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Supplementary Information

A protein crystallisation screening kit designed using polyethylene glycol as major precipitant

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Supplementary Table 1 Formulation of PEG-1

Well	Buffer	Precipitant
A1	0.1M sodium acetate trihydrate pH4.6	20% w/v PEG4000
A2	0.1M Sodium citrate tribasic dihydrate pH5.6	20% w/v PEG4000
A3	0.1M Bis-Tris pH6.5	20% w/v PEG4000
A4	0.1M HEPES pH7.5	20% w/v PEG4000
A5	0.1M sodium acetate trihydrate pH4.6	25% w/v PEG4000
A6	0.1M Sodium citrate tribasic dihydrate pH5.6	25% w/v PEG4000
A7	0.1M Bis-Tris pH6.5	25% w/v PEG4000
A8	0.1M HEPES pH7.5	25% w/v PEG4000
A9	0.1M sodium acetate trihydrate pH4.6	30% w/v PEG4000
A10	0.1M Sodium citrate tribasic dihydrate pH5.6	30% w/v PEG4000
A11	0.1M Bis-Tris pH6.5	30% w/v PEG4000
A12	0.1M HEPES pH7.5	30% w/v PEG4000
B1	0.1M sodium acetate trihydrate pH4.6	10% w/v PEG8000
B2	0.1M Sodium citrate tribasic dihydrate pH5.6	10% w/v PEG8000
B3	0.1M Bis-Tris pH6.5	10% w/v PEG8000
B4	0.1M HEPES pH7.5	10% w/v PEG8000
B5	0.1M sodium acetate trihydrate pH4.6	15% w/v PEG8000
B6	0.1M Sodium citrate tribasic dihydrate pH5.6	15% w/v PEG8000
B7	0.1M Bis-Tris pH6.5	15% w/v PEG8000
B8	0.1M HEPES pH7.5	15% w/v PEG8000
B9	0.1M sodium acetate trihydrate pH4.6	20% w/v PEG8000
B10	0.1M Sodium citrate tribasic dihydrate pH5.6	20% w/v PEG8000
B11	0.1M Bis-Tris pH6.5	20% w/v PEG8000
B12	0.1M HEPES pH7.5	20% w/v PEG8000
C1	0.1M sodium acetate trihydrate pH4.6	10% w/v PEG6000
C2	0.1M Sodium citrate tribasic dihydrate pH5.6	10% w/v PEG6000
C3	0.1M Bis-Tris pH6.5	10% w/v PEG6000
C4	0.1M HEPES pH7.5	10% w/v PEG6000
C5	0.1M sodium acetate trihydrate pH4.6	15% w/v PEG6000

C6	0.1M Sodium citrate tribasic dihydrate pH5.6	15% w/v PEG6000
C7	0.1M Bis-Tris pH6.5	15% w/v PEG6000
C8	0.1M HEPES pH7.5	15% w/v PEG6000
C9	0.1M sodium acetate trihydrate pH4.6	20% w/v PEG6000
C10	0.1M Sodium citrate tribasic dihydrate pH5.6	20% w/v PEG6000
C11	0.1M Bis-Tris pH6.5	20% w/v PEG6000
C12	0.1M HEPES pH7.5	20% w/v PEG6000
D1	0.1M sodium acetate trihydrate pH4.6	20% w/v PEG3350
D2	0.1M Sodium citrate tribasic dihydrate pH5.6	20% w/v PEG3350
D3	0.1M Bis-Tris pH6.5	20% w/v PEG3350
D4	0.1M HEPES pH7.5	20% w/v PEG3350
D5	0.1M sodium acetate trihydrate pH4.6	25% w/v PEG3350
D6	0.1M Sodium citrate tribasic dihydrate pH5.6	25% w/v PEG3350
D7	0.1M Bis-Tris pH6.5	25% w/v PEG3350
D8	0.1M HEPES pH7.5	25% w/v PEG3350
D9	0.1M sodium acetate trihydrate pH4.6	30% w/v PEG3350
D10	0.1M Sodium citrate tribasic dihydrate pH5.6	30% w/v PEG3350
D11	0.1M Bis-Tris pH6.5	30% w/v PEG3350
D12	0.1M HEPES pH7.5	30% w/v PEG3350
E1	0.1M sodium acetate trihydrate pH4.6	15% v/v PEG400
E2	0.1M Sodium citrate tribasic dihydrate pH5.6	15% v/v PEG400
E3	0.1M Bis-Tris pH6.5	15% v/v PEG400
E4	0.1M HEPES pH7.5	15% v/v PEG400
E5	0.1M sodium acetate trihydrate pH4.6	20% v/v PEG400
E6	0.1M Sodium citrate tribasic dihydrate pH5.6	20% v/v PEG400
E7	0.1M Bis-Tris pH6.5	20% v/v PEG400
E8	0.1M HEPES pH7.5	20% v/v PEG400
E9	0.1M sodium acetate trihydrate pH4.6	25% v/v PEG400
E10	0.1M Sodium citrate tribasic dihydrate pH5.6	25% v/v PEG400
E11	0.1M Bis-Tris pH6.5	25% v/v PEG400
E12	0.1M HEPES pH7.5	25% v/v PEG400
F1	0.1M sodium acetate trihydrate pH4.6	15% w/v PEG1000
F2	0.1M Sodium citrate tribasic dihydrate pH5.6	15% w/v PEG1000
F3	0.1M Bis-Tris pH6.5	15% w/v PEG1000
F4	0.1M HEPES pH7.5	15% w/v PEG1000
F5	0.1M sodium acetate trihydrate pH4.6	20% w/v PEG1000
F6	0.1M Sodium citrate tribasic dihydrate pH5.6	20% w/v PEG1000
F7	0.1M Bis-Tris pH6.5	20% w/v PEG1000
F8	0.1M HEPES pH7.5	20% w/v PEG1000
F9	0.1M sodium acetate trihydrate pH4.6	25% w/v PEG1000
F10	0.1M Sodium citrate tribasic dihydrate pH5.6	25% w/v PEG1000
F11	0.1M Bis-Tris pH6.5	25% w/v PEG1000
F12	0.1M HEPES pH7.5	25% w/v PEG1000
G1	0.1M sodium acetate trihydrate pH4.6	10% w/v PEG2000

G2	0.1M Sodium citrate tribasic dihydrate pH5.6	10% w/v PEG2000
G3	0.1M Bis-Tris pH6.5	10% w/v PEG2000
G4	0.1M HEPES pH7.5	10% w/v PEG2000
G5	0.1M sodium acetate trihydrate pH4.6	15% w/v PEG2000
G6	0.1M Sodium citrate tribasic dihydrate pH5.6	15% w/v PEG2000
G7	0.1M Bis-Tris pH6.5	15% w/v PEG2000
G8	0.1M HEPES pH7.5	15% w/v PEG2000
G9	0.1M sodium acetate trihydrate pH4.6	20% w/v PEG2000
G10	0.1M Sodium citrate tribasic dihydrate pH5.6	20% w/v PEG2000
G11	0.1M Bis-Tris pH6.5	20% w/v PEG2000
G12	0.1M HEPES pH7.5	20% w/v PEG2000
H1	0.1M sodium acetate trihydrate pH4.6	15% w/v PEG1500
H2	0.1M Sodium citrate tribasic dihydrate pH5.6	15% w/v PEG1500
H3	0.1M Bis-Tris pH6.5	15% w/v PEG1500
H4	0.1M HEPES pH7.5	15% w/v PEG1500
H5	0.1M sodium acetate trihydrate pH4.6	20% w/v PEG1500
H6	0.1M Sodium citrate tribasic dihydrate pH5.6	20% w/v PEG1500
H7	0.1M Bis-Tris pH6.5	20% w/v PEG1500
H8	0.1M HEPES pH7.5	20% w/v PEG1500
H9	0.1M sodium acetate trihydrate pH4.6	25% w/v PEG1500
H10	0.1M Sodium citrate tribasic dihydrate pH5.6	25% w/v PEG1500
H11	0.1M Bis-Tris pH6.5	25% w/v PEG1500
H12	0.1M HEPES pH7.5	25% w/v PEG1500

Supplementary Table 2 Formulation of PEG-2

Well	Buffer	Precipitant	Additive
A1	0.1M sodium acetate trihydrate pH4.6	20% w/v PEG4000	0.1M Ammonium sulfate
A2	0.1M Sodium citrate tribasic dihydrate pH5.6	20% w/v PEG4000	0.1M Sodium formate
A3	0.1M Bis-Tris pH6.5	20% w/v PEG4000	0.1M Magnesium chloride hexahydrate
A4	0.1M HEPES pH7.5	20% w/v PEG4000	0.1M Sodium malonate
A5	0.1M sodium acetate trihydrate pH4.6	25% w/v PEG4000	10%v/v 2-Methyl-2,4-pentanediol
A6	0.1M Sodium citrate tribasic dihydrate pH5.6	25% w/v PEG4000	10%v/v Ethylene glycol
A7	0.1M Bis-Tris pH6.5	25% w/v PEG4000	10%v/v isopropanol
A8	0.1M HEPES pH7.5	25% w/v PEG4000	0.1M Sodium malonate
A9	0.1M sodium acetate trihydrate pH4.6	30% w/v PEG4000	0.1M glycine
A10	0.1M Sodium citrate tribasic dihydrate pH5.6	30% w/v PEG4000	0.1M Potassium sodium tartrate tetrahydrate
A11	0.1M Bis-Tris pH6.5	30% w/v PEG4000	0.01M EDTA-2Na
A12	0.1M HEPES pH7.5	30% w/v PEG4000	10%v/v Tacsimate PH 7.0
B1	0.1M sodium acetate trihydrate pH4.6	10% w/v PEG8000	0.1M Ammonium sulfate
B2	0.1M Sodium citrate tribasic dihydrate pH5.6	10% w/v PEG8000	0.1M Sodium formate
B3	0.1M Bis-Tris pH6.5	10% w/v PEG8000	0.1M Magnesium chloride hexahydrate
B4	0.1M HEPES pH7.5	10% w/v PEG8000	0.1M Sodium malonate
B5	0.1M sodium acetate trihydrate pH4.6	15% w/v PEG8000	10%v/v 2-Methyl-2,4-pentanediol
B6	0.1M Sodium citrate tribasic dihydrate pH5.6	15% w/v PEG8000	10%v/v Ethylene glycol
B7	0.1M Bis-Tris pH6.5	15% w/v PEG8000	10%v/v isopropanol
B8	0.1M HEPES pH7.5	15% w/v PEG8000	0.1M Sodium malonate
B9	0.1M sodium acetate trihydrate pH4.6	20% w/v PEG8000	0.1M glycine
B10	0.1M Sodium citrate tribasic dihydrate pH5.6	20% w/v PEG8000	0.1M Potassium sodium tartrate tetrahydrate
B11	0.1M Bis-Tris pH6.5	20% w/v PEG8000	0.01M EDTA-2Na
B12	0.1M HEPES pH7.5	20% w/v PEG8000	10%v/v Tacsimate PH 7.0
C1	0.1M sodium acetate trihydrate pH4.6	10% w/v PEG6000	0.1M Ammonium sulfate
C2	0.1M Sodium citrate tribasic dihydrate pH5.6	10% w/v PEG6000	0.1M Sodium formate
C3	0.1M Bis-Tris pH6.5	10% w/v PEG6000	0.1M Magnesium chloride hexahydrate
C4	0.1M HEPES pH7.5	10% w/v PEG6000	0.1M Sodium malonate

C5	0.1M sodium acetate trihydrate pH4.6	15% w/v PEG6000	10%v/v 2-Methyl-2,4-pentanediol
C6	0.1M Sodium citrate tribasic dihydrate pH5.6	15% w/v PEG6000	10%v/v Ethylene glycol
C7	0.1M Bis-Tris pH6.5	15% w/v PEG6000	10%v/v isopropanol
C8	0.1M HEPES pH7.5	15% w/v PEG6000	0.1M Sodium malonate
C9	0.1M sodium acetate trihydrate pH4.6	20% w/v PEG6000	0.1M glycine
C10	0.1M Sodium citrate tribasic dihydrate pH5.6	20% w/v PEG6000	0.1M Potassium sodium tartrate tetrahydrate
C11	0.1M Bis-Tris pH6.5	20% w/v PEG6000	0.01M EDTA-2Na
C12	0.1M HEPES pH7.5	20% w/v PEG6000	10%v/v Tacsimate PH 7.0
D1	0.1M sodium acetate trihydrate pH4.6	20% w/v PEG3350	0.1M Ammonium sulfate
D2	0.1M Sodium citrate tribasic dihydrate pH5.6	20% w/v PEG3350	0.1M Sodium formate
D3	0.1M Bis-Tris pH6.5	20% w/v PEG3350	0.1M Magnesium chloride hexahydrate
D4	0.1M HEPES pH7.5	20% w/v PEG3350	0.1M Sodium malonate
D5	0.1M sodium acetate trihydrate pH4.6	25% w/v PEG3350	10%v/v 2-Methyl-2,4-pentanediol
D6	0.1M Sodium citrate tribasic dihydrate pH5.6	25% w/v PEG3350	10%v/v Ethylene glycol
D7	0.1M Bis-Tris pH6.5	25% w/v PEG3350	10%v/v isopropanol
D8	0.1M HEPES pH7.5	25% w/v PEG3350	0.1M Sodium malonate
D9	0.1M sodium acetate trihydrate pH4.6	30% w/v PEG3350	0.1M glycine
D10	0.1M Sodium citrate tribasic dihydrate pH5.6	30% w/v PEG3350	0.1M Potassium sodium tartrate tetrahydrate
D11	0.1M Bis-Tris pH6.5	30% w/v PEG3350	0.01M EDTA-2Na
D12	0.1M HEPES pH7.5	30% w/v PEG3350	10%v/v Tacsimate PH 7.0
E1	0.1M sodium acetate trihydrate pH4.6	15% v/v PEG400	0.1M Ammonium sulfate
E2	0.1M Sodium citrate tribasic dihydrate pH5.6	15% v/v PEG400	0.1M Sodium formate
E3	0.1M Bis-Tris pH6.5	15% v/v PEG400	0.1M Magnesium chloride hexahydrate
E4	0.1M HEPES pH7.5	15% v/v PEG400	0.1M Sodium malonate
E5	0.1M sodium acetate trihydrate pH4.6	20% v/v PEG400	10%v/v 2-Methyl-2,4-pentanediol
E6	0.1M Sodium citrate tribasic dihydrate pH5.6	20% v/v PEG400	10%v/v Ethylene glycol
E7	0.1M Bis-Tris pH6.5	20% v/v PEG400	10%v/v isopropanol
E8	0.1M HEPES pH7.5	20% v/v PEG400	0.1M Sodium malonate
E9	0.1M sodium acetate trihydrate pH4.6	25% v/v PEG400	0.1M glycine
E10	0.1M Sodium citrate tribasic dihydrate	25% v/v PEG400	0.1M Potassium sodium

	pH5.6		tartrate tetrahydrate
E11	0.1M Bis-Tris pH6.5	25% v/v PEG400	0.01M EDTA-2Na
E12	0.1M HEPES pH7.5	25% v/v PEG400	10%v/v Tacsimate PH 7.0
F1	0.1M sodium acetate trihydrate pH4.6	15% w/v PEG1000	0.1M Ammonium sulfate
F2	0.1M Sodium citrate tribasic dihydrate pH5.6	15% w/v PEG1000	0.1M Sodium formate
F3	0.1M Bis-Tris pH6.5	15% w/v PEG1000	0.1M Magnesium chloride hexahydrate
F4	0.1M HEPES pH7.5	15% w/v PEG1000	0.1M Sodium malonate
F5	0.1M sodium acetate trihydrate pH4.6	20% w/v PEG1000	10%v/v 2-Methyl-2,4-pentanediol
F6	0.1M Sodium citrate tribasic dihydrate pH5.6	20% w/v PEG1000	10%v/v Ethylene glycol
F7	0.1M Bis-Tris pH6.5	20% w/v PEG1000	10%v/v isopropanol
F8	0.1M HEPES pH7.5	20% w/v PEG1000	0.1M Sodium malonate
F9	0.1M sodium acetate trihydrate pH4.6	25% w/v PEG1000	0.1M glycine
F10	0.1M Sodium citrate tribasic dihydrate pH5.6	25% w/v PEG1000	0.1M Potassium sodium tartrate tetrahydrate
F11	0.1M Bis-Tris pH6.5	25% w/v PEG1000	0.01M EDTA-2Na
F12	0.1M HEPES pH7.5	25% w/v PEG1000	10%v/v Tacsimate PH 7.0
G1	0.1M sodium acetate trihydrate pH4.6	10% w/v PEG2000	0.1M Ammonium sulfate
G2	0.1M Sodium citrate tribasic dihydrate pH5.6	10% w/v PEG2000	0.1M Sodium formate
G3	0.1M Bis-Tris pH6.5	10% w/v PEG2000	0.1M Magnesium chloride hexahydrate
G4	0.1M HEPES pH7.5	10% w/v PEG2000	10%v/v Tacsimate PH 7.0
G5	0.1M sodium acetate trihydrate pH4.6	15% w/v PEG2000	10%v/v 2-Methyl-2,4-pentanediol
G6	0.1M Sodium citrate tribasic dihydrate pH5.6	15% w/v PEG2000	10%v/v Ethylene glycol
G7	0.1M Bis-Tris pH6.5	15% w/v PEG2000	10%v/v isopropanol
G8	0.1M HEPES pH7.5	15% w/v PEG2000	10%v/v Tacsimate PH 7.0
G9	0.1M sodium acetate trihydrate pH4.6	20% w/v PEG2000	0.1M glycine
G10	0.1M Sodium citrate tribasic dihydrate pH5.6	20% w/v PEG2000	0.1M Potassium sodium tartrate tetrahydrate
G11	0.1M Bis-Tris pH6.5	20% w/v PEG2000	0.01M EDTA-2Na
G12	0.1M HEPES pH7.5	20% w/v PEG2000	10%v/v Tacsimate PH 7.0
H1	0.1M sodium acetate trihydrate pH4.6	15% w/v PEG1500	0.1M Ammonium sulfate
H2	0.1M Sodium citrate tribasic dihydrate pH5.6	15% w/v PEG1500	0.1M Sodium formate
H3	0.1M Bis-Tris pH6.5	15% w/v PEG1500	0.1M Magnesium chloride hexahydrate
H4	0.1M HEPES pH7.5	15% w/v PEG1500	10%v/v Tacsimate PH 7.0

H5	0.1M sodium acetate trihydrate pH4.6	20% w/v PEG1500	10%v/v 2-Methyl-2,4-pentanediol
H6	0.1M Sodium citrate tribasic dihydrate pH5.6	20% w/v PEG1500	10%v/v Ethylene glycol
H7	0.1M Bis-Tris pH6.5	20% w/v PEG1500	10%v/v isopropanol
H8	0.1M HEPES pH7.5	20% w/v PEG1500	10%v/v Tacsimate PH 7.0
H9	0.1M sodium acetate trihydrate pH4.6	25% w/v PEG1500	0.1M glycine
H10	0.1M Sodium citrate tribasic dihydrate pH5.6	25% w/v PEG1500	0.1M Potassium sodium tartrate tetrahydrate
H11	0.1M Bis-Tris pH6.5	25% w/v PEG1500	0.01M EDTA-2Na
H12	0.1M HEPES pH7.5	25% w/v PEG1500	10%v/v Tacsimate PH 7.0

Supplementary Table 3 Formulation of PEG-3

Well	Buffer	Precipitant	Additive
A1	0.1M citric acid pH3.5	35%v/v PEG 400	0.2M Ammonium sulfate
A2	0.1M Sodium citrate tribasic dehydrate pH4.5	40%v/v PEG 400	0.2M Ammonium sulfate
A3	0.1M BIS-TRIS pH5.5	35%v/v PEG 400	0.1M Ammonium sulfate
A4	0.1M PIPES pH6.5	40%v/v PEG 400	0.1M Ammonium sulfate
A5	0.1M Imidazole pH7.5	35%v/v PEG 400	0.1M Ammonium sulfate
A6	0.1M BICINE pH8.5	40%v/v PEG 400	0.2M Ammonium sulfate
A7	0.1M citric acid pH3.5	40%v/v PEG 550 MME	0.2M 1,6-Hexanediol
A8	0.1M Sodium citrate tribasic dehydrate pH4.5	30%v/v PEG 550 MME	0.1M Potassium thiocyanate
A9	0.1M BIS-TRIS pH5.5	30%v/v PEG 550 MME	0.05M Calcium chloride anhydrous
A10	0.1M BIS-TRIS pH6.5	30%v/v PEG 550 MME	0.05M Calcium chloride anhydrous
A11	0.1M PIPES pH6.5	30%v/v PEG 550 MME	0.2M Calcium chloride anhydrous
A12	0.1M Imidazole pH7.5	40%v/v PEG 550 MME	0.1M Calcium chloride anhydrous
B1	0.1M citric acid pH3.5	30%w/v PEG 1000	0.2M Lithium sulfate monohydrate
B2	0.1M Sodium citrate tribasic dehydrate pH4.5	35%w/v PEG 1000	0.1M Lithium sulfate monohydrate
B3	0.1M BIS-TRIS pH5.5	30%w/v PEG 1000	0.2M Lithium sulfate monohydrate
B4	0.1M PIPES pH6.5	35%w/v PEG 1000	0.1M Lithium sulfate monohydrate
B5	0.1M Imidazole pH7.5	30%w/v PEG 1000	0.2M Lithium sulfate monohydrate
B6	0.1M BICINE pH8.5	35% w/v PEG 1000	0.1M Lithium sulfate monohydrate
B7	0.1M citric acid pH3.5	30% w/v PEG 2000	0.4M Sodium chloride
B8	0.1M Sodium citrate tribasic dehydrate pH4.5	35% w/v PEG 2000	0.2M Sodium chloride
B9	0.1M BIS-TRIS pH5.5	30% w/v PEG 2000	0.4M Sodium chloride
B10	0.1M PIPES pH6.5	35% w/v PEG 2000	0.2M Sodium chloride
B11	0.1M Imidazole pH7.5	30% w/v PEG 2000	0.4M Sodium chloride
B12	0.1M BICINE pH8.5	35% w/v PEG 2000	0.2M Sodium chloride
C1		30% w/v PEG 2000 MME	0.1M Potassium thiocyanate
C2		30% w/v PEG 2000 MME	0.15M Potassium bromide
C3		30% w/v PEG 2000 MME	0.2M Potassium chloride
C4	0.1M citric acid pH3.5	35% w/v PEG 2000 MME	

C5	0.05M Disodium hydrogen Phosphate/ Sodium dihydrogen phosphate pH7.0	35% w/v PEG 2000 MME	
C6	0.1M BICINE pH8.5	35% w/v PEG 2000 MME	
C7	0.05M Disodium hydrogen Phosphate/ Sodium dihydrogen phosphate pH7.0	30% w/v PEG 3350	
C8	0.05M Disodium hydrogen Phosphate/ Sodium dihydrogen phosphate pH7.0	35% w/v PEG 3350	
C9	0.1M citric acid pH3.5	35% w/v PEG 3350	0.15M Lithium sulfate monohydrate
C10	0.1M Sodium citrate tribasic dehydrate pH4.5	30% w/v PEG 3350	0.2M 1,6-Hexanediol
C11	0.1M BIS-TRIS pH5.5	30% w/v PEG 3350	0.2M Potassium sodium tartrate
C12	0.1M PIPES pH6.5	30% w/v PEG 3350	0.15M Lithium sulfate monohydrate
D1	0.1M Imidazole pH7.5	30% w/v PEG 3350	0.1M Potassium phosphate dibasic
D2	0.1M BICINE pH8.5	30% w/v PEG 3350	0.1M Potassium phosphate dibasic
D3	0.1M Sodium citrate tribasic dehydrate pH4.5	25% w/v PEG 4000	0.2M Ammonium sulfate
D4	0.1M BIS-TRIS pH5.5	30% w/v PEG 4000	0.3M Potassium sodium tartrate
D5	0.1M MES pH6.5	28% w/v PEG 4000	0.02M Sodium hydrogen carbonate
D6	0.05M Disodium hydrogen Phosphate/ Sodium dihydrogen phosphate pH7.0	30% w/v PEG 4000	
D7	0.1M Imidazole pH7.5	25% w/v PEG 4000	0.1M Potassium phosphate dibasic
D8	0.1M BICINE pH8.5	25% w/v PEG 4000	0.1M Potassium phosphate dibasic
D9	0.1M citric acid pH3.5	20% w/v PEG 5000 MME	0.1M Potassium thiocyanate
D10	0.1M Sodium citrate tribasic dehydrate pH4.5	30% w/v PEG 5000 MME	0.15M Potassium bromide
D11	0.1M BIS-TRIS pH5.5	20% w/v PEG 5000 MME	0.2M Sodium formate
D12	0.1M PIPES pH6.5	30% w/v PEG 5000 MME	0.1M Potassium phosphate dibasic
E1	0.1M Imidazole pH7.5	20% w/v PEG 5000 MME	0.2M Lithium sulfate monohydrate
E2	0.1M BICINE pH8.5	30% w/v PEG 5000 MME	0.1M Potassium thiocyanate

E3	0.1M citric acid pH3.5	20% w/v PEG 6000	0.15M Lithium sulfate monohydrate
E4	0.1M citric acid pH3.5	25% w/v PEG 6000	0.2M Lithium sulfate monohydrate
E5	0.1M Sodium citrate tribasic dehydrate pH4.5	20% w/v PEG 6000	0.2M Lithium sulfate monohydrate
E6	0.1M PIPES pH6.5	25% w/v PEG 6000	0.2M Lithium sulfate monohydrate
E7	0.05M Disodium hydrogen Phosphate/ Sodium dihydrogen phosphate pH7.0	20% w/v PEG 6000	
E8	0.1M Imidazole pH7.5	30% w/v PEG 6000	0.1M Potassium thiocyanate
E9	0.1M citric acid pH3.5	20% w/v PEG 8000	0.1M Potassium thiocyanate
E10	0.1M Sodium citrate tribasic dehydrate pH4.5	30% w/v PEG 8000	0.2M Potassium bromide
E11	0.1M BIS-TRIS pH5.5	20% w/v PEG 8000	0.2M Sodium chloride
E12	0.1M PIPES pH6.5	30% w/v PEG 8000	0.2M Sodium formate
F1	0.1M Imidazole pH7.5	20% w/v PEG 8000	0.1M Calcium chloride anhydrous
F2	0.1M BICINE pH8.5	30% w/v PEG 8000	0.1M Potassium bromide
F3	0.1M citric acid pH3.5	8% w/v PEG 10000 +8% w/v PEG 1000	0.1M Potassium thiocyanate
F4	0.1M Sodium citrate tribasic dehydrate pH4.5	10% w/v PEG 10000 +10% w/v PEG1000	0.2M Potassium bromide
F5	0.1M BIS-TRIS pH5.5	12% w/v PEG 10000 +12% w/v PEG1000	0.2M Magnesium sulfate
F6	0.1M PIPES pH6.5	10% w/v PEG 10000 +10% w/v PEG1000	0.2M Sodium formate
F7	0.1M Imidazole pH7.5	10% w/v PEG 10000 +10% w/v PEG1000	0.1M Lithium sulfate monohydrate
F8	0.1M BICINE pH8.5	10% w/v PEG 10000 +10% w/v PEG1000	0.1M Potassium thiocyanate
F9	0.1M citric acid pH3.5	8% w/v PEG 20000 +8% v/v PEG 550 MME	0.1M Potassium thiocyanate
F10	0.1M Sodium citrate tribasic dehydrate pH4.5	12% w/v PEG 20000 +12% v/v PEG550 MME	0.1M Potassium bromide
F11	0.1M BIS-TRIS pH5.5	6% w/v PEG 20000 +6% v/vPEG550 MME	0.2M Sodium chloride
F12	0.1M PIPES pH6.5	8% w/v PEG 20000 +8% v/v PEG 550 MME	0.2M Sodium formate
G1	0.1M Imidazole pH7.5	6% w/v PEG 20000 +6% v/vPEG550 MME	0.1M Calcium chloride anhydrous
G2	0.1M BICINE pH8.5	8% w/v PEG 20000 +8% v/v PEG 550 MME	0.2M Potassium bromide

G3		2.0M Ammonium citrate tribasic pH 7.0	
G4		2.0M DL-Malic acid pH 7.0	
G5		2.0M Sodium malonate pH7.0	
G6		1.0M Succinic acid pH7.0	
G7		1.0M Sodium dihydrogen phosphate/ Potassium phosphate dibasic pH 7.0	
G8		35%v/v Jeffamine M-600 pH7.0	
G9		40%v/v Tacsimate pH 7.0	
G10	0.1M HEPES pH7.0	45% v/v Polypropylene glycol P 400	
G11	0.1M HEPES pH7.0	35%v/v Pentaerythritol propoxylate (5/4 PO/OH)	
G12	0.1M HEPES pH7.0	30%v/v Pentaerythritol ethoxylate (15/4 EO/OH)	
H1	0.1M Sodium citrate tribasic dehydrate pH4.5	2.0M Ammonium sulfate	
H2	0.1M Sodium citrate tribasic dehydrate pH4.5	2.0M Ammonium sulfate	0.2M 1,6-Hexanediol
H3	0.1M BIS-TRIS pH5.5	2.0M Ammonium sulfate	
H4	0.1M PIPES pH6.5	2.0M Ammonium sulfate	0.01M EDTA-2Na
H5	0.1M Imidazole pH7.5	3.0M Ammonium sulfate	
H6	0.1M TRIS pH8.5	3.0M Ammonium sulfate	0.01M EDTA-2Na
H7	0.1M BICINE pH9.0	3.0M Ammonium sulfate	0.5M Sodium chloride, 6%v/v Acetone
H8	0.1M Sodium citrate tribasic dehydrate pH4.5	45%v/v 2-Methyl-2,4-pentanediol	0.1M Potassium phosphate dibasic
H9	0.1M Sodium citrate tribasic dehydrate pH5.5	35%v/v 2-Methyl-2,4-pentanediol	0.1M Potassium thiocyanate
H10	0.1M BIS-TRIS pH5.5	45%v/v 2-Methyl-2,4-pentanediol	0.2M Calcium chloride anhydrous
H11	0.1M BIS-TRIS pH5.5	35%v/v 2-Methyl-2,4-pentanediol	0.2M Calcium chloride anhydrous
H12	0.1M Imidazole pH7.5	35%v/v 2-Methyl-2,4-pentanediol	0.1M Potassium bromide

Supplementary Table 4 The buffers systems used for formulating the PEG-3

Buffer system	pKa	Best pH range	pH in the kit
Sodium citrate/citrate	pka1=3.15 pka2=4.77 pka3=6.40	3.0-6.6	3.5, 4.5
Bis-Tris	6.45-6.65	5.45-7.65	5.5, 6.6
HEPES	8.0	6.8-8.2	7.0
Pipes	6.7-6.9	5.7-7.9	6.5
Bicine	8.3	7.3-9.3	8.5, 9.0
MES	6.1	5.1-7.1	6.2
Tris	8.1	7.1-9.1	9.0
Imidazole	7.1	6.1-8.1	7.5
Sodium hydrogen phosphate/ Sodium dihydrogen phosphate dihydrate	—	5.8-8.0	7.0
HEPES Na	7.45-7.65	6.45-8.65	7.0

Note: HEPES Na buffer solution is used to dissolve the protein sample.

Supplementary Table 5 PEGs used in the experiments

No.	Name	Degree of purity	Supplier
1	PEG 400	CP	Xi'an Huabo Chemical Plants
2	PEG 550 MME	GR	Sigma-Aldrich
3	PEG 1000	AR	Tianjin Kermel Chemical Reagent Development Center
4	PEG1500	AR	Beijing SeaskyBio Technology Co. Ltd.
5	PEG 2000	CP	Sinopharm Chemical Reagent Beijing Co.,Ltd
6	PEG 2000 MME	GR	Fluka
7	PEG 3350	GR	Sigma-Aldrich
8	PEG 4000	LR	Tianjin Fuchen Chemical Reagents Factory
9	PEG 5000 MME	GR	Fluka
10	PEG 6000	AR	Tianjin Dongli District Tianda Chemical Reagent Factory
11	PEG 8000	AR	Xi'an Wallsen Biotechnology Co., Ltd.
12	PEG 10000	GR	Beijing Chemical Reagent Company
13	PEG 20000	GR	Sinopharm Chemical Reagent Co., Ltd

Note: GR: Guaranteed Reagent; AR: Analytical Reagent; CP: Chemically Pure (reagent); LR: Laboratory Reagent.

Supplementary Table 6 A list of chemical reagents used in the experiments

No.	Name	Purity	Supplier
1	Sodium acetate trihydrate	AR	Beijing Chemical Plant
2	Glacial acetic acid	AR	Beijing Chemical Plant
3	Sodium citrate tribasic	AR	Tianjin Dongli District Tianda Chemical Reagent Factory
4	Citric acid	AR	Tianjin Dongli District Tianda Chemical Reagent Factory
5	HEPES	AR	Shanghai Yuanye Bio-Technology Co., Ltd
6	Bis-Tris	GR	Shanghai yuanye Bio-Technology Co., Ltd
7	Pipes	GR	Sigma
8	Bicine	GR	Sigma
9	Imidazole	AR	Xi'an Wallsen Biotechnology Co., Ltd.
10	MES	GR	Sigma
11	Tris	GR	Sigma-Aldrich
12	HEPES-Na	AR	Shanghai Kayon Biological Technology Co.,Ltd
13	Sodium dihydrogen phosphate	AR	Tianjin Dongli District Tianda Chemical Reagent Factory
14	Disodium hydrogen phosphate	AR	Tianjin Deng Feng Chemical Reagent Plants
15	Ammonium sulfate	AR	Xi’an Chemical Reagent Plants
16	Sodium formate	AR	Tianjin Fuchen Chemical Reagents Factory
17	Magnesium chloride hexahydrate	AR	Sinopharm Chemical Reagent Co.,Ltd
18	Sodium malonate	GR	Sigma-Aldrich
19	2-Methyl-2,4-pentanediol	GR	Hampton Research
20	Ethylene glycol	AR	Sinopharm Chemical Reagent Co., Ltd
21	Isopropanol	AR	Tianjin Dongli District Tianda Chemical Reagent Factory
22	Glycine	AR	Xi’an Huabo Chemical Plants
23	Potassium sodium tartrate	AR	Shandong Penglai Chemical Reagent Plants
24	EDTA-2Na	AR	Hunan Institute of Geology
25	Tacsimate PH 7.0	GR	Hampton Research
26	Ammonium citrate tribasic	AR	Tianjin Dongli District Tianda Chemical Reagent

			Factory
27	DL-Malic acid	AR	Sinopharm Chemical Reagent Co., Ltd
28	1.2M Succinic acid pH 7.0	GR	Hampton Research
29	Jeffamine M-600	GR	Hampton Research
30	Potassium phosphate dibasic	AR	Tianjin Dongli District Tianda Chemical Reagent Factory
31	Polypropylene glycol P 400	GR	Hampton Research
32	Pentaerythritol propoxylate（5/4 PO/OH）	GR	Aldrich
33	Pentaerythritol ethoxylate（15/4 EO/OH）	GR	Hampton Research
34	Potassium bromide	AR	Tianjin Zhiyuan Chemical Reagen Co. Ltd
35	Calcium chloride anhydrous	AR	Guangdong Shantou Xilong Chemical Plants
36	Potassium thiocyanate	AR	Tianjin Dongli District Tianda Chemical Reagent Factory
37	Sodium chloride	AR	Tianjin Red Rock Chemical Reagent Plants
38	Acetone	AR	Xi’an Huabo Chemical Plants
39	1,6-Hexanediol	AR	Sinopharm Chemical Reagent Co.,Ltd
40	Lithium sulfate	CP	Shanghai Second Reagent Factory
41	Magnesium sulfate	AR	Tianjin Zhiyuan Chemical Reagen Co. Ltd
42	Sodium hydrogen carbonate	AR	Sinopharm Chemical Reagent Co.,Ltd
43	Potassium chloride	AR	Sinopharm Chemical Reagent Co.,Ltd
44	Glycerol	AR	Tianjin Fu Yu Fine Chemical Co., Ltd.
45	Sodium pyrophosphate	AR	Tianjin Dongli District Tianda Chemical Reagent Factory
46	Sodium triphosphate	AR	Tianjin Tianli Chemical Reagents Ltd.
47	L-glutamic acid	GR	Sigma
48	L-alanine	GR	Sigma
49	L-Arginine	GR	Sigma
50	L-Proline	AR	Shanghai Blue Season Science and Technology Development Co., Ltd.
51	Glutathione	GR	Sigma
52	4-Aminobenzoic acid	AR	Sinopharm Chemical Reagent Co., Ltd
53	Ammonium acetate	AR	Tianjin Dongli District Tianda Chemical Reagent

			Factory
54	Cadmium chloride	AR	Tianjin Bodi Chemical Co., Ltd.
55	Cobalt (II) chloride hexahydrate	AR	Tianjin Dongli District Tianda Chemical Reagent Factory
56	Suberic acid	AR	Sinopharm Chemical Reagent Co., Ltd
57	Maleic acid	AR	Tianjin Fuchen Chemical Reagents Factory
58	Glutaric acid	CP	Sinopharm Chemical Reagent Co., Ltd
59	Anchoic acid	CP	Sinopharm Chemical Reagent Co., Ltd
60	Sulfanilic acid	AR	Tianjin Kermel Chemical Reagent Co. Ltd
61	Sebacic acid	CP	Sinopharm Chemical Reagent Co., Ltd
62	Sucrose	AR	Xi'an Huabo Chemical Plants
63	Acetonitrile	AR	Xi'an Huabo Chemical Plants

Note 1: Tacsimate: a mixture of 7 titrated organic acid salts (malonic acid, ammonium citrate tribasic, succinic acid, DL-Malic acid, sodium acetate trihydrate, sodium formate, and ammonium tartrate dibasic), which was developed by Hampton Research Co.

Note 2: HEPES Na buffer solution is used to dissolve the protein sample.