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Supporting information for article:

A drug discovery-oriented non-invasive protocol for protein crystal cryoprotection by dehydration, with application for crystallization screening

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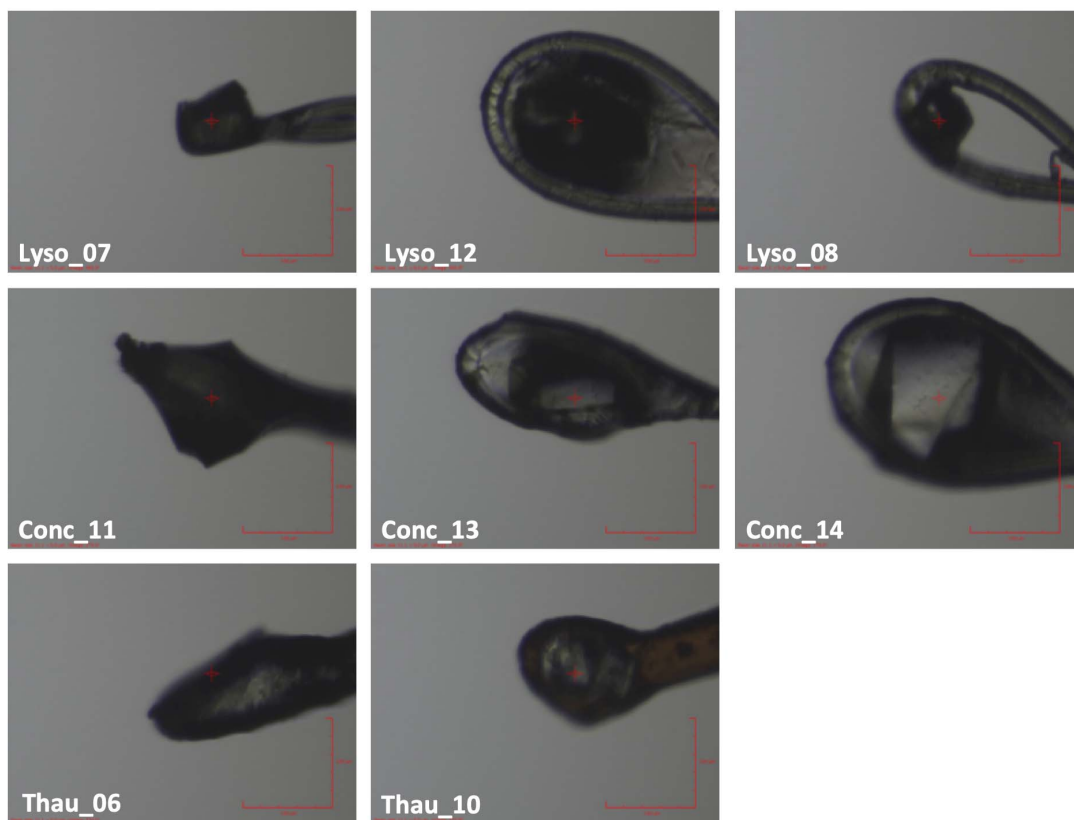


Figure S1. Examples of choices of loop size in comparison to the size of the crystals. Also the X-ray beam size is shown by the red circle with a cross-hair in the middle.

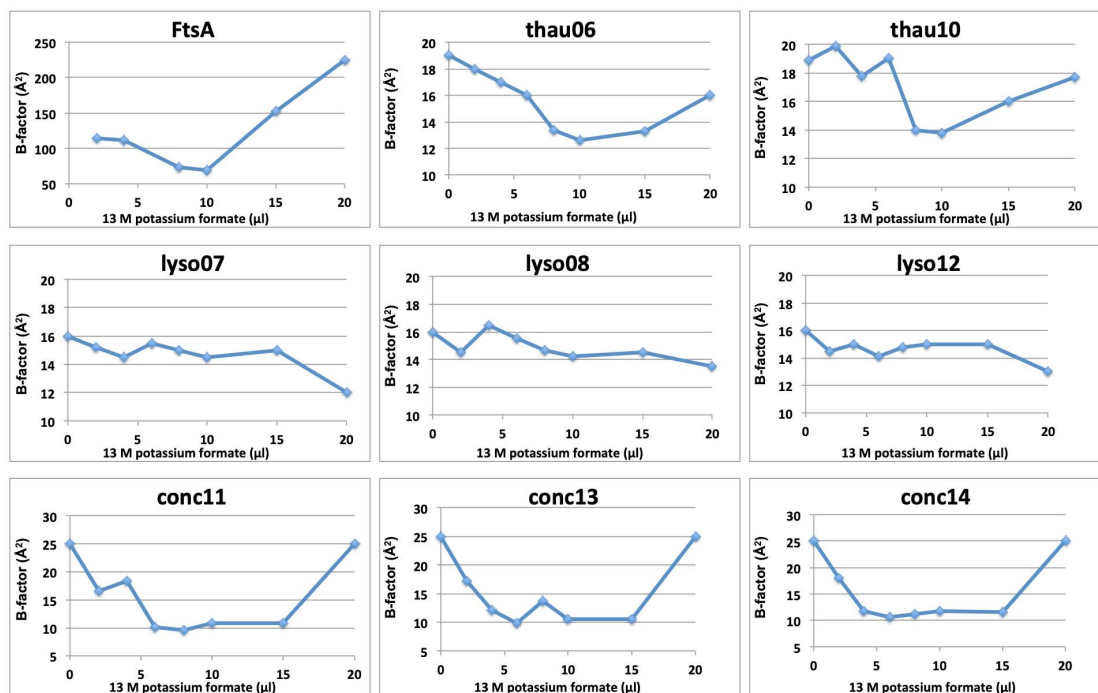


Fig. S2. Correlation between amounts of KF13 used for crystal drop dehydration and average Wilson B-factor.

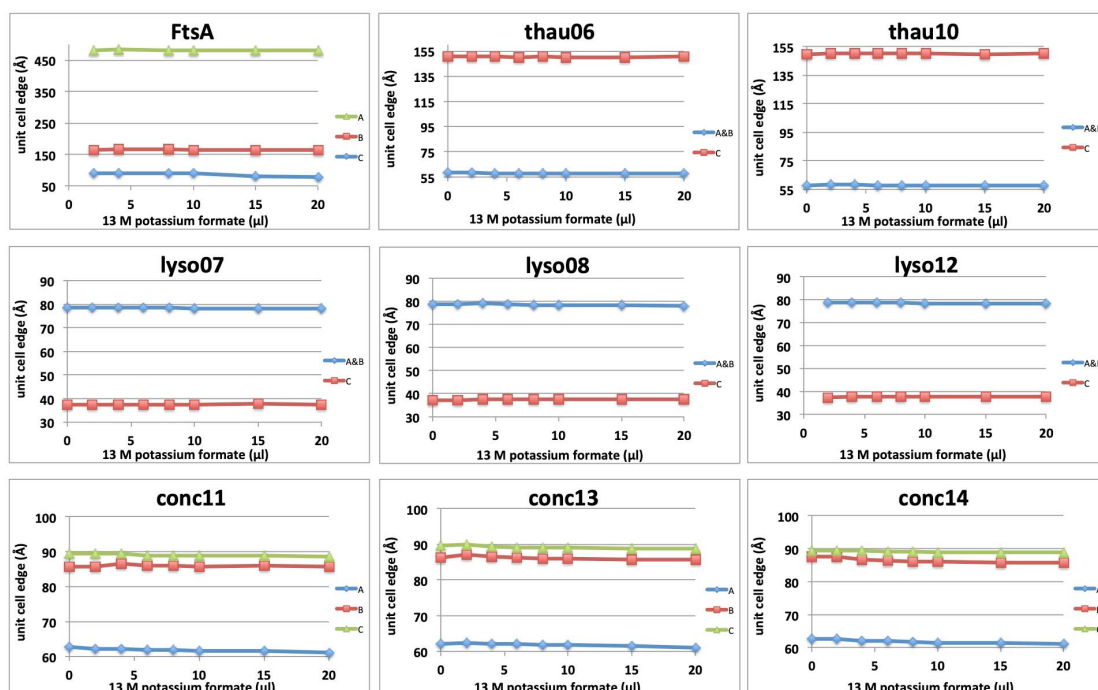


Fig. S3. Correlation between amounts of KF13 used for crystal drop dehydration and unit cell contraction of datasets collected for different crystal samples.

FtsA			
KF13 (ul)	a	b	c
2	90.7	164.1	481.70
4	89.7	165.2	482.75
8	88.9	165.2	481.30
10	88.5	164.5	481.60
15	79.3	164.3	480.70
20	77.9	164.3	480.95

Lyso07			Lyso08			Lyso12		
KF13 (ul)	a = b	c	KF13 (ul)	a = b	c	KF13 (ul)	a = b	c
0	78.8	37.38	0	78.77	37.17	0	unprocessable	unprocessable
2	78.74	37.46	2	78.64	37.32	2	78.69	37.35
4	78.45	37.44	4	79.13	37.69	4	78.56	37.55
6	78.51	37.51	6	78.67	37.60	6	78.56	37.57
8	78.54	37.54	8	78.51	37.54	8	78.54	37.61
10	78.25	37.55	10	78.31	37.58	10	78.29	37.55
15	78.33	37.77	15	78.29	37.62	15	78.29	37.54
20	78.16	37.40	20	78.11	37.40	20	78.24	37.52

Conc11				Conc13				Conc14			
KF13 (ul)	a	b	c	KF13 (ul)	a	b	c	KF13 (ul)	a	b	c
0	62.87	85.56	89.51	0	62.19	86.38	89.54	0	62.60	87.5	89.50
2	62.17	85.59	89.40	2	62.26	86.99	89.80	2	62.60	87.5	89.45
4	62.12	86.57	89.30	4	62.08	86.5	89.24	4	62.09	86.52	89.26
6	61.74	86.09	88.94	6	62.03	86.37	89.21	6	62.00	86.37	89.10
8	61.87	86.13	88.99	8	61.77	86.07	89.03	8	61.68	86.11	89.05
10	61.53	85.76	88.86	10	61.79	86.11	89.07	10	61.51	85.91	88.92
15	61.49	85.85	88.82	15	61.62	85.86	88.90	15	61.49	85.78	88.87
20	61.12	85.66	88.50	20	61.05	85.70	88.70	20	61.04	85.60	88.90

Fig. S4. Tables with values plotted in Fig. S2.

Table S1. Crystallisation conditions in the 96-well plates used to investigate promotion of crystal nucleation in already equilibrated crystals drops. Each table corresponds to a full 96-well plate, each letter corresponds to a row with 12 identical repeats and two drops with different protein concentrations were set up for each condition.

96-well plate rows	Lysozyme (mg/ml)	NaCl (M)	RH (%)
A	20	0.8	97
	10		
B	20	0.7	97.3
	10		
C	20	0.6	97.6
	10		
D	20	0.5	98
	10		
E	20	0.4	98.3
	10		
F	20	0.3	98.7
	10		
G	20	0.2	99.1
	10		
H	20	0.1	99.4
	10		

96-well plate rows	Thaumatococcus (mg/ml)	NaK tartrate (M)	RH (%)
A	12	0.7	95.5
	6		
B	12	0.6	96.2
	6		
C	12	0.5	96.8
	6		
D	12	0.4	97.4
	6		
E	12	0.3	98
	6		
F	12	0.2	98.5
	6		
G	12	0.1	99.1
	6		
H	12	0.05	99.4
	6		