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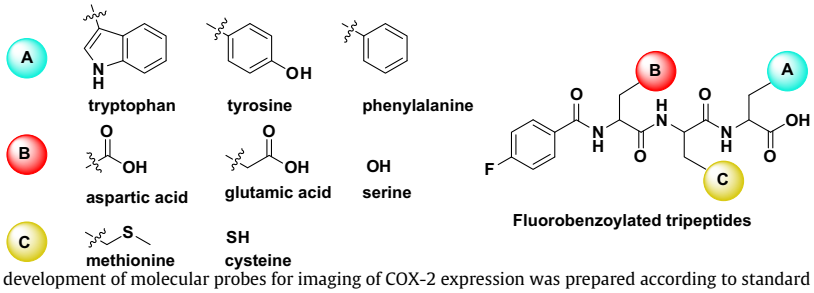
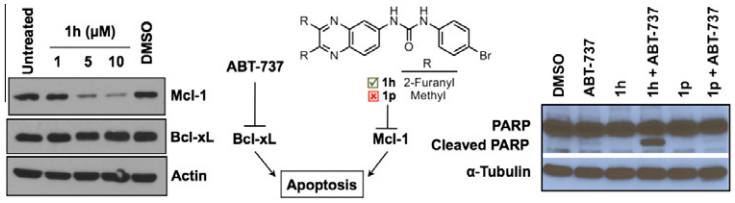
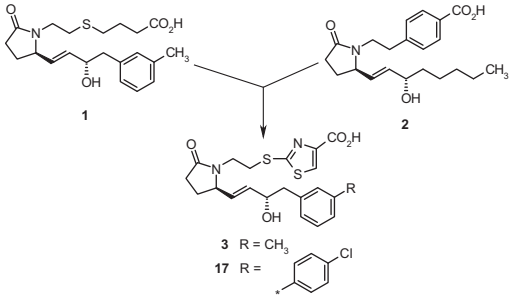
Contents

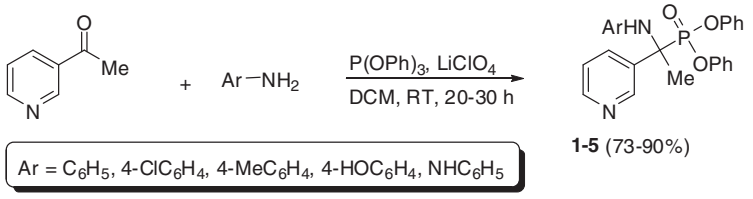
ARTICLES

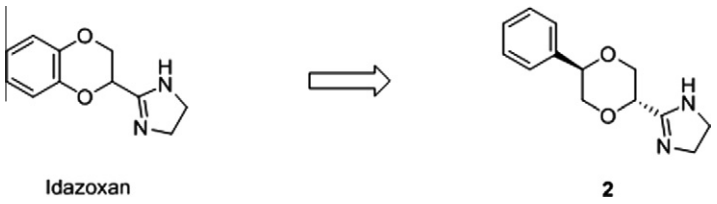


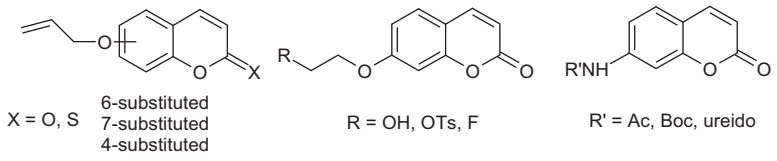
A series of fluorobenzoylated di- and tripeptides as potential leads for the development of molecular probes for imaging of COX-2 expression was prepared according to standard Fmoc-based solid-phase peptide synthesis. All peptides were assessed for their COX-2 inhibitory potency and selectivity profile in a fluorescence-based COX binding assay. Fluorbenzoylated tripeptide FB-Phe-Cys-Ser-OH was further used in molecular modeling docking studies to determine the binding mode within the active site of COX-2.



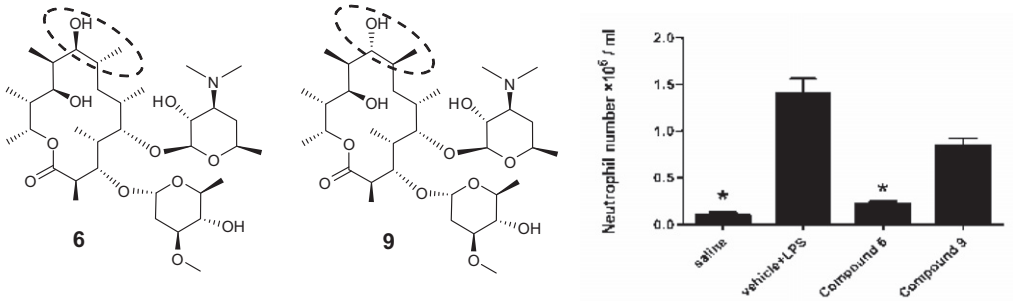


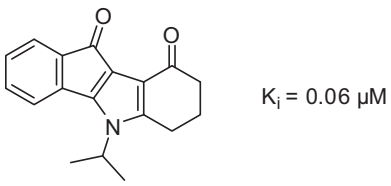


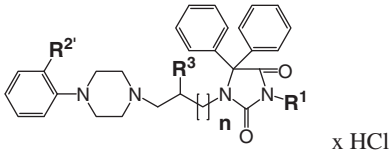




K_I (hCA I)= 8-90 μM; K_I (hCA II) > 200 μM; K_I (hCA IX) = 0.21 – 3.26 μM; K_I (hCA XII) = 0.28 – 2.83 μM

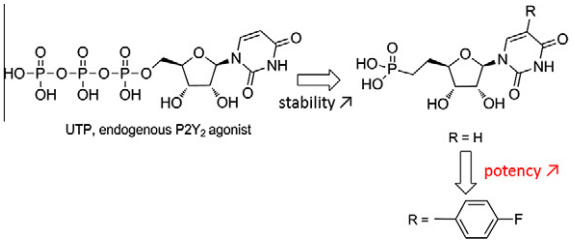


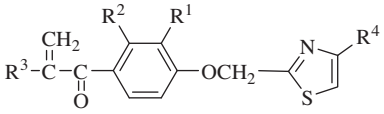




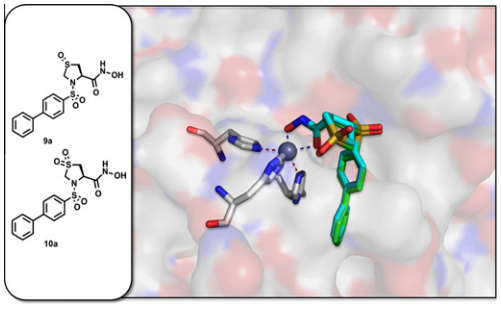
2a-21a

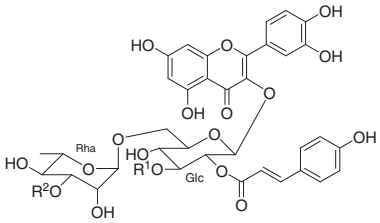
Association between α_1-adrenoceptor affinities, hERG K^+-antagonistic properties and antiarrhythmic activities for a series of phenylpiperazine derivatives of phenytoin (**2a**–**21a**) was investigated. Traditional- or microwave-aided syntheses were carried out.

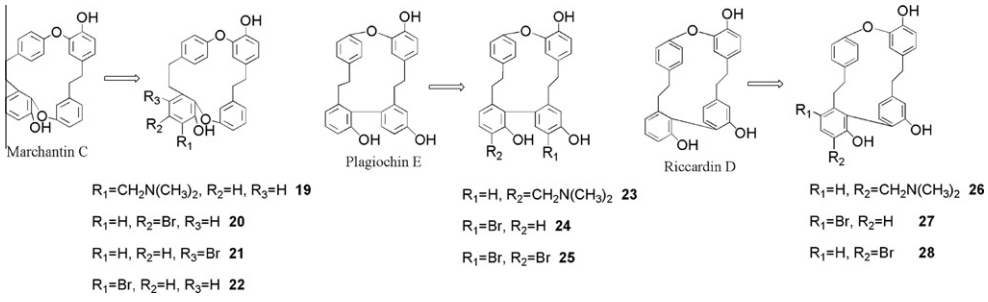


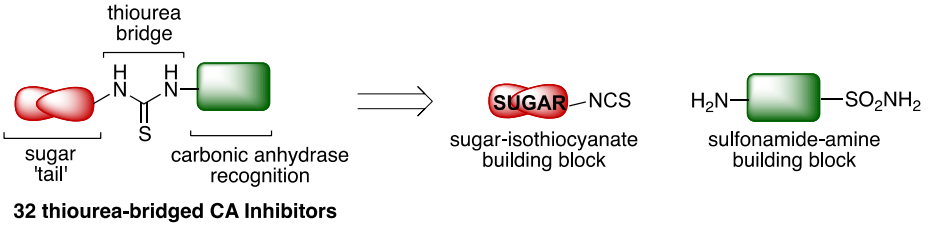


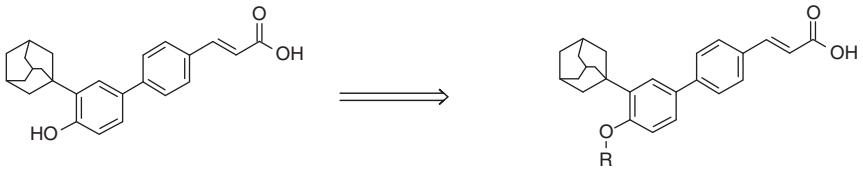
R^1=H, Cl or CH_3; R^2=Cl or CH_3;
R^3 = CH_3 or C_2H_5;
R^4=phenyl, 4-NO_2 phenyl, 2-naphthyl or 4-CF_3 phenyl

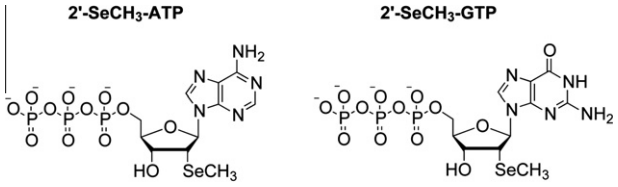


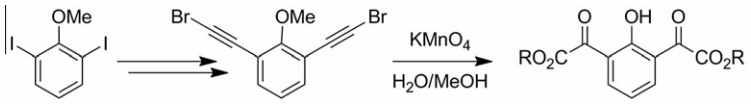


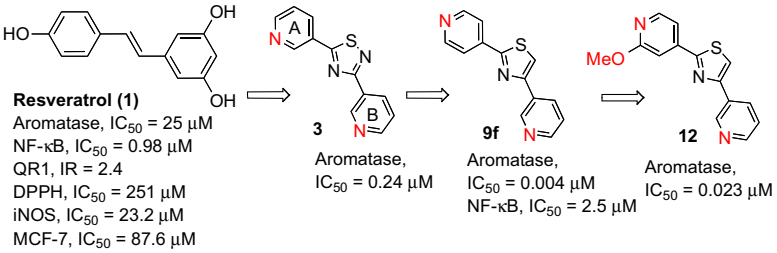


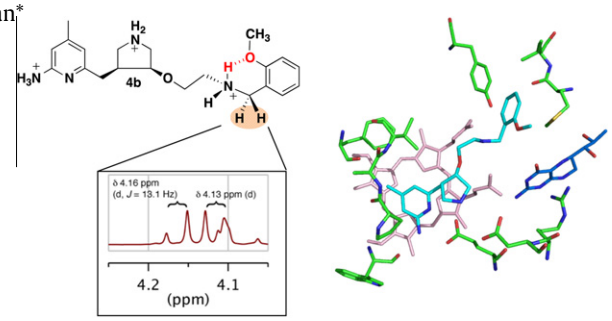


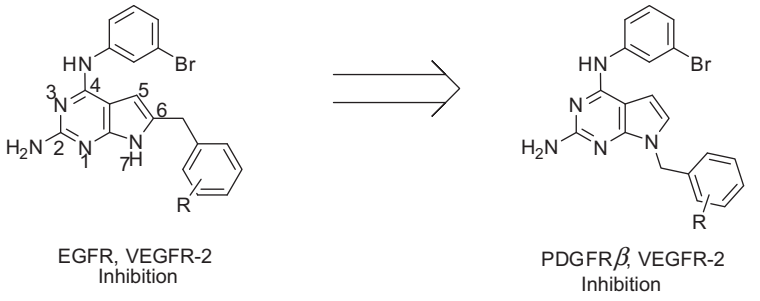


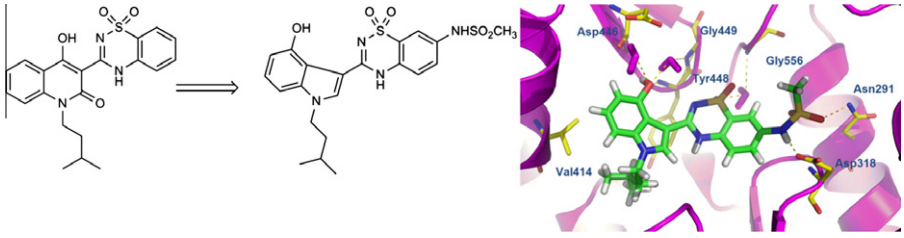












Guided structure-based activity prediction model applied in fragment hopping leads to the discovery of new benzothiadiazines derivatives.

*Corresponding author

Supplementary data available via SciVerse ScienceDirect

COVER

The cover image shows a 2′-methylseleno guanosine 5′-triphosphate, the synthesis of which is described by Santner et al. in this issue. Modified NTPs of this type are potential substrates for engineered RNA polymerases to generate long RNA transcripts for X-ray crystallographic applications. (Background RNA polymerase structure: PDB 2E2I) [Santner, T.; Siegmund, V.; Marx, A.; Micura, R. *Bioorg. Med. Chem. Lett.,* **2012,** *20,* 2416.]

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