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Exploring the Interaction of Natural Monoterpenes Limonene, Naringenin, and Thymol with Cell Cycle-Associated CDKs

بررسی برهمکنش مونوترپن های طبیعی لیمونین، نارینگنین و تیمول با CDK های مرتبط با چرخه سلولی

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Abstract:

مطالعه حاضر برهمکنش مونوترپن های طبیعی با CDK های مرتبط با چرخه سلولی را بررسی کرد. ما بر روی لیمونین، نارینگنین و تیمول تمرکز کردیم و از PubChem برای بدست آوردن کدهای ایزومری SMILES و از SwissTargetPrediction برای برای پیش بینی های موردنظر استفاده کردیم. یافته های ما بیشترین احتمال تعامل با CDK2 و CDK4 را برای نارینگنین نشان داد، در حالی که تیمول کمترین تعامل را با CDK2 نشان داد. در مقابل، لیمونین هیچ اثر متقابلی یا تعاملی نشان نداد. این یافته ها برهمکنش های بالقوه بین مونوترپن های طبیعی و CDK ها را پیشنهاد می کنند، که نشان دهنده نقش احتمالی آنها در تعدیل مسیرهای مرتبط با CDK برای فعالیت ضد سرطانی است.

Abstract:

The current study investigated the interaction of natural monoterpenes with cell cycle-associated CDKs. We focused on Limonene, Naringenin, and Thymol and used PubChem to obtain isomeric SMILES codes and SwissTargetPrediction for target predictions. Our findings revealed the highest probability of interaction with CDK2 and CDK4 for Naringenin, while Thymol exhibited the lowest probability of interaction with CDK2. By contrast, Limonene showed no interaction. These findings suggest potential interactions between natural monoterpenes and CDKs, indicating their possible roles in modulating CDK-related pathways for anticancer activity.

Method & Materials:

To investigate the interaction of natural monoterpenes with cell cycle-associated CDKS, PubChem (https://pubchem.ncbi.nlm.nih.gov), a comprehensive database of chemical substances and their biological

activities, was used to obtain the isomeric SMILES codes of each agent. Then, SwissTargetPrediction (http://www.swisstargetprediction.ch/), an online computational tool equipped with machine learning techniques, was utilized to provide target predictions.

Result & Conclusion:

Based on the analysis using PubChem and SwissTargetPrediction, we examined the interaction of various natural monoterpenes with CDKs. The monoterpenes investigated included limonene, D-limonene, naringenin, hesperidin, perillyl alcohol, thymol, carvacrol, geraniol, terpinolene, linalool, myrcene, and pulegone. Obtained findings indicated several probable interacting monoterpenes; Naringenin was predicted to interact with CDK2 and CDK4 with a probability of approximately 0.1. Conversely, thymol demonstrated a low probability of interaction with CDK2, approximately 0.04. Limonen didn't reveal any interaction with CDKs. These findings suggest potential interactions between natural monoterpenes and CDKs, highlighting their possible roles in modulating CDK-related pathways in the context of anticancer activity.

keywords:: Natural monoterpenes, Cyclin-dependent kinases, Cell cycle