

Organic & Biomolecular Chemistry

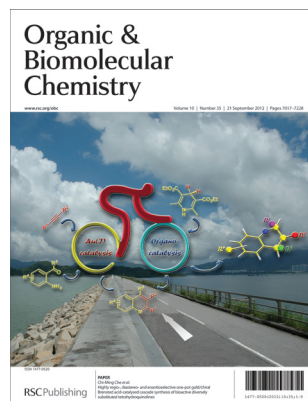
An international journal of synthetic, physical and biomolecular organic chemistry

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Cover

See Chi-Ming Che *et al.*, pp. 7208–7219.

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Inside cover

See Prasat Kittakoop *et al.*, pp. 7220–7226.

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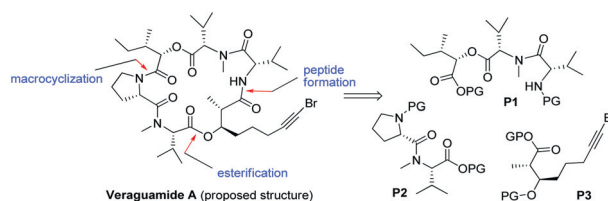
COMMUNICATIONS

7027

Total synthesis of the proposed structure of cyclic hexadepsipeptide veraguamide A

Dongyu Wang, Xian Jia* and Ao Zhang*

We have developed a practical method to assemble the natural product veraguamide A (**1**) by first preparing the three key fragments followed by optimization of the macrocyclization site. Although the synthetic product gave similar optical rotation to that reported for natural product, significant differences in the ^1H and ^{13}C NMR spectra were observed, especially the proton and carbon signals in the two *N*-MeVal moieties.

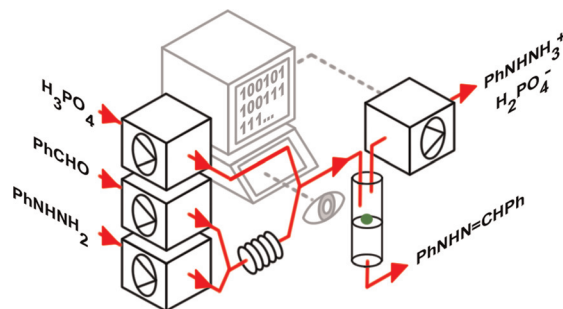


7031

A prototype continuous-flow liquid–liquid extraction system using open-source technology

Matthew O'Brien,* Peter Koos, Duncan L. Browne and Steven V. Ley

A prototype continuous-flow liquid–liquid extraction system was developed using open-source software (Python, OpenCV) for computer-vision based control.



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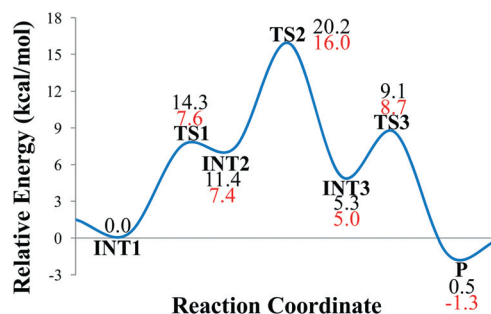
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7037

New insights into the mechanism of the Schiff base hydrolysis catalyzed by type I dehydroquinate dehydratase from *S. enterica*: a theoretical study

Yuan Yao* and Ze-Sheng Li*

The fundamental reaction mechanism for Schiff base hydrolysis catalyzed by type I DHQD from *S. enterica* has been studied by MD simulations and DFT calculations. The new mechanistic insights obtained here will be valuable for the rational design of high-activity inhibitors of type I DHQD as non-toxic antimicrobials, anti-fungals, and herbicides.

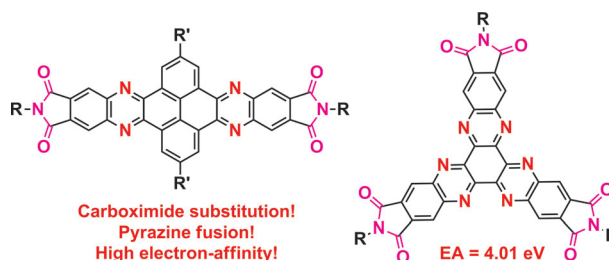


7045

Linear and star-shaped pyrazine-containing acene dicarboximides with high electron-affinity

Jinjun Shao, Jingjing Chang and Chunyan Chi*

Linear and star-shaped pyrazine-containing acenes substituted by dicarboximide groups are synthesized and they show high electron-affinity and ordered self-assembly.

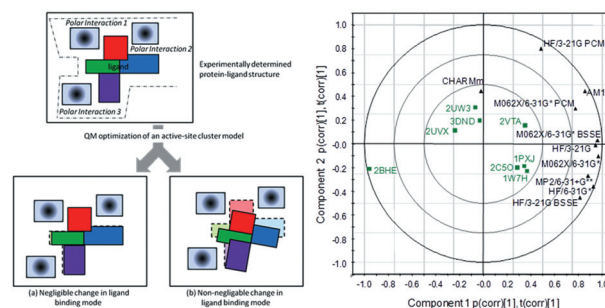


7053

Evaluating the enthalpic contribution to ligand binding using QM calculations: effect of methodology on geometries and interaction energies

Duangkamol Gleeson, Ben Tehan,* M. Paul Gleeson* and Jumras Limtrakul

QM benchmark calculations have been performed on isolated models of protein kinase complexes to assess their geometric and energetic characteristics.

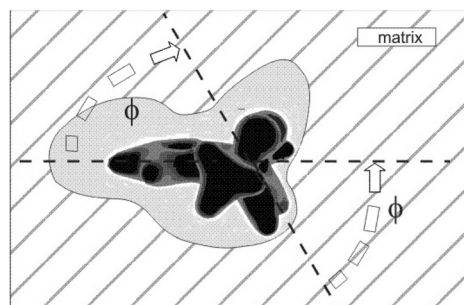


7062

Functionalized derivatives of 1,4-dimethylnaphthalene as precursors for biomedical applications: synthesis, structures, spectroscopy and photochemical activation in the presence of dioxygen

Damir Posavec, Manfred Zabel, Udo Bogner, Günther Bernhardt and Günther Knör*

Controlling the decay kinetics of encapsulated endoperoxides enables a sufficiently high bio-availability to trigger cytostatic and cytotoxic effects on human cancer cells *via* delayed singlet oxygen release.



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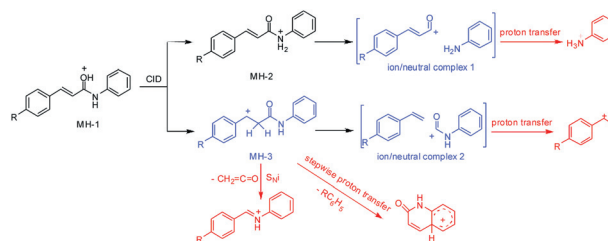
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7070

Intriguing roles of reactive intermediates in dissociation chemistry of *N*-phenylcinnamides

Cheng Guo, Kezhi Jiang, Lei Yue, Ziming Xia, Xiaoxia Wang and Yuanjiang Pan*

Proton transfer and intramolecular nucleophilic substitution reactions mediated by the reactive intermediates resulting from dissociative protonation were discovered and investigated.

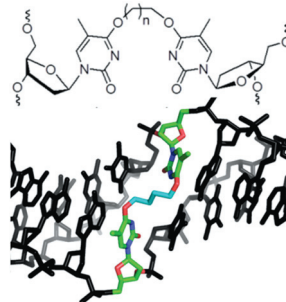


7078

*O*⁴-Alkyl-2'-deoxythymidine cross-linked DNA to probe recognition and repair by *O*⁶-alkylguanine DNA alkyltransferases

Francis P. McManus, Derek K. O'Flaherty, Anne M. Noronha and Christopher J. Wilds*

An approach to synthesize DNA interstrand cross-links linking the *O*⁴ atoms of 2'-deoxythymidine is described. These cross-links were shown to evade repair by various *O*⁶-alkylguanine DNA alkyltransferases.

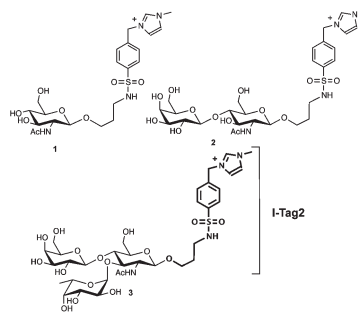


7091

Ionic-liquid-based MS probes for the chemo-enzymatic synthesis of oligosaccharides

M. Carmen Galan,* Anh Tuan Tran, Karen Bromfield, Said Rabbani and Beat Ernst

A new *N*-benzenesulfonyl-based ionic liquid mass spectroscopy label (I-Tag2) for covalent attachment to glycan substrates has been prepared that can be used to monitor oligosaccharide elongation and serve as a purification handle.

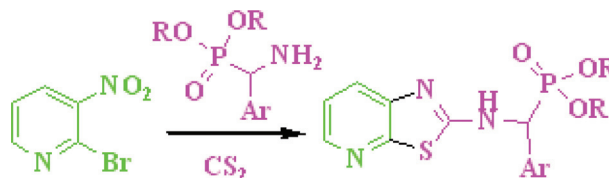


7098

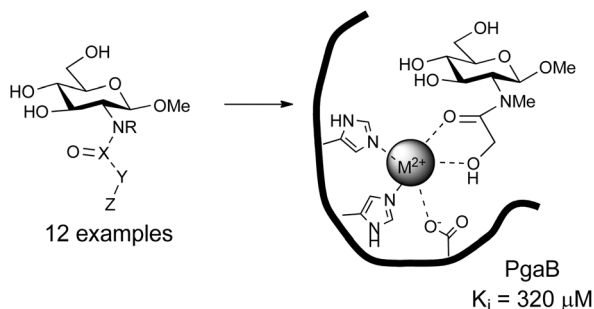
Synthesis and antitumor activity of α -aminophosphonates containing thiazole[5,4-*b*]pyridine moiety

Lijun Gu* and Cheng Jin

A new procedure for synthesis of α -aminophosphonates containing thiazole[5,4-*b*]pyridine moiety. Some compounds are effective against the tested cancer cell lines.



7103

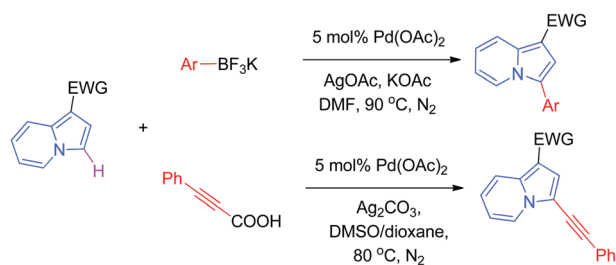


Synthesis and evaluation of inhibitors of *E. coli* PgaB, a polysaccharide de-*N*-acetylase involved in biofilm formation

Anthony Chibba, Joanna Poloczec, Dustin J. Little, P. Lynne Howell and Mark Nitz*

Many medically important biofilm forming bacteria produce similar polysaccharide intracellular adhesins (PIA) consisting of partially de-*N*-acetylated β -(1 \rightarrow 6)-*N*-acetylglucosamine polymers (dPNAG).

7108

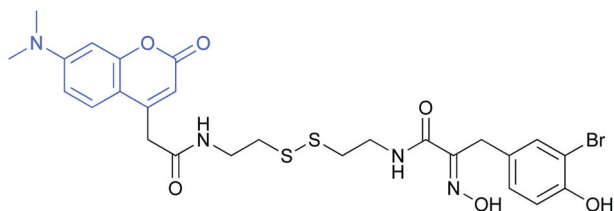


Pd-Catalyzed C-3 functionalization of indolizines via C–H bond cleavage

Baoli Zhao*

New transition metal-catalyzed methods for the arylation of indolizines by direct cleavage of C–H bonds have been developed. A wide range of aryltrifluoroborate salts react with indolizines in the presence of Pd(OAc)₂ catalyst and AgOAc oxidant to give arylated indolizines in high yields. In addition, the indolizines display similar reactivities in the Pd-catalyzed reaction with 3-phenylpropionic acid to afford the corresponding C-3 alkynylated indolizines.

7120

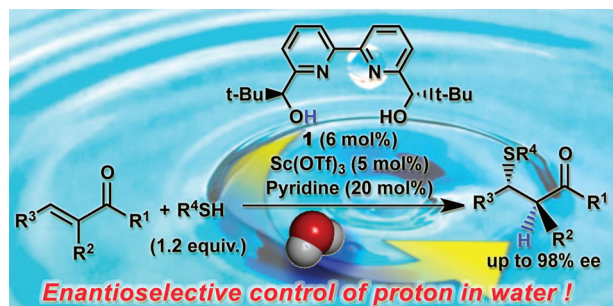


Fluorescent analogs of the marine natural product psammaphin A: synthesis and biological activity

Fabia Hentschel, Florenz Sasse and Thomas Lindel*

New fluorescent analogs of psammaphin A are cytotoxic and cause fluorescence in close proximity of the nuclear envelope of L-929 mouse fibroblast cells, as revealed by fluorescence microscopy.

7134



Chiral-Sc catalyzed asymmetric Michael addition/protonation of thiols with enones in water

Taku Kitanosono, Masaru Sakai, Masaharu Ueno and Shū Kobayashi*

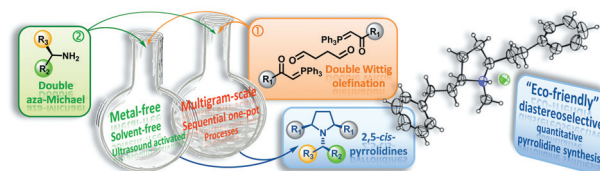
Asymmetric Michael reactions and enantioselective protonations between enones and thiols were catalyzed by a Sc(OTf)₃-chiral 2,2'-bipyridine complex in water.

7148

Solvent-free double aza-Michael under ultrasound irradiation: diastereoselective sequential one-pot synthesis of pyrrolidine *Lobelia* alkaloids analogues

Zacharias Amara, Emmanuelle Drège, Claire Troufflard, Pascal Retailleau and Delphine Joseph*

2,5-*cis*-Pyrrolidines can be prepared by a catalyst-free double aza-Michael addition of liquid primary amines to symmetrical (bis)- α,β -unsaturated compounds. The method proceeds at room temperature in solvent-free conditions and has been extended to the synthesis of bioactive alkaloids.

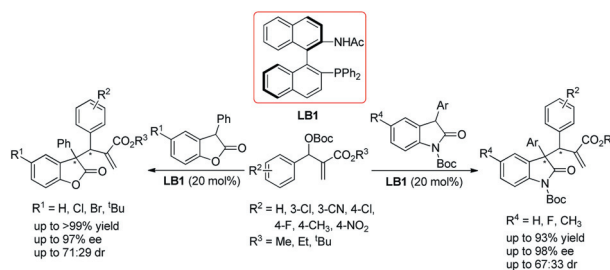


7158

Chiral phosphine-catalyzed asymmetric allylic alkylation of 3-substituted benzofuran-2(3*H*)-ones or oxindoles with Morita–Baylis–Hillman carbonates

De Wang, Yuan-Liang Yang, Jia-Jun Jiang and Min Shi*

An efficient chiral phosphine-catalyzed asymmetric allylic alkylation of MBH carbonates with 3-substituted benzofuran-2(3*H*)-ones or 3-substituted oxindoles is reported.

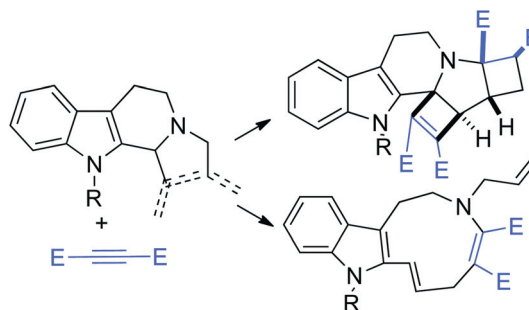


7167

Medium-sized and strained heterocycles from non-catalysed and gold-catalysed conversions of β -carboline

Sandra Medina, Álvaro González-Gómez, Gema Domínguez and Javier Pérez-Castells*

Highly strained polycyclic structures are obtained upon reaction of β -carboline with alkynes. Reaction conditions determine the final product.

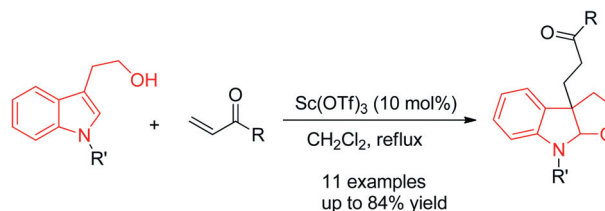


7177

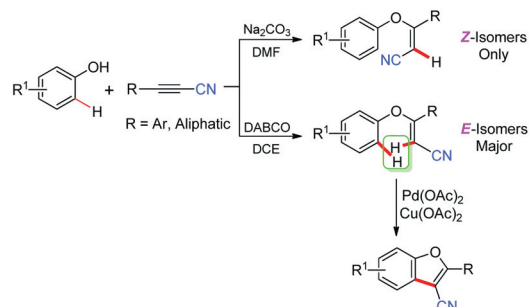
Cascade dearomatization of *N*-substituted tryptophols *via* Lewis acid-catalyzed Michael reactions

Chuan Liu, Wei Zhang, Li-Xin Dai and Shu-Li You*

Lewis acid-catalyzed cascade dearomatization of *N*-substituted tryptophols *via* Michael addition reaction was developed affording furoindoline derivatives in good yields.



7184

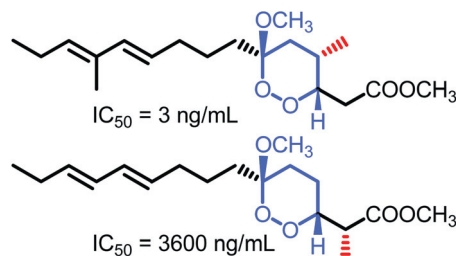


Synthesis of *(Z)*-3-aryloxy-acrylonitriles, *(E)*-3-aryloxy-acrylonitriles and 3-cyanobenzofurans through the sequential reactions of phenols with propiolonitriles

Wei Zhou, Yicheng Zhang, Pinhua Li and Lei Wang*

(Z)/*(E)*-3-Aryloxy-acrylonitriles were prepared via Na₂CO₃/DABCO-promoted additions of phenols to propiolonitriles, and 3-cyanobenzofurans were obtained from palladium-catalyzed C–H functionalization of *(E)*-3-aryloxy-acrylonitriles.

7197

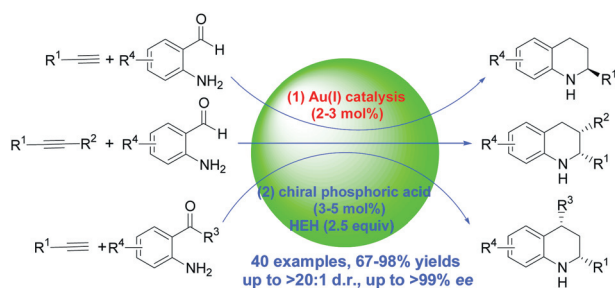
*Trypanosoma b. rhodesiense*

Manadoperoxides, a new class of potent antitrypanosomal agents of marine origin

Giuseppina Chianese, Ernesto Fattorusso, Fernando Scala, Roberta Teta, Barbara Calcinai, Giorgio Bavestrello, Henny A. Dien, Marcel Kaiser, Deniz Tasdemir and Orazio Tagliatalata-Scafati*

Eight endoperoxides, some containing a chlorinated THF ring, were isolated from *Plakortis* cf. *lita*. Among them, manadoperoxide B exhibited ultrapotent trypanocidal activity.

7208

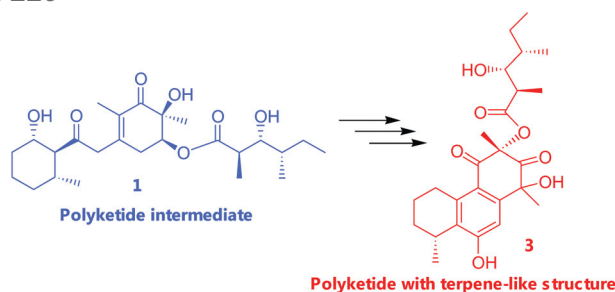


Highly regio-, diastereo- and enantioselective one-pot gold/chiral Brønsted acid-catalysed cascade synthesis of bioactive diversely substituted tetrahydroquinolines

Xin-Yuan Liu, Ya-Ping Xiao, Fung-Ming Siu, Li-Chen Ni, Yong Chen, Lin Wang and Chi-Ming Che*

Au(I)-catalysed reactions of aminobenzaldehydes or aminophenones with alkynes cooperating with chiral Brønsted-acid-catalysed hydrogenation selectively afford various tetrahydroquinolines possessing 2-, 2,3- or 2,4-chiral centers in good to excellent enantioselectivities.

7220



A novel tricyclic polyketide and its biosynthetic precursor azaphilone derivatives from the endophytic fungus *Dothideomycete* sp

Sarath P. D. Senadeera, Suthep Wiyakrutta, Chulabhorn Mahidol, Somsak Ruchirawat and Prasat Kittakoop*

A polyketide 3 possessing a novel terpene-like ring system is co-isolated with its biosynthetic congeners (e.g., 1).