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 Oct;5(10):835–44.

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 Oct;11(20):2775–8.

3.

Kola I, Landis J. Opinion: Can the pharmaceutical industry reduce attrition rates? Nature Reviews Drug Discovery. 2004 Aug;3(8):711–6.

4.

Swinney DC, Anthony J. How were new medicines discovered? Nature Reviews Drug Discovery. 2011 Jun 24;10(7):507–19.

5.

Macarron R, Banks MN, Bojanic D, Burns DJ, Cirovic DA, Garyantes T, et al. Impact of high-throughput screening in biomedical research. Nature Reviews Drug Discovery. 2011 Mar;10(3):188–95.

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 [Internet]. Oxford: BIOS; 2003. Available from: http://www.vlebooks.com/vleweb/product/openreader?id=UCL&isbn=9780203427828

9.

Zvelebil, Marketa J., Baum, Jeremy O. Understanding bioinformatics [Internet]. London: Garland Science; 2008. Available from: https://bibliu.com/app/#/view/books/9781136976964/pdf2htmlex/index.html#page_Cover

10.

Gu, Jenny, Bourne, Philip E. Structural bioinformatics. 2nd ed. Vol. Methods of biochemical analysis. Hoboken, N.J.: Wiley; 2008.

11.

Petsko, Gregory A., Ringe, Dagmar. Protein structure and function. Vol. Primers in biology. 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 Dec;4(12):1221–36.

14.

Overington JP, Al-Lazikani B, Hopkins AL. How many drug targets are there? Nature Reviews Drug Discovery. 2006 Dec;5(12):993–6.

15.

Fitt R, Nodder E. Setting the threshold for industrial application: the UK diverges from Europe. Journal of Intellectual Property Law & Practice. 2010 Jun 4;5(8):560–5.

16.

Ikura M, Inouye M. NMR structure of the histidine kinase domain of the : E. coli: osmosensor EnvZ : Article : Nature. Nature. 1998 Nov 5;396(6706):88–92.

17.

Krohn KA, Link JM. Interpreting enzyme and receptor kinetics: keeping it simple, but not too simple. Nuclear Medicine and Biology. 2003 Nov;30(8):819–26.

18.

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

19.

Jarnagin K. Receptor Binding in Drug Discovery. Encyclopedia of Life Sciences. Chichester: John Wiley & Sons, Ltd; 2001.

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 [Internet]. Vol. Methods of biochemical analysis. Hoboken, N.J.: J. Wiley; 2005. Available from: 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 [Internet]. 9th ed. Edinburgh: Churchill Livingstone; 2019. Available from: 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 Nov;125(5):923–47.

25.

Khawaja X, Dunlop J, Kowal D. Scintillation proximity assay in lead discovery. Expert Opinion on Drug Discovery. 2008 Nov;3(11):1267–80.

26.

Kenakin TP. Cellular assays as portals to seven-transmembrane receptor-based drug discovery. Nature Reviews Drug Discovery. 2009 Jul 17;8(8):617–26.

27.

Dunlop J. High-throughput electrophysiology: an emerging paradigm for ion-channel screening and physiology. Nature Reviews Drug Discovery. 2008 Apr;7(4):358–68.

28.

Hopkins AL, Groom CR. Opinion: The druggable genome. Nature Reviews Drug Discovery. 2002 Sep;1(9):727–30.

29.

Richard M. Durbin. A map of human genome variation from population-scale sequencing. Nature. 2010 Oct 28;467(7319):1061–73.

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 [Internet]. 2003. Available from: 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 [Internet]. 2010 Jul 22;53(14):5061–84. Available from: https://contentstore.cla.co.uk/secure/link?id=fb92e363-cb0b-f011-90cc-c5989c4ef87d

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 [Internet]. 1997 Apr;40(8):1219–29. Available from: https://contentstore.cla.co.uk/secure/link?id=c491b572-220b-f011-90cc-c5989c4ef87d

37.

Willett P, Barnard JM, Downs GM. Chemical Similarity Searching. Journal of Chemical Information and Modeling [Internet]. 1998 Nov 23;38(6):983–96. Available from: https://contentstore.cla.co.uk/secure/link?id=e44202ff-cd0b-f011-90cc-c5989c4ef87d

38.

Welsch ME, Snyder SA, Stockwell BR. Privileged scaffolds for library design and drug discovery. Current Opinion in Chemical Biology. 2010 Jun;14(3):347–61.

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 Jan;23(1–3):3–25.

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 [Internet]. 2002 Jun;45(12):2615–23. Available from: https://contentstore.cla.co.uk/secure/link?id=de13eed7-c90b-f011-90cc-c5989c4ef87d

41.

Blake JF. Identification and Evaluation of Molecular Properties Related to Preclinical Optimization and Clinical Fate. Medicinal Chemistry. 2005 Nov 1;1(6):649–55.

42.

Beck A, Wurch T, Bailly C, Corvaia N. Strategies and challenges for the next generation of therapeutic antibodies. Nature Reviews Immunology. 2010 May;10(5):345–52.

43.

Bradbury ARM, Sidhu S, Dübel S, McCafferty J. Beyond natural antibodies: the power of in vitro display technologies. Nature Biotechnology. 2011 Mar;29(3):245–54.

44.

Nagorsen D, Baeuerle PA. Immunomodulatory therapy of cancer with T cell-engaging BiTE antibody blinatumomab. Experimental Cell Research. 2011 May;317(9):1255–60.

45.

Pillay V, Gan HK, Scott AM. Antibodies in oncology. New Biotechnology. 2011 Sep;28(5):518–29.

46.

Schrama D, Reisfeld RA, Becker JC. Antibody targeted drugs as cancer therapeutics. Nature Reviews Drug Discovery. 2006 Jan 20;5(2):147–59.

47.

Weiner LM, Surana R, Wang S. Monoclonal antibodies: versatile platforms for cancer immunotherapy. Nature Reviews Immunology. 2010 May;10(5):317–27.

48.

Ducry L, Stump B. Antibody−drug conjugates: Linking cytotoxic payloads to monoclonal antibodies. Bioconjugate chemistry. 2010 Jan 20;21(1):5–13.

49.

Alley SC, Okeley NM, Senter PD. Antibody–drug conjugates: targeted drug delivery for cancer. Current Opinion in Chemical Biology. 2010 Aug;14(4):529–37.

50.

Webb S. Pharma interest surges in antibody drug conjugates. Nature Biotechnology. 2011 Apr;29(4):297–8.

51.

Holliger P, Hudson PJ. Engineered antibody fragments and the rise of single domains. Nature Biotechnology. 2005 Sep;23(9):1126–36.

52.

Jinek M, Doudna JA. A three-dimensional view of the molecular machinery of RNA interference. Nature. 2009 Jan 22;457(7228):405–12.

53.

Castanotto D, Rossi JJ. The promises and pitfalls of RNA-interference-based therapeutics. Nature. 2009 Jan 22;457(7228):426–33.

54.

Grimm D. Small silencing RNAs: State-of-the-art. Advanced Drug Delivery Reviews. 2009 Jul;61(9):672–703.

55.

Vaishnaw AK, Gollob J, Gamba-Vitalo C, Hutabarat R, Sah D, Meyers R, et al. A status report on RNAi therapeutics. Silence. 2010;1(1).

56.

Shen J, Samul R, Silva RL, Akiyama H, Liu H, Saishin Y, et al. Suppression of ocular neovascularization with siRNA targeting VEGF receptor 1. Gene Therapy. 2005 Sep 29;13(3):225–34.

57.

Kalluri R, Kanasaki K. RNA interference: Generic block on angiogenesis. Nature. 2008 Apr 3;452(7187):543–5.

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 Oct 15;24(20):2239–63.

60.

Watt FM, Driskell RR. The therapeutic potential of stem cells. Philosophical Transactions of the Royal Society B: Biological Sciences. 2010 Jan 12;365(1537):155–63.

61.

Brignier AC, Gewirtz AM. Embryonic and adult stem cell therapy. Journal of Allergy and Clinical Immunology. 2010 Feb;125(2):S336–44.

62.

Lledo PM, Merkle FT, Alvarez-Buylla A. Origin and function of olfactory bulb interneuron diversity. Trends in Neurosciences. 2008 Aug;31(8):392–400.

63.

Murray CW. Fragment-Based Drug Discovery Applied to Hsp90. Discovery of Two Lead Series with High Ligand Efficiency. Journal of Medicinal Chemistry. 2010 Aug 26;53(16):5942–55.

64.

Hopkins AL, Groom CR, Alex A. Ligand efficiency: a useful metric for lead selection. Drug Discovery Today. 2004 May;9(10):430–1.

65.

Congreve M, Chessari G, Tisi D, Woodhead AJ. Recent Developments in Fragment-Based Drug Discovery. Journal of Medicinal Chemistry [Internet]. 2008 Jul;51(13):3661–80. Available from: https://contentstore.cla.co.uk/secure/link?id=0bbaf30c-e20b-f011-90cc-c5989c4ef87d

66.

Murray CW, Rees DC. The rise of fragment-based drug discovery. Nature Chemistry. 2009 Jun;1(3):187–92.

67.

Baurin N, Aboul-Ela F, Barril X, Davis B, Drysdale M, Dymock B, et al. Design and Characterization of Libraries of Molecular Fragments for Use in NMR Screening against Protein Targets. Journal of Chemical Information and Modeling [Internet]. 2004 Nov 22;44(6):2157–66. Available from: https://contentstore.cla.co.uk/secure/link?id=e3feb169-e40b-f011-90cc-c5989c4ef87d

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 [Internet]. 2010 Aug 26;53(16):5956–69. Available from: https://contentstore.cla.co.uk/secure/link?id=2cf7cd66-e30b-f011-90cc-c5989c4ef87d

69.

DiMasi JA, Hansen RW, Grabowski HG. The price of innovation: new estimates of drug development costs. Journal of Health Economics. 2003 Mar;22(2):151–85.