

Take a 96 well plate and divide up into a 24 well pH/PEG screen, a 24 well PEG/Cation screen and a 48 well PEG/anion screen. Use different PEGs for the different subscreens

PEG/pH (24)	PEG/ Cation (24)
PEG/Anion (48)	

This is the PEG/pH screen.
All wells have 25% PEG 1500

						Succinic acid, Phosphate, glycine system
						Malonic acid, imidazol, boric system
						Propionic acid, cacodylate, Bis-Tris Propane system
						Malic, MES, Tris system
4	5	6	7	8	9	

pH of the buffer system

This is the PEG/cation screen
All wells have 20% PEG 6000

						Acetate pH 5
						MES pH 6
						HEPES pH 7
						Tris pH 8
NaCl	NH ₄ Cl	LiCl	MgCl ₂	CaCl ₂	ZnCl ₂	

200mM of all, except for 10mM ZnCl₂,

This is the PEG/anion screen
All wells have 20% PEG 3350

												No Buffer
												pH 6.5
												pH 7.5
												pH 8.5
NaF	NaBr	NaI	KSCN	NaNO ₃	NaFormate	NaAcetate	Na ₂ SO ₄	Na/Ktartrate	Na/KPO ₄	NaCitrate	NaMalonate	100mM Bis-tris propane

200mM of each

Chemical	Stock	pH	# Additions	Total volume needed	Formula	MW	g/50ml
Water			96	32.4			
PEG 1500	50%		24	12			
PEG 3350	50%		48	19.2			
PEG 6000	50%		24	9.6			
SPG system	1M	4	6	0.35			
SPG system	1M	10	6	0.25			
MIB system	1M	4	6	0.35			
MIB system	1M	10	6	0.25			
PCB system	1M	4	6	0.37			
PCB system	1M	9.5	6	0.23			
MMT system	1M	4	6	0.3			
MMT system	1M	9	6	0.3			
NaAcetate	1M	5	6	0.6	NaAcetate anhydrous	82.03	
MES	1M	6	6	0.6	MES.H2O	213.25	
HEPES	1M	7	6	0.6	HEPES	238.3	
Tris	1M	8	6	0.6	Tris	121.2	
Bis-Tris Propane	1M	6.5	12	1.2	Bis-tris-propane	282.3	
Bis-Tris Propane	1M	7.5	12	1.2			
Bis-Tris Propane	1M	8.5	12	1.2			
NaCl	1M		4	0.8	NaCl	58.44	
NH4Cl	1M		4	0.8	NH4Cl	53.49	
LiCl	1M		4	0.8	LiCl	42.39	
MgCl2	1M		4	0.8	MgCl2.6H2O	203.3	
CaCl2	1M		4	0.8	CaCl2.2H2O	147.02	
ZnCl2	1M		4	0.04	ZnCl2	136.28	
NaF	1M		4	0.8	NaF	41.99	
NaBr	1M		4	0.8	NaBr	102.9	
NaI	1M		4	0.8	NaI	149.9	
KSCN	1M		4	0.8	KSCN	97.18	
NaNO3	1M		4	0.8	NaNO3	84.99	
NaFormate	1M		4	0.8	NaFormate	68.01	
NaAcetate	1M		4	0.8	NaAcetate	82.03	
NaAcetate					NaAcetate.3H2O	136.08	
Na2SO4	1M		4	0.8	Na2SO4.	142	
					Na2SO4.10H2O	322.2	
Na/K Tartrate	1M		4	0.8	K/Na tartrate.4H2O	282.08	
Na/K PO4	1M		4	0.8	Na2HPO4.2H2O	177.99	
					NaH2PO4.H2O	137.99	
					K2HPO4.3H2O	228.23	
					KH2PO4	136.09	
Trisodium Citrate	1M		4	0.8	NaCitrate.2H2O	294.1	
NaMalonate	1M	7	4	0.8	C3H2Na2O4.H2O	166	

1M Sodium acetate buffer pH 5 - dissolve 4.1g of NaC2H3O2 anhydrous in 50ml H2O, add about 26ml 1M acetic acid until pH = 5

1M Acetic acid: 5.75ml of glacial (17.4M) acetic acid made up to 100ml with water

1M MES pH 6 - dissolve 10.66g MES.H2O in 25ml H2O - add NaOH to pH 6 (about 2.07ml 10M), and adjust final volume to 50ml

1M HEPES pH 7 - dissolve 11.92g HEPES in 25ml H2O - add NaOH until pH 7 (about 1.1ml 10M), adjust volume to 50ml

1M Tris pH 8 - dissolve up 6.06g tris add HCl (about 2.75ml 37%) to pH 8, adjust volume to 50ml

1M BisTrisPropane pH 8.5 - dissolve up 14.12g in 25ml H2O - add HCl to pH 8.5, adjust volume to 50ml

1M BisTrisPropane pH 6.5 - dissolve up 14.12g in 25ml H2O - add HCl to pH 6.5, adjust volume to 50ml

1M BisTrisPropane pH 7.5 - dissolve up 14.12g in 25ml H2O - add HCl to pH 7.5, adjust volume to 50ml

1M NaCl - dissolve up 2.92g NaCl in 50ml H2O

1M NH4Cl -dissolve up 2.67g NH4Cl in 50ml H2O

1M LiCl - dissolve up 2.12g LiCl in 50ml H₂O
1M MgCl₂ - dissolve up 10.17g of MgCl₂·6H₂O in 50ml H₂O
1M CaCl₂ - dissolve up 7.35g of CaCl₂·2H₂O in 50ml H₂O
1M ZnCl₂ - dissolve up 6.82g of ZnCl₂ in 50ml H₂O

1M NaF - dissolve up 2.1g of NaF in 50ml H₂O (note 1M is just on the edge of the limit of solubility of NaF)
1M NaBr - dissolve up 5.15g of NaBr in 50ml H₂O
1M NaI - dissolve up 7.5g of NaI in 50ml H₂O
1M KSCN - dissolve up 4.86g in 50ml H₂O
1M NaNO₃ - dissolve up 4.25g in 50ml H₂O
1M NaFormate - dissolve up 3.4g NaCHO₂ in 50ml H₂O
1M NaAcetate - dissolve up 4.1g of NaC₂H₃O₂ anhydrous in 50ml H₂O
1M Na₂SO₄ - dissolve up 7.1g of Na₂SO₄ anhydrous in 50ml H₂O
1M Na/K Tartrate - dissolve 14.1g Na/K tartrate in 50ml H₂O
1M Na/K PO₄ - dissolve 2.22g Na₂HPO₄, 1.72g NaH₂PO₄, 2.85g K₂HPO₄, 1.7g KH₂PO₄ in 50ml H₂O
1M Trisodium Citrate - dissolve 14.7g Na₃Cit in 50ml H₂O
1M NaMalonate - dissolve 8.3g in 50ml H₂O - check pH is close to neutral

Notes: Na/K PO₄ made up by taking 1M Na₂HPO₄, NaH₂PO₄, K₂HPO₄ KH₂PO₄ and mixing them together in the ratio of 1:1:1:1

Reagent position	reagent number	[Salt]	[Salt] units	[stock]	ml salt in 1 ml	Salt	pH	[Buffer]	[Buffer] units	[stock]	ml buffer in 1 ml	Buffer	pH	[Precipitant 1]	[Precipitant 1] units	[stock]	ml precipitant in 1 ml	Precipitant 1	ml H ₂ O in 1 ml
A1	1.000	0.100	0.100 M	1.000	0.100	SPG	4.00	0.000	M	1.000	0.000	SPG	10.000	25.000	%	50.000	0.500	PEG 1.5K	0.400
A2	2.000	0.063	M	1.000	0.063	SPG	4.00	0.017	M	1.000	0.017	SPG	10.000	25.000	%	50.000	0.500	PEG 1.5K	0.400
A3	3.000	0.067	M	1.000	0.067	SPG	4.00	0.033	M	1.000	0.033	SPG	10.000	25.000	%	50.000	0.500	PEG 1.5K	0.400
A4	4.000	0.060	M	1.000	0.050	SPG	4.00	0.050	M	1.000	0.050	SPG	10.000	25.000	%	50.000	0.500	PEG 1.5K	0.400
A5	5.000	0.003	M	1.000	0.033	SPG	4.00	0.067	M	1.000	0.067	SPG	10.000	25.000	%	50.000	0.500	PEG 1.5K	0.400
A6	6.000	0.017	M	1.000	0.017	SPG	4.00	0.063	M	1.000	0.063	SPG	10.000	25.000	%	50.000	0.500	PEG 1.5K	0.400
A7	7.000	0.200	M	1.000	0.200	NaCl	4.00	0.100	M	1.000	0.100	Acetate	5.000	20.000	%	50.000	0.400	PEG 6K	0.300
A8	8.000	0.200	M	1.000	0.200	NH ₄ Cl	4.00	0.100	M	1.000	0.100	Acetate	5.000	20.000	%	50.000	0.400	PEG 6K	0.300
A9	9.000	0.200	M	1.000	0.200	LiCl	4.00	0.100	M	1.000	0.100	Acetate	5.000	20.000	%	50.000	0.400	PEG 6K	0.300
A10	10.000	0.200	M	1.000	0.200	MgCl ₂	4.00	0.100	M	1.000	0.100	Acetate	5.000	20.000	%	50.000	0.400	PEG 6K	0.300
A11	11.000	0.200	M	1.000	0.200	CaCl ₂	4.00	0.100	M	1.000	0.100	Acetate	5.000	20.000	%	50.000	0.400	PEG 6K	0.300
A12	12.000	0.010	M	1.000	0.010	ZnCl ₂	4.00	0.000	M	1.000	0.000	Acetate	5.000	20.000	%	50.000	0.400	PEG 6K	0.400
B1	13.000	0.100	M	1.000	0.100	MIB	4.00	0.000	M	1.000	0.000	MIB	10.000	25.000	%	50.000	0.500	PEG 1.5K	0.400
B2	14.000	0.063	M	1.000	0.063	MIB	4.00	0.017	M	1.000	0.017	MIB	10.000	25.000	%	50.000	0.500	PEG 1.5K	0.400
B3	15.000	0.067	M	1.000	0.067	MIB	4.00	0.033	M	1.000	0.033	MIB	10.000	25.000	%	50.000	0.500	PEG 1.5K	0.400
B4	16.000	0.060	M	1.000	0.050	MIB	4.00	0.050	M	1.000	0.050	MIB	10.000	25.000	%	50.000	0.500	PEG 1.5K	0.400
B5	17.000	0.017	M	1.000	0.033	MIB	4.00	0.067	M	1.000	0.067	MIB	10.000	25.000	%	50.000	0.500	PEG 1.5K	0.400
B6	18.000	0.017	M	1.000	0.017	MIB	4.00	0.063	M	1.000	0.063	MIB	10.000	25.000	%	50.000	0.500	PEG 1.5K	0.400
B7	19.000	0.200	M	1.000	0.200	NaCl	4.00	0.100	M	1.000	0.100	MES	6.000	20.000	%	50.000	0.400	PEG 6K	0.300
B8	20.000	0.200	M	1.000	0.200	NH ₄ Cl	4.00	0.100	M	1.000	0.100	MES	6.000	20.000	%	50.000	0.400	PEG 6K	0.300
B9	21.000	0.200	M	1.000	0.200	LiCl	4.00	0.100	M	1.000	0.100	MES	6.000	20.000	%	50.000	0.400	PEG 6K	0.300
B10	22.000	0.200	M	1.000	0.200	MgCl ₂	4.00	0.100	M	1.000	0.100	MES	6.000	20.000	%	50.000	0.400	PEG 6K	0.300
B11	23.000	0.200	M	1.000	0.200	CaCl ₂	4.00	0.100	M	1.000	0.100	MES	6.000	20.000	%	50.000	0.400	PEG 6K	0.300
B12	24.000	0.010	M	1.000	0.010	ZnCl ₂	4.00	0.000	M	1.000	0.000	MES	6.000	20.000	%	50.000	0.400	PEG 6K	0.400
C1	25.000	0.100	M	1.000	0.100	PCB	4.00	0.000	M	1.000	0.000	PCB	9.500	25.000	%	50.000	0.500	PEG 1.5K	0.400
C2	26.000	0.064	M	1.000	0.082	PCB	4.00	0.018	M	1.000	0.018	PCB	9.500	25.000	%	50.000	0.500	PEG 1.5K	0.400
C3	27.000	0.067	M	1.000	0.064	PCB	4.00	0.036	M	1.000	0.036	PCB	9.500	25.000	%	50.000	0.500	PEG 1.5K	0.400
C4	28.000	0.046	M	1.000	0.046	PCB	4.00	0.054	M	1.000	0.054	PCB	9.500	25.000	%	50.000	0.500	PEG 1.5K	0.400
C5	29.000	0.028	M	1.000	0.028	PCB	4.00	0.072	M	1.000	0.072	PCB	9.500	25.000	%	50.000	0.500	PEG 1.5K	0.400
C6	30.000	0.010	M	1.000	0.010	PCB	4.00	0.060	M	1.000	0.060	PCB	9.500	25.000	%	50.000	0.500	PEG 1.5K	0.400
C7	31.000	0.200	M	1.000	0.200	NaCl	4.00	0.100	M	1.000	0.100	HEPES	7.000	20.000	%	50.000	0.400	PEG 6K	0.300
C8	32.000	0.200	M	1.000	0.200	NH ₄ Cl	4.00	0.100	M	1.000	0.100	HEPES	7.000	20.000	%	50.000	0.400	PEG 6K	0.300
C9	33.000	0.200	M	1.000	0.200	LiCl	4.00	0.100	M	1.000	0.100	HEPES	7.000	20.000	%	50.000	0.400	PEG 6K	0.300
C10	34.000	0.200	M	1.000	0.200	MgCl ₂	4.00	0.100	M	1.000	0.100	HEPES	7.000	20.000	%	50.000	0.400	PEG 6K	0.300
C11	35.000	0.200	M	1.000	0.200	CaCl ₂	4.00	0.100	M	1.000	0.100	HEPES	7.000	20.000	%	50.000	0.400	PEG 6K	0.300
C12	36.000	0.010	M	1.000	0.010	ZnCl ₂	4.00	0.000	M	1.000	0.000	HEPES	7.000	20.000	%	50.000	0.400	PEG 6K	0.400
D1	37.000	0.100	M	1.000	0.100	MMT	4.00	0.000	M	1.000	0.000	MMT	9.000	25.000	%	50.000	0.500	PEG 1.5K	0.400
D2	38.000	0.060	M	1.000	0.080	MMT	4.00	0.020	M	1.000	0.020	MMT	9.000	25.000	%	50.000	0.500	PEG 1.5K	0.400
D3	39.000	0.060	M	1.000	0.060	MMT	4.00	0.040	M	1.000	0.040	MMT	9.000	25.000	%	50.000	0.500	PEG 1.5K	0.400
D4	40.000	0.040	M	1.000	0.040	MMT	4.00	0.060	M	1.000	0.060	MMT	9.000	25.000	%	50.000	0.500	PEG 1.5K	0.400
D5	41.000	0.020	M	1.000	0.020	MMT	4.00	0.080	M	1.000	0.080	MMT	9.000	25.000	%	50.000	0.500	PEG 1.5K	0.400
D6	42.000	0.000	M	1.000	0.000	MMT	4.00	0.100	M	1.000	0.100	MMT	9.000	25.000	%	50.000	0.500	PEG 1.5K	0.400
D7	43.000	0.200	M	1.000	0.200	NaCl	4.00	0.100	M	1.000	0.100	TRIS	8.000	20.000	%	50.000	0.400	PEG 6K	0.300
D8	44.000	0.200	M	1.000	0.200	NH ₄ Cl	4.00	0.100	M	1.000	0.100	TRIS	8.000	20.000	%	50.000	0.400	PEG 6K	0.300
D9	45.000	0.200	M	1.000	0.200	LiCl	4.00	0.100	M	1.000	0.100	TRIS	8.000	20.000	%	50.000	0.400	PEG 6K	0.300
D10	46.000	0.200	M	1.000	0.200	MgCl ₂	4.00	0.100	M	1.000	0.100	TRIS	8.000	20.000	%	50.000	0.400	PEG 6K	0.300
D11	47.000	0.200	M	1.000	0.200	CaCl ₂	4.00	0.100	M	1.000	0.100	TRIS	8.000	20.000	%	50.000	0.400	PEG 6K	0.300
D12	48.000	0.010	M	1.000	0.010	ZnCl ₂	4.00	0.000	M	1.000	0.000	TRIS	8.000	20.000	%	50.000	0.400	PEG 6K	0.400
E1	49.000	0.200	M	1.000	0.200	NaF	4.00	0.100	M	1.000	0.100	TRIS	8.000	20.000	%	50.000	0.400	PEG 3.35K	0.400
E2	50.000	0.200	M	1.000	0.200	NaBr	4.00	0.100	M	1.000	0.100	TRIS	8.000	20.000	%	50.000	0.400	PEG 3.35K	0.400
E3	51.000	0.200	M	1.000	0.200	NaI	4.00	0.100	M	1.000	0.100	TRIS	8.000	20.000	%	50.000	0.400	PEG 3.35K	0.400
E4	52.000	0.200	M	1.000	0.200	KCN	4.00	0.100	M	1.000	0.100	TRIS	8.000	20.000	%	50.000	0.400	PEG 3.35K	0.400
E5	53.000	0.200	M	1.000	0.200	KNO3	4.00	0.100	M	1.000	0.100	TRIS	8.000	20.000	%	50.000	0.400	PEG 3.35K	0.400
E6	54.000	0.200	M	1.000	0.200	NaFormate	4.00	0.100	M	1.000	0.100	TRIS	8.000	20.000	%	50.000	0.400	PEG 3.35K	0.400
E7	55.000	0.200	M	1.000	0.200	NaAcetate	4.00	0.100	M	1.000	0.100	TRIS	8.000	20.000	%	50.000	0.400	PEG 3.35K	0.400
E8	56.000	0.200	M	1.000	0.200	NaSulfate	4.00	0.100	M	1.000	0.100	TRIS	8.000	20.000	%	50.000	0.400	PEG 3.35K	0.400
E9	57.000	0.200	M	1.000	0.200	Na/Ktartrate	4.00	0.100	M	1.000	0.100	TRIS	8.000	20.000	%	50.000	0.400	PEG 3.35K	0.400
E10	58.000	0.200	M	1.000	0.200	Na/Kphosphate	4.00	0.100	M	1.000	0.100	TRIS	8.000	20.000	%	50.000	0.400	PEG 3.35K	0.400
E11	59.000	0.200	M	1.000	0.200	Na/Citrate	4.00	0.100	M	1.000	0.100	TRIS	8.000	20.000	%	50.000	0.400	PEG 3.35K	0.400
E12	60.000	0.200	M	1.000	0.200	Na/Malonnate	4.00	0.100	M	1.000	0.100	TRIS	8.000	20.000	%	50.000	0.400	PEG 3.35K	0.400
F1	61.000	0.200	M	1.000	0.200	NaF	4.00	0.100	M	1.000	0.100	BisTrisPr	6.500	20.000	%	50.000	0.400	PEG 3.35K	0.300
F2	62.000	0.200	M	1.000	0.200	NaBr	4.00	0.100	M	1.000	0.100	BisTrisPr	6.500	20.000	%	50.000	0.400	PEG 3.35K	0.300

<u>System name</u>	<u>Ratio</u>	<u>Chemical Name and source</u>	<u>Formula Weight</u>	<u>Concentration</u>	<u>g</u>	<u>Final volume</u>	<u>High pH</u>	<u>Low pH</u>
Succinic Acid, Sodium Dihydrogen Phosphate, Glycine (SPG)	2 7 7	Succinic Acid (Sigma S9674) Sodium Dihydrogen Phosphate monohydrate (Merck 1.06346) Glycine (Merck 1.04201)	118.1 137.99 75.07	1M 1M 1M	1.48 6.04 3.28	100ml	8.3ml NaOH (pH 10.0)	0.29ml NaOH (pH 4.0)
Citric Acid, HEPES, CHES (CHC)	2 3 4	Citric Acid anhydrous (Fluka 27487) HEPES (Merck 1.10110) CHES (Sigma C2885)	192.43 238.3 207.3	1M 1M 1M	4.28 7.94 9.21	100ml	13.5ml NaOH (pH 10.0)	2.0 ml NaOH (pH 4.0)
Malonic Acid, Imidazol, Boric Acid (MIB)	2 3 3	Sodium Malonate (Sigma M1875) Imidazol (Fluka 56750) Boric Acid (Sigma B9645)	166 68.08 61.83	1M 1M 1M	4.15 2.55 2.32	100ml	3.5 ml NaOH (pH 10.0)	6.3 ml HCl (pH 4.0)
Sodium Propionate, Sodium Cacodylate, Bis-Tris Propane (PCB)	2 1 2	Sodium Propionate (Sigma P1880) Sodium Cacodylate trihydrate (Fluka 20838) Bis-Tris Propane (Sigma B6755)	96.06 214.03 282.3	1M 1M 1M	3.84 4.28 11.29	100ml	1.0 ml HCl (pH 9.5)	12.9 ml HCl (pH 4.0)
Sodium Acetate, ADA, Bicine (AAB)	1 1 1	Sodium Acetate (Merck 1.06268) ADA (Hampton Research 0.5M Stock) Bicine (Fluka 14872)	82.03 190.2 163.18	1M 1M 1M	2.74 6.34 5.44	100ml, of which 66.7ml are 0.5M ADA	5.7ml NaOH (pH 9)	2.95 ml HCl (pH 4)
Malic Acid, MES, Tris (MMT)	1 2 2	DL- Malic Acid (Sigma M1000) MES (Sigma M8250) Tris (Trizma Base, Sigma T1503)	134.1 195.2 121.1	1M 1M 1M	2.68 7.81 5.22	100ml	6.7ml NaOH (pH 9)	2.55ml HCl (pH 4.0)
Sodium Tartrate, Bis-Tris, Glycyl-Glycine (TBG)	3 2 2	Sodium Tartrate dihydrate (Sigma S4797) Bis-Tris (Aldrich 15.666-3) GlycylGlycine (Sigma G1002)	230.1 209.24 132.1	1M 1M 1M	9.86 5.98 3.77	100ml	2.4 ml NaOH (pH 9.0)	5.1 ml HCl (pH 4.0)

Set the pH to either 4 or the upper limit using concentrated (32% = 10M) HCl or 10M NaOH. Numbers under column High pH or Low pH give approximate volumes of concentrated acid or base to pH 100ml 1M buffer.

Scoring sheet

	1	2	3	4	5	6	7	8	9	10	11	12
A	0.2M Li2SO4 Acetate pH 4.5 50% PEG 400	0.2M NH4Cl pH 6.3 20% PEG 3350	Cacodylate pH 6.5 40% MPD 5% PEG 8K	0.2M NaCl Phos-cit pH 4.2 20% PEG 8K	Na/K PO4 pH 6.2 25% 1,2 Propanediol 10% glycerol	0.2M MgCl2 Hepes pH 7.5 70% MPD	1M NaCit Cacodylate pH 6.5	1.6M MgSO4 MES pH 6.5	0.2M MgCl2 Tris pH 8.5 50% ethylene glycol	Hepes pH 7.0 30% Jeffamine ED 2001	0.1M KSCN 30% PEG MME 2K	0.2M AmAc Bis-Tris pH 5.5 45% MPD
B	Citrate pH 5.5 20% PEG 3K	0.2M KFo pH 7.3 20% PEG 3350	Phos-cit pH 4.2 40% Ethanol 5% PEG 1K	1M LiCl Citrate pH 4 20% PEG 6K	Bicine pH 9 10% PEG 20K 2% dioxane	Tris pH 8.5 20% PEG 8K	2M AmSO4 0.2M NaCl Cacodylate pH 6.5	Bicine pH 9.0 10% PEG 6K	Bicine pH 9.0 10% MPD	0.02M MgCl2 Hepes pH 7.5 22% polyacrylic acid 5100	0.15M KBr 30% PEG MME 2K	0.1M AmAc Bis-Tris pH 5.5 17% PEG 10K
C	0.2M AmCit pH 5 20% PEG 3350	0.2M NH4H2PO4 Tris pH 8.5 50% MPD	Acetate pH 4.6 8% PEG 4K	0.2M AmNit. pH 6.3 20% PEG 3350	2M AmSO4 Acetate pH 4.6	0.2M Li2SO4 Tris pH 8.5 40% PEG 400	0.2M NaCl Hepes pH 7.5 10% propanol	1.6M CaAc Cacodylate pH 6.5 14.4% PEG 8K 20% glycerol	0.8M succinate pH 7.0	0.1M CoCl2 tris pH 8.5 20% polyvinyl pyrrolidone K15	2M AmSO4 Bis-Tris pH 5.5	0.2M AmSO4 Bis-Tris pH 5.5 25% PEG 3350
D	20mM CaCl2 NaAc. pH 4.6 30% MPD	0.2M KNO3 pH 6.9 20% PEG 3350	0.2M MgCl2 Tris pH 7 10% PEG 8K	Hepes pH 7 10% PEG 6K	10% PEG 1K 10% PEG 8K	Tris pH 8.0 40% MPD	1.26M AmSO4 0.2M Li2SO4 Tris pH 8.5	Imidazol pH 8 10% PEG 8K	2.1M DL malate pH 7.0	0.2M TMAO Tris pH 8.5 20% PEG MME 2K	3M NaCl Bis-Tris pH 5.5	0.2M NaCl Bis-Tris pH 5.5 25% PEG 3350
E	0.2M MgFo pH 5.9 20% PEG 3350	0.8M AmSO4 Citrate pH 4	Citrate pH 5 20% PEG 6K	0.8M NaH2PO4 0.8M KH2PO4 Hepes pH 7.5	24% PEG 1.5K 20% glycerol	0.17M AmSO4 25.5% PEG 4K 15% glycerol	CAPS pH 10.5 40% MPD	0.05M CsCl MES pH 6.5 30% Jeffamine M- 600	2.4M malonate pH 7.0	5mM CoCl2, CdCl2, MgCl2, NiCl2 Hepes pH 7.5 12% PEG 3350	0.3M MgFo. Bis-Tris pH 5.5	0.2M Li2SO4 Bis-Tris pH 5.5 25% PEG 3350
F	0.2M Li2SO4 Phos-cit pH 4.2 20% PEG 1K	0.2M NaSCN pH 6.9 20% PEG 3350	0.2M MgCl2 Cacodylate pH 6.5 50% PEG 200	Phos-cit pH 4.2 40% PEG 300	0.2M MgCl2 Hepes pH 7.5 30% PEG 400	0.2M CaAc Cacodylate pH 6.5 40% PEG 300	0.2M ZnAc. Imidazol pH 8 20% PEG 3K	3.15M AmSO4 Citrate pH 5.0	1.1M malonate pH 7.0 Hepes pH 7.0 0.5% Jeffamine ED-	0.2M malonate pH 7.0 20% PEG 3350	1M AmSO4 Bis-Tris pH 5.5 1% PEG 3350	0.2M AmAc Bis-Tris pH 5.5 25% PEG 3350
G	CHES pH 9.5 20% PEG 8K	Bicine pH 9 20% PEG 6K	1.6M NaCit	0.2M ZnAc. Acetate pH 4.5 10% PEG 3K	0.2M NaCl Na/K PO4 pH 6.2 50% PEG 200	0.14M CaCl2 Acetate pH 4.6 14% propanol 30% glycerol	0.2M ZnAc. Cacodylate pH 6.5 10% propanol	Tris pH 8.0 20% MPD	1.0M succinate Hepes pH 7 1% PEG MME 2K	0.1M succinate pH 7.0 15% PEG 3350	Bis-Tris pH 5.5 25% PEG 3350	0.2M MgCl2 Bis-Tris pH 5.5 25% PEG 3350
H	0.2M AmFo pH 6.6 20% PEG 3350	Hepes pH 7.5 10% PEG 8K 8% Ethylene Glycol	0.2M Kcit pH 8.3 20% PEG 3350	Tris pH 8.5 20% Ethanol	0.2M Li2SO4 Acetate pH 4.5 30% PEG 8K	0.04M KH2PO4 16% PEG 8K 20% glycerol	1M (NH4)2HPO4 Acetate pH 4.5	Hepes pH 6.5 20% Jeffamine M- 600	Hepes pH 7.0 30% jeffamine M-600 pH 7	0.15M DL- malate pH 7.0 20% PEG 3350	0.2M CaCl2 Bis-Tris pH 5.5 45% MPD	0.2M AmAc Hepes pH 7.5 45% MPD

Reagent number	[Salt1] [Salt1] units	Salt 1	[Buffer] [Buffer] units	Buffer	pH [Precipitant 1]	[Precipitant 1] units	[Stock] ml stock in 1ml	Precipitant 1	ml H2O in 1ml	Reagent number	source screen
1	0.20 M	Li2SO4	0.1 M	acetate	4.5	50 %w/v	100	0.500 PEG 400	0.300	1	W1 cryo #47
2	0.20 M	(NH4)2HC8H16O7 pH 5.0	0.1 M	citrate	5.5	20 %w/v	50	0.400 PEG 3000	0.500	2	W1 #06
3	0.02 M	CaCl2	0.1 M	NaOAcetate	4.6	20 %w/v	50	0.400 PEG 3350	0.520	3	PEG/ion #48
4	0.02 M	Mg(CHO2)2 pH 5.9	0.1 M	NaOAcetate	4.6	30 %w/v	100	0.300 MPD	0.580	4	H1 #01
5	0.20 M	Li2SO4	0.1 M	phosphate-citrate	4.2	20 %w/v	50	0.400 PEG 3350	0.400	5	PEG/ion #20
6	0.20 M	(NH4)CHO2 pH 6.6	0.1 M	CHES	9.5	20 %w/v	50	0.400 PEG 1000	0.400	6	W1 #39
7	0.20 M	(NH4)Cl pH 6.3	0.1 M	phosphate-citrate	4.2	20 %w/v	50	0.400 PEG 8000	0.500	7	W1 #01
8	0.20 M	KCHO2 pH 7.3	0.1 M	tris	8.5	20 %w/v	50	0.400 PEG 3350	0.580	8	PEG/ion #23
9	0.20 M	(NH4)H2PO4	0.1 M	tris	8.5	20 %w/v	50	0.400 PEG 3350	0.560	9	PEG/ion #09
10	0.20 M	(NH4)2SO4	0.1 M	citrate	4.0	20 %w/v	50	0.400 PEG 3350	0.586	10	PEG/ion #22
11	0.20 M	NaSCN pH 6.9	0.1 M	bicine	9.0	20 %w/v	50	0.500 MPD	0.320	11	H2 #43
12	0.80 M	(NH4)2SO4	0.1 M	bicine	4.0	20 %w/v	50	0.400 PEG 3350	0.533	12	PEG/ion #18
13	0.20 M	(NH4)2SO4	0.1 M	bicine	9.0	20 %w/v	50	0.400 PEG 3350	0.671	13	(NH4)2SO4 #01
14	0.20 M	(NH4)2SO4	0.1 M	bicine	9.0	20 %w/v	50	0.400 PEG 6000	0.575	14	PEG/ion #13
15	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.400 PEG 6000	0.500	15	P6K
16	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.200 PEG 8000	0.620	16	H2 #37
17	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.200 PEG 8000	0.080	17	W2cryo #01
18	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.080 Ethylene glycol	0.400	18	W2cryo #01
19	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.400 MPD	0.100	19	W1 cryo #40
20	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.100 PEG 8000	0.400	20	W1 cryo #40
21	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.400 Ethanol	0.400	21	W1 cryo #40
22	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.100 PEG 1000	0.100	22	W1 cryo #40
23	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.160 PEG 4000	0.740	23	H1 #37
24	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.200 PEG 8000	0.600	24	W2 #43
25	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.400 PEG 6000	0.500	25	P6K #14
26	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.400 PEG 200	0.300	26	W2cryo #36
27	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.500 PEG 200	0.000	27	W2cryo #36
28	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.400 PEG 3350	0.000	28	H2 #28
29	0.80 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.400 PEG 3350	0.520	29	PEG/ion #47
30	0.80 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.400 PEG 8000	0.460	30	W1 #31
31	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.400 PEG 6000	0.400	31	P6K/LiCl #13
32	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.400 PEG 3350	0.580	32	PEG/ion #19
33	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.200 PEG 6000	0.700	33	P6K #10
34	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.200 PEG 6000	0.207	34	H1 #35
35	2.00 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.400 PEG 300	0.533	35	H1 #47
36	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.400 PEG 300	0.600	36	H2 #07
37	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.200 PEG 8000	0.200	37	H1 cryo #43
38	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.480 PEG 1500	0.320	38	H1 cryo #43
39	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.200 Ethanol	0.200	39	H1 cryo #43
40	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.200 Ethanol	0.200	40	H1 cryo #43
41	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.250 1,2-propanediol	0.550	41	W2cryo #11
42	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.100 glycerol	0.100	42	W2cryo #11
43	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.333 PEG 20000	0.517	43	H2 #48
44	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.050 dioxane	0.050	44	H2 #48
45	0.17 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.200 PEG 1000	0.329	45	H1 #47
46	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.200 PEG 1000	0.600	46	H2 #07
47	0.14 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.200 PEG 8000	0.200	47	H1 cryo #43
48	0.04 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.480 PEG 1500	0.320	48	H1 cryo #43
49	1.00 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.200 glycerol	0.200	49	H1 cryo #43
50	2.00 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.300 PEG 400	0.500	50	H1 cryo #23
51	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.300 PEG 400	0.360	51	W2cryo #15
52	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.600 PEG 200	0.200	52	W2cryo #15
53	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.700 MPD	0.100	53	W1 #17
54	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.400 PEG 8000	0.500	54	H2 #35
55	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.400 PEG 8000	0.400	55	W2 #03
56	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.400 PEG 400	0.400	56	W1 cryo #38
57	0.17 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.400 MPD	0.500	57	W1 cryo #38
58	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.510 PEG 4000	0.291	58	H1 cryo #31
59	0.20 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.150 glycerol	0.150	59	H1 cryo #31
60	0.14 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.400 PEG 300	0.300	60	W1 cryo #37
61	0.14 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.140 2-propanol	0.350	61	W1 cryo #24
62	0.04 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.300 glycerol	0.300	62	H1 cryo #24
63	1.00 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.320 PEG 8000	0.453	63	H1 cryo #42
64	2.00 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.200 glycerol	0.200	64	H1 cryo #42
65	2.00 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.200 glycerol	0.275	65	W1 #14
66	2.00 M	(NH4)2SO4	0.1 M	HEPES	7.5	10 %w/v	50	0.200 glycerol	0.289	66	W2 #04

count	Chemical	type	pH	Stock	smallest volume/ 1ml	largest volume/ 1ml	# of additions	ml to make up 1ml screen
	acetate	buffer	4.5	1	0.1	0.1	4	0.4
	acetate	buffer	4.6	1	0.07	0.1	4	0.37
	bicine	buffer	9	1	0.1	0.1	4	0.4
	bis-tris	buffer	5.5	1	0.1	0.1	13	1.3
	cacodylate	buffer	6.5	1	0.08	0.1	7	0.68
	CAPS	buffer	10.5	1	0.1	0.1	1	0.1
	CHES	buffer	9.5	1	0.1	0.1	1	0.1
	citrate	buffer	4	1	0.1	0.1	2	0.2
	citrate	buffer	5	1	0.1	0.1	2	0.2
	citrate	buffer	5.5	1	0.1	0.1	1	0.1
	HEPES	buffer	6.5	1	0.1	0.1	1	0.1
	HEPES	buffer	7	1	0.1	0.1	5	0.5
	HEPES	buffer	7.5	1	0.1	0.1	8	0.8
	imidazole	buffer	8	1	0.1	0.1	2	0.2
	MES	buffer	6.5	1	0.1	0.1	2	0.2
	Na/K phosphate	buffer	6.2	1	0.1	0.1	2	0.2
	phosphate-citrate	buffer	4.2	1	0.1	0.1	4	0.4
	tris	buffer	7	1	0.1	0.1	1	0.1
	tris	buffer	8	1	0.1	0.1	2	0.2
20	tris	buffer	8.5	1	0.1	0.1	8	0.8
	1,2 propanediol	organic		100	0.25	0.25	1	0.25
	2-propanol	organic		100	0.1	0.14	3	0.34
	dioxane	organic		40	0.05	0.05	1	0.05
	Ethanol	organic		100	0.2	0.4	2	0.6
	Ethylene glycol	organic		100	0.08	0.5	2	0.58
	glycerol	organic		100	0.1	0.3	6	1.15
7	MPD	organic		100	1	0.7	11	4.35
	Jeffamine M-600	polymer		50	0.4	0.6	3	1.6
	PEG 1000	polymer		50	0.1	0.4	3	0.7
	PEG 10000	polymer		50	0.34	0.34	1	0.35
	PEG 1500	polymer		50	0.48	0.48	1	0.48
	PEG 200	polymer		100	0.5	0.5	2	1
	PEG 20000	polymer		30	0.333	0.333	1	0.333
	PEG 300	polymer		100	0.4	0.4	2	0.8
	PEG 3000	polymer		50	0.2	0.4	3	1
	PEG 3350	polymer		50	0.02	0.5	20	7.96
	PEG 400	polymer		100	0.3	0.5	3	1.2
	PEG 4000	polymer		50	0.16	0.51	2	0.67
	PEG 6000	polymer		50	0.2	0.4	5	1.6
	PEG 8000	polymer		50	0.2	0.6	11	3.308
	PEG MME 2000	polymer		50	0.02	0.6	4	1.62
	polyacrylic acid 5100 sodium salt	polymer		50	0.44	0.44	1	0.44
16	polyvinylpyrrolidone K15	polymer		50	0.4	0.4	1	0.4
	(CH3)3NO (TMAO)	salt		1	0.2	0.2	1	0.2
	(NH4)(C2H3O2)	salt		1	0.1	0.2	4	0.7
	(NH4)2HC6H5O7	salt	5	2.5	0.08	0.08	1	0.8
	(NH4)2HPO4	salt		3.5	0.286	0.286	1	0.286
	(NH4)2SO4	salt		3.5	0.049	0.9	9	3.594
	(NH4)CHO2	salt	6.6	10	0.02	0.02	1	0.02
	(NH4)Cl	salt	6.3	5	0.04	0.04	1	0.04
	(NH4)H2PO4	salt		2.5	0.08	0.08	1	0.08
	(NH4)NO3	salt	6.3	10	0.02	0.2	1	0.02
	C3H4O4 (sodium malonate)	salt	7	3.4	0.059	0.706	3	1.088
	C4H6O4 (sodium succinate)	salt	7	1.2	0.083	0.833	3	1.583
	C4H6O5 (DL-sodium malate)	salt	7	3	0.05	0.7	2	0.75
	Ca(C2H3O2)2	salt		1	0.16	0.2	2	0.36
	CaCl2	salt		1	0.02	0.2	3	0.36
	CdCl2	salt		1	0.005	0.005	1	0.005
	CoCl2	salt		1	0.005	0.1	2	0.105
	CsCl	salt		1	0.05	0.05	1	0.05
	K3C6H5O7	salt	8.3	2.5	0.08	0.08	1	0.08
	KBr	salt		1	0.15	0.15	1	0.15
	KCHO2	salt	7.3	14	0.014	0.014	1	0.014
	KH2PO4	salt		1.5	0.027	0.533	2	0.56
	KNO3	salt	6.9	3	0.067	0.067	1	0.067
	KSCN	salt		8	0.013	0.013	1	0.013
	Li2SO4	salt		2	0.1	0.1	6	0.6
	LiCl	salt		10	0.1	0.1	1	0.1
	Mg(CHO2)2	salt	5.9	1	0.2	0.3	2	0.5
	MgCl2	salt		2	0.003	0.1	8	0.613
	MgSO4	salt		2.5	0.64	0.64	1	0.64
	Na3C6H5O7	salt		1.6	0.625	1	2	1.625
	NaCl	salt		5	0.04	0.6	6	0.8
	NaH2PO4	salt		5	0.16	0.16	1	0.16
	NaSCN	salt	6.9	8	0.025	0.025	1	0.025
	NiCl2	salt		4	0.001	0.001	1	0.001
34	Zn(C2H3O2)2	salt		1	0.2	0.2	3	0.6