

- Abraham, D. J. (Ed.). (2003). **Burgers medicinal chemistry and drug discovery**. New Jersey: Wiley.
- Abraham, E. P. and Chain, E. (1940). **An enzyme from bacteria able to destroy penicillin**. *Nature*, 146, 837.
- Adler, M., Anjum, M., Andersson, D. I., and Sandegren, L. (2013). **Influence of acquired β -lactamases on the evolution of spontaneous carbapenem resistance in *Escherichia coli***. *J Antimicrob Chemother*, 68(1), 51-59.
- Altschul, S. F., Madden, T. L., Schäffer, A. A., Zhang, J., Zhang, Z., Miller, W. and Lipman, D. J. (1997). **Gapped BLAST and PSI-BLAST: a new generation of protein database search programs**. *Nucleic Acids Res.*, 25(17), 3389-3402.
- Ambler, R. P., Coulson, A. F., Frère, J. M., Ghuysen, J. M., Joris, B., Forsman, M., Levesque, R. C., Tiraby, G. and Waley, S. G. (1991). **A standard numbering scheme for the class A beta lactamases**. *Biochem J.*, 276, 269.
- Amyes, S. (2010). **Antibacterial Chemotherapy: Theory, Problems, and Practice**. Oxford University Press.
- Anderson, A. C. (2012). **Structure-based functional design of drugs: from target to lead compound**. In *Molecular Profiling*, 359-36
- Atanasov, B. P., Mustafi, D. and Makinen, M. W. (2000). **Protonation of the β -lactam nitrogen is the trigger event in the catalytic action of class A β -lactamases**. *Proc Natl Acad Sci*, 97(7), 3160-3165.
- Babypadmini, S. and Appalaraju, B. (2004). **Extended spectrum beta-lactamases in urinary isolates of *Escherichia coli* and *Klebsiella pneumoniae* - Prevalence and susceptibility pattern in a tertiary care hospital**. *Indian J Med Microbiol.*, 22, 172-174.

- Baig, M. H., Danishuddin, M., Khan, S., and Khan, A. U. (2012). **Screening of inhibitors for S130G inhibitor resistant mutants of TEM type beta-lactamase.** *Bioinformation*, 8(24), 1225.
- Barry G. H. and Barlow, M. (2005). **Revised Ambler classification of b-lactamases.** *J Antimicrob Chemother*, 1050.
- Bayat, A. (2002). **Science, medicine, and the future: Bioinformatics.** *BMJ: British Medical Journal*, 324(7344). 1018.
- Bebrone, C. (2007). **Metallo-β-lactamases (classification, activity, genetic organization, structure, zinc coordination) and their superfamily.** *Biochem Pharmacol.*, 74(12), 1686-1701.
- Bennett, J. W. and Chung, K. T. (2001). **Alexander Fleming and the discovery of Penicillin.** *Adv app microbial.*, 49, 163-184.
- Berman, H. M., Westbrook, J., Feng, Z., Gilliland, G., Bhat, T. N., Weissig, H., Shindyalov, I. N. and Bourne, P. E. (2000). **The protein data bank.** *Nucleic Acids Res.*, 28(1), 235-242.
- Bethel, C. R., Taracila, M., Shyr, T., Thomson, J. M., Distler, A. M., Hujer, K. M., Endimiani, A., Papp-Wallace, K., Bonnet, R. and Bonomo, R. A. (2011). **Exploring the inhibition of CTX-M-9 by β-lactamase inhibitors and carbapenems.** *Antimicrob Agents Chemother.*, 55(7). 3465-3475.
- Blazquez, J., Baquero, M. R., Canton, R., Alos, I. and Baquero. F. (1993). **Characterization of a new TEM-type β-lactamase resistant to clavulanate, sulbactam, and tazobactam in a clinical isolate of Escherichia coli.** *Antimicrob Agents Chemother.*, 37, 2059-2063.
- Böhm, H. J. (1998). **Prediction of binding constants of protein ligands: a fast method for the prioritization of hits obtained from de novo design or 3D database search programs.** *J Comput Aided Mol Des.*, 12(4). 309-309.

- Bonnet, R. (2004). **Growing group of extended-spectrum β -lactamases: the CTX-M enzymes.** *Antimicrob Agents Chemother.*, 48,1-14.
- Bonomo, R. A. and L. B. Rice. (1999). **Inhibitor resistant class A β -lactamases.** *Front Biosci.*, 4, 34-41.
- Bös, F., and Pleiss, J. (2008). **Conserved water molecules stabilize the Ω -loop in class A β -lactamases.** *Antimicrob Agents Chemother.*, 52(3), 1072-1079.
- Bouthors, A. T., Delettré, J., Mugnier, P., Jarlier, V., and Sougakoff, W. (1999). **Site-directed mutagenesis of residues 164, 170, 171, 179, 220, 237 and 242 in PER-1 β -lactamase hydrolysing expanded-spectrum cephalosporins.** *Protein engineering*, 12(4), 313-318.
- Bradford, P. A. (2001). **Extended-spectrum β -lactamases in the 21st century: characterization, epidemiology, and detection of this important resistance threat.** *Clin.microbiol. rev.*, 14, 933-951.
- Brady, S. F., Stauffer, K. J., Lumma, W. C., Smith, G. M., Ramjit, H. G., Lewis, S. D., Lucas, B. J., Gardell, S. J., Lyle, E. A., Appleby, S. D., Cook, J. J., Holahan, M. A., Stranieri, M. T., Lynch, Jr. J. J., Lin, J. H., Chen, I. W., Vastag, K., Naylor-Olsen, A. M. and Vacca, J. P. (1998). **Solid phase synthesis Interleukin-1b.** *J Med Chem.*, 41, 401-406.
- Brooks, B. R., Bruccoleri, R. E., Olafson, B. D., Swaminathan, S., and Karplus, M. (1983). **CHARMM: A program for macromolecular energy, minimization, and dynamics calculations.** *J Comput Chem.*, 4(2), 187-217.
- *J Comput Chem.* Brown, A. G. (1986). **Clavulanic acid, a novel β -lactamase inhibitor-a case study in drug discovery and development.** *Drug Des Deliv.* 1, 1-21.
- Bush K. (1988) **Beta-lactamase inhibitors from laboratory to clinic.** *Clin Microbiol Rev.* (1):109-23.

- Bush, K. and Jacoby, G. A. (2010). **Updated functional classification of β -lactamases.** *Antimicrob Agents Chemother.*, 54, 969-976.
- Bush, K., and Macielag, M. J. (2010). **New β -lactam antibiotics and β -lactamase inhibitors.** *Expert Opin Ther Pat.*, 20(10), 1277-1293.
- Bush, K., Jacoby, G. A. and Medeiros, A. A. (1995). **A functional classification scheme for β -lactamases and its correlation with molecular structure.** *Antimicrob Agents Chemother.* 39, 1211–1233.
- Buynak, J. D. (2006). **Understanding the longevity of the β -lactam antibiotics and of antibiotic/ β -lactamase inhibitor combinations.** *Biochem Pharmacol.*, 71, 930-940.
- Cantón. R., Morosini. M.I., de la Maza, O.M. and de la Pedrosa, E.G. (2008). **IRT and CMT beta-lactamases and inhibitor resistance.** *Clin Microbiol Infect.* Suppl 1:53-62.
- Chaibi, E. B., Sirot, D., Paul, G., and Labia, R. (1999). **Inhibitor-resistant TEM β -lactamases: phenotypic, genetic and biochemical characteristics.** *J Antimicrob Chemother*, 43(4), 447-458.
- Chambers, H. F. (1997). **Methicillin resistance in staphylococci: molecular and biochemical basis and clinical implications.** *Clin Microbiol Rev.* 10, 781-791.
- Chiu, C. H., Peng, M. Y., Wang, Y. C., and Chang, F. Y. (2009). **Endogenous Endophthalmitis Caused by *Citrobacter koseri*.** *Am J Med Sci.*, 338(6), 509-510.
- Chopra, I., Schofield, C., Everett, M., O'Neill, A., Miller, K., Wilcox, M., Frère, J.M., Dawson, M., Czaplewski, L., Urleb, U., and Courvalin, P. (2008). **Treatment of health-care-associated infections caused by Gram-negative bacteria: a consensus statement.** *Lancet Infect Dis.*, 8, 133-139.
- Collatz, E., Labia, R. and Gutmann, L. (1990). **Molecular evolution of ubiquitous β -lactamases towards extended-spectrum enzymes active against newer β -lactam antibiotics.** *Mol Microbiol.*, 4, 10, 1615-1620.

- Connolly, T. M. (2005). **Database systems: a practical approach to design, implementation, and management.** Pearson Education.
- Crichlow, G.V, Nukaga, M., Doppalapudi, V.R., Buynak, J.D. and Knox, J.R. (2001). **Inhibition of class C beta-lactamases: structure of a reaction intermediate with a cephem sulfone.** *Biochemistry*. 29; 40(21):6233-9.
- Cross, S. S. (2005). **Improved FlexX docking using FlexS-determined base fragment placement.** *J Chem Inf Model.*, 45(4). 993-1001.
- Danishuddin, M., Khan, A., Faheem, M., Kalaiarasan, P., Hassan Baig, M., Subbarao, N., and Khan, A. U. (2013). **Structure-based screening of inhibitors against KPC-2: designing potential drug candidates against multidrug-resistant bacteria.** *J Biomol Struct Dyn.*, (ahead-of-print), 1-10.
- Datta, N. and Kontomichalou, P. (1965). **Penicillinase synthesis controlled by infectious R factors in *Enterobacteriaceae*.** *Nature*, 208, 239-241.
- Davies, J. and Davies, D. (2010). **Origins and evolution of antibiotic resistance.** *Microbiol Mol Biol Rev.* 74, 417-433.
- de Beer, S., Vermeulen, N. P., and Oostenbrink, C. (2010). **The role of water molecules in computational drug design.** *Curr Top Med Chem.*, 10(1), 55-66.
- De Wals, P. Y., Doucet, N. and Pelletier, J. N. (2009). **High tolerance to simultaneous active-site mutations in TEM-1 β -lactamase: Distinct mutational paths provide more generalized β -lactam recognition.** *Protein Sci.*, 18(1), 147-160.
- Dehouck, Y., Grosfils, A., Folch, B., Gilis, D., Bogaerts, P. and Rooman, M. (2009). **Fast and accurate predictions of protein stability changes upon mutations using statistical potentials and neural networks: PoPMuSiC-2.0.** *Bioinformatics*, 25(19), 2537-2543.
- Desiraju G.R. (2005). **C-H...O and other weak hydrogen bonds. From crystal engineering to virtual screening.** *Chem Commun.*, 28, 2995-3001.

- Doman, T. N. McGovern, S. L., Witherbee, B. J., Kastern, T. P., Kurumbail, R., Stallings, W. C. and Connolly, D. T. (2002). **Docking may be competitive with HTS as a discovery method.** *J Med Chem.*, 45, 2213-2221.
- Donowitz, G. R. and Mandell, G. L. (1988). **β -Lactam antibiotics (1).** *N Engl J Med.*, 318, 419-426.
- Doubet, S., Bock, K., and Smith, D. Darvill. A. and Albersheim, P.(1989). **The complex carbohydrate structure database.** *Trends Biochem Sci.*, 14, 475-477.
- Drawz, S. M., and Bonomo, R. A. (2010). **Three decades of β -lactamase inhibitors.** *Clin.microbiol. rev.*, 23(1), 160-201.
- Dror, O., Shulman-Peleg, A., Nussinov, R., & Wolfson, H. J. (2006). **Predicting molecular interactions in silico: I. an updated guide to pharmacophore identification and its applications to drug design.** *Curr Med Chem.*, 3(1), 551-584.
- Dubois, V., Poirel, L., Arpin, C., Coulangue, L., Bebear, C., Nordmann, P., & Quentin, C. (2004). **SHV-49, a novel inhibitor-resistant β -lactamase in a clinical isolate of *Klebsiella pneumoniae*.** *Antimicrob Agents Chemother*, 48(11), 4466-4469.
- EARS-Net (2010) **Antimicrobial resistance surveillance in Europe 2009.** Annual Report of the European Antimicrobial Resistance Surveillance Network (EARS-Net). Stockholm, Sweden: European Centre for Disease Prevention and Control (ECDC).
- Eliopoulos, G. M. and Bush, K. (2001). **New β -lactamases in gram-negative bacteria: diversity and impact on the selection of antimicrobial therapy.** *Clin Infect Dis.*, 32(7), 1085-1089.
- Ellerby, L. M., Escobar, W. A., Fink, A. L., Mitchinson, C., and Wells, J. A. (1990). **The role of lysine-234 in. beta.-lactamase catalysis probed by site-directed mutagenesis.** *Biochemistry*, 29(24). 5797-5806.
- Ewig, C. S., Berry, R., Dinur, U., Hill, J. R., and Hwang, M. J. (2001). **Derivation of class II force fields. VIII. Derivation of a general quantum mechanical force field for organic compounds.** *J Comput Chem.*, 22, 80 1782–1800.

- Fang, X., and Wang, S. (2002). **A web-based 3D-database pharmacophore searching tool for drug discovery.** *J Chem Inf Comput Sci.*, 42(2). 192-198.
- Finlay, J., Miller, L. and Poupard, J. A. (2003). **A review of the antimicrobial activity of clavulanate.** *J Antimicrob Chemother.*, 52, 18-23.
- Fisher, J. F., Meroueh, S. O. and Mobashery, S. (2005). **Bacterial resistance to β -lactam antibiotics: compelling opportunism, compelling opportunity.** *Chem Rev.* 105, 395-424.
- Friesner, R. A., Banks, J. L., Murphy, R. B., Halgren, T. A., Klicic, J. J., Mainz, D. T., and Shenkin, P. S. (2004). **Glide: a new approach for rapid, accurate docking and scoring. 1. Method and assessment of docking accuracy.** *J Med Chem.*, 47(7). 1739-1749.
- G. R. and Mandell, G. L. (1988). **β -Lactam antibiotics (1).** *N Engl J Med.*, 318: 419-426.
- Geddes, A. (2008). **80th Anniversary of the discovery of penicillin: An appreciation of Sir Alexander Fleming.** *Int J Antimicrob Agents*, 32, 373.
- Georgopapadakou, N. H., and Liu, F. Y. (1980). **Penicillin-binding proteins in bacteria.** *Antimicrob Agents Chemother.*, 18(1). 148-157.
- Ghuysen, J. M. (1988). **Bacterial active-site serine penicillin-interactive proteins and domains: mechanism, structure, and evolution.** *Rev Infect Dis.* 10, 726-732.
- Ghuysen, J. M. (1991). **Serine beta-lactamases and penicillin-binding proteins.** *Ann. Rev.s Microbiol.*, 45(1), 37-67.
- Ghuysen, J. M. (1991). **Serine β -lactamases and penicillin-binding proteins.** *Annu Rev Microbiol.*, 45, 37-67.
- Gniadkowski, M. (2008). **Evolution of extended-spectrum β -lactamases by mutation.** *Clin Microbiol Infect.*, 14, 11-32.

- Gohlke, H., Hendlich, M., and Klebe, G. (2000). **Knowledge-based scoring function to predict protein-ligand interactions.** *J Mol Biol.*, 295(2). 337-356.
- Gohlke, H., Hendlich, M., and Kelbe, G. (2000). **Characterization of the proneural gene regulatory network.** *J Mol Biol.* 295, 337-356.
- Goldsworthy, P. D. and McFarlane, A. C. (2002). **Howard Florey, Alexander Fleming and the fairy tale of penicillin.** *Med J.*, 176, 176-178.
- Gong, S., Worth, C., Bickerton, G. R., Lee, S., Tanramluk, D. and Blundell, T. (2009). **Structural and functional restraints in the evolution of protein families and superfamilies.** *Biochem Soc Trans.*, 37(4), 727.
- González-Pons, M., Szeto, A. C., González-Méndez, R., and Serrano, A. E. (2009). **Identification and bioinformatic characterization of a multidrug resistance associated protein (ABCC) gene in Plasmodium berghei.** *Malaria journal*, 8(1). 1.
- Gootz, T. D. (2004). **Global dissemination of beta-lactamases mediating resistance to cephalosporins and carbapenems.** *Expert Rev Anti Infect Ther.*, 2, 317-327.
- Gorbach, S. L. (1994). **Antibiotic treatment of anaerobic infections.** *Clin Infect Dis.*, 4, S305-310.
- Gorbach, S. L. (1994). **Piperacillin/tazobactam in the treatment of polymicrobial infections.** *Intensive Care Med.*, 20(3), S27-S34.
- Güner, O. F. (Ed.). (2000). *Pharmacophore: Perception, Development, and Use in Drug Design (Vol. 2)*. Internatl University Line.
- Gupta, K., and Stamm, W. E. (2002). **Outcomes associated with trimethoprim/sulphamethoxazole (TMP/SMX) therapy in TMP/SMX resistant community-acquired UTI.** *Int J Antimicrob Agents.*, 19(6), 554-556.
- Guyot, A., Barrett, S. P., Threlfall, E. J., Hampton, M. D., and Cheasty, T. (1999). **Molecular epidemiology of multi-resistant Escherichia coli.** *J Hosp Infect.*, 43(1), 39-48.

- Halgren, T. A., Murphy, R. B., Friesner, R. A., Beard, H. S., Frye, L. L., Pollard, W. T., and Banks, J. L. (2004). **Glide: a new approach for rapid, accurate docking and scoring. 2. Enrichment factors in database screening.** *J Med Chem.*, 47(7). 1750-1759.
- Haque, S.F., Ali, S.Z., T.P.M. and Khan, A.U. (2012). **Prevalence of plasmid mediated blaTEM-1 and blaCTX-M-15 type extended spectrum beta-lactamases in patients with sepsis.** *Asian Pac J Trop Med.*, 5.2 (2012), 98-102.
- Hashim, A., Khan, M. S., Khan, M. S., Baig, M. H., and Ahmad, S. (2013). **Antioxidant and α -Amylase Inhibitory Property of Phyllanthus virgatus L.: An In Vitro and Molecular Interaction Study.** *Biomed Res Int.*, 2013.
- Helfand, M. S. and Bonomo, R. A. (2005). **Current challenges in antimicrobial chemotherapy: the impact of extended-spectrum β -lactamases and metallo- β -lactamases on the treatment of resistant Gram-negative pathogens.** *Curr Opin Pharmacol.*, 5, 452-458.
- Helfand, M. S., Bethel, C. R., Hujer, A. M., Hujer, K. M., Anderson, V. E. and Bonomo, R. A. (2003). **Understanding resistance to beta-lactams and beta-lactamase inhibitors in the SHV beta-lactamase: lessons from the mutagenesis of SER-130.** *J Biol Chem.*, 278(52), 52724-52729.
- Hevener, K. E., Zhao, W., Ball, D. M., Babaoglu, K., Qi, J., White, S. W., and Lee, R. E. (2009). **Validation of molecular docking programs for virtual screening against dihydropteroate synthase.** *J Chem Inf Model.*, 49(2), 444-460.
- Holliday, J. and Willet, P. J. (1997). **Identification of common structural features in sets.** *Mol Graphics Modell.* 15, 203–253.
- Holloway, M. K., Wai, J. M., Halgren, T. A., Fitzgerald, P. M., Vacca, J. P., Dorsey, B. D., Levin, R.B., Thompson, W.J., Chen, L.J., and Chen, L. J. (1995). **A priori prediction of activity for HIV-1 protease inhibitors employing energy minimization in the active site.** *J Med Chem.*, 38(2). 305-317.

- Horowitz, S. and Trievel, R. C. (2012). **Carbon-Oxygen Hydrogen Bonding in Biological Structure and Function.** *J Biol Chem.*, 287(50), 41576-41582.
- Hsieh, J. H., Wang, X. S., Teotico, D., Golbraikh, A., and Tropsha, A. (2008). **Differentiation of AmpC beta-lactamase binders vs. decoys using classification kNN QSAR modeling and application of the QSAR classifier to virtual screening.** *J Comput Aided Mol Des.*, 22(9), 593-609.
- Huang, K.Y., Chia, J.H., Chiang, C.Y., Wu, T.L., Su, L.H., Jaing, T.H., Lin, T.Y., and Chiu, C.H., (2009). **Prolonged fecal shedding of CTX-M-15-producing Escherichia coli and recurrent sepsis in a patient after cord blood stem-cell transplantation.** *Scand J Infect Dis.*, 41(3), 224-227.
- Hujer, A. M., Hujer, K. M., Helfand, M. S., Anderson, V. E., and Bonomo, R. A. (2002). **Amino acid substitutions at Ambler position Gly238 in the SHV-1 β -lactamase: exploring sequence requirements for resistance to penicillins and cephalosporins.** *Antimicrob Agents Chemother.*, 46(12), 3971-3977.
- Huletsky, A., Knox, J. R. and Levesque, R. C. (1993). **Role of Ser-238 and Lys-240 in the hydrolysis of third-generation cephalosporins by SHV-type β -lactamases probed by site-directed mutagenesis and three-dimensional modeling.** *J Biol Chem.*, 268, 3690-3697.
- Imtiaz, U., Billings, E. M., Knox, J. R. and Mobashery, S. (1994). **A Structure-Based Analysis of the Inhibition of Class A. beta.-Lactamases by Sulbactam.** *Biochemistry*, 33(19), 5728-5738.
- Irwin, J. J., and Shoichet, B. K. (2005). **ZINC-a free database of commercially available compounds for virtual screening.** *J Chem Inf Model.*, 45(1), 177-182.
- Jacob, F., Joris, B., Lepage, S., Dusart, J. and Frère, J. M. (1990). **Role of the conserved amino acids of the 'SDN' loop (Ser130, Asp131 and Asn132) in a class A beta-lactamase studied by site-directed mutagenesis.** *Biochem. J*, 271, 399-406.

- Jacoby, G. A. and Carreras, I. (1990). **Activities of β -lactam antibiotics against *E. coli* strains producing extended-spectrum β -lactamases.** *Antimicrob Agents Chemother.*, 34, 858-862.
- Jacoby, G. A. and Medeiros, A. A. (1991). **More extended-spectrum beta-lactamases.** *Antimicrob Agents Chemother.*, 35(9). 1697.
- Jacoby, G. A.; Mills, D. M. and Chow, N. (2004). **Role of beta-lactamases and porins in resistance to ertapenem and other beta-lactams in *Klebsiella pneumoniae*.** *Antimicrob Agents Chemother.*, 48, 3203-3206.
- Jan, W.R. and Niels, H. (2007). **Class A carbapenemases.** *J Antimicrob Chemother.* 60, 470–482.
- Jones, G., Willett, P. and Glen, R.C. (1995). **Molecular recognition of receptor sites using a genetic algorithm with a description of desolvation.** *J Mol Biol.* 245, 43-53.
- Jones, G., Willett, P., Glen, R. C., Leach, A. R., and Taylor, R. (1997). **Development and validation of a genetic algorithm for flexible docking.** *J Mol Biol.*, 267(3). 727-748.
- Jones, S., & Thornton, J. M. (1997). **Analysis of protein-protein interaction sites using surface patches.** *J Mol Biol.*, 272(1). 121-132.
- Khan, A.U. and Nordmann, P. (2012). **Spread of carbapenemase NDM-1 producers: the situation in India and what may be proposed.** *Scand J Infect Dis.* 44, 531-535.
- Kitchen, D. B., Decornez, H., Furr, J. R., and Bajorath, J. (2004). **Docking and scoring in virtual screening for drug discovery: methods and applications.** *Nat Rev Drug Discov.*, 3(11), 935-949.
- Knothe, H., Shah, P. D. P., Krcmery, V., Antal, M., and Mitsuhashi, S. (1983). **Transferable resistance to cefotaxime, cefoxitin, cefamandole and cefuroxime in**

- clinical isolates of *Klebsiella pneumoniae* and *Serratia marcescens*. *Infection*, 11(6), 315-317.
- Knowles, J.R. (1985). **Penicillin resistance: the chemistry of β -lactamase inhibition.** *Accounts Chem Res.* 18, 97-104.
 - Knox, J.R. (1995). **Extended-spectrum and inhibitor-resistant TEM-type beta-lactamases: mutations specificity and three-dimensional structure.** *Antimicrob Agents Chemother.*, 39, 2593–2601.
 - Kramer, B., Rarey, M., and Lengauer, T. (1999). **Evaluation of the FLEXX incremental construction algorithm for protein–ligand docking.** *Proteins*, 37(2). 228-241.
 - Kroemer, R.T., Doughty, S.W., Robinson, A.J. and Richards, W.G. (1996). **Prediction of the three-dimensional structure of human interleukin-7 by homology modeling.** *Protein Eng.*, (6):493-8.
 - Kumar, K. M., Lavanya, P., Anbarasu, A. and Ramaiah, S. (2013). **Molecular dynamics and molecular docking studies on E166A point mutant, R274N/R276N double mutant, and E166A/R274N/R276N triple mutant forms of class A β -lactamases.** *J Biomol Struct Dyn.*, (ahead-of-print), 1-16.
 - Kuzin, A. P., Nukaga, M., Nukaga, Y., Hujer, A., Bonomo, R. A. and Knox, J. R. (2001). **Inhibition of the SHV-1 β -lactamase by sulfones: crystallographic observation of two reaction intermediates with tazobactam.** *Biochemistry*, 40(6), 1861-1866.
 - Ladbury, J. E. (1996). **Just add water! The effect of water on the specificity of protein-ligand binding sites And its potential application to drug design.** *Chem. Biol.*, 3, 973-980.
 - Lamotte-Brasseur, J., Dive, G., Dideberg, O., Charlier, P., Frère, J. M., and Ghuysen, J. M. (1991). **Mechanism of acyl transfer by the class A serine beta-lactamase of *Streptomyces albus* G.** *Biochem. J*, 279, 213-221.

- Laskowski, R. A.; Hutchinson, E. G.; Michie, A. D.; Wallace, A. C.; Jones, M. L.; and Thornton, J. M.; (1997). **PDBsum: a Web-based database of summaries and analyses of all PDB structures.** *Trends Biochem. Sci.*, 1997, 22, 488-90.
- Lawton, J. R., Martinez, F. A., and Burks, C. (1989). **Overview of the LiMB database.** *Nucleic Acids Res.*, 17(15). 5885-5889.
- Lee, N., Yuen, K. Y. and Kumana, C. R. (2003). **Clinical role of β -lactam/ β -lactamase inhibitor combinations.** *Drugs*, 63(14), 1511-1524.
- Leflon-Guibout, V., Ternat, G., Heym, B., and Nicolas-Chanoine, M. H. (2002). **Exposure to co-amoxiclav as a risk factor for co-amoxiclav-resistant Escherichia coli urinary tract infection.** *J Antimicrob Chemother.*, 49(2). 367-371.
- Lenfant, F., Labia, R., and Masson, J. M. (1991). **Replacement of lysine 234 affects transition state stabilization in the active site of beta-lactamase TEM1.** *J Biol Chem.*, 266(26). 17187-17194.
- Li, Z., and Lazaridis, T. (2007). **Water at biomolecular binding interfaces.** *Phys Chem Chem Phys.*, 9(5), 573-581.
- Lipinski, C. A. (2004). **Lead-and drug-like compounds: the rule-of-five revolution.** *Drug Discov Today.: Technologies*, 1(4), 337-341.
- Liu, B. and Pop, M. (2009). **ARDB—Antibiotic Resistance Genes Database.** *Nucleic Acids Res.*, 37 D443–D447.
- Livermore, D. M. (1995). **β -Lactamases in laboratory and clinical resistance.** *Clin Microbiol Rev.*, 8, 557-584.
- Livermore, D. M. (2001). **Of Pseudomonas, porins, pumps and carbapenems.** *J Antimicrob Chemother.*, 47(3), 247-250.
- Livermore, D. M. and Williams, J. D. (1996). **Mode of action and mechanisms of bacterial resistance.** In V. Lorian (Ed.). *Antibiotics in Laboratory Medicine*, 4th Ed. New York. *Williams and Wilkins, Baltimore*. 4, 502-578.

- Lu, Y., Wang, Y., Xu, Z., Yan, X., Luo, X., Jiang, H., and Zhu, W. (2009). **C–X···H Contacts in Biomolecular Systems: How They Contribute to Protein–Ligand Binding Affinity.** *J Phys Chem B.*, 113(37), 12615-12621.
- Mandell, G. L. (Ed.). (2005). **Mandell, Douglas, and Bennett's principles and practice of infectious diseases.**
- Martinez, J. L. E., Cercenado, M., Rodriguez-Creixems, M. F., Vicente-Perez, A., Delgado-Iribarren, and Baquero F. (1987). **Resistance to β -lactam/clavulanate.** *Lancet* 2, 1473.
- Martinez, J. L., Vicente, M. F., Delgado-Iribarren, A., Perez-Diaz, J. C., and Baquero, F. (1989). **Small plasmids are involved in amoxicillin-clavulanate resistance in *Escherichia coli*.** *Antimicrob Agents Chemother.*, 33(4), 595.
- Massova, I., and Mobashery, S. (1998). **Kinship and diversification of bacterial penicillin-binding proteins and β -lactamases.** *Antimicrob Agents Chemother.*, 42(1), 1-17.
- Matagne, A., Lamotte-Brasseur, J., and Frere, J. (1998). **Catalytic properties of class A β -lactamases: efficiency and diversity.** *Biochem. J.*, 330, 581-598.
- Matthew, M.; Hedges, R. W. and Smith, J. T. (1979). **Types of β -lactamase determined by plasmids in gram-negative bacteria.** *J Bacteriol.*, 138, 657-662.
- Medeiros, A. A. (1997). **Evolution and dissemination of β -lactamases accelerated by generations of β -lactam antibiotics.** *Clin Infect Dis.*, 24, S19-45.
- Mendonça, N., Manageiro, V., Robin, F., Salgado, M. J., Ferreira, E., Caniça, M., and Bonnet, R. (2008). **The Lys234Arg substitution in the enzyme SHV-72 is a determinant for resistance to clavulanic acid inhibition.** *Antimicrob Agents Chemother.*, 52(5), 1806-1811.
- Meroueh, S. O., Roblin, P., Golemi, D., Maveyraud, L., Vakulenko, S. B., Zhang, Y. and Mobashery, S. (2002). **Molecular Dynamics at the Root of Expansion of**

Function in the M69L Inhibitor-Resistant TEM β -Lactamase from Escherichia coli. *J Am Chem Soc.*, 124(32), 9422-9430.

- Messaoudi, A., Belguith, H., and Hamida, J. B. (2013). **Homology modeling and virtual screening approaches to identify potent inhibitors of VEB-1 β -lactamase.** *Theor Biol Med Model.*, 10(1), 22.
- Minarini, L. A., Gales, A. C., Palazzo, I. C., and Darini, A. L. C. (2007). **Prevalence of community-occurring extended spectrum β -lactamase-producing Enterobacteriaceae in Brazil.** *Curr Microbiol.*, 54(5), 335-341.
- Mohan, V., Gibbs, A. C., Cummings, M. D., Jaeger, E. P., and DesJarlais, R. L. (2005). **Docking: successes and challenges.** *Curr Pharm Des.*, 11(3), 323-333.
- Morris, G.M.; Huey, R and Olson, A.J. (2008). **Using AutoDock for ligand-receptor docking.** *Curr Protoc Bioinformatics.*, Dec;Chapter 8: Unit 8.14. doi: 10.1002/0471250953.bi0814s24.
- Muegge, I. (2006). **PMF scoring revisited.** *J Med Chem.*, 49(20), 5895-5902.
- Murray, P. R. and Pfaller, M. A. (2005). Rosenthal KS (2005) Medical Microbiology, 5th edn. Philadelphia, USA. *Elsevier/Mosby*.
- Naas, T., Poirel, V. and Nordmann, P. (2008). **Minor extended-spectrum β -lactamases.** *Clin. Microbiol. Infect.*, 14, 42–52.
- Nagpal, I., Raj, I., Subbarao, N., and Gourinath, S. (2012). **Virtual screening, identification and in vitro testing of novel inhibitors of O-acetyl-L-serine sulfhydrylase of Entamoeba histolytica.** *PLoS one*, 7(2), e30305.
- Ness, S.; Martin, R.; Kindler, A.M.; Paetzel, M.; Gold, M.; Jensen, S.E.; Jones, J.B.; and Strynadka, N.C. (2000). **Structure-based design guides the improved efficacy of deacylation transition state analogue inhibitors of TEM-1 beta-Lactamase.** *Biochemistry.*, 9;39(18):5312-21.

- Nichols, D. A., Jaishankar, P., Larson, W., Smith, E., Liu, G., Beyrouthy, R. and Chen, Y. (2012). **Structure-based design of potent and ligand-efficient inhibitors of CTX-M class A β -lactamase.** *J Med Chem.*, 8, 2163–2172.
- Nikaido, H. (1998). **Multiple antibiotic resistance and efflux.** *Curr Opin Microbiol.*, 1, 516-523.
- Nisius, L. and Grzesiek, S. (2012). **Key stabilizing elements of protein structure identified through pressure and temperature perturbation of its hydrogen bond network.** *Nat Chem.*, 4(9), 711-717.
- Ohlson, S. (2008). **Designing transient binding drugs: a new concept for drug discovery.** *Drug Discov Today.*, 13(9), 433-439.
- Oliphant, A.R. and Struhl, K. (1989). **An efficient method for generating proteins with altered enzymatic properties: Application to β -lactamase.** *Proc Natl Acad Sci U.S.A.*, 86, 9094-9098.
- Pagan-Rodriguez, D., Zhou, X., Simmons, R., Bethel, C. R., Hujer, A. M., Helfand, M. S. and Bonomo, R. A. (2004). **Tazobactam Inactivation of SHV-1 and the Inhibitor-resistant Ser130→ Gly SHV-1 β -Lactamase INSIGHTS INTO THE MECHANISM OF INHIBITION.** *J Biol Chem.*, 279(19), 19494-19501.
- Page, M.I. (1999). **The reactivity of beta-lactams, the mechanism of catalysis and the inhibition of beta-lactamases.** *Curr Pharm Des.* (11):895-913.
- Page, M. G. (2000). **β -Lactamase inhibitors.** *Drug Resist. Updat.* 3, 109-125.
- Papp-Wallace, K. M., Bethel, C. R., Distler, A. M., Kasuboski, C., Taracila, M., and Bonomo, R. A. (2010). **Inhibitor resistance in the KPC-2 β -lactamase, a preeminent property of this class A β -lactamase.** *Antimicrob Agents Chemother.*, 54(2), 890-897.
- Parasakthi, N. and Ariffin, H. (eds.). (2001). **Consensus Guidelines for the Management of Infections by ESBL-Producing Bacteria.** Joint publication by the Ministry of Health, Malaysia, Academy of Medicine of Malaysia, Malaysian Society

of Infectious Diseases. and Chemotherapy, 2001; available from: <http://www.acadmed.org.my/html/cpg.htm>, accessed on 14-08-09.

- Parthiban, V., Gromiha, M. M. and Schomburg, D. (2006). **CUPSAT: prediction of protein stability upon point mutations.** *Nucleic Acids Res.*, 34(suppl 2), W239-W242.
- Paterson, D. L. and Bonomo, R. A. (2005). **Extended-spectrum β -lactamases: a clinical update.** *Clin Microbiol Rev.*, 18, 657-686.
- Paterson, D. L., Hujer, K. M., Hujer, A. M., Yeiser, B., Bonomo, M. D., Rice, L. B., & Bonomo, R. A. (2003). **Extended-spectrum β -lactamases in *Klebsiella pneumoniae* bloodstream isolates from seven countries: dominance and widespread prevalence of SHV- and CTX-M-type β -lactamases.** *Antimicrob Agents Chemother.*, 47(11), 3554-3560.
- Pattanaik, P., Bethel, C. R., Hujer, A. M., Hujer, K. M., Distler, A. M., Taracila, M. And Bonomo, R. A. (2009). **Strategic design of an effective β -lactamase inhibitor In-1-255, a 6-alkylidene-2'-substituted penicillin sulfone.** *J Biol Chem.*, 284(2), 945-953.
- Payne, D. J., Cramp, R., Winstanley, D. J., and Knowles, D. J. (1994). **Comparative activities of clavulanic acid, sulbactam, and tazobactam against clinically important beta-lactamases.** *Antimicrob Agents Chemother.*, 38(4), 767-772.
- Pfaller, M. A. and Segreti, J. (2006). **Overview of the epidemiological profile and laboratory detection of extended-spectrum β -lactamases.** *Clin Infect Dis.*, 42, S153-163.
- Philippon, A., Labia, R. and Jacoby G. (1989). **Extended-spectrum beta-lactamases.** *Antimicrob Agents Chemother.*, 33(8), 1131.
- Pitton, J. S. (1972). **Mechanisms of bacterial resistance to antibiotics.** *Ergeb Physiol.*, 65, 15-93.

- Poole, K. (2002). **Mechanisms of bacterial biocide and antibiotic resistance.** *J Appl Microbiol.*, 92(s1). 55S-64S.
- Poole, K. (2004). **Efflux-mediated multiresistance in Gram-negative bacteria.** *Clin Microbiol Infect.*, 10(1), 12-26.
- Reading, C. and Cole, M. (1977). **Clavulanic acid: a β -lactamase-inhibiting β -lactam from *Streptomyces clavuligerus*.** *Antimicrob Agents Chemother.*, 11, 852-857.
- Roemer, T., Schneider, T. and Pinho, M. G. (2013). **Auxiliary factors: a chink in the armor of MRSA resistance to β -lactam antibiotics.** *Curr Opin Microbiol.*, 16(5). 538-48.
- Rognan, D. (2007). **Chemogenomic approaches to rational drug design.** *Br J Pharmacol.*, 152(1). 38-52.
- Rolinson, G. N. (1998). **Forty years of β -lactam research.** *J Antimicrob Chemother.*, 41, 589-603.
- Roy, C., Segura, C., Tirado, M., Reig, R., Hermida, M., Teruel, D., and Foz, A. (1985). **Frequency of plasmid-determined beta-lactamases in 680 consecutively isolated strains of Enterobacteriaceae.** *Eur J Clin Microbiol Infect Dis.*, 4(2), 146-147.
- Roy, K. K., Singh, S., and Saxena, A. K. (2011). **Integration-mediated prediction enrichment of quantitative model for Hsp90 inhibitors as anti-cancer agents: 3D-QSAR study.** *Mol divers*, 15(2). 477-489.
- Sader, H. S., Jones, R. N., Gales, A. C., Winokur, P., Kugler, K. C., Pfaller, M. A., and Doern, G. V. (1998). **Antimicrobial susceptibility patterns for pathogens isolated from patients in Latin American medical centers with a diagnosis of pneumonia: analysis of results from the SENTRY Antimicrobial Surveillance Program (1997).** *Diagn Microbiol Infect Dis.*, 32(4), 289-301.
- Sanders, C. C., Iaconis, J. P., Bodey, G. P., and Samonis, G. (1988). **Resistance to ticarcillin-potassium clavulanate among clinical isolates of the family**

- Enterobacteriaceae: role of PSE-1 beta-lactamase and high levels of TEM-1 and SHV-1 and problems with false susceptibility in disk diffusion tests.** *Antimicrob Agents Chemother.*, 32(9), 1365-1369.
- Shakil, S., Ali, S. Z., Akram, M., Ali, S. M., and Khan, A. U. (2010). **Risk factors for extended-spectrum β -lactamase producing Escherichia coli and Klebsiella pneumoniae acquisition in a neonatal intensive care unit.** *J Trop Pediatr.*, 56(2), 90-96.
 - Shakil, S., Khan, R., Zarrilli, R., and Khan, A. U. (2008). **Aminoglycosides versus bacteria—a description of the action, resistance mechanism, and nosocomial battleground.** *J Biomed Sci.*, 15(1), 5-14.
 - Shoichet, B. K. (2004). **Virtual screening of chemical libraries.** *Nature*, 432(7019), 862-865.
 - Singh, R., Suchir, A. and Singh, H. (2008). **DLact: An antimicrobial resistance gene database.** *J Comput Intellig Bioinfo* 1(2-3), 93-108.
 - Sirot, D., Chanal, C., Bonnet, R., De Champs, C. and Bret. L. (2001). **Inhibitor-resistant TEM-33 β -lactamase in a Shigella sonnei isolate.** *Antimicrob Agents Chemother.*, 45, 2179-2180.
 - Smet, A., Martel, A., Persoons, D., Dewulf, J., Heyndrickx, M., Catry, B., Herman, L., Haesebrouck, F. And Butaye, P. (2008). **Diversity of extended-spectrum β -lactamases and class C β -lactamases among cloacal Escherichia coli isolates in Belgian broiler farms.** *Antimicrob Agents Chemother.*, 52(4), 1238-1243.
 - Smith C. (2003). **Hitting the target.** *Nature*, 422, 341–347.
 - Sobel, J.D., Kaye, D. (2004). **Urinary Tract Infection**, Ch.66, p.875 - 905. In Mandel GL, Bennett JE, Dolin RE (eds.), *Mandell Douglas and Bennett's Principles and Practice of Infectious Disease*, vol.1, 6th edition. Churchill Livingstone, New York, NY.

- Spratt, B. G. (1994). **Resistance to antibiotics mediated by target alterations.** *Science* 264: 388-393.
- Sulton, D., Pagan-Rodriguez, D., Zhou, X., Liu, Y., Hujer, A. M., Bethel, C. R. and Bonomo, R. A. (2005). **Clavulanic Acid Inactivation of SHV-1 and the Inhibitor-resistant S130G SHV-1 β -Lactamase INSIGHTS INTO THE MECHANISM OF INHIBITION.** *J Biol Chem.*, 280(42), 35528-35536.
- Sun S, Zhang W, Mannervik B and Andersson DI (2013). **Evolution of Broad Spectrum β -Lactam Resistance in an Engineered Metallo- β -lactamase.** *J Biol Chem.*, 288.4, 2314-2324.
- Sun, H. (2008). **Pharmacophore-based virtual screening.** *Curr med chem*, 15(10). 1018-1024.
- Sussman J.L., Lin D, Jiang. J., Manning, N.O., Prilusky, J., Ritter, O. and Abola, E.E. (1998) **Protein Data Bank (PDB): database of three-dimensional structural information of biological macromolecules.** *Acta Crystallogr D Biol Crystallogr.* 1; 54(Pt 6 Pt 1):1078-84.
- Swaren, P., Golemi, D., Cabantous, S., Bulychev, A., Maveyraud, L., Mobashery, S, and Samama, J. P. (1999). **X-ray structure of the Asn276Asp variant of the Escherichia coli TEM-1 β -lactamase: direct observation of electrostatic modulation in resistance to inactivation by clavulanic acid.** *Biochemistry*, 38(30), 9570-9576.
- Thai, Q.K, Bos F, and Pleiss J. (2009). **The lactamase engineering database: a critical survey of TEM sequences in public databases.** *BMC Genomic*, 10, 390.
- Thai, Q.K. and Pleiss, J. (2010). **SHV Lactamase Engineering Database: a reconciliation tool for SHV β -lactamases in public databases.** *BMC Genomics.* 11, 563.
- Thomas, V. L., Golemi-Kotra, D., Kim, C., Vakulenko, S. B., Mobashery, S., and Shoichet, B. K. (2005). **Structural consequences of the inhibitor-resistant Ser130Gly substitution in TEM β -lactamase.** *Biochemistry*, 44(26), 9330-9338.

- Thompson, Julie D., Toby Gibson, and Des G. Higgins. (2002). **Multiple sequence alignment using ClustalW and ClustalX.** *Curr Protoc Bioinformatics.*: 2-3.
- Thomson, J. M., Distler, A. M., Prati, F., and Bonomo, R. A. (2006). **Probing Active Site Chemistry in SHV β -Lactamase Variants at Ambler Position 244 Understanding unique properties of inhibitor resistance.** *J Biol Chem.*, 281(36), 26734-26744.
- Thomson, J. M., A. M. Distler, and R. A. Bonomo. (2007). **Overcoming resistance to β -lactamase inhibitors: comparing sulbactam to novel inhibitors against clavulanate resistant SHV enzymes with substitutions at Ambler position 244.** *Biochemistry.*, 46,11361-11368.
- Tipper, D. J. and Strominger, J. L. (1965). **Mechanism of action of penicillins: a proposal based on their structural similarity to acyl-D-alanyl-D-alanine.** *Proc Natl Acad Sci USA.* 54, 1133-1141.
- Traxler, P. M. (1997). **Protein tyrosine kinase inhibitors in cancer treatment.** *Exp. Opin. Ther. Patents*, 7, 571-88.
- Tronrud, D. E. (1992). **Conjugate-direction minimization: An improved method for the refinement of macromolecules.** *Acta Crystallographica*, 48, 912–916.
- Tzouvelekis, L. S. and Bonomo, R. A. (1999). **SHV-type β -lactamases.** *Curr Pharm Des.*, 5, 847-864.
- Ulrich, E. L., Markley, J. L., and Kyogoku, Y. (1988). **Creation of a nuclear magnetic resonance data repository and literature database.** *Protein Seq Data Anal.*, 2(1). 23-37.
- Vacca, J. P. and Condra, J. H. (1997). **Clinically effective HIV-1 protease inhibitors.** *Drug Discov Today.*, 2, 261-72.
- Vakulenko, S. B., Geryk, B., Kotra, L. P., Mobashery, S. and Lerner, S. A. (1998). **Selection and characterization of β -lactam- β -lactamase inactivator-resistant**

- mutants following PCR mutagenesis of the TEM-1 β -lactamase gene.** *Antimicrob Agents Chemother.*, 42(7), 1542-1548.
- Vedel, G., Belaouaj, A. Gilly, L. Labia, R. Philippon, A. Nevot, P. and Paul, G. (1992). **Clinical isolates of Escherichia coli producing TRI β -lactamases: novel TEM-enzymes conferring resistance to β -lactamase inhibitors.** *J Antimicrob Chemother.*, 30, 449-462.
 - Vieille, C. and Zeikus, G. J. (2001). **Hyperthermophilic enzymes: sources, uses, and molecular mechanisms for thermostability.** *Microbiol Mol Biol Rev.*, 65(1), 1-43.
 - Wallace, A. C., Laskowski, R. A. and Thornton, J. M. (1995). **LIGPLOT: a program to generate schematic diagrams of protein-ligand interactions.** *Protein Eng.*, 8(2), 127-134.
 - Walsh, T. R., Toleman, M. A., Poirel, L., and Nordmann, P. (2005). **Metallo- β -lactamases: the quiet before the storm?** *Clin. microbiol. rev.*, 18(2), 306-325.
 - Walsh, T. R., MacGowan, A. P., and Bennett, P. M. (1997). **Sequence analysis and enzyme kinetics of the L2 serine beta-lactamase from Stenotrophomonas maltophilia.** *Antimicrob Agents Chemother.*, 41(7), 1460-1464.
 - Wang, W., Sheng, C., Che, X., Ji, H., Cao, Y., Miao, Z, Yao., J. & Zhang, W. (2009). Discovery of highly potent novel antifungal azoles by structure-based rational design. *Bioorg Med Chem Lett.*, 19(20), 5965-5969.
 - Wang, L., Veenstra, D. L., Radmer, R. J. and Kollman, P. A. (1998). **Can one predict protein stability? An attempt to do so for residue 133 of T4 lysozyme using a combination of free energy derivatives, PROFEC, and free energy perturbation methods.** *Proteins.* 32, 438-458.
 - Wang, R., Lai, L., and Wang, S. (2002). **Further development and validation of empirical scoring functions for structure-based binding affinity prediction.** *J Comput Aided Mol Des.*, 16, 11-26

- Wang, X., Minasov, G. and Shoichet, B. K. (2002). **The structural bases of antibiotic resistance in the clinically derived mutant β -lactamases TEM-30, TEM-32, and TEM-34.** *J Biol Chem.*, 277(35), 32149-32156.
- Weldhagen, G. F. (2004). **Integrins and β -lactamases: a novel perspective on resistance.** *Int J Antimicrob Agents*, 23, 556-562.
- Wilke, M. S., Lovering, A. L. and Strynadka, N. C. (2005). **β -lactam antibiotic resistance: a current structural perspective.** *Curr Opin Microbiol.* 8, 525-533.
- Williams, D. H., Stephens, E., O'Brien, D. P. and Zhou, M. (2004). **Understanding Noncovalent Interactions: Ligand Binding Energy and Catalytic Efficiency from Ligand-Induced Reductions in Motion within Receptors and Enzymes.** *Angewandte Chemie International Edition*, 43(48), 6596-6616.
- Williams, H., King, A., Shannon, K., and Phillips, I. (1988). **Amoxicillin/clavulanate resistant Escherichia coli.** *The Lancet*, 331(8580), 304-305.
- Williams, J. D. (1999). **β -Lactamases and β -Lactamase Inhibitors.** *Int J Antimicrob Agents.*, 12, S3-S7.
- Wold, S., and Dunn III, W. J. (1983). **Multivariate quantitative structure-activity relationships (QSAR): conditions for their applicability.** *J Chem Inf Comput Sci.*, 23(1). 6-13.
- Wold, S. and Dunn III, W.J. (1983). **Neural Network in QSAR and Drug Design.** *J Chem Inf Comput Sci.*, 23, 6-13.
- Wu, P. J., Shannon, K. and Phillips, I. (1994). **Effect of hyperproduction of TEM-1 β -lactamase on in vitro susceptibility of Escherichia coli to β -lactam antibiotics.** *Antimicrob Agents Chemother.*, 38, 494-498.
- Wu, P. J., Shannon, K. and Phillips, I. (1995). **Mechanisms of hyperproduction of TEM-1 β -lactamase by clinical isolates of Escherichia coli.** *J Antimicrob Chemother.*, 36, 927-939.

- Yang, S. Y. (2010). **Pharmacophore modeling and applications in drug discovery: challenges and recent advances.** *Drug Discov Today.*, 15(11), 444-450.
- Yang, Y., Rasmussen, B. A. and Shlaes, D. M. (1999). **Class A beta-lactamases--enzyme-inhibitor interactions and resistance.** *Pharmacol Ther.* 83(2):141-51.