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Journal of Physics: Conference Series
Volume 1073, Issue 3, 7 September 2018, Article number 032001
2nd Physics and Technologies in Medicine and Dentistry Symposium, PTMDS 2018; The Margo HotelDepok, West Java; Indonesia; 18 July 2018 through 18 July 2018; Code 139960

In silico analysis of molecular interactions between the anti-apoptotic protein survivin and dentatin, nordentatin, and quercetin (Conference Paper)

(Open Access)

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Abstract

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Survivin is a member of the inhibitor of apoptosis (IAP) family and is reportedly overexpressed in various types of human malignancies. Because the phytochemical compounds dentatin, nordentatin, and quercetin have demonstrated antiproliferative effects in various cancer cell lines, we compared their binding affinities for survivin in silico. Molecular docking analyses were performed using PyMol, Discovery Studio Biovia 2017, AutoDock Vina, and AutoDock Tools version 1.5.4. These computations indicated greater survivin binding affinity of quercetin (ΔG -7.0 kcal/mol) than nordentatin and dentatin (ΔG -6.5 and -5.5 kcal/mol, respectively), but suggest that all three compounds act as ligand inhibitors of survivin. The present data warrant validation using in vitro and in vivo assays.

Indexed keywords

Engineering controlled terms: Binding energy | Cell culture | Cell death | Dentistry | Flavonoids

Engineering uncontrolled terms: Anti-apoptotic protein | Antiproliferative effect | Autodock vinas | Binding affinities | Cancer cell lines | Human malignancies | Inhibitor of apoptosis | Molecular docking

Engineering main heading: Phenols

ISSN: 17426588
Source Type: Conference Proceeding
Original language: English
DOI: 10.1088/1742-6596/1073/3/032001
Document Type: Conference Paper
Sponsors:
Publisher: Institute of Physics Publishing

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