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Molecular dynamics study of autotaxin with potential allosteric inhibitors

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Autotaxin is an enzyme catalyzing the synthesis of lysophosphatidic acid, a lipid signaling molecule involved in several cellular responses such as cellular survival, proliferation, differentiation, and migration. Nevertheless, abnormal expression of autotaxin is correlated with numerous cancer and fibrosis, therefore autotaxin is considered as drug target over years. All of currently studied autotaxin inhibitors bind in the orthosteric site of autotaxin. However, developing allosteric inhibitors can be valuable based on pharmacological aspects, such as more target-specific and cause less side effects. In this work, dynamics of autotaxin in free form and in complex with six ligands are studied by using molecular dynamics approach in order to observe the effect of allosteric binding to orthosteric site. As a result, four of six ligands found to affect the positions of orthosteric site significantly.

Biography

Eko Aditya Rifai is currently a PhD student in Computational Toxicology at Vrije Universiteit Amsterdam, after pursuing his Bachelor's and Master's degrees at Universitas Indonesia and University of Glasgow, respectively. His research interests are using computational methods to discover potential inhibitors of enzymes correlating in human diseases and to examine interactions of drug candidates with target and off-target proteins.

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