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Molecular modeling and computational simulation of photosystem-II reaction centre to address isoproturon resistance in phalaris minor

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Phalaris minor is a notorious weed of wheat crop which has developed resistance against Isoproturon, the only herbicide used to control it over a number of years. Resistance against Isoproturon is due to mutation at binding site reported by Tripathi et al 2004 .The binding site of Isoproturon is proteins of photosytem–II (PS-II) reaction center. In present study we have modeled and simulated PS-II of *Phalaris minor* selecting the crystal structure of PS-II from thermosynechococcus elongates (2AXT.pdb) as template. Loop regions were refined and simulated with Gromacs in vacuum, water and lipid (POPG) environments, to keep the modeled protein in natural environment. In order to preserve compatibility with ligands and cofactors we adapted ffgmx forcefield. System were minimized for 20 ps of steepest decent, equilibrated for pressure with isotropic pressure coupling (Tp=1.0ps) to 1 bar and temperature coupling (T_t =0.1ps) to 310K, using Berendsen protocol and subjected to 100 ps of MD simulation. As a result we obtained best model in lipid biphasic environment, of Ramachandran score in core, allowed, and disallowed regions 80.7, 17.0 and 2.3 respectively and overall quality factor 94.118. Final model contains five chlorophylls, two plastoquinones, two phenophytins and a bicarbonate ion along with cofactor Fe and OEC (Oxygen evolving center). This model shows that binding site of isoproturon shares both D1and D2 proteins. Modeled reaction center was used for cavity prediction, and docking and receptor based pharmacophore modeling for design and development of new isoproturon analogs.