List of References for COMBINE Analysis

January 2008-01-24

1. Ortiz, A.R., et al., *Prediction of drug binding affinities by comparative binding energy analysis.* J. Med. Chem., 1995. **38**: p. 2681-2691.
2. Ortiz, A.R., et al., *Reliability of comparative molecular field analysis models: effects of data scaling and variable selection using a set of human synovial fluid phospholipase A2 inhibitors.* J Med Chem., 1997. **40**: p. 1136-1148.
3. Pastor, M., C. Perez, and F. Gago, *Simulation of alternative binding modes in a structure-based QSAR study of HIV-1 protease inhibitors.* J Mol Graph Model, 1997. **15**(6): p. 364-71, 389.
4. Perez, C., et al., *Comparative binding energy analysis of HIV-1 protease inhibitors: incorporation of solvent effects and validation as a powerful tool in receptor-based drug design.* J. Med. Chem., 1998. **41**: p. 836-852.
5. Wade, R.C., A.R. Oritz, and F. Gago, *Comparative binding energy analysis.* Perspectives in Drug Discovery and Design, 1998. **9**: p. 19-34.
6. Hasegawa, K., T. Kimura, and K. Funatsu, *GA Strategy for Variable Selection in QSAR Studies: Enhancement of Comparative Molecular Binding Energy Analysis by GA-Based PLS Method.* Quantitative Structure-Activity Relationships, 1999. **18**(3): p. 262-272.
7. Lozano, J.J., et al., *3D-QSAR methods on the basis of ligand-receptor complexes. Application of COMBINE and GRID/GOLPE methodologies to a series of CYP1A2 ligands.* J Comput Aided Mol Des, 2000. **14**(4): p. 341-53.
8. Pastor, M., F. Gago, and G. Cruciani, *Comparative binding energy (COMBINE) analysis on a series of glycogen phosphorylase inhibitors: comparison with GRID/GOLPE methods.*, in *Molecular Modeling and Prediction of Bioactivity*, K. Gundertofter and F.S. Jorgensen, Editors. 2000, Kluwer: New York. p. 329-330.
9. Tomic, S., L. Nilsson, and R.C. Wade, *Nuclear receptor-DNA binding specificity: A COMBINE and Free-Wilson QSAR analysis.* J Med Chem, 2000. **43**(9): p. 1780-92.
10. Cuevas, C., et al., *Comparative binding energy (COMBINE) analysis of human neutrophil elastase inhibition by pyridone-containing trifluoromethylketones.* Comb Chem High Throughput Screen, 2001. **4**(8): p. 627-42.
11. Kmunicek, J., et al., *Comparative binding energy (COMBINE) analysis of the substrate specificity of haloalkane dehalogenase from xanthobacter autotrophicus GJ10.* Biochemistry, 2001. **40**: p. 8905-8917.
12. Tomic, S. and R.C. Wade, *COMBINE analysis of nuclear receptor-DNA binding specificity: Comparison of two datasets.* Croat. Chem. Acta, 2001. **74**: p. 295-314.
13. Wade, R.C., *Derivation of QSARs using 3D structural models of protien-ligand complexes by COMBINE analysis*, in *Rational Approaches to Drug Design: 13th European Symposium on Quantitative Structure-Activity Relationships*, H.-D. Holtje and W. Sippl, Editors. 2001, Prous Science S. A.: Barcelona. p. 23-28.
14. Wang, T. and R.C. Wade, *COMBINE 3D-QSAR analysis of influenza neuraminidase inhibitors*, in *Rational Approaches to Drug Design: 13th European Symposium on Quantitative Structure-Activity Relationships*, H.-D. Holtje and W. Sippl, Editors. 2001, Prous Science S. A.: Barcelona. p. 78-82.
15. Wang, T. and R.C. Wade, *Comparative binding energy (COMBINE) analysis of influenza neuraminidase-inhibitor complexes.* J Med Chem, 2001. **44**: p. 961-671.
16. Tomic, S. and B. Kojic-Prodic, *A quantitative model for predicting enzyme enantioselectivity: Application to burkholderia cepacia lipase and 3-(aryloxy)-1,2-propanediol derivatives.* J. Mol. Graph. Model., 2002. **21**(3): p. 241-252.

17. Wang, T. and R.C. Wade, *Comparative binding energy (COMBINE) analysis of OppA-peptide complexes to relate structure to binding thermodynamics.* J. Med. Chem., 2002. **45**: p. 4828-4837.
18. Kmunicek, J., et al., *Comparative binding energy analysis of haloalkane dehalogenase substrates: modelling of enzyme-substrate complexes by molecular docking and quantum mechanical calculations.* J Comput Aided Mol Des, 2003. **17**(5-6): p. 299-311.
19. Damborsky, J., et al., *Rational re-design of haloalkane dehalogenases guided by comparative binding energy analysis*, in *Enzyme Functionality: Design, Engineering and Screening*, A. Svendsen and M. Dekker, Editors. 2004, ISBN:0-8247-4709-7: New York. p. 79-96.
20. Guo, J., et al., *A Docking Score Function for Estimating Ligand-Protein Interactions: Application to Acetylcholinesterase Inhibition.* J. Med. Chem., 2004. **47**(22): p. 5492-5500.
21. Kim, H.J., et al., *Computational studies of COX-2 inhibitors: 3D-QSAR and docking.* Bioorg Med Chem, 2004. **12**(7): p. 1629-41.
22. Martin-Santamaria, S., et al., *Modulation of binding strength in several classes of active site inhibitors of acetylcholinesterase studied by comparative binding energy analysis.* J Med Chem, 2004. **47**(18): p. 4471-82.
23. Murcia, M. and A.R. Ortiz, *Virtual screening with flexible docking and COMBINE-based models. Application to a series of factor Xa inhibitors.* J Med Chem, 2004. **47**(4): p. 805-20.
24. Rodriguez-Barrios, F. and F. Gago, *Chemometrical identification of mutations in HIV-1 reverse transcriptase conferring resistance or enhanced sensitivity to arylsulfonylbenzonitriles.* J Am Chem Soc, 2004. **126**(9): p. 2718-9.
25. Schleinkofer, K., et al., *Comparative structural and energetic analysis of WW domain-peptide interactions.* J Mol Biol, 2004: p. In press.
26. Wade, R.C., S. Henrich, and T. Wang, *Using 3D protein structures to derive 3D-QSARs.* Drug Discovery Today: Technologies, 2004. **1**(3): p. 241-246.
27. Wang, T., et al., *How optimal are the binding energetics of barnase and barstar?* Biophys J, 2004. **87**(3): p. 1618-30.
28. Kmunicek, J., et al., *Quantitative analysis of substrate specificity of haloalkane dehalogenase LinB from Sphingomonas paucimobilis UT26.* Biochemistry, 2005. **44**(9): p. 3390-401.
29. Murcia, M., A. Morreale, and A.R. Ortiz, *COMBINE analysis considering multiple receptors: a step towards structure-activity models for protein families.* J. Med. Chem., 2006. **49**: p. 6241-6253.
30. Peters, M.B. and K.M. Merz, *Semiempirical Comparative Binding Energy Analysis (SE-COMBINE) of a Series of Trypsin Inhibitors.* J. Chem. Theory Comput., 2006. **2**(2): p. 383-399.
31. Lushington, G.H., J.X. Guo, and J.L. Wang, *Whither combine? New opportunities for receptor-based QSAR.* Curr Med Chem, 2007. **14**(17): p. 1863-77.