

參考文獻

- 1 Wunberg, T. *et al.* Improving the hit-to-lead process: data-driven assessment of drug-like and lead-like screening hits. *Drug Discovery Today* **11**, 175-180 (2006).
- 2 Patani, G. A. & LaVoie, E. J. Bioisosterism: A Rational Approach in Drug Design. *Chemical Reviews* **96**, 3147-3176 (1996).
- 3 Ghose, A. K., Viswanadhan, V. N. & Wendoloski, J. J. A knowledge-based approach in designing combinatorial or medicinal chemistry libraries for drug discovery. 1. A qualitative and quantitative characterization of known drug databases. *Journal of Combinatorial Chemistry* **1**, 55-68 (1999).
- 4 Oprea, T. I., Davis, A. M., Teague, S. J. & Leeson, P. D. Is there a difference between leads and drugs? A historical perspective. *Journal of Chemical Information and Computer Sciences* **41**, 1308-1315 (2001).
- 5 Tanrikulu, Y. & Schneider, G. Pseudoreceptor models in drug design: bridging ligand- and receptor-based virtual screening. *Nature Reviews Drug Discovery* **7**, 667-677 (2008).
- 6 Klebe, G. Virtual ligand screening: strategies, perspectives and limitations. *Drug Discovery Today* **11**, 580-594 (2006).
- 7 Congreve, M., Murray, C. W. & Blundell, T. L. Structural biology and drug discovery. *Drug Discovery Today* **10**, 895-907 (2005).
- 8 Carr, R. A., Congreve, M., Murray, C. W. & Rees, D. C. Fragment-based lead discovery: leads by design. *Drug Discovery Today* **10**, 987-992 (2005).
- 9 Tropsha, A. & Golbraikh, A. Predictive QSAR modeling workflow, model applicability domains, and virtual screening. *Current Pharmaceutical Design* **13**, 3494-3504 (2007).
- 10 Lill, M. A. Multi-dimensional QSAR in drug discovery. *Drug Discovery Today* **12**, 1013-1017 (2007).
- 11 Khedkar, S. A., Malde, A. K., Coutinho, E. C. & Srivastava, S. Pharmacophore modeling in drug discovery and development: an overview. *Medicinal Chemistry* **3**, 187-197 (2007).
- 12 Bohacek, R., Boosalis, M. S., McMartin, C., Faller, D. V. & Perrine, S. P. Identification of novel small-molecule inducers of fetal hemoglobin using pharmacophore and 'PSEUDO' receptor models. *Chemical Biology & Drug Design* **67**, 318-328 (2006).
- 13 Ramstrom, O. & Lehn, J. M. Drug discovery by dynamic combinatorial libraries. *Nature Reviews Drug Discovery* **1**, 26-36 (2002).

- 14 Rees, D. C., Congreve, M., Murray, C. W. & Carr, R. Fragment-based lead discovery. *Nature Reviews Drug Discovery* **3**, 660-672 (2004).
- 15 Honorio, K. M., Salum, L. B., Garratt, R. C., Polikarpov, I. & Andricopulo, A. D. Two- and three-dimensional quantitative structure-activity relationships studies on a series of liver x receptor ligands. *The Open Medicinal Chemistry Journal* **2**, 87-96 (2008).
- 16 Carballeira, J. D., Quezada, M. A., Alvarez, E. & Sinisterra, J. V. High throughput screening and QSAR-3D/CoMFA: useful tools to design predictive models of substrate specificity for biocatalysts. *Molecules* **9**, 673-693 (2004).
- 17 Klebe, G., Abraham, U. & Mietzner, T. Molecular similarity indices in a comparative analysis (CoMSIA) of drug molecules to correlate and predict their biological activity. *Journal of Medicinal Chemistry* **37**, 4130-4146 (1994).
- 18 Kubinyi, H., Hamprecht, F. A. & Mietzner, T. Three-dimensional quantitative similarity-activity relationships (3D QSiAR) from SEAL similarity matrices. *Journal of Medicinal Chemistry* **41**, 2553-2564 (1998).
- 19 Sun, H. Pharmacophore-based virtual screening. *Current Medicinal Chemistry* **15**, 1018-1024 (2008).
- 20 Chen, Y. F. *et al.* SiMMap: a web server for inferring site-moiety map to recognize interaction preferences between protein pockets and compound moieties. *Nucleic Acids Research* **38**, W424-430 (2010).
- 21 Chang, S. C., Cheng, Y. Y. & Shih, S. R. Avian influenza virus: the threat of a pandemic. *Chang Gung Medical Journal* **29**, 130-134 (2006).
- 22 Liu, Y., Zhang, J. & Xu, W. Recent progress in rational drug design of neuraminidase inhibitors. *Current Medicinal Chemistry* **14**, 2872-2891 (2007).
- 23 Subbarao, K. *et al.* Characterization of an avian influenza A (H5N1) virus isolated from a child with a fatal respiratory illness. *Science* **279**, 393-396 (1998).
- 24 Tanaka, T. *et al.* Safety of neuraminidase inhibitors against novel influenza A (H1N1) in pregnant and breastfeeding women. *Canadian Medical Association Journal* **181**, 55-58 (2009).
- 25 Russell, R. J. *et al.* The structure of H5N1 avian influenza neuraminidase suggests new opportunities for drug design. *Nature* **443**, 45-49 (2006).
- 26 von Itzstein, M. *et al.* Rational design of potent sialidase-based inhibitors of influenza virus replication. *Nature* **363**, 418-423 (1993).
- 27 Maring, C. J. *et al.* Structure-based characterization and optimization of novel hydrophobic binding interactions in a series of pyrrolidine influenza neuraminidase inhibitors. *Journal of Medicinal Chemistry* **48**, 3980-3990 (2005).

- 28 Burger, R. A. *et al.* Immunological effects of the orally administered neuraminidase inhibitor oseltamivir in influenza virus-infected and uninfected mice. *Immunopharmacology* **47**, 45-52 (2000).
- 29 Klumpp, K. & Graves, B. J. Optimization of small molecule drugs binding to highly polar target sites: lessons from the discovery and development of neuraminidase inhibitors. *Current Topics in Medicinal Chemistry* **6**, 423-434 (2006).
- 30 Meindl, P., Bodo, G., Palese, P., Schulman, J. & Tuppy, H. Inhibition of neuraminidase activity by derivatives of 2-deoxy-2,3-dehydro-N-acetylneuraminic acid. *Virology* **58**, 457-463 (1974).
- 31 Moscona, A. Oseltamivir resistance--disabling our influenza defenses. *The New England Journal of Medicine* **353**, 2633-2636 (2005).
- 32 Sadowski, J., Gasteiger, J. & Klebe, G. Comparison of automatic three-dimensional model builders using 639 x-ray structures. *Journal of Chemical Information and Computer Sciences* **34**, 1000-1008 (1994).
- 33 Xu, X., Zhu, X., Dwek, R. A., Stevens, J. & Wilson, I. A. Structural characterization of the 1918 influenza virus H1N1 neuraminidase. *Journal of Virology* **82**, 10493-10501 (2008).
- 34 Yang, J.-M. & Chen, C.-C. GEMDOCK: a generic evolutionary method for molecular docking. *Proteins: Structure, Function, and Bioinformatics* **55**, 288-304 (2004).
- 35 Yang, J.-M. & Shen, T.-W. A pharmacophore-based evolutionary approach for screening selective estrogen receptor modulators. *Proteins: Structure, Function, and Bioinformatics* **59**, 205-220 (2005).
- 36 Yang, J.-M. Development and evaluation of a generic evolutionary method for protein-ligand docking. *Journal of Computational Chemistry* **25**, 843-857 (2004).
- 37 Yang, J. M., Chen, Y. F., Shen, T. W., Kristal, B. S. & Hsu, D. F. Consensus scoring criteria for improving enrichment in virtual screening. *Journal of Chemical Information and Modeling* **45**, 1134-1146 (2005).
- 38 Hung, H. C. *et al.* Aurintricarboxylic acid inhibits influenza virus neuraminidase. *Antiviral Research* **81**, 123-131 (2009).
- 39 Yang, J. M., Chen, Y. F., Tu, Y. Y., Yen, K. R. & Yang, Y. L. Combinatorial computational approaches to identify tetracycline derivatives as flavivirus inhibitors. *PLoS ONE*, e428 (2007).
- 40 Chin, K. H. *et al.* The cAMP receptor-like protein CLP is a novel c-di-GMP receptor linking cell-cell signaling to virulence gene expression in *Xanthomonas campestris*. *Journal of Molecular Biology* **396**, 646-662 (2010).

- 41 Yang, M.-C. *et al.* Rational design for crystallization of beta-lactoglobulin and vitamin D-3 complex: revealing a secondary binding site *Crystal Growth & Design* **8**, 4268-4276 (2008).
- 42 Ewing, T. J., Makino, S., Skillman, A. G. & Kuntz, I. D. DOCK 4.0: search strategies for automated molecular docking of flexible molecule databases. *Journal of Computer-Aided Molecular Design* **15**, 411-428 (2001).
- 43 Bissantz, C., Folkers, G. & Rognan, D. Protein-based virtual screening of chemical databases. 1. Evaluation of different docking/scoring combinations. *Journal of Medicinal Chemistry* **43**, 4759-4767 (2000).
- 44 Hurt, A. C., Holien, J. K. & Barr, I. G. In vitro generation of neuraminidase inhibitor resistance in A(H5N1) influenza viruses. *Antimicrobial Agents and Chemotherapy* **53**, 4433-4440 (2009).
- 45 Varghese, J. N., Epa, V. C. & Colman, P. M. Three-dimensional structure of the complex of 4-guanidino-Neu5Ac2en and influenza virus neuraminidase. *Protein Science* **4**, 1081-1087 (1995).
- 46 Ghate, A. A. & Air, G. M. Site-directed mutagenesis of catalytic residues of influenza virus neuraminidase as an aid to drug design. *European Journal of Biochemistry* **258**, 320-331 (1998).
- 47 Luo, M. Structural biology: antiviral drugs fit for a purpose. *Nature* **443**, 37-38 (2006).
- 48 Varghese, J. N. *et al.* Structural evidence for a second sialic acid binding site in avian influenza virus neuraminidases. *Proceedings of the National Academy of Sciences of the United States of America* **94**, 11808-11812 (1997).
- 49 Schneider, G. & Fechner, U. Computer-based de novo design of drug-like molecules. *Nature Reviews Drug Discovery* **4**, 649-663 (2005).

附錄

著作

期刊論文

1. Y.-F. Chen, K.-C. Hsu, S.-R. Lin, W.-C. Wang, **Y.-C. Huang** and J.-M. Yang*, " SiMMap: a web server for inferring site-moiety map to recognize interaction preferences between protein pockets and compound moieties," *Nucleic Acids Research*, 2010

