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I obtained my first degree in physics from Stuttgart University and completed my M.Sc. degree with a thesis project at the Max-Planck-Institute for Metal-Research, Stuttgart. I carried out my PhD thesis project "Crystal structures of Aib-containing peptides" at the University of Hohenheim under the supervision of Professor Hans Brückner (Ph.D. degree 1999).

I have worked at IMBB since 1991. I was a member of the Protein Structure/Crystallography group of IMBB as a research technician, the first 11 years in the group of Professor Michalis Kokkinidis and until January 2022 in the group of Dr. Kyriakos Petratos. Briefly, my expertise was

- designing the expression of proteins, protein expression, purification and crystallization of proteins with the methods hanging drop, sitting drop and onyx-nano robot (Douglas instruments)
- collection of diffraction data at our in home X-ray instruments (Enraf-Nonius Cad4 diffractometer, Rigaku rotating anode generator equipped with a Mar-research area detector and Bruker D8 Venture Diffractometer) and in addition at several european synchrotron facilities (Desy Hamburg, ESRF Grenoble, Diamond Didcot)
- crystallization and solving the X-ray structure of natural occurring, very rare peptaibols and also synthetic Aib-containing model peptides with often unusual and unpredictable folding
- secondary structure determination of proteins and peptides with the method of circular dichroism (CD) on a Jasco J-810 spectropolarimeter; determination of the thermal unfolding temperature of proteins
- kinetics of an alcohol dehydrogenase in dependence of the temperature
- unfolding and refolding of a protein in order to substitute the central transition-metal ion by other transition-metal ions and determination of the differences in the geometry of binding
- DNA-isolation of plants for sequencing
- homology modelling of proteins of which no crystal structure is available, and also modelling of enzymes with their substrates

Since 2023 I work in the group of Dr. Inga Siden-Kiamos on a project to develop inhibitors against proteins of the malaria parasites. This involves protein expression, protein purification, structural analysis, homology modelling of a protein trimer and computational work on folding prediction and stability.

Recently I started in Dr. Kotsifakis group the expression of tick salivary molecules for forthcoming structure determination, function insights and function analysis which may be applicable in drug development. Since these protease-inhibitors are produced in E. coli they often turn out to be insoluble under native conditions. The project then demands unfolding of inclusion bodies, refolding to soluble conditions and purification to high purity, and to an amount suitable for the in-home crystallization facility.

## List of publications

Gessmann R, Garcia-Saez I, Simatos G, Mitraki A. Z-Ala-Ile-OH, a dipeptide building block suitable for the formation of orthorhombic microtubes. (2023). *Acta Crystallogr C Struct Chem.* 2023 Jul 1; 79(Pt7): doi: 10.1107/S2053229623004849. PMID: 37345638. [pubmed](#)

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- Gessmann R, Brückner H, Petratos K. The first N-terminal unprotected (Gly-Aib)<sub>n</sub> peptide: H-Gly-Aib-Gly-Aib-OtBu. *Acta Crystallogr C Struct Chem.* 2015 Dec 1;71(Pt 12):1114-7. doi: 10.1107/S2053229615022597. Epub 2015 Nov 28. PMID: 26632841. [pubmed](#)
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