

## VII. REFERÊNCIAS BIBLIOGRÁFICAS

- Alan J. Miller *Subset Selection in Regression*; Chapman and Hall: London, 1990.
- Amaral, A.T.do, Miyazaki, Y., Caprara, L., Oliveira, A.C., In: *Rational Approaches to the Design of Bioactive Compound*, Amsterdam: Elsevier, 1991.
- Amaral, A.T.do, Miyazaki, Y., Capobianco, G., Frey, B.Y., Stachissini, A.S, Miguel, S.R.M., Kawabe, A.B., Tavares, L.C., Gallacci, M., Caprara, L., Oliveira, In: WERMUTH, C. G., Ed. *Trends in QSAR and Molecular Modeling*, 92, Leiden: ESCOM, 1993.
- Amaral, A. T.; Oliveira, A. C.; Neidlein, R.; Gallacci, M.; Caprara, L.; Miyazaki, Y. *European Journal of Medicinal Chemistry* **1997**, 32 433-443.
- Andrews, P. R., Craik, D. J., and Martin, J. L *Journal of Medicinal Chemistry* **1984**, 27, 16484.
- Anzali, S.; Barnickel, G.; Krug, M.; Sadowski, J.; Wagener, M.; Gasteiger, J. *Abstracts of Papers of the American Chemical Society* **1996**, 211 9-CINF.
- Bader, R. F. W.; Matta, C. F. *Journal Of Physical Chemistry A* **2004**, 108, 8385-8394.
- Baker, J. *Journal Of Computational Chemistry* **1986**, 7, 385-395.
- Balaban, A. T.; Devillers, J. *Topological Indices and Related Descriptors in QSAR and QSPR*; Gordon and Breach Science Publishers; Amsterdam, 1999. Dissertação de Mestrado.
- Baroni, M.; Constantino, G.; Cruciani, G.; Riganelli, D. L. V. R.; Clementi, S. *Quantitative Structure-Activity Relationships* **1993**, 12 9-20.
- Baroni, R.V., *Aspectos estruturais, mecanismo de formação e atividade antimicrobiana de benzilidenotiossemocarbonas 2- ou 4-, potencialmente quimioterápicas*. Faculdade de Ciências Farmacêuticas, USP-SP, 1987 [Dissertação de Mestrado]
- Barros Neto, B.; Spacino Scarminio, I.; Bruns, R. E. in *Como Fazer Experimentos*, 2 ed., 2002.
- Basak, S. C.; Gute, B. D.; Grunwald, G. D. *Journal of Chemical Information and Computer Sciences* **1997**, 37, 651-655.
- Belvisi, L.; Bravi, G.; Scolastico, C.; Vulpetti, A.; Salimbeni, A.; Todeschini, R. *Journal of Computer-Aided Molecular Design* **1994**, 8, 211-220.
- Bohm, H. J. *Journal of Computer-Aided Molecular Design* **1992**, 6, 593-606.
- Bohm, H. J. *Journal of Computer-Aided Molecular Design* **1994**, 8, 243-256.
- Broto, P.; Moreau, G.; Vanduycke, C. *European Journal of Medicinal Chemistry* **1984**, 19, 61-65.
- Burden, F. R. *Journal of Chemical Information and Computer Sciences* **1989**, 29, 225-227.
- Burden, F. R. *Quantitative Structure-Activity Relationships* **1997**, 16, 309-314.
- Carbo, R.; Leyda, L.; Arnau, M. *International Journal Of Quantum Chemistry* **1980**, 17, 1185-1189.

- Cheng, E.; Haiduke, R. L. A.; Pires, R.; Ishiki, H.; Bruns, R. E. and Amaral, A. T.-do *Multivariate Analysis of Sets of Antibacterial Nitrofurane Derivatives* 14<sup>th</sup> European Symposium on QSAR: Designing Drugs: processes, problems and solutions, 2002, Bournemouth, Inglaterra.
- Chiyanzu, I.; Hansell, E.; Gut, J.; Rosenthal, P. J.; McKerrow, J. H.; Chibale, K. *Bioorganic & Medicinal Chemistry Letters* **2003**, *13*, 3527-3530.
- Clark, M.; Cramer, R. D. *Quantitative Structure-Activity Relationships* **1993**, *12* 137-145.
- Consonni, V.; Todeschini, R.; Pavan, M. *Journal of Chemical Information and Computer Sciences* **2002**, *42*, 682-692.
- Consonni, V.; Todeschini, R.; Pavan, M.; Gramatica, P. *Journal of Chemical Information and Computer Sciences* **2002**, *42*, 693-705.
- Coura, J. R.; de Castro, S. L. *Memorias Do Instituto Oswaldo Cruz* **2002**, *97*, 3-24.
- Cramer, R. D.; Patterson, D. E.; Bunce, J. D. *Journal Of The American Chemical Society* **1988**, *110* 5959-5967.
- Raminelli, C., *Estudo da relações quantitativa entre a estrutura química e atividade citotóxica de séries de derivados de bases de Mannich*. Instituto de Química, USP, SP, 2001. Dissertação de Mestrado.
- Dearden, J. C.; Bresnen, G. M. *Quantitative Structure-Activity Relationships* **1988**, *7* 133
- Dearden, J. C.; Bradburne, S. J. A.; Abraham, M. H. *QSAR: Rational Approaches to the Design of Bioactive Compound* **1991**, 143-150.
- Dewar, M. J. S.; Zoebisch, E. G.; Healy, E. F.; Stewart, J. J. P. *Journal Of The American Chemical Society* **1985**, *107*, 3902-3909
- Dewar, M. J. S.; Healy, E. F.; Holder, A. J.; Yuan, Y. C. *Journal Of Computational Chemistry* **1990**, *11*, 541-542.
- Diudea, M. V.; Horvath, D.; Graovac, A. *Journal of Chemical Information and Computer Sciences* **1995**, *35*, 129-135.
- Diudea, M. V.; Topan, M.; Graovac, A. *Journal of Chemical Information and Computer Sciences* **1994**, *34*, 1072-1078.
- Du, X. H.; Guo, C.; Hansell, E.; Doyle, P. S.; Caffrey, C. R.; Holler, T. P.; McKerrow, J. H.; Cohen, F. E. *Journal of Medicinal Chemistry* **2002**, *45*, 2695-2707.
- Embrechts, M. J. ANALYZE Program **2001**
- Ertl, P.; Rohde, B.; Selzer, P. *Journal of Medicinal Chemistry* **2000**, *43*, 3714-3717.
- Free, S. M.; Wilson, J. W. *Journal of Medicinal Chemistry* **1964**, *7*, 395-&.
- French, F. A.; Blanz, E. J., Jr.; Shaddix, S. C.; Brockman, R. W. *Journal of Medicinal Chemistry* **1974**, *17*, 172-181.
- Gaillard, P.; Carrupt, P. A.; Testa, B.; Boudon, A. *Journal of Computer-Aided Molecular Design* **1994**, *8*, 83-96.

- Galvez, J.; Garcia, R.; Salabert, M. T.; Soler, R. *Journal of Chemical Information and Computer Sciences* **1994**, *34*, 520-525.
- Gasteiger, J.; Marsili, M. *Organic Magnetic Resonance* **1981**, *15*, 353-360.
- Gasteiger, J.; Sadowski, J.; Schuur, J.; Selzer, P.; Steinhauer, L.; Steinhauer, V. *Journal of Chemical Information and Computer Sciences* **1996**, *36*, 1030-1037.
- Gasteiger, J.; Teckentrup, A.; Terfloth, L.; Spycher, S. *Journal Of Physical Organic Chemistry* **2003**, *16*, 232-245.
- Geary, R. C. *The Incorporated Statistician* **1954**, *5*, 115-145.
- Geladi, P.; Kowalski, B. R. *Analytica Chimica Acta* **1986**, *185* 1-17.
- Ghose, A. K.; Pritchett, A.; Crippen, M. *Journal Of Computational Chemistry* **1988**, *9*, 80-90.
- Ghose, A. K.; Crippen, G. M.; Revankar, G. R.; Mckernan, P. A.; Smee, D. F.; Robins, R. K. *Journal of Medicinal Chemistry* **1989**, *32*, 746-756.
- Gillmor, S. A.; CRAIK, C. S.; FLETTERICK, R. J. *Protein Science* **1997**, *6*, 1603-1611.
- Girault, S.; Davioud-Charvet, E.; Salmon, L.; Berecibar, A.; Debreu, M. A.; Sergheraert, C. *Bioorganic & Medicinal Chemistry Letters* **1998**, *8*, 1175-1180.
- Golbraikh, A.; Tropsha, A. *Journal of Molecular Graphics and Modelling* **2002**, *20*, 269-276.
- Golbraikh, A.; Shen, M.; Xiao, Z. Y.; Xiao, Y. D.; Lee, K. H.; Tropsha, A. *Journal of Computer-Aided Molecular Design* **2003**, *17*, 241-253.
- Golbraikh, A.; Tropsha, A. *Journal of Chemical Information and Computer Sciences* **2003**, *43*, 144-154.
- Good, A. C. *Journal Of Molecular Graphics* **1992**, *10*, 144-151.
- Good, A. C.; So, S. S.; Richards, W. G. *Journal of Medicinal Chemistry* **1993**, *36*, 433-438.
- Graham, J. D. P.; Karrar, M. A. *Journal of Medicinal Chemistry* **1963**, *6*, 103-107.
- Greenbaum, D. C.; Mackey, Z.; Hansell, E.; Doyle, P.; Gut, J.; Caffrey, C. R.; Lehrman, J.; Rosenthal, P. J.; McKerrow, J. H.; Chibale, K. *Journal of Medicinal Chemistry* **2004**, *47*, 3212-3219.
- Guha, R.; Serra, J. R.; Jurs, P. C. *Journal Of Molecular Graphics & Modelling* **2004**, *23*, 1-14.
- Hansch, C.; Maloney, P. P.; Fujita, T. *Nature* **1962**, *194*, 178-&.
- Hansch, C.; Muir, R. M.; Fujita, T.; Maloney, P. P.; Geiger, F.; Streich, M. *Journal Of The American Chemical Society* **1963**, *85*, 2817-2824.
- Hansch, C.; Fujita, T. *Journal Of The American Chemical Society* **1964**, *86* 1616-1626.
- Hansch, C.; Lien, E. J. *Biochemical Pharmacology* **1968**, *17*, 709-720.
- Hansch, C.; Sammes, P. G.; Taylor, J. B. e. *Comprehensive medicinal chemistry: the rational design, mechanistic study and therapeutic application of chemical compounds*; Oxford, 1990.

- Hansch, C.; Leo, A. *Exploring QSAR Fundamentals and Applications in Chemistry and Biology*; Washington, 1995.
- Hansch, C.; Kurup, A.; Garg, R.; Gao, H. *Chemical Reviews* **2001**, *101*, 619-672.
- Hammet, L. P. *Journal Of The American Chemical Society* **1937**, *59*, 96-103.
- Hammett, L. P. *Physical Organic Chemistry. Reaction Rates, Equilibria, and Mechanisms*, New York, McGraw-Hill, 1970.
- Hemmer, M. C.; Steinhauer, V.; Gasteiger, J. *Vibrational Spectroscopy* **1999**, *19*, 151-164.
- Hodgkin, E. E.; Richards, W. G. *International Journal fo Quantum Chemistry: Quantum Biology Symposium* **1987**, *14*, 105-110.
- Honerjager, P. *Herz* **1990**, *15*, 70-78.
- Huang, L.; Ellman, J. A. *Bioorganic & Medicinal Chemistry Letters* **2002**, *12*, 2993-2996.
- Huang, L.; Brinen, L. S.; Ellman, J. A. *Bioorganic & Medicinal Chemistry* **2003**, *11*, 21-29.
- Hubert, M.; Vanden Branden, K. *Journal Of Chemometrics* **2003**, *17*, 537-549.
- Ishiki, H.M. *Relações Qauntitativas estrutura-atividade QSAR/QSAR-3D de dipiridodiazepinonas, inibidoras da transcriptase reversa do virus da imunodeficiência humana do tipo I (HIV-1)*. Ribeirão Preto, SP, 1999. Dissertação de Mestrado
- Ishiki, H.M.; Galembeck, S.E.; AMARAL, A.T.do. Application of two alignments procedures in CoMFA analysis of nevirapine derivative *Proceedings of 13<sup>th</sup> European Symposium on Quantitative Structure-Activity Relationships: Rational Approaches to Drug Design*, Amsterdam: ESCOM, 2001.
- Ishiki, H. M.; Amaral, A. T. do. *Three-Dimensional Quantitative Structure-Activity Relationship Study of Antitumor 2-Formylpyridine Thiosemicarbazones Derivatives as Inhibitors of Ribonucleotide Reductase*. Em fase final de redação.
- Jug, K. *Journal of Organic Chemistry* **1983**, *48*, 1344-1348.
- Karelson, M.; Lobanov, V. S.; Katritzky, A. R. *Chemical Reviews* **1996**, *96*, 1027-1043.
- Klebe, G.; Abraham, U.; Mietzner, T. *Journal of Medicinal Chemistry* **1994**, *37*, 4130-4146.
- Kier, L. B.; Hall, L. H.; Frazer, J. W. *Journal of Mathematical Chemistry* **1991**, *7*, 229-241.
- Kim, K. H. *Quantitative Structure-Activity Relationships* **1992**, *11*, 309-317.
- Kim, K. H.; Greco, G.; Novellino, E. *Perspectives In Drug Discovery And Design* **1998**, *12* 257-315.
- Kim, K. H.; Martin, Y. C. *Journal of Organic Chemistry* **1991**, *56*, 2723-2729.
- Kirchhoff, L. V. *New England Journal of Medicine* **1993**, *329*, 639-644.
- Klebe, G.; Abraham, U. *Journal of Medicinal Chemistry* **1993**, *36*, 70-80.
- Kubinyi, H. *Journal of Mathematical Chemistry* **1976**, *19*, 587-600.

- Kubinyi, H.; Kehrhahn, O. H. *Arzneimittelforschung* **1978**, *28*, 598-601.
- Kubinyi, H. *Quantitative Structure-Activity Relationships* **1988**, *7*, 121-133.
- Kubinyi, H. *Journal Of Cancer Research And Clinical Oncology* **1990**, *116*, 529-537.
- Kubinyi, H. in *QSAR: Hansch Analysis and Related Approaches*, Weinheim, VCH, 1993a.
- Kubinyi, H., in *3D QSAR in Drug Design. Theory, Methods and Applications. ESCOM*: Leiden, 1993b.
- Kubinyi, H. *Quantitative Structure-Activity Relationships* **1994**, *13*, 285-294.
- Kubinyi, H. THE PROGRAM BILIN. **1995**.
- Kubinyi, H. *Drug Discovery Today* **1997**, *2*, 457-467.
- Kubinyi, H.; Hamprecht, F. A.; Mietzner, T. *Journal of Medicinal Chemistry* **1998**, *41*, 2553-2564.
- Lattin, D. L. in *Principles of Medicinal Chemistry*, 4<sup>a</sup> ED., Lippincott Williams & Wilkins, Media, 1995.
- Leardi, R. *Journal Of Chemometrics* **1994**, *8*, 65-79.
- Leardi, R.; Boggia, R.; Terrile, M. *Journal Of Chemometrics* **1992**, *6*, 267-281.
- Lecaille, F.; Bromme, D.; Kaleta, J. *Chemical Review* **2002**, *102*, 4459-4488.
- Li, R. S.; Chen, X. W.; Gong, B. Q.; Selzer, P. M.; Li, Z.; Davidson, E.; Kurzban, G.; Miller, R. E.; Nuzum, E. O.; McKerrow, J. H.; Fletterick, R. J.; Gillmor, S. A.; Craik, C. S.; Kuntz, I. D.; Cohen, F. E.; Kenyon, G. L. *Bioorganic & Medicinal Chemistry* **1996**, *4*, 1421-1427.
- Libow, L. F.; Beltrani, V. P.; Silvers, D. N.; Grossman, M. E. *Cutis* **1991**, *48*, 37-40.
- Lindgren, F.; Eriksson, L.; Hellberg, S.; Jonsson, J.; Sjostrom, M.; Wold, S. *Quantitative Structure-Activity Relationships* **1991**, *10*, 36-42.
- Lipinski, C. A.; Lombardo, F.; Dominy, B. W.; Feeney, P. J. *Advanced Drug Delivery Reviews* **1997**, *23*(1-3), 3-25.
- Livingstone, D. *Data Analysis for Chemists*; Oxford Science Publications, 1995.
- Malvezzi, A., Policastro, D. S, Da Silva, W. C. F. N., Amaral A.T.do. Study of ion-pair formation in a set of [(N,N-dimethylamino)-methyl]-4-substituted benzamide hydrochlorides. *Proceedings of the second log P symposium Lipophilicity in Drug Disposition*, Lausanne, Suíça, 2001.
- Malvezzi, A. "Estudo Comparativo de Parâmetros Hidrofóbicos e relacionados à ionização, de Série de Derivados da Procaína com Atividade Bloqueadora Neuromuscular". 2003. Dissertação de Mestrado.
- Malvezzi, A.; de Rezende, L. Amaral; A. T.-do. *3D QSAR of cathepsin I inhibitors. 15<sup>th</sup> European QSAR & Molecular Modelling Symposium: QSAR & Molecular Modelling in Rational Design of Bioactive Molecules*, em, Istambul, Turquia, 2004.
- Marsili, M.; Gasteiger, J. *Croatia Chemical Acta* **1980**, *53*, 601-614.
- Martin, Y. C.; Lynn, K. R. *Journal of Medicinal Chemistry* **1971**, *14*, 1162-1166.

- Mattioni, B. E.; Jurs, P. C. *Journal of Chemical Information and Computer Sciences* **2002**, *42*, 94-102.
- McGrath, M. E.; Eakin, A. E.; Engel, J. C.; McKerrow, J. H.; Craik, C. S.; Fletterick, R. J. *Journal Of Molecular Biology* **1995**, *247*, 251-259.
- Melo, P. D.; Duran, N.; Haun, M. *Toxicology Letters* **2000**, *116*, 237-242.
- Moon, J. B.; Howe, W. J. *Proteins-Structure Function and Genetics* **1991**, *11*, 314-328.
- Moran, P. A. P. *Biometrika* **1950**, *37*, 17-23.
- Moreau, G.; Broto, P. *Nouveau Journal de Chimie-New Journal of Chemistry* **1980**, *4*, 359-360.
- Moriguchi, I.; Hirono, S.; Liu, Q.; Nakagome, I.; Matsushita, Y. *Chemical & Pharmaceutical Bulletin* **1992**, *40*, 127-130.
- Novellino, E.; Fattorusso, C.; Greco, G. *Pharmaceutica Acta Helvetiae* **1995**, *70* 149-154.
- Otto, M.; Wegscheider, W. *Analytical Chemistry* **1985**, *57*, 63-69.
- Pearlman, R. S.; Smith, K. M. *Journal of Chemical Information and Computer Sciences* **1999**, *39*, 28-35.
- Petitjean, M. *Journal of Chemical Information and Computer Sciences* **1992**, *32*, 331-337.
- Pires, J. R. "Relações Quantitativas entre a Estrutura Química de Derivados Nitrofurânicos e a Atividade Antimicrobiana contra *Caulobacter crescentus* e *Staphylococcus aureus*". 1998. Tese de Doutorado.
- Pires, J. R.; Saito, C.; Gomes, S. L.; Giesbrecht, A. M.; Amaral, A. T. D. *Journal of Medicinal Chemistry* **2001**, *44*, 3673-3681.
- Polak, A.; Richle, R. *Annals Of Tropical Medicine And Parasitology* **1978**, *72*, 45-54.
- Randic, M. *Journal of Chemical Information and Computer Sciences* **1995**, *35*, 373-382.
- Rando, D. G.; Sato, D. N.; Siqueira, L.; Malvezzi, A.; Leite, C. Q. F.; do Amaral, A. T.; Ferreira, E. I.; Tavares, L. C. *Bioorganic & Medicinal Chemistry* **2002**, *10*, 557-560.
- Reynolds, C. A.; Burt, C.; Richards, W. G. *Quantitative Structure-Activity Relationships* **1992**, *11*, 34-35.
- Roush, W. R.; Gonzalez, F. V.; McKerrow, J. H.; Hansell, E. *Bioorganic & Medicinal Chemistry Letters* **1998**, *8*, 2809-2812.
- Roush, W. R.; Hernandez, A. A.; McKerrow, J. H.; Selzer, P. M.; Hansell, E.; Engel, J. C. *Tetrahedron* **2000**, *56*, 9747-9762.
- Roush, W. R.; Cheng, J. M.; Knapp-Reed, B.; Alvarez-Hernandez, A.; McKerrow, J. H.; Hansell, E.; Engel, J. C. *Bioorganic & Medicinal Chemistry Letters* **2001**, *11*, 2759-2762.
- Rucker, G.; Rucker, C. *Journal of Chemical Information and Computer Sciences* **1993**, *33*, 683-695.
- Sadowski, J.; Gasteiger, J. *Chemical Reviews* **1993**, *93*, 2567-2581.
- Sadowski, J.; Gasteiger, J.; Klebe, G. *Journal of Chemical Information and Computer Sciences* **1994**, *34*, 1000-1008.

- Scheidt, K. A.; Roush, W. R.; McKerrow, J. H.; Selzer, P. M.; Hansell, E.; Rosenthal, P. J. *Bioorganic & Medicinal Chemistry* **1998**, *6*, 2477-2494.
- Schonberger, H.; Schwab, C. H.; Hirsch, A.; Gasteiger, J. *Journal Of Molecular Modeling* **2000**, *6*, 379-395.
- Schuur, J. H.; Selzer, P.; Gasteiger, J. *Journal of Chemical Information and Computer Sciences* **1996**, *36*, 334-344.
- Serilevy, A.; Salter, R.; West, S.; Richards, W. G. *European Journal of Medicinal Chemistry* **1994**, *29*, 687-694.
- Seydel, J. K. *International Journal Of Leprosy And Other Mycobacterial Diseases* **1981**, *49*, 90.
- Seydel, J. K.; Trettin, D.; Wassermann, O. *Naunyn-Schmiedebergs Archives Of Pharmacology* **1979**, *307* R1.
- Shoichet, B. K.; Stroud, R. M.; Santi, D. V.; Kuntz, I. D.; Perry, K. M. *Science* **1993**, *259*, 1445-1450.
- Siqueira, L. J. A., *Relação quantitativa entre a estrutura química e o bloqueio da transmissão neuromuscular para série de brometos de [2-(4-benzamido)etil]benzildimetilamônio para-substituídos*. 2001. Dissertação de Mestrado.
- Sousa, W. A. Estudo da Relação Entre a Estrutura Química e a toxicidade Aguda em Série de Cloreto de [2-(Benzoiloxi)Etil]Dimetilamônio Meta-Substituídos, com Atividade Anestésica Local. 4-1-1997. Dissertação de Mestrado.
- Souza, D. H. F.; Garratt, R. C.; Araujo, A. P. U.; Guimaraes, B. G.; Jesus, W. D. P.; Michels, P. A. M.; Hannaert, V.; Oliva, G. *Febs Letters* **1998**, *424*, 131-135.
- Stewart, J. J. P. *Journal of Computer-Aided Molecular Design* **1990**, *4*, 1-45.
- SYBYL program, Tripos Inc. Sybyl program, Tripos Inc. **2002**.
- Taft, R. W. Jr. in *Steric Effects in Organic Chemistry*, M. S. Newman, Ed., New York, Academic Press, 1971.
- Tavares, L. C. *Efeitos de substituintes sobre a polaridade do grupo carbonila e a atividade anestésica local de N,N-[(dimetilamino) metil] benzamidas para-substituídas*. São Paulo, 1987.
- Tavares, L. C. *Relações quantitativas entre a estrutura química e a atividade antimicrobiana de análogos à nifuroxazida*. São Paulo, 1993. Tese de Doutorado.
- Tavares, L.; AMARAL, A. T. *Rev Farm Bioquim.Univ.S.Paulo* **1997**, *33*, 123-129.
- Todeschini, R. *Analytica Chimica Acta* **1997**, *348*, 419-430.
- Todeschini, R.; Consonni, V. *Handbook of Molecular Descriptors*; WILEY - VCH: 2000; Vol. 11.
- Todeschini, R.; Consonni, V.; Maiocchi, A. *Chemometrics and Intelligent Laboratory Systems* **1999**, *46*(1), 13-29.
- Todeschini, R.; Consonni, V.; Mauri, A.; Pavan, M. DRAGON Web 3.0. **2003**.
- Todeschini, R.; Consonni, V.; Mauri, A.; Pavan, M. *Analytica Chimica Acta* **2004**, *515*, 199-208.

- Todeschini, R.; Gramatica, P. *Quantitative Structure-Activity Relationships* **1997**, *16*, 113-119.
- Todeschini, R.; Gramatica, P. *Quantitative Structure-Activity Relationships* **1997**, *16*, 120-125.
- Topliss, J. G.; Costello, R. J. *Journal of Medicinal Chemistry* **1972**, *15*, 1066-1068.
- Topliss, J. G.; Edwards, R. P. *Journal of Medicinal Chemistry* **1979**, *22*, 1238-1244.
- Tropsha, A.; Gramatica, P.; Gombar, V. K. *Qsar & Combinatorial Science* **2003**, *22*, 69-77.
- Unger, S.; Hansch, C. *Journal of Medicinal Chemistry* **1973**, *16*, 745-749.
- Unger, S. H.; Kuchar, C. M. *QSAR in Design of Bioactive Compunds* 1984. Proceedings of the 1st Telesymposium on Medicinal Chemistry.
- Viswanadhan, V. N.; Ghose, A. K.; Revankar, G. R.; Robins, R. K. *Journal of Chemical Information and Computer Sciences* **1989**, *29*, 163-172.
- Voigt, W. H.; Bock, M.; Gonnert, R. *Arzneimittel-Forschung* **1972**, *22*, 1586-&.
- Wakeling, I. N.; Morris, J. J. *Journal Of Chemometrics* **1993**, *7*, 291-304.
- WHO, World Health Organization, <http://www.who.int/tdr/diseases/> acessado em 05/01/2005.
- Wold, S.; Esbensen, K.; Geladi, P. *Chemometrics and Intelligent Laboratory Systems* **1987**, *2*, 37-52.
- Wold, S.; Sjostrom, M.; Eriksson, L. *Chemometrics and Intelligent Laboratory Systems* **2001**, *58*, 109-130.
- Zuccotto, F.; Brun, R.; Pacanowska, D. G.; Perez, L. M. R.; Gilbert, I. H. *Bioorganic & Medicinal Chemistry Letters* **1999**, *9*, 1463-1468.