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#73117 Summary

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Submission

Authors	Yeni Yeni, Rizky Arcintha Rachmania
Title	The Prediction of Pharmacokinetic Properties of Compounds in <i>Hemigraphis alternata</i> (Burm.F.) T. Ander Leaves Using pkCSM
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Title and Abstract

Title	The Prediction of Pharmacokinetic Properties of Compounds in <i>Hemigraphis alternata</i> (Burm.F.) T. Ander Leaves Using pkCSM
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Abstract	<i>The inflammatory process aids in healing and maintains the body's balance. Untreated acute inflammation can cause organ disease, which can lead to a chronic inflammatory phenotype. Hemigraphis alternata is a plant that has anti-inflammatory activity. The compounds contained in H. alternata leaves have been predicted to have an affinity for receptors involved in the inflammatory process. A large number of drug candidates were withdrawn from preclinical trials due to their poor pharmacokinetic profiles. Drug compounds must cross the barriers that exist in the body to reach their biological targets so that they can generate a biological effect. The pharmacokinetic features of 22 compounds in H. alternata leaves were predicted in order to search for</i>
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pharmacokinetic features of 22 components in *H. alternata* leaves were predicted in order to search for inflammatory medication candidates with suitable pharmacokinetic profiles. The pkCSM, a strategy for predicting and optimizing the pharmacokinetic properties of small molecules based on distance-based graph signatures was used in this work. The pkCSM employed 20 predictors separated into four groups: absorption, distribution, metabolism, and excretion. Based on the prediction findings, there are five substances with the best pharmacokinetic features, 8a-methyl-3,4,4a,5,6,7-hexahydro-2H-naphthalene-1,8-dione, (E)-3,7,11,15-tetramethylhexadec-2-en-1-ol, 2-methylenecholestan-3-ol, 5-(hydroxymethyl) furan-2-carbaldehyde and 2,3-dihydro-2,5-dimethyl-5H-1,4-dioxepin.

Indexing

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Supporting Agencies

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Authors: Yeni Yeni, Rizky Arcintha Rachmania

Title: The Prediction of Pharmacokinetic Properties of Compounds in *Hemigraphis alternata* (Burm.F.) T. Ander Leaves Using pkCSM

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Editor: Stalis Ethica

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Submission

Authors: Yeni Yeni, Rizky Arcintha Rachmania

Title: The Prediction of Pharmacokinetic Properties of Compounds in *Hemigraphis alternata* (Burm.F.) T. Ander Leaves Using pkCSM

Section: Articles

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