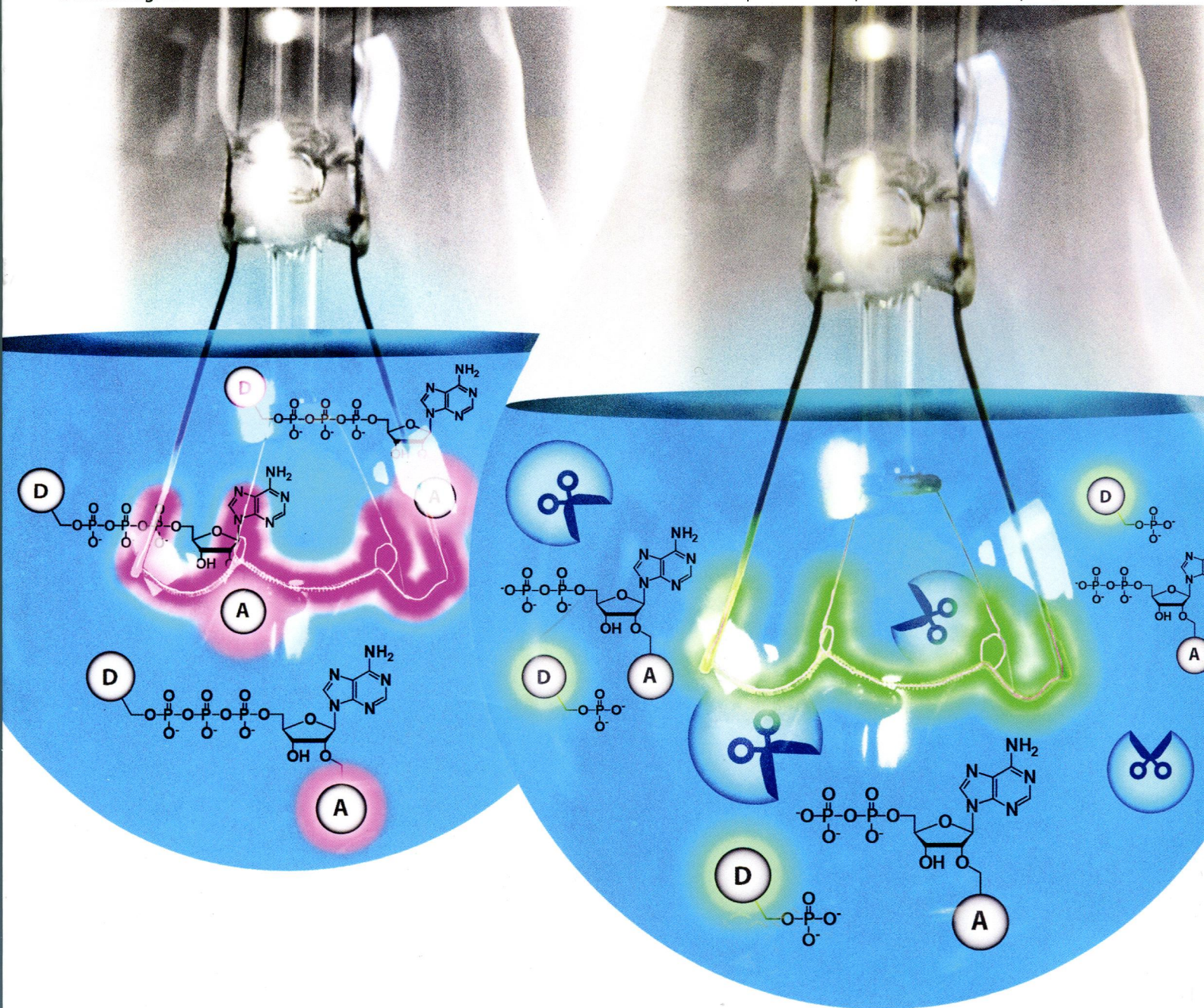


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# Organic & Biomolecular Chemistry

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Volume 11 | Number 48 | 28 December 2013 | Pages 8285–8516



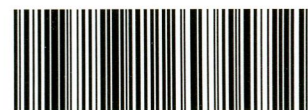
ISSN 1477-0520

RSC Publishing

PAPER

Andreas Marx *et al.*

Synthesis and fluorescence characteristics of ATP-based FRET probes



1477-0520 (2013) 11:48;1-#



# Organic & Biomolecular Chemistry

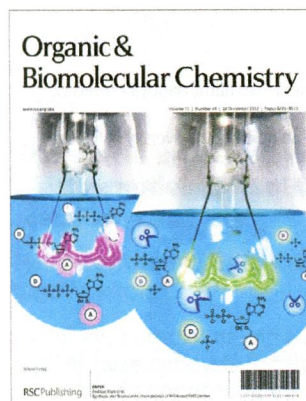
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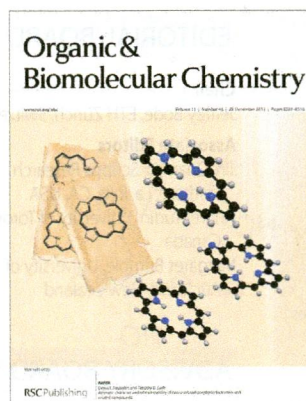
ISSN 1477-0520 CODEN OBCRAK 11(48) 8285–8516 (2013)



### Cover

See Andreas Marx *et al.*,  
pp. 8298–8305.

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8298.



### Inside cover

See Deyaa I. AbuSalim and  
Timothy D. Lash,  
pp. 8306–8323.

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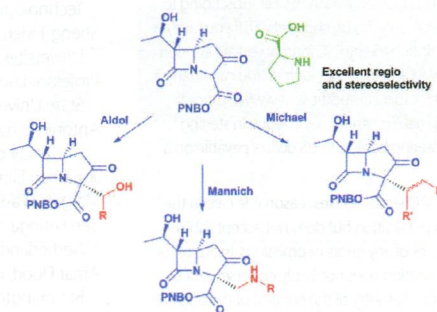
## COMMUNICATION

8294

### Organocatalyzed stereospecific C–C bond formation of $\beta$ -lactams

Sachin A. Pawar, Saba Alapour, Sibusiso Khanyase,  
Zamani E. D. Cele, Srinivas Chitti, Hendrik G. Kruger,  
Thavendran Govender\* and Per I. Arvidsson\*

We report mild, organocatalyzed routes to novel  
carbapenam derivatives through aldol, Mannich and  
Michael C–C bond forming reactions.



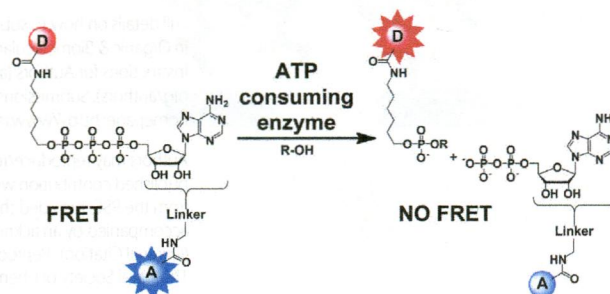
## PAPERS

8298

### Synthesis and fluorescence characteristics of ATP-based FRET probes

Norman Hardt, Stephan M. Hacker and Andreas Marx\*

Syntheses and fluorescence characterizations of seven ATP-  
based FRET probes are presented that hold the potential  
to study ATP consuming enzymes.



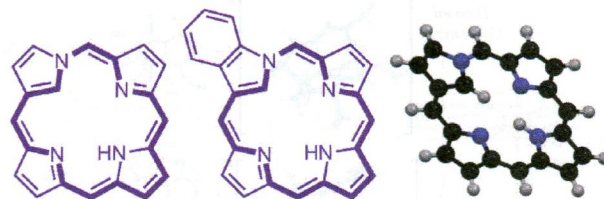


8306

**Aromatic character and relative stability of neo-confused porphyrin tautomers and related compounds**

Deyaa I. AbuSalim and Timothy D. Lash\*

The conformations, relative energies and diatropic characteristics of neo-confused porphyrins and related systems have been assessed.

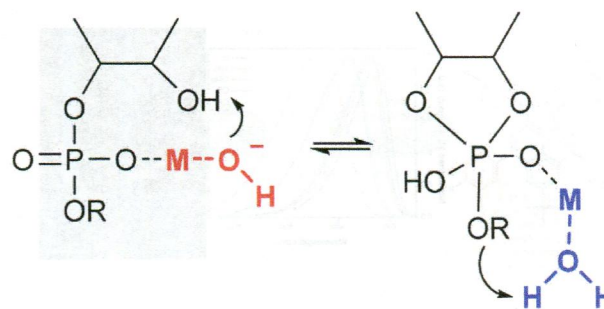


8324

**There is no universal mechanism for the cleavage of RNA model compounds in the presence of metal ion catalysts**

Heidi Korhonen, Timo Koivusalo, Suvi Toivola and Satu Mikkola\*

Metal ion complexes can be intracomplex general acid and/or base catalysts for the cleavage of RNA model compounds depending on the acidity of the aquo ligand and of the leaving group alcohol.

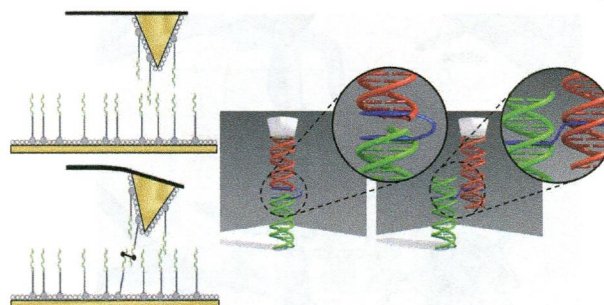


8340

**Non-covalent duplex to duplex crosslinking of DNA in solution revealed by single molecule force spectroscopy**

Benjamin D. Rackham, Lesley A. Howell, Andrew N. Round\* and Mark Searcey\*

A single molecule force spectroscopy assay shows that bisintercalators can crosslink duplex DNA by intermolecular bridging between chromophores or by sequence-specific blunt end ligation.

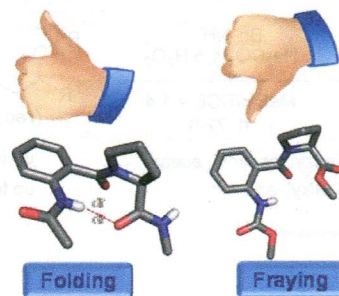


8348

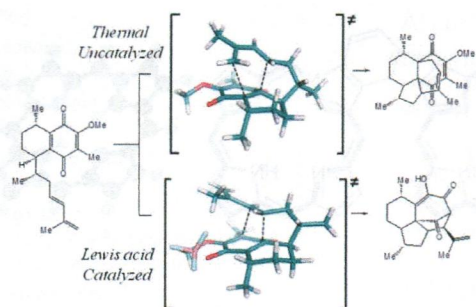
**Ester vs. amide on folding: a case study with a 2-residue synthetic peptide**

Kuruppanthara N. Vijayadas, Roshna V. Nair, Rupesh L. Gawade, Amol S. Kotmale, Panchami Prabhakaran, Rajesh G. Gonnade, Vedavadi G. Puranik, Pattuparambil R. Rajamohanam and Gangadhar J. Sanjayan\*

This article unveils a striking case of comparison of the individual contributions of C-terminal ester vs. amide carbonyl as a H-bonding acceptor in the folding of a synthetic peptide.



8357

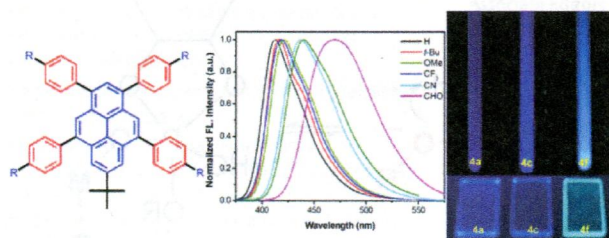


### Theoretical study on the molecular mechanism of the [5 + 2] vs. [4 + 2] cyclization mediated by Lewis acid in the quinone system

Jorge Soto-Delgado,\* José A. Sáez, Ricardo A. Tapia and Luis R. Domingo\*

The molecular mechanism of the quinone involved in the synthesis of *Colombiasin A* and *Elipsaterosin B* has been studied using DFT methods.

8366

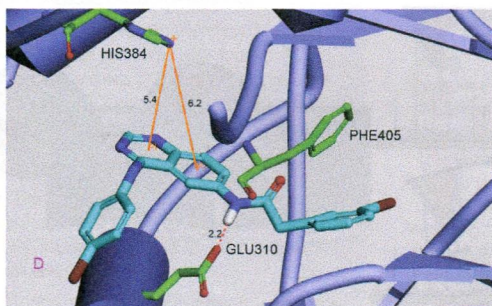


### Synthesis and photophysical properties of novel butterfly-shaped blue emitters based on pyrene

Xing Feng, Jian-Yong Hu,\* Hirotsugu Tomiyasu, Nobuyuki Seto, Carl Redshaw, Mark R. J. Elsegood and Takehiko Yamato\*

The butterfly-shaped pyrene derivatives exhibit good solubility, excellent blue emissions with high quantum efficiency, and long fluorescence lifetimes in solution.

8375

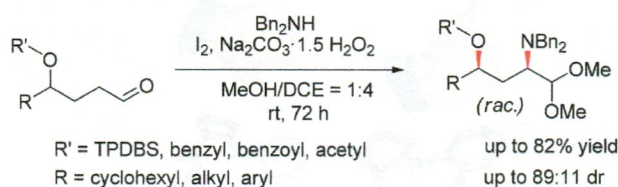


### Discovery of 4,6-substituted-(diaryl-amino)quinazolines as potent c-Src inhibitors

Jing-Ran Li, Dong-Dong Li, Fei Fang, Qian-Ru Du, Lin Lin, Jian Sun, Yong Qian\* and Hai-Liang Zhu\*

A series of 4,6-substituted-(diaryl-amino)quinazolines as c-Src inhibitors have been prepared and their biological activity has also been evaluated. All the compounds displayed potential anti-proliferation activities in five human tumor cell lines.

8387



### Diastereoselective oxidative $\alpha$ -amination of aliphatic aldehydes catalyzed by iodine: synthesis of *syn*- $\gamma$ -hydroxy- $\alpha$ -amino acetals

Yun-Xiao Zhang, An-Qi Zhang, Jie-Sheng Tian and Teck-Peng Loh\*

This paper reports a novel strategy for the synthesis of chiral 1,3-aminoalcohol derivatives with good yields and good diastereoselectivities under very mild conditions.

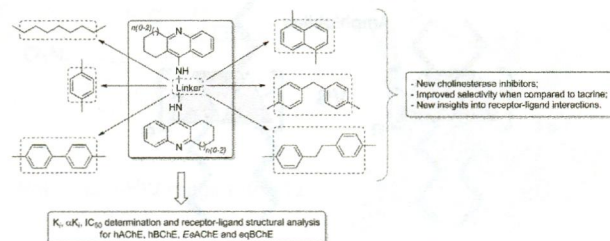


8395

### Synthesis, kinetic studies and molecular modeling of novel tacrine dimers as cholinesterase inhibitors

Roney Anderson Nascimento de Aquino,  
Luzia Valentina Modolo, Rosemeire Brondi Alves and  
Ângelo de Fátima\*

This study presents the synthesis of fifteen new tacrine dimers as well as the  $K_i$  and  $IC_{50}$  results, studies of the kinetic mechanism, and molecular docking analysis of the dimers in relation to the cholinesterases hAChE, hBChE, EeAChE and eqBChE.

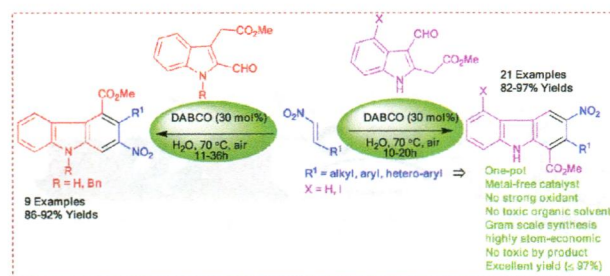


8410

### An organocatalytic highly efficient approach to the direct synthesis of substituted carbazoles in water

Pradeep Kumar Jaiswal, Soumen Biswas,  
Shivendra Singh and Sampak Samanta\*

A DABCO mediated synthesis of substituted carbazoles has been developed by the reaction of methyl 2-(3-formyl-1*H*-indol-2-yl)acetates with  $\beta$ -nitroolefins in water.

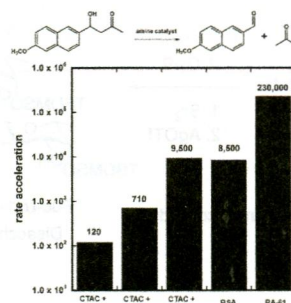


8419

### The effect of the hydrophobic environment on the retro-aldol reaction: comparison to a computationally-designed enzyme

Joshua Schmidt, Clayton Ehasz, Michael Epperson,  
Kimberly Klas, Justin Wyatt, Mirko Hennig and  
Marcello Forconi\*

Non-specific hydrophobic interactions can greatly accelerate the amine-catalysed retro-aldol reaction of an aromatic substrate.

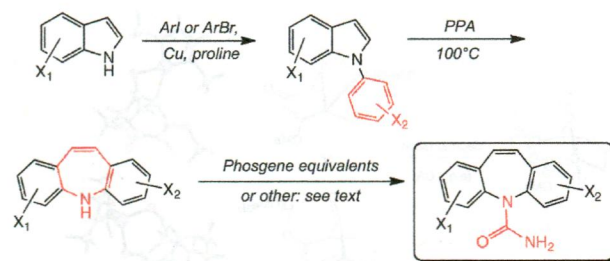


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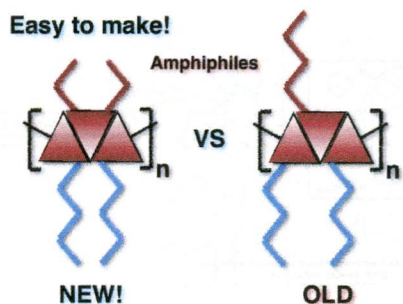
### Convenient syntheses of halo-dibenz[*b,f*]azepines and carbamazepine analogues via *N*-arylindoles

Emma-Claire Elliott, James L. Maggs, B. Kevin Park,  
Paul M. O'Neill and Andrew V. Stachulski\*

The CNS-active drug carbamazepine features a dibenz[*b,f*]azepine ring system bearing an *N*-carboxamide substituent. Here we describe a convenient, three-step synthesis of carbamazepine analogues from *N*-arylindoles.



8435

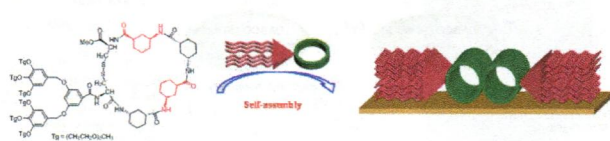


### Designing new symmetrical facial oligothiophene amphiphiles

Dainius Janeliunas, Rienk Eelkema, Belén Nieto-Ortega, Francisco J. Ramírez Aguilar, Juan T. López Navarrete, Lars van der Mee, Marc C. A. Stuart, Juan Casado and Jan H. van Esch\*

An efficient synthesis and the aqueous self-assembly behaviour of curved oligothiophene amphiphiles are reported.

8443

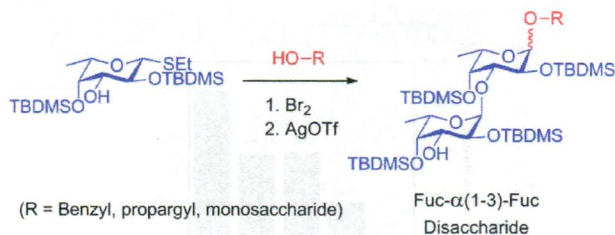


### The self-assembly of cystine-bridged $\gamma$ -peptide-based cyclic peptide–dendron hybrids

Zhizhong Lin, Liangchun Li,\* Yujin Yang, Hongmei Zhan, Yu Hu, Zhiming Zhou, Jin Zhu, Qiwei Wang and Jingen Deng\*

Cystine-bridged  $\gamma$ -peptide-based cyclic peptide–dendron hybrids have been synthesized and self-assembled to amphiphilic nanotubes by hydrogen-bond-mediated parallel stacking, which can form double tubular filaments in aqueous solutions.

8452

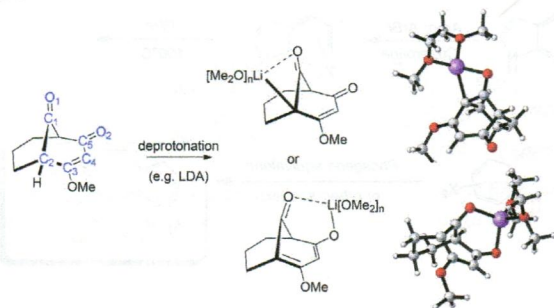


### An unusual glycosylation product from a partially protected fucosyl donor under silver triflate activation conditions

Robin Daly and Eoin M. Scanlan\*

A partially protected fucosyl donor, activated under bromine–silver triflate conditions in the presence of primary alcohols gives difucoside products exclusively.

8458



### Bridgehead enolate or bridgehead organolithium? DFT calculations provide insights into a difficult bridgehead substitution reaction in the synthesis of the polycyclic polyprenylated acylphloroglucinol (PPAP) nemorosone

Christopher J. Hayes\* and Nigel S. Simpkins

DFT calculations reveal three possible structures upon lithiation of bridgehead ketones relating to the PPAP natural product nemorosone.

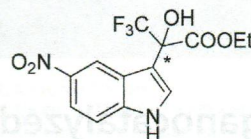


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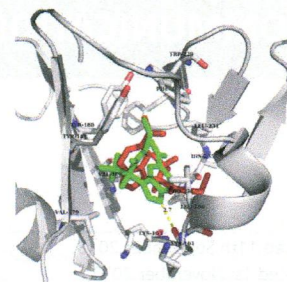
### Enantioselective inhibition of reverse transcriptase (RT) of HIV-1 by non-racemic indole-based trifluoropropanoates developed by asymmetric catalysis using recyclable organocatalysts

Xin Han, Wenjie Ouyang, Bin Liu, Wei Wang,\* Po Tien, Shuwen Wu\* and Hai-Bing Zhou\*

Non-racemic trifluoromethylated indoles were found to be potent and specific inhibitors of reverse transcriptase (RT) of HIV-1 at nanomolar concentrations.



Potent anti-HIV reagent (R)-12  
EC<sub>50</sub> = 19 nM

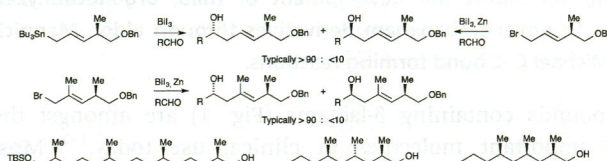


8476

### Development and applications of remote stereocontrol using allylic organobismuth reagents

Norazah Basar, Sam Donnelly, Hasnah M. Sirat and Eric J. Thomas\*

Reactions of aldehydes with 5-benzyloxypent-2-enylstannanes promoted by bismuth(III) iodide and with 5-benzyloxypent-2-enyl bromides promoted by bismuth(III) iodide and zinc, proceed with useful 1,5-stereocontrol. This chemistry has been used to synthesise methylated aliphatic compounds stereoselectively.



## ADDITIONS AND CORRECTIONS

8506

### Additions and corrections published in 2013.