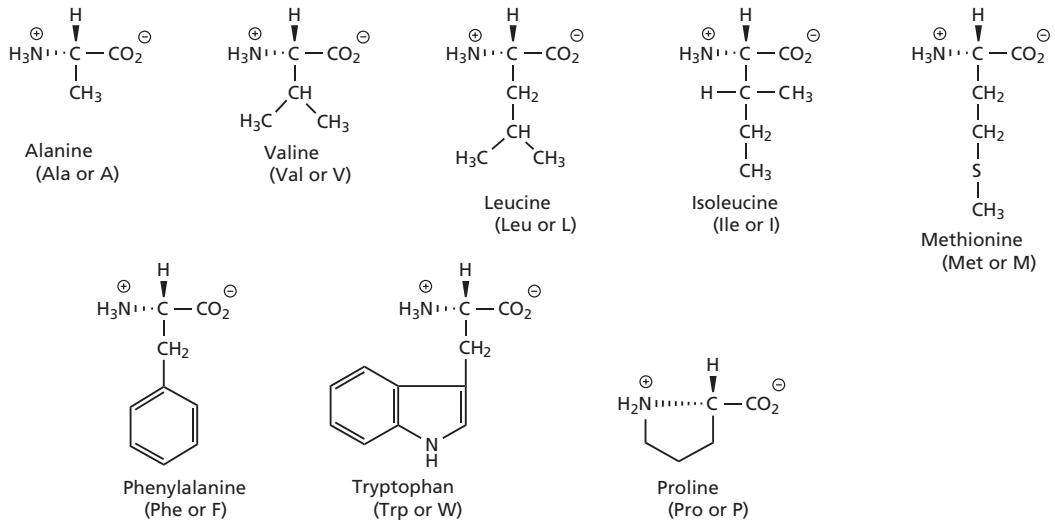


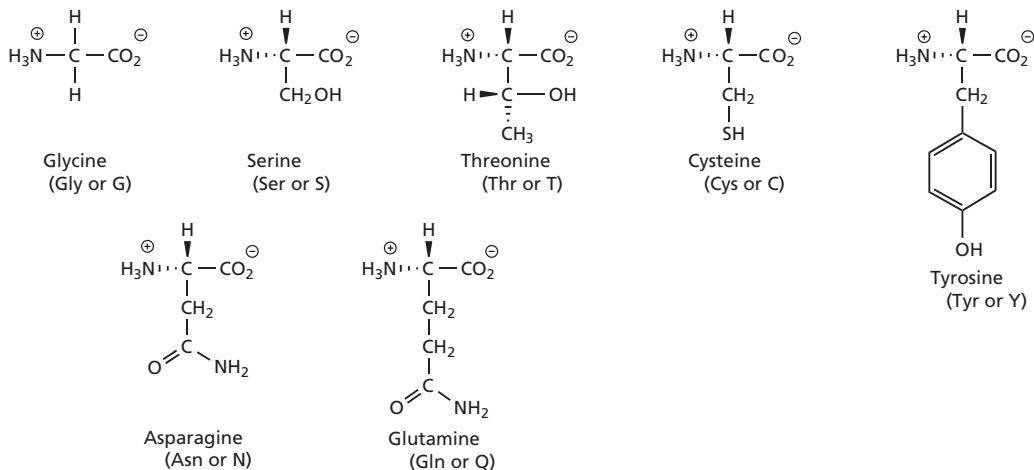
Appendix 1

Essential amino acids

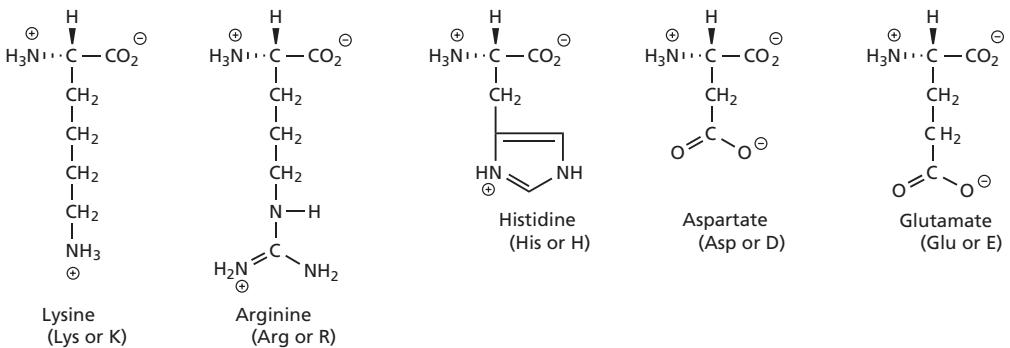
NON POLAR (hydrophobic)



POLAR



IONIZED



Appendix 2

The standard genetic code

UUU	Phe	UCU	Ser	UAU	Tyr	UGU	Cys
UUC	Phe	UCC	Ser	UAC	Tyr	UGC	Cys
UUA	Leu	UCA	Ser	UAA	Stop	UGA	Stop
UUG	Leu	UCG	Ser	UAG	Stop	UGG	Trp
CUU	Leu	CCU	Pro	CAU	His	CGU	Arg
CUC	Leu	CCC	Pro	CAC	His	CGC	Arg
CUA	Leu	CCA	Pro	CAA	Gln	CGA	Arg
CUG	Leu	CCG	Pro	CAG	Gln	CGG	Arg
AUU	Ile	ACU	Thr	AAU	Asn	AGU	Ser
AUC	Ile	ACC	Thr	AAC	Asn	AGC	Ser
AUA	Ile	ACA	Thr	AAA	Lys	AGA	Arg
AUG	Met	ACG	Thr	AAG	Lys	AGG	Arg
GUU	Val	GCU	Ala	GAU	Asp	GGU	Gly
GUC	Val	GCG	Ala	GAC	Asp	GGC	Gly
GUA	Val	GCA	Ala	GAA	Glu	GGA	Gly
GUG	Val	GCG	Ala	GAG	Glu	GGG	Gly

Appendix 3

Statistical data for quantitative structure–activity relationships (QSAR)

To illustrate how statistical terms such as r , s , and F are derived and interpreted, the numerical data in Table A3.1 will be used. There are six compounds in the study ($n = 6$). Y_{exp} is the logarithm of the observed activity for each of the compounds and X is a physicochemical parameter. The QSAR equation derived from the data is:

$$\log(\text{activity}) = Y_{\text{calc}} = k_1 X + k_2 = -0.47 X - 0.022$$

The slope of the line is -0.47 and the intercept with the y -axis is -0.022 .

The correlation coefficient r for the above QSAR equation is calculated using the following equation:

$$r^2 = 1 - \frac{SS_{\text{calc}}}{SS_{\text{mean}}}$$

SS_{calc} is a measure of how much the experimental activity of the compounds varies from the calculated value. For each compound, the difference between the experimental activity and the calculated activity is $Y_{\text{exp}} - Y_{\text{calc}}$ (Fig. A3.1). This is then squared and the values are added together to give the sum of the squares (SS_{calc}).

SS_{mean} is a measure of how much the experimental activity varies from the mean of all the experimental activities and represents the situation where no correlation with X has been attempted (Fig. A3.1).

If there is a correlation between the activity (Y) and the parameter (X), the line of the equation should pass closer to the data points than the line representing the mean. This means that SS_{calc} should be less than SS_{mean} . For a perfect correlation, the calculated values for the activity would be the same as the experimental ones and so SS_{calc} would be zero. This would make $r^2 = 1$.

For the figures shown in Table A3.1, the value of r works out as follows:

$$r^2 = 1 - \frac{SS_{\text{calc}}}{SS_{\text{mean}}} = 1 - \frac{0.1912}{0.5279} = 1 - 0.3622 = 0.638$$

This indicates that only 64% of the variability in activity is due to the parameter X . This is much lower than the minimum acceptable figure of 80% and so the equation is not a particularly good one. Nevertheless, it is possible that X may have some influence on the activity. To check whether there is any significance to the equation

TABLE A3.1

Compound ($n = 6$)	Physicochemical parameter (X)	$\log(\text{act.})_{\text{exp}}$ Y_{exp}	$\log(\text{act.})_{\text{calc}}$ Y_{calc}	$Y_{\text{exp}} - Y_{\text{calc}}$	Square of $Y_{\text{exp}} - Y_{\text{calc}}$	$Y_{\text{exp}} - Y_{\text{mean}}$	Square of $Y_{\text{exp}} - Y_{\text{mean}}$
1	0.23	0.049	-0.129	0.178	0.0317	0.263	0.0692
2	0.23	0.037	-0.129	0.166	0.0276	0.251	0.0630
3	-0.17	0	0.057	-0.057	0.0032	0.214	0.0458
4	0	-0.155	-0.022	-0.133	0.0177	0.059	0.0035
5	1.27	-0.468	-0.613	0.145	0.0210	-0.254	0.0645
6	0.91	-0.745	-0.445	-0.3	0.0900	-0.531	0.2820
Mean value Y_{mean}					Sum of squares SS_{calc}		Sum of squares SS_{mean}
-0.214					0.1912		0.5279

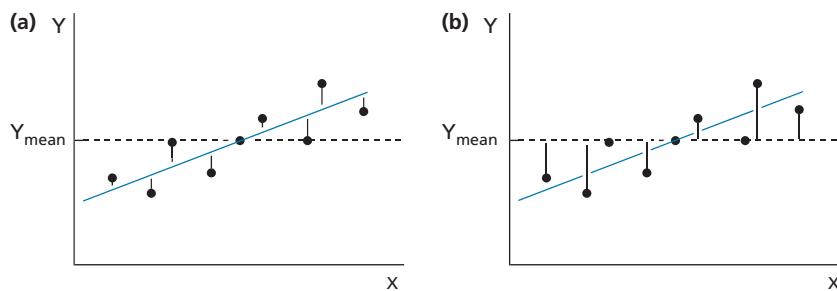


FIGURE A3.1

a statistical test called an *F*-test can be carried out. The equation used for this specific example is as follows:

$$F_{p_2-p_1, n-p_2} = \frac{SS_{\text{mean}} - SS_{\text{calc}}}{SS_{\text{mean}}} \times \frac{n-p_2}{p_2-p_1}$$

where p_2 is the number of parameters involved in the derived QSAR equation (Y and X) and p_1 are the number of parameters involved in the reference equation (Y only in this example). n , SS_{mean} , and SS_{calc} are as described earlier. This gives the following:

$$F_{2-1,6-2} = \frac{0.528 - 0.1912}{0.1912} \times \frac{6-2}{2-1}$$

or $F_{1,4} = \frac{0.528 - 0.1912}{0.1912} \times \frac{6-2}{2-1} = 1.7615 \times 4 = 7.05$

$F_{1,4}$ is now compared against tables of *F* values, which indicate the probability level of a significant correlation. For $F_{1,4}$ the tables show that a value of 4.54 would indicate a probability level of 0.9, whereas 7.71 represents a probability level of 0.95. A value of 21.2 represents a probability level of 0.99. The higher the value of F_{14} , the

closer the probability level approaches 1. The calculated value of 7.05 shows that the probability level is between 0.9 and 0.95.

The standard deviation (s) for the equation is calculated by using the following equation and is dependent on the number of compounds (n) tested.

$$s^2 = \frac{SS_{\text{calc}}}{n-2}$$

This gives a value of 0.218 for the data provided in Table A3.1. The value of s should be as small as possible, but not smaller than the standard deviation of the experimental data.

A QSAR equation can now be derived to see whether the biological activity matches a different physicochemical parameter. Table A3.2 shows values for a different parameter (Z). In this case, the derived equation is:

$$Y_{\text{calc}} = 0.33Z - 0.62$$

TABLE A3.2

Compound ($n = 6$)	Physicochemical parameter (Z)	$\log(\text{act.})_{\text{exp}}$ Y_{exp}	$\log(\text{act.})_{\text{calc}}$ Y_{calc}	$Y_{\text{exp}} - Y_{\text{calc}}$	Square of $Y_{\text{exp}} - Y_{\text{calc}}$	$Y_{\text{exp}} - Y_{\text{mean}}$	Square of $Y_{\text{exp}} - Y_{\text{mean}}$
1	2.03	0.049	0.0499	-0.0009	0.0000	0.263	0.0692
2	1.83	0.037	-0.0161	0.0531	0.0028	0.251	0.0630
3	1.38	0.000	-0.1646	0.1646	0.0271	0.214	0.0458
4	0.90	-0.155	-0.323	0.1680	0.0282	0.059	0.0035
5	1.40	-0.468	-0.158	-0.3100	0.0961	-0.254	0.0645
6	-0.26	-0.745	-0.7058	-0.0392	0.0015	-0.531	0.2820
Mean value Y_{mean}				Sum of squares SS_{calc}		Sum of squares SS_{mean}	
				0.1558		0.5279	

TABLE A3.3

Compound (<i>n</i> = 6)	Physicochemical parameter (X)	Physicochemical parameter (Z)	Log(act.)_{exp}	Y_{exp}	Log(act.)_{calc}	Y_{calc}	Y_{exp}–Y_{calc}	Square of Y_{exp}–Y_{calc}	Y_{exp}–Y_{mean}	Square of Y_{exp}–Y_{mean}
1	0.23	2.03	0.049	0.0493	-0.0003	0.0000			0.263	0.0692
2	0.23	1.83	0.037	-0.0007	0.0377	0.0014			0.251	0.0630
3	-0.17	1.38	0.000	0.0228	-0.0228	0.0005			0.214	0.0458
4	0.00	0.90	-0.155	-0.1550	0.0000	0.0000			0.059	0.0035
5	1.27	1.40	-0.468	-0.4618	-0.0062	0.0000			-0.254	0.0645
6	0.91	-0.26	-0.745	-0.7544	0.0094	0.0001			-0.531	0.2820
Mean value Y _{mean}						Sum of squares SS _{calc}			Sum of squares SS _{mean}	
-0.214						0.0021			0.5279	

710 Appendix 3 Statistical data for quantitative structure–activity relationships (QSAR)

The statistical analysis of this gives the following:

$$n = 6; r = 0.840, s = 0.199, F_{1,4} = 9.6$$

All these results are better than the previous ones, showing that the parameter Z is more important than X in explaining the variation in activity. r is still less than 0.9, however, and further improvements are necessary.

If both of the above parameters are included in the analysis, the equation becomes:

$$Y_{\text{calc}} = -0.34X + 0.25Z - 0.38$$

The corresponding table of results is shown in Table A3.3. The statistical results are $n = 6, r = 0.998, s = 0.028$, and $F_{1,3} = 230.3$. Note that there are three parameters in the QSAR equation and so the F term is $F_{1,3}$ rather than $F_{1,4}$. Comparison with tabulated $F_{1,3}$ values shows that the probability level for this equation is 0.999.

A final check has to be made to ensure that the values for the two parameters (X and Z) are not related in any way. An equation attempting to relate X and Z is derived and assessed statistically. For the values shown, $r^2 = 0.122$, which shows that there is little correlation between X and Z. The final equation is therefore validated.

QSAR equations may also include terms in parenthesis. For example, taking the previous equation:

$$Y_{\text{calc}} = -0.34(\pm 0.08)X + 0.25(\pm 0.05)Z - 0.38(\pm 0.09)$$

The numbers in parenthesis represent the 95% confidence limits for the various parameters. For example, there is 95% confidence that the coefficient for Z lies between the values 0.20 and 0.30. If the number in parenthesis is smaller than the coefficient, it means the parameter is statistically significant in the F -test.

Appendix 4

The action of nerves

The structure of a typical nerve cell or neuron is shown in Fig. A4.1. The nucleus of the cell is found in the large cell body situated at one end of the neuron. Small arms (dendrites) radiate from the cell body and receive messages from other neurons. These messages either stimulate or de-stimulate the neuron. The cell body 'collects' the sum total of these messages.

Ion channels are selective for different ions. There are cationic ion channels for Na^+ , K^+ , and Ca^{2+} ions. When these channels are open, they are generally excitatory and lead to depolarization of the cell.

It is worth emphasizing that the cell body of a neuron receives messages not just from one other neuron, but from a range of different neurons. These pass on different messages (neurotransmitters). Therefore, a message received from a single neuron is unlikely to stimulate a neuron signal by itself, unless other neurons are acting in sympathy.

Assuming that the overall stimulation is great enough, an electrical signal is fired down the length of the neuron (the axon). The axon is covered with sheaths of lipid (myelin sheaths), which act to insulate the signal as it passes down the axon.

The axon leads to a knob-shaped swelling (synaptic button) if the neuron is communicating with another neuron. Alternatively, if the neuron is communicating with a muscle cell, the axon leads to what is known as a neuromuscular endplate, where the end plate is spread like an amoeba over an area of the muscle cell.

Within the synaptic button or neuromuscular endplate there are small globules (vesicles) containing the neurotransmitter chemical. When a signal is received from the axon, the vesicles merge with the cell membrane and release their neurotransmitter into the gap between the neuron and the target cell (synaptic gap). The neurotransmitter binds to a receptor, as described in Chapter 4, and passes on its message. Once the message has been received, the neurotransmitter leaves the receptor and is either broken down enzymatically (e.g. by acetylcholine) or taken up intact by the presynaptic neuron (e.g. noradrenaline). Either way, the neurotransmitter is removed from the synaptic gap and is unable to bind with its receptor a second time.

To date, we have talked about nerves 'firing' and the generation of 'electrical signals' without really considering the mechanism of these processes. The secret behind nerve transmission lies in the movement of ions across cell membranes, but there is an important difference in what happens in the cell body of a neuron compared with the axon. We shall consider what happens in the cell body first.

All cells contain sodium, potassium, calcium, and chloride ions, and it is found that the concentration of these ions is different inside the cell compared with outside. The concentration of potassium inside the cell is larger than the surrounding medium, whereas the concentration of sodium and chloride ions is smaller. Thus, a concentration gradient exists across the membrane.

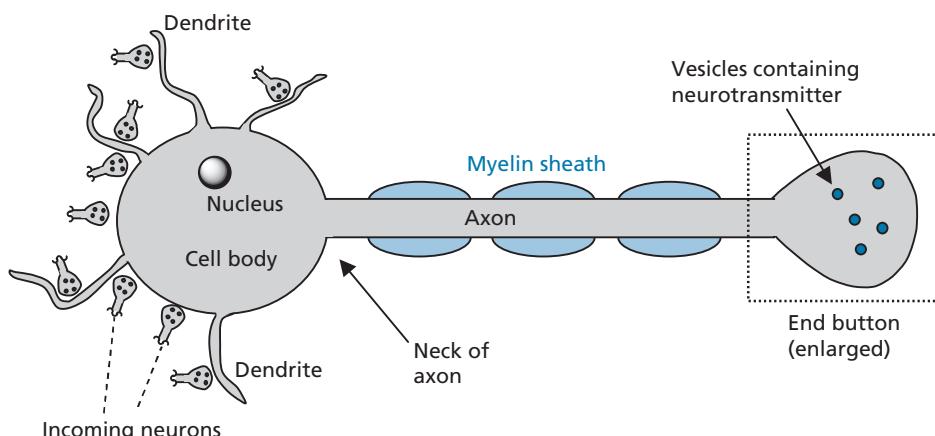


FIGURE A4.1 Structure of a typical nerve cell (neuron).

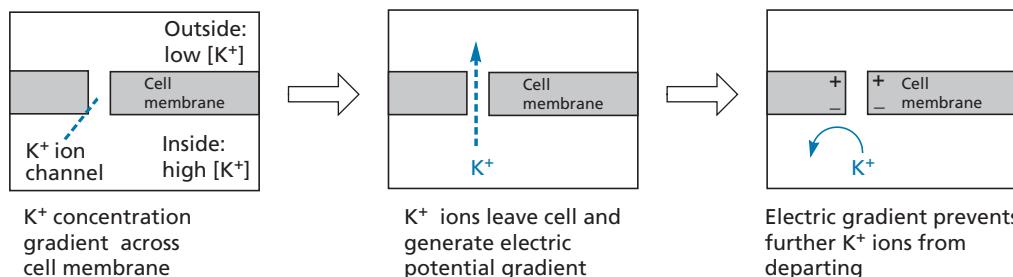


FIGURE A4.2 Generation of electric potential across a cell membrane.

Potassium is able to move down its concentration gradient (i.e. out of the cell), as it can pass through the potassium ion channels (Fig. A4.2). But, if potassium ions can move out of the cell, why does the potassium concentration inside the cell not fall to equal that of the outside? The answer lies in the fact that potassium is a positively charged ion and, as it leaves the cell, an electric potential is set up across the cell membrane. This would not happen if a negatively charged counterion could leave with the potassium ion. However, the counterions in question are large proteins which cannot pass through the cell membrane. As a result, a few potassium ions are able to escape down the ion channels out of the cell and an electric potential builds up across the cell membrane such that the inside of the cell membrane is more negative than the outside. This electric potential (50–80 mV) opposes, and eventually prevents, the flow of potassium ions.

But what about the sodium ions? Could they flow into the cell along their concentration gradient to balance the charged potassium ions that are departing? The answer is that they cannot because they are too big for the potassium ion channels. This appears to be a strange argument, as sodium ions are smaller than potassium ions, but it has to be remembered that we are dealing with an aqueous environment where the ions are solvated (i.e. they have a 'coat' of water molecules). Sodium, being a smaller ion than potassium, has a greater localization of charge and is able to bind its solvating water molecules more strongly. As a result, sodium, along with its water coat, is bigger than a potassium ion with or without its water coat.

Ion channels for sodium do exist, and these channels are capable of removing the water coat around sodium and letting it through. However, the sodium ion channels are mostly closed when the neuron is in the resting state. As a result, the flow of sodium ions across the membrane is very small compared to potassium. Nevertheless, the presence of sodium ion channels is crucial to the transmission of a nerve signal.

To conclude, the movement of potassium across the cell membrane sets up an electric potential across the cell membrane which opposes this flow. Charged protein structures are unable to move across the membrane, while sodium

ions cross very slowly and so an equilibrium is established. The cell membrane is polarized and the electric potential at equilibrium is known as the resting potential.

The number of potassium ions required to establish that potential is of the order of a few million compared with the several hundred billion present in the cell. Therefore, the effect on concentration is negligible.

As mentioned above, potassium ions are able to flow out of potassium ion channels, but not all of these channels are open in the resting state. What would happen if more were to open? The answer is that more potassium ions would flow out of the cell and the electric potential across the cell membrane would become more negative to counter this increased flow. This is known as **hyperpolarization** and the effect is to de-stimulate the neuron (Fig. A4.3).

Suppose, instead, that a few sodium ion channels were to open up. In this case, sodium ions would flow into the cell and, as a result, the electric potential would become less negative. This is known as **depolarization** and results in a stimulation of the neuron.

If chloride ion channels are opened, chloride ions flow into the cell, and the cell membrane becomes hyperpolarized, de-stimulating the neuron.

Ion channels do not open or close by chance. They are controlled by the neurotransmitters released by communicating neurons. The neurotransmitters bind with their receptors and this leads to the opening or closing of ion channels. Such ion channels are known as **ligand-gated ion channels**. For example, acetylcholine controls the sodium ion channel, whereas γ -aminobutyric acid (GABA) and glycine control chloride ion channels. The resulting flow of ions leads to a localized hyperpolarization or depolarization in the area of the ion channel. The cell body collects and sums all this information such that the neck of the axon experiences an overall depolarization or hyperpolarization depending on the sum total of the various excitatory or inhibitory signals received.

We shall now consider what happens at the axon of the neuron (Fig. A4.4). The cell membrane of the axon also has sodium and potassium ion channels, but they are different in character from those in the cell body. The axon

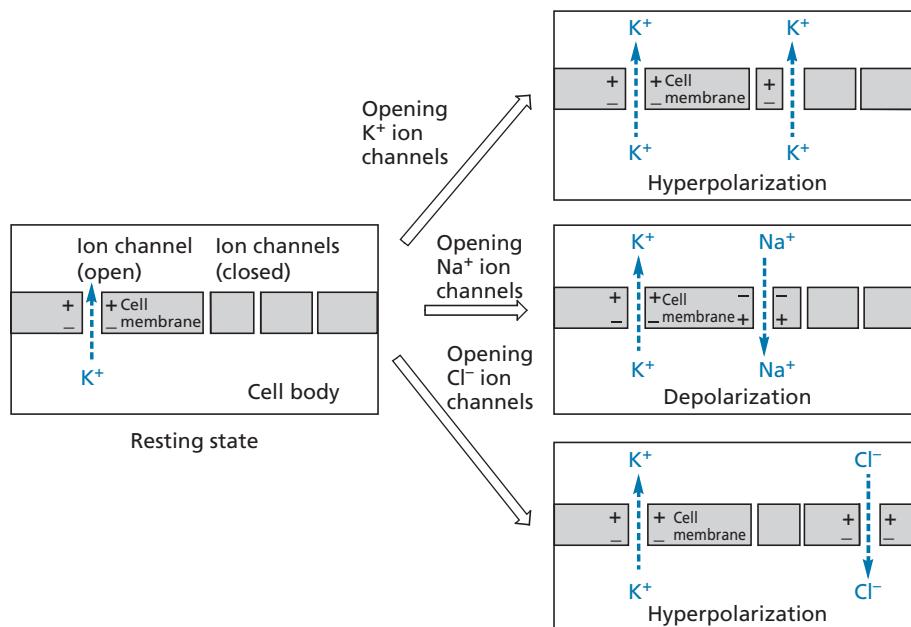


FIGURE A4.3 Hyperpolarization and depolarization.

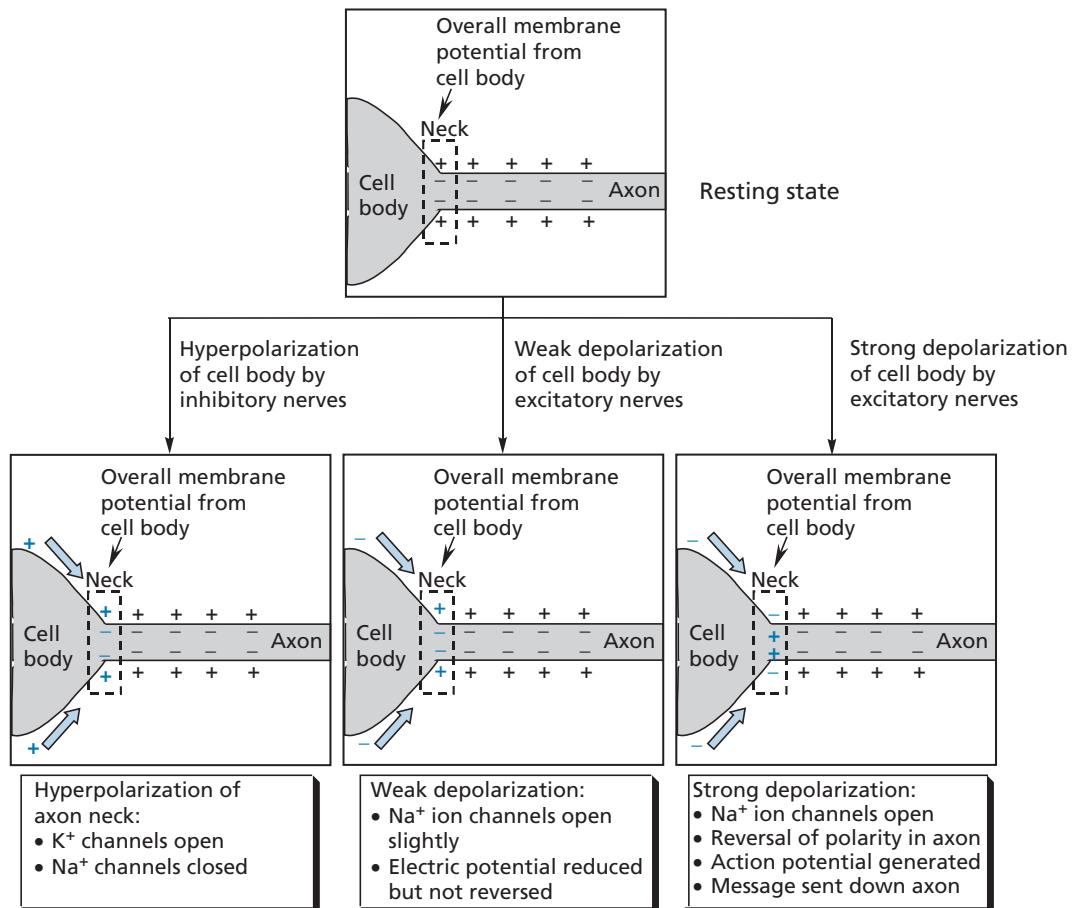


FIGURE A4.4 Hyperpolarization and depolarization effects at the neck of the axon.

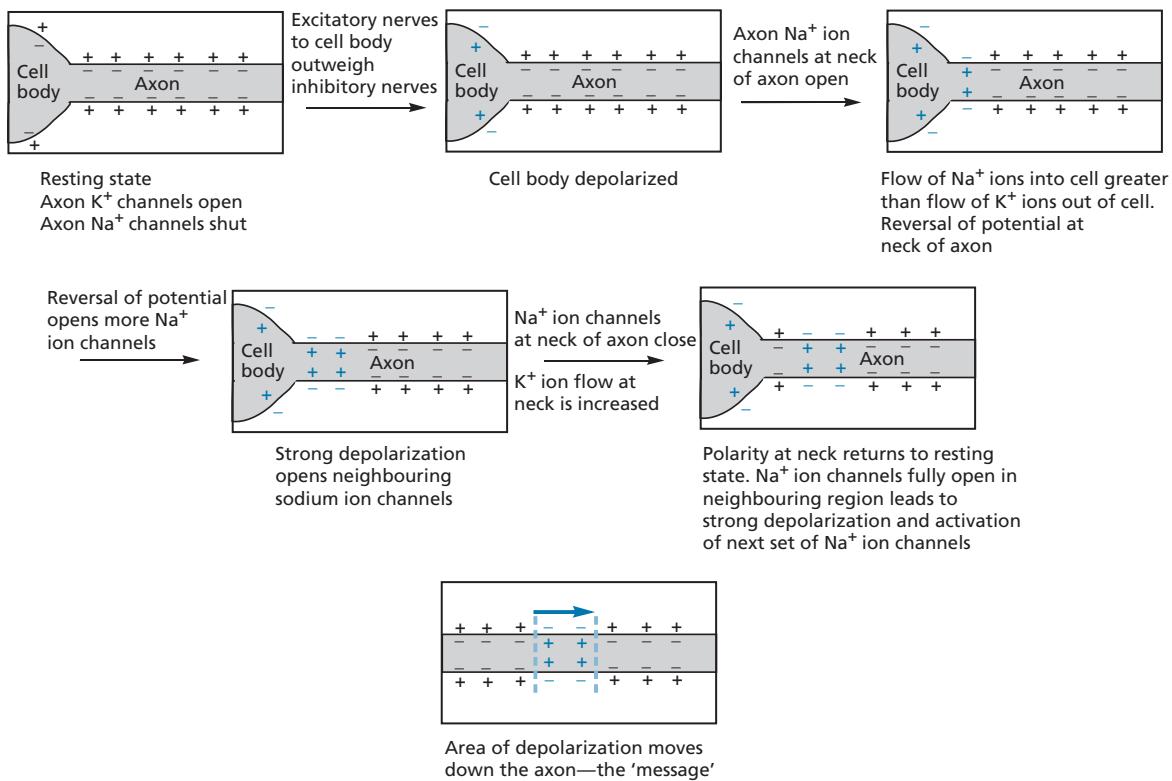


FIGURE A4.5 Generation of an action potential.

ion channels are not controlled by neurotransmitters, but by the electric potential of the cell membrane. Therefore, they are known as **voltage-gated ion channels**.

The sodium ion channels located at the junction of the nerve axon with the cell body are the crucial channels as they are the first channels to experience whether the cell body has been depolarized or hyperpolarized.

If the cell body is strongly depolarized then a signal is fired along the neuron. A specific threshold value has to be reached before this happens, however. If the depolarization from the cell body is weak, only a few sodium channels open up and the depolarization at the neck of the axon does not reach that threshold value. The sodium channels then reclose and no signal is sent.

With stronger depolarization, more sodium channels open up until the flow of sodium ions entering the axon becomes greater than the flow of potassium ions leaving it. This results in a rapid increase in depolarization, which, in turn, opens up more sodium channels, resulting in very strong depolarization at the neck of the axon. The flow of sodium ions into the cell increases dramatically, such that it is far greater than the flow of potassium ions out of the axon, and the electric potential across the

membrane is reversed, such that it is positive inside the cell and negative outside the cell. This process lasts less than a millisecond before the sodium channels reclose and sodium permeability returns to its normal state. More potassium channels then open and permeability to potassium ions increases for a while to speed up the return to the resting state.

The process is known as an action potential and can only take place in the axon of the neuron. The cell membrane of the axon is said to be excitable, unlike the membrane of the cell body. The important point to note is that once an action potential has fired at the neck of the axon it has reversed the polarity of the membrane at that point. This, in turn, has an effect on the neighbouring area of the axon and depolarizes it beyond the critical threshold level. It, too, fires an action potential and so the process continues along the whole length of the axon (Fig. A4.5). The number of ions involved in this process is minute, such that the concentrations are unaffected. Once the action potential reaches the synaptic button or the neuromuscular endplate it causes an influx of calcium ions into the cell and an associated release of neurotransmitter into the synaptic gap. The mechanism of this is not well understood.

Appendix 5

Microorganisms

Bacterial nomenclature

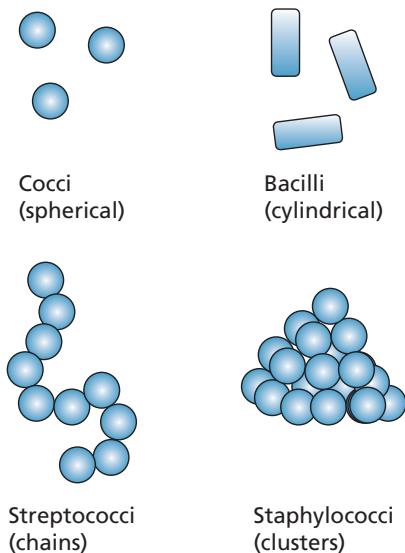


FIGURE A5.1 Bacterial nomenclature.

The Gram-stain

The Gram stain is a staining procedure of great value in the identification of bacteria.

The staining technique involves the addition of a purple dye followed by washing with acetone. Bacteria with a thick cell wall (20–40 nm) absorb the dye and are defined as Gram-positive because they are stained purple. Bacteria with a thin cell wall (2–7 nm) absorb only a small amount of dye, and the excess dye is washed out with acetone. These bacteria are then stained pink with a second dye and are said to be Gram-negative.

- Gram-negative bacteria—these cells have a thin cell wall and are coloured pink.
- Gram-positive bacteria—these cells have a thick cell wall and are coloured purple.

Classifications

Bacteria can be classified as being Gram-positive or Gram-negative depending on what colour they retain on

TABLE A5.1 Some clinically important bacteria

Organism	Gram	Infections
<i>Staphylococcus aureus</i>	Positive	Skin and tissue infections, septicaemia, endocarditis; accounts for about 25% of all hospital infections
<i>Streptococcus</i> species	Positive	Several types—commonly cause sore throats, upper respiratory tract infections, and pneumonia
<i>Escherichia coli</i>	Negative	Urinary tract and wound infections, common in the gastrointestinal tract, and often causes problems after surgery; accounts for about 25% of hospital infections
<i>Proteus</i> species	Negative	Urinary tract infections
<i>Salmonella</i> species	Negative	Food poisoning and typhoid
<i>Shigella</i> species	Negative	Dysentery
<i>Enterobacter</i> species	Negative	Urinary tract and respiratory tract infections, septicaemia
<i>Pseudomonas aeruginosa</i>	Negative	An opportunist pathogen, can cause very severe infections in burn victims and other compromised patients, e.g. cancer patients; commonly causes chest infections in patients with cystic fibrosis
<i>Haemophilus influenzae</i>	Negative	Chest and ear infections, occasionally meningitis in young children
<i>Bacteroides fragilis</i>	Negative	Septicaemia following gastrointestinal surgery

treatment with the Gram-stain procedure. They can also be classed as **aerobic** or **anaerobic** depending on their dependency on oxygen. Aerobic organisms grow in the presence of oxygen, whereas anaerobic organisms do not.

Definitions of different microorganisms

Bacteria are unicellular organisms that have a prokaryotic cell structure. They are diverse in nature and some can carry out photosynthesis. Examples of typical infections are given in Table A5.1.

Blue-green algae are made up of prokaryotic cells that can form multicellular filaments and carry out photosynthesis in the same manner as the eukaryotic algae.

Algae, with the exception of the blue-green algae, are made up of eukaryotic cells and can perform oxygen-evolving photosynthesis. Some are unicellular and some are multicellular. The latter have little, or no, cell differentiation, which sets them apart from higher multicellular organisms, such as plants and animals.

Protozoa are unicellular eukaryotic organisms that are unable to carry out photosynthesis. They are responsible for diseases such as malaria, African sleeping sickness, Chagas' disease, leishmaniasis, and amoebic dysentery.

Fungi are multicellular eukaryotic organisms with little, or no, cell differentiation, which can form long filaments of interconnected cells called mycelia. They, too, are unable to carry out photosynthesis. Fungi are responsible for infections such as athlete's foot, ringworm, aspergillosis, candidiasis, and histoplasmosis.

Appendix 6

Drugs and their trade names

Drug name (Trade name)

abacavir (Ziagen)
abiraterone (Zytiga)
abciximab (ReoPro)
acebutolol (Sectral)
acetorphan (Hidrasec)
aciclovir (Virovir, Zovirax)
aclacinomycin A *see* aclarubicin
aclarubicin (Aclacin, Aclaplastin)
alclometasone dipropionate (Modrasone)
actinomycin D *see* dactinomycin
acyclovir *see* aciclovir
adalimumab (Humira)
adefovir dipivoxil (Hepsera)
adriamycin *see* doxorubicin
agalsidase beta (Fabrazyme)
albuterol *see* salbutamol
aldesleukin (Proleukin)
alemtuzumab (MabCampath)
aliskiren (Tekturna)
allopurinol (Zyloprim)
amantadine (Lysovir, Symmetrel)
aminoglutethimide (Orimeten, Cytadren)
5-aminolevulinic acid (Levulan)
amoxicillin (Amoxil)
amoxicillin with clavulanic acid (Augmentin)
amoxyccillin *see* amoxicillin
amphotericin (Fungilin, Fungizone)
ampicillin (Penbritin)
ampicillin and flucloxacillin (Co-fluampicil)
amprenavir (Agenerase)
amsacrine (Amsidine)
anastrozole (Arimidex)
armodafinil (Nuvigil)
arsenic trioxide (Trisenox)
atazanavir (Reyataz)
atenolol (Tenormin)
atomoxetine (Strattera)
atorvastatin (Lipitor)
atracurium (Tracrium)
azathioprine (Imuran)
azidothymidine *see* zidovudine
azithromycin (Zithromax)
AZT *see* zidovudine
aztreonam (Azactam)
bacitracin and neomycin sulfate (Cicatrin)

bacitracin and polymyxin B sulfate (Polyfax)
beclometasone dipropionate (Beconase, Asmabec Clickhaler, Becodisks, Clenil Modulite, Qvar, Easi-Breathe)
beclometasone dipropionate and formoterol fumarate (Fostair)
belimumab (Benlysta)
bendamustine (Treanda)
benztropine (Cogentin)
benzhexol *see* trihexyphenidyl
benztropine *see* benztropine
benzylpenicillin (Crystapen)
besifloxacin (Besivance)
betamethasone (Betnelan)
betamethasone dipropionate (Diprosone)
betamethasone dipropionate, clotrimazole (Lotriderm)
betamethasone sodium phosphate (Betnesol, Vistamethasone)
betamethasone sodium phosphate, neomycin (Betnesol-N)
betamethasone dipropionate, salicylic acid (Diprosalic)
betamethasone valerate (Betacap, Betesil, Betnovate, Bettamousse)
betamethasone valerate, clioquinol (Betnovate-C)
betamethasone valerate, fusidic acid (Fucibet)
betamethasone valerate, neomycin sulphate (Betnovate-N)
betaxolol (Betoptic)
bethanechol (Myotonine)
bevacizumab (Avastin)
boceprevir (Victrelis)
bortezomib (Velcade)
brentuximab vedotin (Adcetris)
bupivacaine (Marcaine)
buprenorphine (Subutex, Temgesic, Transtec)
bupropion (Zyban)
bupropion and naltrexone (Contrave)
busulfan (Busilvex, Myleran)
busulphan *see* busulfan
capecitabine (Xeloda)
captopril (Capoten)
carbenoxolone (Pyrogastrone)
carbidopa with levodopa *see* co-careldopa
carboplatin (Paraplatin)

carmustine (BCNU, BiCNU, Gliadel)
cefalexin (Ceporex, Keflex, Keftab, Biocef)
cefalothin (Keflin)
ceftaroline fosamil (Teflaro)
cefotaxime (Claforan)
cefoxitin (Mefoxin)
cefprome (Ceffrom)
ceftazidime (Fortum, Kefadim)
ceftobiprole (Zeftera/Zevtera)
ceftriaxone (Rocephin)
cefuroxime (Zinacef, Zinnat, Kefurox)
celecoxib (Celebrex)
cephalexin *see cefalexin*
cephalothin *see cefalothin*
cerivastatin (Baycol)
cetuximab (Erbitux)
chlorambucil (Leukeran)
chloramphenicol (Kemicetine, Chloromycetin)
chlordiazepoxide (Librium)
chloroquine (Avloclor, Nivaquine)
chlorpromazine (Largactil)
chlortetracycline, demeclocycline and tetracycline (Deteclol)
cholestyramine *see colestyramine*
ciclesonide (Alvesco)
ciclosporin (Neoral, Sandimmun)
cidofovir (Vistide)
cilastatin with imipenem (Primaxin)
cilazapril (Vascace)
cimetidine (Dyspamet, Tagamet)
ciprofloxacin (Ciproxin, Ciprobay, Cipro, Ciproxan)
citalopram (Cipramil)
clarithromycin (Clarosip, Klaricid)
clavulanic acid with amoxicillin (Augmentin)
clindamycin (Dalacin C)
clobetasol propionate (Carelux, Dermovate, Etrivex)
clobetasol propionate, neomycin sulphate, nystatin (Dermovate-NN)
clobetasone butyrate (Eumovate)
clobetasone butyrate, oxytetracycline (Trimovate)
clonidine (Catapres, Dixarit)
clozapine (Clozaril)
co-amoxiclav (Augmentin)
co-careldopa (Sinemet, Stalevo)
colestyramine (Questran)
co-trimoxazole (Septrin)
compactin (Mevastatin)
crizotinib (Xalkori)
crisantaspase (Erwinase)
cyclopentolate (Mydriilate)
cyclophosphamide (Endoxana)
cyclosporin *see ciclosporin*
cyproterone acetate (Cyprostat)
dacarbazine (DTIC-Dome)

daclizumab (Zenapax)
dactinomycin (Cosmegen Lyovac)
dalfopristin with quinupristin (Synercid)
daptomycin (Cubicin)
darunavir (Prezita)
dasatinib (Sprycel)
daunorubicin (DaunoXome)
deflazacort (Calcort)
degarelix acetate (Firmagon)
delavirdine (Descriptor)
demeclocycline, chlortetracycline, and tetracycline (Deteclol)
denosumab (Prolia)
depsipeptide (Istodax)
dexamethasone (Maxidex)
dexamethasone, neomycin sulphate (Otomize)
dexamethasone, neomycin sulphate, polymyxin B sulphate (Maxitrol)
dexamethasone sodium metasulphobenzoate, framycetin sulphate, gramicidin (Sofradex)
dexamethasone, tobramycin (Tobradex)
dexlansoprazole (Dexilant)
diazepam (Valium)
didanosine (Videx)
diflucortolone valerate (Nerisone)
dihydrocodeine (DF118 Forte, DHC Continus)
dihydrocodeinone (Hycodan)
digoxin (Lanoxin)
diphenhydramine (Benadryl)
diphenoxylate and atropine sulphate (Co-phenotrope)
dipipanone (diconal)
disulfiram (Antabuse)
dobutamine (Dobutrex, Posject)
docetaxel (Taxotere)
donepezil (Aricept)
doxazosin (Cardura)
doxorubicin (Rubex, Doxil)
doxycycline (Vibramycin)
duloxetine (Cymbalta, Yentreve)
efavirenz (Sustiva)
emtricitabine (Emtriva)
emtricitabine and tenofovir (Truvada)
emtricitabine, tenofovir and efavirenz (Atripla)
enalapril (Innovace)
enfuvirtide (Fuzeon)
epirubicin (Pharmorubicin)
eribulin (Halaven)
erlotinib (Tarceva)
ertapenem (Invanz)
erythromycin (Erymax, Erythrocin, Erythroped)
escitalopram (Cipralex)
esmolol (Brevibloc)
esomeprazole (Nexium)
estramustine (Estracyt)

- etanercept** (Enbrel)
etoposide (Etopophos, Vepesid)
etravirine (Intelence)
everolimus (Zortress, Certican)
ezetimibe (Zetia)
ezetimibe and simvastatin (Vytorin)
famciclovir (Famvir)
famotidine (Pepcid)
fentanyl (Sublimaze, Actiq, Durogesic)
fexofenadine (Allegra, Telfast)
fidaxomicin (Dificlir)
filgrastim (Neupogen)
flucloxacillin (Floxapen)
flucloxacillin and ampicillin (Co-fluampicil)
fluconazole (Diflucan)
fludarabine (Fludara)
fludroxycortide (Haelan)
flumetasone pivalate and clioquinol (Locerten-Vioform)
flunisolide (Synartis)
fluocinolone acetonide (Synalar)
fluocinolone acetonide, clioquinol (Synalar C)
fluocinolone acetonide, neomycin sulphate (Synalar N)
fluocinonide (Metosyn)
fluocortolone (Ultranum Plain)
fluorometholone (FML)
fluorouracil (Efudix)
fluoxetine (Prozac)
fluphenazine decanoate (Modecate)
flutamide (Drogenil)
fluticasone furoate (Avamys)
fluticasone propionate (Cutivate, Flixonase, Flixonase Nasule, Nasofan, Flixotide)
fluticasone propionate and salmeterol (Seretide)
fluvastatin (Lescol)
fluvoxamine (Faverin)
fomivirsen (Vitravene)
formestane (Lentaron)
fosamprenavir (Lexiva, Telzir)
foscarnet (Foscavir)
fulvestrant (Faslodex)
fusidic acid (Fucidin)
gabapentin (Neurontin)
galantamine (Reminyl)
galanthamine see galantamine
ganciclovir (Cymevene)
gefitinib (Iressa)
gemcitabine (Gemzar)
gemtuzumab (Mylotarg)
gentamicin (Cidomycin, Genticin)
glucarpidase (Voraxaze)
goserelin (Zoladex)
granisetron (Kytril)
guanethidine (Ismelin)
halobetasol propionate (Ultravate)
hexamine see methenamine
hydrocodone (Hycodan)
hydrocortisone (Efcortesol, Solu-Cortef, Corlan, Dioderm, Mildison)
hydrocortisone acetate and fusidic acid (Fucidin H)
hydrocortisone and gentamicin (Gentisone)
hydrocortisone and miconazole nitrate (Daktacort)
hydrocortisone, clomitiazole (Canesten)
hydrocortisone, neomycin sulphate and polymyxin B sulphate (Otosporin)
hydrocortisone, nystatin, benzalkonium chloride (Timodine)
hydrocortisone, nystatin, chlorhexidine (Nystaform-HC)
hydrocortisone butyrate (Locoid)
hydromorphone (Palladone)
hyoscine (Scopoderm TTS)
ibritumomab (Zevalin)
idarubicin (Zavedos)
idoxuridine (Herpid)
ifosfamide (Mitoxana)
imatinib (Glivec)
imiglucerase (Cerezyme)
imipenem and cilastatin (Primaxin)
imipramine (Tofranil)
imiquimod (Aldara)
indacaterol (Onbrez)
indinavir (Crixivan)
indometacin (Rimacid)
indomethacin see indometacin
infliximab (Remicade)
 α -interferon (IntronA, Roferon-A, Viraferon)
 γ -interferon (Immukin)
ipratropium (Atrovent, Ipratropium Steri-Neb, Respontin)
irinotecan (Campto, Camptosar)
lamivudine (Epivir, Zeffix)
laninamivir (Inavir)
lansoprazole (Zoton)
lapatinib (Tykerb)
lenalidomide (Revlimid)
L-dopa see levodopa
letrozole (Femera)
levalbuterol (Xopenex)
levobupivacaine (Chirocaine)
levodopa with carbidopa see co-careldopa
levofloxacin (Levaquin, Tavanic)
lidocaine (Xylocaine)
lignocaine see lidocaine
linezolid (Zyvox)
lisinopril (Carace, Zestril, Prinivil)
lithium carbonate (Camcolit, Liskonum, Priadel)
lomustine (CCNU)
loperamide (Imodium)

- lopinavir with ritonavir** (Kaletra)
- losartan** (Cozaar)
- loteprednol etabonate** (Lotemax)
- lovastatin** (Mavacor)
- lucanthone** (Miracil D)
- lumiracoxib** (Prexige)
- lumiracoxib and biomarker** (Joicela)
- malathion** (Derbac-M, Prioderm, Quellada M, Suleo-M)
- maraviroc** (Celsentri)
- medroxyprogesterone acetate** (Farlutal, Provera)
- megestrol acetate** (Megace)
- melphalan** (Alkeran)
- meperidine** *see* pethidine
- mercaptopurine** (Puri-Nethol)
- meropenem** (Meronem)
- mesna** (Uromitexan)
- methadone** (Methadose)
- methenamine** (Hiprex)
- methyldopa** (Aldomet)
- methylphenidate** (Ritalin)
- methylprednisolone** (Medrone, Depo-Medrone, Solu-Medrone)
- metoclopramide** (Maxolon)
- metoprolol** (Betaloc, Lopresor, Corvitol)
- metronidazole** (Flagyl, Metrolyl)
- mirtazepine** (Zispin)
- mitoxantrone** (Novantrone, Onkotrone)
- mivacurium** (Mivacron)
- moclobemide** (Manerix)
- modafinil** (Provigil)
- mometasone furoate** (Nasonex, Asmanex, Elocon)
- morphine** (Oramorph, Sevredol, Morcap, Morphgesic, MST Cintinus, MXL, Zomorph)
- moxifloxacin** (Avelox, Avalox, Vigamox)
- mupirocin** (Bactroban)
- nabiximols** (Sativex)
- nadolol** (Corgard)
- nalidixic acid** (Mictral, Negram, Uriben)
- nalfurafine** (Remitch)
- nalmefene** (Revex, Selincro)
- naloxone** (Narcan)
- naltrexone** (Nalorex)
- naltrexone and bupropion** (Contrave)
- natalizumab** (Tysabri)
- nelfinavir** (Viracept)
- neomycin** (Maxitrol)
- neomycin sulfate and bacitracin** (Cicatrin)
- nevirapine** (Viramune)
- nicotine** (Nicorette, Nicotinell, NiQuitin CQ)
- nilotinib** (Tasigna)
- nitrofurantoin** (Furadantin, Macrobid, Macrodantin)
- nizatidine** (Axid)
- oblimersen** (GenaSense)
- ofatumumab** (Arzerra)
- ofloxacin** (Floxin, Tarivid)
- olanzapine** (Zyprexa)
- omalizumab** (Xolair)
- omeprazole** (Losec, Prilosec)
- ondansetron** (Zofran)
- oseltamivir** (Tamiflu)
- oxaliplatin** (Eloxatin)
- oxamniquine** (Mansil, Vansil)
- oxprenolol** (Trasicor)
- oxycodone** (Oxecta)
- oxytocin** (Syntocinon)
- paclitaxel** (Taxol)
- palivizumab** (Synagis)
- panitumumab** (Vectibix)
- pantoprazole** (Protium)
- paroxetine** (Seroxat)
- pazopanib** (Votrient)
- pegademase** PEG-adenosine deaminase (Adagen)
- pegaptanib** (Macugen)
- pegaspargase** PEG-asparaginase (Oncaspar)
- pegfilgrastim** (Neulasta)
- peginterferon α 2a** PEG-(IFN- α -2a) (Pegasys)
- peginterferon α 2b** PEG-(IFN- α -2b) (Peg-Intron)
- pegvisomant** (Somavert)
- pemetrexed** (Alimta)
- penciclovir** (Vectavir)
- penicillin G** *see* benzylpenicillin
- penicillin V** *see* phenoxyethylpenicillin
- pentazocine** (Fortral)
- pentostatin** (Nipent)
- peramivir** (Raplasta)
- pethidine** (Demerol, Pamergan P100)
- phenelzine** (Nardil)
- phenoxyethylpenicillin** (Apsin)
- phentermine and topiramate** (Qnexa)
- pilocarpine** (Pilogel)
- piperacillin and tazobactam** (Tazocin or Zosyn)
- pleconaril** (Picovir)
- podophyllotoxin** (Condyline, Warticon)
- polymyxin B and bacitracin** (Polyfax)
- polymyxin B and hydrocortisone** (Otosprin)
- pralatrexate** (Folotyn)
- pravastatin** (Pravachol)
- praziquantel** (Cysticide)
- prazosin** (Hypovase)
- prednisolone acetate** (Pred Forte)
- prednisolone sodium phosphate** (Predsol)
- prednisolone sodium phosphate with neomycin sulphate** (Predsol-N)
- probencid** (Probucid, Benuryl)
- promethazine** (Phenergan)
- propranolol** (Inderal)
- propantheline bromide** (Pro-Banthine)
- pseudoephedrine** (Galseud or Sudafed)

pyridostigmine (Mestinon)
pyrimethamine with sulfadoxine (Fansidar)
quinupristin with dalfopristin (Synercid)
rabeprazole (Pariet)
racecadotril (Hidrasec)
raltegravir (Isentress)
raltitrexed (Tomudex)
raloxifene (Evista)
ranibizumab (Lucentis)
ranitidine (Zantac)
reboxetine (Edronax)
ribavirin (Copegus, Rebetol, Virazole)
rifampicin (Rifadin, Rimactane, Rifater, Rifinah, Rimactazid)
rifaximin (Xifaxin)
rilpivirine (Edurant)
rimexolone (Vexol)
risperidone (Risperdal)
ritonavir (Norvir)
rituximab (Rituxan, MabThera)
rivastigmine (Exelon)
rocuronium (Esmeron)
rofecoxib (Vioxx)
romidepsin (Istodax)
rosuvastatin (Crestor)
ruxolitinib (Jakafi)
salbutamol (Ventmax, Ventolin, Volmax, Airomir, Asmasal Clickhaler, Salamol Easi-Breathe, Ventodisks)
salmeterol (Serevent)
saquinavir (Fortovase, Invirase)
selegiline (Deprenyl, Eldepryl, Zelapar)
sertraline (Lustral)
sildenafil (Viagra)
simvastatin (Zocor)
simvastatin and ezetimibe (Vytorin)
sorafenib (Nexavar)
stavudine (Zerit)
suberoylanilide hydroxamic acid see vorinostat
sugammadex (Bridion)
sulfadoxine with pyrimethamine (Fansidar)
sumatriptan (Imigran)
sunitinib (Sutent)
suxamethonium (Anectine)
tacrine (Cognex)
tamoxifen (Nolvadex)
tazobactam with piperacillin (Tazocin or Zosyn)
teicoplanin (Targocid)
telaprevir (Incivek)
telithromycin (Katek)
temocillin (Negaban)

temoporfin (Foscan)
temozolomide (Temodar, Temodal)
temsirolimus (Torisel)
teniposide (Vumon)
tenofovir (Viread)
terazosin (Hytrin)
testosterone propionate (Sustanon 250, Viormone)
tetracycline, chlortetracycline, and demeclocycline (Detecl)
theophylline (Nuelin, Slo-Phyllin, Uniphyllin Continus)
thioguanine see tioguanine
ticarcillin with clavulanic acid (Timentin)
timolol (Betim)
tioconazole (Trosyl)
tioguanine (Lanvis)
tipifarnib (Zarnestra)
tirofiban (Aggrastat)
tobramycin (Nebcin, Tobi)
toceranib (Palladia)
topiramate and phentermine (Qnexa)
topotecan (Hycamtin, Hycamtin)
toremifene (Fareston)
tositumomab (Bexxar)
trastuzumab (Herceptin)
tretinoin (Vesanoid)
triamcinolone acetonide (Kenalog, Nasacort)
triamcinolone acetonide, chlortetracycline (Aureocort)
trihexyphenidyl (Broflex)
trimethoprim (Monotrim, Trimopan)
tropicamide (Mydriacyl)
valaciclovir (Valtrex)
valdecoxib (Bextra)
valganciclovir (Valcyte)
vancomycin (Vancocin)
vandetanib (Caprelsa, Zactima)
varenicline (Chantix)
vasopressin (Pitressin)
vecuronium (Norcuron)
vemurafenib (Zelboraf)
venlafaxine (Fluanxol)
verapamil (Cordilox, Securon)
vinblastine (Velbe)
vincristine (Oncovin)
vindesine (Eldisine)
vinorelbine (Navelbine)
vismodegib (Erivedge)
vorinostat (Zolinza)
zalcitabine (Hivid)
zanamivir (Relenza)
zidovudine (Retrovir)

Appendix 7

Trade names and drugs

Trade name (drug name)

Aclacin (aclarubicin)
Aclaplastin (aclarubicin)
Actiq (fentanyl)
Adagen (pegademase)
Adcetris (brentuximab vedotin)
Agenerase (amprenavir)
Aggrastat (tirofiban)
Airomir (salbutamol)
Aldara (imiquimod)
Aldomet (methyldopa)
Alimta (pemetrexed)
Alkeran (melphalan)
Allegra (fexofenadine)
Alvesco (ciclesonide)
Amoxil (amoxicillin)
Amsidine (amsacrine)
Anectine (suxamethonium)
Antabuse (disulfiram)
Apsin (phenoxymethylpenicillin)
Aricept (donepezil)
Arimidex (anastrozole)
Arzerra (ofatumumab)
Asmabec Clickhaler (beclometasone dipropionate)
Asmanex (mometasone furoate)
Asmasal Clickhaler (salbutamol)
Atripla (emtricitabine, tenofovir & efavirenz)
Atrovent (ipratropium)
Augmentin (amoxicillin with clavulanic acid)
Augmentin (clavulanic acid with amoxicillin)
Augmentin (co-amoxiclav)
Aureocort (triamicinolone acetonide, chlortetracycline)
Avamys (fluticasone furoate)
Avastin (bevacizumab)
Avalox (moxifloxacin)
Avelox (moxifloxacin)
Avlocor (chloroquine)
Axid (nizatidine)
Azactam (aztreonam)
Bactroban (mupirocin)
Baycol (cerivastatin)
BCNU (carmustine)
Becodisks (beclometasone dipropionate)
Beconase (beclometasone dipropionate)
Benadryl (diphenhydramine)
Benlysta (belimumab)
Benuryl (probenecid)

Besivance (besifloxacin)
Betacap (betamethasone valerate)
Betaloc (metoprolol)
Betesil (betamethasone valerate)
Betim (timolol)
Betnelan (betamethasone)
Betnesol (betamethasone sodium phosphate)
Betnesol-N (betamethasone sodium phosphate, neomycin)
Betnovate (betamethasone valerate)
Betnovate-C (betamethasone valerate, clioquinol)
Betnovate-N (betamethasone valerate, neomycin sulphate)
Betoptic (betaxolol)
Bettamousse (betamethasone valerate)
Bextra (valdecoxib)
Bexxar (tositumomab)
BiCNU (carmustine)
Biocef (cefalexin)
Brevibloc (esmolol)
Bridion (sugammadex)
Broflex (trihexyphenidyl)
Budelin Novolizer (budenoside)
Busilvex (busulfan)
Calcort (deflazacort)
Camcolit (lithium carbonate)
Campo (irinotecan)
Camptosar (irinotecan)
Canesten (hydrocortisone, clomitiazole)
Capoten (captopril)
Caprelsa (vandetanib)
Carace (lisinopril)
Cardura (doxazosin)
Carelux (clobetasol propionate)
Catapres (clonidine)
CCNU (lomustine)
Cefrom (cefprirome)
Celebrex (celecoxib)
Celsentri (maraviroc)
Ceporex (cefalexin)
Cerezyme (imiglucerase)
Certican (everolimus)
Chantix (varenicline)
Chirocaine (levobupivacaine)
Chloromycetin (chloramphenicol)
Cicatrin B(acitracin and neomycin sulfate)
Cidomycin (gentamicin)

- Cipralex** (escitalopram)
Cipramil (citalopram)
Cipro (ciprofloxacin)
Ciprobay (ciprofloxacin)
Ciproxan (ciprofloxacin)
Ciproxin (ciprofloxacin)
Claforan (cefotaxime)
Clarosip (clarithromycin)
Clenil Modulite (beclometasone dipropionate)
Clozaril (clozapine)
Co-fluampicil (ampicillin and flucloxacillin)
Cogentin (benztropine)
Cognex (tacrine)
Condylone (podophyllotoxin)
Contrave (bupropion and naltrexone)
Copegus (ribavirin)
Co-phenotrope (diphenoxylate and atropine sulphate)
Cordilox (verapamil)
Corgard (nadolol)
Corlan (hydrocortisone)
Corvitol (metoprolol)
Cosmegen Lyovac (dactinomycin)
Cozaar (losartan)
Crestor (rosuvastatin)
Crixivan (indinavir)
Crystapen (benzylpenicillin)
Cubicin (daptomycin)
Cutivate (fluticasone propionate)
Cymbalta (duloxetine)
Cymevene (gangciclovir)
Cyprostat (cyproterone acetate)
Cysticide (praziquantel)
Cytadren (aminoglutethimide)
DF118 Forte (dihydrocodeine)
DHC Continus (dihydrocodeine)
Daktacort (hydrocortisone and miconazole nitrate)
Dalacin C (clindamycin)
DaunoXome (daunorubicin)
Demerol (pethidine)
Depo-Medrone (methylprednisolone)
Deprenyl (selegiline)
Derbac-M (malathion)
Dermovate (clobetasol propionate)
Dermovate-NN (clobetasol propionate, neomycin sulphate, nystatin)
Detecllo (chlortetracycline, demeclocycline and tetracycline)
Dexilant (dexlansoprazole)
Diconal (dipipanone)
Diflucir (fidaxomicin)
Diflucan (fluconazole)
Dioderm (hydrocortisone)
Diprosalic (betamethasone dipropionate and salicylic acid)
- Diprosone** (betamethasone dipropionate)
Dixarit (clonidine)
Dobutrex (dobutamine)
Doxil (doxorubicin)
Drogenil (flutamide)
DTIC-Dome (dacarbazine)
Durogesic (fentanyl)
Dyspamet (cimetidine)
Easi-Breathe (beclometasone dipropionate)
Edronax (reboxetine)
Edurant (rilpivirine)
Efcortesol (hydrocortisone)
Efudix (fluorouracil)
Eldepryl (selegiline)
Eldisine (vindesine)
Elocon (mometasone furoate)
Eloxatin (oxaliplatin)
Emtriva (emtricitabine)
Enbrel (etanercept)
Endoxana (cyclophosphamide)
Epivir (lamivudine)
Erbitux (cetuximab)
Erivedge (vismodegib)
Erwinase (crisantaspase)
Erymax (erythromycin)
Erythrocin (erythromycin)
Erythroped (erythromycin)
Esmeron (rocuronium)
Estracyt (estramustine)
Etopophos (etoposide)
Etrivex (clobetasol propionate)
Eumovate (clobetasone butyrate)
Evista (raloxifene)
Exelon Rivastigmine
Fabrazyme (agalsidase beta)
Famvir (famciclovir)
Fansidar (sulfadoxine with pyrimethamine)
Fareston (toremifene)
Farlutal (medroxyprogesterone acetate)
Faslodex (fulvestrant)
Faverin (fluvoxamine)
Femera (letrozole)
Firmagon (degarelix acetate)
Flagyl (metronidazole)
Flixonase (fluticasone propionate)
Flixotide (fluticasone propionate)
Floxapen (flucloxacillin)
Floxin (ofloxacin)
Fluanxol (venlafaxine)
Fludara (fludarabine)
FML (fluorometholone)
Folotyn (pralatrexate)
Fortovase (saquinavir)
Fortral (pentazocine)

- Fortum** (ceftazidime)
Foscan (temoporfin)
Foscavir (foscarnet)
Fostair (beclometasone dipropionate and formoterol fumarate)
Fucibet (betamethasone valerate and fusidic acid)
Fucidin (fusidic acid)
Fucidin H (hydrocortisone acetate and fusidic acid)
Fungilin (amphotericin)
Fungizone (amphotericin)
Furadantin (nitrofurantoin)
Fuzeon (enfuvirtide)
Galseud (pseudoephedrine)
Gemzar (gemcitabine)
Genasense (oblimersen)
Genticin (gentamicin)
Gentisone (hydrocortisone and gentamicin)
Gliadel (carmustine)
Glivec (imatinib)
Haelan (fludroxycoertide)
Halaven (eribulin)
Hepsera (adeovir dipivoxil)
Herceptin (trastuzumab)
Herpid (idoxuridine)
Hidrasec (racecadotril or acetorphan)
Hiprex (methenamine)
Hivid (zalcitabine)
Humira (adalimumab)
Hycamtin (topotecan)
Hycamtin (topotecan)
Hycodan (hydrocodone (dihydrocodeinone))
Hypovase (prazosin)
Hytrin (terazosin)
Imigran (sumatriptan)
Immukin γ -(interferon)
Imodium (loperamide)
Imuran (azathioprine)
Inavir (laninamivir)
Incivek (telaprevir)
Inderal (propranolol)
Innovace (enalapril)
Intelence (etravirine)
IntronA α -(interferon)
Invanz (ertapenem)
Invirase (saquinavir)
Ipratropium Steri-Neb (ipratropium)
Iressa (gefitinib)
Isentress (raltegravir)
Ismelin (guanethidine)
Istodax (romidepsin or depsipeptide)
Jakafi (ruxolitinib)
Joicela (lumiracoxib and biomarker)
Kaletra (lopinavir with ritinavir)
Katek (telithromycin)
Kefadim (ceftazidime)
Keflex (cefalexin)
Keflin (cefalothin)
Keftab (cefalexin)
Kefurox (cefuroxime)
Kemicetine (chloramphenicol)
Kenalog (triamcinolone acetonide)
Klaricid (clarithromycin)
Kytril (granisetron)
Lanoxin (digoxin)
Lanvis (tioguanine)
Largactil (chlorpromazine)
Lentaron (formestane)
Lescol (fluvastatin)
Leukeran (chlorambucil)
Levaquin (levofloxacin)
Levulan 5-(aminolevulanic acid)
Lexiva (fosamprenavir)
Librium (chlordiazepoxide)
Lipitor (atorvastatin)
Liskonum (lithium carbonate)
Locoid (hydrocortisone butyrate)
Locorten-Vioform (flumetasone pivalate and clioquinol)
Lopresor (metoprolol)
Losec (omeprazole)
Lotemax (loteprednol etabonate)
Lotiderm (betamethasone dipropionate, clotrimazole)
Lucentis (ranibizumab)
Lustral (sertraline)
Lysovir (amantadine)
MabCampath (alemtuzumab)
MabThera (rituximab)
Macrobid (nitrofurantoin)
Macrodantin (nitrofurantoin)
Marcaine (bupivacaine)
Macugen (pegaptanib)
Manerix (moclobemide)
Mansil (oxamniquine)
Maxidex (dexamethasone)
Maxitrol (dexamethasone, neomycin sulphate and polymyxin B sulphate)
Maxolon (metoclopramide)
Medrone (methylprednisolone)
Mefoxin (cefoxitin)
Megace (megestrol acetate)
Meronem (meropenem)
Mestinon (pyridostigmine)
Methadose (methadone)
Metosyn (fluocinonide)
Metrolyl (metronidazole)
Mevacor (lovastatin)
Mevastatin (compactin)
Mictral (nalidixic acid)

- Mildison** (hydrocortisone)
Mircel D Vlucanthone
Mitoxana (ifosfamide)
Mivacron (mivacurium)
Modecate (fluphenazine decanoate)
Modrasone (alclometasone dipropionate)
Monotrim (trimethoprim)
VMorcap (morphine)
Morphgesic (morphine)
MST Cintinus (morphine)
MXL (morphine)
Mydriacyl (tropicamide)
Mydrilate (cyclopentolate)
Myleran (busulfan)
Mylotarg (gemtuzumab)
Myotonine (bethanechol)
Nalorex (naltrexone)
Narcan (naloxone)
Nardil (phenelzine)
Nasacort (triamcinolone acetonide)
Nasofan (fluticasone propionate)
Nasonex (mometasone furoate)
Navelbine (vinorelbine)
Nebcin (tobramycin)
Negaban (temocillin)
Negram (nalidixic acid)
Neoral (ciclosporin)
Nerisone (diflucortolone valerate)
Neulasta (pegfilgrastim)
Neupogen (filgrastim)
Neurontin (gabapentin)
Nexavar (sorafenib)
Nexium (esomeprazole)
Nicorette (nicotine)
Nicotinell (nicotine)
Nipent (pentostatin)
NiQuitin CQ (nicotine)
Nivaquine (chloroquine)
Nolvadex (tamoxifen)
Norcuron (vecuronium)
Norvir (ritonavir)
Novantrone (mitoxantrone)
Nuelin (theophylline)
Nuvigil (armodafinal)
Nystaform-HC (hydrocortisone, nystatin, chlorhexidine)
Onbrez (indacaterol)
Oncaspars (pegaspargas PEG-asparaginase)
Oncovin (vincristine)
Onkotrone (mitoxantrone)
Oramorph (morphine)
Orimeten (aminoglutethimide)
Otomize (dexamethasone, neomycin sulphate)
Otosporin (hydrocortisone, neomycin sulphate and polymyxin B sulphate)
- Oxecta** (oxycodone)
Palladia (toceranib)
Palladone (hydromorphone)
Pamergan P100 (pethidine)
Paraplatin (carboplatin)
Pariet (rabeprazole)
Peg-Intron (peginterferon a2b)
Pegasys (peginterferon a2a)
Penbritin (ampicillin)
Pepcid (famotidine)
Pharmorubicin (epirubicin)
Phenergan (promethazine)
Picovir (pleconaril)
Pilogel (pilocarpine)
Pitressin (vasopressin)
Polyfax (bacitracin and polymyxin B sulfate)
Posject (dobutamine)
Pravachol (pravastatin)
Pred Forte (prednisolone acetate)
VPredsol (prednisolone sodium phosphate)
Predsol-N (prednisolone sodium phosphate with neomycin sulphate)
Prexige (lumiracoxib)
Prezita (darunavir)
Priadel (lithium carbonate)
Prilosec (omeprazole)
Primaxin (cilastatin with imipenem)
Prinivil (lisinopril)
Prioderm (malathion)
Pro-Banthine (propantheline bromide)
Probucid (probenicid)
Proleukin (aldesleukin)
Prolia (denosumab)
Protium (pantoprazole)
Provera (medroxyprogesterone acetate)
Provigil (modafinil)
Prozac (fluoxetine)
Pulmicort (budesonide)
Puri-Nethol (mercaptopurine)
Pyrogastrone (carbenoxolone)
Qnexa (phentermine and topiramate)
Quellada M (malathion)
Questran (colestyramine)
Qvar (beclometasone dipropionate)
Raplacta (peramivir)
Rebetol (ribavirin)
Relenza (zanamivir)
Remicade (infliximab)
Reminyl (galantamine)
Remitch (nalfurafine)
ReoPro (abciximab)
Rescriptor (delavirdine)
Respon tin (ipratropium)
Retrovir (zidovudine)

- Revex** (nalmefene)
Revlimid (lanalidomide)
Reyataz (atazanavir)
Rhinocort Aqua (budenoside)
Rifadin (rifampicin)
Rifater (rifampicin)
Rifinah (rifampicin)
Rimacid (indometacin)
Rimactane (rifampicin)
Rimactazid (rifampicin)
Risperdal (risperidone)
Ritalin (methylphenidate)
Rituxan (rituximab)
Rocephin (ceftriaxone)
Roferon-A (α -interferon)
Rubex (doxorubicin)
Salamol Easi-Breathe (salbutamol)
Sandimmun (ciclosporin)
Sativex (nabiximols)
Scopoderm TTS (hyoscine)
Sectral (acebutolol)
Securon (verapamil)
Selincro (nalmefene)
Septrin (co-trimoxazole)
Seretide (fluticasone propionate and salmeterol)
Serevent (salmeterol)
Seroxat (paroxetine)
Sevredol (morphine)
Sinemet co-(careldopa)
Slo-Phyllin (theophylline)
Sofradex (dexamethasone sodium metasulphobenzoate, framycetin sulphate and gramicidin)
Solu-Cortef (hydrocortisone)
Solu-Medrone (methylprednisolone)
Somavert (pegvisomant)
Sprycel (dasatinib)
Stalevo (co-careldopa)
Stratter atomoxetine
Sublimaze fentanyl
Subutex buprenorphine
Sudafed pseudoephedrine
Suleo-M malathion
Sustanon 250 (testosterone propionate)
Sustiva (efavirenz)
Sutent (sunitinib)
Symbicort (budenoside and formoterol fumarate)
Symmetrel (amantadine)
Synagis (palivizumab)
Synalar (fluocinolone acetonide)
Synalar C (fluocinolone acetonide, clioquinol)
Synalar N (fluocinolone acetonide, neomycin sulphate)
Synartis (flunisolide)
Synercid (dalfopristin with quinupristine)
- Syntocinon** (oxytocin)
Tagamet (cimetidine)
Tamiflu (oseltamivir)
Tarceva (erlotinib)
Targocid (teicoplanin)
Tarivid (ofloxacin)
Tasigna (nilotinib)
Tavanic (levofloxacin)
Taxol (paclitaxel)
Taxotere (docetaxel)
Tazocin (tazobactam with piperacillin)
VTeflaro (ceftaroline fosamil)
Tekturna (aliskiren)
Telfast (fexofenadine)
Telzir (fosamprenavir)
Temgesic (buprenorphine)
Temodal (temozolomide)
Temodar (temozolomide)
Tenormin (atenolol)
Timentin (ticarcillin with clavulanic acid)
Timodine (hydrocortisone, nystatin, benzalkonium chloride)
Tobi (tobramycin)
Tobradex (dexamethasone, tobramycin)
Tofranil (imipramine)
Tomudex (ralitrexed)
Torisel (temsirolimus)
Tracrium (atracurium)
Transtec (buprenorphine)
Trasicor (oxprenolol)
Treanda (bendamustine)
Trimopan (trimethoprim)
Trimovate (clobetasone butyrate, oxytetracycline)
Trisenox (arsenic trioxide)
Trosyl (tioconazole)
Truvada (emtricitabine and tenofovir)
Tykerb (lapatinib)
Tysabri (natalizumab)
Ultralanum Plain (fluocortolone)
Ultravate (halobetasol propionate)
Uniphyllin Continus (theophylline)
Uriben (nalidixic acid)
Uromitexan (mesna)
Valcyte (valganciclovir)
Valium (diazepam)
Valtrex (valaciclovir)
Vancocin (vancomycin)
Vansil (oxamniquine)
Vascace (cilazapril)
Veasnid (tretinoin)
Vectavir (penciclovir)
Vectibix (panitumumab)
Velbe (vinblastine)
Velcade (bortezomib)

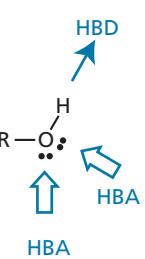
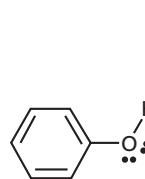
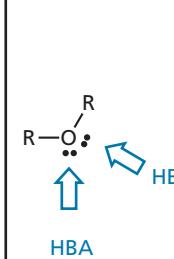
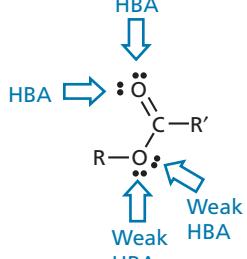
- Ventmax** (salbutamol)
Ventodisks (salbutamol)
Ventolin (salbutamol)
Vepesid (etoposide)
Viagra (sildenafil)
Vibramycin (doxycycline)
Videx (didanosine)
Vigamox (moxifloxacin)
Vioxx (rofecoxib)
Victrelis (boceprevir)
Viracept (nelfinavir)
Viraferon (α -interferon)
Viramune (nevirapine)
Virazole (ribavirin)
Viread (tenofovir)
Virormone (testosterone propionate)
Virovir (aciclovir)
Vistamethasone (betamethasone sodium phosphate)
Vistide (cidofovir)
Vitravene (fomivirsen)
Volmax (salbutamol)
Voraxaze (glucarpidase)
Votrient (pazopanib)
Vumon (teniposide)
Vytorin (ezetimibe and simvastatin)
Warticon (podophyllotoxin)
Xalkori (crizotinib)
Xeloda (lapatinib)
Xifaxin (rifaximin)
Xolair (omalizumab)
Xopenex (levalbuterol)
Xylocaine (lidocaine)
- Yentreve** (duloxetine)
Zactima (vandetanib)
Zantac (ranitidine)
Zarnestra (tipifarnib)
Zavedos (idarubicin)
Zeffix (lamivudine)
Zelapar (selegiline)
Zelboraf (vemurafenib)
Zenapax (daclizumab)
Zerit (stavudine)
Zestril (lisinopril)
Zetia (ezetimibe)
Zevalin (ibritumomab)
Zeftera/Zevtera (ceftobiprole)
Ziagen (abacavir)
Zinacef (cefuroxime)
Zinnat (cefuroxime)
Zispin (mirtazepine)
Zithromax (azithromycin)
Zocor (simvastatin)
Zofran (ondansetron)
Zoladex (goserelin)
Zolinza (vorinostat)
Zomorph (morphine)
Zortress (everolimus)
Zosyn (tazobactam with piperacillin)
Zoton (lansoprazole)
Zovirax (aciclovir)
Zyban (bupropion)
Zyloric (allopurinol)
Zyprexa (olanzapine)
Zytiga (abiraterone)
Zyvox (linezolid)

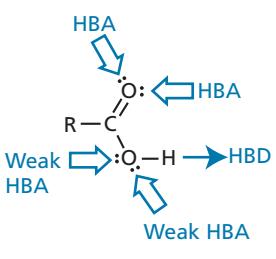
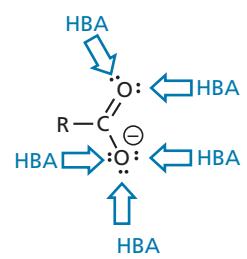
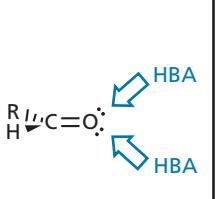
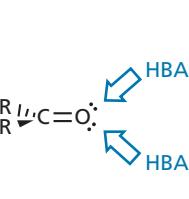
Appendix 8

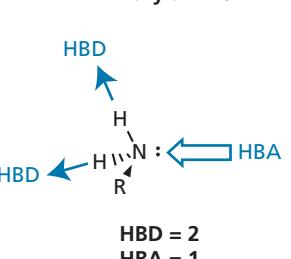
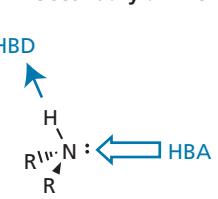
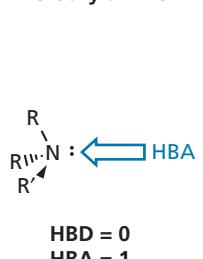
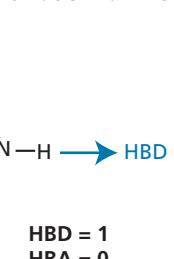
Hydrogen bonding interactions

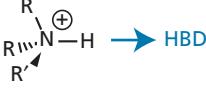
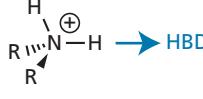
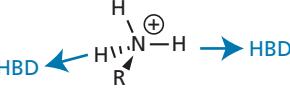
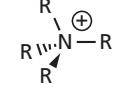
The following table summarizes the possible hydrogen bonding interactions for selected functional groups (see also sections 1.3 and 13.1). The number of hydrogen bond donors (HBDs) and acceptors (HBAs) present in each functional group is given beneath each structure. In medicinal chemistry, the numbers of HBDs and HBAs

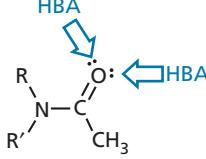
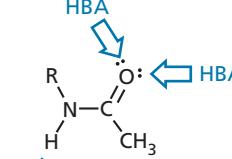
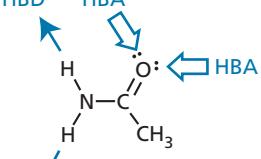
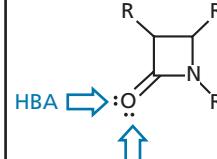
correspond to the number of atoms capable of forming such interactions. Weak HBAs are not included in this text, for example nitrogen atoms that are part of an amide or aniline structure, nitrogen atoms where the lone pair is part of an aromatic sextet, or sp^3 -hybridized oxygen atoms that are linked to an sp^2 -hybridized centre.

Alcohol	Phenol	Ether	Aromatic ether	Ester
 HBD = 1 HBA = 1	 HBD = 1 HBA = 0	 HBD = 0 HBA = 1	 HBD = 0 HBA = 0	 HBD = 0 HBA = 1

Carboxylic acid	Carboxylate ion	Aldehyde	Ketone
 HBD = 1 HBA = 1	 HBD = 0 HBA = 2	 HBD = 0 HBA = 1	 HBD = 0 HBA = 1

Primary amine	Secondary amine	Tertiary amine	Aromatic 2° amine
 HBD = 2 HBA = 1	 HBD = 1 HBA = 1	 HBD = 0 HBA = 1	 HBD = 1 HBA = 0

Aminium ions			Quaternary ammonium ion
 HBD = 1 HBA = 0	 HBD = 2 HBA = 0	 HBD = 3 HBA = 0	 HBD = 0 HBA = 0

Primary amide	Secondary amide	Tertiary amide	β -Lactam
 HBD = 0 HBA = 1	 HBD = 1 HBA = 1	 HBD = 2 HBA = 1	 HBD = 0 HBA = 1

Appendix 9

Drug properties

The properties displayed here were obtained from the websites www.drugbank.ca and www.chemspider.com.

It should be noted that the number of hydrogen bond donors (HBDs) and hydrogen bond acceptors (HBAs) predicted by different software packages often vary

depending on how the rules for determining these centres have been interpreted by different software writers.

pKa values are predicted values except for those marked (exp.), which are experimental. All logP values are experimental values.

Drug	pKa (pred.)	LogP exp.	MWt	Polar surface area	HBD	HBA	Rot. bonds
abacavir	16.71	1.1	286.2	101.9	3	6	4
abiraterone			349.5	33.1	1	2	2
acebutolol	14.6	1.7	336.2	87.7	3	5	10
aciclovir	15.1	-1.56	225.1	114.8	3	7	4
alclometasone	13.86	2.7	408.9	94.8	3	5	2
adefovir dipivoxil		0.8	501.2	167	1	8	15
aliskiren	15.9	3.3	551.4	146	4	7	19
allopurinol	16.5	-1	136.0	65.9	2	5	0
amantadine	-	2.3	151.1	26.0	1	1	0
aminoglutethimide	-	1.3	232.1	72.2	2	3	2
5-aminolevulinic acid	17.16	-1.5	131.1	80.4	2	4	4
amoxicillin	9.5		365.1	133	4	6	4
amphotericin	11.8	0.8	924.1	320	12	17	3
ampicillin	12.0	0.4	349.4	113	3	5	4
amprenavir	14.2	-	505.6	131	3	6	11
amsacrine	17.5	3.8	393.1	80.3	2	5	4
anastrozole		2.4	293.4	78.3	0	4	4
arsenic trioxide	-		197.8	27.7	0	3	0
atazanavir	13.1	4.5	704.4	171	5	7	18
atenolol	16	0.5	266.2	84.6	3	4	8
atomoxetine	-	3.9	255.2	21.3	1	2	6
atorvastatin	11.8	5.7	558.3	112	4	5	12
atracurium	19.6	-	929.1	126	0	10	26
azathioprine	-	0.7	277.0	118	1	6	3
azithromycin	8.74(exp.)	4.02	748.5	180	5	13	7
aztreonam	2.9		435.1	206	3	10	6
bacitracin	3.8	-0.8	1422.7	531	17	20	31

(Continued)

Drug	pKa (pred.)	LogP exp.	MWt	Polar surface area	HBD	HBA	Rot. bonds
beclometasone dipropionate	15.58	1.3	521.0	106.8	1	5	8
bendamustine			358.3	58.4	1	5	9
benztropine	–	4.3	307.2	12.5	0	2	4
benzylpenicillin	2.74(exp.) 12.1	1.5	334.1	86.7	2	4	4
betaxolol	9.4(exp.)	2.4	307.4	50.7	2	4	11
besifloxacin			393.8	86.9	3	6	4
betamethasone	13.48	1.1	392.5	94.8	3	5	2
betamethasone dipropionate			504.6	107.0	1	7	9
betamethasone sodium phosphate			516.4	129.2	4	8	6
betamethasone valerate			476.6	100.9	2	6	9
bethanechol	–		161.2	52.3	1	1	4
boceprevir							
bortezomib	13.8		384.2	124	4	6	9
bupivacaine	8.1(exp.)	3.6	288.2	V32.3	1	2	5
buprenorphine	8.31(exp.) 14.3	3.8	467.3	62.2	2	5	5
bupropion	–	3.6	239.1	29.1	1	2	4
busulfan	–	–0.3	246.0	86.7	0	4	7
capecitabine	12.6	0.4	359.1	121	3	6	7
captopril	10.1	0.6	V217.1	57.6	2	3	3
carbenoxolone	4.7		570.8	118	2	6	6
carbidopa	9.3	–1.9	226.2	116	5	6	4
carboplatin	–		371.0	52.6	0	2	0
carmustine	–	1.5	213.0	61.8	1	2	5
cefalexin	4.5(exp.) 11.9	0	347.1	113	3	5	4
cefalothin	11.7	–0.2	396.0	113	2	5	7
cefotaxime	11.0	–0.5	455.1	174	3	9	8
cefoxitin	11.0	–0.02	427.1	148	3	6	8
cefprome			514.1	207.5	4	11	7
ceftaroline fosamil			684.7	340.1	5	16	9
ceftazidime	3.2	–1.6	546.6	191	3	10	9
ceftobiprole			534.1	249.5	6	14	6
ceftriaxone	3.96	–1.7	554.0	209	4	12	8
cefuroxime	11.0	–0.8	424.4	174	3	7	8
celecoxib	–	3.9	381.1	78	1	3	4
cerivastatin	14.6	3.4	481.2	99.9	3	6	11
chlorambucil	5.75(exp.)	3.9	304.2	40.5	1	3	9
chloramphenicol	13.6	0.7	323.1	115	3	5	6

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Drug	pKa (pred.)	LogP exp.	MWt	Polar surface area	HBD	HBA	Rot. bonds
chlordiazepoxide	4.8(exp.) 16.1	1.7	299.1	48.2	1	4	1
chloroquine	10.1	4.3	319.2	28.2	1	3	8
chlorpromazine	9.3(exp.)	4.9	318.1	6.5	0	2	4
chlortetracycline	2.6	0.3	478.9	243	9	13	10
ciclesonide	15.56		540.7	99.1	1	6	6
ciclosporin			1201.8	279	5	23	16
cidofovir	V7.9	-3.9	279.1	146	4	8	6
cilastatin	4.4		358.2	130	4	6	11
cilazapril	-	-	417.5	99.2	2	6	9
cimetidine	6.8(exp.) 20.0	1	252.3	88.9	3	5	5
ciprofloxacin	6.1	2.3	331.1	72.9	2	6	3
citalopram	-	3.5	324.4	36.3	0	3	5
clarithromycin	8.99(exp.)	1.7	747.5	183	4	13	8
clavulanic acid	15.5	-1.5	199.0	87.1	2	5	2
clindamycin	12.7	1.6	425.0	102	4	6	7
clobetasol	13.65	3	410.9	74.6	2	4	2
clobetasol propionate			467.0	80.7	1	5	6
clobetasone butyrate			479.0	77.5	0	5	6
clonidine	-	2.7	229.0	36.4	2	3	1
clozapine	7.5(exp.)	2.7	326.1	30.9	1	4	0
compactin	14.9		390.2	104	3	5	11
crizotinib			450.3	78.0	3	6	5
cyclopentolate	-	2.4	291.2	49.8	1	3	7
cyclophosphamide	-	0.8	260.0	41.6	1	2	5
cyproterone acetate	17.6		416.2	54.4	1	3	1
dacarbazine	14.0	-1.6	182.2	99.7	2	5	3
dactinomycin	11.1	1.6	1254.6	355	5	16	8
dalfopristin	14.6	-	690.8	176	2	9	7
darunavir	14.2	1.8	547.2	140	3	7	11
dasatinib	10.3	1.8	487.2	106	3	8	7
daunorubicin	11.0	0.1	527.2	186	5	11	4
deflazacort			441.5				
degarelix acetate			1692.3				
delavirdine	12.4	2.8	456.2	110	3	6	5
demeclacycline	4.35	0.2	464.9	182	6	9	2
dexamethasone			392.5	94.8	3	5	5
dexlansoprazole			369.4	87.1	1	5	5
diazepam	3.4(exp.)	2.9	284.1	32.7	0	2	1
didanosine	14.7	-0.2	236.1	88.7	2	6	2

(Continued)

Drug	pKa (pred.)	LogP exp.	MWt	Polar surface area	HBD	HBA	Rot. bonds
diflucortolone valerate			478.6	80.7	1	5	8
dihydrocodeine			301.4	41.9	1		2
dihydrocodeinone			299.4	38.8	0	4	1
digoxin	13.0	2.2	780.9	203	6	13	7
diphenhydramine	8.98(exp.)	3.27	255.2	12.5	0	2	6
diphenoxylate		6.3	452.6	53.3	0	3	9
dipipanone			349.5	20.3	0	2	7
disulfiram	–	1.9	296.1	6.5	0	0	7
dobutamine	10.8	3.6	301.4	72.7	4	4	7
docetaxel	12.0	2.4	807.3	224	5	10	13
donepezil	–	3.6	379.2	38.8	0	4	6
doxazosin	–	2.1	451.2	112	1	9	4
doxorubicin	11.0	–0.5	543.2	206	6	12	5
doxycycline	4.7	–0.2	444.4	182	6	9	2
duloxetine	–	4	297.1	21.3	1	2	6
efavirenz	–	4.6	315.0	38.3	1	2	3
emtricitabine	2.65(exp.)	–1.4	247.0	88.1	2	5	2
enalapril	2.97(exp.) (carboxyl); 5.35(exp.) (amine)	2.1	376.4	95.9	2	5	10
epirubicin	11.0	–0.5	543.2	206	6	12	5
eribulin			729.9	146.4	3	12	6
erlotinib	–	2.7	393.2	74.7	1	7	10
ertapenem	4.0	0.3	475.1	156	5	8	7
erythromycin	8.88(exp.); 12.9	3.06	733.5	194	5	13	7
escitalopram	–	3.5	324.2	36.3	0	3	5
esmolol		1.7	295.4	67.8	2	4	10
esomeprazole	18.3	0.6	345.1	77.1	1	5	5
estramustine	–	5.7	439.2	49.8	1	2	6
etoposide	12.3	1	588.6	161	3	12	5
etravirine			435.3	120.6	3	7	3
everolimus	13.4	–	958.2	204.7	3	13	9
ezetimibe	14.4	4.5	409.4	60.8	2	3	6
famciclovir	–	0.6	321.1	122	1	6	9
famotidine	–	–2.1	337.0	176	4	8	6
fentanyl	–	3.9	336.2	23.6	0	2	6
fexofenadine	13.2	5.6	501.3	81.0	3	5	10
fidaxomicin			1058.0	266.7	7	18	22
flucloxacillin	13.6	3.2	453.1	113	2	5	3
fluconazole	–	0.4	306.1	81.6	1	5	5

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Drug	pKa (pred.)	LogP exp.	MWt	Polar surface area	HBD	HBA	Rot. bonds
fludarabine	6.3	-2.8	365.2	186	5	10	4
fludroxycortide	14.8	0.6	436.5	93.1	2	6	2
flumetasone pivalate			494.6	100.9	2	6	7
flunisolide	14.7	V1.1	434.5	93.1	2	6	2
fluocinolone acetonide	13.9	2.48	452.5	93.1	2	6	2
fluocinonide	14.4	1.9	494.5	99.1	1	6	4
fluocortolone			376.5	74.6	2	4	4
fluorometholone	13.7	V2	376.5	74.6	2	4	1
fluorouracil	8.02(exp.)	-0.8	130.0	58.2	2	2	0
fluoxetine	-	4.6	309.1	21.3	1	2	7
fluphenazine	7.9	4.2	437.2	30.0	1	4	7
flutamide	-	2.6	276.1	74.9	1	3	4
fluticasone furoate			552.6	119.1	1	6	8
fluticasone propionate	14.5	3.4	500.6	80.7	1	4	6
fluvastatin	14.6	4.5		82.7	3	4	8
fluvoxamine	-	3.2	318.2	56.8	1	4	10
fomivirsen							
fosamprenavir	6.3	-	585.2	178	4	8	13
foscarnet	3.5	-2.1		94.8	3	5	1
fulvestrant	19.4	8.9	606.8	57.5	2	3	15
fusidic acid	18.9		516.3	104	3	5	6
gabapentin	-	1.4	171.1	63.3	2	3	3
galantamine	-	1.8	287.2	41.9	1	4	1
ganciclovir	14.3	-1.7	255.1	135	4	8	5
gefitinib	-	3.2	446.2	68.7	1	7	8
gemcitabine	3.6(exp); 14.7		263.1	108	3	6	2
gentamicin	13.2	-3.1	477.6	199.7	8	12	7
gransetron	-	2.6	312.2	50.2	1	3	2
guanethidine	-	0.8	198.2	67.6	2	4	3
halobetasol propionate	14.4	2.9	485.0	80.7	1	4	5
hydrocodone		1.2	299.4	38.8	0	4	1
hydrocortisone	13.9	1.61	362.2	94.8	3	5	2
hydrocortisone acetate			404.5	100.9	2	6	6
hydrocortisone butyrate			432.5	100.9	2	6	8
hydromorphone	18	0.9	285.3	49.8	1	4	0
hyoscine	-	0.8	303.1	62.3	1	4	5
idarubicin	11.0	0.2	479.5	177	5	10	3
idoxuridine	13.9	-0.5	354.1	99.1	3	5	2
ifosfamide	-	0.8	260.0	41.6	1	2	5

(Continued)

Drug	pKa (pred.)	LogP exp.	MWt	Polar surface area	HBD	HBA	Rot. bonds
imatinib	13.5	3	493.3	86.3	2	7	7
imipenem	15.0		299.1	116	3	6	6
imipramine	9.4(exp.)	3.9	280.2	6.48	0	2	4
imiquimod	–	2.7	240.1	56.7	1	3	2
indacaterol	14.1	–	392.5	81.6	4	4	6
indinavir	14.2	2.9	613.4	118	4	7	12
indometacin	4.5(exp.)	3.4	357.1	68.5	1	4	4
ipratropium	–		332.5	46.5	1	2	6
irinotecan	–	3.2	586.3	112	1	6	5
lamivudine	–	–1.4	229.1	88.1	2	5	2
laninamivir			346.3	189.7	8	11	9
lansoprazole	17.3	1.9	369.1	67.9	1	4	6
lapatinib	–	5.4	580.1	106	2	7	11
lenalidomide	15.2	–0.4	259.1	92.5	2	4	1
letrozole	–	2.5	285.1	78.3	0	4	3
levalbuterol	10.3(exp.); 14.2	1.4	239.2	72.7	4	4	5
levobupivacaine	8.1(exp.)	3.6	288.2	32.3	1	2	5
levodopa	2.32(exp.); 9.7	–1.8	197.1	104	4	5	3
levofloxacin	–	2.1	361.1	73.3	1	7	2
lidocaine	8.01(exp.)	2.1	234.2	32.3	1	2	5
linezolid	–	0.9	337.1	71.1	1	5	4
lisinopril	3.8	–0.9	405.5	133	4	7	12
lomustine	–	3	233.1	61.8	1	2	4
loperamide	–	5.5	476.2	43.8	1	3	7
lopinavir	14.0	–	628.4	120	4	5	15
losartan	14.3	6.1	422.2	92.5	2	5	8
loteprednol	14.89	3.4	394.9	83.8	2	4	3
loteprednol etabonate			467.0	99.1	1	7	8
lovastatin	–	4.5	404.3	72.8	1	3	7
lucanthone	–	–	340.2	32.3	1	3	6
lumiracoxib	15.87	3.9	293.7	49.3	2	3	4
malathion	–	2	330.0	71.1	0	2	11
maraviroc	–	–	513.3	63.0	1	4	8
medroxyprogesterone acetate	17.6	3.5	386.2	54.4	1	3	1
megestrol acetate	17.6	3.2	384.2	54.4	1	3	1
melphalan	–	0.4	304.1	66.6	2	4	8
mercaptopurine	11.7	–0.4	152.2	53.1	2	3	0
meropenem	15.0	–0.6	383.2	110	3	6	5

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Drug	pKa (pred.)	LogP exp.	MWt	Polar surface area	HBD	HBA	Rot. bonds
methadone	8.94(exp.)	3.93	309.2	20.3	0	2	7
methylprednisolone	13.9	1.5	374.5	94.8	3	5	2
methyldopa	9.1	-1.7	211.2	104	4	5	3
methylphenidate	8.77(exp)	2.1	233.1	38.3	1	2	4
metoclopramide	9.27(exp.); 18.8	1.8	299.1	67.6	2	4	7
metoprolol	-	1.6	267.2	50.7	2	4	9
metronidazole	-	-0.1	171.1	83.9	1	4	3
mirtazepine	-	2.9	265.2	19.4	0	3	0
mitoxantrone	11.4	-3.1	444.2	163	8	10	12
mivacurium	19.2	-	1028.6	145	0	12	30
moclobemide	-	1.5	268.1	41.6	1	3	4
modafinil	19.3	0.6	273.4	60.2	1	2	5
mometasone	13.85	2.1	427.4	74.6	2	4	2
mometasone furoate			521.4	93.8	1	6	6
morphine	8.21	0.8	285.1	52.9	2	4	0
moxifloxacin	-	2.9	401.2	82.1	2	7	4
mupirocin	13.1	-	500.3	146	4	8	17
nadolol	14.2	1.2	309.2	81.9	4	5	6
nalidixic acid	8.6(exp.)	2.1	232.1	70.5	1	5	2
nalfurafine			476.6	86.4	2	7	7
nalmefene			339.4	52.9	2	4	4
naloxone	13.6	0.6	327.4	70	2	5	2
naltrexone	13.6	0.7	341.2	70	2	5	2
nelfinavir	14.1	6	567.3	102	4	5	10
neomycin	13.2	-7.8	614.3	353	13	19	9
nevirapine	-	2.5	266.1	58.1	1	4	1
nicotine	3.1(exp.)	1.1	162.2	16.1	0	2	1
nilotinib	13.5	-	529.2	97.6	2	6	7
nitrofurantoin	7.2(exp.); 14.9	-0.1	238.0	121	1	5	3
nizatidine	-	1.1	331.1	86.0	2	6	10
ofloxacin	-	2.1	361.1	73.3	1	7	2
olanzapine	-	2.0	312.1	30.9	1	4	1
omeprazole	18.3	0.6	345.1	77.1	1	5	5
ondansetron	-	2.4	293.2	39.8	0	2	2
oseltamivir	-	1	312.2	90.6	2	4	8
oxaliplatin	-	-	397.1	76.7	2	4	0
oxamniquine	18.7	1.5	279.2	90.1	3	5	5
oxprenolol	-	2.1	265.2	50.7	2	4	9
oxycodone	16.2	0.3	315.4	59	1	5	1

(Continued)

Drug	pKa (pred.)	LogP exp.	MWt	Polar surface area	HBD	HBA	Rot. bonds
paclitaxel	12.0	3	853.3	221	4	10	14
pantoprazole	15.8	0.5	383.1	86.3	1	6	7
pazopanib			437.5	95.8	3	9	4
paroxetine	–	3.6	329.1	39.7	1	4	4
pemetrexed	4.22	–1.5	427.4	187.0	6	9	9
penciclovir	15.1	–1.1	253.1	126	4	7	5
pentazocine	8.88(exp.)	3.7	285.2	23.5	1	2	2
pentostatin	5.2(exp.); 13.9	–1.1	268.1	112	4	7	2
peramivir			328.4	151.0	7	8	8
pethidine	8.59(exp.)	2.6	247.3	29.5	0	2	4
phenelzine	–	1.1	136.1	38.0	2	2	3
phenoxycephalothin	2.79(exp); 11.7	1.4	350.4	95.9	2	5	5
phentermine		2.2	149.2	26.0	1	1	2
pilocarpine	6.78(exp.)	1.1	208.1	44.1	0	2	3
piperacillin	11.6	0.3	517.2	159	2	7	6
pleconaril			381.3	74.2	0	6	6
podophyllotoxin	–	1.5	414.4	92.7	1	7	4
polymyxin B	12.0	–4.9		491	18	18	29
pralatrexate			477.5	207.3	7	12	10
pravastatin	14.5	2.2	424.2	124	4	6	11
praziquantel	–	2.5	312.2	40.6	0	2	1
prazosin	–	1.3	383.2	107	1	7	4
prednisolone	13.9	1	360.4	94.8	3	5	2
prednisolone acetate			402.5	100.9	2	6	6
prednisolone sodium phosphate			484.4	129.2	2	8	10
probenecid	3.4(exp.)	2.3	285.1	74.7	1	4	6
promethazine	–	4.4	284.1	6.48	0	2	3
propranolol	–	3	259.2	41.5	2	3	6
propantheline	–	–	447.1	35.5	0	1	7
pseudoephedrine	–	1.4	165.1	32.3	2	2	3
pyridostigmine	–	1.5	181.1	33.4	0	1	2
pyrimethamine	7.34(exp.)	2.7	248.1	77.8	2	4	2
quinine	–	2.6	324.2	45.6	1	4	4
quinupristin	11.5	–	1022.2	231	4	12	10
rabeprazole	17.3	0.6	359.1	77.1	1	5	8
racecadotril			385.5	97.8	1	5	11
raltegravir			444.1	150.0	3	11	7
raltitrexed	4.4	–1.2	458.1	148	4	9	9

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Drug	pKa (pred.)	LogP exp.	MWt	Polar surface area	HBD	HBA	Rot. bonds
raloxifene	9.6	5.2	473.2	70	2	5	7
ranitidine	–	1.3	314.4	86.3	22	5	10
reboxetine	–	3.1	313.2	39.7	1	4	6
ribavirin	12.6	-2.6	244.1	144	4	7	3
rifampicin	8.2	2.7	822.9	220	6	14	5
rifaximin	7.7	2.6	785.9	198.4	5	11	3
rilpivirine			366.4	97.4	2	6	3
rimexolone	19.9	4.2	370.5	54.4	1	3	2
risperidone	–	2.5	410.2	61.9	0	4	4
ritonavir	14.2	3.9	720.3	146	4	6	18
rivastigmine	–	2.3	250.2	32.8	0	2	5
rocuronium			529.8	59	1	4	6
rofecoxib	19.7	3.2	314.1	60.4	0	3	3
romidepsin			540.7	208.3	3	9	8
rosuvastatin	14.6	2.4	481.2	141	3	8	9
ruxolitinib			306.4	83.2	1	6	4
salbutamol	10.3(exp.); 14.1	1.4	239.2	72.7	4	4	5
salmeterol	14.2	4.2	415.6	81.9	4	5	16
saquinavir	14.2	3.8	670.4	167	5	7	13
selegiline	–	2.7	187.3	3.24	0	1	4
sertraline	–	5.1	305.1	12.0	1	1	2
sildenafil	–	1.9	474.2	109	1	8	6
simvastatin	–	4.7	418.3	72.8	1	3	7
sorafenib	14.0	3.8	464.1	92.3	3	3	6
stavudine	14.6	-0.8	224.1	78.9	2	4	2
suberoylanilide hydroxamic acid	9.2(exp.); 14.2	–	264.1	78.4	3	3	8
sugammadex			2178	796.2	24	48	56
sulfadoxine	–	0.7	310.1	116	2	7	4
sumatriptan	17.1	0.8	295.1	65.2	2	3	5
sunitinib	14.2	2.5	398.5	77.2	3	3	7
suxamethonium	–	–	290.2	52.6	0	2	
tacrine	9.95(exp.)	2.2	198.1	38.9	1	2	0
tamoxifen	–	7.1	371.2	12.5	0	2	8
tazobactam	18.6	–	300.1	122	1	7	3
telaprevir	12.4		679.8	179.6	4	8	14
telithromycin	12.8	3.0	812.0	172	1	11	11
temocillin			414.1	187	3	9	6
temoporfin			680.2	138.3	6	8	8

(Continued)

Drug	pKa (pred.)	LogP exp.	MWt	Polar surface area	HBD	HBA	Rot. bonds
temozolomide	–	–2.8	194.1	106	1	5	1
temsirolimus	13.4	–	1029.6	242	4	14	11
teniposide	12.3	1.5	656.7	161	3	12	6
tenofovir	7.9	–1.6	287.1	136	3	8	5
terazosin	–	1.0	387.2	103	1	8	4
testosterone propionate	19.4	3.6	344.2	37.3	1	2	0
tetracycline	3.3(exp.)	–0.3	444.4	182	6	9	2
theophylline	8.81(exp.)	–0.8	180.2	69.3	1	3	0
ticarcillin	4.1	–	384.0	124	3	6	5
timolol	3.9(exp.)	1.2	316.2	79.7	2	7	7
tioconazole	–	4.4	386.0	27.0	0	2	6
tioguanine	13.3	–0.7	167.2	79.1	3	4	0
tipifarnib			489.4				
tirofiban	10.9	1.4	440.6	105	3	6	13
tobramycin	13.1	–5.8	467.3	268	10	14	6
toceranib			396.5	77.2	3	6	5
topiramate		–0.7	339.4	115.5	1	8	3
topotecan	11.7	0.8	421.2	103	2	6	3
toremifene	–	6.8	405.2	12.5	0	2	9
triamcinolone	13.4	0.2	394.4	115.1	4	6	2
triamcinolone acetonide			434.5	93.1	2	6	4
tretinoïn	–	4.2	300.2	37.3	1	2	5
trihexyphenidyl	–	4.5	301.2	23.5	1	2	5
trimethoprim	–	0.6	290.1	106	2	7	5
	–	1.3	284.2	53.4	1	3	6
valaciclovir	–	–0.3	324.2	147	3	8	8
valdecoxib	–	3.2	314.1	86.2	1	3	3
valganciclovir	14.6	–	354.2	167	4	9	9
vancomycin	8.8	–3.1	1447.4	530	19	24	13
vandetanib			475.4	58.5	1	6	5
varenicline		0.9	211.3	37.8	1	3	0
vecuronium	–	–	557.8	55.8	0	3	6
vemurafenib			489.9	100.3	2	6	6
venlafaxine	–	2.8	227.2	32.7	1	3	5
verapamil	8.92(exp.)	4.7	454.3	63.9	0	6	13
vinblastine	14.4	3.9	810.4	154	3	9	10
vincristine	14.4	5.0	824.4	171	3	9	10
vindesine	13.9	2.9	753.9	165	5	9	7

740 Appendix 9 Drug properties

Drug	pKa (pred.)	LogP exp.	MWt	Polar surface area	HBD	HBA	Rot. bonds
vinorelbine	15.0	4.0	778.4	134	2	8	10
vismodegib				421.3			
vorinostat	9.2(exp.); 14.2	–	264.1	78.4	3	3	8
zalcitabine	–	–1.3	211.1	88.1	2	5	2
zanamivir	12.8	–3	332.1	201	7	10	6
zidovudine	9.96	0.05	267.1	108	2	6	3