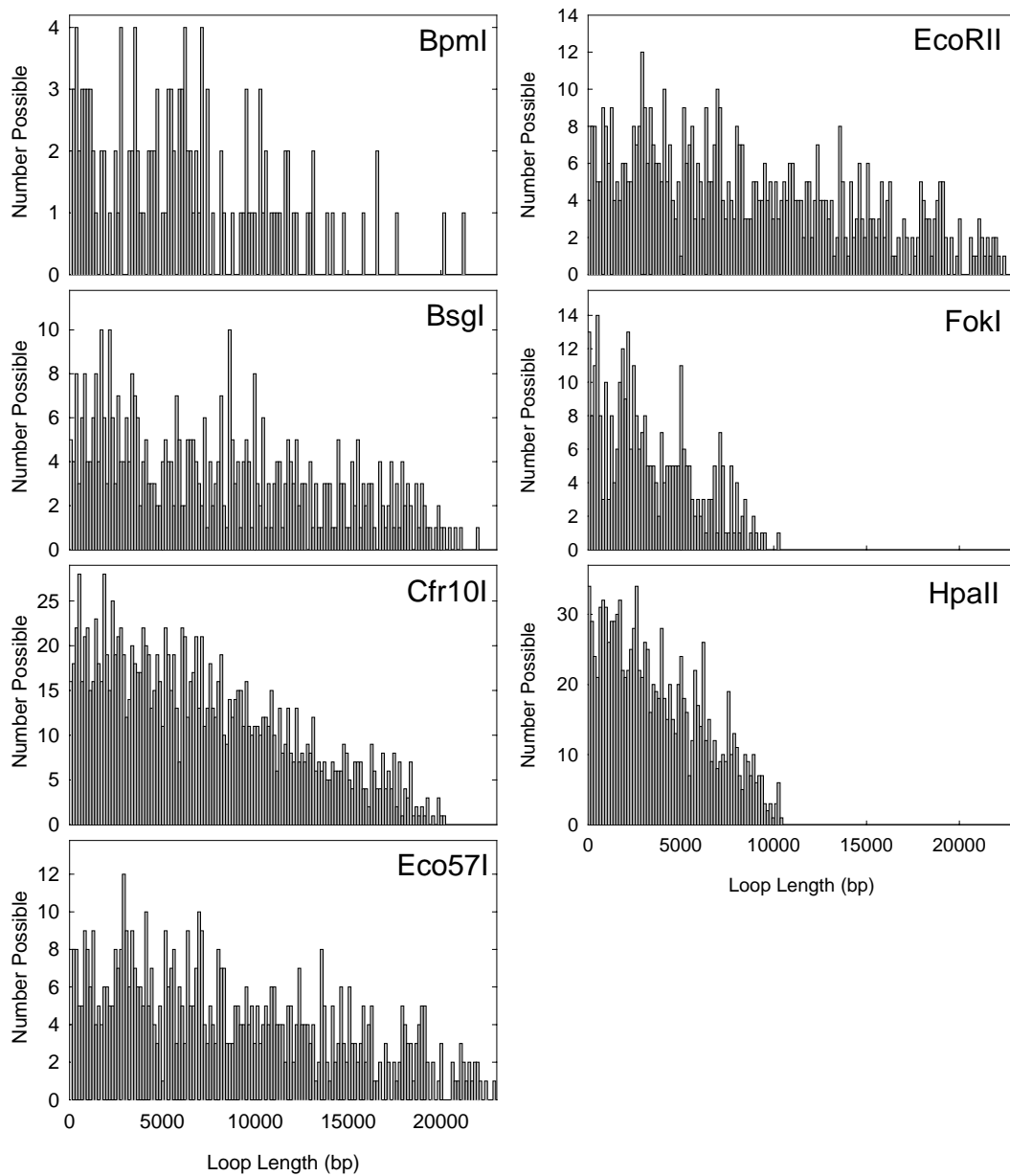


Supplemental Data for “DNA looping by two-site restriction endonucleases: Heterogeneous probability distributions for loop size and unbinding force”

Gregory J. Gemmen, Rachel Millin, Douglas E. Smith

Histograms of possible loop sizes that could be formed by different two-site enzymes computed by considering all possible distances between pairs of binding sites in the DNA template.



Supplemental Data for “DNA looping by two-site restriction endonucleases: Heterogeneous probability distributions for loop size and unbinding force”

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Comparison of the experimental length distributions with theoretical predictions. Theoretical curves (examples shown in Fig. 9) were scaled such that the area under the curve was equal to that under the normalized experimental distribution for each enzyme. In order to compare the shapes of the distributions the sum of the absolute values of the differences between the two distributions was calculated. Theories for which this sum was lowest were in closest agreement with the data. This process was carried out for all enzymes over several loop size ranges (chosen to allow comparison to the maximum number of theories and examination of both peak and tail of the distributions). We focused on comparing the shapes of the distributions as it was unclear how to relate j-factors calculated in theories to number of loops counted in our experiment. Some theoretical predictions reported in the literature were not included because they covered too limited a range for a meaningful comparison.

Model	Code	Code
Du <i>et al.</i> : 100 degree kink with 0.0005 probability	25	K2P1
Du <i>et al.</i> : 100 degree kink with 0.002 probability	"	K2P2
Du <i>et al.</i> : 70 degree kink with 0.0005 probability	"	K1P1
Du <i>et al.</i> : 70 degree kink with 0.002 probability	"	K1P2
Ringrose <i>et al.</i> : 0 nm contact distance	16	R0
Ringrose <i>et al.</i> : 10 nm contact distance	"	R10
Rippe: No curvature, 0 nm contact distance	17	C0R0
Rippe: No curvature, 10 nm contact distance	"	C0R10
Rippe: 120 degree curvature, 10 nm contact distance	"	C120R10
Rippe: 30 degree curvature, 10 nm contact distance	"	C30R10
Rippe: 60 degree curvature, 10 nm contact distance	"	C60R10
Rippe: 90 degree curvature, 10 nm contact distance	"	C90R10
Sankararaman and Marko: circle	19	CIRC
Sankararaman and Marko: 90 degree kink	"	KINK
Sankararaman and Marko: interacting loops, $\beta v=0$ and $\beta \epsilon=10$	18	MB10
Sankararaman and Marko: interacting loops, $\beta v=0$ and $\beta \epsilon=15$	"	MB15
Shimada-Yamakawa: teardrop (Sankararaman and Marko)	13, 19	TEAR
Yan <i>et al.</i> : antiparallel ends	21	AE
Yan <i>et al.</i> : free ends	"	FE
Yan <i>et al.</i> : hinge, $\mu=11$, kink, free ends	"	KHF
Yan <i>et al.</i> : hinge, $\mu=11$, antiparallel ends	"	M11A
Yan <i>et al.</i> : hinge, $\mu=11$, free ends	"	M11F
Yan <i>et al.</i> : hinge, $\mu=11$, parallel ends	"	M11P
Yan <i>et al.</i> : parallel ends	"	PE
Zhang and Crothers: cyclization of homogeneous DNA	67	ZC

Comparison Range: 0-700 bp

Bpml		Bsgl		BspMI		Cfr10I		Eco57I		EcoRII		FokI		HpaII		Sau3AI	
KINK	0.35	K2P2	0.93	MB15	0.56	KINK	0.91	K2P2	1.59	KINK	0.28	KINK	0.48	KINK	0.15	K2P2	0.49
K2P2	0.51	R10	1.07	K2P2	0.57	K2P2	1.38	KINK	2.02	K2P2	0.54	K2P2	0.61	K2P2	0.17	KINK	0.51
MB15	0.61	TEAR	1.13	R10	0.69	MB15	1.7	MB15	2.14	R10	0.62	R10	0.72	MB15	0.23	MB15	0.67
R10	0.63	FE	1.13	KINK	0.7	R10	1.74	R10	2.2	MB15	0.63	MB15	0.75	R10	0.23	R10	0.68
TEAR	0.7	K1P2	1.15	FE	0.75	FE	1.9	FE	2.42	TEAR	0.65	FE	0.77	TEAR	0.25	TEAR	0.77
FE	0.7	K2P1	1.16	TEAR	0.76	TEAR	1.94	TEAR	2.45	FE	0.65	TEAR	0.78	FE	0.25	FE	0.77
R0	0.71	MB15	1.17	R0	0.79	R0	1.98	R0	2.53	K2P1	0.66	R0	0.8	R0	0.26	R0	0.79
K2P1	0.73	R0	1.17	PE	0.82	PE	2.04	PE	2.6	K1P2	0.66	K2P1	0.82	K2P1	0.27	K2P1	0.83
K1P2	0.73	AE	1.21	K2P1	0.85	K2P1	2.05	K2P1	2.61	R0	0.66	K1P2	0.82	K1P2	0.27	K1P2	0.83
MB10	0.73	PE	1.22	K1P2	0.85	K1P2	2.05	K1P2	2.61	AE	0.67	PE	0.82	AE	0.27	PE	0.83
PE	0.74	MB10	1.23	AE	0.86	AE	2.09	AE	2.66	PE	0.67	AE	0.83	PE	0.27	AE	0.86
ZC	0.74	K1P1	1.24	MB10	0.87	MB10	2.13	MB10	2.7	K1P1	0.68	MB10	0.85	ZC	0.27	K1P1	0.87
AE	0.75	ZC	1.25	K1P1	0.88	K1P1	2.15	K1P1	2.74	CIRC	0.68	K1P1	0.86	K1P1	0.28	MB10	0.87
K1P1	0.76	CIRC	1.31	ZC	0.89	ZC	2.16	CIRC	2.79	MB10	0.68	CIRC	0.87	CIRC	0.28	ZC	0.88
CIRC	0.77	KINK	2.19	CIRC	0.91	CIRC	2.18	ZC	2.79	ZC	0.68	ZC	0.87	MB10	0.28	CIRC	0.9

Comparison Range: 0-1000 bp

Bpml		Bsgl		BspMI		Cfr10I		Eco57I		EcoRII		FokI		HpaII		Sau3AI	
KINK	0.66	MB15	1.45	MB15	0.67	KINK	1.28	MB15	2.22	KINK	0.37	KINK	0.53	KINK	0.16	KINK	0.61
R10	0.66	R10	1.5	R10	0.8	MB15	1.86	KINK	2.25	R10	0.64	MB15	0.79	MB15	0.23	MB15	0.69
TEAR	0.72	TEAR	1.62	KINK	0.85	R10	1.91	R10	2.46	TEAR	0.66	R10	0.79	R10	0.26	R10	0.78
FE	0.72	FE	1.65	TEAR	0.86	FE	2.03	FE	2.63	FE	0.66	FE	0.82	TEAR	0.28	TEAR	0.85
R0	0.73	R0	1.69	FE	0.86	TEAR	2.06	TEAR	2.64	R0	0.67	TEAR	0.84	FE	0.28	FE	0.85
MB10	0.74	MB10	1.74	R0	0.89	R0	2.1	R0	2.71	MB10	0.68	R0	0.85	R0	0.28	R0	0.86
PE	0.75	PE	1.83	PE	0.92	PE	2.15	PE	2.76	AE	0.68	PE	0.88	MB10	0.3	PE	0.9
AE	0.77	AE	1.89	MB10	0.94	AE	2.18	MB10	2.81	CIRC	0.69	MB10	0.89	PE	0.3	MB10	0.92
CIRC	0.78	CIRC	2.07	AE	0.95	MB10	2.2	AE	2.83	MB15	0.69	AE	0.9	AE	0.31	AE	0.94
MB15	0.83	KINK	2.73	CIRC	0.99	CIRC	2.25	CIRC	2.97	PE	0.7	CIRC	0.95	CIRC	0.32	CIRC	0.99

Comparison Range: 150-2000 bp

Bpml	Bsgl	BspMI	Cfr10I	Eco57I	EcoRII	FokI	HpaII	Sau3AI									
C30R10	0.29	C60R10	1.47	C60R10	0.52	C60R10	0.62	C120R10	0.96	C60R10	0.22	C120R10	0.25	C120R10	0.09	C120R10	0.24
R10	0.31	C30R10	1.48	MB15	0.55	C120R10	0.72	C90R10	0.98	C90R10	0.23	C90R10	0.25	C90R10	0.1	C90R10	0.25
C0R10	0.31	C0R10	1.61	C30R10	0.56	C90R10	0.73	C60R10	1.31	C120R10	0.24	C60R10	0.29	KINK	0.13	C60R10	0.33
C0R0	0.32	R10	1.75	C90R10	0.57	C30R10	1	KINK	1.64	C30R10	0.25	MB15	0.29	C60R10	0.14	MB15	0.46
TEAR	0.32	C0R0	1.81	C120R10	0.58	C0R10	1.13	C30R10	1.85	R10	0.26	KINK	0.37	MB15	0.15	C30R10	0.49
R0	0.33	TEAR	1.83	C0R10	0.6	R10	1.22	C0R10	2.04	C0R10	0.26	C30R10	0.41	C30R10	0.21	KINK	0.51
FE	0.33	FE	1.85	R10	0.63	C0R0	1.27	MB15	2.16	R0	0.27	C0R10	0.44	C0R10	0.23	C0R10	0.54
AE	0.35	R0	1.87	C0R0	0.65	TEAR	1.27	R10	2.2	C0R0	0.27	R10	0.47	R10	0.24	R10	0.58
PE	0.35	MB15	1.94	TEAR	0.65	FE	1.28	TEAR	2.24	TEAR	0.27	C0R0	0.48	R0	0.25	C0R0	0.6
CIRC	0.36	PE	1.95	FE	0.65	R0	1.3	C0R0	2.25	FE	0.27	TEAR	0.48	C0R0	0.25	TEAR	0.6
C60R10	0.4	AE	1.99	R0	0.66	MB15	1.33	FE	2.29	PE	0.27	FE	0.48	TEAR	0.25	FE	0.61
C90R10	0.73	C90R10	2.02	PE	0.67	PE	1.35	R0	2.31	CIRC	0.28	R0	0.49	FE	0.25	R0	0.62
C120R10	0.77	C120R10	2.05	AE	0.68	AE	1.38	PE	2.38	AE	0.28	PE	0.5	AE	0.26	PE	0.65
MB15	0.86	CIRC	2.13	CIRC	0.7	KINK	1.39	AE	2.43	KINK	0.33	AE	0.51	PE	0.26	AE	0.67
KINK	1.15	KINK	3.25	KINK	0.81	CIRC	1.46	CIRC	2.56	MB15	0.35	CIRC	0.53	CIRC	0.28	CIRC	0.7

Comparison Range: 150-600 bp

Bpml	Bsgl	BspMI	Cfr10I	Eco57I	EcoRII	FokI	HpaII	Sau3AI									
M11A	0.07	M11F	0.4	C30R10	0.26	C60R10	0.22	C120R10	0.46	C120R10	0.07	C60R10	0.1	C60R10	0.02	C60R10	0.07
K2P2	0.1	K2P2	0.47	C60R10	0.26	C120R10	0.39	C90R10	0.46	C90R10	0.07	M11A	0.13	C120R10	0.06	C120R10	0.12
C60R10	0.1	R10	0.47	MB15	0.26	C90R10	0.39	C60R10	0.64	C60R10	0.08	K2P2	0.16	C90R10	0.06	C90R10	0.12
R10	0.11	C30R10	0.49	K2P2	0.28	M11A	0.42	KINK	0.81	KINK	0.09	C120R10	0.16	M11A	0.07	K2P2	0.21
C30R10	0.11	M11A	0.49	C0R10	0.31	K2P2	0.56	KHF	0.83	K2P2	0.1	C90R10	0.16	KHF	0.08	C30R10	0.21
M11F	0.11	C0R10	0.5	R10	0.33	C30R10	0.58	M11A	1.2	KHF	0.1	C30R10	0.17	K2P2	0.09	M11A	0.22
C0R10	0.12	TEAR	0.51	C120R10	0.33	KHF	0.67	K2P2	1.21	M11A	0.1	C0R10	0.2	C30R10	0.1	MB15	0.26
R0	0.14	FE	0.52	C90R10	0.33	KINK	0.69	C30R10	1.24	C0R10	0.11	M11F	0.2	KINK	0.1	C0R10	0.27
C0R0	0.14	K1P2	0.53	M11A	0.33	M11F	0.72	C0R10	1.46	C30R10	0.11	R10	0.21	M11F	0.12	KINK	0.27
TEAR	0.14	K2P1	0.54	M11F	0.33	C0R10	0.73	M11F	1.48	M11F	0.11	MB15	0.21	R10	0.13	KHF	0.28
FE	0.14	C0R0	0.54	FE	0.37	R10	0.77	MB15	1.5	R10	0.12	FE	0.23	C0R10	0.13	R10	0.29
K2P1	0.15	R0	0.55	C0R0	0.38	MB15	0.77	R10	1.52	MB15	0.12	C0R0	0.24	MB15	0.14	M11F	0.29
K1P2	0.15	AE	0.57	TEAR	0.38	FE	0.87	FE	1.68	TEAR	0.12	TEAR	0.24	FE	0.15	C0R0	0.34
MB15	0.15	PE	0.58	R0	0.39	C0R0	0.9	TEAR	1.7	FE	0.12	R0	0.25	C0R0	0.16	TEAR	0.35
C120R10	0.16	K1P1	0.6	PE	0.42	TEAR	0.9	C0R0	1.71	K2P1	0.13	KINK	0.25	TEAR	0.16	FE	0.35
C90R10	0.16	MB10	0.6	KHF	0.43	R0	0.93	R0	1.76	K1P2	0.13	KHF	0.25	K2P1	0.17	R0	0.36
MB10	0.16	MB15	0.63	K1P2	0.44	PE	0.97	PE	1.82	R0	0.13	PE	0.27	K1P2	0.17	K1P2	0.39
PE	0.16	CIRC	0.64	KINK	0.44	K2P1	0.98	K1P2	1.84	C0R0	0.13	K2P1	0.28	R0	0.17	PE	0.39
ZC	0.16	M11P	0.65	K2P1	0.45	K1P2	0.98	K2P1	1.86	AE	0.13	K1P2	0.28	PE	0.17	K2P1	0.4
K1P1	0.17	ZC	0.65	AE	0.45	AE	1	AE	1.88	PE	0.13	AE	0.28	K1P1	0.18	AE	0.41
CIRC	0.17	C60R10	0.75	K1P1	0.47	MB10	1.03	MB10	1.94	K1P1	0.14	MB10	0.29	MB10	0.18	K1P1	0.42
AE	0.17	C120R10	1.29	MB10	0.47	K1P1	1.05	K1P1	1.95	CIRC	0.14	K1P1	0.3	AE	0.18	MB10	0.42
M11P	0.18	C90R10	1.29	ZC	0.48	CIRC	1.06	CIRC	1.98	MB10	0.14	CIRC	0.31	CIRC	0.19	CIRC	0.44
KINK	0.2	KHF	1.66	CIRC	0.49	M11P	1.06	M11P	1.98	M11P	0.14	M11P	0.31	M11P	0.19	ZC	0.44
KHF	0.24	KINK	1.73	M11P	0.49	ZC	1.08	ZC	2.02	ZC	0.14	ZC	0.31	ZC	0.19	M11P	0.45