

BIOGRAPHICAL SKETCH

Provide the following information for the key personnel in the order listed for Form Page 2.
Follow the sample format for each person. **DO NOT EXCEED FOUR PAGES.**

| NAME Curtis M. Breneman | | POSITION TITLE Professor of Chemistry | |
|---|----------------------------------|--|-------------------------|
| EDUCATION/TRAINING <i>(Begin with baccalaureate or other initial professional education, such as nursing, and include postdoctoral training.)</i> | | | |
| INSTITUTION AND LOCATION | DEGREE <i>(if applicable)</i> | YEAR(s) | FIELD OF STUDY |
| University of California, Los Angeles | B.S. | 1980 | Chemistry |
| University of California, Santa Barbara | Ph.D. | 1987 | Chemistry |
| Yale University, New Haven, CT | Post Doc | 1987-89 | Computational Chemistry |

Employment Tandy Corporation Computer Marketing Representative Santa Monica, Los Angeles, Santa Barbara and Beverly Hills, Calif (Full Time) May 1981 - August 1981 (Part Time) June 1975 - April 1981 University of California, Santa Barbara Associate Lecturer, Honors Chemistry Program 1985-1987 Yale University Postdoctoral Research Fellow 1987 - 1989 Research Advisor: Prof. Kenneth B. Wiberg Rensselaer Polytechnic Institute, Troy, New York 7/89 - 6/95 Assistant Professor of Chemistry 7/95 - 11/02 Associate Professor of Chemistry 1/03 - Now Professor of Chemistry Honors and Awards 2003 Nominated for Editor-in-Chief of the Journal of Chemical Information and Computer Science 2002 Re-elected Treasurer of the ACS Division of Computers in Chemistry 1999 Best Paper Award at the SMCia/99 "1999 IEEE Midnight-Sun Workshop on Soft Computing Methods in Industrial Applications for "A Soft Computing Approach for the design of Novel Pharmaceuticals" (Helsinki, Finland, 1999) 1999 Elected Treasurer of the ACS Division of Computers in Chemistry 1999 Nominated for the Board of Directors of the International QSAR Society 1998 Appointed to the Editorial Board, Journal of Computer Graphics and Modelling

Publications relevant to the proposed work

- C.M. Breneman, C.M. Sundling, N. Sukumar, L. Shen, W.P. Katt, and M.J. Embrechts "New Developments in PEST shape/property Hybrid Descriptors", *Journal of Computer-Aided Molecular Design*, 17, 231-240, 2003
- Jinbo Bi, Kristin Bennett, Mark Embrechts, Curt Breneman, Minghu Song; Dimensionality Reduction via Sparse Support Vector Machines" *Journal of Machine Learning Research*, 3(Mar):1229-1243, 2003.
- C. E. Whitehead, C.M. Breneman N. Sukumar and M.D. Ryan, "Transferable Atom Equivalent Multi-Centered Multipole Expansion Method", *J. Comp. Chem. (Special Issue on electron densities and electrostatic potentials) – S. R. Gadre*, Ed.24(4), 512-529 MAR 2003.
- M. Song, C.M. Breneman, J. Bi, N. Sukumar, K.P. Bennett, S. Cramer, and N. Tugcu, "Prediction of Protein Retention Times in Anion-exchange Chromatography Systems using Support Vector Machine Regression", *JCICS (Journal of Chemical Information and Computer Science)*, 42(6), 1347-1357 NOV-DEC 2002. See: <http://dx.doi.org/10.1021/ci025580t>
- C. B. Mazza, C. E. Whitehead, C. M. Breneman and Steven M. Cramer, "Predictive Quantitative Structure-Retention Relationship Models for Ion-Exchange Chromatography" *Chromatographia*, 56(3-4), 147-152, 2002.
- N. Tugcu, C. Mazza, C. Breneman, Y. Sanghvi, J. Moore and S. M. Cramer, "High Throughput Screening and Quantitative Structure-Efficacy Relationship Models for Designing Displacers for Anti-sense Oligonucleotide Purification in Anion-Exchange Systems", *Separation Science and Technology*. 37(7) 1667-1681, 2002
- C. B. Mazza, K. Rege, C. M. Breneman, J. S. Dordick and S. M. Cramer. "High Throughput Screening and Quantitative-Structure Efficacy Relationship Models of Potential Displacer Molecules for Ion Exchange Systems". *Biotechnology and Bioengineering* 80(1), 60-72, 2002
- Mazza, C.B., Sukumar, N., Breneman, C.M. and Cramer, S.M., "Prediction of Protein Retention in Ion-Exchange Systems Using Molecular Descriptors Obtained from Crystal Structure", *Analytical Chemistry*, 73(22) 5457-5461 2001
- Robert H. Kewley, Mark J. Embrechts and Curt Breneman, "Data Strip Mining for the Virtual Design of Pharmaceuticals with Neural Networks," *IEEE Transactions on Neural Networks*, Vol.11, No 3, pp. 668 – 679, May 2000.
- Fabio Arciniegas, Kristin Bennett, Curt Breneman, and Mark J. Embrechts, "Molecular Database Mining using Self-Organizing Maps for the Design of Novel Pharmaceuticals," in *Intelligent Engineering Systems through Artificial Neural Networks: Smart Engineering System Design: Vol. 10*, C. H. Dagli et al., Eds, ASME Press, pp. 477 – 482 (2000).
- Robert Kewley, Mark J. Embrechts, and Curt Breneman, "Neural Network Sensitivity Analysis and Cross-Validation for Data Strip Mining Problems," in *Intelligent Engineering Systems through Artificial Neural Networks*, Vol. 8, Cihan Dagli et al., eds., pp. 391 - 396, ASME Press (1998).
- Mark J. Embrechts, Robert Kewley, Jr., and Curt Breneman, "Computationally Intelligent Data Mining for the Automated Discovery of Novel Pharmaceuticals," in *Intelligent Engineering Systems through Artificial Neural Networks*, Vol. 8, Cihan Dagli et al., eds., pp. 397 - 403, ASME Press (1998).
- C.M. Breneman and M. Rhem, "A QSPR Analysis of HPLC Column Capacity Factors for a set of High-Energy Materials Using Electronic Van der Waals Surface Property Descriptors Computed by the Transferable Atom Equivalent Method." *J. Comp. Chem.* 1997 18(2),182-197.

C.M. Breneman, T.R. Thompson, M. Rhem, and M. Dung, "Electron Density Modeling of Large Systems Using the Transferable Atom Equivalent Method" Computers & Chemistry, 1995, 19(3), 161-179.

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KDI - Automated Design and Discovery of Novel Pharmaceuticals Using Semi-Supervised Learning in Large Molecular Databases.

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Low Molecular Weight Displacers for Protein Purification

National Institute of Health

Co-P.I.'s S. Cramer, J. Moore, C. Breneman, and J. Dordick

funding period 5/1/03-5/1/07

Protein Bioprocessing with Hydrophobic Separations Media

NSF

Co-PI's Dr. Todd Przybycien, Dr. Steven Cramer, Dr. C. Breneman, Dr. Erik Fernandez, Dr. John O'Connell

Funding period 9/02-9/06

Quantitative Combinatorial Design of Displacers and Affinity Ligands

NSF

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Eastman Kodak Company • 2/2000 (Unrestricted gift supporting TAE method development)

Eastman Kodak Company: • 1/1999 (Unrestricted gift supporting TAE method development)

Principal Investigator/Program Director (Last, First, Middle): **Cramer, Steven**