TMSDRDSI: Drug Design MSc

TMSDRDSING01: MSc Drug Design
WIBRG001, WIBRG002, WIBRG003, WIBRG004, 5 + 6

View Online

[1]

Alley, S.C. et al. 2010. Antibody–drug conjugates: targeted drug delivery for cancer. Current Opinion in Chemical Biology. 14, 4 (Aug. 2010), 529–537. DOI:https://doi.org/10.1016/j.cbpa.2010.06.170.

[2]

Baurin, N. et al. 2004. Design and Characterization of Libraries of Molecular Fragments for Use in NMR Screening against Protein Targets. Journal of Chemical Information and Modeling. 44, 6 (Nov. 2004), 2157–2166. DOI:https://doi.org/10.1021/ci049806z.

[3]

Beck, A. et al. 2010. Strategies and challenges for the next generation of therapeutic antibodies. Nature Reviews Immunology. 10, 5 (May 2010), 345–352. DOI:https://doi.org/10.1038/nri2747.

[4]

Bissantz, C. et al. 2010. A Medicinal Chemist's Guide to Molecular Interactions. Journal of Medicinal Chemistry. 53, 14 (Jul. 2010), 5061–5084. DOI:https://doi.org/10.1021/jm100112j.

[5]

Blake, J.F. 2005. Identification and Evaluation of Molecular Properties Related to Preclinical Optimization and Clinical Fate. Medicinal Chemistry. 1, 6 (Nov. 2005), 649–655. DOI:https://doi.org/10.2174/157340605774598081.

[6]

Bradbury, A.R.M. et al. 2011. Beyond natural antibodies: the power of in vitro display technologies. Nature Biotechnology. 29, 3 (Mar. 2011), 245–254. DOI:https://doi.org/10.1038/nbt.1791.

[7]

Brignier, A.C. and Gewirtz, A.M. 2010. Embryonic and adult stem cell therapy. Journal of Allergy and Clinical Immunology. 125, 2 (Feb. 2010), S336–S344. DOI:https://doi.org/10.1016/j.jaci.2009.09.032.

[8]

Castanotto, D. and Rossi, J.J. 2009. The promises and pitfalls of RNA-interference-based therapeutics. Nature. 457, 7228 (Jan. 2009), 426–433. DOI:https://doi.org/10.1038/nature07758.

[9]

Chandra, N. 2009. Computational systems approach for drug target discovery. Expert Opinion on Drug Discovery. 4, 12 (Dec. 2009), 1221–1236. DOI:https://doi.org/10.1517/17460440903380422.

[10]

Colquhoun, D. 1998. 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, 5 (Nov. 1998), 923–947. DOI:https://doi.org/10.1038/sj.bjp.0702164.

[11]

Congreve, M. et al. 2008. Recent Developments in Fragment-Based Drug Discovery. Journal of Medicinal Chemistry. 51, 13 (Jul. 2008), 3661–3680. DOI:https://doi.org/10.1021/jm8000373.

[12]

Copeland, Robert Allen 2005. Evaluation of enzyme inhibitors in drug discovery: a guide for

medicinal chemists and pharmacologists. J. Wiley.

[13]

Cornish-Bowden, Athel 2004. Fundamentals of enzyme kinetics. Portland.

[14]

DiMasi, J.A. et al. 2003. The price of innovation: new estimates of drug development costs. Journal of Health Economics. 22, 2 (Mar. 2003), 151–185. DOI:https://doi.org/10.1016/S0167-6296(02)00126-1.

[15]

Ducry, L. and Stump, B. 2010. Antibody—drug conjugates: Linking cytotoxic payloads to monoclonal antibodies. Bioconjugate chemistry. 21, 1 (Jan. 2010), 5–13. DOI:https://doi.org/10.1021/bc9002019.

[16]

Dunlop, J. 2008. High-throughput electrophysiology: an emerging paradigm for ion-channel screening and physiology. Nature Reviews Drug Discovery. 7, 4 (Apr. 2008), 358–368. DOI:https://doi.org/10.1038/nrd2552.

[17]

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

[18]

Fitt, R. and Nodder, E. 2010. Setting the threshold for industrial application: the UK diverges from Europe. Journal of Intellectual Property Law & Practice. 5, 8 (Jun. 2010), 560–565. DOI:https://doi.org/10.1093/jiplp/jpq061.

[19]

Gasteiger, J. 2003. Handbook of chemoinformatics: from data to knowledge.

[20]

Gibb, Alasdair J. et al. 2011. Textbook of receptor pharmacology. CRC Press.

[21]

Grimm, D. 2009. Small silencing RNAs: State-of-the-art. Advanced Drug Delivery Reviews. 61, 9 (Jul. 2009), 672–703. DOI:https://doi.org/10.1016/j.addr.2009.05.002.

[22]

Gu, Jenny and Bourne, Philip E. 2008. Structural bioinformatics. Wiley.

[23]

Holliger, P. and Hudson, P.J. 2005. Engineered antibody fragments and the rise of single domains. Nature Biotechnology. 23, 9 (Sep. 2005), 1126–1136. DOI:https://doi.org/10.1038/nbt1142.

[24]

Hopkins, A.L. et al. 2004. Ligand efficiency: a useful metric for lead selection. Drug Discovery Today. 9, 10 (May 2004), 430–431. DOI:https://doi.org/10.1016/S1359-6446(04)03069-7.

[25]

Hopkins, A.L. and Groom, C.R. 2002. Opinion: The druggable genome. Nature Reviews Drug Discovery. 1, 9 (Sep. 2002), 727–730. DOI:https://doi.org/10.1038/nrd892.

[26]

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

[27]

Ikura, M. and Inouye, M. 1998. NMR structure of the histidine kinase domain of the : E. coli: osmosensor EnvZ : Article : Nature. Nature. 396, 6706 (Nov. 1998), 88–92. DOI:https://doi.org/10.1038/23968.

[28]

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

[29]

Jarnagin, K. 2001. Receptor Binding in Drug Discovery. John Wiley & Sons, Ltd.

[30]

Jinek, M. and Doudna, J.A. 2009. A three-dimensional view of the molecular machinery of RNA interference. Nature. 457, 7228 (Jan. 2009), 405–412. DOI:https://doi.org/10.1038/nature07755.

[31]

Kalluri, R. and Kanasaki, K. 2008. RNA interference: Generic block on angiogenesis. Nature. 452, 7187 (Apr. 2008), 543–545. DOI:https://doi.org/10.1038/452543a.

[32]

Kenakin, T.P. 2009. Cellular assays as portals to seven-transmembrane receptor-based drug discovery. Nature Reviews Drug Discovery. 8, 8 (Jul. 2009), 617–626. DOI:https://doi.org/10.1038/nrd2838.

[33]

Khawaja, X. et al. 2008. Scintillation proximity assay in lead discovery. Expert Opinion on Drug Discovery. 3, 11 (Nov. 2008), 1267–1280. DOI:https://doi.org/10.1517/17460441.3.11.1267.

[34]

Kola, I. and Landis, J. 2004. Opinion: Can the pharmaceutical industry reduce attrition

rates? Nature Reviews Drug Discovery. 3, 8 (Aug. 2004), 711–716. DOI:https://doi.org/10.1038/nrd1470.

[35]

Krohn, K.A. and Link, J.M. 2003. Interpreting enzyme and receptor kinetics: keeping it simple, but not too simple. Nuclear Medicine and Biology. 30, 8 (Nov. 2003), 819–826. DOI:https://doi.org/10.1016/S0969-8051(03)00132-X.

[36]

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

[37]

Lipinski, C.A. et al. 1997. Experimental and computational approaches to estimate solubility and permeability in drug discovery and development settings. Advanced Drug Delivery Reviews. 23, 1–3 (Jan. 1997), 3–25. DOI:https://doi.org/10.1016/S0169-409X(96)00423-1.

[38]

Lledo, P.-M. et al. 2008. Origin and function of olfactory bulb interneuron diversity. Trends in Neurosciences. 31, 8 (Aug. 2008), 392–400. DOI:https://doi.org/10.1016/j.tins.2008.05.006.

[39]

Macarron, R. et al. 2011. Impact of high-throughput screening in biomedical research. Nature Reviews Drug Discovery. 10, 3 (Mar. 2011), 188–195. DOI:https://doi.org/10.1038/nrd3368.

[40]

Matter, H. 1997. Selecting Optimally Diverse Compounds from Structure Databases: A Validation Study of Two-Dimensional and Three-Dimensional Molecular Descriptors. Journal of Medicinal Chemistry. 40, 8 (Apr. 1997), 1219–1229. DOI:https://doi.org/10.1021/jm960352+.

[41]

Murray, C.W. 2010. Fragment-Based Drug Discovery Applied to Hsp90. Discovery of Two Lead Series with High Ligand Efficiency. Journal of Medicinal Chemistry. 53, 16 (Aug. 2010), 5942–5955. DOI:https://doi.org/10.1021/jm100059d.

[42]

Murray, C.W. and Rees, D.C. 2009. The rise of fragment-based drug discovery. Nature Chemistry. 1, 3 (Jun. 2009), 187–192. DOI:https://doi.org/10.1038/nchem.217.

[43]

Nagorsen, D. and Baeuerle, P.A. 2011. Immunomodulatory therapy of cancer with T cell-engaging BiTE antibody blinatumomab. Experimental Cell Research. 317, 9 (May 2011), 1255–1260. DOI:https://doi.org/10.1016/j.yexcr.2011.03.010.

[44]

Nelson, David L. et al. 2008. Lehninger principles of biochemistry. W.H. Freeman.

[45]

Orengo, Christine Ann et al. 2003. Bioinformatics: genes, proteins and computers. BIOS.

[46]

Overington, J.P. et al. 2006. How many drug targets are there? Nature Reviews Drug Discovery. 5, 12 (Dec. 2006), 993–996. DOI:https://doi.org/10.1038/nrd2199.

[47]

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

[48]

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

[49]

Pillay, V. et al. 2011. Antibodies in oncology. New Biotechnology. 28, 5 (Sep. 2011), 518–529. DOI:https://doi.org/10.1016/j.nbt.2011.03.021.

[50]

Rang, H. P. and Dale, M. Maureen 2019. Pharmacology. Churchill Livingstone.

[51]

Richard M. Durbin 2010. A map of human genome variation from population-scale sequencing. Nature. 467, 7319 (Oct. 2010), 1061–1073. DOI:https://doi.org/10.1038/nature09534.

[52]

Schrama, D. et al. 2006. Antibody targeted drugs as cancer therapeutics. Nature Reviews Drug Discovery. 5, 2 (Jan. 2006), 147–159. DOI:https://doi.org/10.1038/nrd1957.

[53]

Selzer, P. M. et al. 2008. Applied bioinformatics: an introduction. Springer.

[54]

Shen, J. et al. 2005. Suppression of ocular neovascularization with siRNA targeting VEGF receptor 1. Gene Therapy. 13, 3 (Sep. 2005), 225–234. DOI:https://doi.org/10.1038/sj.gt.3302641.

[55]

Smith, R.A. 2001. 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, 20 (Oct. 2001), 2775–2778. DOI:https://doi.org/10.1016/S0960-894X(01)00571-6.

[56]

Stadtfeld, M. and Hochedlinger, K. 2010. Induced pluripotency: history, mechanisms, and applications. Genes & Development. 24, 20 (Oct. 2010), 2239–2263. DOI:https://doi.org/10.1101/gad.1963910.

[57]

Swinney, D.C. and Anthony, J. 2011. How were new medicines discovered? Nature Reviews Drug Discovery. 10, 7 (Jun. 2011), 507–519. DOI:https://doi.org/10.1038/nrd3480.

[58]

Thomas, Gareth 2003. Fundamentals of medicinal chemistry.

[59]

Vaishnaw, A.K. et al. 2010. A status report on RNAi therapeutics. Silence. 1, 1 (2010). DOI:https://doi.org/10.1186/1758-907X-1-14.

[60]

Veber, D.F. et al. 2002. Molecular Properties That Influence the Oral Bioavailability of Drug Candidates. Journal of Medicinal Chemistry. 45, 12 (Jun. 2002), 2615–2623. DOI:https://doi.org/10.1021/jm020017n.

[61]

Watt, F.M. and Driskell, R.R. 2010. The therapeutic potential of stem cells. Philosophical Transactions of the Royal Society B: Biological Sciences. 365, 1537 (Jan. 2010), 155–163. DOI:https://doi.org/10.1098/rstb.2009.0149.

[62]

Webb, S. 2011. Pharma interest surges in antibody drug conjugates. Nature Biotechnology. 29, 4 (Apr. 2011), 297–298. DOI:https://doi.org/10.1038/nbt0411-297.

[63]

Weiner, L.M. et al. 2010. Monoclonal antibodies: versatile platforms for cancer immunotherapy. Nature Reviews Immunology. 10, 5 (May 2010), 317–327. DOI:https://doi.org/10.1038/nri2744.

[64]

Welsch, M.E. et al. 2010. Privileged scaffolds for library design and drug discovery. Current Opinion in Chemical Biology. 14, 3 (Jun. 2010), 347–361. DOI:https://doi.org/10.1016/j.cbpa.2010.02.018.

[65]

Wilhelm, S. 2006. Discovery and development of sorafenib: a multikinase inhibitor for treating cancer. Nature Reviews Drug Discovery. 5, 10 (Oct. 2006), 835–844. DOI:https://doi.org/10.1038/nrd2130.

[66]

Willett, P. et al. 1998. Chemical Similarity Searching. Journal of Chemical Information and Modeling. 38, 6 (Nov. 1998), 983–996. DOI:https://doi.org/10.1021/ci9800211.

[67]

Woodhead, A.J. 2010. 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, 16 (Aug. 2010), 5956–5969. DOI:https://doi.org/10.1021/jm100060b.

[68]

Xiong, Jin 2006. Essential bioinformatics. Cambridge University Press.

[69]

Zvelebil, Marketa J. and Baum, Jeremy O. 2008. Understanding bioinformatics. Garland Science.