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Prediction on binding affinity of Nordentatin and Quercetin against anti-apoptotic BCL-2 Protein (Article)

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Abstract

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Targeting apoptotic cell-death pathways has been a subject of growing interest in discovery of novel anti-cancer agents. Bcl-2 is a member of Bcl-2 family protein that is crucial for cell survival by suppressing apoptosis and its overexpression is frequently detected in many type of cancers. Inactivation of Bcl-2 has been considered as an ideal strategy in anti-cancer therapies. A large number of bioactive compounds derived from natural source including Nordentatin and Quercetin have been reported to possess anticancer activities. Here we report the binding affinities of Nordentatin and Quercetin in silico against anti-apoptotic Bcl-2 protein using molecular docking programs. We demonstrate for the first time that Nordentatin showed optimum binding affinity with Bcl-2, similar to those shown by Quercetin. As the Quercetin has been previously known to play a role in cancer cell apoptosis through down-regulation of Bcl-2, the result indicated that Nordentatin could also be proposed as a prospective anticancer molecule via inhibition of Bcl-2 protein. © 2018, University of Dicle.

Author keywords

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