

DNA PARTITIONS INTO TRIPLETS UNDER TENSION IN THE PRESENCE OF ORGANIC CATIONS, WITH SEQUENCE EVOLUTIONARY AGE PREDICTING THE STABILITY OF THE TRIPLET PHASE

Amirhossein Taghavi, Paul van der Schoot, Joshua T. Berryman

(a) Protozanova *et al.*

Amino Acid	codon · anticodon	$\Delta G_{\tau} / k_B T$
T*	ACC·GGT	1.38
G†	GGT·ACC	1.38
S*	AGT·ACT	1.51
A†	GCC·GGC	1.56
I*	ATC·GAT	1.57
D†	GAT·ATC	1.57
V†	GTC·GAC	1.61
N.	AAT·ATT	1.63
R.	AGA·TCT	2.40
F.	TTC·GAA	2.55
E*	GAA·TTC	2.55
K.	AAA·TTT	2.61
P*	CCC·GGG	3.20
C.	TGT·ACA	3.32
L*	CTC·GAG	3.54
M.	ATG·CAT	4.45
H.	CAT·ATG	4.47
Y.	TAT·ATA	4.57
Q.	CAA·TTG	5.41

(b) Lemkul *et al.*

Amino Acid	codon · anticodon	$\Delta G_{\tau} / k_B T$
S*	AGT·ACT	1.30
T*	ACT·AGT	1.30
A†	GCT·AGC	1.46
D†	GAT·ATC	1.47
I*	ATC·GAT	1.47
R.	CGT·ACG	1.68
E*	GAG·CTC	1.82
L*	CTC·GAG	1.83
V†	GTC·GAC	1.90
N.	AAT·ATT	2.02
K.	AAG·CTT	2.38
Y.	TAT·ATA	3.09
F.	TTC·GAA	3.57
M.	ATG·CAT	3.93
H.	CAT·ATG	3.94
Q.	CAG·CTG	4.32
G†	GGT·ACC	4.81
P*	CCT·AGG	4.82
C.	TGT·ACA	4.96

(c) Protozanova *et al.*

		Base 3				
		T	C	A	G	
T	Base 1	F.	F.	L*	L*	T
		S*	S*	S*	S*	C
		Y.	Y.	X.	X.	A
		C.	C.	X.	Y.	G
C	Base 1	L*	L*	L*	L*	T
		P*	P*	P*	P*	C
		H.	H.	Q.	Q.	A
A	Base 1	R.	R.	R.	R.	G
		I*	I*	I*	M.	T
		T*	T*	T*	T*	C
		N.	N.	K.	K.	A
G	Base 1	S*	S*	R.	R.	G
		V†	V†	V†	V†	T
		A†	A†	A†	A†	C
		D†	D†	E*	E*	A
		G†	G†	G†	G†	G

(d) Lemkul *et al.*

		Base 3				
		T	C	A	G	
T	Base 1	F.	F.	L*	L*	T
		S*	S*	S*	S*	C
		Y.	Y.	X.	X.	A
		C.	C.	X.	Y.	G
C	Base 1	L*	L*	L*	L*	T
		P*	P*	P*	P*	C
		H.	H.	Q.	Q.	A
A	Base 1	R.	R.	R.	R.	G
		I*	I*	I*	M.	T
		T*	T*	T*	T*	C
		N.	N.	K.	K.	A
G	Base 1	S*	S*	R.	R.	G
		V†	V†	V†	V†	T
		A†	A†	A†	A†	C
		D†	D†	E*	E*	A
		G†	G†	G†	G†	G

Figure S1. Triplet formation free energies and triplet disproportionation propensity with Protozanova *et al.*(a,c) and Lemkul *et al.*(b,d) datasets.