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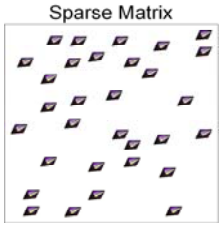


Structure Screen 1 & 2 HT-96 MD1-30

Structure Screen 1 & 2 HT-96 is a 96 reagent, sparse-matrix screen of the classic screen 1, originally published by Jancarik & Kim and the classic extension to this screen, classic screen 2.

The kit contains a 96 × 1ml condition, sparse matrix screen.

Features of Structure Screen 1 & 2 HT-96

- The original sparse-matrix screen 1 and the extension to the original sparse-matrix screen 1 with novel precipitants and combinations.
- Sparse-matrix formula efficiently samples salts, polymers, organics, & pH.
- Proven effective with more than 1,000 biological macromolecules.
- A complete kit designed to provide an effective and rapid screening method for the crystallization of biological macromolecules.
- A simple and practical way to find initial crystallization conditions.

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.

Reproducing Structure Screen Reagents

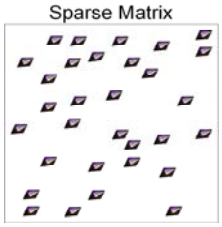
The quoted buffer pH is for a 1.0M stock solution. These reagents have become part of crystal growth folklore and may not necessarily have a final pH in the buffering range of the salts.

Wooh *et al* carried out a comparison of three commercial sparse matrix screens and 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 authors reported that the formulations are not identical as several buffers in Molecular Dimensions' screens use glacial acetic acid to adjust the pH rather than HCl. This formulation was chosen from current practice developed from experience at a major UK research institution. 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 de due to a minor pH difference or simply derived from the chance event of crystal nucleation.



Formulation Notes

Structure Screen 1 & 2 HT-96 reagents are formulated using ultrapure water (>18.0 MΩ) and are sterile-filtered using 0.22 µm filters. No preservatives are added.

Contact Us

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 HT-96 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

References

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

Wooh, J. W., Kidd, R.D., Martin, J.L., Kobe, B. Acta. Cryst. D59, 769-772, (2003).

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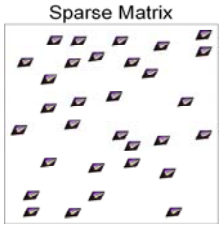
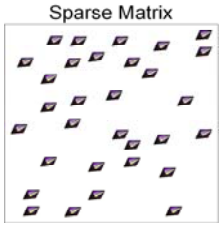


Structure Screen 1 & 2 HT-96 Rows A - D MD1-30

HT#	Salt	Buffer	pH	Precipitant
A1	0.02 M calcium chloride	0.1 M Na acetate	4.6	30 % v/v MPD
A2	0.2 M ammonium acetate	0.1 M Na acetate	4.6	30 % w/v PEG 4000
A3	0.2 M ammonium sulfate	0.1 M Na acetate	4.6	25 % w/v PEG 4000
A4	None	0.1 M Na acetate	4.6	2.0 M sodium formate
A5	None	0.1 M Na acetate	4.6	2.0 M ammonium sulfate
A6	None	0.1 M Na acetate	4.6	8 % w/v PEG 4000
A7	0.2 M ammonium acetate	0.1 M Na citrate	5.6	30 % w/v PEG 4000
A8	0.2 M ammonium acetate	0.1 M Na citrate	5.6	30 % v/v MPD
A9	None	0.1 M Na citrate	5.6	20 % v/v 2-propanol, 20 % w/v PEG 4000
A10	None	0.1 M Na citrate	5.6	1.0 M ammonium dihydrogen phosphate
A11	0.2 M calcium chloride	0.1 M Na acetate	4.6	20 % v/v 2-propanol
A12	None	0.1 M Na cacodylate	6.5	1.4 M sodium acetate
B1	0.2 M sodium citrate	0.1 M Na cacodylate	6.5	30 % v/v 2-propanol
B2	0.2 M ammonium sulfate	0.1 M Na cacodylate	6.5	30 % w/v PEG 8000
B3	0.2 M magnesium acetate	0.1 M Na cacodylate	6.5	20 % w/v PEG 8000
B4	0.2 M magnesium acetate	0.1 M Na cacodylate	6.5	30 % v/v MPD
B5	None	0.1 M imidazole	6.5	1.0 M sodium acetate
B6	0.2 M sodium acetate	0.1 M Na cacodylate	6.5	30 % w/v PEG 8000
B7	0.2 M zinc acetate	0.1 M Na cacodylate	6.5	18 % w/v PEG 8000
B8	0.2 M calcium acetate	0.1 M Na cacodylate	6.5	18 % w/v PEG 8000
B9	0.2 M sodium citrate	0.1 M Na HEPES	7.5	30 % v/v MPD
B10	0.2 M magnesium chloride	0.1 M Na HEPES	7.5	30 % v/v 2-propanol
B11	0.2 M calcium chloride	0.1 M Na HEPES	7.5	28 % v/v PEG 400
B12	0.2 M magnesium chloride	0.1 M Na HEPES	7.5	30 % v/v PEG 400
C1	0.2 M sodium citrate	0.1 M Na HEPES	7.5	20 % v/v 2-propanol
C2	None	0.1 M Na HEPES	7.5	0.8 M K/Na tartrate
C3	None	0.1 M Na HEPES	7.5	1.5 M lithium sulfate
C4	None	0.1 M Na HEPES	7.5	0.8 M sodium dihydrogen phosphate 0.8 M potassium dihydrogen phosphate
C5	None	0.1 M Na HEPES	7.5	1.4 M tri-sodium citrate
C6	None	0.1 M Na HEPES	7.5	2 % v/v PEG 400,2.0 M ammonium sulfate
C7	None	0.1 M Na HEPES	7.5	10 % v/v 2-propanol, 20 % w/v PEG 4000
C8	None	0.1 M Tris	8.5	2.0 M ammonium sulfate
C9	0.2 M magnesium chloride	0.1 M Tris	8.5	30 % w/v PEG 4000
C10	0.2 M sodium citrate	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	0.1 M Tris	8.5	30 % w/v PEG 4000
D2	None	0.1 M Tris	8.5	8 % w/v PEG 8000
D3	None	0.1 M Tris	8.5	2.0 M ammonium dihydrogen phosphate
D4	None	None	None	0.4 M K/Na tartrate
D5	None	None	None	0.4 M ammonium dihydrogen phosphate
D6	0.2 M ammonium sulfate	None	None	30 % w/v PEG 8000
D7	0.2 M ammonium sulfate	None	None	30 % w/v PEG 4000
D8	None	None	None	2.0 M ammonium sulfate
D9	None	None	None	4.0 M sodium formate
D10	0.05 M potassium dihydrogen phosphate	None	None	20 % w/v PEG 8000
D11	None	None	None	30 % w/v PEG 1500
D12	None	None	None	0.2 M magnesium formate



Structure Screen 1 & 2 HT-96 Rows E – H MD1-30

HT#	Salt	Buffer	pH	Precipitant
E1	0.1 M sodium chloride	0.1 M Bicine	9.0	30 % v/v PEG 550 MME
E2	None	0.1 M Bicine	9.0	2.0 M magnesium chloride
E3	2 % v/v dioxane	0.1 M Bicine	9.0	10 % w/v PEG 20,000
E4	0.2 M magnesium chloride	0.1 M Tris	8.5	3.4 M 1,6-hexanediol
E5	None	0.1 M Tris	8.5	25 % v/v *tert*-Butanol
E6	0.01 M nickel chloride	0.1 M Tris	8.5	1.0 M lithium sulfate
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	None	0.1 M Tris	8.5	20 % v/v ethanol
E10	0.01 M nickel chloride	0.1 M Tris	8.5	20 % w/v PEG 2000 MME
E11	0.5 M ammonium sulfate	0.1 M Na HEPES	7.5	30 % v/v MPD
E12	None	0.1 M Na HEPES	7.5	10 % w/v PEG 6000, 5% v/v MPD
F1	None	0.1 M Na HEPES	7.5	20 % v/v Jeffamine M-600
F2	0.1 M sodium chloride	0.1 M Na HEPES	7.5	1.6 M ammonium sulfate
F3	None	0.1 M Na HEPES	7.5	2.0 M ammonium formate
F4	0.05 M cadmium sulfate	0.1 M Na HEPES	7.5	1.0 M sodium acetate
F5	None	0.1 M Na HEPES	7.5	70 % v/v MPD
F6	None	0.1 M Na HEPES	7.5	4.3 M sodium chloride
F7	None	0.1 M Na HEPES	7.5	10 % w/v PEG 8000, 8 % v/v ethylene glycol
F8	None	0.1 M MES	6.5	1.6 M magnesium sulfate
F9	0.1 M sodium dihydrogen phosphate 0.1 M potassium dihydrogen phosphate	0.1 M MES	6.5	2.0 M sodium chloride
F10	None	0.1 M MES	6.5	12 % w/v PEG 20,000
F11	1.6 M ammonium sulfate	0.1 M MES	6.5	10 % v/v dioxane
F12	0.05 M caesium chloride	0.1 M MES	6.5	30 % v/v Jeffamine M-600
G1	0.01 M cobalt chloride	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	0.1 M MES	6.5	25 % v/v PEG 550 MME
G4	None	0.1 M Na HEPES	7.5	20 % w/v PEG 10,000
G5	0.2 M K/Na Tartrate	0.1 M Na citrate	5.6	2.0 M ammonium sulfate
G6	0.5 M ammonium sulfate	0.1 M Na citrate	5.6	1.0 M lithium sulfate
G7	0.5 M sodium chloride	0.1 M Na citrate	5.6	4% v/v polyethyleneimine
G8	None	0.1 M Na citrate	5.6	35 % v/v *tert*-Butanol
G9	0.01 M ferric chloride	0.1 M Na citrate	5.6	10 % v/v Jeffamine M-600
G10	0.01 M manganese chloride	0.1 M Na citrate	5.6	2.5 M 1,6-hexanediol
G11	None	0.1 M Na acetate	4.6	2.0 M sodium chloride
G12	0.2 M sodium chloride	0.1 M Na acetate	4.6	30 % v/v MPD
H1	0.01 M cobalt chloride	0.1 M Na acetate	4.6	1.0 M 1,6-hexanediol
H2	0.1 M cadmium chloride	0.1 M Na acetate	4.6	30 % v/v PEG 400
H3	0.2 M ammonium sulfate	0.1 M Na acetate	4.6	30 % w/v PEG 2000 MME
H4	2.0 M sodium chloride	None	None	10 % w/v PEG 6000
H5	0.01 M CTAB	None	None	0.5 M sodium chloride 0.1 M magnesium chloride
H6	None	None	None	25 % v/v ethylene glycol
H7	None	None	None	35 % v/v dioxane
H8	2.0 M ammonium sulfate	None	None	5 % v/v 2-propanol
H9	None	None	7.0	1.0 M imidazole
H10	None	None	None	10 % w/v PEG 1000, 10% w/v PEG 8000
H11	1.5 M sodium chloride	None	None	10 % v/v ethanol
H12	None	None	6.5	1.6 M sodium citrate

Abbreviations:
Bicine; N,N-Bis(2-hydroxyethyl)glycine, **CTAB**; cetyltrimethylammonium bromide. **HEPES**; N-(2-hydroxyethyl)-piperazine-N'-2-ethanesulfonic acid, **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.

Manufacturer's safety data sheets are available upon request.