

Molecular  
Dimensions



**HELIX™**

**MD1-68**

Crystallize a diverse range of nucleic acid topologies and molecular weights.

This screen targets all types of DNA/RNA, triplexes, quadruplexes, pseudoknots, i-motifs, and large molecular weight nucleic acids.

Developed by Dr. Gary Parkinson from School of Pharmacy, University College London, UK.

MD1- 68 is presented as a 96 x 10 mL conditions.

### Features of HELIX™:

- Crystallize nucleic acid fragments of all molecular weights.
- Ideal for double stranded DNA and RNA, pseudo knots, G-quadruplexes, i-motifs, triplex, ribozymes.
- Optimized for MAD, SAD, SIRAS data collections- no cacodylate.
- Cryo-cooling optimization.
- Screening of additives.
- Adaptable for HT Screening.

MPD, NaCl, and  $(\text{NH}_4)_2\text{SO}_4$  have been used as precipitating agents in HELIX and can be used for any molecular weight target while the size of the PEGs used as crystallization agents tend to follow the molecular weights of the target molecules. Components that have significant impact on crystallization for DNA and RNA are quite restricted and well defined. However, it is still important to explore alternative conditions. HELIX explores the use of PEGs as a precipitating agent.

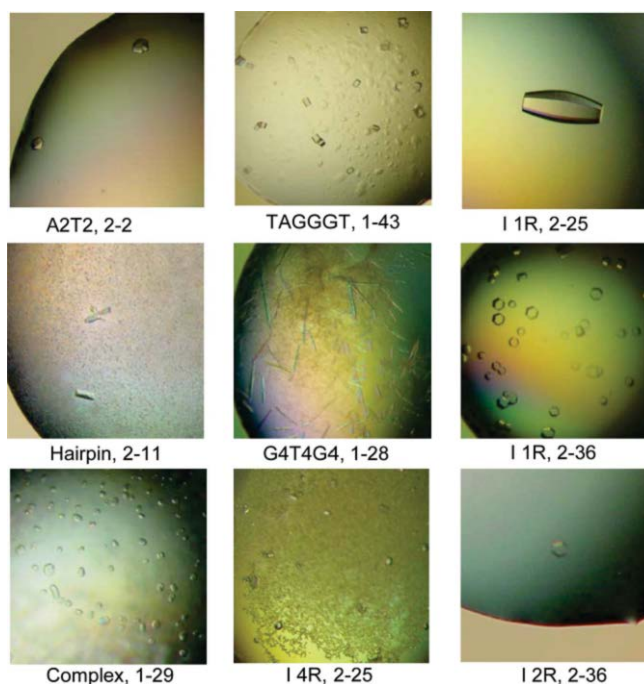
### Introduction

HELIX™ is designed to satisfy the requirements for structural biologists to experimentally determine initial nucleation and crystal growth conditions, and subsequently enable successful cryo-cooling along with the unimpeded collection of anomalous data.

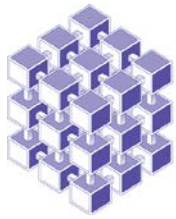
An analysis of the PDB covering the 1324 deposited DNA/RNA crystallization conditions has been crucial in the design of these new 96 conditions.

### HELIX Formulation

A buffering range from pH 4.6 to 8.5, combining ammonium acetate, MES, HEPES, and Bis-Tris, ensures appropriate buffering when setting-up crystallizations from 4 °C to 37 °C. The lower pH conditions, for example, enable protonation of cytosine for the formation of i-motifs and promote triplex DNA formation.



Light micrographs showing nine crystals obtained with HELIX for the sequences assayed. Magnifications differ and crystal sizes vary from 20 to 200 mm.



### **Co-crystallization & Ligand-binding.**

Co-crystallization of ligands to nucleic acids needs to ensure that the electrostatic component of ligand binding associations are not reduced significantly by the use of high salt concentrations. It is for this reason HELIX has limited the use of ammonium sulfate as a precipitating agent, and retained the focus on MPD, PEGs.

Reducing the ionic strength in conditions with precipitants retains the electrostatic component thus promotes the formation of ligand-binding.

### **Cryo-Protection**

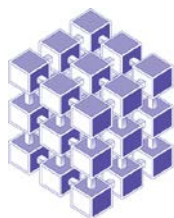
It is now a key requirement to take the initial screening conditions and cryo-protect the crystals for flash-cooling. When flash-cooled the effects of radiation damage on the crystals are limited and allow transportation and long-term storage of the crystal.

HELIX has focused on conditions allowing for an easy transition from the initial well condition towards suitable cryo-conditions. Furthermore, within the kit, 24 conditions have been set aside to enable direct cryo-protection without further modification. For those conditions containing salts known to enhance crystallizations a small percentage of suitable cryo-protectants have been added to aid in subsequent cryo-protection optimization.

### **Why no cacodylate?**

Well apart from the obvious toxicity issue of using cacodylate you might say that nucleic acids would benefit from a chemical that potentially mics a phosphate backbone. Unfortunately the cons outweigh the pros.

The use of cacodylic acid is avoided in HELIX to remove any competing fluorescence signal from the arsenic that will mask the fluorescence emission from selenium, bromine and iodine atoms. The determination of the precise wavelength for the anomalous peak is required to maximize the diffracted anomalous diffraction signal from anomalous scattering elements.



### Instructions for Use:

A range of temperature options are available for screening Nucleic Acids, ranging from 4°C – 37 °C.

Common temperatures are 4°C (18%), 16-20°C (34%), 22-25°C (26%), 37°C (5%).

**Recommended storage for HELIX is 4°C. Or aliquot into deep-well blocks or microplates and freeze until needed.**

**Allow 10 mL tubes to equilibrate to room temperature prior to use.**

### Formulation Notes:

HELIX reagents are formulated using ultrapure water (>18.0 MΩ) and are sterile-filtered using 0.22 μm filters. No preservatives are added.

Final pH may vary from that specified on the datasheet. Molecular Dimensions will be happy to discuss the precise formulation of individual reagents.

Individual reagents and stock solutions for optimization are available from Molecular Dimensions.

Enquiries regarding HELIX formulation, interpretation of results or optimization strategies are welcome. Please e-mail, fax or phone your query to Molecular Dimensions.

Contact and product details can be found at [www.moleculardimensions.com](http://www.moleculardimensions.com)

Manufacturer's safety data sheets are available to download from our website.

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HELIX™

Box 1 Conditions 1 - 48

MD1-68

Tube #	Conc.	Salt 1	Conc.	Salt 2	Conc.	Additive 1	Conc.	Additive 2	Conc.	Buffer	pH	Conc.	Precipitant
1-1	0.05 M	Potassium chloride	0.1 M	Lithium chloride	0.012 M	Spermine tetrahydrochloride			0.05 M	MES	6.5	25 % v/v	PEG 400
1-2					0.001 M	Spermine tetrahydrochloride			0.05 M	MES	6.5	25 % v/v	PEG 400
1-3	0.1 M	Sodium chloride	0.05 M	Lithium chloride	0.01 M	Magnesium chloride hexahydrate			0.05 M	MES	6.5	25 % v/v	PEG 400
1-4	0.2 M	Potassium chloride			0.005 M	Hexamine cobalt(III) chloride			0.05 M	MES	6.5	25 % v/v	PEG 400
1-5	0.1 M	Lithium chloride			0.01 M	Manganese(II) chloride tetrahydrate			0.05 M	MES	6.5	25 % v/v	PEG 400
1-6	0.1 M	Sodium chloride			0.005 M	Strontium chloride hexahydrate			0.05 M	MES	6.5	25 % v/v	PEG 400
1-7	0.05 M	Potassium chloride	0.1 M	Lithium chloride	0.012 M	Spermine tetrahydrochloride			0.05 M	MES	6.5	35 % v/v	MPD
1-8					0.001 M	Spermine tetrahydrochloride			0.05 M	MES	6.5	35 % v/v	MPD
1-9	0.1 M	Sodium chloride	0.1 M	Lithium chloride	0.01 M	Magnesium chloride hexahydrate			0.05 M	MES	6.5	35 % v/v	MPD
1-10	0.2 M	Potassium chloride			0.005 M	Hexamine cobalt(III) chloride			0.05 M	MES	6.5	35 % v/v	MPD
1-11	0.1 M	Lithium chloride			0.01 M	Manganese(II) chloride tetrahydrate			0.05 M	MES	6.5	35 % v/v	MPD
1-12	0.1 M	Sodium chloride			0.005 M	Strontium chloride hexahydrate			0.05 M	MES	6.5	35 % v/v	MPD
1-13	0.05 M	Potassium chloride	0.1 M	Lithium chloride	0.012 M	Spermine tetrahydrochloride			0.05 M	MES	6.5	17 % w/v	PEG 4000
1-14					0.001 M	Spermine tetrahydrochloride			0.05 M	MES	6.5	17 % w/v	PEG 4000
1-15	0.1 M	Sodium chloride	0.05 M	Lithium chloride	0.01 M	Magnesium chloride hexahydrate			0.05 M	MES	6.5	17 % w/v	PEG 4000
1-16	0.2 M	Potassium chloride			0.005 M	Hexamine cobalt(III) chloride			0.05 M	MES	6.5	17 % w/v	PEG 4000
1-17	0.1 M	Lithium chloride			0.01 M	Manganese(II) chloride tetrahydrate			0.05 M	MES	6.5	17 % w/v	PEG 4000
1-18	0.1 M	Sodium chloride			0.005 M	Strontium chloride hexahydrate			0.05 M	MES	6.5	17 % w/v	PEG 4000
1-19	0.05 M	Potassium chloride	0.1 M	Lithium chloride	0.012 M	Spermine tetrahydrochloride			0.05 M	MES	6.5	2.6 M	Sodium malonate dibasic monohydrate
1-20					0.001 M	Spermine tetrahydrochloride			0.05 M	MES	6.5	2.6 M	Sodium malonate dibasic monohydrate
1-21	0.1 M	Sodium chloride	0.05 M	Lithium chloride	0.01 M	Magnesium chloride hexahydrate			0.05 M	MES	6.5	2.6 M	Sodium malonate dibasic monohydrate
1-22	0.2 M	Potassium chloride			0.005 M	Hexamine cobalt(III) chloride			0.05 M	MES	6.5	2.6 M	Sodium malonate dibasic monohydrate
1-23	0.1 M	Lithium chloride			0.01 M	Manganese(II) chloride tetrahydrate			0.05 M	MES	6.5	2.6 M	Sodium malonate dibasic monohydrate
1-24	0.1 M	Sodium chloride			0.002 M	Strontium chloride hexahydrate			0.05 M	MES	6.5	2.6 M	Sodium malonate dibasic monohydrate
1-25	0.1 M	Ammonium sulfate							0.05 M	Bis-Tris	7.0	44 % v/v	PEG 200
1-26	0.2 M	Potassium chloride			0.01 M	Calcium chloride dihydrate			0.05 M	Bis-Tris	7.0	40 % v/v	PEG 400
1-27	0.1 M	Sodium chloride			0.002 M	Spermine tetrahydrochloride			0.05 M	Bis-Tris	7.0	37 % w/v	PEG 1000
1-28	0.1 M	Sodium chloride	0.2 M	Potassium chloride	0.02 M	Magnesium chloride hexahydrate			0.05 M	Bis-Tris	7.0	35 % w/v	PEG 2000
1-29	0.05 M	Potassium chloride			0.005 M	Spermine tetrahydrochloride			0.05 M	Bis-Tris	7.0	33 % w/v	PEG 3350
1-30	0.1 M	Ammonium sulfate	0.1 M	Sodium chloride	1.0 M	Sodium formate			0.05 M	Bis-Tris	7.0	20 % w/v	PEG 8000
1-31					1.0 M	Sodium formate			0.05 M	Bis-Tris	7.0	20 % w/v	PEG 20,000
1-32	0.05 M	Lithium sulfate							0.05 M	Bis-Tris	7.0	40 % v/v	PEG 500 MME
1-33	0.1 M	Sodium citrate tribasic dihydrate							0.05 M	Bis-Tris	7.0	40 % v/v	PEG 500 MME
1-34	0.1 M	Ammonium sulfate			0.002 M	Spermine tetrahydrochloride			0.05 M	Bis-Tris	7.0	40 % v/v	MPD
1-35									0.05 M	Bis-Tris	7.0	35 % v/v	MPD
1-36	0.1 M	Sodium chloride			0.02 M	Magnesium chloride hexahydrate			0.05 M	Bis-Tris	7.0	30 % v/v	MPD
1-37	0.1 M	Potassium chloride							0.05 M	Bis-Tris	7.0	27 % v/v	MPD
1-38						5 % v/v PEG 400			0.05 M	Bis-Tris	7.0	24 % v/v	MPD
1-39	0.2 M	Lithium sulfate							0.05 M	Bis-Tris	7.0	20 % v/v	MPD
1-40						20 % v/v Glycerol		5 % w/v PEG 3350	0.05 M	Bis-Tris	7.0	1.0 M	Ammonium sulfate
1-41						10 % v/v Glycerol		5 % v/v PEG 500 MME	0.05 M	Bis-Tris	7.0	1.2 M	Ammonium sulfate
1-42						25 % v/v Glycerol			0.05 M	Bis-Tris	7.0	1.4 M	Ammonium sulfate
1-43	0.15 M	Potassium chloride				25 % v/v Glycerol			0.05 M	Bis-Tris	7.0	1.6 M	Ammonium sulfate
1-44	0.1 M	Sodium chloride				25 % v/v Glycerol			0.05 M	Bis-Tris	7.0	1.8 M	Ammonium sulfate
1-45						5 % v/v PEG 400			0.05 M	Bis-Tris	7.0	2.0 M	Ammonium sulfate
1-46	0.1 M	Potassium chloride							0.05 M	Bis-Tris	7.0	22 % w/v	PEG 2000 MME
1-47	0.2 M	Lithium chloride							0.05 M	Bis-Tris	7.0	22 % w/v	PEG 2000 MME
1-48	0.1 M	Sodium chloride							0.05 M	Bis-Tris	7.0	22 % w/v	PEG 2000 MME



**HELIX™**      **Box 2 Conditions 1 - 48**      **MD1-68**

Tube #	Conc. Salt 1	Conc. Salt 2	Conc. Additive 1	Conc. Additive 2	Conc. Buffer	pH	Conc. Precipitant
2-1	0.1 M Potassium chloride				0.05 M HEPES	6.5	20 % v/v MPD
2-2			0.005 M Spermine tetrahydrochloride		0.05 M HEPES	6.5	10 % v/v MPD
2-3	0.1 M Sodium chloride	0.2 M Potassium chloride			0.05 M HEPES	6.5	10 % v/v MPD
2-4	0.2 M Sodium chloride				0.05 M HEPES	6.5	25 % v/v MPD
2-5	0.05 M Lithium sulfate				0.05 M HEPES	6.5	15 % v/v MPD
2-6	0.3 M Sodium chloride				0.05 M HEPES	6.5	30 % v/v MPD
2-7	0.05 M Sodium chloride		0.01 M Magnesium chloride hexahydrate		0.05 M HEPES	6.5	25 % v/v PEG 400
2-8	0.2 M Potassium chloride				0.05 M Bis-Tris	7.0	10 % v/v PEG 400
2-9	0.05 M Lithium sulfate				0.05 M HEPES	6.5	18 % w/v PEG 1000
2-10					0.05 M Bis-Tris	7.0	1.5 M Lithium sulfate
2-11	0.1 M Sodium chloride	0.1 M Potassium chloride			0.05 M HEPES	6.5	1.9 M Lithium sulfate
2-12			0.02 M Magnesium chloride hexahydrate		0.05 M Bis-Tris	7.0	15 % w/v PEG 2000 MME
2-13	0.05 M Lithium sulfate				0.05 M HEPES	6.5	10 % w/v PEG 2000 MME
2-14					0.05 M Bis-Tris	7.0	14 % w/v PEG 2000 MME
2-15	0.1 M Lithium chloride				0.05 M Bis-Tris	7.0	10 % v/v PEG 500 MME
2-16	0.05 M Potassium chloride				0.05 M Bis-Tris	7.0	1.1 M Ammonium sulfate
2-17	0.05 M Lithium sulfate				0.05 M HEPES	6.5	1.4 M Ammonium sulfate
2-18	0.1 M Sodium chloride		0.01 M Lithium chloride		0.05 M HEPES	6.5	1.8 M Ammonium sulfate
2-19	0.3 M Lithium sulfate				0.05 M Bis-Tris	7.0	18 % w/v PEG 1000
2-20	0.3 M Sodium chloride				0.05 M HEPES	6.5	15 % w/v PEG 1000
2-21	0.25 M Potassium chloride				0.05 M HEPES	6.5	12 % w/v PEG 1000
2-22	0.1 M Lithium sulfate				0.05 M Bis-Tris	7.0	25 % v/v PEG 350 MME
2-23					0.05 M HEPES	6.5	20 % v/v PEG 350 MME
2-24	0.05 M Lithium sulfate				0.05 M HEPES	6.5	15 % v/v PEG 350 MME
2-25			0.005 M Spermine tetrahydrochloride		0.05 M Sodium acetate	4.5	18 % v/v MPD
2-26	0.1 M Sodium chloride				0.05 M Sodium acetate	4.5	24 % v/v MPD
2-27	0.15 M Potassium chloride				0.05 M Sodium acetate	4.5	32 % v/v MPD
2-28			0.01 M Magnesium chloride hexahydrate		0.05 M Sodium acetate	5.0	21 % v/v MPD
2-29	0.1 M Sodium chloride	0.1 M Potassium chloride	0.005 M Spermine tetrahydrochloride		0.05 M Sodium acetate	5.0	14 % v/v MPD
2-30			0.05 M Lithium chloride		0.05 M Sodium acetate	5.0	15 % v/v PEG 400
2-31					0.05 M MES	5.5	21 % v/v MPD
2-32			0.02 M Magnesium chloride hexahydrate		0.05 M MES	5.5	21 % v/v MPD
2-33					0.05 M MES	5.5	12 % w/v PEG 2000
2-34			0.02 M Magnesium sulfate heptahydrate		0.05 M MES	5.5	21 % v/v MPD
2-35			0.005 M Spermine tetrahydrochloride		0.05 M MES	5.5	15 % v/v PEG 400
2-36			10 % v/v Glycerol		0.05 M MES	5.5	1.5 M Ammonium sulfate
2-37	0.05 M Sodium chloride	0.1 M Potassium chloride	0.01 M Calcium chloride dihydrate		0.05 M Bis-Tris	7.0	25 % w/v PEG 2000
2-38	0.25 M Sodium chloride		0.005 M Spermine tetrahydrochloride		0.05 M Bis-Tris	7.0	20 % w/v PEG 3350
2-39	0.1 M Potassium chloride		0.005 M Barium chloride dihydrate		0.05 M Bis-Tris	7.0	12 % w/v PEG 8000
2-40	0.3 M Sodium chloride				0.05 M Bis-Tris	7.0	8 % w/v PEG 20,000
2-41	0.05 M Sodium chloride	0.2 M Lithium chloride	0.01 M Calcium chloride dihydrate		0.05 M Bis-Tris	7.0	20 % w/v PEG 2000
2-42	0.1 M Potassium chloride		0.002 M Spermine tetrahydrochloride		0.05 M Bis-Tris	7.0	15 % w/v PEG 2000 MME
2-43	0.05 M Potassium chloride	0.1 M Lithium sulfate	0.02 M Magnesium sulfate heptahydrate		0.05 M Bis-Tris	7.0	15 % w/v PEG 2000 MME
2-44	0.1 M Sodium chloride		0.002 M Barium chloride dihydrate		0.05 M Bis-Tris	7.5	6 % w/v PEG 20,000
2-45	0.1 M Potassium chloride		0.002 M Spermine tetrahydrochloride		0.05 M Bis-Tris	7.5	7 % w/v PEG 8000
2-46	0.05 M Lithium sulfate		0.03 M Magnesium sulfate heptahydrate		0.05 M Bis-Tris	8.0	15 % w/v PEG 3350
2-47	0.2 M Sodium chloride				0.05 M Bis-Tris	8.5	9 % w/v PEG 3350
2-48			0.052 M Magnesium chloride hexahydrate		0.05 M Bis-Tris	8.5	18 % w/v PEG 3350



**Abbreviations:**

**MPD:** 2-methyl, 2,4-pentanediol, **PEG:** Poly Ethylene Glycol,

Manufacturer's safety data sheets are available from our website or by scanning the QR code here:



**Ordering details:**

**Catalogue Description**

**Catalogue Code**

HELIX™

MD1-68

HELIX™ HT-96

MD1-69

HELIX™ single reagents

MDSR-68-tube number

HELIX™ HT-96 single reagents

MDSR-69-tube number

For HELIX™ stock reagents visit our Optimization page on our website.