Comment on "Are mechanistic and statistical QSAR approaches really different? MLR studies on 158 cycloalkyl-pyranones [Bhhatarai et al., Mol. Inf. 2010, 29, 511-522]"

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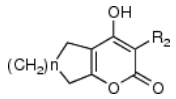
In their study, Bhhatarai et al. [1] develop quantitative structure-activity relationships (QSARs) for the inhibition of HIV protease by 158 so-called 4-OH cycloalkyl-pyranones. Bhhatarai et al. [1] define the 4-OH cycloalkyl-pyranone parent scaffold under study as the following:



By this definition, the numbered compounds studied by Bhhatarai et al. [1] and shown in Figure 1 herein do not appear to be cycloalkyl-pyranones (structures in Figure 1 were generated using the SMILES molecular notation provided in the Supporting Information of ref. [1] and the National Center for Biotechnology Information PubChem online structure generation tool [http://pubchem.ncbi.nlm.nih.gov/edit2/index.html]).

References

[1] B. Bhhatarai, R. Garg, P. Gramatica, Are mechanistic and statistical QSAR approaches really different? MLR studies on 158 cycloalkyl-pyranones, Molecular Informatics 29 (2010) 511–522.

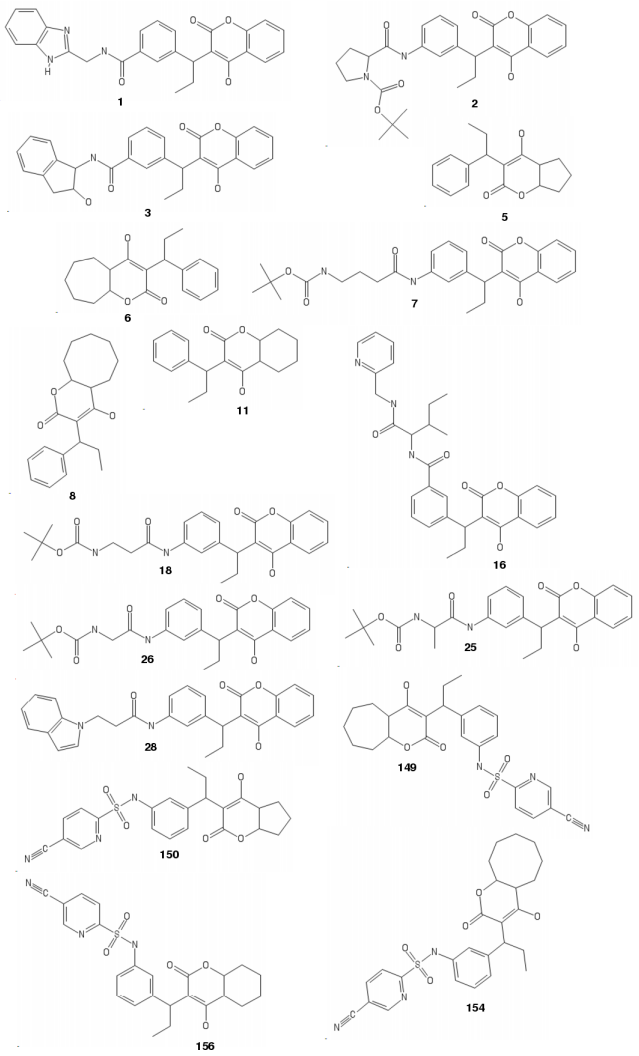


Figure 1: Numbered compounds from ref. [1] that do not appear to be 4-OH cycloalkyl-pyranones as defined by this source.

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