

# TMSDRDSI: Drug Design MSc

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

[View Online](#)



---

Alley, Stephen C, Nicole M Okeley, and Peter D Senter. 2010. 'Antibody-Drug Conjugates: Targeted Drug Delivery for Cancer'. *Current Opinion in Chemical Biology* 14 (4): 529–37. <https://doi.org/10.1016/j.cbpa.2010.06.170>.

Baurin, N., F. Aboul-Ela, X. Barril, B. Davis, M. Drysdale, B. Dymock, H. Finch, 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): 2157–66. <https://doi.org/10.1021/ci049806z>.

Beck, Alain, Thierry Wurch, Christian Bailly, and Nathalie Corvaia. 2010. 'Strategies and Challenges for the next Generation of Therapeutic Antibodies'. *Nature Reviews Immunology* 10 (5): 345–52. <https://doi.org/10.1038/nri2747>.

Bissantz, Caterina, Bernd Kuhn, and Martin Stahl. 2010. 'A Medicinal Chemist's Guide to Molecular Interactions'. *Journal of Medicinal Chemistry* 53 (14): 5061–84. <https://doi.org/10.1021/jm100112j>.

Blake, J. F. 2005. 'Identification and Evaluation of Molecular Properties Related to Preclinical Optimization and Clinical Fate'. *Medicinal Chemistry* 1 (6): 649–55. <https://doi.org/10.2174/157340605774598081>.

Bradbury, Andrew R M, Sachdev Sidhu, Stefan Dübel, and John McCafferty. 2011. 'Beyond Natural Antibodies: The Power of in Vitro Display Technologies'. *Nature Biotechnology* 29 (3): 245–54. <https://doi.org/10.1038/nbt.1791>.

Brignier, Anne C., and Alan M. Gewirtz. 2010. 'Embryonic and Adult Stem Cell Therapy'. *Journal of Allergy and Clinical Immunology* 125 (2): S336–44. <https://doi.org/10.1016/j.jaci.2009.09.032>.

Castanotto, Daniela, and John J. Rossi. 2009. 'The Promises and Pitfalls of RNA-Interference-Based Therapeutics'. *Nature* 457 (7228): 426–33. <https://doi.org/10.1038/nature07758>.

Chandra, Nagasuma. 2009. 'Computational Systems Approach for Drug Target Discovery'. *Expert Opinion on Drug Discovery* 4 (12): 1221–36. <https://doi.org/10.1517/17460440903380422>.

Colquhoun, David. 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): 923–47. <https://doi.org/10.1038/sj.bjp.0702164>.

Congreve, Miles, Gianni Chessari, Dominic Tisi, and Andrew J. Woodhead. 2008. 'Recent Developments in Fragment-Based Drug Discovery'. *Journal of Medicinal Chemistry* 51 (13): 3661–80. <https://doi.org/10.1021/jm8000373>.

Copeland, Robert Allen. 2005. Evaluation of Enzyme Inhibitors in Drug Discovery: A Guide for Medicinal Chemists and Pharmacologists. Vol. Methods of biochemical analysis. Hoboken, N.J.: J. Wiley. <https://onlinelibrary.wiley.com/doi/book/10.1002/9781118540398>.

Cornish-Bowden, Athel. 2004. Fundamentals of Enzyme Kinetics. 3rd ed. London: Portland.

DiMasi, Joseph A, Ronald W Hansen, and Henry G Grabowski. 2003. 'The Price of Innovation: New Estimates of Drug Development Costs'. *Journal of Health Economics* 22 (2): 151–85. [https://doi.org/10.1016/S0167-6296\(02\)00126-1](https://doi.org/10.1016/S0167-6296(02)00126-1).

Ducry, Laurent, and Bernhard Stump. 2010. 'Antibody-drug Conjugates: Linking Cytotoxic Payloads to Monoclonal Antibodies'. *Bioconjugate Chemistry* 21 (1): 5–13. <https://doi.org/10.1021/bc9002019>.

Dunlop, John. 2008. 'High-Throughput Electrophysiology: An Emerging Paradigm for Ion-Channel Screening and Physiology'. *Nature Reviews Drug Discovery* 7 (4): 358–68. <https://doi.org/10.1038/nrd2552>.

Engel, Thomas and Gasteiger, J. 2003. Chemoinformatics: A Textbook.

Fitt, R., and E. Nodder. 2010. 'Setting the Threshold for Industrial Application: The UK Diverges from Europe'. *Journal of Intellectual Property Law & Practice* 5 (8): 560–65. <https://doi.org/10.1093/jiplp/jpq061>.

Gasteiger, J. 2003. Handbook of Chemoinformatics: From Data to Knowledge. <https://onlinelibrary.wiley.com/doi/book/10.1002/9783527618279>.

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

Grimm, Dirk. 2009. 'Small Silencing RNAs: State-of-the-Art'. *Advanced Drug Delivery Reviews* 61 (9): 672–703. <https://doi.org/10.1016/j.addr.2009.05.002>.

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

Holliger, Philipp, and Peter J Hudson. 2005. 'Engineered Antibody Fragments and the Rise of Single Domains'. *Nature Biotechnology* 23 (9): 1126–36. <https://doi.org/10.1038/nbt1142>.

Hopkins, Andrew L., and Colin R. Groom. 2002. 'Opinion: The Druggable Genome'. *Nature Reviews Drug Discovery* 1 (9): 727–30. <https://doi.org/10.1038/nrd892>.

Hopkins, Andrew L., Colin R. Groom, and Alexander Alex. 2004. 'Ligand Efficiency: A Useful Metric for Lead Selection'. *Drug Discovery Today* 9 (10): 430–31. [https://doi.org/10.1016/S1359-6446\(04\)03069-7](https://doi.org/10.1016/S1359-6446(04)03069-7).

'Human Embryonic Stem Cells: Derivation, Culture, and Differentiation: A Review'. n.d.

Ikura, Mitsuhiko, and Masayori Inouye. 1998. 'NMR Structure of the Histidine Kinase Domain of the : E. Coli: Osmosensor EnvZ : Article : Nature'. *Nature* 396 (6706): 88–92. <https://doi.org/10.1038/23968>.

Jarnagin, Kurt. 2001. Receptor Binding in Drug Discovery. *Encyclopedia of Life Sciences*. Chichester: John Wiley & Sons, Ltd. <https://doi.org/10.1038/npg.els.0000056>.

———. n.d. 'Receptor Binding in Drug Discovery'. In eLS.

Jinek, Martin, and Jennifer A. Doudna. 2009. 'A Three-Dimensional View of the Molecular Machinery of RNA Interference'. *Nature* 457 (7228): 405–12. <https://doi.org/10.1038/nature07755>.

Kalluri, Raghu, and Keizo Kanasaki. 2008. 'RNA Interference: Generic Block on Angiogenesis'. *Nature* 452 (7187): 543–45. <https://doi.org/10.1038/452543a>.

Kenakin, Terry P. 2009. 'Cellular Assays as Portals to Seven-Transmembrane Receptor-Based Drug Discovery'. *Nature Reviews Drug Discovery* 8 (8): 617–26. <https://doi.org/10.1038/nrd2838>.

Khawaja, Xavier, John Dunlop, and Dianne Kowal. 2008. 'Scintillation Proximity Assay in Lead Discovery'. *Expert Opinion on Drug Discovery* 3 (11): 1267–80. <https://doi.org/10.1517/17460441.3.11.1267>.

Kola, Ismail, and John Landis. 2004. 'Opinion: Can the Pharmaceutical Industry Reduce Attrition Rates?' *Nature Reviews Drug Discovery* 3 (8): 711–16. <https://doi.org/10.1038/nrd1470>.

Krohn, Kenneth A., and Jeanne M. Link. 2003. 'Interpreting Enzyme and Receptor Kinetics: Keeping It Simple, but Not Too Simple'. *Nuclear Medicine and Biology* 30 (8): 819–26. [https://doi.org/10.1016/S0969-8051\(03\)00132-X](https://doi.org/10.1016/S0969-8051(03)00132-X).

Leach, Andrew R. and Gillet, Valerie J. 2003. An Introduction to Chemoinformatics.

Lipinski, Christopher A., Franco Lombardo, Beryl W. Dominy, and Paul J. Feeney. 1997. 'Experimental and Computational Approaches to Estimate Solubility and Permeability in Drug Discovery and Development Settings'. *Advanced Drug Delivery Reviews* 23 (1–3): 3–25. [https://doi.org/10.1016/S0169-409X\(96\)00423-1](https://doi.org/10.1016/S0169-409X(96)00423-1).

Lledo, Pierre-Marie, Florian T. Merkle, and Arturo Alvarez-Buylla. 2008. 'Origin and Function of Olfactory Bulb Interneuron Diversity'. *Trends in Neurosciences* 31 (8): 392–400. <https://doi.org/10.1016/j.tins.2008.05.006>.

Macarron, Ricardo, Martyn N. Banks, Dejan Bojanic, David J. Burns, Dragan A. Cirovic, Tina Garyantes, Darren V. S. Green, et al. 2011. 'Impact of High-Throughput Screening in Biomedical Research'. *Nature Reviews Drug Discovery* 10 (3): 188–95. <https://doi.org/10.1038/nrd3368>.

Matter, Hans. 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): 1219–29. <https://doi.org/10.1021/jm960352+>.

Murray, Christopher W. 2010. 'Fragment-Based Drug Discovery Applied to Hsp90. Discovery of Two Lead Series with High Ligand Efficiency'. *Journal of Medicinal Chemistry* 53 (16): 5942–55. <https://doi.org/10.1021/jm100059d>.

Murray, Christopher W., and David C. Rees. 2009. 'The Rise of Fragment-Based Drug Discovery'. *Nature Chemistry* 1 (3): 187–92. <https://doi.org/10.1038/nchem.217>.

Nagorsen, Dirk, and Patrick A. Baeuerle. 2011. 'Immunomodulatory Therapy of Cancer with T Cell-Engaging BiTE Antibody Blinatumomab'. *Experimental Cell Research* 317 (9): 1255–60. <https://doi.org/10.1016/j.yexcr.2011.03.010>.

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

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

Overington, John P., Bissan Al-Lazikani, and Andrew L. Hopkins. 2006. 'How Many Drug Targets Are There?' *Nature Reviews Drug Discovery* 5 (12): 993–96.  
<https://doi.org/10.1038/nrd2199>.

Patrick, Graham L. 2017. *An Introduction to Medicinal Chemistry*.

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

Pillay, Vinochani, Hui K. Gan, and Andrew M. Scott. 2011. 'Antibodies in Oncology'. *New Biotechnology* 28 (5): 518–29. <https://doi.org/10.1016/j.nbt.2011.03.021>.

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

Richard M. Durbin. 2010. 'A Map of Human Genome Variation from Population-Scale Sequencing'. *Nature* 467 (7319): 1061–73. <https://doi.org/10.1038/nature09534>.

Schrama, David, Ralph A. Reisfeld, and Jürgen C. Becker. 2006. 'Antibody Targeted Drugs as Cancer Therapeutics'. *Nature Reviews Drug Discovery* 5 (2): 147–59.  
<https://doi.org/10.1038/nrd1957>.

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

Shen, J, R Samul, R L Silva, H Akiyama, H Liu, Y Saishin, S F Hackett, et al. 2005. 'Suppression of Ocular Neovascularization with siRNA Targeting VEGF Receptor 1'. *Gene Therapy* 13 (3): 225–34. <https://doi.org/10.1038/sj.gt.3302641>.

Smith, Roger 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): 2775–78.  
[https://doi.org/10.1016/S0960-894X\(01\)00571-6](https://doi.org/10.1016/S0960-894X(01)00571-6).

Stadtfeld, M., and K. Hochedlinger. 2010. 'Induced Pluripotency: History, Mechanisms, and Applications'. *Genes & Development* 24 (20): 2239–63.  
<https://doi.org/10.1101/gad.1963910>.

Swinney, David C., and Jason Anthony. 2011. 'How Were New Medicines Discovered?' *Nature Reviews Drug Discovery* 10 (7): 507–19. <https://doi.org/10.1038/nrd3480>.

Thomas, Gareth. 2003. *Fundamentals of Medicinal Chemistry*.

Vaishnav, Akshay K, Jared Gollob, Christina Gamba-Vitalo, Renta Hutabarat, Dinah Sah, Rachel Meyers, Tony de Fougerolles, and John Maraganore. 2010. 'A Status Report on RNAi Therapeutics'. *Silence* 1 (1). <https://doi.org/10.1186/1758-907X-1-14>.

Veber, Daniel F., Stephen R. Johnson, Hung-Yuan Cheng, Brian R. Smith, Keith W. Ward, and Kenneth D. Kopple. 2002. 'Molecular Properties That Influence the Oral Bioavailability of Drug Candidates'. *Journal of Medicinal Chemistry* 45 (12): 2615–23.  
<https://doi.org/10.1021/jm020017n>.

Watt, F. M., and R. R. Driskell. 2010. 'The Therapeutic Potential of Stem Cells'. *Philosophical Transactions of the Royal Society B: Biological Sciences* 365 (1537): 155–63.  
<https://doi.org/10.1098/rstb.2009.0149>.

Webb, Sarah. 2011. 'Pharma Interest Surges in Antibody Drug Conjugates'. *Nature Biotechnology* 29 (4): 297–98. <https://doi.org/10.1038/nbt0411-297>.

Weiner, Louis M., Rishi Surana, and Shangzi Wang. 2010. 'Monoclonal Antibodies: Versatile Platforms for Cancer Immunotherapy'. *Nature Reviews Immunology* 10 (5): 317–27.  
<https://doi.org/10.1038/nri2744>.

Welsch, Matthew E, Scott A Snyder, and Brent R Stockwell. 2010. 'Privileged Scaffolds for Library Design and Drug Discovery'. *Current Opinion in Chemical Biology* 14 (3): 347–61.  
<https://doi.org/10.1016/j.cbpa.2010.02.018>.

Wilhelm, Scott. 2006. 'Discovery and Development of Sorafenib: A Multikinase Inhibitor for Treating Cancer'. *Nature Reviews Drug Discovery* 5 (10): 835–44.  
<https://doi.org/10.1038/nrd2130>.

Willett, P., J.M. Barnard, and G.M. Downs. 1998. 'Chemical Similarity Searching'. *Journal of Chemical Information and Modeling* 38 (6): 983–96. <https://doi.org/10.1021/ci9800211>.

Woodhead, Andrew 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): 5956–69.  
<https://doi.org/10.1021/jm100060b>.

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

Zvelebil, Marketa J. and Baum, Jeremy O. 2008. *Understanding Bioinformatics*. London:

Garland Science.

[https://bibliu.com/app/#/view/books/9781136976964/pdf2htmlex/index.html#page\\_Cover](https://bibliu.com/app/#/view/books/9781136976964/pdf2htmlex/index.html#page_Cover).