Towards a new generation of agrochemicals to improve the yield of food crops under water limited conditions

A. Albert[1], L. Infantes[1], J. Lozano-Juste[2], P.L. Rodriguez[2], J.A. Márquez[3], G. Hoffmann[3], I. Cornaciu[3]

[1]Instituto de Química Física Rocasolano CSIC, Madrid, Spain. [2]Instituto de Biología Molecular y Celular de Plantas, CSIC-UPV, Valencia, Spain. [3]European Molecular Biology Laboratory, Grenoble Outstation and Unit of Virus Host-Cell Interactions, Grenoble, France, **xalbert@iqfr.csic.es**

Drought is a major threat to crops. Increasing global warming conditions provokes that ordinary seasonal weather variations have a major influence in crop production areas due to their impact in the decrease of rainfall and the increase of warm periods. Thus, it is required the development of strategies to improve the yield of crops under drought stress. In these situations, the phytohormone Abscisic acid (ABA) and the family of PYR/PYL ABA receptors plays a central role since it controls plant water loss through the regulation of stomata pores [1].

The available structural information on PYR/PYL receptors provides a mechanism of action in ABA sensing. In conditions of sufficient water availability, cytosolic ABA levels are low and the PYR/PYL receptors display an empty, open cavity. On the contrary, drought induces an increase in cytosolic concentration of ABA, which binds to the PYR/PYL receptors. This leads to a structural reorganization that induces the formation of a high-affinity upstream complexes resulting in the activation of ABA mediated stress adaptation [2].

The massive use of small molecules chemical libraries followed by biochemical assays has led to the identification of small synthetic molecules acting as ABA-agonists (binding to the ABA receptor and activating ABA signaling) or ABA-antagonists (occupying the receptor and blocking ABA-mediated responses). This has offered tools to modulate ABA signaling with potential application in crop species agriculture [3]. We have used the Fragment Screening and the integrated Macromolecular Crystallography pipelines at EMBL-ESRF for the identification of fragment molecules that bind to the ABA pocket using crystals of tomato PYR/PYL receptor as a representative target for families of plant receptors [4]. This work constitutes a first step in the identification of new molecules with agronomical interest to help plants coping to water limited conditions.

References

[1] - S.R. Cutler, P.L. Rodriguez, R.R. Finkelstein and S.R. Abrams, Annual review of plant biology *61*, 651-679. (2010).

[2] - J. Santiago, F. Dupeux, A. Round, R. Antoni, S.Y. Park, M. Jamin, S.R. Cutler, P.L. Rodriguez and J.A. Marquez, Nature *462*, 665-668. (2009).

[3] - M. Okamoto, F.C. Peterson, A. Defries, S.Y. Park, A. Endo, E. Nambara, B.F. Volkman and S.R. Cutler, Proceedings of the National Academy of Sciences of the United States of America *110*, 12132-12137. (2013).

[4] - M. Moreno-Alvero, C. Yunta, M. Gonzalez-Guzman, J. Lozano-Juste, J.L. Benavente, V. Arbona, M. Menéndez, M. Martinez-Ripoll, L. Infantes, A. Gomez-Cadenas, P.L. Rodriguez and A. Albert. Molecular Plant. 10, 1250-1253. (2017).