

## Potential of Chemical Compounds from Coloring Plants (*Stenochlaena palutris*) as Competitors for ALK Protein Damage Due To Pesticide Exposure: In Silico Study

<b>Title</b>	Potential of Chemical Compounds from Coloring Plants ( <i>Stenochlaena palutris</i> ) as Competitors for ALK Protein Damage Due To Pesticide Exposure: In Silico Study
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<b>Abstract</b>	Pesticide active ingredients have widespread toxicity effects on target and non-target organisms. Continuous exposure to pesticides causes cancer. Kelakai is thought to have potential cytotoxic activity against the growth of cancer cells. The aim of this research is to examine the potential activity of chemical compounds on Anaplastic Lymphoma Kinase (ALK) proteins exposed to organophosphate pesticides in silico. Protein and ligand preparation with the Chimera program, Docking using SwissDock, as well as virtual screening using the pkCSM web and ProTox. Ethion and neophytadiene have the most negative $\Delta G$ values of -8.62 kcal/mol and -8.39 kcal/mol, respectively. The binding site for ethion and neophytadiene compounds with the ALK protein is right at the active site of the ALK protein. Ethion is the most toxic organophosphate pesticide and has the potential to be cytogenic. Neophytadiene from kelakai compounds has the potential to act as a competitor in inhibiting the ALK protein. The similarity in the type and number of binding residues in ethion and neophytadiene in the ALK protein indicates competition between ethion and neophytadiene.
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