Molecular Dimensions

Soluble Proteins

Structure Screen 1 + 2 HT-96 MD1-30

Structure Screen 1 + 2 HT-96 is a 96 reagent, sparse-matrix screen of Structure Screen 1, and the classic extension to this screen, Structure Screen 2.

Formulated for the crystallization of proteins, peptides, nucleic acids, & water soluble small molecules.

MD1-30 is presented as a 96 x 1 mL conditions in a deep-well block.

Features of Structure Screen 1 + 2:

- Novel precipitants and combinations.
- 96 conditions samples salts, polymers, organics and pH.
- A simple and practical way to find initial crystallization conditions.

Introduction

This classic standard sparse matrix screen lets you:

- Determine initial crystallization conditions.
- Establish the solubility of a macromolecule in a varying range of pH and precipitants,
- Enables screening of greater crystallization space with the enhanced buffer selection.

Originally published in 1991 by Jancarik & Kim from conditions found to be successful in the crystallization of biological macromolecules.

A comparison of three commercial sparse matrix screens, (Wooh *et al,* 2003) reported dramatically different results when comparing Crystal Screens and Structure Screens. In 38 cases the Structure Screens were more successful in producing crystals than the Crystal Screens while the opposite was the case in 26 formulations. The formulations are not identical as in several buffers Molecular Dimensions uses acetic acid to adjust the pH rather than HCl. This formulation was chosen from current practice developed from experience at major UK research institutions. We have now analyzed the results and found the following:

65% could be due to a different buffer counter ion

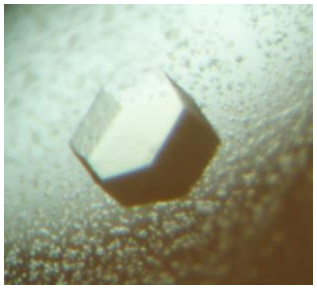
9% could be due to a pH difference probably resulting from glycol oxidation

26% may possibly due to a minor pH difference or simply derived from the chance event of crystal nucleation.

References:

Jancarik, J & Kim, S.H.J. (1991), J.Appl.Cryst. 24, 409-411

Wooh et al, (2003), Acta Cryst , D59, 769 - 772.



Protein crystal grown with Structure Screen courtesy of Laure Yatime.

Sample preparation

The purity of the sample is critical. If particulate or amorphous matter is present centrifugation or micro-filtration is advisable. A sample concentration of 5 - 25 mg/ml is recommended.
Alternatively, set up additional screens to optimize crystal growth.

Interpreting Results

Using a stereo microscope carefully examine the droplets; scan the focal plane for small crystals and record observations. If crystals are obtained during an initial screen the conditions may be optimized by varying the pH and concentrations of precipitant or salt. In the absence of crystals, inspect any droplets with precipitate for microcrystallinity. Use a high power microscope to examine amorphous material between crossed polarizing lenses. True amorphous precipitates do not glow. Birefringent microcrystalline precipitates can glow as a result of the plane of polarization.
It may be possible to use streak seeding to produce larger crystals from microcrystalline precipitates. If the amorphous material is precipitate, repeat the screen, but reduce the sample concentration or dilute the precipitant with water. If the droplets remain clear, leave the screen for a few weeks but continue to observe the samples. Increasing the sample concentration may optimize the conditions.
If small crystals, not suitable for X-ray diffraction are grown, it may be possible to use seeding techniques to grow larger crystals.

Formulation Notes:

Structure Screen 1 + 2 reagents are formulated using ultrapure water (>18.0 MΩ) and are sterile-filtered using 0.22 µm filters. No preservatives are added.

Final pH may vary from that specified on the datasheet. Molecular Dimensions will be happy to discuss the precise formulation of individual reagents.
Individual reagents and stock solutions for optimization are available from Molecular Dimensions.

Enquiries regarding Structure Screen 1 + 2 formulation, interpretation of results or optimization strategies are welcome. Please e-mail, fax or phone your query to Molecular Dimensions.

Contact and product details can be found at www.moleculardimensions.com

Manufacturer's safety data sheets are available to download from our website.

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Structure Screen 1 + 2 Conditions A1 – D12 MD1-30

Well #	Conc.	Units	Salt 1	Conc.	Units	Buffer	pH	Conc.	Units	Precipitant 1	Conc.	Units	Precipitant 2
A1	0.02	M	Calcium chloride dihydrate	0.1	M	Sodium acetate	4.6	30	% v/v	MPD			
A2	0.2	M	Ammonium acetate	0.1	M	Sodium acetate	4.6	30	% w/v	PEG 4000			
A3	0.2	M	Ammonium sulfate	0.1	M	Sodium acetate	4.6	25	% w/v	PEG 4000			
A4	2.0	M	Sodium formate	0.1	M	Sodium acetate	4.6						
A5	2.0	M	Ammonium sulfate	0.1	M	Sodium acetate	4.6						
A6				0.1	M	Sodium acetate	4.6	8	% w/v	PEG 4000			
A7	0.2	M	Ammonium acetate	0.1	M	Sodium citrate	5.6	30	% w/v	PEG 4000			
A8	0.2	M	Ammonium acetate	0.1	M	Sodium citrate	5.6	30	% v/v	MPD			
A9				0.1	M	Sodium citrate	5.6	20	% w/v	PEG 4000	20	% v/v	2-Propanol
A10	1.0	M	Ammonium phosphate monobasic	0.1	M	Sodium citrate	5.6						
A11	0.2	M	Calcium chloride dihydrate	0.1	M	Sodium acetate	4.6	20	% v/v	2-Propanol			
A12	1.4	M	Sodium acetate trihydrate	0.1	M	Sodium cacodylate	6.5						
B1	0.2	M	Sodium citrate tribasic dihydrate	0.1	M	Sodium cacodylate	6.5	30	% v/v	2-Propanol			
B2	0.2	M	Ammonium sulfate	0.1	M	Sodium cacodylate	6.5	30	% w/v	PEG 8000			
B3	0.2	M	Magnesium acetate tetrahydrate	0.1	M	Sodium cacodylate	6.5	20	% w/v	PEG 8000			
B4	0.2	M	Magnesium acetate tetrahydrate	0.1	M	Sodium cacodylate	6.5	30	% v/v	MPD			
B5	1.0	M	Sodium acetate trihydrate	0.1	M	Imidazole	6.5						
B6	0.2	M	Sodium acetate trihydrate	0.1	M	Sodium cacodylate	6.5	30	% w/v	PEG 8000			
B7	0.2	M	Zinc acetate dihydrate	0.1	M	Sodium cacodylate	6.5	18	% w/v	PEG 8000			
B8	0.2	M	Calcium acetate hydrate	0.1	M	Sodium cacodylate	6.5	18	% w/v	PEG 8000			
B9	0.2	M	Sodium citrate tribasic dihydrate	0.1	M	Sodium HEPES	7.5	30	% v/v	MPD			
B10	0.2	M	Magnesium chloride hexahydrate	0.1	M	Sodium HEPES	7.5	30	% v/v	2-Propanol			
B11	0.2	M	Calcium chloride dihydrate	0.1	M	Sodium HEPES	7.5	28	% v/v	PEG 400			
B12	0.2	M	Magnesium chloride hexahydrate	0.1	M	Sodium HEPES	7.5	30	% v/v	PEG 400			
C1	0.2	M	Sodium citrate tribasic dihydrate	0.1	M	Sodium HEPES	7.5	20	% v/v	2-Propanol			
C2	0.8	M	Potasium sodium tartrate tetrahydrate	0.1	M	Sodium HEPES	7.5						
C3	1.5	M	Lithium sulfate	0.1	M	Sodium HEPES	7.5						
C4	0.8	M	Sodium phosphate monobasic monohydrate/	0.1	M	Sodium HEPES	7.5						
	0.8	M	Potasium phosphate monobasic										
C5	1.4	M	Sodium citrate tribasic dihydrate	0.1	M	Sodium HEPES	7.5						
C6	2.0	M	Ammonium sulfate	0.1	M	Sodium HEPES	7.5	2	% v/v	PEG 400			
C7				0.1	M	Sodium HEPES	7.5	20	% w/v	PEG 4000	10	% v/v	2-Propanol
C8	2.0	M	Ammonium sulfate	0.1	M	Tris	8.5						
C9	0.2	M	Magnesium chloride hexahydrate	0.1	M	Tris	8.5	30	% w/v	PEG 4000			
C10	0.2	M	Sodium citrate tribasic dihydrate	0.1	M	Tris	8.5	30	% v/v	PEG 400			
C11	0.2	M	Lithium sulfate	0.1	M	Tris	8.5	30	% w/v	PEG 4000			
C12	0.2	M	Ammonium acetate	0.1	M	Tris	8.5	30	% v/v	2-Propanol			
D1	0.2	M	Sodium acetate trihydrate	0.1	M	Tris	8.5	30	% w/v	PEG 4000			
D2				0.1	M	Tris	8.5	8	% w/v	PEG 8000			
D3	2.0	M	Ammonium phosphate monobasic	0.1	M	Tris	8.5						
D4	0.4	M	Potasium sodium tartrate tetrahydrate										
D5	0.4	M	Ammonium phosphate monobasic										
D6	0.2	M	Ammonium sulfate					30	% w/v	PEG 8000			
D7	0.2	M	Ammonium sulfate					30	% w/v	PEG 4000			
D8	2.0	M	Ammonium sulfate										
D9	4.0	M	Sodium formate										
D10	0.05	M	Potassium phosphate monobasic					20	% w/v	PEG 8000			
D11								30	% w/v	PEG 1500			
D12	0.2	M	Magnesium formate dihydrate										

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Structure Screen 1 + 2 Conditions E1 – H12 MD1-30

Well #	Conc.	Units	Salt 1	Conc.	Units	Buffer	pH	Conc.	Units	Precipitant 1	Conc.	Units	Precipitant 2
E1	0.1	M	Sodium chloride	0.1	M	BICINE	9.0	30	% v/v	PEG 500 MME			
E2	2.0	M	Magnesium chloride hexahydrate	0.1	M	BICINE	9.0						
E3				0.1	M	BICINE	9.0	10	% w/v	PEG 20000	2	% v/v	1,4-Dioxane
E4	0.2	M	Magnesium chloride hexahydrate	0.1	M	Tris	8.5	3.4	M	1,6-Hexanediol			
E5				0.1	M	Tris	8.5	25	% v/v	tert-Butanol			
E6	1.0	M	Lithium sulfate/	0.1	M	Tris	8.5						
	0.01	M	Nickel(II) chloride hexahydrate										
E7	1.5	M	Ammonium sulfate	0.1	M	Tris	8.5	12	% v/v	Glycerol			
E8	0.2	M	Ammonium phosphate monobasic	0.1	M	Tris	8.5	50	% v/v	MPD			
E9				0.1	M	Tris	8.5	20	% v/v	Ethanol			
E10	0.01	M	Nickel(II) chloride hexahydrate	0.1	M	Tris	8.5	20	% w/v	PEG 2000 MME			
E11	0.5	M	Ammonium sulfate	0.1	M	Sodium HEPES	7.5	30	% v/v	MPD			
E12				0.1	M	Sodium HEPES	7.5	10	% w/v	PEG 6000	5	% v/v	MPD
F1				0.1	M	Sodium HEPES	7.5	20	% v/v	Jeffamine® M-600			
F2	1.6	M	Ammonium sulfate/	0.1	M	Sodium HEPES	7.5						
	0.1	M	Sodium chloride										
F3	2.0	M	Ammonium formate	0.1	M	Sodium HEPES	7.5						
F4	1.0	M	Sodium acetate trihydrate	0.1	M	Sodium HEPES	7.5						
	0.05	M	Cadmium sulfate $^{8}/_{3}$-hydrate										
F5				0.1	M	Sodium HEPES	7.5	70	% v/v	MPD			
F6	4.3	M	Sodium chloride	0.1	M	Sodium HEPES	7.5						
F7				0.1	M	Sodium HEPES	7.5	10	% w/v	PEG 8000	8	% v/v	Ethylene glycol
F8	1.6	M	Magnesium sulfate heptahydrate	0.1	M	MES	6.5						
F9	2.0	M	Sodium chloride/	0.1	M	MES	6.5						
	0.1	M	Potassium phosphate monobasic/										
	0.1	M	Sodium phosphate monobasic monohydrate										
F10				0.1	M	MES	6.5	12	% w/v	PEG 20000			
F11	1.6	M	Ammonium sulfate	0.1	M	MES	6.5	10	% v/v	1,4-Dioxane			
F12	0.05	M	Cesium chloride	0.1	M	MES	6.5	30	% v/v	Jeffamine® M-600			
G1	0.01	M	Cobalt(II) chloride hexahydrate	0.1	M	MES	6.5						
	1.8	M	Ammonium sulfate										
G2	0.2	M	Ammonium sulfate	0.1	M	MES	6.5	30	% w/v	PEG 5000 MME			
G3	0.01	M	Zinc sulfate heptahydrate	0.1	M	MES	6.5	25	% v/v	PEG 500 MME			
G4				0.1	M	Sodium HEPES	7.5	20	% w/v	PEG 10000			
G5	2.0	M	Ammonium sulfate	0.1	M	Sodium citrate	5.6						
	0.2	M	Potassium sodium tartrate tetrahydrate										
G6	1.0	M	Lithium sulfate	0.1	M	Sodium citrate	5.6						
	0.5	M	Ammonium sulfate										
G7	0.5	M	Sodium chloride	0.1	M	Sodium citrate	5.6	4	% v/v	Polyethyleneimine			
G8				0.1	M	Sodium citrate	5.6	35	% v/v	tert-Butanol			
G9	0.01	M	Iron(III) chloride hexahydrate	0.1	M	Sodium citrate	5.6	10	% v/v	Jeffamine® M-600			
G10	0.01	M	Manganese(II) chloride tetrahydrate	0.1	M	Sodium citrate	5.6	2.5	M	1,6-Hexanediol			
G11	2.0	M	Sodium chloride	0.1	M	Sodium acetate	4.6						
G12	0.2	M	Sodium chloride	0.1	M	Sodium acetate	4.6	30	% v/v	MPD			
H1	0.01	M	Cobalt(II) chloride hexahydrate	0.1	M	Sodium acetate	4.6	1.0	M	1,6-Hexanediol			
H2	0.1	M	Cadmium chloride hemi(pentahydrate)	0.1	M	Sodium acetate	4.6	30	% v/v	PEG 400			
H3	0.2	M	Ammonium sulfate	0.1	M	Sodium acetate	4.6	30	% w/v	PEG 2000 MME			
H4	2.0	M	Sodium chloride					10	% w/v	PEG 6000			
H5	0.5	M	Sodium chloride/										
	0.1	M	Magnesium chloride hexahydrate/										
	0.01	M	CTAB										
H6								25	% v/v	Ethylene glycol			
H7								35	% v/v	1,4-Dioxane			
H8	2.0	M	Ammonium sulfate					5	% v/v	2-Propanol			
H9				1.0	M	Imidazole	7.0						
H10								10	% w/v	PEG 1000	10	% w/v	PEG 8000
H11	1.5	M	Sodium chloride					10	% v/v	Ethanol			
H12				1.6	M	Sodium citrate	6.5						

Abbreviations:
BICINE; N,N-Bis(2-hydroxyethyl)glycine, **CTAB**; cetyltrimethylammonium bromide, **Sodium HEPES**; 2-(4-(2-Hydroxyethyl)-1-piperazinyl)ethanesulfonic Acid Sodium Salt, **MES**; 2-(N-morpholino)ethanesulfonic acid, **MME**; Monomethylether, **MPD;** 2,4-methyl pentanediol, **PEG**; Polyethylene glycol, **Tris**; 2-Amino-2-(hydroxymethyl)propane-1,3-diol, ***tert*-butanol**; 2-methyl-2-propanol; **Jeffamine M-600®** is titrated to pH 7.0 prior to use.

Manufacturer's safety data sheets are available from our website or by scanning the QR code here:

Re-Ordering details:

Catalogue Description		Catalogue Code
Structure Screen 1	50 x 10 mL	MD1-01
Structure Screen 2	50 x 10 mL	MD1-02
The Structure Screen Combination (Structure Screen 1 + Structure Screen 2)	100 x 50 mL	MD1-03
Structure Screen 1 + 2 HT-96	96 x 1 mL	MD1-30
Eco Screens		
Structure Screen 1 Eco Screen	50 x 10 mL	MD1-01-ECO
Structure Screen 2 Eco Screen	49 x 10 mL	MD1-02-ECO
The Structure Screen Combination Eco Screen (Structure Screen 1 + Structure Screen 2)	99 x 10 mL	MD1-03-ECO
Structure Screen 1 + 2 HT-96 Eco Screen	96 x 1 mL	MD1-30-ECO
Single Reagents		
Structure Screen 1 single reagents	100 mL	MDSR-01-tube number
Structure Screen 2 single reagents	100 mL	MDSR-02-tube number
Structure Screen 1 + 2 HT-96 single reagents	100 mL	MDSR-30 – well number

For Structure Screen stock reagents visit our Optimization page on our website.