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# Bioorganic & Medicinal Chemistry

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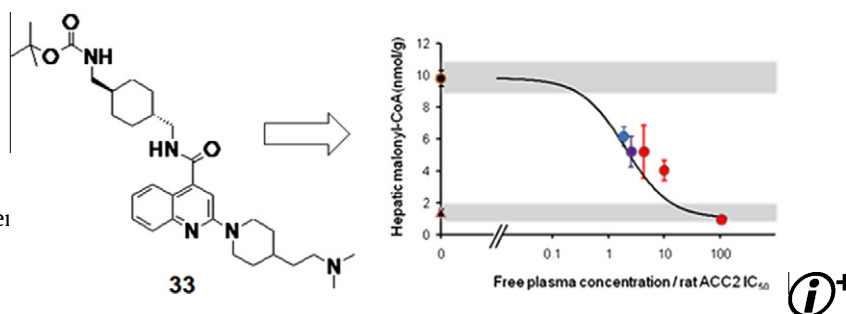
## Bioorganic & Medicinal Chemistry Volume 19, Issue 10, 2011

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#### ARTICLES

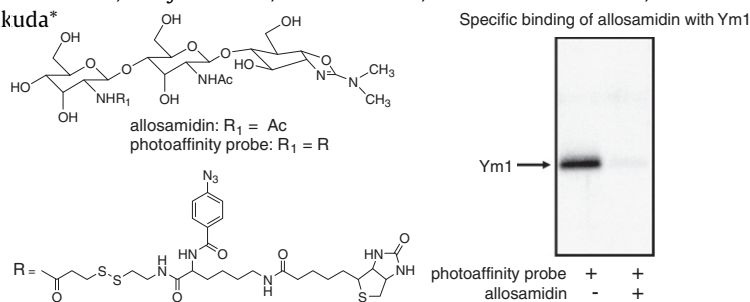
#### Design of small molecule inhibitors of acetyl-CoA carboxylase 1 and 2 showing reduction of hepatic malonyl-CoA levels in vivo in obese Zucker rats pp 3039–3053

Christoffer Bengtsson, Stefan Blaho, David Blomberg Saitton, Kay Brickmann, Johan Broddefalk, Öjvind Davidsson, Tomas Drmota, Rutger Folmer, Kenth Hallberg, Stefan Hallén, Ragnar Hovland, Emre Isin, Petra Johannesson, Bengt Kull, Lars-Olof Larsson, Lars Löfgren, Kristina E. Nilsson, Tobias Noeske, Nick Oakes, Alleyn T. Plowright\*, Volker Schnecke, Pernilla Ståhlberg, Pernilla Sörme, Hong Wan, Eric Wellner, Linda Öster



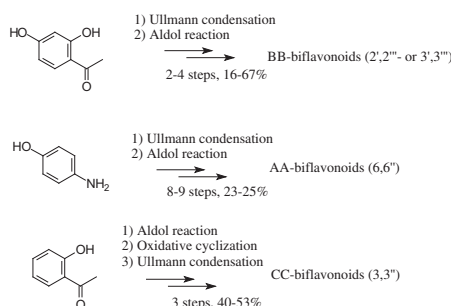
#### Preparation of allosamidin and demethylallosamidin photoaffinity probes and analysis of allosamidin-binding proteins in asthmatic mice pp 3054–3059

Yosuke Sato, Shigeo Suzuki, Seiko Muraoka, Naoya Kikuchi, Naotaka Noda, Takafumi Matsumoto, Hiromasa Inoue\*, Hiromichi Nagasawa, Shohei Sakuda\*



#### Synthesis and antifungal activities of natural and synthetic biflavonoids pp 3060–3073

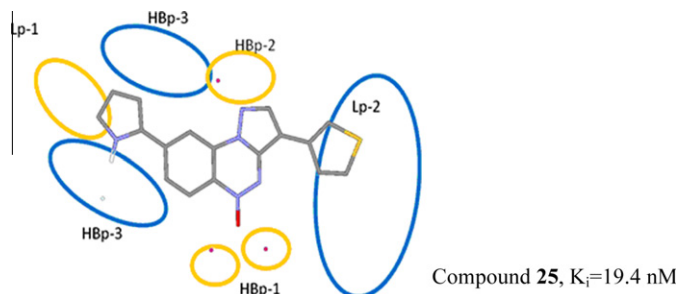
Gabriel Sagrera, Ana Bertucci, Alvaro Vazquez, Gustavo Seoane\*



### New 3-, 8-disubstituted pyrazolo[5,1-c][1,2,4]benzotriazines useful for studying the interaction with the HBp-3 area (hydrogen bond point area) in the benzodiazepine site on the $\gamma$ -aminobutyric acid type A (GABA<sub>A</sub>) receptor

Gabriella Guerrini\*, Giovanna Ciciani, Fabrizio Bruni, Silvia Selleri, Fabrizio Melani, Simona Daniele, Claudia Martini, Annarella Costanzo

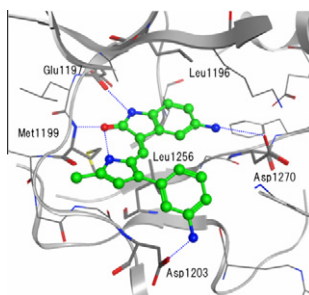
pp 3074–3085



### Virtual screening and further development of novel ALK inhibitors

Masako Okamoto, Hirotatsu Kojima, Nae Saito, Takayoshi Okabe, Yoshiaki Masuda, Toshio Furuya, Tetsuo Nagano\*

pp 3086–3095

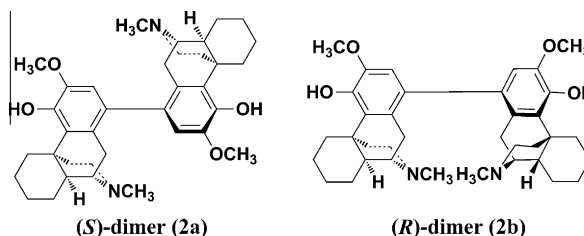


Predicted binding mode of a novel ALK inhibitor: compound **25a**.

### Synthesis and biological evaluation of unique stereodimers of sinomenine analogues as potential inhibitors of NO production

Peng Teng, Hai-Liang Liu, Zhang-Shuang Deng, Zhi-Bing Shi, Yun-Mian He, Li-Li Feng, Qiang Xu, Jian-Xin Li\*

pp 3096–3104



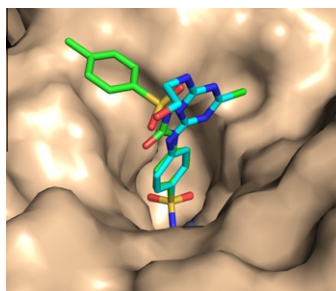
A series of unique stereodimers of sinomenine analogues were synthesized and evaluated on NO production and cytotoxicity. Dimer **2a** and **2b** showed the most potent inhibitory activity on NO production without obvious cytotoxicity and also significantly suppressed mRNA expression of iNOS. Interestingly, (*S*)-dimers displayed a better bioactivity than (*R*)-dimers.



### Sulfonamides incorporating 1,3,5-triazine moieties selectively and potently inhibit carbonic anhydrase transmembrane isoforms IX, XII and XIV over cytosolic isoforms I and II: Solution and X-ray crystallographic studies

Fabrizio Carta, Vladimir Garaj, Alfonso Maresca, Jason Wagner, Balendu Sankara Avvaru, Arthur H. Robbins, Andrea Scozzafava, Robert McKenna\*, Claudiu T. Supuran\*

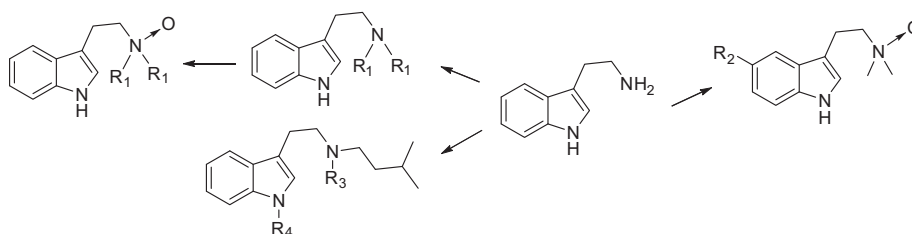
pp 3105–3119



**Tryptamine derivatives as novel non-nucleosidic inhibitors against hepatitis B virus**

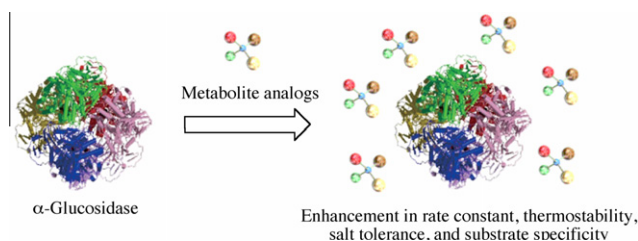
pp 3120–3127

Shi-Jin Qu, Gui-Feng Wang, Wen-Hu Duan, Shan-Yan Yao, Jian-Ping Zuo\*, Chang-Heng Tan\*, Da-Yuan Zhu

**Cellular zwitterionic metabolite analogs simultaneously enhance reaction rate, thermostability, salt tolerance, and substrate specificity of  $\alpha$ -glucosidase**

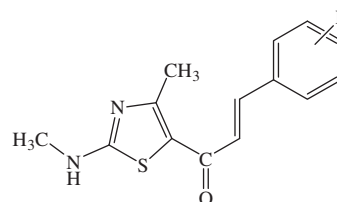
pp 3128–3134

Eisuke Deguchi, Kazuya Koumoto\*

**Thiazole-based chalcones as potent antimicrobial agents. Synthesis and biological evaluation**

pp 3135–3140

K. Liaras, A. Geronikaki\*, J. Glamočlija, A. Ćirić, M. Soković



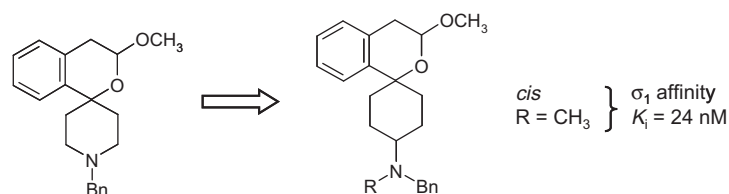
- |                      |              |
|----------------------|--------------|
| 1. H                 | 6. 2-Cl      |
| 2. 4-NO <sub>2</sub> | 7. 4-OMe     |
| 3. 3-NO <sub>2</sub> | 8. 2-OMe     |
| 4. 4-Cl              | 9. 2,6-diCl  |
| 5. 3-Cl              | 10. 2,4-diCl |

A new class of structurally novel thiazole based chalcones were synthesized and evaluated for their antimicrobial and antifungal activity.

**Design, synthesis and pharmacological evaluation of spirocyclic  $\sigma_1$  receptor ligands with exocyclic amino moiety (increased distance 1)**

pp 3141–3151

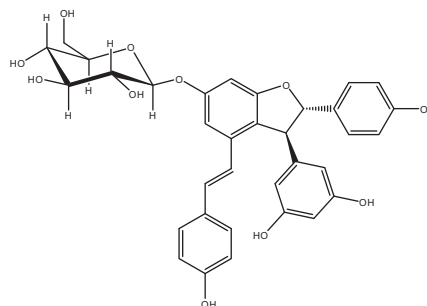
Elisabeth Rack, Roland Fröhlich, Dirk Schepmann, Bernhard Wünsch\*



### Protective effect of $\epsilon$ -viniferin on $\beta$ -amyloid peptide aggregation investigated by electrospray ionization mass spectrometry

pp 3152–3155

Tristan Richard\*, Pascal Poupard, Merian Nassra, Yorgos Papastamoulis, Marie-Laure Igl  sias, St  phanie Krisa, Pierre Waffo-Teguo, Jean-Michel M  rillon, Jean-Pierre Monti

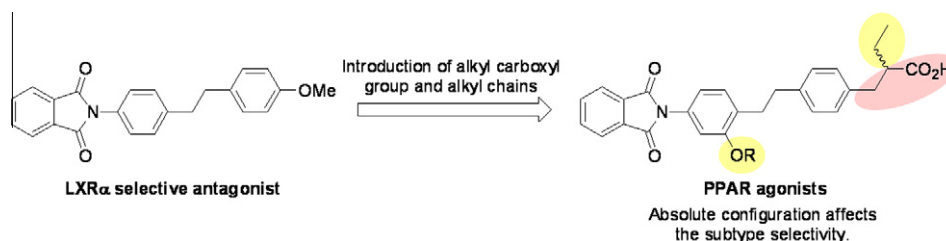


Protective effect mechanism of  $\epsilon$ -viniferin glucoside on  $\beta$ -amyloid peptide aggregation.

### Peroxisome proliferator-activated receptor agonists with phenethylphenylphthalimide skeleton derived from thalidomide-related liver X receptor antagonists: Relationship between absolute configuration and subtype selectivity

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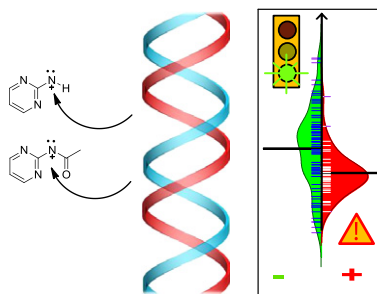
Kazunori Motoshima, Minoru Ishikawa, Yuichi Hashimoto, Kazuyuki Sugita\*



### Avoidance of the Ames test liability for aryl-amines via computation

pp 3173–3182

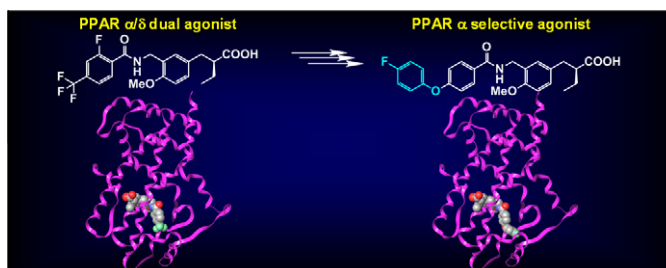
Patrick McCarren, Gregory R. Beberitz, Peter Gedeck, Susanne Glowienke, Melissa S. Grondine, Louise C. Kirman, Jacob Klickstein, Herbert F. Schuster, Lewis Whitehead\*



### Structure-based design, synthesis, and nonalcoholic steatohepatitis (NASH)-preventive effect of phenylpropanoic acid peroxisome proliferator-activated receptor (PPAR) $\alpha$ -selective agonists

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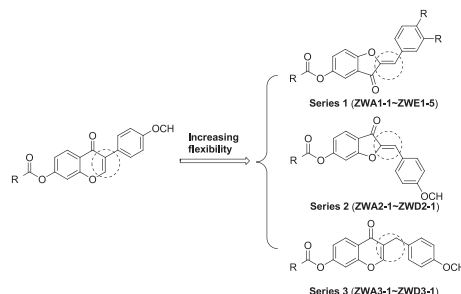
Shintaro Ban, Jun-ichi Kasuga, Izumi Nakagome, Hiromi Nobusada, Fusako Takayama, Shuichi Hirono, Hiromu Kawasaki, Yuichi Hashimoto, Hiroyuki Miyachi\*



### Synthesis and biological evaluation of new flavonoid fatty acid esters with anti-adipogenic and enhancing glucose consumption activities

pp 3192–3203

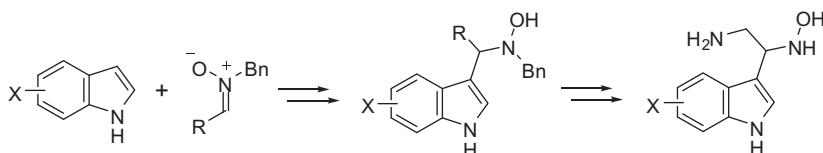
Wei Zhao, Jie Sun, Hua Xiang\*, Yan-yan Zeng, Xiao-bo Li, Hong Xiao, De-ying Chen, Ren-ling Ma



### Synthesis and evaluation of 1-(1*H*-indol-3-yl)ethanamine derivatives as new antibacterial agents

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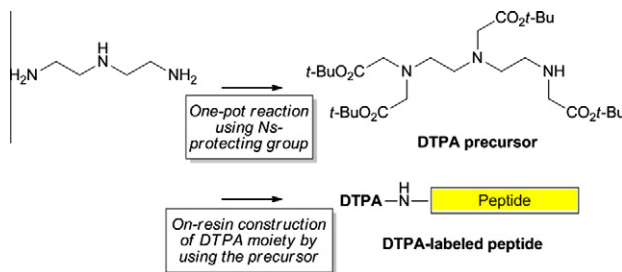
Olga N. Burchak\*, Emmanuelle Le Pihive, Laure Maigre, Xavier Guinchard, Pascale Bouhours, Claude Jolival, Dominique Schneider, Max Maurin, Carmela Giglione, Thierry Meinel, Jean-Marc Paris, Jean-Noël Denis\*



### Concise site-specific synthesis of DTPA–peptide conjugates: Application to imaging probes for the chemokine receptor CXCR4

pp 3216–3220

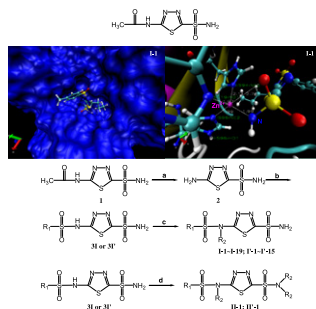
Ryo Masuda, Shinya Oishi\*, Hiroaki Ohno, Hiroyuki Kimura, Hideo Saji, Nobutaka Fujii\*



### Synthesis and evaluation of new carbonic anhydrase inhibitors

pp 3221–3228

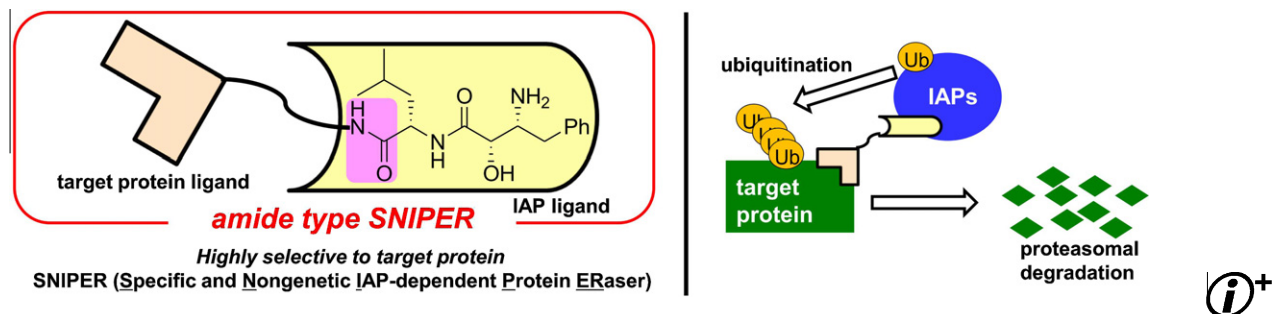
Zhonghai Xiao, Ruifeng Duan, Wenyu Cui, Yanfang Zhang, Shouguo Zhang, Fangjin Chen, Yankun Zhang, Jiaying Liu, Dongxiang Zhang, Yuan Meng, Lin Wang\*, Hai Wang\*



### Development of target protein-selective degradation inducer for protein knockdown

pp 3229–3241

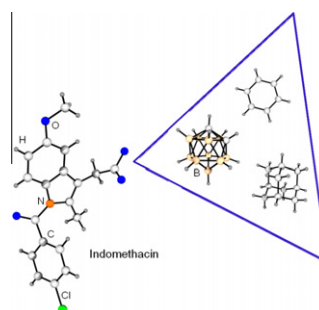
Yukihiro Itoh, Minoru Ishikawa, Risa Kitaguchi, Shinichi Sato, Mikihiro Naito, Yuichi Hashimoto\*



### Synthesis and evaluation of carbaborane derivatives of indomethacin as cyclooxygenase inhibitors

pp 3242–3248

Matthias Scholz, Anna L. Blobaum, Lawrence J. Marnett, Evamarie Hey-Hawkins\*

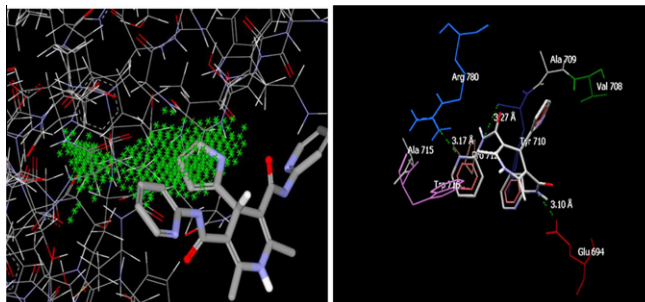


A series of carbaborane esters of indomethacin was constructed and the selectivity of cyclooxygenase inhibition was evaluated. *ortho*-Carbaborane gave the most active inhibitor, whereas the *meta*-carbaborane derivative was, similar to the adamantyl ester, less active.

### Molecular docking studies and in vitro screening of new dihydropyridine derivatives as human MRP1 inhibitors

pp 3249–3254

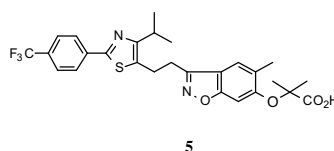
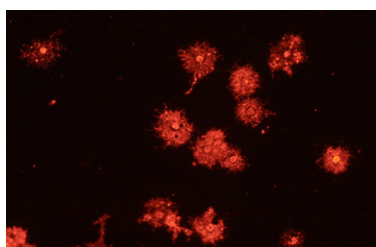
Kalam Sirisha, Maddela Chandra Shekhar, Kulandaivelu Umasankar, Porika Mahendar, Abbagani Sadanandam, Garlapati Achaiah\*, Vanga Malla Reddy\*



### Biological evaluation of novel benzisoxazole derivatives as PPAR $\delta$ agonists

pp 3255–3264

Shogo Sakuma\*, Tsuyoshi Endo, Takashi Kanda, Hideki Nakamura, Satomi Yamasaki, Tomio Yamakawa



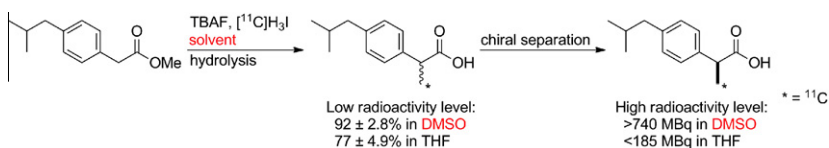
Oligodendrocyte differentiation-stimulating effect of compound 5.



### Efficient synthesis and chiral separation of $^{11}\text{C}$ -labeled ibuprofen assisted by DMSO for imaging of in vivo behavior of the individual isomers by positron emission tomography

pp 3265–3273

Tatsuya Kikuchi, Maki Okada, Nobuki Nengaki, Kenji Furutsuka, Hidekatsu Wakizaka, Toshimitsu Okamura, Ming-Rong Zhang, Koichi Kato\*



### Design, synthesis and inhibition activity of a novel cyclic enediynes amino acid conjugates against MPTpA

pp 3274–3279

Koushik Chandra, Debajyoti Dutta, Analava Mitra, Amit K. Das\*, Amit Basak\*

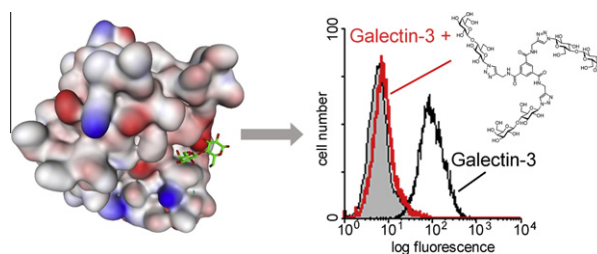
| Compound | Mode of inhibition | $\text{IC}_{50}(\mu\text{M})$ | $K_i(\mu\text{M})$ |
|----------|--------------------|-------------------------------|--------------------|
| 1        | Non-competitive    | $110.2 \pm 10.5$              | $22.5 \pm 1.2$     |
| 2        | Non-competitive    | $235.6 \pm 12.4$              | $101.4 \pm 10.8$   |



### Inhibitory potential of chemical substitutions at bioinspired sites of $\beta$ -D-galactopyranose on neoglycoprotein/cell surface binding of two classes of medically relevant lectins

pp 3280–3287

Denis Giguère, Sabine André, Marc-André Bonin, Marc-André Bellefleur, Alexandre Provencal, Philippe Cloutier, Bernard Pucci, René Roy\*, Hans-Joachim Gabius\*



\*Corresponding author

Supplementary data available via ScienceDirect

**COVER**

The known veterinary anthelmintic and proton ionophore, closantel, was recently discovered to also exhibit potent chitinase inhibition activity and inhibit molting in the parasitic nematode, *Onchocerca volvulus*, the causative agent of the neglected tropical disease onchocerciasis. [C. Gloeckner, A. L. Garner, F. Mersha, Y. Oksov, N. Tricoche, L. M. Eubanks, S. Lustigman, G. F. Kaufmann, K. D. Janda, Repositioning of an existing drug for the neglected tropical disease Onchocerciasis, *Proc. Natl. Acad. Sci., U.S.A.* **2010**, 107, 3424.]

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