APCRP: Development of ResistanceAlert – a prototype computational biology-based early warning system of herbicide resistance for invasive aquatic plant management

Product

Mutations occur randomly or in response to selective pressure; however, not all mutations confer herbicide resistance. As an integral part of invasive aquatic plant management, chemical control through use of registered aquatic herbicides and algicides is widely employed by aquatic plant managers in both private and public water bodies throughout the United States. Although very few cases of herbicide resistance have been confirmed for invasive aquatic plants (except hydrilla), lessons learned from terrestrial weeds serves as an alarming warning. Aquatic herbicide resistance management has therefore received increased attention, especially in light of the fact that all of the aquatic herbicides registered since 2003 (including carfentrazone, penoxsulam, imazamox, flumioxazin, bispyribac, and topramezone) are single site-of-action compounds (i.e., herbicides target a single plant specific enzyme) which have shown potential for weed resistance development in terrestrial systems. Currently, managers and applicators have limited tools and resources to mitigate the evolution and reduce the risk of herbicide resistance in both terrestrial and aquatic weeds. The objective of this research is to develop ResistanceAlert, a macromolecule structural biology-based computational tool that can be used to inform field managers when a mutation is resistance-conferring (Figure 1).

ResistanceAlert enables the prediction of unknown resistance conferred by un-documented new mutations in the aquatic weed or algal population subject to chemical control actions. This tool can empower field managers in decision making with regard to the biotype-specific choice of herbicides. The ResistanceAlert software package consists of a series of computational models that predict the interaction and affinity between a given chemical ligand (herbicide) and its potential binding sites in the target macromolecule (enzyme/protein). As a first step towards this goal, a ResistanceAlert prototype will be developed using the four acetohydroxy acid synthase (AHAS) inhibitors as the testing herbicides and three representative invasive aquatic plants as the target species.

Applications

Many invasive plant control programs rely on single modes of action for a variety of cost, environmental permitting, and efficacy reasons. While cost savings and control efficacy are the two major factors in assessing the success of a chemical control action, the ability to protect the long-term utility of aquatic herbicides is also very important. Recent experiences with fluridone resistance in Florida demonstrates the problems associated with discovering resistance issues after

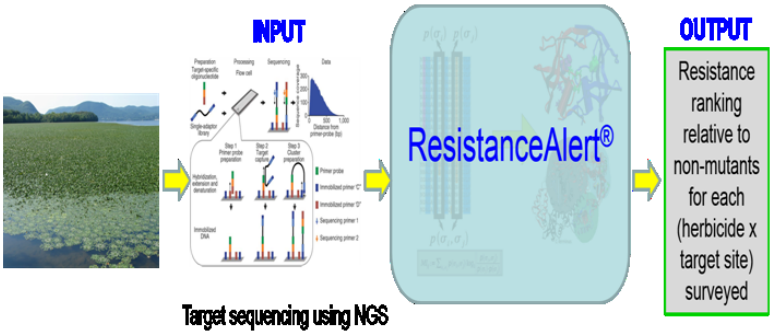

Figure 1: ResistanceAlert is a structural biology-based computational program that predicts resistance-conferring mutations in invasive aquatic plants. By, binding pocket prediction, molecular docking and molecular dynamics, ResistanceAlert characterizes quantitatively the interaction and affinity of a small molecule (herbicide) in a macromolecule (enzyme or receptor).

they have become widespread. As a result, the use of Fluridone has essentially been lost as a hydrilla control tool in many public waters in Florida. The ability to predict herbicide resistance for given management programs will better inform managers which combinations of herbicides and target plants may be particularly susceptible to resistance development. Early intervention with alternate modes of action or management strategies may prevent resistance from becoming widespread and the loss of a control tool.

System Requirements

System Requirements ResistanceAlert is a software package that runs on both Windows and Linux operating systems. More details will be provided when it is fully developed.

Status

ResistanceAlert is funded from FY16 to FY18. If the prototype product meets expectations, we will expand ResistanceAlert to include more aquatic herbicide targets (e.g., 4-hydroxyhenyl-pyruvatedioxygenase or HPPD, protoporphyrinogen oxidase or PPO, phytoene desaturase or PDS, and 5-enolpuruvyl-shikimate-3-phosphase or EPSP).

Get It Here

The source code of ResistanceAlert will be made available for free download. A web link will be provided when it is fully developed.

Documentation and References

A user manual and other information (release updates, journal article citations, technical reports, or other documents) will be provided at a web link when the prototype ResistanceAlert is fully developed.

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Article Sources and Contributors

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