# List of Publications

[1]　E. van Genderen, M.T.B. Clabbers, P.P. Das, A. Stewart, I. Nederlof, K.C. Barentsen, Q. Portillo, N.S. Pannu, S. Nicolopoulos, T. Gruene, and J.P. Abrahams. "Ab initio structure determination of nanocrystals of organic pharmaceutical compounds by electron diffraction at room temperature using a Timepix quantum area direct electron detector". In: *Acta Crystallogr.* A72 (2016), pp. 235–242.

[2]　J. Luebben and T. Gruene. "New Method to compute $R_{complete}$ enables Maximum Likelihood Refinement for Small Data Sets". In: *Proc. Natl. Acad. Sci. U. S. A.* 112 (2015), pp. 8999–9003.

[3]　T. Gruene, G. M. Sheldrick, B. D. Zlatopolskiy, S. I. Kozhushkov, and A. de Meijere. "Structure of Hormaomycin, a Naturally Occurring Cyclic Octadepsipeptide, in the Crystal". In: *Z. Naturforsch., B: J. Chem. Sci.* 69b (2014), pp. 945–949.

[4]　D.A. Köpfer, C. Sing, T. Gruene, G. M. Sheldrick, U. Zachariae, and B. L. de Groot. "Ion Permeation in $K^+$ Channels Occurs by Direct Coulomb Knock-On". In: *Science* 346 (2014), pp. 352–355.

[5]　M. Moreno-Morcillo, N M. I. Taylor, T. Gruene, P. Legrand, U. J. Rashid, F. M. Ruiz, U. Steuerwald, C. W. Müller, and C. Fernández-Tornero. "Solving the RNA polymerase I structural puzzle". In: *Acta Crystallogr* D70 (2014), pp. 2570–2572.

[6]　K. Dalle, T. Gruene, S. Dechert, S. Demeshko, and F. Meyer. "A weakly coupled biologically relevant $Cu_2^{II}(\mu - \eta^1 : \eta^1 - O_2)$ *cis*-peroxo adduct that binds side-on to additional metal ions". In: *J. Am. Chem. Soc.* 136 (2014), pp. 7428–7434.

[7]　T. Gruene. "Structure Determination by X–ray Crystallography: Analysis by X–rays and Neutrons". In: *Crystallogr. Rev.* 20 (2014), pp. 235–236.

[8]　T. Gruene, H. W. Hahn, A. V. Luebben, F. Meilleur, and G. M. Sheldrick. "Refinement of Macromolecular Structures against Neutron Data with SHELXL-2013". In: *J. Appl. Crystallogr.* 47 (2014), pp. 462–466.

[9]　C. Fernández-Tornero, M. Moreno-Morcillo, U. J. Rashid, N M. I. Taylor, F. M. Ruiz, T. Gruene, P. Legrand, U. Steuerwald, and C. W. Müller. "Structure of 14-subunit RNA polymerase I: insight into ribosomal RNA synthesis". In: *Nature* 502.7473 (2013), pp. 644–649.

[10]　T. Gruene. " *mrtailor*: a tool for PDB-file preparation for the generation of external restraints". In: *Acta Crystallogr.* D69 (2013), pp. 1861–1863.

[11]　T. Beck, T. Gruene, and G. M. Sheldrick. "The magic triangle goes MAD: experimental phasing with a bromine derivative". In: *Acta Crystallogr.* D66.4 (2010), pp. 374–380.

[12]　T. Gruene, M.-K. Cho, I. Karyagina, H.-Y. Kim, C. Grosse, K. Giller, M. Zweckstetter, and S. Becker. "Integrated analysis of the conformation of a protein-linked spin label by crystallography, EPR and NMR spectroscopy". In: *J. Biomol. NMR* 49 (2011), pp. 111–119.

[13]   A. A. Bhattacharya, T. Grune, and S. Curry. "Crystallographic analysis reveals common modes of binding of medium and long chain fatty acids to human serum albumin". In: *J Mol Biol* 303.5 (2000), pp. 721–732.

[14]   I. Petitpas, T. Grune, A. A. Bhattacharya, and S. Curry. "Crystal structure of human serum albumin complexed with monosaturated and polyunsaturated fatty acids". In: *J Mol Biol* 314.5 (2000), pp. 955–960.

[15]   T. Grüne, J. Brzeski, A. Eberharter, C. R. Clapier, D. F. V. Corona, P. B. Becker, and C. W. Muller. "Crystal structure and functional analysis of the nucleosome recognition module of the remodeling factor ISWI". In: *Mol. Cell* 12.2 (2003), pp. 449–460.

[16]   T. Gruene and G. M. Sheldrick. "Geometric properties of nucleic acids with potential for autobuilding". In: *Acta Crystallogr.* A67.1 (2011).

[17]   T. Beck, A. Krasauskas, T. Gruene, and G. M. Sheldrick. "A magic triangle for experimental phasing of macromolecules". In: *Acta Crystallogr* D64.11 (2008), pp. 1179–1182.

[18]   T. Grune. " *mtz2sca* and  *mtz2hkl*: facilitated transition from  *CCP4* to the  *SHELX* program suite". In: *J. Appl. Crystallogr.* 41.1 (2008), pp. 217–218.

[19]   Schlicker, C and Fokina, O and Kloft, N and Grüne, T and Becker, S and Sheldrick, GM and Forchhammer, K. "Structural analysis of the PP2C phosphatase tPphA from Thermosynechococcus elongatus: a flexible flap subdomain controls access to the catalytic site." In: *J. Mol. Bio.* 376.2 (2008), pp. 570–81.

[20]   M. R. Conte, T. Grune, J. Ghuman, G. Kelly, A. Ladas, S. Matthews, and S. Curry. "Structure of tandem RNA recognition motifs from polypyrimidine tract binding protein reveals novel features of the RRM fold". In: *EMBO J.* 19.12 (2000), pp. 3132–3141.

[21]   A. Pal, R. Kraetzner, T. Gruene, M. Grapp, K. Schreiber, M. Grønborg, H. Urlaub, S. Becker, A. R. Asif, J. Gärtner, G. M. Sheldrick, and R. Steinfeld. "Structure of Tripeptidyl-peptidase I Provides Insight into the Molecular Basis of Late Infantile Neuronal Ceroid Lipofuscinosis". In: *J. Biol. Chem.* 284 (2009), pp. 3976–3984.

[22]   A. Pal, J. É. Debreczeni, M. Sevvana, T. Gruene, B. Kahle, A. Zeeck, and G. M. Sheldrick. "Structures of viscotoxins A1 and B2 from European mistletoe solved using native data alone". In: *Acta Crystallogr.* D64.9 (2008), pp. 985–992.

[23]   K. F. Hartlepp, C. Fernandez-Tornero, A. Eberharter, T. Grüne, C. W. Müller, and P. W. Becker. "The Histone Fold Subunits of Drosophila CHRAC Facilitate Nucleosome Sliding through Dynamic DNA Interactions". In: *Mol. Cell. Biol.* 25.22 (2005), pp. 9886–9896.

[24]   T. Gruene. "Advanced Applications of Shelxd and Shelxe". In: *Advancing Methods for Biomolecular Crystallography*. Springer, 2012.

[25]   T. Gruene. "Macromolecular Phasing: Solving the Substructure". In: *Advancing Methods for Biomolecular Crystallography*. Springer, 2012.

## Invited Talks

**2015** ECM29 2015, Rovinj, "Xen crystallography: Choose your radiation"

**2014** ESS neutron Laue data processing discussion, Copenhagen, "Quasi-Laue Neutron Diffraction and Modern Data Processing"

**annually since 2008** CCP4 School APS Chicago "Data Processing with XDS"

**annually since 2008** CCP4 School APS Chicago "Macromolecular Phasing with SHELX C/D/E"

**2013** ESS Symposium in Aarhus, "Refinement of Macromolecular Structures from Neutron Data with SHELXL"

**2013** Horizons in Molecular Biology, Göttingen, " Macromolecular Crystallography"

**2012** BER II Users' Meeting, Berlin, "Refinement of Macromolecular Neutron Data with shelxl"

**2012** Bruker AXS Users' Meeting, Bad Herrenalb, "How to Trace Polynucleotides"

**2012** Erice School in Crystallography, "Advanced Applications of SHELXD and SHELXE"

**2012** Erice School in Crystallography, "Macromolecular Phasing: Solving the Substructure"

**2012** Macromolecular Crystallography School, Madrid, "The Shelx Suite: Applications to Macromolecular Crystallography"

**2012** Macromolecular Crystallography School, Madrid, "Fundamentals on Diffraction Data Integration and Data Reduction"