Title: Dataset associated with "An in-frame deletion mutation in the degron tail of auxin co-receptor IAA2 confers resistance to the herbicide 2,4-D in *Sisymbrium orientale*"

Abstract: The natural auxin indole-3-acetic acid (IAA) is a key regulator of many aspects of plant growth and development. Synthetic auxin herbicides such as 2,4-D mimic the effects of IAA by inducing strong auxinic signaling responses in plants. To determine the mechanism of 2,4-D resistance in a *Sisymbrium orientale* (Indian hedge mustard) weed population, we performed a transcriptome analysis of 2,4-D resistant (R) and -susceptible (S) genotypes that revealed an in-frame 27-nucleotide deletion removing 9 amino acids in the degron tail (DT) of the auxin co-receptor Aux/IAA2 (*SoIAA2*). The deletion allele cosegregated with 2,4-D resistance in recombinant inbred lines. Further, this deletion was also detected in several 2,4-D resistant field populations of this species. Arabidopsis transgenic lines expressing the *SoIAA2* mutant allele were resistant to 2,4-D and dicamba. The IAA2-DT deletion reduced binding to TIR1 *in vitro* with both natural and synthetic auxins, causing reduced association and increased dissociation rates. This novel mechanism of synthetic auxin herbicide resistance assigns a new *in planta* function to the DT region of this Aux/IAA co-receptor for its role in synthetic auxin binding kinetics and reveals a potential biotechnological approach to produce synthetic auxin resistant crops using gene editing.

Contact: Todd Gaines, todd.gaines@colostate.edu

Data license: The material is open access and distributed under the terms and conditions of the Creative Commons Public Domain "No rights reserved" (https://creativecommons.org/share-your-work/public-domain/cc0/).

Recommended data citation: Figueiredo, M., A. Küpper, J. Malone, T. Petrovic, A.B. Figueiredo, G. Campagnola, O. Peersen, K. Prasad, E. Patterson, A.S.N. Reddy, M. Kubeš, R. Napier, F. Dayan, C. Preston, and T. Gaines. 2021. Dataset associated with "An in-frame deletion mutation in the degron tail of auxin co-receptor IAA2 confers resistance to the herbicide 2,4-D in *Sisymbrium orientale*." Colorado State University. Libraries. http://dx.doi.org/10.25675/10217/234027

Associated publication: Figueiredo, M., A. Küpper, J. Malone, T. Petrovic, A.B. Figueiredo, G. Campagnola, O. Peersen, K. Prasad, E. Patterson, A.S.N. Reddy, M. Kubeš, R. Napier, F. Dayan, C. Preston, and T. Gaines. 2022. An in-frame deletion mutation in the degron tail of auxin co-receptor *IAA2* confers resistance to the herbicide 2,4-D in *Sisymbrium orientale*. Proceedings of the National Academy of Sciences USA, 119(9), e2105819119. https://doi.org/10.1073/pnas.2105819119

Location where data were collected: Port Broughton, South Australia, Australia

Time period during which data were collected: 2014 to 2021

Format of data files: .tgz, .html, .pdb

File Information:

SoIAA2_full_TIR1_plots.tgz - contains 9 plots in .html format

SoIAA2_full_TIR1_summary.tgz - contains 40 protein models in .pdb format

SoIAA2_short_TIR1_plots.tgz - contains 9 plots in .html format

SoIAA2_short_TIR1_summary.tgz - contains 24 protein models in .pdb format

About the datasets:

Output files from protein docking analysis of the wild-type IAA2 protein and the mutant IAA2 version containing a nine amino acid deletion. These residues were used as docking parameters in HADDOCK 2.4 (https://wenmr.science.uu.nl/haddock2.4/). Docking calculations were performed under expert level, deactivating the DNA/RNA functions and activating the Surface Contact Restrains to enforce contact between the molecules. Degron residues KNNN of SoIAA2 were assigned semiflexible properties during docking whereas the shorter connection in SoIAA2Δ9 was not allowed to be flexible to preserve the structural integrity of PB1. The binding affinities of the SoIAA2/TIR1 and SoIAA2Δ9/TIR1 biological complexes were calculated using PRODIGY (https://bianca.science.uu.nl/prodigy/) for all top 4 poses from the best HADDOCK clusters. Plots are in .html format and protein models are in .pdb format. Files are in TGZ after gzip compression.