

How to Reproduce SaltRx Reagents

SaltRx reagents and optimization conditions based on SaltRx hits can be formulated using volumetric methods and carefully prepared reagent stocks (Table 1). Note the examples below.

Example 1. To prepare 1.0 milliliter of SaltRx reagent 1 in a crystallization plate.

Solution Composition: 1.8 M Sodium acetate trihydrate pH 7.0
0.1 M BIS-TRIS propane pH 7.0

- 450 µl water³
- 100 µl 1.0 M BIS-TRIS propane pH 7.0
(CAS # 64431-96-5, Catalog # HR2-795)
- 450 µl 4.0 M Sodium acetate trihydrate pH 7.0
(CAS # 6131-90-4, Catalog # HR2-763)

Make no pH adjustments. Mix well by aspirating and dispensing the solution multiple times.

Example 2. To prepare 1.0 milliliter of SaltRx reagent 57.

Solution Composition: 0.63 M Sodium phosphate monobasic monohydrate,
1.17 M Potassium phosphate dibasic /pH 6.9

- 550 µl water³
- 157 µl 4.0 M Potassium phosphate dibasic
(CAS # 7758-11-4, Catalog # HR2-635)
- 293 µl 4.0 M Sodium phosphate monobasic monohydrate
(CAS # 10049-21-5, Catalog # HR2-551)

Make no pH adjustments. Mix well. Final pH will be 6.9

Example 3. To prepare 10 milliliters of SaltRx reagent 27.

Solution Composition: 2.0 M Sodium formate
0.1 M Sodium acetate trihydrate pH 4.6

- 6.1 ml water³
- 1.0 ml 1.0 M Sodium acetate trihydrate pH 4.6
(CAS # 6131-90-4, Catalog # HR2-731)
- 2.9 ml 7.0 M Sodium formate
(CAS # 141-53-7, Catalog # HR2-547)

Make no pH adjustments. Mix well.

³ ASTM Type II (laboratory grade) or Type III (analytical grade) water.

Formulation Notes for SaltRx Reagents

1. No additional pH adjustment is made to any reagent after formulation. Use the buffers in Table 1 to reproduce a SaltRx reagent.

2. All Optimize solutions and screen reagents are sterile filtered using 0.22 µm filters into sterile containers.
3. Add water first as this will help maintain the solubility of subsequently added reagents.
4. When formulating reagents using a pipet, add the largest volume last (except water). Use this larger volume setting to aspirate and dispense the reagent until the solution is mixed.
5. When formulating reagents using a pipet, use a clean, sterile pipet tip for each reagent added to the solution.
6. Use the buffers in Table 2 to systematically vary the pH as a crystallization variable.

pH as a Crystallization Variable

The buffers listed in Table 2, can be used to vary the pH as a crystallization variable and are recommended when optimizing a crystal grown from a SaltRx kit.

Optimize™ buffer stocks are supplied as a 100 milliliters sterile filtered solution. Optimize buffers are available as an acid-base pair or titrated to a specific pH.

StockOptions™ buffer kits contain 10 milliliters each of ready to pipet buffers, titrated in 0.1 pH increments over the indicated pH range. The number of reagents offered in a StockOptions buffer kit depends upon the pH range of the buffer. The broader the pH range, the more buffers in the kit.

Online Information

Visit www.hamptonresearch.com and enter one of the following:

- Reagent Catalog Number
- Kit Catalog Number
- CAS Number
- Reagent Name

To obtain reagent specifications, pH titration tables, user guides, certificates of analysis, material safety data sheets (MSDS), and any other additional information.

MakeTray™

MakeTray is a free, web based program at www.hamptonresearch.com which generates both a pipetting worksheet and a reagent formulation document for crystallization set ups. MakeTray allows one to enter general information about the sample and experiment, which is then printed on the pipet worksheet and the reagent formulation document. The plate size can be customized for any number of wells, so MakeTray works for: 24, 48, and 96 well plates. MakeTray is especially useful for the design and formulation of crystal optimization experiments.

Table 1. Recommended reagents for the formulation of SaltRx and Optimization reagents.

Each of these reagents are available as an Optimize™ crystallization grade reagent from Hampton Research. Table 1 provides the common chemical name, the Hampton Research catalog number, supplied stock concentration, the supplied volume, and the CAS number for each reagent. For more information on a specific Optimize reagent, go to

www.hamptonresearch.com. Using Search, enter either the catalog number, CAS number, or chemical name to obtain additional information for the Optimize reagent, including a Certificate of Analysis and MSDS (where applicable).

Salts	Hampton Research Catalog #	Supplied [Stock]	Supplied Volume	CAS #
Ammonium acetate	HR2-565	1.0 M	100 ml	631-61-8
	HR2-799	8.0 M	200 ml	631-61-8
Ammonium chloride	HR2-691	5.0 M	200 ml	12125-02-9
Ammonium citrate dibasic	HR2-685	2.5 M	200 ml	3012-65-5
Ammonium citrate tribasic pH 7.0	HR2-759	2.5 M	200 ml	3458-72-8
Ammonium nitrate	HR2-665	10.0 M	200 ml	6484-52-2
Ammonium phosphate dibasic	HR2-629	3.5 M	200 ml	7783-28-0
Ammonium phosphate monobasic	HR2-555	2.5 M	200 ml	7722-76-1
Ammonium sulfate	HR2-541	3.5 M	200 ml	7783-20-2
Ammonium tartrate dibasic	HR2-679	2.0 M	200 ml	3164-29-2
Lithium sulfate monohydrate	HR2-545	2.0 M	200 ml	10377-48-7
Magnesium formate dihydrate	HR2-537	1.0 M	200 ml	557-39-1
Magnesium sulfate hydrate	HR2-633	2.5 M	200 ml	22189-08-8
DL-Malic acid pH 7.0	HR2-761	3.0 M	200 ml	6915-15-7
Potassium phosphate dibasic	HR2-635	4.0 M	200 ml	7758-11-4
Potassium sodium tartrate tetrahydrate	HR2-539	1.5 M	200 ml	6381-59-5
Potassium thiocyanate	HR2-695	8.0 M	200 ml	333-20-0
Sodium acetate trihydrate pH 7.0	HR2-763	4.0 M	200 ml	6131-90-4
Sodium chloride	HR2-637	5.0 M	200 ml	7647-14-5
Sodium citrate tribasic dihydrate	HR2-549	1.6 M	200 ml	6132-04-3
Sodium formate	HR2-547	7.0 M	200 ml	141-53-7
Sodium malonate pH 7.0	HR2-707	3.4 M	200 ml	141-82-2
Sodium nitrate	HR2-661	7.0 M	200 ml	7631-99-4
Sodium phosphate monobasic monohydrate	HR2-551	4.0 M	200 ml	10049-21-5
Succinic acid pH 7.0	HR2-709	1.2 M	200 ml	110-15-6
Tacsimate pH 7.0	HR2-755	100 %	200 ml	N/A

(Table 1 continued on page 3)

Table 1 (Continued). Recommended reagents for the formulation of SaltRx and Optimization reagents.

Buffers	Hampton Research Catalog #	Supplied [Stock]	Supplied Volume	CAS #
BIS-TRIS propane pH 7.0 ¹	HR2-795	1.0 M	100 ml	64431-96-5
Sodium acetate trihydrate pH 4.6 ¹	HR2-731	1.0 M	100 ml	6131-90-4
Tris pH 8.5 ¹	HR2-725	1.0 M	100 ml	77-86-1
¹ pH titrated using Hydrochloric acid (HR2-581) CAS # 7647-01-0				

Table 2. Recommended buffers for screening the pH of SaltRx and Optimization reagents.

Buffer Solution or Kit	Hampton Research Catalog #	Supplied [Stock]	Supplied Volume	CAS #	pH range
StockOptions™ Bis-Tris propane	HR2-993-**	1.0 M	185 ml	64431-96-5	6.3 - 9.5
StockOptions™ Sodium Acetate kit ⁴	HR2-233	1.0 M	10 ml each	6131-90-4	3.6 - 5.6
StockOptions™ Tris ⁴	HR2-100	1.0 M	10 ml each	77-86-1	7.0 - 9.0
⁴ Individual StockOptions buffers titrated to any pH within the kit's pH range are available in 185 ml volumes from the Hampton Research Custom Shop					
** Refers to the reagent number in the kit. For example, reagent number 1 = HR2-993-01 (pH 6.3)					

Technical Support

Inquiries regarding SaltRx Fundamentals, interpretation of screen results, optimization strategies and general inquiries regarding crystallization are welcome. Please e-mail, fax, or telephone your request to Hampton Research. Fax and e-mail Technical Support are available 24 hours a day. Telephone technical support is available 8:00 a.m. to 5:00 p.m. USA Pacific Standard Time.

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