Published online *Nucleic Acids Research, , Vol. , No.* ***1–3***
doi:10.1093/nar/gkn000

Properties of Gene Expression and Chromatin Structure with Mechanically Regulated Elongation (Supplementary Material)

Stuart A. Sevier [1,3*], Herbert Levine [2,3*]

[1]Department of Physics and Astronomy, Houston, TX 77005, U.S.A. and [2]Department of Bioengineering, Houston, TX 77005, U.S.A. and [3]Center for Theoretical Biological Physics, Rice University, Houston, TX 77005, U.S.A.

SUPPLEMENTARY MATERIAL

Boundary Conditions

In the framework constructed in the RNACs at the ends of genes interact with the closest RNACs on neighboring genes to result in a complete set of LNCs ϕ_i^n for all RNACs at positions $Z_i^{(n)}$. These of course assume that there is at least one RNAC at the neighboring gene; if not we just skip genes until the next RNAC is found.For this to work we must have conditions for all possible gene configurations. We will label genes with positive $+$ and the opposition genes $-$. Thus for any given gene there are 8 possible orientations given neighbors on each side $(\pm,\pm,\pm)$. Explicitly We have

(+,+,+)

$$\begin{aligned} Z_0^{(n)} &\equiv Z_{M_n}^{(n+1)} \quad \phi_0^{(n)} \equiv \phi_{M_n}^{(n+1)} \\ Z_{M_n+1}^{(n)} &\equiv Z_1^{(n-1)} \quad \phi_{M_n+1}^{(n)} \equiv \phi_1^{(n-1)} \end{aligned} \tag{1}$$

(+,+,-)

$$\begin{aligned} Z_0^{(n)} &\equiv Z_1^{(n+1)} \quad \phi_0^{(n)} \equiv \phi_1^{(n+1)} \\ Z_{M_n+1}^{(n)} &\equiv Z_1^{(n-1)} \quad \phi_{M_n+1}^{(n)} \equiv \phi_1^{(n-1)} \end{aligned} \tag{2}$$

(-,+,+)

$$\begin{aligned} Z_0^{(n)} &\equiv Z_{M_n}^{(n+1)} \quad \phi_0^{(n)} \equiv \phi_{M_n}^{(n+1)} \\ Z_{M_n+1}^{(n)} &\equiv Z_{M_n}^{(n-1)} \quad \phi_{M_n+1}^{(n)} \equiv \phi_{M_n}^{(n-1)} \end{aligned} \tag{3}$$

(-,+,-)

$$\begin{aligned} Z_0^{(n)} &\equiv Z_1^{(n+1)} \quad \phi_0^{(n)} \equiv \phi_1^{(n+1)} \\ Z_{M_n+1}^{(n)} &\equiv Z_{M_n}^{(n-1)} \quad \phi_{M_n+1}^{(n)} \equiv \phi_{M_n}^{(n-1)} \end{aligned} \tag{4}$$

(+,-,+)

$$\begin{aligned} Z_{M_n+1}^{(n)} &\equiv Z_{M_n}^{(n+1)} \quad \phi_{M_n+1}^{(n)} \equiv \phi_{M_n}^{(n+1)} \\ Z_0^{(n)} &\equiv Z_1^{(n-1)} \quad \phi_0^{(n)} \equiv \phi_1^{(n-1)} \end{aligned} \tag{5}$$

(+,-,-)

$$\begin{aligned} Z_{M_n+1}^{(n)} &\equiv Z_1^{(n+1)} \quad \phi_{M_n+1}^{(n)} \equiv \phi_1^{(n+1)} \\ Z_0^{(n)} &\equiv Z_1^{(n-1)} \quad \phi_0^{(n)} \equiv \phi_1^{(n-1)} \end{aligned} \tag{6}$$

(-,-,+)

$$\begin{aligned} Z_{M_n+1}^{(n)} &\equiv Z_{M_n}^{(n+1)} \quad \phi_{M_n+1}^{(n)} \equiv \phi_{M_n}^{(n+1)} \\ Z_0^{(n)} &\equiv Z_{M_n}^{(n-1)} \quad \phi_0^{(n)} \equiv \phi_{M_n}^{(n-1)} \end{aligned} \tag{7}$$

(-,-,-)

$$\begin{aligned} Z_{M_n+1}^{(n)} &\equiv Z_1^{(n+1)} \quad \phi_{M_n+1}^{(n)} \equiv \phi_1^{(n+1)} \\ Z_0^{(n)} &\equiv Z_{M_n}^{(n-1)} \quad \phi_0^{(n)} \equiv \phi_{M_n}^{(n-1)} \end{aligned} \tag{8}$$

If the left or right side of the gene contains no additional genes the boundary conditions are set to have either free (torsionally unconstrained) motion by adding an additional LNC matching the end RNACs LNC or fixed (torsionally constrained) motion by an additional static LNC.

Correlation Function

The correlation function shown in main text fig. 8 was calculated using the mRNA content in time of the left $m_L(t)$ and right genes $m_R(t)$ with different orientations using the formula

$$C(\tau) = \overline{m_L(t) \cdot m_R(t+\tau)} - \overline{m_L} \cdot \overline{m_R} \tag{9}$$

*To whom correspondence should be addressed. Email: s.a.sevier@rice.edu

Model Parameters

The model presented introduced a number of parameters. Below is a table summarizing these parameters and the values used to generate the results (unless otherwise noted).

The model contains a number intrinsic parameters dictating the mechanical properties of the RNAP motion. These include well studied mechanical parameters of the RNAP motion (1) as well as unknown parameters of the mRNA drag. Additionally stochastic rates for RNAP initiation, mRNA degradation and DNA relaxation were used. Order of magnitude regimes for initiation and degradation are well established (2) however DNA relaxation rates in the manner used in the model is less constrained.

The model's response to changes in both the mechanical and stochastic parameters are examined in figures 6 and 7 of the main text and S3 of the S.M. Additional theoretical and experimental work is needed to further constrain the parameters, however the qualitative results of the model are robust against changing parameters values.

Symbol	Parameter	Values
η	mRNA drag coefficient	1/20 $pNnm^{\alpha-1}$
α	mRNA drag scaling exponent	1
χ	DNA twisting mobility	10 $spNnm$
δ	hard-core RNAP repulsion distance	15 nm
v	RNAP velocity	20 nm/s
τ_c	RNAP torque cutoff	12 $pNnm$
f	DNA force	1 pN
r	RNAP initiation rate	1/2 min^{-1}
g	DNA super-coiling relaxation rate	1/20 min^{-1}
λ	mRNA degradation rate	1/20 min^{-1}

REFERENCES

1. Jie Ma, Lu Bai, and Michelle D Wang. Transcription under torsion. *Science (New York, N.Y.)*, 340(6140):1580–3, 2013.
2. R. B. Phillips, J. Kondev, J. Theriot, N. Orme, and H. Garcia. *Physical biology of the cell*. Garland Science, 2009.

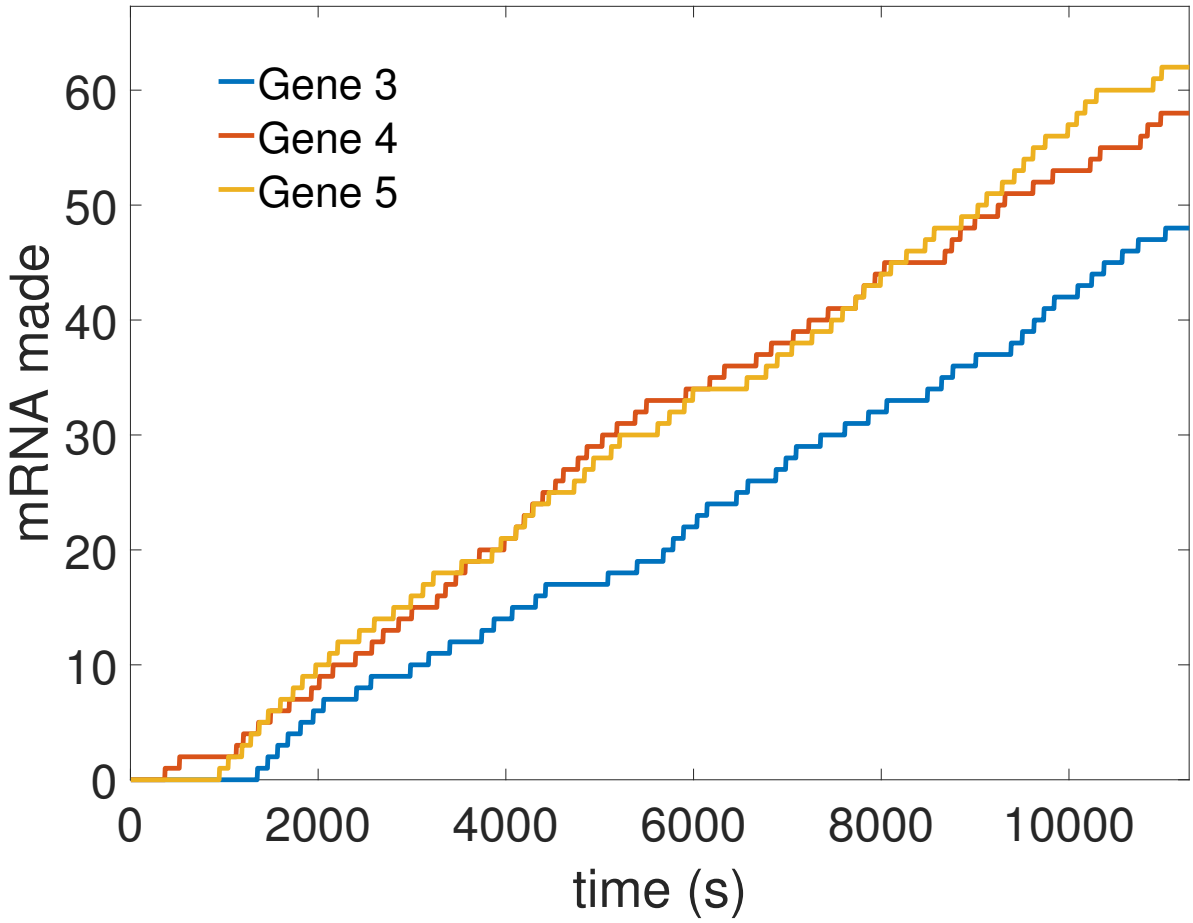

Figure S2. Bursts in production of mRNA shown for three of the genes of the system shown in main text fig.9

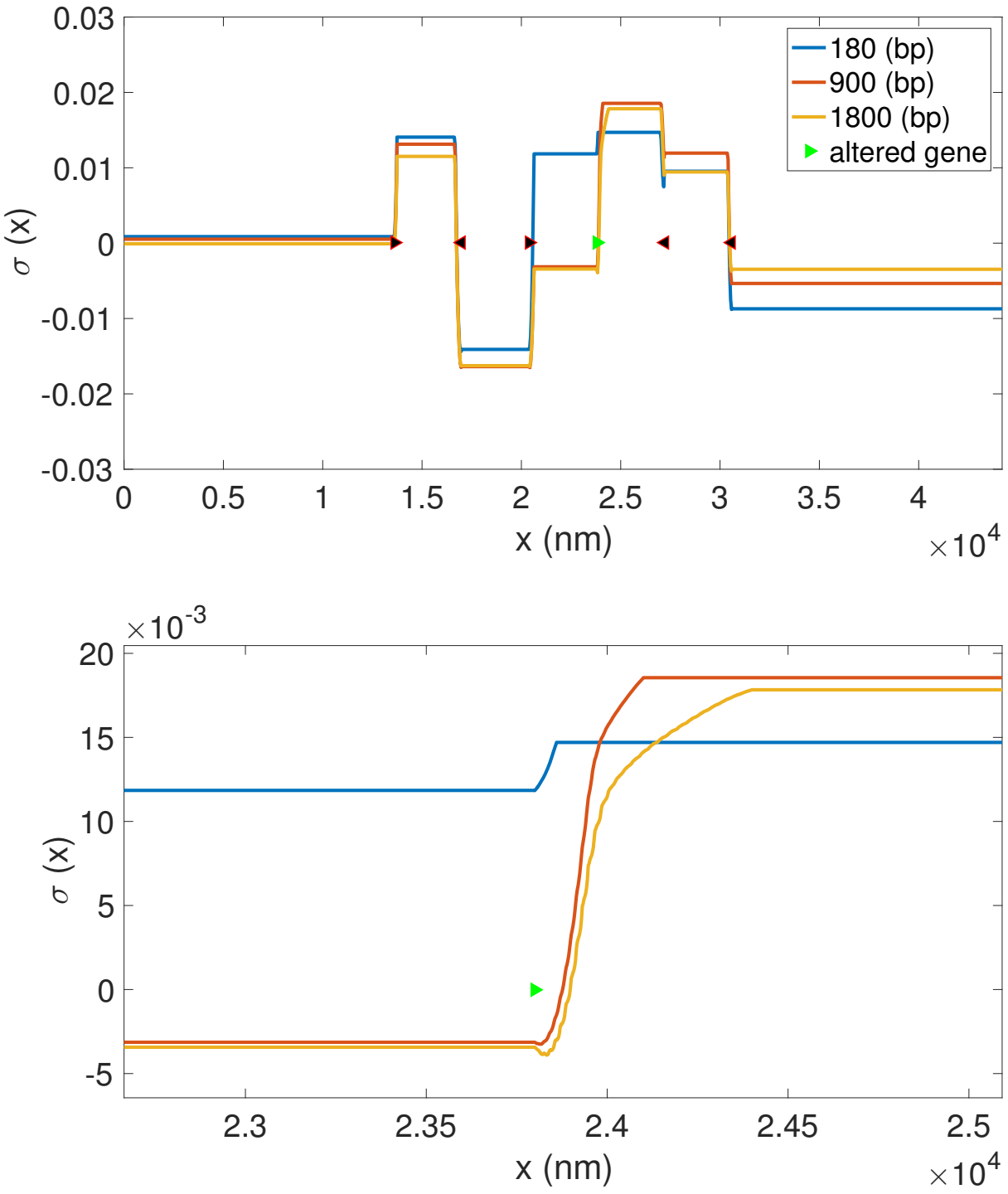

Figure S1. The geometric and compositional structure of the multi-gene system shown in fig.9A (with compositional details in fig.S4) determines the SC structure of a region of DNA (see fig.9B). Changing the length of a particular gene leads to SC structure rearrangement and thus DNA conformational changes. This can be see by changing the length of one particular gene in a multi-gene system at the system level (A) and in detail over the changed region in (B).

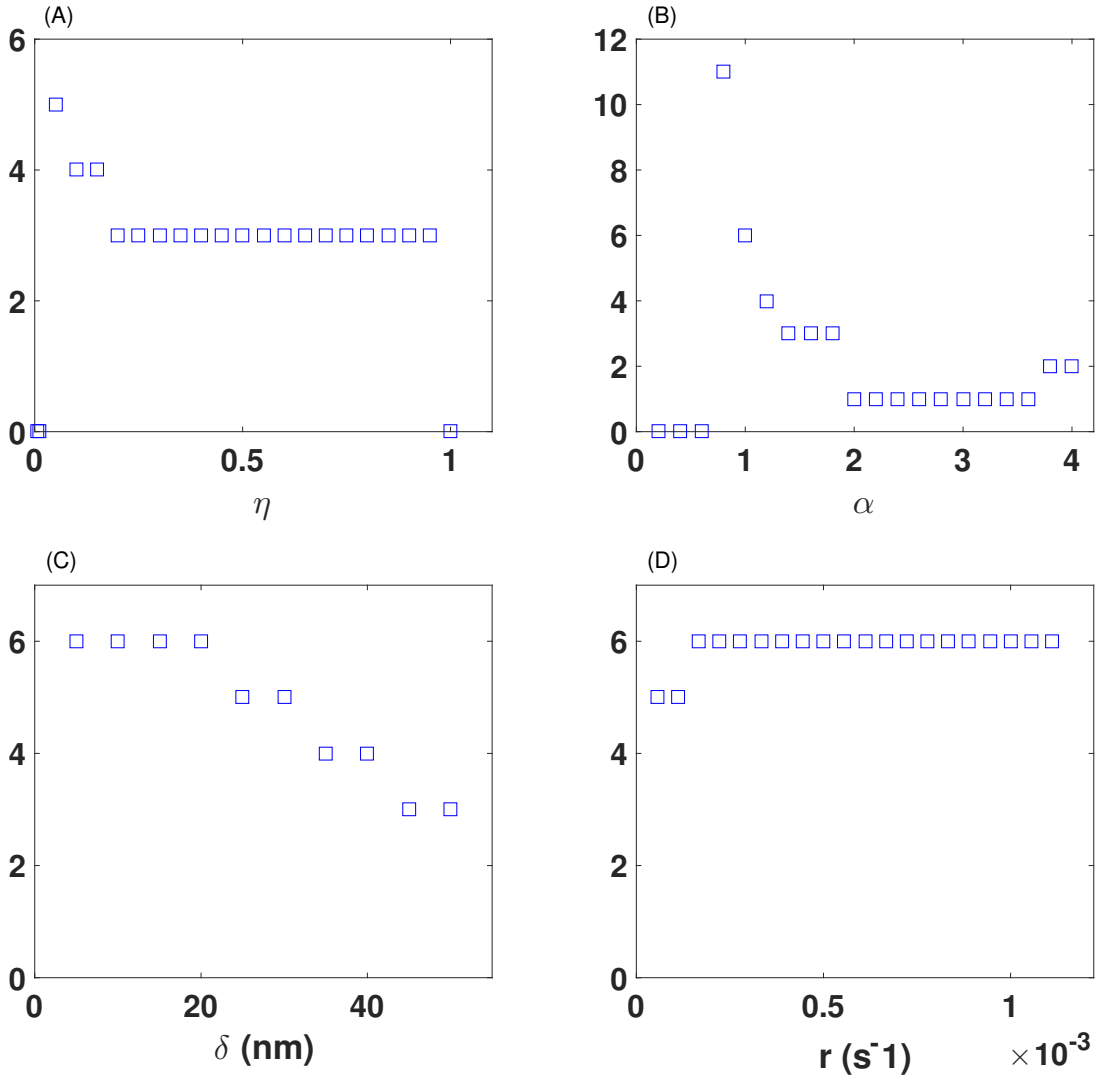

Figure S3. Burst size m_c dependence on drag coefficient η,drag exponent α, RNAC spacing δ, and initiation rate r for an isolated gene with mechanically interacting RNAP. Gene and barrier lengths are 1kbp and 10 kbp respectively. Unless being varied the simulation parameters $\{r,\lambda,g\}=\{2^{-1},1/20,1/20(min^{-1})\}$ were used. The mechanical parameters are $\{v_0,\eta,\alpha,\chi,f\}=\{20,1/20,1,10,1\}$

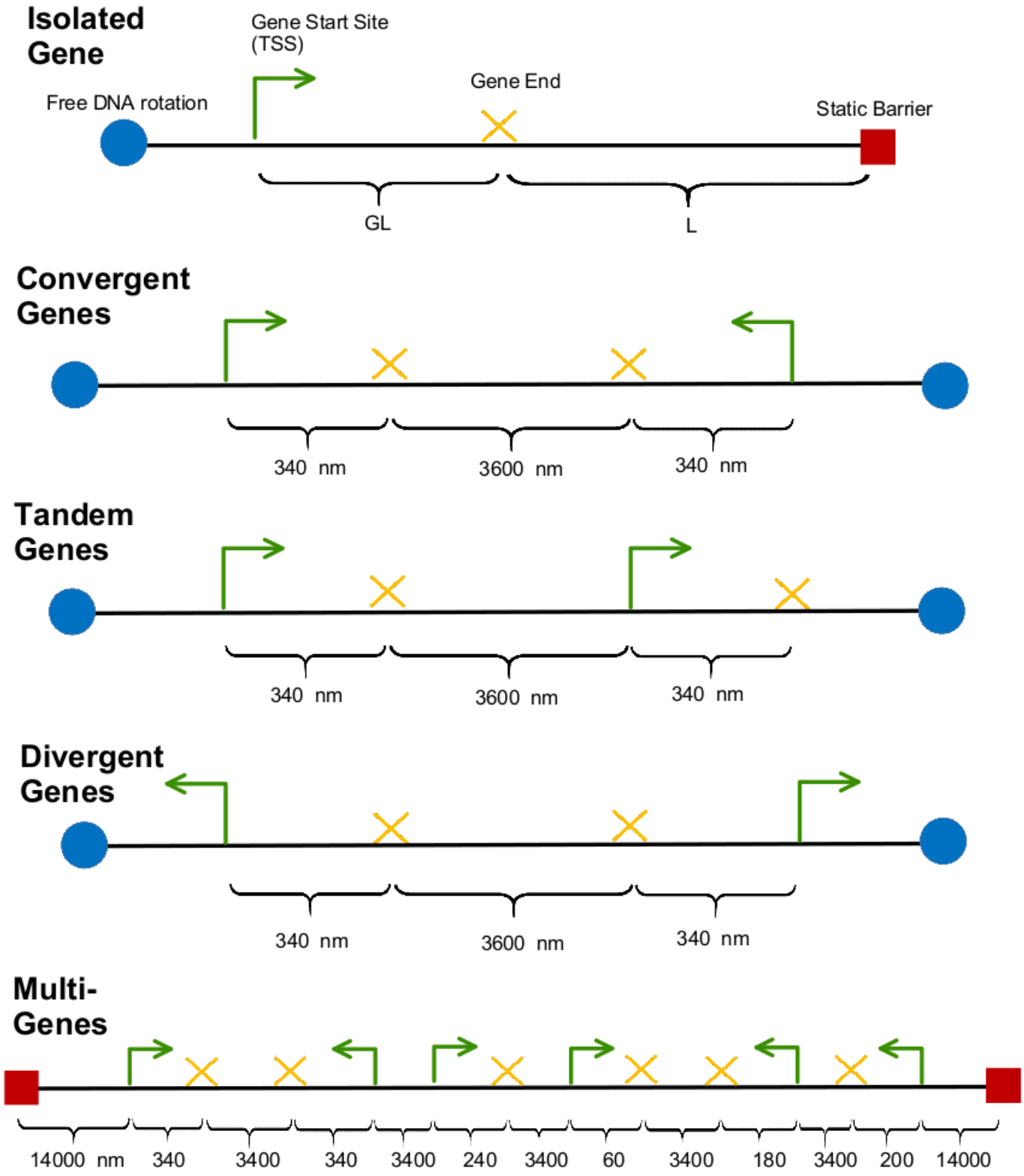

Figure S4. Compositional details for genetic systems used in simulations.