Bioorganic & Medicinal Chemistry 16 (2008) 7081–7094

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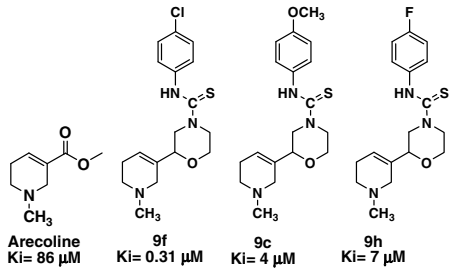
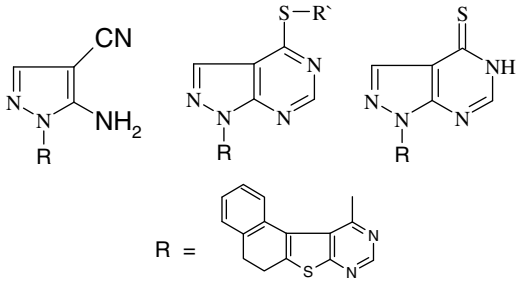
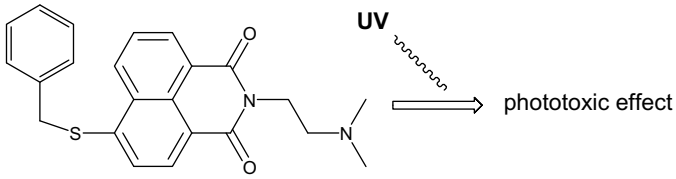
Bioorganic & Medicinal Chemistry Vol. 16, No. 15, 2008

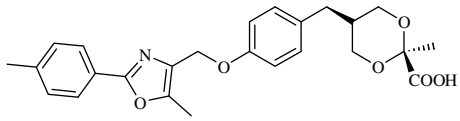
Contents

ARTICLES



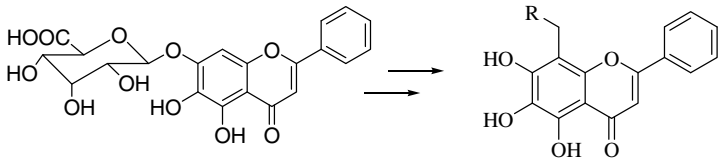




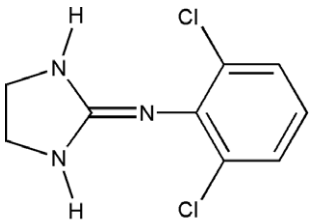


13b

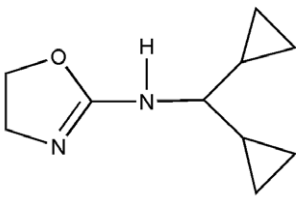
A novel class of PPARα/γ dual agonists containing 1,3-dioxane-2-carboxylic acid was described. Compound **13b** exhibited potent hypoglycemic, hypolipidemic and insulin sensitizing effects in *db*/*db* mice and Zucker *fa*/*fa* rats.



Synthesis and structure–activity relationship of nitrogen-containing flavonoid analogues as CDK1/Cyclin B inhibitors are reported.

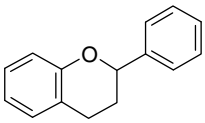


Clonidine

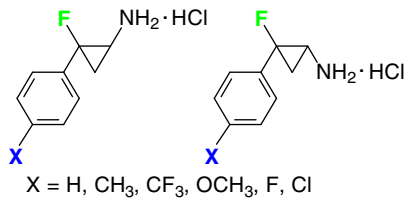


Rilmenidine

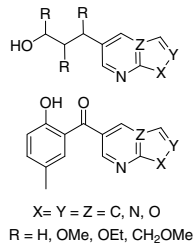
The quantitative structure–activity relationship (QSAR) study of 12 biologically active compounds, including clinically useful clonidine and rilmenidine, was carried out using multilinear regression method on Imidazoline-1 receptor and α_2-adrenergic receptor binding affinities on human platelets.



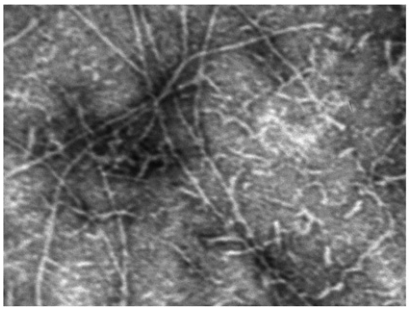
The SAR analysis of flavonoids against influenza virus neuraminidase revealed that for good inhibitory effect, the 4′-OH, 7-OH, C4=O and C2=C3 functionalities were essential.

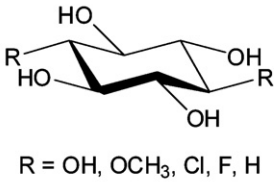


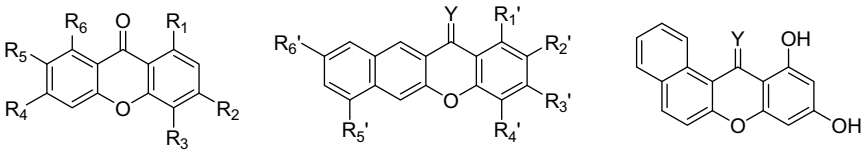
Electron-withdrawing *para*-substituents increase the potency of MAO A inhibition in the *trans*-series, while electron-donating groups have a weak influence on this activity. In contrast, aromatic ring substitution has essentially no effect on inhibition of MAO B. The corresponding *cis*-compounds are 10–100 times less active.



Three different series of pyrazolo[3,4-*b*]pyridines were synthesized and evaluated for their anti-inflammatory activity against TNF-α and IL-6. Several compounds showed promising IL-6 inhibitory activity, amongst which most potent analogue has IC_{50} 0.16 μM and is not cytotoxic (IC_{50} >100 μM).

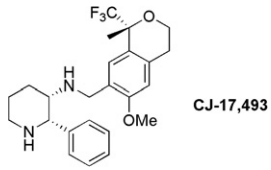


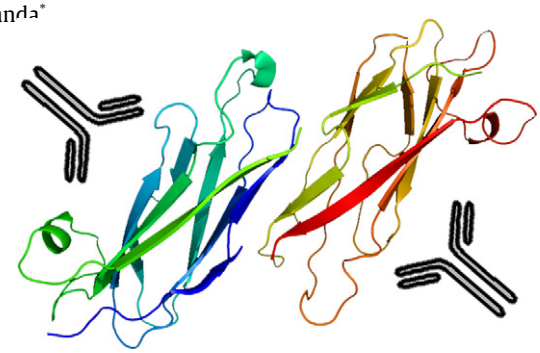


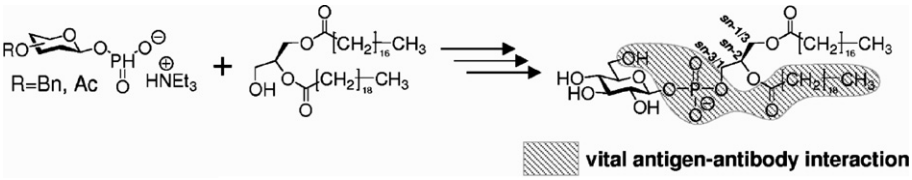


$\mathbf{X_{1-43}}$: R_1, R_2, R_3, R_4, R_5, R_6, R_1', R_2', R_3', R_4', R_5', R_6' = Various substitutions; Y = O, H_2

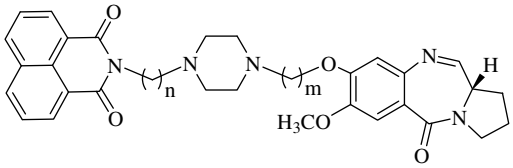
A QSAR model was established by multiple linear regression (MLR) method for a training set of compounds $\mathbf{X_{1-34}}$. The accuracy and predictive power of the proposed QSAR model were verified by LOO validation, Y-randomization, and test group validation with newly synthesized xanthone derivatives $\mathbf{X_{35-43}}$.



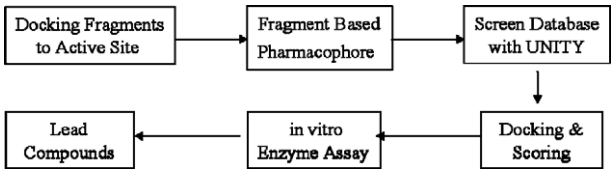


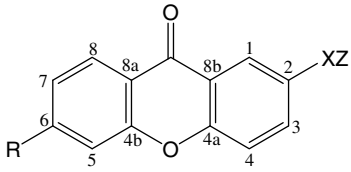


Chemical synthesis of phosphatidyl-β-D-glucoside (PtdGlc) and its analogues was achieved. The proposed structure of natural 6-*O*-Ac PtdGlc was confirmed. The reactivity of monoclonal antibody 'DIM21' towards PtdGlc and its analogues were mapped.

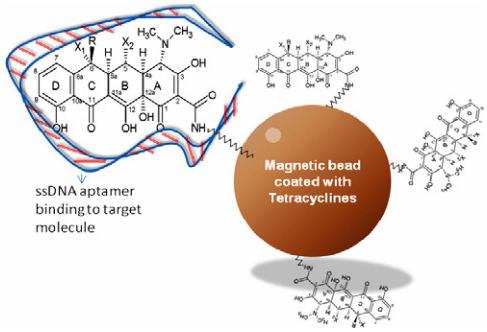


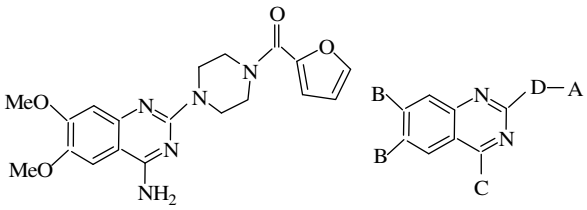
n = 2, 3, 4; m = 2, 3, 4



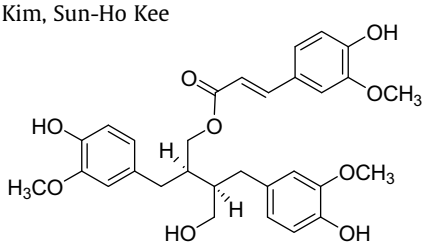


A series of appropriate alkanolamine and amide derivatives of xanthone were prepared and evaluated for anticonvulsant activity using maximal electroshock and subcutaneous pentylenetetrazole-induced seizures, and for neurotoxicity using the rotorod test on mice and rats.



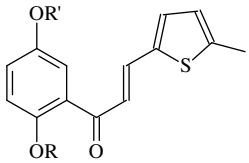


1 Prazosin Structural features studied (A-D)

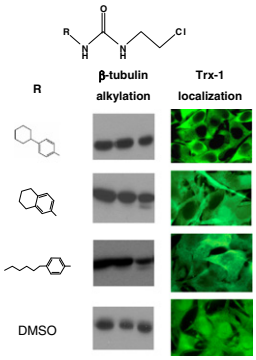


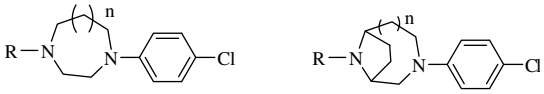
2

A new lignan derivative, hanultarin, was isolated and structure-determined. It inhibited the polymerization of the actin cycloskeleton and also showed cytotoxic effect against human lung carcinoma A549 and other cell lines.

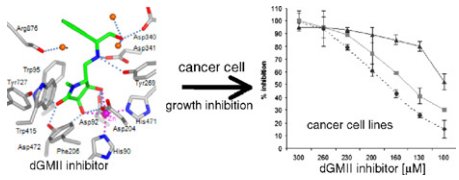


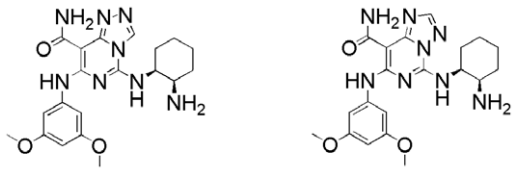
A series of 2′,5′-dialkoxylchalcones has been synthesized and evaluated their cytotoxic, anti-inflammatory and anti-oxidant activities.





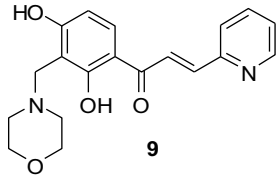
n = 0 or 1





10d **11**

A novel series of 1,2,4-triazolo[4,3-*c*]pyrimidine and 1,2,4-triazolo[1,5-*c*]pyrimidine derivatives were prepared, and their Syk family kinase inhibitory activities were assessed.



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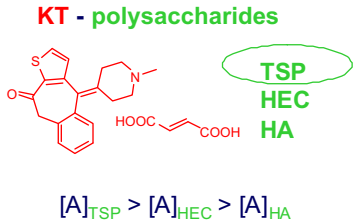
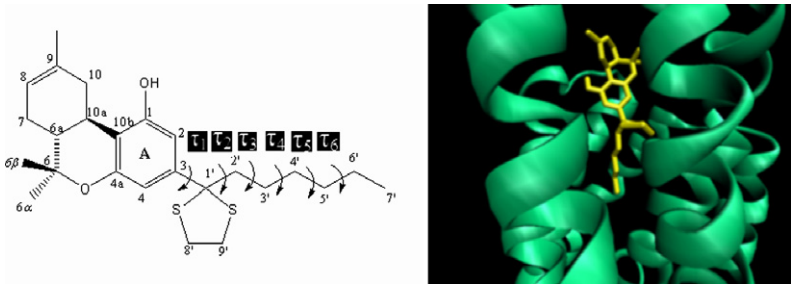
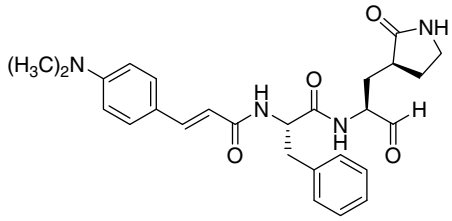
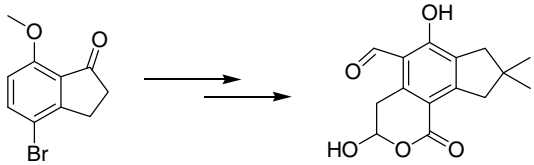


Nuclear magnetic resonance (NMR) spectroscopy demonstrated that, in aqueous solution, ketotifen fumarate bound more strongly to tamarind seed polysaccharide (TSP) than to hydroxyethylcellulose or hyaluronic acid. Results were confirmed by dynamic dialysis technique.

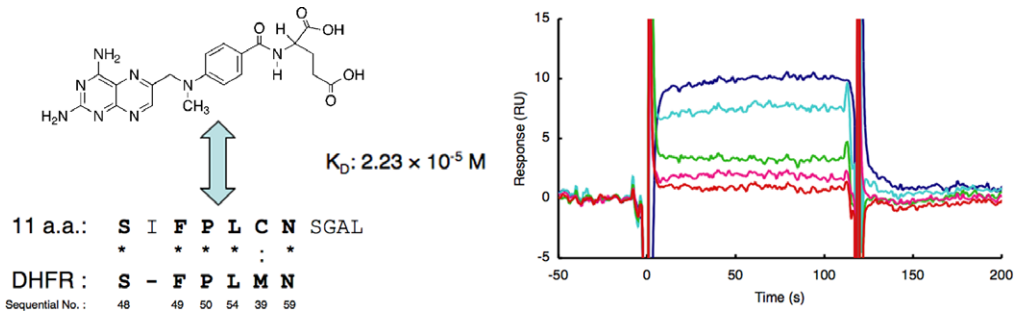


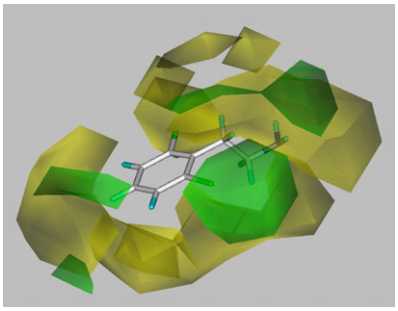


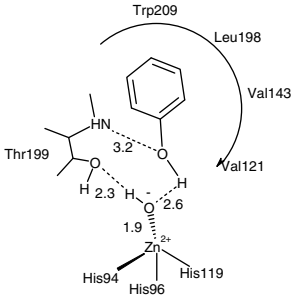
10b

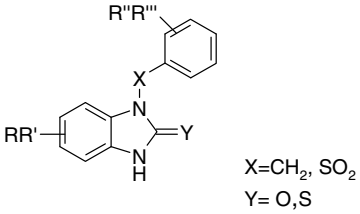


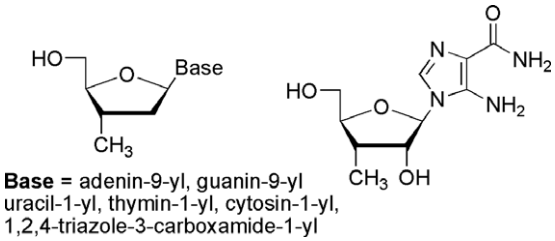
A novel synthesis of the human leukocyte common antigen-related phosphatase (LAR) inhibitor, illudalic acid, has been achieved by a route more amenable to structure modifications. A preliminary study of the structure–activity relationship (SAR) and of the mechanism of action of illudalic acid was conducted.

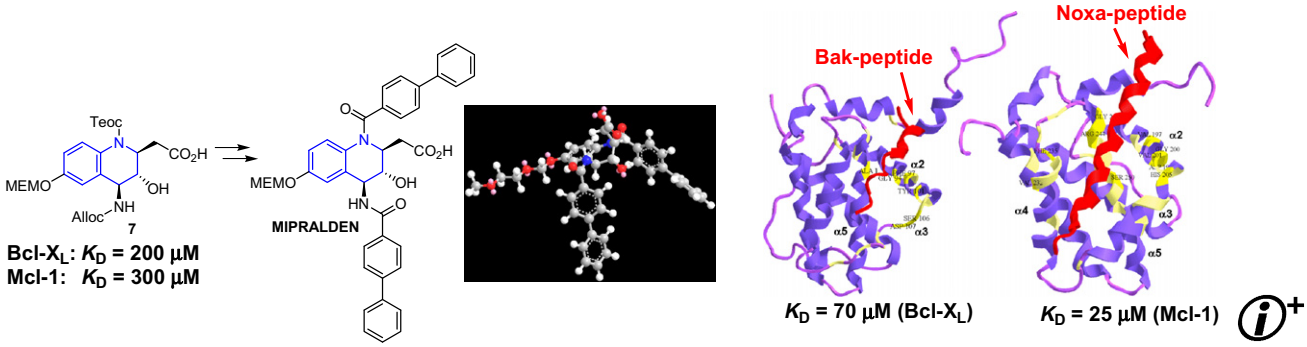


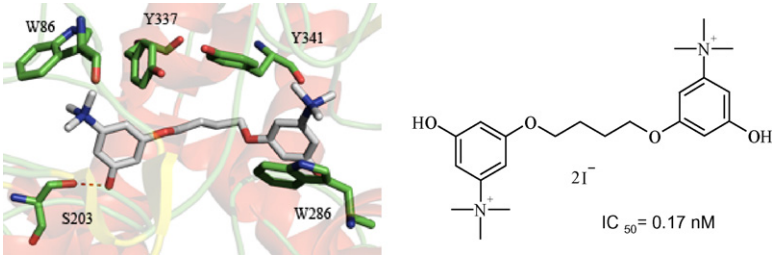


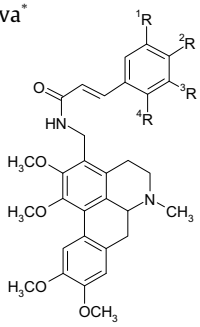




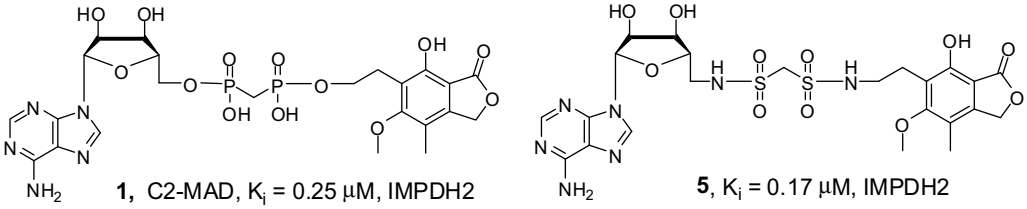


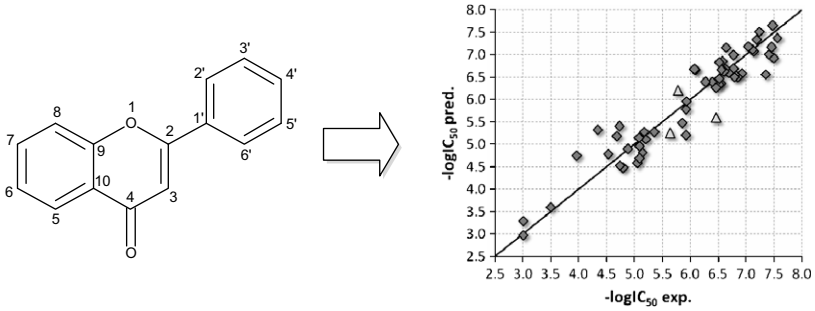


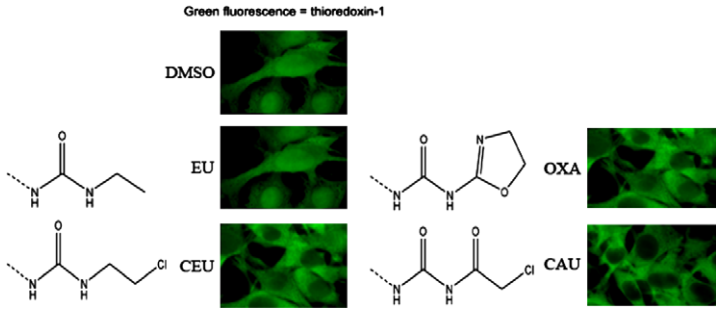


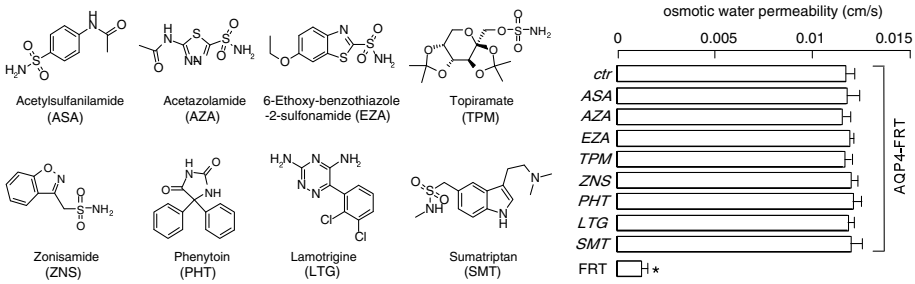


Cinnamoyl-, feruloyl-, sinapoyl-, *o*-, and *p*-coumaroyl amides of 3-aminomethylglaucine were synthesized, and their antiviral activity and antioxidant potential against DPPH* test were estimated.

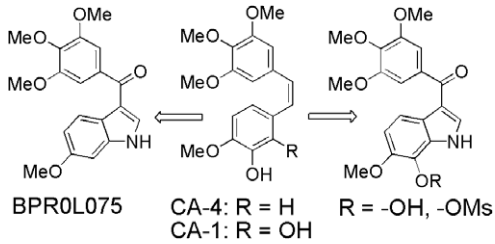


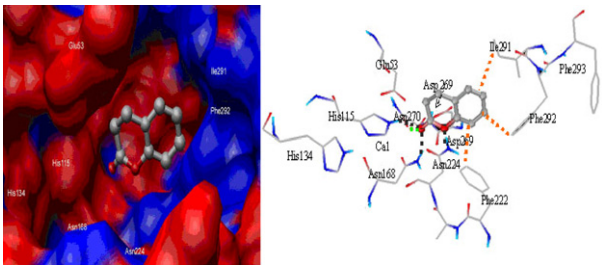


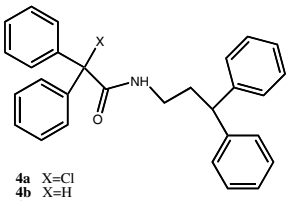




Several antiepileptics, arylsulfonamides, and related small molecules were tested for their ability to inhibit brain water channel AQP4. Multiple functional assays showed no inhibition by these compounds.

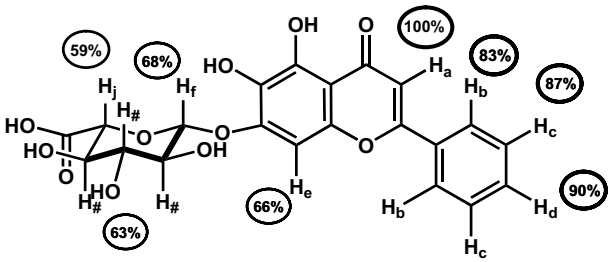






4a X=Cl
4b X=H
4c X=CH_3
4d X=OH

Eleven novel *N*-(3,3-diphenyl)propyl-2,2-diphenylacetamide derivatives and six triphenylacetamides were synthesized and tested as ligands of cannabinoid CB_1 and CB_2 receptors. Compound **4b** was the most potent CB_1 ligand.



*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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