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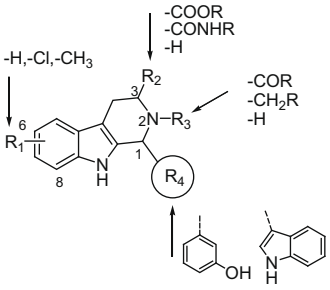
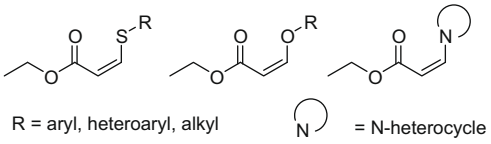
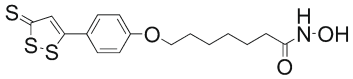
Contents

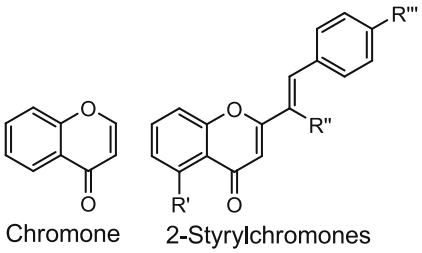
ARTICLES



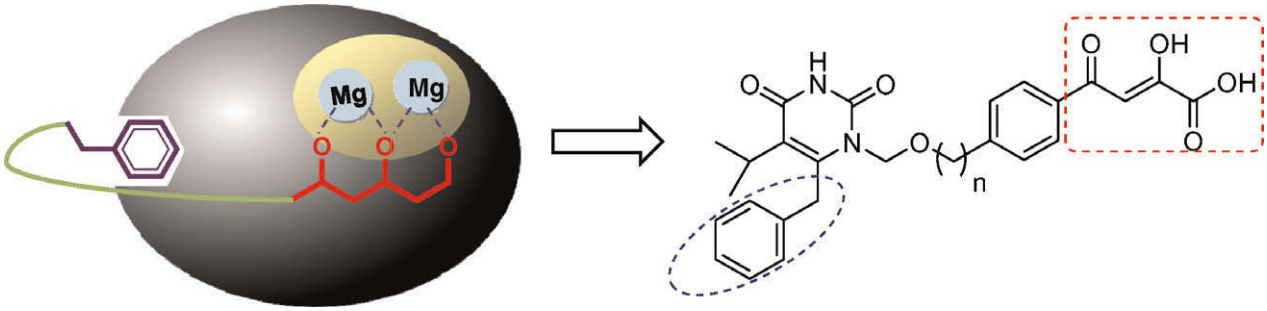




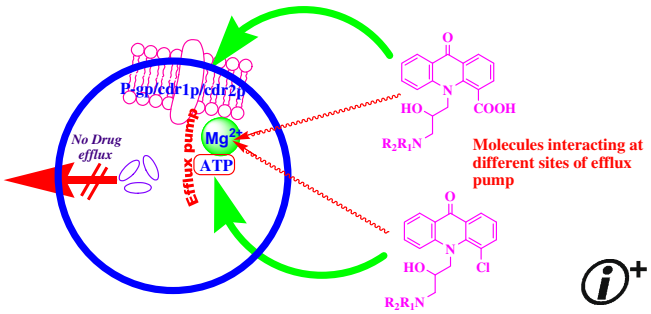
2 (IC_{50}= 0.01 μM)

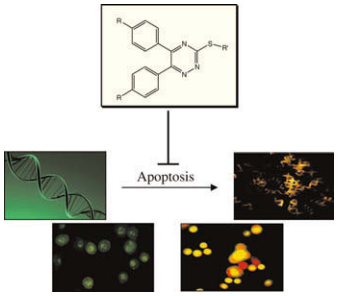


Twelve structure related chromone and (*E*)-2-styrylchromones were tested for their activity against norovirus using the surrogate model MNV/RAW 264.7 cells. (*E*)-5-Hydroxy-2-styrylchromone and (*E*)-4′-methoxy-2-styrylchromone were the most active compounds ($IC_{50} \approx 7\mu M$).

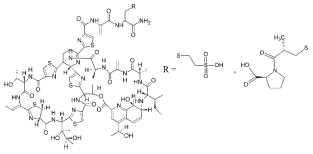


Acridone based molecules are identified for blocking the drug efflux pumps either through interactions with P-gp/cdr1p/cdr2p or interacting with ATP/Mg^{2+}.

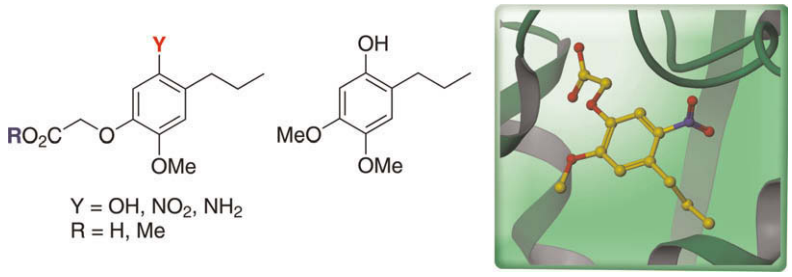


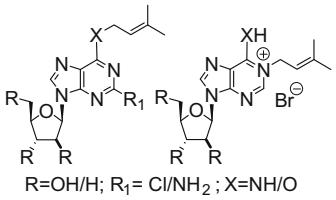


A novel series of 1,2,4-triazine derivatives were synthesized and evaluated for their neuroprotective effect.

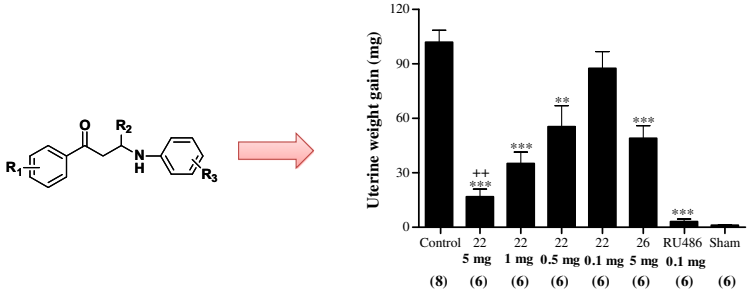


Semi-synthetic, regio-specific analogues of thiostrepton demonstrate the importance of the tail region of this antibiotic in its antibacterial activity and highlight this region as an attractive site for future modification.

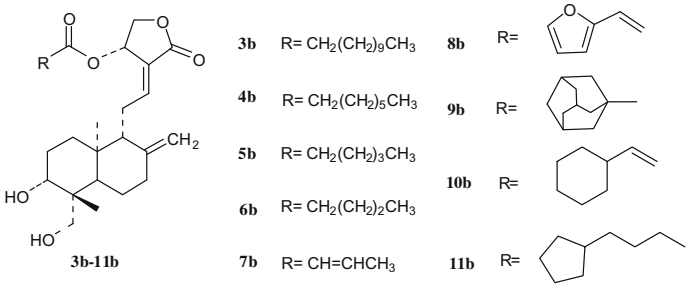


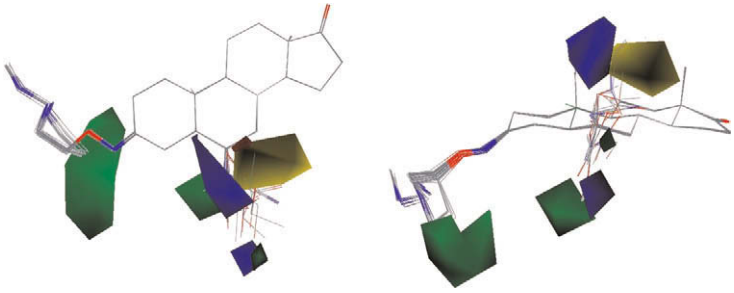


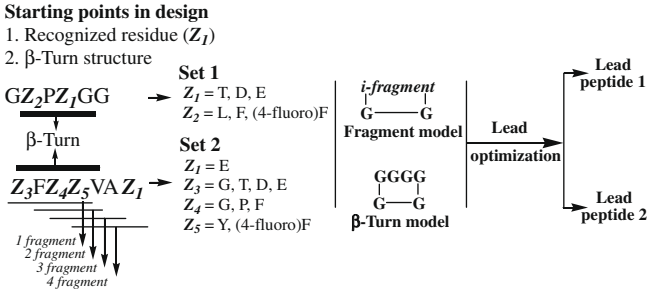
Some novel derivatives of N^6-isopentenyladenosine (iPA) are synthesised and are evaluated for their antiproliferative activity on T24 human bladder carcinoma cells.



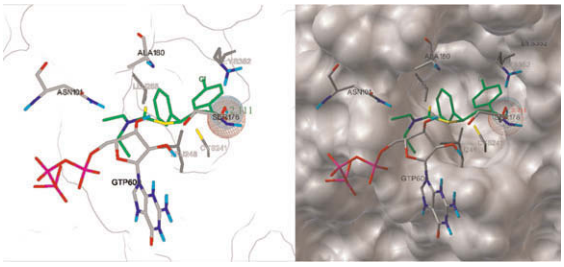
A series of aromatic β-amino-ketone derivatives was identified as a novel class of non-steroidal progesterone receptor antagonists.

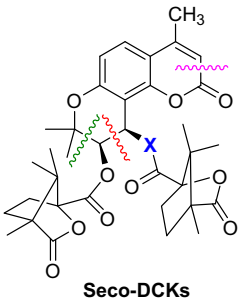


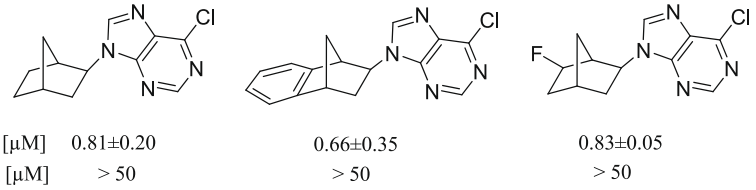




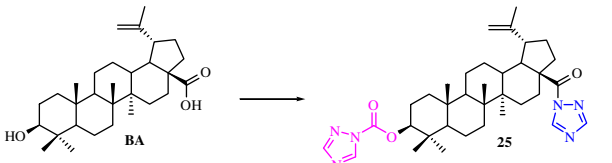
Compound **2n** showed the most potent biological activity in vitro, which inhibited the growth of MCF-7 human breast carcinoma cells with IC_{50} of 0.04 ± 0.01 μM and the polymerization of tubulin with IC_{50} of 6.8 ± 0.6 μM. To understand the tubulin–inhibitor interaction and the selectivity of the most active compound towards tubulin, molecular modeling studies were performed to dock compound **2n** into colchicine binding site and this study provided probable inhibition mechanism. The result indicated that compound **2n** was a potent inhibitor of tubulin polymerization.





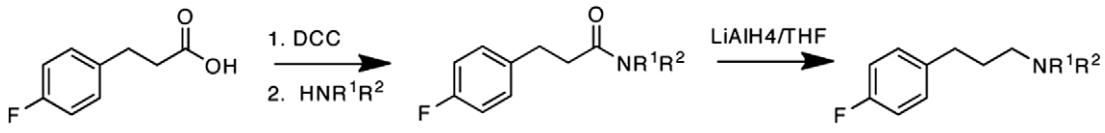


We report synthesis and results of the anti-coxsackievirus B3 screening of the novel 6-chloropurine derivatives.



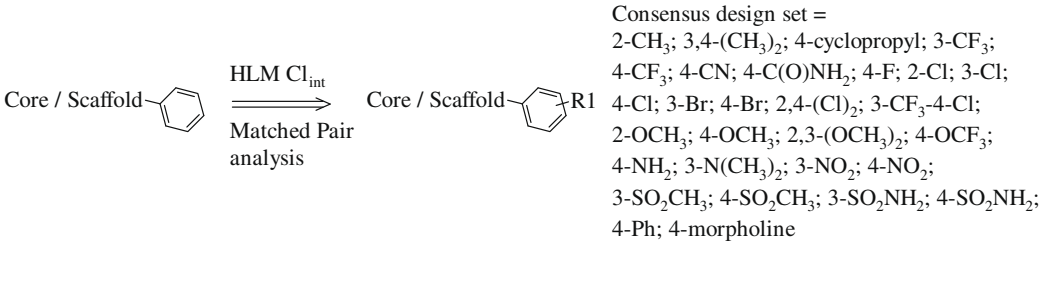
IC_{50} (PC-3) = 21.5 μM
IC_{50} (HT-29) = 12.8 μM

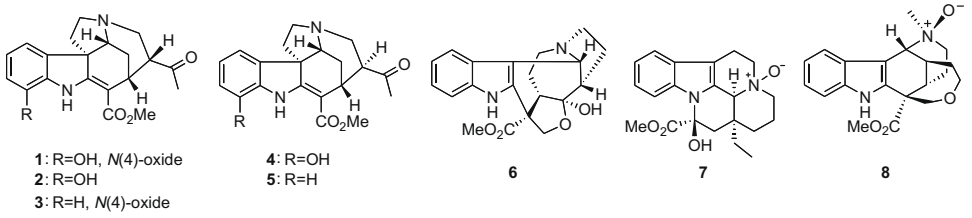
IC_{50} (PC-3) = 1.1 μM
IC_{50} (HT-29) = 1.9 μM

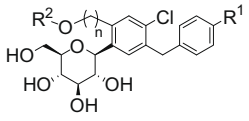


4. $R^1 = R^2$ = n-Butyl
5. $R^1 = R^2$ = n-Octyl
6. R^1 = n-Propyl, R^2 = (4-nitrophenyl)methyl
7. R^1 = n-Propyl, R^2 = (4-nitrophenyl)ethyl
8. R^1 = H, R^2 = n-Propyl

9. $R^1 = R^2$ = n-Butyl
10. $R^1 = R^2$ = n-Octyl
11. R^1 = n-Propyl, R^2 = (4-nitrophenyl)methyl
12. R^1 = n-Propyl, R^2 = (4-nitrophenyl)ethyl
13. R^1 = H, R^2 = n-Propyl

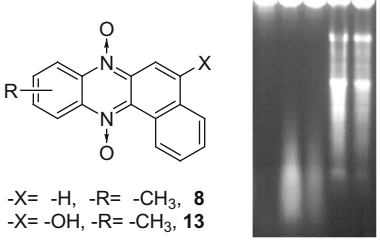


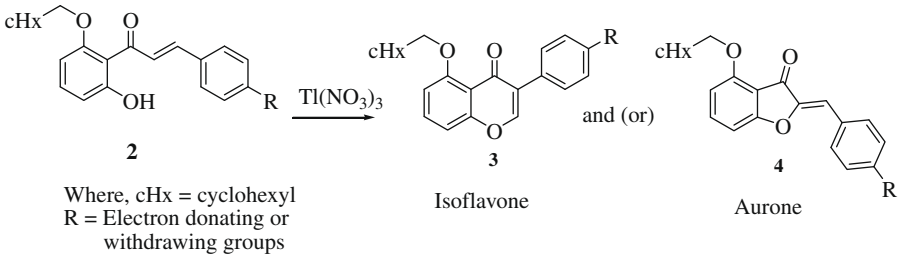


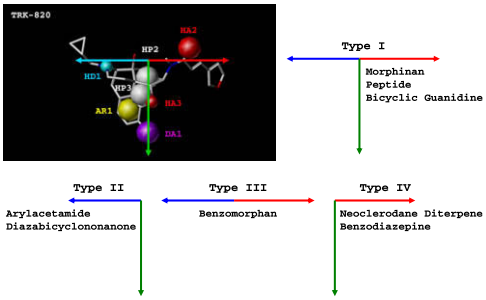


A series of *ortho*-substituted *C*-aryl glucosides have been synthesized and evaluated for inhibition of hSGLT1 and hSGLT2.

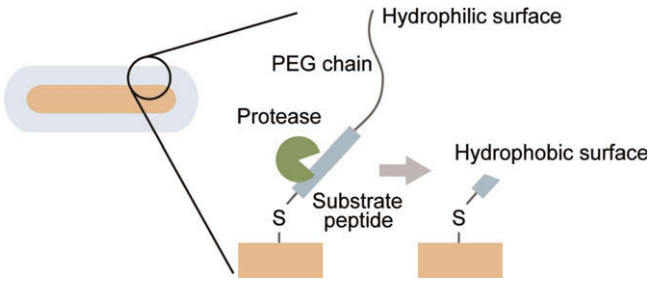
Benzo[*a*]phenazine 7,12-dioxide scaffold has been studied as selective hypoxic cytotoxin and as antiproliferative agents on Caco-2 tumoral cells in normoxia. Electrochemical, DNA-interaction and DNA-damage studies were performed to establish the mode of action.



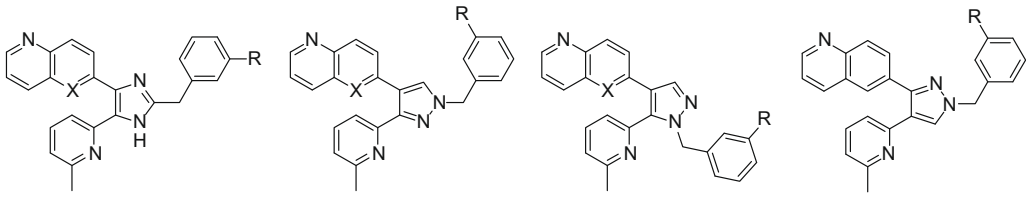


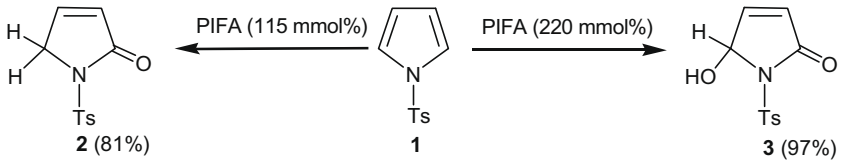


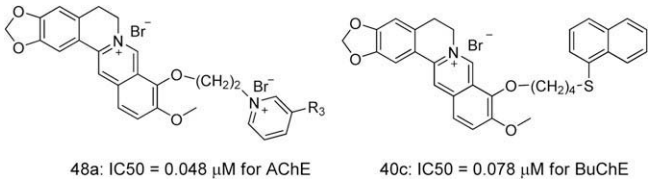
3D-Pharmacophore and classification of binding orientations for κ-agonists. The binding orientations are divided into four types.



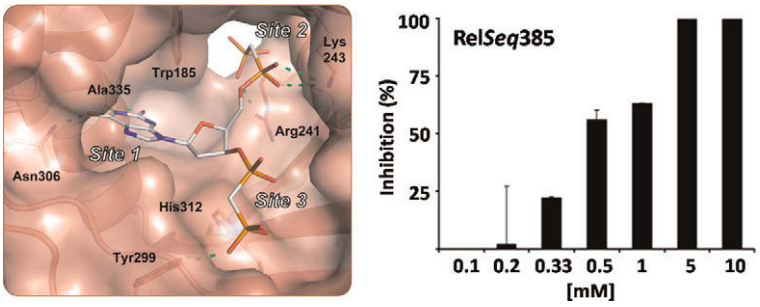
To deliver gold nanorods to tumor, a PEG–peptide conjugate, which contained a substrate sequence for a protease specifically expressed in tumor, was modified.

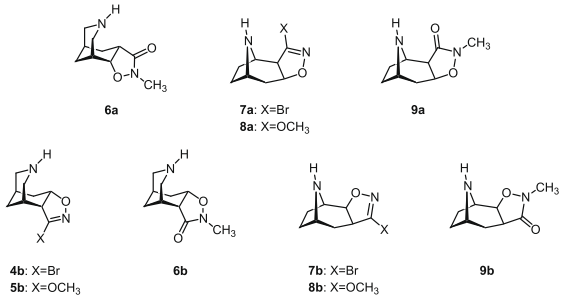


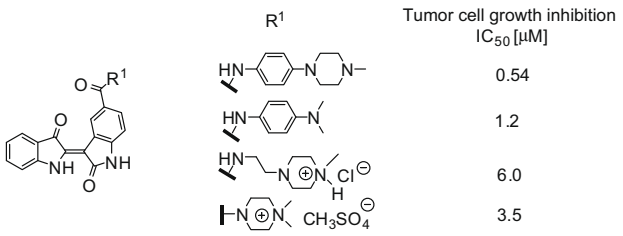




A series of novel berberine derivatives were designed, synthesized, and biologically evaluated as inhibitors of both acetylcholinesterase (AChE) and butyrylcholinesterase (BuChE).

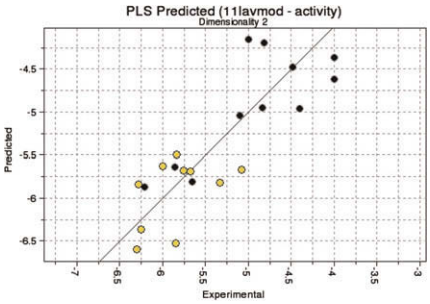


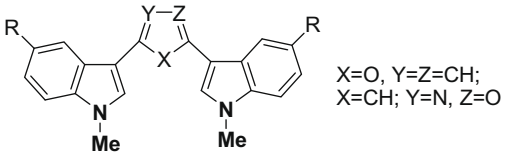




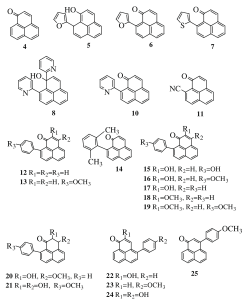
A series of indirubin-5-carboxamides was synthesized and evaluated for tumor cell growth inhibitory activity and solubility. Indirubins carrying amide substituents with basic centers show significantly enhanced solubility without loss of bioactivity.

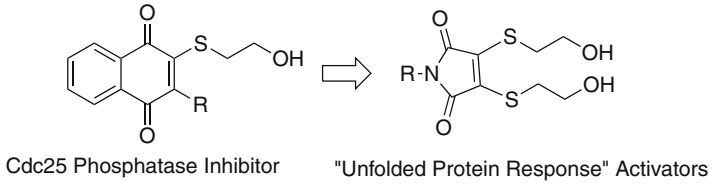
A modeling approach based on physico-chemical and pharmacokinetic properties, called Volsurf+, was used to design new heterocyclic compounds with antiproliferative activity. An Almond model, derived to have an overall structural insight on the above compounds, supported the validity of Volsurf and provided guidelines for the synthesis of new compounds.

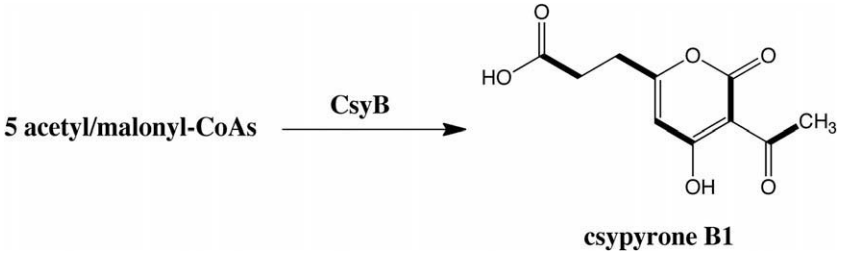


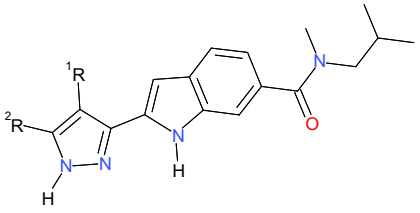


A series of novel 2,5-bis(3′-indolyl)furans and 3,5-bis(3′-indolyl)isoxazoles were synthesized and evaluated as antitumor agents.

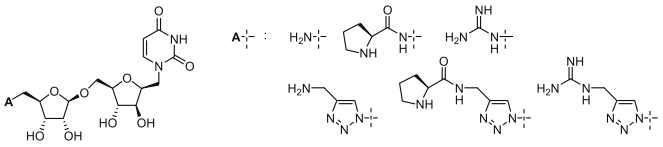


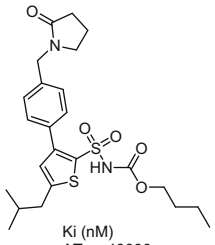






R^1 = Ph, R^2 = H, IC_{50}(ITK) = 0.33 μM
R^1 = Ph, R^2 = $PhCH_2$, IC_{50} (ITK) = 0.56 μM





*Corresponding author

Supplementary data available via ScienceDirect

COVER

An insight into biologically relevant chemical space showing the scaffolds of potential natural-product based inhibitors orbiting their target, the protein structure of protein 11-beta steroid dehydrogenase (PDB code 1xu7). Graphic produced using Pymol (http://www.pymol.org). [M. A. Koch, A. Schuffenhauer, M. Scheck, S. Wetzel, M. Casaulta, A. Odermatt, P. Ertl, H. Waldmann, Charting biologically relevant chemical space: A structural classification of natural products (SCONP), *PNAS* **2005**, *102*, 17272–17277 and S. Wetzel, H. Waldmann, Cheminformatic analysis of natural products and their chemical space, *Chimia* **2007**, *61*(6), 355–360].

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