Breast cancer resistance protein (BCRP/ABCG2): New inhibitors and QSAR studies by a 3D linear solvation energy approach

Titre	Breast cancer resistance protein (BCRP/ABCG2): New inhibitors and QSAR studies by a 3D linear solvation energy approach
Type de publication	Article de revue
Auteur	Nicolle, Edwige [1], Boccard, Julien [2], Guilet, David [3], Dijoux-Franca, Marie-Geneviève [4], Zelefac, Fabien [5], Macalou, Sira [6], Grosselin, Jeanne [7], Schmidt, Julien [8], Carrupt, Pierre-Alain [9], Di Pietro, Attilio [10], Boumendjel, Ahcène [11]
Type	Article scientifique dans une revue à comité de lecture
Année	2009
Langue	Anglais
Date	Jan-08-2009
Numéro	1
Volume	38
Titre de la revue	European Journal of Pharmaceutical Sciences
ISSN	09280987
Mots-clés	3D-QSAR [12], BCRP [13], Flavonoids [14], VolSurf descriptors [15]
Résumé en anglais	A series of compounds derived from naturally occurring flavonoids and synthetic analogs have been evaluated on cell lines overexpressing the wild-type breast cancer resistance protein (BCRP/ABCG2) half-transporter. Human ABCG2-transfected cells were used for screening their inhibitory activity. Five new natural compounds obtained from Morus mesozygia Stapf and one synthetic chromone, comprising a flavonoidic scaffold, were also evaluated. Based on the results obtained with a total of 34 compounds, a 3D linear solvation energy QSAR was investigated by VolSurf descriptors of molecular-interaction fields (MIFs) related to hydrophobic-interaction forces, polarisability and hydrogen-bonding capacity. Accuracy of the constructed 3D-QSAR model was attested by a correlation coefficient r2 of 0.77. Shape parameters and hydrophobicity were revealed to be major physicochemical parameters responsible for the inhibition activity of flavonoid derivatives and synthetic analogs towards ABCG2, whereas hydrogen-bond donor capacity appeared highly unfavorable.
URL de la notice	http://okina.univ-angers.fr/publications/ua10802 [16]
DOI	10.1016/j.ejps.2009.05.012 [17]
Lien vers le document	http://linkinghub.elsevier.com/retrieve/pii/S0928098709001559 [18]
Titre abrégé	European Journal of Pharmaceutical Sciences

Liens

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