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Cytotoxicity Profile Prediction of Different Flavonoids in NCI-H187, LS174T, and MCF7 Cell Lines Using *In Silico* Simulations

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To Editor,

Computer simulation of the effects of a compound, based on its chemical and spatial structure, on biological systems (*in silico* or virtual investigation) is one of the most important and first steps in designing and evaluating the effects of chemical agents.[1]

Cell-line cytotoxicity profile prediction (CLC-Pred) based on chemical structural formula is an online predictive tool for investigating the probability of cytotoxicity of various chemical compounds in healthy and cancer cells based on the structure, which allows this possibility in the form of experimental screening.[2,3] Considering extensive *in vitro* studies evaluating the effects of flavonoids on different tumor cell lines and the lack of comparison between hundreds of different compounds from this family, this study was conducted to comparatively evaluate the effects of flavonoids of different categories on three simulated cell lines in an *in silico* model.

In this study, the CLC-Pred based on the specific spatial chemical structure of more than 2000 flavonoids (families of anthocyanins, benzoflavones, bioflavonoids (flavonoid dimers), catechins, chalcones, flavanones, flavones, flavonolignans, flavonols, isoflavones, and proanthocyanidins) which have been recorded in the PubChem database (https://pubchem.ncbi.nlm.nih.gov/, until November 10, 2022) was performed on three human cancer cell lines of lung (NCI-H187), colon (LS174T), and breast (MCF7), separately.

According to the recommended manner in similar studies, after receiving the molecular structure of each compound in SDF format from the PubChem database, the corresponding file was submitted to the web service for the CLC-Pred (http://way2drug.com/Cell-line/), and the probability of activity (Pa) was estimated (between 0-1). Higher Pa values indicate a great probability of having anti-tumor characteristics in the evaluated cell line.[4]

Compounds whose Pa values were reported as "no activity" or "na" by the software were excluded from the study and consequently a total of 1844, 1608, and 1588 compounds were evaluated for NCI-H187, LS174T, and MCF7 cell lines, respectively. In each cell line, 10 molecules with the highest value of Pa were reported. Their Pa values were presented next to the Pa of known antitumor compounds (doxorubicin, irinotecan, and tamoxifen, respectively).

The CLC-Pred of the flavonoids with the highest Pa values against the investigated cell lines is shown in Figure 1. In the NCI-H187 cell line, tinctormine, caeruleanone B, glycinol, erylysin C, and myristicyclin A obtained a higher Pa score even more than that of doxorubicin. Having evaluated the flavonoids on the LS174T cells, none of the flavonoids had as much Pa as Irinotecan, but the scores of luteolin tetramethyl ether, apigenin 7,4'-dimethyl ether, and luteolin were higher than those of the others, respectively.

It should be noted that even if the predictions are correct, the effect of a flavonoid on the cell culture environment cannot be generalized to a tumor environment and it needs to be included in the discussion.

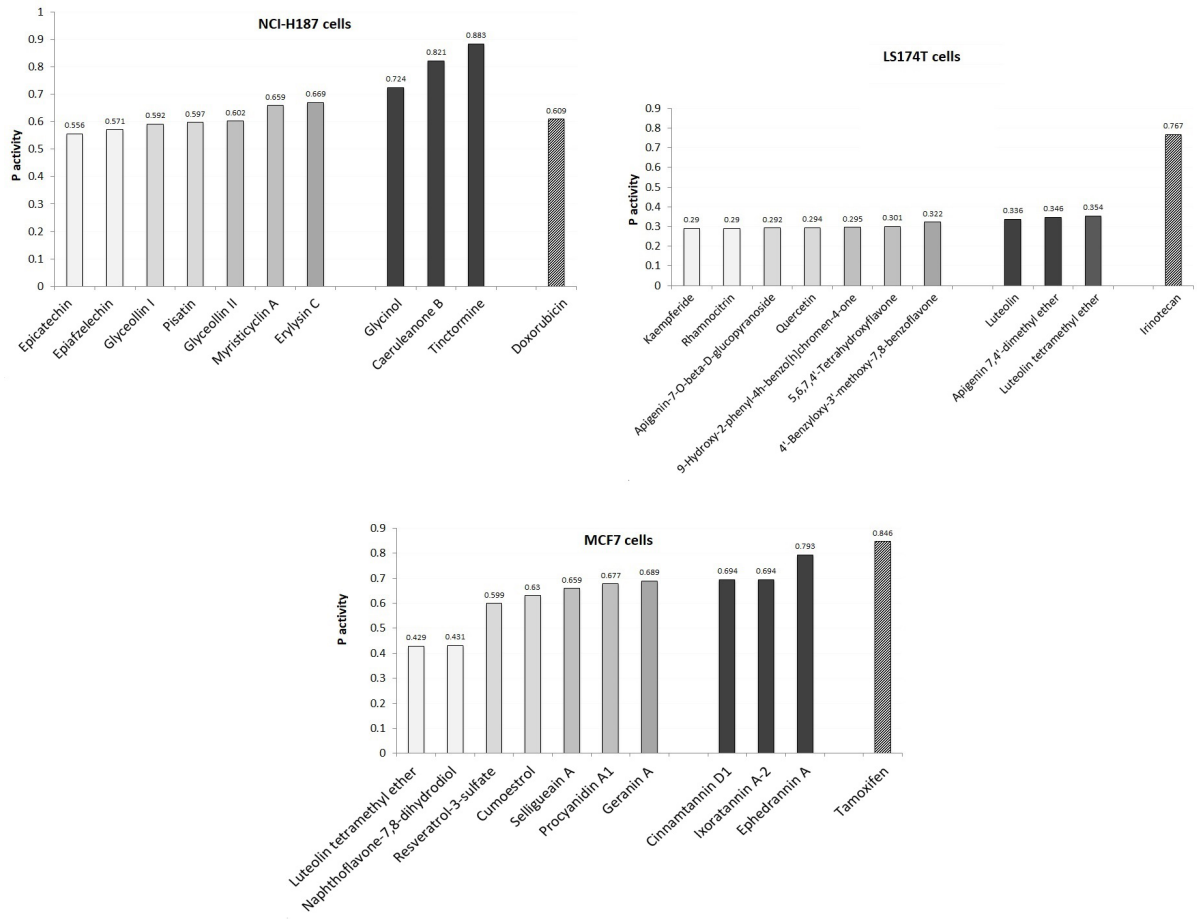

Figure 1. Cell-line Cytotoxicity Profile Prediction of Different Flavonoids in NCI-H187, LS174T, and MCF7 Cell Lines Using *in Silico* Simulation. The probability of activity (Pa) based on the chemical structure and by an online predictive tool (http://way2drug.com/Cell-line/) was estimated

Authors' Contribution

Conceptualization: Mahdi Mashhadi Akbar Boojar.
Data curation: Hasan Amanpour.
Formal analysis: Mahdi Mashhadi Akbar Boojar.
Funding acquisition: Mahdi Mashhadi Akbar Boojar.
Investigation: Mahdi Mashhadi Akbar Boojar.
Methodology: Hasan Amanpour.
Project administration: Hasan Amanpour.
Resources: Mahdi Mashhadi Akbar Boojar.
Software: Mahdi Mashhadi Akbar Boojar.
Supervision: Mahdi Mashhadi Akbar Boojar.
Validation: Mahdi Mashhadi Akbar Boojar.
Visualization: Mahdi Mashhadi Akbar Boojar.
Writing–original draft: Hasan Amanpour.
Writing–review & editing: Mahdi Mashhadi Akbar Boojar.

Competing Interests

No competing financial interests exist.

Ethical Approval

This study has been approved by the Ethical Committee of Baqiyatallah University of Medical Sciences (Code of Ethics: IR.BMSU.BAQ.REC.1398.060).

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