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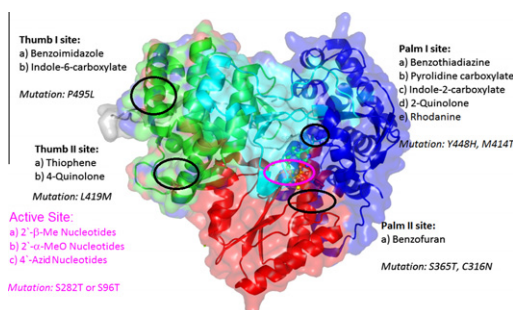
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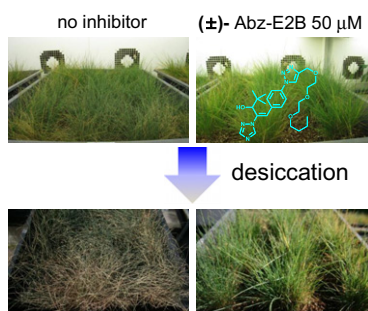
Abdelrahman S. Mayhoub



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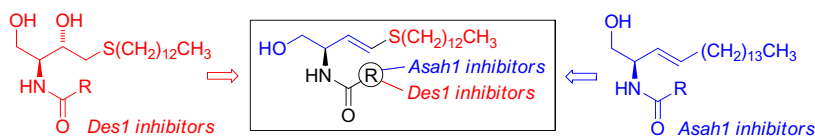
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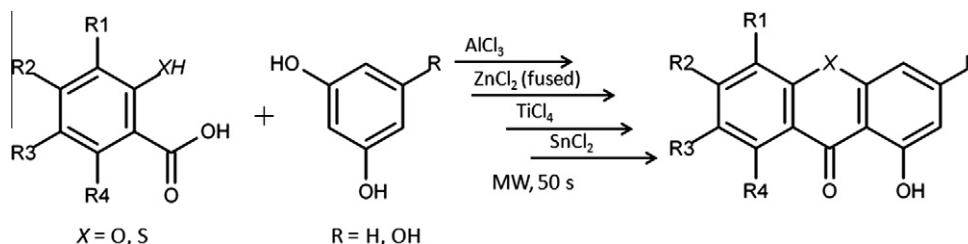
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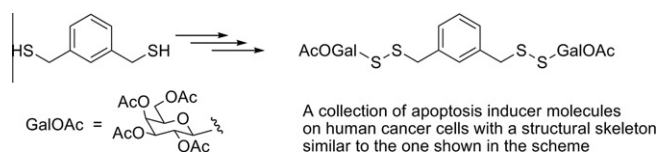
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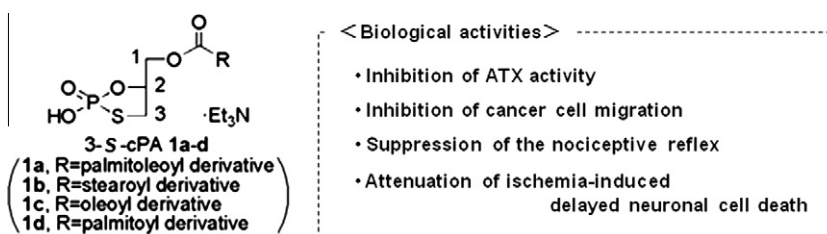
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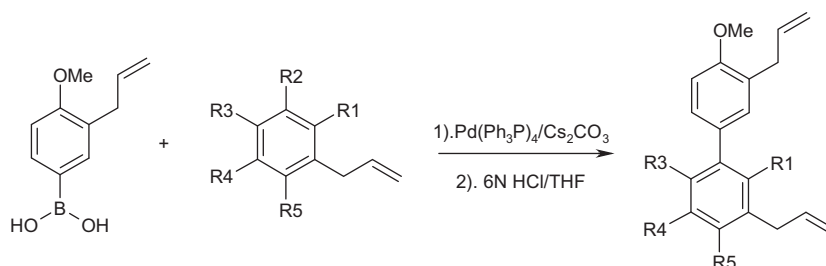
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Jyh Ming Lin*, A. S. Prakasha Gowda, Arun K. Sharma, Shantu Amin

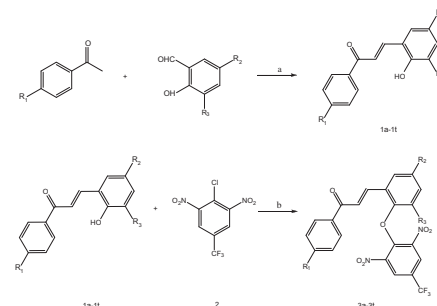


Design, synthesis and biological evaluation of novel chalcone derivatives as antitubulin agents

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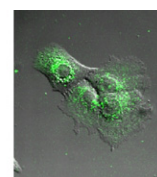
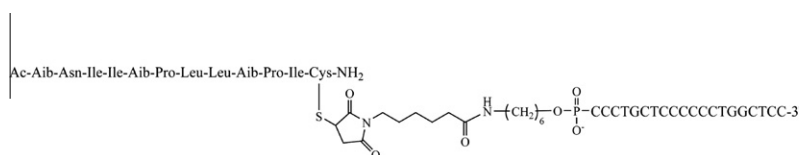
Hui Zhang, Jia-Jia Liu, Jian Sun, Xian-Hui Yang, Ting-Ting Zhao, Xiang Lu, Hai-Bin Gong*, Hai-Liang Zhu*

A series of novel chalcone derivatives have been designed and synthesized, and their biological activities were also evaluated as potential inhibitors of tubulin. These compounds were assayed for growth-inhibitory activity against MCF-7 and A549 cell lines in vitro. Compound **3d** showed the most potent antiproliferative activity against MCF-7 and A549 cell lines with IC_{50} values of 0.03 and 0.95 μ g/mL and exhibited the most potent tubulin inhibitory activity with IC_{50} of 1.42 μ g/mL. Docking simulation was performed to insert compound **3d** into the crystal structure of tubulin at colchicines binding site to determine the probable binding model. Based on the preliminary results, compound **3d** with potent inhibitory activity in tumor growth may be a potential anticancer agent.

**Cellular uptake of covalent conjugates of oligonucleotide with membrane-modifying peptide, peptaibol**

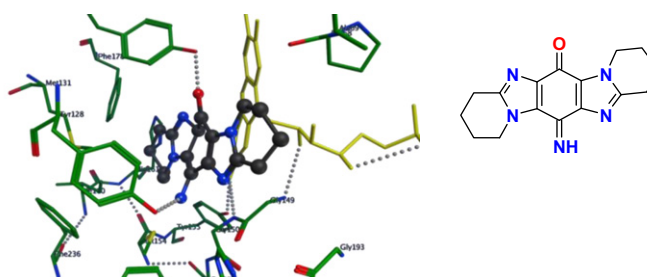
pp 3219–3222

Shun-ichi Wada*, Yasunari Hitora, Saori Yokoe, Osamu Nakagawa, Hidehito Urata

**COMPARE analysis of the toxicity of an iminoquinone derivative of the imidazo[5,4-f]benzimidazoles with NAD(P)H:quinone oxidoreductase 1 (NQO1) activity and computational docking of quinones as NQO1 substrates**

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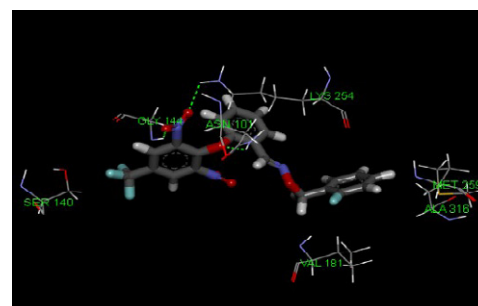
Vincent Fagan, Sarah Bonham, Michael P. Carty, Patricia Saenz-Méndez, Leif A. Eriksson, Fawaz Aldabbagh*

**Synthesis, biological evaluation, and molecular docking studies of 2,6-dinitro-4-(trifluoromethyl)phenoxyalicyclaldoxime derivatives as novel antitubulin agents**

pp 3233–3241

Ting-Ting Zhao, Xiang Lu, Xian-Hui Yang, Li-Ming Wang, Xi Li, Zhong-Chang Wang, Hai-Bin Gong*, Hai-Liang Zhu*

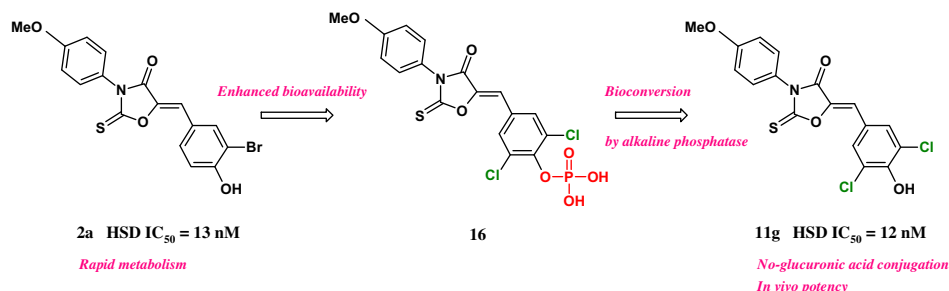
A series of 2,6-dinitro-4-(trifluoromethyl)phenoxyalicyclaldoxime derivatives (**1h–20h**) have been designed and synthesized, and their biological activities were also evaluated as potential antiproliferation and tubulin polymerization inhibitors. Among all the compounds, **2h** showed the most potent activity in vitro, which inhibited the growth of MCF-7, Hep-G2 and A549 cell lines with IC_{50} values of 0.70 ± 0.05 , 0.68 ± 0.02 and 0.86 ± 0.05 μ M, respectively. Compound **2h** also exhibited significant tubulin polymerization inhibitory activity ($IC_{50} = 3.06 \pm 0.05$ μ M). The result of flow cytometry (FCM) demonstrated that compound **2h** induced cell apoptosis. Docking simulation was performed to insert compound **2h** into the crystal structure of tubulin at colchicine binding site to determine the probable binding model. Based on the preliminary results, compound **2h** with potent inhibitory activity in tumor growth may be a potential anticancer agent.



Discovery of potent and orally bioavailable 17 β -hydroxysteroid dehydrogenase type 3 inhibitors

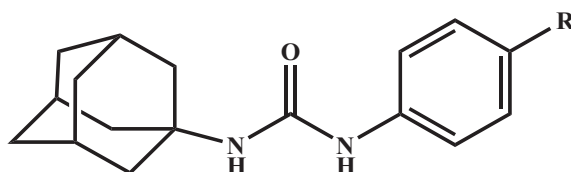
pp 3242–3254

Koichiro Harada*, Hideki Kubo, Jun Abe, Mari Haneta, Arnel Conception, Shinichi Inoue, Satoshi Okada, Kazuhiko Nishioka

**Screening a library of 1600 adamantyl ureas for anti-*Mycobacterium tuberculosis* activity in vitro and for better physical chemical properties for bioavailability**

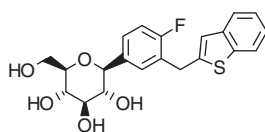
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Michael S. Scherman, Elton J. North, Victoria Jones, Tamara N. Hess, Anna E. Grzegorzewicz, Takeo Kasagami, In-Hae Kim, Oleg Merzlikin, Anne J. Lenaerts, Richard E. Lee, Mary Jackson, Christophe Morisseau*, Michael R. McNeil*

A library of 1600 ureas was screened in vitro for activity against *Mycobacterium tuberculosis*.**Discovery of Ipragliflozin (ASP1941): A novel C-glucoside with benzothiophene structure as a potent and selective sodium glucose co-transporter 2 (SGLT2) inhibitor for the treatment of type 2 diabetes mellitus**

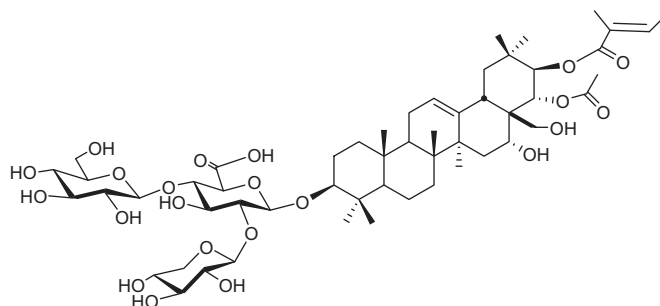
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**14h**; Ipragliflozin (ASP1941)A series of C-glucosides with various heteroaromatics has been synthesized and its inhibitory activity toward SGLTs evaluated and a novel benzothiophene derivative (**14h**; ipragliflozin, ASP1941) was discovered as a highly potent and selective SGLT2 inhibitor that reduced blood glucose levels in a dose-dependent manner in diabetic model mice and rats.**Paviosides A–H, eight new oleanane type saponins from *Aesculus pavia* with cytotoxic activity**

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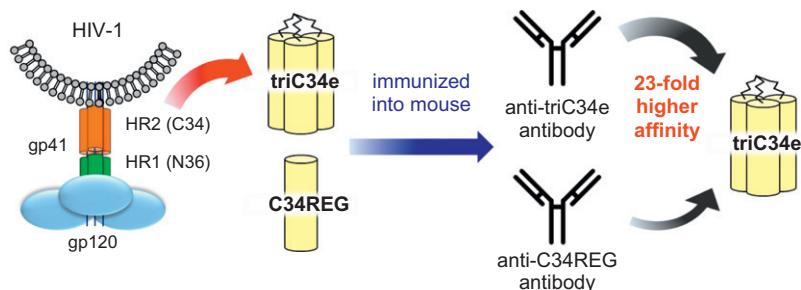
Virginia Lanzotti*, Pasquale Termolino, Marcello Dolci, Paolo Curir



Evaluation of a synthetic C34 trimer of HIV-1 gp41 as AIDS vaccines

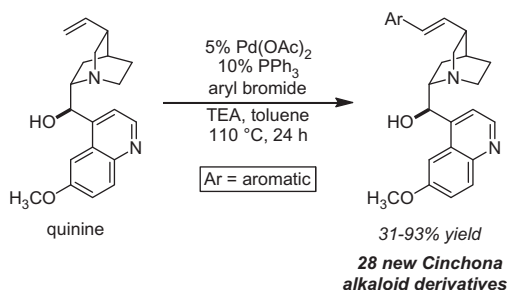
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Chie Hashimoto, Wataru Nomura*, Aki Ohya, Emiko Urano, Kosuke Miyauchi, Tetsuo Narumi, Haruo Aikawa, Jun A. Komano, Naoki Yamamoto, Hirokazu Tamamura*

**Investigating the activity of quinine analogues versus chloroquine resistant *Plasmodium falciparum***

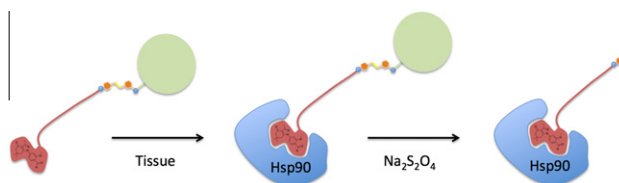
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Theresa Dinio, Alexander P. Gorka, Andrew McGinniss, Paul D. Roepe, Jeremy B. Morgan*

**A highly selective Hsp90 affinity chromatography resin with a cleavable linker**

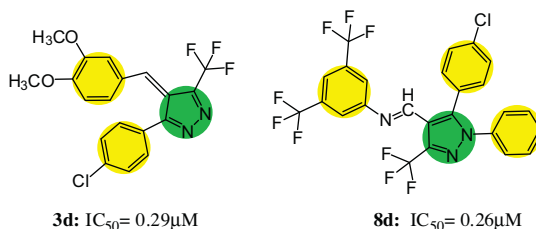
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Philip F. Hughes, Jared J. Barrott, David A. Carlson, David R. Loiselle, Brittany L. Speer, Khaldon Bodoor, Laurreta A. Rund, Timothy A. J. Haystead*

**Synthesis, biological evaluation and molecular modeling study of pyrazole and pyrazoline derivatives as selective COX-2 inhibitors and anti-inflammatory agents. Part 2**

pp 3306–3316

Magda A.-A. El-Sayed, Naglaa I. Abdel-Aziz*, Alaa A.-M. Abdel-Aziz, Adel S. El-Azab, Kamal E. H. ElTahir

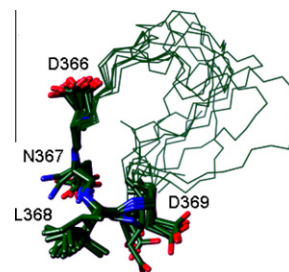


A comparative study of backbone versus side chain peptide cyclization: Application for HIV-1 integrase inhibitors

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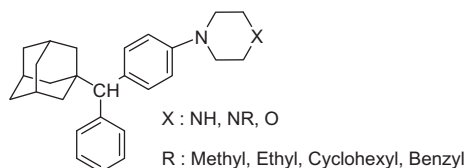
Zvi Hayouka, Aviad Levin, Mattan Hurevich, Deborah E. Shalev, Abraham Loyter, Chaim Gilon, Assaf Friedler*

c(MZ 4K-1) 3D structure is stabilized upon IN binding as c(MZ 4-1). The effect of cyclization type and specifically the bridge and ring sizes on the solution structures of the c(MZ 4-1) analogs was studied by NMR. The backbone RMSD of the IN-bound c(MZ 4K-1) was 1.34 Å and the local RMSD of residues 366–369 was 0.21 Å. This stabilization may correlate between the IN activity of the cyclic peptides and the local RMSD of residues 366–369.

**Synthesis, σ_1 , σ_2 -receptors binding affinity and antiproliferative action of new C1-substituted adamantanes**

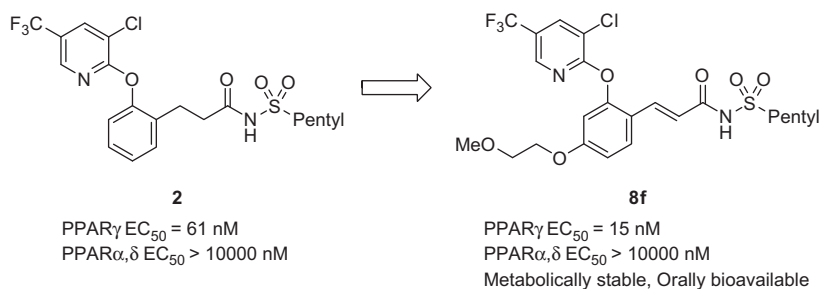
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Stefanos Riganas, Ioannis Papanastasiou, George B. Foscolos*, Andrew Tsotinis, Jean-Jacques Bourguignon, Guillaume Serin, Jean-François Mirjolet, Kostas Dimas, Vassilios N. Kourafalos, Andreas Eleutheriades, Vassilios I. Moutsos, Humaira Khan, Stavroula Georgakopoulou, Angeliki Zaniou, Margarita Prassa, Maria Theodoropoulou, Stavroula Pondiki, Alexandre Vamvakides

**Structure–activity relationships and key structural feature of pyridyloxybenzene-acylsulfonamides as new, potent, and selective peroxisome proliferator-activated receptor (PPAR) γ Agonists**

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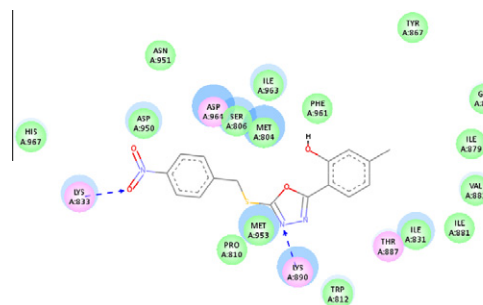
Kentaro Rikimaru*, Takeshi Wakabayashi, Hidenori Abe, Taisuke Tawarashi, Hiroshi Imoto, Jinichi Yonemori, Hideki Hirose, Katsuhito Murase, Takanori Matsuo, Mitsuharu Matsumoto, Chisako Nomura, Hiroko Tsuge, Naoto Arimura, Kazutoshi Kawakami, Junichi Sakamoto, Miyuki Funami, Clifford D. Mol, Gyorgy P. Snell, Kenneth A. Bragstad, Bi-Ching Sang, Douglas R. Dougan, Toshimasa Tanaka, Nozomi Katayama, Yoshiaki Horiguchi, Yu Momose

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

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
Zhi-Ming Zhang, Xue-Wei Zhang, Zong-Zheng Zhao, Ru Yan, Rui Xu, Hai-Bin Gong*, Hai-Liang Zhu*

A series of 1,3,4-oxadiazole derivatives derived from 4-methoxysalicylic acid or 4-methylsalicylic acid (**6a–6z**) have been first synthesized for their potential immunosuppressive activity. Among them, compound **6z** displayed the most potent biological activity against lymph node cells (inhibition = 38.76% for lymph node cells and IC₅₀ = 0.31 μ M for PI3K γ). The preliminary mechanism of compound **6z** inhibition effects was also detected by flow cytometry (FCM) and the compound exerted immunosuppressive activity via inducing the apoptosis of activated lymph node cells in a dose dependent manner. Docking simulation was performed to position compound **6z** into the PI3K γ structure active site to determine the probable binding model.



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*Corresponding author

* Supplementary data available via SciVerse ScienceDirect**COVER**

Dipyrone (metamizol) is a common antipyretic drug and the most popular non-opioid analgesic in many countries. In spite of its long and widespread use, molecular details of its fate in the body are not fully known. Two unknown metabolites were now found, viz. arachidonoyl amides, and positively tested for cannabis receptor binding (CB1 and CB2) and cyclooxygenase inhibition. Two more puzzle pieces of the dipyrone story found! (Rogosch, T.; Sinning, C.; Podlewski, A.; Watzer, B.; Schlosburg, J.; Lichtman, A.H.; Cascio, M.G.; Bisogno, T.; Di Marzo, V.; Nüsing, R.; Imming, P. *Bioorg. Med. Chem.* **2012**, 20, 103–109.)

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