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Organic & Biomolecular Chemistry



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Inside cover See Gevorg Sargsyan and

Milan Balaz, pp. 5533–5540.

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EMERGING AREA

5485

Catalytic methodologies for the β-boration of conjugated electron deficient alkenes

Adam D. J. Calow and Andrew Whiting*

A critical review of the current advances in metal and non-metal catalysed asymmetric β -boration of electron deficient olefins (α , β -unsaturated amides, esters, imines, ketones and nitriles).



PERSPECTIVE

5498

A novel class of tunable cyclopropanation reagents (RXZnCH₂Y) and their synthetic applications

Richard G. Cornwall, O. Andrea Wong, Haifeng Du, Thomas A. Ramirez and Yian Shi*

A novel class of tunable cyclopropanating reagents has been shown to efficiently cyclopropanate alkenes and has been widely used in organic synthesis.



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Keiji Maruoka, Kyoto University, Japan

COMMUNICATIONS

5514

Attack of radicals and protons on ladderane lipids: quantum chemical calculations and biological implications

Dustin H. Nouri and Dean J. Tantillo*

Quantum chemical calculations on possible decomposition processes for ladderane lipids reveal that hydrogen atom abstraction next to the ladderane core can lead to opening of the cyclobutane rings comprising the ladderane substructure and protonation leads directly to fragmentation.

5518

Stereoselective construction of the tetracyclic core of Cryptotrione

Song Chen, Chao Rong, Pengju Feng, Songlei Li and Yian Shi*

An efficient stereoselective approach to the tetracyclic core of Cryptotrione, involving an asymmetric Michael addition, ringclosing metathesis, and subsequent cyclopropanation, is described.





5521

Rhodium(III)-catalyzed oxidative mono- and di-olefination of isonicotinamides

Xiaohong Wei, Feng Wang, Guoyong Song, Zhengyin Du and Xingwei Li*

Rhodium(III) complexes can catalyze the oxidative olefination of secondary isonicotinamides in different selectivity.

5525

Locking high energy 1D chain of dichloromethane molecules containing abnormally short Cl···Cl contacts of 2.524 Å inside organic crystals

Feng Zhou, Haoliang Fu, Wei Qiang Ong, Ruijuan Ye, Weixing Yuan, Yu-Jing Lu, Yan-Ping Huo, Kun Zhang, Haibin Su and Huaqiang Zeng*

Organic helical channels can be used to host 1D chains of dichloromethane molecules containing extraordinarily short intermolecular Cl···Cl contacts of 2.524 Å in length.





New process for crystal data files



Image courtesy of Professor Gang Chen and Dr Rencheng Jin DOI: 10.1039/C2CE06417K

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COMMUNICATIONS

5529

A polyoxapolyaza macrobicyclic receptor for the recognition of zwitterions

Pedro Mateus, Rita Delgado,* Paula Brandão and Vítor Félix

A polyoxapolyaza macrobicyclic receptor designed for zwitterion recognition in aqueous solutions showed preference for substrates containing tetrahedral anionic groups.



PAPERS

5533

Porphyrin–DNA conjugates: porphyrin induced adenine–guanine homoduplex stabilization and interduplex assemblies

Gevorg Sargsyan and Milan Balaz*

The synthesis, self-assembly, stability, and spectroscopic studies of short alternating non-self-complementary DNA sequences 5'-(dGdA)₄ and 5'-(dAdG)₄ with non-charged tetraarylporphyrins covalently linked to the 5' position of deoxyadenosine or deoxyguanosine *via* a phosphate or amide linker is reported.

5541

Total synthesis of dendrobate alkaloid (+)-241D, isosolenopsin and isosolenopsin A: application of a gold-catalyzed cyclization

Nicolas Gouault,* Myriam Le Roch, Gisele de Campos Pinto and Michèle David

A new approach to total syntheses of piperidine alkaloids has been developed from D-alanine *via* a gold-catalyzed 6-endo-dig cyclization process.

5547

Bioorthogonal metal-free click-ligation of *c*RGD-pentapeptide to alginate

Andreas Krause, Andreas Kirschning and Gerald Dräger*

Conjugation of *c*RGD-pentapeptides to modified alginate by employing a metal-free 1,3-dipolar cycloaddition approach is studied in detail using model compounds, ¹H-NMR and ¹⁹F-NMR spectroscopy.







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PAPERS

5554

Novel thieno [2,3-d] pyrimidines: their design, synthesis, crystal structure analysis and pharmacological evaluation

Raju Adepu, D. Rambabu, Bagineni Prasad, Chandana Lakshmi T. Meda, Ajit Kandale, G. Rama Krishna, C. Malla Reddy, Lakshmi N. Chennuru, Kishore V. L. Parsa* and Manojit Pal*

Sequential construction of the thienopyrimidine ring, cyclohexanone moiety and subsequently the fused heterocyclic ring provided novel inhibitors of PDE4.

5570

Polycationic amphiphilic cyclodextrins as gene vectors: effect of the macrocyclic ring size on the DNA complexing and delivery properties

Céline Bienvenu, Álvaro Martínez, José Luis Jiménez Blanco, Christophe Di Giorgio, Pierre Vierling,* Carmen Ortiz Mellet,* Jacques Defaye and José M. García Fernández*

Polycationic amphiphilic cyclodextrins (paCDs) condense DNA to form nanocomplexes (CDplexes) whose transfection capabilities depends on the macrocyclic ring size.

5582

Intramolecular cycloaddition of azomethine vlides, from imines of O-acylsalicylic aldehyde and ethyl diazoacetate, to ester carbonyl - experimental and DFT computational study

Anastasia P. Kadina, Alexander F. Khlebnikov,* Mikhail S. Novikov, Pedro J. Pérez and Dmitry S. Yufit

Intramolecular 1,3-dipolar cycloaddition of alkoxycarbonylsubstituted azomethine ylides to ester carbonyl was realized for the first time.

5592

Iminosugar-ferrocene conjugates as potential anticancer agents

Audrey Hottin, Faustine Dubar, Agata Steenackers, Philippe Delannoy, Christophe Biot and Jean-Bernard Behr*

New iminosugar-ferrocene hybrids display inhibition of fucosidase and inactivation of MDA-MB-231 breast cancer cells proliferation at low micromolar concentrations.









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PAPERS

5598

A theoretical study of carbon–carbon bond formation by a Michael-type addition

Katarzyna Świderek, Anna Pabis and Vicent Moliner*

A theoretical study of the Michael-type addition of 1,3-dicarbonyl compounds to α , β -unsaturated carbonyl compounds has been performed in the gas phase by means of the AM1 semiempirical method and by density functional theory calculations within the B3LYP and M06-2X hybrid functionals.

5606

Highly selective colorimetric sensing pyrophosphate in water by a NBD-phenoxo-bridged dinuclear Zn(II) complex

Shengjun Yang, Guoqiang Feng* and Nicholas H. Williams

A novel effective colorimetric sensor for pyrophosphate (PPi) in pure aqueous solution over a wide pH range is reported.





5613

A tripeptide-like prolinamide-thiourea as an aldol reaction catalyst

Stamatis Fotaras, Christoforos G. Kokotos and George Kokotos*

A tripeptide-like prolinamide-thiourea catalyst with (*S*)-proline, (1S,2S)-diphenylethylenediamine and (*S*)-di-*tert*-butyl aspartate as building blocks provides the products of the reaction between ketones and aromatic aldehydes in high to quantitative yields and high stereoselectivities (up to 99 : 1 dr and 99% ee).

5620

Synthesis of CDE molecular fragments related to sendanin mediated by titanocene(III)

A. Fernández-Mateos,* A. I. Ramos Silvo, R. Rubio González and M. S. J. Simmonds

Fragments of limonoid were synthesized diastereoselectively using the titanocene(III)-promoted cyclization of unsaturated epoxylactones. These compounds show significant antifeedant activity.





Antifeedant activity

PAPERS



fargenone B

5636

5643



fargenone A

temperature-switched mechanism



R¹=H, Me, MeO, CI; R²=Me, n-Pr, Ph



fargenir

A strategy for the synthesis of the fargenone/fargenin family of natural products: synthesis of the tricyclic core

Ross M. Denton* and James T. Scragg

A phosphonium ylide induced cascade reaction afforded the tricyclic core structure of the fargenin/fargenone family of natural products.

Aluminium triflate catalysed *O*-glycosidation: temperature-switched selective Ferrier rearrangement or direct addition with alcohols

D. Bradley G. Williams,* Sandile B. Simelane and Henok H. Kinfe

Temperature-switched mechanism between Ferrier rearrangement and direct addition of alcohols to produce *O*-pseudoglycals or 2-deoxycarbohydrates in Al(OTf)₃-catalysed *O*-glycosylations.

Facile and efficient synthesis of quinolin-2(1*H*)-ones via cyclization of penta-2,4-dienamides mediated by H_2SO_4

Xu Liu, Xin Xin, Dexuan Xiang, Rui Zhang,* Santosh Kumar, Fenguo Zhou and Dewen Dong*

Intramolecular cyclization of penta-2,4-dienamides mediated by concentrated H_2SO_4 (98%) provides access to substituted quinolin-2(1*H*)-ones.



Transformations of diphenylphosphinothioic acid tertiary amides mediated by directed *ortho* metallation

Hajar el Hajjouji, Eva Belmonte, Jesús García-López, Ignacio Fernández, María José Iglesias, Laura Roces, Santiago García-Granda, Anas El Laghdach and Fernando López Ortiz*

An efficient procedure for the *ortho* functionalisation of *P*,*P*-diphenylphosphinothioic amides *via* directed *ortho*-lithiation followed by electrophilic trapping is described.