DAFTAR PUSTAKA

Berman, H.M., Bhat, T.N., Bourne, P.E., Feng, Z., Gilliland, G., Weissig, H., Westbrook, J., 2000. The Protein Data Bank and the challenge of structural genomics. **nature structural biology** 3.

Braga, R.C., Andrade, C.H., 2013. Assessing the Performance of 3D Pharmacophore Models in Virtual Screening: How Good are They? **Current Topics in Medicinal Chemistry** 13, 1127–1138. https://doi.org/10.2174/1568026611313090010

Cereto-Massagué, A., Guasch, L., Valls, C., Mulero, M., Pujadas, G., Garcia-Vallvé, S., 2012. DecoyFinder: an easy-to-use python GUI application for building target-specific decoy sets. **Bioinformatics** 28, 1661–1662. https://doi.org/10.1093/bioinformatics/bts249

Cereto-Massagué, A., Ojeda, M.J., Valls, C., Mulero, M., Garcia-Vallvé, S., Pujadas, G., 2015. Molecular fingerprint similarity search in virtual screening. **Methods** 71, 58–63. https://doi.org/10.1016/j.ymeth.2014.08.005

Chisholm-Burns, M.A., Schwinghammer, T.L., Wells, B.G., Malone, P.M., Kolesar, J.M., DiPiro, J.T., n.d. Pharmacotherapy: Principles & Practice: Fourth Edition 1663.

Dallakyan, S., Olson, A.J., 2015. Small-Molecule Library Screening by Docking with PyRx, in: Hempel, J.E., Williams, C.H., Hong, C.C.

(Eds.), **Chemical Biology**. Springer New York, New York, NY, pp. 243–250. https://doi.org/10.1007/978-1-4939-2269-7_19

Ece, A., Sevin, F., 2013. The discovery of potential cyclin A/CDK2 inhibitors: a combination of 3D QSAR pharmacophore modeling, virtual screening, and molecular docking studies. **Medicinal Chemistry Research** 22, 5832–5843. https://doi.org/10.1007/s00044-013-0571-y

Fischmann, T.O., Hruza, A., Duca, J.S., Ramanathan, L., Mayhood, T., Windsor, W.T., Le, H.V., Guzi, T.J., Dwyer, M.P., Paruch, K., Doll, R.J., Lees, E., Parry, D., Seghezzi, W., Madison, V., 2008. Structure-guided discovery of cyclin-dependent kinase inhibitors. **Biopolymers** 89, 372–379. https://doi.org/10.1002/bip.20868

Gaulton, A., Bellis, L.J., Bento, A.P., Chambers, J., Davies, M., Hersey, A., Light, Y., McGlinchey, S., Michalovich, D., Al-Lazikani, B., Overington, J.P., 2012. ChEMBL: a large-scale bioactivity database for drug discovery. **Nucleic Acids Research** 40, D1100–D1107. https://doi.org/10.1093/nar/gkr777

Irwin, J.J., Sterling, T., Mysinger, M.M., Bolstad, E.S., Coleman, R.G., 2012. ZINC: A Free Tool to Discover Chemistry for Biology. **Journal of Chemical Information and Modeling** 52, 1757–1768. https://doi.org/10.1021/ci3001277

Kemenkes (2015): Situasi Penyakit Kanker. Jakarta: Buletin Jendela Data dan Informasi Kesehatan.

Kumar, R., Garg, P., Bharatam, P.V., 2016. Pharmacoinformatics analysis to identify inhibitors of *Mtb* -ASADH. **Journal of Biomolecular Structure and Dynamics** 34, 1–14. https://doi.org/10.1080/07391102.2015.1005137

Lavecchia, A., Giovanni, C., 2013. Virtual Screening Strategies in Drug Discovery: A Critical Review. **Current Medicinal Chemistry** 20, 2839–2860. https://doi.org/10.2174/09298673113209990001

Lipinski, C.A., Lombardo, F., Dominy, B.W., Feeney, P.J., 2012. Experimental and computational approaches to estimate solubility and permeability in drug discovery and development settings. **Advanced Drug Delivery Reviews** 64, 4–17. https://doi.org/10.1016/j.addr.2012.09.019

Papadatos, G., Overington, J.P., 2014. The ChEMBL database: a taster for medicinal chemists. **Future Medicinal Chemistry** 6, 361–364. https://doi.org/10.4155/fmc.14.8

Park, Y., Hunter, D.J., Spiegelman, D., Bergkvist, L., Berrino, F., van den Brandt, P.A., Buring, J.E., Colditz, G.A., Freudenheim, J.L., Fuchs, C.S., Giovannucci, E., Goldbohm, R.A., Graham, S., Harnack, L., Hartman, A.M., Jacobs, D.R., Kato, I., Krogh, V., Leitzmann, M.F., McCullough, M.L., Miller, A.B., Pietinen, P., Rohan, T.E., Schatzkin, A., Willett, W.C., Wolk, A., Zeleniuch-Jacquotte, A., Zhang, S.M., Smith-Warner, S.A., 2005. Dietary Fiber Intake and Risk of Colorectal Cancer: A Pooled Analysis of Prospective Cohort Studies. **JAMA** 294, 2849. https://doi.org/10.1001/jama.294.22.2849

Peach, M.L., Nicklaus, M.C., 2009. Combining docking with pharmacophore filtering for improved virtual screening. **Journal of Cheminformatics** 1, 6. https://doi.org/10.1186/1758-2946-1-6

Seidel, T., Ibis, G., Bendix, F., Wolber, G., 2010. Strategies for 3D pharmacophore-based virtual screening. Drug Discovery Today: **Technologies** 7, e221–e228. https://doi.org/10.1016/j.ddtec.2010.11.004

Sotriffer, C., n.d. Virtual Screening: Principles Challenges, and Practical Guidelines: Volume 48 496.

Torre, L.A., Bray, F., Siegel, R.L., Ferlay, J., Lortet-Tieulent, J., Jemal, A., 2015. Global cancer statistics, 2012. CA: A Cancer **Journal for Clinicians** 65, 87–108. https://doi.org/10.3322/caac.21262

Trott, O., Olson, A.J., 2009. AutoDock Vina: Improving the speed and accuracy of docking with a new scoring function, efficient optimization, and multithreading. **Journal of Computational Chemistry** NA-NA. https://doi.org/10.1002/jcc.21334

Vyas, V., 2008. Virtual Screening: A Fast Tool for Drug Design. **Scientia Pharmaceutica** 76, 333–360. https://doi.org/10.3797/scipharm.0803-03

Watson, A.J.M., Collins, P.D., 2011. Colon Cancer: A Civilization Disorder. **Digestive Diseases** 29, 222–228. https://doi.org/10.1159/000323926

Wolber, G., Langer, T., 2005. LigandScout: 3-D Pharmacophores Derived from Protein-Bound Ligands and Their Use as Virtual Screening Filters. **Journal of Chemical Information and Modeling** 45, 160–169. https://doi.org/10.1021/ci049885o