Carmay Lim (林小喬)

Distinguished Research Fellow
Institute of Biomedical Sciences (IBMS)
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Education

1976/09 – 1979/06	B.Sc.(Chemistry) with First Class Honors	Royal Holloway College, London University
1979/09 – 1984/03	Ph.D.(Chemical Physics)	University of Minnesota, Minneapolis

Positions

1984/05 – 1986/05	Postdoctoral Fellow	AT&T Bell Laboratories, Murray Hill, New Jersey
1986/08 – 1990/05	Research Associate	Harvard University, Cambridge, Massachusetts
1990/06 – 1994/12	Assistant Professor	Department of Chemistry, Biochemistry, Molecular and Medical Genetics, Univ. of Toronto
	Member	Protein Engineering Network Centers of Excellence, Canada
1995/01 – 1998/12	Assoc. Research Fellow	IBMS, Academia Sinica, Taipei
1995/01 – 1999/06	Assoc. Professor (joint appointment)	Chemistry Department, National Tsing Hua University (NTHU), Hsinchu
1998/12 – 2008/8	Research Fellow	IBMS, Academia Sinica, Taipei
1999/06 – present	Professor (joint appointment)	Chemistry Department, NTHU, Hsinchu
2008/09 – present	Distinguished Research Fellow	IBMS, Academia Sinica, Taipei

Research Fields/Interests

- Computational biophysics/chemistry/biology
- Protein recognition and folding
- Structure-based drug design
- New methods/algorithms for macromolecular systems

Awards

1979	Arnold Spicer Prize (for Best B.Sc. Candidate) from London University
1980	3M Foundation Fellowship
1981	National Science Foundation Fellowship, USA
1982	University of Minnesota Doctoral Dissertation Fellowship
1995–2000	National Science Council Scientist Award (國科會研究獎)
2000–2002	National Science Council Outstanding Scientist Award (國科會傑出研究獎)
2003–2008	Foundation for the Advancement of Outstanding Scholarship Outstanding Scholar Award (傑出人才基金會講座) - one of the 2 recipients awarded in 2003 in all fields; recipients cannot receive any other awards during the award period.
2004	The Chinese Chemical Society Annual Best Article Award 中國化學會會誌論文獎
2007–2011	Academia Sinica Investigator Award (中央研究院深耕計畫)
2008–2011	Human Frontier Science Program (HFSP) Research Award
2009	Ministry of Education 53rd Academic Award (教育部學術獎)
2010–2012	National Science Council Outstanding Scientist Award (國科會傑出研究獎)

Professional Experience

- Presented >100 invited talks at international conferences, and academic/governmental institutions
- Trained 13 post-doctoral fellows, 5 Ph.D. students, and 8 M.S. students
- Currently supervising 6 post-doctoral fellows, 2 Ph.D. students, and 2 Research Assistants
- Experience in collaborating jointly with academia, governmental institutions, pharmaceutical/biotech companies

Professional Service

- Editorial Advisory Board Member of Journal of American Chemical Society (2009–present), Editorial Board Member of Royal Society of Chemistry, Theoretical and Computational Chemistry book series (2009–present), Interdisciplinary Sciences-Computational Life Sciences (2008–present), Journal of Chinese Chemistry Society (2006–present), and Theoretical Chemistry Accounts (2005–present); Advisory Editor of the Journal of Theoretical & Computational Chemistry (2007–present)
- Grant reviewer for National Science Council, Taiwan; National Health Research Institutes, Taiwan; Academia Sinica Thematic Grants, Taiwan; National Science Foundation, USA; Petroleum Research Fund, USA; Research Grants Council, Hong Kong; Japan Society for the Promotion of Science, Japan
- Journal reviewer for 1) Biochemistry, 2) Bioinformatics, 3) Biophysical Journal, 4) Biopolymers, 5) BMC Structural Biology, 6) Computers in Biology and Medicine, 7) European Biophysics Journal, 8) FEBS Letters, 9) Inorganic Chemistry, 10) Journal of the American Chemical Society, 11) Journal of Chinese Chemistry Society, 12) Journal of Computational Chemistry, 13) Journal of Chemical Physics, 14) Journal of Molecular Graphics and Modeling, 15) Journal of Organic

Chemistry, 16) Journal of Physical Chemistry, 17) Journal of Physical Organic Chemistry, 18) Metallomics, 19) Molecular BioSystems, 20) Nucleic Acids Research, 21) Physical Chemistry Chemical Physics, 22) PLoS ONE, 23) Protein Engineering, 24) Protein Science, 25) Proteins, 26) Structure, 27) Theoretical Chemistry Accounts

- Academia Sinica: Ethics Committee, 2006
- TIGP-CBMB, Qualifying Examination Committee
- IBMS: Education Committee, 1997–2000, 2004–2006; Seminar Committee, 1997–1998, 2001–2002, 2006, Chair; Computer & Medical Art Committee, 2003; Appointments, Promotion & Tenure Committee, 2004–2006; General Affairs Committee, 2007; Personnel Committee, 2007–present
- The Biophysical Society of Taiwan, Council member, 1995–present

Current Grants

Title	Period	Source	Current year
Computational studies on Metal Binding and Selectivity in Ion Channels and Nucleic Acids	2009/08–2014/07	NSC	NT$1,194,000
Computational studies on antibody-binding sites and complexes	2006/07–2011/08	NSC	NT$838,000
Academia Sinica Investigator	2007/01–2011/12	AS	NT$3,400,000
Advancing the frontier of enzyme reaction mechanisms in the ADP ribosyltransferase family	2008/06–2012/05	HFSP	US$40,000

Invited Lectures and Presentations

1. 1995/01 Workshop on Molecular Dynamics Simulations, National Sun Yet Sen University, Kaoshiung
2. 1995/02 Chemistry Department, National Tsing-Hua University, Hsin Chu
3. 1995/02 Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei
4. 1995/03 Department of Biochemistry and Biophysics, Columbia University, New York
5. 1995/03 National Institutes of Health, Bethesda
6. 1995/04 National ACS Meeting, Anaheim
7. 1995/05 International Symposium on Biophysics & Structural Biology, Institute of Biomedical Sciences, Academia Sinica, Taipei
8. 1995/06 Institute of Chemistry, Academia Sinica, Taipei
9. 1995/07 Statistical Physics Conference on Nonlinear and Random Processes, Academia Sinica, Taipei
10. 1995/09 High Performance Computing Asia'95 Conference, Taipei
11. 1995/11 Chemistry Department, National Sun Yet Sen University, Kaoshiung
12. 1995/12 International Chemical Conference on Structure and Dynamics of Biological Macromolecules, National Tsing Hua University, Hsinchu
13. 1996/02 2nd CSIRO Symposium on Computational Challenges in Life Sciences, Melbourne

14. 1996/03 Laboratories of Molecular Biophysics, Rockefeller University, New York
15. 1996/03 Department of Chemistry, Yale University, New Haven
16. 1996/04 Department of Biological Sciences, Carnegie Mellon University, Pittsburgh
17. 1996/05 The Biophysical Society of ROC and The 2nd Symposium on Recent Advances in Biophysics, Kenting
18. 1996/05 The 1st Symposium on Genome Research & Analysis, Institute of Biomedical Sciences, Academia Sinica, Taipei
19. 1996/06 Chaired Symposium on Molecular Modeling and Computational Chemistry, Institute of Biological Sciences, Academia Sinica, Taipei
20. 1996/07 Workshop on Structure and Dynamics of Biophysical and Condensed Matter Systems, Telluride, Colorado
21. 1996/12 Department of Chemistry, National Normal University, Taipei
22. 1996/12 Department of Chemistry, National Chung Chen University, Chiayi
23. 1996/12 Mini-Workshop on Protein Structure Determination, Academia Sinica, Taipei
24. 1997/05 The 6th Academia Sinica Workshop on Statistical Physics and Numerical Simulation, Institute of Physics, Academia Sinica, Taipei
25. 1997/08 Chaired Protein Folding Session in the Statistical Physics Conference, Academia Sinica, Taipei
26. 1997/10 Chemistry Department, National Taiwan University, Taipei
27. 1997/11 College of Life Sciences, Tsing-Hua University, Beijing
28. 1997/12 College of Life Sciences, National Tsing-Hua University, Hsinchu
29. 1998/02 Chemistry Department, National Tsing-Hua University, Hsinchu
30. 1998/02 6th Symposium on Recent Advances in Cellular and Molecular Biology, Kenting
31. 1998/03 Institute of Chemistry, Academia Sinica, Taipei
32. 1998/05 Biophysical Chemistry Symposium, Institute of Chemistry, Academia Sinica, Taipei
33. 1998/07 Department of Chemistry, Ohio State University, Columbus, Ohio
34. 1998/07 XIV International Conference of Phosphorus Chemistry, Cincinnati, Ohio
35. 1998/09 Department of Chemistry, National Chung Hsing University, Taichung
36. 1998/11 The Hospital for Sick Children, Toronto
37. 1999/03 Department of Physics & Institute of Astronomy, National Central University, Chungli
38. 1999/03 Center for Complex Systems, National Central University, Chungli
39. 1999/05 The 5th Symposium of the Biophysical Society of Taiwan on Recent Advances in Biophysics, Taichung
40. 1999/06 Advanced School of Proteins, National Central University, Chungli
41. 1999/08 8th International Symposium of the Society of Chinese Bioscientists in America, Hong Kong
42. 2000/03 Department of Chemistry, University of California at San Diego, San Diego
43. 2000/03 Department of Molecular Biology, Scripps Research Institute, San Diego
44. 2000/05 Third East Asian Biophysics Symposium, Kyongju
45. 2000/11 International Symposium on Physical Chemistry and Biophysical Chemistry in the New Millenium, Chungbuk
46. 2000/11 Institute of Korea Chemical Research, Daeduck Research Complex, Taejon

47. 2000/11 Molecular Design Center, Soong-Sil University, Seoul
48. 2001/02 Keynote lecture at the Chemical Society Meeting of Young Scientists, Tao Yuan
49. 2001/05 1st Tsinghua International Conference of Protein Sciences, Beijing
50. 2001/05 Laboratories of Molecular Biophysics, Rockefeller University, New York
51. 2001/06 Midwest Chinese American Science & Technology Association, St Louis
52. 2001/06 Chemistry Department, University of Lund, Lund
53. 2001/08 4th International Conference on Biological Physics, Kyoto
54. 2002/02 NCTS Workshop on Bioinformatics, National Taiwan Normal University, Taipei
55. 2002/03 Physics Department, National Central University, Chungli
56. 2002/04 XIV International Biophysics Congress, Buenos Aires
57. 2002/05 Academia Sinica-Israel Academy meeting, IAMS, Academia Sinica, Taipei
58. 2002/05 Chaired the Bioinformatics and Computational Biophysical session of The 8th Symposium on Recent Advances in Biophysics, Taipei
59. 2002/07 2nd International Conference on Quantum Bioinorganic Chemistry, Lund
60. 2002/08 6th European Conference on Biological Inorganic Chemistry at Lund & Copenhagen
61. 2002/09 World Congress of Theoretical & Computational Chemistry Conference, Taipei
62. 2003/02 Second Asian Joint Workshop for Protein Informatics, Institute for Protein Research, Osaka University, Osaka
63. 2003/03 Physics Department, National Chung Hsing University, Taichung
64. 2003/03 Institute of Biomedical Sciences, National Sun Yet Sen University, Kaoshiung
65. 2003/04 Institute of Atomic and Molecular Physics, Academia Sinica, Taipei
66. 2003/05 Chemistry Department, Tamkang University, Taipei
67. 2003/11 BioResearch Technology Institute, Montreal
68. 2003/11 International Congress of Biochemistry and Molecular Biology, Toronto (International Advisory Committee member)
69. 2003/11 4th East Asian Biophysics Symposium, Taipei (Organizing Committee)
70. 2004/02 Department of Life Sciences, National Taiwan Normal University, Taipei
71. 2004/03 Department of Life Sciences, National Yang Ming University, Taipei
72. 2004/04 The 1st Pacific-Rim International Conference on Protein Science, Pacifico Yokohama
73. 2004/04 Department of Chemistry, Tsing Hua University, Beijing
74. 2004/04 Department of Life Sciences, Nankai University, Tientsin
75. 2004/05 Department of Biochemistry, The Hong Kong University of Science and Technology, Hong Kong
76. 2004/06 The 7th International Conference on Statistical Physics, Institute of Physics, Academia Sinica, Taipei
77. 2004/08 Chinese Academy of Sciences Symposium on Theoretical and Computational Chemistry, Institute of Chemical Physics, Dalian
78. 2004/12 Third Symposium on Advances in Bioinorganic Chemistry, Goa
79. 2005/05 Chemistry Department, University of Minnesota, Minneapolis
80. 2005/09 Workshop on Modeling Interactions in Biomolecules, Prague

81. 2005/12 First Taiwan-Vietnam Quantum Chemistry Conference, Hsinchu
82. 2006/05 Chair of the Bioinformatics and Computational Biophysical session of The 11th Symposium on Recent Advances in Biophysics, Taipei
83. 2006/06 Fifth Cross-Strait Workshop on Biology Inspired Theoretical Science, Taichung
84. 2006/06 Statistical Physics Conference, Academia Sinica, Taipei
85. 2006/09 232nd American Chemical Society National Meeting, San Francisco
86. 2006/12 International Conference on Bioinformatics, New Delhi
87. 2007/06 Third Symposium on Theoretical Biophysics (TheoBio-07), Cetraro
88. 2007/06 International Advisory Board of the XVI Russian International Conference on Chemical Thermodynamics (RCCT2007)
89. 2007/08 Taiwan International Workshop on Biological Physics and Complex Systems, Academia Sinica, Taipei
90. 2007/09 Third Asia-Pacific Conference of Theoretical and Computational Chemists, Beijing
91. 2007/12 Donostia Quantum Chemistry Symposium, San Sebastian
92. 2008/06 College of Chemistry, Beijing Normal University, Beijing
93. 2008/07 Plenary lecture, 6th Congress of the International Society for Theoretical Chemical Physics, Vancouver
94. 2008/08 234th American Chemical Society National Meeting, Philadelphia
95. 2008/11 Dynamics and Spectroscopy of Small Molecules and Biomolecules, Taipei
96. 2009/01 6th Asian Biophysics Association Symposium, Hong Kong
97. 2009/06 9th Human Frontier Science Program Awardees Meeting, Tokyo
98. 2009/06 Joint International Conference of Biophysics & 14th Conference of the Biophysical Society of ROC, National Cheng Kung University, Tainan
99. 2009/09 Modeling Interactions in Biomolecules IV, Prague
100. 2009/10 International Conference on Computational and System Biology, Shanghai
101. 2009/12 Bioinformatics beyond omics data analyses, Ochanomizu University, Tokyo
102. 2010/03 4th Royal Society of Chemistry Editor's symposium, Brussels
103. 2010/03 Laboratoire de Structure et Fonction des Membranes, Universite Libre de Bruxelles
104. 2010/03 Institut de Genetique et de Biologie Moleculaire et Celluaire, Strasbourg University
105. 2010/05 Organizer of Drug/Protein Design session in the 15th Joint Biophysics Conference, IBMS, Academia Sinica, Taipei
106. 2010/06 Department of Chemistry, Harvard University, Cambridge, Massachusetts
107. 2010/06 Institute of Biochemistry, National Chung Hsing University, Taichung
108. 2010/12 The 2010 Mini-Symposium on Chemical Biology, Institute of Biological Chemistry, Academia Sinica, Taipei
109. 2011/01 7th Asian Biophysics Symposium, New Delhi, India
110. 2011/04 Chemistry Department, University of North Carolina, Chapel Hill
111. 2011/06 Nucleic Acid Enzymes & Enzymes in Human Disease, Nankai University, Tianjin
112. 2011/07 The Ninth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC), Santiago de Compostela, Spain
113. 2011/09 Modeling Interactions in Biomolecules V, Kutna Hora

114. 2011/10 Federation of Asian & Oceanian Biochemists and Molecular Biologists, Singapore

115. 2011/10 College of Life Sciences, National Tsing-Hua University, Hsinchu

116. 2011/12 Keynote lecture, Theoretical and Computational Symposium, Annual Meeting of Chinese Chemical Society

Teaching Experience

- Biomolecular Structure, Dynamics, & Function, *Chemistry Department*, NTHU, 1995–2004
- Introduction to Drug Design, *Chemistry Department*, NTHU, 1996
- Physical Chemistry, Statistical Mechanics Section, *Chemistry Department*, NTHU, 1997
- English Scientific Writing & Oral Presentation*, Chemistry Department*, NTHU, 1997
- Introduction to Biochemistry, *Chemistry Department,* NTHU, 1998–2002
- Molecular Biophysics, *Academia Sinica*, 2002–2004
- Structure-Based Drug Design, *College of Life Sciences/Chemistry*, NTHU, 1997-1999; 2005
- General Chemistry, *Electrical Engineering Department*, NTHU, 2007 Spring Semester
- TIGP seminars, Coach, 2003–present

Current Supervision

Postdoctoral Fellows:

Babu, Satheesan	Ph.D. (Chemistry)	University of Hyderabad, India
Dudev, Todor	Ph.D. (Chemistry)	Sofia University, Bulgaria
Lee, Leon	Ph.D. (Chemistry)	National Tsing-Hua University
Sargsyan, Karen	Ph.D. (Physics)	Yerevan Physics Institute, Armenia
Wright, Jon	Ph.D. (Chemistry)	Essex University, U.K.
Wu, Steven	Ph.D. (Chemistry)	National Tsing-Hua University

Ph.D. Student:

Cheng, Yu-Chi	M.S. (Biophysics)	National Chung-Hsing University
Mazmanian, Karine	M.S. (Psychology)	Kiev International University, Ukraine

Research Assistant

Lin, Yeh Fon	M.S. (Biotechnology)	National Taipei University of Technology
Hua, Caesar	Engineering Science	National Taiwan University

Past Supervision (in chronological order)

Postdoctoral Fellows	Graduate Students	Research Assistants
1. Philip Tole	Marios Philippopoulos	Yue-Fang Xiang
2. Shek Ling Chan	Pei-Kun Yang	Marc Roussel
3. Jing Wang	Ming-Hsiang Feng	Brian Tao
4. Wen-Ching Hu	Nai-Yuan Chang	Sergey Filipov
5. Song Liu	Yen-Lin Lin	Alex Lin
6. Madhu Madhusoonan	Li-Ying Chang	Jackie Chen
7. Sergey Noskov	Tammy Cheng	Daphne Kan
8. Dirk Deubel	Yuan-Feng Chao	Donic Lu
9. David Sullivan	Hui-Chung Tai	Minko Dudev
10. Teobald Kupka	Tsung-Ying Yang	Chandan Badapanda
11. Pei-Kun Yang	Backy Chen	Tunell, Ingvar
12. Milos Milcic	Leon Lee	
13. Dmitri Sakharov	Steven Wu	
14. Backy Chen	Gopi Kuppuraj	

Publications *(Corresponding Author Denoted by Asterisk)*

1. The Existence of Straight–Line Paths, Invariant Vectors, and Invariant Tensors Characterizing Nonequilibrium State Distributions during Chemical Reactions.
   Carmay Lim & Donald G. Truhlar, *J. Chem. Phys.* **(1983)** *79*, 3296–3306.

2. Nonequilibrium Effects in Chemical Kinetics: Straight–Line Paths for Homonuclear Diatomic Dissociation–Recombination Process.
   Carmay Lim & Donald G. Truhlar*, *J. Phys. Chem.* **(1983)** *81*, 2683–2699.

3. Study of Mixture Effects in the Nonequilibrium Kinetics of Homonuclear Diatomic Dissociation and Recombination.
   Carmay Lim & Donald G. Truhlar*, *J. Phys. Chem.* **(1984)** *88*, 778–792.

4. Internal–state Nonequilibrium Effects for a Fast, Second–Order Reaction.
   Carmay Lim & Donald G. Truhlar*, *J. Phys. Chem.* **(1985)** *89*, 5–7.

5. New Techniques for the Study of Nonequilibrium Effects in Non–First–Order Systems.
   Carmay Lim & Donald G. Truhlar, *Chem. Phys. Lett.* **(1985)** *114*, 253–257.

6. The Effect of Vibrational–Rotational Disequilibrium on the Rate Constant for an Atom–Transfer Reaction.
   Carmay Lim & Donald G. Truhlar*, *J. Phys. Chem.* **(1986)** *90*, 2616–2634.

7. Molecular Dynamics of Nonequilibrium Infrequent Events: Laser–induced Desorption from Surfaces.
   Carmay Lim & John C. Tully, *J. Chem. Phys.* **(1986)** *85*, 7423–7433.

8. Atom–surface Scattering Dynamics at Hyperthermal Energies.
   Aviv Amirav, Mark J. Cardillo, Paula Trevor, Carmay Lim & John C. Tully, *J. Chem. Phys.* **(1987)** *87*, 1796–1807.

9. Trajectory Studies of Hyperthermal Xenon Scattering from GaAs (110).
   Carmay Lim, John C. Tully, Aviv Amirav, Paula Trevor & Mark J. Cardillo, *J. Chem. Phys.* **(1987)** *87*, 1808–1816.

10. Molecular and Harmonic Dynamics Simulations of Proteins.
    Carmay Lim, Dzung Nguyen, John Straub, Bruce Tidor & Martin Karplus, *John von Neumann National Supercomputer Center, Annual Research Report* **(1988)**.

11. Simulation Analysis of Structures on the Reaction Pathway of RNase A.
    Karen Haydock, Carmay Lim, Axel Brünger & Martin Karplus*, *J. Am. Chem. Soc.* **(1990)** *112*, 3826–3831.

12. Nonexistence of Dianionic Pentacovalent Intermediates in an *ab Initio* Study of the Base–Catalyzed Hydrolysis of Ethylene Phosphate.

Carmay Lim & Martin Karplus*, *J. Am. Chem. Soc.* **(1990)** *112*, 5872–5873.

13. Dianionic Pentacoordinate Species in the Base–Catalyzed Hydrolysis of Ethylene and Dimethyl Phosphate.
Annick Dejaegere, Carmay Lim & Martin Karplus*, *J. Am. Chem. Soc.* **(1991)** *113*, 4353–4355.

14. Absolute pKa Calculations with Continuum Dielectric Methods.
Carmay Lim, Don Bashford & Martin Karplus*, *J. Phys. Chem.* **(1991)** *95*, 5610–5620.

15. Endocyclic and Exocyclic Cleavage of Phosphorane Monoanion: A Detailed Mechanism of the RNase A Transphosphorylation Step.
Carmay Lim* & Philip Tole, *J. Am. Chem. Soc.* **(1992)** *114*, 7245–7252.

16. Concerted Hydroxyl Ion Attack and Pseudorotation in a Quantum Mechanical Study of Methyl Ethylene Phosphate Hydrolysis.
Carmay Lim* & Philip Tole, *J. Phys. Chem.* **(1992)** *96*, 5217–5218.

17. New Insights into the Base–Catalyzed Hydrolysis of Methyl Ethylene Phosphate.
Philip Tole & Carmay Lim*, *J. Phys. Chem.* **(1993)** *97*, 6212–6219.

18. Do Stereoelectronic Effects Control the Structure and Reactivity of TBP Phosphoesters?
Philip Tole & Carmay Lim*, in *ACS Symposium Series No. 539: The Anomeric Effect and Associated Stereoelectronic Effects.* G.R. Thatcher (ed.), Am. Chem. Soc. **(1993)**.

19. Simulation Analysis of the Binding Interactions in the RNase A/3'–UMP Enzyme–Product Complex as a Function of pH.
John Straub, Carmay Lim & Martin Karplus*, *J. Am. Chem. Soc.* **(1994)** *116*, 2591–2599.

20. The Significance of Electrostatic Effects in Phospho–Ester Hydrolysis.
Philip Tole & Carmay Lim*, *J. Am. Chem. Soc.* **(1994)** *116*, 3922–3931.

21. The Double Catalytic Triad, Cys25–His159–Asp158 and Cys25–His159–Asn175, in Papain Catalysis: Role of Asp158 and Asn175.
Jing Wang, YueFang Xiang & Carmay Lim*, *Protein Engineering* **(1994)** *7*, 75–82.

22. Internal Motions in the Molecular Tumbling Regime: Effect on NMR Dipolar Cross–relaxation and Interproton Distance Determination.
Marios Philippopoulos & Carmay Lim*, *J. Phys. Chem.* **(1994)** *98*, 8264–8273.

23. Reducing the Error due to the Uncertainty in the Born Radius in Continuum Dielectric Calculations.
Shek Ling Chan & Carmay Lim*, *J. Phys. Chem.* **(1994)** *98*, 692–695.

24. Conformational Distribution of a Tetrapeptide in Solution Using a Combined Random Search and Continuum Dielectric Approach.
Shek Ling Chan & Carmay Lim*, *J. Phys. Chem.* **(1994)** *98*, 12805–12814.

25. Computational Approaches to the Blood Substitute Problem.
Shek Ling Chan & Carmay Lim*, *Chemistry* **(1994)** *52*, 261–268.

26. Solution Free Energies from a Combined Quantum Mechanical & Continuum Dielectric Approach.
Carmay Lim*, Shek Ling Chan & Philip Tole, in *ACS Symposium Series No. 568: Structure and Reactivity in Aqueous Solution.* C.J. Cramer & G.D. Truhlar (editors), American Chemical Society **(1994)**.

27. Molecular Dynamics Simulation of *E. Coli* Ribonuclease HI in Solution: Correlation with NMR and X–ray Data and Insights into Biological Function.
Marios Philippopoulos & Carmay Lim*, *J. Mol. Biol.* **(1995)** *254*, 771–792.

28. Identifying the Mechanism of Protein Loop Closure: A Molecular Dynamics Simulation of the Bacillus Stearothermophilus LDH Loop in Solution.
Marios Philippopoulos, YueFang Xiang & Carmay Lim*, *Protein Engineering* **(1995)** *8*, 565–573.

29. Discrete, Dynamic Polymer Modeling: A Pseudo–Diatomic Model of Lignin.
Marc Roussel & Carmay Lim*, *J. Comp. Chem.* **(1995)** *16*, 1181–1191.

30. Dynamic Model of Lignin Growing in Restricted Spaces.
Marc Roussel & Carmay Lim*, *Macromolecules* **(1995)** *28*, 370–376.

31. A Commentary on the Relationship Between Continuum Dielectric Theory, and Thermodynamics.
Shek Ling Chan, Wen Ching Hu & Carmay Lim*, *Proceedings of HPC–Asia* **(1995)**.

32. The Binding Mode of an E–64 Analog to the Active site of Cathepsin B.
Ming Hsiang Feng, Shek Ling Chan, YueFang Xiang, Carol P. Huber & Carmay Lim*, *Protein Engineering* **(1996)** *9*, 977–986.

33. Positive Charge at Position 549 is Essential for Phosphatidylinositol 4,5–Bisphosphate but not Phosphatidylinositol–Hydrolyzing Activities of Human Phospholipase C δ 1.
Li-Ping Wang, Carmay Lim, Y.-S. Kuan, Chih-lin Chen, Hwei-Fang Chen & King Klim*, *J. Biol. Chem.* **(1996)** *271*, 24505–24516.

34. Structural Characterization of the Phosphotyrosine Binding Region of a High Affinity SH2 Domain–Phosphopeptide Complex by MD Simulation and Chemical Shift Calculations.
Ming-Hsiang Feng, Marios Philippopoulos, Alexander D. MacKerell Jr. & Carmay Lim*, *J. Am. Chem. Soc.* **(1996)** *118*, 11265–11277.

35. Accuracy and Precision of NMR Relaxation Experiments and MD Simulations for Characterizing Protein Dynamics.
Marios Philippopoulos, Arthur Mandel, Arthur G. Palmer III* & Carmay Lim*, *Proteins: Structure, Function, and Genetics* **(1997)** *28*, 481–493.

36. An *ab Initio* Study of Nucleophilic Attack of Trimethyl Phosphate.
Nai-Yuan Chang & Carmay Lim*, *J. Phys. Chem. A* **(1997)** *101*, 8706–8713.

37. Protein Dynamics: Molecular Dynamics Simulation, NMR Spectroscopy and X–ray Crystallography.
Marios Philippopoulos & Carmay Lim*, *Advances in Computational Life Sciences* **(1998)** *Vol. 2: Humans to Proteins.* M. Michalewicz (Ed.), CSIRO Mathematical & Information Sciences

38. Factors Governing the Enhanced Reactivity of Five–Membered Cyclic Phosphate Esters.
Nai-Yuan Chang & Carmay Lim*, *J. Am. Chem. Soc.* **(1998)** *120*, 2156–2167.

39. Ring Strain Energies from *Ab Initio* Calculations.
Todor Dudev & Carmay Lim*, *J. Am. Chem. Soc.* **(1998)** *120*, 4450–4458.

40. Prediction of an Anti–IgE Binding Site on IgE.
Jon Wright & Carmay Lim*, *Protein Engineering* **(1998)** *11*: 421–427.

41. Exploring the Dynamic Information Content of a Protein NMR Structure: Comparison of a Molecular Dynamics Simulation with the NMR and X–Ray Structures of *E. Coli* RNase HI.
Marios Philippopoulos & Carmay Lim*, *Proteins: Structure, Function & Genetics* **(1999)** *36*: 87–110.

42. Ring Strain vs. Solvent Effects in Phosphate Base Hydrolysis.
Carmay Lim, *Phosphorus, Sulfur & Silicon* **(1999)** *144–146*: 769–773.

43. A New Interpretation of the Effective Born Radius from Simulation and Experiment.
C. Satheesan Babu & Carmay Lim*, *Chem. Phys. Lett.* **(1999)** 310: 225–228.

44. Theory of Ionic Hydration: New Insights from Simulation and Experiment.
C. Satheesan Babu & Carmay Lim*, *J. Phys. Chem. B* **(1999)** 103: 7958–7968.

45. Competitive Binding in Mg Coordination Chemistry: Water vs Ligands of Biological Interest.
Todor Dudev, Jimmy Cowan & Carmay Lim*, *J. Am. Chem. Soc.* **(1999)** 121: 7665–7673.

46. Incremental Binding Free Energies In Mg^{2+} Complexes: A DFT Study.
Todor Dudev & Carmay Lim*, *J. Phys. Chem. A* **(1999)** 103: 8093–8100.

47. Metal Binding in Proteins: The Effect of the Dielectric Medium.
Todor Dudev & Carmay Lim*, *J. Phys. Chem. B* **(2000)** 104: 3692–3694.

48. Tetrahedral vs. Octahedral Zinc Complexes with Ligands of Biological Interest: A DFT/CDM Study.
Todor Dudev & Carmay Lim*, *J. Am. Chem. Soc.* **(2000)** 122: 11146–11153.

49. Design, Synthesis, and SAR of Novel Carbapenem Antibiotics with High Stability to *Xanthomonas maltophilia* Oxyiminocephalosporinase Type II. Gholam H. Hakimelahi*, Ali A. Moosavi-Mohavedi, Shwu-Chen Tsay, Fu-Yuan Tsai, Jon Wright, Todor Dudev, Shahram Hakimelahi & Carmay

Lim*, *J. Med. Chem.* **(2000)** 43: 3632–3640.

50. Conformational Analysis of Long Spacers in PROSITE Patterns.
Kuen-Yi Lin, Jon Wright & Carmay Lim*, *J. Mol. Biol.* **(2000)** 299: 537–548.

51. Metal Selectivity in Metalloproteins: Zn^{2+} vs. Mg^{2+}.
Todor Dudev & Carmay Lim*, *J. Phys. Chem. B* (**2001**) 105: 4446–4452.

52. Modeling Zn^{2+}–Cysteinate Complexes in Proteins.
Todor Dudev & Carmay Lim*, *J. Phys. Chem. B* (**2001**) 105: 10709–10714.

53. Solvation Free Energies of Polar Molecular Solutes: Application of the Two–Sphere Born Radius in Continuum Models of Solvation.
C. Satheesan Babu & Carmay Lim*, *J. Chem. Phys.* **(2001)** 114: 889–899.

54. Incorporating Nonlinear Solvent Response in Continuum Dielectric Models Using A Two–Sphere Description of the Born Radius.
C. Satheesan Babu & Carmay Lim*, *J. Phys. Chem. A* **(2001)** 105*:* 5030–5036.

55. A Fast Method For Predicting Amino Acid Mutations That Lead to Unfolding.
Jon D. Wright & Carmay Lim*, *Prot. Engineering* **(2001)** 14: 479–486.

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