Curriculum Vitae

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Education

Ph.D.: Biochemistry, Rutgers University, New Brunswick, NJ
Advisor: Professor Regina Pietruszko
Degree conferred: August, 1985

B.S.: Chemistry, University of Hawaii, Honolulu, HI
Degree conferred: May, 1981

A.S.: Biology, Gloucester County College, Sewell, NJ
(Now Rowan College of South Jersey)
Degree conferred: May, 1979

Employment Experience

3/08 to Present	**Grollman-Glick Professor of Pharmaceutical Sciences**, University of Maryland, Baltimore, School of Pharmacy, Department of Pharmaceutical Sciences, 20 Penn Street, Baltimore, MD 21201, USA
4/12 to Present	**Co-Founder and Chief Scientific Officer**, SilcsBio, LLC, 8 Market Place, Suite 300, Baltimore, MD 21202, USA
2/17 to Present	**Fellow**, Institute for BioScience and Biotechnology Research, University of Maryland, National Institute of Science and Technology, 9600 Gudelsky Drive, Rockville, MD 20850, USA
8/02 to Present	**Director**, Computer-Aided Drug Design Center, University of Maryland, School of Pharmacy, 20 Penn Street, Baltimore, MD 21201, USA
9/95 to Present	**Member of the Molecular and Structural Biology Program,** Greenebaum Comprehensive Cancer Center, University of Maryland, Baltimore, MD, 21201, USA
4/12 to 6/19	**Adjunct Professor**, University of Maryland, Baltimore, School of Medicine, Department of Anesthesiology, Baltimore, MD 21201, USA
5/04 to 3/08	**Professor**, University of Maryland, Baltimore, School of Pharmacy, Department of Pharmaceutical Sciences, 20 Penn Street, Baltimore, MD 21201, USA
6/97 to 5/04	**Associate Professor**, University of Maryland, Baltimore, School of Pharmacy, Department of Pharmaceutical Sciences
1/02 to 6/02	**Visiting Professor**, The Scripps Research Institute, Department of Molecular Biology, TPC6, 10550 North Torrey Pines Road, LaJolla, CA 92037, USA
6/93 to 6/97	**Assistant Professor:** University of Maryland at Baltimore, School of Pharmacy, Department of Pharmaceutical Sciences, 20 North Pine Street, Baltimore, MD 21201, USA
9/92 to 6/93	**Visiting Assistant Professor:** Swarthmore College, Department of Chemistry, 500 College Ave., Swathmore, PA 19081, USA
4/88 to 7/92	**Research Associate:** Harvard University, Department of Chemistry, 12 Oxford Street, Cambridge, MA 02138, USA Supervisor: Prof. Martin Karplus
9/90 to 6/93	**Consultant:** Polygen Corporation, 200 Fifth Avenue, Waltham, MA 02254, USA

1/86 to 3/88 **Postdoctoral Fellow:** Karolinska Institutet, Department of Medical Biophysics, S104-01, Stockholm, Sweden. Supervisor: Prof. Rudolf Rigler

9/81 to 12/85 **Biochemistry Research Assistant:** Rutgers University, Biochemistry Graduate Program, New Brunswick, NJ, USA, Supervisor: Prof. Regina Pietruszko

11/79 to 6/81 **Lab Assistant:** University of Hawaii, Hawaii Institute of Geophysics, Honolulu, HI, USA. Supervisor: Prof. Donald Thomas

Advisory Boards/Steering Committees

Former:

Lawrence Livermore National Laboratory Biosciences Directorate
Unihart Biotech Pharma N.V.
National Resource for Biomedical SuperComputing, Pittsburgh, PA
Science Gateway Institute, NSF's S2I2 program
The Laufer Center for Physical Quantitative Biology, Stonybrook University, NY.
University of Delaware, NIH COBRE Award
Environmental Sciences Division, Oak Ridge National Laboratory
BioVia (formerly Accelrys Inc.)

Current:

University of Kansas, NIH COBRE Award
The Laufer Center for Physical Quantitative Biology, Stonybrook University, NY
Maryland's Cancer Moonshot Initiative in *Pediatric Cancer Research*

Scientific, Professional and Scholarly Organizations

Federation of American Societies for Experimental Biologies (1988-present)
American Society for Biochemistry and Molecular Biology (1988-1999)
Biophysical Society (2000-present)
American Chemical Society (1992-present)
American Association of Colleges of Pharmacy (1992-1998)
International Society of Quantum Biology and Pharmacology (1992-present)
- Vice President: 2004
- President: 2005-2006
- Web host and advisory board: 2005-present

American Association for the Advancement of Science (1995-present)
Rho Chi Honor Society (1993-present)

Editorial Board Member

Proteins: Structure, Function, and Bioinformatics
Journal of Computational Chemistry
PLoS Computational Biology

Advances and Applications in Bioinformatics and Chemistry
Open Access Bioinformatics, to 2016
Drug Design Reviews, 2002 to 2005

Journals Reviewed For

Biophysical Journal
Bioorganic & Medicinal Chemistry Letters
Biochemistry
Biopolymers
Carbohydrate Research
ChemPhysChem
Journal of Computational Physics
Journal of the American Chemical Society
Journal of Biomolecular Structure and Dynamics
Journal of Computational Chemistry
Journal of Computer-Aided Molecular Modeling
Journal of Chemical Information and Modeling
Journal of Chemical Physics
Journal of Chemical Theory and Computation
Journal of Medicinal Chemistry
Journal of Molecular Graphics and Modeling
Journal of Physical Chemistry A, B and C
Langmuir
Nature Communications
Nucleic Acids Research
Physical Chemistry Chemical Physical
Peptides
Proteins
Proceedings of the Indian National Science Academy
Science Reports
RNA

Honors and Awards

NSF NATO Postdoctoral Research Fellowship, 1987
Karolinska Fellowship for Foreign Researchers, 1986-1987
NIH Postdoctoral Fellowship, 1988-1990
Alumnus of the Year, Gloucester County College (Now Rowan College of South Jersey), Sewell, NJ, ca. 1992
NSF European Centre for Atomic and Molecular Computations Fellowship, 1997
Maryland Chemist of the Year 2006: MD Chapter of the American Chemical Society
Researcher of the Year, University of Maryland, Baltimore, 2012
Inaugural Member, Gloucester County College Hall of Fame (Now Rowan College of South Jersey), Sewell, NJ, 2013

The 16th Annual Goodman Lecture, Oregon Health & Science University, 2013
International Society of Quantum Biology and Pharmacology (ISQBP) Computational Biology Award, 2020
American Chemical Society Award for Computers in Chemical and Pharmaceutical Research, 2022
Inductee, International Wall of Fame For Famous Bioinformaticians and Nobel Laureates, National Center for Bioinformatics, Quaid-i-Azam University, Islamabad, Pakistan, 2023

Publications in Refereed Journals

List of publications in PubMed Central:
http://www.ncbi.nlm.nih.gov/pubmed/?term=Mackerell+A

1. MacKerell, A.D., Jr., Vallari, R.C. and Pietruszko, R., "Human mitochondrial aldehyde dehydrogenase inhibition by diethyldithiocarbamic acid methanethiol mixed disulphide: A derivative of disulfiram," **FEBS Letters** 179:77-81, 1985
2. MacKerell, A.D., Jr., 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, A.D., Jr., McWright, R.S. and Pietruszko, R., Bromoacetophenone as an affinity reagent for human aldehyde dehydrogenase. **Biochemistry** 25:5182-5189, 1986
4. MacKerell, A.D., Jr., and Pietruszko, R., "Chemical modification of human aldehyde dehydrogenase by substrate," **Biophysica Biochimica Acta** 911:306-317, 1986
5. MacKerell, A.D., Jr., 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, A.D., Jr. and Pietruszko, R., Active-site identification of human aldehyde dehydrogenase., **Biochemistry**, 26:5679-5684, 1987
7. MacKerell, A.D., Jr., 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, A.D., Jr., Molecular modeling and dynamics of neuropeptide Y. **Journal of Computer-Aided Molecular Design** 2:55-63, 1988
9. MacKerell, A.D., Jr., 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, A.D., Jr., Hemsen, 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, A.D., Jr., 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, A.D., Jr., 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, A.D., Jr. and Pietruszko, R., Human aldehyde dehydrogenase: Correlation of activity loss with ^{14}C-bromoacetophenone into glutamate 268 and cysteine 302; Quarter-of-the-sites reactivity of aldehyde dehydrogenase., **Biochemical Journal** 266:179-187, 1990.
14. MacKerell, A.D., Jr., 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, A.D., Jr., "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, A.D., Jr. 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, A.D., Jr., and Wiegand, B.C., Intramolecular vibrational coupling of adsorbates probed using HREELS and *ab initio* calculations: ethoxides absorbed 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, A.D., Jr., 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, A.D., Jr., Molecular dynamics simulation analysis of a sodium dodecyl sulfate in aqueous solution: Decreased fluidity of the micelle hydrophobic interior., **Journal of Physical Chemistry**, 99:1846-1855, 1995
20. MacKerell, A.D., Jr., 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, A.D., Jr., 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, A.D., Jr., *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, 10.1021/jp9521971
24. Ho, L.L., MacKerell, A.D., Jr. 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, A.D., Jr., 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, A.D., Jr. 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, A.D., Jr., A Molecular Mechanics Force Field for NAD^+, NADH and the Pyrophosphate Groups of Nucleotides., **Journal of Computational Chemistry**, 18: 221-239, 1997.
28. Li, Y., MacKerell, A.D., Jr., 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, A.D., Jr., 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, A.D., Jr., Molecular Dynamics Simulation of Unsaturated Lipids at Low Hydration: Parametrization and Comparison with Diffraction Studies, **Biophysical Journal**, 73: 2269-2279, 1997.
31. MacKerell, A.D., Jr., "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, A.D., Jr., "Vibrational Spectrum of Methoxy Adsorbed on Metal Surfaces: *Ab initio* Calculations and Experiments" **Surface Science**, 393:141-149, 1997.
33. Yin, D. and MacKerell, A.D., Jr., "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, A.D., Jr., and Wright, J., (-)3β-Substituted Ecgonine Methyl Esters as Inhibitors for Cocaine Binding and Dopamine Uptake., **Journal of Medicinal Chemistry**, 41: 864-876, 1998.
35. MacKerell, A.D., Jr., 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.
36. Foloppe, N. and MacKerell, A.D., Jr., "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 ^{13}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, A.D., Jr., 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, A.D., Jr., Intrinsic Conformational Properties of Deoxyribonucleosides: 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, A.D., Jr., "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, A.D., Jr., Computation of the influence of chemical substitution on the pK_a of pyridine using semiempirical and *ab initio* methods, **Theoretical Chemistry Accounts**, 2000, 103: 483-494.
43. Foloppe, N. and MacKerell, A.D., Jr., 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, A.D., Jr. 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, A.D., Jr., Identification of HIV-1 Integrase Inhibitors via Three-Dimensional Database Searching using ASV and HIV-1 Integrases as Targets., **Bioroganic & Medicinal Chemistry**, 8: 2385-2389, 2000.
46. Barsky, D., Foloppe, N., Ahmadia, S., Wilson, III, D.M., MacKerell, A.D., Jr., 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, A.D., Jr., An Improved Empirical Potential Energy Function for Molecular Simulations of Phospholipids, **Journal of Physical Chemistry B**, 104: 7510-7515, 2000.
48. Ásmundssson, R., Uvdal, P. and MacKerell, A.D., Jr., 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, A.D., Jr., 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, A.D., Jr., 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., Inhibtion 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, A.D., Jr., Banavali, N.B. and Foloppe, N., Development and Current Status of the CHARMM Force Field for Nucleic Acids., **Biopolymers**, 56: 257-265, 2001.
53. Izaguirre, G., Pietruszko, R., Cho, S. and MacKerell, A.D., Jr., Human Aldehyde Dehydrogenase Catalytic Activity and Structural Interactions with Coenzyme Analogs, **Journal of Biomolecular Structure and Dynamics**, 19:429-448, 2001.
54. Banavali, N.B. and MacKerell, A.D., Jr., Reexamination of the Intrinsic, Dynamic, and Hydration Properties of Phosphoramidate DNA, **Nucleic Acids Research**, 29:3219-3230, 2001.
55. Chen, I.-J., Yin, D. and MacKerell, A.D., Jr., Combined *Ab initio*/Empirical Approach for Optimization of Lennard-Jones Parameters for Polar-Neutral Compounds., **Journal of Computational Chemistry**, 23:199-213, 2002.

56. Feller, S.E., Gawrisch, K. and MacKerell, A.D., Jr., 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, A.D., Jr., 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, A.D., Jr., 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, A.D., Jr., "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, A.D., Jr., "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, A.D., Jr., 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 MacKerell, A.D., 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, A.D., Jr., Protein-facilitated base flipping in DNA by cytosine-5-methyltransferase. **Proceedings of the National Academy of Sciences, USA**, 100: 68-73, 2003, PMID: 12506195.
65. Chen, W., Wu, H., Bernard, D., Metcalf, M.D., Deschamps, J., Flippen-Anderson, J., MacKerell, A.D., Jr., 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, A.D., Jr., 2D Conformationally Sampled Pharmacophore: A Novel Approach to Ligand Based Pharmacophore Development Applied to δ Opioid Agonists and Antagonists, **Journal of the American Chemical Society**. 125: 3103-3107, 2003.
67. Feig, M., MacKerell, A.D., Jr., and Brooks, III, C.L., Force field influence on the observation of π-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. PMID: 15273274
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., Bernard, D., Chen, W., Strahan, G.D., Deschamps, J.R., Parrish, D.A., Lewis, J.W. MacKerell, A.D., Jr., and Coop, A., "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, PMID: 16863197
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. Wu, H., Thatcher, L. N., Bernard, D., Parrish, D.A., Deschamps, J.R., Rice, K.C., MacKerell, A.D., Jr., Coop, A., "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, A.D., Jr. "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, A.D., Jr. 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, A.D., Jr. "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, A.D., Jr. "Cooperative binding of DNA and CBFβ to the Runt domain of the CBFα studied via MD simulations," **Nucleic Acids Research**, 33: 4212-4222, 2005, PMCID: PMC1180745.
95. Vorobyov, I.V., Anisimov, V.M., and MacKerell, A.D., Jr. "Polarizable Empirical Force Field for Alkanes Based on the Classical Drude Oscillator Model," **Journal of Physical Chemistry B**, 109: 18988-18999, 2005.
96. 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.
97. Bernard, D.; Coop, A.; MacKerell, A.D., Jr., "Conformationally Sampled Pharmacophore for Peptidic δ Opioid Ligands," **Journal of Medicinal Chemistry**, 48: 7773-7780, 2005, PMCID: PMC2631547
98. Macias, A.T., Mia, M.Y., Xia, G., Hayashi, J. and MacKerell, A.D., Jr., "Lead Validation and SAR Development via Chemical Similarity Searching; Application to Compounds

Targeting the pY+3 Site of the SH2 Domain of $p56^{lck}$," **Journal of Chemical Information and Modeling**, 45: 1759-1766, 2005.

99. Priyakumar, U.D. and MacKerell, A.D., Jr. "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.
100. Buck, M., Bonnet, S., Pastor, R.W. and MacKerell, A.D., Jr. "Importance of the CMAP correction to the CHARMM22 Protein Force Field: dynamics of hen lysozyme" **Biophysical Journal**, 2006, 90: L36-L38, 10.1529/biophysj.105.078154, PMCID: PMC1367299
101. Lamoureux, G., Harder, E., Vorobyov, I.V., Roux, B. and MacKerell, A.D., Jr., "A polarizable model of water for molecular dynamics simulations of biomolecules," **Chemical Physics Letters**, 418: 245-249, 2006.
102. Priyakumar , U.D. and and MacKerell, A.D., Jr. "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, PMCID: PMC2542507
103. Hancock, C.N., Macias, A., MacKerell, A.D., Jr., 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, A.D., Jr. "Computational Approaches for Investigating Base Flipping in Oligonucleotides," **Chemical Reviews**, 2006, 106: 489-505.
105. Banavali, N.B., Huang, N., and MacKerell, A.D., Jr. "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, PMCID: PMC2565643
106. Guvench, O. and MacKerell, A.D., Jr. "Quantum Mechanical Analysis of 1,2-Ethanediol Conformational Energetics and Hydrogen Bonding" **Journal of Physical Chemistry A**, 110: 9934-9939, 2006, DOI: 10.1021/jp0623241, PMID: 16898697
107. Chen, I.-J., Taneja, R., Yin, D., Seo, P.R., Young, D., MacKerell, A.D., Jr., and Polli, J.E., "Chemical Substituent Effect on Pyridine Permeability and Mechanistic Insights from Computational Molecular Descriptors," **Molecular Pharmaceutics**, 3:745-755, 2006, PMCID: PMC2526287
108. Harder, E., Anisimov, V.M., Vorobyov, I.V., Lopes, P.E., Noskov, S., MacKerell, A.D., Jr. 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.
109. 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, PMCID: PMC2531191
110. Chen, F., Hancock, C.N., Macias, A.T., Joh, J., Still, K., Zhong, S., MacKerell, A.D., Jr. 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, PMCID: PMC1857279
111. Macias, A.T., Banavali, N.K. and MacKerell, A.D., Jr., "DNA bending induced by carbocyclic sugar analogs constrained to the north conformation," **Biopolymers**, 85:438-449, 2007, 10.1002/bip.20673, NIHMSID197582

112. Zhong, S., Macias, A.T., MacKerell, A.D., Jr. "Computational identification of the inhibitors of protein-protein interactions," **Current Topics in Medicinal Chemistry,** 7, 63-82, 2007, PMC3173769
113. Mayaan, E., Moser, A., MacKerell, A.D., Jr., 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, NIHMSID # 197800
114. Almond, A. Blundell, C., Higman, V., MacKerell, A.D., Jr., 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.
115. Markowitz, J., MacKerell, A.D., Jr., 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**, 7: 609-616, 2007, PMID: 17584159.
116. 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. DOI: 10.1021/ct600350s
117. Lopes, P., Lamoureux, G., Roux, B., MacKerell, A.D., Jr., Polarizable Empirical Force Field for Aromatic Compounds Based on the Classical Drude Oscillator, **Journal of Physical Chemistry B**, 111:2873-2885, 2007. PMC2519011
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, PMCID: PMC1914444
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 Centeral (BMC) Structural Biology** 7:14, 2007, PMCID: PMC1847519
120. Bernard, D., Coop, A. and MacKerell, A.D., Jr. "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, A.D., Jr. "Polarizable empirical force field for the primary and secondary alcohol series based on the classical Drude model." **Journal of Chemical Theory and Computation**, 3, 1927-1946, 2007, PMCID: PMC2542883
123. Zhong, S. and MacKerell, A.D., Jr. "Binding Response: A Descriptor for Selecting Ligand Binding Site on Protein Surfaces," **Journal of Chemical Information and Modeling**, 47; 2303-2315, 2007, PMID: 17900106.
124. Xie, W., Pu, J, MacKerell, A.D., Jr., Gao, J. "Development of a polarizable intermolecular potential function (PIPF) for liquid amides and alkanes" **Journal of Chemical Theory and Computation**, 3; 1878-1889, 2007. PMCID: PMC2572772
125. Thomas, J.L., Tobias, D.J., MacKerell, A.D., Jr. "Direct Comparisons of Experimental and Calculated Neutron Structure Factors of Pure Solvents as a Method for Force Field Validation" **Journal of Physical Chemistry B (Letter)**, 111:12941-12944, 2007, PMCID: PMC2568990

126. Li, L., Vorobyov, I.V., MacKerell, A.D., Jr., Allen, T.W., "Is arginine charged in a membrane?" **Biophysical Journal**, 94: L11-L13, 2008, PMCID: PMC2157258
127. Priyakumar, U.D., MacKerell, A.D., Jr., "Atomic detail investigation of the structure and dynamics of DNA•RNA hybrids: A molecular dynamics study" **Journal of Physical Chemistry B**, 112: 1515-1524, 2008, NIHMSID 197573
128. Guvench, O. and MacKerell, A.D., Jr., "Automated conformational energy fitting for force-field development," **Journal of Molecular Modeling**, 14, 667-679, 2008, 10.1007/s00894-008-0305-0, PMC2864003
129. Chen, X., Zhong S., Zhu, X., Dziegielewska, B., Ellenberger, T., Wilson, G.M, Bachman, K., MacKerell, A.D., Jr. and Tomkinson, A.E., "Rational Design of Human DNA Ligase Inhibitors that Target Cellular DNA Replication and Repair," **Cancer Research**, 68: 3169-3177, 2008, PMC2734474.
130. Harder, E., Anisimov, V.M., Whitfield, T., MacKerell, A.D., Jr., Roux, B. "Understanding the Dielectric Properties of Liquid Amides from a Polarizable Force Field," **Journal of Physical Chemistry B**, 112:3509-3521. 2008, PMID: 18302362
131. MacKerell, A.D., Jr., Nilsson, L., "Molecular dynamics simulations of nucleic acid-protein complexes," **Current Opinions in Structural Biology**, 18: 194-199, 2008, NIHMSID197576
132. Guvench, O., Greene, S.N., Kamath, G., Brady, J.W., Venable, R.M., Pastor, R.W., MacKerell, A.D., Jr. "Additive empirical force field for hexopyranose monosaccharides" **Journal of Computational Chemistry**, 29: 2543-2564, 2008. NIHMSID 196771
133. Lee, H., Venable, R.M., MacKerell, A.D., Jr., and Pastor, R.W. "Molecular dynamics studies of polyethylene oxide and polyethylene glycol: Hydrodynamic radius and shape anisotropy," **Biophysical Journal**, 95: 1590-1599, 2008, DOI 10.1529/biophysj.108.133025, PMCID: PMC2483782
134. Yu, W.-M., Guvench, O., MacKerell, A.D., Jr., and Qu. C.-K. "Identification of small molecular weight inhibitors of SHP-2 tyrosine phosphatase via in silico screening combined with experimental assay." **Journal of Medicinal Chemistry**, 51: 7396-7404, 2008. PMCID: PMC2645921
135. MacKerell, A.D., Jr., Shim, J.-H., Anisimov, V.M., "Re-evaluation of the reported experimental values of the heat of vaporization of N-methylacetamide." **Journal of Chemical Theory and Computation**, 4; 1307-1312, 2008, DOI: 10.1021/ct8000969, NIHMSID197589
136. Zhong, S. and MacKerell, A.D., Jr. "Pose Scaling: Geometrical Assessment of Ligand Binding Poses," **Journal of Theoretical and Computational Chemistry**, 7: 833–852, 2008.
137. Acharya, C., Seo, P.R., Polli, J.E. MacKerell, A.D., Jr. "Computational Model for Predicting Chemical Substituent Effects on Passive Drug Permeability across Parallel Artificial Membranes," **Molecular Pharmaceutics**, 5, 818–828, 2008, DOI: 10.1021/mp800035h, PMID: 18710255
138. Zhong, S., Chen, X., Zhu, X., Dziegielewska, B., Bachman, K.E., Ellenberger, T., Ballin, J.D., Wilson, G.M., Tomkinson, A.E. and MacKerell, A.D., Jr., "Identification and Validation of Human DNA Ligase Inhibitors using Computer-Aided Drug Design," **Journal of Medicinal Chemistry**, 51; 4553-4562, 2008, PMC2788817
139. Charpentier, T.H., Wilder, P.T., Liriano, M.A., Varney, K.M., Pozharski, E, MacKerell, A.D., Jr., Coop, A., Toth, E.A., Weber, D.J., "Divalent metal ion complexes of S100B in the absence and presence of pentamidine," **Journal of Molecular Biology**, 382:56-73, 2008, PMC2636698

140. Chen, F., MacKerell, A.D., Jr., Luo, Y. and Shapiro, P. "Using Caenorhabditis elegans as a Model Organism for Evaluating Extracellular Signal-Regulated Kinase Docking Domain Inhibitors," **Journal of Cell Communication and Signaling**, 2:81-92. 2008 PMCID: PMC2648047
141. Matthews, M.M., Weber, D.J., Shapiro, P.S., Coop, A., and MacKerell, A.D., Jr., "Inhibition of protein-protein interactions with low molecular weight compounds." **Current Trends in Medicinal Chemistry**, 5, 21-32, 2008, PMC3173769
142, Lopes, P.E.M., Demchuk, E., MacKerell, A.D., Jr. "Reconstruction of the (011) Surface on α-Quartz: a semi-classical ab initio Molecular Dynamics Study," **International Journal of Quantum Chemistry**, 109: 50-64, 2009.
143. Lopes, P.E.M., Lamoureux, G., MacKerell, A.D., Jr., "Polarizable Empirical Force Field for Nitrogen-containing Heteroaromatic Compounds Based on the Classical Drude Oscillator" **Journal of Computational Chemistry**, 30: 1821-1838, 2009, 10.1002/jcc.21183, PMC2704921
144. MacKerell, A.D., Jr. "Contribution of the intrinsic mechanical energy of the phosphodiester linkage to the relative stability of the A, BI and BII forms of duplex DNA," **Journal of Physical Chemistry B** 113: 3235-3244, 2009
145. Harder, E., MacKerell, A.D., Jr. and Roux, B. "Electronic Polarization Effects and the Membrane Dipole Potential" **Journal of the American Chemical Society**, 131; 2760–2761, 2009, PMID: 19199514
146. Guvench, O., and MacKerell, A.D., Jr. "Computational evaluation of protein – small molecule binding," **Current Opinion in Structural Biology**, 19:56–61, 2009. PMC2671234
147. González, P.M., Acharya, C., MacKerell, A.D., Jr. and Polli, J.E., "Inhibition Requirements of the human Apical Sodium-dependent Bile acid Transporter (hASBT) using Aminopiperidine Conjugates of glutamyl-Bile Acids," **Pharmaceutical Research**, 26: 1665-1678, 2009, PMID: 19384469
148. Banavali, N. and MacKerell, A.D., Jr., "Characterizing structural transitions using localized free energy landscape analysis, "**PLOS One**, 4: e5525, 2009, PMC2678196
149. Hatcher, E., Guvench, O., and MacKerell, A.D., Jr. "CHARMM Additive All-Atom Force Field for Acyclic Polyalcohols, Acyclic Carbohydrates and Inositol," **Journal of Chemical Theory and Computation**, 5: 1315-1327, 2009, PMC2760998
150. Brooks, B.R., Brooks, C.L., III, MacKerell, A.D., Jr., Nilsson, L., Petrella, R. J., Roux, B., Won, Y., Archontis, G., Bartels, C., Boresch, S., Caflisch, A., Caves, L., Cui, Q., Dinner, A. R. Feig, M., Fischer, S., Gao, J., Hodoscek, M., Im, W., Kuczera, K.,Lazaridis, T., Ma, J., Ovchinnikov, V., Paci, E., Pastor, R.W., Post, C.B., Pu, J.Z., Schaefer, M., Tidor, B., Venable, R.V., Woodcock, H.L., Wu, X, Yang, W., York, D.M., Karplus, M. "CHARMM: The biomolecular simulation program," **Journal of Computational Chemistry**, 30: 1555-1614, 2009, PMC2810661
151. Guvench, O., and MacKerell, A.D., Jr. "Computational Fragment-Based Binding Site Identification by Ligand Competitive Saturation, **PLoS Computational Biology**, 5: e1000435, 2009, PMC2700966, 10.1371/journal.pcbi.1000435
152. Charpentier, T.H., Wilder, P.T., Liriano, M.A., Varney, K.M., Zhong, S., Coop, A., Pozharski, E., MacKerell, A.D., Jr., Toth, E.A., Weber, D.J. "Small Molecules Bound to Unique Sites in the Target Protein Binding Cleft of Calcium-Bound S100B As Characterized by Nuclear Magnetic Resonance and X-ray Crystallography," **Biochemistry**, 48: 6202-6212, 2009, PMC2804263

153. Sorci, L., Pan, Y., Eyobo, Y. Rodionova, I., Huang, N. Kurnasov, O., Zhong, S., MacKerell, A.D., Jr., Zhang, H., Osterman, A.L., "Targeting NAD biosynthesis in bacterial pathogens. Structure-based development of inhibitors of nicotinate mononucleotide adenylyltransferase NadD," **Chemistry and Biology**, 16:849-61, 2009, PMC2770502.
154. Lopes, P.E.M., B. Roux, R., MacKerell, A.D., Jr., "Molecular modeling and dynamics studies with explicit inclusion of electronic polarizability. Theory and applications." **Theoretical Chemistry Accounts**, 124:11-28, 2009, PMC2888514
155. Hatcher, E., Guvench, O., and MacKerell, A.D., Jr. "CHARMM Additive All-Atom Force Field for Aldopentofuranose Carbohydrates and Fructofuranose." **Journal of Physical Chemistry B**. 113:12466-76, 2009, PMC2741538
156. Guvench, O., Hatcher, E. R., Venable, R. M., Pastor, R. W., MacKerell, A.D., Jr., "Additive Empirical CHARMM Force Field for glycosyl linked hexopyranoses," **Journal of Chemical Theory and Computation**, 5, 2353–2370, 2009, PMC2757763.
157. Burkhard, K., Smith, S., Deshmukh, R., MacKerell, A.D., Jr., Shapiro, P., "Development of extracellular signal-regulated kinase inhibitors," **Current Topics in Medicinal Chemistry**, 9:678-89, 2009, PMCID: PMC2835149
158. Priyakumar, D., Hyeon, C., Thiramuli, D., and MacKerell, A.D., Jr. "Formation of stacking interactions and multiple hydrogen bonds by urea with nucleic acid bases destabilizes RNA" **Journal of the American Chemical Society (Communication)** 131: 17759–17761, 2009, PMC2791195.
159. Cunningham, C.W., Hom, K., Acharya, C., Wilks, A., MacKerell, A.D., Jr., and Coop, A. "Synthesis and Characterization of a Novel Diels-Alder Adduct of Cocaine," **Helvetica Chimica Acta**, 93: 220-226, 2010.
160. Baker, C. and MacKerell, A.D., Jr., "Polarizability Rescaling and atom-based Thole Scaling in the CHARMM Drude Polarizable Force Field for Ethers" **Journal of Molecular Modeling**, 16: 567-576, 2010, PMC2818097
161. Vanommeslaeghe, K., Hatcher, E., Acharya, C., Kundu, S. Zhong, S., Shim, J., E. Darian, E., Guvench, O., Lopes, P., Vorobyov, I., MacKerell, A.D., Jr., "CHARMM General Force Field (CGenFF): A force field for drug-like molecules compatible with the CHARMM all-atom additive biological force fields." **Journal of Computational Chemistry**, 31: 671-90, 2010, PMC2888302, 10.1002/jcc.21367
162. Cerchietti, L.C., Ghetu, A.F., Zhu, X., Da Silva, G.F., Zhong, S., Matthews, M., Bunting, K., Polo, J.M., Farès, C., Arrowsmith, C.H., Yang, S.N., Garcia, M., Coop, A., MacKerell, A.D., Jr. , Privé, G.G., Melnick, A. "A small molecule inhibitor of BCL6 kills DLBCL cells in vitro and in vivo." **Cancer Cell**, 17, 400–411, 2010, PMC2858395
163. Priyakumar, U.D. and MacKerell, A.D., Jr., "Role of the Adenine Ligand on the Stabilization of the Secondary and Tertiary Interactions in the Adenine Riboswitch," **Journal of Molecular Biology**, 396: 1422-1438, 2010, PMC2824916
164. Zhu, X. and MacKerell, A.D., Jr. "Polarizable Empirical Force Field for Sulfur-Containing Compounds Based on the Classical Drude Oscillator Model," **Journal of Computational Chemistry**, 31: 2330-2341, 2010. PMC2923574
165. Yu, H., Whitfield, T.W., Harder, E., Lamoureux, G., Vorobyov, I., Anisimov, V. M., MacKerell, A.D., Jr., and Roux, B. "Simulating Monovalent and Divalent Ions in Aqueous Solution Using a Drude Polarizable Force Field, "**Journal of Chemical Theory and Computation**, 6: 774–786, 2010, PMC2838399

166. Baker, C., Lopes, P., Zhu, X., and MacKerell, A.D., Jr., "Accurate Calculation of Hydration Free Energies using the CHARMM Drude Polarizable Force Field," **Journal of Chemical Theory and Computation**, 6: 1181–1198, 2010, PMC2853947
167. Klauda, J.B., Venable, R.M., Freites, J.A., O'Connor, J.W., Tobias, D.J. Mondragon-Ramirez, C., Igor Vorobyov, I., MacKerell, A.D., Jr.,* and Pastor, R.W.* "Update of the CHARMM all-atom additive force field for lipids: Validation on six lipid types." **Journal of** Physical Chemistry B., 114: 7830–7843, 2010, 10.1021/jp101759q, PMC2922408
168. Rais, R., Acharya, C., Tririya, G, MacKerell, A.D., Jr.,* and Polli, J.* "Molecular Switch Controlling the Binding of Anionic Bile Acid Conjugates to hASBT," **Journal of Medicinal Chemistry**, 53: 4749-4760, 2010, PMC2891776.
169. Huang, N., Kolhatkar, R., Eyobo, Y., Sorci, L, Osterman, A.L, MacKerell, A.D., Jr., and Zhang, H., "Structures of bacterial NaMN adenylyltransferase in complex with inhibitors: implication for structure based drug design and improvement. **Journal of Medicinal Chemistry**, 53: 5229-5239, 2010, PMC2915899.
170. Wilder, P.T., Charpentier, T.H., Liriano, M.A., Gianni, K., Varney, K.M., Pozharski, E., Coop, A., Toth, E.A., MacKerell, A.D., Jr., Weber, D.J. "*In vitro* screening and structural characterization of inhibitors of the S100B-p53 interaction," **International Journal of High Throughput Screening**. 1:109–126, 2010, PMC2995924.
171. Semenyuk, A., Darian, E., Liu, J., Majumdar, A., Cuenoud, B., Miller, P., MacKerell, A.D., Jr., Seidman, M. "Targeting of an interrupted Polypurine:Polypyrimidine sequence in a Triplex forming oligonucleotide containing a novel base analog," **Biochemistry**, 49: 7867-7878, 2010, PMC2935506
172. He, X., Guvench, O., MacKerell, A.D., Jr., and Klein, M.L. "Atomistic Simulation Study of Linear Alkylbenzene Sulfonates at The Water/Air Interface," **Journal of Physical Chemistry B**, 114: 9787-9794, 2010, PMC2924668
173. Raman, P., Guvench, O., MacKerell, A.D., Jr., "CHARMM Additive All-Atom Force Field for Glycosidic Linkages in Carbohydrates Involving Furanoses," **Journal of Physical Chemistry B**, 114: 12981-12994, 2010, PMC2958709
174. West, A.L., St. John, F., Lopes, P.E.M., MacKerell, A.D., Jr., Pozharski, E. and Michel, S.L.J., "Holo-Ni(II)HpNikR is an asymmetric tetramer containing two different nickel binding sites," **Journal of the American Chemical Society**, 132: 14447-14456, 2010, PMC2958704
175. Venable, R.M., Hatcher, E., Guvench, O, MacKerell, A.D., Jr., and Pastor, R.W. "Comparing Simulated and Experimental Translation and Rotation Constants: Range of Validity for Viscosity Scaling," **Journal of Physical Chemistry B**, 114: 12501–12507, 2010, PMC3040444
176. Rais, R., Acharya, C., MacKerell, A.D., Jr., Polli, J., "Structural Determinants for Transport Across the Intestinal Bile Acid Transporter Using C-24 Bile Acid Conjugates" **Molecular Pharmaceutics**, 7:2240-2254, 2010, PMC2997912
177. Acharya, C., Polli, J., Coop, A. and, MacKerell, A.D., Jr., "Recent Advances in Ligand-Based Drug Design: Relevance and Utility of the Conformationally Sampled Pharmacophore Approach," **Current Computer-Aided Drug Design**, 7:10-22, 2011, PMC2975775
178. Hatcher, E., Säwén, E., Widmalm, G.,* and MacKerell, A.D., Jr.* "Conformational properties of Methyl β-maltoside and Methyl α- and β-cellobioside disaccharides," **Journal of Physical Chemistry B**, 115: 597-608, 2011, PMC3077104

179. Abel, S., Dupradeau, F.-Y., Raman, E.P., MacKerell, A.D., Jr. and Marchi, M., "Molecular Simulations of Dodecyl-β-maltoside Micelles in Water: Influence of Headgroup Conformation and the Force field Parameters," **Journal of Physical Chemistry B**, 115: 487–499, 2011, PMC3076730
180. Oashi, T., Ringer, A.L., Raman, E.P., and MacKerell, A.D., Jr., "Automated selection of compounds with physicochemical properties to maximize bioavailability and druglikeness," **Journal of Chemical Information and Modeling**, 51:148-158, 2011, PMC3160130
181. Yap, J.L., Workikar, S., MacKerell, A.D., Jr., Shapiro, P., and Fletcher, S. "Small-Molecule Inhibitors of the ERK Signaling Pathway: Towards Novel Anticancer Therapeutics," **ChemMedChem**, 6: 38-48, 2011.
182. Velvadapu, V., Paul, T., Wagh, B., Klepacki, D., Guvench, O., MacKerell, A.D., Jr., and Andrade, R.B., "Desmethyl Macrolides: Synthesis and Evaluation of 4,8,10-Tridesmethyl Telithromycin," **ACS Medicinal Chemistry Letters**, 2: 68–72, 2011, PMC3105755
183. Baker, C.M., Anisimov, V.M., and MacKerell, A.D., Jr., "Development of CHARMM Polarizable Force Field for Nucleic Acid Bases Based on the Classical Drude Oscillator Model," **Journal of Physical Chemistry, B**. 115; 580–596, 2011, PMC3166616
184. Jiang, W., Hardy, D., Phillips, J., MacKerell, A.D., Jr., Schulten, K., Roux, B., "High-performance Scalable Molecular Dynamics Simulations of a Polarizable Force Field Based on Classical Drude Oscillators in NAMD," **Journal of Physical Chemistry Letters**, 2, 87–92: 2011, PMC3092300
185. Boston, S.R., Deshmukh, R., Strome, S., Priyakumar, U.D., MacKerell, A.D., Jr., and Paul Shapiro, P. "Characterization of ERK Docking Domain Inhibitors that Induce Apoptosis by Targeting Rsk-1 and Caspase-9," **BMC Cancer**, 11: 7, 2011, PMC3025971
186. Denning, E.J., Priyakumar, U.D., Nilsson, L., and MacKerell, A.D., Jr., "Impact of 2'-hydroxyl sampling on the conformational properties of RNA: Update of the CHARMM all-atom additive force field for RNA," **Journal of Computational Chemistry**, 32: 1929-1943, 2011, 10.1002/jcc.21777, PMC3082605
187. Darian, E., Guvench, O. Yu, B., Qu, C.-K., and MacKerell, A.D., Jr., "Structural mechanism associated with domain opening in gain-of-function mutations in SHP2 phosphatase," **Proteins: Structure, Function and Bioinformatics**, 79: 1573–1588, 2011, PMC3076527
188. Busby, B., Oashi, T., Willis, C.D., Borzok, M.A., Kontrogianni-Konstantopoulos, A., MacKerell, A.D., Jr.,* and Bloch, B.J.* "Electrostatic Interactions Mediate Binding of Obscurin to Small Ankyrin 1: Biochemical and Molecular Modeling Studies," **Journal of Molecular Biology,** 408:321-334, 2011, PMC3367564
189. Ringer, A. L. and MacKerell, A.D., Jr. "Calculation of the Vibrational Stark Effect Using a First-Principles QM/MM Approach," **Journal of Physical Chemistry Letters**, 2:553-556, 2011, PMC3058488
190. Pastor, R.W. and MacKerell, A.D., Jr., "Development of the CHARMM Force Field for Lipids," **Journal of Physical Chemistry Letters**, Invited Perspective, 2:1526–1532, 2011, PMC3133452
191. Raman, E.P., Yu, W., Guvench, O. and MacKerell, A.D., Jr., "Reproducing Crystal Binding Modes of Ligand Functional Groups using Site-Identification by Ligand Competitive Saturation (SILCS) Simulations," **Journal of Chemical Information and Modeling**, 51, 877-890, 2011, PMC3090225.

192. Denning, E.J. and MacKerell, A.D., Jr., "Impact of Arsenic/Phosphorous substitution on the intrinsic conformational properties of the phosphodiester backbone of DNA investigated using ab initio quantum mechanical calculations." **Journal of the American Chemical Society (Communication)**, 133:5770-5772, 2011, PMC3076535.
193. Shim, J., and MacKerell, A.D., Jr., "Computational ligand-based rational design: Role of conformational sampling and force fields in model development," **Medicinal Chemistry Communications**, 2: 356-370, 2011, 10.1039/c1md00044f, PMC3123535
194. Shim, J., Coop, A. and Alexander D. MacKerell, A.D., Jr. "Consensus 3D Model of μ-Opioid Receptor Ligand Efficacy based on a Quantitative Conformationally Sampled Pharmacophore" **Journal of Physical Chemistry B**, 115: 7487-7496, 2011, PMC3113728
195. Jo, S., Song, K.C., Desaire, H., MacKerell, A.D., Jr., and Im, W. "Glycan Reader: Automated Sugar Identification and Simulation Preparation for Carbohydrates and Glycoproteins," **Journal of Computational Chemistry**, 32: 3135-3141, 2011, PMC3188666
196. Barr, D., Oashi, T., Burkhard, K., Lucius, S., Samadani, R., Zhang, J., Shapiro, P., MacKerell, A.D., Jr., van der Vaart, A., "The importance of domain closure for the auto-activation of ERK2," **Biochemistry**, 50: 8038-48, 2011, PMC3172398
197. Mallajosyula, S.S. and MacKerell, A.D., Jr. "Influence of Solvent and Intramolecular Hydrogen Bonding on the Conformational Properties of *O*-Linked Glycopeptides," **Journal of Physical Chemistry B**, 115:11215-11229, 2011, PMC3179525
198. Guvench, O., Mallajosyula, S.S. Raman, E.P., Hatcher, E. Vanommeslaeghe, K., Foster, T.J., Jamison II, F.W., and MacKerell, A.D., Jr. "CHARMM additive all-atom force field for carbohydrate derivatives and their utility in polysaccharide and carbohydrate-protein modeling," **Journal of Chemical Theory and Computing**, 7: 3162–3180, 2011, 10.1021/ct200328p, PMC3224046
199. Fribourg, M., Moreno, J.L., Provasi, D., Holloway, T., Mahajan, R., Park, G., Baki, L., Adney, S.K., Hatcher, C., Ruta, J.D., Albizu, L., Li, Z., Shim, J., Fabiato, A., MacKerell, A.D., Jr., Brezina, V., Sealfon, S.C., Filizola, M., González-Maeso, J. and Logothetis, D.E., "Decoding the signalling of a GPCR heteromeric complex reveals the mechanism of action of antipsychotic drugs," **Cell**, 147: 1011-1023, 2011.
200. Xu, Z., Chen, Y.-W., Battu, A., Wilder, P., Weber, D., Yu, W., MacKerell, A.D., Jr. Chen, L.-M., Chai, K., Johnson, M., Lin, C.-Y., "Targeting zymogen activation to control the matriptase-prostasin proteolytic cascade," **Journal of Medicinal Chemistry**, 54: 7567-7578, 2011, PMC3214968
201. Kolhatkar, V., Diao, L., Acharya, C., MacKerell, A.D., Jr., Polli, J. "Identification of novel non-steroidal compounds as substrates or inhibitors of hASBT," **Journal of Pharmaceutical Sciences**, 101: 116-126, 2012, DOI: 10.1002/jps.22728
202. Zhu, X., Lopes, P.E., and MacKerell, A.D., Jr., "Recent developments and applications of the CHARMM force fields," **WIRES Computational Molecular Science**, 2: 167-185, 2012, DOI: 10.1002/wcms.74, PMC3468154
203. Hart, K., Foloppe, N., Baker, C.M., Denning, E.J., Nilsson, L. and MacKerell, A.D., Jr., "Optimization of the CHARMM additive force field for DNA: Improved treatment of the BI/BII conformational equilibrium," **Journal of Chemical Theory and Computation**, 8:348–362, 2012, 10.1021/ct200723y, PMC3285246
204. Underwood, K., D'Souza, D., Mochin-Peters, M., Pierce, A., Kommineni, S., Choe, M., Bennett, J., Gnatt, A., Habtemariam, B., MacKerell, A.D., Jr., and Passaniti, A. "Regulation of RUNX2 transcription factor-DNA interactions and cell proliferation by Vitamin D3

(cholecalciferol) prohormone activity," **Journal of Bone and Mineral Research**, 27: 913-925, 2012, 10.1002/jbmr.1504.
205. Mallajosyula, S.S., Guvench, O., Hatcher, E., MacKerell, A.D., Jr., "CHARMM Additive All-Atom Force Field for Phosphate and Sulfate Linked to Carbohydrates," **Journal of Chemical Theory and Computation**, 8: 759-776, 2012, 10.1021/ct200792v, PMC3367516
206. Yap, J.L., Cao, X., Vanommeslaeghe, A., Jung, K.-Y., Wilder, P.T., Anjan Nan, A., Hom, K., MacKerell, A.D., Jr., Smythe, W.R., and Fletcher, S.,"Relaxation of the rigid backbone of an oligoamide-foldamer-based α-helix mimetic: identification of potent Bcl-x_L inhibitors," **Organic and Biomolecular Chemistry**, 16: 2269-2283, 2012, 10.1039/c2ob07125h
207. Denning, E.J. and MacKerell Jr., A.D. "Intrinsic contribution of the 2'-hydroxyl to RNA conformational heterogeneity," **Journal of the American Chemical Society,** 134: 2800-2806, 2012, PMC3275647, 10.1021/ja211328g
208. Velvadapu, V., Glassford, I., Lee, M., Paul, T., DeBrosse, C., Klepacki, D., Small, M.C., MacKerell, A.D., Jr., and Andrade, R.B., "Desmethyl Macrolides: Synthesis and Evaluation of 4,10-Didesmethyl Telithromycin," **ACS Medicinal Chemistry Letters**, 3: 211-215, 2012, PMC3374412
209. González, P.M., Hussainzada, N., Swaan, P.W., MacKerell Jr., A.D., and Polli, J.E., "Putative irreversible inhibitors of the human sodium-dependent bile acid transporter (hASBT; SLC10A2) support the role of transmembrane domain 7 in substrate binding/translocation," **Pharmaceutical Research**, 29: 1821-1831, 2012, 10.1007/s11095-012-0706-8.
210. Willis, C.D., Oashi, T. Busby, B., MacKerell Jr., A.D. and Bloch, R.J. "Hydrophobic Contribution to Binding of Obscurin and Small Ankyrin 1, **Molecular Membrane Biology**, 29: 36-51, 2012.
211. Raman, E.P., Vanommeslaeghe, K. and MacKerell Jr., A.D., "Site-Specific Fragment Identification Guided by Single-Step Free Energy Perturbation Calculations." **Journal of Chemical Theory and Computation**," 8: 3513-3525, 2012, PMC3490637, 10.1021/ct300088r
212. Maiti, A., Noon, M.S., MacKerell Jr., A.D., Pozharski, E. and Drohat, A.C., "Lesion processing by a repair enzyme is severely curtailed by residues needed to prevent aberrant activity on undamaged DNA," **Proceedings of the National Academy of Sciences**, 109: 8091-8096, 2012, PMC3361372, 10.1073/pnas.1201010109 Article highlighted in Chemical Research in Toxicology.
213. Yu, W., Wu, Z., Chen, H., Liu, X., MacKerell Jr., A.D. and Lin, Z. "Comprehensive Conformational Studies of Five Tripeptides and a Deduced Method for Efficient Determinations of Peptide Structures" **Journal of Physical Chemistry B**., 116: 2269-2283, 2012, PMC3288331, 10.1021/jp207807a, PMC3288331
214. Foster, T.J., MacKerell Jr., A.D. and Guvench, O. "Balancing Target Flexibility and Target Denaturation in Computational Fragment-Based Inhibitor Discovery," **Journal of Computational Chemistry**, 33:1880-91, 2012, 10.1002/jcc.23026, PMC3438888
215. Stavitskaya, L., Shim, J., Healy, J.R., Matsumoto, R.R., MacKerell Jr., A.D., Coop, A. "Deconstructing 14-phenylpropyloxymetopon: minimal requirements for binding to mu opioid receptors," **Bioorganic & Medicinal Chemistry**, 20: 4556–4563, 2012.
216. Zhu, X., Shim, J., Lopes, P.E.M., and MacKerell Jr., A.D. "Intrinsic energy landscapes of amino acid side chains," **Journal of Chemical Information and Modeling**, 52:1559-1572, 2012, PMC3398815

217. Yu, W., He, X., Vanommeslaeghe, K. and MacKerell, A.D., Jr., "Extension of the CHARMM General Force Field to Sulfonyl-Containing Compounds and Its Utility in Biomolecular Simulations," **Journal of Computational Chemistry**, 33: 2451-2468, 2012, 10.1002/jcc.23067, PMC3477297
218. Best, R.B., Zhu, X., Shim, J., Lopes, P.E.M., Mittal, J., Feig, M., and MacKerell Jr., A.D. "Optimization of the additive CHARMM all-atom protein force field targeting improved sampling of the backbone ϕ, ψ and side-chain χ_1 and χ_2 dihedral angles," **Journal of Chemical Theory and Computation**, 8: 3257-3273, 2012, 10.1021/ct300400x, PMC3549273
219. Best, R.B., Mittal, J., Feig, M., and MacKerell Jr., A.D., "Inclusion of many-body effects in the additive CHARMM protein CMAP potential results in enhanced cooperativity of α-helix and β-hairpin formation, **Biophysical Journal**, 103, 1045-1051, 2012, PMC3433603
220. Petty, A., Myshkin, E., Qin, H., Guo, H., Miao, H., Tochtrop, G.P., Hsieh, J.-T., Page, P., Liu, L., Lindner, D.J., Acharya, C., MacKerell, A.D., Jr. Ficker, E., Song, J., and Wang, B. "A Small Molecule Agonist of EphA2 Receptor Tyrosine Kinase Inhibits Tumor Cell Migration in vitro and Prostate Cancer Metastasis in vivo," **PLoS One**, 7: e42120., 2012, PMC3419725.
221. Wagh, B., Paul, T., Glassford, I., DeBrosse, C., Klepacki, D., Small, M.C., MacKerell, A.D., Jr., and Andrade, R.B.,"Desmethyl Macrolides: Synthesis and Evaluation of 4,8-Didesmethyl Telithromycin," **ACS Medicinal Chemistry Letters**, 3:1013–1018, 2012, PMC3763958, DOI: 10.1021/ml200254h.
222. McKnight, L.; Raman, E.; Bezawada, Padmavani; Kudrimoti, Sucheta; Wilder, Paul; Hartman, Kira; Toth, Eric; Coop, Andrew; MacKerell, Alexander; Weber, David "Structure-Based Discovery of a Novel Pentamidine-Related Inhibitor of the Calcium-Binding Protein S100B," **ACS Medicinal Chemistry Letters**, 3: 975–979, 2012, DOI: 10.1021/ml300166s, PMC3524579
223. Vanommeslaeghe, K., and MacKerell Jr., A.D., "Automation of the CHARMM General Force Field (CGenFF) I: bond perception and atom typing," **Journal of Chemical Informationa and Modeling**, 52: 3144–3154, 2012, DOI: 10.1021/ci30036c, PMC3528824
224. Vanommeslaeghe, K., Raman, E.P., and MacKerell Jr., A.D., "Automation of the CHARMM General Force Field (CGenFF) II: Assignment of bonded parameters and partial atomic charges," **Journal of Chemical Informationa and Modeling**, 52: 3155–3168, 2012, DOI: 10.1021/ci3003649, PMC3528813
225. Jain, V., Hilton, B., Lin, B., Patnaik, S., Liang, F., Darian, E., Zou, Y., MacKerell Jr., A.D., and Cho, B.P. "Unusual sequence effects on nucleotide excision repair of arylamine lesions: DNA bending/distortion as a primary recognition factor," **Nucleic Acids Research**, 41: 869-880, 2013, PMC3553991
226. Shim, J., Zhu, X., Best, R.B., and MacKerell Jr., A.D. "$(Ala)_4$-X-$(Ala)_4$ as a model system for the optimization of the χ_1 and χ_2 amino acid side chain dihedral empirical force field parameters." **Journal of Computational Chemistry**, 34: 593-603, 2013, 10.1002/jcc.23178, PMC3570682
227. Luo, Y., Jiang, W., Yu, H., MacKerell, A.D., Jr., and Roux, B., "Simulation study of ion pairing in concentrated aqueous salt solutions with a polarizable force field," **Faraday Discussions**, 160, 135 – 149, 2013, 10.1039/C2FD20068F, PMC3695446

228. Yu, W., Lopes, P.E.M., Roux, B., and MacKerell, A.D., Jr., "Six-site Polarizable Model of Water Based on the Classical Drude Oscillator" **Journal of Chemical Physics**, 138, 034508 2013; http://dx.doi.org/10.1063/1.4774577, PMC3562330
229. Xue, F., MacKerell, A.D., Jr., Heinzl, G., Mbatia, H., and Hom, K. "Room Temperature Catalyst-Free Knoevenagel Condensation: Facile Access to Isatinylidenerhodanines," **Tetrahedron Letters**, 54, 1700-1703, 2013
230. Nagarajan, S., Xue, F., and MacKerell, A.D., Jr. "Impact of substrate protonation and tautomerization states on interactions with the active site of Arginase I," **Journal of Chemical Information and Modeling**, 53: 452–460, 2013, PMC3590304
231. McDonald, A.R., Elizabeth J. Denning, E.J, and MacKerell, A.D., Jr. "Impact of geometry optimization on base-base stacking interaction energies in the canonical A- and B-forms of DNA," **Journal of Physical Chemistry A**, 117: 1560–1568, 2013, PMC3579007.
232. Hom, K., Heinzl, G.A., Eakanunkul, S., Lopes, P.E.M., Xue, F., MacKerell, A.D., Jr., and Angela Wilks, A., "Small Molecule Antivirulents Targeting the Iron-Regulated Heme Oxygenase (HemO) of P. aeruginosa," **Journal of Medicinal Chemistry**, 56: 2097-2109, 2013, PMC3643010
233. Jung, K.-Y., Samadani, R., Chauhan, J., Nevels, K., Yap, J.L., Zhang, J., Worlikar, S., Ensey, M., Shukla, S, Salmo, R., Heinzl, G., Gordon, C., Dukes, T., Lanning, M.E., MacKerell, A.D., Jr., Shapiro, P., and Fletcher, S. "Structural Modifications of (*Z*)-3-(2-aminoethyl)-5-(4-ethoxybenzylidene)thiazolidine-2,4-dione that Improve Selectivity for Inhibiting Melanoma Cells Containing Active ERK Signaling," **Organic & Biomolecular Chemistry**, 11: 3706-3732, 2013, PMC3663054
234. Mallajosyula, S.S., Adams, K.M., Barchi, J.J., and MacKerell, A.D., Jr. "Conformational determinants of the activity of Antiproliferative factor glycopeptide." **Journal of Chemical Information and Modeling**, 53: 1127–1137 2013, 10.1021/ci400147s, PMC3690088
235. Cao, X., Yap, J.L., Newell-Rogers, M.K., Peddaboina, C., Hua, J., Papaconstantinou, H.T., Jupitor, D., Rai, A., Jung, K.-Y., Tubin, R.P., Yu, W., Vanommeslaeghe, K., Wilder, P.T., MacKerell, A.D., Jr., Fletcher, S., and Smythe, W.R., "The novel BH3 α-helix mimetic JY-1-106 induces apoptosis in a subset of cancer cells (lung cancer, colon cancer and mesothelioma) by disrupting Bcl-xL and Mcl-1 protein–protein interactions with Bak," **Molecular Cancer**, 12:42, 2013, 10.1186/1476-4598-12-42, PMC3663763.
236. He, X., Lopes, P.E.M., and MacKerell, A.D., Jr., "Polarizable Empirical Force Field for Acyclic Poly-Alcohols Based on the Classical Drude Oscillator," **Biopolymers**, 99: 724-738, 2013, 10.1002/bip.22286, PMC3902549
237. Lakkaraju, K.S. Xue, F., Faden, A., and MacKerell, A.D., Jr., "Estimation of ligand efficacies of metabotropic glutamate receptors from conformational forces obtained from molecular dynamics simulations," **Journal of Chemical Information and Modeling**, 53: 1337–1349, 2013, PMC3693859
238. Small, M., Andrade, R., and MacKerell, A.D., Jr., "Impact of Ribosomal Modification on the Binding of the Antibiotic Telithromycin using a Combined Grand Canonical Monte Carlo/Molecular Dynamics Simulation Approach," **PLoS Computational Biology**, 9: e1003113, 2013, PMC3681621, 10.1371/journal.pcbi.1003113
239. Yu, B., Liu, W., Yu, W.-M., Loh, M., Alter, S., Guvench, O., MacKerell, A.D., Jr., Tang, L.-D., and Qu, C.-K., "Targeting Protein Tyrosine Phosphatase SHP2 for the Treatment of PTPN11-Associated Malignancies," **Molecular Cancer Therapeutics**, 12:1738-1748, 2013, 10.1158/1535-7163.MCT-13-0049-T, PMC3769526

240. Sandineni, A., Lin, B., MacKerell, A.D., Jr. and Cho, B.P., "Structure and thermodynamic insights on acetylaminofluorene-modified deletion DNA duplexes as models for frameshift mutagenesis," **Chemical Research in Toxicology**, 26: 937-951, 2013, PMC3733349
241. Huang, J., and MacKerell, A.D., Jr. "CHARMM36 all-atom additive protein force field: Validation based on comparison to NMR data," **Journal of Computational Chemistry**, 34: 2135–2145, 2013, PMC3800559
242. Healy, J., Bezawada, P., Shim, J., MacKerell, A.D., Jr., Coop, A., and Matsumoto, R. "Synthesis, Modeling and Pharmacological Evaluation of UMB 425, a Mixed μ Agonist/δ Antagonist Opioid Analgesic with Reduced Tolerance Liabilities," **ACS Chemical Neuroscience**, 4:1256-1266, 2013, PMC3778426
243. Jung, K.-Y., Vanommeslaeghe, K., Lanning, M., Yap, J., Gordon, C., Wilder, P., MacKerell, A.D., Jr., and Fletcher, S., "Amphipathic α-Helix Mimetics Based on a 1,2-Diphenylacetylene Scaffold," **Organics Letters**, 15: 3234–3237, 2013, PMC3663054
244. He, X., Hatcher, E., Eriksson, L., Widmalm, G., and MacKerell, A.D., Jr. "Bifurcated Hydrogen Bonding and Asymmetric Fluctuations in a Carbohydrate Crystal Studied via X-ray Crystallography and Computational Analysis," **Journal of Physical Chemistry B**, 117: 7546–7553, 2013, PMC3771504
245. Shim, J., Coop, A., and MacKerell, A.D., Jr. "Molecular Details of the Activation of the μ Opioid Receptor," **Journal of Physical Chemistry B**, 117; 7907–7917, 2013, PMC3735350
246. Chowdhary, J., Harder, E., Lopes, P.E.M., MacKerell, Jr., A.D, and Roux, B., "A Polarizable Model for Phosphatidylcholine-Containing Biological Membranes," **Journal of Physical Chemistry B**.,117: 9142-9160, 2013. PMC3799809
247. Jain, V., Hilton, B., Lin, B., Jain, A., MacKerell, A.D., Jr., Zou, Y., and Cho, B., "Structural and Thermodynamic Insight into *Escherichia coli* UvrABC-Mediated Incision of Cluster Diacetylaminofluorene Adducts on the *Nar*I Sequence," **Chemical Research in Toxicology**, 26: 1251–1262, 2013, PMC3917139
248. Raman, E.P., and MacKerell, A.D., Jr., "Rapid estimation of hydration thermodynamics of macromolecular regions," **Journal of Chemical Physics**, 139: 055105, 2013, PMC3751957
249. Lin, B., Lopes, P.E.M., Roux, B., and MacKerell, A.D., Jr., "Kirkwood-Buff Analysis of Aqueous N-Methylacetamide and Acetamide Solutions Modeled by the CHARMM Additive and Drude Polarizable Force Fields," **Journal of Chemical Physics**, 139: 084509, 2013, PMC3772949
250. Hatzi, K.; Jiang, Y.; Huang, C.; Garrett-Bakelman, F.; Gearhart, M. D.; Giannopoulou, E. G.; Zumbo, P.; Kirouac, K.; Bhaskara, S.; Polo, J. M., Kormaksson, M., MacKerell, A.D., Jr., Xue, F., Mason, C.E., Hiebert, S.W., Prive, G.G., Cerchietti, L., Bardwell, V.J., Elemento, O., and Melnick, A. "A Hybrid Mechanism of Action for BCL6 in B Cells Defined by Formation of Functionally Distinct Complexes at Enhancers and Promoters," **Cell Reports**, 4, 1-11, 2013, 10.1016/j.celrep.2013.06.016, PMC3854650
251. Denning, E., Thirumali, D., MacKerell, A.D., Jr., "Protonation of Trimethylamine N-Oxide (TMAO) is required for stabilization of RNA tertiary structure," **Biophysical Chemistry**, 184: 8–16, 2013, 10.1016/j.bpc.2013.08.002, PMC3842377
252. Lin, B., He, X., and MacKerell, A.D., Jr., "A Comparative Kirkwood-Buff Study of Aqueous Methanol Solutions Modeled by the CHARMM Additive and Drude Polarizable Force Fields," **Journal of Physical Chemistry B**, 117: 10572-10580, 2013, 10.1021/jp4061889, PMC3787518

253. Varney, K., Bonvin, A.M.J.J., Yu, W., Ateh, E., Oashi, T., Huang, J., Diepeveen-de Buin, M., Bryant, J. Breukink, E., MacKerell, A.D., Jr., and de Leeuw, E., "Turning Defense into Offense: Development of Defensin Mimetics as Novel Antibiotics targeting Lipid II," **PLoS Pathogens**, 9: e1003732, 2013, 10.1371/journal.ppat.1003732, PMC3820767
254. Wagh, B., Paul, T., DeBrosse, C., Klepacki, D., Small, M.C., MacKerell, A.D., Jr., and Andrade, R.B."Desmethyl Macrolides: Synthesis and Evaluation of 4,8,10-Tridesmethyl Cethromycin," **ACS Medicinal Chemistry Letters**, 4: 1114-1118, 2013, 10.1021/ml400337t, PMC3901159
255. Sabit, H., Mallajosyula, S.S., MacKerell, A.D., Jr., and Swaan P.W. "Transmembrane Domain II of the Human Bile Acid Transporter SLC10A2 Coordinates Sodium Translocation," **Journal of Biological Chemistry**, 288: 32349-32404, 2013, PMC3820874, 10.1074/jbc.M113.518555
256. Lopes, P.E.M., Huang, J., Shim, J., Luo, Y., Li, H., Roux, B., and MacKerell, A.D., Jr., "Polarizable Force Field for Peptides and Proteins based on the Classical Drude Oscillator," **Journal of Chemical Theory and Computation**, 9: 5430–5449, 2013, 10.1021/ct400781b, PMC3896220
257. Raman, E.P., Yu, W., Lakkaraju, S.K., and MacKerell, A.D., Jr., "Inclusion of multiple fragment types in the Site Identification by Ligand Competitive Saturation (SILCS) approach," **Journal of Chemical Information and Modeling**, 53: 3384–3398, 2013, 10.1021/ci4005628, PMC3947602
258. Vanommeslaeghe, K., Guvench, O., and MacKerell, A.D., Jr., "Molecular Mechanics," in "Advances in Computational Structure Based Drug Discovery," **Current Pharmaceutical Design,** 20: 3281-3292, 2014, PMC4026342
259. Oyer, J.A., Huang, X., Zheng, Y., Shim, J., Ezponda, T., Allegretta, M., Okot-Kotber, C.I., Patel, J.P., Melnick, A., Levine, R.L., Ferrando, MacKerell, A.D., Jr., Kelleher, N.L., Licht, J.D., and Popovic, R., "Point mutation E1099K in MMSET/NSD2 enhances its methyltranferase activity and leads to altered global chromatin methylation in lymphoid malignancies," **Leukemia**, 28: 198-201, 2014. doi: 10.1038/leu.2013.204, PMC3888226
260. Sun, X., Rai, R., Deschamps, J.R., MacKerell, A.D., Jr., Faden, A.I., and Xue, F. "Boc-protected 1-(3-oxocycloalkyl)ureas via a one-step Curtius rearrangement: mechanism and scope," **Tetrahedron Letters**, 55, 1905-1908, 2014, 10.1016/j.tetlet.2013.12.021
261. Yu, W., Lakkaraju, S.K., Raman, E.P., and MacKerell, A.D., Jr., "Site-Identification by Ligand Competitive Saturation (SILCS) Assisted Pharmacophore Modeling," **Journal of Computer-Aided Molecular Design**, 28: 491-507, 2014, 10.1007/s10822-014-9728-0, PMC4048638
262. Patel, D.S., Pendrill, R., Mallajosyula, S.S., Widmalm, G.* and MacKerell, A.D., Jr.*, "Conformational Properties of α- or β-(1→6)-linked Oligosaccharides: Hamiltonian Replica Exchange MD Simulations and NMR Experiments," **Journal of Physical Chemistry B**., 118: 2851–2871, 2014, 10.1021/jp412051v, PMC3979472
263. Kumar, P., Bojarowski, S.A., Jarzembska, K.N., Domagala, S., Vanommeslaeghe, K., MacKerell, A.D., Jr., and Dominiak, P.A., "A comparative study of transferable aspherical pseudoatom databank and classical force fields for predicting electrostatic interactions in molecular dimers," **Journal of Chemical Theory and Computing**, 10: 1652–1664, 2014, 10.1021/ct4011129, PMC3985931

264. Savelyev, A. and MacKerell, A.D., Jr., "All-Atom Polarizable Force Field for DNA Based on the Classical Drude Oscillator Model," **Journal of Computational Chemistry**, 35: 1219–1239, 2014, DOI: 10.1002/jcc.23611, PMC4075971
265. Lakkaraju, S.K., Raman, E.P., Yu, W., and MacKerell, A.D., Jr., "Sampling of Organic Solutes in Aqueous and Heterogeneous Environments using Oscillating μ_{ex} Grand Canonical-like Monte Carlo-Molecular Dynamics Simulations," **Journal of Chemical Theory and Computing**, 10: 2281–2290, 2014, 10.1021/ct500201y, PMC4053307
266. Venable, R.M., Sodt, A.J., Rogaski, B., Rui, H., Hatcher, E., MacKerell, A.D., Jr., Pastor, R.W. and Klauda, J.B. "CHARMM All-Atom Additive Force Field for Sphingomyelin: Elucidation of Hydrogen Bonding and of Positive Curvature," **Biophysical Journal,** 107: 134-145, 2014, 10.1016/j.bpj.2014.05.034, PMC4119286
267. Lemkul, J.A., Savelyev, A., and MacKerell, A.D., Jr., "Induced Polarization Influences the Fundamental Forces in DNA Base Flipping," **Journal of Physical Chemistry Letters**, 5: 2077–2083 2014, 10.1021/jz5009517, PMC4064933
268. Savelyev, A. and MacKerell, A.D., Jr., "Balancing the interactions of ions, water and DNA in the Drude polarizable force field," **Journal of Physical Chemistry B**, 118: 6742-6757, 2014, 10.1021/jp503469s, PMC4064693
269. Li, T., Yang, D., Zhong, S., Thomas, J.M., Xue, F., Liu, J., Kong, L., Voulalas, P., Hassan, H.E., Park, J.-S., MacKerell, A.D., Jr. and Smith, W., "Novel LRRK2 GTP-binding inhibitors reduced degeneration in Parkinson's disease cell and mouse models," **Human Molecular Genetics**, 23: 6212-6222, 2014, 10.1093/hmg/ddu341.
270. Glassford, I., Miseon, L., Wagh, B., Velvadapu, V., Paul, T., Sandelin, G., DeBrosse, C., Klepacki, D., Small, M.C., MacKerell, A.D., Jr., and Andrade, R.B.," Desmethyl Macrolides: Synthesis and Evaluation of 4-Desmethyl Telithromycin," **ACS Medicinal Chemistry Letters**, 5, 1021-1026, 2014, 10.1021/ml5002097, PMC4160760
271. Huang, J. and MacKerell, A.D., Jr., "Induction of peptide bond dipoles drives cooperative helix formation in the $(AAQAA)_3$ peptide," **Biophysical Journal**, 107: 991-997, 2014, 10.1016/j.bpj.2014.06.038, PMC4142245
272. Huang, J., Lopes, P.E.M., Roux, B. and MacKerell, A.D., Jr., "Recent Advances in Polarizable Force Fields for Macromolecules: Microsecond Simulations of Proteins Using the Classical Drude Oscillator Model," **Journal of Physical Chemistry Letters**, 5: 3144–3150, 2014, 10.1021/jz501315h, PMC4167036
273. Mallajosyula, S., Vanommeslaeghe, K., and MacKerell, A.D., Jr., "Perturbation of Long-Range Water Dynamics as the Mechanism for the Antifreeze Activity of Antifreeze Glycoprotein," **Journal of Physical Chemistry B**, 118: 11696-11706, 2014, 10.1021/jp508128d, PMC4191590
274. Kern, N.R., Lee, H.S., Wu, E.L., Vanommeslaeghe, K., MacKerell, A.D., Jr., Klauda, J.B., Jo, S., and Im, W., "Lipid-Linked Oligosaccharides in Membranes Sample Conformations that Facilitate Binding to Oligosaccharyltransferase," **Biophysical Journal**, 107: 1885-1895, 2014, 10.1016/j.bpj.2014.09.007, PMC4213670
275. Patel, D.S., He, X., and MacKerell, A.D., Jr., "Polarizable Empirical Force Field for Hexopyranose Monosaccharides based on the Classical Drude Oscillator," **Journal of Physical Chemistry B**., 119: 637-652, 2015, 10.1021/jp412696m, PMC4143499
276. Vanommeslaeghe, K., and MacKerell, A.D., Jr., "CHARMM additive and polarizable force fields for biophysics and computer-aided drug design," **Biochimica et Biophysica Acta: General Subjects,** 1850: 861-871, 2015, 10.1016/j.bbagen.2014.08.004, PMC4334745

277. Savelyev, A., and MacKerell, A.D., Jr., "Differential Impact of the Monovalent Ions Li^+, Na^+, K^+ and Rb^+ on DNA Conformational Properties," **Journal of Physical Chemistry Letters**, 6: 212-216, 2015, DOI: 10.1021/jz5024543, PMC4285411
278. Yang, M., and MacKerell, A.D., Jr., "Conformational Sampling of Oligosaccharides Using Hamiltonian Replica Exchange with Two-Dimensional Dihedral Biasing Potentials and the Weighted Histogram Analysis Method (WHAM)," **Journal of Chemical Theory and Computation**, 11: 788–799, 2015, 10.1021/ct500993h, PMC4334390
279. Yu, W., Lakkaraju, S.K., Raman, E.P., Fang, L., and MacKerell, A.D., Jr., "Pharmacophore modeling using Site-Identification by Ligand Competitive Saturation (SILCS) with multiple probe molecules," **Journal of Chemical Information and Modeling**, 55: 407-420, 2015, 10.1021/ci500691p, PMC4339487
280. Raman, E.P. and MacKerell, A.D., Jr., "Spatial Analysis and Quantification of the Thermodynamic Driving Forces in Protein-Ligand Binding: Binding Site Variability," **Journal of the American Chemical Society**, 137: 2608-2621, 2015, DOI: 10.1021/ja512054f, PMC4342289
281. Kasavajhala, K., Bikkina, S., Patil, I., MacKerell, A.D., Jr., and Priyakumar, U.D., "Dispersion Interactions between Urea and Nucleobases Contribute to the Destabilization of RNA by Urea in Aqueous Solution," **Journal of Physical Chemistry B**, 119: 3755-3761, 2015, 10.1021/jp512414f, PMC4352126
282. Fletcher, S.F., Yu, W., Huang, J., Kwasny, S.M., Chauhan, J., Opperman, T.J., MacKerell, A.D., Jr., deLeeuw, E.P.H. "Structure–Activity Relationships of a Small-Molecule Lipid II inhibitor," **Drug Design, Development and Therapy**, 9: 2383-2394, 2015, 10.2147/DDDT.S79504, PMC4422293
283. Lakkaraju, S.K., Yu, W., Raman, E.P., Hershfeld, A.V., Fang, L., Deshpande, D.A., and MacKerell, A.D., Jr., "Mapping Functional Group Free Energy Patterns at Protein Occluded Sites: Nuclear Receptors and G-Protein Coupled Receptors," **Journal of Chemical Information and Modeling**, 55: 700-708, 2015, 10.1021/ci500729k, PMC4372819
284. Samadani, R., Zhang, J., Brophy, A., Oashi, T., Priyakumar, U.D., Raman, E.P., St John, F.J., Jung, K.-Y., Fletcher, S., Pozharski, E., MacKerell, A.D., Jr.,* and Shapiro, P.,* "Small Molecule Inhibitors of ERK-mediated Immediate Early Gene Expression and Proliferation of Melanoma Cells Expressing Mutated BRaf," **Biochemical Journal**, 467: 425-438, 2015, 10.1042/BJ20131571, PMC4643458
285. Vanommeslaeghe, K., Yang, M., and MacKerell, A.D., Jr., "Robustness in the fitting of Molecular Mechanics parameters," **Journal of Computational Chemistry**, 36: 1083-1101, 2015, 10.1002/jcc.23903, PMC4412823
286. He, X., Lakkaraju, S.K., Hanscom, M., Zhao, Z., Wu, J., Stoica, B., MacKerell, A.D., Jr., Faden, A.I. and Xue, F., "Acyl-2-aminobenzimidazoles: a novel class of neuroprotective agents targeting mGluR5," **Bioorganic and Medicinal Chemistry**, 23: 2222-2220, 2015, doi:10.1016/j.bmc.2015.02.054, PMC4697443
287. Savelyev, A., and MacKerell, A.D., Jr., "Competition among Li^+, Na^+, K^+ and Rb^+ Monovalent Ions for DNA in Molecular Dynamics Simulations using the Additive CHARMM36 and Drude Polarizable Force Fields," **Journal of Physical Chemistry B,** 119: 4428–4440, 2015, 10.1021/acs.jpcb.5b00683, PMC4378841
288. Mistry, P., Laird, M.H.W., Schwarz, R.S., Greene, S., Dyson, T., Snyder, G.A., Xiao, T.S., Chauhan, J., Fletcher, S., Toshchakov, V.Y., MacKerell, A.D., Jr.,* and Vogel, S.N.,* "Inhibition of TLR2 Signaling by Novel Small Molecule Inhibitors Targeting a Pocket within

the TLR2 TIR Domain," **Proceedings of the National Academy of Sciences**, USA, 112: 5455–5460, 2015, 10.1073/pnas.1422576112, PMC4418912
289. Lakkaraju, S.K., Mbatia, H., Hanscom, M., Zhao, Z., Wu, J., Stoica, B., MacKerell, A.D., Jr., Faden, A.I. and Xue, F., "Cyclopropyl-containing positive allosteric modulators of metabotropic glutamate receptor subtype 5," **Bioorganic and Medicinal Chemistry**, 25: 2275-2279, 2015, doi:10.1016/j.bmcl.2015.04.042, PMC4690453
290. Mei, Y., Wang, Y., Kumari, P., Shetty, A.C., Clark, D., Gable, T., MacKerell, A.D., Jr., Ma, M.Z., Weber, D., Edelman, M., Mao, L., "piRNA-L-163 interacts with p-ERM proteins in human somatic cells," **Nature Communications**, 6, Article number: 7316, 2015, doi:10.1038/ncomms8316, PMC4557300
291. Lemkul, J.A., Roux, B., van der Spoel, D and MacKerell, A.D., Jr., "Implementation of Extended Lagrangian Dynamics in GROMACS for Polarizable Simulations Using the Classical Drude Oscillator Model," **Journal of Computational Chemistry**, 36: 1480-1486, 2015, 10.1002/jcc.23937, PMC4481176
292. Yang, M., Huang, J., and MacKerell, A.D., Jr., "Enhanced Conformational Sampling Using Replica Exchange with Concurrent Solute Scaling and Hamiltonian Biasing Realized in One Dimension," **Journal of Chemical Theory and Computation**, 11: 2855–2867, 2015, 10.1021/acs.jctc.5b00243, PMC4463548
293. Jana, M. and MacKerell, A.D., Jr., "CHARMM Drude Polarizable Force Field for Aldopentofuranoses and Methyl-aldopentofuranosides," **Journal of Physical Chemistry B**, 119: 7846-7859, 2015, doi: 10.1021/acs.jpcb.5b01767, PMC4483154
294. Yang, W., Sun, X., Yu, W., Rai, R., Deschamps, J., Mitchell, L., Jiang, C., MacKerell, A.D., Jr., Xue, F., "Facile Synthesis of Spirocyclic Lactams from β–keto Carboxylic Acids." **Organic Letters**, 17: 3070-3073, 2015, doi: 10.1021/acs.orglett.5b01350
295. Chen, W., Shi, C., MacKerell, A.D., Jr. and Shen, J. "Conformational Dynamics of Two Natively Unfolded Fragment Peptides: Comparison of the AMBER and CHARMM Force Fields," **The Journal of Physical Chemistry B**, 119: 7902-7910, 2015, 10.1021/acs.jpcb.5b02290, PMC4685472
296. Passaniti, A., Brusgard, J., Choe, M., Chumsri, S., Renoud, K., MacKerell, A.D., Jr, and Sudol, M., "RUNX2 and TAZ-dependent signaling pathways regulate soluble E-Cadherin levels and tumorsphere formation in breast cancer cells," **Oncotarget**, 6: 28132-28150. 2015, doi: 10.18632/oncotarget.4654, 2015.
297. Domene, C., Jorgensen, C., Vanommeslaeghe, K., Schofield, C., MacKerell, A.D., Jr., "Quantifying the binding interaction between the hypoxia-inducible transcription factor and the von Hippel Lindau suppressor," **Journal of Chemical Theory and Computation**, *11:* 3946–3954, 2015, PMC5283694, 10.1021/acs.jctc.5b00411
298. Savelyev, A., and MacKerell, A.D., Jr. "Differential Deformability of the DNA Minor Groove and Altered BI/BII Backbone Conformational Equilibrium by the Monovalent Ions Li+, Na+, K+ and Rb+ via Water-Mediated Hydrogen Bonding," **Journal of Chemical Theory and Computation**, 11: 4473–4485, 2015, 10.1021/acs.jctc.5b00508, PMC4654687
299. Drennen, B., MacKerell, A.D., Jr. and Fletcher, S. "Expedient access to α-helix mimetics based on an Isocinchomeronic acid core," **Tetrahedron Letters**, **2015**, *56*, 6819-6822, 2015. doi:10.1016/j.tetlet.2015.10.020
300. Lee, J., Cheng, X., Swails, J., Yeom, M., Sun, Eastman, P., Lemkul, J., Wei, S., Buckner, J., Jeong, J.Ch., Qi, Y., Jo, S., Pande, V., Case, D., Brooks, C., MacKerell, A, Klauda, J., and Im, W., "CHARMM-GUI Input Generator for NAMD, GROMACS, AMBER, OpenMM,

and CHARMM/OpenMM Simulations using the CHARMM36 Additive Force Field," **Journal of Chemical Theory and Computation**, 12: 405-413, 2015, 10.1021/acs.jctc.5b00935, PMC4712441
301. Wu, E.L., Qi, Y., Park, S., Mallajosyula, S.S., MacKerell, A.D., Jr., Klauda, J.B., and Im, W., "Insight into Early-stage Unfolding of GPI-anchored Human Prion Protein," **Biophysical Journal**, 109: 2090-2100, 2015, 10.1016/j.bpj.2015.10.009, PMC4656879
302. Lakkaraju, S.K., Lemkul, J.A., Huang, J., and MacKerell, A.D., Jr. "DIRECT-ID: An Automated Method to Identify and Quantify Conformational Variations - Application to β2-adrenergic GPCR," **Journal of Computational Chemistry**, 37: 416–425, 2015, 10.1002/jcc.24231, PMC4756637
303. Lemkul, J.A., Huang, J. and MacKerell, A.D., Jr. "Induced Dipole-Dipole Interactions Influence the Unfolding Pathways of Wild-Type and Mutant Amyloid β-Peptides," **Journal of Physical Chemistry B**, 119: 15574–15582, 2015, 10.1021/acs.jpcb.5b09978, PMC4690986
304. Xu, Y., Vanommeslaeghe, K., Aleksandrov, A., MacKerell, A.D., Jr. Nilsson, L., "Additive CHARMM force field for naturally occurring modified ribonucleotides," **Journal of Computational Chemistry**, 37: 896-912, 2016, 10.1002/jcc.24307, PMC4801715
305. Lemkul, J.A., Huang, J., Roux, B., and MacKerell, A.D., Jr. "An Empirical Polarizable Force Field Based on the Classical Drude Oscillator Model: Development History and Recent Applications," **Chemical Reviews**, 116: 4983–5013, 2016, 10.1021/acs.chemrev.5b00505, PMC4865892
306. Lanning, M.E., Yu,W., Yap, J.l., Chauhan, J., Chen, L., Whiting, E., Pidugu, L.S., Atkinson, T, Bailey, H., Li, W., Roth, B.M., Hynicka,L., Chesko, K., Toth, E.A., Shapiro, P., MacKerell, Jr, A.D., Wilder, P.T. and Fletcher, S., "Structure-Based Design of N-Substituted 1-Hydroxy-4-sulfamoyl-2-naphthoates as Selective Inhibitors of the Mcl-1 Oncoprotein," **European Journal of Medicinal Chemistry**," 113: 272-292, 2016, 10.1016/j.ejmech.2016.02.006, PMC4811700
307. Cavalier, M.C., Ansari, M.I., Pierce, A.D., Wilder, P.T., McKnight, L.E., Raman, E.P., Neau, D.B., Bezawada, P., Alasady, M.J., Varney, K.M., Toth, E.A., MacKerell Jr., A.D., Coop, A., Weber, D.J., "Small Molecule Inhibitors of Ca^{2+}-S100B Reveal Two Protein Conformations," **Journal of Medicinal Chemistry**, 59: 592-608, 2016, 10.1021/acs.jmedchem.5b01369, PMC4732916
308. Glassford, I., Teija, C.N., Daher, S.S., Weil, A., Small, M.C., Redhu, S.K., Colussi, D.J., Jacobson, M.A., Childers, W., Buttaro, B., Nicholson, A.W., MacKerell, A.D., Jr., Cooperman, B.S., Andrade, R.B. "Ribosome-templated azide−alkyne cycloadditions: synthesis of potent macrolide antibiotics by *in situ* click chemistry," **Journal of the American Chemical Society**, 138: 3136-3144, 2016, 10.1021/jacs.5b13008, PMC4785600
309. Cavalier, M.C., Melville, Z., Aligholizadeh, E., Raman, E.P., Yu, W., Fang, L., Alasady, M., Pierce, A.D., Wilder, P.T., MacKerell, A.D., Jr. and Weber, D.J. "Novel protein-inhibitor interactions in site 3 of Ca^{2+}-bound S100B as discovered by X-ray crystallography," **Acta Crystallographica Section D**, D72, 753-760, 2016, doi:10.1107/S2059798316005532, PMC4908867
310. Astudillo, L, da Silva, T.G., Wang, Z., Han, X., Jin, K., VanWye, J., Zhu, X., Weaver, K.L., Oashi, T., Lopes, P.E.M., Orton, D., Neitzel, L.R., Lee, E., Landgraf, R., Robbins, D.J., MacKerell, A.D., Jr. and Capobianco, A.J. "Inhibitor of Mastermind Recruitment (IMR-1):

A Small Molecule Inhibitor of the Notch Transcriptional Activation Complex," **Cancer Research**, 76:3593-3603, 2016, doi:10.1158/0008-5472.CAN-16-0061, PMC4911243
311. Feng, Y., Huang, J., Kim, S., Shim, J.-H., MacKerell, A.D., Jr., and Ge, N.-H. "Structure of Penta-Alanine Investigated by Two-Dimensional Infrared Spectroscopy and Molecular Dynamics Simulation," **Journal of Physical Chemistry B**, 120:5325-5339, 2016, 10.1021/acs.jpcb.6b02608, PMC5243129
312. Cardenas, M.G., Yu, W.,* Beguelin, W., Teater, M., Geng, H., Goldstein, R., Oswald, E., Hatzi, K., Yang, S.-N., Cohen, J., Shaknovich, R., Vanommeslaeghe, K., Cheng, H., Liang, D., Cho, H.J., Abbott, J., Cerchietti, L, Cierpicki, T., Xue, F., MacKerell, A.D., Jr., and Melnick, A.M., "Therapeutic targeting of GCB- and ABC-DLBCLs by rationally designed BCL6 inhibitors," **Journal of Clinical Investigation**, 126:3351-336, 2016, 10.1172/JCI85795, PMC5004937
313. Xu, Y., MacKerell, A.D., Jr., and Nilsson, L. "Structural effects of modified ribonucleotides and magnesium in transfer RNAs," **Bioorganic & Medicinal Chemistry**, 24: 4826-4834, 2016, 10.1016/j.bmc.2016.06.037, PMC5052103
314. Soteras Gutiérrez, I., Lin, F.-Y.,* Vanommeslaeghe, K.,Lemkul, J.A., Armacost, K.A., Brooks, Cl., III, and MacKerell, A.D., Jr., "Parametrization of Halogen Bonds in the CHARMM General Force Field: Improved treatment of ligand-protein interactions," **Bioorganic & Medicinal Chemistry**, 24: 4812-4825, 2016, 10.1016/j.bmc.2016.06.034, PMC5053860
315. Yang, M., Angles d'Ortoli, T., Säwén, E., Jana, M., Widmalm, G., and MacKerell, A.D., Jr., "Delineating the conformational flexibility of trisaccharides from NMR spectroscopy experiments and computer simulations," **Physical Chemistry Chemical Physics**, 18: 18776-18794, 2016, 10.1039/c6cp02970a, PMC4945446
316. Heinzl, G., Huang, W., Yu, W, Giardina, B., Zhou, Y, MacKerell, A.D., Jr. Wilks, A., and Xue, F., "Benzimidoguanidines as Allosteric Inhibitors of the Iron-Regulated Heme Oxygenase (HemO) of Pseudomonas aeruginosa," **Journal of Medicinal Chemistry**, 2016, 59:6929-6942, 2016, 10.1021/acs.jmedchem.6b00757, PMC5080841
317. Sarkar, A., Yu, W., Desai, U.R., MacKerell, A.D., Jr., and Mosier, P. "Estimating glycosaminoglycan–protein interaction affinity: Water dominates the specific antithrombin–heparin Interaction," **Glycobiology**, 26: 1041-1047, 2016, 10.1093/glycob/cww073, PMC5072149
318. Chauhan, J., Cardinale, S., Fang, L., Huang, J., Kwasny, S.M., MacKerell, A.D., Jr., Opperman, T.J., Fletcher, S., and Erik P.H. de Leeuw, E.P.H. "Towards Development of Small Molecule Lipid II inhibitors as Novel Antibiotics," **PLoS ONE**, 11: e0164515, 2016, 10.1371/journal.pone.0164515, PMC5077133
319. Khan, H.M., Grauffel, C., Broer, R., MacKerell, A.D., Jr., Havenith, R.W.A., and Reuter, N., "Improving the force field description of tyrosine-choline cation-π interactions: QM investigation of phenol-$N(Me)_4^+$ interactions," **Journal of Chemical Theory and Computation**, 12: 5585-5595, 2016, 10.1021/acs.jctc.6b00654, PMC5148683
320. Huang, J., Rauscher, S., Nawrocki, G., Ran, T., Feig, M, de Groot, B.L., Grubmüller, H., and MacKerell, A.D., Jr., "CHARMM36m: An Improved Force Field for Folded and Intrinsically Disordered Proteins," **Nature Methods**, 14: 71-73, 2016, 10.1038/nmeth.4067, PMC5199616

321. Lemkul, J.A., Lakkaraju, S.K., and MacKerell, A.D., Jr., "Characterization of Mg^{2+} Distributions around RNA in Solution, **ACS Omega**, 1: 680-688, 2016, 10.1021/acsomega.6b00241, PMC5088455
322. Jo, S., Cheng, X., Lee, J., Kim, S., Park, S.-J., Patel, D.S., Beaven, A.H., Lee, K.I., Rui, H., Roux, B., MacKerell, A.D., Jr., Klauda, J.B., Qi, Y., and Im, W. "CHARMM-GUI 10 Years for Biomolecular Modeling and Simulation," **Journal of Computational Chemistry**, 38, 1114-1124, 2016, DOI: 10.1002/jcc.24660, PMC5403596
323. Lemkul, J.A. and MacKerell, A.D., Jr., "Balancing the Interactions of Mg^{2+} in Aqueous Solution and with Nucleic Acid Moieties For a Polarizable Force Field Based on the Classical Drude Oscillator Model," **Journal of Physical Chemistry B**, 120: 11436–11448, 2016, 10.1021/acs.jpcb.6b09262, PMC5148688
324. Huang, J., Lakkaraju, S.K., Coop, A. and MacKerell, A.D., Jr. "Conformational Heterogeneity of Intracellular Loop 3 of the μ-Opioid G-Protein Coupled Receptor," **Journal of Physical Chemistry B**, 120: 11897–11904, 2016, 10.1021/acs.jpcb.6b09351, PMC5148698
325. Raman, E.P., Lakkaraju, S.K., Denny, R.A., and MacKerell, A.D., Jr. "Estimation of relative free energies of binding using pre-computed ensembles based on the single-step free energy perturbation and the site-identification by ligand competitive saturation approaches," **Journal of Computational Chemistry**, 38: 1238-1251, 2017, 10.1002/jcc.24522, PMC5403604
326. Cardenas, M.G., Oswald, E., Yu, W. Xue, F., MacKerell, A.D., Jr. and Melnick, "The expanding role of the BCL6 oncoprotein as a cancer therapeutic target," **Clinical Cancer Research**, 23:885-893, 2017, PMID 27881582, 10.1158/1078-0432.CCR-16-2071, PMC5315622
327. Yang, M., Simon, R., and MacKerell, A.D., Jr. "Conformational Preference of Serogroup B *Salmonella* O Polysaccharide in Presence and Absence of the Monoclonal Antibody Se155-4: Implications for Vaccine Design," **Journal of Physical Chemistry B**, 121: 3412-3423, 2017, DOI: 10.1021/acs.jpcb.6b08955, PMC5407322
328. Small, M.C., Aytenfisu, A.H., Lin, F.-Y. He, X., and MacKerell, A.D., Jr., "Drude Polarizable Force Field for Aliphatic Ketones and Aldehydes, and their Associated Acyclic Carbohydrates," **Journal of Computer-Aided Molecular Design**, 31: 349-363, 2017, 10.1007/s10822-017-0010-0, PMC5392138
329. Huang, J., Mei, Y., Konig, G., Simmonett, A.C., Pickard, F.C., Wu, Q., Wang, L.-P., MacKerell, A.D., Jr., Brooks, B.R., and Shao, Y., "An Estimation of Hybrid Quantum Mechanical Molecular Mechanical (QM/MM) Polarization Energies for Small Molecules Using Polarizable Force-Field Approaches," **Journal of Chemical Theory and Computation**, 13:679-695, 2017,10.1021/acs.jctc.6b01125, PMC5315702
330. Shah, N.G., Tulapurkar, M.E., Ramarathnam, A.,Brophy, Martinez, R., Hom, K., Hodges, T., Samadani, R., Singh, I.S., MacKerell, A.D., Jr., Shapiro, P., and Hasday, J.D., "Novel Non-catalytic Substrate-selective p38α-specific MAPK Inhibitors with Endothelial-Stabilizing and Anti-inflammatory Activity," **The Journal of Immunology**, 198: 3296-3306, 2017, 10.4049/jimmunol.1602059, PMC5649369
331. Liang, D., Yu, W., Nguyen, N., Deschamps, J., Imler, G., Li, Yue; MacKerell, A.D., Jr., Jiang, C., and Xue, F. "Iodobenzene-Catalyzed Synthesis of Phenanthridinones via Oxidative C-H Amidation," **The Journal of Organic Chemistry**, 82 82: 3589-3596, 2017, 10.1021/acs.joc.7b00106

332. Baliban, S.M., Yang, M., Ramachandran, G., Curtis, B., Shridhar, S., Laufer, R.S., Wang, J.Y., Van Druff, J., Higginson, E.E., Hegerle, N., Varney, K.M., Galen, J.E., Tennant, S.M, Lees, A., MacKerell, A.D., Jr., Levine, M.M., and Simon, R., "A *Salmonella* Typhimurium glycoconjugate vaccine that targets invasive infections in sub-Saharan Africa," **PLOS Neglected Tropical Diseases**, 11: e0005493, 2017, doi:10.1371/journal.pntd.0005493, PMC5397072
333. Lemkul, J.A. and MacKerell, A.D., Jr., "Polarizable Force Field for DNA Based on the Classical Drude Oscillator: I. Refinement using Quantum Mechanical Base Stacking and Conformational Energetics," **Journal of Chemical Theory and Computation**, 13: 2053-2071, 2017, 10.1021/acs.jctc.7b00067, PMC5484419
334. Lemkul, J.A. and MacKerell, A.D., Jr., "Polarizable Force Field for DNA Based on the Classical Drude Oscillator: II. Microsecond Molecular Dynamics Simulations of Duplex DNA," **Journal of Chemical Theory and Computation**, 13: 2072-2085 2017, 10.1021/acs.jctc.7b00068, PMC5485260
335. Huang, J., Simmonett, A.C., Pickard, F.C., IV, MacKerell, A.D., Jr., and Brooks, B.R., "Mapping the Drude Polarizable Force Field onto a Multipole and Induced Dipole Model," **Journal of Chemical Physics**, 147, 161702, 2017, 10.1063/1.4984113, PMC5459616
336. Yang, M., Huang, J., Simon, R., Wang, L.-X., and MacKerell, A.D., Jr., "Conformational Heterogeneity of the HIV Envelope Glycan Shield," **Scientific Reports**, 7: 4435, 2017, 10.1038/s41598-017-04532-9, PMC5493700
337. Lin, F.-Y., and MacKerell, A.D., Jr., "Do Halogen-Hydrogen Bond Donor Interactions Dominate the Favorable Contribution of Halogens to Ligand-Protein Binding?" **The Journal of Physical Chemistry B**, 121: 6813-6821, 2017, 10.1021/acs.jpcb.7b04198, PMC5523114
338. Li, H., Chowdhary, J., Huang, L., He, X., MacKerell, A.D., Jr., and Roux, B. "Drude Polarizable Force Field for Molecular Dynamics Simulations of Saturated and Unsaturated Zwitterionic Lipids," **Journal of Chemical Theory and Computation**, 13: 4535-4552, 2017. 10.1021/acs.jctc.7b00262, PMC5595662
339. Klontz, E., Tomich, A., Gunther, S., Lemkul, J.A., Deredge, D., Silverstein, Z., Shaw, J., McElheny, C., Doi, Y., Wintrode, P., MacKerell, A.D., Jr., Sluis-Cremer, N., and Sundberg, E., "Structure and dynamics of FosA-mediated fosfomycin resistance in *Klebsiella pneumoniae* and *Escherichia coli*," **Antimicrobial Agents and Chemotherapy,** 61: e01572-17, 2017, 10.1128/AAC.01572-17, PMC5655077
340. Burns. L.A., Faver, J.C., Zheng, Z., Marshall, M.S., Smith, D.G.A., Vanommeslaeghe, K., MacKerell, A.D., Jr., Merz, K.M., Jr., and Sherrill, C.D., "The BioFragment Database (BFDb): An Open-Data Platform for Computational Chemistry Analysis of Noncovalent Interactions," **Journal of Chemical Physics**, 147:161727, 2017, 10.1063/1.5001028, PMC5656042
341. Huang, J., and MacKerell, A.D., Jr., "Force Field Development and Simulations of Intrinsically Disordered Proteins," **Current Opinion in Structural Biology**, 48:40-48, 2017, 10.1016/j.sbi.2017.10.008, PMC5826789.
342. Re, S., Watabe, S., Nishima, W., Muneyuki, E., Yamaguchi, Y., MacKerell, A.D., Jr., Sugita, Y., "Determinants of Collision Cross Sections of N-Glycans in Ion Mobility Mass Spectroscopy," **Science Reports**, 8, 1164, 2018, 10.1038/s41598-018-20012-0, PMC5786100
343. Yang, M., Aytenfisu, A.H., and MacKerell, A.D., Jr., "Proper Balance of Solvent-Solute and Solute-Solute Interactions in the Treatment of the Diffusion of Glucose using the Drude

Polarizable Force Field," **Carbohydrate Research**, 457:41-50, 2018, 10.1016/j.carres.2018.01.004, PMC5809005
344. Lin, F.-Y. and MacKerell, A.D., Jr., "Polarizable Empirical Force Field for Halogen-containing Compounds Based on the Classical Drude Oscillator," **Journal of Chemical Theory and Computation**, 14: 1083–1098, 2018, 10.1021/acs.jctc.7b01086, PMC5811359, PMC5811359
345. Huang, J., Lemkul, J.A., Eastman, P.K., and MacKerell, A.D., Jr., "Molecular Dynamics Simulations of Explicitly Solvated Drude Polarizable Systems on GPUs: Implementation, Validation, and Benchmark," **Journal of Computational Chemistry**, 39:1682-1689, 2018, 10.1002/jcc.25339, PMC6031474
346. Lin, F.-Y., Lopes, P.E.M., Harder, E., Roux, B.* and MacKerell, A.D., Jr.*, "Polarizable Force Field for Molecular Ions Based on the Classical Drude Oscillator," **Journal of Chemical Information and Modeling**, 58: 993-1004, 2018, 10.1021/acs.jcim.8b00132, PMC5975207
347. Aleksandrov, A., Lin, F.-Y., Roux, B., and MacKerell, A.D., Jr., "Combining the Polarizable Drude Force Field with a Continuum Electrostatic Poisson–Boltzmann Implicit Solvation Model," **Journal of Computational Chemistry**, 39:1707-1719, 2018, 10.1002/jcc.25345, PMC6108925
348. Boulanger, E., Huang, L., Rupakheti, C., MacKerell, A.D., Jr., and Roux, B. "Optimized Lennard-Jones Parameters for Drug-Like Small Molecules," **Journal of Chemical Theory and Computation**, 14: 3121-3131, 2018, 10.1021/acs.jctc.8b00172, 2018, PMC5997559
349. Aytenfisu, A.H., Yang, M., and MacKerell, A.D., Jr., "CHARMM Drude Polarizable Force Field for Glycosidic Linkages Involving Pyranoses and Furanoses," **Journal of Chemical Theory and Computation**, 14: 3132-3143, 2018, 10.1021/acs.jctc.8b00175, PMC5997548
350. Villa, F., MacKerell, A.D., Jr., Roux, B., and Simonson, T., "Classical Drude Polarizable Force Field Model for Methyl Phosphate and its Interactions with Mg^{2+}" **Journal of Physical Chemistry A**, 122: 6147-6155, 2018, 10.1021/acs.jpca.8b04418, PMC6062457
351. Cheng, H., Linhares, B., Yu, W., Cardenas, M., Ai, Y., Jiang, W., Melnick, A., MacKerell, A.D., Jr., Cierpicki, T., Xue, F., "Identification of Thiourea-Based Inhibitors of the BCL6 BTB Domain via NMR-Based Fragment Screening and Computer-Aided Drug Design," **Journal of Medicinal Chemistry**, 61: 7573–7588, 2018, 10.1021/acs.jmedchem.8b00040, PMC6334293
352. Sun, D., Lakkaraju, K., Jo, S., and MacKerell, A.D., Jr., "Determination of Ionic Hydration Free Energies with Grand Canonical Monte Carlo/Molecular Dynamics Simulations in Explicit Water," **Journal of Chemical Theory and Computation**, 14: 5290-5302, 2018, 10.1021/acs.jctc.8b00604, PMC6195813
353. Lemkul, J.A. and MacKerell, A.D., Jr., "Polarizable Force Field for RNA Based on the Classical Drude Oscillator," **Journal of Computational Chemistry**, 39: 2624-2646, 2018, 10.1002/jcc.25709, PMC6284239
354. König, G., Pickard IV, F.C., Huang, J., Thiel, W., MacKerell Jr., A.D., Brooks, B.R., and York, D.M. "A Comparison of QM/MM Simulations with and without the Drude Oscillator Model Based on Hydration Free Energies of Simple Solutes," **Molecules**, 23: 2695, 2018, 10.3390/molecules23102695, PMC6222909
355. Swaroop, A., Oyer, J., Will, C., Huang, X., Yu, W., Troche, C., Bulic, M., Durham, B., Wen, Q., Crispino, J., MacKerell, A.D., Jr., Bennett, R., Kelleher, N., and Licht, J., "An Activating Mutation of the NSD2 Histone Methyltransferase Drives Oncogenic

Reprogramming in Acute Lymphocytic Leukemia," **Oncogene**, 38: 671-686, 2019, 10.1038/s41388-018-0474-y, PMC6358490

356. Lin, F.-Y. and MacKerell Jr., A.D., "Improved Modeling of Halogenated Ligand-Protein Interactions using the Drude Polarizable and CHARMM Additive Empirical Force Fields," **Journal of Chemical Information and Modeling**, 59: 215-218, 2019, 10.1021/acs.jcim.8b00616, PMC6349471
357. Khan, H.M., MacKerell, A.D., Jr., and Reuter, N. "Cation-π interactions between methylated ammonium groups and tryptophan in the CHARMM36 additive force field," **Journal of Chemical Theory and Computation**, 15: 7-12, 2019, 10.1021/acs.jctc.8b00839, PMC6467778
358. Brocke, S.A., Degen, A., MacKerell, A.D., Jr., Dutagaci, B., and Michael Feig, M., "Prediction of Membrane Permeation of Drug Molecules by Combining an Implicit Membrane Model with Machine Learning," **Journal of Chemical Information and Modeling**, 59: 1147-1162, 2019, 10.1021/acs.jcim.8b00648, PMC6433486
359. Yu, W., Jo, S., Lakkaraju, S.K., Weber, D.J., and MacKerell, A.D., Jr., "Exploring protein-protein interactions using the Site-Identification by Ligand Competitive Saturation (SILCS) methodology," **Proteins: Structure, Function and Bioinformatics**, 87: 289-301, 2019, 10.1002/prot.25650, PMC6408985
360. Aytenfisu, A.H., Simon, R., and MacKerell, A.D., Jr., "Impact of branching on the conformational heterogeneity of the lipopolysaccharide from Klebsiella pneumoniae: Implications for vaccine design," **Carbohydrate Research**, 475: 39-47, 2019, 10.1016/j.carres.2019.02.003, PMC6529184
361. Heid, E., Fleck, M., Chatterjee, P., Schröder, C. and MacKerell, A.D., Jr. "Towards Prediction of Electrostatic Parameters for Force Fields that Explicitly Treat Electronic Polarization," **Journal of Chemical Theory and Computation**, 15: 2460-2469, 2019, 10.1021/acs.jctc.8b01289, PMC6473792
362. Ustach, V.D., Lakkaraju, S.K., Jo, S., Yu, W., Jiang, W., and MacKerell, A.D., Jr. "Optimization and Evaluation of the Site-Identification by Ligand Competitive Saturation (SILCS) as a Tool for Target- Based Ligand Optimization," **Journal of Chemical Information and Modeling**, 59: 3018-3035, 2019. 10.1021/acs.jcim.9b00210, PMC6597307
363. Bedrov, D., Piquemal, J.-P., Borodin, O, MacKerell, A.D., Jr., Roux, B., and Schröder, C., "Molecular Dynamics Simulations of Ionic Liquids and Electrolytes Using Polarizable Force Fields," **Chemical Reviews**, 119: 7940-7995, 2019, 10.1021/acs.chemrev.8b00763, PMC6620131
364. Donohue, E., Khorsand S., Mercado, G., Varney, K.M., Wilder P.T., Yu, W., MacKerell Jr., A.D., Alexander, P., Van Q.N., Moree, B., Stephen, A.G., Weber, D.J., Salafsky, J., and McCormick, F., "Second harmonic generation detection of Ras conformational changes and discovery of a novel small-molecule binder," **Proceedings of the National Academy of** Sciences, USA, 116: 17290-17297, 2019, 10.1073/pnas.1905516116, PMC6717309
365. Heid, E., Schmode, S., Chatterjee, P., MacKerell Jr., A.D. and Schröder, C., "Solvation dynamics: improved reproduction of the time-dependent Stokes shift with polarizable empirical force field chromophore models," **Physical Chemistry Chemical Physics**, 21: 17703-17710, 2019, 10.1039/c9cp03000j, PMC6697210
366. Pandey, P., Aytenfisu, A., MacKerell Jr., A.D., and Mallajosyula, S., "Drude Polarizable Force Field Parametrization of Carboxylate and N-acetyl Amine Carbohydrate Derivatives,"

Journal of Chemical Theory and Computation, 15: 5982-5000, 2019, 10.1021/acs.jctc.9b00327, PMC6852669
367. Lin, F.-Y., and MacKerell Jr., A.D., "Improved Modeling of Cation-π and Anion-Ring Interactions Using the Drude Polarizable Empirical Force Field for Proteins," **Journal of Computational Chemistry**, 41: 439-448, 2020, 10.1002/jcc.26067, PMC7322827
368. MacKerell Jr., A.D., "Ions everywhere? Mg^{2+} in the mu-opioid GPCR and atomic details of their impact on function," **Biophysical Journal**, New and Notable, 118: 783-784, 2020, 10.1016/j.bpj.2019.10.017, PMC7036735
369. Xu, X., Ruiz, R., Adipietro, K., Cleveland, T., Grishaev, A., Neu, H., Michel, S., Yu, W., Beckett, B., Rustandi, R.R., MacKerell Jr., A.D., DesGeorges, A., Pozharski, E., and Weber, D.J. "Structure of the cell-binding component of the C. difficile binary toxin reveals a novel macromolecular assembly," **Proceedings of the National Academy of Sciences, USA**, 117:1049-1058, 2020, 10.1073/pnas.191949011758, PMC6969506
370. Kumar, A., Yoluk, O. and MacKerell Jr., A.D. "FFParam: Standalone Package for CHARMM Additive and Drude Polarizable Force Field Parametrization of Small Molecules," **Journal of Computational Chemistry**, 41: 958-970, 2020, 10.1002/jcc.26138, PMC7323454
371. MacKerell Jr., A.D.*, Jo., S., Lakkaraju, S.K., Lind, C., and Yu, W. "Identification and Characterization of Fragment Binding Sites for Allosteric Ligand Design using the Site Identification by Ligand Competitive Saturation Hotspots Approach (SILCS-Hotspots)," **Biochimia et Biophysica Acta**, 1864: 129519, 2020, 10.1016/j.bbagen.2020.129519, PMC7029399
372. Chauhan J., Yu W., Cardinale S., Opperman T., MacKerell, A.D., Jr., Fletcher, S., and de Leeuw, E.P.H. "Optimization of a Benzothiazole Indolene Scaffold Targeting Bacterial Cell Wall Assembly" **Drug Design, Development and Therapy**, 14: 567-574, 2020, 10.2147/DDDT.S226313, PMC7024799
373. Turchi, M., Kognole, A.A, Kumar, A., Cai, Q., Lian, G., and MacKerell, A.D., Jr., Predicting Partition Coefficients of Neutral and Charged Solutes in the Mixed SLES-Fatty Acids Micellar System, **Journal of Physical Chemistry B**, 124: 1653-1664, 2020, 10.1021/acs.jpcb.9b11199, PMC7060100
374. Kognole, A.A. and MacKerell, A.D., Jr., "Mg^{2+} Impacts the Twister Ribozyme through Push-Pull Stabilization of Non-Sequential Phosphate Pairs," **Biophysical Journal**, 6: 1424-1437, 2020, 10.1016/j.bpj.2020.01.021, PMC7091459
375. Goel, H., Yu, W., Ustach, V.D., Aytenfisu, A.H., Sun, D., and MacKerell, A.D., Jr., "Impact of Electronic Polarizability on Protein-Functional Group Interactions," **Physical Chemistry Chemical Physics**, 22: 6848-6860, 2020, 10.1039/D0CP00088D, PMC7194236
376. Lin, F.-Y. Huang, J., Pandey, P., Rupakheti, C., Li, J., Roux, B., and MacKerell, A.D., Jr., "Further Optimization and Validation of the Classical Drude Polarizable Protein Force Field," **Journal of Chemical Theory and Computation**, 16: 3221-3239, 2020, 10.1021/acs.jctc.0c00057, PMC7306265
377. Kognole, A.A., Aytenfisu, A.H., and MacKerell, A.D., Jr., "Balanced Polarizable Drude Force Field Parameters for Molecular Anions: Phosphates, Sulfates, Sulfamates and Oxides," **Journal of Molecular Modeling,** 26:152, 2020, 10.1007/s00894-020-04399-0, PMC7326346

378. Aleksandrov, A., Roux, B., and MacKerell, A.D., Jr., "pK_a Calculations with the Polarizable Drude Force Field and Poisson-Boltzmann Solvation Model," **Journal of Chemical Theory and Computation**, 16: 4655-4668, 2020, 10.1021/acs.jctc.0c00111, PMC7428141
379. Conlon, I.L., Drennen, B., Lanning, M.E., Hughes, S., Rothhaas, R., Wilder, P,T., MacKerell, A.D., Jr., and Fletcher, S. "Rationally Designed Polypharmacology: α-Helix Mimetics as Dual Inhibitors of the Oncoproteins Mcl-1 and HDM2," **ChemMedChem**, 5:1691-1698, 2020, 10.1002/cmdc.202000278, PMC8477420
380. Kognole, A.A. and MacKerell, A.D., Jr., "Contributions and competition of Mg^{2+} and K^+ in folding and stabilization of the Twister Ribozyme," **RNA**, 26:1704-1715, 2020, bioRxiv:10.1101/2020.06.15.152744, 10.1261/rna.076851.120, PMC7566569
381. Rupakheti, C., Lamoureux, G., MacKerell, A.D., Jr., and Roux, B. "Statistical Mechanics of Polarizable Force Fields Based on Classical Drude Oscillators With Dynamical Propagation by the Dual-Thermostat Extended Lagrangian," **Journal of Chemical Physics**, 153: 114108, 2020, 10.1063/5.0019987, PMC7656322
382. Jo, S., Xu, A., Curtis, J., Somani, S., and MacKerell, A.D., Jr. "Computational Characterization of Antibody-Excipient Interactions for Rational Excipient Selection using the Site Identification by Ligand Competitive Saturation (SILCS)-Biologics Approach," **Molecular Pharmaceutics**, 17: 4323-4333, 2020, 10.1021/acs.molpharmaceut.0c00775, PMC7606568
383. Weston, S., Baracco, L., Keller, C., Matthews, K., McGrath, M.E., Logue, J., Liang, J., Dyall, J., Holbrook, M.R., Hensley, L.E., Jahrling, P.B., Yu, W., MacKerell, A.D., Jr., and Frieman, M.B., "The SKI complex is a broad-spectrum, host-directed, antiviral drug target for coronaviruses, influenza and filoviruses," **Proceedings of the National Academies of Sciences, USA**, 117:30687-30698, 2020, 10.1073/pnas.2012939117, PMC7720140
384. Mousaei, M., Kudaibergenova, M., MacKerell, A.D., Jr. and Noskov, S. "Assessing hERG1 Blockade from Bayesian Machine Learning Optimized Site-Identification by Ligand Competitive Saturation (SILCS) Simulations," **Journal of Chemical Information and** Modeling, 60: 6489-6501, 2020, 10.1021/acs.jcim.0c01065, PMC7839320
385. Takimoto. T., Sasaki, H., Tsue, H., Takahashi, H., MacKerell, A.D., Jr., Nakano, K., Okazaki, E., Nakamura, A., Betsuyaku, T., Tachibana, R., Hioki, K., Yoluk, O., and Jo, S. "Simple Synthesis of a Heterocyclophane Exhibiting Anti-c-Met Activity by Acting as a Hatch Blocking Access to the Active Site," **Chemistry - A European Journal**, 27: 1648-1654, 2021, 10.1002/chem.202001382, PMC7887132
386. Somani, S., Jo, S., Thirumangalathu, R., Rodrigues, D., Tanenbaum, L.M., Amin, K., Alexander D. MacKerell, A.D., Jr. and Thakkar, S.V., "Toward Biotherapeutics Formulation Composition Engineering using Site-Identification by Ligand Competitive Saturation (SILCS)," **Journal of Pharmaceutical Sciences**, 110: 1103-1110, 2021, 10.1016/j.xphs.2020.10.051, PMC7897284
387. Diethelm-Varela, B., Kumar, A., Lynch, C., Imler, G., Deschamps, J., Xia, M., MacKerell, A.D., Jr., and Xue, F. "Stereoisomerization of 6-(4-Chlorophenyl)imidazo[2,1-b][1,3]thiazole-5-carbaldehyde-O-(3,4-dichlorobenzyl)oxime (CITCO)," **Tetrahedron**, 79: 131886, 2021, 10.1016/j.tet.2020.131886
388. Solano-Gonzalez, E., Coburn, K., Yu, W., Wilson, G., Nurmemmedov, E., Kesari, S., Chang, E., MacKerell, A.D., Jr., Weber, D., and Carrier, F., "Small molecules inhibitors of the heterogeneous Ribonuclear protein A18 (hnRNP A18); a regulator of protein translation

and an immune checkpoint," **Nucleic Acids Research**, 49:1235-1246 2021, 10.1093/nar/gkaa1254, PMC7897483
389. Parvaiz, N., Ahmad, F., Yu, W., MacKerell, A.D., Jr.,* and Azam, S.S.*, "Discovery of beta-lactamase CMY-10 inhibitors for combination therapy against multi-drug resistant Enterobacteriaceae," **PLoS One**, 16: e0244967, 2021, 10.1371/journal.pone.0244967, PMC7810305
390. Young, B., Yu, W., Vera-Rodriguez, D., Varney, K., MacKerell, A.D., Jr., and Weber, D.J. "Specificity of small molecules binding to S100B versus S100A1 as identified using fragment-based screening by NMR and Site Identification by Ligand Competitive Saturation (SILCS)," **Molecules**, 26:381, 2021, 10.3390/molecules26020381, PMC7828390
391. Ngo, V. Li, H., MacKerell, A.D., Jr., Allen, T.W., Roux, B., and Noskov, S. "Polarization Effects in Water-Mediated Selective Cation Transport Across a Narrow Transmembrane Channel*,"* **Journal of Chemical Theory and Computation**, 17: 1726-1741, 2021, 10.1021/acs.jctc.0c00968, PMC8453344
392. Yu, Y., Krämer, A., Venable, R., Simmonett, A., MacKerell, A.D., Jr., Klauda, J., Pastor, R., and Brooks, B.R., "Semi-Automated Optimization of the CHARMM36 Lipid Force Field to Include Explicit Treatment of Long-Range Dispersion," **Journal of Chemical Theory and Computation**, 17:1562-1580, 2021, 10.1021/acs.jctc.0c01326, PMC8059446
393. Li, S., Zhao, J., Huang, R., Travers, J., Klumpp-Thomas, C., Yu, W., MacKerell, A.D., Jr., S., Sakamuru, Ooka, M., Xue, F., Sipes, N.S., Hsieh, J.-H., Ryan, K., Simeonov, A., Santillo, M.F., Xia, M., "Profiling the Tox21 Program Chemical Collection for Acetylcholinesterase Inhibition," **Environmental Health Perspectives***,* 129: 047008, 2021, 10.1289/EHP6993, PMC8041433
394. Ai, Y., Hwang, L., MacKerell, A.D., Jr., Melnick, A., and Xue, F., "Progress towards B-Cell Lymphoma 6 BTB Domain Inhibitors for the Treatment of Diffuse Large B-Cell Lymphoma and Beyond," **Journal of Medicinal Chemistry**, 64: 4333-4358, 2021, 10.1021/acs.jmedchem.0c01686, PMC8168288
395. Gomes, A.A., da Silva, G.F., Lakkaraju, S.K., MacKerell, A.D., Jr., Magalhaes, M.L.B., "Insights into Glucose-6-phosphate Allosteric Activation of β-Glucosidase A," **Journal of Chemical Information and Modeling**, 61: 1931-1941, 2021, 10.1021/acs.jcim.0c01450, PMC8085047
396. Lind, C., Pandey, P., Pastor, R., and MacKerell, A.D., Jr. "Functional Group Distributions, Partition Coefficients and Resistance Factors in Lipid Bilayers using Site Identification by Ligand Competitive Saturation (SILCS)," **Journal of Chemical Theory and Computation**, 17: 3188-3202, 2021, 10.1021/acs.jctc.1c00089, PMC8212490
397. Li, C., Chong, G., Zong, G., Knorr, D., Bournazos, S., Aytenfisu, A.H., Henry, G., Ravetch, J., MacKerell, A.D., Jr., and Wang, L.-X., "Site-Selective Chemoenzymatic Modification on the Core Fucose of an Antibody Enhances Its Fcγ Receptor Affinity and ADCC Activity," **Journal of the American Chemical Society**, 143: 7828-7838, 2021, PMC8283798, 10.1021/jacs.1c03174
398. Croitoru, A., Park, S.-J., Kumar, A., Lee, J., Im, Wonpil; MacKerell, A.D., Jr., and Aleksandrov, A. "Additive CHARMM36 Force Field for Nonstandard Amino Acids," **Journal of Chemical Theory and Computation**, 17: 3554-3570, 2021, 10.1021/acs.jctc.1c00254, PMC8207570
399. Goel, H., Hazel, A., Ustach, V.D., Jo, S., Yu, W., and MacKerell, A.D., Jr., "Rapid and Accurate Estimation of Protein-Ligand Relative Binding Affinities using Site-Identification

by Ligand Competitive Saturation," **Chemical Science**, 12: 8844-8858, 2021, 10.1039/D1SC01781K, PMC8246086
400. Aytenfisu, A.H., Deredge, D., Klontz, E.H., Du, J., Sundberg, E.J. and MacKerell, A.D., Jr., "Insights into substrate recognition and specificity for IgG by Endoglycosidase S2," **PLoS Computational Biology**, 17: e1009103, 2021, 10.1371/journal.pcbi.1009103, PMC8354483
401. Ernst, O., Khan, M.M., Oyler, B.L., Yoon, S.H., Sun, J., Lin, F.-Y., Manes, N.P., MacKerell, A.D., Jr., Fraser, I.D.C., Ernst, R.K., Goodlett, D.R., and Nita-Lazar, A., "Species-specific endotoxin stimulus determines TLR4- and Caspase11- mediated pathway activation characteristics," **mSystems**, 6: e00306-21, 2021, 10.1128/mSystems.00306-21, PMC8407122
402. Rupakheti, C., MacKerell, A.D., Jr., and Roux, B. "Global Optimization of the Lennard-Jones Parameters for the Drude Polarizable Force Field," **Journal of Chemical Theory and Computation**, 17:7085-7095, 2021, 10.1021/acs.jctc.1c00664, PMC8578466
403. Pane, A.J., Yu, W, Aytenfisu, A.A., Tunyi, J., Venable, R.M., MacKerell, A.D., Jr., and Pastor, R.W., "Development of CHARMM Additive Potential Energy Parameters for α-Methyl Amino Acids," **Journal of Physical Chemistry B**, 125:11687-11696, 2021, 10.1021/acs.jpcb.1c07202, PMC8627904
404. Green, A., Pickard, A., Li, R., MacKerell, A.D., Jr., Bierbach, U., and Cho, S., "Computational and Experimental Characterization of rDNA and rRNA G-Quadruplexes," **Journal of Physical Chemistry B**., 126: 609–619, 2022, PMC8995076, 10.1021/acs.jpcb.1c08340
405. Goel, H., Hazel, A., Yu, W., Jo, S., and MacKerell, A.D., Jr., "Application of Site-Identification by Ligand Competitive Saturation in Computer-Aided Drug Design," **New Journal of Chemistry**, 46: 919-932, 2022, 10.1039/D1NJ04028, PMC8863107
406. Sengul, M.Y. and MacKerell, A.D., Jr., "Accurate modeling of RNA hairpins through the explicit treatment of electronic polarizability with the classical Drude oscillator force field," **Journal of Computational Biophysics and Chemistry**, 21: 1-11, 2022, PMC9231828, 10.1142/S2737416521420060
407. Kognole, A.A., Lee, J., Park, S.-J., Jo, S., Chatterjee, P., Lemkul, J.A., Huang, J., MacKerell, A.D., Jr.,* and Im, W.,* "CHARMM-GUI Drude Prepper for Molecular Dynamics Simulation Using the Classical Drude Polarizable Force Field" **Journal of Computational Chemistry**, 43:359-375, 2022, PMC8741736, 10.1002/jcc.26795
408. Kumar, A., Pandey, P., Chatterjee, P., and MacKerell, A.D., Jr., "Deep Neural Network Model to Predict the Electrostatic Parameters in the Polarizable Classical Drude Oscillator Force Field," **Journal of Chemical Theory and Computation**, 18:1711-1725, 2022, PMC8904317, 10.1021/acs.jctc.1c01166
409. Chatterjee, P., Sengul, M.Y., Kumar, A., and MacKerell, A.D., Jr., "Harnessing Deep Learning for Optimization of Lennard-Jones Parameters for the Polarizable Classical Drude Oscillator Force Field, **Journal of Chemical Theory and Computation**, 18: 2388-2407, 2022, PMC9097857, 10.1021/acs.jctc.2c00115
410. Wang, F., Yu, W., Popescu, C., MacKerell, A.D., and Hoag, S., "Cholecalciferol Complexation with Hydroxypropyl-β-Cyclodextrin (HPBCD) and Its Molecular Dynamics Simulation," **Pharmaceutical Development and Technology (IPHD)**, 27: 389-398, 2022, PMC9233054, 10.1080/10837450.2022.2064492
411. Drennen, B., Goodis, C., Bowen, N., Yu, W., Vickers, G., Wilder, P., MacKerell, A.D., Jr., and Fletcher, S., "Scaffold hopping from indoles to indazoles yields dual MCL-1/BCL-2

inhibitors from MCL-1 selective leads," **RSC Medicinal Chemistry**, 13: 963-969, 2022, PMC9384788, 10.1039/d2md00095d.

412. Goel, H., Yu, W., and MacKerell, A.D., Jr. "hERG Blockade Prediction by Combining Site Identification by Ligand Competitive Saturation and Physicochemical Properties," **MDPI Chemistry**, 4: 630-645, 2022, 10.3390/chemistry4030045 and **Preprints**, 2022050255, 2022 (doi: 10.20944/preprints202205.0255.v1).
413. Kognole, A.A., Hazel, A., and MacKerell, A.D., Jr., "SILCS-RNA: Toward a Structure-Based Drug Design Approach for Targeting RNAs with Small Molecules," **Journal of Chemical Theory and Computation**, 18: 5672-5691, 2022, PMC9474704, 10.1021/acs.jctc.2c00381
414. Orr, A.A., Sharif, S., Wang, J., and MacKerell, A.D., Jr., "Preserving the Integrity of Empirical Force Fields," **Journal of Chemical Information and Modeling**, 62: 3825-3831, 2022, PMC9399073, 10.1021/acs.jcim.2c00615.
415. Chong, G. and MacKerell, A.D., Jr., "Spatial Requirements for ITAM Signaling in an Intracellular Natural Killer Cell Model Membrane" **Biochimica et Biophysica Acta (BBA) – General Subjects**, 1866: 130221, 2022, PMC9420803, 10.1016/j.bbagen.2022.130221, https://authors.elsevier.com/a/1fYoP15Dr%7Eg5ls
416. Kognole, A.A., Aytenfisu, A.H., and MacKerell, A.D., Jr., "Extension of the CHARMM Classical Drude Polarizable Force Field to N- and O-Linked Glycopeptides and Glycoproteins," **Journal of Physical Chemistry B**, 126: 6642-6653, 2022, PMC9463114, 10.1021/acs.jpcb.2c04245
417. Shah, S.D.[*], Lind, C.[*], De Pascali, F., Penn, R.B., MacKerell, A.D., Jr.,* and Deshpande, D.A.,* "In silico identification of a β_2-adrenoceptor allosteric site that selectively augments canonical β_2AR-Gs signaling and function," **Proceedings of the National Academies of Sciences, USA**, 119: e2214024119, 2022, PMC9894167, 10.1073/pnas.2214024119
418. Ruda, A., Aytenfisu, A.H., d'Ortoli, T.A., MacKerell, A.D., Jr.* and Widmalm, G.,* "Glycosidic α-linked mannopyranose disaccharides: An NMR spectroscopy and molecular dynamics simulation study employing additive and Drude polarizable force fields," **Physical Chemistry Chemical Physics**, 25: 3042-3060, 2023, PMC9890503, 10.1039/D2CP05203B
419. Karade, S., Franco, E., Rojas, A., Hanrahan, K., Kolesnikov, A., Yu, W., MacKerell, A.D., Jr., Hill, D., Weber, D., Brown, S., Treston, A., and Mariuzza, R., "Structure-Based Design of Potent Iminosugar Inhibitors of Endoplasmic Reticulum α-Glucosidase I with Anti-SARS-CoV-2 Activity," **Journal of Medicinal Chemistry**, 66:2744-2760, 2023, PMC10278443, 10.1021/acs.jmedchem.2c01750
420. Yu, Y., Venable, R.M., Thirman, J., Chatterjee, P., Kumar, A., Pastor, R.W.,* Roux, R.,* MacKerell, A.D., Jr.,* and Klauda, J.*, "Drude Polarizable Lipid Force Field with Explicit Treatment of Long-Range Dispersion: Parametrization and Validation for Saturated and Mono-unsaturated Zwitterionic Lipids," **Journal of Chemical Theory and Computation**, 19: 2590-2605, 2023, PMC10404126, 10.1021/acs.jctc.3c00203
421. Orr, A., Tao, A., Guvench, O., and MacKerell, A.D., Jr., "Site-Identification by Ligand Competitive Saturation (SILCS)-Biologics Approach for Structure-Based Protein Charge Prediction," **Molecular Pharmaceutics**, 20: 2600-2611, 2023, PMC10159941, 10.1021/acs.molpharmaceut.3c00064.
422. Zhao, M., Kognole, A.A., Jo, S., Tao, A., Hazel, A., and MacKerell, A.D., Jr., "GPU-Specific Algorithms for Improved Solute Sampling in Grand Canonical Monte Carlo

Simulations," **Journal of Computational Chemistry**, 44: 1719-1732, 2023, PMC10330275, 10.1002/jcc.27121

423. Yu, W., Weber, D.J., and MacKerell, A.D., Jr. "An Integrated Covalent Drug Design Workflow using Site-Identification by Ligand Competitive Saturation," **ChemRxiv**, 2023, 10.26434/chemrxiv-2023-sc37c, **Journal of Chemical Theory and Computation**, 19: 3007-3021 article, 2023, PMC10205696, 10.1021/acs.jctc.3c00232
424. Sengul, M.Y. and MacKerell, A.D., Jr. "Influence of Mg^{2+} Distribution on the Stability of Folded States of the Twister Ribozyme Revealed using Grand Canonical Monte Carlo and Generative Deep Learning Enhanced Sampling," **ChemRxiv**, 2023 10.26434/chemrxiv-2023-wkfrk, **ACS Omega,** 8: 19532-19546, 2023, PMC10249389, 10.1021/acsomega.3c00931
425. Bowen, H., Kenedy, M., Johnson, D., MacKerell Jr., A.D., and Akins, D. "Identification of a novel transport system in Borrelia burgdorferi that links the inner and outer membranes," **Pathogens and Disease**, 81: ftad014, 2023, PMC10353723, 10.1093/femspd/ftad014.
426. Devereaux, A.L., Olson, K.M., Chatterjee, P., Saldaña-Shumaker, S.L., Schaefer, A., Plotkin, A., Kandasamy, R., MacKerell Jr., A.D. Traynor, J.R., and Cunningham, C.W., "Nitro-Benzylideneoxymorphone, a Bifunctional Mu and Delta Opioid Receptor Ligand with High Mu Opioid Receptor Efficacy," **Frontiers in Pharmacology**, 14, 2023, PMC10352325, 10.3389/fphar.2023.1230053
427. Pandey, P. and MacKerell, A.D., Jr. "Combining SILCS and Artificial Intelligence for High-Throughput Prediction of Drug Molecule Passive Permeability," **ChemRxiv**, 2023, 10.26434/chemrxiv-2023-rjv6c, **Journal of Chemical Information and Modeling**, 63, 18, 5903–5915, 2023, PMC10352325, 10.1021/acs.jcim.3c00514
428. Ahmad, Faisal, A., Parvaiz, N., MacKerell, A.D., Jr., and Syed, S. "Non-Beta Lactam Ring Inhibitors of the Metallo Beta-Lactamase blaCTX-M15 Protein in Drug Resistant Salmonella typhi are of Potential Utility in Antibacterial Combination Therapy," **Journal of Chemical Information and Modeling**, 63: 6681-6695, 2023, PMC10698858, 10.1021/acs.jcim.3c00780
429. Lázaro-Gorines, R., Pérez, P., Heras-Murillo, I., Adán-Barrientos, I., Albericio, G., Astorgano, D., Flores, S., Luczkowiak, Labiod, N., Harwood, S.L., Segura-Tudela, A., Rubio-Pérez, L, Nugraha, Y., Shang, X., Li, Y., Alfonso, C., Adipietro, K.A., Abeyawardhane, D.L, Navarro,R., Compte, M., Yu, W., MacKerell, A.D., Jr., Sanz, L., Weber, D.J., Blanco, F.J., Esteban, M., Pozharski, E., Godoy-Ruiz, R., Muñoz, I.G., Delgado, R., Sancho, D., García-Arriaza, J., and Álvarez-Vallina, L., "Dendritic Cell-mediated Cross-Priming by a Bispecific Neutralizing Antibody Boosts Cytotoxic T Cell Responses and Protects Mice against SARS-CoV-2," **Advanced Science**, Oct 20:e202304818, 2023,PMC10700188, 10.1002/advs.202304818
430. Brooks, C.L., III, MacKerell, A.D., Jr., Post, C.B., and Nilsson, L., "Biomolecular Dynamics in the 21st Century," **Biochimica et Biophysica Acta (BBA) – General Subjects**, 1868:130534, 2024, 10.1016/j.bbagen.2023.130534

Submitted

Journal: Journal of Chemical Theory and Computation
Manuscript ID: ct-2023-01380c

Title: "Balancing Group I Monoatomic Ion-Polar Compound Interactions for Condensed Phase Simulation in the Polarizable Drude Force Field"
Authors: Nan, Yiling; MacKerell, Alexander
Manuscript Status: Submitted

Title: In Silico Evaluation of Phytoconstituents from Murraya panic-ulata for Potential Inhibitors to Target Aldose Reductase (AKR1B1) with Cytotoxicity and Antioxidant Activity
Authors: Afifa Parvin Shanta *, Fatema- Tuz- Zohora *, Tasnuva Sharmin *, Rumana Mahtarin, Monira Ahsan *, Alexander D. MacKerell

Patents

1) "Immunomodulatory Compounds." Hayashi, J., MacKerell, A.D., Jr. U.S. Patent Number 7,521,463, April 2009.
2) "Methods and Compositions of Trail-Death Receptor Agonists/Activators" Srivastava, R., Shankar, S., MacKerell, A.D., Jr. U.S. Patent Number 7,915,245, March 2011.
3) "Inhibitors of the S100-p53 Protein-Protein Interaction and Method of Inhibiting Cancer Employing the Same," Weber, D.J., Markowitz, J., Carrier, F. and MacKerell Jr., A.D., US. Patent Number 8,053,477, November 2011
4) "Small Molecule Inhibitors of BCL6" Melnick, A.M, MacKerell, A.D., Jr. and Privé, G.G. US Patent Number 8,338,464, December 2012
5) "Compounds that Inhibit Human DNA Ligases and Methods of Treating Cancer" Tomkinson, A.E., Chen, X., MacKerell, A.D., Jr., Dziegeilewska, B., Zhong, S., Wilson, G., US Patent Number 8,445,537, May 2013.
6) "Heme Oxygenase Inhibitors, Screening Methods for Heme Oxygenase Inhibitors and Methods of Use of Heme Oxygenase Inhibitors for Antimicrobial Therapy," Wilks, A., Furci, L., MacKerell, A.D., Jr. and Lopes, P.E.M., Canadian Patent 2,658,877, February 2013, U.S. Patent Number 8,450,368, May 2013.
7) "Small Molecule Inhibitors of LCK SH2 Domain Binding" MacKerell, A.D., Jr., Hayashi, J., Mia, Y., and Xia, G, U.S. Patent Number 8,476,273, July 2013, Japanese Patent Number 5558353
8) "SHP-2 phosphatase inhibitors," Qu, C.-K., Yu, W.-M., Guvench, O., MacKerell, Jr., A.D., U.S. Patent Number 8,673,913, March 2014
9) "Targeting NAD Biosynthesis in Bacterial Pathogens" MacKerell Jr., A.D., Zhang, H., and Osterman, A. U.S. Patent Number 8,785,499, July 2014
10) "Defensin-Like Molecules as Novel Antimicrobial Agents," De Leeuw, E and MacKerell Jr., A.D., U.S. Patent Number 8,796,323, August 2014.
11) "Compounds that Inhibit Human DNA Ligases and Methods of Treating Cancer," Tomkinson, A.E., Dziegielewska, B., Wilson, G., MacKerell, A., Chen, H.X., and Zhong, S., U.S. Patent Number 9,073,896, March 2015
12) "Non-ATP Dependent Inhibitors of Extraceullular Signal-Regulated Kinase (ERK)," Shapiro, S., MacKerell, A.D., Jr. and Fletcher, S., U.S. Patent Number 9,115,122, August 2015

13) “Mixed mu agonist/delta antagonist opioid analgesics with reduced tolerance liabilities and uses thereof,” Coop, A., MacKerell, A.D., Jr. and Matsumoto, R., U.S. Patent Number 9,422,302, August 2016, European Patent Number 2964228, May 2019
14) “Defensin-Like Molecules as Novel Antimicrobial Agents,” De Leeuw, E and MacKerell Jr., A.D., U.S. Patent Number 9,351,963, November 2016.
15) “LRRK2 GTP Binding Inhibitors for Treatment of Parkinson's Disease and Neuroinflammatory Disorders” W. Smith, F. Xue and A.D. MacKerell, Jr., U.S. Patent Number 9,701,627, July 2017.
16) “Compounds that Inhibit Human DNA Ligases and Methods of Treating Cancer,” Tomkinson, A.E., Chen, H.X., Dziegielewska, B., MacKerell, A.D., Jr., Zhong, S. and Wilson, G.M., U.S. Patent Number 9,757,375, September 2017
17) “BCL6 Inhibitors an Anticancer Agents” Melnick, A., Cerchietti, L.C.A., Cardenas, M.G., Xue, F., MacKerell, A.D., Jr., US Patent Number 9,943,506, April 2018
18) “Method for binding site identification by molecular dynamics simulation (SILCS: Site Identification by Ligand Competitive Saturation)” MacKerell, A.D., Jr. and Guvench, O., US Patent Number 10,002,228, June 2018.
19) “RUNX2 Transcription Factor Inhibitors and Uses Thereof ” Passaniti, A. and MacKerell, A.D., Jr. US Patent Number 10,329,246, June 2019.
20) “Inhibitors of the Notch Transcriptional Activation Complex and Methods of Use of the Same, “ Capobianco, A.J., MacKerell, A.D., Jr. and Spyvee, M., U.S. Patent Number 10,501,413, December 2019
21) “Small molecule lipid II inhibitors,” de Leeuw, E., MacKerell, A., Fletcher, S., Jamal, C., U.S. Patent Number 10,941,114, March 2021, European Patent Number EP3393473, June 2022.21)
22) “Small molecule lipid II inhibitors,” de Leeuw, E., MacKerell, A., Fletcher, S., Jamal, C., U.S. Patent Number 10,961,214, March 2021.
23) “Non-ATP/Catalytic Site p38 Mitogen Activated Protein Kinase Inhibitors,” Shapiro, P.S., MacKerell, A.D., Jr., Hasday, J.D., Fletcher, S., Patent Number 11,078,171, August 2021, Japanese Patent No. 7013453, March 2022
24) “Protein Translation Inhibitors of Uses Thereof,” Carrier, F., MacKerell, A.D., Jr., Weber, D.J., Yu, W., U.S. Patent Number 11,510,908, November 2022,
25) “Non-Catalytic Substrate-Selective P38(alpha)-Specific MAPK Inhibitors with Endothelial-Stabilizing and Anti-Inflammatory Activity, and Methods of Use Thereof” Shapiro, P.S., Hasday, J.D., MacKerell, A.D., Jr., US Patent No. 11,357,781, June 2022, Australian Patent number 2019392904, Chinese Patent Number ZL 2017800519068, June 2023, European Patent Number EP 3474835, July 2023, Japanese Patent No. 7372993, November 2023
26) “RUNX2 Transcription Factor Inhibitors and Uses Thereof ,” Passaniti, A., MacKerell, A.D., Jr., U.S. Patent Number 11,634,381, April 2023
27) “Non-ATP/Catalytic Site p38 Mitogen Activated Protein Kinase Inhibitors,” Shapiro, P.S., MacKerell, A.D., Jr., Hasday, J.D., Fletcher, S., U.S. Patent Number 11,718,595, August, 2023, Indian Patent No. 449739, September 2023

Book Chapters

1. Pietruszko, R., Ferencz-Biro, K. and MacKerell, A.D., Jr., 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, A.D., Jr. 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., AlanR. Liss Inc., New York, pp. 67-74, 1985.
3. MacKerell, A.D., Jr., 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, A.D., Jr. , 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, A.D., Jr. 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. , 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, A.D., Jr., 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, A.D., Jr., 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, A.D., Jr., 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, A.D., Jr., 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, pp. 45-69, 2007.

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. 2008 (Methods Mol Biol. 2008;443:63-88. PMID: 18446282)
16. Klauda, J.B., Venable, R.M., MacKerell, A.D., Jr. and Pastor, R.W. "Considerations for Lipid Force Field Development," In **Computational Modeling of Membrane Bilayers**, S. Feller, Editor, Elsevier, Inc. Chapter 1, pp 1-48, 2008.
17. Priyakumar, U.D. and MacKerell, A.D., Jr., "Molecular Modeling of Base Flipping in DNA, " **In DNA and RNA modification Enzymes : Comparative Structure, Mechanism, Functions, Cellular Interactions and Evolution**, Henri Grosjean, Editor, LANDES Biosciences Intelligence Unit, 2009
18. Lopes, P.E.M, Harder, E., Roux, B., and MacKerell, A.D., Jr. "Formalisms for the explicit inclusion of electronic polarizability in molecular modeling and dynamics studies," in "**Multi-scale Quantum Models for Biocatalysis: Modern Techniques and Applications**" Volume editors Darrin York and Tai-Sung Lee; in the series, Challenges and Advances in Computational Chemistry and Physics, Vol. 7, Editor J. Leszczynski, p 219-218, 2009, ISBN: 978-1-4020-9955-7
19. Baker, C.M., Darian, E. and MacKerell, A.D., Jr. "Towards Biomolecular Simulations with Explicit Inclusion of Polarizability: Development of a CHARMM Polarizable Force Field based on the Classical Drude Oscillator Model," **Innovations in Biomolecular Modeling and Simulations**, 2012, **1**, 23-50 , **DOI:**10.1039/9781849735049-00023
20. Zhong, S., Oashi, T., Yu, W., Shapiro, P., and MacKerell, A.D., Jr. "Prospects of modulating protein-protein interactions," In **Protein-Ligand Interactions**, H. Gohlke ED., Methods and Principles in Medicinal Chemistry, Wiley-VCH Verlag Gmbh & Co. KGaA, Weinheim, Germany, p 295-329, 2012, ISBN: 978-3-527-32966-3
21. Hartman, K.G., Wilder, W.T., Varney, K., MacKerell, A.D., Jr., Coop, A., Njar, V., Zimmer, D., Lapidus, R., and Weber, D.J, "Inhibiting S100B in Malignant Melanoma," in **Melanoma – From Early Detection to Treatment**, G. Huynh and T. Duc, editors, INTECH Open Science, Chapter 24, 2013, DOI: 10.5772/55176
22. Yu, W., Guvench, O., and MacKerell, A.D., Jr., "Computational approaches for the design of PPI inhibitors," in **Understanding and exploiting protein—protein interactions as drug targets**, e-book, Future Science Limited, page 90-102, 2013, doi: 10.4155/9781909453463
23. Jo, S., Wu, E.L., Stuhlsatz, D., Klauda, J.B., MacKerell, A.D., Jr., Widmalm, G. and , Im, W., "Lipopolysaccharide Membrane Building and Simulation," in **Glycoinformatics**, Chapter 24, Humana Press, New York, NY, Methods in Molecular Biology, 1273: 391-406, 2015, 10.1007/978-1-4939-2343-4_25.
24. Mallajosyula, S.S., Jo, S., Im, W. and MacKerell, A.D., Jr., "Molecular Dynamics Simulations of Glycoproteins using CHARMM," in **Glycoinformatics**, Chapter 25, Humana Press, New York, NY, Methods in Molecular Biology, 1273: 407-429, 2015, 10.1007/978-1-4939-2343-4_25
25. Lopes, P.E.M., Guvench, O., and MacKerell, A.D., Jr., "Current Status of Protein Force Fields for Molecular Dynamics," In **Molecular Modeling of Proteins**, 2nd edition, A. Kukol, Editor, Humana Press. Chapter 3, pp. 47 -72, 2014; 10.1007/978-1-4939-1465-4_3 (Methods in Molecular Biology, 1215: 47-72, 2014, PMC4554537)

26. Jo, S., Cheng, X., Islam, S.M., Huang, L., Rui, H., Zhu, A., Lee, H.S., Qi, Y., Han, W., Vanommeslaeghe, K., MacKerell, A.D., Jr., Roux, B., and Im, W. "CHARMM-GUI PDB Manipulator for Advanced Modeling and Simulations of Proteins Containing Nonstandard Residues," in **Advances in Protein Chemistry and Structural Biology: Biomolecular Modelling and Simulations**, T. Karabencheva-Christova, Editor, Elsevier, New York, Chapter 8, 235-266, 2014, 10.1016/bs.apcsb.2014.06.002
27. Faller, C.E., Prabhu Raman, E.P., MacKerell, A.D., Jr. and Guvench, O. "Site Identification by Ligand Competitive Saturation (SILCS) Simulations for Fragment-Based Drug Design," in **Fragment-Based Methods in Drug Discovery**, Chapter 7, Anthony E. Klon (ed.), Methods in Molecular Biology, 1289: 75-87, Springer Science+Business Media, New York, 2015, PMC4685950, 10.1007/978-1-4939-2486-8_7
28. Savelyev, A., Roux, B., and MacKerell, A.D., Jr., "Explicit Inclusion of Induced Polarization in Atomistic Force Fields Based on the Classical Drude Oscillator Model," in **Many-Body Effects and Electrostatics in Biomolecules**, Q. Cui and M. Meuwley, Editors, Pan Stanford Publishing, 191-232, 2016, 10.1201/b21343-9
29. Small, M.C., and MacKerell, A.D., Jr., "Force field representation of biomolecular systems," in **in Silico Drug Discovery and Design: Theory, Methods, Challenges and Applications**, Chapter 2, 45-77, CRC Press: Taylor & Francis Group, ISBN (978-1-4822-1783-4), 10.1201/b18799-4
30. Yu, W. and MacKerell, A.D., Jr., "Computer-Aided Drug Design Methods," in Antibiotics, Springer, New York, 2017, **Methods in Molecular Biology**, 1520:85-106, 2017, PMC5248982, 10.1007/978-1-4939-6634-9_5
31. Lin, F.-Y., and MacKerell, A.D., Jr., "Force fields for small molecules," in **Biomolecular Simulations**, Editors: M. Bonomi and C. Camilloni, Springer; Methods in Molecular Biology, 2022: 21-54, 2019, 10.1007/978-1-4939-9608-7_2, PMC6733265
32. Yu W., Weber D.J., Shapiro P., and MacKerell A.D., Jr., (2020) "Developing Kinase Inhibitors Using Computer-Aided Drug Design Approaches." In **Next Generation Kinase Inhibitors**, Shapiro P. Editor, Springer, Ebook, 2020: 81-108, https://doi.org/10.1007/978-3-030-48283-1_5
33. Yu W., Weber D.J., and MacKerell A.D., Jr., (2023) "Computer-Aided Drug Design" An Update," In Antibiotics, Peter Sass, Editor, Chapter 7, p. 123-152, 978-1-0716-2854-6, 514362_2_En, **Methods in Molecular Biology**, 2601: 153-167, PMC9838881, 10.1007/978-1-0716-2855-3
34. Orr, A.A. and MacKerell A.D., Jr., (2024) "Site-Identification by Ligand Competitive Saturation as a Paradigm of co-solvent MD methods," In: **Computational Drug Discovery: Methods and Applications** (ed. Poongavanam, V. and Ramaswamy, V.), Chapter 5, WILEY-VCH. ISBN: 978-3-527-35166-4

Publications in Non-Referred Journals

1. Coop, A., MacKerell, A.D., Jr. and Fletcher, S. "Polypharmacology in Drug Design," **American Association of Pharmaceutical Sciences Newsmagazine**, July, 2015, pp. 14 -18.

Book Editor

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

Compounds in Clinical Trials:

S100b inhibitor

https://ichgcp.net/clinical-trials-registry/NCT00729807

p38 kinase inhibitor

https://clinicaltrials.gov/ct2/show/NCT05795465?term=gen1e&draw=2&rank=2

Invited Lectures

1. "Dynamics of ribonuclease T1 and horse liver alcohol dehydrogenase: Combining experimental and theoretical information," European Society for Photobiology Meeting, Padova, Italy, 1987
2. "Structural and dynamics differences in the free and 2'GMP enzyme forms of ribonuclease T1,"First International Meeting on the Structure and Chemistry of Ribonucleases, Moscow, USSR, 1988
3. "Motivation and Validation for the use of Empirical Force Fields for Computational Studies of Biological Systems," First World Congress on Medicine, Public Health and Biotechnology. Austin, Texas, 1994.
4. "Validation of the use of Empirical Force Fields for Computational Studies of Biological Systems" Department of Microbiology and Immunology, School of Medicine, University of Maryland at Baltimore, Baltimore, MD, 1994.
5. "Validation of the Use of Empirical Force Fields for Computational Studies of Biological Systems" 8th Middle Atlantic Regional Meeting of the Americal Chemical Society Univeristy of Maryland Baltimore County, Catonsville, MD, 1994.
6. "Empirical Force Field Development and Validation for Computational Studies of Biological Membranes,"208th American Chemical Society National Meeting, Washington D.C., 1994
7. "Molecular Dynamics Simulation Studies of Nucleic Acids," Research Seminar, University of Maryland Cancer Center, Department of Developmental Therapeutics, School of Medicine, University of Maryland,Baltimore, Baltimore, MD, 1995
8. "Molecular Dynamics Simulation Studies of Nucleic Acids," Molecular and Cell Biology Graduate Program Seminar Series, University of Maryland at Baltimore, Baltimore, MD, 1995
9. "Molecular Dynamics Simulation Studies of Nucleic Acids," Department of Chemistry and Biochemistry Seminar Series University of Maryland Baltimore County, Catonsville, MD, 1995
10. "Methodological Developments in the Optimization of Lennard-Jones Parameters for Empirical Force Field Calculations," Biophysic Laboratory, Center for Biologics Evaluation & Research, Food and Drug Administration and Laboratory of Structural Biology, Division of Computer Research & Technology, NIH, Bethesda, MD, 1995

11. “Empirical Force Field Parameterization and Simulations of Nucleic Acids,” Laboratory of Medicinal Chemistry, National Cancer Institute, NIH, Bethesda, MD, 1995
12. “Molecular Dynamics Simulation Studies of the EcoRI restriction site dodecamer,” Department of Chemistry, University of Houston, Houston, Texas, 1995
13. "An all-atom empirical energy function for the simulation of nucleic acids, " 210th American Chemical Society National Meeting, Chicago, Il,1995.
14. "MD simulations of the EcoRI recognition sequence in solution: Influence of counterions on stability," 210th American Chemical Society National Meeting, Chicago, Il.,1995.
15. "Combined ab initio/empirical approach for the optimization of Lennard-Jones parameters.” 210th American Chemical Society National Meeting, Chicago, Il,1995.
16. “Computational Approaches to the Study of Biological Systems” Department of Chemistry, Towson State University, Towson, MD, 1995
17. “Empirical Force Field Calculations of Nucleic Acids: Parametrization and Application” Center for Structural Biology Department of Bioscience at Novum, Karolinska Institutet, Huddinge, Sweden, 1996.
18. “Empirical Force Field Calculations of Nucleic Acids: Parametrization and Application” Section de Biphysique des Protéines et de Membranes, Commissariat a l’Energie Atomique, CEA-Saclay, Saclay, France, 1996.
19. “Empirical Force Field Calculations of Nucleic Acids: Parametrization and Application” Laboratoire de Chimie Biophysique, Institut le Bel, Universite Louis Pasteur, Strasbourg, France, 1996.
20. “Validation of Empirical Force Fields Based on Crystal Calculations” 212th American Chemical Society National Meeting, Orlando, FL, 1996.
21. “Use of Ab Initio Calculations to Aid in the Interpretation of the Influcence of Surface Adsorption on the Vibrational Spectra of Alkoxides” 212th American Chemical Society National Meeting, Orlando, FL. 1996.
22. “Lennard-Jones Parameters of Alkanes and Alkenes Based on a Combined Ab Initio-Empirical Optimization Procedure” 212th American Chemical Society National Meeting, Orlando, FL, 1996.
23. “Relationship of Small Molecule Based Parameter Optimization to Condensed Phase Calculations on Proteins and Nucleic Acids” Center Européen de Calcul Atomique et Moléculaire, Workshop: Potential functions for simulation of biomolecules, Lyon, France, 1996.
24. “MD based Potential of Mean Force Calculations on DNA under Tensile Force.” Chemistry Division, Naval Research Laboratory, Washington, DC. 1997
25. “MD based Potential of Mean Force Calculations on DNA under Tensile Force.” Center for Molecular Modeling, Department of Chemistry, University of Pennsylvania, Philadelphia, PA, 1997
26. “Potential of Mean Force Calculations on DNA under Tensile Force.” Center for Advanced Research in Biotechnology, University of Maryland, Rockville, MD, 1997
27. “Structure, Force and Energy of a Double-Stranded DNA Oligonucleotides Under Tensile Loads,” Swiss Federal Institute of Technology, Lausanne, Switzerland, 1997.
28. “Structure, Force and Energy of a Double-Stranded DNA Oligonucleotides Under Tensile Loads” Center Européen de Calcul Atomique et Moléculaire, Workshop: Nucleic Acids, Lyon, France, 1997.

29. “Structure, Force and Energy of a Double-Stranded DNA Oligonucleotides Under Tensile Loads,” Department of Physiology, School of Medicine, Johns Hopkins University, Baltimore, MD, 1997.
30. “Importance of microscopic contributions to condensed phase macroscopic properties in empirical force field calculations,” Computational Chemistry Gordon Conference, Tilton, NH, 1998
31. “Developments in the CHARMM All-Atom Empirical Energy Function for Biological Molecules” 216th American Chemical Society National Meeting, Boston, MA, 1998
32. “Importance of microscopic contributions to condensed phase macroscopic properties in empirical force field calculations” Making and Breaking Potentials, UK Cooperative Computational Project #5 Annual Meeting, Edinburgh, Scotland, 1998
33. “Importance of microscopic contributions to condensed phase macroscopic properties in empirical force field calculations: Application to Nucleic Acids” Department of Chemistry, Georgetown Medical School, Georgetown University, Georgetown, VA, 1998
34. “Mechanical and Environmental Contributions to Opening of Duplex DNA in the TATA Box and Related Oligomers Investigated via Potential of Mean Force Calculations.” Molecular Modeling Interest Group, National Institutes of Health, Bethesda, MD, 1999.
35. “CHARMM empirical force field for biological molecules: Overview of optimization procedures with emphasis on lipid bilayers.” Center Européen de Calcul Atomique et Moléculaire, Workshop: Molecular Dynamics Simulations of Lipid Membranes and Membrane Associated Proteins, Lyon, France, 1999.
36. “Optimization of the CHARMM all-atom nucleic acid force field and investigation of the energetics of DNA deformation.” Department of Biochemistry, University of Zürich, Zürich, Switzerland, 1999.
37. “Optimization of the CHARMM all-atom nucleic acid force field.” Laboratoire de Chimie Biophysique, Institut le Bel, Universite Louis Pasteur, Strasbourg, France, 1999.
38. “HIV Integrase: Identification of Novel Inhibitors and Analysis of Enzyme-Inhibitor Interactions via Ligand Docking.” School of Pharmacy, West Virginia University, Morgantown, WV, 2000.
39. “Balancing Microscopic Contributions with Macroscopic Observables in Empirical Force Fields: Application to Nucleic Acids.” National Institute of Occupational Safety and Health, Morgantown, WV, 2000.
40. “Balancing Microscopic Contributions with Macroscopic Observables in Empirical Force Fields. Application to Nucleic Acids” Department of Chemistry, University of York, York, UK, 2000
41. “Advances in the CHARMM all-atom force field for biological molecules” Canadian Computational Chemistry Conference 4, Bishop University, Quebec, Canada, 2000.
42. “Advances in the CHARMM all-atom force field for biological molecules” 220th American Chemical Society National Meeting, Washington, DC, 2000.
43. “Use of Oligodeoxyribonucleotides with Conformationally Constrained Abasic Sugar Targets to Probe the Mechanism of Base Flipping by *HhaI* DNA (Cytosine C5)-Methyltransferase” Department of Chemistry and Biochemistry, University of Maryland, College Park, MD, 2000
44. “Overview of the CHARMM all-atom force field for biological molecules” 4th Biannual Structural Biology Symposium, Institute of Molecular Biophysics, Florida State University, Tallahassee, FL, 2001

45. “Recent Advances in Biomolecular Molecular Dynamics Simulations: DNA Conformational Transitions and the Impact of Protein Binding” School of Chemical Engineering, Purdue University, West Lafayette, IN, 2001.
46. “Computational Studies of Base Flipping In DNA and Impact of Binding with the (Cytosine-5) Methyltransferase from *Hha*I” Department of Chemistry and Biochemisty, Duquesne University, Pittsburgh, PA, 2001
47. “Base Flipping in DNA and the Impact of Binding to (Cytosine-5) Methyltransferase from *Hha*I” Department of Chemistry, Kansas University, Lawrence, KS, 2001
48. “*Ab initio* Quantum Mechanical Analysis of Nucleic Acid Components” DIMACS Workshop on DNA Sequence and Topology, DIMACS Center, Rutgers University, Piscataway, NJ, 2001.
49. ”Computational Studies of Base Flipping In DNA” Laboratory of Medicinal Chemistry, National Cancer Institute, National Institutes of Health, Frederick, MD, 2001.
50. “Energetic and Structural Details of Base Flipping from Duplex DNA” Horizons in Biophysics 2001, Royal Swedish Academy of Sciences, Nobel Institute of Chemistry, Stockholm, Sweden, 2001.
51. “Energetic and Structural Details of Base Flipping from Duplex DNA” Department of Chemistry and Biochemistry, University of Maryland, College Park, MD, 2001.
52. “Drude Oscillator as a Model for Electronic Polarization in Empirical Force Fields: Application to Dimethylphosphate” Workshop on Polarizability for Biomolecular Simulation, Snowbird, Utah, 2001.
53. “CHARMM Force Fields: Approaches, Recent Developments and the Misery….” Department of Chemistry and Biochemistry, University of California, San Diego, CA, 2002.
54. “ Recent developments in the CHARMM all-atom force field for nucleic acids” 223rd American Chemical Society National Meeting, Orlando, Fl., 2002
55. CHARMM Force Fields: Approaches, Recent Developments and the Misery….” Accelyrs Corporation, San Diego, CA, 2002.
56. “Base Flipping in DNA: Facilitation by the Enzyme Cytosine-5-Methyltransferase” Department of Molecular Biology, The Scripps Research Institute, La Jolla, CA, 2002.
57. “Improved representation of protein backbone conformational energetics and condensed phase simulations of dimethylphosphate using the Shell Model to treat electronic polarizability,” CHARMM Meeting, Department of Chemistry, Harvard University, Cambridge MA, 2002.
58. “Computational Studies of Base Flipping Alone and Complexed to the Cytosine-5-Methyltransferase from *Hha*I” Diffraction Methods In Structural Biology, Gordon Research Conference, New London, CT, 2002
59. “CHARMM biomolecular force field: Recent developments and future directions,” American Chemical Society National Meeting, Boston, MA, 2002
60. “Empirical Force Fields: Overview, parameter optimization & applications,” Department of Physics, University of Cyprus, Nicosia, Cyprus, 2003
61. “Force Fields” Short Course on Force Fields and Molecular Dynamics,” Quantum Theory Project 43rd Sanibel Symposium, University of Florida, St. Augustine, Fl, 2003
62. “Computational Studies of Base Flipping in DNA Alone and Bound to the Cytosine-5-methyltransferase from *Hha*I,” DNA and beyond: Structure, Dynamics and Interactions, École Polytechnique Fédérale de Lausanne, Laussane, Switzerland, 2003.

63. “Computational Studies of Base Flipping in DNA Alone and Bound to the Cytosine-5-methyltransferase from *Hha*I,” Laboratory of Biophysical Chemistry Seminar Series, National Heart, Lung and Blood Institute, NIH, Bethesda, MD, 2003.
64. “Computer-Aided Drug Design: Ligand- and Target-Based Applications,” Chemistry Group, National Institute of Drug Abuse, NIH, Baltimore, MD, 2003.
65. “CHARMM biomolecular force field: Recent developments and future directions,” Annual CHARMM Developers Meeting, The Scripps Reseach Institute, LaJolla, CA, 2003.
66. “Improved Treatment of the Protein Backbone Conformation in the CHARMM All-atom Force Field,” Computing for Biology, IBM-BNL Blue-Gene Science Workshop, Stony Brook, NY, 2003.
67. “CHARMM all-atom empirical force field for biomolecules: Recent enhancements and progress towards inclusion of electronic polarizability” Theoretical and Computational Biophysics Seminar, Beckman Institute, University of Illinois, Urbana-Champaign, IL, 2003
68. “Computational Studies of Base Flipping in DNA Alone and Bound to the Cytosine-5-methyltransferase from *Hha*I,” Department of Chemistry Seminar Series, Pennsylvania State University, State College, PA, 2003
69. “Computational methods used in drug discovery” Department of Medical and Research Technology, University of Maryland School of Medicine, Continuing Education Credits, Baltimore, MD, 2003
70. “Base Flipping in DNA: Accessing Millisecond Events via MD-based Potential of Mean Force Calculations,” 48th Annual Meeting of the Biophysical Society, Baltmore, MD, USA, February 2004
71. “Computational Studies of Base Flipping in DNA Alone and Bound to the Cytosine-5-methyltransferase from HhaI,” 2004 President's Meeting, International Society of Quantum Biology and Pharmacology, Como, Italy, June 2004.
72. “Parameters, parameters, parameters,” Annual CHARMM Developers Meeting, Harvard University, Cambridge, MA, July 2004
73. “Enhancements and Extensions of the CHARMM Biological Empirical Force Fields” Frontiers in Computational Biophysics and Drug Design, Army Research Laboratories Workshop, Beltsville, MD, October 2004
74. “Enhancements and Extensions of the CHARMM Biological Empirical Force Fields” Keck Computational and Theoretical Biology Symposium, Rice University, Houston, TX, December, 2004
75. “Computational Studies of Base Flipping in DNA Alone and Bound to the Cytosine-5-methyltransferase from *Hha*I” World Association of Theoretically Oriented Chemists, 2005 International Meeting, Cape Town, South Africa, January, 2005
76. “Computer-Aided Drug Design: Ligand- and Target-Based Approaches” Howard University, School of Pharmacy, Department of Pharmaceutical Sciences Seminar, March 2005
77. “Computational Studies of Base Flipping in DNA Alone and Bound to the Cytosine-5-methyltransferase from *Hha*I” Molecular Biophysics Seminar Series, Wesleyan University, Middletown, CT, April 2005.
78. “Progress in the CHARMM force fields; Extension to polarizable model based on the classical Drude oscillator,” Annual CHARMM meeting, Weill Medical College, Cornell University, New York, NY, July 2005
79. “Improvements in the CHARMM all-atom force fields for biomolecules” 230th National American Chemical Society Meeting, Washington, DC, August 2005

80. “MD simulation Studies of Base Flipping in DNA,” International Society of Quantum Biology and Pharmacology Gilda Lowe Memorial Meeting, Staten Island, New York, October 2005.
81. “Structure-function relationships of nucleic acids and protein-nucleic acid complexes studied via MD simulations” Bioinformatics Institute Visiting Scientist Lecture Series, Singapore, March 2006.
82. “Computer-aided drug design: Ligand-based approaches on δ-opioid ligands” Bioinformatics Institute Visiting Scientist Lecture Series, Singapore, March 2006.
83. “Computer-aided drug design: Target-based approaches with emphasis on protein-protein interactions” Bioinformatics Institute Visiting Scientist Lecture Series, Singapore, March 2006.
84. “Overview of the CHARMM all-atom force fields including the additive and classical Drude polarizable models,” Validating Modeling and Experimental Methods to Enable Drug Discovery, National Institute of Standards and Technology, Gaithersburg, MD., April, 2006.
85. “Overview of the CHARMM all-atom force fields including the additive and classical Drude polarizable models” Center for Bioinformatics, University of Kansas, Lawrence, Kansas, April, 2006.
86. “MD simulation studies of base flipping in DNA alone and in the presence of the (cytosine-C5)-methyltransferase from HhaI” Department of Chemistry, University of Kansas , Lawrence, Kansas, April, 2006.
87. “CHARMM force fields: 2006” Annual CHARMM Developers Meeting, Harvard University, Cambridge, MA, July 2006.
88. “MD simulation studies of base flipping in DNA alone and in the presence of the (cytosine-C5)-methyltransferase from HhaI” MMTSB Workshop, The Scripps Research Institute, LaJolla, California, August, 2006.
89. “Polarizable empirical force field based on the classical Drude oscillator model” Computational Chemistry Gordon Conference, Les Diablerets, Switzerland, October 2006.
90. “Computer-Aided Drug Design; Targeting the Tyrosine Kinase p56Lck SH2 Domain” Structure Biology Program, St. Jude Children’s Hospital, Memphis, Tennessee. October 2006.
91. “Ligand-based drug discovery using CHARMM; Conformationally sampled pharmacophore (CSP)” Accelyrs User Meeting and Conference 2006, Baltimore, Maryland, November 2006.
92. “Overview of CHARMM force fields and extension to drug-like molecules” Accelyrs User Meeting and Conference 2006, Baltimore, Maryland, November 2006.
93. “Polarizable empirical force field based on the classical Drude oscillator model” Florida State University Workshop 2007 on “Quantitative Computational Biophysics”, Florida State University, Tallahassee, Florida, February 2007.
94. “Computational studies of base flipping in DNA alone and bound to the cytosine-5-methyltransferase from HhaI” Department of Biochemistry and Molecular Biophysics, University of Chicago, Chicago, Illinois, USA, March 2007
95. “Optimization and validation of a polarizable force field based on the classical Drude oscillator” 233rd American Chemical Society National Meeting, Chicago, Illinois, USA, March 2007
96. “Ongoing developments in the CHARMM force fields for lipids” Semiannual Membrane Meeting, University of Utah, Park City, Utah, June 2007

97. “CHARMM force fields: 2007,” Annual CHARMM Developers Meeting, University of Maryland, School of Pharmacy, Baltimore, Maryland, USA, July 2007.
98. “Towards a Polarizable Force Field for Macromolecules: Optimization of a Force Field Based on the Classical Drude Oscillator,” Modeling Interactions in Biomolecules III, Prague, Czech Republic, September, 2007
99. “Computational studies of base flipping in DNA bound to the cytosine-5-methyltransferase from HhaI” FEBS Workshop on “DNA and RNA Modification Enzymes,” Centre Paul Langevin, Aussois, France, September 2007
100. “Advances in the CHARMM force fields for biological and pharmaceutical compounds” Accelrys Science Forum, Cambridge, MA, USA, October 2007.
101. “Development of a polarizable force field based on the classical Drude oscillator” 16th Conference on Current Trends in Computational Chemistry (CCTCC), Jackson State University, Jackson, MS, USA, November, 2007.
102. “Computational studies of base flipping in DNA alone and bound to the cytosine-5-methyltransferase from HhaI,” Institute for Structural Biology and Drug Discovery, Virginia Commonwealth University, Richmond, VA, USA, November, 2007.
103. “Development of a polarizable force field based on the classical Drude oscillator” American Physical Society March Meeting 2008, New Orleans, LA. March, 2008
104. “Computational studies of base flipping in DNA bound to the cytosine-5-methyltransferase from HhaI” Baltimore Area Repair Symposium (BARS), Baltimore, MD, March 2008
105. “Introduction and overview of CADD capabilities” Computer-Aided Drug Design Forum, School of Pharmacy, University of Maryland, Baltimore, MD, June 2008.
106. “The additive and Drude-based polarizable CHARMM force fields” Annual CHARMM Developers Meeting, Harvard University, Cambridge, MA, July 2008.
107. “Development of a Polarizable Empirical Force Field Based on the Classical Drude Oscillator” International Society of Theoretical Chemical Physics - VI, Vancouver, Canada, July 2008
108. “Inclusion of free energies of solvation during force field optimization” American Chemical Society 236th National Meeting, Philadelphia, PA, August 2008
109. “Optimization of a Polarizable Empirical Force Field Based on the Classical Drude Oscillator”American Chemical Society 236th National Meeting, Philadelphia, PA, August 2008
110. “Development of a Polarizable Force Field for Biological Molecules Based on the Classical Drude Oscillator.” Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, October 2008
111. “Optimization of a Polarizable Empirical Force Field Based on the Classical Drude Oscillator (and more....).” Department of Pharmaceutical Sciences, School of Pharmacy, University of California San Fransisco, San Fransisco, CA, February 2009.
112. “Optimization of a polarizable force field based on the classical Drude oscillator and application to biological macromolecules,” 237th American Chemical Society National Meeting, Salt Lake City, Utah, March 2009.
113. “Computational Studies of Base Flipping in DNA Alone and Bound to the Cytosine-5-methyltransferase from *Hha*I” Department of Biomedical and Pharmaceutical Sciences, College of Pharmacy, University of Rhode Island, Kingston, Rhode Island, April 2009.
114. “CHARMM force fields: 2009,” Annual CHARMM Developers Meeting, Karolinska Institutet, Stockholm Sweden, June 2009

115. “Optimizing ligand-protein interactions via SILCS: Site Identification by Ligand Competitive Saturation,” Biomolecular Simulations: Advanced Methods and Applications, Karolinska Institutet, Stockholm Sweden, June 2009
116. “CHARMM General Force Field (CGenFF) for pharmaceutical compounds; Development and use in drug design,” Accelyrs Users Group Meeting, Tokyo, Japan, July 2009
117. “Optimization of a polarizable force field based on the classical Drude oscillator and application to biological macromolecules,” Biomolecular Modeling and Simulations, Safed, Summer Workshop, Research workshop of the Israel Science Foundation, Safed, Israel, September, 2009
118. “Optimizing ligand-protein interactions via SILCS: Site Identification by Ligand Competitive Saturation,” Department of Chemistry, State University of New York, Stony Brook, October 2009
119 “Optimizing ligand-protein interactions via SILCS: Site Identification by Ligand Competitive Saturation,” Structural Biology and Chemistry Symposium, Dedicated to the memory of Dr. Nikos M. Oikonomakos, Institute of Organic and Pharmaceutical Chemistry, National Hellenic Research Foundation, Athens, Greece, October 2009
120. “Optimizing ligand-protein interactions via SILCS: Site Identification by Ligand Competitive Saturation,” Department of Chemistry and Biochemistry, Biophysics Program, Ohio State University, Columbus, Ohio, November 2009.
121. “Optimizing ligand-protein interactions via SILCS: Site Identification by Ligand Competitive Saturation,” Department of Chemistry and Biochemistry, University of Maryland, Baltimore County, Catonsville, Maryland, February, 2010
121. “Optimizing ligand-protein interactions via SILCS: Site Identification by Ligand Competitive Saturation,” 54th Annual Meeting of the Biophysical Society, San Fransisco, CA, February 2010.
122. “Optimizing ligand-protein interactions via SILCS: Site Identification by Ligand Competitive Saturation” Centre de recherché en modélisation moléculaire (CERMM) Seminar, Concordia University, Montreal, Canada, March 2010.
123. “Optimization of a polarizable force field based on the classical Drude oscillator and application to biological macromolecules,” Advances in the Implementation of Polarizable Force Fields for Molecular Simulations,” Center Européen de Calcul Atomique et Moléculaire, CECAM-HQ-EPFL, Lausanne, Switzerland, June 2010.
124. “Polarizable Empirical Force Field based on the Classical Drude Oscillator: Validation via Peptide Folding Simulations,” International Society for Quantum Biology and Pharmacology President’s Meeting, Cetraro, Italy, June 2010.
125. “Site Identification by Ligand Competitive Saturation (SILCS): Computational free energy-based approach for optimization of ligand-protein interactions,” Department of Physiology & Biophysics, School of Medicine, Case Western Reserve University, Cleveland, Ohio, November, 2010
126. “Site Identification by Ligand Competitive Saturation (SILCS): Computational free energy-based approach for optimization of ligand-protein interactions,” Bergen Centre for Computational Sciences, Faculty of Mathematics and Natural Sciences, University of Bergen, Bergen, Norway, November, 2010.
127. “Optimization of a polarizable force field based on the classical Drude oscillator and application to biological macromolecules,” Quantum Theory Project, University of Florida, Gainesville, Florida, December, 2010.

128. “An Overview of Force Fields & Molecular Mechanics Force Field Parameter Optimization,” Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Mahidol University, Bangkok, Thailand, January, 2011.
129. “Optimization of a polarizable force field based on the classical Drude oscillator,” Molecular Biophysics Unit, Indian Institute of Science, Bangalore, India, January, 2011.
130. “Progress towards a comprehensive polarizable macromolecular force field based on the CHARMM classical Drude oscillator model.” 241st American Chemical Society National Meeting, Anaheim, CA, March 2011.
131. “CHARMM all-atom additive force field for carbohydrates: Parameter optimization overview and utilization for simulations of heterogeneous systems.” 241st American Chemical Society National Meeting, Anaheim, CA, March 2011.
132. “CHARMM additive and polarizable force fields for biomolecules and medicinal compounds,” Bioleap Inc., Ewing, NJ, April 2011.
133. “Progress towards a comprehensive polarizable macromolecular force field based on the CHARMM classical Drude oscillator model,” Unité de Bioinformatique Structurale, Institut Pasteur, Paris, France, May 2011.
134. “Site Identification by Ligand Competitive Saturation (SILCS): Computational approach for optimization of inhibitors of protein-protein interactions including BCL6, ERK and S100B,” Institut Pasteur, Paris, France, May 2011.
135. “CHARMM additive and polarizable force fields for biomolecules and medicinal compounds,” Accelrys Inc. User Group Meeting, Jersey City, NJ, May 2011.
136. “Trials and tribulations of a being a principle investigator in a postdoctoral-fellow “dominated” laboratory,” Office of Career Development, University of Maryland, School of Medicine, Baltimore, MD, May 2011.
137. “A tale with no end: Ongoing developments in the CHARMM additive and Drude force fields,” Annual CHARMM developers Meeting, University of Wisconsin, Madison, WI, July 2011.
138. “Role of the 2'OH on RNA conformational heterogeneity; Relevance to nucleic acid force field optimization,” Center Européen de Calcul Atomique et Moléculaire, Workshop: Dynamics of Protein-Nucleic Acid Interactions: Integrating Simulations with Experiments, CECAM-ETHZ, Zurich, Switzerland, September 2011.
139. “A tale with no end: Ongoing developments in the CHARMM additive and Drude force fields,” Department of Biochemistry, University of Zurich, September, 2011.
140. “Progress towards a comprehensive polarizable macromolecular force field based on the CHARMM classical Drude oscillator model,” Lausanne Biomolecular Modeling Seminars, Swiss Institute of Bioinformatics, Ecole Polytechnique Federale Lausanne, Laussanne, Switzerland, October, 2011
141. “Site Identification by Ligand Competitive Saturation (SILCS): Computational approach for optimization of inhibitors of protein-protein interactions including BCL6, ERK and S100B,” Biozentrum, Basel, Switzerland, October, 2011.
142. “Progress towards a comprehensive polarizable macromolecular force field based on the CHARMM classical Drude oscillator model,” Department of Physical Chemistry, University of Basel, Basel, Switzerland, October, 2011.
143. “Progress towards a comprehensive polarizable macromolecular force field based on the CHARMM classical Drude oscillator model,” Competence Center for Computational

Chemistry (C4) of ETH Zurich, the University of Zurich and the IBM Research Laboratory, Zurich, Switzerland, October, 2011.

144. "Site Identification by Ligand Competitive Saturation (SILCS): Computational approach for optimization of inhibitors of protein-protein interactions including BCL6, ERK and S100B," University of Southern Florida, Department of Chemistry, Tampa, Florida, November, 2011
145. "Progress towards a comprehensive polarizable macromolecular force field based on the CHARMM classical Drude oscillator model," Department of Physics and Astronomy, University of Delaware, Newark, Delaware, February, 2012.
146. "Progress towards a comprehensive polarizable macromolecular force field based on the CHARMM classical Drude oscillator model," Instituto de Química, Universidade de São Paulo, São Paulo, Brazil, March 2012.
147. "Computer-Aided Drug Design: Ligand-Based Approaches." In the workshop on "Advanced Topics in Computational Biology – Agrochemical and Drug Design", Embrapa Agriculture Informatics, University of Campinas, UNICAMP, Campinas, São Paulo, Brazil, April, 2012.
148. "The CHARMM Force Field," Center Européen de Calcul Atomique et Moléculaire, Workshop: Advances in Biomolecular Modelling and Simulations using CHARMM, University College Dublin, Dublin, Ireland, June 2012.
149. "Site Identification by Ligand Competitive Saturation (SILCS): Computational approach for optimization of inhibitors of protein-protein interactions including BCL6, ERK and S100B," University of Maryland Greenebaum Cancer Center, Molecular and Structural Biology Program, Baltimore, MD, June 2012.
150. "Contribution of the 2'-hydroxyl to the conformational properties of RNA," President's Meeting of the International Society of Quantum Biology and Pharmacology, Stockholm Sweden, June 2012
151. "Ongoing developments in the CHARMM additive and Drude force fields," Annual CHARMM developers Meeting, Computational Biophysics Section of the Laboratory of Computational Biology, National Heart, Blood and Lung Institute, National Institutes of Health, Rockville, MD, July 2012.
152. "Towards a comprehensive polarizable macromolecular force field based on the CHARMM classical Drude oscillator model," Computational Chemistry Gordon Conference, Mount Snow, Vermont, July 2012
153. "From Balls on Springs to Drugs and Things," University of Maryland Baltimore Research of the Year Seminar, Baltimore, MD, October, 2012
154. "Site Identification by Ligand Competitive Saturation (SILCS): Computational approach for optimization of inhibitors of protein-protein interactions including BCL6, ERK and S100B," Sealy Center for Structural Biology and Molecular Biophysics, University of Texas Medical Branch, Galveston, TX, October, 2012
155. "Identification and Optimization of Inhibitors of Protein-Protein Interactions: ERK, S100B and BTB domain Containing Proteins" Department of Pharmacology, Weill Cornell Medical School, New York, NY, December, 2012
156. "Progress towards a comprehensive polarizable macromolecular force field based on the CHARMM classical Drude oscillator model" Physics and Chemistry Seminar Series, Wake Forest University, Winston-Salem, NC, February, 2013

157. “Contribution of the 2’-hydroxyl to the conformational properties of RNA,” University of Maryland, College Park, Department of Chemistry and Biochemistry Seminar, College Park, MD, February, 2013
158. “Site Identification by Ligand Competitive Saturation (SILCS): Computational approach for optimization of inhibitors of protein-protein interactions including BCL6, ERK and S100B,” Institute of Bioscience & Biotechnology Research, Rockville, MD, February, 2013
159. “Progress towards a comprehensive polarizable macromolecular force field based on the CHARMM classical Drude oscillator model” Center for Molecular Biophysics, Oak Ridge National Laboratory, Oak Ridge, TN, March, 2013
160. “Progress towards a comprehensive polarizable macromolecular force field based on the CHARMM classical Drude oscillator model” 245th American Chemical Society National Meeting, New Orleans, LA, April 2013.
161. “Site Identification by Ligand Competitive Saturation (SILCS): Mapping fragment binding sites including consideration of protein flexibility and fragment desolvation using an explicit solvent representation” 245th American Chemical Society National Meeting, New Orleans, LA, April 2013.
162. “Intrinsic contribution of the 2'-hydroxyl to RNA conformational heterogeneity,” 245th American Chemical Society National Meeting, New Orleans, LA, April 2013.
163. “Site Identification by Ligand Competitive Saturation (SILCS): Structure-Based Free Energy Computational Approach for Ligand Discovery and Optimization,” Cambridge Healthtech Institute’s 8th Annual Drug Discovery Chemistry Meeting, San Diego, CA., April 2013.
164. “Site Identification by Ligand Competitive Saturation (SILCS): Structure-Based Free Energy Computational Approach for the Identification and Optimization of Ligands Targeting Proteins including Inhibitors of Protein-Protein Intearctions,” Drug Discovery & Therapy World Congress 2013, Boston, MA, USA, June 2013.
165. “Site Identification by Ligand Competitive Saturation (SILCS): Structure-Based Free Energy Computational Approach for Ligand Discovery and Optimization,” Cambridge Healthtech Institute and BIO-IT World’s 13th Structure-Based Drug Design Meeting, Boston, MA, June 2013.
166. “RNA Conformational Heterogeneity,” RNA Dynamics, Telluride Scientific Research Conference, Telluride, CO, USA, July 2013.
167. “Site Identification by Ligand Competitive Saturation (SILCS): Computational approach to the identification and optimization of ligands targeting proteins, RNA and other macromolecules,” 2nd International Conference on Medicinal Chemistry & Computer-Aided Drug Designing, Las Vegas, NV, USA, October 2013.
168. “Toward opioid analgesics with decreased adverse side effects: From ligand-based to GPCR-based computer-aided drug design,” The 16th Annual Goodman Lecture, The Department of Physiology and Pharmacology, Oregon Health & Sciences University, Portland, OR, USA, October 2013.
169. “Development of a Polarizable Force Field for Macromolecules based on the Classical Drude Oscillator,” Workshop on Polarizable Force Fields from Biomacromolecules, 58th Annual Meeting of the Biophysical Society, San Fransisco, CA, USA, February 2014.
170. “Site Identification by Ligand Competitive Saturation (SILCS): Computational approach to to the identification and optimization of ligands,” Oak Ridge National Laboratory Science Focus Area Advisory Committee Site Visit, Oak Ridge, TN, USA, April 2014.

171. “Development of a Polarizable Force Field for Macromolecules based on the Classical Drude Oscillator,” Department of Biochemistry, Cellular and Molecular Biology, Univesity of Tennessee and Center for Molecular Biophysics, Oak Ridge National Laboratory, Oak Ridge, TN, USA, April 2014.
172. “CHARMM Force Fields: From the Additive CHARMM Force Field to the Polarizable Drude Force Field for Biomolecules,” Dassault Systemes, Accelerate 2014 Users Group Meeting, Washington DC, USA, May 2014.
173. “The CHARMM Force Field,” Centre Européen de Calcul Atomique et Moléculaire, Workshop: Advances in Biomolecular Modelling and Simulations using CHARMM, University College Dublin, Dublin, Ireland, June 2014.
174. “Polarizable Force Field for Macromolecules based on the Classical Drude Oscillator,” 2014 International Society of Quantum Biology and Pharmacology (ISQBP) President’s Meeting, Telluride Science Research Center, Telluride, CO, June 2014.
175. “A Drude polarizable force field for macromolecules” Annual CHARMM Developers Meeting, Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, July 2014.
176. “Computer-Aided Drug Design: Molecular modeling and the design of inhibitors targeting BCL6,” College of Pharmacy, Ewha Womans University, Seoul, Korea, September 2014.
177. “Site Identification by Ligand Competition Saturation (SILCS),” Korean Institute for Advanced Sciences, Computational Sciences, Seoul, Korea, September 2014.
178. “Site Identification by Ligand Competition Saturation (SILCS),” Mini-Symposium on Computational Biology, Department of Chemistry, Seoul National University, Seoul, Korea, September 2014.
179. “A Polarizable Force Field for Simulations of Peptides and Proteins Based on the Classical Drude Oscillator,” The 14th KIAS Conference on Protein Structure and Function, Korean Institute for Advanced Sciences, Seoul, Korea, September 2014.
180. “A Polarizable Force Field for Simulations of Macromolecules Based on the Classical Drude Oscillator,” Workshop on Computer Modeling and Simulation of Biomolecular Systems,” Theoretical Molecular Sciences Laboratory, RIKEN Institute, Wako, Saitama 351-0198, Japan, September 2014.
181. “A Polarizable Force Field for Simulations of Macromolecules Based on the Classical Drude Oscillator,” Department of Chemistry, University of Virginia, Charlottesville, VA, October 2014.
182. “A Polarizable Force Field for Simulations of Macromolecules Based on the Classical Drude Oscillator,” Department of Chemistry, University of New Orleans, New Orleans, LA, November 2014.
183. “A Polarizable Force Field for Simulations of Macromolecules Based on the Classical Drude Oscillator,” echeminfo, Drug Discovery USA 2015, Baltimore, MD, February 2015.
184. “RNA conformational heterogeneity: Role of the 2’OH and Impact of TMAO,” Department of Biochemistry and Molecular Biology, School of Medicine, University of Maryland, Baltimore, MD, March 2015.
185. “Ligand Design Targeting GPCRs and Protein-Protein Interactions Using the Site Identification by Ligand Competitive Saturation (SILCS) Approach,” Center for Computational Biology and Bioinformatics, Indiana University School of Medicine in Indianapolis, Indianapolis, IN, April, 2015.

186. “Role of explicit polarization in the conformational heterogeneity of peptides and DNA studied using the classical Drude oscillator force field,” Challenges in Large-Scale Biomolecular Computing, Telluride Science Research Center, Telluride, CO, June 2015.
187. “Explicit treatment of polarization using the classical Drude oscillator,” Development and Deployment of Chemical Software for Advanced Potential Energy Surfaces, Telluride Science Research Center, Telluride, CO, June 2015.
188. “Status of the CHARMM36 and Drude force fields and enhanced sampling methods for complex carbohydrates,” Annual CHARMM Meeting, Universitaet Wien, Vienna, Austria, July, 2015.
189. “Ligand Design using Site Identification by Ligand Competitive Saturation (SILCS),” American Association of Pharmaceutical Sciences (AAPS) Online Webinar, July, 2015.
190. “A Polarizable Force Field for Simulations of Macromolecules Based on the Classical Drude Oscillator,” Biochemistry and Molecular Biophysics, Kansas State University, Manhattan, KS, October, 2015
191. “A Polarizable Force Field for Simulations of Macromolecules Based on the Classical Drude Oscillator,” Center for Computational Biology, The University of Kansas, Lawrence, KS, October, 2015
192. “Novel Site Identification by Ligand Competitive Saturation (SILCS) CADD Approach,” Clinical Sciences and Drug Discover-2015 Conference, Baltimore, MD, November, 2015.
193. “Grand Canonical Solute Sampling in Combination with the Site Identification by Ligand Competitive Saturation (SILCS) Ligand Design Methodology,” Mathematical Challenges in Drug and Protein Design, Mathematical and Biosciences Institute, Ohio State University, Columbus, OH, December, 2015.
194. “Functional Group Affinity Mapping and Rapid Estimation of Relative Ligand Affinities by Site Identification by Ligand Competitive Saturation (SILCS),” Grand Rounds, Conte Grant Research Group, Maryland Psychiatric Research Center, Spring Grove, MD, January 2016.
195. “Polarizable Force Field for RNA Based on the Classical Drude Oscillator,” 251st American Chemical Society National Meeting, San Diego, CA, March 2016.
196. “Grand Canonical Solute Sampling in Combination with the Site Identification by Ligand Competitive Saturation (SILCS) Ligand Design Methodology,” 251st American Chemical Society National Meeting, San Diego, CA, March 2016.
197. “Role of Explicit Polarization on the Conformational Heterogeneity of Biological Molecules Studied using the Classical Drude Oscillator Force Field,” Beyond point charges: novel electrostatic developments in force fields, Center Européen de Calcul Atomique et Moléculaire, CECAM-HQ-EPFL, Lausanne, Switzerland, April 2016.
198. “Rapid Estimation of Relative Binding Affinities: Evaluation Across Multiple Gene Family Targets, “ 2016 Workshop on Free Energy Methods in Drug Design: Targeting Cancer, Boston, MA, May 2016.
199. “Overview of the Classical Drude Oscillator Polarizable Force Field for Biomolecules,” International Society of Quantum Biology and Pharmacology (ISQBP) President’s Meeting, Bergen, Norway, June, 2016
200. “Updates of the CHARMM36 and Drude force fields and additional extensions to CHARMM,” Annual CHARMM Meeting, University of Michigan, Ann Arbor, MI, USA, July 2016.
201. “Ongoing Developments in the Drude Polarizable Force Field for Biomolecules,” 252nd American Chemical Society National Meeting, Philadelphia, PA, August 2016.

202. “Computational Chemistry: From Balls on Springs to Opioids and Things,” University of Maryland Baltimore School of Nursing, Baltimore, MD, September 2016.
203. “Electronic Polarization in Macromolecular Structure and Dynamics: Development and Application of a Polarizable Force Field based on the Classical Drude Oscillator,” Biophysics Colloquim, Cornell University, Ithaca, NY, September 2016.
204. “Electronic Polarization in Macromolecular Structure and Dynamics: Development and Application of a Polarizable Force Field based on the Classical Drude Oscillator,” Molecular Biophysics Unit, Indian Institute of Science, Bangalore, India, December, 2016.
205. “SILCS/SSFEP for Ligand Development: Rapid Estimation of Relative Ligand Binding Affinities Using Pre-Computed Conformational Ensembles,” Molecular Biophysics Unit, Indian Institute of Science, Bangalore, India, December, 2016.
206. “Electronic Polarization in Macromolecular Structure and Dynamics: Development and Application of a Polarizable Force Field based on the Classical Drude Oscillator,” 15th International Theoretical Chemistry Symposium, University of Hyderabad, Hyderabad, India, December, 2016.
207. “Computational Chemistry: From Balls on Springs to Drugs and Things,” Oak Ridge International School, Hyderabad, India, December, 2016.
208. “SILCS/SSFEP for Ligand Development: Rapid Estimation of Relative Ligand Binding Affinities Using Pre-Computed Conformational Ensembles,” Indian Institute of Information Technology, Hyderabad, India, December, 2016.
209. “Targeting BCL6 for the treatment of DLBCL using the Site Identification by Ligand Competitive Saturation (SILCS) Technology,” 2nd International Cancer Study & Therapy Conference, Baltimore, MD, USA, February 2017.
210. “Electronic Polarization in Macromolecular Structure and Dynamics: Development and Application of a Polarizable Force Field based on the Classical Drude Oscillator,” Lectures in Computational Biophysics at Johns Hopkins University, Baltimore, MD, USA, February 2017.
211. “Electronic Polarization in Macromolecular Structure and Dynamics: Development and Application of a Polarizable Force Field based on the Classical Drude Oscillator,” Centre for Molecular Simulations, University of Calgary, Alberta, Canada, March, 2017.
212. “SILCS/SSFEP for Ligand Development: Rapid Estimation of Relative Ligand Binding Affinities Using Pre-Computed Conformational Ensembles,” Molecular and Structural Biology Program Meeting, University of Maryland. Marlene and Stewart Greenebaum Comprehensive Cancer Center, Baltimore, MD, USA, March 2017.
213. “Rapid Estimation of Relative Ligand Binding Affinities Using Pre-Computed Conformational Ensembles” Center Européen de Calcul Atomique et Moléculaire, CECAM-HQ-EPFL, Lausanne, Switzerland, June 2017.
214. “Can CADD Drive Drug Design and Development? Rapid Estimation of Relative Ligand Binding Affinities Based on Pre-Computed Conformational Ensembles.” Drug Discovery and Therapy World Congress, Boston, MA, USA, July 2017.
215. “Updates of the CHARMM36 and Drude force fields etc…” Annual CHARMM Meeting, Harvard University, Cambridge, MA, USA, July 2017.
216. “Modeling the conformational heterogeneity of complex carbohydrates: Enhanced sampling, methods of analyses and towards a polarizable force field,” 254st American Chemical Society National Meeting, Washington DC, USA, August 2017.

217. “Can CADD Drive Drug Design and Development? Rapid Estimation of Relative Ligand Binding Affinities Based on Pre-Computed Conformational Ensembles.” Department of Cell and Molecular Biology, Uppsala University, Uppsala, Sweden, October 2017.
218. “Electronic Polarization in Macromolecular Structure and Dynamics: Development and Application of a Polarizable Force Field based on the Classical Drude Oscillator,” Department of Biochemistry and Biophysics, Science for Life Laboratory, Stockholm University, Stockholm, Sweden, October 2017.
219. “Electronic Polarization in Macromolecular Structure and Dynamics: Development and Application of a Polarizable Force Field based on the Classical Drude Oscillator,” University of Maryland/National Institute of Standards and Technology, Institute of Bioscience and Biotechnology, Rockville, MD, USA, October 2017.
220. “Conformational heterogeneity of complex carbohydrates in vaccine antigens,” Institute of Human Virology, University of Maryland, Baltimore. General Staff Seminar, Baltimore, MD, USA, February 2018.
221. “Complimentary Base Specificity in Base Excision by Thymine DNA Glycosylase,” Epigenetics and Multiscale Genomics, Center Européen de Calcul Atomique et Moléculaire, CECAM-HQ-EPFL, Lausanne, Switzerland, May 2018.
222. “Updates of the C36 and Drude force fields, CHARMM-Psi4 interface and more,” Annual CHARMM Meeting, University of Chicago, Chicago, USA, July 2018.
223. “Development and Application of a Polarizable Force Field based on the Classical Drude Oscillator,” 256th American Chemical Society National Meeting, Boston, MA, USA, August 2018.
224. “Can CADD Drive GPCR Drug Design? Rapid Estimation of Relative Ligand Binding Affinities Based on Pre-Computed Conformational Ensembles.” Center for Computational Biology, University of Kansas, Lawrence, KS, USA, October 2018
225. “Electronic Polarization in Macromolecular Structure and Dynamics: Development and Application of the Drude Polarizable Force Field,” Dalian University of Technology, Dalian, China, October, 2018
226. “Electronic Polarization in Macromolecular Structure and Dynamics: Development and Application of the Drude Polarizable Force Field,” Shenyang Pharmaceutical University, Shenyang, China, October, 2018.
227. “Can CADD Drive GPCR Drug Design? Rapid Estimation of Relative Binding Affinities Based on Pre-Computed Conformational Ensembles,” Westlake Masters Forum, Westlake University, Hangzhou, China, 2018.
228. “Electronic Polarization in Macromolecular Structure and Dynamics: Development and Application of the Drude Polarizable Force Field,” NYU-ECNU Center for Computational Chemistry, East China Normal University, Shanghai, October, 2018.
229. “Can CADD Drive GPCR Drug Design? Rapid Estimation of Relative Binding Affinities Based on Pre-Computed Conformational Ensembles,” Graduate School of Peking University, Peking University, Shenzhen, China, 2018.
230. “Electronic Polarization in Macromolecular Structure and Dynamics: Development and Application of the Drude Polarizable Force Field,” Xtal-Pi, Shenzhen Jingtai Technology Co., Ltd., Shenzhen, China, 2018.
231. “Can CADD Drive GPCR Drug Design?” National Institute of Biological Sciences (NIBS), Beijing, China, 2018.

232. “Rapid Estimation of Relative Binding Affinities Based on Pre-Computed Conformational Ensembles, Application to GPCRs,” 5th AEGIS Workshop, Institut Pasteur, Paris, France November, 2018.
233. “the trouble with the French is that they don't have a word for entrepreneur,” George W. Bush, ca. 2004,” 5th AEGIS Workshop, Institut Pasteur, Paris, France, November, 2018.
234. “Electronic Polarization in Macromolecular Structure and Dynamics: Development and Application of the Drude Polarizable Force Field,” Theoretical and Computational Biophysics Seminar, Beckman Institute, University of Illinois, Urbana-Champaign, IL, January, 2019.
235. “Site Identification by Ligand Competitive Saturation (SILCS) for ligand affinity rank ordering, update of the Drude polarizable force field and a mix of the two…” Free Energy calculations, Entering the fourth decade of adventure in chemistry and biophysics (2019), Sante Fe, New Mexico, USA, June 2019.
236. “Status and code availability of the additive C36 and polarizable Drude force fields,” CHARMM-Tinker Meeting, Institut Pasteur, Paris, France, July 2019.
237. “Electronic Polarization in Macromolecular Structure and Dynamics: Development and Application of the Drude Polarizable Force Field,” Department of Pharmaceutical Sciences, College of Pharmacy, University of New England, Portland, Maine, USA, October 2019.
238. “Electronic Polarization in Macromolecular Structure and Dynamics: Development and Application of the Drude Polarizable Force Field,” University of Maryland, College Park, Department of Chemistry and Biochemistry Seminar, College Park, MD, November, 2019
239. “Benchmarks….” Path to a Machine Learned (ML) Organic Force Field, Flatiron Institute, New York, NY, December, 2019
240. “Electronic Polarization in Macromolecular Structure and Dynamics: Development and Application of the Drude Polarizable Force Field,” Beyond Point Charges: Novel Electrostatic Developments in Force Fields , Center Européen de Calcul Atomique et Moléculaire, CECAM-HQ-EPFL, Lausanne, Switzerland, December 2019.
241. “Ligand discovery and design using Site Identification by Ligand Competitive Saturation (SILCS),” Cancer Chemical and Structural Boology (CCSB) Program, The Sidney Kimmel Comprehensive Cancer Center and the Department of Pharmacology, The Johns Hopkins University, Baltimore, MD, USA, January 2020.
242. “DRUDE,” CHARMM NIH Mini Meeting, National Heart, Lung, and Blood Insitute, NIH, Bethesda, MD, USA, January 2020.
243. “Update of the Drude Force Field and Grand Canonical Sampling,” Annual CHARMM Meeting, Online Zoom Meeting, Boston University, Boston, MA, July 2020.
244. “Polarizable Force Field Based on the Classical Drude Oscillator,” BioVia Conference 2020, Online Zoom Meeting, September 2020.
245. “Computer-Aided Drug Design at UMB,” Molecular and Structural Biology Program 2020 Annual Retreat, University of Maryland Marlene and Stewart Greenebaum Comprehensive Cancer Center, Baltimore, MD, Online Zoom Meeting, October 2020.
246. “Site Identification by Ligand Competitive Saturation (SILCS): Ligand design and more,” Computational Biology Unit, University of Bergen, Bergen, Norway, Zoom Seminar, February 2021.
247. “Status of the Classical Drude Oscillator Polarizable Force Field,” American Chemical Society National Meeting, Virtual, April 2021.

248. “CHARMM Additive and Drude Polarizable Force Fields: The Long and Winding Road….to….Hey Jude,” Computational Biology Award Lecture, International Society for Quantum Biology and Pharmacology President’s Meeting, Virtual meeting based in Strasbourg, France, June-July 2021
249. “Ligand discovery and design using Site Identification by Ligand Competitive Saturation (SILCS),” Virtual Workship Presentation, Advanced Molecular Dynamics Simulations AMDS 2021 (gctatku.org.np), Indian Institutes of Science and Education Pune, Kathmandu University-Nepal, and Green Club of Thoughts-Kathmandu University, India, July 2021
250. “Development in the additive C36 and Drude polarizable force fields,” Annual CHARMM Meeting, Virtual Meeting, Michigan State University, East Lansing, MI, July 2021
251. “Site Identification by Ligand Competitive Saturation (SILCS): Utilization in Ligand Design and Development,” Sergei Noskov Memorial Symposium –Protein-Ligand Interactions: Theory Meets the Experiment, IUPAC- CCCE 2021 Virtual Meeting, Canada, August 2021
252. “Electronic response in proteins and their environment using the classical Drude oscillator polarizable force field,” American Chemical Society Fall National Meeting, Virtual Meeting based in Atlanta, GA, August 2021
253. “CGenFF and Drude force field: Development and application,” Center Européen de Calcul Atomique et Moléculaire, CECAM-FR-GSO, CHARMM-GUI CECAM School, Virtual/Live Workshop, Toulouse, France, September 2021.
254. “Drude General Force Field (DGenFF): Extension of the Drude Polarizable Force Field to Drug-like Molecules using Machine Learning,” 2021 BIOVIA Conference, Dassault Systemes, USA, Virtual, September 2021.
255. “Extension of the CHARMM36 force field to LJ-PME and current status of the Drude polarizable force field,” NAMD Developers Workshop, University of Illinois at Urbana-Champaign, Illinois, USA, Hybrid meeting, September 2021.
256. “Modeling the IgG-Endoglycosidase S2 Complex using SILCS, replica-exchange and microsecond MD simulations,” EMBO Workshop: Advances and challenges in bimolecular simulations, Virtual meeting, Brno, Czech Republic, October 2021.
257. “Pre-Computed Conformational Ensembles in Drug Design: Site Identification by Ligand Competitive Saturation (SILCS) and Single-Step Free Energy Perturbation (SSFEP),” Pfizer Virtual Seminar, November 2021.
258. “Computer Aided Drug Design: From the Lab to the Clinic,” Seminar with Paul Shapiro for the Baltimore Underground Science Space (BUGSS, https://bugssonline.org/) Seminar, Virtual, January 2022.
259. “Pre-Computed Conformational Ensembles in Drug Design: Site Identification by Ligand Competitive Saturation (SILCS),” American Chemical Society National Meeting, Symposium in honor of Prof. Charles Brooks, San Diego, CA, March 2022
260. “From CHARMM to SILCS: Confluence of force fields and computer aided drug design,” American Chemical Society National Meeting, American Chemical Society Award for Computers in Chemical and Pharmaceutical Research Symposium in honor of Prof. Alexander MacKerell, San Diego, CA, March 2022
261. “Pre-Computed Conformational Ensembles in Drug Design: Site Identification by Ligand Competitive Saturation (SILCS),” International Conference in Advances in Pharmaceutical

Medicinal Chemistry-2022, Virtual Conference, School of Pharmacy, D Y Patil Deemed to be University, Nerul, Navi Mumbai, India, April 2022

262. "Site Identification by Ligand Competitive Saturation (SILCS): From ligand design to modeling of macromolecular interactions," International Society for Quantum Biology and Pharmacology President's Meeting, Innsbruck Austria, July 2022
263. "Ongoing development of the additive C36 and Drude polarizable force fields," Annual CHARMM Meeting, Harvard University, Cambridge, MA, July 2022
264. "Site Identification by Ligand Competitive Saturation (SILCS): Overview and extension to RNA," REVIR Therapeutics, Virtual Seminar, October 2022.
265. "Pre-Computed Conformational Ensembles in Drug Design and More: Site Identification by Ligand Competitive Saturation (SILCS)," Department of Physiology and Membrane Biology, School of Medicine, University of California Davis, Rosetta Brainstorm Virtual Seminar, March 2023
266. "SILCS as a Platform Technology for Computational Investigations of Free Energies of Intermolecular Interactions," American Chemical Society National Meeting, American Chemical Society Award for Computers in Chemical and Pharmaceutical Research Symposium in honor of Prof. Jiali Gao, Indianapolis, IN, March 2023
267. "Introduction to Site Identification by Ligand Competitive Saturation (SILCS) and its Application in Drug Design and Development," CCPBioSim Industry Series Seminar, Virtual seminar, April 2023
268. "Introduction to Site Identification by Ligand Competitive Saturation (SILCS) and its Application in Drug Design and Development," Computer-Aided Drug Design Group, Center for Cancer Research, National Cancer Institute, Virtual seminar, July 2023.
269. "Introduction to Site Identification by Ligand Competitive Saturation (SILCS) and its Application in Drug Design and Development," Eli Lilly and Company, Virtual Multi-site seminar, July 2023.
270. "Developments in the CHARMM force fields and Oscillating μ_{ex} GCMC," Annual CHARMM Meeting, University of Michigan, Ann Arbor, MI, July 2023
271. "Overview of the Classical Drude Oscillator Polarizable Force Field," Department of Chemistry, Stanford University, Stanford, CA, January 2024.

Grants and Contracts (funding levels are approximate).

Ongoing

Principal Investigator

NIGMS R35 GM131710 05/01/2019-04/30/2024 6.12 calendar
Macromolecular Conformational Heterogeneity $3,653,8383 (Total award)
Investigations will be undertaken on the conformational properties of biological macromolecules, including DNA, RNA, carbohydrates and proteins, to relate their structural and dynamic properties to their biological functions. This information will be applied to facilitate the development of novel therapies for diseases including antibiotic resistant bacterial infections and cancer based on both small molecule therapeutics and vaccines. Facilitating these efforts will be the development of improved theoretical force fields and conformational sampling methods

R44GM130198 08/10/2021-07/31/2023
0.24 calendar
SilcsBio LLC (SBIR Subcontract) $796,682 (total award)

Computational Methods for Optimizing Biologics Formulation
Studies will involve the development of a rational formulation design technology using computational methods that will allow screening of a large number of excipient/buffer combinations that will result in accelerated and improved biopharmaceutical development thereby facilitating bringing these agents to market as well as improving clinical outcomes.

Waxman Research Foundation (MacKerell) 7/01/06-6/31/2023
Subcontract from Albert Einstein College of Medicine and Cornell Weill School of Medicine
~$850,000 Total Costs
Chemical Intervention for Transcription Therapy
Compounds that bind to the proteins BTB containing proteins, including BCL6, Kaiso and Bach2 will be identified and optimized to develop novel anticancer agents. This is a collaborative grant from a private foundation with Drs. Ari Melnick, Albert Einstein College of Medicine and Gil Prive, University of Toronto that is renewed on an annual basis.

Co-Investigator

R01AG068130 (Tsukamoto) 07/01/2020-06/30/2025 0.24 calendar
Johns Hopkins University / NIH $37,402
Development of GCPII inhibitors for the treatment of age-related cognitive disorders
For this project, Dr. MacKerell's lab will provide:
1) SILCS FragMaps and identity of potential allosteric binding pockets on GCPII
2) Lists of compounds that are potential inhibitors of GCPII for biological evaluation.
Role: Co-Investigator

NIH R21 AI161313-01 (Xue, Wilks, MPI) 1/22/21-12/31/23 (NCE) 0.24 calendar
Pseudomonas aeruginosa heme sensing inhibitors targeting HasAp $424,875 (Total award)
Major goal: The goal of our research is to synthesize and test a series of GaSal analogs using established assays, to identify, validate, and characterize potent inhibitors of heme signaling and iron homeostasis as a potential treatment for MDR *P. aeruginosa* infections.

2004548643 (PI: Davis) 05/31/19 – 04/30/24 0.6 Calendar
Johns Hopkins University/ NIH (Prime) $896,655 (Total Award)
Johns Hopkins Institute for Clinical and Translational Research
To train future translational clinical scientists; amplification of community and collaboration across Baltimore; unifying translational endeavors and pilot scientific awards; expansion of joint drug development and repurposing programs.

Completed Grants

Principle Investigator

R44GM130198

R43GM130198 03/05/19-02/29/20 0.24 calendar
SilcsBio LLC (SBIR Subcontract) $74,250
Computational Methods for Optimizing Biologics Formulation
Studies will involve the development of a rational formulation design technology using computational methods that will allow screening of a large number of excipient/buffer combinations that will result in accelerated and improved biopharmaceutical development thereby facilitating bringing these agents to market as well as improving clinical outcomes.

Following three grants converted to NIGMS R35 GM131710, 05/01/2019

R01 GM072558 (Roux and MacKerell, Co-PIs) 02/01/06 – 06/30/20
NIH/NIGMS - University of Chicago
$1,588,875 Total Costs – to ADM, $594,507 total costs: 2016-2020
Polarizable Force Field for Proteins and Lipids
The major goal of this project is the development of an empirical force field for proteins and lipids that explicitly treats electronic polarizability.

R01 GM070855 (MacKerell) 09/01/05 –11/31/18
NIH/NIGMS
$3,368,846 Total Costs
Carbohydrate Force Field for Molecular Recognition
To develop empirical force field parameters for carbohydrates and undertake structure-function studies of complex carbohydrates including glycosylated proteins including the antiproliferative factor and the HIV envelope complex.

R01 GM051501 (MacKerell) 09/01/96 – 06/31/21
NIH/NIGMS
$4,851,950 Total Costs
Energetics of Oligonucleotide Conformational Heterogeneity
Investigate structure-function relationships in DNA and RNA and develop a polarizable empirical force field for nucleic acids.

Leukemia and Lymphoma Foundation (MacKerell) 07/01/15-06/30/18
Weill Medical College Subcontract (Melnick, Prime) $1,800,000 total
Structural biology of BCL-6 Small Molecule Inhibitors $727,698 to UMB
The project will involve structure-based drug design targeting the transcription repressor BCL6 with efforts including molecular modeling and medicinal chemistry.

2R44GM109635-03 (MacKerell, Malone, CoPI) 9/19/16-8/31/18
SilcsBio LLC (SBIR Subcontract to UMB) $1,008,920 Direct/$1,225,638 Total
$219,600/$307,220 Direct/Total to UMB
Pre-computed free energy maps for rapid structure-based ligand design

Computer code will be developed and tested for the extraction of 3D pharmacophores from SILCS FragMaps and the calculation of SILCS Grid Free Energy (GFE) scores for use in database screening.

R43GM109635 (MacKerell, Malone, CoPI) 11/01/14-04/30/16
SilcsBio LLC (SBIR Subcontract to UMB) $188,720 Direct/$229,9258 Total
$82,053 Total to UMB
Pre-computed free energy maps for rapid structure-based ligand design
Computer code will be developed and tested for the extraction of 3D pharmacophores from SILCS FragMaps and the calculation of SILCS Grid Free Energy (GFE) scores for use in database screening.

(MacKerell) 11/01/15-02/29/16 0.24 Calendar
Pfizer Inc $37,930
Validation of the SSFEP and SILCS computational methodologies
Work will involve testing of the CADD SSFEP and SILCS technologies against a collection of experimental data on therapeutically relevant proteins.

Maryland Industrial Partnership Award #5212 08/1/13 – 08/31/14
$136,899 Total Costs
Validation of SILCS™ Molecular Modeling Software
Validate the SILCS technology for its utility in the identification of potential therapeutic chemicals and for optimization of those chemicals into candidates for New Drug Applications (NDAs)

NSF CHE-0823198 (MacKerell) 09/01/08-08/31/14
$665,367 Total Costs
Extensible Cyberenvironments for Empiriical & Semi-Empiricals Hamiltonians Parameter Optimization & Dissemination
Cyberenvironments will be created to automate the process of parameterization for classical molecular mechanics (MM) and semi-empirical (SE) Hamiltonians and allow for wide dissemination of the developed parameters.

American Chemical Society (MacKerell and Thorpe (UMBC)) 2012
Project Grant for Divisional Enhancement for support of a symposium at the ACS Mid-Atlantic Regional Meeting (MARM)
$5000 total costs
Frontiers in the Application of Computational Chemistry to Biological Systems.

R01 GM070855-03S1 Minority Supplement to Carlos A. Ramirez 06/01/06-08/30/10
$140,000 Total costs

University of Maryland College Park (MacKerell and Yu, CoPIs) 12/15/2008-12/14/09
$96,287 total costs
Engineering paramagnetic Complexes for Multi-Chromic 19F MRI

NIH/NCI R01 CA95200 (MacKerell) 2002-2005

$703,471 total costs
p56lck Inhibitors as Potential Immunosuppressive Drugs
Co-I, Hayashi

Center for Disease Control, 258699 (MacKerell) 2003-2004
$50,000 direct costs
Charmm force field for silicates

Lawrence Livermore National Laboratory 1998-1999
$8,700 total costs
Empirical Force Field Parameterization of Modified Nucleic Acids

University of Maryland School of Pharmacy Designated Research Initiative Fund
(MacKerell) $100,000 total costs 1998-2000
Rational Drug Design of Therapeutic Agents for the Treatment of Diabetes via Antibodies as 3D Surrogates for the Insulin Receptor
CoI; Hayashi, Serrero

The Procter & Gamble Company International Program for Animal Alternatives
(MacKerell) $100,000 direct costs 1995-1996
Predicting the Absorption and Disposition of Drugs based on the Thermodynamic Solvation Contributions of Chemical Substituents
Co-I; Polli, Young

University of Maryland. School of Pharmacy Designated Research Initiative Fund
$10,000 total costs 1995
Molecular Alterations of the T-Antigen II Origin of Replication due to the Incorporation of the Antineoplastic Agent AraC

American Cancer Society, Maryland Division, Inc. 1995-1996
$30,000 total costs
Molecular Mechanism of Antineoplastic Nucleosides

University of Maryland, School of Pharmacy Designated Research Initiative Fund 1994
$10,000 total costs
Molecular Mechanism of Antineoplastic Nucleosides

American Association of Colleges of Pharmacy Grant Program for Young Investigators 1993
$7,500 total costs
Rational Drug Design: Database of the Energy Contributions of Halogen Atoms to Drug Molecule Aqueous Solvation, Lipid Solubility and Receptor Binding

University of Maryland Biomedical Research Support Grant 1993
$10,000 total costs
Energetic contributions of halogen atoms to drug solvation and binding

American Cancer Society/University of Maryland Institutional Research Grant 1993
$10,000 total costs
Energetic based rational design of inhibitors for Dihydrofolate Reductase

Co-Investigator

Leukemia and Lymphoma Society (Melnick PI). 7/01/15-06/30/20 0.48 Calendar
Subcontract from Weill Cornell Medical College $80,000
Design and synthesis of inhibitors of the BTB domain of BCL6
Work will involve design of novel inhibitors of BCL6 and subsequent optimization for the development of therapeutic agents to treat Diffuse Large B-Cell Lymphoma.

National Academy of Sciences 10003290 (MacKerell, UMB PI) 7/1/2017-8/31/2020
Pakistan – United States Science and Technology Cooperation Program 2016: Phase 7
$442,266 Total
$159,150 to UMB
Molecular Characterization and Drug Design Targeting Emerging Pathogenic Bacteria of Pakistan and Development of an Access Application for the Health Care Industry
Perform in silico database screening again putative bacterial target proteins with the goal of developing novel antibiotics and the development of a web utility to collect information on emerging infectious bacterial strains in Pakistan.

NIH R21AI135082 (PI: Deshpande) 12/20/17-11/30/20
Biased agonism and conformational heterogeneity of beta adrenergic receptors in Bronchodilation $154,500 Total Costs to UMB
Investigate the conformational properties of the beta adrenergic receptor and identify novel agonists using computational chemistry methods that may be developed into novel treatments for asthma

NIH R01 GM072711-11A1 (PI: Drohat) 06/01/16-04/30/2020
Mechanism of Glycosylase Enzymes in DNA Repair and Demethylation $44,033/year
Apply a combination of computational and experimental methods to elucidate the catalytic mechanism and specificity of base excision repair enzymes including DNA glycosylases.

NIH R01AI123820 (Ernst, Goodlett, CoPIs) 09/01/2016-08/31/2020
Protection Against Gram-Negative Sepsis Conferred by Lipid A-Based Structural Variants
$40,000 to MacKerell Lab
Molecular modeling applied to determine structure-activity relationships of variants of Lipid A with the goal of designing novel therapeutics for the treatment of sepsis.

NIH R21 NS096620-01 (Smith) 09/01/16-08/31/18
LRRK2 dimerization and therapeutic evaluation $40,111 to UMB
Johns Hopkins University
Computer-aided drug design (CADD) database screening will be performed targeting the crystal structure of LRRK2 to identify compounds with a high probability of having biological activity including inhibition of LRRK2 GTP binding and dimerization activities.

F32 GM109632 (Lemkul) 3/1/14-2/28/17
NIH/NIGMS Postdoctoral Fellowship $159,906 Total Costs
Exploring RNA Folding and Dynamics Using a Polarizable Force Field
Mentor: MacKerell

NIH/NCI R01 CA107331 (Weber) 07/01/06-4/30/16
$5,260,578 Total Costs, $925,180 Total Costs to ADM and AC
Restoration of Tumor Suppression Activity in Malignant Melanoma
To synthesize new compounds that bind S100B at nM concentrations and restore p53 activity in malignant melanoma.
CoI: MacKerell, Coop

0314-009 (DeLeeuw)
Maryland Technology Development Corporation 06/13/14-03/12/15
Lead optimization of Defensin Mimetics as Novel Antibiotics targeting Lipid II

N/A (Xue) 07/01/14-06/30/15
Leukemia Research Foundation $100,000
Small molecule BCL6 inhibitors for diffuse large B-cell lymphoma (DLBCL)
The objective of this proposal is to design and synthesize inhibitors targeting the BCL6 BTB domain with improved potency and drug-like characteristics for the treatment of DLBCL.

Melnick-Janssen06102014 (MacKerell) 07/01/14-06/30/15
Weill Medical College Subcontract/Janssen Biotech (Prime) $80,000 Direct
Structural biology of BCL-6 Small Molecule Inhibitors
The project will involve molecular modeling and dynamics studies of BCL6-inhibitor interactions, including SILCS simulations, in order to predict chemical modifications of the inhibitors to improve their biological efficacy.

NIH/NIAID R01 AI080968-01 (Andrade) 07/15/09-06/30/13
Temple University - no cost extension
$278,795 Total Costs – to ADM
Discovery of Novel Macrolide Antibodies
Optimization of erythromycin analogs to minimize bacterial resistance.
CoI: MacKerell

R01 DA013581 and DA013583 (Coop) 02/01/01-01/31/13
NIH-NIDA no cost extension
$2,283,650 Total Costs
Opioids with Delta Antagonist and Mu Agonist Activity
Determine structure-function relationships of opioid analogs
CoI; MacKerell, Wang

NIH/NIMH R21 MH092940 (Wang) 07/21/11-6/30/13

$412,500 Total Costs
Exploring the role of HINT1 protein in neuronal function
To identify and characterize novel low molecular weight inhibitors of the HINT1 protein
CoI: MacKerell

F32 GM090669 (Ringer) 12/1/09-11/31/12
NIH/NIGMS Postdoctoral Fellowship
$144,462 Total Costs
Validating polarizability models in macromolecular force fields: The Stark Effect
Mentor: MacKerell

NIH R21 HL082670 (MacKerell) 07/01/07 – 06/30/09
Case Western Reserve University (Subcontract with Prof. C.K., Qu)
$250,000 direct costs, $115,000 direct costs to ADM
"SHP-2 Inhibitors as Potential Therapeutic Agents for JMML and Noonan Syndrome"
Computer-aided drug design will be combined with biological assays to identify inhibitors of SHP-2 phosphatase

F32 CA119771 (Guvench) 06/1/06-05/31/09
NIH Postdoctoral Fellowship
$240,000 total costs
Development of tyrosine phosphatase SHP-2 inhibitors for leukemia therapy
Mentor

NIH/NCI R01 CA120215 (Shapiro) 04/01/06 – 03/31/11
$1,000,000 total costs, $325,000 direct costs to ADM
Substrate Specific ERK docking Domain inhibitors
The goal of this project is to identify through computer modeling low molecular weight inhibitors that disrupt ERK interactions with substrate proteins involved in cell proliferation. The efficacy of these inhibitors will be tested in vitro, cell based, and animal assays.
CoI; MacKerell

NIH/NIDDK R01 DK067530 (Polli) 09/10/05 – 08/31/10
$1,000,000 total costs, $200,000 direct costs to ADM
Substrate requirements of the bile acid transporter
The substrate requirements for the human apical sodium-dependent bile acid transporter will be determined.
CoI; MacKerell, Coop

NIH/NCI R21 CA 10529-01 (Shapiro) 2004 – 2006
$270,000 total costs, $100,000 direct costs to ADM
Development of ERK docking domain inhibitors
CoI; MacKerell

Tobacco Related Diseases Research Grant (Shapiro) 2005-2006
Greenebaum Cancer Center/State of Maryland

$50,000 total direct costs, $5000 direct costs to ADM
Development of novel MAP Kinase inhibitors to inhibit airway smooth muscle cell proliferation associated with asthma
CoI; MacKerell

NIH R21CA95350-01 (Passaniti) 2002-2004
$300,000 direct costs, $50,000 to ADM
Runx-specific angiogenesis inhibitors
CoI: MacKerell

Congressionally Directed Medical Research Program (CDMRP) (Srivistava)2002-2003
$222,750 total costs
Development of Novel Death Receptor-5 Binding Molecules

NIH/NCI R21CA91240-01 (Sussman) 2000-2002
$300,000 total costs
High - Throughput Assay Targeting β-Catenin and TCF

DoD Concept Award (Serrero) 2000-2001
$50,000 direct costs, $15,000 direct costs to ADM
Identification of PC-Cell Derived Growth Factor antagonists that inhibit breast cancer tumorigenesis via computer-aided rational drug design

NIH/NIDA R01 DA 05195 (Aldrich) 1998-2001
$500,000 direct costs, $15,000 direct costs to ADM
Dynphorin Analogs as Kappa Opioid Receptor Antagonists

Swedish Natural Science Research Council (Uvdal, Lund Univ. Sweden) 1995-1997
576,000 Swedish Krona (approx. $81,000 US); 0 costs to ADM (free trips to Sweden!)
Absorption and Reaction of Organic Compounds on Solid Surfaces

S10 NCRR-BRS (Weber, UM Medicine) 1995
NIH Shared Instrumentation Grant for a 600 MHz NMR Spectrometer"
NIH $400,000
CoI, MacKerell, Guiles others

Computational Grants

ACCESS (formally XSEDE)/National Resource Allocations Committee/National Partnership Alliance for Computing Infrastructure 1993 to present
Support renewed on an annual basis.
~2,000,000 CPU hours/year
"Atomic detail investigations of the structural and dynamic properties of biological systems."

DoD High-Performance Computing Modernization Plan 1998 to 2012

Support renewed on an annual basis. All computing resources to ADM with DoD acting PIs; Lee, Kim, Deschamps
~500,000 CPU Hrs/year
"Molecular Dynamics Simulations of the Inter- and Intramolecular Forces"

National Cancer Institute Supercomputing Facility 1995 – 2000, 2005 - 2009
Support renewed on an annual basis from 1995 – 2000 and support restarted in 2005.
"Antiviral Nucleosides: Free energies of solvation and conformational contributions to biological efficacy"
Current allocation is unlimited

Creative Endeavors

Contributor, American Chemical Society Careers Office: "Chemical Careers in Brief" 1994, American Chemical Society. Was interviewed and one page description of my scientific background, including quotes, was prepared for distribution to high school students to motivate them to consider careers in chemistry.

Designer "Making Your Own Medicines" video game as part of the Medicines: The Inside Story Museum Exhibit, 1996. The game allowed non-scientific users to actively alter a drug structures and see how that would change its biological activity. The game was included as part of a CDROM distributed by the Medicines: The Inside Story organization.

Subject of an American Chemical Society Education Division Careers in Chemistry Video (A video aimed at providing college chemistry students with a sampling of career profiles), 1997. IV Teaching

Teaching and Mentoring

Courses taught and managed

Drugs and Biologics Discovery. REG614
Course manager
6 credit on line course part of the Masters in Regulatory Sciences programs
~40 students
2017 to present

Medicinal Chemistry I, PHAR 533
2 credits
90 - 160 students
Course manager: MacKerell (2010 to 2013) and Xue (11 to 15 lectures)
2010 to present

Pharmaceutical Chemistry, PHAR 531
2-3 credits

120 students
Course manager: MacKerell (30 lectures)
1993 to 2010

Principle of Drug Design and Development, PHAR 600
3 credits
~15 students
Manager of module 2, 1995 to 2007
Course manager: 2008 to present
7 lectures
1995 to present

Drug Design, PHAR 751
3 credits
~5 students
Course manager: MacKerell (8 lectures)
1994 to ~2010

Biochemistry, PHAR511
3 credits
120 students
Course manager: Michel (MacKerell, 3 to 8 lectures)
1993 to present

Advanced Educational Opportunities, PHMY 510
1 credit
~25 students
Course manager: Luo, Shen (MacKerell, 1 lecture)
1996 to 2001

Pharmacy Practice and Education, PHAR516
2 credit
~15 students
Coursemaster: Anderson (MacKerell, 1 lecture)
1995 to 2005

Principles of Pharmaceutical Sciences, PHNT 512
3 credits
~25 students
Course manager: Weiner (MacKerell, 1 lecture)
1996 to 2001

Recent Advances in Pharmacology, PHMY551
1 credit
~5 students
Course manager: Shen (MacKerell, 2 lectures)

1995 to present

Biological Chemistry, Swarthmore College, CHEM 38
3 credits
~75 students
Course manager: MacKerell (all lectures)
1992-1993

Organic Chemistry Laboratories, Swarthmore College
Course manager: Paley (MacKerell 15 laboratory introductory lectures)
1992-1993

Advanced Biochemistry Seminar, Swarthmore College, CHEM 108b
1 Credits
~15 students
Course manager: MacKerell
Course involved student presentations and discussions.
1992-1993

New Courses and Teaching Methods Devised and Instituted

Pharmaceutical Chemistry, PHAR531
1993
Developed entire course as part of all Pharm.D. curriculum. Course content was developed to facilitate the transition from the basic science chemistry courses (i.e. Biochemistry, Drug Chemistry, Physical Chemistry) to the pharmacologically related science courses (e.g. Principles of Drug Action, Pharmacology, Medicinal Chemistry). Efforts included development of computer-based laboratories designed to facilitate understanding of drug structure to function. These efforts have resulted in the following publications.

MacKerell, A.D., Jr. "A Computer Laboratory Exercise to Aid in the Instruction of Drug-Receptor Interactions" Contribution to the AACP Section of Teachers of Chemistry "1994-1995 Task Force on Teaching Problem Solving in Medicinal/Natural Products Chemistry Courses Final Report."

Coop, A. and MacKerell, A.D., Jr. "The Future of Opioid Analgesics" **American Journal of Pharmaceutical Education**, 2002, 66, 153-156

Principle of Drug Design and Development, PHAR600
1995
Collaborated with Drs. Eddington and Moreton to design the flagship course for the Department of Pharmaceutical Sciences Graduate Program. Emphasis placed on broad exposure to all aspects of pharmaceutical sciences, allowing graduates of our program to be able to interpret results from and collaborate with scientists not in their area of specialization.

Drug Design, PHAR 751

1994
Restructured the graduate program Drug Design course, including conversion from a 2 semester to a 1 semester course. Emphasis included presentation of methods followed by reviews of scientific literature that employed the respective methods. Instituted a grant writing project for the students to facilitate their writing abilities, with emphasis on peer review.

Doctoral/Masters Students

1. Daxu Yin
Parametrization for Empirical Force Field Calculations & A Theoretical Study of Membrane Permeability of Pyridine Derivatives
Ph.D., 1998

2. I-Jen Chen
Computational Investigation of Molecular Interactions and Its Application to Drug Design
Ph.D., 2001

3. Nilesh Banavali
Theoretical Studies of DNA and modified DNA analogs
Ph.D., 2001

4. Niu Huang
Computational Chemistry in Structural Biology and Drug Design
Ph.D., 2003

5. Denzil Bernard
Computational Studies of δ-opioid receptor ligands: Development of the Conformationally Sampled Pharmacophore (CSP) Method
Ph.D., 2006

6. Carlos Ramirez-Mondragon, Non-thesis M.S., 2008

7. Chayan Acharya
3D QSAR Study to Improve Intestinal Absorption of Oral Drug Candidates via Ligand-based Drug Design: Use and Relevance of Conformationally Sampled Pharmacophore Approach
Ph.D., 2009

8. Xiao Zhu
Development of Additive and Polarizable Force Field Parameters for Polypeptides
Ph.D., 2012

9. Jihyun Shim
The use of conformational sampling in CHARMM protein force field optimization and ligand-based drug design
Ph.D., 2013

10. Meagan Small
Molecular Modelling of Macrolide Antibiotic Conformational Sampling and Interactions in the 50S Ribosomal Subunit for the Development of Novel Antibiotics
Ph.D., 2015

11. Fang-Yu Lin
Development of the Drude Polarizable Force Field for Molecular Dynamics Simulation
Ph.D., 2019

12. Payal Chatterjee
Development of the Lennard-Jones Parameters for the Polarizable Classical Drude Oscillator Force Field
Ph.D, 2022

Current graduate students:
Suliman Sharif

Postdoctoral Fellows

1. Dr. Riad Manaa, 1996
2. Dr. Nicolas Foloppe, 1997-1999
3. Dr. Susil Silva, 1998-2000
4. Dr. Moushine Tazi, 2001-2002
5. Dr. Seung Choi, 2002
6. Dr. Yongping Pan, 2001-2003
7. Dr. Alba Macias, 2002-2005
8. Dr. Igor Vorobyov, 2003-2007
9. Dr. Victor Anisimov, 2003-2008
10. Dr. Sabsinkar Kundu, 2004-2005
11. Dr. Pedro Lopes, 2004-2008
12. Dr. Deva Priyakumar, 2004-2008
13. Dr. Shijun Zhong, 2004-2011
14. Dr. Olgun Guvench, 2005-2009
15. Dr. Shannon Greene, 2005-2006
16. Dr. Ganesh Kamath, 2006-2008
17. Dr. Kenno Vanommeslaeghe, 2006-2011
18. Dr. Elizabeth Hatcher, 2007-2010
19. Dr. Eva Darien, 2008-2011
20. Dr. Taiji Oashi, 2008-2011
21. Dr. Chris Baker, 2008-2011
22. Dr. Prabhu Raman, 2008-2015
23. Dr. Ashley Ringer, 2009-2011
24. Dr. Sairam S. Mallajosyula, 2009-2013
25. Dr. Wenbo Yu, 2009-2016
26. Dr. Elizabeth Denning, 2010-2013
27. Dr. Xibing He, 2010-2013

28. Dr. Randy Bin Lin, 2011-2013
29. Dr. Shanthi Nagarajan, 2011-2012
30. Dr. Sirish Kaushik Lakkaraju, 2011-2018
31. Dr. Arghya Barman, 2012-2013
32. Dr. Dhilon S. Patel, 2012-2014
33. Dr. Alexey Savelyev, 2012-2015
34. Dr. Jing Huang, 2012-2017
35. Dr. Igancio Soteras Gutiérrez, 2012-2015
36. Dr. Justin Lemkul, 2013-2017
37. Dr. Lei Fang, 2013-2015
38. Dr. Ming-Jun Yang 2013-2016
39. Dr. Madhurima Jana 2013-2014
40. Dr. Asaminew H. Aytenfisu 2015-2021
41. Dr. Goutam Mukherjee, 2016
42. Dr. Yunxiang Sun, 2016
43. Dr. Delin Sun, 2016-2017
44. Dr. Ozge Yulok, 2017-2019
45. Dr. Wenjuan Jiang, 2017
46. Dr. Sreya Mukerjee, 2017-2018
47. Dr. Shalini Aswathi, 2017
48. Dr. Anmol Kumar, 2017-present
49. Dr. Abhishek Kognole, 2017-2022
50. Dr. Christoffer Lind, 2018-2021
51. Dr. Himanshu Goal, 2018-2022
52. Dr. Gene Chong, 2019-2021
53. Dr. Poonam Pandey, 2019-2021
54. Dr. Anthony Hazel, 2019-2021
55. Dr. Mert Sengul, 2020-2022
56. Dr. Mingtian Zhao, 2020-present
57. Dr. Asuka Orr, 2021-present
58. Dr. Yiling Nan, 2022-present
59. Dr. Negar Parvizi, 2022
60. Dr. Prabin Baril, 2022-present
61. Dr. Shashi Kumar, 2022-present
62. Dr. Anastasia Croitoru, 2023-present
63. Dr. Erik Nordquist

Research Associates

Dr. Pedro Lopes, 2008-2011
Dr. Kenno Vanommeslaeghe, 2011-2015

Research Assistant Professors

Dr. Pedro Lopes, 2011-2014
Dr. Wenbo Yu, 2016-present

Faculty Mentored

Dr. Angela Wilks (tenured, 2003)
Dr. Andrew Coop (tenured, 2003)
Dr. Adrian Batchelor
Dr. Michael Shapiro
Dr. Steven Fletcher (tenured, 2016)
Dr. Wanli Smith
Dr. Fengtian Xue (tenured, 2018)
Dr. Ian Thorpe (UMBC)
Dr. Jana Shen (Full Professor, 2019)
Dr. Bruce Yu (Full Professor, 2015)
Dr. Saif Hasan (IBBR)
Dr. Ryan Pearson
Dr. Daniel Deredge

Visiting Scientists

Dr. Daniel Barsky, Lawrence Livermore National Laboratory, 1997
Dr Carmen Domene, Physical and Theoretical Chemistry Laboratory, University of Oxford, 2010, 2011
Dr. Jutarat Pimthon, Faculty of Pharmacy, Mahidol University, Bangkok, Thailand, 2012
Mr. Eliot Boulanger, Ph.D. Student, Prof. Walter Thiel, Max-Planck-Institut für Kohlenforschung, 2012.
Prof. Atef Abdelmonem Abdelhafez, Professor of Medicinal Chemistry, Assiut University, Assuit, Egypt; 2014-2015
Mr. You Xu, Ph.D. student, Prof. Lennart Nilsson, Karolinska Insitutet, Stockholm, Sweden, 2015
Ting Ran, Ph.D. student, China Pharmaceutical University, 1 year student internship, 2015-2016
Yue Zhou, Ph.D. student, Beijing University of Technology, College: Life science and Bio-engineering, 1 year student internship, 2015-2016
Dr. Aparoy Polamarasetty, 2016-2017, Visiting Faculty, "Raman Fellowship for Postdoctoral Research for Indian Scholars in United States of America," Centre for Computational Biology and Bioinformatics, School of Life Sciences, Central University of Himachal Pradesh
Poonam Pandy, Ph.D. student, 2017, Indian Institute of Technology Gandhinagar
Dr. Tatsuya Takimoto, 2018-2019, Visiting Faculty, Faculty of Pharmaceutical Sciences Kobe Gakuin University, Japan
Esther Heid, Ph.D. student, 2018, University of Vienna
Prof. Bryan Kolaczkowski, 2019, Sabbatical, Molecular and Cellular Biology University of Florida, Gainseville.

Dr. Miroslava Nedyalkova, 2019-2020, Fulbright Fellow, Sofia University, Bulgaria.

Graduate Students Supervised/Thesis committee participant)

Name	Degree Sought	Major Res advisor	Advanced to Candidacy	Thesis Defended
1) Biao Yang	Ph.D.	Wright	y	y
2) Yanglong Li	Ph.D.	Callery	y	y
3) Chunhua Yan	Ph.D.	Guiles	y	y
4) Deepa Meehta	Ph.D.	Guiles	y	y
5) Daxu Yin	Ph.D.	MacKerell	y	y
6) Faye Rogers	Ph.D.	Callery	y	y
7) I-Jen Chen	Ph.D.	MacKerell	y	y
8) Vasanthakumar Rajappan (UMBC, Dept. of Chemistry and Biochemistry)	Ph.D.	Hosmane	y	y
9) Bindi Dangi	Ph.D.	Guiles	y	y
10) Brita Schulze (Univ. of Miami, Dept of Chemistry)	Ph.D.	Evanseck	y	y
11) Niu Huang	Ph.D.	MacKerell	y	y
12) Rajneesh Taneja	Ph.D.	Polli	y	y
13) Balvinder Vig	Ph.D.	Aldrich	y	y
14) Chris Sasiela	Ph.D.	Aldrich	y	y
15) Nilesh Banavali	Ph.D.	MacKerell	y	y
16) Nazim Shahzad	Ph.D.	Guiles	y	y
17) Alba Macias (Univ. of Miami, Dept of Chemistry)	Ph.D.	Evanseck	y	y
18) Rahul Desmuhk	Ph.D.	Wilks	y	y
19) Kshitij Patkar	Ph.D.	Aldrich	y	y
20) Michelle Kuttel (University of Cape Town, South Africa)	Ph.D.	Naidoo	y	y
21) Lanxuan Doan (UMBC, Dept. of Chemistry and Biochemistry)	Ph.D.	Whalen	y	y
22) Denzil Bernard	Ph.D.	MacKerell	y	y
23) Meng Qiao	Ph.D.	Passaniti	y	y
24) Linn Thatcher	Ph.D.	Coop	y	y
25) Matt Metcalf	Ph.D.	Coop	y	y
26) Lena Bockrath	Ph.D.	Wilks	y	y
27) Pablo Gonzalez	Ph.D.	Polli	y	y
28) Kim Burkhard	Ph.D.	Wilks	y	y
29) Chris Cunningham	Ph.D.	Coop	y	y
30) Trudy Smith	Ph.D.	Coop	y	y
31) Fengming Chen	Ph.D.	Shapiro	y	y
32) Chayan Acharya	Ph.D.	MacKerell	y	y
33) Marilyn Matthews	Ph.D.	Coop	y	y
34) Rahul Desmuck	Ph.D.	Shapiro	y	y
35) Carlos Ramirez	Ph.D.	MacKerell	n	n: Non-thesis MS, 2008

36) Torben Brömstrep (University of Bergen, Norway, Thesis opponent)				
	Ph.D.	Reuter	y	y
37) Abby West	Ph.D.	Wilks	y	y
38) Ji Hyun Shim	Ph.D.	MacKerell	y	y
39) Xiao Zhu	Ph.D.	MacKerell	y	y
40) Laura Dosangh	Ph.D.	Luo	y	y
41) Rana Rais	Ph.D.	Polli	y	y
42) Sarice Smith	Ph.D.	Shapiro	y	y
43) Lidiya Stavitskaya	Ph.D.	Coop	y	y
44) Maura J. O Neill	Ph.D.	Wilks	y	y
45) Katherine Joyner	Ph.D.	Yu	y	y
46) Jeremy Yang	Ph.D.	Fletcher	y	y
47) Jun Zhang	Ph.D.	Shapiro	y	y
48) Meagan Small	Ph.D.	MacKerell	y	y
49) Jodian Brown (UMBC, Dept. of Chemistry and Biochemistry)				
	Ph.D.	Thorpe	y	y
50) Rachita Rao	Ph.D.	Xue	n	n: Non-thesis MS, 2015
51) Maryanna Lanning	Ph.D.	Fletcher	y	y
52) Shivangi Awasthi	Ph.D.	Goodlett	y	y
53) Matt Welch	Ph.D.	Swaan	y	
54) Zhi (Shane) Yue	Ph.D	Shen	y	y
55) Fang-Yu Lin	Ph.D.	MacKerell	y	y
56) Cheng-Chuih Tsai	Ph.D.	Shen	y	y
57) Tyler Gable (UMB Dental School)				
	Ph.D.	Mao	y	y
58) Ivie Conlon	Ph.D.	Fletcher	y	y
59) Chad Johnson	Ph.D.	Coop	y	y
60) Christoffer Lind (Uppsala University, Sweden, Thesis opponent)				
	Ph.D.	Åqvist	y	y
61) Payal Chatterjee	Ph.D.	MacKerell	y	
62) Jack Henderson	Ph.D.	Shen	y	y
63) Garrick Centola	Ph.D.	Xue/Wilks	y	y
64) Peter Merkel	Ph.D.	Yu	n	n: Non-thesis MS, 2019
65) Blaine J. Dow (UMB School of Medicine)				
	Ph.D.	Drohat	y	y
66) Kyle Kihn	Ph.D	Wintrode/Deredge	y	y
67) Benjamin M. Diethelm Varela				
	Ph.D	Xue	y	n: Non-thesis MS, 2021
68) Alexandria Chan	Ph.D	Fletcher	y	
69) Suliman Sarif	Ph.D.	MacKerell	y	
70) Ryan Lazar (University of South Africa, External thesis evaluation)				
	M.S.	Kuttel	y	y
71) Aarion Romany	Ph.D.	Shen	y	

Pharm.D., Undergraduate, and High School Students

The following students performed significant research projects in my laboratory beyond laboratory rotations.

Spencer Lieske (SoP, Pharm.D. student)
First author on a Journal of Medicinal Chemistry paper

Dr. Aleksandra Gelman (now Besselman) (SoP Pharm.D. student)
Poster presented with Dr. Besselman as coauthor
Coauthor on a Journal of Organic Chemistry paper

Dr. Sam Cho (Univ. of Maryland Baltimore County undergraduate student)
Coauthor on three published papers (Journal of Biomolecular Structure and Dynamics and Journal of Chemical Information and Computer Science)

Dr. Bahru Habtemariam (SoP Pharm.D. student)
First author publication, Nucleic Acids research

Xiao Zhu (University of Montreal undergraduate student)
Work included CADD studies leading to the current Waxman foundation grant. Currently a graduate student in my laboratory following completion of his B.S. and M.S. degrees from the University of Montreal

Muhammad Saad Noon (B.S. Bioinformatics)
Lab assistant working on molecular simulations of RUNT transcription factor-DNA interactions, Thymidine Glycoylase and hydrogel forming peptides. Coauthor on a paper in the Proceedings of the National Academy of Sciences, USA.

Sherry Chen (SoP Pharm.D. student)
Empirical force field parametrization and computer-aided drug design

Frank Horrigan (Math, Science, Computer science magnet program at Poolsville High School)
Empirical force field development including development of machine learning models

Sevien Schulhoff (Friends School of Baltimore, High School Senior)
Empirical force field development of a perfluoroalcohol

Service

Committee Service

Departmental

Molecular Modeling Committee — Chair, 1993-2000
BMCH Graduate Program Unification Steering Committee — Chair, 1994

Immunology Faculty Search Committee	Chair, 1994-1995
Pharmaceutics Solids Faculty Search Committee	Member, 1995-1996
Department Chairperson Search Committees (2nd and 3rd searches)	Member, 1997 and 1998
Drug Design Research Focus Group	Chair, 1999-2001
Biochemistry Faculty Search Committee	Chair, 2001
Tenure Review, Teaching Peer Review Committee, Angela Wilks	Member, 2002-2003
Cellular and Biological Chemistry Division	Chair, 2003-2006
Pharmaceutical Science Department Executive Council	Member, 2003-2006
	2008 to 2011
Chemistry Faculty Search	Member, 2007-2009
Nanotechnology Research Faculty Search	Member, 2015
CADD Research Faculty Search	Chair, 2016
PSC Leadership Group	2020
Mass Spectrometry Faculty Search	Chair, 2020-2021
KUDOS (Awards) Committee	2023

School of Pharmacy

School Yearbook (Terra Mariae)	Faculty Advisor; 1993 to present
Computer Informatics Search Committee	Member, 1995
Computer Advisory Group	Member, 1995-2000
Student Affairs Committee	Member, 1996-2000
Admission Committee	Member, 1993-1996
	Chair, 2002-2004
	Member, 2006-2008
Fire Warden	1998 to present
Accreditation Curriculum Committee	Member, 2000
Faculty Retreat Organizing Committee	Member, 2001
5-year Post-tenure Review of Myron Weiner	Chair, 2001
Graduate Studies and Research Committee	Chair, 2004-2005
	Member, 2008-2010
Strategic Initiative	Member, 2004-2006
5-Year Post-tenure Review of Hamid Ghandehari	Chair, 2006
5-Year Post-tenure Review of Gary Buterbaugh	Chair, 2007
5-Year Post-tenure Review of Bruce Stuart	Member, 2009
Tenure Review of Sarah Michel	Chair, 2010
Faculty Affairs Committee	2009-2011
Chair	2010-2011
Promotion Review of Bruce Yu	Chair, 2011
5-Year Post-tenure Review of Angela Wilks	Member, 2012
Tenure Review of Patrick Wintrode	Chair, 2012
Promotion Review of Bruce Yu	Chair, 2013
Tenure Review of Steven Fletcher	Chair, 2015
Assessment Committee	2016-2022
Incentive Evaluation Committee	2020

University

Greenebaum Cancer Center, Drug Discovery Working Group	Chair, 2002-2006
Scientific Review Board, Office of Research and Development	Member, 2002-present
UMB Conflict of Interest Committee	Member, 2007-present
Center for Biomolecular Therapeutics Advisory Board	Member, 2012-present
Research Computing Committee	Member, 2011-present

National

Computer-Aided Drug Design (CADD) Center, University of Maryland, Baltimore, School of Pharmacy: Director 2002–present

The CADD center is the first organized research center in the Department of Pharmaceutical Sciences. It is an organization designed to foster collaboration between biological scientists with scientists in computational chemistry, synthetic chemistry and structural biology on a local, national and international level. It should be noted that CADD Center related activities started in 1998, although it did not become an official center until 2002.

Multiple academic and industrial promotion reviews.

Pittsburgh Supercomputing Center Workshop on Molecular Modeling, 1995, 1997 and 1999. Lecturer for a workshop in the background and application of molecular modeling methods to biological systems. The workshop is open to both academic and industrial participants.

MMTSB Workshop on Molecular Modeling, 2006, The Scripps Research Institute, La Jolla, Ca. Workshop lecturer and the development and application of force fields to molecules of biological interest.

Grant Reviewing

Research Corporation, *ad hoc* reviewer (1995, 1997)
NSF *ad hoc* reviewer (2 to 5 reviews annually, 1994-present)
Pittsburgh Supercomputing Center, *ad hoc* reviewer, 1995, 1996
Cornell Supercomputing Center, *ad hoc* reviewer, 1996
Lawrence Livermore National Laboratory, Material Research Institute, University Collaborative Research Program, *ad hoc* reviewer (1999, 2000)
American Chemical Society Petroleum Research Foundation, *ad hoc* reviewer (2000, 2001, 2003, 2005)

NIH Study Section Permanent member, MSFB, 2006 to 2010 (Attended 12 committee meetings)
NIH *ad hoc* review committees
Physical Biochemistry (1999)
Research Resource Site Visit (2000)
Postdoctoral Fellowships (2001)
BBCA (Molecular and Cellular Biophysics) (2003)

Special Emphasis Panel/ ZRG1 BMBI: Biomaterials and Biointerfaces (2004)
Special Emphasis Panel/ ZRG1 MABS (2004)
MSFB (Molecular Structure and Function), ad hoc (2005)
Special Emphasis Panel/ZRG1 BCMB-P (2011)
P01 review (2012)
MSFD (2013)
ZRG1/BCMB-B (2013)
ZRG1/IMST Small Business Review (2013)
NIH Director's New Innovator Award Program (DP2) Panel (2015)
NIH Director's New Innovator Award Program (DP2) Panel (2016)
Special Emphasis Panel/ ZRG1 (2016)
NIH XO2 (2016)
NIH Director's New Innovator Award Program (DP2) Panel (2017)
Special Emphasis Panel for the review of 12 RM1 grant applications (2018)

S06 proposal for Florida A&M University (2006)
NSF *ad hoc* reviewer, 1 to 5 proposals annually since 2002
American Chemical Society Computational Chemistry Section Chemical Computing Group's Excellence Awards, 2 to 5 proposals annually since 2006

Lawrence Livermore National Laboratory, Biotechnology and Biology Research Program (BBRP) Directorate Review Committee
Member, 2002 – 2005

National Resource for Biomedical Supercomputing Research Resource
Pittsburgh Supercomputing Center
Advisory Board Member, 2008 to 2012, Chair, 2011

Biogeochemical and Molecular Mechanisms Controlling Contaminant Transformation in the Environment, Environmental Sciences Division
Oak Ridge National Laboratory
Advisory Board Member, 2011 to 2019

Fellowship reviews: American Chemical Society Computational Chemistry Division, Annually, 2012 to present

University of Delaware NIH COBRE Executive Advisory Committee, 2016

University of Kansas NIH COBRE Executive Advisory Committee, "Chemical Biology for Infectious Diseases" 2016-present

Grant Review: Blue Waters, 2018
Grant Review: RESEARCH CORPORATION FOR SCIENCE ADVANCEMENT, 2020

<u>International</u>

Grant Review, Swiss Federal Institute of Technology Grant Review, Zurich, Switzerland, 2000
Grant Review, Civilian Research And Development Foundation for the Independent States of the Former Soviet Union, 2003

National Hellenic Research Foundation, European Young Investigator Award (2004)

International Society of Quantum Biology and Pharmacology (ISQBP)
Vice President: 2003-2004
President: 2005-2006: Duties include overseeing ISQBP function and organization of the semiannual ISQBP President's meeting: http://isqbp.umaryland.edu/ISQBP/
Advisor Board and Web-page management 2006- present

Grant Review, Netherlands, Chemische Wetenschappen, 2007

Workshop lecturer: CERMM (Centre de recherché en modélisation moléculaire/PROTEO Workshop "CHARMM: Chemistry at HARvard Molecular Mechanics," Concordia University, Montreal, Canada, March 2010. Lecture on "CGenFF: The CHARMM General Force Field.

Grant Review, Italy, 2010

Workshop lecturer: Series of 7 lectures as part of the MOLECULAR DYNAMICS SIMULATIONS & MOLECULAR DOCKIING STUDIES Workshop, Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Mahidol University, Bangkok, Thailand, January, 2011.

Grant Review, European Research Council, 2012
Grant Review, Czech Science Foundation, 2012
Grant Review, Poland, National Research Foundation, 2013
Grant Review, Deutsche Forschungsgemeinschaft (German Research Foundation), 2013
Grant Review, Swiss National Research Foundation, 2013
Grant Review, European Union, LinkSCEEM/Cy-Tera Production 2013
Grant Review, Singapore, A*STAR, Agency for Science, Technology and Resarch, 2014
Grant Review, Swiss National Research Foundation, 2014
Grant Review, Chile, Fondo Nacional de Desarrollo Científico y Tecnológico (FONDECYT), 2015
Grant Review, Denmark BRAINSTRUC: Complex Structural Aspects of Signaling, Inflammation and Disease in the Brain, 2016
Grant Review, Marsden Fund, New Zealand, 2016
Grant Review, Israel Science Foundation, 2017
Grant Review, Netherlands Organization for Scientific Research, 2017
Grant Review, Deutsche Forschungsgemeinschaft (German Research Foundation), 2016, 2018
Grant Review, Swiss National Research Foundation, 2016, 2017, 2020, 2021
Grant Review, Czech Science Foundation, 2019
Grant Review, Agence nationale de la recherche, France, 2019, 2021

Session Chair or Symposium or Meeting Organizer

Organizer and Session Chair, Computational Chemistry Symposium on Molecular Modeling Using Empirical Force Fields, Atlantic Regional Meeting of the Americal Chemical Society, Univeristy of Maryland Baltimore County, MD. 1994.

Organizer, Molecular Modeling: Applications in the Pharmaceutical Industry. Conference sponsored by Advanstar Communications, New Brunswick, NJ. 1994

Session Chair, Computational Chemistry Symposium on Molecular Mechanics parameters and parameterization, American Chemical Society 216th National Meeting, Boston, MA, August 1998

Session Chair, Structure and Dynamics of Nucleic Acids, Biophysical Society 44th Annual Meeting, New Orleans, LA, February, 2000

Session Chair, Computational Chemistry Symposium on Current Status of Molecular Force Fields; Beyond Conventional Molecular Mechanics, American Chemical Society National Meeting, Washington, DC August 2000.

Session Organizer and Chair, "More Than Intuition – Theoretical Analysis of Structure in Understanding Function," Diffraction Methods In Structural Biology, Gordon Research Conference, New London, CT, July 2002

Session Chair, "Carbohydrate Modeling," Quantum Theory Project 43rd Sanibel Symposium, University of Florida, St. Augustine, Fl, February, 2003.

Session Organizer and Chair, 7th Congress of the World Association of Theoretically Oriented Chemists (WATOC), Cape Town, South Africa, January 2005.

Organizer "2006 International Society of Quantum Biology and Pharmacology (ISQBP) President's Meeting" Strausborg, France, July 2006

Session Chair, "Measures of Accuracy and Reliability in Molecular Simulation: Force Fields/Simulation Methods" 233rd American Chemical Society National Meeting, Chicago, Illinois, USA, Session Chair, March 2007

Organizer "Annual CHARMM Developers Meeting," School of Pharmacy, University of Maryland, Baltimore, July 2007.

Session Chair, "Pharma/Biotechnology Session" Accelrys Science Forum, Cambridge, MA, USA, October 2007

Organizer "Computer-Aided Drug Design Forum," School of Pharmacy, University of Maryland, Baltimore, June, 2008.

Session Chair, "Advances in the Implementation of Polarizable Force Fields for Molecular Simulations," Center Européen de Calcul Atomique et Moléculaire, CECAM-HQ-EPFL, Lausanne, Switzerland, June 2010.

Organizer "Computer-Aided Drug Design Symposium," School of Pharmacy, University of Maryland, Baltimore, June, 2010.

Session Chair, International Society for Quantum Biology and Pharmacology President's Meeting, Cetraro, Italy, June 2010.

Organizer, "Computational Biosciences" Mid-Atlantic Regional Meeting (MARM) of the American Chemical Society, University of Maryland Baltimore County, Maryland, May 2012.

Organizer, "Computer-Aided Drug Design Symposium," School of Pharmacy, University of Maryland, Baltimore, June 2012.

Organizer, "Workshop on Polarizable Force Fields from Biomacromolecules," 58th Annual Meeting of the Biophysical Society, San Fransisco, CA, USA, February 2014.
Organizer, "Computer-Aided Drug Design Symposium," School of Pharmacy, University of Maryland, Baltimore, June 2014.
Organizer, "Computer-Aided Drug Design Symposium," School of Pharmacy, University of Maryland, Baltimore, May 2016.
Session Chair, International Society for Quantum Biology and Pharmacology President's Meeting, Bergen, Norway, June 2016.
Session Chair (Presider), 252nd American Chemical Society National Meeting, Physical Chemistry Section, Advanced Potential Energy Surfaces, Classical Simulation Methods and Software, Philadelphia, PA, August 21, 2016.
International Advisory Board Member, Drug Discovery and Therapy World Congress 2017 and Global Biotechnology Congress 2017 (10th – 13th July, 2017, Boston, USA)
Session Chair, Cancer Drug Discovery, Development and Delivery, 2nd International Cancer Study & Therapy Conference, Baltimore, MD, February 20-22, 2017.
Organizing Committee and Session Chair, International Society for Quantum Biology and Pharmacology President's Meeting, Barcelona, Spain, June 2018
Session Chair, Molecular and Structural Biology Program 2018 Annual Retreat, University of Maryland Marlene and Stewart Greenbaum Comprehensive Cancer Center, University of Maryland Baltimore, MD, USA, October 2018
Organizer and Presenter, Hands-on Project, SILCS and SSFEP approaches, 5th AEGIS Workshop, Institut Pasteur, Paris, France, November, 2018.
Organizer, "Computer-Aided Drug Design Symposium," School of Pharmacy, University of Maryland, Baltimore, May 2023

I hereby declare that details mentioned in the document are true to the best of my knowledge.
Place : Baltimore MD, USA
Date : January 24, 2024

Sincerely,

Alexander D. MacKerell Jr.