

TMSDRDSI: Drug Design MSc

TMSDRDSING01: MSc Drug Design

WIBRG001, WIBRG002, WIBRG003, WIBRG004, 5 + 6

View Online



1

Wilhelm S. Discovery and development of sorafenib: a multikinase inhibitor for treating cancer. *Nature Reviews Drug Discovery* 2006;**5**:835–44. doi:10.1038/nrd2130

2

Smith RA. Discovery of heterocyclic ureas as a new class of raf kinase inhibitors: identification of a second generation lead by a combinatorial chemistry approach. *Bioorganic & Medicinal Chemistry Letters* 2001;**11**:2775–8. doi:10.1016/S0960-894X(01)00571-6

3

Kola I, Landis J. Opinion: Can the pharmaceutical industry reduce attrition rates? *Nature Reviews Drug Discovery* 2004;**3**:711–6. doi:10.1038/nrd1470

4

Swinney DC, Anthony J. How were new medicines discovered? *Nature Reviews Drug Discovery* 2011;**10**:507–19. doi:10.1038/nrd3480

5

Macarron R, Banks MN, Bojanic D, et al. Impact of high-throughput screening in biomedical research. *Nature Reviews Drug Discovery* 2011;**10**:188–95. doi:10.1038/nrd3368

6

Selzer, P. M., Rohwer, A., Marhöfer, R. J. Applied bioinformatics: an introduction. Berlin: : Springer 2008.

7

Xiong, Jin. Essential bioinformatics. New York: : Cambridge University Press 2006.

8

Orengo, Christine Ann, Thornton, Janet M., Jones, David Tudor. Bioinformatics: genes, proteins and computers. Oxford: : BIOS 2003.
<http://www.vlebooks.com/vleweb/product/openreader?id=UCL&isbn=9780203427828>

9

Zvelebil, Marketa J., Baum, Jeremy O. Understanding bioinformatics. London: : Garland Science 2008.
https://bibliu.com/app/#/view/books/9781136976964/pdf2htmllex/index.html#page_Cover

10

Gu, Jenny, Bourne, Philip E. Structural bioinformatics. 2nd ed. Hoboken, N.J.: : Wiley 2008.

11

Petsko, Gregory A., Ringe, Dagmar. Protein structure and function. London: : New Science 2004.

12

Nelson, David L., Cox, Michael M., Lehninger, Albert L. Lehninger principles of biochemistry . 5th ed. Basingstoke: : W.H. Freeman 2008.

13

Chandra N. Computational systems approach for drug target discovery. Expert Opinion on Drug Discovery 2009;**4**:1221–36. doi:10.1517/17460440903380422

14

Overington JP, Al-Lazikani B, Hopkins AL. How many drug targets are there? Nature Reviews Drug Discovery 2006;**5**:993–6. doi:10.1038/nrd2199

15

Fitt R, Nodder E. Setting the threshold for industrial application: the UK diverges from Europe. Journal of Intellectual Property Law & Practice 2010;**5**:560–5. doi:10.1093/jiplp/jpq061

16

Ikura M, Inouye M. NMR structure of the histidine kinase domain of the : E. coli: osmosensor EnvZ : Article : Nature. Nature 1998;**396**:88–92. doi:10.1038/23968

17

Krohn KA, Link JM. Interpreting enzyme and receptor kinetics: keeping it simple, but not too simple. Nuclear Medicine and Biology 2003;**30**:819–26. doi:10.1016/S0969-8051(03)00132-X

18

Jarnagin K. Receptor Binding in Drug Discovery. In: eLS.

19

Jarnagin K. Receptor Binding in Drug Discovery. Chichester: : John Wiley & Sons, Ltd 2001. doi:10.1038/npg.els.0000056

20

Cornish-Bowden, Athel. Fundamentals of enzyme kinetics. 3rd ed. London: : Portland 2004.

21

Copeland, Robert Allen. Evaluation of enzyme inhibitors in drug discovery: a guide for medicinal chemists and pharmacologists. Hoboken, N.J.: : J. Wiley 2005.
<https://onlinelibrary.wiley.com/doi/book/10.1002/9781118540398>

22

Gibb, Alasdair J., Foreman, John C., Johansen, Torben. Textbook of receptor pharmacology. 3rd ed. Boca Raton, FL: : CRC Press 2011.

23

Rang, H. P., Dale, M. Maureen. Pharmacology. 9th ed. Edinburgh: : Churchill Livingstone 2019. <https://elsevierelibrary.co.uk/product/9780702074462>

24

Colquhoun D. Binding, gating, affinity and efficacy: The interpretation of structure-activity relationships for agonists and of the effects of mutating receptors. British Journal of Pharmacology 1998;**125**:923–47. doi:10.1038/sj.bjp.0702164

25

Khawaja X, Dunlop J, Kowal D. Scintillation proximity assay in lead discovery. Expert Opinion on Drug Discovery 2008;**3**:1267–80. doi:10.1517/17460441.3.11.1267

26

Kenakin TP. Cellular assays as portals to seven-transmembrane receptor-based drug discovery. Nature Reviews Drug Discovery 2009;**8**:617–26. doi:10.1038/nrd2838

27

Dunlop J. High-throughput electrophysiology: an emerging paradigm for ion-channel screening and physiology. Nature Reviews Drug Discovery 2008;**7**:358–68.
doi:10.1038/nrd2552

28

Hopkins AL, Groom CR. Opinion: The druggable genome. *Nature Reviews Drug Discovery* 2002;**1**:727–30. doi:10.1038/nrd892

29

Richard M. Durbin. A map of human genome variation from population-scale sequencing. *Nature* 2010;**467**:1061–73. doi:10.1038/nature09534

30

Thomas, Gareth. *Fundamentals of medicinal chemistry*. 2003.

31

Patrick, Graham L. *An introduction to medicinal chemistry*. 2017.

32

Leach, Andrew R., Gillet, Valerie J. *An introduction to chemoinformatics*. 2003.

33

Engel, Thomas, Gasteiger, J. *Chemoinformatics: a textbook*. 2003.

34

Gasteiger, J. *Handbook of chemoinformatics: from data to knowledge*. 2003.
<https://onlinelibrary.wiley.com/doi/book/10.1002/9783527618279>

35

Bissantz C, Kuhn B, Stahl M. A Medicinal Chemist's Guide to Molecular Interactions. *Journal of Medicinal Chemistry* 2010;**53**:5061–84. doi:10.1021/jm100112j

36

Matter H. Selecting Optimally Diverse Compounds from Structure Databases: A Validation Study of Two-Dimensional and Three-Dimensional Molecular Descriptors. *Journal of Medicinal Chemistry* 1997;**40**:1219–29. doi:10.1021/jm960352+

37

Willett P, Barnard JM, Downs GM. Chemical Similarity Searching. *Journal of Chemical Information and Modeling* 1998;**38**:983–96. doi:10.1021/ci9800211

38

Welsch ME, Snyder SA, Stockwell BR. Privileged scaffolds for library design and drug discovery. *Current Opinion in Chemical Biology* 2010;**14**:347–61. doi:10.1016/j.cbpa.2010.02.018

39

Lipinski CA, Lombardo F, Dominy BW, et al. Experimental and computational approaches to estimate solubility and permeability in drug discovery and development settings. *Advanced Drug Delivery Reviews* 1997;**23**:3–25. doi:10.1016/S0169-409X(96)00423-1

40

Veber DF, Johnson SR, Cheng H-Y, et al. Molecular Properties That Influence the Oral Bioavailability of Drug Candidates. *Journal of Medicinal Chemistry* 2002;**45**:2615–23. doi:10.1021/jm020017n

41

Blake JF. Identification and Evaluation of Molecular Properties Related to Preclinical Optimization and Clinical Fate. *Medicinal Chemistry* 2005;**1**:649–55. doi:10.2174/157340605774598081

42

Beck A, Wurch T, Bailly C, et al. Strategies and challenges for the next generation of

therapeutic antibodies. *Nature Reviews Immunology* 2010;**10**:345–52. doi:10.1038/nri2747

43

Bradbury ARM, Sidhu S, Dübel S, et al. Beyond natural antibodies: the power of in vitro display technologies. *Nature Biotechnology* 2011;**29**:245–54. doi:10.1038/nbt.1791

44

Nagorsen D, Baeuerle PA. Immunomodulatory therapy of cancer with T cell-engaging BiTE antibody blinatumomab. *Experimental Cell Research* 2011;**317**:1255–60. doi:10.1016/j.yexcr.2011.03.010

45

Pillay V, Gan HK, Scott AM. Antibodies in oncology. *New Biotechnology* 2011;**28**:518–29. doi:10.1016/j.nbt.2011.03.021

46

Schrama D, Reisfeld RA, Becker JC. Antibody targeted drugs as cancer therapeutics. *Nature Reviews Drug Discovery* 2006;**5**:147–59. doi:10.1038/nrd1957

47

Weiner LM, Surana R, Wang S. Monoclonal antibodies: versatile platforms for cancer immunotherapy. *Nature Reviews Immunology* 2010;**10**:317–27. doi:10.1038/nri2744

48

Ducry L, Stump B. Antibody–drug conjugates: Linking cytotoxic payloads to monoclonal antibodies. *Bioconjugate chemistry* 2010;**21**:5–13. doi:10.1021/bc9002019

49

Alley SC, Okeley NM, Senter PD. Antibody–drug conjugates: targeted drug delivery for cancer. *Current Opinion in Chemical Biology* 2010;**14**:529–37.

doi:10.1016/j.cbpa.2010.06.170

50

Webb S. Pharma interest surges in antibody drug conjugates. *Nature Biotechnology* 2011;**29**:297–8. doi:10.1038/nbt0411-297

51

Holliger P, Hudson PJ. Engineered antibody fragments and the rise of single domains. *Nature Biotechnology* 2005;**23**:1126–36. doi:10.1038/nbt1142

52

Jinek M, Doudna JA. A three-dimensional view of the molecular machinery of RNA interference. *Nature* 2009;**457**:405–12. doi:10.1038/nature07755

53

Castanotto D, Rossi JJ. The promises and pitfalls of RNA-interference-based therapeutics. *Nature* 2009;**457**:426–33. doi:10.1038/nature07758

54

Grimm D. Small silencing RNAs: State-of-the-art. *Advanced Drug Delivery Reviews* 2009;**61**:672–703. doi:10.1016/j.addr.2009.05.002

55

Vaishnaw AK, Gollob J, Gamba-Vitalo C, et al. A status report on RNAi therapeutics. *Silence* 2010;**1**. doi:10.1186/1758-907X-1-14

56

Shen J, Samul R, Silva RL, et al. Suppression of ocular neovascularization with siRNA targeting VEGF receptor 1. *Gene Therapy* 2005;**13**:225–34. doi:10.1038/sj.gt.3302641

57

Kalluri R, Kanasaki K. RNA interference: Generic block on angiogenesis. *Nature* 2008;**452**:543–5. doi:10.1038/452543a

58

Human embryonic stem cells: Derivation, culture, and differentiation: A review.

59

Stadtfeld M, Hochedlinger K. Induced pluripotency: history, mechanisms, and applications. *Genes & Development* 2010;**24**:2239–63. doi:10.1101/gad.1963910

60

Watt FM, Driskell RR. The therapeutic potential of stem cells. *Philosophical Transactions of the Royal Society B: Biological Sciences* 2010;**365**:155–63. doi:10.1098/rstb.2009.0149

61

Brignier AC, Gewirtz AM. Embryonic and adult stem cell therapy. *Journal of Allergy and Clinical Immunology* 2010;**125**:S336–44. doi:10.1016/j.jaci.2009.09.032

62

Lledo P-M, Merkle FT, Alvarez-Buylla A. Origin and function of olfactory bulb interneuron diversity. *Trends in Neurosciences* 2008;**31**:392–400. doi:10.1016/j.tins.2008.05.006

63

Murray CW. Fragment-Based Drug Discovery Applied to Hsp90. Discovery of Two Lead Series with High Ligand Efficiency. *Journal of Medicinal Chemistry* 2010;**53**:5942–55. doi:10.1021/jm100059d

64

Hopkins AL, Groom CR, Alex A. Ligand efficiency: a useful metric for lead selection. *Drug*

Discovery Today 2004;**9**:430–1. doi:10.1016/S1359-6446(04)03069-7

65

Congreve M, Chessari G, Tisi D, et al. Recent Developments in Fragment-Based Drug Discovery. *Journal of Medicinal Chemistry* 2008;**51**:3661–80. doi:10.1021/jm8000373

66

Murray CW, Rees DC. The rise of fragment-based drug discovery. *Nature Chemistry* 2009;**1**:187–92. doi:10.1038/nchem.217

67

Baurin N, Aboul-Ela F, Barril X, et al. Design and Characterization of Libraries of Molecular Fragments for Use in NMR Screening against Protein Targets. *Journal of Chemical Information and Modeling* 2004;**44**:2157–66. doi:10.1021/ci049806z

68

Woodhead AJ. Discovery of (2,4-Dihydroxy-5-isopropylphenyl)-[5-(4-methylpiperazin-1-ylmethyl)-1,3-dihydroisoindol-2-yl]methanone (AT13387), a Novel Inhibitor of the Molecular Chaperone Hsp90 by Fragment Based Drug Design. *Journal of Medicinal Chemistry* 2010;**53**:5956–69. doi:10.1021/jm100060b

69

DiMasi JA, Hansen RW, Grabowski HG. The price of innovation: new estimates of drug development costs. *Journal of Health Economics* 2003;**22**:151–85. doi:10.1016/S0167-6296(02)00126-1