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# Bioorganic & Medicinal Chemistry

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## Bioorganic & Medicinal Chemistry Volume 20, Issue 4, 2012

### Contents

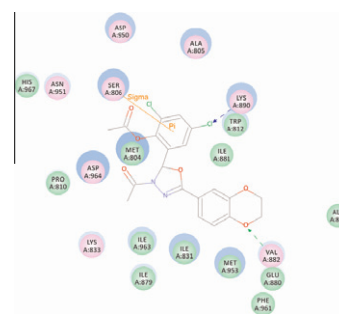
#### ARTICLES

#### Synthesis, molecular docking and biological evaluation of 1,3,4-oxadiazole derivatives as potential immunosuppressive agents

pp 1373–1379

Ru Yan, Zhi-Ming Zhang, Xian-Ying Fang, Yang Hu, Hai-Liang Zhu\*

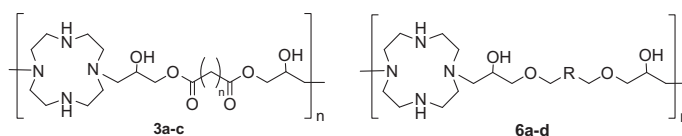
A series of novel 1,3,4-oxadiazole derivatives (**5a–5s**) have been designed, synthesized and evaluated for their immunosuppressive activity. Most of these synthesized compounds were proved to have potent immunosuppressive activity and low toxicity. Among them, compounds (**5m–5r**) showed the most potent biological activity against lymph node cells. The results of flow cytometry (FCM) and western blotting demonstrated that compound **5q** induce cell apoptosis by the inhibition of PI3 K/AKT pathway. Molecular docking was performed to position compound **5q** into PI3 K binding site in order to explore the potential target.



#### Biodegradable cyclen-based linear and cross-linked polymers as non-viral gene vectors

pp 1380–1387

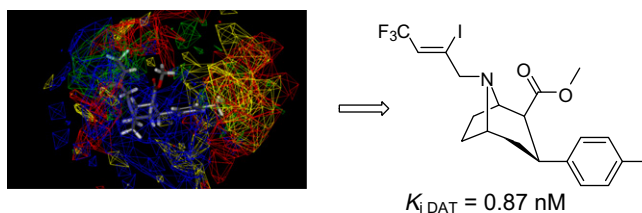
Shuo Li, Yu Wang, Shan Wang, Ji Zhang\*, Shi-Fei Wu, Bo-Lin Wang, Wen Zhu\*, Xiao-Qi Yu\*



#### QSAR study and synthesis of new phenyltropanes as ligands of the dopamine transporter (DAT)

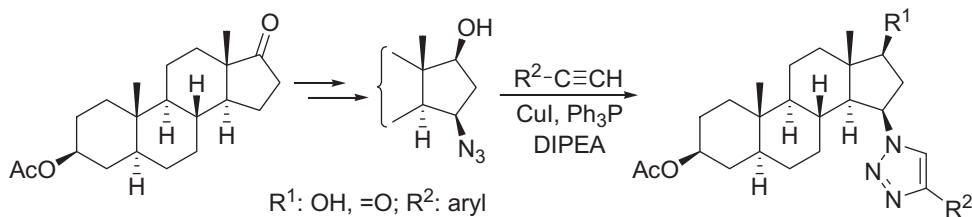
pp 1388–1395

Sylvie Mavel\*, Zoya Mincheva, Nathalie Méheux, Yvan Carcenac, Denis Guilloteau, Mohamed Abarbri, Patrick Emond



## A facile ‘click’ approach to novel 15 $\beta$ -triazolyl-5 $\alpha$ -androstane derivatives, and an evaluation of their antiproliferative activities in vitro pp 1396–1402

Zalán Kádár, Judit Molnár, Gyula Schneider, István Zupkó\*, Éva Frank\*



## Cloning, characterization and sulfonamide inhibition studies of an $\alpha$ -carbonic anhydrase from the living fossil sponge *Astrosclera willeyana* pp 1403–1410

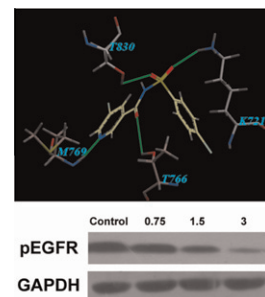
Anna Ohradanova, Daniela Vullo, Silvia Pastorekova, Jaromir Pastorek, Daniel J. Jackson, Gert Wörheide, Claudiu T. Supuran\*



Astrosclerin:  $k_{\text{cat}} = 0.9 \times 10^6 \text{ s}^{-1}$  and  $k_{\text{cat}}/K_m = 1.1 \times 10^8 \text{ M}^{-1} \times \text{s}^{-1}$ ,  $K_i(\text{acetazolamide}) = 51 \text{ nM}$ .

## Design, synthesis and biological evaluation of *N*-phenylsulfonylnicotinamide derivatives as novel antitumor inhibitors pp 1411–1416

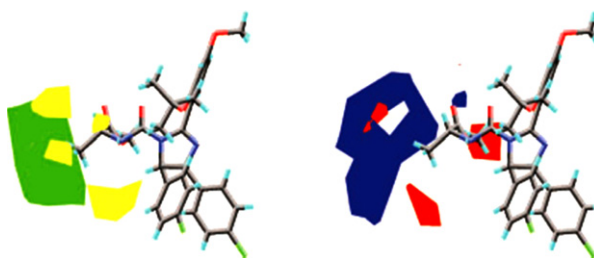
Hui Zhang, Xiang Lu, Li-Rong Zhang, Jia-Jia Liu, Xian-Hui Yang, Xiao-Ming Wang\*, Hai-Liang Zhu\*



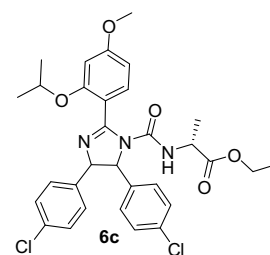
A series of novel *N*-phenylsulfonylnicotinamide derivatives (1–24) have been synthesized and evaluated as potential EGFR tyrosine kinase (TK) inhibitors. Among all the compounds, compound **10** (5-bromo-*N*-(4-chlorophenylsulfonyl)nicotinamide) showed the most potent growth inhibitory activity against EGFR TK and antiproliferative activity of MCF-7 cancer cell line in vitro, with  $\text{IC}_{50}$  value of 0.09 and 0.07  $\mu\text{M}$ . Docking simulation was performed to insert compound **10** into the EGFR TK active site to determine the probable binding model.

## Design, synthesis and CoMFA studies of *N*1-amino acid substituted 2,4,5-triphenyl imidazoline derivatives as p53–MDM2 binding inhibitors pp 1417–1424

Chunqi Hu, Xiaoxue Dou, Yizhe Wu, Lei Zhang, Yongzhou Hu\*



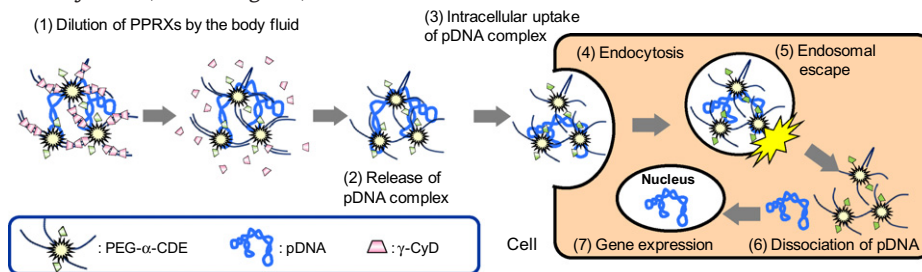
Twenty-three novel *N*1-amino-acid substituted 2,4,5-triphenyl imidazoline derivatives were designed and synthesized as p53–MDM2 binding inhibitors. And statistically significant CoMFA model with high predict abilities was established.



### Polypseudorotaxanes of pegylated $\alpha$ -cyclodextrin/polyamidoamine dendrimer conjugate with cyclodextrins as a sustained release system for DNA

pp 1425–1433

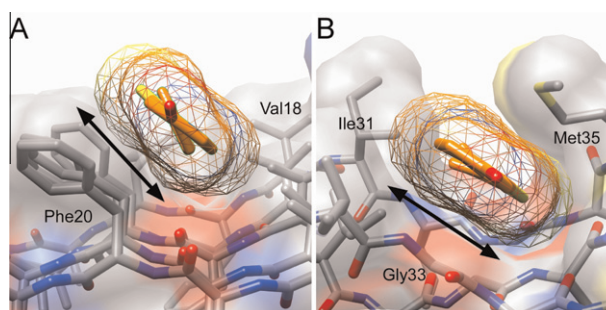
Keiichi Motoyama, Kayoko Hayashida, Taishi Higashi, Hidetoshi Arima\*

Proposed scheme for gene transfer mechanism of PEG- $\alpha$ -CDE/ $\gamma$ -CyD PPRX suspension after intramuscular injection to mice.

### QSAR studies for prediction of cross- $\beta$ sheet aggregate binding affinity and selectivity

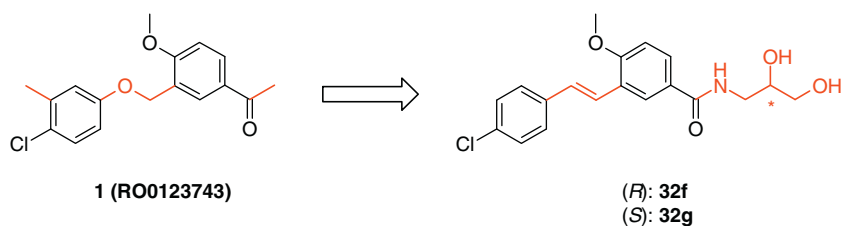
pp 1434–1441

Katryna Cisek, Jeff Kuret\*



### Angiogenesis inhibitors identified by cell-based high-throughput screening: Synthesis, structure–activity relationships and biological evaluation of 3-[(*E*)-styryl]benzamides that specifically inhibit endothelial cell proliferation

Kihito Hada\*, Atsushi Suda, Kohsuke Asoh, Takuo Tsukuda, Masami Hasegawa, Yasuko Sato, Kotaro Ogawa, Shino Kuramoto, Yuko Aoki, Nobuo Shimma, Tsutomu Ishikawa, Hiroshi Koyano



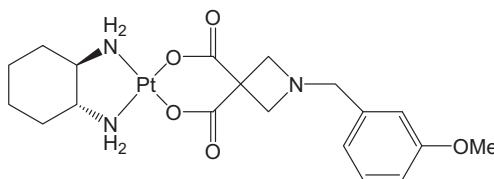
Orally available, in vivo active angiogenesis inhibitors which specifically inhibit endothelial cell proliferation are reported.



### In vitro biological evaluation of platinum(II) complexes with 1-(methoxy substituted benzyl) azetidine-3,3-dicarboxylato ligands

pp 1461–1467

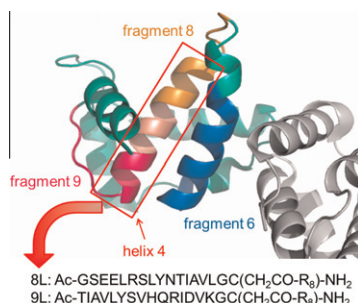
Runting Yin, Shaohua Gou\*, Yanyan Sun, Xia Liu



### Conjugation of cell-penetrating peptides leads to identification of anti-HIV peptides from matrix proteins

pp 1468–1474

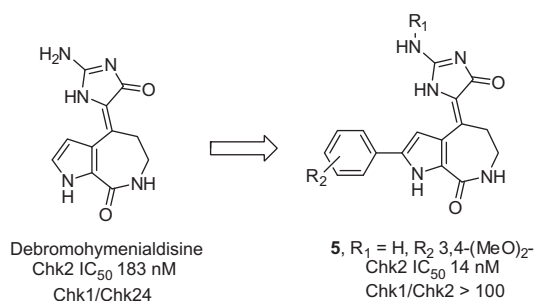
Tetsuo Narumi, Mao Komoriya, Chie Hashimoto, Honggui Wu, Wataru Nomura, Shintaro Suzuki, Tomohiro Tanaka, Joe Chiba, Naoki Yamamoto, Tsutomu Murakami\*, Hirokazu Tamamura\*



### Synthesis and evaluation of debromohymenialdisine-derived Chk2 inhibitors

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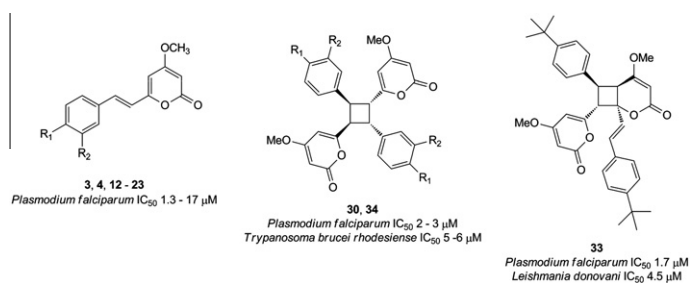
Rahman Shah Zaib Saleem, Theresa A. Lansdell, Jetze J. Tepe\*



### Synthesis and antimalarial and antituberculosis activities of a series of natural and unnatural 4-methoxy-6-styryl-pyran-2-ones, dihydro analogues and photo-dimers

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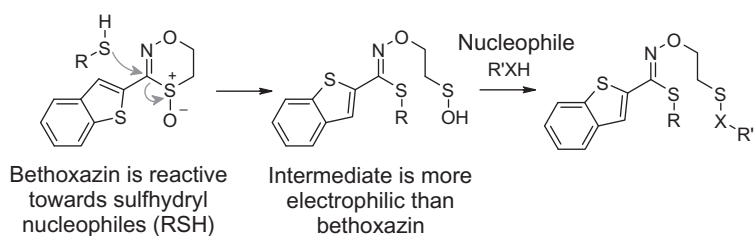
Stephen T. McCracken, Marcel Kaiser, Helena I. Boshoff, Peter D. W. Boyd, Brent R. Copp\*



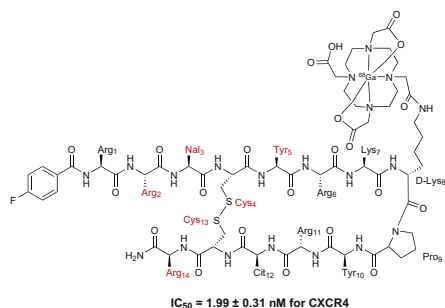
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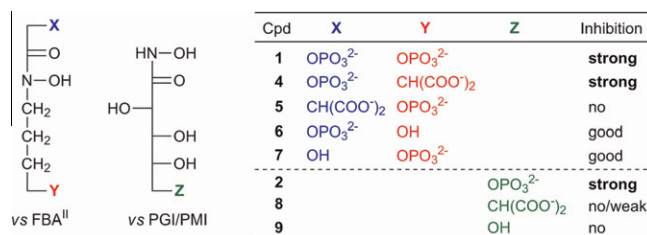
Gaik-Lean Chee\*, Bharat Bhattarai, R. Daniel Gietz, Samaa Alrushaid, John L. Nitiss, Brian B. Hasinoff



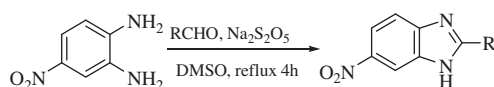
Ute Hennrich\*, Lisa Seyler, Martin Schäfer, Ulrike Bauder-Wüst, Michael Eisenhut, Wolfhard Semmler, Tobias Bäuerle



Stéphanie Desvergues, Stéphanie Courtiol-Legourd, Racha Daher, Maciej Dabrowski, Laurent Salmon\*, Michel Therisod\*

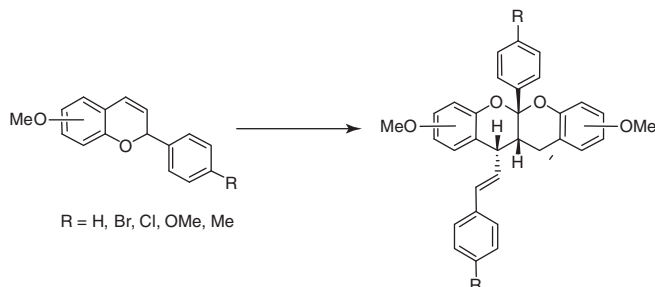


K. M. Khan\*, Zarbad Shah, V. U. Ahmad, N. Ambreen, M. Khan, M. Taha, F. Rahim, S. Noreen, S. Perveen, M. I. Choudhary, W. Voelter



Synthesis of 6-nitrobenzimidazole derivatives **1–30** showed excellent phosphodiesterase inhibitory activities some of which are superior to the standard EDTA and thus are potential molecules for the development of a new class of phosphodiesterase inhibitors. A structure–activity relationship is evaluated.

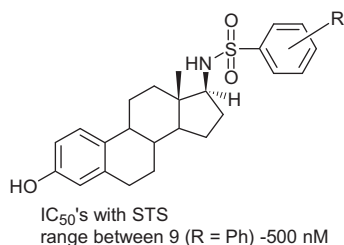
Ruth Devakaram, David StC. Black, Vanida Choomuenwai, Rohan A. Davis, Naresh Kumar\*



### 17 $\beta$ -Arylsulfonamides of 17 $\beta$ -aminoestra-1,3,5(10)-trien-3-ol as highly potent inhibitors of steroid sulfatase

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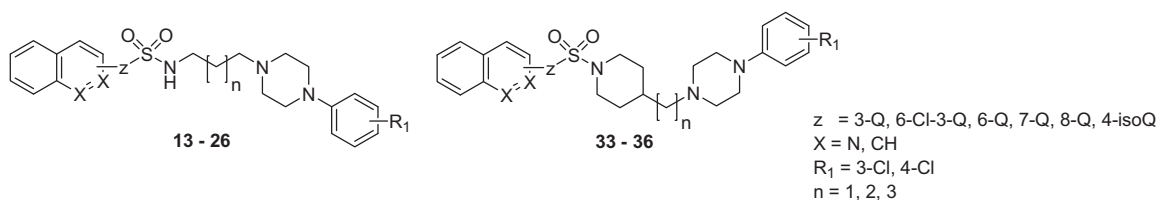
Yaser A. Mostafa, Scott D. Taylor\*



### Quinoline- and isoquinoline-sulfonamide derivatives of LCAP as potent CNS multi-receptor—5-HT<sub>1A</sub>/5-HT<sub>2A</sub>/5-HT<sub>7</sub> and D<sub>2</sub>/D<sub>3</sub>/D<sub>4</sub>—agents: The synthesis and pharmacological evaluation

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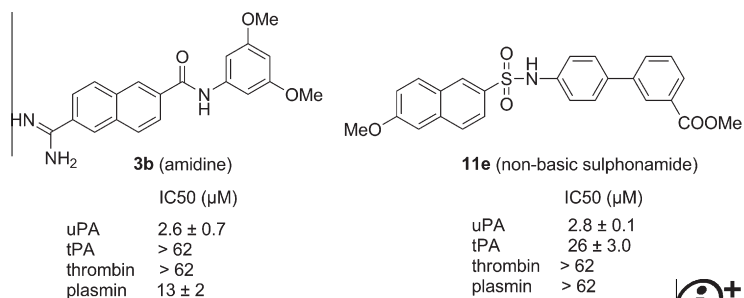
Paweł Zajdel\*, Krzysztof Marciniak, Andrzej Maślankiewicz, Grzegorz Satała, Beata Duszyńska, Andrzej J. Bojarski, Anna Partyka, Magdalena Jastrzębska-Wiesek, Dagmara Wróbel, Anna Wesołowska, Maciej Pawłowski



### Synthesis and evaluation of non-basic inhibitors of urokinase-type plasminogen activator (uPA)

pp 1557–1568

Muthusamy Venkatraj, Jonas Messagie, Jurgen Joossens, Anne-Marie Lambeir, Achiel Haemers, Pieter Van der Veken, Koen Augustyns\*



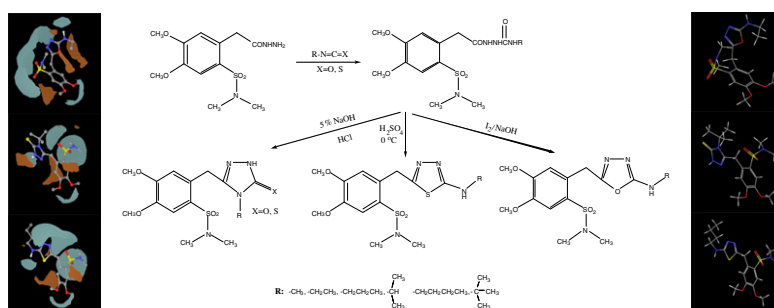
A series of non-basic naphthamides and naphthalene sulfonamides were synthesized and evaluated for uPA inhibition. Several non-basic compounds showed comparable uPA inhibition and selectivity with reference amidines.



## Synthesis of novel sulfonamide-1,2,4-triazoles, 1,3,4-thiadiazoles and 1,3,4-oxadiazoles, as potential antibacterial and antifungal agents. Biological evaluation and conformational analysis studies

pp 1569–1583

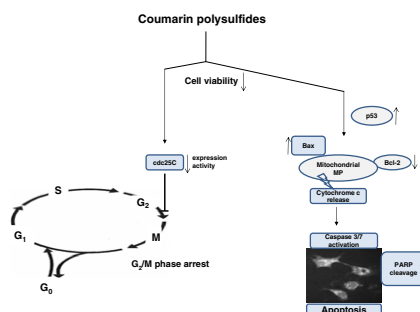
P. Zoumpoulakis\*, Ch. Camoutsis, G. Pairas, M. Soković, J. Glamočlija, C. Potamitis, A. Pitsas



**Coumarin polysulfides inhibit cell growth and induce apoptosis in HCT116 colon cancer cells**

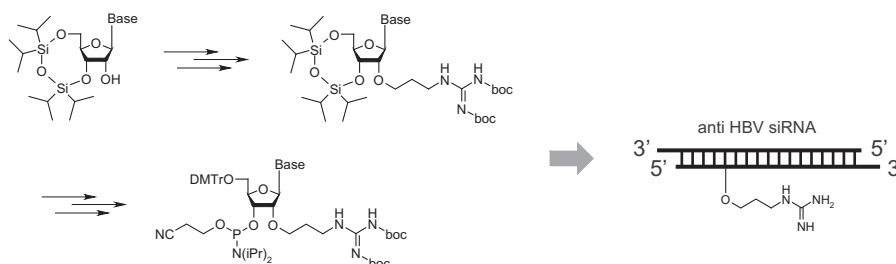
pp 1584–1593

Nathaniel Edward Bennett Saidu, Sergio Valente, Emilie Bana, Gilbert Kirsch, Denyse Bagrel, Mathias Montenarh\*

**Synthesis of 2'-O-guanidinopropyl-modified nucleoside phosphoramidites and their incorporation into siRNAs targeting hepatitis B virus**

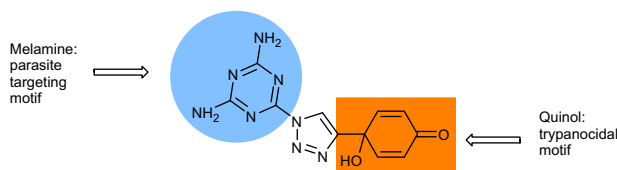
pp 1594–1606

Jolanta Brzezinska, Jennifer D'Onofrio, Maximilian C. R. Buff, Justin Hean, Abdullah Ely, Musa Marimani, Patrick Arbuthnot, Joachim W. Engels\*

**Quinol derivatives as potential trypanocidal agents**

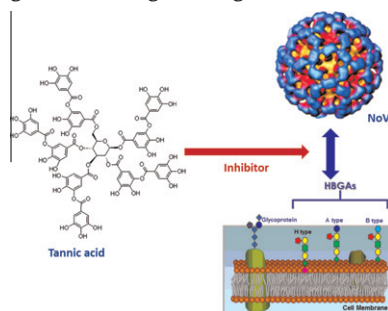
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Amy Capes, Stephen Patterson, Susan Wyllie, Irene Hallyburton, Iain T. Collie, Andrew J. McCarroll, Malcolm F. G. Stevens, Julie A. Frearson, Paul G. Wyatt, Alan H. Fairlamb, Ian H. Gilbert\*

**Tannic acid inhibited norovirus binding to HBGA receptors, a study of 50 Chinese medicinal herbs**

pp 1616–1623

Xu-Fu Zhang, Ying-Chun Dai, Weiming Zhong, Ming Tan, Zhi-Ping Lv, Ying-Chun Zhou\*, Xi Jiang\*

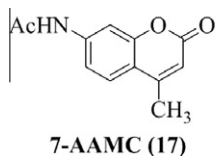


Tannic acid, a common composition of Chinese Gall and Pomegranate, has proven to be a strong inhibitor in the binding of NoV to HBGA receptors.

# Substrate specificity of acetoxy derivatives of coumarins and quinolones towards Calreticulin mediated transacetylation: Investigations on antiplatelet function

pp 1624–1638

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



Compound	IC <sub>50</sub> values (μM)	
	ADP	AA
7-AAMC	145±2.4	77±3.0
ASA	Nil	80±2.5



\*Corresponding author

Supplementary data available via SciVerse ScienceDirect

## COVER

Astrosclerin, a carbonic anhydrase from a living fossil sponge and human carbonic anhydrase II have similar catalytic activity and affinity for sulfonamide inhibitors, although their last common ancestor lived more than 550 million years ago. [Ohradanova, A.; Vullo, D.; Pastorekova, S.; Pastorek, J.; Jackson, D.J.; Wörheide, Supuran, C.T. *Bioorg. Med. Chem.* **2012**, 20, 1403–1410.]

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