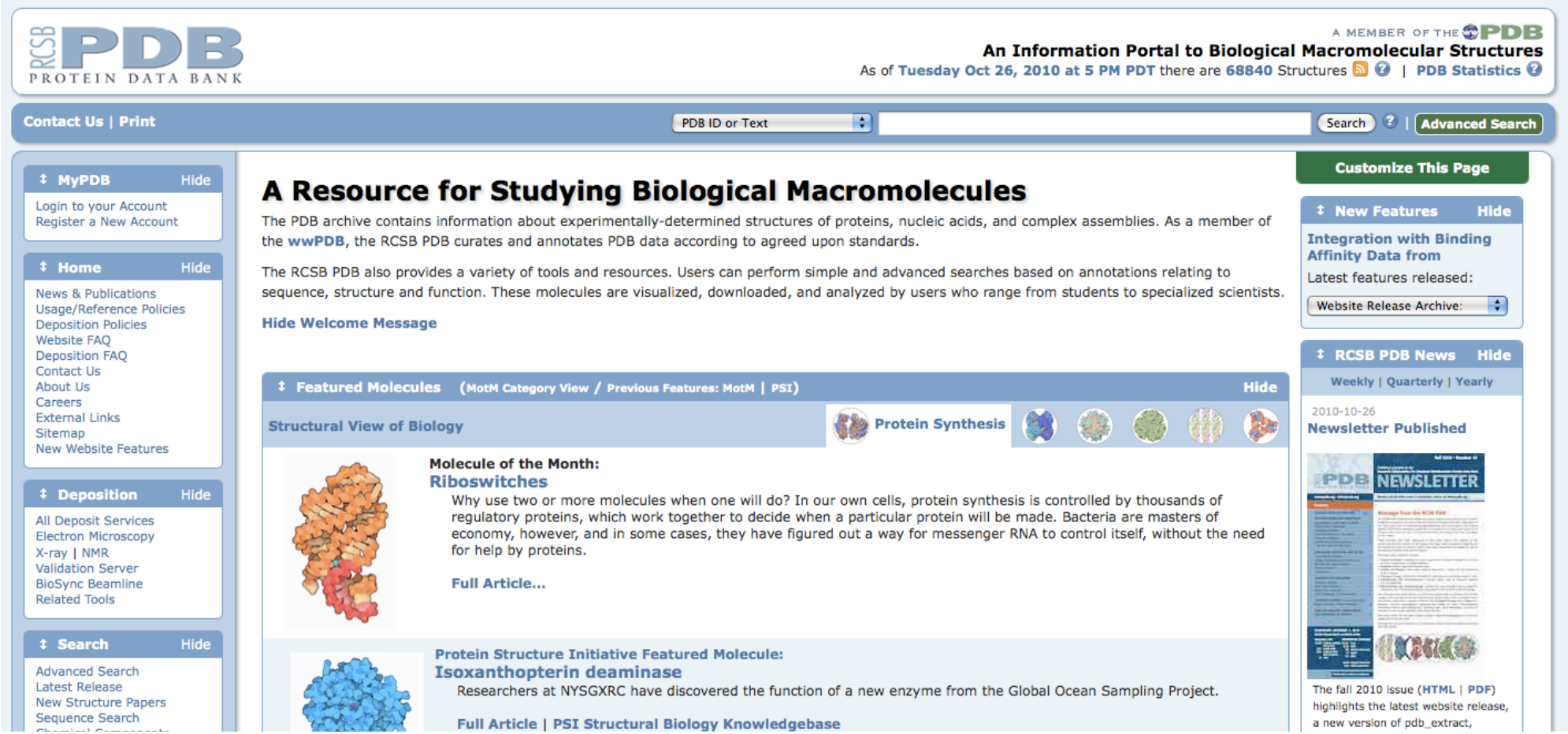
2010-10-27

MACROMOLECULES AS RANDOM WALKS

Ref.: Phys. Biol. Of the Cell

Macromolecular Structure



http://www.rcsb.org/pdb/home/

Multimolecular Structure

VIPERdb

Main | Data | Utilities | Links | Help | Contact Us | Find a Virus

Virus Particle ExploreR 2

X-RAY Entries | Cryo-EM Models | Enter PDBID

Close this Introduction and start using VIPERdb²

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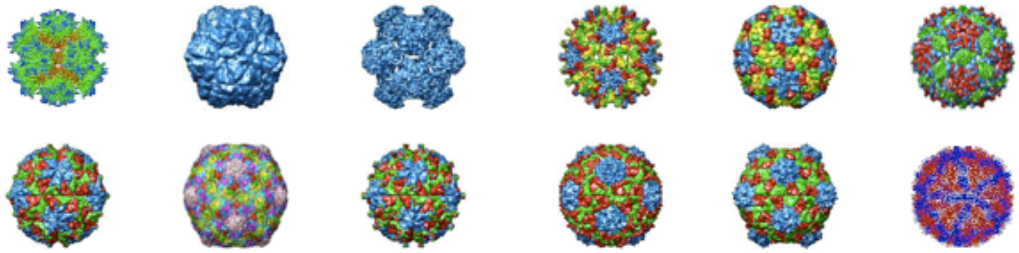
WELCOME

VIPERdb is a database for icosahedral virus capsid structures . The emphasis of the resource is on providing data from structural and computational analyses on these systems, as well as high quality renderings for visual exploration. In addition, all virus capsids are placed in a single icosahedral orientation convention, facilitating comparison between different structures. The web site includes powerful search utilities , links to other relevant databases, background information on virus capsid structure, and useful database interface tools.

You have different options on how to start using VIPERdb. You can jump to any section in the site using the Top Menu. If you are looking for a specific entry, you can look for it on the X-Ray or Cryo-EM drop-down lists on the top, or type its PDB-ID in the correspondig field above. If you are not sure, you can access the Search Page here and look for it by Name. All virus entries are grouped into Families , you can see a list here with links to all their members.

All database information (from 289 viruses) is accessed through the Info Page, which shows all pertinent data using different database interfaces (Biodata, 3D Structure, 2D Φ-Ψ Maps) for each individually selected entry.

If you are new to VIPERdb, you can get familiar with the site by accessing the Info Page for some of the most popular spherical viruses. Here is just a small sample (click images to open corresponding Info Page):



Visitor locations — ClustrMaps — Click to see

1 online

MMTSB

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http://viperdb.scripps.edu/

Structure

Molecule of N atoms

For the i-th atom

$\mathbf{r}_i = (x_i, y_i, z_i)$

No dynamics

Alternative view: Statistical description of structure
Avg. shape
Avg. size

Random Walk Model of a Polymer

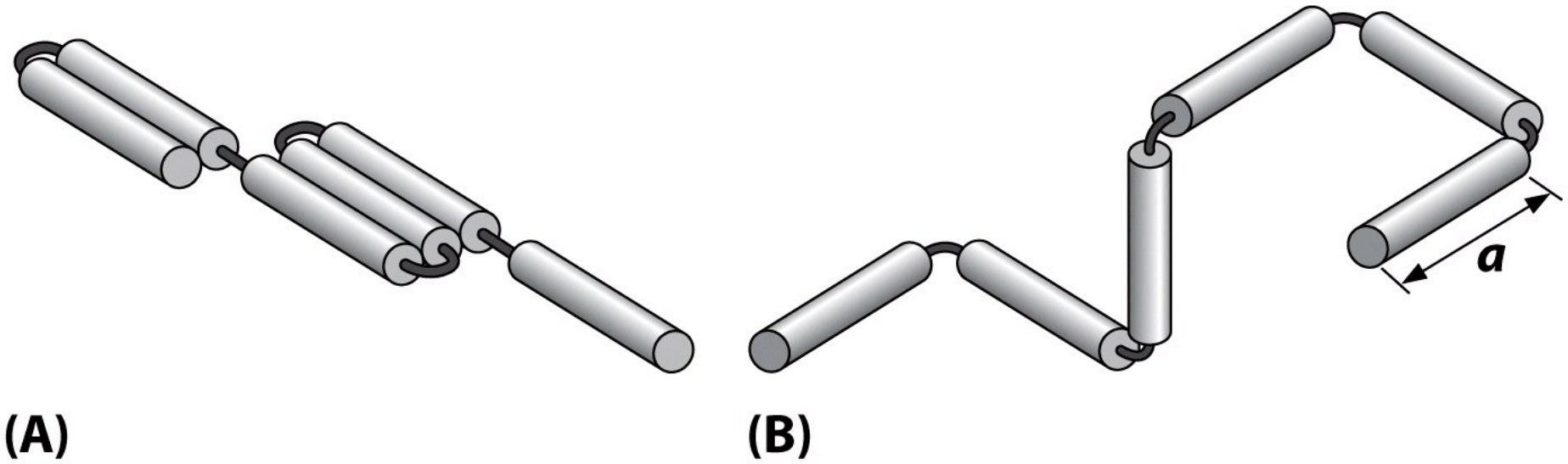
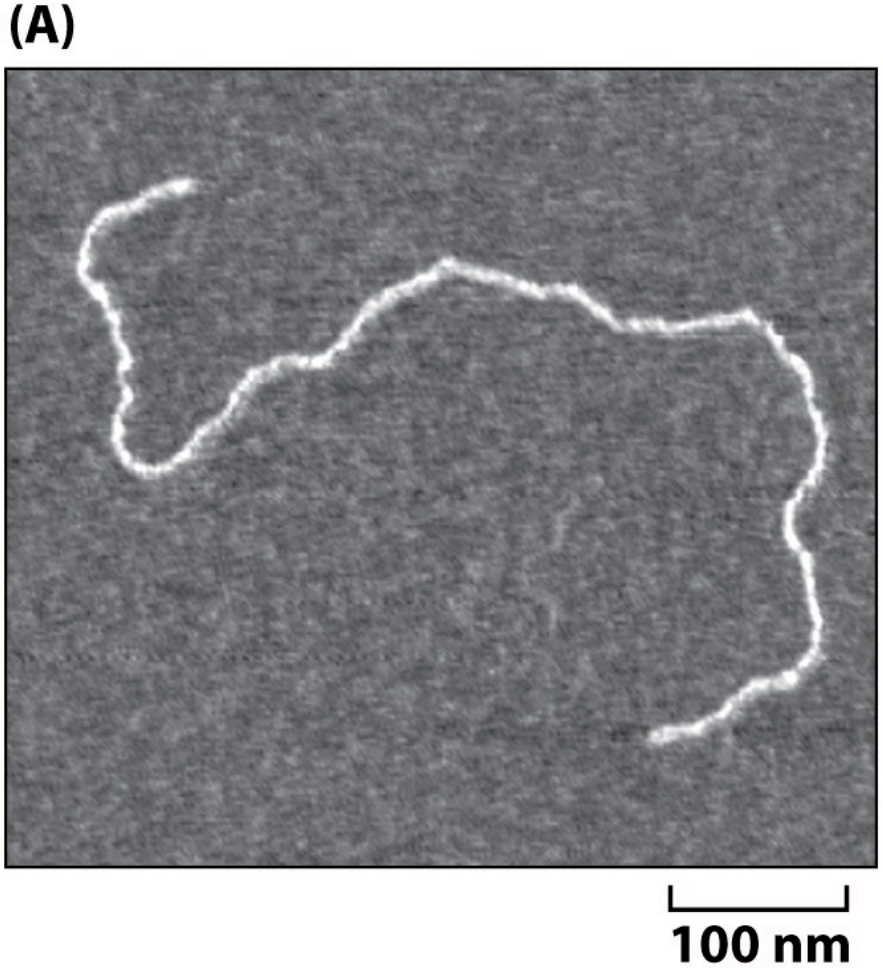


Figure 8.1 Physical Biology of the Cell (© Garland Science 2009)

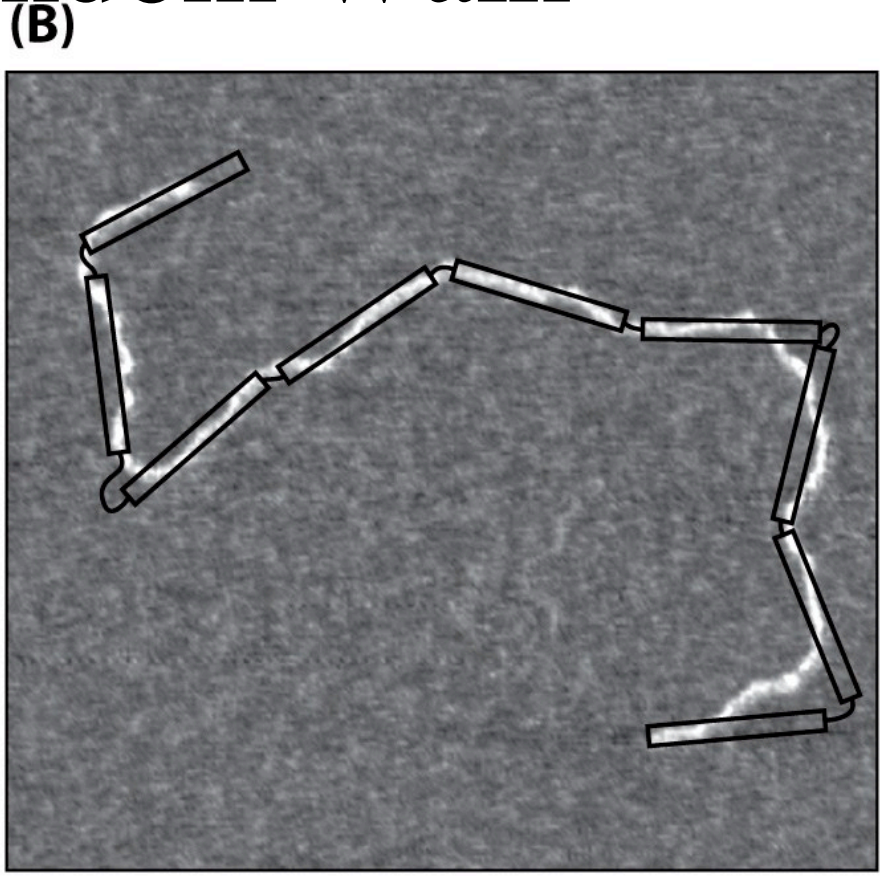
a = segment length

Kuhn Segments: rigid rods
Flexible hinges

DNA as a Random Walk



AFM image of DNA on a surface in air



Fitted segments for the DNA molecule

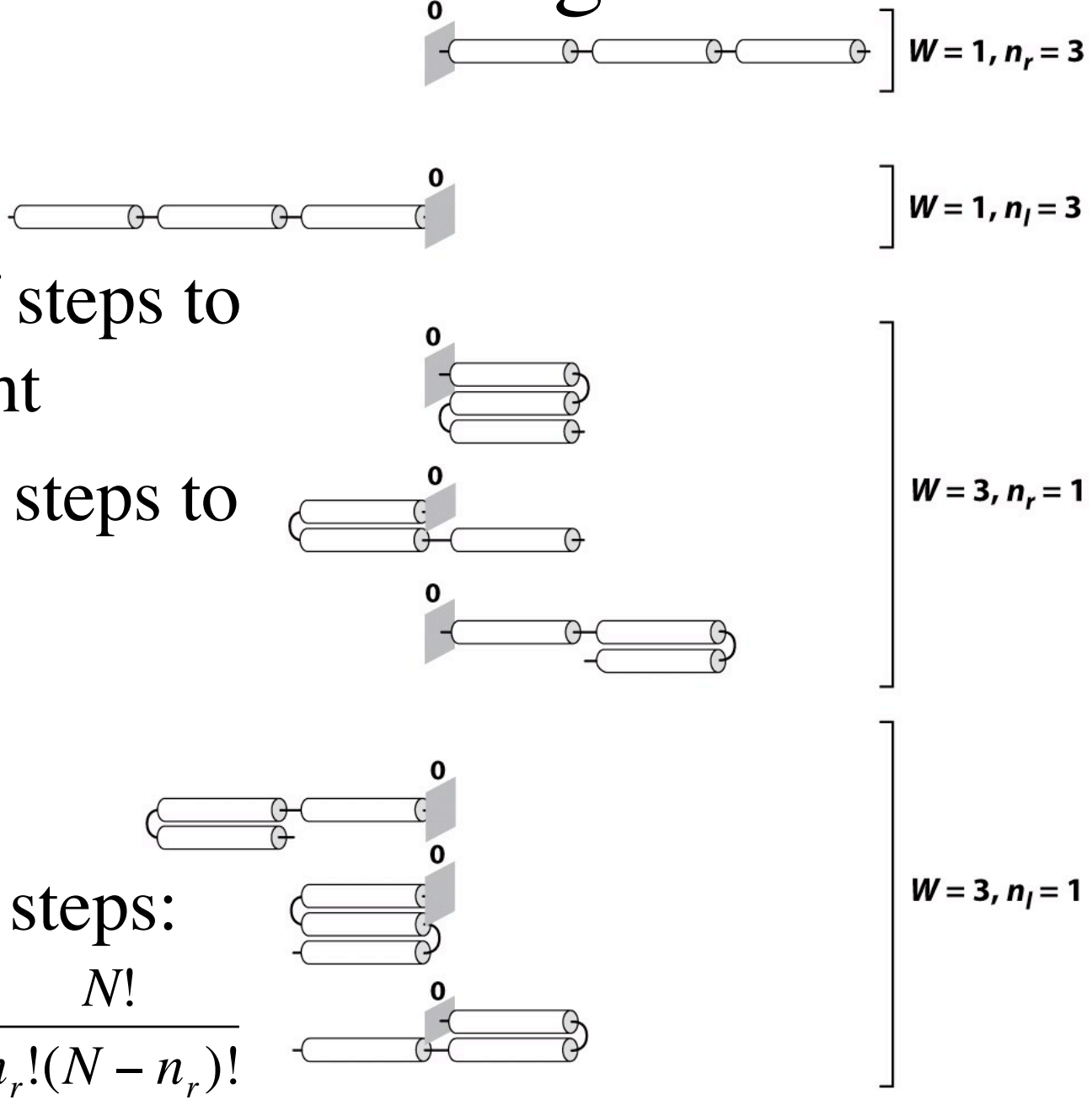
Random Walk Size

Mean distance of walker $\langle R \rangle$

Variance of walk $\langle R^2 \rangle$

Relation of variance $\langle R^2 \rangle$ with segment length (a) and number of steps (N)

RW Configurations



n_r=no. of steps to the right

n_l=no. of steps to the left

p_r

P_l

For right steps:

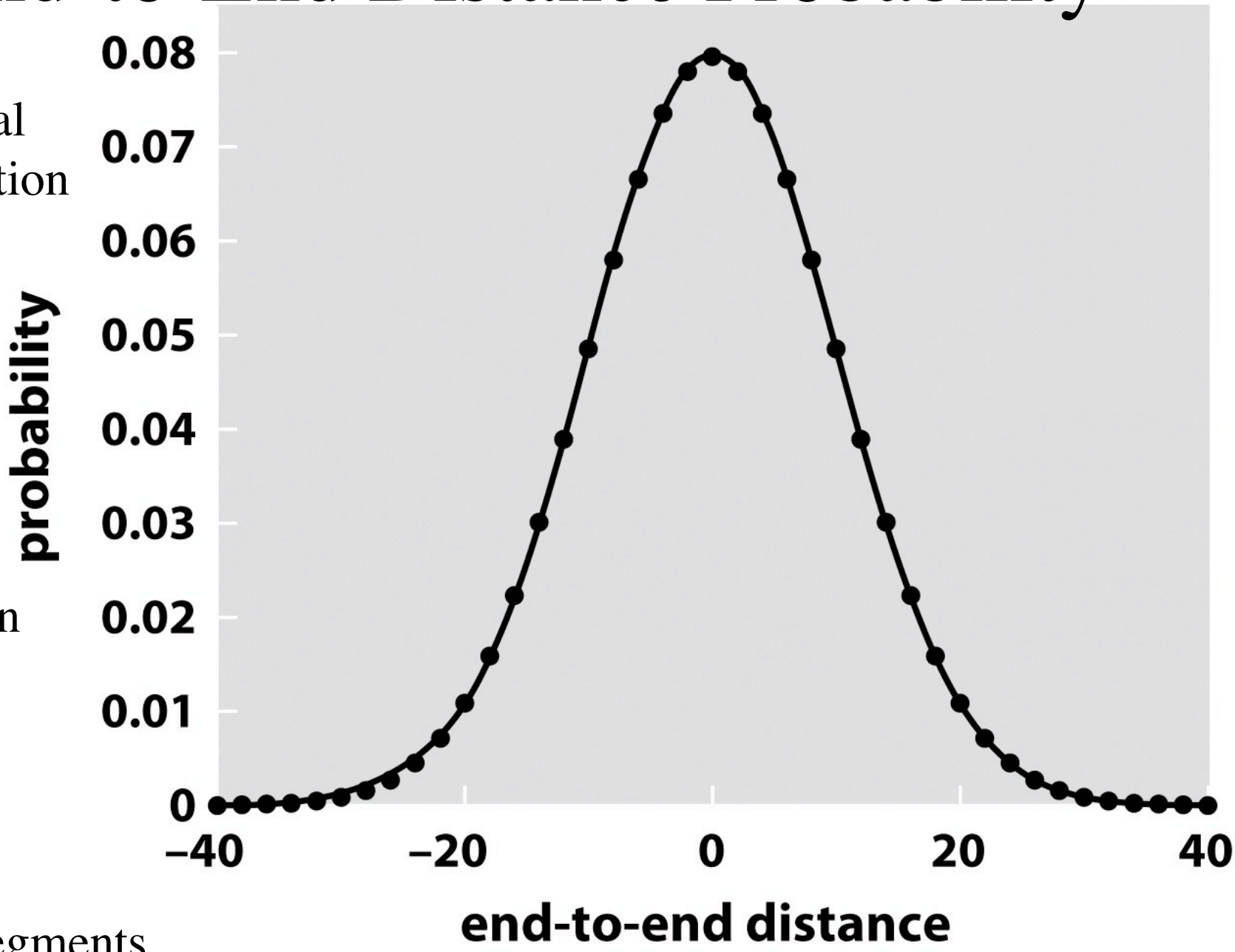
$$W(n_r;N) = \frac{N!}{n_r!(N-n_r)!}$$

Figure 8.3 Physical Biology of the Cell (© Garland Science 2009)

End-to-End Distance Probability

- R by Binomial distribution

— R by approx. Gaussian distribution



1D, 100 segments

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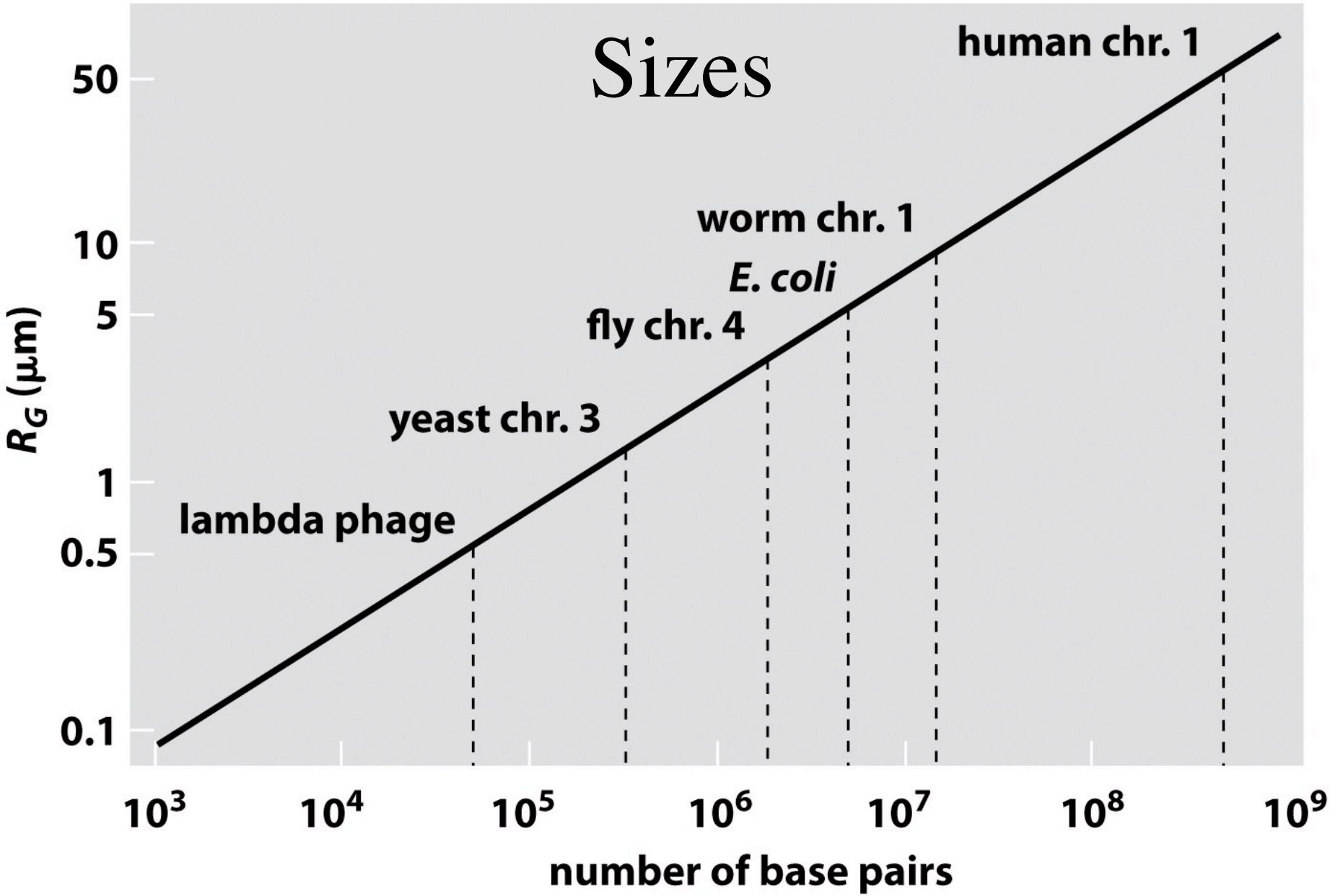
Estimates of Genomic DNA Sizes



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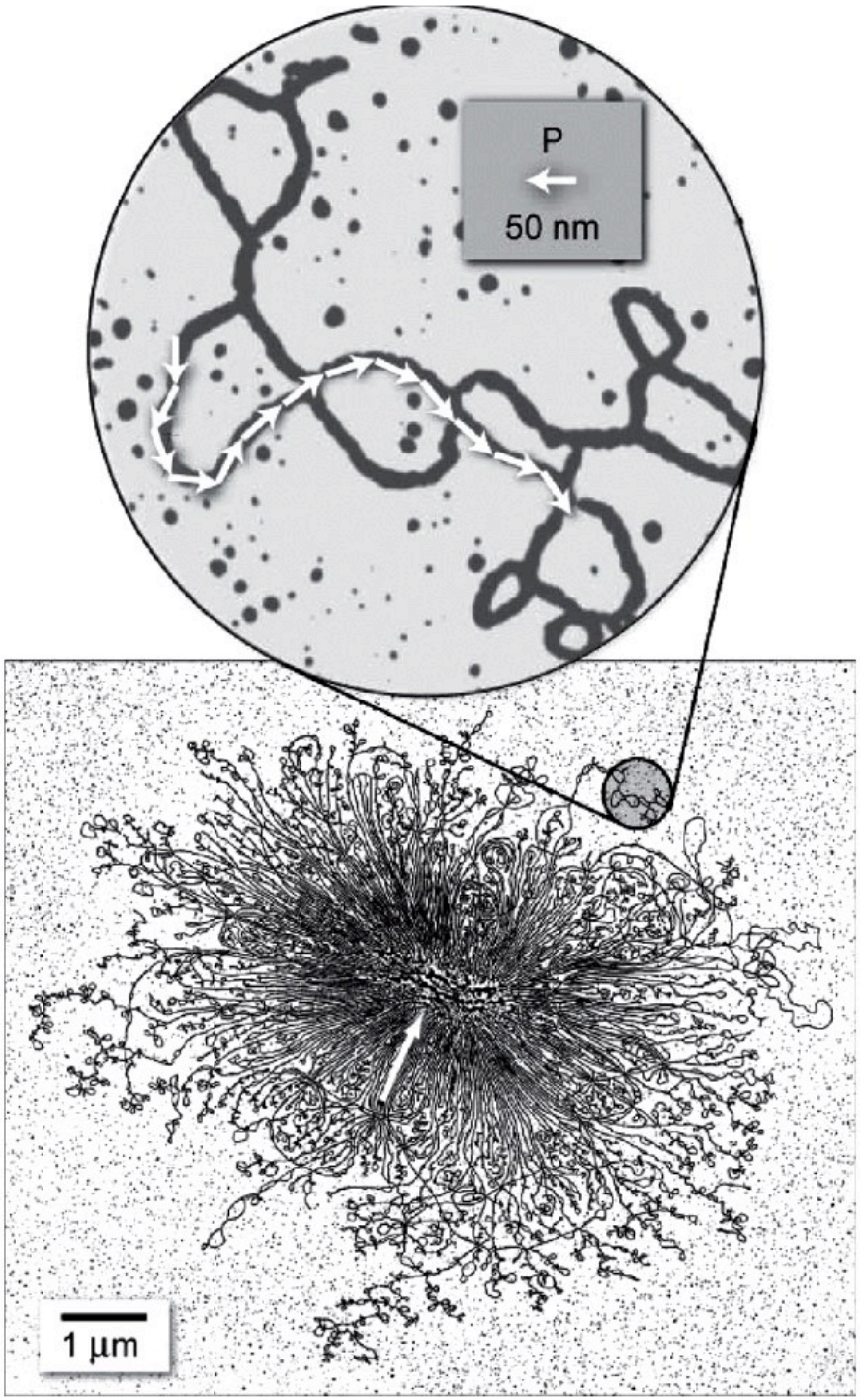
Bacterial Genome



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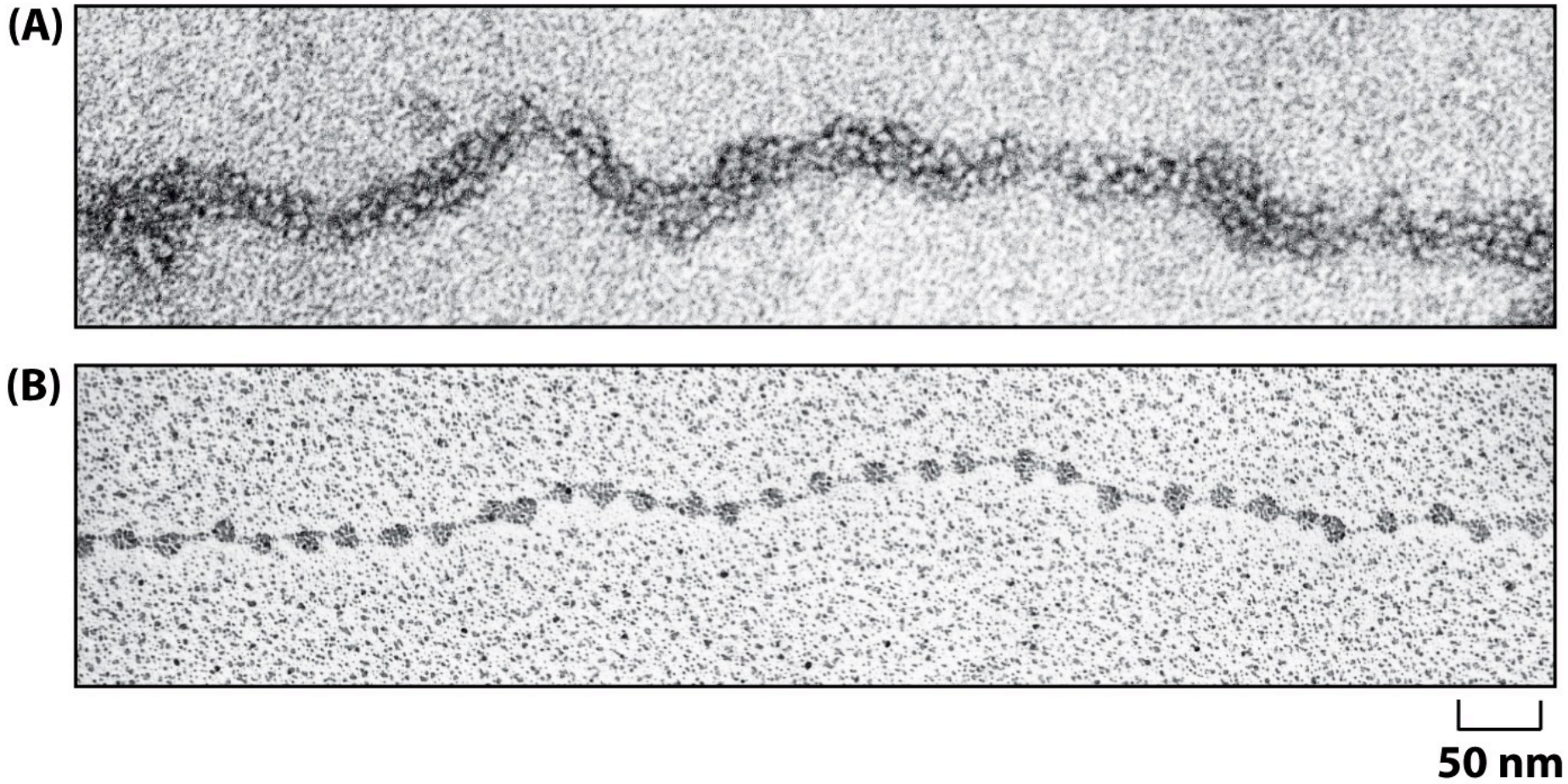
Chromatin



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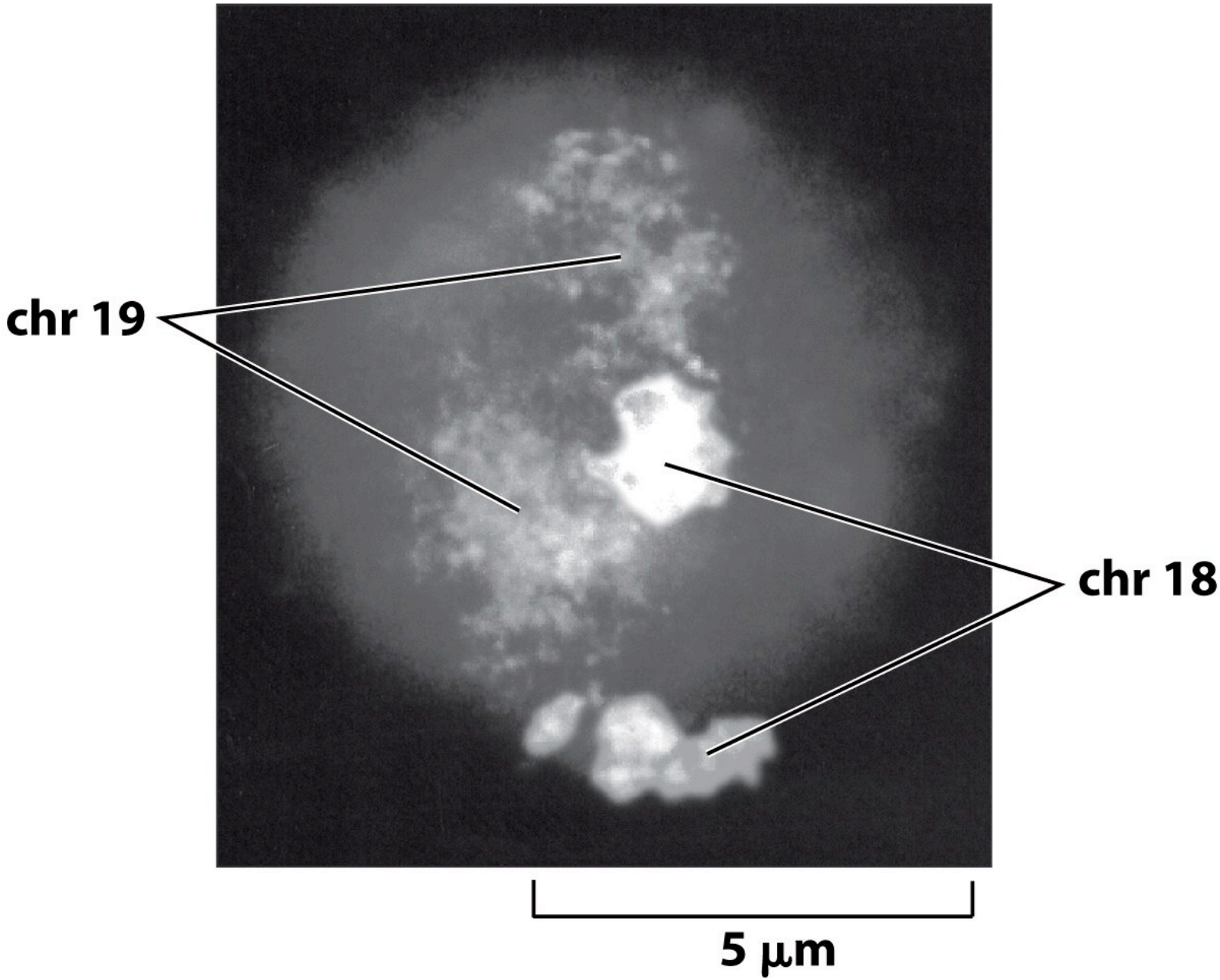

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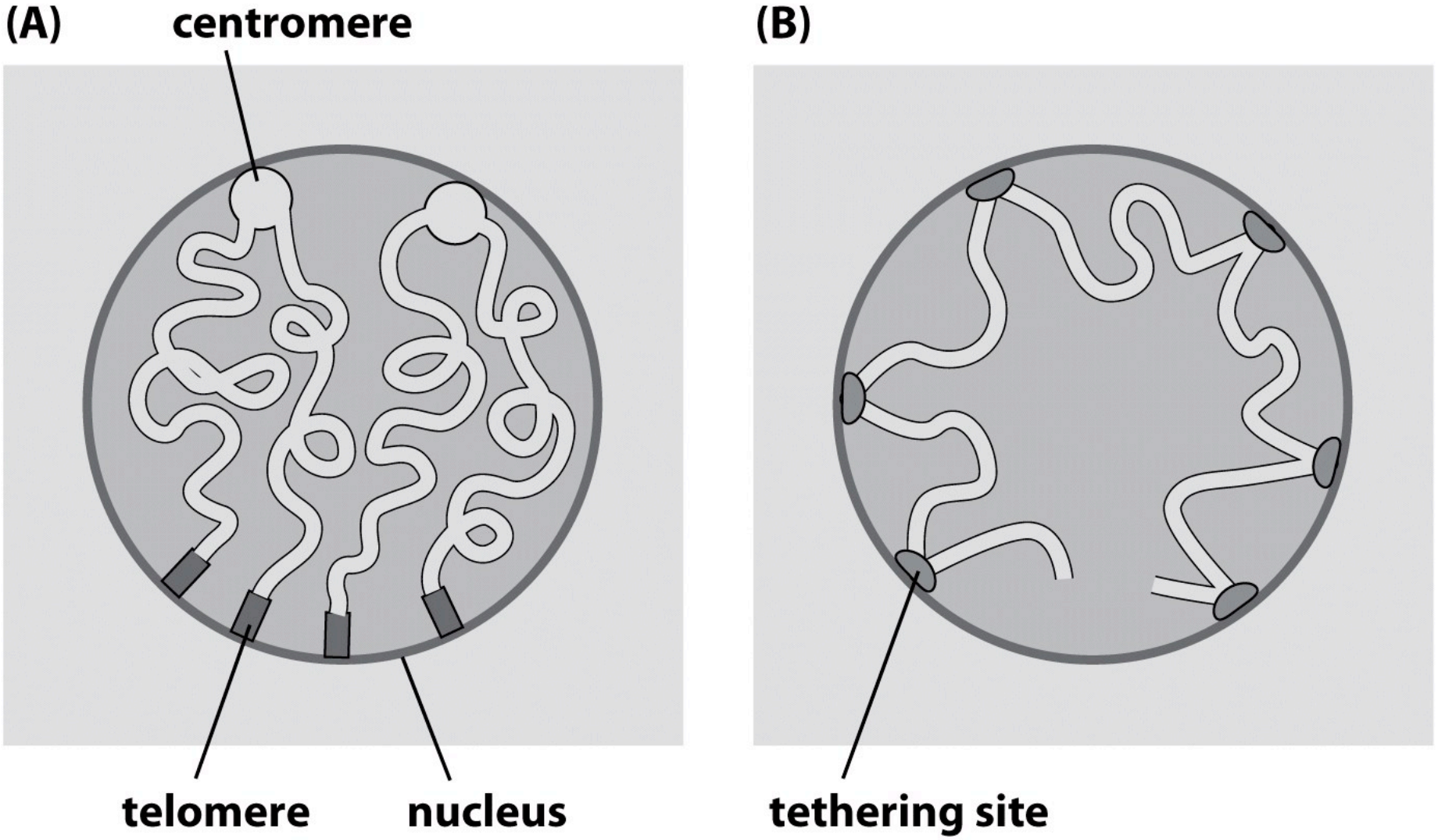

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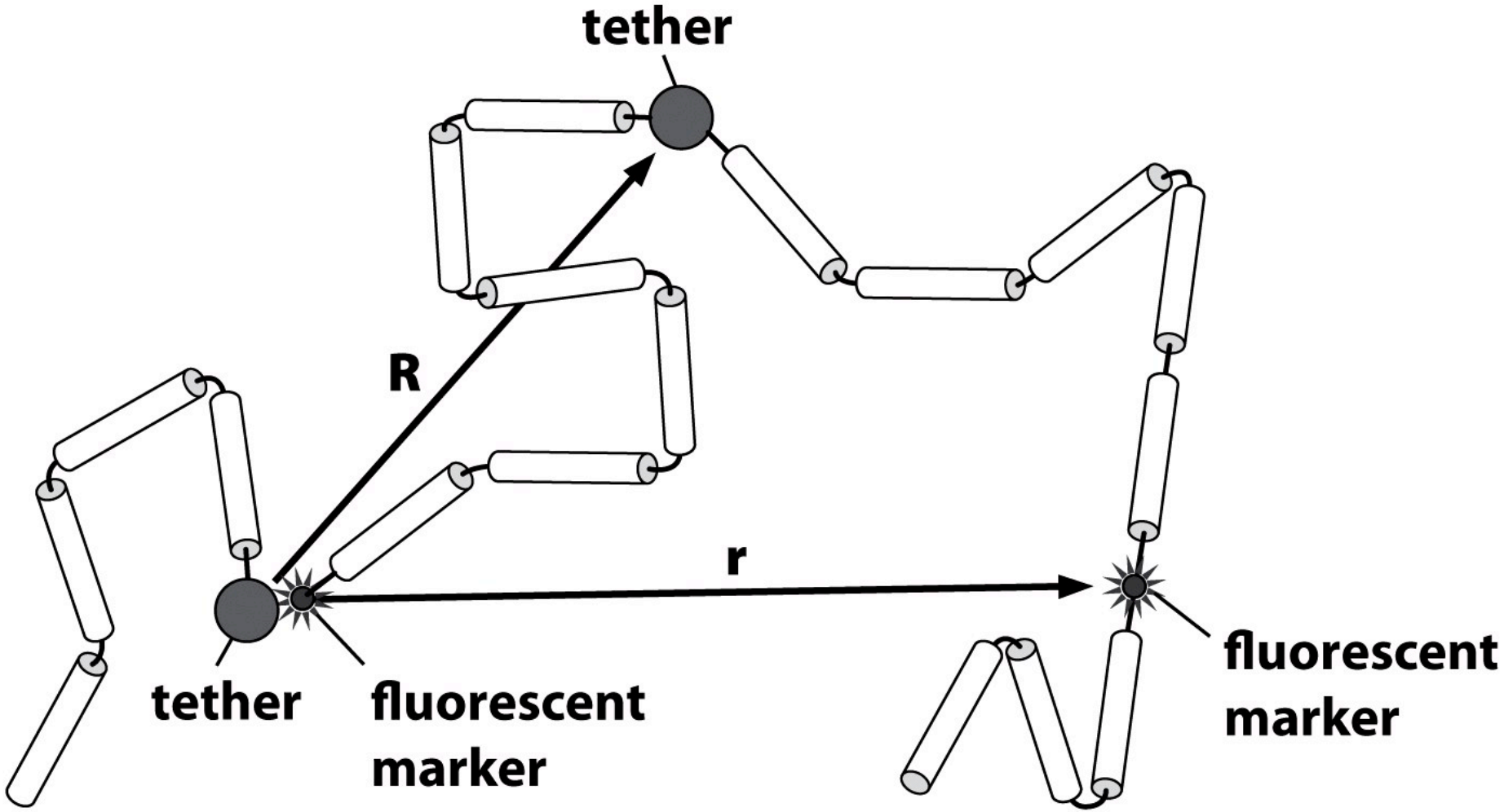

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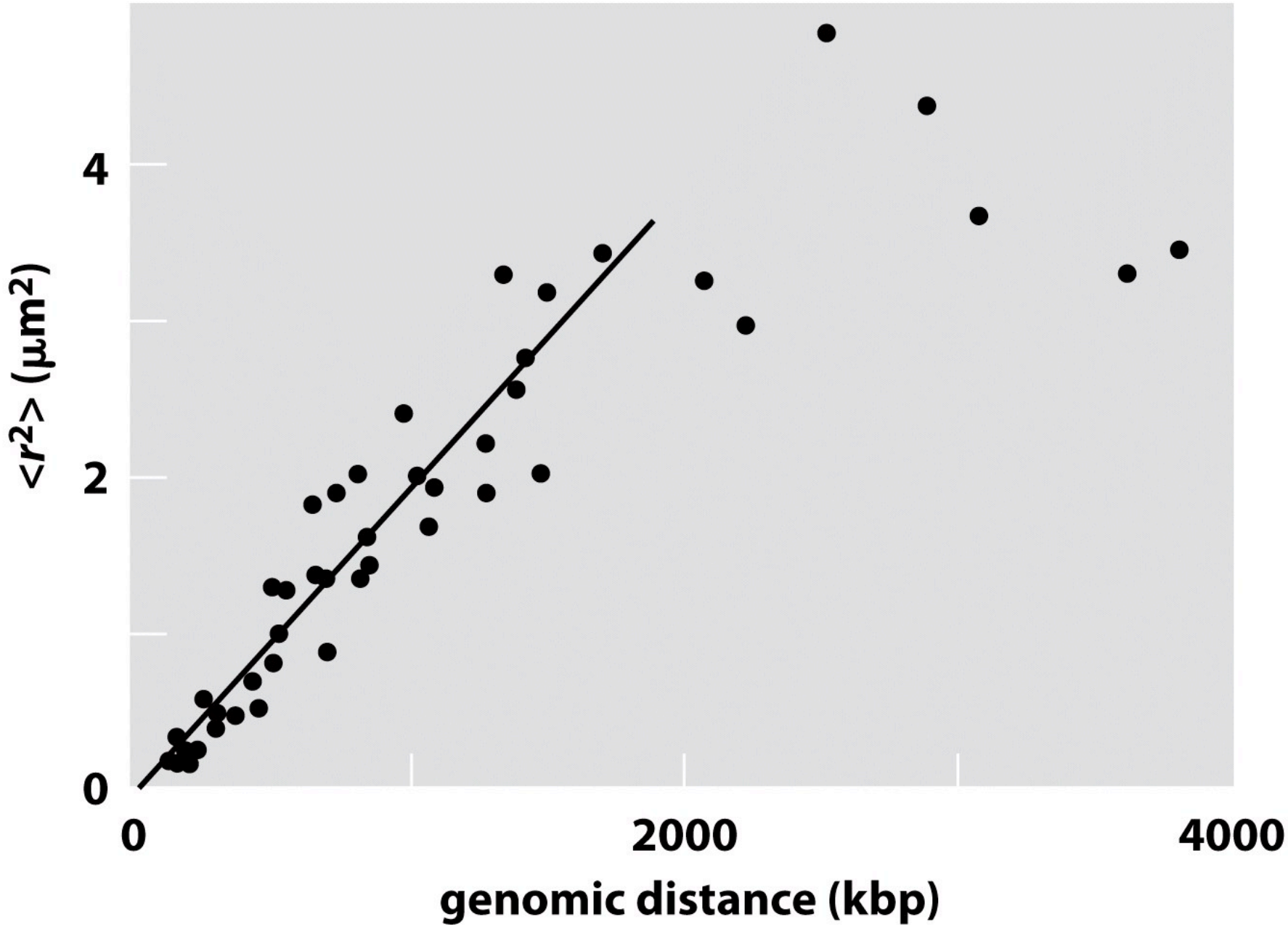

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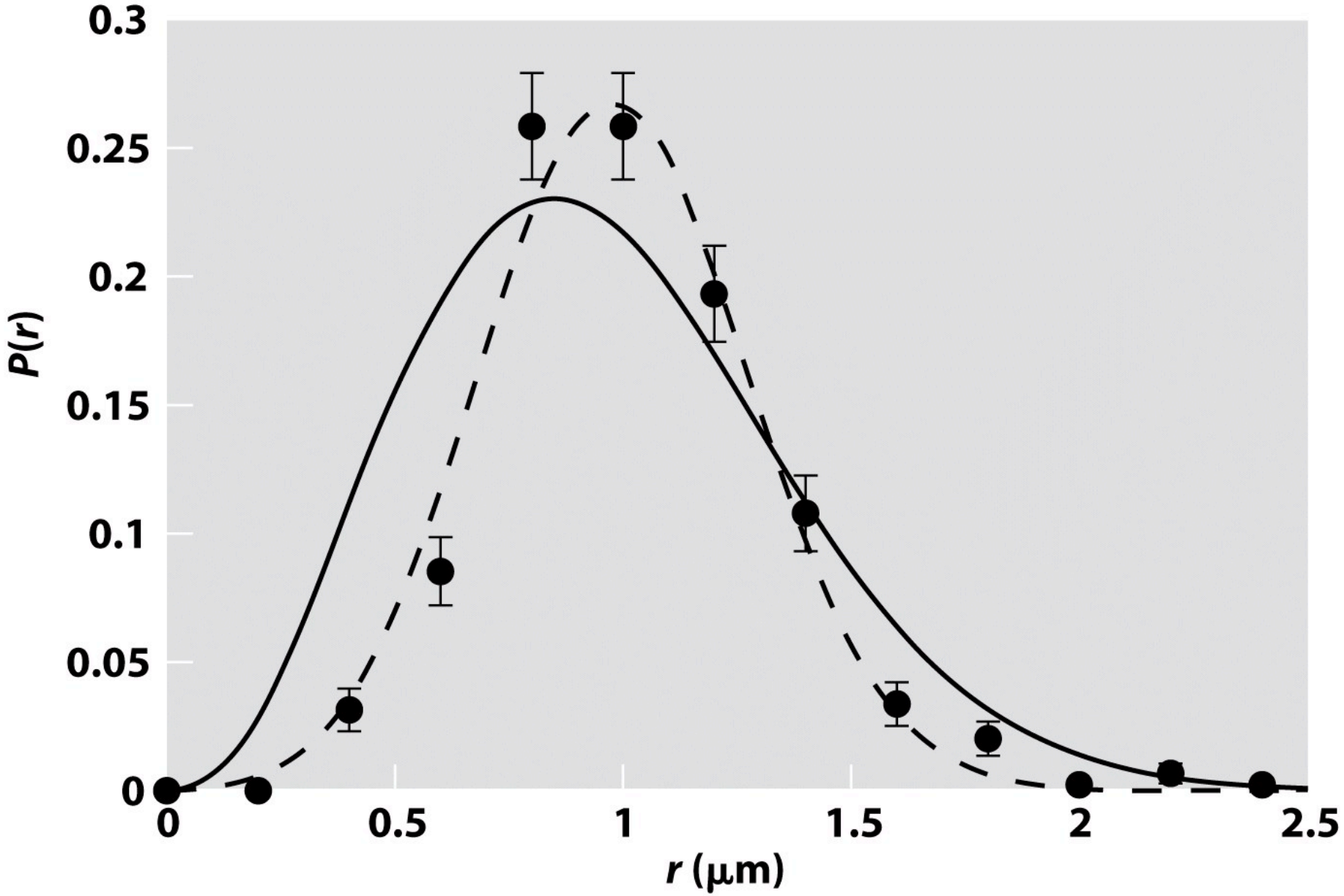

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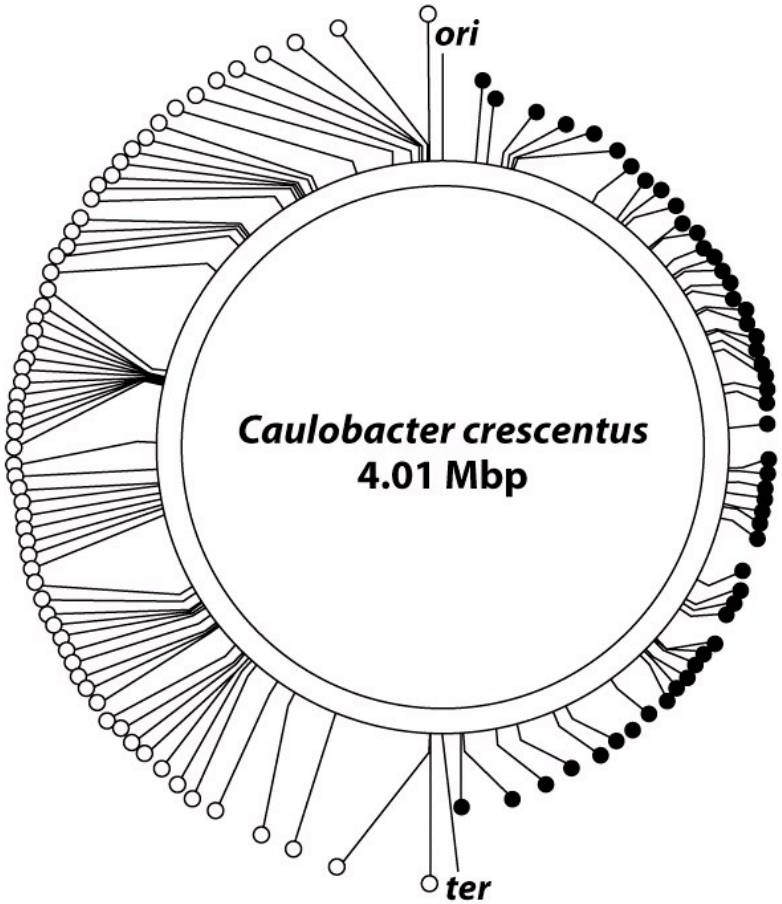

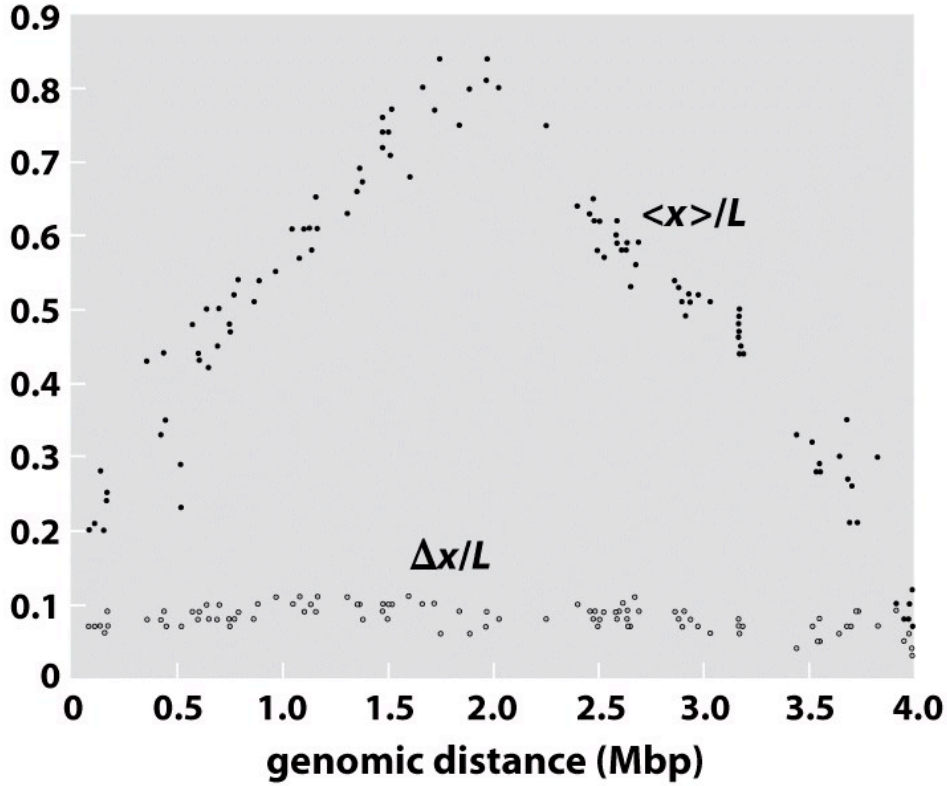

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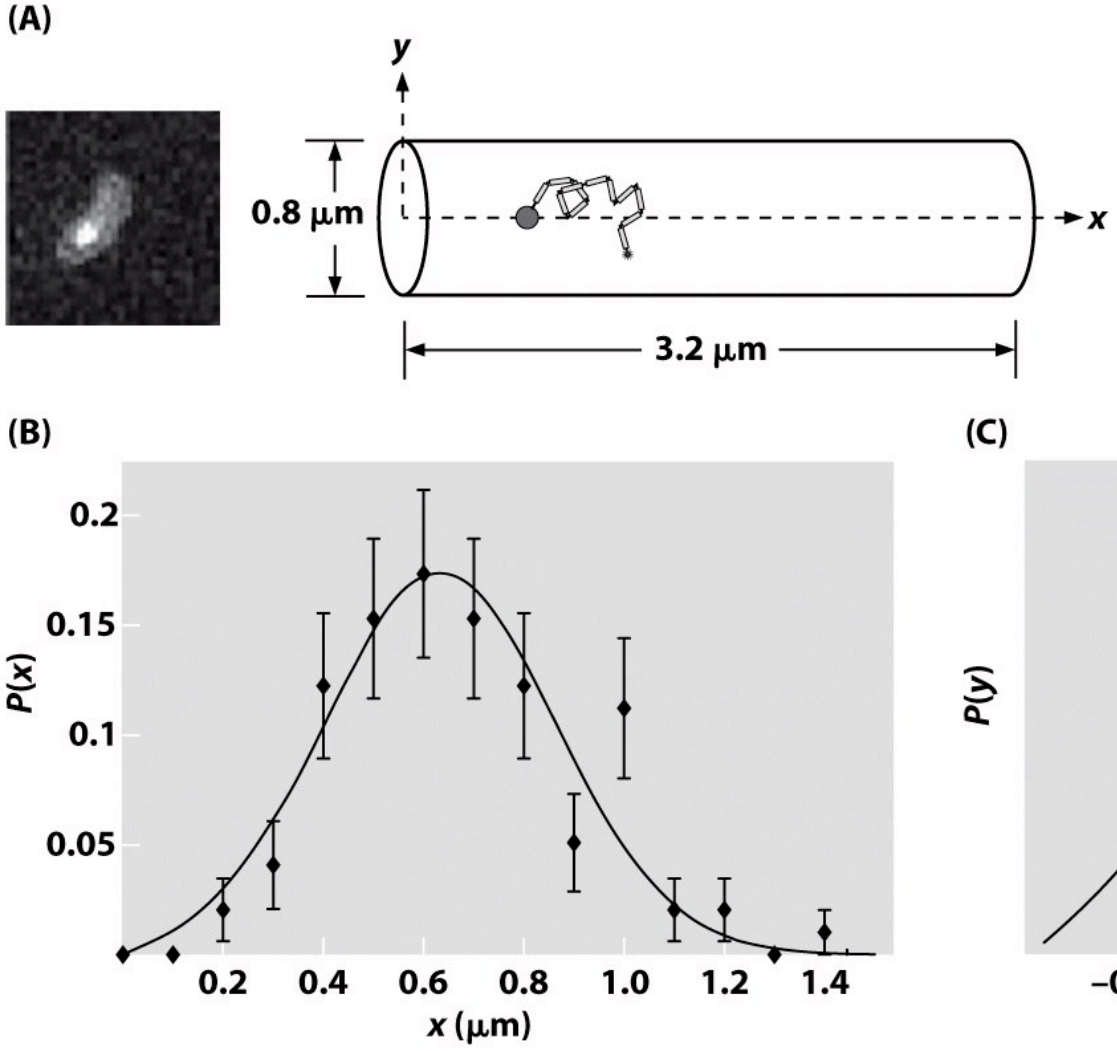

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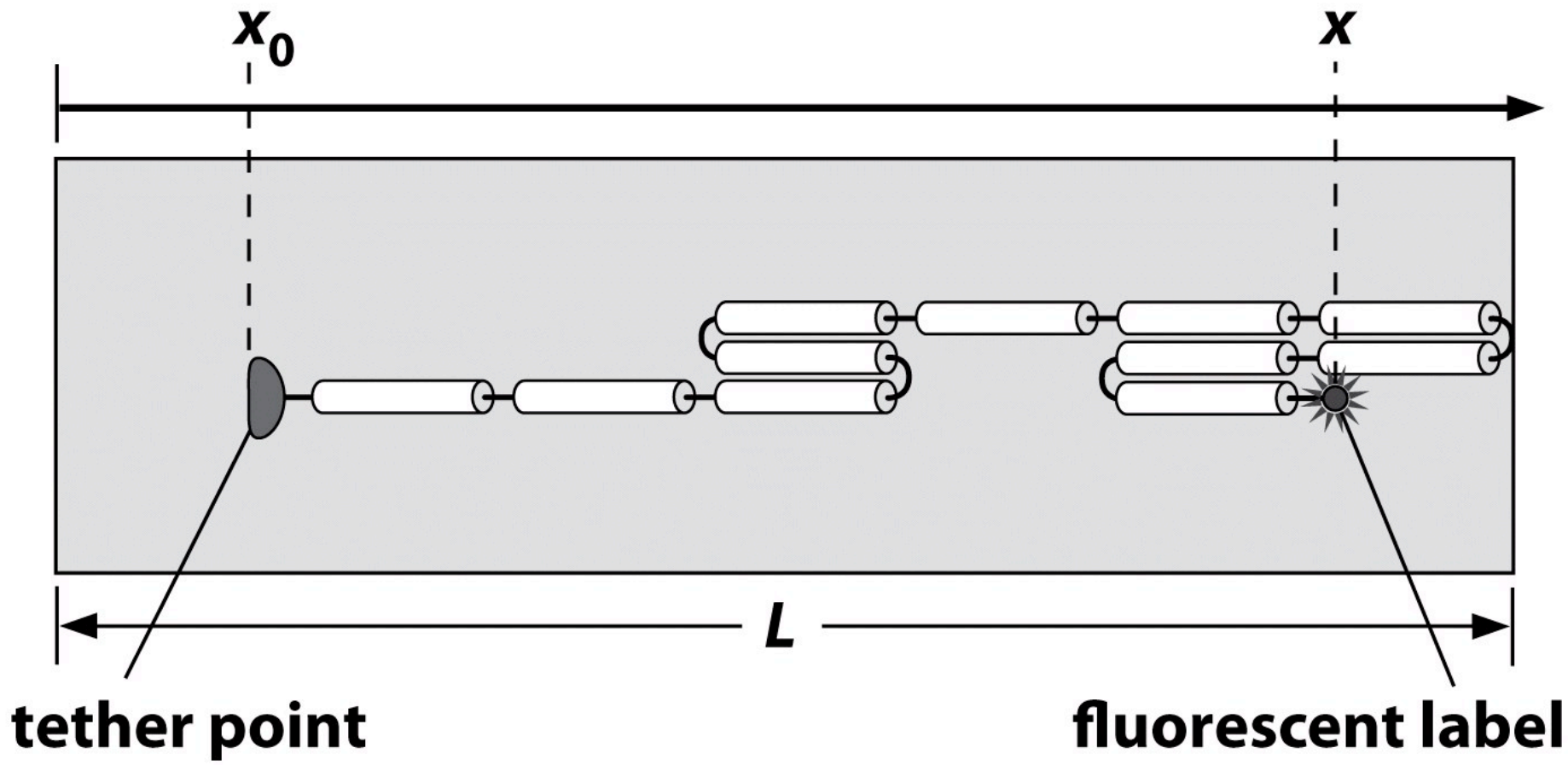
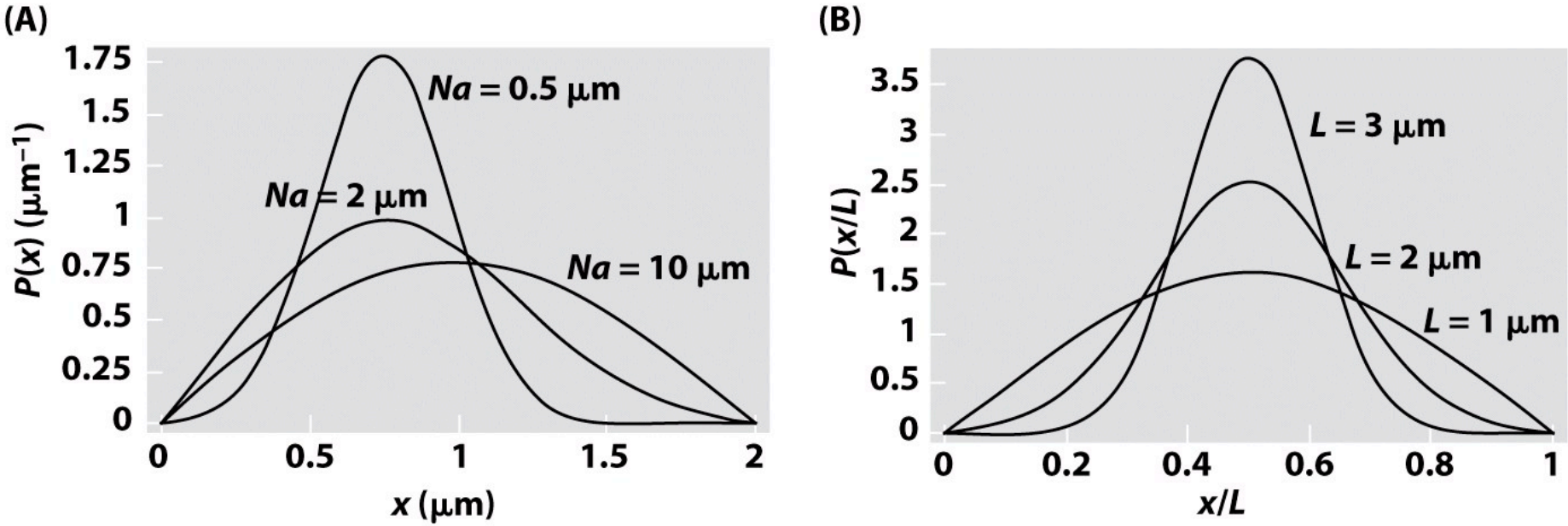


Figure 8.15 Physical Biology of the Cell (© Garland Science 2009)



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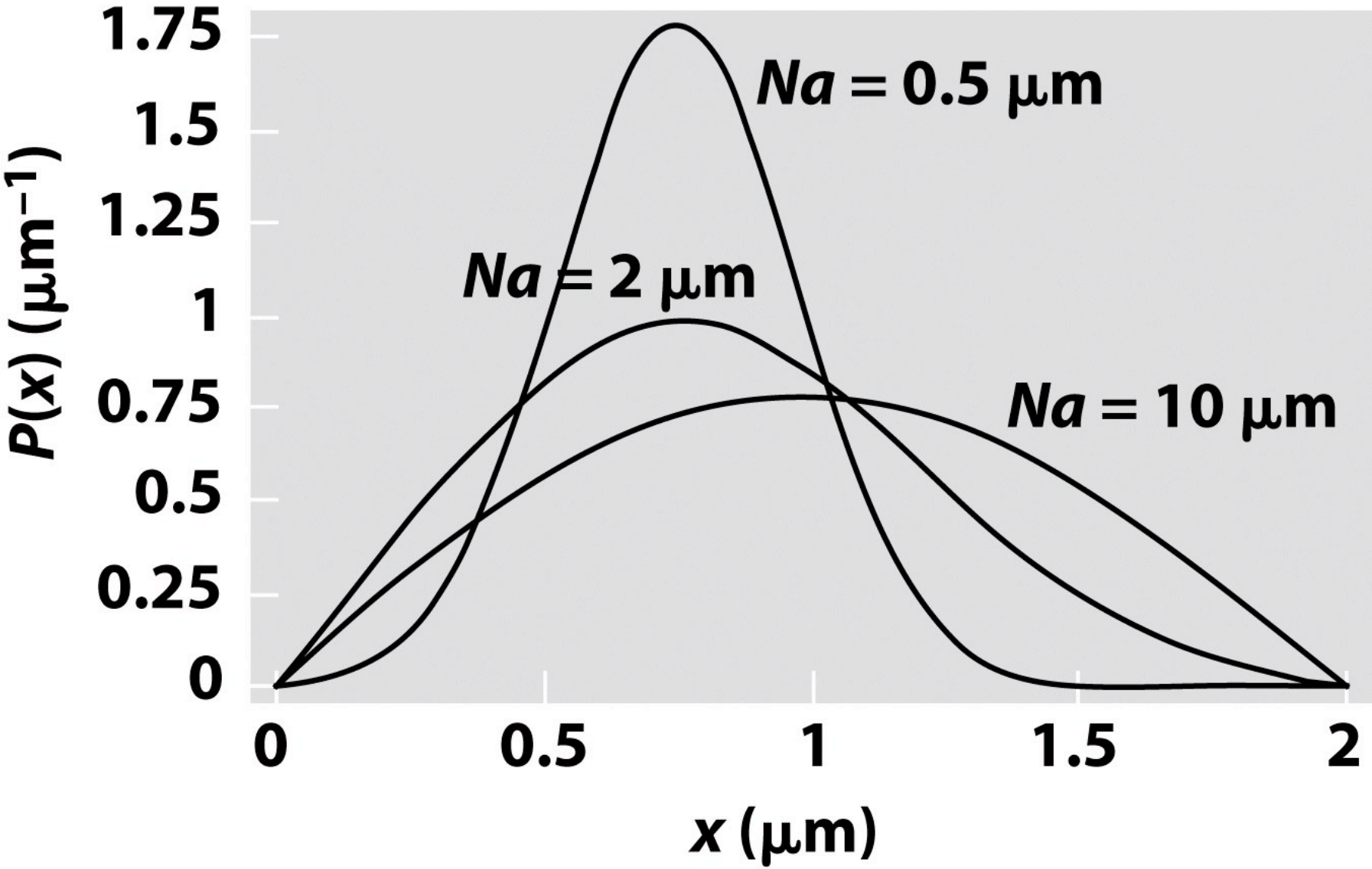

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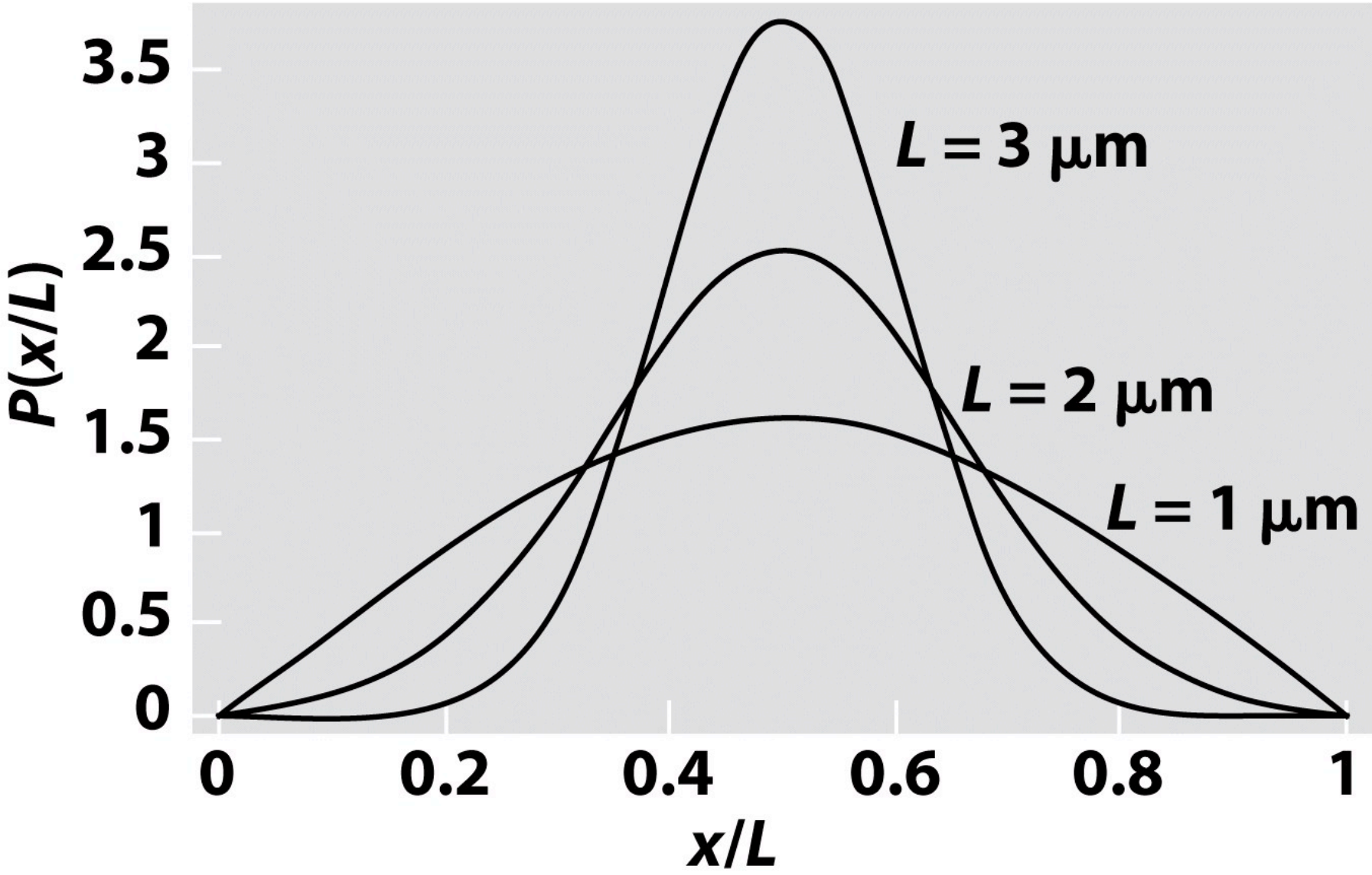

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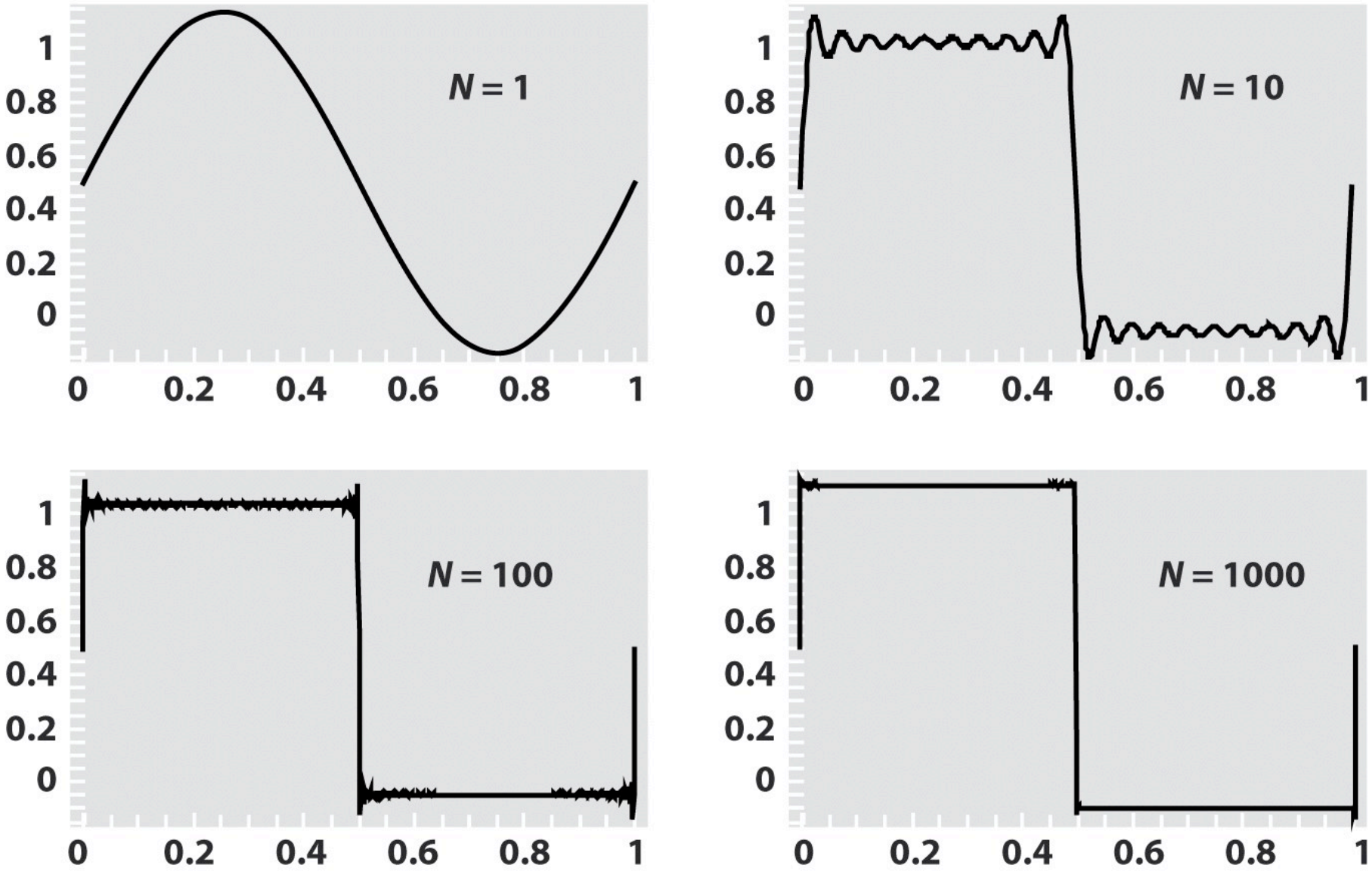

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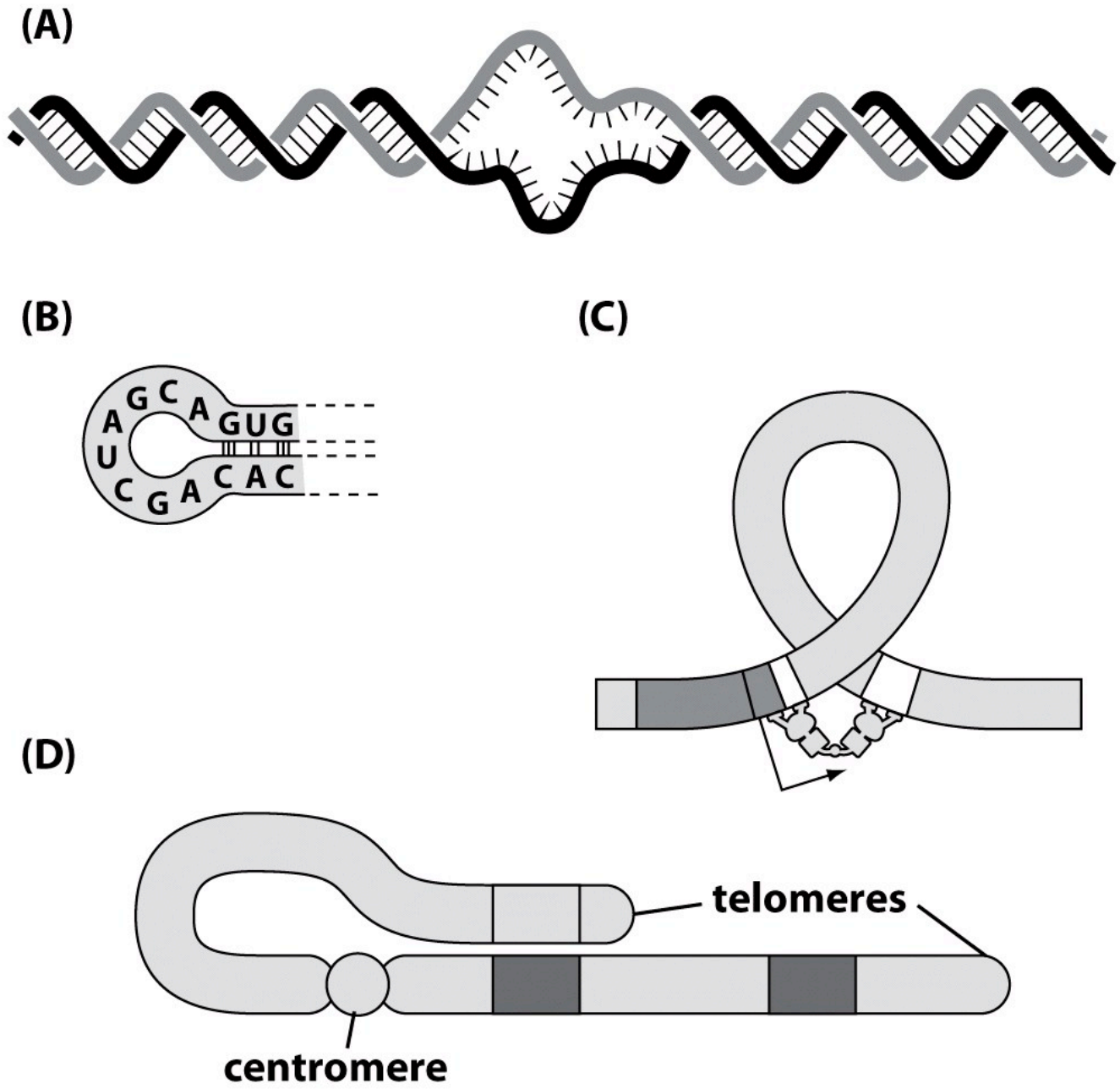

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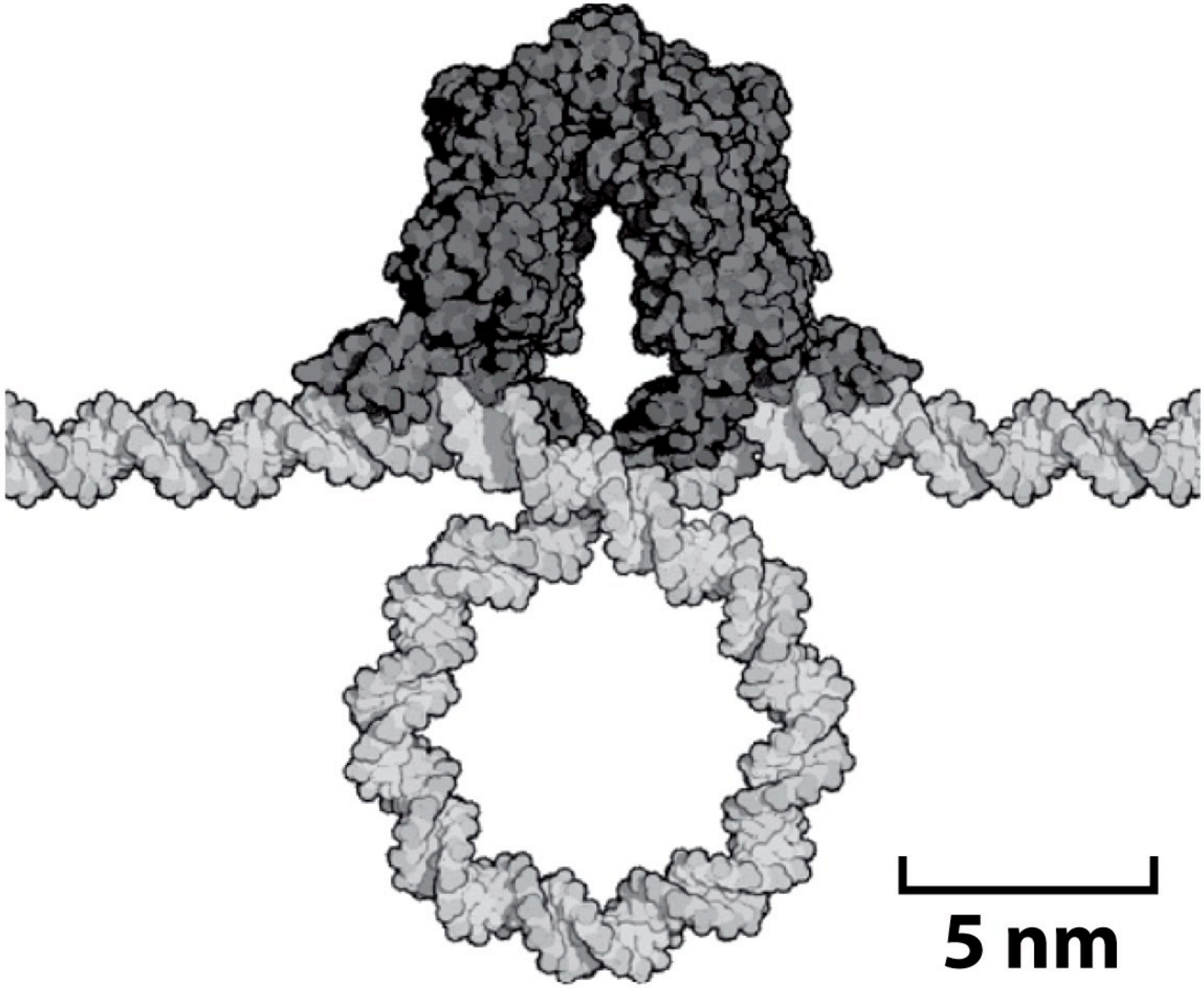

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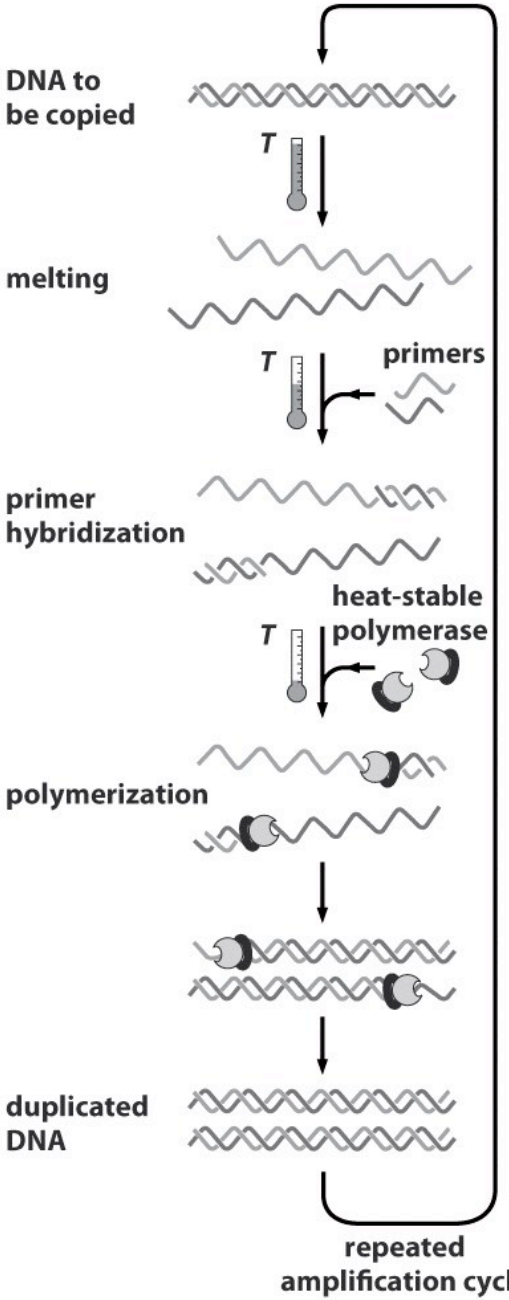

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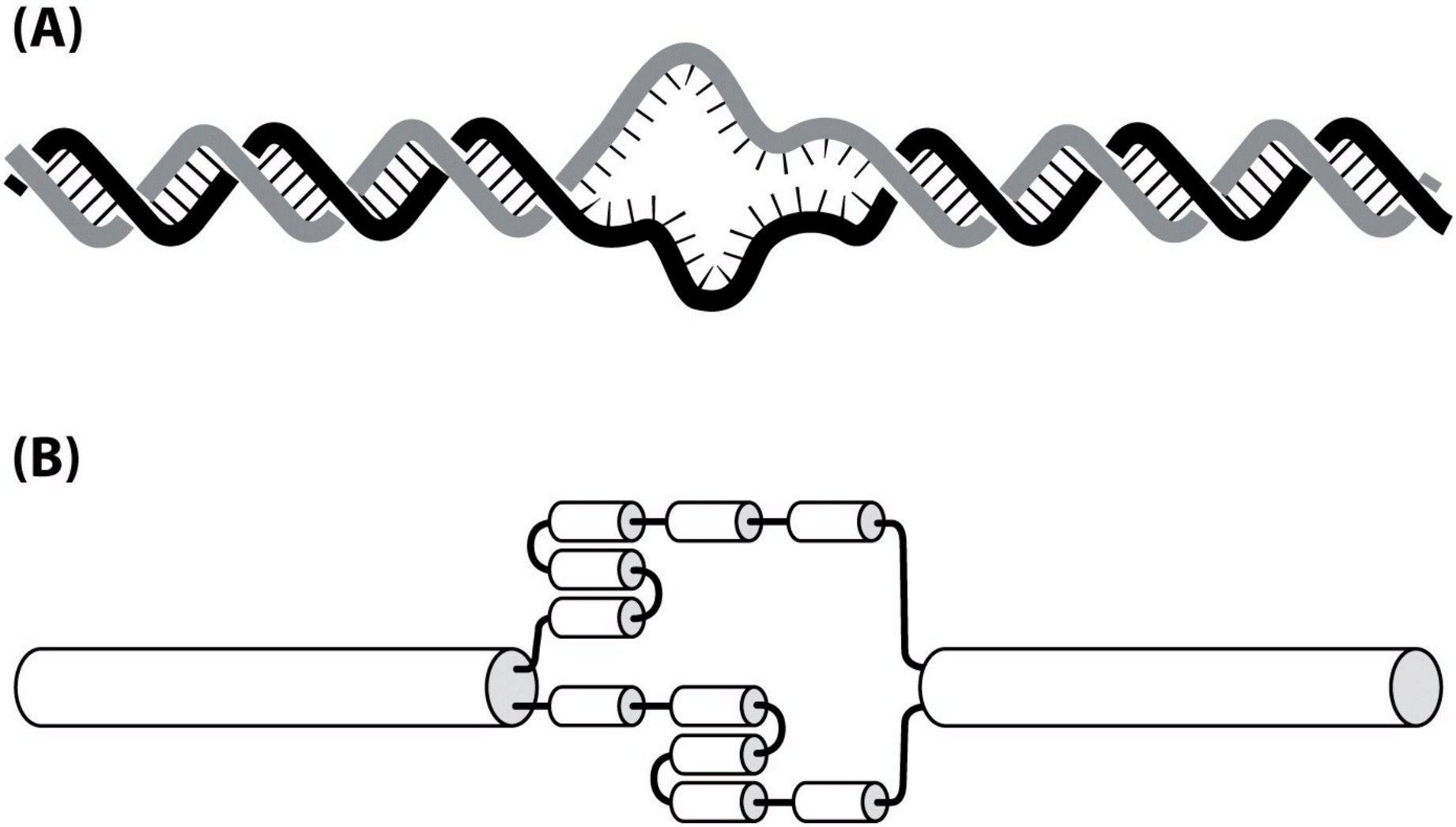

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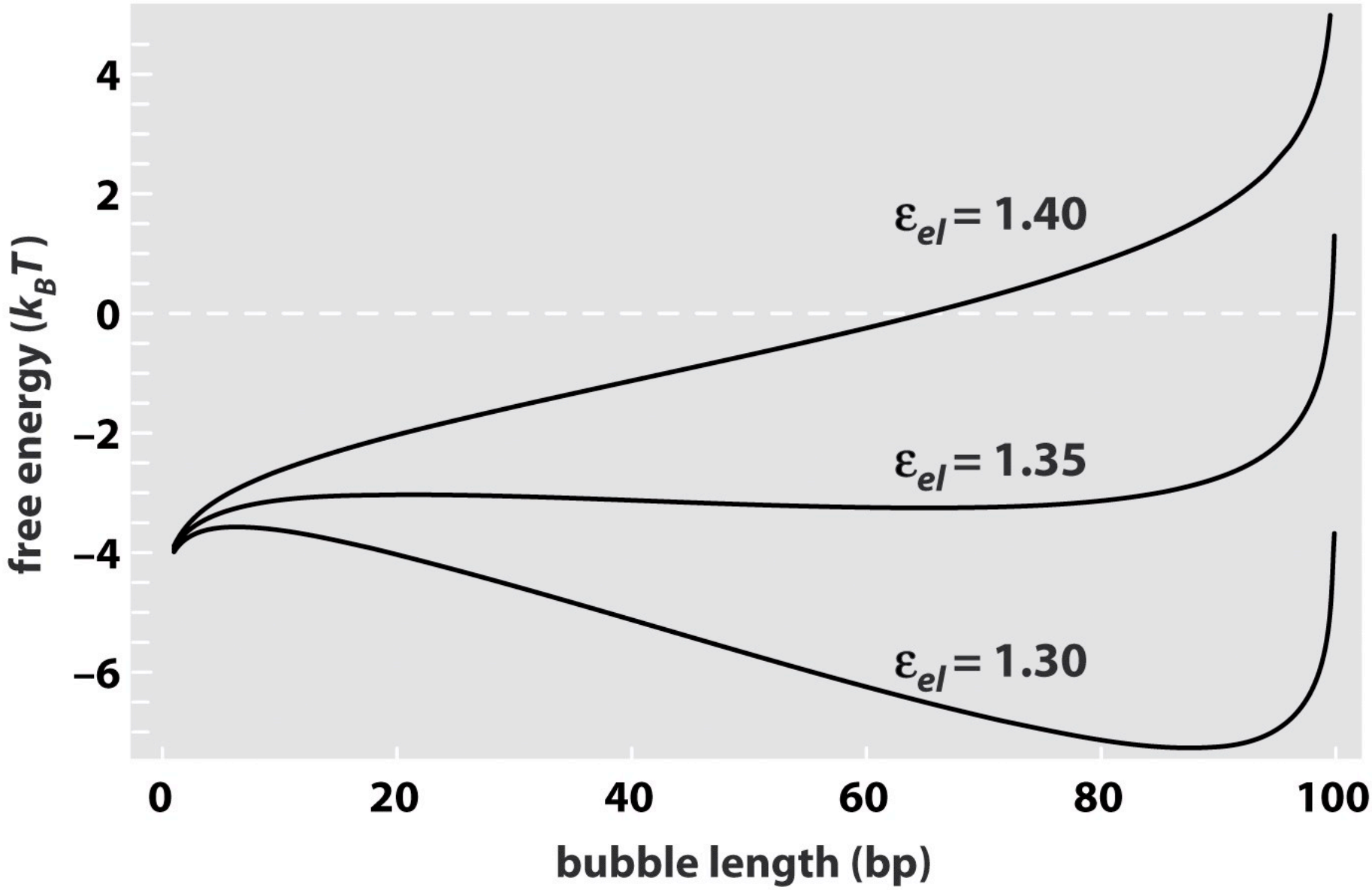

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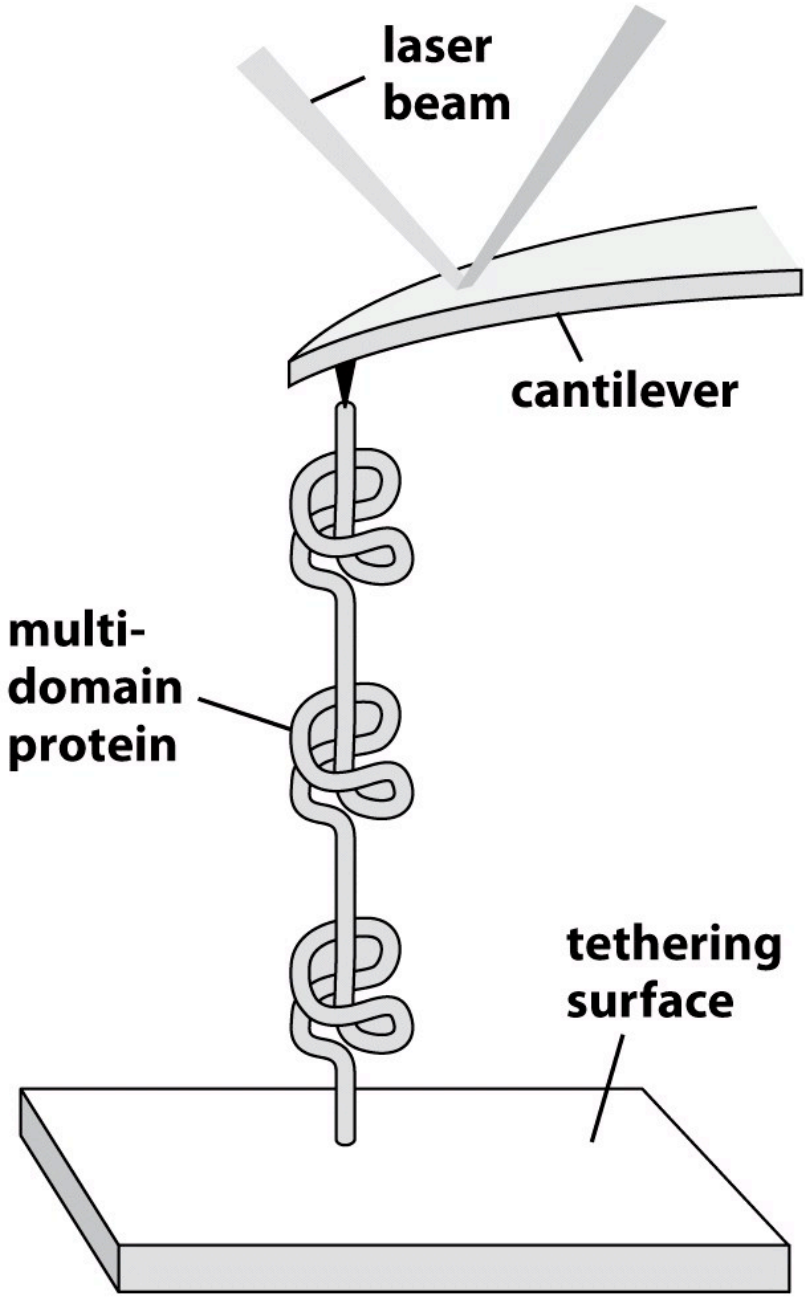

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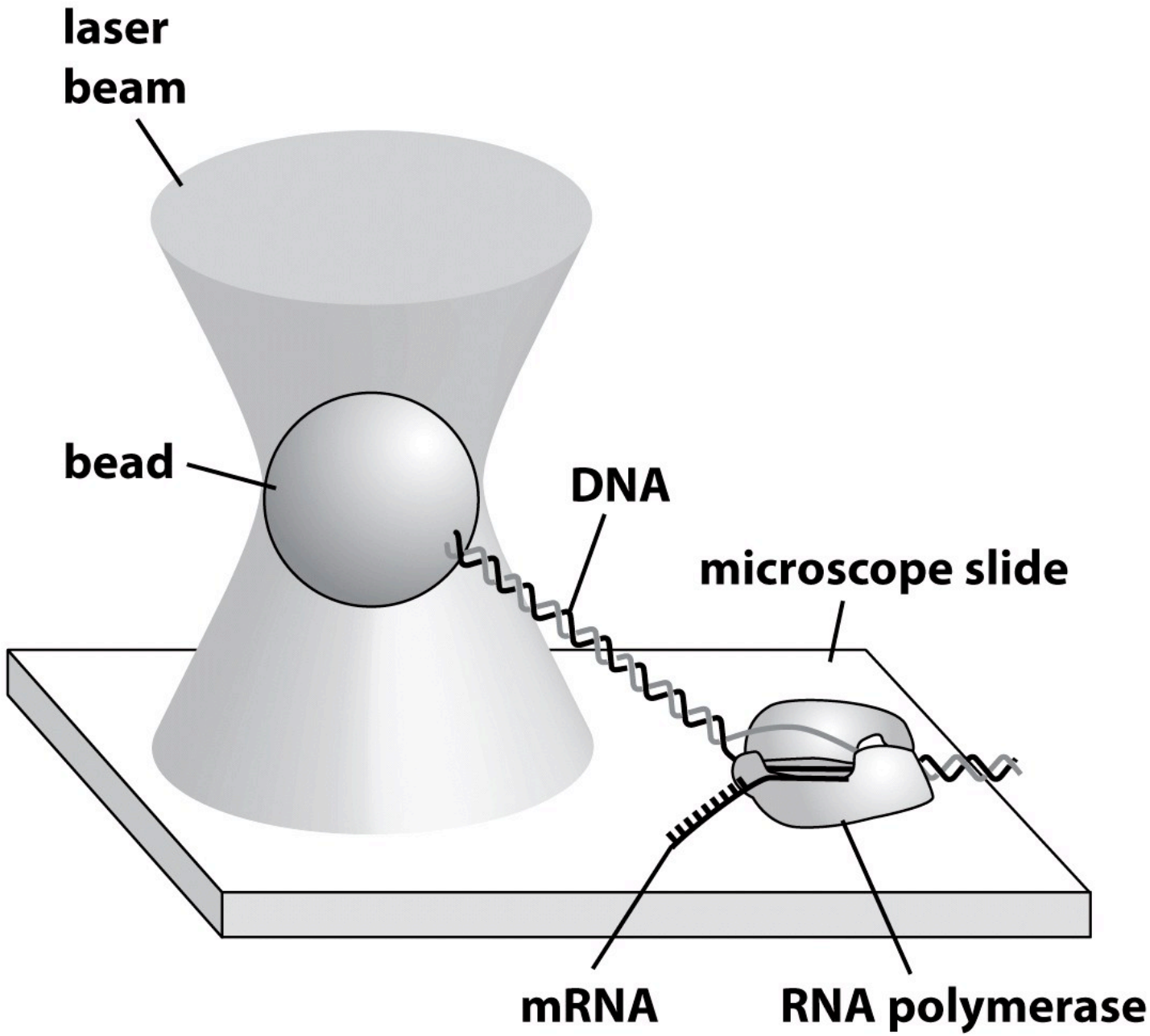

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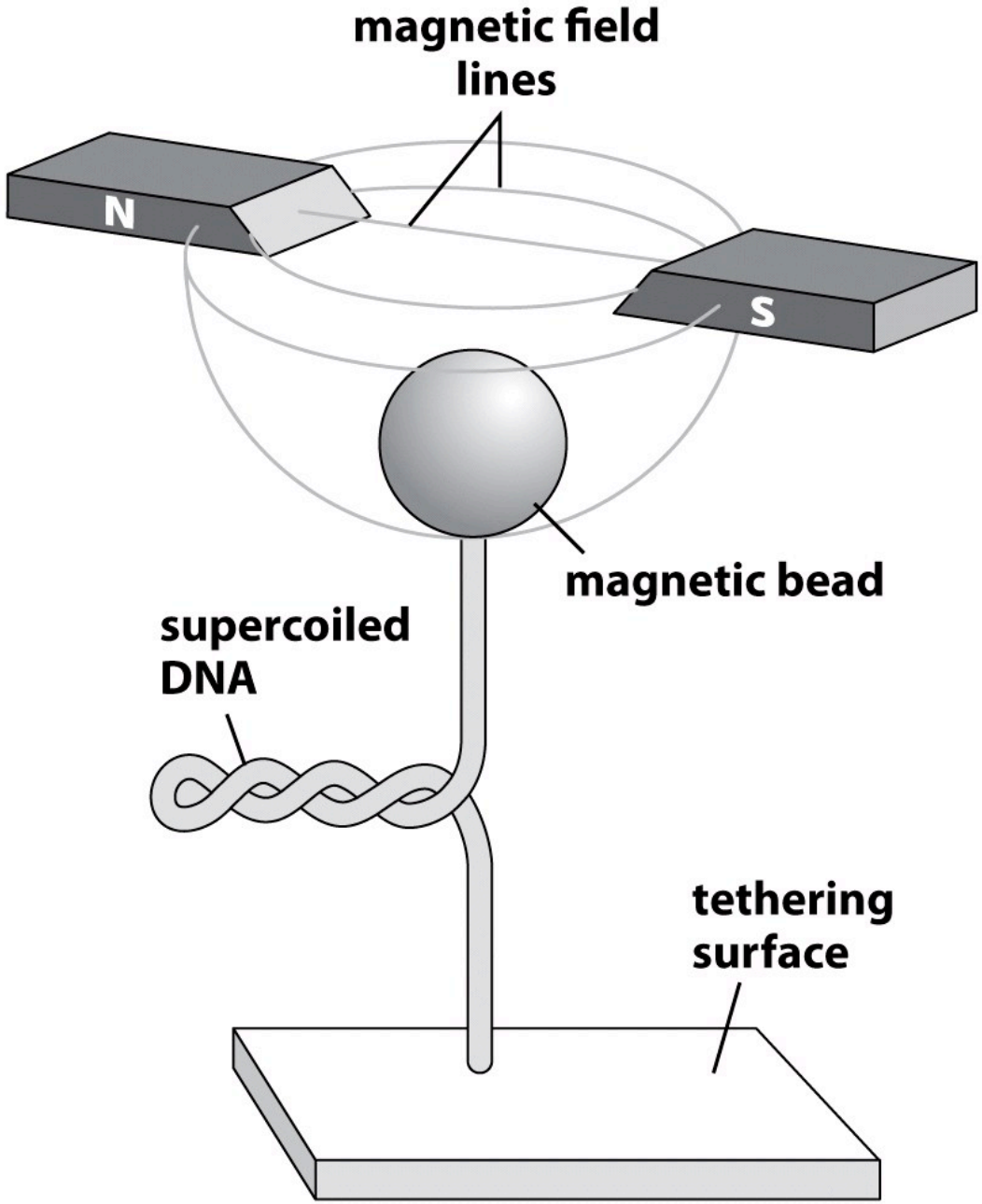

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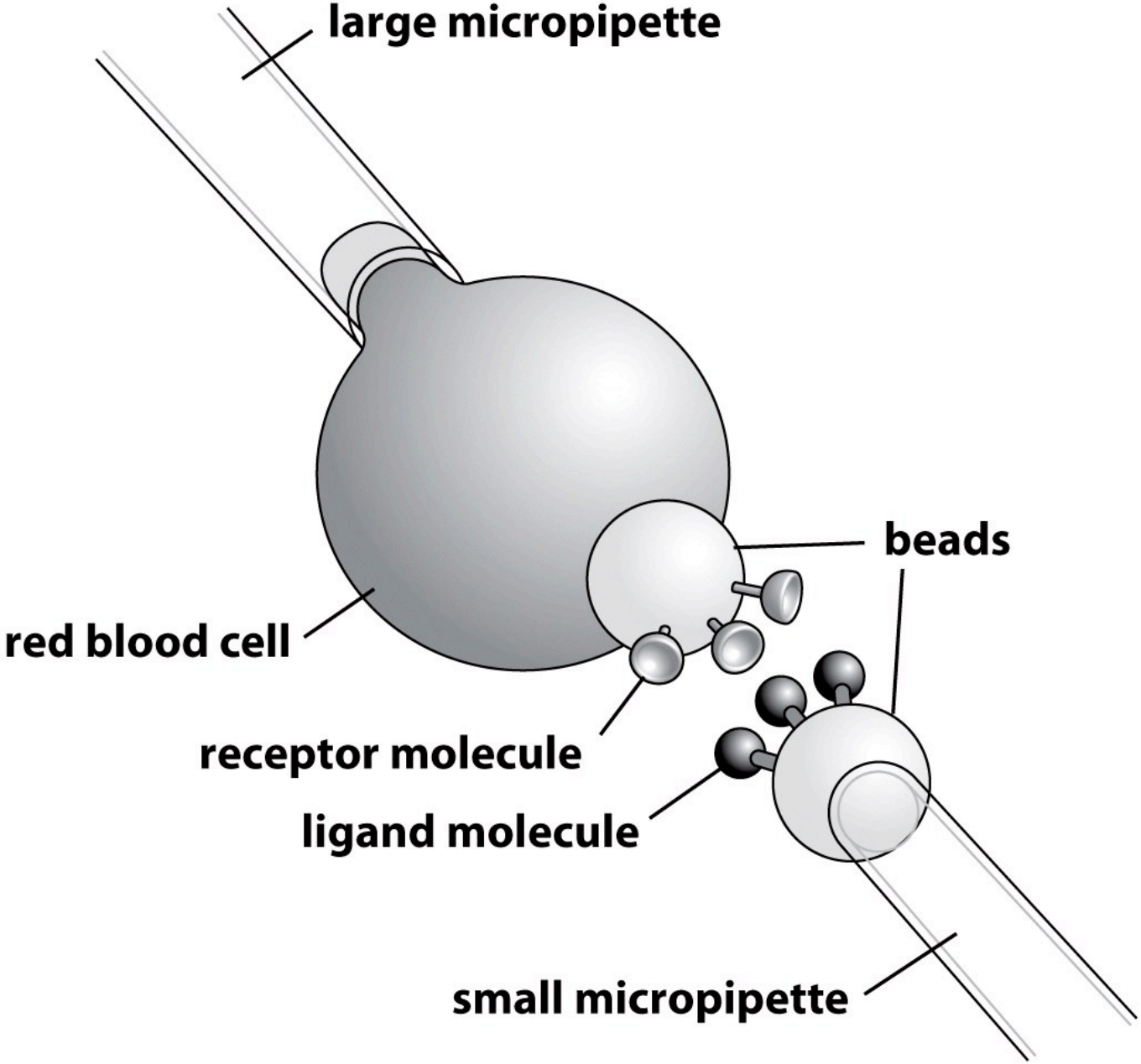

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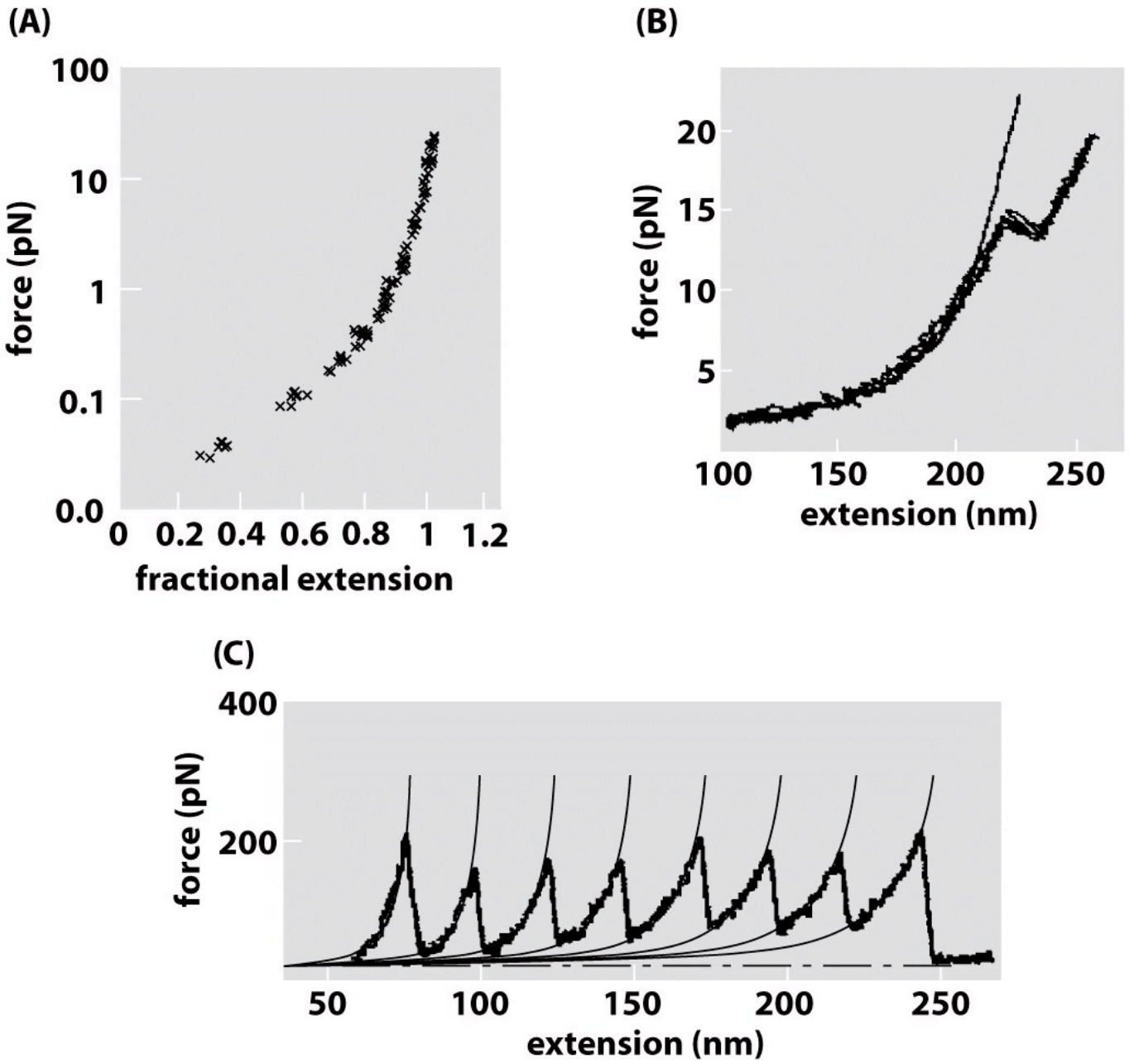

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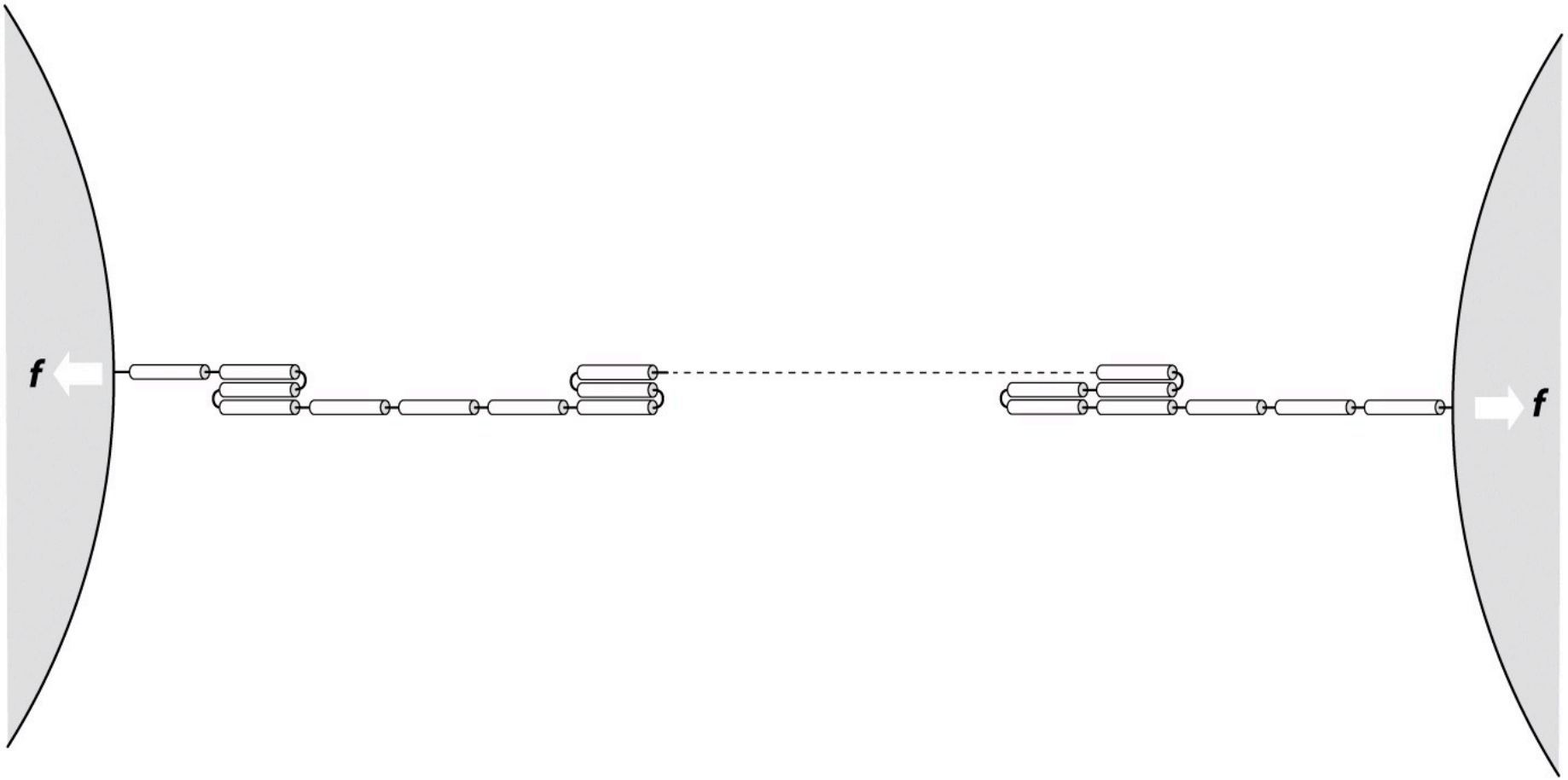

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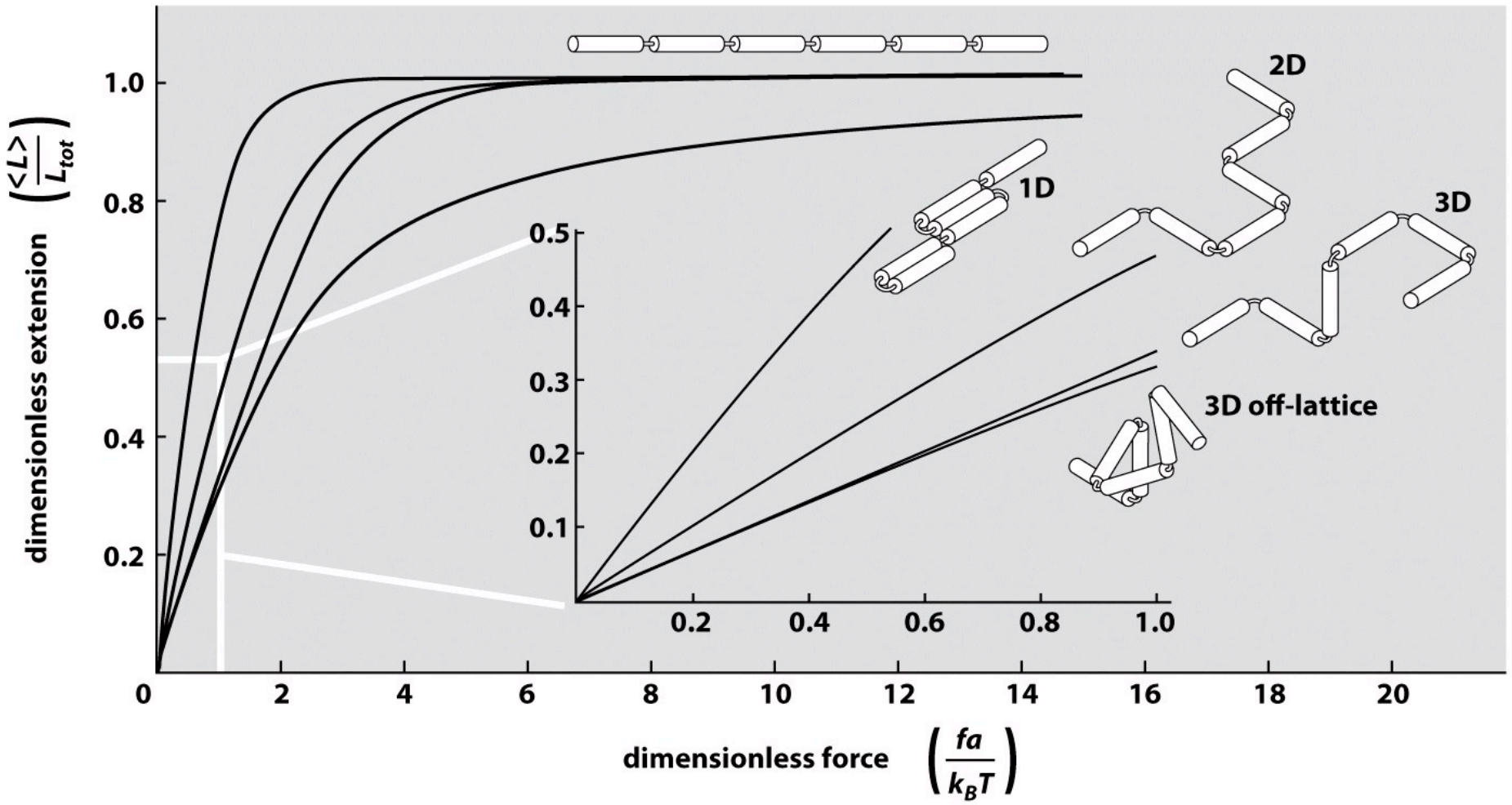

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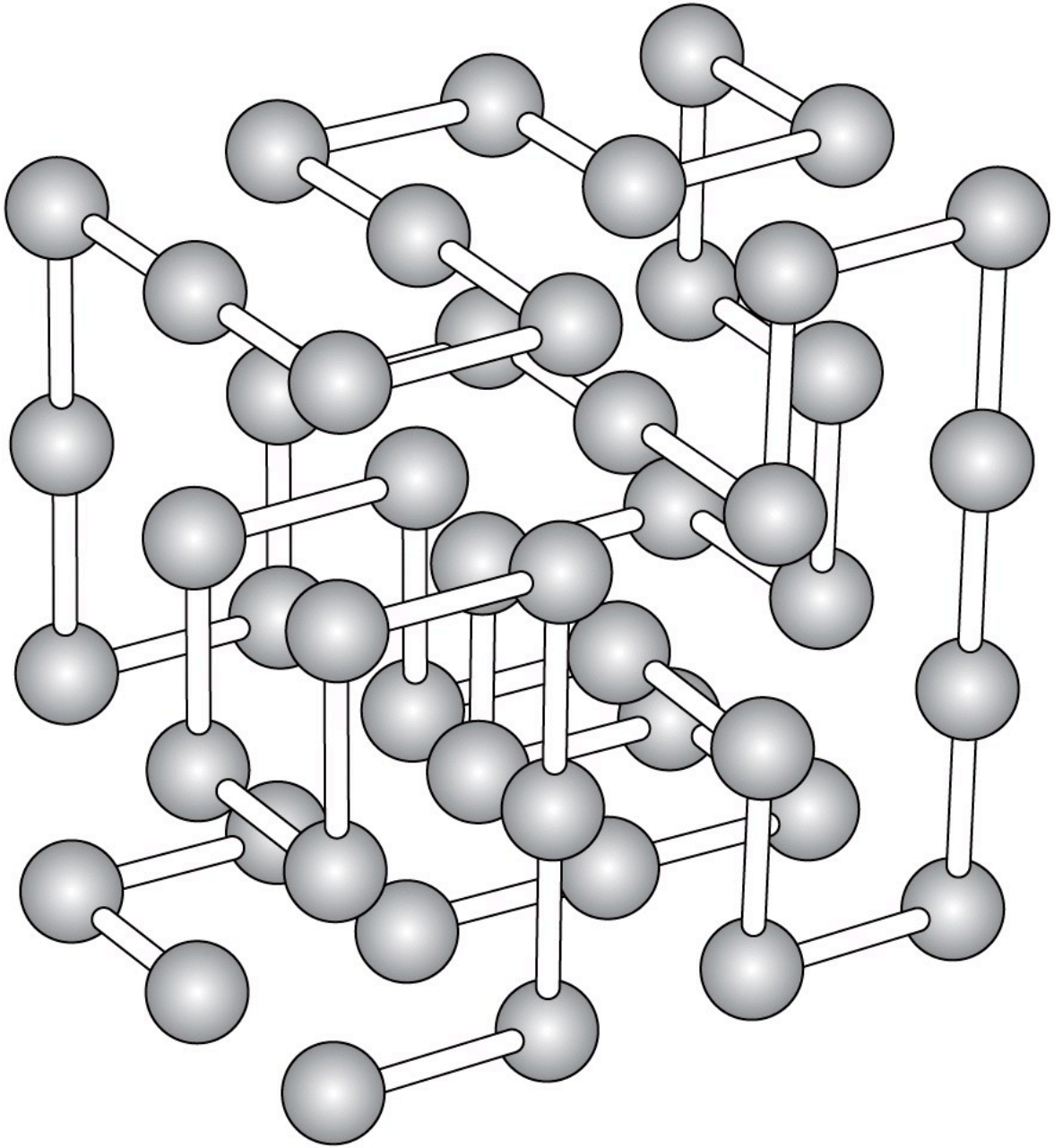

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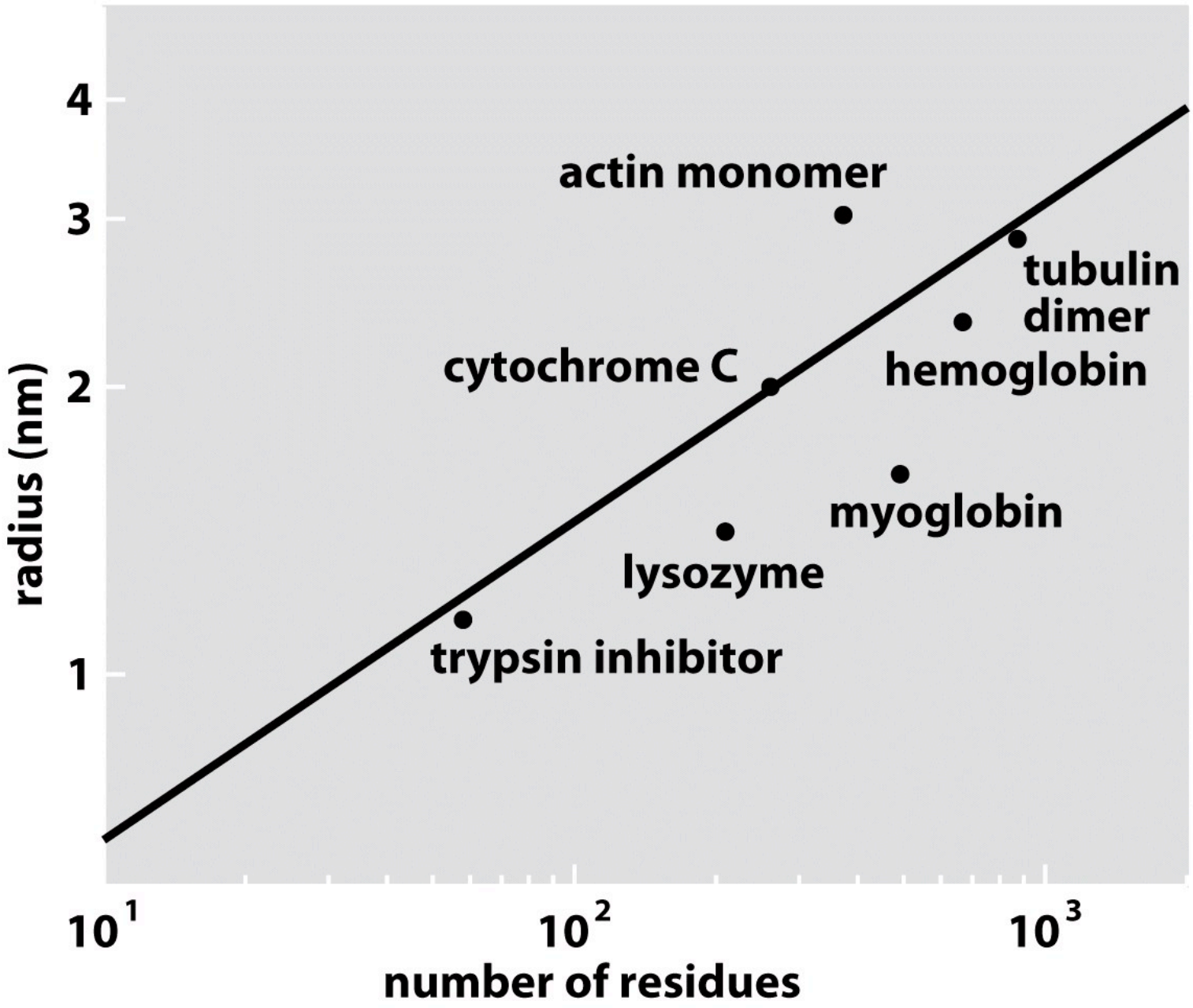

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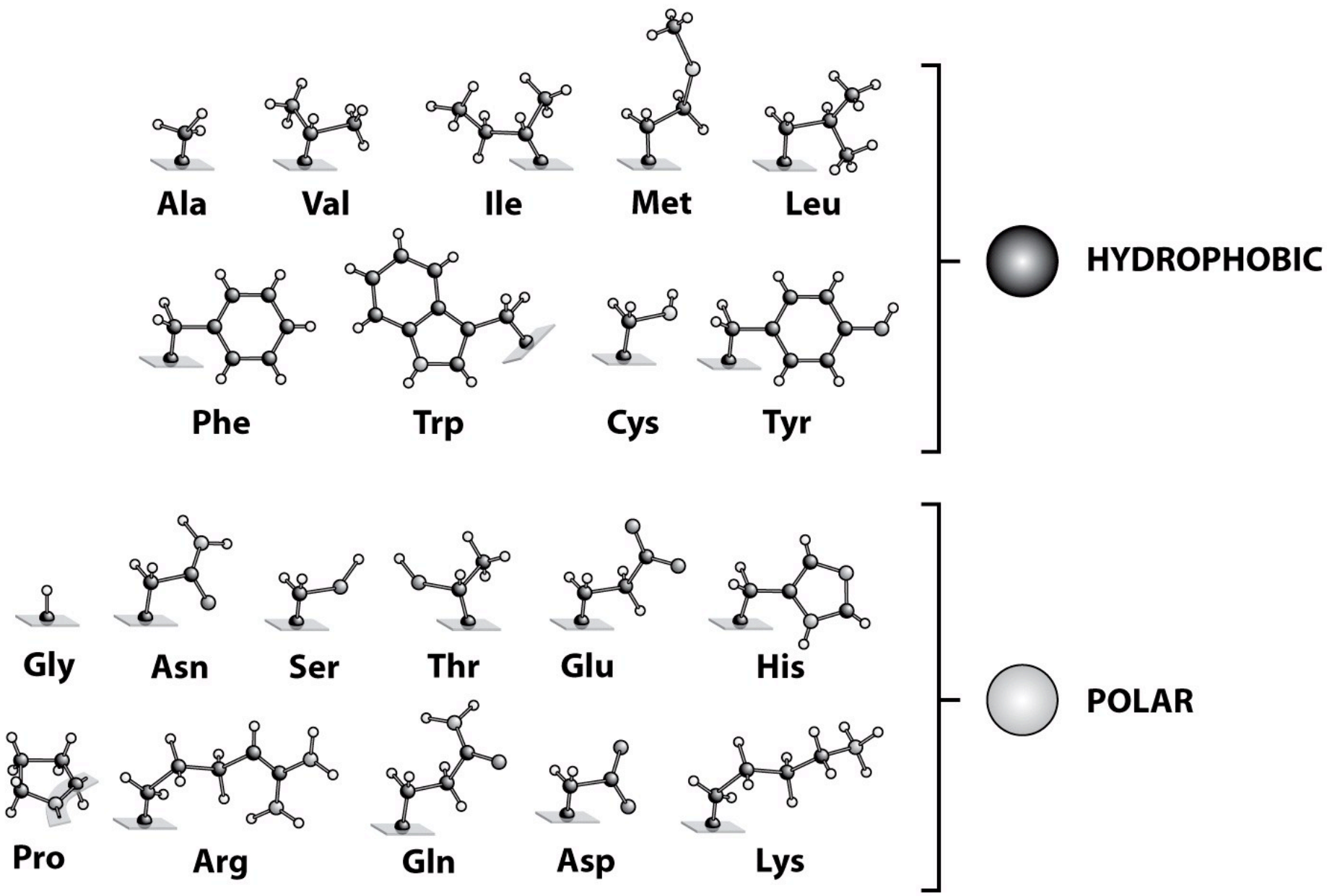

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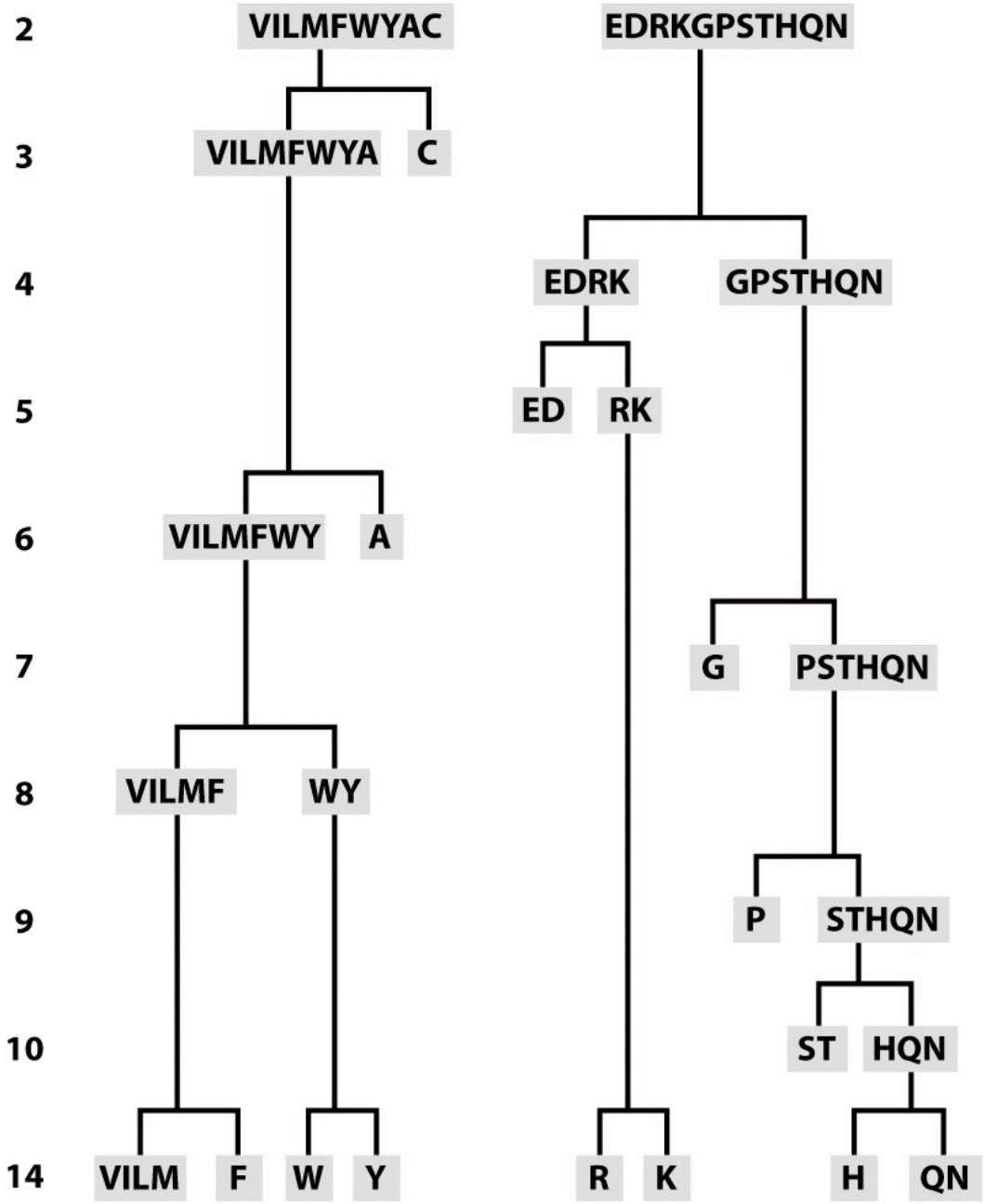

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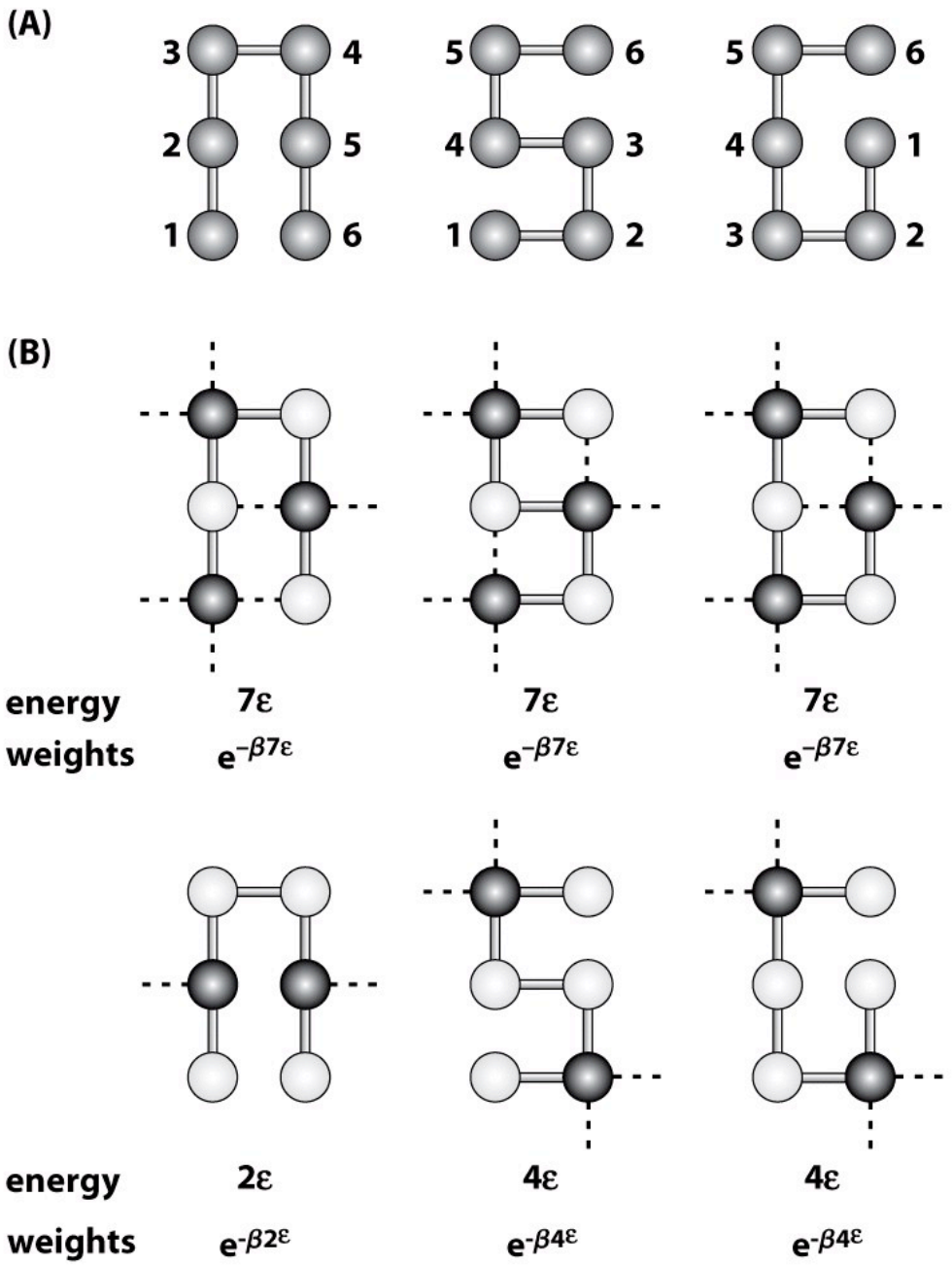

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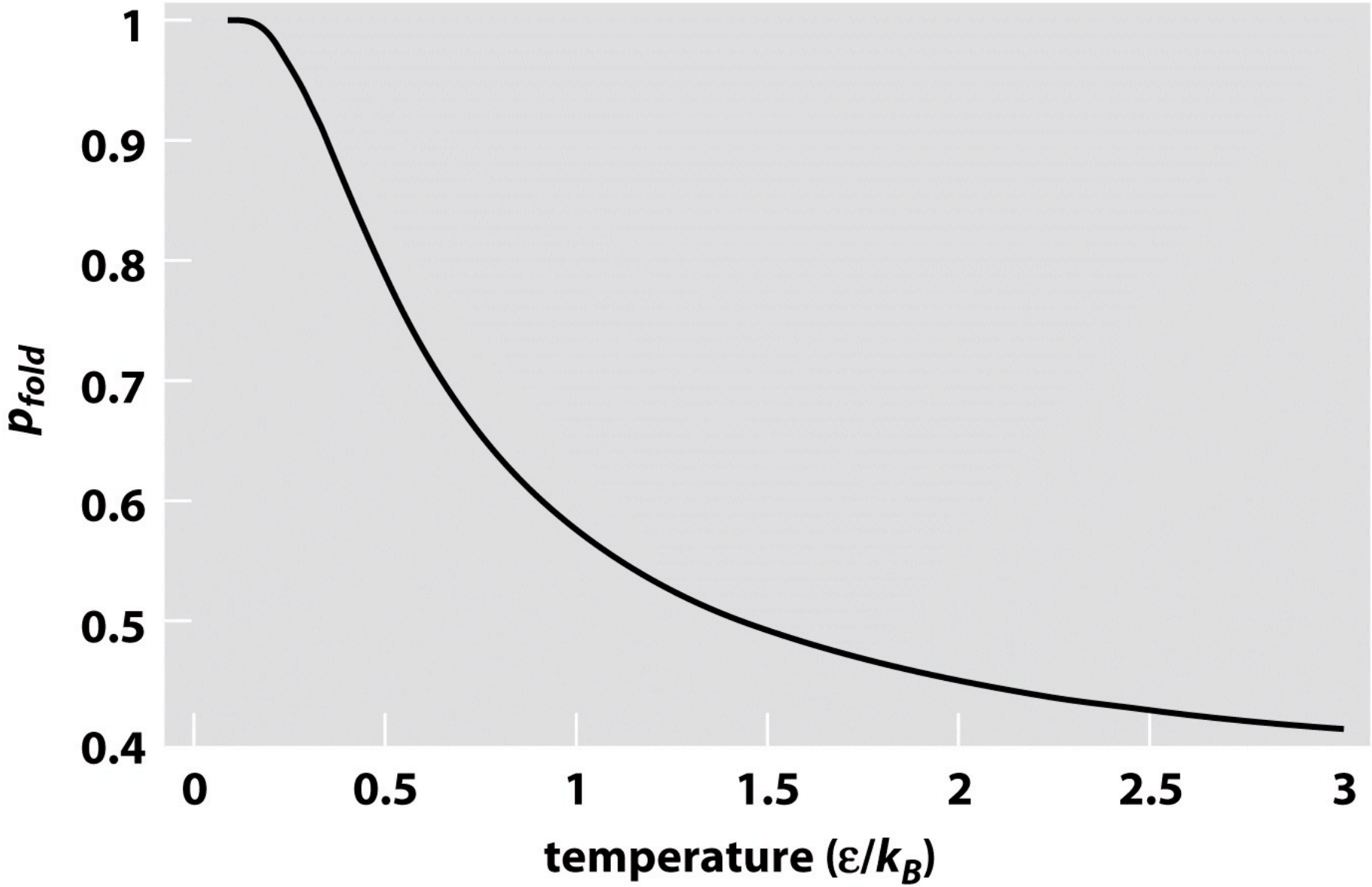

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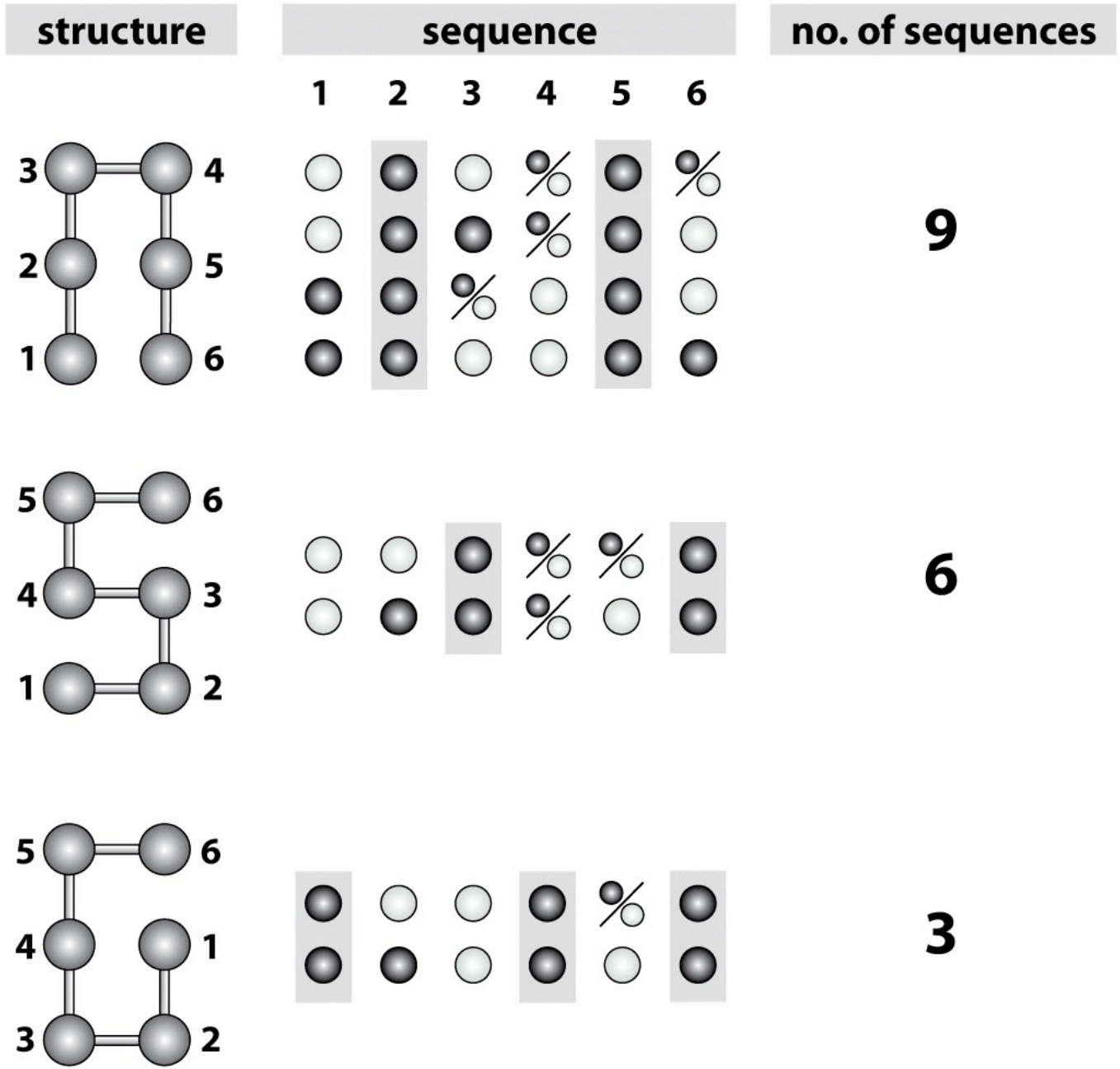

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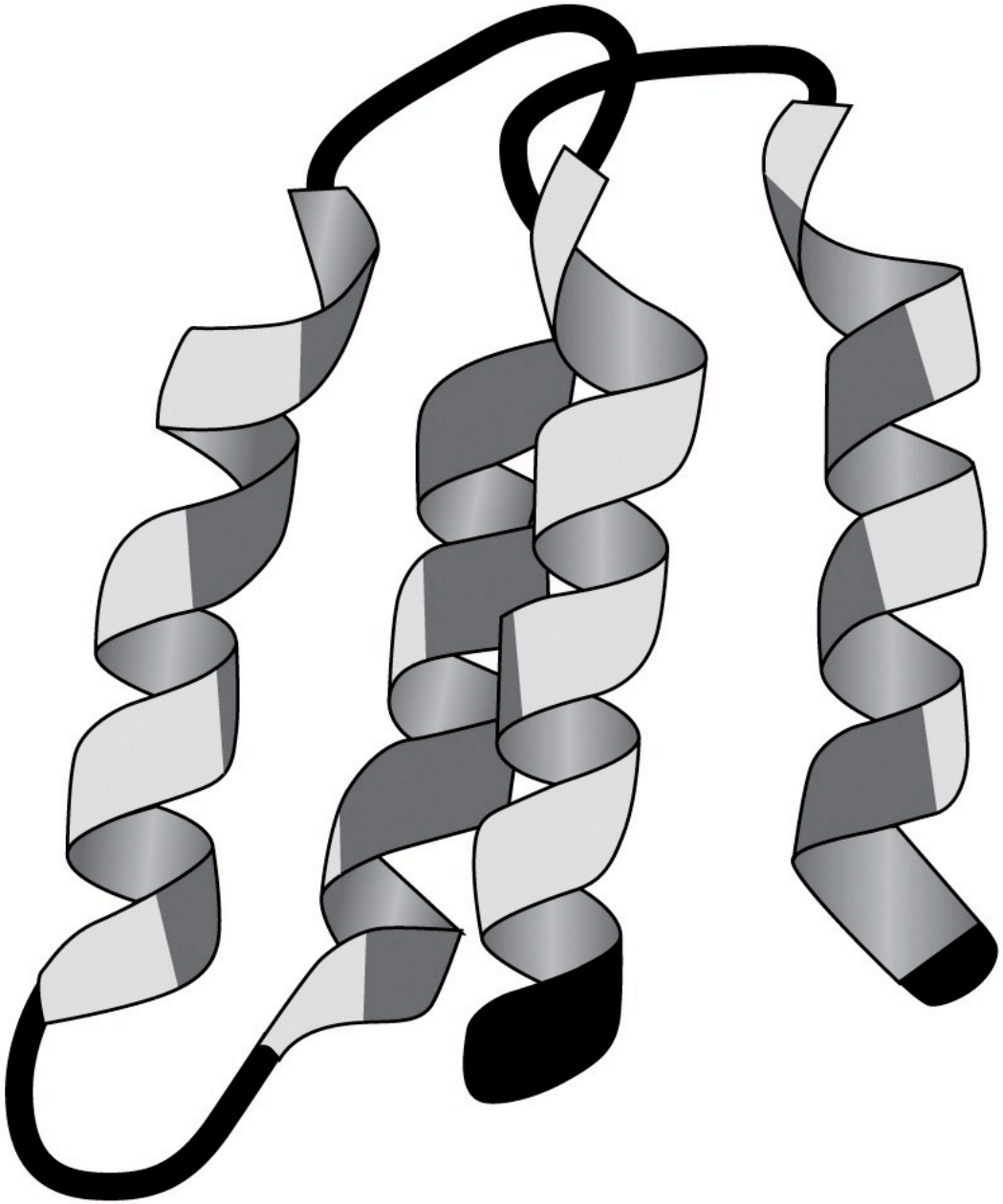

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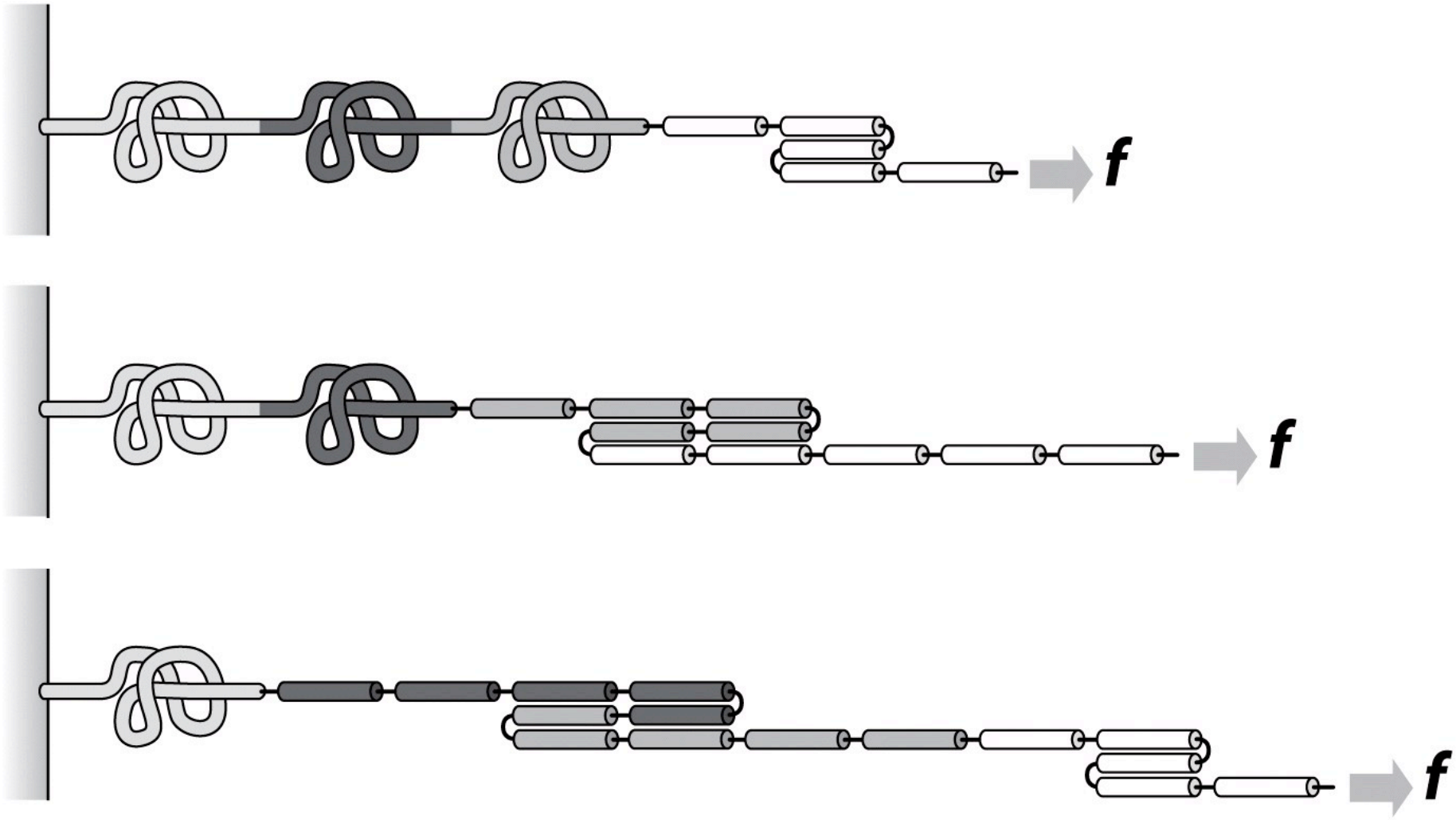

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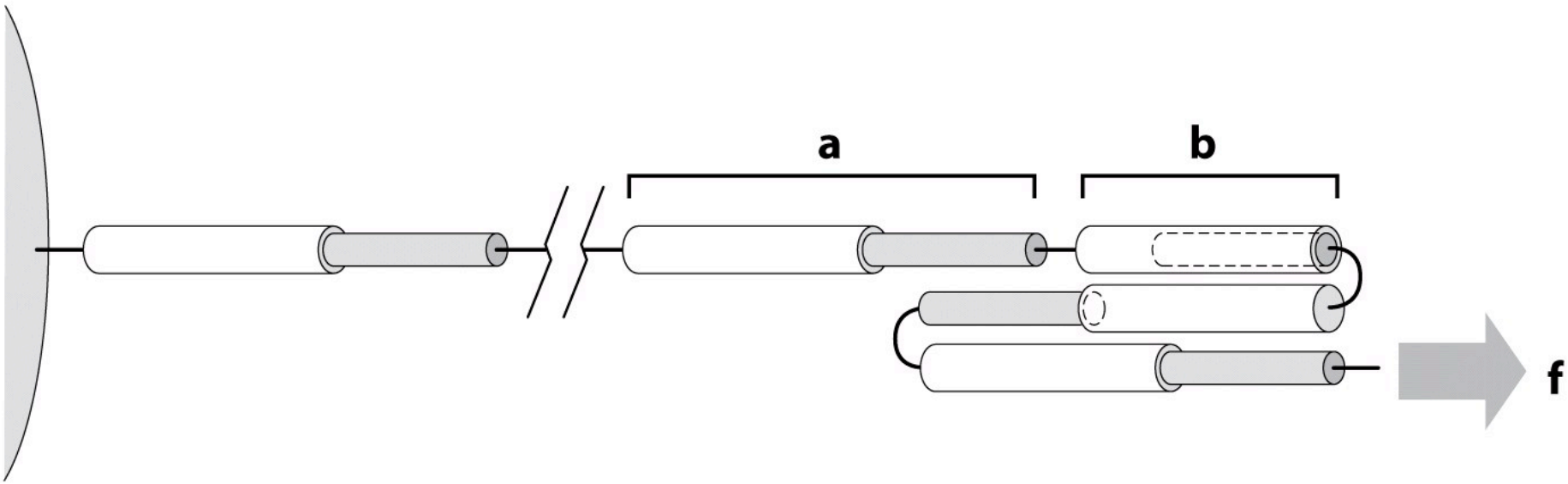

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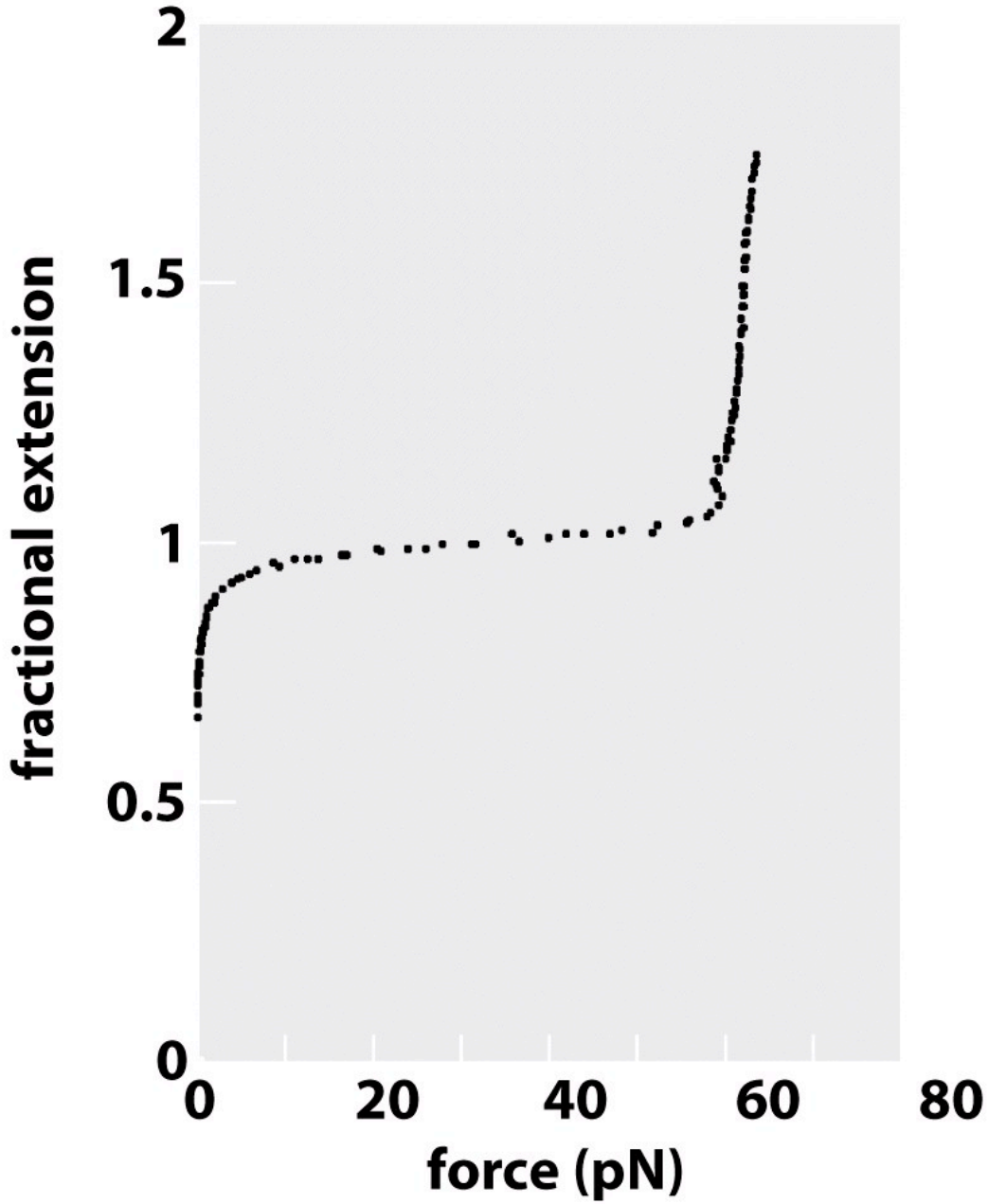

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