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Design and synthesis of novel potent anticoagulant and anti-tyrosinase pyranopyrimidines and pyranotriazolopyrimidines: insights from molecular docking and SAR analysis

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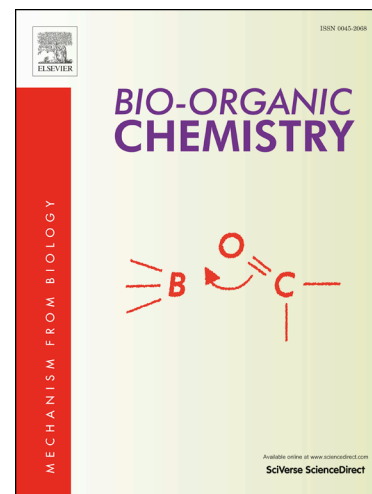
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**Design and synthesis of novel potent anticoagulant  
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insights from molecular docking and SAR analysis**

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**Abstract**

Pyrimidine-fused compounds are of great interest for the discovery of potent bioactive agents. This study describes the synthesis of novel pyranopyrimidines **3a-f** and pyranotriazolopyrimidines **4a-d** derivatives *via* the cyclocondensation reaction of  $\alpha$ -functionalized iminoether **2**, which was obtained from 2-amino-3-cyanopyrane **1**, with a series of primary aromatic amines and hydrazides, respectively. Structures of all synthesized compounds were established on the basis of spectroscopic methods including <sup>1</sup>H NMR, <sup>13</sup>C NMR and ES-HRMS. They were finally tested for their anticoagulant and anti-tyrosinase activities. Significant results have been obtained and the structure-activity relationship (SAR) was discussed with the help of molecular docking analysis.

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