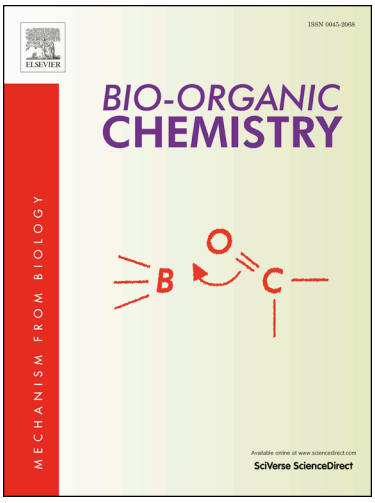

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PII: S0045-2068(18)30812-5
DOI: https://doi.org/10.1016/j.bioorg.2018.10.004
Reference: YBIOO 2538

To appear in: *Bioorganic Chemistry*

Received Date: 2 August 2018
Revised Date: 21 September 2018
Accepted Date: 4 October 2018

Please cite this article as: M. Debbabi, V.D. Nimbarte, S. Chekir, S. Chortani, A. Romdhane, H. Ben jannet, Design and synthesis of novel potent anticoagulant and anti-tyrosinase pyranopyrimidines and pyranotriazolopyrimidines: insights from molecular docking and SAR analysis, *Bioorganic Chemistry* (2018), doi: https://doi.org/10.1016/j.bioorg.2018.10.004

Design and synthesis of novel potent anticoagulant and anti-tyrosinase pyranopyrimidines and pyranotriazolopyrimidines : 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 α-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 ^{1}H NMR, ^{13}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.