

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(10):835-844. 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(20):2775-2778. 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(8):711-716. doi:10.1038/nrd1470

4.

Swinney DC, Anthony J. How were new medicines discovered? *Nature Reviews Drug Discovery*. 2011;10(7):507-519. 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(3):188-195. doi:10.1038/nrd3368

6.

Selzer, P. M., Rohwer, A., Marhöfer, R. J. Applied Bioinformatics: An Introduction. Springer; 2008.

7.

Xiong, Jin. Essential Bioinformatics. Cambridge University Press; 2006.

8.

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

9.

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

10.

Gu, Jenny, Bourne, Philip E. Structural Bioinformatics. Vol Methods of biochemical analysis. 2nd ed. Wiley; 2008.

11.

Petsko, Gregory A., Ringe, Dagmar. Protein Structure and Function. Vol Primers in biology. New Science; 2004.

12.

Nelson, David L., Cox, Michael M., Lehninger, Albert L. Lehninger Principles of Biochemistry . 5th ed. W.H. Freeman; 2008.

13.

Chandra N. Computational systems approach for drug target discovery. *Expert Opinion on Drug Discovery*. 2009;4(12):1221-1236. doi:10.1517/17460440903380422

14.

Overington JP, Al-Lazikani B, Hopkins AL. How many drug targets are there? *Nature Reviews Drug Discovery*. 2006;5(12):993-996. 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(8):560-565. 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(6706):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(8):819-826. 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. John Wiley & Sons, Ltd; 2001. doi:10.1038/npg.els.0000056

20.

Cornish-Bowden, Athel. *Fundamentals of Enzyme Kinetics*. 3rd ed. Portland; 2004.

21.

Copeland, Robert Allen. Evaluation of Enzyme Inhibitors in Drug Discovery: A Guide for Medicinal Chemists and Pharmacologists. Vol Methods of biochemical analysis. 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. CRC Press; 2011.

23.

Rang, H. P., Dale, M. Maureen. Pharmacology. 9th ed. 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(5):923-947. 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(11):1267-1280. 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(8):617-626. 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(4):358-368. doi:10.1038/nrd2552

28.

Hopkins AL, Groom CR. Opinion: The druggable genome. *Nature Reviews Drug Discovery*. 2002;1(9):727-730. doi:10.1038/nrd892

29.

Richard M. Durbin. A map of human genome variation from population-scale sequencing. *Nature*. 2010;467(7319):1061-1073. 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(14):5061-5084. 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(8):1219-1229. doi:10.1021/jm960352+

37.

Willett P, Barnard JM, Downs GM. Chemical Similarity Searching. *Journal of Chemical Information and Modeling*. 1998;38(6):983-996. 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(3):347-361. doi:10.1016/j.cbpa.2010.02.018

39.

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

40.

Veber DF, Johnson SR, Cheng HY, Smith BR, Ward KW, Kopple KD. Molecular Properties That Influence the Oral Bioavailability of Drug Candidates. *Journal of Medicinal Chemistry*. 2002;45(12):2615-2623. doi:10.1021/jm020017n

41.

Blake JF. Identification and Evaluation of Molecular Properties Related to Preclinical Optimization and Clinical Fate. *Medicinal Chemistry*. 2005;1(6):649-655. doi:10.2174/157340605774598081

42.

Beck A, Wurch T, Bailly C, Corvaia N. Strategies and challenges for the next generation of therapeutic antibodies. *Nature Reviews Immunology*. 2010;10(5):345-352. doi:10.1038/nri2747

43.

Bradbury ARM, Sidhu S, Dübel S, McCafferty J. Beyond natural antibodies: the power of in vitro display technologies. *Nature Biotechnology*. 2011;29(3):245-254. 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(9):1255-1260. doi:10.1016/j.yexcr.2011.03.010

45.

Pillay V, Gan HK, Scott AM. Antibodies in oncology. *New Biotechnology*. 2011;28(5):518-529. 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(2):147-159. doi:10.1038/nrd1957

47.

Weiner LM, Surana R, Wang S. Monoclonal antibodies: versatile platforms for cancer immunotherapy. *Nature Reviews Immunology*. 2010;10(5):317-327. doi:10.1038/nri2744

48.

Ducry L, Stump B. Antibody–drug conjugates: Linking cytotoxic payloads to monoclonal antibodies. *Bioconjugate chemistry*. 2010;21(1):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(4):529-537. doi:10.1016/j.cbpa.2010.06.170

50.

Webb S. Pharma interest surges in antibody drug conjugates. *Nature Biotechnology*. 2011;29(4):297-298. doi:10.1038/nbt0411-297

51.

Holliger P, Hudson PJ. Engineered antibody fragments and the rise of single domains. *Nature Biotechnology*. 2005;23(9):1126-1136. doi:10.1038/nbt1142

52.

Jinek M, Doudna JA. A three-dimensional view of the molecular machinery of RNA interference. *Nature*. 2009;457(7228):405-412. doi:10.1038/nature07755

53.

Castanotto D, Rossi JJ. The promises and pitfalls of RNA-interference-based therapeutics. *Nature*. 2009;457(7228):426-433. doi:10.1038/nature07758

54.

Grimm D. Small silencing RNAs: State-of-the-art. *Advanced Drug Delivery Reviews*. 2009;61(9):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(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(3):225-234. doi:10.1038/sj.gt.3302641

57.

Kalluri R, Kanasaki K. RNA interference: Generic block on angiogenesis. *Nature*. 2008;452(7187):543-545. doi:10.1038/452543a

58.

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

59.

Stadtfield M, Hochedlinger K. Induced pluripotency: history, mechanisms, and applications. *Genes & Development*. 2010;24(20):2239-2263. 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(1537):155-163. 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(2):S336-S344. doi:10.1016/j.jaci.2009.09.032

62.

Lledo PM, Merkle FT, Alvarez-Buylla A. Origin and function of olfactory bulb interneuron diversity. *Trends in Neurosciences*. 2008;31(8):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(16):5942-5955. doi:10.1021/jm100059d

64.

Hopkins AL, Groom CR, Alex A. Ligand efficiency: a useful metric for lead selection. *Drug Discovery Today*. 2004;9(10):430-431. doi:10.1016/S1359-6446(04)03069-7

65.

Congreve M, Chessari G, Tisi D, Woodhead AJ. Recent Developments in Fragment-Based Drug Discovery. *Journal of Medicinal Chemistry*. 2008;51(13):3661-3680. doi:10.1021/jm8000373

66.

Murray CW, Rees DC. The rise of fragment-based drug discovery. *Nature Chemistry*. 2009;1(3):187-192. 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(6):2157-2166. 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(16):5956-5969. 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(2):151-185. doi:10.1016/S0167-6296(02)00126-1