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Mechanism of isoproturon resistance in phalaris minor: In silico design, synthesis and testing of some novel herbicides for regaining sensitivity

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Phalaris minor, a major weed growing in wheat fields has acquired resistance towards the only accessible herbicide isoproturon. D1 protein encoded by PsbA gene, the binding site for isoproturon has shown to be having four mutations. D1 protein of both susceptible and resistant biotypes has been modeled, volume and area of active site of both types has been simulated. Isoproturon was docked at the active site of both D1 proteins. Simulation of resistant D1 protein indicates that the resistance is due to alteration in secondary structure near the binding site, resulting in loss in cavity area, volume and change in binding position, loss of hydrogen bonds, hydrophobic interaction and complete loss of hydrophobic sites. To regain sensitivity in resistant biotype new analogs of isoproturon molecule have been designed, synthesized, characterized and tested through pot assay. Among these eighteen analogues we found the triazole analog as having potential to replace isoproturon.