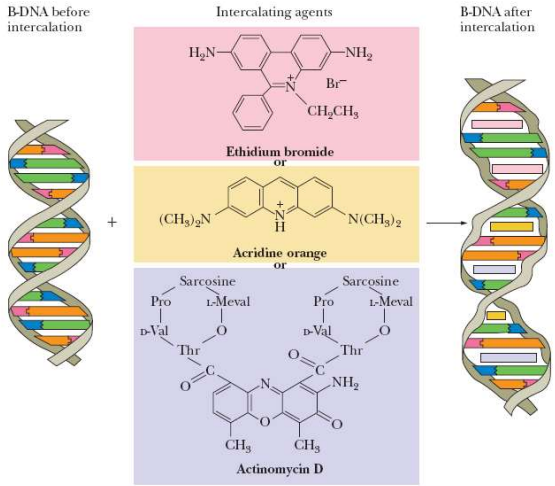

FIGURE 11.14 The structures of ethidium bromide, acridine orange, and actinomycin D, three intercalating agents, and their effects on DNA structure.

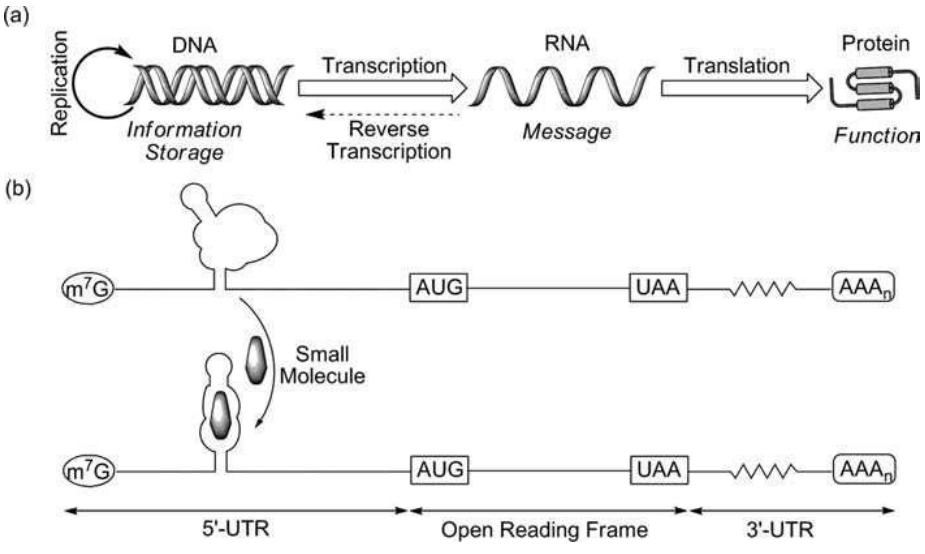

Figure 6.1 *(a) The central dogma of biology. (b) RNA binders could affect the translation of mRNA by binding at the 5'-untranslated region and interfering with ribosome scanning, a process preceding translation*

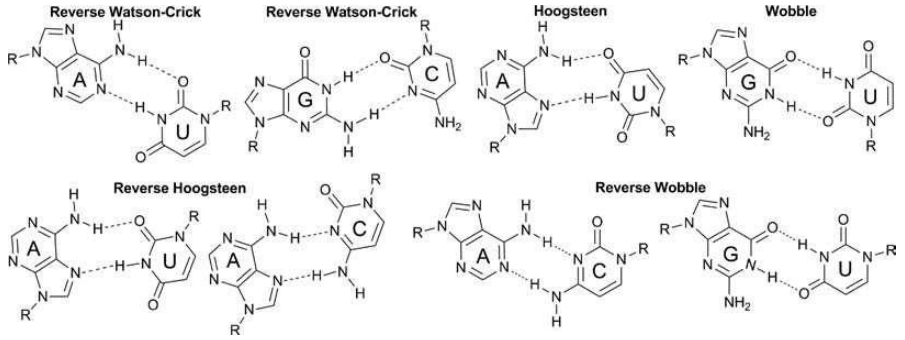

Figure 6.4 *Non-canonical hydrogen bonding base pairs. DNA: R=deoxy-D-ribose. RNA: R=D-ribose*

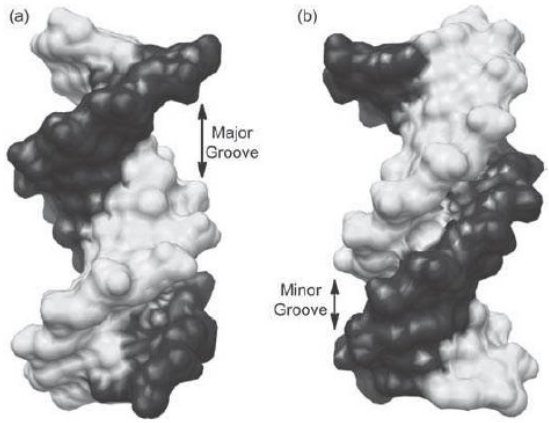

Figure 6.5 *X-ray crystal structure views of the (a) major groove and (b) minor groove of the Dickerson–Drew B-DNA dodecamer. Each strand is shaded separately, and each view is rotated approximately 180° from one another. Major and minor groove widths are the distances between inter-strand phosphates. PDB ID: 2BNA*

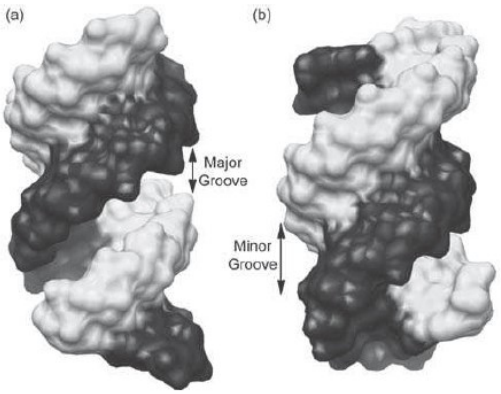

Figure 6.6 *Views of the (a) major groove and (b) minor groove of a representative A-form RNA duplex. The RNA duplex is an X-ray crystal structure of the self complementary 14-mer sequence 5′-U(UA)$_6$A-3′. Each strand is shaded differently, and each view is rotated approximately 180° from one another. Major and minor groove widths are the distances between inter-strand phosphates. PDB ID: 1RNA*

Table 6.1 *Physical characteristics of B-form DNA and A-form RNA*

Characteristic	DNA (B-form)	RNA (A-form)
Base pairs per helical turn	10	11
Helical twist per base pair (°)	36	32.7
Distance between base pair (helical rise) (Å)	3.4	2.8
Pitch height (full helical turn) (Å)	34	32.7
Helix diameter (Å)	20	26
Major groove width (Å)	11.7	4.7
Major groove depth (Å)	8.8	12.9
Minor groove width (Å)	5.7	10.8
Minor groove depth (Å)	7.5	3.3

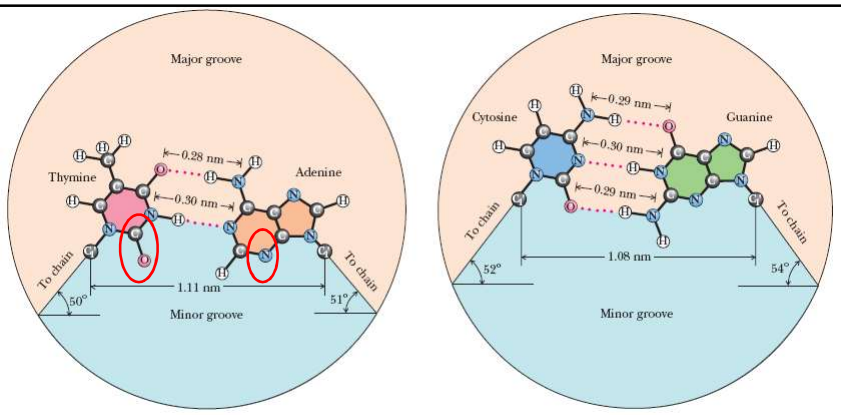

FIGURE 11.8 Watson–Crick A:T and G:C base pairs. All H bonds in both base pairs are straight.

In an A-T base pair, the N3 of adenine and the O2 of thymine both point towards the minor groove, resulting in an overall negative potential. In comparison, the minor groove of G-C is less densely charged, as the contribution from N3 in guanine and O2 carbonyl of cytosine is partially neutralized by the exocyclic N2 amino functionality.

In the major groove, there is less of a difference in electrostatic potential between A-T and G-C bases pairs. In A-T, a negative potential is contributed by O4 of thymine and N7 of adenine; however, positive electrostatic potential is provided by the exocyclic 6-amino functionality of adenine. Similarly, in G-C, positive potential from the exocyclic amine at N4 of cytosine partially diminishes the negative potential contributions from N7 and O6 of guanine.

$$\Delta G_{\text{obs}} = \Delta G_{\text{DNA}} + \Delta G_{\text{r+t}} + \Delta G_{\text{hyd}} + \Delta G_{\text{pe}} + \Delta G_{\text{mol}} \sqrt{a^2 + b^2}$$

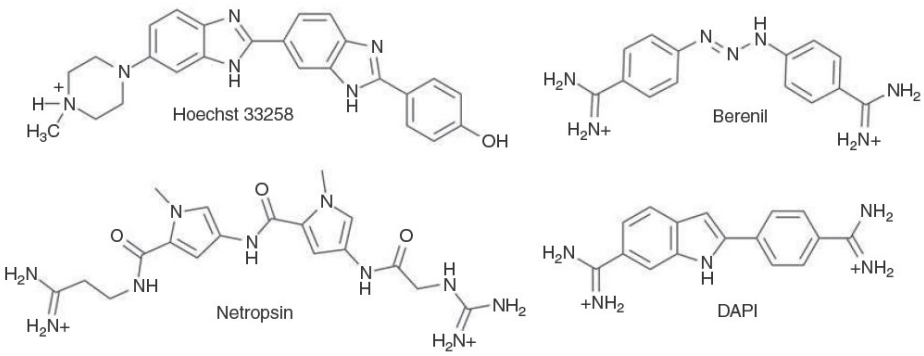

Figure 6.7 *Examples of groove binders. Most groove binders adopt a 'crescent'-shaped form*

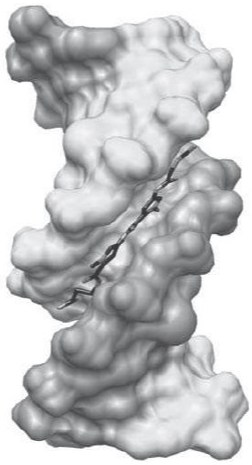

Figure 6.8 *X-ray crystal structure of a 1:1 netropsin–DNA complex. Netropsin resides in the minor groove of the DNA helix. PDB ID: 6BNA*

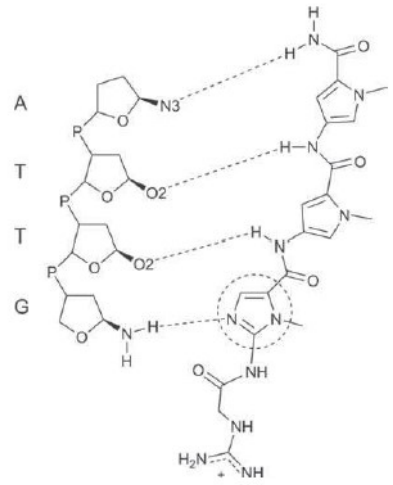

Figure 6.9 *Schematic representation of the hydrogen-bonding contacts between a PyPyIm 'lexitropsin' and ATTG bases in the minor groove of DNA. The additional imidazole (circled) nitrogen allows for hydrogen bonding with the N2 of guanosine, which normally clashes with a pyrrole hydrogen. The nucleic acid structure has been minimized with base identities indicated along the left column. The DNA sugar–phosphate backbone is represented by a reduced ribose and 'P' (for phosphorus). Only the purine or pyrimidine atoms involved in hydrogen bonding are indicated. Hydrogen bonding is represented by dashed lines*

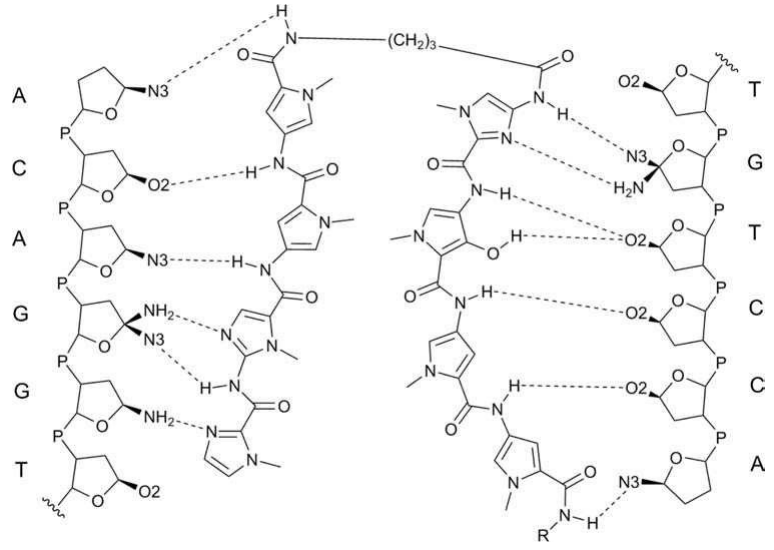

Figure 6.11 *Schematic representation of the hydrogen-bonding contacts between a sequence-selective hairpin polyamide in the minor groove of DNA. Note: the hydroxypyrrole allows for discrimination of an T·A base pair over A·T due to additional hydrogen-bonding interactions. The nucleic acid structure has been minimized with base identities indicated along the left and right columns. The DNA sugar–phosphate backbone is represented by a reduced ribose and 'P' (for phosphate). Only the purine or pyrimidine atoms involved in hydrogen bonding are indicated. Hydrogen bonding is represented by dashed lines*

Table 6.2 *Dervan's pairing rules for sequence selective targeting with polyamides*

Pair[a]	G·C	C·G	T·A	A·T
Im/Py	√	×	×	×
Py/Im	×	√	×	×
Hp/Py	×	×	√	×
Py/Hp	×	×	×	√

[a] Im = imidazole; Py = pyrrole; Hy = hydroxypyrrole

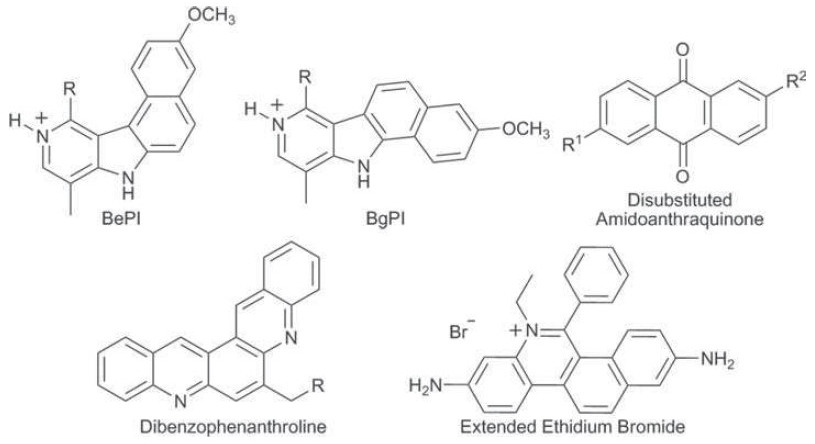

Figure 6.12 *Representative structures of triple helix binders*

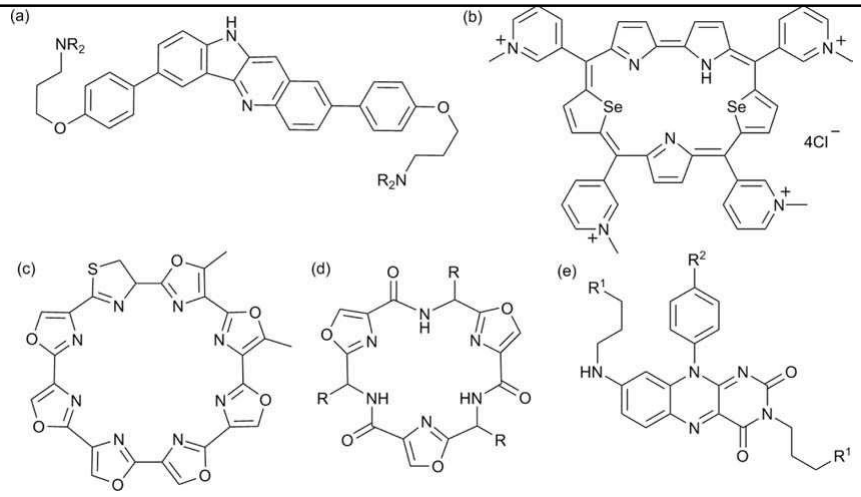

Figure 6.14 *Scaffolds of G-quadruplex binders from the recent literature: (a) 2,7-disubstituted indoloquinolines [61]; (b) Se2SAP [62]; (c) telomstatin [62]; (d) oxazole-based peptide macrocycles [63]; (e) isoalloxazine ligands [64]*