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

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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.

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