

Donald F. Weaver

Medicinal Chemistry

1. A. Y. Jin, F. Y. Leung, D. F. Weaver. "Three variations of genetic algorithm for searching biomolecular conformation space: Comparison of GAP 1.0, 2.0, and 3.0. *Journal of Computational Chemistry*: 20 (13), 1999: 1329-1342A
2. P. Milne, M. Ho, D. F. Weaver. Interaction of anticonvulsant drugs with metals: a semi-empirical molecular orbital study of phenytoin-zinc(II) complexation. *Journal of Molecular Structure (Theochem)* 492:19-28. 1999
3. I. Shamovksy, G. Ross, R. Riopelle, D. Weaver. The interaction of neurotrophins with the p75NTR common neurotrophin receptor: a comprehensive molecular modeling study. *Protein Sci* 1999. 8(11):2223-33
4. I. Shamovsky, G. Ross, R. Riopelle, D. Weaver. "Theoretical and Biochemical Studies on the Selectivity of Nerve Growth Factor for Transition Metal Cations." *J. Am. Chem. Soc.* 1999; 121(42); 9797-9806.
5. G. Duan, V. Smith, D. Weaver. "An ab initio and data mining study on aromatic-amide interactions" *Chem Phys Letters* 310: 323-332. 1999.
6. S. Marone, I. Rozas, D. Weaver*. "Theoretical Structural Analyses of Tricyclic Neuroactive Drugs: Quantum Pharmacologic Descriptors for Clustering Anticonvulsant, Antidepressant, and Antipsychotic Activities", *Journal of Molecular Structure (Theochem)* 467, 25-30 (1999).
7. G. Duan, V. H. Smith, Jr., D.F. Weaver. "A Data Mining and *Ab Initio* Study of the Interaction between the Aromatic and Backbone Amide Groups in Proteins." *Int. J Quant Chem* (2000)
8. M. W. Jones, W. T. Blume, A. Guberman, M. A. Lee, N. Pillay, D. F. Weaver, F. Veloso, T. A. H. Holdich. Ramacemide Hydrochloride as an add-on therapy in epilepsy: A randomized, placebo-controlled trial of three dose levels (300, 600 and 800 mg/day) in a bid regimen. submitted *Epilepsia*. 2000.
9. G. Duan, V. H. Smith, Jr., and D. F. Weaver. "Characterization of Aromatic-Amide(Side-Chain) Interactions in Proteins through Systematic ab Initio Calculations and Data Mining Analyses", *J. Phys Chem. A* 104: 4521-4532. 2000.

10. M. Ho, B. J. Clark, D.F. Weaver, V. H. Smith, Jr., C. Gatti, R. P. Sagar, and R. O. Esquivel, "Shannon Information Entropies of molecules and functional groups in the Self-Consistent Reaction Field", J. Chem. Phys., accepted
11. D. Weaver. "Epilepsy: A Handbook for Patients and their Families" Key-Porter Books. in press.
12. S Kim, D. Weaver. "Theoretical Studies on Alzheimer's Disease: structures of β -amyloid Aggregates", *Theochem* 527: 127-138 (2000).
13. D. Weaver. *Epilepsy Research in the 21st Century*. Lumina. Spring 2000. 8.
14. J. Bruni, A. Guberman, L. Vachon, C. Desforges, M. A. Lee, R. McLachlan, A. Ogunyemi, N. Pillay, S. Purves, M. Sadler, E. Starreveld, D. Weaver. Vigabatrin as add-on therapy for adult complex partial seizures: a double-blind, placebo-controlled multicentre study. *Seizure* 9: 224-232 2000.
15. A. Guberman, J. Bruni, M. Jones, M. A. Lee, R. McLachlan, A. Ogunyemi, N. Pillay, M. Sadler, E. Starreveld, D. Weaver. "Long-term open multicentre, add-on trial of vigabatrin in adult resistant partial epilepsy" *Seizure* 9(2): 112-118. 2000.
16. A. Pollard, D. Mewhort, D. Weaver, (editors). *High Performance Computing Systems and Applications*. Kluwer Academic Publishers. 2000.
17. I. L. Shamovsky, G. M. Ross, R. J. Riopelle and D. F. Weaver. "Molecular Modeling of the Interaction of Neurotrophins with the P75^{NTR} Common Neurotrophin Receptor" in *High Performance Computing Systems and Applications*. eds. A. Pollard, D.J.K. Mewhort and D.F. Weaver, Kluwer Academic, Massachusetts, 2000, pp.99-113.
18. M. Ho, H. L. Schmider, D. F. Weaver, V. H. Smith, Jr., R. P. Sagar and R. O. Esquivel, "Shannon Entropy of Chemical Changes: S_N2 Displacement Reactions", *Int. J. Quantum Chem.*, 77, 376 (2000).
19. D. Weaver. "A Clinical Examination Technique for Mild Upper Motor Neuron Paresis of the Arm". *Neurology* 54(2): 531. 2000.