

## Supplemental table S1

<b>ROSETTA CODE</b>	<b>AMBER CODE</b>	<b>NAME</b>
A20	2AG	2-allyl-glycine
A33	AHP	2-amino-heptanoic acid
A44	IGL	2-indanyl-glycine_puck1
A45	IGL	2-indanyl-glycine
A48	MFO	2-methyl-phenylalanine
A69	TY2	3-amino-tyrosine
A84	TMB	3-methyl-biphenylalanine
ABA	ABA	2-Aminobutyric acid
APA	HOX	4-amino-phenylalanine
B21	D4P	4-hydroxy-phenylglycine
B27	4PH	4-methyl-phenylalanine
B30	BFA	Biphenylalanine
B31	TP4	4-tert-butyl-phenylalanine
B36	HRP	5-hydroxytryptophan
B38	TR6	6-methyl-tryptophan
B40	MTR	5-methyl-tryptophan
B44	ANT	3-(9-anthryl)-alanine
B47	IIL	allo-isoleucine
B53	DAB	diaminobutyric_acid
B57	RML	(R)-alpha-methylleucine
B58	MPH	(R)-alpha-methyl-phenylalanine
B67	ALN	1-naphthylalanine
B74	NAL	2-naphthylalanine
B96	DIF	3,3-diphenylalanine
B99	ALC	Cyclohexylalanine
C01	CP3	3-cyclopentylalanine
C04	VAH	Hydroxynorvaline
C20	ESC	Ethionine
C27	HPE	homophenylalanine
C30	HSE	homoserine
C36	OMW	1-methyltryptophan
C42	004	phenylglycine
C43	BB8	phenyl-serine
C55	BUG	t-butyl-leucine
F30	HSE	homoserine
mpa	4PH	4-methylphenylalanine
NLU	NLE	Norleucine
NVL	NVA	norvaline

Table S1. Rosetta–Amber non-canonical amino acid code conversion table