

which were filled with other atoms from the boron group (In and Tl) by 3 to 5 at.%. The binary convex hulls for these systems were also calculated.

From our results we compare the mechanical and energetical stability of different types of theoretical heptagonal approximants, in relation to the stable modifications of Gallium. We could draw conclusions about the mechanisms of heptagonal ordering in Gallium from the structure types decomposing during relaxation. We were also able to estimate the influence of doping on the stability of our approximants.

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**Keywords:** gallium, quasicrystal, calculation

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### A novel structure: PSPC1/NONO heterodimer, members of the DBHS protein family

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Proteins of the Drosophila Behavior and Human Splicing (DBHS) family share a common domain structure: two RNA recognition motifs (RRMs), a NONA/Paraspeckle (NOPS) domain followed by a coiled-coil region. Paraspeckle Protein Component 1 (PSPC1) and Non-POU domain-containing octamer-binding protein (NONO) are members of this family and have a highly similar sequences within the DBHS domain. PSPC1 and NONO form a heterodimer and they are co-localised to paraspeckles, a dynamic sub-ribonuclear bodies in eukaryotic cells [1]. These proteins will be recruited to paraspeckles at the point of transcription of a long non-coding RNA, called NEAT1 which forms the structural scaffold of these bodies [2,3,4]. Within paraspeckles, PSPC1 and NONO are involved in transcriptional regulation by confining RNA to the nucleus, preventing subsequent protein production [2,3,4]. However, the mechanisms at the molecular level behind these processes are still unclear. Structural analysis of PSPC1 and NONO and investigation of RNA binding partners will broaden the knowledge about their functions in transcriptional control. Here we present the first paraspeckle protein structure, the PSPC1/NONO heterodimer. This structure highlights the DBHS domain with a novel arrangement of four different RRM. Furthermore, we describe a new protein-protein interaction domain (NOPS). We also observe the first example of an anti-parallel right handed heterodimeric coiled-coil. This PSPC1/NONO structure provides us with new insights into the functions of paraspeckle assembly as well as possible RNA binding modes.

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### Structural basis of inhibition mechanism by carrot EDGP against endoglucanase

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Plant cell wall is composed of various polysaccharides such as cellulose, hemicellulose and pectin. Cellulose microfibrils are linked via hemicellulose. The network of cellulose-hemicellulose provides tensile strength. Carrot extracellular dermal glycoprotein (EDGP) is one of proteinous inhibitor to protect cell wall. To penetrate and use plant cell walls nutritionally, pathogen secretes cell wall degrading enzymes. These enzymes including endoglucanases, xylanase and polygalacturonases are classified into glycoside hydrolase (GH) families. EDGP shows inhibitory activity against xyloglucan specific endo- $\beta$ -1,4-glucanase (XEG) from *Aspergillus aculeatus*. XEG belongs to GH12 family. XEG specifically cleaves xyloglucan that is a major hemicellulose of dicots. Xyloglucan consists of  $\beta$ -linked glucose backbone substituted with xylose side-chains. The degradation of xyloglucan is great damage for dicotyledonous plants. Thus, inhibition of XEG by EDGP is important in plant defense system. Until now, the homologous proteins of EDGP were found in various plants. The tomato homolog (xyloglucan specific endo- $\beta$ -1,4-glucanase inhibitor protein, XEGIP) and tobacco homolog (Necturin IV, NEC4) also inhibit XEG. In contrast, the homologous protein from wheat (*Triticum aestivum* xylanase inhibitor, TAXI) inhibits GH11 xylanases. Interestingly, a soybean homolog (Basic 7S globulin, Bg7S) lacks inhibitory activity for both GH11 and GH12 enzymes.

To clarify the inhibition mechanism of EDGP against GH12 endoglucanase, we work on structure determination of EDGP and EDGP in complex with GH12 enzyme by X-ray crystallography. EDGP and the inhibition complex with FI-CMCase, which is GH12 endoglucanase from *Aspergillus aculeatus*, were successfully crystallized. Hexagonal crystal of EDGP belonged to space group *P6*<sub>3</sub>, with unit cell parameters  $a = b = 130.4$ ,  $c = 44.5$  Å and  $\beta = 120^\circ$ . Monoclinic crystal of EDGP complex with FI-CMCase belonged to space group *C2* and unit cell parameters  $a = 169.5$ ,  $b = 143.0$ ,  $c = 63.0$  Å and  $\beta = 110.9^\circ$ . The crystal structure of EDGP was determined by SIRAS method using iodine derivative crystal, and the crystal structure of EDGP~FI-CMCase complex was determined by molecular replacement. The structure of EDGP~FI-CMCase complex reveals that Arg423 of EDGP intrudes into the active site of FI-CMCase. The arginine residue is conserved in homologous proteins that have inhibitory activity for GH12 enzymes. This work provides structural basis of inhibition mechanism by EDGP and its homologous proteins against GH12 enzymes.

**Keywords:** plant, inhibitor, structure

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### Architecture of the mediator head module

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