The Ligand-Friendly Screen Eco version 10 mL and HT-96 MD1-121-ECO and MD1-122-ECO

The Ligand-Friendly Screen (LFS) is a semi-systematic screen based on the PACT*premier* screen and optimized for compound-binding studies

MD1-121-ECO is presented as 96 x 10 mL conditions./MD-122-ECO is presented as 96 x 1 mL conditions.

PCTP buffer has been replaced by PMTP buffer in this kit.

The LFS is designed to provide crystals that are directly usable for compound binding studies:

- Identify more tight-binding ligands, as it contains no components that are likely to bind at protein-ligand interaction sites.
- Near physiological pH conditions ensure you are studying the active form of your protein.
- More hits for rarely-crystallising proteins. The semi-systematic format of the screen provides multiple trials of similar conditions - an important factor for difficult cases.
- Increased hit rate for ligand co-crystallisations – the semi-systematic format efficiently screens around related conditions when complex formation alters crystallisation conditions.

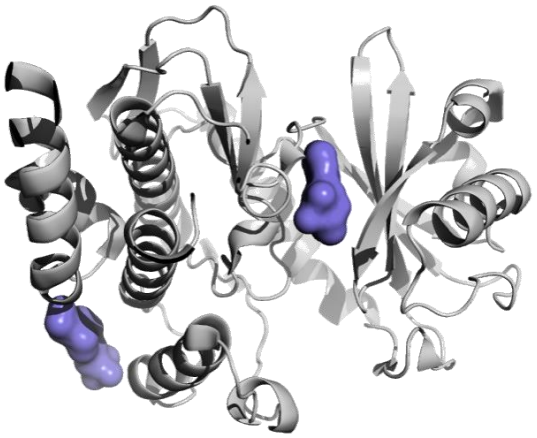
Introduction

The Ligand-Friendly Screen (LFS)[1] has been one of the two primary coarse screens of the Structural Genomics Consortium (SGC) in Oxford since 2004; at last count, it had produced 190 novel structures over 10 years.

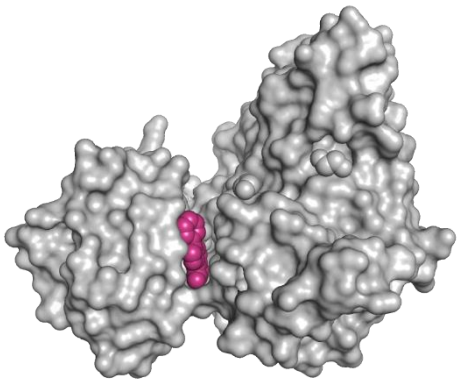
The screen was developed at the SGC in the Protein Crystallography group of Prof. Frank von Delft, which also developed one of our most successful screens of 2017, the BCS screen. LFS was designed by Dr Janet Newman (who since then set up the Collaborative Crystallization Centre, CSIRO, Australia) and Frank von Delft, as a modification of Dr Newman's popular PACT screen[2]: it screens combinations of PEG (1K to 6K), salts and buffers at near-physiological pH in a semi-systematic manner.

Structures crystallised in LFS conditions include:

- Haspin in complex with a range of halo-aromatic inhibitors including the complex with 5-



iodotubercidin (PDBID: 6G34)[3]:



- CLK3 in complex with a new inhibitor chemotype (PDBID: 6FT7)[4].

References

1. Ng, J. T *et al. Acta Cryst* D**72**: 224-235 (2015).
2. Newman, J. *et al. Acta Cryst D***61**: 1426-1431 (2015).
3. Heroven *et al. Angew. Chem. Int. Ed. Engl.* **57**: 7220-7224 (2018).
4. Walter, A. *et al. PLoS One* **13**: e0196761 (2018)

Formulation Notes

The Ligand-Friendly 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 The Ligand-Friendly 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.

Abbreviations

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, **MES**; 2-(N-morpholino)ethanesulfonic acid, **MIB**; Sodium malonate dibasic monohydrate, imidazole, boric acid, **MMT**; DL-Malic acid, MES monohydrate, **MPD**; 2-methyl-2,4-pentanediol, **PEG**; Polyethylene glycol, **PMPT**; Sodium propionate, MES, bis-tris propane, **Tris**; 2-Amino-2-(hydroxymethyl)propane-1,3-diol, **SPG**; succinic acid, sodium phosphate monobasic monohydrate, glycine.

Images produced using PyMol.

RE-ORDERING INFORMATION

	Pack Size	Description
MD1-121	96 x 10 mL	The LFS
MD1-122	96 x 1 mL	The LFS HT-96
MD1-122-FX	96 x 100 µL	The LFS FX-96 pre-filled plate
Eco Screens		
MD1-121-ECO	96 x 10 mL	The LFS ECO
MD1-122-ECO	96 x 1 mL	The LFS ECO HT-96
Single Reagents		
MDSR-121-tube number	100 mL	The LFS single reagents
MDSR-121-ECO-tube number	100 mL	The LFS ECO single reagents
MDSR-122-well number	100 mL	The LFS HT-96 single reagents
MDSR-122-ECO-well number	100 mL	The LFS ECO HT-96 single reagents

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Well #	Tube #	Conc.		Buffer	Conc.		Salt	Conc.		Precipitant 1	Conc.		Precipitant 2
A1	1-1	0.1	M	SPG pH 6				30	% w/v	PEG 1000			
A2	1-2	0.1	M	SPG pH 7				30	% w/v	PEG 1000			
A3	1-3	0.1	M	SPG pH 8				30	% w/v	PEG 1000			
A4	1-4	0.1	M	SPG pH 6				55	% v/v	MPD			
A5	1-5	0.1	M	SPG pH 7				55	% v/v	MPD			
A6	1-6	0.1	M	SPG pH 8				55	% v/v	MPD			
A7	1-7				0.2	M	Sodium chloride	20	% w/v	PEG 6000	10	% v/v	Ethylene glycol
A8	1-8				0.2	M	Ammonium chloride	20	% w/v	PEG 6000	10	% v/v	Ethylene glycol
A9	1-9				0.2	M	Lithium chloride	20	% w/v	PEG 6000	10	% v/v	Ethylene glycol
A10	1-10				0.1	M	Magnesium chloride hexahydrate	20	% w/v	PEG 6000	10	% v/v	Ethylene glycol
A11	1-11				0.1	M	Calcium chloride dihydrate	20	% w/v	PEG 6000	10	% v/v	Ethylene glycol
A12	1-12				0.01	M	Zinc chloride	20	% w/v	PEG 6000	10	% v/v	Ethylene glycol
B1	1-13	0.1	M	MIB pH 6				30	% w/v	PEG 1000			
B2	1-14	0.1	M	MIB pH 7				30	% w/v	PEG 1000			
B3	1-15	0.1	M	MIB pH 8				30	% w/v	PEG 1000			
B4	1-16	0.1	M	MIB pH 6				55	% v/v	MPD			
B5	1-17	0.1	M	MIB pH 7				55	% v/v	MPD			
B6	1-18	0.1	M	MIB pH 8				55	% v/v	MPD			
B7	1-19	0.1	M	MES pH 6	0.2	M	Sodium chloride	20	% w/v	PEG 6000	10	% v/v	Ethylene glycol
B8	1-20	0.1	M	MES pH 6	0.2	M	Ammonium chloride	20	% w/v	PEG 6000	10	% v/v	Ethylene glycol
B9	1-21	0.1	M	MES pH 6	0.2	M	Lithium chloride	20	% w/v	PEG 6000	10	% v/v	Ethylene glycol
B10	1-22	0.1	M	MES pH 6	0.1	M	Magnesium chloride hexahydrate	20	% w/v	PEG 6000	10	% v/v	Ethylene glycol
B11	1-23	0.1	M	MES pH 6	0.1	M	Calcium chloride dihydrate	20	% w/v	PEG 6000	10	% v/v	Ethylene glycol
B12	1-24	0.1	M	MES pH 6	0.01	M	Zinc chloride	20	% w/v	PEG 6000	10	% v/v	Ethylene glycol
C1	1-25	0.1	M	PMTP pH 6				30	% w/v	PEG 1000			
C2	1-26	0.1	M	PMTP pH 7				30	% w/v	PEG 1000			
C3	1-27	0.1	M	PMTP pH 8				30	% w/v	PEG 1000			
C4	1-28	0.1	M	PMTP pH 6				60	% v/v	MPD			
C5	1-29	0.1	M	PMTP pH 7				60	% v/v	MPD			
C6	1-30	0.1	M	PMTP pH 8				60	% v/v	MPD			
C7	1-31	0.1	M	HEPES pH 7	0.2	M	Sodium chloride	20	% w/v	PEG 6000	10	% v/v	Ethylene glycol
C8	1-32	0.1	M	HEPES pH 7	0.2	M	Ammonium chloride	20	% w/v	PEG 6000	10	% v/v	Ethylene glycol
C9	1-33	0.1	M	HEPES pH 7	0.2	M	Lithium chloride	20	% w/v	PEG 6000	10	% v/v	Ethylene glycol
C10	1-34	0.1	M	HEPES pH 7	0.1	M	Magnesium chloride hexahydrate	20	% w/v	PEG 6000	10	% v/v	Ethylene glycol
C11	1-35	0.1	M	HEPES pH 7	0.1	M	Calcium chloride dihydrate	20	% w/v	PEG 6000	10	% v/v	Ethylene glycol
C12	1-36	0.1	M	HEPES pH 7	0.01	M	Zinc chloride	20	% w/v	PEG 6000	10	% v/v	Ethylene glycol
D1	1-37	0.1	M	MMT pH 6				30	% w/v	PEG 1000			
D2	1-38	0.1	M	MMT pH 7				30	% w/v	PEG 1000			
D3	1-39	0.1	M	MMT pH 8				30	% w/v	PEG 1000			
D4	1-40	0.1	M	MMT pH 6				60	% v/v	MPD			
D5	1-41	0.1	M	MMT pH 7				60	% v/v	MPD			
D6	1-42	0.1	M	MMT pH 8				60	% v/v	MPD			
D7	1-43	0.1	M	tris pH 7.5	0.2	M	Sodium chloride	20	% w/v	PEG 6000	10	% v/v	Ethylene glycol
D8	1-44	0.1	M	tris pH 7.5	0.2	M	Ammonium chloride	20	% w/v	PEG 6000	10	% v/v	Ethylene glycol
D9	1-45	0.1	M	tris pH 7.5	0.2	M	Lithium chloride	20	% w/v	PEG 6000	10	% v/v	Ethylene glycol
D10	1-46	0.1	M	tris pH 7.5	0.1	M	Magnesium chloride hexahydrate	20	% w/v	PEG 6000	10	% v/v	Ethylene glycol
D11	1-47	0.1	M	tris pH 7.5	0.1	M	Calcium chloride dihydrate	20	% w/v	PEG 6000	10	% v/v	Ethylene glycol
D12	1-48	0.1	M	tris pH 7.5	0.01	M	Zinc chloride	20	% w/v	PEG 6000	10	% v/v	Ethylene glycol

Well #	Tube #	Conc.		Buffer	Conc.		Salt	Conc.		Precipitant 1	Conc.		Precipitant 2
E1	2-1				0.2	M	Sodium fluoride	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
E2	2-2				0.2	M	Sodium bromide	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
E3	2-3				0.2	M	Sodium iodide	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
E4	2-4				0.2	M	Potassium thiocyanate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
E5	2-5				0.2	M	Sodium nitrate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
E6	2-6				0.2	M	Sodium formate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
E7	2-7				0.2	M	Sodium acetate trihydrate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
E8	2-8				0.2	M	Sodium sulfate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
E9	2-9				0.2	M	Potassium sodium tartrate tetrahydrate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
E10	2-10				0.02	M	sodium potassium phosphate pH 7.5	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
E11	2-11				0.2	M	Potassium citrate tribasic monohydrate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
E12	2-12				0.2	M	Sodium malonate dibasic monohydrate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
F1	2-13	0.1	M	Bis Tris Propane pH 6.5	0.2	M	Sodium fluoride	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
F2	2-14	0.1	M	Bis Tris Propane pH 6.5	0.2	M	Sodium bromide	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
F3	2-15	0.1	M	Bis Tris Propane pH 6.5	0.2	M	Sodium iodide	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
F4	2-16	0.1	M	Bis Tris Propane pH 6.5	0.2	M	Potassium thiocyanate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
F5	2-17	0.1	M	Bis Tris Propane pH 6.5	0.2	M	Sodium nitrate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
F6	2-18	0.1	M	Bis Tris Propane pH 6.5	0.2	M	Sodium formate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
F7	2-19	0.1	M	Bis Tris Propane pH 6.5	0.2	M	Sodium acetate trihydrate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
F8	2-20	0.1	M	Bis Tris Propane pH 6.5	0.2	M	Sodium sulfate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
F9	2-21	0.1	M	Bis Tris Propane pH 6.5	0.2	M	Potassium sodium tartrate tetrahydrate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
F10	2-22	0.1	M	Bis Tris Propane pH 6.5	0.02	M	Sodium potassium phosphate pH 7.5	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
F11	2-23	0.1	M	Bis Tris Propane pH 6.5	0.2	M	Potassium citrate tribasic monohydrate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
F12	2-24	0.1	M	Bis Tris Propane pH 6.5	0.2	M	Sodium malonate dibasic monohydrate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
G1	2-25	0.1	M	Bis Tris Propane pH 7.5	0.2	M	Sodium fluoride	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
G2	2-26	0.1	M	Bis Tris Propane pH 7.5	0.2	M	Sodium bromide	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
G3	2-27	0.1	M	Bis Tris Propane pH 7.5	0.2	M	Sodium iodide	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
G4	2-28	0.1	M	Bis Tris Propane pH 7.5	0.2	M	Potassium thiocyanate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
G5	2-29	0.1	M	Bis Tris Propane pH 7.5	0.2	M	Sodium nitrate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
G6	2-30	0.1	M	Bis Tris Propane pH 7.5	0.2	M	Sodium formate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
G7	2-31	0.1	M	Bis Tris Propane pH 7.5	0.2	M	Sodium acetate trihydrate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
G8	2-32	0.1	M	Bis Tris Propane pH 7.5	0.2	M	Sodium sulfate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
G9	2-33	0.1	M	Bis Tris Propane pH 7.5	0.2	M	Potassium sodium tartrate tetrahydrate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
G10	2-34	0.1	M	Bis Tris Propane pH 7.5	0.02	M	Sodium potassium phosphate pH 7.5	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
G11	2-35	0.1	M	Bis Tris Propane pH 7.5	0.2	M	Potassium citrate tribasic monohydrate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
G12	2-36	0.1	M	Bis Tris Propane pH 7.5	0.2	M	Sodium malonate dibasic monohydrate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
H1	2-37	0.1	M	Bis Tris Propane pH 8.5	0.2	M	Sodium fluoride	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
H2	2-38	0.1	M	Bis Tris Propane pH 8.5	0.2	M	Sodium bromide	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
H3	2-39	0.1	M	Bis Tris Propane pH 8.5	0.2	M	Sodium iodide	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
H4	2-40	0.1	M	Bis Tris Propane pH 8.5	0.2	M	Potassium thiocyanate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
H5	2-41	0.1	M	Bis Tris Propane pH 8.5	0.2	M	Sodium nitrate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
H6	2-42	0.1	M	Bis Tris Propane pH 8.5	0.2	M	Sodium formate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
H7	2-43	0.1	M	Bis Tris Propane pH 8.5	0.2	M	Sodium acetate trihydrate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
H8	2-44	0.1	M	Bis Tris Propane pH 8.5	0.2	M	Sodium sulfate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
H9	2-45	0.1	M	Bis Tris Propane pH 8.5	0.2	M	Potassium sodium tartrate tetrahydrate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
H10	2-46	0.1	M	Bis Tris Propane pH 8.5	0.02	M	Sodium potassium phosphate pH 8.5	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
H11	2-47	0.1	M	Bis Tris Propane pH 8.5	0.2	M	Potassium citrate tribasic monohydrate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol
H12	2-48	0.1	M	Bis Tris Propane pH 8.5	0.2	M	Sodium malonate dibasic monohydrate	20	% w/v	PEG 3350	10	% v/v	Ethylene glycol