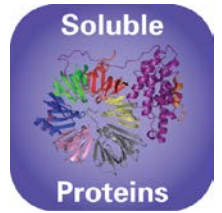


Molecular Dimensions



JCSG-plus™ HT-96 Eco screen

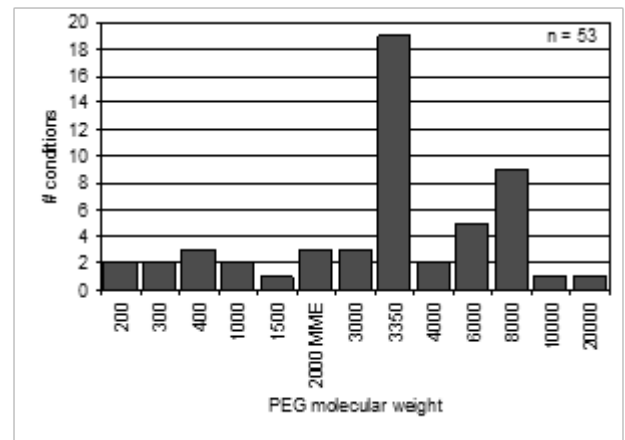
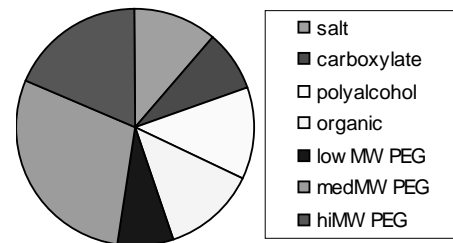
MD1-40-ECO

JCSG-plus is the screen of choice for initial screening experiments. The most complete sparse matrix screen available today.

MD1-40-ECO is presented as 96 x 1 mL cacodylate-free/dioxane-free conditions in a deep-well block.

Features of JCSG-plus: HT-96

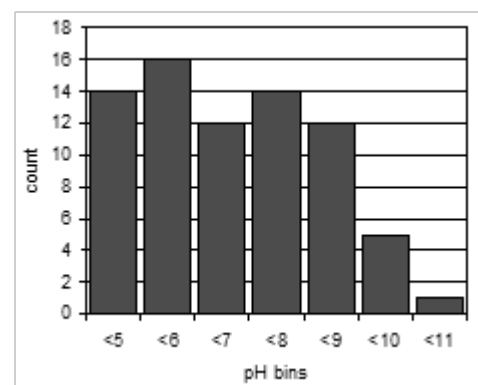
- Optimized sparse matrix screen without cacodylate (MES used instead) or dioxane.
- Reduced redundancy.
- Screens classic PEG and salt conditions.
- Access more areas of crystallization space.
- Neutralised organic acids: Formate, acetate, citrate, succinate, malate, malonate.
- More organic and polyalcohol conditions
- Precipitant synergy.
- Wide pH range 4.0 – 10.0.
- Cacodylate and dioxane-free.



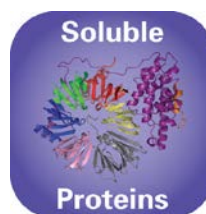
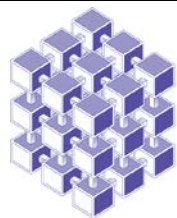
Introduction

Commercially available sparse matrix screens are devised using conditions based on previously successful crystallization conditions. Since increasing numbers of researchers now use commercially available sparse matrix screens, the same sub-sets of conditions are used repeatedly. A number of structural genomics initiatives have published results of data-mining exercises using internally consistent datasets and analysing negative results as well as positive hits. The results have been startling!

Members of the Joint Centre for Structural Genomics analysed the crystallization of over 500 different proteins against commercially available sparse matrix screens totalling 480 conditions, compiled to sample a wide range of precipitant, buffer, additive and pH. The **core screen (JCSG)** was developed when data mining revealed massive redundancy between clusters of conditions in commercial screens, particularly where high molecular weight PEGs are used as precipitants (1). Using a novel algorithm, members of the JCSG identified "conditions most essential for promoting crystal formation for the most diverse set of proteins. **JCSG+ supersedes the JCSG Core Screen and Index screens.**



Analysis of precipitants used in JCSG-plus



In-filling the optimized screen

The second issue to come to light was that even extensive suites of sparse matrix screens represent incomplete coverage of crystallisation space – 480 conditions failed to crystallise 15% of the target proteins.

The **JCSG-plus** screen is supplemented with additional conditions to provide a more complete coverage of crystallisation space and improved chemical complementarity (2).

- i. In-filling the pH profile
- ii. introduce conditions using neutralised organic acids as the precipitant (3)
- iii. expanded range of organic and polyalcohol conditions
- iv. precipitant synergy

Usage

JCSG-*plus* is designed for the rapid, efficient screening for crystallization leads of a new protein or preparation. In the first instance, drops should be set-up using equal volumes of protein solution and reagent. Protein samples should be in a minimal solvent system containing a low concentration of buffer. Starting protein concentrations should be between 5 mg/ml and 40 mg/ml. Protein concentration can be varied in subsequent rounds depending on initial results.

The conditions in JCSG-*plus* are compatible with all commonly used crystallisation methods, sitting drop, hanging drop, sandwich drop, microbatch, vapour microbatch and microdialysis.

The JCSG-*plus* sparse matrix screen is highly effective when used alongside a systematic screen such as PACT-*premier*. The two screens provide a thorough exploration of crystallization conditions and the unique design of PACT-*premier* facilitates rational interpretation of results from both itself and JCSG-*plus* assisting the design of subsequent experiments.

Formulation Notes:

JCSG-*plus* reagents are formulated using ultrapure water (>18.0 MΩ) and are sterile-filtered using 0.22 μm filters. No preservatives are added.

50% Stock solutions of Jeffamine are adjusted to pH 7.0 using HCl prior to inclusion in the reagents. 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 JCSG-*plus* formulation, interpretation of results or optimization strategies are welcome. Please e-mail, fax or phone your query to Molecular Dimensions.

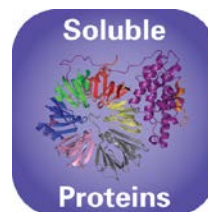
Contact and product details can be found at www.moleculardimensions.com

References.

1. Page *et al* (2003). Shotgun crystallization strategy for structural genomics: an optimized two-tiered crystallization screen against the *Thermotoga maritima* proteome. *Acta Cryst.* **D59**, 1028-1037
2. Newman *et al* (2005). Towards rationalization of crystallization screening for small- to medium-sized academic laboratories: the PACT/JCSG+ strategy. *Acta Cryst.* **D61**, 1426-1431
3. McPherson *et al* (2001). A comparison of salts for the crystallisation of macromolecules, *Protein Science* **10**, 418422
4. Crystallization of Nucleic Acids and Proteins, Edited by A. Ducruix and R. Giegé, The Practical Approach Series, Oxford Univ. Press, 1992
5. Protein Crystallization Techniques Strategies & Tips, Edited by Terese Bergfors, IUL 1999
6. Methods and Results in the Crystallization of Membrane Proteins, Edited by So Iwata, IUL 2003.

Hints & Tips:

The JCSG-*plus* sparse matrix screen is highly effective when used alongside a systematic screen such as PACT-*premier*. The two screens provide a thorough exploration of crystallization conditions and the unique design of PACT-*premier* facilitates rational interpretation of results from both itself and JCSG-*plus* assisting the design of subsequent experiments.

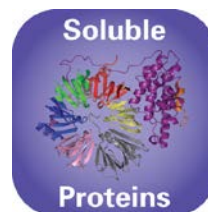


JCSG-plus HT-96 Eco Screen

Wells A1- D12

MD1-40-ECO

Well #	Conc.	Salt	Conc.	Buffer	pH	Conc.	Precipitant
A1	0.2 M	Lithium sulfate	0.1 M	Sodium acetate	4.5	50 % w/v	PEG 400
A2		None	0.1 M	Sodium citrate	5.5	20 % w/v	PEG 3000
A3	0.2 M	Ammonium citrate dibasic		None	-	20 % w/v	PEG 3350
A4	0.02 M	Calcium chloride dihydrate	0.1 M	Sodium acetate	4.6	30 % v/v	MPD
A5	0.2 M	Magnesium formate dihydrate		None	-	20 % w/v	PEG 3350
A6	0.2 M	Lithium sulfate	0.1 M	Phosphate/citrate	4.2	20 % w/v	PEG 1000
A7		None	0.1 M	CHES	9.5	20 % w/v	PEG 8000
A8	0.2 M	Ammonium formate		None	-	20 % w/v	PEG 3350
A9	0.2 M	Ammonium chloride		None	-	20 % w/v	PEG 3350
A10	0.2 M	Potassium formate		None	-	20 % w/v	PEG 3350
A11	0.2 M	Ammonium phosphate monobasic	0.1 M	Tris	8.5	50 % v/v	MPD
A12	0.2 M	Potassium nitrate		None	-	20 % w/v	PEG 3350
B1	0.8 M	Ammonium sulfate	0.1 M	Citrate	4.0		None
B2	0.2 M	Sodium thiocyanate		None	-	20 % w/v	PEG 3350
B3		None	0.1 M	BICINE	9.0	20 % w/v	PEG 6000
B4		None	0.1 M	HEPES	7.5	10 % w/v	PEG 8000 8 % v/v Ethylene glycol
B5		None	0.1 M	MES	6.5	40 % v/v	MPD 5 % w/v PEG 8000
B6		None	0.1 M	Phosphate/citrate	4.2	40 % v/v	Ethanol 5 % w/v PEG 1000
B7		None	0.1 M	Sodium acetate	4.6	8 % w/v	PEG 4000
B8	0.2 M	Magnesium chloride hexahydrate	0.1 M	Tris	7.0	10 % w/v	PEG 8000
B9		None	0.1 M	Citrate	5.0	20 % w/v	PEG 6000
B10	0.2 M	Magnesium chloride hexahydrate	0.1 M	MES	6.5	50 % v/v	PEG 200
B11	1.6 M	Sodium citrate tribasic dihydrate		None	6.5		None
B12	0.2 M	Potassium citrate tribasic monohydrate		None	-	20 % w/v	PEG 3350
C1	0.2 M	Sodium chloride	0.1 M	Phosphate/citrate	4.2	20 % w/v	PEG 8000
C2	1.0 M	Lithium chloride	0.1 M	Citrate	4.0	20 % w/v	PEG 6000
C3	0.2 M	Ammonium nitrate		None	-	20 % w/v	PEG 3350
C4		None	0.1 M	HEPES	7.0	10 % w/v	PEG 6000
C5	0.8 M	Sodium phosphate monobasic monohydrate	0.1 M	Sodium HEPES	7.5		None
C6		None	0.1 M	Phosphate/citrate	4.2	40 % v/v	PEG 300
C7	0.2 M	Zinc acetate dihydrate	0.1 M	Sodium acetate	4.5	10 % w/v	PEG 3000
C8		None	0.1 M	Tris	8.5	20 % v/v	Ethanol
C9		None	0.1 M	Sodium/potassium phosphate	6.2	25 % v/v	1,2-Propandiol 10 %v/v Glycerol
C10		None	0.1 M	BICINE	9.0	10 % w/v	PEG 20,000
C11	2.0 M	Ammonium sulfate	0.1 M	Sodium acetate	4.6		None
C12		None		None	-	10 % w/v	PEG 1000 10 % w/v PEG 8000
D1		None		None	-	24 % w/v	PEG 1500 20 % v/v Glycerol
D2	0.2 M	Magnesium chloride hexahydrate	0.1 M	Sodium HEPES	7.5	30 % v/v	PEG 400
D3	0.2 M	Sodium chloride	0.1 M	Sodium/potassium phosphate	6.2	50 % v/v	PEG 200
D4	0.2 M	Lithium sulfate	0.1 M	Sodium acetate	4.5	30 % w/v	PEG 8000
D5		None	0.1 M	HEPES	7.5	70 % v/v	MPD
D6	0.2 M	Magnesium chloride hexahydrate	0.1 M	Tris	8.5	20 % w/v	PEG 8000
D7	0.2 M	Lithium sulfate	0.1 M	Tris	8.5	40 % v/v	PEG 400
D8		None	0.1 M	Tris	8.0	40 % v/v	MPD
D9	0.17 M	Ammonium sulfate		None	-	26 % w/v	PEG 4000 15 % v/v Glycerol
D10	0.2 M	Calcium acetate hydrate	0.1 M	MES	6.5	40 % v/v	PEG 300
D11	0.14 M	Calcium chloride dihydrate	0.1 M	Sodium acetate	4.6	14 % v/v	2-Propanol 30 % v/v Glycerol
D12	0.04 M	Potassium phosphate monobasic		None	-	16 % w/v	PEG 8000 20 % v/v Glycerol



JCSG-plus HT-96 Eco Screen

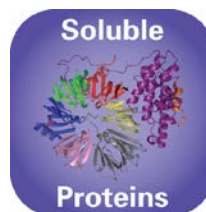
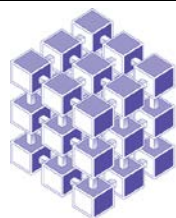
Wells E1 – H12

MD1-40-ECO

Well #	Conc.	Salt	Conc.	Buffer	pH	Conc.	Precipitant
E1	1.0 M	Sodium citrate tribasic dihydrate	0.1 M	MES	6.5		None
E2	2.0 M	Ammonium sulfate	0.1 M	MES	6.5		None
	0.2 M	Sodium chloride					
E3	0.2 M	Sodium chloride	0.1 M	HEPES	7.5	10 % v/v	2-Propanol
E4	1.26 M	Ammonium sulfate	0.1 M	Tris	8.5		None
	0.2 M	Lithium sulfate					
E5		None	0.1 M	CAPS	10.5	40 % v/v	MPD
E6	0.2 M	Zinc acetate dihydrate	0.1 M	Imidazole	8.0	20 % w/v	PEG 3000
E7	0.2 M	Zinc acetate dihydrate	0.1 M	MES	6.5	10 % v/v	2-Propanol
E8	1.0 M	Ammonium phosphate dibasic	0.1 M	Sodium acetate	4.5		None
E9	1.6 M	Magnesium sulfate heptahydrate	0.1 M	MES	6.5		None
E10		None	0.1 M	BICINE	9.0	10 % w/v	PEG 6000
E11	0.16 M	Calcium acetate hydrate	0.08 M	MES	6.5	14.4 % w/v	PEG 8000
						20 % v/v	Glycerol
E12		None	0.1 M	Imidazole	8.0	10 % w/v	PEG 8000
F1	0.05 M	Cesium chloride	0.1 M	MES	6.5	30 % v/v	Jeffamine® M-600
F2	3.2 M	Ammonium sulfate	0.1 M	Citrate	5.0		None
F3		None	0.1 M	Tris	8.0	20 % v/v	MPD
F4		None	0.1 M	HEPES	7.5	20 % v/v	Jeffamine® M-600
F5	0.2 M	Magnesium chloride hexahydrate	0.1 M	Tris	8.5	50 % v/v	Ethylene glycol
F6		None	0.1 M	BICINE	9.0	10 % v/v	MPD
F7	0.8 M	Succinic acid pH 7.0		None			None
F8	2.1 M	DL-Malic acid pH 7.0		None			None
F9	2.4 M	Sodium malonate dibasic monohydrate pH 7.0		None			None
F10	1.1 M	Sodium malonate dibasic monohydrate	0.1 M	HEPES	7.0	0.5 % v/v	Jeffamine® ED-2003
F11	1.0 M	Succinic acid	0.1 M	HEPES	7.0	1 % w/v	PEG 2000 MME
F12		None	0.1 M	HEPES	7.0	30 % v/v	Jeffamine® M-600
G1		None	0.1 M	HEPES	7.0	30 % v/v	Jeffamine® ED-2003
G2	0.02 M	Magnesium chloride hexahydrate	0.1 M	HEPES	7.5	22 % w/v	Poly(acrylic acid sodium salt) 5100
G3	0.01 M	Cobalt(II) chloride hexahydrate	0.1 M	Tris	8.5	20 % w/v	Polyvinylpyrrolidone
G4	0.2 M	TMAO	0.1 M	Tris	8.5	20 % w/v	PEG 2000 MME
G5	0.005 M	Cobalt(II) chloride hexahydrate	0.1 M	HEPES	7.5	12 % w/v	PEG 3350
	0.005 M	Cadmium chloride hemi(pentahydrate)					
	0.005 M	Magnesium chloride hexahydrate					
	0.005 M	Nickel(II) chloride hexahydrate					
G6	0.2 M	Sodium malonate dibasic monohydrate		None		20 % w/v	PEG 3350
G7	0.1 M	Succinic acid		None		15 % w/v	PEG 3350
G8	0.15 M	DL-Malic acid		None		20 % w/v	PEG 3350
G9	0.1 M	Potassium thiocyanate		None		30 % w/v	PEG 2000 MME
G10	0.15 M	Potassium bromide		None		30 % w/v	PEG 2000 MME
G11	2.0 M	Ammonium sulfate	0.1 M	BIS-Tris	5.5		None
G12	3.0 M	Sodium chloride	0.1 M	BIS-Tris	5.5		None
H1	0.3 M	Magnesium formate dihydrate	0.1 M	BIS-Tris	5.5		None
H2	1.0 M	Ammonium sulfate	0.1 M	BIS-Tris	5.5	1 % w/v	PEG 3350
H3		None	0.1 M	BIS-Tris	5.5	25 % w/v	PEG 3350
H4	0.2 M	Calcium chloride dihydrate	0.1 M	BIS-Tris	5.5	45 % v/v	MPD
H5	0.2 M	Ammonium acetate	0.1 M	BIS-Tris	5.5	45 % v/v	MPD
H6	0.1 M	Ammonium acetate	0.1 M	BIS-Tris	5.5	17 % w/v	PEG 10,000
H7	0.2 M	Ammonium sulfate	0.1 M	BIS-Tris	5.5	25 % w/v	PEG 3350
H8	0.2 M	Sodium chloride	0.1 M	BIS-Tris	5.5	25 % w/v	PEG 3350
H9	0.2 M	Lithium sulfate	0.1 M	BIS-Tris	5.5	25 % w/v	PEG 3350
H10	0.2 M	Ammonium acetate	0.1 M	BIS-Tris	5.5	25 % w/v	PEG 3350
H11	0.2 M	Magnesium chloride hexahydrate	0.1 M	BIS-Tris	5.5	25 % w/v	PEG 3350
H12	0.2 M	Ammonium acetate	0.1 M	HEPES	7.5	45 % v/v	MPD

Abbreviations: Bis Tris; Bis-(2-hydroxyethyl)imino-tris(hydroxymethyl)methane, **CAPS**; N-Cyclohexyl-3-aminopropanesulfonic acid, **CHES**; 2-(N-Cyclohexylamino)ethane Sulfonic Acid, **HEPES**; 2-(4-(2-Hydroxyethyl)-1-piperazinyl)ethanesulfonic Acid, **Na 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 (2K, 6K, 8K and 10K correspond to the molecular weight, in thousands of Daltons, of PEG), **TMAO**: Trimethylamine N-oxide, **Tris**; 2-Amino-2-(hydroxymethyl)propane-1,3-diol.

N.B. Jeffamine ED-2001 has been superseded with Jeffamine ED-2003. Polyvinylpyrrolidone K15 is called Polyvinylpyrrolidone.



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



Re-Ordering details:

Catalogue Description Code	Pack size	Catalogue
JCSG- <i>plus</i>	96 x 10 mL	MD1-37
JCSG- <i>plus</i> HT-96	96 x 1 mL	MD1-40
Eco screens		
JCSG- <i>plus</i> Eco Screen	96 x 10 mL	MD1-37-ECO
JCSG- <i>plus</i> HT-96 Eco Screen	96 x 1 mL	MD1-40-ECO
Green screens (contain fluorescent green dye- ideal for UV)		
JCSG- <i>plus</i> Green screen	96 x 10 mL	MD1-56
JCSG- <i>plus</i> HT-96 Green screen	96 x 1 mL	MD1-53
Combo Packs		
Super2 Combo Value Pack (JCSG- <i>plus</i> + PACT- <i>premier</i>)	2 x 96 x 10 mL	MD1-75
Super2 Combo HT-96 Value Pack (JCSG- <i>plus</i> HT-96 + PACT- <i>premier</i> HT-96)	2 x 96 x 10 mL	MD1-75-HT
Single Reagents		
JCSG- <i>plus</i> single reagents	100 mL	MDSR-37-tube number
JCSG- <i>plus</i> single reagents	100 mL	MDSR-40-well number

For JCSG-*plus* stock solutions please visit the Optimization section on our website.