# A molecular docking and ADMET study of a promising compound of the Brazilian semi arid with inhibitory potencial of IKK-B

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**Abstract**

The enzyme IKK-$\beta$ modulates nuclear transcription factor (NF-?B) action directly affecting the transcription response of genes encoding proteins important for immune and inflammatory response. The Brazilian semi-arid compounds can be configured as scafolds for new anti-inflammatory agents. Several binders isolated from Brazilian semi arid plants were evaluated, selecting the best complexes with the IKK-$\beta$ structure and their ADMET characteristics. Binder structures were designed and deposited in the Semi arid Molecule Database (SAM Database), hosted in the Laboratory of Bioinformatics and Computational Chemistry (LBQC-UESB). The enzyme structure was downloaded from PDB database (4KIK) and computational chemistry tools (Marvin Sketch, Autodock Vina, Pymol 1.7, Discovery Studio 4.0 and Osiris Property Explorer) were used to prepare the structures of the compounds for the molecular docking assay and evaluation of their ADMET characteristics. The SAM0850 binder (-6.5kcal/mol) had lower affinity energy with IKK-$\beta$, when compared to ATP (-7.3 kcal/mol), estaurosporine (-7, 7kcal/mol), GSK-7 (-9, 5kcal/mol) and higher affinity energy than acetylsalicylic acid (-5.8kcal/mol) and mesalasin (-5.5kcal/mol)/mol). The compound SAM0850 did not demonstrate toxicity in the silicon prediction, the molecular dynamics of the complexes and in vitro tests assays wiil be the next steps.

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