Structure-based Classification of the Plant Non-specific Lipid Transfer Protein Superfamily Towards its Functional Characterization

Cécile FLEURY\textsuperscript{1}, Marie-Françoise GAUTIER\textsuperscript{3}, Jean-François DUFAYARD\textsuperscript{1}, Franck MOLINA\textsuperscript{2}, Manuel RUIZ\textsuperscript{1} and Frédéric DE LAMOTTE\textsuperscript{1}

\textsuperscript{1}UMR AGAP CIRAD/INRA, avenue Agropolis, 34398, Montpellier, Cedex 5, France
\textsuperscript{2} SysDiag, UMR3145 CNRS/Bio-Rad, 1682 rue de La Valsière, CS 61003, Montpellier, Cedex 4, France

\texttt{cecile.fleury@cirad.fr}

\section*{CONTEXT}
non-specific Lipid Transfer Proteins (\textit{nsLTPs}) :
\begin{itemize}
  \item small proteins : 50 to 150 amino acid residues (including signal peptide)
  \item 8 cysteine motif backbone : C-Xn-C-Xn-CC-Xn-CXn-CXn-C-Xn-C
  \item no glycine/proline rich N-terminal region (< 40%)
  \item > 70 ligands (lipids, hydrophobic compounds)
  \item roles in plant defense mechanism: resistance to biotic stresses and abiotic, plant germination, etc.
  \item \(\alpha\)-helical folding pattern (4-5 helices)
  \item 4 disulfide bonds
  \item hydrophobic cavity (35-350 Å\textsuperscript{3})
  \item 32 experimental structures (10 seq.)
\end{itemize}

800 \textit{nsLTPs} from 100 plant species

\section*{Figure 1: Homology modeling of the 800 \textit{nsLTPs} with no known structure.}

\section*{Figure 2: Dendrogram generated on the basis of structural comparison of all the \textit{nsLTPs} of the new dataset. As the tree is ultrametric, one can group the structures according to a maximal RMS distance of 1.8 Å. By doing so, the superfamily is split into 10 groups, among which 3 main clusters arise that contain 509, 261 and 29 proteins, respectively.}

\section*{Figure 3: Structure-based sequence alignment of the reference proteins of the 3 main structural clusters. The original alignment has been performed on the whole set of protein structures, but only the 3 representative proteins are shown here. The class-specific evolutionarily important residues are highlighted in one colour for each cluster, while the important residues roughly conserved among the whole superfamily are underlined.}

\section*{Figure 4: Experimentally determined three-dimensional structures of cluster 2 (up : maize type I \textit{nsLTP}) and cluster 3 (down : wheat type II \textit{nsLTP}) representative proteins. Class-specific evolutionarily important residues are highlighted in red on each structure and a natural ligand is bound inside the cavity.}