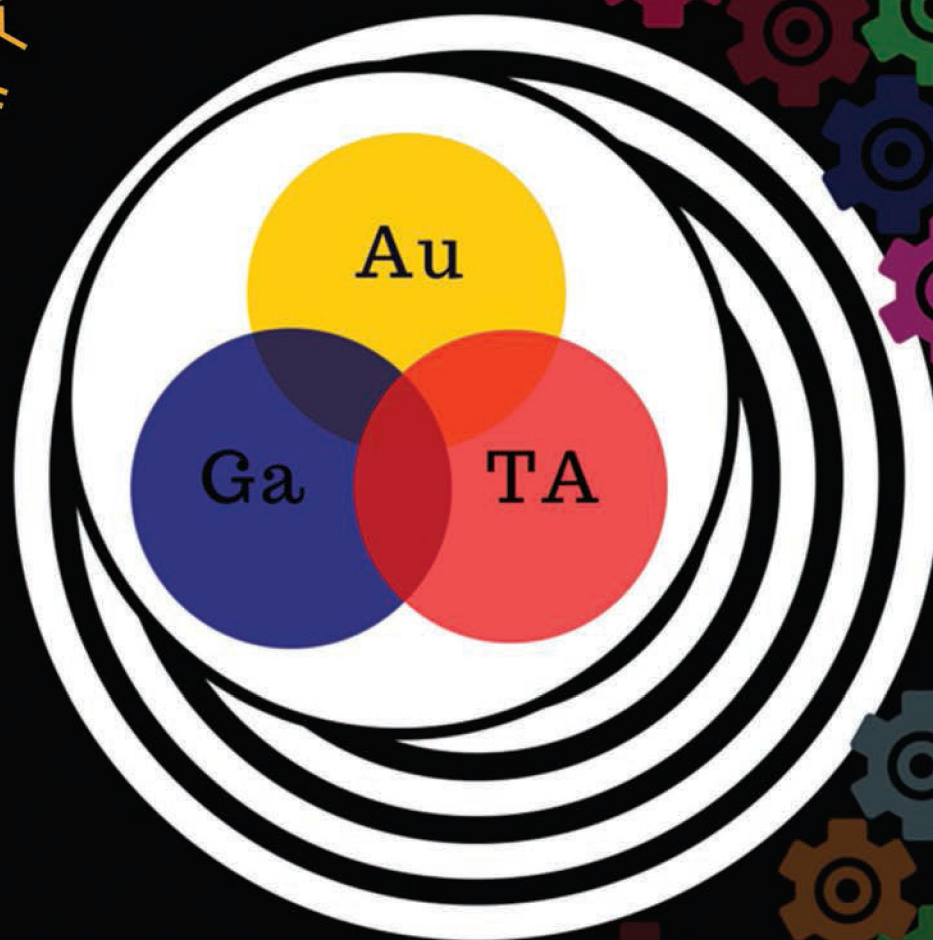


# Organic & Biomolecular Chemistry

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Synergistic Catalysis

ISSN 1477-0520



PAPER

Ayan Datta *et al.*

Mechanistic insights into the synergistic catalysis by Au(I), Ga(III), and counterions in the Nakamura reaction

# Organic & Biomolecular Chemistry

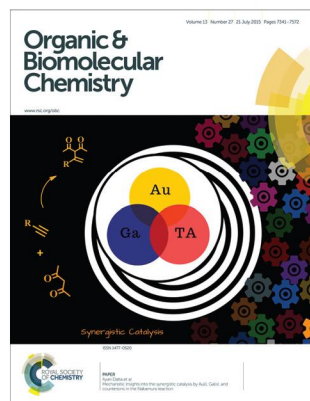
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## IN THIS ISSUE

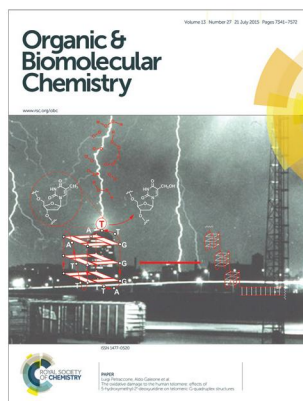
ISSN 1477-0520 CODEN OBCRAK 13(27) 7341–7572 (2015)



### Cover

See Ayan Datta *et al.*, pp. 7412–7420.

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### Inside cover

See Luigi Petraccone, Aldo Galeone *et al.*, pp. 7421–7429.

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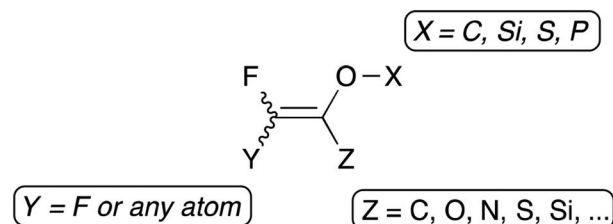
## REVIEW

7351

### Fluorinated enol ethers: their synthesis and reactivity

M. Decostanzi, J.-M. Campagne and E. Leclerc\*

This review sums up the methods for the preparation of fluorinated enol ethers as well as their numerous synthetic applications.



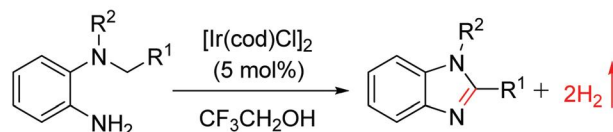
## COMMUNICATIONS

7381

### Synthesis of benzimidazoles *via* iridium-catalyzed acceptorless dehydrogenative coupling

Xiang Sun, Xiao-Hui Lv, Lin-Miao Ye, Yu Hu, Yan-Yan Chen, Xue-Jing Zhang and Ming Yan\*

Benzimidazoles were prepared in good yields *via* the iridium-catalyzed acceptorless dehydrogenative coupling of tertiary amines and arylamines.





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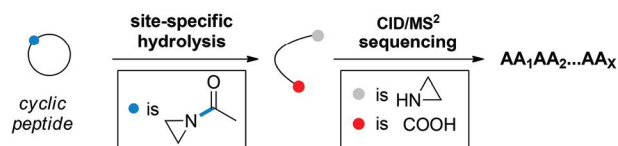
## COMMUNICATIONS

7384

**Twisted amide electrophiles enable cyclic peptide sequencing**

Serge Zaretsky, Vishal Rai, Gerald Gish, Matthew W. Forbes, Michael Kofler, Joy C. Y. Yu, Joanne Tan, Jennifer L. Hickey, Tony Pawson and Andrei K. Yudin\*

Preserving the electrophilic carbonyl group of an aziridine amide in a macrocycle enables cyclic peptide sequencing by chemoselective linearization and tandem mass spectrometry.

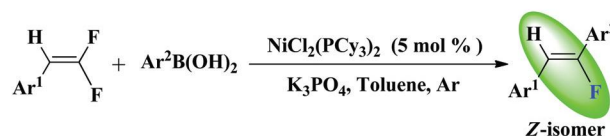


7389

**Nickel-catalyzed Suzuki–Miyaura type cross-coupling reactions of (2,2-difluorovinyl)-benzene derivatives with arylboronic acids**

Yang Xiong, Tao Huang, Xinfei Ji, Jingjing Wu\* and Song Cao\*

An unprecedented highly stereoselective example of nickel-catalyzed Suzuki–Miyaura type cross-coupling reactions of (2,2-difluorovinyl)benzene derivatives with arylboronic acids was developed.

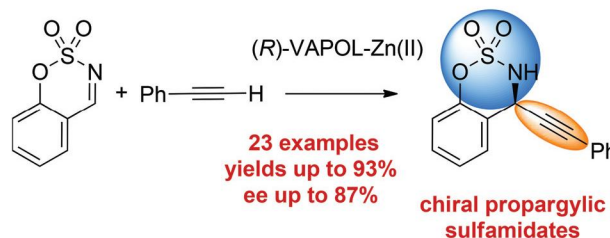


7393

**Enantioselective alkylation of benzo[e][1,2,3]-oxathiazine 2,2-dioxides catalysed by (R)-VAPOL-Zn complexes: synthesis of chiral propargylic cyclic sulfamidates**

Lode De Munck, Alicia Monleón, Carlos Vila, M. Carmen Muñoz and José R. Pedro\*

An enantioselective alkylation of cyclic benzoxathiazine 2,2-dioxides catalysed by (R)-VAPOL-Zn(II) complexes is described.

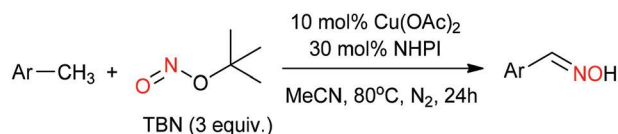


7397

**Copper(II)-promoted direct conversion of methylarenes into aromatic oximes**

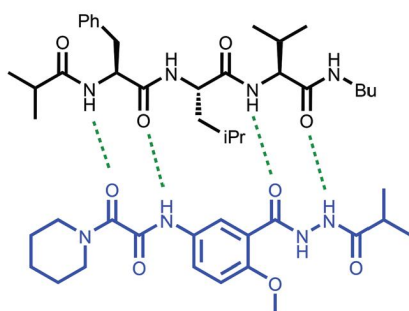
Jiatao Yu and Ming Lu\*

A simple and efficient catalytic system for direct conversion of methylarenes into aromatic oximes has been developed, with Cu(OAc)₂ as catalyst, NHPI (*N*-hydroxyphthalimide) as additive, *tert*-butyl nitrite (TBN) as both the nitrogen source and the oxidant. The process proceeds under mild conditions, tolerates a wide range of substrates, affording the corresponding aromatic oximes in 63–86% yields.



## COMMUNICATIONS

7402

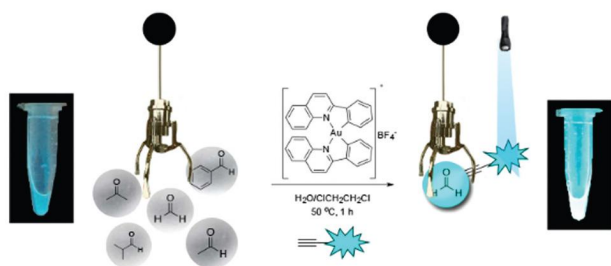


### A model $\beta$ -sheet interaction and thermodynamic analysis of $\beta$ -strand mimetics

Colin W. Robinson, Carl S. Rye, Nicola E. A. Chessum and Keith Jones\*

Two novel  $\beta$ -strand mimetics are synthesized and their binding to a model peptide is studied in detail by  $^1\text{H}$  NMR.

7408



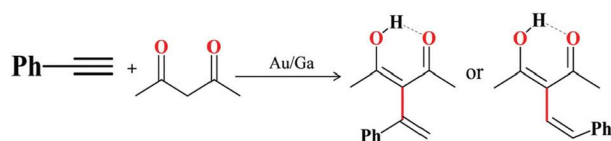
### Visual detection of formaldehyde by highly selective fluorophore labeling *via* gold(III) complex-mediated three-component coupling reaction

Kong-Fan Wong, Jie-Ren Deng, Xiao-Qun Wei, Shi-Ping Shao, Da-Peng Xiang\* and Man-Kin Wong\*

Visual fluorescence detection of formaldehyde by a highly selective gold(III) complex-mediated three component coupling reaction has been described.

## PAPERS

7412



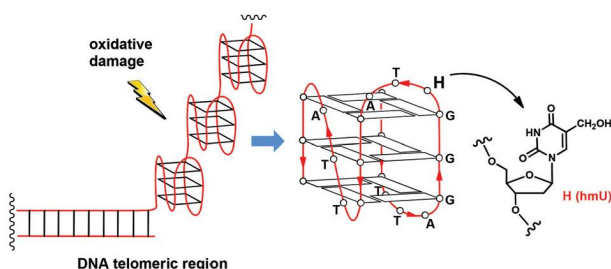
*Au with TA ligand : Low Barrier and High Selectivity*

### Mechanistic insights into the synergistic catalysis by Au(I), Ga(III), and counterions in the Nakamura reaction

Rameswar Bhattacharjee, A. Nijamudheen and Ayan Datta\*

DFT calculations explain the origin of Au/Ga dual catalyzed regioselectivity of Nakamura reactions. The role of the counterions and the triazole ligand is shown to be significant.

7421



### The oxidative damage to the human telomere: effects of 5-hydroxymethyl-2'-deoxyuridine on telomeric G-quadruplex structures

Antonella Virgilio, Veronica Esposito, Luciano Mayol, Concetta Giancola, Luigi Petraccone\* and Aldo Galeone\*

The effects of 5-hydroxymethyl-2'-deoxyuridine on two human telomeric G-quadruplexes have been investigated. Reported results suggest a possible protecting effect of the loop residues on the other parts of the structure.



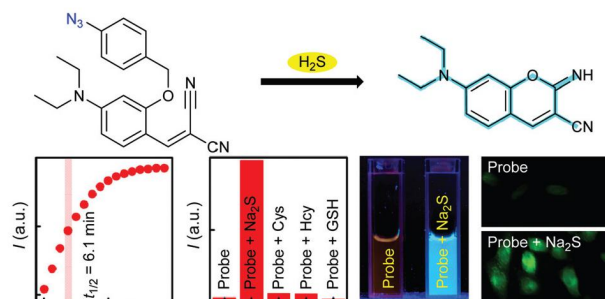
## PAPERS

7430

### Hydrogen sulfide mediated cascade reaction forming an iminocoumarin: applications in fluorescent probe development and live-cell imaging

Pratryush Kumar Mishra, Tanmoy Saha and Pinaki Talukdar\*

The study on a fluorescent probe that undergoes a H<sub>2</sub>S mediated cascade reaction to form an iminocoumarin fluorophore is reported.

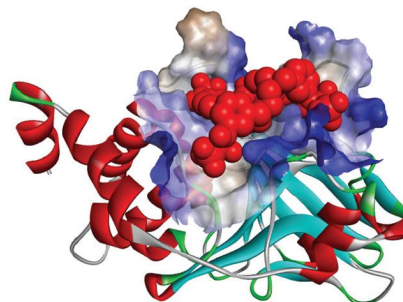


7437

### Phosphonate derivatives of tetraazamacrocycles as new inhibitors of protein tyrosine phosphatases

Oleksandr L. Kobzar, Michael V. Shevchuk, Alesya N. Lyashenko, Vsevolod Yu. Tanchuk, Vadim D. Romanenko, Sergei M. Kobelev, Alexei D. Averin, Irina P. Beletskaya, Andriy I. Vovk\* and Valery P. Kukhar\*

$\alpha,\alpha$ -Difluoro- $\beta$ -ketophosphonate derivatives of tetraazamacrocycles were synthesized and found to be potential inhibitors of protein tyrosine phosphatases.

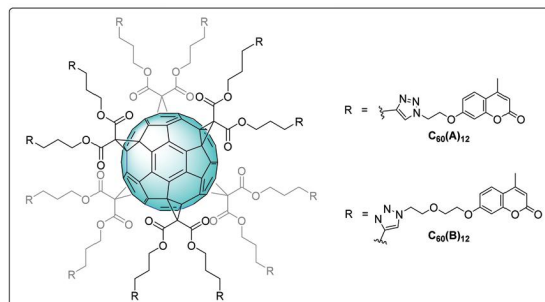


7445

### Exploring carbonic anhydrase inhibition with multimeric coumarins displayed on a fullerene scaffold

Marta Abellán-Flos, Muhammet Tanç, Claudiu T. Supuran\* and Stéphane P. Vincent\*

This study reports the first synthesis of multimeric suicide inhibitors of carbonic anhydrases.

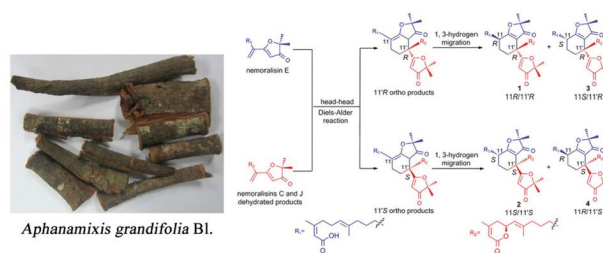


7452

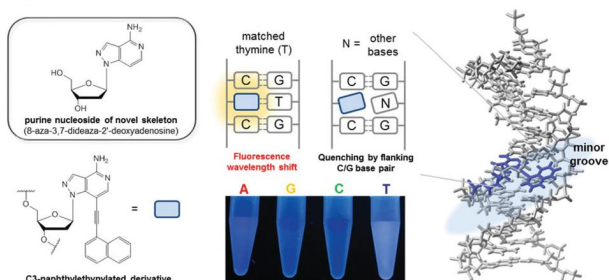
### Anti-inflammatory diterpene dimers from the root barks of *Aphanamixis grandifolia*

Hong-Jian Zhang, Yang-Mei Zhang, Jian-Guang Luo, Jun Luo\* and Ling-Yi Kong\*

14 new diterpene dimers, aphanamenes C–P (**1–14**), were isolated from the root barks of *A. grandifolia* Bl. Their structures were elucidated by spectroscopic analyses and CD exciton chirality method. In addition, all the compounds exhibited significant inhibition of nitric oxide production (IC<sub>50</sub> 7.75–38.23  $\mu$ M).



7459

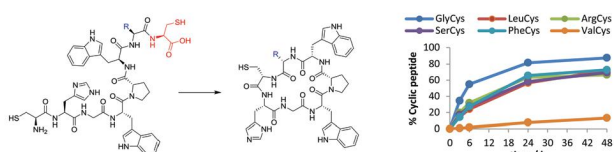


### Synthesis of 8-aza-3,7-dideaza-2'-deoxyadenosines possessing a new adenosine skeleton as an environmentally sensitive fluorescent nucleoside for monitoring the DNA minor groove

Azusa Suzuki, Mio Saito, Ryuzi Katoh and Yoshio Saito\*

Fluorescent ODN probes containing <sup>3n7z</sup>A (**2**) acted as effective reporter probes for homogeneous single nucleotide polymorphism (SNP) typing.

7469

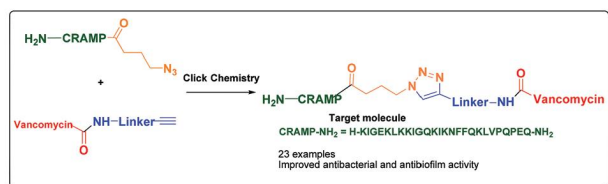


### Expanding the scope of N → S acyl transfer in native peptide sequences

Ben Cowper, Leila Shariff, Wenjie Chen, Samantha M. Gibson, Wei-Li Di and Derek Macmillan\*

A wider variety of Xaa-Cys motifs than originally envisaged were capable of undergoing efficient N → S acyl transfer to form thioesters and cyclic peptides, and our findings are applied to synthesis of wild-type Sunflower Trypsin Inhibitor-1 (SFTI-1).

7477

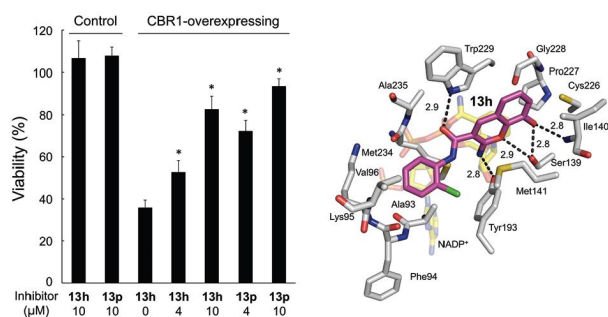


### Evaluation of the antibacterial and antibiofilm activities of novel CRAMP–vancomycin conjugates with diverse linkers

Nigam M. Mishra, Yves Briers, Chris Lamberigts, Hans Steenackers, Stijn Robijns, Bart Landuyt, Jos Vanderleyden, Liliane Schoofs, Rob Lavigne, Walter Luyten and Erik V. Van der Eycken\*

Conjugates of CRAMP (cathelicidin-related antimicrobial peptides) and vancomycin were synthesised using click chemistry with diverse hydrophilic and hydrophobic linkers.

7487



### Synthesis of 8-hydroxy-2-iminochromene derivatives as selective and potent inhibitors of human carbonyl reductase 1

D. Hu, N. Miyagi, Y. Arai, H. Oguri, T. Miura, T. Nishinaka, T. Terada, H. Gouda, O. El-Kabbani, S. Xia, N. Toyooka, A. Hara, T. Matsunaga, A. Ikari and S. Endo\*

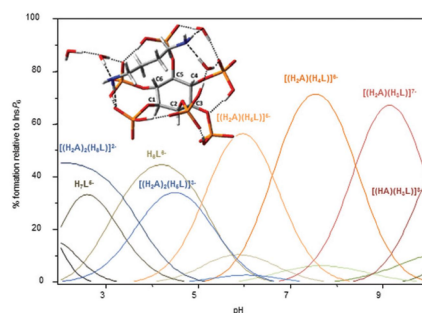
Human carbonyl reductase 1 (CBR1), a member of the short-chain dehydrogenase/reductase superfamily, reduces anthracycline anticancer drugs to their less potent anticancer C-13 hydroxy metabolites, which are linked with pathogenesis of cardiotoxicity, a side effect of the drugs.

7500

### Interaction of *myo*-inositol hexakisphosphate with biogenic and synthetic polyamines

Julia Torres, Claudia Giorgi, Nicolás Veiga, Carlos Kremer\* and Antonio Bianchi\*

*myo*-Inositol hexakisphosphate (phytate) forms very stable adducts with biogenic and synthetic polyamines in aqueous solution.

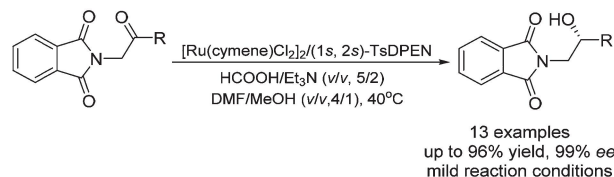


7513

### Highly enantioselective asymmetric transfer hydrogenation (ATH) of $\alpha$ -phthalimide ketones

Zhou Xu,\* Yong Li, Jing Liu, Nan Wu, Ke Li, Songlei Zhu, Rongli Zhang and Yi Liu\*

Optically active amino alcohols are obtained in good yield and excellent ee via an efficient asymmetric transfer hydrogenation (ATH) of  $\alpha$ -phthalimide ketones.

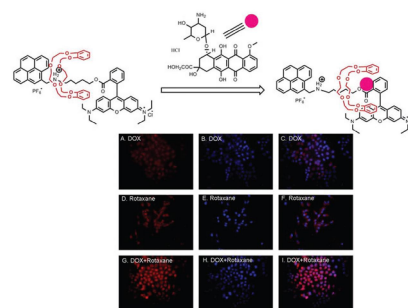


7517

### Synthesis and evaluation of a novel Rhodamine B pyrene [2]rotaxane as an intracellular delivery agent for doxorubicin

Jiaxin Shi, Yuan Xu, Xinlong Wang, Luyong Zhang, Jing Zhu,\* Tao Pang\* and Xiaofeng Bao\*

RhBPy [2]rotaxane has been demonstrated to be an efficient transport agent for delivering the cancer drug doxorubicin (DOX) into tumor cells.

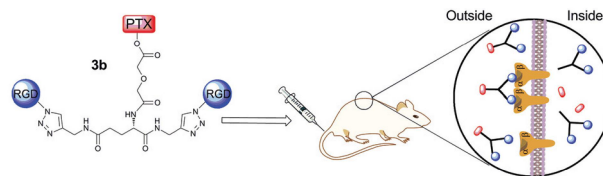


7530

### Design, synthesis and biological evaluation of novel dimeric and tetrameric cRGD–paclitaxel conjugates for integrin-assisted drug delivery

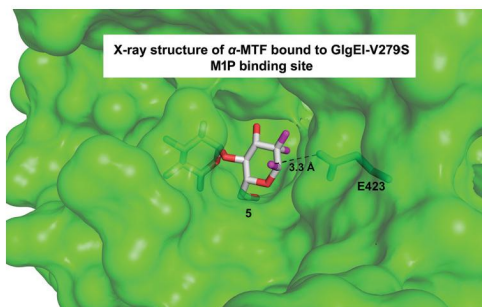
A. Bianchi, D. Arosio, P. Perego, M. De Cesare, N. Carenini, N. Zaffaroni, M. De Matteo and L. Manzoni\*

Novel RGD–PTX multivalent conjugates, presenting enhanced binding for an  $\alpha_v\beta_3$  integrin, have been reported. *In vivo* evaluation of **3b** showed tumor growth inhibition through administering one-third of the PTX dose.





7542

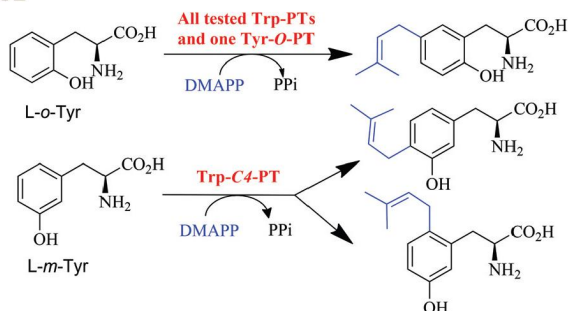


### Synthesis of 2-deoxy-2,2-difluoro- $\alpha$ -maltosyl fluoride and its X-ray structure in complex with *Streptomyces coelicolor* GlgE1-V279S

Sandeep Thanna, Jared J. Lindenberger, Vishwanath V. Gaitonde, Donald R. Ronning\* and Steven J. Sucheck\*

*Mycobacterium tuberculosis* (Mtb) GlgE is a genetically validated TB drug target involved in  $\alpha$ -glucan biosynthesis. The *Streptomyces coelicolor* (Sco) GlgE1-V279S variant described here is used as a model enzyme for structure-based inhibitor design.

7551

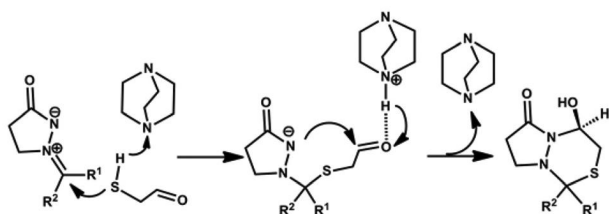


### Tryptophan prenyltransferases showing higher catalytic activities for Friedel–Crafts alkylation of *o*- and *m*-tyrosines than tyrosine prenyltransferases

Aili Fan, Xiulan Xie and Shu-Ming Li\*

Better conversion of L-*o*- and L-*m*-tyrosine to their C-prenylated derivatives by tryptophan prenyltransferases (Trp-PTs) than tyrosine O-prenyltransferases (Tyr-O-PT).

7558



### Theoretical investigations of the reaction between 1,4-dithiane-2,5-diol and azomethine imines: mechanisms and diastereoselectivity

Linjie Zheng, Yan Qiao,\* Mengxue Lu and Junbiao Chang\*

The detailed mechanism of the DABCO-catalyzed reaction between 1,4-dithiane-2,5-diol and azomethine imines.