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# Computational Analysis of Potential Inhibitors Selected Based on Structural Similarity for the Src SH2 Domain

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**Abstract :** The inhibition of SH2 domain regulated protein-protein interactions is an attractive target for developing an effective chemotherapeutic approach in the treatment of disease. Molecular simulation is a useful tool for developing new drugs and for studying molecular recognition. In this study, we searched potential drug compounds for the inhibition of SH2 domain by performing structural similarity search in PubChem Compound Database. A total of 37 compounds were screened from the database, and then we used the LibDock docking program to evaluate the inhibition effect. The best three compounds (AP22408, CID 71463546 and CID 9917321) were chosen for MD simulations after the LibDock docking. Our results show that the compound CID 9917321 can produce a more stable protein-ligand complex compared to other two currently known inhibitors of Src SH2 domain. The compound CID 9917321 may be useful for the inhibition of SH2 domain based on these computational results. Subsequently experiments are needed to verify the effect of compound CID 9917321 on the SH2 domain in the future studies.

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