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### IN THIS ISSUE

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#### **EMERGING AREA**

#### 2579

### Induced cross-linking reactions to target genes using modified oligonucleotides

#### Fumi Nagatsugi\* and Shuhei Imoto

This short review highlights recently developed novel cross-linking reactions, focusing particularly on nucleoside derivatives developed by our group.



### PERSPECTIVE

### 2586

### Organic reactions mediated by electrochemically generated ArS<sup>+</sup>

Kouichi Matsumoto, Seiji Suga and Jun-ichi Yoshida\*

"ArS\*" which is generated by the electrochemical oxidation of ArSSAr serves as a highly reactive reagent for stoichiometric reactions and an initiator for cationic chain reactions.



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### Poly(vinyl)chloride supported palladium nanoparticles: catalyst for rapid hydrogenation reactions

### Hosahalli P. Hemantha and Vommina V. Sureshbabu\*

Palladium nanoparticles supported over poly(vinyl)chloride matrix (PVC-Pd<sup>o</sup>) are prepared through an efficient and inexpensive protocol. The catalyst works exceptionally well for reduction and hydrogenation reactions.



#### 2602

### Benzaldehyde lyase catalyzed enantioselective self and cross condensation reactions of acetaldehyde derivatives

Peruze Ayhan, İlke Şimşek, Burçe Çifçi and Ayhan S. Demir\*

Benzaldehyde lyase catalyzed synthesis of protected 1,3,4-trihydroxy-2-butanone in high enantiomeric excesses



### 2606

### Novel hemicyanine dye as colorimetric and fluorometric dual-modal chemosensor for mercury in water

Yuanyuan Li, Song He, Yan Lu\* and Xianshun Zeng\*

A novel hemicyanine-based colorimetric and fluorometric chemosensor shows a specific aqueous  $Hg^{2+}$  selectivity in conjunction with a visible colorimetric change from red to colorless.



### 2610

### A ratiometric near-infrared pH-responsive fluorescent dye based on distyryl BODIPY

Hui He and Dennis K. P. Ng\*

We report herein a novel bis[4-(dimethylamino)phenylethynyl] substituted distyryl BODIPY which exhibits remarkable and reversible pH-responsive spectral changes.



### Dinuclear zinc catalyzed asymmetric Friedel–Crafts amidoalkylation of indoles with aryl aldimines

Bei-Lei Wang, Nai-Kai Li, Jin-Xin Zhang, Guo-Gui Liu, Teng Liu, Qi Shen\* and Xing-Wang Wang\*

The Friedel–Crafts amidoalkylation of indoles with N-sulfonyl aldimines could be efficiently catalyzed by Trost's dinuclear zinc catalysts to generate enantiomerically enriched 3-indolyl methanamines in good to excellent yields with moderate to high enantiomeric ratios, without the bis- and tris(indolyl)methanes (BIMs and TIMs) being generated.

### 2618



### Rational design of BINOL-based diimidazolyl ligands: homochiral channel-like mono-component organic frameworks by hydrogen-bond-directed self-assembly

Li Yang, Fei Yang, Jingbo Lan, Ge Gao, Jingsong You\* and Xiaoyu $\mathrm{Su}^*$ 

The conformationally rigid BINOL-based diimidazolyl ligands bearing both hydrogen-bond-acceptors and -donators self-assemble into homochiral channel-like mono-component organic frameworks *via*  $O-H\cdots N$  hydrogen bonds.

### PAPERS

#### 2622



### Formation and regulation of fullerene-incorporation in liposomes under the phase transition temperature

Atsushi Ikeda,\* Yoshihiko Kawai, Jun-ichi Kikuchi, Motofusa Akiyama, Eiji Nakata, Yoshihiro Uto and Hitoshi Hori

The fullerene-exchange reaction was found to occur efficiently by the addition of small amounts of lipids bearing  $\pi$ -moieties, which act as a gate when hydrophobic  $C_{70}$  migrates into the hydrophilic liposome surface.



### Signal control by self-assembly of fluorophores in a molecular beacon—a model study

Sarah M. Biner, Dominic Kummer, Vladimir L. Malinovskii and Robert Häner\*

Pyrene excimer fluorescence is efficiently regulated by formation of  $\pi$ -stacked aggregates between dialkynylpyrene and perylenediimide residues located in the stem region of a molecular beacon.

### 2634

### Neutral species from "non-protic" N-heterocyclic ionic liquids

Oldamur Hollóczki and László Nyulászi\*

Possible isomerisation of 1,2,3-trialkylimidazolium and 1-alkylpyridinium ion pairs by proton transfer and by the nucleophilic addition of the anion to the cation have been investigated at the B3LYP/6-31+G\* and B3LYP/6-311+G\*\* levels of density functional theory.

#### 2641

### Comprehensive screening of octopus amphiphiles as DNA activators in lipid bilayers: implications on transport, sensing and cellular uptake

Javier Montenegro, Andrea Fin and Stefan Matile\*

A systematic screening of dynamic amphiphiles as activators of DNA in lipid bilayers shows that activity shifts with increasing tail number to decreasing tail length and increases with *cis*-unsaturated and branched tails to ultimately maximize with the fragrant jasminaldehyde.

#### 2648

Promoting the formation and stabilization of human telomeric G-quadruplex DNA, inhibition of telomerase and cytotoxicity by phenanthroline derivatives

Lihua Wang, Ye Wen, Jie Liu, Jun Zhou, Can Li and Chunying Wei\*

Four new di-substituted phenanthroline-based compounds have been designed and prepared, and they have been shown to induce the formation of anti-parallel structure of human telomeric G-quadruplex DNA by CD spectra.

### 2654

### Protecting-group-free synthesis of a dual CCK1/CCK2 receptor antagonist

Jing Liu, Xiaohu Deng,\* Anne E. Fitzgerald, Zachary S. Sales, Hariharan Venkatesan and Neelakandha S. Mani

An efficient, protecting-group-free synthesis of the dual CCK1/CCK2 receptor antagonist **1** is developed.









Human telomeric sequence

Inducement and stabilization of anti-parallel structure





### Overcoming challenges in the palladium-catalyzed synthesis of electron deficient *ortho*-substituted aryl acetonitriles



Molly C. Brannock, William J. Behof, Gregory Morrison and Christopher B. Gorman\*

Highly electron deficient monoaryl, di-aryl and bis-diaryl acetonitriles were effectively synthesized using a palladium-mediated coupling pathway.



# Laccase-catalyzed phenol oxidation. Rapid assignment of ring-proton deficient polycyclic benzofuran regioisomers by experimental <sup>1</sup>H–<sup>13</sup>C long-range coupling constants and DFT-predicted product formation

Heiko Leutbecher, Gerhard Greiner, Robert Amann, Andreas Stolz, Uwe Beifuss\* and Jürgen Conrad\*

Based on experimental  ${}^{1}H{-}{}^{13}C$  long-range coupling constants a rule of thumb was developed for an easy and unambiguous differentiation of ring-proton deficient polycyclic benzofuran regioisomers.

### <sup>15</sup>N-labeled ionic probe attachment mass spectrometry of carbon clusters

Fumihiro Ito and Kentaro Yamaguchi\*

An ionization method that uses metal-complex-based ionization probes, including Sar-TMpybox, was developed for isotope ratio analysis and the effective ionization of unsubstituted carbon clusters. Applications using cold-spray ionization mass spectrometry are reported.

2680

2674



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573.13

572.9

### Synthesis of novel functional polycyclic chromones through Michael addition and double cyclizations

Yang Liu, Liping Huang, Fuchun Xie, Xuxing Chen and Youhong Hu\*

The synthesis of novel functional polycyclic chromones have been achieved *via* a Michael addition/ cyclization/ $8\pi$ -electrocyclization/ elimination cascade.

### 2685

#### Intramolecular Diels-Alder chemistry of 4-vinylimidazoles

Yong He, Pasupathy Krishnamoorthy, Heather M. Lima, Yingzhong Chen, Haiyan Wu, Rasapalli Sivappa, H. V. Rasika Dias\* and Carl J. Lovely\*

A comprehensive investigation of the intramolecular Diels–Alder reaction of 4-vinylimidazoles is described. The use of pseudo dimeric derivatives provides rapid stereocontrolled access to the polysubstituted tetrahydrobenzimidazole core found in the oroidin alkaloid ageliferin.

### 2702

Stereoselective control in the Staudinger reactions involving monosubstituted ketenes with electron acceptor substituents: experimental investigation and theoretical rationalization

Hengzhen Qi, Xinyao Li and Jiaxi Xu\*

The *exo*-attack of imines to ketenes and the isomerization of iminiums, rather than the torquoelectronic effect, control the stereoselectivity.

### 2715

A general approach to high-yielding asymmetric synthesis of chiral 3-alkyl-4-nitromethylchromans *via* cascade Barbas–Michael and acetalization reactions

Dhevalapally B. Ramachary,\* M. Shiva Prasad and R. Madhavachary

Chiral 4-nitromethylchromans as drug intermediates were achieved through cascade Barbas–Michael and acetalization reactions on 2-(2-nitrovinyl)phenols with aldehydes in the presence of a catalytic amount of (R)-DPPOTMS/PhCO<sub>2</sub>H.

#### 2722

## Synthesis of benzo- and naphtho-fused bicyclo[n.3.1]alkane frameworks with a bridgehead nitrogen function by palladium-catalyzed intramolecular $\alpha'$ -arylation of $\alpha$ -nitroketones

Giorgio Giorgi, Swarupananda Maiti, Pilar López-Alvarado and J. Carlos Menéndez\*

Intramolecular Pd-catalyzed *C*-arylation reactions were used for the construction of fused bicyclic systems bearing a bridgehead nitro group. Fused indane systems were alternative products in some cases.









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### 2731

## Asymmetric *syn*-selective direct aldol reaction of protected hydroxyacetone catalyzed by primary amino acid derived bifunctional organocatalyst in the presence of water

Akshay Kumar, Sarbjit Singh, Vikas Kumar and Swapandeep Singh Chimni\*

The organocatalyst **1g** catalyzes the direct aldol reaction of O-protected (di)hydroxyacetone with aromatic aldehydes in high enantioselectivity (up to 97%).

2743

### Stannylated allyl carbonates as versatile building blocks for the diversity oriented synthesis of allylic amines and amides

Christian Bukovec and Uli Kazmaier\*

In DMF and with [allylPdCl]<sub>2</sub> as catalyst the stannylated allyl amines formed can be directly coupled with electrophiles according to the Stille protocol, giving rise to highly functionalized building blocks in excellent yields.





### 2751

### Structure and unimolecular chemistry of protonated sulfur betaines, $(CH_3)_2S^+(CH_2)_nCO_2H$ (*n* = 1 and 2)

Ellie Jung-Hwa Yoo, Linda Feketeová, George N. Khairallah, Jonathan M. White and Richard A. J. O'Hair\*

The number of methylene "spacers" has a profound effect on the unimolecular chemistry of protonated sulfur betaines  $(CH_3)_2S^*(CH_2)_nCO_2H$ :

### 2760

A DFT study on the mechanism of gold(III)-catalyzed synthesis of highly substituted furans *via* [3, 3]-sigmatropic rearrangements and/or [1, 2]-acyloxy migration based on propargyl ketones

Ran Fang,\* Lizi Yang and Yongcheng Wang

Substituted furan can be prepared after [3,3]-sigmatropic rearrangements and/or [1,2]-acyloxy migration. This interesting Au(III)-catalyzed way is fully supported by a computational study justifying the formation of each intermediate.







(-)-(1



2784



2790



### Phenazinolins A–E: novel diphenazines from a tin mine tailings-derived *Streptomyces* species

Zhang-Gui Ding, Ming-Gang Li, Jie Ren, Jiang-Yuan Zhao, Rong Huang, Qing-Zhong Wang, Xiao-Long Cui, Hua-Jie Zhu\* and Meng-Liang Wen\*

Phenazinolins A–E (1–5), which possess a carbon skeleton unique to diphenazines (the azabicyclo[3.3.1]nonadienol moiety 1–3 and the oxabicycle[3.3.1]nonadienol moiety in 4 and 5), were isolated from tin mine tailings-derived *Streptomyces diastaticus* YIM DT26, with 1–3 exhibited appreciable cytotoxicity and antibiotic effects.

### Thiourea catalyzed organocatalytic enantioselective Michael addition of diphenyl phosphite to nitroalkenes

Ana Alcaine, Eugenia Marqués-López, Pedro Merino, Tomás Tejero and Raquel P. Herrera\*

The simple operational procedure makes this new approach very accessible and attractive for the synthesis of optically active  $\beta$ -aminophosphonic acids

### Sequential two-step multienzyme synthesis of tumor-associated sialyl T-antigens and derivatives

Kam Lau, Hai Yu, Vireak Thon, Zahra Khedri, Meghan E. Leon, Bao K. Tran and Xi Chen\*

 $\alpha$ 2–3-Sialylated  $\beta$ 1–3-galactosides containing natural and non-natural sialic acids were synthesized from simple monosaccharides by sequential two-step multienzyme reactions.

### Pyridinium derivatives of histamine are potent activators of cytosolic carbonic anhydrase isoforms I, II and VII

Khyati Dave, Andrea Scozzafava, Daniela Vullo, Claudiu T. Supuran\* and Marc A. Ilies\*

Pyridinium histamines act as nanomolar activators of cytosolic isoforms of carbonic anhydrase hCA I, II and VII.

### 2801

### Stereoselective synthesis of polyhydroxylated aminocyclohexanes

#### Sajjad Ahmad, Lynne H. Thomas and Andrew Sutherland\*

A new approach for the synthesis of dihydroconduramine derivatives has been developed using a one-pot tandem asymmetric synthesis of an *N*-(cyclohexenyl)trichloroacetamide followed by stereoselective oxidation of the cyclohexene ring.



#### 2809

#### Total synthesis of the Amaryllidaceae alkaloid clivonine

Helmut Haning, Carles Giró-Mañas, Victoria L. Paddock, Christian G. Bochet, Andrew J. P. White, Gerald Bernardinelli, Inderjit Mann, Wolfang Oppolzer and Alan C. Spivey\*

Two syntheses of the Amaryllidaceae alkaloid clivonine (1) are described.



### 2821

### A one pot three-step process for the synthesis of an array of arylated benzimidazoribosyl nucleosides

Jolanta Hałuszczak, Simon J. F. Macdonald and Marie E. Migaud\*

A three-step one pot reaction/purification protocol was developed to facilitate rapid access to benzimidazole-based nucleosides, for which benzoylated benzimidazoribosyl nucleosides incorporating boronic esters were key reaction intermediates.

#### 2832

### An anomalous hydration/dehydration sequence for the mild generation of a nitrile oxide

Nagatoshi Nishiwaki,\* Kazuya Kobiro, Hideyuki Kiyoto, Shotaro Hirao, Jun Sawayama, Kazuhiko Saigo, Yoshikazu Okajima, Toshiharu Uehara, Asaka Maki and Masahiro Ariga

Mild generation of functionalized nitrile oxide is provided upon treatment of nitroisoxazolone with water, which contains an anomalous hydration/dehydration sequence.





without using any special reagents, conditions, and maniulations!





### Incorporation of porphyrin acetylides into duplexes of the simplified nucleic acid GNA

Hui Zhou, Andrew T. Johnson, Olaf Wiest and Lilu Zhang\*

Porphyrin-acetylide modified GNA duplexes were synthesized and the resulting duplexes containing one or two porphyrins were studied by UV-melting, UV-vis, fluorescence and CD spectroscopy.

### Rhodamine-based highly sensitive colorimetric off-on fluorescent chemosensor for Hg<sup>2+</sup> in aqueous solution and for live cell imaging

Hengguo Wang, Yapeng Li, Shufei Xu, Yanchun Li, Chen Zhou, Xiaoliang Fei, Lei Sun, Chaoqun Zhang, Yaoxian Li, Qingbiao Yang\* and Xiaoyi Xu\*

A novel reversible rhodamine-based chemosensor is prepared for the selective and sensitive detection of  $Hg^{2+}$  in aqueous and living cells.

#### 2856



### Synthesis of novel deoxynucleoside *S*-methylphosphonic acids using *S*-(diisopropylphosphonomethyl)isothiouronium tosylate, a new equivalent of mercaptomethylphosphonate

Ivana Kóšiová, Miloš Buděšínský, Natalya Panova and Ivan Rosenberg\*

A new synthetic equivalent of diisopropyl mercaptomethylphosphonate, the *S*-(diisopropylphosphonomethyl)isothiouronium tosylate, was introduced for the straightforward synthesis of *5'*-deoxynucleoside-*5'*-thiomethylphosphonates, novel nucleoside-*5'*-phosphate analogues.

## Fluorinated substrates result in variable leakage of a reaction intermediate during catalysis by dehydroquinate synthase

Leonardo Negron and Emily J Parker\*

Fluorine-substituted substrates result in unusual premature and variable release of a reaction intermediate by dehydroquinate synthase.



### 2868

## Cascade reaction of $\beta$ , $\gamma$ -unsaturated $\alpha$ -ketoesters with phenols in trityl chloride/TFA system. Highly selective synthesis of 4-aryl-2*H*-chromenes and their applications

Yan-Chao Wu,\* Hui-Jing Li, Li Liu, Zhe Liu, Dong Wang and Yong-Jun Chen\*

Condensation of  $\beta$ , $\gamma$ -unsaturated  $\alpha$ -ketoesters with phenols in TFA afforded 4-aryl-2*H*-chromenes, which reacted with various amino-containing nucleophiles in high selectivity.

#### 2878

### Molecular assembly of a squaraine dye with cationic surfactant and nucleotides: its impact on aggregation and fluorescence response

Yongqian Xu, Andrey Malkovskiy, Qiuming Wang and Yi Pang\*

A biomolecule ATP is used as a building block for the nano assembly, which influences the aggregate structure of a squaraine dye to give a fluorescence signal.

### 2885

### The SAMP alkylation: A computational study

Rainer Koch\*

Based on the available experimental evidence, quantum chemical calculations are employed to suggest a reaction mechanism for the SAMP alkylation.







### 2892

#### Structural effects on the photodissociation of alkoxyamines

Davy-Louis Versace, Yohann Guillaneuf, Denis Bertin, Jean Pierre Fouassier, Jacques Lalevée\* and Didier Gigmes\*

The search for photosensitive alkoxyamines remains a challenge. We investigate the effect of alkoxyamine structure on the photodissociation process.





### Novel biotinylated bile acid amphiphiles: Micellar aggregates formation and interaction with hepatocytes

Luca Rizzi, Marta Braschi, Miriam Colombo, Nadia Vaiana, Gianpaolo Tibolla, Giuseppe Danilo Norata, Alberico Luigi Catapano, Sergio Romeo\* and Davide Prosperi\*

Amphiphilic bile acids linked through an oligoethylene glycol to a biotin moiety are shown to have potential as a drug delivery system against liver diseases.



2920



Barbara Buchs (née Levrand), Wolfgang Fieber, Florence Vigouroux-Elie, Nampally Sreenivasachary, Jean-Marie Lehn\* and Andreas Herrmann\*

Combination of rheology data with dynamic headspace analysis of fragrance evaporation suggests that reversible hydrazone formation has a stronger influence on the release of volatiles than the absolute stability of the gel.

### Nitroxide biradicals as thread units in paramagnetic cucurbituril-based rotaxanes

Elisabetta Mileo, Costanza Casati, Paola Franchi, Elisabetta Mezzina and Marco Lucarini\*

The first example of paramagnetic rotaxane containing cucurbit[6]urils has been reported.



2925



Soluble polymer supported divergent synthesis of tetracyclic benzene-fused pyrazino/diazepino indoles: an advanced synthetic approach to bioactive scaffolds

Po-Tsung Lin, Deepak B. Salunke, Li-Hsun Chen and Chung-Ming Sun\*

The synthesis of structurally diverse benzene-fused pyrazino/diazepino indoles as VEGFR-3 inhibitors is disclosed.

### 2938

### A highly sensitive water-soluble system to sense glucose in aqueous solution

Liheng Feng,\* Fei Liang, Yue Wang, Ming Xu and Xiaoju Wang\*

A highly sensitive sensing switch for glucose is formed by the water soluble conjugated polymer PP–S-BINOL and a boronic acid-functionalized benzyl viologen *o*-BBV.

#### 2943

## MS/MS fragmentation-guided search of TMG-chitooligomycins and their structure–activity relationship in specific $\beta$ -N-acetylglucosaminidase inhibition

Hirokazu Usuki, Yukihiro Yamamoto, Yuya Kumagai, Teruhiko Nitoda, Hiroshi Kanzaki and Tadashi Hatanaka\*

A MS/MS fragmentation-guided search was developed and adapted for the screening of putative GH20 GlcNAcase inhibitors, TMG-chitooligomycins [TMG-(GlcNAc)<sub>n</sub>].

### 2952

### Assessing the whole range of CuAAC mechanisms by DFT calculations—on the intermediacy of copper acetylides

David Cantillo,\* Martín Ávalos, Reyes Babiano, Pedro Cintas, José L. Jiménez and Juan C. Palacios

An in-depth mechanistic study of the Cu(I)-catalyzed alkyne-azide click cycloaddition (CuAAC) *via* DFT calculations and isotopic labeling finally unveils the intermediacy of copper acetylides, ruling out the alternative participation of  $\pi$ -complexes in accelerating the transformation.

### 2959

### Photochemical [2 + 2] cycloaddition reactions of 6-alkenyl-3-phenylcyclohex-2-en-1-ones: using biradical conformation control to account for exceptions to the "rule of five"

Stephen A. Bradley, Brian J. Bresnan, Sylvia M. Draper, Niall W. A. Geraghty,\* Mark Jeffares, Thomas McCabe, T. Brian H. McMurry\* and John E. O'Brien

The conformation of 1,4-biradical intermediates plays a product determining role in intramolecular [2 + 2] cycloaddition reactions.









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### 2969

### Reactivity of *endo*-3-bromocamphor with sulfur-centered nucleophiles by an electron transfer mechanism. Electrophilic behaviour of the 3-camphoryl radical

Jorge G. Uranga and Ana N. Santiago\*

The  $pK_a$  and proton affinities of the conjugated acids can predict the reactivity of ArS<sup>-</sup> with 3-camphoryl radicals.

#### 2975

### Disubstituted 2-phenyl-benzopyranopyrimidine derivatives as a new type of highly selective ligands for telomeric G-quadruplex DNA

Wei-Bin Wu, Shu-Han Chen, Jin-Qiang Hou, Jia-Heng Tan, Tian-Miao Ou, Shi-Liang Huang, Ding Li, Lian-Quan Gu and Zhi-Shu Huang\*

A series of disubstituted 2-phenyl-benzopyranopyrimidine (PBPP) derivatives were found to be a new type of highly selective ligand for telomeric G-quadruplex DNA.

### 2987

### Iodination of anilines and phenols with 18-crown-6 supported ICl<sub>2</sub><sup>-</sup>

Hannah W. Mbatia, Olbelina A. Ulloa, Daniel P. Kennedy, Christopher D. Incarvito and Shawn C. Burdette\*

An ICl<sub>2</sub> trihalide supported by an 18-crown-6 macrocycle forms a columnar supramolecular structure in the solid state. This reagent,  $\{[K\cdot(18-C-6)]ICl_2\}_n$  iodinates anilines and phenols efficiently under mild conditions.

### 2992

### Synthesis, characterization and structures of 2-(3,5-dimethylpyrazol-1-yl)ethylseleno derivatives and their probable glutathione peroxidase (GPx) like activity

Ananda S. Hodage, Prasad P. Phadnis, Amey Wadawale, K. I. Priyadarsini and Vimal K. Jain\*

Glutathione peroxidase (GPx) like catalytic activity of 2-(3,5-dimethylpyrazol-1-yl)ethylseleno derivatives has been investigated





 $\Delta T_{\rm m} = 16.5 \,{}^{\rm o}{\rm C}$  11b  $\kappa_{\rm D} = 4.5 \,{}_{\rm \mu}{\rm M}$  $\Delta G = -19.5 \,{\rm kcal \, mol}^{-1}$ 









#### 3011 $R_2$ $R_1$ $R_3$ $C \equiv N$ NHase pH7 buffer, MeOH $R_1$ $R_3$ $R_1$ $R_3$ $R_1$ $R_2$ $R_1$ $R_3$ $R_1$ $R_2$ $R_1$ $R_3$ $R_3$ $R_1$ $R_3$ $R_1$ $R_2$ $R_3$ $R_3$ $R_3$ $R_1$ $R_3$ 
$$\label{eq:R1=C2H5} \begin{split} R_1 = & C_2 H_5, Ph, PhCH_2, 6-(CH_3 O) naphthyl, 3-(COOH)Ph, 4-(NO_2)Ph \\ R_2 = & CH_3, C_2 H_5, OH, NH_2, OAc, Cl, N_3 \\ R_3 = & H, CH_3 \end{split}$$

\ OMe

NDMM

BnO

HC

Dor

BnC

C

Don

ÓН

OMe

OMe

NDMM

NDMM

only product

Determined experimentally

$$E$$
 up to  $> 100$ 

BnC

Dor

BnO

Don

OMe

0

H\_C

ÓН

óн

Determined by DFT calculations

much more stable than

Synthesis and evaluation of 5-lipoxygenase translocation inhibitors from acylnitroso hetero-Diels-Alder cycloadducts

Joshua K. Bolger, Wen Tian, William R. Wolter, Wonhwa Cho, Mark A. Suckow and Marvin J. Miller\*

Regioselective oxazine ring opening reactions generate potent 5-lipoxygenase inhibitors with antitumor properties.

### Probing the enantioselectivity of a diverse group of purified cobalt-centred nitrile hydratases

S. van Pelt, M. Zhang, L. G. Otten, J. Holt, D. Y. Sorokin, F. van Rantwijk, G. W. Black, J. J. Perry\* and R. A. Sheldon\*

Four purified cobalt containing nitrile hydratases were screened for their enantioselectivity towards a range of chiral nitriles showing that they can exhibit high E values for some substrates.

### Regioselectivity of the glycosylation of *N*-dimethylmaleoyl-protected hexosamine acceptors. An experimental and DFT approach

María I. Colombo,\* Edmundo A. Rúveda and Carlos A. Stortz\*

The experimental outcomes of the regioselectivity of the glycosylation of hexosamine diol acceptors were rationalized by DFT calculations.



3020

Don

HC

OBr

ÓН

0



## Optimized strategies to synthesize $\beta$ -cyclodextrin-oxime conjugates as a new generation of organophosphate scavengers

Romain Le Provost, Timo Wille, Ludivine Louise, Nicolas Masurier, Susanne Müller, Georg Reiter, Pierre-Yves Renard, Olivier Lafont, Franz Worek and François Estour\*

A series of  $\beta$ -CD derivatives was prepared. The obtained compounds were able to detoxify the highly deadly chemical warfare agent GF.

2576 | Org. Biomol. Chem., 2011, 9, 2559-2578

### 3033

### A novel hydrazide type organocatalyst for enantioselective Diels-Alder reactions

Ichiro Suzuki,\* Masafumi Ando, Rumiko Shimabara, Ai Hirata and Kei Takeda

Facile enantioselective Diels–Alder reaction were realized by a novel hydrazide-type twin-core catalyst.



#### 3041

### Synthesis and biological activity of 2-aminoimidazole triazoles accessed by Suzuki–Miyaura cross-coupling

Samuel Reyes, Robert W. Huigens III, Zhaoming Su, Michel L. Simon and Christian Melander\*

A 2-aminoimidazole triazole (2-AIT) lead compound was diversified *via* Suzuki-Miyaura cross-coupling to produce derivatives with enhanced biofilm modulation and antibacterial properties



### 3050

### Bifunctional primary amine-thiourea–TfOH (BPAT·TfOH) as a chiral phase-transfer catalyst: the asymmetric synthesis of dihydropyrimidines

Yangyun Wang, Jipan Yu, Zhiwei Miao\* and Ruyu Chen\*

An enantioselective Biginelli reaction has been developed by using a bifunctional primary amine-thiourea–TfOH (BPAT·TfOH) as a chiral phase-transfer catalyst and *t*-BuNH<sub>2</sub>·TFA as an additive in saturated brine at room temperature.



### 42nd National Organic Chemistry Symposium Princeton University, June 5-9, 2011

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