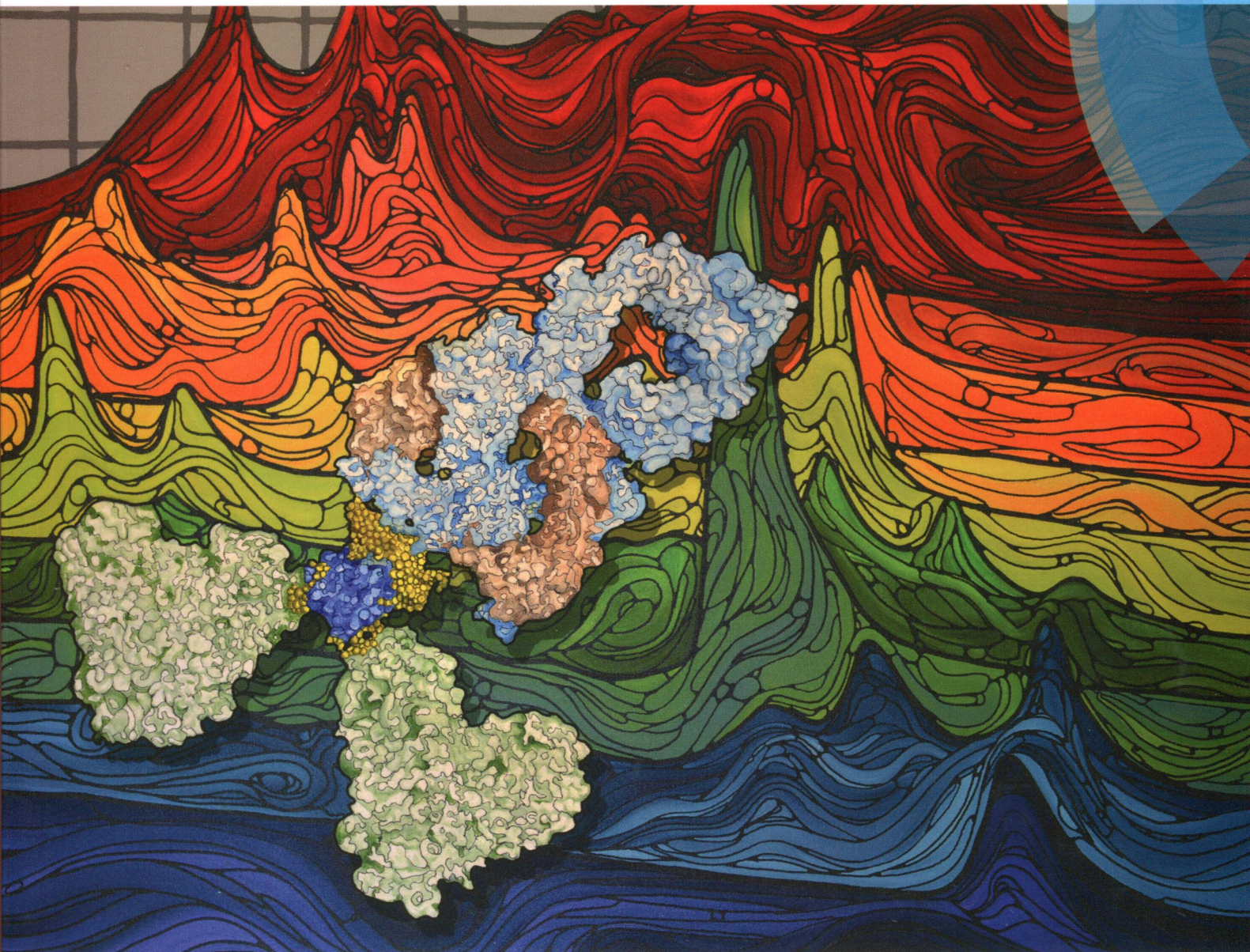


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PAPER

Justin J. Bailey and David R. Bundle

Synthesis of high-mannose 1-thio glycans and their conjugation to protein

Organic & Biomolecular Chemistry

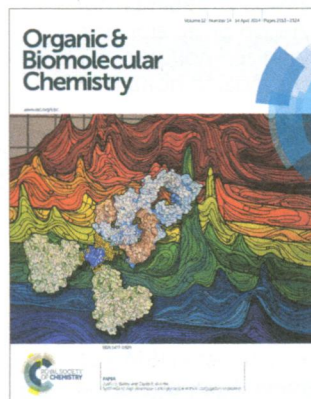
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IN THIS ISSUE

ISSN 1477-0520 CODEN OBCRAK 12(14) 2153–2324 (2014)

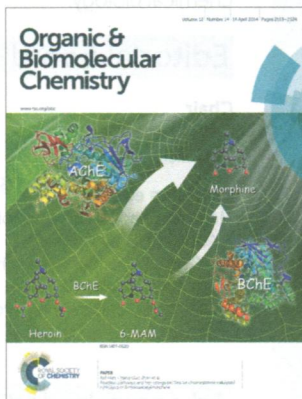


Cover

See Justin J. Bailey and David R. Bundle, pp. 2193–2213.

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The authors gratefully acknowledge Tammie Hunter from White Cap Art (whitecapart.com) for preparing the cover image.



Inside cover

See Keli Han, Chang-Guo Zhan *et al.*, pp. 2214–2227.

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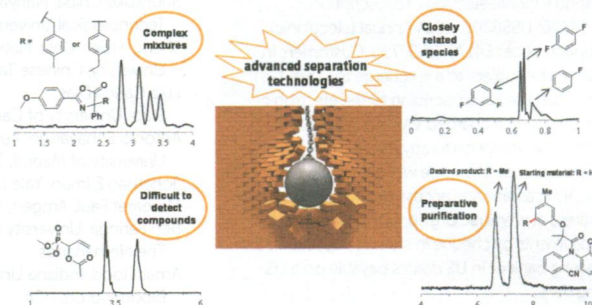
REVIEW

2161

Support of academic synthetic chemistry using separation technologies from the pharmaceutical industry

Erik L. Regalado,* Marisa C. Kozlowski, John M. Curto, Tobias Ritter, Michael G. Campbell, Anthony R. Mazzotti, Bruce C. Hamper, Christopher D. Spilling, Michael P. Mannino, Li Wan, Jin-Quan Yu, Jinchu Liu and Christopher J. Welch*

State-of-the-art separation tools from the pharmaceutical industry are applied to intractable separation problems from academic synthetic chemistry, showing fast and useful results.



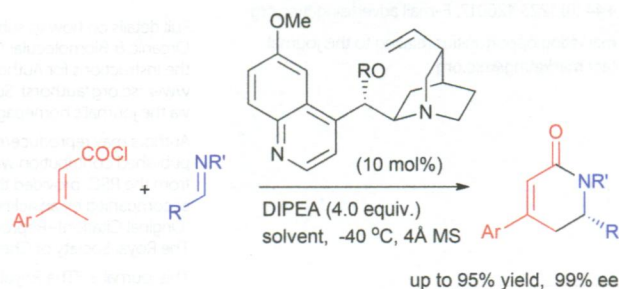
COMMUNICATIONS

2167

Organocatalytic [4 + 2] cyclocondensation of α,β -unsaturated acyl chlorides with imines: highly enantioselective synthesis of dihydropyridinone and piperidine derivatives

Wen-Qiang Jia, Xiang-Yu Chen, Li-Hui Sun and Song Ye*

The cinchona alkaloid-catalyzed [4 + 2] cyclocondensation of α,β -unsaturated acyl chlorides with aldimines is developed to give the corresponding substituted dihydropyridinones in good yields with high to excellent enantioselectivities.



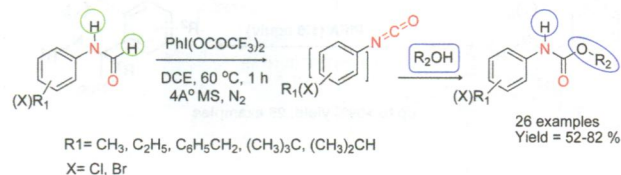
Федеральное государственное
бюджетное учреждение науки
Центральная научная библиотека
Уральского отделения
Российской академии наук (ЦНБ УрО РАН)

2172

Metal free oxidative coupling of aryl formamides with alcohols for the synthesis of carbamates

N. Veera Reddy, K. Rajendra Prasad, P. Sudhir Reddy, M. Lakshmi Kantam and K. Rajender Reddy*

A new method under metal free conditions has been developed for the direct transformation of *N*-aryl formamides to corresponding *N*-aryl carbamates with alcohols using hypervalent iodine reagents as oxidants. The reaction has been postulated to go through the formation of isocyanate intermediates.

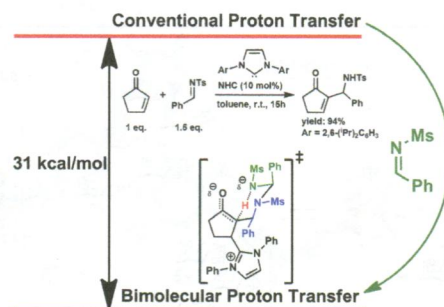


2176

The mechanism of the NHC catalyzed aza-Morita–Baylis–Hillman reaction: insights into a new substrate-catalyzed bimolecular pathway

Pritha Verma, Pragya Verma and Raghavan B. Sunoj*

The first mechanistic study on the NHC-catalyzed aza-MBH reaction between cyclopentenone and *N*-mesylbenzaldimine using density functional theory reveals that a bimolecular mechanism, involving two molecules of benzaldimine in the proton transfer, is energetically more preferred over the conventional direct proton transfer.

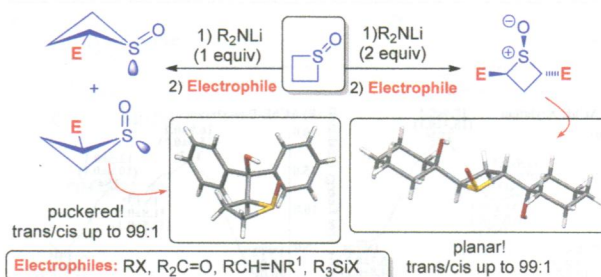


2180

Straightforward access to 4-membered sulfurated heterocycles: introducing a strategy for the single and double functionalization of thietane 1-oxide

Laura Carroccia, Leonardo Degennaro, Giuseppe Romanazzi, Corrado Cuocci, Luisa Pisano and Renzo Luisi*

A strategy for the stereoselective functionalization of thietane 1-oxide has been developed by using the corresponding organometallic intermediates that reacted with electrophiles leaving intact the 4-membered ring.

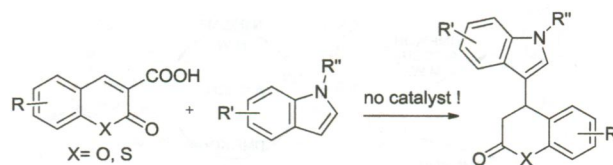


2185

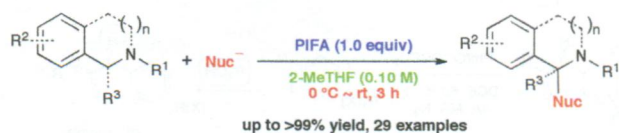
Catalyst-free tandem Michael addition/ decarboxylation of (thio)coumarin-3-carboxylic acids with indoles: facile synthesis of indole-3-substituted 3,4-dihydro(thio)coumarins

Zhuzhou Shao, Lubin Xu, Liang Wang, Hongtao Wei and Jian Xiao*

The tandem Michael addition/decarboxylation of (thio)-coumarin-3-carboxylic acids with indoles gives biologically important indole-3-substituted dihydrocoumarins in good to excellent yields under catalyst-free conditions.



2189



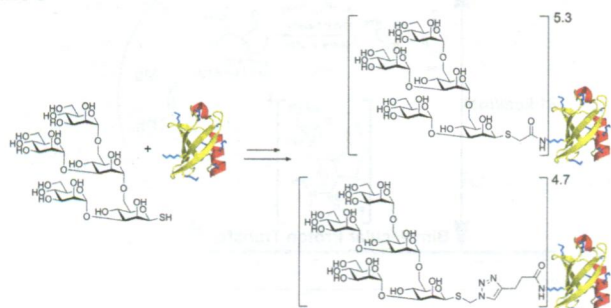
Direct sp^3 C–H bond arylation, alkylation, and amidation of tetrahydroisoquinolines mediated by hypervalent iodine(III) under mild conditions

Wataru Muramatsu,* Kimihiro Nakano and Chao-Jun Li*

We have developed a method for the sp^3 C–H bond functionalization of tetrahydroisoquinolines (THIQs) mediated by [bis(trifluoroacetoxy)iodo]benzene (PIFA).

PAPERS

2193

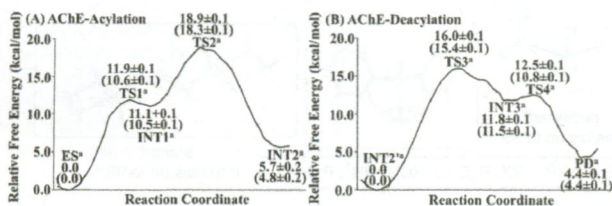


Synthesis of high-mannose 1-thio glycans and their conjugation to protein

Justin J. Bailey* and David R. Bundle

Mannosylthiol derivatives of the high-mannose structure $\text{Man}_9\text{GlcNAc}_2$ were synthesized and conjugated to ubiquitin in high copy number as determined by LC-UV-MS.

2214

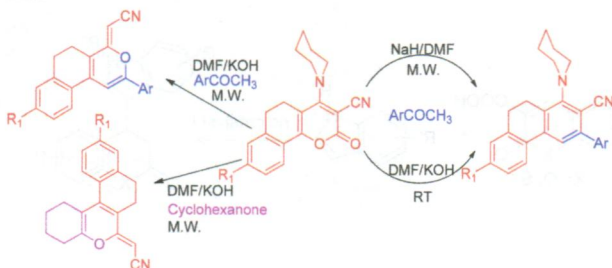


Reaction pathways and free energy profiles for cholinesterase-catalyzed hydrolysis of 6-monoacetylmorphine

Yan Qiao, Keli Han* and Chang-Guo Zhan*

Reaction-coordinate calculations revealed the detailed reaction pathways for acetylcholinesterase (AChE)- and butyrylcholinesterase (BChE)-catalyzed hydrolysis of 6-monoacetylmorphine (6-MAM) to morphine and the corresponding free energy profiles in good agreement with the available experimental kinetic data.

2228



Microwave assisted base dependent regioselective synthesis of partially reduced chromenes, isochromenes and phenanthrenes

Pratik Yadav, Surjeet Singh, Satya Narayan Sahu, Firasat Hussain and Ramendra Pratap*

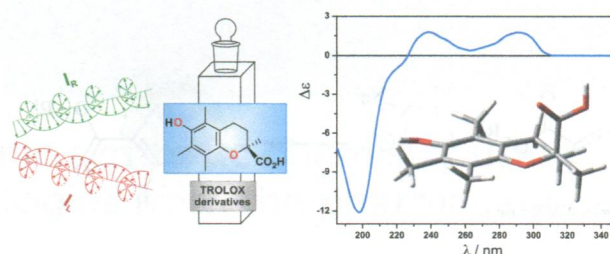
Microwave assisted base directed regioselective synthesis of partially reduced chromenes, isochromenes and phenanthrenes has been reported.

2235

Chromane helicity rule – scope and challenges based on an ECD study of various trolox derivatives

Marcin Górecki,* Agata Suszczyńska, Magdalena Woźnica, Aneta Baj, Michał Wolniak, Michał K. Cyrański, Stanisław Witkowski and Jadwiga Frelek*

The validity of the chromane helicity rule is examined using a set of natural (*S*)-trolox derivatives.

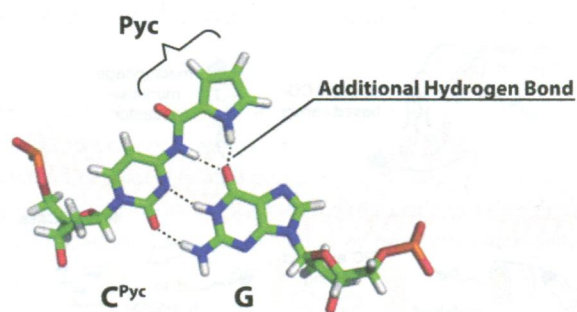


2255

A new modified cytosine base capable of base pairing with guanine using four hydrogen bonds

Ken Yamada, Yoshiaki Masaki, Hirosuke Tsunoda, Akihiro Ohkubo, Kohji Seio and Mitsuo Sekine*

Oligonucleotides, containing 4-*N*-(1*H*-pyrrol-2-ylcarbonyl)deoxycytidine (dC^{Pyc}) and related derivatives, were synthesized *via* deprotection using 1.5 M NaOMe/MeOH.

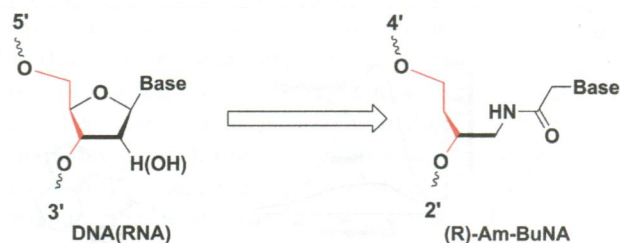


2263

Design, synthesis and properties of artificial nucleic acids from (*R*)-4-amino-butane-1,3-diol

Pengfei Li, Jingjing Sun, Meng Su, Xiaogai Yang and Xinjing Tang*

A new artificial nucleic acid analogue with (*R*)-4-amino-butane-1,3-diol as the scaffold was developed.

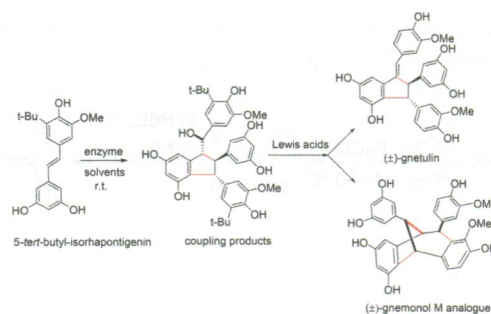


2273

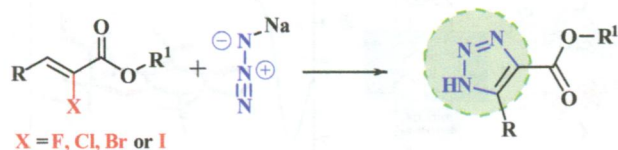
Enzyme-promoted regioselective coupling oligomerization of isorhapontigenin towards the first synthesis of (±)-gnetulin

Wenling Li,* Shixia Yang, Teng Lv and Yadong Yang

The first synthesis of two isorhapontigenin dimers—(±)-gnetulin and (±)-gnemonol M analogue—has been achieved through different structural modifications of the coupling products, which were obtained from the enzyme-promoted oxidative coupling reactions of 5-*tert*-butyl-isorhapontigenin.



2280

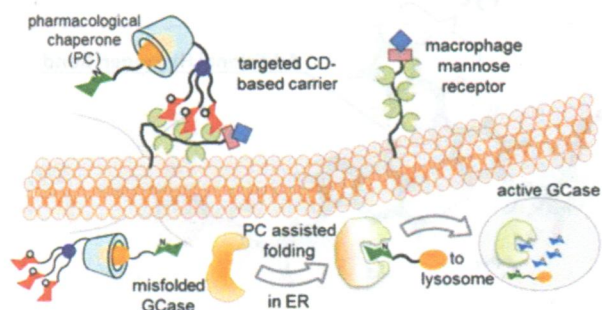


α -Haloacrylates as acceptors in the [3 + 2] cycloaddition reaction with NaN_3 : an expedient approach to *N*-unsubstituted 1,2,3-triazole-4-carboxylates

John Kallikat Augustine,* Chandrakantha Boodappa and Srinivasa Venkatachaliah

An expedient synthesis of *N*-unsubstituted 1,2,3-triazole-4-carboxylates has been demonstrated through [3 + 2] cycloaddition of sodium azide with α -haloacrylates.

2289

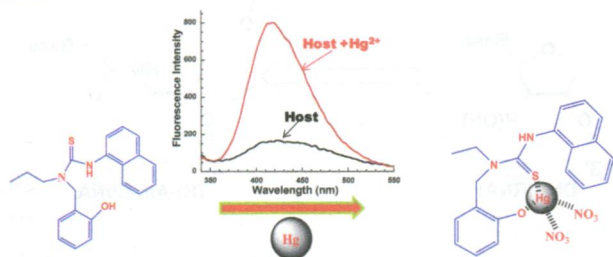


Targeted delivery of pharmacological chaperones for Gaucher disease to macrophages by a mannosylated cyclodextrin carrier

Julio Rodríguez-Lavado, Mario de la Mata, José L. Jiménez-Blanco, M. Isabel García-Moreno, Juan M. Benito, Antonio Díaz-Quintana, José A. Sánchez-Alcázar, Katsumi Higaki, Eiji Nanba, Kousaku Ohno, Yoshiyuki Suzuki, Carmen Ortiz Mellet* and José M. García Fernández*

Efficient delivery of pharmacological chaperones for Gaucher disease to macrophages has been achieved.

2302

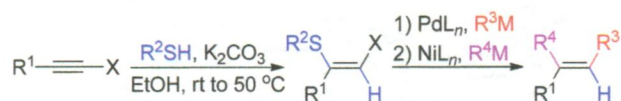


Fluorometric sensing of Hg^{2+} ions in aqueous medium by nano-aggregates of a tripodal receptor

Ajнеш Singh, Simanpreet Kaur, Narinder Singh* and Navneet Kaur*

Two new tripodal receptors (1–2) have been synthesized and characterized by various spectroscopic techniques.

2310



A regio- and stereoselective entry to (*Z*)- β -halo alkenyl sulfides and their applications to access stereodefined trisubstituted alkenes

Ge Liu, Lichun Kong, Ji Shen and Gangguo Zhu*

A regio- and stereoselective synthesis of (*Z*)- β -halo alkenyl sulfides via K_2CO_3 -promoted hydrothiolation of haloalkynes has been reported, permitting a new entry to trisubstituted alkenes featuring the iterative cross-coupling of carbon–halide and carbon–sulfur bonds.