




Michael Levitt

Robert W. and Vivian K. Cahill Professor of Cancer Research

Structural Biology

 NIH Biosketch available Online

 Curriculum Vitae available Online

Bio

BIO

The world-wide COVID-19 corona virus pandemic has hijacked all our academic attention. Please see Presentations.

Is it possible to understand the molecular structure and function of proteins and nucleic acids in enough detail to make accurate predictions about structure and function? We are mounting a two-pronged attack on this problem using both molecular dynamics simulation and molecular modeling. (i) Simulation attempts to reproduce the structural, thermodynamic and dynamic properties of a macromolecule in as accurate a way as possible. Starting with simple but realistic expressions for the interactions between atoms and classical laws of motion, we calculate a trajectory that specifies the position and velocity of every atom as a function of time. The time-step between calculated structures is small at 10-15 seconds, and we need to reduce hundreds of thousands of sets of atomic coordinates into a simple coherent description. We have simulated with reasonable fidelity the measurable static and dynamic properties of the several different proteins surrounded by thousands of water molecules. Simulation at different temperatures has allowed exploration of the pathways of protein denaturation of entire proteins and small fragments of protein secondary structure (alpha-helices and beta-hairpins). Companion studies of DNA double-helix segments in solution preserve the classical double helix while still showing a wide repertoire of interesting motions. (ii) Molecular modeling attempts to build a model of a macromolecule using known three-dimensional structures and energy minimization as complementary guidelines. Specific examples of this work include the automatic modeling of antibody variable domains, the general modeling of homologous proteins and studies of DNA base-pair mismatches. Questions we are trying to answer include: How can a protein be stabilized by a single amino acid change? How does the sequence of DNA cause local variations of double-helix conformation and stability? Extensive use is made of sophisticated programming, sequence and structural data bases, and computer graphics.

ACADEMIC APPOINTMENTS

- Professor, Structural Biology
- Member, Bio-X
- Member, Wu Tsai Neurosciences Institute

ADMINISTRATIVE APPOINTMENTS

- Chair, Department of Structural Biology, (1993-2004)
- Associate Chair, Department of Structural Biology, (2005-2010)

HONORS AND AWARDS

- Nobel Prize in Chemistry, Nobel Foundation (2013)
- Member, American Academy of Arts & Sciences (2010)
- Blaise Pascal Professor of Research, Fondation de l'Ecole Normale Supérieure, Paris, France (2003-2004)

- Member, Editorial Board Proc. Natl. Acad. Sci. USA (2002)
- Member, The US National Academy of Science (2002)
- Fellow, The Royal Society (2001)
- Co-director of Program in Mathematics and Molecular Biology, Mathematics and Molecular Biology (1997-2002)
- Anniversary Prize, Federation of European Biochemical Societies (1986)
- Member, European Molecular Biology Organization. (1981)

BOARDS, ADVISORY COMMITTEES, PROFESSIONAL ORGANIZATIONS

- Member, National Academy of Sciences (2013 - present)

PROFESSIONAL EDUCATION

- PhD, Gonville and Caius College, Cambridge, Structural Biology (1971)

LINKS

- Levitt Site: <http://csb.stanford.edu/levitt/>

Research & Scholarship

CURRENT RESEARCH AND SCHOLARLY INTERESTS

I pioneered of computational biology setting up the conceptual and theoretical framework for a field that I am still actively involved in at all levels. More specifically, I still write and maintain computer programs of all types including large simulation packages and molecular graphics interfaces. I have also developed a high-level of expertise in Perl scripting, as well as in the advanced use of the Office Suite of programs (Word, Excel and PowerPoint), which is more important and rare than it may seem. My research focuses on three different but inter-related areas of research. First, we are interested in predicting the folding of a polypeptide chain into a protein with a unique native-structure with particular emphasis on how the hydrophobic forces affect the pathway. We expect hydrophobic interactions to energetically favor structure that are more native-like. In this way, the same stabilizing interactions that exist in the final folded state the search tractable. Second we are interested in predicting protein structure from sequence without regard for the process of folding. Such prediction relies on the well-established paradigms that similar protein sequences imply similar three-dimensional structures. We have focused on the hardest problem in homology modeling: the refinement of a near-native structure to make it more precisely like the actual native structure of protein. We have also focused on how the general similarity of all protein sequences resulting from their evolution from common ancestor sequence affects the nature of the protein universe. Third, we are focusing on mesoscale modeling of large macromolecular complexes such as RNA polymerase and the mammalian chaperonin. In this work, done in close collaboration with experimentalists, we use new morphing strategies combined with normal mode analysis in torsion angle space to overcome problems caused by the size and complexity of these critical, biomedically important systems. All this work depends on the way a molecular structure is represented in terms of the force-field that allows calculation of the potential energy of the system. We employ a very wide variety of such energy functions that extend from knowledge-based statistical potentials for a single interaction center per residue to quantum-mechanical force-fields that include inductive effects as well as polarization.

Teaching

GRADUATE AND FELLOWSHIP PROGRAM AFFILIATIONS

- Biomedical Data Science (Phd Program)
- Biophysics (Phd Program)
- Structural Biology (Phd Program)

Publications

PUBLICATIONS

- **Single-residue effects on the behavior of a nascent polypeptide chain inside the ribosome exit tunnel.** *bioRxiv : the preprint server for biology*
Pardo-Avila, F., Kudva, R., Levitt, M., von Heijne, G.
2024
- **Panel stacking is a threat to consensus statement validity.** *Journal of clinical epidemiology*
Kepp, K. P., Aavitsland, P., Ballin, M., Balloux, F., Baral, S., Bardosh, K., Bauchner, H., Bendavid, E., Bhopal, R., Blumstein, D. T., Boffetta, P., Bourgeois, F., Brufsky, et al
2024: 111428
- **The Determination of Free Energy of Hydration of Water Ions from First Principles.** *Journal of chemical theory and computation*
Butin, O., Pereyaslavets, L., Kamath, G., Illarionov, A., Sakipov, S., Kurnikov, I. V., Voronina, E., Ivahnenko, I., Leontyev, I., Nawrocki, G., Darkhovskiy, M., Olevanov, M., Cherniavskiy, et al
2024
- **Neural Network Corrections to Intermolecular Interaction Terms of a Molecular Force Field Capture Nuclear Quantum Effects in Calculations of Liquid Thermodynamic Properties.** *Journal of chemical theory and computation*
Kurnikov, I. V., Pereyaslavets, L., Kamath, G., Sakipov, S. N., Voronina, E., Butin, O., Illarionov, A., Leontyev, I., Nawrocki, G., Darkhovskiy, M., Olevanov, M., Ivahnenko, I., Chen, et al
2024
- **Combining Force Fields and Neural Networks for an Accurate Representation of Bonded Interactions.** *The journal of physical chemistry. A*
Kamath, G., Illarionov, A., Sakipov, S., Pereyaslavets, L., Kurnikov, I. V., Butin, O., Voronina, E., Ivahnenko, I., Leontyev, I., Nawrocki, G., Darkhovskiy, M., Olevanov, M., Cherniavskiy, et al
2024
- **Variability in excess deaths across countries with different vulnerability during 2020-2023.** *Proceedings of the National Academy of Sciences of the United States of America*
Ioannidis, J. P., Zonta, F., Levitt, M.
2023; 120 (49): e2309557120
- **Combining Force Fields and Neural Networks for an Accurate Representation of Chemically Diverse Molecular Interactions.** *Journal of the American Chemical Society*
Illarionov, A., Sakipov, S., Pereyaslavets, L., Kurnikov, I. V., Kamath, G., Butin, O., Voronina, E., Ivahnenko, I., Leontyev, I., Nawrocki, G., Darkhovskiy, M., Olevanov, M., Cherniavskiy, et al
2023
- **Variability in excess deaths across countries with different vulnerability during 2020-2023.** *medRxiv : the preprint server for health sciences*
Ioannidis, J. P., Zonta, F., Levitt, M.
2023
- **What Really Happened During the Massive SARS-CoV-2 Omicron Wave in China?** *JAMA internal medicine*
Ioannidis, J. P., Zonta, F., Levitt, M.
2023
- **Flaws and uncertainties in pandemic global excess death calculations.** *European journal of clinical investigation*
Ioannidis, J. P., Zonta, F., Levitt, M.
2023: e14008
- **Excess death estimates from multiverse analysis in 2009-2021.** *European journal of epidemiology*
Levitt, M., Zonta, F., Ioannidis, J. P.
2023
- **AlphaFold accelerates artificial intelligence powered drug discovery: efficient discovery of a novel CDK20 small molecule inhibitor.** *Chemical science*
Ren, F., Ding, X., Zheng, M., Korzinkin, M., Cai, X., Zhu, W., Mantsyzov, A., Aliper, A., Aladinskiy, V., Cao, Z., Kong, S., Long, X., Man Liu, et al
2023; 14 (6): 1443-1452

- **Estimates of COVID-19 deaths in Mainland China after abandoning zero COVID policy.** *European journal of clinical investigation*
Ioannidis, J. P., Zonta, F., Levitt, M.
2023: e13956
- **Estimates of COVID-19 deaths in Mainland China after abandoning zero COVID policy.** *medRxiv : the preprint server for health sciences*
Ioannidis, J. P., Zonta, F., Levitt, M.
2023
- **AlphaFold accelerates artificial intelligence powered drug discovery: efficient discovery of a novel CDK20 small molecule inhibitor** *CHEMICAL SCIENCE*
Ren, F., Ding, X., Zheng, M., Korzinkin, M., Cai, X., Zhu, W., Mantsyzov, A., Aliper, A., Aladinskiy, V., Cao, Z., Kong, S., Long, X., Man Liu, et al
2023
- **Protein-Ligand Binding Free-Energy Calculations with ARROW#A Purely First-Principles Parameterized Polarizable Force Field.** *Journal of chemical theory and computation*
Nawrocki, G., Leontyev, I., Sakipov, S., Darkhovskiy, M., Kurnikov, I., Pereyaslavets, L., Kamath, G., Voronina, E., Butin, O., Illarionov, A., Olevanov, M., Kostikov, A., Ivahnenko, et al
2022
- **Virus spread on a scale-free network reproduces the Gompertz growth observed in isolated COVID-19 outbreaks.** *Advances in biological regulation*
Zonta, F., Levitt, M.
2022: 100915
- **Comparison of pandemic excess mortality in 2020-2021 across different empirical calculations.** *Environmental research*
Levitt, M., Zonta, F., Ioannidis, J. P.
2022: 113754
- **Accurate determination of solvation free energies of neutral organic compounds from first principles.** *Nature communications*
Pereyaslavets, L., Kamath, G., Butin, O., Illarionov, A., Olevanov, M., Kurnikov, I., Sakipov, S., Leontyev, I., Voronina, E., Gannon, T., Nawrocki, G., Darkhovskiy, M., Ivahnenko, et al
1800; 13 (1): 414
- **SARS-CoV-2 Omicron variant: viral spread dynamics, disease burden, and vaccine effectiveness.** *Current medicine (Cham, Switzerland)*
Sun, S., Wu, J., Chen, R., Levitt, M.
2022; 1 (1): 14
- **Probing Interplays between Human XBP1 α Translational Arrest Peptide and 80S Ribosome.** *Journal of chemical theory and computation*
Di Palma, F., Decherchi, S., Pardo-Avila, F., Succi, S., Levitt, M., von Heijne, G., Cavalli, A.
2021
- **The Gompertz Growth of COVID-19 Outbreaks is Caused by Super-Spreaders.** *ArXiv*
Zonta, F., Scaiewicz, A., Levitt, M.
2021
- **Insights on cross-species transmission of SARS-CoV-2 from structural modeling.** *bioRxiv : the preprint server for biology*
Rodrigues, J. P., Barrera-Vilarmau, S., Teixeira, J. M., Seckel, E., Kastritis, P., Levitt, M.
2020
- **Interfacea: Open-Source Library for Protein Interface Analysis**
Rodrigues, J., Levitt, M.
CELL PRESS.2020: 516A
- **Insights on cross-species transmission of SARS-CoV-2 from structural modeling** *bioRxiv*
Rodrigues, J. P., Barrera-Vilarmau, S., Teixeira, J. M., Seckel, E., Kastritis, P., Levitt, M.
2020
- **Insights on cross-species transmission of SARS-CoV-2 from structural modeling.** *PLoS computational biology*
Rodrigues, J. P., Barrera-Vilarmau, S. n., M C Teixeira, J. n., Sorokina, M. n., Seckel, E. n., Kastritis, P. L., Levitt, M. n.
2020; 16 (12): e1008449
- **Solving the structure of Lgl2, a difficult blind test of unsupervised structure determination.** *Proceedings of the National Academy of Sciences of the United States of America*

- Ufimtsev, I. S., Almagor, L., Weis, W. I., Levitt, M.
2019
- **Unsupervised determination of protein crystal structures.** *Proceedings of the National Academy of Sciences of the United States of America*
Ufimtsev, I. S., Levitt, M.
2019
 - **Automatic Inference of Sequence from Low-Resolution Crystallographic Data.** *Structure (London, England : 1993)*
Ben-Aharon, Z., Levitt, M., Kalisman, N.
2018
 - **On the importance of accounting for nuclear quantum effects in ab initio calibrated force fields in biological simulations.** *Proceedings of the National Academy of Sciences of the United States of America*
Pereyaslavets, L., Kurnikov, I., Kamath, G., Butin, O., Illarionov, A., Leontyev, I., Olevanov, M., Levitt, M., Kornberg, R. D., Fain, B.
2018
 - **Proteomic analysis of monolayer-integrated proteins on lipid droplets identifies amphipathic interfacial alpha-helical membrane anchors.** *Proceedings of the National Academy of Sciences of the United States of America*
Pataki, C. I., Rodrigues, J., Zhang, L., Qian, J., Efron, B., Hastie, T., Elias, J. E., Levitt, M., Kopito, R. R.
2018
 - **Unique function words characterize genomic proteins.** *Proceedings of the National Academy of Sciences of the United States of America*
Scaiewicz, A., Levitt, M.
2018; 115 (26): 6703–8
 - **The solution structure of monomeric CCL5 in complex with a doubly sulfated N-terminal segment of CCR5** *FEBS JOURNAL*
Abayev, M., Rodrigues, J. M., Srivastava, G., Arshava, B., Jaremko, L., Jaremko, M., Naider, F., Levitt, M., Anglister, J.
2018; 285 (11): 1988–2003
 - **An analysis and evaluation of the WeFold collaborative for protein structure prediction and its pipelines in CASP11 and CASP12.** *Scientific reports*
Keasar, C. n., McGuffin, L. J., Wallner, B. n., Chopra, G. n., Adhikari, B. n., Bhattacharya, D. n., Blake, L. n., Bortot, L. O., Cao, R. n., Dhanasekaran, B. K., Dimas, I. n., Faccioli, R. A., Faraggi, et al
2018; 8 (1): 9939
 - **Emerging #-Sheet Rich Conformations in Supercompact Huntingtin Exon-1 Mutant Structures.** *Journal of the American Chemical Society*
Kang, H., Vázquez, F. X., Zhang, L., Das, P., Toledo-Sherman, L., Luan, B., Levitt, M., Zhou, R.
2017; 139 (26): 8820-8827
 - **Future of fundamental discovery in US biomedical research.** *Proceedings of the National Academy of Sciences of the United States of America*
Levitt, M., Levitt, J. M.
2017
 - **Sequential allosteric mechanism of ATP hydrolysis by the CCT/TRiC chaperone is revealed through Arrhenius analysis** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Gruber, R., Levitt, M., Horovitz, A.
2017; 114 (20): 5189-5194
 - **The language of the protein universe** *CURRENT OPINION IN GENETICS & DEVELOPMENT*
Scaiewicz, A., Levitt, M.
2015; 35: 50-56
 - **Birth and Future of Multiscale Modeling for Macromolecular Systems (Nobel Lecture)** *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION*
Levitt, M.
2014; 53 (38): 10006-10018
 - **WeFold: A competition for protein structure prediction** *PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS*
Khoury, G. A., Liwo, A., Khatib, F., Zhou, H., Chopra, G., Bacardit, J., Bortot, L. O., Faccioli, R. A., Deng, X., He, Y., Krupa, P., Li, J., Mozolewska, et al
2014; 82 (9): 1850-1868
 - **Deformable elastic network refinement for low-resolution macromolecular crystallography.** *Acta crystallographica. Section D, Biological crystallography*
Schröder, G. F., Levitt, M., Brunger, A. T.

2014; 70: 2241-2255

- **Deformable elastic network refinement for low-resolution macromolecular crystallography** *ACTA CRYSTALLOGRAPHICA SECTION D-BIOLOGICAL CRYSTALLOGRAPHY*
Schroeder, G. F., Levitt, M., Brunger, A. T.
2014; 70: 2241-2255
- **Redundancy-weighting for better inference of protein structural features.** *Bioinformatics*
Yanover, C., Vanetik, N., Levitt, M., Kolodny, R., Keasar, C.
2014; 30 (16): 2295-2301
- **Millisecond dynamics of RNA polymerase II translocation at atomic resolution** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Silva, D., Weiss, D. R., Avila, F. P., Da, L., Levitt, M., Wang, D., Huang, X.
2014; 111 (21): 7665-7670
- **Training-free atomistic prediction of nucleosome occupancy** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Minary, P., Levitt, M.
2014; 111 (17): 6293-6298
- **Architecture of an RNA Polymerase II Transcription Pre-Initiation Complex** *SCIENCE*
Murakami, K., Elmlund, H., Kalisman, N., Bushnell, D. A., Adams, C. M., Azubel, M., Elmlund, D., Levi-Kalisman, Y., Liu, X., Gibbons, B. J., Levitt, M., Kornberg, R. D.
2013; 342 (6159): 709-?
- **Architecture of an RNA polymerase II transcription pre-initiation complex.** *Science*
Murakami, K., Elmlund, H., Kalisman, N., Bushnell, D. A., Adams, C. M., Azubel, M., Elmlund, D., Levi-Kalisman, Y., Liu, X., Gibbons, B. J., Levitt, M., Kornberg, R. D.
2013; 342 (6159): 1238724-?
- **The crystal structures of the eukaryotic chaperonin CCT reveal its functional partitioning.** *Structure*
Kalisman, N., Schröder, G. F., Levitt, M.
2013; 21 (4): 540-549
- **The Crystal Structures of the Eukaryotic Chaperonin CCT Reveal Its Functional Partitioning** *STRUCTURE*
Kalisman, N., Schroeder, G. F., Levitt, M.
2013; 21 (4): 540-549
- **On the Universe of Protein Folds** *ANNUAL REVIEW OF BIOPHYSICS, VOL 42*
Kolodny, R., Pereyaslavets, L., Samson, A. O., Levitt, M.
2013; 42: 559-582
- **Evolutionarily consistent families in SCOP: sequence, structure and function** *BMC STRUCTURAL BIOLOGY*
Pethica, R. B., Levitt, M., Gough, J.
2012; 12
- **KoBaMIN: a knowledge-based minimization web server for protein structure refinement** *NUCLEIC ACIDS RESEARCH*
Rodrigues, J. P., Levitt, M., Chopra, G.
2012; 40 (W1): W323-W328
- **KoBaMIN: a knowledge-based minimization web server for protein structure refinement.** *Nucleic acids research*
Rodrigues, J. P., Levitt, M., Chopra, G.
2012; 40 (Web Server issue): W323-8
- **Multiscale natural moves refine macromolecules using single-particle electron microscopy projection images** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Zhang, J., Minary, P., Levitt, M.
2012; 109 (25): 9845-9850
- **Improving the accuracy of macromolecular structure refinement at 7 Å resolution.** *Structure*

-
- Brunger, A. T., Adams, P. D., Fromme, P., Fromme, R., Levitt, M., Schröder, G. F.
2012; 20 (6): 957-966
- **Improving the Accuracy of Macromolecular Structure Refinement at 7 angstrom Resolution** *STRUCTURE*
Brunger, A. T., Adams, P. D., Fromme, P., Fromme, R., Levitt, M., Schroeder, G. F.
2012; 20 (6): 957-966
 - **Comparative modeling and protein-like features of hydrophobic-polar models on a two-dimensional lattice** *PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS*
Moreno-Hernandez, S., Levitt, M.
2012; 80 (6): 1683-1693
 - **Modeling nucleic acids** *CURRENT OPINION IN STRUCTURAL BIOLOGY*
Sim, A. Y., Minary, P., Levitt, M.
2012; 22 (3): 273-278
 - **EVALUATING MIXTURE MODELS FOR BUILDING RNA KNOWLEDGE-BASED POTENTIALS** *JOURNAL OF BIOINFORMATICS AND COMPUTATIONAL BIOLOGY*
Sim, A. Y., Schwander, O., Levitt, M., Bernauer, J.
2012; 10 (2)
 - **Application of DEN refinement and automated model building to a difficult case of molecular-replacement phasing: the structure of a putative succinyl-diaminopimelate desuccinylase from *Corynebacterium glutamicum*** *ACTA CRYSTALLOGRAPHICA SECTION D-BIOLOGICAL CRYSTALLOGRAPHY*
Brunger, A. T., Das, D., Deacon, A. M., Grant, J., Terwilliger, T. C., Read, R. J., Adams, P. D., Levitt, M., Schroeder, G. F.
2012; 68: 391-403
 - **Modeling and design by hierarchical natural moves** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Sim, A. Y., Levitt, M., Minary, P.
2012; 109 (8): 2890-2895
 - **Subunit order of eukaryotic TRiC/CCT chaperonin by cross-linking, mass spectrometry, and combinatorial homology modeling** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Kalisman, N., Adams, C. M., Levitt, M.
2012; 109 (8): 2884-2889
 - **Symmetry-free cryo-EM structures of the chaperonin TRiC along its ATPase-driven conformational cycle** *EMBO JOURNAL*
Cong, Y., Schroeder, G. F., Meyer, A. S., Jakana, J., Ma, B., Dougherty, M. T., Schmid, M. F., Reissmann, S., Levitt, M., Ludtke, S. L., Frydman, J., Chiu, W.
2012; 31 (3): 720-730
 - **Optimized Torsion-Angle Normal Modes Reproduce Conformational Changes More Accurately Than Cartesian Modes** *BIOPHYSICAL JOURNAL*
Bray, J. K., Weiss, D. R., Levitt, M.
2011; 101 (12): 2966-2969
 - **Remarkable patterns of surface water ordering around polarized buckminsterfullerene** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Chopra, G., Levitt, M.
2011; 108 (35): 14455-14460
 - **Fully differentiable coarse-grained and all-atom knowledge-based potentials for RNA structure evaluation** *RNA-A PUBLICATION OF THE RNA SOCIETY*
Bernauer, J., Huang, X., Sim, A. Y., Levitt, M.
2011; 17 (6): 1066-1075
 - **Cryo-EM Structure of a Group II Chaperonin in the Prehydrolysis ATP-Bound State Leading to Lid Closure** *STRUCTURE*
Zhang, J., Ma, B., DiMaio, F., Douglas, N. R., Joachimiak, L. A., Baker, D., Frydman, J., Levitt, M., Chiu, W.
2011; 19 (5): 633-639
 - **Normal Modes of Prion Proteins: From Native to Infectious Particle** *BIOCHEMISTRY*
Samson, A. O., Levitt, M.
2011; 50 (12): 2243-2248
-

- **Clustering to identify RNA conformations constrained by secondary structure** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Sim, A. Y., Levitt, M.
2011; 108 (9): 3590-3595
- **To what extent does the citation advantage of collaboration depend on the citation counting system?** *13th Conference of the International-Society-for-Scientometrics-and-Infometrics (ISSI)*
Levitt, J. M., Thelwall, M., Levitt, M.
INT SOC SCIENTOMETRICS & INFORMETRICS-ISSI.2011: 398-408
- **RNA polymerase II trigger loop residues stabilize and position the incoming nucleotide triphosphate in transcription** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Huang, X., Wang, D., Weiss, D. R., Bushnell, D. A., Kornberg, R. D., Levitt, M.
2010; 107 (36): 15745-15750
- **Consistent refinement of submitted models at CASP using a knowledge-based potential** *PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS*
Chopra, G., Kalisman, N., Levitt, M.
2010; 78 (12): 2668-2678
- **Conformational Optimization with Natural Degrees of Freedom: A Novel Stochastic Chain Closure Algorithm** *JOURNAL OF COMPUTATIONAL BIOLOGY*
Minary, P., Levitt, M.
2010; 17 (8): 993-1010
- **MOTIF-EM: an automated computational tool for identifying conserved regions in CryoEM structures** *BIOINFORMATICS*
Saha, M., Levitt, M., Chiu, W.
2010; 26 (12): i301-i309
- **Super-resolution biomolecular crystallography with low-resolution data** *NATURE*
Schroeder, G. F., Levitt, M., Brunger, A. T.
2010; 464 (7292): 1218-U146
- **Mechanism of folding chamber closure in a group II chaperonin** *NATURE*
Zhang, J., Baker, M. L., Schroeder, G. F., Douglas, N. R., Reissmann, S., Jakana, J., Dougherty, M., Fu, C. J., Levitt, M., Ludtke, S. J., Frydman, J., Chiu, W.
2010; 463 (7279): 379-U130
- **Insights into the intra-ring subunit order of TRiC/CCT: a structural and evolutionary analysis.** *Pacific Symposium on Biocomputing. Pacific Symposium on Biocomputing*
Kalisman, N., Levitt, M.
2010: 252-259
- **Nature of the protein universe** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Levitt, M.
2009; 106 (27): 11079-11084
- **Structural Basis of Transcription: Backtracked RNA Polymerase II at 3.4 Angstrom Resolution** *SCIENCE*
Wang, D., Bushnell, D. A., Huang, X., Westover, K. D., Levitt, M., Kornberg, R. D.
2009; 324 (5931): 1203-1206
- **Outcome of a Workshop on Applications of Protein Models in Biomedical Research** *STRUCTURE*
Schwede, T., Sali, A., Honig, B., Levitt, M., Berman, H. M., Jones, D., Brenner, S. E., Burley, S. K., Das, R., Dokholyan, N. V., Dunbrack, R. L., Fidelis, K., Fiser, et al
2009; 17 (2): 151-159
- **Generalized ensemble methods for de novo structure prediction** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Shmygelska, A., Levitt, M.
2009; 106 (5): 1415-1420
- **Can Morphing Methods Predict Intermediate Structures?** *JOURNAL OF MOLECULAR BIOLOGY*
Weiss, D. R., Levitt, M.

2009; 385 (2): 665-674

- **Protein segment finder: an online search engine for segment motifs in the PDB** *NUCLEIC ACIDS RESEARCH*
Samson, A. O., Levitt, M.
2009; 37: D224-D228
- **Solvent dramatically affects protein structure refinement** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Chopra, G., Summa, C. M., Levitt, M.
2008; 105 (51): 20239-20244
- **Inhibition mechanism of the acetylcholine receptor by alpha-neurotoxins as revealed by normal-mode dynamics** *BIOCHEMISTRY*
Samson, A. O., Levitt, M.
2008; 47 (13): 4065-4070
- **How hydrophobic Buckminsterfullerene affects surrounding water structure** *JOURNAL OF PHYSICAL CHEMISTRY B*
Weiss, D. R., Raschke, T. M., Levitt, M.
2008; 112 (10): 2981-2990
- **Probing protein fold space with a simplified model** *JOURNAL OF MOLECULAR BIOLOGY*
Minary, P., Levitt, M.
2008; 375 (4): 920-933
- **Combining efficient conformational sampling with a deformable elastic network model facilitates structure refinement at low resolution** *STRUCTURE*
Schroeder, G. F., Brunger, A. T., Levitt, M.
2007; 15 (12): 1630-1641
- **Simulations of RNA base pairs in a nanodroplet reveal solvation-dependent stability** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Sykes, M. T., Levitt, M.
2007; 104 (30): 12336-12340
- **Growth of novel protein structural data** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Levitt, M.
2007; 104 (9): 3183-3188
- **Near-native structure refinement using in vacuo energy minimization** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Summa, C. M., Levitt, M.
2007; 104 (9): 3177-3182
- **Discussion of "equi-energy sampler" by Kou, Zhou and Wong** *ANNALS OF STATISTICS*
Minary, P., Levitt, M.
2006; 34 (4): 1636-1641
- **Spatial regulation and the rate of signal transduction activation** *PLOS COMPUTATIONAL BIOLOGY*
Batada, N. N., Shepp, L. A., Siegmund, D. O., Levitt, M.
2006; 2 (5): 343-349
- **Theory and simulation - Accuracy and reliability in modelling proteins and complexes** *CURRENT OPINION IN STRUCTURAL BIOLOGY*
Janin, J., Levitt, M.
2006; 16 (2): 139-141
- **An atomic environment potential for use in protein structure prediction** *JOURNAL OF MOLECULAR BIOLOGY*
Summa, C. M., Levitt, M., DeGrado, W. F.
2005; 352 (4): 986-1001
- **Describing RNA structure by libraries of clustered nucleotide doublets** *JOURNAL OF MOLECULAR BIOLOGY*
Sykes, M. T., Levitt, M.
2005; 351 (1): 26-38

- **Nonpolar solutes enhance water structure within hydration shells while reducing interactions between them** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Raschke, T. M., Levitt, M.
2005; 102 (19): 6777-6782
- **Comprehensive evaluation of protein structure alignment methods: Scoring by geometric measures** *JOURNAL OF MOLECULAR BIOLOGY*
Kolodny, R., Koehl, P., Levitt, M.
2005; 346 (4): 1173-1188
- **Inverse kinematics in biology: The protein loop closure problem** *INTERNATIONAL JOURNAL OF ROBOTICS RESEARCH*
Kolodny, R., Guibas, L., Levitt, M., Koehl, P.
2005; 24 (2-3): 151-163
- **Diffusion of nucleoside triphosphates and role of the entry site to the RNA polymerase II active center** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Batada, N. N., Westover, K. D., Bushnell, D. A., Levitt, M., Kornberg, R. D.
2004; 101 (50): 17361-17364
- **The area derivative of a space-filling diagram** *DISCRETE & COMPUTATIONAL GEOMETRY*
Bryant, R., Edelsbrunner, H., Koehl, P., Levitt, M.
2004; 32 (3): 293-308
- **Detailed hydration maps of benzene and cyclohexane reveal distinct water structures** *JOURNAL OF PHYSICAL CHEMISTRY B*
Raschke, T. M., Levitt, M.
2004; 108 (35): 13492-13500
- **Improved protein structure selection using decoy-dependent discriminatory functions.** *BMC structural biology*
Wang, K., Fain, B., Levitt, M., Samudrala, R.
2004; 4: 8-?
- **Simulating protein evolution in sequence and structure space** *CURRENT OPINION IN STRUCTURAL BIOLOGY*
Xia, Y., Levitt, M.
2004; 14 (2): 202-207
- **Funnel-like organization in sequence space determines the distributions of protein stability and folding rate preferred by evolution** *PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS*
Xia, Y., Levitt, M.
2004; 55 (1): 107-114
- **The ASTRAL Compendium in 2004** *NUCLEIC ACIDS RESEARCH*
Chandonia, J. M., Hon, G., Walker, N. S., Lo Conte, L., Koehl, P., Levitt, M., Brenner, S. E.
2004; 32: D189-D192
- **Funnel sculpting for in silico assembly of secondary structure elements of proteins** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Fain, B., Levitt, M.
2003; 100 (19): 10700-10705
- **A novel approach to decoy set generation: Designing a physical energy function having local minima with native structure characteristics** *JOURNAL OF MOLECULAR BIOLOGY*
Kearar, C., Levitt, M.
2003; 329 (1): 159-174
- **Protein decoy assembly using short fragments under geometric constraints** *BIOPOLYMERS*
Kolodny, R., Levitt, M.
2003; 68 (3): 278-285
- **Evidence of turn and salt bridge contributions to beta-hairpin stability: MD simulations of C-terminal fragment from the B1 domain of protein G** *BIOPHYSICAL CHEMISTRY*
Tsai, J., Levitt, M.

2002; 101: 187-201

- **Sequence variations within protein families are linearly related to structural variations** *JOURNAL OF MOLECULAR BIOLOGY*
Koehl, P., Levitt, M.
2002; 323 (3): 551-562
- **Small libraries of protein fragments model native protein structures accurately** *JOURNAL OF MOLECULAR BIOLOGY*
Kolodny, R., Koehl, P., Guibas, L., Levitt, M.
2002; 323 (2): 297-307
- **Roles of mutation and recombination in the evolution of protein thermodynamics** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Xia, Y., Levitt, M.
2002; 99 (16): 10382-10387
- **Design of an optimal Chebyshev-expanded discrimination function for globular proteins** *PROTEIN SCIENCE*
Fain, B., Xia, Y., Levitt, M.
2002; 11 (8): 2010-2021
- **A comprehensive analysis of 40 blind protein structure predictions.** *BMC structural biology*
Samudrala, R., Levitt, M.
2002; 2: 3-?
- **Protein topology and stability define the space of allowed sequences** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Koehl, P., Levitt, M.
2002; 99 (3): 1280-1285
- **Within the twilight zone: A sensitive profile-profile comparison tool based on information theory** *JOURNAL OF MOLECULAR BIOLOGY*
Yona, G., Levitt, M.
2002; 315 (5): 1257-1275
- **Improved recognition of native-like protein structures using a family of designed sequences** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Koehl, P., Levitt, M.
2002; 99 (2): 691-696
- **ASTRAL compendium enhancements** *NUCLEIC ACIDS RESEARCH*
Chandonia, J. M., Walker, N. S., Conte, L. L., Koehl, P., Levitt, M., Brenner, S. E.
2002; 30 (1): 260-263
- **Peter Kollman - Obituary** *NATURE STRUCTURAL BIOLOGY*
Levitt, M., Daggett, V.
2001; 8 (8): 662-662
- **Quantification of the hydrophobic interaction by simulations of the aggregation of small hydrophobic solutes in water** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Raschke, T. M., Tsai, J., Levitt, M.
2001; 98 (11): 5965-5969
- **Determination of optimal Chebyshev-expanded hydrophobic discrimination function for globular proteins** *IBM JOURNAL OF RESEARCH AND DEVELOPMENT*
Fain, B., Xia, Y., Levitt, M.
2001; 45 (3-4): 525-532
- **The birth of computational structural biology** *NATURE STRUCTURAL BIOLOGY*
Levitt, M.
2001; 8 (5): 392-393
- **A novel method for sampling alpha-helical protein backbones** *JOURNAL OF MOLECULAR BIOLOGY*
Fain, B., Levitt, M.

2001; 305 (2): 191-201

- **De novo protein design** *4th NATO Advanced-Study-Institute on Dynamics, Structure and Function of Biological Macromolecules*
Koehl, P., Levitt, M.
I O S PRESS.2001: 57-75
- **Extracting knowledge-based energy functions from protein structures by error rate minimization: Comparison of methods using lattice model** *JOURNAL OF CHEMICAL PHYSICS*
Xia, Y., Levitt, M.
2000; 113 (20): 9318-9330
- **Constructing side chains on near-native main chains for ab initio protein structure prediction** *PROTEIN ENGINEERING*
Samudrala, R., Huang, E. S., Koehl, P., Levitt, M.
2000; 13 (7): 453-457
- **Decoys 'R' Us: A database of incorrect conformations to improve protein structure prediction** *PROTEIN SCIENCE*
Samudrala, R., Levitt, M.
2000; 9 (7): 1399-1401
- **Ab initio construction of protein tertiary structures using a hierarchical approach** *JOURNAL OF MOLECULAR BIOLOGY*
Xia, Y., Huang, E. S., Levitt, M., Samudrala, R.
2000; 300 (1): 171-185
- **Towards a complete map of the protein space based on a unified sequence and structure analysis of all known proteins.** *Proceedings. International Conference on Intelligent Systems for Molecular Biology*
Yona, G., Levitt, M.
2000; 8: 395-406
- **Expectations from structural genomics** *PROTEIN SCIENCE*
Brenner, S. E., Levitt, M.
2000; 9 (1): 197-200
- **The ASTRAL compendium for protein structure and sequence analysis** *NUCLEIC ACIDS RESEARCH*
Brenner, S. E., Koehl, P., Levitt, R.
2000; 28 (1): 254-256
- **Probing structure-function relationships of the DNA polymerase alpha-associated zinc-finger protein using computational approaches.** *Pacific Symposium on Biocomputing. Pacific Symposium on Biocomputing*
Samudrala, R., Xia, Y., Levitt, M., Cotton, N. J., Huang, E. S., Davis, R.
2000: 179-190
- **De novo protein design. I. In search of stability and specificity** *JOURNAL OF MOLECULAR BIOLOGY*
Koehl, P., Levitt, M.
1999; 293 (5): 1161-1181
- **De novo protein design. II. Plasticity in sequence space** *JOURNAL OF MOLECULAR BIOLOGY*
Koehl, P., Levitt, M.
1999; 293 (5): 1183-1193
- **Structure-based conformational preferences of amino acids** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Koehl, P., Levitt, M.
1999; 96 (22): 12524-12529
- **Hierarchy of structure loss in MD simulations of src SH3 domain unfolding** *JOURNAL OF MOLECULAR BIOLOGY*
Tsai, J., Levitt, M., Baker, D.
1999; 291 (1): 215-225
- **Theory and simulation - Can theory challenge experiment? Editorial overview** *CURRENT OPINION IN STRUCTURAL BIOLOGY*
Koehl, P., Levitt, M.
1999; 9 (2): 155-156

- **A brighter future for protein structure prediction.** *Nature structural biology*
Koehl, P., Levitt, M.
1999; 6 (2): 108-111
- **A combined approach for ab initio construction of low resolution protein tertiary structures from sequence.** *Pacific Symposium on Biocomputing. Pacific Symposium on Biocomputing*
Samudrala, R., Xia, Y., Levitt, M., Huang, E. S.
1999: 505-516
- **Ab initio protein structure prediction using a combined hierarchical approach** *3rd Meeting on the Critical Assessment of Techniques for Protein Structure Prediction (CASP3)*
Samudrala, R., Xia, Y., Huang, E., Levitt, M.
WILEY-BLACKWELL.1999: 194-198
- **The PRESAGE database for structural genomics** *NUCLEIC ACIDS RESEARCH*
Brenner, S. E., Barken, D., Levitt, M.
1999; 27 (1): 251-253
- **Accuracy of side-chain prediction upon near-native protein backbones generated by ab initio folding methods** *PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS*
Huang, E. S., Koehl, P., Levitt, M., Pappu, R. V., Ponder, J. W.
1998; 33 (2): 204-217
- **Simulating water and the molecules of life** *SCIENTIFIC AMERICAN*
Gerstein, M., Levitt, M.
1998; 279 (5): 100-105
- **A unified statistical framework for sequence comparison and structure comparison** *Colloquium on Computational Biomolecular Science*
Levitt, M., Gerstein, M.
NATL ACAD SCIENCES.1998: 5913-20
- **Comprehensive assessment of automatic structural alignment against a manual standard, the scop classification of proteins** *PROTEIN SCIENCE*
Gerstein, M., Levitt, M.
1998; 7 (2): 445-456
- **Simulating the minimum core for hydrophobic collapse in globular proteins** *PROTEIN SCIENCE*
Tsai, J., Gerstein, M., Levitt, M.
1997; 6 (12): 2606-2616
- **A structural census of the current population of protein sequences** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Gerstein, M., Levitt, M.
1997; 94 (22): 11911-11916
- **Calibration and testing of a water model for simulation of the molecular dynamics of proteins and nucleic acids in solution** *JOURNAL OF PHYSICAL CHEMISTRY B*
Levitt, M., Hirshberg, M., Sharon, R., Laidig, K. E., Daggett, V.
1997; 101 (25): 5051-5061
- **Factors affecting the ability of energy functions to discriminate correct from incorrect folds** *JOURNAL OF MOLECULAR BIOLOGY*
Park, B. H., Huang, E. S., Levitt, M.
1997; 266 (4): 831-846
- **Competitive assessment of protein fold recognition and alignment accuracy** *PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS*
Levitt, M.
1997: 92-104
- **Packing as a structural basis of protein stability: understanding mutant properties from wildtype structure.** *Pacific Symposium on Biocomputing. Pacific Symposium on Biocomputing*
Lee, C., Levitt, M.

1997: 245-255

- **A retrospective analysis of CASP2 threading predictions** *PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS*
Marchler-Bauer, A., Levitt, M., Bryant, S. H.
1997: 83-91
- **Protein folding: The endgame** *ANNUAL REVIEW OF BIOCHEMISTRY*
Levitt, M., Gerstein, M., Huang, E., Subbiah, S., Tsai, J.
1997; 66: 549-579
- **Finite-difference solution of the Poisson-Boltzmann equation: Complete elimination of self-energy** *JOURNAL OF COMPUTATIONAL CHEMISTRY*
Zhou, Z. X., Payne, P., Vasquez, M., Kuhn, N., Levitt, M.
1996; 17 (11): 1344-1351
- **Keeping the shape but changing the charges: A simulation study of urea and its iso-steric analogs** *JOURNAL OF CHEMICAL PHYSICS*
Tsai, J., Gerstein, M., Levitt, M.
1996; 104 (23): 9417-9430
- **Energy functions that discriminate X-ray and near-native folds from well-constructed decoys** *JOURNAL OF MOLECULAR BIOLOGY*
Park, B., Levitt, M.
1996; 258 (2): 367-392
- **From structure to sequence and back again** *JOURNAL OF MOLECULAR BIOLOGY*
Hinds, D. A., Levitt, M.
1996; 258 (1): 201-209
- **Using a hydrophobic contact potential to evaluate native and near-native folds generated by molecular dynamics simulations** *JOURNAL OF MOLECULAR BIOLOGY*
Huang, E. S., Subbiah, S., Tsai, J., Levitt, M.
1996; 257 (3): 716-725
- **Through the breach.** *Current opinion in structural biology*
LEVITT
1996; 6 (2): 193-194
- **Theory and simulation through the breach** *CURRENT OPINION IN STRUCTURAL BIOLOGY*
Levitt, M.
1996; 6 (2): 193-194
- **Using iterative dynamic programming to obtain accurate pairwise and multiple alignments of protein structures.** *Proceedings / ... International Conference on Intelligent Systems for Molecular Biology ; ISMB. International Conference on Intelligent Systems for Molecular Biology*
Gerstein, M., Levitt, M.
1996; 4: 59-67
- **Packing as a structural basis of protein stability: Understanding mutant properties from wildtype structure** *2nd Pacific Symposium on Biocomputing (PSB)*
Lee, C., Levitt, M.
WORLD SCIENTIFIC PUBL CO PTE LTD.1996: 245-255
- **Simulating the dynamics of the DNA double helix in solution** *NATO Advanced Study Institute / International-School-of-Biological-Magnetic-Resonances 2nd Course on Dynamics and the Problem of Recognition in Biological Macromolecules*
Hirshberg, M., Levitt, M.
PLENUM PRESS DIV PLENUM PUBLISHING CORP.1996: 173-191
- **RECOGNIZING NATIVE FOLDS BY THE ARRANGEMENT OF HYDROPHOBIC AND POLAR RESIDUES** *JOURNAL OF MOLECULAR BIOLOGY*
Huang, E. S., Subbiah, S., Levitt, M.
1995; 252 (5): 709-720
- **POTENTIAL-ENERGY FUNCTION AND PARAMETERS FOR SIMULATIONS OF THE MOLECULAR-DYNAMICS OF PROTEINS AND NUCLEIC-ACIDS IN SOLUTION** *COMPUTER PHYSICS COMMUNICATIONS*
Levitt, M., Hirshberg, M., Sharon, R., Daggett, V.
1995; 91 (1-3): 215-231

- **THE VOLUME OF ATOMS ON THE PROTEIN SURFACE - CALCULATED FROM SIMULATION, USING VORONOI POLYHEDRA** *JOURNAL OF MOLECULAR BIOLOGY*
Gerstein, M., Tsai, J., Levitt, M.
1995; 249 (5): 955-966
- **THE COMPLEXITY AND ACCURACY OF DISCRETE STATE MODELS OF PROTEIN-STRUCTURE** *JOURNAL OF MOLECULAR BIOLOGY*
Park, B. H., Levitt, M.
1995; 249 (2): 493-507
- **STRUCTURAL DIVERSITY IN A CONSERVED CHOLERA-TOXIN EPITOPE INVOLVED IN GANGLIOSIDE BINDING** *PROTEIN SCIENCE*
Shoham, M., Scherf, T., Anglister, J., Levitt, M., Merritt, E. A., Hol, W. G.
1995; 4 (5): 841-848
- **SIMULATION OF PROTEIN-FOLDING PATHWAYS - LOST IN (CONFORMATIONAL) SPACE** *TRENDS IN BIOTECHNOLOGY*
Hinds, D. A., Levitt, M.
1995; 13 (1): 23-27
- **EXPLORING CONFORMATIONAL SPACE WITH A SIMPLE LATTICE MODEL FOR PROTEIN-STRUCTURE** *JOURNAL OF MOLECULAR BIOLOGY*
Hinds, D. A., Levitt, M.
1994; 243 (4): 668-682
- **DIFFERENT PROTEIN SEQUENCES CAN GIVE RISE TO HIGHLY SIMILAR FOLDS THROUGH DIFFERENT STABILIZING INTERACTIONS** *PROTEIN SCIENCE*
Laurents, D. V., Subbiah, S., Levitt, M.
1994; 3 (11): 1938-1944
- **PROTEIN FOLDING[--]UNFOLDING DYNAMICS** *CURRENT OPINION IN STRUCTURAL BIOLOGY*
Daggett, V., Levitt, M.
1994; 4 (2): 291-295
- **WATER - NOW YOU SEE IT, NOW YOU DONT** *STRUCTURE*
Levitt, M., Park, B. H.
1993; 1 (4): 223-226
- **PROTEIN UNFOLDING PATHWAYS EXPLORED THROUGH MOLECULAR-DYNAMICS SIMULATIONS** *JOURNAL OF MOLECULAR BIOLOGY*
Daggett, V., Levitt, M.
1993; 232 (2): 600-619
- **STRUCTURAL SIMILARITY OF DNA-BINDING DOMAINS OF BACTERIOPHAGE REPRESSORS AND THE GLOBIN CORE** *CURRENT BIOLOGY*
Subbiah, S., Laurents, D. V., Levitt, M.
1993; 3 (3): 141-148
- **REALISTIC SIMULATIONS OF NATIVE-PROTEIN DYNAMICS IN SOLUTION AND BEYOND** *ANNUAL REVIEW OF BIOPHYSICS AND BIOMOLECULAR STRUCTURE*
Daggett, V., Levitt, M.
1993; 22: 353-380
- **INDUCED PEPTIDE CONFORMATIONS IN DIFFERENT ANTIBODY COMPLEXES - MOLECULAR MODELING OF THE 3-DIMENSIONAL STRUCTURE OF PEPTIDE ANTIBODY COMPLEXES USING NMR-DERIVED DISTANCE RESTRAINTS** *BIOCHEMISTRY*
Scherf, T., Hiller, R., Naider, F., Levitt, M., Anglister, J.
1992; 31 (30): 6884-6897
- **ACCURATE MODELING OF PROTEIN CONFORMATION BY AUTOMATIC SEGMENT MATCHING** *JOURNAL OF MOLECULAR BIOLOGY*
Levitt, M.
1992; 226 (2): 507-533
- **A MODEL OF THE MOLTEN GLOBULE STATE FROM MOLECULAR-DYNAMICS SIMULATIONS** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Daggett, V., Levitt, M.

- 1992; 89 (11): 5142-5146
- **A LATTICE MODEL FOR PROTEIN-STRUCTURE PREDICTION AT LOW RESOLUTION** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Hinds, D. A., Levitt, M.
1992; 89 (7): 2536-2540
 - **MOLECULAR-DYNAMICS SIMULATIONS OF HELIX DENATURATION** *JOURNAL OF MOLECULAR BIOLOGY*
Daggett, V., Levitt, M.
1992; 223 (4): 1121-1138
 - **A MOLECULAR-DYNAMICS SIMULATION OF THE C-TERMINAL FRAGMENT OF THE L7/L12 RIBOSOMAL-PROTEIN IN SOLUTION** *CHEMICAL PHYSICS*
Daggett, V., Levitt, M.
1991; 158 (2-3): 501-512
 - **STRUCTURAL AND KINETIC-STUDIES OF THE FAB FRAGMENT OF A MONOCLONAL ANTI-SPIN LABEL ANTIBODY BY NUCLEAR-MAGNETIC-RESONANCE** *JOURNAL OF MOLECULAR BIOLOGY*
Theriault, T. P., Leahy, D. J., Levitt, M., McConnell, H. M., Rule, G. S.
1991; 221 (1): 257-270
 - **ACCURATE PREDICTION OF THE STABILITY AND ACTIVITY EFFECTS OF SITE-DIRECTED MUTAGENESIS ON A PROTEIN CORE** *NATURE*
Lee, C., Levitt, M.
1991; 352 (6334): 448-451
 - **REAL-TIME INTERACTIVE FREQUENCY FILTERING OF MOLECULAR-DYNAMICS TRAJECTORIES** *JOURNAL OF MOLECULAR BIOLOGY*
Levitt, M.
1991; 220 (1): 1-4
 - **ENHANCED STABILITY OF SUBTILISIN BY 3 POINT MUTATIONS** *BIOTECHNOLOGY AND APPLIED BIOCHEMISTRY*
Narhi, L. O., STABINSKY, Y., Levitt, M., Miller, L., Sachdev, R., Finley, S., Park, S., Kolvenbach, C., Arakawa, T., Zukowski, M.
1991; 13 (1): 12-24
 - **Protein Folding** *Curr. Opinions Struct. Biol.*
Levitt M
1991; 1: 224-229
 - **NMR-DERIVED MODEL FOR A PEPTIDE-ANTIBODY COMPLEX** *BIOCHEMISTRY*
Zilber, B., Scherf, T., Levitt, M., Anglister, J.
1990; 29 (43): 10032-10041
 - **CONFORMATIONS OF IMMUNOGLOBULIN HYPERVARIABLE REGIONS** *NATURE*
Chothia, C., Lesk, A. M., Tramontano, A., Levitt, M., SMITHGILL, S. J., Air, G., Sheriff, S., Padlan, E. A., Davies, D., TULIP, W. R., Colman, P. M., Spinelli, S., Alzari, et al
1989; 342 (6252): 877-883
 - **A HUMANIZED ANTIBODY THAT BINDS TO THE INTERLEUKIN-2 RECEPTOR** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Queen, C., Schneider, W. P., Selick, H. E., PAYNE, P. W., Landolfi, N. F., Duncan, J. F., AVDALOVIC, N. M., Levitt, M., Junghans, R. P., Waldmann, T. A.
1989; 86 (24): 10029-10033
 - **PROBING ANTIBODY DIVERSITY BY 2D NMR - COMPARISON OF AMINO-ACID SEQUENCES, PREDICTED STRUCTURES, AND OBSERVED ANTIBODY ANTIGEN INTERACTIONS IN COMPLEXES OF 2 ANTIPEPTIDE ANTIBODIES** *BIOCHEMISTRY*
Levy, R., ASSULIN, O., Scherf, T., Levitt, M., Anglister, J.
1989; 28 (18): 7168-7175
 - **STABILIZATION OF PHAGE-T4 LYSOZYME BY ENGINEERED DISULFIDE BONDS** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Matsumura, M., Becktel, W. J., Levitt, M., Matthews, B. W.
1989; 86 (17): 6562-6566

- **MOLECULAR-DYNAMICS OF MACROMOLECULES IN WATER** *CHEMICA SCRIPTA*
Levitt, M.
1989; 29A: 197-203
- **ACCURATE SIMULATION OF PROTEIN DYNAMICS IN SOLUTION** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Levitt, M., Sharon, R.
1988; 85 (20): 7557-7561
- **AROMATIC RINGS ACT AS HYDROGEN-BOND ACCEPTORS** *JOURNAL OF MOLECULAR BIOLOGY*
Levitt, M., Perutz, M. F.
1988; 201 (4): 751-754
- **CONTRIBUTION OF TRYPTOPHAN RESIDUES TO THE COMBINING SITE OF A MONOCLONAL ANTI DINITROPHENYL SPIN-LABEL ANTIBODY** *BIOCHEMISTRY*
Anglister, J., Bond, M. W., Frey, T., Leahy, D., Levitt, M., McConnell, H. M., Rule, G. S., Tomasello, J., Whittaker, M.
1987; 26 (19): 6058-6064
- **THE PREDICTED STRUCTURE OF IMMUNOGLOBULIN-D1.3 AND ITS COMPARISON WITH THE CRYSTAL-STRUCTURE** *SCIENCE*
Chothia, C., Lesk, A. M., Levitt, M., AMIT, A. G., Mariuzza, R. A., Phillips, S. E., Poljak, R. J.
1986; 233 (4765): 755-758
- **HELIX TO HELIX PACKING IN PROTEINS** *JOURNAL OF MOLECULAR BIOLOGY*
Chothia, C., Levitt, M., Richardson, D.
1981; 145 (1): 215-250
- **PERIODICITY OF DEOXYRIBONUCLEASE-I DIGESTION OF CHROMATIN** *SCIENCE*
Prunell, A., Kornberg, R. D., Lutter, L., Klug, A., Levitt, M., CRICK, F. H.
1979; 204 (4395): 855-858
- **CONFORMATION OF AMINO-ACID SIDE-CHAINS IN PROTEINS** *JOURNAL OF MOLECULAR BIOLOGY*
Janin, J., Wodak, S., Levitt, M., MAIGRET, B.
1978; 125 (3): 357-386
- **STRUCTURE OF PROTEINS - PACKING OF ALPHA-HELICES AND PLEATED SHEETS** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Chothia, C., Levitt, M., Richardson, D.
1977; 74 (10): 4130-4134
- **STRUCTURE OF NUCLEOSOME CORE PARTICLES OF CHROMATIN** *NATURE*
Finch, J. T., Lutter, L. C., Rhodes, D., Brown, R. S., Rushton, B., Levitt, M., Klug, A.
1977; 269 (5623): 29-36
- **STRUCTURAL PATTERNS IN GLOBULAR PROTEINS** *NATURE*
Levitt, M., Chothia, C.
1976; 261 (5561): 552-558

PRESENTATIONS

- First prediction that coronavirus COVID-19 outbreak in China was slowing made on 2 February 2020 - Online Distribution