Macromolecular Crystallography Products

- Crystallization Screens
- Crystallization Optimization
- Cryo Screens
- Phasing

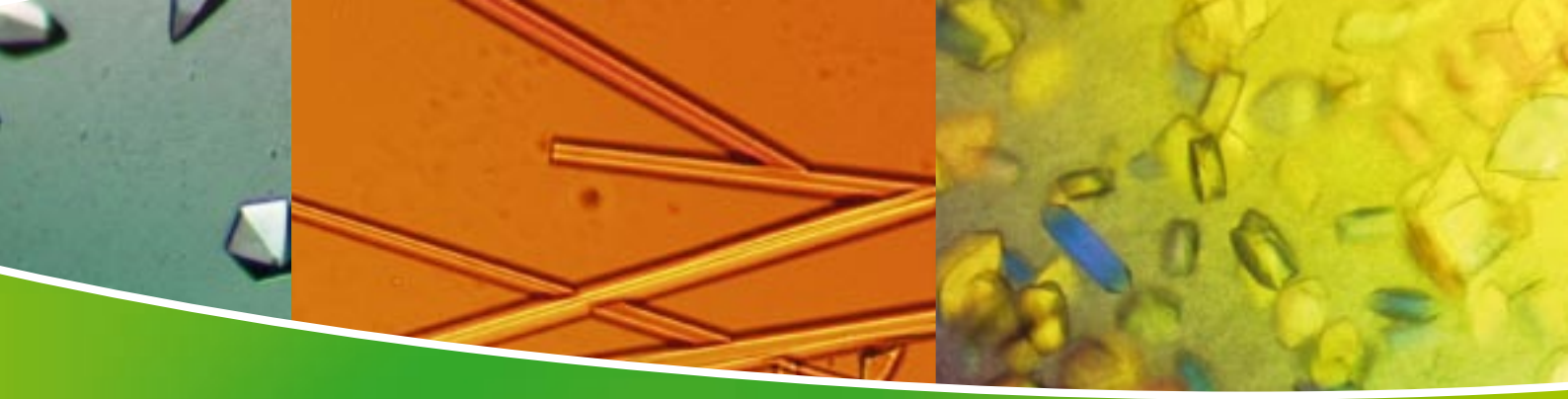
JENA BIOSCIENCE

www.jenabioscience.com

Grow your crystals with ***Jena Bioscience*** Products

Jena Bioscience was founded in 1998 by scientists who wanted to share their ideas and experience with the life science community. Over the years, Jena Bioscience has developed from a local start-up company into an established business with a global distribution network. We deliver products and services to leading industrial players and universities in more than 40 countries.

Our macromolecular crystallography product portfolio comprises an extensive assortment of tools for protein crystallization. High quality reagents and excellent customer service help the researcher to find tailor-made solutions in the areas of crystal screening, crystallization optimization, cryo-crystallography and phasing.



Crystallization Screens

Despite intensive research, the crystallization of biological macromolecules remains a process of trial and error. Nucleation and crystal growth are influenced by the interaction of many variables, such as temperature, pH, precipitant and salt concentration. Testing all possible combinations would be too time consuming and would require enormous amounts of sample. Our **JBScreen** products are designed for efficient and flexible screening of crystallization conditions for proteins, peptides, nucleic acids, macromolecular complexes and water-soluble small molecules.

JBScreen Classic

JBScreen Classic covers 240 unique conditions. Their composition results from data mining of several thousands of successfully crystallized proteins. The ten individual **JBScreen Classic** kits (bulk and ampoules) represent specific precipitant classes, organized by precipitant type and concentration. This systematic arrangement grants easy access to all relevant information and is already a first step to a refinement of the crystallization conditions: Once you get a hit, you immediately see the effects caused by the composition of adjoining reagents. This simplifies the development of rational strategies for further improvement of crystal quality. Numerous proteins have been successfully crystallized using **JBScreen Classic**, for examples see [1–7].

JBScreen Classic is available in a variety of formats to satisfy your specific needs:

JBScreen Classic HTS
two pre-filled 96 deep-well blocks

JBScreen Classic bulk
ten individual kits, 24 conditions each, supplied in 10 ml volumes

JBScreen Classic ampoules
ten individual kits, 24 conditions each, supplied as 0.7 ml single shots in individual vials

JBScreen Basic

JBScreen Basic has been formulated to comply with our customers' continuous interest in this particular sparse-matrix screen. The method involves screening with an intentional bias towards conditions that were proven successful in the crystallization of biological macromolecules. The reagents of **JBScreen Basic** have been selected based upon the protocol of Jancarik & Kim [8] and others [9]. Visit our website to read more about the improvements we have made, such as the elimination of cacodylate.

The **JBScreen Basic** kits 1–4 are designed to fit the 24-well plate format for screening a large range of pH, salts and precipitants. Each condition of the 96 unique reagents is supplied in 10 ml quantities. For high-throughput users, we offer all 96 conditions in a pre-filled deep well block.

Grow your crystals with *Jena Bioscience* Products

JBScreen Membrane

The **JBScreen Membrane** screens 1–3 cover 72 of the most promising reagents for crystallization of membrane proteins. Their composition was devised by an exhaustive analysis of crystallization conditions of successfully determined membrane protein structures.

The **JBScreen Membrane** crystallization buffers are organized by type and concentration of the precipitant to facilitate the refinement of successful crystallization conditions. Each kit contains 24 sterile solutions, supplied in 10 ml volumes. All reagents are also available in a pre-filled deep well block.

Crystallization Optimization

Our crystallization optimization product line accompanies the researcher throughout the entire crystallization procedure.

Effective solutions are offered for each stage of the process, e.g. optimization of the buffer composition to confine protein aggregation prior to the crystallization set-up, modification of protein surface residues to enhance crystallization or efficient refinement of initial crystallization conditions.

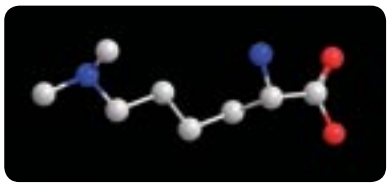
JBS Solubility Kit

The **JBS Solubility Kit** is a pre-crystallization screen to improve the composition of the initial protein buffer solution prior to performing crystallization set-ups [10]. Since the highly complex properties of proteins are dependent on their environment, buffer solutions play an important role, i.e. influencing the solubility and the aggregation behavior of the protein sample. Studies have shown that aggregation of the protein may inhibit nucleation and crystal growth. Therefore, the **JBS Solubility Kit** has been developed to investigate protein samples towards their homogeneity and monodispersity prior to crystallization trials, employing hanging drop vapor diffusion experiments combined with dynamic light scattering.

The **JBS Solubility Kit** contains 24 buffer solutions at different pH-values for setting up hanging drop vapor diffusion experiments in order to monitor the aggregation and precipitation of the protein sample and 14 additives used for further optimization employing dynamic light scattering.

JBS Methylation Kit

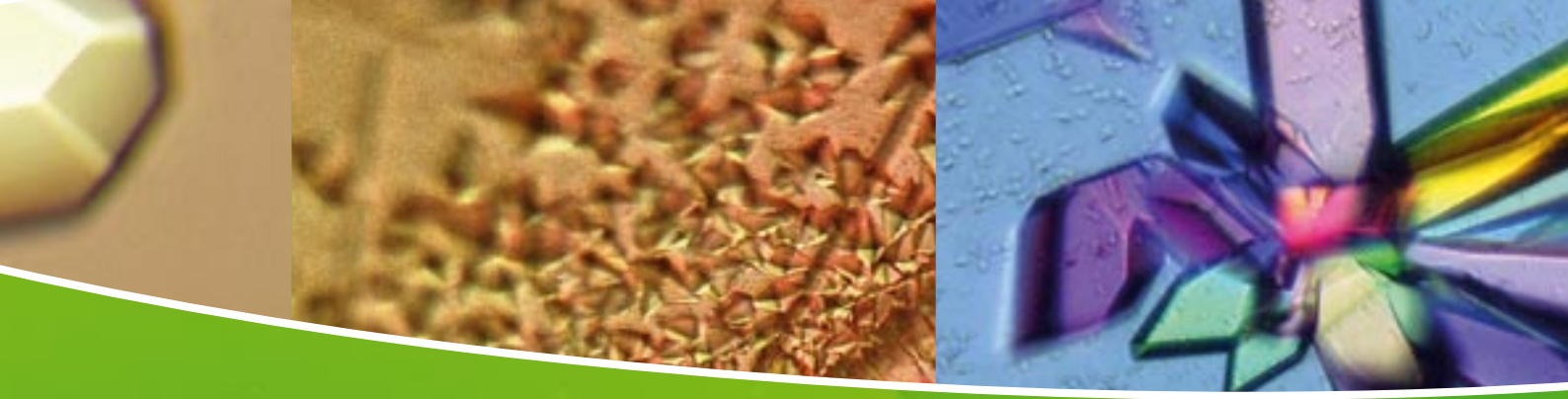
Surface engineering of biological macromolecules provides a powerful technique to deal with proteins which are reluctant to crystallize or which yield poorly diffracting crystals [11,12]. The **JBS Methylation Kit** offers a straightforward tool for the selective methylation of lysine residues. The method does not require laborious cloning/expression/purification, but chemically substitutes the protons of the amino group of lysine residues with methyl groups. The result is a surface-engineered protein within 24 hours, ready for crystallization.



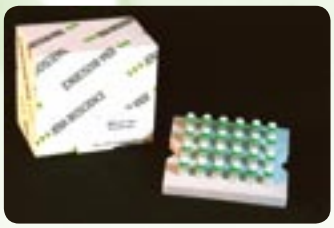
Ball-and-Stick representation of a methylated lysine residue

JBScreen Plus

JBScreen Plus solutions are most useful in the optimization of preliminary crystallization conditions, where specific interactions between the additives and the biological macromolecule may assist in the initial crystallization of the sample and may help to



improve the size and diffraction quality of the crystals. **JBScreen Plus** comprises 5 kits, including kosmotropic (structure-stabilizing) and chaotropic (structure-disturbing) additives, salts, volatile and non-volatile organics and other compounds. Each kit contains 24 different additives, supplied as ready-to-use, sterile filtered aliquots with adjusted concentration.



JBScreen Detergents

The **JBScreen Detergents** kits 1 and 2 cover a great variety of detergents that have been successfully used for the crystallization of membrane proteins. Each kit contains 12 detergents, supplied as stock solutions at 5 or 10 times the reported CMC (Critical Micellar Concentration), with 100 or 200 µl per compound.

JBScreen Detergents is an ideal supplement to the **JBScreen Membrane** screens.

Auxiliary Products

Furthermore, **JBScreen Buffer Kits** containing ready-made buffer solutions with preset pH-values and **JBScreen Single Stocks** – individual stock solutions of the **JBScreen** components – can be purchased for the convenient reproduction and optimization of crystallization conditions.

Cryo Screens

The employment of cryo-techniques is not only used to carefully preserve and store crystals for later analysis but also to reduce radiation damage, caused by intense x-ray sources, since the diffusion of active radicals is decelerated. Therefore, cryocooling prolongs crystal lifetime and facilitates straightforward data collection [13].

However, the use of cryoprotectants is crucial to prevent crystals from cracking and to protect them from the damaging effects of ice formation during the cryocooling process. The appropriate cryoprotectant will guarantee that the thin layer of mother liquor, which surrounds the protein, will form an amorphous glass without the formation of water ice. Thus, x-ray data, free of "ice rings", can be collected.

JBScreen Cryo

JBScreen Cryo is designed for efficient crystal screening in cryo conditions. The unique formulations of the **JBScreen Cryo** reagents are based on an extensive data base search [14] and contain sufficiently large concentrations of cryoprotectants so that crystals can be directly transferred into liquid nitrogen.

JBScreen Cryo includes 4 kits, offering 96 different crystallization conditions in total (24 each), available in the standard 10 ml bulk format. For high-throughput users, the **JBScreen Cryo HTS** contains all 96 conditions in a pre-filled deep well block.

JBScreen Cryo Pro

JBScreen Cryo Pro is the most convenient and most material-saving tool on the market for producing effective cryoprotectants from your crystallization reservoir solution, while utilizing just a minimum amount of your precious crystals. The kit contains 12 different compounds, divided into sugar/amino acid based cryoprotectants, alcohol based cryoprotectants, and an oil based cryoprotectant.

Grow your crystals with *Jena Bioscience* Products

Three pre-dispensed samples of each solid and 50 µl of each liquid formulation are ready to be diluted with the reservoir solution. Crystals soaked in this reservoir-solution/cryoprotectant mixture can be transferred to a liquid nitrogen bath or cryogenic gas stream.

Phasing

In contrast to the amplitude, the phase of scattered x-rays cannot be measured directly. Phase determination is one of the most difficult tasks in macromolecular crystallography and known as the "phase problem". Multiple isomorphous replacement (MIR), multiple wavelength anomalous dispersion (MAD) and single wavelength anomalous dispersion (SAD) are powerful techniques for initial phase determination of novel macromolecular crystal structures. These methods require the incorporation of heavy atoms into the crystal lattice.

JBScreen Heavy

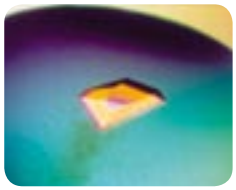
The search for suitable heavy-atom derivatives is often a tedious process and usually requires screening of a broad range of heavy atoms. **JBScreen Heavy** will shorten this process: It contains a collection of 24 of the most successful heavy-atom compounds, selected from data mining of heavy-atom derivatized protein crystals, which have been successfully employed in structure determination of biological macromolecules. Each of the 24 heavy-atom compounds is supplied in three identical solid aliquots – enough material for the preparation of 3x100 µl of a 100 mM stock solution. This will avoid tedious calculating and weighing – simply add 100 µl of water or buffer (or more, for a more diluted solution) to the individual aliquot, and you are ready to prepare your set-ups.

JBS Halo Kits

The search for suitable heavy-atom derivatives by conventional trial-and-error approaches can be quite cumbersome and binding of heavy atoms often results in disrupting the crystal lattice. Halogenated ATP and GTP analogs however, provide an alternative method that allows rational incorporation of heavy atoms into a large number of physiologically relevant enzymes, exploiting the natural affinity of the protein to these nucleotides [15,16].

The **JBS Halo-ATP Kit** contains 12 halogenated adenosine nucleotides and the **JBS Halo-GTP Kit** contains 6 halogenated guanosine nucleotides in form of lyophilized sodium salts.

Moreover, a large selection of halogenated nucleotides, e.g. non-hydrolyzable analogs, can be found on our website.



Crystal of human TMP-kinase co-crystallized with 2'Br-ADP

References

[1] Mueller *et al.* (2005) Crystallization and preliminary x-ray diffraction analysis of human growth and differentiation factor 5 (GDF-5). *Acta Cryst. F* **61**:134.

[2] Park *et al.* (2005) Crystallization and preliminary x-ray crystallographic analysis of peptide deformylase (PDF) from Bacillus cereus in ligand-free and actinonin bound forms. *Acta Cryst. F* **61**:150.

[3] Ferraroni *et al.* (2005) Crystallization and preliminary structure analysis of the blue laccase from the ligninolytic fungus Panus tigrinus. *Acta Cryst. F* **61**:205.

[4] Irimia *et al.* (2004) Methanoarchaeal sulfolactate dehydrogenase: prototype of a new family of NADH-dependent enzymes. *EMBO J.* **23**:1234.

[5] Vallazza *et al.* (2004) First look at RNA in L-configuration. *Acta Cryst. D* **60**:1.

[6] Kundrot (2004) Which strategy for a protein crystallization project? *Cell. Mol. Life Sci.* **61**:525.

[7] Vorup-Jensen *et al.* (2003) Structure and allosteric regulation of the aXb2 integrin I domain. *Proc. Natl. Acad. Sci. USA* **100**:1873.

[8] Jancarik and Kim (1991) Sparse matrix sampling: a screening method for crystallization of proteins. *J. Appl. Cryst.* **4**:409.

[9] Cudney *et al.* (1994) Screening and optimization strategies for macromolecular crystal growth. *Acta Cryst. D* **50**:414.

[10] Jancarik *et al.* (2004) Optimum solubility (OS) screening: an efficient method to optimize buffer conditions for homogeneity and crystallization of proteins. *Acta Cryst. D* **60**: 1670.

[11] Kurinov *et al.* (2000) X-ray crystallographic analysis of pokeweed antiviral protein-II after reductive methylation of lysine residues. Biochem. *Biophys. Res. Comm.* **275**:549.

[12] Kobayashi *et al.* (1999) Crystallization and improvement of crystal quality for x-ray diffraction of maltooligosyl trehalose synthase by reductive methylation of lysine residues. *Acta Cryst. D* **55**:931.

[13] Garman (1999) Cool data: quantity AND quality. *Acta Cryst. D* **55**:1641.

[14] http://idb.exst.jaxa.jp/db_data/protein/search-e.php

[15] Naber *et al.* (1995) A novel adenosine-triphosphate analog with a heavy-atom to target the nucleotide-binding site of proteins. *Protein Sci.* **4**:1824.

[16] Gruen *et al.* (1999) 2'-Halo-ATP and -GTP analogues: Rational phasing tools for protein crystallography. *Protein Sci.* **8**:2524.

Copyright

Crystal pictures are by courtesy of Dr. Alexey Rak, Max-Planck-Institute for Molecular Physiology, Dortmund
Product photographs were taken by Tilo Bössel, http://www.tiloboessel.de

JENA BIOSCIENCE

You have the following options to order products directly from Jena Bioscience:

Mail orders

Please send your mail orders to the following address:
Jena Bioscience GmbH
Loebstedter Strasse 78
07749 Jena
Germany

Telephone orders

We will accept telephone orders from Monday to Friday between 8:00 AM and 4:00 PM Central European Time.
+49 - (0)3641 - 46 49 52

24 hour fax ordering

Download our fax order form from our website at
http://www.jenabioscience.com
Please send your fax orders to:
+49 - (0)3641 - 46 49 91

Online ordering

Please direct your e-mail orders to:
orders@jenabioscience.com

Products can also be ordered through our online shop at
http://www.jenabioscience.com

Please provide us with the following information when ordering:

- Your name, name of your institution
- Billing and shipping address
- PO number (if applicable)
- Catalog number of products and quantity needed
- Contact person and contact data for questions (phone/fax number, e-mail address)

For inquiries or further information,
please contact: xtals@jenabioscience.com

Jena Bioscience GmbH
Loebstedter Str. 78
07749 Jena, Germany
Phone +49 (0)3641-46 49 52
Fax +49 (0)3641-46 49 91
www.jenabioscience.com