Molecular Dimensions ACHIEVE MORE.

Additive screen

Membrane and Soluble Proteins

The Hippocrates™ Additive Screen MD1–118

The Hippocrates Additive Screen is a new 48-condition additive screen, containing a library of unique drug-like compounds to enhance protein stability and crystallisability.

MD1-118 is presented as 48 x 100 µL conditions.

Let the unique, drug-like compounds in Hippocrates Additive screen cure your crystallisation problems:

- Expand the range of chemical space screened with these unique additives.
- Enhance stability and solubility of protein for crystallization with the drug-like compounds including phytochemicals, anitbiotics and vitamins.
- No bias to particular reagents of macromolecule classes.
- Use in protein stability screen assays.

Introduction

The Hippocrates Additive Screen contains a library of drug-like compounds for use in protein crystallization optimization experiments (Table 1). The compounds include antibiotics, vitamins, dipeptides, nucleosides, phytochemicals, anesthetic alkaloids and cholic acid derivatives. Some can be found bound to proteins and may aid protein stability and solubility. The Hippocrates Additive screen contains all the compounds found in the Morpheus® III screen, plus three additional compounds: Rosmarinic acid and gallotannin (both Phytochemicals), and dibucaine hydrochloride (an anesthetic alkaloid).

How to use The Hippocrates Additive Screen:

Additives may alter hydration and intermolecular interactions between protein molecules or between protein molecule and solvent/ligands. The additives in The Hippocrates Additive Screen may also be used in protein stability assays.

The Hippocrates Additive Screen is provided in an easy-to-use 48-well low-profile block that is compatible with dispensing robots.

Recommended set-up: Set-up your optimization screen and add 10% (v/v) of additive in reservoir or drop.

References

1. Gorrec, F (2009), The MORPHEUS protein crystallization screen *J Appl Cryst* 42, 1035-1042

2. Gorrec, F (2013), The current approach to initial crystallization screening of proteins is under-sampled *J Appl Cryst* 46, 795-797.

3. Gorrec, F (2015), The Morpheus II protein crystallization screen, ICCBM15 proceedings (Special Issue Acta Cryst F71, p. 831-837).

Please note

The screen must be frozen upon arrival.

Gently mix the screen before use (invert the block several times then spin down <1000 rpm).

Formulation Notes:

The Hippocrates Additive Screen reagents are formulated using ultrapure water (>18.0 MΩ), except as specifically stated below, and are sterile-filtered using 0.22 µm filters. No preservatives are added. Material Safety Datasheets are available from our website.

(-)-menthol, caffeic acid, gallic acid monohydrate, N-vanillylnonanamide (capsaicin synthetic), thymol, rosmarinic acid, esculin hydrate, quinine hemisulfate monohydrate and tryptamine are all dissolved in 50% EtOH and 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 The Hippocrates Additive Screen 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

RE-ORDERING INFORMATION

Code	Pack Size	Description
MD1-116	96 x 10 mL	Morpheus III
MD1-117	96 x 1 mL	Morpheus III HT-96
MD1-118	48 x 100 µL	Hippocrates™ additive screen
MD1-91	96 x 10 mL	Morpheus II
MD1-92	96 x 1 mL	Morpheus II HT-96
MD1-46	96 x 10 mL	Morpheus
MD1-47	96 x 1 mL	Morpheus HT-96
MD1-93	48 x 100 µL	The Morpheus® Additive screen

Hippocrates, Morpheus III, Morpheus II and Morpheus have been designed and developed by Fabrice GORREC, in collaboration with the scientists at the Medical Research Council Laboratory of Molecular Biology (LMB) at Cambridge and is manufactured exclusively under license from LifeARC by Molecular Dimensions Limited.

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Table 1: List of Drug-like compounds in Hippocrates

Ligand Name	Mix	PDB ID	No of Structures*
Ala-Ala	Dipeptides	n/a	-
Ala-Gln	Dipeptides	n/a	1
Gly-Glu	Dipeptides	n/a	-
Gly-L-Ala	Dipeptides	n/a	-
Gly-L-Asp	Dipeptides	n/a	-
Gly-Sar	Dipeptides	n/a	-
L-Carnosine	Dipeptides	n/a	-
Leu-Ala hydrate	Dipeptides	n/a	1
Sodium-L-ascorbate	Vitamins	ASC	33
Choline chloride	Vitamins	CHT	37
D-Panthenol	Vitamins	MV2	1
Pyridoxine hydrochloride	Vitamins	UEG	3
Thiamine hydrochloride	Vitamins	VIB	12
Cytidine	Nucleosides	CTN	23
Inosine	Nucleosides	NOS	14
Ribavirin	Nucleosides	RBV	3
Thymidine	Nucleosides	THM	45
Uridine	Nucleosides	URI	27
Menthol	Phytochemicals 1	n/a	-
Caffeic acid	Phytochemicals 1	DHC	9
D-Quinic acid	Phytochemicals 1	QIC	3
Shikimic acid	Phytochemicals 1	SKM	36
Gallic acid monohydrate	Phytochemicals 1	GDE	9
N-Vanillylnonanamide	Phytochemicals 1	n/a	-
Thymol	Phytochemicals 1	IPB	1
D-Salicin	Phytochemicals 2	SAO	1
Esculin hydrate	Phytochemicals 2	n/a	-
Quinine hemisulfate salt monohydrate	Phytochemicals 2	QI9	3
Tryptamine	Phytochemicals 2	TSS	7
Arbutin	Phytochemicals 2	n/a	-
Rosmarinic acid #	Phytochemicals 2	ROA	2
Gallotannin(Tannic acid) #	Phytochemicals 2	n/a	-
Ampicillin sodium salt	Antibiotics	AIC	8
Apramycin sulfate salt	Antibiotics	AM2	7
Bacitracin	Antibiotics	n/a	-
Dihydrostreptomycin sesquisulfate	Antibiotics	SRY	19
Gentamicin sulfate	Antibiotics	51G	3
Spectinomycin dihydrohloride pentahydrate	Antibiotics	SCM	3
CHAPS	Cholic acid derivatives	CPS	60
CHAPSO	Cholic acid derivatives	1N7	9
Sodium glycocholate hydrate	Cholic acid derivatives	GCH	4
Taurocholic acid sodium salt hydrate	Cholic acid derivatives	TCH	8
Lidocaine hydrochloride	Anesthetic alkaloids	LQZ	2
Procaine hydrochloride	Anesthetic alkaloids	n/a	-
Proparacaine hydrochloride	Anesthetic alkaloids	n/a	-
Tetracaine hydrochloride	Anesthetic alkaloids	TE4	2
Dibucaine Hydrochloride(Cinchocaine) #	Anesthetic alkaloids	n/a	-

*No of Structures requested in April 2018

#These compounds are only in Hippocrates and do NOT appear in the Morpheus® III screen or Morpheus III mixes.

This is a 48-well screen. Only columns 1-6 in each row are filled. Columns 7-12 are deliberately left empty.

Well No.	Screen ID	Conc.	Units	Ligand
A1	1	50	%	Ethanol
A2	2	6	%	Ala-Ala
A3	3	6	%	Ala-Gln
A4	4	6	%	Gly-Glu
A5	5	6	%	Gly-L-Ala
A6	6	6	%	Gly-L-Asp
B1	7	6	%	Gly-Sar
B2	8	6	%	L-Carnosine
B3	9	6	%	Leu-Ala hydrate
B4	10	9	%	(+)-Sodium L-ascorbate
B5	11	9	%	Choline Chloride
B6	12	9	%	D-Panthenol (provitamin B5)
C1	13	9	%	Pyridoxine hydrochloride
C2	14	9	%	Thiamine hydrochloride
C3	15	9	%	Cytidine
C4	16	2	%	Inosine
C5	17	6	%	Ribavirin
C6	18	6	%	Thymidine
D1	19	6	%	Uridine
D2	20	1.5	%	(-)-Menthol†
D3	21	1.5	%	Caffeic acid †
D4	22	1.5	%	D-(−)-Quinic acid
D5	23	1.5	%	Gallic acid monohydrate†
D6	24	0.5	%	N-vanillylnonanamide (capsaicin synthetic)†
E1	25	1.5	%	Shikimic acid
E2	26	1.5	%	Thymol†
E3	27	1.5	%	Rosmarinic acid† #
E4	28	1.5	%	D-(−)-Salicin
E5	29	0.5	%	Esculin hydrate †
E6	30	1.5	%	Gallotannin (tannic acid) #
F1	31	1.5	%	p-Arbutin
F2	32	1	%	Quinine hemisulfate salt monohydrate†
F3	33	1.5	%	Tryptamine†
F4	34	3	%	Ampicillin sodium salt
F5	35	3	%	Apramycin sulfate salt
F6	36	3	%	Bacitracin (baciim)
G1	37	3	%	Dihydrostreptomycin sesquisulfate
G2	38	3	%	gentamicin sulfate
G3	39	3	%	Spectinomycin dihydrochloride pentahydrate
G4	40	9	%	CHAPS hydrate
G5	41	9	%	CHAPSO
G6	42	9	%	Sodium glycocholate hydrate
H1	43	9	%	Taurocholic acid sodium salt hydrate
H2	44	6	%	Dibucaine hydrochloride (Cinchocaine) #
H3	45	6	%	Lidocaine hydrochloride monohydrate (Xylocaine)
H4	46	6	%	Procaine hydrochloride (Novocaine)
H5	47	6	%	Proparacaine hydrochloride (Proxymetacaine)
H6	48	6	%	Tetracaine hydrochloride (Amethocaine)

†These compounds are dissolved in 50% EtOH.

These compounds are only in Hippocrates and do NOT appear in the Morpheus® III screen or Morpheus III mixes.

*Some solutions in the vitamin and phytochemicals 1 classes may darken with age.