

Applications

Detergent Screen is a ready to use formulation of 96 mild detergent reagents for use in protein solubility and crystallization studies. Manipulate sample-sample and sample-solvent interactions, including non-specific aggregation due to hydrophobic interactions, to alter sample solubility, or obtain or improve crystalline samples.

Features

- Developed at Hampton Research
- For use with either membrane or soluble proteins
- Compatible with vapor diffusion, microbatch, and free interface diffusion methods
- 96 Deep Well block format
- Classification of Detergents in screen
 - Ionic detergents
 - Zwitterionic detergents
 - Non-ionic detergents
 - Non-detergent Sulfobetaines
- Ionic detergents contain a head group with a net charge and are either anionic (negative charge) or cationic (positive charge). Ionic detergents are useful for dissociating sample-sample interactions. The CMC of ionic detergents is reduced by increasing the ionic strength of the reagent and is unaffected by temperature changes.
- Non-ionic detergents contain an uncharged hydrophilic head group. Non-ionic detergents manipulate sample-sample, sample-reagent, and sample-solvent interactions and are widely used in protein crystallization. Non-ionic detergents are non-denaturing and allow the solubilized protein to retain native structure, enzymatic activity and function. The CMC of non-ionic detergents is not significantly altered by changes in ionic strength although the CMC increases with increasing temperature.
- Zwitterionic detergents contain combined properties of ionic and non-ionic detergents and are useful for disrupting and manipulating sample-sample interactions.
- Non-detergent Sulfobetaines (NDSB) are non-denaturing protein solubilizing reagents used successfully for both the solubilization and crystallization of proteins.¹ NDSB reagents are zwitterionic, possess good solubility in water, do not alter significantly the pH or viscosity of reagent, and can easily be removed by dialysis since they do not form micelles. NDSB reagents are efficient in preventing non-specific interactions between proteins. They will not however, disrupt strongly aggregated proteins.

Application

For crystallization to take place, a protein must be soluble in aqueous solution. Ideally the sample should be homogenous, monodisperse, and in a state of aggregation conducive to interactions which will promote the nucleation and subsequent growth of a crystal. Unfavorable aggregation

can compete with, obstruct, and prevent the normal ordering or the sample into a crystal. Many proteins, typically membrane proteins, membrane associated proteins, and soluble proteins contain hydrophobic residues on the surface which can lead to non-specific aggregation, a deterrent to solubility and crystallization. Mild, biological detergents can perturb and manipulate hydrophobic sample-sample and sample-solvent interactions. Incorporating detergents into the solubilization or crystallization reagent during screening and optimization is a popular and effective strategy for identifying conditions which promote and enhance solubility and crystallization.³ Besides improving the crystallization properties for some proteins and nucleic acids, detergents have also been shown to alleviate problems of twinning and secondary nucleation and can also produce different crystal forms.^{4,5}

Since it can be difficult to impossible a priori to predict and select which detergent or solubilizing agent will minimize the general nonspecific interactions yet at the same time sustain the specific interactions necessary for crystallization, the screening of a portfolio of detergent and solubilizing reagents is an efficient and effective strategy to identify the appropriate and best detergent reagent. The Detergent Screen is a set of solubilization and crystallization specific, mild, biological detergent reagents in a ready to use format at concentrations appropriate for solubility and crystallization screens. The Detergent Screen format allows one to identify a detergent effect as well as help select the best detergent reagent.

Sample Preparation

The protein sample should be homogenous, as pure as is practically possible (>95%), and free of amorphous material. Remove amorphous material by centrifugation or microfiltration prior to use. The recommended sample concentration is 5 to 25 mg/ml in dilute (25 mM or less) buffer. For initial screens, the sample should be free of unnecessary additives in order to observe the effect of the Detergent Screen reagents. However, agents that promote and preserve sample solubility, stability, and homogeneity can and should be included in the sample buffer. For additional sample preparation recommendations see Hampton Research Crystal Growth 101 – Sample Preparation for Crystallization.

Preparing the Deep Well Block for Use

Allow the Deep Well Block and reagents to stabilize at room temperature. If reagents precipitate during cold storage, warm the sealed block at up to 50°C for up to 60 minutes, inverting the block several times to solubilize the reagents.

Centrifuge the block at 500 rpm for 5 minutes to remove stray drops from the film before removing the sealing film. The film can be removed by grasping a corner of the film and gently peeling the film from the plate. Alternatively, the film can be left intact and pierced to access reagents.

For storage, reseal using AlumaSeal II Sealing Film.

Performing the Screen

Example 1 - Detergent reagent in drop only

Vapor Diffusion Crystallization: Detergent Reagents need only appear in the crystallization drop. Detergent Reagents DO NOT need to be dispensed into the reservoir for vapor diffusion. It is recommended the crystallization drop be built by adding Sample first, followed by Detergent Reagent and finally the Crystallization Reagent. This procedure allows the Detergent Reagent to interact with the sample prior to the addition of Crystallization Reagent to the drop.

Reservoir

Pipette the appropriate volume of Crystallization Reagent into the plate reservoir.

Drop

The recommended drop ratio is:

5 parts Sample : 1 part Detergent Reagent : 4 parts Crystallization Reagent

Example: 500 nl protein + 100 nl Detergent Reagent + 400 nl Crystallization Reagent. Seal the plate.

Example 2 - Detergent reagent in drop and reservoir

Vapor Diffusion Crystallization: Detergent Reagents need only appear in the crystallization drop. However, some prefer to mix the drop in two steps and this requires adding the Detergent Reagent to the Crystallization Reagent in the reservoir.

Reservoir

It is recommended the initial or final concentration of Detergent Reagent in the drop be 10 to 30% of the concentration supplied in the Detergent Screen. Pipette the appropriate volume of crystallization reagent into the plate reservoir, for example 90 μ l. Pipette 10 μ l of Detergent Reagent to the reservoir.

Drop

The recommended drop ratio for initial screens is:

1 part sample: 1 part Detergent Reagent / Crystallization Reagent, although other drop ratios might be worth evaluating during optimization.

Example 500 nl protein + 500 nl Detergent Reagent / Crystallization Reagent. Seal the plate.

Examine the Drop

After setting the screen, carefully examine the drops under 10 to 100 x magnifications. Examine drops each day for seven days and then for once each week thereafter. Record all observations and be particularly careful to scan the focal plane of the drop for the presence of small crystals.

There are many different ways to score observations, but one should primarily be concerned whether the drop is clear, contains a precipitate or phase separation, or crystals. Adding magnitude to observations can also prove useful, such as 1+ yellow/brown fine precipitate, 2+ phase separation, or 3+ small bipyramid crystals. One may also employ a numerical scoring scheme such as 0 = Clear, 1 = skin/precipitate, 2 = light precipitate, 3 = granular precipitate, 4 = precipitate/phase separation, 5 = phase separation, 6 = quasicrystals, 7 = micro crystals, 8 = needle clusters, 9 = plates, 10 = single crystal(s).

Interpretation

Detergent Screen results with crystals or improved crystals should be pursued for further optimization. In the absence of crystals, or when performing solubility experiments, one should look at differences in solubility between the control drops and those drops with the Detergent Reagent – paying particular attention to results changing from precipitate to clear (increased solubility) and precipitate to crystalline. During optimization one should evaluate, in addition to the primary crystallization variables, the Detergent Reagent class and concentration; the variation of the type, the type and concentration of the primary Crystallization Reagent; the potential evaluation of amphipathic additives (such as 1,2,3-Heptanetriol) as well as salts and polyethylene glycols; pH and buffer type; temperature; and other chemical and physical crystallization variables.

Group the results of the Detergent Screen reagents by the appearance of the drop compared to that of the original / control drop. One might group detergents by clear drops, drops with precipitate, drops with phase separation, and drops with crystals. Within each group, review the Detergent Reagent and look for similarities in class, structure, chain length, head group, or CMC. If one or more specific detergents or classes of detergents or a CMC can be identified as producing a desirable change in solubility or crystallization, one should pursue further optimization with this detergent or group of detergents. This may mean varying detergent concentration, drop ratio, Crystallization Reagent type and concentration, pH, buffer type, temperature, and other crystallization variables to determine the best use of the Detergent Reagent.

Formulation & Storage

The Detergent Screen reagent formulations are designed to be compatible with most crystallization reagents and yet allow one to screen the detergent at an appropriate concentration for solubility and crystallization studies.

Each solution is formulated in sterile filtered, deionized Type 1+ ultrapure water: 18.2 megaohm-cm resistivity at 25°C, < 5 ppb Total Organic Carbon, bacteria free (<1 Bacteria (CFU/ml)), pyrogen free (<0.03 Endotoxin (EU/ml)), RNase-free (< 0.01 ng/mL) and DNase-free (< 4 pg/ μ L) and filled (0.250 milliliter per reagent) into sterile, thermal sealed polypropylene blocks.

The kit should be stored at -20°C. Best if used within 12 months of receipt. The block and reagents must be allowed to equilibrate to room temperature and mixed prior to removal of the sealing film and use of the reagents.

Individual Detergent Screen reagents are available through the Hampton Research Custom Shop in 0.5 ml volumes at the same concentration supplied in the kit.

References and Further Reading

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7. The effects of neutral detergents on the crystallization of soluble proteins. A. McPherson et al. 1986, *J. Crystal Growth*, 76, 547-553.
8. Kuhlbrand, W., *Quarterly Rev. Biophys.*, 21, 429, 1988.
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11. Screening and optimization strategies for macromolecular crystal growth. R. Cudney, S. Patel, K. Weisgraber, Y. Newhouse and A. McPherson. 1994, *Acta Cryst. D50*, 414-423.

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Well #	[actual] Detergent	Synonyms	M _r	CMC	Type ¹
1. (A01)	1.0 mM 14:0 Lyso PG	1-myristoyl-2-hydroxy-sn-glycero-3-phospho-(1'-rac-glycerol) (sodium salt) / 1-tetradecanoyl-sn-glycero-3-phospho-(1'-rac-glycerol) (sodium salt)	478.49	0.036 mM	I
2. (A02)	6.0 mM 16:0 Lyso PG	1-palmitoyl-2-hydroxy-sn-glycero-3-phospho-(1'-rac-glycerol) (sodium salt) / 1-hexadecanoyl-sn-glycero-3-phospho-(1'-rac-glycerol) (sodium salt)	506.543	0.6 mM	I
3. (A03)	5.0 mM 18:0 Lyso PG	1-stearoyl-2-hydroxy-sn-glycero-3-phospho-(1'-rac-glycerol) (sodium salt) / 1-octadecanoyl-sn-glycero-3-phospho-(1'-rac-glycerol) (sodium salt)	534.596	N/A	I
4. (A04)	5.0 mM 18:1 Lyso PG	1-oleoyl-2-hydroxy-sn-glycero-3-phospho-(1'-rac-glycerol) (sodium salt) / 1-oleoy-sn-glycero-3-phospho-(1'-rac-glycerol) (sodium salt)	532.58	N/A	I
5. (A05)	10.0 mM CTAB	Hexadecyltrimethylammonium bromide / Cetrimonium bromide / Cetyltrimethylammonium bromide / Palmityltrimethylammonium bromide	364.45	1 mM	I
6. (A06)	1% w/v BAM	Benzyltrimethylammonium bromide / Benzyltrimethylammonium bromide	384.44	N/A	I
7. (A07)	1.0 mM Dodecyltrimethylammonium chloride		263.89	0.046 mM	I
8. (A08)	150.0 mM Sodium cholate hydrate	3 α ,7 α ,12 α -Trihydroxy-5 β -cholan-24-oic acid, sodium salt / Cholalic acid sodium salt	430.55	15 mM	I
9. (A09)	60.0 mM Deoxycholic acid sodium salt	3 α ,12 α -Dihydroxy-5 β -cholan-24-oic acid, monosodium salt / 3 α ,12 α -Dihydroxy-5 β -cholan-24-oic acid sodium salt / 7-Deoxycholic acid sodium salt / Sodium deoxycholate	414.55	6 mM	I
10. (A10)	5.0 mM MSDH	(S)-O-methyl-serine dodecylamide hydrochloride	322.91	N/A	I
11. (A11)	146.0 mM N-Lauroylsarcosine sodium salt	Sodium lauroyl sarcosine / Sarkosyl NL / N-Methyl-N-(1-oxododecyl)-glycine, sodium salt / N-Dodecanoyl-N-methylglycine sodium salt	293.38	14.6 mM	I
12. (A12)	100.0 mM Sodium dodecyl sulfate	SDS / Sulfuric acid monododecyl ester sodium salt / Dodecyl sulfate sodium salt / Lauryl sulfate sodium salt / Sodium lauryl sulfate	288.38	10 mM	I
13. (B01)	100.0 mM Lithium dodecyl sulfate	LDS / Dodecyl lithium sulfate / Dodecyl sulfate lithium salt / Lauryl sulfate lithium salt / Lithium lauryl sulfate	272.33	10 mM	I
14. (B02)	400.0 mM APO 8	Dimethyloctylphosphine oxide	190.27	40 mM	N
15. (B03)	5.0 mM APO 9	Dimethylnonylphosphine oxide	204.10	N/A	N
16. (B04)	47.0 mM APO 10	Dimethyldodecylphosphine oxide	218.30	4.66 mM	N
17. (B05)	5.0 mM APO 11	Dimethylundecylphosphine oxide	232.30	N/A	N
18. (B06)	5.7 mM APO 12	Dimethyldodecylphosphine oxide	246.40	0.568 mM	N
19. (B07)	80.0 mM Tetraethylene glycol mono-octyl ether	Octyl tetraethylene glycol ether / Octyltetraglycol / C ₈ E ₄	306.44	8 mM	N
20. (B08)	71.0 mM Pentaethylene glycol mono-octyl ether	C ₈ E ₅ / Octyl pentaethylene glycol ether / Octylpentaglycol	350.49	7.1 mM	N
21. (B09)	1.1 mM C ₁₂ E ₈	Polyoxyethylene(8)dodecyl ether / 3,6,9,12,15,18,21,24-octa-oxahexatriacontan-1-ol / Octaethyleneglycol Mono-n-dodecyl Ether	538.77	0.11 mM	N
22. (B10)	0.8 mM C ₁₂ E ₉	Nonaethylene glycol monododecyl ether / Dodecyl nonaethylene glycol ether / Dodecylnonaglycol / Polidocanol / Polyoxyethylene (9) lauryl ether	582.81	0.08 mM	N
23. (B11)	1% v/v Brij® 35	C ₁₂ E ₂₃ / α -Dodecyl- ω -hydroxy-poly(oxy-1,2-ethanediyl) / Polyethylene glycol (23) monododecyl ether / Polyoxyethylene [23] lauryl ether	1,198	0.091 mM	N
24. (B12)	1% v/v Brij® 56	Polyoxyethylene (10) cetyl ether	683	0.077 mM	N

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Well #	[actual] Detergent	Synonyms	M _r	CMC	Type ¹
25. (C01)	1% v/v Brij® 58	Polyethylene glycol (20) monohexadecyl ether / C16E20 / α -Dodecyl-w-hydroxy-poly(oxy-1,2-ethanediyl)	1,122	0.08 mM	N
26. (C02)	1% v/v Genapol® X-080	Iso-tridecyl alcohol polyglycol ether (8EO) / Oligoethylene glycol monoalkyl ether / Polyethylene glycol monoalkyl ether	552.78	0.15 mM	N
27. (C03)	1.8 mM Facade®-EM	3 α -hydroxy-7 α ,12 α -di-((O- β -D-maltosyl)-2-hydroxyethoxy)-cholane / 3 α -hydroxy-7 α ,12 α -di-((O- β -D-maltopyranosyl)ethoxy)-cholane	1,115.256	0.18 mM	N
28. (C04)	9.7 mM Facade®-EPC	3 α -hydroxy-7 α ,12 α -di-(((2-(trimethylamino)ethyl)phosphoryl)ethoxy)-cholane	796.948	0.97 mM	N
29. (C05)	1.9 mM Facade®-TEG	3 α ,7 α ,12 α -tri-((O- β -D-glucopyranosyl)ethoxy)-cholane	997.168	0.19 mM	N
30. (C06)	1.9 mM Facade®-TEM	3 α ,7 α ,12 α -tri-((O- β -D-maltopyranosyl)ethoxy)-cholane	1,483.59	0.19 mM	N
31. (C07)	0.13 mM Facade®-TFA1	Tandem Facial Amphiphile-1	2,148.416	0.013 mM	N
32. (C08)	790.0 mM MEGA-8	Octanoyl-N-methylglucamide	321.42	79 mM	N
33. (C09)	250.0 mM MEGA-9	Nonanoyl-N-methylglucamide	335.44	25 mM	N
34. (C10)	70.0 mM MEGA-10	Decanoyl-N-methylglucamide	349.47	7 mM	N
35. (C11)	3.7 mM Mal(11.1)	Dodecan-2-yloxy- β -D-maltoside / 2-dodecyl- β -D-maltopyranoside	510.615	0.37 mM	N
36. (C12)	1.1 mM Mal(11.2)	Tridecan-3-yloxy- β -D-maltoside / 3-tridecyl- β -D-maltopyranoside	524.642	0.11 mM	N
37. (D01)	105.0 mM N,N-Dimethyldecylamine-N-oxide	DDAO	201.35	10.48 mM	N
38. (D02)	18.0 mM n-Decyl- β -D-maltoside	n-Decyl- β -D-maltopyranoside / decyl 4-O- α -D-glucopyranosyl- β -D-glucopyranoside / DM	482.562	1.8 mM	N
39. (D03)	2.0 mM n-Dodecyl- β -D-maltoside	n-Dodecyl- β -D-maltopyranoside / Lauryl maltoside / Dodecyl 4-O- α -D-glucopyranosyl- β -D-glucopyranoside / DDM	510.615	0.2 mM	N
40. (D04)	1.0 mM n-Hexadecyl- β -D-maltoside	n-Hexadecyl- β -D-maltopyranoside / Cetyl β -D-maltoside / Hexadecyl- β -D-maltoside	566.72	0.0006 mM	N
41. (D05)	1.0 mM n-Tetradecyl- β -D-maltoside	n-Tetradecyl- β -D-maltopyranoside	538.67	0.01 mM	N
42. (D06)	1.0 mM Tridecyl- β -D-maltoside	n-Tridecyl- β -D-maltopyranoside	524.64	0.033 mM	N
43. (D07)	5.9 mM Undecyl- β -D-maltoside	Undecyl- β -D-maltopyranoside	496.59	0.59 mM	N
44. (D08)	195.0 mM Methyl-6-O-(N-heptylcarbamoyl)- α -D-glucopyranoside	6-O-(N-Heptylcarbamoyl)-methyl- α -D-glucopyranoside / HECAMEG	335.4	19.5 mM	N
45. (D09)	5.0 mM IPTG	Isopropyl-beta-D-thiogalactopyranoside	238.31	N/A	N
46. (D10)	25.0 mM n-Decanoylsucrose	α -D-Glucopyranoside / β -D-Fructofuranosyl Monodecanoate / Sucrose Monocaprato	496.55	2.5 mM	N
47. (D11)	65.0 mM n-Nonyl- β -D-glucoside	n-Nonyl- β -D-glucopyranoside	306.395	6.5 mM	N
48. (D12)	200.0 mM n-Octyl- β -D-glucoside	n-Octyl- β -D-glucopyranoside	292.37	20 mM	N

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New formulation

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Solutions for Crystal Growth

Well #	[actual] Detergent	Synonyms	M _r	CMC	Type ¹
49. (E01)	90.0 mM n-Octyl-β-D-thioglucofuranoside	n-Octyl-β-D-thioglucofuranoside / OSGP	308.44	9 mM	N
50. (E02)	10% w/v Pluronic® F-68	Polyoxyethylene-polyoxypropylene block copolymer	~8,350	0.04 mM	N
51. (E03)	10% w/v Pluronic® F-127	Polyoxyethylene-polyoxypropylene block copolymer	~12,600	3.97 mM	N
52. (E04)	3.0 mM Sucrose monolaurate	β-D-Fructofuranosyl-α-D-glucopyranoside monododecanoate / Lauroyl sucrose / Dodecanoyl sucrose / Sucrose monododecanoate / n-Monododecanoate-α-D-glucopyranoside / β-D-Fructofuranosylsucrose Monolaurate	524.61	0.3 mM	N
53. (E05)	0.9 mM Thesit®	Polyethylene glycol 400 dodecyl ether / Polyethylene glycol dodecyl ether / Hydroxypolyethoxydodecane / Lauromacrogol / Macrogol lauryl ether / Polidocanol	582.90	0.09 mM	N
54. (E06)	1% v/v Triton® X-100	4-(1,1,3,3-Tetramethylbutyl)phenyl-polyethylene glycol / t-Octylphenoxyethoxyethanol / Polyethylene glycol tert-octylphenyl ether	647	0.9 mM	N
55. (E07)	1% v/v Triton® X-114	t-Octylphenoxyethoxyethanol / (1,1,3,3-Tetramethylbutyl)phenyl-polyethylene glycol / Polyethylene glycol tert-octylphenyl ether	536	0.2 mM	N
56. (E08)	1% v/v Nonylphenyl polyethylene glycol		N/A	300 μM	N
57. (E09)	1% v/v Tween® 20	Polyoxyethylenesorbitan monolaurate	1,228	0.059 mM	N
58. (E10)	1% v/v Tween® 80	Polyoxyethylenesorbitan monooleate / Poly(oxy-1,2-ethanediyl) derivs., (Z)-sorbitan mono-9-octadecanoate	1,310	0.012 mM	N
59. (E11)	0.18 mM GDN	Glyco-diosgenin	1,165.315	18 μM	N
60. (E12)	80.0 mM CHAPS	3-[(3-Cholamidopropyl)-dimethylammonio]-1-propane sulfonate / N,N-Dimethyl-3-sulfo-N-[3-[[[3α,5β,7α,12α]-3,7,12-trihydroxy-24-oxocholan-24-yl] amino] propyl]-1-propanaminium hydroxide, inner salt	614.89	8 mM	Z
61. (F01)	80.0 mM CHAPSO	3-[(3-Cholamidopropyl)dimethylammonio]-2-hydroxy-1-propanesulfonate	630.89	8 mM	Z
62. (F02)	29.0 mM BIG CHAP	[N,N'-Bis(3-D-gluconamidopropyl)cholamide]	878.10	2.9 mM	Z
63. (F03)	14.0 mM Deoxy BIG CHAP	N,N-bis-(3-D-Gluconamidopropyl)deoxycholamide	862.10	1.4 mM	Z
64. (F04)	43.0 mM DDMAB	N-Dodecyl-N,N-(dimethylammonio)butyrate	299.50	4.3 mM	Z
65. (F05)	20.0 mM LDAO	Lauryldimethylamine-N-oxide / DDAO / N,N-Dimethyl-1-dodecanamine-N-oxide / n-Dodecyl-N,N-dimethylamine-N-oxide / n-Dodecyl-N,N-dimethyl-amine-N-oxide	229.402	2 mM	Z
66. (F06)	10% w/v Sulfobetaine 8	n-Octyl-N,N-dimethyl-3-ammonio-1-propanesulfonate	279.44	330 mM	Z
67. (F07)	400.0 mM Sulfobetaine 10	n-Decyl-N,N-dimethyl-3-ammonio-1-propanesulfonate / Zwittergent 3-10	307.50	40 mM	Z
68. (F08)	40.0 mM Sulfobetaine 12	n-Dodecyl-N,N-dimethyl-3-ammonio-1-propanesulfonate / Zwittergent 3-12	335.55	4 mM	Z
69. (F09)	4.0 mM Sulfobetaine 14	n-Tetradecyl-N,N-dimethyl-3-ammonio-1-propanesulfonate / Zwittergent 3-14	363.61	0.4 mM	Z
70. (F10)	0.6 mM Sulfobetaine 16	n-Hexadecyl-N,N-dimethyl-3-ammonio-1-propanesulfonate / Zwittergent 3-16	391.65	0.06 mM	Z
71. (F11)	150.0 mM 06:0 PC (DHPC)	1,2-dihexanoyl-sn-glycero-3-phosphocholine / 1,2-dicaproyl-sn-glycero-3-phosphocholine	453.507	15 mM	Z
72. (F12)	14.0 mM 07:0 PC (DHPC)	1,2-diheptanoyl-sn-glycero-3-phosphocholine	481.56	1.4 mM	Z

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Well #	[actual] Detergent	Synonyms	M _r	CMC	Type ¹
73. (G01)	5.0 mM 06:0 Lyso PC	1-hexanoyl-2-hydroxy-sn-glycero-3-phosphocholine / 1-hexanoyl-sn-glycero-3-phosphocholine	355.364	N/A	Z
74. (G02)	5.0 mM 07:0 Lyso PC	1-heptanoyl-2-hydroxy-sn-glycero-3-phosphocholine / 1-heptanoyl-sn-glycero-3-phosphocholine	369.391	N/A	Z
75. (G03)	60.0 mM 08:0 Lyso PC	1-octanoyl-2-hydroxy-sn-glycero-3-phosphocholine / 1-octanoyl-sn-glycero-3-phosphocholine	383.417	60 mM	Z
76. (G04)	5.0 mM 09:0 Lyso PC	1-nonanoyl-2-hydroxy-sn-glycero-3-phosphocholine / 1-nonanoyl-sn-glycero-3-phosphocholine	397.444	N/A	Z
77. (G05)	80.0 mM 10:0 Lyso PC	1-decanoyl-2-hydroxy-sn-glycero-3-phosphocholine / 1-decanoyl-sn-glycero-3-phosphocholine	411.471	8 mM	Z
78. (G06)	5.0 mM 11:0 Lyso PC	1-undecanoyl-2-hydroxy-sn-glycero-3-phosphocholine / 1-undecanoyl-sn-glycero-3-phosphocholine	425.497	N/A	Z
79. (G07)	9.0 mM 12:0 Lyso PC	1-lauroyl-2-hydroxy-sn-glycero-3-phosphocholine / 1-dodecanoyl-sn-glycero-3-phosphocholine	439.524	0.9 mM	Z
80. (G08)	5.0 mM 13:0 Lyso PC	1-tridecanoyl-2-hydroxy-sn-glycero-3-phosphocholine / 1-tridecanoyl-sn-glycero-3-phosphocholine	453.55	N/A	Z
81. (G09)	1.0 mM 14:0 Lyso PC	1-myristoyl-2-hydroxy-sn-glycero-3-phosphocholine / 1-tetradecanoyl-sn-glycero-3-phosphocholine	467.577	0.09 mM	Z
82. (G10)	5.0 mM 15:0 Lyso PC	1-pentadecanoyl-2-hydroxy-sn-glycero-3-phosphocholine / 1-pentadecanoyl-sn-glycero-3-phosphocholine	481.603	N/A	Z
83. (G11)	1.0 mM 16:0 Lyso PC	1-palmitoyl-2-hydroxy-sn-glycero-3-phosphocholine / 1-hexadecanoyl-sn-glycero-3-phosphocholine	495.63	8.3 μM	Z
84. (G12)	1.0 mM 17:0 Lyso PC	1-heptadecanoyl-2-hydroxy-sn-glycero-3-phosphocholine / 1-heptadecanoyl-sn-glycero-3-phosphocholine	509.657	N/A	Z
85. (H01)	1.0 mM 18:0 Lyso PC	1-stearoyl-2-hydroxy-sn-glycero-3-phosphocholine / 1-octadecanoyl-sn-glycero-3-phosphocholine	523.683	0.4 μM	Z
86. (H02)	1.0 mM 18:1 Lyso PC	1-oleoyl-2-hydroxy-sn-glycero-3-phosphocholine / 1-(9Z-octadecenoyl)-sn-glycero-3-phosphocholine	521.667	0.002 mM	Z
87. (H03)	110.0 mM MAPCHO-10	n-decylphosphocholine / FOS-Choline-10	323.409	11 mM	Z
88. (H04)	11.0 mM MAPCHO-12	n-dodecylphosphocholine / FOS-Choline-12	351.462	1.1 mM	Z
89. (H05)	1.2 mM MAPCHO-14	n-tetradecylphosphocholine / FOS-Choline-14	379.515	0.12 mM	Z
90. (H06)	1.0 mM MAPCHO-16	n-hexadecylphosphocholine / FOS-choline 16	407.568	0.013 mM	Z
91. (H07)	500.0 mM NDSB-195	Dimethylethylammonium-1-propane sulfonate	195.30	N/A	NS
92. (H08)	500.0 mM NDSB-201	3-(1-Pyridino)-1-propane sulfonate	201.26	N/A	NS
93. (H09)	500.0 mM NDSB-211	Dimethyl-2-hydroxyethylammonium-1-propane sulfonate	211.30	N/A	NS
94. (H10)	500.0 mM NDSB-221	3-(1-Methylpiperidinium)-1-propane sulfonate	221.34	N/A	NS
95. (H11)	500.0 mM NDSB-256	Dimethylbenzylammonium-1-propane sulfonate	257.37	N/A	NS
96. (H12)	500.0 mM NDSB-256-4T	3-(4-tert-Butyl-1-pyridino)-1-propane sulfonate	257.35	N/A	NS

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¹ **N** = Non ionic / **I** = Ionic / **Z** = Zwitterionic / **NS** = Non-detergent Sulfobetaines

Sample: _____ Sample Concentration: _____
 Sample Buffer: _____ Date: _____
 Reservoir Volume: _____ Temperature: _____
 Drop Volume: Total _____ μ l Sample _____ μ l Reservoir _____ μ l Additive _____ μ l

- 1 Clear Drop
- 2 Phase Separation
- 3 Regular Granular Precipitate
- 4 Birefringent Precipitate or Microcrystals
- 5 Posettes or Spherulites
- 6 Needles (1D Growth)
- 7 Plates (2D Growth)
- 8 Single Crystals (3D Growth < 0.2 mm)
- 9 Single Crystals (3D Growth > 0.2 mm)

Detergent Screen™ - HR2-407 Scoring Sheet

		Date:	Date:	Date:	Date:
1. (A01)	1.0 mM 14:0 Lyso PG	Ionic			
2. (A02)	6.0 mM 16:0 Lyso PG	Ionic			
3. (A03)	5.0 mM 18:0 Lyso PG	Ionic			
4. (A04)	5.0 mM 18:1 Lyso PG	Ionic			
5. (A05)	10.0 mM CTAB	Ionic			
6. (A06)	1% w/v BAM	Ionic			
7. (A07)	1.0 mM Dodecyltrimethylammonium chloride	Ionic			
8. (A08)	150.0 mM Sodium cholate hydrate	Ionic			
9. (A09)	60.0 mM Deoxycholic acid sodium salt	Ionic			
10. (A10)	5.0 mM MSDH	Ionic			
11. (A11)	146.0 mM N-Lauroylsarcosine sodium salt	Ionic			
12. (A12)	100.0 mM Sodium dodecyl sulfate	Ionic			
13. (B01)	100.0 mM Lithium dodecyl sulfate	Ionic			
14. (B02)	400.0 mM APO 8	Non-ionic			
15. (B03)	5.0 mM APO 9	Non-ionic			
16. (B04)	47.0 mM APO 10	Non-ionic			
17. (B05)	5.0 mM APO 11	Non-ionic			
18. (B06)	5.7 mM APO 12	Non-ionic			
19. (B07)	80.0 mM Tetraethylene glycol mono-octyl ether	Non-ionic			
20. (B08)	71.0 mM Pentaethylene glycol mono-octyl ether	Non-ionic			
21. (B09)	1.1 mM C ₁₂ E ₈	Non-ionic			
22. (B10)	0.8 mM C ₁₂ E ₉	Non-ionic			
23. (B11)	1% v/v Brij® 35	Non-ionic			
24. (B12)	1% v/v Brij® 56	Non-ionic			
25. (C01)	1% v/v Brij® 58	Non-ionic			
26. (C02)	1% v/v Genapol® X-080	Non-ionic			
27. (C03)	1.8 mM Facade®-EM	Non-ionic			
28. (C04)	9.7 mM Facade®-EPC	Non-ionic			
29. (C05)	1.9 mM Facade®-TEG	Non-ionic			
30. (C06)	1.9 mM Facade®-TEM	Non-ionic			
31. (C07)	0.13 mM Facade®-TFA1	Non-ionic			
32. (C08)	790.0 mM MEGA-8	Non-ionic			
33. (C09)	250.0 mM MEGA-9	Non-ionic			
34. (C10)	70.0 mM MEGA-10	Non-ionic			
35. (C11)	3.7 mM Mal(11.1)	Non-ionic			
36. (C12)	1.1 mM Mal(11.2)	Non-ionic			
37. (D01)	105.0 mM N,N-Dimethyldecylamine-N-oxide	Non-ionic			
38. (D02)	18.0 mM n-Decyl- β -D-maltoside	Non-ionic			
39. (D03)	2.0 mM n-Dodecyl- β -D-maltoside	Non-ionic			
40. (D04)	1.0 mM n-Hexadecyl- β -D-maltoside	Non-ionic			
41. (D05)	1.0 mM n-Tetradecyl- β -D-maltoside	Non-ionic			
42. (D06)	1.0 mM Tridecyl- β -D-maltoside	Non-ionic			
43. (D07)	5.9 mM Undecyl- β -D-maltoside	Non-ionic			
44. (D08)	195.0 mM Methyl 6-O-(N-heptylcarbamoyl)- α -D-glucopyranoside	Non-ionic			
45. (D09)	5.0 mM IPTG	Non-ionic			
46. (D10)	25.0 mM n-Decanoylsucrose	Non-ionic			
47. (D11)	65.0 mM n-Nonyl- β -D-glucoside	Non-ionic			
48. (D12)	200.0 mM n-Octyl- β -D-glucoside	Non-ionic			

New formulation. Refer to Detergent Screen documents for updated formulation.



Solutions for Crystal Growth

34 Journey
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Sample: _____ Sample Concentration: _____
 Sample Buffer: _____ Date: _____
 Reservoir Volume: _____ Temperature: _____
 Drop Volume: Total _____ μ l Sample _____ μ l Reservoir _____ μ l Additive _____ μ l

- 1 Clear Drop
- 2 Phase Separation
- 3 Regular Granular Precipitate
- 4 Birefringent Precipitate or Microcrystals
- 5 Posettes or Spherulites
- 6 Needles (1D Growth)
- 7 Plates (2D Growth)
- 8 Single Crystals (3D Growth < 0.2 mm)
- 9 Single Crystals (3D Growth > 0.2 mm)

Detergent Screen™ - HR2-407 Scoring Sheet

Detergent Screen™ - HR2-407 Scoring Sheet		Date:	Date:	Date:	Date:
49. (E01) 90.0 mM n-Octyl- β -D-thioglucopyranoside	Non-ionic				
50. (E02) 10% w/v Pluronic® F-68	Non-ionic				
51. (E03) 10% w/v Pluronic® F-127	Non-ionic				
52. (E04) 3.0 mM Sucrose monolaureate	Non-ionic				
53. (E05) 0.9 mM Thesit®	Non-ionic				
54. (E06) 1% v/v Triton® X-100	Non-ionic				
55. (E07) 1% v/v Triton® X-114	Non-ionic				
56. (E08) 1% v/v Nonylphenyl polyethylene glycol	Non-ionic				
57. (E09) 1% v/v Tween® 20	Non-ionic				
58. (E10) 1% v/v Tween® 80	Non-ionic				
59. (E11) 0.18 mM GDN	Non-ionic				
60. (E12) 80.0 mM CHAPS	Zwitterionic				
61. (F01) 80.0 mM CHAPSO	Zwitterionic				
62. (F02) 29.0 mM BIG CHAP	Zwitterionic				
63. (F03) 14.0 mM Deoxy BIG CHAP	Zwitterionic				
64. (F04) 43.0 mM DDMAB	Zwitterionic				
65. (F05) 20.0 mM LDAO	Zwitterionic				
66. (F06) 10% w/v Sulfobetaine 8	Zwitterionic				
67. (F07) 400.0 mM Sulfobetaine 10	Zwitterionic				
68. (F08) 40.0 mM Sulfobetaine 12	Zwitterionic				
69. (F09) 4.0 mM Sulfobetaine 14	Zwitterionic				
70. (F10) 0.6 mM Sulfobetaine 16	Zwitterionic				
71. (F11) 150.0 mM 06:0 PC (DHPC)	Zwitterionic				
72. (F12) 14.0 mM 07:0 PC (DHPC)	Zwitterionic				
73. (G01) 5.0 mM 06:0 Lyso PC	Zwitterionic				
74. (G02) 5.0 mM 07:0 Lyso PC	Zwitterionic				
75. (G03) 60.0 mM 08:0 Lyso PC	Zwitterionic				
76. (G04) 5.0 mM 09:0 Lyso PC	Zwitterionic				
77. (G05) 80.0 mM 10:0 Lyso PC	Zwitterionic				
78. (G06) 5.0 mM 11:0 Lyso PC	Zwitterionic				
79. (G07) 9.0 mM 12:0 Lyso PC	Zwitterionic				
80. (G08) 5.0 mM 13:0 Lyso PC	Zwitterionic				
81. (G09) 1.0 mM 14:0 Lyso PC	Zwitterionic				
82. (G10) 5.0 mM 15:0 Lyso PC	Zwitterionic				
83. (G11) 1.0 mM 16:0 Lyso PC	Zwitterionic				
84. (G12) 1.0 mM 17:0 Lyso PC	Zwitterionic				
85. (H01) 1.0 mM 18:0 Lyso PC	Zwitterionic				
86. (H02) 1.0 mM 18:1 Lyso PC	Zwitterionic				
87. (H03) 110.0 mM MAPCHO-10	Zwitterionic				
88. (H04) 11.0 mM MAPCHO-12	Zwitterionic				
89. (H05) 1.2 mM MAPCHO-14	Zwitterionic				
90. (H06) 1.0 mM MAPCHO-16	Zwitterionic				
91. (H07) 500.0 mM NDSB-195	Non-detergent Sulfobetaines				
92. (H08) 500.0 mM NDSB-201	Non-detergent Sulfobetaines				
93. (H09) 500.0 mM NDSB-211	Non-detergent Sulfobetaines				
94. (H10) 500.0 mM NDSB-221	Non-detergent Sulfobetaines				
95. (H11) 500.0 mM NDSB-256	Non-detergent Sulfobetaines				
96. (H12) 500.0 mM NDSB-256-4T	Non-detergent Sulfobetaines				

New formulation. Refer to Detergent Screen documents for updated formulation.

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