Abstract: ERK2 is a mitogen-activated protein kinase. When ERK2 undergoes dual phosphorylation, it interchanges between two states “L”, loose, and “R”, rigid. These two configurations are then kept at these distinct states by an inhibitor. Based on HX-MS data, coupling occurs at the activation loop and activation site when interchanging between L and R states. Thus inhibitor binding controls the configurations of the Glycine rich activation loop and active site. The structure of dually phosphorylated ERK2 fluctuates L⇌R to form an adequate active site based on inhibitors. Using Partial Optimum Order Likelihood (POOL), electrostatics forming at these active sites are calculated. These electrostatic calculations give insight on configurations, location of activation loops, and active sites as well as other genomic properties, furthering our knowledge of protein-kinase interactions.

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