

chemoinformatics

October 12, 2009

References

- [1] J. Aires-de Sousa and J. Gasteiger. Prediction of enantiomeric excess in a combinatorial library of catalytic enantioselective reactions. *J Comb Chem*, 7(2):298–301, 2005.
- [2] Rieko Arimoto, Madhu-Ashni Prasad, and Eric M Gifford. Development of CYP3A4 inhibition models: comparisons of machine-learning techniques and molecular descriptors. *J Biomol Screen*, 10(3):197–205, Apr 2005.
- [3] A. M. Aronov. Predictive in silico modeling for hERG channel blockers. *Drug Discov. Today*, 10(2):149–155, Jan 2005.
- [4] J. Bajorath. Selected concepts and investigations in compound classification, molecular descriptor analysis, and virtual screening. *J Chem Inf Comput Sci*, 41(2):233–245, 2001.
- [5] H.-J. Böhm, G. Schneider, R. Mannhold, H. Kubinyi, and G. Folkers. *Protein-ligand interactions*. Wiley, 2003.
- [6] F. Bonachéra and D. Horvath. Fuzzy tricentric pharmacophore fingerprints. 2. application of topological fuzzy pharmacophore triplets in quantitative structure-activity relationships. *J. Chem. Inf. Model.*, 48(2):409–425, Feb 2008.
- [7] F. Bonachéra, B. Parent, F. Barbosa, N. Froloff, and D. Horvath. Fuzzy tricentric pharmacophore fingerprints. 1. topological fuzzy pharmacophore triplets and adapted molecular similarity scoring schemes. *J. Chem. Inf. Model.*, 46(6):2457–2477, 2006.
- [8] Karsten M. Borgwardt and Hans-Peter Kriegel. Shortest-path kernels on graphs. In *ICDM '05: Proceedings of the Fifth IEEE International Conference on Data Mining*, pages 74–81, Washington, DC, USA, 2005. IEEE Computer Society.
- [9] Hans Briem and Judith Günther. Classifying ”kinase inhibitor-likeness” by using machine-learning methods. *Chembiochem*, 6(3):558–66, Mar 2005.

- [10] F.K. Brown. Chemoinformatics : What is it and How does it Impact Drug Discovery. *Annual Reports in Med. Chem.*, 33:375–384, 1998.
- [11] R. D. Brown and Y. C. Martin. The information content of 2D and 3D structural descriptors relevant to ligand-receptor binding. *J Chem Inf Comput Sci*, 37:1–9, 1997.
- [12] Robert D. Brown and Yvonne C. Martin. Use of Structure-Activity Data To Compare Structure-Based Clustering Methods and Descriptors for Use in Compound Selection. *J Chem Inf Comput Sci*, 36:572–584, 1996.
- [13] R. Burbidge, M. Trotter, B. Buxton, and S. Holden. Drug design by machine learning: support vector machines for pharmaceutical data analysis. *Comput. Chem.*, 26(1):4–15, December 2001.
- [14] D. Butina, M. D. Segall, and K. Frankcombe. Predicting ADME properties in silico: methods and models. *Drug Discov Today*, 7(11 Suppl):S83–S88, Jun 2002.
- [15] E. Byvatov, U. Fechner, J. Sadowski, and G. Schneider. Comparison of support vector machine and artificial neural network systems for drug/nondrug classification. *J Chem Inf Comput Sci*, 43(6):1882–9, 2003.
- [16] Evgeny Byvatov and Gisbert Schneider. SVM-based feature selection for characterization of focused compound collections. *J Chem Inf Comput Sci*, 44(3):993–9, 2004.
- [17] R. Carbó, L. Leyda, and M. Arnau. How similar is a molecule to another - an electron-density measure of similarity between 2 molecular structures. *Int. J. Quantum Chem.*, 17:1185–1189, 1980.
- [18] A. Cavalli, E. Poluzzi, F. De Ponti, and M. Recanatini. Toward a pharmacophore for drugs inducing the long QT syndrome: insights from a CoMFA study of HERG K(+) channel blockers. *J. Med. Chem.*, 45(18):3844–3853, Aug 2002.
- [19] X. Chen, A. Russinko III, and S. S. Young. Recursive Partitioning Analysis of a Large Structure-Activity Data Set Using Three-Dimensional Descriptors. *J Chem Inf Comput Sci*, 38:1054–1062, 1998.
- [20] G. Cianchetta, Y. Li, J. Kang, D. Rampe, A. Fravolini, G. Cruciani, and R. J. Vaz. Predictive models for hERG potassium channel blockers. *Bioorg. Med. Chem. Lett.*, 15(15):3637–3642, Aug 2005.
- [21] A. Coi, I. Massarelli, L. Murgia, M. Saraceno, V. Calderone, and A. M. Bianucci. Prediction of hERG potassium channel affinity by the CODESSA approach. *Bioorg. Med. Chem.*, 14(9):3153–3159, May 2006.

- [22] A.K. Debnath, R.L. Lopez de Compadre, G. Debnath, A.J. Schusterman, and C. Hansch. Structure-activity relationship of mutagenic aromatic and heteroaromatic nitro compounds. correlation with molecular orbital energies and hydrophobicity. *Journal of Medicinal Chemistry*, 34(2):786–797, 1991.
- [23] M. Deshpande, M. Kuramochi, N. Wale, and G. Karypis. Frequent Substructure-Based Approaches for Classifying Chemical Compounds. *IEEE Transactions on Knowledge and Data Engineering*, 17(8):1036–1050, August 2005.
- [24] J. Drews. Drug Discovery: A Historical Perspective. *Science*, 287:1960–1964, March 2000.
- [25] E. Dubus, I. Ijjaali, F. Petitet, and A. Michel. In Silico Classification of hERG Channel Blockers: a Knowledge-Based Strategy. *Chem. Med. Chem.*, 1(6):622–630, Jun 2006.
- [26] R. Farid, T. Day, R. A. Friesner, and R. A. Pearlstein. New insights about HERG blockade obtained from protein modeling, potential energy mapping, and docking studies. *Bioorg. Med. Chem.*, 14(9):3160–3173, May 2006.
- [27] P. Finn, S. Muggleton, D. Page, and A. Srinivasan. Pharmacophore discovery using the inductive logic programming language Progol. *Machine Learning*, 30:241–270, 1998.
- [28] A. F. Fliri, W. T. Loging, P. F. Thadeio, and R. A. Volkmann. Analysis of drug-induced effect patterns to link structure and side effects of medicines. *Nat. Chem. Biol.*, 1(7):389–397, Dec 2005.
- [29] A. F. Fliri, W. T. Loging, P. F. Thadeio, and R. A. Volkmann. Biological spectra analysis: Linking biological activity profiles to molecular structure. *Proc. Natl. Acad. Sci. USA*, 102(2):261–266, Jan 2005.
- [30] Anton F Fliri, William T Loging, Peter F Thadeio, and Robert A Volkmann. Biospectra analysis: model proteome characterizations for linking molecular structure and biological response. *J. Med. Chem.*, 48(22):6918–6925, Nov 2005.
- [31] H. Fröhlich, J. K. Wegner, F. Sieker, and A. Zell. Optimal assignment kernels for attributed molecular graphs. In *Proceedings of the 22nd international conference on Machine learning*, pages 225 – 232, New York, NY, USA, 2005. ACM Press.
- [32] J. Gasteiger and T. Engel, editors. *Cheminformatics : a Textbook*. Wiley, New York, NY, USA, 2003.

- [33] I. Halperin, B. Ma, H. Wolfson, and R. Nussinov. Principles of docking: An overview of search algorithms and a guide to scoring functions. *Proteins*, 47(4):409–443, Jun 2002.
- [34] C. Helma, T. Cramer, S. Kramer, and L. De Raedt. Data mining and machine learning techniques for the identification of mutagenicity inducing substructures and structure activity relationships of noncongeneric compounds. *J. Chem. Inf. Comput. Sci.*, 44(4):1402–11, 2004.
- [35] J. D. Holliday and P. Willett. Using a genetic algorithm to identify common structural features in sets of ligands. *J. Mol. Graph. Model.*, 15(4):221–232, Aug 1997.
- [36] D. Horvath and C. Jeandenans. Neighborhood behavior of in silico structural spaces with respect to in vitro activity spaces—a benchmark for neighborhood behavior assessment of different in silico similarity metrics. *J. Chem. Inf. Comput. Sci.*, 43(2):691–698, 2003.
- [37] T. Horváth, T. Gärtner, and S. Wrobel. Cyclic pattern kernels for predictive graph mining. In *Proceedings of the tenth ACM SIGKDD international conference on Knowledge discovery and data mining*, pages 158–167, New York, NY, USA, 2004. ACM Press.
- [38] W. L. Jorgensen. The many roles of computation in drug discovery. *Science*, 303(5665):1813–1818, Mar 2004.
- [39] H. Kashima, K. Tsuda, and A. Inokuchi. Kernels for graphs. In B. Schölkopf, K. Tsuda, and J.P. Vert, editors, *Kernel Methods in Computational Biology*, pages 155–170. MIT Press, The MIT Press, Cambridge, Massachusetts, 2004.
- [40] G. M. Keserü. Prediction of hERG potassium channel affinity by traditional and hologram qSAR methods. *Bioorg. Med. Chem. Lett.*, 13(16):2773–2775, Aug 2003.
- [41] H. Kubinyi. Comparative Molecular Field Analysis. In J. Gasteiger, editor, *Handbook of Chemoinformatics. From Data to Knowledge, Volume 4*, pages 1555–1574. Wiley-VCH, Weinheim, 2003.
- [42] C. Lemmen and T. Lengauer. Computational methods for the structural alignment of molecules. *J. Comput. Aided. Mol. Des.*, 14(3):215–232, Mar 2000.
- [43] H. Li, C. Ung, C. Yap, Y. Xue, Z. Li, Z. Cao, and Y. Chen. Prediction of genotoxicity of chemical compounds by statistical learning methods. *Chem. Res. Toxicol.*, 18(6):1071–1080, Jun 2005.
- [44] P. Lind and T. Maltseva. Support vector machines for the estimation of aqueous solubility. *J Chem Inf Comput Sci*, 43(6):1855–9, 2003.

- [45] C. A. Lipinski, F. Lombardo, B. W. Dominy, and P. J. Feeney. Experimental and computational approaches to estimate solubility and permeability in drug discovery and development settings. *Adv. Drug. Deliv. Rev.*, 46(1-3):3–26, Mar 2001.
- [46] H. X. Liu, R. S. Zhang, X. J. Yao, M. C. Liu, Z. D. Hu, and B. T. Fan. QSAR and classification models of a novel series of COX-2 selective inhibitors: 1,5-diarylimidazoles based on support vector machines. *J Comput Aided Mol Des*, 18(6):389–99, Jun 2004.
- [47] P. Mahé, L. Ralaivola, V. Stoven, and J.-P. Vert. The pharmacophore kernel for virtual screening with support vector machines. Technical Report Technical Report HAL:ccsd-00020066, Ecole des Mines de Paris, march 2006.
- [48] P. Mahé, L. Ralaivola, V. Stoven, and J.-P. Vert. The pharmacophore kernel for virtual screening with support vector machines. *J. Chem. Inf. Model.*, 46(5):2003–2014, 2006.
- [49] P. Mahé, N. Ueda, T. Akutsu, J.-L. Perret, and J.-P. Vert. Extensions of marginalized graph kernels. In R. Greiner and D. Schuurmans, editors, *Proceedings of the Twenty-First International Conference on Machine Learning (ICML 2004)*, pages 552–559. ACM Press, 2004.
- [50] P. Mahé, N. Ueda, T. Akutsu, J.-L. Perret, and J.-P. Vert. Graph kernels for molecular structure-activity relationship analysis with support vector machines. *J. Chem. Inf. Model.*, 45(4):939–51, 2005.
- [51] P. Mahé and J.-P. Vert. Graph kernels based on tree patterns for molecules. Technical Report ccsd-00095488, HAL, September 2006.
- [52] C. Manly, S. Louise-May, and J. Hammer. The impact of informatics and computational chemistry on synthesis and screening. *Drug Discov. Today*, 6(21):1101–1110, Nov 2001.
- [53] H. Matter and T. Pötter. Comparing 3D pharmacophore triplets and 2D fingerprints for selecting diverse compound subsets. *J. Chem. Inf. Comput. Sci.*, 39(6):1211–1225, 1999.
- [54] Christian Merkwirth, Harald Mauser, Tanja Schulz-Gasch, Olivier Roche, Martin Stahl, and Thomas Lengauer. Ensemble methods for classification in cheminformatics. *J Chem Inf Comput Sci*, 44(6):1971–8, 2004.
- [55] S. Miertus, G. Fassina, and P.F. Seneci. Concepts of Combinatorial Chemistry and Combinatorial Technologies. *Chemické Listy*, 94:1104–1110, 2000.
- [56] G. Moreau and P. Broto. Autocorrelation of molecular structures: Application to SAR studies. *Nouv. J. Chim.*, 757:764, 1980.

- [57] K.-R. Müller, G. Rätsch, S. Sonnenburg, S. Mika, M. Grimm, and N. Heinrich. Classifying 'drug-likeness' with Kernel-based learning methods. *J Chem Inf Model*, 45(2):249–53, 2005.
- [58] R. Pearlstein, R. Vaz, and D. Rampe. Understanding the structure-activity relationship of the human ether-a-go-go-related gene cardiac K⁺ channel. A model for bad behavior. *J. Med. Chem.*, 46(11):2017–2022, May 2003.
- [59] R. A. Pearlstein, R. J. Vaz, J. Kang, X.-L. Chen, M. Preobrazhenskaya, A. E. Shchekotikhin, A. M. Korolev, L. N. Lysenkova, O. V. Miroshnikova, J. Hendrix, and D. Rampe. Characterization of HERG potassium channel inhibition using CoMSiA 3D QSAR and homology modeling approaches. *Bioorg Med Chem Lett*, 13(10):1829–1835, May 2003.
- [60] S. D. Pickett, J. S. Mason, and I. M. McLay. Diversity profiling and design using 3D pharmacophores : Pharmacophores-Derived Queries (PQD). *J. Chem. Inf. Comput. Sci.*, 36(6):1214–1223, 1996.
- [61] L. Ralaivola, S. J. Swamidass, H. Saigo, and P. Baldi. Graph kernels for chemical informatics. *Neural Netw.*, 18(8):1093–1110, Sep 2005.
- [62] J. Ramon and T. Gärtner. Expressivity versus efficiency of graph kernels. In T. Washio and L. De Raedt, editors, *Proceedings of the First International Workshop on Mining Graphs, Trees and Sequences*, pages 65–74, 2003.
- [63] O. Roche, G. Trube, J. Zuegge, P. Pfimlin, A. Alanine, and G. Schneider. A virtual screening method for prediction of the HERG potassium channel liability of compound libraries. *Chembiochem*, 3(5):455–459, May 2002.
- [64] G. Rücker and C. Rücker. Counts of All Walks as Atomic and Molecular Descriptors. *J Chem Inf Comput Sci*, 33:683–695, 1993.
- [65] J. Saeh, P. Lyne, B. Takasaki, and D. Cosgrove. Lead hopping using SVM and 3D pharmacophore fingerprints. *J Chem Inf Model*, 45(4):1122–1133, Jul 2005.
- [66] M. Song and M. Clark. Development and evaluation of an in silico model for hERG binding. *J. Chem. Inf. Model.*, 46(1):392–400, 2006.
- [67] J. J. Sutherland, L. A. O'Brien, and D. F. Weaver. Spline-fitting with a genetic algorithm: a method for developing classification structure-activity relationships. *J. Chem. Inf. Comput. Sci.*, 43(6):1906–1915, 2003.
- [68] M. Tobita, T. Nishikawa, and R. Nagashima. A discriminant model constructed by the support vector machine method for HERG potassium channel inhibitors. *Bioorg. Med. Chem. Lett.*, 15(11):2886–90, Jun 2005.
- [69] R. Todeschini and V. Consonni. *Handbook of Molecular Descriptors*. Wiley-VCH, New York, 2002.

- [70] J. Xu and A. Hagler. Chemoinformatics and Drug Discovery. *Molecules*, 7:566–600, 2002.
- [71] L. Xue and J. Bajorath. Molecular descriptors in chemoinformatics, computational combinatorial chemistry, and virtual screening. *Comb. Chem. High. Throughput Screen.*, 3(5):363–372, Oct 2000.
- [72] X. J. Yao, A. Panaye, J. P. Doucet, R. S. Zhang, H. F. Chen, M. C. Liu, Z. D. Hu, and B. T. Fan. Comparative study of QSAR/QSPR correlations using support vector machines, radial basis function neural networks, and multiple linear regression. *J Chem Inf Comput Sci*, 44(4):1257–66, 2004.
- [73] C. W. Yap, C. Z. Cai, Y. Xue, and Y. Z. Chen. Prediction of torsade-causing potential of drugs by support vector machine approach. *Toxicol Sci*, 79(1):170–7, May 2004.
- [74] C. W. Yap and Y. Z. Chen. Prediction of Cytochrome P450 3A4, 2D6, and 2C9 Inhibitors and Substrates by Using Support Vector Machines. *J Chem Inf Model*, 45(4):982–92, 2005.
- [75] V. V. Zernov, K. V. Balakin, A. A. Ivaschenko, N. P. Savchuk, and I. V. Pletnev. Drug discovery using support vector machines. The case studies of drug-likeness, agrochemical-likeness, and enzyme inhibition predictions. *J Chem Inf Comput Sci*, 43(6):2048–56, 2003.