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# Organic & Biomolecular Chemistry

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**PAPER**

Webster L. Santos *et al.*

Targeting folded RNA: a branched peptide boronic acid that binds to a large surface area of HIV-1 RRE RNA



1477-0520 (2013) 11:37;1-3

# Organic & Biomolecular Chemistry

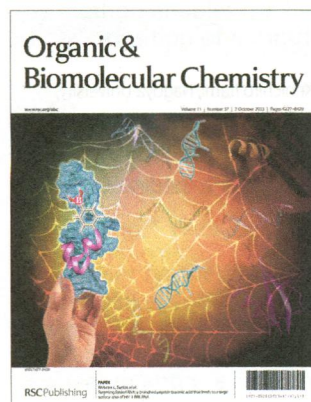
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## IN THIS ISSUE

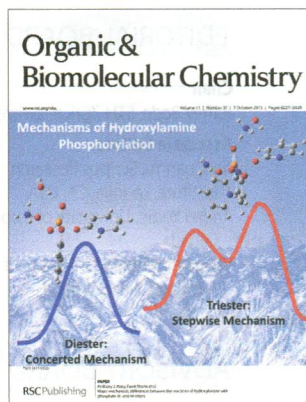
ISSN 1477-0520 CODEN OBCRAK 11(37) 6227–6428 (2013)



### Cover

See Webster L. Santos *et al.*, pp. 6263–6271.

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### Inside cover

See Anthony J. Kirby, Faruk Nome *et al.*, pp. 6272–6284.

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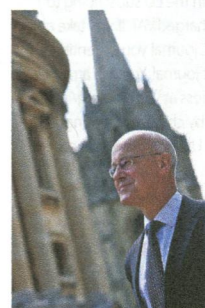
## PROFILE

6236

### In celebration of the 60<sup>th</sup> birthday of Professor Andrew D. Hamilton FRS

Sam Thompson, Andrew J. Wilson and Alan R. Battersby

An on-line collection of articles celebrating the 60th birthday of Professor Andrew D. Hamilton FRS has been published featuring contributions from students and colleagues past and present.



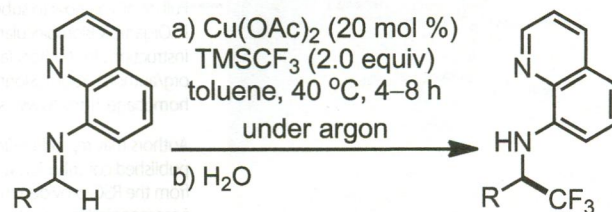
## COMMUNICATIONS

6242

### Copper(II)-catalyzed trifluoromethylation of *N*-aryl imines

Yong-Qiang Zhang, Ji-Dan Liu and Hao Xu\*

We describe a copper(II)-catalyzed trifluoromethylation of *N*-aryl imines in the absence of external Lewis-base activators. This unique transformation presumably proceeds through cooperative activation.



15 examples, 47–81 % yield

R: alkyl, alkenyl, aryl, and hetero-aryl groups

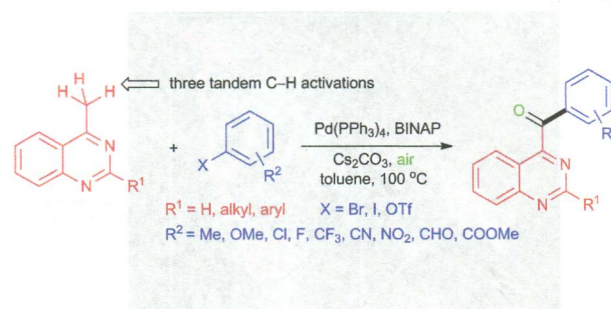
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бюджетное учреждение науки  
Центральная научная библиотека  
Уральского отделения  
Российской академии наук (ЦНБ УрО РАН)

6246

### Pd(0)-catalyzed benzylic arylation–oxidation of 4-methylquinazolines via $sp^3$ C–H activation under air conditions

Dan Zhao, Min-Xue Zhu, Yue Wang, Qi Shen and Jian-Xin Li\*

An efficient and selective Pd(0)-catalyzed  $sp^3$  C–H bond arylation–oxidation of 4-methylquinazolines is reported. The method enables the introduction of arylketone at the benzylic position of 4-methylquinazolines.

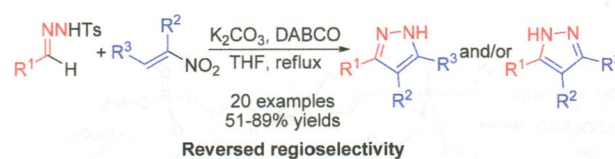


6250

### DABCO-promoted synthesis of pyrazoles from tosylhydrazones and nitroalkenes

Meng Tang,\* Wen Zhang and Yuanfang Kong

An efficient synthesis of pyrazoles from tosylhydrazones and nitroalkenes was developed. Compared with the previously reported results, this methodology proceeded with a sequential Baylis–Hillman/intramolecular cyclization mechanism and the regioselectivity was reversed.

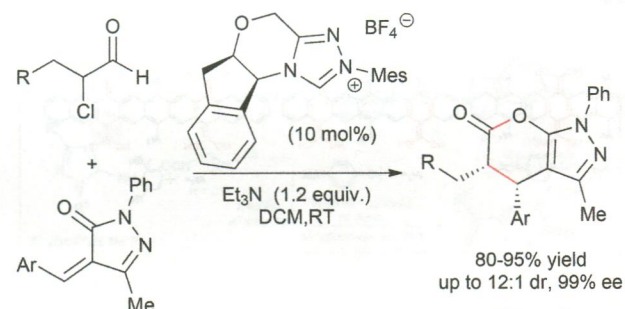


6255

### N-Heterocyclic carbene-catalyzed highly enantioselective synthesis of substituted dihydropyranopyrazolones

Han-Ming Zhang, Hui Lv and Song Ye\*

Multisubstituted dihydropyrano[2,3-c]pyrazol-6-(1H)-ones were synthesized enantioselectively via the N-heterocyclic carbene-catalyzed [4 + 2] annulation of  $\alpha$ -chloroaldehydes and pyrazolone-derived oxodienes.

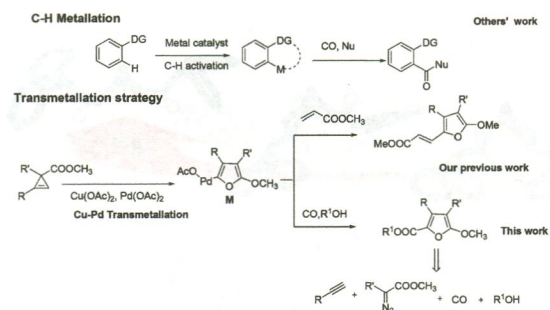


6258

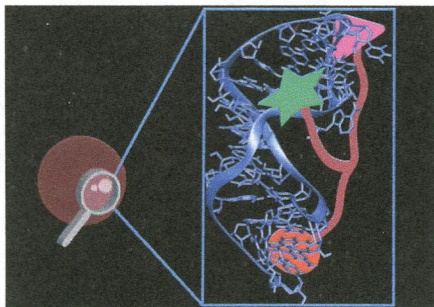
### Modular synthesis of all-substituted furans through oxidative carbonylation of cyclopropenes with tandem metal relay catalysis

Chuanling Song, Shuli Dong, Lei Feng, Xianglong Peng, Mingchao Wang, Jianwu Wang and Zhenghu Xu\*

A modular synthesis of tetrasubstituted furan carboxylates using a tandem cycloisomerization/oxidative carbonylation sequence of cyclopropenes has been successfully developed.



5263

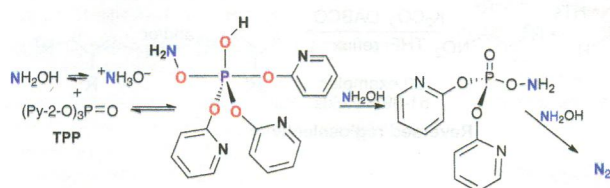


### Targeting folded RNA: a branched peptide boronic acid that binds to a large surface area of HIV-1 RRE RNA

Wenyu Zhang, David I. Bryson, Jason B. Crumpton, Jessica Wynn and Webster L. Santos\*

A branched peptide boronic acid recognizes the three dimensional architecture of HIV-1 RRE RNA through a large surface area interaction.

6272

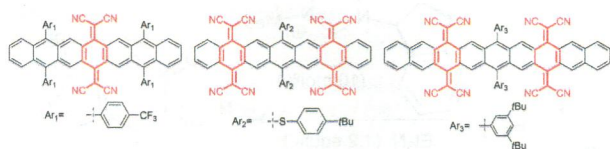


### Major mechanistic differences between the reactions of hydroxylamine with phosphate di- and tri-esters

Michelle Medeiros, Eduardo H. Wanderlind, José R. Mora, Raphael Moreira, Anthony J. Kirby\* and Faruk Nome\*

Hydroxylamine reacts with the diester anion **DPP<sup>-</sup>** by the expected concerted  $S_N2(P)$  mechanism, but with the triester **TPP** by an addition–elimination process, with breakdown of the phosphorane intermediate rate-determining.

6285

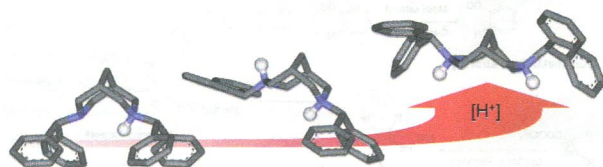


### TCNQ-embedded heptacene and nonacene: synthesis, characterization and physical properties

Qun Ye, Jingjing Chang, Kuo-Wei Huang, Gaole Dai and Chunyan Chi\*

Three acene-TCNQ derivatives have been successfully prepared with two TCNQ moieties on the heptacene and nonacene backbone for the first time.

6292



### Protonation-triggered conformational modulation of an *N,N'*-dialkylbispidine: first observation of the elusive boat–boat conformer

Sara Norrehed, Máté Erdélyi, Mark E. Light and Adolf Gogoll\*

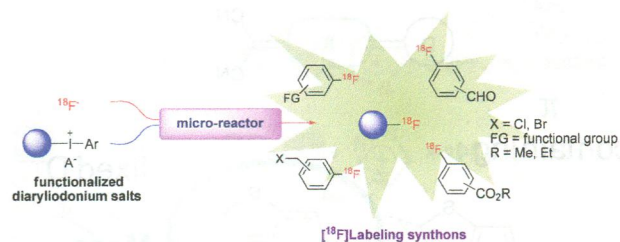
Finally caught: the boat–boat conformer of bispidine.

6300

### Single-step syntheses of no-carrier-added functionalized [ $^{18}\text{F}$ ]fluoroarenes as labeling synthons from diaryliodonium salts

Joong-Hyun Chun and Victor W. Pike\*

Functionalized [ $^{18}\text{F}$ ]fluoroarenes as labeling synthons are rapidly accessible from the single-step microfluidic radiofluorination of corresponding functionalized diaryliodonium salts.

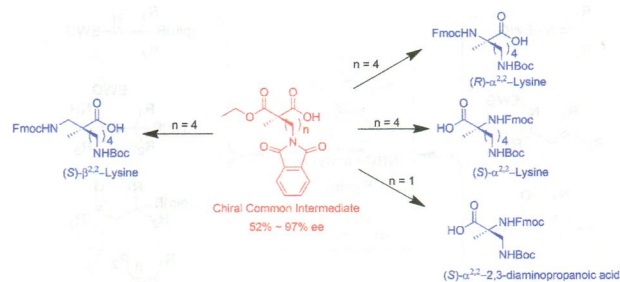


6307

### Novel synthesis of various orthogonally protected C $^{\alpha}$ -methyllysine analogues and biological evaluation of a Vapreotide analogue containing (S)- $\alpha$ -methyllysine

Souvik Banerjee, Walker J. Wiggins, Jessie L. Geoghegan, Catherine T. Anthony, Eugene A. Woltering and Douglas S. Masterson\*

An enantiodivergent strategy for the preparation of various unnatural lysine analogues is presented.

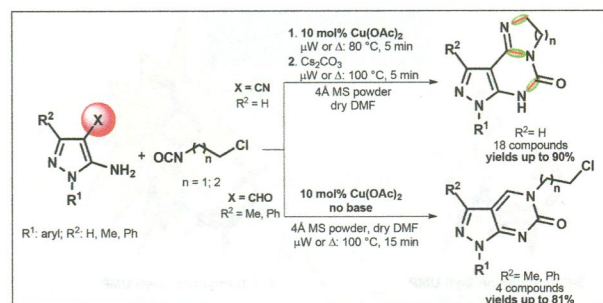


6320

### Synthesis of novel pyrazole-based heterocycles via a copper(II)-catalysed domino annulation

Márió Gyuris, László G. Puskás, Gábor K. Tóth and Iván Kanizsai\*

Pyrazole-based  $\beta$ -aminonitriles and  $\beta$ -amino-carbaldehydes as bifunctional building blocks are introduced in a facile copper(II)-catalysed one-pot domino generation of multiple N-containing heterobi- and tricycles.

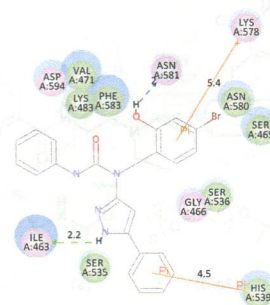


6328

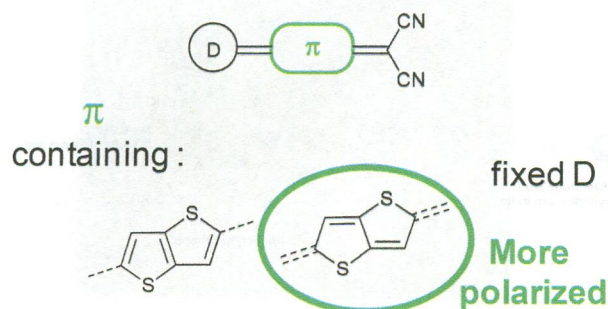
### Synthesis, biological evaluation and molecular docking of novel 5-phenyl-1H-pyrazol derivatives as potential BRAF<sup>V600E</sup> inhibitors

Jing-Jun Dong, Qing-Shan Li, Shu-Fu Wang, Cui-Yun Li, Xin Zhao, Han-Yue Qiu, Meng-Yue Zhao and Hai-Liang Zhu\*

A series of novel 5-phenyl-1H-pyrazol derivatives were designed and synthesized, among which 1-(4-bromo-2-hydroxybenzyl)-3-phenyl-1-(5-phenyl-1H-pyrazol-3-yl)urea exhibited the most potent inhibitory activity with an IC<sub>50</sub> value of 0.19  $\mu\text{M}$  for BRAF<sup>V600E</sup>.



6338

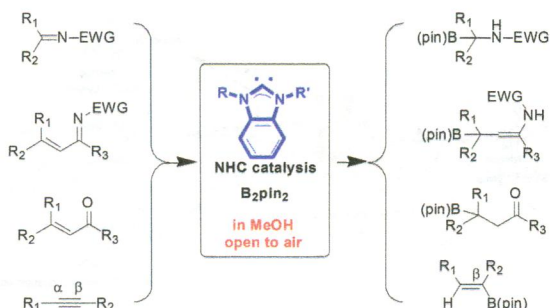


### Push–pull systems bearing a quinoid/aromatic thieno[3,2-*b*]thiophene moiety: synthesis, ground state polarization and second-order nonlinear properties

A. B. Marco, R. Andreu,\* S. Franco, J. Garín, J. Orduna, B. Villacampa, B. E. Diosdado, J. T. López Navarrete and J. Casado

The polarization of the ground state of Donor– $\pi$ –acceptor systems with a thieno[3,2-*b*]thiophene unit and their second-order nonlinear optical responses have been studied.

6350

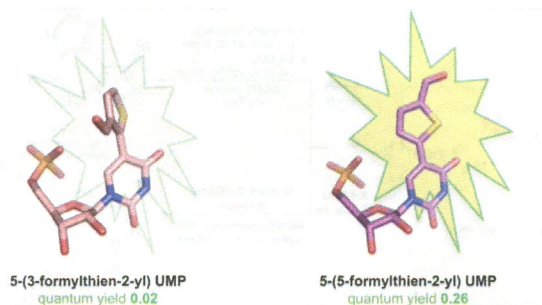


### Metal free catalytic hydroboration of multiple bonds in methanol using N-heterocyclic carbenes under open atmosphere

Kun Wen, Jinbo Chen, Feng Gao, Pinaki S. Bhadury, Erkang Fan and Zhihua Sun\*

An easy to operate method of catalytic hydroboration of unsaturated compounds has been developed with wide substrate scope.

3557

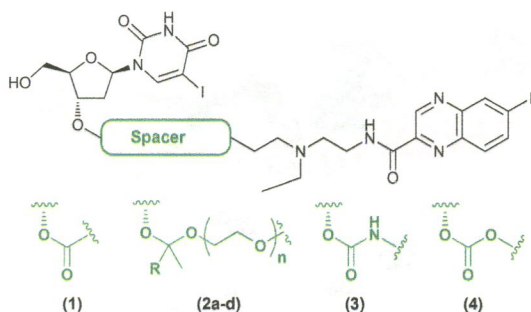


### Exploring the role of the 5-substituent for the intrinsic fluorescence of 5-aryl and 5-heteroaryl uracil nucleotides: a systematic study

Thomas Pesnot, Lauren M. Tedaldi, Pablo G. Jambrina, Edina Rosta and Gerd K. Wagner\*

The interplay of structure, conformation and fluorescence in a series of 5-substituted UMP fluorophores has been investigated.

6372



### Spacer optimization of new conjugates for a melanoma-selective delivery approach

Mathieu André, Sébastien Tarrit, Marie-Joelle Couret, Marie-Josèphe Galmier, Eric Débiton, Jean-Michel Chezal and Emmanuelle Mounetou\*

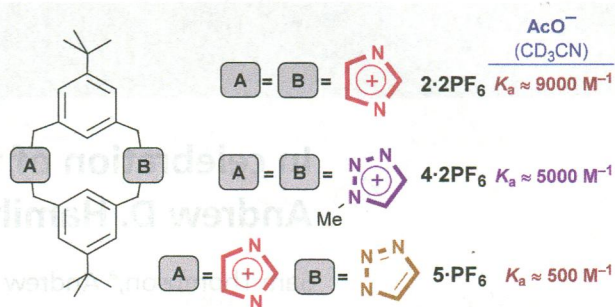
A series of seven conjugates with various linkers connecting the 5-iodo-2'-deoxyuridine (IUdR) to the ICF 01012 melanoma-carrier were synthesized and their stability evaluated for potential intratumoural specific drug release.

6385

### [1<sub>4</sub>]Heterophane prototypes containing azolium and/orazole anion-binding motifs

Neus Mesquida,\* Immaculada Dinarès, Anna Ibáñez and Ermitas Alcalde\*

Comparative study of the synthesis and anion-binding properties of [1<sub>4</sub>]heterophane models containing imidazolium, triazole and/or triazolium units showing a particular preference for acetate.

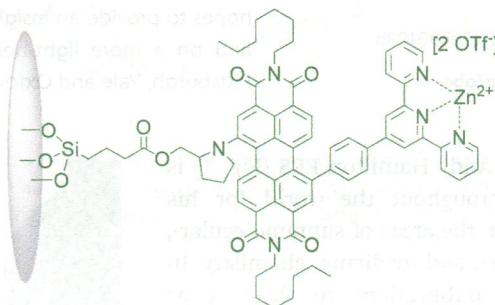


6397

### Supramolecular assemblies of bay-substituted perylene diimides in solution and on a solid substrate

Essi Sariola-Leikas,\* Marja Niemi, Helge Lemmetyinen and Alexander Efimov

Perylene diimides with terpyridine groups and silane anchors at the bay-region were synthesized. Supramolecular complexes were constructed via the terpyridine moieties and zinc ions both in solution and on a surface.

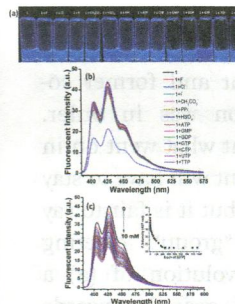


6407

### Selective detection of guanosine-5'-triphosphate and iodide by fluorescent benzimidazolium-based cyclophanes

Nisar Ahmed, Bahareh Shirinfar, Il Seung Youn, Muhammad Yousuf and Kwang S. Kim\*

New fluorescent benzimidazolium-based receptors selectively display the effective fluorescence quenching effect for biologically important anions, GTP and I<sup>-</sup>, in aqueous solution of physiological pH 7.4.



6414

### Structure–activity studies of 4-phenyl-substituted 2'-benzoylpyridine thiosemicarbazones with potent and selective anti-tumour activity

Adeline Y. Lukmantara,\* Danuta S. Kalinowski, Naresh Kumar\* and Des R. Richardson\*

The synthesis of novel substituted 2'-benzoylpyridine thiosemicarbazones as anti-tumour agents and their structure–activity relationships are discussed.

