

CURRICULUM VITAE

BIOGRAPHICAL

Name: Lee Wei Yang

Birth Year: 1976

Current position: Professor & Director
Inst. of Bioinformatics and Structural Biology,
Director, PhD program in Biomedical Artificial Intelligence
National Tsing Hua University

Birth Place: Taiwan

Honorary Professor, Dept. Mathematical Sciences,
University Liverpool (2019-2022, Dual PhD degree program)
Visiting Scholar, Tokyo Institute of Technology, Japan (2023)
Visiting Professor, University of Pittsburgh, USA (2022)
Visiting Professor, IPR, Osaka University, Japan (2018)
Program Coordinator (IDP3, TG4.3),
Physics Division,
National Center of Theoretical Sciences (NCTS)



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Personal [highlight](#) and [news](#)

RESEARCH INTEREST

We use a spectrum of physics models to study protein/RNA conformational changes and the consequent protein-drug and protein-protein interaction; The dynamics features are used to understand biomolecular functions, predict enzyme active sites, protein-DNA binding sites and protein-protein binding interfaces etc. Normal mode analysis, time-dependent linear response theory and molecular dynamics simulations are used to refine X-ray/NMR-determined structure complexes, understand intra-/intermolecular signal communication, design antimicrobial peptides/ anticancer drugs, explore protease degradation mechanism, study down-regulation of autophagic flux to suppress tumors in xenografted mice, design peptide drugs/ antimicrobial peptides and understand ribosomal helicase activities in unwinding secondary structures of mRNA. We also develop new bioinformatics tools such as fast comparison tools for long text strings and chromosome identification using algorithms implemented for Next Generation Sequencing

The techniques we used in research include but are not limited to Machine Learning Algorithms, Protein Dynamics, Polymer Physics, Molecular mechanics, Coarse-Grained modeling and simulations, Enzymology, Active site prediction, Physical model-based prediction/analysis of NMR relaxation data and temperature factors of X-ray determined structures, Structure Refinement, DNA Polymerase, Homology modeling, Biological and dynamics database/online calculation tools development, Statistical analysis of biomolecular traits in dynamics, Computational techniques for large matrix decomposition, Linear response theory, Normal Mode Analysis, Langevin Dynamics, Theoretical reconciliation of lock-and-key and induce-fit paths on substrate binding.

Wet labs techniques involved in our researches include basic biochemistry/molecular biology/cell culture/biophysics techniques as well as optical tweezers, FRET, fluorescence anisotropy, NMR spectroscopy, x-ray crystallography.

EDUCATION AND TRAINING

POSTGRADUATE:

Postdoctoral Fellow in Dr Shakhnovich's lab, Dept. of Chemistry and Chemical Biology, Harvard University, Boston (2010- 2011)

Postdoctoral Scientist in Dr Chachisvilis's lab, La Jolla Bioeng. Inst, San Diego (2009-2010)

JSPS Researcher in Dr. Akio Kitao's lab, Inst. of Molecular and Cellular Bioscience., University of Tokyo (2006- 2009)

Research Associate in Dr. Ivet Bahar's lab, Dept. of Computational Biology, School of Medicine, University of Pittsburgh (2005- 2006)

GRADUATE:

Ph.D. in Molecular Genetics and Biochemistry (MGB), School of Medicine, University of Pittsburgh (Sept.,2001-Jun.,2005); Dissertation title: Biomolecular dynamics revealed by elastic network models and the study of mechanical key sites for ligand binding

M.S. in Chemical Engineering, National Tsing Hua University (NTHU), Taiwan, (1997-1999); Thesis title: "Application of immobilized D-hydantoinase on ion exchanger"

UNDERGRADUATE:

B.S. in Chemical Engineering, National Taiwan University (NTU), Taiwan (1993-1997)

APPOINTMENTS and POSITIONS

ACADEMIC:

Year

Division Director of International Students, Office of Global Affairs, National Tsing Hua University, Hsinchu, Taiwan, Aug, 2016- Jan, 2019

Visiting Professor, Institute of Protein Research, Osaka University, Japan, Aug, 2018 – Oct, 2018

Associate Professor in Institute of Bioinformatics and Structural Biology, National Tsing Hua University, Hsinchu, Taiwan 2015- 2018

Assistant Professor in Institute of Bioinformatics and Structural Biology, National Tsing Hua University, Hsinchu, Taiwan 2011- 2015

Postdoctoral fellow, Dept of Chemistry and Chemical Biology, Harvard 2010-2011

Postdoctoral researcher, La Jolla Bioengineering Institute 2009-2010

Visiting Scholar, University of Pittsburgh 2009

JSPS foreigner researcher, University of Tokyo and JAEA 2006-2009

TA - Microbiology lab of 1st year Pitt Med students 2004, Spring/2005

- BBSI summer class in CCBB, Univ. of Pitt 2003

- Undergraduate classes, NTHU 1997-1999

RA - Dr. Ivet Bahar's lab (elastic network model), University of Pittsburgh 2002-Summer/2005

- Dr. Richard Wood's lab (DNA repair), University of Pittsburgh 2002

- Dr. Leaf Huang's lab (nonviral gene therapy), University of Pittsburgh 2001

- Dr. P.H.Liang's lab (PCR/mutation/Enzyme kinetics), Academia Sinica 2000

NON-ACADEMIC:

Division Director of International students, Office of Global Affairs,

National Tsing Hua University 2016-

Academic Affair Members in TIGP Bioinformatics Program (since 2012),

Recruitment Committee Members in TIGP CBMB Program (since 2017),

hosted by Academia Sinica, Taiwan. 2012-

Vice director, UPitt chapter of Tsu-chi charity group 2004

Process Engineer, CTCI Corp. Taipei, Taiwan 2000

Chem. Plant Investigator, Ping-Ching Tech. Taipei, Taiwan 1997

Investigator, Council of Aboriginal Affairs Taipei City Hall 1996

Engineering School Student Representative (NTU) 1996

Director, Star-Rain Group (help Autistic children in NTU) 1995

CERTIFICATION, LISCENSURE AND PROGRAMMING SKILLS

SPECIALITY CERTIFICATION:

Certified UNIX programmer (1999)

MEDICAL or OTHER PROFESSIONAL LISCENSURE:

Certified researcher for laboratory small animals (2001)

PROGRAMMING SKILLS:

OS: Windows, UNIX, Linux, SGI-based; Programming languages: C/C++, FORTRAN, PERL, JAVA, MATLAB; Professional Software: Mathematica, Midas, Chimera, VMD, SwissPDBViewer, Rasmol, Chime, Jmol, MOE, InsightII, NAMD, UHBD, Kaliedagraph, origin, Cygwin, Apache/Tomcat

MEMBERSHIPS IN PROFESSIONAL AND SCIENTIFIC SOCIETIES

Organization

Year

台灣學術倫理教育學會(Taiwan Association for Academic Ethics Education)

since 2021

Board member of Taiwanese Society for Computational Neuroscience (sfCN)

(理事) since 2020

ACS member, USA since 2019

Biophysical Society of R.O.C. since 2011

Biophysics Society since 2004

ISMB since 2006

Biophysical Society of Japan since 2008

Others

Board member of 李昭仁教授生醫工程基金會 (董事) since 2022
Board member of Praexisio Taiwan Inc. (董事) since 2020

AWARD & HONORS

1999: China Technical Consultants, INC. Scholarship
1999: The Phi Tau Phi honorary members (2 students each college)
2001 - 2003: Scholarship for INTBP students of School of Medicine
2003 - 2005: Research fellowship
2006: DCB Best Student Award + Annual Retreat Best Poster Award
2006: Stephen L. Phillips Scientific Achievement Award
2006 - 2009: JSPS fellowship for foreign researchers
2011: 國立清華大學新聘教師激勵研究專案補助
2012: 101 年傑出學術研究出版獎勵
2012- 2013: 計畫薪資(102N1707E1)激勵新聘助理教授
2012- 2015: 獲教學績優獎勵
2017: Ta-You Wu Memorial Award 吳大猷先生紀念獎 (national award; 300,000 NTD)
2017-2018: International Collaboration Research of IPR, Osaka University (funding : 400,000 JP Yen)
2019: 108 年第 1 梯次中研院短期訪問學人 (subsidy:150,000 NTD)(2019)
2019-2020: Awarded 48,000 node-hours computation resources by High Performance Computing Infrastructure (HPCI), Japan, for the year 2019-2020
2022: 2022 國家新創獎 (初創企業組)

Research Funds Granted from MOST and Private Sector, Taiwan (in NTD; since 2011)

計畫名稱 (Project Names) ▲▼	起訖日期 ▲▼	擔任工作	經費總額 ▲▼
應用分子動力模擬與轉錄體分析研發氨基糖?類抗生素及順鉑耳毒性之保護策略(111-2314-B-303-022-)	2022/08/01~ 2023/07/31	共同主持人	1,000,000
細菌與哺乳類細胞中 -1 轉譯軌道移轉的機制與調控—以電腦輔助的光鉗篩藥平台來開發抗病毒藥物來調控偽節造成的框架轉移並以冷凍電顯觀察核糖體構型變化(3/3)(111-2311-B-007-001-)	2022/08/01~ 2023/07/31	主持人	1,800,000
克服現時肺癌治療之困境：藥物投遞、精準標靶與抗藥性(111-2628-B-038-020-MY3)	2022/08/01~ 2025/07/31	共同主持人	4,650,000
以可藥動態組輔助新適應症拓展及安全新藥之開發(1/3)(111-2113-M-007-016-)	2022/08/01~ 2023/07/31	主持人	2,800,000
細菌與哺乳類細胞中 -1 轉譯軌道移轉的機制與調控—以電腦輔助的光鉗篩藥平台來開發抗病毒藥物來調控偽節造成的框架轉移並以冷凍電顯觀察核糖體構型變化(2/3)(110-2311-B-007-008-)	2021/08/01~ 2022/10/31	主持人	1,800,000
細菌與哺乳類細胞中 -1 轉譯軌道移轉的機制與調控—以電腦輔助的光鉗篩藥平台來開發抗病毒藥物來調控偽節造成的框架轉移並以冷凍電顯觀察核糖體構型變化(1/3)(109-2311-B-007-008-)	2020/08/01~ 2021/07/31	主持人	1,800,000

結合以第一原理及巨量資料驅動的抗癌及抗菌胜?設計(3/3)(109-2113-M-007-002-)	2020/08/01~ 2021/07/31	主持人	1,560,000
藉由對核醣體與訊息核糖核酸間相互作用的動力學分析 來探究轉譯讀取軌道恆定維持的調控機制—探究功能性訊息核糖核酸及其解旋中間態對於核醣體構型改變及+1/-1 轉譯軌道移轉之影響(3/3)(108-2313-B-007-001 -)	2019/08/01~ 2020/07/31	主持人	1,260,000
結合以第一原理及巨量資料驅動的抗癌及抗菌胜肽設計(2/3)(108-2113-M-007-005 -)	2019/08/01~ 2020/07/31	主持人	2,120,000
藉由對核醣體與訊息核糖核酸間相互作用的動力學分析 來探究轉譯讀取軌道恆定維持的調控機制—探究功能性訊息核糖核酸及其解旋中間態對於核醣體構型改變及+1/-1 轉譯軌道移轉之影響(2/3)(107-2313-B-007-001-)	2018/08/01~ 2019/07/31	主持人	1,260,000
結合以第一原理及巨量資料驅動的抗癌及抗菌胜肽設計(1/3)(107-2113-M-007-015-)	2018/08/01~ 2019/07/31	主持人	1,200,000
藉由對核醣體與訊息核糖核酸間相互作用的動力學分析 來探究轉譯讀取軌道恆定維持的調控機制—探究功能性訊息核糖核酸及其解旋中間態對於核醣體構型改變及+1/-1 轉譯軌道移轉之影響(1/3)(106-2313-B-007-001-)	2017/08/01~ 2018/07/31	主持人	1,200,000
利用癌症標的蛋白的異構調控現象以及新的 FDA 核准用藥篩選平台來專一性地抑制 ATG4B(106-2113-M-007-022-)	2017/08/01~ 2018/07/31	主持人	1,425,000
第一原理結合大數據來設計抗菌及抗癌 α - 螺旋胜?(105-2113-M-007-017-)	2016/08/01~ 2017/07/31	主持人	1,600,000
開發 ATG4s 及 ATG4B 專一性抑制劑用以治療癌症(105-2311-B-075B-001-)	2016/08/01~ 2017/07/31	共同主持人	1,000,000
以適切的線性響應理論來量化的預測遠端的點突變對酵素的基質結合以及催化速率的影響(104-2113-M-007-019-)	2015/08/01~ 2016/07/31	主持人	1,800,000
核醣體轉譯過程中訊息核糖核酸結構之解旋與折疊及其對-1 轉譯框架移轉的調控機制—建構核醣體對外界干擾進行響應的動態模擬(子計畫四)(3/3)(103-2627-M-007-001-)	2014/08/01~ 2015/07/31	主持人	1,150,000
核醣體轉譯過程中訊息核糖核酸結構之解旋與折疊及其對-1 轉譯框架移轉的調控機制—建構核醣體對外界干擾進行響應的動態模擬(子計畫四)(2/3)(102-2627-M-007-003-)	2013/08/01~ 2014/07/31	主持人	2,128,000
核醣體轉譯過程中訊息核糖核酸結構之解旋與折疊及其對-1 轉譯框架移轉的調控機制—建構核醣體對外界干擾進行響應的動態模擬(子計畫四)(1/3)(101-2627-M-007-010-)	2012/08/01~ 2013/07/31	主持人	1,570,000
量化的預測異構調控對酵素活性的影響 (100-2112-M-007-020-)	2011/08/01~ 2012/07/31	主持人	535,000

107 產學合作績優教師遴選資料核對表

系所	生資所		姓名	楊立威		
產學計畫名稱	執行起時	執行迄時	計畫 總金額	管理費 金額	管理費 合計	核算 點數
具隱私保護功能的全文比對搜尋引擎研究計畫	2018/09/01	2019/08/31	940,000	188,000	349,500	2
光鉗節藥研究	2018/08/01	2019/07/31	807,500	161,500		

Know-How 技轉技術名稱	合約 簽訂日	技轉金 入帳日	技轉金額	Know-How 技轉金額 合計	核算 點數
光鉗節藥研究	2018/08/20	2018/09/12	142,500	142,500	1

Tech. Name	專利名稱/ Patent name	Licensor	Licensee	Effective Data	Royalty	MOST fund no.
電腦輔助之藥物開發服務		N T H U 100%	Praexisio Taiwan Inc.	2020/07/01	200,000	
電腦輔助之蛋白質活性調控設計及可藥點預測服務		N T H U 100%	Praexisio Taiwan Inc.	2020/07/01	300,000	MOST104-2113-M007-019
據隱私保護功能的全文搜尋引擎、據隱私保護功能的剽竊偵測應用及軟體產品	文字比對方法、系統及其電腦程式產品	N T H U 60%; NCTU 40%	Praexisio Taiwan Inc.	2020/07/01	300,000	

Patent Granted

類別	專利名稱	國別	專利號碼	發明人	專利權人	專利核准日期	科技部計畫編號
A	評估抗菌胜肽之抗菌力之系統及其使用方法	中華民國	I557587	蔡政育,李紅春,程家維,游輝元,楊立威	國立清華大學 100%	2016/11/11	105-2113-M-007-017-
A	評估抗菌胜肽之抗菌力之系統及其使用方法	中國	3376320	蔡政育,李紅春,程家維,游輝元,楊立威	國立清華大學 100%	2019/05/14	105-2113-M-007-017-107-2113-M-007-015-
A	In silico design of peptides equilibrated in a lipid bilayer with partition free energies indicating probability of antimicrobial activity	美國	10,810,329	蔡政育,李紅春,程家維,游輝元,楊立威	國立清華大學 100%	2020/10/20	105-2113-M-007-017-107-2113-M-007-015-

A	METHOD FOR THE TREATMENT OF ATG4-RELATED DISORDERS	美國	10,583,123	蔡昆霖,徐志文,劉佩芬,楊立威	國立清華大學 100%	2020/03/10 (~2037-12-15)	105-2311-B-075B-001-106-2113-M-007-022-107-2113-M-007-015-
A	治療 ATG4 相關病症的方法	中華民國	I732084	蔡昆霖,徐志文,劉佩芬,楊立威	國立清華大學 100%	2021/07/01(~2037/12/25)	105-2311-B-075B-001-106-2113-M-007-022-107-2113-M-007-015
A	文字比對方法、系統及其電腦程式產品	中華民國	I719537	楊立威,洪瑞鴻,Emmanuel Salawu,張芄瑜	國立清華大學 60%, 國立陽明交通大學 40%	2021/02/21(~2039/07/15)	https://patentscope.wipo.int/search/en/detail.jsf?docId=US31529214 8 (歐、中專利申請中)
A	PRIVACY-KEPT TEXT COMPARISON METHOD, SYSTEM AND COMPUTER PROGRAM PRODUCT	美國	11232157	Lee-Wei Yang, Jui-Hung Hung, Emmanuel Oluwatobi Salawu, Yuan-Yu Chang	國立清華大學 60%, 國立陽明交通大學 40%	2022/01/25(~2040-02-14)	https://patentscope.wipo.int/search/en/detail.jsf?docId=US31529214 8 (歐、中專利申請中)

Technique Transfer

編號/名稱	起迄	總金額/管理費
108A0232V9 具隱私保護功能的全文比對搜尋引擎研究	2019/11/15 2020/11/14	1,187,500 237,500

國際產學營運總中心 敬啟 108 年 4 月 8 日

107 產學合作績優教師遴選資料核對表

系所	生資所		姓名	楊立威		
產學計畫名稱	執行起時	執行迄時	計畫 總金額	管理費 金額	管理費 合計	核算 點數
具隱私保護功能的全文比對搜尋引擎研究計畫	2018/09/01	2019/08/31	940,000	188,000	349,500	2
光鉗篩藥研究	2018/08/01	2019/07/31	807,500	161,500		

Know-How 技轉技術名稱	合約 簽訂日	技轉金 入帳日	技轉金額	Know-How 技轉金額 合計	核算 點數
光鉗篩藥研究	2018/08/20	2018/09/12	142,500	142,500	1

技術名稱	專利名稱	授權單位	被授權單位	簽約日期	權利金, 衍生利	科技部計畫編號
電腦輔助之藥物開發服務		國立清華大學 100%	普睿思股份有限公司	2020/07/01	200,000	
電腦輔助之蛋白活性調控設計及可藥點預測服務		國立清華大學 100%	普睿思股份有限公司	2020/07/01	300,000	MOST104-2113-M 007-019
據隱私保護功能的全文搜尋引擎、據隱私保護功能的剽竊偵測應用及軟體產品	文字比對方法、系統及其電腦程式產品	國立清華大學 60% 交大 40%	普睿思股份有限公司	2020/07/01	300,000	

Peer Review / Editorial Experience in Scientific Journals

Peer Review:

1. Proceedings of the National Academy of Sciences of the USA (PNAS) (1 manuscript)
2. Nucleic Acid Research (2 manuscripts)
3. Bioinformatics (6 manuscripts)
4. PLoS Computational Biology (1 manuscript)
5. Journal Molecular Biology (1 manuscript)
6. Biophysical Journal (3 manuscripts)
7. Proteins: Structure, Function and Bioinformatics (14 manuscripts)
8. Scientific Reports (3 manuscripts)
9. BioMed Research International (1 manuscript)
10. Journal of Biomolecular Structure & Dynamics (1 manuscript)
11. International Journal of Molecular Sciences (1 manuscript)

Editorial:

1. Special Issue Editor of *International Journal of Molecular Sciences* (IF=6.2) (2023-)
2. Associate Editor of *Frontiers in Molecular Biosciences* (IF=6.1) (2022-)
3. Associate Editor of *Biophysics and Physicobiology* (2022-)
4. Guest Editor of a thematic issue “Conformational allostery- and folding-controlled Medication” in *Current Medicinal Chemistry* (2019-2020; IF=3.5)
<https://benthamscience.com/journals/current-medicinal-chemistry/special-issues/>
<https://benthamscience.com/journal-files/special-issue-details/CMC-SII20170522-01.pdf>
5. Lead Guest Editor for a Special Issue “Theoretical and Experimental Advances in Understanding Biomolecular Dynamics, Interactions, and Allostery” in *BioMed Research International* (2014-2015; IF=2.7) <http://www.hindawi.com/journals/bmri/si/621813/cfp/>
6. Lead Guest Editor for a Special Issue “Functional Dynamics of Proteins” in *Computational and Mathematical Methods in Medicine* (2012; IF=1.0)
<http://www.hindawi.com/journals/cmmm/si/891327/>

PUBLICATIONS (IF: Impact Factor/Journal Ranking) [times cited as of Feb 2020]

Journals

Yuan-Yu Chang, Christopher Llynard Ortiz, Wen-Guey Wu*, Lee-Wei Yang* (202x) Salt bridges formed by phosphorylated Y73 stabilizes the dimerization interface of PIP2-bestriding FGF2 monomers. (to be submitted)

Justin Chan, Jinhao Zou, Rong-Long Pan, Hui-Hsu Tsai*, Tzu-Ying Liu*, Lee-Wei Yang* (2023) Mechanochemical coupling found in PHT1;1 facilitates inorganic phosphate transport. (to be submitted)

Po-Chun Chen, Ahmed Ragab, Hsiu-Ting Hsu, Yu-Ling Lu, Shalaka Patil and Kung-Yao Chang*, Jin-Der Wen* and Lee-Wei Yang* (202x) An accurate and efficient predictor for -1 Programmed Ribosomal Frameshifting (-1PRF) signals in viral genomes. (to be submitted)

Yuan-Yu Chang^{1,2,¶}, Bob-Son Huang^{1,3,¶}, Ching-Tang Hsu¹, Mihir Janel¹, Yuan-Da He¹, Che Lin^{3,6*}, Lee-Wei Yang^{1,2,6,7,*} (2023) Deep Architectures for Protein Dynamics Prediction that Facilitates the Flexible Protein Docking. (to be submitted)

Tzong-Huah Wu^{1,2,3,†}, Emmanuel Oluwatobi Salawu^{3,4,†}, Christopher Ortiz³, Yuan-Da He³, Chung-Ke Chang⁵, Tai-Huang Huang⁵, Lee-Wei Yang^{3,4,6,*} and Joseph Jen-Tse Huang^{1,7,*} (2023) Possible dsDNA Unwinding Activities Evolved from Potent RNA-Recognition Motifs Leveraging a Guanine-Binding Specificity. (to be submitted)

Emmanuel Oluwatobi Salawu^{1,2,§}, Manuel Maestre Reyna^{3,§,*}, Yuan-Yu Chang¹, Shun Sakuraba^{4,5}, and Lee-Wei Yang^{1,2,6,*} (2023) Water Molecules Actively Facilitate DNA-Kinking Induced by a Sequence General DNA-Bending Protein Sac7d. (to be submitted)

Bang-Chieh Huang, Chi-Hong Chang-Chein, Lee-Wei Yang* (2024) Intramolecular Communication and Allosteric Sites in Enzymes Unraveled by Time-Dependent Linear Response Theory. *bioRxiv* doi: <https://doi.org/10.1101/677617>

Kun-Lin Tsai, Chi-Yuan Kao, Yuan-Yu Chang, Tzu-Kuan Lin, Sui-Yuan Chang and Lee-Wei Yang (2024) DRDOCK leverages conformational dynamics and prioritizes favored binding properties of FDA-approved drugs in drug repurposing automation. *bioRxiv* doi: <https://www.biorxiv.org/content/10.1101/2021.01.31.429052v4>; <https://dyn.life.nthu.edu.tw/drdoack/>

0. Yu-Ying Cheng#, Anindita Ganguly#, Yi-Yun Cheng#, Christopher Llynard D. Ortiz, Arnab Pala, Pramod Shah, Lee-Wei Yang*, Zong-Hong Lin* (2024) Development of Label-Free Triboelectric Nanosensor as a Drug Screening Platform. *Nano Energy* (being peer reviewed)

1. Cheng-Yu Tsai, Ying-Chang Lu, Yen-Hui Chan, Navaneethan Radhakrishnan, Yuan-Yu Chang, Shu-Wha Lin, Tien-Chen Liu, Chuan-Jen Hsu, Pei-Lung Chen, Lee-Wei Yang*, Chen-Chi Wu* (2023) Simulation-Predicted and -Explained Inheritance Model of Pathogenicity Confirmed by Transgenic Mice Models. *Computational and Structural Biotechnology Journal*, 21, 5698–5711 <https://www.sciencedirect.com/science/article/pii/S2001037023004415> (5-yr IF: 6.3; Ranking: 60/285 in Biochemistry & Molecular Biology)

2. Yuan-Yu Chang, Sheng-Tang Wong, Emmanuel Oluwatobi Salawu, Ming-Hsuan Liao, Jui-Hung Hung* and Lee-Wei Yang* (2023) Full-privacy secured search engine empowered by efficient genome-mapping algorithms. *IEEE Journal of Biomedical and Health Informatics*, 27, issue 10, 5155-5164 <https://ieeexplore.ieee.org/document/10198547/> (5-yr IF: 7.7; Ranking: 4/67 in Mathematical & Computational Biology)

3. Anupam Banerjee, Satyaki Saha, Nathan C. Tvedt, Lee-Wei Yang and Ivet Bahar (2023) Mutually Beneficial Confluence of Structure-Based Modeling of Protein Dynamics and Machine Learning Methods. *Current Opinion in Structural Biology*, 78, 102517. <https://doi.org/10.1016/j.sbi.2022.102517> (5-yr IF: 7.5; Ranking: 34/297 in Biochemistry & Molecular Biology)

4. Hsuan Cheng, Yu-Lin Kao, Ting Chen, Lohitaksh Sharma, Wen-Ting Yang, Yi-Chien Chuang, Shih-Han Huang, **Hong-Rui Lin**, Yao-Shen Huang, Ching-Lin Kao, **Lee-Wei Yang**, Rachel Bearon, Hui-Chun Cheng, Kuo-Chiang Hsia, and Yu-Chun Lin* (2022) Actin filaments form a size-dependent diffusion barrier around centrosomes. *EMBO Reports*. 24, e54935 <https://doi.org/10.15252/embr.202254935> (5-yr IF: 10.4; Ranking: 48/297 in Biochemistry & Molecular Biology)
5. **Cheng-Yu Tsai**, Emmanuel O Salawu, **Hongchun Li**, Guan-Yu Lin, Ting-Yu Kuo, **Liyin Voon**, **Adarsh Sharma**, **Kai-Di Hu**, **Yi-Yun Cheng**, **Sobha Sahoo**, **Lutimba Stuart**, **Chih-Wei Chen**, **Yuan-Yu Chang**, **Yu-Lin Lu**, **Ximai Ke**, **Christopher Llynard D. Ortiz**, Bai-Shan Fang, Chen-Chi Wu, Chung-Yu Lan*, Hua-Wen Fu*, **Lee-Wei Yang*** (2022) Helical Structure Motifs Made Searchable to Facilitate the Functional Peptide Design. *Nature Communications* 13, Article number: 102 (5-yr IF: 15.8; Ranking: 4/72 in Multidisciplinary Sciences)
6. Wentong Fang, Chengheng Liao, Giada Zurlo, Jeremy Simon, Travis Ptacek, Youqiong Ye, Leng Han, Cheng Fan, **Christopher Ortiz**, **Hong-Rui Lin**, Ujjawal Manocha, William Kim, and **Lee-Wei Yang** and Qing Zhang (2021) ZHX2 Promotes HIF1 α Oncogenic Signaling in Triple-Negative Breast Cancer. *eLife*, 10:e70412 <https://elifesciences.org/articles/70412> (5-yr IF: 9.1; Ranking: 5/93 in Biology)
7. K K DurgaRao Viswanadham, Roland Böttger, Lukas Hohenwarter, Anne Nguyen, Elham Rouhollahi, Alexander Smith, **Yi-Hsuan Tsai**, **Yuan-Yu Chang**, **Christopher Llynard Ortiz**, **Lee-Wei Yang**, Liliana Jimenez, Siyuan Li, Chan Hur, Shyh-Dar Li (2021) An Effective and Safe Enkephalin Analog for Antinociception. *Pharmaceutics*, 13, 927- (IF: 6.1)
8. **Justin Chan**, **Hong-Rui Lin**, Kazuhiro Takemura, **Kai-Chun Chang**, **Yuan-Yu Chang**, Yasumasa Joti, Akio Kitao* and **Lee-Wei Yang*** (2020) An efficient timer and sizer of biomacromolecular motions. *Structure*, 28, 259-269 (<https://doi.org/10.1016/j.str.2019.10.020>) (IF: 5.9; Ranking: 9/72 in Biophysics)
9. **Justin Chan**, **Jinhao Zou**, **Christopher Llynard Ortiz**, **Chi-Hong Chang Chien**, Rong-Long Pan, **Lee-Wei Yang*** (2020) DR-SIP: Protocols for Higher Order Structure Modeling with Distance Restraints- and Cyclic Symmetry-Imposed Packing. *Bioinformatics*, 36, 449–461. <https://doi.org/10.1093/bioinformatics/btz579> (5-yr IF: 9.9; ranked 3/59 in Mathematical & Computational Biology)
10. **Bang-Chieh Huang** and **Lee-Wei Yang** (2019) Molecular dynamics simulations and linear response theories jointly describe biphasic responses of myoglobin relaxation and reveal evolutionarily conserved frequent communicators. *Biophysics and Physicobiology*, 16, 473-484
11. **Kai-Chun Chang** , **Emmanuel Oluwatobi Salawu**, **Yuan-Yu Chang**, Jin-Der Wen and **Lee-Wei Yang*** (2019) Resolution-exchanged structural modeling and simulations jointly unravel that subunit rolling underlies the mechanism of programmed ribosomal frameshifting. *Bioinformatics*, 35, p945–952. doi: 10.1093/bioinformatics/bty762. (5-yr IF: 9.9; ranked 3/59 in Mathematical & Computational Biology) [1]
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16. **Chandrasekaran, Aravind, Chan, Justin**, Lim, Carmay*, **Yang, Lee-Wei*** (2016) Protein dynamics and contact topology reveal protein-DNA binding orientation. *Journal of Chemical Theory and Computation*. 12, 5269–5277 (IF: 5.8; Ranking: 5/35 in Atomic, Molecular & Chemical Physics) [7]
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21. **Hongchun Li**, Shun Sakuraba, **Aravind Chandrasekaran and Lee-Wei Yang*** (2014) Molecular binding sites are located near the interface of intrinsic dynamics domains (IDDs) *J. Chem. Inf. Model*. 54 (8), 2275-2285. (IF: 4.3; Ranking: 3/100 in Computer Science) [15]
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41. Seki, M., Masutani, C., **Yang, L.-W.**, Schuffert, A., Iwai, S., Bahar, I. and Wood, R.D. (2004) High efficiency bypass of DNA damage by a single human DNA polymerase. *EMBO J.* 23, 4484-4494. (IF: 8.9; Ranking: 20/275 in **Biochemistry & Molecular Biology**) [185]
42. Liu, X., Karimi, H., **Yang, L.-W.**, Bahar, I. (2004) Protein functional motion query and visualization" IEEE Proceedings, 28th Annual International Computer Software and Applications Conference - (COMPSAC'04)
43. Pan, J.J., Kuo, T.H., Chen, Y.K., **Yang, L.-W.**, Liang P.H. (2002) Insight into the activation mechanism of Escherichia coli octaprenyl pyrophosphate synthase derived from pre-steady-state kinetic analysis. *Biochim Biophys Acta.* 1594, 64-73. (IF: 2.8 Ranking: 165/275 in **Biochemistry & Molecular Biology**) [25]
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45. Yang, L.-W. (楊立威) and Chu, I.M. (朱一民) (2000) 以陰離子交換樹脂固定 D-hydantoinase 進行光學分割反應之研究. 化工 47:2=208, p24-33

[1] Annual best student paper (ref 28) award in School of Medicine (for the year 2005-2006), Univ. of Pittsburgh.

Book Chapters

Rader, A.J., Chennubhotla, C., **Yang, L.-W.**, Bahar, I. (2005) "The Gaussian Network Model: Theory and Applications." Normal Mode Analysis: Theory and Applications to Biological and Chemical Systems. Chap 3, CRC Press, London. [8]

Invited/Selected Platform Talks in the International Conferences (110+)

"Integrate Systemic Benefit in the Small-Molecule Drug Design", National Institute of Quantum Science and Technology (QST), Chiba, Japan (Feb 6, 2024)

"Ribosome Rolls to Exercise Translational Control that can Potentially be Modulated by Small-Molecule Drugs", 量子生命, National Institute of Quantum Science and Technology (QST), Chiba, Japan (Jan 19, 2024)

"Science", 樹心學堂 (to senior high school students), Taipei (Dec 16, 2023)

"Integration of on-target and systemic chemical fragments of old drugs in CADD to save the environment and lives", 2023 ACS Global Innovation Imperatives - 7th International Conference on Computation for Science and Technology (ICCST), Kuala Lumpur, Malaysia <https://www.7thiccst2023.com/page-scientific-program-2> (Dec 9, 2023)

"NVIDIA-NTHU JIC and joint research centers outlining NTHU's industry-university collaboration strategy and outlook", IC之音訪問, Hsinchu, Taiwan (Dec 1, 2023)

"Data Science Application in Chemistry", serving as a moderator in the open discussion session, Annual Meeting of Theoretical and Computational Chemistry (理論/計算化學研究交流研討會), Taipei (Nov 26, 2023)

"Systemic Feedback to Drug a Dancing Target on its Multiple Sites" (keynote speaker), the 6th International Conference on Molecular Simulation (ICMS 2023), National Taiwan University, Taipei, Taiwan (Oct 6-9, 2023)

"Drug Design and Screening for the Dancing Targets", National Sun Yat-Sen University, Kaohsiung, Taiwan (July 19, 2023)

"Ribosome Rolls to Exercise Translational Control", Nucleic Acids : Prospect and Therapeutic Applications (2023 核酸結構研究前景與醫學應用國際研討會研討會), National Chung-Hsing University, Taichung, Taiwan (July 7, 2023)

"Drug the dancing targets", Korean Biophysical Society (KBPS) and Korean Society for Protein Science (KSPS) Joint Conference, Busan, Korea (June 22-23, 2023)

"Drug the dancing targets", US BIO 2023, Boston (June 5-8, 2023)

"Safer drug discovery hitting the dancing targets while leveraging systemic effects and multisite targeting.", NTHU BME Day, Hsinchu, Taiwan (Apr 21, 2023)

"Revisit the design of small molecule drugs - evidence from leveraging dancing targets, systemic effects, safer chemical space and multisite targeting", Tokyo Institute of Technology, Tokyo (Jan 19, 2023)

Chairing a session at 111 年理論/計算化學研究成果分享與交流研討會(Dec 17, 2022)

“[Druggable DynOmics](#)”, Multiomics and Precision Medicine Joint Conference 2022 (多體學及精準醫學聯合會議), Chang, Yung-Fa Foundation International Convention Center, 張榮發基金會國際會議廳, Taipei (Nov 20, 2022)

“Drug Discovery Driven by Linear Response Theories, Molecular Mechanics and Bioinformatics”, 2022 NCTS Forum and Annual Meeting 國家理論科學研究中心物理領域成果發表暨研討會, NTU, Taiwan (Nov 19, 2022)

“Drug the Dancing Target by Beneficial Systemic Effects”, 2022 TSBMB Autumn Camp, 2022 台灣生物化學及分子生物學學會生化秋令營, Beipu, Hsinchu (Nov 4, 2022)

“Helical structure motifs made searchable for functional peptide design”, 5th World Chemistry Conference and Exhibition, London, UK (Oct 5, 2022)

“Druggable DynOmics - past, now and the future”, to Poly-omics and Precision Medicine Research Group, NTU hospital, Taipei ([online](#); Oct 5, 2022)

“Drugging the dancing target by leveraging beneficial systemic effects”, Taiwan Theoretical and Computational Molecular Sciences Association, T2COMSA monthly talk (<https://www.t2comsa.tw/2021seminarlist/>), Academia Sinica, Taipei (Sept 29, 2022)

“Drugging the dancing targets by leveraging beneficial off-target effects”, DCSB Seminar, School of Medicine, Univ of Pittsburgh (Aug 30, 2022)

Chairing a Bioinformatics session at ABA-APPA-TBS Joint Congress Program Meeting. NCKU, Tainan (June 24, 2022)

“在分子層面解密生命”, NTU Hospital Hsinchu Branch, Chu-Bei, Taiwan (Apr 1, 2022)

“Small subunit rolling underlies the mechanism of programmed ribosomal frameshifting”, Taiwan Cryo-EM Symposium 2022, Academia Sinica, Taipei (Mar 24, 2022)

“First-principle-based and Data-driven Drug Design Platform Using a Multi-site Targeting Strategy [S41686]”, [Nvidia GTC Conference 2022](#), San Jose (turned online due to COVID19) (Mar 21-24, 2022) <https://www.nvidia.com/gtc/session-catalog/?tab.day=20220323#/session/16385155433000015Zik>

“A First-principle-based and Data-driven Drug Design Platform Leverages Favorable Off-Target Effects and Redefines Specificity Through Multi-Site Targeting”, 2022化學年會(ROC Chemical Society Annual Meeting), NTNU, Taipei (Mar 12-13, 2022)

“Billiard Ball Therapy - Leveraging therapeutic synergy using multi-site drugging in a single disease protein target”, 2021 Asian Federation of Biotechnology (AFOB) Virtual Conference, Seoul, Korea (Nov 1-4, 2021)

“Medicinal Chemistry Says Hello to the Jiggling and Wiggling of Atoms”, TIGP CBMB Faculty Presentation 2020 Autumn, IBC, Academia Sinica, Taipei (Jan 5, 2021)

“Billiard Ball Therapy – drug cocktails targeting the new sites in old/new disease targets” School of Medicine, NTU, Taipei, Taiwan (Dec 23, 2020)

“Billiard Ball Therapy - toward a rational repurposing of FDA drugs that target multiple sites in a disease-modulating protein”理論/計算化學研究成果分享與交流研討會, MOST, Taipei, Taiwan (Dec 12, 2020)

“獵殺舞動的蛋白”, Dept Med Sci Ind, CJC, Tainan, Taiwan (Nov 23, 2020)

“*In silico* design and repurposing of medicine”, iPhD Seminar, NTHU, Hsinchu (May 20, 2020)

“Explore alternative druggable sites in known drug targets, facilitated by Stat Mech theories, Simulations and AI”, Department of Chemistry, Fu Jen Catholic University, Taipei County, Taiwan (March 26, 2020)

“Explore the alternative druggable sites in known drug targets, facilitated by Stat Mech theories, Mechanics Simulations and AI”, Chemical Engineering Department, NTHU, Hsinchu, Taiwan (Dec 25, 2019)

Cross-strait Theoretical Chemistry Conference 海峽兩岸理論與計算化學 CTCC-8, session chair, Academia Sinica, Taipei (Dec 8 2019)

“How to distinguish Agonists from Antagonists for opium receptors?” *1st Members of General Assembly of Taiwan Computational Neuroscience Society*, NTHU, Hsinchu, Taiwan (Nov 16 2019)

“Programmed Ribosomal Frameshifting is Facilitated by 30S Rolling and Evenly Distributed Unfolding Intermediates of Pseudoknots”, *2019 NTHU-Osaka U International Symposium*, Osaka University (Toyonaka campus), Osaka, Japan (Oct 7-10, 2019)

“As Central Dogma Goes off the Rails - Programmed Ribosomal Frameshifting Facilitated by Pseudoknot-Induced 30S Rolling”, the 7th Hong Kong and Cross-Strait Life Science Culture Day, Peking University, Beijing (Sept 2-7, 2019)

“Turn ENM into an efficient timer and sizer of biomacromolecular functional motion”, *Paul Flory's "Statistical Mechanics of Chain Molecules: The 50th Anniversary of Polymer Chemistry"@ ACS Meeting*, San Diego (Aug 27-29, 2019)

“First-Principle-Based and Data-Driven Design of Therapeutics”, *The 23rd International Annual Symposium on Computational Science and Engineering (ANSCE23)*, Chiang Mai, Thailand (June 27-29, 2019)

“Molecular Dynamics Simulations - Theoretical Basis and Trajectory Analysis”, *3rd Taiwan-Philippines Workshop on Computational Chemistry and Physics Program*, Academia Sinica, Taipei, Taiwan (June 21-25, 2019)

“Allosteric drug development for cancer treatment”, School of Medicine, University of North Carolina, Chapel Hill, USA (Apr 2nd, 2019)

“Computer-Aided Design of Orthosteric and Allosteric ATG4 Inhibitors to Suppress Autophagy and Sensitize Cancer Cells to Chemotherapy”, Advanced Drug Delivery Symposium & Annual Meeting of Biomaterials and Controlled Releases Society, National Tsing Hua University, Hsinchu, Taiwan (March 28, 2019)

“Simulation-Aided and Data-Driven Design of Antimicrobial Peptides”, School of Life Science and Technology, Tokyo Institute of Technology, Tokyo, Japan (March 11, 2019)

“Ribosome is signaled to roll to promote programmed ribosomal frameshifting” TARA International symposium: Biological and Structural Mechanisms of Cellular Dynamics, University of Tsukuba, Ibaraki, Japan (March 8, 2019)

“First-principle-based and data-driven design of antimicrobial peptides and protein drugs”, Dept. of Physics, National Central University, Taoyuan, Taiwan (Feb 19, 2019)

“Development of orthosteric/allosteric anti-cancer drugs”, Dept. of Biochemistry, Chulalongkorn University, Bangkok, Thailand (Jan 21, 2019)

“Programmed Ribosomal Frameshifting Facilitated by Pseudoknot-Induced 30S Rolling”, *The 2nd Taiwan-Thailand-Vietnam Workshop on Theoretical and Computational Chemistry*, Thailand Science Park, Pathum Thani Thailand (Jan 16-20, 2019) – One of the three **Plenary Speakers** (representing Taiwan)

“First-principle and data-driven approach to design antimicrobial peptides”, Dept. Che. & Mat. Eng., NYUST, Yunlin, Taiwan (Dec 27th, 2018)

“Mechanobiological studies on water-catalyzed dsDNA bending and programmed ribosomal frameshifting facilitated by pseudoknot-induced 30S rolling.”, *The 8th NTHU-UoL Bilateral Workshop*, Taoyuan, Taiwan (Nov 28, 2018)

“How ribosome rolls to promote programmed frameshifting?”, Institute of Atomic and Molecular Sciences (IAMS), Taipei <https://www.iam.s.sinica.edu.tw/tw/?link=history&type=s> (Nov 15, 2018)

“Computer aided cancer drug development”, Department of Marine Biotechnology and Resources, NSYSU, Kaohsiung, Taiwan (Oct 29, 2018)

“Find and Drug Allosteric Sites Using First-Principle-Based Simulations and Data Driven Approaches”, AS-IIT Delhi Bilateral Meeting, Academia Sinica, Taipei (Oct 4, 2018)

“Resolution-exchanged structural modeling and simulations jointly unravel that subunit rolling underlies the mechanism of programmed ribosomal frameshifting”, <http://www.kansai.qst.go.jp/seminar-2018k17.html> 第45回 KPSI セミナー 関西光科学研究 所 (QST), Kyoto (Sept 26, 2018)

“Computer-aided design of anti-cancer and antimicrobial peptides”, Che. Eng. Dept. NCKU, Tainan (May 4th, 2018)

“Structural and dynamics-based design of anti-cancer and antimicrobial peptides”, National Taiwan University College of Medicine Graduate Institute of Medical Genomics and Proteomics, Taipei (Apr 9th, 2018)

“ATP-Independent dsDNA Helicases Could be Evolved from Potent RNA-Recognition Motifs Leveraging a Guanine-Binding Specificity”, Protein Research Institute/Osaka University, Osaka, Japan (March 27th 2018) (funded visiting and lecture by IPR)

“First-principle-based and data-driven design of therapeutic peptides”, ISGC, Academia Sinica, Taipei (March 20, 2018) <http://event.twgrid.org/isgc2018/program>

“Joint first-principle-based and data-driven methods aid the development of antimicrobial peptides” Dept. of Chemistry, National Taiwan Normal University, Taipei (March 5, 2018) <http://www.chem.ntnu.edu.tw/app/news.php?Sn=1616>

“Rational Design of Allosteric Drugs that Drug the Protein Targets of FDA-Approved Drugs”, Winter meeting of Theoretical/Computational Chemistry, KMU@Kaohsiung (Jan 30- 31, 2018) <https://goo.gl/57tFzR>

“Structural and dynamics-based drug design”, Graduate Institute of Biochemical and Biomedical Engineering, Chang Gung University, Taoyuan (Oct 17, 2017) <http://ibbe.cgu.edu.tw/files/11-1052-8358-1.php?Lang=zh-tw>

“DynOmics: dynamics of structural proteome and beyond”, as a Plenary Speaker, 11th Central and Eastern European Proteomic Conference (CEEPC), Kosice, Slovakia (Sept 28, 2017) <http://lbmi.uvm.sk/ceepe2017/Kosice/Welcome.html> http://lbmi.uvm.sk/ceepe2017/Kosice/Scientific_program_files/Scientific%20Program_1.pdf

“Evolving through jiggling-wiggling atoms – the functional molecular mechanics of proteins studied by first-principle-based and data-driven methods”, Computational Biology Workshop, National Center for Theoretical Sciences (Physics Division), Hsinchu (July 29, 2017) <http://phys.cts.nthu.edu.tw/actnews/intro.php?Sn=364&OSn=770>

“How does water help bend the dsDNA?”, Taiwan-Thailand 2017 Workshop on Theoretical and Computational Chemistry, National Taiwan University (June 16, 2017) <http://phys.cts.nthu.edu.tw/actnews/intro.php?Sn=344&OSn=787>

“Translation frame shift and maintenance are explained by resolution exchanged simulations and linear response theories”, 22nd Biophysics Conference, I-Shou University, Kaohsiung (May 18, 2017) <http://biophys.sinica.edu.tw/Symposium/22BC/program.htm>

“Mechanism of Ribosomal Reading Frame Shifting Is Explained by Resolution-Exchanged Mechanical Models That Agree Closely with Single Molecule and Structural Biology Data”, 17th RIES-Hokudai International Symposium on 柔, Sapporo, Hokkaido (Dec 13-14, 2016) <https://www.es.hokudai.ac.jp/symposium/2016/>

“How are structured DNA and RNA bent and unwound by small and large nanomachines?”, the third international conference on computational science and engineering (ICCSE-3), Ho Chi Min City, Vietnam (Nov 28-29, 2016) <http://conference.icst.org.vn/all-speakers-page-5.html>

“A Re-purposed FDA Drug Inhibits ATG Proteins to Regulate Autophagic Flux and Sensitize Tumor Cells to Chemotherapy”, Session Chair and invited speaker in International Drug Discovery Science & Technology-2016, Nanjing, China (Nov 18th, 2016) http://www.iddst.com/iddst2016/ScientificProgram_F3-1-6.asp

“A First-Principle-Based Computational Platform to Design and Evaluate New Variants of Antimicrobial Peptides”, Session Chair and invited speaker in International Congress of Medichem-2016, Nanjing, China (Nov 17th, 2016) <http://www.bitcongress.com/icm2016/ScientificProgram4.asp>

"GNM 2.0- A database housing protein dynamics data of >11,000 PDB structures revealing dynamics prerequisites for protein functions and interactions", World Bioinformatics 2016, Rome, Italy (Oct 25th 2016)
<http://bioinformatics.conferenceseries.com/scientific-program.php?day=2&sid=2567&date=2016-10-25>

"Ribosomal reading frame shift and maintenance are explained by resolution-exchanged mechanical models ", Protein Research Institute/Osaka University, Osaka, Japan (Sept 28th 2016)

"Determinants for structured DNA and RNA being bent and unwound by small and large nanomachines" Graduate Institute of Applied Physics, National Chengchi University, Taipei (Sept 12th 2016)

"Resolution exchanged mechanical models reveal how structured mRNA allosterically induces programmed ribosomal frameshifting", Research Center for the Mathematics on Chromatin Live Dynamics (RcMcD), Hiroshima University, Higashihiroshima, Japan (Sept 5th 2016)

"Resolution exchanged mechanical models reveal how structured mRNA allosterically induces programmed ribosomal frameshifting, Å, 2016 NCTS International Workshop on Critical Phenomena and Complex Systems, Hsinchu (July 3rd , 2016)
<http://phys.cts.nthu.edu.tw/actnews/intro.php?Sn=282&OSn=636>

"Programmed ribosomal frameshifting revealed by mechanical models and linear response theories", Department of Mechanical Engineering at the National Cheng Kung University, Tainan (May 31st 2016)
http://apps.acad.ncku.edu.tw/lecture/main/show_list_down.php?no=201604110029

"A first-principle-based computational platform to design and evaluate a repertoire of new antimicrobial peptides" 2016 _____, NCHU, Taichung (May 6th, 2016) <https://predtox.wikispaces.com>

Organizer and session chair in , Å "Conference on Time in Biological Systems and Beyond", NCTS, Hsinchu (Mar 28th-29th, 2016)

"Big data in structural biology that drive the design of protein binders and peptide blockers" The Third EITA-Bio Conference (EITA-Bio 2015), NTU, Taipei (Oct 25th, 2015) <http://www.eitc.org/eita/eita-venture-community/eita-venture-forum/year-2015/eita-bio-2015/program-eita-bio-2015-at-ntu-pdf-1>

"Communication property as a newly identified, important physical trait that governs the allosteric regulation of enzyme activity", _____, NCTU, Hsinchu (Aug 18th, 2015) <http://alibaba.phys.nctu.edu.tw/invitedspeakers/invitedspeakers.html>

"Structural Dynamic Model of Programmed Ribosomal Frameshifting", 2015 NCTS International Workshop on Critical Phenomena and Complex Systems, NTHU, Hsinchu (Aug 17th, 2015)

"Theories describing sensors and responders reveal important allosteric sites in enzymes", Biophysical Society (US) Thematic Meeting, New Biological Frontiers Illuminated by Molecular Sensors and Actuators, NTU, Taipei (June 30, 2015)
<https://www.biophysics.org/2015taiwan/Program/Speakers/tabid/5382/Default.aspx>

"Mechanical network in enzymes", GSB Seminar (jointly held by Academia Sinica and National Taiwan University), LS college, NTU, Taipei (June 30, 2015)

Chairing a session on "protein dynamics" in the 20th Biophysics Conference in Taiwan, Academia Sinica, Taipei (May 12th, 2015)
<http://www.ibc.sinica.edu.tw/biophysicsconf20/committees.aspx>

"Mechanical characteristics of enzyme catalysis", Department of Chemistry, NTU, Taipei (Mar 26th, 2015)

As a Keynote Speaker - "Allosteric Regulation Sites for Enzyme Catalysis are Co-localized with Communication Centers of Mechanical Signals" 8th AYRCOB NCTU, Hsinchu <http://2015.ayrcob.org/program/keynote-speaker/> (Jan 2015)

"Molecular binding sites are located near the interface of intrinsic dynamics domains (IDDs) ", TIGP Bioinformatics seminar series, IIS, Academia Sinica, Taipei (2014)

"Intramolecular communication based on time-dependent linear response theories", Modeling of Biomolecular Systems Interactions, Dynamics, and Allostery Meeting, Istanbul, Turkey, (2014)

"Development of antimicrobial/anticancer peptides using computers". _____, Xiamen University, Xiamen (2014)

"Computer-aided design of antimicrobial peptides" Department of Microbiology and Immunology, School of Medicine, NCKU, Tainan (2014)

"Time-dependent linear response theories used to gain insight on ligand binding and allosteric regulations in proteins", Physics Department Seminar, NCTU, Hsinchu (2014)

"Molecular responses to ligand perturbations can be described by linear response theories", TIGP Bioinformatics seminar IIS, Academia Sinica, Taipei (2014)

"Ultrafast molecular responses to ligand perturbations revealed by linear response theories - Reconsider Induced-Fit Phenomenon". iCeMs, NCTU, Hsinchu (2013)

"Compute the life", to students at College of Engineering, NTHU, Hsinchu (2013)

"Protein Design Principles Imposed by Intrinsic Dynamics - Studies on Protein-Protein Docking Orientations", Physics Department Seminar, NCTU, Hsinchu (2013)

"Protein-Ligand interactions treated as perturbations of protein intrinsic dynamics - Reconsider Induced-Fit Phenomenon", NCTS Critical Phenomena and Complex Systems Focus group, Academia Sinica, Taipei (2012)

"Characterization of membrane-penetrating physiochemical properties of antimicrobial peptides", NCCP Symposium held by National Center of High-performance Computer, Hsinchu (2012)

"Protein intrinsic dynamics and enzyme catalysis", to TIGP students, Inst. Information Science, Academia Sinica, Taipei (2012)

"Mechanically important residues are conserved in the evolution", International Symposium on Evolutionary Genomics and Bioinformatics, National Sun Yet-Sen University, Kaohsiung (2012)

"Protein intrinsic dynamics and enzyme catalysis", Physics Dept, National Tsing Hua University, Hsinchu (2012)

"Catalytic Chemistry Coupled with Mechanically Important Residues", Chemistry Dept, National Central University, Jhongli, Taiwan (2012)

"Protein intrinsic dynamics and enzyme catalysis", Chemistry Dept, National Taiwan University, Taipei (2012)

"Dynamics Imposed Constraints on Protein-Protein Docking Orientations", IBMS, Academia Sinica, Taipei, the 17th Biophysics Conference (2012)

"Protein design principles imposed by Protein Intrinsic Dynamics", App Math Dept, National Hsinchu University of Education, Hsinchu (2012)

"Protein Functional Dynamics - Intrinsic and Perturbed", Dept of Biotechnology, National Chiao Tung University, Hsinchu (2012)

"Protein in the move - the dynamics of protein-ligand binding", Physics Dept, National Taiwan Normal University, Taipei (2012)

"Protein design principles imposed by Protein Intrinsic Dynamics", Biophys Dept, Fudan University, Shanghai (2012)

"Protein-Ligand interactions treated as perturbations of protein intrinsic dynamics - Reconsider Induced-Fit Phenomenon", Biosoft 4th Annual Meeting, Beijing (2012)

"Preferred ways for protein to rotate - Enzyme Catalysis Power Designed to Distribute along Rotation Axes Identified by a New Elastic Network Model", Pepcon 2012, Beijing (2012)

"A dynamic story of Proteins - a Study on Dynamics Imposed Constraint on Protein-Protein Docking Orientations", Biophysics Journal Club, Phys Dept, National Chung Hsing University, Taichung (2012)

"Protein in the move - Intrinsic dynamics-imposed protein-protein docking orientation", Math Dept, National Taiwan University (2011)

"The interplay between intrinsic and perturbed protein dynamics is summarized by a simple linear response theory", 2011 Taiwan-Japan joint workshop on Numerical Analysis and Scientific Computation, Math Dept, National Taiwan University (2011)

"Population-shift or Induce-fit? Insight from Linear Response Theory and Simple Models", Dept Chemical Biology, Harvard Univ, Boston, USA (Apr, 2009)

"Protein Conformational Changes Explained by Population-shift and Induce-fit" JAEA, Kyoto, Japan (2008)

"Dynamics portal - An integral effort on developing/organizing dynamics web servers/databases and its significance to mediate systematic analyses to map experimental and computational characterized dynamics." Japan Biophysics Annual meeting, Yokohama, Japan (2007)

"Dynamics era: How information on conformational dynamics can be used to gain a deeper understanding of biological events at the molecular level?" Highlights (Papers) Track, in ISMB/ECCB Annual Conference, Vienna, Austria (2007)

"Dynamics and shape of the enzyme predispose the location of active sites" in Discussion on theory and simulation of biomolecular nano-machines, Kobe University, Kobe, Japan (2006)

"How to predict enzyme active sites without detailed atomic coordinates?" in Annual Meeting of the Biophysical Society, Long Beach, CA, USA (2005)

"Enzyme Active Site Prediction Based on Gaussian Network Model and its Implementation online" in 40th IUPAC Congress, Beijing, China (2005)

"iGNM" in 2nd Biological Language Conference, CMU, Pittsburgh PA, USA (2004)

Poster Abstracts

Yang, L.-W, Kitao, A, G_, N." Linear Response of Biomolecules To External Perturbations: Revisit Induce-fit ". Biophysical Society's 53rd Annual Meeting. Boston, USA (2009)

Yang, L.-W, Kitao, A, G_, N. "_____". the 46th Annual Meeting of Biophysical Society of Japan, Fukuoka, Japan (2008)

Yang, L.-W, Kitao, A, G_, N." Induce-fit Revisit: Protein Conformational Changes in Response to External Perturbations, Examined Using Linear Response Theories (LRT) ". InCoB 2008. Taipei, Taiwan (2008)

Yang, L.-W, Eyal, E, Bahar, I, Kitao, A."A PCA analysis of NMR on ubiquitin proteins and the webserver tool". Japan Biophysics Annual meeting. Yokohama, Japan (2007)

Yang, L.-W., Rader, A.J., Liu, X., Jursa, CJ, Chen, SC, Karimi, H and Bahar, I. "oGNM: Online Computation of Protein Dynamics Using Gaussian Network Model" in ISMB/ECCB Annual Conference, Vienna, Austria (2007)

Yang, L.-W., Kitao, A. and Bahar, I. "The dynamic predisposition of (the location of) enzyme active sites" in AFP-Biosapiens Annual Conference, Vienna, Austria (2007)

Yang, L.-W. and Bahar, I. " oGNM: Online Computation of Protein Dynamics Using Gaussian Network Model " DCB Annual Retreat, Pittsburgh, PA (2006)

Yang, L.-W. and Bahar, I. "oGNM " RECOMB 2006, Venice, Italy (2006)

Yang, L.-W. and Bahar, I. " COMPACT, A Low Frequency Conformational Dynamics Based Enzyme Active Site Predictor, Correctly Predicts Chain Elongation Sites in Two Prenyltransferases" Annual Meeting of the Biophysical Society, Salt Lake City UT (2006)

Yang, L.-W. and Bahar, I. "Coupling between enzymes' global dynamics and catalytic activity" Annual Meeting of the Biophysical Society, Baltimore MD (2004)

Yang, L.-W. and Bahar, I. "Enzyme global dynamics and its catalytic activity" BGSA Symposium, Pittsburgh PA (2004)

Yang, L.-W. and Bahar, I. "Enzyme active site dynamics and prediction algorithm" Science 2004, Pittsburgh PA (2004)
Yang, L.-W. and Bahar, I. "Enzyme active site dynamics" Science 2003, Pittsburgh (2003)

In the thesis committees of degree students (Master/PhD students **NOT from my lab)**

范楷柏、劉奎麟、鄭好英(國立清華大學醫工所碩士/林宗宏教授指導, 2022), Nuzhat Parvee (國立清華大學化學系博士/余靖教授指導, 2022), 吳崇璋(國立清華大學化學系碩士/余靖教授指導, 2022), 林鈺子(國立清華大學醫工所碩士/林宗宏教授指導, 2022), 黃詩淳(中興大學基因體暨生物資訊學研究所碩士/侯明宏教授指導, 2022), 王彥翔(國立清華大學服科所碩士/Soumya Ray 教授指導, 2022), 劉子齊(國立清華大學電機系博士/劉奕汶教授指導, 2021), 蘇冠璇(輔大化學研究所碩士/楊小青教授教授指導, 2021), 張維宸(國立交通大學資訊工程研究所碩士/洪瑞鴻教授教授指導, 2020), 楊仲棋(非論文研究計畫考核/清大生資所博士班三年級/莊永仁教授指導, 2020), Roshan Babarao Satange (國立中興大學基因體暨生物資訊學研究所博士/侯明宏教授指導, 2020), 王宇軒(國立交通大學資訊工程研究所碩士/洪瑞鴻教授教授指導, 2020), 杜睿芸(台灣大學分子與細胞生物學研究所碩士/溫進德教授指導, 2020), 李翊廷(台灣大學分子與細胞生物學研究所碩士/溫進德教授指導, 2020), 袁子鈞(國立中興大學基因體暨生物資訊學研究所碩士/侯明宏教授指導, 2020), Nikhil Pathak (TIGP Bioinformatics PhD program/交通大學生物資訊及系統生物研究所楊進木教授指導, 2020), 江蘇峰(台大基因體與系統生物學程博士, 蔡懷寬教授與日本大阪大學的岡田真理子教授指導, 2019), 陳君豪(國立交通大學資訊工程研究所碩士/洪瑞鴻教授教授指導, 2019), 曾靜儀(國立中興大學基因體暨生物資訊學研究所碩士/侯明宏教授指導, 2019), 陳宥宏(交通大學生物資訊及系統生物研究所博士/羅惟正教授指導, 2019), 高毓霖(清大分醫所碩士/林玉俊教授指導, 2018), 吳宗澤(台灣大學分子與細胞生物學研究所碩士/溫進德教授指導, 2018), 李安益(台灣大學分子與細胞生物學研究所碩士/溫進德教授指導, 2018), 楊善閔(清大生資所碩士/殷獻生教授指導, 2018), 張凱鈞(台灣大學分子與細胞生物學研究所博士/溫進德教授指導, 2018), 黃柏升(清華大學通訊所碩士/林澤教授指導, 2018), 胡顯騰(中興大學生物化學系博士/張功耀教授指導, 2018), 范藝耀(交通大學物理研究所碩士/吳天鳴教授指導, 2017), 廖駿嘉(交通大學物理研究所碩士/吳天鳴教授指導, 2017), 吳宗樺(PhD proposal defense; TIGP CBMB program 博士候選人/黃人則教授/副研究員指導, 2017), Nikhil Pathak (PhD proposal defense; TIGP Bioinformatics program 博士候選人/楊進木教授指導, 2017), 謝伯思(台灣大學分子與細胞生物學研究所碩士/溫進德教授指導, 2016), 許瓊方(台灣大學分子與細胞生物學研究所碩士/溫進德教授指導, 2016), Thejkiran Pitti (PhD proposal defense; TIGP Bioinformatics program 博士候選人/宋定懿研究員指導, 2016), 李健賓(中央大學化學系博士/蔡惠旭教授指導, 2015), 鄧德明(交大物理所博士/張正宏教授指導, 2014), 蕭寶岳(清大生資所博士/羅中泉教授指導, 2014), 蔡政育(清大生技所碩士/程家維教授指導, 2014), 黃韻芳(清大生資所碩士/呂平江教授指導, 2014), 吳海寶(清大生資所碩士/孫玉珠教授指導, 2014), 張智閔&林玉鳳(交大生資所博班資格考/黃鎮剛教授指導, 2014), 曾彥皆(清大分醫所碩士/林志侯教授指導, 2012), 游輝元(清大生技所博士/程家維教授指導, 2012), 施宣誠(TIGP/清大生資所博士/黃明經教授指導, 2012), 王乃娟(清大生資所碩士/呂平江教授指導, 2011)。