

## [P39] Search of new inhibitors of PI3K $\delta$

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The enzyme family Phosphatidylinositol-4,5-bisphosphate 3-kinase (PI3K) is involved in multiple cellular pathway (cellular proliferation, growth, survival). This family can be separated in 3 classes (I, II and III) [1]. Class I possesses 4 different isoforms : PI3K $\alpha$ , PI3K $\beta$ , PI3K $\delta$  and PI3K $\gamma$ . In this project, we focus our work on the isoform PI3K $\delta$ , because this is mainly localized in B-cells. This type of cells are responsible for the cancer B-cell lymphoma. We are in partnership with the team of Pr. A. Boumendjel, MEDCHEM, from l'Université Joseph Fourier de Grenoble. They have discovered a molecule with a specific activity for our target of interest, a chalcone modified from plants called MBL. This study aimed to find a calibration curve to obtain the best scoring function ; the correct pose of MBL in the protein PI3K, to explain it's affinity and specificity toward PI3K $\delta$ , using molecular docking, molecular dynamics, and scoring methods.

### Bibliography:

[1] A.B; S.M; O.W. Nature Chemical Biology 6 (2010) 117-124.