Molecular docking and in silico ADME study of Novel N9-substituted Purines targeting CK1 and abl-tyrosine kinase. Iten M. Fawzy1, Khairia M. Youssef 1, Nasser S. M. Ismail2, Deena S. Lasheen2 and Khaled A. M. Abouzid2

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Abstract

Novel N9-substituted purines were designed with anticipated anticancer activity based on the idea presented by recent publications were new compounds were synthesized combining the purine system in their structure in order to explore possible interactions with the different regions of the ATP binding site in several disease-related protein kinases especially cancer [1]. The study was supported by an in silico molecular docking study against both casein kinase-1 (CK1) and Bcr-abl-tyrosine kinase together with an in silico ADME study to assure the bioavailability of these compounds.

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