

MOLECULAR DIMENSIONS MONOGRAPH SERIES[®]

Buffers make a difference

Woo et al Acta Cryst. (2003) D59, 769 – 772, Comparison of three commercial sparse matrix screens, reported dramatically different results when comparing Crystal Screens and Structure Screens. In 38 cases the Structure Screens were more successful in producing crystals than the Crystal Screens while the opposite was the case in 26 formulations. The authors reported that the formulations are not identical as in several buffers Molecular Dimensions uses glacial acetic acid to adjust the pH rather than HCl. This formulation was chosen from current practice developed from experience at a major UK research institution. We have analysed the results and found the following...

- 65% could be due to a different buffer counter ion
- 9% could be due to a pH difference probably resulting from Glycol oxidation
- 26% may possibly be due to minor pH differences or simply from the chance event of crystal nucleation
- Buffers compositions that may not be obvious are listed below

Structure Screen 1 & 2 Buffers

Buffer	Concentrate	Reagent used	Adjusted to pH with:
Sodium acetate	2M pH 4.6	Sodium acetate	Glacial acetic acid
Tri-sodium citrate	1M pH 5.6	Tri-sodium citrate	Glacial acetic acid
Sodium cacodylate	0.5M pH 6.5	Cacodylic acid sodium salt trihydrate	Glacial acetic acid
Imidazole	1M pH 6.5	Imidazole	Glacial acetic acid
MES	1M pH 6.5	2-morpholinoethanesulphonic acid monohydrate	10M sodium hydroxide
Sodium HEPES	1M pH 7.5	4-(2-hydroxyethyl)piperazine -1-ethanesulphonic acid sodium salt	Glacial acetic acid
Tris HCl	1M pH 8.5	TRIZMA base (Tris[hydroxymethyl]aminomethane)	Hydrochloric acid
Tris	1M pH 8.5	TRIZMA base (Tris[hydroxymethyl]aminomethane)	Glacial acetic acid
Bicine	1M pH 9.0	N,N-bis(2-hydroxyethyl)glycine	10M sodium hydroxide

Clear Strategy Screen Buffers

Buffer	Concentrate	Reagent used	Adjusted to pH with:
1) Sodium acetate	1M pH 4.5	Sodium acetate	Glacial acetic acid
2) Sodium acetate	1M pH 5.5	Sodium acetate	Glacial acetic acid
3) Sodium cacodylate	1M pH 6.5	Cacodylic acid sodium salt trihydrate	Glacial acetic acid
4) Tris	1M pH 7.5	TRIZMA base (Tris[hydroxymethyl]aminomethane)	Glacial acetic acid
5) Tris	1M pH 8.5	TRIZMA base (Tris[hydroxymethyl]aminomethane)	Glacial acetic acid