Molecular Dimensions

Soluble Proteins

Structure Screen 1 MD1-01

Structure Screen 1 is formulated for the crystallization of proteins, peptides, nucleic acids, & water soluble small molecules. This classic screen was originally published by Jancarik & Kim from conditions found to be successful in the crystallization of biological macromolecules.

MD1-01 is presented as a 50 x 10 mL conditions.

Features of Structure Screen 1:

- The classic standard sparse matrix screen: for the crystallization of proteins, peptides, nucleic acids and , water soluble small molecules.
- Sparse matrix formula efficiently samples salts, polymers, organics, & pH.
- Proven effective with more than 1,000 biological macromolecules.
- 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

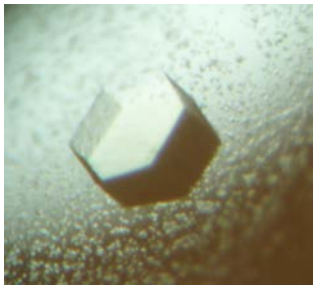
9% could be due to a pH difference probably resulting from glycol oxidation

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 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 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 Conditions 1-50 MD1-01

Tube #	Conc.	Units	Salt 1	Conc.	Units	Buffer	pH	Conc.	Units	Precipitant 1
1	0.02	M	Calcium chloride dihydrate	0.1	M	Sodium acetate	4.6	30	% v/v	MPD
2	0.2	M	Ammonium acetate	0.1	M	Sodium acetate	4.6	30	% w/v	PEG 4000
3	0.2	M	Ammonium sulfate	0.1	M	Sodium acetate	4.6	25	% w/v	PEG 4000
4	2.0	M	Sodium formate	0.1	M	Sodium acetate	4.6			
5	2.0	M	Ammonium sulfate	0.1	M	Sodium acetate	4.6			
6				0.1	M	Sodium acetate	4.6	8	% w/v	PEG 4000
7	0.2	M	Ammonium acetate	0.1	M	Sodium citrate	5.6	30	% w/v	PEG 4000
8	0.2	M	Ammonium acetate	0.1	M	Sodium citrate	5.6	30	% v/v	MPD
9				0.1	M	Sodium citrate	5.6	20	% w/v	PEG 4000/
								20	% v/v	2-Propanol
10	1.0	M	Ammonium phosphate monobasic	0.1	M	Sodium citrate	5.6			
11	0.2	M	Calcium chloride dihydrate	0.1	M	Sodium acetate	4.6	20	% v/v	2-Propanol
12	1.4	M	Sodium acetate trihydrate	0.1	M	Sodium cacodylate	6.5			
13	0.2	M	Sodium citrate tribasic dihydrate	0.1	M	Sodium cacodylate	6.5	30	% v/v	2-Propanol
14	0.2	M	Ammonium sulfate	0.1	M	Sodium cacodylate	6.5	30	% w/v	PEG 8000
15	0.2	M	Magnesium acetate tetrahydrate	0.1	M	Sodium cacodylate	6.5	20	% w/v	PEG 8000
16	0.2	M	Magnesium acetate tetrahydrate	0.1	M	Sodium cacodylate	6.5	30	% v/v	MPD
17	1.0	M	Sodium acetate trihydrate	0.1	M	Imidazole	6.5			
18	0.2	M	Sodium acetate trihydrate	0.1	M	Sodium cacodylate	6.5	30	% w/v	PEG 8000
19	0.2	M	Zinc acetate dihydrate	0.1	M	Sodium cacodylate	6.5	18	% w/v	PEG 8000
20	0.2	M	Calcium acetate hydrate	0.1	M	Sodium cacodylate	6.5	18	% w/v	PEG 8000
21	0.2	M	Sodium citrate tribasic dihydrate	0.1	M	Sodium HEPES	7.5	30	% v/v	MPD
22	0.2	M	Magnesium chloride hexahydrate	0.1	M	Sodium HEPES	7.5	30	% v/v	2-Propanol
23	0.2	M	Calcium chloride dihydrate	0.1	M	Sodium HEPES	7.5	28	% v/v	PEG 400
24	0.2	M	Magnesium chloride hexahydrate	0.1	M	Sodium HEPES	7.5	30	% v/v	PEG 400
25	0.2	M	Sodium citrate tribasic dihydrate	0.1	M	Sodium HEPES	7.5	20	% v/v	2-Propanol
26	0.8	M	Potasium sodium tartrate tetrahydrate	0.1	M	Sodium HEPES	7.5			
27	1.5	M	Lithium sulfate	0.1	M	Sodium HEPES	7.5			
28	0.8	M	Sodium phosphate monobasic monohydrate/	0.1	M	Sodium HEPES	7.5			
	0.8	M	Potasium phosphate monobasic							
29	1.4	M	Sodium citrate tribasic dihydrate	0.1	M	Sodium HEPES	7.5			
30	2.0	M	Ammonium sulfate	0.1	M	Sodium HEPES	7.5	2	% v/v	PEG 400
31				0.1	M	Sodium HEPES	7.5	20	% w/v	PEG 4000/
								10	% v/v	2-Propanol
32	2.0	M	Ammonium sulfate	0.1	M	Tris	8.5			
33	0.2	M	Magnesium chloride hexahydrate	0.1	M	Tris	8.5	30	% w/v	PEG 4000
34	0.2	M	Sodium citrate tribasic dihydrate	0.1	M	Tris	8.5	30	% v/v	PEG 400
35	0.2	M	Lithium sulfate	0.1	M	Tris	8.5	30	% w/v	PEG 4000
36	0.2	M	Ammonium acetate	0.1	M	Tris	8.5	30	% v/v	2-Propanol
37	0.2	M	Sodium acetate trihydrate	0.1	M	Tris	8.5	30	% w/v	PEG 4000
38				0.1	M	Tris	8.5	8	% w/v	PEG 8000
39	2.0	M	Ammonium phosphate monobasic	0.1	M	Tris	8.5			
40	0.4	M	Potasium sodium tartrate tetrahydrate							
41	0.4	M	Ammonium phosphate monobasic							
42	0.2	M	Ammonium sulfate					30	% w/v	PEG 8000
43	0.2	M	Ammonium sulfate					30	% w/v	PEG 4000
44	2.0	M	Ammonium sulfate							
45	4.0	M	Sodium formate							
46	0.05	M	Potassium phosphate monobasic							
47								30	% w/v	PEG 1500
48	0.2	M	Magnesium formate dihydrate							
49	1.0	M	Lithium sulfate					2	% w/v	PEG 8000
50	0.5	M	Lithium sulfate					15	% w/v	PEG 8000

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Abbreviations:
Sodium HEPES; 2-(4-(2-Hydroxyethyl)-1-piperazinyl)ethanesulfonic Acid Sodium Salt, **MES**; 2-(N-morpholino)ethanesulfonic acid, **MPD;** 2,4-methyl pentanediol, **PEG**; Polyethylene glycol, **Tris**; 2-Amino-2-(hydroxymethyl)propane-1,3-diol.

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

Ordering details:

Catalogue Description		Catalogue Code
Structure Screen 1	(50 x 10 mL kit)	MD1-01
Structure Screen 2	(50 x 10 mL kit)	MD1-02
The Structure Screen Combination (Contains structure screen 1 & 2)	(100 x 50 mL)	MD1-03
Structure Screen 1 &2 HT-96	(96 x 1 mL)	MD1-30
Eco Screen (Cacodylate and dioxane-free) versions		
Structure Screen 1	(50 x 10 mL kit)	MD1-01-ECO
Structure Screen 2	(49 x 10 mL kit)	MD1-02-ECO
The Structure Screen Combination	(100 x 50 mL)	MD1-03-ECO
Structure Screen 1 &2 HT-96	(96 x 1 mL)	MD1-30-ECO
Single Reagents		
Structure Screen 1	(100 mL)	MDSR-01 - tube number
Structure Screen 2	(100 mL)	MDSR-02 - tube number
Structure Screen 1 & 2 HT-96	(100 mL)	MDSR-30 – well number

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