Molecular Dimensions

Soluble Proteins

Structure Screen 2 MD1-02

Structure Screen 2 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.

MD1-02 is presented as 50 x 10 mL conditions.

Features of Structure Screen 2:

- 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

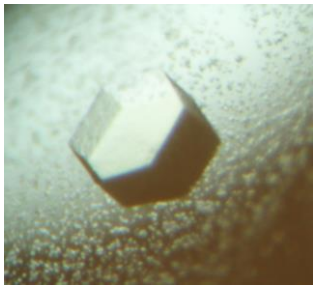
9% could be due to a pH difference probably resulting from glycol oxidation

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 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 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 2 Conditions 1-49 MD1-02

Tube #	Conc.	Salt	Conc.	Buffer	pH	Conc.	Precipitant
1	0.1 M	Sodium chloride	0.1 M	BICINE	9.0	30 % v/v	PEG 500 MME
2	2.0 M	Magnesium chloride hexahydrate	0.1 M	BICINE	9.0		
3			0.1 M	BICINE	9.0	10 % w/v	PEG 20000
						2 % v/v	1,4-Dioxane
4	0.2 M	Magnesium chloride hexahydrate	0.1 M	Tris	8.5	3.4 M	1,6-Hexanediol
5			0.1 M	Tris	8.5	25 % v/v	tert-Butanol
6	1.0 M	Lithium sulfate	0.1 M	Tris	8.5		
	0.01 M	Nickel(II) chloride hexahydrate					
7	1.5 M	Ammonium sulfate	0.1 M	Tris	8.5	12 % v/v	Glycerol
8	0.2 M	Ammonium phosphate monobasic	0.1 M	Tris	8.5	50 % v/v	MPD
9			0.1 M	Tris	8.5	20 % v/v	Ethanol
10	0.01 M	Nickel(II) chloride hexahydrate	0.1 M	Tris	8.5	20 % w/v	PEG 2000 MME
11	0.5 M	Ammonium sulfate	0.1 M	Sodium HEPES	7.5	30 % v/v	MPD
12			0.1 M	Sodium HEPES	7.5	10 % w/v	PEG 6000
						5 % v/v	MPD
13			0.1 M	Sodium HEPES	7.5	20 % v/v	Jeffamine® M-600
14	1.6 M	Ammonium sulfate	0.1 M	Sodium HEPES	7.5		
	0.1 M	Sodium chloride					
15	2.0 M	Ammonium formate	0.1 M	Sodium HEPES	7.5		
16	1.0 M	Sodium acetate trihydrate	0.1 M	Sodium HEPES	7.5		
	0.05 M	Cadmium sulfate $^{8}/_{3}$-hydrate					
17			0.1 M	Sodium HEPES	7.5	70 % v/v	MPD
18	4.3 M	Sodium chloride	0.1 M	Sodium HEPES	7.5		
19			0.1 M	Sodium HEPES	7.5	10 % w/v	PEG 8000
						8 % v/v	Ethylene glycol
20	1.6 M	Magnesium sulfate heptahydrate	0.1 M	MES	6.5		
21	2.0 M	Sodium chloride	0.1 M	MES	6.5		
	0.1 M	Potassium phosphate monobasic					
	0.1 M	Sodium phosphate monobasic monohydrate					
22			0.1 M	MES	6.5	12 % w/v	PEG 20000
23	1.6 M	Ammonium sulfate	0.1 M	MES	6.5	10 % v/v	1,4-Dioxane
24	0.05 M	Cesium chloride	0.1 M	MES	6.5	30 % v/v	Jeffamine® M-600
25	0.01 M	Cobalt(II) chloride hexahydrate	0.1 M	MES	6.5		
	1.8 M	Ammonium sulfate					
26	0.2 M	Ammonium sulfate	0.1 M	MES	6.5	30 % w/v	PEG 5000 MME
27	0.01 M	Zinc sulfate heptahydrate	0.1 M	MES	6.5	25 % v/v	PEG 500 MME
28			0.1 M	Sodium HEPES	7.5	20 % w/v	PEG 10000
29	2.0 M	Ammonium sulfate	0.1 M	Sodium citrate	5.6		
	0.2 M	Potassium sodium tartrate tetrahydrate					
30	1.0 M	Lithium sulfate	0.1 M	Sodium citrate	5.6		
	0.5 M	Ammonium sulfate					
31	0.5 M	Sodium chloride	0.1 M	Sodium citrate	5.6	4 % v/v	Polyethyleneimine
32			0.1 M	Sodium citrate	5.6	35 % v/v	tert-Butanol
33	0.01 M	Iron(III) chloride hexahydrate	0.1 M	Sodium citrate	5.6	10 % v/v	Jeffamine® M-600
34	0.01 M	Manganese(II) chloride tetrahydrate	0.1 M	Sodium citrate	5.6	2.5 M	1,6-Hexanediol
35	2.0 M	Sodium chloride	0.1 M	Sodium acetate	4.6		
36	0.2 M	Sodium chloride	0.1 M	Sodium acetate	4.6	30 % v/v	MPD
37	0.01 M	Cobalt(II) chloride hexahydrate	0.1 M	Sodium acetate	4.6	1.0 M	1,6-Hexanediol
38	0.1 M	Cadmium chloride hemi(pentahydrate)	0.1 M	Sodium acetate	4.6	30 % v/v	PEG 400
39	0.2 M	Ammonium sulfate	0.1 M	Sodium acetate	4.6	30 % w/v	PEG 2000 MME
40	2.0 M	Sodium chloride				10 % w/v	PEG 6000
41	0.5 M	Sodium chloride					
	0.1 M	Magnesium chloride hexahydrate					
	0.01 M	CTAB					
42						25 % v/v	Ethylene glycol
43						35 % v/v	1,4-Dioxane
44	2.0 M	Ammonium sulfate				5 % v/v	2-Propanol
45			1.0 M	Imidazole	7.0		
46						10 % w/v	PEG 1000
						10 % w/v	PEG 8000
47	1.5 M	Sodium chloride				10 % v/v	Ethanol
48			1.6 M	Sodium citrate	6.5		
49						15 % w/v	Polyvinylpyrrolidone
50	2.0 M	Urea					

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.