Molecular Dimensions

Soluble Proteins

# SG1 Screen MD1-88

**From the CSRIO - the C3 ShotGun (SG1) Screen** - a set of 96 conditions that occur with highest, non-redundant frequency amongst all PDB deposits.

SG1 Screen uses the ShotGun approach to gather all the most successful conditions from all the early commercially available screens.

MD1-88 is presented as 96 x 10 mL conditions.

**Features of SG1 (ShotGun) Screen:**

- 96 of the most successful conditions from all the early commercially available screens.
- Provides a great start for easy optimization.
- Save money and time.

## Introduction

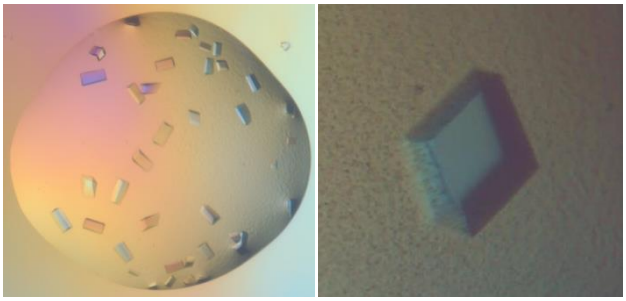
Commercial crystallization screening offers more than 15000 crystallization conditions for screening of new crystallization targets. Some conditions have been far more successful than others.

**SG1 (ShotGun) Screen** is designed by Janet Newman *et al* from **CSIRO** and represents the most successful, non-redundant frequently reported crystallization conditions* from all the early commercially available crystallization screens.

The term "shotgun screening" was coined early in the Structural Genomics era and refers to the process of setting up experiments using pre-mixed cocktails until a crystal of sufficient quality is obtained. The best place to start screening is within the context of previously successful crystallization space. "*Although only 14% of successful crystallization conditions from, the PDB are identical to a commercial condition, almost 40% of the PDB conditions can be obtained by trivial optimization of a commercial cocktail.*" (Fazio *et al*) So this is a reasonable place to commence screening.

However, that does leave 60% of deposits not covered in this screen and requiring additional screening tools.

Molecular Dimensions has always recommended JCSG-*plus*™ and PACT *premier*™ as powerful non-redundant screens containing 384 conditions that combine a sparse matrix approach with a systematic screen to give maximum information. The recent introduction of Morpheus®, MIDAS™ and The PGA Screen™ provide the opportunity to explore even wider crystallization space with the use of ligand screening and novel precipitants.



**Images of HSP90 (N-term domain) crystallized in C3 for MecRx from SG1 (ShotGun) Screen** *(courtesy of J.Newman, CSIRO)*

**Reference:**

Fazio VJ, Peat TS & Newman J (2014). A drunken search in Crystallization Space. Acta Cryst. F70:1303-1311

**These are conditions from commercially available crystallization screens that have been included in the REMARK280 field of the PDB ID code. It is therefore, biased slightly towards the earlier generation of classic screens, and not the later releases, such as Morpheus®, MIDAS™ etc. REMARK280 is a non-mandatory field in the PDB record and should only contain data associated with the crystallization cocktail and not the chemistry associated with protein formulation, the cryoprotectant or soaking solutions.*

**Formulation Notes:**

SG1 Screen 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 SG1 Screen 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 from our website or by scanning the QR code here:

## Re-Ordering details:

| Catalogue Description | | Catalogue Code |
|---|---|---|
| SG1 Screen | 96 x 10 mL | MD1-88 |
| SG1 Screen HT-96 | 96 x 1 mL | MD1-89 |
| SG1 Screen FX-96 | 96 x 80 µL | MD1-89-FX |
| **Eco Screens** | | |
| SG1 Eco Screen | 96 x 10 mL | MD1-88-ECO |
| SG1 Screen HT-96 Eco Screen | 96 x 1 mL | MD1-89-ECO |
| **Single Reagents** | | |
| SG1 Screen single reagent | 100 mL | MDSR-88-tube number |
| SG1 Screen HT-96 single reagent | 100 mL | MDSR-89-well number |

For SG1 Screen stock reagents visit our Optimization page on our website.

*Developed by Janet Newman (CSIRO) and manufactured under licence by Molecular Dimensions Ltd. Molecular Dimensions operates an ethical approach to all its products by making sure the inventors of its products receive the appropriate acknowledgments/rewards for their hard work. We hope you appreciate their hard work too and only buy the 'real-thing' anything else that is not licenced does not acknowledge or support the inventor and institute.

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# SG1 Screen Box 1 Conditions 1 - 48 MD1-88

| Tube # | Conc. | Salt1 | Conc. | Salt2 | Conc. | Buffer | pH | Conc. | Precipitant1 | Conc. | Precipitant2 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1-1 | 0.2 M | Magnesium chloride hexahydrate | | | 0.1 M | Tris | 8.5 | 30 % w/v | PEG 4000 | | |
| 1-2 | 2.0 M | Ammonium sulfate | | | | | | | | | |
| 1-3 | 0.2 M | Sodium acetate trihydrate | | | | | | 20 % w/v | PEG 3350 | | |
| 1-4 | 2.0 M | Ammonium sulfate | | | 0.1 M | Tris | 8.5 | | | | |
| 1-5 | 0.2 M | Sodium citrate tribasic dihydrate | | | | | | 20 % w/v | PEG 3350 | | |
| 1-6 | | | | | 0.1 M | Sodium HEPES | 7.5 | 20 % w/v | PEG 4000 | 10 % v/v | 2-Propanol |
| 1-7 | 2.0 M | Ammonium sulfate | | | 0.1 M | Sodium HEPES | 7.5 | 2 % v/v | PEG 400 | | |
| 1-8 | 1.4 M | Sodium citrate tribasic dihydrate | | | 0.1 M | Sodium HEPES | 7.5 | | | | |
| 1-9 | 0.2 M | Sodium acetate trihydrate | | | 0.1 M | Tris | 8.5 | 30 % w/v | PEG 4000 | | |
| 1-10 | 0.2 M | Lithium sulfate | | | 0.1 M | Tris | 8.5 | 30 % w/v | PEG 4000 | | |
| 1-11 | 4.0 M | Sodium formate | | | | | | | | | |
| 1-12 | 0.2 M | Magnesium acetate tetrahydrate | | | 0.1 M | Sodium cacodylate | 6.5 | 20 % w/v | PEG 8000 | | |
| 1-13 | | | | | 0.1 M | Bis-Tris | 5.5 | 25 % w/v | PEG 3350 | | |
| 1-14 | | | | | 0.1 M | MES | 6.5 | 12 % w/v | PEG 20000 | | |
| 1-15 | 0.2 M | Magnesium chloride hexahydrate | | | 0.1 M | Bis-Tris | 5.5 | 25 % w/v | PEG 3350 | | |
| 1-16 | 0.2 M | Ammonium sulfate | | | 0.1 M | MES | 6.5 | 30 % w/v | PEG 5000 MME | | |
| 1-17 | 0.2 M | Calcium chloride dihydrate | | | | | | 20 % w/v | PEG 3350 | | |
| 1-18 | | | | | 0.1 M | Sodium HEPES | 7.5 | 20 % w/v | PEG 10000 | | |
| 1-19 | 0.2 M | Sodium formate | | | | | | 20 % w/v | PEG 3350 | | |
| 1-20 | 0.2 M | Ammonium sulfate | | | 0.1 M | Bis-Tris | 5.5 | 25 % w/v | PEG 3350 | | |
| 1-21 | 1.6 M | Sodium citrate tribasic dihydrate | | | | | | | | | |
| 1-22 | 0.2 M | Calcium chloride dihydrate | | | 0.1 M | Sodium HEPES | 7.5 | 28 % v/v | PEG 400 | | |
| 1-23 | 0.2 M | Ammonium chloride | | | | | | 20 % w/v | PEG 3350 | | |
| 1-24 | 0.2 M | Magnesium formate dihydrate | | | | | | 20 % w/v | PEG 3350 | | |
| 1-25 | 0.2 M | Ammonium sulfate | | | 0.1 M | Sodium acetate | 4.6 | 25 % w/v | PEG 4000 | | |
| 1-26 | 1.4 M | Sodium malonate dibasic monohydrate pH 7.0 | | | | | | | | | |
| 1-27 | 0.2 M | Lithium sulfate | | | 0.1 M | Bis-Tris | 5.5 | 25 % w/v | PEG 3350 | | |
| 1-28 | 0.2 M | Potassium sodium tartrate tetrahydrate | | | | | | 20 % w/v | PEG 3350 | | |
| 1-29 | 0.2 M | Ammonium sulfate | | | 0.1 M | Sodium cacodylate | 6.5 | 30 % w/v | PEG 8000 | | |
| 1-30 | 2.0 M | Ammonium sulfate | | | 0.1 M | Sodium acetate | 4.6 | | | | |
| 1-31 | | | | | 0.1 M | Sodium HEPES | 7.5 | 25 % w/v | PEG 3350 | | |
| 1-32 | 0.2 M | Magnesium chloride hexahydrate | | | 0.1 M | Bis-Tris | 6.5 | 25 % w/v | PEG 3350 | | |
| 1-33 | 0.2 M | Magnesium chloride hexahydrate | | | 0.1 M | Tris | 8.5 | 25 % w/v | PEG 3350 | | |
| 1-34 | 0.2 M | Magnesium chloride hexahydrate | | | 0.1 M | Sodium HEPES | 7.5 | 25 % w/v | PEG 3350 | | |
| 1-35 | 0.2 M | Sodium acetate trihydrate | | | 0.1 M | Sodium cacodylate | 6.5 | 30 % w/v | PEG 8000 | | |
| 1-36 | 0.2 M | Sodium acetate trihydrate | | | 0.1 M | Bis-Tris | 5.5 | 25 % w/v | PEG 3350 | | |
| 1-37 | 1.5 M | Lithium sulfate | | | 0.1 M | Sodium HEPES | 7.5 | | | | |
| 1-38 | | | | | 0.1 M | Sodium citrate | 5.5 | 20 % w/v | PEG 3000 | | |
| 1-39 | | | | | | | | 25 % w/v | PEG 1500 | | |
| 1-40 | 0.2 M | Potassium thiocyanate | | | | | | 20 % w/v | PEG 3350 | | |
| 1-41 | 0.2 M | Sodium acetate trihydrate | | | 0.1 M | Sodium cacodylate | 6.5 | 18 % w/v | PEG 8000 | | |
| 1-42 | 0.2 M | Lithium sulfate | | | 0.1 M | Sodium HEPES | 7.5 | 25 % w/v | PEG 3350 | | |
| 1-43 | 0.2 M | Ammonium sulfate | | | | | | 30 % w/v | PEG 8000 | | |
| 1-44 | | | | | 0.1 M | Bis-Tris | 6.5 | 20 % w/v | PEG 5000 MME | | |
| 1-45 | 0.2 M | Ammonium sulfate | | | 0.1 M | Sodium acetate | 4.6 | 30 % w/v | PEG 2000 MME | | |
| 1-46 | 0.2 M | Lithium sulfate | | | 0.1 M | Bis-Tris | 6.5 | 25 % w/v | PEG 3350 | | |
| 1-47 | | | | | 0.1 M | Sodium acetate | 4.6 | 8 % w/v | PEG 4000 | | |
| 1-48 | 2.0 M | Ammonium sulfate | | | 0.1 M | Bis-Tris | 6.5 | | | | |

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# SG1 Screen Box 2 Conditions 1 - 48 MD1-88

| Tube # | Conc. | Salt1 | Conc. | Salt2 | Conc. | Buffer | pH | Conc. | Precipitant1 |
|---|---|---|---|---|---|---|---|---|---|
| 2-1 | 2.0 M | Ammonium sulfate | | | 0.1 M | Bis-Tris | 5.5 | | |
| 2-2 | | | | | | | | 25 % w/v | PEG 3350 |
| 2-3 | 0.2 M | Magnesium chloride hexahydrate | | | 0.1 M | Sodium HEPES | 7.5 | 30 % v/v | PEG 400 |
| 2-4 | 2.0 M | Ammonium sulfate | | | 0.1 M | Sodium HEPES | 7.5 | | |
| 2-5 | 3.5 M | Sodium formate | | | | | | | |
| 2-6 | 1.6 M | Magnesium sulfate heptahydrate | | | 0.1 M | MES | 6.5 | | |
| 2-7 | 0.2 M | Magnesium chloride hexahydrate | | | | | | 20 % w/v | PEG 3350 |
| 2-8 | 0.2 M | Ammonium sulfate | | | | | | 30 % w/v | PEG 4000 |
| 2-9 | 0.1 M | Potassium thiocyanate | | | | | | 30 % w/v | PEG 2000 MME |
| 2-10 | 0.2 M | Sodium malonate dibasic monohydrate pH7 | | | | | | 20 % w/v | PEG 3350 |
| 2-11 | 2.0 M | Sodium formate | | | 0.1 M | Sodium acetate | 4.6 | | |
| 2-12 | 0.2 M | Ammonium sulfate | | | 0.1 M | Sodium HEPES | 7.5 | 25 % w/v | PEG 3350 |
| 2-13 | 0.2 M | Potassium sodium tartrate tetrahydrate | 2.0 M | Ammonium sulfate | 0.1 M | Sodium citrate | 5.6 | | |
| 2-14 | 0.2 M | Sodium acetate trihydrate | | | 0.1 M | Sodium HEPES | 7.5 | 25 % w/v | PEG 3350 |
| 2-15 | 0.2 M | Ammonium sulfate | | | | | | 20 % w/v | PEG 3350 |
| 2-16 | 1.0 M | Sodium citrate tribasic dihydrate | | | 0.1 M | Sodium cacodylate | 6.5 | | |
| 2-17 | 0.2 M | Ammonium sulfate | | | 0.1 M | Bis-Tris | 6.5 | 25 % w/v | PEG 3350 |
| 2-18 | 0.2 M | Ammonium nitrate | | | | | | 20 % w/v | PEG 3350 |
| 2-19 | 0.2 M | Sodium thiocyanate | | | | | | 20 % w/v | PEG 3350 |
| 2-20 | 0.2 M | Potassium nitrate | | | | | | 20 % w/v | PEG 3350 |
| 2-21 | | | | | 0.1 M | Sodium HEPES | 7.5 | 20 % w/v | PEG 8000 |
| 2-22 | 0.2 M | Magnesium acetate tetrahydrate | | | | | | 20 % w/v | PEG 3350 |
| 2-23 | | | | | 0.1 M | Bis-Tris | 6.5 | 25 % w/v | PEG 3350 |
| 2-24 | 0.02 M | Calcium chloride dihydrate | | | 0.1 M | Sodium acetate | 4.6 | 30 % v/v | MPD |
| 2-25 | 0.2 M | Sodium acetate trihydrate | | | 0.1 M | MES | 6.0 | 20 % w/v | PEG 8000 |
| 2-26 | 0.2 M | Sodium sulfate | | | | | | 20 % w/v | PEG 3350 |
| 2-27 | 0.01 M | Zinc sulfate heptahydrate | | | 0.1 M | MES | 6.5 | 25 % v/v | PEG 550 MME |
| 2-28 | 0.2 M | Sodium tartrate dibasic dihydrate | | | | | | 20 % w/v | PEG 3350 |
| 2-29 | | | | | | | | 60 % v/v | T-mate pH 7.0 |
| 2-30 | 0.5 M | Ammonium sulfate | 1.0 M | Lithium sulfate | 0.1 M | Sodium citrate | 5.6 | | |
| 2-31 | | | | | | | | 30 % w/v | PEG 1500 |
| 2-32 | 0.2 M | Magnesium chloride hexahydrate | | | 0.1 M | Tris | 8.5 | 20 % w/v | PEG 8000 |
| 2-33 | 0.2 M | Ammonium tartrate dibasic | | | | | | 20 % w/v | PEG 3350 |
| 2-34 | 0.2 M | Sodium fluoride | | | | | | 20 % w/v | PEG 3350 |
| 2-35 | 0.2 M | Sodium chloride | 2.0 M | Ammonium sulfate | 0.1 M | Sodium cacodylate | 6.5 | | |
| 2-36 | 0.1 M | Sodium chloride | 1.6 M | Ammonium sulfate | 0.1 M | Sodium HEPES | 7.5 | | |
| 2-37 | 0.2 M | Ammonium formate | | | | | | 20 % w/v | PEG 3350 |
| 2-38 | 0.2 M | Lithium citrate tribasic tetrahydrate | | | | | | 20 % w/v | PEG 3350 |
| 2-39 | 0.2 M | Ammonium iodide | | | | | | 20 % w/v | PEG 3350 |
| 2-40 | 0.2 M | Sodium acetate trihydrate | | | 0.1 M | Bis-Tris | 6.5 | 25 % w/v | PEG 3350 |
| 2-41 | | | | | | | | 30 % w/v | PEG 4000 |
| 2-42 | | | | | 0.1 M | Tris | 8.5 | 25 % w/v | PEG 3350 |
| 2-43 | 0.2 M | Ammonium fluoride | | | | | | 20 % w/v | PEG 3350 |
| 2-44 | 0.1 M | Sodium acetate trihydrate | | | 0.1 M | Bis-Tris | 5.5 | 17 % w/v | PEG 10000 |
| 2-45 | 0.2 M | Sodium acetate trihydrate | | | 0.1 M | Imidazole | 8.0 | 10 % w/v | PEG 8000 |
| 2-46 | 0.2 M | Ammonium sulfate | | | 0.1 M | Tris | 8.5 | 25 % w/v | PEG 3350 |
| 2-47 | | | | | 0.1 M | CHES | 9.0 | 20 % w/v | PEG 8000 |
| 2-48 | 4.3 M | Sodium chloride | | | 0.1 M | Sodium HEPES | 7.5 | | |

**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, **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, **T-mate;** Sodium malonate dibasic monohydrate, Ammonium citrate dibasic, Succinic acid, DL-Malic acid, Sodium acetate trihydrate, Sodium formate, Ammonium tartrate tribasic.