



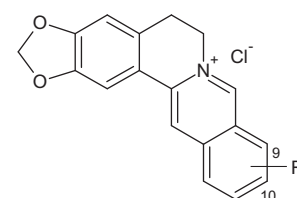
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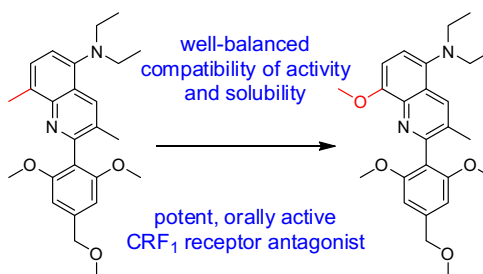


Compound **1** might become a promising candidate for the treatment of metabolic syndrome.

1: R = 10, 11-dimethoxy;

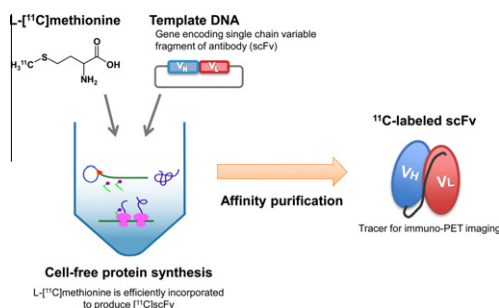
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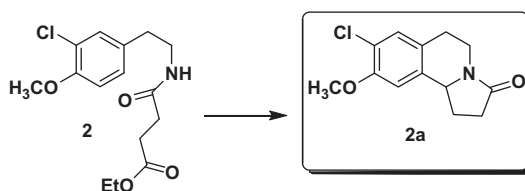


Toxic protein with its molecular mass of 23 kDa isolated from *Chlorophyllum molybdites* is a member of the deuterolysin family of zinc proteases.

Synthesis of new antimicrobial pyrrolo[2,1-*a*]isoquinolin-3-ones

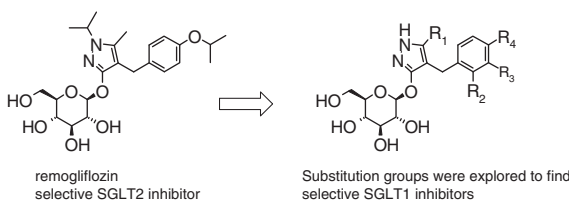
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**Structure–activity relationship studies of 4-benzyl-1*H*-pyrazol-3-yl β-*D*-glucopyranoside derivatives as potent and selective sodium glucose co-transporter 1 (SGLT1) inhibitors with therapeutic activity on postprandial hyperglycemia**

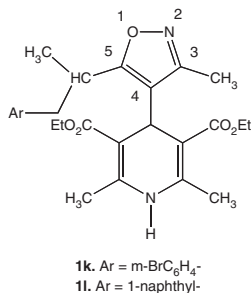
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**4-Isoxazolyl-1,4-dihydropyridines exhibit binding at the multidrug-resistance transporter**

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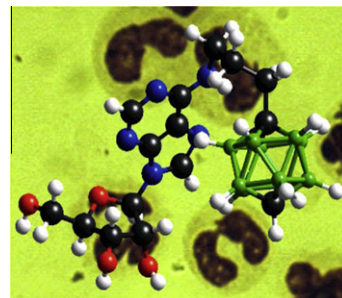
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Effect of adenosine modified with a boron cluster pharmacophore on reactive oxygen species production by human neutrophils pp 6621–6629

Katarzyna Bednarska, Agnieszka B. Olejniczak, Agnieszka Piskala, Magdalena Klink, Zofia Sulowska, Zbigniew J. Lesnikowski*

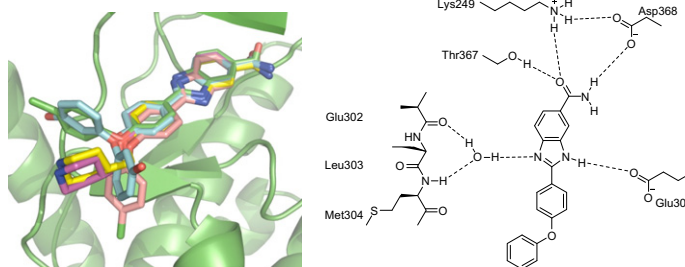
New chemistries were developed and series of adenosine/boron cluster conjugates was synthesized and screened for activity as inhibitors of reactive oxygen species (ROS) production in neutrophils. The high activity and affinity of the selected compounds for adenosine receptor A_{2A} was established. This study extends the range of innovative molecules available for testing as agents affecting inflammatory processes.



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Unconstrained rigid docking, flexible side chain docking and protein crystal structure determinations reveal a water-mediated hinge binding mode for a series of benzimidazole ligands of the protein kinase CHK2. This binding mode is different from those previously postulated in the literature and may provide a useful approach to selective small molecule inhibitor design.



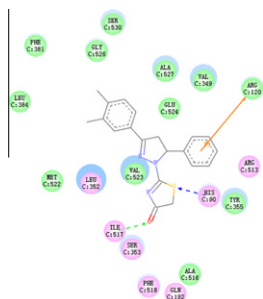
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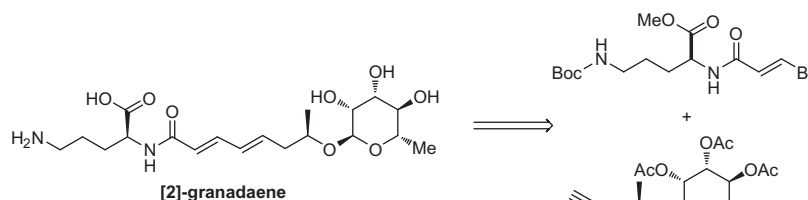
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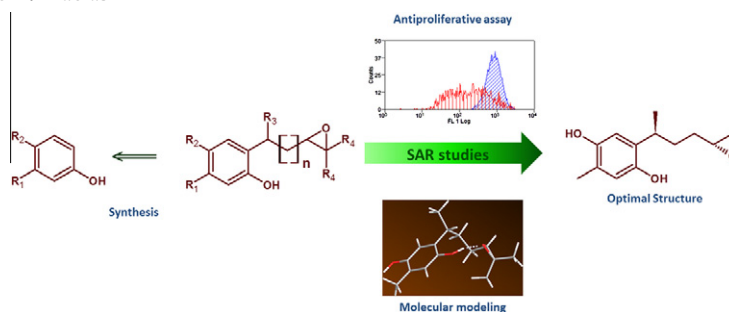
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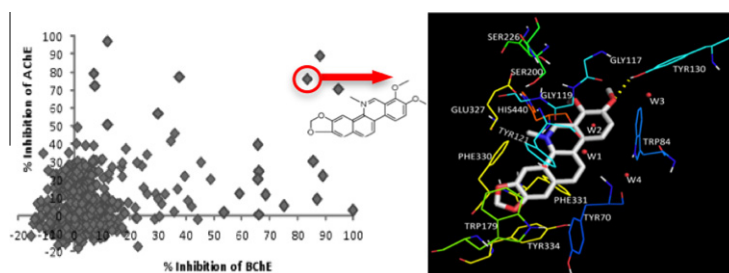
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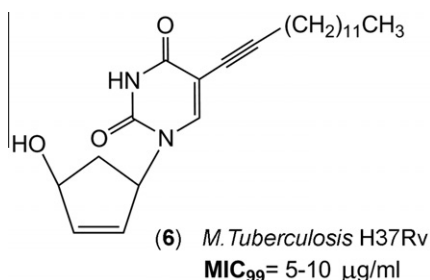
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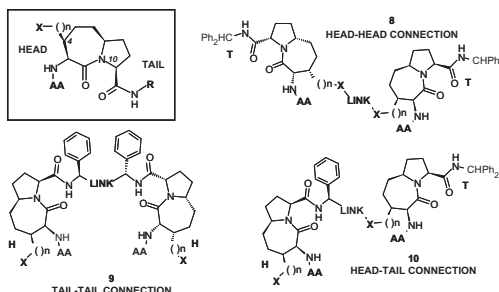
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Homo- and heterodimeric Smac mimetics/IAP inhibitors as in vivo-active pro-apoptotic agents. Part I: Synthesis

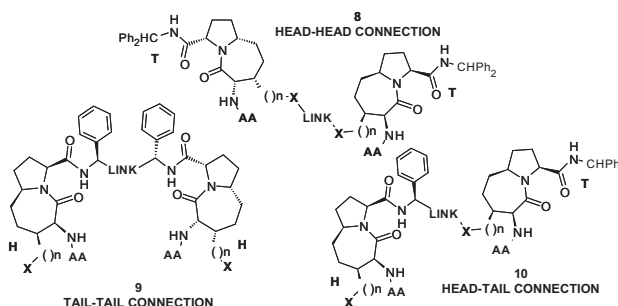
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**Dimeric Smac mimetics/IAP inhibitors as in vivo-active pro-apoptotic agents. Part II: Structural and biological characterization**

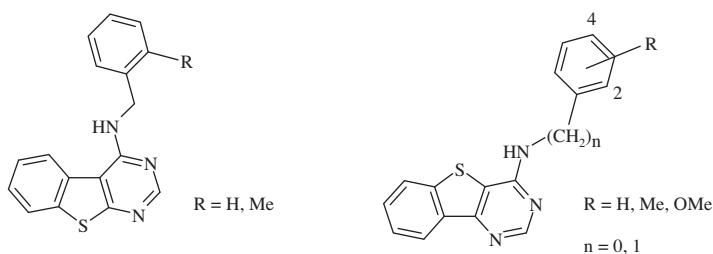
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**Synthesis and evaluation of apoptosis induction of thienopyrimidine compounds on KRAS and BRAF mutated colorectal cancer cell lines**

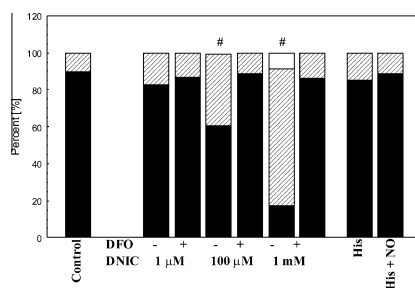
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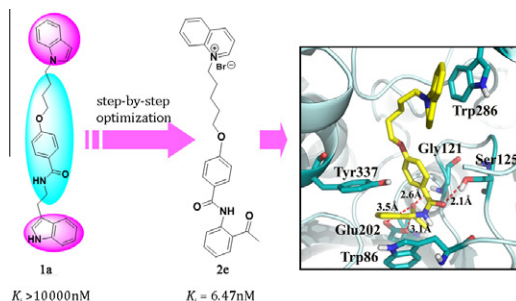


Nicking of the plasmid DNA by HIS-DNIC. Filled box—supercoiled form (CCC); hatched box—open circular form (OC); empty box—linear form (L).



Design, synthesis, and bioevaluation of benzamides: Novel acetylcholinesterase inhibitors with multi-functions on butylcholinesterase, A β aggregation, and β -secretase pp 6739–6750

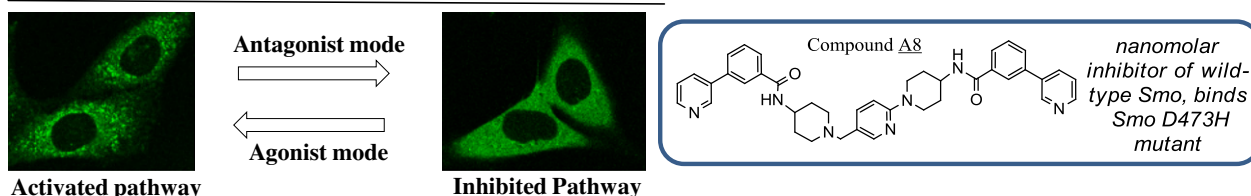
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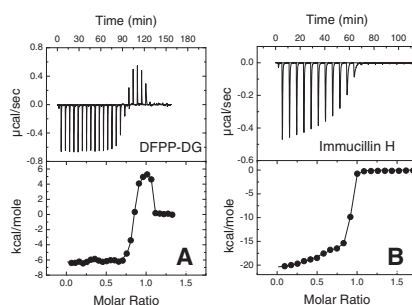
Jiangbo Wang, Robert A. Mook Jr.*, Jiuyi Lu, David M. Gooden, Anthony Ribeiro, Anchen Guo, Larry S. Barak, H. Kim Lysterly, Wei Chen*

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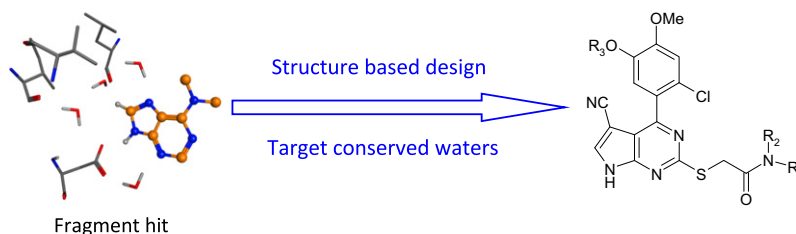
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Targeting conserved water molecules: Design of 4-aryl-5-cyanopyrrolo[2,3-d]pyrimidine Hsp90 inhibitors using fragment-based screening and structure-based optimization pp 6770–6789

Nicholas G. M. Davies, Helen Browne, Ben Davis, Martin J. Drysdale, Nicolas Foloppe, Stephanie Geoffrey, Ben Gibbons, Terance Hart, Roderick Hubbard, Michael Rugaard Jensen, Howard Mansell, Andrew Massey, Natalia Matassova, Jonathan D. Moore, James Murray, Robert Pratt, Stuart Ray, Alan Robertson, Stephen D. Roughley, Joseph Schoepfer, Kirsten Scriven, Heather Simmonite, Stephen Stokes, Allan Surgenor, Paul Webb, Mike Wood, Lisa Wright, Paul Brough*



*Corresponding author

+ Supplementary data available via SciVerse ScienceDirect

COVER

Fragment library screening against the molecular Chaperone Hsp90 identified several purine based hits, which bound to the ATP site. Computer aided design utilised structural information from ligand-protein X-ray crystallography to propose the rational displacement of a structurally conserved water molecule. Subsequent structure-based elaboration of the initial hits led to potent and biologically active inhibitors. [Davies, N.G.M.; Browne, H.; Davis, B.; Drysdale, M.J.; Foloppe, N.; Geoffrey, S.; Gibbons, B.; Hart, T.; Hubbard, R.; Rugaard Jensen, M.; Mansell, H.; Massey, A.; Matassova, N.; Moore, J.D.; Murray, J.; Pratt, R.; Ray, S.; Robertson, A.; Roughley, S.D.; Schoefer, J.; Scriven, K.; Simmonite, H.; Stokes, S.; Surgenor, A.; Webb, P.; Wood, M.; Wright, L.; Brough, P. [*Bioorg. Med. Chem.* **2012**, 20, 6770–6789.]

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