

Supplementary material

Figure S1 Summary of outcomes using the three screens, shown as a Venn diagram. WS, CS and PSS, number of proteins crystallized only using only WS, CS and PSS, respectively. Cross-sections, number of proteins crystallized using 2 or 3 screens.

Figure S2 (a) Relative success for different precipitant classes, calculated as in Fig. 2. We classified the precipitants in the following categories: volatile organic solvents (2-propanol, ethanol and t-butanol); non-volatile organic solvents (1,4-butanediol, 1,6-hexanediol, glycerol, ethylene glycol, dioxane and 2-methyl-2,4-pentanediol (MPD)); polymers (PEG 400, PEG 1000, PEG 1500, PEG 3000, PEG 4000, PEG 6000, PEG 8000, PEG 10,000, PEG 20,000, PEG MME 550, PEG MME 2000, PEG MME 5000, Jeffamine M-600, polyethyleneimine and polyvinylpyrrolidone); salts (ammonium sulphate, lithium sulphate, magnesium sulphate, ammonium formate, magnesium formate, sodium formate, sodium citrate, magnesium chloride, sodium chloride, sodium acetate, ammonium phosphate, sodium/potassium phosphate and sodium/potassium tartrate); and "other" precipitants (imidazole, urea and combined precipitants (10% isopropanol and 20% PEG 4000; 20% isopropanol and 20% PEG 4000; 2% PEG 400 and 2 M ammonium sulphate; 10% PEG 6000 and 5% MPD; 10% PEG 8000 and 8% ethylene glycol; 0.5 M sodium chloride and 0.01 M magnesium chloride; and 10% PEG 1000 and 10% PEG 8000)). A component was considered a precipitant if regarded as such by the manufacturer. (b) Relative success for various salts, calculated as in Fig. 2. (c) Relative success for various organic solvents, calculated as in Fig. 2. (d) Relative success for "other" precipitants, calculated as in Fig. 2. The polymers Jeffamine M-600, polyethyleneimine and polyvinylpyrrolidone are also shown here.

Figure S3 Relative crystallisation success as a function of pH.

Table S1 Formulations in each crystallisation screen.

Number	Precipitant	Buffer (100 mM)	Additive
Wizard Screens I and II (WS)			
1	20% (w/v) PEG-8000	CHES pH 9.5	
2	10% (v/v) 2-Propanol	HEPES pH 7.5	0.2 M sodium chloride
3	15% (v/v) ethanol	CHES pH 9.5	
4	35% (v/v) MPD	Imidazole pH 8.0	0.2 M magnesium chloride
5	30% (v/v) PEG-400	CAPS pH 10.5	
6	20% (w/v) PEG-3000	Citrate pH 5.5	
7	10% (w/v) PEG-8000	MES pH 6.0	0.2 M zinc acetate
8	2.0 M ammonium sulphate	Citrate pH 5.5	
9	1.0 M ammonium phosphate	Acetate pH 4.5	
10	20% (w/v) PEG-2000 MME	Tris pH 7.0	
11	20% (v/v) 1,4-butanediol	MES pH 6.0	0.2 M lithium sulphate
12	20% (w/v) PEG-1000	Imidazole pH 8.0	0.2 M cadmium acetate
13	1.26 M ammonium sulphate	Cacodylate pH 6.5	
14	1.0 M sodium citrate	Cacodylate pH 6.5	
15	10% (w/v) PEG-3000	Imidazole pH 8.0	0.2 M lithium sulphate
16	2.5 M sodium chloride	Na/K phosphate pH 6.2	
17	30% (w/v) PEG-8000	Acetate pH 4.5	0.2 M lithium sulphate
18	1.0 M K/Na tartrate	Imidazole pH 8.0	0.2 M sodium chloride
19	20% (w/v) PEG-1000	Tris pH 7.0	
20	0.4 M Na phosphate/1.6 M K phosphate	Imidazole pH 8.0	0.2 M sodium chloride
21	20% (w/v) PEG-8000	HEPES pH 7.5	
22	10% (v/v) 2-Propanol	Tris pH 8.5	
23	15% (v/v) Ethanol	Imidazole pH 8.0	0.2 M magnesium chloride
24	35% (v/v) MPD	Tris pH 7.0	0.2 M sodium chloride
25	30% (v/v) PEG-400	Tris pH 8.5	0.2 M magnesium chloride
26	10% (w/v) PEG-3000	CHES pH 9.5	
27	1.2 M Na phosphate/0.8 M K phosphate	CAPS pH 10.5	0.2 M lithium sulphate
28	20% (w/v) PEG-3000	HEPES pH 7.5	0.2 M sodium chloride
29	10% (w/v) PEG-8000	CHES pH 9.5	0.2 M sodium chloride
30	1.26 M ammonium sulphate	Acetate pH 4.5	0.2 M sodium chloride
31	20% (w/v) PEG-8000	Phosphate-citrate pH 4.2	0.2 M sodium chloride
32	10% (w/v) PEG-3000	Na/K phosphate pH 6.2	
33	2.0 M ammonium sulphate	CAPS pH 10.5	0.2 M lithium sulphate
34	1.0 M ammonium phosphate	Imidazole pH 8.0	
35	20% (v/v) 1,4-butanediol	Acetate pH 4.5	
36	1.0 M sodium citrate	Imidazole pH 8.0	
37	2.5 M sodium chloride	Imidazole pH 8.0	
38	1.0 M K/Na tartrate	CHES pH 9.5	0.2 M lithium sulphate
39	20% (w/v) PEG-1000	Phosphate-citrate pH 4.2	0.2 M lithium sulphate
40	10% (v/v) 2-Propanol	MES pH 6.0	0.2 M calcium acetate
41	30% (w/v) PEG-3000	CHES pH 9.5	
42	15% (v/v) Ethanol	Tris pH 7.0	
43	35% (v/v) MPD	Na/K phosphate pH 6.2	
44	30% (v/v) PEG-400	Acetate pH 4.5	0.2 M calcium acetate
45	20% (w/v) PEG-3000	Acetate pH 4.5	
46	10% (w/v) PEG-8000	Imidazole pH 8.0	0.2 M calcium acetate
47	1.26 M ammonium sulphate	Tris pH 8.5	0.2 M lithium sulphate
48	20% (w/v) PEG-1000	Acetate pH 4.5	0.2 M zinc acetate
49	10% (w/v) PEG-3000	Acetate pH 4.5	0.2 M zinc acetate
50	35% (v/v) MPD	MES pH 6.0	0.2 M lithium sulphate
51	20% (w/v) PEG-8000	Tris pH 8.5	0.2 M magnesium chloride
52	2.0 M ammonium sulphate	Cacodylate pH 6.5	0.2 M sodium chloride
53	20% (v/v) 1,4-butanediol	HEPES pH 7.5	0.2 M sodium chloride
54	10% (v/v) 2-propanol	Phosphate-citrate pH 4.2	0.2 M lithium sulphate
55	30% (w/v) PEG-3000	Tris pH 7.0	0.2 M sodium chloride
56	10% (w/v) PEG-8000	Na/K phosphate pH 6.2	0.2 M sodium chloride
57	2.0 M ammonium sulphate	Phosphate-citrate pH 4.2	
58	1.0 M ammonium phosphate	Tris pH 8.5	
59	10% (v/v) 2-Propanol	Cacodylate pH 6.5	0.2 M zinc acetate
60	30% (v/v) PEG-400	Cacodylate pH 6.5	0.2 M lithium sulphate
61	15% (v/v) ethanol	Citrate pH 5.5	0.2 M lithium sulphate
62	20% (w/v) PEG-1000	Na/K phosphate pH 6.2	0.2 M sodium chloride
63	1.26 M ammonium sulphate	HEPES pH 7.5	
64	1.0 M sodium citrate	CHES pH 9.5	
65	2.5 M sodium chloride	Tris pH 7.0	0.2 M magnesium chloride
66	20% (w/v) PEG-3000	Tris pH 7.0	0.2 M calcium acetate
67	1.6 M Na phosphate/0.4 M K phosphate	Phosphate-Citrate pH 4.2	
68	15% (v/v) ethanol	MES pH 6.0	0.2 M zinc acetate
69	35% (v/v) MPD	Acetate pH 4.5	
70	10% (v/v) 2-propanol	Imidazole pH 8.0	
71	15% (v/v) ethanol	HEPES pH 7.5	0.2 M magnesium chloride
72	30% (w/v) PEG-8000	Imidazole pH 8.0	0.2 M sodium chloride
73	35% (v/v) MPD	HEPES pH 7.5	0.2 M sodium chloride
74	30% (v/v) PEG-400	CHES pH 9.5	
75	10% (w/v) PEG-3000	Cacodylate pH 6.5	0.2 M magnesium chloride
76	20% (w/v) PEG-8000	MES pH 6.0	0.2 M calcium acetate

77	1.26 M ammonium sulphate	CHES pH 9.5	0.2 M sodium chloride
78	20% (v/v) 1,4-butanediol	Imidazole pH 8.0	0.2 M zinc acetate
79	1.0 M sodium citrate	Tris pH 7.0	0.2 M sodium chloride
80	20% (w/v) PEG-1000	Tris pH 8.5	
81	1.0 M ammonium phosphate	Citrate pH 5.5	0.2 M sodium chloride
82	10% (w/v) PEG-8000	Imidazole pH 8.0	
83	0.8 M Na phosphate/1.2 M K phosphate	Acetate pH 4.5	
84	10% (w/v) PEG-3000	Phosphate-citrate pH 4.2	0.2 M sodium chloride
85	1.0 M K/Na tartrate	Tris pH 7.0	0.2 M lithium sulphate
86	2.5 M sodium chloride	Acetate pH 4.5	0.2 M lithium sulphate
87	20% (w/v) PEG-8000	CAPS pH 10.5	0.2 M sodium chloride
88	20% (w/v) PEG-3000	Imidazole pH 8.0	0.2 M zinc acetate
89	2.0 M ammonium sulphate	Tris pH 7.0	0.2 M lithium sulphate
90	30% (v/v) PEG-400	HEPES pH 7.5	0.2 M sodium chloride
91	10% (w/v) PEG-8000	Tris pH 7.0	0.2 M magnesium chloride
92	20% (w/v) PEG-1000	Cacodylate pH 6.5	0.2 M magnesium chloride
93	1.26 M ammonium sulphate	MES pH 6.0	
94	1.0 M ammonium phosphate	Imidazole pH 8.0	0.2 M sodium chloride
95	2.5 M sodium chloride	Imidazole pH 8.0	0.2 M zinc acetate
96	1.0 M K/Na tartrate	MES pH 6.0	
Crystal Screen and Crystal Screen 2 (CS)			
1	30% v/v MPD	Na acetate pH 4.6	0.02 M calcium chloride
2	0.4 M Na/K tartrate		
3	0.4 M ammonium phosphate		
4	2.0 M ammonium sulphate	Tris HCl pH 8.5	
5	30% v/v MPD	Na Hepes pH 7.5	0.2 M sodium citrate
6	30% w/v PEG 4000	Tris HCl pH 8.5	0.2 M magnesium chloride
7	1.4 M sodium acetate	Na cacodylate pH 6.5	
8	30% v/v isopropanol	Na cacodylate pH 6.5	0.2 M sodium citrate
9	30% w/v PEG 4000	Na citrate pH 5.6	0.2 M ammonium acetate
10	30% w/v PEG 4000	Na acetate pH 4.6	0.2 M ammonium acetate
11	1.0 M ammonium phosphate	Na citrate pH 5.6	
12	30% v/v isopropanol	Na Hepes pH 7.5	0.2 M magnesium chloride
13	30% v/v PEG 400	Tris HCl pH 8.5	0.2 M sodium citrate
14	28% v/v PEG 400	Na Hepes pH 7.5	0.2 M calcium chloride
15	30% w/v PEG 8000	Na cacodylate pH 6.5	0.2 M ammonium sulphate
16	1.5M lithium sulphate	Na Hepes pH 7.5	
17	30% w/v PEG 4000	Tris HCl pH 8.5	0.2 M lithium sulphate
18	20% w/v PEG 8000	Na cacodylate pH 6.5	0.2 M magnesium acetate
19	30% v/v isopropanol	Tris HCl pH 8.5	0.2 M ammonium acetate
20	25% w/v PEG 4000	Na acetate pH 4.6	0.2 M ammonium sulphate
21	30% v/v MPD	Na cacodylate pH 6.5	0.2 M magnesium acetate
22	30% w/v PEG 4000	Tris HCl pH 8.5	0.2 M sodium acetate
23	30% v/v PEG 400	Na Hepes pH 7.5	0.2 M magnesium chloride
24	20% v/v isopropanol	Na acetate pH 4.6	0.2 M calcium chloride
25	1.0 M sodium acetate	imidazole pH 6.5	
26	30% v/v MPD	Na citrate pH 5.6	0.2 M ammonium acetate
27	20% v/v isopropanol	Na Hepes pH 7.5	0.2 M sodium citrate
28	30% w/v PEG 8000	Na cacodylate pH 6.5	0.2 M sodium acetate
29	0.8 M Na/K tartrate	0.1M Na Hepes pH 7.5	
30	30% w/v PEG 8000		0.2 M ammonium sulphate
31	30% w/v PEG 4000		0.2 M ammonium sulphate
32	2.0 M ammonium sulphate		
33	4.0 M sodium formate		
34	2.0 M sodium formate	Na acetate pH 4.6	
35	0.8 M Na/K phosphate	Na Hepes pH 7.5	
36	8% w/v PEG 8000	Tris HCl pH 8.5	
37	8% w/v PEG 4000	Na acetate pH 4.6	
38	1.4 M sodium citrate	Na Hepes pH 7.5	
39	2% v/v PEG 400, 2.0 M ammonium sulphate	Na Hepes pH 7.5	
40	20% v/v isopropanol, 20% w/v PEG 4000	Na citrate pH 5.6	
41	10% v/v isopropanol, 20% w/v PEG 4000	Na Hepes pH 7.5	
42	20% w/v PEG 8000		0.05 M potassium phosphate
43	30% w/v PEG 1500		
44	0.2 M magnesium formate		
45	18% w/v PEG 8000	Na cacodylate pH 6.5	0.2 M zinc acetate
46	18% w/v PEG 8000	Na cacodylate pH 6.5	0.2 M calcium acetate
47	2.0 M ammonium sulphate	Na acetate pH 4.6	
48	2.0 M Ammonium phosphate	Tris HCl pH 8.5	
49	10% w/v PEG 6000		2.0 M sodium chloride
50	0.01 M Hexacetyltrimethylammonium bromide (CTAB)		0.5 M sodium chloride, 0.01 M magnesium chloride
51	25% v/v ethylene glycol		
52	35% v/v dioxane		
53	5% v/v isopropanol		2.0 M ammonium sulphate
54	1.0M imidazole pH 7.0		
55	10% w/v PEG 1000, 10% w/v PEG 8000		
56	10% v/v ethanol		1.5 M sodium chloride

57	2.0 M sodium chloride	Na acetate pH 4.6	
58	30% v/v MPD	Na acetate pH 4.6	0.2 M sodium chloride
59	1.0 M 1,6 hexanediol	Na acetate pH 4.6	0.01 M cobalt chloride
60	30% v/v PEG 400	Na acetate pH 4.6	0.1M cadmium chloride
61	30% w/v PEG MME 2000	Na acetate pH 4.6	0.2 M ammonium sulphate
62	2.0 M ammonium sulphate	Na citrate pH 5.6	0.2M K/Na tartrate
63	1.0 M lithium sulphate	Na citrate pH 5.6	0.5M ammonium sulphate
64	2% w/v polyethyleneimine	Na citrate pH 5.6	0.5 M sodium chloride
65	35% v/v tert-butanol	Na citrate pH 5.6	
66	10% v/v Jeffamine M-600	Na citrate pH 5.6	0.01 M ferric chloride
67	2.5 M 1,6 hexanediol	Na citrate pH 5.6	
68	1.6 M magnesium sulphate	MES pH 6.5	
69	2.0 M sodium chloride	MES pH 6.5	0.2 M Na/K phosphate
70	12% w/v PEG 20,000	MES pH 6.5	
71	10% v/v dioxane	MES pH 6.5	1.6 M ammonium sulphate
72	30% v/v Jeffamine M-600	MES pH 6.5	0.05 M caesium chloride
73	1.8 M ammonium sulphate	MES pH 6.5	0.01 M cobalt chloride
74	30% w/v PEG MME 5000	MES pH 6.5	0.2 M ammonium sulphate
75	25% v/v PEG MME 550	MES pH 6.5	0.01 M zinc sulphate
76	1.6 M sodium citrate pH 6.5		
77	30% v/v MPD	Hepes pH 7.5	0.5 M ammonium sulphate
78	10% w/v PEG 6000, 5% v/v MPD	Hepes pH 7.5	
79	20% v/v Jeffamine M-600	Hepes pH 7.5	
80	1.6 M ammonium sulphate	Hepes pH 7.5	0.1 M sodium chloride
81	2.0 M ammonium formate	Hepes pH 7.5	
82	1.0 M sodium acetate	Hepes pH 7.5	0.05 M cadmium sulphate
83	70% v/v MPD	Hepes pH 7.5	
84	4.3 M sodium chloride	Hepes pH 7.5	
85	10% w/v PEG 8000, 8% v/v ethylene glycol	Hepes pH 7.5	
86	20% w/v PEG 10,000	Hepes pH 7.5	
87	3.4 M 1,6 hexanediol	Tris pH 8.5	0.2 M magnesium chloride
88	25% v/v tert-butanol	Tris pH 8.5	
89	1.0 M lithium sulphate	Tris pH 8.5	0.01 M nickel (II) chloride
90	12% v/v glycerol	Tris pH 8.5	1.5 M ammonium sulphate
91	50% v/v MPD	Tris pH 8.5	0.2 M ammonium phosphate
92	20% v/v ethanol	Tris pH 8.5	
93	20% w/v PEG MME 2000	Tris pH 8.5	0.01 M nickel (II) chloride
94	20% w/v PEG MME 550	Bicine pH 9.0	0.1 M sodium chloride
95	2.0 M magnesium chloride	Bicine pH 9.0	
96	10% w/v PEG 20,000	Bicine pH 9.0	2% v/v dioxane
Personal Structure Screens 1 and 2 (PSS)			
1	15% w/v polyvinylpyrrolidone		
2	2.0 M Urea		
3	25% w/v PEG 4000	Na acetate pH 4.6	0.2 M ammonium sulphate
4	2.0 M sodium formate	Na acetate pH 4.6	
5	2.0 M ammonium sulphate	Na acetate pH 4.6	
6	8% w/v PEG 4000	Na acetate pH 4.6	
7	30% w/v PEG 4000	Na citrate pH 5.6	0.2 M ammonium acetate
8	30% v/v MPD	Na citrate pH 5.6	0.2 M ammonium acetate
9	20% w/v iso-propanol, 20% w/v PEG 4000	Na citrate pH 5.6	
10	1.0 M ammonium phosphate	Na citrate pH 5.6	
11	20% v/v iso-propanol	Na acetate pH 4.6	0.2M calcium chloride
12	1.4 M sodium acetate	Na cacodylate pH 6.5	
13	30% v/v isopropanol	Na cacodylate pH 6.5	0.2 M sodium citrate
14	30% w/v PEG 8000	Na cacodylate pH 6.5	0.2 M ammonium sulphate
15	20% w/v PEG 8000	Na cacodylate pH 6.5	0.2 M magnesium acetate
16	30% v/v MPD	Na cacodylate pH 6.5	0.2 M magnesium acetate
17	1.0 M sodium acetate	Imidazole pH 6.5	
18	30% w/v PEG 8000	Na cacodylate pH 6.5	0.2 M sodium acetate
19	18% w/v PEG 8000	Na cacodylate pH 6.5	0.2 M zinc acetate
20	18% w/v PEG 8000	Na cacodylate pH 6.5	0.2 M calcium acetate
21	30% v/v MPD	Na Hepes pH 7.5	0.2 M sodium citrate
22	30% v/v isopropanol	Na Hepes pH 7.5	0.2 M magnesium chloride
23	28% v/v PEG 400	Na Hepes pH 7.5	0.2 M calcium chloride
24	30% v/v PEG 400	Na Hepes pH 7.5	0.2 M magnesium Chloride
25	20% v/v isopropanol	Na Hepes pH 7.5	0.2 M sodium citrate
26	0.8 M K, Na tartrate	Na Hepes pH 7.5	
27	1.5 M lithium sulphate	Na Hepes pH 7.5	
28	0.8 M Na/K phosphate	Na Hepes pH 7.5	
29	1.4 M sodium citrate	Na Hepes pH 7.5	
30	2% v/v PEG 400, 2.0 M ammonium sulphate	Na Hepes pH 7.5	
31	10% v/v isopropanol, 20% w/v PEG 4000	Na Hepes pH 7.5	
32	2.0 M ammonium sulphate	Tris HCl pH 8.5	
33	30% w/v PEG 4000	Tris HCl pH 8.5	0.2 M magnesium chloride
34	30% v/v PEG 400	Tris HCl pH 8.5	0.2 M sodium citrate
35	30% w/v PEG 4000	Tris HCl pH 8.5	0.2 M lithium sulphate
36	30% v/v 2-propanol	Tris HCl pH 8.5	0.2 M ammonium acetate

37	30% w/v PEG 4000	Tris HCl pH 8.5	0.2 M sodium acetate
38	8% w/v PEG 8000	Tris HCl pH 8.5	
39	2.0 M ammonium phosphate	Tris HCl pH 8.5	
40	0.4 M K, Na tartrate		
41	0.4 M ammonium phosphate		
42	30% w/v PEG 8000		0.2 M ammonium sulphate
43	30% w/v PEG 4000		0.2 M ammonium sulphate
44	2.0 M ammonium sulphate		
45	4.0 M sodium formate		
46	20% w/v PEG 8000		0.05 M potassium phosphate
47	30% w/v PEG 1500		
48	0.2 M magnesium formate		
49	30% v/v PEG MME 550	Bicine pH 9.0	0.1 M sodium chloride
50	2.0 M magnesium chloride	Bicine pH 9.0	
51	10% w/v PEG 20,000	Bicine pH 9.0	2% w/v dioxane
52	3.4 M 1,6 hexanediol	Tris pH 8.5	0.2 M magnesium chloride
53	25% v/v tert-butanol	Tris pH 8.5	
54	1.0 M lithium sulphate	Tris pH 8.5	0.01 M nickel (II) chloride
55	12% v/v glycerol	Tris pH 8.5	1.5 M ammonium sulphate
56	50% v/v MPD	Tris pH 8.5	0.2 M ammonium phosphate
57	20% v/v ethanol	Tris pH 8.5	
58	20% w/v PEG MME 2000	Tris pH 8.5	0.01 M nickel (II) chloride
59	30% v/v MPD	Hepes pH 7.5	0.5 M ammonium sulphate
60	10% w/v PEG 6000, 5% v/v MPD	Hepes pH 7.5	
61	20% v/v Jeffamine M-600	Hepes pH 7.5	
62	1.6 M ammonium sulphate	Hepes pH 7.5	0.1 M sodium chloride
63	2.0 M ammonium formate	Hepes pH 7.5	
64	1.0 M sodium acetate	Hepes pH 7.5	0.05 M cadmium sulphate
65	70% v/v MPD	Hepes pH 7.5	
66	4.3 M sodium chloride	Hepes pH 7.5	
67	10% w/v PEG 8000, 8% v/v ethylene glycol	Hepes pH 7.5	
68	1.6 M magnesium sulphate	MES pH 6.5	
69	2.0 M sodium chloride	MES pH 6.5	0.1M Na, K phosphate
70	12% w/v PEG 20,000	MES pH 6.5	
71	10% v/v dioxane	MES pH 6.5	1.6 M ammonium sulphate
72	30% v/v Jeffamine M-600	MES pH 6.5	0.05 M caesium chloride
73	1.8 M ammonium sulphate	MES pH 6.5	0.01 M cobalt chloride
74	30% w/v PEG MME 5000	MES pH 6.5	0.2 M ammonium sulphate
75	25% v/v PEG MME 550	MES pH 6.5	0.01 M zinc sulphate
76	20% w/v PEG 10,000	Hepes pH 7.5	
77	2.0 M ammonium sulphate	Na citrate pH 5.6	0.2 M K/Na tartrate
78	1.0 M lithium sulphate	Na citrate pH 5.6	0.5 M ammonium sulphate
79	4% v/v polyethyleneimine	Na citrate pH 5.6	0.5 M sodium chloride
80	35% v/v tert-butanol	Na citrate pH 5.6	
81	10% v/v Jeffamine M-600	Na citrate pH 5.6	0.01 M ferric chloride
82	2.5 M 1,6 hexanediol	Na citrate pH 5.6	0.01 M manganese chloride
83	2.0 M sodium chloride	Na acetate pH 4.6	
84	30% v/v MPD	Na acetate pH 4.6	0.2 M sodium chloride
85	1.0 M 1,6 hexanediol	Na acetate pH 4.6	0.01 M cobalt chloride
86	30% v/v PEG 400	Na acetate pH 4.6	0.1 M cadmium chloride
87	30% w/v PEG MME 2000	Na acetate pH 4.6	0.2 M ammonium sulphate
88	10% w/v PEG 6000		2.0 M sodium chloride
89	0.5 M sodium chloride, 0.1 M magnesium chloride		0.01 M CTAB
90	25% v/v ethylene glycol		
91	35% v/v dioxane		
92	5% v/v isopropanol		2.0 M ammonium sulphate
93	1.0 M imidazole pH 7.0		
94	10% w/v PEG 1000, 10% w/v PEG 8000		
95	10% v/v ethanol		1.5 M sodium chloride
96	1.6 M sodium citrate pH 6.5		

Table S2 Formulations resulting in successful crystallisations in the three screens (WS, Wizard Screens I and II; CS, Crystal Screen and Crystal Screen 2; PSS, Personal Structure Screens 1 and 2).

Protein	WS	CS	PSS
Myoglobin	-	36	68
Lysozyme	2, 6, 10, 26, 34, 45, 46, 86, 87, 88, 93, 94	3, 5, 9, 17, 28, 30, 34, 35, 38, 48, 49, 56, 57, 61, 69, 71, 81, 83, 86, 93, 95	3, 4, 7, 9, 14, 15, 18, 26, 27, 29, 30, 31, 35, 36, 42, 52, 63, 66, 69, 73, 74, 76, 83, 88, 89
Catalase	56, 61, 75, 84, 89, 91	35	56, 71, 75, 89, 91
Xylanase	44, 45, 46, 48, 49, 76, 78, 79, 88, 89, 91, 95	1, 3, 6, 14, 16, 24, 45, 60, 76, 89	11, 19, 27, 33, 46, 54, 56, 75
Phosphorylase B	75	14, 41	5, 56
Pepsin	-	-	46
MBP-Chk2	-	-	4, 51, 96
Glucose isomerase	4, 6, 10, 12, 25, 31, 45, 46, 51, 52, 55, 66, 72, 75, 76, 77, 82, 89, 91, 92	1, 2, 14, 15, 17, 28, 30, 33, 37, 39, 40, 42, 44, 46, 55, 74, 76, 83, 86, 87, 91, 92	7, 9, 11, 14, 15, 18, 20, 23, 24, 29, 30, 31, 32, 33, 35, 41, 52, 71, 74, 76, 85
α -lactalbumin	6, 20, 31, 57	4, 14, 24, 26, 47, 53, 61, 62	6, 20, 31, 57
Trypsin	17, 20	2, 24, 25, 27, 20, 30, 31, 44, 74, 87, 95	5, 14, 42, 43, 46, 74, 76
Haemoglobin	-	-	-
Subtilisin Carlsberg	37, 72	-	54, 76
Ribonuclease A	17, 18, 23, 48, 57, 71	6, 23, 24, 30, 31, 60, 61	3, 5, 42, 43, 82
Ribonuclease inhibitor	13, 14, 72, 88	1, 6, 16, 17, 24, 26, 37	- [†]
Elastase	21, 40, 41, 69, 70, 80, 82	39, 43, 52, 71, 78, 83, 85, 86	9, 31, 36, 38, 46, 51, 53, 57, 60, 65, 67, 70, 73, 76, 90, 95
DsbG	1, 8, 10	9, 16, 62, 74	7, 14, 20, 38, 40, 46, 74, 91
Dun1-FHA	-	-	35, 46, 77, 92
Importin- α	-	50	21
MBP-gp36	11, 12	-	64, 68

[†] Not analysed due to limited amount of protein.

Table S3 The matched conditions in CS and PSS. The formulations are ordered according to CS; original formulation numbers in PSS are also shown (these numbers were used in Fig. 1a-c and Table 1). Formulations 50, 64, 67 and 94 are similar but not identical, while the other formulations are identical as listed by the manufacturers. CS formulations 1 and 10 do not have a match in PSS in our set-up. The pH was measured as described in Experimental Methods.

Number (Crystal Screen (CS))	Formulation (CS)	Measured pH (CS)	Number (Personal Structure Screen (PSS))	Formulation (PSS)	Measured pH (PSS)
1	30% v/v MPD 0.1 M Na Acetate pH 4.6 0.02 M calcium chloride	5.02	-		
2	0.4 M Na/K tartrate	6.70	40	0.4 M K, Na tartrate	6.67
3	0.4 M ammonium phosphate	4.29	41	0.4 M ammonium phosphate	4.21
4	2.0 M ammonium sulphate 0.1 M Tris HCl pH 8.5	8.46	32	2.0 M ammonium sulphate 0.1 M Tris HCl pH 8.5	8.43
5	30% v/v MPD 0.1M Na HEPES pH 7.5 0.2 M sodium citrate	7.36	21	30% v/v MPD 0.1 M Na HEPES pH 7.5 0.2 M sodium citrate	7.63
6	30% w/v PEG 4000 0.1M Tris HCl pH 8.5 0.2 M magnesium chloride	8.50	33	30% w/v PEG 4000 0.1 M Tris HCl pH 8.5 0.2 M magnesium chloride	6.23
7	1.4 M sodium acetate 0.1M Na cacodylate pH 6.5	6.78	12	1.4 M sodium acetate 0.1 M Na cacodylate pH 6.5	6.95
8	30% v/v isopropanol 0.1 M Na cacodylate pH 6.5 0.2 M sodium citrate	6.99	13	30% v/v isopropanol 0.1 M Na cacodylate pH 6.5 0.2 M sodium citrate	7.08
9	30% w/v PEG 4000 0.1 M Na citrate pH 5.6 0.2 M ammonium acetate	6.46	7	30% w/v PEG 4000 0.1 M Na citrate pH 5.6 0.2 M ammonium acetate	6.23
10	30% w/v PEG 4000 0.1 M Na acetate pH 4.6 0.2 M ammonium acetate	5.79	-		
11	1.0 M ammonium phosphate 0.1 M Na citrate pH 5.6	4.96	10	1.0 M ammonium phosphate 0.1 M Na citrate pH 5.6	5.56
12	30% v/v isopropanol 0.1 M Na HEPES pH 7.5 0.2 M magnesium chloride	7.09	22	30% v/v isopropanol 0.1 M Na HEPES pH 7.5 0.2 M magnesium chloride	7.05
13	30% v/v PEG 400 0.1 M Tris HCl pH 8.5 0.2 M sodium citrate	9.09	34	30% v/v PEG 400 0.1 M Tris HCl pH 8.5 0.2 M sodium citrate	8.43
14	28% v/v PEG 400 0.1M Na HEPES pH 7.5 0.2 M calcium chloride	7.28	23	28% v/v PEG 400 0.1 M Na HEPES pH 7.5 0.2 M calcium chloride	6.97
15	30% w/v PEG 8000 0.1 M Na cacodylate pH 6.5 0.2 M ammonium sulphate	6.60	14	30% w/v PEG 8000 0.1 M Na cacodylate pH 6.5 0.2 M ammonium sulphate	6.49
16	1.5 M lithium sulphate 0.1 M Na HEPES pH 7.5	7.84	27	1.5 M lithium sulphate 0.1 M Na HEPES pH 7.5	7.82
17	30% w/v PEG 4000 0.1M Tris HCl pH 8.5 0.2 M lithium sulphate	8.79	35	30% w/v PEG 4000 0.1 M Tris HCl pH 8.5 0.2 M lithium sulphate	7.34
18	20% w/v PEG 8000 0.1M Na cacodylate pH 6.5 0.2 M magnesium acetate	6.50	15	20% w/v PEG 8000 0.1 M Na cacodylate pH 6.5 0.2 M magnesium acetate	6.40
19	30% v/v isopropanol 0.1M Tris HCl pH 8.5 0.2 M ammonium acetate	8.53	36	30% v/v 2-propanol 0.1 M Tris HCl pH 8.5 0.2 M ammonium acetate	8.31
20	25% w/v PEG 4000 0.1 M Na acetate pH 4.6 0.2 M ammonium sulphate	5.06	3	25% w/v PEG 4000 0.1 M Na acetate pH 4.6 0.2 M ammonium sulphate	4.43
21	30% v/v MPD 0.1 M Na cacodylate pH 6.5 0.2 M magnesium acetate	6.53	16	30% v/v MPD 0.1 M Na cacodylate pH 6.5 0.2 M magnesium acetate	6.53
22	30% w/v PEG 4000 0.1 M Tris HCl pH 8.5 0.2 M sodium acetate	8.74	37	30% w/v PEG 4000 0.1 M Tris HCl pH 8.5 0.2 M sodium acetate	8.08
23	30% v/v PEG 400 0.1M Na HEPES pH 7.5 0.2 M magnesium chloride	7.32	24	30% v/v PEG 400 0.1 M Na HEPES pH 7.5 0.2 M magnesium chloride	6.90
24	20% v/v isopropanol 0.1 M Na acetate pH 4.6 0.2 M calcium chloride	4.72	11	20% v/v iso-propanol 0.1M Na acetate pH 4.6 0.2M calcium chloride	4.56
25	1.0 M sodium acetate 0.1 M imidazole pH 6.5	7.06	17	1.0 M sodium acetate 0.1 M imidazole pH 6.5	7.00

26	30% v/v MPD 0.1 M Na citrate pH 5.6 0.2 M ammonium acetate	6.47	8	30% v/v MPD 0.1 M Na citrate pH 5.6 0.2 M ammonium acetate	6.38
27	20% v/v isopropanol 0.1M Na HEPES pH7.5 0.2 M sodium citrate	7.46	25	20% v/v isopropanol 0.1 M Na HEPES pH 7.5 0.2 M sodium citrate	7.63
28	30% w/v PEG 8000 0.1M Na cacodylate pH 6.5 0.2 M sodium acetate	6.81	18	30% w/v PEG 8000 0.1 M Na cacodylate pH 6.5 0.2 M sodium acetate	6.59
29	0.8 M Na/K tartrate 0.1M Na HEPES pH7.5	7.75	26	0.8 M K, Na tartrate 0.1 M Na HEPES pH 7.5	7.83
30	30% w/v PEG 8000 0.2 M ammonium sulphate	5.07	42	30% w/v PEG 8000 0.2 M ammonium sulphate	3.09
31	30% w/v PEG 4000 0.2 M ammonium sulphate	4.91	43	30% w/v PEG 4000 0.2 M ammonium sulphate	3.00
32	2.0 M ammonium sulphate	4.88	44	2.0 M ammonium sulphate	4.49
33	4.0 M sodium formate	7.22	45	4.0 M sodium formate	7.28
34	2.0 M sodium formate 0.1 M Na acetate pH 4.6	5.50	4	2.0 M sodium formate 0.1 M Na acetate pH 4.6	4.91
35	0.8 M Na/K phosphate 0.1 M Na HEPES pH7.5	4.63	28	0.8 M Na/K phosphate 0.1 M Na HEPES pH 7.5	4.75
36	8% w/v PEG 8000 0.1 M Tris HCl pH 8.5	8.49	38	8% w/v PEG 8000 0.1 M Tris HCl pH 8.5	8.02
37	8% w/v PEG 4000 0.1 M Na acetate pH 4.6	4.83	6	8% w/v PEG 4000 0.1 M Na acetate pH 4.6	4.15
38	1.4 M sodium citrate 0.1 M Na HEPES pH 7.5	7.92	29	1.4 M sodium citrate 0.1 M Na HEPES pH 7.5	7.89
39	2% v/v PEG 400, 2.0 M ammonium sulphate 0.1 M Na HEPES pH 7.5	7.79	30	2% v/v PEG 400, 2.0 M ammonium sulphate 0.1 M Na HEPES pH 7.5	7.70
40	20% v/v isopropanol, 20% w/v PEG 4000 0.1 M Na citrate pH 5.6	6.32	9	20% v/v iso-propanol. 20% w/v PEG 4000 0.1 M Na citrate pH 5.6	6.44
41	10% v/v isopropanol, 20% w/v PEG 4000 0.1 M Na HEPES pH 7.5	7.17	31	10% v/v isopropanol, 20% w/v PEG 4000 0.1 M Na HEPES pH 7.5	7.05
42	20% w/v PEG 8000 0.05 M potassium phosphate	5.50	46	20% w/v PEG 8000 0.05 M potassium phosphate	4.15
43	30% w/v PEG 1500	6.29	47	30% w/v PEG 1500	3.12
44	0.2 M magnesium formate	6.16	48	0.2 M magnesium formate	6.39
45	18% w/v PEG 8000 0.1M Na cacodylate pH 6.5 0.2 M zinc acetate	5.88	19	18% w/v PEG 8000 0.1 M Na cacodylate pH 6.5 0.2 M zinc acetate	5.55
46	18% w/v PEG 8000 0.1M Na cacodylate pH 6.5 0.2 M calcium acetate	6.48	20	18% w/v PEG 8000 0.1 M Na cacodylate pH 6.5 0.2 M calcium acetate	6.43
47	2.0 M ammonium sulphate 0.1 M Na acetate pH 4.6	4.88	5	2.0 M ammonium sulphate 0.1 M Na acetate pH 4.6	4.42
48	2.0 M Ammonium phosphate 0.1M Tris HCl pH 8.5	4.24	39	2.0 M ammonium phosphate 0.1 M Tris HCl pH 8.5	4.90
49	10% w/v PEG 6000 2.0 M sodium chloride	3.43	88	10% w/v PEG 6000 2.0 M sodium chloride	2.62
50	0.01 M Hexacethyltrimethylammonium bromide (CTAB) 0.5 M sodium chloride, 0.01 M magnesium chloride	4.28	89	0.5 M sodium chloride, 0.1 M magnesium chloride 0.01 M CTAB	3.84
51	25% v/v ethylene glycol	7.51	90	25% v/v ethylene glycol	6.23
52	35% v/v dioxane	4.70	91	35% v/v dioxane	5.04
53	5% v/v isopropanol 2.0 M ammonium sulphate	4.50	92	5% v/v isopropanol 2.0 M ammonium sulphate	4.76
54	1.0M imidazole pH 7.0	7.21	93	1.0 M imidazole pH 7.0	6.98
55	10% w/v PEG 1000, 10% w/v PEG 8000	6.60	94	10% w/v PEG 1000, 10% w/v PEG 8000	2.82
56	10% v/v ethanol 1.5 M sodium chloride	3.98	95	10% v/v ethanol 1.5 M sodium chloride	3.58
57	2.0 M sodium chloride 0.1 M Na acetate pH 4.6	4.44	83	2.0 M sodium chloride 0.1 M Na acetate pH 4.6	4.07
58	30% v/v MPD 0.1 M Na acetate pH 4.6 0.2 M sodium chloride	5.04	84	30% v/v MPD 0.1 M Na acetate pH 4.6 0.2 M sodium chloride	4.74
59	1.0 M 1,6 hexanediol 0.1 M Na acetate pH 4.6 0.01 M cobalt chloride	4.82	85	1.0 M 1,6 hexanediol 0.1 M Na acetate pH 4.6 0.01 M cobalt chloride	4.58
60	30% v/v PEG 400 0.1 M Na acetate pH 4.6 0.1M cadmium chloride	4.75	86	30% v/v PEG 400 0.1 M Na acetate pH 4.6 0.1 M cadmium chloride	4.42
61	30% w/v PEG MME 2000 0.1 M Na acetate pH 4.6 0.2 M ammonium sulphate	5.06	87	30% w/v PEG MME 2000 0.1 M Na acetate pH 4.6 0.2 M ammonium sulphate	4.49
62	2.0 M ammonium sulphate 0.1 M Na citrate pH 5.6 0.2M K/Na tartrate	5.84	77	2.0 M ammonium sulphate 0.1 M Na citrate pH 5.6 0.2 M K/Na tartrate	5.84

63	1.0 M lithium sulphate 0.1 M Na citrate pH 5.6 0.5 M ammonium sulphate	5.35	78	1.0 M lithium sulphate 0.1 M Na citrate pH 5.6 0.5 M ammonium sulphate	5.39
64	2% w/v polyethyleneimine 0.1 M Na citrate pH 5.6 0.5 M sodium chloride	5.72	79	4% v/v polyethyleneimine 0.1 M Na citrate pH 5.6 0.5 M sodium chloride	10.60
65	35% v/v tert-butanol 0.1 M Na citrate pH 5.6	6.29	80	35% v/v tert-butanol 0.1 M Na citrate pH 5.6	6.24
66	10% v/v Jeffamine M-600 0.1 M Na citrate pH 5.6 0.01 M ferric chloride	5.41	81	10% v/v Jeffamine M-600 0.1 M Na citrate pH 5.6 0.01 M ferric chloride	10.27
67	2.5 M 1,6 hexanediol 0.1 M Na citrate pH 5.6	6.27	82	2.5 M 1,6 hexanediol 0.1 M Na citrate pH 5.6 0.01 M manganese chloride	9.21
68	1.6 M magnesium sulphate 0.1 M MES pH 6.5	6.73	68	1.6 M magnesium sulphate 0.1 M MES pH 6.5	6.84
69	2.0 M sodium chloride 0.1 M MES pH 6.5 0.2 M Na/K phosphate	5.47	69	2.0 M sodium chloride 0.1 M MES pH 6.5 0.1 M Na, K phosphate	3.73
70	12% w/v PEG 20,000 0.1 M MES pH 6.5	6.64	70	12% w/v PEG 20,000 0.1 M MES pH 6.5	6.65
71	10% v/v dioxane 0.1 M MES pH 6.5 1.6 M ammonium sulphate	6.99	71	10% v/v dioxane 0.1 M MES pH 6.5 1.6 M ammonium sulphate	7.02
72	30% v/v Jeffamine M-600 0.1 M MES pH 6.5 0.05 M cesium chloride	6.65	72	30% v/v Jeffamine M-600 0.1 M MES pH 6.5 0.05 M caesium chloride	10.88
73	1.8 M ammonium sulphate 0.1 M MES pH 6.5 0.01 M cobalt chloride	7.03	73	1.8 M ammonium sulphate 0.1 M MES pH 6.5 0.01 M cobalt chloride	7.37
74	30% w/v PEG MME 5000 0.1 M MES pH 6.5 0.2 M ammonium sulphate	6.43	74	30% w/v PEG MME 5000 0.1 M MES pH 6.5 0.2 M ammonium sulphate	6.49
75	25% v/v PEG MME 550 0.1 M MES pH 6.5 0.01 M zinc sulphate	6.34	75	25% v/v PEG MME 550 0.1 M MES pH 6.5 0.01 M zinc sulphate	6.36
76	1.6 M sodium citrate pH 6.5	6.92	96	1.6 M sodium citrate pH 6.5	6.74
77	30% v/v MPD 0.1 M Hepes pH 7.5 0.5 M ammonium sulphate	7.51	59	30% v/v MPD 0.1 M Hepes pH 7.5 0.5 M ammonium sulphate	7.42
78	10% w/v PEG 6000, 5% v/v MPD 0.1 M Hepes pH 7.5	7.29	60	10% w/v PEG 6000, 5% v/v MPD 0.1 M Hepes pH 7.5	7.31
79	20% v/v Jeffamine M-600 0.1 M Hepes pH 7.5	7.69	61	20% v/v Jeffamine M-600 0.1 M Hepes pH 7.5	10.69
80	1.6 M ammonium sulphate 0.1 M Hepes pH 7.5 0.1 M sodium chloride	7.94	62	1.6 M ammonium sulphate 0.1 M Hepes pH 7.5 0.1 M sodium chloride	7.82
81	2.0 M ammonium formate 0.1 M Hepes pH 7.5	7.63	63	2.0 M ammonium formate 0.1 M Hepes pH 7.5	7.64
82	1.0 M sodium acetate 0.1 M Hepes pH 7.5 0.05 M cadmium sulphate	7.50	64	1.0 M sodium acetate 0.1 M Hepes pH 7.5 0.05 M cadmium sulphate	7.44
83	70% v/v MPD 0.1 M Hepes pH 7.5	7.42	65	70% v/v MPD 0.1 M Hepes pH 7.5	7.41
84	4.3 M sodium chloride 0.1 M Hepes pH 7.5	8.03	66	4.3 M sodium chloride 0.1 M Hepes pH 7.5	7.88
85	10% w/v PEG 8000, 8% v/v ethylene glycol 0.1 M Hepes pH 7.5	7.73	67	10% w/v PEG 8000, 8% v/v ethylene glycol 0.1 M Hepes pH 7.5	7.50
86	20% w/v PEG 10,000 0.1 M Hepes pH 7.5	7.58	76	20% w/v PEG 10,000 0.1 M Hepes pH 7.5	7.46
87	3.4 M 1,6 hexanediol 0.1 M Tris pH 8.5 0.2 M magnesium chloride	8.40	52	3.4 M 1,6 hexanediol 0.1 M Tris pH 8.5 0.2 M magnesium chloride	8.48
88	25% v/v tert-butanol 0.1 M Tris pH 8.5	8.73	53	25% v/v tert-butanol 0.1 M Tris pH 8.5	8.81
89	1.0 M lithium sulphate 0.1 M Tris pH 8.5 0.01 M nickel (II) chloride	8.97	54	1.0 M lithium sulphate 0.1 M Tris pH 8.5 0.01 M nickel (II) chloride	9.07
90	12% v/v glycerol 0.1 M Tris pH 8.5 1.5 M ammonium sulphate	8.57	55	12% v/v glycerol 0.1 M Tris pH 8.5 1.5 M ammonium sulphate	8.48
91	50% v/v MPD 0.1 M Tris pH 8.5 0.2 M ammonium phosphate	6.47	56	50% v/v MPD 0.1 M Tris pH 8.5 0.2 M ammonium phosphate	6.34
92	20% v/v ethanol 0.1 M Tris pH 8.5	8.56	57	20% v/v ethanol 0.1 M Tris pH 8.5	8.52
93	20% w/v PEG MME 2000 0.1 M Tris pH 8.5 0.01 M nickel (II) chloride	8.46	58	20% w/v PEG MME 2000 0.1 M Tris pH 8.5 0.01 M nickel (II) chloride	8.61
94	20% w/v PEG MME 550 0.1 M Bicine pH 9.0 0.1 M sodium chloride	9.10	49	30% w/v PEG MME 550 0.1 M Bicine pH 9.0 0.1 M sodium chloride	8.95

95	2.0 M magnesium chloride 0.1 M Bicine pH 9.0	7.61	50	2.0 M magnesium chloride 0.1 M Bicine pH 9.0	6.83
96	10% w/v PEG 20,000 0.1 M Bicine pH 9.0 2% v/v dioxane	9.72	51	10% w/v PEG 20,000 0.1 M Bicine pH 9.0 2% w/v dioxane	9.36

Figure S1

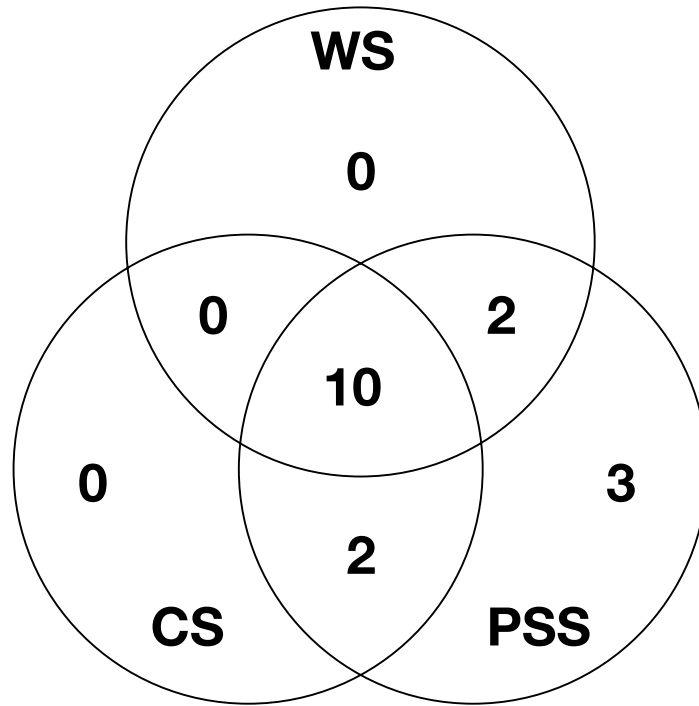


Figure S2a

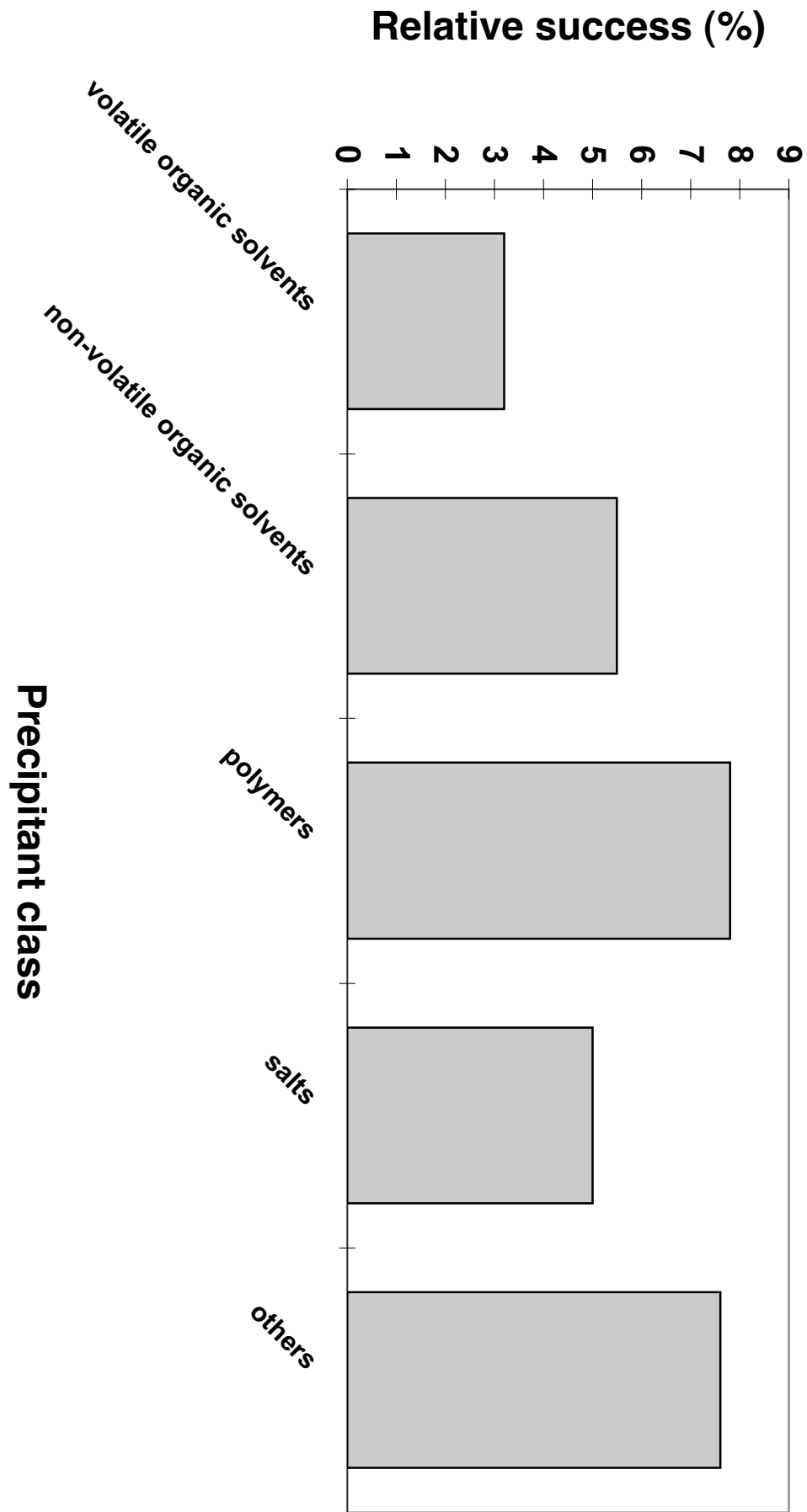


Figure S2b

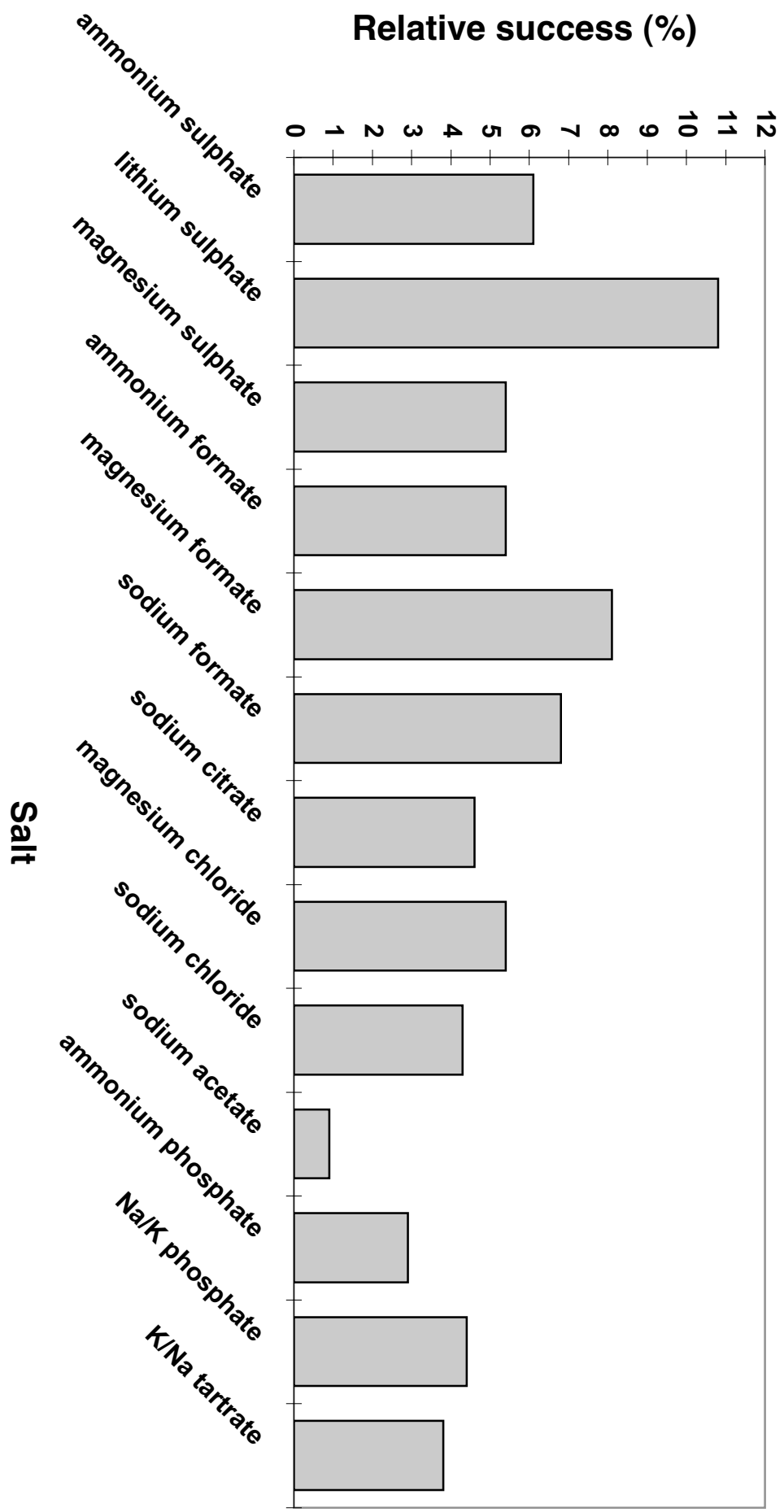


Figure S2c

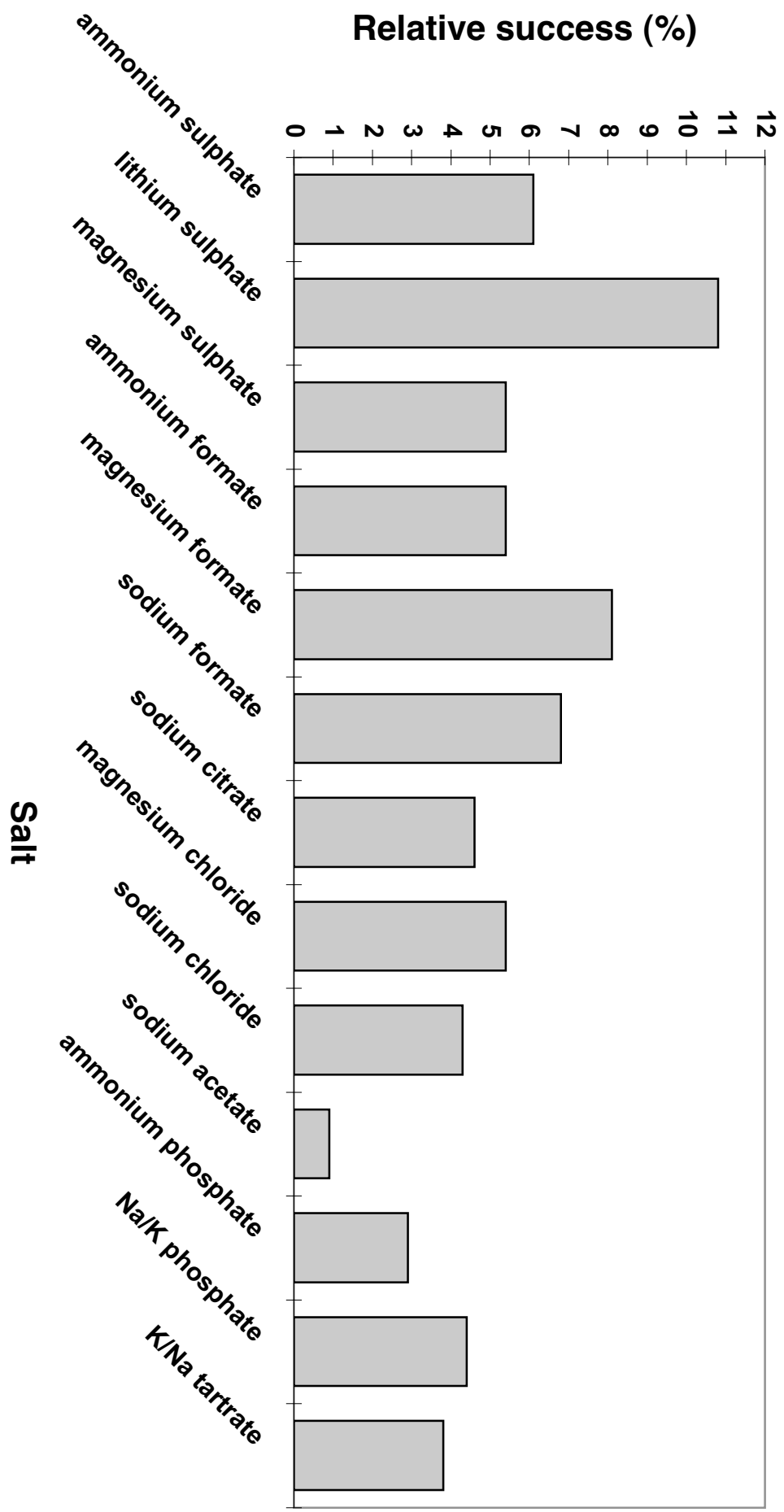


Figure S2d

Relative success (%)

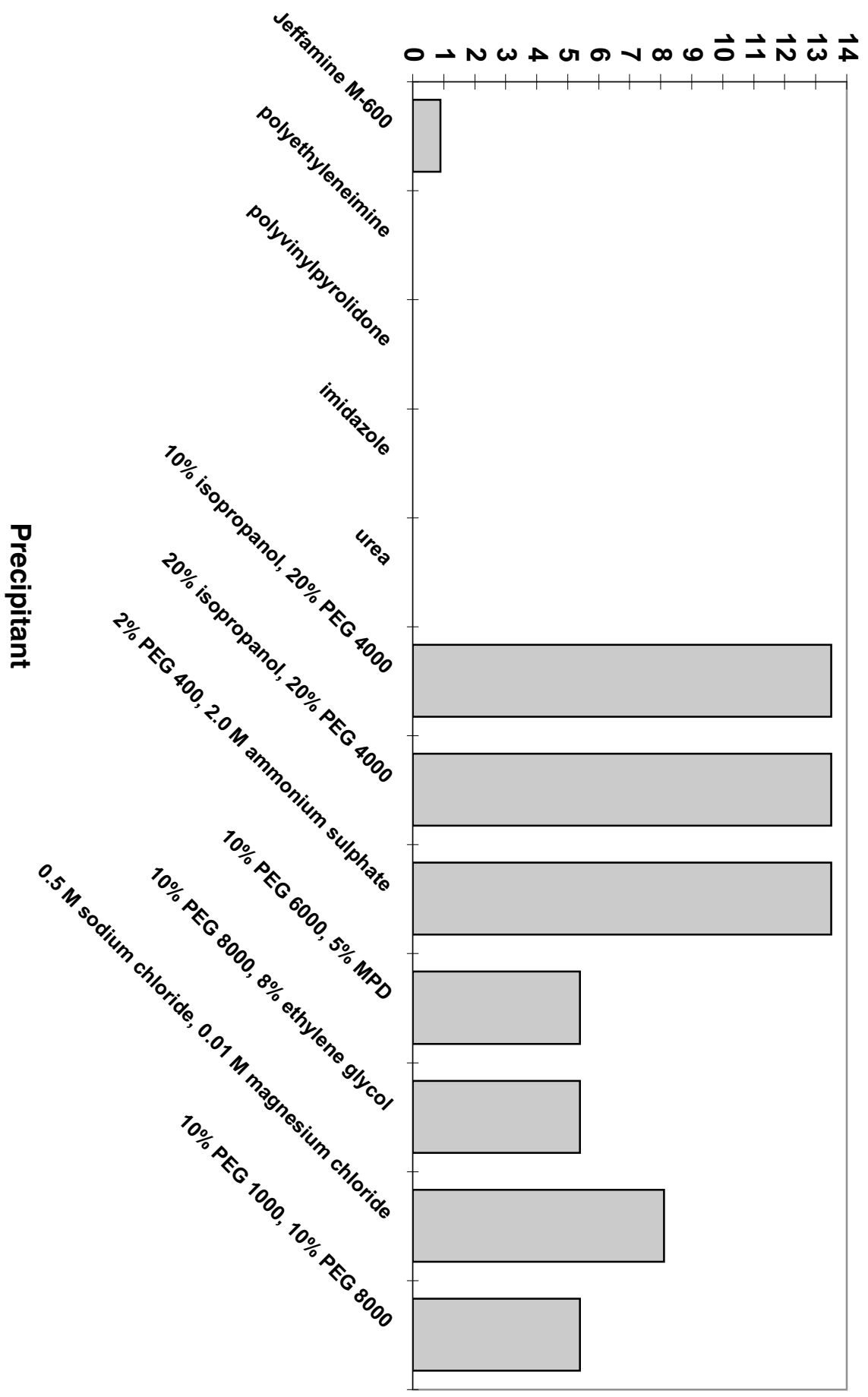


Figure S3

