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P. Metrangolo* 1985

Crystal Structure of the DFNKF
Segment of Human Calcitonin Unveils
Aromatic Interactions between
Phenylalanines

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"To obtain the reported crystal required six months, and the crystals were tiny..." - Read more about the story behind the cover in the Cover Profile and about the research itself on page 2051 ff. (DOI: 10.1002/chem.201604639).

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Crystal Structure of the DFNKF Segment of Human Calcitonin Unveils Aromatic Interactions between Phenylalanines



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Invited for the cover of this issue is the group of Pierangelo Metrangolo at the Politecnico di Milano. The image depicts the steric zipper formed by the amyloidogenic peptide, DFNKF. Read the full text of the article at 10.1002/chem.201604639.

What is the most significant result of this study?

Iodination of the benzene ring *p*-position of Phe2 in the human calcitonin-derived amyloidogenic sequence DFNKF allowed its first ever high-resolution crystal structure determination. The structure unveils aromatic–aromatic interactions as key structural factors. This is important as it may shed new light on the formation mechanism of amyloid fibrils. Furthermore, we demonstrate that iodination promotes peptide crystallization by introducing secondary contacts that stabilize the overall packing.

What time consuming dead-ends delayed the results before this breakthrough?

Obtaining high-quality single crystals of fibril-forming peptides is rather difficult. To obtain the reported crystal required six months and the crystals were tiny, which complicated the data acquisition.

What other topics are you working on at the moment?

Besides our research on protein and peptide crystallography, we are working on the effects of halogenation on the self-assembly of amyloidogenic peptides. In particular, we are exploiting halogen bonding as key noncovalent interaction to direct self-assembly and nanostructure control in peptide and proteins.

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