Identification of lead molecule against Acetyl-CoA carboxylases of *Phalaris minor*

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ABSTRACT

Phalaris minor is an aggressive winter weed and is one of the major biotic reductions in wheat crop production. After the withdrawal of isoproturon around the year 1995, FOP, DEN and DIM group of herbicides were the only choices of herbicide to check the growth of *Phalaris minor* in wheat crops. However, this group of herbicides also developed resistance by the year 2005. The ACCase protein of *P. minor* and wheat share almost 93% of sequence similarity. This imposes a great challenge to design a selective herbicide against *P. minor* and therefore, it is pertinent to identify the lead molecule against ACCase of *P. minor*. To model the structure of protein, target template alignment has been performed. Based upon which model has been generated. To validate the model structure, several validations for stereochemical arrangement, quality and compactness has been performed. Modelled protein has been docked with the reference DEN group molecule to get a better predicted binding affinity and ligand efficiency. Identification of hit molecule and prioritisation of hit through Virtual screening of several small molecule databases has been used and 757 molecules were identified and filter out through ADME. The threshold was set to be the binding affinity of reference DIM group and filtering was done. It has been followed by filtering molecules based on the properties and descriptors of known reference herbicide molecules in order to sort molecules and to remove the false positive result. Further, it has been followed by simulation studies.

Keywords: *Phalaris minor*, acetyl-CoA carboxyl, Molecular Docking, Molecular Dynamic Simulation,

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