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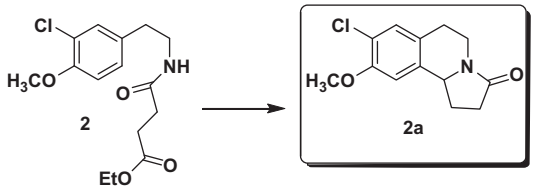
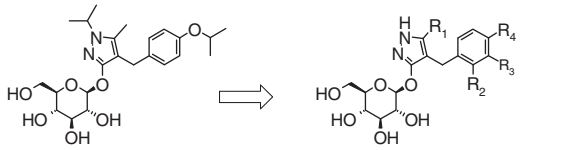
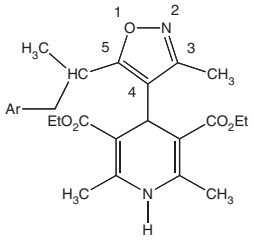
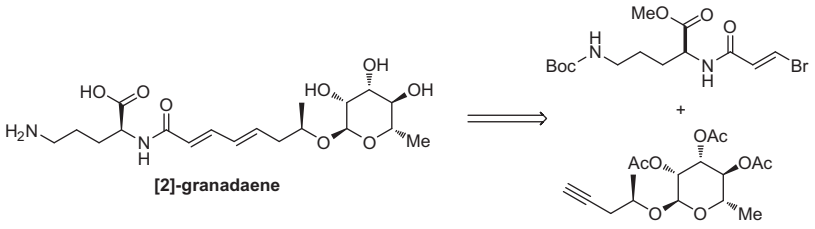
ARTICLES

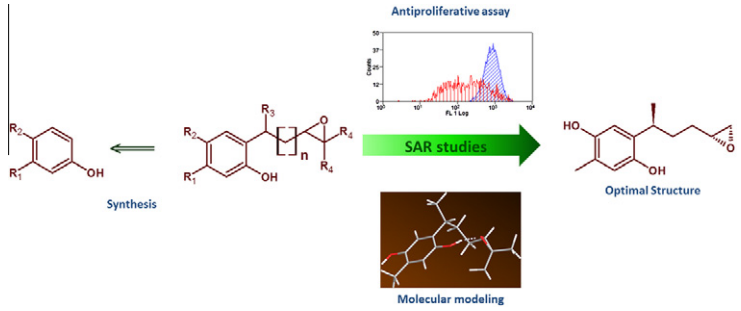


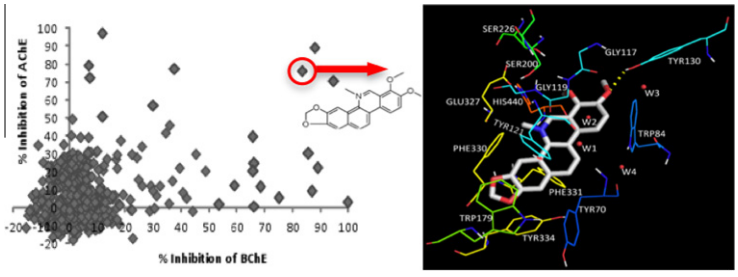


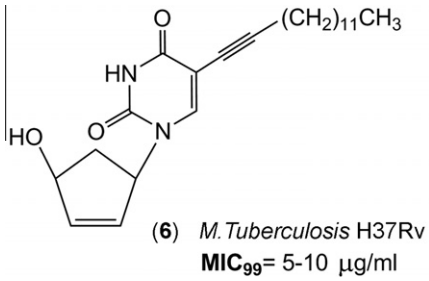


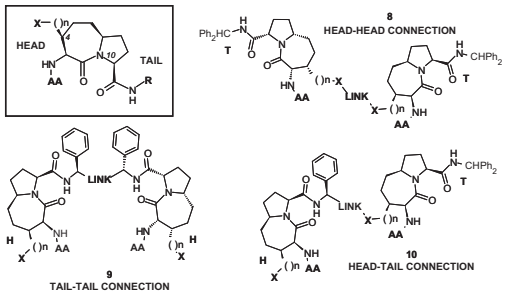
1k. Ar = m-BrC_6H_4-
1l. Ar = 1-naphthyl-

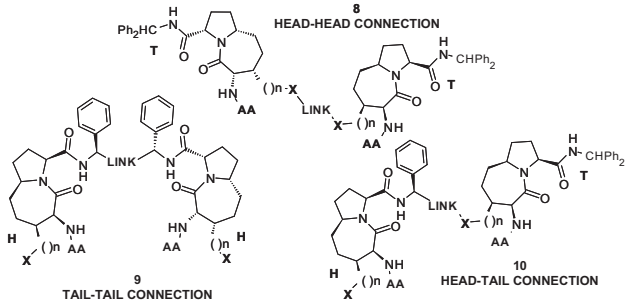


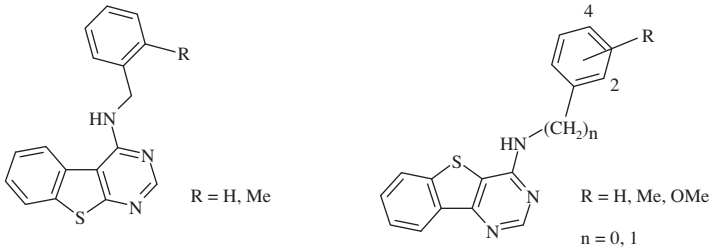


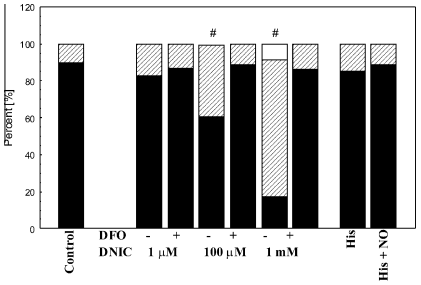




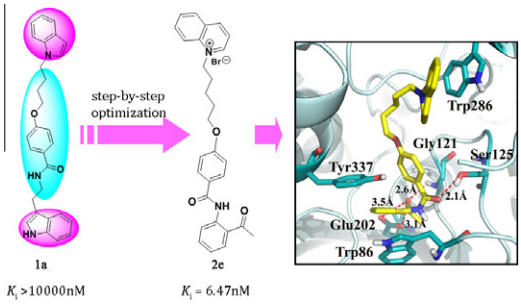


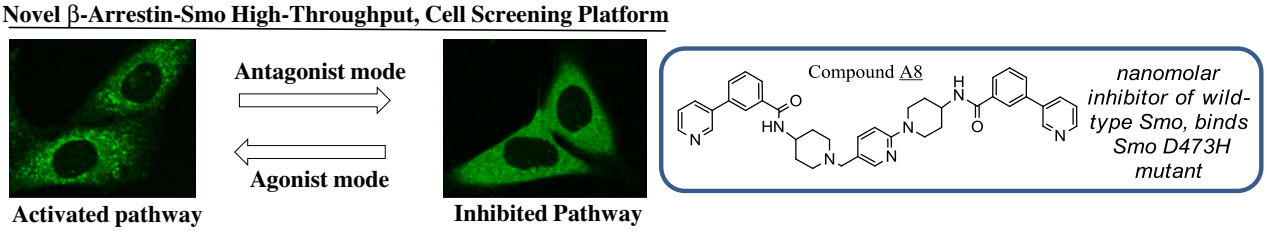


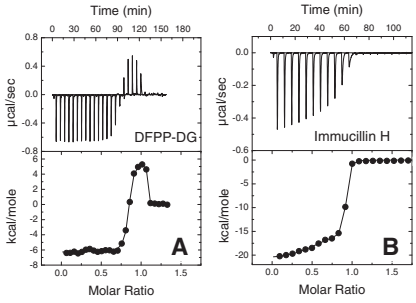


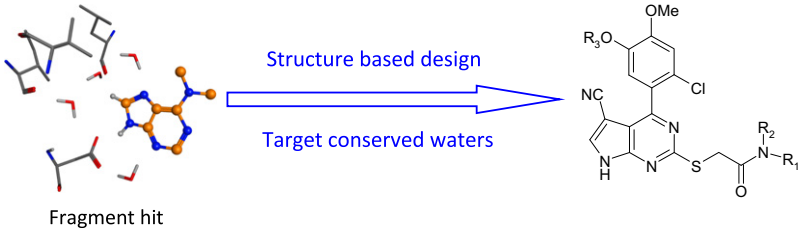


Nicking of the plasmid DNA by HIS-DNIC. Filled box—supercoiled form (CCC); hatched box—open cicrular form (OC); empty box—linear form (L).









*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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