

JBScreen PACT ++

Background

JBScreen PACT++ is a crystallization screen facilitating systematic **pH**, **anion-** and **cation** testing in the presence of polyethylene glycol (PEG) [1].

The 96 unique reagents incorporate three screens in one. For each sub-screen a different PEG concentration is chosen and the PEG concentration is kept constant within each screen.

1. PEG/pH Screen

The *PEG/pH Screen* comprises 24 conditions. 4 broad range buffer systems are screened against 25% w/v PEG 1500. Each buffer system is adjusted to 6 distinct pH values, allowing to screen a pH range from pH 4 to pH 9 without changing the chemical nature of the reagent solution [2].

The exact composition of the broad range buffer systems is described in Tab. 1.

In contrast to the crystal screen PACT, published on the SPINE website [3], JBScreen PACT++ does not contain cacodylate. According to our philosophy to omit the use of cacodylate, the buffer system PCB (Propionate, Cacodylate, Bis-Tris Propane) was replaced by TBG (Tartrate, Bis-Tris, Glycylglycine), which is described by Newman *et al.* [2], too.

Abbr.	Buffer composition	Ratio	pH low	pH high
SPG	Succinic Acid	2	4.0	10.0
	Sodium dihydrogen Phosphate	7		
	Glycine	7		
MIB	Malonic Acid	2	4.0	10.0
	Imidazole	3		
	Boric Acid	3		
TBG	Sodium Tartrate dihydrate	3	4.0	9.0
	Bis-Tris	2		
	Glycylglycine	2		
MMT	L-Malic Acid	1	4.0	9.0
	MES	2		
	Tris	2		

Table 1: Broad range buffer systems used in the PEG/pH Screen

2. PEG/Cation Screen

The 24 conditions of the *PEG/Cation Screen* are designed to screen 6 different cations against 20% w/v PEG 6000 at 4 distinct pH values. All cations (Na⁺, NH₄⁺, Li⁺, Mg²⁺, Ca²⁺ and Zn²⁺) have chloride as counter ion. Acetate, MES, HEPES and Tris are the buffers used, adjusted to pH 5, pH 6, pH 7 and pH 8, respectively.

3. PEG/Anion Screen

The *PEG/Anion Screen* comprises 48 conditions. 12 different anions, i.e. fluoride, bromide, iodide, thiocyanate, nitrate, formate, acetate, sulphate, tartrate, phosphate, citrate and malonate, are screened against 20% w/v PEG 3350. Either sodium or potassium are present as counter ion.

In order to evaluate the effect of the pH, the 12 anions are screened against PEG using Bis-Tris Propane buffer at pH values of 6.5, 7.5 and 8.5. Furthermore one set of anions is screened without any buffer solution.

Please consult our formulation sheets for the exact composition of **JBScreen PACT++**.

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Instructions

The layout of the screen is designed for setting up a 96 well plate. Pipette the solutions starting with A1 horizontally to A12, then the 2nd row from B1 to B12 down to H1 to H12. Then your plate is divided into 3 sub-screens as depicted in Figure 1.

	1	2	3	4	5	6	7	8	9	10	11	12
A												
B			24 well						24 well			
C		25% PEG 1500						20% PEG 6000				
D		vs pH						vs Cations				
E												
F						24 well						
G					20% PEG 3350							
H					vs Anions							

Figure 1: JBScreen PACT++ consists of three sub-screens, each containing a different PEG.

References

- [1] Newman *et al.* (2005) Towards rationalization of crystallization screening for small- to medium-sized academic laboratories: the PACT/JCSC+ strategy. *Acta Cryst. D* **61**:1426.
- [2] Newman (2004) Novel buffer systems for macromolecular crystallization. *Acta Cryst. D* **60**:610.
- [3] <http://www.spineurope.org>