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### **Contents**

### February 2012

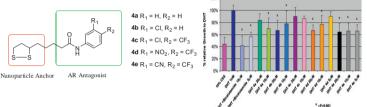
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#### **Preliminary Communications**

### A comparative assessment of $\alpha$ -lipoic acid N-phenylamides as non-steroidal androgen receptor antagonists both on and off gold nanoparticles

pp 1-5

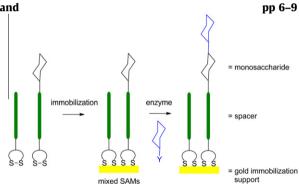
Luke C. Henderson,\* Jarrad M. Altimari, Gail Dyson, Linden Servinis, Birunthi Niranjan and Gail P. Risbridger



Mixed SAMs and MALDI-ToF MS: Preparation of *N*-glycosylamine derivative and thioctic acid methyl ester bearing 1,2-dithiolane groups and detection of enzymatic reaction on Au

Hani Mutlak A. Hassan\* and Beatrice A. Maltman

Herein, we report an enzymatic galactosylation reaction of  $\beta$ -glucopyranosylamide **4** and thioctic acid methyl ester **5** bearing 1,2-dithiolane groups to form a new system of mixed self-assembled monolayers (SAMs) on gold. Characterization of the enzymatic activity was conveniently achieved by mass spectrometry.

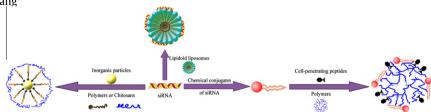


#### **Review Paper**

### Non-viral vectors for the mediation of RNAi

pp 10-18

Shubiao Zhang,\* Yinan Zhao, Defu Zhi and Shufen Zhang\*

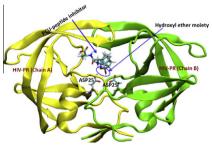


#### **Regular Articles**

### Pentacycloundecane derived hydroxy acid peptides: A new class of irreversible non-scissile ether bridged type isoster as potential HIV-1 wild type C-SA protease inhibitors

pp 19-29

Rajshekhar Karpoormath, Yasien Sayed, Patrick Govender, Thavendran Govender, Hendrik G. Kruger, Mahmoud E.S. Soliman\* and Glenn E.M. Maguire\*



### Synthesis and anti-inflammatory properties of some aromatic and heterocyclic aromatic curcuminoids

pp 30-38

Riyad El-Khatib, M. Akram Khan,\* K.D. Rainsford and M.W. Whitehouse

A variety of aromatic and heterocyclic aromatic curcuminoids were synthesised and characterised for their *in vivo* anti-inflammatory activities. Three curcuminoids were found to have quite potent anti-inflammatory activity compared with natural curcumin.

acetylacetone 
$$\frac{B(OC_4H_9)_3}{Boric \ oxide}$$
  $\frac{B_{ing}}{Boric \ oxide}$   $\frac{H_c}{H_b}$   $\frac{H_c}{H_a}$   $\frac{H_c}{H_b}$ 

1,7-bis(Ring)-1,6-heptadiene-3,5-dione (enol form)

#### Role of histidine 225 in adenosylcobalamin-dependent ornithine 4,5-aminomutase

pp 39-47

Caitlyn Makins, François N. Miros, Nigel S. Scrutton and Kirsten R. Wolthers\*

#### First general methods toward aldehyde enolphosphates

pp 48-56

Nicolas Barthes\* and Claude Grison

# Characterization of covalent Ene adduct intermediates in "hydride equivalent" transfers in a dihydropyridine model for NADH reduction reactions

pp 57-66

R. Daniel Libby\* and Ryan A. Mehl

Characterization of a covalent adduct in a dihydropyridine reduction reaction provides a flexible transition state model that could accommodate a range of mechanistic paths for NADH hydride equivalent transfers.

$$\begin{array}{c|c} & & & \\ & & &$$

# 2,4-Diaryl-5,6-dihydro-1,10-phenanthroline and 2,4-diaryl-5,6-dihydrothieno[2,3-h] quinoline derivatives for topoisomerase I and II inhibitory activity, cytotoxicity, and structure—activity relationship study

pp 67-78

Pritam Thapa, Radha Karki, Han Young Yoo, Pil-Hoon Park, Eunyoung Lee, Kyung-Hwa Jeon, Younghwa Na, Won-Jea Cho, Youngjoo Kwon\* and Eung-Seok Lee\*

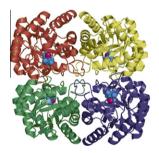
2,4-Diaryl-5,6-dihydro-1,10-phenanthroline and 2,4-diaryl-5,6-dihydrothieno[2,3-h] quinoline derivatives as rigid analogs of 2,4,6-trisubstituted pyridines were prepared, and evaluated for topoisomerase I and II inhibitory activities as well as cytotoxicities against several human cancer cell lines. Structure–activity relationship study showed that [2,2';6',2"]-terpyridine skeleton is important for the cytotoxicity against several human cancer cell lines.

quinoline moiety 
$$\begin{array}{c} R_2 \\ R_1 \text{ and } R_2 = \text{phenyl.} \\ R_1 \\ N \\ \end{array}$$
 quinoline moiety  $\begin{array}{c} R_2 \\ R_2 \\ R_3 \\ \end{array}$   $\begin{array}{c} R_1 \text{ and } R_2 = \text{phenyl.} \\ 2, 3 \text{ or } 4 \text{- pyridyl.} \\ \end{array}$  2, 3 or 4 - pyridyl.

# Structure and characterization of the 3-deoxy-p-arabino-heptulosonate 7-phosphate synthase from $Aeropyrum\ pernix$

pp 79-86

Lily Zhou, Jing Wu, Vijayalakshmi Janakiraman, Igor A. Shumilin, Ronald Bauerle, Robert H. Kretsinger and Ronald W. Woodard\*



A. pernyx DAH7PS
PEP: Cyan Spheres
Mn<sup>2+</sup>: Magenta Sphere

### $Is of or sythia side, \ an \ antioxidant \ and \ antibacterial \ phenylethanoid \ glycoside \ is olated \ from \ For sythia \ suspensa$

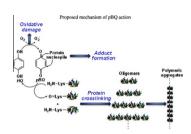
pp 87-91

Huanhuan Qu, Yongmin Zhang, Xiaoyun Chai and Wenji Sun\*

#### Modifications of ribonuclease A induced by p-benzoquinone

Jisook Kim,\* Albert R. Vaughn, Chris Cho, Titus V. Albu and Ethan A. Carver

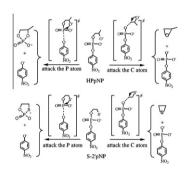
Proposed mechanism of pBQ action.



#### Density functional calculations on the effect of sulfur substitution for 2-hydroxypropyl-pnitrophenyl phosphate: C-O vs. P-O bond cleavage

Futing Xia and Hua Zhu\*

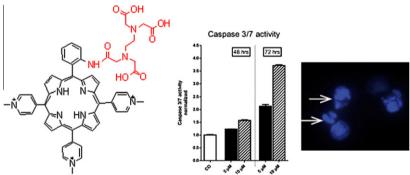
The intra-molecular attack at the phosphorus atom is more accessible for 2'-hydroxypropyl-p-nitrophenyl phosphate (HPpNP), while the intra-molecular attack at the beta carbon atom is more accessible for its analogous compound 2-thiouridyl-p-nitrophenyl phosphate (s-2'pNP).



### A water soluble tri-cationic porphyrin-EDTA conjugate induces apoptosis in human

neuroendocrine tumor cell lines

Gert Schwach, Patchanita Thamyongkit, Lorenz Michael Reith, Bernhard Svejda, Günther Knör, Roswitha Pfragner\* and Wolfgang Schoefberger\*



#### Monoamine oxidase inhibition by C4-substituted phthalonitriles

pp 114-124

pp 108-113

Clarina I. Manley-King, Jacobus J. Bergh and Jacobus P. Petzer\*

$$R = C_6H_5CH_2O - \\ \hline \\ IC_{50} \\ (MAO-B) \\ \hline \\ higher potency \\ \hline \\ R = C_6H_5CH_2O - \\ \hline \\ CN \\ 4 \\ \hline \\ CN \\ 0.785 \ \mu M \\ 6.63 \ \mu M \\ \hline \\ \\ lower potency \\ \hline \\ \hline \\ \\ IOMETRIC PORTON | Potency | Potenc$$

pp 92-98

pp 99-107

# 3-Alkyl- and 3-amido-isothiazoloquinolin-4-ones as ligands for the benzodiazepine site of $\mathsf{GABA}_A$ receptors

pp 125-130

Jakob Nilsson, Elsebet Østergaard Nielsen, Tommy Liljefors, Mogens Nielsen and Olov Sterner\*

### Calreticulin transacetylase: A novel enzyme-mediated protein acetylation by acetoxy derivatives of 3-alkyl-4-methylcoumarins

pp 131-136

Sarah Jalal, Karam Chand, Abha Kathuria, Prabhjot Singh, Nivedita Priya, Bhavna Gupta, Hanumantharao G. Raj and Sunil K. Sharma\*

$$R = n-C_3H_7/n-C_7H_{15}/n-C_9H_{19}$$
  
 $R' = H/OAc$ 

# Synthesis and evaluation of aryl boronic acids as fluorescent artificial receptors for biological carbohydrates

pp 137-142

Sandra Craig

