MemGoldMeso™ 10 mL and HT-96* MD1-114, MD1-115

MemGoldMeso is rational sparse-matrix screen based on a hand-curated database of *in meso* phase crystallization conditions data-mined from the Protein Data Bank.

MD1-114 is presented as 96 x 10 mL conditions./MD-115 is presented as 96 x 1 mL conditions.

The most comprehensive LCP crystallisation screen:

- Based on a survey of the crystallisation conditions for mesophase structures in the PDB up to March 2017 – a more recent analysis than those used for other screens on the market.
- More structures from which to identify optimum *in meso* crystallisation conditions
- Wider range of proteins used in screen development, reducing bias to GPCR and rhodopsin conditions.
- Conditions taken from a hand-curated database to ensure no false positives from unrelated structures contributed to the formulation.
- From the trusted developers of our popular MemGold and MemGold2 screens, Prof. Simon Newstead and Dr Joanne Parker of Oxford University.

Introduction

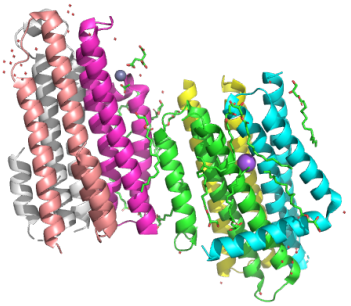
The protein environment for LCP crystallisation is strikingly different from that for other common crystallisation methods. Unsurprisingly, therefore, successful mesophase crystallisation conditions are very different to those for vapour diffusion. In addition, many classic crystallisation conditions can destabilize sponge phases. As a result, a screen specifically optimized for *in meso* phase crystallisation is an important factor in maximising the chances of success.

Prof. Simon Newstead of Oxford University, maintains a hand-curated database (1) of α-helical membrane protein structures and their crystallization conditions, which has already resulted in the development of our popular **MemGold**™ (2) and **MemGold**™ 2 (2,3) screens.

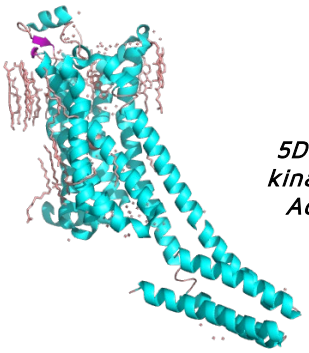
MemGoldMeso™ utilises Prof. Newstead and Dr Joanne Parker's hand-curated database to identify the optimum conditions for *in meso* phase crystallisation.

The conditions for this screen were developed from almost twice as many successful crystallisations as were available for earlier meso phase screens, resulting in a much more statistically robust identification of optimum conditions. In addition, a wider range of protein structures were available, resulting in a reduction in bias towards GPCR and rhodopsin-crystallising conditions.

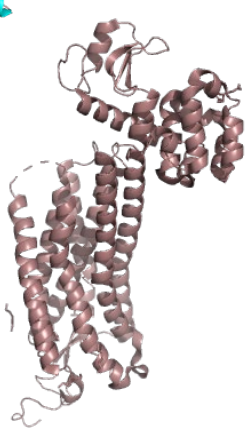
Examples of structures solved from crystals grown in conditions similar to those in MemGoldMeso include:



5K2C: A2a adenosine receptor. Batyuk, A et al. Sci. Adv. 2: e160092 (2016).



5DWK: Diacylglycerol kinase. Olieric, V et al. Acta Cryst D72: 421 (2016).



5T04: Neurotensin receptor. Krumm, BE. et al. Sci. Rep. 6: 38564 (2016).

Formulation Notes

MemGoldMeso™ 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 MemGoldMeso™ 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:

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RE-ORDERING INFORMATION

	Pack Size	Description
MD1-114	96 x 10 mL	MemGoldMeso
MD1-115	96 x 1 mL	MemGoldMeso HT-96
Eco Screens		
MD1-114-ECO	96 x 10 mL	MemGoldMeso ECO
MD1-115-ECO	96 x 1 mL	MemGoldMeso ECO HT-96
Single Reagents		
MDSR-114-tube number	100 mL	MemGoldMeso single reagents
MDSR-114-ECO-tube number	100 mL	MemGoldMeso ECO single reagents
MDSR-115-well number	100 mL	MemGoldMeso HT-96 single reagents
MDSR-115-ECO-well number	100 mL	MemGoldMeso ECO HT-96 single reagents

For MemChannel™ stock solutions please visit the Optimization section on our website.

*Developed by Prof. Simon Newstead and Dr Joanne Parker of Oxford University and exclusively licensed to Molecular Dimensions Ltd by Oxford University Innovation.

Abbreviations

ADA; 2-[(2-amino-2-oxoethyl)-(carboxymethyl)amino]acetic acid, **BICINE**; N,N-Bis(2-hydroxyethyl)glycine, **Bis-Tris**; 2-[Bis(2-hydroxyethyl)amino]-2-(hydroxymethyl)propane-1,3-diol, **Bis-tris propane;** 2,2'-(Propane-1,3-diyldiimino)bis[2-(hydroxymethyl)propane-1,3-diol], **HEPES**; N-(2-hydroxyethyl)-piperazine-N'-2-ethanesulfonic acid, **MME**; Monomethylether, **MOPS;** 3-Morpholinopropane-1-sulfonic acid, **PEG**; Polyethylene glycol, **Tricine;** N-(2-Hydroxy-1,1-bis(hydroxymethyl)ethyl)glycine, **Tris**; 2-Amino-2-(hydroxymethyl)propane-1,3-diol.

Images produced using LiteMol from the European Bioinformatics Institute and available to download from GitHub.

Manufacturer's safety data sheets are available from our website: moldim.com/memchannel-msds

References

1. Parker, JL and Newstead, S. Membrane protein crystallisation: current trends and future perspectives. *Adv. Exp. Med. Biol.* **922**: 61-72 (2016).
2. Newstead, S., Ferrandon, S., Iwata, S. Rationalizing alpha-helical membrane protein crystallization. *Protein Science* **17**: 466-472 (2008).
3. Parker, J. and Newstead, S. Current trends in alpha helical membrane protein crystallisation: an up-date. *Protein Science* **21**: 1358-1365 (2012).

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Well #	Tube #	Conc.		Salt 1	Conc.		Salt 2	Conc.		Buffer	pH	Conc.		Precipitant 1
A1	1-1	0.175	M	Sodium acetate trihydrate				0.100	M	MES monohydrate	6.50	42	% v/v	PEG 400
A2	1-2	0.100	M	Sodium chloride	0.100	M	Lithium nitrate	0.100	M	Sodium citrate	5.50	4	% v/v	MPD
A3	1-3	0.200	M	Lithium sulfate				0.100	M	MES monohydrate	6.80	25	% v/v	PEG 400
A4	1-4	0.075	M	Sodium malonate dibasic monohydrate				0.100	M	Sodium cacodylate	6.00	40	% v/v	PEG 300
A5	1-5	0.400	M	Lithium chloride				0.100	M	Tris	7.20	30	% v/v	PEG 400
A6	1-6	0.075	M	Sodium chloride				0.100	M	BICINE	9.00	32	% v/v	PEG 600
A7	1-7	0.100	M	Sodium succinate dibasic hexahydrate				0.100	M	MES monohydrate	6.30	32	% v/v	PEG 300
A8	1-8	0.100	M	Sodium chloride	0.060	M	Magnesium acetate tetrahydrate	0.050	M	Sodium citrate	6.30	5	% v/v	MPD
A9	1-9	0.200	M	Lithium sulfate				0.100	M	Sodium citrate	5.50	30	% v/v	PEG 400
A10	1-10	0.100	M	Magnesium sulfate heptahydrate	0.100	M	Sodium sulfate	0.050	M	MOPS	6.00	31	% v/v	PEG 500 MME
A11	1-11	0.150	M	Sodium chloride				0.900	M	Sodium/potassium phosphate dibasic	5.00			
A12	1-12	0.350	M	Magnesium chloride hexahydrate	0.150	M	Sodium malonate dibasic monohydrate	0.100	M	HEPES	7.50	33	% v/v	PEG 400
B1	1-13							1.000	M	Sodium/potassium phosphate dibasic	5.00	0.3	M	D-Trehalose
B2	1-14	0.220	M	Lithium sulfate				0.100	M	HEPES	7.00	28	% v/v	PEG 500 DME
B3	1-15	0.070	M	Ammonium fluoride				0.100	M	HEPES	8.00	32	% v/v	PEG 400
B4	1-16	0.200	M	Lithium sulfate				0.100	M	Phosphate/Citrate	4.20	10	% w/v	PEG 1000
B5	1-17	0.300	M	Ammonium phosphate monobasic	0.010	M	Magnesium chloride hexahydrate	0.100	M	Sodium citrate	4.50	30	% v/v	PEG 400
B6	1-18	0.300	M	Ammonium acetate				0.100	M	Bis-Tris	7.60	30	% v/v	PEG 400
B7	1-19							0.100	M	Sodium citrate	3.60	34	% v/v	PEG 400
B8	1-20	0.560	M	Ammonium sulfate				0.080	M	HEPES	7.50	18	% v/v	Jeffamine® M-600
B9	1-21	0.200	M	Sodium formate				0.100	M	Tris	8.00	27	% v/v	PEG 400
B10	1-22							0.100	M	Bis-Tris	5.50	25	% w/v	PEG 3350
B11	1-23							0.050	M	Sodium acetate	5.00	22	% v/v	Pentaethylene glycol
B12	1-24	0.180	M	Potassium sodium tartrate tetrahydrate				0.100	M	MES monohydrate	6.00	17	% v/v	PEG 400
C1	1-25	0.450	M	Potassium nitrate				0.100	M	Sodium citrate	6.00	30	% v/v	PEG 400
C2	1-26	0.040	M	Magnesium chloride hexahydrate				0.100	M	Tris	8.50	30	% v/v	PEG 400
C3	1-27	0.100	M	Sodium acetate trihydrate	0.100	M	Ammonium fluoride	0.100	M	MES monohydrate	6.00	30	% v/v	PEG 500 DME
C4	1-28	0.100	M	Ammonium phosphate monobasic				0.100	M	HEPES	7.50	45	% v/v	PEG 300
C5	1-29							1.100	M	Sodium/potassium phosphate dibasic	5.10			
C6	1-30	0.150	M	Ammonium sulfate				0.100	M	HEPES	7.50	10	% v/v	PEG 400
C7	1-31	0.100	M	Sodium chloride				0.100	M	Tris	8.50	24	% v/v	PEG 350 MME
C8	1-32	0.300	M	Ammonium phosphate dibasic				0.100	M	Tris	8.00	28	% v/v	PEG 400
C9	1-33							0.100	M	Sodium/potassium phosphate dibasic	5.60	32	% w/v	PEG 2000
C10	1-34	0.350	M	Ammonium acetate				0.100	M	Sodium citrate	5.00	35	% v/v	PEG 400
C11	1-35	0.300	M	Lithium sulfate				0.100	M	HEPES	7.00	35	% v/v	PEG 400
C12	1-36	0.100	M	Ammonium chloride	0.010	M	Calcium chloride dihydrate	0.100	M	MES monohydrate	6.50	10	% v/v	Pentaerythritol propoxylate (5/4 PO/OH
D1	1-37	0.250	M	Ammonium phosphate dibasic				0.100	M	MES monohydrate	6.00	28	% v/v	PEG 400
D2	1-38	0.080	M	Sodium citrate tribasic dihydrate				0.100	M	Tricine	8.30	36	% v/v	PEG 400
D3	1-39	0.100	M	Magnesium chloride hexahydrate				0.050	M	Sodium citrate	5.50	5	% v/v	MPD
D4	1-40	0.400	M	Sodium chloride				0.100	M	HEPES	7.00	20	% v/v	PEG 400
D5	1-41	0.300	M	Potassium formate				0.100	M	Bis-Tris	7.00	28	% v/v	PEG 400
D6	1-42	0.200	M	Sodium formate				0.100	M	Sodium citrate	6.00	31	% v/v	PEG 400
D7	1-43	0.350	M	Magnesium sulfate heptahydrate				0.100	M	Tris	8.30	28	% v/v	PEG 550 MME
D8	1-44	0.100	M	Potassium sodium tartrate tetrahydrate	0.100	M	Potassium nitrate	0.100	M	Tris	8.80	30	% v/v	PEG 550 MME
D9	1-45							0.100	M	BICINE	9.00	2	M	Ammonium sulfate
D10	1-46	0.100	M	Sodium chloride	0.100	M	Lithium sulfate	0.100	M	Sodium citrate	4.50	18	% v/v	PEG 400
D11	1-47	0.100	M	Sodium chloride	0.100	M	Potassium nitrate	0.100	M	Sodium citrate	5.50	8	% v/v	MPD
D12	1-48							0.050	M	ADA	5.80	0.6	M	Potassium sodium tartrate tetrahydrate

Well #	Tube #	Conc.		Salt 1	Conc.		Salt 2	Conc.		Buffer	pH	Conc.		Precipitant 1
E1	2-1	0.350	M	Ammonium formate				0.100	M	Tris	8.50	18	% v/v	1,4-Butanediol
E2	2-2	0.075	M	EDTA				0.100	M	MES monohydrate	6.00	25	% v/v	PEG 300
E3	2-3	0.050	M	Ammonium citrate dibasic				0.100	M	HEPES	6.80	28	% v/v	PEG 400
E4	2-4	0.200	M	Sodium malonate dibasic monohydrate				0.100	M	Sodium acetate	4.50	12	% w/v	PEG 3350
E5	2-5	0.025	M	Zinc sulfate heptahydrate				0.100	M	Sodium citrate	5.00	27	% v/v	PEG 550 MME
E6	2-6							0.100	M	Tris	7.50	14	% v/v	PEG 400
E7	2-7	0.100	M	Ammonium nitrate				0.100	M	MES monohydrate	6.50	27	% v/v	PEG 500 DME
E8	2-8	0.200	M	Ammonium phosphate dibasic				0.100	M	HEPES	6.80	24	% v/v	PEG 400
E9	2-9	0.400	M	Ammonium phosphate monobasic				0.100	M	ADA	7.00	34	% v/v	PEG 400
E10	2-10	0.050	M	Magnesium citrate tribasic nonahydrate				0.100	M	Sodium acetate	4.00	42	% v/v	PEG 200
E11	2-11	0.400	M	Potassium citrate monobasic				0.100	M	Sodium citrate	6.00	28	% v/v	PEG 400
E12	2-12	0.120	M	Sodium chloride				0.100	M	MOPS	6.00	35	% v/v	PEG 400
F1	2-13	0.175	M	Ammonium formate				0.100	M	Sodium cacodylate	6.50	35	% v/v	PEG 400
F2	2-14	0.200	M	Sodium chloride				0.100	M	MES monohydrate	6.80	35	% v/v	PEG 400
F3	2-15	0.050	M	Sodium chloride	0.050	M	Magnesium acetate tetrahydrate	0.100	M	MES monohydrate	6.50	35	% v/v	PEG 200
F4	2-16	0.100	M	Sodium citrate tribasic dihydrate				0.100	M	MES monohydrate	6.00	32	% w/v	PEG 1000
F5	2-17	0.220	M	Potassium nitrate				0.100	M	Sodium citrate	6.00	30	% v/v	PEG 400
F6	2-18							0.525	M	Sodium malonate	5.60	3	% w/v	PEG 6000
F7	2-19	0.160	M	Lithium sulfate	0.004	M	Strontium chloride hexahydrate	0.100	M	ADA	6.50	40	% v/v	PEG 400
F8	2-20	0.100	M	Sodium thiocyanate	0.020	M	Calcium chloride dihydrate	0.050	M	MES monohydrate	6.50	30	% v/v	PEG 400
F9	2-21	0.025	M	Magnesium sulfate heptahydrate				0.100	M	Sodium cacodylate	6.50	42	% v/v	PEG 300
F10	2-22	0.075	M	Magnesium sulfate heptahydrate				0.100	M	BICINE	8.00	30	% v/v	PEG 400
F11	2-23	0.050	M	Magnesium chloride hexahydrate	0.150	M	Sodium chloride	0.100	M	Sodium citrate	6.00	30	% v/v	PEG 500 DME
F12	2-24	0.025	M	Ammonium formate				0.100	M	Sodium cacodylate	6.00	25	% v/v	PEG 400
G1	2-25	0.100	M	Ammonium citrate dibasic				0.100	M	HEPES	8.00	20	% v/v	PEG 350 MME
G2	2-26	0.002	M	Cadmium chloride hemi(pentahydrate)				0.100	M	Sodium cacodylate	6.00	28	% v/v	PEG 500 DME
G3	2-27	0.175	M	Potassium sodium tartrate tetrahydrate				0.100	M	Bis-Tris propane	6.50	32	% v/v	PEG 400
G4	2-28	0.080	M	Ammonium phosphate dibasic				0.100	M	HEPES	7.50	32	% v/v	PEG 300
G5	2-29	0.450	M	Sodium chloride				0.100	M	Sodium cacodylate	6.50	39	% v/v	PEG 400
G6	2-30	0.120	M	Ammonium phosphate dibasic				0.100	M	Sodium acetate	5.00	28	% v/v	PEG 400
G7	2-31	0.050	M	Sodium thiocyanate				0.100	M	Sodium citrate	5.00	25	% v/v	PEG 400
G8	2-32	0.100	M	Magnesium acetate tetrahydrate				0.100	M	ADA	6.50	39	% v/v	PEG 400
G9	2-33	0.040	M	EDTA				0.100	M	HEPES	7.00	15	% v/v	PEG 300
G10	2-34							0.075	M	Sodium acetate	4.50	1.5	M	Sodium chloride
G11	2-35	0.120	M	Magnesium formate dihydrate	0.100	M	Sodium chloride	0.100	M	Tris	8.50	33	% v/v	PEG 600
G12	2-36							0.100	M	Sodium cacodylate	6.50	30	% v/v	PEG 550 MME
H1	2-37	0.200	M	Sodium malonate dibasic monohydrate				0.100	M	Tris	8.00	29	% v/v	PEG 400
H2	2-38	0.150	M	Sodium sulfate				0.100	M	Bis-Tris	6.30	35	% v/v	PEG 400
H3	2-39	0.100	M	Sodium acetate trihydrate				0.100	M	Bis-Tris propane	8.30	25	% v/v	PEG 300
H4	2-40	0.175	M	Magnesium chloride hexahydrate				0.100	M	Sodium citrate	5.00	30	% v/v	PEG 400
H5	2-41	0.550	M	Ammonium sulfate				0.050	M	ADA	7.00	26	% v/v	PEG 550 MME
H6	2-42	0.030	M	Ammonium formate				0.050	M	HEPES	7.50	38	% v/v	PEG 200
H7	2-43	0.100	M	Ammonium sulfate	0.200	M	Sodium citrate tribasic dihydrate	0.100	M	HEPES	8.00	35	% v/v	PEG 200
H8	2-44	0.150	M	Potassium sodium tartrate tetrahydrate				0.100	M	Bis-Tris propane	6.50	25	% v/v	PEG 400
H9	2-45	0.250	M	Potassium formate	0.010	M	Zinc sulfate heptahydrate	0.100	M	Sodium acetate	4.00	28	% v/v	PEG 550 MME
H10	2-46							0.100	M	Tris	8.00	44	% v/v	PEG 400
H11	2-47	0.050	M	Lithium citrate hydrate				0.080	M	HEPES	7.00	20	% v/v	PEG 400
H12	2-48							3.000	M	Sodium/potassium phosphate dibasic	5.50			