

## **Understanding Auxin perception and selectivity**

Mussa Quareshy<sup>1</sup> and Richard Napier<sup>1</sup>

<sup>1</sup>*University of Warwick*

Auxin (Indole-3-acetic acid) can be considered one of the most important hormones in plant development as it coordinates plant responses through transcriptional regulation. Auxin binds Transport Inhibitor Response 1 (TIR1) of which there are 5 other homologues; Auxin Signalling F-Box (AFB1 – 5). TIR1 and AFB5 are the most distantly related in terms of sequence homology and are studied in this work.

Currently 25 molecules are marketed as synthetic auxins and there is still a drive to discover new auxin-like molecules, in particular from an agrochemical perspective to overcome weed-based resistance and reduce field dose. Interestingly, there is as yet no definitive descriptor that defines an auxin chemically and until recently there has been no compound that has complete selectivity for one of the individual receptorproteins.

We will present our work using purified TIR1 and AFB5 and compound screening by SPR, *in-silico* docking, kinetic parameterization and 3D QSAR modelling to identify and synthesize potential novel auxins or anti-auxins. This has yielded a novel class of auxin molecule, which has also shown selectivity between some of the auxin receptors. It is a potential scaffold for receptor-specific auxins and thus a new generation of herbicides. We also present our work on auxin- molecular field descriptors as a tool in the search for rationally designed novel auxins.