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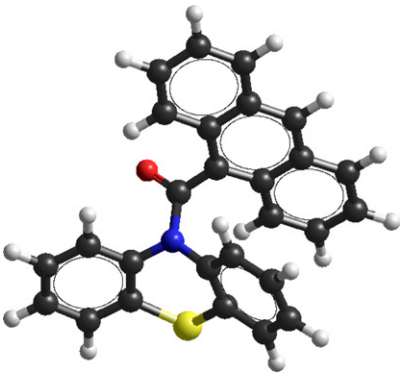

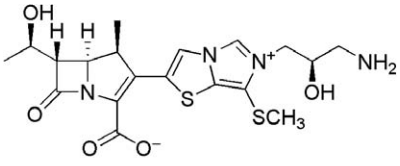

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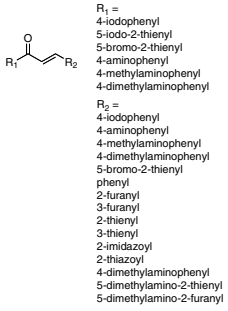

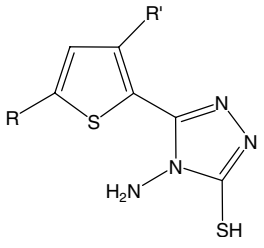

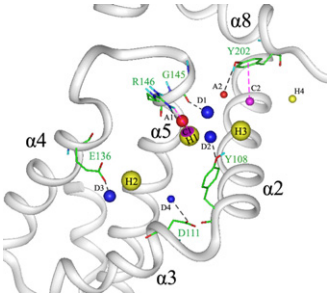

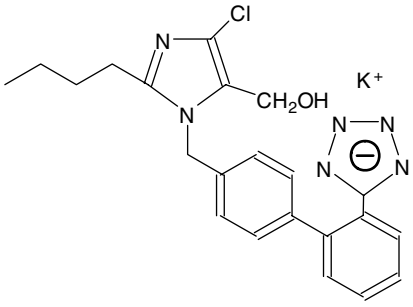

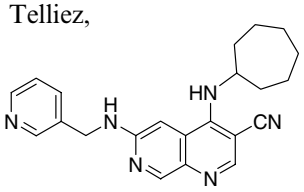

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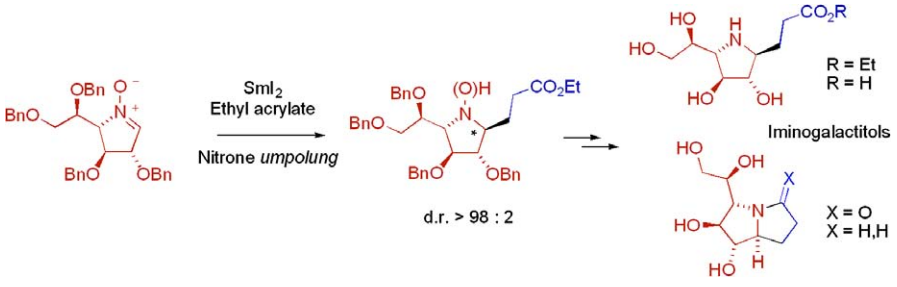
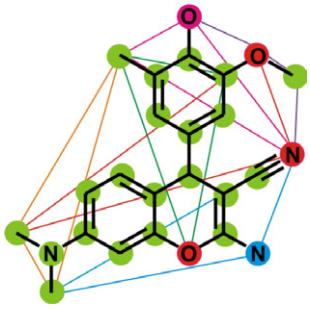
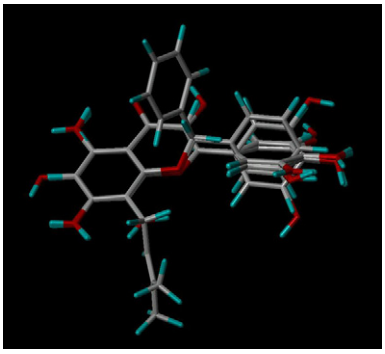
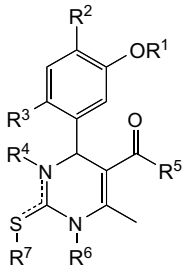


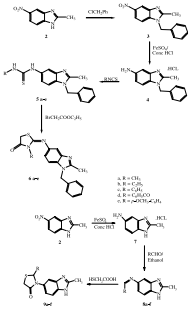


A predictive CoMFA model of flavonoid inhibitors of the PIM-1 kinase is reported. Shown is the alignment rule for the training set of compounds used to build the CoMFA model.



Monastrol is a specific allosteric inhibitor of Eg5, a kinesin responsible for the formation and maintenance of the bipolar spindle. In contrast to anticancer drugs that perturb mitosis and all target tubulin, it does not display any neurotoxicity and thus is thought to have antitumor potential. A series of analogs have been synthesized and tested for inhibition of Eg5 in vitro and for arresting mitosis of cultured cells. One compound was more potent than parent monastrol by a fivefold factor. Structure–activity relationships led to the preparation of an affinity matrix for unprecedentedly fast and efficient purification of full-length Eg5 from eukaryotic cells. The question of monastrol-targets other than Eg5 is discussed.





OTHER CONTENTS

*Corresponding author
ⓘ+ Supplementary data available via ScienceDirect

COVER

Terfenadine (an antihistamine pulled from the market in 1997) bound to a model of an open form of the homo-tetrameric pore domain of hERG, produced using Schrödinger's "Induced Fit Docking" technology [Farid, R.; Day, T.; Friesner, R. A.; Pearlstein, R. A. *Bioorg. Med. Chem*. **2006,** *14*, 3160–3173].

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