

**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

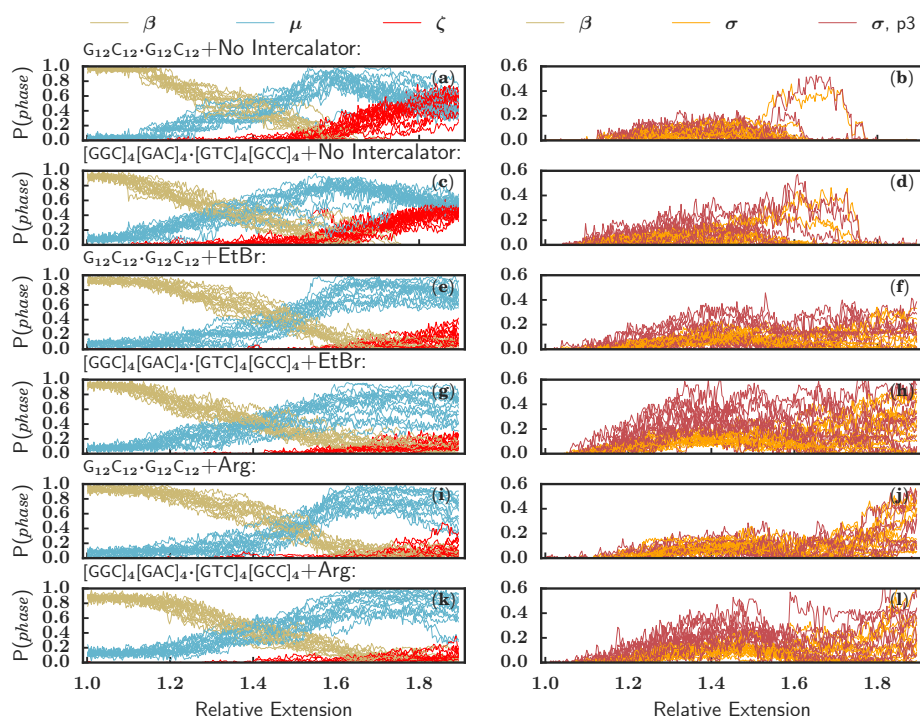
(c) Protozanova *et al.*

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

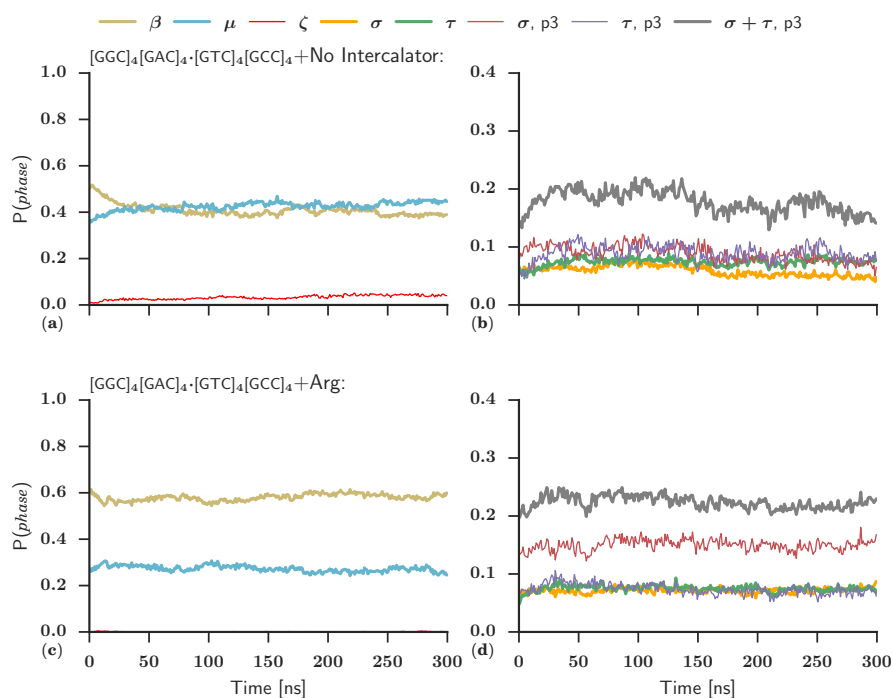
(d) Lemkul *et al.*

		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	Base 1	C.	C.	X.	Y.	G
		L*	L*	L*	L*	T
		P*	P*	P*	P*	C
A	Base 1	H.	H.	Q.	Q.	A
		R.	R.	R.	R.	G
		I*	I*	I*	M.	T
G	Base 1	T*	T*	T*	T*	C
		N.	N.	K.	K.	A
		S*	S*	R.	R.	G
G	Base 1	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.



**Figure S2.** Inter-run variation of the proportion of different local conformations of different phases. Trends are consistent between replicates up to extensions of  $>1.5$ , where (especially without intercalator) strong kinetic lock-in becomes evident.



**Figure S3.** Proportion of each classified conformation versus time, at constant extension of 1.45, averaged over 16 replicates and also smoothed over a 1ns window. The proportion of each conformation remained approximately constant over 300ns.