Supporting information for article:

Lessons from ten years of crystallization experiments at the SGC

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Table S1  Crystallization conditions of our modified version of JCSG+.

| Row | Col | Condition |
|-----|-----|-----------|
| A   | 1   | 50% PEG400 -- 0.2M lithium sulfate -- 0.1M acetate pH 4.5 |
| A   | 2   | 20% PEG3000 -- 0.1M citrate pH 5.5 |
| A   | 3   | 20% PEG3350 -- 0.2M ammonium citrate dibasic |
| A   | 4   | 30% MPD -- 0.02M calcium chloride -- 0.1M acetate pH 4.5 |
| A   | 5   | 20% PEG3350 -- 0.2M magnesium formate |
| A   | 6   | 20% PEG1000 -- 0.2M lithium sulfate -- 0.1M citrate pH 4.2 |
| A   | 7   | 20% PEG8000 -- 0.1M CAPSO pH 9.5 |
| A   | 8   | 20% PEG3350 -- 0.2M ammonium formate |
| A   | 9   | 20% PEG3350 -- 0.2M ammonium chloride |
| A   | 10  | 20% PEG3350 -- 0.2M potassium formate |
| A   | 11  | 50% MPD -- 0.2M ammonium phosphate dibasic -- 0.1M tris pH 8.5 |
| A   | 12  | 20% PEG3350 -- 0.2M potassium nitrate |
| B   | 1   | 0.8M ammonium sulfate -- 0.1M citrate pH 4.2 |
| B   | 2   | 20% PEG3350 -- 0.2M potassium thiocyanate |
| B   | 3   | 20% PEG6000 -- 0.1M bicine pH 9.0 |
| B   | 4   | 10% PEG8000 -- 8% ethylene glycol -- 0.1M HEPES pH 7.5 |
| B   | 5   | 40% MPD -- 5% PEG8000 -- 0.1M cacodylate pH 6.5 |
| B   | 6   | 5% PEG1000 -- 40% ethanol -- 0.1M citrate pH 4.2 |
| B   | 7   | 8% PEG4000 -- 0.1M acetate pH 4.5 |
| B   | 8   | 10% PEG8000 -- 0.2M magnesium chloride -- 0.1M HEPES pH 7.0 |
| B   | 9   | 20% PEG6000 -- 0.1M citrate pH 5.0 |
| B   | 10  | 50% PEG200 -- 0.2M magnesium chloride -- 0.1M cacodylate pH 6.5 |
| B   | 11  | 1.6M sodium citrate tribasic |
| B   | 12  | 20% PEG3350 -- 0.2M potassium citrate tribasic |
| C   | 1   | 20% PEG8000 -- 0.2M sodium chloride -- 0.1M citrate pH 4.2 |
| C   | 2   | 20% PEG6000 -- 0.8M lithium chloride -- 0.1M citrate pH 4.2 |
| C   | 3   | 20% PEG3350 -- 0.2M ammonium nitrate |
|   |   |   |
|---|---|---|
| C | 4 | 10% PEG6000 -- 0.1M HEPES pH 7.0 |
| C | 5 | 0.8M sodium phosphate monobasic -- 0.8M potassium phosphate dibasic -- 0.1M HEPES pH 7.5 |
| C | 6 | 40% PEG300 -- 0.1M citrate pH 4.2 |
| C | 7 | 10% PEG3000 -- 0.2M zinc acetate -- 0.1M acetate pH 4.5 |
| C | 8 | 20% ethanol -- 0.1M tris pH 8.5 |
| C | 9 | 25% 1,2-propanediol -- 10% glycerol -- 0.1M sodium/potassium phosphate pH 7.5 |
| C | 10 | 10% PEG20000 -- 2%(v/v) dioxane -- 0.1M bicine pH 9.0 |
| C | 11 | 2M ammonium sulfate -- 0.1M acetate pH 4.5 |
| C | 12 | 10% PEG1000 -- 10% PEG8000 |
| D | 1 | 25% PEG1000 -- 20% glycerol |
| D | 2 | 30% PEG400 -- 0.2M magnesium chloride -- 0.1M HEPES pH 7.5 |
| D | 3 | 50% PEG200 -- 0.2M sodium chloride -- 0.1M sodium/potassium phosphate pH 7.5 |
| D | 4 | 30% PEG8000 -- 0.2M lithium sulfate -- 0.1M acetate pH 4.5 |
| D | 5 | 60% MPD -- 0.1M HEPES pH 7.5 |
| D | 6 | 20% PEG8000 -- 0.2M magnesium chloride -- 0.1M tris pH 8.5 |
| D | 7 | 40% PEG400 -- 0.2M lithium sulfate -- 0.1M tris pH 8.5 |
| D | 8 | 40% MPD -- 0.1M tris pH 8.0 |
| D | 9 | 0.15M ammonium sulfate -- 25% PEG4000 -- 15% glycerol |
| D | 10 | 40% PEG300 -- 0.2M calcium acetate -- 0.1M cacodylate pH 6.5 |
| D | 11 | 30% glycerol -- 15% 2-propanol -- 0.15M calcium chloride -- 0.1M acetate pH 4.5 |
| D | 12 | 16% PEG8000 -- 0.04M potassium phosphate dibasic -- 20% glycerol |
| E | 1 | 1M sodium citrate tribasic -- 0.1M cacodylate pH 6.5 |
| E | 2 | 2M ammonium sulfate -- 0.2M sodium chloride -- 0.1M cacodylate pH 6.5 |
| E | 3 | 10% 2-propanol -- 0.2M sodium chloride -- 0.1M HEPES pH 7.5 |
| E | 4 | 1.26M ammonium sulfate -- 0.2M lithium sulfate -- 0.1M tris pH 8.5 |
| E | 5 | 40% MPD -- 0.1M CAPS pH 10.5 |
| E | 6 | 20% PEG3000 -- 0.2M zinc acetate -- 0.1M HEPES pH 7.5 |
| E | 7 | 10% 2-propanol -- 0.2M zinc acetate -- 0.1M cacodylate pH 6.5 |
|   |   |   |
|---|---|---|
| E  | 8 | 0.8M ammonium phosphate dibasic -- 0.1M acetate pH 4.5 |
| E  | 9 | 1.6M magnesium sulfate -- 0.1M MES pH 6.5 |
| E  | 10 | 10% PEG6000 -- 0.1M bicine pH 9.0 |
| E  | 11 | 16% PEG8000 -- 20% glycerol -- 0.16M calcium acetate -- 0.1M cacodylate pH 6.5 |
| E  | 12 | 10% PEG8000 -- 0.1M tris pH 8.0 |
| F  | 1 | 30% Jeffamine M-600 -- 0.05M cesium chloride -- 0.1M MES pH 6.5 |
| F  | 2 | 3M ammonium sulfate -- 0.1M citrate pH 5.0 |
| F  | 3 | 20% MPD -- 0.1M tris pH 8.0 |
| F  | 4 | 20% Jeffamine M-600 -- 0.1M HEPES pH 7.5 |
| F  | 5 | 50% ethylene glycol -- 0.2M magnesium chloride -- 0.1M tris pH 8.5 |
| F  | 6 | 10% MPD -- 0.1M bicine pH 9.0 |
| F  | 7 | 0.8M succinic acid |
| F  | 8 | 2.1M DL- malic acid |
| F  | 9 | 2.4M sodium malonate |
| F  | 10 | 1.2M sodium malonate -- 0.5% Jeffamine ED-2003 -- 0.1M HEPES pH 7.0 |
| F  | 11 | 1M succinic acid -- 1% PEG2000MME -- 0.1M HEPES pH 7.0 |
| F  | 12 | 30% Jeffamine M-600 -- 0.1M HEPES pH 7.0 |
| G  | 1 | 30% Jeffamine ED-2003 -- 0.1M HEPES pH 7.0 |
| G  | 2 | 22% polyacrylic acid 5100 -- 0.02M magnesium chloride -- 0.1M HEPES pH 7.5 |
| G  | 3 | 20% polyvinylpyrrolidone -- 0.01M cobalt chloride -- 0.1M tris pH 8.5 |
| G  | 4 | 20% PEG2000MME -- 0.2M trimethylamine N-oxide -- 0.1M tris pH 8.5 |
| G  | 5 | 12% PEG3350 -- 0.005M cobalt chloride -- 0.005M cadmium chloride -- 0.005M nickel chloride -- 0.005M magnesium chloride -- 0.1M HEPES pH 7.5 |
| G  | 6 | 20% PEG3350 -- 0.2M sodium malonate |
| G  | 7 | 20% PEG3350 -- 0.1M succinic acid |
| G  | 8 | 20% PEG3350 -- 0.15M DL- malic acid |
| G  | 9 | 30% PEG2000MME -- 0.1M potassium thiocyanate |
| G  | 10 | 30% PEG2000MME -- 0.15M potassium bromide |
| G  | 11 | 2M ammonium sulfate -- 0.1M bis-tris pH 5.5 |
|   |   |   |
|---|---|---|
| G | 12 | 3M sodium chloride -- 0.1M bis-tris pH 5.5 |
| H | 1  | 0.3M magnesium formate -- 0.1M bis-tris pH 5.5 |
| H | 2  | 1% PEG3350 -- 1M ammonium sulfate -- 0.1M bis-tris pH 5.5 |
| H | 3  | 25% PEG3350 -- 0.1M bis-tris pH 5.5 |
| H | 4  | 45% MPD -- 0.2M calcium chloride -- 0.1M bis-tris pH 5.5 |
| H | 5  | 45% MPD -- 0.2M ammonium acetate -- 0.1M bis-tris pH 5.5 |
| H | 6  | 0.1M ammonium acetate -- 0.1M bis-tris pH 5.5 -- 16%(w/v) PEG10000 |
| H | 7  | 25% PEG3350 -- 0.2M ammonium sulfate -- 0.1M bis-tris pH 5.5 |
| H | 8  | 25% PEG3350 -- 0.2M sodium chloride -- 0.1M bis-tris pH 5.5 |
| H | 9  | 25% PEG3350 -- 0.2M lithium sulfate -- 0.1M bis-tris pH 5.5 |
| H | 10 | 25% PEG3350 -- 0.2M ammonium acetate -- 0.1M bis-tris pH 5.5 |
| H | 11 | 25% PEG3350 -- 0.2M magnesium chloride -- 0.1M bis-tris pH 5.5 |
| H | 12 | 45% MPD -- 0.2M ammonium acetate -- 0.1M HEPES pH 7.5 |
Table S2  Crystallization conditions of the Ligand Friendly Screen (LFS)

| Row | Col | Condition                                      |
|-----|-----|-----------------------------------------------|
| A   | 1   | 30% PEG1000 -- 0.1M SPG pH 6.0                 |
| A   | 2   | 30% PEG1000 -- 0.1M SPG pH 7.0                 |
| A   | 3   | 30% PEG1000 -- 0.1M SPG pH 8.0                 |
| A   | 4   | 60% MPD -- 0.1M SPG pH 6.0                    |
| A   | 5   | 60% MPD -- 0.1M SPG pH 7.0                    |
| A   | 6   | 60% MPD -- 0.1M SPG pH 8.0                    |
| A   | 7   | 20% PEG6000 -- 10% ethylene glycol -- 0.2M sodium chloride |
| A   | 8   | 20% PEG6000 -- 10% ethylene glycol -- 0.2M ammonium chloride |
| A   | 9   | 20% PEG6000 -- 10% ethylene glycol -- 0.2M lithium chloride |
| A   | 10  | 20% PEG6000 -- 10% ethylene glycol -- 0.1M magnesium chloride |
| A   | 11  | 20% PEG6000 -- 10% ethylene glycol -- 0.1M calcium chloride |
| A   | 12  | 20% PEG6000 -- 10% ethylene glycol -- 0.01M zinc chloride |
| B   | 1   | 30% PEG1000 -- 0.1M MIB pH 6.0                 |
| B   | 2   | 30% PEG1000 -- 0.1M MIB pH 7.0                 |
| B   | 3   | 30% PEG1000 -- 0.1M MIB pH 8.0                 |
| B   | 4   | 60% MPD -- 0.1M MIB pH 6.0                    |
| B   | 5   | 60% MPD -- 0.1M MIB pH 7.0                    |
| B   | 6   | 60% MPD -- 0.1M MIB pH 8.0                    |
| B   | 7   | 20% PEG6000 -- 10% ethylene glycol -- 0.1M MES pH 6.0 -- 0.2M sodium chloride |
| B   | 8   | 20% PEG6000 -- 10% ethylene glycol -- 0.1M MES pH 6.0 -- 0.2M ammonium chloride |
| B   | 9   | 20% PEG6000 -- 10% ethylene glycol -- 0.1M MES pH 6.0 -- 0.2M lithium chloride |
| B   | 10  | 20% PEG6000 -- 10% ethylene glycol -- 0.1M MES pH 6.0 -- 0.1M magnesium chloride |
| B   | 11  | 20% PEG6000 -- 10% ethylene glycol -- 0.1M MES pH 6.0 -- 0.1M calcium chloride |
| B   | 12  | 20% PEG6000 -- 10% ethylene glycol -- 0.1M MES pH 6.0 -- 0.01M zinc chloride |
| C   | 1   | 30% PEG1000 -- 0.1M PCB pH 6.0                 |
| C   | 2   | 30% PEG1000 -- 0.1M PCB pH 7.0                 |
| C   | 3   | 30% PEG1000 -- 0.1M PCB pH 8.0                 |
C  4  60% MPD -- 0.1M PCB pH 6.0
C  5  60% MPD -- 0.1M PCB pH 7.0
C  6  60% MPD -- 0.1M PCB pH 8.0
C  7  20% PEG6000 -- 10% ethylene glycol -- 0.1M HEPES pH 7.0 -- 0.2M sodium chloride
C  8  20% PEG6000 -- 10% ethylene glycol -- 0.1M HEPES pH 7.0 -- 0.2M ammonium chloride
C  9  20% PEG6000 -- 10% ethylene glycol -- 0.1M HEPES pH 7.0 -- 0.2M lithium chloride
C 10  20% PEG6000 -- 10% ethylene glycol -- 0.1M HEPES pH 7.0 -- 0.1M magnesium chloride
C 11  20% PEG6000 -- 10% ethylene glycol -- 0.1M HEPES pH 7.0 -- 0.1M calcium chloride
C 12  20% PEG6000 -- 10% ethylene glycol -- 0.1M HEPES pH 7.0 -- 0.01M zinc chloride
D  1  30% PEG1000 -- 0.1M MMT pH 6.0
D  2  30% PEG1000 -- 0.1M MMT pH 7.0
D  3  30% PEG1000 -- 0.1M MMT pH 8.0
D  4  60% MPD -- 0.1M MMT pH 6.0
D  5  60% MPD -- 0.1M MMT pH 7.0
D  6  60% MPD -- 0.1M MMT pH 8.0
D  7  20% PEG6000 -- 10% ethylene glycol -- 0.1M tris pH 7.5 -- 0.2M sodium chloride
D  8  20% PEG6000 -- 10% ethylene glycol -- 0.1M tris pH 7.5 -- 0.2M ammonium chloride
D  9  20% PEG6000 -- 10% ethylene glycol -- 0.1M tris pH 7.5 -- 0.2M lithium chloride
D 10  20% PEG6000 -- 10% ethylene glycol -- 0.1M tris pH 7.5 -- 0.1M magnesium chloride
D 11  20% PEG6000 -- 10% ethylene glycol -- 0.1M tris pH 7.5 -- 0.1M calcium chloride
D 12  20% PEG6000 -- 10% ethylene glycol -- 0.1M tris pH 7.5 -- 0.01M zinc chloride
E  1  20% PEG3350 -- 10% ethylene glycol -- 0.2M sodium fluoride
E  2  20% PEG3350 -- 10% ethylene glycol -- 0.2M sodium bromide
E  3  20% PEG3350 -- 10% ethylene glycol -- 0.2M sodium iodide
E  4  20% PEG3350 -- 10% ethylene glycol -- 0.2M potassium thiocyanate
E  5  20% PEG3350 -- 10% ethylene glycol -- 0.2M sodium nitrate
E  6  20% PEG3350 -- 10% ethylene glycol -- 0.2M sodium formate
E  7  20% PEG3350 -- 10% ethylene glycol -- 0.2M sodium acetate
E  8  20% PEG3350 -- 10% ethylene glycol -- 0.2M sodium sulfate
E  9  20% PEG3350 -- 10% ethylene glycol -- 0.2M sodium/potassium tartrate
|   |   |   |
|---|---|---|
| E 10 | 20% PEG3350 -- 10% ethylene glycol -- 0.2M sodium/potassium phosphate |
| E 11 | 20% PEG3350 -- 10% ethylene glycol -- 0.2M potassium citrate tribasic |
| E 12 | 20% PEG3350 -- 10% ethylene glycol -- 0.2M sodium malonate |
| F  1 | 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 6.5 -- 0.2M sodium fluoride |
| F  2 | 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 6.5 -- 0.2M sodium bromide |
| F  3 | 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 6.5 -- 0.2M sodium iodide |
| F  4 | 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 6.5 -- 0.2M potassium thiocyanate |
| F  5 | 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 6.5 -- 0.2M sodium nitrate |
| F  6 | 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 6.5 -- 0.2M sodium formate |
| F  7 | 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 6.5 -- 0.2M sodium acetate |
| F  8 | 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 6.5 -- 0.2M sodium sulfate |
| F  9 | 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 6.5 -- 0.2M sodium/potassium tartrate |
| F 10 | 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 6.5 -- 0.02M sodium/potassium phosphate |
| F 11 | 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 6.5 -- 0.2M potassium citrate tribasic |
| F 12 | 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 6.5 -- 0.2M sodium malonate |
| G  1 | 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 7.5 -- 0.2M sodium fluoride |
| G  2 | 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 7.5 -- 0.2M sodium bromide |
| G  3 | 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 7.5 -- 0.2M sodium iodide |
| G  4 | 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 7.5 -- 0.2M potassium thiocyanate |
| G  5 | 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 7.5 -- 0.2M sodium nitrate |
| G  6 | 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 7.5 -- 0.2M sodium formate |
| G  7 | 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 7.5 -- 0.2M sodium acetate |
| G  8 | 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 7.5 -- 0.2M sodium sulfate |
| G  9 | 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 7.5 -- 0.2M sodium/potassium tartrate |
G 10 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 7.5 -- 0.02M sodium/potassium phosphate

G 11 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 7.5 -- 0.2M potassium citrate tribasic

G 12 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 7.5 -- 0.1M sodium malonate

H 1 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 8.5 -- 0.2M sodium fluoride

H 2 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 8.5 -- 0.2M sodium bromide

H 3 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 8.5 -- 0.2M sodium iodide

H 4 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 8.5 -- 0.2M potassium thiocyanate

H 5 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 8.5 -- 0.2M sodium nitrate

H 6 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 8.5 -- 0.2M sodium formate

H 7 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 8.5 -- 0.2M sodium acetate

H 8 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 8.5 -- 0.2M sodium sulfate

H 9 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 8.5 -- 0.2M sodium/potassium tartrate

H 10 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 8.5 -- 0.02M sodium/potassium phosphate

H 11 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 8.5 -- 0.2M potassium citrate tribasic

H 12 20% PEG3350 -- 10% ethylene glycol -- 0.1M bis-tris-propane pH 8.5 -- 0.2M sodium malonate