Synthesis, antiplatelet aggregation activity, and molecularmodeling study of novel substituted-piperazine analogues. Khairia M. Youssef • Mohamed A. Al-Omar • Hussein I. El-Subbagh • Laila A. Abou-zeid • Abdel-Galil M. Abdel-Gader •

khairia M. Youssef

Abstract

New carbamoylpyridine and carbamoylpiperidine analogues containing nipecotic acid scaffold were designed, synthesized, and evaluated for their platelet aggregation inhibitory activity. Molecular modeling investigation was performed and the impact of lipophilicity on activity was also discussed. Structure activity relationship among this series was obtained. N1-[1-(4-bromobenzyl)-3-piperidinocarbonyl]-N4-(2-chlorophenyl)-piperazine hydrobromide (20), and 1,4-bis-[3-[N4-(2-chlorophenyl)-N1-(piperazinocarbonyl)]-piperidin-1-yl-methyl]-benzene dibromide (30) are the most active antiplatelet aggregating compounds in this study, both at concentration of 0.06 lM.

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