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| **1.** | **References & Suggested Reading** |

This section contains a list of the references to general theory, algorithms and implementation details which have been of use during the development of the TINKER package. Methods described in some of the references have been implemented in detail within the TINKER source code. Other references contain useful background information although the algorithms themselves are now obsolete. Still other papers contain ideas or extensions planned for future inclusion in TINKER. References for specific force field parameter sets are provided in an earlier section of this User's Guide. This list is heavily skewed toward biomolecules in general and proteins in particular. This bias reflects our group's major interests; however an attempt has been made to include methods which should be generally applicable.

**PARTIAL LIST OF MOLECULAR MECHANICS SOFTWARE PACKAGES**

AMBER Peter Kollman, University of California, San Francisco

AMMP Rob Harrison, Thomas Jefferson University, Philadelphia

ARGOS Andy McCammon, University of California, San Diego

BOSS William Jorgensen, Yale University

BRUGEL Shoshona Wodak, Free University of Brussels

CFF Shneior Lifson, Weizmann Institute

CHARMM Martin Karplus, Harvard University

CHARMM/GEMM Bernard Brooks, National Institutes of Health, Bethesda

DELPHI Bastian van de Graaf, Delft University of Technology

DISCOVER Molecular Simulations Inc., San Diego

DL\_POLY W. Smith & T. Forester, CCP5, Daresbury Laboratory

ECEPP Harold Scheraga, Cornell University

ENCAD Michael Levitt, Stanford University

FANTOM Werner Braun, University of Texas, Galveston

FEDER/2 Nobuhiro Go, Kyoto University

GROMACS Herman Berendsen, University of Groningen

GROMOS Wilfred van Gunsteren, BIOMOS and ETH, Zurich

IMPACT Ronald Levy, Rutgers University

MACROMODEL Schodinger, Inc., Jersey City, New Jersey

MM2/MM3/MM4 N. Lou Allinger, University of Georgia

MMC Cliff Dykstra, Indiana Univ.≠Purdue Univ. at Indianapolis

MMFF Tom Halgren, Merck Research Laboratories, Rahway

MMTK Konrad Hinsen, Inst. of Structural Biology, Grenoble

MOIL Ron Elber, Cornell University

MOLARIS Arieh Warshal, University of Southern California

MOLDY Keith Refson, Oxford University

MOSCITO Dietmar Paschek & Alfons Geiger, Universit‰t Dortmund

NAMD Klaus Schulten, University of Illinois, Urbana

OOMPAA Andy McCammon, University of California, San Diego

ORAL Karel Zimmerman, INRA, Jouy-en-Josas, France

ORIENT Anthony Stone, Cambridge University

PCMODEL Kevin Gilbert, Serena Software, Bloomington, Indiana

PEFF Jan Dillen, University of Pretoria, South Africa

Q Johan ≈qvist, Uppsala University

SIBFA Nohad Gresh, INSERM, CNRS, Paris

SIGMA Jan Hermans, University of North Carolina

SPASIBA Gerard Vergoten, UniversitÈ de Lille

SPASMS David Spellmeyer and the Kollman Group, UCSF

TINKER Jay Ponder, Washington University, St. Louis

XPLOR/CNS Axel Br¸nger, Stanford University

YAMMP Stephen Harvey, University of Alabama, Birmingham

YASP Florian Mueller-Plathe, ETH Zentrum, Zurich

YETI Angelo Vedani, Biografik-Labor 3R, Basel

**AMBER** D. A Pearlman, D. A. Case, J. W. Caldwell, W. S. Ross, T. E. Cheatham III, S. DeBolt, D. Ferguson, G. Seibel and P. Kollman, AMBER, a Package of Computer Programs for Applying Molecular Mechanics, Normal Mode Analysis, Molecular Dynamics and Free Energy Calculations to Simulate the Structural and Energetic Properties of Molecules, ***Comp. Phys. Commun.***, *91*, 1-41 (1995)

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