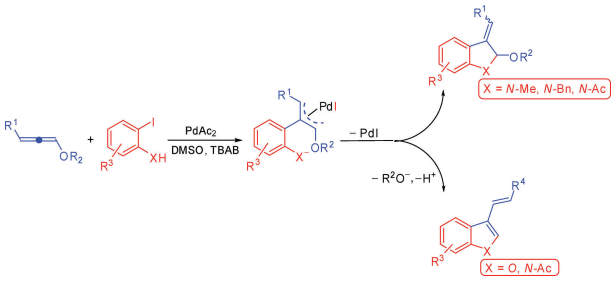


2020

Heck reaction on protected 3-alkyl-1,2-dien-1-ols: an approach to substituted 3-alkenylindoles, 2-alkoxy-3-alkylidene-2,3-dihydrobenzofuranes and -indolidines

Tommaso Boi, Annamaria Deagostino,* Cristina Prandi, Silvia Tabasso, Antonio Toppino and Paolo Venturello

Two different heterocyclic frameworks were obtained in the benzoannulation of 3-alkyl-1,2-dienols and *o*-iodophenols or protected *o*-iodoanilines, in dependence of the nucleophilic properties of the attaching heteroatom.

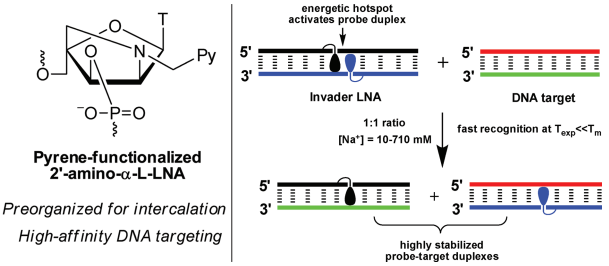


2028

Invader LNA: Efficient targeting of short double stranded DNA

Sujay P. Sau, T. Santhosh Kumar and Patrick J. Hrdlicka*

Energetically activated double stranded Invader LNA probes enable recognition of short isosequential dsDNA-targets at low experimental temperatures, at a variety of ionic strengths, and with good mismatch discrimination.

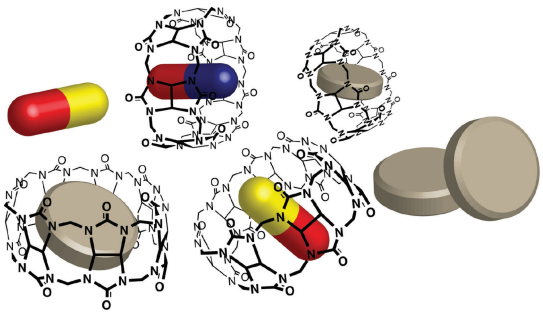


2037

Toxicity of cucurbit[7]uril and cucurbit[8]uril: an exploratory *in vitro* and *in vivo* study

Vanya D. Uzunova, Carleen Cullinane, Klaudia Brix, Werner M. Nau* and Anthony I. Day*

The molecular container cucurbit[7]uril shows a low cytotoxicity (IC_{50} = 0.53 mM) and high tolerated intravenous and oral dosage of at least 250 mg kg^{-1}, which makes it an ideal candidate for potential pharmaceutical applications.

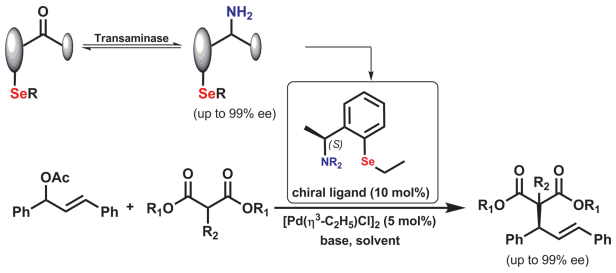


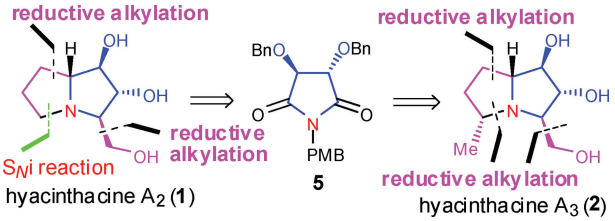
2043

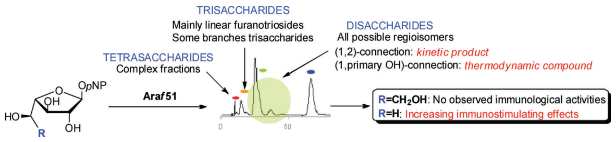
ω-Transaminases as efficient biocatalysts to obtain novel chiral selenium-amine ligands for Pd-catalysis

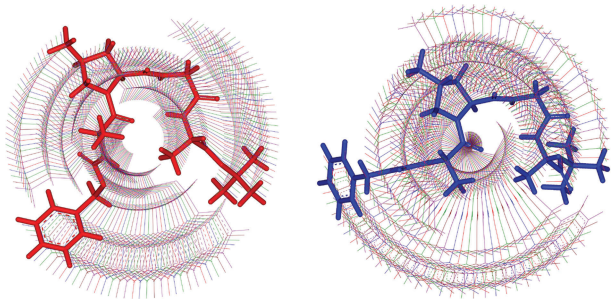
Leandro H. Andrade,* Alexandre V. Silva, Priscila Milani, Dominik Koszelewski and Wolfgang Kroutil

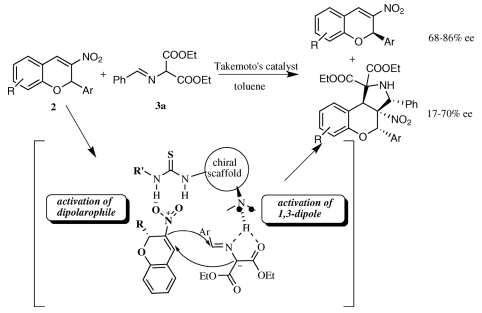
Modulated chiral selenium-amines were efficiently synthesized by using ω-transaminases as tools for asymmetric induction. New chiral selenium compounds were evaluated as ligands in the palladium-catalyzed asymmetric alkylation.











ICOS 18

18th International Conference on Organic Synthesis
Bergen, Norway, August 1st – 6th, 2010

Conference chair:

Professor Leiv K. Sydnes
leiv.sydnes@kj.uib.no

Invited speakers:

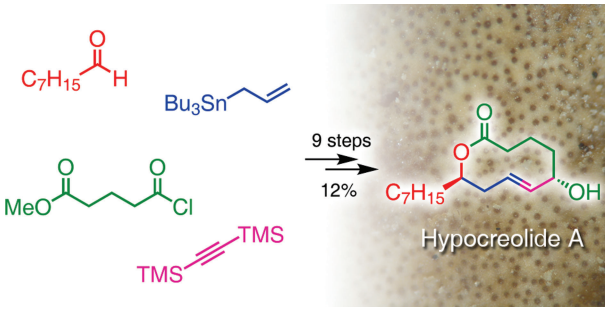
Varinder K. Aggarwal, UK
Helen E. Blackwell, USA
Christian Bochet, Switzerland
David Y.-K. Chen, Singapore
Karol Grela, Poland
Antonio Guarna, Italy
Henk Hiemstra, The Netherlands
Ari M. P. Koskinen, Finland
Mark Lautens, Canada
Anita Maguire, Ireland
Vakhid A. Mamedov, Russia
José L. Mascareñas, Spain
Frank E. McDonald, USA
Hans Reissig, Germany
Dieter Schinzer, Germany
Tony K. M. Shing, Hong Kong
Snorri Th. Sigurdsson, Iceland
Mats Tilset, Norway

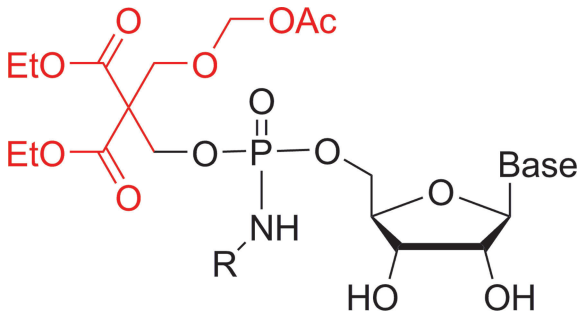
Plenary speakers:

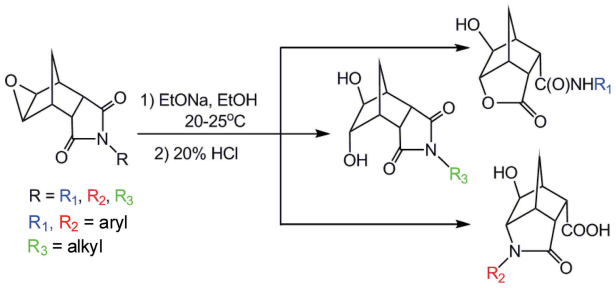
Prof. Jan E. Bäckvall, Sweden
Prof. Martin Banwell, Australia
Prof. Valery V. Fokin, USA
Prof. Karl A. Jørgensen, Denmark
Nobel Laureate Robert H. Grubbs, USA
Prof. Paul Knochel, Germany
Prof. Steven Ley, UK
Prof. Johann Mulzer, Austria
Prof. Samir Zard, France
Prof. Dieter Seebach, Switzerland
Prof. Victor Snieckus, Canada
Prof. Michinori Suginome, Japan

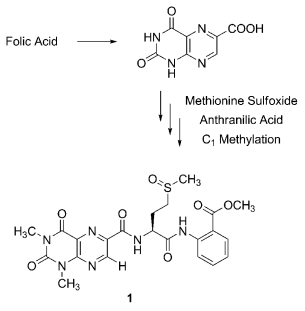
In addition to these speakers the winner of the 2010 Thieme–IUPAC Prize in Synthetic Organic Chemistry, Prof. Phil Baran, will receive the prize and deliver the Prize Lecture.

Register and submit abstract through www.ICOS-18.no









BIT's 1st Annual International Conference of

Medichem-2010

Theme: Smart Chemistry in Drug Discovery

Highlights

- Organize up to 150 + Oral Presentations on the Latest Tech Trend of Medicinal Chemistry Development
- Bring together 80 + Project Posters on New Technologies Implemented in Industrial Manufacturing
- Network with 300 + Colleagues and Friends in China and Beyond
- Meet with 100 + Leading Suppliers from all over the World

Time: May 18-20, 2010
Place: International Convention Center
Beijing, China

Renowned Speakers

Dr. Herbert Treutlein, Co-Founder and CEO, Qubist Molecular Design Pty. Ltd., Australia

Dr. Thomas Ryckmans, Senior Principle, Pfizer Discovery Chemistry, Global Research and Development, UK

Dr. Thomas Ruckle, Director of Discovery Project Management at Merck Serono, Switzerland

Dr. Spiros Liras, Executive Director and Department Head, CVMED Medicinal Chemistry, Pfizer, USA

Dr. Jiaan Yang, Vice President of Drug Discovery Technology, Sundia MediTech Company, Ltd., China

Dr. Tony Wood, Vice President, Pfizer Global Research & Development, UK

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Email: grace@webbitmail.cn

Programmed Tracks at a Glance

- Track 1: Target Structure and Fragment Based Drug Design and Synthesis
- Track 2: Application of New Technologies and Tools for Medichem Studies
- Track 3: Case Studies of Medichem on Drug Candidates on Major Diseases
- Track 4: Medichem R & D Outsourcing Alliance Trend

*Call for Co-organizers
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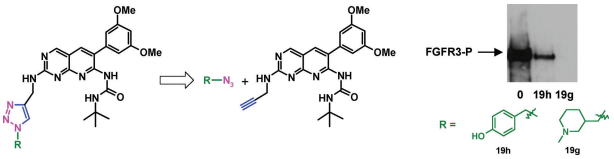

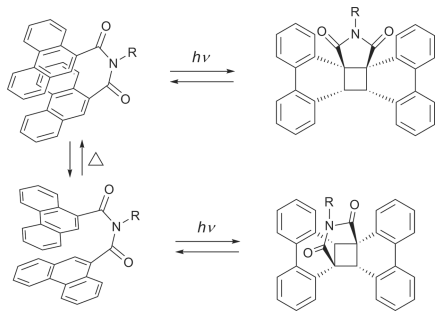

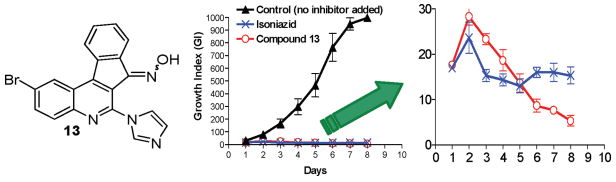

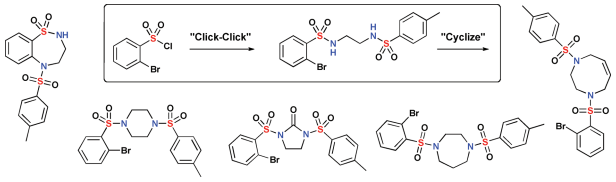

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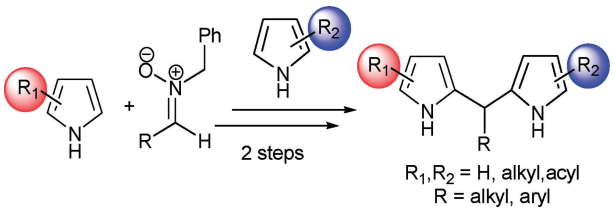
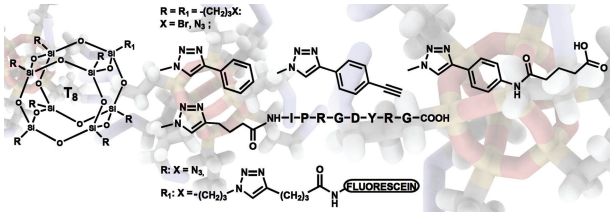


An efficient method for the synthesis of unsymmetrical 2,2′-bis(pyrrolyl)alkanes

Marie Laure Murat-Onana, Christophe Berini, Frédéric Minassian,* Nadia Pelloux-Léon* and Jean-Noël Denis

A new strategy for the preparation of unsymmetrical 2,2′-bis(pyrrolyl)alkanes has been developed, and it has also been extended to the synthesis of tripyrromethanes and *N*-confused dipyrromethanes.

2212

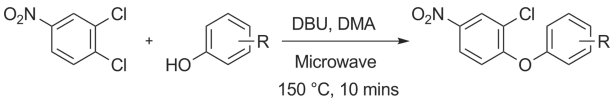


Towards click bioconjugations on cube-octameric silsesquioxane scaffolds

Sebastian Fabritz, Dirk Heyl, Viktor Bagutski, Martin Empting, Eckhard Rikowski, Holm Frauendorf, Ildiko Balog, Wolf-Dieter Fessner, Jörg. J. Schneider, Olga Avrutina and Harald Kolmar*

Synthesis and click conjugations on octaazido octasilsesquioxane scaffold without cage rearrangements are described, including effective transformation into an octaalkyne POSS framework and an octaconjugate of a fully unprotected functional peptide.

2219

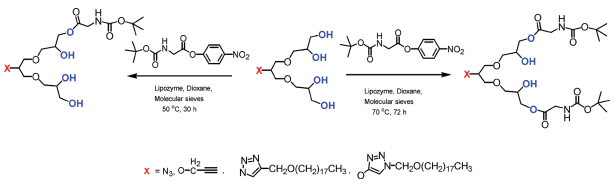


The application of stop-flow microwave technology to scaling-out S_NAr reactions using a soluble organic base

Jameel A. Marafie and Jonathan D. Moseley*

Substituted diaryl ethers have been prepared by S_NAr reaction in combination with a soluble organic base, with productivities of >0.5 kg per day using an automated stop-flow microwave reactor.

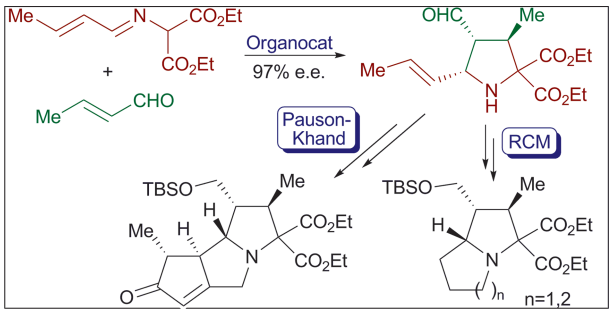
2228

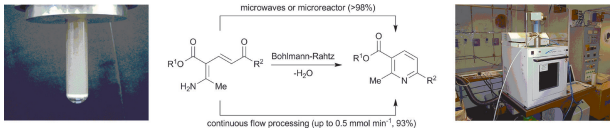


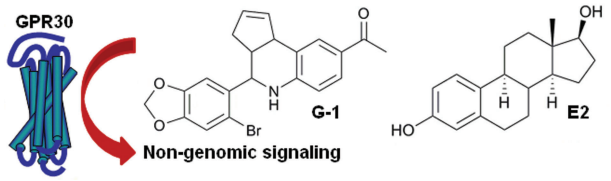
Novel chemoenzymatic methodology for the regioselective glycine loading on polyhydroxy compounds

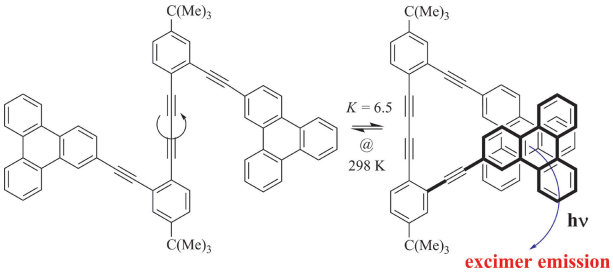
Shashwat Malhotra, Marcelo Calderón, Ashok K. Prasad, Virinder S. Parmar* and Rainer Haag*

We present a temperature-dependent chemo-enzymatic methodology which offers efficient and controlled loading of amino acid (glycine) on polyhydroxy compounds and represents a platform for the selective amino acid attachment (decoration) to the dendritic polyglycerol (PG) scaffolds.









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