

Supplementary Table S1. Chemicals, and the associated concentration information, which were found in the 321 crystallization conditions extracted from the crystallization communications published 2012. Only the 73 chemicals that were found more than once are shown in the table. There were another 71 chemicals that were found only once in the conditions parsed from these papers.

Frequency	Chemical	UNITS	Most common concentration	Minimum concentration	Maximum concentration	Standard deviation in concentration
79	POLYETHYLENE GLYCOL 3350	W/V	20.0000	0.7500	28.0000	7.3628
64	SODIUM HEPES AMMONIUM	M	0.1000	0.0200	0.1000	0.0453
61	SULFATE	M	0.2000	0.0500	3.6000	1.0064
43	TRIS CHLORIDE	M	0.1000	0.0200	0.8500	0.3338
41	POLYETHYLENE GLYCOL 4000	W/V	20.0000	8.0000	30.0000	7.2155
40	SODIUM CITRATE - CITRIC ACID	M	0.1000	0.0100	1.6000	0.6993
36	SODIUM ACETATE MAGNESIUM	M	0.1000	0.0500	2.8000	0.8966
33	CHLORIDE	M	0.2000	0.0010	0.4000	0.1348
29	MES	M	0.1000	0.0400	0.5000	0.1673
26	POLYETHYLENE GLYCOL 8000	W/V	30.0000	1.0000	30.0000	8.3007
24	GLYCEROL	W/V	6.3000	2.2680	31.5000	10.0147
23	SODIUM CHLORIDE	M	0.2000	0.0060	3.0000	1.0390
22	BIS-TRIS	M	0.1000	0.0500	0.1000	0.0241
22	POLYETHYLENE GLYCOL 400	W/V	2.2520	2.0000	34.9060	11.4205
21	POLYETHYLENE GLYCOL 6000	W/V	14.0000	5.0000	42.0000	12.1977
21	LITHIUM SULFATE SODIUM	M	0.2000	0.0500	1.8000	0.5530
20	CACODYLATE	M	0.1000	0.0200	0.1000	0.0386
18	2-METHYL-2,4-PENTANEDIOL AMMONIUM	W/V	4.6270	1.8508	46.2700	14.8432
16	ACETATE	M	0.2000	0.0100	0.3500	0.1005
14	BIS-TRIS PROPANE	M	0.1000	0.0001	0.1000	0.0431
12	2-PROPANOL	W/V	7.8550	0.6011	15.7100	4.5530
11	CALCIUM CHLORIDE	M	0.2000	0.0080	0.4000	0.1445
10	ETHYLENE GLYCOL POLYETHYLENE	V/V	5.0000	5.0000	45.0000	14.5204
10	GLYCOL 1000 POLYETHYLENE	W/V	44.8000	5.0000	44.8000	12.6858
9	GLYCOL MONOMETHYL ETHER 2000	W/V	1.0000	1.0000	30.0000	8.6312
9	POTASSIUM SODIUM TARTRATE	M	0.2000	0.0250	1.0000	0.3356
9	FORMATE	M	0.2000	0.1600	4.0000	1.4258
8	IMIDAZOLE LITHIUM	M	0.1000	0.0290	0.1000	0.0297
7	CHLORIDE	M	1.0000	0.2000	1.0000	0.3765
7	TACSIMATE POTASSIUM	V/V	5.0000	2.0000	45.0000	15.7116
7	CHLORIDE MAGNESIUM	M	0.2000	0.0500	0.3000	0.0875
7	SULFATE	M	0.2000	0.0050	1.6000	0.5574
6	SPERMINE	M	0.0060	0.0005	0.0130	0.0043
6	MAGNESIUM	M	0.1000	0.0050	0.1000	0.0367

	ACETATE					
6	POLYETHYLENE GLYCOL MONOMETHYL ETHER 5000	W/V	12.0000	10.0000	30.0000	7.1134
6	POLYETHYLENE GLYCOL 20000	W/V	10.0000	10.0000	15.0000	1.9003
6	POLYETHYLENE GLYCOL 1500	W/V	25.0000	20.0000	25.0000	2.6300
4	CHES SODIUM PHOSPHATE	M	0.1000	0.1000	0.1200	0.0112
4	CALCIUM ACETATE TRI-AMMONIUM CITRATE	M	0.1700	0.1700	0.3250	0.0652
4	POTASSIUM THIOCYANATE MANGANESE (II) CHLORIDE	M	0.2000	0.1000	0.2000	0.0428
3	GALACTOSE SUCCINATE- PHOSPHATE- GLYCINE	M	0.0010	0.0001	0.0010	0.0004
3	POTASSIUM PHOSPHATE- SODIUM PHOSPHATE	M	0.2500	0.2500	36.0320	18.8588
3	POLYETHYLENE GLYCOL 300	W/V	10.0000	0.1000	10.0000	5.2178
3	TCEP	M	1.2000	0.0600	1.2000	0.5282
3	SODIUM IODIDE	M	35.4375	35.4375	45.0000	3.9052
3	ETHANOL	W/V	0.0010	0.0010	0.1000	0.0447
3	DITHIOTHREITOL	M	0.1300	0.0300	0.1400	0.0497
3	POLYETHYLENE GLYCOL 10000	W/V	11.0502	7.8930	12.0000	1.7555
3	POLYETHYLENE GLYCOL 600	W/V	0.0050	0.0010	0.0050	0.0021
3	POLYETHYLENE GLYCOL MONOMETHYL ETHER 550	W/V	17.0000	17.0000	20.0000	1.2472
3	POLYETHYLENE GLYCOL 2000	W/V	28.0000	20.1600	41.0000	8.5944
3	SODIUM MES	M	20.0000	20.0000	49.2300	12.4148
3	SERINE POTASSIUM PHOSPHATE PHOSPHATE- CITRATE	M	42.0000	12.0000	42.0000	12.3918
3	GUANIDINE HYDROCHLORIDE	M	0.1000	0.1000	0.1000	0.0000
3	SODIUM FLUORIDE	M	0.1250	0.0200	0.1250	0.0442
2	POLYETHYLENE GLYCOL 3000 AMMONIUM CHLORIDE	M	1.3400	0.4000	1.3400	0.4954
2	MES-IMIDAZOLE SODIUM MALONATE	M	0.1000	0.1000	0.2400	0.0700
2	UREA N-OCTYL-B-D- GLUCOPYRANOSID E	M	0.0200	0.0100	0.0200	0.0050
2	TRIMETHYLAMINE N-OXIDE	W/V	0.5000	0.0050	0.5000	0.2475
2	SPERMIDINE	W/V	15.0200	3.0000	15.0200	6.0100
2		M	0.0020	0.0020	0.0100	0.0040

2	SODIUM THIOCYANATE	M	0.2000	0.1820	0.2000	0.0090
2	AMMONIUM PHOSPHATE	M	0.5000	0.2000	0.5000	0.1500
2	SODIUM SUCCINATE	M	1.0000	0.0500	1.0000	0.4750
2	POTASSIUM ACETATE	M	2.0000	0.4000	2.0000	0.8000

Supplementary Table S2. Buffer chemicals, and the associated pH information, which were found in the 321 crystallization conditions extracted from the crystallization communications published 2012.

Frequency	Buffer chemical	Average pH	Most common pH	Minimum pH	Maximum pH	Standard Deviation of pH
63	SODIUM HEPES	7.37	7.5	6	8.5	0.54
41	TRIS CHLORIDE	8.17	8.5	7	9	0.53
33	SODIUM CITRATE - CITRIC ACID	5.24	5	3.5	7.8	0.79
31	MES	6.16	6.5	5.5	7	0.47
26	SODIUM ACETATE	4.67	4.6	4	5.5	0.45
23	BIS-TRIS	5.94	5.5	5.5	7	0.52
20	SODIUM CACODYLATE	6.29	6.5	4.5	7	0.77
13	BIS-TRIS PROPANE	7.25	6.5	5.5	8.8	0.95
5	IMIDAZOLE	7.44	8	6.2	8	0.83
4	CHES	9.15	9.5	8.6	9.5	0.39
3	SUCCINATE-PHOSPHATE-GLYCINE	8.08	9.15	6	9.15	1.47
3	SODIUM MES	6.28	6.75	6	6.75	0.33
3	PHOSPHATE-CITRATE	4.20	4.2	4.2	4.2	0.00
3	POTASSIUM PHOSPHATE-SODIUM PHOSPHATE	6.50	7	5.5	7	0.79
1	SODIUM SUCCINATE	5.5	5.5	5.5	5.5	0.00
2	MES-IMIDAZOLE	6.50	6.5	6.5	6.5	0.00
1	POTASSIUM MES	5.90	5.9	5.9	5.9	0.00
1	SODIUM MALONATE	4.00	4	4	4	0.00
1	CAPS	10.00	10	10	10	0.00
1	BICINE	9.00	9	9	9	0.00
1	ADA	6.60	6.6	6.6	6.6	0.00
1	SODIUM TRICINE	8.40	8.4	8.4	8.4	0.00
1	MOPS	7.00	7	7	7	0.00
1	MALATE-MES-TRIS	4.00	4	4	4	0.00