Molecular Dimensions

Soluble Proteins

PACT *premier*™ HT-96 / FX-96 MD1-36 / MD1-36-FX

PACT *premier* is a pH, Anion, Cation crystallization trial devised to test pH within a PEG/Ion screen.

MD1-36 is presented as 96 x 1 mL conditions / MD1-36-FX is presented as 96 x 100 µL conditions

Features of PACT *premier*™:

- A modern, comprehensive PEG/ion screen.
- This 96-well screen is really 3 screens in one:
  - 24-well pH/PEG screen
  - 24-well cation/PEG screen
  - 48-well anion/PEG screen

Rationale for a new PEG/Ion screen

The first step in crystallization is often to reach for a commercially available "sparse matrix" kit, and hope that one of the conditions produces something that looks harvestable, or optimizable. If no obvious leads come out of the screen, it is hard to learn anything from the negative (precipitate and clear) results.

There are a few screens that try to test crystallization space in a more rational manner – for example, the Clear Strategy™ Screen and The Solubility Tool Kit.

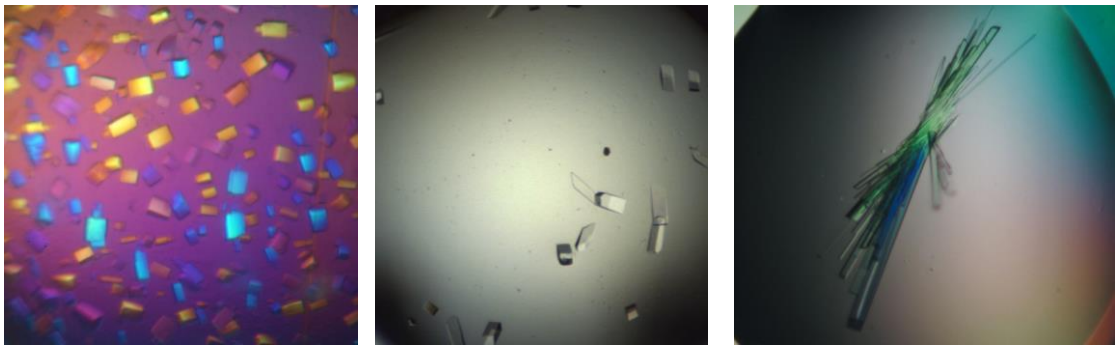
Traditional PEG/Ion screens provide a logical test of seven cations and eleven anions using PEG 3350 as the precipitation agent. However, the user has no control over pH and hence cannot determine the effect of one cation or anion over another.

For this reason the PEG/ION/pH (PACT) screen has been developed to systematically test the effect of pH, anions and cations, using PEG as the precipitant. This screen has been implemented very successfully at the Netherlands Cancer Institute (NKI), and at the Oxford Protein Production Facility (OPPF).

PACT *premier*™

pH/PEG screen

This consists of four broad range buffer systems (1) versus PEG 1500. These buffers allow one to scan the pH range from 4 to 9, without changing the chemistry of the system, so effectively isolating the effect of pH from the effect of the buffer that causes the change in pH.



Protein crystals grown successfully with PACT *premier*™.

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Cation/PEG screen

This is made up of six cations (all with chloride counter ions) that are combined with PEG 6000 at four different pHs: Acetate pH 5.0, MES pH 6.0, HEPES pH 7.0 and Tris pH 8.0. The cations tested are Na^+, NH_4^+, Li^+, Mg^{2+}, Ca^{2+} and Zn^{2+}. The zinc ion is tested at lower concentration than the other cations in the screen (0.01 M *vs.* 0.2 M)

Anion/PEG screen

This is made up of 12 anions, with either sodium or potassium counter ions, which are tested at 0.2 M against PEG 3350. The anions include fluoride, bromine, iodide, thiocyanate, nitrate, formate, acetate, sulfate, tartrate, phosphate, citrate and malonate. The phosphate solution is tested at a concentration of 0.02 M. Chloride is not included here as it is the counter ion in the cation screen. Three sets of reagents are tested at pH 6.5, 7.5, and 8.5 with the Bis-Tris propane buffer system whilst one set of reagents is tested without buffering.

References:

(1)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.

Formulation Notes

PACT *premier*™ 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 **PACT *premier*™** 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

PACT *premier*™ - when used together with JCSG-*plus*™ as a primary screening strategy is an extremely powerful and successful combination (i.e. a combination of a modern sparse matrix approach and an information yielding systematic trial).

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PACT *premier*™ HT-96 / FX-96 Conditions A1-D12 MD1-36 / MD1-36-FX

Well #	Conc.	Salt	Conc.	Buffer	pH	Conc.	Precipitant
A1			0.1 M	SPG	4.0	25 % w/v	PEG 1500
A2			0.1 M	SPG	5.0	25 % w/v	PEG 1500
A3			0.1 M	SPG	6.0	25 % w/v	PEG 1500
A4			0.1 M	SPG	7.0	25 % w/v	PEG 1500
A5			0.1 M	SPG	8.0	25 % w/v	PEG 1500
A6			0.1 M	SPG	9.0	25 % w/v	PEG 1500
A7	0.2 M	Sodium chloride	0.1 M	Sodium acetate	5.0	20 % w/v	PEG 6000
A8	0.2 M	Ammonium chloride	0.1 M	Sodium acetate	5.0	20 % w/v	PEG 6000
A9	0.2 M	Lithium chloride	0.1 M	Sodium acetate	5.0	20 % w/v	PEG 6000
A10	0.2 M	Magnesium chloride hexahydrate	0.1 M	Sodium acetate	5.0	20 % w/v	PEG 6000
A11	0.2 M	Calcium chloride dihydrate	0.1 M	Sodium acetate	5.0	20 % w/v	PEG 6000
A12	0.01 M	Zinc chloride	0.1 M	Sodium acetate	5.0	20 % w/v	PEG 6000
B1			0.1 M	MIB	4.0	25 % w/v	PEG 1500
B2			0.1 M	MIB	5.0	25 % w/v	PEG 1500
B3			0.1 M	MIB	6.0	25 % w/v	PEG 1500
B4			0.1 M	MIB	7.0	25 % w/v	PEG 1500
B5			0.1 M	MIB	8.0	25 % w/v	PEG 1500
B6			0.1 M	MIB	9.0	25 % w/v	PEG 1500
B7	0.2 M	Sodium chloride	0.1 M	MES	6.0	20 % w/v	PEG 6000
B8	0.2 M	Ammonium chloride	0.1 M	MES	6.0	20 % w/v	PEG 6000
B9	0.2 M	Lithium chloride	0.1 M	MES	6.0	20 % w/v	PEG 6000
B10	0.2 M	Magnesium chloride hexahydrate	0.1 M	MES	6.0	20 % w/v	PEG 6000
B11	0.2 M	Calcium chloride dihydrate	0.1 M	MES	6.0	20 % w/v	PEG 6000
B12	0.01 M	Zinc chloride	0.1 M	MES	6.0	20 % w/v	PEG 6000
C1			0.1 M	PCTP	4.0	25 % w/v	PEG 1500
C2			0.1 M	PCTP	5.0	25 % w/v	PEG 1500
C3			0.1 M	PCTP	6.0	25 % w/v	PEG 1500
C4			0.1 M	PCTP	7.0	25 % w/v	PEG 1500
C5			0.1 M	PCTP	8.0	25 % w/v	PEG 1500
C6			0.1 M	PCTP	9.0	25 % w/v	PEG 1500
C7	0.2 M	Sodium chloride	0.1 M	HEPES	7.0	20 % w/v	PEG 6000
C8	0.2 M	Ammonium chloride	0.1 M	HEPES	7.0	20 % w/v	PEG 6000
C9	0.2 M	Lithium chloride	0.1 M	HEPES	7.0	20 % w/v	PEG 6000
C10	0.2 M	Magnesium chloride hexahydrate	0.1 M	HEPES	7.0	20 % w/v	PEG 6000
C11	0.2 M	Calcium chloride dihydrate	0.1 M	HEPES	7.0	20 % w/v	PEG 6000
C12	0.01 M	Zinc chloride	0.1 M	HEPES	7.0	20 % w/v	PEG 6000
D1			0.1 M	MMT	4.0	25 % w/v	PEG 1500
D2			0.1 M	MMT	5.0	25 % w/v	PEG 1500
D3			0.1 M	MMT	6.0	25 % w/v	PEG 1500
D4			0.1 M	MMT	7.0	25 % w/v	PEG 1500
D5			0.1 M	MMT	8.0	25 % w/v	PEG 1500
D6			0.1 M	MMT	9.0	25 % w/v	PEG 1500
D7	0.2 M	Sodium chloride	0.1 M	Tris	8.0	20 % w/v	PEG 6000
D8	0.2 M	Ammonium chloride	0.1 M	Tris	8.0	20 % w/v	PEG 6000
D9	0.2 M	Lithium chloride	0.1 M	Tris	8.0	20 % w/v	PEG 6000
D10	0.2 M	Magnesium chloride hexahydrate	0.1 M	Tris	8.0	20 % w/v	PEG 6000
D11	0.2 M	Calcium chloride dihydrate	0.1 M	Tris	8.0	20 % w/v	PEG 6000
D12	0.002 M	Zinc chloride	0.1 M	Tris	8.0	20 % w/v	PEG 6000

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PACT *premier*™ HT-96 / FX-96 Conditions E1-H12 MD1-36 / MD1-36-FX

Well #	Conc.	Salt	Conc.	Buffer	pH	Conc.	Precipitant
E1	0.2 M	Sodium fluoride				20 % w/v	PEG 3350
E2	0.2 M	Sodium bromide				20 % w/v	PEG 3350
E3	0.2 M	Sodium iodide				20 % w/v	PEG 3350
E4	0.2 M	Potassium thiocyanate				20 % w/v	PEG 3350
E5	0.2 M	Sodium nitrate				20 % w/v	PEG 3350
E6	0.2 M	Sodium formate				20 % w/v	PEG 3350
E7	0.2 M	Sodium acetate trihydrate				20 % w/v	PEG 3350
E8	0.2 M	Sodium sulfate				20 % w/v	PEG 3350
E9	0.2 M	Potassium sodium tartrate tetrahydrate				20 % w/v	PEG 3350
E10	0.02 M	Sodium/potassium phosphate				20 % w/v	PEG 3350
E11	0.2 M	Sodium citrate tribasic dihydrate				20 % w/v	PEG 3350
E12	0.2 M	Sodium malonate dibasic monohydrate				20 % w/v	PEG 3350
F1	0.2 M	Sodium fluoride	0.1 M	Bis-Tris propane	6.5	20 % w/v	PEG 3350
F2	0.2 M	Sodium bromide	0.1 M	Bis-Tris propane	6.5	20 % w/v	PEG 3350
F3	0.2 M	Sodium iodide	0.1 M	Bis-Tris propane	6.5	20 % w/v	PEG 3350
F4	0.2 M	Potassium thiocyanate	0.1 M	Bis-Tris propane	6.5	20 % w/v	PEG 3350
F5	0.2 M	Sodium nitrate	0.1 M	Bis-Tris propane	6.5	20 % w/v	PEG 3350
F6	0.2 M	Sodium formate	0.1 M	Bis-Tris propane	6.5	20 % w/v	PEG 3350
F7	0.2 M	Sodium acetate trihydrate	0.1 M	Bis-Tris propane	6.5	20 % w/v	PEG 3350
F8	0.2 M	Sodium sulfate	0.1 M	Bis-Tris propane	6.5	20 % w/v	PEG 3350
F9	0.2 M	Potassium sodium tartrate tetrahydrate	0.1 M	Bis-Tris propane	6.5	20 % w/v	PEG 3350
F10	0.02 M	Sodium/potassium phosphate	0.1 M	Bis-Tris propane	6.5	20 % w/v	PEG 3350
F11	0.2 M	Sodium citrate tribasic dihydrate	0.1 M	Bis-Tris propane	6.5	20 % w/v	PEG 3350
F12	0.2 M	Sodium malonate dibasic monohydrate	0.1 M	Bis-Tris propane	6.5	20 % w/v	PEG 3350
G1	0.2 M	Sodium fluoride	0.1 M	Bis-Tris propane	7.5	20 % w/v	PEG 3350
G2	0.2 M	Sodium bromide	0.1 M	Bis-Tris propane	7.5	20 % w/v	PEG 3350
G3	0.2 M	Sodium iodide	0.1 M	Bis-Tris propane	7.5	20 % w/v	PEG 3350
G4	0.2 M	Potassium thiocyanate	0.1 M	Bis-Tris propane	7.5	20 % w/v	PEG 3350
G5	0.2 M	Sodium nitrate	0.1 M	Bis-Tris propane	7.5	20 % w/v	PEG 3350
G6	0.2 M	Sodium formate	0.1 M	Bis-Tris propane	7.5	20 % w/v	PEG 3350
G7	0.2 M	Sodium acetate trihydrate	0.1 M	Bis-Tris propane	7.5	20 % w/v	PEG 3350
G8	0.2 M	Sodium sulfate	0.1 M	Bis-Tris propane	7.5	20 % w/v	PEG 3350
G9	0.2 M	Potassium sodium tartrate tetrahydrate	0.1 M	Bis-Tris propane	7.5	20 % w/v	PEG 3350
G10	0.02 M	Sodium/potassium phosphate	0.1 M	Bis-Tris propane	7.5	20 % w/v	PEG 3350
G11	0.2 M	Sodium citrate tribasic dihydrate	0.1 M	Bis-Tris propane	7.5	20 % w/v	PEG 3350
G12	0.2 M	Sodium malonate dibasic monohydrate	0.1 M	Bis-Tris propane	7.5	20 % w/v	PEG 3350
H1	0.2 M	Sodium fluoride	0.1 M	Bis-Tris propane	8.5	20 % w/v	PEG 3350
H2	0.2 M	Sodium bromide	0.1 M	Bis-Tris propane	8.5	20 % w/v	PEG 3350
H3	0.2 M	Sodium iodide	0.1 M	Bis-Tris propane	8.5	20 % w/v	PEG 3350
H4	0.2 M	Potassium thiocyanate	0.1 M	Bis-Tris propane	8.5	20 % w/v	PEG 3350
H5	0.2 M	Sodium nitrate	0.1 M	Bis-Tris propane	8.5	20 % w/v	PEG 3350
H6	0.2 M	Sodium formate	0.1 M	Bis-Tris propane	8.5	20 % w/v	PEG 3350
H7	0.2 M	Sodium acetate trihydrate	0.1 M	Bis-Tris propane	8.5	20 % w/v	PEG 3350
H8	0.2 M	Sodium sulfate	0.1 M	Bis-Tris propane	8.5	20 % w/v	PEG 3350
H9	0.2 M	Potassium sodium tartrate tetrahydrate	0.1 M	Bis-Tris propane	8.5	20 % w/v	PEG 3350
H10	0.02 M	Sodium/potassium phosphate	0.1 M	Bis-Tris propane	8.5	20 % w/v	PEG 3350
H11	0.2 M	Sodium citrate tribasic dihydrate	0.1 M	Bis-Tris propane	8.5	20 % w/v	PEG 3350
H12	0.2 M	Sodium malonate dibasic monohydrate	0.1 M	Bis-Tris propane	8.5	20 % w/v	PEG 3350

Abbreviations:
HEPES; N-(2-hydroxyethyl)-piperazine-N'-2-ethanesulfonic acid, **MES**; 2-(N-morpholino)ethanesulfonic acid, **PEG**; Polyethylene glycol, **Tris**; 2-Amino-2-(hydroxymethyl)propane-1,3-diol, **SPG buffer**; Succinic Acid, sodium phosphate monobasic monohydrate, Glycine, **MIB buffer**; Sodium malonate dibasic monohydrate, Imidazole, Boric acid, **PCTP buffer**; Sodium propionate, Sodium cacodylate trihydrate, Bis-Tris propane, **MMT buffer**; DL-Malic acid, MES monohydrate, Tris.

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
PACT *premier*™	96 x 10 mL	MD1-29
PACT *premier*™ HT-96	96 x 1 mL	MD1-36
PACT *premier*™ FX-96	96 x 100 µL	MD1-36-FX
Eco Screens		
PACT *premier*™ Eco Screen	96 x 10 mL	MD1-29-ECO
PACT *premier*™ HT-96 Eco Screen	96 x 1 mL	MD1-36-ECO
Green Screens (contain fluorescent green dye - ideal for UV)		
PACT *premier*™ Green Screen	96 x 10 mL	MD1-55
PACT *premier*™ HT-96 Green Screen	96 x 1 mL	MD1-52
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		
PACT *premier*™ single reagents	100 mL	MDSR-29-tube number
PACT *premier*™ HT-96 single reagents	100 mL	MDSR-36-well number

For PACT *premier*™ stock solutions please visit the Optimization section on our website.