Molecular Dimensions

Soluble Proteins

# JCSG-*plus*™ HT-96 MD1-40

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

MD1-40 is presented as 96 x 1 mL conditions in a deep-well block.

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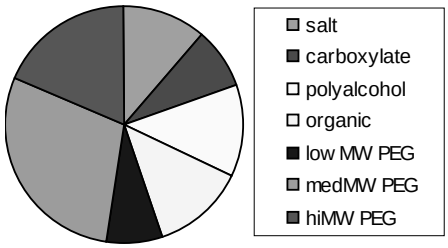
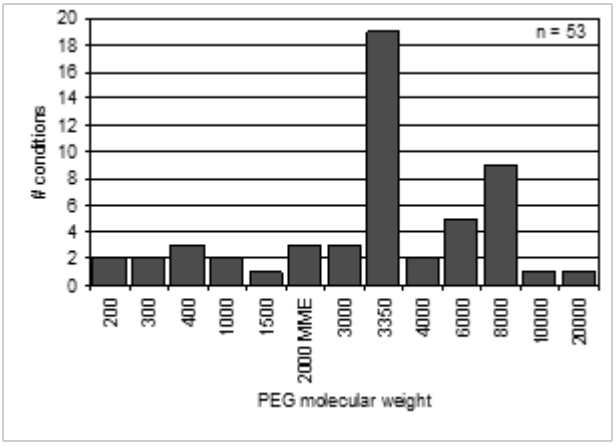
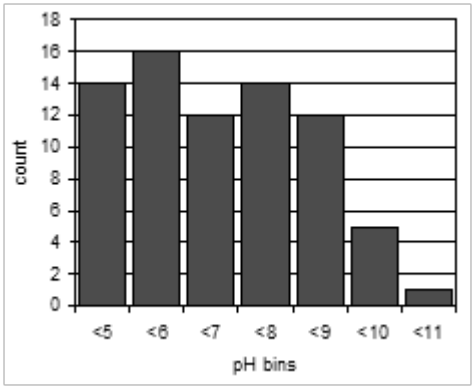
**Features of JCSG-*plus: HT-96***

- Optimized sparse matrix screen.
- 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.




***Analysis of precipitants used in JCSG-plus***

**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 JSCG Core Screen and Index screens.**

## 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.

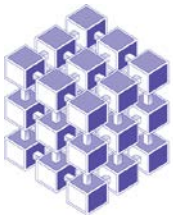
Contact and product details can be found at www.moleculardimensions.com

**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.



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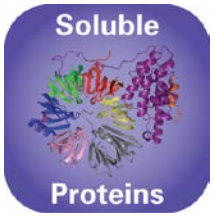


# JCSG-*plus* HT-96 Wells A1- D12 MD1–40

| 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 | Sodium cacodylate | 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 | Sodium cacodylate | 6.5 | 50 % v/v | PEG 200 |
| B11 | 1.6 M | Sodium citrate tribasic dihydrate pH 6.5 | | None | | | 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 |
| | 0.8 M | Potassium phosphate monobasic | | 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 |
| | | | | | | 2 % v/v | 1,4-Dioxane |
| 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 | | 25.5 % w/v | PEG 4000 |
| | | | | | | 15 % v/v | Glycerol |
| D10 | 0.2 M | Calcium acetate hydrate | 0.1 M | Sodium cacodylate | 6.5 | 40 % v/v | PEG 300 |
| D11 | 0.14 M | Calcium chloride dihydrate | 0.07 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 Wells E1 – H12 MD1–40

| Well # | Conc. | Salt | Conc. | Buffer | pH | Conc. | Precipitant |
|---|---|---|---|---|---|---|---|
| E1 | 1.0 M | Sodium citrate tribasic dihydrate | 0.1 M | Sodium cacodylate | 6.5 | | None |
| E2 | 2.0 M | Ammonium sulfate | 0.1 M | Sodium cacodylate | 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 | Sodium cacodylate | 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 | Magneisum 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 | Sodium cacodylate | 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. Polyvinylpyrolidone K15 is called Polyvinylpyrolidine.**

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

## Re-Ordering details:

| Catalogue Description | Pack size | Catalogue Code |
|---|---|---|
| JCSG-*plus* | 96 x 10 mL | MD1-37 |
| JCSG-*plus* HT-96 | 96 x 1 mL | MD1-40 |
| **Eco Screens** | | |
| JCSG-*plus* Eco Screen | 96 x 10 mL | MD1-37-ECO |
| JCSG-*plus* HT-96 Eco Screen | 96 x 1 mL | MD1-40-ECO |
| **Green screens** (contain fluorescent green dye- ideal for UV) | | |
| JCSG-*plus* Green screen | 96 x 10 mL | MD1-56 |
| JCSG-*plus* HT-96 Green screen | 96 x 1 mL | MD1-53 |
| **Combo Packs** | | |
| Super2 Combo Value Pack (JCSG-*plus* + PACT-*premier*) | 2 x 96 x 10 mL | MD1-75 |
| Super2 Combo HT-96 Value Pack (JCSG-*plus* HT-96 + PACT-*premier* HT-96) | 2 x 96 x 10 mL | MD1-75-HT |

| **Single Reagents** | | |
|---|---|---|
| JCSG-*plus* single reagents | 100 mL | MDSR-37-tube number |
| JCSG-*plus* single reagents | 100 mL | MDSR-40-well number |

For JCSG-plus stock solutions please visit the Optimization section on our website.
ECO screens contain no cacodylate, dioxane or azide etc.