tion of transgenic plants over-expressing or silencing RLCK_VIA genes. The identification of altered phenotypes in these transgenic plants can be very helpful in order to determine the developmental role of RLCK class VI members in Arabidopsis.

Jurca M, Bottka S, Feher A (2008). Characterization of a family of Arabidopsis receptor-like cytoplasmic kinases (RLCK class VI). Plant Cell Reports 27:739-748.
Murase K, Shiba H, Iwano M, Che F, Watanabe M, Isogai A, Takayama S (2004) A membrane-anchored protein kinase involved in Brassica self-incompatibility signaling. Science 303:1516-1519.
Shiu S, Karlowski W, Pan R, Tzeng Y, Mayer K, Li W (2004) Comparative analysis of the receptor-like kinase family in Arabidopsis and rice. Plant Cell 16:1220-1234.
Zhou J, Loh Y, Bresan R, Martin G (1995) The tomato gene Pti1 encodes a serine/threonine kinase that is phosphorylated by Pto and is involved in the hypersensitive response. Cell 83:925-935.

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Structural analysis of antimicrobial peptides by molecular dynamics methods

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Cationic antimicrobial peptides (AMPs) play an important role in the innate immune system. There are several experimental methods for investigating the secondary structures of these small molecules but they are not precise enough to provide reliable information. Accordingly, we chose molecular dynamics methods to investigate the structural properties of some AMPs. Three types of peptides were studied: peptides rich in His (alloferon-1 and -2), peptides rich in Trp and Arg (indolicidin and tritrpticin) and cyclic peptides containing a disulfide bridge (bactenecin and tigerinin-1).

Alloferon-1 and -2 isolated from insects are rich in His and they possess antiviral and antitumor activities with immunomodulatory effect (Chernysh 2002). The secondary structure of alloferons has not been examined yet. Indolicidin and tritrpticin are peptides containing aromatic residues isolated from bovine neutrophils (Selsted 1992; Lawyer 1996). They possess broad spectrum of antibacterial, antifungal and hemolytic activities. Both indolicidin and tritrpticin are known to be flexible in aqueous solution and adopt either helical (poly-proline II helix) or turn structures in membrane mimic environment. Bactenecin and tigerinin-1 are cyclic peptides with serious antimicrobial activity (Romeo 1988; Sai 2001). Bactenecin was isolated from bovine neutrophils and tigerinin-1 was isolated from the skin of Rana tigerina. Each of them tends to adopt β-turn conformation. Because of the controversial assumptions and the lack of reasonable information about the secondary structures of these AMPs our goal was to perform conformational analysis of these peptides.

To explore the conformational spaces of molecules simulated annealing calculations were performed using implicit solvent model. For peptides containing Pro residues, torsional restraints were applied to keep the Xxx-Pro peptide bonds either in *cis* or *trans* configurations. The evolving secondary structures and the intramolecular interactions were examined.

For indolicidin and tritrpticin, it was observed that the *cis-trans* isomerisation plays a key role in the distribution of secondary structural elements (Kerényi 2007). For *trans* isomers, mainly type I and III β-turns were identified. Nevetheless, 3_{10}- and poly-proline II helical segments also appeared along the sequence of peptides possessing *trans* Xxx-Pro peptide bonds. In *cis* isomers, type VI β-turns were observed in specific tetrapeptide units. The stabilizing intramolecular interactions were in good agreement with the structural data: the observed H-bonds play a role in the stabilization of type I and III β-turns, as well as of 3_{10}-helical segments, while the proline-aromatic interactions participate in the stabilization of type VI β-turns. In alloferons, type I, II, II' and III β-turns were the most frequent structural elements. These secondary structures were also stabilized by backbone H-bonds. In the cyclic peptides (bactenecin and tigerinin-1), type I and III β-turns could be found in major population. In the *cis* isomers of tigerinin-1, type VI β-turns were also identified. In every peptide examined, minor populations of backbone-sidechain and sidechain-sidechain H-bonds were also found.

The results obtained from modelling the secondary structures and stabilizing intramolecular interactions were coherent and the conclusions derived from these calculations coincided with the data published so far.

Chernysh S, Kim SI, Bekker G, Pleskach VA, Filatova NA, Anikin VB, Platonov VG, Bulet P (2002) Antiviral and antitumor peptides from insects. Proc Nat Acad Sci USA 99(20):12628-12632.
Kerényi Á, Rákhely G, Leitgeb B (2007) Peptides 2006. In Proceedings of the 29th European Peptide Symposium., eds. Rolka K, Rekowski P, Silberring J), Kenes International, pp. 222.
Lawyer C, Pai S, Watabe M, Borgia P, Mashimo T, Eagleton L, Watabe, K (1996) Antimicrobial activity of a 13 amino acid tryptophan-rich peptide derived from a putative porcine precursor protein of a novel family of antibacterial peptides. FEBS Lett 390:95-98.
Romeo D, Skerlavaj B, Bolognesi M, Gennaro R (1988) Structure and bactericidal activity of an antibiotic dodecapeptide purified from bovine neutrophils. J Biol Chem 263:9573-9575.
Sai KP, Jaganadham MV, Vairamani M, Raju NP, Devi AS, Nagaraj R, Sitaram N (2001) Tigerinins: novel antimicrobial peptides from the Indian frog Rana tigerina. J Biol Chem 276:2701-2707.
Selsted ME, Novotny MJ, Morris WL, Tang YQ, Smith W, Cullor JS (1992) Indolicidin, a novel bactericidal tridecapeptide amide from neutrophils. J Biol Chem 267:4292-4295.

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