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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 toxico-pathology 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, Gjermandsen, 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 5α-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 5alpha-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 Disrupters: 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

UNIVERSITAS GADJAH MADA
STUDI KOMPUTASIONAL MEKANISME AKSI PYRETHROID PADA ENZIM GONADAL STEROIDOGENIK YANG TERLIBAT DALAM BIOSINTESIS HORMON REPRODUKTIF
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Universitas Gadjah Mada, 2016 | Diunduh dari http://etd.repository.ugm.ac.id/

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., Terfloth, 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, P450scc: 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 P450c17 (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

UNIVERSITAS GADJAH MADA
STUDI KOMPUTASIONAL MEKANISME AKSI PYRETHROID PADA ENZIM GONADAL STEROIDOGENIK YANG TERLIBAT DALAM BIOSINTESIS HORMON REPRODUKTIF
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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 N Y 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 17β-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 3β-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 17β-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 P45017α) 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.

UNIVERSITAS GADJAH MADA
STUDI KOMPUTASIONAL MEKANISME AKSI PYRETHROID PADA ENZIM GONADAL STEROIDOGENIK YANG TERLIBAT DALAM BIOSINTESIS HORMON REPRODUKTIF
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Universitas Gadjah Mada, 2016 | Diunduh dari http://etd.repository.ugm.ac.id/

Flores, E., Bratoeff, E., Cabeza, M., Ramirez, E., Quiroz, A., Heuze, I., **2003**. Steroid 5α-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 17β–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 17β-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, ***ExpToxicol Pathol***, **63**(1-2): 131–135. DOI

Gingras, S., Moriggl, R., Groner, B., Simard, J., **1999**. Induction of 3β-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 N Y 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

UNIVERSITAS GADJAH MADA
STUDI KOMPUTASIONAL MEKANISME AKSI PYRETHROID PADA ENZIM GONADAL STEROIDOGENIK YANG TERLIBAT DALAM BIOSINTESIS HORMON REPRODUKTIF
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Universitas Gadjah Mada, 2016 | Diunduh dari http://etd.repository.ugm.ac.id/

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 17β-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 17β-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-subtituted methyleneimidazoyl 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

UNIVERSITAS
GADJAH MADA
STUDI KOMPUTASIONAL MEKANISME AKSI PYRETHROID PADA ENZIM GONADAL STEROIDOGENIK YANG TERLIBAT DALAM BIOSINTESIS HORMON REPRODUKTIF
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Universitas Gadjah Mada, 2016 | Diunduh dari http://etd.repository.ugm.ac.id/

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 17β-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 5α-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., Gonzàlez-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 ^{3}H-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

UNIVERSITAS GADJAH MADA
STUDI KOMPUTASIONAL MEKANISME AKSI PYRETHROID PADA ENZIM GONADAL STEROIDOGENIK YANG TERLIBAT DALAM BIOSINTESIS HORMON REPRODUKTIF
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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: Elsivier; 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 17β-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 3β-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 insecticidedes 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

UNIVERSITAS
GADJAH MADA
STUDI KOMPUTASIONAL MEKANISME AKSI PYRETHROID PADA ENZIM GONADAL STEROIDOGENIK YANG TERLIBAT DALAM BIOSINTESIS HORMON REPRODUKTIF
BAMBANG SULISTYO ARI SUDARMANTO, Prof. Dr. Sri Noegrohati, Apt.
Universitas Gadjah Mada, 2016 | Diunduh dari http://etd.repository.ugm.ac.id/

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., Hartamann, C., Lefrançois, J.M., Tessier, S., Tric, B., Teutsch, G., **2001**. Biphenyls as surrogates of the steroidal backbone. Part 2: discovery af a novel family of non-steroidal 5alpha-reductase inhibitors, ***Bioorg Med Chem Lett***, 11(13): 1713–1716. PubMed

Lertkiatmongkol, P., Jenwitheesuk, E., Rongnoparut, 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 alpha-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 beta-hydroxysteroid dehydrogenase/delta$^{5\rightarrow4}$ isomerase from placenta: expression in nonsteroidogenic cells of a protein that catalyzes the dehydrogenation/isomerization of C_{21} and C_{19} 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 17β-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., Côtè, J., Bérubé, D., Gagné, R., Labrie, F., **1989**. Characterization of cDNAs for Human Estradiol 17β-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 deltametrin and α-cypermetrin, ***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 17β-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

UNIVERSITAS GADJAH MADA
STUDI KOMPUTASIONAL MEKANISME AKSI PYRETHROID PADA ENZIM GONADAL STEROIDOGENIK YANG TERLIBAT DALAM BIOSINTESIS HORMON REPRODUKTIF
BAMBANG SULISTYO ARI SUDARMANTO, Prof. Dr. Sri Noegrohati, Apt.
Universitas Gadjah Mada, 2016 | Diunduh dari http://etd.repository.ugm.ac.id/

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 17β-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 (Ca^{2+} + Mg^{2+})-ATPase, ***Biochem Biophys Acta***, **1028**: 58-66. DOI

Miller, T.A., Salgado, V.L., **1985**. *The mode of action pf 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 adrenarche, ***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

UNIVERSITAS GADJAH MADA
STUDI KOMPUTASIONAL MEKANISME AKSI PYRETHROID PADA ENZIM GONADAL STEROIDOGENIK YANG TERLIBAT DALAM BIOSINTESIS HORMON REPRODUKTIF
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Universitas Gadjah Mada, 2016 | Diunduh dari http://etd.repository.ugm.ac.id/

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 17β-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., Hartamann, 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

UNIVERSITAS GADJAH MADA
STUDI KOMPUTASIONAL MEKANISME AKSI PYRETHROID PADA ENZIM GONADAL STEROIDOGENIK YANG TERLIBAT DALAM BIOSINTESIS HORMON REPRODUKTIF
BAMBANG SULISTYO ARI SUDARMANTO, Prof. Dr. Sri Noegrohati, Apt.
Universitas Gadjah Mada, 2016 | Diunduh dari http://etd.repository.ugm.ac.id/

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 17β-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 17β-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 Mg^{2+} 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., Neugebaeuer, A., Biemel, K., Streiber, M., Maas, R., Hartmann, R.W., **2006**. Novel 5α-Reductase Inhibitors: Synthesis, Structure−Activity Studies, and Pharmacokinetic Profile of Phenoxybenzoylphenyl Acetic Acids, ***J Med Chem***, 49(2): 748–759.

UNIVERSITAS GADJAH MADA
STUDI KOMPUTASIONAL MEKANISME AKSI PYRETHROID PADA ENZIM GONADAL STEROIDOGENIK YANG TERLIBAT DALAM BIOSINTESIS HORMON REPRODUKTIF
BAMBANG SULISTYO ARI SUDARMANTO, Prof. Dr. Sri Noegrohati, Apt.
Universitas Gadjah Mada, 2016 | Diunduh dari http://etd.repository.ugm.ac.id/

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, 17α-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 17β-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 Fernadez-Bolanos, J.G., **2011**, ***RSC Green Chemistry No.11: Green Trens 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

UNIVERSITAS
GADJAH MADA
STUDI KOMPUTASIONAL MEKANISME AKSI PYRETHROID PADA ENZIM GONADAL STEROIDOGENIK YANG TERLIBAT DALAM BIOSINTESIS HORMON REPRODUKTIF
BAMBANG SULISTYO ARI SUDARMANTO, Prof. Dr. Sri Noegrohati, Apt.
Universitas Gadjah Mada, 2016 | Diunduh dari http://etd.repository.ugm.ac.id/

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., Orengo, 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

UNIVERSITAS GADJAH MADA
STUDI KOMPUTASIONAL MEKANISME AKSI PYRETHROID PADA ENZIM GONADAL STEROIDOGENIK YANG TERLIBAT DALAM BIOSINTESIS HORMON REPRODUKTIF
BAMBANG SULISTYO ARI SUDARMANTO, Prof. Dr. Sri Noegrohati, Apt.
Universitas Gadjah Mada, 2016 | Diunduh dari http://etd.repository.ugm.ac.id/

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 P450scc (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

Volkmann, J., Müller, D., Feuerstacke, C., Kliesch, S., Bergmann, M., Müchlfeld, C., Middendorff, R., **2011**. Disturbed spermatogenesisassociated with thickened lamina propia 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 P450scc (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

UNIVERSITAS
GADJAH MADA
STUDI KOMPUTASIONAL MEKANISME AKSI PYRETHROID PADA ENZIM GONADAL STEROIDOGENIK YANG TERLIBAT DALAM BIOSINTESIS HORMON REPRODUKTIF
BAMBANG SULISTYO ARI SUDARMANTO, Prof. Dr. Sri Noegrohati, Apt.
Universitas Gadjah Mada, 2016 | Diunduh dari http://etd.repository.ugm.ac.id/

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