

## Publications in Refereed Journals

1. MacKerell, Jr., A.D., Vallari, R.C. and Pietruszko, R., Human mitochondrial aldehyde dehydrogenase inhibition by diethylthiocarbamic acid methanethiol mixed disulphide: A derivative of disulfiram., **FEBS Letters** 179:77-81, 1985
2. MacKerell, Jr., A.D., Blatter, E.E. and Pietruszko, R., Human aldehyde dehydrogenase: Kinetic identification of the isozymes for which biogenic aldehydes and acetaldehyde compete. **Alcoholism: Clinical and Experimental Research** 10:266-277, 1986
3. MacKerell, Jr., A.D., McWright, R.S. and Pietruszko, R., Bromoacetophenone as an affinity reagent for human aldehyde dehydrogenase. **Biochemistry** 25:5182-5189, 1986
4. MacKerell, Jr., A.D., and Pietruszko, R., Chemical modification of human aldehyde dehydrogenase by substrate., **Biophysica Biochemica Acta** 911:306-317, 1986
5. MacKerell, Jr., A.D., Rigler, R., Nilsson, L., Hahn, U. and Saenger, W., Protein Dynamics: A time-resolved fluorescence, energetic and molecular dynamics study of ribonuclease T1. **Biophysical Chemistry** 26:247-261, 1987
6. Abriola, D.P., Fields, R., Stein, S., MacKerell, Jr., A.D. and Pietruszko, R., Active-site identification of human aldehyde dehydrogenase., **Biochemistry**, 26:5679-5684, 1987
7. MacKerell, Jr., A.D., Nilsson, L., Rigler, R. and Saenger, W., Molecular dynamic simulations of ribonuclease T1: Analysis of the effect of solvent on the structure, fluctuations and active site of the free enzyme., **Biochemistry**, 27:4547-4556, 1988
8. MacKerell, Jr., A.D., Molecular modeling and dynamics of neuropeptide Y. **Journal of Computer-Aided Molecular Design** 2:55-63, 1988
9. MacKerell, Jr., A.D., Rigler, R., Nilsson, L., Heinemann, U. and Saenger, W., Molecular dynamic simulations of ribonuclease T1: Effect of solvent on the interaction with 2'GMP., **European Biophysics Journal** 16:287-297, 1988
10. MacKerell, Jr. A.D., Hensen, A., Lacroix, J.S. and Lundberg, J.M., Analysis of structure-function relationships of neuropeptide Y using molecular dynamics simulations and pharmacological activity measurements., **Regulatory Peptides** 25:295-313, 1989
11. MacKerell, Jr., A.D., Nilsson, L., Rigler, R. Heinemann, U. and Saenger, W., Molecular dynamic simulations of ribonuclease T1: Comparison of the free enzyme and the 2'GMP-enzyme complex., **Proteins: Structure, Function and Genetics** 6:20-31, 1989
12. Chen, E., Soderberg, P.G., MacKerell, Jr., A.D., Lindstrom, B. and Tengroth, B.M., Inactivation of lactate dehydrogenase by UV radiation in the 300 nm wavelength region., **Radiation and Environmental Biophysics** 28:185-191. 1989.
13. Abriola, D.P., MacKerell, Jr., A.D. and Pietruszko, R., Human aldehyde dehydrogenase: Correlation of activity loss with <sup>14</sup>C-bromoacetophenone into glutamate 268 and cysteine 302; Quarter-of-the-sites reactivity of aldehyde dehydrogenase., **Biochemical Journal** 266:179-187, 1990.
14. MacKerell, Jr., A.D., Rigler, R., Hahn, U. and Saenger, W., Thermodynamic analysis of the equilibrium, association, and dissociation of 2'GMP and 3'GMP with Ribonuclease T1 at pH 5.3., **Biochimica et Biophysica Acta** 1073:357-365, 1991.
15. MacKerell, Jr., A.D., Principles and methods in molecular modeling and dynamics of biologically active peptides: Application to neuropeptide Y., **Methods in Enzymology** 202:449-470, 1991.

16. MacKerell, Jr., A.D. and Karplus, M., Importance of attractive van der Waals contribution in empirical energy function models for the heat of vaporization of polar liquids., **Journal of Physical Chemistry** 95:10559-10560, 1991.
17. Uvdal, P., MacKerell Jr. A.D. and Wiegand, B.C., Intramolecular vibrational coupling of adsorbates probed using HREELS and *ab initio* calculations: ethoxides adsorbed on Mo(110)., **Journal of Electron Spectroscopy and Related Phenomena**, 64/65: 193-199, 1993.
18. Yang, B., Wright, J., Eldefrawi, M.E., Poi, S., and MacKerell Jr., A.D., Conformational, aqueous solvation and  $pK_a$  contributions to the binding of cocaine, WIN and a WIN vinyl analog. **Journal of the American Chemical Society**, 116:8722-8732, 1994.
19. MacKerell Jr., A.D., Molecular dynamics simulation analysis of a sodium dodecyl sulfate micelle in aqueous solution: Decreased fluidity of the micelle hydrophobic interior., **Journal of Physical Chemistry**, 99:1846-1855, 1995
20. MacKerell, Jr., A.D., Sommer, M.S. and Karplus, M., pH Dependence of binding reactions from free energy simulations and macroscopic continuum electrostatic calculations: Application to 2'GMP/3'GMP binding to ribonuclease T1., **Journal of Molecular Biology**, 247:774-807, 1995.
21. Uvdal, P., MacKerell, Jr., A.D., Wiegand, B.C. and Friend, C.M., Surface-induced alteration of adsorbate intramolecular vibrational coupling: 2-propoxide on Mo(110) as determined by *ab initio* calculations and experiments., **Physical Review B**, 51:7844-7848, 1995.
22. MacKerell, Jr. A.D., Wiorkiewicz, J.K. and Karplus, M., All-atom empirical energy function for the simulation of nucleic acids., **Journal of the American Chemical Society**, 117:11946-11975, 1995.
23. Yin, D. and MacKerell, Jr., A.D., *Ab initio* calculations on the use of Helium and Neon as probes of van der Waals surfaces of molecules., **Journal of Physical Chemistry**, 100:2588-2596, 1996.
24. Ho, L.L., MacKerell, Jr., A.D. and Bash, P.A., Proton and Hydride Transfers in Solution (I): Hybrid, QM/MM Free Energy Perturbation Study. **Journal of Physical Chemistry**, 100:4466-4475, 1996.
25. Bash, P.A., Ho, L.L., MacKerell, Jr., A.D., Levine, D. and Hallstrom, P., Progress toward Chemical Accuracy in the Computer Simulations of Condensed Phase Reactions. **Proceedings of the National Academy of Sciences, USA**, 93: 3698-3703, 1996,
26. Feng, M.-H., Philippopoulos, M., MacKerell, Jr., A.D. and Lim, C., Structural Characterization of the Phosphotyrosine Binding Region of a High-Affinity SH2 Domain-Phosphopeptide Complex by Molecular Dynamics Simulation and Chemical Shift Calculations., **Journal of the American Chemical Society**, 118: 11265-11277, 1996.
27. Pavelites, J.J., Bash, P.A., Gao, J., and MacKerell, Jr., A.D., A Molecular Mechanics Force Field for NAD<sup>+</sup>, NADH and the Pyrophosphate Groups of Nucleotides., **Journal of Computational Chemistry**, 18: 221-239, 1997.
28. Li, Y., MacKerell, Jr., A.D., Egorin, M.J., Ballesteros, M.F., Rosen, D.M., Wu, Y.-Y., Blamble, D.A. and Callery, P.S., Structure-Function Relationships of Polyamine Transport Inhibitors in L1210 Murine Leukemia Cells, **Cancer Investigation**, 57: 234-239, 1997.
29. MacKerell, Jr., A.D., Influence of Magnesium Ions on Duplex DNA Structural, Dynamic and Solvation Properties. **Journal of Physical Chemistry B**, 101: 646-650, 1997.

30. Feller., S.E., Yin, D., Pastor, R.W. and MacKerell, Jr., A.D., Molecular Dynamics Simulation of Unsaturated Lipids at Low Hydration: Parametrization and Comparison with Diffraction Studies., **Biophysical Journal**, 73: 2269-2279, 1997.
31. MacKerell, Jr., A.D., Influence of Water and Sodium on the Energetics of Dimethylphosphate and its Implications For DNA Structure., **Journal de Chimie Physique**, 94:1436-1447, 1997.
32. Uvdal, P. and MacKerell, Jr., A.D., Vibrational Spectrum of Methoxy Adsorbed on Metal Surfaces: *Ab initio* Calculations and Experiments., **Surface Science**, 393:141-149, 1997.
33. Yin, D. and MacKerell, Jr. A.D., Combined *Ab initio*/Empirical Approach for the Optimization of Lennard-Jones Parameters. **Journal of Computational Chemistry**, 19: 334-338, 1998.
34. Lieske, S., Yang, B., Eldefrawi, M.E. and MacKerell Jr., A.D., and Wright, J., (-)3 $\beta$ -Substituted Ecgonine Methyl Esters as Inhibitors for Cocaine Binding and Dopamine Uptake., **Journal of Medicinal Chemistry**, 41: 864-876, 1998.
35. MacKerell Jr., A.D., Bashford, D., Bellott, M., Dunbrack Jr., R.L., Evanseck, J., Field, M.J., Fischer, S., Gao, J., Guo, H., Ha, S., Joseph, D., Kuchnir, L., Kuczera, K., Lau, F.T.K., Mattos, C., Michnick, S., Ngo, T., Nguyen, D.T., Prodhom, B., Reiher, III, W. E., Roux, B., Schlenkrich, M., Smith, J., Stote, R., Straub, J., Watanabe, M., Wiorkiewicz-Kuczera, J., Yin, D., and Karplus, M. All-atom empirical potential for molecular modeling and dynamics studies of protein., **Journal of Physical Chemistry B**, 102: 3586-3616, 1998.

<http://pubs.acs.org/journals/jpchax/promo/editors/articles1000.html>

36. Foloppe, N. and MacKerell, Jr. A.D., Conformational Properties of the Deoxyribose and Ribose Moieties of Nucleic Acids: A Quantum Mechanical Study., **Journal of Physical Chemistry B**, 102: 6669-6678, 1998.
37. Uvdal, P., Åsmundsson, R. and MacKerell, A.D., Jr., Experimental vibrational shifts induced by <sup>13</sup>C isotopic substitution assigned by *ab initio* calculations., **Physical Review Letters**, 82: 125-128, 1999.
38. Pastor, N., MacKerell, A.D., Jr., and Weinstein, H., TIT for TAT: The Properties of Inosine and Adenosine in TATA Box DNA., **Journal of Biomolecular Structure & Design**, 16: 787-810, 1999.
39. Lee, G.U. and MacKerell, Jr., A.D., Force, Energy and Structure of Double-stranded DNA Oligonucleotides under Tensile Load., **European Journal of Biophysics**, 28: 415-426, 1999,
40. Foloppe, N. and MacKerell, Jr., A.D., Intrinsic Conformational Properties of Deoxyribosnucleosides: Implicated role for cytosine in the equilibrium between the A, B and Z forms of DNA, **Biophysical Journal**, 76: 3206-3218, 1999.
41. Foloppe, N. and MacKerell, Jr. A.D., Contribution of the Phosphodiester Backbone and Glycosyl Linkage Intrinsic Torsional Energetics to DNA Structure and Dynamics., **Journal of Physical Chemistry B**, 103: 10955-10964, 1999.
42. Chen, I.-J. and MacKerell, Jr., A.D., Computation of the influence of chemical substitution on the pK<sub>a</sub> of pyridine using semiempirical and *ab initio* methods, **Theoretical Chemistry Accounts**, 2000, 103: 483-494.
43. Foloppe, N. and MacKerell, Jr., A.D., All-atom empirical force field for nucleic acids: 1) Parameter optimization based on small molecule and condensed phase macromolecular target data., **Journal of Computational Chemistry**, 21: 86-104, 2000.

44. MacKerell, Jr., A.D. and Banavali, N., All-atom empirical force field for nucleic acids: 2) Application to molecular dynamics simulations of DNA and RNA in solution., **Journal of Computational Chemistry**, 21: 105-120, 2000.
45. Chen, I.J., Neamati, N., Nicklaus, M.C., Orr, A., Anderson, L., Barchi, Jr., J.J., Kelley, J.A., Pommier, Y., and MacKerell, Jr. A.D., Identification of HIV-1 Integrase Inhibitors via Three-Dimensional Database Searching using ASV and HIV-1 Integrases as Targets., **Bioorganic & Medicinal Chemistry**, 8: 2385-2389, 2000.
46. Barsky, D., Foloppe, N., Ahmadi, S., Wilson, III, D.M., MacKerell, Jr., A.D., New Insights into the Structure of Abasic DNA from Molecular Dynamics Simulations., **Nucleic Acids Research**, 28: 2613-2626, 2000.
47. Feller, S.E. and MacKerell, Jr., A.D., An Improved Empirical Potential Energy Function for Molecular Simulations of Phospholipids., **Journal of Physical Chemistry B**, 104: 7510-7515, 2000.
48. Ásmundsson, R., Uvdal, P. and MacKerell, Jr. A.D., Binary combination and overtone modes in the C-H stretch region in ethoxy adsorbed on Cu(100): Experimental and calculated vibrational spectra., **Journal of Chemical Physics**, 113:1258-1267, 2000.
49. Wang, P., Nicklaus, M.C., Marquez, V.E., Brank, A.S., Christman, J., Banavali, N.K. and MacKerell, Jr., A.D., Use of Oligodeoxyribonucleotides with Conformationally Constrained Abasic Sugar Targets to Probe the Mechanism of Base Flipping by HhaI DNA (Cytosine C5)-Methyltransferase., **Journal of the American Chemical Society**, 122:12422-12434, 2000.
50. Banavali, N.B. and MacKerell, Jr., A.D., Reevaluation of Stereoelectronic Contributions to the Conformational Properties of the Phosphodiester and N3'-Phosphoramidate Moieties of Nucleic Acids., **Journal of the American Chemical Society**, 123:6747-6755, 2001.
51. Marquez, V.E., Wang, P., Nicklaus, M.C., Maier, M., Manoharan, M., Christman, J.K., Banavali, N.K., and MacKerell, A.D., Jr., Inhibition of (Cytosine C5)-Methyltransferase by Oligonucleotides Containing Flexible (Cyclopentane) and Conformationally Constrained (Bicyclo[3.1.0]hexane) abasic sites., **Nucleosides, Nucleotides and Nucleic Acids**, 20:451-450, 2001.
52. MacKerell, Jr., A.D., Banavali, N.B. and Foloppe, N., Development and Current Status of the CHARMM Force Field for Nucleic Acids., **Biopolymers**, 56: 257-265, 2001.
53. Chen, I.-J., Yin, D. and MacKerell, Jr., A.D., Combined *Ab initio*/Empirical Approach for Optimization of Lennard-Jones Parameters for Polar-Neutral Compounds., **Journal of Computational Chemistry**, 23:199-213, 2002.
54. Izaguirre, G., Pietruszko, R., Cho, S. and MacKerell, Jr., A.D., Human Aldehyde Dehydrogenase Catalytic Activity and Structural Interactions with Coenzyme Analogs, **Journal of Biomolecular Structure and Dynamics**, 19:429-448, 2001.
55. Banavali, N.B. and MacKerell, Jr., A.D., Reexamination of the Intrinsic, Dynamic, and Hydration Properties of Phosphoramidate DNA, **Nucleic Acids Research**, 29:3219-3230, 2001.
56. Feller, S.E., Gawrisch, K. and MacKerell, Jr., A.D., Polyunsaturated Fatty Acids in Lipid Bilayers: Intrinsic and Environmental Contributions to their Unique Physical Properties., **Journal of the American Chemical Society**, 124:318-326, 2002.
57. Foloppe, N., Nilsson, L. and MacKerell, Jr., A.D., Ab initio conformational analysis of nucleic acid components: Intrinsic energetic contributions to nucleic acid structure and dynamics. **Biopolymers**, 61: 61-76, 2002.

58. Chen, I-J., Neamati, N. and MacKerell, Jr. A.D., Structure-Based Inhibitor Design Targeting HIV-1 Integrase., **Current Drug Targets - Infectious Disorders**, 2: 217-234, 2002.
59. Foloppe, N., Hartmann, B., Nilsson, L. and MacKerell, Jr., A.D., Intrinsic Conformational Energetics Associated with the Glycosyl Torsion in DNA: a Quantum Mechanical Study, **Biophysical Journal**, 82: 1554-1569, 2002.
60. Banavali, N.K. and MacKerell, Jr., A.D., Free Energy and Structural Pathways of Base Flipping in a DNA GCGC containing sequence., **Journal of Molecular Biology**, 319: 141-160, 2002.
61. Huang, N., and MacKerell, Jr., A.D. , An *Ab Initio* Quantum Mechanical Study of Hydrogen-Bonded Complexes of Biological Interest, **Journal of Physical Chemistry A**, 106; 7820-7827, 2002.
62. Andersson, M.P., Uvdal, P. and MacKerell, Jr., A.D., Fundamental, Binary Combination and Overtone Modes in Methoxy Adsorbed on Cu(100): Infrared Spectroscopy and *ab initio* Calculations. **Journal of Physical Chemistry B**, 106: 5200-5211, 2002.
63. Pan, Y., Huang, N., Cho, S. and A. D. MacKerell, Jr., Consideration of molecular weight during compound selection in virtual database screening., **Journal of Chemical Information and Computer Science**, 43: 267-272, 2003.
64. Huang, N. Banavali, N.K., and MacKerell, Jr., A.D., Protein-facilitated base flipping in DNA by cytosine-5-methyltransferase. **Proceedings of the National Academy of Sciences, USA**, 100: 68-73, 2003.
65. Chen, W., Wu, H., Bernard, D., Metcalf, M.D., Deschamps, J., Flippen-Anderson, J., MacKerell, Jr., A.D. and Coop, A., Rearrangement of 5-Trimethylsilylthebaine on Treatment with L-Selectride: An Efficient Synthesis of (+)-Bractazonine, **Journal of Organic Chemistry**, 68: 1929-1932, 2003.
66. Bernard, D., Coop, A. and MacKerell, Jr., A.D. , 2D Conformationally Sampled Pharmacophore: A Novel Approach to Ligand Based Pharmacophore Development Applied to  $\delta$  Opioid Agonists and Antagonists, **Journal of the American Chemical Society**. 125: 3103-3107, 2003.
67. Feig, M., MacKerell, Jr., A.D., and Brooks, III, C.L., Force field influence on the observation of  $\pi$ -helical protein structures in molecular dynamics simulations, **Journal of Physical Chemistry B**, 107: 2831-2836, 2003.
68. Lamoureux, G., MacKerell, A.D., Jr., Roux, B., A simple polarizable model of water based on classical Drude oscillators, **Journal of Chemical Physics**, 119: 5185-5197, 2003
69. Pan, Y. and MacKerell, A.D., Jr., Altered structural fluctuations in duplex RNA versus DNA: A conformational switch involving base pair opening. **Nucleic Acids Research**, 31: 7131-7140, 2003
70. Huang, N. and MacKerell, A.D., Jr., Atomistic view of base flipping in DNA. **Philosophical Transactions of The Royal Society, London, A**, 362: 1439-1460, 2004
71. MacKerell, A.D., Jr., Feig, M. and Brooks, III, C.L., Improved treatment of the protein backbone in empirical force fields, **Journal of the American Chemical Society**, 126:698-699, 2004.
72. Rosen, G.M, Beselman, A., Tsai, P., Pou, S., Mailer, C. Ichikawa, K., Robinson, B.H., Nielsen, R., Halpern, H. and MacKerell, A.D. Jr., Influence of Structure on the EPR Spectrum of Spin Trapped Adducts of 5,5-Dimethyl-1-Pyrroline-N-Oxide, **Journal of Organic Chemistry**, 69: 1321-1330, 2004.

73. Macias, A., Hernandez, R.J., Mehta, A.K., MacKerell, A.D., Jr., Ticku, M.K. and Coop, A., 3-Chloropropanoic acid (UMB66): a ligand for the gamma-hydroxybutyric acid receptor lacking a 4-hydroxyl group, **Bioorganic & Medicinal Chemistry**, 12: 1643-1647, 2004.
74. Huang, N., Nagarsekar, A., Xia, G., Hayashi, J., MacKerell, A.D., Jr., Identification of Non-phosphate containing Small Molecular Weight Inhibitors of the Tyrosine Kinase p56 LCK SH2 Domain via In silico Screening against the pY+3 site. **Journal of Medicinal Chemistry**, 47: 3502-3511, 2004
75. MacKerell, A.D., Jr., Feig, M., Brooks, C.L., III, Extending the treatment of backbone energetics in protein force fields: limitations of gas-phase quantum mechanics in reproducing protein conformational distributions in molecular dynamics simulations, **Journal of Computational Chemistry**, 25: 1400-1415, 2004.
76. Patel, S., MacKerell, A.D., Jr., Brooks, C.L., III, CHARMM fluctuating charge force field for proteins: II Protein/solvent properties from molecular dynamics simulations using a nonadditive electrostatic model, **Journal of Computational Chemistry**, 25: 1504-1514, 2004
77. MacKerell, A.D., Jr., Empirical Force Fields for Biological Macromolecules: Overview and Issues, **Journal of Computational Chemistry**, 25: 1584-1604, 2004
78. Horton, J.R., Ratner, G., Banavali, N.K., Huang, H., Choi, Y., Maier, M.A., Marquez, V.E., MacKerell, A.D., Jr, and Cheng, X. "Caught in the act: visualization of an intermediate in the DNA base-flipping pathway induced by HhaI methyltransferase," **Nucleic Acids Research**, 32: 3877-3886, 2004.
79. Mason, P. E., Neilson, G. W., Enderby, J. E., Saboungi, M.-L., Dempsey, C. E.; MacKerell, A. D., Jr., Brady, J. W. "The Structure of Aqueous Guanidinium Chloride Solutions," **Journal of the American Chemical Society**, 126: 11462-11470, 2004, DOI: 10.1021/ja040034x
80. Markowitz, J., Chen, I., Gitti, R., Baldisseri, D. M., Pan, Y., Udan, R., Carrier, F., MacKerell, A. D., Jr., Weber, D. J., "Identification and Characterization of Small Molecule Inhibitors of the Calcium-Dependent S100B-p53 Tumor Suppressor Interaction," **Journal of Medicinal Chemistry**, 47; 5085-5093, 2004.
81. Wymore, T. ,Hempel, J., Cho, S.C., MacKerell, A.D., Jr., Nicholas, H.B. Jr., Deerfield, D.W., II, "Molecular recognition of aldehydes by aldehyde dehydrogenase and mechanism of nucleophile activation, **Proteins: Structure, Function, and Bioinformatics**, 57: 758-777, 2004
82. Pitman, M.C., Frank Suits, F., MacKerell, A.D., Jr., Feller, S.E., "Molecular Level Organization of Saturated and Polyunsaturated Fatty Acids in a Phosphatidylcholine Bilayer Containing Cholesterol, **Biochemistry**, 43:15318-15328, 2004
83. Huang, N, MacKerell, A.D., Jr., "Specificity in Protein-DNA Interactions: Energetic Recognition by the (Cytosine-C5)-methyltransferase from HhaI." **Journal of Molecular Biology**. 345: 265-274, 2005
84. Wu, H., D. Bernard, W. Chen, G.D. Strahan, J.R. Deschamps, D.A. Parrish, J.W. Lewis, A.D. MacKerell, Jr., and A. Coop, "Functionalization of the 6,14-bridge of the orvinols. 2. Preparation of 18- and 19-hydroxyl substituted thevinols and their treatment with benzyl bromide. **Journal of Organic Chemistry**, 70: 1907-1910, 2005
85. Klauda, J.B., Brooks, B.R., MacKerell, A.D., Jr., Richard M. Venable, R.M. and Pastor, R.W., An Ab Initio Study on the Torsional Surface of Alkanes and its Effect on Molecular

- Simulations of Alkanes and a DPPC Bilayer, **Journal of Physical Chemistry B**, 109; 5300-5311, 2005
86. MacKerell, A.D., Jr., "Empirical Force Fields for Proteins: Current Status and Future Directions," **Annual Reports in Computational Chemistry**, 1: 91-102, 2005
  87. Anisimov, V.M., Lamoureux, G., Vorobyov, I.V., Huang, N., Roux, B. and MacKerell, A.D., Jr. "Determination of Electrostatic Parameters for a Polarizable Force Field Based on the Classical Drude Oscillator," **Journal of Chemical Theory and Computing**, 1: 153-168, 2005.
  88. Pan, Y., Priyakumar, D. and MacKerell, A.D., Jr., "Conformational Determinants of Tandem GU Mismatches in RNA: Insights from molecular dynamics simulations and quantum mechanical calculations," **Biochemistry**, 44: 1433-1443, 2005.
  89. Boresch, S., Leitgeb, M., Beselman, A., MacKerell, A.D., Jr., "Unexpected relative aqueous solubilities of a phosphotyrosine analogue and two phosphonate derivatives" **Journal of the American Chemical Society**, 127; 4640-4648, 2005
  90. H. Wu, L. N. Thatcher, D. Bernard, D. A. Parrish, J. R. Deschamps, K. C. Rice, A. D. MacKerell Jr., A. Coop: The Position of Coordination of the Lithium Ion Determines the Regioselectivity of Demethylations of 3,4-Dimethoxymorphinans with L-Selectride, **Organic Letters**, 7, 2531-2534, 2005
  91. Bernard, D., Coop, A. and MacKerell, Jr., A.D. "Computer-Aided Drug Design: Structure-Activity Relationships of Delta Opioid Ligands." **Drug Design Reviews**, 2005, 2: 277-291.
  92. Hancock, C.N., Macias, A. Lee, E.K., Yu, S.Y., MacKerell, Jr., A.D. and Shapiro, P. "Identification of novel extracellular signal-regulated kinase (ERK) docking domain inhibitors," **Journal of Medicinal Chemistry**, 2005, 48; 4586-4595.
  93. Macias, A.T. and MacKerell, Jr., A.D. "CH/pi Interactions Involving Aromatic Amino Acids: Refinement of the CHARMM Tryptophan Force field," **Journal of Computational Chemistry**, 2005, 26: 1452-1463.
  94. Habtemariam, B., Anisimov, V.M., and MacKerell, Jr., A.D. "Cooperative binding of DNA and CBF $\beta$  to the Runt domain of the CBF $\alpha$  studied via MD simulations," **Nucleic Acids Research**, 33: 4212-4222, 2005.
- <http://nar.oxfordjournals.org/cgi/reprint/33/13/4212?ijkey=UTMV7oMutgQrEd2&keytype=ref>
95. Vorobyov, I.V., Anisimov, V.M., and MacKerell, Jr., A.D. "Polarizable Empirical Force Field for Alkanes Based on the Classical Drude Oscillator Model," **Journal of Physical Chemistry B**, 109: 18988-18999, 2005.
  96. Priyakumar, U.D. and MacKerell, Jr., A.D. "Base Flipping in a GCGC Containing DNA Dodecamer: A Comparative Study of the Performance of the Nucleic Acid Force Fields, CHARMM, AMBER and BMS," **Journal of Chemical Theory and Computing**, 2006, 2:187-200.
  97. Markowitz, J., MacKerell, A. D., Jr., Carrier, F., Charpentier, T.H., Weber, D. J. Design of Inhibitors of S100B," **Current Topics in Medicinal Chemistry**, 2005, 5: 1093-1108.
  98. Bernard, D.; Coop, A.; MacKerell, A. D., Jr., "Conformationally Sampled Pharmacophore for Peptidic  $\delta$  Opioid Ligands," **Journal of Medicinal Chemistry**, 2005, 48: 7773-7780.
  99. Macias, A.T., Mia, M.Y., Xia, G., Hayashi, J. and MacKerell, Jr., A.D., "Lead Validation and SAR Development via Chemical Similarity Searching; Application to Compounds Targeting the pY+3 Site of the SH2 Domain of p56<sup>lck</sup>," **Journal of Chemical Information and Modeling**, 2005, 45: 1759-1766.

100. Buck, M., Bonnet, S., Pastor, R.W. and MacKerell, Jr., A.D. "Importance of the CMAP correction to the CHARMM22 Protein Force Field: dynamics of hen lysozyme" **Biophysical Journal**, 2006, 90: L36-L38, On line: Dec. 16, 2005, doi:10.1529/biophysj.105.078154.
101. Lamoureux, G., Harder, E., Vorobyov, I.V., Roux, B. and MacKerell, Jr., A.D. "A polarizable model of water for molecular dynamics simulations of biomolecules," **Chemical Physics Letters**, 2006, 418: 245-249.
102. Priyakumar, U.D. and MacKerell, Jr., A.D. "NMR Imino Proton Exchange Experiments on Duplex DNA Primarily Monitor the Opening of Purine Bases" **Journal of the American Chemical Society** (Communication), 2006, 128:678-679.
103. Hancock, C.N., Macias, A., MacKerell, Jr. A.D., and Shapiro, P., "Mitogen Activated Protein (MAP) Kinases: Development of ATP and Non-ATP Dependent Inhibitors," **Medicinal Chemistry**, 2006, 2, 213-222.
104. Priyakumar, U.D. and MacKerell, Jr., A.D. "Computational Approaches for Investigating Base Flipping in Oligonucleotides," **Chemical Reviews**, 2006, 106: 489-505.
105. Banavali, N.B., Huang, N., and MacKerell, Jr., A.D. "Conserved Patterns in Backbone Torsional Changes Allow For Single Base Flipping from Duplex DNA with Minimal Distortion of the Double Helix" **Journal of Physical Chemistry B**, 2006, 110: 10997-11004.
106. Guvench, O. and MacKerell, Jr., A.D. "Quantum Mechanical Analysis of 1,2-Ethanediol Conformational Energetics and Hydrogen Bonding" **Journal of Physical Chemistry A**, 2006, 110: 9934-9939, ASAP Article; DOI: 10.1021/jp0623241
107. Mayaan, E., Moser, A., MacKerell, Jr., A.D., York, D.M., "CHARMM force field parameters for simulation of reactive intermediates in native and thio-substituted ribozymes," **Journal of Computational Chemistry**, 28: 495-507, 2007.
108. Chen, I.-J., Taneja, R., Yin, D., Seo, P.R., Young, D., MacKerell, Jr., A.D., and Polli, J.E., "Chemical Substituent Effect on Pyridine Permeability and Mechanistic Insights from Computational Molecular Descriptors" **Molecular Pharmaceutics**, 3:745-755, 2006.
109. Harder, E., Anisimov, V.M., Vorobyov, I.V., Lopes, P.E., Noskov, S., MacKerell, Jr., A.D. and Roux, B. "Atomic Level Anisotropy in the Electrostatic Modeling of Lone Pairs for a Polarizable Force Field based on the Classical Drude Oscillator," **Journal of Chemical Theory and Computation**, 2; 1587-1597. 2006.
110. Lopes, P.E.M., Murashov, V. Tazi, M. Demchuk, E. MacKerell, A. D., Jr. "Development of an Empirical Force Field for Silica. Application to the Quartz-Water Interface," **Journal of Physical Chemistry B**, 110: 2782-2792, 2006.
111. Zhong, S., Macias, A.T., MacKerell, Jr., A.D. "Computational identification of the inhibitors of protein-protein interactions," **Current Topics in Medicinal Chemistry**, 7, 63-82, 2007.
112. Chen, F., Hancock, C.N., Macias, A.T., Joh, J., Still, K., Zhong, S., MacKerell, Jr., A.D. Shapiro, P.S., "Characterization of ATP independent ERK inhibitors identified through in silico analysis of the active ERK2 structure," **Bioorganic and Medicinal Chemistry Letters**, 16:6281-627, 2006.
113. Almond, A. ; Blundell, C., Higman, V., MacKerell, Jr., A.D., Day, A. "Using molecular dynamics simulations to provide new insights into protein structure on the nanosecond timescale: comparison with experimental data and biological inferences for the hyaluronan-binding Link module of TSG-6," **Journal of Chemical Theory and Computation**, 3:1-16, 2007.

114. Markowitz, J., MacKerell, Jr., A.D., and Weber, D.J. "A search for inhibitors of S100B, a member of the S100 family of calcium-binding proteins," **Mini-Reviews in Medicinal Chemistry**, In Press, 2007.
115. Vorobyov, I.V., Anisimov, V.M., Greene, S., Venable, R.M., Moser, A., Pastor, R.W. and MacKerell, A.D., Jr., Additive and Classical Drude Polarizable Force Fields for Linear and Cyclic Ethers, **Journal of Chemical Theory and Computation**, 3: 1120-1133, 2007.
116. Lopes, P., Lamoureux, G., Roux, B., MacKerell, Jr., A.D., Polarizable Empirical Force Field for Aromatic Compounds Based on the Classical Drude Oscillator, **Journal of Physical Chemistry B**, 111:2873-2885, 2007
117. Macias, A.T., Banavali, N.K. and MacKerell, Jr. A.D. "DNA bending induced by carbocyclic sugar analogs constrained to the north conformation," **Biopolymers**, DOI 10.1002/bip.20673, 2006
118. Woodcock, H.L., Moran, D., Pastor, R.W., MacKerell, A.D., Jr. Brooks, B.R., "Ab initio modeling of glycosyl torsions and anomeric effects in a model carbohydrate: 2-Ethoxy Tetrahydropyran" **Biophysical Journal**, 93: 1-10, 2007
119. Guvench, O., Qu, C.K., MacKerell, A.D., Jr., "Tyr66 acts as a conformational switch in the closed-to-open transition of the SHP-2 N-SH2-domain phosphotyrosine-peptide binding cleft" **BioMed Central (BMC) Structural Biology** 7:14, 2007.
120. Bernard, D., Coop, A. and MacKerell, Jr., A.D. "Quantitative Conformationally Sampled Pharmacophore for  $\delta$  Opioid Ligands: Reevaluation of Hydrophobic Moieties Essential for Biological Activity," **Journal of Medicinal Chemistry**, 50: 1799-1809, 2007.
121. Furci, L.M., Lopes, P., Eakanunkul, S., Zhong, S., MacKerell, A.D., Jr., Wilks, A., "Inhibition of the Bacterial Heme Oxygenases from *Pseudomonas aeruginosa* (*pa*-HO) and *Neisseria meningitidis* (*nm*-HO): A Novel Antimicrobial Target," **Journal of Medicinal Chemistry**, 50: 3804-3813, 2007.
122. Anisimov, V.M., Vorobyov, I.V., Roux, B., and MacKerell, Jr., A.D. "Polarizable empirical force field for the primary and secondary alcohol series based on the classical Drude model." **Journal of Chemical Theory and Computation**, In Press, 2007.
123. Zhong, S. and MacKerell, Jr., A.D. "Binding Response: A Descriptor for Selecting Ligand Binding Site on Protein Surfaces," **Journal of Chemical Information and Modeling**, In Press, 2007.
124. Xie, W., Pu, J, MacKerell, Jr., A.D., Gao, J. "Development of a polarizable intermolecular potential function (PIPF) for liquid amides and alkanes" **Journal of Chemical Theory and Computation**, In Press, 2007.
125. Thomas, J.L., Tobias, D.J., MacKerell, Jr., A.D. "Direct Comparisons of Experimental and Calculated Neutron Structure Factors of Pure Solvents as a Method for Force Field Validation" **Journal of Physical Chemistry**, 111:12941-12944, 2007.
126. Li, L., Vorobyov, I.V., MacKerell, Jr., A.D., Allen, T.W., "Is arginine charged in a membrane?" **Biophysical Journal**, In press, 2007.
127. Priyakumar, U.D., MacKerell, Jr., A.D., "Atomic detail investigation of the structure and dynamics of DNA•RNA hybrids: A molecular dynamics study" **Journal of Physical Chemistry**, In Press, 2008
128. Guvench, O. and MacKerell, Jr., A.D., "Automated conformational energy fitting for force-field development," **Journal of Molecular Modeling**, Submitted.
129. Chen, X., Zhong, S., Dziegielewska, B., Ellenberger, T., Wilson, G.M, MacKerell, Jr.\*, A.D., and Tomkinson, A.E.\*, "Structure-based identification of human DNA ligase inhibitors," **Cancer Research**, Submitted.

130. Guvench, O., Greene, S.N., Kamath, G., Brady, J.W., Venable, R.M., Pastor, R.W., and MacKerell, Jr., A.D. "Additive empirical force field for hexopyranose monosaccharides," **Journal of Computational Chemistry**, Submitted.

## Book Chapters

1. Pietruszko, R., Ferencz-Biro, K. and MacKerell, Jr., A.D., Chemical modification of human aldehyde dehydrogenase., In **Enzymology of Carbonyl Metabolism 2**, H. Weiner and T.G. Flynn EDS., Alan R. Liss Inc., New York, pp. 29-41, 1985.
2. Pietruszko, R., MacKerell, Jr., A.D. and Ferencz-Biro, K., Adducts of propionaldehyde and 3,4-dihydroxyphenylacetaldehyde with human liver aldehyde dehydrogenase., In **Aldehyde Adducts in Alcoholism** M.A. Collins ED., Alan R. Liss Inc., New York, pp. 67-74, 1985.
3. MacKerell, Jr., A.D., Rigler, R., Hahn, U. and Saenger, W., Ribonuclease T1: Interaction with 2'GMP and 3'GMP as studied by time resolved fluorescence spectroscopy., In **Structure, Dynamics and Function of Biomolecules** A.Ehrenberg, R. Rigler, A. Graslund and L. Nilsson EDS., Springer Series in Biophysics, Vol. 1., Springer-Verlag, pp. 260-264, 1987.
4. Pietruszko, R., and MacKerell, Jr., A.D. , Stoichiometry of chemical modification of human aldehyde dehydrogenase: Evidence for "Quarter of the sites" reactivity., In **Enzymology and Molecular Biology of Carbonyl Metabolism: Aldehyde Dehydrogenase, Aldo-Keto Reductase and Alcohol Dehydrogenase** H. Weiner ED., Progress in Clinical and Biological Research, Vol.232, Alan R. Liss Inc., New York, pp. 37-52., 1987.
5. Rigler, R., MacKerell, A., Vogel, H. and Nilsson, L, Picosecond spectroscopy of molecular dynamics of proteins and enzymes., In **Laser Spectroscopy VIII (EICOLS 87)** W. Persson and S. Svanberg EDS. pp. 242-244, 1988.
6. Schlenkrich, M., Brickmann, J. MacKerell, Jr., A.D. and Karplus, M., An Empirical Potential Energy Function for Phospholipids: Criteria for Parameter Optimization and Applications., In **"Biological Membranes: A Molecular Perspective from Computation and Experiment"** K.M. Merz, Jr. and B. Roux, Eds. Birkhäuser, Boston, 1996
7. MacKerell Jr., A.D., Observations on the A versus B equilibrium in molecular dynamics simulations of duplex DNA and RNA. ACS Symposium Series, "**Molecular Modeling and Structural Determination of Nucleic Acids**, N.B. Leontis, Ed., pp. 304-311, 1997.
8. MacKerell, Jr., A.D., Protein Force Fields., In **Encyclopedia of Computational Chemistry**, P. v.R.Schleyer, N.L Allinger, T. Clark, J. Gasteiger, P.A. Kollman, H.F. Schaefer III, P.R. Schreiner, Editors, John Wiley & Sons, Chichester, 1998.
9. MacKerell, Jr., A.D., Brooks, B., Brooks, III, C.B., Nilsson, L., Roux, B., Won, Y. and Karplus, M., CHARMM: The Energy Function and Its Parametrization with an Overview of the Program, In **Encyclopedia of Computational Chemistry**, P. v.R.Schleyer, N.L Allinger, T. Clark, J. Gasteiger, P.A. Kollman, H.F. Schaefer III, P.R. Schreiner, Editors, John Wiley & Sons, Chichester, Vol. 1, 271-277, 1998.
10. MacKerell, Jr., A.D., Atomistic Models and Force Fields, In **Computational Biochemistry and Biophysics**, O. Becker, A.D. MacKerell, Jr., B. Roux and M. Watanabe, Editors, Marcel Dekker Inc., New York, 7-38, 2001.

11. MacKerell, Jr., A.D., Nilsson, L, Nucleic Acid Simulations., In **Computational Biochemistry and Biophysics**, O. Becker, A.D. MacKerell, Jr., B. Roux and M. Watanabe, Editors, Marcel Dekker Inc., New York, 441-463, 2001.
12. MacKerell, A.D., Jr., “Interatomic Potentials: Molecules,” In **Handbook of Materials Modeling**, S. Yip, Editor, Lancaster Publishing Services, Lancaster, UK, 2005
13. MacKerell, A.D., Jr., “Empirical Force Fields,” In **Computational Methods for Protein Structure Prediction and Modeling I: Basic Characterization**, Ying Xu, Dong Xu, Jie Liang, Editors, Springer, New York, In Press
14. MacKerell, A.D., Jr. and Nilsson, L. “Theoretical Studies of Nucleic Acids and Nucleic Acid-Protein Complexes using CHARMM,” In **Computational Studies of RNA and DNA**, J. Sponer and F. Lankas, Eds., Springer, Netherlands, pp. 73-94, 2006.
15. Guvench, O. and MacKerell, A.D., Jr., “Comparison of protein force fields for molecular dynamics simulations,” In **Molecular Modeling of Proteins**, A. Kukol, Editor, Humana Press, Submitted.
16. Klauda, J.B., Venable, R.M., MacKerell, Jr., A.D. and Pastor, R.W. “Considerations for Lipid Force Field Development, In **Computational Modeling of Membrane Bilayers**, S. Feller, Editor, Elsevier, Inc. In Press.

### Book Editor

**Computational Biochemistry and Biophysics**, O. Becker, A.D. MacKerell, Jr., B. Roux and M. Watanabe, Editors, Marcel Dekker Inc., New York, 2001.