

Macromolecular Crystallography

Catalog No. 3 Distributor Edition

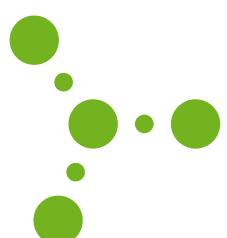


- ▶ *How to get started*
- ▶ *Initial Screening*
- ▶ *Hit Optimization*
- ▶ *Phasing*



IFTA AG
Certified QMS according to
DIN EN ISO 9001
Reg. No. IC 03214 034

www.jenabioscience.com



Jena Bioscience

Imprint

Design and Layout by:

timespin - Digital Communication GmbH
Sophienstrasse 1
07743 Jena
www.timespin.de

Copyright:

Please contact Jena Bioscience if you want to use texts and/or images in any format or media.



Table of Contents

How to get started	2
<i>Teaching</i>	2
<i>JBS Crystallization Freshman Kits</i>	2
<i>Crystallization Model Proteins</i>	3
<i>Crystal Handling Kit</i>	3
Initial Screening	4
<i>Crystallization Screens</i>	4
<i>Cryo Screens</i>	8
<i>Crystal Dyes</i>	9
Hit Optimization	10
<i>Chemical Environment</i>	11
<i>Input Protein</i>	16
<i>Thermodynamics / Kinetics</i>	17
Phasing	18
<i>Phasing Kits</i>	18
<i>Halogenated and Mercurated Nucleotides and Oligonucleotides</i>	19
Appendix – Screen Formulations	20



How to get started

Teaching

Protein Crystallization Starter Kit



Product	Cat. No.
Proteinkristallisations Starter Kit, Deutsche Version	CS-401DE
Protein Crystallization Starter Kit, English Version	CS-401EN
Kit d' initiation à la cristallisation des protéines, version française	CS-401FR

The **Protein Crystallization Starter Kit** is designed to introduce students to the field of protein crystallization. It contains all material you need to start to grow great looking Lysozyme crystals – a real highlight in Biology or Chemistry courses!

Two different experiments can be carried out using the Protein Crystallization Starter Kit:

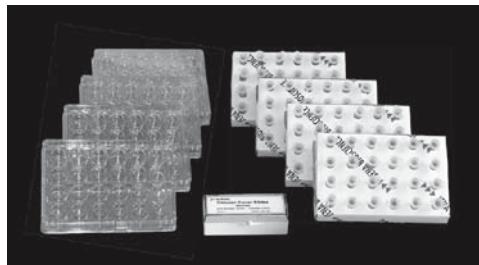
- Growing Lysozyme crystals using the hanging-drop method, demonstrating the dependence of nucleation and crystal growth on salt concentration and buffer pH
- Growing Lysozyme crystals within minutes using the batch crystallization method

The kit contains two crystallization plates, cover slides, a microscope slide, a syringe pre-filled with sealing grease, all necessary buffer and salt stock solutions and a small tube containing pre-filtered Lysozyme solution.

No pipettes necessary! – If you don't have pipettes, simply use the included microcapillaries to pipette your crystallization drops!

JBS Crystallization Freshman Kits

JBS Crystallization Freshman Kit - Junior



Product	Cat. No.
JBS Crystallization Freshman Kit – Junior	CSK-101

The **JBS Crystallization Freshman Kit – Junior** is addressed to newcomers in the field of protein crystallography. It is designed for screening of initial crystallization conditions of proteins, peptides, nucleic acids and macromolecular complexes in order to grow single crystals suitable for X-ray diffraction analysis.

The **JBS Crystallization Freshman Kit – Junior** contains the required material to crystallize your protein under investigation using the "Hanging Drop Method":

- four 24-well crystallization plates
- 100 thick siliconized cover slides
- 1ml each of 96 unique **JBScreen JCSG++** screening reagents
- a detailed User Guide

JBS Crystallization Freshman Kit – Scholar



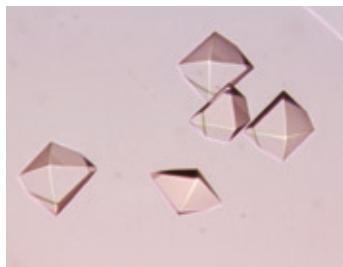
Product	Cat. No.
JBS Crystallization Freshman Kit – Scholar	CSK-102

The **JBS Crystallization Freshman Kit – Scholar** is the extended version of our JBS Crystallization Freshman Kit - Junior. It is addressed to newcomers in the field of protein crystallography who are interested in a rather extensive screening of one or more proteins, peptides, nucleic acids or macromolecular complexes in order to grow single crystals suitable for X-ray diffraction analysis.

The **JBS Crystallization Freshman Kit – Scholar** contains the required material for crystallization screening using the "Hanging Drop Method":

- forty 24-well crystallization plates
- 1000 thick siliconized cover slides
- five **JBScreen Classic Kits**, each containing 24 reagents at 10 ml
 - JBScreen Classic 1 (PEG 400 to PEG 3000 based)
 - JBScreen Classic 2 (PEG 4000 based)
 - JBScreen Classic 4 (PEG 5000 MME to 8000 based)
 - JBScreen Classic 6 (Ammonium Sulfate based)
 - JBScreen Classic 7 (MPD based)
- a detailed User Guide

Crystallization Model Proteins



Crystal Handling Kit



Product	Cat. No.
Lysozyme	CO-401
Lipase B	CO-402
Xylanase	CO-403
Proteinase K	CO-404

Our **Crystallization Model Proteins** can be utilized in crystallization experiments as well as crystallization training and demos.

We offer 4 proteins which can be easily crystallized within days as lyophilized powder or in a stabilization buffer:

- Lysozym (*Chicken egg white*)
- Lipase B (*Candida antarctica*)
- Xylanase (*Trichoderma longibrachiatum*)
- Proteinase K (*Tritirachium album*)

Product	Cat. No.
Crystal Handling Kit	CO-150

The **Crystal Handling Kit** will help you to acquire skills in protein crystallization, crystal mounting and data collection.

Each kit contains:

- 4 proteins, i.e. Lysozyme, Lipase B, Xylanase and Proteinase K
- optimized solubilization and crystallization buffers for each protein
- MicroMounts™ and Goniometer Bases, as well as
- a user manual with instructions for protein crystallization using the hanging-drop vapor diffusion method and crystal mounting using MiTeGen's MicroMounts™



Initial Screening

Crystallization Screens

The products of the **JBScreen family** are designed for efficient and flexible screening of crystallization conditions for proteins, peptides, nucleic acids, macromolecular complexes and water-soluble small molecules.



A broad sampling of crystallization space and select formulations proven to maximize the rate of success make JBScreen's the number one choice for academic and industrial labs around the world.

The high-quality reagents are prepared with great care ensuring elaborate and reproducible crystallization experiments.

- Chemicals used are of MicroSelect grade for Molecular Biology.
- Buffers are prepared as 1 M stock solutions. The pH is adjusted to the value indicated in the specification of the particular condition (23°C; Fisher pH electrode). pH values indicated are those of the buffer used, not those of the final JBScreen condition!
- Percentages given are w/v or v/v values as indicated in the data sheets.
- The final volume is adjusted with >18 MΩ × cm⁻¹ water.
- Solutions are sterile filtered (0.2 µm filter) and filled under sterile conditions.
- All screens contain a detailed production report.



IFTA AG
Certified QMS according to
DIN EN ISO 9001
Reg. No. IC 03214 034

The production of our screening reagents is examined by a stringent quality management system which is certified by **DIN EN ISO 9001**.

All our Screens include a detailed production report and data sheets.

The formulations of the unique reagents are listed in the appendix. → Please see page 20

JBScreen Classic

Product	Cat. No.
JBScreen Classic 1	CS-101L
JBScreen Classic 2	CS-102L
JBScreen Classic 3	CS-103L
JBScreen Classic 4	CS-104L
JBScreen Classic 5	CS-105L
JBScreen Classic 6	CS-106L
JBScreen Classic 7	CS-107L
JBScreen Classic 8	CS-108L
JBScreen Classic 9	CS-109L
JBScreen Classic 10	CS-110L
JBScreen Classic 1–5	CS-112L
JBScreen Classic 6–10	CS-113L
JBScreen Classic 1–10	CS-114L
JBScreen Classic HTS I S (1.0 ml per well)	CS-201S
JBScreen Classic HTS I L (1.7 ml per well)	CS-201L
JBScreen Classic HTS II S (1.0 ml per well)	CS-202S
JBScreen Classic HTS II L (1.7 ml per well)	CS-202L

Formats:

Bulk – 1Kit contains 24 screening solutions at 10 ml aliquots.

HTS – a **compressed JBScreen Classic** delivered in 2 x 96 well master blocks (HTS I & HTS II).

HTS S: 1.0 ml per well

HTS L: 1.7 ml per well

The **JBScreen Classic** crystallization screening kits represent a comprehensive statistical compilation of the most successful crystallization conditions published.

The full JBScreen Classic system comprises 10 screening kits covering 240 conditions, with each kit containing 24 reagent formulations grouped according to precipitant type and concentration. The organization of the JBScreen Classic maximizes flexibility by allowing the user to selectively screen against specific precipitant classes. A zone-organized layout of the individual kit formulations also provides an opportunity to visualize the effects of conditions neighbouring a particular hit!

Numerous **literature citations** show that JBScreen Classic has been successfully employed in crystallization experiments:

Marcia *et al.* (2009) The structure of *Aquifex aeolicus* sulfide:quinone oxidoreductase, a basis to understand sulfide detoxification and respiration. *Proc. Natl. Acad. Sci.* **106**:9625.

Dunstan *et al.* (2009) Structure of the Thiotreptone Resistance Methyltransferase S-Adenosyl-L-methionine Complex and Its Interaction with Ribosomal RNA. *J. Biol. Chem.* **284**: 17013.

Vulliez-LeNormand *et al.* (2008) Structures of synthetic O-antigen fragments from serotype 2a *Shigella flexneri* in complex with a protective monoclonal antibody. *Proc. Natl. Acad. Sci.* **105**:9976.

Okada *et al.* (2007) Crystal Structure of the γ-Glutamyltranspeptidase Precursor Protein from *Escherichia coli*. *J. Biol. Chem.* **282**:2433.

Smatanová *et al.* (2006) New techniques for membrane protein crystallization tested on photosystem II core complex of *Pisum sativum*. *Photosynth. Res.* **90**:255.

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

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

Vorup-Jensen *et al.* (2003) Structure and allosteric regulation of the αXβ2 integrin I domain. *Proc. Natl. Acad. Sci. USA* **100**:1873.

JBScreen Basic

Product	Cat. No.
JBScreen Basic 1	CS-121
JBScreen Basic 2	CS-122
JBScreen Basic 3	CS-123
JBScreen Basic 4	CS-124
JBScreen Basic 1–4	CS-125
JBScreen Basic HTS S (1.0 ml per well)	CS-203S
JBScreen Basic HTS L (1.7 ml per well)	CS-203L

Applications: Crystallization screening for proteins, peptides, nucleic acids, macromolecular complexes and water-soluble small molecules.

Formats:

Bulk – 1 Kit contains 24 screening solutions at 10 ml aliquots

HTS – 96 solutions of **JBScreen Basic 1–4** delivered in a 96 well masterblock (HTS I & HTS II).

HTS S: 1.0 ml per well

HTS L: 1.7 ml per well

JBScreen Basic has been formulated to comply with our customers' continuous interest in this particular sparse-matrix screen. The reagents of JBScreen Basic were selected based upon the protocol of Jancarik & Kim [1] and others [2]. Visit our web page to read more about the improvements we have made, such as the elimination of harmful cacodylate.



JBScreen Basic has been used to crystallize various proteins with the **CyBi®-Crystal Creator** from CyBio AG [3]. Samples of Insulin, Alcohol Dehydrogenase, Phospholipase A2, Trypsin and Lysozyme at 10 mg/ml were crystallized using protein volumes as low as 0.1 µl.

All five proteins applied in the crystallization experiment yielded either micro crystals or well-shaped small crystals. Both the reagent selection and the software-controlled robotic system with its Graphical User Interface enabled easy and very efficient walk-away automation of the crystallization experiment.

Protein	No. of Hits produced by JBScreen Basic	
	room temperature	4°C
Insulin	7	4
Alcohol Dehydrogenase	7	2
Phospholipase A2	0	2
Trypsin	1	1
Lysozyme	1	17

References:

- [1] Jancarik & Kim (1991) Sparse matrix sampling: a screening method for crystallization of proteins. *J. Appl. Cryst.* **4**:409.
- [2] Cudney *et al.* (1994) Screening and optimization strategies for macromolecular crystal growth. *Acta Cryst. D* **50**:414.
- [3] Kenkles *et al.* (2007) Application Note: Fully automated sitting drop protein crystallization with CyBi®-Crystal Creator using JBScreen Basic HTS Kit, www.cybio-ag.com

Selected Literature Citations of JBScreen Basic

- Kumar *et al.* (2009) Crystallization and preliminary X-ray diffraction analysis of human seminal plasma protein PSP94. *Acta Cryst. F* **65**:389.
- Squina *et al.* (2009) Expression, purification, crystallization and preliminary crystallographic analysis of an endo-1,5- α -L-arabinanase from hyperthermophilic Thermotoga petrophila. *Acta Cryst. F* **65**:902.
- Fehnle *et al.* (2006) Examination of Key Intermediates in the Catalytic Cycle of Aspartate- β -semialdehyde Dehydrogenase from a Gram-positive Infectious Bacteria. *J. Biol. Chem.* **281**:31031.
- Küttner *et al.* (2006) Crystallization and preliminary X-ray characterization of two thermostable DNA nucleases. *Acta Cryst. F* **62**:1290.

JBScreen Membrane

Product	Cat. No.
JBScreen Membrane 1	CS-301L
JBScreen Membrane 2	CS-302L
JBScreen Membrane 3	CS-303L
JBScreen Membrane 1–3	CS-306L
JBScreen Membrane 1–3 & Detergents 1–2	CS-307L
JBScreen Membrane HTS S (1.0 ml per well)	CS-305S
JBScreen Membrane HTS L (1.7 ml per well)	CS-305L

Applications: Effective crystallization screening for membrane proteins.

Formats:

Bulk – 1 Kit contains 24 screening solutions at 10 ml aliquots

HTS – 72 solutions of **JBScreen Membrane 1–3** delivered in a 96 well masterblock

HTS S: 1.0 ml per well

HTS L: 1.7 ml per well

The **JBScreen Membrane** crystallization screening kits represent a compilation of the most successful published crystallization conditions for obtaining well-diffracting membrane protein crystals.

Similar to JBScreen Classic, the JBScreen Membrane kits are organized in terms of precipitant type and concentration. The powerful conditions and sensible layout make JBScreen Membrane a first choice for crystallization screening of membrane proteins. When used in combination with the **JBScreen Detergents** kits, a further dramatic enhancement of membrane protein crystallization potential is realized.

Selected Literature Citations of JBScreen Membrane

- Cherezov *et al.* (2006) In Meso Structure of the Cobalamin Transporter, BtuB, at 1.95 Å Resolution. *J. Mol. Biol.* **364**:716.

JBScreen Kinase

Product	Cat. No.
JBScreen Kinase 1	CS-131
JBScreen Kinase 2	CS-132
JBScreen Kinase 3	CS-133
JBScreen Kinase 4	CS-134
JBScreen Kinase 1–4	CS-135
JBScreen Kinase HTS S (1.0 ml per well)	CS-204S
JBScreen Kinase HTS L (1.7 ml per well)	CS-204L

Applications: Crystallization screening for protein kinases.

Formats:

Bulk – 1 Kit contains 24 screening solutions at 10 ml aliquots

HTS – 96 solutions of **JBScreen Kinase 1–4** delivered in a 96 well masterblock

HTS S: 1.0 ml per well

HTS L: 1.7 ml per well

JBScreen Kinase is a highly specialized screen formulated for the determination of initial crystallization conditions of protein kinases.

Through the use of advanced data mining, crystallization conditions of kinases have been identified from published structures. Data evaluation and verification resulted in the formulation of 96 unique reagents, highly effective for the crystallization of kinases.

JBScreen Kinase utilizes a variety of different precipitating agents, i.e. various molecular weight PEG's, MPD and Ammonium Sulfate, in combination with buffers covering a pH range from 3.1 – 10.0 and numerous additives.



JBScreen Phosphatase

Product	Cat. No.
JBScreen Phosphatase 1	CS-171
JBScreen Phosphatase 2	CS-172
JBScreen Phosphatase 3	CS-173
JBScreen Phosphatase 4	CS-174
JBScreen Phosphatase 1–4	CS-175
JBScreen Phosphatase HTS S (1.0 ml per well)	CS-208S
JBScreen Phosphatase HTS L (1.7 ml per well)	CS-208L

Applications: Crystallization screening for phosphatases.

Formats:

Bulk – 1Kit contains 24 screening solutions at 10 ml aliquots

HTS – 96 solutions of **JBScreen Phosphatase 1–4** delivered in a 96 well masterblock

HTS S: 1.0 ml per well

HTS L: 1.7 ml per well

JBScreen Phosphatase is a highly specialized crystallization screen ideally suited for phosphatases. 96 conditions have been selected from a comprehensive survey of successfully crystallized phosphatases.

JBScreen Phosphatase utilizes a variety of different precipitating agents, i.e. various molecular weight PEGs, MPD and Ammonium Sulfate, in combination with buffers covering a pH range from 4.0–11.0 and numerous additives. The reagents have been selected and indexed according to the main precipitant.

JBScreen PEG/Salt

Product	Cat. No.
JBScreen PEG/Salt 1	CS-141
JBScreen PEG/Salt 2	CS-142
JBScreen PEG/Salt 3	CS-143
JBScreen PEG/Salt 4	CS-144
JBScreen PEG/Salt 1–4	CS-145
JBScreen PEG/Salt HTS S (1.0 ml per well)	CS-205S
JBScreen PEG/Salt HTS L (1.7 ml per well)	CS-205L

Applications: Crystallization screening for soluble proteins.

Formats:

Bulk – 1Kit contains 24 screening solutions at 10 ml aliquots

HTS – 96 solutions of **JBScreen PEG/Salt 1–4** delivered in a 96 well masterblock

HTS S: 1.0 ml per well

HTS L: 1.7 ml per well

JBScreen PEG/Salt is an effective and universal reagent kit designed for initial screening of crystallization conditions of biological macromolecules.

It comprises high-purity PEG 3350 and PEG 5000 MME, each combined with 48 different salts, thus covering a range of anions and cations most frequently used in biocrystallography. The unique combination of the reagents allows screening of PEG versus ionic strength, ion type and pH.

JBScreen Nuc-Pro

Product	Cat. No.
JBScreen Nuc-Pro 1	CS-181
JBScreen Nuc-Pro 2	CS-182
JBScreen Nuc-Pro 3	CS-183
JBScreen Nuc-Pro 4	CS-184
JBScreen Nuc-Pro 1–4	CS-185
JBScreen Nuc-Pro HTS S (1.0 ml per well)	CS-209S
JBScreen Nuc-Pro HTS L (1.7 ml per well)	CS-209L

Applications: Crystallization screening for preliminary crystallization conditions of nucleic acids and protein-nucleic acid complexes.

Formats:

Bulk – 1Kit contains 24 screening solutions at 10 ml aliquots

HTS – 96 solutions of **JBScreen Nuc-Pro 1–4** delivered in a 96 well masterblock

HTS S: 1.0 ml per well

HTS L: 1.7 ml per well

JBScreen Nuc-Pro is a highly effective sparse matrix screen based upon extensive screening of the PDB [1], with focus on entries by structural genomic initiatives, the BMCD [2] and other protocols [3–5]. Reported crystallization conditions for various RNAs, DNAs as well as protein-nucleic acid complexes were compiled and analyzed for rate of recurrence.

The 96 conditions selected cover a variety of polymers, mono- and divalent metal ions, organics, alcohols and buffers of a pH range from 4.0 to 8.5. The organization of the reagents into individual kits is based upon the main precipitant, i.e. various molecular weight PEGs, Salts, alcohols (MPD and 2-Propanol).

References:

- [1] Berman *et al.* (2000) The Protein Data Bank. *Nucleic Acids Research* **28**:235.
- [2] Gilliland *et al.* (1994) The Biological Macromolecule Crystallization Database, Version 3.0: New Features, Data, and the NASA Archive for Protein Crystal Growth Data. *Acta Cryst. D* **50**:408.
- [3] Doudna *et al.* (1993) Crystallization of ribozymes and small RNA motifs by a sparse matrix approach. *Proc. Natl. Sci. USA* **90**:7829.
- [4] Scott *et al.* (1995) Rapid Crystallization of Chemically Synthesized Hammerhead RNAs using a Double Screening Procedure. *J. Mol. Biol.* **250**:327.
- [5] Ke *et al.* (2004) Crystallization of RNA and RNA-protein complexes. *Methods* **34**:408.

JBScreen Pentaerythritol

Product	Cat. No.
JBScreen Pentaerythritol 1 (PEP 426 based)	CS-191
JBScreen Pentaerythritol 2 (PEP 629 based)	CS-192
JBScreen Pentaerythritol 3 (PEE 270 based)	CS-193
JBScreen Pentaerythritol 4 (PEE 797 based)	CS-194
JBScreen Pentaerythritol 1–4	CS-195
JBScreen Pentaerythritol HTS S (1.0 ml per well)	CS-210S
JBScreen Pentaerythritol HTS L (1.7 ml per well)	CS-210L

Applications: Crystallization screening of peptides, proteins, membrane proteins and macromolecular complexes based on pentaerythritol polymers as precipitants.

Formats:

Bulk – 1Kit contains 24 screening solutions at 10 ml aliquots

HTS – 96 solutions of **JBScreen Pentaerythritol 1–4** delivered in a 96 well masterblock

HTS S: 1.0 ml per well

HTS L: 1.7 ml per well

JBScreen Pentaerythritol has been designed for efficient crystallization screening of biological macromolecules based on pentaerythritol polymers as precipitants. The screen was developed by Ulrike Demmer from the Max-Planck-Institute for Biophysics in Frankfurt.

The choice of a suitable precipitant is of crucial importance for the crystallization of proteins.

JBScreen Pentaerythritol utilizes two novel precipitating agents, i.e. pentaerythritol propoxylate and pentaerythritol epoxylate. Both are branched polymers containing a pentaerythritol backbone. Thus they differ from more traditional precipitants like MPD and PEG's in size and nature.

In addition, pentaerythritol polymers function as cryoprotectants. Protein crystals grown in high concentrations of these precipitants can be frozen directly from the crystallization drop. The successful application of pentaerythritol polymers to yield protein crystals was first described by Gulick *et al.*

JBScreen Pentaerythritol comprises of 96 unique conditions, based on 4 different pentaerythritol polymers as precipitating agent:

- Pentaerythritol propoxylate 426 (5/4 PO/OH)
- Pentaerythritol propoxylate 629 (17/8 PO/OH)
- Pentaerythritol ethoxylate 270 (3/4 EO/OH)
- Pentaerythritol ethoxylate 797 (15/4 EO/OH)



The 4 polymers are arranged to a grid screen, thus allowing screening i) of three different precipitant concentrations, ii) four different pH values and iii) with and without the addition of salts, i.e. magnesium chloride, ammonium sulfate, potassium chloride.

The advantage of **JBScreen Pentaerythriol** not only lies in the novel 96 conditions but also in the systematic arrangement of the unique reagents, which enables the user to compare individual conditions directly. Even if initial screening may not always yield crystals, valuable information about the protein under investigation can be obtained from the scoring sheet.

All **JBScreen Pentaerythritol** screening kits include a detailed production report and data sheets.

References:

Gulick *et al.* (2002) Pentaerythritol propoxylate: a new crystallization agent and cryoprotectant induces crystal growth of 2-methylcitrate dehydratase. *Acta Cryst. D* **58**:306.

JBScreen JCSG ++

Product	Cat. No.
JBScreen JCSG++ 1	CS-151
JBScreen JCSG++ 2	CS-152
JBScreen JCSG++ 3	CS-153
JBScreen JCSG++ 4	CS-154
JBScreen JCSG++ 1–4	CS-155
JBScreen JCSG++ HTS S (1.0 ml per well)	CS-206S
JBScreen JCSG++ HTS L (1.7 ml per well)	CS-206L

Applications: Crystallization screening for biological macromolecules.

Formats:

Bulk – 4 Kits containing 24 screening solutions each at 10 ml aliquots

HTS – 96 solutions of **JBScreen JCSG++ 1–4** delivered in a 96 well masterblock

HTS S: 1.0 ml per well

HTS L: 1.7 ml per well

JBScreen JCSG++ is a optimized sparse matrix screen developed by researchers from the Joint Center for Structural Genomics (JCSG) [1] and from the European Genomics Consortium [2].

96 reagents have been selected with the aim and to maximize the coverage of the crystallization parameter space and to reduce the redundancy of crystallization conditions within commercially available crystallization screens. Thus, a core set of 66 conditions used by the JCSG for high-throughput structural determination [1] was extended to 96 screening conditions in order to round off the pH profile and to incorporate different precipitants such as succinate, malonate and formate.

When **JBScreen JCSG ++** is used along with **JBScreen PACT ++**, the benefits of a sparse matrix screen can be combined with the systematic investigation the precipitation behaviour of the protein.

References:

[1] Page *et al.* (2004) Shotgun crystallization strategy for structural genomics: an optimized two-tiered crystallization screen against the *Thermotoga maritima* proteome. *Acta Cryst. D* **59**:1028.

[2] Newman *et al.* (2005) Towards rationalization of crystallization screening for small- to medium-sized academic laboratories: the PACT/JCSG+ strategy. *Acta Cryst. D* **61**:1426.

JBScreen PACT++

Product	Cat. No.
JBScreen PACT++ 1	CS-161
JBScreen PACT++ 2	CS-162
JBScreen PACT++ 3	CS-163
JBScreen PACT++ 4	CS-164
JBScreen PACT++ 1–4	CS-165
JBScreen PACT++ HTS S (1.0 ml per well)	CS-207S
JBScreen PACT++ HTS L (1.7 ml per well)	CS-207L

Applications: Crystallization screen facilitating systematic pH, anion- and cation testing in the presence of polyethylene glycol (PEG).

Formats:

Bulk – 4 Kits containing 24 screening solutions each at 10 ml aliquots

HTS – 96 solutions of **JBScreen PACT++ 1–4** delivered in a 96 well masterblock

HTS S: 1.0 ml per well

HTS L: 1.7 ml per well

JBScreen PACT++ is based on the work of Newman *et al.* [1]. The 96 unique crystallization conditions combine three mini-screens in one:

1. 24-condition PEG/pH screen
2. 24-condition PEG/cation screen
3. 48-condition PEG/anion screen

This systematic approach aims to alter individual components of the crystallization conditions, i.e. pH, anions and cations, independently from the others in order to obtain more information of the precipitation behaviour of the protein.

When **JBScreen PACT ++** is used along with **JBScreen JCSG ++**, systematic investigation of the precipitation behaviour of the protein can be combined with a sparse matrix screen in order to enhance the success rate of protein crystallization.

References:

[1] Newman *et al.* (2005) Towards rationalization of crystallization screening for small- to medium-sized academic laboratories: the PACT/JCSG+ strategy. *Acta Cryst. D* **61**:1426.



Cryo Screens

JBScreen Cryo

Product	Cat. No.
JBScreen Cryo 1	CC-103
JBScreen Cryo 2	CC-104
JBScreen Cryo 3	CC-105
JBScreen Cryo 4	CC-106
JBScreen Cryo 1–4	CC-107
JBScreen Cryo HTS S (1.0 ml per well)	CC-201S
JBScreen Cryo HTS L (1.7 ml per well)	CC-201L

Applications: Crystallization screening for proteins, peptides, nucleic acids, macromolecular complexes and water-soluble small molecules with cryo-ready reagents.

Formats:

Bulk – 1 Kit contains 24 screening solutions at 10 ml aliquots

HTS – 96 solutions of **JBScreen Cryo 1–4** delivered in a 96 well masterblock

HTS S: 1.0 ml per well

HTS L: 1.7 ml per well

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, cryo cooling prolongs crystal lifetime and facilitates straightforward data collection [1].

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 cryo cooling process. The right 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 is designed for efficient crystal screening in the presence of various cryoprotectants. The unique formulations of the JBScreen Cryo reagents are based on an extensive data base search [2] and contain sufficiently high concentrations of cryoprotectants allowing direct transfer of crystals from the crystallization drop into liquid nitrogen.

References:

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

[2] http://idb.ebstjaxa.jp/db_data/protein/search-e.php

Individual Screen Conditions



Product	Cat. No.
Individual Jena Bioscience Screen Condition, 10 ml	CS-IND-10ML
Individual Jena Bioscience Screen Condition, 100 ml	CS-IND-100ML

Applications: Convenient reproduction and optimization of crystallization conditions.

Formats:

Jena Bioscience individual conditions: 10 ml and 100 ml volumes

Access to individual screen conditions in larger volumes is important when it comes to reproducing initial hits and starting crystallization optimization, or for soaking experiments.

Individual conditions are available for the following Jena Bioscience screens...

- JBScreen Classic
- JBScreen Basic
- JBScreen Membrane
- JBScreen Kinase
- JBScreen Phosphatase
- JBScreen Nuc-Pro
- JBScreen PEG/Salt
- JBScreen Pentaerytritol
- JBScreen Cryo
- JBScreen PACT++
- JBScreen JCSG++

Solutions are made from identical chemicals as the conditions in the original screens.

Upon ordering, please indicate which condition from which screen you wish to purchase!

JBScreen Cryo Pro



Product	Cat. No.
JBScreen Cryo Pro	CC-102

Applications: Screening for suitable cryo conditions.

Kit contents: 12 compounds, either at 3 solid aliquots or at 50 µl aliquots each

JBScreen Cryo Pro is the most convenient tool on the market for producing effective cryoprotectants from your crystallization reservoir solution. The kit contains 12 different compounds, divided into sugar/amino acid-based cryoprotectants, alcohol-based cryoprotectants, and an oil-based cryoprotectant.

Three predispensed 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 directly transferred to a liquid nitrogen bath or cryogenic gas stream.

Crystal Dyes



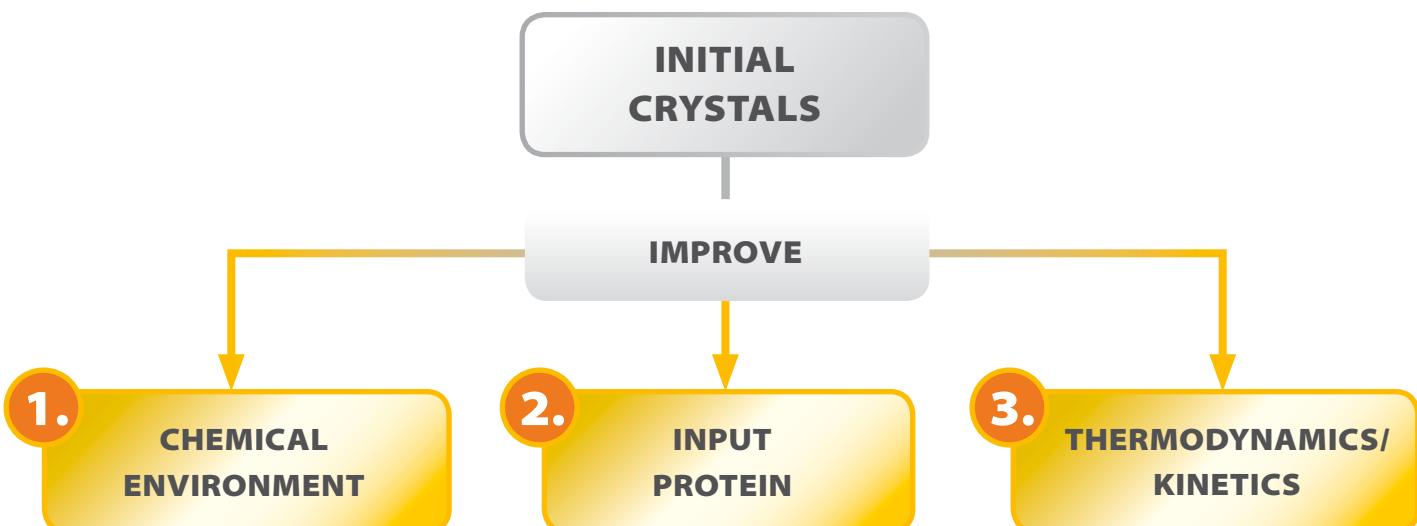
Product	Cat. No.	Amount
JBS True Blue	CO-301	300 µl
JBS Deep Purple	CO-302	300 µl
JBS Xtal Green	CO-303	300 µl
JBS Bright Red	CO-304	300 µl
JBS Rainbow Set of JBS Deep Purple, JBS True Blue, JBS Xtal Green and JBS Bright Red	CO-305	4 × 300 µl
JBS Black Light Fluorescent Crystal Dye	CO-306	300 µl

With the help of **JBS Crystal Dyes** you can discriminate between macromolecular crystals and salt crystals within minutes. Whatever suits your taste, you can stain your crystals blue, purple, green or red. All our crystal dyes are small molecules which are able to permeate the solvent channels of proteins and thus, staining them. In contrast, salt crystals will remain colorless.

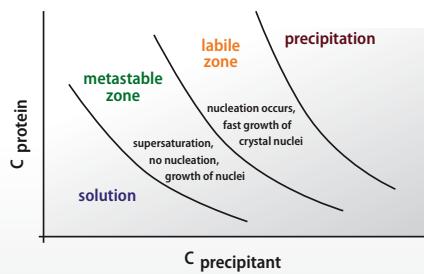
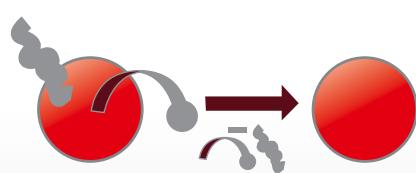
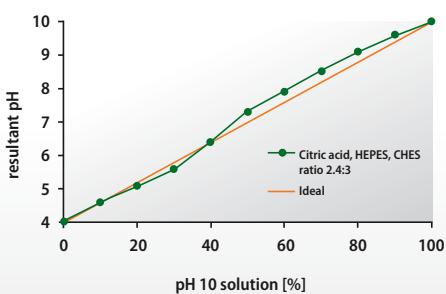
Our **JBS Black Light** is a nonspecific fluorescent crystal dye used for the detection of protein crystals in crystallization trials. The fluorescence signal can be exploited to contrast protein crystals above background artifacts and enables the detection of microcrystals, even if they are located under a protein skin. Thus, the dye is suitable for automatic crystal detection.

Hit Optimization

Strategies to optimize initial crystallization hits:



JBScreen pH-2D-Buffer system 2: Citric Acid, HEPES, CHES



Chemical Environment

Kits and screens to optimize the chemical composition of your crystallization reagents, i.e. buffer pH, precipitant and additive composition.

Input Protein

Get your protein ready for crystallization! Consider to optimize the solubilization buffer, alter the protein surface or modify the sequence by truncation or mutagenesis. Or try a new mode of production.

Thermodynamics / Kinetics

Do not discard bad diffracting crystals! They can be very useful, too. Try to improve diffraction by varying the solvent content or use your initial crystals for seeding.



Chemical Environment

Screens & Stock Solutions

JBS Custom Screen



Let us mix your screens!

JBS Custom Screens are designed by you! – Devise your own crystallization screens for initial screening or for optimization of a successful crystallization condition and let us prepare them for you.

Simply, send an xls sheet to orders@jenabioscience.com containing your required screening composition and format. We will come back to you with a quote and delivery time.

Please contact xtals@jenabioscience.com with questions or inquiries.

JBScreen Single Stocks



Applications: Reagents, consistent with Jena Bioscience screens, for reproduction and optimization of screening conditions.

Formats: JBScreen Single Stocks are available at 100 ml aliquots

Single stock solutions of the **JBScreen** components, i.e. polymers, buffers and salts are ideal for the optimization of your crystallization conditions.

Using the same chemicals as utilized in the JBScreens ensures higher reproducibility of your experiments. **JBScreen Single Stocks** are ready for use: the concentration is adjusted and they are sterile filtered.

Polymers

Product	Cat. No.	Price (€)
Pentaerythritol ethoxylate (3/4 EO/OH), 60 % w/v PEE 270	CSS-372	25,—
Pentaerythritol ethoxylate (3/4 EO/OH), 100 % v/v PEE 270	CSS-373	30,—
Pentaerythritol ethoxylate (15/4 EO/OH), 60 % w/v PEE 797	CSS-374	25,—
Pentaerythritol ethoxylate (15/4 EO/OH), 100 % v/v PEE 797	CSS-375	30,—
Pentaerythritol propoxylate (17/8 PO/OH), 60 % w/v PEP 629	CSS-376	25,—
Pentaerythritol propoxylate (17/8 PO/OH), 100 % v/v PEP 629	CSS-377	30,—

Pentaerythritol propoxylate (5/4 PO/OH),
60 % w/v
PEP 426

Pentaerythritol propoxylate (5/4 PO/OH),
100 % v/v
PEP 426

Polyethyleneglycol 200, 50 % v/v

Polyethyleneglycol 200, 50 % w/v

Polyethyleneglycol 300, 50 % v/v

Polyethyleneglycol 400, 50 % v/v

Polyethyleneglycol 400, 50 % w/v

Polyethyleneglycol 400, 75 % w/v

Polyethyleneglycol 400, 100 % v/v

Polyethyleneglycol 550 Monomethylether,
50 % v/v

Polyethyleneglycol 550 Monomethylether,
50 % w/v

Polyethyleneglycol 600, 50 % v/v

Polyethyleneglycol 600, 50 % w/v

Polyethyleneglycol 1000, 50 % w/v

Polyethyleneglycol 1500, 50 % w/v

Polyethyleneglycol 2000, 50 % w/v

Polyethyleneglycol 2000 Monomethylether,
50 % w/v

Polyethyleneglycol 3000, 50 % w/v

Polyethyleneglycol 3350, 50 % w/v

Polyethyleneglycol 4000, 50 % w/v

Polyethyleneglycol 5000 Monomethylether,
50 % w/v

Polyethyleneglycol 6000, 50 % w/v

Polyethyleneglycol 8000, 50 % w/v

Polyethyleneglycol 10000, 50 % w/v

Polyethyleneglycol 20000, 50 % w/v

Polyethylenimine, 50 % w/v

Jeffamine M-600, 50 % v/v, pH 7.0

CSS-196 55,—

Organics

Product

1,3-Propanediol, 50 % v/v

CSS-104 40,—

1,4-Dioxane, 50 % v/v

CSS-107 20,—

1,4-Dioxane, 50 % w/v

CSS-106 20,—

1,6-Hexanediol, 5 M

CSS-109 20,—

2,3-Butandiol, 50 % v/v

CSS-113 40,—

2-Methyl-2,4-Pentanediol, 50 % v/v

MPD CSS-328 20,—

2-Methyl-2,4-Pentanediol, 50 % w/v

MPD CSS-115 20,—

2-Methyl-2,4-Pentanediol, 100 % v/v

MPD CSS-117 25,—

2-Propanol, 50 % w/v

Iso-Propanol CSS-118 20,—

2-Propanol, 100 % v/v

Iso-Propanol CSS-119 25,—

Ethanol, 50 % v/v

Ethylalkohol CSS-330 25,—



Ethanol, 66 % w/v Ethylalkohol	CSS-179	30,—	Citrate/ Phosphate pH 5.0, 1 M 1M di-Potassium hydrogen Phosphate adjusted with Citric acid	CSS-341	45,—
Ethylene glycol, 50 % v/v 1,2-Ethanediol	CSS-182	20,—	Citric Acid pH 3.1, 1 M	CSS-162	35,—
Ethylene glycol, 50 % w/v 1,2-Ethanediol	CSS-336	20,—	Citric Acid pH 4.2, 1 M	CSS-342	35,—
Ethylene glycol, 100 % v/v 1,2-Ethanediol	CSS-183	25,—	Citric Acid pH 5.0, 1 M	CSS-343	35,—
Glycerol, 50 % v/v Glycerin	CSS-329	10,—	di-Potassium hydrogen Phosphate pH 7.0, 5 M	CSS-073	30,—
Glycerol, 50 % w/v Glycerin	CSS-186	10,—	Glycine pH 9.5, 1 M Glycocol	CSS-089	35,—
Glycerol, 80 % v/v Glycerin	CSS-332	15,—	Glycine, 1 M Glycocol	CSS-189	30,—
Glycerol, 80 % w/v Glycerin	CSS-187	15,—	HEPES pH 7.5, 1 M 4-(2-Hydroxyethyl)piperazine-1-ethanesulfonic acid	CSS-192	35,—
Glycerol, 100 % v/v Glycerin	CSS-188	20,—	HEPES, 1 M 4-(2-Hydroxyethyl)piperazine-1-ethanesulfonic acid	CSS-360	30,—
L-Glutathion reduced, 0.16 M	CSS-199	80,—	Imidazole pH 6.5, 1 M	CSS-095	45,—
Methanol, 50 % w/v	CSS-224	25,—	Imidazole pH 7.0, 1 M	CSS-355	45,—
Propylene Glycol, 50 % v/v 1,2-Propanediol	CSS-280	20,—	Imidazole pH 7.5, 1 M	CSS-344	45,—
tert-Butanol, 50 % v/v 2-Methyl-2-propanol	CSS-311	10,—	Imidazole pH 8.0, 1 M	CSS-345	45,—
tert-Butanol, 50 % w/v 2-Methyl-2-propanol	CSS-310	10,—	Imidazole pH 9.0, 1 M	CSS-346	45,—
Triethyleneglycol, 50 % w/v	CSS-314	20,—	Imidazole, 1 M	CSS-195	40,—
Xylitol, 50 % w/v Xylite	CSS-322	20,—	Lithium Acetate Dihydrate pH 7.5, 1 M	CSS-000	35,—

Buffers

Product	Cat. No.	Price (€)			
ADA pH 6.0, 1 M N-(2-Acetamido) iminodiacetic acid, N-(Carbamoylmethyl)iminodiacetic acid	CSS-125	70,—	Sodium Acetate pH 4.6, 1 M	CSS-283	35,—
ADA pH 6.5, 1 M N-(2-Acetamido) iminodiacetic acid, N-(Carbamoylmethyl)iminodiacetic acid	CSS-338	70,—	Potassium Phosphate, 1 M 1M di-Potassium hydrogen Phosphate adjusted with 1M Potassium dihydrogen Phosphate to pH 8.0	CSS-273	35,—
Bicine pH 9.0, 1 M N,N-Bis(2-hydroxyethyl) glycine	CSS-147	35,—	Sodium dihydrogen Phosphate, 5 M	CSS-087	35,—
Bicine pH 9.5, 1 M N,N-Bis (2-hydroxyethyl) glycine	CSS-339	35,—	Sodium Phosphat pH 6.2, 1 M 1M di-Sodium hydrogen Phosphate adjusted with 1M Sodium dihydrogen Phosphate	CSS-297	30,—
Bis-Tris pH 6.5, 1 M 2-Bis (2-hydroxyethyl) amino-2-(hydroxymethyl)-1,3-propanediol	CSS-148	50,—	Sodium Phosphat pH 6.7, 1 M 1M di-Sodium hydrogen Phosphate adjusted with 1M Sodium dihydrogen Phosphate	CSS-348	30,—
Bis-Tris pH 7.0, 1 M 2-Bis (2-hydroxyethyl) amino-2-(hydroxymethyl)-1,3-propanediol	CSS-340	50,—	Sodium Phosphat pH 6.8, 1 M 1M di-Sodium hydrogen Phosphate adjusted with 1M Sodium dihydrogen Phosphate	CSS-349	30,—
Bis-Tris-Propan pH 7.0, 1M	CSS-149	95,—	Sodium Phosphat pH 7.0, 1 M 1M di-Sodium hydrogen Phosphate adjusted with 1M Sodium dihydrogen Phosphate	CSS-350	30,—
CAPS pH 10, 1 M 3-(Cyclohexylamino)-1-1propanesulfonic acid	CSS-156	35,—	Sodium Potassium Phosphate pH 6.5, 1 M	CSS-299	30,—
CHES pH 9.5, 1 M 2-(Cyclohexylamino)ethanesulfonic acid	CSS-160	70,—	Sodium Potassium Phosphate pH 7.5, 1 M	CSS-351	30,—
Citrate/ Phosphate pH 4.4, 1 M 1M di-Potassium hydrogen Phosphate adjusted with Citric acid	CSS-161	45,—	Succinic Acid, 0.5 M	CSS-307	20,—
			Tricine pH 8.0, 1 M N-[Tris(hydroxymethyl)methyl]glycine	CSS-313	35,—
			Tris (Tris-Acetate) pH 8.0, 1 M 2-Amino-2-(hydroxymethyl)-1,3-propanediol	CSS-337	30,—
			Tris pH 7.5, 1 M 2-Amino-2-(hydroxymethyl)-1,3-propanediol	CSS-320	35,—



Tris pH 8.0, 1 M	CSS-353	35,—
2-Amino-2-(hydroxymethyl)-1,3-propanediol		
Tris pH 8.5, 1 M	CSS-354	35,—
2-Amino-2-(hydroxymethyl)-1,3-propanediol		
tri-Sodium Citrate Dihydrate pH 4.8, 1 M	CSS-318	30,—
tri-Sodium Citrate Dihydrate pH 5.6, 1 M	CSS-352	30,—

Salts

Product	Cat. No.	Price (€)
Ammonium Acetate, 1 M	CSS-128	30,—
Ammonium Acetate, 5 M	CSS-129	30,—
Ammonium Bromide, 1 M	CSS-130	30,—
Ammonium Chloride, 5 M	CSS-131	30,—
Ammonium dihydrogen Phosphate, 1 M	CSS-132	30,—
Ammonium dihydrogen Phosphate, 3 M	CSS-133	30,—
Ammonium Fluoride, 10 M	CSS-134	35,—
Ammonium Formate, 2.5 M	CSS-135	35,—
Ammonium Formate, 5 M	CSS-136	40,—
Ammonium Iodide, 1 M	CSS-137	30,—
Ammonium Nitrate, 10 M	CSS-138	35,—
Ammonium Sulfate, 1 M	CSS-142	35,—
Ammonium Sulfate, 5 M	CSS-143	40,—
Cadmium Chloride, 1 M	CSS-151	40,—
Cadmium Sulfate, 1 M	CSS-152	40,—
Calcium Acetate Hydrate, 1 M	CSS-153	30,—
Calcium Chloride Dihydrate, 1 M	CSS-154	30,—
Calcium Chloride Dihydrate, 5 M	CSS-155	35,—
Cesium Chloride, 1 M	CSS-157	40,—
Cesium Chloride, 2 M	CSS-158	50,—
Cobalt(II) Chloride Hexahydrate, 1 M	CSS-163	40,—
di-Ammonium hydrogen Phosphate, 3.5 M	CSS-171	30,—
di-Ammonium Tartrate, 2 M	CSS-172	30,—
di-Potassium hydrogen Phosphate, 5 M	CSS-173	30,—
di-Sodium hydrogen Phosphate, 0.5 M	CSS-174	30,—
Ferric(III) Chloride Hexahydrate, 1 M	CSS-184	40,—
Hexadecyltrimethylammonium Bromide, 0.008 M	CSS-331	20,—
Cetyltrimethylammonium bromide		
Lithium Acetate Dihydrate, 1 M	CSS-200	30,—
Lithium Bromide, 1 M	CSS-201	60,—
Lithium Chloride, 1 M	CSS-335	30,—
Lithium Chloride, 5 M	CSS-202	35,—
Lithium Chloride, 10 M	CSS-356	40,—
Lithium Citrate Hydrate, 1.5 M	CSS-203	30,—
Lithium Nitrate, 8 M	CSS-204	40,—
Lithium Sulfate, 1 M	CSS-206	30,—
Lithium Sulfate, 2.5 M	CSS-207	35,—
Magnesium Acetate Tetrahydrate, 1 M	CSS-210	35,—
Magnesium Chloride Hexahydrate, 1 M	CSS-211	35,—
Magnesium Chloride Hexahydrate, 2.5 M	CSS-212	40,—
Magnesium Formate Dihydrate, 0.2 M	CSS-213	30,—
Magnesium Nitrate Hexahydrate, 1 M	CSS-214	35,—

Magnesium Sulfate Heptahydrate, 1 M	CSS-215	30,—
Magnesium Sulfate Heptahydrate, 2.5 M	CSS-216	35,—
Nickel Sulfate Hexahydrate, 1 M	CSS-227	35,—
Nickel(II) Chloride Hexahydrate, 1 M	CSS-228	40,—
Potassium Acetate, 5 M	CSS-262	35,—
Potassium Bromide, 4 M	CSS-264	40,—
Potassium Chloride, 1 M	CSS-265	35,—
Potassium Chloride, 4 M	CSS-371	40,—
Potassium dihydrogen Phosphate, 1 M	CSS-268	30,—
Potassium Formate, 10 M	CSS-269	80,—
Potassium Iodide, 1 M	CSS-270	35,—
Potassium L-Tartrate Monobasic, 0.025 M	CSS-271	30,—
Potassium Nitrate, 1 M	CSS-272	35,—
Potassium Phosphate, 1 M 1M di-Potassium hydrogen Phosphate/1M Potassium dihydrogen Phosphate	CSS-274	35,—
Potassium Sulfate 0.5 M	CSS-275	30,—
Potassium Thiocyanate, 2 M	CSS-276	45,—
Potassium/Sodium Tartrate-4-hydrate, 1 M	CSS-277	35,—
Potassium/Sodium Tartrate-4-hydrate, 2 M	CSS-278	40,—
Sodium Acetate, 2.5 M	CSS-284	40,—
Sodium Bromide, 3 M	CSS-285	40,—
Sodium Chloride, 1 M	CSS-333	35,—
Sodium Chloride, 5 M	CSS-286	40,—
Sodium dihydrogen Phosphate, 5 M	CSS-287	35,—
Sodium Fluoride, 1 M	CSS-290	30,—
Sodium Formate, 5 M	CSS-291	35,—
Sodium Iodide, 1 M	CSS-293	30,—
Sodium Malonate, 2 M Malonic acid Disodium salt Monohydrate	CSS-217	45,—
Sodium Nitrate, 7 M	CSS-294	30,—
Sodium Sulfate, 1 M	CSS-300	35,—
Sodium Tartrate dibasic Dihydrate, 1 M	CSS-301	35,—
Sodium Thiocyanate, 8 M	CSS-303	30,—
tri-Potassium Citrate Monohydrate, 2.5 M	CSS-266	30,—
tri-Sodium Citrate Dihydrate, 1.6 M	CSS-319	30,—
Zinc Acetate Dihydrate, 1 M	CSS-324	35,—
Zinc Chloride, 1 M	CSS-325	30,—
Zinc Sulfate Heptahydrate, 1 M	CSS-326	35,—



Buffers

JBScreen pH-2D



Product	Cat. No.
JBScreen pH-2D	CS-701

Applications: Extended broad range pH-screening independent of the chemical nature of the components of the buffer system

Kit contents: 6 broad range buffer systems, each consisting of a low pH and a high pH buffer at 10 ml aliquots.

JBScreen pH-2D is designed to sample a broad pH-range without changing the buffering environment [1]. This ensures pH-screening independent of the chemical nature of the components of the buffer system.

JBScreen pH-2D contains six extended range buffer systems, each composed of a mixture of three individual buffers with a distinct chemical nature and well separated pKa values. Each buffer system is composed of a low-pH and a high-pH stock solution, supplied in 10 ml volumes. The low-pH stock solution is preset at pH 4.0 and the high-pH solution at either pH 9.0 or 10.0. Thus, mixtures of the low-pH and high-pH stock solutions in different proportions allow to cover the entire pH range from 4.0–9.0 or 4.0–10.0, respectively. The composition of the buffer systems assures a virtually linear distribution of the resulting pH vs. the percentage of high pH / low pH stock.

Larger volumes of the buffers are available upon request.

References:

- [1] Newman (2004) Novel buffer systems for macromolecular crystallization. *Acta Cryst. D* **60**:610.

JBScreen Buffer Kits



Product	Cat. No.
JBScreen Buffer Kit Sodium Acetate	CO-101
JBScreen Buffer Kit Sodium Citrate	CO-102
JBScreen Buffer Kit MES	CO-103
JBScreen Buffer Kit HEPES	CO-104
JBScreen Buffer Kit Tris-HCl	CO-105

Applications: Titrated buffer stocks for pH modulation, reproduction and optimization of crystallization set-ups.

Kit contents: The JBScreen Buffer Kits contain ready-made 1M buffer solutions with preset pH values at 0.1 unit increments at 10 ml aliquots.

- JBScreen Buffer Kit Sodium Acetate, pH 3.5 – 5.6
- JBScreen Buffer Kit Sodium Citrate, pH 3.7 – 6.0
- JBScreen Buffer Kit MES, pH 5.6 – 6.7
- JBScreen Buffer Kit HEPES, pH 6.8 – 8.2
- JBScreen Buffer Kit Tris-HCl, pH 7.1 – 9.0

JBScreen Buffer Kits are designed for convenient reproduction and optimization of crystallization conditions. The solutions can be used to reformulate conditions of the **JBScreen family**, e.g. JBScreen Classic, JBScreen Basic, JBScreen Cryo, and other commercially available crystallization screens.

Furthermore, JBScreen Buffer Kits can be employed for the straightforward preparation of custom screen solutions for the refinement and optimization of initial crystallization conditions. The JBScreen Buffer Kit formulations will help to save time preparing accurate and high-quality reagents for the reproducible production of single protein crystals.

Additives and Detergents

JBScreen Plus



JBScreen Detergents



Product	Cat. No.
JBScreen Plus Kosmotropic	CS-501
JBScreen Plus Chaotropic	CS-502
JBScreen Plus Salts	CS-503
JBScreen Plus Additives	CS-504
JBScreen Plus Volatiles	CS-505
JBScreen Plus Complete (all 5 kits)	CS-506
JBScreen Plus HTS S (200 µl per well)	CS-507S
JBScreen Plus HTS L (1.0 ml per well)	CS-507L

Applications: Additive screening to manipulate sample-sample and sample-solvent interactions.

Formats:

Bulk – 1Kit contains 24 screening solutions at 1 ml aliquots

HTS – 96 solutions of JBScreen Plus (kosmotropic, chaotropic, salts, additives) delivered in a 96 well masterblock

HTS S: 250 µl per well

HTS L: 1.0 ml per well

JBScreen Plus is an additive screen most useful in the optimization of preliminary crystallization conditions. JBScreen Plus consists of 5 individual kits, JBScreen Plus Kosmotropic, JBScreen Plus Chaotropic, JBScreen Plus Salts, JBScreen Plus Additives and JBScreen Plus Volatiles. The selection of the additives is based on the Hofmeister series which reflects the ability of ions to stabilize the structure of proteins. Hence, ions can be classified as either kosmotropic or chaotropic. The former having structure stabilizing properties. Thus, they may assist in, e.g. crystallizing proteins with a high proportion of flexible loop regions. The latter showing structure disturbing properties which may assist in the crystallization of large complexes allowing them to rearrange to form favorable crystal contacts [1].

The 96 solutions of **JBScreen Plus HTS**, comprising the reagents of the kosmotropic, chaotropic, salts and additive kit, are supplied in a sterile deep well block containing either 200 µl (JBScreen Plus HTS S) or 1 ml (JBScreen Plus HTS L). JBScreen Plus HTS S is particularly designed for low volume users. The screening reagents can be added directly to the additives in the deep well block before starting a vapor diffusion experiment, while JBScreen Plus HTS L will enable you to transfer any desired volume of additive solution to your plate.

References:

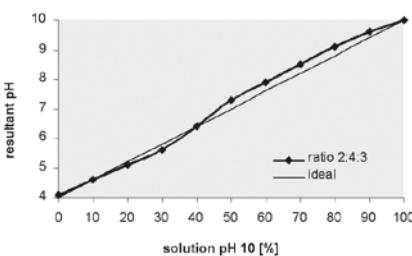
- [1] Collins (2004) Ions from the Hofmeister series and osmolytes: effects on proteins in solution and in the crystallization process. *Methods* **34**:300.

Product	Cat. No.
JBScreen Detergents 1	CD-101
JBScreen Detergents 2	CD-102
JBScreen Detergents 1 & 2	CD-103

Applications: Optimization of solubility of membrane proteins as well as additive screening with detergents and detergent mixtures.

Kit contents: 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.

Membrane protein crystallization remains one of the most formidable challenges of modern-day crystallography. To help speed and simplify the process, Jena Bioscience has assembled a collection of the 24 most successful detergents used in membrane protein crystallization.



Plot of the pH-curve for buffer system Citric Acid, HEPES, CHES, which comprises two stock solutions preset at pH 4.0 and 10.0, respectively. The two stock solutions were mixed in different ratios ranging from 10:0 to 0:10 and the resulting pH values were measured.

JBScreen Detergents can be used throughout the protein purification process or can be added afterwards by dialysis on ion-exchange chromatography. Detergent exchange can be vital for obtaining well-diffracting membrane protein crystals [1]. JBScreen Detergents are also valuable for additive screening with detergents and detergent mixtures [2,3] in combination with the JBScreen Membrane kit.

References:

- [1] Rosenow *et al.* (2003) The influence of detergents and amphiphiles on the solubility of the light-harvesting I complex. *Acta Cryst. D* **59**:1422.
[2] Adir (1999) Crystallization of the oxygen-evolving reaction centre of photosystem II in nine different detergent mixtures. *Acta Cryst. D* **55**:891.
[3] Koronakis *et al.* (2000) Crystal structure of the bacterial membrane protein TolC central to multidrug efflux and protein export. *Nature* **405**:914.



Input Protein

Existing Protein

JBS Solubility Kit



Product	Cat. No.
JBS Solubility Kit	CO-310

Applications: Pre-crystallization screen to improve the composition of the initial protein buffer solution prior to performing crystallization set-ups.

Kit contents: 24 buffer solutions at 10 ml aliquots + 14 additives at 250 µl aliquots

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 [1]. 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 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.

References:

- [1] 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.

JBSolution Detergent Test Kit



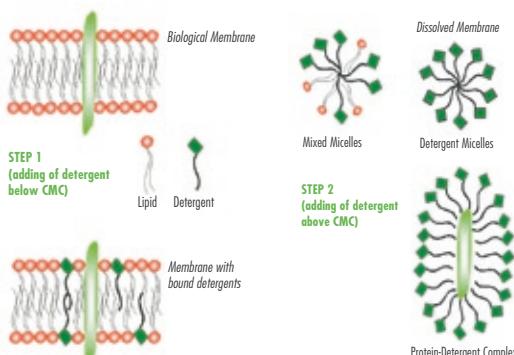
Product	Cat. No.
JBSolution Detergent Test Kit	DK-101

Applications: Dissolving hydrophobic proteins out of the biological lipid bilayer.

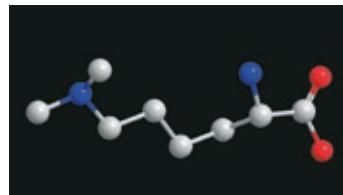
Kit contents: Assembly of 27 detergents as 4 ml stock solutions + 3 buffer solutions at 10 ml aliquots, each at two pH values.

The **JBSolution Detergent Test Kit** is designed to optimize the solubilization of membrane proteins. Compounds assembled in the kit range from ionic to non-ionic to zwitter-ionic detergents. These detergents have non-denaturing as well as denaturing properties. The arrangement is based on years of experience. The kit contains 4 ml stock solutions of 27 detergents and 3 buffers at 1 M concentration (Tris-HCl, HEPES Sodium Salt, Sodium Phosphate Buffer), each at two different pH-values (7.5 and 8.0).

Solubilization of Cell Membranes:



JBS Methylation Kit



Ball-and-Stick representation of a methylated lysine residue.

Product	Cat. No.
JBS Methylation Kit	CS-510

Applications: Surface engineering by selective methylation of lysine residues to alter crystallization properties of proteins.

Formats: All reagents required, sufficient for at least 6 methylation experiments.

Surface engineering of proteins can be a powerful technique for dealing with proteins that yield no or poorly diffracting crystals. In particular, reductive methylation of proteins has emerged as a standard procedure in several large scale facilities and research programs, i.e. the Midwest Centre of Structural genomics [1] and the Structural Proteomics In Europe (SPINE) program [2,3].

The **JBS Methylation Kit** is designed for **selective methylation of lysine residues**. The method does not require laborious cloning/expression/purification but chemically replaces the protons of the amino group of all lysine residues with methyl groups. The result is a surface-engineered protein within 24 hours ready for crystallization.

Just follow the manual step-by-step. No background in chemistry necessary.

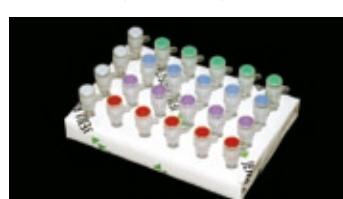
References:

- [1] Kim *et al.* (2008) Large-scale evaluation of protein reductive methylation for improving protein crystallization. *Nature Methods* **5**:853.
[2] Fogg *et al.* (2006) Application of the use of high-throughput technologies to the determination of protein structures of bacterial and viral pathogens. *Acta Cryst. D* **62**:1196.
[3] Walter *et al.* (2006) Lysine methylation as a routine rescue strategy for protein crystallization. *Structure* **14**:1617.

Reference for successful application of the JBS Methylation Kit:

Shi *et al.* (2006) Expression, crystallization and preliminary crystallographic studies of a novel bifunctional N-acetylglutamate synthase/kinase from *Xanthomonas campestris* homologous to vertebrate N-acetylglutamate synthase. *Acta Cryst. D* **62**:1218.

JBS Floppy-Choppy



Product	Cat. No.
JBS Floppy-Choppy (In situ proteolysis as rescue technique in protein crystallization)	CO-110

JBS Floppy-Choppy is the rescue kit for proteins which are recalcitrant to crystallization. It enables the researcher to modify the protein target by *in situ* proteolysis to improve its crystallization behavior.

The method implies the addition of trace amounts of protease to the protein solution immediately prior to crystallization. Thus, the crystallization experiment is very straightforward. It can be set up without evaluating the efficacy of proteolysis, without stopping the proteolysis reaction and without purification of any proteolyzed protein fragments.

In situ proteolysis is one of the most efficacious crystallization rescue strategies used at structural genomic centers [1,2].

Make a new / better Protein

Random Mutagenesis Kits

Product	Cat. No.	Amount
JBS dNTP-Mutagenesis Kit Random Mutagenesis by dNTP Analogs	PP-101	15 reactions
JBS Error-Prone Kit Random Mutagenesis by Error-Prone PCR	PP-102	15 reactions
JBS DNA-Shuffling Kit Random Mutagenesis by DNA Shuffling	PP-103	15 reactions

Within three billion years of evolution, nature has produced a plethora of proteins simply by repeated cycles of random mutagenesis followed by *in vivo* selection for superior function of the encoded proteins. This example of natural evolution has guided researchers within the last two decades to develop strategies for *in vitro* permutation of proteins.

Among the variety of strategies applied, three major powerful techniques have emerged.

LEXSY – Eukaryotic protein expression in *Leishmania tarentolae*

The unicellular kinetoplast protozoan *Leishmania tarentolae*, isolated from the Moorish gecko *Tarentola mauritanica*, not pathogenic to mammals (Biosafety level 1) – was turned into the protein-producing host of our eukaryotic protein expression system LEXSY:

- eukaryotic host as easy to handle as *E. coli*: no specific labware, no cell biology equipment required.
- fully eukaryotic protein expression machinery with post-translational modifications, including glycosylation and disulfide bond formation
- shuttle vectors: cloning in *E. coli*, expression in LEXSY host
- constitutive or inducible, intracellular or secretory expression of target proteins
- stable expression strains for constant protein production

Find all tools required for protein expression with LEXSY (expression kits, LEXSY host, cultivation kits and tools, shuttle vectors and more) in our General Catalog or at our website www.jenabioscience.com.

Thermodynamics / Kinetics

Dehydration Salts & Crystal Dehydration and Salvage Kit



Product	Cat. No.
Dehydration Salts	CO-121
Crystal Dehydration and Salvage Kit	CO-122

Dehydration has been used as a tool for inducing structural changes in protein crystals since the earliest days of protein crystallography. Though neglected, dehydration remains a powerful tool for improving or at least modifying the diffraction properties of protein crystals.

- Dehydration removes excess solvent, tightens packing of protein molecules, and reduces the size of solvent channels. As a result, it sometimes improves crystal order and diffraction resolution.
- By removing excess solvent, dehydration can make successful flash cooling easier, especially for crystals with large initial solvent contents.
- When sufficiently dehydrated, many protein crystals undergo structural transformations, yielding alternative crystal packings that may be difficult or impossible to achieve directly during crystal growth.

Of all post-crystallization treatments, dehydration has proven to be the most effective in improving crystal diffraction properties. Of course, dehydration also often severely degrades crystal diffraction, but (amazingly!) original crystal order can usually be fully recovered just by rehydrating.

Dehydration Salts and the **Crystal Dehydration and Salvage Kit** have been designed for an easy, controlled and reliable way to dehydrate protein crystals and thus provide an efficient tool for altering / improving their diffraction properties.

The **Dehydration Salts** contain 12 saturated salt solutions, 1 ml each, producing relative humidities in the range of 22.5 to 97.3 %.

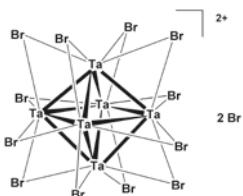
The **Crystal Dehydration and Salvage Kit**, shown on the left, is composed of the 12 dehydration salts, MiTeGen's goniometer bases and RT Tubing.



Phasing

Phasing Kits

Tantalum Cluster Derivatization Kit



proteros 

Product	Cat. No.
Tantalum Cluster Derivatization Kit	PK-103

Applications: Heavy atom derivatization of biological macromolecules for isomorphous and/or anomalous phasing methods.

Kit contents: 6 pre-weighted solid aliquots of hexantantalum tetradecabromide at 1 mg.

The **Tantalum Bromide Cluster**, manufactured by Proteros biostructures GmbH, is utilized for the preparation of heavy-atom derivatives for structure determination of biological macromolecules by X-ray analysis.

The electron-rich compound can be employed in single and multiple isomorphous replacement (SIR and MIR) experiments in order to induce measurable changes of the diffraction intensities required for phase calculation.

Furthermore, the Tantalum Bromide Cluster contains two strong anomalous scatterers suitable for multiple anomalous diffraction (MAD) experiments. Tantalum Bromide Clusters have been successfully employed in several structural studies because of their high electron-density, solubility in aqueous solutions and stability over a wide pH range [1-4].

[1] Knäblein *et al.* (1997) Ta6Br122+, a tool for phase determination of large biological assemblies by X-ray crystallography. *J.Mol.Biol.* **270**:1.

[2] Yonath *et al.* (1998) Crystallographic studies on the ribosome, a large macromolecular assembly exhibiting severe nonisomorphism, extreme beam sensitivity and no internal symmetry. *Acta Cryst. A* **54**:945.

[3] Gomis-Rüth *et al.* (2001) Solving a 300 kDa multimeric protein by low-resolution MAD phasing and averaging/phase extension. *Acta Cryst. D* **57**:800.

[4] Szczepanowski *et al.* (2005) Crystal structure of a fragment of mouse ubiquitin-activating enzyme. *J. Biol. Chem.* **280**:22006.

JBS Magic Triangle



Product	Cat. No.
JBS Magic Triangle	PK-104

Applications: Heavy atom derivatization of biological macromolecules for anomalous and/or isomorphous phasing methods.

Kit contents:

- 6 pre-weighted solid aliquots of I3C (33 mg each)
- 6 aliquots of lithium hydroxide solution (60 µl each)

JBS Magic Triangle is a phasing kit developed in co-operation with Tobias Beck in the research group of Prof. George M. Sheldrick, Georg-August University Göttingen.

I3C – the magic triangle – is depicted above. The three iodine atoms form an equilateral triangle with a side length of 6.0 Å and can be readily identified in the anomalous electron density map [1].

The researchers in the Sheldrick group have successfully demonstrated that I3C can be utilized for heavy-atom derivatization of biological macromolecules. Experimental phases for several proteins have been derived using single-wavelength anomalous dispersion (SAD) or single isomorphous replacement plus anomalous scattering (SIRAS) methods [1,2].

References:

- [1] Beck *et al.* (2008) A magic triangle for experimental phasing of macromolecules. *Acta Cryst. D* **64**:1179.
- [2] Sippel *et al.* (2008) Structure determination of the cancer-associated Mycoplasma hyorhinis protein Mh-p37. *Acta Cryst. D* **64**:1172.

JBS Halo Kits

Halogenated and Mercurated Nucleotides and Oligonucleotides

We offer a wide variety of halogenated and mercurated nucleotides as well as modified DNA oligonucleotides suitable for phasing experiments. Please consult our General Catalog or our website www.jenabioscience.com

Product	Cat. No.
JBS Halo-ATP Kit	PK-101
JBS Halo-GTP Kit	PK-102

Applications: Halogenated ATP and GTP analogs for incorporation of heavy atoms into nucleotide binding enzymes in order to identify nucleotide binding sites with the help of isomorphous/anomalous difference electron density.

Kit contents:

- **JBS Halo-ATP Kit** – 12 halogenated adenosine nucleotides in form of lyophilized sodium salts
- **JBS Halo-GTP Kit** – 6 halogenated guanosine nucleotides in form of lyophilized sodium salts

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.

The **JBS Halo-ATP Kit** contains 12 halogenated Adenosine nucleotides (50 units [1 µl of a 10 mM solution] as lyophilized sodium salts):

- 2'-Iodo-ADP, 2'-Iodo-ATP, 2'-Iodo-AppNH₂ (2'-Iodo-AMPPNP)
- 2'-Bromo-ADP, 2'-Bromo-ATP, 2'-Bromo-AppNH₂ (2'-Bromo-AMPPNP)
- 8-Iodo-ADP, 8-Iodo-ATP, 8-Iodo-AppNH₂ (8-Iodo-AMPPNP)
- 8-Bromo-ADP, 8-Bromo-ATP, 8-Bromo-AppNH₂ (8-Bromo-AMPPNP)

The **JBS Halo-GTP Kit** contains 6 halogenated Guanosine nucleotides (50 units [1 µl of a 10 mM solution] as lyophilized sodium salts):

- 8-Iodo-GDP, 8-Iodo-GTP, 8-Iodo-GppNH₂ (8-Iodo-GMPPNP)
- 8-Bromo-GDP, 8-Bromo-GTP, 8-Bromo-GppNH₂ (8-Bromo-GMPPNP)



Crystal of human TMP-kinase co-crystallized with 2'Br-ADP/ATP
(courtesy of N. Ostermann)

The protein under investigation can either be co-crystallized with the respective analog, or the nucleotide can be added directly to the crystallization drops containing pre-grown crystals. Since it is difficult to predict a priori which one of the Halo-nucleotides will give the highest quality derivative crystals, it is advisable to screen them all in parallel.

References:

- Gruen *et al.* (1999) 2'-Halo-ATP and -GTP analogues: Rational phasing tools for protein crystallography. *Protein Sci.* **8**:2524.
- Gruen *et al.* (1999) Synthesis of 2'-iodo- and 2'-bromo-ATP and GTP analogues as potential phasing tools for X-ray crystallography. *Nucleos. Nucleot.* **18**:137.
- 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.



Appendix – Screen Formulations

Crystallization Screens

JBScreen Classic

Classic 1		Precipitant 1	Buffer	pH	Additive
bulk	HTS I				
A 1	A 1	15% w/v PEG 400	100 mM Sodium Acetate	4.6	100 mM Calcium Chloride
A 2	—	15% w/v PEG 400	100 mM MES Sodium Salt	6.5	None
A 3	A 2	15% w/v PEG 400	100 mM HEPES Sodium Salt	7.5	200 mM Magnesium Chloride
A 4	—	15% w/v PEG 400	100 mM Tris-HCl	8.5	200 mM Sodium Citrate
A 5	A 3	25% w/v PEG 400	100 mM Sodium Acetate	4.6	100 mM Magnesium Chloride
A 6	A 4	25% w/v PEG 400	100 mM Tris-HCl	8.5	200 mM Lithium Sulfate
B 1	—	28% w/v PEG 400	100 mM HEPES Sodium Salt	7.5	200 mM Calcium Chloride
B 2	A 5	30% w/v PEG 400	100 mM Sodium Acetate	4.6	100 mM Calcium Chloride
B 3	A 6	30% w/v PEG 400	100 mM MES Sodium Salt	6.5	100 mM Sodium Acetate
B 4	—	30% w/v PEG 400	100 mM MES Sodium Salt	6.5	100 mM Magnesium Chloride
B 5	A 7	30% w/v PEG 400	100 mM HEPES Sodium Salt	7.5	200 mM Magnesium Chloride
B 6	A 8	30% w/v PEG 400	100 mM Tris-HCl	8.5	200 mM Sodium Citrate
C 1	A 9	30% w/v PEG 550 MME	100 mM Bicine	9.0	100 mM Sodium Chloride
C 2	A 10	25% w/v PEG 550 MME	100 mM MES Sodium Salt	6.5	10 mM Zinc Sulfate
C 3	A 11	25% w/v PEG 1000	100 mM HEPES Sodium Salt	7.5	None
C 4	A 12	30% w/v PEG 1000	100 mM Tris-HCl	8.5	None
C 5	B 1	15% w/v PEG 1500	None		None
C 6	B 2	20% w/v PEG 1500	100 mM HEPES Sodium Salt	7.5	None
D 1	B 3	30% w/v PEG 1500	None		None
D 2	B 4	20% w/v PEG 2000 MME	100 mM Tris-HCl	8.5	10 mM Nickel (II) Chloride
D 3	B 5	25% w/v PEG 2000 MME	None		None
D 4	—	30% w/v PEG 2000 MME	100 mM MES Sodium Salt	6.5	100 mM Sodium Acetate
D 5	B 6	20% w/v PEG 3000	100 mM HEPES Sodium Salt	7.5	200 mM Sodium Acetate
D 6	B 7	30% w/v PEG 3000	100 mM Tris-HCl	8.5	200 mM Lithium Sulfate

Classic 2		Precipitant 1	Buffer	pH	Additive
bulk	HTS I				
A 1	B 8	4% w/v PEG 4000	100 mM Sodium Acetate	4.6	None
A 2	B 9	8% w/v PEG 4000	None		None
A 3	B 10	8% w/v PEG 4000	100 mM Sodium Acetate	4.6	None
A 4	B 11	10% w/v PEG 4000	100 mM MES Sodium Salt	6.5	200 mM Magnesium Chloride
A 5	B 12	12% w/v PEG 4000	100 mM HEPES Sodium Salt	7.5	100 mM Sodium Acetate
A 6	—	12% w/v PEG 4000	100 mM Tris-HCl	8.5	None
B 1	C 1	16% w/v PEG 4000	100 mM Tris-HCl	8.5	200 mM Lithium Sulfate
B 2	C 2	16% w/v PEG 4000	100 mM Tris-HCl	8.5	200 mM Sodium Acetate
B 3	—	16% w/v PEG 4000	100 mM Tris-HCl	8.5	200 mM Magnesium Chloride
B 4	C 3	18% w/v PEG 4000	100 mM Sodium Acetate	4.6	None
B 5	C 4	20% w/v PEG 4000	100 mM Tris-HCl	8.5	200 mM Lithium Sulfate
B 6	C 5	20% w/v PEG 4000	100 mM Tris-HCl	8.5	200 mM Calcium Chloride
C 1	—	22% w/v PEG 4000	100 mM HEPES Sodium Salt	7.5	100 mM Sodium Acetate
C 2	C 6	25% w/v PEG 4000	100 mM Sodium Acetate	4.6	None
C 3	C 7	25% w/v PEG 4000	100 mM MES Sodium Salt	6.5	200 mM Magnesium Chloride
C 4	C 8	25% w/v PEG 4000	100 mM Tris-HCl	8.5	200 mM Calcium Chloride
C 5	C 9	30% w/v PEG 4000	None		None
C 6	C 10	30% w/v PEG 4000	100 mM Sodium Acetate	4.6	100 mM Magnesium Chloride
D 1	—	30% w/v PEG 4000	100 mM MES Sodium Salt	6.5	None
D 2	C 11	30% w/v PEG 4000	100 mM HEPES Sodium Salt	7.5	200 mM Calcium Chloride
D 3	—	30% w/v PEG 4000	100 mM Tris-HCl	8.5	200 mM Lithium Sulfate
D 4	C 12	30% w/v PEG 4000	100 mM Tris-HCl	8.5	200 mM Sodium Acetate
D 5	D 1	30% w/v PEG 4000	100 mM Tris-HCl	8.5	200 mM Magnesium Chloride
D 6	D 2	35% w/v PEG 4000	None		None



Classic 3		Precipitant 1	Precipitant 2	Buffer	pH	Additive
bulk	HTS I					
A 1	D 3	8% w/v PEG 4000	800 mM Lithium Chloride	100 mM Tris-HCl	8.5	None
A 2	D 4	10% w/v PEG 4000	20% w/v 2-Propanol	None		None
A 3	D 5	10% w/v PEG 4000	10% w/v 2-Propanol	100 mM Sodium Citrate	5.6	None
A 4	—	10% w/v PEG 4000	5% w/v 2-Propanol	100 mM HEPES Sodium Salt	7.5	None
A 5	D 6	10% w/v PEG 4000	20% w/v 2-Propanol	100 mM HEPES Sodium Salt	7.5	None
A 6	D 7	12% w/v PEG 4000	None	100 mM Sodium Acetate	4.6	200 mM Ammonium Sulfate
B 1	—	15% w/v PEG 4000	None	None		200 mM Ammonium Sulfate
B 2	D 8	15% w/v PEG 4000	None	100 mM Sodium Citrate	5.6	200 mM Ammonium Sulfate
B 3	D 9	16% w/v PEG 4000	10% w/v 2-Propanol	100 mM HEPES Sodium Salt	7.5	200 mM Ammonium Sulfate
B 4	D 10	20% w/v PEG 4000	None	None		200 mM Ammonium Sulfate
B 5	D 11	20% w/v PEG 4000	10% w/v Glycerol	None		200 mM Magnesium Sulfate
B 6	—	20% w/v PEG 4000	5% w/v 2-Propanol	None		100 mM Sodium Citrate
C 1	D 12	20% w/v PEG 4000	20% w/v 2-Propanol	None		100 mM Sodium Citrate
C 2	E 1	20% w/v PEG 4000	None	100 mM MES Sodium Salt	6.5	600 mM Sodium Chloride
C 3	E 2	20% w/v PEG 4000	10% w/v 2-Propanol	100 mM HEPES Sodium Salt	7.5	None
C 4	E 3	22% w/v PEG 4000	None	None		200 mM Ammonium Sulfate 100 mM Sodium Acetate
C 5	—	25% w/v PEG 4000	None	100 mM Sodium Acetate	4.6	200 mM Ammonium Sulfate
C 6	E 4	25% w/v PEG 4000	None	100 mM Sodium Citrate	5.6	200 mM Ammonium Sulfate
D 1	E 5	25% w/v PEG 4000	200 mM Lithium Sulfate	100 mM HEPES Sodium Salt	7.5	100 mM Sodium Acetate
D 2	E 6	25% w/v PEG 4000	8% w/v 2-Propanol	None		100 mM Sodium Acetate
D 3	E 7	30% w/v PEG 4000	None	None		200 mM Ammonium Sulfate
D 4	—	30% w/v PEG 4000	None	100 mM Sodium Acetate	4.6	200 mM Ammonium Sulfate
D 5	E 8	30% w/v PEG 4000	None	100 mM Sodium Citrate	5.6	100 mM Ammonium Sulfate
D 6	E 9	32% w/v PEG 4000	None	100 mM Tris-HCl	8.5	800 mM Lithium Chloride
Classic 4		Precipitant 1	Precipitant 2	Buffer	pH	Additive
bulk	HTS I					
A 1	E 10	25% w/v PEG 5000 MME	None	100 mM Tris-HCl	8.5	200 mM Lithium Sulfate
A 2	E 11	30% w/v PEG 5000 MME	None	100 mM MES Sodium Salt	6.5	200 mM Ammonium Sulfate
A 3	E 12	3% w/v PEG 6000	None	100 mM Tris-HCl	8.5	100 mM Potassium Chloride
A 4	F 1	10% w/v PEG 6000	None	None		10 mM Magnesium Chloride
A 5	F 2	12% w/v PEG 6000	2.0 M Sodium Chloride	None		None
A 6	F 3	15% w/v PEG 6000	5% w/v Glycerol	None		None
B 1	F 4	15% w/v PEG 6000	50 mM Potassium Chloride	None		10 mM Magnesium Chloride
B 2	—	16% w/v PEG 6000	None	None		10 mM Sodium Citrate
B 3	F 5	20% w/v PEG 6000	None	50 mM Imidazole-HCl	8.0	None
B 4	F 6	25% w/v PEG 6000	None	100 mM HEPES Sodium Salt	7.5	100 mM Lithium Chloride
B 5	F 7	28% w/v PEG 6000	500 mM Lithium Chloride	100 mM Tris-HCl	8.5	None
B 6	F 8	30% w/v PEG 6000	1.0 M Lithium Chloride	None		100 mM Sodium Acetate
C 1	—	33% w/v PEG 6000	None	None		10 mM Sodium Citrate
C 2	F 9	2% w/v PEG 8000	500 mM Lithium Sulfate	None		None
C 3	F 10	2% w/v PEG 8000	1.0 M Lithium Sulfate	None		None
C 4	F 11	4% w/v PEG 8000	None	None		None
C 5	F 12	8% w/v PEG 8000	200 mM Lithium Chloride	None		50 mM Magnesium Sulfate
C 6	—	8% w/v PEG 8000	None	100 mM Tris-HCl	8.5	None
D 1	G 1	10% w/v PEG 8000	None	100 mM MES Sodium Salt	6.5	200 mM Zinc Acetate
D 2	G 2	10% w/v PEG 8000	None	100 mM HEPES Sodium Salt	7.5	200 mM Calcium Acetate
D 3	G 3	10% w/v PEG 8000	None	None		50 mM Magnesium Acetate 100 mM Sodium Acetate
D 4	G 4	10% w/v PEG 8000	None	None		200 mM Magnesium Acetate
D 5	G 5	10% w/v PEG 8000	10% w/v Ethylene Glycol	100 mM HEPES Sodium Salt	7.5	None
D 6	—	10% w/v PEG 8000	10% w/v PEG 1000	None		None



Classic 5		Precipitant 1	Precipitant 2	Buffer	pH	Additive
bulk	HTS I					
A 1	—	12% w/v PEG 8000	5% w/v Glycerol	None		100 mM Potassium Chloride
A 2	G 6	12% w/v PEG 8000	10% w/v Glycerol	None		500 mM Potassium Chloride
A 3	G 7	15% w/v PEG 8000	None	None		200 mM Ammonium Sulfate
A 4	G 8	15% w/v PEG 8000	500 mM Lithium Sulfate	None		None
A 5	G 9	15% w/v PEG 8000	None	100 mM MES Sodium Salt	6.5	200 mM Sodium Acetate
A 6	—	15% w/v PEG 8000	None	None		50 mM Ammonium Sulfate 100 mM Sodium Citrate
B 1	G 10	18% w/v PEG 8000	None	100 mM HEPES Sodium Salt	7.5	200 mM Calcium Acetate
B 2	G 11	18% w/v PEG 8000	2% w/v 2-Propanol	100 mM HEPES Sodium Salt	7.5	100 mM Sodium Acetate
B 3	G 12	18% w/v PEG 8000	None	100 mM Tris-HCl	8.5	200 mM Lithium Sulfate
B 4	—	20% w/v PEG 8000	None	100 mM HEPES Sodium Salt	7.5	None
B 5	H 1	20% w/v PEG 8000	None	100 mM MES Sodium Salt	6.5	200 mM Magnesium Acetate
B 6	H 2	20% w/v PEG 8000	None	100 mM CHES	9.5	None
C 1	—	22% w/v PEG 8000	None	100 mM MES Sodium Salt	6.5	200 mM Ammonium Sulfate
C 2	H 3	25% w/v PEG 8000	None	None		200 mM Lithium Chloride
C 3	H 4	30% w/v PEG 8000	None	None		200 mM Ammonium Sulfate
C 4	H 5	8% w/v PEG 10000	None	100 mM Sodium Acetate	4.6	None
C 5	H 6	14% w/v PEG 10000	None	100 mM Imidazole-HCl	8.0	None
C 6	—	16% w/v PEG 10000	None	100 mM Tris-HCl	8.5	None
D 1	H 7	18% w/v PEG 10000	20% w/v Glycerol	100 mM Tris-HCl	8.5	100 mM Sodium Chloride
D 2	H 8	20% w/v PEG 10000	None	100 mM HEPES Sodium Salt	7.5	None
D 3	H 8	30% w/v PEG 10000	None	100 mM Tris-HCl	8.5	None
D 4	H 10	10% w/v PEG 20000	None	100 mM MES Sodium Salt	6.5	None
D 5	H 11	17% w/v PEG 20000	None	100 mM Tris-HCl	8.5	100 mM Magnesium Chloride
D 6	H 12	20% w/v PEG 20000	None	None		None

Classic 6		Precipitant 1	Precipitant 2	Buffer	pH	Additive
bulk	HTS II					
A 1	A 1	500 mM Ammonium Sulfate	1.0 M Lithium Sulfate	None		100 mM Sodium Citrate
A 2	—	1.0 M Ammonium Sulfate	None	None		None
A 3	A 2	1.0 M Ammonium Sulfate	None	100 mM Sodium Acetate	4.6	None
A 4	A 3	1.0 M Ammonium Sulfate	2% w/v PEG 400	100 mM HEPES Sodium Salt	7.5	None
A 5	A 4	1.0 M Ammonium Sulfate	None	100 mM Tris-HCl	8.5	None
A 6	A 5	1.2 M Ammonium Sulfate	3% w/v 2-Propanol	None		50 mM Sodium Citrate
B 1	A 6	1.5 M Ammonium Sulfate	15% w/v Glycerol	100 mM Tris-HCl	8.5	None
B 2	—	1.6 M Ammonium Sulfate	500 mM Lithium Chloride	None		None
B 3	A 7	1.6 M Ammonium Sulfate	1.0 M Lithium Sulfate	None		None
B 4	A 8	1.6 M Ammonium Sulfate	None	100 mM HEPES Sodium Salt	7.5	200 mM Sodium Chloride
B 5	A 9	1.6 M Ammonium Sulfate	2% w/v PEG 1000	100 mM HEPES Sodium Salt	7.5	None
B 6	A 10	1.8 M Ammonium Sulfate	None	100 mM MES Sodium Salt	6.5	None
C 1	A 11	2.0 M Ammonium Sulfate	2.0 M Sodium Chloride	None		None
C 2	A 12	2.0 M Ammonium Sulfate	None	100 mM Sodium Acetate	4.6	None
C 3	B 1	2.0 M Ammonium Sulfate	5% w/v PEG 400	100 mM MES Sodium Salt	6.5	None
C 4	B 2	2.0 M Ammonium Sulfate	None	100 mM Tris-HCl	8.5	None
C 5	—	2.2 M Ammonium Sulfate	None	None		None
C 6	B 3	2.2 M Ammonium Sulfate	20% w/v Glycerol	None		None
D 1	B 4	2.4 M Ammonium Sulfate	None	None		100 mM Sodium Citrate
D 2	B 5	3.0 M Ammonium Sulfate	1% w/v MPD	None		None
D 3	B 6	3.0 M Ammonium Sulfate	10% w/v Glycerol	None		None
D 4	B 7	3.5 M Ammonium Sulfate	None	100 mM HEPES Sodium Salt	7.5	None
D 5	B 8	3.5 M Ammonium Sulfate	1% w/v MPD	100 mM MES Sodium Salt	6.5	None
D 6	—	3.5 M Ammonium Sulfate	None	None		None



Classic 7		Precipitant 1	Precipitant 2	Buffer	pH	Additive
bulk	HTS II					
A 1	B 9	10% w/v MPD	None	100 mM HEPES Sodium Salt	7.5	100 mM Sodium Citrate
A 2	B 10	12% w/v MPD	None	100 mM Tris-HCl	8.5	50 mM Magnesium Chloride
A 3	—	15% w/v MPD	None	100 mM Sodium Acetate	4.6	20 mM Calcium Chloride
A 4	B 11	15% w/v MPD	5% w/v PEG 4000	100 mM Imidazole-HCl	8.0	None
A 5	B 12	15% w/v MPD	None	100 mM Sodium Citrate	5.6	200 mM Ammonium Acetate
A 6	—	15% w/v MPD	None	100 mM MES Sodium Salt	6.5	200 mM Magnesium Acetate
B 1	C 1	15% w/v MPD	None	100 mM HEPES Sodium Salt	7.5	200 mM Sodium Citrate
B 2	C 2	20% w/v MPD	None	100 mM HEPES Sodium Salt	7.5	100 mM Sodium Citrate
B 3	C 3	20% w/v MPD	None	100 mM Imidazole-HCl	8.0	None
B 4	C 4	20% w/v MPD	4% w/v Glycerol	None		200 mM Sodium Chloride
B 5	C 5	30% w/v MPD	None	100 mM Sodium Acetate	4.6	20 mM Calcium Chloride
B 6	C 6	30% w/v MPD	None	100 mM Sodium Citrate	5.6	200 mM Ammonium Acetate
C 1	—	30% w/v MPD	None	100 mM MES Sodium Salt	6.5	200 mM Magnesium Acetate
C 2	C 7	30% w/v MPD	None	100 mM HEPES Sodium Salt	7.5	500 mM Ammonium Sulfate
C 3	C 8	30% w/v MPD	None	100 mM HEPES Sodium Salt	7.5	200 mM Sodium Citrate
C 4	—	30% w/v MPD	5% w/v PEG 4000	100 mM HEPES Sodium Salt	7.5	None
C 5	C 9	30% w/v MPD	10% w/v PEG 4000	100 mM Imidazole-HCl	8.0	None
C 6	C 10	30% w/v MPD	20% w/v Ethanol	None		None
D 1	—	35% w/v MPD	None	None		None
D 2	C 11	35% w/v MPD	None	100 mM Imidazole-HCl	8.0	None
D 3	C 12	40% w/v MPD	None	100 mM Tris-HCl	8.5	None
D 4	D 1	47% w/v MPD	None	100 mM HEPES Sodium Salt	7.5	None
D 5	D 2	47% w/v MPD	2% w/v tert-Butanol	None		None
D 6	D 3	50% w/v MPD	None	None		None

Classic 8		Precipitant 1	Precipitant 2	Buffer	pH	Additive
bulk	HTS II					
A 1	—	50% w/v MPD	15% w/v Ethanol	None		10 mM Sodium Acetate
A 2	D 4	50% w/v MPD	20% w/v 2-Propanol	None		50 mM Sodium Chloride 50 mM Sodium Acetate
A 3	D 5	50% w/v MPD	None	100 mM Tris-HCl	8.5	100 mM Ammonium dihydrogen Phosphate
A 4	D 6	55% w/v MPD	None	None		None
A 5	D 7	60% w/v MPD	None	100 mM Sodium Acetate	4.6	10 mM Calcium Chloride
A 6	—	60% w/v MPD	None	None		20 mM Sodium Acetate
B 1	D 8	70% w/v MPD	None	100 mM MES Sodium Salt	6.5	None
B 2	D 9	70% w/v MPD	None	100 mM Tris-HCl	8.5	None
B 3	D 10	20% w/v Methanol	None	100 mM Tris-HCl	8.5	10 mM Calcium Chloride
B 4	D 11	2% w/v Ethanol	None	100 mM Tris-HCl	8.5	None
B 5	—	5% w/v Ethanol	5% w/v MPD	100 mM HEPES Sodium Salt	7.5	None
B 6	D 12	5% w/v Ethanol	5% w/v MPD	100 mM Tris-HCl	8.5	200 mM Sodium Chloride
C 1	E 1	10% w/v Ethanol	None	100 mM Tris-HCl	8.5	None
C 2	E 2	12% w/v Ethanol	4% w/v PEG 400	100 mM Sodium Acetate	4.6	None
C 3	E 3	14% w/v Ethanol	5% w/v Glycerol	100 mM Tris-HCl	8.5	None
C 4	E 4	18% w/v Ethanol	None	100 mM Tris-HCl	8.5	None
C 5	—	20% w/v Ethanol	None	None		None
C 6	E 5	20% w/v Ethanol	10% w/v Glycerol	None		None
D 1	E 6	30% w/v Ethanol	10% w/v PEG 6000	None		100 mM Sodium Acetate
D 2	E 7	45% w/v Ethanol	None	None		None
D 3	E 8	50% w/v Ethanol	None	None		100 mM Sodium Acetate
D 4	E 9	60% w/v Ethanol	1.5% w/v PEG 6000	None		50 mM Sodium Acetate
D 5	E 10	60% w/v Ethanol	None	None		100 mM Sodium Chloride
D 6	—	2% w/v 2-Propanol	None	100 mM Tris-HCl	8.5	10 mM Magnesium Sulfate
D 6	—	2% w/v 2-Propanol	None	100 mM Tris-HCl	8.5	10 mM Magnesium Sulfate



Classic 9		Precipitant 1	Buffer	pH	Additive
bulk	HTS II				
A 1	E 11	5% w/v 2-Propanol	100 mM HEPES Sodium Salt	7.5	None
A 2	E 12	10% w/v 2-Propanol	100 mM Sodium Acetate	4.6	200 mM Calcium Chloride
A 3	F 1	10% w/v 2-Propanol	100 mM HEPES Sodium Salt	7.5	200 mM Sodium Citrate
A 4	F 2	10% w/v 2-Propanol	100 mM Tris-HCl	8.5	10 mM Magnesium Chloride
A 5	—	12% w/v 2-Propanol	100 mM Tris-HCl	8.5	50 mM Sodium Chloride
A 6	F 3	15% w/v 2-Propanol	100 mM MES Sodium Salt	6.5	200 mM Sodium Citrate
B 1	—	15% w/v 2-Propanol	100 mM HEPES Sodium Salt	7.5	200 mM Sodium Citrate
B 2	F 4	15% w/v 2-Propanol	100 mM HEPES Sodium Salt	7.5	200 mM Magnesium Chloride
B 3	F 5	15% w/v 2-Propanol	100 mM Tris-HCl	8.5	200 mM Ammonium Acetate
B 4	F 6	20% w/v 2-Propanol	100 mM Sodium Acetate	4.6	200 mM Calcium Chloride
B 5	—	20% w/v 2-Propanol	100 mM HEPES Sodium Salt	7.5	200 mM Sodium Citrate
B 6	F 7	25% w/v 2-Propanol	100 mM HEPES Sodium Salt	7.5	100 mM Magnesium Chloride
C 1	F 8	30% w/v 2-Propanol	100 mM MES Sodium Salt	6.5	200 mM Sodium Citrate
C 2	—	30% w/v 2-Propanol	100 mM HEPES Sodium Salt	7.5	200 mM Magnesium Chloride
C 3	F 9	30% w/v 2-Propanol	100 mM Tris-HCl	8.5	200 mM Ammonium Acetate
C 4	F 10	25% w/v tert-Butanol	100 mM Tris-HCl	8.5	100 mM Calcium Chloride
C 5	F 11	35% w/v tert-Butanol	100 mM Sodium Citrate	5.6	None
C 6	F 12	200 mM Ammonium dihydrogen Phosphate	None		None
D 1	G 1	200 mM Potassium / Sodium Tartrate	None		None
D 2	G 2	200 mM Magnesium Acetate	None		None
D 3	G 3	400 mM Ammonium dihydrogen Phosphate	None		None
D 4	—	400 mM Potassium / Sodium Tartrate	None		None
D 5	G 4	400 mM Potassium / Sodium Tartrate	100 mM Tris-HCl	8.5	None
D 6	G 5	500 mM Ammonium dihydrogen Phosphate	None		200 mM Sodium Citrate

Classic 10		Precipitant 1	Precipitant 2	Buffer	pH	Additive
bulk	HTS II					
A 1	G 6	500 mM Sodium Acetate	None	100 mM Imidazole-HCl	8.0	None
A 2	G 7	700 mM Sodium Citrate	None	100 mM HEPES Sodium Salt	7.5	None
A 3	—	700 mM Lithium Sulfate	None	100 mM Tris-HCl	8.5	None
A 4	G 8	800 mM Potassium / Sodium Chloride	None	100 mM HEPES Sodium Salt	7.5	None
A 5	G 9	1.0 M Ammonium dihydrogen Phosphate	None	100 mM Sodium Citrate	5.6	None
A 6	G 10	1.0 M Ammonium dihydrogen Phosphate	None	100 mM Tris-HCl	8.5	None
B 1	G 11	1.0 M Lithium Sulfate	None	100 mM Tris-HCl	8.5	10 mM Nickel (II) Chloride
B 2	G 12	1.0 M Sodium Acetate	None	100 mM Imidazole-HCl	8.0	None
B 3	—	1.0 M Sodium Formate	None	100 mM Sodium Acetate	4.6	None
B 4	H 1	1.4 M Sodium Acetate	None	100 mM MES Sodium Salt	6.5	None
B 5	—	1.4 M Sodium Citrate	None	100 mM HEPES Sodium Salt	7.5	None
B 6	H 2	1.5 M Lithium Sulfate	None	100 mM Tris-HCl	8.5	None
C 1	H 3	None	None	1.5 M Sodium Citrate	6.5	None
C 2	H 4	1.6 M Magnesium Sulfate	None	100 mM MES Sodium Salt	6.5	None
C 3	H 5	1.6 M Potassium / Sodium Tartrate	None	100 mM MES Sodium Salt	6.5	None
C 4	H 6	2.0 M Ammonium Formate	None	100 mM MES Sodium Salt	6.5	None
C 5	H 7	2.0 M Ammonium dihydrogen Phosphate	None	100 mM Tris-HCl	8.5	None
C 6	—	2.0 M Sodium Formate	None	None		None
D 1	—	2.0 M Magnesium Chloride	None	100 mM Tris-HCl	8.5	None
D 2	H 8	2.0 M Sodium Chloride	None	100 mM MES Sodium Salt	6.5	200 mM Sodium Acetate
D 3	H 9	2.0 M Sodium Formate	None	100 mM Sodium Acetate	4.6	None
D 4	H 10	1.0 M Ammonium dihydrogen Phosphate	30% w/v Glycerol	100 mM Tris-HCl	8.5	None
D 5	H 11	4.0 M Sodium Chloride	None	100 mM HEPES Sodium Salt	7.5	None
D 6	H 12	3.0 M Sodium Formate	None	None		None



JBScreen Basic

Basic 1		Precipitant 1	Precipitant 2	Buffer	pH	Additive
bulk	HTS					
A 1	A 1	25% v/v Ethylene Glycol	None	None		None
A 2	A 2	12% v/v Glycerol anhydrous	1.5 M Ammonium Sulfate	100 mM Tris-HCl	8.5	None
A 3	A 3	1.0 M 1,6-Hexanediol	None	100 mM Sodium Acetate	4.6	10 mM Cobalt(II) Chloride
A 4	A 4	2.5 M 1,6-Hexanediol	None	100 mM Sodium Citrate	5.6	None
A 5	A 5	3.4 M 1,6-Hexanediol	None	100 mM Tris-HCl	8.5	200 mM Magnesium Chloride
A 6	A 6	30% v/v MPD	None	100 mM Sodium Acetate	4.6	200 mM Sodium Chloride
B 1	A 7	30% v/v MPD	None	100 mM Sodium Citrate	5.6	200 mM Ammonium Acetate
B 2	A 8	30% v/v MPD	None	100 mM Sodium Acetate	4.6	20 mM Calcium Chloride
B 3	A 9	30% v/v MPD	500 mM Ammonium Sulfate	100 mM HEPES Sodium Salt	7.5	None
B 4	A 10	30% v/v MPD	None	100 mM HEPES Sodium Salt	7.5	200 mM Sodium Citrate
B 5	A 11	50% v/v MPD	None	100 mM Tris-HCl	8.5	200 mM Ammonium dihydrogen Phosphate
B 6	A 12	70% v/v MPD	None	100 mM HEPES Sodium Salt	7.5	None
C 1	B 1	2% v/v Polyethylenimine	None	100 mM Sodium Citrate	5.6	500 mM Sodium Chloride
C 2	B 2	2% v/v PEG 400	2.0 M Ammonium Sulfate	100 mM HEPES Sodium Salt	7.5	None
C 3	B 3	28% v/v PEG 400	None	100 mM HEPES Sodium Salt	7.5	200 mM Calcium Chloride
C 4	B 4	30% v/v PEG 400	None	100 mM Tris-HCl	8.5	200 mM Sodium Citrate
C 5	B 5	30% v/v PEG 400	None	100 mM HEPES Sodium Salt	7.5	200 mM Magnesium Chloride
C 6	B 6	30% v/v PEG 400	None	100 mM Sodium Acetate	4.6	100 mM Calcium Chloride
D 1	B 7	20% w/v PEG 550 MME	None	100 mM Bicine	9.5	100 mM Sodium Chloride
D 2	B 8	25% w/v PEG 550 MME	None	100 mM MES Sodium Salt	6.5	10 mM Zinc Sulfate
D 3	B 9	10% w/v PEG 1000	10% w/v PEG 8000	None		None
D 4	B 10	30% w/v PEG 1500	None	None		None
D 5	B 11	20% w/v PEG 2000 MME	None	100 mM Tris-HCl	8.5	10 mM Nickel(II) Chloride
D 6	B 12	30% w/v PEG 2000 MME	None	100 mM Sodium Acetate	4.6	200 mM Ammonium Sulfate

Basic 2		Precipitant 1	Precipitant 2	Buffer	pH	Additive
bulk	HTS					
A 1	C 1	8% w/v PEG 4000	None	100 mM Sodium Acetate	4.6	None
A 2	C 2	20% w/v PEG 4000	20% v/v 2-Propanol	100 mM Sodium Citrate	5.6	None
A 3	C 3	20% w/v PEG 4000	10% v/v 2-Propanol	100 mM HEPES Sodium Salt	7.5	None
A 4	C 4	25% w/v PEG 4000	None	100 mM Sodium Acetate	4.6	200 mM Ammonium Sulfate
A 5	C 5	30% w/v PEG 4000	None	None		200 mM Ammonium Sulfate
A 6	C 6	30% w/v PEG 4000	None	100 mM Sodium Acetate	4.6	200 mM Ammonium Acetate
B 1	C 7	30% w/v PEG 4000	None	100 mM Sodium Citrate	5.6	200 mM Ammonium Acetate
B 2	C 8	30% w/v PEG 4000	None	100 mM Tris-HCl	8.5	200 mM Sodium Acetate
B 3	C 9	30% w/v PEG 4000	None	100 mM Tris-HCl	8.5	200 mM Lithium Sulfate
B 4	C 10	30% w/v PEG 4000	None	100 mM Tris-HCl	8.5	200 mM Magnesium Chloride
B 5	C 11	30% w/v PEG 5000 MME	None	100 mM MES Sodium Salt	6.5	200 mM Ammonium Sulfate
B 6	C 12	10% w/v PEG 6000	2.0 M Sodium Chloride	None		None
C 1	D 1	10% w/v PEG 6000	5% v/v MPD	100 mM HEPES Sodium Salt	7.5	None
C 2	D 2	2% w/v PEG 8000	1.0 M Lithium Sulfate	None		None
C 3	D 3	8% w/v PEG 8000	None	100 mM Tris-HCl	8.5	None
C 4	D 4	10% w/v PEG 8000	8% v/v Ethylene Glycol	100 mM HEPES Sodium Salt	7.5	None
C 5	D 5	15% w/v PEG 8000	500 mM Lithium Sulfate	None		None
C 6	D 6	18% w/v PEG 8000	None	100 mM MES Sodium Salt	6.5	200 mM Calcium Acetate
D 1	D 7	18% w/v PEG 8000	None	100 mM MES Sodium Salt	6.5	200 mM Zinc Acetate
D 2	D 8	20% w/v PEG 8000	None	None		50 mM Potassium dihydrogen Phosphate
D 3	D 9	20% w/v PEG 8000	None	100 mM MES Sodium Salt	6.5	200 mM Magnesium Acetate
D 4	D 10	30% w/v PEG 8000	None	100 mM MES Sodium Salt	6.5	200 mM Sodium Acetate
D 5	D 11	30% w/v PEG 8000	None	None		200 mM Ammonium Sulfate
D 6	D 12	30% w/v PEG 8000	None	100 mM MES Sodium Salt	6.5	200 mM Ammonium Sulfate



Basic 3		Precipitant 1	Precipitant 2	Buffer	pH	Additive
bulk	HTS					
A 1	E 1	10% w/v PEG 10000	2% v/v 1.4-Dioxane	100 mM Bicine	9.5	None
A 2	E 2	20% w/v PEG 10000	None	100 mM HEPES Sodium Salt	7.5	None
A 3	E 3	12% w/v PEG 20000	None	100 mM MES Sodium Salt	6.5	None
A 4	E 4	5% v/v 2-Propanol	2.0 M Ammonium Sulfate	None		None
A 5	E 5	20% v/v 2-Propanol	None	100 mM HEPES Sodium Salt	7.5	200 mM Sodium Citrate
A 6	E 6	20% v/v 2-Propanol	None	100 mM Sodium Acetate	4.6	200 mM Calcium Chloride
B 1	E 7	30% v/v 2-Propanol	None	100 mM HEPES Sodium Salt	7.5	200 mM Magnesium Chloride
B 2	E 8	30% v/v 2-Propanol	None	100 mM Tris-HCl	8.5	200 mM Ammonium Acetate
B 3	E 9	10% v/v 1.4-Dioxane	1.6 M Ammonium Sulfate	100 mM MES Sodium Salt	6.5	None
B 4	E 10	35% v/v 1.4-Dioxane	None	None		None
B 5	E 11	10% v/v Ethanol	1.5 M Sodium Chloride	None		None
B 6	E 12	20% v/v Ethanol	None	100 mM Tris-HCl	8.5	None
C 1	F 1	25% v/v tert-Butanol	None	100 mM Tris-HCl	8.5	None
C 2	F 2	35% v/v tert-Butanol	None	100 mM Sodium Citrate	5.6	None
C 3	F 3	None	None	1.0 M Imidazole-HCl	7.0	None
C 4	F 4	1.0 M Lithium Sulfate	None	100 mM Tris-HCl	8.5	10 mM Nickel(II) Chloride
C 5	F 5	1.5 M Lithium Sulfate	None	100 mM HEPES Sodium Salt	7.5	None
C 6	F 6	400 mM Potassium / Sodium Tartrate	None	None		None
D 1	F 7	800 mM Potassium / Sodium Tartrate	None	100 mM HEPES Sodium Salt	7.5	None
D 2	F 8	1.4 M Sodium Citrate	None	100 mM HEPES Sodium Salt	7.5	None
D 3	F 9	None	None	1.6 M Sodium Citrate	6.5	None
D 4	F 10	10% v/v Jeffamine M-600	None	100 mM Sodium Citrate	5.6	10 mM Ferric(III) Chloride
D 5	F 11	20% v/v Jeffamine M-600	None	100 mM HEPES Sodium Salt	7.5	None
D 6	F 12	30% v/v Jeffamine M-600	None	100 mM MES Sodium Salt	6.5	50 mM Cesium Chloride

Basic 4		Precipitant 1	Precipitant 2	Buffer	pH	Additive
bulk	HTS					
A 1	G 1	800 mM Sodium dihydrogen Phosphate	800 mM Potassium dihydrogen Phosphate	100 mM HEPES Sodium Salt	7.5	None
A 2	G 2	400 mM Ammonium dihydrogen Phosphate	None	None		None
A 3	G 3	1.0 M Ammonium dihydrogen Phosphate	None	100 mM Sodium Citrate	5.6	None
A 4	G 4	2.0 M Ammonium dihydrogen Phosphate	None	100 mM Tris-HCl	8.5	None
A 5	G 5	2.0 M Ammonium Formate	None	100 mM Sodium Acetate	4.6	None
A 6	G 6	4.0 M Ammonium Formate	None	100 mM HEPES Sodium Salt	7.5	None
B 1	G 7	2.0 M Ammonium Formate	None	None		None
B 2	G 8	500 mM Ammonium Sulfate	1.0 M Lithium Sulfate	100 mM Sodium Citrate	5.6	None
B 3	G 9	1.6 M Ammonium Sulfate	None	100 mM HEPES Sodium Salt	7.5	100 mM Sodium Chloride
B 4	G 10	1.8 M Ammonium Sulfate	None	100 mM MES Sodium Salt	6.5	10 mM Cobalt(II) Chloride
B 5	G 11	2.0 M Ammonium Sulfate	None	100 mM Tris-HCl	8.5	None
B 6	G 12	2.0 M Ammonium Sulfate	None	None		None
C 1	H 1	2.0 M Ammonium Sulfate	None	100 mM Sodium Acetate	4.6	None
C 2	H 2	2.0 M Ammonium Sulfate	None	100 mM Sodium Citrate	5.6	200 mM Potassium / Sodium Tartrate
C 3	H 3	200 mM Magnesium Formate	None	None		None
C 4	H 4	1.6 M Magnesium Sulfate	None	100 mM MES Sodium Salt	6.5	None
C 5	H 5	2.0 M Magnesium Chloride	None	100 mM Bicine	9.5	None
C 6	H 6	1.0 M Sodium Acetate	None	100 mM Imidazole-HCl	6.5	None
D 1	H 7	1.0 M Sodium Acetate	None	100 mM HEPES Sodium Salt	7.5	50 mM Cadmium Sulfate
D 2	H 8	1.4 M Sodium Acetate	None	100 mM MES Sodium Salt	6.5	None
D 3	H 9	500 mM Sodium Chloride	10 mM Magnesium Chloride	None		10 mM Hexadecyltrimethylammonium Bromide
D 4	H 10	2.0 M Sodium Chloride	None	100 mM Sodium Acetate	4.6	None
D 5	H 11	2.0 M Sodium Chloride	None	100 mM MES Sodium Salt	6.5	200 mM Sodium/Potassium dihydrogen Phosphate
D 6	H 12	4.3 M Sodium Chloride	None	100 mM HEPES Sodium Salt	7.5	None



JBScreen Membrane

Membrane 1		Precipitant 1	Precipitant 2	Buffer	pH	Additive
bulk	HTS					
A 1	A 1	15% w/v PEG 400	15% w/v Glycerol	100 mM HEPES Sodium Salt	7.5	200 mM Calcium Chloride
A 2	A 2	20% w/v PEG 400	100 mM Sodium Chloride	100 mM Sodium Citrate	5.6	20 mM Magnesium Chloride
A 3	A 3	25% w/v PEG 400	None	50 mM Sodium Acetate	4.6	50 mM Magnesium Acetate
A 4	A 4	30% w/v PEG 400	50 mM Sodium Sulfate	50 mM Tris-HCl	8.5	50 mM Lithium Sulfate
A 5	A 5	48% w/v PEG 400	None	100 mM HEPES Sodium Salt	7.5	200 mM Calcium Chloride
A 6	A 6	20% w/v PEG 550 MME	None	10 mM Tris-HCl	7.5	None
B 1	A 7	30% w/v PEG 550 MME	None	50 mM Tris-HCl	8.5	100 mM Magnesium Chloride
B 2	A 8	35% w/v PEG 600	None	None		None
B 3	A 9	28% w/v PEG 1000	10% w/v Glycerol	100 mM Tricine	8.0	350 mM Sodium Chloride
B 4	A 10	10% w/v PEG 1500	5% w/v Ethanol	100 mM Sodium Chloride		100 mM Magnesium Chloride
B 5	A 11	30% w/v PEG 1500	None	None		None
B 6	A 12	5% w/v PEG 2000	None	None		None
C 1	B 1	10% w/v PEG 2000	None	50 mM Tris-HCl	8.5	500 mM Magnesium Chloride
C 2	B 2	15% w/v PEG 2000	None	None		None
C 3	B 3	15% w/v PEG 2000	None	None		100 mM Lithium Chloride
C 4	B 4	15% w/v PEG 2000	None	100 mM Sodium Phosphate	6.2	20 mM Sodium Citrate
C 5	B 5	15% w/v PEG 2000	None	100 mM Sodium Phosphate	6.8	500 mM Sodium Chloride
C 6	B 6	15% w/v PEG 2000	None	20 mM Bis Tris	7.0	None
D 1	B 7	15% w/v PEG 2000	None	50 mM HEPES Sodium Salt	7.5	100 mM Magnesium Chloride
D 2	B 8	20% w/v PEG 2000	2% w/v MPD	100 mM Tris-HCl	8.0	300 mM Magnesium Nitrate
D 3	B 9	25% w/v PEG 2000	15% w/v Glycerol	100 mM Bis-Tris	9.0	300 mM Magnesium Chloride
D 4	B 10	30% w/v PEG 2000	None	200 mM Sodium Phosphate	6.2	500 mM Sodium Chloride
D 5	B 11	8% w/v PEG 2000 MME	None	100 mM Sodium Acetate	4.6	None
D 6	B 12	10% w/v PEG 2000 MME	20% w/v Glycerol	100 mM Sodium Citrate	5.6	3% w/v PEG 200

Membrane 2		Precipitant 1	Precipitant 2	Buffer	pH	Additive
bulk	HTS					
A 1	C 1	12% w/v PEG 2000 MME	None	50 mM Tris-HCl	7.5	500 mM Sodium Chloride
A 2	C 2	10% w/v PEG 3350	None	50 mM Sodium Citrate	5.6	150 mM Sodium Chloride
A 3	C 3	2% w/v PEG 4000	None	50 mM Tris-HCl	7.5	None
A 4	C 4	5% w/v PEG 4000	None	None		None
A 5	C 5	5% w/v PEG 4000	None	None		100 mM Potassium Chloride
A 6	C 6	5% w/v PEG 4000	10% w/v Glycerol	50 mM MES Sodium Salt	6.5	100 mM Sodium Chloride
B 1	C 7	5% w/v PEG 4000	None	50 mM Sodium Phosphate	6.7	None
B 2	C 8	10% w/v PEG 4000	None	50 mM Tris-HCl	8.5	500 mM Sodium Chloride
B 3	C 9	12% w/v PEG 4000	None	100 mM ADA	6.5	100 mM Lithium Sulfate
B 4	C 10	12% w/v PEG 4000	None	50 mM Sodium Phosphate	6.8	None
B 5	C 11	12% w/v PEG 4000	20% w/v Glycerol	50 mM MOPS	7.0	500 mM Potassium Chloride
B 6	C 12	15% w/v PEG 4000	None	10 mM Tris-HCl	7.5	100 mM Lithium Chloride
C 1	D 1	20% w/v PEG 4000	None	100 mM Bis Tris	7.0	500 mM Sodium Chloride
C 2	D 2	20% w/v PEG 4000	None	100 mM Sodium Phosphate	7.0	500 mM Sodium Chloride
C 3	D 3	20% w/v PEG 4000	150 mM Zinc Acetate	50 mM Tris-HCl	7.5	50 mM Zinc Chloride
C 4	D 4	22% w/v PEG 4000	None	50 mM Tricine	8.0	None
C 5	D 5	22% w/v PEG 4000	None	50 mM Tris-HCl	8.5	500 mM Sodium Chloride
C 6	D 6	30% w/v PEG 4000	None	None		None
D 1	D 7	10% w/v PEG 5000 MME	None	100 mM Sodium Citrate	5.6	100 mM Magnesium Acetate
D 2	D 8	5% w/v PEG 6000	None	None		100 mM Magnesium Sulfate
D 3	D 9	10% w/v PEG 6000	150 mM Zinc Acetate	50 mM Tris-HCl	7.5	50 mM Zinc Chloride
D 4	D 10	15% w/v PEG 6000	None	50 mM Sodium Succinate	6.5	None
D 5	D 11	12% w/v PEG 8000	10% w/v MPD	None		25 mM Potassium dihydrogen Phosphate
D 6	D 12	8% w/v PEG 10000	None	100 mM Sodium Citrate	5.6	100 mM Magnesium Acetate



Membrane 3		Precipitant 1	Precipitant 2	Buffer	pH	Additive
bulk	HTS					
A 1	E 1	700 mM Ammonium Sulfate	None	1.0 M Sodium / Potassium Phosphate	7.5	None
A 2	E 2	1.0 M Ammonium Sulfate	None	50 mM MES Sodium Salt	6.5	100 mM Zinc Acetate
A 3	E 3	1.2 M Ammonium Sulfate	None	50 mM Tris-HCl	7.5	None
A 4	E 4	1.2 M Ammonium Sulfate	None	100 mM Tris-HCl	8.5	None
A 5	E 5	1.4 M Ammonium Sulfate	4% w/v 2-Propanol	None		100 mM Ammonium Acetate
A 6	E 6	2.0 M Ammonium Sulfate	None	None		None
B 1	E 7	2.0 M Ammonium Sulfate	None	100 mM Sodium Citrate	5.6	None
B 2	E 8	2.5 M Ammonium Sulfate	2% PEG 5000 MME	100 mM HEPES Sodium Salt	7.5	None
B 3	E 9	3.0 M Ammonium Sulfate	None	None		None
B 4	E 10	3.5 M Ammonium Sulfate	None	None		None
B 5	E 11	3.5 M Ammonium Sulfate	None	50 mM Sodium/ Potassium Phosphate	7.5	250 mM Sodium Chloride
B 6	E 12	25% w/v MPD	None	100 mM Bis-Tris	7.0	None
C 1	F 1	30% w/v MPD	None	300 mM Sodium Citrate	5.6	None
C 2	F 2	25% w/v Ethylene Glycol	None	None		100 mM Ammonium Sulfate 100 mM Glycine
C 3	F 3	30% w/v 2-Propanol	20% w/v Glycerol	100 mM Sodium Acetate	4.6	200 mM Calcium Chloride
C 4	F 4	None	None	50 mM Potassium Phosphate	8.0	None
C 5	F 5	None	None	100 mM Sodium Citrate	4.8	None
C 6	F 6	1.0 M Potassium Phosphate	None	None	6.5	1% w/v 1,4-Dioxane
D 1	F 7	1.0 M Sodium Citrate	None	None		None
D 2	F 8	None	None	1.0 M Sodium Citrate	5.6	500 mM Lithium Chloride
D 3	F 9	1.5 M Sodium Chloride	None	100 mM Sodium Acetate	4.6	None
D 4	F 10	None	None	1.5 M Potassium Phosphate	7.0	None
D 5	F 11	1.5 M Lithium Sulfate	None	100 mM HEPES Sodium Salt	7.5	None
D 6	F 12	2.0 M Sodium Chloride	None	None		100 mM Sodium Formate



JBScreen Kinase

Kinase 1		Precipitant	Buffer	pH	Additive 1	Additive 2
bulk	HTS					
A 1	A 1	1.0 M Ammonium Sulfate	100 mM Sodium Citrate	5.6	200 mM Magnesium Acetate	10 mM DTT
A 2	A 2	1.3 M Ammonium Sulfate	100 mM Sodium Citrate	5.6	None	None
A 3	A 3	1.3 M Ammonium Sulfate	100 mM Tris-HCl	8.5	None	None
A 4	A 4	1.8 M Ammonium Sulfate	100 mM MES Sodium Salt	6.5	25 mM Cobalt (II) Chloride	None
A 5	A 5	2.0 M Ammonium Sulfate	100 mM Citric Acid	3.1	200 mM Sodium Chloride	None
A 6	A 6	2.0 M Ammonium Sulfate	100 mM Sodium Acetate	4.6	50 mM Magnesium Chloride	None
B 1	A 7	2.0 M Ammonium Sulfate	100 mM Sodium Acetate	4.6	None	None
B 2	A 8	2.0 M Ammonium Sulfate	100 mM HEPES Sodium Salt	7.5	2% v/v PEG 550 MME	None
B 3	A 9	2.0 M Ammonium Sulfate	100 mM HEPES Sodium Salt	7.5	None	None
B 4	A 10	2.0 M Ammonium Sulfate	100 mM Tris-HCl	8.5	6 mM Magnesium Chloride	None
B 5	A 11	1.5 M Lithium Sulfate	100 mM Tris-HCl	8.5	10 mM Nickel Sulfate	None
B 6	A 12	1.0 M Lithium Chloride	100 mM Citric Acid	4.2	None	None
C 1	B 1	2.0 M Sodium Chloride	100 mM Sodium Acetate	4.6	None	None
C 2	B 2	2.0 M Sodium Chloride	100 mM MES Sodium Salt	6.5	200 mM Sodium/Potassium Phosphate	None
C 3	B 3	3.3 M Sodium Chloride	100 mM HEPES Sodium Salt	7.5	1% v/v Glycerol	None
C 4	B 4	1.2 M Sodium Acetate	100 mM MES Sodium Salt	6.5	6.25 mM Calcium Chloride	None
C 5	B 5	3.7 M Sodium Formate	100 mM Bicine	9.5	2% w/v PEG 3000	None
C 6	B 6	500 mM Sodium Malonate	50 mM PIPES	6.0	1.6% v/v Glycerol	10 mM DTT
D 1	B 7	500 mM di-Sodium hydrogen Phosphate	100 mM CAPS	10.0	500 mM di-Potassium hydrogen Phosphate	100 mM Lithium Sulfate
D 2	B 8	1.2 M Sodium Tartrate	100 mM Tris-HCl	8.5	5 mM DTT	None
D 3	B 9	1.0 M Potassium / Sodium Tartrate	100 mM MES Sodium Salt	6.5	None	None
D 4	B 10	30% v/v Jeffamine M-600	100 mM MES Sodium Salt	6.5	50 mM Cesium Chloride	None
D 5	B 11	40% v/v MPD	100 mM MES Sodium Salt	6.5	None	None
D 6	B 12	50% v/v MPD	100 mM HEPES Sodium Salt	7.5	None	None

Kinase 2		Precipitant	Buffer	pH	Additive 1	Additive 2	Additive 3
bulk	HTS						
A 1	C 1	10% v/v PEG 400	50 mM Tris-HCl	8.5	300 mM Sodium Chloride	1 mM DTT	1mM EDTA
A 2	C 2	15% v/v PEG 400	100 mM HEPES Sodium Salt	7.5	200 mM Calcium Chloride	None	None
A 3	C 3	25% v/v PEG 400	100 mM MES Sodium Salt	6.5	10% v/v 2-Propanol	None	None
A 4	C 4	25% v/v PEG 400	100 mM Tris-HCl	8.5	150 mM Sodium Citrate	None	None
A 5	C 5	15% v/v PEG 550 MME	100 mM Sodium Acetate	4.6	5% v/v Ethylene Glycol	None	None
A 6	C 6	20% v/v PEG 550 MME	100 mM Bicine	9.0	100 mM Sodium Chloride	None	None
B 1	C 7	20% w/v PEG 1000	100 mM Tris-HCl	8.5	1 mM DTT	None	None
B 2	C 8	35% w/v PEG 1000	100 mM HEPES Sodium Salt	7.5	50 mM Lithium Sulfate	None	None
B 3	C 9	12% w/v PEG 2000	100 mM MES Sodium Salt	6.5	200 mM Magnesium Acetate	None	None
B 4	C 10	25% w/v PEG 2000	100 mM Sodium Acetate	4.6	100 mM Magnesium Chloride	None	None
B 5	C 11	30% w/v PEG 2000	100 mM Sodium Acetate	4.6	50 mM Magnesium Chloride	None	None
B 6	C 12	24% w/v PEG 2000 MME	100 mM Citrate/Phosphate	5.0	None	None	None
C 1	D 1	12% w/v PEG 3350	100 mM MES Sodium Salt	6.5	500 mM Sodium Chloride	None	None
C 2	D 2	12% w/v PEG 3350	50 mM Sodium Citrate	5.6	200 mM Ammonium Sulfate	50 mM Magnesium Sulfate	None
C 3	D 3	15% w/v PEG 3350	100 mM Imidazole-HCl	7.5	250 mM Ammonium Sulfate	10 mM Cadmium Chloride	None
C 4	D 4	20% w/v PEG 3350	150 mM D,L-Malic Acid	7.0	None	None	None
C 5	D 5	20% w/v PEG 3350	100 mM HEPES Sodium Salt	7.5	200 mM Sodium Chloride	20 mM Glutathione	None
C 6	D 6	20% w/v PEG 3350	100 mM Tris-HCl	8.5	120 mM Sodium Chloride	5 mM DTT	None
D 1	D 7	20% w/v PEG 3350	None		200 mM Potassium Nitrate	None	None
D 2	D 8	22% w/v PEG 3350	None		100 mM Ammonium Formate	None	None
D 3	D 9	24% w/v PEG 3350	100 mM Citric Acid	5.0	None	None	None
D 4	D 10	30% w/v PEG 3350	100 mM Sodium Acetate	4.6	200 mM Ammonium Acetate	None	None
D 5	D 11	30% w/v PEG 3350	200 mM Ammonium Acetate	5.6	20% v/v 2-Propanol	200 mM Calcium Chloride	None
D 6	D 12	32.5% w/v PEG 3350	100 mM Tris-HCl	8.5	200 mM Magnesium Chloride	500 mM Sodium Chloride	None



Kinase 3		Precipitant	Buffer	pH	Additive 1	Additive 2	Additive 3
bulk	HTS						
A 1	E 1	8% w/v PEG 4000	50 mM MES Sodium Salt	6.5	10 mM Magnesium Chloride	10 mM DTT	None
A 2	E 2	10% w/v PEG 4000	50 mM PIPES	7.0	10 mM DTT	None	None
A 3	E 3	10% w/v PEG 4000	100 mM HEPES Sodium Salt	7.5	200 mM Magnesium Chloride	15% v/v Ethylene Glycol	10% v/v 2-Propanol
A 4	E 4	10% w/v PEG 4000	100 mM HEPES Sodium Salt	7.5	None	None	None
A 5	E 5	15% w/v PEG 4000	100 mM HEPES Sodium Salt	7.5	10% v/v 2-Propanol	None	None
A 6	E 6	15% w/v PEG 4000	75 mM Tris-HCl	8.5	75 mM Sodium Acetate	200 mM Sodium Chloride	1% w/v PEG 6000
B 1	E 7	15% w/v PEG 4000	100 mM L-Malic Acid	5.5	200 mM Ammonium Sulfate	None	None
B 2	E 8	20% w/v PEG 4000	100 mM Bis-Tris	6.5	100 mM Sodium Chloride	None	None
B 3	E 9	20% w/v PEG 4000	100 mM HEPES Sodium Salt	7.5	200 mM Magnesium Chloride	None	None
B 4	E 10	20% w/v PEG 4000	100 mM Tris-HCl	8.5	200 mM Magnesium Chloride	None	None
B 5	E 11	25% w/v PEG 4000	100 mM MES Sodium Salt	6.5	200 mM Magnesium Chloride	None	None
B 6	E 12	25% w/v PEG 4000	100 mM Tris-HCl	8.5	100 mM Lithium Sulfate	None	None
C 1	F 1	28% w/v PEG 4000	200 mM Lithium Acetate	7.5	None	None	None
C 2	F 2	30% w/v PEG 4000	100 mM MES Sodium Salt	6.5	200 mM Sodium Acetate	None	None
C 3	F 3	30% w/v PEG 4000	150 mM Tris-HCl	8.5	200 mM Ammonium Sulfate	None	None
C 4	F 4	8% w/v PEG 5000 MME	100 mM HEPES Sodium Salt	7.5	10% v/v 2-Propanol	None	None
C 5	F 5	25% w/v PEG 5000 MME	100 mM MES Sodium Salt	6.5	200 mM Ammonium Sulfate	None	None
C 6	F 6	30% w/v PEG 5000 MME	100 mM HEPES Sodium Salt	7.5	200 mM Ammonium Sulfate	None	None
D 1	F 7	30% w/v PEG 5000 MME	100 mM ADA	6.5	100 mM Ammonium Sulfate	None	None
D 2	F 8	20% w/v PEG 6000	100 mM MES Sodium Salt	6.5	None	None	None
D 3	F 9	28% w/v PEG 6000	100 mM MES Sodium Salt	6.5	10 mM DTT	None	None
D 4	F 10	30% w/v PEG 6000	100 mM HEPES Sodium Salt	7.5	175 mM Lithium Sulfate	None	None
D 5	F 11	30% w/v PEG 6000	100 mM PIPES	7.0	10 mM DTT	None	None
D 6	F 12	32% w/v PEG 6000	100 mM MES Sodium Salt	6.5	None	None	None

Kinase 4		Precipitant	Buffer	pH	Additive 1	Additive 2
bulk	HTS					
A 1	G 1	7% w/v PEG 8000	100 mM MES Sodium Salt	6.5	20% v/v Ethylene Glycol	None
A 2	G 2	7% w/v PEG 8000	100 mM MES Sodium Salt	6.5	150 mM Calcium Acetate	16% v/v Ethylene Glycol
A 3	G 3	10% w/v PEG 8000	100 mM Tris-HCl	8.5	10% v/v PEG 200	None
A 4	G 4	12% w/v PEG 8000	100 mM HEPES Sodium Salt	7.5	None	None
A 5	G 5	12% w/v PEG 8000	100 mM Tris-HCl	8.5	250 mM Sodium Tartrate	None
A 6	G 6	16% w/v PEG 8000	100 mM HEPES Sodium Salt	7.5	100 mM Potassium dihydrogen Phosphate	None
B 1	G 7	16% w/v PEG 8000	100 mM HEPES Sodium Salt	7.5	150 mM Sodium Chloride	2% v/v Ethylene Glycol
B 2	G 8	18% w/v PEG 8000	100 mM MES Sodium Salt	6.5	200 mM Magnesium Acetate	None
B 3	G 9	18% w/v PEG 8000	100 mM MES Sodium Salt	6.5	None	None
B 4	G 10	18% w/v PEG 8000	100 mM Tris-HCl	8.5	None	None
B 5	G 11	20% w/v PEG 8000	100 mM Citric Acid	5.0	100 mM Magnesium Acetate	None
B 6	G 12	20% w/v PEG 8000	100 mM Tris-HCl	8.5	200 mM Magnesium Chloride	2% v/v Ethylene Glycol
C 1	H 1	22% w/v PEG 8000	100 mM Tris-HCl	8.5	2% v/v Ethylene Glycol	None
C 2	H 2	25% w/v PEG 8000	100 mM Sodium Acetate	4.6	50 mM Magnesium Chloride	None
C 3	H 3	30% w/v PEG 8000	100 mM MES Sodium Salt	6.5	200 mM Ammonium Sulfate	4% v/v 1,3-Propanediol
C 4	H 4	30% w/v PEG 8000	100 mM HEPES Sodium Salt	7.5	10 mM DTT	20% v/v Glycerol
C 5	H 5	9% w/v PEG 8000	100 mM MES Sodium Salt	6.5	200 mM Zinc Acetate	None
C 6	H 6	16% w/v PEG 10000	100 mM Bis-Tris	6.5	300 mM Ammonium Sulfate	5% v/v Ethylene Glycol
D 1	H 7	10% w/v PEG 10000	100 mM HEPES Sodium Salt	7.5	8% v/v Ethylene Glycol	None
D 2	H 8	15% w/v PEG 10000	100 mM HEPES Sodium Salt	7.5	5 mM DTT	None
D 3	H 9	15% w/v PEG 10000	100 mM Tris-HCl	8.5	None	None
D 4	H 10	12% w/v PEG 20000	100 mM MES Sodium Salt	6.5	None	None
D 5	H 11	10% w/v PEG 20000	100 mM HEPES Sodium Salt	7.5	100 mM Ammonium Formate	None
D 6	H 12	15% w/v PEG 20000	None		10 mM Potassium Tartrate	None



JBScreen Phosphatase

Phosphatase 1		Precipitant 1	Precipitant 2	Buffer	pH	Additive 1	Additive 2
bulk	HTS						
A1	A1	15 % v/v PEG 400	None	50 mM Sodium Citrate	5.6	200 mM Sodium Tartrate	200 mM Ammonium Sulfate
A2	A2	22 % v/v PEG 400	None	100 mM Tris-HCl	8.5	200 mM Lithium Sulfate	None
A3	A3	25 % v/v PEG 400	None	100 mM HEPES Sodium Salt	7.5	200 mM Calcium Chloride	None
A4	A4	25 % v/v PEG 550 MME	None	100 mM MES Sodium Salt	6.5	10 mM Zinc Sulfate	None
A5	A5	27 % w/v PEG 1500	10 % v/v MPD	10 mM Imidazole-HCl	7.0	220 mM Sodium Nitrate	None
A6	A6	30% w/v PEG 1500	None	100 mM Bis-Tris	6.5	400 mM Potassium Fluoride	None
B1	A7	8 % w/v PEG 2000 MME	None	10 mM Tris-HCl	7.0	10 mM Nickel (II) Chloride	None
B2	A8	16% w/v PEG 2000 MME	None	100 mM Sodium Acetate	4.6	400 mM Ammonium Sulfate	None
B3	A9	8 % w/v PEG 3350	None	None		100 mM Sodium Acetate	None
B4	A10	10 % w/v PEG 3350	None	100 mM HEPES Sodium Salt	7.5	200 mM Ammonium Acetate	None
B5	A11	10 % w/v PEG 3350	None	100 mM HEPES Sodium Salt	7.5	50 mM Ammonium Acetate	15 mM Sodium Chloride
B6	A12	10 % w/v PEG 3350	None	100 mM MES Sodium Salt	6.5	20 mM Zinc Acetate	None
C1	B1	15 % w/v PEG 3350	None	None		200 mM Sodium Fluoride	None
C2	B2	15 % w/v PEG 3350	None	100 mM Bis-Tris	6.5	50 mM Glycine	200 mM Sodium Formate
C3	B3	15 % w/v PEG 3350	5 % v/v Glycerol	100 mM Bis-Tris	7.0	200 mM Magnesium Formate	None
C4	B4	20 % w/v PEG 3350	None	None		200 mM Potassium Fluoride	None
C5	B5	20 % w/v PEG 3350	None	100 mM MES Sodium Salt	6.5	100 mM Ammonium Chloride	None
C6	B6	20 % w/v PEG 3350	None	10 mM Tris-HCl	8.0	200 mM Potassium Sulfate	None
D1	B7	20 % w/v PEG 3350	None	None		100 mM Sodium Citrate	None
D2	B8	22 % w/v PEG 3350	None	100 mM HEPES Sodium Salt	7.5	200 mM Calcium Chloride	None
D3	B9	25 % w/v PEG 3350	None	100 mM Tris-HCl	8.5	200 mM Magnesium Chloride	None
D4	B10	25 % w/v PEG 3350	10 % v/v 2-Propanol	100 mM Sodium Citrate	4.8	100 mM Lithium Chloride	None
D5	B11	30 % w/v PEG 3350	None	None		200 mM Ammonium Nitrate	None
D6	B12	30 % w/v PEG 3350	None	None		200 mM Ammonium dihydrogen Phosphate	None

Phosphatase 2		Precipitant 1	Precipitant 2	Buffer	pH	Additive 1	Additive 2
bulk	HTS						
A1	C1	8 % w/v PEG 4000	None	50 mM HEPES Sodium Salt	7.0	22 mM Lithium Sulfate	0.1 % v/v β-Mercaptoethanol
A2	C2	10 % w/v PEG 4000	None	100 mM HEPES Sodium Salt	7.5	50 mM Ammonium Acetate	None
A3	C3	10 % w/v PEG 4000	10 % v/v Glycerol	50 mM Sodium Succinate	5.5	3 mM Magnesium Chloride	50 mM Tris-Phosphate pH 7.5
A4	C4	12 % w/v PEG 4000	10 % v/v 2-Propanol	100 mM Sodium Citrate	5.6	None	None
A5	C5	12 % w/v PEG 4000	None	200 mM Imidazole Malate	6.0	2 mM Zinc Acetate	None
A6	C6	15 % w/v PEG 4000	None	100 mM HEPES Sodium Salt	7.0	200 mM Magnesium Chloride	None
B1	C7	15 % w/v PEG 4000	15 % v/v PEG 400	50 mM MES Sodium Salt	6.5	200 mM Magnesium Sulfate	50 mM Ammonium Sulfate
B2	C8	15 % w/v PEG 4000	None	85 mM MES Sodium Salt	6.5	170 mM Sodium Acetate	None
B3	C9	20 % w/v PEG 4000	5 % v/v 2-Propanol	100 mM Bicine	9.0	None	None
B4	C10	22 % w/v PEG 4000	10 % v/v 2-Propanol	100 mM Tris-HCl	8.5	200 mM Lithium Sulfate	0.5 % v/v β-Mercaptoethanol
B5	C11	25 % w/v PEG 4000	None	100 mM Bis-Tris Propane	6.5	200 mM di-Ammonium Tartrate	None
B6	C12	30 % w/v PEG 4000	None	100 mM Sodium Acetate	4.6	None	None
C1	D1	30 % w/v PEG 4000	None	100 mM Sodium Citrate	5.6	200 mM Ammonium Acetate	None
C2	D2	30 % w/v PEG 4000	None	100 mM Tris-HCl	7.5	100 mM Cesium Chloride	250 mM Lithium Sulfate
C3	D3	35 % w/v PEG 4000	None	100 mM MES Sodium Salt	6.0	None	None
C4	D4	42 % w/v PEG 4000	None	50 mM Tris-HCl	8.0	100 mM Sodium Perchlorate	None
C5	D5	8 % w/v PEG 6000	10 % v/v 2-Propanol	100 mM Citric Acid	4.0	50 mM Ammonium dihydrogen Phosphate	None
C6	D6	10 % w/v PEG 6000	4 % v/v MPD	100 mM HEPES Sodium Salt	7.5	None	None
D1	D7	10 % w/v PEG 6000	None	100 mM MES Sodium Salt	6.5	None	None
D2	D8	12 % w/v PEG 6000	None	100 mM Sodium Acetate	4.6	None	None
D3	D9	12 % w/v PEG 6000	None	100 mM Tris-Acetate	8.0	None	None
D4	D10	12 % w/v PEG 6000	2% v/v Glycerol	None		25 mM Sodium Phosphate	None
D5	D11	15 % w/v PEG 6000	None	50 mM Sodium Phosphate	7.0	25 mM Potassium Chloride	5 mM Magnesium Sulfate
D6	D12	20 % w/v PEG 6000	None	100 mM Bicine	9.0	None	None



Phosphatase 3		Precipitant 1	Precipitant 2	Buffer	pH	Additive 1	Additive 2
bulk	HTS						
A1	E1	8 % w/v PEG 8000	None	None		100 mM Potassium Phosphate	0.2 % v/v β-Mercaptoethanol
A2	E2	10 % w/v PEG 8000	None	100 mM HEPES Sodium Salt	7.5	200 mM Magnesium Acetate	None
A3	E3	10 % w/v PEG 8000	None	100 mM MES Sodium Salt	6.5	200 mM Potassium Chloride	100 mM Magnesium Acetate
A4	E4	10 % w/v PEG 8000	None	100 mM Tris-HCl	8.5	50 mM Sodium Chloride	None
A5	E5	12 % w/v PEG 8000	None	50 mM Sodium Acetate	5.0	300 mM Ammonium Acetate	None
A6	E6	12 % w/v PEG 8000	None	100 mM Tris-HCl	6.3	200 mM Lithium Sulfate	None
B1	E7	12 % w/v PEG 8000	None	100 mM HEPES Sodium Salt	7.5	200 mM Sodium Acetate	None
B2	E8	13 % w/v PEG 8000	15 % v/v Glycerol	100 mM MOPS	7.0	500 mM Ammonium Sulfate	None
B3	E9	15 % w/v PEG 8000	None	100 mM Potassium Phosphate	4.6	None	None
B4	E10	15 % w/v PEG 8000	None	100 mM Sodium Phosphate	4.6	None	None
B5	E11	15 % w/v PEG 8000	None	100 mM Sodium Succinate	5.5	250 mM Lithium Sulfate	None
B6	E12	18 % w/v PEG 8000	None	100 mM HEPES Sodium Salt	7.0	100 mM Potassium dihydrogen Phosphate	None
C1	F1	18 % w/v PEG 8000	None	None		200 mM Lithium Sulfate	None
C2	F2	18 % w/v PEG 8000	5 % v/v 1,4-Dioxane	100 mM Tris-HCl	8.0	200 mM Sodium Fluoride	None
C3	F3	25 % w/v PEG 8000	5 % v/v Jeffamine M600	90 mM MES Sodium Salt	6.0	90 mM Magnesium Acetate	None
C4	F4	25 % w/v PEG 8000	None	100 mM Tris-HCl	8.5	200 mM Magnesium Sulfate	None
C5	F5	5 % w/v PEG 10000	None	100 mM HEPES Sodium Salt	7.5	200 mM Magnesium Chloride	None
C6	F6	10 % w/v PEG 10000	None	50 mM Sodium Acetate	5.0	None	None
D1	F7	10 % w/v PEG 10000	None	100 mM HEPES Sodium Salt	7.5	None	None
D2	F8	15 % w/v PEG 10000	None	100 mM Bis-Tris	5.5	100 mM Ammonium Acetate	5 mM LDAO
D3	F9	15 % w/v PEG 10000	None	60 mM Glycine	9.0	20 mM Sodium Citrate	None
D4	F10	20 % w/v PEG 10000	5 % v/v PEG 550 MME	100 mM Sodium Citrate	5.6	None	None
D5	F11	12 % w/v PEG 20000	None	100 mM MES Sodium Salt	6.5	None	None
D6	F12	17 % w/v PEG 20000	None	100 mM Tris-HCl	8.5	100 mM Magnesium Chloride	None

Phosphatase 4		Precipitant 1	Precipitant 2	Buffer	pH	Additive 1	Additive 2
bulk	HTS						
A1	G1	500 mM Ammonium Sulfate	None	100 mM HEPES Sodium Salt	7.5	200 mM Lithium Sulfate	None
A2	G2	1.0 M Ammonium Sulfate	None	100 mM MES Sodium Salt	6.5	100 mM Potassium Chloride	None
A3	G3	1.0 M Ammonium Sulfate	800 mM Potassium Chloride	100 mM HEPES Sodium Salt	7.0	None	None
A4	G4	1.3 M Ammonium Sulfate	None	100 mM CHES	9.5	200 mM Sodium Chloride	None
A5	G5	1.3 M Ammonium Sulfate	None	100 mM Sodium Acetate	5.5	None	None
A6	G6	1.3 M Ammonium Sulfate	5 % v/v Glycerol	100 mM Maleic Acid	6.5	1 mM Magnesium Chloride	5 mM Zinc Chloride
B1	G7	1.5 M Ammonium Sulfate	None	100 mM Tris-HCl	8.5	200 mM Lithium Sulfate	None
B2	G8	1.7 M Ammonium Sulfate	None	100 mM MES Sodium Salt	6.0	None	None
B3	G9	1.7 M Ammonium Sulfate	4 % v/v MPD	100 mM HEPES Sodium Salt	7.5	None	None
B4	G10	1.7 M Ammonium Sulfate	2 % v/v PEG 400	100 mM Tris-HCl	7.5	None	None
B5	G11	2.0 M Ammonium Sulfate	None	100 mM Tris-HCl	8.5	None	None
B6	G12	2.0 M Ammonium Sulfate	10 % v/v PEG 400	50 mM HEPES Sodium Salt	7.0	50 mM Zinc Sulfate	None
C1	H1	2.0 M Ammonium Sulfate	None	100 mM Sodium Citrate	5.6	200 mM Potassium/Sodium Tartrate	None
C2	H2	2.2 M Ammonium Sulfate	6 % v/v PEG 400	100 mM Bis-Tris	6.5	None	None
C3	H3	2.4 M Ammonium Sulfate	None	100 mM HEPES Sodium Salt	7.0	None	None
C4	H4	2.4 M Ammonium Sulfate	None	100 mM Tris-HCl	8.0	10 mM Magnesium Chloride	5 mM Zinc Sulfate
C5	H5	500 mM Lithium Sulfate	10 % v/v PEG 400	100 mM Imidazole-HCl	8.0	None	None
C6	H6	1.5 M Lithium Sulfate	None	100 mM HEPES Sodium Salt	7.5	None	None
D1	H7	2.0 M Lithium Sulfate	2 % v/v PEG 400	100 mM Tris-Acetate	8.0	0.1 % v/v β-Mercaptoethanol	None
D2	H8	20 % v/v MPD	None	100 mM MES Sodium Salt	6.5	None	None
D3	H9	35 % v/v MPD	None	100 mM Sodium Acetate	4.6	None	None
D4	H10	1.4 M Sodium Formate	None	100 mM MES Sodium Salt	6.0	None	None
D5	H11	3.0 M Sodium Formate	None	100 mM Tris-HCl	8.0	None	None
D6	H12	1.0 M Sodium Tartrate	None	100 mM Tris-HCl	8.5	None	None



JBScreen Nuc-Pro

Nuc-Pro 1		Precipitant 1	Precipitant 2	Buffer	pH	Additive 1	Additive 2
bulk	HTS						
A1	A1	20 % v/v PEG 200	None	50 mM HEPES Sodium Salt	7.5	200 mM Potassium Chloride	25 mM Magnesium Sulfate
A2	A2	50 % v/v PEG 200	None	100 mM Tris-HCl	8.0	None	None
A3	A3	5 % v/v PEG 400	None	50 mM PIPES	7.0	30 mM Magnesium Chloride	None
A4	A4	5 % v/v PEG 400	None	20 mM MES Sodium Salt	5.8	15 mM Magnesium Formate	2 mM Cobalt (II) Chloride
A5	A5	10 % v/v PEG 400	None	50 mM HEPES Sodium Salt	7.0	100 mM Potassium Chloride	None
A6	A6	15 % v/v PEG 400	None	50 mM MES Sodium Salt	6.5	80 mM Magnesium Acetate	15 mM Magnesium Chloride
B1	A7	15 % v/v PEG 400	None	100 mM Tris-HCl	8.0	80 mM Calcium Chloride	20 mM Sodium Chloride
B2	A8	20 % v/v PEG 400	None	50 mM Bis-Tris-Propane	6.8	60 mM Magnesium Chloride	None
B3	A9	25% v/v PEG 400	None	100 mM Sodium Citrate	5.6	130 mM Sodium Chloride	60 mM Magnesium Chloride
B4	A10	30 % v/v PEG 400	None	100 mM HEPES Sodium Salt	7.5	200 mM Calcium Chloride	None
B5	A11	30 % v/v PEG 400	None	50 mM Tris-HCl	8.5	100 mM Potassium Chloride	10 mM Magnesium Chloride
B6	A12	25 % v/v PEG 550 MME	None	50 mM HEPES Sodium Salt	7.0	10 mM Magnesium Chloride	None
C1	B1	20 % w/v PEG 1000	None	50 mM MES Sodium Salt	6.5	200 mM Magnesium Chloride	100 mM Sodium Chloride
C2	B2	30 % w/v PEG 2000 MME	None	100 mM Sodium Acetate	4.6	200 mM Ammonium Sulfate	None
C3	B3	10 % w/v PEG 3350	None	100 mM MES Sodium Salt	6.5	100 mM Calcium Chloride	13 % v/v Glycerol
C4	B4	25 % w/v PEG 3350	None	50 mM MES Sodium Salt	6.0	200 mM Sodium Formate	10 % v/v Glycerol
C5	B5	30 % w/v PEG 3350	None	50 mM Sodium Succinate	5.5	100 mM Sodium Chloride	None
C6	B6	35 % w/v PEG 3350	None	50 mM Tris-HCl	7.5	50 mM Potassium Chloride	None
D1	B7	5 % w/v PEG 4000	None	50 mM HEPES Sodium Salt	7.0	200 mM Ammonium Sulfate	20 mM Magnesium Acetate
D2	B8	5 % w/v PEG 4000	None	50 mM MES Sodium Salt	6.0	5 mM Magnesium Sulfate	None
D3	B9	10 % w/v PEG 4000	None	50 mM MES Sodium Salt	6.5	200 mM Ammonium Acetate	10 mM Calcium Chloride
D4	B10	10 % w/v PEG 4000	None	50 mM Imidazole-HCl	7.2	20 mM Zinc Sulfate	None
D5	B11	15 % w/v PEG 4000	None	50 mM Tris-HCl	7.5	150 mM Potassium Chloride	20 mM Magnesium Chloride
D6	B12	15 % w/v PEG 4000	None	50 mM Sodium Citrate	5.0	100 mM Sodium Chloride	20 mM Ammonium Sulfate

Nuc-Pro 2		Precipitant 1	Precipitant 2	Buffer	pH	Additive 1	Additive 2
bulk	HTS						
A1	C1	20 % w/v PEG 4000	None	100 mM Sodium Citrate	5.6	100 mM Potassium Chloride	10 % v/v 2-Propanol
A2	C2	20 % w/v PEG 4000	None	50 mM MOPS	7.0	100 mM Sodium Chloride	None
A3	C3	20 % w/v PEG 4000	None	100 mM HEPES Sodium Salt	7.5	None	None
A4	C4	24 % w/v PEG 4000	None	50 mM Sodium Succinate	5.5	60 mM Magnesium Chloride	30 mM Sodium Chloride
A5	C5	25 % w/v PEG 4000	None	50 mM Sodium Citrate	5.0	50 mM Ammonium Sulfate	None
A6	C6	30 % w/v PEG 4000	None	50 mM MES Sodium Salt	6.5	80 mM Magnesium Acetate	None
B1	C7	30 % w/v PEG 4000	None	50 mM Tris-HCl	8.5	150 mM Ammonium Chloride	10 mM Calcium Chloride
B2	C8	32 % w/v PEG 4000	None	100 mM Tris-HCl	8.5	5 % v/v Glycerol	None
B3	C9	36% w/v PEG 4000	None	50 mM Sodium Acetate	5.0	None	None
B4	C10	5 % w/v PEG 6000	None	20 mM Bis-Tris	6.0	60 mM Ammonium Citrate	20 mM Magnesium Chloride
B5	C11	10 % w/v PEG 6000	None	50 mM Citric Acid	4.0	100 mM Sodium Chloride	None
B6	C12	10 % w/v PEG 6000	None	50 mM HEPES Sodium Salt	7.0	200 mM Ammonium Acetate	150 mM Magnesium Acetate
C1	D1	15 % w/v PEG 6000	None	10 mM Tris-HCl	7.5	None	None
C2	D2	18 % w/v PEG 6000	None	50 mM Sodium Acetate	5.0	None	None
C3	D3	20 % w/v PEG 6000	None	50 mM Bis-Tris-Propane	7.0	7 % v/v MPD	5 % v/v Tert-Butanol
C4	D4	20 % w/v PEG 6000	None	50 mM L-Malic Acid	5.0	30 mM Calcium Chloride	None
C5	D5	5 % w/v PEG 8000	None	50 mM HEPES Sodium Salt	7.5	20 mM Magnesium Chloride	None
C6	D6	10 % w/v PEG 8000	None	100 mM Tris-HCl	8.0	10 % v/v Glycerol	1 mM TCEP
D1	D7	10 % w/v PEG 8000	None	50 mM MES Sodium Salt	6.5	200 mM Potassium Chloride	100 mM Magnesium Acetate
D2	D8	15 % w/v PEG 8000	None	50 mM Bis-Tris-Propane	6.8	100 mM Ammonium Sulfate	10 % v/v Glycerol
D3	D9	15 % w/v PEG 8000	None	100 mM MES Sodium Salt	6.5	200 mM Calcium Acetate	None
D4	D10	18 % w/v PEG 8000	None	100 mM Tris-HCl	8.0	200 mM Magnesium Formate	None
D5	D11	20 % w/v PEG 8000	None	10 mM Tris-HCl	7.5	10 mM Calcium Chloride	None
D6	D12	15 % w/v PEG 20000	None	100 mM MES Sodium Salt	6.5	80 mM Mangan (II) Chloride	None



Nuc-Pro 3		Precipitant 1	Precipitant 2	Buffer	pH	Additive 1	Additive 2
bulk	HTS						
A1	E1	1.2 M Ammonium Sulfate	None	100 mM HEPES Sodium Salt	7.5	2 % w/v PEG 400	None
A2	E2	20 mM Calcium Chloride	None	100 mM Glycine	8.0	None	None
A3	E3	2 M Lithium Chloride	None	50 mM MES Sodium Salt	6.0	200 mM Calcium Acetate	1 mM Cobalt (II) Chloride
A4	E4	600 mM Lithium Sulfate	None	50 mM MES Sodium Salt	6.0	10 mM Magnesium Chloride	None
A5	E5	1 M Lithium Sulfate	8 % w/v PEG 400	50 mM HEPES Sodium Salt	7.5	None	None
A6	E6	1 M Lithium Sulfate	None	None		50 mM Sodium Citrate	3 % v/v 2-Propanol
B1	E7	1.2 M Lithium Sulfate	None	50 mM MES Sodium Salt	6.5	30 mM Magnesium Chloride	None
B2	E8	1.2 M Lithium Sulfate	None	50 mM MES Sodium Salt	6.5	50 mM Magnesium Chloride	2 mM Cobalt (II) Chloride
B3	E9	1.5 M Lithium Sulfate	None	50 mM Tris-HCl	8.5	5 % w/v Glycerol	None
B4	E10	1.6 M Lithium Sulfate	2 % w/v PEG 1000	50 mM HEPES Sodium Salt	7.5	None	None
B5	E11	1.7 M Lithium Sulfate	None	50 mM HEPES Sodium Salt	7.0	50 mM Magnesium Sulfate	None
B6	E12	1.7 M Lithium Sulfate	None	None		10 % w/v Glycerol	None
C1	F1	2 M Lithium Sulfate	None	None		3 % w/v MPD	None
C2	F2	5 mM Magnesium Chloride	None	50 mM MES Sodium Salt	6.5	2.5 mM Cobalt (II) Chloride	None
C3	F3	40 mM Magnesium Chloride	None	50 mM MES Sodium Salt	6.0	None	None
C4	F4	80 mM Magnesium Chloride	None	50 mM HEPES Sodium Salt	7.5	None	None
C5	F5	200 mM Sodium Chloride	None	50 mM Bis-Tris-Propane	7.0	None	None
C6	F6	400 mM Sodium Chloride	None	50 mM Bis-Tris-Propane	6.8	None	None
D1	F7	600 mM Sodium Chloride	None	50 mM MES Sodium Salt	6.0	100 mM Ammonium Acetate	5 mM Magnesium Sulfate
D2	F8	2.5 M Sodium Chloride	None	50 mM Tris-HCl	7.5	200 mM Magnesium Chloride	None
D3	F9	1.8 M Sodium Formate	None	100 mM Tris-HCl	8.0	None	None
D4	F10	2 M Sodium Formate	None	100 mM Sodium Acetate	4.6	None	None
D5	F11	100 mM Sodium Phosphate anhydrous	None	None		80 mM Sodium Chloride	None
D6	F12	1 M Sodium Tartrate	None	50 mM Tris-HCl	7.5	30 mM Magnesium Chloride	None

Nuc-Pro 4		Precipitant 1	Precipitant 2	Buffer	pH	Additive 1	Additive 2
bulk	HTS						
A1	G1	10 % w/v 1.6 Hexandiol	None	50 mM MES Sodium Salt	6.5	20 mM Magnesium Chloride	None
A2	G2	20 % w/v 1.6 Hexandiol	None	50 mM HEPES Sodium Salt	7.0	50 mM Ammonium Chloride	10 mM Magnesium Chloride
A3	G3	35 % w/v 1.6 Hexandiol	None	50 mM Tris-HCl	8.5	75 mM Magnesium Sulfate	None
A4	G4	10 % v/v MPD	None	50 mM Tris-HCl	7.5	50 mM Ammonium Acetate	None
A5	G5	10 % v/v MPD	None	50 mM HEPES Sodium Salt	7.0	80 mM Potassium Chloride	10 mM Magnesium Sulfate
A6	G6	15 % v/v MPD	None	50 mM ADA	6.5	100 mM Sodium Acetate	None
B1	G7	15 % v/v MPD	None	50 mM Sodium Succinate	5.5	10 mM Magnesium Acetate	None
B2	G8	18 % v/v MPD	None	20 mM MES Sodium Salt	5.8	10 mM Magnesium Chloride	None
B3	G9	23 % v/v MPD	None	50 mM MES Sodium Salt	6.0	100 mM Sodium Chloride	None
B4	G10	26 % v/v MPD	None	50 mM PIPES	7.0	65 mM Magnesium Chloride	1 mM Cobalt (III) Hexamine
B5	G11	27 % v/v MPD	None	20 mM MES Sodium Salt	5.8	400 mM Sodium Chloride	120 mM Calcium Chloride
B6	G12	35 % v/v MPD	None	20 mM Bis-Tris	6.0	50 mM Sodium Chloride	10 mM Calcium Chloride
C1	H1	50 % v/v MPD	None	100 mM Sodium Citrate	5.6	10 mM Magnesium Chloride	None
C2	H2	5 % v/v 2-Propanol	None	50 mM Tris-HCl	7.5	10 mM Magnesium Chloride	None
C3	H3	5 % v/v 2-Propanol	None	50 mM MES Sodium Salt	6.5	100 mM Calcium Acetate	None
C4	H4	9 % v/v 2-Propanol	None	50 mM Imidazole	7.2	15 mM Magnesium Acetate	15 mM Magnesium Chloride
C5	H5	10 % v/v 2-Propanol	None	50 mM MES Sodium Salt	6.5	80 mM Ammonium Acetate	None
C6	H6	10 % v/v 2-Propanol	None	50 mM Sodium Succinate	5.5	2 mM Cobalt (II) Chloride	None
D1	H7	13 % v/v 2-Propanol	None	50 mM MOPS	7.0	200 mM Potassium Chloride	6 mM Cobalt (III) Hexamine
D2	H8	15 % v/v 2-Propanol	None	50 mM MES Sodium Salt	6.0	20 mM Magnesium Chloride	None
D3	H9	10 % v/v 1.4-Dioxane	None	50 mM HEPES Sodium Salt	7.5	None	None
D4	H10	10 % v/v Ethanol	None	50 mM MES Sodium Salt	6.5	20 mM Magnesium Chloride	1 mM Cobalt (II) Chloride
D5	H11	20 % v/v Ethylen Glycol	5 % w/v PEG 3350	None		20 mM Magnesium Chloride	None
D6	H12	15 % v/v Glycerol	None	100 mM Sodium Acetate	4.6	200 mM Sodium Chloride	None



JBScreen PEG/Salt

PEG/Salt 1		Precipitant	Salt	PEG/Salt 2		Precipitant	Salt
bulk	HTS			bulk	HTS		
A 1	A 1	20% w/v PEG 3350	200 mM Ammonium Acetate	A 1	C 1	20% w/v PEG 3350	200 mM Potassium Acetate
A 2	A 2	20% w/v PEG 3350	200 mM Ammonium Chloride	A 2	C 2	20% w/v PEG 3350	200 mM Potassium Chloride
A 3	A 3	20% w/v PEG 3350	200 mM Ammonium Fluoride	A 3	C 3	20% w/v PEG 3350	200 mM Potassium Fluoride
A 4	A 4	20% w/v PEG 3350	200 mM Ammonium Formate	A 4	C 4	20% w/v PEG 3350	200 mM Potassium Iodide
A 5	A 5	20% w/v PEG 3350	200 mM Ammonium Iodide	A 5	C 5	20% w/v PEG 3350	200 mM Potassium Nitrate
A 6	A 6	20% w/v PEG 3350	200 mM Ammonium Nitrate	A 6	C 6	20% w/v PEG 3350	200 mM Potassium dihydrogen Phosphate
B 1	A 7	20% w/v PEG 3350	200 mM Ammonium dihydrogen Phosphate	B 1	C 7	20% w/v PEG 3350	200 mM di-Potassium hydrogen Phosphate
B 2	A 8	20% w/v PEG 3350	200 mM di-Ammonium hydrogen Phosphate	B 2	C 8	20% w/v PEG 3350	200 mM Potassium Sulfate
B 3	A 9	20% w/v PEG 3350	200 mM Ammonium Sulfate	B 3	C 9	20% w/v PEG 3350	200 mM Potassium Thiocyanate
B 4	A 10	20% w/v PEG 3350	200 mM Ammonium Sulfito	B 4	C 10	20% w/v PEG 3350	200 mM Potassium / Sodium Tartrate
B 5	A 11	20% w/v PEG 3350	200 mM Calcium Acetate	B 5	C 11	20% w/v PEG 3350	200 mM Sodium Acetate
B 6	A 12	20% w/v PEG 3350	200 mM Calcium Chloride	B 6	C 12	20% w/v PEG 3350	200 mM Sodium Chloride
C 1	B 1	20% w/v PEG 3350	200 mM di-Ammonium Tartrate	C 1	D 1	20% w/v PEG 3350	200 mM Sodium Citrate
C 2	B 2	20% w/v PEG 3350	200 mM Potassium Formate	C 2	D 2	20% w/v PEG 3350	200 mM Sodium Fluoride
C 3	B 3	20% w/v PEG 3350	200 mM Lithium Acetate	C 3	D 3	20% w/v PEG 3350	200 mM Sodium Formate
C 4	B 4	20% w/v PEG 3350	200 mM Lithium Chloride	C 4	D 4	20% w/v PEG 3350	200 mM Sodium Iodide
C 5	B 5	20% w/v PEG 3350	200 mM Lithium Citrate	C 5	D 5	20% w/v PEG 3350	200 mM Sodium Isothiocyanate
C 6	B 6	20% w/v PEG 3350	200 mM Lithium Nitrate	C 6	D 6	20% w/v PEG 3350	200 mM Sodium Nitrate
D 1	B 7	20% w/v PEG 3350	200 mM Lithium Sulfate	D 1	D 7	20% w/v PEG 3350	200 mM Sodium dihydrogen Phosphate
D 2	B 8	20% w/v PEG 3350	200 mM Magnesium Acetate	D 2	D 8	20% w/v PEG 3350	200 mM di-Sodium hydrogen Phosphate
D 3	B 9	20% w/v PEG 3350	200 mM Magnesium Chloride	D 3	D 9	20% w/v PEG 3350	200 mM Sodium Sulfate
D 4	B 10	20% w/v PEG 3350	200 mM Magnesium Formate	D 4	D 10	20% w/v PEG 3350	200 mM di-Sodium Tartrate
D 5	B 11	20% w/v PEG 3350	200 mM Magnesium Nitrate	D 5	D 11	20% w/v PEG 3350	200 mM tri-Potassium Citrate
D 6	B 12	20% w/v PEG 3350	200 mM Magnesium Sulfate	D 6	D 12	20% w/v PEG 3350	200 mM Zinc Acetate

PEG/Salt 3		Precipitant	Salt	PEG/Salt 4		Precipitant	Salt
bulk	HTS			bulk	HTS		
A 1	E 1	20% w/v PEG 5000 MME	200 mM Ammonium Acetate	A 1	G 1	20% w/v PEG 5000 MME	200 mM Potassium Acetate
A 2	E 2	20% w/v PEG 5000 MME	200 mM Ammonium Chloride	A 2	G 2	20% w/v PEG 5000 MME	200 mM Potassium Chloride
A 3	E 3	20% w/v PEG 5000 MME	200 mM Ammonium Fluoride	A 3	G 3	20% w/v PEG 5000 MME	200 mM Potassium Fluoride
A 4	E 4	20% w/v PEG 5000 MME	200 mM Ammonium Formate	A 4	G 4	20% w/v PEG 5000 MME	200 mM Potassium Iodide
A 5	E 5	20% w/v PEG 5000 MME	200 mM Ammonium Iodide	A 5	G 5	20% w/v PEG 5000 MME	200 mM Potassium Nitrate
A 6	E 6	20% w/v PEG 5000 MME	200 mM Ammonium Nitrate	A 6	G 6	20% w/v PEG 5000 MME	200 mM Potassium dihydrogen Phosphate
B 1	E 7	20% w/v PEG 5000 MME	200 mM Ammonium dihydrogen Phosphate	B 1	G 7	20% w/v PEG 5000 MME	200 mM di-Potassium hydrogen Phosphate
B 2	E 8	20% w/v PEG 5000 MME	200 mM di-Ammonium hydrogen Phosphate	B 2	G 8	20% w/v PEG 5000 MME	200 mM Potassium Sulfate
B 3	E 9	20% w/v PEG 5000 MME	200 mM Ammonium Sulfate	B 3	G 9	20% w/v PEG 5000 MME	200 mM Potassium Thiocyanate
B 4	E 10	20% w/v PEG 5000 MME	200 mM Ammonium Sulfito	B 4	G 10	20% w/v PEG 5000 MME	200 mM Potassium / Sodium Tartrate
B 5	E 11	20% w/v PEG 5000 MME	200 mM Calcium Acetate	B 5	G 11	20% w/v PEG 5000 MME	200 mM Sodium Acetate
B 6	E 12	20% w/v PEG 5000 MME	200 mM Calcium Chloride	B 6	G 12	20% w/v PEG 5000 MME	200 mM Sodium Chloride
C 1	F 1	20% w/v PEG 5000 MME	200 mM di-Ammonium Tartrate	C 1	H 1	20% w/v PEG 5000 MME	200 mM Sodium Citrate
C 2	F 2	20% w/v PEG 5000 MME	200 mM Potassium Formate	C 2	H 2	20% w/v PEG 5000 MME	200 mM Sodium Fluoride
C 3	F 3	20% w/v PEG 5000 MME	200 mM Lithium Acetate	C 3	H 3	20% w/v PEG 5000 MME	200 mM Sodium Formate
C 4	F 4	20% w/v PEG 5000 MME	200 mM Lithium Chloride	C 4	H 4	20% w/v PEG 5000 MME	200 mM Sodium Iodide
C 5	F 5	20% w/v PEG 5000 MME	200 mM Lithium Citrate	C 5	H 5	20% w/v PEG 5000 MME	200 mM Sodium Isothiocyanate
C 6	F 6	20% w/v PEG 5000 MME	200 mM Lithium Nitrate	C 6	H 6	20% w/v PEG 5000 MME	200 mM Sodium Nitrate
D 1	F 7	20% w/v PEG 5000 MME	200 mM Lithium Sulfate	D 1	H 7	20% w/v PEG 5000 MME	200 mM Sodium dihydrogen Phosphate
D 2	F 8	20% w/v PEG 5000 MME	200 mM Magnesium Acetate	D 2	H 8	20% w/v PEG 5000 MME	200 mM di-Sodium hydrogen Phosphate
D 3	F 9	20% w/v PEG 5000 MME	200 mM Magnesium Chloride	D 3	H 9	20% w/v PEG 5000 MME	200 mM Sodium Sulfate
D 4	F 10	20% w/v PEG 5000 MME	200 mM Magnesium Formate	D 4	H 10	20% w/v PEG 5000 MME	200 mM di-Sodium Tartrate
D 5	F 11	20% w/v PEG 5000 MME	200 mM Magnesium Nitrate	D 5	H 11	20% w/v PEG 5000 MME	200 mM tri-Potassium Citrate
D 6	F 12	20% w/v PEG 5000 MME	200 mM Magnesium Sulfate	D 6	H 12	20% w/v PEG 5000 MME	200 mM Zinc Acetate



JBScreen Pentaerythritol

Pentaerythritol 1		Precipitant	Buffer	pH	Additive
bulk	HTS				
A 1	A 1	25 % w/v PEP 426	100 mM Sodium Acetate	4.6	None
A 2	A 2	35 % w/v PEP 426	100 mM Sodium Acetate	4.6	None
A 3	A 3	45 % w/v PEP 426	100 mM Sodium Acetate	4.6	None
A 4	A 4	25 % w/v PEP 426	100 mM MES	6.5	None
A 5	A 5	35 % w/v PEP 426	100 mM MES	6.5	None
A 6	A 6	45 % w/v PEP 426	100 mM MES	6.5	None
B 1	A 7	25 % w/v PEP 426	100 mM HEPES	7.5	None
B 2	A 8	35 % w/v PEP 426	100 mM HEPES	7.5	None
B 3	A 9	45 % w/v PEP 426	100 mM HEPES	7.5	None
B 4	A 10	25 % w/v PEP 426	100 mM Tris	8.5	None
B 5	A 11	35 % w/v PEP 426	100 mM Tris	8.5	None
B 6	A 12	45 % w/v PEP 426	100 mM Tris	8.5	None
C 1	B 1	25 % w/v PEP 426	100 mM Sodium Acetate	4.6	50 mM Magnesium Chloride
C 2	B 2	35 % w/v PEP 426	100 mM Sodium Acetate	4.6	200 mM Ammonium Sulfate
C 3	B 3	45 % w/v PEP 426	100 mM Sodium Acetate	4.6	400 mM Potassium Chloride
C 4	B 4	25 % w/v PEP 426	100 mM MES	6.5	50 mM Magnesium Chloride
C 5	B 5	35 % w/v PEP 426	100 mM MES	6.5	200 mM Ammonium Sulfate
C 6	B 6	45 % w/v PEP 426	100 mM MES	6.5	400 mM Potassium Chloride
D 1	B 7	25 % w/v PEP 426	100 mM HEPES	7.5	50 mM Magnesium Chloride
D 2	B 8	35 % w/v PEP 426	100 mM HEPES	7.5	200 mM Ammonium Sulfate
D 3	B 9	45 % w/v PEP 426	100 mM HEPES	7.5	400 mM Potassium Chloride
D 4	B 10	25 % w/v PEP 426	100 mM Tris	8.5	50 mM Magnesium Chloride
D 5	B 11	35 % w/v PEP 426	100 mM Tris	8.5	200 mM Ammonium Sulfate
D 6	B 12	45 % w/v PEP 426	100 mM Tris	8.5	400 mM Potassium Chloride

Pentaerythritol 2		Precipitant	Buffer	pH	Additive
bulk	HTS				
A 1	C 1	25 % w/v PEP 629	100 mM Sodium Acetate	4.6	None
A 2	C 2	35 % w/v PEP 629	100 mM Sodium Acetate	4.6	None
A 3	C 3	45 % w/v PEP 629	100 mM Sodium Acetate	4.6	None
A 4	C 4	25 % w/v PEP 629	100 mM MES	6.5	None
A 5	C 5	35 % w/v PEP 629	100 mM MES	6.5	None
A 6	C 6	45 % w/v PEP 629	100 mM MES	6.5	None
B 1	C 7	25 % w/v PEP 629	100 mM HEPES	7.5	None
B 2	C 8	35 % w/v PEP 629	100 mM HEPES	7.5	None
B 3	C 9	45 % w/v PEP 629	100 mM HEPES	7.5	None
B 4	C 10	25 % w/v PEP 629	100 mM Tris	8.5	None
B 5	C 11	35 % w/v PEP 629	100 mM Tris	8.5	None
B 6	C 12	45 % w/v PEP 629	100 mM Tris	8.5	None
C 1	D 1	25 % w/v PEP 629	100 mM Sodium Acetate	4.6	50 mM Magnesium Chloride
C 2	D 2	35 % w/v PEP 629	100 mM Sodium Acetate	4.6	200 mM Ammonium Sulfate
C 3	D 3	45 % w/v PEP 629	100 mM Sodium Acetate	4.6	300 mM Potassium Chloride
C 4	D 4	25 % w/v PEP 629	100 mM MES	6.5	50 mM Magnesium Chloride
C 5	D 5	35 % w/v PEP 629	100 mM MES	6.5	200 mM Ammonium Sulfate
C 6	D 6	45 % w/v PEP 629	100 mM MES	6.5	300 mM Potassium Chloride
D 1	D 7	25 % w/v PEP 629	100 mM HEPES	7.5	50 mM Magnesium Chloride
D 2	D 8	35 % w/v PEP 629	100 mM HEPES	7.5	200 mM Ammonium Sulfate
D 3	D 9	45 % w/v PEP 629	100 mM HEPES	7.5	300 mM Potassium Chloride
D 4	D 10	25 % w/v PEP 629	100 mM Tris	8.5	50 mM Magnesium Chloride
D 5	D 11	35 % w/v PEP 629	100 mM Tris	8.5	200 mM Ammonium Sulfate
D 6	D 12	45 % w/v PEP 629	100 mM Tris	8.5	300 mM Potassium Chloride



Pentaerythritol 3		Precipitant	Buffer	pH	Additive
bulk	HTS				
A 1	E 1	25 % w/v PEE 270	100 mM Sodium Acetate	4.6	None
A 2	E 2	35 % w/v PEE 270	100 mM Sodium Acetate	4.6	None
A 3	E 3	45 % w/v PEE 270	100 mM Sodium Acetate	4.6	None
A 4	E 4	25 % w/v PEE 270	100 mM MES	6.5	None
A 5	E 5	35 % w/v PEE 270	100 mM MES	6.5	None
A 6	E 6	45 % w/v PEE 270	100 mM MES	6.5	None
B 1	E 7	25 % w/v PEE 270	100 mM HEPES	7.5	None
B 2	E 8	35 % w/v PEE 270	100 mM HEPES	7.5	None
B 3	E 9	45 % w/v PEE 270	100 mM HEPES	7.5	None
B 4	E 10	25 % w/v PEE 270	100 mM Tris	8.5	None
B 5	E 11	35 % w/v PEE 270	100 mM Tris	8.5	None
B 6	E 12	45 % w/v PEE 270	100 mM Tris	8.5	None
C 1	F 1	25 % w/v PEE 270	100 mM Sodium Acetate	4.6	50 mM Magnesium Chloride
C 2	F 2	35 % w/v PEE 270	100 mM Sodium Acetate	4.6	200 mM Ammonium Sulfate
C 3	F 3	45 % w/v PEE 270	100 mM Sodium Acetate	4.6	400 mM Potassium Chloride
C 4	F 4	25 % w/v PEE 270	100 mM MES	6.5	50 mM Magnesium Chloride
C 5	F 5	35 % w/v PEE 270	100 mM MES	6.5	200 mM Ammonium Sulfate
C 6	F 6	45 % w/v PEE 270	100 mM MES	6.5	400 mM Potassium Chloride
D 1	F 7	25 % w/v PEE 270	100 mM HEPES	7.5	50 mM Magnesium Chloride
D 2	F 8	35 % w/v PEE 270	100 mM HEPES	7.5	200 mM Ammonium Sulfate
D 3	F 9	45 % w/v PEE 270	100 mM HEPES	7.5	400 mM Potassium Chloride
D 4	F 10	25 % w/v PEE 270	100 mM Tris	8.5	50 mM Magnesium Chloride
D 5	F 11	35 % w/v PEE 270	100 mM Tris	8.5	200 mM Ammonium Sulfate
D 6	F 12	45 % w/v PEE 270	100 mM Tris	8.5	400 mM Potassium Chloride

Pentaerythritol 4		Precipitant	Buffer	pH	Additive
bulk	HTS				
A 1	G 1	25 % w/v PEE 797	100 mM Sodium Acetate	4.6	None
A 2	G 2	35 % w/v PEE 797	100 mM Sodium Acetate	4.6	None
A 3	G 3	45 % w/v PEE 797	100 mM Sodium Acetate	4.6	None
A 4	G 4	25 % w/v PEE 797	100 mM MES	6.5	None
A 5	G 5	35 % w/v PEE 797	100 mM MES	6.5	None
A 6	G 6	45 % w/v PEE 797	100 mM MES	6.5	None
B 1	G 7	25 % w/v PEE 797	100 mM HEPES	7.5	None
B 2	G 8	35 % w/v PEE 797	100 mM HEPES	7.5	None
B 3	G 9	45 % w/v PEE 797	100 mM HEPES	7.5	None
B 4	G 10	25 % w/v PEE 797	100 mM Tris	8.5	None
B 5	G 11	35 % w/v PEE 797	100 mM Tris	8.5	None
B 6	G 12	45 % w/v PEE 797	100 mM Tris	8.5	None
C 1	H 1	25 % w/v PEE 797	100 mM Sodium Acetate	4.6	50 mM Magnesium Chloride
C 2	H 2	35 % w/v PEE 797	100 mM Sodium Acetate	4.6	200 mM Ammonium Sulfate
C 3	H 3	45 % w/v PEE 797	100 mM Sodium Acetate	4.6	400 mM Potassium Chloride
C 4	H 4	25 % w/v PEE 797	100 mM MES	6.5	50 mM Magnesium Chloride
C 5	H 5	35 % w/v PEE 797	100 mM MES	6.5	200 mM Ammonium Sulfate
C 6	H 6	45 % w/v PEE 797	100 mM MES	6.5	400 mM Potassium Chloride
D 1	H 7	25 % w/v PEE 797	100 mM HEPES	7.5	50 mM Magnesium Chloride
D 2	H 8	35 % w/v PEE 797	100 mM HEPES	7.5	200 mM Ammonium Sulfate
D 3	H 9	45 % w/v PEE 797	100 mM HEPES	7.5	400 mM Potassium Chloride
D 4	H 10	25 % w/v PEE 797	100 mM Tris	8.5	50 mM Magnesium Chloride
D 5	H 11	35 % w/v PEE 797	100 mM Tris	8.5	200 mM Ammonium Sulfate
D 6	H 12	45 % w/v PEE 797	100 mM Tris	8.5	400 mM Potassium Chloride



JBScreen Cryo

Cryo 1		Cryoprotectant 1	Cryoprotectant 2	Cryoprotectant 3	Buffer	pH	Additive 1	Additive 2
bulk	HTS							
A 1	A 1	2.8% v/v Glycerol	32% w/v PEG 8000	None	100 mM Tris-HCl	8.5	200 mM Cesium Chloride	None
A 2	A 2	5.0% v/v Glycerol	None	None	100 mM Sodium Citrate	5.6	3.2 M Sodium Formate	None
A 3	A 3	5.0% v/v Glycerol	20% w/v PEG 4000	None	None		None	None
A 4	A 4	10% v/v Glycerol	15% w/v PEG 5000 MME	10% w/v Xylitol	None		None	None
A 5	A 5	10% v/v Glycerol	28% w/v PEG 8000	None	50 mM MES Sodium Salt	6.5	100 mM Ammonium Acetate	None
A 6	A 6	10% v/v Glycerol	25% w/v PEG 4000	4.5% v/v 2-Propanol	18 mM MES Sodium Salt	6.5	None	None
B 1	A 7	10% v/v Glycerol	20% v/v PEG 400	10% w/v PEG 8000	50 mM Tris-HCl	8.5	100 mM Sodium Chloride	None
B 2	A 8	10% v/v Glycerol	15% w/v PEG 6000	None	100 mM MES Sodium Salt	6.5	1.0 M Lithium Chloride	None
B 3	A 9	15% v/v Glycerol	15% w/v PEG 5000 MME	None	None		None	None
B 4	A 10	15% v/v Glycerol	20% w/v PEG 6000	None	100 mM MES Sodium Salt	6.5	None	None
B 5	A 11	15% v/v Glycerol	30% w/v PEG 8000	None	100 mM MES Sodium Salt	6.5	200 mM Sodium Acetate	None
B 6	A 12	15% v/v Glycerol	None	None	100 mM Tris-HCl	8.5	2.5 M Sodium Chloride	200 mM Lithium Sulfate
C 1	B 1	15% v/v Glycerol	15% w/v PEG 20000	None	None		None	None
C 2	B 2	15% v/v Glycerol	35% w/v PEG 4000	None	100 mM Tris-Acetate	8.0	100 mM Sodium Citrate	None
C 3	B 3	15% v/v Glycerol	15% w/v PEG 8000	None	None		500 mM Lithium Sulfate	None
C 4	B 4	20% v/v Glycerol	16% v/v Ethylene Glycol	20% w/v PEG 6000	30 mM Tris-HCl	8.5	100 mM Sodium Acetate	None
C 5	B 5	20% v/v Glycerol	None	None	None		2.0 M Ammonium Sulfate	None
C 6	B 6	20% v/v Glycerol	20% w/v PEG 4000	10% v/v 2-Propanol	50 mM Sodium Acetate	4.6	100 mM Sodium Chloride	None
D 1	B 7	20% v/v Glycerol	None	None	100 mM MES Sodium Salt	6.5	2.5 M Ammonium Sulfate	None
D 2	B 8	20% v/v Glycerol	15% w/v PEG 8000	None	100 mM MES Sodium Salt	6.5	160 mM Zinc Acetate	None
D 3	B 9	20% v/v Glycerol	15% w/v PEG 8000	None	80 mM Tris-HCl	8.5	920 mM Sodium Chloride	None
D 4	B 10	20% v/v Glycerol	6% v/v 2-Propanol	None	None		1.8 M Ammonium Sulfate	None
D 5	B 11	20% v/v Glycerol	None	None	100 mM MES Sodium Salt	6.5	1.8 M Ammonium Sulfate	None
D 6	B 12	20% v/v Glycerol	20% w/v PEG 6000	None	100 mM MES Sodium Salt	6.5	None	None

Cryo 2		Cryoprotectant 1	Cryoprotectant 2	Cryoprotectant 3	Buffer	pH	Additive 1	Additive 2
bulk	HTS							
A 1	C 1	20% v/v Glycerol	16% w/v PEG 8000	None	80 mM MES Sodium Salt	6.5	160 mM Magnesium Acetate	None
A 2	C 2	20% v/v Glycerol	7% w/v PEG 8000	None	100 mM MES Sodium Salt	6.5	None	None
A 3	C 3	24% v/v Glycerol	None	None	None		2.3 M Ammonium Sulfate	None
A 4	C 4	25% v/v Glycerol	None	None	None		750 mM Sodium Bromide	None
A 5	C 5	25% v/v Glycerol	None	None	100 mM Sodium Citrate	5.6	1.2 M Ammonium dihydrogen Phosphate	None
A 6	C 6	25% v/v Glycerol	None	None	None		1.5 M Ammonium Sulfate	None
B 1	C 7	25% v/v Glycerol	None	None	100 mM MES Sodium Salt	6.5	2.2 M Ammonium Sulfate	None
B 2	C 8	25% v/v Glycerol	None	None	100 mM Sodium / Potassium Phosphate	6.5	2.5 M Ammonium Sulfate	None
B 3	C 9	30% v/v Glycerol	None	None	None		1.26 M Ammonium dihydrogen Phosphate	None
B 4	C 10	30% v/v Glycerol	None	None	100 mM Sodium Acetate	4.6	2.0 M Ammonium Sulfate	None
B 5	C 11	30% v/v Glycerol	None	None	50 mM MES Sodium Salt	6.5	2.3 M Ammonium Sulfate	None
B 6	C 12	30% v/v Glycerol	None	None	None		2.0 M Ammonium Sulfate	None
C 1	D 1	30% v/v Glycerol	15% w/v PEG 4000	5% v/v 2-Propanol	100 mM HEPES Sodium Salt	7.5	None	None
C 2	D 2	30% v/v Glycerol	20% w/v PEG 4000	20% v/v 2-Propanol	100 mM Tris-HCl	8.5	None	None
C 3	D 3	30% v/v Glycerol	None	None	50 mM MES Sodium Salt	6.5	1.2 M Ammonium Sulfate	None
C 4	D 4	30% v/v Glycerol	15% w/v PEG 6000	None	500 mM Tris-HCl	8.5	None	None
C 5	D 5	30% v/v Glycerol	None	None	None		2.0 M Ammonium Sulfate	None
C 6	D 6	30% v/v Glycerol	30% w/v PEG 1500	None	50 mM MES Sodium Salt	6.5	None	None
D 1	D 7	30% v/v Glycerol	None	None	100 mM Sodium / Potassium Phosphate	6.5	1.0 M Ammonium Sulfate	None
D 2	D 8	30% v/v Glycerol	30% w/v PEG 4000	None	100 mM Sodium Acetate	4.6	None	None
D 3	D 9	30% v/v Glycerol	None	None	100 mM MES Sodium Salt	6.5	1.4 M Sodium Acetate	None
D 4	D 10	30% v/v Glycerol	None	None	150 mM HEPES Sodium Salt	7.5	1.6 M Sodium dihydrogen Phosphate	450 mM di-Potassium hydrogen Phosphate
D 5	D 11	35% v/v Glycerol	None	None	20 mM HEPES Sodium Salt	7.5	None	None
D 6	D 12	35% v/v Glycerol	7% w/v PEG 6000	None	50 mM MES Sodium Salt	6.5	None	None



Cryo 3		Cryoprotectant 1	Cryoprotectant 2	Cryoprotectant 3	Buffer	pH	Additive 1	Additive 2
bulk	HTS							
A 1	E 1	10% v/v PEG 200	24% w/v PEG 3000	None	100 mM Sodium Citrate	5.6	None	None
A 2	E 2	20% v/v PEG 200	20% w/v PEG 4000	10% v/v 2-Propanol	100 mM HEPES Sodium Salt	7.5	None	None
A 3	E 3	30% v/v PEG 200	5% w/v PEG 3000	None	100 mM MES Sodium Salt	6.5	None	None
A 4	E 4	40% v/v PEG 300	5% w/v PEG 1000	None	100 mM Tris-HCl	8.5	None	None
A 5	E 5	20% v/v PEG 400	30% w/v PEG 4000	None	100 mM Sodium Citrate	5.6	50 mM Ammonium Acetate	None
A 6	E 6	30% v/v PEG 400	11% w/v PEG 20000	None	100 mM Potassium Phosphate	8.0	None	None
B 1	E 7	10% v/v PEG 400	20% w/v PEG 5000 MME	None	None		None	None
B 2	E 8	34% v/v PEG 400	None	None	100 mM HEPES Sodium Salt	7.5	100 mM Sodium Chloride	200 mM Calcium Chloride
B 3	E 9	40% v/v PEG 400	5% w/v PEG 3000	None	100 mM MES Sodium Salt	6.5	None	None
B 4	E 10	35% v/v PEG 600	None	None	100 mM PIPES	7.0	100 mM Sodium Chloride	None
B 5	E 11	30% w/v PEG 1000	None	None	100 mM Phosphate / Citrate	4.4	110 mM Lithium Sulfate	None
B 6	E 12	40% w/v PEG 1500	None	None	100 mM ADA	6.0	None	None
C 1	F 1	17% w/v PEG 1500	10% v/v MPD	None	50 mM PIPES	7.0	None	None
C 2	F 2	35% w/v PEG 3350	None	None	None		300 mM Potassium Thiocyanate	None
C 3	F 3	25% w/v PEG 4000	18% v/v MPD	None	100 mM Sodium Acetate	4.6	200 mM Ammonium Sulfate	None
C 4	F 4	25% w/v PEG 4000	30% v/v Ethylene Glycol	None	None		None	None
C 5	F 5	20% w/v PEG 4000	20% v/v MPD	10% v/v 2-Propanol	50 mM Sodium Citrate	5.6	None	None
C 6	F 6	10% w/v PEG 4000	20% v/v Ethylene Glycol	None	55 mM ADA	6.0	105 mM Sodium Chloride	None
D 1	F 7	2% w/v PEG 4000	25% v/v MPD	None	100 mM HEPES Sodium Salt	7.5	None	None
D 2	F 8	20% w/v PEG 8000	20% v/v MPD	None	100 mM HEPES Sodium Salt	7.5	200 mM Rubidium Bromide	None
D 3	F 9	28% w/v PEG 8000	None	None	100 mM Glycine	9.5	10 mM Calcium Chloride	None
D 4	F 10	10% w/v PEG 8000	15% v/v MPD	None	100 mM MES Sodium Salt	6.5	550 mM Ammonium Sulfate	None
D 5	F 11	25% w/v PEG 8000	30% v/v Ethylene Glycol	None	150 mM ADA	6.0	80 mM Ammonium Sulfate	None
D 6	F 12	10% w/v PEG 20000	5.6% v/v Ethylene Glycol	30% v/v 2,3-Butanediol	100 mM HEPES Sodium Salt	7.5	None	None

Cryo 4		Cryoprotectant 1	Buffer	pH	Additive 1
bulk	HTS				
A 1	G 1	20% v/v Ethylene Glycol	100 mM HEPES Sodium Salt	7.5	1.6 M Lithium Sulfate
A 2	G 2	25% v/v Ethylene Glycol	100 mM HEPES Sodium Salt	7.5	200 mM Sodium / Potassium Phosphate
A 3	G 3	25% v/v Ethylene Glycol	100 mM HEPES Sodium Salt	7.5	1.0 M Potassium / Sodium Tartrate
A 4	G 4	40% v/v Ethylene Glycol	100 mM Sodium Acetate	4.6	None
A 5	G 5	40% v/v Ethylene Glycol	100 mM Tris-HCl	8.5	None
A 6	G 6	40% v/v Ethylene Glycol	100 mM Imidazole-HCl	9.0	200 mM Calcium Acetate
B 1	G 7	40% v/v Ethylene Glycol	100 mM MES Sodium Salt	6.5	200 mM Zinc Acetate
B 2	G 8	50% v/v Ethylene Glycol	100 mM Tris-HCl	8.5	200 mM Magnesium Chloride
B 3	G 9	50% v/v Ethylene Glycol	100 mM HEPES Sodium Salt	7.5	200 mM Lithium Sulfate
B 4	G 10	35% v/v 2-Propanol	100 mM Tris-HCl	8.5	None
B 5	G 11	35% v/v 2-Propanol	100 mM Sodium Acetate	4.6	None
B 6	G 12	35% v/v 2-Propanol	100 mM Imidazole-HCl	9.0	200 mM Zinc Acetate
C 1	H 1	40% v/v 1,2-Propanediol	100 mM Imidazole-HCl	9.0	None
C 2	H 2	40% v/v 1,2-Propanediol	100 mM Sodium Acetate	4.6	None
C 3	H 3	40% v/v 1,2-Propanediol	100 mM Sodium Citrate	5.6	200 mM Sodium Chloride
C 4	H 4	40% v/v 1,2-Propanediol	100 mM Sodium Acetate	4.6	50 mM Calcium Acetate
C 5	H 5	35% v/v MPD	100 mM Tris-HCl	8.5	None
C 6	H 6	30% v/v MPD	100 mM Sodium Acetate	4.6	20 mM Calcium Chloride
D 1	H 7	30% v/v MPD	100 mM HEPES Sodium Salt	7.5	200 mM Sodium Citrate
D 2	H 8	30% v/v MPD	100 mM Sodium Citrate	5.6	200 mM Ammonium Acetate
D 3	H 9	35% v/v MPD	100 mM MES Sodium Salt	6.5	200 mM Ammonium Sulfate
D 4	H 10	40% v/v MPD	100 mM Sodium Citrate	5.6	None
D 5	H 11	40% v/v MPD	100 mM MES Sodium Salt	6.5	200 mM Ammonium Sulfate
D 6	H 12	40% v/v MPD	100 mM Imidazole-HCl	9.0	200 mM Magnesium Chloride



JBScreen PACT ++

PACT++ 1		Precipitant 1	Buffer	pH	Salt
bulk	HTS				
A 1	A1	25% w/v PEG 1500	100 mM SPG Buffer	4.0	None
A 2	A2	25% w/v PEG 1500	100 mM SPG Buffer	5.0	None
A 3	A3	25% w/v PEG 1500	100 mM SPG Buffer	6.0	None
A 4	A4	25% w/v PEG 1500	100 mM SPG Buffer	7.0	None
A 5	A5	25% w/v PEG 1500	100 mM SPG Buffer	8.0	None
A 6	A6	25% w/v PEG 1500	100 mM SPG Buffer	9.0	None
B 1	A7	20% w/v PEG 6000	100 mM Sodium Acetate	5.0	200 mM Sodium Chloride
B 2	A8	20% w/v PEG 6000	100 mM Sodium Acetate	5.0	200 mM Ammonium Chloride
B 3	A9	20% w/v PEG 6000	100 mM Sodium Acetate	5.0	200 mM Lithium Chloride
B 4	A10	20% w/v PEG 6000	100 mM Sodium Acetate	5.0	200 mM Magnesium Chloride
B 5	A11	20% w/v PEG 6000	100 mM Sodium Acetate	5.0	200 mM Calcium Chloride
B 6	A12	20% w/v PEG 6000	100 mM Sodium Acetate	5.0	10 mM Zinc Chloride
C 1	B1	25% w/v PEG 1500	100 mM MIB Buffer	4.0	None
C 2	B2	25% w/v PEG 1500	100 mM MIB Buffer	5.0	None
C 3	B3	25% w/v PEG 1500	100 mM MIB Buffer	6.0	None
C 4	B4	25% w/v PEG 1500	100 mM MIB Buffer	7.0	None
C 5	B5	25% w/v PEG 1500	100 mM MIB Buffer	8.0	None
C 6	B6	25% w/v PEG 1500	100 mM MIB Buffer	9.0	None
D 1	B7	20% w/v PEG 6000	100 mM MES Sodium Salt	6.0	200 mM Sodium Chloride
D 2	B8	20% w/v PEG 6000	100 mM MES Sodium Salt	6.0	200 mM Ammonium Chloride
D 3	B9	20% w/v PEG 6000	100 mM MES Sodium Salt	6.0	200 mM Lithium Chloride
D 4	B10	20% w/v PEG 6000	100 mM MES Sodium Salt	6.0	200 mM Magnesium Chloride
D 5	B11	20% w/v PEG 6000	100 mM MES Sodium Salt	6.0	200 mM Calcium Chloride
D 6	B12	20% w/v PEG 6000	100 mM MES Sodium Salt	6.0	10 mM Zinc Chloride

PACT++ 2		Precipitant 1	Buffer	pH	Salt
bulk	HTS				
A 1	C1	25% w/v PEG 1500	100 mM TBG Buffer	4.0	None
A 2	C2	25% w/v PEG 1500	100 mM TBG Buffer	5.0	None
A 3	C3	25% w/v PEG 1500	100 mM TBG Buffer	6.0	None
A 4	C4	25% w/v PEG 1500	100 mM TBG Buffer	7.0	None
A 5	C5	25% w/v PEG 1500	100 mM TBG Buffer	8.0	None
A 6	C6	25% w/v PEG 1500	100 mM TBG Buffer	9.0	None
B 1	C7	20% w/v PEG 6000	100 mM HEPES Sodium Salt	7.0	200 mM Sodium Chloride
B 2	C8	20% w/v PEG 6000	100 mM HEPES Sodium Salt	7.0	200 mM Ammonium Chloride
B 3	C9	20% w/v PEG 6000	100 mM HEPES Sodium Salt	7.0	200 mM Lithium Chloride
B 4	C10	20% w/v PEG 6000	100 mM HEPES Sodium Salt	7.0	200 mM Magnesium Chloride
B 5	C11	20% w/v PEG 6000	100 mM HEPES Sodium Salt	7.0	200 mM Calcium Chloride
B 6	C12	20% w/v PEG 6000	100 mM HEPES Sodium Salt	7.0	10 mM Zinc Chloride
C 1	D1	25% w/v PEG 1500	100 mM MMT Buffer	4.0	None
C 2	D2	25% w/v PEG 1500	100 mM MMT Buffer	5.0	None
C 3	D3	25% w/v PEG 1500	100 mM MMT Buffer	6.0	None
C 4	D4	25% w/v PEG 1500	100 mM MMT Buffer	7.0	None
C 5	D5	25% w/v PEG 1500	100 mM MMT Buffer	8.0	None
C 6	D6	25% w/v PEG 1500	100 mM MMT Buffer	9.0	None
D 1	D7	20% w/v PEG 6000	100 mM Tris HCl	8.0	200 mM Sodium Chloride
D 2	D8	20% w/v PEG 6000	100 mM Tris HCl	8.0	200 mM Ammonium Chloride
D 3	D9	20% w/v PEG 6000	100 mM Tris HCl	8.0	200 mM Lithium Chloride
D 4	D10	20% w/v PEG 6000	100 mM Tris HCl	8.0	200 mM Magnesium Chloride
D 5	D11	20% w/v PEG 6000	100 mM Tris HCl	8.0	200 mM Calcium Chloride
D 6	D12	20% w/v PEG 6000	100 mM Tris HCl	8.0	10 mM Zinc Chloride



PACT++ 3		Precipitant 1	Buffer	pH	Salt
bulk	HTS				
A 1	E1	20% w/v PEG 3350	None		200 mM Sodium Fluoride
A 2	E2	20% w/v PEG 3350	None		200 mM Sodium Bromide
A 3	E3	20% w/v PEG 3350	None		200 mM Sodium Iodide
A 4	E4	20% w/v PEG 3350	None		200 mM Potassium Thiocyanate
A 5	E5	20% w/v PEG 3350	None		200 mM Sodium Nitrate
A 6	E6	20% w/v PEG 3350	None		200 mM Sodium Formate
B 1	E7	20% w/v PEG 3350	None		200 mM Sodium Acetate
B 2	E8	20% w/v PEG 3350	None		200 mM Sodium Sulfate
B 3	E9	20% w/v PEG 3350	None		200 mM Potassium/Sodium Tartrate
B 4	E10	20% w/v PEG 3350	None		200 mM Sodium/Potassium Phosphate
B 5	E11	20% w/v PEG 3350	None		200 mM Sodium Citrate
B 6	E12	20% w/v PEG 3350	None		200 mM Sodium Malonate
C 1	F1	20% w/v PEG 3350	100 mM Bis-Tris Propane	6.5	200 mM Sodium Fluoride
C 2	F2	20% w/v PEG 3350	100 mM Bis-Tris Propane	6.5	200 mM Sodium Bromide
C 3	F3	20% w/v PEG 3350	100 mM Bis-Tris Propane	6.5	200 mM Sodium Iodide
C 4	F4	20% w/v PEG 3350	100 mM Bis-Tris Propane	6.5	200 mM Potassium Thiocyanate
C 5	F5	20% w/v PEG 3350	100 mM Bis-Tris Propane	6.5	200 mM Sodium Nitrate
C 6	F6	20% w/v PEG 3350	100 mM Bis-Tris Propane	6.5	200 mM Sodium Formate
D 1	F7	20% w/v PEG 3350	100 mM Bis-Tris Propane	6.5	200 mM Sodium Acetate
D 2	F8	20% w/v PEG 3350	100 mM Bis-Tris Propane	6.5	200 mM Sodium Sulfate
D 3	F9	20% w/v PEG 3350	100 mM Bis-Tris Propane	6.5	200 mM Potassium/Sodium Tartrate
D 4	F10	20% w/v PEG 3350	100 mM Bis-Tris Propane	6.5	200 mM Sodium/Potassium Phosphate
D 5	F11	20% w/v PEG 3350	100 mM Bis-Tris Propane	6.5	200 mM Sodium Citrate
D 6	F12	20% w/v PEG 3350	100 mM Bis-Tris Propane	6.5	200 mM Sodium Malonate

PACT++ 4		Precipitant 1	Buffer	pH	Salt
bulk	HTS				
A 1	G1	20% w/v PEG 3350	100 mM Bis-Tris Propane	7.5	200 mM Sodium Fluoride
A 2	G2	20% w/v PEG 3350	100 mM Bis-Tris Propane	7.5	200 mM Sodium Bromide
A 3	G3	20% w/v PEG 3350	100 mM Bis-Tris Propane	7.5	200 mM Sodium Iodide
A 4	G4	20% w/v PEG 3350	100 mM Bis-Tris Propane	7.5	200 mM Potassium Thiocyanate
A 5	G5	20% w/v PEG 3350	100 mM Bis-Tris Propane	7.5	200 mM Sodium Nitrate
A 6	G6	20% w/v PEG 3350	100 mM Bis-Tris Propane	7.5	200 mM Sodium Formate
B 1	G7	20% w/v PEG 3350	100 mM Bis-Tris Propane	7.5	200 mM Sodium Acetate
B 2	G8	20% w/v PEG 3350	100 mM Bis-Tris Propane	7.5	200 mM Sodium Sulfate
B 3	G9	20% w/v PEG 3350	100 mM Bis-Tris Propane	7.5	200 mM Potassium/Sodium Tartrate
B 4	G10	20% w/v PEG 3350	100 mM Bis-Tris Propane	7.5	200 mM Sodium/Potassium Phosphate
B 5	G11	20% w/v PEG 3350	100 mM Bis-Tris Propane	7.5	200 mM Sodium Citrate
B 6	G12	20% w/v PEG 3350	100 mM Bis-Tris Propane	7.5	200 mM Sodium Malonate
C 1	H1	20% w/v PEG 3350	100 mM Bis-Tris Propane	8.5	200 mM Sodium Fluoride
C 2	H2	20% w/v PEG 3350	100 mM Bis-Tris Propane	8.5	200 mM Sodium Bromide
C 3	H3	20% w/v PEG 3350	100 mM Bis-Tris Propane	8.5	200 mM Sodium Iodide
C 4	H4	20% w/v PEG 3350	100 mM Bis-Tris Propane	8.5	200 mM Potassium Thiocyanate
C 5	H5	20% w/v PEG 3350	100 mM Bis-Tris Propane	8.5	200 mM Sodium Nitrate
C 6	H6	20% w/v PEG 3350	100 mM Bis-Tris Propane	8.5	200 mM Sodium Formate
D 1	H7	20% w/v PEG 3350	100 mM Bis-Tris Propane	8.5	200 mM Sodium Acetate
D 2	H8	20% w/v PEG 3350	100 mM Bis-Tris Propane	8.5	200 mM Sodium Sulfate
D 3	H9	20% w/v PEG 3350	100 mM Bis-Tris Propane	8.5	200 mM Potassium/Sodium Tartrate
D 4	H10	20% w/v PEG 3350	100 mM Bis-Tris Propane	8.5	200 mM Sodium/Potassium Phosphate
D 5	H11	20% w/v PEG 3350	100 mM Bis-Tris Propane	8.5	200 mM Sodium Citrate
D 6	H12	20% w/v PEG 3350	100 mM Bis-Tris Propane	8.5	200 mM Sodium Malonate



JBScreen JCSG ++

JCSG++ 1		Precipitant 1	Precipitant 2	Buffer	pH	Salt	pH
bulk	HTS						
A 1	A1	50% v/v PEG 400	None	100 mM Sodium Acetate	4.5	200 mM Lithium Sulfate	
A 2	A2	20% w/v PEG 3000	None	100 mM Sodium Citrate	5.5	None	
A 3	A3	20% w/v PEG 3350	None	None		200 mM di-Ammonium hydrogen Citrate	5.0
A 4	A4	30% v/v MPD	None	100 mM Sodium Acetate	4.6	20 mM Calcium Chloride	
A 5	A5	20% w/v PEG 3350	None	None		200 mM Magnesium Formate	5.9
A 6	A6	20% w/v PEG 1000	None	100 mM Phosphate / Citrate	4.2	200 mM Lithium Sulfate	
B 1	A7	20% w/v PEG 8000	None	100 mM CHES	9.5	None	
B 2	A8	20% w/v PEG 3350	None	None		200 mM Ammonium Formate	6.6
B 3	A9	20% w/v PEG 3350	None	None		200 mM Ammonium Chloride	6.3
B 4	A10	20% w/v PEG 3350	None	None		200 mM Potassium Formate	7.3
B 5	A11	50% v/v MPD	None	100 mM Tris-HCl	8.5	200 mM Ammonium dihydrogen Phosphate	
B 6	A12	20% w/v PEG 3350	None	None		200 mM Potassium Nitrate	6.9
C 1	B1	None	None	100 mM Citric Acid	4.0	800 mM Ammonium Sulfate	
C 2	B2	20% w/v PEG 3550	None	None		200 mM Sodium Thiocyanate	6.9
C 3	B3	20% w/v PEG 6000	None	100 mM Bicine	9.0	None	
C 4	B4	10% w/v PEG 8000	8% v/v Ethylene Glycol	100 mM HEPES Sodium Salt	7.5	None	
C 5	B5	40% v/v MPD	5% w/v PEG 8000	100 mM MES Sodium Salt	6.5	None	
C 6	B6	40% v/v Ethanol	5% w/v PEG 1000	100 mM Phosphate / Citrate	4.2	None	
D 1	B7	8% w/v PEG 4000	None	100 mM Sodium Acetate	4.6	None	
D 2	B8	10% w/v PEG 8000	None	100 mM Tris-HCl	7.0	200 mM Magnesium Chloride	
D 3	B9	20% w/v PEG 6000	None	100 mM Citric Acid	5.0	None	
D 4	B10	50% v/v PEG 200	None	100 mM MES Sodium Salt	6.5	200 mM Magnesium Chloride	
D 5	B11	None	None	None		1.6 M Sodium Citrate	
D 6	B12	20% w/v PEG 3350	None	None		200 mM Potassium Citrate	8.3

JCSG++ 2		Precipitant 1	Precipitant 2	Buffer	pH	Salt	pH
bulk	HTS						
A 1	C1	20% w/v PEG 8000	None	100 mM Phosphate / Citrate	4.2	200 mM Sodium Chloride	
A 2	C2	20% w/v PEG 6000	None	100 mM Citric Acid	4.0	1.0 M Lithium Chloride	
A 3	C3	20% w/v PEG 3350	None	None		200 mM Ammonium Nitrate	6.3
A 4	C4	10% w/v PEG 6000	None	100 mM HEPES Sodium Salt	7.0	None	
A 5	C5	800 mM Sodium dihydrogen Phosphate	800 mM Potassium dihydrogen Phosphate	100 mM HEPES Sodium Salt	7.5	None	
A 6	C6	40% v/v PEG 300	None	100 mM Phosphate / Citrate	4.2	None	
B 1	C7	10% w/v PEG 3000	None	100 mM Sodium Acetate	4.5	200 mM Zinc Acetate	
B 2	C8	20% v/v Ethanol	None	100 mM Tris-HCl	8.5	None	
B 3	C9	25% v/v 1,2-Propanediol	10% v/v Glycerol	100 mM Sodium / Potassium Phosphate	6.2	None	
B 4	C10	10% w/v PEG 20000	2% v/v 1,4-Dioxane	100 mM Bicine	9.0	None	
B 5	C11	None	None	100 mM Sodium Acetate	4.6	2.0 M Ammonium Sulfate	
B 6	C12	10% w/v PEG 1000	10% w/v PEG 8000	None		None	
C 1	D1	24% w/v PEG 1500	20% v/v Glycerol	None		None	
C 2	D2	30% v/v PEG 400	None	100 mM HEPES Sodium Salt	7.5	200 mM Magnesium Chloride	
C 3	D3	50% v/v PEG 200	None	100 mM Sodium / Potassium Phosphate	6.2	200 mM Sodium Chloride	
C 4	D4	30% w/v PEG 8000	None	100 mM Sodium Acetate	4.5	200 mM Lithium Sulfate	
C 5	D5	70% v/v MPD	None	100 mM HEPES Sodium Salt	7.5	None	
C 6	D6	20% w/v PEG 8000	None	100 mM Tris-HCl	8.5	200 mM Magnesium Chloride	
D 1	D7	40% v/v PEG 400	None	100 mM Tris-HCl	8.5	200 mM Lithium Sulfate	
D 2	D8	40% v/v MPD	None	100 mM Tris-HCl	8.0	None	
D 3	D9	25.5% w/v PEG 4000	15% v/v Glycerol	None		170 mM Ammonium Sulfate	
D 4	D10	40% v/v PEG 300	None	100 mM MES Sodium Salt	6.5	200 mM Calcium Acetate	
D 5	D11	14% v/v 2-Propanol	30% v/v Glycerol	70 mM Sodium Acetate	4.6	140 mM Calcium Chloride	
D 6	D12	16% w/v PEG 8000	20% v/v Glycerol	None		40 mM Potassium dihydrogen Phosphate	



JCSG++ 3		Precipitant 1		Precipitant 2		Buffer		pH	Salt		pH
bulk	HTS										
A 1	E1	None		None		100 mM MES Sodium Salt		6.5	1.0 M Sodium Citrate		
A 2	E2	2.0 M Ammonium Sulfate		None		100 mM MES Sodium Salt		6.5	200 mM Sodium Chloride		
A 3	E3	10% v/v 2-Propanol		None		100 mM HEPES Sodium Salt		7.5	200 mM Sodium Chloride		
A 4	E4	1.26 M Ammonium Sulfate		None		100 mM Tris-HCl		8.5	200 mM Lithium Sulfate		
A 5	E5	40% v/v MPD		None		100 mM CAPS		10.5	None		
A 6	E6	20% w/v PEG 3000		None		100 mM Imidazole-HCl		8.0	200 mM Zinc Acetate		
B 1	E7	10% v/v 2-Propanol		None		100 mM MES Sodium Salt		6.5	200 mM Zinc Acetate		
B 2	E8	None		None		100 mM Sodium Acetate		4.5	1.0 M di-Ammonium hydrogen Phosphate		
B 3	E9	None		None		100 mM MES Sodium Salt		6.5	1.6 M Magnesium Sulfate		
B 4	E10	10% w/v PEG 6000		None		100 mM Bicine		9.0	None		
B 5	E11	14.4% w/v PEG 8000		20% v/v Glycerol		80 mM MES Sodium Salt		6.5	160 mM Calcium Acetate		
B 6	E12	10% w/v PEG 8000		None		100 mM Imidazole-HCl		8.0	None		
C 1	F1	30% v/v Jeffamine M-600		None		100 mM MES Sodium Salt		6.5	50 mM Cesium Chloride		
C 2	F2	None		None		100 mM Citric Acid		5.0	3.15 M Ammonium Sulfate		
C 3	F3	20% v/v MPD		None		100 mM Tris-HCl		8.0	None		
C 4	F4	20% v/v Jeffamine M-600		None		100 mM HEPES Sodium Salt		7.5	None		
C 5	F5	50% v/v Ethylene Glycol		None		100 mM Tris-HCl		8.5	200 mM Magnesium Chloride		
C 6	F6	10% v/v MPD		None		100 mM Bicine		9.0	None		
D 1	F7	None		None		None			800 mM Succinic Acid		7.0
D 2	F8	None		None		None			2.1 M D,L-Malic Acid		7.0
D 3	F9	None		None		None			2.4 M Sodium Malonate		7.0
D 4	F10	0.5% w/v Jeffamine ED-2001 pH 7.0		None		100 mM HEPES Sodium Salt		7.0	1.1 M Sodium Malonate		7.0
D 5	F11	1%w/v PEG 2000 MME		None		100 mM HEPES Sodium Salt		7.0	1.0 M Succinic Acid		7.0
D 6	F12	30 %v/v Jeffamine M-600 pH 7.0		None		100 mM HEPES Sodium Salt		7.0	None		

JCSG++ 4		Precipitant 1		Buffer		pH	Salt		pH
bulk	HTS								
A 1	G1	30% w/v Jeffamine ED-2001 pH 7.0		100 mM HEPES Sodium Salt		7.0	None		
A 2	G2	22% w/v Polyacrylic Acid 5100 Sodium Salt		100 mM HEPES Sodium Salt		7.5	200 mM Magnesium Chloride		
A 3	G3	20% w/v Polyvinylpyrrolidone K 15		100 mM Tris-HCl		8.5	100 mM Cobalt Chloride		
A 4	G4	20% w/v PEG 2000 MME		100 mM Tris-HCl		8.5	200 mM Trimethylamine N-oxide		
A 5	G5	12% w/v PEG 3350		100 mM HEPES Sodium Salt		7.5	5 mM Cobalt Chloride, 5 mM Cadmium Chloride, 5 mM Magnesium Chloride, 5 mM Nickel Chloride		
A 6	G6	20% w/v PEG 3350		None			200 mM Sodium Malonate		7.0
B 1	G7	15% w/v PEG 3350		None			100 mM Succinic Acid		7.0
B 2	G8	20% w/v PEG 3350		None			150 mM D,L-Malic Acid		7.0
B 3	G9	30% w/v PEG 2000 MME		None			100 mM Potassium Thiocyanate		
B 4	G10	30% w/v PEG 2000 MME		None			150 mM Potassium Bromide		
B 5	G11	None		100 mM Bis-Tris		5.5	2.0 M Ammonium Sulfate		
B 6	G12	None		100 mM Bis-Tris		5.5	3.0 M Sodium Chloride		
C 1	H1	None		100 mM Bis-Tris		5.5	300 mM Magnesium Formate		
C 2	H2	1% w/v PEG 3550		100 mM Bis-Tris		5.5	1.0 M Ammonium Sulfate		
C 3	H3	25% w/v PEG 3350		100 mM Bis-Tris		5.5	None		
C 4	H4	45% v/v MPD		100 mM Bis-Tris		5.5	200 mM Calcium Chloride		
C 5	H5	45% v/v MPD		100 mM Bis-Tris		5.5	200 mM Ammonium Acetate		
C 6	H6	17% w/v PEG 10000		100 mM Bis-Tris		5.5	100 mM Ammonium Acetate		
D 1	H7	25% w/v PEG 3350		100 mM Bis-Tris		5.5	200 mM Ammonium Sulfate		
D 2	H8	25% w/v PEG 3350		100 mM Bis-Tris		5.5	200 mM Sodium Chloride		
D 3	H9	25% w/v PEG 3350		100 mM Bis-Tris		5.5	200 mM Lithium Sulfate		
D 4	H10	25% w/v PEG 3350		100 mM Bis-Tris		5.5	200 mM Ammonium Acetate		
D 5	H11	25% w/v PEG 3350		100 mM Bis-Tris		5.5	200 mM Magnesium Chloride		
D 6	H12	45% v/v MPD		100 mM HEPES		7.5	200 mM Ammonium Acetate		



JBS Optimization Screens and Reagents

JBS Solubility Kit

Buffer Kit		
No.	Buffer	pH
1	Glycine	3.0
2	Citric Acid	3.2
3	PIPPS	3.7
4	Citric Acid	4.0
5	Sodium Acetate	4.5
6	Sodium / Potassium Phosphate	5.0
7	Sodium Citrate	5.5
8	Sodium / Potassium Phosphate	6.0
9	Bis-Tris	6.0
10	MES	6.2
11	ADA	6.5
12	Bis-Tris Propane	6.5
13	Ammonium Acetate	7.0
14	MOPS	7.0
15	Sodium / Potassium Phosphate	7.0
16	HEPES	7.5
17	Tris	7.5
18	EPPS	8.0
19	Imidazole	8.0
20	Bicine	8.5
21	Tris	8.5
22	CHES	9.0
23	CHES	9.5
24	CAPS	10.0

Additive Kit		
No.	Additive	Concentrated Stock Solution
1	Sodium Chloride	80 mM
2	Sodium Chloride	200 mM
3	Sodium Chloride	400 mM
4	Glycerol	20%
5	Glycerol	40%
6	CHAPS	8 mM
7	Octyl Glucopyranoside	0.4 %
8	Octyl Glucopyranoside	4%
9	Dodecyl Maltoside	0.4 %
10	Dodecyl Maltoside	4%
11	BME	40 mM
12	DTT	4 mM
13	DTT	20 mM
14	TCEP	120 mM

JBScreen pH-2D

No	Buffer composition	Ratio	pH low	pH high
1	Succinic Acid : Sodium dihydrogen Phosphate : Glycine	2:7:7	4.0	10.0
2	Citric acid : HEPES : CHES	2:3:4	4.0	10.0
3	Malonic Acid : Imidazole : Boric Acid	2:3:3	4.0	10.0
4	Sodium Acetate : ADA : Bicine	1:1:1	4.0	9.0
5	L-Malic Acid : MES : Tris	1:2:2	4.0	9.0
6	Sodium Tartrate dihydrate : Bis-Tris : Glycylglycine	3:2:2	4.0	9.0

JBScreen Plus

JBScreen Kosmotropic			
bulk	HTS	Compound	Classification
A 1	A1	1.0 M Trimethylamine N-oxide	Zwitterion
A 2	A2	1.0 M Proline	Zwitterion
A 3	A3	0.1 M Ectoine	Zwitterion
A 4	A4	1.0 M Glycine	Zwitterion
A 5	A5	0.1 M Betaine monohydrate	Zwitterion
A 6	A6	0.1 M Taurine	Zwitterion
B 1	A7	2.0 M Glycerol	Polyalcohol
B 2	A8	2.0 M Erythritol	Polyalcohol
B 3	A9	2.0 M Xylitol	Polyalcohol
B 4	A10	2.0 M Adonitol	Polyalcohol
B 5	A11	0.8 M Mannitol	Polyalcohol
B 6	A12	1.0 M Sorbitol	Polyalcohol
C 1	B1	0.2 M Aluminium Chloride	Kosmotropic Cation
C 2	B2	0.2 M Magnesium Chloride	Kosmotropic Cation
C 3	B3	0.2 M Calcium Chloride	Kosmotropic Cation
C 4	B4	2.0 M Lithium Chloride	Kosmotropic Cation
C 5	B5	1.0 M Manganese (II) Chloride	Kosmotropic Cation
C 6	B6	1.0 M Zinc Chloride	Kosmotropic Cation
D 1	B7	2.0 M Sodium Malonate	Kosmotropic Anion
D 2	B8	2.0 M Sodium Citrate	Kosmotropic Anion
D 3	B9	2.0 M Sodium Fluoride	Kosmotropic Anion
D 4	B10	2.0 M Ammonium Sulfate	Kosmotropic Anion
D 5	B11	1.0 M Ammonium Phosphate dibasic	Kosmotropic Anion
D 6	B12	1.0 M Ammonium Formate	Kosmotropic Anion

JBScreen Chaotropic			
bulk	HTS	Compound	Classification
A 1	C1	1.0 M Urea	Non-ionic
A 2	C2	4.0 M DMSO	Non-ionic
A 3	C3	4.0 M DMF	Non-ionic
A 4	C4	1.0 M Pyridine	Non-ionic
A 5	C5	0.5 M ϵ -Caprolactam	Non-ionic
A 6	C6	0.1 M Phenol	Non-ionic
B 1	C7	2.0 M Trimethylammonium Chloride	Chaotropic Cation
B 2	C8	2.0 M Guanidinium Chloride	Chaotropic Cation
B 3	C9	2.0 M Tetramethylammonium Chloride	Chaotropic Cation
B 4	C10	1.0 M Cesium Chloride	Chaotropic Cation
B 5	C11	1.0 M Rubidium Chloride	Chaotropic Cation
B 6	C12	1.0 M Potassium Chloride	Chaotropic Cation
C 1	D1	2.0 M Potassium Thiocyanate	Chaotropic Anion
C 2	D2	2.0 M Potassium Cyanate	Chaotropic Anion
C 3	D3	1.0 M Potassium Nitrate	Chaotropic Anion
C 4	D4	1.0 M Potassium Acetate	Chaotropic Anion
C 5	D5	1.0 M Potassium Iodide	Chaotropic Anion
C 6	D6	1.0 M Potassium Bromide	Chaotropic Anion
D 1	D7	2.0 M Sodium trichloroacetate	Chaotropic Anion
D 2	D8	2.0 M Sodium Thiocyanate	Chaotropic Anion
D 3	D9	2.0 M Sodium Perchlorate	Chaotropic Anion
D 4	D10	2.0 M Sodium Nitrate	Chaotropic Anion
D 5	D11	1.0 M Sodium Iodide	Chaotropic Anion
D 6	D12	2.0 M Sodium Bromide	Chaotropic Anion



JBScreen Plus Salts			
bulk	HTS	Compound	Classification
A 1	E1	1.0 M Lithium Citrate	Lithium Salt
A 2	E2	2.0 M Lithium Acetate	Lithium Salt
A 3	E3	2.0 M Lithium Bromide	Lithium Salt
A 4	E4	2.0 M Lithium Salicylate	Lithium Salt
A 5	E5	2.0 M Lithium Nitrate	Lithium Salt
A 6	E6	2.0 M Lithium Perchlorate	Lithium Salt
B 1	E7	2.0 M Ammonium Fluoride	Ammonium Salt
B 2	E8	2.0 M Ammonium Chloride	Ammonium Salt
B 3	E9	2.0 M Ammonium Bromide	Ammonium Salt
B 4	E10	2.0 M Ammonium Nitrate	Ammonium Salt
B 5	E11	2.0 M Ammonium Thiocyanate	Ammonium Salt
B 6	E12	2.0 M Ammonium Trifluoroacetate	Ammonium Salt
C 1	F1	2.0 M Ammonium Tartrate dibasic	Ammonium Salt
C 2	F2	0.7 M Potassium Sulfate	Sulfate
C 3	F3	2.0 M Sodium Sulfate	Sulfate
C 4	F4	2.0 M Lithium Sulfate	Sulfate
C 5	F5	2.0 M Magnesium Sulfate	Sulfate
C 6	F6	1.0 M Beryllium Sulfate	Sulfate
D 1	F7	0.1 M Barium Chloride	Multivalent Cation
D 2	F8	0.1 M Strontium Chloride	Multivalent Cation
D 3	F9	0.1 M Cadmium Chloride	Multivalent Cation
D 4	F10	0.1 M Cobalt (II) Chloride	Multivalent Cation
D 5	F11	0.1 M Copper (II) Chloride	Multivalent Cation
D 6	F12	0.1 M Yttrium (III) Chloride	Multivalent Cation

JBScreen Volatiles			
bulk	HTS	Compound	Classification
A 1	-	10.0 M Methanol	Small Alcohol
A 2	-	5.0 M Ethanol	Small Alcohol
A 3	-	5.0 M 2-Propanol	Small Alcohol
A 4	-	5.0 M 1-Propanol	Small Alcohol
A 5	-	1.0 M 1-Butanol	Small Alcohol
A 6	-	5.0 M tert-Butanol	Small Alcohol
B 1	-	5.0 M Ethylene Glycol	Small Alcohol
B 2	-	5.0 M 1,3-Propandiol	Small Alcohol
B 3	-	4.0 M 1,4-Butanediol	Small Alcohol
B 4	-	4.0 M 1,2-Butanediol	Small Alcohol
B 5	-	4.0 M 2,2,2-Trifluoroethanol	Small Alcohol
B 6	-	2.0 M Hexafluoro-2-propanol	Small Alcohol
C 1	-	4.0 M γ -Butyrolactone	Non-ionic Chaotropic
C 2	-	10.0 M Acetonitrile	Non-ionic Chaotropic
C 3	-	1.5 M Propionitrile	Non-ionic Chaotropic
C 4	-	0.4 M tert-Butyl Methyl Ether	Non-ionic Chaotropic
C 5	-	4.0 M Dioxane	Non-ionic Chaotropic
C 6	-	4.0 M Tetrahydrofuran	Non-ionic Chaotropic
D 1	-	5.0 M Acetone	Organic Volatile
D 2	-	2.5 M Ethyl Methyl Ketone	Organic Volatile
D 3	-	1.0 M 3-Pentanone	Organic Volatile
D 4	-	0.5 M Methyl Acetate	Organic Volatile
D 5	-	0.3 M Ethyl Acetate	Organic Volatile
D 6	-	0.05 M Dichloromethane	Organic Volatile

JBScreen Additives			
bulk	HTS	Compound	Classification
A 1	G1	2.0 M 6-Aminocaproic Acid	Linker Molecule
A 2	G2	2.0 M Ethanolamine	Linker Molecule
A 3	G3	2.0 M 1,6-Diaminohexane	Linker Molecule
A 4	G4	2.0 M 1,8-Diaminoctane	Linker Molecule
A 5	G5	1.0 M 1,2,3-Hexanetriol	Polyalcohol
A 6	G6	0.1 M Spermidine trihydrochloride	Polyamine
B 1	G7	0.5 M PPG 400	Organic Hydrophilic Polymer
B 2	G8	1.0 M PEG 200	Organic Hydrophilic Polymer
B 3	G9	0.5 M PEG 600	Organic Hydrophilic Polymer
B 4	G10	0.02 M Dextran Sulfate	Organic Hydrophilic Polymer
B 5	G11	1 % w/v Polyvinyl Alcohol	Organic Hydrophilic Polymer
B 6	G12	5 % w/v Polyvinylpyrrolidone K15	Organic Hydrophilic Polymer
C 1	H1	1.0 M D,L-Fructose	Carbohydrate
C 2	H2	1.0 M D,L-Glucose	Carbohydrate
C 3	H3	1.0 M D,L-Mannose	Carbohydrate
C 4	H4	0.6 M Lactose	Carbohydrate
C 5	H5	1.0 M Sucrose	Carbohydrate
C 6	H6	1.0 M Trehalose	Carbohydrate
D 1	H7	0.1 M DTT	Reducing Agent
D 2	H8	0.1 M L-Cysteine	Reducing Agent
D 3	H9	0.1 M EDTA Sodium Salt	Chelator
D 4	H10	0.1 M ATP disodium Salt	Co-factor
D 5	H11	1.0 M Benzamidine Hydrochloride	Amphiphilic Molecule
D 6	H12	0.3 M Glycyl-glycyl-glycine	Amphiphilic Molecule



JBScreen Detergents

JBScreen Detergents 1				
No.	Detergent	CMC(mM)	conc. stock solution (mM)(5 or 10 x CMC)	Amount
D 1-1	3-(N,N-Dimethylpalmitylammonio)propane-sulfonate (ZWITTERGENT® 3-16)	0.06	0.6	100 µl
D 1-2	Nonaethylene glycol monododecyl ether (C12E9)	0.08	0.8	100 µl
D 1-3	Octaethylene glycol monododecyl ether (C12E8)	0.11	1.1	100 µl
D 1-4	Dodecyl-β-D-glucopyranoside	0.13	1.3	100 µl
D 1-5	3-(N,N-Dimethylmyristylammonio)propane-sulfonate (ZWITTERGENT® 3-14)	0.4	4	100 µl
D 1-6	Dodecyl-β-D-maltoside	0.6	6	100 µl
D 1-7	Decyl-β-D-maltopyranoside	1.8	18	100 µl
D 1-8	N,N-Dimethyldodecylamine N-oxide (LDAO)	2.0	20	100 µl
D 1-9	3-(Dodecyldimethylammonio)propane-sulfonate (ZWITTERGENT® 3-12)	4.0	40	100 µl
D 1-10	Nonyl-β-D-glucopyranoside	6.5	65	100 µl
D 1-11	N-Decanoyl-N-methylglucamine(MEGA-10)	7.0	70	100 µl
D 1-12	Tetraethylene glycol monoocetyl ether (C8E4)	7.0	70	100 µl

JBScreen Detergents 2				
No.	Detergent	CMC(mM)	conc. Stock solution (mM)(5 or 10 x CMC)	Amount
D 2-1	Pentaethylene glycol monoocetyl ether (C8E5)	7.1	71	100 µl
D 2-2	3-[(3-Cholamidopropyl)dimethylammonio]-1-propanesulfonate (CHAPS)	8.0	80	100 µl
D 2-3	3-[(3-Cholamidopropyl)dimethylammonio]-2-hydroxy-1-propanesulfonate (CHAPSO)	8.0	80	100 µl
D 2-4	Pentaethylene glycol monododecyl ether (C10E5)	0.81	8.1	100 µl
D 2-5	N,N-Dimethyldecylamine-N-oxide (DDAO)	10.4	104	100 µl
D 2-6	Octyl-β-D-glucopyranoside	25	250	100 µl
D 2-7	N-Nonanoyl-N-methylglucamine (MEGA-9)	25	250	100 µl
D 2-8	3-(Decyldimethylammonio)propane-1-sulfonate (ZWITTERGENT® 3-10)	40	400	100 µl
D 2-9	Heptyl-β-D-glucopyranoside	79	790	100 µl
D 2-10	N-Octanoyl-N-methylglucamine (MEGA-8)	79	790	100 µl
D 2-11	Hexyl-β-D-glucopyranoside	250	1250	200 µl
D 2-12	3-(N,N-Dimethyoctylammonio)propane-sulfonate (ZWITTERGENT® 3-8)	330	1650	200 µl

JBsolution Detergent Test Kit

Detergent	Molecular Mass (g/mol)	Concentration (equals stock solution)	Critical Micellar Concentration (CMC)
Non-ionic detergents			
Brij® 35	1199.76 g/mol	33.3 mM	0.09 mM
Deoxy-BIGCHAP	862.1 g/mol	46.4 mM	1.1 – 1.4 mM
HECAMEG	335.39 g/mol	119.3 mM	19.5 mM
MEGA-8	321.42 g/mol	124.5 mM	58 mM
MEGA-9	335.5 g/mol	119.2 mM	19 – 25 mM
n-Octyl-β-D-glucopyranoside	292.38 g/mol	136.8 mM	25 – 30 mM
Pluronic F-68	~ 8300 g/mol	4.8 mM	17.9 mM
Sucrose monolaurate	524.60 g/mol	76.3 mM	0.4 mM
Triton® X-100	~ 625 g/mol	64.0 mM	0.2 – 0.9 mM
Triton® X-114	~527 g/mol	75.9 mM	0.35 mM
Tween®20	~ 1228 g/mol	32.6 mM	0.059 mM
Tween®80	~ 1310 g/mol	30.5 mM	0.012 mM
Nonidet P40	603.3 g/mol	66.3 mM	0.05 – 0.30 mM
Anionic detergents			
N-Lauroylsarcosin-sodium salt	293.4 g/mol	136.0 mM	13.7 mM
Lithiumdodecyl sulfate	272.3 g/mol	147.0 mM	8.7 mM
Sodium cholate	430.6 g/mol	92.9 mM	14 mM
Sodium deoxycholate	414.6 g/mol	96.5 mM	10 mM
SDS (Sodiumdodecylsulfate)	288.4 g/mol	138.7 mM	7 – 10 mM

Cationic detergents			
Cetylpyridinium chloride	358.0 g/mol	111.7 mM	0.12 mM
Cetyltrimethylammonium bromide	364.5 g/mol	109.8 mM	1 mM
Zwitterionic detergents			
CHAPS	614.9 g/mol	65.1 mM	6 – 10 mM
CHAPSO	630.9 g/mol	63.4 mM	8 mM
Sulfobetaine SB8	279.6 g/mol	143.1 mM	330 mM
Sulfobetaine SB10	307.6 g/mol	130.2 mM	25 – 40 mM
Sulfobetaine SB12	335.6 g/mol	119.3 mM	2 – 4 mM
Sulfobetaine SB14	363.6 g/mol	110.0 mM	0.2 mM
Sulfobetaine SB16	391.6 g/mol	51.1 mM	0.01 – 0.06 mM

JBScreen Cryo Pro

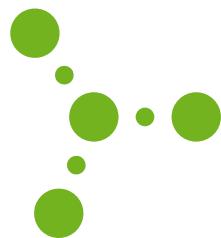
No.	Cryoprotectant
Cryo-1	Sucrose/Xylitol
Cryo-2	Sucrose/Glucose
Cryo-3	Sucrose
Cryo-4	Xylitol
Cryo-5	Taurine
Cryo-6	Glycerol
Cryo-7	Pentaerythritol propoxylate (5/4 PO/OH)
Cryo-8	Pentaerythritol ethoxylate (15/4 EO/OH)
Cryo-9	Ethylene glycol
Cryo-10	MPD
Cryo-11	PEG 400
Cryo-12	Mineral Oil

www.jenabioscience.com



IFTA AG
Certified QMS according to
DIN EN ISO 9001
Reg. No. IC 03214 034

Jena Bioscience GmbH
Loebstedter Strasse 80
D-07749 Jena
Germany
phone: +49-3641-6285 000
fax: +49-3641-6285 100
e-mail: info@jenabioscience.com
www.jenabioscience.com



Jena Bioscience

A decorative graphic in the bottom left corner features a series of green circles of varying sizes arranged in a cluster, with smaller dots interspersed between them.