

Supplementary Figure 3 A. Sequence alignment of AtNIP5;1, AtNIP6;1 and AtNIP7;1 protein sequences. The Ar/R residues are highlighted with the position nomenclature (H2, H5, LE<sub>1</sub> and LE<sub>2</sub>) of Wallace and Roberts (ref. 21 main text). The position of Tyr81 of AtNIP7;1 and the corresponding Asn and Cys in AtNIP5;1 and AtNIP6;1 respectively are indicated by an asterisk. B. Homology models of AtNIP5;1, AtNIP6;1 and AtNIP7;1 viewed down the pore axis from the extracellular vestibule. The ar/R residues are indicated by a ball and stick representation with the blue residue indicating the conserved Arg at position LE2. The position of the Asn (gray), Cys (yellow) and Tyr (yellow) from the asterisked position in the sequence in panel A is shown in space filling representation. The orange atoms in AtNIP 6;1 and AtNIP7;1 show the position of sulfhydryl S and phenolic O atoms respectively. The distance (2.84 Å) between the Tyr 81 hydroxyl and the closest guanidinium nitrogen atom of Arg220 is indicated in the AtNIP7;1 structure by a green dotted line.