MOL2NET, International Conference Series on Multidisciplinary Sciences
http://sciforum.net/conference/mol2net-03

QSAR of natural sesquiterpene lactones as inhibitors of Myb-dependent gene expression

Gloria Castellano [a,*], Lucía Redondo [a], Francisco Torrens [b]

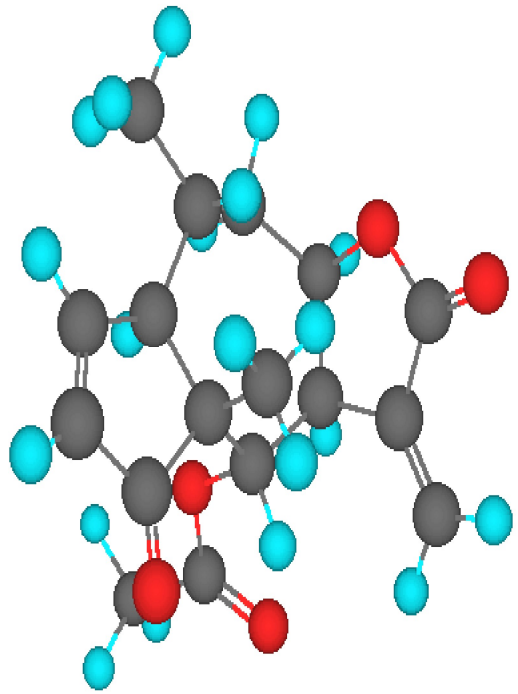
[a] Departamento de Ciencias Experimentales y Matemáticas, Facultad de Veterinaria y Ciencias Experimentales, Universidad Católica de Valencia *San Vicente Mártir*, Guillem de Castro-94, E-46001 València, Spain

[b] Institut Universitari de Ciència Molecular, Universitat de València, Edifici d'Instituts de Paterna, P. O. Box 22085, E-46071 València, Spain

* Corresponding author. Tel.: +34 963 544 431; fax: +34 963 543 274.

E-mail address: gloria.castellano@ucv.es (G. Castellano)

Graphical Abstract



Abstract. Protein c-Myb is a therapeutic target. Some sesquiterpene lactones suppress Myb-dependent gene expression, which results in a mechanism for their potential anti-cancer activity. Database ChEMBL is representative of lactones for physicochemical and physiochemical properties. We studied a dataset with 31 natural lactones are discussed in terms of quantitative structure–activity relationships, which objective is to predict inhibitors of Myb-induced gene expression. Several constitutional descriptors are related to structure–activity. Coefficients standard errors result acceptable in almost all equations. After cross-validation, linear equations for lactones, pseudoguaianolides and germacranolides are the most predictive. Most descriptors are constitutional variables.