

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* **5**, 835–844 (2006).

2.

Smith, R. A. 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* **11**, 2775–2778 (2001).

3.

Kola, I. & Landis, J. Opinion: Can the pharmaceutical industry reduce attrition rates? *Nature Reviews Drug Discovery* **3**, 711–716 (2004).

4.

Swinney, D. C. & Anthony, J. How were new medicines discovered? *Nature Reviews Drug Discovery* **10**, 507–519 (2011).

5.

Macarron, R. et al. Impact of high-throughput screening in biomedical research. *Nature Reviews Drug Discovery* **10**, 188–195 (2011).

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).

9.

Zvelebil, Marketa J. & Baum, Jeremy O. Understanding bioinformatics. (Garland Science, 2008).

10.

Gu, Jenny & Bourne, Philip E. Structural bioinformatics. vol. Methods of biochemical analysis (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. (W.H. Freeman, 2008).

13.

Chandra, N. Computational systems approach for drug target discovery. Expert Opinion on Drug Discovery **4**, 1221-1236 (2009).

14.

Overington, J. P., Al-Lazikani, B. & Hopkins, A. L. How many drug targets are there? *Nature Reviews Drug Discovery* **5**, 993–996 (2006).

15.

Fitt, R. & Nodder, E. Setting the threshold for industrial application: the UK diverges from Europe. *Journal of Intellectual Property Law & Practice* **5**, 560–565 (2010).

16.

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

17.

Krohn, K. A. & Link, J. M. Interpreting enzyme and receptor kinetics: keeping it simple, but not too simple. *Nuclear Medicine and Biology* **30**, 819–826 (2003).

18.

Jarnagin, K. Receptor Binding in Drug Discovery. in eLS.

19.

Jarnagin, K. Receptor Binding in Drug Discovery. *Encyclopedia of Life Sciences* (John Wiley & Sons, Ltd, 2001). doi:10.1038/npg.els.0000056.

20.

Cornish-Bowden, Athel. *Fundamentals of enzyme kinetics*. (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).

22.

Gibb, Alasdair J., Foreman, John C., & Johansen, Torben. Textbook of receptor pharmacology. (CRC Press, 2011).

23.

Rang, H. P. & Dale, M. Maureen. Pharmacology. (Churchill Livingstone, 2019).

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* **125**, 923–947 (1998).

25.

Khawaja, X., Dunlop, J. & Kowal, D. Scintillation proximity assay in lead discovery. *Expert Opinion on Drug Discovery* **3**, 1267–1280 (2008).

26.

Kenakin, T. P. Cellular assays as portals to seven-transmembrane receptor-based drug discovery. *Nature Reviews Drug Discovery* **8**, 617–626 (2009).

27.

Dunlop, J. High-throughput electrophysiology: an emerging paradigm for ion-channel screening and physiology. *Nature Reviews Drug Discovery* **7**, 358–368 (2008).

28.

Hopkins, A. L. & Groom, C. R. Opinion: The druggable genome. *Nature Reviews Drug Discovery* **1**, 727–730 (2002).

29.

Richard M. Durbin. A map of human genome variation from population-scale sequencing. *Nature* **467**, 1061-1073 (2010).

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).

35.

Bissantz, C., Kuhn, B. & Stahl, M. *A Medicinal Chemist's Guide to Molecular Interactions*. *Journal of Medicinal Chemistry* **53**, 5061-5084 (2010).

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* **40**, 1219-1229 (1997).

37.

Willett, P., Barnard, J. M. & Downs, G. M. Chemical Similarity Searching. *Journal of Chemical Information and Modeling* **38**, 983–996 (1998).

38.

Welsch, M. E., Snyder, S. A. & Stockwell, B. R. Privileged scaffolds for library design and drug discovery. *Current Opinion in Chemical Biology* **14**, 347–361 (2010).

39.

Lipinski, C. A., Lombardo, F., Dominy, B. W. & Feeney, P. J. Experimental and computational approaches to estimate solubility and permeability in drug discovery and development settings. *Advanced Drug Delivery Reviews* **23**, 3–25 (1997).

40.

Veber, D. F. et al. Molecular Properties That Influence the Oral Bioavailability of Drug Candidates. *Journal of Medicinal Chemistry* **45**, 2615–2623 (2002).

41.

Blake, J. F. Identification and Evaluation of Molecular Properties Related to Preclinical Optimization and Clinical Fate. *Medicinal Chemistry* **1**, 649–655 (2005).

42.

Beck, A., Wurch, T., Bailly, C. & Corvaia, N. Strategies and challenges for the next generation of therapeutic antibodies. *Nature Reviews Immunology* **10**, 345–352 (2010).

43.

Bradbury, A. R. M., Sidhu, S., Dübel, S. & McCafferty, J. Beyond natural antibodies: the power of in vitro display technologies. *Nature Biotechnology* **29**, 245–254 (2011).

44.

Nagorsen, D. & Baeuerle, P. A. Immunomodulatory therapy of cancer with T cell-engaging BiTE antibody blinatumomab. *Experimental Cell Research* **317**, 1255–1260 (2011).

45.

Pillay, V., Gan, H. K. & Scott, A. M. Antibodies in oncology. *New Biotechnology* **28**, 518–529 (2011).

46.

Schrama, D., Reisfeld, R. A. & Becker, J. C. Antibody targeted drugs as cancer therapeutics. *Nature Reviews Drug Discovery* **5**, 147–159 (2006).

47.

Weiner, L. M., Surana, R. & Wang, S. Monoclonal antibodies: versatile platforms for cancer immunotherapy. *Nature Reviews Immunology* **10**, 317–327 (2010).

48.

Ducry, L. & Stump, B. Antibody–drug conjugates: Linking cytotoxic payloads to monoclonal antibodies. *Bioconjugate chemistry* **21**, 5–13 (2010).

49.

Alley, S. C., Okeley, N. M. & Senter, P. D. Antibody-drug conjugates: targeted drug delivery for cancer. *Current Opinion in Chemical Biology* **14**, 529–537 (2010).

50.

Webb, S. Pharma interest surges in antibody drug conjugates. *Nature Biotechnology* **29**, 297–298 (2011).

51.

Holliger, P. & Hudson, P. J. Engineered antibody fragments and the rise of single domains. *Nature Biotechnology* **23**, 1126–1136 (2005).

52.

Jinek, M. & Doudna, J. A. A three-dimensional view of the molecular machinery of RNA interference. *Nature* **457**, 405–412 (2009).

53.

Castanotto, D. & Rossi, J. J. The promises and pitfalls of RNA-interference-based therapeutics. *Nature* **457**, 426–433 (2009).

54.

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

55.

Vaishnaw, A. K. et al. A status report on RNAi therapeutics. *Silence* **1**, (2010).

56.

Shen, J. et al. Suppression of ocular neovascularization with siRNA targeting VEGF receptor 1. *Gene Therapy* **13**, 225–234 (2005).

57.

Kalluri, R. & Kanasaki, K. RNA interference: Generic block on angiogenesis. *Nature* **452**, 543–545 (2008).

58.

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

59.

Stadtfeld, M. & Hochedlinger, K. Induced pluripotency: history, mechanisms, and applications. *Genes & Development* **24**, 2239–2263 (2010).

60.

Watt, F. M. & Driskell, R. R. The therapeutic potential of stem cells. *Philosophical Transactions of the Royal Society B: Biological Sciences* **365**, 155–163 (2010).

61.

Brignier, A. C. & Gewirtz, A. M. Embryonic and adult stem cell therapy. *Journal of Allergy and Clinical Immunology* **125**, S336–S344 (2010).

62.

Lledo, P.-M., Merkle, F. T. & Alvarez-Buylla, A. Origin and function of olfactory bulb interneuron diversity. *Trends in Neurosciences* **31**, 392–400 (2008).

63.

Murray, C. W. Fragment-Based Drug Discovery Applied to Hsp90. Discovery of Two Lead Series with High Ligand Efficiency. *Journal of Medicinal Chemistry* **53**, 5942–5955 (2010).

64.

Hopkins, A. L., Groom, C. R. & Alex, A. Ligand efficiency: a useful metric for lead selection. *Drug Discovery Today* **9**, 430–431 (2004).

65.

Congreve, M., Chessari, G., Tisi, D. & Woodhead, A. J. Recent Developments in Fragment-Based Drug Discovery. *Journal of Medicinal Chemistry* **51**, 3661–3680 (2008).

66.

Murray, C. W. & Rees, D. C. The rise of fragment-based drug discovery. *Nature Chemistry* **1**, 187–192 (2009).

67.

Baurin, N. et al. Design and Characterization of Libraries of Molecular Fragments for Use in

NMR Screening against Protein Targets. *Journal of Chemical Information and Modeling* **44**, 2157–2166 (2004).

68.

Woodhead, A. J. 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* **53**, 5956–5969 (2010).

69.

DiMasi, J. A., Hansen, R. W. & Grabowski, H. G. The price of innovation: new estimates of drug development costs. *Journal of Health Economics* **22**, 151–185 (2003).