

2010-10-27

MACROMOLECULES AS RANDOM WALKS

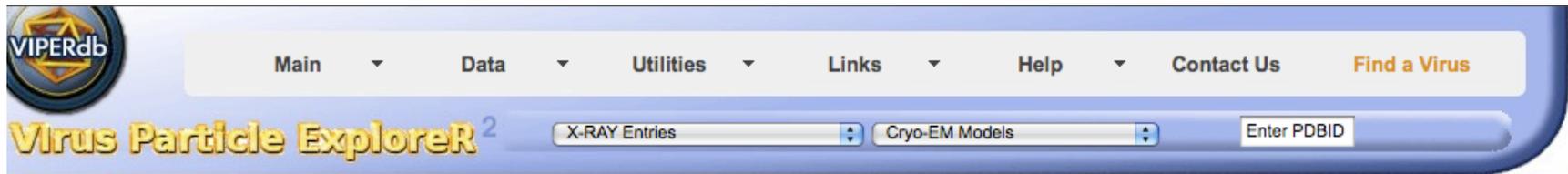
Ref.: Phys. Biol. Of the Cell

Macromolecular Structure

The screenshot shows the RCSB PDB website homepage. At the top left is the RCSB PDB logo (Protein Data Bank). At the top right, it states "A MEMBER OF THE PDB" and "An Information Portal to Biological Macromolecular Structures". Below this, it says "As of Tuesday Oct 26, 2010 at 5 PM PDT there are 68840 Structures" with links to RSS, help, and PDB Statistics. A search bar is located below the header, with "PDB ID or Text" as a placeholder and "Search" and "Advanced Search" buttons. On the left side, there are three main navigation menus: "MyPDB" (Login, Register), "Home" (News, Policies, FAQ, Contact, About, Careers, Links, Sitemap, Features), and "Deposition" (Services, Microscopy, X-ray, NMR, Validation, Beamline, Tools). The main content area features a large heading "A Resource for Studying Biological Macromolecules" followed by introductory text. Below this is a "Featured Molecules" section with a "Structural View of Biology" header and a "Protein Synthesis" feature. The "Molecule of the Month" is "Riboswitches", with a description and a "Full Article..." link. Another featured molecule is "Isoxanthopterin deaminase", with a description and a "Full Article | PSI Structural Biology Knowledgebase" link. On the right side, there is a "Customize This Page" section with "New Features" and "Integration with Binding Affinity Data from" (Latest features released: Website Release Archive). Below that is the "RCSB PDB News" section, showing the "2010-10-26 Newsletter Published" with a thumbnail of the newsletter and a note that the fall 2010 issue highlights the latest website release and a new version of pdb_extract.

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

Multimolecular Structure



The image shows the top navigation bar of the VIPERdb website. It includes the VIPERdb logo on the left, followed by a menu with items: Main, Data, Utilities, Links, Help, Contact Us, and Find a Virus. Below the menu is a search bar with two dropdown menus: 'X-RAY Entries' and 'Cryo-EM Models', and a text input field labeled 'Enter PDBID'.

Close this Introduction and start using VIPERdb²
Do not show this message again

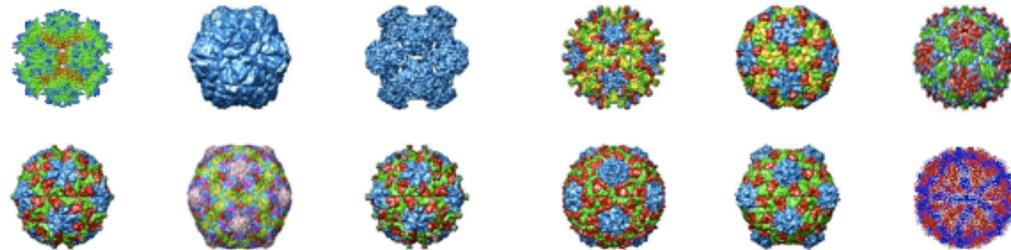
WELCOME

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 corresponding 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 \$\Phi\$ - \$\Psi\$ 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](#)):



1 online



Main | Data & Analysis | Utilities | Search | Contact Us |
Help | Links | Mailing List | Cite VIPERdb | Disclaimer

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<http://viperdbscripps.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

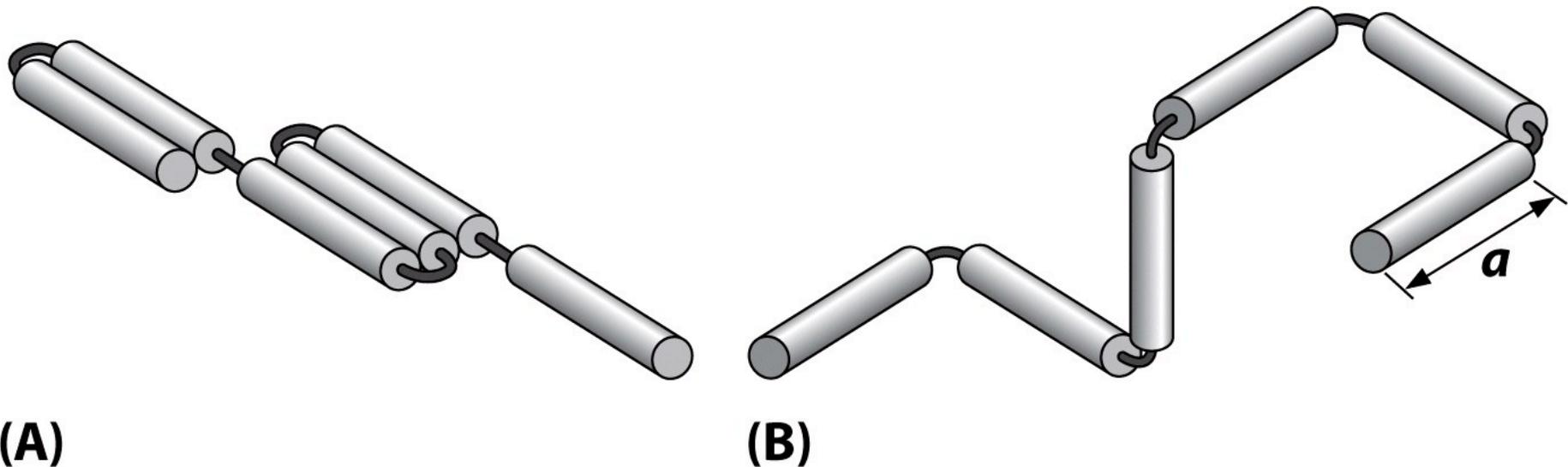


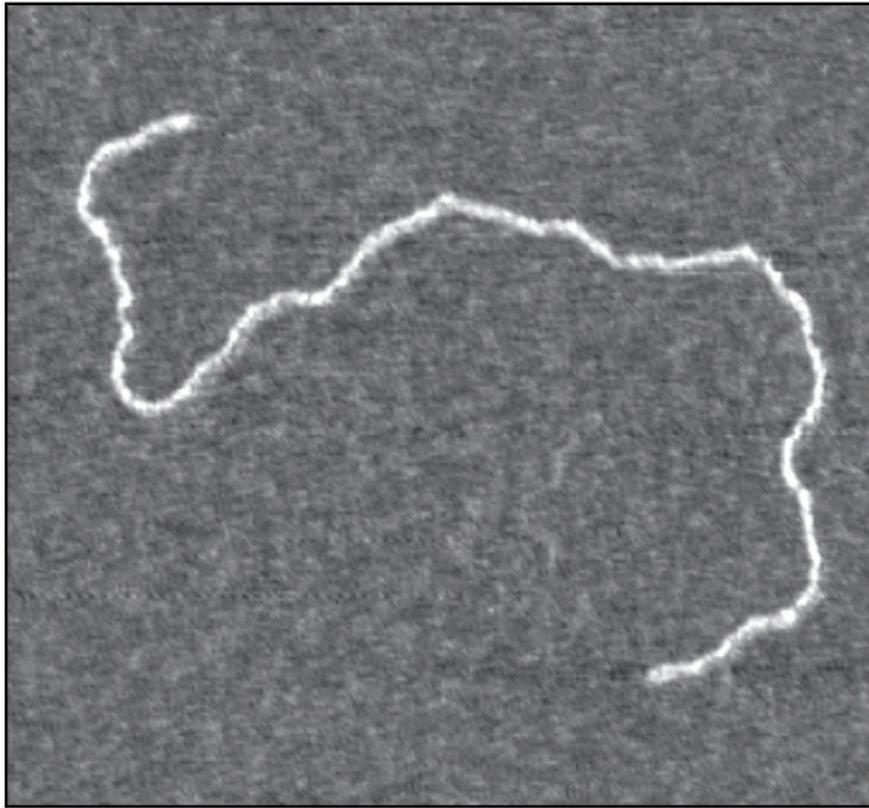
Figure 8.1 Physical Biology of the Cell (© Garland Science 2009)

a = segment length

Kuhn Segments: rigid rods
Flexible hinges

DNA as a Random Walk

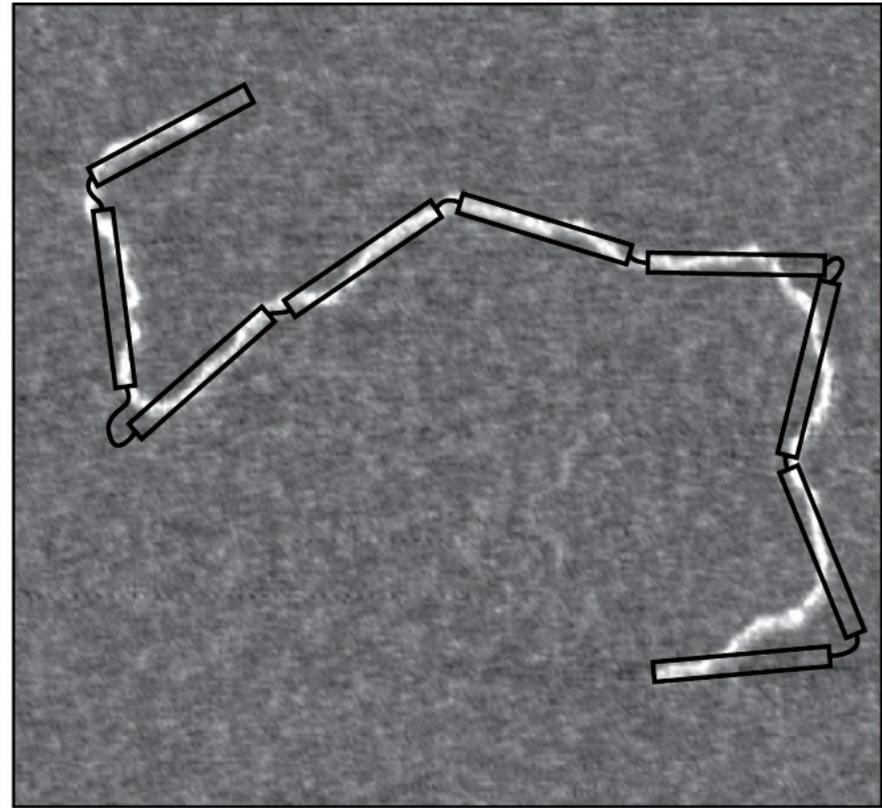
(A)



100 nm

AFM image of DNA on a surface in air

(B)



Fitted segments for the DNA molecule

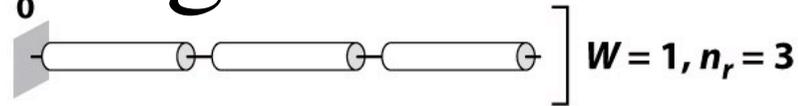
Random Walk Size

Mean distance of walker $\langle R \rangle$

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

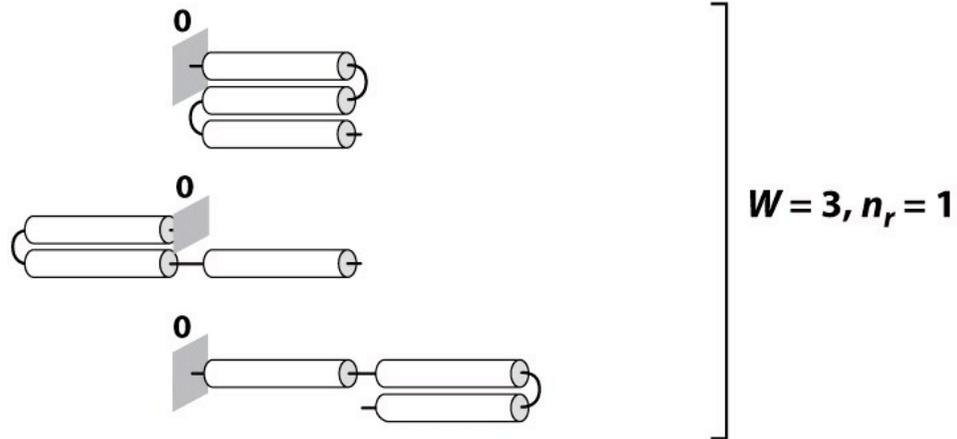
Relation of variance $\langle R^2 \rangle$ with segment length (a) and number of steps (N)

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:

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

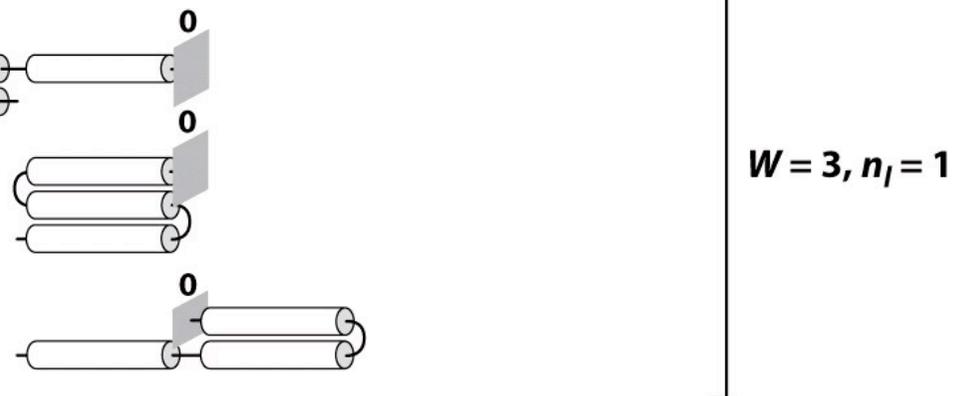


Figure 8.3 Physical Biology of the Cell (© Garland Science 2009)

End-to-End Distance Probability

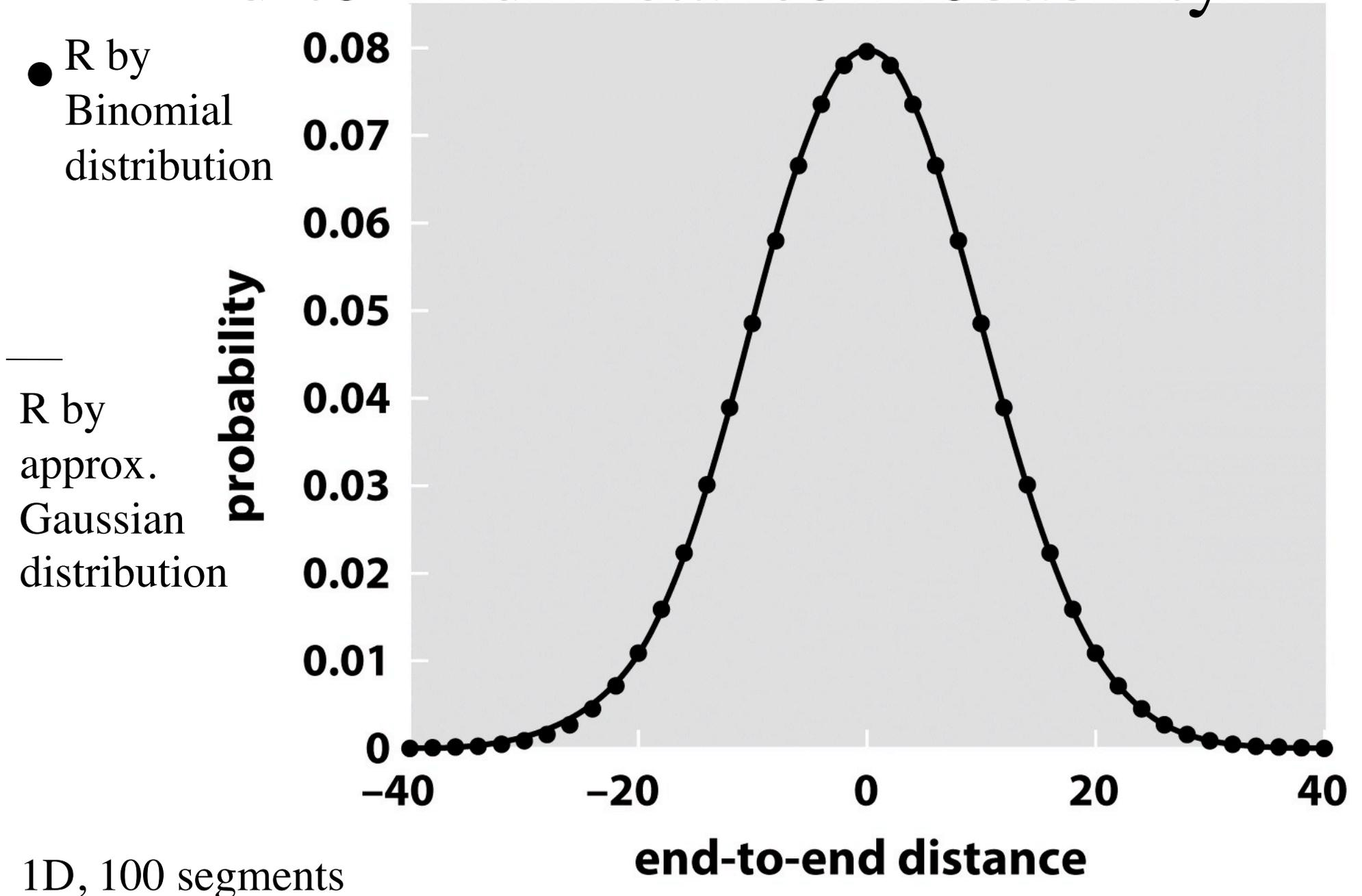
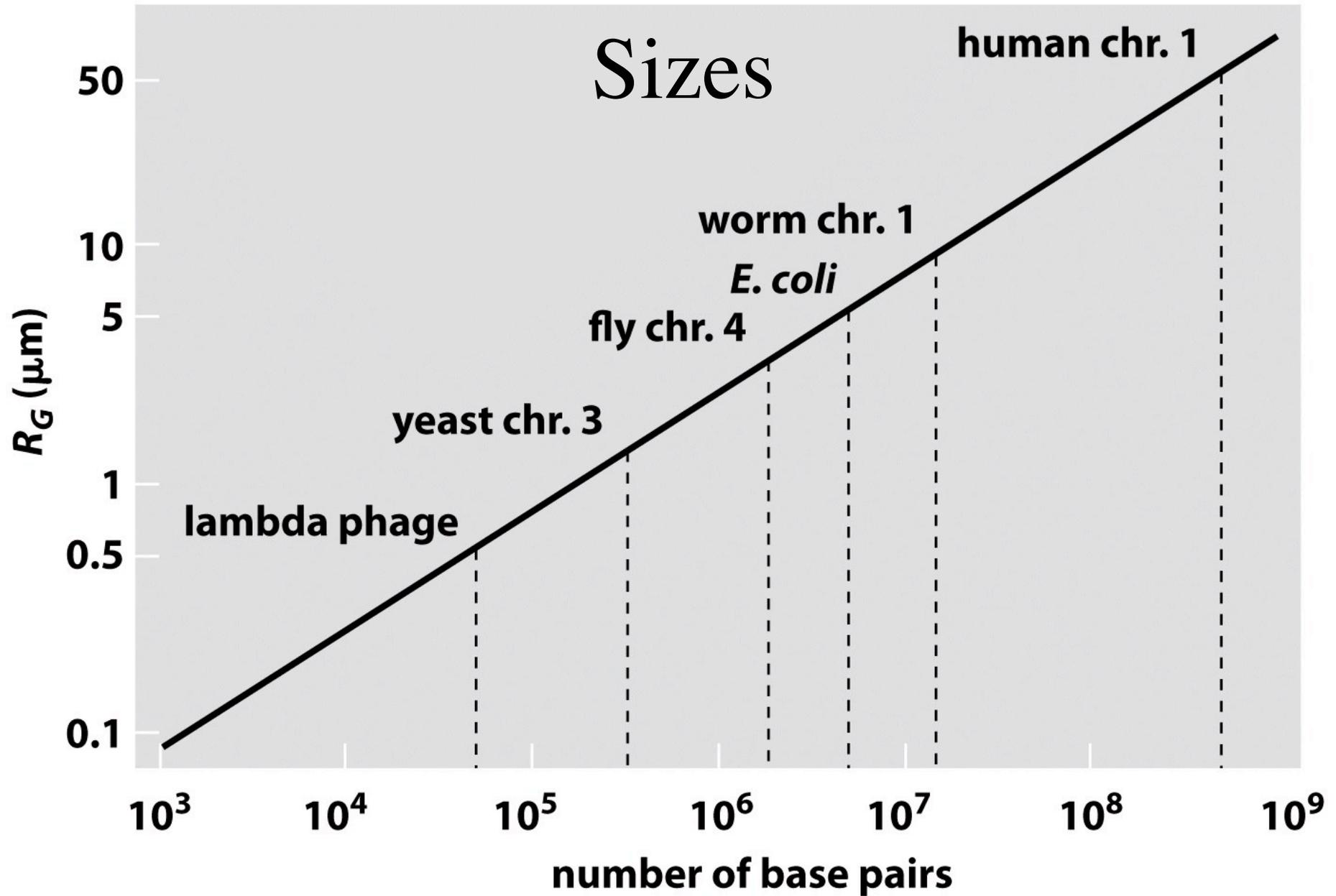


Figure 8.4 Physical Biology of the Cell (© Garland Science 2009)

Estimates of Genomic DNA



Bacterial Genome

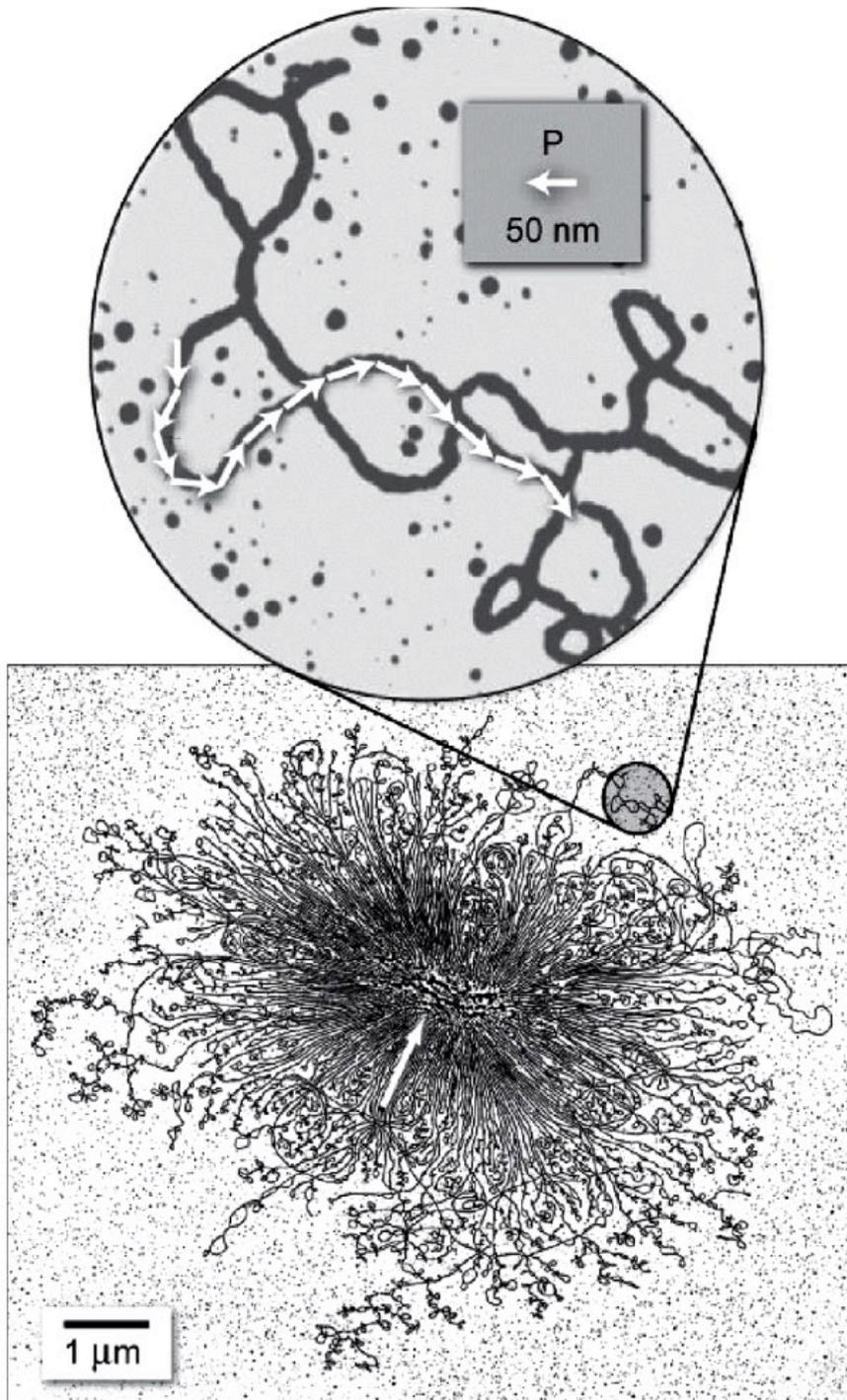
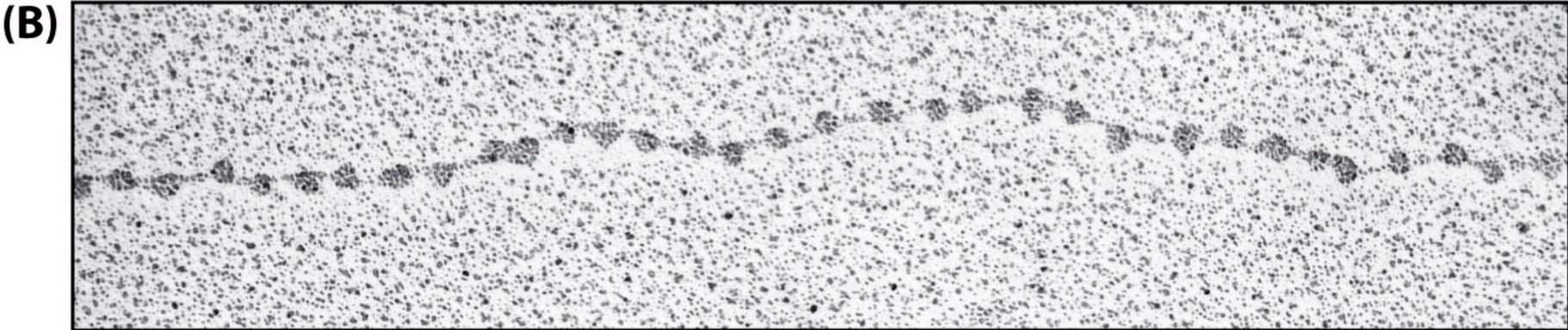
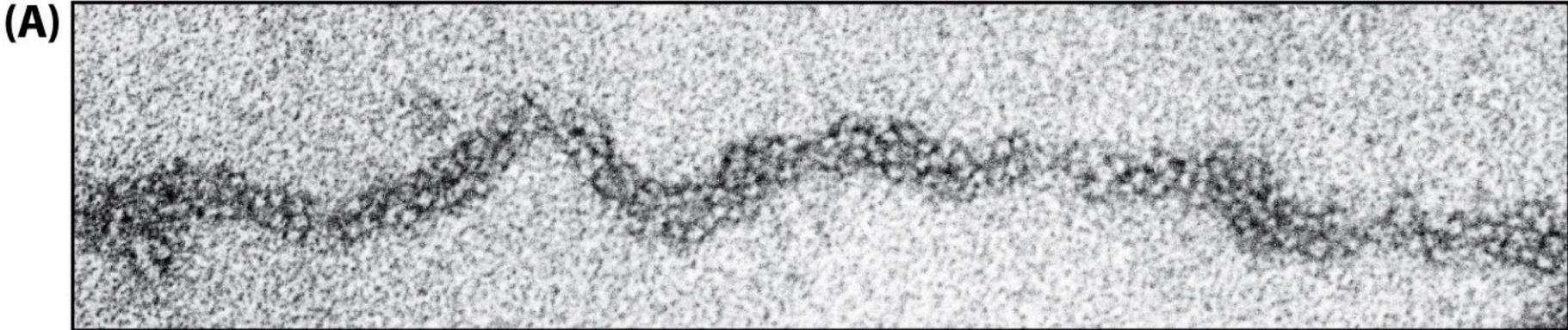


Figure 8.6 Physical Biology of the Cell (© Garland Science 2009)

Chromatin



50 nm

Figure 8.7 Physical Biology of the Cell (© Garland Science 2009)

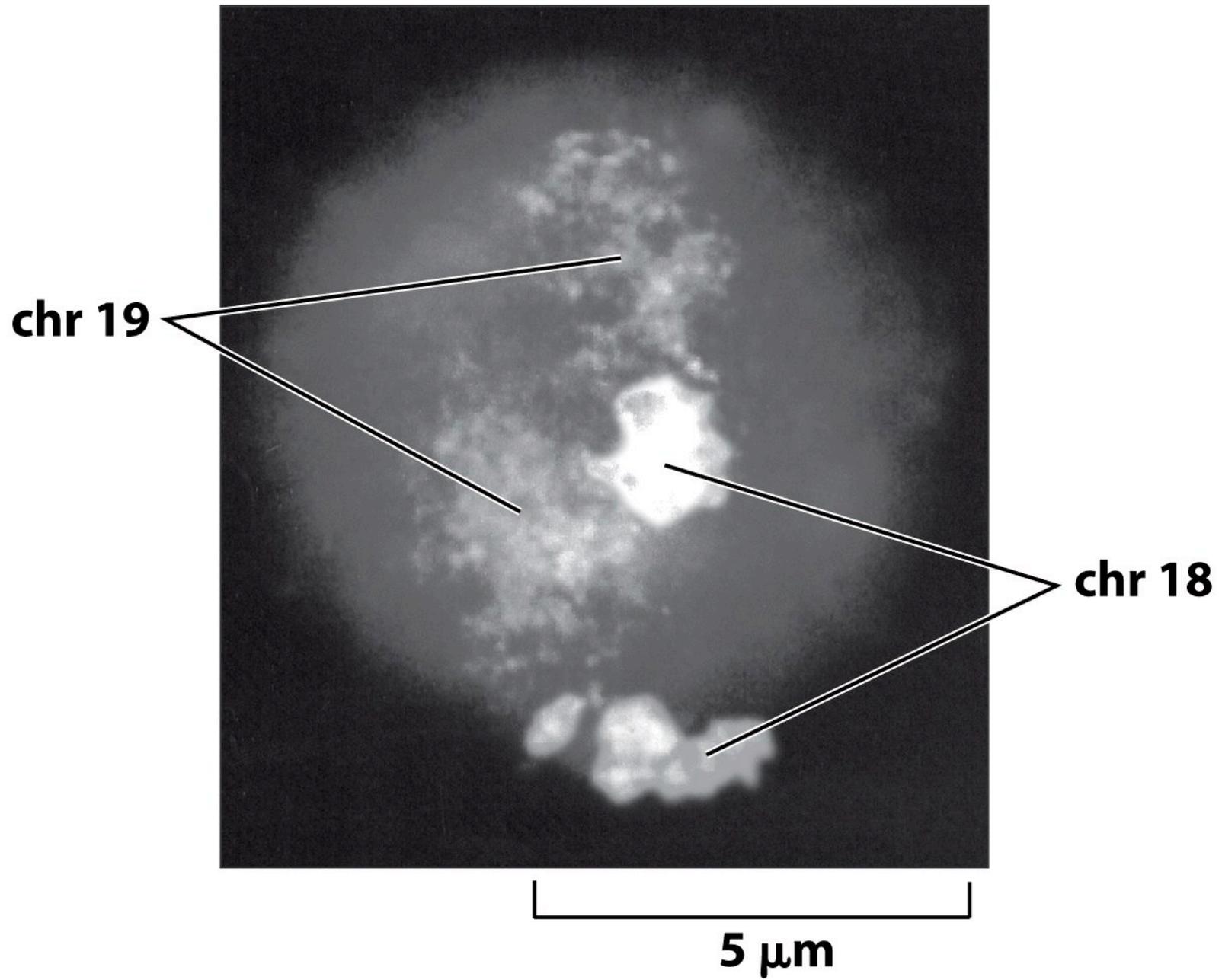


Figure 8.8 Physical Biology of the Cell (© Garland Science 2009)

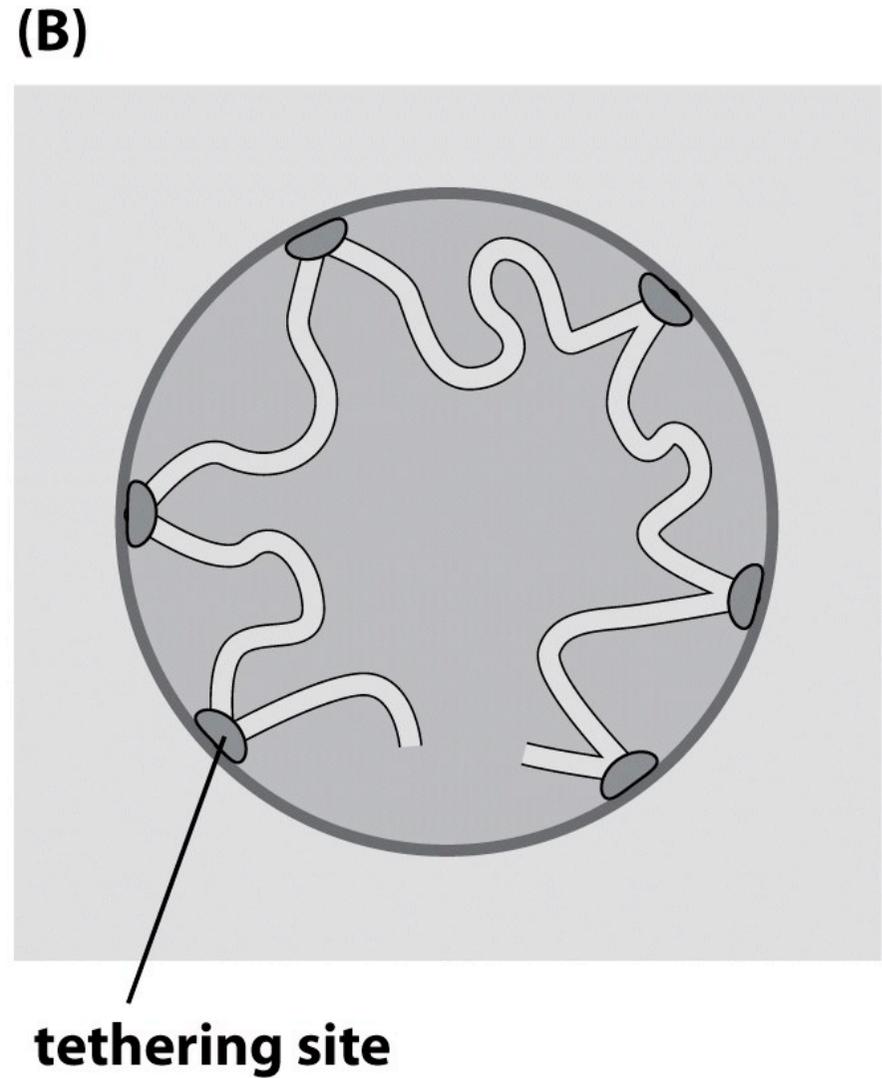
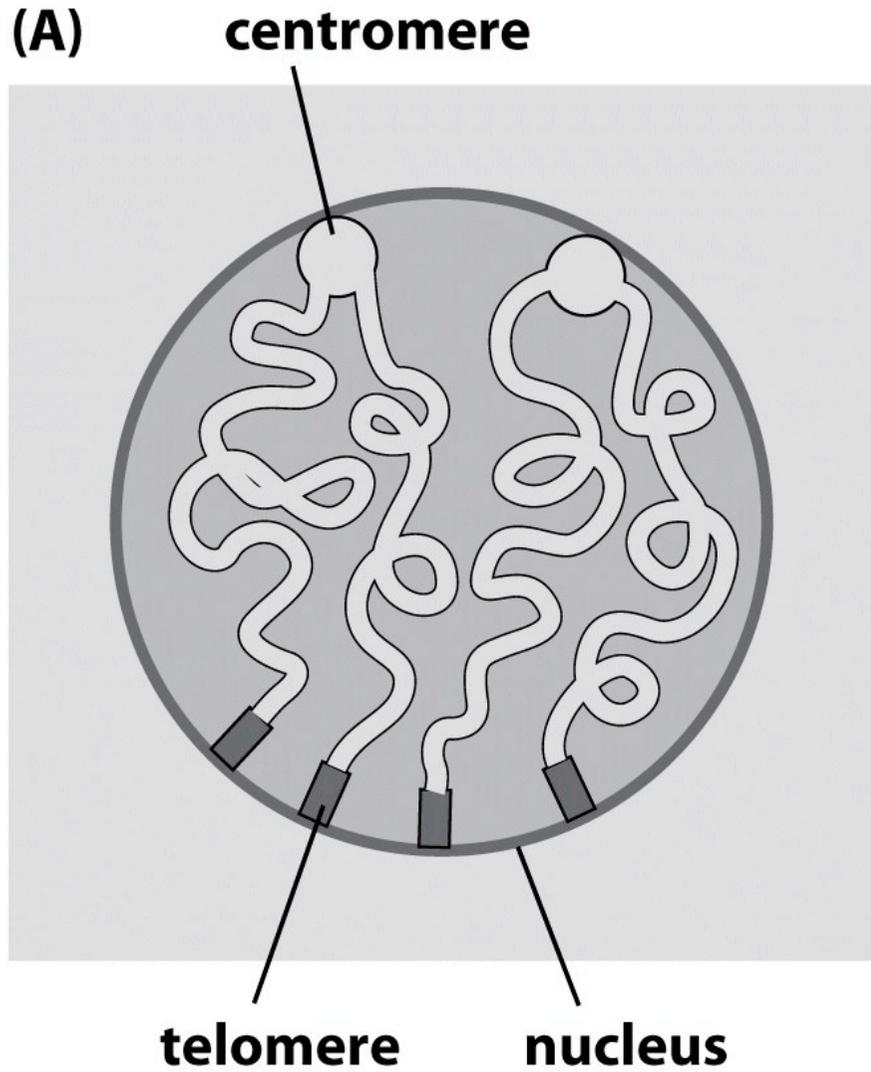


Figure 8.9 Physical Biology of the Cell (© Garland Science 2009)

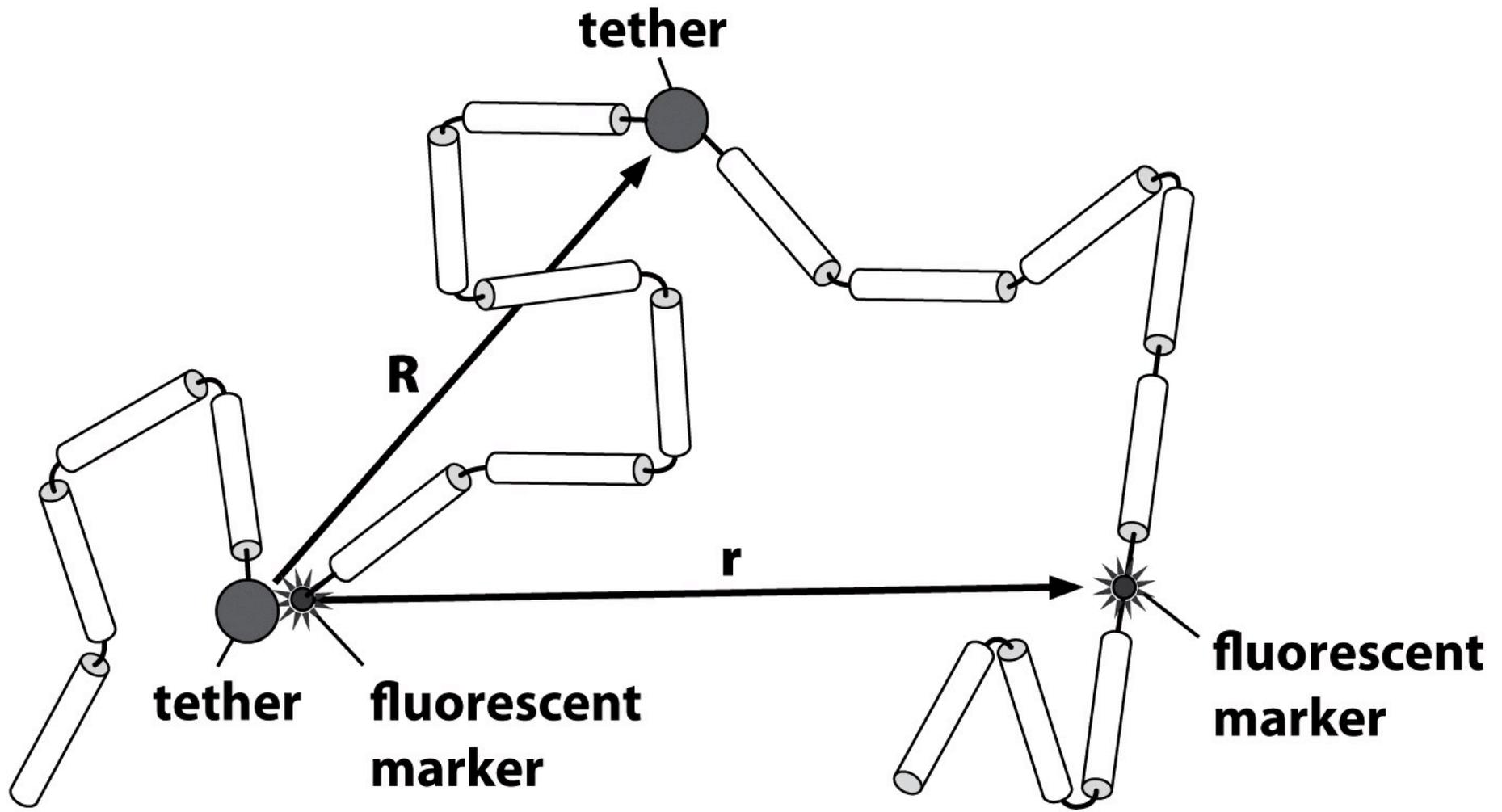


Figure 8.10 Physical Biology of the Cell (© Garland Science 2009)

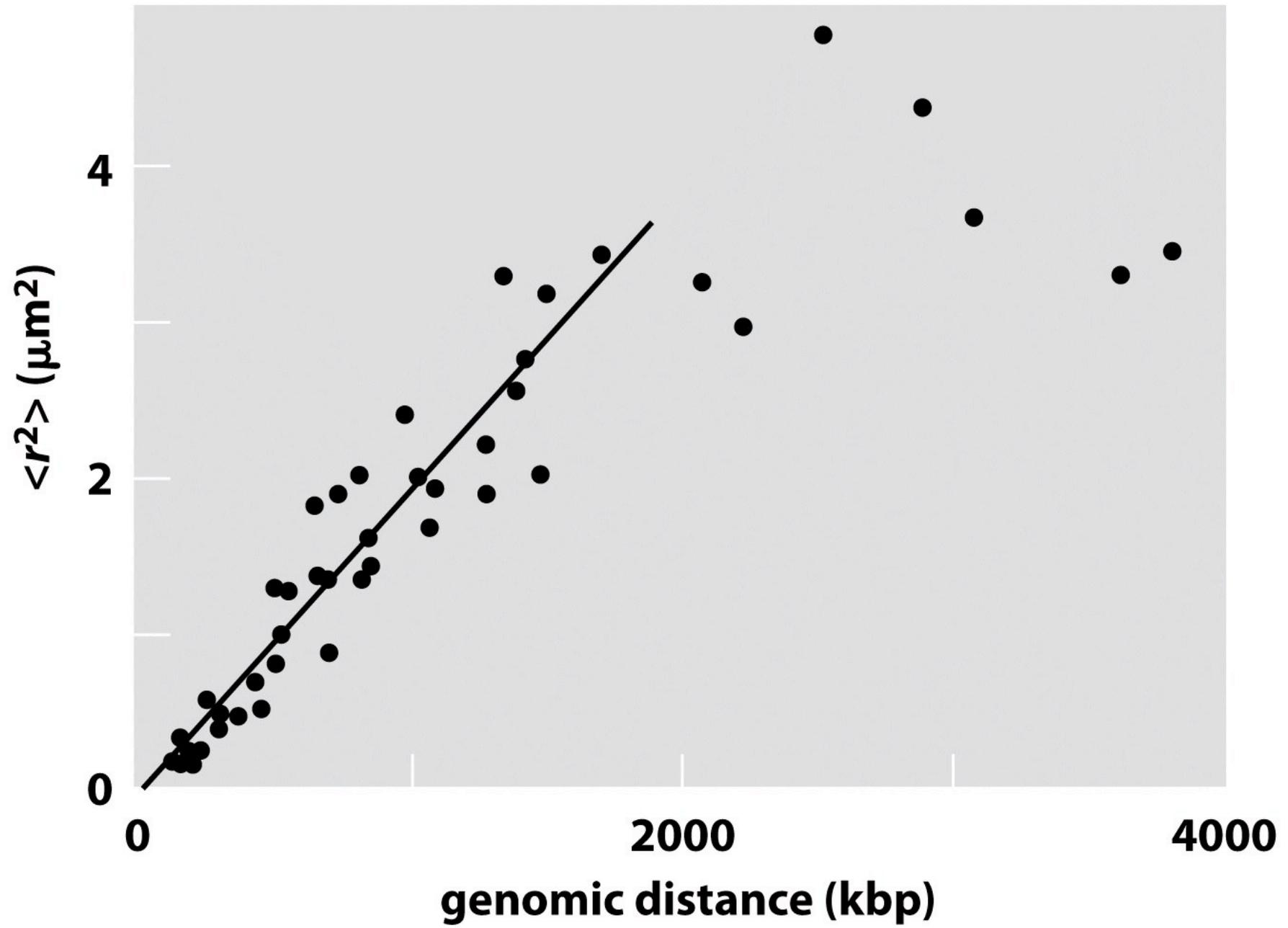


Figure 8.11 Physical Biology of the Cell (© Garland Science 2009)

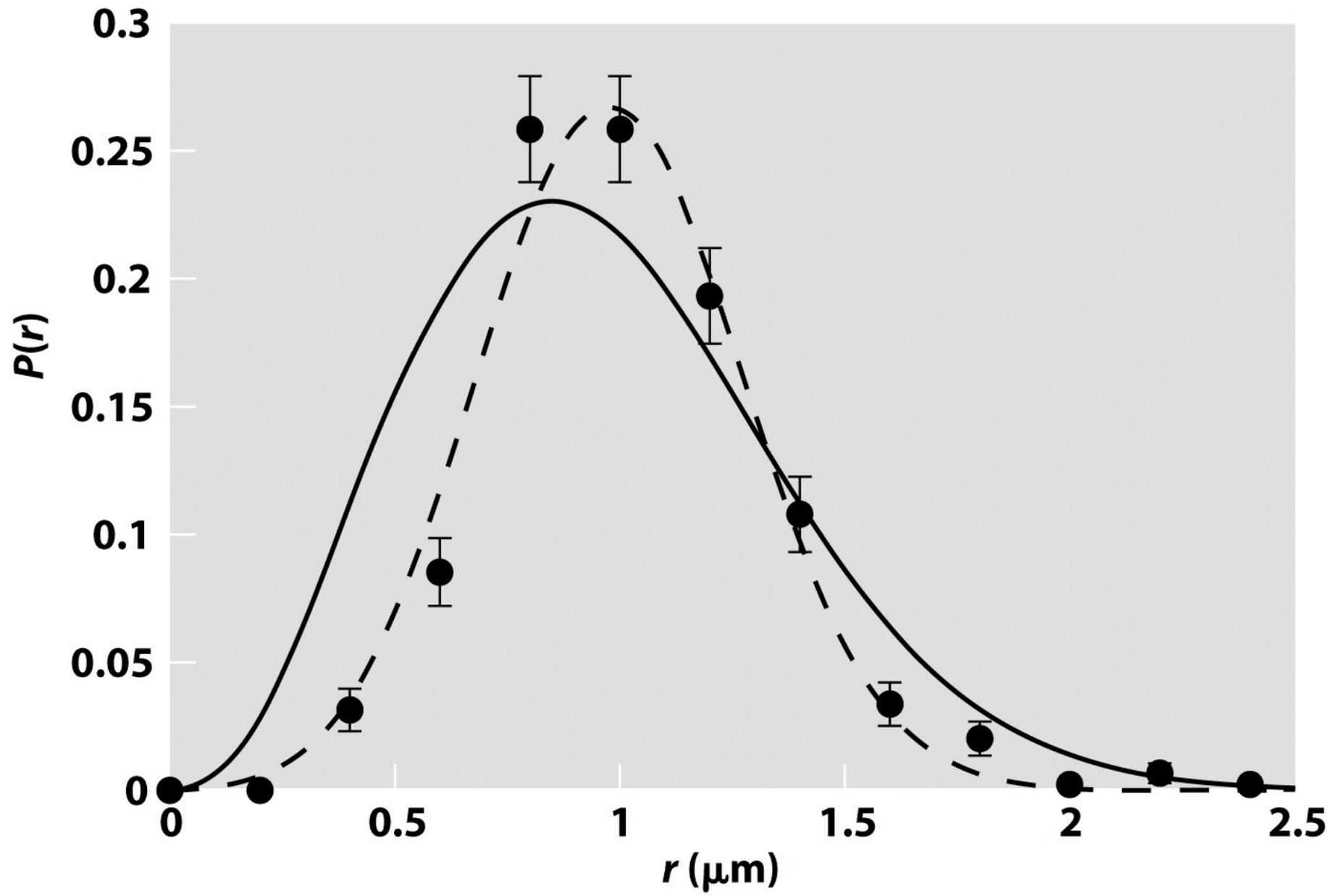


Figure 8.12 Physical Biology of the Cell (© Garland Science 2009)

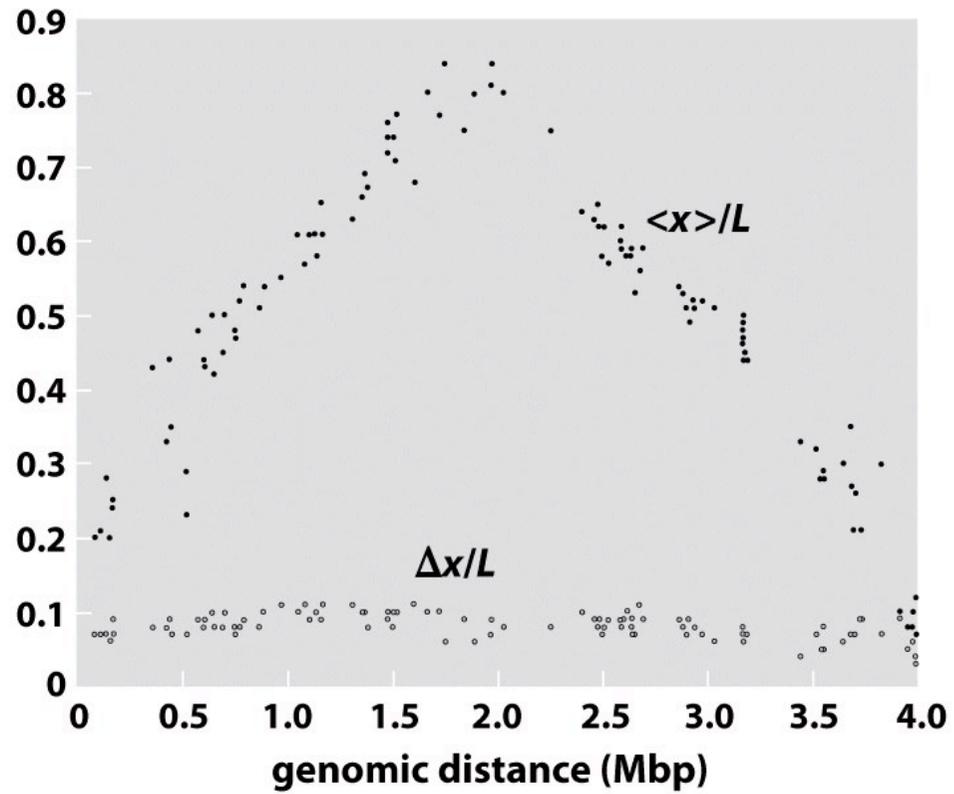
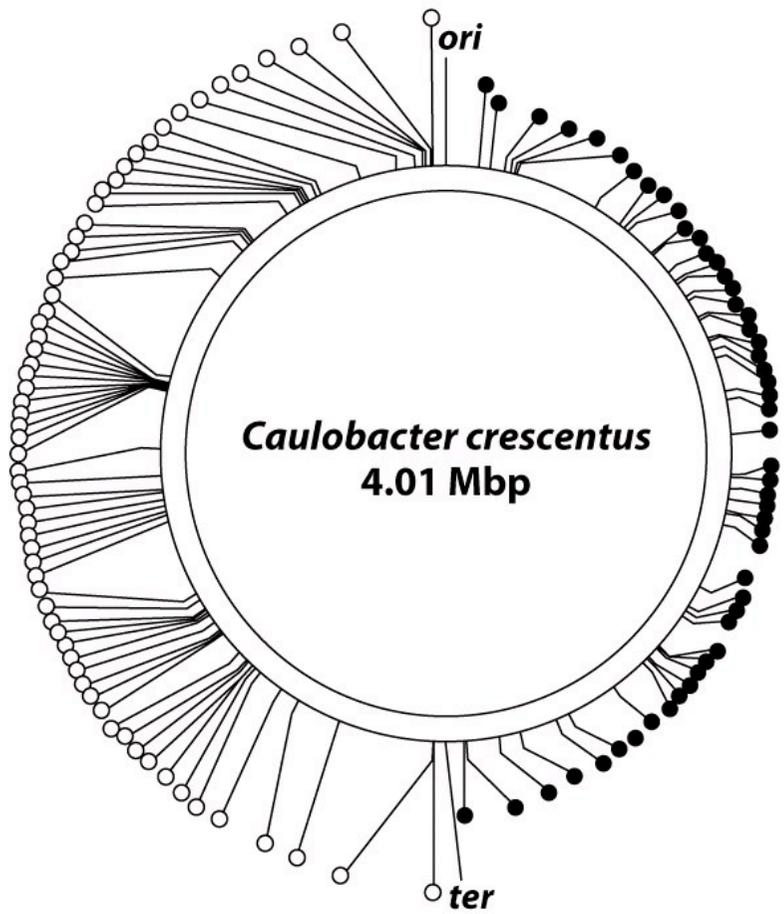
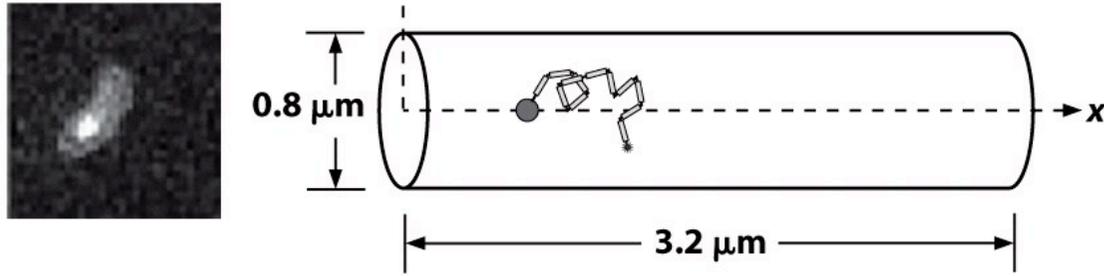
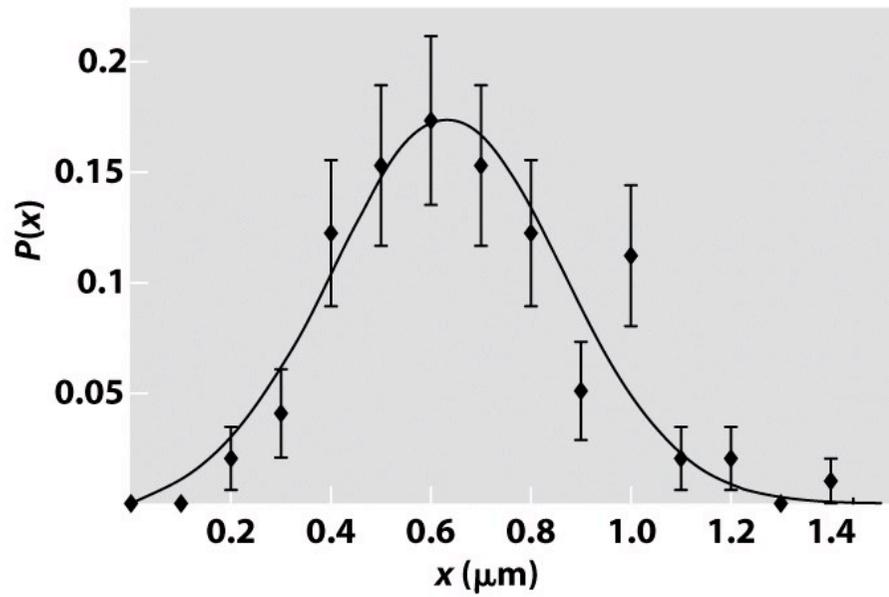


Figure 8.13 Physical Biology of the Cell (© Garland Science 2009)

(A)



(B)



(C)

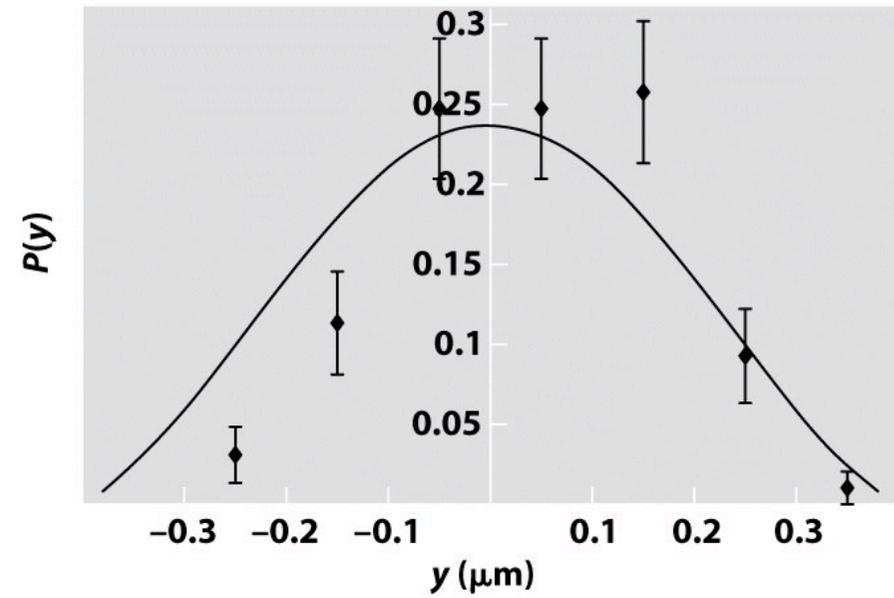


Figure 8.14 Physical Biology of the Cell (© Garland Science 2009)

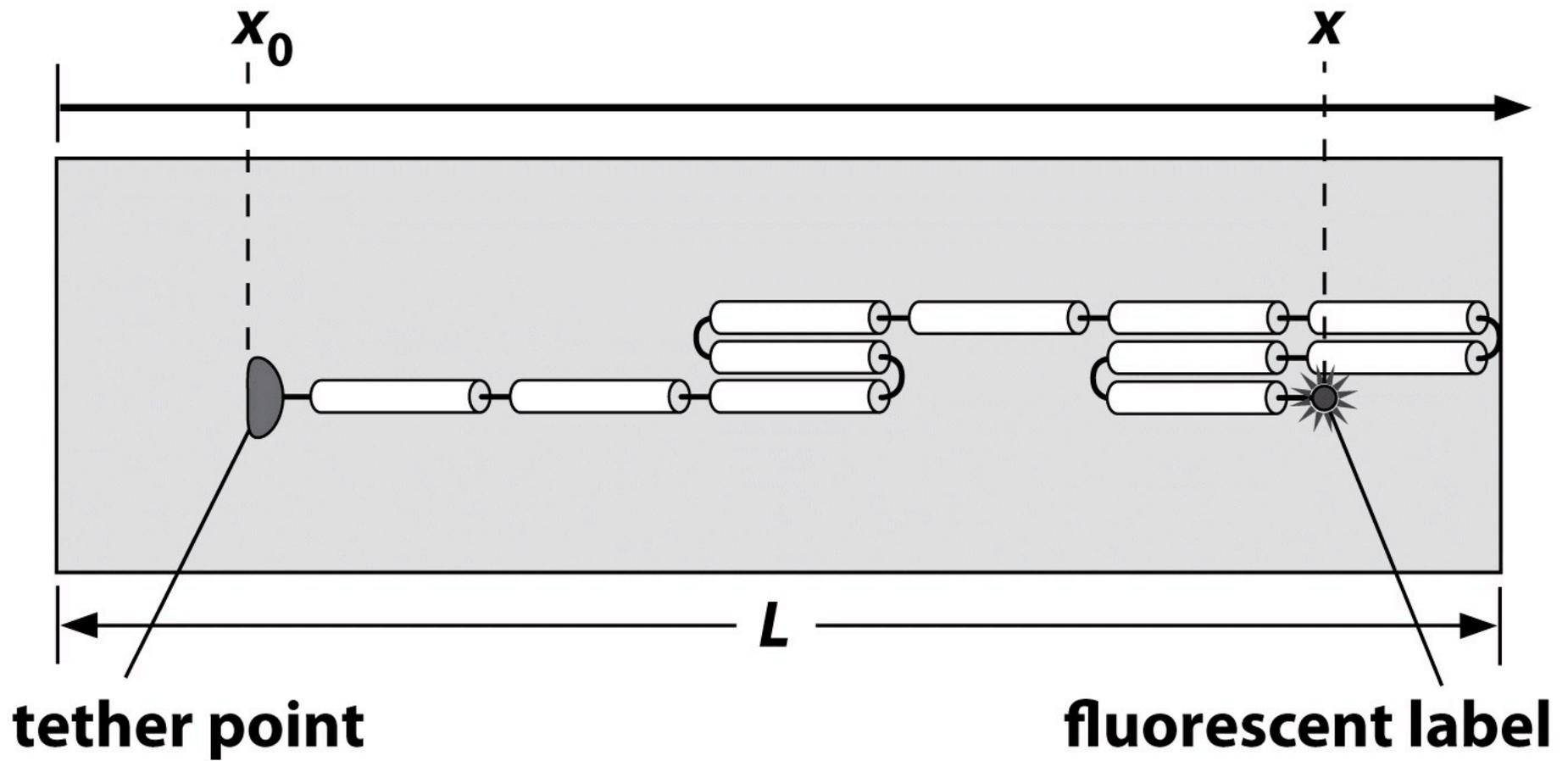


Figure 8.15 Physical Biology of the Cell (© Garland Science 2009)

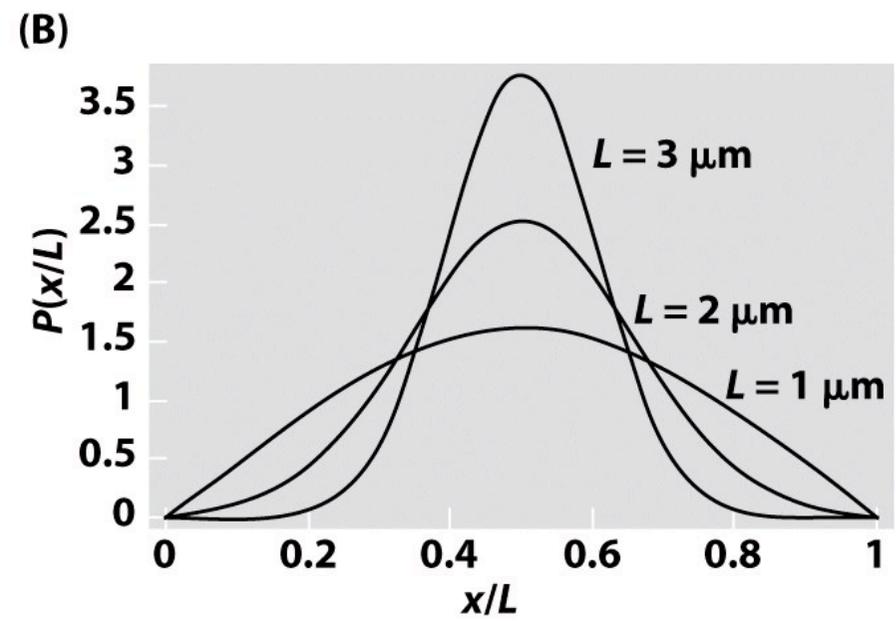
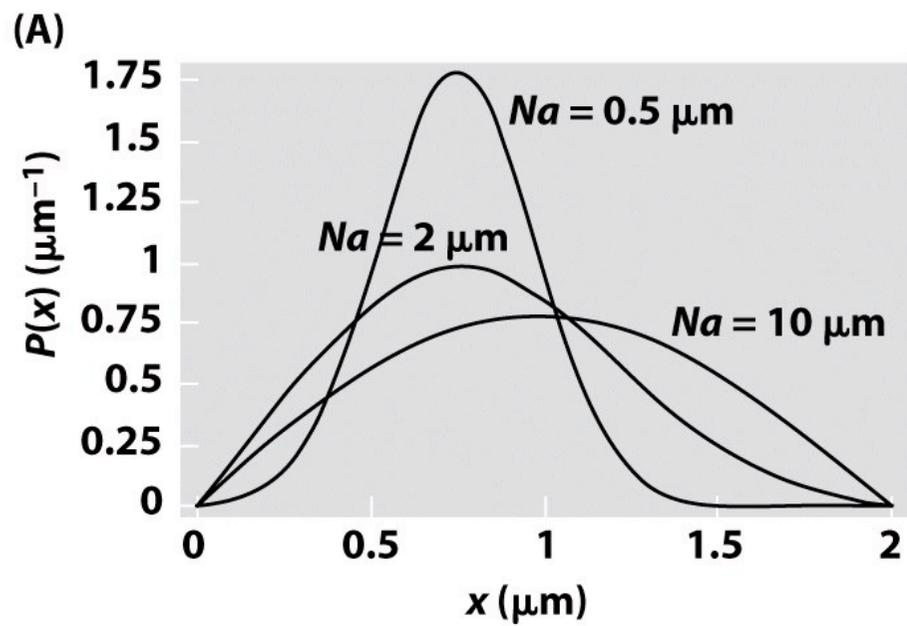


Figure 8.16 Physical Biology of the Cell (© Garland Science 2009)

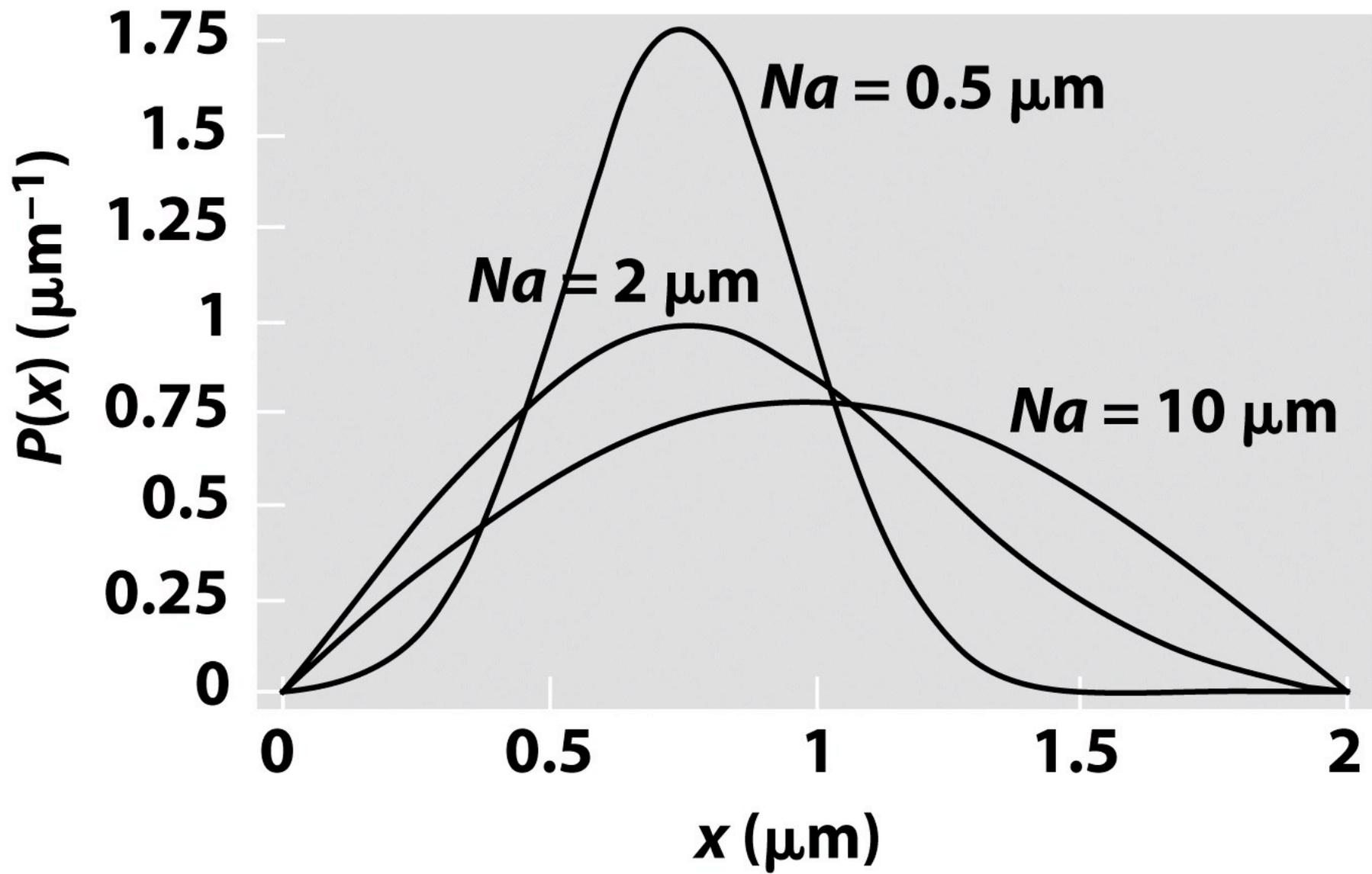


Figure 8.16a Physical Biology of the Cell (© Garland Science 2009)

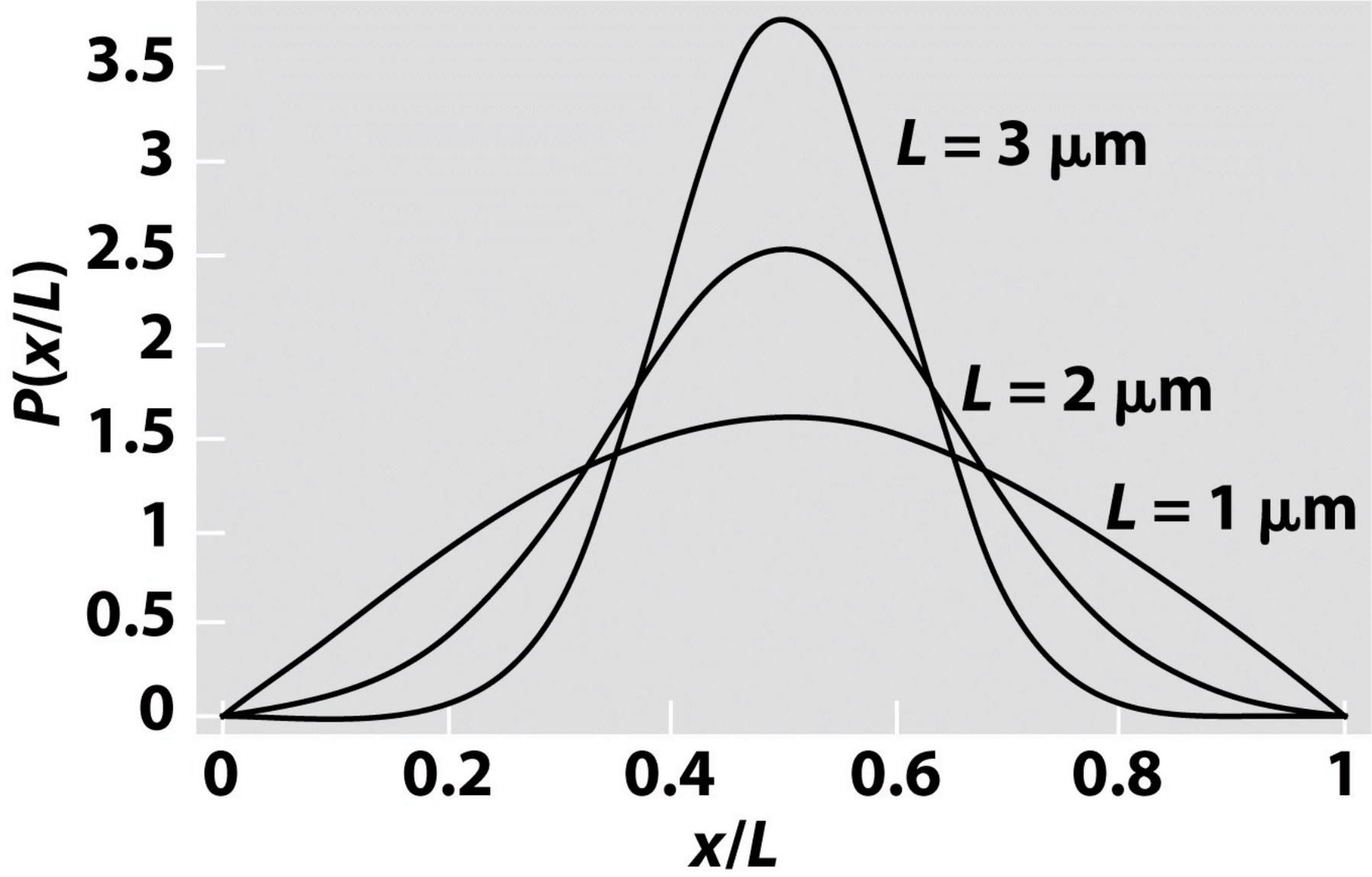


Figure 8.16b Physical Biology of the Cell (© Garland Science 2009)

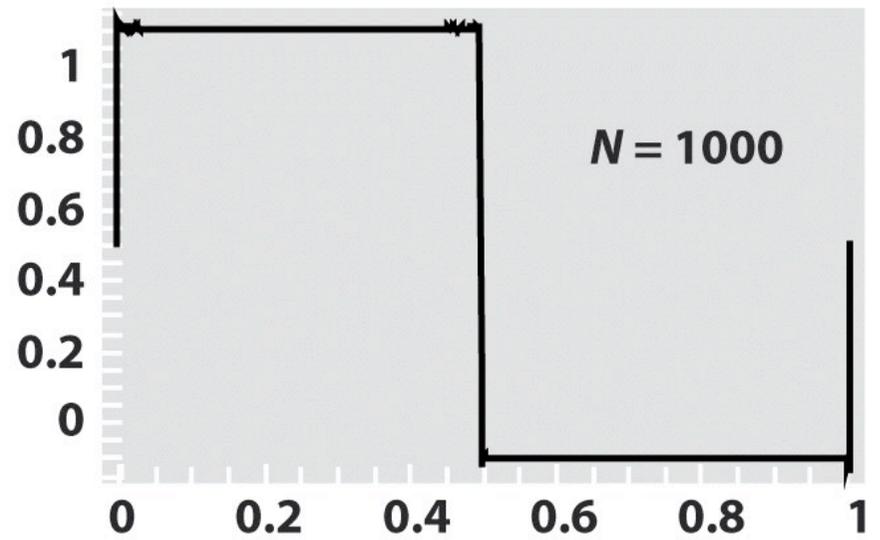
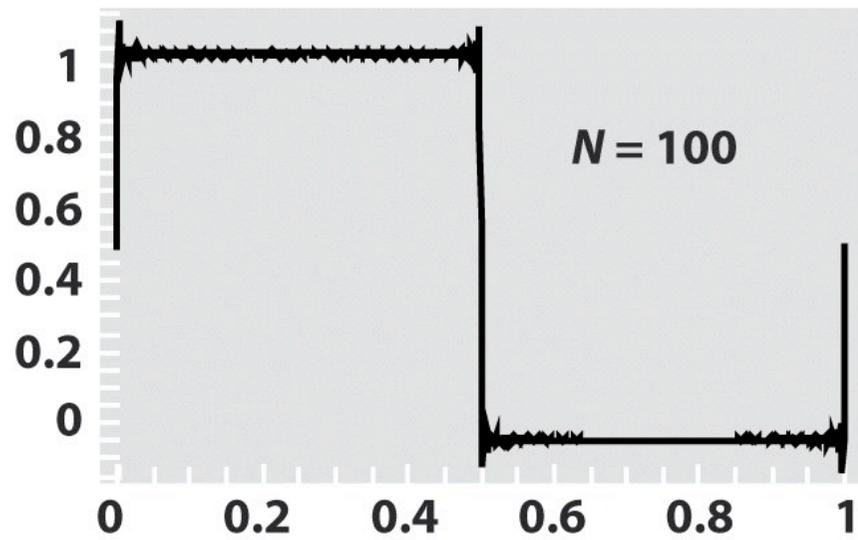
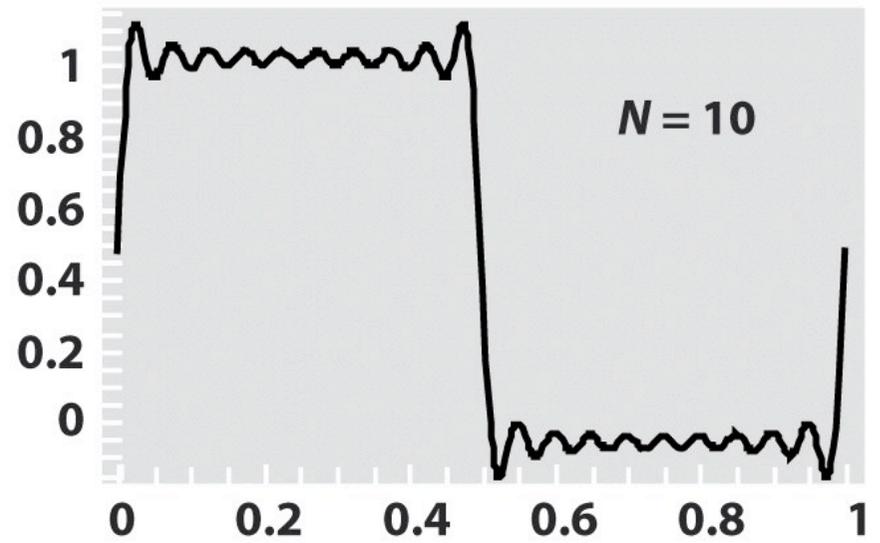
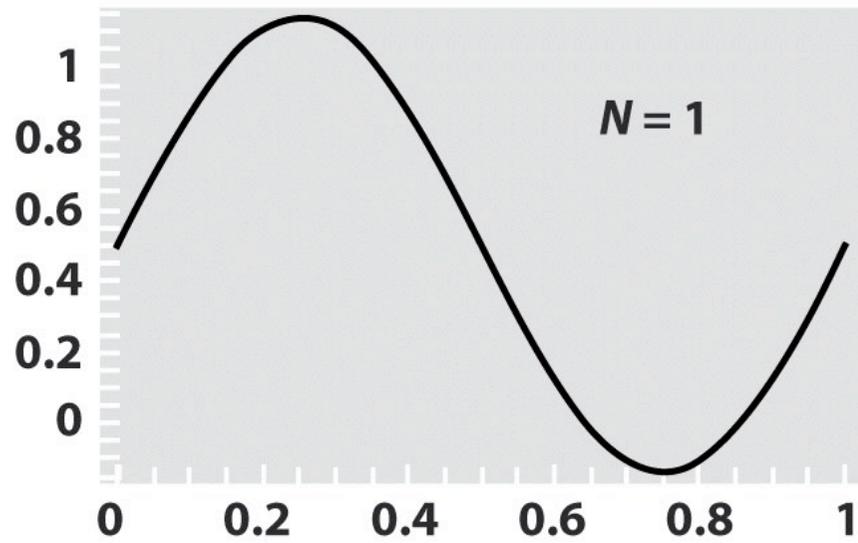


Figure 8.17 Physical Biology of the Cell (© Garland Science 2009)

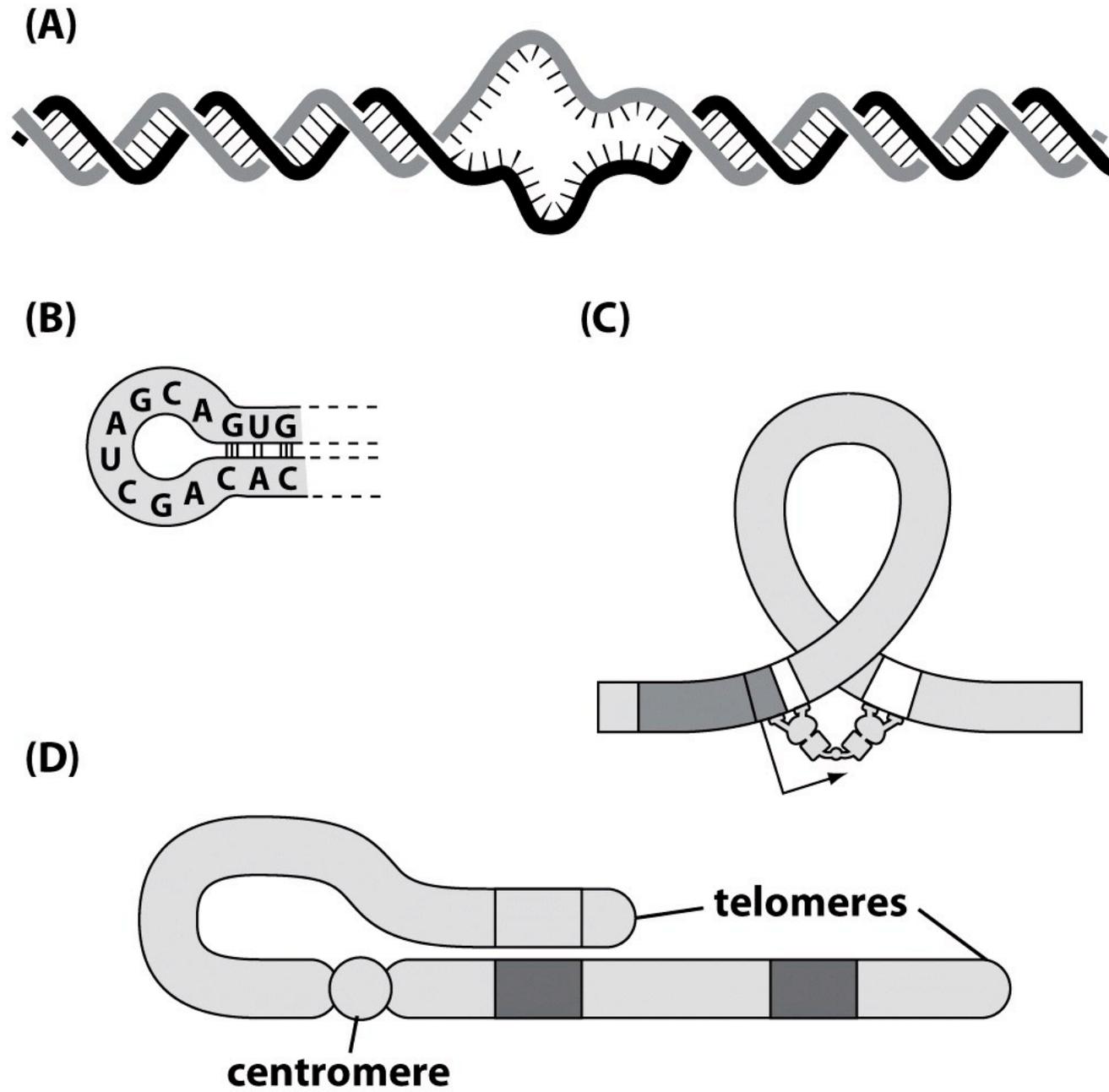


Figure 8.18 Physical Biology of the Cell (© Garland Science 2009)

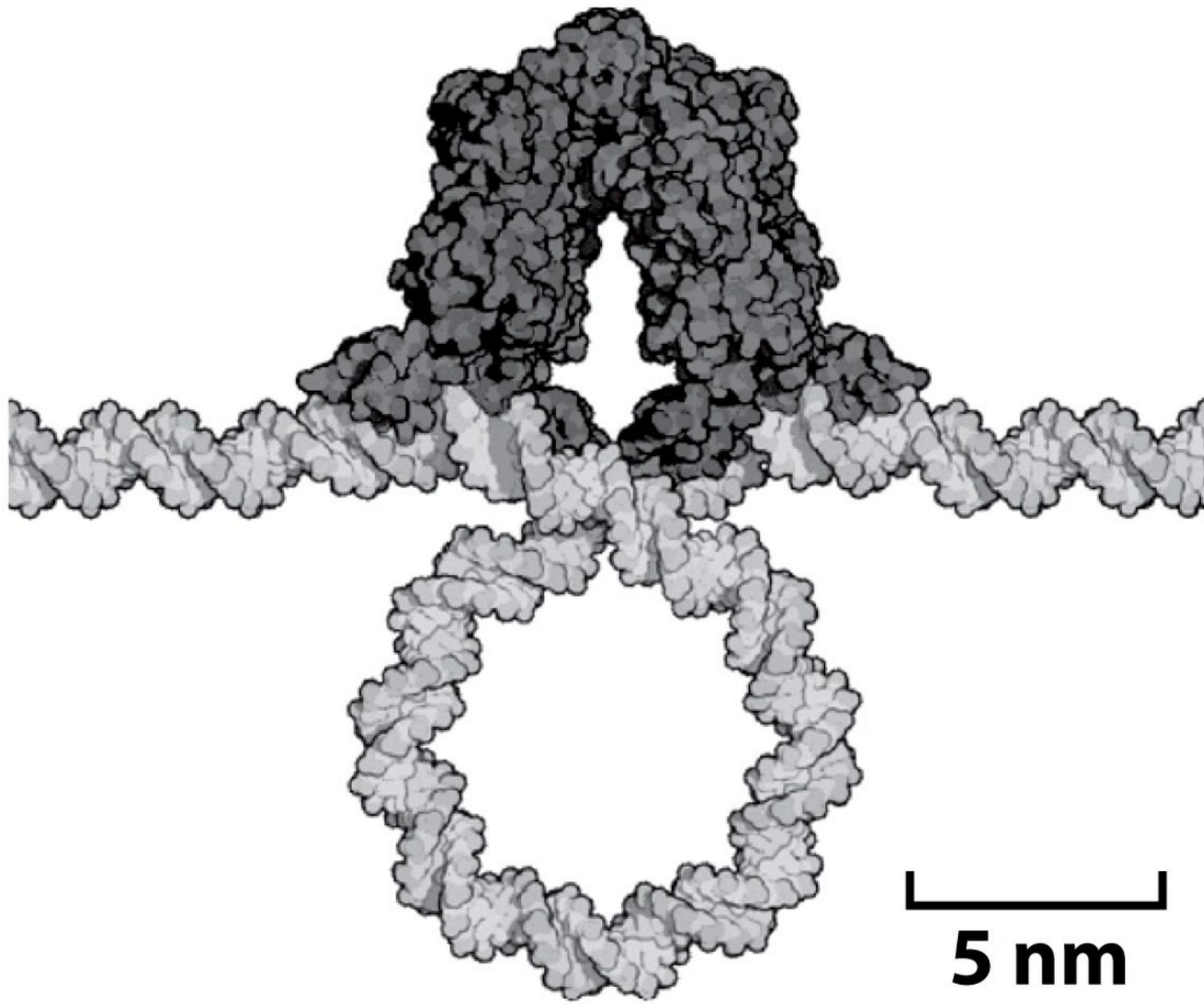


Figure 8.19 Physical Biology of the Cell (© Garland Science 2009)

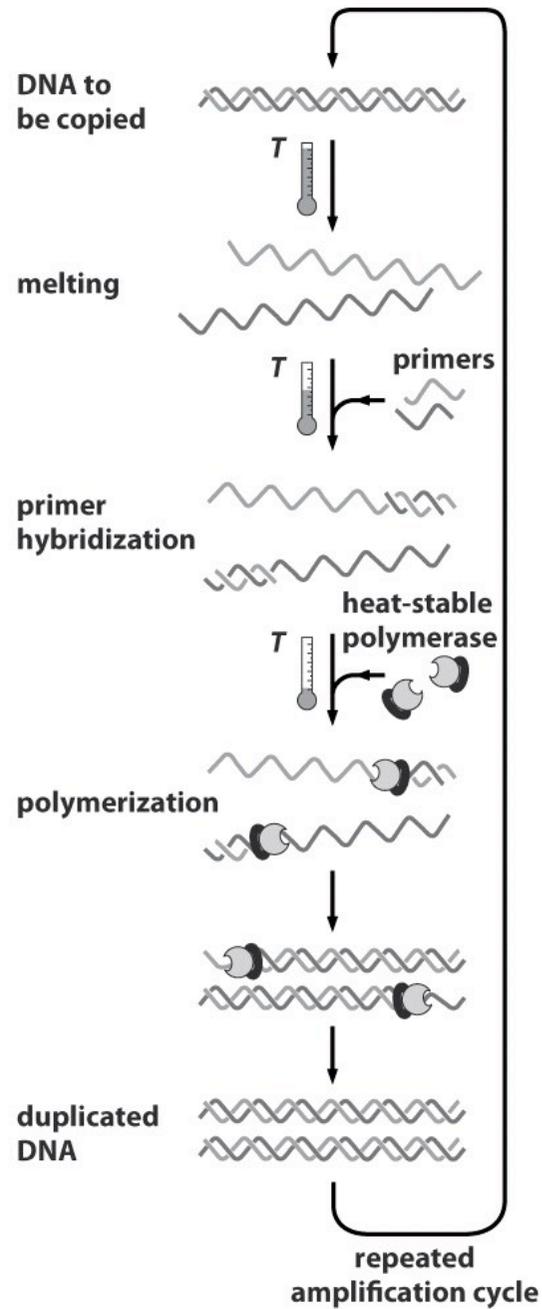
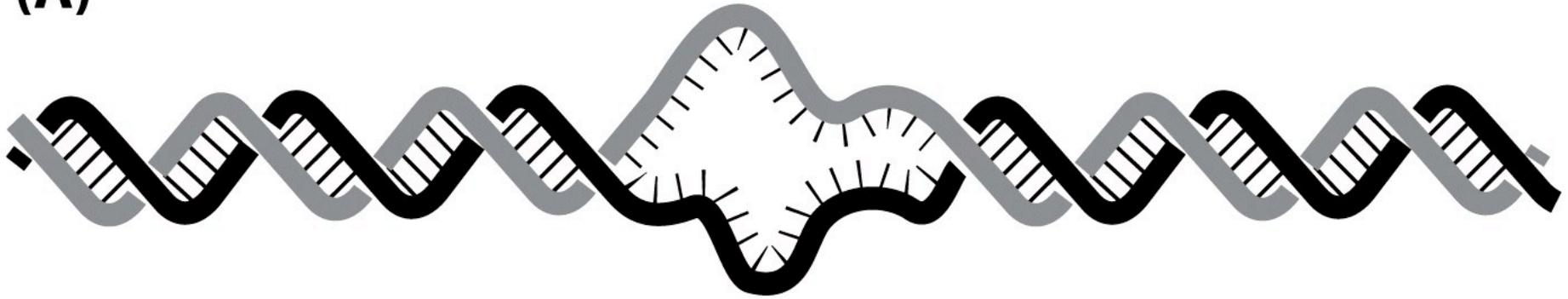


Figure 8.20 Physical Biology of the Cell (© Garland Science 2009)

(A)



(B)

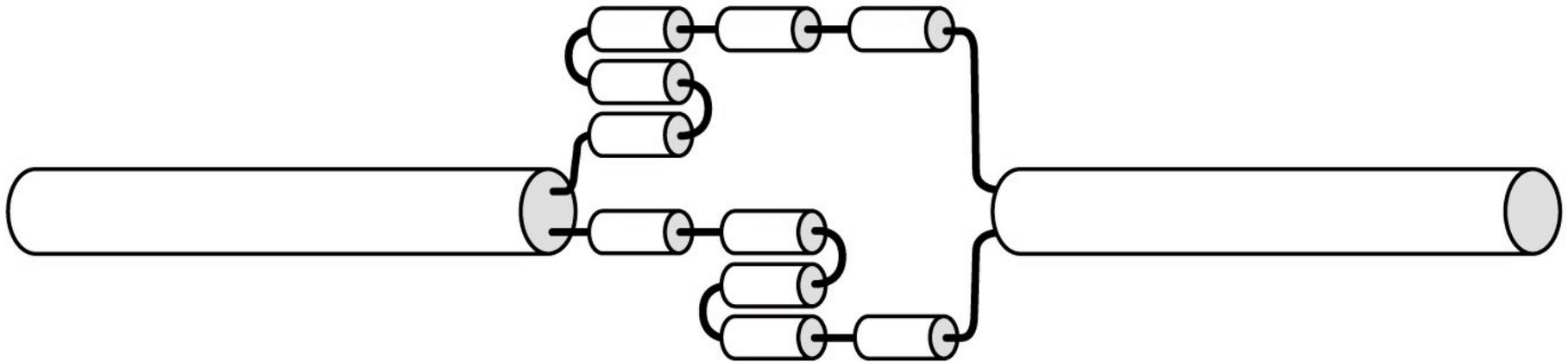


Figure 8.21 Physical Biology of the Cell (© Garland Science 2009)

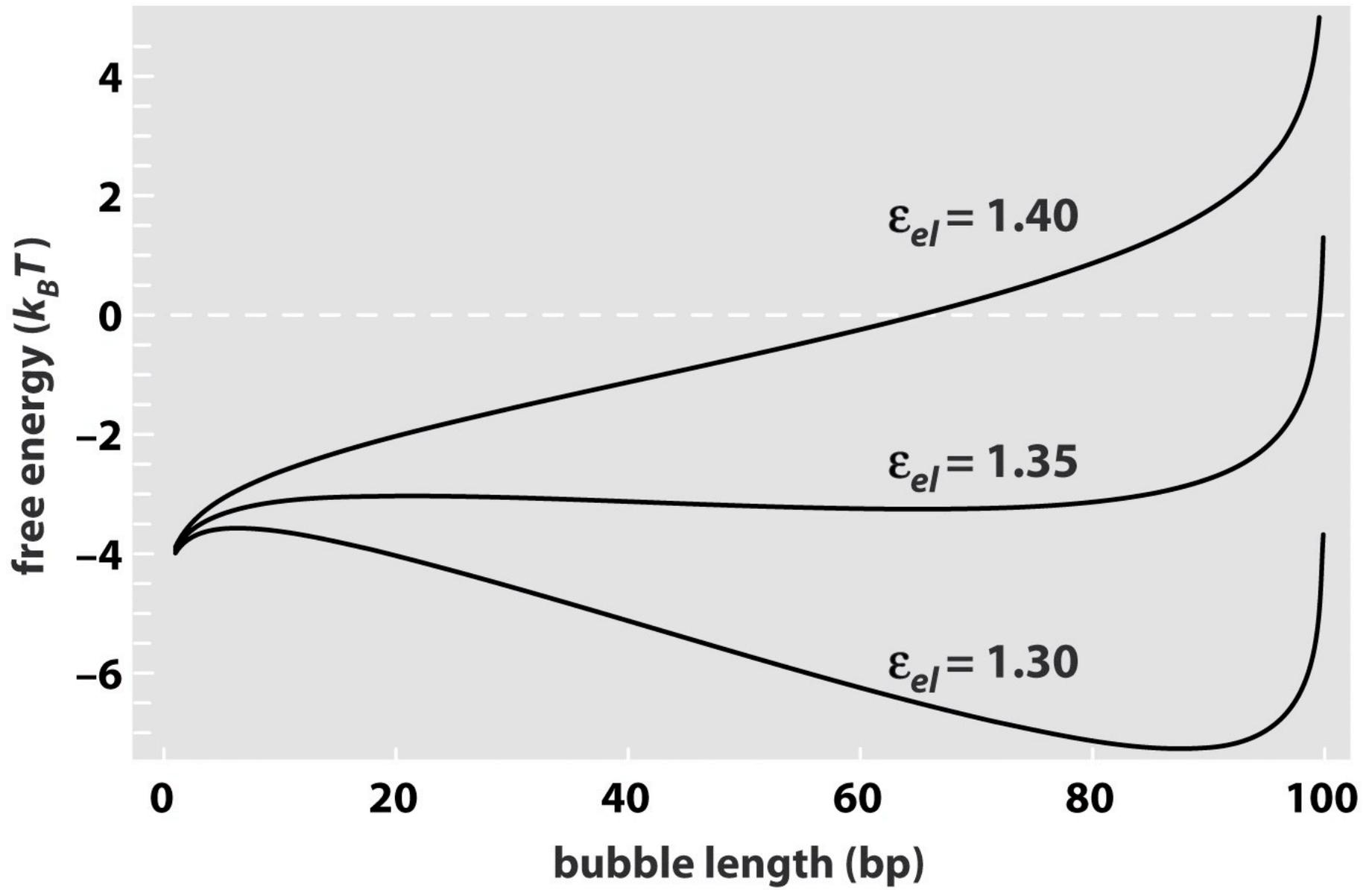


Figure 8.22 Physical Biology of the Cell (© Garland Science 2009)

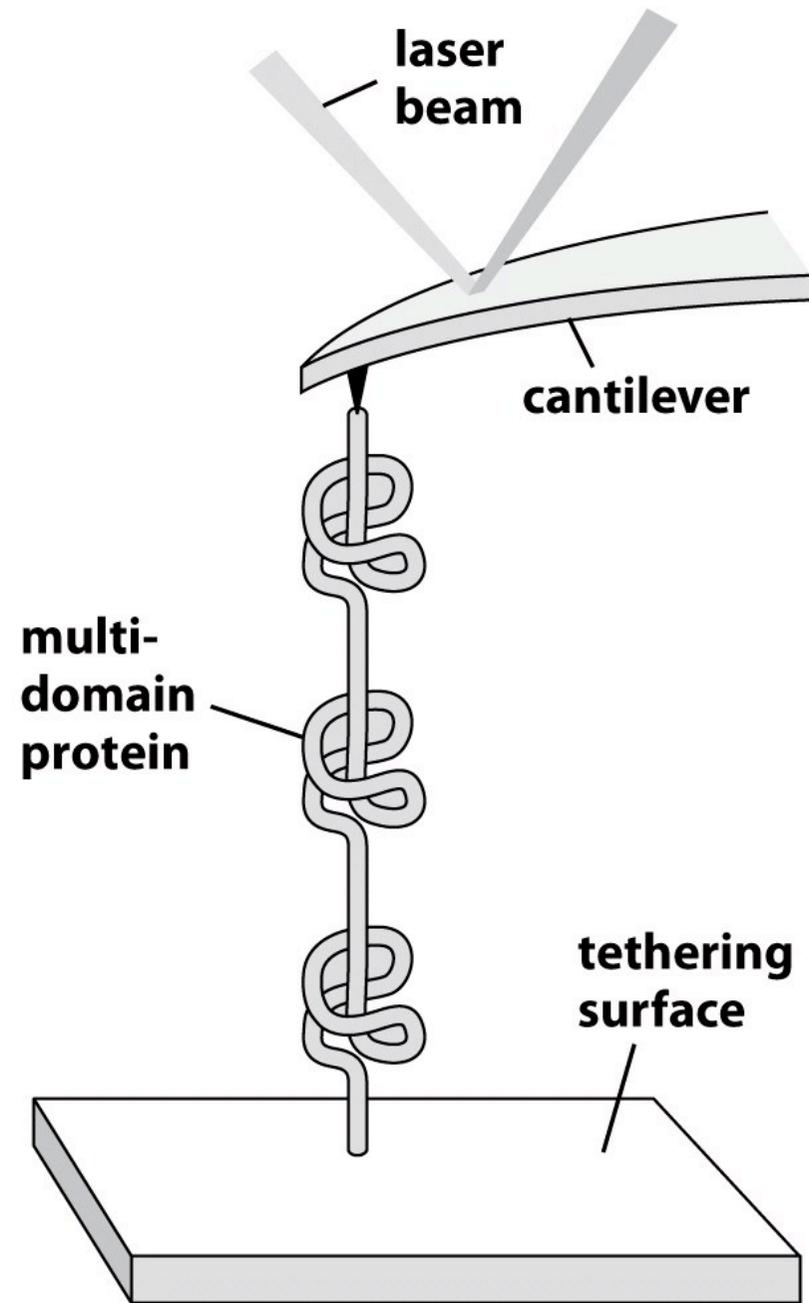


Figure 8.23a Physical Biology of the Cell (© Garland Science 2009)

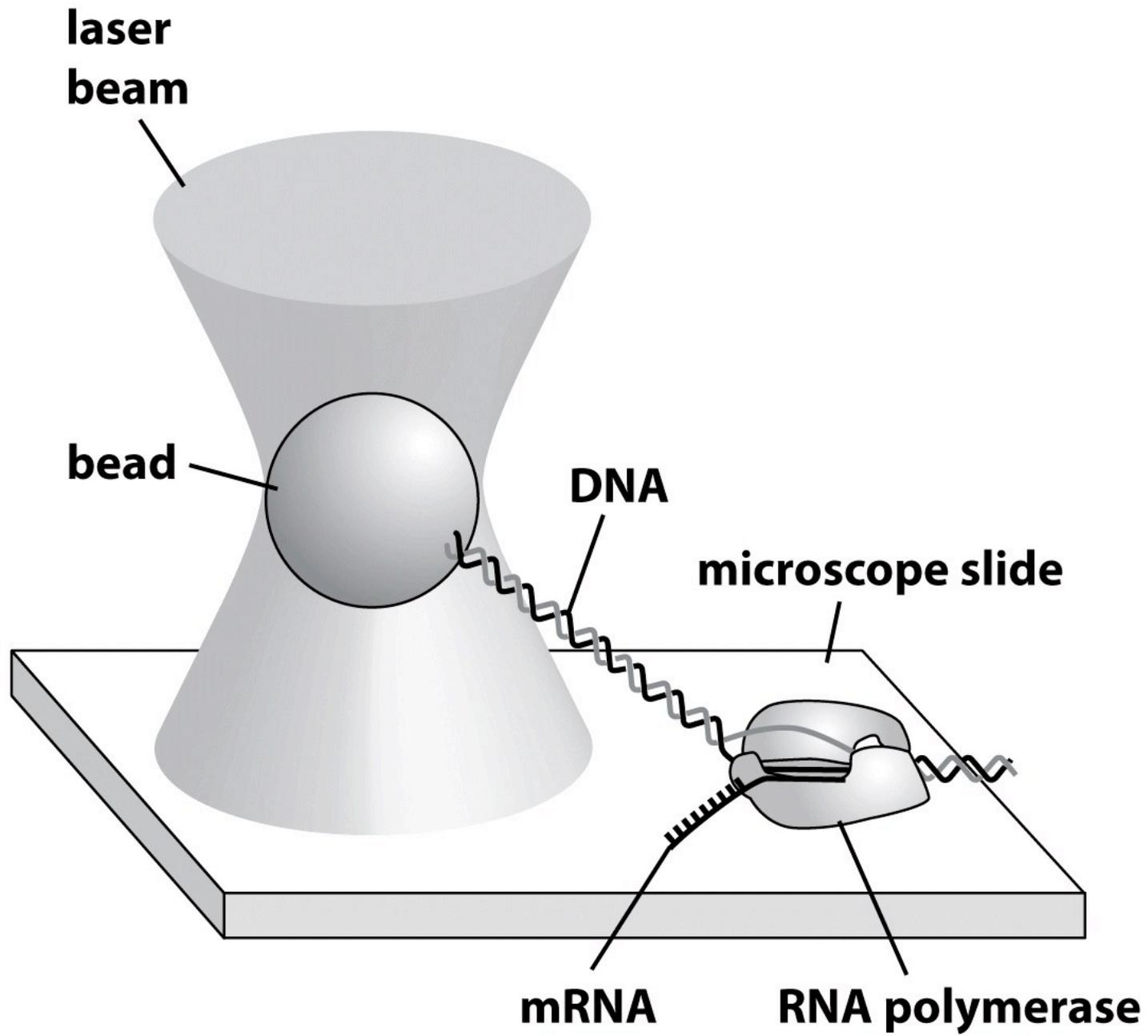


Figure 8.23b Physical Biology of the Cell (© Garland Science 2009)

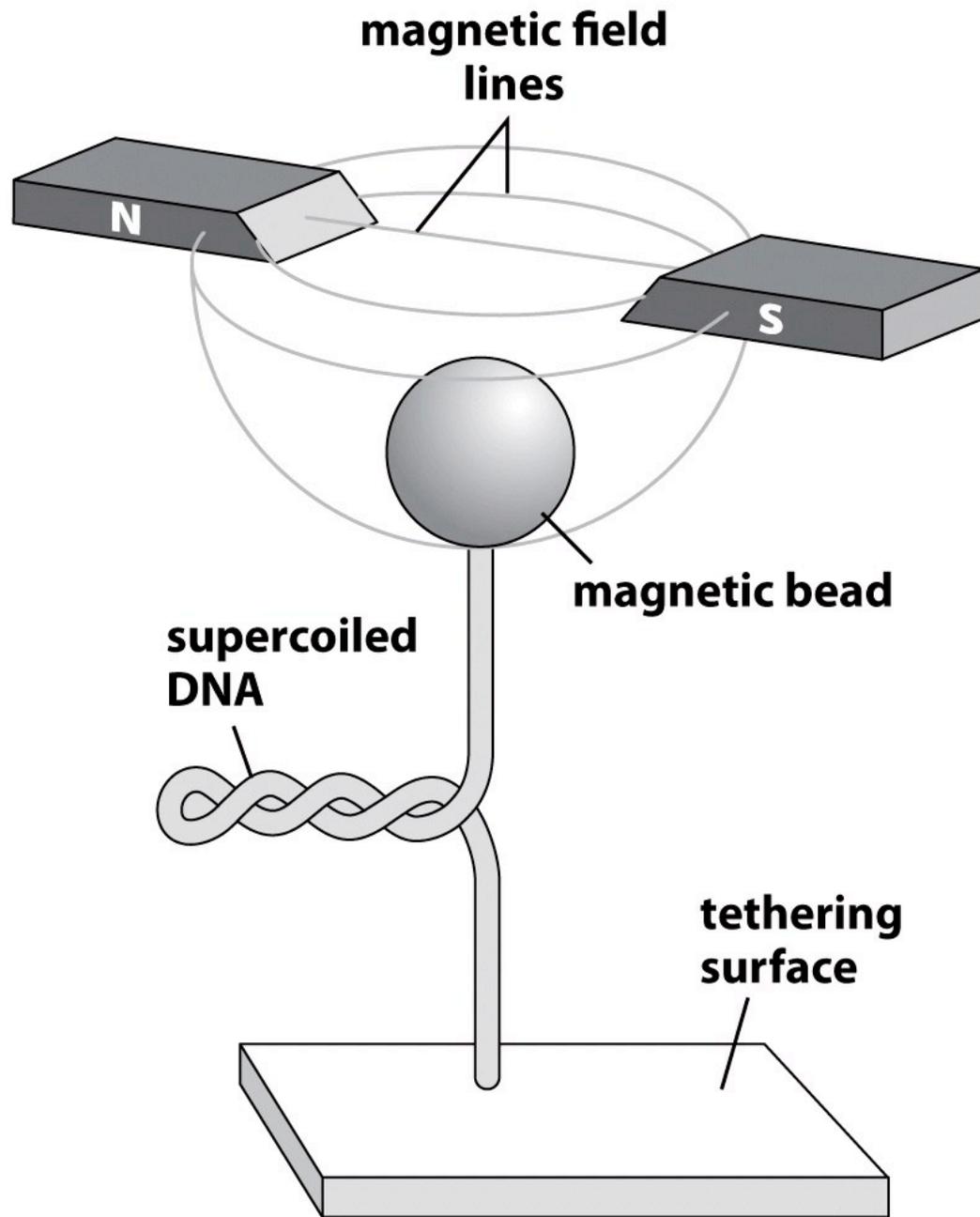


Figure 8.23c Physical Biology of the Cell (© Garland Science 2009)

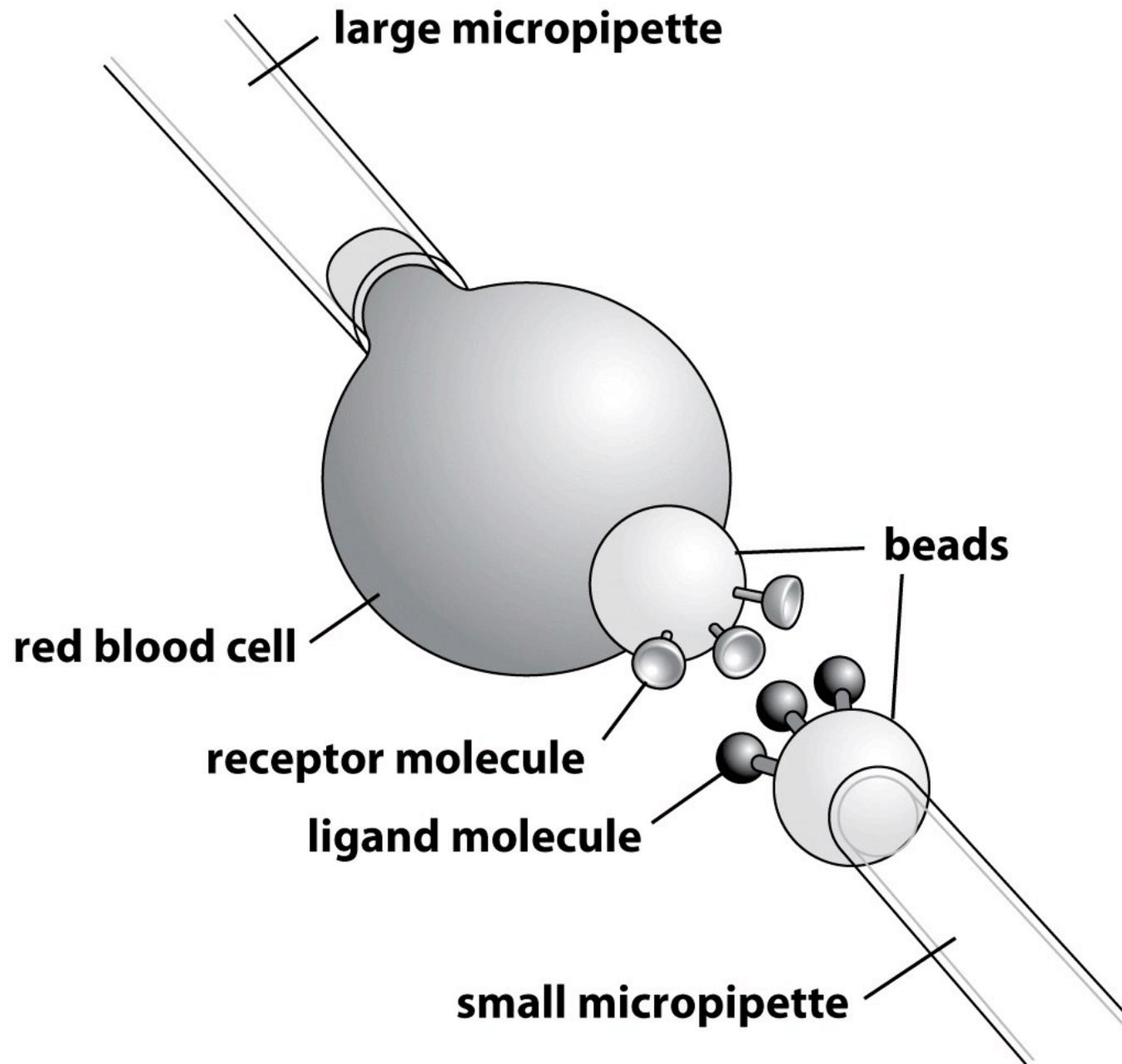


Figure 8.23d Physical Biology of the Cell (© Garland Science 2009)

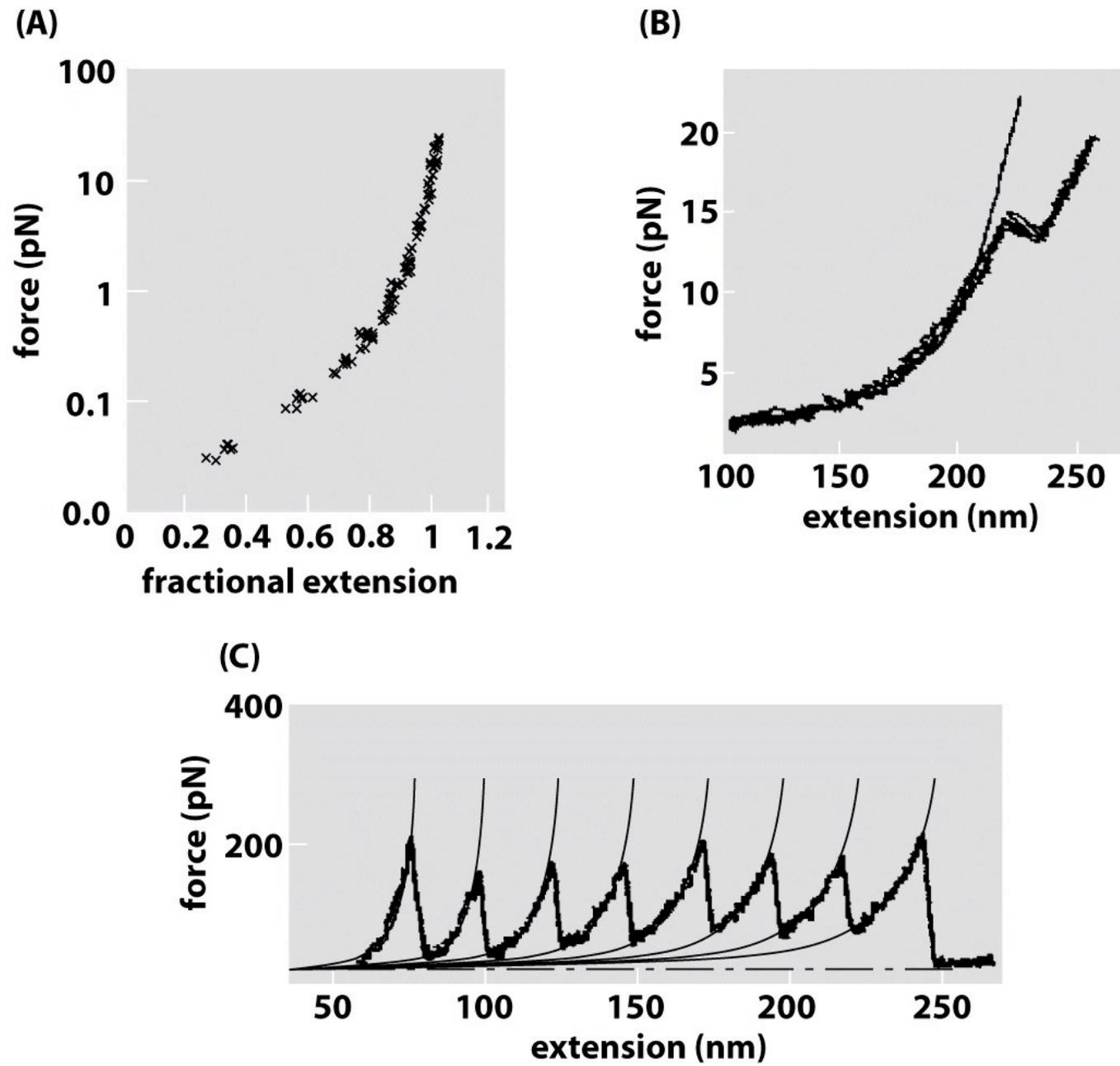


Figure 8.24 Physical Biology of the Cell (© Garland Science 2009)

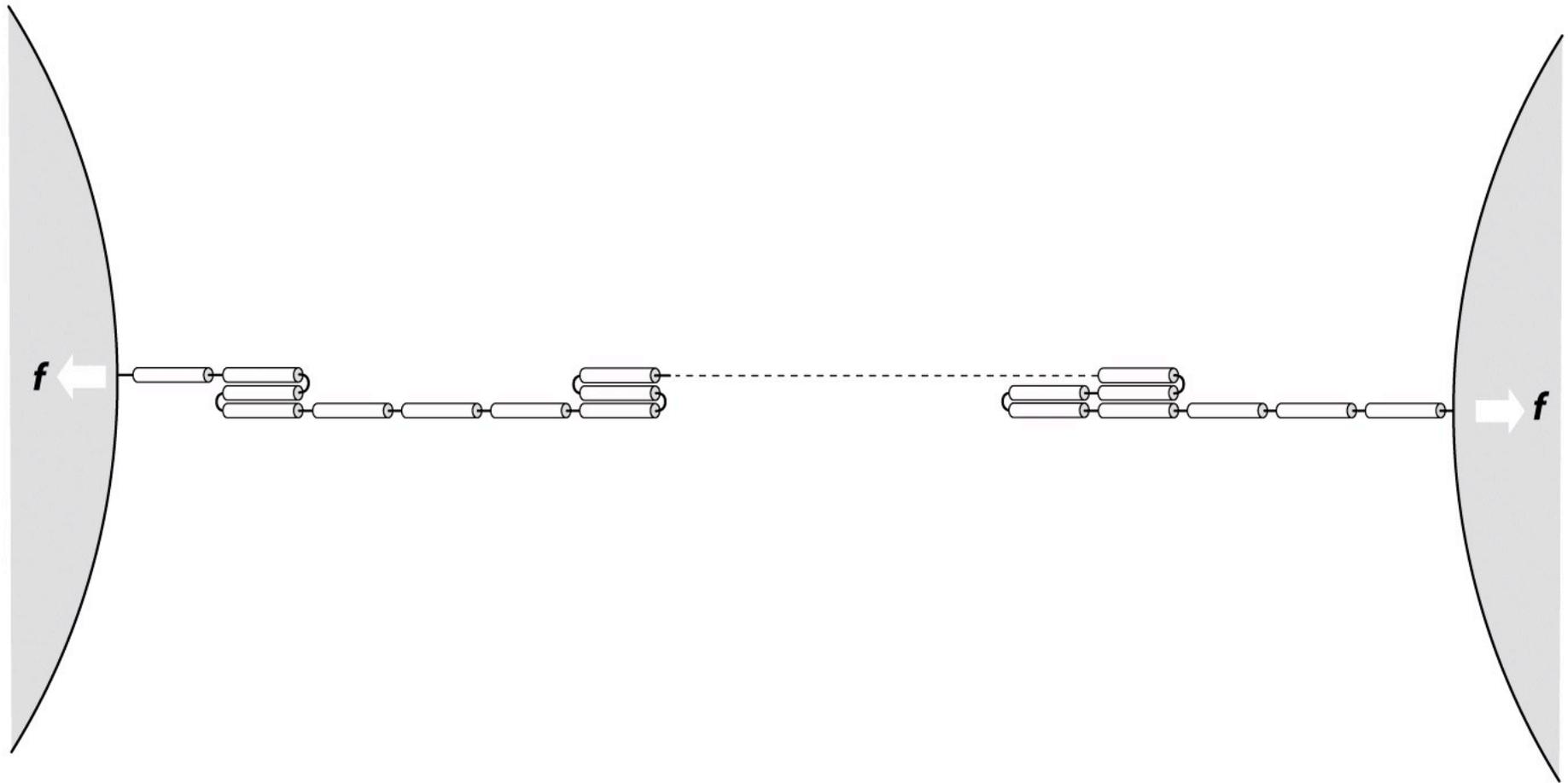


Figure 8.25 Physical Biology of the Cell (© Garland Science 2009)



Figure 8.26 Physical Biology of the Cell (© Garland Science 2009)

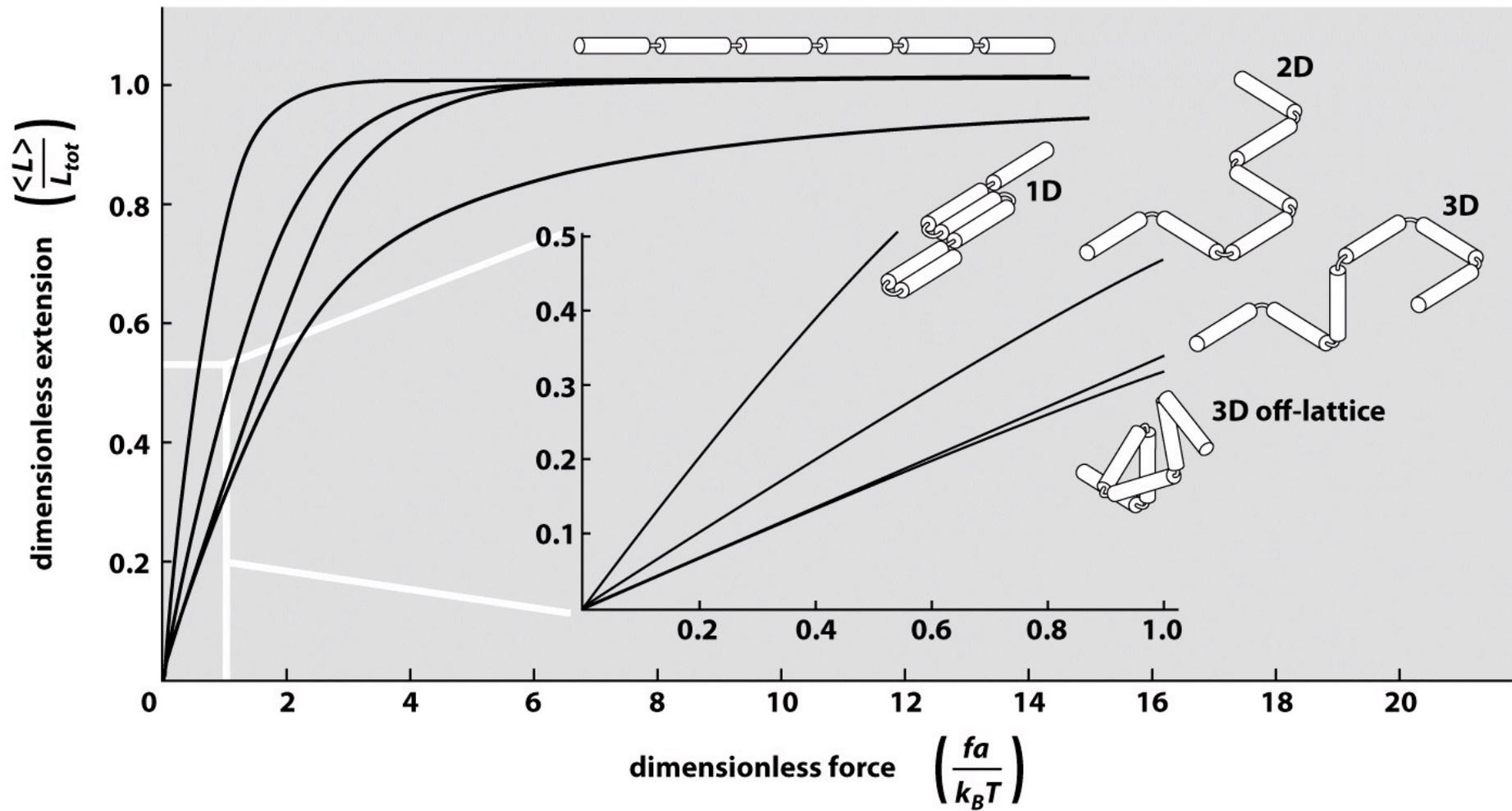


Figure 8.27 Physical Biology of the Cell (© Garland Science 2009)

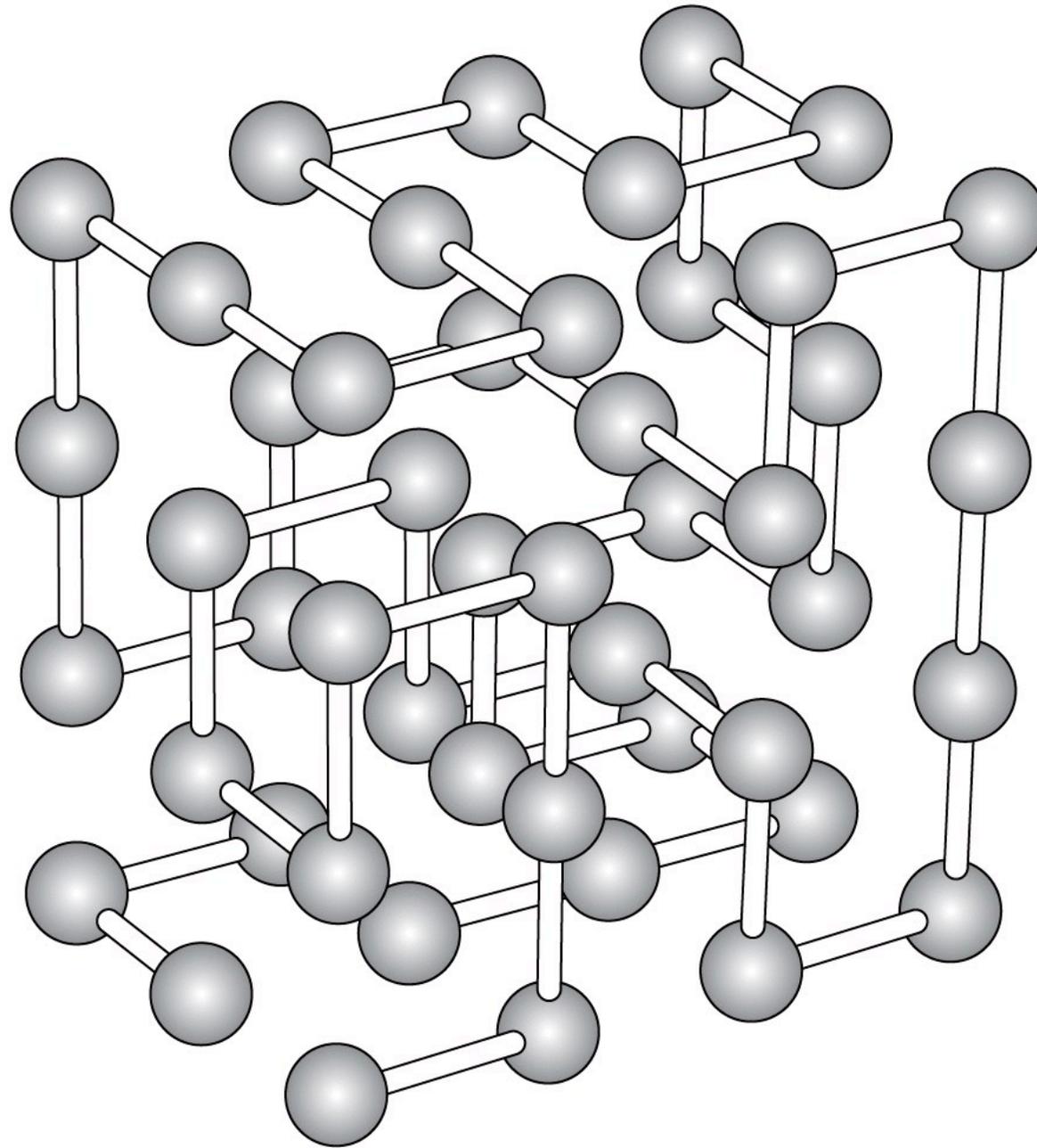


Figure 8.28 Physical Biology of the Cell (© Garland Science 2009)

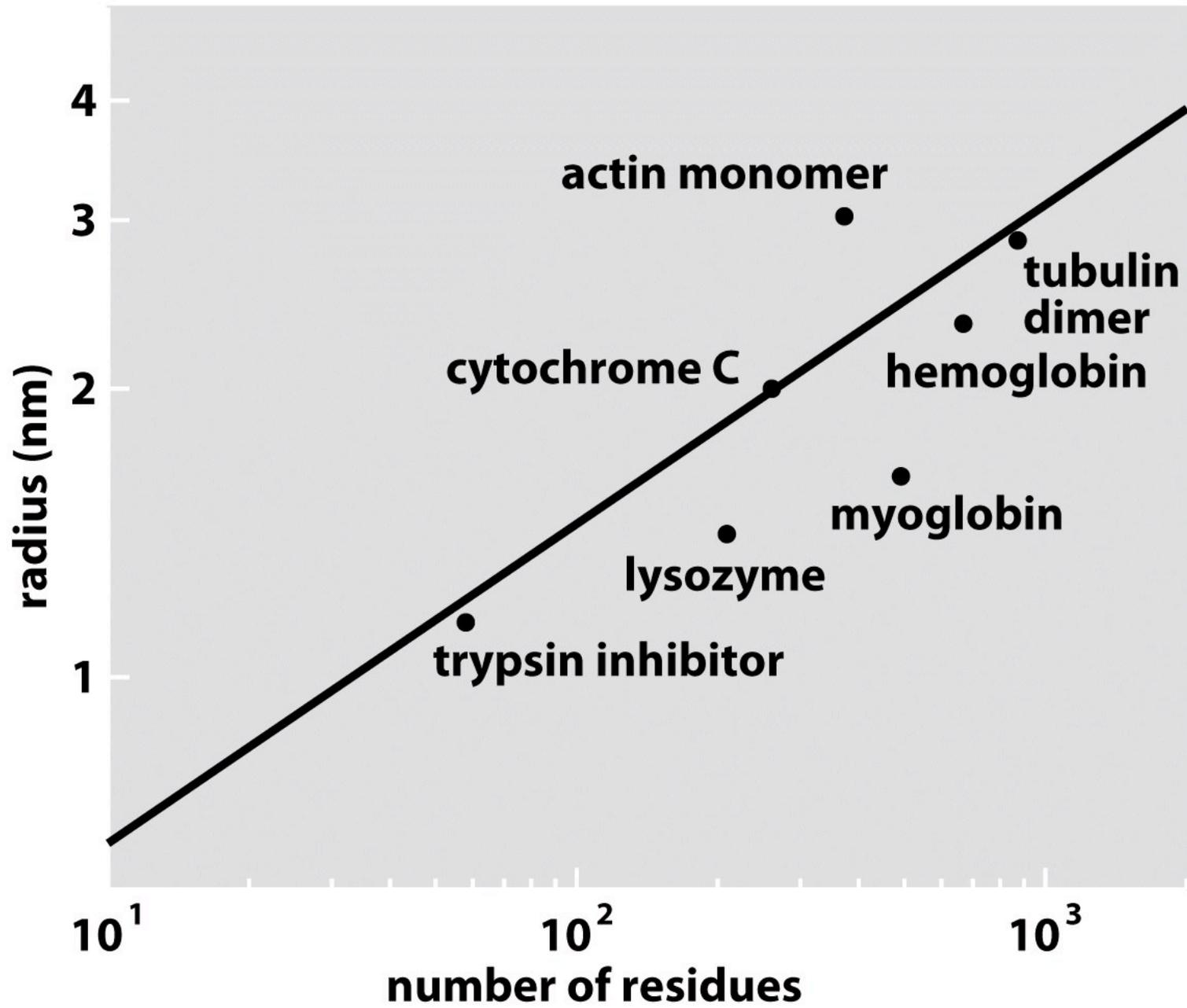


Figure 8.29 Physical Biology of the Cell (© Garland Science 2009)

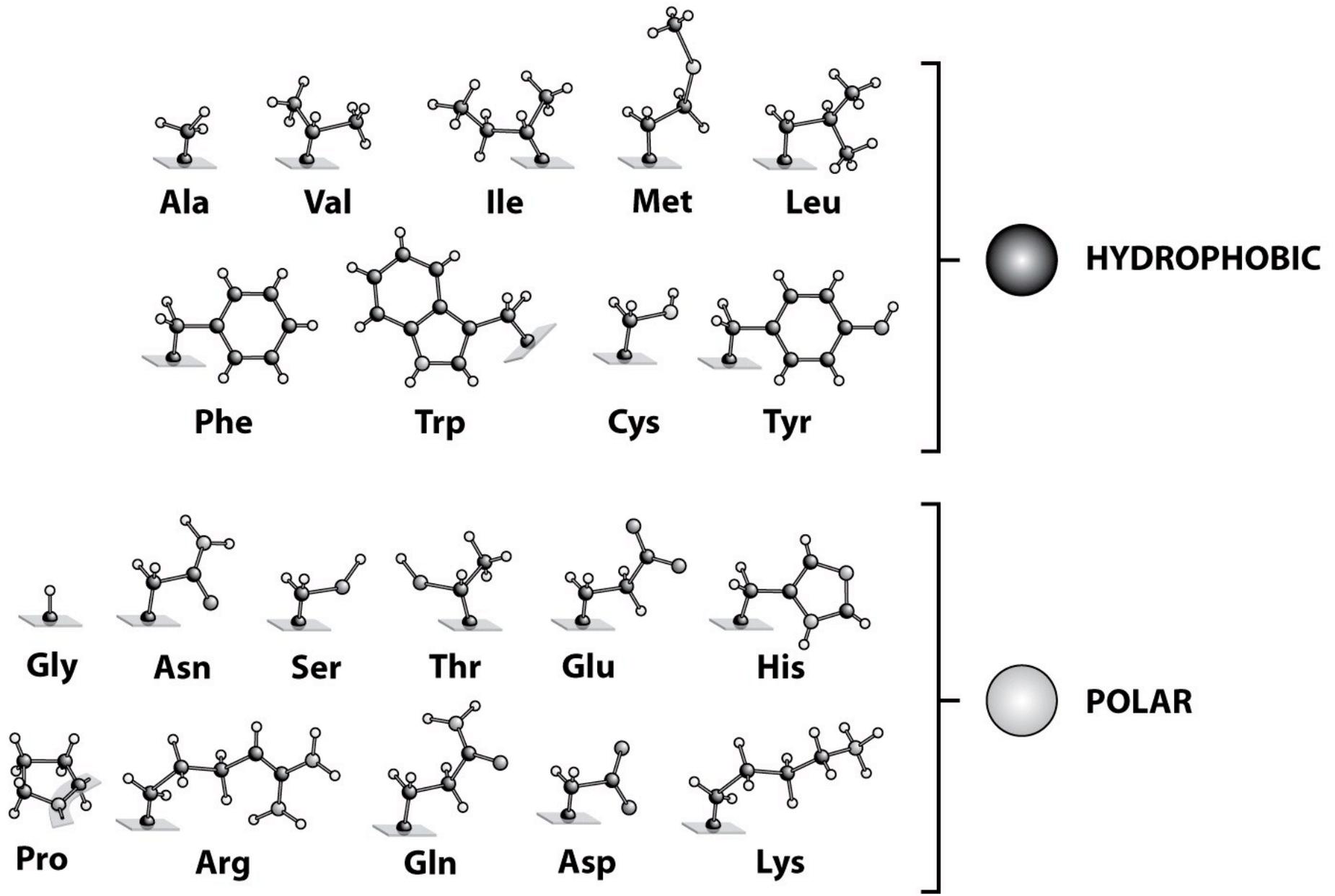


Figure 8.30 Physical Biology of the Cell (© Garland Science 2009)

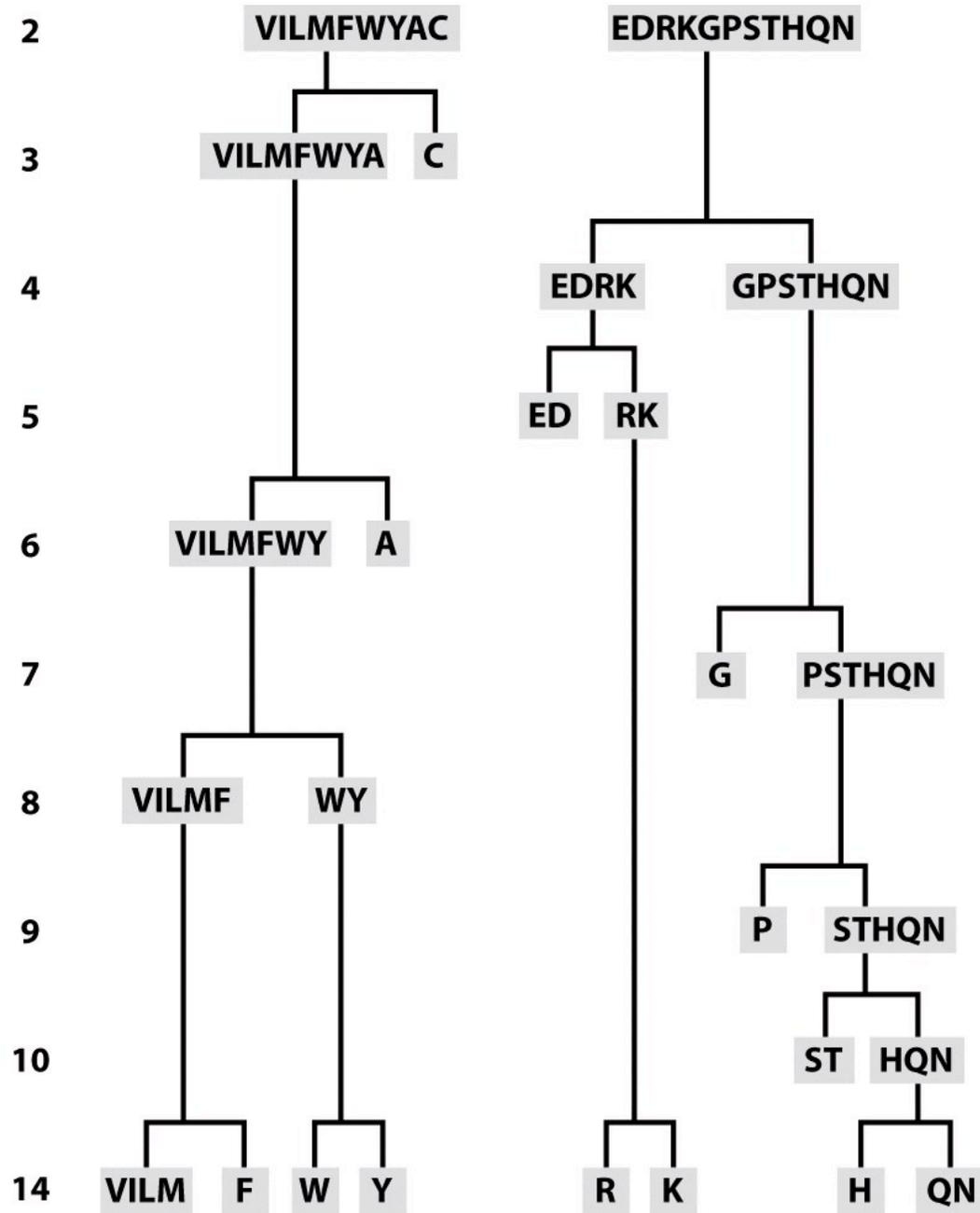


Figure 8.31 Physical Biology of the Cell (© Garland Science 2009)

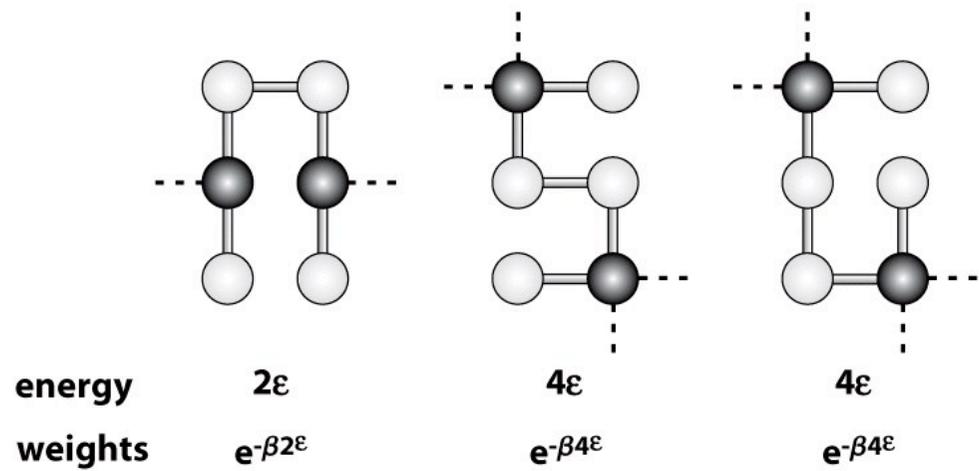
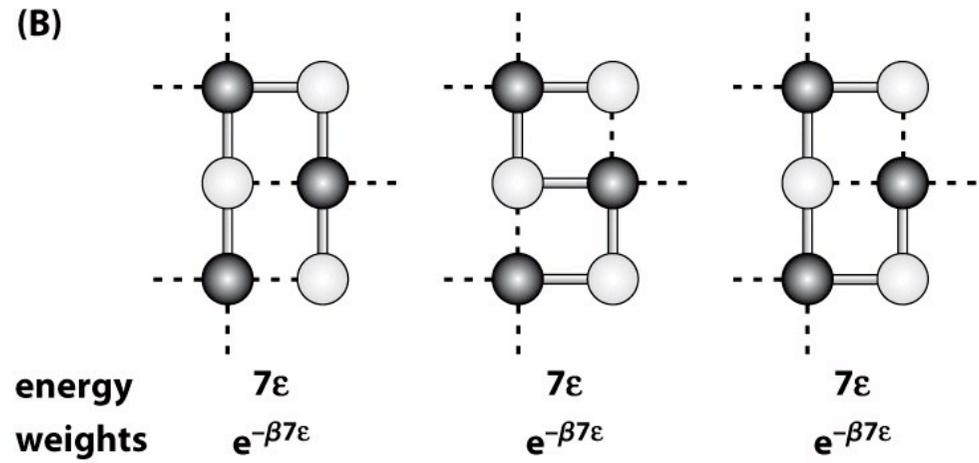
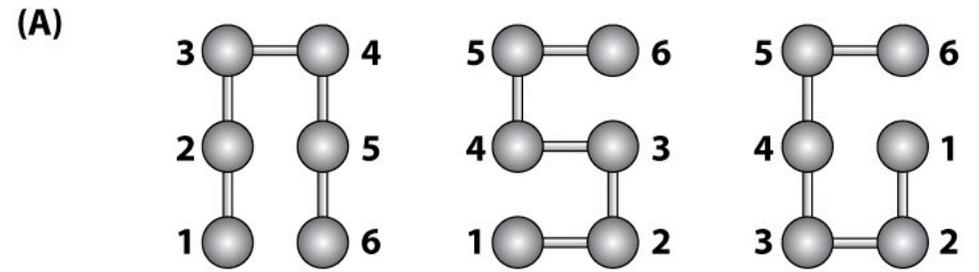


Figure 8.32 Physical Biology of the Cell (© Garland Science 2009)

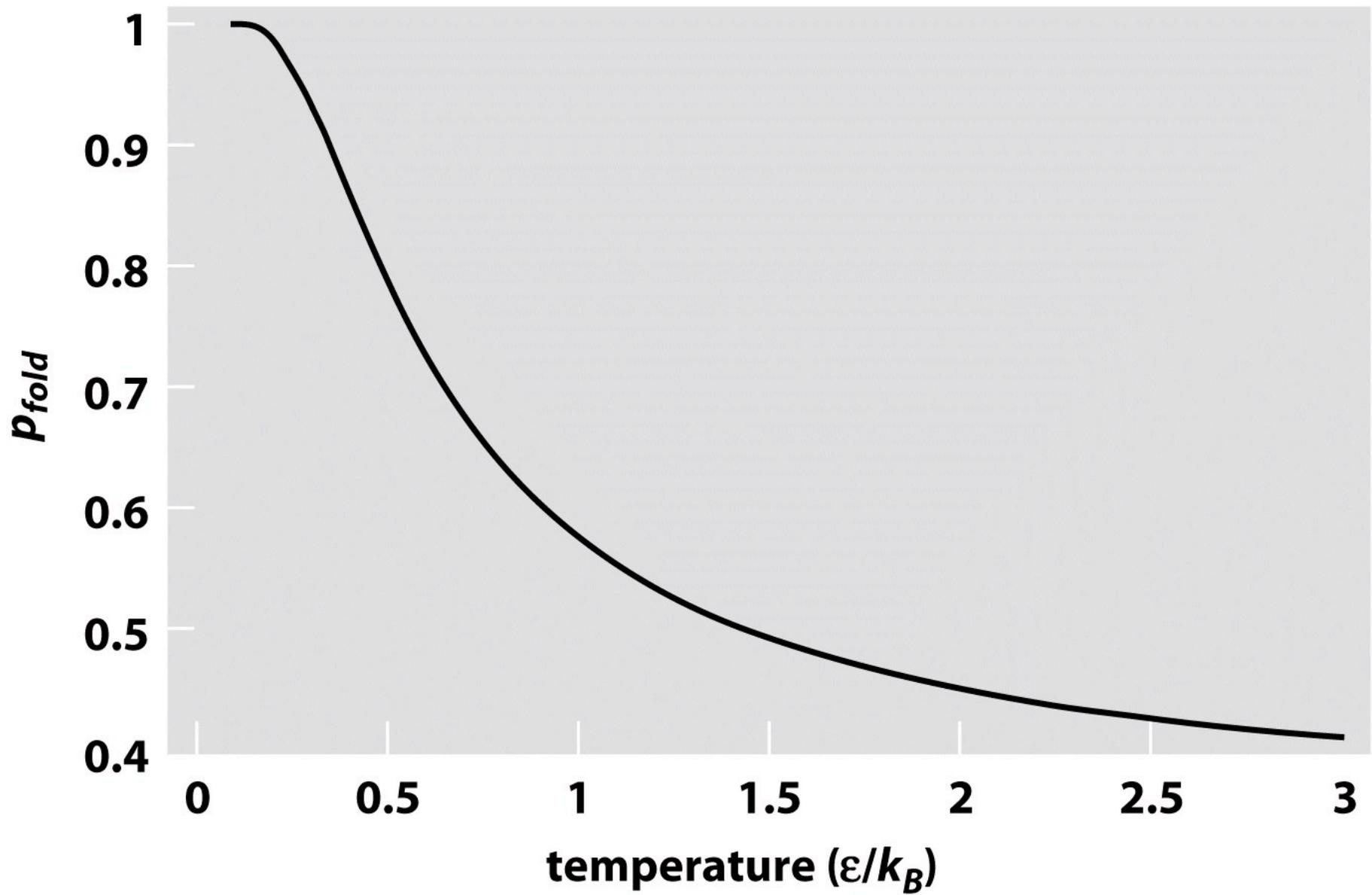


Figure 8.33 Physical Biology of the Cell (© Garland Science 2009)

structure	sequence						no. of sequences
	1	2	3	4	5	6	
	○	●	○	⊗	●	⊗	9
	○	●	●	⊗	●	○	
	●	●	⊗	○	●	○	
	●	●	○	○	●	●	
	○	○	●	⊗	⊗	●	6
	○	●	●	⊗	○	●	
	●	○	○	●	⊗	●	3
	●	●	○	●	○	●	

Figure 8.34 Physical Biology of the Cell (© Garland Science 2009)

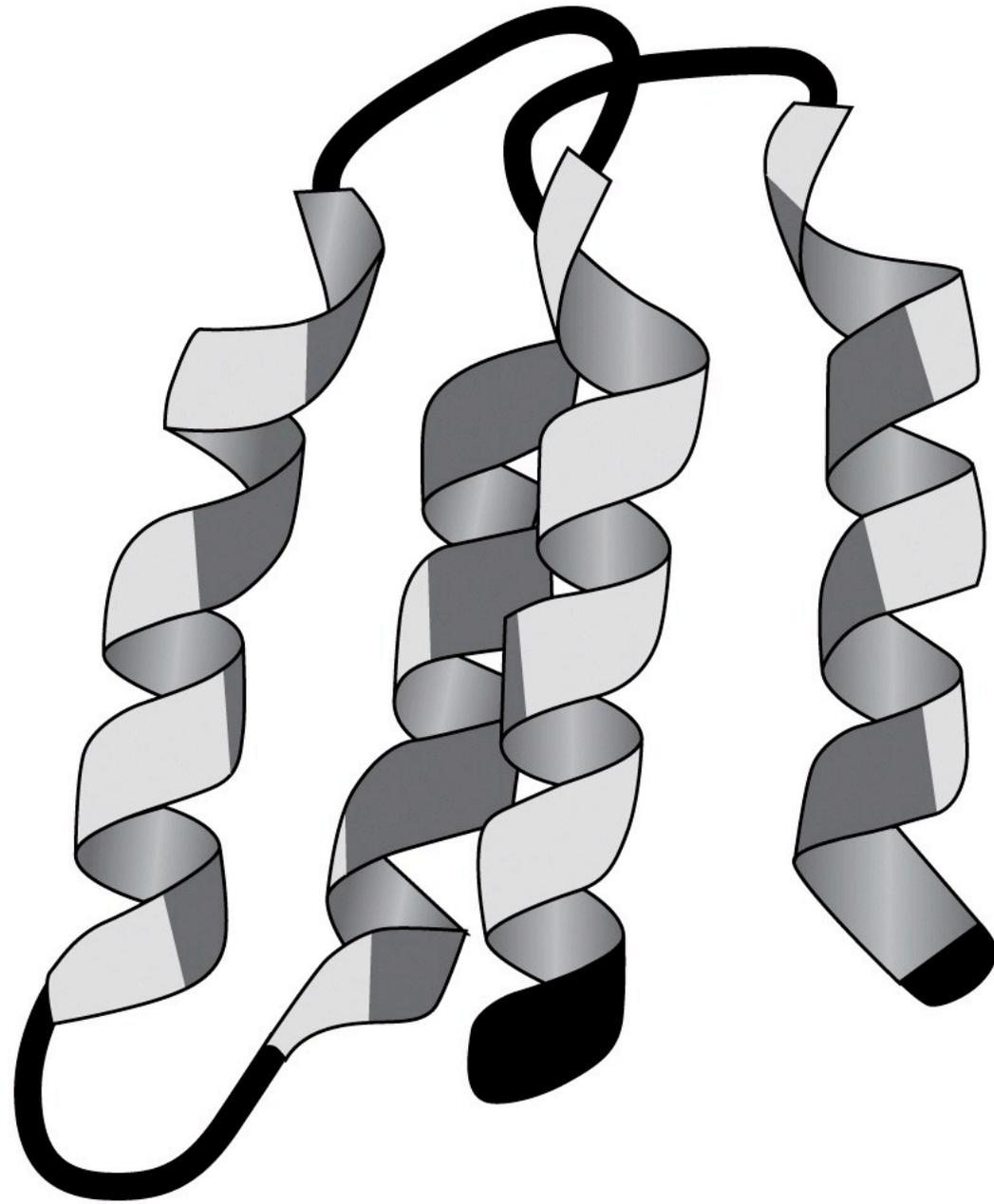


Figure 8.35 Physical Biology of the Cell (© Garland Science 2009)

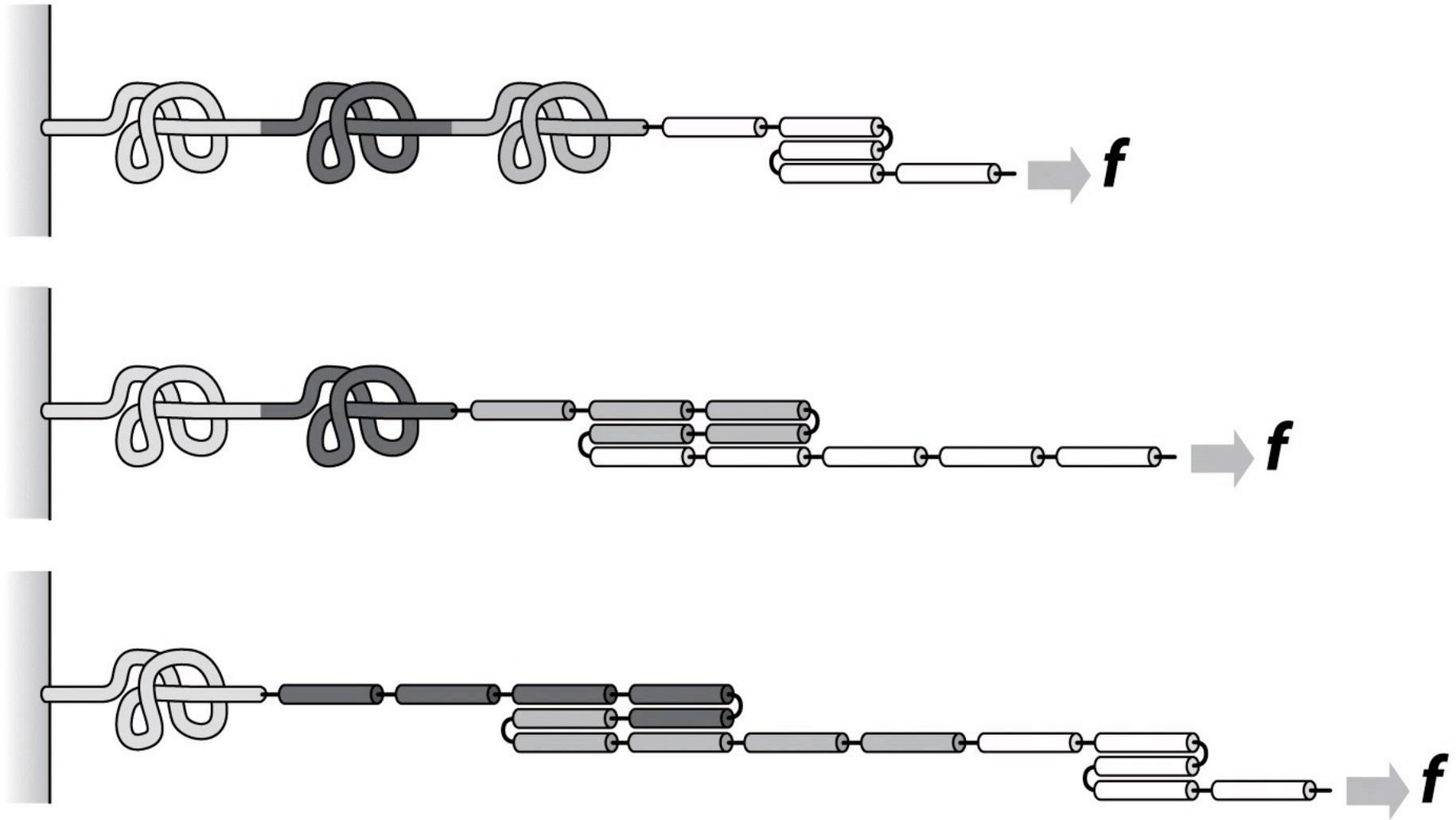


Figure 8.36 Physical Biology of the Cell (© Garland Science 2009)

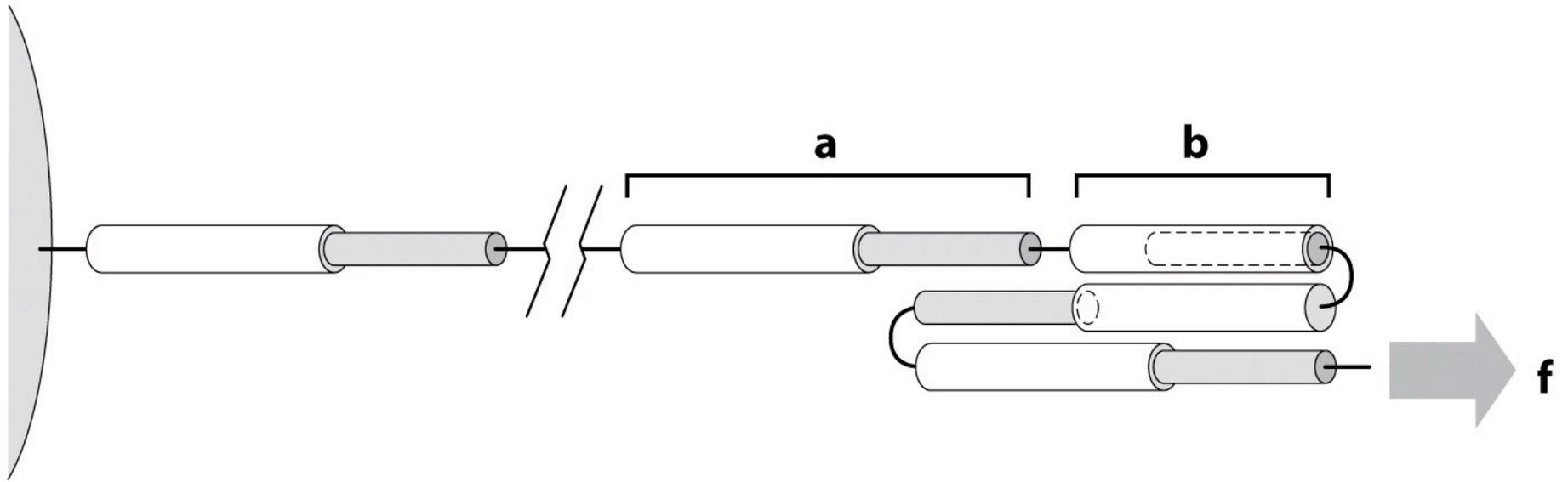


Figure 8.37a Physical Biology of the Cell (© Garland Science 2009)

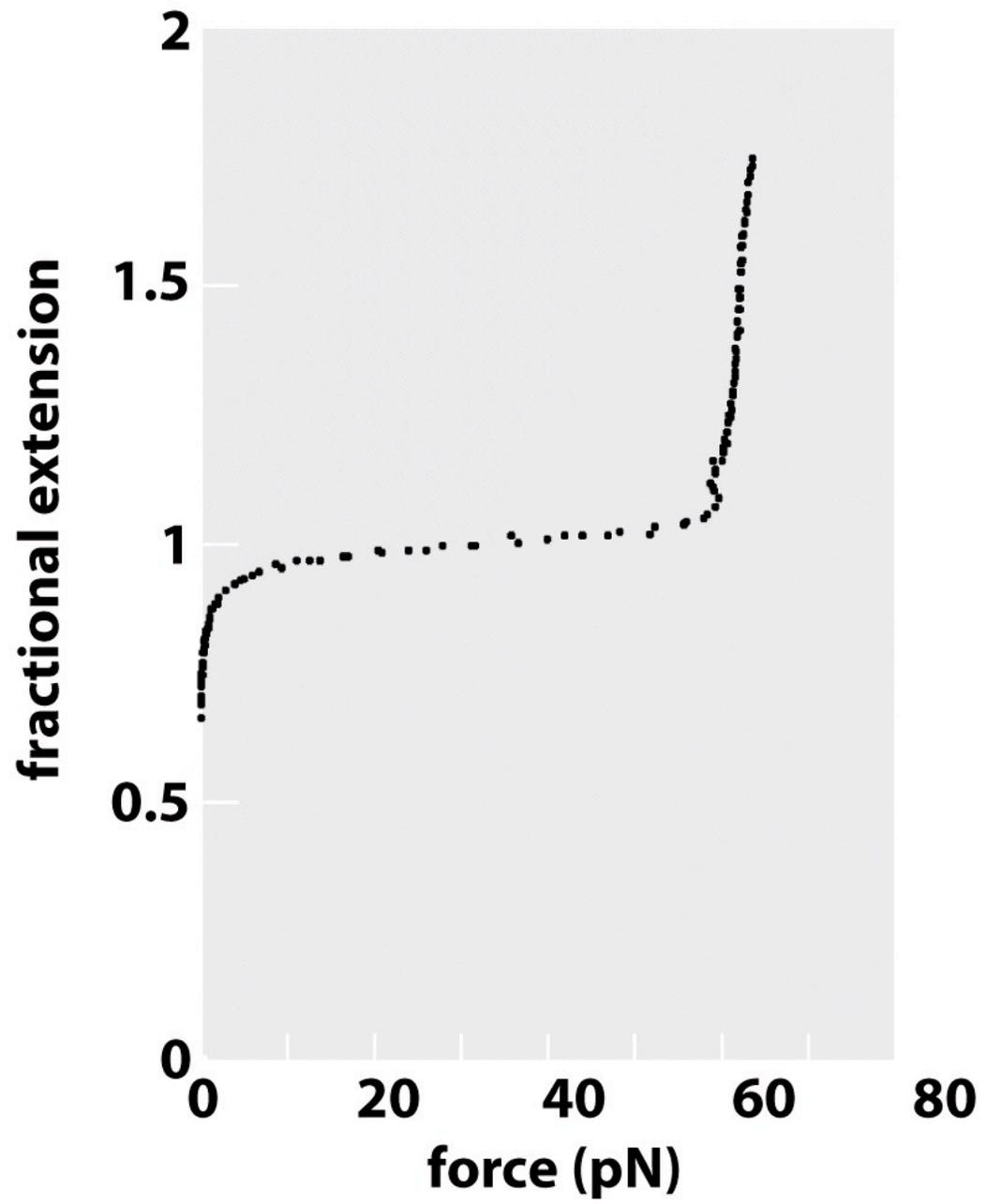


Figure 8.37b Physical Biology of the Cell (© Garland Science 2009)