

DAFTAR PUSTAKA

- Abbassy, M.A., Eldefrawi, M.E., Eldefrawi, A.T., **1983**. Pyrethroid action on the nicotinic acetylcholine receptor/channel, *Pestic Biochem Physiol*, **19**(3): 299–308. [DOI](#)
- Aggarwal, A.K., Auchus, R.J., **2005**. Minireview: Cellular redox state regulates hydroxysteroid dehydrogenase activity and intracellular hormone potency, *Endocrinology*, **146**(6): 2531–2538. [DOI](#)
- Ahmad, L., Khan, A., Khan, M.Z., **2012**. Pyrethroid-induced reproductive toxicopathology in non-target species, *Pak Vet J*, **32**(1): 1–9. [link](#)
- Ahmad, M., Hussain, I., Khan, A., Najib-ur-Rehman, **2009**. Deleterious effects of cypermethrin on semen characteristics and testes of dwarf goats (*Capra hircus*), *Exp Toxicol Pathol*, **61**(4): 339–346. [DOI](#)
- Andersen, H.R., Vinggaard, A.M., Rasmussen, T.H, Gjermansen, I.M., Bonefeld-Jørgensen, E.C., **2002**. Effects of Currently Used Pesticides in Assays for Estrogenicity, Androgenicity, and Aromatase Activity in Vitro, *Toxicol Appl Pharmacol*, **179**(1): 1–12. [DOI](#)
- Andersson, S., Berman, D.M., Jenkins, E.P., Russell, D.W., **1991**. Deletion of steroid 5 α -reductase 2 gene in male pseudohermaphroditism, *Nature*, **354**: 159–161. [DOI](#)
- Andersson, S., Russell, D.W., **1990**. Structural and biochemical properties of cloned and expressed human and rat steroid 5 α -reductases, *Proc Natl Acad Sci USA*, **87**(10): 3640–3644. [PMCID](#)
- Andrews, P.R., Craik, D.J. and Martin, J.L., **1984**. Functional group contributions to drug–receptor interactions, *J Med Chem*, **27**(12): 1648–1657. [DOI](#)
- Anger, T., Madge, D.J., Mulla, M., Riddall, D., **2001**. Medicinal Chemistry of Neuronal Voltage-Gated Sodium Channel Blockers, *J Med Chem*, **44**(2): 115–137. [DOI](#)
- Apweiler, R., Bairoch, A., Wu, C.H., Barker, W.C., Boeckmann, B., Ferro, S., Gasteiger, E., Huang, H., Lopez, R., Magrane, M., Martin, M.J., Natale, D.A., O’Donovan, C., Redaschi, N., Yeh, L.-S.L., **2004**. UniProt: the Universal Protein knowledgebase. *Nucleic Acids Res*, **32**(suppl_1): D115–D119. [DOI](#)
- Attwood, T.K., **2002**. The PRINTS database: A resource for identification of protein families. *Brief Bioinform*, **3**(3): 252–263. [DOI](#)
- Auchus, R.J., Lee, T.C., Miller, W.L., **1998**. Cytochrome b5 augments the 17,20-lyase activity of human P450c17 without direct electron transfer, *J Biol Chem*, **273**: 3158–3165. [DOI](#)
- Benkert, P., Biasini, M., Schwede, T., **2010**. Toward the estimation of the absolute quality of individual protein structure models. *Bioinformatics*, **27**(3): 343–350. [DOI](#)
- Berman, H.M., Westbrook, J., Feng, Z., Gilliland, G., Bhat, T.N., Weissig, H., Shindyalov, I.N., Bourne, P.E., **2000**. The Protein Data Bank, *Nucleic Acid Res*, **28**(1): 235–242. [DOI](#)
- Botham, C., Holmes, P., **2005**. *Chemicals Purported to be Endocrine Disruptors: A Compilation of Published Lists*, IEH Web Report W20, Leicester, UK. [link](#)
- Bradberry, S.M., Cage, S.A., Proudfoot, A.T., Vale, J.A., **2005**. Poisoning due to pyrethroids, *Toxicol Rev*, **24**(2): 93–106. [DOI](#)
- Brodie, A., Inkster, S., **1993**. Aromatase in the human testis, *J Steroid Biochem Mol Biol*, **44**(4-6): 549–555. [DOI](#)
- Brook, C.G., **1999**. Mechanism of puberty, *Horm Res*, **51**(Suppl 3): 52–54. [DOI](#)

- Brueggemeier, R.W., **2002**. Overview of the pharmacology of the aromatase inactivator exemestane, *Breast Cancer Res Treat*, **74**(2): 177–185. [DOI](#)
- Casida, J.E., **1980**. Pyrethrum flowers and pyrethroid insecticides. *Environ Health Perspect*, **34**: 189–202. [DOI](#)
- Catterall, W.A., Goldin, A.L., Waxman, S.G., **2005^a**. International Union of Pharmacology. XLVII. Nomenclature and Structure-Function Relationships of Voltage-Gated Sodium Channels, *Pharmacol Rev*, **57**(4): 397–409. [DOI](#)
- Catterall, W.A., Perez-Reyes, E., Snutch, T.P., Striessnig, J., **2005^b**. International Union of Pharmacology. XLVIII. Nomenclature and Structure-Function Relationships of Voltage-Gated Calcium Channels, *Pharmacol Rev*, **57**(4): 411–425. [DOI](#)
- Chen, S.Y., Zhang, Z.W., He, F.S., Yao, P.P., Wu, Y.Q., Sun, J.X., Liu, L.H., Li, Q.G., **1991**. An epidemiological study on occupational acute pyrethroid poisoning in cotton farmers, *Br J Ind Med*, **48**(2): 77–81. [DOI](#)
- Cherkasov, A., Muratov, E.N., Fourches, D., Varnek, A., Baskin, I.I., Cronin, M., Dearden, J., Gramatica, P., Martin, Y.C., Todeschini, R., Consonni, V., Kuz'min, V.E., Cramer, R., Benigni, R., Yang, C., Rathman, J., Terflath, L., Gasteiger, J., Richard, A., Tropsha, A., **2014**. QSAR Modeling: Where Have You Been? Where Are You Going To?, *J Med Chem*, **57**(12): 4977-5010 [DOI](#)
- Chinn, K., Narahashi, T., **1989**. Temperature-dependent subconducting states and kinetics of deltamethrin-modified sodium channels of neuroblastoma cells, *Pflügers Arch Eur J Physiol*, **413**: 571–579. [DOI](#)
- Chung, B.C., Matteson, K.J., Voutilainen, R., Mohandas, T.K., Miller, W.L., **1986**. Human cholesterol side-chain cleavage enzyme, P450_{scc}: cDNA cloning, assignment of the gene to chromosome 15, and expression in the placenta, *Proc Natl Acad Sci USA*, **83**(23): 8962–8966. [DOI](#)
- Chung, B.C., Picado-Leonard, J., Haniu, M., Bienkowski, M., Hall, P.F., Shively, J.E., Miller, W.L., **1987**. Cytochrome P450_{c17} (steroid 17 alpha-hydroxylase/17,20 lyase): cloning of human adrenal and testis cDNAs indicates the same gene is expressed in both tissues, *Proc Natl Acad Sci USA*, **84**(2): 407–411. [DOI](#)
- Clark, J.M., **1995**. Effects and mechanisms of action of pyrethrin and pyrethroid insecticides, in: Chang, L.W., Dyer, R.S. (Eds.), *Handbook of Neurotoxicology*, Taylor & Francis, pp. 511–546.
- Corpet, F., Servant, F., Gouzy, J., Kahn, D., **2000**. ProDom and ProDom-CG: tools for protein domain analysis and whole genome comparisons. *Nucleic Acids Res*, **28**(1): 267–269. [DOI](#)
- Craig, Z.R., Wang, W., Flaws, J.A., **2011**. Endocrine-disrupting chemicals in ovarian function: effects on steroidogenesis, metabolism and nuclear receptor signaling, *Reproduction*, **142**: 633–646. [DOI](#)
- Crombie, L., Harper, S.H., Elad, D., Ginsburg, D., Bell, F., Jefferies, P.R., Davies, D.W., Hammick, D.L., **1954**. The chrysanthemum carboxylic acids. VI. The configurations of the chrysanthemic acids, *J Chem Soc Resumed*: 470–475.
- Cross, J.B., Thompson, D.C., Rai, B.K., Baber, J.C., Fan, K.Y., Hu, Y., Humblet, C., **2009**. Comparison of Several Molecular Docking Programs: Pose Prediction and Virtual Screening Accuracy, *J Chem Inf Model*, **49**(6): 1455–1474. [DOI](#)
- Crow, J.A., Borazjani, A., Potter, P.M., Ross, M.K., **2007**. Hydrolysis of Pyrethroids by Human and Rat Tissues: Examination of Intestinal, Liver and Serum Carboxylesterases, *Toxicol Appl Pharmacol*, **221**(1): 1–12. [DOI](#)
- de Castro, E., Sigrist, C.J.A., Gattiker, A., Bulliard, V., Langendijk-Genevaux, P.S., Gasteiger, E., Bairoch, A., Hulo, N., **2006**. ScanProsite: detection of PROSITE

- signature matches and ProRule-associated functional and structural residues in proteins. *Nucleic Acids Res*, **34** (suppl_2): W362–W365. DOI
- Devaud, L.L., Murray, T.F., **1988**. Involvement of peripheral-type benzodiazepine receptors in the proconvulsant actions of pyrethroid insecticides, *J Pharmacol Exp Ther*, **247**(1): 14–22. link
- Diel, F., Detscher, M., Borck, H., Schrimpf, D., Diel, E., Hoppe, H.W., **1998**. Effects of permethrin on human basophils and lymphocytes in vitro, *Inflamm Res*, **47** (suppl_1): 11–12. DOI
- Dong, K., **2007**. Insect sodium channels and insecticide resistance, *Invert Neurosci*, **7**: 17–30. DOI
- Duax, W.L., Thomas, J., Pletnev, V., Addlagatta, A., Huether, R., Habegger, L., Weeks, C.M., **2005**. Determining Structure and Function of Steroid Dehydrogenase Enzymes by Sequence Analysis, Homology Modeling, and Rational Mutational Analysis, *Ann NY Acad Sci*, **1061**: 135–148. DOI
- Dufort, I., Rheault, P., Huang, X.-F., Soucy, P., Luu-The, V., **1999**. Characteristics of a Highly Labile Human Type 5 17 β -Hydroxysteroid Dehydrogenase, *Endocrinology*, **140**(2): 568–574. DOI
- Dunn, W.J. and Rogers, D., **1994**, Genetic Partial Least Squares in QSAR, in: Devillers, J. (Ed.), *Genetic Algorithms in Molecular Modeling*, Academic Press, London, pp. 109–130.
- Dupont, E., Zhao, H.-F., Rhéaume, E., Simard, J., Luuthe, V., Labrie, F., Pelletier, G., **1990**. Localization of 3 β -Hydroxysteroid Dehydrogenase/ Δ^5 - Δ^4 -Isomerase in Rat Gonads and Adrenal Glands by Immunocytochemistry and in Situ Hybridization, *Endocrinology*, **127**(3): 1394–1403. DOI
- Ehrlich, P., **1909**. Über den jetzigen Stand der Chemotherapie, *Berichte Dtsch Chem Ges*, **42**: 17–47. DOI
- Engeli, R.T., Rhouma, B.B., Sager, C.P., Tsachaki, M., Birk, J., Fakhfakh, F., Keskes, L., Belguith, N., Odermatt, A., **2016**. Biochemical analyses and molecular modeling explain the functional loss of 17 β -hydroxysteroid dehydrogenase 3 mutant G133R in three Tunisian patients with 46, XY Disorders of Sex Development. *J Steroid Biochem Mol Biol*, **155**(Pt A): 147-54. DOI
- Eil, C., Nisula, B.C., **1990**. The binding properties of pyrethroids to human skin fibroblast androgen receptors and to sex hormone binding globulin, *J Steroid Biochem*, **35**(3-4): 409-414. DOI
- Ertel, E.A., Campbell, K.P., Harpold, M.M., Hofmann, F., Mori, Y., Perez-Reyes, E., Schwartz, A., Snutch, T.P., Tanabe, T., Birnbaumer, L., Tsien, R.W., Catterall, W.A., **2000**. Nomenclature of Voltage-Gated Calcium Channels, *Neuron*, **25**(3): 533–535. DOI
- Fan, Y.-S., Sasi, R., Lee, C., Winter, J.S.D., Waterman, M.R., Lin, C.C., **1992**. Localization of the human CYP17 gene (cytochrome P45017 α) to 10q24.3 by fluorescence in situ hybridization and simultaneous chromosome banding, *Genomics*, **14**(4): 1110–1111. DOI
- Finn, R.D., Bateman, A., Clements, J., Coggill, P., Eberhardt, R.Y., Eddy, S.R., Heger, A., Hetherington, K., Holm, L., Mistry, J., Sonnhammer, E.L.L., Tate, J., Punta, M., **2014**. Pfam: the protein families database. *Nucleic Acids Res*, **42**(D1): D222–D230. DOI
- Fujitani, Y., **1909**. Chemistry and Pharmacology of Insect Powder, *Arch Exp Pathol Pharmacol*, **61**: 47–75.

- Flores, E., Bratoeff, E., Cabeza, M., Ramirez, E., Quiroz, A., Heuze, I., **2003**. Steroid 5 α -Reductase Inhibitors. *Mini-Rev Med Chem*, **3**(3): 225–237. [DOI](#)
- Gallivan, J.P., Dougherty, D.A., **1999**. Cation- π interactions in structural biology, *Proc Natl Acad Sci USA*, **96**(17): 9459-9464. [DOI](#)
- Gassner, B., Wüthrich, A., Scholtysik, G., Solioz, M., **1997**. The Pyrethroids Permethrin and Cyhalothrin are Potent Inhibitors of the Mitochondrial Complex I, *J Pharmacol Exp Ther*, **281**(2): 855–860. [link](#)
- 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 Res*, **40**(D1): D1100–D1107. [DOI](#)
- Geissler, W.M., Davis, D.L., Wu, L., Bradshaw, K.D., Patel, S., Mendonca, B.B., Elliston, K.O., Wilson, J.D., Russell, D.W., Andersson, S., **1994**. Male pseudohermaphroditism caused by mutations of testicular 17 β -hydroxysteroid dehydrogenase 3, *Nat Genet*, **7**: 34–39. [DOI](#)
- Ghosh, D., Pletnev, V.Z., Zhu, D.-W., Wawrzak, Z., Duax, W.L., Pangborn, W., Labrie, F., Lin, S.-X., **1995**. Structure of human estrogenic 17 β -hydroxysteroid dehydrogenase at 2.20 Å resolution, *Structure*, **3**(5): 503–513. [DOI](#)
- Ghosh, D., Griswold, J., Erman, M., and Pangborn, W., **2009**, Structural basis for androgen specificity and oestrogen synthesis in human aromatase, *Nature*, **457**: 219–223. [DOI link](#)
- Gill, S.A., Rizvi, F., Khan, M.Z., Khan, A., **2011**. Toxic effects of cypermethrin and methamidophos on bovine corpus luteal cells and progesterone production, *Exp Toxicol Pathol*, **63**(1-2): 131–135. [DOI](#)
- Gingras, S., Moriggl, R., Groner, B., Simard, J., **1999**. Induction of 3 β -Hydroxysteroid Dehydrogenase/ Δ^5 - Δ^4 Isomerase Type 1 Gene Transcription in Human Breast Cancer Cell Lines and in Normal Mammary Epithelial Cells by Interleukin-4 and Interleukin-13, *Mol Endocrinol*, **13**(1): 66–81. [DOI](#)
- Godin, P.J., Sleeman, R.J., Snarey, M., Thain, E.M., **1966**. The jasmolins, new insecticidally active constituents of *Chrysanthemum cinerariaefolium* VIS., *J Chem Soc C Org*, **1966**: 332–334. [DOI](#)
- Gough, J., Karplus, K., Hughey, R., Chothia, C., **2001**. Assignment of homology to genome sequences using a library of hidden Markov models that represent all proteins of known structure1. *J Mol Biol*, **313**(4): 903–919. [DOI](#)
- Graham-Lorence, S.E., Peterson, J.A., **1996**. Structural alignments of P450s and extrapolations to the unknown, *Methods Enzymol*, **272**: 315-326. [DOI](#)
- Guerriero, G., **2009**. Vertebrate sex steroid receptors: evolution, ligands, and neurodistribution, *Ann NY Acad Sci*, **1163**: 154–168. [DOI](#)
- Gund, P., **1977**. Three-Dimensional Pharmacophoric Pattern Searching, in: Hahn, P.F.E., Kersten, H., Kersten, W., Szybalski, W. (Eds.), **Progress in Molecular and Subcellular Biology**, *Progress in Molecular and Subcellular Biology*, Springer Berlin Heidelberg, pp. 117–143. [DOI](#)
- Hackett, J.C., Brueggemeier, R.W., Hadad, C.M., **2005**. The Final Catalytic Step of Cytochrome P450 Aromatase: A Density Functional Theory Study, *J Am Chem Soc*, **127**(14): 5224–5237. [DOI](#)
- Hagiwara, N., Irisawa, H., Kameyama, M., **1988**. Contribution of two types of calcium currents to the pacemaker potentials of rabbit sino-atrial node cells, *J Physiol*, **395**(1): 233–253. [DOI](#)

- Hansch, C., Maloney, P.P., Fujita, T., Muir, R.M., **1962**. Correlation of Biological Activity of Phenoxyacetic Acids with Hammett Substituent Constants and Partition Coefficients. *Nature*, **194**: 178–180. [DOI](#)
- Hanukoglu, I., **1992**. Steroidogenic enzymes: structure, function, and role in regulation of steroid hormone biosynthesis, *J Steroid Biochem Mol Biol*, **43**(8): 779–804. [DOI](#)
- Harada, K., Kubo, H., Tanaka, A., Nishioka, K., **2012^a**. Identification of oxazolidinediones and thiazolidinediones as potent 17 β -hydroxysteroid dehydrogenase type 3 inhibitors, *Bioorg Med Chem Lett*, **22**(1): 504–507. [DOI](#)
- Harada, K., Kubo, H., Abe, J., Haneta, M., Conception, A., Inoue, S., Okada, S., Nishioka, K., **2012^b**. Discovery of potent and orally bioavailable 17 β -hydroxysteroid dehydrogenase type 3 inhibitors, *Bioorg Med Chem*, **20**(10): 3242–3254. [DOI](#)
- Hart, C.P., **2005**. Finding the target after screening the phenotype, *Drug Discov Today*, **10**(7): 513–519. [DOI](#)
- He, F., Wang, S., Liu, L., Chen, S., Zhang, Z., Sun, J., **1989**. Clinical manifestations and diagnosis of acute pyrethroid poisoning, *Arch Toxicol*, **63**(1): 54–58. [DOI](#)
- He, J., Chen, J., Liu, R., Wang, S., Song, L., Chang, H.C., Wang, X., **2004**. Alterations of FSH-stimulated progesterone production and calcium homeostasis in primarily cultured human luteinizing-granulosa cells induced by fenvalerate, *Toxicology*, **203**(1-3): 61–68. [DOI](#)
- He, J., Chen, J-F., Liu, R., Song, L., Chang, H.C., Wang, X-R., **2006**. Fenvalerate-induced alterations in calcium homeostasis in rat ovary, *Biomed Environ Sci*, **19**(1): 15-20. [link](#)
- Hemmer, M.C., Gasteiger, J., **2000**, Prediction of three-dimensional molecular structures using information from infrared spectra, *Analytica Chimica Acta*, **420**(2): 145-154. [DOI](#)
- Hildebrand, M.E., McRory, J.E., Snutch, T.P., Stea, A., **2004**. Mammalian voltage-gated calcium channels are potently blocked by the pyrethroid insecticide allethrin, *J Pharmacol Exp Ther*, **308**(3): 805–813. [DOI](#)
- Hille, U.E., Hu, Q., Vock, C., Negri, M., Bartels, M., Müller-Vieira, U., Lauterbach, T., Hartmann, R.W., **2009**. Novel CYP17 inhibitors: synthesis, biological evaluation, structure-activity relationships and modelling of methoxy- and hydroxy-substituted methyleneimidazolyl biphenyl, *Eur J Med Chem*, **44**(7): 2765–2775. [DOI](#)
- Hosokawa, M., Maki, T., Satoh, T., **1990**. Characterization of molecular species of liver microsomal carboxylesterases of several animal species and humans, *Arch Biochem Biophys*, **277**(1): 219–227. [DOI](#)
- Hu, M.-C., Hsu, N.-C., El Hadj, N.B., Pai, C.-I., Chu, H.-P., Wang, C.-K.L., Chung, B.-C., **2002**. Steroid deficiency syndromes in mice with targeted disruption of Cyp11a1, *Mol Endocrinol*, **16**(8): 1943–1950. [DOI](#)
- Hu, Q., Yin, L., Jagusch, C., Hille, U.E., Hartmann, R.W., **2010**. Isopropylidene substitution increases activity and selectivity of biphenylmethylene 4-pyridine type CYP17 inhibitors, *J Med Chem*, **53**(13): 5049–5053. [DOI](#)
- Huang, H., Fleming, C.D., Nishi, K., Redinbo, M.R., Hammock, B.D., **2005**. Stereoselective hydrolysis of pyrethroid-like fluorescent substrates by human and other mammalian liver carboxylesterases, *Chem Res Toxicol*, **18**(9): 1371–1377. [DOI](#)

- Hubbard, T.J.P., Ailey, B., Brenner, S.E., Murzin, A.G., Chothia, C., **2000**. SCOP: a Structural Classification of Proteins database, *Nucleic Acids Res*, **28**(1): 257–259. [DOI](#)
- Inano, H., Tamaoki, B., **1986**. Testicular 17 β -hydroxysteroid dehydrogenase: molecular properties and reaction mechanism, *Steroids*, **48**(1-2): 3–26. [DOI](#)
- Inouye, Y., Takeshiya, Y., Ohno, M., **1955**. Studies on Synthetic Pyrethroids. Part V. Synthesis of Geometrical Isomers of Chrysanthemum Dicarboxylic Acid, *Bull Agric Chem Soc Jpn*, **19**(3): 193–199. [DOI](#)
- Jefferys, B.R., Kelley, L.A., Sternberg, M.J.E., **2010**. Protein Folding Requires Crowd Control in a Simulated Cell, *J Mol Biol*, **397**(5): 1329–1338. [DOI](#)
- Jenkins, E.P., Hsieh, C.-L., Milatovich, A., Normington, K., Berman, D.M., Francke, U., Russell, D.W., **1991**. Characterization and chromosomal mapping of a human steroid 5 α -reductase gene and pseudogene and mapping of the mouse homologue, *Genomics*, **11**(4): 1102–1112. [DOI](#)
- Jin, Y., Wang, L., Ruan, M., Liu, J., Yang, Y., Zhou, C., Xu B., Fu, Z., **2011**. Cypermethrin exposure during puberty induces oxidative stress and endocrine disruption in male mice, *Chemosphere*, **84**(1): 124–130. [DOI](#)
- Jones, D.T., **1999**. Protein secondary structure prediction based on position-specific scoring matrices, *J Mol Biol*, **292**(2): 195–202. [DOI](#)
- Jones, D.T., **2007**. Improving the accuracy of transmembrane protein topology prediction using evolutionary information, *Bioinformatics*, **23**(5): 538–44. [DOI](#)
- Jones, P., Binns, D., Chang, H-Y., Fraser, M., Li, W., McAnulla, C., McWilliam, H., Maslen, J., Mitchell, A., Nuka, G., Pesseat, S., Quinn, A.F., Sangrador-Vegas, A., Scheremetjew, M., Yong, S-Y., Lopez, R., Hunter, S., **2014**. InterProScan 5: genome-scale protein function classification, *Bioinformatics*, **30**(9): 1236–1240. [DOI](#)
- Jorgensen, W.L., **1991**. Rusting of the lock and key model for protein-ligand binding. *Science*, **254**(5034): 954–955. [DOI](#) [PMID](#).
- Jörnvall, H., Persson, B., Krook, M., Atrian, S., González-Duarte, R., Jeffery, J., Ghosh, D., **1995**. Short-chain dehydrogenases/reductases (SDR), *Biochemistry (Mosc)*, **34**(18): 6003–6013. [DOI](#)
- Kadous, A., Matsumura, F., Enan, E., **1994**. High affinity binding of ³H-verapamil to rat brain synaptic membrane is antagonized by pyrethroid insecticides. *J Environ Sci Health B*, **29**(5): 855-871. [DOI](#)
- Kallberg, Y., Oppermann, U., Persson, B., **2010**. Classification of the short-chain dehydrogenase/reductase superfamily using hidden Markov models, *FEBS J*, **277**(10): 2375–2386. [DOI](#)
- Kamat, A., Hinshelwood, M.M., Murry, B.A., Mendelson, C.R., **2002**. Mechanisms in tissue-specific regulation of estrogen biosynthesis in humans, *Trends Endocrinol Metab*, **13**(3): 122–128. [DOI](#)
- Katsuda, Y. **1999**, Development of and future prospects for pyrethroid chemistry, *Pestic Sci*, **55**(8): 775–782. [DOI](#)
- Katsuda, Y., Chikamoto, T., Inouye, Y., **1958**. The Absolute Configuration of Naturally Derived Pyrethrolone and Cinerolone, *Bull Agric Chem Soc Jpn*, **22**(6): 427–428. [DOI](#)
- Kelley, L.A., Mezulis, S., Yates, C.M., Wass, M.N., Sternberg, M.J.E., **2015**. The Phyre2 web portal for protein modeling, prediction and analysis. *Nat Protoc*, **10**: 845–858. [DOI](#)

- Khambay, B.P.S, Jewess, P.J., **2010**. *Pyrethroids*. In *Insect Control Biological and Synthetic Agents*, Edited by Gilbert LI and Gill SS: Oxford, UK: Elsevier; pp. 1–29.
- Kim, I.Y., Shin, J.H., Kim, H.S., Lee, S.J., Kang, I.H., Kim, T.S., Moon, H.J., Choi, K.S., Moon, A., Han, S.Y., **2004**. Assessing estrogenic activity of pyrethroid insecticides using in vitro combination assays, *J Reprod Dev*, **50**(2): 245-255. [DOI](#)
- Kitchen, D.B., Decornez, H., Furr, J.R., Bajorath, J., **2004**. Docking and scoring in virtual screening for drug discovery: methods and applications. *Nat Rev Drug Discov*, **3**(11): 935–949. [DOI](#)
- Kongsbak, K., Vinggaard, A.M., Hadrup, N., Audouze, K., **2014**. A Computational Approach to Mechanistic and Predictive Toxicology of Pesticides, *ALTEX*, **31**(1): 11-22. [DOI](#)
- Kowalczyk-Bronisz, S.H., Giełdanowski, J., Bubak, B., **1990**. Immunological profile of animals exposed to pesticide—deltamethrin, *Arch Immunol Ther Exp (Warsz)*, **38**(3-4): 229–238.
- Kuntz, I.D., Blaney, J.M., Oatley, S.J., Langridge, R., Ferrin, T.E., **1982**. A geometric approach to macromolecule-ligand interactions. *J Mol Biol*, **161**(2): 269–88. [DOI](#) [PMID](#).
- Labrie, F., Luu-The, V., Lin, S.-X., Claude, L., Simard, J., Breton, R., Bélanger, A., **1997**. The key role of 17 β -hydroxysteroid dehydrogenases in sex steroid biology, *Steroids*, **62**(1): 148–158. [DOI](#)
- Labrie, F., Simard, J., Luu-The, V., Bélanger, A., Pelletier, G., **1992**. Structure, function and tissue-specific gene expression of 3 β -hydroxysteroid dehydrogenase/5-ene-4-ene isomerase enzymes in classical and peripheral intracrine steroidogenic tissues, *J Steroid Biochem Mol Biol*, **43**(8): 805–826. [DOI](#)
- Labute, P., **2009**. Protonate3D: Assignment of ionization states and hydrogen coordinates to macromolecular structures, *Proteins*, **75**(1): 187–205. [DOI](#)
- Labute, P., **2010**. LowModeMD - Implicit Low Mode Velocity Filtering Applied to Conformational Search of Macrocycles and Protein Loops, *J Chem Inf Model*, **50**(5): 792–800. [DOI](#)
- Lachance, Y., Luu-The, V., Labrie, C., Simard, J., Dumont, M., de Launoit, Y., Guérin, S., Leblanc, G., Labrie, F., **1990**. Characterization of human 3 beta-hydroxysteroid dehydrogenase/delta 5-delta 4-isomerase gene and its expression in mammalian cells, *J Biol Chem*, **265**: 20469–20475. [link](#)
- LaForge, F.B., Barthel, W.F., **1945**. Constituents of Pyrethrum Flowers. XVIII. The Structure and Isomerism of Pyrethrolone, *J Org Chem*, **10**: 114–120. [DOI](#)
- Laskowski, R.A., MacArthur, M.W., Moss, D., Thornton, J.M., **1993**. PROCHECK: a program to check the stereochemical quality of protein structures, *J Appl Cryst*, **26**: 283-291. [DOI](#)
- Lawrence, L.J., Casida, J.E., **1983**. Stereospecific action of pyrethroid insecticides on the gamma-aminobutyric acid receptor-ionophore complex, *Science*, **221**(4618): 1399-1401. [DOI](#).
- Leach, A.R., **2001**, *Molecular Modelling: Principles and Applications*, 2nd edition, Pearson Education Ltd., London. [ISBN](#)
- Lee, T.C., Miller, W.L., Auchus, R.J., **1999**. Medroxyprogesterone acetate and dexamethasone are competitive inhibitors of different human steroidogenic enzymes, *J Clin Endocrinol Metab*, **84**(6): 2104–2110. [DOI](#)

- Leng, G., Ranft, U., Sugiri, D., Hadnagy, W., Berger-Preiß, E., Idel, H., **2003**. Pyrethroids used indoors – Biological monitoring of exposure to pyrethroids following an indoor pest control operation, *Int J Hyg Environ Health*, **206**(2): 85–92. [DOI](#)
- Lengauer, T., Rarey, M., **1996**. Computational methods for biomolecular docking, *Curr Opin Struct Biol*, **6**(3): 402–6. [DOI PubMed](#)
- Lesuisse, D., Gourvest, J.F., Albert, E., Doucet, B., Hartmann, C., Lefrançois, J.M., Tessier, S., Tric, B., Teutsch, G., **2001**. Biphenyls as surrogates of the steroidal backbone. Part 2: discovery of a novel family of non-steroidal 5 α -reductase inhibitors, *Bioorg Med Chem Lett*, **11**(13): 1713–1716. [PubMed](#)
- Lertkiatmongkol, P., Jenwitheesuk, E., Rongneparut, P., **2011**. Homology modeling of mosquito cytochrome P450 enzymes involved in pyrethroid metabolism: insights into differences in substrate selectivity, *BMC Res Notes*, **4**: 321. [DOI](#)
- Liang, G., Tang, L., Kang, L., Mei, H., Li, Z., **2008**, Using multidimensional patterns of amino acid attributes for QSAR analysis of peptides, *Amino Acids*, **37**(4): 583–5891 [DOI](#)
- Lin, D., Black, S.M., Nagahama, Y., Miller, W.L., **1993**. Steroid 17 α -hydroxylase and 17,20-lyase activities of P450c17: contributions of serine106 and P450 reductase, *Endocrinology*, **132**(6): 2498–2506. [DOI](#)
- Litchfield, M.H., **1985**. *The Pyrethroid Insecticides*, J.P. Leahey (eds), Taylor & Francis, Philadelphia, PA, pp. 99-150.
- Lorence, M.C., Murry, B.A., Trant, J.M., Mason, J.I., **1990**. Human 3 β -hydroxysteroid dehydrogenase/delta^{5 \rightarrow 4} isomerase from placenta: expression in nonsteroidogenic cells of a protein that catalyzes the dehydrogenation/isomerization of C₂₁ and C₁₉ steroids, *Endocrinology*, **126**(5): 2493–2498. [DOI](#)
- Lu, S., Liu, H.-C., Chen, Y.-D., Yuan, H.-L., Sun, S.-L., Gao, Y.-P., Yang, P., Zhang, L., Lu, T., **2011**. Combined Pharmacophore Modeling, Docking, and 3D-QSAR Studies of PLK1 Inhibitors, *Int J Mol Sci*, **12**(12): 8713–8739. [DOI](#)
- Luu-The, V., **2001**. Analysis and characteristics of multiple types of human 17 β -hydroxysteroid dehydrogenase, *J Steroid Biochem Mol Biol*, **76**(1-5): 143–151. [DOI](#)
- Luu-The, V., Bélanger, A., Labrie, F., **2008**. Androgen biosynthetic pathways in the human prostate, *Best Pract Res Clin Endocrinol Metab*, **22**(2): 207–221. [DOI](#)
- Luu-The, V., Labrie, C., Zhao, H.F., Couët, J., Lachance, Y., Simard, J., Leblanc, G., Côté, J., Bérubé, D., Gagné, R., Labrie, F., **1989**. Characterization of cDNAs for Human Estradiol 17 β -Dehydrogenase and Assignment of the Gene to Chromosome 17: Evidence of two mRNA Species with Distinct 5'-Termini in Human Placenta, *Mol Endocrinol*, **3**(8): 1301–1309. [DOI](#)
- Madsen, C., Claesson, M.H., Röpke, C., **1996**. Immunotoxicity of the pyrethroid insecticides deltamethrin and α -cypermethrin, *Toxicology*, **107**(3): 219–227. [DOI](#)
- Martel, C., Rhéaume, E., Takahashi, M., Trudel, C., Couët, J., Luu-The, V., Simard, J., Labrie, F., **1992**. Distribution of 17 β -hydroxysteroid dehydrogenase gene expression and activity in rat and human tissues, *J Steroid Biochem Mol Biol*, **41**(3-8): 597–603. [DOI](#)
- Marti-Renom, M.A., Stuart, A.C., Fiser, A., Sanchez, R., Melo, F., Sali, A., **2000**. Comparative protein structure modeling of genes and genomes. *Annu Rev Biophys Biomol Struct*, **29**: 291–325. [DOI](#)

- Matsuo, N., Mori, T., 2012. *Pyrethroids: From Chrysanthemum to Modern Industrial Insecticide*, Springer, Berlin. DOI
- McCarthy, A.R., Thomson, B.M., Shaw, I.C., Abell, A.D., 2006. Estrogenicity of pyrethroid insecticide metabolites, *J Environ Monit*, **8**(1): 197–202. DOI
- McGregor, M.J., Luo, Z., Jiang, X., 2006. Chapter 3. *Virtual Screening in Drug Discovery*, in: Huang, Z. (Ed.), *Drug Discovery Research*, John Wiley & Sons, Inc., pp. 63–88.
- McKeever, B.M., Hawkins, B.K., Geissler, W.M., Wu, L., Sheridan, R.P., Mosley, R.T., Andersson, S., 2002. Amino acid substitution of arginine 80 in 17 β -hydroxysteroid dehydrogenase type 3 and its effect on NADPH cofactor binding and oxidation/reduction kinetics. *Biochimica et Biophysica Acta (BBA) - Proteins and Proteomics*, **1601**(1): 29-37. DOI
- Meeker, J.D., Barr, D.B., Hauser, R., 2008. Human semen quality and sperm DNA damage in relation to urinary metabolites of pyrethroid insecticides, *Hum Reprod*, **23**(8): 1932-1940. DOI
- Mendieta, M.A.E.P-B., Negri, M., Jagusch, C., Hille, U.E., Müller-Vieira, U., Schmidt, D., Hansenc, K., Hartmann, R.W., 2008. Synthesis, biological evaluation and molecular modelling studies of novel ACD- and ABD-ring steroidomimetics as inhibitors of CYP17, *Bioorg Med Chem Lett*, **18**: 267-273. DOI
- Michelangeli, F., Robson, M.J., East, J.M., Lee, A.G., 1990. Fluorescence and kinetic studies of the interactions of pyrethroids with the (Ca²⁺ + Mg²⁺)-ATPase, *Biochem Biophys Acta*, **1028**: 58-66. DOI
- Miller, T.A., Salgado, V.L., 1985. *The mode of action of pyrethroids on insect*, in: John P. Leahey (Ed.), *The Pyrethroid Insecticides*. Taylor & Francis, London; Philadelphia, pp. 43–93.
- Miller, W.L., 1988. Molecular Biology of Steroid Hormone Synthesis, *Endocr Rev*, **9**(3): 295–318. DOI
- Miller, W.L., 2005. Minireview: regulation of steroidogenesis by electron transfer, *Endocrinology*, **146**: 2544–2550. DOI
- Miller, W.L., 2009. Androgen synthesis in adrenarache, *Rev Endocr Metab Disord*, **10**: 3–17. DOI
- Mitchell, J.C., Dupuis, G., Towers, G.H.N., 1972. Allergic Contact Dermatitis from Pyrethrum (*Chrysanthemum Spp.*), *Br J Dermatol*, **86**: 568–573. DOI
- Molecular Operating Environment (MOE), 2015.10; Chemical Computing Group Inc., 1010 Sherbrooke St. West, Suite #910, Montreal, QC, Canada, H3A 2R7, 2015.
- Moitessier, N., Englebienne, P., Lee, D., Lawandi, J., Corbeil, C.R., 2008. Towards the development of universal, fast and highly accurate docking/scoring methods: a long way to go, *Br J Pharmacol*, **153**(S1): S7–S26. DOI
- National Research Council, 2007. *Toxicity Testing in the 21st Century: A Vision and a Strategy*, The National Academies Press, Washington DC. DOI
- Nakajin, S., Shively, J.E., Yuan, P.M., Hall, P.F., 1981. Microsomal cytochrome P-450 from neonatal pig testis: two enzymatic activities (17 alpha-hydroxylase and c17,20-lyase) associated with one protein, *Biochemistry (Mosc)*, **20**(14): 4037–4042. DOI
- Narahashi, T., 1996. Neuronal Ion Channels as the Target Sites of Insecticides, *Pharmacol. Toxicol.*, **79**(1): 1–14. DOI
- Narahashi, T., 2002. Nerve membrane ion channels as the target site of insecticides. *Mini Rev Med Chem*, **2**: 419–432. DOI

- Normington, K., Russell, D.W., **1992**. Tissue distribution and kinetic characteristics of rat steroid 5 alpha-reductase isozymes. Evidence for distinct physiological functions, *J Biol Chem*, **267**(27): 19548–19554. [link](#)
- O'Reilly, A.O., Khambay, B.P.S., Williamson, M.S., Field, L.M., Wallace, B.A., Davies, T.G.E., **2006**. Modelling insecticide-binding sites in the voltage-gated sodium channel, *Biochem J*, **396**(2): 255–263. [DOI](#)
- Oliva, A., Spira, A., Multigner, L., **2001**. Contribution of environmental factors to the risk of male infertility, *Hum Reprod Oxf Engl*, **16**(8): 1768–1776. [DOI](#)
- Oortgiesen, M., van Kleef, R.G.D.M., Vijverberg, H.P.M., **1989**. Effects of pyrethroids on neurotransmitter-operated ion channels in cultured mouse neuroblastoma cells, *Pestic Biochem Physiol*, **34**(2): 164–173. [DOI](#)
- Ortiz, A.R., Pisabarro, M.T., Gago, F., Wade, R.C., **1995**. Prediction of Drug Binding Affinities by Comparative Binding Energy Analysis, *J Med Chem.*, **38**(14): 2681-2691. [DOI](#)
- Payne, A.H., Hales, D.B., **2004**. Overview of Steroidogenic Enzymes in the Pathway from Cholesterol to Active Steroid Hormones, *Endocr Rev*, **25**(6): 947–970. [DOI](#)
- Payne, A.H., Youngblood, G.L., **1995**. Regulation of expression of steroidogenic enzymes in Leydig cells, *Biol Reprod*, **52**(2): 217–225. [DOI](#)
- Pelletier, G., Luu-The, V., Tětu, B., Labrie, F., **1999**. Immunocytochemical Localization of Type 5 17 β -Hydroxysteroid Dehydrogenase in Human Reproductive Tissues, *J Histochem Cytochem*, **47**(6): 731–737. [DOI](#)
- Penning, T.M., Burczynski, M.E., Jez, J.M., Lin, H.-K., Ma, H., Moore, M., Ratnam, K., Palackal, N., **2001**. Structure-function aspects and inhibitor design of type 5 17 β -hydroxysteroid dehydrogenase (AKR1C3), *Mol Cell Endocrinol*, **171**(1-2): 137–149. [DOI](#)
- Perry, M.J., **2008**. Effects of environmental and occupational pesticide exposure on human sperm: a systematic review. *Hum Reprod Update*, **14**(3): 233–242. [DOI](#)
- Perry, M.J., Venners, S.A., Barr, D.B. Xu, X., **2007**. Environmental pyrethroid and organophosphorus insecticide exposures and sperm concentration, *Reprod Toxicol*, **23**(1): 113-118. [DOI](#)
- Persson, B., Kallberg, Y., Bray, J.E., Bruford, E., Dellaporta, S.L., Favia, A.D., Duarte, R.G., Jörnvall, H., Kavanagh, K.L., Kedishvili, N., Kisiela, M., Maser, E., Mindnich, R., Orchard, S., Penning, T.M., Thornton, J.M., Adamski, J., Oppermann, U., **2009**. The SDR (short-chain dehydrogenase/reductase and related enzymes) nomenclature initiative, *Chem Biol Interact*, **178**(1-3): 94-98. [DOI](#)
- Picard, F., Barassin, S., Mokhtarian, A., Hartmann, R.W., **2002**. Synthesis and evaluation of 2'-substituted 4-(4'-carboxy- or 4'-carboxymethylbenzylidene)-N-acylpiperidines: highly potent and in vivo active steroid 5alpha-reductase type 2 inhibitors, *J Med Chem*, **45**(16): 3406–3417.
- Pikuleva, I.A., **2006**. Cholesterol-metabolizing cytochromes P450. *Drug Metab Dispos Biol Fate Chem*, **34**(4): 513–520. [DOI](#)
- Pine, M.D., Hiney, J.K., Lee, B., Les Dees, W., **2008**. The Pyrethroid Pesticide Esfenvalerate Suppresses the Afternoon Rise of Luteinizing Hormone and Delays Puberty in Female Rats, *Environ Health Perspect*, **116**(9): 1243–1247. [DOI](#)

- Plewczynski, D., Lazniewski, M., Augustyniak, R., Ginalski, K., **2011**, Can We Trust Docking Results? Evaluation of Seven Commonly Used Programs on PDBbind Database, *J Comput Chem*, **32**(4): 742–755. [DOI](#)
- Portier, C.J., **2002**. Endocrine dismodulation and cancer, *Neuro Endocrinol Lett*, **23**(Suppl 2): 43–47. [PubMed](#)
- Qiu, W., Zhou, M., Labrie, F., Lin, S.-X., **2004**. Crystal Structures of the Multispecific 17 β -Hydroxysteroid Dehydrogenase Type 5: Critical Androgen Regulation in Human Peripheral Tissues, *Mol Endocrinol*, **18**(7): 1798–1807. [DOI](#)
- Quinkler, M., Sinha, B., Tomlinson, J.W., Bujalska, I.J., Stewart, P.M., Arlt, W., **2004**. Androgen generation in adipose tissue in women with simple obesity – a site-specific role for 17 β -hydroxysteroid dehydrogenase type 5, *J Endocrinol*, **183**: 331–342. [DOI](#)
- Rabbani, B., Mahdieh, N., Haghi Ashtiani, M.T., Setoodeh, A., Rabbani, A., **2012**. In silico structural, functional and pathogenicity evaluation of a novel mutation: An overview of HSD3B2 gene mutations, *Gene*, **503**(2): 215–221. [DOI](#)
- Ramachandran, K.I., Deepa, G., and Krishnan Namboori. P.K., **2008**, *Computational Chemistry and Molecular Modeling Principles and Applications*, Springer-Verlag GmbH. [DOI](#)
- Ratnasooriya, W.D., Ratnayake, S.S.K., Jayatunga, Y.N.A., **2002**. Effects of pyrethroid insecticide ICON (lambda cyhalothrin) on reproductive competence of male rats, *Asian J Androl*, **4**(1): 35-41. [link](#)
- Ray, D.E., Forshaw, P.J., **2000**. Pyrethroid insecticides: poisoning syndromes, synergies, and therapy, *J Toxicol Clin Toxicol*, **38**(2): 95–101. [DOI](#)
- Reddy, P.M., Philip, G.H., Bashamohideen, M., **1991**. Inhibition of Mg²⁺ and Na⁺-K⁺ ATPases in selected tissues of fish, *Cyprinus carpio* under fenvalerate toxicity, *Biochem Int*, **23**(4): 715–721. [PubMed](#)
- Rester, U., **2008**. From virtuality to reality - Virtual screening in lead discovery and lead optimization: a medicinal chemistry perspective, *Curr Opin Drug Discov Devel*, **11**(4): 559–568. [PubMed](#)
- Roessink, I., Arts, G.H.P., Belgers, J.D.M., Bransen, F., Maund, S.J., Brock, T.C.M., **2005**. Effects of lambda-cyhalothrin in two ditch microcosm systems of different trophic status, *Environ Toxicol Chem SETAC*, **24**(7): 1684–1696. [DOI](#)
- Rollinger, J.M., Schuster, D., Danzl, B., Schwaiger, S., Markt, P., Schmidtke, M., Gertsch, J., Raduner, S., Wolber, G., Langer, T., Stuppner, H., **2009**. In silico Target Fishing for Rationalized Ligand Discovery Exemplified on Constituents of *Ruta graveolens*, *Planta Med*, **75**(3): 195–204. [DOI](#)
- Ruigt, G.S., Neyt, H.C., Van der Zalm, J.M., Van den Bercken, J., **1987**. Increase of sodium current after pyrethroid insecticides in mouse neuroblastoma cells, *Brain Res*, **437**(2): 309–322. [DOI](#)
- Saito, R., Terasaki, N., Yamazaki, M., Masutomi, N., Tsutsui, N., Okamoto, M., **2016**. Estimation of the Mechanism of Adrenal Action of Endocrine-Disrupting Compounds Using a Computational Model of Adrenal Steroidogenesis in NCI-H295R Cells, *J Toxicol*, **2016**: Article ID 4041827, 19 pages, [DOI](#)
- Salem, O.I., Frotscher, M., Scherer, C., Neugebauer, A., Biemel, K., Streiber, M., Maas, R., Hartmann, R.W., **2006**. Novel 5 α -Reductase Inhibitors: Synthesis, Structure–Activity Studies, and Pharmacokinetic Profile of Phenoxybenzoylphenyl Acetic Acids, *J Med Chem*, **49**(2): 748–759.

- Sanborn, M., Kerr, K.J., Sanin, L.H., Cole, D.C., Bassil, K.L., Vakil, C., **2007**. Non-cancer health effects of pesticides. *Can Fam Physician*, **53**(10): 1712–1720. [PMC](#)
- Santen, R.J., **1987**. Aromatase: future perspectives. Miami, Florida, March 4-7, 1987. Proceedings. I, *Steroids*, **50**(1-3): 1–323.
- Sapre, N.S., Gupta, S., Sapre, N., **2008**. Assessing ligand efficiencies using template-based molecular docking and Tabu-clustering on tetrahydroimidazo-[4,5,1-jk][1,4]-benzodiazepin-2(1H)-one and-thione (TIBO) derivatives as HIV-1RT inhibitors, *J Chem Sci*, **120**(4): 395–404. [DOI](#)
- Sasano, H., Okamoto, M., Mason, J.I., Simpson, E.R., Mendelson, C.R., Sasano, N., Silverberg, S.G., **1989**. Immunolocalization of aromatase, 17 α -hydroxylase and side-chain-cleavage cytochromes P-450 in the human ovary, *J Reprod Fertil*, **85**(1): 163–169. [DOI](#)
- Satoh, T., Hosokawa, M., **1998**. The Mammalian Carboxylesterases: From Molecules to Functions, *Annu Rev Pharmacol Toxicol*, **38**(1): 257–288. [DOI](#)
- Sawicki, M.W., Erman, M., Puranen, T., Vihko, P., Ghosh, D., **1999**. Structure of the ternary complex of human 17 β -hydroxysteroid dehydrogenase type 1 with 3-hydroxyestra-1,3,5,7-tetraen-17-one (equilin) and NADP⁺, *Proc Natl Acad Sci USA*, **96**(3): 840–845. [DOI](#)
- Schechter, M.S., Green, N., LaForge, F.B., **1949**. Constituents of Pyrethrum Flowers. XXIII. Cinerolone and the Synthesis of Related Cyclopentenolones. *J Am Chem Soc*, **71**(9): 3165–3173. [DOI](#)
- Schleier, J.J., Peterson, R.K., *Ch#3: Pyrethrins and Pyrethroid Insecticides*, In: Lopez, O. and Fernandez-Bolanos, J.G., **2011**, *RSC Green Chemistry No.11: Green Trends in Insect Control*, Royal Society of Chemistry, [DOI](#)
- Scollon, E.J., Starr, J.M., Godin, S.J., DeVito, M.J., Hughes, M.F., **2009**. In Vitro Metabolism of Pyrethroid Pesticides by Rat and Human Hepatic Microsomes and Cytochrome P450 Isoforms, *Drug Metab Dispos*, **37**(1): 221–228. [DOI](#)
- Scott, H.M., Mason, J.I., Sharpe, R.M., **2009**. Steroidogenesis in the Fetal Testis and Its Susceptibility to Disruption by Exogenous Compounds, *Endocr Rev*, **30**(7): 883–925. [DOI](#)
- Shafer, T.J., Meyer, D.A., **2004**. Effects of pyrethroids on voltage-sensitive calcium channels: a critical evaluation of strengths, weaknesses, data needs, and relationship to assessment of cumulative neurotoxicity, *Toxicol Appl Pharmacol*, **196**: 303–318. [DOI](#)
- Shafer, T.J., Meyer, D.A., Crofton, K.M., **2005**. Developmental neurotoxicity of pyrethroid insecticides: critical review and future research needs, *Environ Health Perspect*, **113**(2): 123–136. [DOI](#)
- Sharma, S., Basu, A., Agrawal, R.K., **2013**. Pharmacophore Modeling and Docking Studies on Some Nonpeptide-Based Caspase-3 Inhibitors, *BioMed Res Int*, **2013**: Article ID 306081, 15 pages. [DOI](#)
- Shoichet, B.K., **2004**. Virtual screening of chemical libraries, *Nature*, **432**(7019): 862–865. [DOI](#)
- Sillitoe, I., Cuff, A.L., Dessailly, B.H., Dawson, N.L., Furnham, N., Lee, D., Lees, J.G., Lewis, T.E., Studer, R.A., Rentzsch, R., Yeats, C., Thornton, J.M., Orengo, C.A., **2012**. New functional families (FunFams) in CATH to improve the mapping of conserved functional sites to 3D structures, *Nucleic Acids Res*, **41**: D490–D498. [DOI](#)

- Sillitoe, I., Lewis, T.E., Cuff, A., Das, S., Ashford, P., Dawson, N.L., Furnham, N., Laskowski, R.A., Lee, D., Lees, J.G., Lehtinen, S., Studer, R.A., Thornton, J., Orenge, C.A., **2015**. CATH: comprehensive structural and functional annotations for genome sequences, *Nucleic Acids Res*, **43**: D376–D381. [DOI](#)
- Simpson, E.R., Clyne, C., Rubin, G., Boon, W.C., Robertson, K., Britt, K., Speed, C., Jones, M., **2002**. Aromatase—a Brief Overview, *Annu Rev Physiol*, **64**: 93–127. [DOI](#)
- Simpson, E.R., Mahendroo, M.S., Means, G.D., Kilgore, M.W., Hinshelwood, M.M., Graham-Lorence, S., Amarneh, B., Ito, Y., Fisher, C.R., Michael, M.D., Mendelson, C.R., Bulun, S.E., **1994**. Aromatase Cytochrome P450, The Enzyme Responsible for Estrogen Biosynthesis, *Endocr Rev*, **15**(3): 342–355. [DOI](#)
- Singh, S., Kumar, V., Thakur, S., Banerjee, B.D., Chandna, S., Rautela, R.S., Grover, S.S., Rawat, D.S., Pasha, S.T., Jain, S.K., Ichhpujani, R.L., Rai, A., **2011**. DNA damage and cholinesterase activity in occupational workers exposed to pesticides, *Environ Toxicol Pharmacol*, **31**(2): 278–285. [DOI](#)
- Soderlund, D.M., Casida, J.E., **1977**. Effects of pyrethroid structure on rates of hydrolysis and oxidation by mouse liver microsomal enzymes, *Pestic Biochem Physiol*, **7**(4): 391–401. [DOI](#)
- Soderlund, D.M., Clark, J.M., Sheets, L.P., Mullin, L.S., Piccirillo, V.J., Sargent, D., Stevens, J.T., Weiner, M.L., **2002**. Mechanisms of pyrethroid neurotoxicity: implications for cumulative risk assessment, *Toxicology*, **171**(1): 3–59. [DOI](#)
- Söding, J., **2005**. Protein homology detection by HMM-HMM comparison, *Bioinformatics*, **21**(7): 951–960. [DOI](#)
- Solati, J., Hijakhani, R., Zaiem, R.T., **2010**. Effects of Cypermethrin on Sexual Behaviour and Plasma Concentrations of Pituitary-Gonadal Hormones, *Int J Fertil Steril*, **4**(1): 23–28. [link](#)
- Someya, T., Yoshino, M., **1990**. Characterization of two types of calcium channel in smooth muscle cell membrane of guinea-pig taenia coli, *Sapporo Med J*, **59**: 177–188.
- Song, J.H., Narahashi, T., **1996**. Modulation of sodium channels of rat cerebellar Purkinje neurons by the pyrethroid tetramethrin, *J Pharmacol Exp Ther*, **277**(1): 445–453. [link](#)
- Staudinger, H., Ruzicka, L., **1924**. Insektentötende Stoffe I. Über Isolierung und Konstitution des wirksamen Teiles des dalmatinischen Insektenpulvers. *Helv Chim Acta*, **7**(1): 177–201. [DOI](#)
- Strushkevich, N., MacKenzie, F., Cherkesova, T., Grabovec, I., Usanov, S., Park, H.-W., **2011**. Structural basis for pregnenolone biosynthesis by the mitochondrial monooxygenase system, *Proc Natl Acad Sci USA*, **108**(25): 10139–10143. [DOI](#)
- Sun, H., Xu, X.-L., Xu, L.-C., Song, L., Hong, X., Chen, J.-F., Cui, L.-B., Wang, X.-R., **2007**. Antiandrogenic activity of pyrethroid pesticides and their metabolite in reporter gene assay. *Chemosphere*, **66**(3): 474–479. [DOI](#)
- Symington, S.B., Clark, J.M., **2005**. Action of deltamethrin on N-type (Cav2.2) voltage-sensitive calcium channels in rat brain, *Pestic Biochem Physiol*, **82**(1): 1–15. [DOI](#)
- Terwindt, G.M., Ophoff, R.A., Haan, J., Sandkuijl, L.A., Frants, R.R., Ferrari, M.D., **1998**. Migraine, ataxia and epilepsy: a challenging spectrum of genetically determined calcium channelopathies, *Eur J Hum Genet*, **6**(4): 297–307. [DOI](#)

- Thigpen, A.E., Silver, R.I., Guileyardo, J.M., Casey, M.L., McConnell, J.D., Russell, D.W., **1993**. Tissue distribution and ontogeny of steroid 5 alpha-reductase isozyme expression, *J Clin Invest*, **92**(2): 903–910. [DOI](#)
- Thomas, J.L., Boswell, E.L., Scaccia, L.A., Pletnev, V., Umland, T.C., **2005**. Identification of key amino acids responsible for the substantially higher affinities of human type 1 3beta-hydroxysteroid dehydrogenase/isomerase (3beta-HSD1) for substrates, coenzymes, and inhibitors relative to human 3beta-HSD2, *J Biol Chem*, **280**(22): 21321–21328. [DOI](#)
- Thomas, J.L., Duax, W.L., Addlagatta, A., Scaccia, L.A., Frizzell, K.A., Carloni, S.B., **2004**. Serine-124 completes the Tyr, Lys and Ser triad responsible for the catalysis of human type 1 3beta-hydroxysteroid dehydrogenase, *J Mol Endocrinol*, **33**(1): 253–261. [DOI](#)
- Toda, K., Shizuta, Y., **1993**. Molecular cloning of a cDNA showing alternative splicing of the 5'-untranslated sequence of mRNA for human aromatase P-450, *Eur J Biochem*, **213**(1): 383–389. [DOI](#)
- Todd, G.D., Wohlers, D., Citra, M.J., **2003**, *Toxicological Profile for Pyrethrins and Pyrethroids*, Agency for Toxic Substances and Disease Registry (ASTDR), Atlanta. [link](#)
- Ullah, M.S., Ahmad, M., Ahmad, N., Khan, M.Z., Ahmad, I., **2006**. Toxic effects of cypermethrin in female rabbits, *Pak Vet J*, **26**(4): 193-196. [link](#)
- Usanov, S.A., Graham, S.E., Lepesheva, G.I., Azeva, T.N., Strushkevich, N.V., Gilep, A.A., Estabrook, R.W., Peterson, J.A., **2002**. Probing the interaction of bovine cytochrome P450_{scc} (CYP11A1) with adrenodoxin: evaluating site-directed mutations by molecular modeling. *Biochemistry (Mosc)*, **41**(26): 8310–8320. [DOI](#)
- Usherwood, P.N.R., Davies, T.G.E., Mellor, I.R., O'Reilly, A.O., Peng, F., Vais, H., Khambay, B.P.S., Field, L.M., Williamson, M.S., **2007**. Mutations in DIIS5 and the DIIS4–S5 linker of *Drosophila melanogaster* sodium channel define binding domains for pyrethroids and DDT, *FEBS Lett*, **581**(28): 5485–5492. [DOI](#)
- Vijverberg, H.P., van den Bercken, J., **1990**. Neurotoxicological effects and the mode of action of pyrethroid insecticides, *Crit Rev Toxicol*, **21**(2): 105–126. [DOI](#)
- Volkman, J., Müller, D., Feuerstacke, C., Kliesch, S., Bergmann, M., Müchlfeld, C., Middendorff, R., **2011**. Disturbed spermatogenesis associated with thickened lamina propria of seminiferous tubules is not caused by dedifferentiation of myofibroblast, *Hum Reprod*, **26**(6): 1450-1461. [DOI](#)
- Voutilainen, R., Tapanainen, J., Chung, B.C., Matteson, K.J., Miller, W.L., **1986**. Hormonal regulation of P450_{scc} (20,22-desmolase) and P450c17 (17 alpha-hydroxylase/17,20-lyase) in cultured human granulosa cells, *J Clin Endocrinol Metab*, **63**(1): 202–207. [DOI](#)
- Wakeling, E.N., Atchison, W.D., Neal, A.P., **2012**. *Pyrethroids and Their Effects on Ion Channels*, in: Soundararajan, R.P. (Ed.), *Pesticides - Advances in Chemical and Botanical Pesticides*, InTech. [DOI](#)
- Walsh, L.P., Stocco, D.M., **2000**. Effects of Lindane on Steroidogenesis and Steroidogenic Acute Regulatory Protein Expression, *Biol Reprod*, **63**(4): 1024–1033. [DOI](#)
- Walters, W.P., Stahl, M.T., Murcko, M.A., **1998**. Virtual screening—an overview, *Drug Discov Today*, **3**(4): 160–178. [DOI](#)
- Wang, L.M., Liu, W.P., Yang, C.X., Pan, Z.Y., Gan, J.Y., Xu, C., Zhao, M.R., Schlenk, D., **2007**. Enantioselectivity in estrogenic potential and uptake of bifenthrin, *Environ Sci Tech*, **41**(17): 6124–6128. [DOI](#)

- Wang, M., Roberts, D.L., Paschke, R., Shea, T.M., Masters, B.S.S., Kim, J.-J.P., **1997**. Three-dimensional structure of NADPH-cytochrome P450 reductase: Prototype for FMN- and FAD-containing enzymes, *Proc Natl Acad Sci USA*, **94**(16): 8411–8416. [link](#)
- Ward, J.J., Sodhi, J.S., McGuffin, L.J., Buxton, B.F., Jones, D.T., **2004**. Prediction and functional analysis of native disorder in proteins from the three kingdoms of life, *J Mol Biol*, **337**(3): 635–645. [DOI](#)
- Wermuth, C.G., Ganellin, C.R., Lindberg, P., Mitscher, L.A., **1998**. Glossary of terms used in medicinal chemistry (IUPAC Recommendations 1998), *Pure Appl Chem*, **70**(5): 1129–1143. [DOI](#)
- Whitehead, S.A., Rice, S., **2006**. Endocrine-disrupting chemicals as modulators of sex steroid synthesis, *Best Pract Res Clin Endocrinol Metab*, **20**(1): 45–61. [DOI](#)
- Wiederstein, M., Sippl, M.J., **2007**. ProSA-web: interactive web service for the recognition of errors in three-dimensional structures of proteins, *Nucleic Acids Res*, **35**: W407–W410. [DOI](#)
- Xu, D., Zhang, Y., **2011**. Improving the Physical Realism and Structural Accuracy of Protein Models by a Two-Step Atomic-Level Energy Minimization, *Biophys J*, **101**(10): 2525–2534. [DOI](#)
- Xu, L.-C., Sun, H., Chen, J.-F., Bian, Q., Song, L., Wang, X.-R., **2006**. Androgen receptor activities of p,p'-DDE, fenvalerate and phoxim detected by androgen receptor reporter gene assay, *Toxicol Lett*, **160**(2): 151–157. [DOI](#)
- Xue, L.A., Kuliopulos, A., Mildvan, A.S., Talalay, P., **1991**. Catalytic mechanism of an active-site mutant (D38N) of delta 5-3-ketosteroid isomerase. Direct spectroscopic evidence for dienol intermediates, *Biochemistry (Mosc)*, **30**(20): 4991–4997. [DOI](#)
- Yamamoto, R., **1923**. The insecticidal principle in *Chrysanthemum cinerariaefolium*. Part II and part III. On the constitution of pyrethronic acid, *J Chem Soc Jpn*, **44**: 311–330.
- Yamashita, M., Tanaka, J. and Ando Y, **1997**. Human mortality in organophosphate poisonings. *Vet Hum Toxicol*, **39**: 84-85. [PubMed](#)
- Yang, X., Iwamoto, K., Wang, M., Artwohl, J., Mason, J.I., Pang, S., **1993**. Inherited congenital adrenal hyperplasia in the rabbit is caused by a deletion in the gene encoding cytochrome P450 cholesterol side-chain cleavage enzyme, *Endocrinology*, **132**(5): 1977–1982. [DOI](#)
- Ye, L., Su, Z.-J., Ge, R.-S., **2011**. Inhibitors of Testosterone Biosynthetic and Metabolic Activation Enzymes, *Molecules*, **16**(12): 9983–10001. [DOI](#)
- Zhang, J., Zhu, W., Zheng, Y., Yang, J. Zhu, X. **2008**. The antiandrogenic activity of pyrethroid pesticides cyfluthrin and beta-cyfluthrin, *Reprod Toxicol*, **25**(4): 491-496. [DOI](#)
- Zhang, X., Zhao, W., Jing, R., Wheeler, K., Smith, G.A., Stallones, L., Xiang, H., **2011**. Work-related pesticide poisoning among farmers in two villages of Southern China: a cross-sectional survey. *BMC Public Health*, **11**: 429. [DOI](#)