Molecular Dimensions

Soluble Proteins

SG1 Screen™ MD1-88

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

SG1 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

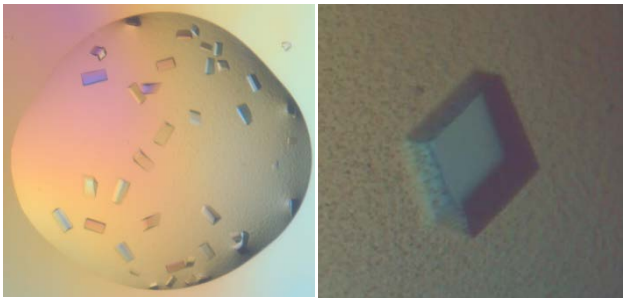
Commercial crystallization screening offers more than 15000 crystallization conditions for screening of new crystallization targets. Some conditions have been far more successful than others.

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 PGA 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 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 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:

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 x 80 uL (pre-filled plate)	MD1-89-FX
SG1 Screen™ ECO	96 x 10 mL Eco screen	MD1-88-ECO
SG1 Screen™ HT-96 ECO	96 x 1 mL Eco screen	MD1-89-ECO

Single Reagents

SG1 Screen™	(100 mL)	MDSR-88 - tube number
SG1 Screen™ HT-96	(100 mL)	MDSR-89 - tube number
SG1 Screen™ ECO	(100 mL)	MDSR-88-ECO - well number
SG1 Screen™ HT-96 ECO	(100 mL)	MDSR-89 ECO - 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, **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), **T-mate;** Sodium malonate, Ammonium citrate, Succinic acid, DL-Malic acid, Sodium acetate, Sodium formate, Ammonium tartrate.