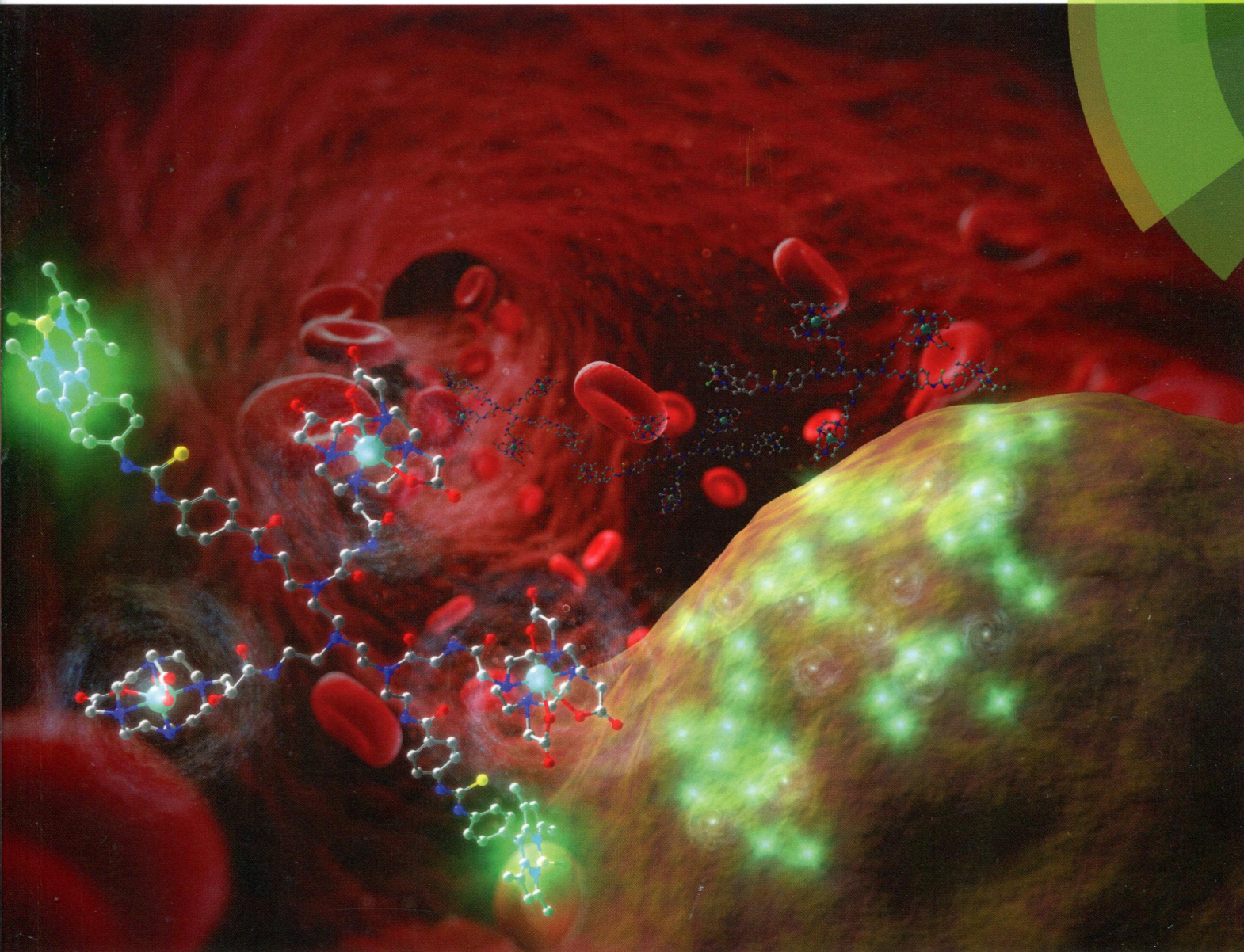


M
0-72/6

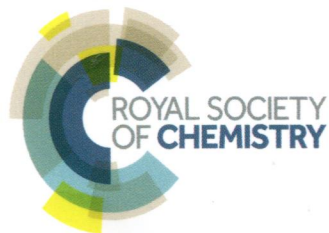
Volume 12 | Number 43 | 21 November 2014 | Pages 8564–8784

Organic & Biomolecular Chemistry

www.rsc.org/obc



ISSN 1477-0520



PAPER

Kenjiro Hanaoka *et al.*

A design strategy for small molecule-based targeted MRI contrast agents: their application for detection of atherosclerotic plaques

Organic & Biomolecular Chemistry

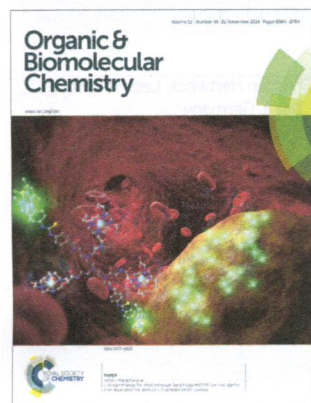
An international journal of synthetic, physical and biomolecular organic chemistry

www.rsc.org/obc

The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

IN THIS ISSUE

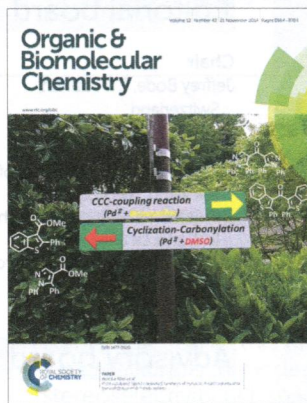
ISSN 1477-0520 CODEN OBCRAK 12(43) 8564–8784 (2014)



Cover

See Kenjiro Hanaoka et al., pp. 8611–8618.

Image reproduced by permission of Kenjiro Hanaoka from *Org. Biomol. Chem.*, 2014, **12**, 8611.



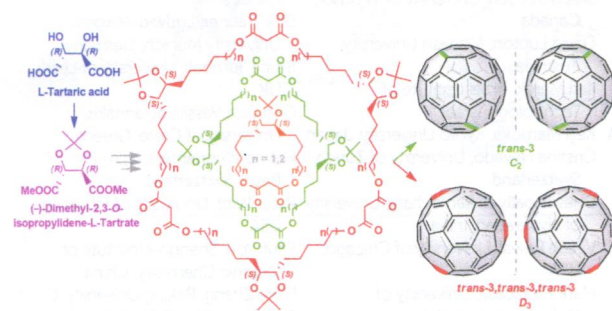
Inside cover

See Keisuke Kato et al., pp. 8619–8626.

Image reproduced by permission of Keisuke Kato from *Org. Biomol. Chem.*, 2014, **12**, 8619.

PERSPECTIVE

8574



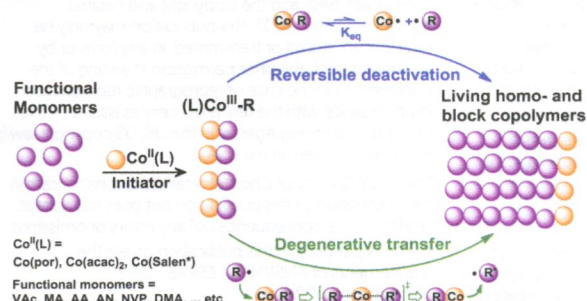
The journey of L-tartaric acid in the world of enantiomerically pure bis- and trisadducts of C₆₀ with the inherently chiral *trans*-3 and all-*trans*-3 addition patterns

Nikos Chronakis

The journey of L-tartaric acid through its derivative (–)-dimethyl-2,3-O-isopropylidene-L-tartrate in the synthesis of enantiomerically pure diols, *cyclo*-[*n*]-malonates and finally, inherently chiral *trans*-3 bisadducts and all-*trans*-3 trisadducts of C₆₀ is presented.

REVIEW

8580



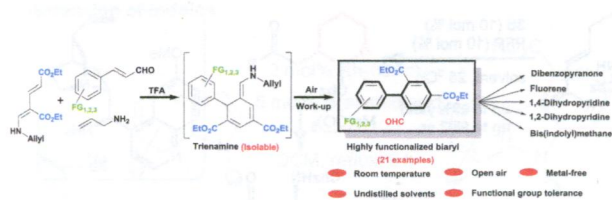
Reversible deactivation radical polymerization mediated by cobalt complexes: recent progress and perspectives

Chi-How Peng,* Tsung-Yao Yang, Yaguang Zhao and Xuefeng Fu*

The current status and future perspective of cobalt mediated radical polymerization that showed efficient control of vinyl acetate and acrylate polymerization are described.

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

8588

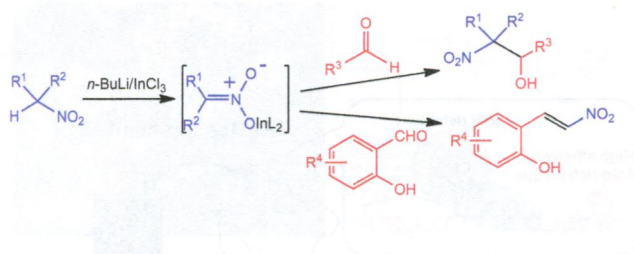


A metal-free one-pot cascade synthesis of highly functionalized biaryl-2-carbaldehydes

Chandrasekhar Challa, Jamsheena Vellekkatt, Jaice Ravindran and Ravi S. Lankalapalli*

A metal-free one-pot cascade annulation of acyclic substrates dienaminodioate, cinnamaldehydes and allyl amine was achieved for the synthesis of polyfunctional biaryl-2-carbaldehydes.

8593

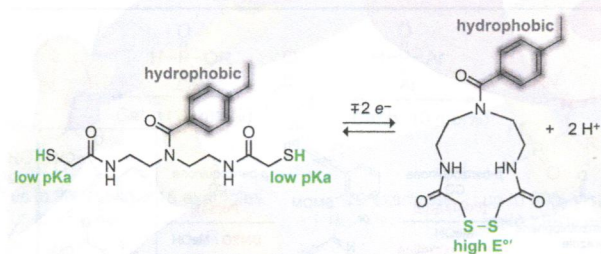


Preparation of indium nitronates and their Henry reactions

Raquel G. Soengas,* Rita Acúrcio and Artur M. S. Silva*

Indium nitronates were readily prepared from commercially available nitroalkanes by transmetalation of the corresponding lithium nitronates with indium salts. The Henry reaction of this nitronates with aldehydes afforded β -nitroalkanols in moderate to high yields and excellent stereoselectivity (when using chiral aldehydes).

8598

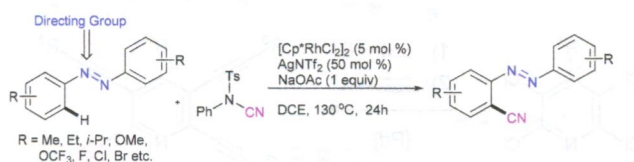


Organocatalysts of oxidative protein folding inspired by protein disulfide isomerase

John C. Lukesh III, Kristen A. Andersen, Kelly K. Wallin and Ronald T. Raines*

Organocatalysts derived from ethylenetriamine and containing a hydrophobic moiety effect the isomerization of non-native protein disulfide bonds to native ones.

8603



Rhodium-catalyzed *ortho*-cyanation of symmetrical azobenzenes with *N*-cyano-*N*-phenyl-*p*-toluenesulfonamide

Jie Han, Changduo Pan, Xuefeng Jia* and Chengjian Zhu*

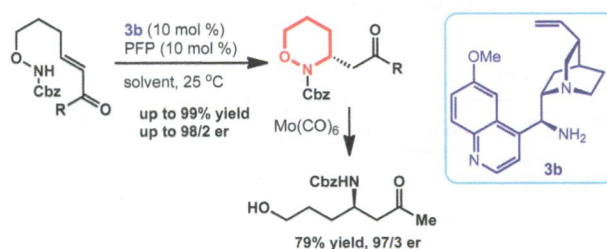
A rhodium(III)-catalyzed *ortho*-cyanation of symmetrical azobenzenes with NCTS via *azo*-group-directed C(sp²)-H bond activation is described.

8607

Enantioselective synthesis of 3-substituted 1,2-oxazinanones via organocatalytic intramolecular aza-Michael addition

Shuanghua Cheng and Shouyun Yu*

A highly enantioselective intramolecular 6-*exo*-trig aza-Michael addition was developed to afford chiral 3-substituted 1,2-oxazinanones in high yields (up to 99% yield) and good enantioselectivities (up to 98/2 er).



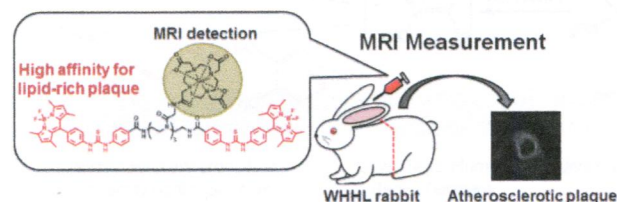
PAPERS

8611

A design strategy for small molecule-based targeted MRI contrast agents: their application for detection of atherosclerotic plaques

S. Iwaki, K. Hokamura, M. Ogawa, Y. Takehara, Y. Muramatsu, T. Yamane, K. Hirabayashi, Y. Morimoto, K. Hagsawa, K. Nakahara, T. Mineno, T. Terai, T. Komatsu, T. Ueno, K. Tamura, Y. Adachi, Y. Hirata, M. Arita, H. Arai, K. Umemura, T. Nagano and K. Hanaoka*

Atherosclerotic plaques were clearly visualized in T_1 -weighted MR images after intravenous injection of **2BDP3Gd** *in vivo*.

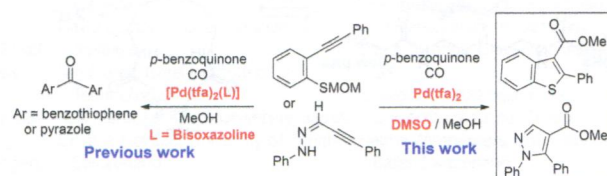


8619

Pd(II)-catalyzed ligand controlled synthesis of pyrazole-4-carboxylates and benzo[*b*]thiophene-3-carboxylates

Yogesh Daulat Dhage, Hiroki Daimon, Cheng Peng, Taichi Kusakabe, Keisuke Takahashi, Yuichiro Kanno, Yoshio Inouye and Keisuke Kato*

A simple change of the ligand and solvent allows controlled, effective switching between cyclization–carbonylation–cyclization–coupling (CCC-coupling) and cyclization–carbonylation reactions.

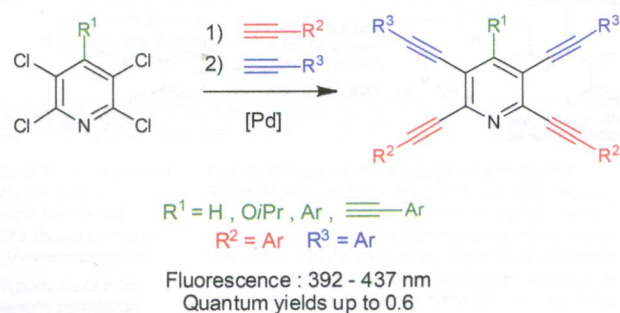


8627

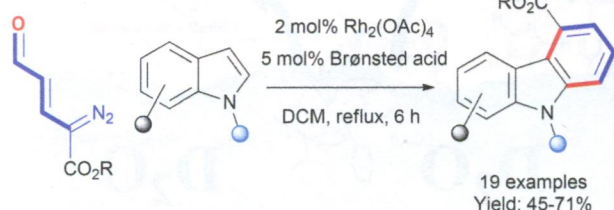
Synthesis of fluorescent 2,3,5,6-tetraalkynylpyridines by site-selective Sonogashira-reactions of 2,3,5,6-tetrachloropyridines

Peter Ehlers, Andranik Petrosyan, Antje Neubauer, Timo Bröse, Stefan Lochbrunner, Taniel V. Ghochikyan, Ashot S. Saghyan and Peter Langer*

4-Substituted 2,3,5,6-tetraalkynylpyridines were prepared by tetra-fold Sonogashira reactions of the corresponding 2,3,5,6-tetrachloropyridines.



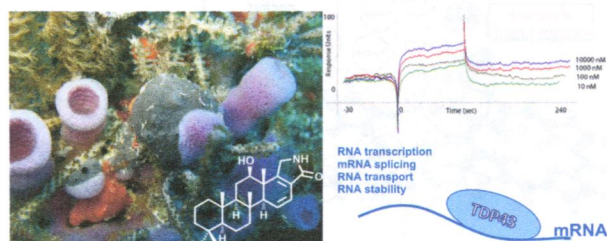
8641

 π -Extension of IndolesRegioselective π -extension of indoles with rhodium enalcarbenoids – synthesis of substituted carbazoles

Kuldeep Singh Rathore, Mandeep Harode and Sreenivas Katukojvala*

An efficient Rh(II) carboxylate and Brønsted acid catalyzed direct π -extension of indoles to 4-substituted carbazoles is developed.

8646

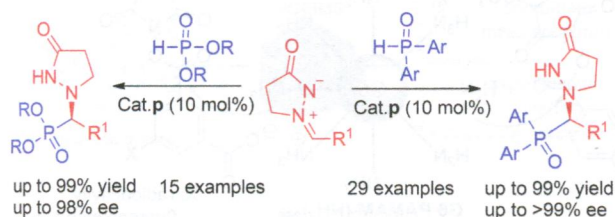


Scalarane sesterterpenes from Thorectidae sponges as inhibitors of TDP-43 nuclear factor

Carmen Festa, Chiara Cassiano, Maria Valeria D'Auria, Cécile Debitus, Maria Chiara Monti and Simona De Marino*

The chemical analysis of two Thorectidae sponges led to the isolation of five new scalarane derivatives along with fifteen known compounds. Their binding capability to TDP-43 was assessed by bio-physical techniques and resulted in the identifications of potent inhibitors.

8656

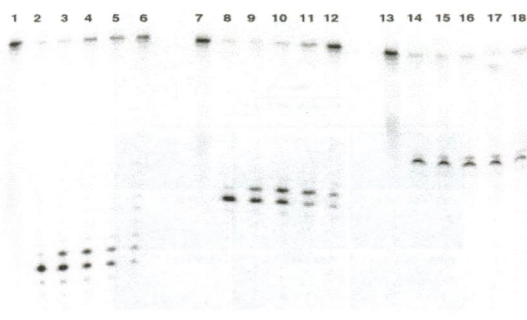


Highly enantioselective phosphination and hydrophosphonylation of azomethine imines: using chiral squaramide as a hydrogen bonding organocatalyst

Ling-Pei Kong, Nai-Kai Li, Shao-Yun Zhang, Xiang Chen, Min Zhao, Ya-Fei Zhang and Xing-Wang Wang*

Highly enantioselective phosphination and hydrophosphonylation reactions of azomethine imines are respectively reported in this paper.

8671



Effects of (5'S)-5',8-cyclo-2'-deoxyadenosine on the base excision repair of oxidatively generated clustered DNA damage. A biochemical and theoretical study

Boleslaw T. Karwowski,* Sophie Bellon, Peter O'Neill, Martine E. Lomax and Jean Cadet

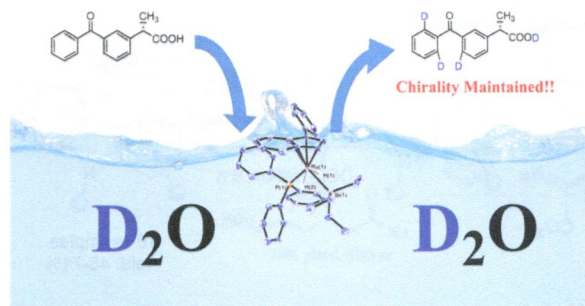
Rejoining of an AP-site in ds-DNA containing the (5'S)-cdA in the complementary strand. Distance between AP-site and (5'S)-cdA, lanes: (1–6) –8 bases; (7–12) no (5'S)-cdA (control); (13–18) +8 bases.

8683

Regioselective ruthenium catalysed H–D exchange using D₂O as the deuterium source

Lorenzo Piola, José A. Fernández-Salas, Simone Manzini and Steven P. Nolan*

An efficient and convenient ruthenium catalysed method for a regioselective H/D exchange using D₂O is described.

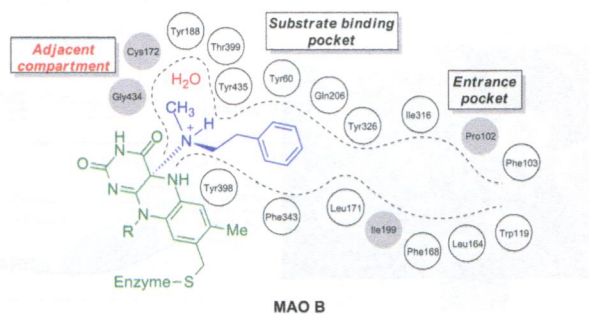


8689

Profiling substrate specificity of two series of phenethylamine analogs at monoamine oxidase A and B

Egon Heuson, Morten Storgaard, Tri H. V. Huynh, Franck Charmantray, Thierry Gefflaut* and Lennart Bunch*

The membrane bound enzyme *monoamine oxidase* exists in two splice variants designated A and B (MAO-A and MAO-B) and are key players in the oxidative metabolism of monoamines in mammals.

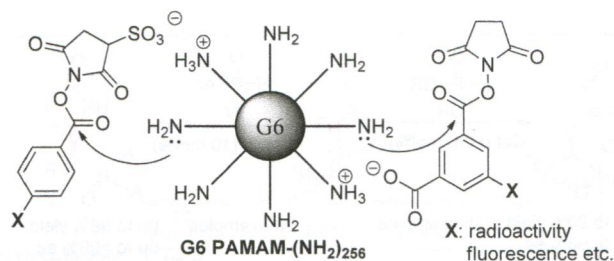


8696

Utilizing electrostatic interactions to facilitate F-18 radiolabeling of poly(amido)amine (PAMAM) dendrimers

Dong Zhou,* Sung Hoon Kim, Vincent M. Carroll, Carmen S. Dence and John A. Katzenellenbogen

Electrostatic interactions facilitate conjugation reactions of cationic poly(amido)amine (PAMAM) dendrimers with anionic NHS reagents.

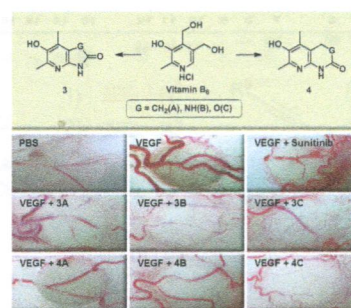


8702

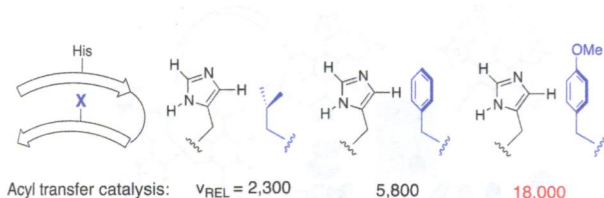
Pyridoxine-derived bicyclic amido-, ureido-, and carbamato-pyridinols: synthesis and antiangiogenic activities

Hyunji Lee, Dong-Guk Kim, Suhrid Banskota, You Kyoung Lee, Tae-gyu Nam,* Jung-Ae Kim* and Byeong-Seon Jeong*

Preparation of a series of five- and six-membered cyclic amide-, urea-, and carbamate-fused bicyclic pyridinols and their inhibitory capacities against VEGF-induced angiogenesis are described.



8711

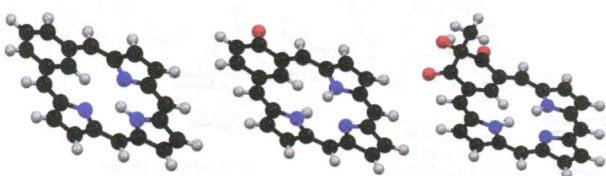


Cross-strand histidine–aromatic interactions enhance acyl-transfer rates in beta-hairpin peptide catalysts

M. Matsumoto, S. J. Lee, M. R. Gagné* and M. L. Waters*

A His–aryl interaction in a beta-hairpin catalyst provides rate enhancements of up to 18 000 for acyl transfer catalysis.

8719

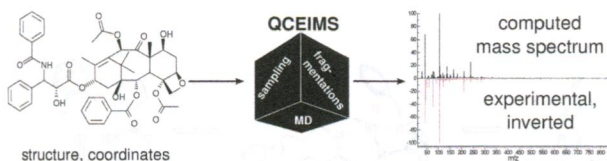


Relative stability of benziporphyrin and naphthiporphyrin tautomers and the emergence of macrocyclic diatropicity

Deyya I. AbuSalim and Timothy D. Lash*

The conformations and relative stabilities of a series of benziporphyrin and naphthiporphyrin tautomers were calculated and the diatropic properties of each of these species were assessed. The results were in good agreement with experimental observations and allow favorable delocalization pathways to be identified.

8737

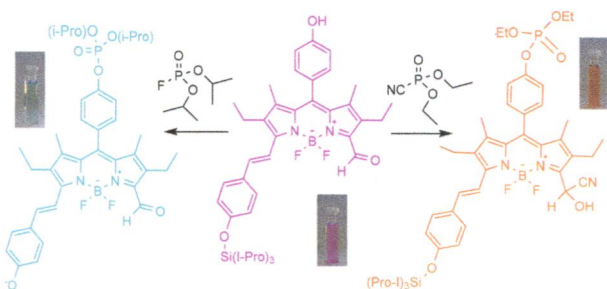


First principles calculation of electron ionization mass spectra for selected organic drug molecules

Christoph Alexander Bauer and Stefan Grimme*

The QCEIMS method provides automated calculation of EI mass spectra and requires only structural information (3D coordinates) as the input.

8745



Selective chromo-fluorogenic detection of DFP (a Sarin and Soman mimic) and DCNP (a Tabun mimic) with a unique probe based on a boron dipyrromethene (BODIPY) dye

Andrea Barba-Bon, Ana M. Costero,* Salvador Gil, Ramón Martínez-Mañez* and Félix Sancenón

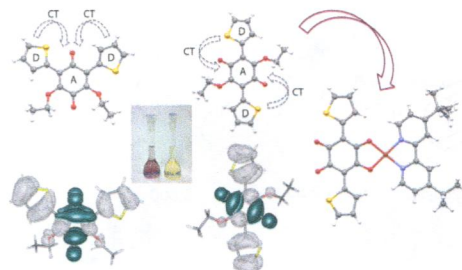
A new naked eye colorimetric BODIPY probe able to discriminate DCNP and DFP nerve agent mimics with good LODs.

8752

Thiophene-benzoquinones: synthesis, crystal structures and preliminary coordination chemistry of derived anilate ligands

Matteo Atzori, Flavia Pop, Thomas Cauchy, Maria Laura Mercuri and Narcis Avarvari*

The Stille coupling strategy allowed the preparation of electron-rich substituted anilate derivatives, which were fully characterized, and their coordination ability was investigated.



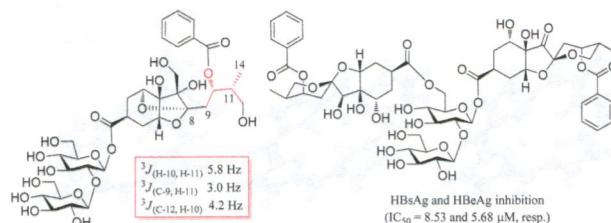
Donor-Acceptor Thiophene-Anilates

8764

Anti-hepatitis B virus activities and absolute configurations of sesquiterpenoid glycosides from *Phyllanthus emblica*

Jun-Jiang Lv, Ya-Feng Wang, Jing-Min Zhang, Shan Yu, Dong Wang, Hong-Tao Zhu, Rong-Rong Cheng, Chong-Ren Yang, Min Xu* and Ying-Jun Zhang*

The sesquiterpenoid glycoside dimers isolated from *Phyllanthus emblica* have anti-HBV activities towards HBsAg and HBeAg secretions inhibition.



8775

Robust asymmetric synthesis of unnatural alkenyl amino acids for conformationally constrained α -helix peptides

Boris Aillard, Naomi S. Robertson, Adam R. Baldwin, Siobhan Robins and Andrew G. Jamieson*

The efficient asymmetric synthesis of unnatural alkenyl amino acids required for peptide 'stapling' has been achieved using alkylation of a fluorine-modified Ni^{II} Schiff

