Bibliography

[1] Protein Data Bank (PBD). http://www.rcsb.org/pdb/.

[2] *Amira – User's Guide and Reference Manual* as well as *Amira Programmer's Guide*. Zuse Institute Berlin (ZIB) and Indeed - Visual Concepts GmbH, Berlin, http://www.amiravis.com, 2001.

[3] *AmiraMol, AmiraDeconv - Extensions for Amira 3.1.* Zuse Institute Berlin (ZIB) and Mercury Computer Systems - TGS Group, http://amira.zib.de/Amira31-MolDeconv-manual.pdf, 2003.

[4] Tipranavir. Boehringer Ingelheim Pharmaceuticals, Inc., 2005. Anti-Viral Drugs Advisory Committee (AVDAC) Briefing Document.

[5] Tatsuya Akutsu. A polynomial time algorithm for finding a largest common subgraph of almost trees of bounded degree. *IEICE Trans. Fundamentals E76-A*, pages 1488–1493, 1993.

[6] Tatsuya Akutsu. Protein structure alignment using dynamic programming and iterative improvement. *IEICE Transactions on Information and Systems*, 12:1629–1636, 1996.

[7] Mike P. Allen and Dominic J. Tildesley. *Computer Simulations of Liquids.* Clarendon, Oxford, 1987.

[8] Mathias Alterman. *Design and Synthesis of HIV-1 Protease Inhibitors.* PhD thesis, University of Uppsala, Sweden, 2001.

[9] Peter Atkins and Julio de Paula. *Physical Chemistry.* Oxford, 7 edition, 2002.

[10] Dukka Bahadur K.C., Tatsuya Akutsu, Etsuji Tomita, Tomokazu Seki, and Asao Fujiyama. Point matching under non-uniform distortions and protein side chain packing based on an efficient maximum clique algorithm. *Genome Informatics*, 13:143–152, 2002.

[11] Maha T. Barakat and Philip M. Dean. Molecular structure matching by simulated annealing, III. The incorporation of null correspondences into the matching problem. *Journal of Computer-Aided Molecular Design*, 5:107–117, 1991.

[12] Gill Barequet and Micha Sharir. Partial surface matching by using directed footprints. *Computational Geometry*, 12(1-2):45–62, 1999.

[13] Markus Bauer, Gunnar W. Klau, and Knut Reinert. Fast and accurate structural RNA alignment by progressive Lagrangian optimization. In *Computational Life Sciences: First International Symposium, CompLife 2005*, volume 3695 of *Lecture Notes on Computer Science*, pages 217–228, Konstanz, Germany, 2005. Springer.

[14] Markus Bauer, Gunnar W. Klau, and Knut Reinert. Multiple structural RNA alignment with Lagrangian relaxation. In *Algorithms in Bioinformatics, 5th International Workshop, WABI 2005, Proceedings*, pages 303–314, 2005.

[15] Daniel Baum. Multiple Semi-flexible 3D Superposition of Drug-sized Molecules. In *Computational Life Sciences: First International Symposium, CompLife 2005*, volume 3695 of *Lecture Notes on Computer Science*, pages 198–207, Konstanz, Germany, 2005. Springer.

[16] Daniel Baum and Hans-Christian Hege. A Point-Matching Based Algorithm for 3D Surface Alignment of Drug-Sized Molecules. In *Computational Life Sciences: Second International Symposium, CompLife 2006*, volume 4216 of *Lecture Notes on Computer Science*, pages 183–193, Cambridge, UK, 2006. Springer.

[17] Daniel Runge (Baum). Algorithms and methods for the visualization of molecular surfaces and interfaces. Diploma thesis, Humboldt Universität zu Berlin and Zuse Institute Berlin (ZIB), 1999.

[18] Barnard Chemical Information Ldt., http://www.bci1.demon.co.uk.

[19] Niko Beerenwinkel. *Computational Analysis of HIV Drug Resistance Data*. Doctoral thesis, Universität des Saarlandes, Germany, 2004.

[20] Guy W. Bemis and Irwin D. Kuntz. A fast and efficient method for 2D and 3D molecular shape description. *Journal of Computer-Aided Molecular Design*, 6(6):607–628, 1992.

[21] Andreas Bender. *Studies on Molecular Similarity*. PhD thesis, Darwin College, University of Cambridge, UK, 2005.

[22] Andreas Bender, Andreas Klamt, Karin Wichmann, Michael Thormann, and Robert C. Glen. Molecular similarity searching using COSMO screening charges (COSMO/3PP). In *Computational Life Sciences: First International Symposium, CompLife 2005*, volume 3695 of *Lecture Notes on Computer Science*, pages 175–185, Konstanz, Germany, 2005. Springer.

[23] Andreas Bender, Hamse Y. Mussa, Gurprem S. Gill, and Robert C. Glen. Molecular surface point environments for virtual screening and the elucidation of binding patterns (MOLPRINT 3D). *Journal of Medicinal Chemistry*, 47:6569–6583, 2004.

[24] Denise D. Beusen and Garland R. Marshall. Pharmacophores definition using the active analog approach. In Osman F. Güner, editor, *Pharmacophore - Perception, Development, and Use in Drug Design*, pages 24–45. IUL Biotechnology Series, 1999.

[25] Denise D. Beusen and E. F. Berkley Shands. Systematic search strategies in conformational analysis. *Drug Discovery Today*, 1(10):429–437, 1996.

[26] Jonas Boström. Reproducing the conformations of protein-bound ligands: A critical evaluation of several popular conformational searching tools. *Journal of Computer-Aided Molecular Design*, 15(12):1137–1152, 2001.

[27] Heinrich Braun and Martin Riedmiller. Rprop: A fast and robust backpropagation learning strategy. In *Proceedings of the Fourth Australian Conference on Neural Networks*, pages 598–591, 1993.

[28] Andrew T. Brint and Peter Willett. Algorithms for the identification of three-dimensional maximal common substructures. *Journal of Chemical Information and Computer Sciences*, 27:152–158, 1987.

[29] Andrew T. Brint and Peter Willett. Pharmacophoric pattern matching in files of 3d chemical structures: comparison of geometric searching algorithms. *Journal of Molecular Graphics*, 5(1):49–56, 1987.

[30] Coen Bron and Joep Kerbosch. Algorithm 457: Finding all cliques of an undirected graph. *Communications of the ACM*, 16(9):575–577, 1973.

[31] Alberto Caprara and Giuseppe Lancia. Structural alignment of large-size proteins via Lagrangian relaxation. In *RECOMB*, pages 100–108, 2002.

[32] Raymond E. Carhart, Dennis H. Smith, and R. Venkataraghavan. Atom pairs as molecular features in structure-activity studies: Definition and applications. *Journal of Chemical Information and Computer Sciences*, 25:64–73, 1985.

[33] George Chang, Wayne C. Guida, and W. Clark Still. An internal coordinate Monte-Carlo method for searching conformational space. *Journal of the Association of Computing Machinery*, 111:4379–4386, 1989.

[34] Thomas H. Cormen, Charles E. Leiserson, Ronald L. Rivest, and Clifford Stein. *Introduction to Algorithms.* MIT Press and McGraw-Hill, 2nd edition, 2001.

[35] David A. Cosgrove, Denis M. Bayada, and A. Peter Johnson. A novel method of aligning molecules by local surface shape similarity. *Journal of Computer-Aided Molecular Design*, 14(6):573–591, 2000.

[36] Gordon M. Crippen. *Distance Geometry and Conformational Calculations.* J. Wiley, New York, 1981.

[37] Daylight Chemical Information Systems, Inc., http://www.daylight.com.

[38] *Daylight Theory Manual, Daylight Version 4.9, Release Date 04/17/06.* Daylight Chemical Information Systems, Inc., http://www.daylight.com/dayhtml/doc/theory/index.html, 2006.

[39] Mark de Berg, Otfried Schwarzkopf, Marc van Kreveld, and Mark Overmars. *Computational Geometry: Algorithms and Applications.* Springer, 1997.

[40] Philip M. Dean and P. Callow. Molecular recognition: Identification of local minima for matching in rotational 3-space by cluster analysis. *Journal of Molecular Graphics*, 5(3):159–164, 1987.

[41] Philip M. Dean and P.-L. Chau. Molecular recognition: Optimized searching through rotational 3-space for pattern matches on molecular surfaces. *Journal of Molecular Graphics*, 5(3):152–158, 1987.

[42] Peter Deuflhard. From molecular dynamics to conformation dynamics in drug design. In M. Kirkilionis, S. Krömker, R. Rannacher, and F. Tomi, editors, *Trends in Nonlinear Analysis*, pages 269–287. Springer, 2003.

[43] Peter Deuflhard, Michael Dellnitz, Oliver Junge, and Christof Schütte. Computation of essential molecular dynamics by subdivision techniques. In P. Deuflhard et al., editor, *Lecture Notes in Computational Science and Engineering*, volume 4, pages 98–115. Springer, 1998.

[44] Peter Deuflhard, Wilhelm Huisinga, Alexander Fischer, and Christof Schütte. Identification of almost invariant aggregates in reversible nearly uncoupled markov chains. *Linear Algebra and its Applications*, 315:39–59, 2000.

[45] Peter Deuflhard and Marcus Weber. Robust Perron cluster analysis in conformation dynamics. In M. Dellnitz, S. Kirkland, M. Neumann, and Ch. Schütte, editors, *Lin. Alg. Appl. - Special Issue on Matrices and Mathematical Biology*, volume 398, pages 161–184. Elsevier, 2005.

[46] Oliver Deussen, Stefan Hiller, Cornelius W. A. M. van Overveld, and Thomas Strothotte. Floating points: A method for computing stipple drawings. *Comput. Graph. Forum*, 19(3), 2000.

[47] James Devillers, editor. *Genetic Algorithms in Molecular Modeling.* Academic Press, 1996.

[48] Reinhard Diestel. *Graph Theory.* Springer, 1997.

[49] John H. Van Drie. Future directions in pharmacophore discovery. In Osman F. Güner, editor, *Pharmacophore - Perception, Development, and Use in Drug Design*, pages 515–530. IUL Biotechnology Series, 1999.

[50] John H. Van Drie, David Weininger, and Yvonne C. Martin. ALADDIN: An integrated tool for computer-assisted molecular design and pharmacophore recognition

from geometric, steric, and substructure searching of three-dimensional molecular structures. *Journal of Computer-Aided Molecular Design*, 3:225–251, 1989.

[51] Qiang Du, Vance Faber, and Max Gunzburger. Centroidal Voronoi tesselations: Applications and algorithms. *SIAM Rev.*, 41(4):637–677, 1999.

[52] Bruce S. Duncan and Arthur J. Olson. Approximation and characterization of molecular surfaces. *Biopolymers*, 33(2):219–229, 1993.

[53] Bruce S. Duncan and Arthur J. Olson. Shape analysis of molecular surfaces. *Biopolymers*, 33(2):231–238, 1993.

[54] Paul Ehrlich. *Dtsch. Chem. Ges.*, 42:17, 1909.

[55] Thomas E. Exner, Matthias Keil, and Jürgen Brickmann. Pattern recognition strategies for molecular surfaces. I. Pattern generation using fuzzy set theory. *Journal of Computational Chemistry*, 23(12):1176–1187, 2002.

[56] Thomas E. Exner, Matthias Keil, and Jürgen Brickmann. Pattern recognition strategies for molecular surfaces. II. Surface complementarity. *Journal of Computational Chemistry*, 23(12):1188–1197, 2002.

[57] Paul W. Finn, Lydia E. Kavraki, Jean-Claude Latombe, Rajeev Motwani, Christian R. Shelton, Suresh Venkatasubramanian, and A. Yao. RAPID: Randomized pharmacophore identification for drug design. In *Proceedings of the thirteenth annual symposium on Computational geometry*, pages 324–333. ACM Press, 1997.

[58] Alexander Fischer, Christof Schütte, Peter Deuflhard, and Frank Cordes. Hierarchical uncoupling-coupling of metastable conformations. In Tamar Schlick and Hin Hark Gan, editors, *Computational Methods for Macromolecules: Challenges and Applications, Proceedings of the 3rd International Workshop on Algorithms for Macromolecular Modeling, New York, Oct. 12–14, 2000*, volume 24 of *Lecture Notes in Computational Science and Engineering*, pages 235–259, Berlin, 2002. Springer.

[59] Daan Frenkel and Berend Smit. *Understanding Molecular Simulations: From Algorithms to Applications*. Academic Press, San Diego, 1996.

[60] Andrew S. Glassner, editor. *An introduction to ray tracing*. Academic Press Ltd., London, UK, 1989.

[61] David E. Goldberg. *Genetic Algorithms in Search, Optimization, and Machine Learning*. Addison-Wesley Professional, January 1989.

[62] Brian B. Goldman and W. Todd Wipke. Quadratic shape descriptors. 1. Rapid superposition of dissimilar molecules using geometrically invariant surface descriptors. *Journal of Chemical Information and Computer Sciences*, 40(3):644–658, 2000.

[63] Deborah Goldman, Sorin Istrail, and Christos H. Papadimitriou. Algorithmic aspects of protein structure similarity. In *FOCS*, pages 512–522, 1999.

[64] V. E. Golender and A. B. Rozenblit. *Logical and Combinatorial Algorithms for Drug Design*. Research Studies Press, 1983.

[65] Andrew C. Good, Edward E. Hodgkin, and W. Graham Richards. Utilization of Gaussian functions for the rapid evaluation of molecular similarity. *Journal of Chemical Information and Computer Sciences*, 32(3):188–191, 1992.

[66] Peter J. Goodford. A computational procedure for determining energetically favorable binding sites on biologically important macromolecules. *Journal of Medicinal Chemistry*, 28:849–857, 1985.

[67] J. Andrew Grant, M. A. Gallardo, and Barry T. Pickup. A fast method of molecular shape comparison: A simple application of a Gaussian description of molecular shape. *Journal of Computational Chemistry*, 17(14):1653–1666, 1996.

[68] J. Andrew Grant and Barry T. Pickup. Gaussian shape methods. In W. Gunsteren and P. K. Weiner, editors, *Computer Simulation of Biomolecular Systems*, volume 3. Kluwer, 1997.

[69] Peter Gund. *Progress in Molecular and Subcellular Biology*, 5:117–143, 1977.

[70] Osman F. Güner, editor. *Pharmacophore - Perception, Development, and Use in Drug Design*. IUL Biotechnology Series, La Jolla, 1999.

[71] Aysam Gürler. Selection and flexible optimization of binding modes from conformation ensembles. Master thesis, Freie Universität Berlin and Zuse Institute Berlin (ZIB), 2006.

[72] Dan Gusfield. *Algorithms on Strings, Trees, and Sequences - Computer Science and Computational Biology*. Cambridge University Press, 1997.

[73] Thomas A. Halgren. Merck molecular force field. I-V. *Journal of Computational Chemistry*, 17(5&6):490–641, 1996.

[74] Sandra Handschuh. *Entwicklung und Einsatz computergestützter Methoden zur Ermittlung struktureller Ähnlichkeiten: Analyse biologisch relevanter Ligand-Rezeptor Wechselwirkungen*. Doctoral thesis, Friedrich-Alexander-Universität Erlangen-Nürnberg, 1999.

[75] Sandra Handschuh, Markus Wagener, and Johann Gasteiger. Superposition of three-dimensional chemical structures allowing for conformational flexibility by a hybrid method. *Journal of Chemical Information and Computer Sciences*, 38:220–232, 1998.

[76] Timothy F. Havel, Irwin D. Kuntz, and Gordon M. Crippen. Effect of distance constraints on macromolecular conformation. *Biopolymers*, 18:73–81, 1979.

[77] Hans-Christian Hege, Tobias Höllerer, and Detlev Stalling. Volume rendering – mathematical models and algorithmic aspects. TR 93-07, Zuse Institute Berlin, 1993.

[78] Wolfgang Heiden and Jürgen Brickmann. Segmentation of protein surfaces using fuzzy logic. *Journal of Molecular Graphics*, 12(2):106–115, 1994.

[79] Stefan Hiller, Oliver Deussen, and Alexander Keller. Tiled blue noise samples. In *VMV*, pages 265–272, 2001.

[80] Edward E. Hodgkin and W. Graham Richards. Molecular similarity based on electrostatic potential and electric field. *International Journal of Quantum Chemistry*, 32:517–545, 1987.

[81] Christian Hofbauer. *Molecular Surface Comparison. A Versatile Drug Discovery Tool*. PhD thesis, Technische Universität Wien, 2004.

[82] John D. Holliday, C.-Y. Hu, and Peter Willett. Grouping of coefficients for the calculation of inter-molecular similarity and dissimilarity using 2D fragment bitstrings. *Journal of American Chemical Society*, 5(2):155–166, 2002.

[83] Liisa Holm and Chris Sander. 3-d lookup: Fast protein structure database searches at 90% reliability. In Christopher J. Rawlings, Dominic A. Clark, Russ B. Altman, Lawrence Hunter, Thomas Lengauer, and Shoshana J. Wodak, editors, *Proceedings of the Third International Conference on Intelligent Systems for Molecular Biology, Cambridge, United Kingdom, July 16-19, 1995*, pages 179–187, 1995.

[84] Mamoru Hosaka. *Modeling of curves and surfaces in CAD/CAM*. Springer, 1992.

[85] Kazuhiko Iwase and Shuichi Hirono. Estimation of active conformations of drugs by a new molecular superposing procedure. *Journal of Computer-Aided Molecular Design*, 13(5):499–512, 1999.

[86] P. Jaccard. Étude comparative de la distribution florale dans une portion des Alpes et des Jura. *Bull. Soc. Vaudoise Sci. Nat.*, 37:547–579, 1901.

[87] Ajay N. Jain. Morphological similarity: A 3D molecular similarity method correlated with protein-ligand recognition. *Journal of Computer-Aided Molecular Design*, 14:199–213, 2000.

[88] Wolfgang Kabsch. A solution for the best rotation to relate two sets of vectors. *Acta Crystallographica A*, 32:922–923, 1976.

[89] Wolfgang Kabsch. A discussion of the solution for the best rotation to relate two sets of vectors. *Acta Crystallographica A*, 34:827–828, 1978.

[90] Alan Kalvin, Edith Schonberg, Jacob T. Schwartz, and Micha Sharir. Two-dimensional model-based boundary matching using footprints. *International Journal of Robotics Research*, 5(4):38–55, 1987.

[91] George Karypis and Vipin Kumar. *METIS, a Software Package for Partitioning Unstructured Graphs and Computing Fill-Reduced Orderings of Sparse Matrices*. University of Minnesota, Department of Computer Science, 1998.

[92] George Karypis and Vipin Kumar. Multilevel k-way partitioning scheme for irregular graphs. *Journal of Parallel and Distributed Computing*, 48(1):96–129, 1998.

[93] Ephraim Katchalski-Katzir, Isaac Shariv, Miriam Einstein, Asher A. Friesem, Claude Aflalo, and Ilya A. Vakser. Molecular surface recognition: Determination of geometric fit between proteins and their ligands by correlation techniques. *Proceedings of the National Academy of Sciences USA*, 89:2195–2199, 1992.

[94] Arie Kaufman, editor. *Volume Visualization*. IEEE Computer Society Press, 1991.

[95] Simon K. Kearsley and Graham M. Smith. An alternative method for the alignment of molecular structures: Maximizing electrostatic and steric overlap. *Tetrahedron Computer Methodology*, 3:615–633, 1990.

[96] Stefan Kirchner. An FPTAS for computing the similarity of three-dimensional point sets. *To appear in International Journal of Computational Geometry and Applications*.

[97] Stefan Kirchner. Ein Approximationsalgorithmus zur Berechnung der Ähnlichkeit dreidimensionaler Punktmengen. Diploma thesis, Humboldt Universität zu Berlin, Department of Computer Science, 2003.

[98] Scott Kirkpatrick, D. Gelatt Jr., and M. P. Vecchi. Optimization by simulated annealing. *Science*, 220(4598):671–680, 1983.

[99] Gerhard Klebe, Thomas Mietzner, and Frank Weber. Different approaches toward an automatic structural alignment of drug moleculars: Applications to sterol mimics, thrombin and thermolysin inhibitors. *Journal of Computer-Aided Molecular Design*, 8(6):751–778, 1994.

[100] Jan J. Koenderink. *Solid Shape*. MIT Press, Cambridge, USA, 1990.

[101] Andreas Krämer, Hans W. Horn, and Julia E. Rice. Fast 3d molecular superposition and similarity search in databases of flexible molecules. *Journal of Computer-Aided Molecular Design*, 17(1):13–38, 2003.

[102] Hugo Kubinyi, editor. *3D QSAR in Drug Design. Volume 1: Theory Methods and Applications*. Springer, 1993.

[103] Frederick S. Kuhl, Gordon M. Crippen, and Donald K. Friesen. A combinatorial algorithm for calculating ligand binding. *Journal of Computational Chemistry*, 5:24–34, 1984.

[104] Paul Labute, Chris Williams, Miklos Feher, Elizabeth Sourial, and Jonathan M. Schmidt. Flexible alignment of small molecules. *Journal of Medicinal Chemistry*, 44(10):1483–1490, 2001.

[105] Yehezkel Lamdan and Haim J. Wolfson. Geometric hashing: A general and efficient model-based recognition scheme. In *Second International Conference on Computer Vision*, pages 238–249. IEEE Computer Society Press, 1988.

[106] Giuseppe Lancia, Robert D. Carr, Brian Walenz, and Sorin Istrail. 101 optimal PDB structure alignments: A branch-and-cut algorithm for the maximum contact map overlap problem. In *RECOMB*, pages 193–202, 2001.

[107] Andrew R. Leach. *Molecular Modelling: Principles and Applications*. Prentice Hall, 2001.

[108] Steve Leicester, John Finney, and Robert Bywater. A quantitative representation of molecular surface shape. II: Protein classification using Fourier shape descriptors and classical scaling. *Journal of Mathematical Chemistry*, 16(1):343–365, 1994.

[109] Christian Lemmen, Claus Hiller, and Thomas Lengauer. RigFit: A new approach to superimposing ligand molecules. *Journal of Computer-Aided Molecular Design*, 12(5):491–502, 1998.

[110] Christian Lemmen and Thomas Lengauer. Time-efficient flexible superposition of medium-sized molecules. *Journal of Computer-Aided Molecular Design*, 11(4):357–368, 1997.

[111] Christian Lemmen and Thomas Lengauer. FLEXS: a method for fast flexible ligand superposition. *Journal of Medicinal Chemistry*, 41(23):4502–4520, 1998.

[112] Christian Lemmen and Thomas Lengauer. Computational methods for the structural alignment of molecules. *Journal of Computer-Aided Molecular Design*, 14:215–232, 2000.

[113] Stuart P. Lloyd. Least squares quantization in PCM. *IEEE Transactions on Information Theory*, 28(2):129–136, 1982.

[114] Harald Martens and Tormod Naes. *Multivariate calibration*. Wiley, Chichester, 1991.

[115] Yvonne C. Martin, Mark G. Bures, Elisabeth Danaher, Jerry DeLazzer, and Isabella Lico. A fast new approach to pharmacophore mapping and its application to dopaminergic and benzodiazepine agonists. *Journal of Computer-Aided Molecular Design*, 7:83–102, 1993.

[116] Yvonne C. Martin, Mark G. Bures, and Peter Willett. Searching databases of three-dimensional structures. In Kenny B. Lipkowitz, editor, *Reviews in Computational Chemistry*, volume 1, pages 213–263. Elsevier Science Publishers B.V., 1990.

[117] Brian B. Masek, Arshad Merchant, and James B. Matthew. Molecular shape comparison of angiotensin II receptor antagonists. *Journal of Medicinal Chemistry*, 36(9):1230–1238, 1993.

[118] Brian B. Masek, Arshad Merchant, and James B. Matthew. Molecular skins: A new concept for the quantitative shape matching of a protein with its small molecule mimics. *Proteins*, 17:193–202, 1993.

[119] Brian B. Masek, Arshad Merchant, and James B. Matthew. Molecular surface comparisons. In Philip M. Dean, editor, *Molecular Similarity in Drug Discovery*. Blackey Academic and Professional, New York, 1995.

[120] Nelson L. Max and Elizabeth D. Getzoff. Spherical harmonic molecular surfaces. *IEEE Computer Graphics and Applications*, 8(4):42–50, 1988.

[121] Michael McCool and Eugene Fiume. Hierarchical Poisson disk sampling distributions. *Graphics Interface*, pages 94–105, 1992.

[122] James J. McGregor. Backtrack search algorithms and the maximal common subgraph problem. *Software - Practice and Experience*, 12(1):23–34, 1982.

[123] Alan J. McMahon and Paul M. King. Optimization of Carbó molecular similarity index using gradient methods. *Journal of Computational Chemistry*, 18(2):151–158, 1997.

[124] Colin McMartin and Regine S. Bohacek. Flexible matching of test ligands to a 3d pharmacophore using a molecular superposition force field: Comparison of predicted and experimental conformations of inhibitors of three enzymes. *Journal of Computer-Aided Molecular Design*, 9(3):237–250, 1995.

[125] Holger Meyer, Frank Cordes, and Marcus Weber. ConFlow: A new space-based application for complete conformational analysis of molecules. Unpublished manuscript.

[126] Paul G. Mezey. *Shape in Chemistry*. VCH, 1993.

[127] Michael D. Miller, Robert P. Sheridan, and Simon K. Kearsley. SQ: A program for rapidly producing pharmacophorically relevant molecular superpositions. *Journal of Medicinal Chemistry*, 42(9):1505–1514, 1999.

[128] Donald R. Morrison. Patricia - practical algorithm to retrieve information coded in alphanumeric. *Journal of the Association of Computing Machinery*, 15(4):514–534, 1968.

[129] Richard M. Murray, Zexiang Li, and S. Shankar Sastry. *A Mathematical Introduction to Robotic Manipulation*. CRC Press, 1994.

[130] J. Willem M. Nissink, Marcel L. Verdonk, Jan Kroon, Thomas Mietzner, and Gerhard Klebe. Superposition of molecules: Electron density fitting by application of Fourier transforms. *Journal of Computational Chemistry*, 18(5):638–645, 1997.

[131] Ruth Nussinov and Haim-J. Wolfson. Efficient detection of three-dimensional structural motifs in biological macromolecules by computer vision techniques. *Proceedings of the National Academy of Sciences USA*, 88:10495–10499, 1991.

[132] International Union of Biochemistry and Molecular Biology. *Enzyme Nomenclature. Recommendations (1992) of the Nomenclature Committee of the International Union of Biochemistry and Molecular Biology.* Academic Press, Inc., London, 1992.

[133] Yumiko Ohta, Yasuyuki Ogura, and Akiyoshi Wada. Thermostable protease from thermophilic bacteria. I. Thermostability, physicochemical properties, and amino acid composition. *Journal of Biological Chemistry*, 241(24):5919–5925, 1966.

[134] Panos M. Pardalos and Jue Xue. The maximum clique problem. *Journal of Global Optimization*, 4:301–328, 1994.

[135] Martin F. Parretti, Romano T. Kroemer, Jeffrey H. Rothman, and W. Graham Richards. Alignment of molecules by the Monte Carlo optimization of molecular similarity indices. *Journal of Computational Chemistry*, 18(11):1344–1353, 1997.

[136] M. Pastor, G. Cruciani, I. McLay, S. Pickett, and S. Clementi. GRid-INdependent descriptors (GRIND): A novel class of alignment-independent three-dimensional molecular descriptors. *Journal of Medicinal Chemistry*, 43(17):3233–3243, 2000.

[137] Daniela Pelz. *Functional characterization of Drosophila melanogaster Olfactory Receptor Neurons.* Doctoral thesis, Freie Universität Berlin, 2005.

[138] Xavier Pennec. Multiple registration and mean rigid shape - Application to the 3D case. In K.V. Mardia, C.A. Gill, and Dryden I.L., editors, *Image Fusion and Shape Variability Techniques (16th Leeds Annual Statistical Workshop)*, pages 178–185. University of Leeds, UK, July 1996.

[139] Catherine A. Pepperrell, Peter Willett, and Robin Taylor. Implementation and use of an atom-mapping procedure for similarity searching in databases of 3-d. *Tetrahedron Computer Methodology*, 3:575, 1990.

[140] Tim D. J. Perkins, J. E. J. Mills, and Philip M. Dean. Molecular surface-volume and property matching to superpose flexible dissimilar molecules. *Journal of Computer-Aided Molecular Design*, 9(6):479–490, 1995.

[141] Andrew R. Poirrette, Peter J. Artymiuk, David W. Rice, and Peter Willett. Comparison of protein surfaces using a genetic algorithm. *Journal of Computer-Aided Molecular Design*, 11(6):557–569, 1997.

[142] Matthias Rarey and J. Scott Dixon. Feature trees: A new molecular similarity measure based on tree matching. *Journal of Computer-Aided Molecular Design*, 12(5):471–490, 1998.

[143] John W. Raymond, Eleanor J. Gardiner, and Peter Willett. Rascal: Calculation of graph similarity using maximum common edge subgraphs. *The Computer Journal*, 45(6):631–644, 2002.

[144] John W. Raymond and Peter Willett. Effectiveness of graph-based and fingerprint-based similarity measures for virtual screening of 2D chemical structure databases. *Journal of Computer-Aided Molecular Design*, 16(1):59–71, 2002.

[145] John W. Raymond and Peter Willett. Maximum common subgraph isomorphism algorithms for the matching of chemical structures. *Journal of Computer-Aided Molecular Design*, 16(7):521–533, 2002.

[146] Jacqueline D. Reeves and Robert W. Doms. Human immunodeficiency virus type 2. *The Journal of General Virology*, 83(6):1253–1265, 2002.

[147] Penny Rheingans and Shrikant Joshi. Visualization of molecules with positional uncertainty. In E. Gröller, H. Löffelmann, and W. Ribarsky, editors, *Data Visualization '99, Proceedings of the Joint EUROGRAPHICS - IEEE TCVG Symposium on Visualization*, pages 299–306. Springer, Vienna, 1999.

[148] F. M. Richards. Areas, volumes, packing and protein structure. *Ann. Rev. Biophys. Bioeng.*, 6:151–176, 1977.

[149] Isidore Rigoutsos, Daniel E. Platt, Andrea Califano, and David Silverman. Representation and matching of small flexible molecules in large databases of 3d molecular information. In *Pattern Discovery in Biomolecular Data*, pages 111–129. Oxford University Press, 1999.

[150] David W. Ritchie and Graham J. L. Kemp. Fast computation, rotation, and comparison of low resolution spherical harmonic molecular surfaces. *Journal of Computational Chemistry*, 20(4):383–395, 1999.

[151] S. Kashif Sadiq, Stefan J. Zasada, and Peter V. Coveney. Grid assisted ensemble molecular dynamics simulations of HIV-1 proteases reveal novel conformations of the inhibitor saquinavir. In *Computational Life Sciences: Second International Symposium, CompLife 2006*, volume 4216 of *Lecture Notes on Computer Science*, pages 151–161, Cambridge, UK, 2006. Springer.

[152] Hanan Samet. An overview of quadtrees, octrees, and related hierarchical data structures. In Rae A. Earnshaw, editor, *Theoretical Foundations of Computer Graphics and CAD*, pages 51–68. Springer, Berlin, Heidelberg, 1988.

[153] Martin Saunders. Stochastic exploration of molecular mechanics energy surfaces. hunting for the global minimum. *Journal of American Chemical Society*, 109(10):3150–3152, 1987.

[154] Kristina Schädler and Fritz Wysotzki. A connectionist approach to structural similarity determination as a basis of clustering, classification and feature detection. In

Principles of Data Mining and Knowledge Discovery, First European Symposium, PKDD '97, Trondheim, Norway, June 24-27, 1997, Proceedings, pages 254–264, 1997.

[155] Johannes Schmidt-Ehrenberg, Daniel Baum, and Hans-Christian Hege. Visualizing dynamic molecular conformations. In *Proceedings of IEEE Visualization 2002*, pages 235–242, 2002.

[156] Jacob T. Schwartz and Micha Sharir. Identification of partially obscured objects in two and three dimensions by matching noisy characteristic. *International Journal of Robotics Research*, 6(2):29–44, 1987.

[157] Robert P. Sheridan, Michael D. Miller, Dennis J. Underwood, and Simon K. Kearsley. Chemical similarity using geometric atom pair descriptors. *Journal of Chemical Information and Computer Sciences*, 36:128–136, 1996.

[158] Robert P. Sheridan, Ramaswamy Nilakantan, Andrew Rusinko III, Norman Bauman, Kevin S. Haraki, and R. Venkataraghavan. 3DSEARCH: A system for three-dimensional substructure searching. *Journal of Chemical Information and Computer Sciences*, 29:255–260, 1989.

[159] Nikolaus Stiefl and Knut Baumann. Mapping property distributions of molecular surfaces: Algorithm and evaluation of a novel 3D quantitative structure-activity relationship technique. *Journal of Medicinal Chemistry*, 46(8):1390–1407, 2003.

[160] George C. Stockman. Object recognition and localization via pose clustering. *Computer Vision, Graphics, and Image Processing*, 40(3):361–387, 1987.

[161] Lubert Stryer. *Biochemistry*. W. H. Freeman and Company, New York, 1995.

[162] H. A. Stuart. *Z. phys. Chem.*, 27:350, 1927.

[163] Martin Thimm. *Algorithmen im Wirkstoffdesign*. Doctoral thesis, Humboldt Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät II, 2006.

[164] Maxim Totrov and Ruben Abagyan. The contour-buildup algorithm to calculate the analytical molecular surface. *Journal of Structural Biology*, 116:138–143, 1995.

[165] Tripos Inc., http://www.tripos.com.

[166] David A. Van Veldhuizen. *Multiobjective Evolutionary Algorithms: Classification, Analyses, and New Innovations*. PhD thesis, Faculty of the Graduate School of Engineering of the Air Force Institute of Technology, Air University, 1999.

[167] Leroy G. Wade. *Organic Chemistry*. Prentice Hall, New Jersey, 1987.

[168] Markus Wagener and Johann Gasteiger. The determination of maximum common substructures by a genetic algorithm: Application in synthesis design and for the structural analysis of biological activity. *Angew. Chem. Int. Ed. Engl.*, 33:1189–1192, 1994.

[169] Lionel Walter and Marcus Weber. ConfJump: a fast biomolecular sampling method which drills tunnels through high mountains. ZIB Report 06-26, Zuse Institute Berlin (ZIB), 2006.

[170] Marcus Weber. *Meshless Methods in Conformation Dynamics*. Doctoral thesis, Freie Universität Berlin, 2006.

[171] Hassler Whitney. Congruent graphs and the connectivity of graphs. *American Journal of Mathematics*, 54:150–168, 1932.

[172] Peter Willett. Similarity searching in chemical databases using molecular fields and data fusion. In Ramon Carbó-Dorca, Xavier Gironés, and Paul G. Mezey, editors, *Fundamentals of Molecular Similarity*, pages 51–66. Kluwer Academic/Plenum Publishers, 2001.

[173] Haim J. Wolfson and Isidore Rigoutsos. Geometric hashing: An overview. *IEEE Computational Science and Engineering*, 4(4):10–21, 1997.

[174] A. K. C. Wong and F. A. Akinniyi. An algorithm for the largest common subgraph isomorphism using the implicit net. In *Proceedings of IEEE Systems, Man, & Cybernetics*, pages 197–201, 1983.

[175] Shengang Yuan, Chongzhi Zheng, Xia Zhao, and Fanyou Zeng. Identification of maximal common substructures in structure/activity studies. *Analytica Chimica Acta*, 235(1):239–241, 1990.

[176] Carl-Dieter Zachmann, Wolfgang Heiden, Michael Schlenkrich, and Jürgen Brickmann. Topological analysis of complex molecular surfaces. *Journal of Computational Chemistry*, 13(1):76–84, 1992.

[177] Randy J. Zauhar, Guillermo Moyna, LiFeng Tian, ZhiJian Li, and William J. Welsh. Shape signatures: a new approach to computer-aided ligand- and receptor-based drug design. *Journal of Medicinal Chemistry*, 46(26):5674–5690, 2003.

[178] D. Zhang and M. Herbert. Harmonic maps and their applications in surface matching. In *Proceedings of IEEE Conference on Computer Vision and Pattern Recognition*. IEEE Computer Society Press, 1999.