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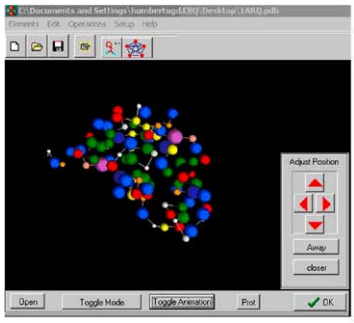
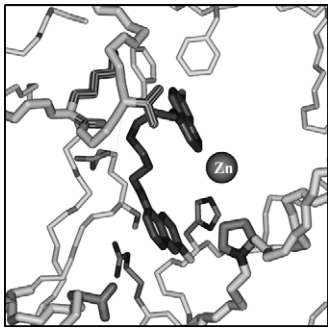
# Contents

## ARTICLES

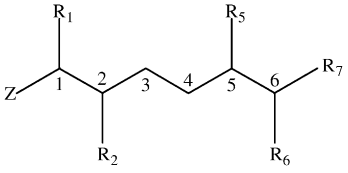




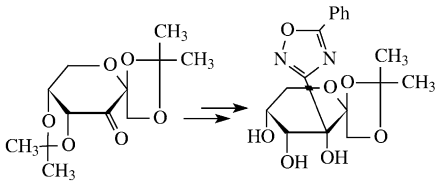

Molecular dynamics simulations were used to explore how residue motion in and around the botulinum neurotoxin serotype A light chain (BoNT/A LC) substrate binding cleft might affect inhibitor binding. Results from these studies indicate that surface loop reorientations toward the substrate binding cleft may facilitate small molecule binding by creating additional inhibitor-residue contacts. Based on molecular docking studies, our common pharmacophore model for BoNT/A LC inhibitors has been refined via the inclusion of these potential contact residues.

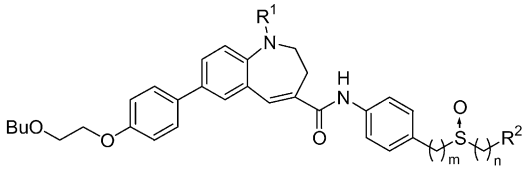




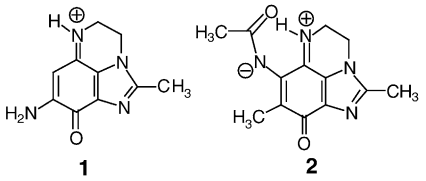

The antimycobacterial activity of nitro/acetamido alkenol derivatives and chloro/amino alkenol derivatives has been analyzed through combinatorial protocol in multiple linear regression (CP-MLR) using different topological descriptors obtained from Dragon software.







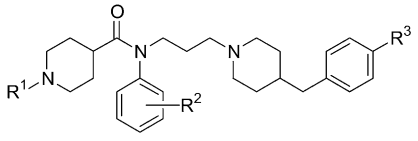




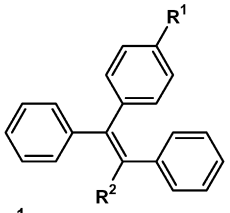
**1** **2**

**Imidazoquinoxalinones**

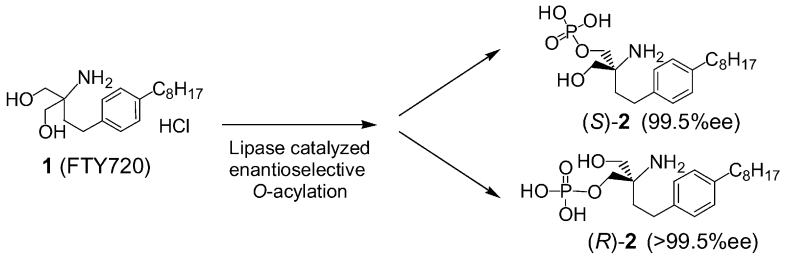




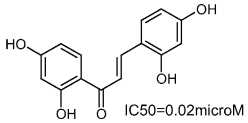




**$R^1$** = $NHSO_2Me$, $N_3$
**$R^2$** = Me, Et,*n*-Butyl, *n*-Hexyl, Cyclohexyl,*n*-Octyl



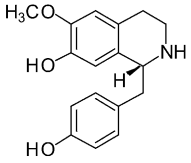


2,4,2',4'-tetrahydroxychalcone

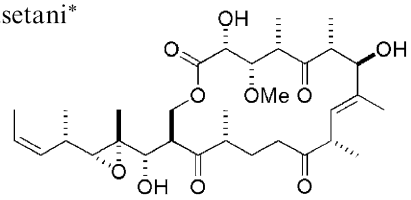
Chalcones with tetra-substituted hydroxyl groups were synthesized and tested as tyrosinase inhibitors towards designing novel whitening agents, resulting with the most potent inhibitor, with $IC_{50}$ of 0.02 μM concn.






(+)-1(*R*)-Coclaurine (**1**) and (−)-1(*S*)-norcoclaurine (**3**), together with quercetin 3-*O*-β-D-glucuronide (**4**), were isolated from the leaves of *Nelumbo nucifera* (Nymphaceae), and identified as anti-HIV principles. These compounds can serve as new leads for further development of anti-AIDS agents.





13-deoxytedanolide

By using radiolabeled ligand derived from 13-deoxytedanolide, the ribosome was identified as the target molecule of 13-deoxytedanolide. As expected, 13-deoxytedanolide inhibited polypeptide elongation at low concentration.

## OTHER CONTENTS



*Corresponding author
ⓘ+ Supplementary data available via ScienceDirect

## COVER

Peptide libraries on phage and on solid phase beads were screened as ligands for members of the galectin family of endogenous lectins relevant in e.g. cancer. The phage libraries were screened in microtiter plates whereas the on-bead library hits were identified by a colorimetric method. The galectins normally bind β-galactosides, as exemplified by the space filling models, in each of its two binding sites. The peptides identified from the phage did not bind to the sugar binding site whereas the on-bead library derived peptides did, as illustrated by the arrows pointing to the respective parts of the protein. [André, S.; Arnusch, C. J.; Kuwabara, I.; Russwurm, R.; Kaltner, H.; Gabius, H.-J.; Pieters, R. J. *Bioorg. Med. Chem.* **2005**, *13*, 563–573].

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