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QSAR methods to determine the biological activity of coumarin derivatives

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This work is based on coumarinic derivaties with a biological activity such as antioxydant and anticancerigenic [1]activities through QSAR methods. These compounds have as nucleus 2-oxo-2H-chromen-3-yl

4-Xbenzoate [2] which are analogous to 3-bromophenyl 6-acetoxymethyl-2-oxo-2H-1-benzopyran-3-carboxylate, which is considered as a power inhibitor of tumor proliferation and angiogenis, present some water solubility and stability problems. The QSAR methods used, allows prediction of biological activities of news compounds and to conceive more actives ones against any given infection.

Here, we report the strucutral determination, prediction of biological activities and conception of biological molecules against cancer.

[1] Lacy, A. & O'Kennedy, R. (2004).Curr. Pharm. Des.10, 3797-3811

[2] Ziki, E., Yoda, J., Djande´, A., Saba, A. & Kakou-Yao, R. (2016). Acta Cryst.E72, 1562–1564

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