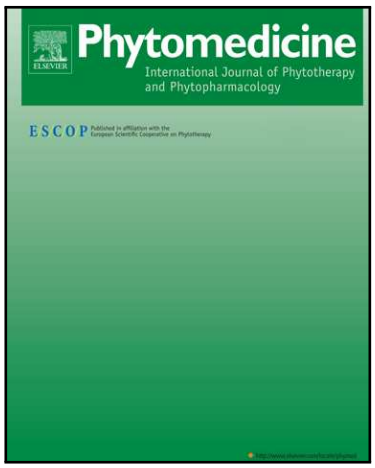

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Ilkay Erdogan Orhan , Dariusz Jedrejek , F. Sezer Senol , Ramin Ekhteiari Salmas , Serdar Durdagi , Iwona Kowalska , Lukasz Pecio , Wieslaw Oleszek

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Molecular modeling and *in vitro* approaches towards cholinesterase inhibitory effect of some natural xanthohumol, naringenin, and acyl phloroglucinol derivatives

Ilkay Erdogan Orhan[a,*], Dariusz Jedrejek[b], F. Sezer Senol[a], Ramin Ekhteiari Salmas[c], Serdar Durdagi[c], Iwona Kowalska[b], Lukasz Pecio[b], Wieslaw Oleszek[b]

[a]Department of Pharmacognosy, Faculty of Pharmacy, Gazi University, 06330 Ankara, Turkey
[b]Institute of Soil Science and Plant Cultivation, State Research Institute, Czartoryskich 8, 24-100 Pulawy, Poland
[b]Computational Biology and Molecular Simulations Laboratory, Department of Biophysics, School of Medicine, Bahcesehir University, 34349 Istanbul, Turkey

*Corresponding author:
Ilkay Erdogan Orhan, Ph.D.
E-mail address: (iorhan@gazi.edu.tr)

ABSTRACT

Background: Many natural products, particularly phenolic compounds, have been reported to have a strong inhibition against acetylcholinesterase (AChE) and butyrylcholinesterase (BChE), the key enzymes in the pathology of Alzheimer's disease (AD).

Hypothesis: Therefore, we hypothesized that some xanthahumol, naringenin, and acyl phloroglucinol derivatives (**1-14**) isolated from *Humulus lupulus* L. (hops) may have an inhibitory potential against AChE and BChE.

Methods: Inhibitory potential of compounds **1-14** were tested against AChE and BChE using ELISA microtiter assay. Different molecular docking simulations, including IFD and GOLD protocols, were implemented to verify the interactions between the ligands and the active site amino acids and also their binding energies inside the catalytic crevices of AChE and BChE. ADME/Tox analysis were used to determine pharmacological activities of the compounds.