

PACT *premier*[™]

MD1-29

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

MD1-29 contains 96 x 10 mL reagents.

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

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).

Rationale for a new PEG/Ion screen

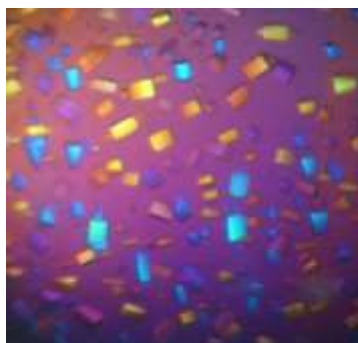
The first step in crystallization is often to reach for a commercially available "sparse matrix" kit, and hope that one of the conditions produces something that looks harvestable, or optimizable. If no obvious leads come out of the screen, it is hard to learn anything from the negative (precipitate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

There are a few screens that try to test crystallization space in a more rational manner – for example, the Clear Strategy[™] Screens.

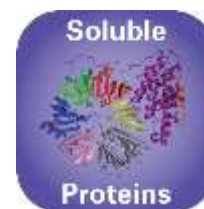
PACT *premier*[™]

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*[™].



PACT premier™

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⁺, NH₄⁺, Li⁺, Mg²⁺, Ca²⁺ and Zn²⁺. 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.

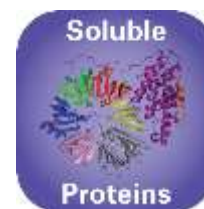
Final pH may vary from that specified on the datasheet. Molecular Dimensions will be happy to discuss the precise formulation of individual reagents.

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

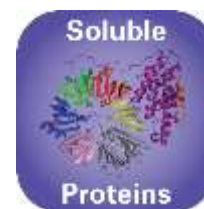
PACT premier™ when used together with JCSG-plus™ as a primary screening strategy is an extremely powerful and successful combination (i.e. a combination of a modern sparse matrix approach and an information yielding systematic trial).



PACT premier™

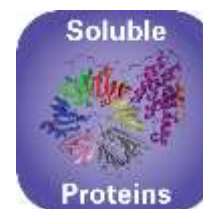
Conditions 1-48 (Box 1) MD1-29

Tube #	Conc.	Salt	Conc.	Buffer	pH	Conc.	Precipitant
1-1			0.1 M	SPG	4.0	25 % w/v	PEG 1500
1-2			0.1 M	SPG	5.0	25 % w/v	PEG 1500
1-3			0.1 M	SPG	6.0	25 % w/v	PEG 1500
1-4			0.1 M	SPG	7.0	25 % w/v	PEG 1500
1-5			0.1 M	SPG	8.0	25 % w/v	PEG 1500
1-6			0.1 M	SPG	9.0	25 % w/v	PEG 1500
1-7	0.2 M	Sodium chloride	0.1 M	Sodium acetate	5.0	20 % w/v	PEG 6000
1-8	0.2 M	Ammonium chloride	0.1 M	Sodium acetate	5.0	20 % w/v	PEG 6000
1-9	0.2 M	Lithium chloride	0.1 M	Sodium acetate	5.0	20 % w/v	PEG 6000
1-10	0.2 M	Magnesium chloride hexahydrate	0.1 M	Sodium acetate	5.0	20 % w/v	PEG 6000
1-11	0.2 M	Calcium chloride dihydrate	0.1 M	Sodium acetate	5.0	20 % w/v	PEG 6000
1-12	0.01 M	Zinc chloride	0.1 M	Sodium acetate	5.0	20 % w/v	PEG 6000
1-13			0.1 M	MIB	4.0	25 % w/v	PEG 1500
1-14			0.1 M	MIB	5.0	25 % w/v	PEG 1500
1-15			0.1 M	MIB	6.0	25 % w/v	PEG 1500
1-16			0.1 M	MIB	7.0	25 % w/v	PEG 1500
1-17			0.1 M	MIB	8.0	25 % w/v	PEG 1500
1-18			0.1 M	MIB	9.0	25 % w/v	PEG 1500
1-19	0.2 M	Sodium chloride	0.1 M	MES	6.0	20 % w/v	PEG 6000
1-20	0.2 M	Ammonium chloride	0.1 M	MES	6.0	20 % w/v	PEG 6000
1-21	0.2 M	Lithium chloride	0.1 M	MES	6.0	20 % w/v	PEG 6000
1-22	0.2 M	Magnesium chloride hexahydrate	0.1 M	MES	6.0	20 % w/v	PEG 6000
1-23	0.2 M	Calcium chloride dihydrate	0.1 M	MES	6.0	20 % w/v	PEG 6000
1-24	0.01 M	Zinc chloride	0.1 M	MES	6.0	20 % w/v	PEG 6000
1-25			0.1 M	PCTP	4.0	25 % w/v	PEG 1500
1-26			0.1 M	PCTP	5.0	25 % w/v	PEG 1500
1-27			0.1 M	PCTP	6.0	25 % w/v	PEG 1500
1-28			0.1 M	PCTP	7.0	25 % w/v	PEG 1500
1-29			0.1 M	PCTP	8.0	25 % w/v	PEG 1500
1-30			0.1 M	PCTP	9.0	25 % w/v	PEG 1500
1-31	0.2 M	Sodium chloride	0.1 M	HEPES	7.0	20 % w/v	PEG 6000
1-32	0.2 M	Ammonium chloride	0.1 M	HEPES	7.0	20 % w/v	PEG 6000
1-33	0.2 M	Lithium chloride	0.1 M	HEPES	7.0	20 % w/v	PEG 6000
1-34	0.2 M	Magnesium chloride hexahydrate	0.1 M	HEPES	7.0	20 % w/v	PEG 6000
1-35	0.2 M	Calcium chloride dihydrate	0.1 M	HEPES	7.0	20 % w/v	PEG 6000
1-36	0.01 M	Zinc chloride	0.1 M	HEPES	7.0	20 % w/v	PEG 6000
1-37			0.1 M	MMT	4.0	25 % w/v	PEG 1500
1-38			0.1 M	MMT	5.0	25 % w/v	PEG 1500
1-39			0.1 M	MMT	6.0	25 % w/v	PEG 1500
1-40			0.1 M	MMT	7.0	25 % w/v	PEG 1500
1-41			0.1 M	MMT	8.0	25 % w/v	PEG 1500
1-42			0.1 M	MMT	9.0	25 % w/v	PEG 1500
1-43	0.2 M	Sodium chloride	0.1 M	Tris	8.0	20 % w/v	PEG 6000
1-44	0.2 M	Ammonium chloride	0.1 M	Tris	8.0	20 % w/v	PEG 6000
1-45	0.2 M	Lithium chloride	0.1 M	Tris	8.0	20 % w/v	PEG 6000
1-46	0.2 M	Magnesium chloride hexahydrate	0.1 M	Tris	8.0	20 % w/v	PEG 6000
1-47	0.2 M	Calcium chloride dihydrate	0.1 M	Tris	8.0	20 % w/v	PEG 6000
1-48	0.002 M	Zinc chloride	0.1 M	Tris	8.0	20 % w/v	PEG 6000



PACT premier™ Conditions 1-48 (Box 2) MD1-29

Tube #	Conc.	Salt	Conc.	Buffer	pH	Conc.	Precipitant
2-1	0.2 M	Sodium fluoride				20 % w/v	PEG 3350
2-2	0.2 M	Sodium bromide				20 % w/v	PEG 3350
2-3	0.2 M	Sodium iodide				20 % w/v	PEG 3350
2-4	0.2 M	Potassium thiocyanate				20 % w/v	PEG 3350
2-5	0.2 M	Sodium nitrate				20 % w/v	PEG 3350
2-6	0.2 M	Sodium formate				20 % w/v	PEG 3350
2-7	0.2 M	Sodium acetate trihydrate				20 % w/v	PEG 3350
2-8	0.2 M	Sodium sulfate				20 % w/v	PEG 3350
2-9	0.2 M	Potassium sodium tartrate tetrahydrate				20 % w/v	PEG 3350
2-10	0.02 M	Sodium/potassium phosphate				20 % w/v	PEG 3350
2-11	0.2 M	Sodium citrate tribasic dihydrate				20 % w/v	PEG 3350
2-12	0.2 M	Sodium malonate dibasic monohydrate				20 % w/v	PEG 3350
2-13	0.2 M	Sodium fluoride	0.1 M	Bis-Tris propane	6.5	20 % w/v	PEG 3350
2-14	0.2 M	Sodium bromide	0.1 M	Bis-Tris propane	6.5	20 % w/v	PEG 3350
2-15	0.2 M	Sodium iodide	0.1 M	Bis-Tris propane	6.5	20 % w/v	PEG 3350
2-16	0.2 M	Potassium thiocyanate	0.1 M	Bis-Tris propane	6.5	20 % w/v	PEG 3350
2-17	0.2 M	Sodium nitrate	0.1 M	Bis-Tris propane	6.5	20 % w/v	PEG 3350
2-18	0.2 M	Sodium formate	0.1 M	Bis-Tris propane	6.5	20 % w/v	PEG 3350
2-19	0.2 M	Sodium acetate trihydrate	0.1 M	Bis-Tris propane	6.5	20 % w/v	PEG 3350
2-20	0.2 M	Sodium sulfate	0.1 M	Bis-Tris propane	6.5	20 % w/v	PEG 3350
2-21	0.2 M	Potassium sodium tartrate tetrahydrate	0.1 M	Bis-Tris propane	6.5	20 % w/v	PEG 3350
2-22	0.02 M	Sodium/potassium phosphate	0.1 M	Bis-Tris propane	6.5	20 % w/v	PEG 3350
2-23	0.2 M	Sodium citrate tribasic dihydrate	0.1 M	Bis-Tris propane	6.5	20 % w/v	PEG 3350
2-24	0.2 M	Sodium malonate dibasic monohydrate	0.1 M	Bis-Tris propane	6.5	20 % w/v	PEG 3350
2-25	0.2 M	Sodium fluoride	0.1 M	Bis-Tris propane	7.5	20 % w/v	PEG 3350
2-26	0.2 M	Sodium bromide	0.1 M	Bis-Tris propane	7.5	20 % w/v	PEG 3350
2-27	0.2 M	Sodium iodide	0.1 M	Bis-Tris propane	7.5	20 % w/v	PEG 3350
2-28	0.2 M	Potassium thiocyanate	0.1 M	Bis-Tris propane	7.5	20 % w/v	PEG 3350
2-29	0.2 M	Sodium nitrate	0.1 M	Bis-Tris propane	7.5	20 % w/v	PEG 3350
2-30	0.2 M	Sodium formate	0.1 M	Bis-Tris propane	7.5	20 % w/v	PEG 3350
2-31	0.2 M	Sodium acetate trihydrate	0.1 M	Bis-Tris propane	7.5	20 % w/v	PEG 3350
2-32	0.2 M	Sodium sulfate	0.1 M	Bis-Tris propane	7.5	20 % w/v	PEG 3350
2-33	0.2 M	Potassium sodium tartrate tetrahydrate	0.1 M	Bis-Tris propane	7.5	20 % w/v	PEG 3350
2-34	0.02 M	Sodium/potassium phosphate	0.1 M	Bis-Tris propane	7.5	20 % w/v	PEG 3350
2-35	0.2 M	Sodium citrate tribasic dihydrate	0.1 M	Bis-Tris propane	7.5	20 % w/v	PEG 3350
2-36	0.2 M	Sodium malonate dibasic monohydrate	0.1 M	Bis-Tris propane	7.5	20 % w/v	PEG 3350
2-37	0.2 M	Sodium fluoride	0.1 M	Bis-Tris propane	8.5	20 % w/v	PEG 3350
2-38	0.2 M	Sodium bromide	0.1 M	Bis-Tris propane	8.5	20 % w/v	PEG 3350
2-39	0.2 M	Sodium iodide	0.1 M	Bis-Tris propane	8.5	20 % w/v	PEG 3350
2-40	0.2 M	Potassium thiocyanate	0.1 M	Bis-Tris propane	8.5	20 % w/v	PEG 3350
2-41	0.2 M	Sodium nitrate	0.1 M	Bis-Tris propane	8.5	20 % w/v	PEG 3350
2-42	0.2 M	Sodium formate	0.1 M	Bis-Tris propane	8.5	20 % w/v	PEG 3350
2-43	0.2 M	Sodium acetate trihydrate	0.1 M	Bis-Tris propane	8.5	20 % w/v	PEG 3350
2-44	0.2 M	Sodium sulfate	0.1 M	Bis-Tris propane	8.5	20 % w/v	PEG 3350
2-45	0.2 M	Potassium sodium tartrate tetrahydrate	0.1 M	Bis-Tris propane	8.5	20 % w/v	PEG 3350
2-46	0.02 M	Sodium/potassium phosphate	0.1 M	Bis-Tris propane	8.5	20 % w/v	PEG 3350
2-47	0.2 M	Sodium citrate tribasic dihydrate	0.1 M	Bis-Tris propane	8.5	20 % w/v	PEG 3350
2-48	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 <i>premier</i> [™]	96 x 10 mL	MD1-29
PACT <i>premier</i> [™] HT-96	96 x 1 mL	MD1-36
Eco Screens		
PACT <i>premier</i> [™] Eco Screen	96 x 10 mL	MD1-29-ECO
PACT <i>premier</i> [™] HT-96 Eco Screen	96 x 1 mL	MD1-36-ECO
Green Screens (contain fluorescent green dye - ideal for UV)		
PACT <i>premier</i> [™] Green Screen	96 x 10 mL	MD1-55
PACT <i>premier</i> [™] HT-96 Green Screen	96 x 1 mL	MD1-52
Combo Packs		
Super2 Combo Value Pack (JCSG- <i>plus</i> [™] + PACT <i>premier</i> [™])	2 x 96 x 10 mL	MD1-75
Super2 Combo HT-96 Value Pack (JCSG- <i>plus</i> [™] HT-96 + PACT <i>premier</i> [™] HT-96)	2 x 96 x 10 mL	MD1-75-HT
Single Reagents		
PACT <i>premier</i> [™] single reagents	100 mL	MDSR-29-tube number
PACT <i>premier</i> [™] HT-96 single reagents	100 mL	MDSR-36-well number

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