

Stock solutions of the MORPHEUS screens

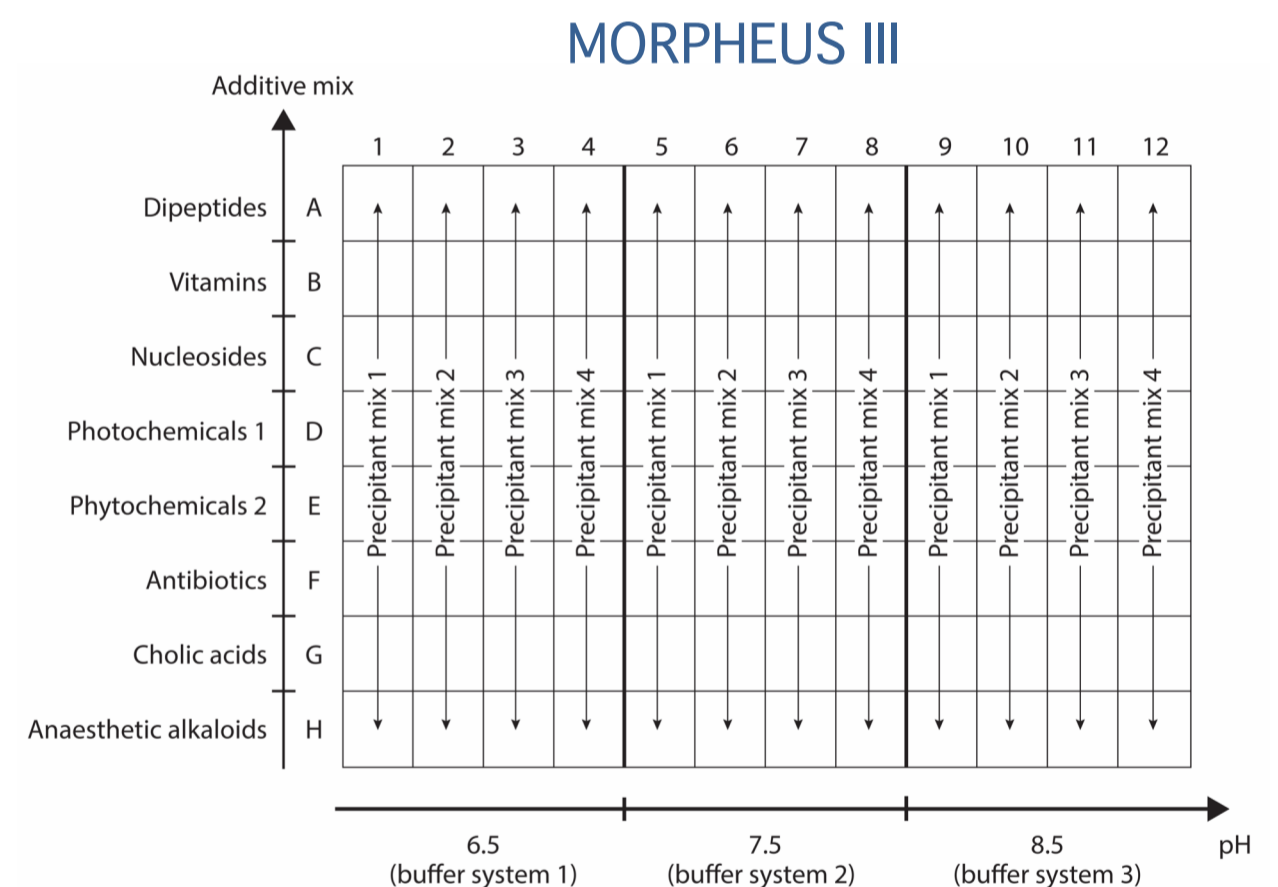
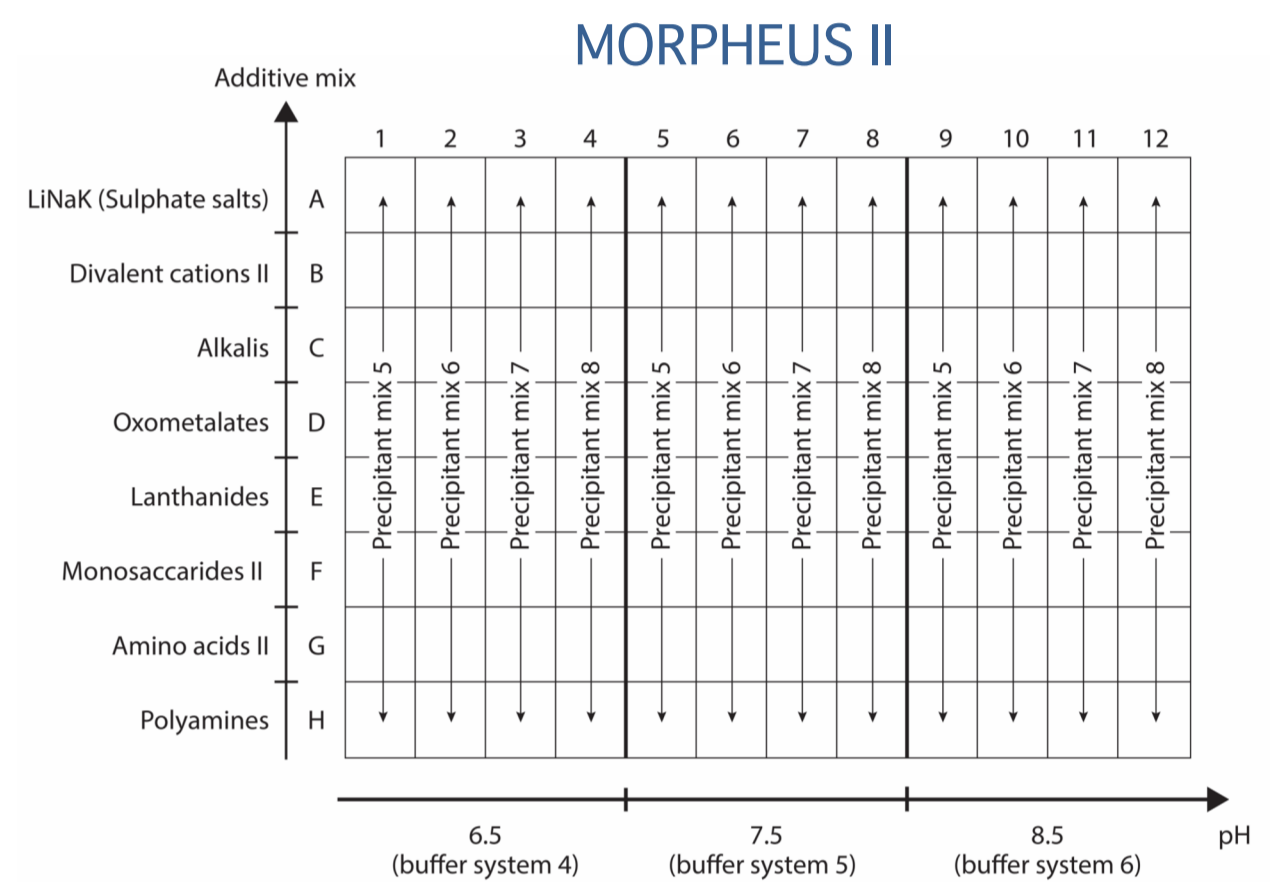
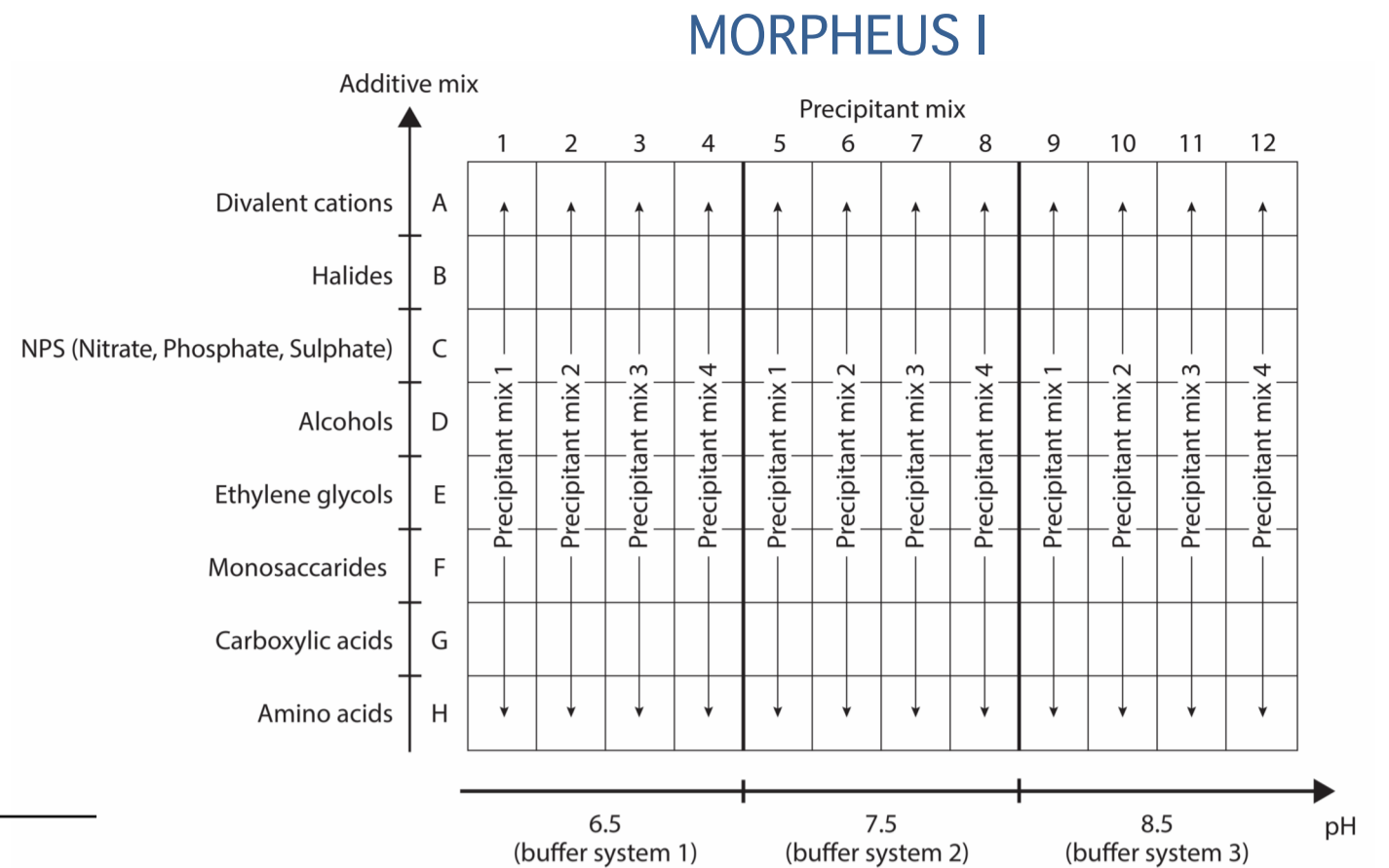
The screens: Three 96-condition initial screens (3-D grids)
+ Two additive screens (single reagents)

Screening Kit Name (and LMB name)	RT	4°C	-20°C	Catalogue Number (MDL)	Comments (reagents integrated)
MORPHEUS I ('LMB17')		✓		MD1-46 (tubes, 10 mL)	All reagents highly represented in the PDB
MORPHEUS II ('LMB20')	✓			MD1-91 (tubes, 10 mL)	Glycerol-like cryoprotectants and heavy-atoms
MORPHEUS III ('LMB22')		✓		MD1-116 (tubes, 10 mL)	Drug-like compounds as additives
MORPHEUS additive ('Addit01')			✓	MD1-93 (plate, 100 µL)	The 95 reagents found in MORPHEUS I & II
HIPPOCRATES ('Addit03')			✓	MD1-118 (plate, 100 µL)	The 44 (+3) additives found in MORPHEUS III

The 38 stock solutions (by alphabetical order)

Stock Name	Initial Screen	CN (100/250 mL)	Description
Alcohols	MORPHEUS I	MD2-100-73	Mix of 6 additives (conc. 0.2 M each)
Alkalis	MORPHEUS II	MD2-100-233	Mix of 4 additives (conc. 10 mM each)
Amino acids	MORPHEUS I	MD2-100-77	Mix of 5 additives (conc. 0.2 M each)
Amino acids II	MORPHEUS II	MD2-100-237	Mix of 5 additives (0.2 M each)
Anesthetic alkaloids	MORPHEUS III	MD2-100-320	Mix of 4 additives (conc. 2 %w/v each)
Antibiotics	MORPHEUS III	MD2-100-318	Mix of 6 additives (conc. 1 %w/v each)
Buffer system 1	MORPHEUS I & III	MD2-100-100	Two stocks: 1 M MES (acid, pKa 6.2) and 1 M imidazole (base, pKa 6.9)
Buffer system 2	MORPHEUS I & III	MD2-100-101	Two stocks: 1 M MOPS (acid, pKa 7.3) and 1 M Sodium-HEPES (base, pKa 7.6)
Buffer system 3	MORPHEUS I & III	MD2-100-102	Two stocks: 1 M bicine (acid, pKa 8.4) and 1 M Trizma-base (pKa 8.20)
Buffer system 4	MORPHEUS II	MD2-100-243	Two stocks: 1 M MOPSO (acid, pKa 6.9) and 1 M bis-tris (base, pKa 6.5)
Buffer system 5	MORPHEUS II	MD2-100-244	Two stocks: 1 M BES (acid, pKa 7.1) and 1 M TEA* (base, pKa 7.8)
Buffer system 6	MORPHEUS II	MD2-100-245	Two stocks: 1 M GlyGly (acid, pKa 8.2) and 1 M AMPD* (base, pKa 8.8)
Carboxylic acids	MORPHEUS I	MD2-100-76	Mix of 5 additives (conc. 0.2 M each)
Cholic acid derivatives	MORPHEUS III	MD2-100-319	Mix of 4 additives (conc. 3 %w/v each)
Dipeptides	MORPHEUS III	MD2-100-313	Mix of 8 additives (conc. 2 %w/v each)
Divalent cations II	MORPHEUS II	MD2-100-232	Mix of 4 additives (5 mM each)
Divalent cations	MORPHEUS I	MD2-100-70	Mix of 2 additives (conc. 0.3 M each)
Ethylene Glycols	MORPHEUS I	MD2-100-74	Mix of 4 additives (conc. 0.3 M each)
Halides	MORPHEUS I	MD2-100-71	Mix of 3 additives (conc. 0.3 M each)
Lanthanides	MORPHEUS II	MD2-100-235	Mix of 4 additives (5 mM each)
LiNaK	MORPHEUS II	MD2-100-231	Mix of 3 additives (SO4 salts, 0.3 M each)
Monosaccharides	MORPHEUS I	MD2-100-75	Mix of 6 additives (conc. 0.2 M each)
Monosaccharides II	MORPHEUS II	MD2-100-236	Mix of 5 additives (0.2 M each)
NPS	MORPHEUS I	MD2-100-72	Mix of 3 additives (NO3, PO4 and SO4, conc. 0.3 M each)
Nucleosides	MORPHEUS III	MD2-100-315	Mix of 5 additives (conc. 2 %w/v each)
Oxometalates	MORPHEUS II	MD2-100-234	Mix of 4 additives (5 mM each)
Phytochemicals 1	MORPHEUS III	MD2-100-316	Mix of 7 additives (conc. 0.5 %w/v each in 50 %v/v EtOH)
Phytochemicals 2	MORPHEUS III	MD2-100-317	Mix of 5 additives (conc. 0.5 %w/v each in 50 %v/v EtOH)
Polyamines	MORPHEUS II	MD2-100-238	Mix of 4 additives (powder: Add DW to reach 0.1 M each)
Precipitant mix 1	MORPHEUS I & III	MD2-250-81	Mix of 2 reagents (total conc. 60%, cryo: PEGMME500)
Precipitant mix 2	MORPHEUS I & III	MD2-250-82	Mix of 2 reagents (total conc. 60%, cryo: ethylene glycol)
Precipitant mix 3	MORPHEUS I & III	MD2-250-83	Mix of 2 reagents (total conc. 60%, cryo: glycerol)
Precipitant mix 4	MORPHEUS I & III	MD2-250-84	Mix of 3 reagents (total conc. 75%, cryo: MPD)
Precipitant mix 5	MORPHEUS II	MD2-250-239	Mix of 3 reagents (total conc. 72%, cryo: glycerol-like, NDSB256)
Precipitant mix 6	MORPHEUS II	MD2-250-240	Mix of 2 reagents (total conc. 65%, cryo: glycerol-like)
Precipitant mix 7	MORPHEUS II	MD2-250-241	Mix of 2 reagents (total conc. 60%, cryo: glycerol-like)
Precipitant mix 8	MORPHEUS II	MD2-250-242	Mix of 3 reagents (total conc. 62%, cryo: tris-like, NDSB195)
Vitamins	MORPHEUS III	MD2-100-314	Mix of 5 additives (conc. 3 %w/v each)

*AMPD: 2-amino-2-methyl-1,3-propanediol; TEA: triethanolamine



For every condition, a mix of additives, a mix of precipitants and a buffer system are combined using the following fixed ratio:

0.5 stock precipitants + 0.1 stock additives + 0.1 stock buffer system + 0.3 water

The 6 buffer systems: acid-to-base ratios for the corresponding pH range

System 1			System 2			System 3			System 4			System 5		System 6			
pH	MES	Imidazole	pH	MOPS	Na-HEPES	pH	Bicine	Trizma-base	pH	MOPSO	Bis-tris	pH	BES	TEA	pH	Glygly	AMPD
3.1	100	0	3.4	100	0	5.0	100	0	2.3	100	0	2.8	100	0	5.6	100	0
6.0	71	29	7.0	72	28	8.0	67	33	6.0	87	13	7.0	68	32	8.0	80	20
6.1	68	32	7.1	67	33	8.1	62	38	6.1	85	15	7.1	65	35	8.1	78	22
6.2	65	35	7.2	63	37	8.2	56	44	6.2	81	19	7.2	63	38	8.2	75	25
6.3	62	38	7.3	59	41	8.3	50	50	6.3	78	22	7.3	60	40	8.3	72	28
6.4	58	42	7.4	55	45	8.4	45	55	6.4	74	26	7.4	58	42	8.4	69	31
6.5	56	44	7.5	50	50	8.5	39	61	6.5	69	31	7.5	56	44	8.5	66	34
6.6	53	47	7.6	46	54	8.6	34	66	6.6	64	36	7.6	55	45	8.6	63	37
6.7	50	50	7.7	42	58	8.7	28	72	6.7	59	41	7.7	53	47	8.7	61	39
6.8	47	53	7.8	37	63	8.8	24	76	6.8	53	47	7.8	52	48	8.8	58	42
6.9	44	56	7.9	33	67	8.9	19	81	6.9	48	52	7.9	51	49	8.9	55	45
7.0	41	59	8.0	29	71	9.0	16	84	7.0	42	58	8.0	50	50	9.0	52	48
10.2	0	100	10.9	0	100	10.8	0	100	11.5	0	100	13.1	0	100	11.9	0	100