

Induction of crystal nucleation by orientation-controlled binding of His₆-tagged proteins to functionalized gold nanoparticles

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Primer name	Primer sequence (5'→3')
<i>A. acidocaldarius</i> acetyl-CoA carboxylase ligase forward	TACTTCCAATCCAATGCAATGGCCCAGGATGACACCC
<i>A. acidocaldarius</i> acetyl-CoA carboxylase ligase reverse	TTATCCACTTCCAATGTTATTAGACCTGCTCGCGCTCGGA
<i>A. prevotii</i> nitric oxide reductase forward	TACTTCCAATCCAATGCAATGATTAATACTTACAAGAAGAA A
<i>A. prevotii</i> nitric oxide reductase reverse	TTATCCACTTCCAATGTTATTATTCATCAAATACACTTTCTCCT A

Table S1. Primers for cloning

Well	Solutions (salt + buffer + precipitant)
A1	0.2 M Potassium Sodium Tartrate 20 % (w/v) PEG 3350
A2	0.15 M Potassium Bromide 30 % (w/v) PEG 2000 MME
A3	0.2 M Sodium Chloride 0.1 M Na ₂ HPO ₄ : Citric Acid, pH 4.2 20 % (w/v) PEG 8000
A4	0.1 M Sodium Acetate: Acetic Acid, pH 4.5 0.8 / 1.2 M NaH ₂ PO ₄ /K ₂ HPO ₄
A5	0.2 M Lithium Sulfate 0.1 M CAPS: NaOH, pH 10.5 1.2 / 0.8 M NaH ₂ PO ₄ /K ₂ HPO ₄
A6	0.1 M Sodium Cacodylate: HCl, pH 6.5 1.26 M Ammonium Sulfate
A7	0.2 M Sodium Chloride 0.1 M Na ₂ HPO ₄ : Citric Acid, pH 4.2 10 % (w/v) PEG 3000
A8	0.2 M Potassium Formate, pH 7.3 20 % (w/v) PEG 3350
A9	0.1 M Sodium Citrate: HCl, pH 5 20 % (w/v) PEG 6000
A10	0.2 M Ammonium Nitrate, pH 6.3 20 % (w/v) PEG 3350
A11	0.2 M Lithium Chloride 20 % (w/v) PEG 3350
A12	0.1 M Sodium Citrate: Citric Acid, pH 5.5 40 % (v/v) PEG 600
B1	0.1 M MES: NaOH, pH 6.5 12 % (w/v) PEG 20000
B2	0.2 M Potassium Acetate 20 % (w/v) PEG 3350
B3	0.2 M Ammonium Citrate Dibasic 20 % (w/v) PEG 3350
B4	1.8 M NaH ₂ PO ₄ /K ₂ HPO ₄ , pH 8.2
B5	0.2 M Ammonium Sulfate 0.1 M Sodium Cacodylate: HCl, pH 6.5 30 % (w/v) PEG 8000
B6	0.2 M Sodium Formate 20 % (w/v) PEG 3350
B7	0.1 M Bis-Tris Propane: HCl, pH 7 2.8 M Sodium Acetate, pH 7.0
B8	60 % (v/v) Microlytic Mix*, pH 7.0
B9	1 M Ammonium Sulfate 0.1 M Bis-Tris: HCl, pH 5.5 1 % (w/v) PEG 3350
B10	1.1 M Sodium Malonate, pH 7.0 0.1 M HEPES: NaOH, pH 7 0.5 % (w/v) Jeffamine ED-2001, pH 7.0
B11	0.2 M Lithium Sulfate 0.1 M Bis-Tris: HCl, pH 6.5 25 % (w/v) PEG 3350

B12 3 M Sodium Chloride 0.1 M Bis-Tris: HCl, pH 5.5

C1 0.8 M Succinic Acid, pH 7.0

C2 35 % (v/v) Microlytic Mix*, pH 7.0

C3 0.2 M Ammonium Acetate 0.1 M HEPES: NaOH, pH 7.5 25 % (w/v) PEG 3350

C4 0.2 M Ammonium Citrate Tribasic, pH 7.0 20 % (w/v) PEG 3350

C5 0.2 M Sodium Citrate 20 % (w/v) PEG 3350

C6 0.1 M Bicine: NaOH, pH 9 20 % (w/v) PEG 6000

C7 0.1 M Tris: HCl, pH 8.5 1.5 M Ammonium Phosphate Dibasic

C8 0.1 M Bis-Tris Propane: HCl, pH 7 1.8 M Magnesium Sulfate

C9 0.2 M Sodium Fluoride 20 % (w/v) PEG 3350

C10 0.2 M Sodium Nitrate 20 % (w/v) PEG 3350

C11 0.1 M Bis-Tris Propane: HCl, pH 7 1.3 M Ammonium Tartrate Dibasic

C12 0.1 M Tris: HCl, pH 8.5 1.4 M Ammonium Tartrate Dibasic

D1 0.1 M Tris: HCl, pH 8.5 1.5 M Ammonium Sulfate

D2 0.2 M Lithium Sulfate 0.1 M Tris: HCl, pH 8.5 1.26 M Ammonium Sulfate

D3 0.2 M Lithium Sulfate 0.1 M CAPS: NaOH, pH 10.5 1 M Ammonium Sulfate

D4 0.2 M Calcium Acetate Hydrate 0.1 M Sodium Acetate: Acetic Acid, pH 4.5 30 % (v/v) PEG
400

D5 0.1 M Tris: HCl, pH 8.5 3 M Sodium Chloride

D6 2.8 M Sodium Acetate: HCl, pH 7

D7 1.1 M Ammonium Tartrate Dibasic, pH 7.0

D8 0.2 M Potassium Nitrate, pH 6.9 20 % (w/v) PEG 3350

D9 1 M Lithium Chloride 0.1 M Sodium Citrate: HCl, pH 4 20 % (w/v) PEG 6000

D10 0.2 M Lithium Citrate Tribasic 20 % (w/v) PEG 3350

D11 0.1 M Tris: HCl, pH 8.5 1.5 M Lithium Sulfate

D12 0.2 M Ammonium Sulfate 20 % (w/v) PEG 3350

E1 0.1 M Bis-Tris Propane: HCl, pH 7 1.8 M Sodium Acetate, pH 7.0

E2 0.1 M Bis-Tris Propane: HCl, pH 7 3.2 M Sodium Chloride

E3 0.1 M Bis-Tris Propane: HCl, pH 7 1.5 M Lithium Sulfate

E4 1.6 M Ammonium Sulfate 0.1 M MES: NaOH, pH 6.5 10 % (v/v) Dioxane

E5 0.2 M Lithium Sulfate 0.1 M Sodium Acetate: Acetic Acid, pH 4.5 30 % (w/v) PEG 8000

E6 0.1 M Sodium Acetate: Acetic Acid, pH 4.5 1 M Ammonium Phosphate Dibasic

E7 0.2 M Lithium Sulfate 0.1 M Na₂HPO₄: Citric Acid, pH 4.2 20 % (w/v) PEG 1000

E8 0.1 M CHES: NaOH, pH 9.5 20 % (w/v) PEG 8000

E9 0.1 M CHES: NaOH, pH 9.5 1 M Sodium Citrate

E10 0.1 M Na₂HPO₄: Citric Acid, pH 4.2 1.6 / 0.4 M Na₂HPO₄/K₂HPO₄

E11 0.2 M Magnesium Chloride 0.1 M Sodium Cacodylate: HCl, pH 6.5 10 % (w/v) PEG 3000

E12 E12 0.2 M Lithium Sulfate 0.1 M Sodium Cacodylate: HCl, pH 6.5 30 % (v/v) PEG 400

F1 0.2 M Sodium Chloride 0.1 M Imidazole: HCl, pH 8 1 M Ammonium Phosphate Dibasic

F2 0.1 M Bis-Tris: HCl, pH 6.5 3 M Sodium Chloride

F3 0.1 M HEPES: NaOH, pH 7.5 3 M Sodium Chloride

F4 1 M Na₂HPO₄/K₂HPO₄, pH 6.9

F5 0.02 M Magnesium Chloride 0.1 M HEPES: NaOH, pH 7.5 22 % (w/v) Polyacrylic Acid 5100

F6 0.2 M Sodium Malonate, pH 7.0 20 % (w/v) PEG 3350

F7 0.15 M DL-Malic Acid, pH 7.0 20 % (w/v) PEG 3350

F8 0.2 M Ammonium Phosphate Monobasic 0.1 M Tris: HCl, pH 8.5 50 % (v/v) MPD

F9 0.1 M HEPES: NaOH, pH 7 10 % (w/v) PEG 6000

F10 24 % (w/v) PEG 1500, 20 % (v/v) Glycerol

F11 0.2 M Sodium Tartrate Dibasic 20 % (w/v) PEG 3350

F12 0.2 M Lithium Nitrate 20 % (w/v) PEG 3350

G1 0.2 M Sodium Phosphate Dibasic 20 % (w/v) PEG 3350

G2 0.1 M Tris: HCl, pH 8.5 2.4 M Ammonium Phosphate Dibasic

- G3 0.2 M Sodium Chloride 0.1 M Imidazole: HCl, pH 8 0.4 / 1.6 M NaH₂PO₄/K₂HPO₄
- G4 0.2 M Calcium Acetate Hydrate 0.1 M MES: NaOH, pH 6 10 % (w/v) Isopropanol
- G5 0.2 M Sodium Chloride 0.1 M CHES: NaOH, pH 9.5 1.26 M Ammonium Sulfate
- G6 0.2 M Sodium Chloride 0.1 M Sodium Citrate: Citric Acid, pH 5.5 1 M Ammonium Phosphate
Dibasic
- G7 0.1 M Tris: HCl, pH 7 15 % (w/v) Ethanol
- G8 0.1 M Tris: HCl, pH 7 20 % (w/v) PEG 1000
- G9 0.2 M Sodium Chloride 0.1 M Na₂HPO₄/KH₂PO₄, pH 6.2 20 % (w/v) PEG 1000
- G10 0.2 M Sodium Chloride 0.1 M CAPS: NaOH, pH 10.5 20 % (w/v) PEG 8000
- G11 0.1 M HEPES: NaOH, pH 7 30 % (v/v) Jeffamine ED-2001, pH 7.0
- G12 0.2 M Calcium Chloride 0.1 M Bis-Tris: HCl, pH 5.5 45 % (v/v) MPD
- H1 0.2 M Calcium Chloride 0.1 M Bis-Tris: HCl, pH 6.5 45 % (v/v) MPD
- H2 0.2 M Potassium Chloride 0.05 M HEPES: NaOH, pH 7.5 35 % (v/v) Pentaerythritol
Propoxylate 5/4 PO/OH
- H3 0.2 M Trimethylamine N-Oxide 0.1 M Tris: HCl, pH 8.5 20 % (w/v) PEG 2000 MME
- H4 0.2 M Ammonium Acetate 0.1 M Tris: HCl, pH 8.5 25 % (w/v) PEG 3350
- H5 0.1 M Succinic Acid, pH 7.0 15 % (w/v) PEG 3350
- H6 0.1 M Sodium Citrate: HCl, pH 4 0.8 M Ammonium Sulfate
- H7 0.1 M Bicine: NaOH, pH 9 10 % (w/v) PEG 20000, 2 % (v/v) Dioxane
- H8 0.2 M Magnesium Chloride 0.1 M HEPES: NaOH, pH 7.5 30 % (v/v) PEG 400
- H9 0.1 M Sodium Acetate: HCl, pH 4.6 2.5 M Ammonium Sulfate
- H10 0.2 M Sodium Chloride 20 % (w/v) PEG 3350
- H11 0.1 M Tris: HCl, pH 8.5 2.5 M Ammonium Sulfate
- H12 0.2 M Zinc Acetate 0.1 M Sodium Acetate: Acetic Acid, pH 4.5 10 % (w/v) PEG 3000

*(1)Microlytic Mix is comprised of 1.8305 M Malonic Acid, 0.25 M Ammonium Citrate Tribasic, 0.12

M Succinic Acid, 0.3 M DL-Malic Acid, 0.4 M Sodium Acetate Trihydrate, 0.5 M Sodium Formate,

0.16 M Ammonium Tartrate Dibasic. Microlytic Mix at pH 7.0 is titrated with HCl. This mix is available from Anatrace, Product Nos. OPTIMIZE-131 and OPTIMIZE-132.¹

Table S2. Components of MCSG 2T crystal screening solution. MCSG 2T crystallization suite has 96 solutions. All 96 conditions have a different constituent of salt, buffer, and precipitant.

Supplementary References

1. A. McPherson and B. Cudney, *Journal of structural biology*, 2006, **156**, 387-406.